Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Anthanthrene Dye-Sensitized Solar Cells: Influence of the Number of Anchoring Groups and Substitution Motif

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Table S1. Dye-1 M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength f_{calc}	Major contributions [%]M06-2X		μ [Debye]	Character
S_0					0.0009	
S_1	439.84	0.0001	HOMO-1 → LUMO	3	0.0016	π → π*
			HOMO → LUMO+1	90		π → π* CT
			HOMO→ LUMO+4	7		π → π*
S_2	438.83	0.6770	HOMO → LUMO	96	9.7808	π → π* CT
			HOMO → LUMO+2	4		π → π* CT
S_3	397.43	0.3172	HOMO-1→ LUMO+1	7	4.1505	π → π*
			HOMO → LUMO	2		π → π* CT
			HOMO → LUMO+2	85		π → π* CT
			HOMO → LUMO+4	6		π → π*
S_4	359.89	0.1320	HOMO-3→ LUMO	4	1.5650	π → π*
			HOMO-3 → LUMO+2	9		π → π*
			HOMO-2 → LUMO	25		π → π*
			HOMO-2 → LUMO+2	8		π → π*
			HOMO-1 → LUMO+1	5		π → π*
			HOMO-1 → LUMO+3	49		π → π*
S_5	340.43	0.0000	HOMO-4 → LUMO+2	3	0.0011	π → π*
			HOMO-3 → LUMO+1	7		π → π*
			HOMO-2 → LUMO+1	21		π → π* CT
			HOMO-1 → LUMO	69		π → π* CT
S_6	339.43	1.6266	HOMO-4 → LUMO+1	5	18.1774	π → π*
			HOMO-3 → LUMO	10		π → π*
			HOMO-2 → LUMO	16		π → π*
			HOMO-2 → LUMO+2	4		π → π*
			HOMO-1 → LUMO+1	40		π → π* CT
			HOMO → LUMO	4		π → π* CT
			HOMO → LUMO+2	9		π → π* CT
			HOMO → LUMO+3	11		π → π*
S_7	325.68	0.0000	HOMO-2 → LUMO+1	2	0.009	π → π*
			HOMO-1 → LUMO	3		π → π* CT
			HOMO-1 → LUMO+2	22		π → π
			HOMO → LUMO+1	4		π → π* CT
			HOMO → LUMO+4	66		π → π*
			HOMO → LUMO+7	2		π → π*
S_8	309.65	0.0000	HOMO-4 → LUMO	13	0.009	π → π* CT
			HOMO-3 → LUMO+1	6		π → π* CT
			HOMO-2 → LUMO+1	10		π → π*
			HOMO-2 → LUMO	3		π → π*
			HOMO-1 → LUMO+2	40		π → π*
			HOMO → LUMO+1	3		π → π*
			HOMO → LUMO+4	25		π → π*
S_9	294.55	0.2999	HOMO-3 → LUMO	6	2.9091	π → π* CT
			HOMO-2 → LUMO	34		π → π*
			HOMO-2 → LUMO+2	14		π → π*
			HOMO-1 → LUMO+1	19		π → π* CT
			HOMO → LUMO+3	27		π → π*
S_{10}	281.20	0.0000	HOMO-7 → LUMO	3	0.0009	π → π*
			HOMO-3 → LUMO+1	29		π → π* CT
			HOMO-3 → LUMO+4	48		π → π*
			HOMO-2 → LUMO+1	7		π → π*
			HOMO-2 → LUMO+4	5		π → π*

			HOMO-1 → LUMO	7	π → π*
			HOMO-1 → LUMO+2	3	π → π*
			HOMO-1 → LUMO+3	3	π → π*

Table S2. Dye-2 M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength f_{calc}	Major contributions [%]M06-2X		μ [Debye]	Character
S_0					9.0788	
S_1	449.47	0.3298	HOMO-2 → LUMO HOMO-1 → LUMO HOMO → LUMO HOMO→ LUMO+1	2 9 85 4	10.9990	π → π* π → π* CT π → π* CT π → π* CT
S_2	414.47	0.2511	HOMO-2 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+1 HOMO → LUMO+2	3 6 89 2	10.4267	π → π* π → π* CT π → π* CT π → π* CT
S_3	365.29	0.0143	HOMO-3 → LUMO HOMO-3 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO-1 → LUMO+2 HOMO → LUMO HOMO → LUMO+2 HOMO → LUMO+3	6 21 13 24 3 3 28 2	9.1465	π → π* CT π → π* π → π* CT π → π* CT π → π* CT π → π* π → π*
S_4	360.08	0.0181	HOMO-4 → LUMO+1 HOMO-3 → LUMO+1 HOMO-2 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO-1 → LUMO+2 HOMO → LUMO HOMO → LUMO+2 HOMO → LUMO+3	3 3 6 6 23 25 2 3 17 12	9.2066	π → π* π → π* π → π* π → π* π → π* CT π → π* CT π → π* CT π → π* CT π → π* π → π*

S_5	344.84	1.5337	HOMO-4 → LUMO 10 HOMO-2 → LUMO 58 HOMO-1→ LUMO 5 HOMO-1 → LUMO+1 6 HOMO → LUMO 3 HOMO → LUMO+1 3 HOMO → LUMO+3 15	15.8728	π → π* CT π → π* π → π* CT π → π* CT π → π* CT π → π*
S_6	332.73	0.1028	HOMO-2 → LUMO 10 HOMO-2 → LUMO+1 3 HOMO-1 → LUMO 8 HOMO-1 → LUMO+3 6 HOMO → LUMO+2 18 HOMO → LUMO+3 54	9.3997	π → π* π → π* π → π* CT π → π* CT π → π* π → π*
S_7	329.94	0.0138	HOMO-2 → LUMO 11 HOMO-1 → LUMO 45 HOMO-1 → LUMO+1 28 HOMO-1 → LUMO+3 5 HOMO → LUMO 5 HOMO → LUMO+1 2 HOMO → LUMO+3 4	9.1948	π → π* π → π* CT π → π* CT π → π* π → π* CT π → π* CT π → π*
S_8	309.35	0.0370	HOMO-4 → LUMO 11 HOMO-3 → LUMO 3 HOMO-3 → LUMO+1 7 HOMO-2 → LUMO+1 69 HOMO-1 → LUMO+1 3 HOMO → LUMO+3 7	9.1001	π → π* CT π → π* CT π → π* π → π* π → π* CT π → π*
S_9	306.91	0.0216	HOMO-1 → LUMO+2 2 HOMO-1 → LUMO+4 73 HOMO-1 → LUMO+9 3 HOMO → LUMO+4 22	9.1495	π → π* CT π → π* π → π* CT π → π* CT
S_{10}	299.59	0.8485	HOMO-3 → LUMO 10 HOMO-3 → LUMO+1 11 HOMO-1→ LUMO+1 9 HOMO-1 → LUMO+3 20 HOMO-1 → LUMO+5 25 HOMO-1 → LUMO+7 4	12.3383	π → π* CT π → π* π → π* CT π → π*

HOMO → LUMO+2	6	$\pi \rightarrow \pi^*$
HOMO → LUMO+3	3	CT
HOMO → LUMO+5	12	$\pi \rightarrow \pi^*$
		CT
		$\pi \rightarrow \pi^*$
		$\pi \rightarrow \pi^*$
		$\pi \rightarrow \pi^*$
		CT

Dye-2 CAM-B3LYP/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength f_{calc}	Major contributions [%]		μ [Debye]	Character
S_0					9.3353	
S_1	444.39	0.4310	HOMO-2 → LUMO HOMO-1 → LUMO HOMO → LUMO HOMO→ LUMO+1	2 7 75 16	11.8163	π → π* π → π* CT π → π* CT π → π* (CT)
S_2	412.65	0.2136	HOMO-2 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO HOMO → LUMO+1 HOMO→ LUMO+2	5 5 10 76 4	10.4772	π → π* π → π* CT π → π* CT π → π* (CT)
S_3	364.59	0.0055	HOMO-3 → LUMO HOMO-3 → LUMO+1 HOMO-2 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO+1 HOMO-1 → LUMO+2 HOMO → LUMO+2 HOMO → LUMO+3	6 28 3 3 3 4 44 9	9.3611	π → π* CT π → π* π → π* π → π* π → π* CT π → π* CT π → π* π → π*
S_4	348.49	0.0181	HOMO-4 → LUMO+1 HOMO-2 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO HOMO → LUMO+3	4 8 8 20 44 7 9	9.4168	π → π* π → π* π → π* π → π* CT π → π* CT π → π* CT π → π*
S_5	343.92	1.5337	HOMO-4 → LUMO HOMO-2 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO HOMO → LUMO+3	17 59 2 3 19	16.1671	π → π* (CT) π → π* π → π* CT π → π* CT π → π*
S_6	328.32	0.1028	HOMO-2 → LUMO HOMO-1 → LUMO HOMO-1 → LUMO+1	4 9 8	9.7727	π → π* π → π* CT

			HOMO-1 → LUMO+2	2		π → π*
			HOMO-1 → LUMO+3	7		CT
			HOMO-1 → LUMO+1	3		π → π*
			HOMO → LUMO+1	4		CT
			HOMO → LUMO+2	19		π → π*
			HOMO → LUMO+3	44		π → π*
						CT
						π → π*
						(CT)
						π → π*
						π → π*
						π → π*
			HOMO-3 → LUMO+1	2		π → π*
			HOMO-2 → LUMO	3		π → π*
			HOMO-2 → LUMO+1	10		π → π*
S_7	318.58	0.0138	HOMO-1 → LUMO	62	9.3913	CT
			HOMO-1 → LUMO+1	12		π → π*
			HOMO-1 → LUMO+3	4		CT
			HOMO → LUMO	7		π → π*
						π → π*
						CT
						π → π*
			HOMO-6 → LUMO+1	3		CT
			HOMO-4 → LUMO	12		π → π*
			HOMO-3 → LUMO+1	4		(CT)
			HOMO-2 → LUMO+1	50		π → π*
S_8	307.14	0.0370	HOMO-1 → LUMO	3	9.4823	π → π*
			HOMO-1 → LUMO+1	9		π → π*
			HOMO-1 → LUMO+3	5		π → π*
			HOMO-1 → LUMO+5	6		CT
			HOMO → LUMO+3	8		π → π*
						π → π*
						π → π*
			HOMO-1 → LUMO+4	81		π → π*
S_9	303.83	0.0216	HOMO → LUMO+4	19	9.4204	π → π*
						CT
						π → π*
			HOMO-3 → LUMO	14		CT
			HOMO-3 → LUMO+1	15		π → π*
			HOMO-1→ LUMO+1	16		π → π*
			HOMO-1 → LUMO+3	9		CT
S_{10}	294.60	0.8485	HOMO-1 → LUMO+5	25	12.5728	π → π*
			HOMO → LUMO+2	9		π → π*
			HOMO → LUMO+3	3		π → π*
			HOMO → LUMO+5	9		π → π*
						CT

Table S3. Dye-3 M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength f_{calc}	Major contributions [%]		μ [Debye]	Character
S_0					0.0001	
S_1	430.60	0.6210	HOMO → LUMO+1 HOMO→ LUMO+2	94 6	0.6211	π → π* CT π → π*
S_2	410.58	0.0000	HOMO → LUMO+2	100	0.0001	π → π*
S_3	405.59	0.1215	HOMO → LUMO+1 HOMO→ LUMO+2	6 94	0.1216	π → π* CT π → π*
S_4	356.76	0.0227	HOMO-5 → LUMO HOMO-5 → LUMO+2 HOMO-4 → LUMO HOMO-4 → LUMO+2 HOMO-2 → LUMO HOMO-2 → LUMO+2 HOMO → LUMO+3	12 11 5 2 14 10 45	1.5650	π → π* π → π* CT π → π* π → π* CT π → π* CT
S_5	348.14	0.0000	HOMO-6 → LUMO HOMO-6 → LUMO+2 HOMO-1 → LUMO HOMO-1 → LUMO+2 HOMO → LUMO+4	6 5 47 32 10	0.0011	π → π* π → π* π → π* CT π → π* CT π → π*
S_6	323.03	0.0000	HOMO-4 → LUMO+1 HOMO-3 → LUMO HOMO-3 → LUMO+2 HOMO-1 → LUMO HOMO-1 → LUMO+2 HOMO → LUMO+4	5 5 3 8 4 75	18.1774	π → π* π → π* CT π → π* π → π* CT π → π* CT π → π*
S_7	321.71	1.4585	HOMO-5 → LUMO HOMO-5 → LUMO+2 HOMO-4 → LUMO HOMO-4 → LUMO+2 HOMO-3 → LUMO+1	7 6 22 15 50	0.009	π → π* π → π* CT π → π* π → π* CT π → π* CT
S_8	316.64	0.0000	HOMO-5→ LUMO+1 HOMO-4 → LUMO+1 HOMO-3 → LUMO HOMO-3 → LUMO+2	10 30 25 17	0.009	π → π* π → π* π → π* CT

			HOMO → LUMO+4	18		π → π* π → π*
S_9	303.08	0.6550	HOMO−2 → LUMO HOMO−2 → LUMO+2 HOMO−1 → LUMO+4 HOMO → LUMO+3	48 26 5 21	2.9091	π → π* CT π → π* CT π → π* (CT) π → π*
S_{10}	293.88	0.0000	HOMO−2 → LUMO+1 HOMO−1 → LUMO HOMO−1 → LUMO+2	11 36 53	0.0009	π → π* π → π* CT π → π*

Table S4. Dye-4 M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength f_{calc}	Major contributions [%]		μ [Debye]	Character
S_0					10.1014	
S_1	436.90	0.2390	HOMO-1 → LUMO HOMO → LUMO HOMO → LUMO+1	4 85 11	11.4537	π → π* CT π → π* CT π → π*
S_2	421.96	0.5155	HOMO → LUMO HOMO → LUMO+1	11 89	12.9188	π → π* CT π → π*
S_3	363.39	0.0092	HOMO-4 → LUMO+1 HOMO-3 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	8 10 4 58 17 3	10.1448	π → π* π → π* CT π → π* CT π → π* π → π*
S_4	358.29	0.0114	HOMO-4 → LUMO+1 HOMO-3 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	14 16 3 34 19 14	10.1541	π → π* π → π* CT π → π* CT π → π* π → π*
S_5	341.98	0.0363	HOMO-6 → LUMO+2 HOMO-5 → LUMO HOMO-2 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	8 6 3 58 3 7 15	10.2624	π → π* CT π → π* π → π* CT π → π* (CT) π → π* CT π → π* π → π*
S_6	326.44	0.0158	HOMO-6 → LUMO+2 HOMO-2 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	3 23 21 53	10.1683	π → π* CT π → π* (CT) π → π* π → π*
S_7	324.24	0.0003	HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO	89 6 5	10.1025	π → π* CT π → π* CT π → π*

						CT
S_8	322.77	1.0124	HOMO−5 → LUMO HOMO−2→ LUMO+1	97 3	14.3337	π → π* π → π* (CT)
S_9	307.42	0.0230	HOMO−1 → LUMO+2 HOMO−1 → LUMO+3 HOMO−1 → LUMO+4 HOMO−1 → LUMO+6 HOMO−1 → LUMO+7 HOMO−1 → LUMO+8 HOMO → LUMO+4	20 4 52 5 8 3 8	10.1930	π → π* CT π → π* CT π → π* π → π* CT π → π* π → π* π → π* CT
S_{10}	299.35	0.7436	HOMO−3 → LUMO HOMO−3 → LUMO+1 HOMO−2 → LUMO HOMO−1 → LUMO+5 HOMO → LUMO+2 HOMO → LUMO+3	10 43 23 2 15 7	12.9843	π → π* CT π → π* CT π → π* CT π → π* π → π* π → π*

Dye-4 CAM-B3LYP/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength f_{calc}	Major contributions [%]		μ [Debye]	Character
S_0					10.4030	
S_1	433.29	0.5852	HOMO → LUMO HOMO → LUMO+1	45 55	11.8904	π → π* CT π → π*
S_2	419.28	0.1924	HOMO → LUMO HOMO → LUMO+1	54 46	10.8920	π → π* CT π → π*
S_3	361.89	0.0076	HOMO-4 → LUMO+1 HOMO-2 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	24 26 41 9	10.4223	π → π* π → π* (CT) π → π* π → π*
S_4	347.09	0.0096	HOMO-6 → LUMO+1 HOMO-5 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+4	7 3 25 2 50 13	10.4274	π → π* π → π* π → π* (CT) π → π* CT π → π* CT π → π* CT
S_5	339.42	0.0866	HOMO-6 → LUMO+2 HOMO-5 → LUMO HOMO-2 → LUMO+1 HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	5 7 30 2 43 5 8	10.6231	π → π* π → π* π → π* (CT) π → π* CT π → π* CT π → π* π → π*
S_6	325.59	0.9266	HOMO-5 → LUMO HOMO-2 → LUMO+1 HOMO → LUMO+3	92 5 3	12.7582	π → π* π → π* CT π → π*
S_7	323.12	0.0147	HOMO-6 → LUMO+1 HOMO-2 → LUMO+1 HOMO → LUMO+2 HOMO → LUMO+3	5 23 15 57	10.4404	π → π* π → π* π → π* π → π* π → π* CT
S_8	305.24	0.0003	HOMO-2 → LUMO HOMO-1 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO	2 90 4 4	10.4038	π → π* CT π → π* CT π → π* CT

			HOMO−1 → LUMO+2	14		π → π* CT
			HOMO−1 → LUMO+3	5		π → π* CT
S_9	303.68	0.0228	HOMO−1 → LUMO+4	70	10.4610	π → π*
			HOMO−1 → LUMO+9	3		π → π* CT
			HOMO → LUMO+4	8		π → π* CT
			HOMO−3 → LUMO	3		π → π* CT
			HOMO−3 → LUMO+1	56		π → π*
S_{10}	295.48	1.2210	HOMO−1 → LUMO+5	7	13.5065	(CT)
			HOMO → LUMO+2	27		π → π*
			HOMO → LUMO+3	7		π → π*
						π → π*

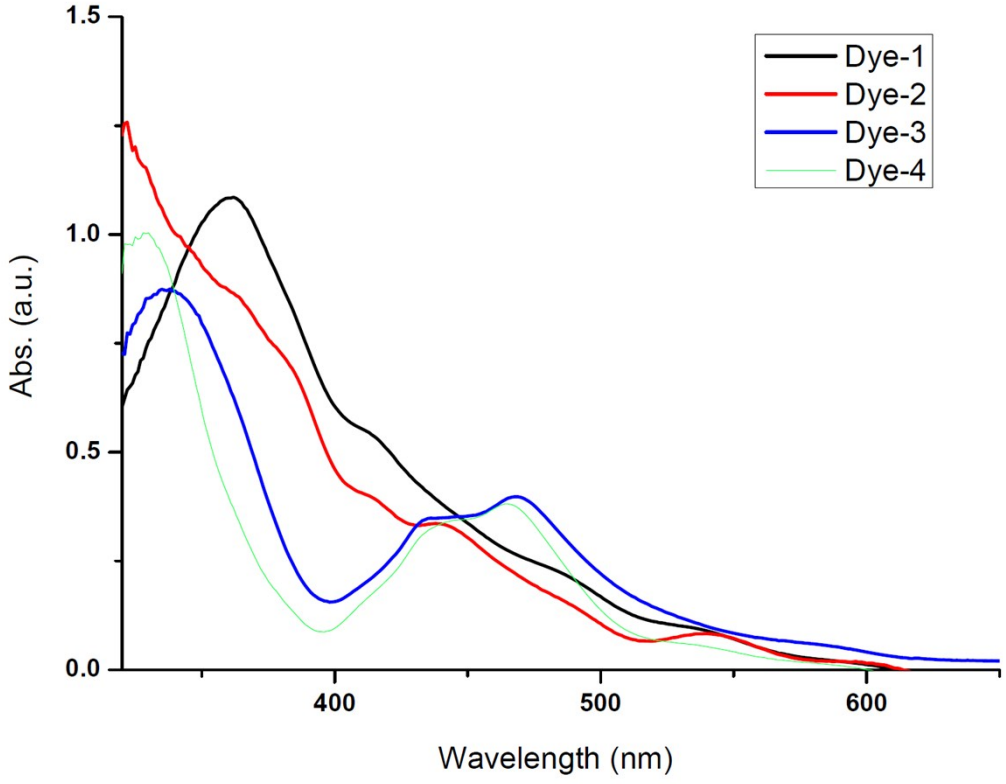

Figure S1 Optical absorption spectra of **Dye-1** to **Dye-4** adsorbed on TiO_2 films.

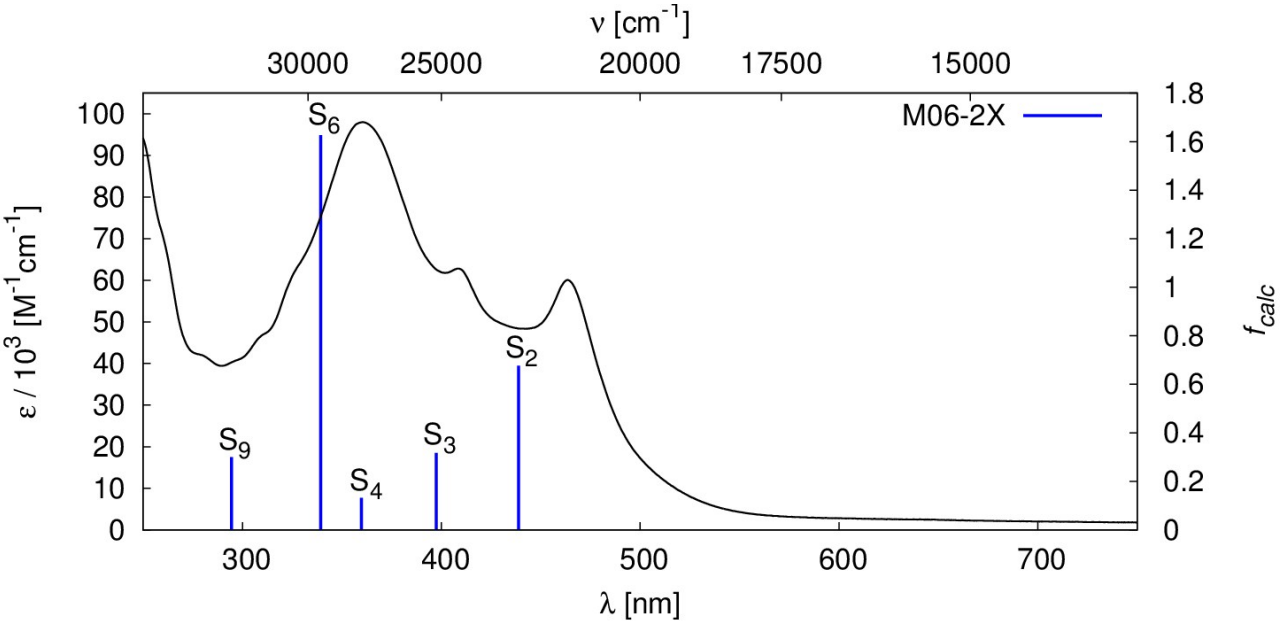

Figure S2 Optical absorption spectrum of Dye-1 together with the calculated electronic excitations (stick plot).

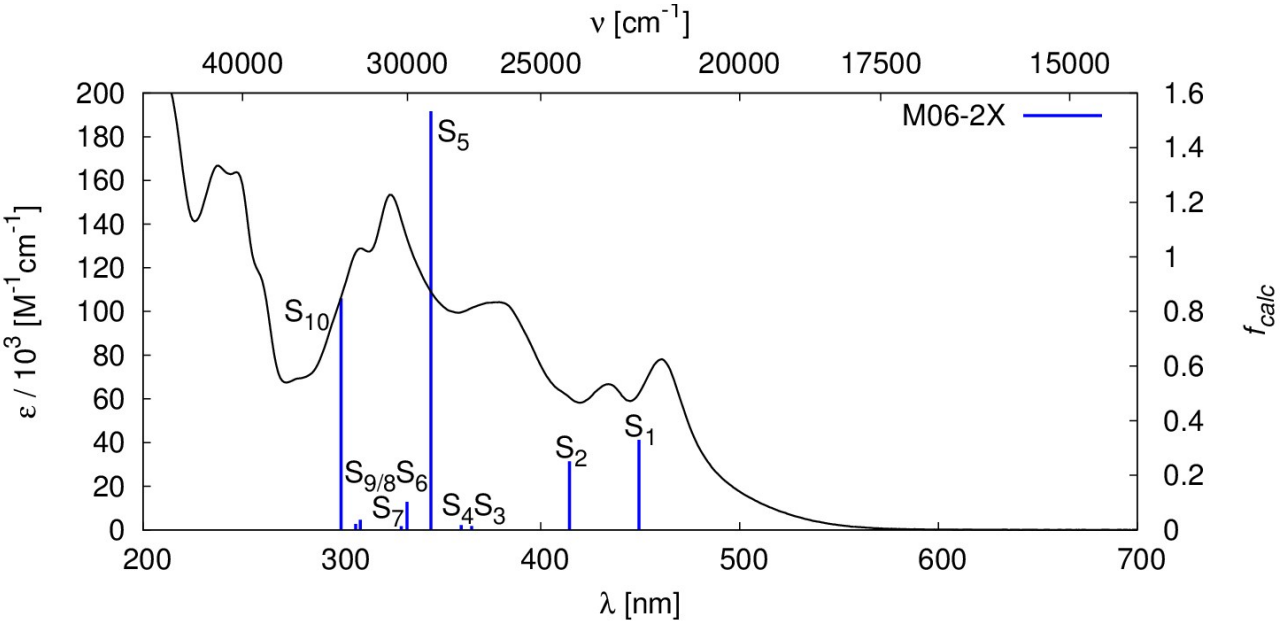

Figure S3 Optical absorption spectrum of Dye-2 together with the calculated electronic excitations (stick plot).

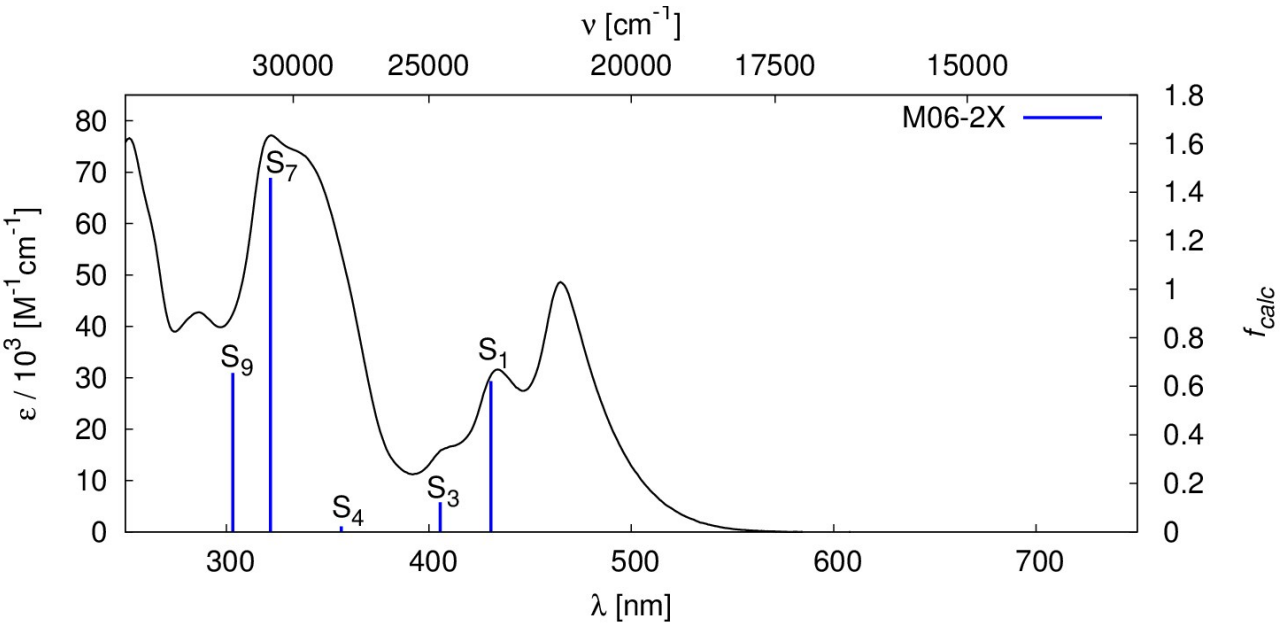

Figure S4 Optical absorption spectrum of **Dye-3** together with the calculated electronic excitations (stick plot).

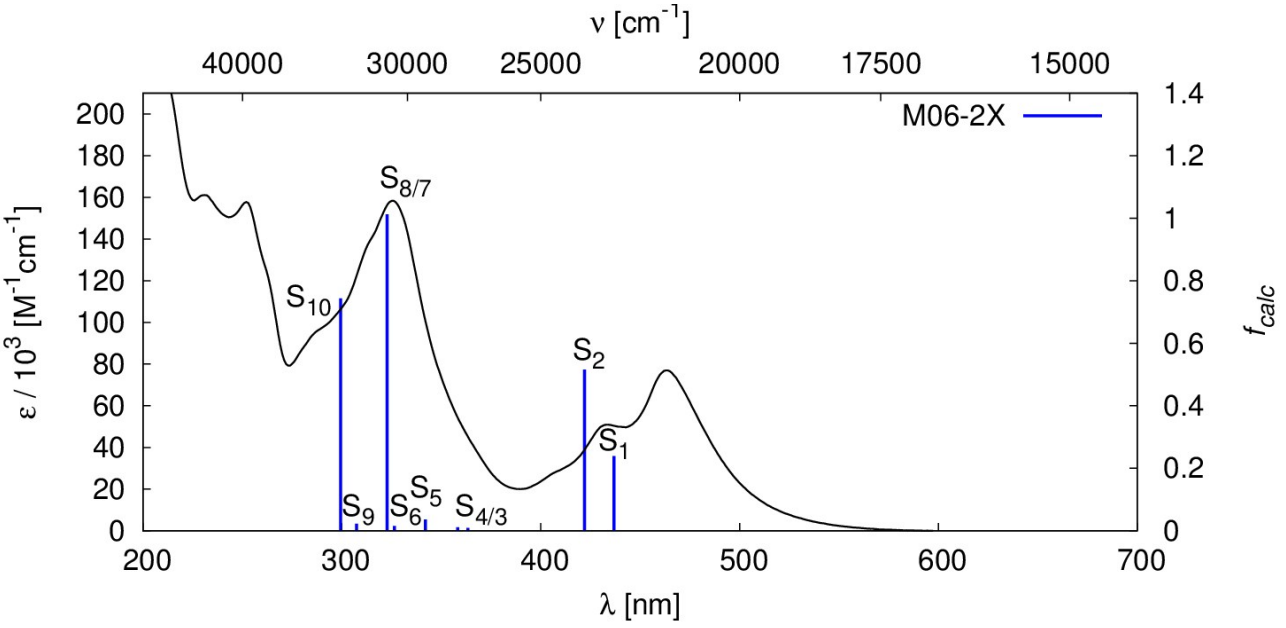

Figure S5 Optical absorption spectrum of **Dye-4** together with the calculated electronic excitations (stick plot).