Supporting Information for:

Heuristics from Modeling of Spectral Overlap in Förster Resonance Energy Transfer (FRET)

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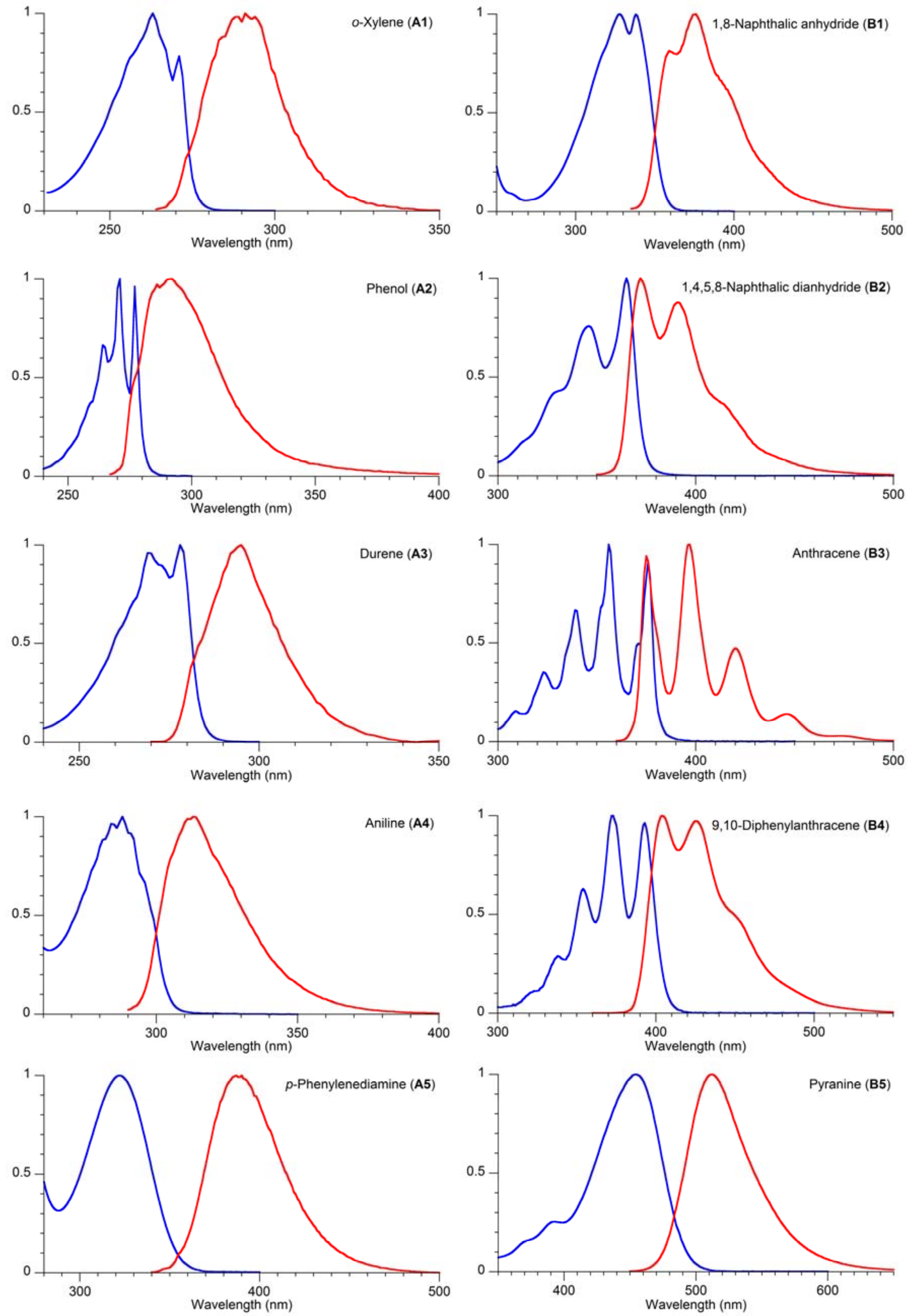
A. Gaussian distributions. The Gaussian distribution is given by equation S1 where x is the wavelength, μ is the mean value (the wavelength at the peak of the band), and δ is the standard deviation. The fwhm is given by equation S2.[S1]

$$y = \frac{1}{\delta\sqrt{2\pi}} e^{-(x-u)^2/2\delta^2} \quad \text{(eq S1)}$$

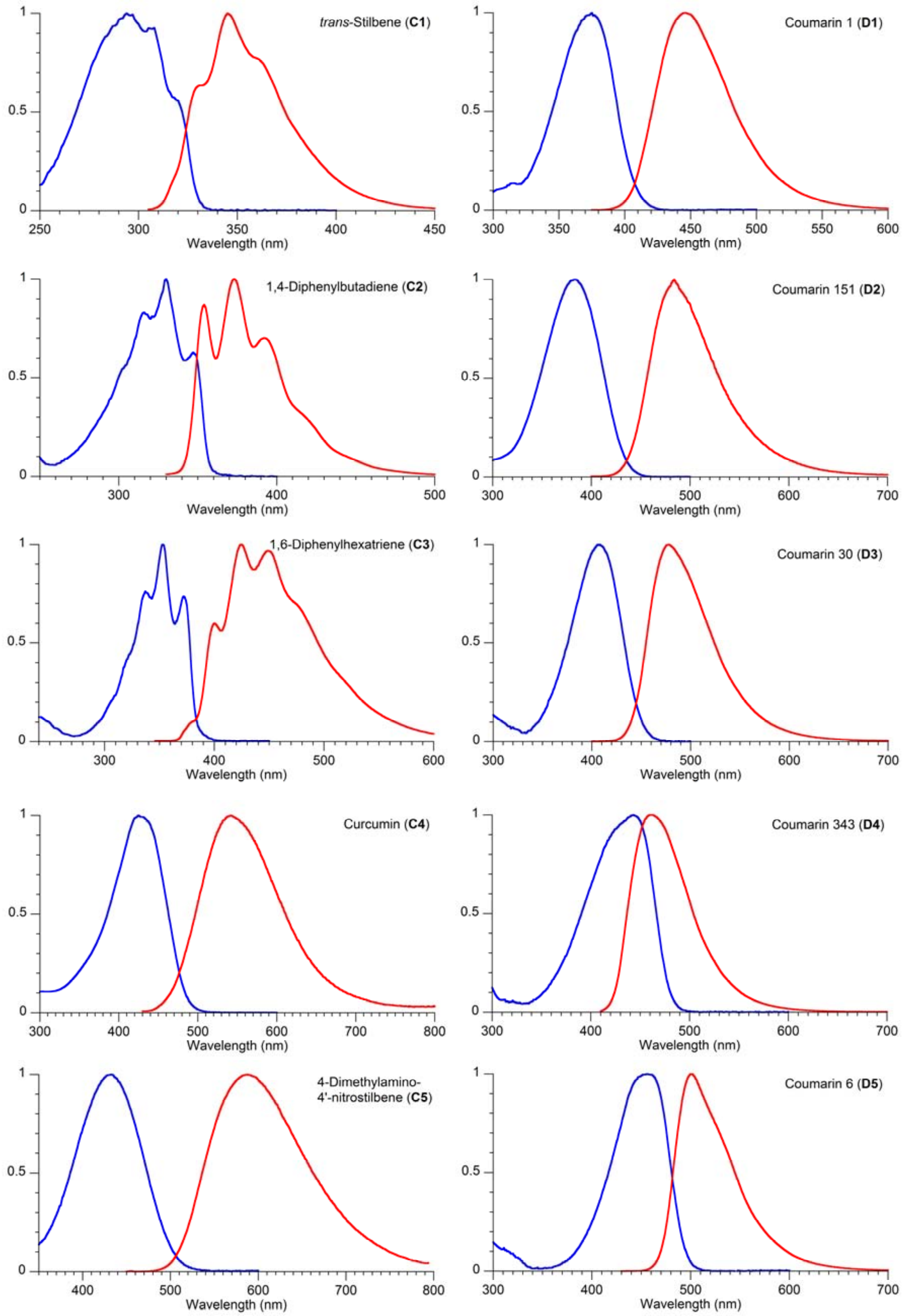
$$\text{fwhm} = 2\sqrt{2\ln 2}\,\delta \approx 2.3548\,\delta \quad \text{(eq S2)}$$

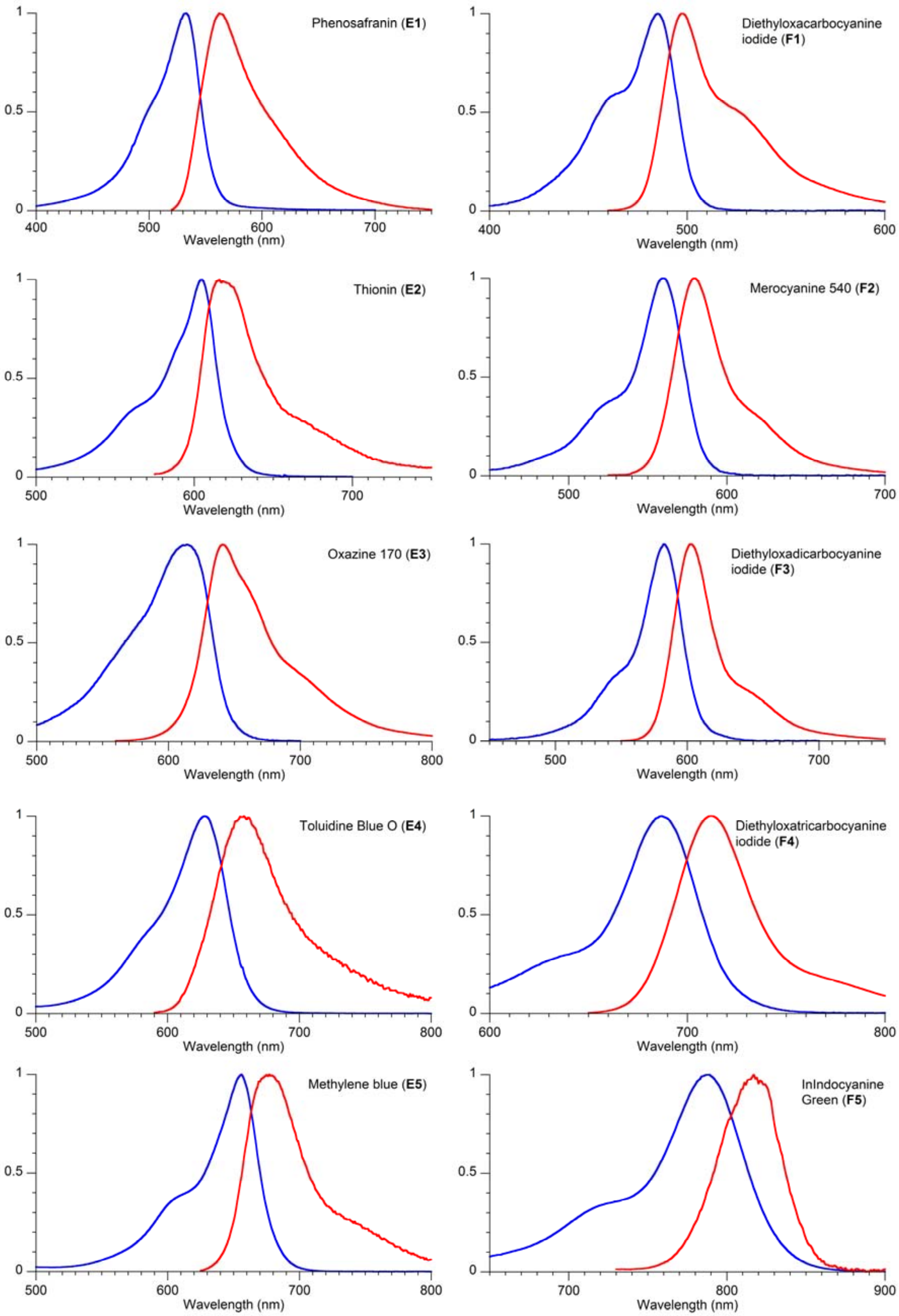
(S1) http://mathworld.wolfram.com/GaussianFunction.html

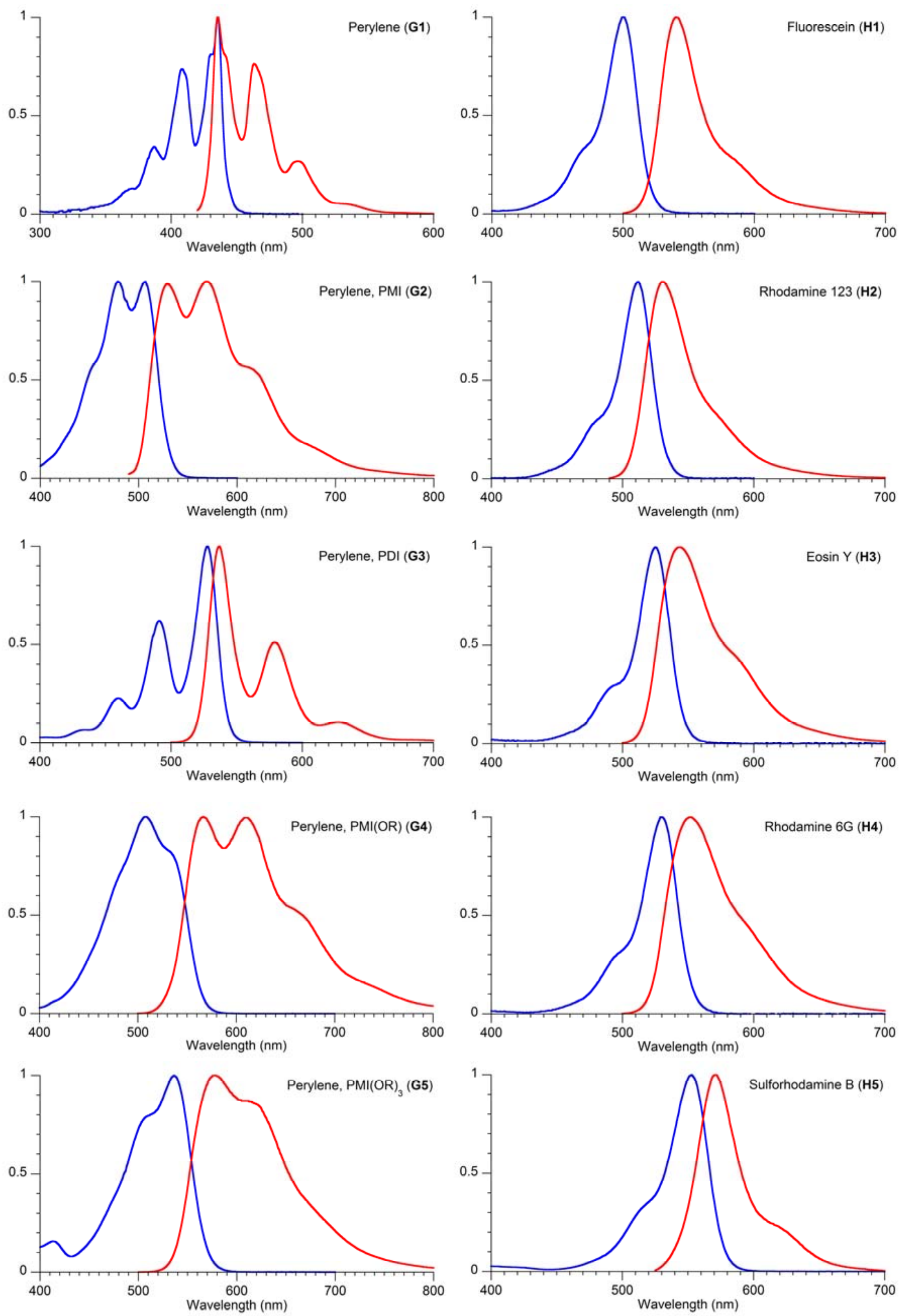
B. Spectra and spectral data. The following six pages of spectra (for all 60 compounds) pertain to Figure S1.

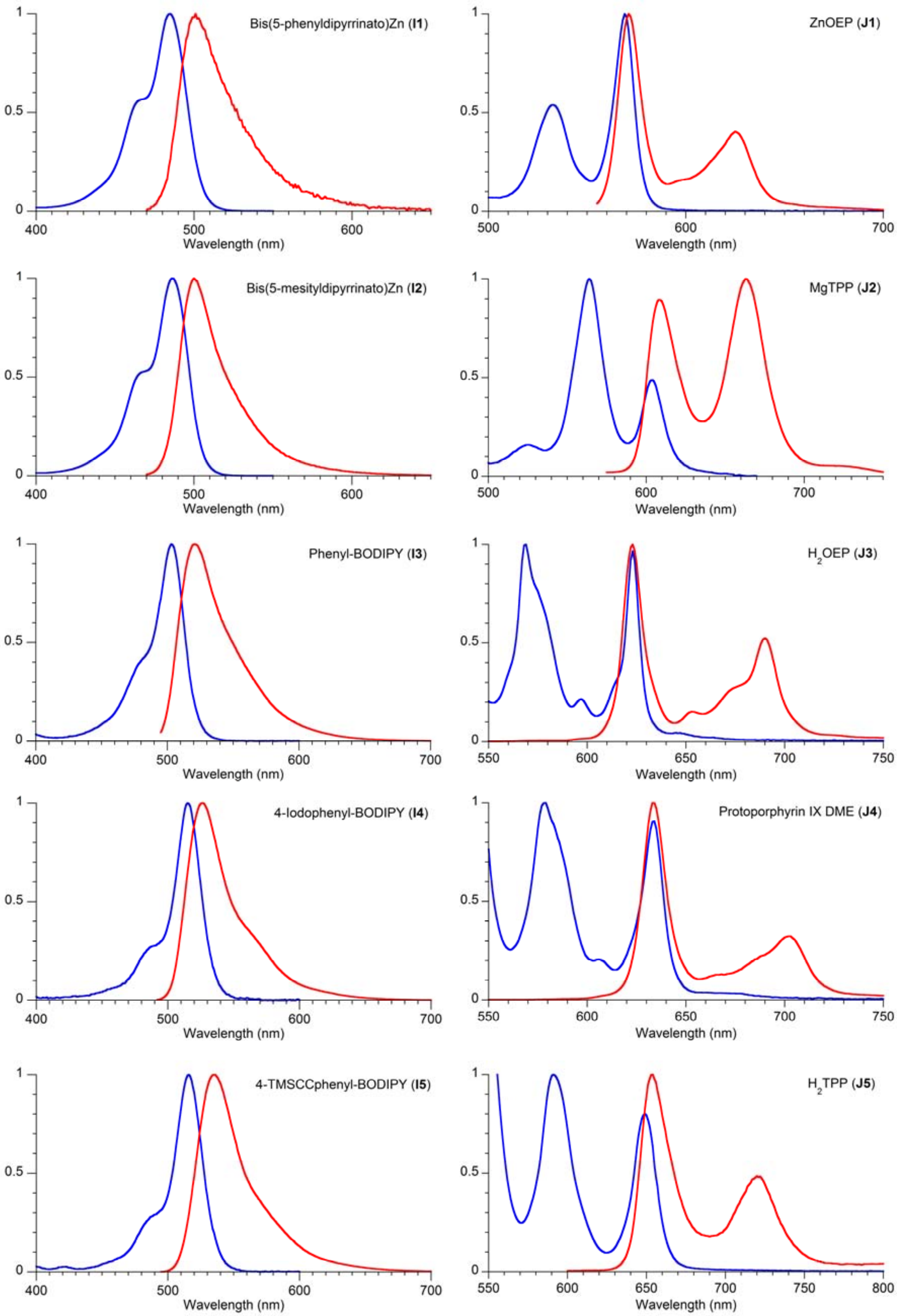


o-Xylene (A1)
1,8-Naphthalic anhydride (B1)
Phenol (A2)
1,4,5,8-Naphthalic dianhydride (B2)
Durene (A3)
Anthracene (B3)
Aniline (A4)
9,10-Diphenylanthracene (B4)
p-Phenylenediamine (A5)
Pyranine (B5)
Wavelength (nm)


trans-Stilbene (C1)
Coumarin 1 (D1)
1,4-Diphenylbutadiene (C2)
Coumarin 151 (D2)
1,6-Diphenylhexatriene (C3)
Coumarin 30 (D3)
Curcumin (C4)
Coumarin 343 (D4)
4-Dimethylamino-4'-nitrostilbene (C5)
Coumarin 6 (D5)
Wavelength (nm)


Phenosafranin (**E1**)
Diethyloxacarbocyanine iodide (**F1**)
Thionin (**E2**)
Merocyanine 540 (**F2**)
Oxazine 170 (**E3**)
Diethyloxadicarbocyanine iodide (**F3**)
Toluidine Blue O (**E4**)
Diethyloxatricarbocyanine iodide (**F4**)
Methylene blue (**E5**)
InIndocyanine Green (**F5**)
Wavelength (nm)
0
0.5
1


Perylene (**G1**)
Fluorescein (**H1**)
Perylene, PMI (**G2**)
Rhodamine 123 (**H2**)
Perylene, PDI (**G3**)
Eosin Y (**H3**)
Perylene, PMI(OR) (**G4**)
Rhodamine 6G (**H4**)
Perylene, PMI(OR)$_3$ (**G5**)
Sulforhodamine B (**H5**)
Wavelength (nm)


Bis(5-phenyldipyrrinato)Zn (I1)
ZnOEP (J1)
Bis(5-mesityldipyrrinato)Zn (I2)
MgTPP (J2)
Phenyl-BODIPY (I3)
H_2OEP (J3)
4-Iodophenyl-BODIPY (I4)
Protoporphyrin IX DME (J4)
4-TMSCCphenyl-BODIPY (I5)
H_2TPP (J5)
Wavelength (nm)

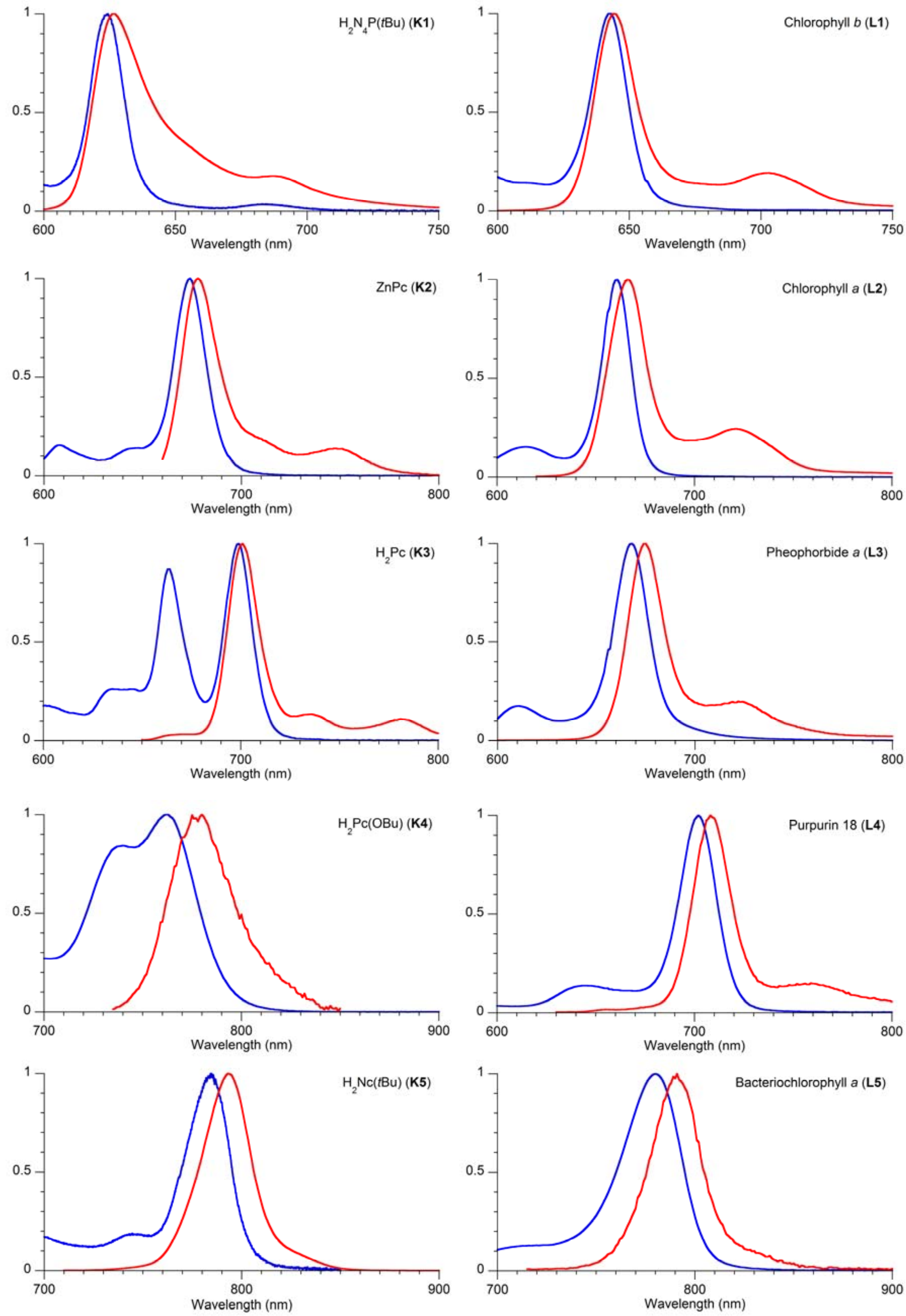


Figure S1. Absorption (blue line) and fluorescence (red line) spectra of 60 compounds.

Table S1. Spectral data for 60 compounds in wavenumbers.[a]

ID	compound	λ_{abs} (cm^{-1})	λ_{flu} (cm^{-1})	λ_{avg} (cm^{-1})[b]	fwhm (cm^{-1})[c]	Stokes (cm^{-1})	Stokes/ fwhm[b]
A1	*o*-Xylene	38023	34364	36194	3204	3659	1.14
A2	Phenol	36900	34247	35573	3150	2654	0.84
A3	Durene	35971	33898	34935	2807	2073	0.74
A4	Aniline	34722	31949	33336	3278	2773	0.85
A5	*p*-Phenylenediamine	30864	25641	28253	3430	5223	1.52
B1	1,8-Naphthalic anhydride	30488	26596	28542	3819	3892	1.02
B2	1,4,5,8-Naphthalic dianhydride	27397	26882	27139	2655	516	0.19
B3	Anthracene	26667	26667	26667	640	0	0
B4	9,10-Diphenylanthracene	26810	23474	25142	3327	3335	1
B5	Pyranine	22026	19531	20779	2396	2495	1.04
C1	*trans*-Stilbene	34043	28986	31514	5225	5057	0.97
C2	1,4-Diphenylbutadiene	30303	26810	28556	4380	3493	0.8
C3	1,6-Diphenylhexatriene	28309	23585	25947	4875	4724	0.97
C4	Curcumin	23529	18450	20990	4140	5079	1.23
C5	4-DMA-4'-nitrostilbene	23148	17007	20077	4226	6141	1.45
D1	Coumarin 1	26810	22371	24591	3389	4438	1.31
D2	Coumarin 151	26042	20661	23351	3843	5381	1.4
D3	Coumarin 30	24510	20921	22715	3238	3589	1.11
D4	Coumarin 343	22472	21645	22058	3511	827	0.24
D5	Coumarin 6	21786	20000	20893	2791	1786	0.64
E1	Phenosafranin	18762	17794	18278	1817	968	0.53
E2	Thionin	16529	16234	16381	1006	295	0.29
E3	Oxazine 170	16313	15601	15957	1566	713	0.46
E4	Toluidine Blue O	15924	15198	15561	1391	726	0.52
E5	Methylene blue	15244	14771	15007	1046	473	0.45
F1	Diethyloxacarbocyanine iodide	20619	20080	20349	1681	538	0.32
F2	Merocyanine 540	17857	17271	17564	1065	586	0.55
F3	Diethyloxadicarbocyanine iodide	17182	16556	16869	997	626	0.63
F4	Diethyloxatricarbocyanine iodide	14535	14045	14290	910	490	0.54
F5	Indocyanine Green	12674	12240	12457	827	434	0.52
G1	Perylene	22936	22936	22936	842	0	0
G2	Perylene, PMI	20877	17575	19226	3379	3302	0.98
G3	Perylene, PDI	18939	18622	18781	723	317	0.44
G4	Perylene, PMI(OR)	19724	16393	18059	3267	3330	1.02
G5	Perylene, $PMI(OR)_3$	18657	17301	17979	2747	1356	0.49
H1	Fluorescein	20000	18519	19259	1171	1481	1.26
H2	Rhodamine 123	19531	18797	19164	1224	734	0.6
H3	Eosin Y	19048	18382	18715	1389	665	0.48
H4	Rhodamine 6G	18868	18116	18492	1490	752	0.5
H5	Sulforhodamine B	18083	17513	17798	1125	570	0.51
I1	Bis(5-phenyldipyrrinato)Zn	20619	19960	20289	1524	658	0.43
I2	Bis(5-mesityldipyrrinato)Zn	20534	20000	20267	1338	534	0.4
I3	Phenyl-BODIPY	19881	19194	19537	1308	687	0.53
I4	4-Iodophenyl-BODIPY	19380	19011	19196	1083	368	0.34
I5	4-TMSCCphenyl-BODIPY	19380	18657	19018	1113	723	0.65
J1	ZnOEP	17575	17513	17544	400	62	0.15
J2	MgTPP	16556	16420	16488	557	136	0.24
J3	H_2OEP	16051	16051	16051	258	0	0
J4	Protoporphyrin IX DME	15773	15773	15773	336	0	0
J5	H_2TPP	15408	15291	15349	459	118	0.26

K1	H_2N_4P(*t*Bu)	16026	15974	16000	518	51	0.1
K2	ZnPc	14837	14728	14782	448	109	0.24
K3	H_2Pc	14306	14265	14286	347	41	0.12
K4	H_2Pc(OBu)	13106	12821	12963	811	286	0.35
K5	H_2Nc(*t*Bu)	12755	12610	12683	442	145	0.33
L1	Chlorophyll *b*	15552	15528	15540	411	24	0.06
L2	Chlorophyll *a*	15129	15015	15072	454	114	0.25
L3	Pheophorbide *a*	14970	14815	14892	455	155	0.34
L4	Purpurin 18	14245	14124	14185	453	121	0.27
L5	Bacteriochlorophyll *a*	12821	12642	12731	520	178	0.34

[a]Structures and compound names are shown in Figure 1. Significant figures are not taken into consideration. [b]Average peak wavelength position of the absorption and fluorescence spectra. [c]Average fwhm of the absorption and fluorescence spectra.

Table S2. Values of J for distinct wavelength and fwhm for Gaussian distributions with perfect overlap (Stokes shift = 0).[a]

	Wavelength (nm)																
fwhm	200	250	300	350	400	450	500	550	600	650	700	750	800	850	900	950	1000
5	1.13	2.76	5.73	10.6	18.1	29.0	44.2	64.7	91.6	126	170	224	290	369	464	576	707
10	1.13	2.76	5.73	10.6	18.1	29.0	44.2	64.7	91.7	126	170	224	290	369	464	576	707
20	1.14	2.77	5.74	10.6	18.1	29.0	44.2	64.8	91.7	126	170	224	290	369	464	576	707
30	1.15	2.78	5.76	10.7	18.2	29.1	44.3	64.8	91.8	126	170	224	290	369	464	576	707
40	1.16	2.80	5.78	10.7	18.2	29.1	44.3	64.9	91.9	126	170	224	290	370	464	576	708
50	1.17	2.82	5.81	10.7	18.3	29.2	44.4	65.0	92.0	127	170	224	290	370	465	577	708
60	1.19	2.85	5.85	10.8	18.3	29.3	44.5	65.1	92.1	127	170	225	291	370	465	577	708
70	1.21	2.88	5.90	10.8	18.4	29.4	44.7	65.3	92.3	127	171	225	291	370	465	578	709
80	1.23	2.92	5.95	10.9	18.5	29.5	44.8	65.4	92.5	127	171	225	291	371	466	578	710
90	1.26	2.96	6.01	11.0	18.6	29.6	45.0	65.6	92.8	128	171	225	292	371	466	579	710
100	1.29	3.00	6.07	11.1	18.7	29.8	45.2	65.9	93.0	128	172	226	292	372	467	579	711

[a]A factor of 10^{14} needs to be included when $\varepsilon_{(A)} = 100{,}000\ M^{-1}\cdot cm^{-1}$.

Table S3. Values of J/λ^4 (nm^4) and the molar absorption coefficient ($\varepsilon_{(A)}$) for distinct wavelength and fwhm for Gaussian distributions with perfect overlap (Stokes shift = 0).

	Wavelength (nm)																
fwhm	200	250	300	350	400	450	500	550	600	650	700	750	800	850	900	950	1000
5	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707
10	0.708	0.708	0.708	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707
20	0.711	0.710	0.709	0.708	0.708	0.708	0.708	0.708	0.708	0.707	0.707	0.707	0.707	0.707	0.707	0.707	0.707
30	0.716	0.713	0.711	0.710	0.709	0.709	0.708	0.708	0.708	0.708	0.708	0.708	0.708	0.708	0.708	0.707	0.707
40	0.722	0.717	0.714	0.712	0.711	0.710	0.710	0.709	0.709	0.709	0.708	0.708	0.708	0.708	0.708	0.708	0.708
50	0.731	0.722	0.718	0.715	0.713	0.712	0.711	0.710	0.710	0.709	0.709	0.709	0.709	0.708	0.708	0.708	0.708
60	0.742	0.729	0.722	0.718	0.716	0.714	0.713	0.712	0.711	0.710	0.710	0.710	0.709	0.709	0.709	0.709	0.708
70	0.754	0.737	0.728	0.722	0.719	0.716	0.715	0.713	0.712	0.712	0.711	0.710	0.710	0.710	0.709	0.709	0.709
80	0.769	0.746	0.734	0.727	0.722	0.719	0.717	0.715	0.714	0.713	0.712	0.711	0.711	0.710	0.710	0.710	0.710
90	0.785	0.757	0.742	0.732	0.727	0.722	0.720	0.717	0.716	0.714	0.713	0.713	0.712	0.711	0.711	0.711	0.710
100	0.804	0.769	0.750	0.738	0.731	0.726	0.722	0.720	0.718	0.716	0.715	0.714	0.713	0.712	0.712	0.711	0.711

Table S4. Values of *J* for distinct wavelength and fwhm for Lorentzian distributions with perfect overlap (Stokes shift = 0).[a]

	Wavelength (nm)																
fwhm	200	250	300	350	400	450	500	550	600	650	700	750	800	850	900	950	1000
5	0.80	1.96	4.07	7.53	12.8	20.6	31.3	45.9	65.1	89.5	120	159	205	262	329	408	501
10	0.81	1.97	4.10	7.56	12.9	20.7	31.4	46.0	65.3	89.7	121	159	206	262	329	409	502
20	0.83	2.00	4.16	7.63	13.0	20.8	31.6	46.3	66.0	90.2	121	160	207	263	331	410	504
30	0.85	2.04	4.24	7.72	13.1	21.0	31.9	46.6	66.6	90.7	122	161	208	264	332	412	505
40	0.89	2.10	4.33	7.84	13.3	21.3	32.2	47.0	67.3	91.3	123	162	209	266	334	414	508
50	0.93	2.16	4.44	7.97	13.5	21.6	32.5	47.4	68.1	92.0	124	163	210	267	335	416	510
60	0.98	2.24	4.55	8.13	13.7	21.9	32.9	47.9	69.0	92.8	125	164	212	269	337	418	512
70	1.04	2.33	4.68	8.31	13.9	22.2	33.3	48.4	69.8	93.6	126	165	213	271	339	420	515
80	1.11	2.43	4.82	8.51	14.2	22.6	33.7	48.9	70.8	94.5	127	166	215	272	341	423	518
90	1.19	2.55	4.97	8.73	14.5	23.0	34.2	49.6	71.8	95.4	128	168	216	274	344	425	521
100	1.28	2.68	5.13	8.98	14.8	23.4	34.7	50.2	72.8	96.4	129	169	218	276	346	428	524

[a]A factor of 10^{14} needs to be included when $\varepsilon_{(A)}$ = 100,000 $M^{-1}\cdot cm^{-1}$.

Table S5. Values of J/λ^4 (nm^4) and the molar absorption coefficient ($\varepsilon_{(A)}$) for distinct wavelength and fwhm for Lorentzian distributions with perfect overlap (Stokes shift = 0).

	Wavelength (nm)																
fwhm	200	250	300	350	400	450	500	550	600	650	700	750	800	850	900	950	1000
5	0.503	0.502	0.503	0.502	0.501	0.502	0.501	0.501	0.502	0.501	0.501	0.501	0.501	0.501	0.501	0.501	0.501
10	0.507	0.505	0.506	0.504	0.503	0.504	0.503	0.503	0.504	0.502	0.502	0.502	0.502	0.502	0.502	0.502	0.502
20	0.517	0.513	0.514	0.509	0.507	0.508	0.506	0.506	0.509	0.505	0.505	0.505	0.504	0.504	0.504	0.504	0.504
30	0.533	0.523	0.524	0.515	0.513	0.513	0.510	0.509	0.514	0.508	0.508	0.508	0.507	0.507	0.506	0.506	0.505
40	0.553	0.537	0.535	0.522	0.519	0.519	0.515	0.513	0.520	0.512	0.511	0.511	0.510	0.509	0.509	0.508	0.508
50	0.579	0.553	0.548	0.531	0.526	0.526	0.520	0.518	0.526	0.515	0.515	0.514	0.513	0.512	0.511	0.511	0.510
60	0.611	0.573	0.562	0.542	0.534	0.533	0.526	0.523	0.532	0.520	0.519	0.518	0.516	0.515	0.514	0.513	0.512
70	0.649	0.596	0.578	0.554	0.544	0.541	0.532	0.529	0.539	0.524	0.523	0.522	0.520	0.518	0.517	0.516	0.515
80	0.693	0.623	0.595	0.567	0.554	0.550	0.539	0.535	0.546	0.529	0.527	0.526	0.524	0.522	0.520	0.519	0.518
90	0.744	0.653	0.614	0.582	0.566	0.560	0.547	0.542	0.554	0.534	0.532	0.530	0.528	0.526	0.524	0.522	0.521
100	0.803	0.687	0.634	0.599	0.578	0.570	0.556	0.549	0.562	0.540	0.537	0.535	0.532	0.529	0.527	0.525	0.524

Table S6. Relationship between the degree of overlap (%) and the ratio of Stokes shift/fwhm.[a]

λ_{abs} (nm)	λ_{flu} (nm)	λ_{avg} (nm)[b]	Stokes (nm)	fwhm (nm)	Stokes/ fwhm	J [b] ($M^{-1}\cdot cm^{-1}\cdot nm^4$)	Overlap (%)[c]
λ_{avg} = 400 nm, fwhm = 20 nm							
400	400	400	0	20	0	1.813E+10	100.00
399	401	400	2	20	0.1	1.788E+10	98.62
398	402	400	4	20	0.2	1.715E+10	94.61
397	403	400	6	20	0.3	1.600E+10	88.27
396	404	400	8	20	0.4	1.452E+10	80.11
395	405	400	10	20	0.5	1.282E+10	70.71
394	406	400	12	20	0.6	1.100E+10	60.71
393	407	400	14	20	0.7	9.190E+09	50.70
392	408	400	16	20	0.8	7.464E+09	41.18
391	409	400	18	20	0.9	5.897E+09	32.53
390	410	400	20	20	1	4.532E+09	25.00
389	411	400	22	20	1.1	3.387E+09	18.69
388	412	400	24	20	1.2	2.462E+09	13.58
387	413	400	26	20	1.3	1.741E+09	9.61
386	414	400	28	20	1.4	1.197E+09	6.61
385	415	400	30	20	1.5	8.011E+08	4.42
384	416	400	32	20	1.6	5.212E+08	2.88
383	417	400	34	20	1.7	3.299E+08	1.82
382	418	400	36	20	1.8	2.031E+08	1.12
381	419	400	38	20	1.9	1.216E+08	0.67
380	420	400	40	20	2	7.081E+07	0.39
λ_{avg} = 400 nm, fwhm = 80 nm							
400	400	400	0	80	0	1.849E+10	100.00
396	404	400	8	80	0.1	1.824E+10	98.62
392	408	400	16	80	0.2	1.750E+10	94.61
388	412	400	24	80	0.3	1.633E+10	88.27
384	416	400	32	80	0.4	1.482E+10	80.11
380	420	400	40	80	0.5	1.308E+10	70.71
376	424	400	48	80	0.6	1.123E+10	60.71
372	428	400	56	80	0.7	9.376E+09	50.70
368	432	400	64	80	0.8	7.616E+09	41.18
364	436	400	72	80	0.9	6.017E+09	32.53
360	440	400	80	80	1	4.624E+09	25.00
356	444	400	88	80	1.1	3.456E+09	18.69
352	448	400	96	80	1.2	2.512E+09	13.58
348	452	400	104	80	1.3	1.776E+09	9.61
344	456	400	112	80	1.4	1.222E+09	6.61
340	460	400	120	80	1.5	8.173E+08	4.42
336	464	400	128	80	1.6	5.318E+08	2.88
332	468	400	136	80	1.7	3.366E+08	1.82
328	472	400	144	80	1.8	2.072E+08	1.12

324	476	400	152	80	1.9	1.241E+08	0.67
320	480	400	160	80	2	7.224E+07	0.39
λ_{avg} = 600 nm, fwhm = 20 nm							
600	600	600	0	20	0	9.170E+10	100.00
599	601	600	2	20	0.1	9.043E+10	98.62
598	602	600	4	20	0.2	8.675E+10	94.61
597	603	600	6	20	0.3	8.094E+10	88.27
596	604	600	8	20	0.4	7.346E+10	80.11
595	605	600	10	20	0.5	6.484E+10	70.71
594	606	600	12	20	0.6	5.567E+10	60.71
593	607	600	14	20	0.7	4.649E+10	50.70
592	608	600	16	20	0.8	3.776E+10	41.18
591	609	600	18	20	0.9	2.983E+10	32.53
590	610	600	20	20	1	2.292E+10	25.00
589	611	600	22	20	1.1	1.713E+10	18.69
588	612	600	24	20	1.2	1.246E+10	13.58
587	613	600	26	20	1.3	8.808E+09	9.61
586	614	600	28	20	1.4	6.058E+09	6.61
585	615	600	30	20	1.5	4.052E+09	4.42
584	616	600	32	20	1.6	2.637E+09	2.88
583	617	600	34	20	1.7	1.669E+09	1.82
582	618	600	36	20	1.8	1.027E+09	1.12
581	619	600	38	20	1.9	6.151E+08	0.67
580	620	600	40	20	2	3.582E+08	0.39
λ_{avg} = 600 nm, fwhm = 80 nm							
600	600	600	0	80	0	9.252E+10	100.00
596	604	600	8	80	0.1	9.125E+10	98.62
592	608	600	16	80	0.2	8.753E+10	94.61
588	612	600	24	80	0.3	8.167E+10	88.27
584	616	600	32	80	0.4	7.412E+10	80.11
580	620	600	40	80	0.5	6.542E+10	70.71
576	624	600	48	80	0.6	5.617E+10	60.71
572	628	600	56	80	0.7	4.691E+10	50.70
568	632	600	64	80	0.8	3.810E+10	41.18
564	636	600	72	80	0.9	3.010E+10	32.53
560	640	600	80	80	1	2.313E+10	25.00
556	644	600	88	80	1.1	1.729E+10	18.69
552	648	600	96	80	1.2	1.257E+10	13.58
548	652	600	104	80	1.3	8.887E+09	9.61
544	656	600	112	80	1.4	6.112E+09	6.61
540	660	600	120	80	1.5	4.089E+09	4.42
536	664	600	128	80	1.6	2.661E+09	2.88
532	668	600	136	80	1.7	1.684E+09	1.82
528	672	600	144	80	1.8	1.037E+09	1.12
524	676	600	152	80	1.9	6.206E+08	0.67
520	680	600	160	80	2	3.614E+08	0.39

λ_{avg} = 800 nm, fwhm = 20 nm							
800	800	800	0	20	0	2.8973E+11	100.00
799	801	800	2	20	0.1	2.8574E+11	98.62
798	802	800	4	20	0.2	2.7410E+11	94.61
797	803	800	6	20	0.3	2.5574E+11	88.27
796	804	800	8	20	0.4	2.3209E+11	80.11
795	805	800	10	20	0.5	2.0487E+11	70.71
794	806	800	12	20	0.6	1.7589E+11	60.71
793	807	800	14	20	0.7	1.4689E+11	50.70
792	808	800	16	20	0.8	1.1931E+11	41.18
791	809	800	18	20	0.9	9.4259E+10	32.53
790	810	800	20	20	1	7.2432E+10	25.00
789	811	800	22	20	1.1	5.4138E+10	18.69
788	812	800	24	20	1.2	3.9357E+10	13.58
787	813	800	26	20	1.3	2.7830E+10	9.61
786	814	800	28	20	1.4	1.9141E+10	6.61
785	815	800	30	20	1.5	1.2804E+10	4.42
784	816	800	32	20	1.6	8.3314E+09	2.88
783	817	800	34	20	1.7	5.2728E+09	1.82
782	818	800	36	20	1.8	3.2458E+09	1.12
781	819	800	38	20	1.9	1.9434E+09	0.67
780	820	800	40	20	2	1.1318E+09	0.39
λ_{avg} = 800 nm, fwhm = 80 nm							
800	800	800	0	80	0	2.912E+11	100.00
796	804	800	8	80	0.1	2.872E+11	98.62
792	808	800	16	80	0.2	2.755E+11	94.61
788	812	800	24	80	0.3	2.570E+11	88.27
784	816	800	32	80	0.4	2.333E+11	80.11
780	820	800	40	80	0.5	2.059E+11	70.71
776	824	800	48	80	0.6	1.768E+11	60.71
772	828	800	56	80	0.7	1.476E+11	50.70
768	832	800	64	80	0.8	1.199E+11	41.18
764	836	800	72	80	0.9	9.474E+10	32.53
760	840	800	80	80	1	7.280E+10	25.00
756	844	800	88	80	1.1	5.441E+10	18.69
752	848	800	96	80	1.2	3.956E+10	13.58
748	852	800	104	80	1.3	2.797E+10	9.61
744	856	800	112	80	1.4	1.924E+10	6.61
740	860	800	120	80	1.5	1.287E+10	4.42
736	864	800	128	80	1.6	8.374E+09	2.88
732	868	800	136	80	1.7	5.300E+09	1.82
728	872	800	144	80	1.8	3.262E+09	1.12
724	876	800	152	80	1.9	1.953E+09	0.67
720	880	800	160	80	2	1.137E+09	0.39

[a]See text and Figure 8. [b]J here is calculated for the given Stokes shift. [c]Degree of overlap = 100 x $J / J_{G\text{-}0}$. The J in the numerator is calculated here for the given Stokes shift (column 7 in this table).

C. Assessing the degree of overlap. We explored a handful of methods for assessing the degree of overlap (in %) of experimental spectra, which often deviate substantially from elegant Gaussian distributions (Figures S2–S6). The methods were applied first to Merocyanine 540 owing to the nature of the absorption and fluorescence spectra (Figure S2). The methods are as follows:

Method I: The experimental spectra are implicitly approximated by Gaussian distributions and the degree of overlap is based on the experimental Stokes shift and average fwhm. The resulting Stokes shift/fwhm value is used with the graph in Figure 8 and the companion equation to obtain the degree of overlap (in %), here termed Overlap-I. The validity of this approach here is illustrated by the close match of the Gaussian distributions for the Merocyanine 540 spectra, with Overlap-I of 67% (Figure S3). The values for Stokes/fwhm in Table S7 are calculated on the basis of wavelength (nm); the values differ by <2% upon calculation on the basis of wavenumbers (cm^{-1}) as shown in Table S1.

Method II: The approach is based on the idealized full utilization of the fluorescence spectrum. Assume that the absorption spectrum is flat (i.e., constant ε and independent of λ; the value of $\varepsilon_{(A)}$ equals that of the value at the experimental λ_{abs}) whereupon a model J value is calculated (Figure AS4). The experimental J value divided by the model J value provides the Overlap-II, which is independent of the shape of the absorption spectrum. For Merocyanine 540, the model J value is 1.73×10^{16} $M^{-1} \cdot cm^{-1} \cdot nm^4$, which resulted in Overlap-II = 21%.

Method III: Here the absorption spectrum is taken to be identical with that of the fluorescence spectrum, in which case the spectra are perfectly overlapped (Figure S5). The resulting model J value is calculated by replacing the experimental absorption spectrum with the fluorescence spectrum. The experimental J value divided by the model J value provides the Overlap-III. For Merocyanine 540, the model J value is 9.64×10^{15} $M^{-1} \cdot cm^{-1} \cdot nm^4$, which resulted in Overlap-III = 38%.

Method IV: A model J value is calculated with perfectly overlapped Gaussian distributions centered at λ_{avg}. For Merocyanine 540, the λ_{avg} is 569 nm with average fwhm of 35 nm as shown in Figure S6, with $\varepsilon_{(A)}$ = 138,000 $M^{-1} \cdot cm^{-1}$ and the fluorescence spectrum integrated area of 1. The Overlap-IV is then given by the experimental J divided by the model J. The model J value for Merocyanine 540 is 1.03×10^{16} $M^{-1} \cdot cm^{-1} \cdot nm^4$, which corresponds to Overlap-IV = 36%.

Method V: Here a simple approximation of Method IV is instituted. A model J value is not calculated by assessed by the overlap of the spectra; instead, equation 5 is used to give a value for the model J. The Overlap-V is then given by the experimental J divided by the model J ($J_{G\text{–}0}$) as described in equation 6. Thus, the Overlap-V is the same as the "degree of overlap" described in the main body of the paper. For Merocyanine 540, the Overlap-V is 36%.

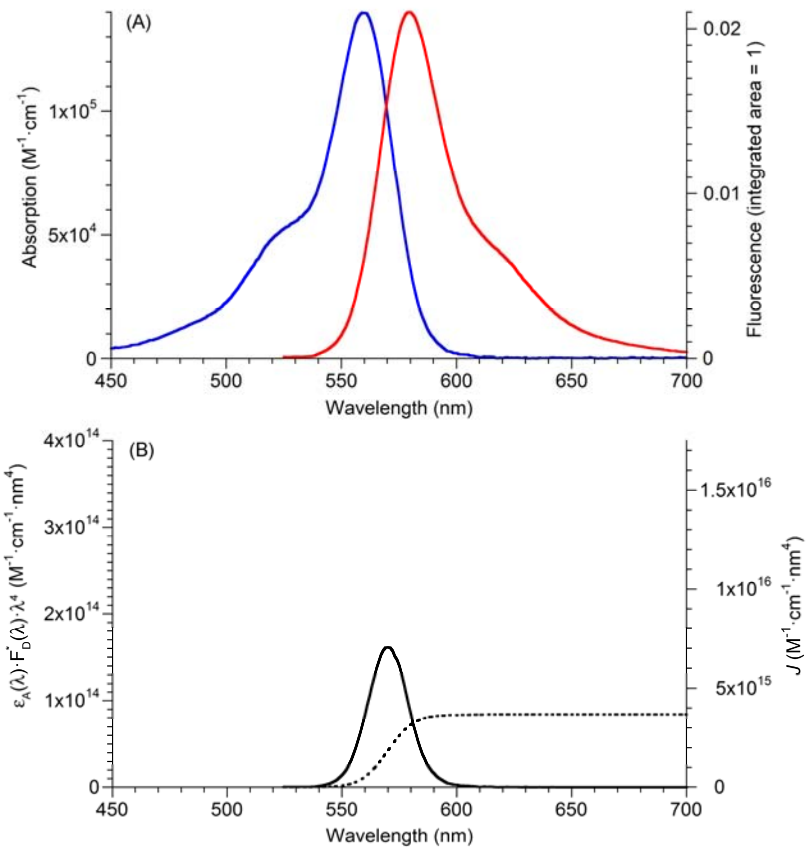


Figure S2. Data for Merocyanine 540. (A) Absorption spectrum (blue line, scale shown on the left y-axis) and fluorescence spectrum (red line, scale shown on the right y-axis). (B) Integrand of the *J* calculation, equation 3 (solid line, left vertical scale). The magnitude of the integration over the specified wavelength region (dotted line, right vertical scale) here equals 3.67×10^{15} $M^{-1} \cdot cm^{-1} \cdot nm^{4}$.

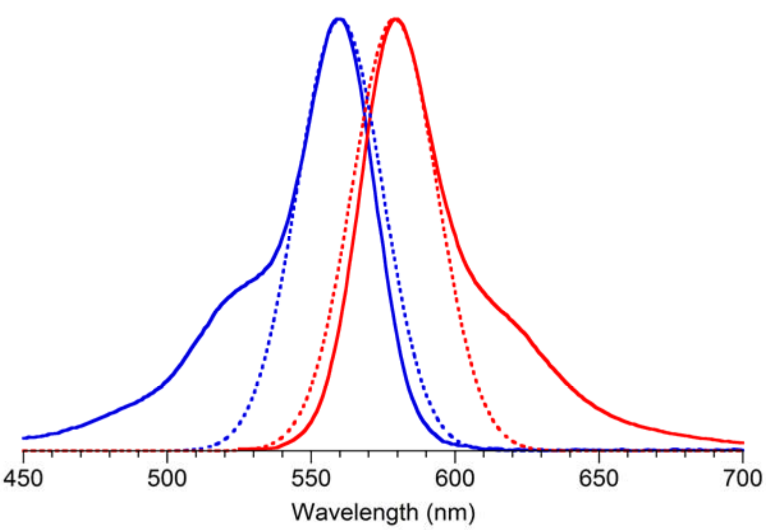


Figure S3. Method I. Absorption spectrum (solid blue line) and fluorescence spectrum (solid red line) of Merocyanine 540, along with respective Gaussian fits (dotted lines).

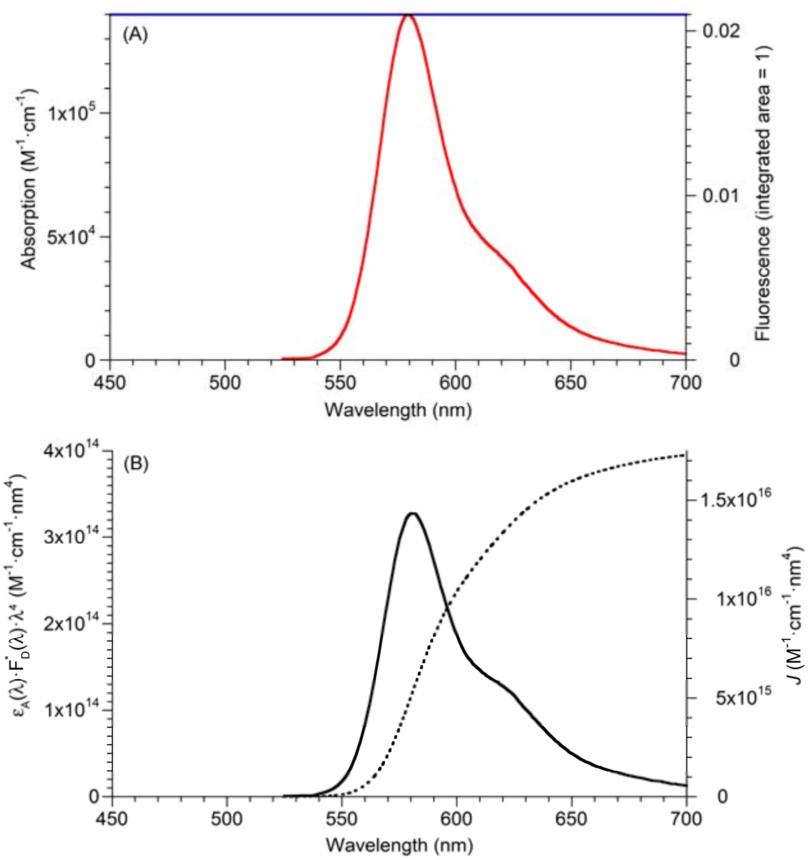


Figure S4. Method II. Model overlap of absorption and fluorescence spectra. (A) A model absorption spectrum of uniform intensity across the entire wavelength region (blue line, left vertical scale), and the experimental fluorescence spectrum of Merocyanine 540 (red line, right vertical scale). (B) Integrand of the *J* calculation, equation 3 (solid line, left vertical scale). The magnitude of the integration over the specified wavelength region (dotted line, right vertical scale) here equals 1.73×10^{16} $M^{-1} \cdot cm^{-1} \cdot nm^4$.

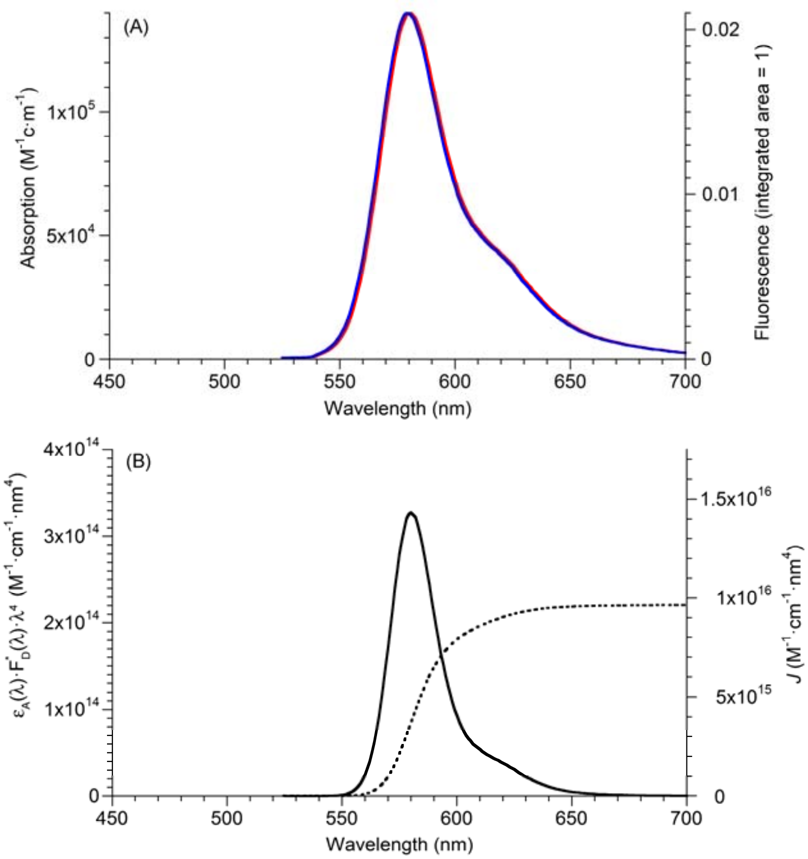


Figure S5. Method III. Model overlap of the absorption and fluorescence spectra. (A) The model absorption spectrum is assumed to be identical to the fluorescence spectrum (blue line, left vertical scale) of Merocyanine 540 (red line, right vertical scale shown). (B) Integrand of the J calculation, equation 3 (solid line, scale shown on the left side of the y-axis). The magnitude of the integration over the specified wavelength region (dotted line, scale shown on the right side of the y-axis) here equals 9.64×10^{15} $M^{-1}{\cdot}cm^{-1}{\cdot}nm^4$.

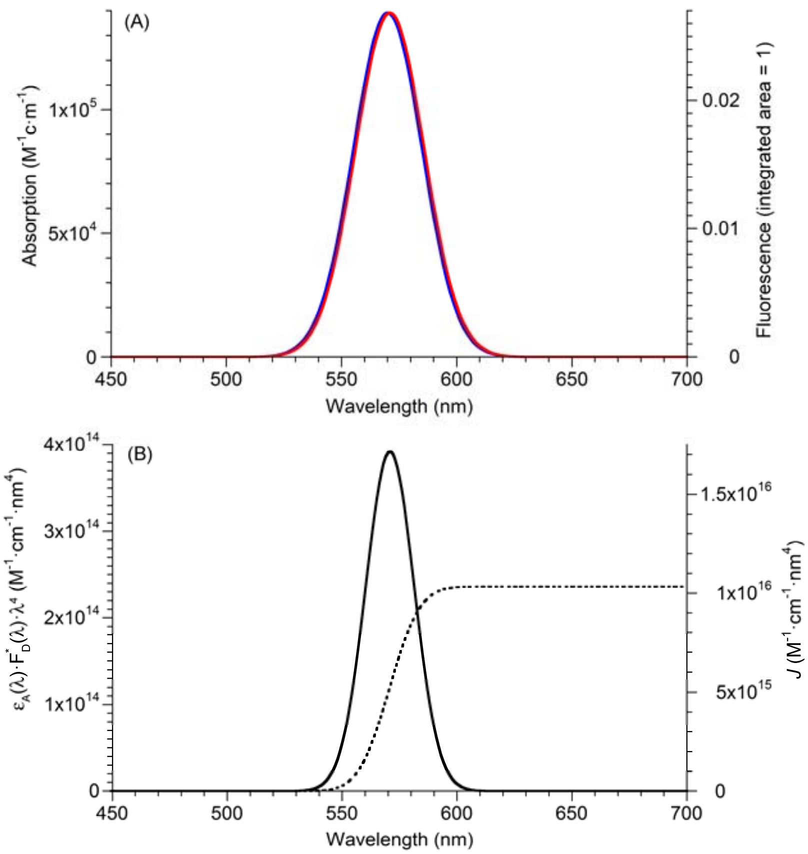


Figure S6. Method IV. Perfect overlap of absorption and fluorescence spectra given by Gaussian distributions centered at the experimental λ_{avg} for Merocyanine 540. (A) A model absorption spectrum (blue line, left vertical scale) and a model fluorescence spectrum (red line, right vertical scale). (B) Integrand of the *J* calculation, equation 3 (solid line, scale shown on the left side of the y-axis). The magnitude of the integration over the specified wavelength region (dotted line, scale shown on the right side of the y-axis) here equals 1.03×10^{16} $M^{-1} \cdot cm^{-1} \cdot nm^{4}$.

Table S7. Degree of overlap assessed via distinct methods

ID	compound	exptl J ($M^{-1}\cdot cm^{-1}\cdot nm^4$)[a]	Stokes/ fwhm[b]	Overlap-I (%)[c]	model J method II[d]	Overlap-II (%)[e]	model J method III[f]	Overlap-III (%)[e]	model J method IV[f]	Overlap-IV (%)[e]	$J/\varepsilon\cdot\lambda^4$ [(g)]	Overlap-V (%)[h]
A1	*o*-Xylene	4.18E+10	1.12	18	1.89E+12	2	1.29E+12	3	1.06E+12	4	0.028	4
A2	Phenol	7.84E+11	0.79	40	2.00E+13	4	1.23E+13	6	1.05E+13	8	0.054	8
A3	Durene	7.99E+10	0.74	47	1.71E+12	5	1.07E+12	8	1.03E+12	8	0.055	8
A4	Aniline	7.99E+11	0.83	38	1.91E+13	4	1.19E+13	7	1.03E+13	8	0.056	8
A5	*p*-Phenylenediamine	2.07E+11	1.53	8	4.33E+13	0.5	2.83E+13	0.7	1.99E+13	1	0.007	1
B1	1,8-Naphthalic anhydride	7.54E+12	1.02	24	2.71E+14	3	1.65E+14	5	1.33E+14	6	0.041	6
B2	Naphthalic dianhydride	6.92E+13	0.19	95	7.59E+14	9	4.40E+14	16	4.03E+14	17	0.123	17
B3	Anthracene	2.79E+13	0	100[i]	2.63E+14	11	1.27E+14	22	1.40E+14	23	0.143	23
B4	9,10-Diphenylanthracene	3.92E+13	1	25	4.94E+14	8	3.20E+14	12	2.56E+14	15	0.110	16
B5	Pyranine	4.73E+13	1.05	22	1.68E+15	3	1.03E+15	5	8.37E+14	6	0.040	6
C1	*trans*-Stilbene	1.27E+13	0.99	26	4.76E+14	3	2.80E+14	5	2.09E+14	6	0.043	6
C2	1,4-Diphenylbutadiene	3.30E+13	0.8	41	7.61E+14	4	4.27E+14	8	3.63E+14	9	0.066	9
C3	1,6-Diphenylhexatriene	1.59E+13	0.93	30	3.85E+15	0.4	2.31E+15	1	1.36E+15	1	0.008	1
C4	Curcumin	4.71E+13	1.22	13	6.12E+15	0.8	3.65E+15	1	2.18E+15	2	0.016	2
C5	4-DMA-4'-nitrostilbene	8.56E+12	1.46	5	4.01E+15	0.2	2.53E+15	0.3	1.23E+15	0.6	0.005	0.7
D1	Coumarin 1	6.02E+12	1.3	10	1.10E+15	0.5	6.86E+14	0.9	4.74E+14	1	0.009	1
D2	Coumarin 151	2.29E+12	1.43	6	1.17E+15	0.2	6.69E+14	0.3	4.32E+14	0.5	0.004	0.5
D3	Coumarin 30	1.57E+14	1.11	18	3.51E+15	5	2.12E+15	7	1.49E+15	11	0.075	11
D4	Coumarin 343	7.53E+14	0.24	92	2.43E+15	31	1.54E+15	49	1.35E+15	56	0.402	57
D5	Coumarin 6	2.37E+14	0.64	57	4.21E+15	6	2.49E+15	10	2.05E+15	12	0.083	12
E1	Phenosafranin	4.14E+14	0.53	68	4.40E+15	9	2.46E+15	17	2.28E+15	18	0.129	18
E2	Thionin	2.79E+15	0.29	89	1.32E+16	21	7.38E+15	38	7.66E+15	36	0.258	36
E3	Oxazine 170	2.74E+15	0.46	75	1.68E+16	16	9.25E+15	30	9.12E+15	30	0.213	30
E4	Toluidine Blue O	3.05E+15	0.52	69	1.61E+16	19	9.23E+15	33	8.98E+15	34	0.241	34
E5	Methylene blue	2.05E+15	0.45	76	9.73E+15	21	5.74E+15	36	5.71E+15	36	0.255	36
F1	Diethyloxacarbocyanine[j]	1.98E+15	0.32	87	1.12E+16	18	5.71E+15	35	6.20E+15	32	0.227	32
F2	Merocyanine 540	3.67E+15	0.54	67	1.73E+16	21	9.64E+15	38	1.03E+16	36	0.253	36
F3	Diethyloxadicarbocyanine[j]	8.05E+15	0.63	58	3.54E+16	23	1.91E+16	42	2.08E+16	39	0.275	39
F4	Diethyloxatricarbocyanine[j]	1.88E+16	0.53	68	6.03E+16	31	3.68E+16	51	3.74E+16	50	0.357	50
F5	Indocyanine Green	4.12E+16	0.53	68	8.52E+16	48	5.91E+16	70	5.72E+16	72	0.511	72
G1	Perylene	2.86E+14	0	100[i]	1.83E+15	16	9.05E+14	32	9.84E+14	29	0.205	29
G2	Perylene, PMI	2.31E+14	0.96	28	3.86E+15	6	2.36E+15	10	1.74E+15	13	0.096	14
G3	Perylene, PDI	9.24E+14	0.43	77	5.20E+15	18	2.35E+15	39	2.86E+15	32	0.230	32
G4	Perylene, PMI(OR)	2.09E+14	1.01	24	4.97E+15	4	3.12E+15	7	2.25E+15	9	0.067	10

G5	Perylene, PMI(OR)$_3$	3.17E+14	0.49	72	6.06E+15	5	3.79E+15	8	2.76E+15	12	0.082	12
H1	Fluorescein	1.29E+14	1.25	11	9.14E+15	1.4	4.97E+15	3	4.78E+15	3	0.019	3
H2	Rhodamine 123	1.26E+15	0.59	62	8.01E+15	16	4.44E+15	28	4.51E+15	28	0.198	28
H3	Eosin Y	2.04E+15	0.48	73	1.18E+16	17	6.76E+15	30	6.51E+15	31	0.223	31
H4	Rhodamine 6G	1.96E+15	0.5	71	1.28E+16	15	7.56E+15	26	7.05E+15	28	0.197	28
H5	Sulforhodamine B	2.95E+15	0.5	71	1.16E+16	25	6.51E+15	45	7.00E+15	42	0.299	42
I1	Bis(5-phenyldipyrrinato)Zn	1.42E+15	0.43	77	8.52E+15	17	4.76E+15	30	4.82E+15	29	0.208	29
I2	Bis(5-mesityldipyrrinato)Zn	1.66E+15	0.49	81	8.25E+15	20	4.58E+15	36	4.85E+15	34	0.243	34
I3	Phenyl-BODIPY	6.81E+14	0.51	70	4.67E+15	15	2.68E+15	25	2.63E+15	26	0.184	26
I4	4-Iodophenyl-BODIPY	1.36E+15	0.33	86	5.22E+15	26	2.93E+15	47	3.08E+15	44	0.314	44
I5	4-TMSCCphenyl-BODIPY	7.47E+14	0.65	56	4.61E+15	16	2.61E+15	29	2.65E+15	28	0.200	28
J1	ZnOEP	1.31E+15	0.15	97	5.30E+15	25	2.25E+15	58	3.04E+15	43	0.304	43
J2	MgTPP	3.06E+14	0.24	92	2.08E+15	15	1.40E+15	22	1.01E+15	30	0.215	30
J3	H$_2$OEP	2.55E+14	0	100[i]	1.22E+15	21	5.01E+14	51	7.07E+14	36	0.255	36
J4	Protoporphyrin IX DME	3.35E+14	0	100[i]	1.05E+15	32	4.06E+14	83	6.90E+14	49	0.344	48
J5	H$_2$TPP	2.09E+14	0.25	92	1.06E+15	20	6.07E+14	35	6.01E+14	35	0.247	35
K1	H$_2$N$_4$P(*t*Bu)	3.80E+15	0.1	99	1.29E+16	29	6.44E+15	59	7.83E+15	47	0.344	48
K2	ZnPc	2.51E+16	0.24	92	6.66E+16	38	3.36E+16	75	4.19E+16	60	0.425	60
K3	H$_2$Pc	1.80E+16	0.12	98	4.28E+16	42	2.08E+16	87	2.75E+16	65	0.463	65
K4	H$_2$Pc(OBu)	2.23E+16	0.35	84	5.07E+16	44	3.30E+16	68	3.37E+16	66	0.469	66
K5	H$_2$Nc(*t*Bu)	5.32E+16	0.32	87	1.07E+17	50	6.81E+16	78	7.38E+16	72	0.512	72
L1	Chlorophyll *b*	4.18E+15	0.06	99	1.12E+16	37	5.24E+15	80	7.01E+15	60	0.423	60
L2	Chlorophyll *a*	5.76E+15	0.25	92	1.94E+16	30	9.17E+15	63	1.19E+16	49	0.345	49
L3	Pheophorbide *a*	3.69E+15	0.33	86	1.03E+16	36	4.96E+15	75	6.42E+15	58	0.408	57
L4	Purpurin 18	4.49E+15	0.26	91	1.15E+16	39	5.74E+15	78	7.31E+15	61	0.434	61
L5	Bacteriochlorophyll *a*	1.91E+16	0.34	85	3.65E+16	52	2.20E+16	87	2.49E+16	77	0.544	77

[a]The *J* here is the experimental value taken from Table 1. [b]Calculated from the data (Stokes shift and fwhm) in nm shown in Table 1. [c]Calculated from the equation shown in Figure 8. [d]See text and Figure A3. [e]Experimental *J*/model *J* x 100 (%). [e]See text and Figure S5. [f]See text and Figure S6. [g]The *J* here is the experimental value. [h]$J/\varepsilon_{(A)}\cdot\lambda^4$/0.71 x 100 (%), where the λ term employed is λ_{avg}. [i]100% derives given the Stokes shift = 0. [j]Iodide salt.

D. Evaluation of Methods to Assess the Degree of Overlap. The advantages and disadvantages of Methods I–V for assessing the degree of overlap are described above for homo-transfer with Merocyanine 540, where the overlap in methods I–V is 67%, 21%, 38%, 36% and 36%, respectively. The methods were next evaluated for homo-transfer with 60 fluorophores having various types of spectra (Table S7). Representative spectra are displayed in Figure S7 along with superposed Gaussian distributions to illustrate the advantages and disadvantages of the methods. The methods are further explored as follows in the context of the 60 fluorophores.

Method I affords results the accuracy of which depends on the shape of the experimental absorption and fluorescence spectra – if close to Gaussian distributions, the calculated results will closely match reality; if not, the results will be offset [e.g., perylene (**G1**), wherein the absorption and fluorescence spectra each exhibit several sharp bands; Figure S7 panel A]. Method I is based purely on the Stokes shift/fwhm ratio; therefore, the definition of the Stokes shift is a key factor; for example, with 1,4-diphenylbutadiene (**C2**), the Gaussian spectra can be used to capture solely the 0–0 (origin) transitions (Figure S7 panel B) or the most intense peaks (Figure S7 panel C) thereby enveloping the entire manifold of transitions. The value of Overlap-I was 63% in the former (Stokes shift = 7 nm, fwhm = 12 nm) versus 41% in the latter (Stokes shift = 43 nm, fwhm = 54 nm). Both gave a much larger overlap compared with the other methods (~9%). The other limitation of this method is the value of the average fwhm, given that the fwhm values of the absorption spectrum and the fluorescence spectrum are treated as equal; in some case the results will not be accurate [e.g., Rhodamine 6G (**H4**), Figure S7 panel D]. Overall, it is difficult to gauge the degree of overlap solely using Gaussian distributions. In general, Method I generally provides the largest values for the degree of overlap.

Method II is very simple but the assumption that the full shape of the fluorescence band overlaps the absorption is not generally realized in practice. Method II generally provides the smallest values for the degree of overlap.

Method III has a minor drawback because setting $\lambda_{flu} = \lambda_{abs}$ for the *J* calculation causes the integrated area to shift to longer wavelength compared to the true overlapped area; in other words, the model *J* value tends to be larger because the resulting Stokes shift is zero. Hence, the degree of overlap calculated by method III tends to be small for fluorophores with a large Stokes shift [e.g., *p*-phenylenediamine (**A5**), Pyranine (**B5**), Figure S1]. The values obtained herein do not reflect the shape of the peaks; for example, a large tailing or splitting of a second (or third) peak is not captured [e.g., protoporphyrin IX dimethyl ester (**J4**), Figure S7 panel E].

Method IV, which is based on Gaussian curve-fitting of the overlapped spectral region, affords a result for the degree of overlap that is independent of the overall shape of the experimental spectra.

Method V, a simple approximation of Method IV, across the 60 compounds considered here, provides the most useful estimate of the degree of overlap, although an error of up to ~10% may arise due to the approximation inherent in equation 5 that gives rise to equation 6. Method V gives essentially the same value as for method IV in all cases examined but does not require handling Gaussian distributions; indeed, for Merocyanine 540, the value for the degree of overlap was 36% in both methods.

Several points emerge from the above considerations. First, for homo-transfer, short-wavelength shoulders in the absorption spectrum do not overlap with the fluorescence spectrum and thus are immaterial concerning the *J* value (Figure S7 panel A). The absorption spectrum is based on intensity ($\varepsilon_{(A)}$ at λ_{abs}), thereby the non-overlapped region of the absorption spectrum can be simply ignored. Second, the presence of an absorption spectrum tailing toward longer wavelength is quite rare and is not considered here. Third, tailing or splitting of the fluorescence spectrum can dramatically affect the degree of overlap. The y-axis of the fluorescence spectrum is based on an integrated area = 1; thus, only a fraction of the total area of the fluorescence spectrum is utilized. For example, perylene (**G1**) exhibits almost no Stokes shift and in principle can exhibit a high value of *J*. However, the non-overlapped area of the fluorescence spectrum (>450 nm) contributes to the integrated area in the normalization process, thus the degree of overlap is smaller than that expected. A similar observation can be made for 1,4-diphenylbutadiene (**C2**). The Gaussian overlays for Indocyanine Green (**F5**) are unusual given that the fluorescence band is more narrow than the absorption band (Figure S7 panel F). A large degree of overlap accrues despite the sizable Stokes shift owing to the rather broad bands.

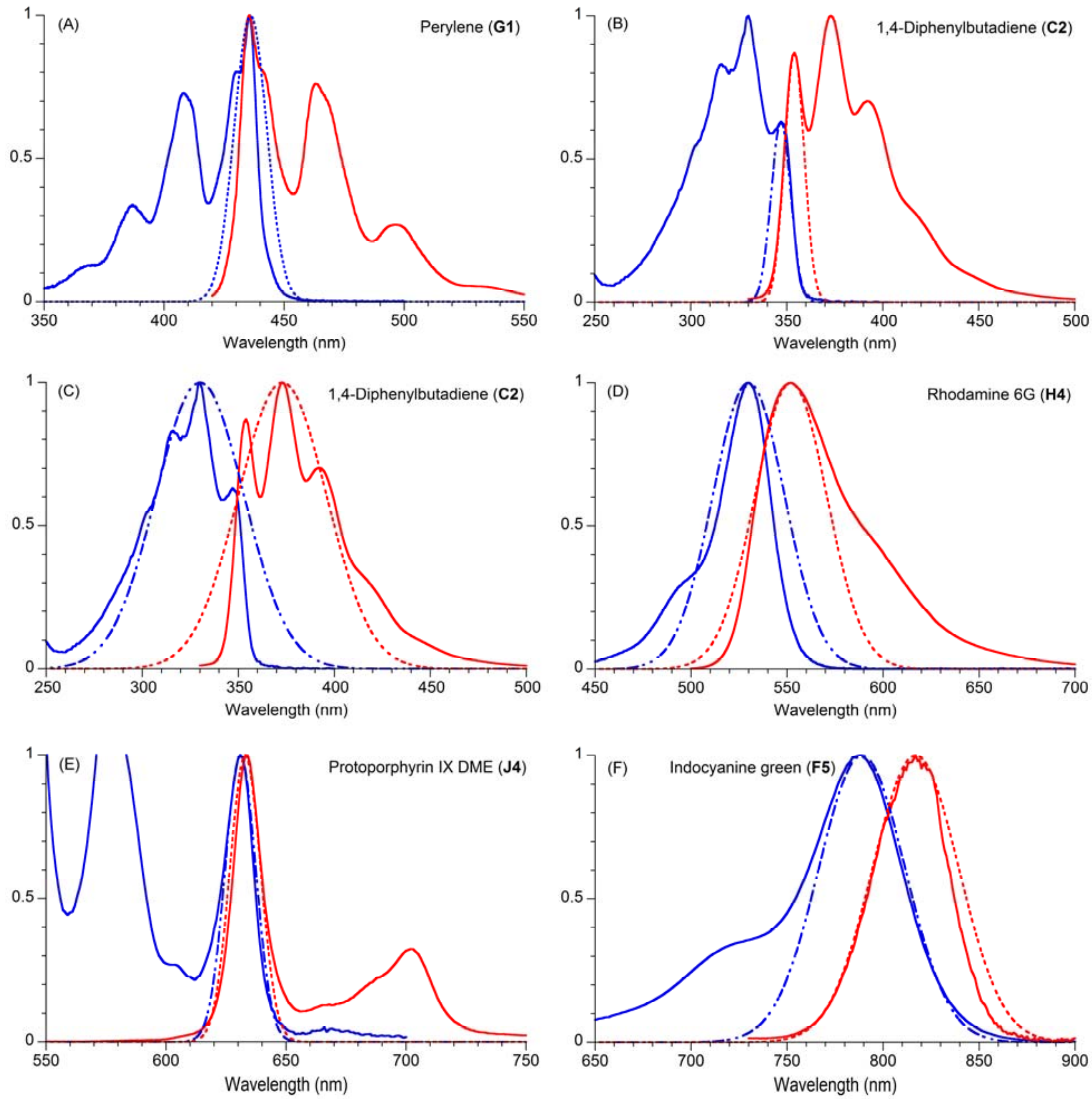


Figure S7. Absorption (blue line) and fluorescence (red line) spectra along with Gaussian fits of each for representative compounds.