Table S1. Cartesian transition dipole moment (μ) vector components of dyes in implicit water solvent. Vertical excited state calculations were done using the ground state geometry. Dye structures are shown in Figure 4 of the main text.

Dye	μ_x (Debye)	μ_y (Debye)	μ_z (Debye)
Cy3	12.25	0.00	0.00
Cy5	15.35	0.00	0.00
Cy5-CN	15.66	-0.24	0.00
Cy5-NMe2	15.81	-0.74	-0.01
Cy5-Cl	-15.74	0.00	0.00
Cy5-hex	16.22	0.00	0.00
Cy5-Peg	-16.19	0.00	0.00
Cy5-tBu	-15.90	0.00	0.00
Cy5.5	-15.57	0.00	0.00
Cy7	17.62	0.00	0.00
1	1.03	8.98	0.86
2	-7.81	0.43	-0.50
3	-20.25	0.00	0.10
4	7.97	0.42	-0.25
5	-20.17	0.00	0.32
6	13.99	0.21	0.13
7	4.68	9.57	0.49
8	-15.45	1.08	0.20
9	-14.67	-0.46	0.13
10	16.15	1.02	0.23
11	-14.00	0.30	-0.03
12	-10.84	-2.63	1.56
13	-3.47	7.98	-3.88
14	9.23	-1.43	0.00
15	8.51	-6.10	-0.27

Table S2. Gibbs free energy of solvation (ΔG_{solv}) of dyes in implicit water and n-octanol solvents. The values of ΔG_{solv} were determined using Equation (2) with the dye geometry relaxed in implicit solvent and vacuum. Dye structures are shown in Figure 4 of the main text.

Dye	$\Delta G_{solv}^{n-octanol}$ (Hartree)	ΔG_{solv}^{water} (Hartree)
Cy3	-0.0743	-0.0655
Cy5	-0.0735	-0.0626
Cy5-CN	-0.0831	-0.0739
Cy5-NMe2	-0.0728	-0.0618
Cy5-Cl	-0.0812	-0.0690
Cy5-hex	-0.0806	-0.0597
Cy5-Peg	-0.0966	-0.0845
Cy5-tBu	-0.0734	-0.0567
Cy5.5	-0.0785	-0.0650
Cy7	-0.0740	-0.0596
1	-0.0329	-0.0169
2	-0.0845	-0.0886
3	-0.0738	-0.0612
4	-0.0251	-0.0263
5	-0.0757	-0.0632
6	-0.0737	-0.0625
7	-0.0344	-0.0131
8	-0.0780	-0.0685
9	-0.0479	-0.0377
10	-0.0745	-0.0653
11	-0.0715	-0.0587
12	-0.0478	-0.0201
13	-0.0431	-0.0561
14	-0.0260	-0.0225
15	-0.0433	-0.0189