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Electronic Supplementary Information

Study of the chemical reactivity with relation to the experimental parameters of efficiency in coumarin derivatives for dye sensitized solar cells using DFT.

Rody Soto-Rojo,[a,b] Jesús Baldenebro-López[b] and Daniel Glossman-Mitnik[a]

[a] *Laboratorio Virtual NANOCOSMOS – Departamento de Medio Ambiente y Energía - Centro de Investigación en Materiales Avanzados, Miguel de Cervantes 120, Complejo Industrial Chihuahua, Chihuahua, Chih. 31136, México.*

[b] *Facultad de Ingeniería Mochis – Universidad Autónoma de Sinaloa – Prol. Ángel Flores y Fuente de Poseidón, S.N, C.P. 81223 Los Mochis, Sinaloa, México.*

E-mail: daniel.glossman@cimav.edu.mx

This electronic supplementary information has the aim of providing to the reader the theoretical results called out using different chemical models as: PBE0/6-31G(d), PBE0/MIDIY, M06/MIDIY, B3LYP/6-31G(d), B3LYP/MIDIY and CAM-B3LYP/6-31G(d). Above allow to compare with the chemical model reported in the paper, which was the most accurate, however the theoretical levels showed here could be a good alternative (with exception of CAM-B3LYP), it because the results were similar among them. Then, each result showed in the paper was presented in the present material, except the HOMO and LUMO orbitals and NTO analysis.

According to the comparison between the theoretical and experimental λ_{max} shown in the table S1, the levels of calculation more accurate are with the PBE0 and M06 functionals. It can be noted that both functionals show very similar results and hence any could be used in this study. B3LYP functional is a good option but with less accurate than the above, however the rest of calculated molecular properties exhibit the same trend. CAM-B3LYP is further from the experimental data.

Table S1. Comparison between the theoretical and experimental maximum absorption wavelengths with the different levels of calculation.

Molecule	PBE0		M06		B3LYP		CAM-B3LYP	Experimental
	6-31G(d)	MIDIY	6-31G(d)	MIDIY	6-31G(d)	MIDIY	6-31G(d)	
C343	**375**	**368**	**376**	**369**	**385**	**377**	**355**	**442**
	12	18	66	73	57	65	87	
NKX-2398	**400**	**393**	**400**	**395**	**412**	**404**	**373**	**451**
	51	58	51	57	39	47	78	
NKX-2388	**424**	**412**	**424**	**414**	**434**	**421**	**401**	**493**
	69	81	69	79	59	72	92	
NKX-2311	**497**	**463**	**494**	**464**	**512**	**476**	**452**	**504**
	7	41	10	40	8	28	52	
NKX-2586	**523**	**512**	**519**	**512**	**540**	**529**	**462**	**506**
	17	6	13	6	34	23	44	
NKX-2753	**533**	**520**	**525**	**519**	**553**	**540**	**454**	**492**
	41	28	33	27	61	48	38	
NKX-2593	**587**	**573**	**576**	**573**	**615**	**601**	**474**	**510**
	77	63	66	63	105	91	36	
NKX-2807	**570**	**549**	**560**	**550**	**602**	**578**	**467**	**566**
	4	17	6	16	36	12	99	
NKX-2883	**671**	**646**	**651**	**648**	**720**	**702**	**468**	**552**
	119	94	99	96	168	150	84	

All units are in nm. Cell contents: theoretical λ_{max} and the difference between experimental and theoretical λ_{max}.

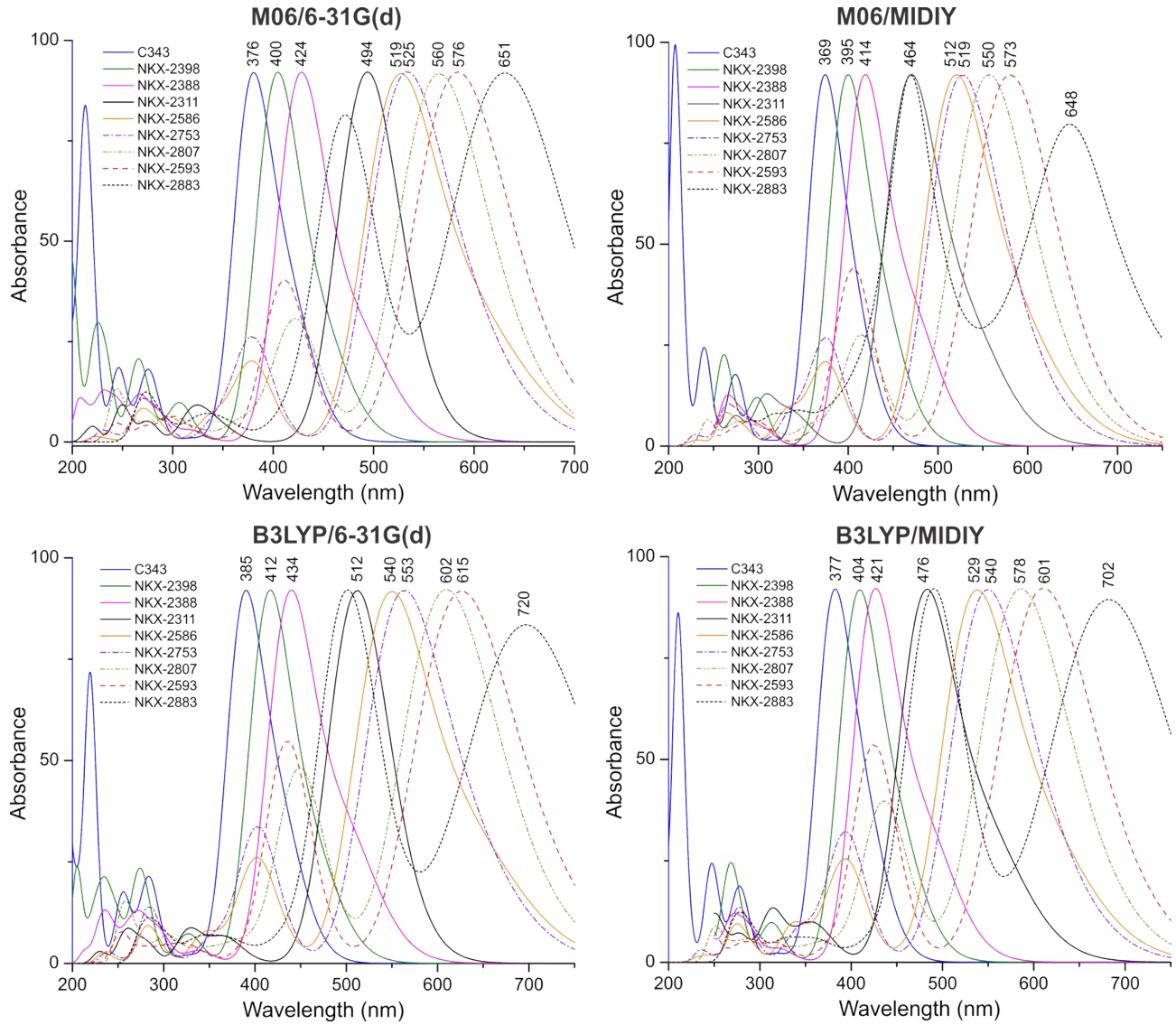

Figure S1 (a). Theoretical UV-Vis spectra of coumarin derivatives dyes using M06 and B3LYP functionals with 6-31G(d) and MIDIY basis sets.

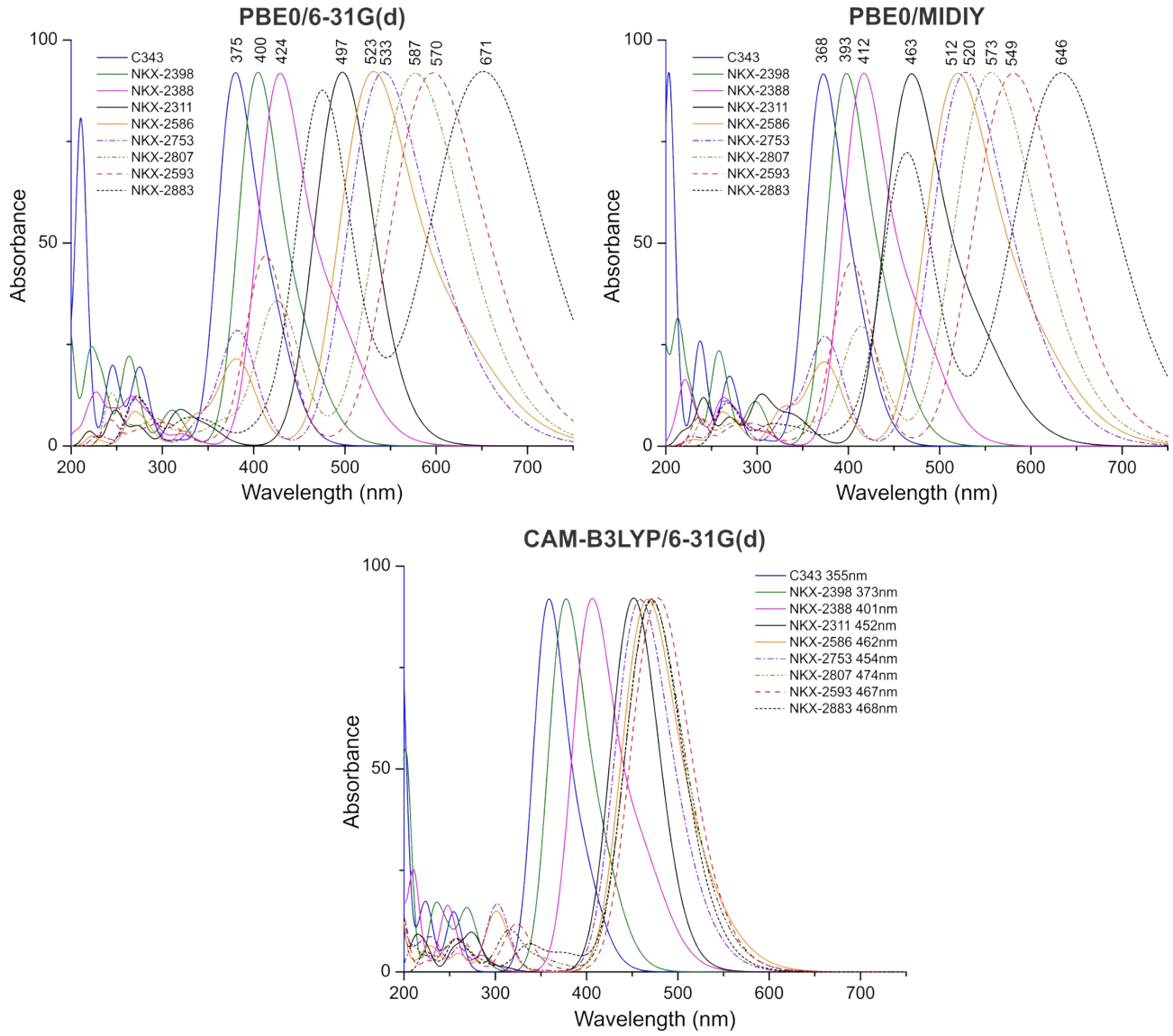

Figure S1 (b). Theoretical UV-Vis spectra of coumarin derivatives dyes using PBE0 functional with 6-31G(d) and MIDIY basis sets, and at CAM-B3LYP/6-31G(d).

Table S2. Absorption wavelengths, oscillator strength (f) and the orbitals involved in the transitions of coumarins using M06/6-31G(d) and M06/MIDIY.

M06/6-31G(d)				M06/MIDIY			
Molecule	λ_{max} (nm)	f	Transitions H=HOMO L=LUMO (%)	Molecule	λ_{max} (nm)	f	Transitions H=HOMO L=LUMO (%)
C343	376	0.6484	H→L(97)	C343	369	0.6210	H→L(97)
	275	0.0995	H→L+1(84)		273	0.0984	H→L+1(86)
	219	0.1070	H→L+3(74)		209	0.1122	H-5→L(73) H→L+3(13) H-1→L+1(8)
	211	0.4694	H-1→L+1(75)		205	0.5447	H-1→L+1(72) H→L+3(10) H-1→L+2(7)
NKX-2398	400	0.9909	H→L(99)	NKX-2398	395	0.9559	H→L(99)
	306	0.0867	H→L+1(83)		298	0.1009	H→L+1(85) H-1→L(10)
	264	0.1828	H-2→L(55) H→L+2(31)		260	0.2041	H-2→L(59) H→L+2(25) H→L+3(12)
	223	0.1551	H-2→L+1(84)		218	0.3177	H-2→L+1(57) H-5→L(19) H-1→L+1(6)
NKX-2388	424	1.1066	H→L(99)	NKX-2388	414	1.1176	H→L(99)
	265	0.0991	H→L+2(72)		263	0.1105	H→L+2(77) H-2→L(13)
	245	0.0792	H-1→L+1(88)		236	0.0498	H-1→L+1(65) H-5→L(16) H-4→L+1(6)
	229	0.0511	H-2→L+1(57) H-7→L(24)		222	0.1185	H-2→L+1(72) H-7→L(7) H-8→L(5)
NKX-2311	494	1.7517	H→L(99)	NKX-2311	464	1.4693	H→L(100)
	321	0.1478	H-1→L(63)		306	0.2011	H-2→L(39) H-1→L(34) H→L+1(17)
	276	0.0961	H→L+2(80)		273	0.0917	H→L+2(78) H→L+3(6) H-2→L+1(5)
	252	0.0817	H-2→L+1(79)		243	0.0917	H-2→L+1(42) H-5→L(33) H-1→L+1(13)
NKX-2586	519	1.8326	H→L(100)	NKX-2586	512	1.7652	H→L(100)
	381	0.3357	H→L+1(49) H-1→L(44)		378	0.3355	L-1→L(48) H→L+1(42) H-2→L(9)
	336	0.1348	H-1→L(52) H→L+1(41)		329	0.1781	H-1→L(49) H→L+1(36) H-2→L(36)
	269	0.0703	H-3→L(36) H-1→L+1(35)		264	0.0712	H-5→L(44) H-1→L+1(31) H→L+3(15)
NKX-2753	525	1.5791	H→L(100)	NKX-2753	519	1.5150	H→L(100)
	380	0.4221	H→L+1(54) H-1→L(43)		377	0.4217	H→L+1(49) H-1→L(45)
	286	0.0572	H→L+2(51) H-2→L+1(21)		284	0.0568	H→L+2(66)
	268	0.1028	H-2→L+1(63) H→L+2(28)		264	0.0870	H-2→L+1(70) H→L+2(20)
NKX-2593	576	1.4079	H→L(100)	NKX-2593	573	1.3476	H→L(100)
	412	0.7190	H-1→L(52) H→L+1(47)		407	0.7580	H→L+1(50) H-1→L(49)
	314	0.0437	H→L+2(88)		310	0.0449	H→L+2(90)
	245	0.0441	H→L+6(46) H-1→L+2(25)		241	0.0402	H→L+5(31) H-1→L+2(31) H-7→L(25)
NKX-2807	560	1.3953	H→L(100)	NKX-2807	550	1.4542	H→L(100)
	423	0.5691	H→L+1(74) H-1→L(24)		416	0.5387	H→L+1(73) H-1→L(26)
	367	0.0854	H-1→L(60) H→L+1(19) H-2→L(18)		357	0.0855	H-1→L(47) H-2→L(35)
	244	0.1027	H-4→L+1(51) H-2→L+2(29)		243	0.0614	H-3→L+1(51)
NKX-2883	651	0.9998	H→L(99)	NKX-2883	648	1.0692	H→L(100)
	476	1.2480	H→L+1(50) H-1→L(48)		469	1.2382	H→L+1(55) H-1→L(43)
	325	0.0515	H-3→L(42) H-1→L+1(27)		317	0.0489	H-3→L(45) H-1→L+1(25)
	273	0.0855	H-1→L+2(28) H-5→L(21)		268	0.0859	H→L+5(30)

Table S3. Absorption wavelengths, oscillator strength (f) and the orbitals involved in the transitions of coumarins using B3LYP/6-31G(d) and B3LYP/MIDIY.

B3LYP/6-31G(d)				B3LYP/MIDIY			
Molecule	λ_{max} (nm)	f	Transitions H=HOMO L=LUMO (%)	Molecule	λ_{max} (nm)	f	Transitions H=HOMO L=LUMO (%)
C343	385	0.6286	H→L(97)	C343	377	0.6159	H→L(97)
	283	0.1185	H→L+1(89)		277	0.1037	H→L+1(89)
	257	0.0620	H→L+2(93)		248	0.0920	H→L+2(71) H-3→L(25)
	219	0.2373	H-1→L+1(52) H-2→L+1(18)		209	0.4918	H-1→L+1(79)
NKX-2398	412	0.9701	H→L(99)	NKX-2398	404	0.9444	H→L(99)
	271	0.1902	H-2→L(53) H→L+2(32)		266	0.2064	H-2→L(56) H→L+2(26) H→L+3(13)
	248	0.0856	H-1→L+1(92)		239	0.0527	H-1→L+1(82) H-5→L(6)
	234	0.1173	H-2→L+1(77)		227	0.1010	H-2→L+1(62) H-5→L(25)
NKX-2388	434	1.0866	H→L(100)	NKX-2388	442	1.1149	H→L(100)
	272	0.0872	H→L+2(81)		268	0.0958	H→L+2(81) H-2→L(9)
	258	0.0546	H-1→L+1(86)		248	0.0303	H-1→L+1(75) H-5→L(9) H-4→L+1(6)
	243	0.0427	H-2→L+1(57) H-5→L(23)		228	0.0437	H-2→L+1(37) H→L+3(20) H-6→L(11) H-5→L(11) H-7→L(7)
NKX-2311	512	1.6962	H→L(100)	NKX-2311	476	1.4232	H→L(100)
	328	0.1540	H-1→L(51) H-2→L(25)		312	0.2102	H-2→L(38) H-1→L(33) H→L+1(17)
	283	0.0808	H→L+2(74)		278	0.0739	H→L+2(71) H-1→L+1(9) H-2→L+1(7)
	265	0.0808	H-2→L+1(75)		250	0.0770	H-5→L(45) H-2→L+1(26) H-1→L+1(17)
NKX-2586	540	1.7173	H→L(100)	NKX-2586	529	1.6831	H→L(100)
	405	0.3880	H→L+1(45) H-1→L(43)		396	0.3864	L-1→L(45) H→L+1(41)
	344	0.1631	H-1→L(51) H→L+1(38)		336	0.1987	H-1→L(49) H→L+1(34)
	281	0.0787	H-2→L+1(40)		273	0.0827	H-2→L+1(45)
NKX-2753	553	1.4608	H→L(100)	NKX-2753	540	1.4404	H→L(100)
	404	0.4903	H→L+1(50) H-1→L(43)		395	0.4740	H→L+1(47) H-1→L(44)
	350	0.1070	H→L(53) H→L+1(37)		341	0.1410	H-1→L(51) H→L+1(32)
	281	0.1073	H-2→L+1(42) H→L+2(31)		275	0.9500	H-2→L+1(57) H→L+2(25)
NKX-2593	615	1.2766	H→L(100)	NKX-2593	601	1.2742	H→L(100)
	435	0.8581	H-1→L(52) H→L+1(46)		425	0.8349	H-1→L(51) H→L+1(47)
	333	0.0441	H→L+2(89)		324	0.0409	H→L+2(90)
	255	0.0725	H→L+5(32) H-7→L(28)		248	0.0513	H-7→L(29) H→L+5(29) H-1→L+2(24)
NKX-2807	602	1.1882	H→L(100)	NKX-2807	578	1.3189	H→L(100)
	449	0.7925	H→L+1(68) H-1→L(31)		437	0.7060	H→L+1(66) H-1→L(32)
	378	0.0702	H-1→L(59) H→L+1(24)		366	0.0709	H-1→L(50) H-2→L(23) H→L+1(22)
	256	0.1269	H-2→L+2(69)		334	0.2730	H→L+2(68) H-1→L+1(29)
NKX-2883	720	0.8896	H→L(100)	NKX-2883	702	0.9501	H→L(100)
	503	1.4034	H-1→L(51) H→L+1(48)		493	1.3759	H→L+1(51) H-1→L(49)
	336	0.0595	H-3→L(36) H-1→L+1(24)		326	0.0532	H-3→L(39) H-1→L+1(24)
	281	0.0490	H-1→L+2(20) H→L+6(18)		275	0.0509	H-4→L+1(42) H→L+5(19)

Table S4. Absorption wavelengths, oscillator strength (f) and the orbitals involved in the transitions of coumarins using PBE0/6-31G(d) and PBE0/MIDIY.

PBE0/6-31G(d)				PBE0/MIDIY			
Molecule	λ_{max} (nm)	f	Transitions H=HOMO L=LUMO (%)	Molecule	λ_{max} (nm)	f	Transitions H=HOMO L=LUMO (%)
C343	375	0.6602	H→L(98)	C343	368	0.6520	H→L(98)
	274	0.1108	H→L+1(87)		269	0.0990	H→L+1(88)
	247	0.0737	H→L+2(90)		239	0.0909	H→L+2(65) H-3→L(31)
	209	0.3285	H-1→L+1(56) H-2→L+1(18)		202	0.5590	H-1→L+1(79)
NKX-2398	400	1.0081	H→L(99)	NKX-2398	393	0.9858	H→L(99)
	261	0.2018	H-2→L(63) H→L+2(23)		256	0.2128	H-2→L(62) H→L+2(22)
	236	0.0940	H-1→L+1(90)		228	0.0394	H-1→L+1(47) H→L+3(29)
	223	0.1392	H-2→L+1(76)		216	0.0963	H-2→L+1(56) H-5→L(30)
NKX-2388	424	1.1281	H→L(100)	NKX-2388	412	1.1574	H→L(100)
	264	0.0918	H→L+2(82)		259	0.1027	H→L+2(80)
	246	0.0674	H-1→L+1(88)		238	0.0245	H-1→L+1(45) H-4→L+1(24) H-3→L+1(19)
	226	0.0378	H-2→L+1(27) H-7→L(26)		220	0.0958	H-2→L(67)
NKX-2311	497	1.7706	H→L(100)	NKX-2311	463	1.5085	H→L(100)
	318	0.1600	H-1→L(52) H-2→L(30)		302	0.2081	H-2→L(41) H-1→L(35)
	274	0.0910	H→L+2(81)		269	0.0865	H→L+2(78)
	252	0.0683	H-2→L+1(70)		240	0.0878	H-2→L+1(40) H-5→L(35)
NKX-2586	523	1.8465	H→L(100)	NKX-2586	512	1.8153	H→L(100)
	383	0.3403	H→L+1(46) H-1→L(44)		376	0.3390	L-1→L(46) H→L+1(43)
	334	0.1559	H-1→L(52) H→L+1(38)		326	0.1950	H-1→L(51) H→L+1(33)
	268	0.0801	H-1→L+1(27) H-3→L(24) H-2→L(19)		261	0.0727	H-3→L(41) H-1→L+1(29) H→L+3(19)
NKX-2753	533	1.5829	H→L(100)	NKX-2753	520	1.5668	H→L(100)
	383	0.4455	H→L+1(51) H-1→L(43)		376	0.4294	H→L+1(50) H-1→L(44)
	340	0.1042	H-1→L(54) H→L+1(36)		331	0.1441	H-1→L(52) H→L+1(30)
	269	0.1016	H-2→L+1(64) H→L+2(28)		262	0.0874	H-2→L+1(69) H→L+2(22)
NKX-2593	587	1.3881	H→L(100)	NKX-2593	573	1.3892	H→L(100)
	413	0.8026	H-1→L(50) H→L+1(49)		404	0.7870	H→L+1(51) H-1→L(48)
	316	0.0463	H→L+2(91)		308	0.0445	H→L+2(91)
	244	0.0444	H→L+6(29) H-1→L+2(19)		264	0.0362	H→L+3(53) H-2→L+1(19)
NKX-2807	570	1.3596	H→L(100)	NKX-2807	549	1.4899	H→L(100)
	427	0.6647	H→L+1(74) H-1→L(25)		415	0.5817	H→L+1(73) H-1→L(26)
	364	0.0939	H-1→L(59) H→L+1(19) H-2→L(19)		352	0.0919	H-1→L(49) H-2→L(32)
	243	0.0909	H-2→L+2(59) H-9→L(24)		241	0.0599	H-3→L+1(56)
NKX-2883	671	1.0136	H→L(100)	NKX-2883	646	1.1547	H→L(100)
	478	1.3436	H→L+1(54) H-1→L(45)		467	1.2669	H→L+1(58) H-1→L(41)
	323	0.0586	H-3→L(42) H-1→L+1(26)		313	0.0562	H-3→L(48) H-1→L+1(24)
	270	0.0858	H→L+6(30)		265	0.0949	H→L+5(56)

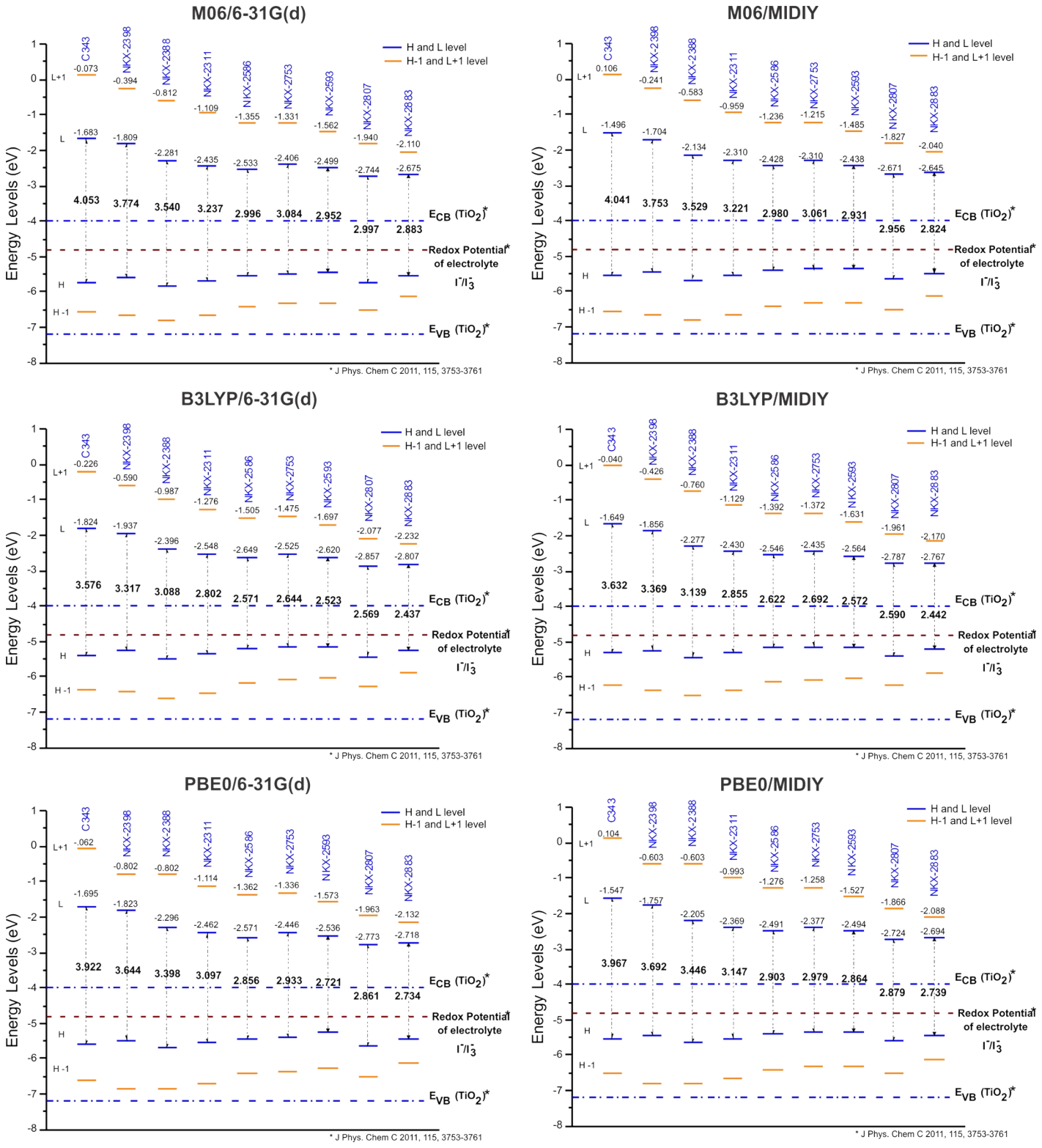

Figure S2. Orbital energy levels of coumarins using M06, PBE0 and B3LYP functionals with 6-31G(d) and MIDIY basis sets.

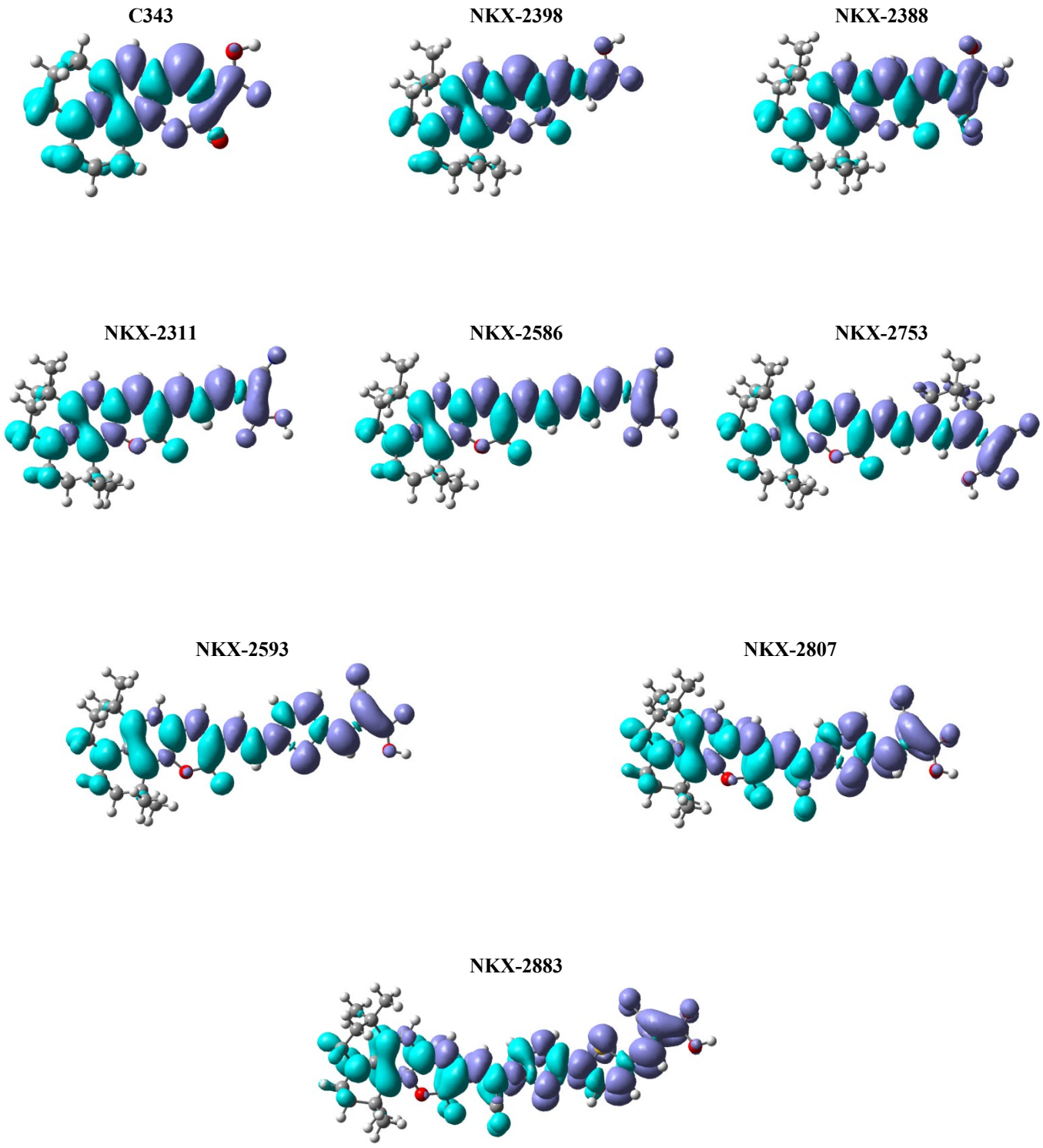

Figure S3. Electron Density Difference Maps (EDDMs) for the first excited singlet state of coumarin molecules with M06/6-31G(d) level of calculation. Cyan color indicates the electron density loss in transition and the purple color the electron density gain in transition.

Table S5. Chemical reactivity of coumarin derivates using M06, PBE0 and B3LYP functionals with 6-31G(d) and MIDIY basis sets.

	M06/6-311G(d)						M06/MIDIY					
MOLECULE	A	I	h	ω	ω-	ω+	A	I	h	ω	ω-	ω+
C343	0.32	7.03	3.36	2.02	4.27	0.60	0.37	7.43	3.53	2.16	4.55	0.65
NKX-2398	0.60	6.74	3.07	2.19	4.41	0.74	0.43	6.68	3.13	2.02	4.18	0.63
NKX-2388	1.11	6.94	2.91	2.78	5.16	1.13	0.90	6.85	2.97	2.52	4.83	0.96
NKX-2311	1.34	6.71	2.69	3.01	5.36	1.34	1.15	6.63	2.74	2.76	5.05	1.16
NKX-2586	1.51	6.53	2.51	3.21	5.54	1.52	1.34	6.43	2.55	2.96	5.22	1.34
NKX-2753	1.41	6.45	2.52	3.06	5.35	1.41	1.26	6.38	2.56	2.86	5.09	1.26
NKX-2593	1.48	6.41	2.46	3.15	5.43	1.49	1.37	6.38	2.51	2.99	5.24	1.37
NKX-2807	1.77	6.68	2.46	3.64	6.06	1.83	1.65	6.62	2.49	3.44	5.82	1.68
NKX-2883	1.76	6.44	2.34	3.58	5.92	1.83	1.69	6.39	2.35	3.47	5.78	1.74
	B3LYP/6-311G(d)						B3LYP/MIDIY					
MOLECULE	A	I	h	ω	ω-	ω+	A	I	h	ω	ω-	ω+
C343	0.25	6.89	3.32	1.92	4.12	0.55	0.05	6.79	3.37	1.73	3.86	0.44
NKX-2398	0.53	6.59	3.03	2.09	4.25	0.69	0.42	6.58	3.08	1.99	4.13	0.62
NKX-2388	1.03	6.78	2.87	2.66	4.97	1.06	0.89	6.73	2.92	2.48	4.75	0.94
NKX-2311	1.27	6.55	2.64	2.90	5.18	1.27	1.12	6.51	2.69	2.71	4.95	1.13
NKX-2586	1.44	6.35	2.46	3.09	5.34	1.45	1.31	6.32	2.50	2.91	5.13	1.31
NKX-2753	1.40	6.28	2.46	2.97	5.19	1.36	1.25	6.26	2.51	2.81	5.00	1.25
NKX-2593	1.40	6.25	2.40	3.08	5.31	1.46	1.33	6.22	2.44	2.92	5.11	1.33
NKX-2807	1.70	6.52	2.39	3.55	5.91	1.79	1.64	6.48	2.42	3.41	5.74	1.68
NKX-2883	1.80	6.25	2.25	3.57	5.85	1.85	1.71	6.23	2.26	3.48	5.75	1.78
	PBE0/6-311G(d)						PBE0/MIDIY					
MOLECULE	A	I	h	ω	ω-	ω+	A	I	h	ω	ω-	ω+
C343	0.28	6.94	3.33	1.96	4.18	0.57	0.10	6.87	3.38	1.79	3.96	0.47
NKX-2398	0.56	6.65	3.05	2.14	4.32	0.71	0.48	6.67	3.10	2.06	4.23	0.66
NKX-2388	1.08	6.84	2.88	2.72	5.06	1.10	0.96	6.82	2.93	2.58	4.89	1.00
NKX-2311	1.32	6.62	2.65	2.97	5.29	1.32	1.19	6.61	2.71	2.81	5.10	1.20
NKX-2586	1.49	6.43	2.47	3.17	5.46	1.50	1.38	6.42	2.52	3.02	5.28	1.38
NKX-2753	1.40	6.37	2.48	3.04	5.29	1.41	1.31	6.37	2.53	2.91	5.15	1.31
NKX-2593	1.48	6.34	2.43	3.14	5.40	1.49	1.41	6.37	2.48	3.05	5.31	1.42
NKX-2807	1.76	6.61	2.42	3.61	6.01	1.82	1.69	6.59	2.45	3.50	5.88	1.73
NKX-2883	1.77	6.36	2.30	3.60	5.92	1.85	1.73	6.36	2.31	3.54	5.85	1.80

A=electron affinity, I=ionization potential, h=chemical hardness, ω=electrophilicity index, ω-=electrodonating power, and ω+=electroaccepting power. All units are in eV.

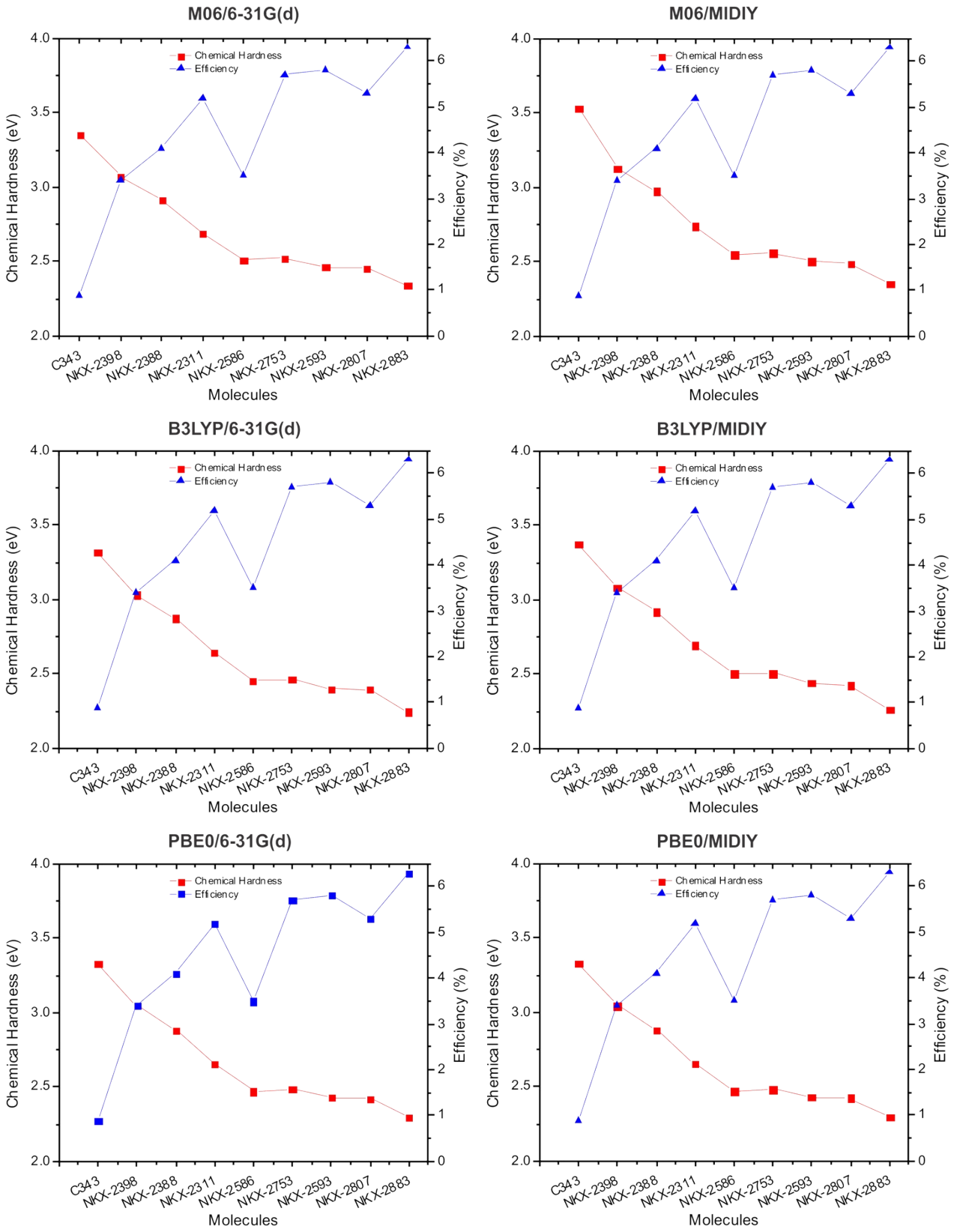

Figure S4. Chemical Hardness and experimental efficiency of coumarin molecules using M06, PBE0 and B3LYP functionals with 6-31G(d) and MIDIY basis sets. All graphs show that the lower chemical hardness, the higher conversion efficiency.

Table S6. Pearson correlation and P-Value of coumarin derivatives between the theoretical molecular properties and chemical reactivity, the oscillator streng and driving force of the electron injection (inject).

	M06/6-31G(d)				M06/MIDIY			
PARAMETER	**Jsc**	**Voc**	**η**	**inject**	**Jsc**	**Voc**	**η**	**inject**
Chemical	-0.960	-0.774	-0.977	0.955	-0.974	-0.804	0.987	0.971
Hardness	0.001	0.041	0	0.001	0	0.029	0	0
Electrophilicity	0.912	0.700	0.937	-0.990	0.808	0.533	0.848	-0.948
	0.004	0.080	0.002	0	0.028	0.218	0.016	0.001
Electron-	0.897	0.689	0.921	-0.993	0.726	0.431	0.772	-0.908
donator power	0.006	0.087	0.003	0	0.065	0.334	0.042	0.005
Electron-	0.911	0.691	0.938	-0.982	0.838	0.573	0.876	-0.956
acceptor power	0.004	0.086	0.002	0	0.019	0.178	0.01	0.001
Oscillator	0.717	0.845	0.693	-0.622	0.841	0.896	0.815	-0.721
strength	0.070	0.017	0.084	0.136	0.018	0.006	0.025	0.068
inject	-0.923	-0.738	-0.942		-0.938	-0.747	-0.957	
	0.003	0.058	0.002		0.002	0.054	0.001	
	B3LYP/6-31G(d)				**B3LYP/MIDIY**			
PARAMETER	**Jsc**	**Voc**	**η**	**inject**	**Jsc**	**Voc**	**η**	**inject**
Chemical	-0.954	-0.760	-0.972	0.955	-0.951	-0.752	-0.970	0.971
Hardness	0.001	0.048	0	0.001	0.001	0.051	0	0
Electrophilicity	0.901	0.676	0.929	-0.986	0.903	0.679	0.931	-0.984
	0.006	0.095	0.003	0	0.005	0.094	0.002	0
Electron-	0.888	0.667	0.916	-0.990	0.898	0.679	0.925	-0.986
donator power	0.008	0.102	0.004	0	0.006	0.093	0.003	0
Electron-	0.896	0.664	0.926	-0.975	0.890	0.655	0.921	-0.974
acceptor power	0.006	0.104	0.003	0	0.007	0.110	0.003	0
Oscillator	0.653	0.824	0.625	-0.537	0.778	0.873	0.745	-0.634
strength	0.112	0.023	0.134	0.214	0.039	0.010	0.055	0.126
inject	-0.919	-0.727	-0.939		-0.938	-0.744	-0.957	
	0.003	0.064	0.002		0.002	0.055	0.001	
	PBE0/6-31G(d)				**PBE0/MIDIY**			
PARAMETER	**Jsc**	**Voc**	**η**	**inject**	**Jsc**	**Voc**	**η**	**inject**
Chemical	-0.959	-0.771	-0.976	0.960	-0.955	-0.762	-0.973	0.973
Hardness	0.001	0.042	0	0.001	0.001	0.046	0	0
Electrophilicity	0.909	0.692	0.935	-0.989	0.915	0.694	0.941	-0.988
	0.005	0.085	0.002	0	0.004	0.084	0.002	0
Electron-	0.896	0.682	0.922	-0.992	0.911	0.695	0.936	-0.991
donator power	0.006	0.091	0.003	0	0.004	0.083	0.002	0
Electron-	0.906	0.681	0.934	-0.980	0.903	0.672	0.932	-0.979
acceptor power	0.005	0.092	0.002	0	0.005	0.098	0.002	0
Oscillator	0.711	0.848	0.687	-0.615	0.866	0.904	0.844	-0.764
strength	0.073	0.016	0.088	0.141	0.012	0.005	0.017	0.045
inject	-0.925	-0.737	-0.944		-0.942	-0.755	-0.960	
	0.003	0.059	0.001		0.001	0.050	0.001	

Cell contents: Pearson correlation and P-Value.