Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Antioxidant properties of several Coumarin-Chalcone hybrids from theoretical insights.

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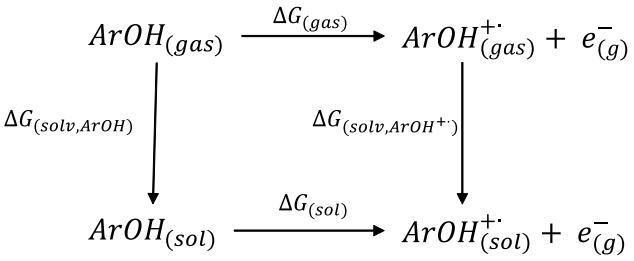
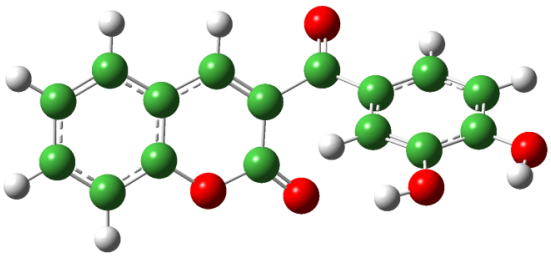
- Figure S1. Born-Haber thermodynamic cycle used to calculate $\Delta G_{(sol)}$ for a one-electron oxidation of a given phenolic species ArOH.
- Figure S2. B3LYP optimized geometries of all the considered coumarin-chalcone hybrids.
- Figure S3. Spin densities of the most stable radical species formed by H removal from the neutral form of each compound.
- Table S4. Bond dissociation enthalpies (BDE), O-H proton dissociation enthalpies (PDE), proton affinities (PA), electron transfer enthalpies (ETE) and adiabatic ionization potentials (IP) are reported in kcal/mol.
- Table S5. Energies of HOMO and LUMO for all compounds investigated, expressed in eV.
- Figure S6. Molecular surface contour plots for the highest occupied and lowest unoccupied molecular orbitals of all the investigated coumarin-chalcone derivatives.
- Figure S7. Molecular surface contour plots for the two highest occupied and lowest unoccupied molecular orbitals of coumarin and chalcone.
- Table S8. Main excitation energies (ΔE), oscillator strengths (f) and MO contribution (%) computed for **1**-**3**, **5**-**8** and **10** compounds in methanol by using three different exchange and correlation functionals. All electronic states belong to ^{1}A.


$ArOH_{(gas)}$
$\Delta G_{(gas)}$
$ArOH^{+\cdot}_{(gas)} + e^-_{(g)}$
$\Delta G_{(solv,ArOH)}$
$\Delta G_{(solv,ArOH^{+\cdot})}$
$ArOH_{(sol)}$
$\Delta G_{(sol)}$
$ArOH^{+\cdot}_{(sol)} + e^-_{(g)}$



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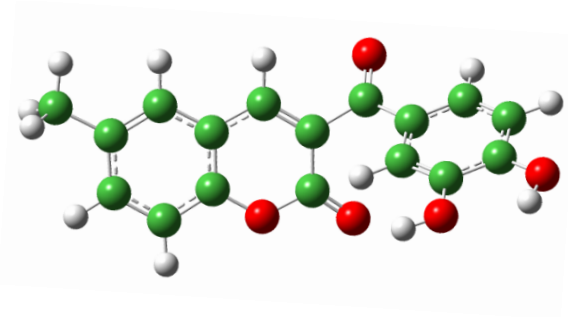

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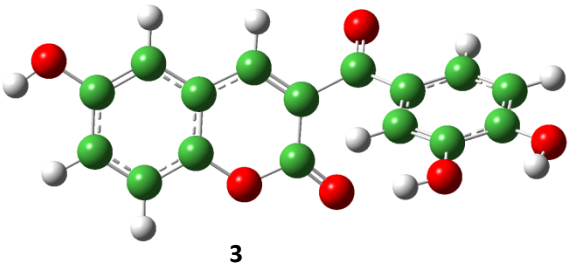

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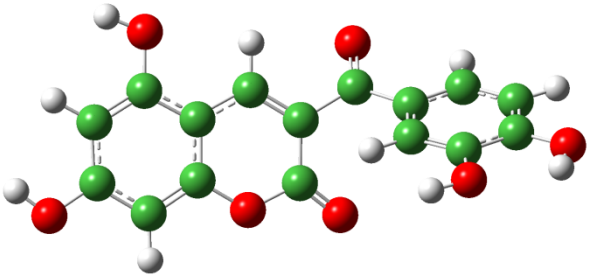

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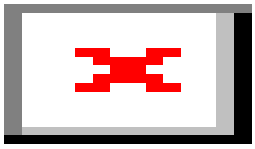

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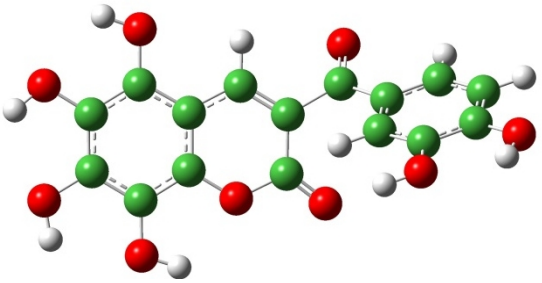

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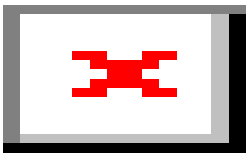

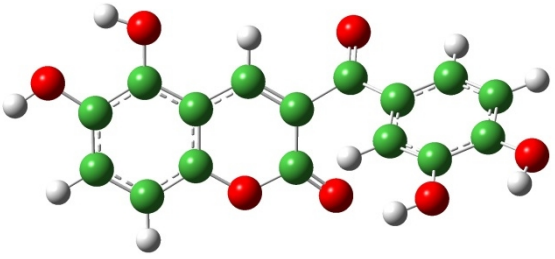

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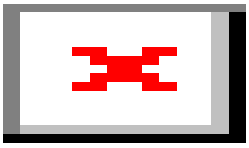

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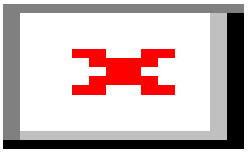

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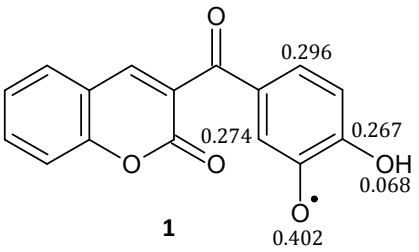

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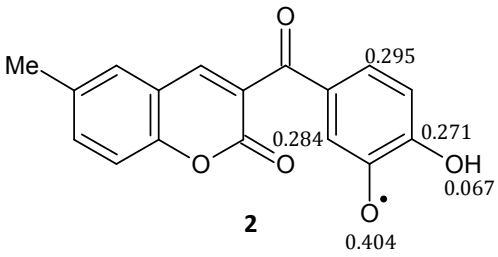

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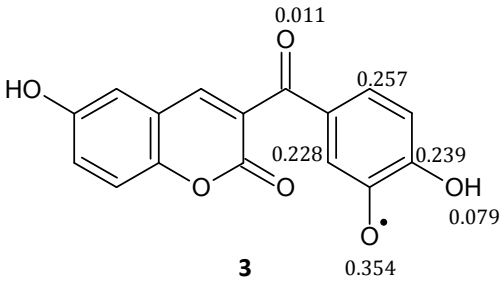

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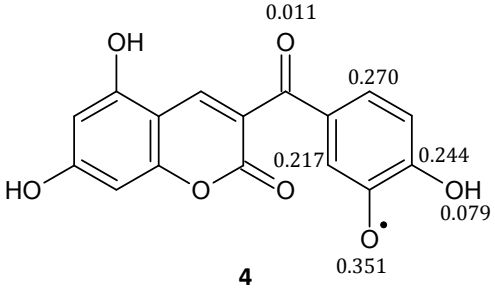

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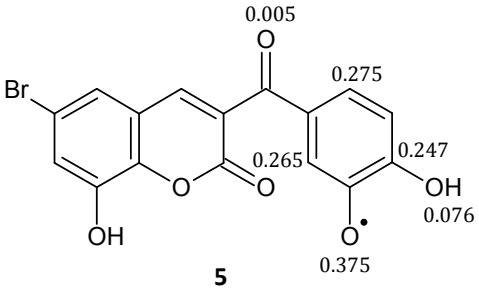

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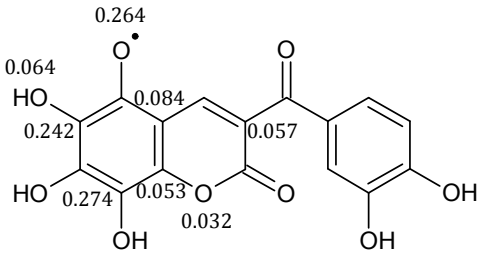

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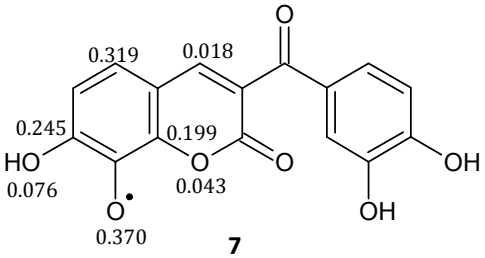

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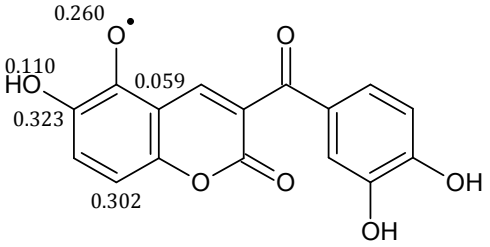

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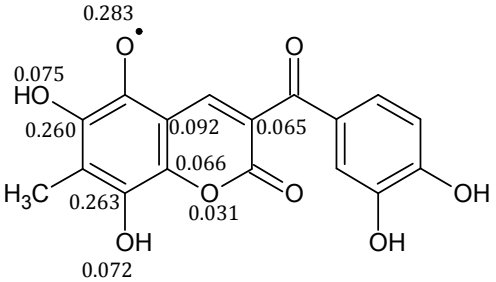

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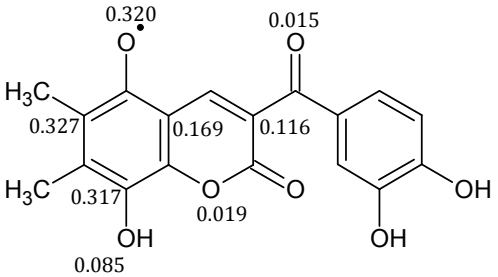

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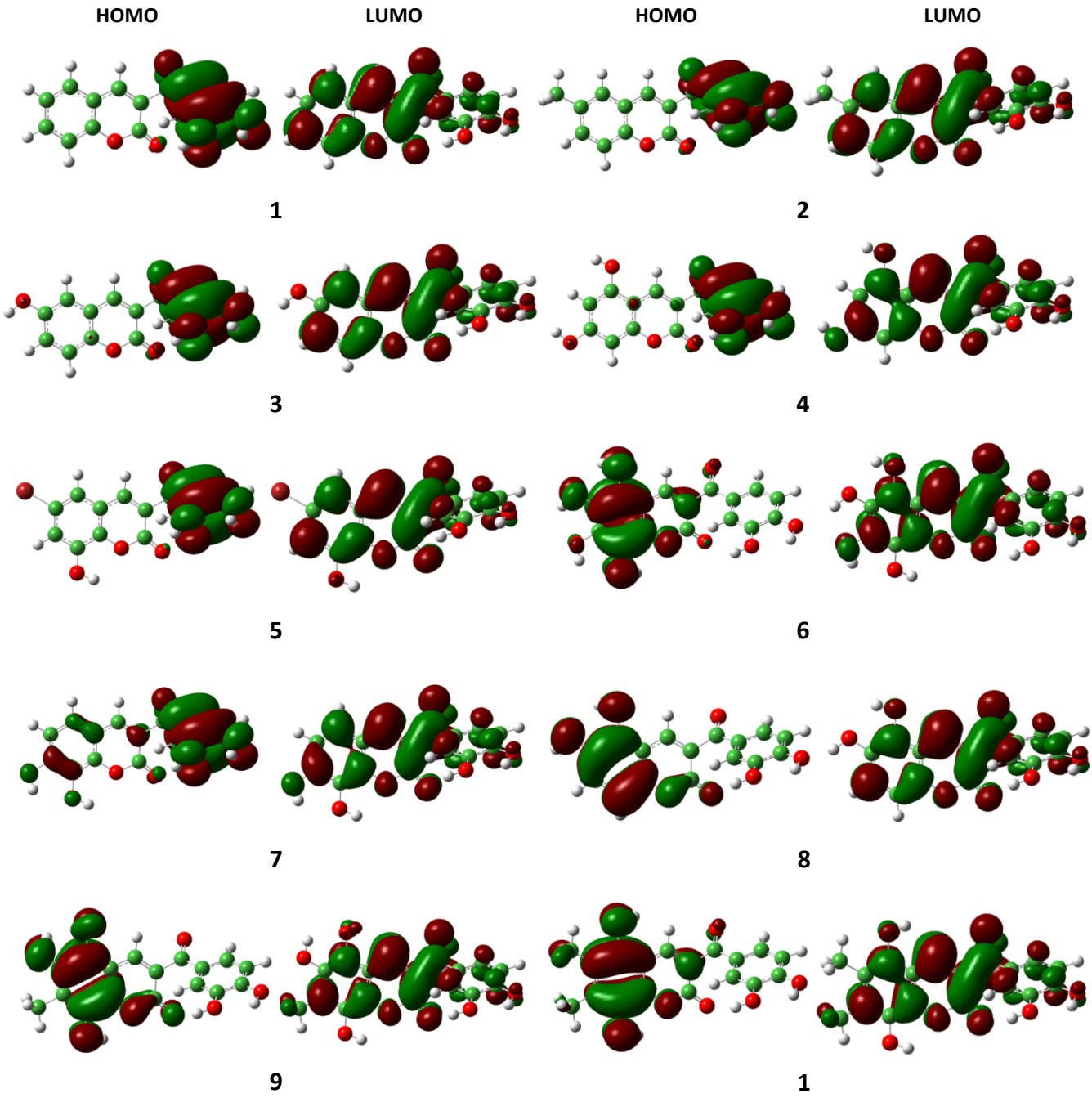
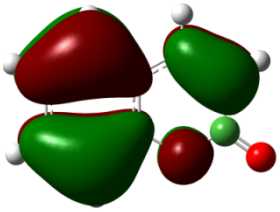
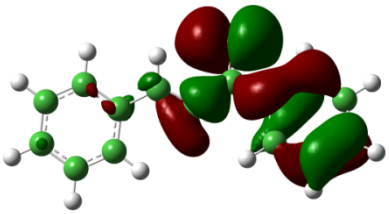
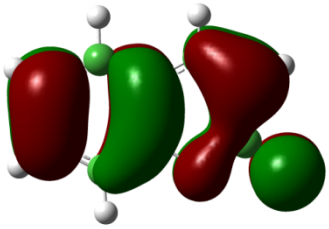
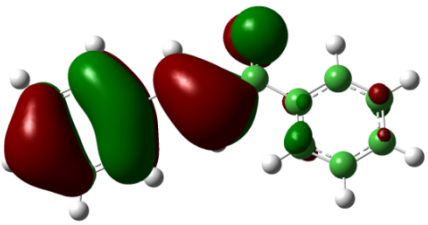
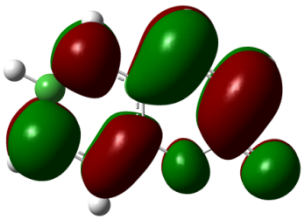
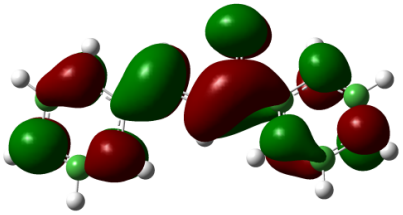
Compound	Site	BDE	PDE	PA	ETE	IP
DHMCoumarin	6OH	80.42	266.91	290.58	106.00	129.67
	7OH	80.96	267.45	287.59	109.53	
Helichrysetin	4OH	84.48	269.41	290.91	109.74	131.23
	4'OH	90.09	275.02	290.59	115.66	
	6'OH	99.48	284.41	296.30	119.35	
1	3'OH	82.27	257.43	293.01	105.43	141.00
	4'OH	82.39	257.55	287.94	110.61	
2	3'OH	82.28	264.72	293.11	105.33	133.72
	4'OH	82.39	264.83	288.14	110.41	
3	6OH	87.22	269.46	294.26	109.12	133.92
	3'OH	82.37	264.61	292.75	105.78	
	4'OH	82.48	264.72	287.78	110.86	
4	5OH	87.88	271.78	287.20	116.85	132.27
	7OH	89.27	273.17	287.28	118.15	
	3'OH	81.76	265.66	293.01	104.92	
	4'OH	81.84	265.67	288.94	108.91	
5	8OH	87.60	269.59	288.98	114.78	134.18
	3'OH	82.42	264.40	291.70	106.88	
	4'OH	82.52	264.51	287.61	110.07	
6	5OH	73.90	266.97	287.26	102.80	123.09
	6OH	74.95	268.02	289.05	102.06	
	7OH	77.35	270.42	282.81	110.70	
	8OH	74.59	267.66	293.89	96.87	
	3'OH	81.87	274.94	292.08	105.95	
	4'OH	81.75	274.82	287.69	110.22	
7	7OH	82.36	265.75	397.58	112.43	132.78
	8OH	80.75	264.13	397.59	107.49	
	3'OH	82.18	265.56	289.42	105.43	
	4'OH	82.17	265.55	286.10	109.74	
8	5OH	78.05	263.51	397.53	108.51	130.70
	6OH	79.35	264.82	287.83	103.85	
	3'OH	82.12	267.58	289.86	105.65	
	4'OH	82.13	267.59	291.67	110.61	
9	5OH	70.45	265.24	286.70	99.91	121.37
	6OH	74.27	269.07	291.71	98.72	
	8OH	77.12	271.92	294.07	99.22	
	3'OH	82.39	277.18	292.84	105.71	
	4'OH	82.28	277.07	288.28	110.17	
10	5OH	75.54	266.69	288.04	102.67	125.01
	8OH	78.19	269.34	295.44	98.91	
	3'OH	82.05	273.20	292.42	105.79	
	4'OH	81.93	273.09	286.97	111.13	

Compound	ε_{HOMO}	ε_{LUMO}	ΔE_{H-L}
1	-0.237	-0.098	0.139
2	-0.237	-0.096	0.141
3	-0.237	-0.098	0.139
4	-0.235	-0.094	0.141
5	-0.238	-0.102	0.136
6	-0.226	-0.096	0.130
7	-0.236	-0.096	0.140
8	-0.234	-0.098	0.136
9	-0.224	-0.099	0.125
10	-0.228	-0.099	0.129


HOMO
LUMO
HOMO
LUMO
1
2
3
4
5
6
7
8
9
1

	coumarin	chalcone
HOMO-1		
HOMO		
LUMO		

Comp.	MO contribution	*B3LYP*			*PBE0*			*wB97XD*		
		ΔE		*f*	ΔE		*f*	ΔE		*f*
		eV	nm		eV	nm		eV	nm	
1	H → L (70%)	3.27	379	0.060	3.45	359	0.076	3.91	317	0.069
	H-1 → L (53%)	3.59	345	0.167	3.67	337	0.152	4.13	300	0.611
	H-3 → L (43%); H-4 → L (31%)	3.83	324	0.126	3.94	315	0.193	4.61	269	0.149
	H → L+1 (46%); H-4 → L(22%)	4.05	306	0.301	4.20	295	0.296			
2	H → L (70%)	3.30	376	0.070	3.48	357	0.090	3.89	318	0.134
	H-1 → L (62%)	3.54	350	0.214	3.64	341	0.208	4.05	306	0.382
	H → L+1 (44%); H-3 → L (15%)	4.03	308	0.385	4.16	298	0.385	4.31	288	0.223
3	H → L (69%)	3.26	380	0.092	3.43	362	0.204	3.80	326	0.257
	H-1 → L (69%)	3.33	372	0.099	3.47	358	0.020	4.27	290	0.392
	H → L+1 (42%); H-4 → L (32%)	4.00	310	0.200	4.15	299	0.368			
	H-1 → L+1 (52%)	4.07	305	0.242	4.26	291	0.113	4.56	272	0.221
	H-3 → L (42%); H → L+1 (30%)	4.28	290	0.155	4.41	281	0.125			
5	H → L (70%)	3.17	391	0.043	3.35	370	0.056	4.20	295	0.634
	H-2 → L (49%); H-4 → L (41%);	3.60	344	0.131	4.02	308	0.318	4.41	281	0.174
	H → L+1 (43%); H-2 → L (36%)	3.91	317	0.485	4.04	307	0.239	4.91	252	0.116
6	H → L (70%)	2.94	421	0.059	3.07	404	0.067	3.53	350	0.181
	H-1 → L (70%)	3.28	378	0.148	3.46	359	0.335	3.80	327	0.385
	H-2 → L (65%)	3.39	365	0.361	3.50	254	0.208	4.34	286	0.112
	H-1 → L+1 (58%); H-3 → L (24%)	4.15	299	0.139	4.32	287	0.160			
7	H → L (70%)	3.28	377	0.148	3.46	358	0.293	3.81	325	0.454
	H-1 → L(66%)	3.40	365	0.322	3.51	353	0.234			
	H-4 → L(52%); H-4 → L+1 (21%)	3.80	326	0.177	3.89	319	0.191	4.00	310	0.388
	H → L+1 (52%); H-1 → L+1 (27%)	4.15	299	0.113	4.32	286	0.122			
8	H → L (70%)	3.10	400	0.026	3.23	384	0.030	3.72	334	0.053
	H-2 → L (67%); H-4 → L+1(15%)	3.54	350	0.228	3.63	342	0.216	3.87	321	0.128
	H-4 → L(49%); H-2 → L(34%)	3.84	323	0.209	3.94	315	0.323	4.08	304	0.683
	H → L+1(65%)	4.01	309	0.168	4.24	292	0.123			
10	H → L (70%)	2.81	442	0.092	2.93	424	0.103	3.39	366	0.192
	H-2 → L (61%)	3.50	354	0.321	3.59	345	0.309	3.85	322	0.188
	H-4 → L (53%); H-2 → L (27%)	3.80	326	0.214	3.84	323	0.110	4.01	309	0.479
	H-1 → L+1 (61%)	4.13	300	0.112	3.95	314	0.146			