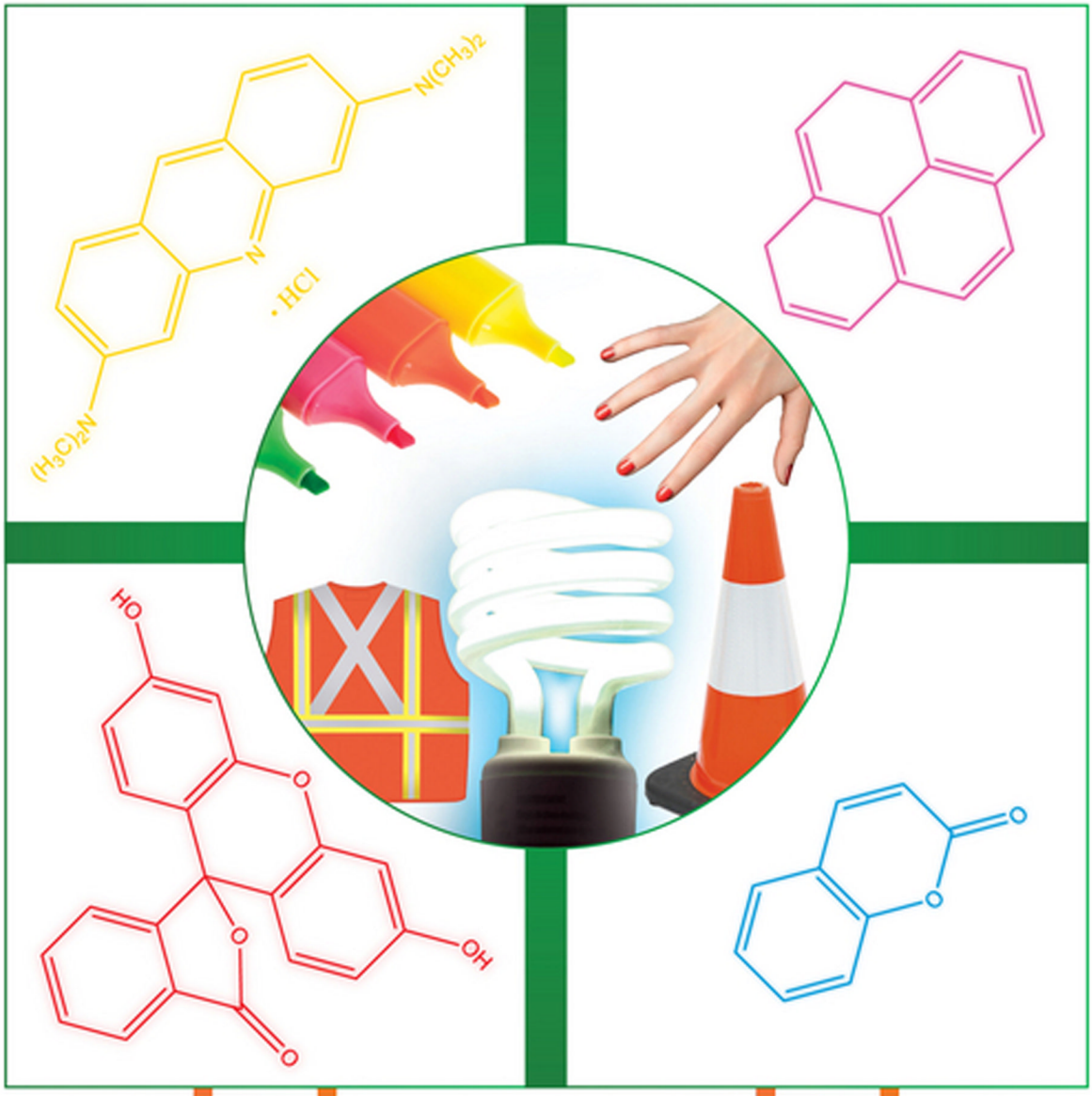
HANDBOOK OF FLUORESCENT DYES AND PROBES



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R. W. Sabnis, Ph.D.

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Dedicated To
My Wife
Mrs. Madhuri R. Sabnis

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Contents

PREFACE xv

ABOUT THE AUTHOR xvii

ACRIDINE HOMODIMER 1

ACRIDINE ORANGE (AO) 3

ACRIDINE ORANGE 10-DODECYL BROMIDE (DODECYL-ACRIDINE ORANGE (DAO)) 10

ACRIDINE ORANGE 10-NONYL BROMIDE (NONYL-ACRIDINE ORANGE (NAO)) 12

ALEXA FLUOR 350 CARBOXYLIC ACID SUCCINIMIDYL ESTER (AMCA-S) 15

ALEXA FLUOR 430 CARBOXYLIC ACID SUCCINIMIDYL ESTER 17

ALEXA FLUOR 488 CARBOXYLIC ACID SUCCINIMIDYL ESTER 20

ALEXA FLUOR 514 CARBOXYLIC ACID SUCCINIMIDYL ESTER 23

ALEXA FLUOR 532 CARBOXYLIC ACID SUCCINIMIDYL ESTER 25

ALEXA FLUOR 555 CARBOXYLIC ACID SUCCINIMIDYL ESTER 28

ALEXA FLUOR 594 CARBOXYLIC ACID SUCCINIMIDYL ESTER 30

ALEXA FLUOR 633 CARBOXYLIC ACID SUCCINIMIDYL ESTER 33

ALEXA FLUOR 660 CARBOXYLIC ACID SUCCINIMIDYL ESTER 35

ALEXA FLUOR 680 CARBOXYLIC ACID SUCCINIMIDYL ESTER 38

ALEXA FLUOR 700 CARBOXYLIC ACID SUCCINIMIDYL ESTER 40

ALEXA FLUOR 750 CARBOXYLIC ACID SUCCINIMIDYL ESTER 42

ALEXA FLUOR 790 CARBOXYLIC ACID SUCCINIMIDYL ESTER 45

9-AMINO-6-CHLORO-2-METHOXYACRIDINE (ACMA) 46

4-AMINO-5-METHYLAMINO-2′,7′-DIFLUOROFLUORESCEIN (DAFFM) 50

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4-AMINO-5-METHYLAMINO-2′,7′-DIFLUOROFLUORESCEIN DIACETATE (DAF-FM DA) 52

7–AMINO-4-METHYLCOUMARIN (AMC) (COUMARIN 120) (COUMARIN 440) 54

8-AMINOPYRENE-1,3,6-TRISULFONIC ACID TRISODIUM SALT (APTS) 63

7-ANILINOCOUMARIN-4-ACETIC ACID (ACAA) 65

9-ANTHROYLNITRILE 66

BOBO 1 69

BOBO 3 71

BODIPY FL C_5-CERAMIDE (C_5-DMB-CERAMIDE) 74

BODIPY FL C_5-GANGLIOSIDE GM1 77

BODIPY FL C_5-LACTOSYLCERAMIDE 79

BODIPY FL C_5-SPHINGOMYELIN (C_5-DMB-SPHINGOMYELIN) 81

BODIPY FL C_5-SUCCINIMIDYL ESTER 83

BODIPY TR CERAMIDE 85

BO-PRO 1 87

BO-PRO 3 89

4-BROMOMETHYL-6,7-DIMETHOXYCOUMARIN 91

5-(BROMOMETHYL)FLUORESCEIN 93

4-BROMOMETHYL-7-METHOXYCOUMARIN 95

CALCEIN BLUE AM 101

5-CARBOXY-2′,7′-DICHLOROFLUORESCEIN 102

6-CARBOXY-2′,7′-DICHLOROFLUORESCEIN 104

5-CARBOXY-2′,7′-DICHLOROFLUORESCEIN DIACETATE 106

6-CARBOXY-2′,7′-DICHLOROFLUORESCEIN DIACETATE 108

5-CARBOXYFLUORESCEIN 110

6-CARBOXYFLUORESCEIN 114

5-CARBOXYFLUORESCEIN DIACETATE **119**

6-CARBOXYFLUORESCEIN DIACETATE **121**

5-CARBOXYFLUORESCEIN SUCCINIMIDYL ESTER **125**

6-CARBOXYFLUORESCEIN SUCCINIMIDYL ESTER **129**

5-CARBOXYNAPHTHOFLUORESCEIN **132**

6-CARBOXYNAPHTHOFLUORESCEIN **134**

CASCADE BLUE ACETYL AZIDE TRISODIUM SALT **136**

CASCADE BLUE HYDRAZIDE TRISODIUM SALT **138**

3-CYANO-7-ETHOXYCOUMARIN (7-ETHOXYCOUMARIN-3-CARBONITRILE) **139**

3-CYANO-7-HYDROXYCOUMARIN (3-CYANOUMBELLIFERONE) **141**

4′,6-DIAMIDINO-2-PHENYLINDOLE DIHYDROCHLORIDE (DAPI) **145**

7-DIETHYLAMINOCOUMARIN-3-CARBONYL AZIDE **148**

7-DIETHYLAMINOCOUMARIN-3-CARBOXYLIC ACID (DAC) (DEAC) **149**

7-DIETHYLAMINOCOUMARIN-3-CARBOXYLIC ACID HYDRAZIDE (DCCH) **153**

7-DIETHYLAMINOCOUMARIN-3-CARBOXYLIC ACID SUCCINIMIDYL ESTER (DEAC SE) **155**

4-[4-(DIETHYLAMINO)STYRYL]-*N*-METHYLPYRIDINIUM IODIDE (4-Di-2-ASP) **157**

3,3′-DIETHYLOXACARBOCYANINE IODIDE ($DiOC_2(3)$) **160**

3,3′-DIHEPTYLOXACARBOCYANINE IODIDE ($DiOC_7(3)$) **163**

3,3′-DIHEXYLOXACARBOCYANINE IODIDE ($DiOC_6(3)$) **165**

DIHYDRORHODAMINE 123 (DHR 123) **169**

DIHYDRORHODAMINE 6G (DHR 6G) **173**

6,7-DIMETHOXYCOUMARIN-4-ACETIC ACID **175**

7-DIMETHYLAMINOCOUMARIN-4-ACETIC ACID (DMACA) **176**

7-DIMETHYLAMINOCOUMARIN-4-ACETIC ACID SUCCINIMIDYL ESTER (DMACA SE) **178**

7-DIMETHYLAMINO-4-METHYLCOUMARIN-3-ISOTHIOCYANATE (DACITC) **180**

2-[4-(DIMETHYLAMINO)STYRYL]-*N*-ETHYLPYRIDINIUM IODIDE (DASPEI) **181**

4-[4-(DIMETHYLAMINO)STYRYL]-*N*-METHYLPYRIDINIUM IODIDE (4-Di-1-ASP) (DASPMI) **183**

3,3′-DIMETHYL-α-NAPHTHOXACARBOCYANINE IODIDE (JC-9) **186**

3,3′-DIPENTYLOXACARBOCYANINE IODIDE ($DiOC_5(3)$) **187**

3,3′-DIPROPYLTHIADICARBOCYANINE IODIDE ($DiSC_3(5)$) **189**

ETHIDIUM BROMIDE (HOMIDIUM BROMIDE) **193**

ETHIDIUM HOMODIMER-1 (EthD-1) **199**

ETHIDIUM HOMODIMER-2 (EthD-2) **203**

FLUORESCEIN **205**

FLUORESCEIN DIACETATE (FDA) **213**

FLUOROSCEIN-5-ISOTHIOCYANATE (FITC) **219**

FLUORESCEIN-5-THIOSEMICARBAZIDE **224**

4-HEPTADECYL-7-HYDROXYCOUMARIN (4-HEPTADECYLUMBELLIFERONE) **227**

HEXIDIUM IODIDE **229**

HOECHST 33258 **231**

HOECHST 33342 **238**

HOECHST 34580 **244**

7-HYDROXYCOUMARIN-3-CARBOXYLIC ACID (UMBELLIFERONE-3-CARBOXYLIC ACID) **246**

7-HYDROXYCOUMARIN-3-CARBOXYLIC ACID SUCCINIMIDYL ESTER **250**

7-HYDROXY-4-METHYLCOUMARIN-3-ACETIC ACID **252**

8-HYDROXYPYRENE-1,3,6-TRISULFONIC ACID TRISODIUM SALT (HPTS) (PYRANINE) **253**

JOJO 1 **263**

JO-PRO 1 **265**

LOLO 1 **267**

LYSOSENSOR BLUE DND 167 **269**

LYSOSENSOR BLUE DND 192 **271**

LYSOSENSOR GREEN DND 153 **272**

LYSOSENSOR GREEN DND 189 **273**

LYSOSENSOR YELLOW/BLUE DND 160 (PDMPO) **275**

MARINA BLUE (6,8-DIFLUORO-7-HYDROXY-4-METHYLCOUMARIN) (DiFMU) **277**

7-METHOXYCOUMARIN-3-CARBONYL AZIDE **280**

7-METHOXYCOUMARIN-3-CARBOXYLIC ACID **281**

7-METHOXYCOUMARIN-3-CARBOXYLIC ACID SUCCINIMIDYL ESTER **285**

8-METHOXYPYRENE-1,3,6-TRISULFONIC ACID TRISODIUM SALT (MPTS) **287**

NBD C_6-CERAMIDE **289**

NBD METHYLHYDRAZINE (MNBDH) **293**

NUCLEAR YELLOW (HOECHST S 769121) **295**

OREGON GREEN 488 (2′,7′-DIFLUOROFLUORESCEIN) **297**

OREGON GREEN 488 CADAVERINE **300**

OREGON GREEN 488 CARBOXYLIC ACID **302**

OREGON GREEN 514 CARBOXYLIC ACID **304**

OREGON GREEN 488 CARBOXYLIC ACID DIACETATE **306**

OREGON GREEN 488 CARBOXYLIC ACID SUCCINIMIDYL ESTER **308**

OREGON GREEN 514 CARBOXYLIC ACID SUCCINIMIDYL ESTER **310**

OREGON GREEN 488 MALEIMIDE **312**

PACIFIC BLUE (6,8-DIFLUORO-7-HYDROXYCOUMARIN-3-CARBOXYLIC ACID) **315**

PACIFIC BLUE C_5-MALEIMIDE **317**

PACIFIC BLUE SUCCINIMIDYL ESTER **318**

POPO 1 **320**

POPO 3 **322**

PO-PRO 1 **324**

PO-PRO 3 **326**

PROPIDIUM IODIDE (PI) **328**

1-PYRENEBUTANOIC ACID HYDRAZIDE (PBH) **334**

1-PYRENEBUTANOIC ACID SUCCINIMIDYL ESTER **336**

1-PYRENEDECANOIC ACID (PDA) **340**

1-PYRENEDODECANOIC ACID (PDDA) **343**

1-PYRENEHEXADECANOIC ACID **346**

1-PYRENEHEXANOIC ACID (PHA) **348**

1-PYRENESULFONYL CHLORIDE **350**

1,3,6,8-PYRENETETRASULFONIC ACID TETRASODIUM SALT **352**

N-**(1-PYRENYL)IODOACETAMIDE** **355**

N-**(1-PYRENYL)MALEIMIDE** **357**

QSY 7 CARBOXYLIC ACID SUCCINIMIDYL ESTER **361**

QSY 9 CARBOXYLIC ACID SUCCINIMIDYL ESTER **364**

QSY 21 CARBOXYLIC ACID SUCCINIMIDYL ESTER **366**

REDOXSENSOR RED CC-1 **369**

RESAZURIN SODIUM SALT (ALAMAR BLUE) **370**

RHODAMINE 6G (RH 6G) **373**

RHODAMINE 110 (RH 110) **380**

RHODAMINE 123 (RH 123) **384**

5,5′,6,6′-TETRACHLORO-1,1′,3,3′-TETRAETHYLBENZIMIDAZOLOCARBOCYANINE IODIDE (JC-1) **389**

TETRAMETHYLRHODAMINE ETHYL ESTER PERCHLORATE (TMRE) **394**

TETRAMETHYLRHODAMINE METHYL ESTER PERCHLORATE (TMRM) **396**

TO-PRO 1 **398**

TO-PRO 3 **400**

TO-PRO 5 **403**

TOTO 1 **405**

TOTO 3 **408**

TRUE BLUE (TRUE BLUE CHLORIDE) **411**

VITA BLUE **413**

YO-PRO 1 **415**

YO-PRO 3 **419**

YOYO 1 **421**

YOYO 3 **425**

APPENDIX A INDEX OF CAS REGISTRY NUMBERS **427**

APPENDIX B INDEX OF ACRIDINES **431**

APPENDIX C INDEX OF ANTHRACENES **433**

APPENDIX D INDEX OF BORON CO-ORDINATION COMPOUNDS/DYES **435**

APPENDIX E INDEX OF COUMARINS **437**

APPENDIX F INDEX OF CYANINES/STYRYLS **439**

APPENDIX G INDEX OF HETEROCYCLES **441**

APPENDIX H INDEX OF PYRENES **443**

APPENDIX I INDEX OF XANTHENES **445**

Preface

Fluorescence has been a fascination for individuals for a long time. This book is intended as a reference guide on fluorescent dyes used in medicine, life science, imaging science, cell biology, labeling technology, clinical science, biological chemistry, dye chemistry, biological staining, color chemistry, environmental science, forensic science, organic chemistry, histochemistry, cytochemistry, medicinal chemistry, adhesives, agriculture, coatings, devices, electronics, petroleum, photography, plastics, polymers, security, textile and toys. There are hundreds of fluorescent dyes reported but this book mainly focuses on those dyes, which are widely used in various industrial and academic research.

There is no book available in the market directly on fluorescent dyes and probes, which provides information (such as CAS Registry Numbers, synthesis, various properties, safety/toxicity data and a wide variety of applications) in one source, even though use of fluorescent dyes is wide spread, growing rapidly and has exploded in the past decade. There was a need to publish a book that provided an immediate incentive for compiling the notes to update the scientific community with the wealth of information on fluorescent dyes and probes. To remedy this situation, we have undertaken an ambitious and monumental task of assembling in one publication all the critical data relevant in the field of fluorescent dyes. The dyestuff literature, particularly on fluorescent dyes, is largely in patents. The book provides systematic and up-to-date library of information on 150+ fluorescent dyes and probes as a reference handbook. The book is compiled as a resource guide for chemist and non-chemist in industry as well as in university.

Apart from supplying specific data, the comprehensive, interdisciplinary and comparative nature of the book will provide the user with an easy overview of the state of the art, pinpointing the gaps in the fluorescent dyes knowledge and providing a basis for further research. In addition, it will enable the researcher to use the book in most facile and user-friendly manner.

Fluorescent dyes and probes are arranged alphabetically by the most commonly used name. Again, the choice of primary name is somewhat arbitrary, but an effort has been made to strike a balance between names that are easily recognizable and names that are chemically informative. The detail information of each fluorescent dye or probe is covered in the following order: CAS registry number, chemical structure, CA index name, other names, Merck index number (Merck Index 15th Edition, 2013), chemical/dye class, molecular formula, molecular weight, physical form, solubility, melting point, boiling point, pK_a, absorption (λ max), emission (λ max), molar extinction coefficient, quantum yield, synthesis, imaging/labeling applications, biological/medical applications, industrial applications, safety/toxicity and references. Where there are discrepancies between different values, the author used his judgment on selecting the most likely value.

Numerous recent references have been provided on various synthetic methods, imaging/labeling applications, biological/medical applications, industrial applications and safety/toxicity data. Space and format limitations prevent giving all the references for each dye. This is the first ever book which provides safety/toxicity data with reference to acute toxicity, aquatic toxicity, carcinogenicity, cytotoxicity, chronic toxicity, ecotoxicity, genotoxicity, hematotoxicity, hepatotoxicity, immunotoxicity, microbial toxicity, mutagenicity, nephrotoxicity, neurotoxicity, nucleic acid damage, oral toxicity, phototoxicity, phytotoxicity, skin toxicity, reproductive toxicity, and so on.

Several appendixes have been provided at the end of the book for scientists to conveniently and easily find a dye as per their need. These appendixes include CAS Registry Numbers, Acridines, Anthracenes, Boron co-ordination compounds/dyes, Coumarins, Cyanines/Styryls, Heterocycles, Pyrenes and Xanthenes.

Omissions as well as errors of fact and interpretation are inevitable in dealing with so vast a subject as fluorescent dyes. I shall be glad to have my attention drawn to errors and to incorporate suggestions for improvement when a revision becomes possible.

I express my profound respect and appreciation to my Guru/Mentor/Advisor, Prof. D. W. Rangnekar, who brought me to this wonderful world of Color Science in the Department of Dyestuffs Technology, Institute of Chemical Technology (ICT), where I laid the foundation stone for my research career in Dye Chemistry.

It is a pleasure to make grateful acknowledgement to Dr. Alan Fanta, Dr. Doina Ene, and Dr. Jeffrey Talkington for extremely useful discussions, encouragement and inspiration.

Words are inadequate to express my sincere appreciation to my wife Madhuri and daughter Anika. It would not have been possible to write this book without their encouragement and patience. It is a great pleasure to express my gratitude and appreciation to John Wiley & Sons Inc., for giving me an opportunity to write this book.

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About the Author

Ram W. Sabnis is a Senior Patent Agent in USA. His interests include dyes, pigments, organic chemistry, heterocycles, polymers, synthesis, formulations, coatings and patents. Presently, he focuses on drafting and prosecuting US and international patents. He is a registered patent agent with US Patent and Trademark Office (USPTO). Prior to entering the legal (patents) field, he was a research chemist for Ascadia, General Electric, Brewer Science, U.S. Textiles and Thermo Fisher (Molecular Probes) in USA. He also worked as a Patent Agent at Squire Patton Boggs L.L.P. and Senior Manager at Pfizer Inc. (Wyeth).

Dr. Sabnis was born and raised in Mumbai, India. He received his Ph.D. in Organic Chemistry (Dye Chemistry) from Institute of Chemical Technology (ICT) (formerly UDCT), Mumbai, India. He is a Chartered Colourists, Fellow of Society of Dyers and Colourists (CCol FSDC).

Dr. Sabnis is one of the world's foremost experts in dyes, inventing world's first colored bubbles (non-staining) and color changing dye system with many applications. He has immensely contributed to color science and technology for the past 25 years, particularly, dyes for biomedicine, personal care products, health/beauty products, electronics (displays, OLEDs), inks, paints, plastics, textiles and toys/bubbles.

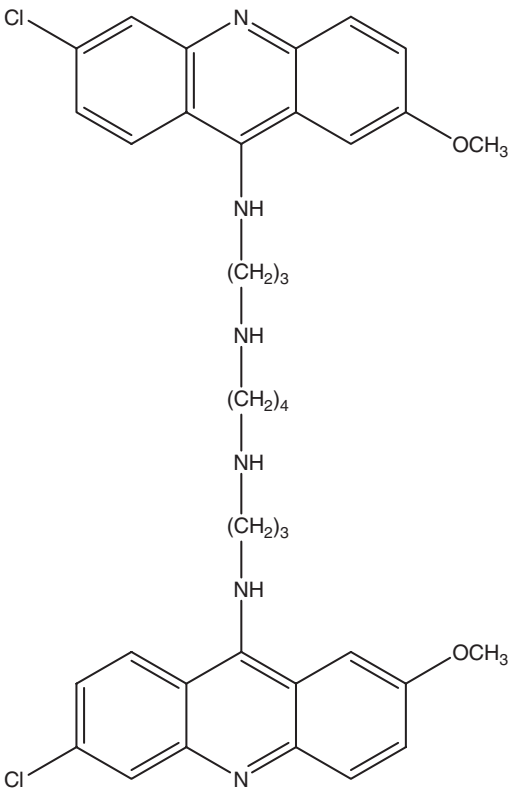
He has over 200 publications which include books, book chapters, encyclopedia chapters, patents, reviews, papers, and symposia presentations. He is also an inventor of several US and international patents (issued/published). Dr. Sabnis is the recipient of Pfish Award, Perkin Innovation Award, Grand Innovation Award, Competitive Spirit Award and Best Doctoral Thesis Award. Dr. Sabnis is awarded the Gold Medal for "Outstanding service to the coloration industry" by the Society of Dyers and Colourists, Bradford, U.K.

He has written two books on color chemistry, namely, "*Handbook of Biological Dyes and Stains*" and "*Handbook of Acid-Base Indicators.*" He will continue to focus his activities on fascinating dye chemistry as well as demanding intellectual property in the years to come.

ACRIDINE HOMODIMER

CAS Registry Number 57576-49-5

Chemical Structure



CA Index Name 1,4-Butanediamine, *N*,*N*′-bis[3-[(6-chloro-2-methoxy-9-acridinyl)amino]propyl]-

Other Names Acridine homodimer; NSC 219743

Merck Index Number Not listed

Chemical/Dye Class Acridine

Molecular Formula $C_{38}H_{42}Cl_2N_6O_2$

Molecular Weight 685.69

Physical Form Orange-brown powder or yellow solid

Solubility Soluble in water, *N*,*N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 169–170 °C[2]

Boiling Point (Calcd.) 885.4 ± 65.0 °C Pressure: 760 Torr

pKa (Calcd.) 10.63±0.19 Most Basic Temperature: 25 °C

Absorption (λmax) 431 nm (H_2O/DNA); 418 nm (MeOH)

Emission (λmax) 498 nm (H_2O/DNA); 500 nm (MeOH)

Molar Extinction Coefficient 12,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Nucleic acids;[1–9] chromosomes[10]

Biological/Medical Applications Detecting nucleic acids;[1–9] diagnosis and selective tissue necrosis;[11] treating cancer,[11] malformed proteins causing neurodegenerative disease,[13] prion disease[12]

Industrial Applications Not reported

Safety/Toxicity Neurotoxicity[13]

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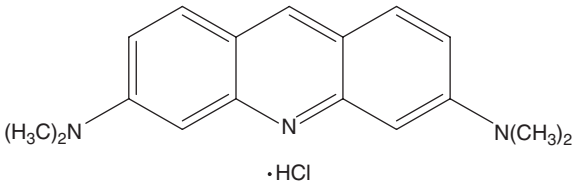
ACRIDINE ORANGE (AO)

CAS Registry Number 65-61-2

Chemical Structure



CA Index Name 3,6-Acridinediamine, N^3,N^3,N^6,N^6-tetramethyl-, hydrochloride (1:1)

Other Names 3,6-Acridinediamine, *N*,*N*,*N*′,*N*′-tetramethyl-, monohydrochloride; Acridine Orange R; Acridine, 3,6-bis(dimethylamino)-, hydrochloride; Acridine, 3,6-bis(dimethylamino)-, monohydrochloride; 3,6-Bis(dimethylamino)acridine hydrochloride; Acridine Orange; AO; Acridine Orange N; Acridine Orange NO; Acridine Orange NS; Basic Orange 14; Basic Orange 3RN; C.I. 46005; C.I. Basic Orange 14; Rhoduline Orange NO; Sumitomo Acridine Orange NO; Sumitomo AcridineOrange RK conc

Merck Index Number Not listed

Chemical/Dye Class Acridine

Molecular Formula $C_{17}H_{20}ClN_3$

Molecular Weight 301.82

Physical Form Orange solid

Solubility Soluble in water, dimethyl sulfoxide, ethanol, methanol

Absorption (λ_{max}) 500 nm (H_2O/DNA); 460 nm (H_2O/RNA); 489 nm (MeOH)

Emission (λ_{max}) 526 nm (H_2O/DNA); 650 nm (H_2O/RNA); 520 nm (MeOH)

Molar Extinction Coefficient 53,000 cm^{-1} M^{-1} (H_2O/DNA); 64,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–8]

Imaging/Labeling Applications Bacteria;[9–15] blood smears;[16–18] casein;[19] cells/tissues;[20–23] chromosomes;[24,25] endospores;[26] lignin;[27,107] liposomes;[28] lysosomes;[29–35] micronucleus;[36–38] microorganisms;[39–49] mucin;[50] nuclei;[51] nucleic acids;[52–74] parasites;[75–79] sperms;[80,81] tumors;[82,83] yeast[84–88]

Biological/Medical Applications Analyzing/counting/measuring microorganisms;[39–49] analyzing/detecting/identifying nucleic acids;[52–74] counting/detecting cells/tissues;[20–23] detecting parasites;[75–79] measuring phagosome-lysosome fusion;[31,33] for photodynamic therapy;[82,83] monitoring atmospheric/indoor bioaerosols;[89,90] apoptosis assay;[91–97] cytotoxicity assay;[98,99] genotoxicity assay;[99] as temperature sensor;[100,101] dental materials for crowns and bridges[102]

Industrial Applications Adhesives;[103] aluminophosphate crystalline materials;[104] detecting clay particles;[105] display device;[106] evaluating fiber surface characteristics;[107] glass matrixes;[108] imaging material;[109] inks;[110,111] lasers;[112] recording materials;[113–115] photoresists;[116,117] textiles;[118] thin films;[119,120] tracers for hydrology;[121] wiring boards[122]

Safety/Toxicity Carcinogenicity;[123–125] cytotoxicity;[126,127] DNA damage;[128] embryotoxicity;[129] genotoxicity;[130–134] mutagenicity;[135–138] photodynamic toxicity;[139] phototoxicity[140–142]

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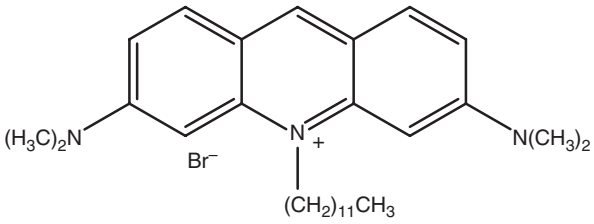
ACRIDINE ORANGE 10-DODECYL BROMIDE (DODECYL-ACRIDINE ORANGE (DAO))

CAS Registry Number 41387-42-2

Chemical Structure



CA Index Name Acridinium, 3,6-bis(dimethylamino)-10-dodecyl-, bromide (1:1)

Other Names Acridinium, 3,6-bis(dimethylamino)-10-dodecyl-, bromide; 10-Dodecylacridine Orange Bromide; 3,6-Bis(dimethylamino)-10-dodecylacridinium bromide; AO 10 Dodecylbromide; Acridine orange 10-dodecyl bromide; Dodecyl-Acridine Orange; BDA; D 455; DADAB; DAO

Merck Index Number Not listed

Chemical/Dye Class Acridine

Molecular Formula $C_{29}H_{44}BrN_3$

Molecular Weight 514.59

Physical Form Orange solid

Solubility Soluble in dimethyl sulfoxide, ethanol, methanol

Melting Point >250 °C

Absorption (λ_{max}) 495 nm (MeOH)

Emission (λ_{max}) 520 nm (MeOH)

Molar Extinction Coefficient 87,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Chloride ions;[5] keratin fibers/hairs;[6,7] Langmuir-Blodgett (LB) monolayers;[23] micelles;[2–4,8,9] mitochondrial membranes;[10] proteins[11–14]

Biological/Medical Applications Analyzing chloride ions;[5] characterizing drug binding sites on glycoproteins;[14] opthalmic devices (intraocular lenses (IOL))[15]

Industrial Applications Determining cationic surfactants;[16] electroluminescent devices;[17–19] Langmuir-Blodgett films;[20,23] photographic imaging system;[21] photoresists;[22] semiconductor electrodes;[23–25] silica-surfactant composite films[26]

Safety/Toxicity No data available

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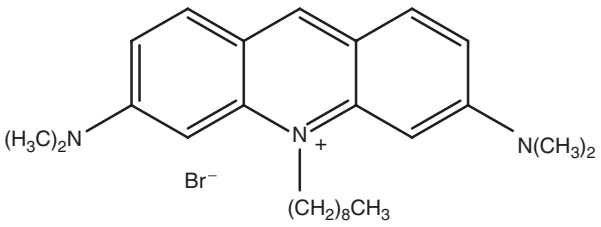
ACRIDINE ORANGE 10-NONYL BROMIDE (NONYL-ACRIDINE ORANGE (NAO))

CAS Registry Number 75168-11-5

Chemical Structure



CA Index Name Acridinium, 3,6-bis(dimethylamino)-10-nonyl-, bromide (1:1)

Other Names Acridinium, 3,6-bis(dimethylamino)-10-nonyl-, bromide; Acridine Orange 10-nonyl bromide; 3,6-bis-(dimethylamino)-10-nonylacridinium bromide; 10-nonyl acridine orange; A 1372; Nonyl-Acridine Orange; NAO

Merck Index Number Not listed

Chemical/Dye Class Acridine

Molecular Formula $C_{26}H_{38}BrN_3$

Molecular Weight 472.50

Physical Form Orange solid or brown solid[2]

Solubility Soluble in dichloromethane, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol; slightly soluble in water; insoluble in hexanes, toluene

Melting Point ≥250 °C

Absorption (λ_{max}) 495 nm (MeOH)

Emission (λ_{max}) 519 nm (MeOH)

Molar Extinction Coefficient 84,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Mitochondria;[1–23,29,36,37] cardiolipin;[22–29] blood cells;[30] cells;[31] liposomes;[32] lipid membranes;[33] nerve terminals;[34] peptides[35]

Biological/Medical Applications Analyzing mitochondria;[1–23,29,36,37] assessing/measuring cardiolipin (content);[22–29] assessing/recording membrane potential;[17–22] apoptosis assay;[36,37] hematotoxicity assay;[30] detecting prostate cancer;[14] diagnosing/treating arthritic disorders,[15] type 2 diabetes;[16] testing cardiotoxicity of compounds;[31] opthalmic devices (intraocular lenses (IOL))[38]

Industrial Applications Not reported

Safety/Toxicity Mitochondrial toxicity[39]

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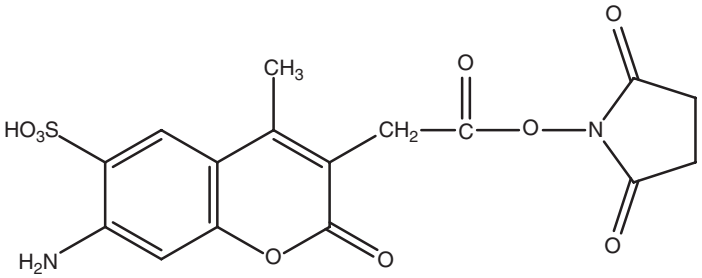
ALEXA FLUOR 350 CARBOXYLIC ACID SUCCINIMIDYL ESTER (AMCA-S)

CAS Registry Number 200554-19-4

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-acetic acid, 7-amino-4-methyl-2-oxo-6-sulfo-, 3-(2,5-dioxo-1-pyrrolidinyl) ester

Other Names 2*H*-1-Benzopyran-6-sulfonic acid, 7-amino-3-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl] -4-methyl-2-oxo-; 7-amino-3-((((succinimidyl)oxy)-carbonyl)methyl)-4-methylcoumarin-6-sulfonic acid; AMCA-S; Alexa 350 carboxylic acid succinimidyl ester; Alexa Fluor 350 carboxy acid succinimidyl ester; Alexa Fluor 350 succinimidyl ester; Alexa Fluor 350NHS; Sulfosuccinimidyl-7-amino-4-methylcoumarin-3-acetic acid

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{16}H_{14}N_2O_9S$

Molecular Weight 410.35

Physical Form Pale yellow precipitate[2] or yellow/orange solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

pKa (Calcd.) -0.46±0.20 Most Basic Temperature: 25 °C

Absorption (λ_{max}) 346 nm (Buffer pH 7); 353 nm (MeOH)

Emission (λ_{max}) 445 nm (Buffer pH 7); 438 nm (MeOH)

Molar Extinction Coefficient 19,000 cm^{-1} M^{-1} (Buffer pH 7); 20,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Amines;[3,7,24] neomycin;[4] nucleic acids;[5–7] peptides;[8–11] proteins;[1,2,10,12–19] silane coupling agent;[20–24] silica particles/beads[20–24]

Biological/Medical Applications Analyzing peptides;[8–11] detecting mutations;[25] detecting/identifying nucleic acids;[5–7] detecting/isolating/purifying proteins;[1,2,10,12–19] investigating location of phosphatidylinositol-4,5-bisphosphate ($PI(4,5)P_2$) in cell membranes;[4] colloidal diagnostic devices;[20] multiplex genetic analysis;[25] as nucleic acid hybridization probe;[7] useful for synthesizing nucleic acid,[21,22] peptides[20,22]

Industrial Applications Poly(vinyl alcohol)-coated microfluidic devices;[3] self-assembled monolayers;[26] silica particles/beads[20–24]

Safety/Toxicity No data available

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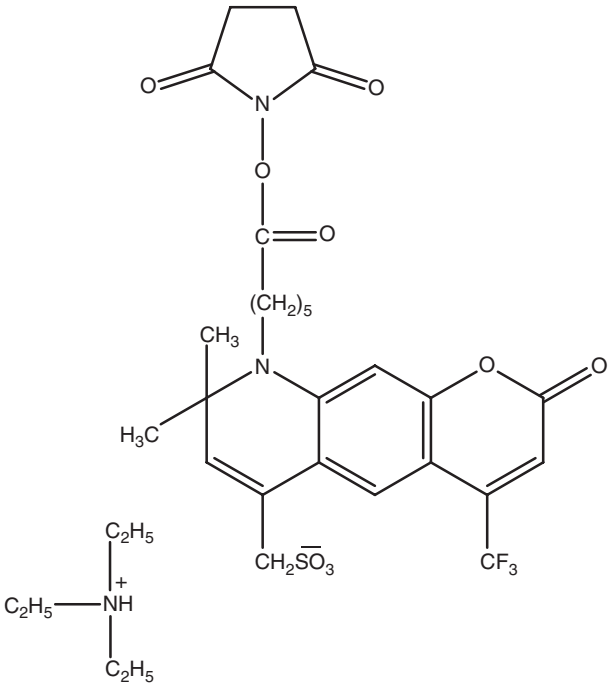
ALEXA FLUOR 430 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 467233-94-9

Chemical Structure



CA Index Name 2*H* -Pyrano[3,2-*g*]quinoline-9(8*H*)-hexanoic acid, 8,8-dimethyl-2-oxo-6-(sulfomethyl)-4-(trifluoromethyl)-, 2,5-dioxo-1-pyrrolidinyl ester, compd. with *N*,*N*-diethylethanamine (1:1)

Other Names 2*H*-Pyrano[3,2-*g*]quinoline-6-methanesulfonic acid, 9-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-8,9-dihydro-8,8-dimethyl-2-oxo-4-(trifluoromethyl)-, compd. with *N*,*N*-diethylethanamine (1:1); Alexa 430; Alexa 430 succinimidyl ester; Alexa Fluor 430; Alexa Fluor 430 NHS; Alexa Fluor 430 NHS ester; Alexa Fluor 430 carboxylic acid SE; Alexa Fluor 430 carboxylic acid succinimidyl ester; Alexa Fluor 430 SE; Alexa Fluor 430 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Heterocycle

Molecular Formula $C_{32}H_{42}F_3N_3O_9S$

Molecular Weight 701.75

Physical Form Yellow solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 430 nm (Buffer pH 7); 425 nm (MeOH)

Emission (λ_{max}) 545 nm (Buffer pH 7); 530 nm (MeOH)

Molar Extinction Coefficient 15,000 cm^{-1} M^{-1} (Buffer pH 7); 16,200 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[16,24] antibodies;[2,3] bacteria;[4] cells;[5,6] chromosomes;[7,8] glucose;[9] histone deacetylases;[10] microorganisms;[2,11] nucleic acids/nucleotides;[12–16] proteins/peptides;[17–25] quantum dots;[26] silane coupling agents;[27–29] viruses[30,31]

Biological/Medical Applications Analyzing sugar flux;[9] assaying retinol-binding protein-transthyretin interaction;[21] detecting chromosomal aberration;[7,8] detecting/quantifying biotinylated proteins;[23] identifying microorganisms;[2,11] monitoring reorganization of matrigel[22]

Industrial Applications Explosives detection polymers;[32] nanowalled polymeric microtubes;[33] photoresists;[34] silica particles/beads;[27–29] optical waveguides[35,36]

Safety/Toxicity No data available

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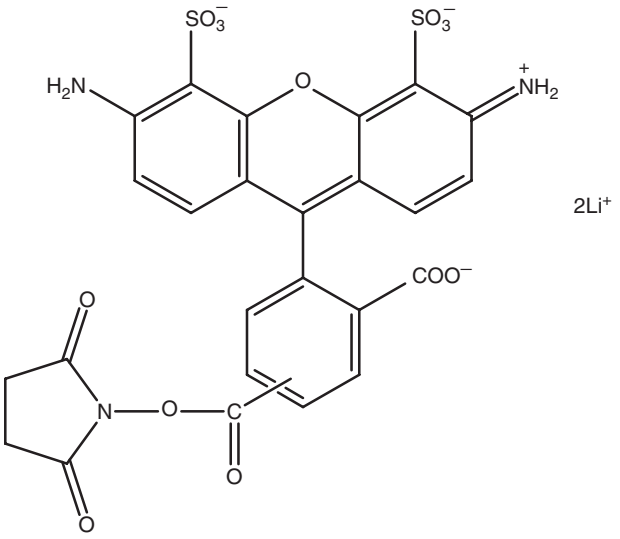
ALEXA FLUOR 488 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 222164-96-7

Chemical Structure



CA Index Name Xanthylium, 3,6-diamino-9-[2-carboxy-4(*or* 5)-[[(2,5-dioxo-1-pyrrolidinyl)oxy] carbonyl]phenyl]-4,5-disulfo-, inner salt, lithium salt (1:2)

Other Names Xanthylium, 3,6-diamino-9-[2-carboxy-4 (*or* 5)-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]phenyl]-4,5-disulfo-, inner salt, dilithium salt; Alexa 488; Alexa 488 succinimidyl ester; Alexa Fluor 488; Alexa Fluor 488 NHS; Alexa Fluor 488 NHS ester; Alexa Fluor 488 carboxylic acid SE; Alexa Fluor 488 carboxylic acid succinimidyl ester; Alexa Fluor 488 SE; Alexa Fluor 488 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{15}Li_2N_3O_{13}S_2$

Molecular Weight 643.41

Physical Form Orange solid

Solubility Soluble in water, dimethyl sulfoxide

Absorption (λmax) 494 nm (Buffer pH 7)

Emission (λmax) 517 nm (Buffer pH 7)

Molar Extinction Coefficient 73,000 cm^{-1} M^{-1} (Buffer pH 7)

Quantum Yield 0.92 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[2–5,21,29,42] antibodies;[6–12] cells/tissues;[12–15] chromosomes;[16,17] cyclodextrins;[18] histone deacetylases;[19] insulin-saccharide conjugates;[20] liposomes/lysozymes;[34] nucleic acids/nucleotides;[21–29] polymersomes;[30] proteins/peptides;[3–5,9,11,31–44] receptor-like kinases (RLKs) microbeads;[45] silane coupling agents;[46] cowpea mosaic virus (CPMV);[47] dengue virus[48]

Biological/Medical Applications Analyzing/profiling amyloid-β peptides;[3,4] assessing/evaluating protein-lipid interactions;[35] characterizing submicron protein aggregates/conjugates;[32,33] detecting/quantifying proteins;[41] detecting chromosomal aberration;[16,17] labeling/detecting nucleic acids;[21–29] measuring protein dynamics;[37,38] patterning wide range of proteins;[36] tracing adenosine A2A receptors *in vitro*;[39] visualizing vasculature/blood flow in living mouse and chick embryos[47] polymersomes in biomedical or cosmetic applications[30]

Industrial Applications Photoresists;[49] silica particles/beads[46]

Safety/Toxicity No data available

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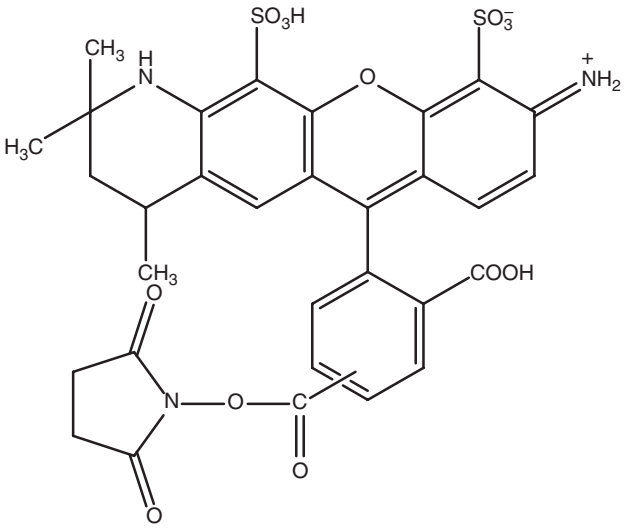
ALEXA FLUOR 514 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 918946-23-3

Chemical Structure



CA Index Name [1]Benzopyrano[3,2-*g*]quinolin-11-ium, 9-amino-6-[2-carboxy-4(*or* 5)-[[(2,5-dioxo-1-pyrrolidinyl)-oxy]carbonyl]-phenyl]-1,2,3,4-tetrahydro-2,2,4-trimethyl-10,12-disulfo-, inner salt

Other Names Alexa 514; Alexa 514 succinimidyl ester; Alexa Fluor 514; Alexa Fluor 514 NHS; Alexa Fluor 514 NHS ester; Alexa Fluor 514 carboxylic acid SE; Alexa Fluor 514 carboxylic acid succinimidyl ester; Alexa Fluor 514 SE; Alexa Fluor 514 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{31}H_{27}N_3O_{13}S_2$

Molecular Weight 713.69

Physical Form Red solid

Solubility Soluble in water, dimethyl sulfoxide

Absorption (λ_{max}) 517 nm (Buffer pH 7)

Emission (λ_{max}) 542 nm (Buffer pH 7)

Molar Extinction Coefficient 80,000 cm^{-1} M^{-1} (Buffer pH 7)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[2] antibodies;[3,4] cells;[5–7] chromosomes;[8,9] histone deacetylases;[10] microorganisms;[11] nucleic acids;[4,12] proteins[4]

Biological/Medical Applications Analyzing/detecting analytes;[4] detecting chromosomal aberration;[8,9] identifying/characterizing microorganisms;[11] imaging cells;[5–7] labeling amines/amino groups[2]

Industrial Applications Photoresists[13]

Safety/Toxicity No data available

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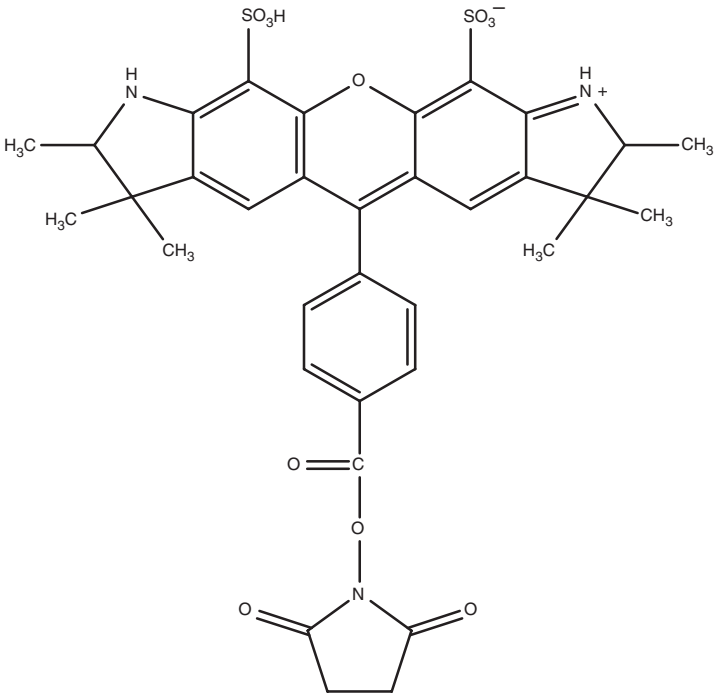
ALEXA FLUOR 532 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 477876-64-5

Chemical Structure



CA Index Name Pyrano[3,2-*f*:5,6-*f*′]diindol-11-ium, 5-[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]phenyl]-1,2,3,7,8,9-hexahydro-2,3,3,7,7,8-hexamethyl-10,12-disulfo-, inner salt

Other Names Alexa 532; Alexa 532 succinimidyl ester; Alexa Fluor 532; Alexa Fluor 532 NHS; Alexa Fluor 532 NHS ester; Alexa Fluor 532 carboxylic acid SE; Alexa Fluor 532 carboxylic acid succinimidyl ester; Alexa Fluor 532 SE; Alexa Fluor 532 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{34}H_{33}N_3O_{11}S_2$

Molecular Weight 723.77

Physical Form Red solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λmax) 530 nm (Buffer pH 7); 532 nm (MeOH)\

Emission (λmax) 555 nm (Buffer pH 7); 558 nm (MeOH)

Molar Extinction Coefficient 81,000 cm^{-1} M^{-1} (Buffer pH 7); 89,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.61 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[22,23,27,29,30,32,37] antibodies;[2–4,33,34] benzodiazepines;[4,5] cells/tissues;[6–8,24] chromosomes;[9,10] flagellar filaments;[11] histone deacetylases;[12] microorganisms;[13] muscimol;[14,15] nucleic acids/nucleotides;[3,16–23] proteins/peptides[3,24–38]

Biological/Medical Applications Analyzing/detecting analytes;[3] counting cells;[24] detecting chromosomal aberration;[9,10] identifying/characterizing microorganisms;[13] labeling/detecting nucleic acids;[3,16–23] measuring albumin diffusion rates and concentration profiles;[28] probing the charge-transfer dynamics in DNA;[17] quantifying proteins[24]

Industrial Applications Photoresists[39]

Safety/Toxicity No data available

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ALEXA FLUOR 555 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 886046-94-2

Chemical Structure Not reported

CA Index Name Alexa Fluor 555 carboxylic acid succinimidyl ester

Other Names Alexa 555; Alexa 555 succinimidyl ester; Alexa Fluor 555; Alexa Fluor 555 NHS; Alexa Fluor 555 NHS ester; Alexa Fluor 555 carboxylic acid SE; Alexa Fluor 555 carboxylic acid succinimidyl ester; Alexa Fluor 555 SE; Alexa Fluor 555 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1250

Physical Form Purple solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λmax) 555 nm (MeOH)

Emission (λmax) 572 nm (MeOH)

Molar Extinction Coefficient 155,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.10 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Antibodies;[2–6] bicyclononynes;[7] cells;[8,9] chromosomes;[10,11] dendrimers;[12] endosomes;[13] histone deacetylases;[14] nucleic acids;[4,15] proteins;[4,5,7,16–21] cowpea mosaic virus (CPMV)[22]

Biological/Medical Applications Analyzing/detecting analytes;[4] detecting chromosomal aberration;[10,11] encapsulating proteins inside surface-tethered liposomes;[18] investigating late endosome-lysosome retrograde fusion events;[13] visualizing living melanoma cells,[7] vasculature/blood flow in living mouse and chick embryos[22]

Industrial Applications Not reported

Safety/Toxicity No data available

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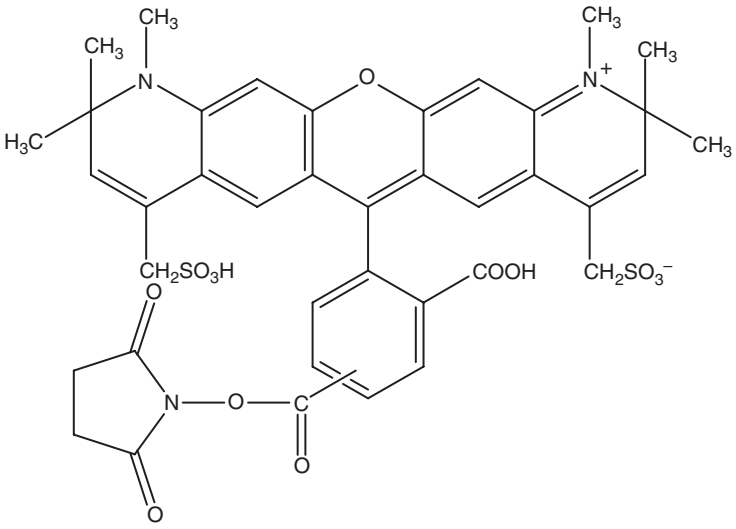
ALEXA FLUOR 594 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 295348-87-7

Chemical Structure



CA Index Name Pyrano[3,2-*g*:5,6-*g*']diquinolin-13-ium, 6-[2-carboxy-4(*or* 5)-[[(2,5-dioxo-1-pyrrolidinyl)-oxy]carbonyl]phenyl]-1,2,10,11-tetrahydro-1,2,2,10,10,11-hexamethyl-4,8-bis(sulfomethyl)-, inner salt

Other Names Alexa 594; Alexa 594 succinimidyl ester; Alexa Fluor 594; Alexa Fluor 594 NHS; Alexa Fluor 594 NHS ester; Alexa Fluor 594 carboxylic acid SE; Alexa Fluor 594 carboxylic acid succinimidyl ester; Alexa Fluor 594 SE; Alexa Fluor 594 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{39}H_{37}N_3O_{13}S_2$

Molecular Weight 819.85

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide

Absorption (λ_{max}) 590 nm (Buffer pH 7)

Emission (λ_{max}) 617 nm (Buffer pH 7)

Molar Extinction Coefficient 92,000 cm^{-1} M^{-1} (Buffer pH 7)

Quantum Yield 0.66 (Buffer pH 7.2)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Amines/amino groups;[21,25] antibodies;[4,5] biotin;[6] cells/tissues;[7–10] chromosomes;[11,12] cyclodextrin/dextran;[13–15] dendrimers;[16] glucose;[17] histone deacetylases;[18] hydrogen peroxide;[19] nucleic acids/nucleotides;[1,5,20,21] proteins/peptides;[5,22–26] quantum dots;[27,28] dengue virus[29]

Biological/Medical Applications Analyzing/detecting analytes;[5] characterizing submicron protein aggregates in human serum/plasma;[23] detecting chromosomal aberration;[11,12] detecting/quantifying biotin derivatives;[6] measuring blood glucose;[17] hydrogen peroxide sensor[19]

Industrial Applications Photoresists[30]

Safety/Toxicity No data available

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ALEXA FLUOR 633 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 1132773-86-4

Chemical Structure Not reported

CA Index Name Alexa Fluor 633 carboxylic acid succinimidyl ester

Other Names Alexa 633; Alexa 633 succinimidyl ester; Alexa Fluor 633; Alexa Fluor 633 NHS; Alexa Fluor 633 NHS ester; Alexa Fluor 633 carboxylic acid SE; Alexa Fluor 633 carboxylic acid succinimidyl ester; Alexa Fluor 633 SE; Alexa Fluor 633 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1200

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 621 nm (MeOH)

Emission (λ_{max}) 639 nm (MeOH)

Molar Extinction Coefficient 159,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[11,18] antibodies;[2,3,18] cells;[4,5] chromosomes;[6,7] histone deacetylases;[8] liposomes;[9,10] nanoparticles;[11] nucleic acids/nucleotides;[3,12–17] polymersomes;[18] proteins[3,9,18–20]

Biological/Medical Applications Analyzing/detecting analytes;[3] detecting chromosomal aberration;[6,7] investigating degradation of liposomal subcompartments in PEGylated capsosomes;[9] labeling/detecting nucleic acids;[12–17] patterning wide range of proteins;[19] studying molecule-membrane interactions or molecule-molecule interactions[10]

Industrial Applications Not reported

Safety/Toxicity No data available

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ALEXA FLUOR 660 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 422309-89-5

Chemical Structure Not reported

CA Index Name Alexa Fluor 660 carboxylic acid succinimidyl ester

Other Names Alexa 660; Alexa 660 succinimidyl ester; Alexa Fluor 660; Alexa Fluor 660 NHS; Alexa Fluor 660 NHS ester; Alexa Fluor 660 carboxylic acid SE; Alexa Fluor 660 carboxylic acid succinimidyl ester; Alexa Fluor 660 SE; Alexa Fluor 660 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1100

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 668 nm (MeOH); 660 nm (Buffer pH 7)

Emission (λ_{max}) 698 nm (MeOH); 689 nm (Buffer pH 7)

Molar Extinction Coefficient 132,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.37 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[15,25,27] antibodies;[2–6,30] bacteria;[7] blood vessels;[8] cells;[9–11] chromosomes;[12,13] Cu(II);[14] dendrimers;[15,16] epidermal growth factor receptor (EGFR);[30] folate;[17,18] histone deacetylases;[19] kinases;[20] nucleic acids/nucleotides;[21–27] proteins;[5,28–32] tumors;[30,33,34] Zn(II) cytochrome c[35]

Biological/Medical Applications Analyzing/detecting nucleic acids;[21–27] assessing epithelial neoplasia;[30] detecting chromosomal aberration;[12,13] detecting/confirming lymph nodes;[36,37] fluorescent labels in kinases (FLiK) assay;[20] glucose sensor for diabetic monitoring;[16] identifying stent thrombosis;[8] measuring/quantifying folate;[17,18] understanding lymph node metastasis;[34] as temperature sensor[38,39]

Industrial Applications Not reported

Safety/Toxicity No data available

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ALEXA FLUOR 680 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 948558-33-6

Chemical Structure Not reported

CA Index Name Alexa Fluor 680 carboxylic acid succinimidyl ester

Other Names Alexa 680; Alexa 680 succinimidyl ester; Alexa Fluor 680; Alexa Fluor 680 NHS; Alexa Fluor 680 NHS ester; Alexa Fluor 680 carboxylic acid SE; Alexa Fluor 680 carboxylic acid succinimidyl ester; Alexa Fluor 680 SE; Alexa Fluor 680 succinimidyl ester; Sulfo-NHS-AF680

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1150

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 684 nm (MeOH)

Emission (λ_{max}) 707 nm (MeOH)

Molar Extinction Coefficient 183,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.36 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[16,21,28,29] antibodies;[2–6] blood vessels;[7] cells;[8–13,23,26] chromosomes;[14,15] dendrimers;[16] histone deacetylase;[17] nucleic acids/nucleotides;[4,18–22] proteins/peptides;[4,23–34] tetanus toxin (TTc)[34]

Biological/Medical Applications Analyzing/detecting analytes;[4] counting cells;[23,26] detecting chromosomal aberration;[14,15] identifying stent thrombosis;[7] imaging of fast retrograde axonal transport in living animals;[34] monitoring mTORC1 activation;[25] quantifying proteins[23,27,30]

Industrial Applications Not reported

Safety/Toxicity No data available

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ALEXA FLUOR 700 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 1246956-22-8

Chemical Structure Not reported

CA Index Name Alexa Fluor 700 carboxylic acid succinimidyl ester

Other Names Alexa 700; Alexa 700 succinimidyl ester; Alexa Fluor 700; Alexa Fluor 700 NHS; Alexa Fluor 700 NHS ester; Alexa Fluor 700 carboxylic acid SE; Alexa Fluor 700 carboxylic acid succinimidyl ester; Alexa Fluor 700 SE; Alexa Fluor 700 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1400

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 702 nm (MeOH)

Emission (λ_{max}) 723 nm (MeOH)

Molar Extinction Coefficient 205,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.25 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[11] antibodies;[2,3] blood vessels;[4] cells;[5–8] chromosomes;[9,10] dendrimers;[11] histone deacetylases;[12] Hodgkin and Reed Sternberg (HRS) cells;[13] nucleic acids;[3,14,15] proteins[3,16,17]

Biological/Medical Applications Analyzing/detecting analytes;[3] detecting chromosomal aberration;[9,10] diagnosing classical Hodgkin lymphoma (CHL) in lymph nodes;[13] fluorescent cell barcoding;[7] identifying stent thrombosis[4]

Industrial Applications Not reported

Safety/Toxicity No data available

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ALEXA FLUOR 750 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 697795-06-5

Chemical Structure Not reported

CA Index Name Alexa Fluor 750

Other Names Alexa 750; Alexa 750 NHS; Alexa 750 succinimidyl ester; Alexa Fluor 750; Alexa Fluor 750 NHS; Alexa Fluor 750 NHS ester; Alexa Fluor 750 carboxylic acid SE; Alexa Fluor 750 carboxylic acid succinimidyl ester; Alexa Fluor 750 SE; Alexa Fluor 750 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1300

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 753 nm (MeOH)

Emission (λ_{max}) 782 nm (MeOH)

Molar Extinction Coefficient 290,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.12 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino groups;[2,3,11,21] amyloid-β (Aβ) peptides;[4] atherosclerotic plaque;[5] antibodies;[6–12] blood vessels;[13] caries in tooth enamel;[14] cells;[15–18] chromosomes;[19,20] dendrimers;[21] glucose;[22–24] histone deacetylases;[25] liposomes;[26] nanoparticles;[27–29] nucleic acids;[10,30–34] phospholipid micelles;[43] proteins/peptides;[10,23,24,26,35–41] quantum dots;[42] tumors[26,43,44]

Biological/Medical Applications Analyzing/detecting analytes;[10] detecting chromosomal aberration;[19,20] fluorescent cell barcoding;[17] glucose sensor;[22–24] homing/trafficking human hematopoietic stem cells (HSC);[28] identifying carious lesion;[14] imaging/identifying stent thrombosis;[13] quantifying proteins;[39] understanding lymph node metastasis;[44] use in agriculture and plant cultivation[45]

Industrial Applications Not reported

Safety/Toxicity No data available

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ALEXA FLUOR 790 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 950891-33-5

Chemical Structure Not reported

CA Index Name Alexa Fluor 790 carboxylic acid succinimidyl ester

Other Names Alexa 790; Alexa 790 succinimidyl ester; Alexa Fluor 790; Alexa Fluor 790 NHS; Alexa Fluor 790 NHS ester; Alexa Fluor 790 carboxylic acid SE; Alexa Fluor 790 carboxylic acid succinimidyl ester; Alexa Fluor 790 SE; Alexa Fluor 790 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Not reported

Molecular Formula Not reported

Molecular Weight ~1750

Physical Form Blue solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 784 nm (MeOH)

Emission (λ_{max}) 814 nm (MeOH)

Molar Extinction Coefficient 260,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Antibodies;[2] blood vessels;[3] cells;[4–6] chromosomes;[7,8] histone deacetylases;[9] proteins;[10] tetanus toxin (TTc)[10]

Biological/Medical Applications Detecting chromosomal aberration;[7,8] detecting/imaging cells;[4–6] identifying stent thrombosis;[3] imaging retrograde axonal transport in living animals;[10] treating ocular diseases[11]

Industrial Applications Not reported

Safety/Toxicity No data available

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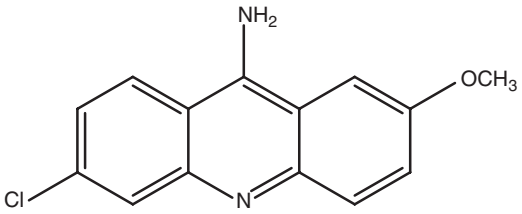
9-AMINO-6-CHLORO-2-METHOXYACRIDINE (ACMA)

CAS Registry Number 3548-09-2

Chemical Structure



CA Index Name 9-Acridinamine, 6-chloro-2-methoxy-

Other Names Acridine, 9-amino-6-chloro-2-methoxy-; 2-Methoxy-6-chloro-9-aminoacridine; 3-Chloro-7-methoxy-9-aminoacridine; 6-Chloro-9-amino-2-methoxyacridine; 9-Amino-3-chloro-7-methoxyacridine; 9-Amino-6-chloro-2-methoxyacridine; G 185; NSC 15300

Merck Index Number Not listed

Chemical/Dye Class Acridine

Molecular Formula $C_{14}H_{11}ClN_2O$

Molecular Weight 258.70

Physical Form Yellow crystals;[15] Yellow cubic crystals;[17] Orange-yellow crystals;[16] Yellow solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 341 °C;[3] 281 °C;[16] 274 °C;[4,10,17] 273 °C;[15] 272 °C;[9] 265–267 °C;[13] 250 °C[8]

Boiling Point (Calcd.) 475.1±35.0 °C, pressure: 760 Torr

pK_a 8.6, temperature: 22 °C

pK_a (Calcd.) 8.69 ± 0.10, most basic, temperature: 25 °C

Absorption (λ_{max}) 412 nm (MeOH acidified with a trace of HCl)

Emission (λ_{max}) 471 nm (MeOH acidified with a trace of HCl)

Molar Extinction Coefficient 8200 cm^{-1} M^{-1} (MeOH acidified with a trace of HCl)

Synthesis Synthetic methods[1–17]

Imaging/Labeling Applications Cancer cells;[18] chromosome;[19] membranes;[20–28] microorganisms;[29] nucleic acids/nucleic acid bases[30–49]

Biological/Medical Applications Analyzing membrane architecture;[28] antimalarial activity;[13,50,51] anti-prion activity;[3] antiviral activity;[54] bactericidal activity;[52,53] detecting cancer cells,[18] measuring microorganisms;[29] studying proton-pumping activity of various membrane-bound ATPases,[20,21,26,27] structure and function of membranes;[28] treating malformed forms of proteins causing neurodegenerative diseases;[55] as temperature sensor[56,57]

Industrial Applications Not reported

Safety/Toxicity Genotoxicity;[58–60] mutagenicity[58,61–64]

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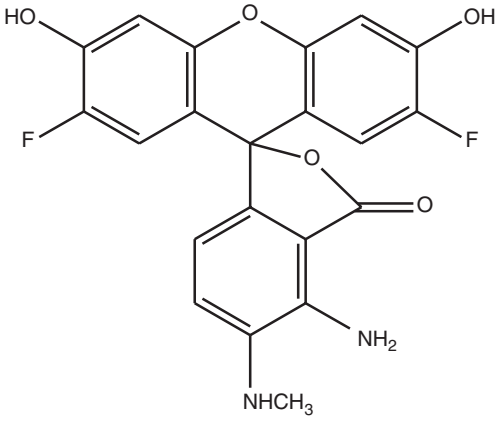
4-AMINO-5-METHYLAMINO-2′,7′-DIFLUOROFLUORESCEIN (DAF-FM)

CAS Registry Number 254109-20-1

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-3-one, 4-amino-2′,7′-difluoro-3′,6′-dihydroxy-5-(methylamino)-

Other Names 4-Amino-5-methylamino-2′,7′-difluorofluorescein; DAF-FM

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{14}F_2N_2O_5$

Molecular Weight 412.35

Physical Form Brown solid; White to beige powder

Solubility Soluble in dimethyl sulfoxide, methanol

Melting Point 265 °C[2]

Boiling Point (Calcd.) 693.7 ± 55.0 °C, pressure: 760 Torr

pK_a (Calcd.) 8.19 ± 0.20, most acidic, temperature: 25 °C; 4.23 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 487 nm (Buffer pH 8.0)

Emission (λ_{max}) Fluorescence is very weak; 515 nm (Buffer pH 7.4) (of benzotriazole)

Molar Extinction Coefficient 84,000 cm^{-1} M^{-1} (Buffer pH 8.0)

Quantum Yield 0.005 (Buffer pH 7.4)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Bacteria;[3] microorganisms;[3] nitric oxide ions[1,2,4–18]

Biological/Medical Applications Detecting bacteria/microorganisms;[3] nitric oxide indicator[1,2,4–18]

Industrial Applications Not reported

Safety/Toxicity No data available

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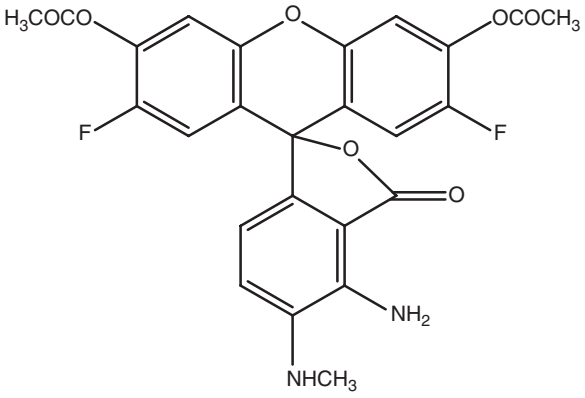
4-AMINO-5-METHYLAMINO-2′,7′-DIFLUOROFLUORESCEIN DIACETATE (DAF-FM DA)

CAS Registry Number 254109-22-3

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]-xanthen]-3-one, 3′,6′-bis(acetyloxy)-4-amino-2′,7′-difluoro-5-(methylamino)-

Other Names 4-Amino-5-methylamino-2′,7′-difluorofluorescein diacetate; DAF-FM DA

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{18}F_2N_2O_7$

Molecular Weight 496.42

Physical Form Orange/yellow solid

Solubility Soluble in dimethyl sulfoxide

Melting Point 135 °C[1]

Boiling Point (Calcd.) 695.7 ± 55.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.20 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 365 nm (MeOH)

Emission (λ_{max}) None

Synthesis Synthetic method[1]

Imaging/Labeling Applications Bacteria;[2] microorganisms;[2] nitric oxide ions[1,3–20]

Biological/Medical Applications Detecting bacteria/microorganisms;[2] nitric oxide indicator[1,3–20]

Industrial Applications Not reported

Safety/Toxicity No data available

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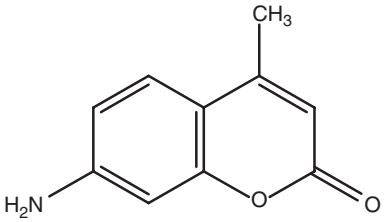
7–AMINO-4-METHYLCOUMARIN (AMC) (COUMARIN 120) (COUMARIN 440)

CAS Registry Number 26093-31-2

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-2-one, 7-amino-4-methyl-

Other Names Coumarin, 7-amino-4-methyl-; (4-Methyl-2-oxo-2*H*-chromen-7-yl)amine; 1: PN: JP2013135660 PAGE: 3 claimed sequence; 4-Methyl-7-aminocoumarin; 7-AMC; 7-Amino-4-methyl-2*H*-chromen-2-one; 7-Amino-4-methylcoumarin; C 120; Coumarin 120; Coumarin 440; NSC 45796; AMC

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{10}H_9NO_2$

Molecular Weight 175.18

Physical Form Yellow needles;[49] Yellow crystals;[1,26] Yellow solid; Brown crystals;[14] Brown solid;[12] Colorless solid;[19] Cream colored glistening needles[51]

Solubility Soluble in acetone, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 226–227 °C;[30,31,50] 226 °C;[48,51] 224–226 °C;[15,21] 223–226 °C;[4,17] 223–225 °C;[2] 223 °C;[44] 222–224 °C (decompose);[47] 222–224 °C;[6] 222–223 °C;[16] 221–225 °C;[26] 221–224 °C;[35] 221–223 °C;[19,22,28] 220–224 °C;[13,42,49] 220–222 °C;[14,20,38] 219–222 °C;[29] 219–220 °C[43]

Boiling Point (Calcd.) 378.3 ± 37.0 °C, pressure: 760 Torr

pK_a (Calcd.) 1.89 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 351 nm (MeOH); 342 nm (Buffer pH 7)

Emission (λ_{max}) 430 nm (MeOH); 441 nm (Buffer pH 7)

Molar Extinction Coefficient 18,000 cm^{-1} M^{-1} (MeOH); 16,000 cm^{-1} M^{-1} (Buffer pH 7)

Synthesis Synthetic methods[1–51]

Imaging/Labeling Applications Amyloid β peptide;[52] bacteria;[53] carbohydrates/sugars;[54–63] cells;[64] cellulose nanocrystals;[65] clay mineral;[66] metal ions (copper ions,[67,68] mercury ions,[69,70] zinc ions;[71]) nitrite;[72] nucleic acids/nucleotides;[73,74] proteins;[75–78] silica nanoparticles[79,80]

Biological/Medical Applications Identifying bacteria;[53] measuring urinary kallikrein levels;[81] monitoring platinum(iv) reduction and platinum(ii) reactions in cancer cells;[82] as a substrate for measuring adipinylamidases activity,[83] aromatic amino acid decarboxylases activity,[84] histone deacetylases activity,[85–93] hydrolases/esterases activity,[94–97] β-lactamases activity,[98] microbial nitroreductases activity,[99] penicillin G acylases activity,[100,101] proteases/proteinases/peptidases activity,[26,102–135] glutamyltransferases activity,[136] tryptophanases activity;[137] as an effective antitubercular agent;[138] use as temperature sensor[139,140]

Industrial Applications For authentification;[141] dye lasers;[45,142–163,172] color display devices;[164–166] inks;[167] monitoring underlying corrosion on coated aluminum;[168] photoinitiating systems;[169] recording materials;[170] semiconductor devices;[171] dye-sensitized solar cells (DSCs);[172,173] mesoporous silica fibers;[174] SiO_2 sonogel hybrid materials;[175] textiles;[176] waveguides;[177,178] whitening agents[179,180]

Safety/Toxicity Mutagenicity[181]

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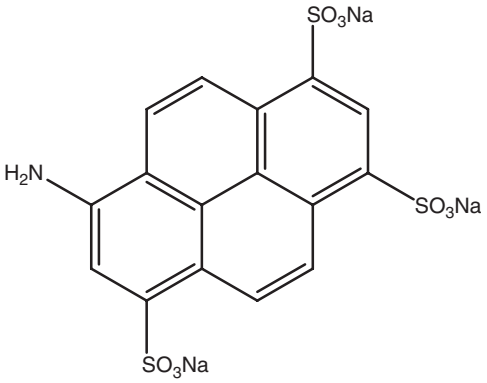
8-AMINOPYRENE-1,3,6-TRISULFONIC ACID TRISODIUM SALT (APTS)

CAS Registry Number 196504-57-1

Chemical Structure



CA Index Name 1,3,6-Pyrenetrisulfonic acid, 8-amino-, sodium salt (1:3)

Other Names 8-Aminopyrene-1,3,6-trisulfonic acid, trisodium salt; APTS; 1,3,6-Pyrenetrisulfonic acid, 8-amino-, trisodium salt; Trisodium 8-aminopyrene-1,3,6-trisulfonate

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{16}H_8NNa_3O_9S_3$

Molecular Weight 523.39

Physical Form Yellow solid;[2] Brown powder (crude); Orange powder (pure);[3] Orange solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point ≥250 °C

Absorption (λ_{max}) 424 nm (Buffer pH 7.0); 424 nm, 383 nm (H_2O)

Emission (λ_{max}) 505 nm (Buffer pH 7.0)

Molar Extinction Coefficient 19,000 cm^{-1} M^{-1} (Buffer pH 7.0); 20,600 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Cyclen 1;[4] glycoproteins;[5] glucose/monosaccharides;[3,6] oligosaccharides;[7–10] polysaccharides[11,12]

Biological/Medical Applications Analysizing monosaccharides;[3,6] detecting oligosaccharides;[7–10] separating polysaccharides;[11,12] ultrathin protein films[13]

Industrial Applications Not reported

Safety/Toxicity No data available

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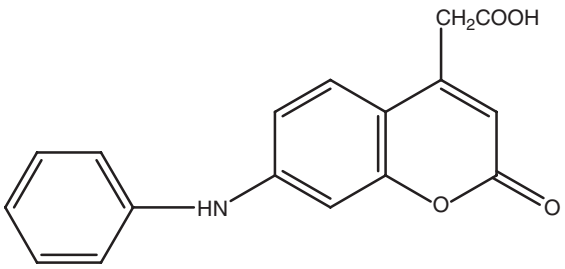
7-ANILINOCOUMARIN-4-ACETIC ACID (ACAA)

CAS Registry Number 82412-15-5

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(phenylamino)-

Other Names 2*H*-1-Benzopyran-4-acetic acid, 7-anilino-2-oxo-; 7-Anilinocoumarin-4-acetic acid; 7-Phenylaminocoumarin-4-acetic acid; ACAA

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{17}H_{13}NO_4$

Molecular Weight 295.29

Physical Form Pale yellow needles[2]

Solubility Soluble in water, cyclohexane, dimethyl sulfoxide, ethanol

Melting Point 186–189 °C (decompose);[2] 183.5–184.5 °C;[1] >160 °C (decompose)[3]

Boiling Point (Calcd.) 545.5 ± 50.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.22 ± 0.10, most acidic, temperature: 25 °C; −1.59 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 262 nm, 375 nm (H_2O); 269 nm, 376 nm (EtOH); 272 nm, 378 nm (Cyclohexane)

Emission (λ_{max}) 459 nm (H_2O); 458 nm (EtOH); 404 nm (Cyclohexane); 475 nm (Phosphate Buffer pH 7.4 in the presence of human serum albumin (HSA))

Molar Extinction Coefficient 4,150 cm^{-1} $M,^{-1}$ 4,350 cm^{-1} M^{-1} (H_2O); 4,220 cm^{-1} M^{-1} (EtOH); 4,160 cm^{-1} $M,^{-1}$ 4,440 cm^{-1} M^{-1} (Cyclohexane)

Quantum Yield <0.01 (H_2O); 0.01 (EtOH); 0.32 (Cyclohexane); 0.06 (Phosphate Buffer pH 7.4 in the presence of human serum albumin (HSA))

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Human serum albumin (HSA);[2,4–6] iron chelators[1]

Biological/Medical Applications Evaluating iron chelators;[1] as a probe for human serum albumin (HAS) binding sites;[2] studying binding sites of bile acids on human serum albumin,[6] drug-albumin interactions;[2] ultrafiltration assays of ligand binding to human serum albumin[5]

Industrial Applications Not reported

Safety/Toxicity No data available

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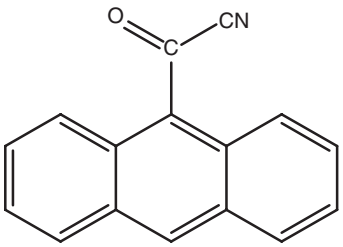
9-ANTHROYLNITRILE

CAS Registry Number 85985-44-0

Chemical Structure



CA Index Name 9-Anthraceneacetonitrile, α-oxo-

Other Names 9-Anthracenecarbonyl cyanide; 9-Anthroylnitrile; 9-AN; α-Oxo-anthracene-9-acetonitrile; ANN

Merck Index Number Not listed

Chemical/Dye Class Anthracene

Molecular Formula $C_{16}H_9NO$

Molecular Weight 231.25

Physical Form Orange-yellow needles;[1] Orange powder[2]

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, methanol

Melting Point 143–144 °C[1]

Boiling Point (Calcd.) 426.8±14.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 361 nm, 380 nm, 344 nm (MeOH)

Emission (λ_{max}) 470 nm (MeOH)

Molar Extinction Coefficient 7500 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Alcohols;[1,2,7,17,19] aloesin;[3] analytes;[4] bile acid *N*-acetylglucosaminides;[5,6] carnitine enantiomers;[7] corticosteroids;[8] cortisol;[9] cortisone;[9] farnesyl pyrophosphate (FPP);[10] hydroxy steroids;[1,2] archaeal ether core lipids;[11] *N*-terminal peptide segment of myosin subfragment-1 (S-1);[12] serine-181;[13,14] thyroid hormones;[15] triamcinolone (TMC)[16]

Biological/Medical Applications Analyzing primary/secondary/tertiary alcohols;[17] detecting aloesin,[3] analytes,[4] cortisol/cortisone in biological fluids,[9] farnesyl pyrophosphate (FPP),[10] archaeal ether core lipids,[11] thyroid hormones in pharmaceutical preparations,[15] small quantities of triamcinolone (TMC);[16] identifying serine 181;[13,14] reagents for hydroxy steroids;[1,2] separating/characterizing bile acid *N*-acetylglucosaminides;[5,6] separating carnitine enantiomers in pharmaceuticals;[7] reagents for alcohols/hydroxyl groups[1,2,7,17,19]

Industrial Applications Analyzing chemical compositions for carbonized distillate of coal-tar refined soft pitch;[18] detecting absolute amount of resin-bound hydroxyl groups[19]

Safety/Toxicity No data available

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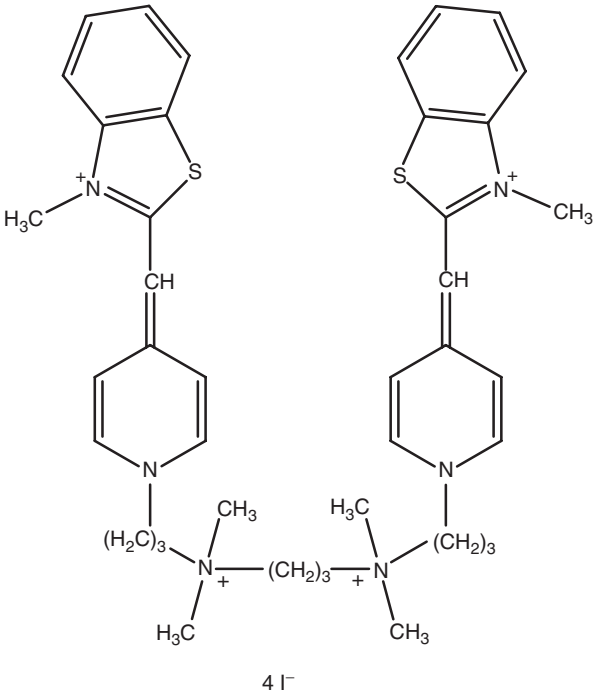
BOBO 1

CAS Registry Number 169454-13-1

Chemical Structure



CA Index Name Benzothiazolium, 2,2′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidenemethylidyne]]bis[3-methyl-, iodide (1:4)

Other Names Benzothiazolium, 2,2′-[1,3-propanediyl-bis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidenemethylidyne]]bis[3-methyl-, tetraiodide; BOBO 1; BOBO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{41}H_{54}I_4N_6S_2$

Molecular Weight 1202.66

Physical Form Yellow-brown powder[2]

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 462 nm (H_2O/DNA)

Emission (λ_{max}) 481 nm (H_2O/DNA)

Molar Extinction Coefficient 113,600 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.22 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–12] cells;[2,11,12] bacteria;[12] chromosome spreads;[2] nuclei;[13–16] micronuclei;[17] megakaryocyte;[18] microorganisms;[19–21] sperms;[11,22] hairs[23]

Biological/Medical Applications Detecting nucleic acids,[1–12] cells;[2,11,12] classifying/counting megakaryocytes;[18] counting erythroblasts,[15,16] sperms;[11,22] characterizing DNA/lipid complexes (lipoplexes);[9,10] detecting/measuring microorganisms;[19–21] as temperature sensor[24,25]

Industrial Applications Not reported

Safety/Toxicity No data available

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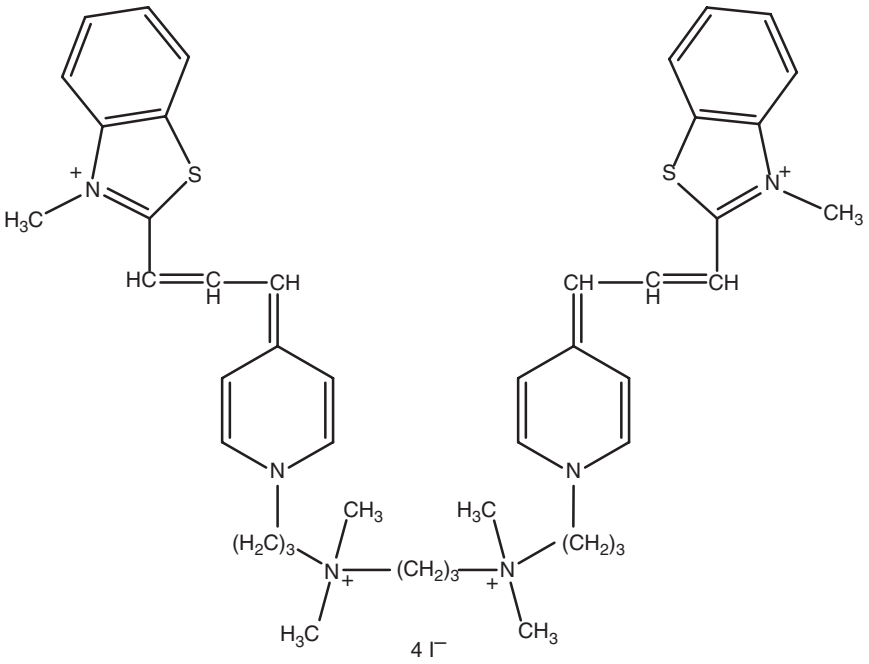
BOBO 3

CAS Registry Number 169454-17-5

Chemical Structure



CA Index Name Benzothiazolium, 2,2′-[1,3-propanediylbis-[(dimethyliminio)-3, 1-propanediyl-1(4*H*)-pyridinyl-4-ylidene-1-propen-1-yl-3-ylidene]]bis[3-methyl-, iodide (1:4)

Other Names Benzothiazolium, 2,2′-[1,3-propanediyl-bis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidene-1-propen-1-yl-3-ylidene]]bis[3-methyl-, tetraiodide; BOBO 3; BOBO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{45}H_{58}I_4N_6S_2$

Molecular Weight 1254.73

Physical Form Yellow-brown powder; Purple powder[2]

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 570 nm (H_2O/DNA)

Emission (λ_{max}) 602 nm (H_2O/DNA)

Molar Extinction Coefficient 147,800 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.39 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–13] cells;[1,2,12,13] bacteria;[13,14] chromosome spreads;[2] nuclei;[15–18] megakaryocytes;[19] microorganisms;[20,21] sperms;[12,22] hairs[23]

Biological/Medical Applications Detecting nucleic acids,[1–13] cells,[1,2,12,13] microorganisms;[20,21] IDH1/IDH2 mutations;[24] JAK2 gene mutation;[25] PIK3CA mutation;[26] B-type Raf Kinase (BRAF) mutation;[27] Mucin 1;[28] thrombin;[29] classifying/counting megakaryocytes;[19] counting erythroblasts,[17,18] sperms;[12,22] nucleic acid sequencing;[30] as temperature sensor;[31,32] biophotonic wire assemblies[33]

Industrial Applications Semiconductor nanocrystal[34]

Safety/Toxicity No data available

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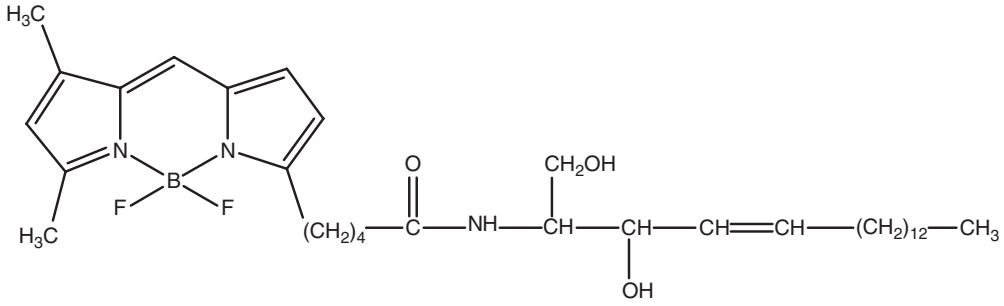
BODIPY FL C_5-CERAMIDE (C_5-DMB-CERAMIDE)

CAS Registry Number 133867-53-5

Chemical Structure



CA Index Name Boron, [5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene-κ*N*)methyl]-*N*-[(1*S*,2*R*,3*E*)-2-hydroxy-1-(hydroxymethyl)-3-heptadecen-1-yl]-1*H*-pyrrole-2-pentanamidato-κN^1]difluoro-, (*T*-4)-

Other Names Boron, [5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene)-methyl]-*N*-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-1*H*-pyrrole-2-pentanamidato-N^1,N^5] difluoro-, [*T*-4-[*R*-[*R**,*S**-(*E*)]]]-; Boron, [5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene-κ*N*)methyl]-*N*-[(1*S*,2*R*,3*E*)-2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-1*H*-pyrrole-2-pentanamidato-κN^1]difluoro-, (*T*-4)-; 1*H*-Pyrrole-2-pentanamide, 5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene)methyl]-*N*-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, boron complex, [*R*-[*R**,*S**-(*E*)]]-; BODIPY FL C_5-ceramide; BODIPY FL C_5-cer; C_5-DMB-ceramide; C_5-DMB-cer

Merck Index Number Not listed

Chemical/Dye Class Boron co-ordination compound/dye

Molecular Formula $C_{34}H_{54}BF_2N_3O_3$

Molecular Weight 601.63

Physical Form Orange solid

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 505 nm (MeOH)

Emission (λ_{max}) 511 nm (MeOH)

Molar Extinction Coefficient 91,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Golgi apparatus;[1–9,28] antigen presenting cells (APCs);[10] bacteria;[11] cytoplasmic membranes;[28] exosome subpopulations;[12] glycoproteins;[13] lipids;[14–17] lipid bilayers;[18] lipoproteins;[19] live cells;[20] Madin-Darby canine kidney (MDCK) cells;[21] myelin;[22] nucleic acids;[27] Pc 4;[28] sphingolipid[23–26]

Biological/Medical Applications Analyzing lipoproteins;[19] characterizing exosome subpopulations;[12] detecting trogocytosis;[10] identifying nucleic acids;[27] inhibiting glycoprotein traffic;[13] investigating sphingolipid transport and metabolism;[23–26] measuring rate of myelination;[22] modulating peptidolytic activity of cathepsin D;[29] monitoring live cells;[20] as a substrate for measuring hydrolytic enzyme activity,[30] inositol phosphorylceramide synthase activity[31]

Industrial Applications Not reported

Safety/Toxicity No data available

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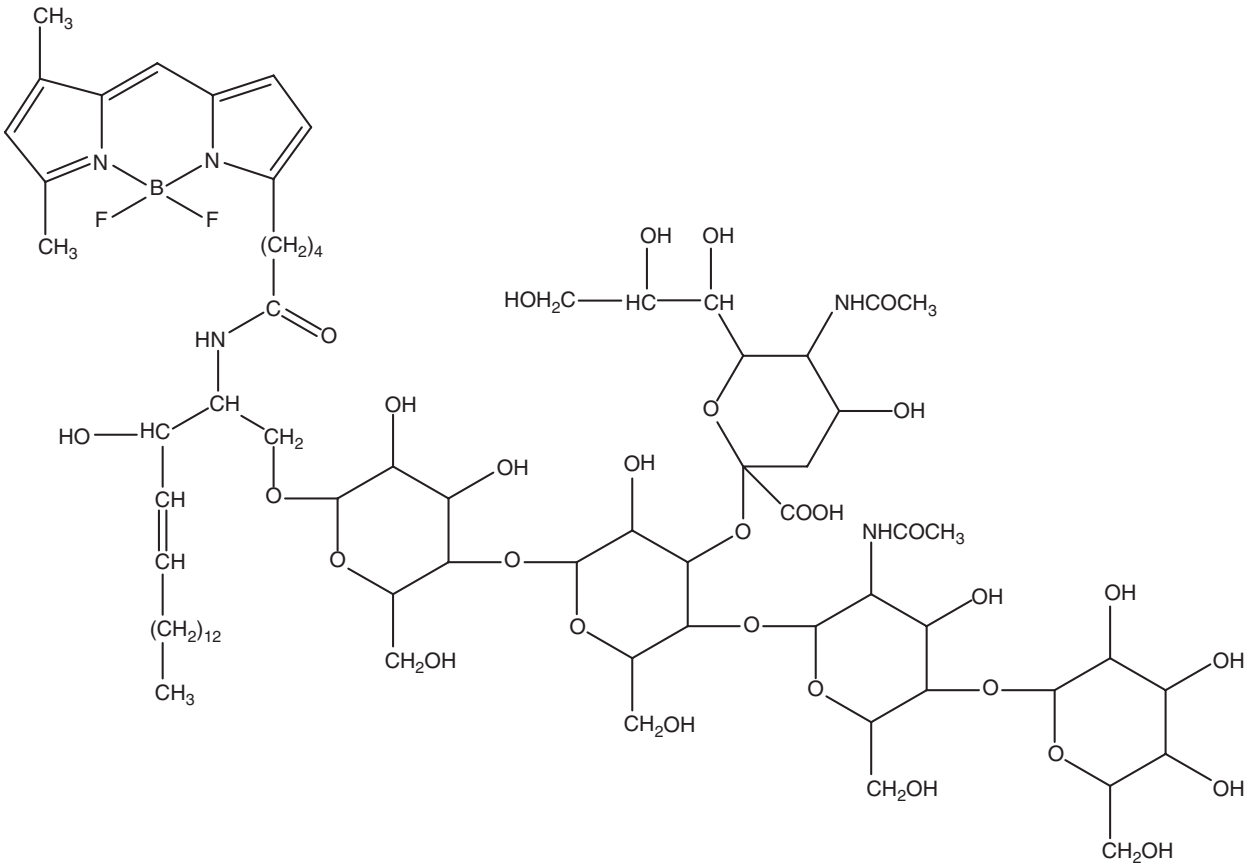
BODIPY FL C_5-GANGLIOSIDE GM1

CAS Registry Number 908143-55-5

Chemical Structure



CA Index Name Boron, [5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene-κ*N*)methyl]-*N*-[(1*S*,2*R*,3*E*)-1-[[[*O*-β-D-galactopyranosyl-(1→4)-2-*O*-(acetylamino)-2-deoxy-β-D-galactopyranosyl-(1→4)-*O*-[*N*-acetyl-α-neuraminosyl-(2→3)]-*O*-β-D-galactopyranosyl-(1→4)-β-D-glucopyranosyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-1*H*-pyrrole-2-pentanamidato-κ*N*[1]]difluoro-, (*T*-4)-

Other Names BODIPY FL C_5-ganglioside GM_1; BODIPY FL C_5-GM_1; BO-GM1

Merck Index Number Not listed

Chemical/Dye Class Boron co-ordination compound/dye

Molecular Formula $C_{71}H_{114}BF_2N_5O_{31}$

Molecular Weight 1582.50

Physical Form Orange solid

Solubility Soluble in dimethyl sulfoxide, ethanol, methanol

Absorption (λ_{max}) 505 nm (MeOH)

Emission (λ_{max}) 512 nm (MeOH)

Molar Extinction Coefficient 80,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amyloid beta-protein;[2] antigen presenting cells (APCs);[3] cholera toxin (CT);[4,5] bilayer lipid membranes;[1] laminin-1;[8] lipid rafts[5–9]

Biological/Medical Applications Detecting lipid rafts in live red blood cells (RBCs) membranes,[6] protein toxin,[4,5] trogocytosis;[3] investigating binding of laminin-1 to BO-GM1 for neurite outgrowth[8]

Industrial Applications Not reported

Safety/Toxicity No data available

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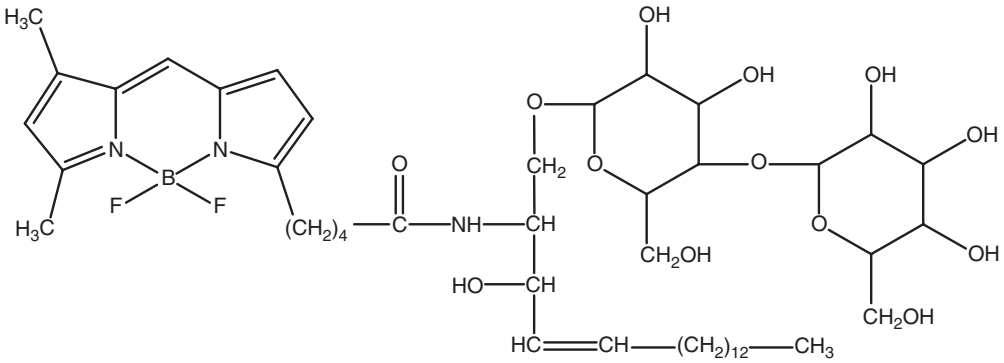
BODIPY FL C_5-LACTOSYLCERAMIDE

CAS Registry Number 251955-11-0

Chemical Structure



CA Index Name Boron, [5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene-κ*N*)methyl]-*N*-[(1*S*,2*R*,3*E*)-1-[[(4-*O*-β-D-galactopyranosyl-β-D-glucopyranosyl)oxy]methyl]-2-hydroxy-3-heptadecenyl]-1*H*-pyrrole-2-pentanamidato-κ*N*^{1}]difluoro-, (*T*-4)-

Other Names BODIPY FL C_5-lactosylceramide; BODIPY FL C_5-LacCer; BODIPY LacCer; *N*-(4,4-Difluoro-5,7-dimethyl-4-bora-3a,4a-diaza-*s*-indacene-3-pentanoyl)sphingosyl 1-β-D-lactoside

Merck Index Number Not listed

Chemical/Dye Class Boron co-ordination compound/dye

Molecular Formula $C_{46}H_{74}BF_2N_3O_{13}$

Molecular Weight 925.91

Physical Form Orange solid

Solubility Soluble in dimethyl sulfoxide, ethanol, methanol

Absorption (λ_{max}) 505 nm (MeOH)

Emission (λ_{max}) 511 nm (MeOH)

Molar Extinction Coefficient 80,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Golgi apparatus;[1,3,5,11,12] antigen presenting cells (APCs);[4] caveolae;[5,6] cellular organelles;[8] endosomes;[11] glycosphingolipids (GSLs);[1,2,6,7,9] lipids;[10] lysosomes;[11] oligodendrocytes;[15] plasma membrane micrometric domains[16]

Biological/Medical Applications Analyzing glycosphingolipid transport;[1,2] detecting Niemann-Pick C (NPC) variants,[11] trogocytosis;[4] diagnosing diseases/disorders associated with an alteration in sialyltransferase activity such as neurological disorders, inflammatory disorders, and cancers;[9] differentiating oligodendrocytes;[15] investigating mechanism of endocytosis,[6] sphingolipid transport/metabolism;[12–14] monitoring glycosphingolipid metabolism;[7] as a substrate for measuring sialyltransferase activity;[1,9] visualizing cellular organelles[8]

Industrial Applications Not reported

Safety/Toxicity No data available

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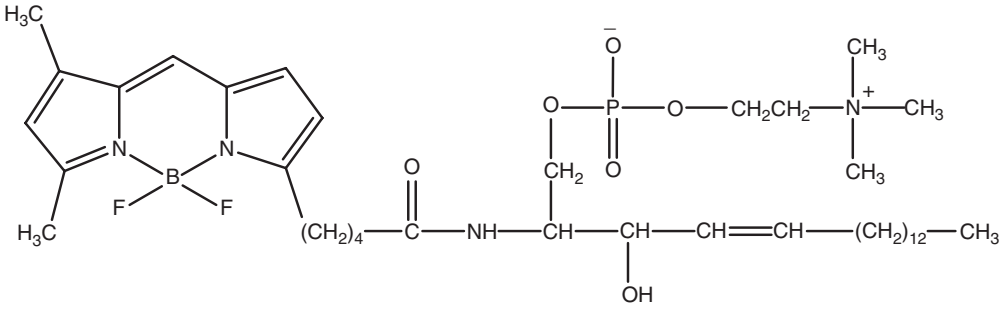
BODIPY FL C_5-SPHINGOMYELIN (C_5-DMB-SPHINGOMYELIN)

CAS Registry Number 191853-29-9

Chemical Structure



Physical Form Orange solid

Solubility Soluble in chloroform, methanol

Absorption (λ_{max}) 505 nm (MeOH)

Emission (λ_{max}) 512 nm (MeOH)

Molar Extinction Coefficient 77,000 cm^{-1} M^{-1} (MeOH)

CA Index Name Boron, [(7*S*)-13-[2-[(3,5-dimethyl-1*H*-pyrrol-2-yl-κ*N*)-methylene]-2*H*-pyrrol-5-yl-κ*N*]-4-hydroxy-7-[(1*R*,2*E*)-1-hydroxy-2-hexadecenyl]-*N*,*N*,*N*-trimethyl-9-oxo-3,5-dioxa-8-aza-4-phosphatridecan-1-aminium 4-oxidato(2-)]-difluoro-, (*T*-4)-

Other Names BODIPY FL C_5-sphingomyelin; BODIPY FL C_5-SM; C_5-DMB-sphingomyelin; C_5-DMB-SM; N-(4,4-difluoro-5,7-dimethyl-4-bora-3a,4a-diaza-*s*-indacene-3-pentanoyl)sphingosyl phospho choline

Merck Index Number Not listed

Chemical/Dye Class Boron co-ordination compound/dye

Molecular Formula $C_{39}H_{66}BF_2N_4O_6P$

Molecular Weight 766.75

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Golgi apparatus;[4,17] antigen presenting cells (APCs);[5] endosomes;[6,11] immobilized enzymes;[7] lipids;[8–13] lipid bilayer membranes;[14] low-density lipoproteins;[6] lysosomes;[11] plasma membrane micrometric domains[15,16]

Biological/Medical Applications Detecting trogocytosis;[5] distinguishing unique populations of early endosomes from one another;[6,11] examing lipid bilayer membranes;[14] investigating sphingolipid transport and metabolism;[1,9–12,17,18] measuring spontaneous transfer and transbilayer movement of lipids in lipid vesicles;[13] studying enzymic reactions,[7] membrane lipid traffic along the endocytic pathway[9–12]

Industrial Applications Not reported

Safety/Toxicity No data available

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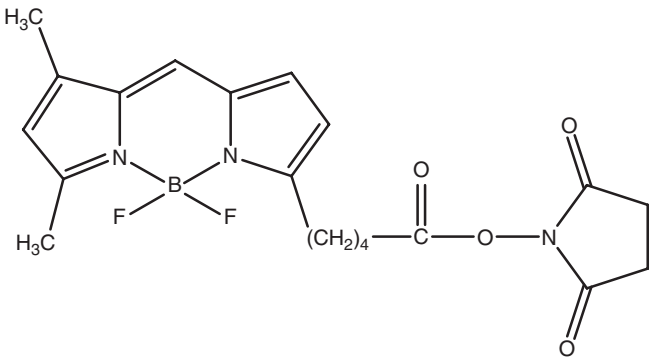
BODIPY FL C_5-SUCCINIMIDYL ESTER

CAS Registry Number 133867-52-4

Chemical Structure



CA Index Name Boron, [1-[[5-[5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene-κ*N*)methyl]-1*H*-pyrrol-2-yl-κ*N*]-1-oxopentyl]oxy]-2,5-pyrrolidinedionato]difluoro-, (*T*-4)-

Other Names Boron, [1-[[5-[5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene)methyl]-1*H*-pyrrol-2-yl]-1-oxopentyl] oxy]-2,5-pyrrolidinedionato]difluoro-, (*T*-4)-; 2,5-Pyrrolidinedione, 1-[[5-[5-[(3,5-dimethyl-2*H*-pyrrol-2-ylidene)methyl]-1*H*-pyrrol-2-yl]-1-oxopentyl]oxy]-, boron complex; BODIPY FL-C_5-SE; BODIPY FL C_5-succinimidyl ester; BODIPY FL C_5-N-hydroxysuccinimidyl (NHS) ester; BODIPY FL C_5- NHS ester; BODIPY-NHS ester

Merck Index Number Not listed

Chemical/Dye Class Boron co-ordination compound/dye

Molecular Formula $C_{20}H_{22}BF_2N_3O_4$

Molecular Weight 417.22

Physical Form Orange solid

Solubility Soluble in acetonitrile, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 504 nm (MeOH)

Emission (λ_{max}) 511 nm (MeOH)

Molar Extinction Coefficient 87,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Glycosphingolipids (GSLs);[2,3] nucleoside triphosphates;[4–6] oligonucleotides;[7] pladienolide[8]

Biological/Medical Applications Dyed polymer microparticles;[9,10] purifying oligonucleotides;[7] regulating meiosis;[11] as a substrate for measuring lysophospholipase D (lysoPLD) activity,[12–14] phospholipases A (PLA) activity[15]

Industrial Applications For synthesizing boron dipyrromethene difluoride (BODIPY) ceramide analogs;[16] for synthesizing lactosylceramide stereoisomers[3]

Safety/Toxicity No data available

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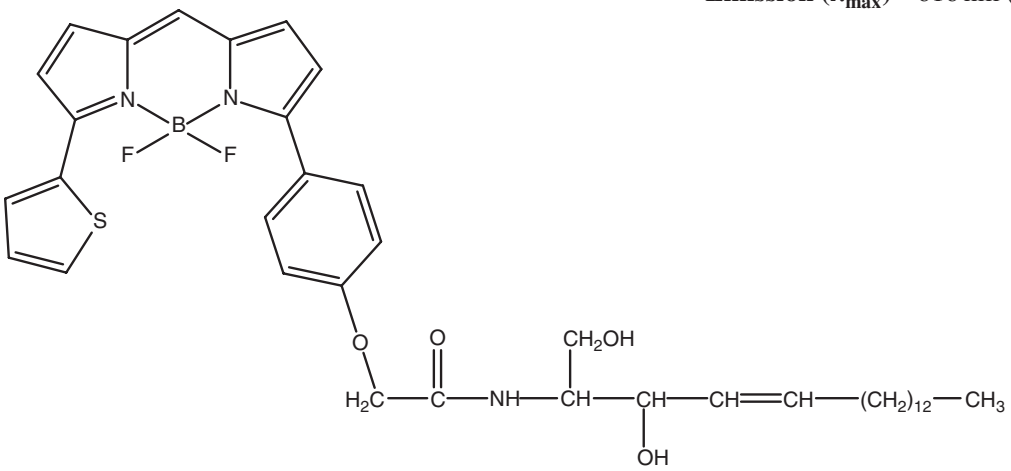
BODIPY TR CERAMIDE

CAS Registry Number 571186-05-5

Chemical Structure



CA Index Name Boron, difluoro[*N*-[(1*S*,2*R*,3*E*)-2-hydroxy-1-(hydroxymethyl)-3-heptadecen-1-yl]-2-[4-[5-[[5-(2-thienyl)-2*H*-pyrrol-2-ylidene-κ*N*]methyl]-1*H*-pyrrol-2-yl-κ*N*]phenoxy]acetamidato]-, (*T*-4)-

Other Names Boron, difluoro[*N*-[(1*S*,2*R*,3*E*)-2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-2-[4-[5-[[5-(2-thienyl)-2*H*-pyrrol-2-ylidene-κ*N*]methyl]-1*H*-pyrrol-2-yl-κ*N*]phenoxy]acetamidato]-, (*T*-4)-; BODIPY TR ceramide; Bodipy TR C5 ceramide

Merck Index Number Not listed

Chemical/Dye Class Boron co-ordination compound/dye

Molecular Formula $C_{39}H_{50}BF_2N_3O_4S$

Molecular Weight 705.71

Physical Form Purple solid

Solubility Soluble in chloroform, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 589 nm (MeOH)

Emission (λ_{max}) 616 nm (MeOH)

Molar Extinction Coefficient 65,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Golgi apparatus;[1–6] cells;[7,9,10] liposomes;[8] live malaria blood stage parasites;[9,10] PC-3 prostate cancer cells;[11] sphingomyelin[2]

Biological/Medical Applications Demonstrating sphingomyelin intracellular distribution;[2] mapping whole cell architecture;[10] revealing modular features of exomembrane system of malaria parasite;[10] studying malaria blood stages biology[9]

Industrial Applications Not reported

Safety/Toxicity No data available

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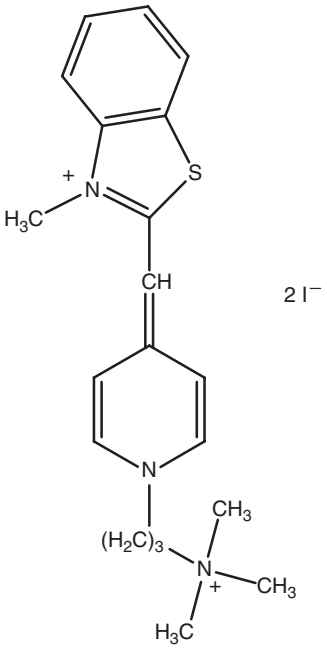
BO-PRO 1

CAS Registry Number 157199-57-0

Chemical Structure



CA Index Name Benzothiazolium, 3-methyl-2-[[1-[3-(trimethylammonio)propyl]-4(1*H*)-pyridinylidene] methyl]-,iodide (1:2)

Other Names Benzothiazolium, 3-methyl-2-[[1-[3-(trimethylammonio)propyl]-4(1*H*)-pyridinylidene] methyl]-, diiodide; BO-PRO 1; BO-PRO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{20}H_{27}I_2N_3S$

Molecular Weight 595.32

Physical Form Solid

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 462 nm (H_2O/DNA)

Emission (λ_{max}) 481 nm (H_2O/DNA)

Molar Extinction Coefficient 58,100 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.16 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–10] cells;[1,2,10] bacteria;[2] nuclei;[11–13] cytoplasm;[13] megakaryocyte;[14] microorganisms;[15] sperms[10,16]

Biological/Medical Applications Detecting nucleic acids,[1–10] cells,[1,2,10] microorganisms,[15] classifying/counting megakaryocyte;[14] counting erythroblasts,[11,12] sperms;[10,16] nucleic acids amplification;[9] nucleic acid sequencing;[17] as temperature sensor[18,19]

Industrial Applications Not reported

Safety/Toxicity No data available

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8. Erikson, G. H.; Daksis, J. I.; Kandic, I.; Picard, P. Nucleic acid multiplex formation. PCT Int. Appl. WO 2002103051, 2002.
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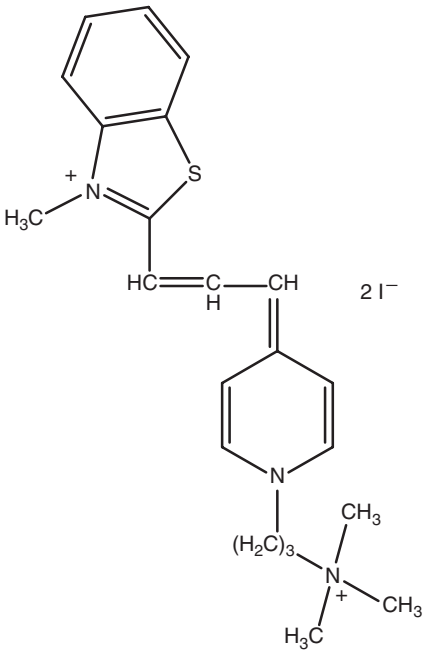
BO-PRO 3

CAS Registry Number 173357-16-9

Chemical Structure



CA Index Name Benzothiazolium, 3-methyl-2-[3-[1-[3-(trimethylammonio)propyl]-4(1*H*)-pyridinylidene]-1-propen-1-yl]-, iodide (1:2)

Other Names Benzothiazolium, 3-methyl-2-[3-[1-[3-(trimethylammonio)propyl]-4(1*H*)-pyridinylidene]-1-propenyl]-, diiodide; BO-PRO 3; BO-PRO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{22}H_{29}I_2N_3S$

Molecular Weight 621.36

Physical Form Solid

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 575 nm (H_2O/DNA)

Emission (λ_{max}) 599 nm (H_2O/DNA)

Molar Extinction Coefficient 80,900 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.62 (H_2O/DNA)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Nucleic acids;[1–10] cells;[1,10] bacteria;[1] microorganisms;[11] sperms[10]

Biological/Medical Applications Detecting nucleic acids,[1–10] cells,[1,10] microorganisms;[11] nucleic acids amplification;[9] as temperature sensor[12,13]

Industrial Applications Photonic fabric display[14]

Safety/Toxicity No data available

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12. Bousseksou, A.; Salmon, L.; Molnar, G.; Cobo, S. Materials with thermochromic spin transition doped with one or more fluorescent agents for use as temperature sensor. Fr. Demande FR 2952371, 2011.
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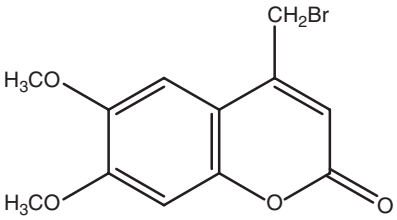
4-BROMOMETHYL-6,7-DIMETHOXYCOUMARIN

CAS Registry Number 88404-25-5

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-2-one, 4-(bromomethyl)-6,7-dimethoxy-

Other Names 4-Bromomethyl-6,7-dimethoxycoumarin; 4-(Bromomethyl)-6,7-dimethoxycoumarin; 4-(Bromomethyl)-6,7-dimethoxy-2-oxo-2*H*-benzopyran; BrCU; 4-Bdmc; BDMC; BrDMC; Brmdmc; Br-Mdmc; Brdmc-4,6,7

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{12}H_{11}BrO_4$

Molecular Weight 299.12

Physical Form Yellow crystals or powder

Solubility Soluble in acetonitrile, dichloromethane, *N,N*-dimethylformamide, methanol

Melting Point 208 °C[1]

Boiling Point (Calcd.) 417.1 ± 45.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 348 nm (MeOH)

Emission (λ_{max}) 425 nm (MeOH)

Molar Extinction Coefficient 10,631 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.24 (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Bacteria;[2] bile acid;[3] calcium-magnesium-ATPase;[4] myosin ATPase;[5] carboxylic acids;[1,6,7,9–11] cyclosporine;[8] fatty acids;[1,9–11,] lauric acid metabolites;[10,11] metail ions;[12–17] proteins;[18–20] sulfhydryl groups[5,19,20]

Biological/Medical Applications Analyzing bile acid;[3] anticancer agents;[21,22] identifying bacteria;[2] identifying/measuring lauric acid metabolites;[10,11] measuring cyclosporine;[8] studying/monitoring early stages of protein folding;[18] treating gastrointestinal diseases;[23] derivatization reagent for carboxylic acids;[1,6,7,9–11] as a substrate for measuring lauric acid hydroxylase activity[10,11]

Industrial Applications Electrostatic imaging process;[24] resists;[25] printed circuit boards;[26] semiconductor devices[26]

Safety/Toxicity No data available

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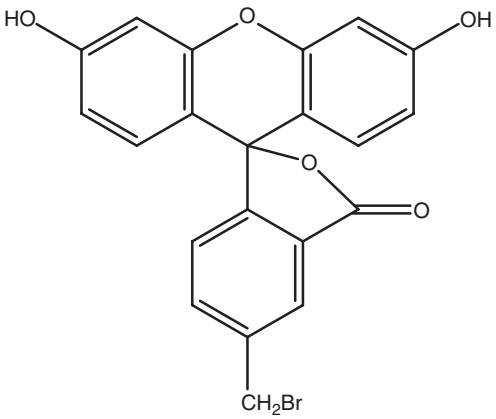
5-(BROMOMETHYL)FLUORESCEIN

CAS Registry Number 148942-72-7

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-3-one, 5-(bromomethyl)-3′,6′-dihydroxy-

Other Names 5-(Bromomethyl)fluorescein; 5-BMF; BMF; BrF

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{13}BrO_5$

Molecular Weight 425.23

Physical Form Orange solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 681.8 ± 55.0 °C, pressure: 760 Torr

pK_a (Calcd.) 9.33 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 492 nm (Buffer pH 9.0)

Emission (λ_{max}) 515 nm (Buffer pH 9.0)

Molar Extinction Coefficient 81,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Acidic fibroblast growth factor;[2] calcium-ATPase/calcium-magnesium-ATPase of sarcoplasmic reticulum at Glu-439;[3,4] cefuroxime;[5] γ-cholesteryloxybutyric acid (CBA);[5,6] fatty acids;[5,7–9] jasmonic acid (JA);[10] oleic acid;[5] palmitic acid;[5,8,9] prostaglandin E_2 (PGE_2);[5] retinoic acid;[11,12] nucleic acids;[13–15] proteins;[16–20] thiols[11,12,14,21,22]

Biological/Medical Applications Analyzing fatty acids;[5,7–9] analyzing/detecting/quantitating proteins;[16–20] analyzing/measuring retinoic acid concentration in biological samples;[11,12] determining/separating/quantifying jasmonic acid (JA);[10] inhibiting/monitoring glutathione S-transferase omega 1 (GSTO1) activity;[23] labeling of thiols;[11,12,14,21,22] labeling/purifying nucleic acids;[13–15] derivatization reagent for carboxylic acids[3–12]

Industrial Applications Not reported

Safety/Toxicity No data available

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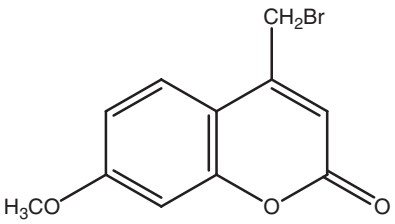
4-BROMOMETHYL-7-METHOXYCOUMARIN

CAS Registry Number 35231-44-8

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-2-one, 4-(bromomethyl)-7-methoxy-

Other Names 4-(Bromomethyl)-7-methoxy-2*H*-chromen-2-one; 4-(Bromomethyl)-7-methoxy-2*H*-chromene-2-one; 4-Bromomethyl-7-methoxy-2-oxo-2*H*-benzopyran; 4-Bromomethyl-7-methoxycoumarin; 7-Methoxy-4-(bromomethyl)coumarin; BMC; Br-Mmc; BrMMC

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{11}H_9BrO_3$

Molecular Weight 269.09

Physical Form Pale yellow crystals/needles[8]

Solubility Soluble in acetone, acetonitrile, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 214–215 °C;[4] 209–210 °C (decompose);[10] 208–209 °C;[8] 206–208 °C (decompose);[5] 205–207 °C;[6] 204 °C[11]

Boiling Point (Calcd.) 385.3 ± 42.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 330 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 13,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–11]

Imaging/Labeling Applications Amino acids;[12,13] bile acids;[14–17] biotin and its analogs;[18] carboxylic acids;[19–37] cyclosporins;[38] dalapon;[39] ethosuximide;[40,41] fatty acids;[42–52] fusilade;[53,54] immunoglobulins;[55] luminol derivatives;[56] mercury ions;[57,58] nitric oxide;[59,60] penicillins;[61,62] phosphoric acid;[63] picomole;[64] prostaglandins;[65–70] pyrimidine nucleobases;[8,71–82] steviol;[83] surfactants;[84–86] thromboxanes[87,88]

Biological/Medical Applications Analyzing/detecting carboxylic acids;[19–37] analyzing/labeling fatty acids;[42–52] detecting nitric oxide;[59,60] detecting/separating bile acids;[14–17] labeling pyrimidine nucleobases;[8,71–82] anticancer agents;[4,89,90] biomedical trace analysis;[37,49] herbicides;[34,39,53,54,64] as a substrate for measuring histone acetyltransferases (HATs) activity,[91] peptidases activity,[92,93] sirtuin activity[94]

Industrial Applications Detection of nitrated explosives;[95] measuring ultraviolet ray power;[56] photoacid generators;[96] polyurethane foams;[97] photoresists;[98] silica nanoparticles[99]

Safety/Toxicity Mutagenicity[100]

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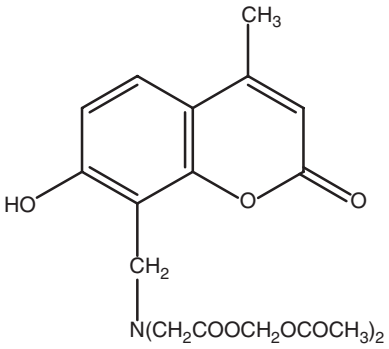
CALCEIN BLUE AM

CAS Registry Number 168482-84-6

Chemical Structure



CA Index Name Glycine, *N*-[2-[(acetyloxy)methoxy]-2-oxoethyl]-*N*-[(7-hydroxy-4-methyl-2-oxo-2*H*-1-benzopyran-8-yl)methyl]-, (acetyloxy)methyl ester

Other Names Calcein Blue AM, Calcein Blue acetoxymethyl ester; CellTrace Calcein Blue AM

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{21}H_{23}NO_{11}$

Molecular Weight 465.41

Physical Form Colorless Solid

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, ethyl acetate, methanol

Boiling Point (Calcd.) 617.0 ± 55.0 °C, pressure: 760 Torr

pK_a (Calcd.) 7.76 ± 0.20, most acidic, temperature: 25 °C; 2.51 ± 0.50, most basic, temperature: 25 °C

Absorption (λ_{max}) 322 nm (DMSO)

Emission (λ_{max}) 437 nm (DMSO)

Molar Extinction Coefficient 13,000 cm^{-1} M^{-1} (DMSO)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Bacteria;[1,3] cells[1,2]

Biological/Medical Applications Cell viability assay;[1,2] cytotoxicity assay;[1,4] monitoring bacterial transport;[1,3] as a substrate for measuring esterases activity[1,2]

Industrial Applications Not reported

Safety/Toxicity No data available

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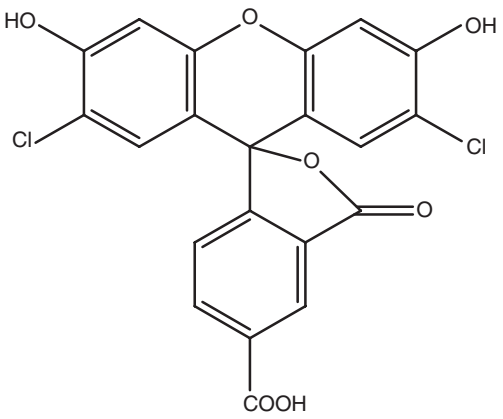
5-CARBOXY-2′,7′-DICHLOROFLUORESCEIN

CAS Registry Number 142975-81-3

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 2′,7′-dichloro-3′,6′-dihydroxy-3-oxo-

Other Names 5-Carboxy-2′,7′-dichlorofluorescein; Carboxy-DCF; 5-CDCF

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{10}Cl_2O_7$

Molecular Weight 445.21

Physical Form Orange solid[4]

Solubility Insoluble in water, soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point >250 °C

Boiling Point (Calcd.) 732.3 ± 60.0 °C, pressure: 760 Torr

pK_a 4.8, temperature: 22 °C

pK_a (Calcd.) 3.72 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 495 nm (Buffer pH 4.0); 504 nm (Buffer pH 8.0)

Emission (λ_{max}) 529 nm (Buffers pH 4.0, pH 8.0)

Molar Extinction Coefficient 38,000 cm^{-1} M^{-1} (Buffer pH 4.0); 107,000 cm^{-1} M^{-1} (Buffer pH 8.0)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Bacteria;[6,7] dideoxynucleotides;[8] lysosomes;[2] mitochondria;[9] nucleic acids;[10] protein-2 (MRP2, ABCC2);[11–13] protein-5 (MRP5, ABCC5)[13]

Biological/Medical Applications Assessing reactive oxygen species (ROS) generation in isolated-perfused rat heart tissue;[14] detecting nucleic acids;[10] detecting/quantifying bacteria;[6,7] evaluating multimeric complexes;[15] monitoring blood gas;[16] monitoring/measuring analytes concentration;[17] multidrug resistance-associated protein-2 (MRP2, ABCC2) substrates;[11–13] multidrug resistance-associated protein-5 (MRP5, ABCC5) substrates;[13] screening mitochondrial permeability transition;[9] studying hepatic disposition;[18,19] a substrate for measuring aryl sulfatase activity,[2] acid phosphatase activity,[2] β-galactosidase activity,[2] lipase activity[2]

Industrial Applications Fiber optic sensor for sol–gel material;[20] planar laser-induced fluorescence (PLIF) measurements in aqueous flows[21]

Safety/Toxicity Metabolic toxicity[22]

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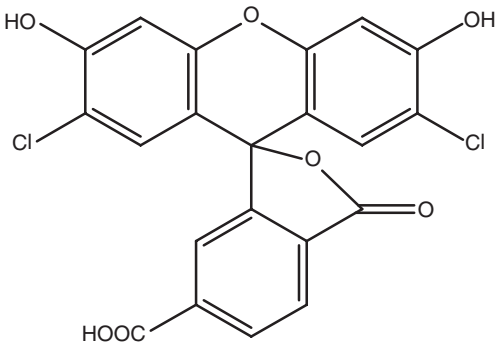
22. Sinclair, J. A.; Henderson, C.; Tettey, J. N. A.; Grant, M. H. The influence of the choice of digestion enzyme used to prepare rat hepatocytes on xenobiotic uptake and efflux. *Toxicol. In Vitro* **2013**, *27*, 451–457.

6-CARBOXY-2′,7′-DICHLOROFLUORESCEIN

CAS Registry Number 144316-86-9

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-6-carboxylic acid, 2′,7′-dichloro-3′,6′-dihydroxy-3-oxo-

Other Names 6-Carboxy-2′,7′-dichlorofluorescein; Carboxy-DCF

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{10}Cl_2O_7$

Molecular Weight 445.21

Physical Form Orange solid;[6] Yellow solid[3]

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point >250 °C

Boiling Point (Calcd.) 742.4 ± 60.0 °C pressure: 760 Torr

pK_a 4.8 Temperature: 22 °C

pK_a (Calcd.) 3.51 ± 0.20 most acidic, temperature: 25 °C

Absorption (λ_{max}) 495 nm (Buffer pH 4.0); 504 nm (Buffer pH 8.0)

Emission (λ_{max}) 529 nm (Buffers pH 4.0, pH 8.0)

Molar Extinction Coefficient 38,000 cm^{-1} M^{-1} (Buffer pH 4.0); 107,000 cm^{-1} M^{-1} (Buffer pH 8.0)

Quantum Yield 0.67 (Buffer pH 7.4)

Synthesis Synthetic methods[1–7]

Imaging/Labeling Applications Bacteria;[8,9] lysosomes;[4] mitochondria;[10] proteins;[3] protein-2 (MRP2, ABCC2);[11–13] protein-5 (MRP5, ABCC5)[13]

Biological/Medical Applications Assessing reactive oxygen species (ROS) generation in isolated-perfused rat heart tissue;[14] detecting/quantifying bacteria;[8,9] monitoring blood gas;[15] monitoring/measuring analytes concentration;[16] multidrug resistance-associated protein-2 (MRP2, ABCC2) substrates;[11–13] multidrug resistance-associated protein-5 (MRP5, ABCC5) substrates;[13] screening mitochondrial permeability transition;[10] studying hepatic disposition;[17,18] a substrate for measuring aryl sulfatase activity,[4] acid phosphatase activity,[4] β-galactosidase activity,[4] lipase activity[4]

Industrial Applications Fiber optic sensor for sol–gel material;[19] planar laser-induced fluorescence (PLIF) measurements in aqueous flows[20]

Safety/Toxicity Metabolic toxicity[21]

REFERENCES

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19. Manyam, U. H.; Shahriari, M. R.; Morris, M. J. A complete spectrum fiber optic pH sensor based on a novel fluorescent indicator doped porous sol–gel material. *Proc. SPIE- Int. Soc. Opt. Eng.* **1999**, *3540*, 10–18.
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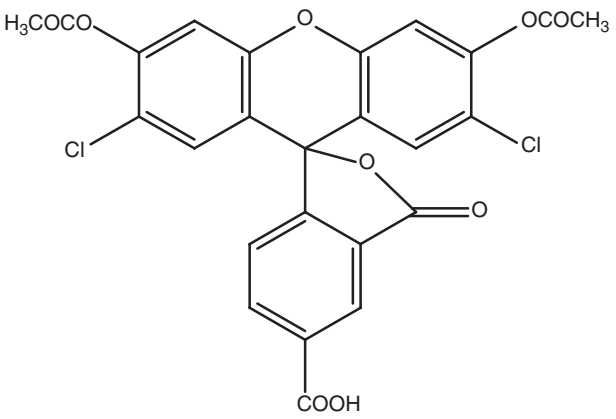
21. Sinclair, J. A.; Henderson, C.; Tettey, J. N. A.; Grant, M. H. The influence of the choice of digestion enzyme used to prepare rat hepatocytes on xenobiotic uptake and efflux. *Toxicol. In Vitro* **2013**, *27*, 451–457.

5-CARBOXY-2′,7′-DICHLORO-FLUORESCEIN DIACETATE

CAS Registry Number 144489-09-8

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 3′,6′-bis(acetyloxy)-2′,7′-dichloro-3-oxo-

Other Names 5-Carboxy-2′,7′-dichlorofluorescein diacetate; Carboxy-DCFDA; 5-CDCF DA

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{14}Cl_2O_9$

Molecular Weight 529.28

Physical Form Light brown solid;[1] Off-white solid

Solubility Insoluble in water; soluble acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 178–180 °C[1]

Boiling Point (Calcd.) 743.3 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.70 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) <300 nm (Buffer pH 4.0); 292 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 6,000 (MeOH) $cm^{-1}\,M^{-1}$

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Caco-2 cell;[11] lysosomes;[3] microparticles;[4] protein-2 (MRP2);[10] vacuoles;[5] yeast cells[6]

Biological/Medical Applications Assessing reactive oxygen species (ROS) generation;[7,8] counting yeast cells;[6] identifying vacuolar system;[5] monitoring blood gas;[9] multidrug resistance-associated protein-2 (MRP2) substrates;[10,11] studying hepatic disposition;[12] a substrate for measuring esterase activity[3]

Industrial Applications Not reported

Safety/Toxicity Metabolic toxicity[13]

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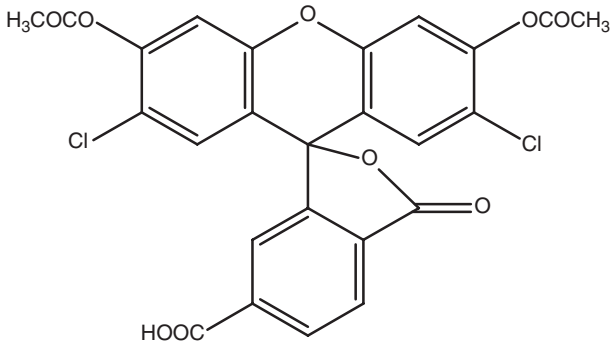
6-CARBOXY-2′,7′-DICHLORO-FLUORESCEIN DIACETATE

CAS Registry Number 144489-10-1

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-6-carboxylic acid, 3′,6′-bis(acetyloxy)-2′,7′-dichloro-3-oxo-

Other Names 3′,6′-Diacetyl-2′,7′-dichloro-6-carboxyfluorescein; 6-Carboxy-2′,7′-dichlorofluorescein diacetate; Carboxy-DCFDA; 6-CDCF DA

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{14}Cl_2O_9$

Molecular Weight 529.28

Physical Form Off-white solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

Melting Point >300 °C (decompose)[2]

Boiling Point (Calcd.) 751.5 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.49 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) <300 nm (Buffer pH 4.0); 292 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 6,000 (MeOH) $cm^{-1}\,M^{-1}$

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Caco-2 cell;[13] lysosomes;[4] proteins;[1] protein-2 (MRP2);[12] vacuoles;[5] yeast cells[6,7]

Biological/Medical Applications Assessing reactive oxygen species (ROS) generation;[8,9] counting/detecting yeast cells;[6,7] diagnosing Cowden syndrome;[10] identifying vacuolar system;[5] monitoring blood gas;[11] multidrug resistance-associated protein-2 (MRP2) substrates;[12,13] studying hepatic disposition;[14] a substrate for measuring esterase activity[4]

Industrial Applications Not reported

Safety/Toxicity Metabolic toxicity[15]

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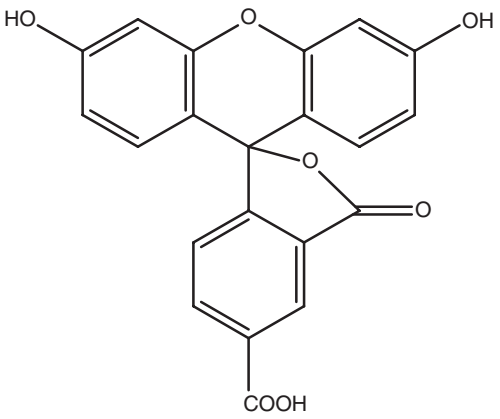
5-CARBOXYFLUORESCEIN

CAS Registry Number 76823-03-5

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 3′,6′-dihydroxy-3-oxo-

Other Names 5-Carboxyfluorescein; 5-FAM; FAM; FAM (dye); FAM 494/520

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{12}O_7$

Molecular Weight 376.32

Physical Form Orange solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 368–372 °C[4]

Boiling Point (Calcd.) 725.2 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.80 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 492 nm (Buffer pH 9.0)

Emission (λ_{max}) 518 nm (Buffer pH 9.0)

Molar Extinction Coefficient 79,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications β-Amyloid peptides;[6,7] bacteria;[8–10] cell;[11] dendrimers;[12] liposomes;[13–17] metal ions (lead ions,[18] mercury ions,[19–21] silver ions;[22]) microorganisms;[23,24] nucleic acids/nucleotides;[25–44] proteins/peptides;[45–55] quantum dots;[56] viruses[57,58]

Biological/Medical Applications Authenticating canned products;[59] detecting/measuring citrate;[60,61] as a substrate for measuring phospholipase activity;[62] use in ophthalmology[63]

Industrial Applications Colored or luminescent products;[64] as geothermal tracers;[65] microfabricated electrophoresis devices;[66,67] porous polymer monoliths;[68] separation devices;[69] thin-film polymer light emitting diodes[70]

Safety/Toxicity Genotoxicity;[71] membrane toxicity;[72] ophthalmic toxicity;[73] pulmonary toxicity[74]

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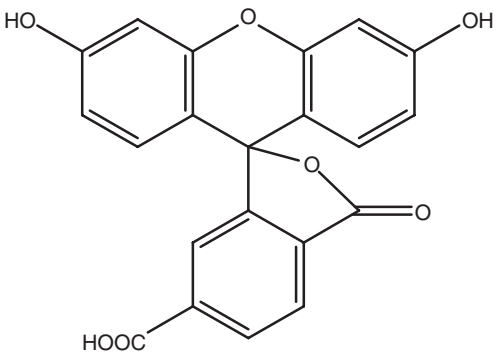
6-CARBOXYFLUORESCEIN

CAS Registry Number 3301-79-9

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-6-carboxylic acid, 3′,6′-dihydroxy-3-oxo-

Other Names Spiro[phthalan-1,9′-xanthene]-6-carboxylic acid, 3′,6′-dihydroxy-3-oxo-; Terephthalic acid, (3,6,9-trihydroxyxanthen-9-yl)-, γ-lactone; 6-Carboxyfluorescein; 6-FAM; Fluorescein, 6-carboxy-

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{12}O_7$

Molecular Weight 376.32

Physical Form Orange solid

Solubility Soluble in acetone, chloroform, dichloromethane, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point >360 °C;[5] 352–356 °C[4]

Boiling Point (Calcd.) 736.4 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.58 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 492 nm (Buffer pH 9.0)

Emission (λ_{max}) 515 nm (Buffer pH 9.0)

Molar Extinction Coefficient 81,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Ammonia gas;[6,7] antibodies;[8,9] axons;[10] bacteria;[11,12] cornea;[13] cytoplasm;[14] insulin;[15] islet cells;[16] liposomes;[17–33,74] myosin subfragment 1;[34] nucleic acids/nucleotides;[35–44] proteins/peptides;[45–48] protoplasts;[49] silver nanoparticles;[50] symplast;[51–54] viruses[55–69]

Biological/Medical Applications Diagnosing bladder cancer;[70] evaluating corneal endothelial barrier function;[13] as a substrate for measuring protein kinase activity,[71] methyltransferase activity,[72] phospholipase activity,[73,74] rhodanese activity,[75] sulfotransferase activity;[76] use in ophthalmology[77]

Industrial Applications Not reported

Safety/Toxicity Cytotoxicity;[78] genotoxicity;[79,80] immunotoxicity;[80] membrane toxicity;[81–83] neurotoxicity;[84] nucleic acid damage;[85] ophthalmic toxicity;[86–90] pulmonary toxicity[91,92]

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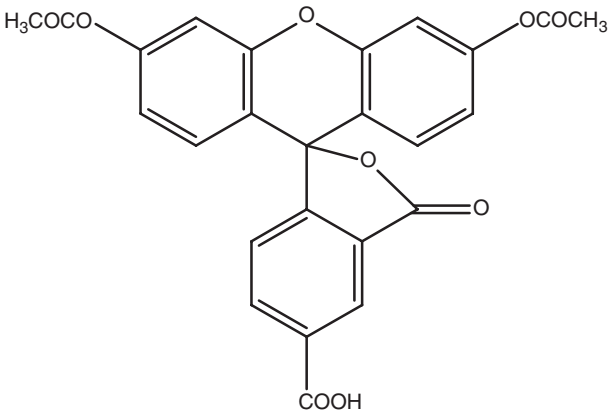
5-CARBOXYFLUORESCEIN DIACETATE

CAS Registry Number 79955-27-4

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 3′,6′-bis(acetyloxy)-3-oxo-

Other Names 5-Carboxyfluorescein diacetate; 5-CFDA

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{16}O_9$

Molecular Weight 460.39

Physical Form Colorless solid

Solubility Soluble in acetone, acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 693.1 ± 55.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.77 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 290 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 5,500 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Bacteria;[5–9,11,12,19] bone marrow stromal cells;[10] cells;[11,12,15,16,18–21] chloroplasts;[13] endospores;[14] eosinophils;[22] fungi;[15,16] low-density lipoprotein (LDL);[17] microorganisms;[18–21] neutrophils;[22] proteins;[2] protein kinase C;[4] sperms;[23] tumors;[24–26] yeasts[19,27,28]

Biological/Medical Applications Analyzing intracellular glutathione levels in cells;[29] assessing gap junctional intercellular communication in cells;[29] characterizing antifungal activity of micafungin,[15] caspofungin;[16] counting/detecting/evaluating microorganisms;[18–21] detecting cells;[11,12,15,16,18–21] detecting/measuring intracellular pH in yeast;[27] determining extracellular/intracellular pH in bacteria under CO_2 treatment;[8] evaluating/measuring keratinocytes growth rate;[30] identifying cancerous cells[24–26] measuring gas (carbon dioxide or ammonia) concentration in body fluids;[31] screening xenobiotic phloem mobility in plants;[32] studying low-density lipoprotein (LDL)/cholesterol metabolism;[17] as a substrate for measuring esterase activity[18,19,24,28]

Industrial Applications Not reported

Safety/Toxicity No data available

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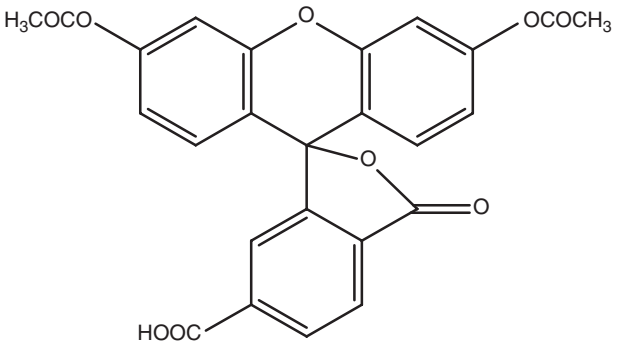
6-CARBOXYFLUORESCEIN DIACETATE

CAS Registry Number 3348-03-6

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-6-carboxylic acid, 3′,6′-bis(acetyloxy)-3-oxo-

Other Names Spiro[phthalan-1,9′-xanthene]-6-carboxylic acid, 3′,6′-dihydroxy-3-oxo-, diacetate; Terephthalic acid, (3,6,9-trihydroxyxanthen-9-yl)-, γ-lactone, diacetate; 6-Carboxyfluorescein diacetate; 6-CFDA

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{16}O_9$

Molecular Weight 460.39

Physical Form Light yellow or off-white solid

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 152–153 °C[4]

Boiling Point (Calcd.) 701.6 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.55 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 290 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 6,150 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Bacteria;[5–24,28,29,42] cells;[5,7,13,14,17,19,20,25–30,41,42,45,46,52,58,59] chloroplasts;[31] eosinophils;[48] fungi;[32–38] low-density lipoprotein (LDL);[39] microorganisms;[40–47] neutrophils;[48] protein kinase C;[3] sperms;[49] tumors;[50,51] yeasts[42,47,52–58]

Biological/Medical Applications Analyzing/detecting cells;[5,7,13,14,17,19,20,25–30,41,42,45,46,52,58,59] counting/detecting/evaluating microorganisms;[40–47] detecting/measuring bacteria;[5–24,28,29,42] quantifying adhesion of tumor cells to endothelial monolayers;[50] measuring gas (carbon dioxide or ammonia) concentration in body fluids;[61] monitoring intracellular nitric oxide production;[62] screening xenobiotic phloem mobility in plants;[63,64] studying low-density lipoprotein (LDL)/cholesterol metabolism;[39] apoptosis assay;[59] method for antifungal susceptibility testing;[35,37] as a substrate for measuring esterase activity[5,14,17,22,24,33,41,42,51,55,57,58,60]

Industrial Applications Not reported

Safety/Toxicity Hepatotoxicity;[65] ploem mobility of xenobiotics;[64] retinal toxicity[66]

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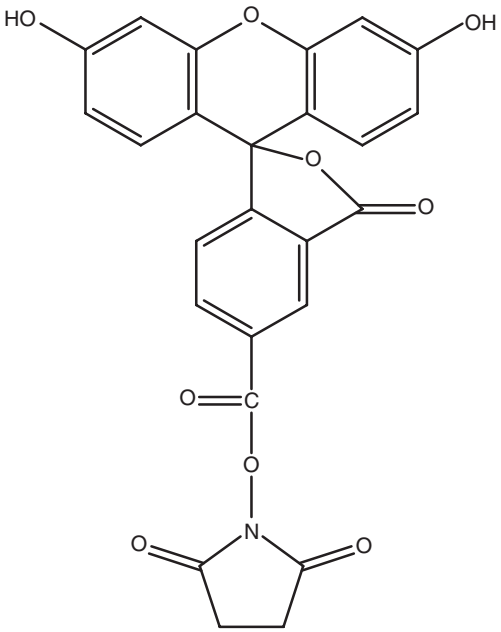
5-CARBOXYFLUORESCEIN SUCCINIMIDYL ESTER

CAS Registry Number 92557-80-7

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 3′,6′-dihydroxy-3-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[(3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-5-yl)carbonyl]oxy]-; Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene], 2,5-pyrrolidinedione deriv.; 5-Carboxyfluorescein *N*-hydroxysuccinimide ester; 5-Carboxyfluorescein *N*-succinimidyl ester; 5-Carboxyfluorescein NHS ester; 5-Carboxyfluorescein succinimidyl ester; 5-CFSE; CFSE; 5-FAM, SE

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{15}NO_9$

Molecular Weight 473.39

Physical Form Orange solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 778.7 ± 70.0 °C, pressure: 760 Torr

pK_a (Calcd.) 9.31 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 494 nm (Buffer pH 9)

Emission (λ_{max}) 520 nm (Buffer pH 9)

Molar Extinction Coefficient 78,000 cm^{-1} M^{-1} (Buffer pH 9)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Actin;[6] amino acids;[7,8] antibodies;[9] bacteria;[10] peptide chloromethyl ketones;[11] herbicides;[12] histamine H1/H2 receptor antagonists;[13,14] lymphocytes;[15,16] metal ions (Fe(III);[17] Pt(IV);[18]) nanoparticles;[19–24] nucleic acids/nucleotides;[25–34] pheomelanin;[35] polystyrene latex particles;[36] proteins/peptides;[37–41] risedronate;[42] serotonin;[43] stem cells[44,45]

Biological/Medical Applications Analyzing/assessing T cell function proliferation;[15,16] detecting degree of cross-linked allogeneic tissue;[46] determining phosphorus-containing amino acid herbicides;[12] evaluating/studying mesenchymal stem cells subpopulations proliferative activity;[45] locating/investigating hemopoietic stem cell niche *in situ*;[44] monitoring bacterial pathogens;[23] multiplexed cancer cell monitoring;[21] quantifying serotonin;[43] for synthesizing vasopressin analogs;[47] as a substrate for measuring histone acetyltransferases (HATs) activity,[48] kinase activity,[49,50] phosphatase activity[50]

Industrial Applications Abrasives;[19] platings[19]

Safety/Toxicity No data available

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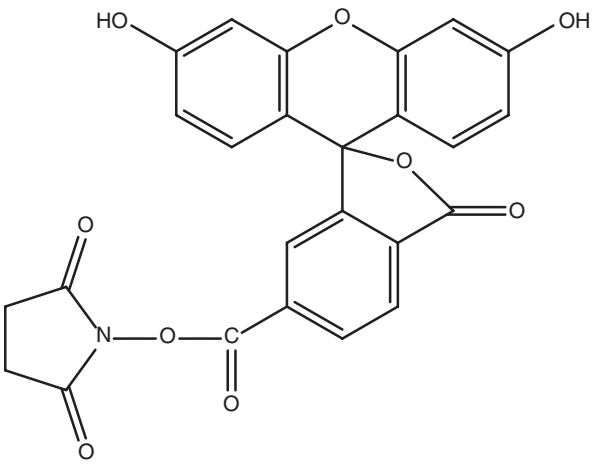
6-CARBOXYFLUORESCEIN SUCCINIMIDYL ESTER

CAS Registry Number 92557-81-8

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-6-carboxylic acid, 3′,6′-dihydroxy-3-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[(3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-6-yl)carbonyl]oxy]-; Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene], 2,5-pyrrolidinedione deriv.; 6-Carboxyfluorescein *N*-hydroxysuccinimide ester; 6-Carboxyfluorescein succinimidyl ester; Fluorescein-6-carboxylic acid *N*-succinimidyl ester; 6-CFSE; CFSE; 6-FAM, SE

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{15}NO_9$

Molecular Weight 473.39

Physical Form Orange solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

Boiling Point (Calcd.) 788.1 ± 70.0 °C, pressure: 760 Torr

pK_a (Calcd.) 9.31 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 496 nm (Buffer pH 9)

Emission (λ_{max}) 516 nm (Buffer pH 9)

Molar Extinction Coefficient 83,000 cm^{-1} M^{-1} (Buffer pH 9)

Synthesis Synthetic methods[1–6]

Imaging/Labeling Applications Amantadine;[16] aminoglycosides;[7] anti-digoxin;[8] baclofen;[9] bacteria;[10] peptide chloromethyl ketones;[11] gabapentin;[12] herbicides;[13] histamine H1/H2 receptor antagonists;[14,15] memantine[16] metal ions (Fe(III));[17] nanoparticles;[18] nucleic acids/nucleotides;[19–23] phosphatidylethanolamine;[24] proteins/peptides;[5,25–35] risedronate;[36] amino functionalized rhodamine spirolactams[37]

Biological/Medical Applications Analyzing aminoglycosides;[7] analyzing/determining gabapentin;[12] detecting/analyzing baclofen in human plasma at micromolar level;[9] determining phosphorus-containing amino acid herbicides;[13] multiplex genetic analysis;[19] visualizing/detecting proteins;[5,25–35] for synthesizing vancomycin analogs,[38] vasopressin analogs;[39] as a substrate for measuring kinase activity,[40,41] phosphatase activity[41]

Industrial Applications Not reported

Safety/Toxicity No data available

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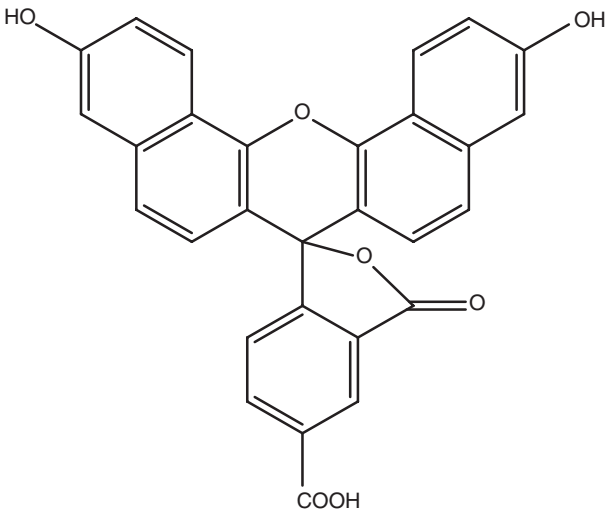
5-CARBOXYNAPHTHO-FLUORESCEIN

CAS Registry Number 145103-60-2

Chemical Structure



CA Index Name Spiro[7H-dibenzo[c,h]xanthene-7,1′(3′H)-isobenzofuran]-5′-carboxylic acid, 3,11-dihydroxy-3′-oxo-

Other Names Spiro[7H-dibenzo[c,h]xanthene-7,1′(3′H)-isobenzofuran]-5′-carboxylic acid, 3,6a-dihydro-11-hydroxy-3,3′-dioxo-; 5-Carboxynaphthofluorescein; CNF

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{29}H_{16}O_7$

Molecular Weight 476.44

Physical Form Purple solid or dark blue crystalline powder

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 845.9 ± 65.0 °C, pressure: 760 Torr

pK_a 7.6, temperature: 22 °C

pK_a (Calcd.) 3.68 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 512 nm (Buffer pH 6.0); 598 nm (Buffer pH 10.0)

Emission (λ_{max}) 563 nm (Buffer pH 6.0); 668 (Buffer pH 10.0)

Molar Extinction Coefficient 11,000 $cm^{-1}\,M^{-1}$ (Buffer pH 6.0); 49,000 $cm^{-1}\,M^{-1}$ (Buffer pH 10.0)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Live cells;[3,4] oligonucleotides[5]

Biological/Medical Applications Evaluating multimeric complexes (proteins, peptides, antibody molecules, small/large molecules);[6] fluorosensor for measurement of near-neutral pH values;[7] organic electroluminescence (OEL)-based biochips;[8,9] optical sensors for bio-medical applications;[10–12] substrates for assaying esterase;[2] studying protein crystal nucleation;[13] as temperature sensor[14,15]

Industrial Applications Adhesive;[16] electronic device manufacturing;[16] fabricating multiplexed arrays of chemosensors[17]

Safety/Toxicity No data available

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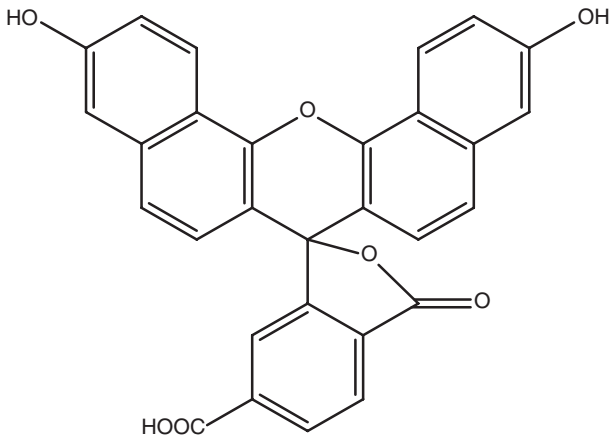
6-CARBOXYNAPHTHO-FLUORESCEIN

CAS Registry Number 145103-61-3

Chemical Structure



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Synthesis Synthetic methods[1–4]

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Biological/Medical Applications Fluorosensor for measurement of near-neutral pH values;[4] organic electroluminescence (OEL)-based biochips;[7,8] optical sensors for bio-medical applications;[9–11] substrates for assaying esterase;[2] studying protein crystal nucleation[12]

Industrial Applications Not reported

Safety/Toxicity No data available

REFERENCES

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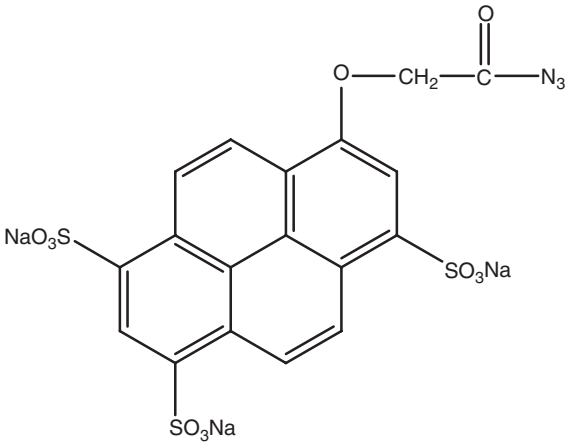
CASCADE BLUE ACETYL AZIDE TRISODIUM SALT

CAS Registry Number 138039-58-4

Chemical Structure



CA Index Name 1,3,6-Pyrenetrisulfonic acid, 8-(2-azido-2-oxoethoxy)-, sodium salt (1:3)

Other Names 1,3,6-Pyrenetrisulfonic acid, 8-(2-azido-2-oxoethoxy)-, trisodium salt; Cascade Blue Acetyl Azide; Cascade Blue acetyl azide trisodium salt

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{18}H_8N_3Na_3O_{11}S_3$

Molecular Weight 607.42

Physical Form Tan powder;[1,2] Yellow solid

Solubility Soluble in water, methanol

Absorption (λ_{max}) 396 nm, 376 nm (MeOH)

Emission (λ_{max}) 410 nm (MeOH)

Molar Extinction Coefficient 29,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Bacteria;[3] cells;[4,5] cyclodextrin;[6] nuclei;[1] nucleic acids;[7–9] proteins[3–5,10–14]

Biological/Medical Applications Detecting/identifying proteins;[3–5,10–14] detecting/quantifying bacteria;[3] diagnosing/treating chronic lymphocytic leukemia (CLL)[7]

Industrial Applications Not reported

Safety/Toxicity No data available

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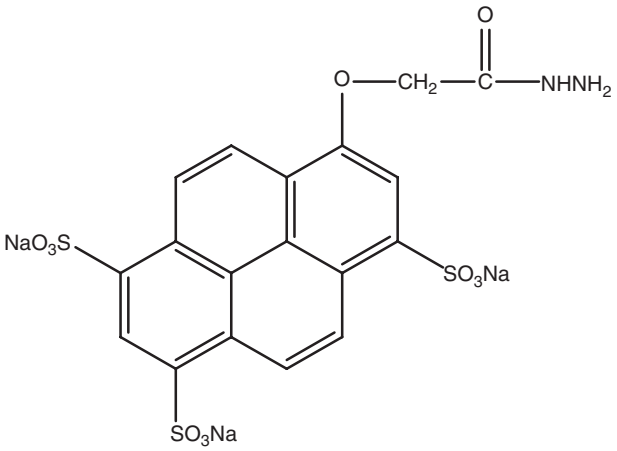
CASCADE BLUE HYDRAZIDE TRISODIUM SALT

CAS Registry Number 137182-38-8

Chemical Structure



CA Index Name Acetic acid, 2-[(3,6,8-trisulfo-1-pyrenyl)oxy]-, hydrazide, sodium salt (1 : 3)

Other Names Acetic acid, [(3,6,8-trisulfo-1-pyrenyl) oxy]-, 1-hydrazide, trisodium salt; Cascade Blue hydrazide trisodium salt

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{18}H_{11}N_2Na_3O_{11}S_3$

Molecular Weight 596.44

Physical Form Yellow powder[1,2]

Solubility Soluble in water

Absorption (λ_{max}) 399 nm, 376 nm (H_2O)

Emission (λ_{max}) 421 nm (H_2O)

Molar Extinction Coefficient 30,000 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Cytoplasm;[3] nuclei;[1,3] nucleic acid[4]

Biological/Medical Applications Cosmetics;[5,6] reagents for modifying aldehydes/ketones[1,2,7]

Industrial Applications Solid-state materials[8]

Safety/Toxicity No data available

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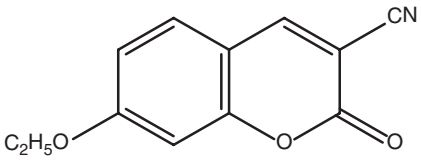
3-CYANO-7-ETHOXYCOUMARIN (7-ETHOXYCOUMARIN-3-CARBONITRILE)

CAS Registry Number 117620-77-6

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carbonitrile, 7-ethoxy-2-oxo-

Other Names 3-Cyano-7-ethoxycoumarin; 7-Ethoxycoumarin-3-carbonitrile; 7-Ethoxy-2-oxo-2H-chromene-3-carbonitrile

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{12}H_9NO_3$

Molecular Weight 215.20

Physical Form Off-white solid

Solubility Soluble in acetone, acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 212 °C[1,2]

Boiling Point (Calcd.) 396.8 ± 42.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 356 nm (Buffer pH 7); 355 nm (MeOH)

Emission (λ_{max}) 411 nm (Buffer pH 7); 411 nm (MeOH)

Molar Extinction Coefficient 20,000 cm^{-1} M^{-1} (Buffer pH 7); 22,500 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Cytochrome P 450 enzymes[1–23]

Biological/Medical Applications As a substrate for measuring cytochrome P 450 enzymes activity;[1–11] cytochrome P450 inhibition assays;[12–16] drug design;[17,18] drug metabolism;[17–23] treating viral or parasite infections[24]

Industrial Applications Not reported

Safety/Toxicity No data available

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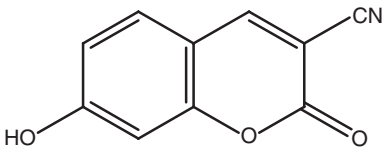
3-CYANO-7-HYDROXYCOUMARIN (3-CYANOUMBELLIFERONE)

CAS Registry Number 19088-73-4

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carbonitrile, 7-hydroxy-2-oxo-

Other Names Coumarin, 3-cyano-7-hydroxy-; 3-Cyano-7-hydroxycoumarin; 3-Cyanoumbelliferone; 7-Hydroxy-3-cyanocoumarin; 7-Hydroxycoumarin-3-carbonitrile

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{10}H_5NO_3$

Molecular Weight 187.15

Physical Form Yellow solid[1] or powder

Solubility Soluble in acetonitrile, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 273–275 °C;[7] 270–272 °C;[10] 262 °C;[14] 252–254 °C;[2] 250–252 °C;[4] 249–251 °C;[5,8] 246–248 °C[1]

Boiling Point (Calcd.) 436.6 ± 45.0 °C, pressure: 760 Torr

pK_a (Calcd.) 7.03 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 408 nm (Buffer pH 9); 408 nm (MeOH)

Emission (λ_{max}) 450 nm (Buffer pH 9); 450 nm (MeOH)

Molar Extinction Coefficient 43,000 cm^{-1} M^{-1} (Buffer pH 9)

Synthesis Synthetic methods[1–14]

Imaging/Labeling Applications Esters;[15] ethers;[16–25] phosphates;[26–32] microorganisms;[33] proteins[34]

Biological/Medical Applications Detecting microorganisms,[33] nucleic acids;[26–32] inhibiting cell proliferation/tumor growth;[10] reference standard for esters;[15] ethers,[16–25] phosphates substrates;[26–32] as a substrate for measuring nucleic acid polymerases activity;[26–32] treating viral or parasite infections[35]

Industrial Applications Electroluminescent device;[36] laser dyes;[37,38] modified polyester for food containers/beverage bottles;[11] monitoring of cationic photopolymerization processes;[39] textiles;[12] thin films[40]

Safety/Toxicity No data available

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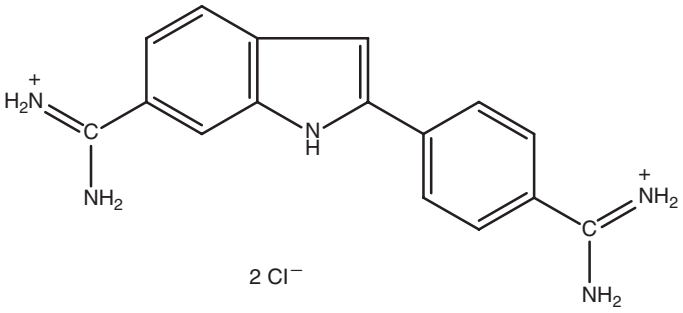
4′,6-DIAMIDINO-2-PHENYLINDOLE DIHYDROCHLORIDE (DAPI)

CAS Registry Number 28718-90-3

Chemical Structure



CA Index Name 1*H*-Indole-6-carboximidamide, 2-[4-(aminoiminomethyl)-phenyl]-, hydrochloride (1 : 2)

Other Names 1*H*-Indole-6-carboximidamide, 2-[4-(aminoiminomethyl)-phenyl]-, dihydrochloride; Indole-6-carboxamidine, 2-(*p*-amidinophenyl)-, dihydrochloride; 4′,6-Diamidino-2-phenylindole dihydrochloride; 6-Amidino-2-(4-amidinophenyl)-indole dihydrochloride; FxCycle Violet; DAPI

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Indole

Molecular Formula $C_{16}H_{17}Cl_2N_5$

Molecular Weight 350.25

Physical Form Yellow powder[4,5] or solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 360–362 °C (decompose)[4,5]

Absorption (λ_{max}) 358 nm (H_2O/DNA); 342 nm (H_2O); 348 nm (MeOH)

Emission (λ_{max}) 461 nm (H_2O/DNA); 450 nm (H_2O); 457 nm (MeOH)

Molar Extinction Coefficient 24,000 cm^{-1} M^{-1} (H_2O/DNA); 28,000 cm^{-1} M^{-1} (H_2O); 31,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.34 (H_2O/DNA)

Synthesis Synthetic methods[1–6]

Imaging/Labeling Applications Nucleic acids;[1,7–18,29] cells;[1,19–22] nuclei;[23] antigens;[24] bacteria;[25–28] chromosomes;[29] endotoxins;[30] microorganisms;[31] neuron-specific nuclear protein NeuN;[32] polynucleotides;[33] proteins;[34] mesenchymal stem cells[35]

Biological/Medical Applications Detecting nucleic acids,[1,7–18,29] cells,[1,19–22] neuron-specific nuclear protein NeuN;[28] identifying/quantifying bacteria;[25–28] monitoring microorganisms;[31] quantifying proteins;[34] nuclear apoptosis assay;[36] treating Alzheimer's disease,[37,38] Down's syndrome,[37] type II diabetes,[37,38] cerebral amyloid angiopathy,[38] ischemic disease;[39] monitoring atmospheric/indoor bioaerosols[40,41]

Industrial Applications Not reported

Safety/Toxicity Neurotoxicity[42]

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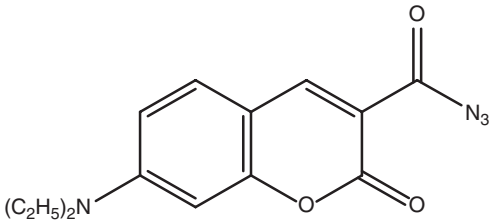
7-DIETHYLAMINOCOUMARIN-3-CARBONYL AZIDE

CAS Registry Number 157673-16-0

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carbonyl azide, 7-(diethylamino)-2-oxo-

Other Names 7-Diethylaminocoumarin-3-carbonyl azide

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{14}H_{14}N_4O_3$

Molecular Weight 286.29

Physical Form Orange solid

Solubility Soluble in acetonitrile, *N,N*-dimethylformamide, methanol

Absorption (λ_{max}) 436 nm (MeOH)

Emission (λ_{max}) 478 nm (MeOH)

Molar Extinction Coefficient 57,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Alcohols;[2] cyclic ketones;[3] epolactaene derivatives;[4] iejimalide carbamate derivatives;[5] lysophospholipids;[6] macrolide analogs;[7] platelet-activating factor acetylhydrolase (PAF-AH);[6,8] phosphonic acid-based NAALADase inhibitors;[9] uronium salts;[10] vinblastine analog[11]

Biological/Medical Applications Detecting lysophospholipids,[6] uronium salts;[10] identifying macrolide analogs;[7] measuring platelet-activating factor acetylhydrolase (PAF-AH) activity;[6,8] reagents for alcohols/hydroxyl groups[1,2,12]

Industrial Applications Polyelectrolytes[12]

Safety/Toxicity No data available

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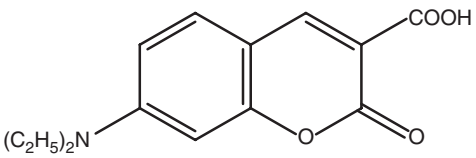
7-DIETHYLAMINOCOUMARIN-3-CARBOXYLIC ACID (DAC) (DEAC)

CAS Registry Number 50995-74-9

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-(diethylamino)-2-oxo-

Other Names 3-Carboxy-7-(diethylamino)coumarin; 7-(Diethylamino)-3-(carboxy)coumarin; 7-Diethylaminocoumarin-3-carboxylic acid; Coumarin D 1421; D 1421; DAC; DCCA; 7-DCCA; DEAC

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{14}H_{15}NO_4$

Molecular Weight 261.27

Physical Form Bright orange solid;[11] Orange crystals;[13] Orange crystalline solid;[27] Orange laths;[37,38] Orange powder;[4] Orange solid[2,3,6,9,12,16,20,28,35]

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide,

Melting Point 243–248 °C;[16] 231–232 °C;[37,38] 230–232 °C;[13] 230 °C;[2] 229–231 °C;[27] 228 °C;[35] 227–229 °C;[40] 224–225.5 °C;[30] 224–225 °C;[10,18] 222.4–223.3 °C;[7] 222–224 °C;[33] 220 °C;[39] 217–218 °C;[32] 215–217 °C;[36] 214–215 °C;[17]

Boiling Point (Calcd.) 464.7 ± 45.0 °C, pressure: 760 Torr

pK_a (Calcd.) −98.36 ± 0.20, most acidic, temperature: 25 °C; 6.06 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 409 nm (Buffer pH 9.0)

Emission (λ_{max}) 473 nm (Buffer pH 9.0)

Molar Extinction Coefficient 34,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–41]

Imaging/Labeling Applications Alcohols;[42] ATP;[43] copper ions;[22,44–46] iron ions;[3,30] fluoride ions;[7] cyclodextrins (CDs)/dextrans;[47–49] hydrogen peroxide;[50] hydrogen sulfide;[51] hypochlorite;[52] lysine;[28,29] nitric oxide;[53] nucleotides/nucleic acids;[35,54–56] proteins/amino acids;[9,37,38,57–60] sulfide ions;[61] thiols[62]

Biological/Medical Applications Detecting hydrogen peroxide;[50] evaluating iron ions;[3,30] cysteine cathepsins inhibitors;[8] β-glucosidase inhibitors;[63,64] human monoamine oxidase inhibitors;[15] *N*-Methyl-D-aspartate receptors (NMDARs) inhibitors;[65] phosphate assay;[37,60] probing actomyosin mechanism;[55] treating cancer/antitumor activity;[5] treating cognitive deficits or schizophrenia;[65] as a substrate for measuring protein kinase activity[66,67]

Industrial Applications Epoxy resins photoluminescent devices;[68] lithographic plate materials;[69] oil-repellent copolymers/coatings;[19,20,70,71] polymer matrices;[72] silica nanoparticles for imaging, security, and sensing applications[73,74]

Safety/Toxicity No data available

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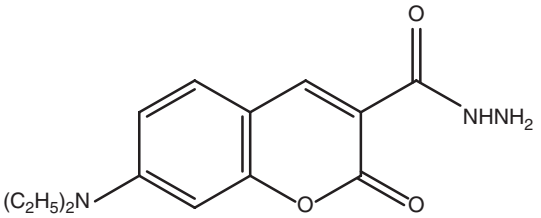
7-DIETHYLAMINOCOUMARIN-3-CARBOXYLIC ACID HYDRAZIDE (DCCH)

CAS Registry Number 100343-98-4

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-(diethylamino)-2-oxo-, hydrazide;

Other Names 7-Diethylaminocoumarin-3-carboxylic acid hydrazide; DCCH; 7-Diethylaminocoumarin-3-carbohydrazide; CHH; 7-Diethylamino-2-oxo-2*H*-chromene-3-carbohydrazide

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{14}H_{17}N_3O_3$

Molecular Weight 275.30

Physical Form Orange needles;[1] Yellow crystals[2]

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, methanol

Melting Point 162–165 °C;[2] 160–165 °C[1]

pK_a (Calcd.) 10.95 ± 0.20, most acidic, temperature: 25 °C; 3.01 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 420 nm (MeOH)

Emission (λ_{max}) 468 nm (MeOH)

Molar Extinction Coefficient 46,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Cellulose fibre interfaces;[3,4] copper,[5,6] iron;[6] sugar chains;[7–11] skin;[12] hair;[12] tetrahydroprogesterones[13]

Biological/Medical Applications Analyzing/detecting/quantifying sugar chains;[7–11] detecting copper,[5,6] iron,[6] hydrogen peroxide;[6] analyzing skin/hair;[12] detecting/labeling/quantifying biological carbonyl compounds (aldehydes and/or ketones)[13–15]

Industrial Applications Cellulosic materials/paper;[3,4] detecting carboxylic acids[16]

Safety/Toxicity No data available

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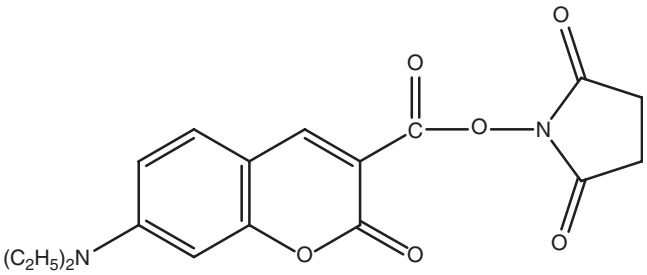
7-DIETHYLAMINOCOUMARIN-3-CARBOXYLIC ACID SUCCINIMIDYL ESTER (DEAC SE)

CAS Registry Number 139346-57-9

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-(diethylamino)-2-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[[7-(diethylamino)-2-oxo-2*H*-1-benzopyran-3-yl]carbonyl] oxy]-; 7-(Diethylamino)-coumarin-3-carboxylic acid *N*-succinimidyl ester; 7-Diethylaminocoumarin-3-carboxylic acid succinimidyl ester; 7-Ethylaminocoumarin-3-carboxylic acid succinimidyl ester; DCCS; DEAC SE

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{18}H_{18}N_2O_6$

Molecular Weight 358.35

Physical Form Yellow solid;[4–6] Bright yellow solid;[1] Organge solid;[3] Orange powder[2]

Solubility Soluble in acetonitrile, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 559.3 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 2.60 ± 0.20, most basic, temperature: 25 °C

Absorption (λmax) 442 nm (Buffer pH 9)

Emission (λmax) 483 nm (Buffer pH 9)

Molar Extinction Coefficient 64,000 cm^{-1} M^{-1} (Buffer pH 9)

Synthesis Synthetic methods[1–7]

Imaging/Labeling Applications Amino acids;[2,6–9] analytes;[10] azobenzene photoswitching *in vivo*;[11] leucine;[2] lysines;[6–8] small molecules;[12,13] metal ions;[13] transition metal complexes;[14] nucleic acids;[15,16] peptide analog;[11] proteins;[4,17–20] silane coupling agent;[24] silica particles/beads;[24] uronium salts[21]

Biological/Medical Applications Detecting amino acids,[2,6–9] hydrogen peroxide,[5] metal ions/small molecules;[12,13] detecting/identifying uronium salts;[21] identifying chromosome,[15] genome;[16] monitoring proteolysis;[6] quantifying analytes;[10] as a substrate for measuring extracellular matrix metalloprotease (MMP-1) activity,[6] proteases activity;[22] measuring lysosomal membrane potential *in situ*;[23] colloidal diagnostic devices;[24] useful for synthesizing peptides[24]

Industrial Applications Silica particles/beads[24]

Safety/Toxicity No data available

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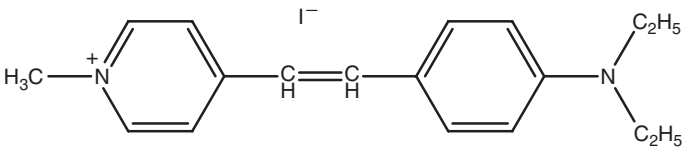
4-[4-(DIETHYLAMINO)STYRYL]-*N*-METHYLPYRIDINIUM IODIDE (4-Di-2-ASP)

CAS Registry Number 105802-46-8

Chemical Structure



CA Index Name Pyridinium, 4-[2-[4-(diethylamino) phenyl]ethenyl]-1-methyl-, iodide (1 : 1)

Other Names Pyridinium, 4-[2-[4-(diethylamino) phenyl]ethenyl]-1-methyl-, iodide; 4-Di-2-ASP; 4-[4-(Diethylamino)styryl]-1-methylpyridinium iodide; 4-[4-Diethylamino)styryl]-*N*-methylpyridinium iodide; D289

Merck Index Number Not listed

Chemical/Dye Class Styryl

Molecular Formula $C_{18}H_{23}IN_2$

Molecular Weight 394.30

Physical Form Red solid

Solubility Soluble in water, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 231.3–232 °C;[2] 226 °C;[1] 221–222 °C[4]

Absorption (λ_{max}) 488 nm (MeOH); 484.7 nm (DMSO); 471 nm (H_2O)

Emission (λ_{max}) 607 nm (MeOH)

Molar Extinction Coefficient 48,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Amyloid plaques;[6] axons;[17,27,28,38] blood cells (erythrocytes, reticulocytes, blood platelets);[7] blood vessels;[13] ganglia;[16,20,22] Merkel cells;[28] mitochondria;[27,38] myelinated fibers;[10] nerve fibers;[16,22,28] nerve plexuses;[20,22] nerve terminals;[10,14,23,24,26,27,30,38] neuroepithelial bodies (NEBs);[8,9] neuromuscular junctions (NMJs);[14,19,21,24–27,29] neurons;[11–13,15,18,22] polylactic acid (PLA) particles[31]

Biological/Medical Applications Assessing nerve ultrastructure;[15] characterizing Merkel cells and mechanosensory axons;[28] diagnosing of Hirschsprung's disease;[20] identifying neuroepithelial bodies (NEBs);[8.9] investigating stability and release properties of biodegradable polylactic acid (PLA) particles;[31] measuring blood cells (erythrocytes, reticulocytes, blood platelets);[7] visualizing nerve terminals and myelinated fibers[10]

Industrial Applications Bentonite clay;[32] characterizing supramolecular materials;[33] visualizing mesopores and defects in porous molecular sieves;[33] nonlinear optical devices/materials;[34,35] photographic materials/systems;[36] photoresists[37]

Safety/Toxicity Neurotoxicity[27]

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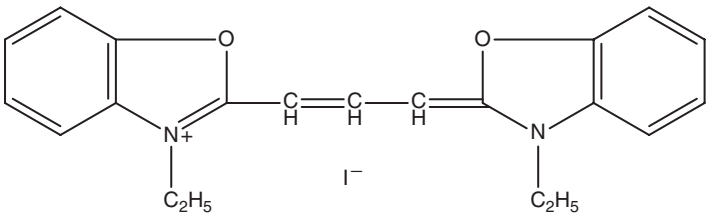
3,3′-DIETHYLOXACARBOCYANINE IODIDE ($DiOC_2(3)$)

CAS Registry Number 905-96-4

Chemical Structure



CA Index Name Benzoxazolium, 3-ethyl-2-[3-(3-ethyl-2(3*H*)-benzoxazolylidene)-1-propen-1-yl]-, iodide (1:1)

Other Names 3-Ethyl-2-[3-(3-ethyl-2-benzoxazolinylidene)propenyl]-benzoxazolium iodide; Benzoxazolium, 3-ethyl-2-[3-(3-ethyl-2(3*H*)-benzoxazolylidene)-1-propenyl]-, iodide; Benzoxazolium, 3-ethyl-2-[3-(3-ethyl-2-benzoxazolinylidene)propenyl]-, iodide; 3,3′-Diethyloxadicarbocyanine iodide; 3,3′-Diethyl-2,2′-oxacarbocyanine iodide; 3,3′-Diethyloxacarbocyanine iodide; 3-Ethyl-2-[3-ethyl-2(3*H*)-benzoxazolylidene)-1-propenyl] benzoxazolium iodide); 3-Ethyl-2-[3-(3-ethyl-3H-benzoxazol-2-ylidene)propenyl]benzoxazolium iodide; DOC; DOC (dye); DOCCI; DOCI; DiOC 2; DiOC 2(3); DODCI; G 1745; NK 85

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{21}H_{21}IN_2O_2$

Molecular Weight 460.31

Physical Form Dark red crystals or powder; Red-violet crystalline powder;[2] Orange solid[9]

Solubility Soluble in acetone, acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 287 °C;[8] 279 °C;[2] 272–273 °C;[4] 210 °C (decompose)[9]

Absorption (λ_{max}) 482 nm (MeOH); 478 nm (H_2O)

Emission (λ_{max}) 497 nm (MeOH); 496 nm (H_2O)

Molar Extinction Coefficient 165,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.04 (MeOH)

Synthesis Synthetic methods[1–9]

Imaging/Labeling Applications Bacteria;[10,11] cells;[10,12,13] hairs;[14] hepatocytes;[15] malaria infected cells;[16] mitochondria;[17–19,25] nucleic acids;[20–22] P-glycoprotein;[23,24] sperms[25]

Biological/Medical Applications Analyzing sperm motility;[25] assessing/determining P-glycoprotein expression and/or function;[23,24] detecting malaria infected cells,[16] prostate cancer;[17] inhibiting mitosis and cell growth;[12,13] measuring/monitoring membrane potential;[4,10,11,25,26] treating cancer;[24] cytotoxicity assay;[26] as temperature sensor[27,28]

Industrial Applications Displays;[29] dye laser;[30–34] electroluminescent devices;[35,36] electrophotographic material;[37] imaging materials;[38] light emitting diode lens;[39] micelles;[40] microemulsions;[40] mortar composition;[41] nonlinear optical materials;[42] photographic materials;[6,9,43–45] polymer nanocomposites (PNCs);[46] recording materials;[47–50] solar panels;[51] thin films[52]

Safety/Toxicity As substrate to evaluate efflux pump activity in leukemias;[53] toxicity[54]

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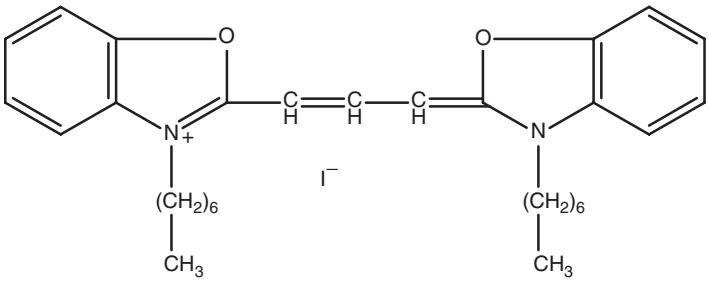
3,3′-DIHEPTYLOXACARBOCYANINE IODIDE (DiOC$_7$(3))

CAS Registry Number 53213-83-5

Chemical Structure



CA Index Name Benzoxazolium, 3-heptyl-2-[3-(3-heptyl-2(3*H*)-benzoxazolylidene)-1-propen-1-yl]-, iodide (1:1)

Other Names Benzoxazolium, 3-heptyl-2-[3-(3-heptyl-2(3*H*)-benzoxazolylidene)-1-propenyl]-, iodide; 3,3′-Diheptyloxacarbocyanine iodide; D 378; DiOC$_7$(3)

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{31}H_{41}IN_2O_2$

Molecular Weight 600.58

Physical Form Red powder or crystals

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 194–197 °C[2]

Absorption (λ_{max}) 482 nm (MeOH)

Emission (λ_{max}) 504 nm (MeOH)

Molar Extinction Coefficient 148,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Mitochondria;[1,3,4] bacteria;[5] cells;[6,7] fungi;[8] tumors[9–11]

Biological/Medical Applications Analyzing cells;[6,7] distinguishing between viable and non-viable bacteria;[5] identifying/quantifying transient perfusion in tumors;[10] marking murine tumor vasculature;[11] measuring/monitoring membrane potential;[1,2,12] mitochondria stain;[1,3,4] cytotoxicity assays[12,13]

Industrial Applications Not reported

Safety/Toxicity No data available

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tumor models. *Int. J. Radiat. Oncol., Biol., Phys.* **2001**, *49*, 799–808.

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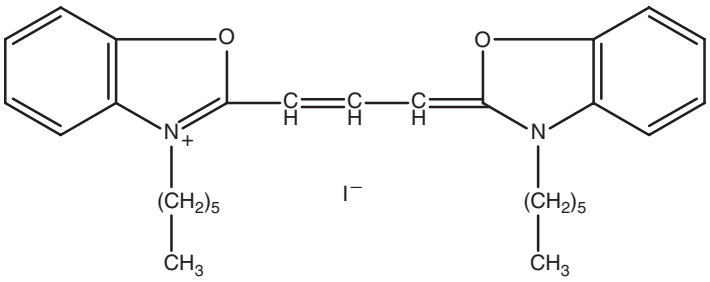
3,3′-DIHEXYLOXACARBOCYANINE IODIDE ($DiOC_6(3)$)

CAS Registry Number 53213-82-4

Chemical Structure



CA Index Name Benzoxazolium, 3-hexyl-2-[3-(3-hexyl-2(3*H*)-benzoxazolylidene)-1-propen-1-yl]-, iodide (1:1)

Other Names Benzoxazolium, 3-hexyl-2-[3-(3-hexyl-2(3*H*)-benzoxazolylidene)-1-propenyl]-, iodide; 3,3′-Dihexyloxacarbocyanine iodide; D 273; $DiOC_6(3)$; Dioc6; NK 2280

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{29}H_{37}IN_2O_2$

Molecular Weight 572.53

Physical Form Red powder or crystals

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 222–224 °C[3]

Absorption (λ_{max}) 484 nm (MeOH)

Emission (λ_{max}) 501 nm (MeOH)

Molar Extinction Coefficient 154,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Mitochondria;[1,2,6–24,59,60,70] endoplasmic reticulum;[1,2,20,25–45] astrocytes;[46] bacteria;[47–50] *Bacillus* spores;[51] cells;[4] fungi;[48,52] lymphocytes;[53,54] monocytes;[55] myelin sheath;[56] nucleic acids;[57] presynaptic nerve terminals;[58] sperms[59–61]

Biological/Medical Applications Analyzing germinating *Bacillus* spores;[51] assessing bacterial viability;[50] detecting prostate cancer,[9] diagnosing bipolar/unipolar disorders;[62] identifying myelin sheath;[56] measuring/monitoring membrane potential;[1–3,6,10–18,21,24,51,53,54,59–66,70] monitoring bacterial batch cultures;[47] apoptosis assays;[67–70] autophagy assays;[71] in photodynamic therapy[72]

Industrial Applications Carbon nanotubes;[73,74] Copper electrodeposition;[75] dye sensitized photographic imaging system;[76,77] photoresists[78]

Safety/Toxicity Phototoxicity[79]

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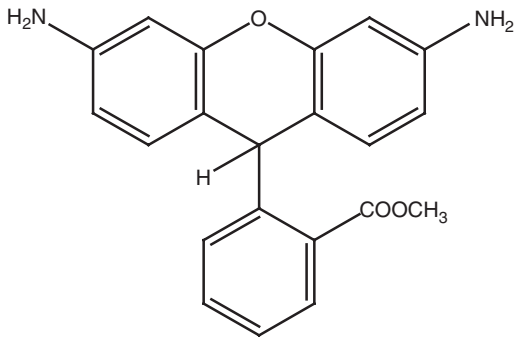
DIHYDRORHODAMINE 123 (DHR 123)

CAS Registry Number 109244-58-8

Chemical Structure



CA Index Name Benzoic acid, 2-(3,6-diamino-9*H*-xanthen-9-yl)-, methyl ester

Other Names D 23806; D 632; DHR; DHR 123; Dihydrorhodamine 123

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{18}N_2O_3$

Molecular Weight 346.38

Physical Form Pinkish-white solid[2,3]

Solubility Insoluble in water; soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 163–165 °C[2,3]

Boiling Point (Calcd.) 526.9 ± 50.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.70 ± 0.40, most basic, temperature: 25 °C

Absorption (λ_{max}) 289 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 7100 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Cells;[1–4] high density lipoprotein (HDL);[5] leukocytes (neutrophils, lymphocytes, monocytes);[6–24] mitochondria;[25–29] sperms[30,31]

Biological/Medical Applications Analyzing/measuring oxidative/respiratory burst activity;[1,6–24] assessing the oxidative properties of high density lipoprotein (HDL);[5] generating/detecting/measuring reactive oxygen species;[1,4,6–26,30–48,56,66] generating/detecting/measuring reactive nitrogen species;[1,10,31,46–50] producing/detecting/measuring peroxynitrite;[51–54] apoptosis assays;[8] autophagy assays;[34] chronic granulomatous disease (CGD) assay;[55] screening antioxidant activity[56]

Industrial Applications Not reported

Safety/Toxicity Benzene-mediated toxicity;[57] cytotoxicity;[58] hepatotoxicity;[59] lung toxicity;[60,61] nephrotoxicity;[62] neurotoxicity;[63–65] skin toxicity[66]

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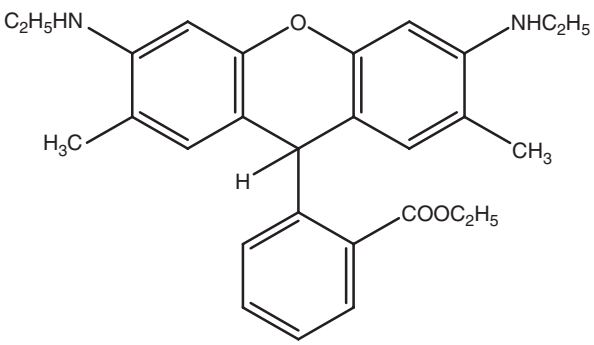
DIHYDRORHODAMINE 6G (DHR 6G)

CAS Registry Number 217176-83-5

Chemical Structure



CA Index Name Benzoic acid, 2-[3,6-bis(ethylamino)-2,7-dimethyl-9*H*-xanthen-9-yl]-, ethyl ester

Other Names D 633; DHR 6G; Dihydrorhodamine 6G; d-R 6G

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{28}H_{32}N_2O_3$

Molecular Weight 444.57

Physical Form Light pink solid

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 572.4 ± 50.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.97 ± 0.40, most basic, temperature: 25 °C

Absorption (λ_{max}) 296 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 11,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Fungi;[3] mitochondria;[4,5] nucleic acids[6–9]

Biological/Medical Applications Detecting intracellular hydrogen peroxide in tumor cells,[4] 5-methylcytosine,[10] nucleic acids;[7,8] detecting/identifying gene duplications;[8] detecting/quantifying fungi;[3] generating/detecting/monitoring reactive oxygen species (ROS);[11–15] measuring hydrogen peroxide production in eukaryotic cells;[16] measuring/monitoring membrane potential;[5] nucleic acid ligation assays;[6] nucleic acids sequencing;[9] nanocomposite particles for biomedical applications;[17] skin care products[18]

Industrial Applications Light-transmitting materials/construction boards[19]

Safety/Toxicity No data available

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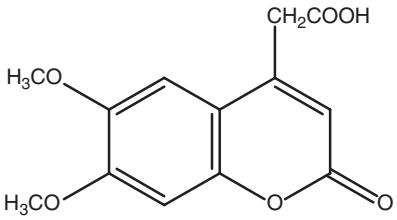
6,7-DIMETHOXYCOUMARIN-4-ACETIC ACID

CAS Registry Number 88404-26-6



CA Index Name 2*H*-1-Benzopyran-4-acetic acid, 6,7-dimethoxy-2-oxo-

Other Names 6,7-Dimethoxy-4-coumarinyl acetic acid; 6,7-Dimethoxycoumarin-4-acetic acid; (6,7-Dimethoxy-2-oxo-2*H*-chromen-4-yl)acetic acid

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{13}H_{12}O_6$

Molecular Weight 264.23

Physical Form Light tan solid

Solubility Soluble in dimethyl sulfoxide, ethanol, methanol, tetrahydrofuran

Melting Point 218 °C;[1] 174.5–175 °C[2]

Boiling Point (Calcd.) 498.0 ± 45.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.12 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 340 nm (MeOH)

Emission (λ_{max}) 415 nm (MeOH)

Molar Extinction Coefficient 12,800 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.36 (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Cyclic peptides[3–5]

Biological/Medical Applications Reagent for carboxylic acids;[1] as a substrate for measuring proteinases activity[3–5]

Industrial Applications Not reported

Safety/Toxicity No data available

REFERENCES

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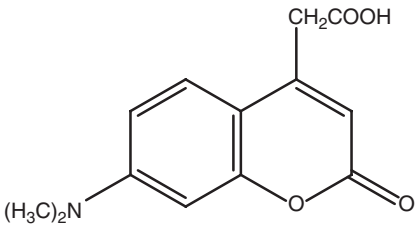
7-DIMETHYLAMINOCOUMARIN-4-ACETIC ACID (DMACA)

CAS Registry Number 80883-54-1

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-4-acetic acid, 7-(dimethylamino)-2-oxo-

Other Names 7-(Dimethylamino)coumarin-4-acetic acid; Coumarin D 126; D 126; DMACA

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{13}H_{13}NO_4$

Molecular Weight 247.25

Physical Form Yellow crystals;[5] Yellow needles;[7] Yellow precipitate;[3] Yellow solid;[1] Light yellow solid[2]

Solubility Soluble in *N,N*-dimethylformamide, methanol

Melting Point 168 °C;[7] 166–167 °C;[5] 163.5–164.5 °C[4]

Boiling Point (Calcd.) 497.6 ± 45.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.27 ± 0.10, most acidic, temperature: 25 °C; 1.70 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 370 nm (MeOH)

Emission (λ_{max}) 459 nm (MeOH)

Molar Extinction Coefficient 22,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–7]

Imaging/Labeling Applications Antibodies;[1] bovine pancreatic trypsin inhibitor (BPTI);[13,14] iron chelators;[4] natural products;[2,8] oligo[(R)-3-hydroxybutanoic acids] (OHB);[9] proteins;[1,3,10–14] toxins[8]

Biological/Medical Applications Distinguishing producer and nonproducer strains;[8] evaluating iron chelators;[4] synthesizing didemnin,[5] neovibsanin derivatives;[15] studying natural product biology;[2] as a substrate for measuring/monitoring β-secretase activity[16]

Industrial Applications Not reported

Safety/Toxicity No data available

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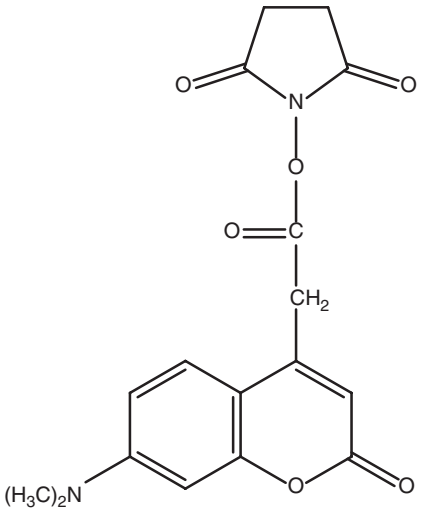
7-DIMETHYLAMINOCOUMARIN-4-ACETIC ACID SUCCINIMIDYL ESTER (DMACA SE)

CAS Registry Number 96686-59-8

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-4-acetic acid, 7-(dimethylamino)-2-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[[7-(dimethylamino)-2-oxo-2*H*-1-benzopyran-4-yl]acetyl] oxy]-; 7-Dimethylaminocoumarin-4-acetic acid, succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{17}H_{16}N_2O_6$

Molecular Weight 344.32

Physical Form Yellow solid

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 552.3 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 1.60 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 376 nm (MeOH)

Emission (λ_{max}) 468 nm (MeOH)

Molar Extinction Coefficient 22,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Analytes;[2] bovine pancreatic trypsin inhibitor (BPTI) derivatives;[1,10] oligonucleotides;[3,4] proteins/ fusion proteins;[1,5–10] silane coupling agent;[19] silica particles/beads;[19] taxol[11]

Biological/Medical Applications Amine reactive probe;[1,6,10,17,18] detecting oligonucleotides;[3,4] detecting/isolating proteins/fusion proteins;[1,5–10] quantifying analytes;[2] nucleic acid sequencing;[3,4] as a substrate for measuring angiotensin I-converting enzyme (ACE) activity,[12] glutathione and/or glutathione transferase activity,[13] chloramphenicol acetyltransferase activity,[14,15] proteases activity;[16] visualizing biomolecular dynamics in living cells,[5] taxol-microtubule system in cultured cells;[11] colloidal diagnostic devices;[19] useful for synthesizing peptides[19]

Industrial Applications Cations/metal ion sensing by self-assembled monolayers on glass;[17,18] silica particles/beads[19]

Safety/Toxicity No data available

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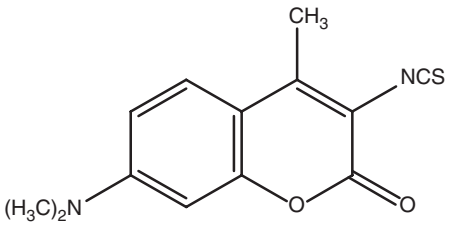
7-DIMETHYLAMINO-4-METHYLCOUMARIN-3-ISOTHIOCYANATE (DACITC)

CAS Registry Number 74802-04-3

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-2-one, 7-(dimethylamino)-3-isothiocyanato-4-methyl-

Other Names 7-(Dimethylamino)-4-methylcoumarin-3-isothiocyanate; DACITC

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{13}H_{12}N_2O_2S$

Molecular Weight 260.31

Physical Form Yellow needles[1]

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, methanol

Melting Point 200–201 °C[1]

Boiling Point (Calcd.) 475.6 ± 45.0 °C, pressure: 760 Torr

pK_a (Calcd.) 1.17 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 400 nm (MeOH)

Emission (λ_{max}) 476 nm (MeOH)

Molar Extinction Coefficient 36,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Alcohols;[1] amines;[1] silica shells[2]

Biological/Medical Applications Fluorescent acylating reagent for alcohols and primary amines[1]

Industrial Applications Superparamagnetic iron oxide-silica nanoparticles coating[2]

Safety/Toxicity No data available

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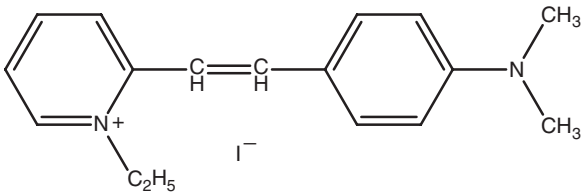
2-[4-(DIMETHYLAMINO)STYRYL]-*N*-ETHYLPYRIDINIUM IODIDE (DASPEI)

CAS Registry Number 3785-01-1

Chemical Structure



CA Index Name Pyridinium, 2-[2-[4-(dimethylamino) phenyl]ethenyl]-1-ethyl-, iodide (1:1)

Other Names 2-[*p*-(Dimethylamino)styryl]-1-ethylpyridinium iodide; Pyridinium, 2-[2-[4-(dimethylamino)phenyl]ethenyl]-1-ethyl-, iodide; Pyridinium, 2-[*p*-(dimethylamino)styryl]-1-ethyl-, iodide; 2-[4-(Dimethylamino)styryl]-1-ethylpyridinium iodide; 2-[4-(Dimethylamino)styryl]-N-ethylpyridinium iodide; D 426; DASPEI; NK 557; Pinaflavol

Merck Index Number Not listed

Chemical/Dye Class Styryl

Molecular Formula $C_{17}H_{21}IN_2$

Molecular Weight 380.27

Physical Form Bright red crystals[4]

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 258–259 °C;[4] 255 °C[5]

Absorption (λ_{max}) 461 nm (MeOH)

Emission (λ_{max}) 589 nm (MeOH)

Molar Extinction Coefficient 39,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–8]

Imaging/Labeling Applications Amyloid plaques;[9–11] axons;[25] bacteria;[12] epidermal cells;[13] hairs;[14–17] mitochondria;[1,18–25,34] nerve terminals;[25,26] neuromuscular junctions;[25] phospholipid vesicles/liposomes[27]

Biological/Medical Applications Analyzing mitochondria;[21] detecting prostate cancer;[21] diagnosing/treating amyloidosis disorder;[9–11] measuring/monitoring membrane potential[1,18–25,27]

Industrial Applications Color proofing materials;[32] holographic materials;[32] monitoring photopolymerization processes;[28] platemaking materials;[32] optoelectronic devices;[29] photographic materials/systems;[30–32] photoresists;[32] thermal cure monitoring of phenolic resole resins[33]

Safety/Toxicity Mitochondrial toxicity[34]

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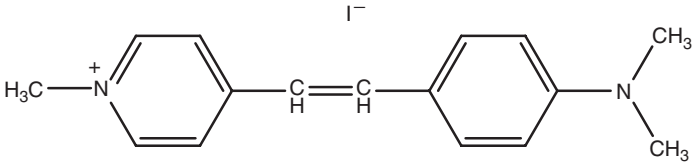
4-[4-(DIMETHYLAMINO)STYRYL]-*N*-METHYLPYRIDINIUM IODIDE (4-Di-1-ASP) (DASPMI)

CAS Registry Number 959-81-9

Chemical Structure



CA Index Name Pyridinium, 4-[2-[4-(dimethylamino) phenyl]ethenyl]-1-methyl-, iodide (1 : 1)

Other Names 4-[*p*-(Dimethylamino)styryl]-1-methylpyridinium iodide; Pyridinium, 4-[2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-, iodide; Pyridinium, 4-[*p*-(dimethylamino)styryl]-1-methyl-, iodide; 1-Methyl 4-(4-dimethylamino styryl) pyridinium iodide; 4-[2-[4-(Dimethylamino)phenyl]-ethenyl]-1-methylpyridinium iodide; 4-[4-(Dimethylamino)-α-styryl]-1-methylpyridinium iodide; 4-[4-(Dimethylamino)styryl]-1-methylpyridinium iodide; 4-[4-(Dimethylamino) styryl]-*N*-methylpyridinium iodide; 4′-Dimethylamino-1-methylstilbazolium iodide; 4′-Dimethylamino-*N*-methyl-4-stilbazolium iodide; D 288; DASPMI; 4-Di-1-ASP; ω-(*N*′-Methylpyridyl-4′)-4-dimethylaminostyrene iodide

Merck Index Number Not listed

Chemical/Dye Class Styryl

Molecular Formula $C_{16}H_{19}IN_2$

Molecular Weight 366.24

Physical Form Greenish purple solid;[2] Purple solid; Red needles[16]

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 262–263 °C;[6] 261–262 °C;[17] 261 °C;[7,8] 259 °C;[12] 258–259 °C;[20] 256–258 °C;[16] 255.5–256.2 °C;[11] 240–242 °C[2]

Absorption (λ_{max}) 475 nm (MeOH); 472 nm (DMSO); 505 nm ($CHCl_3$); 450 nm (H_2O)

Emission (λ_{max}) 605 nm (MeOH)

Molar Extinction Coefficient 45,000 cm^{-1} M^{-1} (MeOH); 42,000 cm^{-1} M^{-1} (DMSO); 58,000 cm^{-1} M^{-1} ($CHCl_3$)

Synthesis Synthetic methods[1–21]

Imaging/Labeling Applications Amyloid plaques[22–24] epithelial cells;[25] mitochondria;[1,26–32] nerve terminals;[33] nucleic acids;[4,34–36] proteins[37]

Biological/Medical Applications Analyzing/monitoring protein aggregation;[37] analyzing/visualizing mitochondria;[1,26–32] detecting nucleic acids,[4,34–36] prostate cancer,[29] diagnosing/treating amyloidosis disorder;[22–24] measuring/monitoring membrane potential;[1,30,32] treating bacterial infection[38]

Industrial Applications Electrochromic materials;[39] glass;[40] nonlinear optical (NLO) materials;[1,2,7,8,14,41–43] photoconductors;[44,45] thin films[46]

Safety/Toxicity No data available

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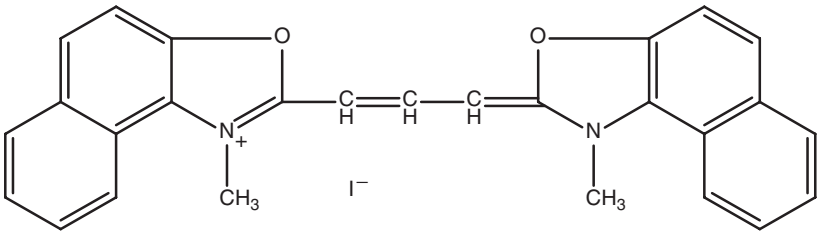
3,3′-DIMETHYL-α-NAPHTHOXACARBOCYANINE IODIDE (JC-9)

CAS Registry Number 522592-13-8

Chemical Structure



CA Index Name Naphth[1,2-*d*]oxazolium, 1-methyl -2-[3-(1-methylnaphth-[1,2-*d*]oxazol-2(1*H*)-ylidene)-1-propen-1-yl]-, iodide (1 : 1)

Other Names Naphth[1,2-*d*]oxazolium, 1-methyl -2-[3-(1-methylnaphth-[1,2-*d*]oxazol-2(1*H*)-ylidene)-1-propenyl]-, iodide; D 22421; DiNOC$_1$(3); 3,3′-Dimethyl -α-naphthoxacarbocyanine iodide; JC 9

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{27}H_{21}IN_2O_2$

Molecular Weight 532.38

Physical Form Red solid

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide

Absorption (λ_{max}) 522 nm ($CHCl_3$)

Emission (λ_{max}) 535 nm ($CHCl_3$)

Molar Extinction Coefficient 143,000 cm^{-1} M^{-1} ($CHCl_3$)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Mitochondria;[1–6] proteins;[7] sperms;[3] yeast cells[7]

Biological/Medical Applications Assessing sperm quality;[3] detecting ligated products;[8] identifying proteins;[7] measuring *in vivo* hematotoxicity;[5] measuring/monitoring membrane potential;[1–6] apoptosis assay;[5,9] as temperature sensor[10,11]

Industrial Applications Not reported

Safety/Toxicity No data available

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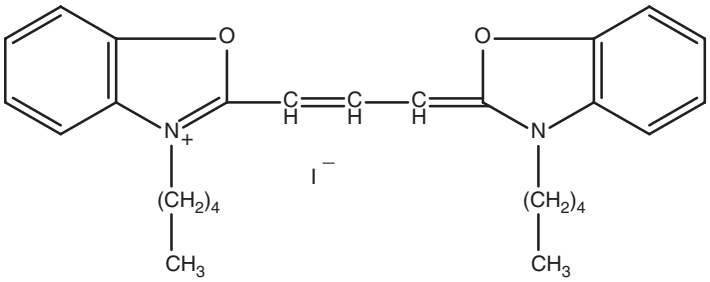
3,3′-DIPENTYLOXACARBOCYANINE IODIDE (DiOC$_5$(3))

CAS Registry Number 53213-81-3

Chemical Structure



CA Index Name Benzoxazolium, 3-pentyl-2-[3-(3-pentyl-2(3*H*)-benzoxazolylidene)-1-propen-1-yl]-, iodide (1 : 1)

Other Names Benzoxazolium, 3-pentyl-2-[3-(3-pentyl-2(3*H*)-benzoxazolylidene)-1-propenyl]-, iodide; 3,3′-Dipentyloxacarbocyanine iodide; DiOC$_5$(3); NK 2453

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{27}H_{33}IN_2O_2$

Molecular Weight 544.47

Physical Form Red powder or solid

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 214–215 °C[2]

Absorption (λ_{max}) 484 nm (MeOH)

Emission (λ_{max}) 500 nm (MeOH)

Molar Extinction Coefficient 155,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Mitochondria;[3–7] bacteria;[8,15,16,28] cells;[9] endoplasmic reticulum;[10] fungi;[27] hairs;[11] intraocular tissue;[12] lymphocytes;[13,14] leukocytes;[15] squamous epithelial cells;[15] microorganisms;[15,16,25–28] parasites;[26] platelets;[13] monocytes;[17] retina tissue;[18] sperms;[19] yeasts[25]

Biological/Medical Applications Detecting prostate cancer;[3] detecting/quantitating microorganisms,[15] leukocytes,[15] squamous epithelial cells;[15] measuring/monitoring membrane potential;[1,2,4,7,8,13,14,19–23,25–28] mitochondria stain;[3–7] cytotoxicity assay;[23,24] susceptibility assay[25–28]

Industrial Applications Photoresists[29]

Safety/Toxicity No data available

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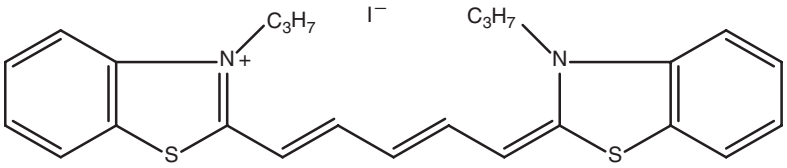
3,3′-DIPROPYLTHIADICARBOCYANINE IODIDE ($DiSC_3(5)$)

CAS Registry Number 53213-94-8

Chemical Structure



CA Index Name Benzothiazolium, 3-propyl-2-[5-(3-propyl-2(3*H*)-benzothiazolylidene)-1,3-pentadien-1-yl]-, iodide (1 : 1)

Other Names Benzothiazolium, 3-propyl-2-[5-(3-propyl-2(3*H*)-benzothiazolylidene)-1,3-pentadienyl]-, iodide; 3,3′-Dipropyl-2,2′-thiadicarbocyanine iodide; 3,3′-Dipropylthiadicarbocyanine iodide; Di-S-C_3-5; $DiSC_3(5)$; NK 2251

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{25}H_{27}IN_2S_2$

Molecular Weight 546.53

Physical Form Green powder or solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 248–249 °C[2]

Absorption (λ_{max}) 651 nm (MeOH)

Emission (λ_{max}) 675 nm (MeOH)

Molar Extinction Coefficient 258,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Adipocytes;[3] bacteria;[4–7] brush border membrane vesicles (BBMV);[8–12] cells;[13] Ehrlich ascites tumor cells;[57–59] epithelial cells;[14] erythrocytes;[15–21] granulocytes;[22,23] leukocytes;[24] lipid membranes/lipid bilayer membranes;[25–27] liposomes;[26,28,29] lymphocytes;[30,31] lysosomes;[32,33] microorganisms;[34] mitochondria;[30,35–41] mycoplasma membranes;[42] neuroblastoma cells;[43,44] neutrophils;[45,46] platelets;[47,48] proteins;[49] sperms;[50,51] yeast[52–55]

Biological/Medical Applications Detecting prostate cancer,[35] calcium-binding proteins;[49] measuring/monitoring membrane potential;[1–7,10–24,27–33,36–61] studying conformational changes,[49] neutrophil activation;[45] as anticancer agents;[56–59] cytotoxicity assays;[60] for photodynamic therapy[62]

Industrial Applications Not reported

Safety/Toxicity No data available

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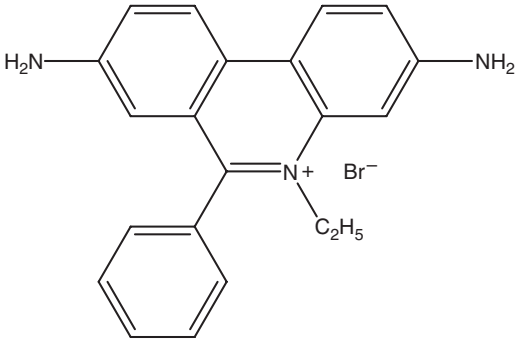
ETHIDIUM BROMIDE (HOMIDIUM BROMIDE)

CAS Registry Number 1239-45-8

Chemical Structure



CA Index Name Phenanthridinium, 3,8-diamino-5-ethyl-6-phenyl-, bromide (1 : 1)

Other Names 3,8-Diamino-5-ethyl-6-phenylphenanthridinium bromide; Phenanthridinium, 3,8-diamino-5-ethyl-6-phenyl-, bromide; 2,7-Diamino-10-ethyl-9-phenylphenanthridinium bromide; 2,7-Diamino-9-phenyl-10-ethylphenanthridinium bromide; 2,7-Diamino-9-phenylphenanthridine ethobromide; Dromilac; Ethidium bromide; Homidium bromide

Merck Index Number 4769

Chemical/Dye Class Heterocycle; Phenanthridine

Molecular Formula $C_{21}H_{20}BrN_3$

Molecular Weight 394.31

Physical Form Dark red crystals;[2,4,5] Dark red elongated plates[6]

Solubility Soluble in water, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 261–264 °C (decompose);[2] 248–249 °C (decompose);[6] 238–240 °C[4,5]

Absorption (λmax) 518 nm (H_2O/DNA); 480 nm (H_2O)

Emission (λmax) 605 nm (H_2O/DNA); 620 nm (H_2O)

Molar Extinction Coefficient 5,200 cm^{-1} M^{-1} (H_2O/DNA); 5,600 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1–6]

Imaging/Labeling Applications Nucleic acids;[1,2,7–46] bacteria;[47–50] cells;[51,52] chromatin;[53–56] chromosomes;[57–59] leukocytes;[60] microorganisms;[61–64] nerve terminals;[65] ribosomes;[66,67] sperms;[68–71] tumors;[72–74] yeast[75]

Biological/Medical Applications Assessing sperms quality;[70,71] detecting nucleic acids,[1,2,7–46] classifying/counting leukocytes;[60] counting sperms;[69] apoptosis assay;[76,77] cytotoxicity assay;[78,79] mitochondria toxicity assay;[80] as a substrate for measuring ribonuclease activity;[81,82] studying multidrug resistance;[83] as temperature sensor;[84,85] treating horses with pyroplasmosis;[86] treating trypanosomiasis[12,87]

Industrial Applications Electroluminescent displays;[88] photoresists[89]

Safety/Toxicity Carcinogenicity;[90–92] chromosome aberration;[93] genotoxicity;[94–97] DNA damage;[98] embryotoxicity;[99] genotoxicity;[100–104] mitochondrial toxicity;[105] mutagenicity;[106–113] neurotoxicity;[114,115] phototoxicity[116]

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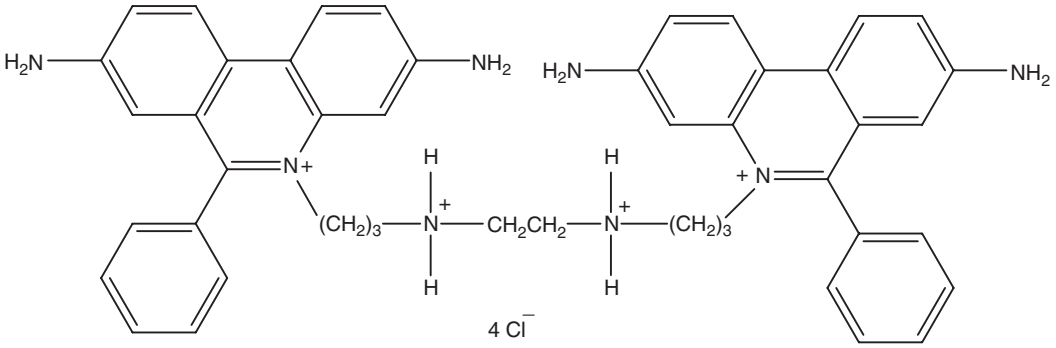
ETHIDIUM HOMODIMER-1 (EthD-1)

CAS Registry Number 61926-22-5

Chemical Structure



CA Index Name Phenanthridinium, 5,5′-[1,2-ethanediylbis(imino-3,1-propanediyl)]bis[3,8-diamino-6-phenyl-, chloride, hydrochloride (1 : 2: 2)

Other Names Phenanthridinium, 5,5′-[1,2-ethanediyl-bis(imino-3,1-propanediyl)]bis[3,8-diamino-6-phenyl-, dichloride, dihydrochloride; 5,5′-(4,7-Diazadecamethylene)bis(3,8-diamino-6-phenylphenanthridinium) dichloride dihydrochloride; EthD 1; Ethidium homodimer; Ethidium homodimer 1

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Phenanthridine

Molecular Formula $C_{46}H_{50}Cl_4N_8$

Molecular Weight 856.77

Physical Form Purple crystals;[2] Red solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 275 °C[2,3]

Absorption (λ_{max}) 528 nm (H_2O/DNA); 493 nm (H_2O)

Emission (λ_{max}) 617 nm (H_2O/DNA); 631 nm (H_2O)

Molar Extinction Coefficient 7000 cm^{-1} M^{-1} (H_2O/DNA); 9100 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–18] cells;[4,18–24] nuclei;[28–31] algae;[26] bacteria;[4] leukocytes;[32] megakaryocytes;[33] microorganisms;[34–39] oligonucleotides;[45] sperms;[18,40–43,58] Schwann cells (SCs) in whole nerves[44]

Biological/Medical Applications Detecting nucleic acids,[1–18] cell viability assay;[4,18–24] cytotoxicity assay;[24–27,52] classifying/counting leukocytes,[32] megakaryocyte;[33] counting erythroblasts;[30,31] detecting/counting sperms;[18,40–43,58] detecting/measuring microorganisms;[34–39] nucleic acid amplification;[45] evaluating freshness of a fish product;[46] as temperature sensor[47,48]

Industrial Applications For authentification[49]

Safety/Toxicity Cytotoxicity;[50–52] gastric toxicity;[53] neurotoxicity;[54,55] phototoxicity;[56,57] retinal toxicity;[56,57] reproductive toxicity;[58] tumor necrosis factor activity[59]

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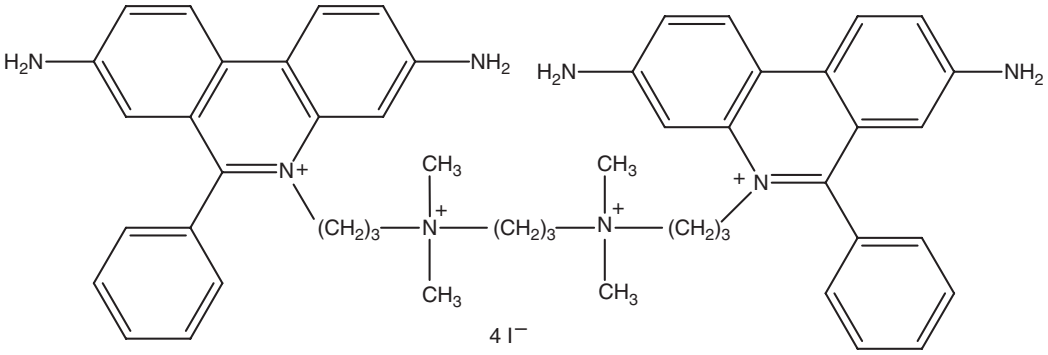
ETHIDIUM HOMODIMER-2 (EthD-2)

CAS Registry Number 180389-01-9

Chemical Structure



CA Index Name Phenanthridinium, 5,5′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl]]bis [3,8-diamino-6-phenyl-, iodide (1 : 4)

Other Names Phenanthridinium, 5,5′-[1,3-propanediyl-bis-[(dimethyliminio)-3,1-propanediyl]]bis[3,8-diamino-6-phenyl-, tetraiodide; EthD 2; Ethidium homodimer 2

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Phenanthridine

Molecular Formula $C_{51}H_{60}I_4N_8$

Molecular Weight 1292.71

Physical Form Purple crystals or red solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 535 nm (H_2O/DNA); 498 (H_2O)

Emission (λ_{max}) 624 nm (H_2O/DNA); 631 (H_2O)

Molar Extinction Coefficient 8000 cm^{-1} M^{-1} (H_2O/DNA); 10,800 (H_2O)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–9] cells;[1,2,9] nuclei;[10,11] bacteria;[,2] leukocytes;[12] megakaryocyte;[13] microorganisms;[14] oligonucleotides;[15] sperms[9,16]

Biological/Medical Applications Detecting nucleic acids,[1–9] cells,[1,2,9] microorganisms;[14] classifying/counting leukocytes,[12] megakaryocyte;[13] counting erythroblasts,[10,11] sperms;[9,16] nucleic acids amplification[15]

Industrial Applications Not reported

Safety/Toxicity No data available

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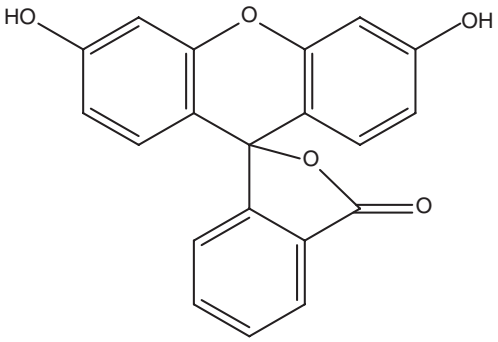
FLUORESCEIN

CAS Registry Number 2321-07-5

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-3-one, 3′,6′-dihydroxy-

Other Names Fluorescein; 3,6-Dihydroxyspiro[xanthene-9,3′-phthalide]; 3′,6′-Dihydroxyfluoran; 3′,6′-Fluorandiol; 9-(*o*-Carboxyphenyl)-6-hydroxy-3-isoxanthenone; Benzoic acid, 2-(6-hydroxy-3-oxo-3*H*-xanthen-9-yl)-; C.I. 45350:1; C.I. Solvent Yellow 94; D and C Yellow No. 7; D&C Yellow No. 7; Fluorescein acid; Japan Yellow 201; Japan Yellow No. 201; NSC 667256; Resorcinolphthalein; Solvent Yellow 94; Yellow fluorescein

Merck Index Number 4192

Chemical/Dye Class Xanthene

Molecular Formula $C_{20}H_{12}O_5$

Molecular Weight 332.31

Physical Form Red crystalline solid;[12] Reddish mass;[22] Red powder[3,21,24]

Solubility Insoluble in water, benzene, chloroform, ether; Soluble in acetone, *N,N*-dimethylformamide, dimethyl sulfoxide, hot ethanol, glacial acetic acid

Melting Point >350 °C;[27] 314–316 °C;[21,24] 312–315 °C;[3] >300 °C[12]

Boiling Point (Calcd.) 620.8 ± 55.0 °C, pressure: 760 Torr

pK_a 6.4, temperature: 22 °C

pK_a (Calcd.) 9.35 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 473 nm (Buffer pH 5.0); 490 nm (Buffer pH 9.0)

Emission (λ_{max}) 514 nm (Buffers pH 5.0, pH 9.0)

Molar Extinction Coefficient 34,000 cm^{-1} M^{-1} (Buffer pH 5.0); 93,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–29]

Imaging/Labeling Applications Amyloid-β peptides;[30] antibodies;[31–35] bacteria;[36] brain;[37] chromosomes;[38,39] cornea;[40–43] cyanide;[44] dental plaque;[45,46] dextran;[47–49] fibrin;[50] hairs;[51–54] hydrogen peroxide;[55] insects;[56] liposomes;[57] lymphocytes;[58–60] metal ions (aluminum ions,[61] arsenic ions,[62] chromium ions,[61] copper ions,[63] iron ions,[61] lead ions,[64] mercury ions,[65,66] palladium ions,[67] silver ions,[68] zinc ions;[69]) nucleic acids/nucleotides;[70–79] plasma;[80,81] polylactic acid (PLA) microspheres;[82] proteins;[83–96] protoplasm;[97] silica nanoparticles;[98–100] steroids[101]

Biological/Medical Applications Detecting chromosomal aberration;[38,39] diagnosing corneal diseases;[40] marking/detecting insects;[56] as antitumor agent;[102] as antihistaminic agent;[103] use in agriculture and plant cultivation;[104] use in cosmetics;[105–109] use in ophthalmology;[40–43,110,111] as a substrate for measuring α-amylases activity,[112] elastases activity,[113] esterases activity,[114,115] β-glucuronidases activity,[116] horseradish peroxidases activity,[117] kinases activity,[118,119] monoamine oxidases (MAOs) activity,[120] phosphatases activity,[121] phospholipases activity,[122] proteases/proteinases activity,[123,124] telomerases activity activity[125]

Industrial Applications Aerosol products;[126] bar code systems;[127] cathode-ray tube;[128] color filters;[129,130] corrosion inhibitors;[131] detecting cracks on concrete;[132] dye lasers;[133–140] electrophotographic materials;[141,142] glass articles;[143] liquid-crystal displays;[144] light emitting diode;[145] metal oxide particles;[146] organic light-emitting device (OLED);[147] paints;[148,149] papers;[150–153] photoconductive materials;[154] photoresists;[155] photosensitive materials;[156,157] recording materials;[158–160] rubber;[161,162] textiles;[163,164] thin films;[165] toners;[166,167] for water tracing (tracers for hydrology)[168–170]

Safety/Toxicity Acute toxicity;[171] cytotoxicity;[172,173] mutagenicity;[172,174,175] ophthalmic toxicity;[176,177] phototoxicity;[178] skin toxicity[179,180]

Handbook of Fluorescent Dyes and Probes, First Edition. R. W. Sabnis.
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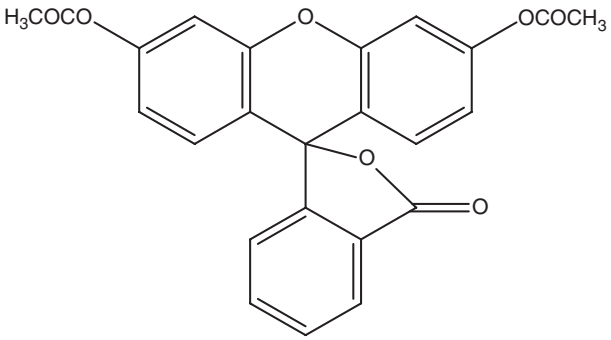
FLUORESCEIN DIACETATE (FDA)

CAS Registry Number 596-09-8

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]-xanthen]-3-one, 3′,6′-bis(acetyloxy)-

Other Names Fluorescein, diacetate; 3′,6′-Diacetylfluorescein; F 1303; FDA; Fluorescein 3′,6′-diacetate; MFCD 5062; NSC 4726; NSC 667259

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{24}H_{16}O_7$

Molecular Weight 416.38

Physical Form White crystals[5,9,10] or colorless solid; Beige crystals[11]

Solubility Soluble in acetone, chloroform, dimethyl sulfoxide, ethanol, methanol

Melting Point 205–206 °C;[17] 205 °C;[11,16] 203–205.5 °C;[5] 203–205 °C;[15] 202–203 °C;[2] 202 °C;[8] 199–203 °C[9,10]

Boiling Point (Calcd.) 604.7 ± 55.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 289 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 5300 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–17]

Imaging/Labeling Applications Algae;[18,115–117] bacteria;[19–25] cells;[26–33] corneal endothelium;[34] cysts;[35,36] embryo;[37,128] hepatocytes;[38,39] hyphae;[40,41] marine plankton;[42] membrane integrity/permeability;[43–50] microorganisms;[51–57] microspores;[58] oocytes;[59] perborate;[60,61] pollen;[62–65] protoplasts;[66–69] seeds;[70] sperms;[43,45] spores;[71] teliospores;[72] tumors;[73,74] yeasts[75]

Biological/Medical Applications Assessing membrane integrity/permeability;[43–50] detecting/counting microorganisms;[51–57] measuring microbial activity;[76–86] as a substrate for measuring acylases activity,[101] amidases activity,[87] aminopeptidases activity,[97] arylsulfatases activity,[87] chymotrypsin activity,[101] esterases activity;[88–100] galactosidases activity,[87] glucosidases activity,[87,97] lipases activity,[2,8,89,101] phosphatases activity,[97] proteases activity;[89] cell viability assay;[26–33] cytotoxicity assay;[46,117,120–125,130] implantable medical devices;[102] as temperature sensor;[103,104] treating ischemic disease[105]

Industrial Applications Display devices;[106] electrophotography;[107,108] laser dyes;[109,110] papers;[111] petroleum markers,[3,9,10] recording materials[112,113]

Safety/Toxicity Acute toxicity;[114] algal toxicity;[115–117] aluminum toxicity;[118] arsenic toxicity;[119] cytotoxicity;[46,117,120–125,130] ecotoxicity;[126,127] embryotoxicity;[128] marine toxicity;[129] nephrotoxicity;[130] neurotoxicity;[131–133] phytotoxicity[134]

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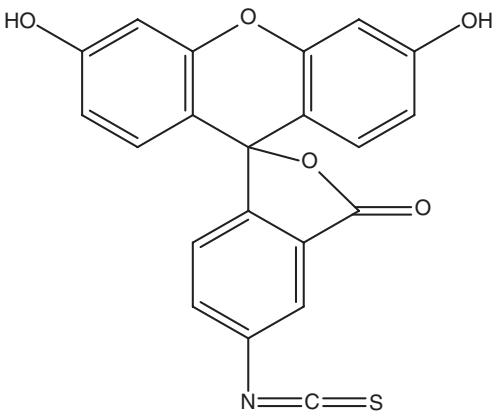
FLUOROSCEIN-5-ISOTHIOCYANATE (FITC)

CAS Registry Number 3326-32-7

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-3-one, 3′,6′-dihydroxy-5-isothiocyanato-

Other Names Fluorescein, 5-isothiocyanato-; 5-Isothiocyanatofluorescein; FITC isomer I; Fitc isomer 1; Fluorescein 5-isothiocyanate; Fluorescein isothiocyanate isomer 1; Fluorescein isothiocyanate isomer I; Fluoroscein-5-isothiocyanate

Merck Index Number 4120

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{11}NO_5S$

Molecular Weight 389.38

Physical Form Orange-yellow crystal;[2,6] Orange solid[9]

Solubility Soluble in acetone, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point >193 °C (decompose);[2] >160 °C (decompose)[6]

Boiling Point (Calcd.) 708.6 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 9.31 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 494 nm (Buffer pH 9.0)

Emission (λ_{max}) 519 nm (Buffer pH 9.0)

Molar Extinction Coefficient 77,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–9]

Imaging/Labeling Applications Amino groups;[10] antibodies;[11–15] biotin;[16] cells;[17,18] cellulose nanocrystals;[19,20] α-cobratoxin;[21] dendrimers;[22–25,80] dextrans;[26,27] digoxin;[28] enzymes: ATPase,[29–33] soybean lipoxygenase;[34] heparins;[35,36] Hodgkin and Reed Sternberg (HRS) cells;[37] insulin;[38] nanoparticles (gold nanoparticles,[39] silica nanoparticles;[40,41]) nucleotides/nucleic acids;[12,42–47] paclitaxel;[48,49] PEO-PCL-PEO triblock copolymers;[50] polymersomes;[51] proteins/peptides;[5,7,9,12,52–66] strychnine;[67] sugar chains;[68] thiol groups[69,70]

Biological/Medical Applications Analyzing sugar chain;[68] detecting iodide/iodate or total iodine;[39] detecting/imaging thiols;[69,70] detecting/quantifying biotin derivatives;[16] diagnosing classical Hodgkin lymphoma (CHL) in lymph nodes;[37] cellulose nanocrystals for bioimaging applications;[20] treating neuroinflammation;[23] treating/diagnosing cancer;[24] PEO-PCL-PEO triblock copolymers for topical delivery;[50] polymersomes in biomedical or cosmetic applications;[51] apoptosis assay;[71] as a substrate for measuring heparanase activity,[72] human immunodeficiency virus 1 (HIV-1) proteinase activity,[73] kinase activity,[74] phosphatase activity,[74] β-lactamase activity,[75] transglutaminase (TG2) activity;[76] implantable drug-delivery devicess[77]

Industrial Applications Gel coating/gel monolith for fiber-optic sensor applications;[78] ultrathin films[79]

Safety/Toxicity Cytotoxicity;[80,81] genotoxicity;[82] membrane toxicity;[83] neurotoxicity;[84] ophthalmic toxicity;[85] phototoxicity;[86] pulmonary toxicity;[87] skin toxicity[88–92]

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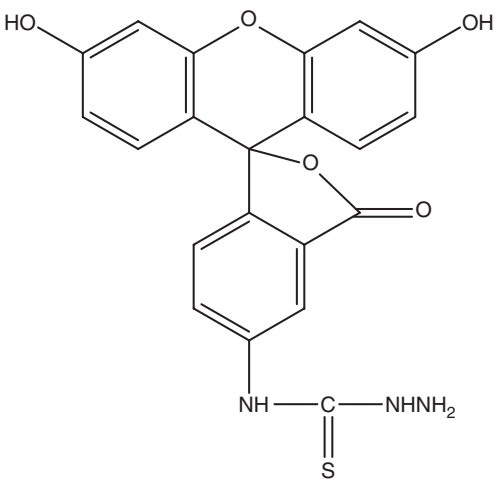
FLUORESCEIN-5-THIOSEMICARBAZIDE

CAS Registry Number 76863-28-0

Chemical Structure



CA Index Name Hydrazinecarbothioamide, *N*-(3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-5-yl)-

Other Names Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene], hydrazinecarbothioamide deriv.; Fluorescein-5-thiosemicarbazide; 5-FTSC; FTSC; FTZ;

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{15}N_3O_5S$

Molecular Weight 421.43

Physical Form Yellow solid[1]

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide

Boiling Point (Calcd.) 723.8 ± 70.0 °C, pressure: 760 Torr

pK_a (Calcd.) 9.33 ± 0.20, most acidic, temperature: 25 °C; 1.76 ± 0.19, most basic, temperature: 25 °C

Absorption (λ_{max}) 492 nm (Buffer pH 9.0)

Emission (λ_{max}) 516 nm (Buffer pH 9.0)

Molar Extinction Coefficient 85,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Carbonyl groups (aldehydes/ketones/carboxylic acids);[1,3,4,7,9–12,] cellulose fibre interfaces;[5,6] dendrimer surface;[7] glycosaminoglycan;[8] hairs;[9–12] hyaluronic acid;[8] lipobeads;[13] nanoparticles;[14] nucleic acids;[2,15–20,] polysaccharides;[21] proteins;[9–12,22–31] sterols[32]

Biological/Medical Applications Analyzing low-molecular mass aldehydes in urine,[3] drinking waters;[4] assaying glycosaminoglycan-degrading enzyme activity;[8] detecting sterols;[32] measuring/quantifying degree of hair damage[9–12]

Industrial Applications Characterizing soft material interfaces;[6] understanding fibrous network structures;[6] in nanodevice preparation;[7] functionalizing/ encapsulatiing particles by initiated chemical vapor deposition (iCVD);[33,34] functional polymer coatings;[33] high refractive index coatings;[34] papers[5]

Safety/Toxicity No data available

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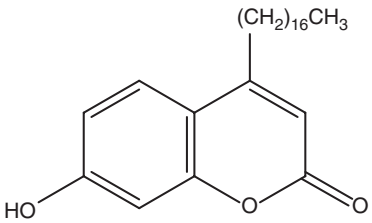
4-HEPTADECYL-7-HYDROXYCOUMARIN (4-HEPTADECYLUMBELLIFERONE)

CAS Registry Number 26038-83-5

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-2-one, 4-heptadecyl-7-hydroxy-

Other Names Coumarin, 4-heptadecyl-7-hydroxy-; 4-Heptadecyl-7-hydroxycoumarin; 4-heptadecyl-hydroxycoumarin; heptadecyl-hydroxycoumarin; 4-Heptadecylumbelliferone; 7-hydroxy-4-heptadecyl coumarin; C17HC; C17-HC; HC; HHC; HUF

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{26}H_{40}O_3$

Molecular Weight 400.59

Physical Form Off-white solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 95 °C

Boiling Point (Calcd.) 544.7 ± 45.0 °C, pressure: 760 Torr

pK_a 8.9, temperature: 22 °C

pK_a (Calcd.) 8.02 ± 0.20, most acidic, tempeature: 25 °C

Absorption (λ_{max}) 325 nm ($MeOH/H^+$); 366 nm ($MeOH/OH^-$)

Emission (λ_{max}) 385 nm ($MeOH/H^+$); 453 nm ($MeOH/OH^-$)

Molar Extinction Coefficient 15,000 $cm^{-1}\,M^{-1}$ ($MeOH/H^+$); 20,000 $cm^{-1}\,M^{-1}$ ($MeOH/OH^-$)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Erythrocytes;[4,5] lipids;[6–10] liposomes;[21–24] proteins[24]

Biological/Medical Applications Analyzing protein orientations in proteoliposomes;[24] characterizing interactions of cationic lipids with nucleic acids;[6] investigating lipid assemblies;[10] measuring surface potential in biomembranes;[7,8,13–23,] studying/evaluating human erythrocyte exovesiculation;[4,5] studying lipid bilayers properties;[7] Langmuir-Blodgett films;[2,11,12,] as a biological pH indicator;[1,7–20,22,23] as a probe of membrane surfaces[7,8,13–23,]

Industrial Applications Not reported

Safety/Toxicity No data available

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Handbook of Fluorescent Dyes and Probes, First Edition. R. W. Sabnis.
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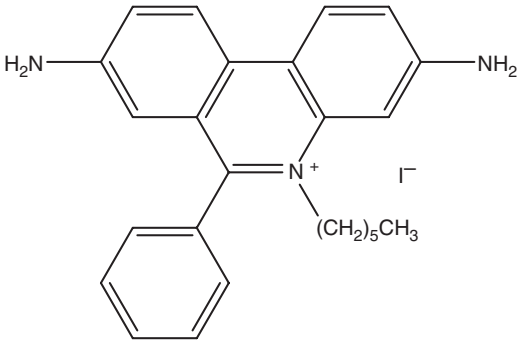
HEXIDIUM IODIDE

CAS Registry Number 211566-66-4

Chemical Structure



CA Index Name Phenanthridinium, 3,8-diamino-5-hexyl-6-phenyl-, iodide (1:1)

Other Names Phenanthridinium, 3,8-diamino-5-hexyl-6-phenyl-, iodide; Hexidium iodide

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Phenanthridine

Molecular Formula $C_{25}H_{28}IN_3$

Molecular Weight 497.42

Physical Form Red solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 518 nm (H_2O/DNA); 482 nm (H_2O)

Emission (λ_{max}) 600 nm (H_2O/DNA); 625 nm (H_2O)

Molar Extinction Coefficient 3900 cm^{-1} M^{-1} (H_2O/DNA); 5500 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1,3,4] nuclei;[5–7] bacteria;[8–11] fungi;[12] microorganisms;[13,14] mold;[8,15] oligonucleotides;[16] polynucleotides;[17] yeast[8]

Biological/Medical Applications Detecting nucleic acids,[1,3,4] bacteria,[8–11] microorganisms;[13,14] molds,[8,15] nucleic acid binding proteins,[18] yeast;[8] analyzing polynucleotides;[17] nucleic acids amplification;[16] measuring membrane/transmembrane potential[19,20]

Industrial Applications Not reported

Safety/Toxicity No data available

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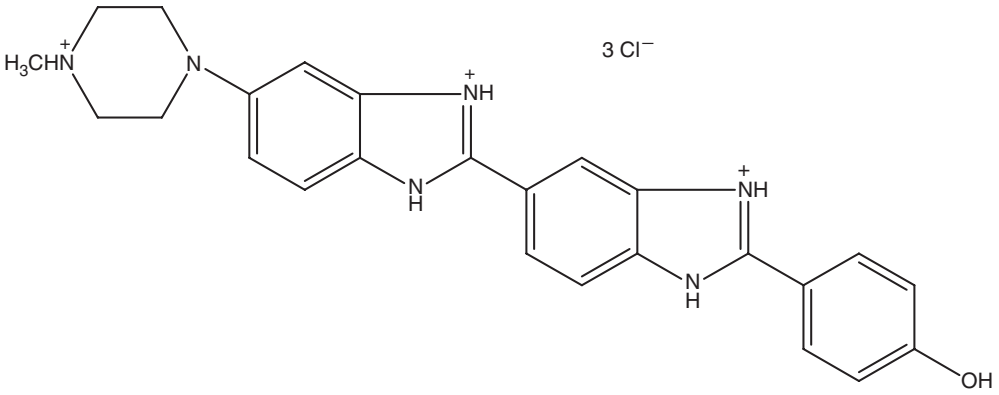
HOECHST 33258

CAS Registry Number 23491-45-4

Chemical Structure



CA Index Name Phenol, 4-[6-(4-methyl-1-piperazinyl)[2,6′-bi-1*H*-benzimidazol]-2′-yl]-, hydrochloride (1:3)

Other Names Phenol, 4-[5-(4-methyl-1-piperazinyl)[2,5′-bi-1*H*-benzimidazol]-2′-yl]-, trihydrochloride; Phenol, *p*-[5-[5-(4-methyl-1-piperazinyl)-2-benzimidazolyl]-2-benzimidazolyl]-, trihydrochloride; 2-[2-(4-Hydroxyphenyl)-6-benzimidazolyl]-6-(1-methyl-4-piperazinyl)-benzimidazole trihydrochloride; 2-[2-(4-Hydroxyphenyl)-6-benzimidazolyl]-6-(1-methyl-4-piperazyl)-benzimidazole trihydrochloride; 2-[2-(4-Hydroxyphenyl)-6-benzimidazolyl]-6-(1-methyl-4-piperazyl)benzimidazole trichloride; 2-[2-(4-Hydroxyphenyl)-6-benzimidazolyl]-6-(1-methyl-4-piperazyl)benzimidazole-3HCl; 2′-(4-Hydroxyphenyl)-5-(4-methyl-1-piperazinyl)-2,5′-bi-1*H*-benzimidazole; 4-[5-[5-(4-Methyl-1-piperazinyl)-2-benzimidazolyl]-2-benzimidazolyl]phenol trihydrochloride; Bisbenzimide; Bisbenzimide (quenchant); Bisbenzimide trihydrochloride; H 33258; HOE 33258; Ho 33258; Hoechst 33258; NSC 322921; Pibenzimol hydrochloride

Merck Index Number 1250

Chemical/Dye Class Heterocycle; Benzimidazole

Molecular Formula $C_{25}H_{27}Cl_3N_6O$

Molecular Weight 533.88

Physical Form Yellow to green powder or solid

Solubility Soluble in water, *N,N*-dimethylformamide, ethanol, methanol

Melting Point 280 °C (decompose)[4,5]

Absorption (λ_{max}) 352 nm (H_2O/DNA); 357 nm (MeOH/H^+)

Emission (λ_{max}) 461 nm (H_2O/DNA); 536 nm (MeOH/H^+)

Molar Extinction Coefficient 40,000 cm^{-1} M^{-1} (H_2O/DNA); 47,000 cm^{-1} M^{-1} (MeOH/H^+)

Quantum Yield 0.42 (H_2O/DNA)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Nucleic acids;[1,6–55] cells;[1,55–59] chromatin;[60–63] chromosomes;[64–83] embryos;[84] lymphocytes;[85] microorganisms;[86,87] myoglobin;[88] nuclei;[89–95] parasites;[96,97] protoplasts;[98,99] sperms[100–105]

Biological/Medical Applications Analyzing cell division;[106] as anticancer agent;[1,2,107–110] as antimicrobial agent;[110,111] counting/identifying cells;[1,55–59] detecting/measuring microorganisms;[86,87] detecting/quantifying nucleic acids;[1,6–55] measuring membrane potential;[112,113] studying multidrug resistance;[114] apoptosis assay;[115,116] cell cycle assay;[117–123] cell proliferation assay[124]

Industrial Applications Photoresists;[125] thin films[126]

Safety/Toxicity Cytotoxicity;[127,128] DNA damage;[129] genotoxicity;[130] radiotoxicity[131]

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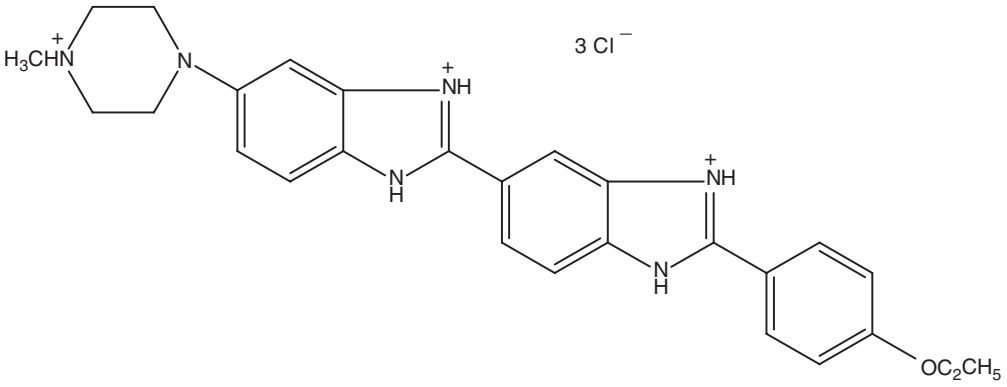
HOECHST 33342

CAS Registry Number 875756-97-1

Chemical Structure



CA Index Name 2,5′-Bi-1*H*-benzimidazole, 2′-(4-ethoxyphenyl)-5-(4-methyl-1-piperazinyl)-, hydrochloride (1:3)

Other Names 2,5′-Bi-1*H*-benzimidazole, 2′-(4-ethoxyphenyl)-5-(4-methyl-1-piperazinyl)-, trihydrochloride; 2,5′-Bibenzimidazole, 2′-(*p*-ethoxyphenyl)-5-(4-methyl-1-piperazinyl)-, trihydrochloride; 2′-(4-Ethoxyphenyl)-5-(4-methyl-1-piperazinyl)-2,5′-bi-1H-benzimidazole trihydrochloride; 2-[2-(4-Ethoxyphenyl)-6-benzimidazolyl]-6-(1-methyl-4-piperazinyl)benzimidazole trihydrochloride; Bisbenzimide; HOE 33342; Ho 342; Hoechst 33342; Hoechst 33342 trihydrochloride; NSC 334072

Merck Index Number 1250

Chemical/Dye Class Heterocycle; Benzimidazole

Molecular Formula $C_{27}H_{31}Cl_3N_6O$

Molecular Weight 561.94

Physical Form Yellow to green powder or solid

Solubility Soluble in water, *N,N*-dimethylformamide, methanol

Melting Point >300 °C

Boiling Point (Calcd.) 725.9 ± 70.0 °C, pressure: 760 Torr

pK_a (Calcd.) 11.08 ± 0.69, most acidic, temperature: 25 °C; 7.66 ± 0.42, most basic, temperature: 25 °C

Absorption (λ_{max}) 350 nm (H_2O/DNA); 357 nm (MeOH/H^+)

Emission (λ_{max}) 461 nm (H_2O/DNA); 538 nm (MeOH/H^+)

Molar Extinction Coefficient 45,000 cm^{-1} M^{-1} (H_2O/DNA); 43,000 cm^{-1} M^{-1} (MeOH/H^+)

Quantum Yield 0.38 (H_2O/DNA)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Nucleic acids;[6–21] β-amyloid (Aβ) plaques;[22] bacteria;[23,24] cells;[25–31] chromatin;[32,33] lymphocytes;[34–36] microorganisms;[37,38] nucleus;[39–41] neurons;[42] parasites;[43,44] sperms;[45–52] stem cells;[53–62] tumors[63–71]

Biological/Medical Applications Detecting β-amyloid (Aβ) plaques;[22] detecting/measuring microorganisms;[37,38] identifying/counting cells;[25–31] studying multidrug resistance;[72] apoptosis assay;[73–83] cell cycle assay;[83–85] cell proliferation assay;[86] measuring membrane potential;[87–89] treating disc degenerative disease,[90] erectile dysfunction[91]

Industrial Applications Photoresists[92]

Safety/Toxicity Carcinogenicity;[93] cardiotoxicity;[94] cytotoxicity;[95,99,100] DNA damage;[96–100] genotoxicity;[101–103] metabolic toxicity;[104] mutagenicity;[100] neurotoxicity;[105–107] phototoxicity;[108,109] reproductive toxicity[110–112]

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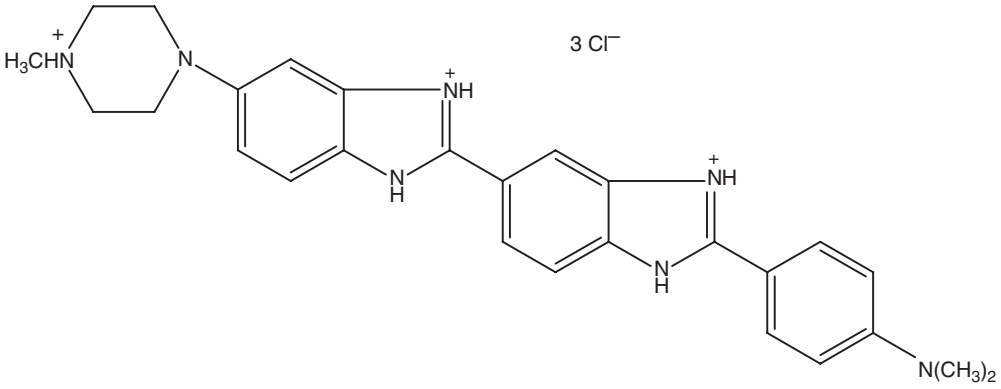
HOECHST 34580

CAS Registry Number 23555-00-2

Chemical Structure



CA Index Name Benzenamine, *N*,*N*-dimethyl-4-[5-(4-methyl-1-piperazinyl)[2,5′-bi-1*H*-benzimidazol]-2′-yl]-, hydrochloride (1:3)

Other Names 2,5′-Bibenzimidazole, 2′-[*p*-(dimethylamino)-phenyl]-5-(4-methyl-1-piperazinyl)-, trihydrochloride; HOE 34580; Hoechst 34580; Proamine

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Benzimidazole

Molecular Formula $C_{27}H_{32}Cl_3N_7$

Molecular Weight 560.96

Physical Form Light brown powder;[5] Yellow powder or solid

Solubility Soluble in dimethyl sulfoxide

Melting Point 225–226 °C (decompose);[2–5] 210 °C[6,7]

Boiling Point (Calcd.) 733.2 ± 70.0 °C, pressure: 760 Torr

pK_a (Calcd.) 10.97±0.10, most acidic, temperature: 25 °C; 7.66 ± 0.42, most basic, temperature: 25 °C

Absorption (λ_{max}) 392 nm (H_2O/DNA)

Emission (λ_{max}) 440 nm (H_2O/DNA)

Molar Extinction Coefficient 47,000 cm^{-1} M^{-1} (H_2O/DNA)

Synthesis Synthetic methods[1–7]

Imaging/Labeling Applications Nucleic acids;[1–13] cells;[13] nuclei;[14,15] microorganisms;[16] oligonucleotides;[17] polynucleotides;[18] sperms[13]

Biological/Medical Applications Detecting nucleic acids,[1–13] cells,[13] microorganisms;[16] analyzing polynucleotides;[18] nucleic acid amplification;[17] nucleic acid sequencing;[19] radioprotectors;[2–4] as temperature sensor[20,21]

Industrial Applications Not reported

Safety/Toxicity No data available

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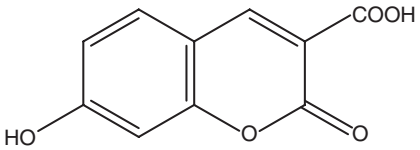
7-HYDROXYCOUMARIN-3-CARBOXYLIC ACID (UMBELLIFERONE-3-CARBOXYLIC ACID)

CAS Registry Number 779-27-1

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-hydroxy-2-oxo-

Other Names 3-Carboxy-7-hydroxycoumarin; 3-Carboxyumbelliferone; 7-Hydroxycoumarin-3-carboxylic acid; NSC 115545; Umbelliferone-3-carboxylic acid; HCC; 7-OHCCA; 7-OH-C-3-COOH

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{10}H_6O_5$

Molecular Weight 206.15

Physical Form Yellow solid;[1,16,17] Orange solid;[14] Off-white powder[2]

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 283–284 °C;[16] 271 °C (decompose);[27] 264–265 °C;[26] 263.4–265.3 °C;[1] 262–266 °C;[14] 262–263 °C;[8,24] 262 °C (decompose);[25] 261–263 °C;[20] 260–262 °C;[3] 259–262 °C;[7] 259–260 °C;[4] 258–259 °C;[13] 248–250 °C (decompose)[19]

Boiling Point (Calcd.) 474.8 ± 45.0 °C, pressure: 760 Torr

pK_a 7.04 ± 0.02, temperature: 23 °C

pK_a (Calcd.) 1.98 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 386 nm (Buffer pH 10.0); 339 nm (Buffer pH 4.0)

Emission (λ_{max}) 448 nm (Buffer pH 10.0, 4.0)

Molar Extinction Coefficient 29,000 cm^{-1} M^{-1} (Buffer pH 10.0); 19,000 cm^{-1} M^{-1} (Buffer pH 4.0)

Synthesis Synthetic methods[1–27]

Imaging/Labeling Applications Amines;[28,29] antibodies;[30] bacteria;[31,32] hairs/keratinous fibers;[33,34] hydroxyl radicals;[10,12,15,35–44] nucleic acids;[44,45] palladium;[46] photoactive yellow protein[47–55]

Biological/Medical Applications Chemical dosimeter for radiation therapy;[56] detecting bacteria;[31,32] detecting/sensing hydroxyl radicals;[10,12,15,35–44] studying nucleic acids;[44,45] as a substrate for measuring carboxylesterases activity,[57] cellulases activity,[58] β-galactosidases activity,[21,59,60] glycosidases activity,[61] glycosyltransferases activity,[62–64] hydrolases activity,[65] 4-hydroxycinnamate decarboxylases activity,[66] β-lactamases activity,[9,67] phosphatases activity,[57] sulfatases activity;[57] treating cancer/antitumor activity[68–70]

Industrial Applications Carbon-dioxide sensor;[71,72] chemical sensors based on non-linear optics;[73] monitoring of cationic photopolymerization processes;[74] nanomaterials[75]

Safety/Toxicity No data available

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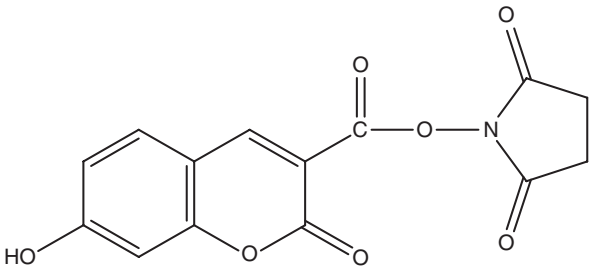
7-HYDROXYCOUMARIN-3-CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 134471-24-2

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-hydroxy-2-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[(7-hydroxy-2-oxo-2*H*-1-benzopyran-3-yl)carbonyl]oxy]-; 7-Hydroxycoumarin-3-carboxylic acid *N*-succinimidyl ester; 7-Hydroxycoumarin-3-carboxylic acid succinimidyl ester; HCC-NHS; HCCS

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{14}H_9NO_7$

Molecular Weight 303.22

Physical Form Yellow solid[3]

Solubility Soluble in acetonitrile, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 558.9 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 7.09 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 419 nm (MeOH)

Emission (λ_{max}) 447 nm (MeOH)

Molar Extinction Coefficient 36,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Analytes;[5] cells;[3] NPTX-594 toxin analogs;[6–8] nucleic acids;[9] peptides;[10] proteins[1,11–14]

Biological/Medical Applications Analyzing peptides;[10] detecting/measuring/sensing hydroxyl radicals;[2,4,15–21] identifying genome;[9] quantifying analytes;[5] as a substrate for measuring glutathione and/or glutathione transferase activity,[22] glycosyltransferases activity;[23] viscosity sensors[24]

Industrial Applications Not reported

Safety/Toxicity No data available

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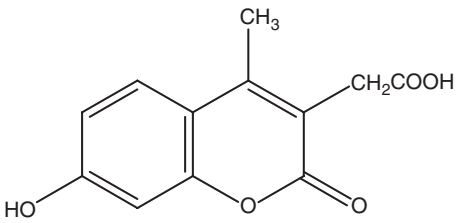
7-HYDROXY-4-METHYLCOUMARIN-3-ACETIC ACID

CAS Registry Number 5852-10-8

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-acetic acid, 7-hydroxy-4-methyl-2-oxo-

Other Names 7-Hydroxy-4-methyl-2-oxo-2*H*-1-benzopyran-3-acetic acid; 7-Hydroxy-4-methylcoumarin-3-acetic acid; 7-Hydroxy-4-methyl-3-coumarinylacetic acid; 4-Methylumbelliferone-3-acetic acid

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{12}H_{10}O_5$

Molecular Weight 234.20

Physical Form Yellow solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

Melting Point 268–269 °C;[1] 268 °C;[5] 265–268 °C;[3] 265–266 °C;[4] 265 °C;[6]

Boiling Point (Calcd.) 512.9 ± 50.0 °C, pressure: 760 Torr

pK_a (Calcd.) 3.78 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 360 nm (Buffer pH 10.0)

Emission (λ_{max}) 455 nm (Buffer pH 10.0)

Molar Extinction Coefficient 19,000 cm^{-1} M^{-1} (Buffer pH 10.0)

Synthesis Synthetic methods[1–6]

Imaging/Labeling Applications Botulinum neurotoxins (BoNTs);[7] nucleic acids;[8] steroids;[9,10]

Biological/Medical Applications Detecting nucleic acids;[8] detecting/monitoring botulinum neurotoxins (BoNTs);[7] assaying steroids;[9,10] as a substrate for measuring proteinases activity[11]

Industrial Applications Not reported

Safety/Toxicity No data available

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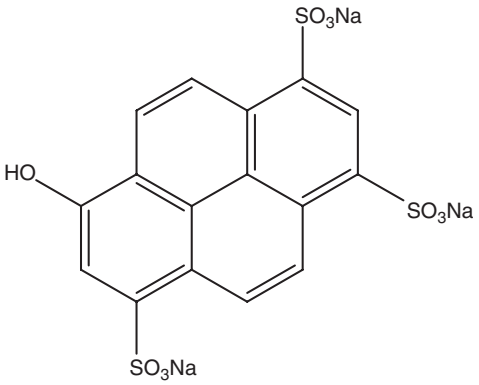
8-HYDROXYPYRENE-1,3,6-TRISULFONIC ACID TRISODIUM SALT (HPTS) (PYRANINE)

CAS Registry Number 6358-69-6

Chemical Structure



CA Index Name 1,3,6-Pyrenetrisulfonic acid, 8-hydroxy-, sodium salt (1:3)

Other Names 1,3,6-Pyrenetrisulfonic acid, 8-hydroxy-, trisodium salt; 11389 Green; 8-Hydroxy-1,3,6-pyrenetrisulfonic acid trisodium salt; C.I. 59040; C.I. Solvent Green 7; D and C Green No. 8; D&C Green 8; D&C Green No. 8; Fluka 56360; Green 204; Green No. 204; HPTS; Japan Green 204; Japan Green No. 204; Keyacid Pyranine 10G; PY; Pyranine; Pyranine 10G; Pyranine 120; Pyranine Concentrated; Pyranine conk; Pyrene 1; Sanolin Pyranine Green; Solvent Green 7; Trisodium 1-hydroxy-3,6,8-pyrenetrisulfonate; Trisodium 8-hydroxypyrene-1,3,6-trisulfonate; Yellow Pyracide G

Merck Index Number 8065

Chemical/Dye Class Pyrene

Molecular Formula $C_{16}H_7Na_3O_{10}S_3$

Molecular Weight 524.37

Physical Form Yellow solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide; slightly soluble in glacial acetic acid

Melting Point >300 °C

pK_a 7.3, temperature: 22 °C

Absorption (λ_{max}) 403 nm (Buffer pH 4.0); 454 nm (Buffer pH 9.0)

Emission (λ_{max}) 511 nm (Buffers pH 4.0, 9.0)

Molar Extinction Coefficient 20,000 cm^{-1} M^{-1} (Buffer pH 4.0); 24,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Bile acids;[2] living cells/tissues;[3–5] chitosan;[6] cornea;[7] cyclen 1;[8] cytochrome c/cytochrome o;[9–11] domes;[12] eye shadows;[13] fungi;[14] ferric/ferrous derivatives of hemoglobin;[15] lipids;[16,40] liposomes;[17–31] proteoliposomes;[32,33] microorganism;[34] mitochondria;[35,36] myoglobin;[37] plant cells;[38,39] prostaglandins;[40] yeast[41–44]

Biological/Medical Applications Antiperspirants;[45] bath preparations;[46–51] cleansing products;[52,53] cosmetics;[54–61] contact lens;[62] hair dyes;[63–75,201] hygiene products/soaps;[76,77] food products;[78] controlled-release system for proteins;[79] drug delivery;[80] in ophthalmology/retinal surgery;[81] sugar sensors (glucose, fructose, lactose, sucrose);[82–90] as a substrate for measuring acetylcholinesterase (AChE) activity,[21] carbonic anhydrase activity,[91] esterases activity,[92,93] β-glucuronidase activity,[94] lipase activity,[95] acidic/alkaline phosphatases activity,[96–98] pyrophosphatase activity,[99] sucrose phosphorylase (SPO) activity,[100] phosphoglucomutase (PGM) activity;[100] treating cancer,[101] infection,[101] immune/autoimmune disease,[101] mastitis,[76] tonsillitis,[76] tuberculosis[102]

Industrial Applications Adhesives;[103,104] agro-chemicals;[61] ammonia sensor;[105] carbon dioxide sensor;[106–115] oxygen sensor;[115,116] anionic surfactants sensor;[117] measuring the size of the organoclay aggregates;[118] detecting cracks/flaws in metallic surfaces,[119] refrigerant leaking;[120] detergents;[121–123] correction fluid;[124] highlighters;[125–127] inks;[127–139,144,145] markers;[140–142] paints;[142,144,145] pencils;[143] toners;[146] chemically amplified resist;[147] color filters;[148] chemiluminescent materials;[149] electrophoretic display (EPD) film materials;[150] electroluminescent displays/materials;[151,152] fuel cell;[153,154] lasers;[155–158] liquid crystal displays;[159] luminescent materials;[160–162] nanoparticles;[163] papers;[164–166] photoresist processes;[167] photonic ionic liquids;[168] soils;[169] solar cell;[170] sol–gel materials/processes/thin films;[171–181] sonophotoluminescence;[182–184] water tracers;[185–194,198] evaluating liquid water flow in wood during drying[195]

Safety/Toxicity Acute intravenous toxicity;[196] cytotoxicity;[197] ecotoxicity;[198,199] phototoxicity;[200] skin toxicity[201]

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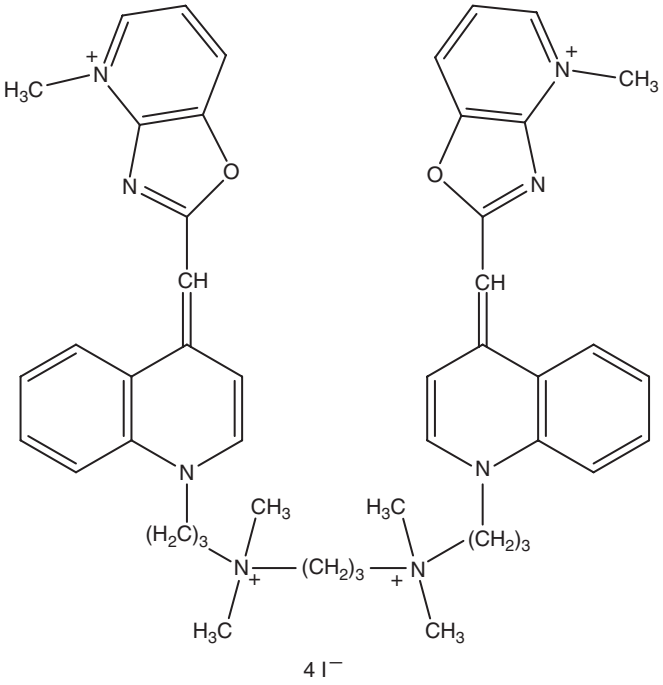
JOJO 1

CAS Registry Number 305801-87-0

Chemical Structure



CA Index Name Oxazolo[4,5-*b*]pyridinium, 2,2′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-quinolinyl-4-ylidenemethylidyne]]bis[4-methyl-, iodide (1 : 4)

Other Names Oxazolo[4,5-*b*]pyridinium, 2,2′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-quinolinyl-4-ylidenemethylidyne]]bis[4-methyl-, tetraiodide; JOJO 1; JOJO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{47}H_{56}I_4N_8O_2$

Molecular Weight 1272.63

Physical Form Yellow-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 529 nm (H_2O/DNA)

Emission (λ_{max}) 545 nm (H_2O/DNA)

Molar Extinction Coefficient 171,400 $cm^{-1}\,M^{-1}$ (H_2O/DNA)

Quantum Yield 0.44 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–7] cells;[7] sperms;[7] hairs[8]

Biological/Medical Applications Detecting nucleic acids,[1–7] cells,[7] oligonucleotides;[2] nucleic acid nanochannel device;[9,10] nucleic acid sequencing;[11,12] as temperature sensor[13,14]

Industrial Applications Not reported

Safety/Toxicity No data available

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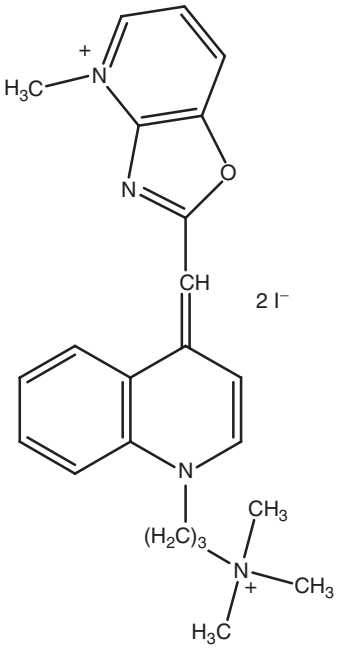
JO-PRO 1

CAS Registry Number 305801-86-9

Chemical Structure



CA Index Name Quinolinium, 4-[(4-methyloxazolo [4,5-*b*]pyridin-2(4*H*)-ylidene)methyl]-1-[3-(trimethylammonio)propyl]-, iodide (1 : 2)

Other Names Quinolinium, 4-[(4-methyloxazolo[4,5-*b*] pyridin-2(4*H*)-ylidene)methyl]-1-[3-(trimethylammonio) propyl]-, diiodide; JO-PRO 1; JO-PRO 1 iodide

Merck Index Numbe Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{23}H_{28}I_2N_4O$

Molecular Weight 630.31

Physical Form Yellow-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 530 nm (H_2O/DNA)

Emission (λ_{max}) 546 nm (H_2O/DNA)

Molar Extinction Coefficient 94,400 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.38 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–9] cells;[9] sperms[9]

Biological/Medical Applications Detecting nucleic acids,[1–9] cells;[9] apoptosis;[2] nucleic acid sequencing;[10] as temperature sensor[11,12]

Industrial Applications Not reported

Safety/Toxicity No data available

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2. Haugland, R. P.; Yue, S. T. Aza-benzazolium-containing cyanine dyes and their use in fluorescent biological stains. PCT Int. Appl. WO 2000066664, 2000.
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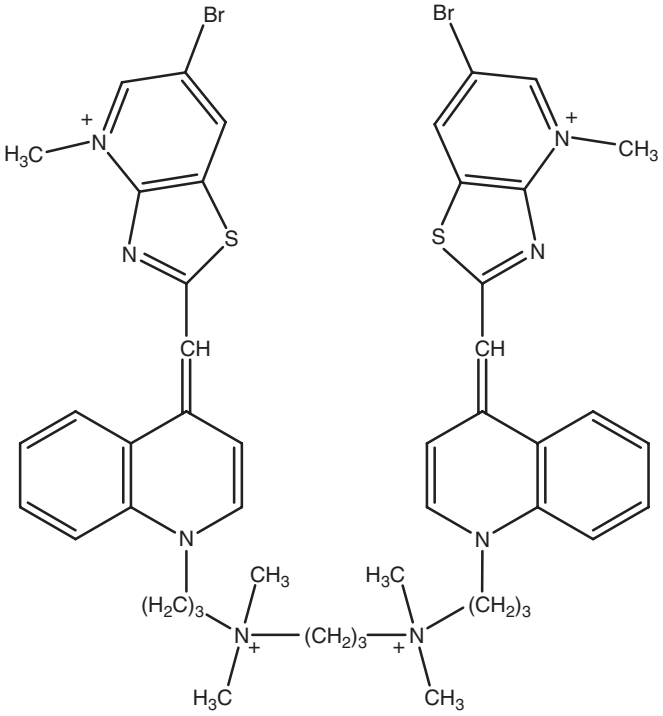
LOLO 1

CAS Registry Number 305802-06-6

Chemical Structure



Physical Form Yellow-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 565 nm (H_2O/DNA)

Emission (λ_{max}) 579 nm (H_2O/DNA)

CA Index Name Thiazolo[4,5-*b*]pyridinium, 2,2′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-quinolinyl-4-ylidenemethylidyne]]bis[6-bromo-4-methyl-, iodide (1 : 4)

Other Names Thiazolo[4,5-*b*]pyridinium, 2,2′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl-1(4*H*)-quinolinyl-4-ylidenemethylidyne]]bis[6-bromo-4-methyl-, tetraiodide; LOLO 1; LOLO iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{47}H_{54}Br_2I_4N_8S_2$

Molecular Weight 1462.54

Molar Extinction Coefficient 108,400 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.40 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–7] cells;[7] sperms;[7] microorganisms;[8] hairs[9]

Biological/Medical Applications Detecting nucleic acids,[1–7] cells,[7] microorganisms;[8] nucleic acid nanochannel device;[10] nucleic acid sequencing;[11,12] as temperature sensor[13,14]

Industrial Applications Not reported

Safety/Toxicity No data available

REFERENCES

1. Sabnis, R. W. *Handbook of Biological Dyes and Stains*; John Wiley & Sons Inc.: Hoboken, **2010**; pp 264–265.
2. Haugland, R. P.; Yue, S. T. Aza-benzazolium-containing cyanine dyes and their use in fluorescent biological stains. PCT Int. Appl. WO 2000066664, 2000.

Handbook of Fluorescent Dyes and Probes, First Edition. R. W. Sabnis.

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3. Exner, M.; Rogers, A. Methods for detecting nucleic acids using multiple signals. U.S. Pat. Appl. Publ. US 2007172836, 2007.
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10. Tegenfeldt, J.; Reisner, W.; Flyvbjerg, H. Method for the mapping of the local AT/GC ratio along DNA. PCT Int. Appl. WO 2010042007, 2010.
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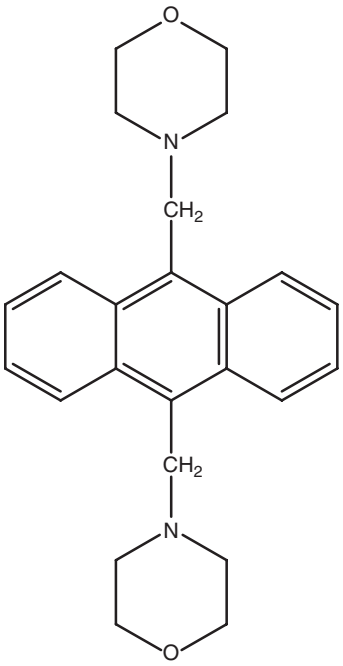
LYSOSENSOR BLUE DND 167

CAS Registry Number 101821-61-8

Chemical Structure



CA Index Name Morpholine, 4,4′-[9,10-anthracenediylbis(methylene)]bis-

Other Names Morpholine, 4,4′-(9,10-anthrylenedimethylene)di-; DND 167; LysoSensor Blue DND 167

Merck Index Number Not listed

Chemical/Dye Class Anthracene

Molecular Formula $C_{24}H_{28}N_2O_2$

Molecular Weight 376.49

Physical Form Yellow plates[2]

Solubility Insoluble in water; soluble in dimethyl sulfoxide

Melting Point 243 °C (decompose);[2] 229–230 °C[3]

Boiling Point (Calcd.) 546.5 ± 45.0 °C, pressure: 760 Torr

pK_a 5.1, temperature: 22 °C

pK_a (Calcd.) 6.97 ± 0.10, most basic, temperature: 25 °C

Absorption (λ_{max}) 373 nm, 394 nm (Buffers pH 3.0, pH 7.0)

Emission (λ_{max}) 425 nm, 401 nm (Buffers pH 3.0, pH 7.0)

Molar Extinction Coefficient 11,000 cm^{-1} M^{-1} (Buffers pH 3.0, pH 7.0)

Quantum Yield 0.80 (Buffer pH 3.0)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Lysosomes;[1,4–8] acidic vesicles[5]

Biological/Medical Applications Analysizing of autophagic and necrotic cell death in *Dictyostelium discoideum*;[6] detecting nucleic acids;[9] measuring/controlling multidrug resistance;[7,8] sensing cholesterol composition of subcellular organelle membranes;[10] as temperature sensor[11,12]

Industrial Applications Not reported

Safety/Toxicity No data available

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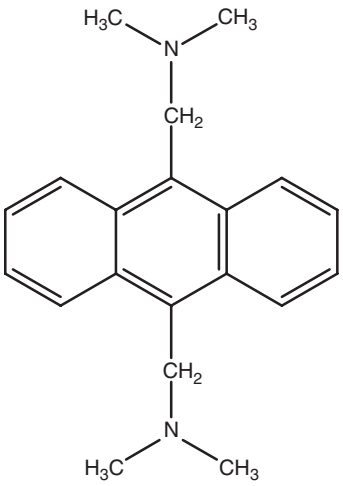
LYSOSENSOR BLUE DND 192

CAS Registry Number 166821-89-2

Chemical Structure



CA Index Name 9,10-Anthracenedimethanamine, N9,N9,N10,N10-tetramethyl-

Other Names 9,10-Anthracenedimethanamine, N,N,N′,N′-tetramethyl-; LysoSensor Blue DND 192; LysoSensor DND 192

Merck Index Number Not listed

Chemical/Dye Class Anthracene

Molecular Formula $C_{20}H_{24}N_2$

Molecular Weight 292.42

Physical Form Yellow crystalline powder[2]

Solubility Insoluble in water; soluble in dimethyl sulfoxide

Melting Point >300 °C (decompose)[2]

Boiling Point (Calcd.) 418.0 ± 25.0 °C, pressure: 760 Torr

pK_a 7.5, temperature: 22 °C

pK_a (Calcd.) 9.11 ± 0.28 most basic, temperature: 25 °C

Absorption (λ_{max}) 374 nm (Buffers pH 5.0, 9.0)

Emission (λ_{max}) 424 nm (Buffers pH 5.0, 9.0)

Molar Extinction Coefficient 11,000 cm^{-1} M^{-1} (Buffers pH 5.0, 9.0)

Quantum Yield 0.88 (Buffer pH 4.0)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Lysosomes;[1,3] acidic vesicles[1,3]

Biological/Medical Applications As temperature sensor;[4,5] for ratiometric pH measurements[6]

Industrial Applications Qualification of cooking oils;[7] quantitative temperature gradient focusing[8]

Safety/Toxicity No data available

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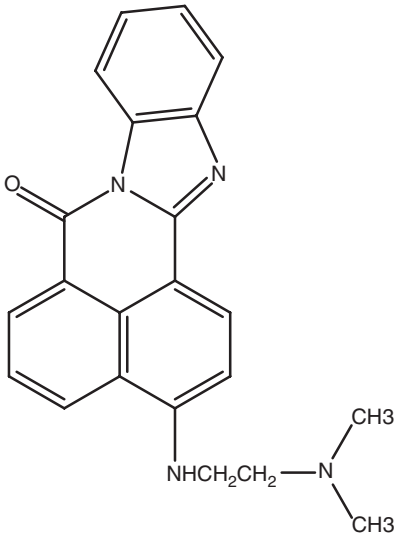
LYSOSENSOR GREEN DND 153

CAS Registry Number 231632-16-9

Chemical Structure



CA Index Name 7H-Benzimidazo[2,1-a]benz[de] isoquinolin-7-one, 3-[[2-(dimethylamino)ethyl]amino]-

Other Names DND 153; LysoSensor Green DND 153

Merck Index Number Not listed

Chemical/Dye Class Heterocycle

Molecular Formula $C_{22}H_{20}N_4O$

Molecular Weight 356.42

Physical Form Orange solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide, methanol

Boiling Point (Calcd.) 660.9 ± 65.0 °C, pressure: 760 Torr

pK_a 7.5, temperature: 22 °C

pK_a (Calcd.) 9.10 ± 0.28, most basic, temperature: 25 °C

Absorption (λ_{max}) 442 nm (Buffers pH 5.0, pH 9.0)

Emission (λ_{max}) 505 nm (Buffers pH 5.0, pH 9.0)

Molar Extinction Coefficient 17,000 cm^{-1} M^{-1} (Buffers pH 5.0, pH 9.0)

Quantum Yield 0.34 (Buffer pH 4.0)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Lysosomes;[1,2] acidic vesicles;[1] living cells;[3] intestinal mucosa[4,5]

Biological/Medical Applications Detecting nucleic acids;[6] examining colitis;[2] test reagent for intestinal mucosa;[4,5] visualizing lysosomes[1]

Industrial Applications Not reported

Safety/Toxicity No data available

REFERENCES

1. Lin, H.; Herman, P.; Kang, J. S.; Lakowicz, J. R. Fluorescence lifetime characterization of novel low-pH probes. *Anal. Biochem.* **2001**, *294*, 118–125.
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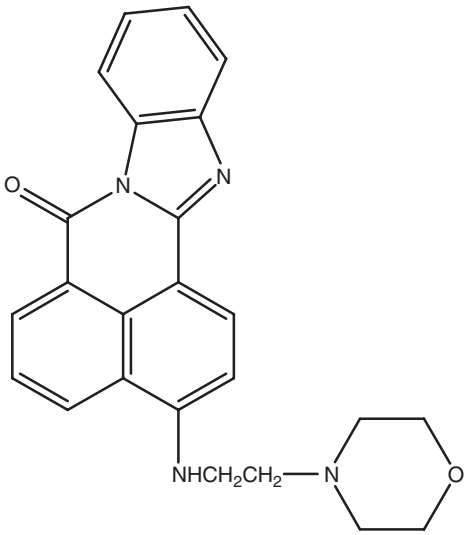
LYSOSENSOR GREEN DND 189

CAS Registry Number 152584-38-8

Chemical Structure



CA Index Name 7H-Benzimidazo[2,1-a]benz[de] isoquinolin-7-one, 3-[[2-(4-morpholinyl)ethyl]amino]-

Other Names DND 189; LysoSensor Green DND 189

Merck Index Number Not listed

Chemical/Dye Class Heterocycle

Molecular Formula $C_{24}H_{22}N_4O_2$

Molecular Weight 398.46

Physical Form Red crystals[2]

Solubility Insoluble in water; soluble in dimethyl sulfoxide

Melting Point 254–258 °C[2]

Boiling Point (Calcd.) 730.4 ± 70.0 °C, pressure: 760 Torr

pK_a 5.2, temperature: 22 °C

pK_a (Calcd.) 6.89 ± 0.10, most basic, temperature: 25 °C

Absorption (λ_{max}) 443 nm (Buffers pH 3.0, 7.0)

Emission (λ_{max}) 505 nm (Buffers pH 3.0, 7.0)

Molar Extinction Coefficient 16,000 cm^{-1} M^{-1} (Buffers pH 3.0, 7.0)

Quantum Yield 0.41 (Buffer pH 3.0); 0.48 (Buffer pH 4.4)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Lysosomes;[1–6] acidic vesicles;[3] amyloid oligomers;[7] endosomes;[5,6] intestinal mucosa[8,9]

Biological/Medical Applications As an amyloid aggregation probe;[7] detecting nucleic acids;[10] examining colitis;[4] test reagent for intestinal mucosa;[8,9] visualizing lysosomes[1–6]

Industrial Applications Not reported

Safety/Toxicity No data available

REFERENCES

1. Sabnis, R. W. *Handbook of Acid–base Indicators*; CRC Press: Boca Raton, **2008**; p 209.
2. de Silva, A. P. Gunaratne, H. Q. N.; Lynch, P. L. M.; Patty, A. J.; Spence, G. L. Luminescence and charge transfer. Part 3. The use of chromophores with ICT (internal charge transfer) excited states in the construction of fluorescent PET (photoinduced electron transfer) pH sensors and related absorption pH sensors with aminoalkyl side chains. *J. Chem. Soc., Perkin Trans. 2* **1993**, 1611–1616.
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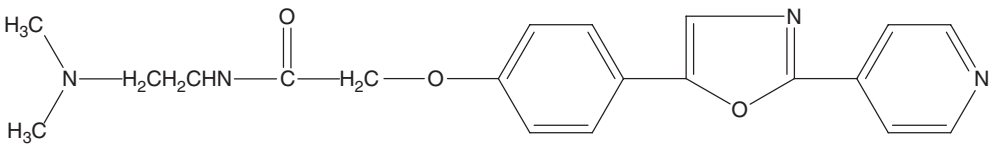
LYSOSENSOR YELLOW/BLUE DND 160 (PDMPO)

CAS Registry Number 231632-18-1

Chemical Structure



CA Index Name Acetamide, N-[2-(dimethylamino) ethyl]-2-[4-[5-(4-pyridinyl)-2-oxazolyl]phenoxy]-

Other Names DND 160; L 7545; Lyso Sensor DND 160; LysoSensor Yellow/Blue DND 160; 2-(4-Pyridyl)-5-{[4-(2-dimethylaminoethylaminocarbamoyl)-methoxy] phenyl}-oxazole; PDMPO

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Oxazole

Molecular Formula $C_{20}H_{22}N_4O_3$

Molecular Weight 366.41

Physical Form Pale yellow solid[2]

Solubility Insoluble in water; soluble in dimethyl sulfoxide, methanol

Melting Point 141–142 °C[2]

pK_a 4.2, temperature: 22 °C

pK_a (Calcd.) 14.25 ± 0.46, most acidic, temperature: 25 °C; 8.36 ± 0.10, most basic, temperature: 25 °C

Absorption (λ_{max}) 384 nm (Buffer pH 3.0); 329 nm (Buffer pH 7.0)

Emission (λ_{max}) 540 nm (Buffer pH 3.0); 440 nm (Buffer pH 7.0)

Molar Extinction Coefficient 21,000 cm^{-1} M^{-1} (Buffer pH 3.0); 23,000 cm^{-1} M^{-1} (Buffer pH 7.0)

Quantum Yield 0.31 (Buffer pH 3.0); 0.34 (Buffer pH 7.7)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Lysosomes;[1–4] acidic vesicles;[4–6] silica/silica deposits[7–12]

Biological/Medical Applications Detecting nucleic acids;[13] biosensor system for liquid analytes;[14] regulating acidity within the lumen and tubulovesicle compartment of gastric parietal cells;[6] studying silica deposition;[7–12] treating age-related macular degeneration;[3] visualizing lysosomes[1–4]

Industrial Applications Recording medium[15,16]

Safety/Toxicity No data available

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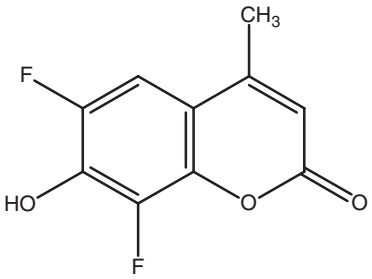
MARINA BLUE (6,8-DIFLUORO-7-HYDROXY-4-METHYLCOUMARIN) (DiFMU)

CAS Registry Number 215868-23-8

Chemical Structure



CA Index Name 2H-1-Benzopyran-2-one, 6,8-difluoro-7-hydroxy-4-methyl-

Other Names 6,8-Difluoro-7-hydroxy-4-methylcoumarin; 6,8-Difluoro-4-methylumbelliferon; DiFMU; Marina Blue

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{10}H_6F_2O_3$

Molecular Weight 212.15

Physical Form Colorless needles;[3] white solid[1]

Solubility Insoluble in water; soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide

Melting Point 154–155 °C[1]

Boiling Point (Calcd.) 332.3 ± 42.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C

pK_a (Calcd.) 5.50 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 358 nm (Buffers pH 10.0, pH 9.0)

Emission (λ_{max}) 455 nm (Buffer pH 10.0); 452 nm (Buffer pH 9.0)

Molar Extinction Coefficient 17,500 cm^{-1} M^{-1} (Buffer pH 10.0); 18,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Quantum Yield 0.89 (Buffer pH 10.0)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Aβ-proteins;[4,5] bacteria;[6] histone deacetylase;[7] nucleic acids;[14–20] peptides;[8] proteins;[9–12] sugar chains[13]

Biological/Medical Applications Amplifying/detecting nucleic acid sequences;[14–18] analyzing peptides,[8] sugar chains;[13] detecting bacteria;[6] detecting/quantifying nucleic acids;[19,20] a substrate for measuring acyl protein thioesterase (APT1) activity,[1,30] α-amylase activity,[21] aryl sulfatases activity,[22] β-galactosidases activity,[3,23,29] guanidinobenzoatase activity,[3] β-lactamase activity,[24] lipase activity,[25] phosphatases activity,[3,26–29] phospholipase LYPLAL1 activity,[30] protein kinases activity,[31] xylanase activity;[32] diagnosing/treating traumatic brain injury;[4] treating amyloidogenic disease;[5] as temperature sensor[33,34]

Industrial Applications Detecting/quantifying/measuring metals (beryllium, chromium, lead)[35]

Safety/Toxicity No data available

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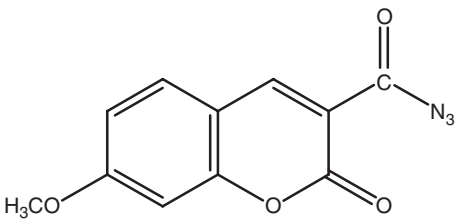
7-METHOXYCOUMARIN-3-CARBONYL AZIDE

CAS Registry Number 97632-67-2

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carbonyl azide, 7-methoxy-2-oxo-

Other Names 7-Methoxycoumarin-3-carbonyl azide

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{11}H_7N_3O_4$

Molecular Weight 245.19

Physical Form Pale yellow needles[1]

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, methanol

Melting Point 170–171 °C[1]

Absorption (λ_{max}) 360 nm (MeOH)

Emission (λ_{max}) 415 nm (MeOH)

Molar Extinction Coefficient 25,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Alcohols;[1,2] biomacromolecules;[3,4] glycerophospholipids;[5] 7α-hydroxycholesterol[6]

Biological/Medical Applications Analyzing molecular species of glycerophospholipids;[5] detecting 7α-hydroxycholesterol in dog plasma;[6] encapsulating/microencapsulating biomacromolecules;[3,4] reagent for alcohols[1,2]

Industrial Applications Poly(propargyl acrylate) (pPA) polymer coatings/fims;[7] poly(propargyl methacrylate) (PPMA) polymer coatings/fims[8]

Safety/Toxicity No data available

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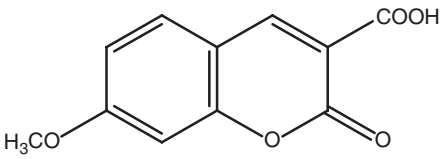
7-METHOXYCOUMARIN-3-CARBOXYLIC ACID

CAS Registry Number 20300-59-8

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-methoxy-2-oxo-

Other Names 3-Carboxy-7-methoxycoumarin; 7-methoxy-2-oxo-2*H*-chromene-3-carboxylic acid; 7-methoxy-2*H*-chromene-3-carboxylic acid; 7-methoxy-3-carboxycoumarin; 7-methoxycoumarin-3-carboxylic acid

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{11}H_8O_5$

Molecular Weight 220.18

Physical Form White crystals;[11] white crystalline solid;[10] white glistening flakes;[36] off-white solid[19,21] or colorless solid; Orange crystals;[17] pale greenish-yellow plates[35]

Solubility Soluble in acetone, acetonitrile, *N,N*-dimethylformamide, dimethyl sulfoxide

Melting Point 231–233 °C;[17] 208–210 °C;[19] 203 °C;[27] 198–199 °C;[33] 197–199 °C;[21] 195 °C;[35,36] 193–195 °C;[3,13] 193–194 °C;[7,14,18] 192–194 °C;[25,34] 192–193 °C;[12,24,26,32] 192 °C;[28] 191.5–192.5 °C;[22] 190–191 °C;[6] 190–195 °C;[10] 178 °C;[2] 176–177 °C;[29,30] 169 °C[11]

Boiling Point (Calcd.) 424.4 ± 45.0 °C, pressure: 760 Torr

pK_a (Calcd.) 1.92 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 336 nm (Buffer pH 9.0)

Emission (λ_{max}) 402 nm (Buffer pH 9.0)

Molar Extinction Coefficient 20,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–36]

Imaging/Labeling Applications Iron chelators;[22] lysine;[23,37] peptides;[38–41] proteins;[42,43] ribonucleopeptide (RNP);[44–48] sulfenic acids;[21,49] thiols[50]

Biological/Medical Applications Assaying thiols;[50] evaluating iron chelators;[22] identifying/mapping sulfenic acid modifications;[21,49] as a substrate for measuring peptidases activity,[51] proteases/proteinases activity;[39–41] as *Mycobacterium bovis* (BCG) inhibitors;[5] human monoamine oxidase inhibitors;[9] *N*-Methyl-D-aspartate receptors (NMDARs) inhibitors;[52] dopamine sensors;[44] viscosity sensors;[53] treating cancer/antitumor activity;[1] treating cognitive deficits or schizophrenia[52]

Industrial Applications For organic light-emitting device applications[54]

Safety/Toxicity No data available

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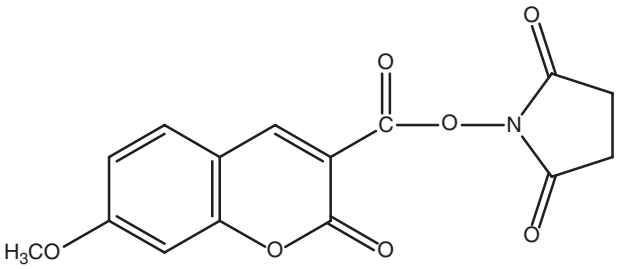
7-METHOXYCOUMARIN-3-CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 150321-92-9

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 7-methoxy-2-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[(7-methoxy-2-oxo-2*H*-1-benzopyran-3-yl)carbonyl]oxy]-; 7-Methoxycoumarin-3-carboxylic acid succinimidyl ester; Succinimidyl 7-methoxy-2*H*-chromene-3-carboxylate; MCCS

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{15}H_{11}NO_7$

Molecular Weight 317.25

Physical Form White solid[1,2]

Solubility Soluble in acetonitrile, *N,N*-dimethylformamide, methanol

Boiling Point (Calcd.) $522.4 \pm 60.0\,^{\circ}C$, pressure: 760 Torr

Absorption (λ_{max}) 358 nm (MeOH)

Emission (λ_{max}) 410 nm (MeOH)

Molar Extinction Coefficient 26,000 $cm^{-1}\,M^{-1}$ (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Amino acids;[2,3] analytes;[4] lysines;[2,3] peptides;[5–8] silane coupling agent;[16] silica particles/beads[16]

Biological/Medical Applications Analyzing/screening peptides;[5–8] monitoring proteolysis;[2] quantifying analytes;[4] as ligands and/or substrates for transport proteins;[9] as a substrate for measuring extracellular matrix metalloprotease (MMP-1) activity,[2] reverse transcriptase (RT) polymerase activity,[10] proteases activity;[11] viscosity sensor;[12–15] colloidal diagnostic devices;[16] useful for synthesizing peptides[16]

Industrial Applications Silica particles/beads[16]

Safety/Toxicity No data available

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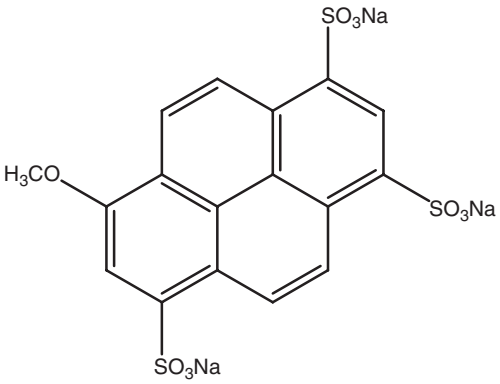
8-METHOXYPYRENE-1,3,6-TRISULFONIC ACID TRISODIUM SALT (MPTS)

CAS Registry Number 82962-86-5

Chemical Structure



CA Index Name 1,3,6-Pyrenetrisulfonic acid, 8-methoxy-, sodium salt (1:3)

Other Names 8-Methoxypyrene-1,3,6-trisulfonic acid, trisodium salt; MPTS; 1,3,6-Pyrenetrisulfonic acid, 8-methoxy-, trisodium salt; Trisodium 8-methoxy-1,3,6-pyrenetrisulfonate

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{17}H_9Na_3O_{10}S_3$

Molecular Weight 538.41

Physical Form Light brown to beige crystals or yellow solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 253–260 °C (decompose); 217 °C (decompose)[1]

Absorption (λ_{max}) 404 nm (Buffer pH 8.0); 404 nm (H_2O)

Emission (λ_{max}) 435 nm (Buffer pH 8.0); 431 nm (H_2O)

Molar Extinction Coefficient 29,000 cm^{-1} M^{-1} (Buffer pH 8.0); 27,000 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Lung tissue;[3] reversed micelles[1,5,6]

Biological/Medical Applications Detecting glucose;[4] measuring lipase activity[2]

Industrial Applications Assessing the interior of the reversed micelles;[1] evaluating critical micelle concentrations (CMC) of non-ionic detergents;[5] investigating decarboxylation reaction of 6-nitro-1,2-benzisoxazole-3-carboxylate in cationic and anionic reversed micelles with particular attention to the microenvironmental effects[6]

Safety/Toxicity No data available

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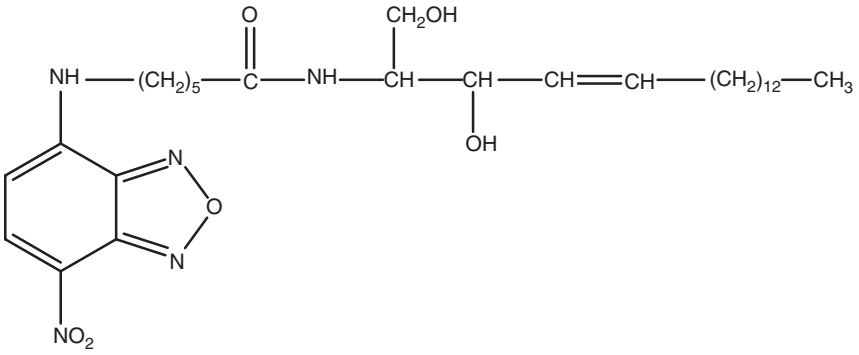
NBD C_6-CERAMIDE

CAS Registry Number 86701-10-2

Chemical Structure



Absorption (λ_{max}) 466 nm (MeOH)

Emission (λ_{max}) 536 nm (MeOH)

CA Index Name Hexanamide, *N*-[2-hydroxy-1-(hydroxymethyl)-3-heptadecen-1-yl]-6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-

Other Names Hexanamide, *N*-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-; Hexanamide, *N*-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-6-[(7-nitro-4-benzofurazanyl)amino]-; 2,1,3-Benzoxadiazole, hexanamide deriv.; 6-((N-(7-Nitrobenz-2-Oxa-1,3-Diazol-4-yl)amino)hexanoyl)Sphingosine; N-(6-[(7-nitrobenzo-2-oxa-1,3-diazo1-4-yl)amino]caproy1)-sphingosine; NBD C_6-ceramide

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Benzoxadiazole

Molecular Formula $C_{30}H_{49}N_5O_6$

Molecular Weight 575.74

Physical Form Orange powder or solid

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

pK_a (Calcd.) 13.81 ± 0.20, most acidic, temperature: 25 °C; −0.77 ± 0.70, most basic, temperature: 25 °C

Molar Extinction Coefficient 22,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Golgi apparatus;[1,2,4–28,31,44–46,48,55] cells;[18,28] erythrocytes;[29,30] fibroblasts;[3] lipids;[31–34] lipopolysaccharides;[35] lipoproteins;[36–40] lysosomes;[3] sphingolipids;[5,6,9,27,41–47] vacuoles[44,48]

Biological/Medical Applications Selective stain for Golgi apparatus;[1,2,4–28,31,44–46,48,55] analyzing/evaluating lipoprotein profile;[36–40] examining the biogenesis of Golgi structure and function;[11] monitoring cholesterol at the Golgi apparatus of living cells;[13] studying sphingolipid transport and metabolism mechanisms;[5,6,9,27,41–47] as a substrate for measuring inositol phosphorylceramide synthase (IPC synthase) activity,[49–53] sphingomyelinase activity,[54] sphingomyelin synthase activity;[55] treating fungal infections[56] visualizing formation and dynamics of vacuoles[44,48]

Industrial Applications Not reported

Safety/Toxicity Fungal toxicity;[56] tumor necrosis[57]

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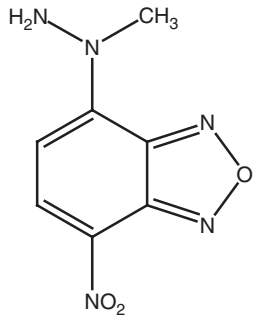
NBD METHYLHYDRAZINE (MNBDH)

CAS Registry Number 214147-22-5

Chemical Structure



CA Index Name 2,1,3-Benzoxadiazole, 4-(1-methylhydrazinyl)-7-nitro-

Other Names 2,1,3-Benzoxadiazole, 4-(1-methylhydrazino)-7-nitro-; *N*-methyl-4-hydrazino-7-nitrobenzofurazan; MNBDH; NBD methylhydrazine; 4-(1-Methylhydrazino)-7-nitrobenzofurazan; 4-(1-methylhydrazino)-7-nitro-benzooxadiazole; 4-(*N*-methylhydrazino)-7-nitro-1,2,3-benzooxadiazole; 4-(*N*-Methylhydrazino)-7-nitro-2,1,3-benzooxadiazole (MNBDH)

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Benzoxadiazole

Molecular Formula $C_7H_7N_5O_3$

Molecular Weight 209.16

Physical Form Brown powder or solid

Solubility Soluble in acetonitrile, chloroform, *N*,*N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 160 °C

Boiling Point (Calcd.) 425.7 ± 55.0 °C, pressure 760 Torr

pKa (Calcd.) 2.07 ± 0.30, most basic, temperature: 25 °C

Absorption (λ_{max}) 487 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 24,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Nitrite ions;[1,4] aldehyde-functionalized DNA[5]

Biological/Medical Applications Detecting nitrite in water,[1,4] creatinine in body fluids,[12] telmisartan;[13] quantifying aldehyde-functionalized (carbonyl compound) DNA;[5] analyzing microperoxidases (microperoxidase substrate);[14] analyzing/detecting peroxidases (peroxidase substrate)[15,16]

Industrial Applications Monitoring/detecting/measuring/quantifying aldehydes and/or ketones (carbonyl compounds) in air/smoke[1,2,6–11]

Safety/Toxicity No data available

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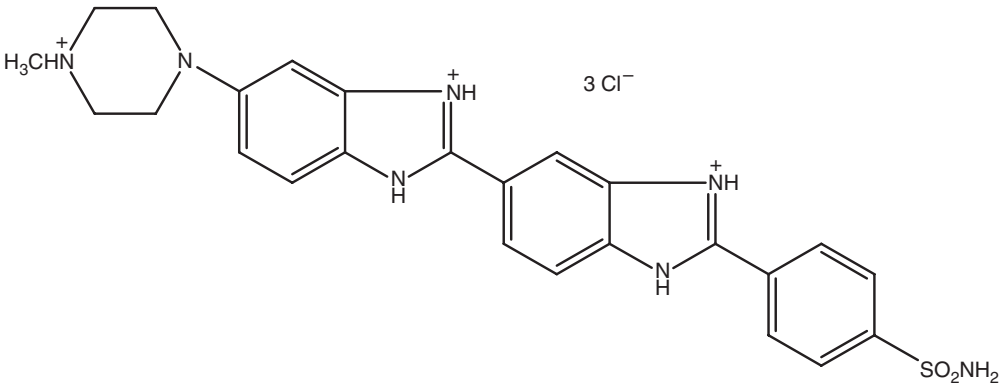
NUCLEAR YELLOW (HOECHST S 769121)

CAS Registry Number 74681-68-8

Chemical Structure



Molecular Weight 596.96

Physical Form Yellow solid or powder

Solubility Soluble in water, dimethyl sulfoxide

Melting Point >300 °C

Absorption (λ_{max}) 355 nm (H_2O/DNA)

CA Index Name Benzenesulfonamide, 4-[5-(4-methyl-1-piperazinyl)[2,5′-bi-1*H*-benzimidazol]-2′-yl]-, hydrochloride (1:3)

Other Names Benzenesulfonamide, 4-[5-(4-methyl-1-piperazinyl)[2,5′-bi-1*H*-benzimidazol]-2′-yl]-, trihydrochloride; 4-[5-(4-Methyl-1-piperazinyl)[2,5′-bi-1*H*-benzimidazol]-2′-yl]-benzenesulfonamide; Hoechst S 769121; Hoechst S 769121 trihydrochloride; Nuclear yellow; NY; 2-(4-sulfamylphenyl)-6-(6-(4-methylpiperazino)-2-benzimidazolyl)benzimidazoletrishydrochloride

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Benzimidazole

Molecular Formula $C_{25}H_{28}Cl_3N_7O_2S$

Emission (λ_{max}) 495 nm (H_2O/DNA)

Molar Extinction Coefficient 36,000 cm^{-1} M^{-1} (H_2O/DNA)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Nucleic acids;[1,4–9] cells;[1,8] nuclei;[1,2,9–15] neurons;[1,3,12–19] chromosomes;[20] lysosomes;[21] sperms[8]

Biological/Medical Applications Detecting/analyzing/quantifying nucleic acid;[1,4–9] cells;[1,8] retrograde neuronal tracer[1,3,12–19]

Industrial Applications Not reported

Safety/Toxicity No data available

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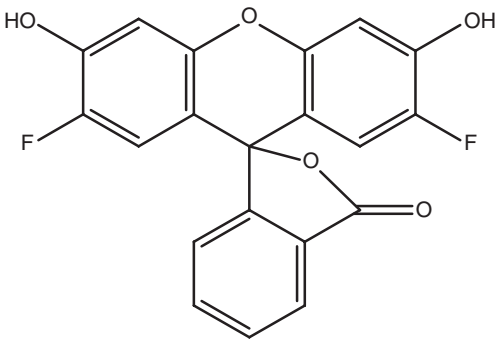
OREGON GREEN 488 (2′,7′-DIFLUOROFLUORESCEIN)

CAS Registry Number 195136-58-4

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-3-one, 2′,7′-difluoro-3′,6′-dihydroxy-

Other Names 2′,7′-Difluorofluorescein; Oregon Green 488

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{20}H_{10}F_2O_5$

Molecular Weight 368.29

Physical Form Orange powder[1–3]

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

Boiling Point (Calcd.) 591.7 ± 50.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C[2,3]

pKa (Calcd.) 8.22 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 490 nm (Buffer pH 9.0)

Emission (λ_{max}) 514 nm (Buffer pH 9.0)

Molar Extinction Coefficient 87,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Quantum Yield 0.97 (Buffer pH 9.0)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Amyloid Aβ peptides;[4] apoplast;[5] bacteria;[6,7] cells;[8] cetuximab;[9] CNA35;[10] cortisol;[11] melatonin;[11] secretory IgA;[11] PAMAM dendrimers;[12] fimbrin;[13] fungi;[14] hair follicles;[15,16] nucleic acids;[17–23] plant cells;[24] proteins[2,3,20,25–30,] TiO_2 nanoparticles;[34] tumors[29]

Biological/Medical Applications Detecting atherosclerosis;[10] detecting/monitoring amyloid Aβ production/accumulation/aggregation/disaggregation;[4] diagnosing Alzheimer's disease;[4] estimating/measuring concentration of cortisol, melatonin, secretory IgA in body fluids;[11] evaluating cetuximab-based imaging probe to target epidermal growth factor receptor (EGFR);[9] examining biodistribution of proteins;[27] investigating/measuring protein-protein and protein-nucleic acid interactions;[20] measuring pH of apoplast at the root surface;[5] visualizing hair follicles;[15,16] as a substrate for measuring β-lactamase activity,[30] phosphatases activity[31,32]

Industrial Applications As geothermal tracers;[33] TiO_2 nanoparticles for light energy conversion[34]

Safety/Toxicity Cytotoxicity;[35] mutagenicity;[35] tissue toxicity[35]

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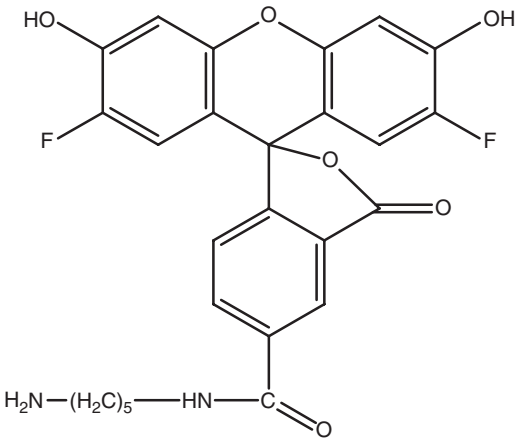
OREGON GREEN 488 CADAVERINE

CAS Registry Number 886210-16-8

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxamide, *N*-(5-aminopentyl)-2′,7′-difluoro-3′,6′-dihydroxy-3-oxo-

Other Names Oregon Green 488 cadaverine; Oregon Green cadaverine

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{26}H_{22}F_2N_2O_6$

Molecular Weight 496.46

Physical Form Orange solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

Boiling Point (Calcd.) 723.7 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 8.19 ± 0.20, most acidic, temperature: 25 °C; 10.52 ± 0.10, most basic, temperature: 25 °C

Absorption (λ_{max}) 494 nm (Buffer pH 9.0)

Emission (λ_{max}) 521 nm (Buffer pH 9.0)

Molar Extinction Coefficient 75,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Autophagosomes;[2] dextrin;[3] N-(2-hydroxypropyl)-methacrylamide (HPMA) copolymers;[3,4] p(HPMA)-b-p(LLA) copolymers;[5] p(HPMA)-co-p(LMA) copolymers;[6] polyethylene glycol (PEG);[3] poly(β-amino ester);[7] diamond nanoparticles;[8] nanohydrogel particles;[9] thymosin b4;[10] vinyl polymers[11]

Biological/Medical Applications Defining polymer localization to late endocytic intracellular compartments;[3] detecting/measuring amount of autophagic activity;[2] *in vitro* evaluating N-(2-hydroxypropyl)-methacrylamide (HPMA) folate conjugates;[4] exhibiting tendency to interact with model cell membranes;[6] high-throughput drug screening;[2] identifying autophagosomes;[2] investigating cationic polymers in promoting surface-mediated gene delivery;[7] studying cellular uptake in human cervix adenocarcinoma (HeLa) cells;[5] nanodiamond as drug delivery vehicles;[8] as a platform for proper siRNA delivery systems;[9] tracing hydrogels during complexation with siRNA or cell uptake experiments[9]

Industrial Applications Diamond nanoparticles;[8] dye-functionalized polymer[11]

Safety/Toxicity No data available

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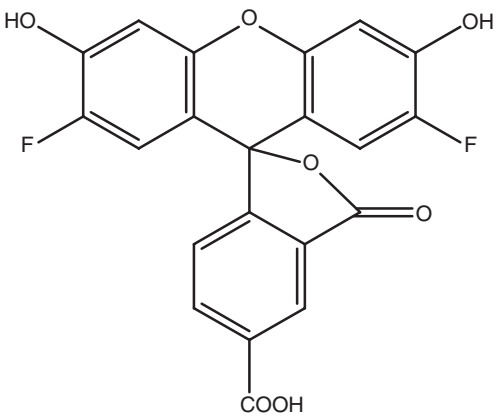
OREGON GREEN 488 CARBOXYLIC ACID

CAS Registry Number 195136-52-8

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 2′,7′-difluoro-3′,6′-dihydroxy-3-oxo-

Other Names Oregon Green 488 carboxylic acid

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{10}F_2O_7$

Molecular Weight 412.30

Physical Form Orange powder[2–4]

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

Boiling Point (Calcd.) 693.9 ± 55.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C

pK_a (Calcd.) 3.71 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 478 nm (Buffer pH 3.0); 492 nm (Buffer pH 9.0)

Emission (λ_{max}) 518 nm (Buffers pH 3.0, 9.0)

Molar Extinction Coefficient 27,000 cm^{-1} M^{-1} (Buffer pH 3.0); 85,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Quantum Yield 0.92 (Buffer pH 9.0)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Actin analogs;[5] liposomes;[1–4] RNA polymerase (RNAP);[6] vasotocin (Arginine8-vasotocin (AVT))[7]

Biological/Medical Applications Analysizing single cells;[8] detecting intracellular analytes,[9] undetectable analytes;[10] as marker for Arginine8-vasotocin (AVT) target neurons;[7] measuring phagosomal pH;[11] monitoring melting of duplex DNA;[6] temperature gradient focusing;[12,13] studying actin dynamics in plant cells[5]

Industrial Applications Silica nanoparticles;[14] temperature gradient focusing (TGF) in a PDMS/glass hybrid microfluidic chip[15]

Safety/Toxicity No data available

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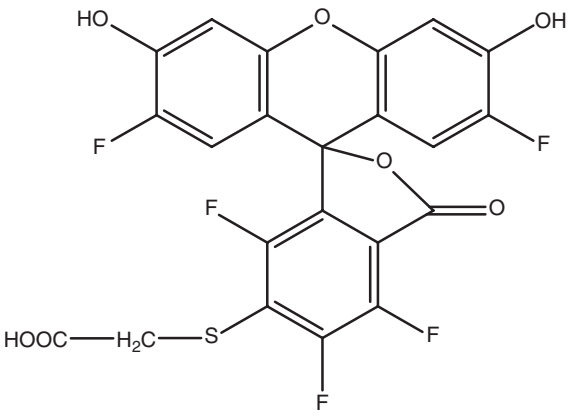
OREGON GREEN 514 CARBOXYLIC ACID

CAS Registry Number 198139-49-0

Chemical Structure



CA Index Name Acetic acid, 2-[(2′,4,5,7,7′-pentafluoro-3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-6-yl)thio]-

Other Names Acetic acid, [(2′,4,5,7,7′-pentafluoro-3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-6-yl)thio]-; Oregon Green 514 carboxylic acid 6-isomer

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{22}H_9F_5O_7S$

Molecular Weight 512.36

Physical Form Orange solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

Boiling Point (Calcd.) 703.2 ± 60.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C

pK_a (Calcd.) 3.01 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 489 nm (Buffer pH 3.0); 506 nm (Buffer pH 9.0)

Emission (λ_{max}) 526 nm (Buffers pH 3.0, 9.0)

Molar Extinction Coefficient 26,000 cm^{-1} M^{-1} (Buffer pH 3.0); 86,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Beads;[4,5] cortisol;[6] melatonin;[6] secretory IgA;[6] monocytes;[7] nucleic acids;[8–10] peptides;[11–14] polynucleotides;[15] proteins[1–3,10,16,17,]

Biological/Medical Applications Analyzing protein distribution in hydrogel beads;[16] estimating/measuring concentration of cortisol, melatonin, secretory IgA in body fluids;[6] identifying beads;[4,5] investigating/measuring protein-protein and protein-nucleic acid interactions;[10] monitoring pH changes in acidic environments;[19] tracing pH in different cellular compartments;[19] treating/diagnosing disease states mediated by monocytes;[7] treating apoptosis related diseases[18]

Industrial Applications As geothermal tracers;[20] sol–gel thin films;[21–23] ultrathin liquid films[24]

Safety/Toxicity No data available

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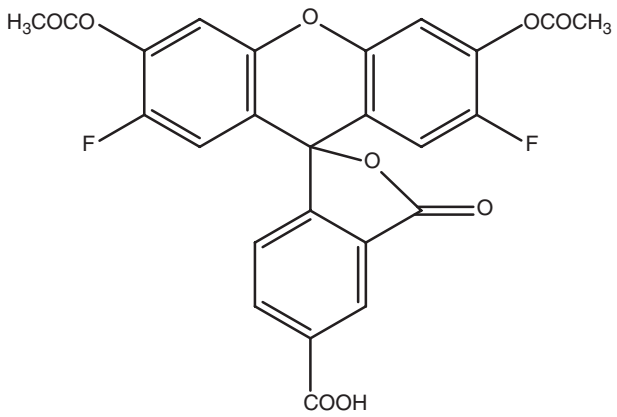
OREGON GREEN 488 CARBOXYLIC ACID DIACETATE

CAS Registry Number 195136-74-4

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 3′,6′-bis(acetyloxy)-2′,7′-difluoro-3-oxo-

Other Names Oregon Green 488 carboxylic acid diacetate

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{14}F_2O_9$

Molecular Weight 496.37

Physical Form Colorless crystals;[2] Off-white solid[3,4]

Solubility Insoluble in water; soluble in dimethyl sulfoxide, methanol

Boiling Point (Calcd.) $691.5 \pm 55.0\,^{\circ}C$, pressure: 760 Torr

pK_a (Calcd.) 3.69 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 298 nm (MeOH); < 300 nm (Buffer pH 3.0)

Emission (λ_{max}) None

Molar Extinction Coefficient 8,000 $cm^{-1}\,M^{-1}$ (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Sodium ions[5]

Biological/Medical Applications Analyzing single cells;[6–9] detecting electrical lysis of cells;[10] locating anion transport mechanism in fungi (*Pisolithus tinctorius*);[11] measuring gap junction mediated diffusion[12]

Industrial Applications Not reported

Safety/Toxicity No data available

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2. Sun, W.; Gee, K. R.; Klaubert, D. H.; Haugland, R. P. Synthesis of fluorinated fluoresceins. *J. Org. Chem.* **1997**, *62*, 6469–6475.
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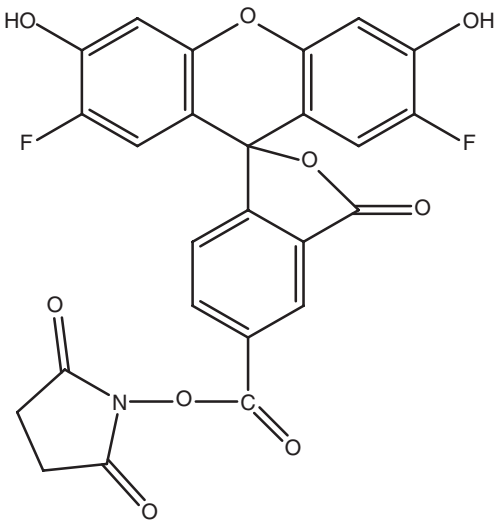
OREGON GREEN 488 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 198139-51-4

Chemical Structure



CA Index Name Spiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthene]-5-carboxylic acid, 2′,7′-difluoro-3′,6′-dihydroxy-3-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[(2′,7′-difluoro-3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-5-yl)carbonyl]oxy]-; Oregon Green 488 NHS ester; Oregon Green 488 carboxylic acid succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{13}F_2NO_9$

Molecular Weight 509.37

Physical Form Yellow/orange solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

Boiling Point (Calcd.) 752.9 ± 70.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C

pK_a (Calcd.) 8.17 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 480 nm (Buffer pH 3.0); 495 nm (Buffer pH 9.0)

Emission (λ_{max}) 521 nm (Buffers pH 3.0, 9.0)

Molar Extinction Coefficient 24,000 cm^{-1} M^{-1} (Buffer pH 3.0); 76,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Cells;[4] cellulose nanocrystals;[3] microorganisms;[4,5] microspheres;[1,2] nucleic acids;[6,7] proteins;[1,2,8–21] small molecules[22]

Biological/Medical Applications Analyzing tag-fused G-protein coupled receptor (GPCR);[10] detecting cells,[4] microorganisms;[4,5] detecting/isolating/purifying proteins;[1,2,8–21] detecting/measuring nitric oxide;[20,21] detecting/monitoring protein-protein interactions in real time;[15] measuring farnesyltransferase activity;[17] visualizing formation/orientation of collagen fibers in tissue[14]

Industrial Applications Not reported

Safety/Toxicity No data available

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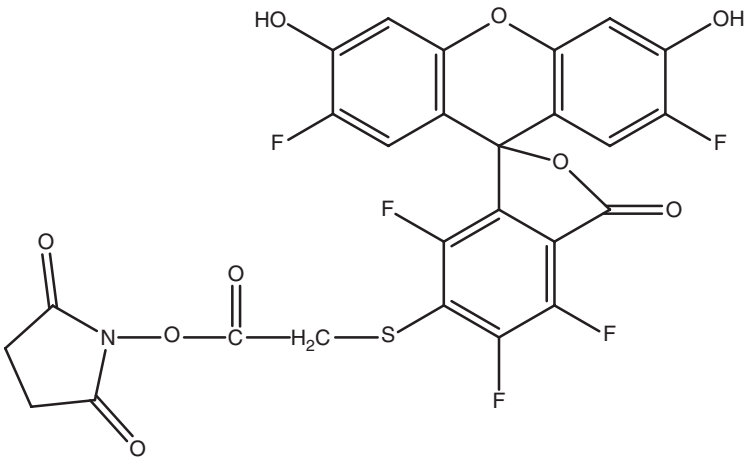
OREGON GREEN 514 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 198139-53-6

Chemical Structure



CA Index Name Acetic acid, 2-[(2′,4,5,7,7′-pentafluoro-3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-6-yl)thio]-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[[(2′,4,5,7,7′-pentafluoro-3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-6-yl)thio]acetyl]oxy]-; Oregon Green 514; Oregon Green 514 carboxylic acid succinimidyl ester; Oregon Green 514 succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{26}H_{12}F_5NO_9S$

Molecular Weight 609.43

Physical Form Yellow solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

Boiling Point (Calcd.) 741.4 ± 70.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C

pK_a (Calcd.) 8.07 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 506 nm (Buffer pH 9.0)

Emission (λ_{max}) 526 nm (Buffers 9.0)

Molar Extinction Coefficient 85,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Androgens;[3] bacteria;[4,5] beads;[6,7] α-bungarotoxin;[1,2] cobalamin;[8] microspheres;[1,2] microorganisms;[9] monocytes;[10] nucleic acids;[11–15] peptides;[16,17] proteins;[1,2,5,13,18–23] tumors[13]

Biological/Medical Applications Detecting/measuring nitric oxide;[23] detecting/diagnosing human immunodeficiency virus (HIV) infection;[19] detecting/identifying nucleic acids;[11–15] diagnosing/treating diseases associated with androgens;[3] identifying beads;[6,7] *in vitro* and *in vivo* imaging of transcobalamin receptors on cancer cells;[8] investigating/measuring protein-protein and protein-nucleic acid interactions;[15] treating/diagnosing disease states mediated by monocytes;[10] treating/preventing cancers of central nervous system;[13] monolayer-functionalized microfluidics devices;[24] as temperature sensor[25,26]

Industrial Applications Not reported

Safety/Toxicity No data available

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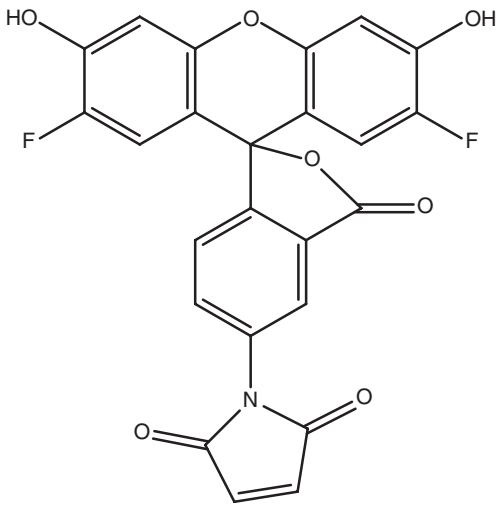
OREGON GREEN 488 MALEIMIDE

CAS Registry Number 328085-55-8

Chemical Structure



CA Index Name 1*H*-Pyrrole-2,5-dione, 1-(2′,7′-difluoro-3′,6′-dihydroxy-3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]-5-yl)-

Other Names Oregon Green 488 maleimide

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{24}H_{11}F_2NO_7$

Molecular Weight 463.35

Physical Form Orange/yellow solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

Boiling Point (Calcd.) 740.5 ± 60.0 °C, pressure: 760 Torr

pK_a 4.7, temperature: 22 °C

pK_a (Calcd.) 8.17 ± 0.20, most acidic, temperature: 25 °C; −2.30 ± 0.20 most basic, temperature: 25 °C

Absorption (λ_{max}) 491 nm (Buffer pH 9.0)

Emission (λ_{max}) 515 nm (Buffer pH 9.0)

Molar Extinction Coefficient 81,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Actin filaments;[2] cathepsin D;[3] diamond nanoparticles;[4] metal ions (Zn(II), Cu(II), Co(II), Ni(II), Cd(II));[5] proteins;[6–21] titin molecules;[2] TonB N-terminus;[22] tumors[23]

Biological/Medical Applications Analyzing/monitoring proteins translocation;[20] detecting localized cathepsin D activity *in vivo*;[3] detecting/monitoring protein-protein interactions in real time;[15] imaging angiogenesis;[17] measuring protein expression;[18] monitoring collagen formation in live tissue cultures;[14] probing protein conformations;[10] providing affinity purification;[18] studying intranuclear protein,[11] ribonucleoprotein particle mobility,[11] protein folding at the single molecule level;[21] visualizing proteins;[18] photoluminescent sensors for detecting/quantitating metal ions in an aqueous sample;[5] viral nanoparticles (VNPs) for biomedical applications;[6,23] Western blot identification[18]

Industrial Applications Diamond nanoparticles[4]

Safety/Toxicity No data available

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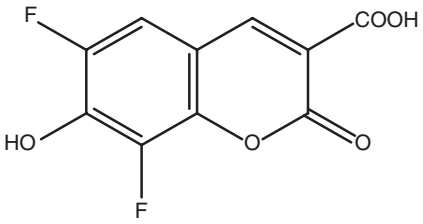
PACIFIC BLUE (6,8-DIFLUORO-7-HYDROXYCOUMARIN-3-CARBOXYLIC ACID)

CAS Registry Number 215868-31-8

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 6,8-difluoro-7-hydroxy-2-oxo-

Other Names 3-Carboxy-6,8-difluoro-7-hydroxycoumarin; 6,8-Difluoro-7-hydroxycoumarin-3-carboxylic acid; Pacific Blue

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{10}H_4F_2O_5$

Molecular Weight 242.13

Physical Form Green powder[2]

Solubility Soluble in ethyl acetate

Boiling Point (Calcd.) 422.0 ± 45.0 °C, pressure: 760 Torr

pK_a 3.7, temperature: 22 °C

pK_a (Calcd.) 1.40 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 400 nm (Buffers pH 10.0)

Emission (λ_{max}) 447 nm (Buffer pH 10.0)

Molar Extinction Coefficient 29500 cm^{-1} M^{-1} (Buffer pH 10.0)

Quantum Yield 0.75 (Buffer pH 10.0)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Antibodies;[3,4] bacteria;[5] chromosomes;[6,7] histone deacetylase;[8] Hodgkin and Reed Sternberg (HRS) cells;[9] microorganisms;[10,11] nucleotides/nucleic acids;[12–19] peptides/proteins;[20–22] silver particles;[23] T lymphocyte antigens[24]

Biological/Medical Applications Analyzing JAK2 gene mutation;[25] analyzing/identifying peptides/proteins;[20–22] detecting chromosomal aberration;[6,7] diagnosing classical Hodgkin lymphoma (CHL) in lymph nodes;[9] identifying/characterizing microorganisms;[10,11] treating human immunodeficiency virus (HIV) infection,[4] ocular diseases;[26] as temperature sensors[27,28]

Industrial Applications Automotive paints[29]

Safety/Toxicity No data available

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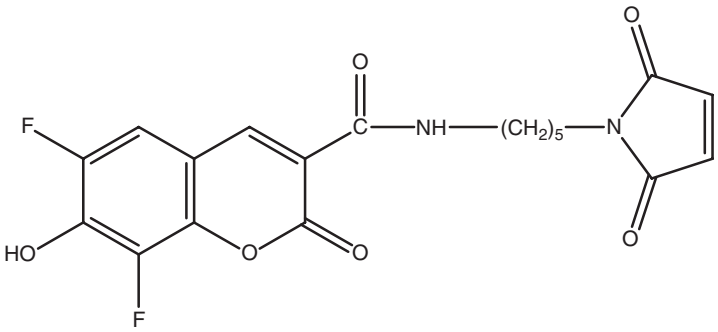
PACIFIC BLUE C_5-MALEIMIDE

CAS Registry Number 934216-71-4

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxamide, *N*-[5-(2,5-dihydro-2,5-dioxo-1*H*-pyrrol-1-yl)pentyl]-6,8-difluoro-7-hydroxy-2-oxo-

Other Names Pacific Blue C_5-Maleimide; Pacific Blue maleimide

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{19}H_{16}F_2N_2O_6$

Molecular Weight 406.34

Physical Form Off-white solid

Solubility Soluble in dimethyl sulfoxide

Boiling Point (Calcd.) 681.4 ± 55.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.99 ± 0.20, most acidic, temperature: 25 °C; −1.54 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 402 nm (Buffer pH 9.0)

Emission (λ_{max}) 451 nm (Buffer pH 9.0)

Molar Extinction Coefficient 40,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Quantum Yield 0.78 (Buffer pH 7.2)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amino acid;[2] cardiac troponin I (cTnI);[3,4] MHC tetramers;[5] pathogen;[6] proteins;[3,4] thiols[7]

Biological/Medical Applications Analyzing/detecting of thiols;[7] detecting pathogen;[6] labeling amino acids;[2] producing MHC tetramers;[5]

Industrial Applications Not reported

Safety/Toxicity No data available

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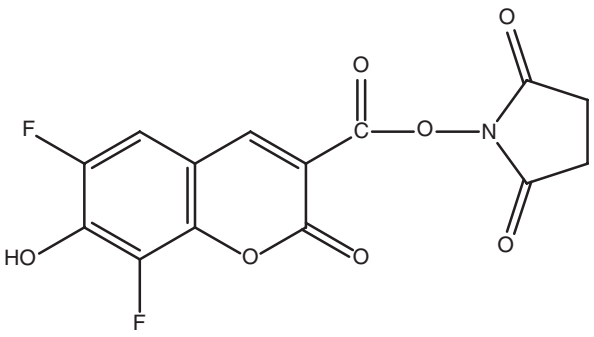
PACIFIC BLUE SUCCINIMIDYL ESTER

CAS Registry Number 215868-33-0

Chemical Structure



CA Index Name 2*H*-1-Benzopyran-3-carboxylic acid, 6,8-difluoro-7-hydroxy-2-oxo-, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[[(6,8-difluoro-7-hydroxy-2-oxo-2*H*-1-benzopyran-3-yl)carbonyl]oxy]-; Pacific Blue succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Coumarin

Molecular Formula $C_{14}H_7F_2NO_7$

Molecular Weight 339.20

Physical Form Greenish powder[1] or yellow solid

Solubility Soluble in acetonitrile, *N,N*-dimethylformamide, ethyl acetate

Boiling Point (Calcd.) 518.9 ± 60.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.60 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 416 nm (Buffer pH 9.0)

Emission (λ_{max}) 451 nm (Buffer pH 9.0)

Molar Extinction Coefficient 46,000 cm^{-1} M^{-1} (Buffer pH 9.0)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Amines/amino acids;[2–4] cells;[5,6] mercury;[7] nucleic acids;[4] pancreatic β-cells;[8] proteins[9–12]

Biological/Medical Applications Analyzing cells;[5,6,8] analyzing/detecting amines/amino acids;[2–4] fluorescent cell barcoding;[6] imaging/labeling proteins;[9–12] measuring/quantifying mercury concentration in a sample[7]

Industrial Applications Not reported

Safety/Toxicity No data available

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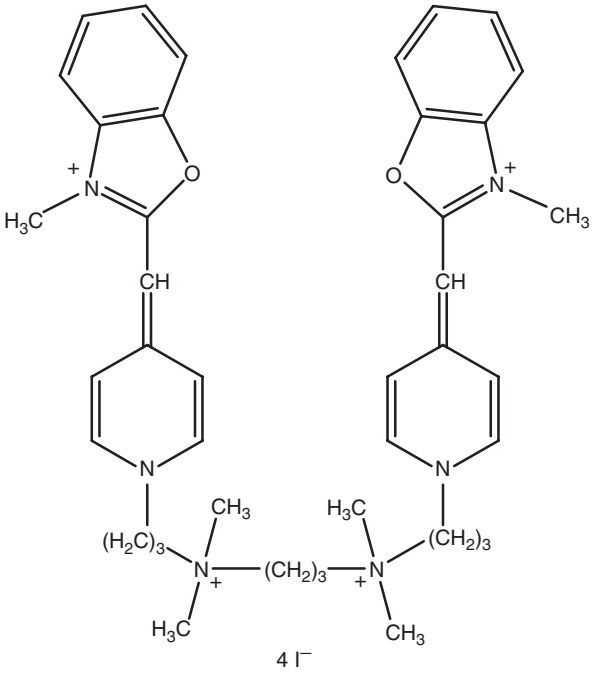
POPO 1

CAS Registry Number 169454-15-3

Chemical Structure



CA Index Name Benzoxazolium, 2,2′-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidenemethylidyne]]bis[3-methyl-, iodide (1 : 4)

Other Names Benzoxazolium, 2,2′-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidenemethylidyne]]bis[3-methyl-, tetraiodide; POPO 1; POPO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{41}H_{54}I_4N_6O_2$

Molecular Weight 1170.53

Physical Form Yellow-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 434 nm (H_2O/DNA)

Emission (λ_{max}) 456 nm (H_2O/DNA)

Molar Extinction Coefficient 92,400 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.60 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–12] cells;[2,11,12] bacteria;[12] chromosome spreads;[2] nuclei;[13,14] megakaryocytes;[15] microorganisms;[16–18] sperms;[11,19] hairs[20]

Biological/Medical Applications Detecting nucleic acids,[1–12] cells,[2,11,12] JAK2 gene mutation;[21] classifying/counting megakaryocytes;[15] counting erythroblasts;[13,14] sperms;[11,19] detecting/measuring microorganisms;[16–18] nucleic acid hybridization;[22] nucleic acids nanochannel device;[23] nanosensor platforms for diagnostic applications;[24] as temperature sensor[25,26]

Industrial Applications Not reported

Safety/Toxicity No data available

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purple oxazole dimer POPO-1. *J. Biomed. Opt.* **1997**, *2*, 125–130.

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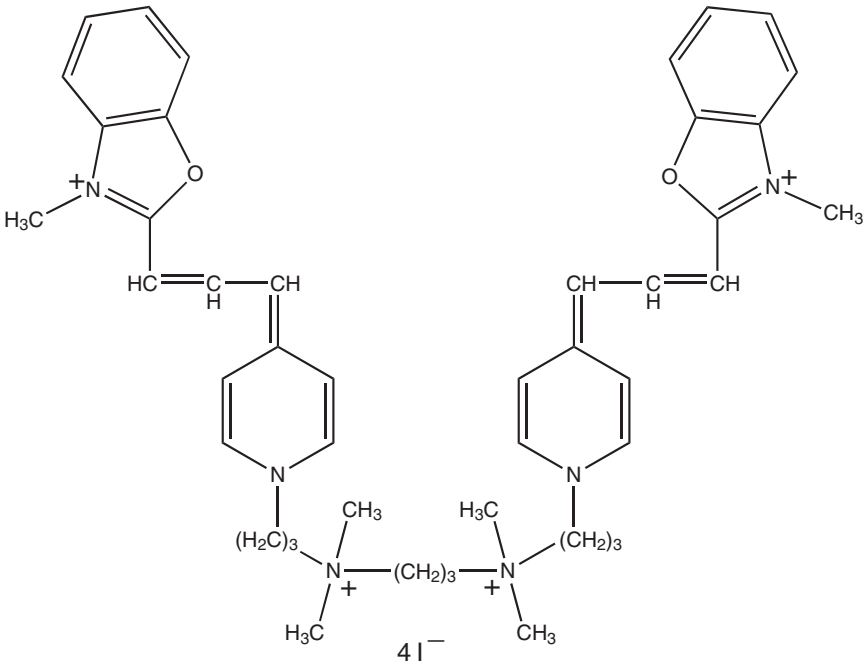
POPO 3

CAS Registry Number 154757-99-0

Chemical Structure



CA Index Name Benzoxazolium, 2,2′-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidene-1-propen-1-yl-3-ylidene]]bis[3-methyl-, iodide (1 : 4)

Other Names Benzoxazolium, 2,2′-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl-1(4*H*)-pyridinyl-4-ylidene-1-propen-1-yl-3-ylidene]]bis[3-methyl-, tetraiodide; POPO 3; POPO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{45}H_{58}I_4N_6O_2$

Molecular Weight 1222.61

Physical Form Yellow-brown powder

Solubility Soluble in *N,N*-dimethylformamide

Absorption (λ_{max}) 534 nm (H_2O/DNA)

Emission (λ_{max}) 570 nm (H_2O/DNA)

Molar Extinction Coefficient 146,400 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.46 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–12] cells;[2,10–12] bacteria;[10] chromosome spreads;[2] nuclei;[13,14] megakaryocyte;[15] microorganisms;[16–18] reticulocytes;[11,19] sperms[12,20]

Biological/Medical Applications Detecting nucleic acids,[1–12] cells,[2,10–12] microorganisms,[16–18] IDH1/IDH2 mutations,[21] JAK2 gene mutation,[22] PIK3CA mutation,[23] B-type Raf Kinase (BRAF) mutation,[24] classifying/counting megakaryocytes;[15] counting erythroblasts,[13,14] reticulocytes,[11,19] sperms;[12,20] quantifying nucleic acids;[9] nucleic acid amplification;[25] nucleic acid hybridization;[26] nucleic acid nanochannel device;[27] as temperature sensor[28,29]

Industrial Applications Photonic fabric display[30]

Safety/Toxicity No data available

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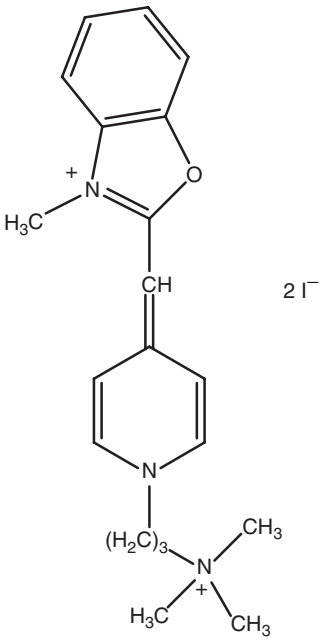
PO-PRO 1

CAS Registry Number 157199-56-9

Chemical Structure



CA Index Name Benzoxazolium, 3-methyl-2-[[1-[3-(trimethylammonio)-propyl]-4(1*H*)-pyridinylidene] methyl]-, iodide (1:2)

Other Names Benzoxazolium, 3-methyl-2-[[1-[3-(trimethylammonio)-propyl]-4(1*H*)-pyridinylidene] methyl]-, diiodide; PO-PRO 1; PO-PRO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{20}H_{27}I_2N_3O$

Molecular Weight 579.26

Physical Form Yellow-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 435 nm (H_2O/DNA)

Emission (λ_{max}) 455 nm (H_2O/DNA)

Molar Extinction Coefficient 50,100 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.39 (H_2O/DNA)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Nucleic acids;[1–10] cells;[1–3,10,11] bacteria;[3] microorganisms;[12,13] proteins;[14,15] sperms[10]

Biological/Medical Applications Detecting nucleic acids,[1–10] cells;[1–3,10,11] counting/detecting microorganisms;[12,13] nucleic acids amplification;[9] nucleic acid hybridization;[16] nucleic acid sequencing;[17] as temperature sensor[18,19]

Industrial Applications Not reported

Safety/Toxicity No data available

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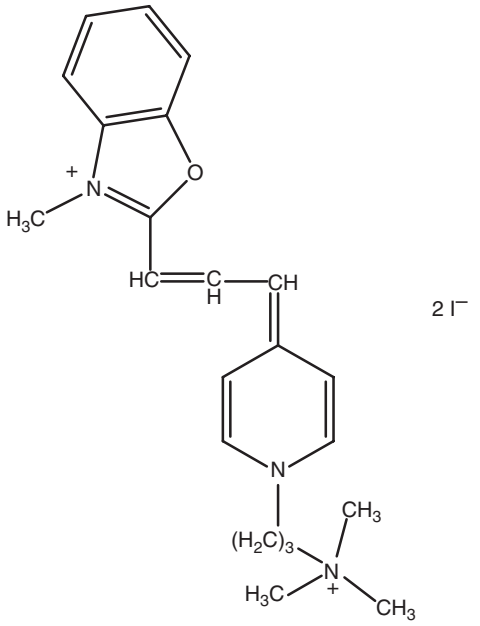
PO-PRO 3

CAS Registry Number 161016-55-3

Chemical Structure



CA Index Name Benzoxazolium, 3-methyl-2-[3-[1-[3-(trimethylammonio)-propyl]-4(1*H*)-pyridinylidene]-1-propen-1-yl]-, iodide (1 : 2)

Other Names Benzoxazolium, 3-methyl-2-[3-[1-[3-(trimethylammonio)-propyl]-4(1*H*)-pyridinylidene]-1-propenyl]-, diiodide; PO-PRO 3; PO-PRO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{22}H_{29}I_2N_3O$

Molecular Weight 605.30

Physical Form Yellow-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 539 nm (H_2O/DNA)

Emission (λ_{max}) 567 nm (H_2O/DNA)

Molar Extinction Coefficient 87,900 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.57 (H_2O/DNA)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Nucleic acids;[1–11] cells;[2,3,10,11] bacteria;[3] reticulocytes;[11,12] sperms;[10] nuclei;[13] cytoplasm[13]

Biological/Medical Applications Detecting nucleic acids,[1–11] cells;[2,3,10,11] counting reticulocytes;[11,12] nucleic acid amplification;[8] nucleic acid hybridization;[14] as temperature sensor[15,16]

Industrial Applications Not reported

Safety/Toxicity No data available

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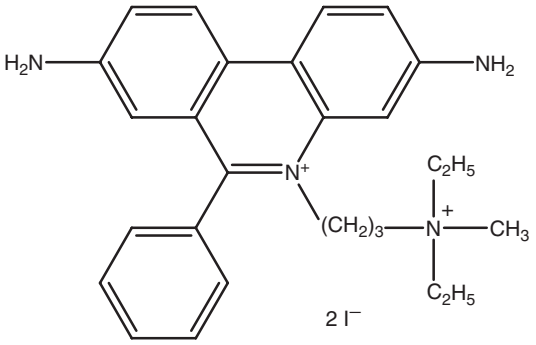
16. Bousseksou, A.; Salmon, L.; Molnar, G.; Cobo, S. Heat-sensitive spin-transition materials doped with one or more fluorescent agents for use as temperature sensor. PCT Int. Appl. WO 2011058277, 2011.

PROPIDIUM IODIDE (PI)

CAS Registry Number 25535-16-4

Chemical Structure



CA Index Name Phenanthridinium, 3,8-diamino-5-[3-(diethylmethylammonio)propyl]-6-phenyl-, iodide (1:2)

Other Names 3,8-Diamino-5-(3-diethylaminopropyl)-6-phenylphenanthridinium iodide methiodide; Phenanthridinium, 3,8-diamino-5-[3-(diethylmethylammonio)propyl]-6-phenyl-, diiodide; Ammonium, [3-(3,8-diamino-6-phenyl-5-phenanthridinio)-propyl]diethylmethyl-, diiodide; 3,8-Diamino-5-(diethylmethylaminopropyl)-6-phenyl-phenanthridinium diiodide; Propidium diiodide; Propidium iodide; PI

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Phenanthridine

Molecular Formula $C_{27}H_{34}I_2N_4$

Molecular Weight 668.40

Physical Form Red powder or solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 220–225 °C (decompose)

Absorption (λ_{max}) 535 nm (H_2O/DNA); 493 nm (H_2O)

Emission (λ_{max}) 617 nm (H_2O/DNA); 636 nm (H_2O)

Molar Extinction Coefficient 5400 cm^{-1} M^{-1} (H_2O/DNA); 5900 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–27] acetylcholinesterase;[28,29] bacteria;[30–34] cells;[35–44] chromosomes;[45,46] fungi;[47,48] liposomes;[49] leukocytes;[50,51] megakaryocytes;[52] microorganisms;[53–63] neurons;[64] nuclei;[65–68] parasites;[69–71] protozoa;[72] sperms;[73–79] stem cells;[80,81] yeasts;[82–85]

Biological/Medical Applications Analyzing/counting cells;[35–44] detecting nucleic acids;[1–27] apoptosis assays;[86–102] cytotoxicity assays;[103–107] measuring/monitoring microorganisms;[53–63] monitoring atmospheric/indoor bioaerosols;[108,109] as temperature sensor;[110,111] treating ischemic diseases,[112] viral diseases[113]

Industrial Applications Electroluminescent displays;[114] photoresists[115,116]

Safety/Toxicity Cytotoxicity;[117,118] embryotoxicity;[119] mutagenicity;[120] neurotoxicity;[121,122] phototoxicity;[123] reproductive toxicity[124]

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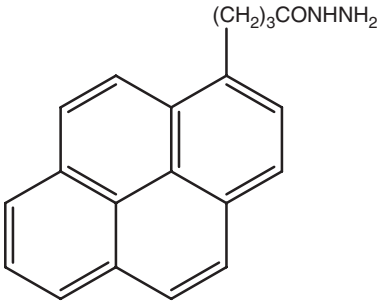
1-PYRENEBUTANOIC ACID HYDRAZIDE (PBH)

CAS Registry Number 55486-13-0

Chemical Structure



CA Index Name 1-Pyrenebutanoic acid, hydrazide

Other Names Pyrenebutyric acid hydrazide; 1-Pyrenebutyric acid hydrazide; Pyrenebutyrylhydrazine; 1-Pyrenebutyrylhydrazine; Pyrene butanoic acid hydrazide; 4-(1-Pyrene)butanoic acid hydrazide; 4-(1-Pyrene)butyric acid hydrazide; 4-(1-Pyrene)butyryl hydrazide; PBH

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{20}H_{18}N_2O$

Molecular Weight 302.37

Physical Form Yellow needles;[2] white powder[1]

Solubility Soluble in water, acetonitrile, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 167–171 °C

Boiling Point (Calcd.) 588.8 ± 29.0 °C, pressure: 760 Torr

pK_a (Calcd.) 13.22 ± 0.35, most acidic, temperature: 25 °C; 3.23 ± 0.10, most basic, temperature: 25 °C

Absorption (λ_{max}) 341 nm, 325 nm (MeOH)

Emission (λ_{max}) 376 nm, 396 nm (MeOH)

Molar Extinction Coefficient 43,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[2,3] collagen;[4,5] chitosan;[6,7] oligonucleotide;[8,9] oligosaccharides;[10–13] polynucleotide;[3] carboxylic acids[14–17]

Biological/Medical Applications Detecting/labeling/quantifying biological carbonyl compounds (aldehydes and/or ketones);[2–5,10–13,18] analyzing/detecting/measuring carboxylic acids;[14–17] treating inflammation,[11] autoimmune diseases,[11] allergic diseases,[11] viral diseases,[11] cancer,[11] infectious diseases,[11] heart diseases[11]

Industrial Applications Chemosensor materials;[19] lubricants[20]

Safety/Toxicity No data available

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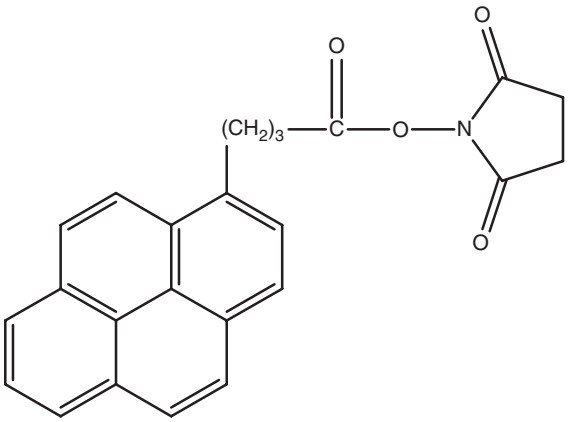
1-PYRENEBUTANOIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 114932-60-4

Chemical Structure



CA Index Name 1-Pyrenebutanoic acid, 2,5-dioxo-1-pyrrolidinyl ester

Other Names 2,5-Pyrrolidinedione, 1-[1-oxo-4-(1-pyrenyl)butoxy]-; 1-Pyrenebutanoic acid succinimidyl ester; 1-Pyrenebutyric acid *N*-hydroxysuccinimide ester; 4-Pyrenebutanoate *N*-hydroxysuccinimidyl ester; 4-(1-Pyrene)butanoic acid succimidyl ester; 4-(1-Pyrene)butyric acid *N*-hydroxysuccinimide ester; *N*-(1-Pyrene)-butyryloxysuccinimide; Succinimidyl 1-Pyrenebutanoate; 1-Succinimidyl pyrenebutyrate; PANHS; PBASE; PBSE; PNHS; PSE; PyBHS; Py-Boc; PYS

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{24}H_{19}NO_4$

Molecular Weight 385.41

Physical Form Yellow solid[1–4]

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 132–136 °C; 131–133 °C[5]

Boiling Point (Calcd.) 590.9 ± 43.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 340 nm, 325 nm (MeOH)

Emission (λ_{max}) 376 nm, 396 nm (MeOH)

Molar Extinction Coefficient 43,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–7]

Imaging/Labeling Applications Cellulose;[8] cyclodextrin-based polyrotaxanes;[9–12] histamine/histidine;[13–17] lysozymes;[18] nucleic acids;[6,7,19–33] polyamines;[34–38] proteins;[4,39–41] poly(dimethylsiloxane) (PDMS) oligomers[58–62]

Biological/Medical Applications Characterizing cyclodextrin-based polyrotaxanes;[9–12] detecting nucleic acids,[6,7,19–33] polyamines;[34–38] immobilizing proteins;[4,39–41] probing lysozyme in human serum;[18] as a substrate for measuring polymerases activity,[42] recombinases activity,[43] topoisomerases activity[43]

Industrial Applications Carbon nanotubes (single-wall carbon nanotubes (SWCNT) and multi-wall carbon nanotubes (MWCNTs));[1,2,44–53] cellulose materials for bulky paper sheets;[8] graphene-based polymer nanocomposites materials/films;[54–56] photonic materials;[55] photovoltaic devices;[56] polyaniline systems;[57] poly(dimethylsiloxane) (PDMS) oligomers;[58–62] poly(propylene imine) dendrimers;[63,64] thin-films[65]

Safety/Toxicity No data available

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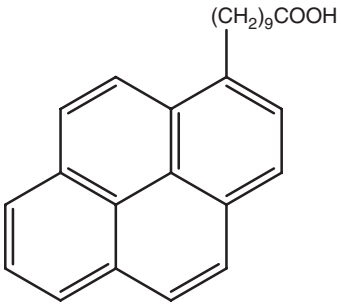
1-PYRENEDECANOIC ACID (PDA)

CAS Registry Number 64701-47-9

Chemical Structure



CA Index Name 1-Pyrenedecanoic acid

Other Names 10-(1-Pyrene)decanoic acid; 10-(1-Pyrenyl)decanoic acid; PDA; PyDA

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{26}H_{28}O_2$

Molecular Weight 372.50

Physical Form Light yellow crystals[2,3]

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 110 °C[3]; 104–108.5 °C[1]; 99 °C[2]

Boiling Point (Calcd.) 576.4 ± 19.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.78 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 341 nm, 325 nm (MeOH)

Emission (λ_{max}) 377 nm, 396 nm (MeOH)

Molar Extinction Coefficient 43,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Liponucleotides;[1] glycosphingolipids;[4] lipids;[5–9] sphingomyelin;[10,11] sphingosines[12]

Biological/Medical Applications Analyzing lipid aggregates;[5] diagnosis of Niemann-Pick disease in cultured cells,[10,11] Wolman disease;[14] as substrates for ceramidase activity,[13] cholesteryl esterases activity,[14] lipase activity,[15–17] phospholipases A2 activity,[18,19] sphingomyelinase activity,[10] sphingosine kinases 1 and 2 activity,[12] synthetase activity[20]

Industrial Applications Electroluminescent material;[21] oxygen sensing material;[22–27] Langmuir-Blodgett films;[28–30] laser-assisted vacuum-deposited films/ vacuum-deposited films[31–35]

Safety/Toxicity No data available

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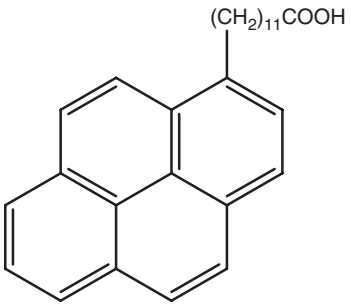
1-PYRENEDODECANOIC ACID (PDDA)

CAS Registry Number 69168-45-2

Chemical Structure



CA Index Name 1-Pyrenedodecanoic acid

Other Names 12-(1-Pyrene)dodecanoic acid; 12-(1-Pyrenyl)dodecanoic acid; P 12; P 12 (photosensitizer); PDDA

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{28}H_{32}O_2$

Molecular Weight 400.55

Physical Form Pale yellow solid[2]

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 123–125 °C[1]; 110–111 °C[2]

Boiling Point (Calcd.) 594.5 ± 19.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.78 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 341 nm, 325 nm (MeOH)

Emission (λ_{max}) 377 nm, 396 nm (MeOH)

Molar Extinction Coefficient 44,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Membranes;[3,4] fatty acid;[5–11] gangliosides;[12] lipids;[13–16] sphingomyelin[17–19]

Biological/Medical Applications Lipid probe;[13–16] diagnosis of Niemann-Pick disease;[17,19] studying transport of fatty acids;[10,11] membrane probe;[3,4] as substrates for sphingomyelinase activity[19]

Industrial Applications Oxygen sensing material;[20–23] Langmuir-Blodgett films;[24–27] liquid crystal orienting film;[28] self-assembled monolayer films;[29] vacuum-deposited films[30–34]

Safety/Toxicity Cytotoxicity;[35–39] phototoxicity[35–39]

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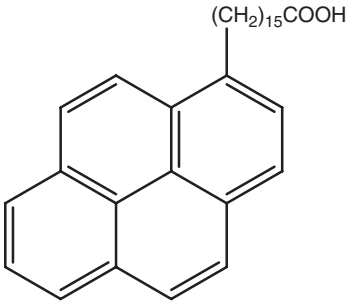
1-PYRENEHEXADECANOIC ACID

CAS Registry Number 90936-84-8

Chemical Structure



CA Index Name 1-Pyrenehexadecanoic acid

Other Names 16-(1-Pyrenyl)hexadecanoic acid; Pyrenehexadecanoic acid; PHA; PHD; PHDA; PyHA; PY-HDA

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{32}H_{40}O_2$

Molecular Weight 456.66

Physical Form Solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) $631.5 \pm 24.0\,^{\circ}C$, pressure: 760 Torr

pK_a (Calcd.) 4.78 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 341 nm, 325 nm (MeOH)

Emission (λ_{max}) 377 nm, 396 nm (MeOH)

Molar Extinction Coefficient 43,000 $cm^{-1}\,M^{-1}$ (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Lipids;[1–7] fatty acids;[8,9] membranes;[6,10,11] inverted micelles[12]

Biological/Medical Applications Lipid probe;[1–7] membrane probe[6,10,11]

Industrial Applications Characterizing inverted micelles;[12] electrooptical displays;[13] electronic systems for optical information processing (organic photoconductors);[14,15] Langmuir-Blodgett films;[16–21] self-assembled monolayer films;[22,23] nano-structured silica films;[24] vacuum-deposited films[25,26]

Safety/Toxicity No data available

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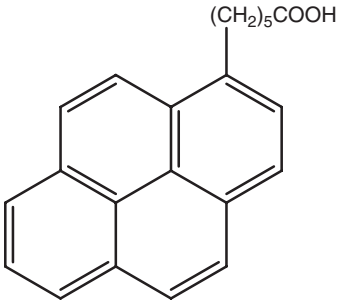
1-PYRENEHEXANOIC ACID (PHA)

CAS Registry Number 90936-85-9

Chemical Structure



CA Index Name 1-Pyrenehexanoic acid

Other Names 1-Pyrenehexanoic acid; 6-(1-Pyrenyl)-hexanoic acid; 6-(Pyren-1-yl)-hexanoic acid; 6-Pyrenylhexanoic acid; PHA

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{22}H_{20}O_2$

Molecular Weight 316.39

Physical Form Solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 200–201 °C[2]

Boiling Point (Calcd.) 552.2 ± 29.0 °C, pressure: 760 Torr

pK_a (Calcd.) 4.77 ± 0.10, most acidic, temperature: 25 °C

Absorption (λ_{max}) 341 nm, 325 nm (MeOH)

Emission (λ_{max}) 377 nm, 396 nm (MeOH)

Molar Extinction Coefficient 42,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Fibroblasts;[3,4] galactosylceramide;[14] glucose oxidase (GOx);[6] horseradish peroxidase (HRP);[6,7] laccase;[5] lipids;[3] lysozyme crystal;[8] nucleic acids;[9–11] paromomycin;[9] phosphatidylcholine;[14] proteins;[12,13] sphingomyelin;[14] sphingosines[15]

Biological/Medical Applications Assessing role of membrane domains in lipid trafficking/sorting;[14] characterizing interactions/mass transfer of surfactants inside crystaline protein matrixes;[8] investigating transport/metabolism of cellular lipids;[3] monitoring domain formation in membranes;[14] implantable biocathodes/composite electrodes;[5–7] nucleic acid hybridization probe;[10,11] as a substrate for measuring cholesterylester hydrolase (CEH) activity,[16] sphingosine kinases 1 and 2 activity[15]

Industrial Applications Boron-doped diamond (BDD) substrates;[17] Langmuir-Blodgett films;[18] thin films;[19] vacuum-deposited films[20,21]

Safety/Toxicity No data available

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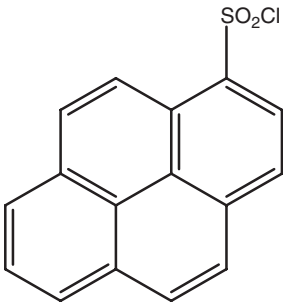
1-PYRENESULFONYL CHLORIDE

CAS Registry Number 61494-52-8

Chemical Structure



CA Index Name 1-Pyrenesulfonyl chloride

Other Names 3-Pyrenesulfonyl chloride; PSC; PSCL

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{16}H_9ClO_2S$

Molecular Weight 300.76

Physical Form Bright yellow crystals;[3] Orange crystals[4]

Solubility Soluble in acetonitrile, chloroform, *N,N*-dimethylformamide, methanol, xylenes

Melting Point 172–174 °C;[5] 172–173 °C;[4] 163–166 °C (decompose)[3]

Boiling Point (Calcd.) 472.0 ± 14.0 °C, pressure: 760 Torr

Absorption (λ_{max}) 350 nm (MeOH)

Emission (λ_{max}) 380 nm (MeOH)

Molar Extinction Coefficient 28,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Estrogens;[6] oligosaccharides;[7,8] phospholipids;[9,10] cationic polyacrylamides (C-PAM);[11] 2-(arylsulfonyl)-methacrylates;[12] ribonucleopeptide;[13,14] sphingosines;[15,16] sugar chains[17]

Biological/Medical Applications Quantitating estrogens;[6] as substrates for acetylcholinesterase activity,[18] arylsulfatase A activity,[19] phosphatase activity,[15] sphingosine kinases 1 and 2 activity[15,16]

Industrial Applications Analysizing sugar chains;[17] Detecting dicarboxylic acids,[5,24,25] picric acid;[26] functionalized fluorescent polymers;[11,12] sensor for copper ions,[20,21] lead ions,[22] mercury ions;[22,23] self-assembled monolayer film;[27,28] composite materials;[30] glass fibers;[29–31] silica microfibers[32]

Safety/Toxicity No data available

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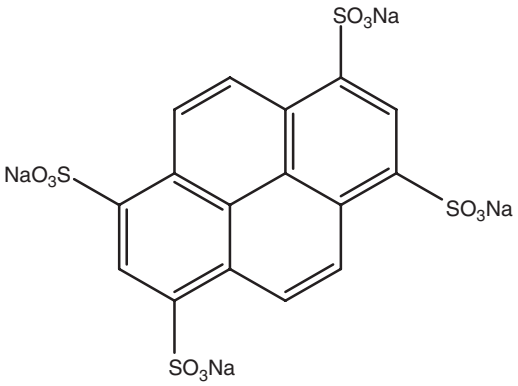
1,3,6,8-PYRENETETRASULFONIC ACID TETRASODIUM SALT

CAS Registry Number 59572-10-0

Chemical Structure



CA Index Name 1,3,6,8-Pyrenetetrasulfonic acid, sodium salt (1:4)

Other Names 1,3,6,8-Pyrenetetrasulfonic acid, tetrasodium salt; 1,3,6,8-Pyrenetetrasulfonic acid tetra-Na salt; Tetrasodium 1,3,6,8-pyrenetetrasulfonate; Tetra-Na 1,3,6,8-pyrenetetrasulfonate; Tetrasodium pyrenetetrasulfonate; tetrasodium 1,3,6,8-pyrenetetrasulfonate; Na_4PS_4; PSA; 4- PSA; PTS; PTSA; PY; Py-4; PyTS; SPA; TPA; Trasar 23299

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{16}H_6Na_4O_{12}S_4$

Molecular Weight 610.43

Physical Form Yellow powder[1,3]

Solubility Soluble in water

Absorption (λ_{max}) 374 nm (H_2O)

Emission (λ_{max}) 403 nm (H_2O)

Molar Extinction Coefficient 51,000 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Cyclen 1;[4] polyelectrolytes;[5–8] metal-polyethylenimine complexes;[9] proteins/peptides[10–12]

Biological/Medical Applications Characterizing water-in-oil-in-water (W/O/W) emulsions;[13–15] as a substrate for measuring lipase activity;[13,16] air-breathing biocathodes for zinc/oxygen batteries;[17] graphene-coated biochar for various environmental applications;[18] plants or plant parts identification labels[19]

Industrial Applications Assessing interaction between sulfonated polystyrene and poly(ethylacrylate-co-4-vinylpyridine) ionomers;[20] carbon nanotube;[21] evaluating/studying influence of incorporation of counterions into polypyrrole;[22] examining salt group association of sulfonated polystyrene ionomers;[23] fabricating graphene-based nanoelectronic devices;[24] graphene/polymer dispersions for graphene/polymer nanocomposites,[25] organic solar cells,[25] conductive films,[25] ink-jet-printed electronic devices;[25] graphene-zeolite based microcapsules;[26] investigating electrical breakdown/permeability control of bilayer-corked capsule membrane;[27] light filters;[2] monitoring wastewater treatment;[28] poly(arylene sulfide) blends in UV weathering;[29] pulp and papermaking processes;[30] thermosensitive polymer gels;[31–33] thin films;[6,7] TiO_2-based materials;[6] tracing corrosive materials;[34] ureasil gels for water purification[35]

Safety/Toxicity No data available

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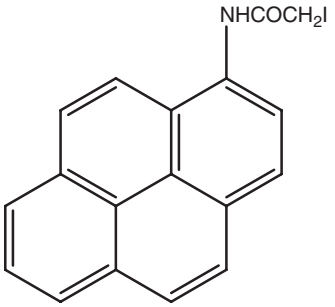
N-(1-PYRENYL)IODOACETAMIDE

CAS Registry Number 76936-87-3

Chemical Structure



CA Index Name Acetamide, 2-iodo-*N*-1-pyrenyl-

Other Names *N*-(1-Pyrenyl)iodoacetamide; NPIA; PIA; PIAA

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{18}H_{12}INO$

Molecular Weight 385.20

Physical Form Yellow–green solid

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Boiling Point (Calcd.) $587.1 \pm 33.0\,^{\circ}C$, pressure: 760 Torr

pK_a (Calcd.) 12.90 ± 0.30, most acidic, temperature: $25\,^{\circ}C$; -0.01 ± 0.70, most basic, temperature: $25\,^{\circ}C$

Absorption (λ_{max}) 339 nm (MeOH)

Emission (λ_{max}) 384 nm (MeOH)

Molar Extinction Coefficient 26,000 $cm^{-1}\,M^{-1}$ (MeOH)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Actin;[2–10] RNA polymerase;[11] gelsolin;[12] histone H4;[13] α-lipoic acid;[14] myosin;[15] nucleic acid;[16] oxytocin;[17] proteins;[18–22] spectrin;[23] tropomyosins;[24–26] thiols[1–26]

Biological/Medical Applications Analyzing α-lipoic acid;[14] characterizing/monitoring spectrin structural changes;[23] determing oxytocin in human urine;[17] monitoring association-dissociation equilibria of protein subunits transitions;[20] nucleic acid hybridization probe;[16] studying local/global tropomyosin unfolding[24]

Industrial Applications Not reported

Safety/Toxicity No data available

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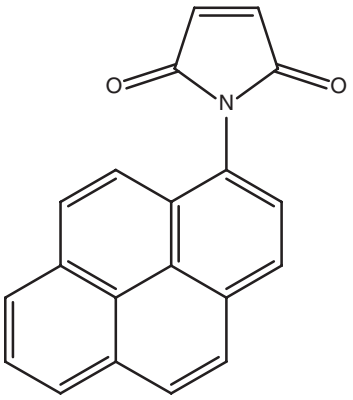
N-(1-PYRENYL)MALEIMIDE

CAS Registry Number 42189-56-0

Chemical Structure



CA Index Name 1*H*-Pyrrole-2,5-dione, 1-(1-pyrenyl)-

Other Names *N*-(1-Pyrenyl)maleimide; MPy; MalPy; Mal-pyrene; NPM; *N*-(1-Pyrene)maleimide; *N*-(3-pyrene)maleimide; *N*-(3-pyrenyl)maleimide; PM; PMI; pyrene-TM

Merck Index Number Not listed

Chemical/Dye Class Pyrene

Molecular Formula $C_{20}H_{11}NO_2$

Molecular Weight 297.31

Physical Form Yellow needles;[2] Gold needles[1]

Solubility Soluble in chloroform, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 239–240 °C;[2] 235–237 °C; 223–225 °C[1]

Boiling Point (Calcd.) 526.8 ± 19.0 °C, pressure: 760 Torr

pK_a (Calcd.) −1.21 ± 0.20, most basic, temperature: 25 °C

Absorption (λ_{max}) 338 nm, 325 nm (MeOH)

Emission (λ_{max}) 375 nm, 396 (MeOH)

Molar Extinction Coefficient 40,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nicotinic acetylcholine receptor (AChR);[5–7] actin;[8–11] antibodies;[12,13] cells;[14,37] chloroplast coupling factor;[15,16] cellobiohydrolase I (CBH I);[17] dehydrogenases;[18–23] luciferase;[24] 4-aminobutyrate aminotransferase;[25] glutathione S-transferase;[26] histone acetyltransferases (HATs);[27] phosphotransferase;[28] immunoglobulin;[29,30] myosin;[31] nucleic acids;[3,35,41] profilin;[32] proteins;[1,3,33–42] ribosomes;[43,44] radio-fluorogenic gel;[67] sarcoplasmic reticulum ATPase;[45–51] α-synuclein;[52] tropomyosins;[53–56] tubulin;[57,58] thiols[1–60,65]

Biological/Medical Applications Analyzing molecular aspects of muscle contraction;[31] detecting nucleic acids,[3,35,41] proteins;[1,3,33–42] determining/evaluating cell activity;[14,37] diagnosing/treating Parkinson's disease;[52] monitoring/studying ribosomal structure and conformation;[43,44] studying nicotinic acetylcholine receptor (AChR) structure;[5] sulfhydryl reagent[1–60,65]

Industrial Applications Dendrimers;[61,62] dye functionalized single-wall carbon nanotube (SWNT) conjugated polymer devices;[63,64] photovoltaic cells;[63,64] polymer-coated gold electrodes;[65] fluorescent polymers;[66] radio-fluorogenic gel;[67] in sequence-controlled polymerizations;[68] rubber[69]

Safety/Toxicity Cytotoxicity;[70] peroxidative damage[71]

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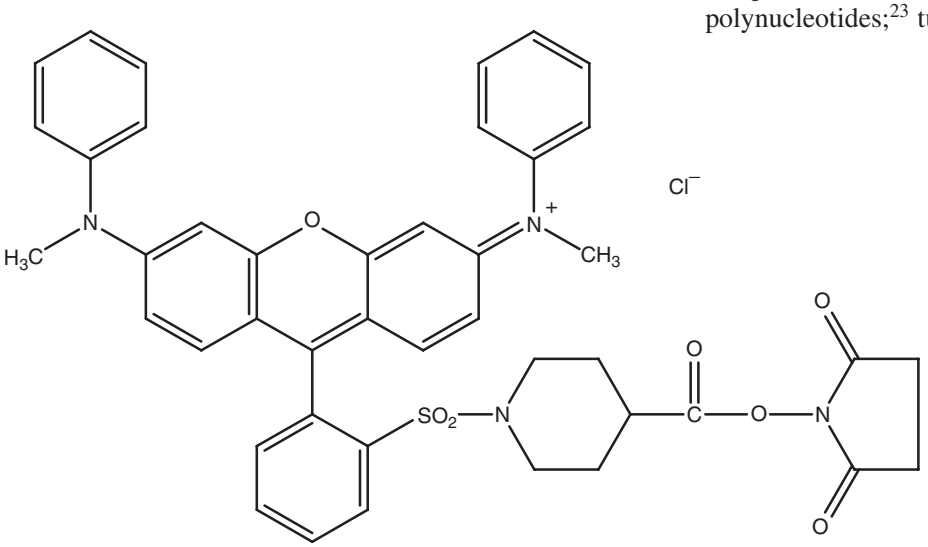
QSY 7 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 304014-12-8

Chemical Structure



CA Index Name Xanthylium, 9-[2-[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]-carbonyl]-1-piperidinyl]sulfonyl] phenyl]-3,6-bis(methylphenylamino)-, chloride (1:1)

Other Names Xanthylium, 9-[2-[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]-carbonyl]-1-piperidinyl]sulfonyl] phenyl]-3,6-bis(methylphenylamino)-, chloride; QSY 7; QSY 7 carboxylic acid succinimidyl ester; QSY 7 succinimidyl ester; QSY 7NHS; QSY 7SE

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{43}H_{39}ClN_4O_7S$

Molecular Weight 791.32

Physical Form Purple solid

Solubility Soluble in dimethyl sulfoxide, methanol

Absorption (λ_{max}) 560 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 90,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.0009 (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–10] cells;[11] oligonucleotides;[1–4,20] avidin;[12,13] trastuzumab;[12] bacteria;[14] spores;[14] cathepsin;[15–17] G-protein-coupled receptors (GPCRs);[18] microorganisms;[19] proteins;[11,21,22] polynucleotides;[23] tumors[12,15–17]

Biological/Medical Applications Fluorescence quencher;[1–4,11–34] detecting nucleic acids,[1–10] microorganisms,[19] membrane protein internalization,[21,22] analytes;[33] imaging/detecting/identifying cancer;[12,15–17] diagnosing active wound infection;[27] assays for measuring/detecting/imaging nuclease activity,[3,4] ligase activity,[3,4] topoisomerase activity,[3,4] phospholipase activity,[3,4] clostridial toxin activity,[25,26] human neutrophil elastase activity,[27] protease activity,[15–17,25,26,30,31] peptidylarginine deiminase (PAD) activity,[28] phosphoinositide kinase activity,[29] phosphatase activity,[29] gamma-secretase activity;[32] nucleic acid sequencing[34]

Industrial Applications Not reported

Safety/Toxicity No data available

Handbook of Fluorescent Dyes and Probes, First Edition. R. W. Sabnis.
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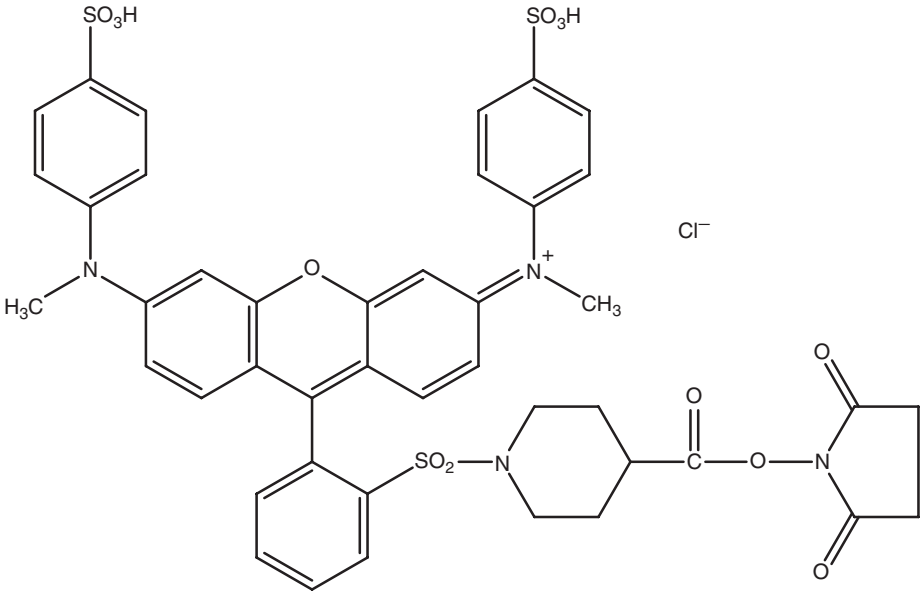
QSY 9 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 700834-40-8

Chemical Structure



CA Index Name Xanthylium, 9-[2-[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]-carbonyl]-1-piperidinyl]sulfonyl] phenyl]-3,6-bis[methyl(4-sulfophenyl)amino]-, chloride (1:1)

Other Names Xanthylium, 9-[2-[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy]-carbonyl]-1-piperidinyl]sulfonyl] phenyl]-3,6-bis[methyl(4-sulfophenyl)amino]-, chloride; QSY 9; QSY 9 carboxylic acid succinimidyl ester

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{43}H_{39}ClN_4O_{13}S_3$

Molecular Weight 951.43

Physical Form Purple solid

Solubility Soluble in water, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 562 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 88,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.002 (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–6] oligonucleotides;[1–4] antibody;[7] G-protein-coupled receptors (GPCRs);[8] microorganisms;[9] peptides;[10] proteins;[11–13] polynucleotides[14]

Biological/Medical Applications Fluorescence quencher;[1–4,7,8,13–20] detecting nucleic acids,[1–6] microorganisms,[9] membrane protein internalization;[11,12] G-protein-coupled receptors (GPCRs) assay;[8] ligand assays;[7,8,13] bioaffinity assay;[18] peptide substrates;[10] measuring/detecting analytes;[18,19] nucleic acid sequencing;[20] assays for measuring/detecting nuclease activity,[3,4] ligase activity,[3,4] topoisomerase activity,[3,4] phospholipase activity,[3,4] caspase activity,[16] phosphoinositide kinase activity,[17] phosphatase activity[17]

Industrial Applications Not reported

Safety/Toxicity No data available

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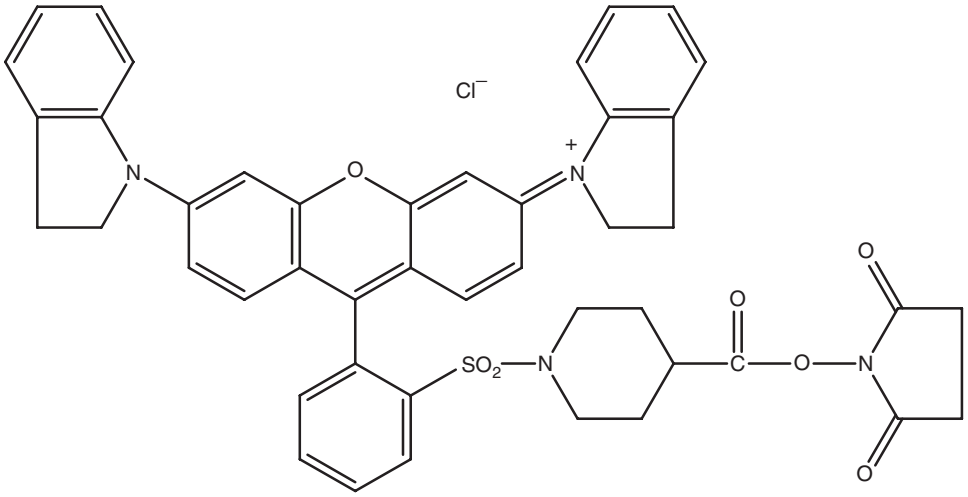
QSY 21 CARBOXYLIC ACID SUCCINIMIDYL ESTER

CAS Registry Number 304014-13-9

Chemical Structure



CA Index Name Xanthylium, 3,6-bis(2,3-dihydro-1*H*-indol-1-yl)-9-[2-[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy] carbonyl]-1-piperidinyl]-sulfonyl]phenyl]-, chloride (1:1)

Other Names Xanthylium, 3,6-bis(2,3-dihydro-1*H*-indol-1-yl)-9-[2-[[4-[[(2,5-dioxo-1-pyrrolidinyl)oxy] carbonyl]-1-piperidinyl]-sulfonyl]phenyl]-, chloride; QSY 21; QSY 21 carboxylic acid succinimidyl ester; QSY 21NHS

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{45}H_{39}ClN_4O_7S$

Molecular Weight 815.34

Physical Form Purple solid

Solubility Soluble in dimethyl sulfoxide, methanol

Absorption (λ_{max}) 661 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 90,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.0002 (MeOH)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–8] cells;[9] oligonucleotides;[1–4] bacteria;[10,11] cathepsin;[12–15] protein-coupled receptors (GPCRs);[19] microorganisms;[20] oligopeptides;[21] proteins;[22,23] polynucleotides[24]

Biological/Medical Applications Fluorescence quencher;[1–4,9–19,21,24–32] detecting nucleic acids,[1–8] microorganisms,[20] membrane protein internalization,[22,23] analytes;[30] detecting/imaging cells,[9] bacteria,[10,11] apoptosis;[32] imaging/detecting/identifying cancer;[12–18,27] diagnosing active wound infection;[28] assays for measuring/detecting/imaging nuclease activity,[3,4] ligase activity,[3,4] topoisomerase activity,[3,4] phospholipase activity,[3,4] β-lactamase activity,[9–11] caspase activity,[26] lysophospholipase D (LysoPLD) activity,[27] human neutrophil elastase activity,[28] saccharide activity;[29] nucleic acid sequencing;[31] as a quantum dot quencher;[33] glucose monitoring[34,35]

Industrial Applications Not reported

Safety/Toxicity No data available

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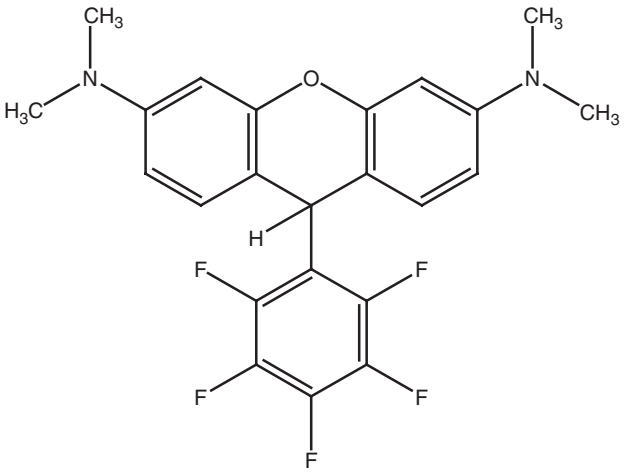
REDOXSENSOR RED CC-1

CAS Registry Number 296277-09-3

Chemical Structure



CA Index Name 9*H*-Xanthene-3,6-diamine, N^3,N^3,N^6,N^6-tetramethyl-9-(2,3,4,5,6-pentafluorophenyl)-

Other Names 9*H*-Xanthene-3,6-diamine, *N*,*N*,*N*′,*N*′-tetramethyl-9-(pentafluorophenyl)-; R 14060; RedoxSensor; RedoxSensor CC 1; RedoxSensor Red; RedoxSensor Red CC 1

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{23}H_{19}F_5N_2O$

Molecular Weight 434.40

Physical Form Colorless solid

Solubility Soluble in dimethyl sulfoxide, methanol

Boiling Point (Calcd.) $445.1 \pm 45.0\,^{\circ}C$, pressure: 760 Torr

pK_a (Calcd.) 4.83 ± 0.40, most basic, temperature: 25 °C

Absorption (λ_{max}) 239 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 52,000 $cm^{-1}\,M^{-1}$ (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Mitochondria;[1–4] lysosomes;[1,2,5] cells;[5] semiconductor nanocrystal (quantum dot)[5]

Biological/Medical Applications Detecting prostate cancer[4] generating/detecting reactive oxygen species (ROS)[1,2,6–9]

Industrial Applications Assaying reactive oxidants in smoke[9]

Safety/Toxicity No data available

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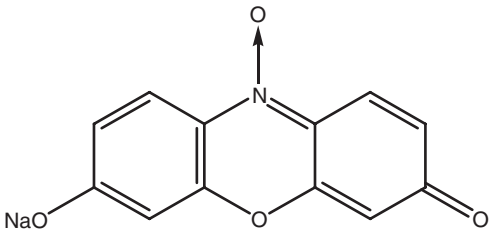
RESAZURIN SODIUM SALT (ALAMAR BLUE)

CAS Registry Number 62758-13-8

Chemical Structure



CA Index Name 3*H*-Phenoxazin-3-one, 7-hydroxy-, 10-oxide, sodium salt (1:1)

Other Names Alamar Blue; 3*H*-Phenoxazin-3-one, 7-hydroxy-, 10-oxide, sodium salt; 7-hydroxy-3*H*-Phenoxazin-3-one 10-oxide, sodium salt; Resazurin sodium salt; Sodium resazurin

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Phenoxazine

Molecular Formula $C_{12}H_6NNaO_4$

Molecular Weight 251.17

Physical Form Dark green to black powder or purple solid

Solubility Soluble in water, methanol

Absorption (λ_{max}) 604 nm (MeOH)

Emission (λ_{max}) None

Molar Extinction Coefficient 60,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications D-Arabinitol;[4] bacteria;[5–9] bile acids;[10–14] cells;[32–35] hairs;[15] hypoxic cells;[16] microorganisms;[17–19] sperms;[20–29] yeasts[30,31]

Biological/Medical Applications Analyzing/evaluating sperm parameters;[20–29] detecting bacteria,[5–9] D-arabinitol in vaginal fluid,[4] yeasts;[30,31] determining malt quality for use in beer production;[49] diagnosing *Candida* vaginitis;[4] evaluating/quantitating/measuring glucose, 2-deoxy-D-glucose (2DG), glucose 6-phosphate, 2-deoxy-D-glucose 6- phosphate (DG6P);[45,46] locating hidden microorganism contaminated surfaces in industrial water systems;[17] measuring mitochondrial metabolic activity;[47,48] as cell viability assay reagent;[32–35] as cytotoxicity assay reagent;[36–44] as a substrate for measuring dehydrogenases activity,[50,51] β-glucosidase activity,[52] glutathione transferase activity,[53] glycosidases activity,[54] hydrolases activity;[55,56] testing/characterizing microorganisms[18,19]

Industrial Applications Electrochemichromic solutions/devices (mirrors, glazings, partitions, filters, displays, lenses);[57,58] oxygen-barrier packaging materials;[59] oxidation-reduction (redox) indicator[1–3,5–9,17–19,30,31,49,57,58]

Safety/Toxicity No data available

Certification/Approval Certified by Biological Stain Commission (BSC)

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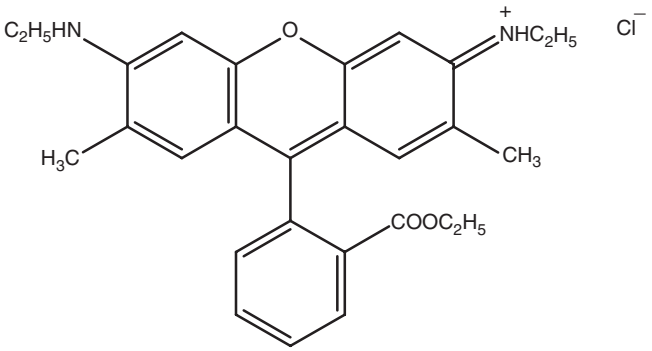
RHODAMINE 6G (RH 6G)

CAS Registry Number 989-38-8

Chemical Structure



CA Index Name Xanthylium, 9-[2-(ethoxycarbonyl) phenyl]-3,6-bis(ethylamino)-2,7-dimethyl-, chloride (1:1)

Other Names Benzoic acid, *o*-[6-(ethylamino)-3-(ethylimino)-2,7-dimethyl-3*H*-xanthen-9-yl]-, ethyl ester, monohydrochloride; Rhodamine 6GCP; Xanthylium, 9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethyl-, chloride; Aizen Rhodamine 6GCP; Basic Red 1; Basonyl Red 482; Basonyl Red 483; C.I. 45160; C.I. Basic Red 1; Calcozine Red 6G; Calcozine Rhodamine 6GX; Eljon Pink Toner; Exciton 590; Fanal Pink B; Fanal Pink GFK; Fanal Red 25532; Flexo Red 482; Heliostable Brilliant Pink B extra; Mitsui Rhodamine 6GCP; NSC 36345; Nyco Liquid Red GF; R 634; R 6G; Rh 6G; Rhodamin 6G; Rhodamine 4GD; Rhodamine 4GH; Rhodamine 5GDN; Rhodamine 5GDN Extra; Rhodamine 5GL; Rhodamine 6G; Rhodamine 6G Extra; Rhodamine 6G Extra Base; Rhodamine 6G chloride; Rhodamine 6GB; Rhodamine 6GBN; Rhodamine 6GD; Rhodamine 6GDN; Rhodamine 6GDN Extra; Rhodamine 6GEx ethyl ester; Rhodamine 6GH; Rhodamine 6GO; Rhodamine 6GX; Rhodamine 6JH; Rhodamine 6JH-SA; Rhodamine 6JH-SA Extra 1150; Rhodamine 6Zh-DN; Rhodamine F 5G; Rhodamine F 5GL; Rhodamine GDN; Rhodamine GDN Extra; Rhodamine Y 20–7425; Rhodamine Zh; Silosuper Pink B; Vali Fast Red 1308

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{28}H_{31}ClN_2O_3$

Molecular Weight 479.01

Physical Form Red crystals, powder or solid

Solubility Soluble in water, ethanol, methanol

Absorption (λ_{max}) 528 nm (MeOH)

Emission (λ_{max}) 551 nm (MeOH)

Molar Extinction Coefficient 105,000 cm^{-1} M^{-1} (MeOH)

Quantum Yield 0.95 (1.0 N H_2SO_4)[5]

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Mitochondria;[1,6–10] cells;[11,12] hairs;[13,14] metal ions: copper ions;[15–17] gold ions;[18] iron ions;[19,20] mercury ions;[21–25] palladium ions;[26] rhodium ions;[27] vanadium ions;[28] nitrite ions;[29] microorganisms;[30] nucleic acids;[31–34] proteins[35,36]

Biological/Medical Applications Analyzing cells;[11,12] analyzing/labeling nucleic acids;[31–34] characterizing multidrug resistance;[37] as a substrate for measuring phospholipase activity,[38] protease activity;[39] measuring membrane potential;[40] treating amyloidosis,[41] cancer[41,42]

Industrial Applications Clays;[43–46] colored bubbles;[47,48] color filters;[49–58] detergents;[59,60] drawing materials;[61] dye lasers;[62–73] electroluminescent (EL) displays;[52,53,55,58,74–77] glass materials;[78,79] inks;[80–94] laser devices/laser materials;[95–97] light-emitting diode devices/materials;[54,56,98–100] liquid crystals;[101] liquid crystal displays;[50,102] luminescent materials;[103] metal oxide particles;[104] petroleum products;[105] photographic materials;[106] photoresists;[107] photovoltaic devices;[108] polymer films;[109] printing materials;[110] recording materials;[111,112] silica gel;[113] solar cells;[114,115] sol–gel materials;[116] sputtered gold films;[117] textiles;[118] thin films;[119,120] toners;[121–123] tracers for hydrology;[124] waveguides[125–127]

Safety/Toxicity Carcinogenicity;[128–132] cardiotoxicity;[133] DNA damage;[134] ecotoxicity;[135] genotoxicity;[136] mutagenicity;[130,134,137–139] phototocicity;[140,141] reproductive toxicity[142]

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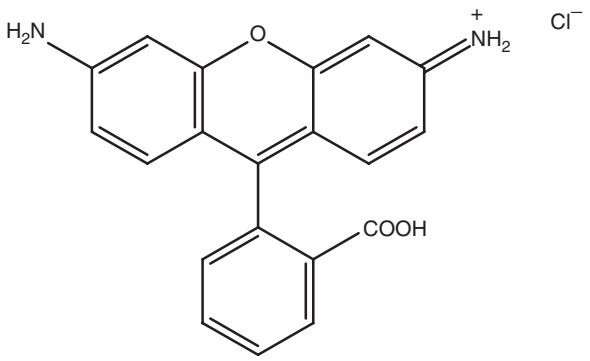
RHODAMINE 110 (RH 110)

CAS Registry Number 13558-31-1

Chemical Structure



CA Index Name Xanthylium, 3,6-diamino-9-(2-carboxyphenyl)-, chloride (1:1)

Other Names Benzoic acid, 2-(6-amino-3-imino-3*H*-xanthen-9-yl)-, monohydrochloride; Benzoic acid, *o*-(6-amino-3-imino-3*H*-xanthen-9-yl)-, monohydrochloride; Xanthylium, 3,6-diamino-9-(2-carboxyphenyl)-, chloride; R 110; RH 110; Rh 110; rh 110; Rho 110; Rhod 110; Rhodamine 110; Rhodamine 560; Rhodamine N

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{20}H_{15}ClN_2O_3$

Molecular Weight 366.80

Physical Form Green or red or reddish-green solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point >380 °C (decompose)[2]

Absorption (λ_{max}) 499 nm (MeOH); 496 nm (H_2O)

Emission (λ_{max}) 521 nm (MeOH); 520 nm (H_2O)

Molar Extinction Coefficient 92,000 cm^{-1} M^{-1} (MeOH); 83,000 cm^{-1} M^{-1} (H_2O)

Quantum Yield 0.92 (1.0 N H_2SO_4)[3]

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Actin filaments;[4] amino acids;[5] amyloid Aβ peptides;[6] bacteria;[7] cells;[8] glycopeptide;[9] hairs;[10,11] metal ions (copper ions,[12] iron ions,[12] chromium ions,[13] lead ions,[13] mercury(II) ions,[14] nitrite ions[15]); microorganisms;[16] monosaccharides;[17] nucleic acids;[18–25] proteins;[26,27] protoplasts;[28] sperms;[29] starch granules;[30] superoxide anions;[31] thiols[32]

Biological/Medical Applications Detecting risk of Alzheimer's disease and stroke;[33] evaluating/testing sperm quality;[29] identifying bacteria;[7] as a substrate for measuring aromatase activity,[34] azoreductase activity,[35] phospholipase activity,[36] proteases activity (caspase activity, cathepsin C activity, elastase activity proteinase activity);[37–49] implantable drug-delivery devices[50]

Industrial Applications Color filters;[51,52] liquid crystal displays;[51,52] dye lasers;[53–63] electroluminescent displays;[64–67] inks;[68,69] light-emitting diode (LED);[70–72] papermaking process;[73] recording materials;[74,75] solar cells;[76] silica thin films;[77] sol–gel titania films;[78] waveguides[79]

Safety/Toxicity Mutagenicity[80]

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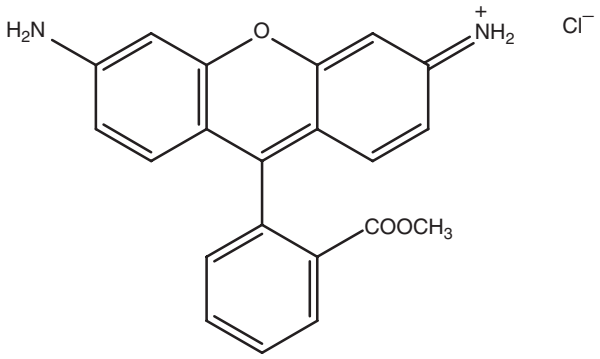
RHODAMINE 123 (RH 123)

CAS Registry Number 62669-70-9

Chemical Structure



CA Index Name Xanthylium, 3,6-diamino-9-[2-(methoxycarbonyl)phenyl]-, chloride (1:1)

Other Names Benzoic acid, 2-(6-amino-3-imino-3*H*-xanthen-9-yl)-, methyl ester, monohydrochloride; Xanthylium, 3,6-diamino-9-[2-(methoxycarbonyl)phenyl]-, chloride; R 22420; R 302; R 123; RH 123; Rh 123; rh 123; Rho 123; Rhod 123; Rhodamine 123

Merck Index Number 8306

Chemical/Dye Class Xanthene

Molecular Formula $C_{21}H_{17}ClN_2O_3$

Molecular Weight 380.83

Physical Form Red powder or solid Brown solid[3]

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, ether, methanol

Absorption (λ_{max}) 507 nm (MeOH); 500 nm (H_2O)

Emission (λ_{max}) 529 nm (MeOH); 530 nm (EtOH)

Molar Extinction Coefficient 101,000 cm^{-1} M^{-1} (MeOH); 75,000 cm^{-1} M^{-1} (H_2O)

Quantum Yield 0.90 (1.0 N H_2SO_4)[99]

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Mitochondria;[4–16] bacteria;[17–19] cells;[20–22] mercury ions;[23,24] microorganisms;[25] P-glycoprotein;[26–40] retina;[41] sperm;[42–45] stem cells;[46–52] tumors[54,55]

Biological/Medical Applications Characterizing/identifying stem cells;[46–52] detecting Hg(II) ions;[23,24] evaluating sperm quality/motility;[42–45] measuring/monitoring membrane potential;[4–16] as a substrate for measuring P-glycoprotein activity;[26–40] anticancer drug;[55–57] apoptosis assay;[58,59] cytotoxicity assay;[60] implantable medical device;[61–63] for photodynamic therapy;[64] treating disc degenerative diseases,[51] erectile dysfunction,[52] epilepsy,[53] prostate cancer;[65–67] as temperature sensor[68,69]

Industrial Applications Colored bubbles;[70,71,76] color filters;[72] liquid crystal displays;[72] light-emitting diodes;[73] luminescent materials;[74] nanophotonic composites;[75] paints;[76,77] semiconductor electrodes;[78] solar cells[79]

Safety/Toxicity Acute toxicity;[80] aluminum toxicity;[81] cardiotoxicity;[82] cellular toxicity;[83] cytotoxicity;[84–89] metabolic toxicity;[90] mitochondrial toxicity;[84,91] mutagenicity;[92] nephrotoxicity;[93] neurotoxicity;[94–96] ocular toxicity;[97] phototoxicity;[3] reproductive toxicity[98]

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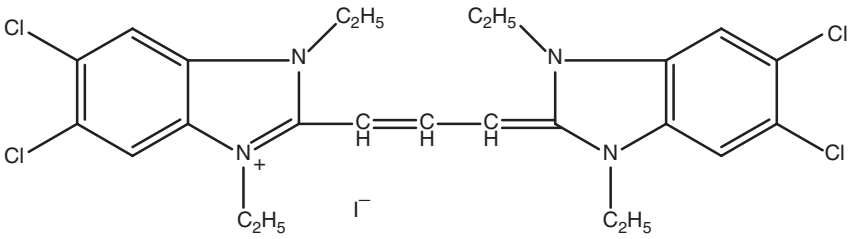
5,5′,6,6′-TETRACHLORO-1,1′,3,3′-TETRAETHYLBENZIMIDAZOLOCARBOCYANINE IODIDE (JC-1)

CAS Registry Number 3520-43-2

Chemical Structure



CA Index Name 1*H*-Benzimidazolium, 5,6-dichloro-2-[3-(5,6-dichloro-1,3-diethyl-1,3-dihydro-2*H*-benzimidazol-2-ylidene)-1-propen-1-yl]-1,3-diethyl-, iodide (1:1)

Other Names 1*H*-Benzimidazolium, 5,6-dichloro-2-[3-(5,6-dichloro-1,3-diethyl-1,3-dihydro-2*H*-benzimidazol-2-ylidene)-1-propenyl]-1,3-diethyl-, iodide; 5,6-Dichloro-2-[3-(5,6-dichloro-1,3-diethyl-2-benzimidazolinylidene)propenyl]-1,3-diethylbenzimidazolium iodide; Benzimidazolium, 5,6-dichloro-2-[3-(5,6-dichloro-1,3-diethyl-2-benzimidazolinylidene)propenyl]-1,3-diethyl-, iodide; Benzimidazolocarbocyanine iodide, 5,5′,6,6′-tetrachloro-1,1′,3,3′-tetraethyl-; Imidacarbocyanine iodide, 1,1′,3,3′-tetraethyl-5,5′,6,6′-tetrachloro-; 1,1′,3,3′-Tetraethyl-5,5′,6,6′-tetrachlorobenzimidazolocarbocyanine iodide; 1,1′,3,3′-Tetraethyl-5,5′,6,6′-tetrachloroimidacarbocyanine iodide; 5,5′,6,6′-Tetrachloro-1,1′,3,3′-tetraethylbenzimidazolocarbocyanine iodide; Bis(5,6-dichloro-1,3-di-ethyl-2-benzimidazole)trimethinecyanine iodide; $CBIC_2$; $CBIC_2$(3); JC 1; NK 1420

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{25}H_{27}Cl_4IN_4$

Molecular Weight 652.23

Physical Form Reddish lustrous crystals[7,9]

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Melting Point 275–278 °C[7,9]

Absorption (λ_{max}) 514 nm (MeOH)

Emission (λ_{max}) 529 nm (MeOH)

Molar Extinction Coefficient 195,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1–10]

Imaging/Labeling Applications Amyloid plaque;[11] astrocytes;[12,30] bacteria;[13] fungi;[13–15] hairs;[16] insect cells;[17] mitochondria;[1,17–43,46,47,52–54,56–58,60–63,65,78,79] neurons;[45–47] P-glycoprotein (P-gp);[66–68] proteins;[48] retina tissue;[49] sperms;[50–58] α-synuclein;[59] yeast cells[48]

Biological/Medical Applications Analyzing mitochondrial morphology and function;[19,20,36,54,56,58,65] assessing sperm integrity;[56] detecting prostate cancer;[19] diagnosing/treating Alzheimer′s disease;[60] evaluating sperm motility and chemotaxis;[51] measuring *in vivo* hematotoxicity;[26] measuring/monitoring membrane potential;[1,13,17,21–44,46,52,53,56–58,61–64,78] apoptosis assay;[26,61–63] cytotoxicity assay;[23,64,65] P-glycoprotein (P-gp) activity acute myeloid leukemia (AML) assay;[66–68] multidrug resistance assay;[69,70] as temperature sensor[71,72]

Industrial Applications Langmuir-Blodgett films;[73] lasing systems;[74] nonlinear optical materials;[75] photographic materials[1,2,7–10,76–79]

Safety/Toxicity Hepatotoxicity;[80] mitochondrial toxicity[81]

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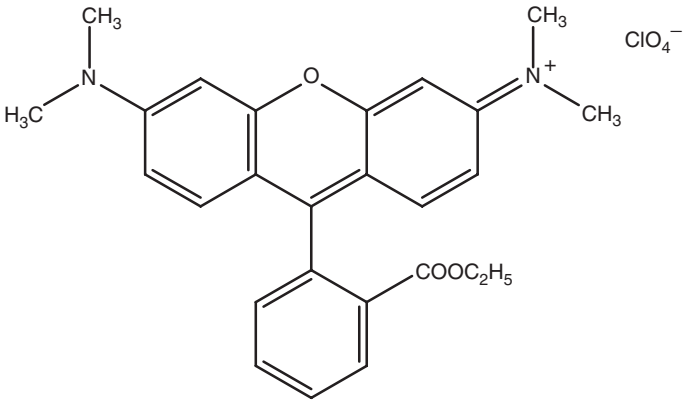
TETRAMETHYLRHODAMINE ETHYL ESTER PERCHLORATE (TMRE)

CAS Registry Number 115532-52-0

Chemical Structure



CA Index Name Xanthylium, 3,6-bis(dimethylamino)-9-[2-(ethoxycarbonyl)phenyl]-, perchlorate (1:1)

Other Names Xanthylium, 3,6-bis(dimethylamino)-9-[2-(ethoxycarbonyl)phenyl]-, perchlorate; T 669; Tetramethylrhodamine ethyl ester perchlorate; TMRE

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{26}H_{27}ClN_2O_7$

Molecular Weight 514.95

Physical Form Dark green crystals[2]

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 264–266 °C (decompose)[2]

Absorption (λ_{max}) 549 nm (MeOH)

Emission (λ_{max}) 574 nm (MeOH)

Molar Extinction Coefficient 109,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Mitochondria;[1–14,16,17] cells[1–4,15,20]

Biological/Medical Applications Monitoring/measuring membrane potential;[1–8] detecting/measuring analytes or metabolites;[15] cell viability assays;[1–4,15,20] apoptosis assays;[16–19] multidrug resistance assays[20]

Industrial Applications Semi-conducting polymer nanoparticles[21]

Safety/Toxicity Carcinogenicity[22]

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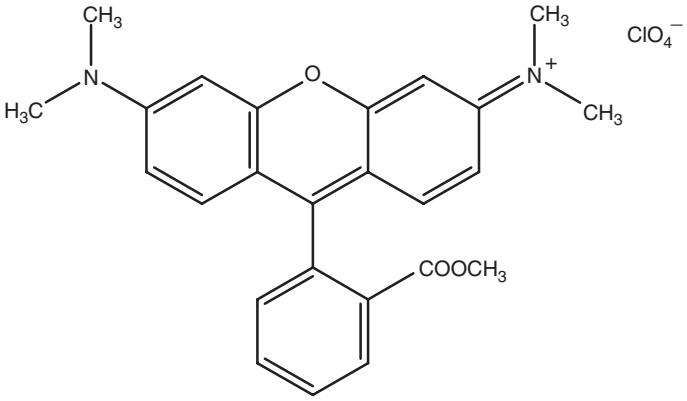
TETRAMETHYLRHODAMINE METHYL ESTER PERCHLORATE (TMRM)

CAS Registry Number 115532-50-8

Chemical Structure



CA Index Name Xanthylium, 3,6-bis(dimethylamino)-9-[2-(methoxycarbonyl)phenyl]-, perchlorate (1:1)

Other Names Xanthylium, 3,6-bis(dimethylamino)-9-[2-(methoxycarbonyl)phenyl]-, perchlorate; T 668; TMRM; Tetramethylrhodamine methyl ester perchlorate

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{25}H_{25}ClN_2O_7$

Molecular Weight 500.93

Physical Form Dark green crystals[2]

Solubility Soluble in *N,N*-dimethylformamide, dimethyl sulfoxide, ethanol, methanol

Melting Point 274–276 °C (decompose)[2]

Absorption (λ_{max}) 549 nm (MeOH)

Emission (λ_{max}) 573 nm (MeOH)

Molar Extinction Coefficient 115,000 cm^{-1} M^{-1} (MeOH)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Mitochondria;[1–7,10,11] cells[1–6,8,9,12]

Biological/Medical Applications Monitoring/measuring membrane potential;[1–7] detecting/measuring analytes or metabolites;[9] cell viability assays;[1–6,8,9,12] apoptosis assays;[10,11] multidrug resistance assays[12]

Industrial Applications Not reported

Safety/Toxicity No data available

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2. Ehrenberg, B.; Montana, V.; Wei, M. D.; Wuskell, J. P.; Loew, L. M. Membrane potential can be determined in individual cells from the Nernstian distribution of cationic dyes. *Biophys. J.* **1988**, *53*, 785–794.
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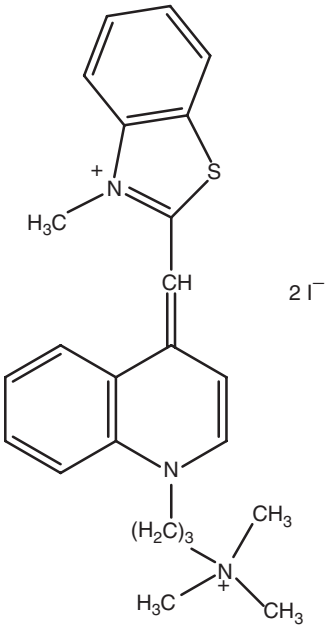
TO-PRO 1

CAS Registry Number 157199-59-2

Chemical Structure



CA Index Name Quinolinium, 4-[(3-methyl-2(3*H*)-benzothiazolylidene)-methyl]-1-[3-(trimethylammonio) propyl]-, iodide (1:2)

Other Names Quinolinium, 4-[(3-methyl-2(3*H*)-benzothiazolylidene)-methyl]-1-[3-(trimethylammonio) propyl]-, diiodide; TO-PRO 1; TO-PRO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{24}H_{29}I_2N_3S$

Molecular Weight 645.38

Physical Form Red-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 515 nm (H_2O/DNA)

Emission (λ_{max}) 531 nm (H_2O/DNA)

Molar Extinction Coefficient 62,800 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.25 (H_2O/DNA)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–17] cells;[1–3,17] nuclei;[18–20] bacteria;[3,4,21,22] cytoplasm;[20] eggs of zooplankton species;[23] leukocytes;[24] megakaryocyte;[25] microorganisms;[26,27] reticulocytes;[28] sperms[17,29]

Biological/Medical Applications Detecting nucleic acids,[1–17] cells,[1–3,17] classifying/counting leukocytes,[24] megakaryocytes;[25] counting erythroblasts,[18,19] sperms;[17,29] detecting/measuring microorganisms;[26,27] detecting location of cancer cells/tissues;[30] nucleic acids amplification;[16] nucleic acid sequencing;[31] as temperature sensor[32,33]

Industrial Applications Not reported

Safety/Toxicity No data available

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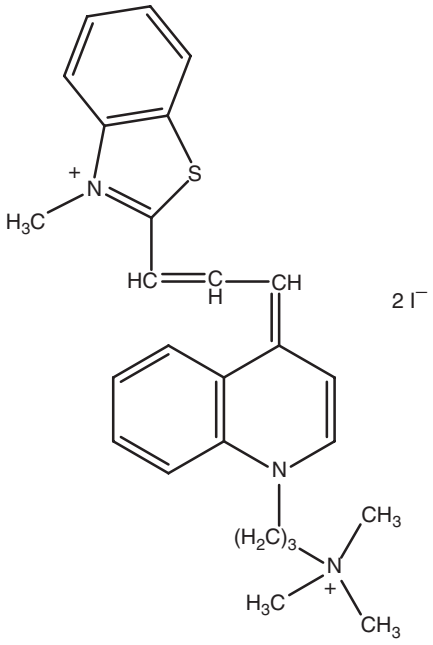
TO-PRO 3

CAS Registry Number 157199-63-8

Chemical Structure



CA Index Name Quinolinium, 4-[3-(3-methyl-2(3*H*)-benzothiazolylidene)-1-propen-1-yl]-1-[3-(trimethylammonio)propyl]-, iodide (1:2)

Other Names Quinolinium, 4-[3-(3-methyl-2(3*H*)-benzothiazolylidene)-1-propenyl]-1-[3-(trimethylammonio) propyl]-, diiodide; TO-PRO 3; TO-PRO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{26}H_{31}I_2N_3S$

Molecular Weight 671.42

Physical Form Red-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 642 nm (H_2O/DNA)

Emission (λ_{max}) 661 nm (H_2O/DNA)

Molar Extinction Coefficient 102,000 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.11 (H_2O/DNA)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–19] cells;[1–3,18–20] nuclei;[21–23] bacteria;[3,24–26] leukocytes;[27] liposomes;[28,29] microorganisms;[30–32] reticulocytes;[18,33] sperms[19]

Biological/Medical Applications Detecting nucleic acids,[1–19] cells,[1–3,18–20] microorganisms;[30–32] IDH1/IDH2 mutations,[34] JAK2 gene mutation,[35] PIK3CA mutation,[36] B-type Raf Kinase (BRAF) mutation;[37] classifying/counting leukocytes;[27] counting reticulocytes;[18,33] detecting/counting bacteria;[3,24–26] cytotoxicity assay;[38–40] drug delivery;[28,29] as temperature sensor[41,42]

Industrial Applications Not reported

Safety/Toxicity No data available

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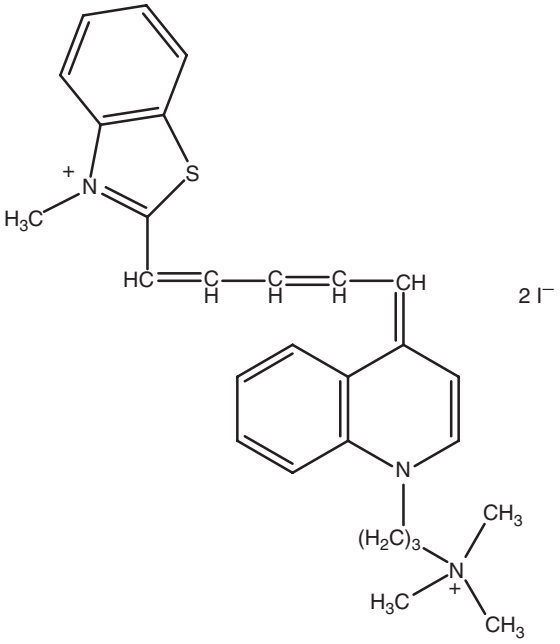
TO-PRO 5

CAS Registry Number 177027-61-1

Chemical Structure



CA Index Name Quinolinium, 4-[5-(3-methyl-2(3*H*)-benzothiazolylidene)-1,3-pentadien-1-yl]-1-[3-(trimethylammonio)propyl]-, iodide (1:2)

Other Names Quinolinium, 4-[5-(3-methyl-2(3*H*)-benzothiazolylidene)-1,3-pentadienyl]-1-[3-(trimethylammonio)propyl]-, diiodide; 3-methyl-2-[5-[1-[3-(trimethylammonio)propyl]-4(1*H*)-quinolinylidene]-1,3-pentadienyl]benzothiazolium diiodide; TO-PRO 5; TO-PRO 5 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{28}H_{33}I_2N_3S$

Molecular Weight 697.46

Physical Form Red-brown powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 748 nm (H_2O/DNA)

Emission (λ_{max}) 768 nm (H_2O/DNA)

Molar Extinction Coefficient 108,500 cm^{-1} M^{-1} (H_2O/DNA)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–11] cells;[1–3,11] bacteria;[3] proteins;[12] sperms[11]

Biological/Medical Applications Detecting nucleic acids,[1–11] cells[1–3,11]

Industrial Applications Not reported

Safety/Toxicity No data available

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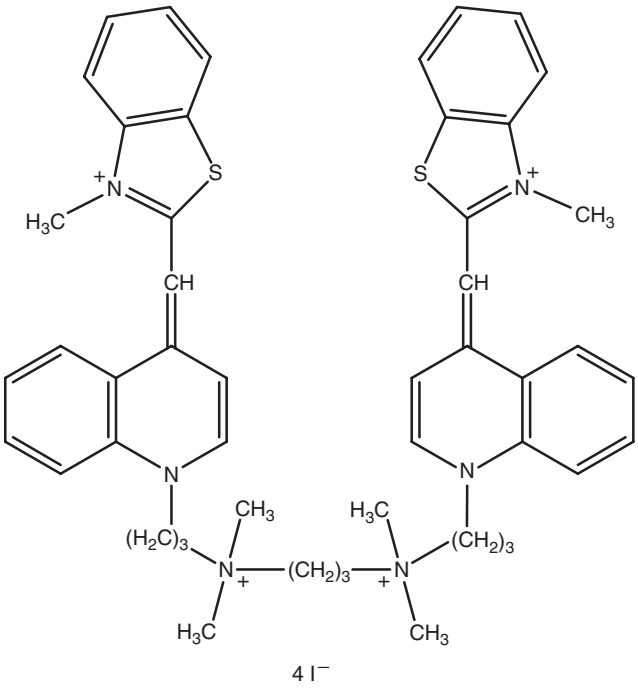
TOTO 1

CAS Registry Number 143413-84-7

Chemical Structure



CA Index Name Quinolinium, 1,1′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl]]bis[4-[(3-methyl-2 (3*H*)-benzothiazolylidene)methyl]-, iodide (1:4)

Other Names Quinolinium, 1,1′-[1,3-propanediylbis [(dimethyliminio)-3,1-propanediyl]]bis[4-[(3-methyl-2 (3*H*)-benzothiazolylidene)methyl]-, tetraiodide; TOTO 1; TOTO 1 iodide

Merck Index Number 9460

Chemical/Dye Class Cyanine

Molecular Formula $C_{49}H_{58}I_4N_6S_2$

Molecular Weight 1302.78

Physical Form Red powder[3,4]

Solubility Soluble in dimethyl sulfoxide

Melting Point 281 °C[2]

Absorption (λ_{max}) 514 nm (H_2O/DNA)

Emission (λ_{max}) 533 nm (H_2O/DNA)

Molar Extinction Coefficient 117,000 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.34 (H_2O/DNA)

Synthesis Synthetic methods[1–7]

Imaging/Labeling Applications Nucleic acids;[1–23] cells;[4,6,21–24] nuclei;[25,26] bacteria;[3,21,27–29] chromosoms;[30] chromosome spreads;[4] leukocytes;[31] micronuclei;[32] megakaryocyte;[33] microorganisms;[34,35] reticulocytes;[22] sperms[23,36]

Biological/Medical Applications Detecting nucleic acids,[1–23] cells,[4,6,21–24] characterizing chromosoms;[30] classifying/counting leukocytes,[31] megakaryocytes;[33] counting erythroblasts,[25,26] sperms;[23,36] detecting/measuring microorganisms;[34,35] detecting location of cancer cells/tissues;[37] nucleic acids amplification;[38] nanosensor platforms for diagnostic applications;[39] detecting/quantifying nuclease activity;[40,41] as temperature sensor[42,43]

Industrial Applications Marker systems for product authentication[44]

Safety/Toxicity No data available

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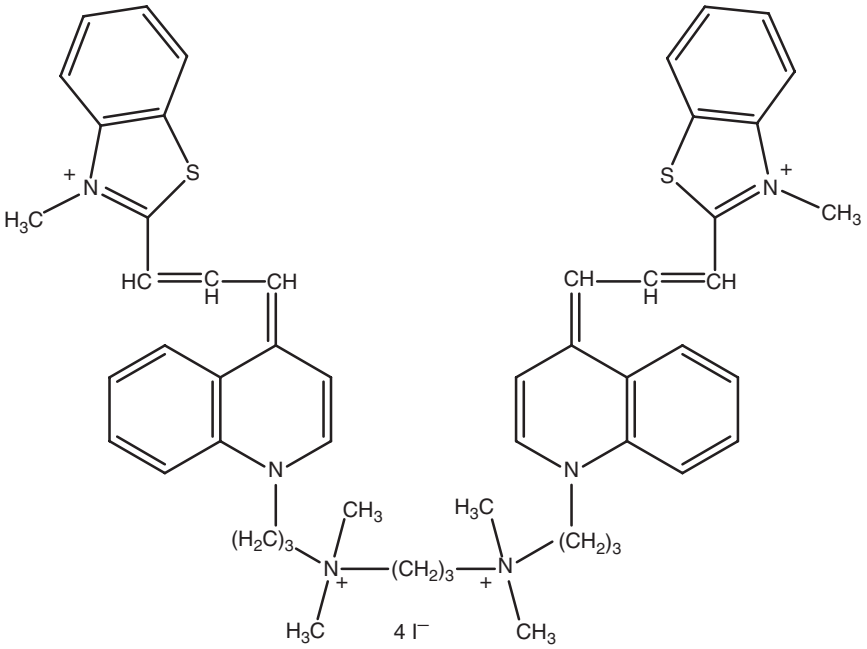
TOTO 3

CAS Registry Number 166196-17-4

Chemical Structure



CA Index Name Quinolinium, 1,1'-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl]]bis[4-[3-(3-methyl-2(3*H*)-benzothiazolylidene)-1-propen-1-yl]-, iodide (1:4)

Other Names Quinolinium, 1,1'-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl]]bis[4-[3-(3-methyl-2(3*H*)-benzothiazolylidene)-1-propenyl]-, tetraiodide; TOTO 3; TOTO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{53}H_{62}I_4N_6S_2$

Molecular Weight 1354.85

Physical Form Red powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 642 nm (H_2O/DNA)

Emission (λ_{max}) 660 nm (H_2O/DNA)

Molar Extinction Coefficient 154,100 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.06 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–14] cells;[2,12–14] nuclei;[15–19] bacteria;[12,20,21] chromosome spreads;[2] cytoplasm;[19] leukocytes;[22] megakaryocyte;[23] microorganisms;[24–26] porous wall hollow glass microspheres (PW-HGMs);[27] proteins;[28] reticulocytes;[13,29] sperms;[14,30] hairs[31]

Biological/Medical Applications Detecting nucleic acids,[1–14] cells,[2,12–14] microorganisms,[24–26] IDH1/IDH2 mutations,[32] JAK2 gene mutation,[33] PIK3CA mutation,[34] B-type Raf Kinase (BRAF) mutation;[35] classifying/counting leukocytes,[22] megakaryocytes;[23] counting erythroblasts,[17,18] reticulocytes;[13,29] sperms;[14,30] detecting/counting bacteria;[12,20,21] detecting/quantifying nuclease activity;[36,37] quantifying proteins;[28] monitoring ultrasound-mediated local drug delivery *in vivo*;[38] as temperature sensor[39,40]

Industrial Applications Semiconductor devices[41]

Safety/Toxicity No data available

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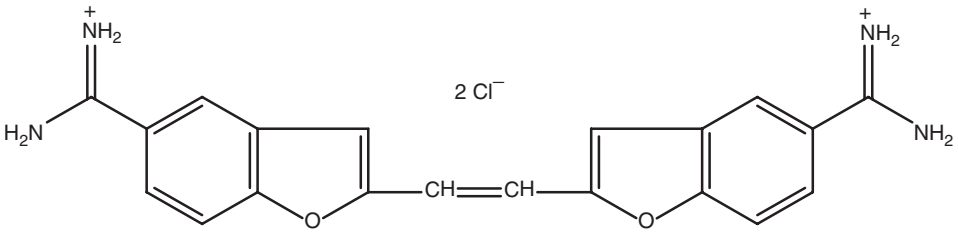
TRUE BLUE (TRUE BLUE CHLORIDE)

CAS Registry Number 71431-30-6

Chemical Structure



CA Index Name 5-Benzofurancarboximidamide, 2,2′-(1*E*)-1,2-ethenediylbis-, hydrochloride (1:2)

Other Names 5-Benzofurancarboximidamide, 2,2′-(1,2-ethenediyl)bis-, dihydrochloride, (*E*)-; 5-Benzofurancarboximidamide, 2,2′-(1*E*)-1,2-ethenediylbis-, dihydrochloride; NCI 240899; True Blue; True Blue chloride

Merck Index Number Not listed

Chemical/Dye Class Heterocycle; Benzofuran

Molecular Formula $C_{20}H_{18}Cl_2N_4O_2$

Molecular Weight 417.29

Physical Form Yellow solid

Solubility Soluble in water, *N,N*-dimethylformamide, dimethyl sulfoxide, methanol

Absorption (λ_{max}) 375 nm (H_2O)

Emission (λ_{max}) 403 nm (H_2O)

Molar Extinction Coefficient 68,000 cm^{-1} M^{-1} (H_2O)

Synthesis Synthetic method[1]

Imaging/Labeling Applications Analytes;[2] antibodies;[3] antigens;[3] axons;[4,5] cytoplasm;[5] endotoxins (lipopolysaccharides) (LPS);[6,7] keratin;[8] class III β-tubulin;[8] motoneural projections;[9] neurons[4,5,10–12,14–28]

Biological/Medical Applications Retrograde neuronal tracer;[4,5,10–12,14–28] detecting analytes,[2] axonal transport;[4,5] detecting/removing/inactivating/detoxifying endotoxins (lipopolysaccharides) (LPS);[6,7] evaluating a test element for antigens or antibodies;[3] assays for gene induction;[13] identifying genes related to malfunctions of central nervous system;[14] reducing the risk of iatrogenic nerve injury during a surgical procedure of the head or neck;[10] studying changes in motoneural projections;[9] preventing/treating septic shoc;[7] as temperature sensor[29,30]

Industrial Applications Not reported

Safety/Toxicity No data available

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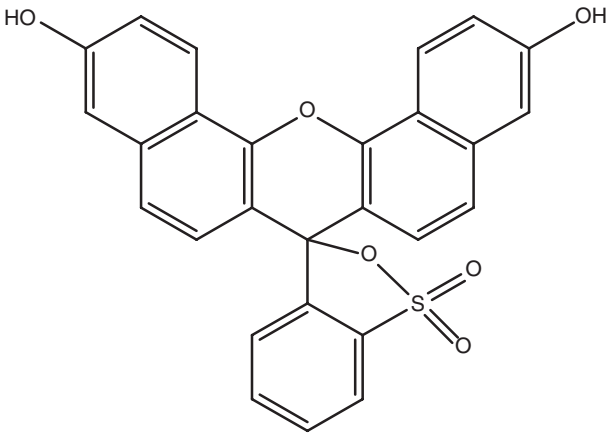
VITA BLUE

CAS Registry Number 122079-36-1

Chemical Structure



CA Index Name Spiro[3*H*-2,1-benzoxathiole-3,7′-[7*H*]dibenzo[*c*,*h*]xan-thene]-3′,11′-diol, 1,1-dioxide

Other Names Vita Blue

Merck Index Number Not listed

Chemical/Dye Class Xanthene

Molecular Formula $C_{27}H_{16}O_6S$

Molecular Weight 468.48

Physical Form Purple powder[1,2]

Solubility Soluble in dimethyl sulfoxide

Boiling Point (Calcd.) $756.2 \pm 60.0\,^{\circ}C$, pressure: 760 Torr

pK_a 7.56 ± 0.03, temperature: 22 °C

pK_a (Calcd.) 8.73 ± 0.20, most acidic, temperature: 25 °C

Absorption (λ_{max}) 609 nm (Buffer pH 9.5)

Emission (λ_{max}) 665 nm (Buffer pH 9.5)

Molar Extinction Coefficient $36{,}000\,cm^{-1}\,M^{-1}$ (Buffer pH 9.5)

Quantum Yield 0.15 (Buffer pH 9.5)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Cells;[1,2] stem cells[3–6]

Biological/Medical Applications Detecting/identifying cells;[1,2] discriminating between live and dead cells;[1,2] enhancing muscle stem cell activity;[3] increasing stem cell proliferation;[3–6] preventing/repairing cell damage due to aging, injury or disease (stroke, heart attack or coronary artery disease);[4–6] as a substrate for measuring alkaline phosphatases activity,[7] esterase activity,[1,2,7] peptidases/proteases activity,[7] kinases activity,[7] sulfatases activity;[7] treating stroke[6]

Industrial Applications Not reported

Safety/Toxicity No data available

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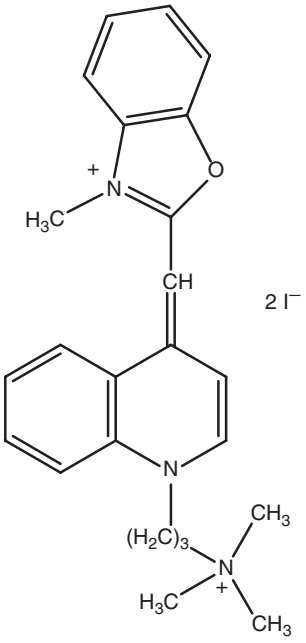
YO-PRO 1

CAS Registry Number 152068-09-2

Chemical Structure



CA Index Name Quinolinium, 4-[(3-methyl-2(3*H*)-benzoxazolylidene)-methyl]-1-[3-(trimethylammonio) propyl]-, iodide (1:2)

Other Names Quinolinium, 4-[(3-methyl-2(3*H*)-benzoxazolylidene) methyl]-1-[3-(trimethylammonio)propyl]-, diiodide; Oxazole yellow; YO-PRO 1; YO-PRO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{24}H_{29}I_2N_3O$

Molecular Weight 629.32

Physical Form Orange-red powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 491 nm (H_2O/DNA)

Emission (λ_{max}) 509 nm (H_2O/DNA)

Molar Extinction Coefficient 52,000 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.44 (H_2O/DNA)

Synthesis Synthetic methods[1–4]

Imaging/Labeling Applications Nucleic acids;[1–21] cells;[3,4,20–22] nuclei;[23–26] bacteria;[2,3,27] islets;[28] marine prokaryotes;[29] megakaryocyte;[30] micronuclei;[31] microorganisms;[32–36] reticulocytes;[20,37] sperms;[21,38–41] viruses[42,43]

Biological/Medical Applications Detecting nucleic acids,[1–21] cells,[3,4,20–22] bacteria,[2,3,27] microorganisms,[32–36] IDH1/IDH2 mutations,[44] PIK3CA mutation,[45] B-type Raf Kinase (BRAF) mutation;[46] analyzing marine prokaryotes;[29] classifying/counting megakaryocytes;[30] counting erythroblasts,[25,26] reticulocytes,[20,37] sperms,[21,38–41] viruses;[42,43] nucleic acids amplification;[19] nucleic acid hybridization;[47] nucleic acid sequencing;[48] apoptosis assay;[49–52] monitoring atmospheric/indoor bioaerosols;[53–55] as temperature sensor[56,57]

Industrial Applications Not reported

Safety/Toxicity Cytotoxicity;[58] neurotoxicity;[59] phototoxicity;[60] vasotoxicity[61]

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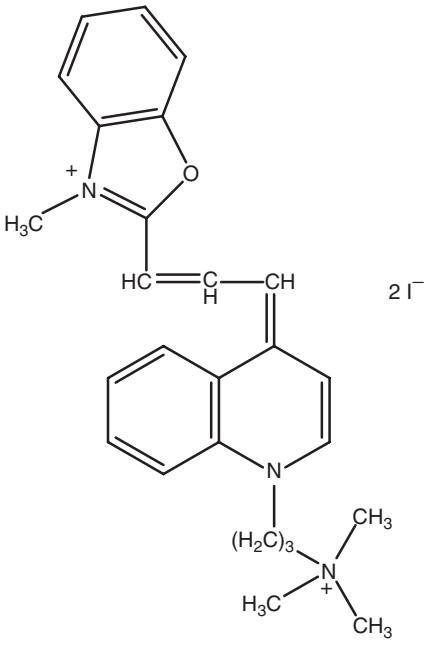
YO-PRO 3

CAS Registry Number 157199-62-7

Chemical Structure



CA Index Name Quinolinium, 4-[3-(3-methyl-2(3*H*)-benzoxazolylidene)-1-propen-1-yl]-1-[3-(trimethylammonio)propyl]-, iodide (1:2)

Other Names Quinolinium, 4-[3-(3-methyl-2(3*H*)-benzoxazolylidene)-1-propenyl]-1-[3-(trimethylammonio) propyl]-, diiodide; YO-PRO 3; YO-PRO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{26}H_{31}I_2N_3O$

Molecular Weight 655.36

Physical Form Orange-red powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 612 nm (H_2O/DNA)

Emission (λ_{max}) 631 nm (H_2O/DNA)

Molar Extinction Coefficient 100,100 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.16 (H_2O/DNA)

Synthesis Synthetic methods[1–3]

Imaging/Labeling Applications Nucleic acids;[1–11] cells;[1–3,11] nuclei;[12] bacteria;[3] cytoplasm;[12] microorganisms;[13] reticulocytes;[14] sperms[11]

Biological/Medical Applications Detecting nucleic acids;[1–11] cells;[1–3,11] microorganisms;[13] counting reticulocytes;[14] nucleic acids amplification;[10] nucleic acid hybridization[15]

Industrial Applications Not reported

Safety/Toxicity No data available

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using fluorescent dyes and kit useful therein. Eur. Pat. Appl. EP 684316, 1995.

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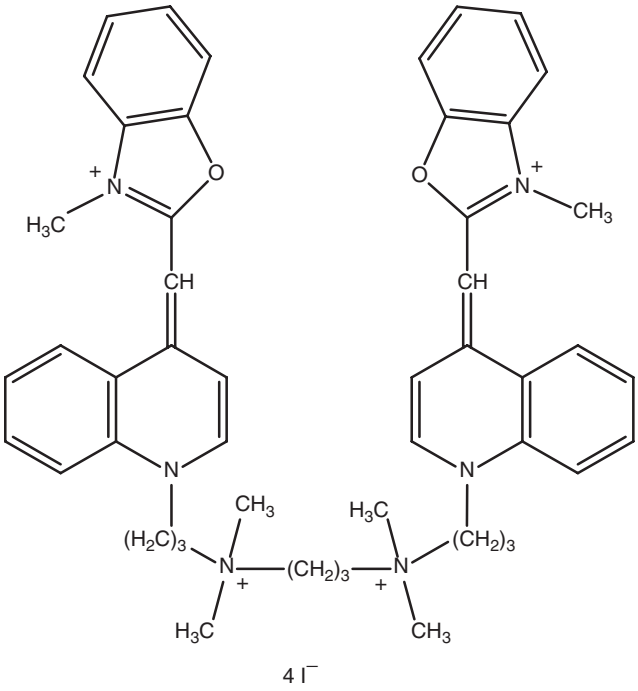
YOYO 1

CAS Registry Number 143413-85-8

Chemical Structure



CA Index Name Quinolinium, 1,1′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl]]bis[4-[(3-methyl-2(3*H*)-benzoxazolylidene)methyl]-, iodide (1:4)

Other Names Quinolinium, 1,1′-[1,3-propanediylbis[(dimethyliminio)-3,1-propanediyl]]bis[4-[(3-methyl-2(3*H*)-benzoxazolylidene)methyl]-, tetraiodide; YOYO 1; YOYO 1 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{49}H_{58}I_4N_6O_2$

Molecular Weight 1270.65

Physical Form Orange-red powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 491 nm (H_2O/DNA)

Emission (λ_{max}) 509 nm (H_2O/DNA)

Molar Extinction Coefficient 98,900 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.52 (H_2O/DNA)

Synthesis Synthetic methods[1–5]

Imaging/Labeling Applications Nucleic acids;[1–31] cells;[1–3,29–33] nuclei;[34–38] atherosclerotic plaque;[39] bacteria;[4,29,40] chromosomes;[41] chromosome spreads;[3] cytoplasm;[38] erythrocytes;[42–44] marine prokaryotes;[45] megakaryocyte;[46] micronuclei;[47] microorganisms;[48–50] reticulocytes;[30,51] sperms[31,52,53]

Biological/Medical Applications Detecting nucleic acids,[1–31] cells,[1–3,29–33] bacteria;[4,29,40] analyzing marine prokaryotes;[45] characterizing atherosclerotic plaque,[39] chromosomes;[41] classifying/counting megakaryocytes;[46] counting erythroblasts,[36,37] reticulocytes,[30,51] sperms;[31,52,53] detecting/measuring microorganisms;[48–50] detecting/quantifying nuclease activity;[54–56] evaluating freshness of a fish product;[57] nucleic acid amplification;[58] nucleic acid hybridization;[59] nucleic acid mapping;[60,61] nucleic acid sequencing;[62] nanosensor platforms for diagnostic applications;[63] as temperature sensor[64,65]

Industrial Applications Not reported

Safety/Toxicity Double-strand breaks in DNA/chromatin;[66] phototoxicity[67]

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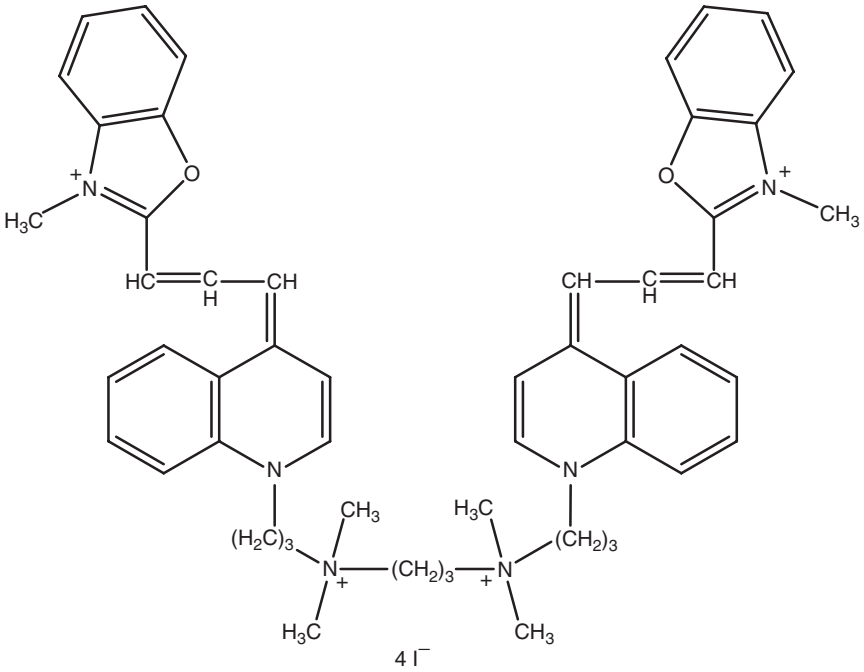
YOYO 3

CAS Registry Number 156312-20-8

Chemical Structure



CA Index Name Quinolinium, 1,1′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl]]bis[4-[3-(3-methyl-2(3*H*)-benzoxazolylidene)-1-propen-1-yl]-, iodide (1:4)

Other Names Quinolinium, 1,1′-[1,3-propanediylbis-[(dimethyliminio)-3,1-propanediyl]]bis[4-[3-(3-methyl-2(3*H*)-benzoxazolylidene)-1-propenyl]-, tetraiodide; YOYO 3; YOYO 3 iodide

Merck Index Number Not listed

Chemical/Dye Class Cyanine

Molecular Formula $C_{53}H_{62}I_4N_6O_2$

Molecular Weight 1322.73

Physical Form Orange-red powder

Solubility Soluble in dimethyl sulfoxide

Absorption (λ_{max}) 612 nm (H_2O/DNA)

Emission (λ_{max}) 631 nm (H_2O/DNA)

Molar Extinction Coefficient 167,000 cm^{-1} M^{-1} (H_2O/DNA)

Quantum Yield 0.15 (H_2O/DNA)

Synthesis Synthetic methods[1,2]

Imaging/Labeling Applications Nucleic acids;[1–11] cells;[1–3,11] bacteria;[3] chromosome spreads;[2] nuclei;[12–14] cytoplasm;[14] microorganisms;[15,16] porous wall hollow glass microspheres;[17] reticulocytes;[18] sperms[11,19]

Biological/Medical Applications Detecting nucleic acids,[1–11] cells,[1–3,11] microorganisms;[15,16] counting erythroblasts,[12,13] reticulocytes,[18] sperms;[11,19] nucleic acid hybridization;[20] nucleic acid nanochannel device;[21] nucleic acid sequencing[22,23]

Industrial Applications Analyzing polymers[17]

Safety/Toxicity No data available

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APPENDIX A
INDEX OF CAS REGISTRY NUMBERS

CAS Registry Number	Dye	Page Number
65-61-2	Acridine Orange (AO)	3
596-09-8	Fluorescein diacetate (FDA)	213
779-27-1	7-Hydroxycoumarin-3-carboxylic acid (Umbelliferone-3-carboxylic acid)	246
905-96-4	3,3′-Diethyloxacarbocyanine iodide ($DiOC_2(3)$)	160
959-81-9	4-[4-(Dimethylamino)styryl]-*N*-methylpyridinium iodide (4-Di-1-ASP) (DASPMI)	183
989-38-8	Rhodamine 6G (RH 6G)	373
1239-45-8	Ethidium bromide (Homidium bromide)	193
2321-07-5	Fluorescein	205
3301-79-9	6-Carboxyfluorescein	114
3326-32-7	Fluoroscein-5-isothiocyanate (FITC)	219
3348-03-6	6-Carboxyfluorescein diacetate	121
3520-43-2	5,5′,6,6′-Tetrachloro-1,1′,3,3′-tetraethylbenzimidazolocarbocyanine iodide (JC-1)	389
3548-09-2	9-Amino-6-chloro-2-methoxyacridine (ACMA)	46
3785-01-1	2-[4-(Dimethylamino)styryl]-*N*-ethylpyridinium iodide (DASPEI)	181
5852-10-8	7-Hydroxy-4-methylcoumarin-3-acetic acid	252
6358-69-6	8-Hydroxypyrene-1,3,6-trisulfonic acid trisodium salt (HPTS) (Pyranine)	253
13558-31-1	Rhodamine 110 (RH 110)	380
19088-73-4	3-Cyano-7-hydroxycoumarin (3-Cyanoumbelliferone)	141
20300-59-8	7-Methoxycoumarin-3-carboxylic acid	281
23491-45-4	Hoechst 33258	231
23555-00-2	Hoechst 34580	244
25535-16-4	Propidium iodide (PI)	328
26038-83-5	4-Heptadecyl-7-hydroxycoumarin (4-Heptadecylumbelliferone)	227
26093-31-2	7-Amino-4-methylcoumarin (AMC) (Coumarin 120) (Coumarin 440)	54
28718-90-3	4′,6-Diamidino-2-phenylindole dihydrochloride (DAPI)	145
35231-44-8	4-Bromomethyl-7-methoxycoumarin	95
41387-42-2	Acridine orange 10-dodecyl bromide (Dodecyl-Acridine Orange (DAO))	10
42189-56-0	*N*-(1-Pyrenyl)maleimide	357
50995-74-9	7-Diethylaminocoumarin-3-carboxylic acid (DAC) (DEAC)	149
53213-81-3	3,3′-Dipentyloxacarbocyanine iodide ($DiOC_5(3)$)	187
53213-82-4	3,3′-Dihexyloxacarbocyanine iodide ($DiOC_6(3)$)	165
53213-83-5	3,3′-Diheptyloxacarbocyanine iodide ($DiOC_7(3)$)	163
53213-94-8	3,3′-Dipropylthiadicarbocyanine iodide ($DiSC_3(5)$)	189
55486-13-0	1-Pyrenebutanoic acid hydrazide (PBH)	334
57576-49-5	Acridine Homodimer	1
59572-10-0	1,3,6,8-Pyrenetetrasulfonic acid tetrasodium salt	352
61494-52-8	1-Pyrenesulfonyl chloride	350
61926-22-5	Ethidium Homodimer-1 (EthD-1)	199
62669-70-9	Rhodamine 123 (RH 123)	384
62758-13-8	Resazurin sodium salt (Alamar Blue)	370
64701-47-9	1-Pyrenedecanoic acid (PDA)	340

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CAS Registry Number	Dye	Page Number
69168-45-2	1-Pyrenedodecanoic acid (PDDA)	343
71431-30-6	True Blue (True Blue chloride)	411
74681-68-8	Nuclear Yellow (Hoechst S 769121)	295
74802-04-3	7-Dimethylamino-4-methylcoumarin-3-isothiocyanate (DACITC)	180
75168-11-5	Acridine Orange 10-nonyl bromide (Nonyl-Acridine Orange (NAO))	12
76823-03-5	5-Carboxyfluorescein	110
76863-28-0	Fluorescein-5-thiosemicarbazide	224
76936-87-3	*N*-(1-Pyrenyl)iodoacetamide	355
79955-27-4	5-Carboxyfluorescein diacetate	119
80883-54-1	7-Dimethylaminocoumarin-4-acetic acid (DMACA)	176
82412-15-5	7-Anilinocoumarin-4-acetic acid (ACAA)	65
82962-86-5	8-Methoxypyrene-1,3,6-trisulfonic acid trisodium salt (MPTS)	287
85985-44-0	9-Anthroylnitrile	66
86701-10-2	NBD C_6-ceramide	289
88404-25-5	4-Bromomethyl-6,7-dimethoxycoumarin	91
88404-26-6	6,7-Dimethoxycoumarin-4-acetic acid	175
90936-84-8	1-Pyrenehexadecanoic acid	346
90936-85-9	1-Pyrenehexanoic acid (PHA)	348
92557-80-7	5-Carboxyfluorescein succinimidyl ester	125
92557-81-8	6-Carboxyfluorescein succinimidyl ester	129
96686-59-8	7-Dimethylaminocoumarin-4-acetic acid succinimidyl ester (DMACA SE)	178
97632-67-2	7-Methoxycoumarin-3-carbonyl azide	280
100343-98-4	7-Diethylaminocoumarin-3-carboxylic acid hydrazide (DCCH)	153
101821-61-8	LysoSensor Blue DND 167	269
105802-46-8	4-[4-(Diethylamino)styryl]-*N*-methylpyridinium iodide (4-Di-2-ASP)	157
109244-58-8	Dihydrorhodamine 123 (DHR 123)	169
114932-60-4	1-Pyrenebutanoic acid succinimidyl ester	336
115532-50-8	Tetramethylrhodamine methyl ester perchlorate (TMRM)	396
115532-52-0	Tetramethylrhodamine ethyl ester perchlorate (TMRE)	394
117620-77-6	3-Cyano-7-ethoxycoumarin (7-Ethoxycoumarin-3-carbonitrile)	139
122079-36-1	Vita Blue	413
133867-52-4	BODIPY FL C_5-succinimidyl ester	83
133867-53-5	BODIPY FL C_5-ceramide (C_5-DMB-ceramide)	74
134471-24-2	7-Hydroxycoumarin-3-carboxylic acid succinimidyl ester	250
137182-38-8	Cascade Blue hydrazide trisodium salt	138
138039-58-4	Cascade Blue acetyl azide trisodium salt	136
139346-57-9	7-Diethylaminocoumarin-3-carboxylic acid succinimidyl ester (DEAC SE)	155
142975-81-3	5-Carboxy-2′,7′-dichlorofluorescein	102
143413-84-7	TOTO 1	405
143413-85-8	YOYO 1	421
144316-86-9	6-Carboxy-2′,7′-dichlorofluorescein	104
144489-09-8	5-Carboxy-2′,7′-dichlorofluorescein diacetate	106
144489-10-1	6-Carboxy-2′,7′-dichlorofluorescein diacetate	108
145103-60-2	5-Carboxynaphthofluorescein	132
145103-61-3	6-Carboxynaphthofluorescein	134
148942-72-7	5-(Bromomethyl)fluorescein	93
150321-92-9	7-Methoxycoumarin-3-carboxylic acid succinimidyl ester	285
152068-09-2	YO-PRO 1	415
152584-38-8	LysoSensor Green DND 189	273
154757-99-0	POPO 3	322

CAS Registry Number	Dye	Page Number
156312-20-8	YOYO 3	425
157199-56-9	PO-PRO 1	324
157199-57-0	BO-PRO 1	87
157199-59-2	TO-PRO 1	398
157199-62-7	YO-PRO 3	419
157199-63-8	TO-PRO 3	400
157673-16-0	7-Diethylaminocoumarin-3-carbonyl azide	148
161016-55-3	PO-PRO 3	326
166196-17-4	TOTO 3	408
166821-89-2	LysoSensor Blue DND 192	271
168482-84-6	Calcein Blue AM	101
169454-13-1	BOBO 1	69
169454-15-3	POPO 1	320
169454-17-5	BOBO 3	71
173357-16-9	BO-PRO 3	89
177027-61-1	TO-PRO 5	403
180389-01-9	Ethidium Homodimer-2 (EthD-2)	203
191853-29-9	BODIPY FL C_5-sphingomyelin (C_5-DMB-sphingomyelin)	81
195136-52-8	Oregon Green 488 carboxylic acid	302
195136-58-4	Oregon Green 488 (2′,7′-Difluorofluorescein)	297
195136-74-4	Oregon Green 488 carboxylic acid diacetate	306
196504-57-1	8-Aminopyrene-1,3,6-trisulfonic acid trisodium salt (APTS)	63
198139-49-0	Oregon Green 514 carboxylic acid	304
198139-51-4	Oregon Green 488 carboxylic acid succinimidyl ester	308
198139-53-6	Oregon Green 514 carboxylic acid succinimidyl ester	310
200554-19-4	Alexa Fluor 350 carboxylic acid succinimidyl ester (AMCA-S)	15
211566-66-4	Hexidium iodide	229
214147-22-5	NBD methylhydrazine (MNBDH)	293
215868-23-8	Marina Blue (6,8-Difluoro-7-hydroxy-4-methylcoumarin) (DiFMU)	277
215868-31-8	Pacific Blue (6,8-Difluoro-7-hydroxycoumarin-3-carboxylic acid)	315
215868-33-0	Pacific Blue succinimidyl ester	318
217176-83-5	Dihydrorhodamine 6G (DHR 6G)	173
222164-96-7	Alexa Fluor 488 carboxylic acid succinimidyl ester	20
231632-16-9	LysoSensor Green DND 153	272
231632-18-1	LysoSensor Yellow/Blue DND 160 (PDMPO)	275
251955-11-0	BODIPY FL C_5-lactosylceramide	79
254109-20-1	4-Amino-5-methylamino-2′,7′-difluorofluorescein (DAF-FM)	50
254109-22-3	4-Amino-5-methylamino-2′,7′-difluorofluorescein diacetate (DAF-FM DA)	52
295348-87-7	Alexa Fluor 594 carboxylic acid succinimidyl ester	30
296277-09-3	RedoxSensor Red CC-1	369
304014-12-8	QSY 7 carboxylic acid succinimidyl ester	361
304014-13-9	QSY 21 carboxylic acid succinimidyl ester	366
305801-86-9	JO-PRO 1	265
305801-87-0	JOJO 1	263
305802-06-6	LOLO 1	267
328085-55-8	Oregon Green 488 maleimide	312
422309-89-5	Alexa Fluor 660 carboxylic acid succinimidyl ester	35
467233-94-9	Alexa Fluor 430 carboxylic acid succinimidyl ester	17
477876-64-5	Alexa Fluor 532 carboxylic acid succinimidyl ester	25
522592-13-8	3,3′-Dimethyl-α-naphthoxacarbocyanine iodide (JC-9)	186

CAS Registry Number	Dye	Page Number
571186-05-5	BODIPY TR ceramide	85
697795-06-5	Alexa Fluor 750 carboxylic acid succinimidyl ester	42
700834-40-8	QSY 9 carboxylic acid succinimidyl ester	364
875756-97-1	Hoechst 33342	238
886046-94-2	Alexa Fluor 555 carboxylic acid succinimidyl ester	28
886210-16-8	Oregon Green 488 cadaverine	300
908143-55-5	BODIPY FL C_5-ganglioside GM1	77
918946-23-3	Alexa Fluor 514 carboxylic acid succinimidyl ester	23
934216-71-4	Pacific Blue C_5-maleimide	317
948558-33-6	Alexa Fluor 680 carboxylic acid succinimidyl ester	38
950891-33-5	Alexa Fluor 790 carboxylic acid succinimidyl ester	45
1132773-86-4	Alexa Fluor 633 carboxylic acid succinimidyl ester	33
1246956-22-8	Alexa Fluor 700 carboxylic acid succinimidyl ester	40

APPENDIX B
INDEX OF ACRIDINES

Dye	Page Number
Acridine Homodimer	1
Acridine Orange (AO)	3
Acridine Orange 10-dodecyl bromide (Dodecyl-Acridine Orange (DAO))	10
Acridine Orange 10-nonyl bromide (Nonyl-Acridine Orange (NAO))	12
9-Amino-6-chloro-2-methoxyacridine (ACMA)	46

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APPENDIX C
INDEX OF ANTHRACENES

Dye	Page Number
9-Anthroylnitrile	66
LysoSensor Blue DND 167	269
LysoSensor Blue DND 192	271

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APPENDIX D
INDEX OF BORON CO-ORDINATION COMPOUNDS/DYES

Dye	Page Number
BODIPY FL C_5-ceramide (C_5-DMB-ceramide)	74
BODIPY FL C_5-ganglioside GM1	77
BODIPY FL C_5-lactosylceramide	79
BODIPY FL C_5-sphingomyelin (C_5-DMB-sphingomyelin)	81
BODIPY FL C_5-succinimidyl ester	83
BODIPY TR ceramide	85

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APPENDIX E
INDEX OF COUMARINS

Dye	Page Number
Alexa Fluor 350 carboxylic acid succinimidyl ester (AMCA-S)	15
7-Amino-4-methylcoumarin (AMC) (Coumarin 120) (Coumarin 440)	54
7-Anilinocoumarin-4-acetic acid (ACAA)	65
4-Bromomethyl-6,7-dimethoxycoumarin	91
4-Bromomethyl-7-methoxycoumarin	95
Calcein Blue AM	101
3-Cyano-7-ethoxycoumarin (7-Ethoxycoumarin-3-carbonitrile)	139
3-Cyano-7-hydroxycoumarin (3-Cyanoumbelliferone)	141
7-Diethylaminocoumarin-3-carbonyl azide	148
7-Diethylaminocoumarin-3-carboxylic acid (DAC) (DEAC)	149
7-Diethylaminocoumarin-3-carboxylic acid hydrazide (DCCH)	153
7-Diethylaminocoumarin-3-carboxylic acid succinimidyl ester (DEAC SE)	155
6,7-Dimethoxycoumarin-4-acetic acid	175
7-Dimethylaminocoumarin-4-acetic acid (DMACA)	176
7-Dimethylaminocoumarin-4-acetic acid succinimidyl ester (DMACA SE)	178
7-Dimethylamino-4-methylcoumarin-3-isothiocyanate (DACITC)	180
4-Heptadecyl-7-hydroxycoumarin (4-Heptadecylumbelliferone)	227
7-Hydroxycoumarin-3-carboxylic acid (Umbelliferone-3-carboxylic acid)	246
7-Hydroxycoumarin-3-carboxylic acid succinimidyl ester	250
7-Hydroxy-4-methylcoumarin-3-acetic acid	252
Marina Blue (6,8-Difluoro-7-hydroxy-4-methylcoumarin) (DiFMU)	277
7-Methoxycoumarin-3-carbonyl azide	280
7-Methoxycoumarin-3-carboxylic acid	281
7-Methoxycoumarin-3-carboxylic acid succinimidyl ester	285
Pacific Blue (6,8-Difluoro-7-hydroxycoumarin-3-carboxylic acid)	315
Pacific Blue C_5-maleimide	317
Pacific Blue succinimidyl ester	318

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APPENDIX F
INDEX OF CYANINES/STYRYLS

Dye	Page Number
BOBO 1	69
BOBO 3	71
BO-PRO 1	87
BO-PRO 3	89
4-[4-(Diethylamino)styryl]-*N*-methylpyridinium iodide (4-Di-2-ASP)	157
3,3′-Diethyloxacarbocyanine iodide ($DiOC_2(3)$)	160
3,3′-Diheptyloxacarbocyanine iodide ($DiOC_7(3)$)	163
3,3′-Dihexyloxacarbocyanine iodide ($DiOC_6(3)$)	165
2-[4-(Dimethylamino)styryl]-*N*-ethylpyridinium iodide (DASPEI)	181
4-[4-(Dimethylamino)styryl]-*N*-methylpyridinium iodide (4-Di-1-ASP) (DASPMI)	183
3,3′-Dimethyl-α-naphthoxacarbocyanine iodide (JC-9)	186
3,3′-Dipentyloxacarbocyanine iodide ($DiOC_5(3)$)	187
3,3′-Dipropylthiadicarbocyanine iodide ($DiSC_3(5)$)	189
JOJO 1	263
JO-PRO 1	265
LOLO 1	267
POPO 1	320
POPO 3	322
PO-PRO 1	324
PO-PRO 3	326
5,5′,6,6′-Tetrachloro-1,1′,3,3′-tetraethylbenzimidazolocarbocyanine iodide (JC-1)	389
TO-PRO 1	398
TO-PRO 3	400
TO-PRO 5	403
TOTO 1	405
TOTO 3	408
YO-PRO 1	415
YO-PRO 3	419
YOYO 1	421
YOYO 3	425

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APPENDIX G
INDEX OF HETEROCYCLES

Dye	Page Number
Alexa Fluor 430 carboxylic acid succinimidyl ester	17
4′,6-Diamidino-2-phenylindole dihydrochloride (DAPI)	145
Ethidium bromide (Homidium bromide)	193
Ethidium Homodimer-1 (EthD-1)	199
Ethidium Homodimer-2 (EthD-2)	203
Hexidium iodide	229
Hoechst 33258	231
Hoechst 33342	238
Hoechst 34580	244
LysoSensor Green DND 153	272
LysoSensor Green DND 189	273
LysoSensor Yellow/Blue DND 160 (PDMPO)	275
NBD C_6-ceramide	289
NBD methylhydrazine (MNBDH)	293
Nuclear Yellow (Hoechst S 769121)	295
Propidium iodide (PI)	328
Resazurin sodium salt (Alamar Blue)	370
True Blue (true blue chloride)	411

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APPENDIX H
INDEX OF PYRENES

Dye	Page Number
8-Aminopyrene-1,3,6-trisulfonic acid trisodium salt (APTS)	63
Cascade Blue acetyl azide trisodium salt	136
Cascade Blue hydrazide trisodium salt	138
8-Hydroxypyrene-1,3,6-trisulfonic acid trisodium salt (HPTS) (Pyranine)	253
8-Methoxypyrene-1,3,6-trisulfonic acid trisodium salt (MPTS)	287
1-Pyrenebutanoic acid hydrazide (PBH)	334
1-Pyrenebutanoic acid succinimidyl ester	336
1-Pyrenedecanoic acid (PDA)	340
1-Pyrenedodecanoic acid (PDDA)	343
1-Pyrenehexadecanoic acid	346
1-Pyrenehexanoic acid (PHA)	348
1-Pyrenesulfonyl chloride	350
1,3,6,8-Pyrenetetrasulfonic acid tetrasodium salt	352
N-(1-Pyrenyl)iodoacetamide	355
N-(1-Pyrenyl)maleimide	357

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APPENDIX I
INDEX OF XANTHENES

Dye	Page Number
Alexa Fluor 488 carboxylic acid succinimidyl ester	20
Alexa Fluor 514 carboxylic acid succinimidyl ester	23
Alexa Fluor 532 carboxylic acid succinimidyl ester	25
Alexa Fluor 594 carboxylic acid succinimidyl ester	30
4-Amino-5-methylamino-2′,7′-difluorofluorescein (DAF-FM)	50
4-Amino-5-methylamino-2′,7′-difluorofluorescein diacetate (DAF-FM DA)	52
5-(Bromomethyl)fluorescein	93
5-Carboxy-2′,7′-dichlorofluorescein	102
6-Carboxy-2′,7′-dichlorofluorescein	104
5-Carboxy-2′,7′-dichlorofluorescein diacetate	106
6-Carboxy-2′,7′-dichlorofluorescein diacetate	108
5-Carboxyfluorescein	110
6-Carboxyfluorescein	114
5-Carboxyfluorescein diacetate	119
6-Carboxyfluorescein diacetate	121
5-Carboxyfluorescein succinimidyl ester	125
6-Carboxyfluorescein succinimidyl ester	129
5-Carboxynaphthofluorescein	132
6-Carboxynaphthofluorescein	134
Dihydrorhodamine 123 (DHR 123)	169
Dihydrorhodamine 6G (DHR 6G)	173
Fluorescein	205
Fluorescein diacetate (FDA)	213
Fluoroscein-5-isothiocyanate (FITC)	219
Fluorescein-5-thiosemicarbazide	224
Oregon Green 488 (2′,7′-Difluorofluorescein)	297
Oregon Green 488 cadaverine	300
Oregon Green 488 carboxylic acid	302
Oregon Green 514 carboxylic acid	304
Oregon Green 488 carboxylic acid diacetate	306
Oregon Green 488 carboxylic acid succinimidyl ester	308
Oregon Green 514 carboxylic acid succinimidyl ester	310
Oregon Green 488 maleimide	312
QSY 7 carboxylic acid succinimidyl ester	361
QSY 9 carboxylic acid succinimidyl ester	364
QSY 21 carboxylic acid succinimidyl ester	366

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Dye	Page Number
RedoxSensor Red CC-1	369
Rhodamine 6G (RH 6G)	373
Rhodamine 110 (RH 110)	380
Rhodamine 123 (RH 123)	384
Tetramethylrhodamine ethyl ester perchlorate (TMRE)	394
Tetramethylrhodamine methyl ester perchlorate (TMRM)	396
Vita Blue	413

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