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Database of Absorption and Fluorescence Spectra of >300 Common Compounds for use in PhotochemCAD

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ABSTRACT

The design of new molecules for photochemical studies typically requires knowledge of spectral features of pertinent chromophores beginning with the absorption spectrum (λ_{abs}) and accompanying molar absorption coefficient (ϵ , $\text{M}^{-1}\text{cm}^{-1}$) and often extending to the fluorescence spectrum (λ_{em}) and fluorescence quantum yield (Φ_f), where the fluorescence properties may be of direct relevance or useful as proxies to gain insight into the nature of the first excited singlet state. PhotochemCAD databases, developed over a period of 30 years, are described here. The previous databases for 150 compounds have been expanded to encompass 339 compounds for which absorption spectra (including ϵ values), fluorescence spectra (including Φ_f values) and references to the primary literature have been included where available (551 spectra altogether). The compounds exhibit spectra in the ultraviolet, visible, and/or near-infrared spectral regions. The compound classes and number of members include acridines (21), aromatic hydrocarbons (41), arylmethane dyes (11), azo dyes (18), biomolecules (18), chlorins/bacteriochlorins (16), coumarins (14), cyanine dyes (19), dipyrins (7), heterocycles (26), miscellaneous dyes (13), oligophenylenes (13), oligopyrroles (6), perylenes (5), phthalocyanines (11), polycyclic aromatic hydrocarbons (16), polyenes/polyynes (10), porphyrins (34), quinones (24), and xanthenes (15). A database of 31 solar spectra also is included.

INTRODUCTION

Studies in photochemistry inevitably start with the absorption of light, and with that quantum step arises the qualitative issue of wavelength of absorption and the quantitative issue of the intensity of absorption. The absorption spectrum of a compound thus is the first expression of possible photoactivity. Following absorption, fluorescence emission may be of central importance as occurs in various fluorometric analytical procedures (e.g., flow cytometry); regardless, the nature and intensity of the fluorescence spectrum provide information concerning the properties of the excited singlet state. Hence, knowledge of absorption and fluorescence spectra of diverse compounds is essential to photochemical studies and is an integral to the molecular design of photofunctional molecules.

Our effort to assemble databases of absorption and fluorescence spectral data began in the mid-late 1980s. While a number of databases were available at that time for absorption (1-17) and fluorescence (11,18-25) the assembled data typically were qualitative and spare (e.g., tabulations of selected wavelengths of absorption spectra) without quantitative features, and most that were available emphasized compounds with ultraviolet absorption (although some data were available for selected dyestuffs (24-28). Moreover, pointers to the original literature where the spectra were collected often were not available. Yet, even if data were available in printed collections, digital data were needed for use in calculations. Hence, PhotochemCAD – a program with integrated spectral databases for diverse photophysical calculations – grew out of an effort to have at one's metaphorical if not literal fingertips the spectral data needed for diverse studies in photochemistry. A key objective was to collect in one location the fundamental photochemical parameters of a representative set of compounds [e.g., absorption and fluorescence spectra, molar absorption coefficient (ϵ), fluorescence quantum yield (Φ_f)] accompanied by references to the

original literature where such data were first reported, and provide the capability to perform a variety of calculations that employ absorption and fluorescence spectra.

The biggest challenge in developing PhotochemCAD concerned the laborious assembly of the databases rather than software development for the various calculational modules. In that era, computer-based searching of the literature resided, if at all, in the province of science librarians and was not commonly available to individual patrons, at least without prohibitively steep fees; regardless, even with computer-based search tools, finding fundamental photophysical data (e.g., spectra, ϵ , Φ_f values) often was not assured. Hence, the first database, of spectral data for 125 compounds, was assembled by (1) manual searching the literature by one of us (JSL) to find photophysical data for each compound, (2) acquiring a sample of each compound, (3) recording the absorption spectrum and fluorescence spectrum of each compound, and (4) combining the recorded spectra with photophysical data from the available literature.

The first version (PhotochemCAD 1) contained spectral data for 125 compounds (29). PhotochemCAD 2 chiefly featured revisions to the user interface whereas the spectral databases only included a few additional compounds, to 150 total (30). A small database of naturally occurring (or naturally derived) tetrapyrrole macrocycles (free base and metal chelates) (31, 32) was added several years ago. Here, the spectral database has been more than doubled, containing 551 absorption and fluorescence spectra for 339 compounds. The compounds selected include those with absorption ranging from the ultraviolet (200–400 nm) across the visible (400–700 nm) into the near-infrared (700–1000 nm) spectral regions. The spectra are accompanied by the molecular structure and references to the original scientific literature. The databases are best employed with the revised program, PhotochemCAD 3. The features of PhotochemCAD 3 have been described in detail in the companion paper (33). The comprehensive description of the

absorption and fluorescence spectral databases of PhotochemCAD 3 provided herein should prove useful for diverse studies in photochemistry.

MATERIALS AND METHODS

The absorption and fluorescence database includes the literature values for ϵ and the wavelength maximum (to which the ϵ corresponds) where such values could be located. Values reported without a literature citation were obtained by one of the authors. The wavelength maximum of the absorption spectrum in the database often is slightly shifted from the reported maximum in the literature. These small differences are within the range of variation expected in experimental work. The literature molar absorption coefficient values have been used and applied to the wavelength maximum observed upon collecting the absorption spectrum. These discrepancies between the literature values (λ , ϵ) and our observed value (λ) are likely to be inconsequential for most considerations. Such discrepancies have been noted for each compound.

Terminology. Values in the database have been drawn from literature dating from the mid-20th century. In so doing, present terminology has been adopted. Thus, molar absorption coefficient (ϵ) is used in place of extinction coefficient; absorbance (A) in lieu of optical density (OD). The term fluorescence quantum yield (Φ_f) has its usual definition of (number of photons emitted)/(number of photons absorbed). All other photochemical terms are used in accord with standard IUPAC recommendations (34,35).

Absorption spectra. Absorption spectra were collected using a Cary III UV-Vis spectrophotometer (a double-beam scanning instrument) or an HP 8453 UV-Vis spectrophotometer (a single-beam scanning instrument). Cary III: Data were obtained using a spectral bandwidth of 1.0 nm, a signal averaging time of 0.133 sec, a data interval of 0.250 nm, and a scan rate of 112.500 nm/min. HP 8453: Data were obtained using a spectral bandwidth of

1.0 nm. A known limitation of this diode-array spectrometer is the appearance of a spike at ~655 nm, due to an imbalance in the lamp intensity from recording the respective blank and sample. A manual data-smoothing procedure has been applied to remove the instrumental spike in many of the spectra. Regardless of instrument, other spectra have been manually corrected for any significant baseline offset due to an imbalance between the blank and sample.

Fluorescence spectra. Fluorescence spectra were collected in accord with standard protocols (36-43) using a Spex Fluoromax (DM3000 software) or PTI QM-4/2003 SE (Felix 32 software) instrument. In general, samples were prepared in 1-cm pathlength quartz cells with absorbance < 0.1 at the wavelength of excitation to achieve uniform illumination across the sample, and with absorbance < 0.1 at all wavelengths in the emission scan in order to avoid the inner-filter effect. The dark counts were subtracted and the spectra were corrected for wavelength-dependent variations in optical and photomultiplier sensitivity. Spex Fluoromax: The excitation and emission monochromators were set at 1 mm, giving a spectral bandwidth of 4.25 nm. The data interval was 0.5 nm and the integration time was 2.0 sec. PTI QM-4/2003 SE: The excitation and emission monochromators were set at 0.25 mm, giving a spectral bandwidth of 1 nm. The data interval was 1 nm and the integration time was 1 sec.

The Φ_f values have been taken from the literature with citation. Recently, the Φ_f of meso-tetraphenylporphyrin (**H₂TPP**) has been determined to be 0.070 (44). Although **H₂TPP** has been widely used as a standard, the values employed, often 0.11, have ranged as large as 0.15 (45). The user is urged to choose the value of the Φ_f with care, not only for **H₂TPP**, but for all compounds in the database.

RESULTS AND DISCUSSION

Solar spectra

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This file contains a collection of 31 solar spectra. The spectra were obtained courtesy of the National Science Foundation (NSF) and National Renewable Energy Laboratory (NREL). The NSF data were collected as part of the NSF Polar Programs UV Radiation Monitoring Network (1995–1997); information concerning this effort is available in the report by Booth et al. (46). Collection of solar spectral irradiance data might seem a trivial undertaking. The challenge of obtaining accurate solar irradiance data across the UV/Vis/near-IR spectrum is delineated by Booth et al. (46), and more generally, in a scholarly treatise by Kostkowski (47).

Absorption and fluorescence spectral databases

There are multiple spectra in the databases. Provisions are included for inputting new absorption and fluorescence spectra, as well as printing spectra and the results of calculations. The databases also contain the molecular structure of the given compound. The spectra and accompanying structures in the database can be perused to assess structure–property relationships.

The Master Molecular database includes 339 absorption spectra, one for each compound. Each spectrum is entered with information concerning compound name, compound class, molecular structure, CAS# (if available), instrument used to collect the data, solvent, molar absorption coefficient (ϵ , in $\text{M}^{-1}\text{cm}^{-1}$), wavelength for the ϵ value, literature reference, date, filename, and investigator. An example is provided below.

[1 Absorption]

Name=Naphthalene

Class=polycyclic aromatic hydrocarbon

CAS#=91-20-3

Structure=naphthalene.str.bmp

Instrument=Cary 3

Solvent=cyclohexane

Epsilon=6000

Wavelength=275

Reference=276 nm, ϵ =6000, cyclohexane (11)

Date=06-09-1995

File=naphthalene.abs.txt

Investigator=RAF (Ru-Chun Amy Fuh)

The Master Molecular database includes 240 fluorescence spectra. Each member is entered with the same information as for the absorption spectral data, except Φ_f replaces ϵ . The number of spectral sets (absorption and fluorescence) may exceed the number of compounds because several compounds might be examined in more than one solvent.

Data export and import

Export. All the spectral data in PhotochemCAD 3 are stored as text files. The text files are not protected and can be readily opened and used in other software programs. Created data (e.g., blackbody radiation, Gaussian distribution, spectra simulation) or modified/altered data (e.g., spectrum math, converted into energy-based scale) can be readily exported from the 'DataEditor' window, which can be accessed through the 'List' button in "selected spectral files"

Import. All the information (other than the spectral files) are stored in a database file (PCAD3.db); the '.db' extension is required to read in the PhotochemCAD program. To view a database file, the file extension of '.db' needs to be renamed to ".txt", then converted to a text file, which can be read and edited by common spreadsheet editor programs. The database file consists of three main parts: compound (Entry, Name, CAS #, corresponding structure file,

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class), absorption spectra (corresponding absorption spectra file, epsilon, wavelength for epsilon, reference, solvent, instrument, date acquired data, investigator), and fluorescence spectra (corresponding fluorescence spectra file, fluorescence quantum yield, reference, solvent, instrument, date acquired data, investigator); for these the header (1st row) is clearly labeled. After modification of the database file, the file extension needs to be converted back to ‘db’ for use in the PhotochemCAD program.

Compounds in spectral databases

The databases at present are composed of absorption spectra, fluorescence spectra, and solar spectra. The absorption/fluorescence database contains spectra for 339 compounds. The compounds chosen – while idiosyncratic – are aimed to encompass very common compounds, including natural and synthetic, and to span the ultraviolet, visible and near-IR spectral regions. The latter region is perhaps the most active at present in terms of development of new chromophores and compounds (48). While the molecular photosciences may never have a universal basis set of chromophores, the dataset here should provide a general overview for a very large variety thereof. The Master Molecular database is organized into subgroups of compounds (series A–T). A representative member from each structure class A–T is provided in Figure 1. The following provides a brief description of each subgroup of the absorption/fluorescence database, with the structure of each compound provided in Figures S1–S21. The structure, name, synonyms and registry number (CAS or Colour Index if available) of each compound are provided in Table 1. A set of “Other references” provides additional literature pertaining to the spectral data or other notable features for the various compounds. Some photophysical data in the paper were present in the Help files of PhotochemCAD 1 (29) or PhotochemCAD 2 (30) but did not appear in the manuscripts themselves; such data are also

listed here with citations of the prior publication. Data reported here for the first time are denoted with the number symbol #.

A-series: Aromatic hydrocarbons (41 compounds) include benzene and derivatives, as well as acylbenzenes such as benzophenone. Tetraphenylmethane is placed in this family, as is the organometallic compound ferrocene. Omitted here, however, are oligophenylenes, which constitute a separate group.

B-series: Oligophenylenes (13 compounds) include biphenyl, p-terphenyl, p-quinquephenyl and p-quinquephenyl; 1,3,5-triphenylbenzene; and the laser dyes PPO and POPOP.

C-series: Polycyclic Aromatic Hydrocarbons (16 compounds) include the series naphthalene, anthracene, tetracene and pentacene; arene clusters such as 9,10-diphenylanthracene and rubrene; and multi-annulated structures such as triphenylene and pyrene.

D-series: Polyenes/Polyyenes (10 compounds) include alkenes such as the series trans-stilbene, 1,4-diphenylbutadiene, and 1,6-diphenylhexatriene; the natural product β -carotene; and the styryl dye 4-dimethylamino-4'-nitrostilbene. Alkynes in the group include 1,2-diphenylacetylene and 1,4-diphenylbutadiyne.

E-series: Heterocycles (26 compounds) include diverse heteroatom-substituted compounds that do not naturally fall into other dye classes. Such compounds include the classic parent structures pyrrole and pyridine; bipy compounds such as tris(2,2'-bipyridyl)ruthenium(II); other parent heterocycles such as quinoline, benzothiazole and benzotriazole; dyes such as Thiazole Orange and Thioflavin T; quinolone derivatives such as Carbofuran 124 and quinine sulfate, the latter with its black-light induced mesmerizing eerie blue fluorescence; and a dye from antiquity, indigo.

F-series: Biomolecules (18 compounds) include amino acids with aromatic side chains, nucleic acid bases, riboflavin and folic acid.

G-series: Quinones (24 compounds) include the parent compound 1,4-benzoquinone and derivatives therefrom, such as p-chloranil (2,3,5,6-tetrachloro-1,4-benzoquinone), DDQ (2,3-dichloro-5,6-dicyano-1,4-benzoquinone); hydroquinones such as hydroquinone itself (1,4-dihydroxybenzene) and 2,3,5,6-tetrachloro-1,4-hydroquinone; and the series 1,4-naphthoquinone, 9,10-anthraquinone, 5,12-naphthacenequinone, and 6,13-pentacenequinone. Other members that are not exactly quinones, but have some resemblance, include tetracyanoethylene and 7,7,8,8-tetracyanoquinodimethane.

H-series: Coumarins (14 compounds) include a series of dyes ranging from “coumarin” itself, which is essentially non-fluorescent, to derivatives bearing a range of substituents. The latter constitute dyes such as Coumarin 314 and Coumarin 343.

I-series: Acridines (21 compounds) are anthracenes with a nitrogen substituent at the 9-position. Further 9,10-diaza or 9-aza-10-thia substitution affords phenazines or phenothiazines, respectively. Peripheral substitution leads to prominent members of this class, including common dyes Acridine Orange and Toluidine Blue O. The dyes Cresyl Violet and Nile Red stem from annulation with an additional benzo group.

J-series: Azo dyes (18 compounds) constitute a sizable class of dyes and indicators such as Congo Red, Acid Orange 7 and Sudan I. The parent member, azobenzene, also is included. The family is readily divided into dyes with one or two azo groups.

K-series: Cyanine dyes (19 compounds) date to the work of Brooker for use in the photographic process. The cyanines included here bear dimethylcarba, oxa, and thia substituents in the indole nucleus and polyene chains of 3, 5 or 7 carbons in length. Well-known members of the cyanine family include Indocyanine Green (ICG), Pinacyanol iodide (Quinaldine Blue or 1,1'-diethyl-2,2'-carabocyanine iodide) and Merocyanine 540.

L-series: Arylmethane dyes (11 compounds) include well-known dimethylamino-substituted compounds such as Malachite Green and Crystal Violet. Indicator dyes included are phenolphthalein and related members such as Phenol Red and Cresol Red.

M-series: Perylenes (5 compounds) include perylene itself and derivatives. The latter include 3,4,9,10-perylenetetracarboxylic dianhydride and bis(imides) derived therefrom such as various red pigments. Several perylene-monoimides also are included.

N-series: Xanthenes (15 compounds) include members of the fluorescein and rhodamine family of dyes. Included here are fluorescein itself and halogenated derivatives thereof, such as Eosin B and Rose Bengal. Rhodamine dyes include Rhodamine 123, Rhodamine B and Rhodamine G.

O-series: Miscellaneous dyes (13 compounds) include those compounds that don't easily fit in other categories, such as ethidium bromide, squarylium dye III, 4'-6-dimidino-2-phenylindole (DAPI), Hoechst 33258, Lucifer Yellow CH, and others.

P-series: Dipyrins (7 compounds) include a large class of chromophores, of which a handful is included here. 5-Phenyldipyrin is a free base chromophore, to be contrasted with the difluoroboron complexes (known commercially as BODIPY[®] dyes). A dipyrromethane (a dihydrodipyrin) is included for comparison.

Q-series: Porphyrins (34 compounds) entail fully unsaturated, cyclic tetrapyrroles with alternating pyrrole and methylenedioxy groups. Representative members include heme, meso-tetraphenylporphyrin and tetrabenzoporphyrin.

R-series: Oligopyrroles (6 compounds) include linear tetrapyrroles such as bilins; cyclic tetrapyrroles with an A-D ring junction (corrole, vitamin B₁₂, and expanded cyclic tetrapyrroles (sapphyrin).

S-series: Phthalocyanines (11 compounds) include free base and metal chelates.

T-series: Chlorins/Bacteriochlorins (16 compounds) include dihydroporphyrins and tetrahydroporphyrins. Classic members include chlorophyll a, chlorophyll b, and bacteriochlorophyll a. Spectra for several hundred chlorins also have been assembled as part of a comparative study (49) and constitute part of a new database of tetrapyrrole spectra, which will be described elsewhere.

<Figure 1>

SUPPORTING INFORMATION

Additional Supporting Information is available in the online version of this article:

Figures S1-S21. The compounds in the series A–T.

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Table 1. Compounds in the Master Molecular database.

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
A-1	Benzene	71-43-2		210 (255 nm) cyclohexane (11)	0.053, hexane (50)	(11,51,52)
A-2	Toluene	108-88-3		2860 (265 nm) cyclohexane (11)	0.17, cyclohexane (11)	(51,53)
A-3	o-Xylene	95-47-6		254 (262 nm) ethanol (54)	0.17, hexane (55)	(51,53)
A-4	m-Xylene	108-38-3		284 (266 nm) cyclohexane (11)	0.13, hexane (55)	(51,53)
A-5	p-Xylene	106-42-3		770 (274 nm) cyclohexane (11)	0.22, hexane (55)	(51,53)
A-6	Mesitylene	108-67-8	1,3,5-Trimethylbenzene	180 (274 nm) ethyl acetate (56)	0.088, hexane (55)	(51,53)
A-7	Durene	95-93-2	1,2,4,5-Tetramethylbenzene	214 (279 nm) ethyl acetate (56)	0.3, hexane (55)	(51,53,54,57-60)
A-8	Pentamethylbenzene	700-12-9		629 (280 nm) ethyl acetate (56)	0.075, hexane (55)	(51,53)
A-9	Hexamethylbenzene	87-85-4		214 (273 nm) ethyl acetate (56)	< 0.01, hexane (55)	(51,53,57,61)
A-10	Phenol	108-95-2		2340 (271 nm) cyclohexane (11)	0.075, hexane (62)	(63)
A-11	Anisole	100-66-3	Methoxybenzene	620 (270 nm) cyclohexane (64)	0.45, cyclohexane (64)	(65)
A-12	Benzonitrile	100-47-0	Phenyl cyanide	11650 (230 nm) n-heptane (66)	0.23, cyclohexane (64)	(64)
A-13	Benzaldehyde	100-52-7	Phenylmethanal	1350 (282 nm) ethanol (67)	ND, cyclohexane (#)	(68,69)
A-14	Benzoic acid	65-85-0		1010 (272 nm) methanol (70)	ND (71)	(69)
A-15	Acetophenone	98-86-2	Methyl phenyl ketone	1050 (280 nm) ethanol (67)	0.001, toluene (72)	(68,69,73-75)
A-16	Aniline	62-53-3		1760 (287.5 nm) cyclohexane (76)	0.17, cyclohexane (76)	(77)
A-17	N,N-Dimethylaniline	121-69-7		14900 (251 nm) cyclohexane (64)	0.19, cyclohexane (64)	(65,78-83)
A-18	Phenylhydrazine Hydrochloride	59-88-1		490 (275 nm) phosphate buffer	ND, PBS (#)	

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
				(pH 7) (84)		
A-19	Chlorobenzene	108-90-7		222 (272 nm) cyclohexane (85)	0.0042, cyclohexane (86)	(87)
A-20	Iodobenzene	591-50-4		13200 (229 nm) cyclohexane (65)	ND, cyclohexane (88)	(65)
A-21	Nitrobenzene	98-95-3		8140 (260 nm) ethanol (89)	ND, ethanol (88)	(90)
A-22	Styrene	100-42-5	Phenylethylene; Vinylbenzene	14700 (245 nm) cyclohexane (91)	0.22, cyclohexane (92)	(93-95)
A-23	Phenylacetylene	536-74-3	Ethynylbenzene	15900 (245 nm) n- heptane (66)	0.11, benzene (96)	(97-99)
A-24	1,4-Diethynylbenzene	935-14-8		28200 (275 nm) chloroform (100)	0.19, chloroform (#)	(101,102)
A-25	Phenylpropargyl aldehyde	2579-22-8	Phenylpropionaldehyde; 3- Phenyl-2-propynal	5000 (279 nm) ethanol (103)	ND, ethanol (#)	(103)
A-26	Phenylboronic acid	98-80-6	Benzeneboronic acid	9520 (220 nm) hexane (104)	0.26, cyclohexane (#)	(105)
A-27	Vanillin	121-33-5	4-Hydroxy-3- methoxybenzaldehyde	9770 (232.6 nm) cyclohexane (106)	ND, cyclohexane (#)	(106,107)
A-28	3-Hydroxyacetophenone	121-71-1	m-Acetylphenol	2500 (310 nm) ethanol (108)	ND, ethanol (#)	(109)
A-29	Ethyl 4-(dimethylamino)benzoate	10287-53-3	Parbenate	23200 (310 nm) alcohol (110)	0.29, cyclohexane (111)	
A-30	Gallacetophenone	528-21-2	2',3',4'-Trihydroxyacetophenone	12500 (296 nm) methanol (112)	ND, methanol (#)	
A-31	Terephthalic acid	100-21-0	Benzene-1,4-dicarboxylic acid; 1,4-dicarboxybenzene	17000 (231 nm) dichloromethane (113)	0.0057, ethanol (#)	(115)
A-32	p-Phenylenediamine	106-50-3	1,4-Benzenediamine; 1,4- Diaminobenzene; 1,4- Phenylenediamine	1780 (321 nm) acetonitrile (116)	0.065, acetonitrile (116)	
A-33	Tetraphenylmethane	630-76-2		1910 (256 nm) chloroform (117)	0.24, cyclohexane (#)	(117,118)
A-34	N-Phenylbenzylamine	103-32-2	N-Benzylaniline; N-Benzyl-N- phenylamine	13200 (248 nm) acetonitrile (119)	0.164, cyclohexane (120)	
A-35	trans-Chalcone	614-47-1	Benzylideneacetophenone; 1,3- Diphenyl-2-propen-3-one	ϵ = 28000 (302 nm) cyclohexane (121)	ND (122)	(123)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
A-36	Benzophenone	119-61-9	Diphenyl ketone	19400 (248 nm) cyclohexane (124)	ND, ethanol (#)	(69,125,126)
A-37	4,4'-Dihydroxybenzophenone	611-99-4		15200 (291.5 nm) chloroform (126)	ND, chloroform (#)	
A-38	Diethyl phthalate	84-66-2		ϵ = 1260 (277 nm) NS (127)	0.015, NS (127)	(128)
A-39	1,2,4,5-Tetracyanobenzene	712-74-3	TCNB; Pyromellitic acid tetranitrile	3400 (316 nm) chloroform (129)	0.21, chloroform (#)	(129,130)
A-40	Hexafluorobenzene	392-56-3		684 (230 nm) ethanol (131)	0.035, ethanol (132)	(131-133)
A-41	Ferrocene	102-54-5	Bis(cyclopentadienyl)iron; Di(cyclopentadienyl)iron	96 (437 nm) cyclohexane (134)	ND (134)	(135)
B-1	Biphenyl	92-52-4		16000 (247 nm) cyclohexane (11)	0.18, cyclohexane (11)	
B-2	p-Terphenyl	92-94-4		33800 (276 nm) cyclohexane (11)	0.93, cyclohexane (11)	(52,117,136)
B-3	p-Quaterphenyl	135-70-6	1,4-Diphenylbenzene	41000 (294 nm) cyclohexane (11)	0.89, cyclohexane (11)	(136,137)
B-4	p-Quinquephenyl	3073-05-0		62500 (311 nm) THF (138)	0.89, cyclohexane (139)	(140)
B-5	1,3,5-Triphenylbenzene	612-71-5		60000 (252 nm) cyclohexane (11)	0.27, cyclohexane (11)	
B-6	Benzidine	92-87-5	4,4'-Diaminobiphenyl	40700 (282 nm) methanol (141)	0.16, chloroform (142)	(77,142)
B-7	3,3'-Dimethylbenzidine	119-93-7	o-Tolidine	21800 (285 nm) ethanol (143)	0.33, ethanol (#)	(144)
B-8	3,3',5,5'-Tetramethylbenzidine	54827-17-7	TMB	16000 (288 nm) ethanol (145)	0.29, ethanol (#)	(146)
B-9	2,5-Diphenyloxazole	92-71-7	PPO	35700 (302 nm) cyclohexane (11)	1, cyclohexane (11)	(136)
B-10	1,4-Bis(5-phenyl-2-oxazolyl)benzene	1806-34-4	POPOP; 1,4-Bis[2-(5-phenyloxazolyl)]benzene; 1,4-Bis(5-phenyloxazol-2-yl)benzene	47000 (358 nm) cyclohexane (11)	0.93, cyclohexane (11)	(136)
B-11	1,2,3,4,5-Pentaphenyl-1,3-cyclopentadiene	2519-10-0		11000 (336 nm) acetonitrile (147)	0.0028, dioxane (148)	(148,149)
B-12	rac-BINAP	98327-87-8	(\pm)-2,2'-Bis(diphenylphosphino)-1,1'-binaphthalene	9800 (228 nm) acetonitrile (150)		(150,151)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
B-13	(R)-BINOL	18531-94-7	(R)-(+)-1,1'-Bi(2-naphthol); (R)-(+)-1,1'-Binaphthyl-2,2'-diol	6510 (333 nm) chloroform (152)	0.1, THF (153)	(153)
C-1	Naphthalene	91-20-3		6000 (276 nm) cyclohexane (11)	0.23, cyclohexane (11)	(50,52)
C-2	Anthracene	120-12-7	Paranaphthalene	9700 (358 nm) cyclohexane (11)	0.36, cyclohexane (11)	(50,154)
C-3	Tetracene	92-24-0	Naphthacene; 2,3-Benzanthracene; Benz[b]anthracene	10000 (476 nm) benzene (11)	0.13, benzene (155)	(156,157)
C-4	Pentacene	135-48-8	Benzo[b]naphthacene	7200 (574 nm) THF (158)	0.13, THF (158)	(159)
C-5	Phenanthrene	85-01-8		15700 (293 nm) cyclohexane (11)	0.125, ethanol (50)	
C-6	Pyrene	129-00-0	Benzo[def]phenanthrene	54000 (333 nm) cyclohexane (11)	0.32, cyclohexane (11)	(50)
C-7	Triphenylene	217-59-4	9,10-Benzophenanthrene	18200 (287 nm) cyclohexane (11)	0.08, cyclohexane (11)	(50,160)
C-8	9,10-Diphenylanthracene	1499-10-1		14000 (373 nm) cyclohexane (11)	1, cyclohexane (11)	(137,154,161)
C-9	9,10-Bis(phenylethynyl)anthracene	10075-85-1		35400 (455 nm) cyclohexane (11)	1, cyclohexane (11)	
C-10	Rubrene	517-51-1	5,6,11,12-Tetraphenyltetracene	11800 (528 nm) benzene (11)	0.54, chloroform (162)	(162,163)
C-11	1,8-Naphthalic anhydride	81-84-5		7760 (339 nm) ethanol (164)	0.32, acetonitrile (#)	(165,166)
C-12	2-Aminonaphthalene	91-59-8	2-Naphthylamine	2140 (344 nm) acetonitrile (167)	0.91, acetonitrile (167)	(168)
C-13	2,3-Diaminonaphthalene	771-97-1	2,3-Naphthalenediamine	50100 (245 nm) methanol (169)	0.54, methanol (169)	
C-14	8-Anilino-1-naphthalenesulfonic acid	82-76-8	ANS	3740 (375 nm) methanol (168)	0.24, methanol (170)	(170-172)
C-15	1,4,5,8-Naphthalenetetracarboxylic dianhydride	81-30-1	NTCDA	30600 (363.5 nm) acetonitrile (173)	0.13, acetonitrile (173)	(165)
C-16	Pyranine	6358-69-6	8-Hydroxypyrene-1,3,6-trisulfonic acid trisodium salt, HPTS	21600 (456 nm) NaOH aq (0.01 M) (174)	1, water (pH 10) (175)	(174)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
D-1	1,2-Diphenylacetylene	501-65-5	1,2-Diphenylethyne; Tolan	27600 (283 nm) ethanol (176)	0.0034, 3-methylpentane (177)	(177)
D-2	cis-Stilbene	645-49-8	cis-1,2-Diphenylethylene; Isostilbene	10200 (276 nm) cyclohexane (178)	0.00008, hexane (179)	
D-3	trans-Stilbene	103-30-0	trans-1,2-Diphenylethylene	28200 (297 nm) cyclohexane (178)	0.04, hexane (180)	(121,181-185)
D-4	1,4-Diphenylbutadiyne	886-66-8		27800 (327 nm) ethanol (176)	0.0016, ethanol (29)	(99)
D-5	1,4-Diphenylbutadiene	538-81-8	trans,trans-1,4-Diphenyl-1,3-butadiene	33000 (330 nm) hexane (186)	0.42, cyclohexane (187)	(187-190)
D-6	1,6-Diphenylhexatriene	1720-32-7	1,6-Diphenyl-1,3,5-hexatriene	82400 (353 nm) cyclohexane (187)	0.65, cyclohexane (187)	(11,184,187-190)
D-7	4-Dimethylamino-4'-nitrostilbene	2844-15-7	N,N-Dimethyl-4'-nitro-4-stilbenamine; DANS	27000 (436 nm) benzene (191)	0.7, benzene (191)	(192)
D-8	Curcumin	458-37-7	Natural Yellow 3	55000 (422 nm) ethanol (193)	0.063, ethanol (194)	(194,195)
D-9	all trans-Retinal	116-31-4	Vitamin A aldehyde	43500 (383 nm) ethanol (196)	$< 10^{-5}$, 3-methylpentane (197)	(198-201)
D-10	Beta-carotene	7235-40-7	Provitamin A	139500 (452 nm) hexane (202)	< 0.0001 (203)	(204)
E-1	Pyridine	110-86-1		1800 (252 nm) isooctane (205)	ND, acetonitrile (#)	(206)
E-2	Pyridine N-oxide	694-59-7		14300 (275 nm) dichloromethane (207)		(208,209)
E-3	2-Acetylpyridine	1122-62-9		3250 (267 nm) cyclohexane (210)	ND, cyclohexane (#)	
E-4	4-Dimethylaminopyridine	1122-58-3	DMAP	13300 (257 nm) acetonitrile (211)	0.017, acetonitrile (212)	
E-5	4-(4-Nitrobenzyl)pyridine	1083-48-3		12300 (265 nm) ethanol (213)		
E-6	1,3,5-Triazine	290-87-9	s-Triazine	890 (272 nm) ethanol (214)	ND, water (215)	(206,216)
E-7	Phthalimide	85-41-6		1860 (290 nm) ethanol (164)	ND, ethanol (#)	(164,217,218)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
E-8	2,2'-Bipyridine	366-18-7	2,2'-Bipyridyl; 2,2'-Dipyridine; 2,2'-Dipyridyl	11200 (282 nm) hexane (219)	ND, acetonitrile (#)	(220)
E-9	4,4'-Bipyridine	553-26-4	4,4'-Bipyridyl; 4,4'-Dipyridine; 4,4'-Dipyridyl	12600 (236 nm) hexane (219)	ND, acetonitrile (#)	(220,221)
E-10	Quinoline	91-22-5		2560 (313 nm) hexane (222)	0.01, ethanol (#)	(223,224)
E-11	8-Quinoline carboxylic acid	86-59-9		5750 (318 nm) ethanol (225)	0.02, ethanol (#)	
E-12	3-Quinoline carboxaldehyde	13669-42-6		1330 (246 nm) methanol (226)	ND, ethanol (#)	
E-13	Benzothiazole	95-16-9		1350 (294 nm) methanol (227)		(228)
E-14	Benzotriazole	95-14-7		4680 (274 nm) Tris- HCl buffer (pH 7.2) (229)	ND, ethanol (#)	(230,231)
E-15	2-Methylbenzoxazole	95-21-6		4640 (277 nm) cyclohexane (52)	0.05, cyclohexane (52)	
E-16	Pyrrole	109-97-7		15000 (210 nm) hexane (232)		
E-17	Pyrrole-2-carboxaldehyde	1003-29-8	2-Formylpyrrole	15600 (289 nm) hexane (233)	ND, hexane (#)	(234,235)
E-18	Thiazole Orange	107091-89-4		58500 (498 nm) methanol (236)	0.003 (237)	(238-240)
E-19	Thioflavin T	2390-54-7		36000 (412 nm) water (241)	0.0004, water (242)	(243-246)
E-20	Tris(2,2'-bipyridyl)ruthenium(II)	65034-88-0	Ru(bpy) ₃ ; Tris(2,2'- bipyridyl)dichlororuthenium(II)	14600 (452 nm) water (247)	0.042, water (248)	
E-21	4-Chloro-7-nitrobenzofurazan	10199-89-0	NBD	8130 (332 nm) cyclohexane (249)	ND, acetonitrile (250)	(250-253)
E-22	7-Benzylamino-4-nitrobenz-2- oxa-1,3-diazole	18378-20-6	4-Benzylamino-7- nitrobenzofurazan, Benzylamino- NBD	19700 (462 nm) ethanol (254)	0.36, ethanol (254)	(255)
E-23	Carbostyryl 124	19840-99-4	7-Amino-4-methyl-2- hydroxyquinoline	16000 (340 nm) water (pH 5 to 9) (256)	0.97, water (pH 5 to 9) (256)	
E-24	Quinoline Yellow	8004-92-0	Acid Yellow 3	22700 (414 nm) Trsi-HCl buffer	ND, PBS (#)	

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
				(257)		
E-25	2,3,5-Triphenyltetrazolium Chloride	298-96-4	Tetrazolium Red	25600 (247 nm) water (258)	ND, PBS (#)	(259)
E-26	Quinine sulfate	207671-44-1		5700 (345 nm) H ₂ SO ₄ aq (0.05 M) (260)	0.546, H ₂ SO ₄ aq (1 N) (154)	(261)
F-1	L-Alanine	56-41-7		9 (261 nm) methanol (262)		
F-2	L-Phenylalanine	63-91-2		195 (257.6 nm) water (263)	0.022, water (38)	
F-3	L-Tyrosine	60-18-4		1405 (274.8 nm) phosphate buffer (pH 7, 0.1 M) (263)	0.13, phosphate buffer (pH 7, 0.1 M) (38)	
F-4	L-Histidine	71-00-1		5700 (206 nm) phosphate buffer (pH 7, 0.1 M) (263)		
F-5	L-Tryptophan	73-22-3		5579 (279 nm) phosphate buffer (pH 7, 0.1 M) (263)	0.12, phosphate buffer (pH 7, 0.1 M) (38)	(154,264)
F-6	Adenine	73-24-5		13000 (260.5 nm) water (pH 7) (265)	0.00026, water (266)	(267)
F-7	Guanine	73-40-5		10700 (246 nm) water (265)	0.0003, water (266)	(267)
F-8	Cytosine	71-30-7		6100 (267 nm) water (265)	0.000082, water (266)	(267)
F-9	Thymine	65-71-4		7900 (264.5 nm) water (265)	0.000102, water (266)	(267)
F-10	Uracil	66-22-8		8200 (259.5 nm) water (265)	0.000035, water (268)	(267,268)
F-11	2-Amino-4-methylpyrimidine	108-52-1		4270 (292 nm) ethanol (269)	0.00032, isooctane (270)	
F-12	2,4-dihydroxy-6-methylpyrimidine	626-48-2	6-Methyluracil	9300 (257 nm) water (268)	0.000062, water (268)	
F-13	D-(-)-Salicin	138-52-3		130 (269 nm) water (271)		(272,273)
F-14	Riboflavin	83-88-5	Vitamin B2	33000 (270 nm) ethanol (274)	0.3, ethanol (274)	(275,276)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
F-15	L-Ascorbic acid	50-81-7	Vitamin C	14000 (267 nm) aqueous buffer (pH 6.9) (277)		(278)
F-16	DL-alpha-Tocopherol	10191-41-0	Vitamin E	2990 (292 nm) ethanol (279)	0.14, ethanol (#)	(280-283)
F-17	Vitamin K1	84-80-0	2-Methyl-3-phytyl-1,4-naphthoquinone, Phylloquinone	3160 (328 nm) ethanol (284)		
F-18	Folic acid	59-30-3	Vitamin B9	25200 (280 nm) water (285)	< 0.005, water (286)	(287,288)
G-1	1,4-Benzoquinone	106-51-4		17000 (240 nm) cyclohexane (289)		(290-294)
G-2	Hydroquinone	123-31-9		10000 (294 nm) acetonitrile (63)	0.16, acetonitrile (#)	(63)
G-3	2,3,5,6-Tetrachloro-1,4-benzoquinone	118-75-2	p-Chloranil	22400 (292 nm) chloroform (295)		(290,296-298)
G-4	Tetrachlorohydroquinone	87-87-6	2,3,5,6-Tetrachloro-1,4-benzenediol	6600 (310 nm) diethyl ether (299)	ND, acetonitrile (#)	(296,297)
G-5	2,3,5,6-Tetramethyl-1,4-benzoquinone	527-17-3	Duroquinone	24500 (268 nm) chloroform (300)	ND, acetonitrile (#)	(290,301-303)
G-6	2,3-Dichloro-5,6-dicyano-1,4-benzoquinone	84-58-2	DDQ	12300 (280 nm) acetonitrile (304)		(305)
G-7	3,4,5,6-Tetrachloro-1,2-benzoquinone	2435-53-2	o-Chloranil	1480 (457 nm) chloroform (306)	ND, chloroform (#)	(290,307)
G-8	2,5-Diphenyl-1,4-benzoquinone	844-51-9		10500 (341 nm) carbon tetrachloride (301)	ND, acetonitrile (#)	(308)
G-9	2,5-Di-tert-butyl-1,4-benzoquinone	2460-77-7		15100 (261 nm) n-heptane (292)	ND, acetonitrile (#)	(301)
G-10	Tetracyanoethylene	670-54-2	TCNE	14500 (267.7 nm) chloroform (295)		(309,310)
G-11	7,7,8,8-Tetracyanoquinodimethane	1518-16-7	TCNQ	42700 (401 nm) dichloromethane (311)		(312-315)
G-12	1,4-Naphthoquinone	130-15-4	α -Naphthoquinone	2840 (328 nm) n-heptane (292)	ND, ethanol (#)	(282,316)
G-13	1,4-Naphthoquinone-2-sulfonic acid, Potassium salt	34169-62-5		3060 (345 nm) water (#)		

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
G-14	2,3-Dichloro-1,4-naphthoquinone	117-80-6	Dichlone	3200 (343 nm) dichloromethane (317)	ND, ethanol (#)	
G-15	2-Methyl-1,4-naphthoquinone	58-27-5	Menadione, Vitamin K3	2190 (330 nm) ethanol (318)	ND, ethanol (#)	(316,319)
G-16	9,10-Phenanthrenequinone	84-11-7		4900 (324 nm) chloroform (320)	ND (321)	(322)
G-17	1,2-Naphthoquinone	524-42-5	β -Naphthoquinone	1710 (396 nm) methanol (323)	ND, methanol (#)	(324,325)
G-18	1,2-Naphthoquinone-4-sulfonic acid, sodium salt	521-24-4		1030 (370 nm) methanol (326)		
G-19	9,10-Anthraquinone	84-65-1		56800 (250.5 nm) n-heptane (292)		(311,327,328)
G-20	Alizarin	72-48-0	1,2-Dihydroxyanthraquinone, Mordant Red 11	4900 (421 nm) acetonitrile (329)	0.002, acetonitrile (329)	(330-333)
G-21	Alizarin Red S	130-22-3		3280 (420 nm) acetonitrile (334)	0.001, 75% methanol, 10 mM HEPES (pH 7.1) (333)	
G-22	1,4-Anthraquinone	635-12-1		9300 (299 nm) ethanol (335)	ND, ethanol (#)	(164)
G-23	5,12-Naphthacenequinone	1090-13-7	Tetracenequinone	5750 (389 nm) dioxane (336)	0.43, benzene (#)	(337,338)
G-24	6,13-Pentacenequinone	3029-32-1	6,13-Pentacenequinone	14500 (403 nm) dioxane (336)	0.54, benzene (#)	(337)
H-1	Coumarin	91-64-5		5700 (311 nm) ethanol (339)	0.0032, water (340)	(341-344)
H-2	4-Hydroxycoumarin	1076-38-6		6000 (308 nm) ethanol (345)	0.003, ethanol (#)	(342,346-348)
H-3	7-Hydroxycoumarin	93-35-6	Umbelliferone	16800 (330 nm) ethanol (341)	0.08, methanol (349)	(345,346,349-354)
H-4	7-Hydroxy-4-(trifluoromethyl)coumarin	575-03-1	4-Trifluoromethylumbelliferone	12600 (338 nm) ethanol (355)	0.2, ethanol (355)	(354,356,357)
H-5	7-Methoxycoumarin-4-acetic acid	62935-72-2		11820 (320 nm) methanol (358)	0.18, methanol (358)	
H-6	Coumarin 1	91-44-1	7-(Diethylamino)-4-methylcoumarin	23500 (373 nm) ethanol (359)	0.5, ethanol (359)	(26,357,360,361)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
H-7	Coumarin 6	38215-36-0		54000 (454 nm) ethanol (359)	0.78, ethanol (359)	(26,361-366)
H-8	Coumarin 7	27425-55-4	3-(2-Benzimidazolyl)-7-(diethylamino)coumarin	52500 (438 nm) methanol (367)	0.82, methanol (367)	(26,362,363,365,366,368)
H-9	Coumarin 30	41044-12-6		54000 (425 nm) 30% ethanol in water (366)	0.8, ethanol (366)	(26,361,366,369,370)
H-10	Coumarin 151	53518-15-3	7-Amino-4-(trifluoromethyl)coumarin	17000 (382 nm) ethanol (359)	0.53, ethanol (359)	(26,355,357)
H-11	Coumarin 314	55804-66-5		46800 (436 nm) ethanol (359)	0.68, ethanol (359)	(26,371)
H-12	Coumarin 343	55804-65-4		44300 (446 nm) ethanol (359)	0.63, ethanol (359)	(26)
H-13	Calcein Blue	54375-47-2	4-Methylumbelliferone-8-methyliminodiacetic acid	16100 (360 nm) aqueous buffer (pH 9) (372)	0.59, PBS (#)	(372,373)
H-14	Urolithin B	1139-83-9	3-Hydroxy-6H-benzo[c]chromen-6-one	8910 (305 nm) ethanol (374)	0.21, DMF (375)	
I-1	Acridine	260-94-6		13800 (355 nm) ethanol (376)	0.0079, ethanol (377)	(378-380)
I-2	Proflavine hydrochloride	952-23-8	3,6-Diaminoacridine hydrochloride	39900 (444 nm) water (pH 7) (381)	0.34, water (pH 4) (382)	(383)
I-3	Acridine Orange	65-61-2, 494-38-2	Basic Orange 14	27000 (435 nm) ethanol (basic) (384)	0.2, ethanol (basic) (159)	(383)
I-4	Acridine Yellow G	135-49-9	3,6-Diamino-2,7-dimethylacridine	39400 (461 nm) ethanol (11)	0.47, ethanol (385)	(385)
I-5	Acridone	578-95-0	9(10H)-Acridanone, 9,10-Dihydro-9-oxoacridine	15000 (398 nm) methanol (386)	0.72, ethanol (50)	(52,387-389)
I-6	Phenazine	92-82-0		12600 (363 nm) ethanol (376)	ND, ethanol (376)	(378)
I-7	Phenosafranin	81-93-6		35600 (520 nm) water (390)	0.2, methanol (391)	(392-394)
I-8	Neutral Red	553-24-2	Basic Red 5	15500 (460 nm) ethanol (376)	0.044, ethanol (395)	(395)
I-9	Janus Green B	2869-83-2		35000 (608 nm) water (396)	ND, PBS (#)	(397)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
I-10	Phenothiazine	92-84-2	10H-Phenothiazine	4700 (316 nm) cyclohexane (398)	0.006, cyclohexane (398)	(399-402)
I-11	Thionin	26754-93-8	Thionine, 3,7-Diaminophenothiazin-5-Ium Chloride	77600 (602 nm) ethanol (401)	0.04, ethanol (#)	
I-12	Methylene blue	61-73-4		40700 (654 nm) ethanol (401)	0.04, ethanol (385)	(385,396,403)
I-13	Azure II	37247-10-2		81300 (657 nm) water (404)	0.04, ethanol (#)	
I-14	Toluidine Blue O	92-31-9	Basic Blue 17	74000 (627 nm) ethanol (403)	0.076, ethanol (403)	(405,406)
I-15	Phenoxathiin	262-20-4		28500 (238 nm) ethanol (407)	ND, ethanol (#)	(408,409)
I-16	Phenoxazine	135-67-1		7900 (318 nm) ethanol (410)	0.025, ethanol (411)	(378,399)
I-17	Oxazine 1	24796-94-9	Oxazine 725, Oxazine 1 perchlorate	117000 (641 nm) ethanol (378)	0.11, ethanol (412)	(26,412-416)
I-18	Cresyl Violet perchlorate	41830-80-2	Cresyl violet 670	28000 (602 nm) ethanol (378)	0.54, methanol (417)	(26,385,412,413,418)
I-19	Nile Red	7385-67-3	Nile Blue A Oxazone, Oxazine 17	38000 (518 nm) dioxane (419)	0.7, dioxane (420)	(334,419,421-425)
I-20	Nile Blue	53340-16-2	Nile Blue A perchlorate	67000 (625 nm) methanol (426)	0.27, ethanol (412)	(378,412,427-429)
I-21	Oxazine 170	62669-60-7	Oxazine 720, Oxazine 170 perchlorate	83000 (620 nm) methanol (26)	0.63, methanol (412)	(413,430,431)
J-1	Azobenzene	103-33-3		22400 (313 nm) benzene (432)		(433-438)
J-2	Acid Red 2	493-52-7	Methyl Red, 4-Dimethylaminoazobenzene-2'-carboxylic Acid	18500 (430 nm) PBS (pH 7.5) (436)		(396,439-441)
J-3	Methyl orange	547-58-0	Acid Orange 52	25900 (460 nm) PBS (pH 7.5) (436)		(442-448)
J-4	Orange G	1936-15-8	Acid Orange 10	20900 (480 nm) PBS (pH 7.5) (436)	ND, PBS (#)	(449,450) <u>ENREF 403</u>
J-5	Orange II	633-96-5	Acid Orange 7	15400 (480 nm) PBS (pH 7.5) (436)		(447,451,452)
J-6	Acid Red 88	1658-56-6	Acid Red A, Fast Red, 2-	11700 (510 nm)	ND, PBS (#)	(450,451,453) <u>EN</u>

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
			Naphthol Red	PBS (pH 7.5) (436)		<u>REF 405</u>
J-7	Sudan I	842-07-9	1-Phenylazo-2-naphthol	14500 (476 nm) ethanol (454)	ND, ethanol (#)	(455-459)
J-8	Sudan II	3118-97-6	Solvent Orange 7, 1-(2,4-Xylyldylazo)-2-naphthol	15800 (494 nm) ethanol (454)	ND, ethanol (#)	(455,458,460)
J-9	Acid Violet 3	1681-60-3		36000 (552 nm) water (461)		
J-10	Acid Red 1	3734-67-6	Azophloxine	31900 (530 nm) water (450)		(462)
J-11	Acid Red 14	3567-69-9	Azo Rubine, Carmoisine	24000 (510 nm) water (450)	0.0007, PBS (#)	(463-465)
J-12	Acid Blue 92	3861-73-2	Acid Blue A,	32300 (570 nm) water (450)		
J-13	Sudan III	85-86-9	Solvent Red 23	30000 (512 nm) NS (466)		(455,467)
J-14	Sudan IV	85-83-6	Solvent Red 24	32500 (515 nm) ethanol (460)		(455,467-469)
J-15	Acid Black 1	1064-48-8	Naphthol Blue Black	51600 (619 nm) MOPS buffer (pH 7.4, 25 mM) (462)	ND, PBS (#)	(470)
J-16	Ponceau S	6226-79-5	Acid Red 112	42000 (520 nm) water (471)		(469,472,473)
J-17	Congo Red	573-58-0	Direct Red 28	48000 (500 nm) water (474)		(436,444,446,475,476)
J-18	Benzopurpurin 4B	992-59-6	Direct Red 2, Benzopurpurin	23900 (497 nm) water (449)		
J-19	Evans Blue	314-13-6	Direct Blue 53	86000 (606 nm) water (477)		(475,478,479)
K-1	1,1'-Diethyl-2,2'-cyanine iodide	977-96-8	DEC	54000 (525 nm) ethanol (480)	0.001, ethanol (480)	(481)
K-2	1,1'-Diethyl-2,2'-carbocyanine iodide	605-91-4	Pinacyanol iodide, DECC	128000 (605 nm) methanol (482)	0.001, methanol (482)	(481,483,484)
K-3	1,1'-Diethyl-2,2'-dicarbocyanine iodide	14187-31-6	DDI	227000 (710 nm) ethanol (485)	0.0028, ethanol (485)	(481)
K-4	1,1'-Diethyl-4,4'-cyanine iodide	4727-49-5		75000 (nm NR) alcohol (486)	ND, ethanol (#)	
K-5	1,1'-Diethyl-4,4'-carbocyanine	4727-50-8	DCI, Cryptocyanine,	211000 (709 nm)	0.007, ethanol (485)	(481)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
	iodide		Kryptocyanin	ethanol (485)		
K-6	1,1'-Diethyl-4,4'-dicarbocyanine iodide	18300-31-7		213000 (nm NR) alcohol (486)	0.033, DMSO (481)	
K-7	3,3'-Diethyloxacarbocyanine iodide	905-96-4	DOC, DOCI	149000 (483 nm) ethanol (487)	0.05, methanol (488)	(489,490)
K-8	3,3'-Diethyloxadibocarbocyanine iodide	14806-50-9	DODC, DODCI	237000 (579.5 nm) ethanol (487)	0.49, ethanol (491)	(26,480,490,492-494)
K-9	3,3'-Diethyloxatricarbocyanine iodide	15185-43-0	DOTC, DOTCI	220000 (684 nm) ethanol (487)	0.49, ethanol (26)	(413,495)
K-10	1,1'-Diethyl-3,3,3',3'-tetramethylindocarbocyanine iodide	14696-39-0		133000 (546 nm) ethanol (487)	0.07, methanol (488)	(496-498)
K-11	1,1'-Diethyl-3,3,3',3'-tetramethylindodicarbocyanine iodide	17094-16-5, 15185-46-3		200000 (639 nm) ethanol (487)	0.4, methanol (488)	(488,496,499)
K-12	1,1'-Diethyl-3,3,3',3'-tetramethylindotricarbocyanine iodide	15185-47-4	HITCI	240000 (741 nm) ethanol (487)	0.28, ethanol (488)	(495,496,500)
K-13	Indocyanine Green	3599-32-4	ICG, Cardiogreen	194000 (782 nm) ethanol (501)	0.05, ethanol (501)	(481,502,503)
K-14	3,3'-Diethylthiacarbocyanine iodide	905-97-5	DTC, DTICI	161000 (557 nm) ethanol (487)	0.05, ethanol (480)	(480,483,489,490,494,496,504,505)
K-15	3,3'-Diethylthiadibocarbocyanine iodide	514-73-8	DTDC, DTDCI	249000 (652 nm) ethanol (487)	0.35, ethanol (491)	(26,481,490,494,504,506)
K-16	3,3'-Diethylthiatricarbocyanine iodide	3071-70-3	DTTC, DTTCI	212000 (758 nm) ethanol (487)	0.36, DMSO (481)	(495,504)
K-17	Merocyanine 540	62796-23-0		138000 (559 nm) ethanol (507)	0.39, ethanol (507)	(396,508-510)
K-18	4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran, [DCM]	51325-91-8		42000 (465 nm) methanol (511)	0.43, methanol (512)	(496,512,513)
K-19	Stains all	7423-31-6	3,3'-Diethyl-9-methyl-4,5,4',5'-dibenzothiacarbocyanine	96500 (575 nm) ethanol (514)		(515)
L-1	Auramine O	2465-27-2	Basic Yellow 2, Pyocyaninum aureum	25300 (431 nm) water (cacodylate buffer) (516)	0.03, glycerol (517)	(451)
L-2	Malachite Green	2437-29-8	Basic Green 4	77200 (616 nm)		(396,431,518)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
				water (cacodylate buffer) (516)		
L-3	Crystal violet	548-62-9	Basic Violet 3	75800 (590 nm) water (cacodylate buffer) (516)	0.019, glycerol (517)	(393,431,519-521)
L-4	p-Fuchsin	632-99-5	Basic Fuchsin	80600 (545 nm) water (cacodylate buffer) (516)	ND, ethanol (#)	(393,522)
L-5	Methyl violet	8004-87-3	Basic Violet 1	84300 (579 nm) methanol (520)		(523,524)
L-6	Methyl Green	7114-03-6		77800 (630 nm) water (cacodylate buffer) (516)		(524)
L-7	Methyl blue	28983-56-4	Acid Blue 93	12250 (598 nm) water (525)		(526)
L-8	Phenolphthalein	77-09-8		21500 (550 nm) water (pH 12.2) (527)		(528,529)
L-9	Phenol Red	143-74-8	Phenolsulfonphthalein	40000 (560 nm) water (pH 9.0) (527)		(530,531)
L-10	Cresol Red	1733-12-6		46300 (570 nm) water (pH 9.4) (527)		(470,530,532)
L-11	Thymol Blue	76-61-9		17600 (595 nm) water (pH 9.7) (527)		(530,531)
M-1	Perylene	198-55-0		38500 (438 nm) cyclohexane (11)	0.94, cyclohexane (11)	(11,50,385)
M-2	Perylene, PMI	165550-61-8	N-(2,6-diisopropylphenyl)perylene-3,4-dicarboximide	32000 (506 nm) toluene (533)	0.91, toluene (533)	(534)
M-3	Perylene, PMI(OR)		9-(4-tert-butylphenoxy)-N-(2,6-diisopropylphenyl)-3,4-perylenedicarboximide	32000 (532 nm) toluene (533)	0.82, toluene (533)	
M-4	Perylene, PMI(OR) ₃	468083-01-4	1,6,9-tris(4-tert-butylphenoxy)-N-(2,6-diisopropyl-4-	40000 (536 nm) toluene (533)	0.86, toluene (533)	

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
			ethynylphenyl)-3,4- perylene dicarboximide			
M-5	Perylene, PDI	83054-80-2	N,N'-Bis(2,5-di-tert- butylphenyl)-3,4,9,10- perylene dicarboximide	50000 (525 nm) chloroform (535)	0.97, toluene (536)	(535-537)
N-1	Fluorescein	2321-07-5		92300 (499 nm) ethanol (basic) (538)	0.97, ethanol (basic) (538)	(539-541)
N-2	2',7'-Dichlorofluorescein	76-54-0		75000 (501.5 nm) water (542)	0.58, 30% Tris buffered in DMSO (543)	(542-544)
N-3	3,4,5,6-Tetrachlorofluorescein	6262-21-1		65500 (511 nm) phosphate buffer (pH 8) (545)	0.65, PBS (#)	(544)
N-4	Eosin B	548-24-3	Acid Red 91, Saffrosine, Safrosin	95000 (530 nm) DMF (546)	0.63, ethanol (547)	
N-5	Eosin Y	17372-87-1 (548-26-5)	Acid Red 87	112000 (526 nm) ethanol (basic) (538)	0.67, ethanol (538)	(334,444,540,546- 549)
N-6	Phloxine B	18472-87-2	Acid Red 92	83000 (538 nm) phosphate buffer (pH 7.4) (550)	0.67, ethanol (#)	
N-7	Erythrosine B	16423-68-0		107000 (532 nm) ethanol (551)	0.08, ethanol (549)	(540,549,552,553)
N-8	Rose bengal	11121-48-5	Acid Red 94, 4,5,6,7-Tetrachloro- 2',4',5',7'-tetraiodofluorescein	90400 (560 nm) ethanol (basic) (538)	0.11, ethanol (basic) (538)	(540,546,547,549,55 4)
N-9	Xantphos	161265-03-8	4,5-Bis(diphenylphosphino)-9,9- dimethylxanthene	23700 (262 nm) dichloromethane (555)	0.16, dichloromethane (#)	(555,556)
N-10	Rhodamine 123	62669-70-9		85700 (507 nm) ethanol (557)	0.86, ethanol (557)	(557-559)
N-11	Rhodamine B	81-88-9		106000 (545 nm) methanol (560)	0.7, ethanol (561)	(393,541,559,562- 568)
N-12	Sulforhodamine B	3520-42-1	Acid Red 52	99000 (565 nm) phosphate buffer (pH 7.4) (550)	0.7, ethanol (#)	

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
N-13	Rhodamine 6G	989-38-8		116000 (530 nm) ethanol (563)	0.95, ethanol (559)	(541,563,569-571)
N-14	Rhodamine 101 inner salt	41175-43-3 (116450-56-7)		95000 (568 nm) ethanol (572)	0.98, ethanol (572)	(563-565)
N-15	Sulforhodamine 101	60311-02-6		110000 (577 nm) methanol (573)	0.9, ethanol (574)	(26,430,573)
O-1	Dansylglycine	1091-85-6	[5-(Dimethylamino)naphthalene-1-sulfonyl]glycine	4300 (340 nm) 60% ethanol (water) (575)	0.66, dioxane (576)	(576-578)
O-2	Lucifer Yellow CH	67769-47-5	Lucifer Yellow CH dilithium salt	24200 (280 nm) water (579)	0.21, water (579)	
O-3	Piroxicam	36322-90-4		13000 (326 nm) hexane (580)	0.035, hexane (580)	
O-4	1,2,3,4,5-Pentamethylcyclopentadiene	4045-44-7		12200 (240 nm) ethanol (581)		
O-5	Ethidium Bromide	1239-45-8		5680 (478 nm) aq HCl (pH 3) (582)	0.039, water (583)	(584)
O-6	4',6-Diamidino-2-phenylindole, [DAPI]	28718-90-3	DAPI	27800 (343 nm) water (585)	0.043, water (586)	(583,585,587)
O-7	Hoechst 33258	23491-45-4		40100 (341 nm) water (pH 5.5) (588)	0.35, DMF (586)	(516,583,589)
O-8	Squarylium dye III	43134-09-4		309000 (627.6 nm) dichloromethane (590)	0.65, dichloromethane (590)	
O-9	Ellagic Acid Dihydrate	133039-73-3		12200 (356 nm) water (pH 7) (591)	ND, Tris buffer (pH 7.4) (592)	(591,593)
O-10	Betalamic Acid	18766-66-0		27000 (424 nm) water (594)		
O-11	Betanin	7659-95-2		65000 (536 nm) water (595)	0.0007, H ₂ O (596)	(597,598)
O-12	Rutin trihydrate	153-18-4		11750 (358 nm) methanol (599)	0.0114, methanol (600)	(601-603)
O-13	Hesperidin	520-26-3		17800 (284 nm) methanol (604)	ND, methanol (#)	
P-1	5-Phenyldipyrromethane	107798-98-1	meso-Phenyl-2,2'-dipyrromethane	36000 (208 nm)	ND, hexane (#)	

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
				hexane (605)		
P-2	5-Phenyldipyrin	118762-53-1	meso-Phenyl-2,2'-dipyrromethene	19000 (432 nm) toluene (606)		(607)
P-3	N,N'-Difluoroboryl-1,9-dimethyl-5-phenyldipyrin	865479-43-2		54000 (503 nm) toluene (608)	0.053, toluene (608)	
P-4	N,N'-Difluoroboryl-1,9-dimethyl-5-(4-iodophenyl)dipyrin			59000 (514 nm) toluene (608)	0.23, toluene (608)	
P-5	N,N'-Difluoroboryl-1,9-dimethyl-5-[(4-(2-trimethylsilylethynyl)phenyl)dipyrin			48800 (516 nm) toluene (608)	0.078, toluene (608)	
P-6	Bis(5-phenyldipyrinato)zinc			115000 (485 nm) toluene (609)	0.006, toluene (609)	(606)
P-7	Bis(5-mesityldipyrinato)zinc			115000 (487 nm) toluene (609)	0.36, toluene (609)	(606)
Q-1	H ₂ P	101-60-0	Porphine; Porphin	261000 (395 nm) benzene (610)	0.043, toluene (611)	(612-615)
Q-2	MgP		Magnesium porphine	487,000 (402 nm) benzene (610)	0.0084, ethanol (617)	(615, 616)
Q-3	ZnP		Zinc porphine	380000 (398 nm) ethanol (617)	0.058, propanol (618)	(613-616)
Q-4	H ₂ OEP	2683-82-1	Octaethylporphyrin; 2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine	159000 (400 nm) benzene (619)	0.13, benzene (613)	
Q-5	MgOEP	20910-35-4	Magnesium octaethylporphyrin	408000 (408.5 nm) dichloromethane (620)	0.15, toluene (29)	
Q-6	CuOEP	14409-63-3	Copper(II) octaethylporphyrin	31300 (562 nm) toluene (621)		(622)
Q-7	ZnOEP	17632-18-7	Zinc octaethylporphyrin; 2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine zinc(II)	417000 (407 nm) dioxane (623)	0.045, benzene (613)	(617,618)
Q-8	H ₂ TPP	917-23-7	Tetraphenylporphyrin; 5,10,15,20-Tetraphenyl-21H,23H-porphine	443000 (419 nm) toluene (624)	0.11, toluene (625)	(611,612,626-631)
Q-9	MgTPP	14640-21-2	Magnesium tetraphenylporphyrin; 5,10,15,20-	562000 (426 nm) toluene (632)	0.15, toluene (633)	(613,618,631,634,635)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
			Tetraphenyl-21H,23H-porphine magnesium(II)			
Q-10	ZnTPP	14074-80-7	Zinc tetraphenylporphyrin; 5,10,15,20-Tetraphenyl- 21H,23H-porphine zinc(II)	574000 (422 nm) toluene (629)	0.033, toluene (633)	(617,624,626,630,631,636)
Q-11	H ₂ TMP	56396-12-4	Tetramesitylporphyrin; 5,10,15,20-Tetramesityl- 21H,23H-porphine	427000 (418 nm) toluene (637)	0.088, toluene (638)	(626)
Q-12	MgTMP		Magnesium tetramesitylporphyrin; 5,10,15,20-Tetramesityl- 21H,23H-porphine magnesium(II)	446700 (428 nm) toluene (639)	0.17, toluene (638)	
Q-13	ZnTMP		Zin tetramesitylporphyrin; 5,10,15,20-Tetramesityl- 21H,23H-porphine zinc(II)	385000 (420 nm) toluene (29)	0.039, toluene (638)	(626)
Q-14	H ₂ TTP	14527-51-6	Tetrakis(4-methylphenyl)porphyrin [TTP]	495000 (422 nm) benzene (640)	0.12, benzene (641)	(642,643)
Q-15	(o-H ₂ NPh) ₂ P	52199-35-6	Tetrakis(o-aminophenyl)porphyrin; 5,10,15,20-Tetrakis(2-aninophenyl)-21H,23H-porphine	186000 (422 nm) toluene (29)	0.091, toluene (29)	(644)
Q-16	(ODC)H ₂ P	37083-37-7	Tetrakis(2,6-dichlorophenyl)porphyrin; 5,10,15,20-Tetrakis(2,6-dichlorophenyl)-21H,23H-porphine	299000 (418.5 nm) benzene (627)	0.0019, toluene (638)	
Q-17	C ₆ F ₅ -H ₂ P	25440-14-6	Tetrakis(pentafluorophenyl)porphyrin	236900 (416 nm) benzene (645)	0.032, benzene (645)	(646,647)
Q-18	N-Confused tetraphenylporphyrin		N-Confused H ₂ TPP	159000 (438 nm) chloroform (648)	0.00156, chloroform (648)	(648,649)
Q-19	H ₄ TPP ₂₊		Diprotonated-tetraphenylporphyrin	431000 (445 nm) chloroform + HCl (650)	0.14, benzene + TFA (613)	
Q-20	ZnTMP.+		Zinc tetramesitylporphyrin radical cation	190000 (409 nm) dichloromethane (651)		(651)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
Q-21	Protoporphyrin IX dimethyl ester	5522-66-7	Protoporphyrin IX	166000 (406.5 nm) chloroform (652)	0.1, methanol (653)	(653-656)
Q-22	Hematin	15489-90-4		85000 (383 nm) acetic acid (657)		
Q-23	Tetrabenzoporphine	52952-31-5		11500 (661.5 nm) (658)	0.41, DMF (611)	(659,660)
Q-24	H ₂ TBP(CO ₂ Bu)		Benzoporphyrin(CO ₂ Bu) ₈	324000 (447 nm) DMF (661)	0.27, DMF (661)	(30)
Q-25	ZnTBP(CO ₂ Bu)		Zn-Benzoporphyrin(CO ₂ Bu) ₈	437000 (452 nm) pyridine (661)	0.15, pyridine (661)	(30)
Q-26	PdTBP(CO ₂ Bu)		Pd-Benzoporphyrin(CO ₂ Bu) ₈	302000 (426 nm) DMF (661)	0.23, DMF (661)	(30)
Q-27	H ₂ TBP(CO ₂ Me)Ph		TBP-meso-tetra(4-COOMe-phenyl)-Fb	220000 (469 nm) DMF (662)	0.027, DMF (662)	(30)
Q-28	ZnTBP(CO ₂ Me)Ph		TBP-meso-tetra(4-COOMe-phenyl)-Zn	300000 (471 nm) DMF (32)	0.01, DMF (30)	
Q-29	PdTBP(CO ₂ Me)Ph		TBP-meso-tetra(4-COOMe-phenyl)-Pd	240000 (444 nm) DMF (662)	0.106, DMF (662)	(30)
Q-30	ZnTCPH(CO ₂ Me)Ph		TCPH-meso-tetra(4-COOMe-phenyl)-Zn	210000 (453 nm) DMF (30)	0.0005, DMF (30)	
Q-31	PdTCPH(CO ₂ Me)Ph		TCPH-meso-tetra(4-COOMe-phenyl)-Pd	200000 (428 nm) DMF (30)	< 0.0005, DMF (30)	(662)
Q-32	H ₂ TBP(CO ₂ Bu)Ph		TBP-meso-tetraphenyl-beta-octa(COOMe)-Fb	229000 (483 nm) DMF (661)	0.018, DMF (661)	(30)
Q-33	ZnTBP(CO ₂ Bu)Ph		TBP-meso-tetraphenyl-beta-octa(COOMe)-Zn	389000 (487 nm) DMF (661)	0.03, DMF (661)	(30)
Q-34	PdTBP(CO ₂ Bu)Ph		TBP-meso-tetraphenyl-beta-octa(COOMe)-Pd	250000 (460 nm) DMF (661)	0.03, DMF (661)	(30)
R-1	Ph-Corrole	246231-45-8	5,10,15-Triphenylcorrole	110000 (415 nm) dichloromethane (663)	0.14, dichloromethane (30)	(664)
R-2	C ₆ F ₅ -Corrole	262280-80-8	5,10,15-Tris(pentafluorophenyl)corrole	114000 (408 nm) dichloromethane (665)	0.11, dichloromethane (30)	
R-3	Sapphyrin		Tetraphenyl sapphyrin	74900 (493 nm) dichloromethane (666)		

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
R-4	Bilirubin	635-65-4		55000 (450.8 nm) NS (667)		(668)
R-5	Biliverdin dimethyl ester	10035-62-8		56200 (376 nm) ethanol (669)		(669-672)
R-6	Cyanocobalamin	68-19-9	synthetic form of Vitamin B12	27500 (360.5 nm) borate buffer (pH 10) (673)		(674,675)
S-1	H ₂ Pc	574-93-6	Phthalocyanine; 29H,31H-Phthalocyanine	162000 (698 nm) chloronaphthalene (676)	0.6, chloronaphthalene (625)	(611)
S-2	MgPc	1661-03-6	Magnesium phthalocyanine; Cyanide Ionophore II	87100 (674.5 nm) pyridine (676)	0.48, pyridine (625)	(611)
S-3	FePc	132-16-1	Iron(II) phthalocyanine	69200 (656 nm) o-dichlorobenzene (676)		
S-4	ZnPc	14320-04-8	Zinc phthalocyanine	281800 (672 nm) pyridine (676)	0.3, chloronaphthalene (625)	(611)
S-5	H ₂ Pc(OBu)	116453-73-7	1,4,8,11,15,18,22,25-Octabutoxy-29H,31H-phthalocyanine	134000 (761 nm) toluene (677)	0.13, chloroform (162)	(162,678,679)
S-6	H ₂ Pc(tBu)	35984-93-1	2,9,16,23-Tetra-tert-butyl-29H,31H-phthalocyanine	178000 (697 nm) benzene (680)	0.77, benzene (680)	
S-7	ZnPc(tBu)	39001-65-5	Zinc 2,9,16,23-tetra-tert-butyl-29H,31H-phthalocyanine	380000 (675 nm) benzene (680)	0.37, benzene (680)	(681,682)
S-8	H ₂ Nc(OnBu)	105528-25-4	5,9,14,18,23,27,32,36-Octabutoxy-2,3-naphthalocyanine	181000 (862 nm) toluene (677)	0.17, chloroform (162)	(162)
S-9	H ₂ Nc(tBu)	58687-99-3	2,11,20,29-Tetra-tert-butyl-2,3-naphthalocyanine; Tetra-tert-butyl-naphthalocyanine	26900 (784 nm) chlorobenzene (683)	0.01, chloroform (29)	
S-10	H ₂ N ₄ P(tBu)	64987-70-8	2,7,12,17-Tetra-tert-butyl-5,10,15,20-tetraaza-21H,23H-porphine; Tetra-tert-butyl-tetraazaporphine	72600 (624 nm) chlorobenzene (684)	0.21, chloroform (29)	(685)
S-11	Boron subphthalocyanine chloride	36530-06-0		63000 (564 nm) benzene (686)	0.25, benzene (686)	
T-1	Chlorophyll a	479-61-8		111700 (428.5 nm) diethyl ether (687)	0.32, diethyl ether (688)	(689,690)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ε (λ)	EMISSION Φ_f	OTHER REFS
T-2	Chlorophyll b	519-62-0		160000 (453 nm) diethyl ether (691)	0.117, diethyl ether (688)	(690,692)
T-3	Pheophorbide a	15664-29-6		44500 (667 nm) ethanol (693)	0.28, ethanol (693)	(694,695)
T-4	Pyropheophorbide a	24533-72-0		45000 (669 nm) dichloromethane (696)	0.31, DMF (697)	
T-5	Pyropheophorbide a methyl ester	6453-67-4	Methyl pyropheophorbide a	47100 (668 nm) dichloromethane (698)	0.21, dichloromethane (699)	(697,700-703)
T-6	Chlorin e ₆	19660-77-6		55000 (667 nm) diethyl ether (704)	0.16, ethanol (705)	(706)
T-7	Purpurin 18	25465-77-4		41800 (695 nm) acetone (707)	0.08, toluene (706)	(706,708)
T-8	H ₂ TPC	2669-65-0	meso-Tetraphenylchlorin	42000 (652 nm) benzene (709)	0.28, toluene (710)	(711-715)
T-9	H ₂ C-1		17,18-Dihydro-5-(4-methylphenyl)-10-mesityl-18,18-dimethylporphyrin,	89100 (414 nm) toluene (716)	0.26, toluene (717)	(718)
T-10	CuC-1		Copper(II)-17,18-dihydro-10-mesityl-18,18-dimethyl-5-(4-methylphenyl)porphyrin	162000 (408 nm) toluene (717)		(718)
T-11	ZnC-1		Zinc(II)-17,18-Dihydro-10-mesityl-18,18-dimethyl-5-(4-methylphenyl)porphyrin	186000 (412 nm) toluene (716)	0.083, toluene (717)	(718)
T-12	H ₂ COxo-1		17,18-Dihydro-18,18-dimethyl-5-(4-methylphenyl)-10-mesityl-17-oxoporphyrin	174000 (414 nm) toluene (717)	0.13, toluene (717)	(718)
T-13	MgCOxo-1		Magnesium(II)-17,18-dihydro-18,18-dimethyl-5-(4-methylphenyl)-10-mesityl-17-oxoporphyrin	191000 (425 nm) toluene (717)	0.1, toluene (717)	(718)
T-14	CuCOxo-1		Copper(II)-17,18-dihydro-18,18-dimethyl-5-(4-methylphenyl)-10-mesityl-17-oxoporphyrin	174000 (419 nm) toluene (717)		(718)
T-15	ZnCOxo-1		Zinc(II)-17,18-dihydro-18,18-dimethyl-5-(4-methylphenyl)-10-	209000 (423 nm) toluene (717)	0.04, toluene (717)	(718)

ID	COMPOUND	CAS	SYNONYM	ABSORPTION ϵ (λ)	EMISSION Φ_f	OTHER REFS
			mesityl-17-oxoporphyrin			
T-16	Bacteriochlorophyll a	17499-98-8		92000 (781 nm) toluene (719)	0.2, toluene (719)	

#: data reported herein.

Abbreviations: DMF, N,N-dimethylformamide; DMSO, dimethylsulfoxide; MOPS, 3-(N-morpholino)propylsulfonic acid; ND, not detected; NR, not reported; NS, solvent not specified; PBS, phosphate-buffered saline; TFA, trifluoroacetic acid; THF, tetrahydrofuran.

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FIGURE CAPTION

Figure 1. Representative member of each structure class A–T.

