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Table S1: The calculated C-C d(1-4) and C-P d5 bond lengths in Å, angles CCCC and CCPO α(1-5) in (°) by different functional and basis set.

Basis set	Functional	d1	d2	d3	d4	d5	α1	α2	α3	α4	α5
6-31g(d)	B3LYP	1.449	1.454	1.456	1.447	1.778	18.9	3.2	1.4	2.0	3.0
	B3PW91	1.447	1.451	1.452	1.445	1.775	20.4	3.8	1.6	5.1	2.1
	BHANDH	1.436	1.441	1.442	1.435	1.751	7.3	2.1	1.3	0.8	4.7
	CAM-B3LYP	1.456	1.461	1.462	1.455	1.773	30.7	13.7	11.7	25.1	2.0
	M062X	1.455	1.460	1.461	1.453	1.774	24.7	14.3	13.6	15.4	1.5
	ωB97XD	1.459	1.463	1.464	1.458	1.778	38.4	21.9	21.4	35.4	2.6
6-31+g(d)	B3LYP	1.452	1.456	1.458	1.448	1.778	24.1	8.2	3.0	1.7	5.3
	B3PW91	1.449	1.452	1.454	1.446	1.775	25.8	9.0	2.1	4.3	6.0
	BHANDH	1.438	1.443	1.444	1.436	1.751	14.7	2.4	2.0	0.3	7.6
	CAM-B3LYP	1.459	1.463	1.463	1.457	1.773	37.6	19.9	18.5	31.3	4.7
	M062X	1.457	1.461	1.462	1.456	1.775	29.5	18.0	17.4	24.3	4.8
	ωB97XD	1.461	1.465	1.465	1.460	1.778	44.4	26.2	26.0	43.4	3.7
6-311g(d)	B3LYP	1.451	1.455	1.456	1.448	1.777	30.7	7.6	3.6	22.9	3.4
	B3PW91	1.447	1.451	1.452	1.445	1.773	30.2	6.9	4.0	23.0	2.3
	BHANDH	1.436	1.441	1.442	1.434	1.749	21.5	2.9	1.9	8.7	1.7
	CAM-B3LYP	1.457	1.461	1.462	1.456	1.772	40.9	19.6	18.6	36.8	1.7
	M062X	1.456	1.460	1.461	1.455	1.773	32.6	18.9	18.6	28.7	0.3
	ωB97XD	1.459	1.463	1.464	1.458	1.775	45.4	25.9	26.0	41.2	4.6
6-311+g(d)	B3LYP	1.450	1.455	1.457	1.448	1.777	28.5	11.4	8.1	19.9	5.7
	B3PW91	1.447	1.451	1.452	1.445	1.772	28.4	10.8	7.7	20.2	5.9
	BHANDH	1.436	1.441	1.442	1.434	1.749	17.8	2.5	5.2	3.6	8.1
	CAM-B3LYP	1.457	1.461	1.462	1.456	1.772	40.5	22.7	22.0	35.6	5.9
	M062X	1.456	1.460	1.461	1.454	1.772	31.2	20.4	19.9	26.2	5.9
	ωB97XD	1.460	1.463	1.464	1.459	1.775	46.1	27.6	27.6	43.9	5.6

Table S2: HOMO energies in (eV) of the most stable conformation exp. -5.50 eV

Basis-set\Functional	B3LYP	B3PW91	BHandH	CAM-B3LYP	M062X	ωB97XD
6-31g(d)	-5.03	-5.16	-5.82	-6.36	-6.29	-7.05
6-31+g(d)	-5.26	-5.34	-6.00	-6.63	-6.50	-7.28
6-311g(d)	-5.30	-5.38	-6.03	-6.67	-6.54	-7.30
6-311+g(d)	-5.34	-5.40	-6.06	-6.74	-6.58	-7.36

Table S3: LUMO energies in (eV) of the most stable conformation exp -3.55 eV

Basis-set\Functional	B3LYP	B3PW91	BHandH	CAM-B3LYP	M062X	ωB97XD
6-31g(d)	-2.85	-2.94	-1.87	-1.70	-2.04	-1.10
6-31+g(d)	-3.08	-3.12	-2.10	-1.91	-2.23	-1.27
6-311g(d)	-3.02	-3.07	-2.04	-1.84	-2.16	-1.21
6-311+g(d)	-3.10	-3.13	-2.13	-1.92	-2.24	-1.28

Table S4: Energies de gap de la conformation la plus stable exp. 1.95 eV

Basis-set\Functional	B3LYP	B3PW91	BHandH	CAM-B3LYP	M062X	ωB97XD
6-31g(d)	2.17	2.22	3.9	4.72	4.27	6.02
6-31+g(d)	2.28	2.3	3.99	4.83	4.38	6.09
6-311g(d)	2.19	2.22	3.95	4.66	4.25	5.95
6-311+g(d)	2.25	2.28	3.93	4.82	4.34	6.08

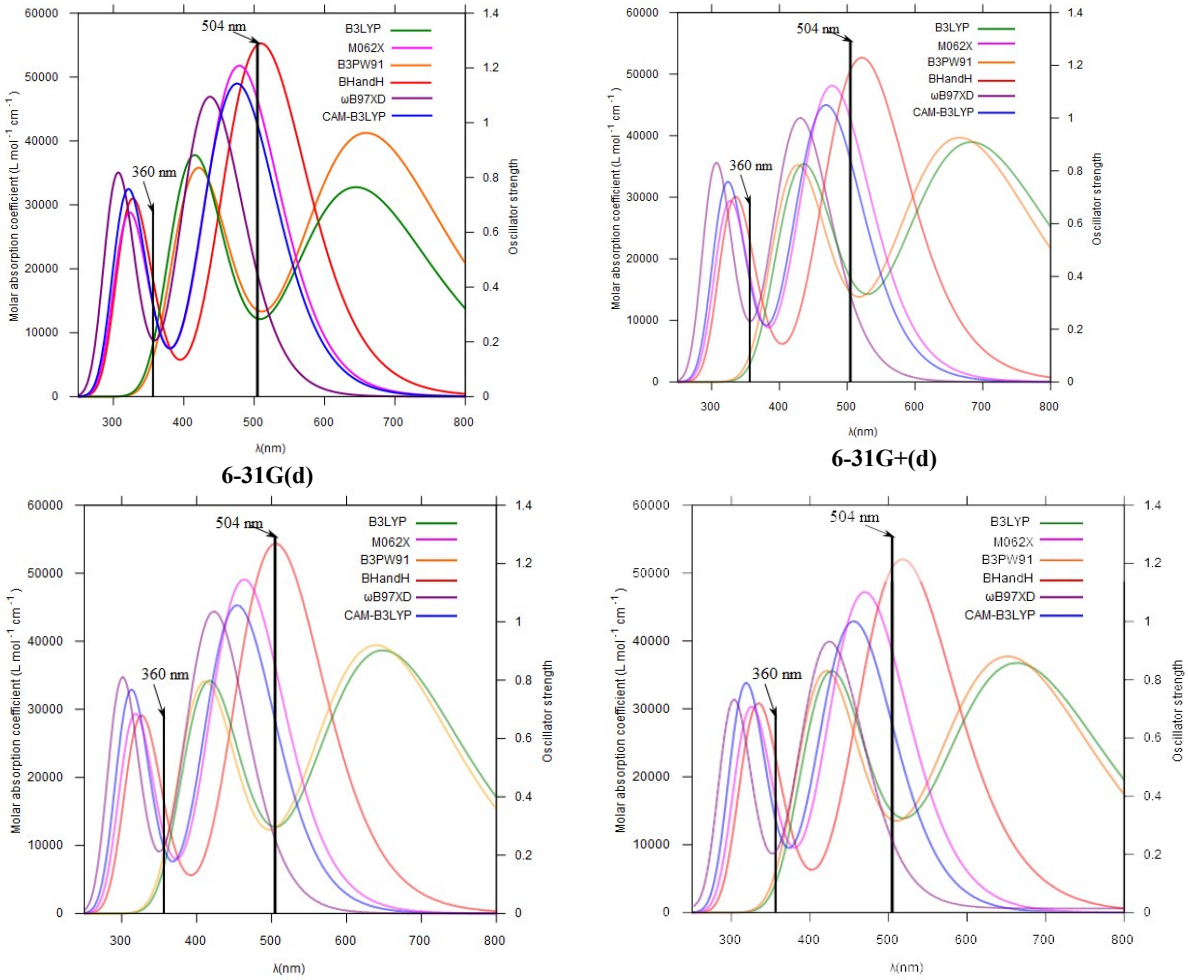

Figure S1: the photo-spectra of the studied dye in various functionals and basis sets

Table S 5: Δ_{inj} in (eV) in various functionals and basis sets

Basis-set\Functional	B3LYP	B3PW91	BHandH	CAM-B3LYP	M062X	ωB97XD
6-31G(d)	-0.894	-0.722	-0.614	-0.249	-0.301	0.213
6-31+G(d)	-0.555	-0.522	-0.378	-0.017	-0.097	0.399
6-311G(d)	-0.613	-0.560	-0.425	-0.062	-0.138	0.367
6-311+G(d)	-0.529	-0.503	-0.336	0.017	-0.061	0.434

Table S 6: Δ_{rec} in (eV) in various functionals and basis sets

Basis-set\Functional	B3LYP	B3PW91	BHandH	CAM-B3LYP	M062X	ωB97XD
6-31G(d)	-1.030	-1.160	-1.820	-2.360	-2.290	-3.050
6-31+G(d)	-1.260	-1.340	-2.000	-2.630	-2.500	-3.280
6-311G(d)	-1.300	-1.380	-2.030	-2.670	-2.540	-3.300
6-311+G(d)	-1.340	-1.400	-2.060	-2.740	-2.580	-3.360

Table S 7: Δ_{reg} in (eV) in various functionals and basis sets

Basis-set\Functional	B3LYP	B3PW91	BHandH	CAM-B3LYP	M062X	ωB97XD
6-31G(d)	-0.230	-0.360	-1.020	-1.560	-1.490	-2.250
6-31+G(d)	-0.460	-0.540	-1.200	-1.830	-1.700	-2.480
6-311G(d)	-0.500	-0.580	-1.230	-1.870	-1.740	-2.500
6-311+G(d)	-0.540	-0.600	-1.260	-1.940	-1.780	-2.560