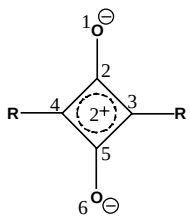
Table A: E_2 energies of Croconates Obtained at B3LYP/6-311+G(d,p) and BLYP/TZP Methods.

Mol. No.	[a]E_2 in kcal/mol	[b]E_2 in kcal/mol
40	10.1	14.11
41	7.8	12.11
42	16.1	18.10
43	17.1	18.96
44	13.7	17.26
45	14.4	17.41
46	14.2	17.22
47	14.0	17.09
48	14.3	17.18
49	12.5	15.39

[a] at B3LYP/6-311+G(d, p), [b] at BLYP/TZP



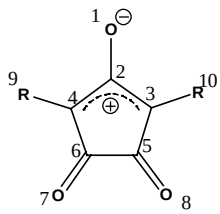


Table B: Optimized singlet geometrical parameters of Symmetrical Squaraines using the B3LYP/ 6-311+G(d,p) Method.

Mol. No.	Bond lengths (A^0)				Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	C_3-R= C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
1	1.226	1.474	1.474	1.410	135.4	135.4	89.2
2	1.226	1.474	1.474	1.410	135.4	135.4	89.1
3	1.238	1.462	1.466	1.404	133.2	136.2	90.5
4	1.227	1.477	1.478	1.420	136.6	133.5	90.0
5	1.227	1.473	1.473	1.409	135.4	135.4	89.3
6	1.228	1.474	1.479	1.393	133.7	136.3	89.9
7	1.227	1.475	1.481	1.391	133.7	136.3	90.0
8	1.227	1.478	1.476	1.404	134.8	134.8	90.2
9	1.223	1.475	1.474	1.414	135.5	135.6	88.9
10	1.226	1.474	1.473	1.410	135.4	135.4	89.2
11	1.221	1.481	1.481	1.399	134.9	134.9	90.1
12	1.226	1.482	1.473	1.401	137. 7	132.2	90.1
13	1.223	1.472	1.476	1.389	135.2	135. 7	89.2
14	1.229	1.478	1.472	1.393	136.5	133. 7	90.1
15	1.226	1.473	1.474	1.393	134.3	136.1	89.6
16	1.247	1.459	1.459	1.402	133.9	133.9	92.2
17	1.244	1.459	1.459	1.404	134.0	133.9	92.0
18	1.241	1.472	1.468	1.423	135.7	131.8	92.6
19	1.225	1.475	1.473	1.398	136.3	134.2	89.5

Table C: Optimized singlet geometrical parameters of Unsymmetrical Squaraines using the B3LYP/6-311+G(d,p) Method.

Mol. No.	Bond lengths (A^0)						Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	O_6-C_5	C_3-R	C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
20	1.224	1.466	1.482	1.229	1.410	1.393	136.3	133.9	89.9
21	1.223	1.471	1.482	1.233	1.409	1.393	135.8	134.6	89.6
22	1.227	1.476	1.479	1.229	1.390	1.401	133.1	136.9	90.0
23	1.227	1.467	1.481	1.224	1.415	1.387	135.6	135.1	89.3
24	1.224	1.465	1.447	1.218	1.392	1.425	132.4	136.8	90.8
25	1.242	1.449	1.469	1.220	1.403	1.352	131.7	137.9	90.4
26	1.235	1.472	1.458	1.236	1.390	1.417	132.5	137.2	90.3
27	1.224	1.470	1.478	1.225	1.418	1.404	135.8	135.1	89.0
28	1.228	1.465	1.475	1.219	1.409	1.414	135.3	135.2	89.6
29	1.218	1.480	1.485	1.227	1.420	1.381	138.2	133.2	88.6
30	1.236	1.478	1.470	1.221	1.391	1.402	134.7	135.1	90.3
31	1.249	1.450	1.452	1.219	1.404	1.392	134.6	134.0	91.4
32	1.224	1.467	1.480	1.223	1.422	1.379	136.8	134.0	89.2
33	1.242	1.457	1.456	1.220	1.404	1.389	133.6	135. 6	90.8
34	1.232	1.466	1.465	1.222	1.392	1.390	133.6	136.6	89.9
35	1.227	1.495	1.461	1.227	1.343	1.396	137.2	133.8	88.9
36	1.224	1.478	1.471	1.225	1.406	1.418	135.2	135.8	89.0
37	1.243	1.465	1.449	1.220	1.393	1.422	132.4	136.8	90.8
38	1.224	1.461	1.453	1.221	1.398	1.414	132.7	136.5	90.8
39	1.226	1.489	1.468	1.227	1.471	1.412	137.1	133.6	89.3

Table D: Optimized singlet geometrical parameters of Croconates using the B3LYP/6-311+G(d,p) Method.

Mol. No.	Bond lengths (A^0)							Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	C_5-O_8	C_6-O_7	C_3-R	C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
40	1.239	1.462	1.476	1.218	1.225	1.394	1.397	128.2	123.7	108.2
41	1.238	1.464	1.478	1.218	1.224	1.393	1.396	128.1	123.5	108.3
42	1.262	1.460	1.460	1.228	1.228	1.426	1.426	123.8	123.8	112.4
43	1.276	1.449	1.449	1.216	1.216	1.428	1.428	123.7	123.7	112.7
44	1.236	1.465	1.465	1.223	1.223	1.389	1.389	126.8	126.8	106.4
45	1.253	1.454	1.460	1.218	1.235	1.393	1.401	127.7	123.7	108.6
46	1.241	1.450	1.466	1.220	1.225	1.392	1.393	127.0	125.2	107.7
47	1.240	1.449	1.461	1.220	1.225	1.392	1.393	127.0	125.3	107.7
48	1.241	1.450	1.466	1.221	1.225	1.392	1.393	127.0	125.2	107.8
49	1.241	1.459	1.477	1.220	1.225	1.394	1.396	128.3	123.3	108.4

Table E: Optimized triplet geometrical parameters of Croconates using the B3LYP/6-311+G(d,p) Method.

Mol. No.	Bond lengths (A^0)							Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	C_5-O_8	C_6-O_7	C_3-R	C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
40	1.230	1.475	1.495	1.216	1.223	1.387	1.388	127.6	123.2	109.2
41	1.230	1.476	1.496	1.215	1.222	1.385	1.386	127.7	123.1	109.2
42	1.256	1.472	1.473	1.232	1.232	1.444	1.444	123.8	123.8	112.5
43	1.265	1.464	1.464	1.218	1.218	1.438	1.438	123.5	123.5	113.0
44	1.229	1.482	1.482	1.223	1.223	1.391	1.391	126.3	126.3	107.3
45	1.243	1.464	1.481	1.217	1.236	1.401	1.403	127.5	123.1	109.4
46	1.233	1.466	1.482	1.219	1.224	1.394	1.395	126.3	124.7	108.9
47	1.233	1.466	1.482	1.219	1.223	1.393	1.394	126.3	124.8	108.9
48	1.233	1.466	1.482	1.220	1.224	1.395	1.395	126.3	124.8	108.9
49	1.232	1.473	1.496	1.218	1.224	1.391	1.391	127.8	123.0	109.2

Table F: Optimized singlet and triplet geometrical parameters of symmetrical squaraines using the BLYP/TZP Method (triplet geometrical parameters are given in parenthesis).

Mol. No.	Bond lengths (A^0)				Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	C_3-R= C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
1	1.243(1.240)	1.482(1.495)	1.482(1.495)	1.411(1.402)	135.4(134.6)	135.39(134.6)	89.22(90.7)
2	1.242(1.239)	1.483(1.496)	1.483(1.496)	1.412(1.403)	135.4(134.6)	135.38(134.6)	89.24(90.8
3	1.256(1.252)	1.468(1.479)	1.475(1.483)	1.406(1.406)	133.1(132.6)	136.18(135.7)	90.69(91.7)
4	1.243(1.240)	1.489(1.502)	1.487(1.502)	1.423(1.416)	133.4(132.9)	136.52(135.7)	90.06(91.5)
5	1.244(1.242)	1.483(1.494)	1.483(1.494)	1.409(1.401)	135.3(134.7)	135.34(134.7)	89.30(90.6)
6	1.244(1.238)	1.483(1.493)	1.491(1.493)	1.395(1.380)	133.3(132.9)	136.68(132.9)	90.06(91.0)
7	1.243(1.238)	1.484(1.493)	1.493(1.505)	1.393(1.378)	133.3(133.0)	136.56(136.1)	90.14(91.0)
8	1.243(1.238)	1.490(1.503)	1.486(1.498)	1.407(1.405)	134.8(134.2)	134.74(134.1)	90.33(91.6)
9	1.241(1.237)	1.485(1.500)	1.485(1.500)	1.415(1.404)	135.4(134.5)	135.66(134.6)	88.99(90.9)
10	1.243(1.240)	1.483(1.496)	1.482(1.495)	1.410(1.403)	135.5(134.7)	135.33(134.6)	89.19(90.7)
11	1.245(1.241)	1.490(1.500)	1.486(1.494)	1.405(1.403)	134.6(134.2)	134.69(134.0)	90.65(91.7)
12	1.242(1.237)	1.495(1.507)	1.483(1.497)	1.403(1.394)	138.1(137.2)	131.72(131.6)	90.21(91.3)
13	1.239(1.235)	1.481(1.491)	1.486(1.499)	1.389(1.380)	135.0(134.2)	135.81(135.4)	89.23(90.4)
14	1.245(1.238)	1.488(1.502)	1.481(1.493)	1.394(1.381)	136.6(136.1)	133.25(133.0)	90.10(90.9)
15	1.243(1.238)	1.483(1.494)	1.483(1.499)	1.395(1.387)	134.2(133.9)	136.13(135.2)	89.68(90.9)
16	1.265(1.261)	1.466(1.474)	1.466(1.474)	1.406(1.416)	133.8(133.5)	133.81(133.5)	92.38(93.0)
17	1.263(1.258)	1.467(1.477)	1.467(1.477)	1.409(1.414)	133.9(133.5)	133.88(133.4)	92.23(93.1)
18	1.258(1.255)	1.482(1.484)	1.476(1.487)	1.428(1.430)	135.5(135.2)	131.67(131.3)	92.80(93.5)
19	1.241(1.237)	1.486(1.500)	1.483(1.500)	1.401(1.395)	136.5(133.6)	133.96(133.3)	89.59(91.1)

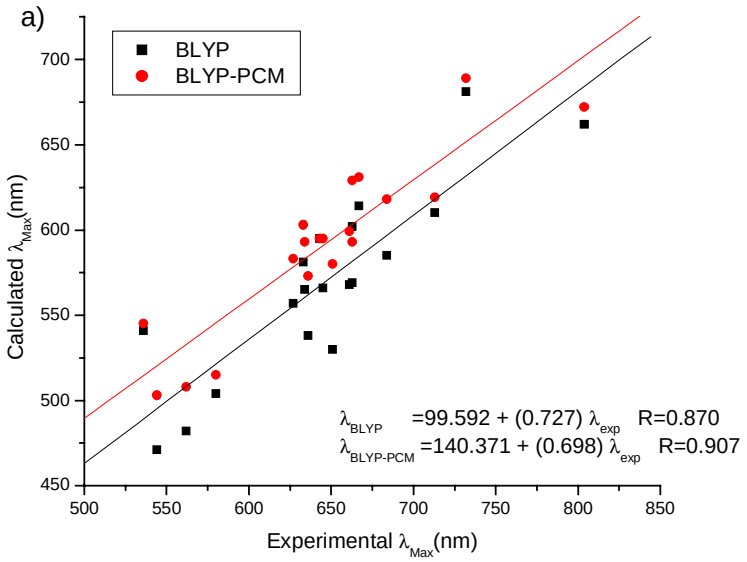
Table G: Optimized singlet and triplet geometrical parameters of unsymmetrical squaraines using the BLYP/TZP Method (triplet geometrical parameters are given in parenthesis).

Mol. No.	Bond lengths (A^0)						Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	O_6-C_5	C_3-R	C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
20	1.244(1.237)	1.475(1.483)	1.500(1.504)	1.241(1.239)	1.410(1.407)	1.394(1.377)	133.1(135.6)	137.3(133.6)	89.6(90.9
21	1.239(1.236)	1.481(1.489)	1.492(1.505)	1.249(1.243)	1.411(1.406)	1.393(1.374)	136.0(135.3)	136.0(133.9)	89.8(90.8)
22	1.242(1.236)	1.482(1.494)	1.491(1.505)	1.246(1.240)	1.391(1.378)	1.403(1.394)	132.4(132.5)	137.5(136.6)	90.1(91.0)
23	1.243(1.239)	1.478(1.493)	1.489(1.499)	1.240(1.236)	1.410(1.404)	1.392(1.387)	135.4(134.5)	135.1(134.6)	89.5(90.9)
24	1.263(1.257)	1.468(1.467)	1.458(1.485)	1.235(1.233)	1.346(1.410)	1.420(1.402)	132.2(132.7)	136. 7(135.1)	91.1(92.2)
25	1.259(1.255)	1.455(1.466)	1.479(1.489)	1.236(1.235)	1.405(1.409)	1.36(1.379)	131.4(131.2)	138.0(137.1)	90.6(91.7)
26	1.254(1.246)	1.477(1.483)	1.466(1.491)	1.252(1.248)	1.395(1.406)	1.418(1.402)	132.4(132.5)	137.0(135.7)	90.6(91.8)
27	1.241(1.238)	1.480(1.500)	1.487(1.493)	1.242(1.239)	1.418(1.403)	1.407(1.404)	135.7(134.4)	135.1(135.8)	89.2(90.8)
28	1.236(1.241)	1.485(1.486)	1.497(1.500)	1.245(1.234)	1.410(1.403)	1.415(1.405)	134.0 (134.6)	136.0(134.3)	88.7(91.1)
29	1.243(1.240)	1.481(1.500)	1.475(1.479)	1.233(1.231)	1.420(1.404)	1.383(1.381)	136.3(135.0)	133.3(133.4)	89.8(91.0)
30	1.251(1.234)	1.489(1.497)	1.482(1.498)	1.237(1.243)	1.396(1.394)	1.405(1.393)	134.6(134.3)	135.0(134.2)	90.4(91.5)
31	1.264(1.234)	1.459(1.501)	1.466(1.505)	1.236(1.259)	1.406(1.405)	1.396(1.392)	133.9(134.3)	134.8(135.4)	91.3(90.1)
32	1.240(1.237)	1.477(1.501)	1.487(1.488)	1.240(1.235)	1.421(1.404)	1.381(1.384)	136.8(135.2)	133.9(134.0)	89.3(90.8)
33	1.258(1.254)	1.465(1.475)	1.469(1.481)	1.237(1.234)	1.406(1.405)	1.391(1.381)	133.0(132.6)	136.2(135.4)	90.9(91.9)
34	1.248(1.243)	1.476(1.488)	1.473(1.486)	1.238(1.234)	1.395(1.392)	1.391(1.380)	133.8(133.4)	136.2(135.4)	90.0(91.2)
35	1.243(1.239)	1.494(1.503)	1.465(1.483)	1.244(1.238)	1.352(1.375)	1.397(1.385)	136.1(135.6)	133.7(132.7	89.6(90.8)
36	1.240(1.238)	1.486(1.493)	1.481(1.500)	1.241(1.238)	1.408(1.404)	1.419(1.403)	135.1(134.7)	135.7(134.5)	89.2(90.9)
37	1.261(1.255)	1.470(1.469)	1.459(1.486)	1.236(1.234)	1.397(1.409)	1.422(1.402)	132.3(132.7)	136.7(134.1)	91.0(92.2)
38	1.262(1.257)	1.466(1.471)	1.462(1.481)	1.238(1.236)	1.401(1.407)	1.415(1.402)	132.6(132.6	136.4(135.3)	91.1(92.2)
39	1.242(1.238)	1.501(1.519)	1.475(1.491)	1.244(1.241)	1.420(1.414)	1.412(1.404)	137.4(136.5)	133.3(132.7)	89.4(90.9)

Table H: Optimized singlet and triplet geometrical parameters of croconates using the BLYP/TZP Method (triplet geometrical parameters are given in parenthesis).

Mol. No.	Bond lengths (A^0)							Bond angles (^{0})		
	O_1-C_2	C_2-C_3	C_2-C_4	C_5-O_8	C_6-O_7	C_3-R	C_4-R	O_1-C_2-C_3	O_1-C_2-C_4	C_3-C_2-C_4
40	1.255(1.249)	1.470(1.481)	1.486(1.501)	1.235(1.234)	1.242(1.241)	1.398(1.394)	1.400(1.395)	128.4(127.9)	123.3(122.8)	108.2(109.2)
41	1.255(1.249)	1.471(1.479)	1.488(1.499)	1.235(1.233)	1.242(1.241)	1.397(1.391)	1.399(1.393)	128.4(128.0)	123.2(122.7)	108.5(109.3)
42	1.280(1.275)	1.466(1.477)	1.466(1.477)	1.248(1.252)	1.248(1.252)	1.432(1.454)	1.432(1.455)	123.7(126.7)	123.7(123.7)	112.6(112.7)
43	1.292(1.287)	1.455(1.465)	1.455(1.465)	1.233(1.234)	1.233(1.235)	1.434(1.446)	1.435(1.440)	123.6(123.4)	123.6(123.4)	112.9(113.2)
44	1.252(1.246)	1.473(1.485)	1.473(1.485)	1.241(1.241)	1.241(1.241)	1.392(1.395)	1.392(1.396)	126.8(126.4)	126.8(126.4)	106.3(107.2)
45	1.270(1.264)	1.460(1.467)	1.470(1.484)	1.235(1.235)	1.255(1.255)	1.400(1.407)	1.405(1.408)	128.0(127.8)	123.3(122.8)	108.7(109.4)
46	1.258(1.251)	1.455(1.469)	1.475(1.486)	1.237(1.236)	1.244(1.242)	1.396(1.399)	1.397(1.401)	127.1(126.3)	125.0(124.8)	107.9(108.9)
47	1.257(1.251)	1.454(1.469)	1.474(1.486)	1.236(1.236)	1.243(1.241)	1.396(1.399)	1.397(1.400)	127.0(126.2)	125.1(124.8)	107.9(108.9)
48	1.257(1.252)	1.455(1.469)	1.477(1.488)	1.238(1.237)	1.244(1.243)	1.396(1.400)	1.397(1.401)	126.9(126.3)	125.4(124.9)	107.8(108.8)
49	1.257(1.250)	1.467(1.477)	1.487(1.503)	1.237(1.235)	1.243(1.242)	1.399(1.398)	1.401(1.398)	128.5(128.1)	123.0(122.7)	108.5(109.2)

Figure A: Calculated versus Experimental λ_{Max} (nm) for Symmetrical squaraines using a) BLYP/PCM-BLYP at 6-311G(d,p) level and b) LB94/COSMO-LB94 at TZ2P level.



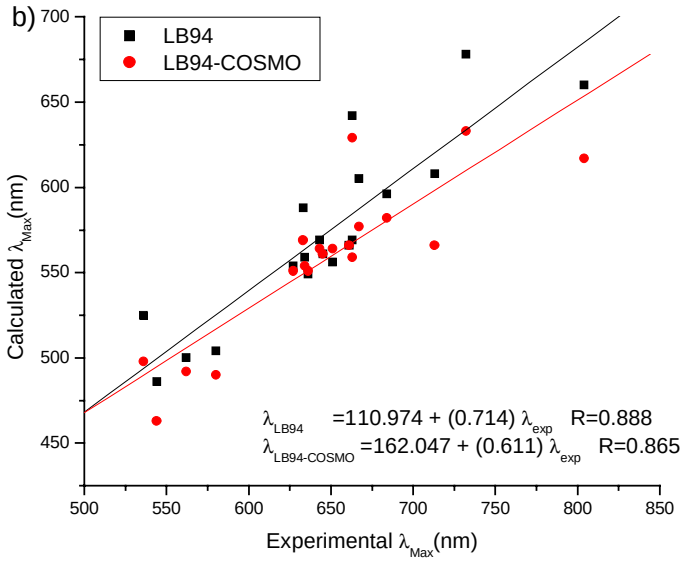
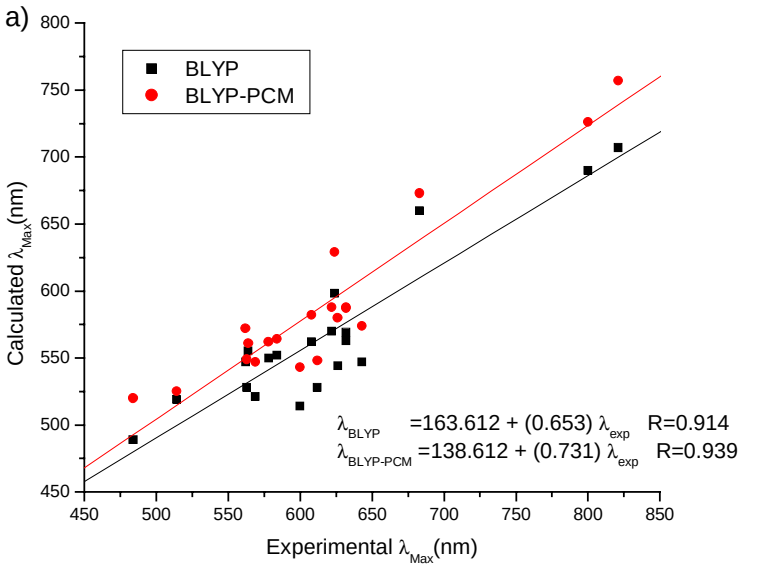


Figure B: Calculated versus Experimental λ_{Max} (nm) for Unsymmetrical squaraines using a) BLYP/PCM-BLYP at 6-311G(d,p) level and b) LB94/COSMO-LB94 at TZ2P level.



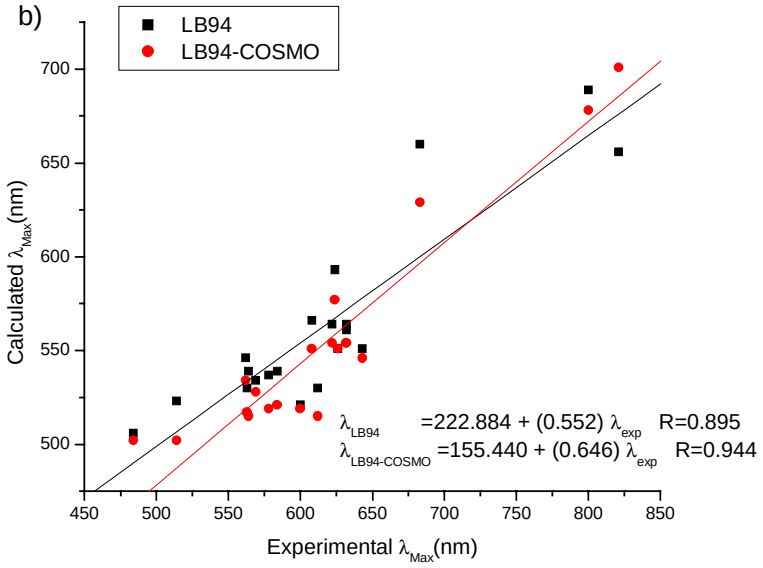
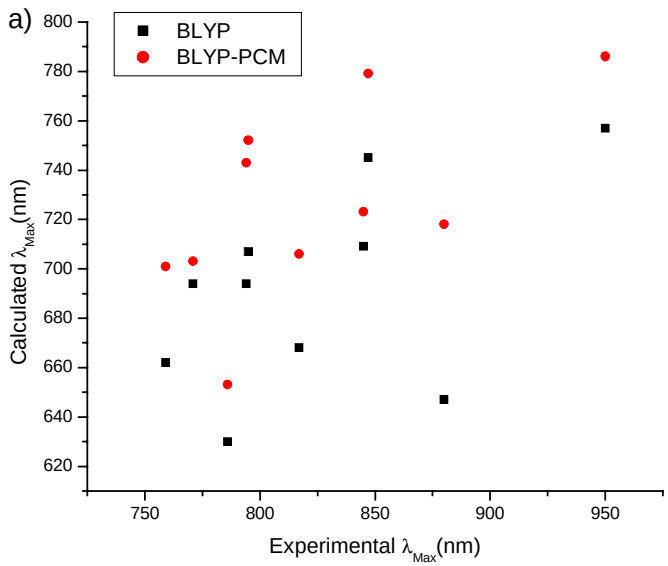
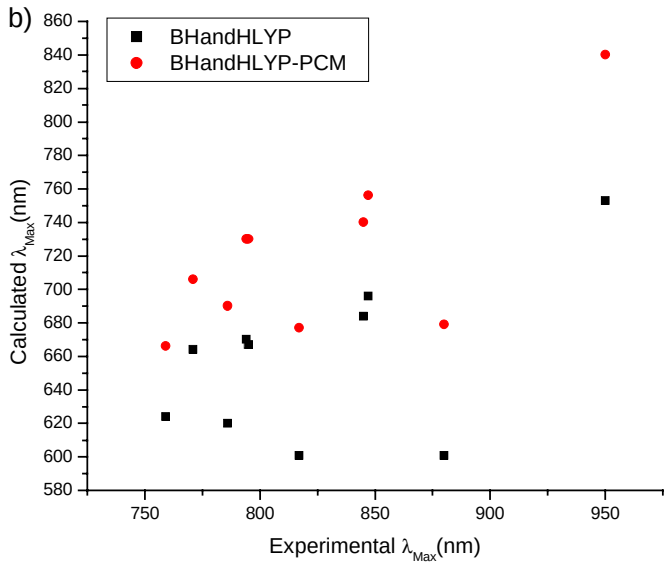


Figure C: Calculated versus Experimental λ_{Max} (nm) for Croconates using a) BLYP/PCM-BLYP at 6-311G(d,p) level, b) BHandHLYP/PCM-BHandHLYP at 6-311G(d,p) level and c) LB94/COSMO-LB94 at TZ2P level.





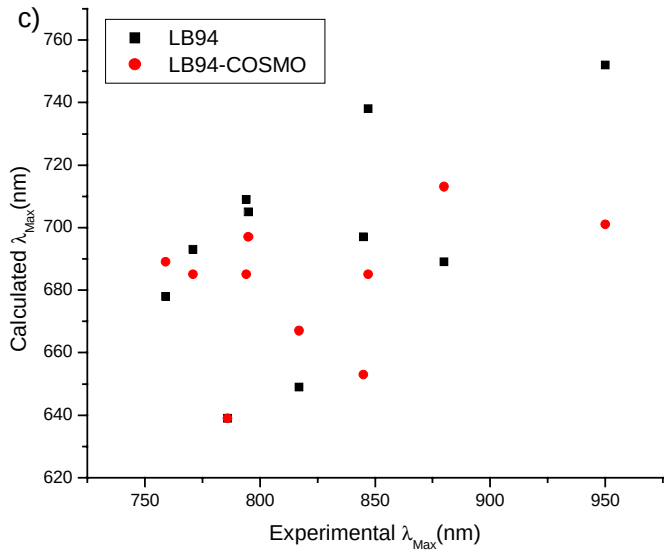


Table I: Calculated λ_{Max} (in nm), Oscillator strengths (*f*) of Symmetrical Squaraines.

Mol. No.	TD-B3LYP/ 6-311G(d,p)		TD-BLYP/ 6-311G(d,p)		TD-LB94/TZ2P	
	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*
1	528	1.521	565	1.292	559	1.565
2	524	1.361	557	1.210	554	1.411
3	509	1.450	538	1.244	549	1.383
4	533	1.310	595	1.639	569	1.093
5	536	1.532	568	1.344	566	1.544
6	583	1.200	610	1.005	608	1.095
7	640	1.346	662	1.173	660	1.228
8	488	0.908	504	0.754	504	0.827
9	503	0.924	541	0.751	525	0.903
10	531	1.432	566	1.215	561	1.292
11	563	0.954	585	0.824	596	0.769
12	545	1.375	581	1.158	588	1.234
13	548	1.365	569	1.233	569	1.329
14	617	1.476	681	1.034	678	1.118
15	575	1.269	614	1.084	605	1.267
16	500	1.718	530	1.705	556	1.668
17	462	1.026	482	0.937	500	0.935
18	567	0.898	602	0.779	642	0.710
19	471	0.777	471	0.777	486	0.713

Table J: Calculated λ_{Max} (in nm), Oscillator strengths (*f*) of Unsymmetrical Squaraines.

Mol. No.	TD-B3LYP/ 6-311G(d,p)		TD-BLYP/ 6-311G(d,p)		TD-LB94/TZ2P	
	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*
20	656	1.177	707	0.999	656	1.196
21	639	1.156	690	0.975	689	1.069
22	613	1.276	660	1.029	660	1.103
23	555	1.198	598	1.015	593	1.145
24	504	1.180	547	0.940	546	1.034
25	484	1.164	521	0.999	534	1.035
26	464	0.980	489	0.928	506	0.949
27	513	1.210	552	0.973	539	1.265
28	531	1.368	569	1.135	564	1.453
29	536	1.186	570	1.000	564	1.207
30	527	1.388	562	1.226	566	1.391
31	492	1.260	514	1.038	521	1.206
32	519	1.026	555	0.804	539	1.027
33	521	1.340	547	1.140	551	1.29
34	510	1.130	528	1.014	530	1.097
35	484	0.985	519	0.863	523	0.938
36	512	1.137	550	0.923	537	1.155
37	493	1.178	528	0.911	530	0.876
38	512	1.415	544	1.222	551	1.374
39	526	1.311	563	1.073	561	0.812

Table K: Calculated λ_{Max} (in nm) and Oscillator strengths (*f*) of Croconates.

Mol. No.	TD-B3LYP/ 6-311G(d,p)		TD-BLYP/ 6-311G(d,p)		TD-BHandHLYP/ 6-311G(d,p)		TD-LB94/TZ2P	
	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*
40	689	0.961	709	0.782	684	1.200	697	0.906
41	751	1.07	757	0.948	753	1.321	752	0.979
42	621	1.202	647	1.111	601	1.358	689	0.944
43	624	1.053	668	0.287	601	1.328	649	1.094
44	622	1.094	630	1.001	620	1.287	639	1.008
45	641	1.068	662	0.997	624	1.203	678	1.008
46	678	1.031	694	0.950	664	1.210	693	1.091
47	686	1.028	694	0.992	670	1.207	709	0.983
48	687	1.141	707	1.061	667	1.335	705	1.203
49	712	1.293	745	0.970	696	1.566	738	1.026

Table L: Calculated λ_{Max} (in nm) and Oscillator strengths (*f*) including solvent for symmetrical Squaraines.

Mol. No.	TD-PCM-B3LYP/ 6-311G(d,p)		TD-PCM-BLYP/ 6-311G(d,p)		TD-COSMO-LB94/ TZ2P	
	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*
1	563	1.990	593	1.902	554	1.805
2	554	1.841	583	1.739	551	1.645
3	546	1.805	573	1.741	551	1.593
4	566	1.710	595	1.640	564	1.508
5	575	2.002	599	1.951	566	1.743
6	603	1.530	619	1.394	566	1.362
7	681	1.697	672	1.643	617	1.455
8	511	1.141	515	1.099	490	0.923
9	516	1.311	545	1.218	498	1.232
10	566	1.894	595	1.808	561	1.640
11	600	1.194	618	1.088	582	0.838
12	569	1.661	603	1.522	569	1.422
13	583	1.734	593	1.690	559	1.399
14	643	1.896	689	1.562	633	1.348
15	601	1.611	631	1.492	577	1.477
16	544	1.996	580	1.757	564	1.610
17	487	1.233	508	1.175	492	0.989
18	596	1.096	629	1.003	629	0.742
19	492	1.061	503	0.939	463	0.862

Table M: Calculated λ_{Max} (in nm) and Oscillator strengths (*f*) including solvent for Unsymmetrical Squaraines.

Mol. No.	TD-PCM-B3LYP/ 6-311G(d,p)		TD-PCM-BLYP/ 6-311G(d,p)		TD-COSMO-LB94/ TZ2P	
	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*
20	706	1.504	757	1.318	701	0.702
21	680	1.513	726	1.311	678	1.157
22	640	1.593	673	1.45	629	1.209
23	590	1.503	629	1.375	577	1.285
24	527	1.491	572	1.162	534	1.158
25	510	1.431	547	1.337	528	1.201
26	493	1.219	520	1.177	502	0.984
27	536	1.665	564	1.587	521	1.533
28	562	1.85	588	1.834	554	1.774
29	563	1.59	588	1.541	554	1.370
30	553	1.696	582	1.61	551	1.453
31	523	1.566	543	1.46	519	1.339
32	534	1.397	561	1.293	515	1.203
33	558	1.682	574	1.699	546	1.463
34	539	1.45	548	1.407	515	1.234
35	495	1.201	525	1.112	502	1.092
36	533	1.573	562	1.496	519	1.482
37	518	1.547	549	1.424	517	0.842
38	550	1.784	580	1.687	551	1.589
39	565	1.583	587	1.723	554	1.531

Table N: Calculated λ_{Max} (in nm) and Oscillator strengths (*f*) including solvent for Croconates.

Molecule	TD-PCM-B3LYP/ 6-311G(d,p)		TD-PCM-BLYP/ 6-311G(d,p)		TD-PCM-BHandHLYP/ 6-311G(d,p)		TD-COSMO-LB94/TZ2P	
	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*	$\lambda_{Max.}$	*f*
40	721	1.243	723	1.111	740	1.449	653	1.054
41	805	1.381	786	1.317	840	1.596	701	1.145
42	693	1.415	718	1.311	679	1.578	713	0.879
43	688	1.483	706	1.304	677	1.655	667	1.214
44	674	1.405	653	1.453	690	1.578	639	1.041
45	679	1.260	701	1.180	666	1.373	689	0.259
46	707	1.320	703	1.306	706	1.469	685	0.616
47	729	1.346	743	1.165	730	1.491	685	0.811
48	733	1.510	752	1.471	730	1.619	697	0.724
49	749	1.679	779	0.313	756	1.876	685	0.913