

Supporting Information

Electrophilicity ω and Nucleophilicity N Scales for Cationic and Anionic Species

Luis R. Domingo,^{1*} Mar Ríos-Gutiérrez² and Patricia Pérez³

¹ Avd. Tirso de Molina 20, 46015, Valencia, Spain.

² Department of Organic Chemistry, University of Valencia, Dr. Moliner 50, 46100 Burjassot, Valencia, Spain.

³ Universidad Andres Bello, Facultad de Ciencias Exactas, Departamento de Ciencias Químicas, Centro de Química Teórica & Computacional. Av. República 275, 8370146, Chile.

E-mail: luisrdomingo@gmail.com

DOI: 10.58332/ scirad2025v4i1a01

Index

- S3** Figure S1 with the plot of the B3LYP/6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo for the set of twelve selected molecules.
- S4** Figure S2 with the plot of the MPWB1K/6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo for the set of twelve selected molecules.
- S5** Figure S3 with the plot of the M06-2X /6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo for the set of twelve selected molecules.
- S6** Figure S4 with the plot of the ω B97X-D/6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo for the set of twelve selected molecules.
- S7** Table S1 with the B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in vacuo of compounds **1-20**.
- S8** Table S2 with the B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for compounds **1-20**.
- S9** Table S3 with the B3LYP/6-311G(d.p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for compounds **1-20**.
- S10** Table S4 with the MPWB1K/6-311G(d.p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for compounds **1-20**.
- S11** Table S5 with the M06-2X/6-311G(d.p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for compounds **1-20**.

- S12** Table S6 with the ω B97X-D/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for compounds **1-20**.
- S13** Table S7 with the B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in vacuo for cationic species **21 – 25** and anionic species **26 – 30**.
- S14** Table S8 with the B3LYP/6-311++G(d,p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in vacuo for cationic species **21 – 25** and anionic species **26 – 30**.
- S15** Table S9 with the B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for cationic species **21 – 25** and anionic species **26 – 30**. **S8**.
- S16** Table S10 with the B3LYP/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for cationic species **21 – 25** and anionic species **26 – 30**.
- S17** Table S11 with the MPWB1K/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω , and nucleophilicity N indices computed in DMSO for cationic species **21 – 25** and anionic species **26 – 30**.
- S18** Table 12 with the M06-2X/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for cationic species **21 – 25** and anionic species **26 – 30**.
- S19** Table 13 with the ω B97X-D/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices computed in DMSO for cationic species **21 – 25** and anionic species **26 – 30**.

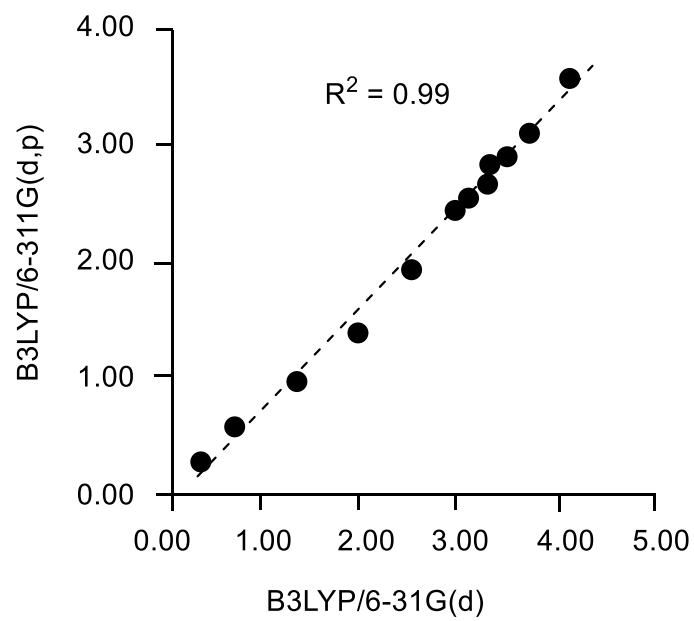


Fig. S1. Plot of the B3LYP/6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo, in eV, for the set of twelve selected molecules.

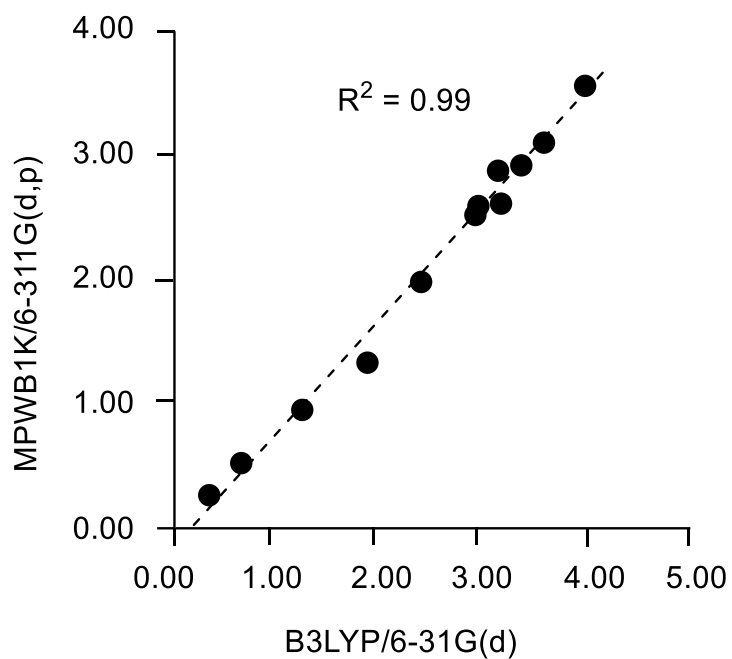


Fig. S2. Plot of the MPWB1K/6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo, in eV, for the set of twelve selected molecules.

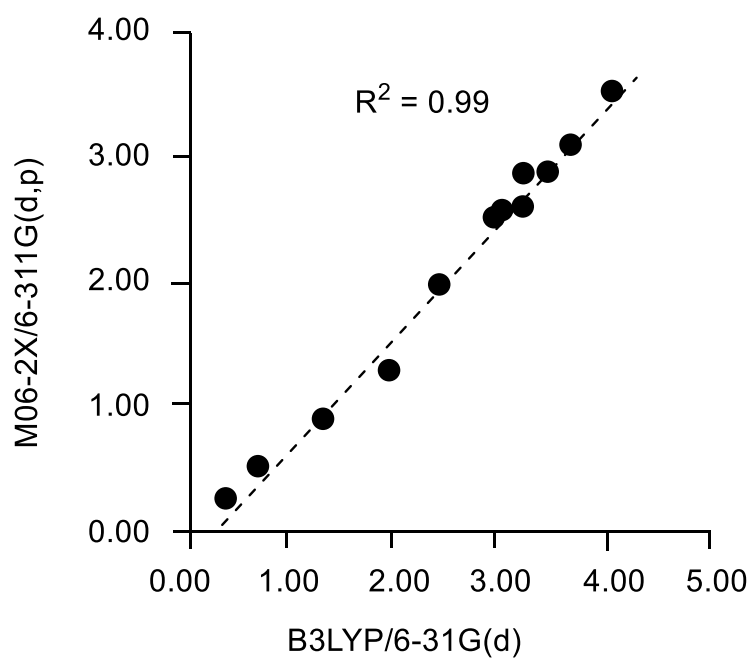


Fig. S3. Plot of the M06-2X /6-311G(d,p) nucleophilicity *N* indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity *N* indices computed in vacuo, in eV, for the set of twelve selected molecules.

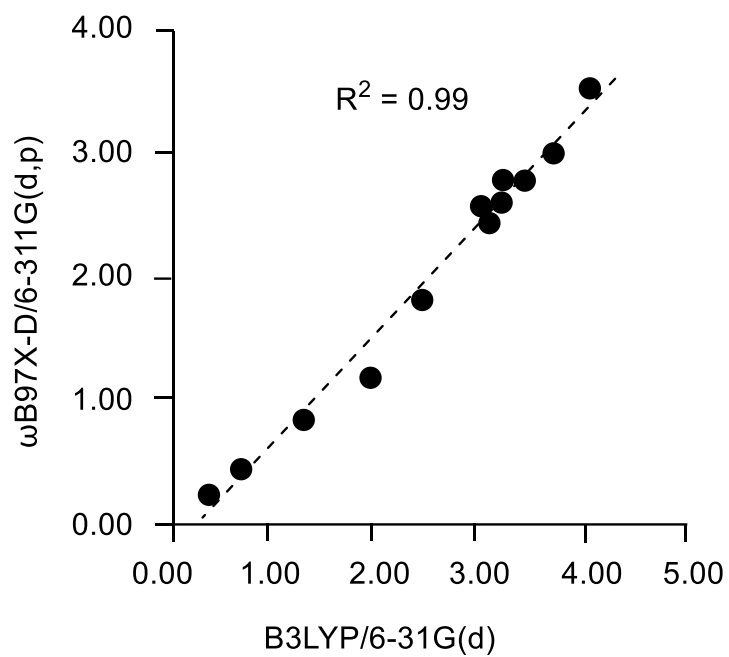


Fig. S4. Plot of the ω B97X-D/6-311G(d,p) nucleophilicity N indices computed in DMSO versus the standard B3LYP/6-31G(d) nucleophilicity N indices computed in vacuo, in eV, for the set of twelve selected molecules.

Table S1. B3LYP/6-31G(d) total electronic energy and ε_{H} and ε_{L} energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in vacuo for compounds **1-20**.

	Energy	ε_{H}	ε_{L}	μ	η	ω	N
1	-447.518342	-0.3352	-0.1823	-7.04	4.16	5.96	0.00
2	-355.295391	-0.3230	-0.1498	-6.43	4.71	4.39	0.33
3	-516.484645	-0.3352	-0.1205	-6.20	5.84	3.29	0.00
4	-263.062686	-0.3112	-0.1037	-5.64	5.65	2.82	0.65
5	-283.087901	-0.2958	-0.0957	-5.33	5.45	2.61	1.07
6	-191.911972	-0.2571	-0.0650	-4.38	5.23	1.84	2.12
7	-170.831551	-0.2892	-0.0563	-4.70	6.34	1.74	1.25
8	-231.234882	-0.2479	-0.0569	-4.15	5.20	1.66	2.38
9	-306.466612	-0.2719	-0.0452	-4.31	6.17	1.51	1.72
10	-155.992140	-0.2290	-0.0225	-3.42	5.62	1.04	2.89
11	-195.310448	-0.2261	-0.0191	-3.34	5.63	0.99	2.97
12	-194.101062	-0.2115	-0.0099	-3.01	5.49	0.83	3.37
13	-232.248651	-0.2463	0.0037	-3.30	6.80	0.80	2.42
14	-78.587459	-0.2666	0.0188	-3.37	7.77	0.73	1.87
15	-230.020584	-0.2245	0.0197	-2.79	6.64	0.58	3.01
16	-77.325646	-0.2819	0.0524	-3.12	9.10	0.54	1.45
17	-235.856670	-0.2178	0.0373	-2.46	6.94	0.43	3.19
18	-193.110421	-0.2185	0.0384	-2.45	6.99	0.43	3.18
19	-210.165894	-0.2015	0.0510	-2.05	6.87	0.31	3.64
20	-212.562351	-0.1884	0.0507	-1.87	6.51	0.27	4.00

Table S2. B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for compounds **1-20**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
1	-447.530042	-0.3214	-0.1664	-6.64	4.22	5.22	0.38
2	-355.307554	-0.3115	-0.1354	-6.08	4.79	3.86	0.64
3	-516.501059	-0.3201	-0.1126	-5.89	5.65	3.07	0.41
4	-263.072842	-0.3023	-0.0914	-5.36	5.74	2.50	0.89
5	-283.095004	-0.3009	-0.0975	-5.42	5.53	2.65	0.93
6	-191.917624	-0.2613	-0.0643	-4.43	5.36	1.83	2.01
7	-170.838534	-0.2863	-0.0519	-4.60	6.38	1.66	1.33
8	-231.240804	-0.2539	-0.0581	-4.25	5.33	1.69	2.21
9	-306.472037	-0.2801	-0.0485	-4.47	6.30	1.59	1.50
10	-155.994093	-0.2319	-0.0254	-3.50	5.62	1.09	2.81
11	-195.312260	-0.2293	-0.0225	-3.43	5.63	1.04	2.88
12	-194.103077	-0.2155	-0.0133	-3.11	5.50	0.88	3.26
13	-232.251256	-0.2507	-0.0008	-3.42	6.80	0.86	2.30
14	-78.588637	-0.2696	0.0160	-3.45	7.77	0.77	1.79
15	-230.023575	-0.2282	0.0154	-2.90	6.63	0.63	2.91
16	-77.329018	-0.2874	0.0481	-3.26	9.13	0.58	1.30
17	-235.857620	-0.2202	0.0354	-2.52	6.95	0.45	3.13
18	-193.114242	-0.2233	0.0334	-2.58	6.99	0.48	3.04
19	-210.172014	-0.2083	0.0458	-2.21	6.91	0.35	3.45
20	-212.565390	-0.1928	0.0447	-2.02	6.46	0.31	3.88

Table S3. B3LYP/6-311G(d,p) total electronic energy and ε_H and ε_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for compounds **1-20**.

	Energy	ε_H	ε_L	μ	η	ω	N
1	-447.642879	-0.3299	-0.1727	-6.84	4.28	5.47	0.15
2	-355.399196	-0.3200	-0.1419	-6.28	4.85	4.08	0.41
3	-516.656779	-0.3291	-0.1209	-6.12	5.66	3.31	0.17
4	-191.974076	-0.2688	-0.0724	-4.64	5.35	2.02	1.81
5	-283.176849	-0.3096	-0.1038	-5.62	5.60	2.82	0.70
6	-263.142812	-0.3109	-0.0990	-5.58	5.77	2.70	0.66
7	-170.886789	-0.2956	-0.0610	-4.85	6.38	1.84	1.08
8	-231.307768	-0.2629	-0.0668	-4.49	5.34	1.89	1.97
9	-306.560597	-0.2892	-0.0570	-4.71	6.32	1.76	1.25
10	-156.040659	-0.2424	-0.0370	-3.80	5.59	1.29	2.52
11	-195.368456	-0.2394	-0.0344	-3.72	5.58	1.24	2.61
12	-194.155992	-0.2264	-0.0245	-3.41	5.50	1.06	2.96
13	-232.311381	-0.2609	-0.0138	-3.74	6.72	1.04	2.02
14	-78.615226	-0.2806	0.0011	-3.80	7.66	0.94	1.49
15	-230.086603	-0.2385	0.0026	-3.21	6.56	0.79	2.63
16	-77.358189	-0.3017	0.0306	-3.69	9.04	0.75	0.91
17	-235.923458	-0.2279	0.0244	-2.77	6.86	0.56	2.92
18	-193.172594	-0.2330	0.0185	-2.92	6.84	0.62	2.78
19	-210.232471	-0.2193	0.0315	-2.55	6.82	0.48	3.15
20	-212.627375	-0.2006	0.0291	-2.33	6.25	0.44	3.66

Table S4. MPWB1K/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for compounds **1-20**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
1	-447.414306	-0.3681	-0.1416	-6.94	6.16	3.90	0.00
2	-355.213384	-0.3582	-0.1075	-6.34	6.82	2.94	0.26
3	-516.451750	-0.3683	-0.0824	-6.13	7.78	2.42	-0.01
4	-262.999670	-0.3489	-0.0608	-5.58	7.84	1.98	0.52
5	-283.030745	-0.3597	-0.0606	-5.72	8.14	2.01	0.22
6	-191.864140	-0.3204	-0.0306	-4.78	7.88	1.45	1.29
7	-170.784844	-0.3340	-0.0207	-4.83	8.52	1.37	0.92
8	-231.173390	-0.3142	-0.0262	-4.63	7.84	1.37	1.46
9	-306.398267	-0.3342	-0.0169	-4.78	8.64	1.32	0.92
10	-155.933377	-0.2764	0.0013	-3.74	7.56	0.93	2.49
11	-195.237184	-0.2735	0.0033	-3.68	7.53	0.90	2.57
12	-194.042271	-0.2612	0.0138	-3.37	7.48	0.76	2.90
13	-232.176956	-0.2957	0.0223	-3.72	8.65	0.80	1.97
14	-78.554208	-0.3198	0.0439	-3.75	9.90	0.71	1.31
15	-229.969802	-0.2729	0.0458	-3.09	8.67	0.55	2.59
16	-77.304094	-0.3437	0.0749	-3.66	11.39	0.59	0.66
17	-235.762723	-0.2626	0.0637	-2.71	8.88	0.41	2.87
18	-193.056377	-0.2724	0.0602	-2.89	9.05	0.46	2.60
19	-210.118832	-0.2533	0.0739	-2.44	8.90	0.33	3.12
20	-212.488317	-0.2374	0.0678	-2.31	8.31	0.32	3.55

Table S5. M06-2X/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for compounds **1-20**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
1	-447.479643	-0.3840	-0.1362	-7.08	6.74	3.72	0.00
2	-355.264245	-0.3744	-0.1022	-6.48	7.41	2.84	0.26
3	-516.471013	-0.3836	-0.0772	-6.27	8.34	2.36	0.01
4	-263.036640	-0.3654	-0.0564	-5.74	8.41	1.96	0.51
5	-283.052672	-0.3765	-0.0545	-5.86	8.76	1.96	0.21
6	-191.881939	-0.3396	-0.0258	-4.97	8.54	1.45	1.21
7	-170.807869	-0.3507	-0.0165	-5.00	9.09	1.37	0.91
8	-231.195494	-0.3327	-0.0218	-4.82	8.46	1.37	1.40
9	-306.425902	-0.3511	-0.0129	-4.95	9.20	1.33	0.90
10	-155.951735	-0.2933	0.0038	-3.94	8.09	0.96	2.47
11	-195.260187	-0.2903	0.0055	-3.87	8.05	0.93	2.55
12	-194.059654	-0.2793	0.0157	-3.59	8.03	0.80	2.85
13	-232.199488	-0.3123	0.0227	-3.94	9.12	0.85	1.95
14	-78.563827	-0.3367	0.0465	-3.95	10.43	0.75	1.29
15	-229.989291	-0.2898	0.0480	-3.29	9.19	0.59	2.56
16	-77.318501	-0.3604	0.0785	-3.84	11.94	0.62	0.64
17	-235.788642	-0.2797	0.0657	-2.91	9.40	0.45	2.84
18	-193.076206	-0.2897	0.0613	-3.11	9.55	0.51	2.57
19	-210.138404	-0.2704	0.0754	-2.65	9.41	0.37	3.09
20	-212.513886	-0.2552	0.0671	-2.56	8.77	0.37	3.51

Table S6. ω B97X-D/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for compounds **1-20**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
1	-447.461178	-0.4047	-0.1060	-6.95	8.13	2.97	-1.89
2	-355.254712	-0.3955	-0.0720	-6.36	8.80	2.30	-1.64
3	-516.491614	-0.4058	-0.0459	-6.15	9.80	1.93	-1.92
4	-263.035882	-0.3875	-0.0254	-5.62	9.85	1.60	-1.42
5	-283.076183	-0.3952	-0.0272	-5.75	10.01	1.65	-1.63
6	-191.901210	-0.3505	0.0036	-4.72	9.64	1.16	-0.42
7	-170.816016	-0.3734	0.0142	-4.89	10.55	1.13	-1.04
8	-231.223422	-0.3441	0.0085	-4.57	9.60	1.09	-0.24
9	-306.452542	-0.3722	0.0188	-4.81	10.64	1.09	-1.01
10	-155.975923	-0.3174	0.0360	-3.83	9.62	0.76	0.48
11	-195.292779	-0.3141	0.0382	-3.75	9.59	0.73	0.57
12	-194.083818	-0.3034	0.0495	-3.45	9.60	0.62	0.87
13	-232.222045	-0.3363	0.0573	-3.80	10.71	0.67	-0.03
14	-78.580882	-0.3609	0.0789	-3.84	11.97	0.62	-0.70
15	-230.003867	-0.3147	0.0799	-3.19	10.74	0.48	0.56
16	-77.322339	-0.3836	0.1091	-3.73	13.41	0.52	-1.32
17	-235.841401	-0.3029	0.0993	-2.77	10.94	0.35	0.88
18	-193.101247	-0.3106	0.0954	-2.93	11.05	0.39	0.67
19	-210.156796	-0.2953	0.1074	-2.56	10.96	0.30	1.09
20	-212.551230	-0.2765	0.1038	-2.35	10.35	0.27	1.60

Table S7. B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in vacuo for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
21	-39.480387	-0.7883	-0.4854	-17.33	8.24	18.22	-12.33
22	-157.554197	-0.5868	-0.3231	-12.38	7.17	10.68	-6.85
23	-116.972214	-0.5736	-0.3820	-13.00	5.21	16.21	-6.49
24	-270.662267	-0.4595	-0.3253	-10.68	3.65	15.61	-3.38
25	-154.090735	-0.5059	-0.2207	-9.89	7.76	6.30	-4.65
26	-39.790295	0.1372	0.3726	6.94	6.41	3.76	12.85
27	-157.757749	0.1030	0.2775	5.18	4.75	2.82	11.92
28	-117.241696	0.1027	0.3082	5.59	5.59	2.79	11.91
29	-270.921301	0.0636	0.2036	3.64	3.81	1.74	10.85
30	-153.207231	0.0602	0.3105	5.04	6.81	1.87	10.76

Table S8. B3LYP/6-311++G(d,p) total electronic energy and ε_{H} and ε_{L} energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in vacuo for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ε_{H}	ε_{L}	μ	η	ω	N
21	-39.491472	-0.7872	-0.4872	-17.34	8.16	18.42	-11.93
22	-157.596766	-0.5893	-0.3245	-12.43	7.21	10.73	-6.54
23	-117.001545	-0.5786	-0.3873	-13.14	5.21	16.59	-6.25
24	-270.725072	-0.4665	-0.3323	-10.87	3.65	16.17	-3.20
25	-154.147989	-0.5143	-0.2404	-10.27	7.45	7.07	-4.50
26	-39.856214	0.0655	0.1399	2.79	2.03	1.93	11.27
27	-157.840056	0.0466	0.1115	2.15	1.77	1.31	10.76
28	-117.314066	0.0547	0.1258	2.46	1.94	1.56	10.98
29	-271.017948	0.0317	0.1033	1.84	1.95	0.86	10.35
30	-153.289946	0.0133	0.1316	1.97	3.22	0.60	9.85

Table S9. B3LYP/6-31G(d) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
21	-39.595246	-0.5616	-0.2554	-11.12	8.33	7.41	-6.54
22	-157.639859	-0.4183	-0.1517	-7.76	7.25	4.15	-2.64
23	-117.064462	-0.3902	-0.1976	-8.00	5.24	6.10	-1.88
24	-270.739275	-0.3092	-0.1729	-6.56	3.71	5.80	0.33
25	-154.193194	-0.3226	-0.0299	-4.80	7.96	1.44	-0.04
26	-39.908180	-0.0899	0.1664	1.04	6.97	0.08	6.30
27	-157.847320	-0.0736	0.1169	0.59	5.18	0.03	6.74
28	-117.338814	-0.0822	0.1273	0.61	5.70	0.03	6.50
29	-271.005919	-0.0954	0.0461	-0.67	3.85	0.06	6.15
30	-153.308504	-0.1323	0.1177	-0.20	6.80	0.00	5.14

Table S10. B3LYP/6-311G(d,p) total electronic energy and ϵ_{H} and ϵ_{L} energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ϵ_{H}	ϵ_{L}	μ	η	ω	N
21	-39.606177	-0.5610	-0.2576	-11.14	8.26	7.51	-6.29
22	-157.681774	-0.4214	-0.1537	-7.83	7.29	4.20	-2.50
23	-117.093583	-0.3953	-0.2026	-8.13	5.24	6.31	-1.79
24	-270.801034	-0.3158	-0.1793	-6.74	3.72	6.10	0.38
25	-154.248506	-0.3287	-0.0384	-4.99	7.90	1.58	0.03
26	-39.945248	-0.1187	0.0804	-0.52	5.42	0.02	5.74
27	-157.910781	-0.0970	0.0609	-0.49	4.30	0.03	6.33
28	-117.391798	-0.1027	0.0787	-0.33	4.94	0.01	6.18
29	-271.089126	-0.1114	0.0280	-1.13	3.79	0.17	5.94
30	-153.367183	-0.1494	0.0895	-0.81	6.50	0.05	4.91

Table S11. MPWB1K/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
21	-39.572938	-0.6117	-0.2067	-11.13	11.02	5.63	-6.63
22	-157.569711	-0.4667	-0.1137	-7.90	9.61	3.25	-2.69
23	-117.010673	-0.4321	-0.1643	-8.11	7.29	4.52	-1.75
24	-270.642032	-0.3500	-0.1489	-6.79	5.47	4.21	0.49
25	-154.160768	-0.3677	0.0068	-4.91	10.19	1.18	0.01
26	-39.902307	-0.1584	0.1158	-0.58	7.46	0.02	5.70
27	-157.790596	-0.1311	0.0951	-0.49	6.16	0.02	6.44
28	-117.302624	-0.1332	0.1128	-0.28	6.69	0.01	6.39
29	-270.926686	-0.1379	0.0631	-1.02	5.47	0.09	6.26
30	-153.275821	-0.1857	0.1247	-0.83	8.45	0.04	4.96

Table S12. M06-2X/6-311G(d,p) total electronic energy and ϵ_H and ϵ_L energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ϵ_H	ϵ_L	μ	η	ω	N
21	-39.577632	-0.6254	-0.1903	-11.10	11.84	5.20	-6.57
22	-157.580258	-0.4793	-0.1075	-7.98	10.12	3.15	-2.59
23	-117.018654	-0.4466	-0.1577	-8.22	7.86	4.30	-1.70
24	-270.662466	-0.3665	-0.1465	-6.98	5.99	4.07	0.48
25	-154.172296	-0.3844	0.0096	-5.10	10.72	1.21	-0.01
26	-39.912192	-0.1721	0.1208	-0.70	7.97	0.03	5.77
27	-157.814295	-0.1463	0.0966	-0.68	6.61	0.03	6.47
28	-117.322300	-0.1477	0.1146	-0.45	7.14	0.01	6.43
29	-270.961137	-0.1531	0.0634	-1.22	5.89	0.13	6.28
30	-153.293926	-0.2013	0.1276	-1.00	8.95	0.06	4.97

Table S13. ω B97X-D/6-311G(d,p) total electronic energy and ε_{H} and ε_{L} energies, in a.u., electronic chemical potential μ , chemical hardness η , and electrophilicity ω and nucleophilicity N indices, in eV, computed in DMSO for cationic species **21** – **25** and anionic species **26** – **30**.

	Energy	ε_{H}	ε_{L}	μ	η	ω	N
21	-39.606177	-0.5610	-0.2576	-11.14	8.26	7.51	-6.29
22	-157.681774	-0.4214	-0.1537	-7.83	7.29	4.20	-2.50
23	-117.093583	-0.3953	-0.2026	-8.13	5.24	6.31	-1.79
24	-270.801034	-0.3158	-0.1793	-6.74	3.72	6.10	0.38
25	-154.248506	-0.3287	-0.0384	-4.99	7.90	1.58	0.03
26	-39.945248	-0.1187	0.0804	-0.52	5.42	0.02	5.74
27	-157.910781	-0.0970	0.0609	-0.49	4.30	0.03	6.33
28	-117.391798	-0.1027	0.0787	-0.33	4.94	0.01	6.18
29	-271.089126	-0.1114	0.0280	-1.13	3.79	0.17	5.94
30	-153.367183	-0.1494	0.0895	-0.81	6.50	0.05	4.91