SUPPLIMENTARY MATERIALS

The interplay between diradical character and stability in organic molecules

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Table S1. Dataset used for the K-means clustering of quinone methides: REPE [β] – resonance energy per π-electron, ΔE_i [β^{-1}] and ΔE_{ij} [β^{-1}] – Hückel reactivity indices, P – generalized stability index, I [eV] – vertical ionization potential, A [eV] – vertical electron affinity, χ [eV] – electronegativity, η [eV] – hardness, δ [eV^{-1}] – softness, ω [eV] – electrophilicity, f^{-}_{max} – largest atomic Fukui index for electrophilic attack, f^{+}_{max} largest atomic Fukui index for nucleophilic attack, f^{0}_{max} – largest atomic Fukui index for radical attack; Lab_s – laboratory stability and its corresponding code.

	REPE	ΔE_i	ΔE_{ij}	P	I	A	χ	η	δ	ω	DRC	f^{-}_{max}	f^{+}_{max}	f^{0}_{max}	Code	LAB_s
Ia	0.0340	1.6139	0.471	19.6	8.71	0.49	4.60	8.22	0.12	1.28	0.114	0.120	0.160	0.140	1	unstable
Ib	0.0442	1.2240	0.275	57.4	7.26	1.05	4.16	6.22	0.16	1.39	0.198	0.059	0.048	0.054	3	stable
IIa	0.0338	1.5847	0.451	20.7	8.29	0.59	4.44	7.70	0.13	1.28	0.152	0.127	0.152	0.140	1	unstable
IIb	0.0356	1.2670	0.292	42.1	6.92	1.07	4.00	5.86	0.17	1.36	0.257	0.078	0.059	0.066	2	moderately stable
IIIa	0.0472	1.3277	0.387	40.2	8.03	0.61	4.32	7.42	0.13	1.26	0.107	0.096	0.127	0.111	2	moderately stable
IIIb	0.0410	1.0853	0.264	67.7	6.99	0.88	3.93	6.11	0.16	1.27	0.140	0.059	0.058	0.050	3	stable
IVa	0.0470	1.3868	0.421	35.2	7.81	0.58	4.19	7.23	0.14	1.22	0.114	0.108	0.137	0.122	4	-
IVb	0.0414	1.1182	0.280	57.8	6.77	1.03	3.90	5.74	0.17	1.32	0.201	0.074	0.049	0.061	3	stable
Va	0.0255	1.9846	0.595	9.4	7.67	1.17	4.42	6.51	0.15	1.50	0.275	0.138	0.127	0.133	4	-
Vb	0.0395	1.4574	0.319	37.2	6.64	1.52	4.08	5.12	0.20	1.62	0.375	0.077	0.051	0.064	2	moderately stable
VIa	0.0274	1.9117	0.526	11.9	7.16	1.32	4.24	5.84	0.17	1.54	0.394	0.090	0.125	0.107	1	unstable
VIb	0.0329	1.4998	0.326	29.4	6.22	1.56	3.89	4.66	0.21	1.63	0.508	0.080	0.046	0.063	2	moderately stable
VIIa	0.0470	1.3772	0.423	35.3	8.24	0.52	4.38	7.72	0.13	1.24	0.095	0.139	0.135	0.137	4	-
VIIb	0.0480	1.0643	0.259	76.2	7.03	1.03	4.03	6.00	0.17	1.35	0.183	0.063	0.049	0.056	3	stable
VIII	0.0277	1.8897	0.590	10.9	7.19	1.36	4.28	5.83	0.17	1.57	0.416	0.117	0.106	0.111	4	-
IX	0.0271	1.8806	0.543	11.6	7.46	1.29	4.37	6.17	0.16	1.55	0.348	0.108	0.111	0.109	4	-
X	0.0510	0.9220	0.242	9.3	7.26	1.22	4.24	6.05	0.17	1.49	0.346	0.125	0.122	0.124	4	-
XIa	0.0267	1.9819	0.633	60.0	7.87	0.47	4.17	7.40	0.14	1.17	0.072	0.127	0.100	0.114	3	stable
XIb	0.0539	1.1758	0.334	100.0	7.20	0.60	3.90	6.61	0.15	1.15	0.074	0.049	0.046	0.043	3	stable
XII	0.0539	1.2410	0.376	50.5	7.71	0.59	4.15	7.12	0.14	1.21	0.084	0.080	0.120	0.100	2	moderately stable
XIII	0.0305	2.2465	0.665	8.9	7.10	1.54	4.32	5.56	0.18	1.68	0.393	0.120	0.112	0.116	4	-

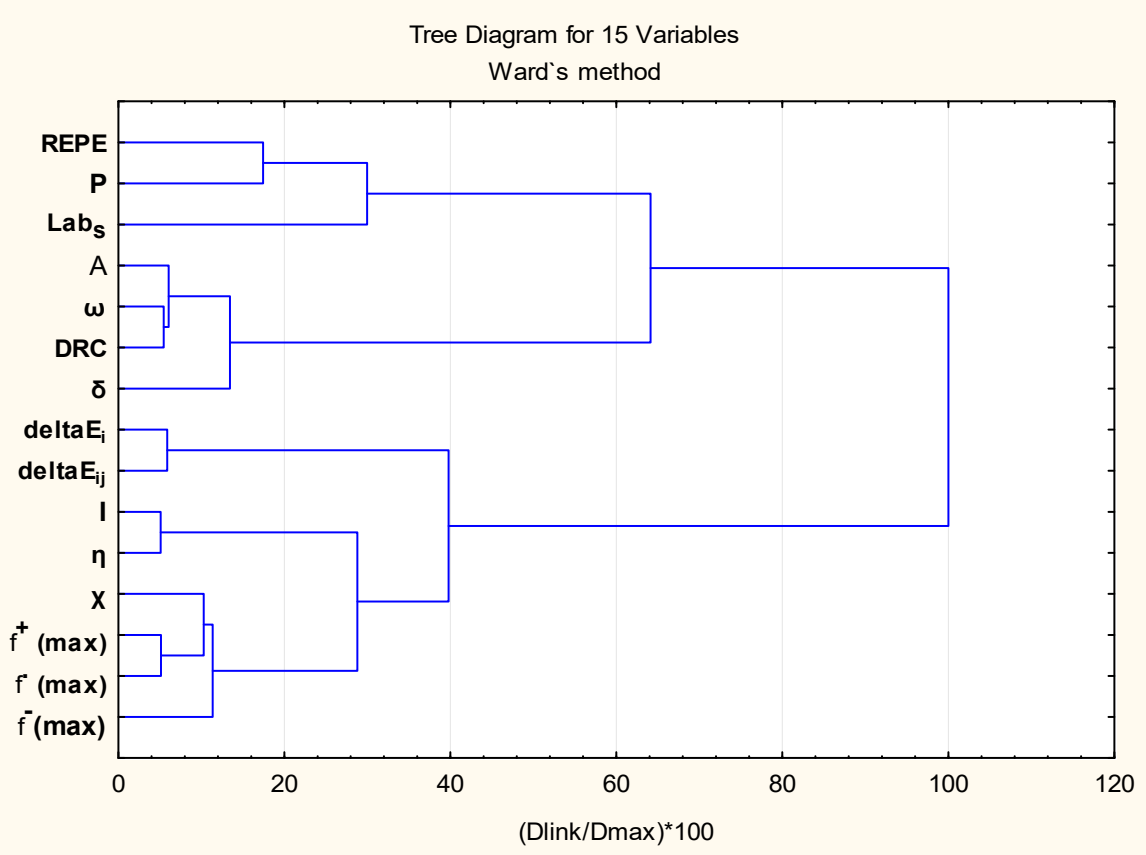

Figure S1. Hierarchical clustering for the variable – dendrogram representation. REPE [β] – resonance energy per π-electron, DeltaE$_i$ [β^{-1}] and DeltaE$_{ij}$ [β^{-1}] – Hückel reactivity indices, P – generalized stability index, I [eV] – vertical ionization potential, A [eV] – vertical electron affinity, χ [eV] – electronegativity, η [eV] – hardness, δ [eV^{-1}] – softness, ω [eV] – electrophilicity, f^{-}_{max} – largest atomic Fukui index for electrophilic attack, f^{+}_{max} largest atomic Fukui index for nucleophilic attack, f^{0}(max) – largest atomic Fukui index for radical attack; Lab$_s$ – laboratory stability.

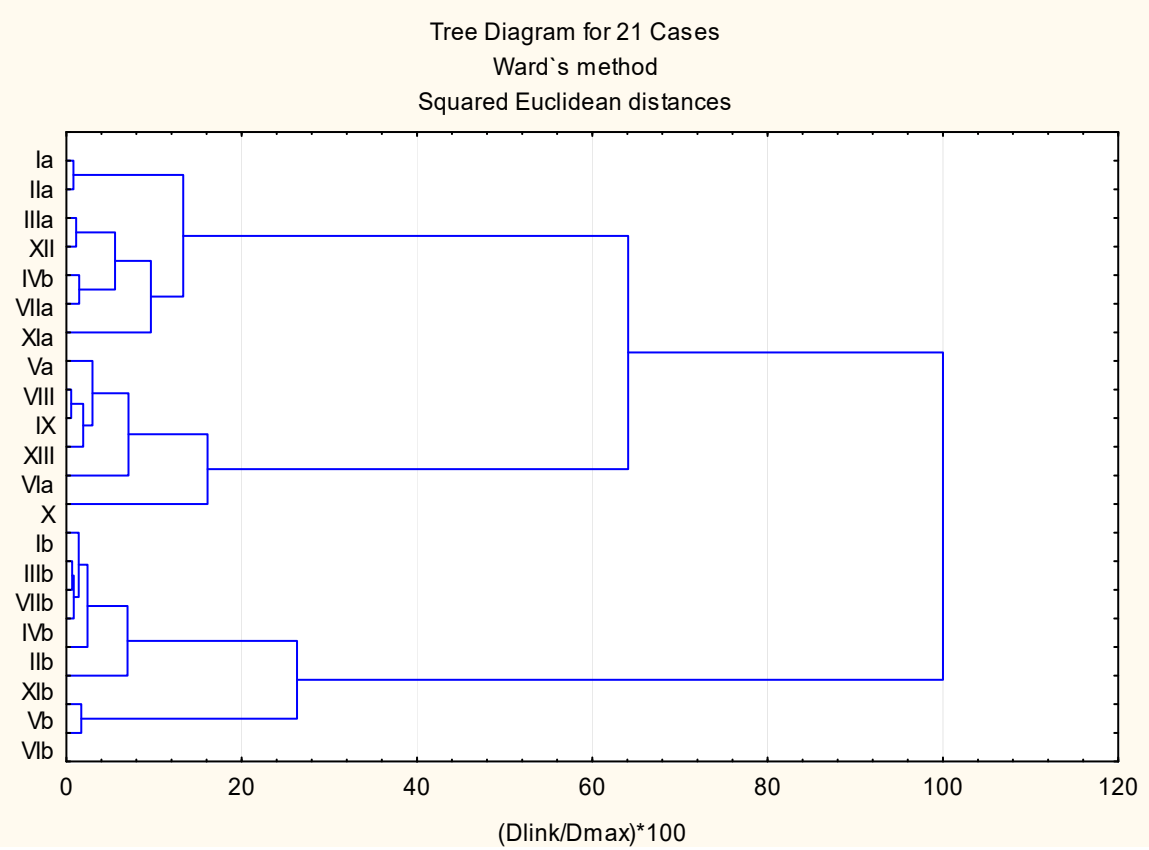

Figure S2. Hierarchical clustering of the objects – a dendrogram representation.

Tables S2-S4: Members distribution in the obtained clusters from K-means clustering:

	Members of Cluster Number 3 (Jul_second.sta) and Distances from Respective Cluster Center Cluster contains 7 cases
	Distance
Ia	0,706200
IIa	0,530343
IIIa	0,329001
IVa	0,484408
VIIa	0,505363
XIa	0,773103
XII	0,659780

	Members of Cluster Number 2 (Jul_second.sta) and Distances from Respective Cluster Center Cluster contains 6 cases
	Distance
Ib	0,316211
IIb	0,489626
IIIb	0,180973
IVb	0,280261
VIIb	0,203413
XIb	0,662530

	Members of Cluster Number 1 (Jul_second.sta) and Distances from Respective Cluster Center Cluster contains 8 cases
	Distance
Va	0,803030
Vb	0,841881
VIa	0,607413
VIb	1,071743
VIII	0,392537
IX	0,462811
X	0,974783
XIII	0,639119