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**Why naturally occurring quinone redox systems lack amino groups:
consideration using 1,4-naphthoquinone derivatives**

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Starting compounds and experimental procedures

1,4-Naphthoquinone (**3a**) (Lancaster Synthesis, 97+%) was further purified by column chromatography (Al_2O_3 , Brockmann activity II and CHCl_3) and recrystallized from hexane. And its nitrogen derivatives **5-8** were prepared as described previously [M.P. Vlasenko, A.F. Pozharskii, O.P. Demidov, V.A. Ozeryanskii G.S. Borodkin, *Mendeleev Commun.*, 2023, **33**, 197].

The cyclic voltammetry of compounds **3a,5-8** was measured with the use of three-electrode configuration (glassy carbon working electrode $d = 2$ mm, Pt counter electrode, Ag/Ag^+ reference electrode (0.01 M AgNO_3 in CH_3CN), 0.1 M Bu_4NPF_6 , $C = 5$ mM) and potentiostat – galvanostat Elins P-45X. The difference between E_{pa} and E_{pc} is broadened due to the uncompensated resistance of the solvents used and the structural features of the electrochemical cell. R_{ohmic} was determined using ferrocene as a standard and was 4100 Ω for methylene chloride and 6400 Ω for THF.

ESR spectra were recorded on X-band Bruker EMX Plus spectrometer (9.65 GHz). The theoretical spectra were calculated using the Bruker WinEPR Simfonia v.1.25 program. The radical anions were obtained by reduction of solutions in THF over a potassium mirror under anaerobic conditions.

ESR spectra of radical anions

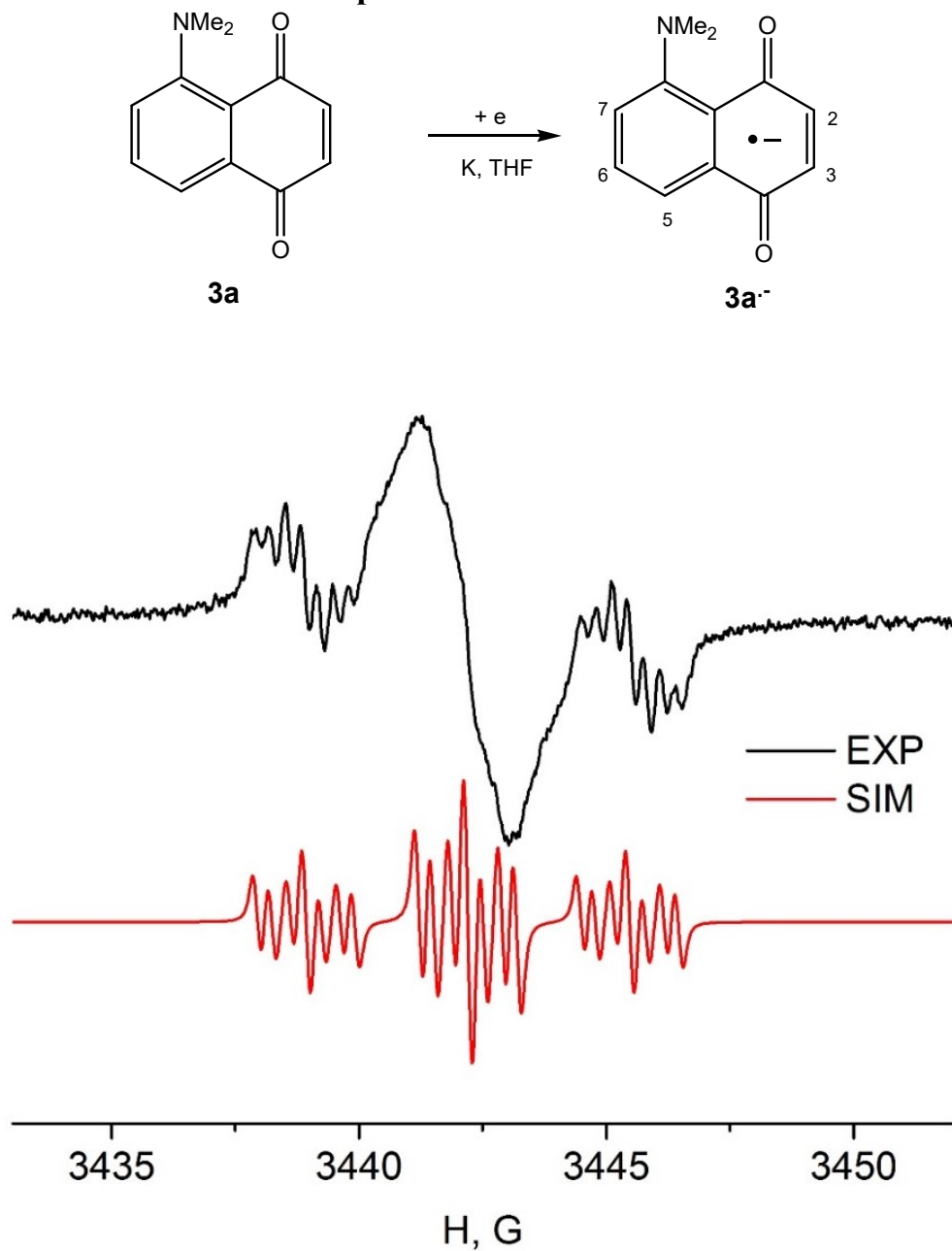


Figure S1. ESR spectra of radical anion **3a⁻** in THF (experimental (*black*), calculated (*red*), $g = 2.001$, $a(\text{H}_{2,3}) = 3.27$ G, $a(\text{H}_5) = 0.30$ G, $a(\text{H}_6) = 1.01$ G, $a(\text{H}_8) = 0.67$ G).

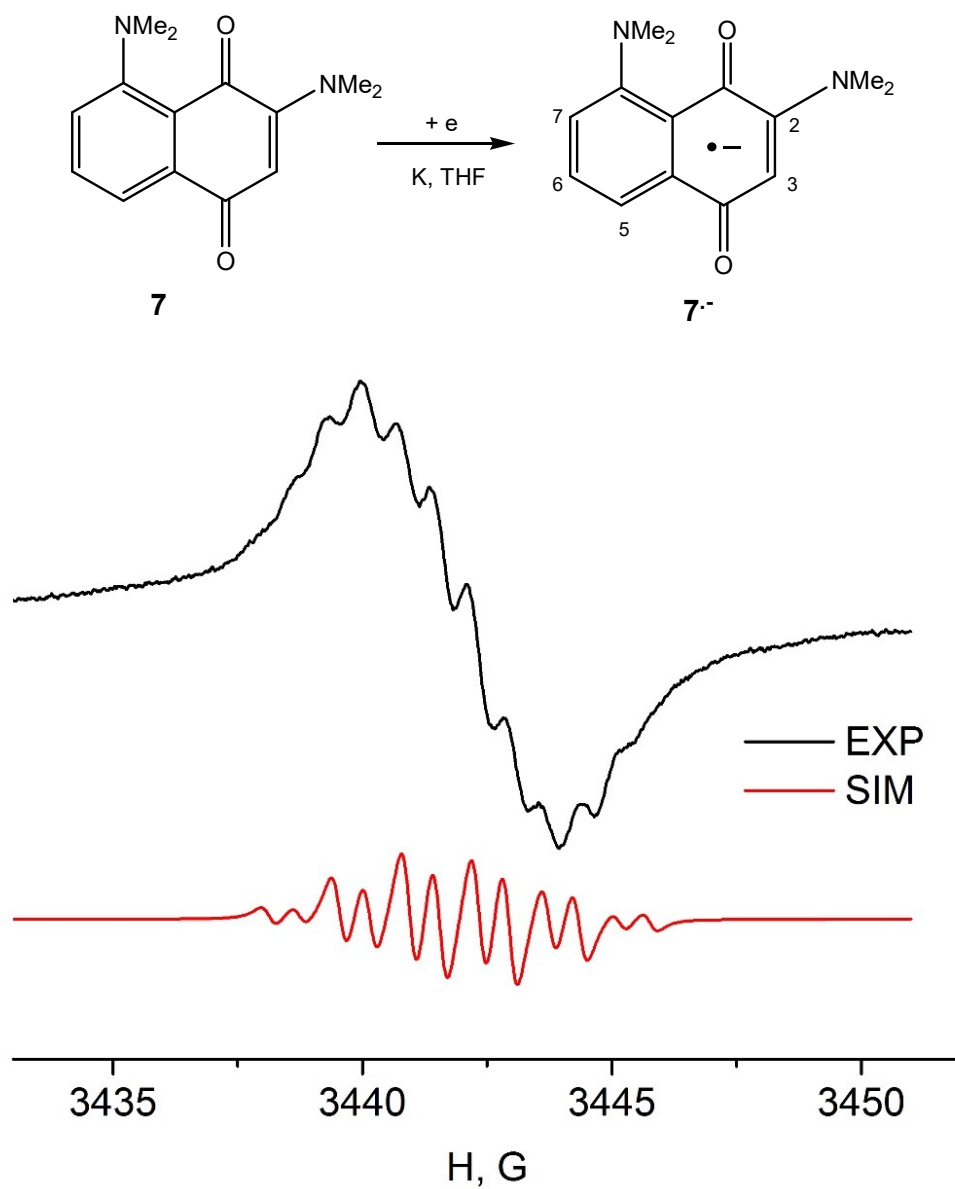


Figure S2. ESR spectra of radical anion of **7** (experimental (*black*), calculated (*red*), $g = 2.001$, $a(\text{N}_2) = 1.38 \text{ G}$, $a(\text{H}_5) = 0.61 \text{ G}$, $a(\text{H}_{3,6,7}) = 1.42 \text{ G}$).

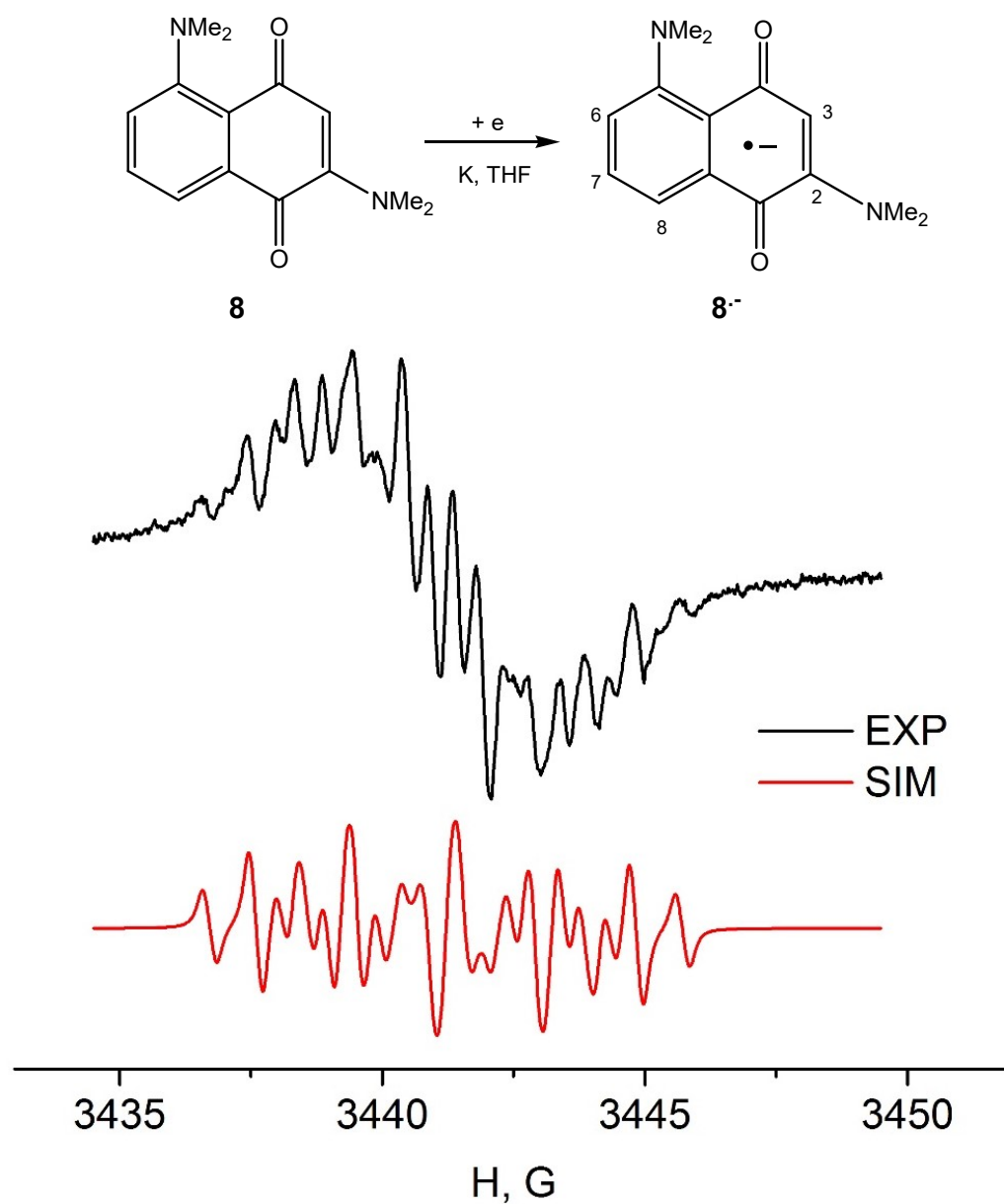


Figure S3. ESR spectra of radical anion of **8** (experimental (*black*), calculated (*red*), $g = 2.002$, $a(\text{N}_2) = 2.00$ G, $a(\text{H}_3) = 1.86$ G, $a(\text{H}_7) = 1.38$ G, $a(\text{H}_{6,8}) = 0.88$ G).

Quantum chemical calculations

The density functional theory (DFT)^{S1} calculations were performed by means of Gaussian 16 program package^{S2} using the B3LYP functional^{S3} and 6-311++G(d,p) basis set. The discussed structures, to which minima on the potential energy surface (PES) correspond, are found by means of full geometry optimization without imposing symmetric constraints. The character of the found stationary points was ascertained by calculating the force constant matrix.

S1 W. Kohn and L. J. Sham, *Phys. Rev.*, 1965, **140**, A1133.

S2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H.P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16 Revision A.03*, Gaussian, Wallingford, CT, 2016.

S3 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.

Table S1. Total energies (E_T) of compounds **3a**, **5-8**

Compound	E_T (a.u.)
3a	-535.258580
5	-669.253602
6	-724.644970
7	-803.264174
8	-803.262874

Table S2. Total (E_T) and relative (ΔE) energies of isomeric radical anions **3a**, **5-8** in the gas state

Radical anion	E_T (a.u.)	ΔE (kcal/mol)	Radical anion	E_T (a.u.)	ΔE (kcal/mol)
3R	-535.332317	-	7Rii	-803.315913	2.5
5Ri	-669.319948	0.0	7Riii	-803.316728	0.7
5R	-669.318927	0.6	8R	-803.320157	0.6
6R	-724.702428	0.0	8Ri	-803.321185	0.0
6Ri	-724.701465	0.6	8Rii	-803.317803	2.1
7R	-803.319865	0.0	8Riii	-803.316869	2.7
7Ri	803.316728	2.0			

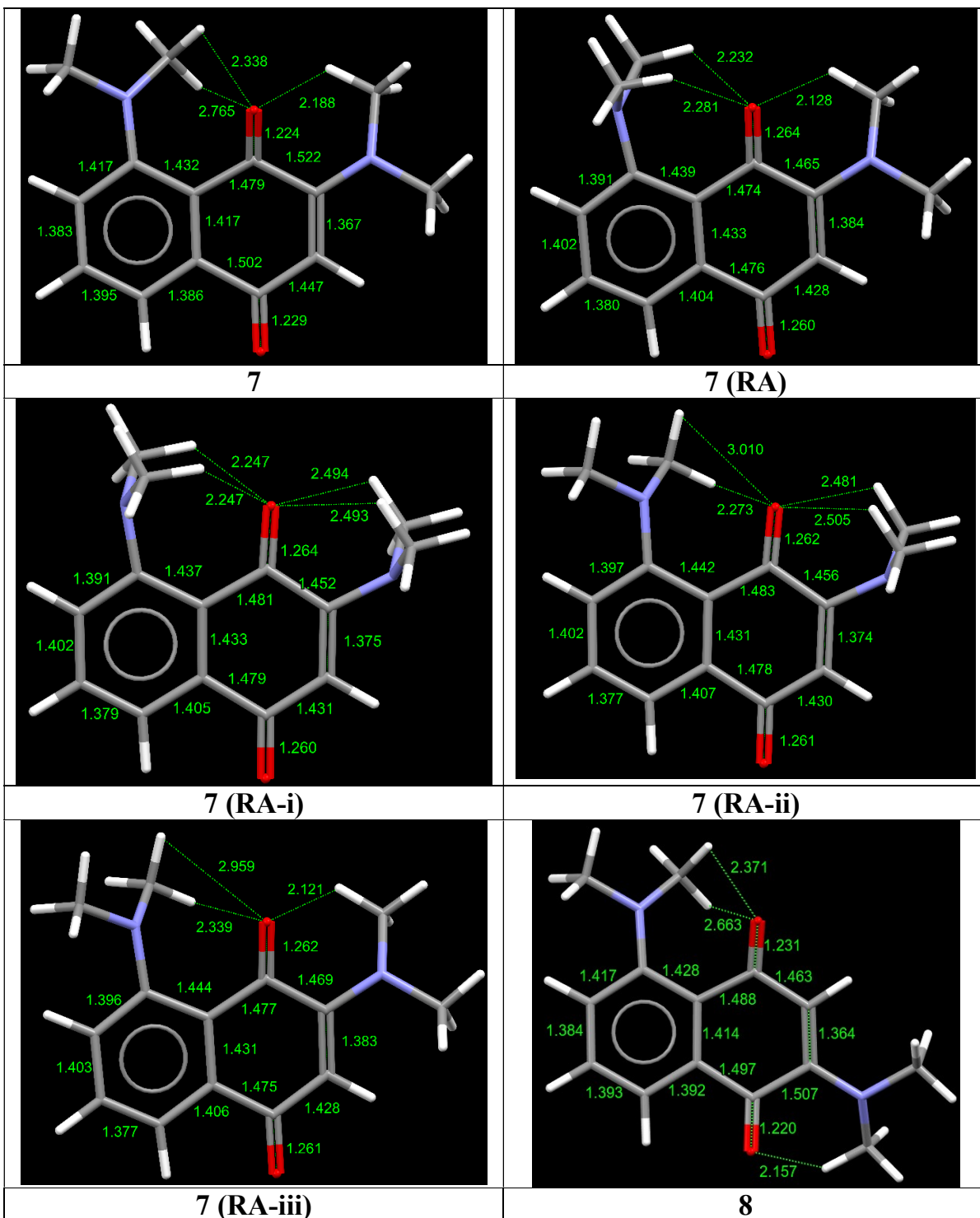
Table S3. Selected geometrical parameters of 1,4-naphthoquinone¹⁴ and its derivatives⁶ in the crystal state.

Comp.	Bond lengths and distances, Å						Angles (°)		
	C(1)=O	C(4)=O	N(5)...O(4)	$\Delta N(5)$	$\Delta O(1)$	$\Delta O(4)$	NMe ₂ -ring	$\Sigma N(5)$	θ
3a	1.222	1.223	-	-	+0.025	-0.052	-	-	1.0
3b	1.232	1.233	-	+0.042 ^a	+0.045	-0.012	-	-	0.38
5	1.223	1.231	2.897	+0.404	+0.210	-0.458	39.8	355.8	7.9
6	1.240	1.228	2.851	+0.418 +0.180 ^b	+0.122	-0.465	41.4 12.5 ^b	355.6 359.9 ^b	10.0
7	1.240	1.229	2.935	+0.455 +0.022 ^c	+0.173	-0.805	33.1 19.3 ^c	357.5 357.8 ^c	7.8
8	1.218	1.238	2.843	-0.463 -0.234 ^d	+0.452	+0.580	40.6 18.2 ^d	354.8 359.9 ^d	9.1

^a 2-Me; ^b 3-NH₂; ^c 3-NMe₂; ^d 2-NMe₂**Table S4.** Selected geometrical parameters of 1,4-naphthoquinone and its derivatives in the gas state (calculation data)

Com	Bond lengths and distances, Å						Angles (°)		
	C(1)=O	C(4)=O	N(5)...O(4)	$\Delta N(5)$	$\Delta O(1)$	$\Delta O(4)$	NMe ₂ -ring	$\Sigma N(5)$	θ
3a	1.220	1.220	-	-	0	0	-	-	0
5	1.222	1.228	2.874	-0.422	-0.175	+0.438	40.7	357.5	9.8
6	1.220	1.229	2.857	-0.412	-0.188	+0.403	42.1 24.1 ^a	356.9 356.1 ^a	10.2
7	1.229	1.224	+2.885	+0.391 +0.064 ^b	+0.078	-0.688	36.2 24.0 ^b	358.1 357.1 ^b	7.8
8	1.220	1.231	2.873	+0.374 +0.221 ^c	-0.158	-0.510	40.0 38.0 ^c	357.0 353.4 ^c	12.2

^a 3-NH₂; ^b 3-NMe₂; ^c 2-NMe₂



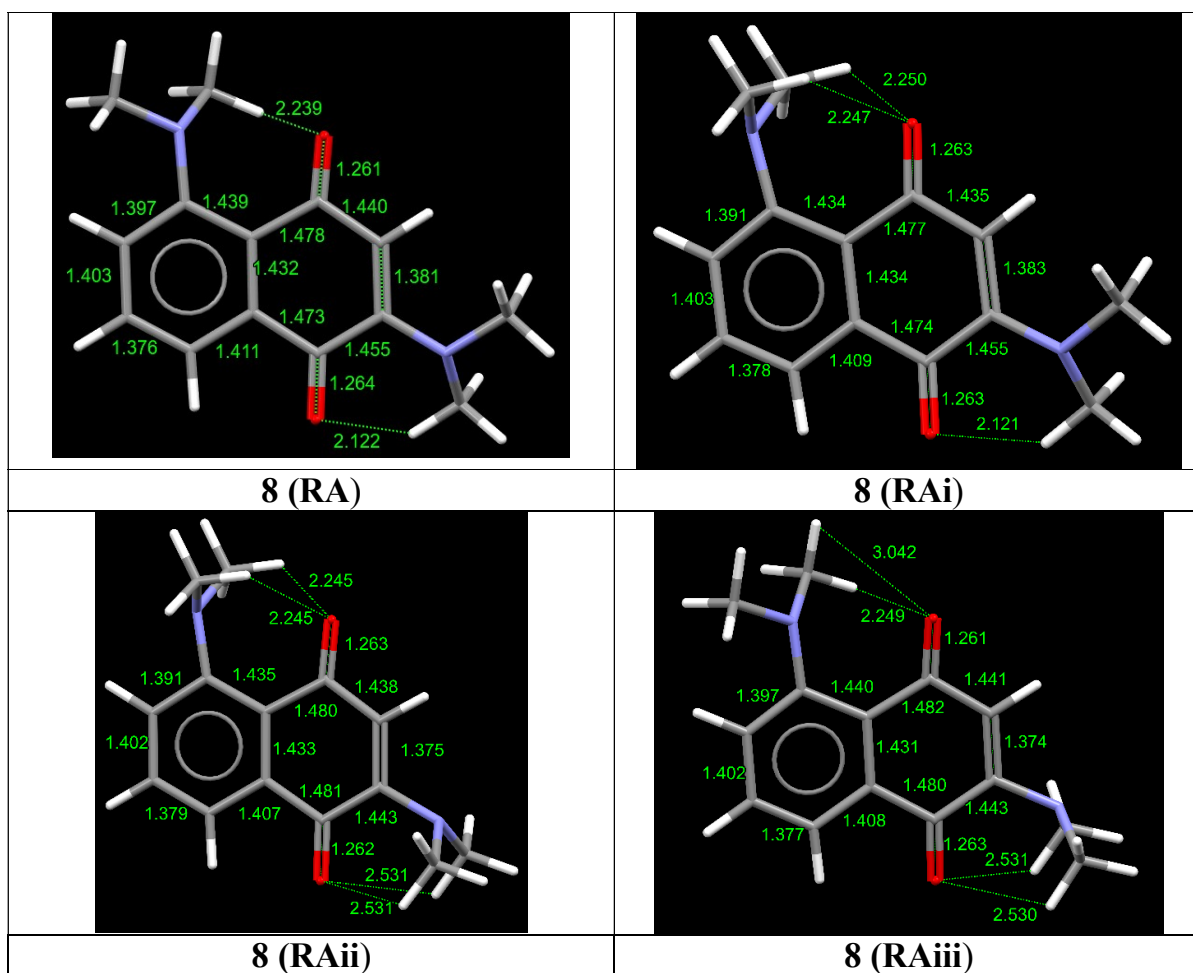


Figure S4. Bond lengths and some CH...O and NH...O contacts (Å) in 1,4-naphthoquinones and their radical anions (according to gas-phase calculated data using the DFT method in the approximation B3LYP/6-311++G(d,p))

Table S5. Bond lengths and some CH...O and NH...O contacts (Å) in 1,4-naphthoquinones and their radical anions (according to gas-phase calculated data using the DFT method in the approximation B3LYP/6-311++G(d,p))

Particle type	Bond	Bond lengths, Å	Particle type	Bond	Bond lengths, Å
3a	CH... O	-	7 (RA-i)	CH... O	2.247 2.247 2.493 2.494
3a (RA)	CH... O	-	7 (RA-ii)	CH... O	2.273 2.481 2.505
5	CH... O	2.329	7 (RA-iii)	CH... O	2.121 2.339
5 (RA)	CH... O	2.244 2.244	8	CH... O	2.157 2.371
5 (RAi)	CH... O	2.249	8 (RA)	CH... O	2.122 2.239
6	CH... O NH... O	2.370 2.161	8 (RAi)	CH... O	2.121 2.247 2.250
6 (RA)	CH... O CH... O NH...O	2.225 2.273 2.119	8 (RAii)	CH... O	2.245 2.245
6 (RAi)	CH... O NH...O	2.272 2.108	8 (RAiii)	CH... O	2.249
7	CH... O	2.188 2.338			

Table S6. Energies (E) of singly occupied molecular orbital (SOMO) of isomeric radical anions **3a** and **5-8** (in the gas state, eV)

Radical anion	E (SOMO)	Radical anion	E (SOMO)
3R	-0.47	7Rii	-0.48
5R	-0.56	7Riii	-0.30
5Ri	-0.39	8R	-0.30
6R	-0.42	8Ri	-0.44
6Ri	-0.25	8Rii	-0.65
7R	-0.42	8Riii	-0.49
7Ri	-0.65		

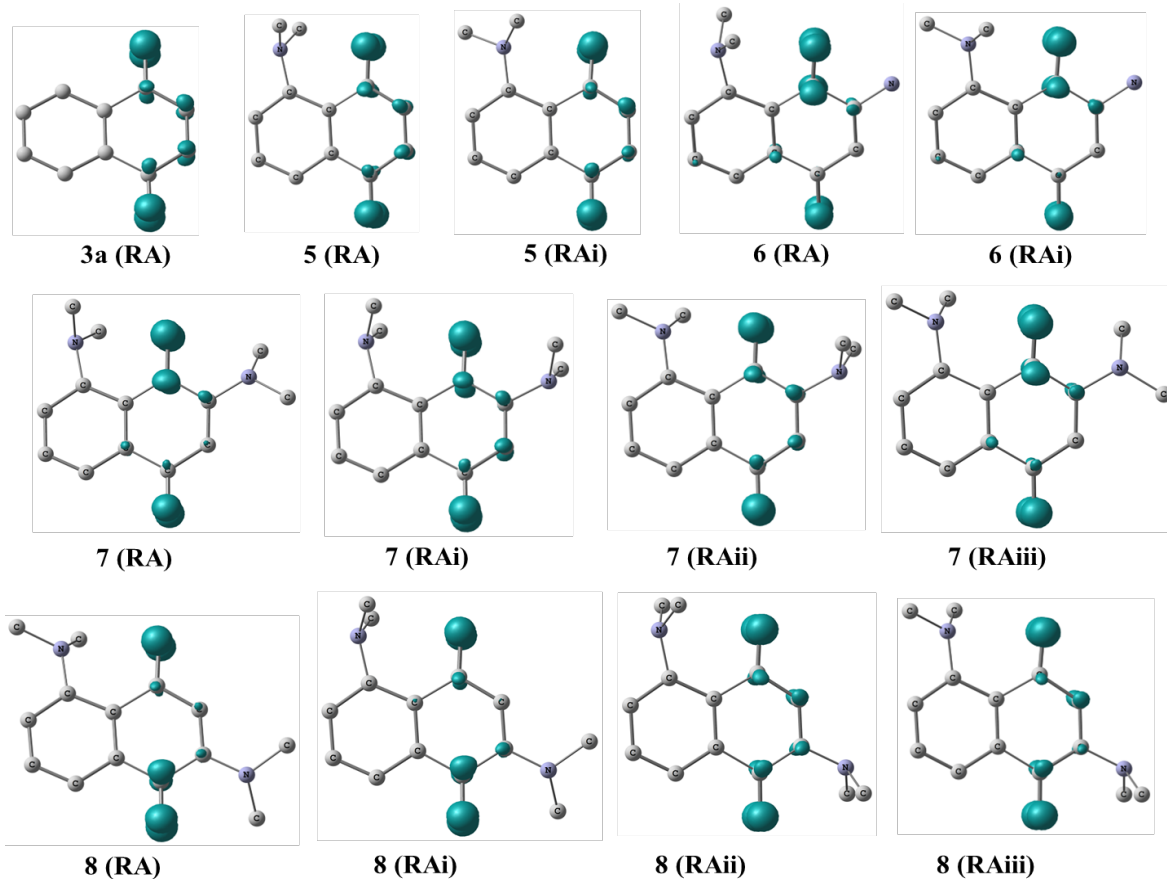


Figure S5. Spin density distribution in isomers of the radical anions (according to gas-phase calculated data using the DFT method in the approximation B3LYP/6-311++G(d,p)). Hydrogen atoms are omitted, cut off = $0.012 \text{ e } \text{\AA}^{-3}$.

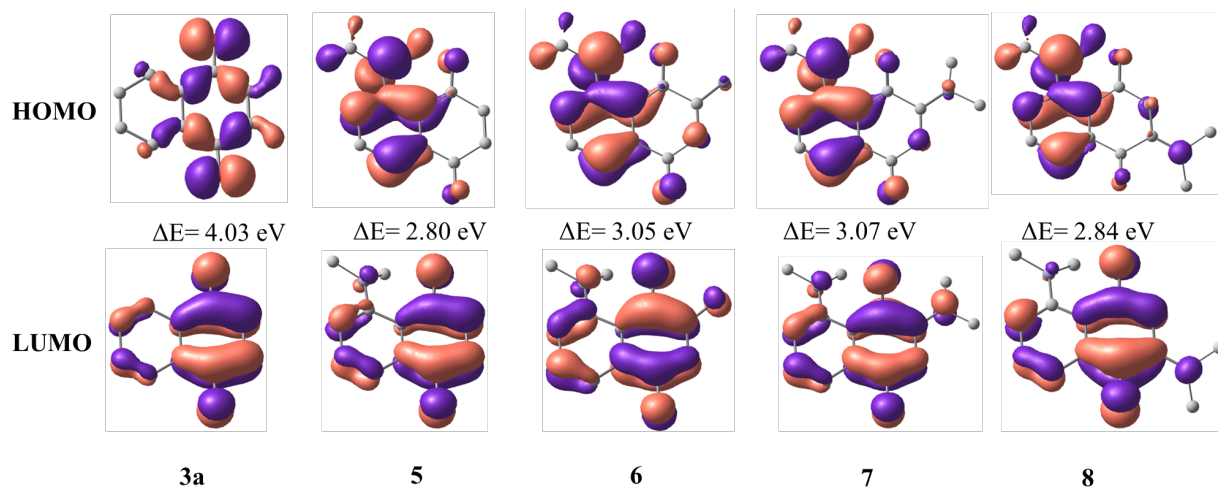


Figure S6. HOMO and LUMO orbitals of the compounds **3a**, **5-8** (according to gas-phase calculated data using the DFT method in the approximation B3LYP/6-311++G(d,p)). Hydrogen atoms are omitted, cut off = $0.038 \text{ e } \text{\AA}^{-3}$.

Cartesian coordinates of the compounds **3a**, **5-8** and isomers of their radical anions calculated using the DFT method in the approximation B3LYP/6-311++G(d,p)).

3a

H	-0.021328000	-0.030696000	-2.817454000
C	-0.021328000	0.473779000	-1.858857000
C	-0.021328000	1.862280000	-1.772046000
C	-0.021328000	2.487857000	-0.522861000
C	-0.021328000	1.725526000	0.640952000
C	-0.021328000	0.331079000	0.562507000
C	-0.021328000	-0.298918000	-0.695311000
C	-0.021328000	-1.788171000	-0.797311000
C	-0.021328000	-2.555687000	0.471826000
C	-0.021328000	-1.956099000	1.670194000
C	-0.021328000	-0.479436000	1.816571000
H	-0.021328000	2.459559000	-2.676704000
H	-0.021328000	3.570018000	-0.459378000
H	-0.021328000	2.190922000	1.619095000
H	-0.021328000	-2.517718000	2.598350000
H	-0.021328000	-3.635219000	0.365352000
O	-0.021328000	-2.367911000	-1.870898000
O	-0.021328000	0.032661000	2.923611000

5

C	0.248123000	0.012589000	-1.839192000
C	0.584159000	1.385625000	-1.725156000
C	0.532245000	2.046471000	-0.512603000
C	0.138351000	1.377588000	0.646839000
C	-0.120291000	0.015715000	0.588683000
C	-0.008852000	-0.709156000	-0.629417000
C	0.054194000	-2.185901000	-0.550325000
C	-0.319715000	-2.828625000	0.738495000
C	-0.577486000	-2.138905000	1.855061000
C	-0.486882000	-0.667013000	1.871608000
H	0.830649000	1.947725000	-2.615449000
H	0.766770000	3.104580000	-0.474865000
H	0.048175000	1.887840000	1.596716000
H	-0.841149000	-2.615089000	2.793100000
H	-0.341689000	-3.912887000	0.709188000
O	0.453637000	-2.910312000	-1.457441000
O	-0.696796000	-0.041319000	2.899860000
N	0.162924000	-0.560156000	-3.086187000
C	0.801480000	0.063024000	-4.235811000
H	1.779378000	0.462286000	-3.965082000

H	0.956459000	-0.700456000	-5.000334000
H	0.196375000	0.868780000	-4.677282000
C	-0.858638000	-1.545553000	-3.419650000
H	-1.378857000	-1.218012000	-4.326741000
H	-0.432890000	-2.538718000	-3.578353000
H	-1.593305000	-1.614666000	-2.618315000

6

C	0.247651000	0.002505000	-1.847610000
C	0.610827000	1.366576000	-1.722372000
C	0.560319000	2.015836000	-0.504183000
C	0.141887000	1.345498000	0.648195000
C	-0.148352000	-0.005800000	0.580489000
C	-0.042348000	-0.719706000	-0.644199000
C	-0.014595000	-2.185418000	-0.581567000
C	-0.402579000	-2.852677000	0.722652000
C	-0.664396000	-2.133556000	1.845850000
C	-0.547553000	-0.694354000	1.862922000
H	0.873498000	1.930978000	-2.606378000
H	0.815336000	3.068955000	-0.454680000
H	0.054411000	1.848119000	1.602349000
H	-0.950334000	-2.611475000	2.776714000
O	0.350118000	-2.921641000	-1.495105000
O	-0.755310000	-0.035132000	2.878402000
N	0.169032000	-0.564214000	-3.099453000
C	0.835436000	0.054936000	-4.235161000
H	1.819967000	0.426093000	-3.949310000
H	0.978751000	-0.703906000	-5.006844000
H	0.255950000	0.880818000	-4.674164000
C	-0.892173000	-1.496610000	-3.461488000
H	-1.406418000	-1.116081000	-4.351689000
H	-0.504283000	-2.497267000	-3.664415000
H	-1.623784000	-1.570833000	-2.658452000
N	-0.469213000	-4.203176000	0.623277000
H	-0.101605000	-4.610831000	-0.225197000
H	-0.540569000	-4.774015000	1.448436000

7

C	0.166557000	0.011076000	-1.783228000
C	0.525871000	1.381331000	-1.774151000
C	0.674485000	2.083081000	-0.592124000
C	0.459830000	1.461395000	0.637902000
C	0.159726000	0.108736000	0.668790000
C	0.064403000	-0.656017000	-0.520374000
C	0.120126000	-2.129026000	-0.396754000

C	-0.257835000	-2.752157000	0.939864000
C	-0.273730000	-1.960608000	2.053771000
C	-0.031293000	-0.534839000	2.011910000
H	0.637335000	1.908540000	-2.711474000
H	0.929433000	3.136668000	-0.630627000
H	0.536721000	1.997760000	1.574370000
H	-0.483790000	-2.356728000	3.037840000
O	0.546523000	-2.848758000	-1.290545000
O	-0.023059000	0.144617000	3.036206000
N	-0.097185000	-0.605314000	-2.986918000
C	0.368098000	-0.024938000	-4.237113000
H	1.376012000	0.375915000	-4.124558000
H	0.409148000	-0.812940000	-4.991262000
H	-0.291388000	0.771727000	-4.612468000
C	-1.115215000	-1.633299000	-3.132014000
H	-1.743711000	-1.390760000	-3.995442000
H	-0.679793000	-2.627457000	-3.269129000
H	-1.756480000	-1.657796000	-2.250019000
N	-0.419053000	-4.112468000	0.993429000
C	-0.488260000	-4.754501000	2.297707000
H	0.328855000	-4.409789000	2.933243000
H	-1.439869000	-4.560220000	2.813555000
H	-0.387993000	-5.831839000	2.159031000
C	-1.064578000	-4.884464000	-0.070298000
H	-0.555514000	-5.844975000	-0.183449000
H	-2.115983000	-5.076556000	0.185128000
H	-1.009491000	-4.362523000	-1.017156000

8

C	0.163509000	0.010511000	-1.789340000
C	0.413775000	1.405201000	-1.800516000
C	0.480180000	2.142374000	-0.631620000
C	0.291041000	1.528966000	0.604288000
C	0.103976000	0.150832000	0.655465000
C	0.095005000	-0.637721000	-0.518515000
C	0.209754000	-2.110744000	-0.338865000
C	-0.080717000	-2.669858000	0.981492000
C	-0.291656000	-1.936964000	2.112266000
C	-0.038493000	-0.453931000	2.017338000
H	0.505968000	1.919437000	-2.747498000
H	0.649041000	3.212201000	-0.686360000
H	0.306738000	2.092668000	1.527151000
O	0.548584000	-2.870414000	-1.246530000
O	0.095046000	0.230685000	3.018338000
N	-0.017811000	-0.653222000	-2.984354000

C	0.455939000	-0.074960000	-4.230593000
H	1.432359000	0.391264000	-4.093436000
H	0.573264000	-0.877622000	-4.961557000
H	-0.237463000	0.668768000	-4.653352000
C	-1.028543000	-1.691260000	-3.146314000
H	-1.676860000	-1.424974000	-3.990134000
H	-0.581735000	-2.672257000	-3.321361000
H	-1.650811000	-1.757941000	-2.255232000
N	-0.534432000	-2.493001000	3.346788000
C	-1.419178000	-1.850672000	4.323933000
H	-1.389951000	-0.773105000	4.218289000
H	-2.451854000	-2.207705000	4.201565000
H	-1.083352000	-2.104795000	5.331962000
C	-0.497570000	-3.942479000	3.463070000
H	-0.528391000	-4.205999000	4.520921000
H	-1.347165000	-4.429370000	2.960818000
H	0.427930000	-4.334423000	3.037346000
H	-0.108660000	-3.750983000	0.989238000

3 (RA)

H	-0.021328000	-0.047698000	-2.805348000
C	-0.021328000	0.465570000	-1.850169000
C	-0.021328000	1.847368000	-1.770838000
C	-0.021328000	2.477795000	-0.511477000
C	-0.021328000	1.713433000	0.642220000
C	-0.021328000	0.306139000	0.583680000
C	-0.021328000	-0.330462000	-0.688286000
C	-0.021328000	-1.802277000	-0.809999000
C	-0.021328000	-2.522251000	0.433390000
C	-0.021328000	-1.905108000	1.666210000
C	-0.021328000	-0.477775000	1.835441000
H	-0.021328000	2.445857000	-2.677517000
H	-0.021328000	3.562313000	-0.447346000
H	-0.021328000	2.171217000	1.625316000
H	-0.021328000	-2.495429000	2.578842000
H	-0.021328000	-3.606473000	0.359225000
O	-0.021328000	-2.376211000	-1.933453000
O	-0.021328000	0.077818000	2.967746000

5R (RA)

C	-0.008319000	0.220422000	-1.856311000
C	-0.021890000	1.601203000	-1.690366000
C	-0.032142000	2.201847000	-0.423844000
C	-0.028761000	1.401553000	0.698902000
C	-0.015186000	0.000198000	0.587787000

C	-0.004484000	-0.631949000	-0.700685000
C	0.009825000	-2.112604000	-0.763699000
C	0.011838000	-2.808238000	0.495452000
C	0.001431000	-2.192161000	1.721791000
C	-0.012645000	-0.766685000	1.855977000
H	-0.024301000	2.204501000	-2.591734000
H	-0.042606000	3.284363000	-0.334441000
H	-0.036344000	1.814674000	1.700758000
H	0.003535000	-2.770747000	2.641306000
H	0.022460000	-3.891952000	0.418580000
O	0.020007000	-2.766996000	-1.844553000
O	-0.022394000	-0.188648000	2.976056000
N	0.000501000	-0.196841000	-3.239293000
C	1.233717000	-0.808763000	-3.722195000
H	2.085174000	-0.211967000	-3.382301000
H	1.363846000	-1.845616000	-3.387116000
H	1.227701000	-0.786400000	-4.820051000
C	-1.217559000	-0.831916000	-3.730708000
H	-1.203712000	-0.810429000	-4.828502000
H	-1.330895000	-1.870743000	-3.395644000
H	-2.082431000	-0.250648000	-3.397821000

5 (RAi)

C	1.111108000	0.859904000	-0.233803000
C	0.899937000	2.216196000	-0.492243000
C	-0.385900000	2.775278000	-0.499005000
C	-1.477813000	1.983329000	-0.223324000
C	-1.319646000	0.606041000	0.021290000
C	-0.021276000	-0.000848000	-0.005633000
C	0.077207000	-1.476691000	0.113529000
C	-1.162732000	-2.181668000	0.325117000
C	-2.393157000	-1.581949000	0.408263000
C	-2.559167000	-0.167399000	0.263775000
H	1.749394000	2.865024000	-0.664164000
H	-0.507665000	3.835912000	-0.701243000
H	-2.486534000	2.377302000	-0.199379000
H	-3.293825000	-2.166393000	0.575407000
H	-1.062589000	-3.259857000	0.414948000
O	1.156278000	-2.125214000	0.028573000
O	-3.686686000	0.395386000	0.324861000
N	2.439945000	0.364177000	-0.228580000
C	3.451344000	1.123417000	-0.928564000
H	3.091922000	1.416181000	-1.917187000
H	3.784391000	2.037757000	-0.396442000
H	4.333006000	0.486936000	-1.059082000

C	2.940297000	-0.177619000	1.026204000
H	3.794591000	-0.832382000	0.827785000
H	3.268335000	0.631056000	1.708711000
H	2.179394000	-0.778595000	1.511590000

6 (RA)

C	-0.029089000	0.205212000	-1.839882000
C	-0.068787000	1.586184000	-1.687257000
C	-0.080337000	2.201480000	-0.427575000
C	-0.034295000	1.410409000	0.703948000
C	0.007042000	0.012310000	0.607817000
C	-0.005746000	-0.637076000	-0.673669000
C	-0.015274000	-2.099486000	-0.721578000
C	0.076221000	-2.808393000	0.547704000
C	0.106795000	-2.169238000	1.767702000
C	0.058588000	-0.748056000	1.883212000
H	-0.079500000	2.179840000	-2.595212000
H	-0.112281000	3.284173000	-0.348758000
H	-0.027995000	1.833465000	1.701813000
H	0.172010000	-2.739200000	2.690983000
O	-0.119166000	-2.793574000	-1.782862000
O	0.066110000	-0.155587000	2.993212000
N	0.001596000	-0.231812000	-3.215710000
C	1.212197000	-0.919278000	-3.651729000
H	2.084845000	-0.370392000	-3.286316000
H	1.271535000	-1.959314000	-3.306858000
H	1.244880000	-0.905558000	-4.749374000
C	-1.234710000	-0.806342000	-3.734724000
H	-1.183502000	-0.818538000	-4.831576000
H	-1.421138000	-1.826971000	-3.375343000
H	-2.074369000	-0.166611000	-3.447694000
N	0.146607000	-4.196456000	0.427991000
H	-0.125825000	-4.484934000	-0.506841000
H	-0.288332000	-4.718698000	1.174167000

6 (RAi)

6	1.439349000	0.410294000	-0.057526000
6	1.839191000	1.746419000	-0.095818000
6	0.911182000	2.798822000	-0.072838000
6	-0.435683000	2.517607000	0.015939000
6	-0.890640000	1.189228000	0.040693000
6	0.032202000	0.092497000	-0.026808000
6	-0.494733000	-1.268945000	-0.146654000
6	-1.944377000	-1.424492000	-0.073692000
6	-2.813304000	-0.364018000	0.048210000

6	-2.360043000	0.987638000	0.098256000
1	2.895213000	1.985215000	-0.115541000
1	1.263233000	3.826112000	-0.102631000
1	-1.187175000	3.296873000	0.055627000
1	-3.886248000	-0.529321000	0.106275000
8	0.200913000	-2.316083000	-0.329889000
8	-3.148177000	1.966292000	0.184457000
7	2.429759000	-0.606069000	-0.070173000
6	3.741130000	-0.270415000	-0.575792000
1	3.657490000	0.276325000	-1.517260000
1	4.357205000	0.333462000	0.121526000
1	4.287701000	-1.200394000	-0.766054000
6	2.503503000	-1.469721000	1.098894000
1	3.023058000	-2.397181000	0.837752000
1	3.053978000	-0.979637000	1.926024000
1	1.508752000	-1.739928000	1.435840000
7	-2.382219000	-2.750108000	-0.117105000
1	-1.630428000	-3.353683000	-0.437843000
1	-3.264107000	-2.895764000	-0.586495000

7 (RA)

C	-0.044543000	0.199787000	-1.828271000
C	-0.003549000	1.582816000	-1.689474000
C	0.150659000	2.209162000	-0.444368000
C	0.232393000	1.428240000	0.690104000
C	0.196030000	0.027664000	0.603891000
C	0.090059000	-0.633682000	-0.662686000
C	0.176672000	-2.103382000	-0.724425000
C	0.189133000	-2.826700000	0.549827000
C	0.234959000	-2.152656000	1.757700000
C	0.272126000	-0.729321000	1.869256000
H	-0.118758000	2.170102000	-2.594340000
H	0.179832000	3.292872000	-0.378530000
H	0.323966000	1.857314000	1.681095000
H	0.249852000	-2.686991000	2.699434000
O	0.277604000	-2.730309000	-1.817770000
O	0.342549000	-0.144669000	2.983319000
N	-0.259192000	-0.239482000	-3.186123000
C	0.918033000	-0.699138000	-3.913935000
H	1.740264000	0.002499000	-3.746974000
H	1.239616000	-1.705197000	-3.614679000
H	0.690499000	-0.699194000	-4.988300000
C	-1.464783000	-1.013311000	-3.448133000
H	-1.688649000	-0.957723000	-4.522125000
H	-1.379668000	-2.068626000	-3.158675000

H	-2.303593000	-0.562754000	-2.910261000
N	0.258855000	-4.238560000	0.500976000
C	0.573493000	-4.939861000	1.727590000
H	1.454431000	-4.502579000	2.201236000
H	-0.249757000	-4.934743000	2.466882000
H	0.794015000	-5.984144000	1.484657000
C	-0.745710000	-4.938333000	-0.293752000
H	-0.407815000	-5.963648000	-0.480046000
H	-1.718848000	-4.989118000	0.229644000
H	-0.864795000	-4.432787000	-1.247957000

7 (RAi)

C	0.011079000	0.217498000	-1.858807000
C	-0.024403000	1.597594000	-1.688977000
C	-0.068744000	2.196477000	-0.422488000
C	-0.077688000	1.393679000	0.698251000
C	-0.043092000	-0.006450000	0.581986000
C	0.002423000	-0.637681000	-0.703448000
C	0.037684000	-2.116732000	-0.776121000
C	0.023292000	-2.840809000	0.482874000
C	-0.020618000	-2.205876000	1.701901000
C	-0.056066000	-0.782391000	1.841592000
H	-0.016306000	2.202891000	-2.588946000
H	-0.095541000	3.278525000	-0.332028000
H	-0.111296000	1.803232000	1.701008000
H	-0.029260000	-2.800818000	2.609075000
O	0.078751000	-2.751876000	-1.867770000
O	-0.096069000	-0.213873000	2.965296000
N	0.054033000	-0.192320000	-3.242881000
C	1.304818000	-0.778349000	-3.709901000
H	2.141251000	-0.179136000	-3.338710000
H	1.440647000	-1.820103000	-3.392679000
H	1.323629000	-0.733927000	-4.806989000
C	-1.144656000	-0.834057000	-3.769492000
H	-1.112361000	-0.788928000	-4.866240000
H	-1.248073000	-1.881377000	-3.458429000
H	-2.024520000	-0.274137000	-3.439672000
N	0.055745000	-4.286491000	0.484339000
C	-1.130135000	-4.912412000	-0.097143000
H	-2.024552000	-4.483046000	0.361446000
H	-1.196953000	-4.783443000	-1.187136000
H	-1.114891000	-5.985108000	0.133779000
C	1.295338000	-4.857967000	-0.038164000
H	1.317182000	-5.930447000	0.193232000
H	1.409033000	-4.725204000	-1.123809000

H	2.146280000	-4.389178000	0.462616000
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7 (RAii)

6	1.897655000	-0.283215000	0.066454000
6	2.991326000	0.581359000	0.153887000
6	2.836328000	1.974674000	0.137620000
6	1.578871000	2.520408000	0.009835000
6	0.444099000	1.690622000	-0.057058000
6	0.566149000	0.266095000	0.000113000
6	-0.662549000	-0.560915000	0.080589000
6	-1.933514000	0.145804000	0.009518000
6	-2.016550000	1.512361000	-0.108580000
6	-0.868474000	2.364829000	-0.147587000
1	3.991656000	0.170378000	0.203865000
1	3.713551000	2.612292000	0.203803000
1	1.413002000	3.590136000	-0.027473000
1	-2.993262000	1.981911000	-0.162642000
8	-0.652366000	-1.814813000	0.221274000
8	-0.960307000	3.619171000	-0.241499000
7	2.132906000	-1.681134000	0.067612000
6	1.744677000	-2.421108000	-1.123786000
1	0.800505000	-2.053903000	-1.509940000
1	2.520045000	-2.345132000	-1.911218000
1	1.606012000	-3.477387000	-0.872698000
6	3.379708000	-2.162493000	0.617929000
1	3.287387000	-3.239606000	0.793677000
1	4.257005000	-2.013467000	-0.043964000
1	3.587207000	-1.676959000	1.573571000
7	-3.173089000	-0.595777000	0.075606000
6	-3.388922000	-1.512097000	-1.041123000
1	-3.234626000	-0.975020000	-1.980664000
1	-2.721794000	-2.386425000	-1.022086000
1	-4.429772000	-1.859675000	-1.019555000
6	-3.420660000	-1.229174000	1.369236000
1	-4.457872000	-1.586986000	1.398158000
1	-2.745891000	-2.073418000	1.572618000
1	-3.299335000	-0.486116000	2.161531000

7 (RAiii)

6	-1.986350000	-0.145286000	-0.072863000
6	-2.987324000	0.828053000	-0.092320000
6	-2.690623000	2.198659000	-0.043531000
6	-1.379643000	2.607630000	0.059910000
6	-0.336427000	1.664700000	0.063648000
6	-0.601116000	0.262625000	-0.043931000

6	0.519731000	-0.679760000	-0.234858000
6	1.875972000	-0.129892000	-0.106498000
6	2.090089000	1.222712000	0.083461000
6	1.039800000	2.187852000	0.152939000
1	-4.025853000	0.522231000	-0.110154000
1	-3.499660000	2.923573000	-0.059390000
1	-1.101943000	3.652320000	0.129456000
1	3.090714000	1.625366000	0.181955000
8	0.353324000	-1.894967000	-0.531383000
8	1.269046000	3.419822000	0.296777000
7	-2.362952000	-1.509336000	-0.093965000
6	-1.953402000	-2.338927000	1.026805000
1	-0.976369000	-2.037943000	1.387966000
1	-2.681389000	-2.271633000	1.859289000
1	-1.881152000	-3.384453000	0.710677000
6	-3.679913000	-1.855701000	-0.573318000
1	-3.701524000	-2.930817000	-0.782262000
1	-4.496043000	-1.646791000	0.148449000
1	-3.900825000	-1.323841000	-1.500966000
7	2.961695000	-1.021309000	-0.282431000
6	4.279005000	-0.448158000	-0.458924000
1	4.256316000	0.329062000	-1.225108000
1	4.699447000	-0.005102000	0.464087000
1	4.961688000	-1.238552000	-0.787185000
6	2.989349000	-2.222206000	0.546237000
1	3.702315000	-2.937380000	0.121286000
1	3.307103000	-1.998011000	1.582179000
1	2.002118000	-2.676152000	0.550788000

8 (RA)

C	0.145624000	-0.068947000	-1.781000000
C	0.350066000	1.312011000	-1.827380000
C	0.385812000	2.088685000	-0.659456000
C	0.196084000	1.495468000	0.567067000
C	0.001759000	0.101196000	0.669250000
C	-0.000298000	-0.718220000	-0.505494000
C	-0.066065000	-2.183785000	-0.323707000
C	-0.217302000	-2.660633000	1.026080000
C	-0.269988000	-1.874909000	2.160722000
C	-0.132806000	-0.431608000	2.035559000
H	0.455814000	1.804814000	-2.785322000
H	0.544269000	3.161083000	-0.734641000
H	0.205266000	2.063493000	1.488682000
O	-0.005523000	-3.017833000	-1.267676000
O	-0.098899000	0.340325000	3.036148000

N	0.111535000	-0.795926000	-2.999118000
C	0.737466000	-0.202799000	-4.159466000
H	1.723988000	0.188162000	-3.902387000
H	0.864848000	-0.980864000	-4.919749000
H	0.151253000	0.615703000	-4.624765000
C	-1.137812000	-1.461232000	-3.338471000
H	-1.868960000	-0.746994000	-3.765788000
H	-0.945818000	-2.245132000	-4.077934000
H	-1.561923000	-1.941117000	-2.463453000
N	-0.361525000	-2.437464000	3.455849000
C	-1.383473000	-1.896025000	4.347016000
H	-1.373456000	-0.810888000	4.282814000
H	-2.391066000	-2.277540000	4.094820000
H	-1.157266000	-2.192850000	5.377187000
C	-0.235537000	-3.874576000	3.571059000
H	-0.139493000	-4.132393000	4.630484000
H	-1.103887000	-4.429535000	3.167643000
H	0.658251000	-4.222154000	3.049103000
H	-0.293473000	-3.739013000	1.091011000

8 (RAi)

6	-2.234009000	0.402123000	0.017034000
6	-2.665019000	1.724162000	0.006472000
6	-1.764811000	2.798815000	-0.045251000
6	-0.411333000	2.544831000	-0.084590000
6	0.079920000	1.223894000	-0.071229000
6	-0.829126000	0.116123000	-0.024124000
6	-0.254928000	-1.245086000	-0.021158000
6	1.176817000	-1.345761000	-0.042846000
6	2.061782000	-0.284063000	-0.088750000
6	1.545024000	1.075332000	-0.133476000
1	-3.735509000	1.894680000	0.039934000
1	-2.136301000	3.819621000	-0.053576000
1	0.320525000	3.342167000	-0.128489000
8	-0.952252000	-2.297403000	0.016471000
8	2.292269000	2.088454000	-0.237043000
7	-3.309840000	-0.559950000	0.074353000
6	-3.440823000	-1.309328000	1.319033000
1	-3.342928000	-0.620414000	2.163036000
1	-4.447783000	-1.745861000	1.359689000
1	-2.699363000	-2.111895000	1.421635000
6	-3.532192000	-1.355354000	-1.128181000
1	-2.800381000	-2.163435000	-1.254118000
1	-4.539743000	-1.789575000	-1.078522000
1	-3.495693000	-0.699095000	-2.002509000

7	3.459225000	-0.481996000	-0.176586000
6	4.299849000	0.259656000	0.759388000
1	3.955516000	1.289488000	0.809237000
1	4.282576000	-0.190599000	1.769698000
1	5.334969000	0.248017000	0.400855000
6	3.932905000	-1.832759000	-0.392200000
1	5.000199000	-1.793493000	-0.631437000
1	3.809925000	-2.491712000	0.488054000
1	3.407658000	-2.291219000	-1.232422000
1	1.536166000	-2.366959000	-0.011588000

8 (RAii)

6	-2.209029000	0.479033000	0.000083000
6	-2.533466000	1.831385000	0.000120000
6	-1.553500000	2.833817000	0.000107000
6	-0.222521000	2.474247000	0.000073000
6	0.160178000	1.120661000	0.000008000
6	-0.829115000	0.083762000	-0.000019000
6	-0.367117000	-1.322763000	-0.000205000
6	1.055156000	-1.533643000	-0.000224000
6	2.005900000	-0.540472000	-0.000175000
6	1.615891000	0.848997000	0.000016000
1	-3.588138000	2.084496000	0.000208000
1	-1.845290000	3.880131000	0.000156000
1	0.571945000	3.211054000	0.000096000
8	-1.147631000	-2.315362000	-0.000394000
8	2.456239000	1.790252000	0.000165000
7	-3.358808000	-0.394787000	0.000137000
6	-3.595348000	-1.151896000	1.225040000
1	-3.476525000	-0.486573000	2.085052000
1	-4.633831000	-1.508633000	1.219812000
1	-2.923080000	-2.011550000	1.339188000
6	-3.595692000	-1.151397000	-1.224978000
1	-2.922989000	-2.010606000	-1.340006000
1	-4.633927000	-1.508838000	-1.219224000
1	-3.477908000	-0.485576000	-2.084756000
7	3.399480000	-0.922690000	-0.000186000
6	4.115367000	-0.527445000	-1.212871000
1	3.566821000	-0.887822000	-2.086821000
1	4.244193000	0.561107000	-1.302891000
1	5.103504000	-1.004160000	-1.213985000
6	4.114895000	-0.528550000	1.213159000
1	5.103271000	-1.004760000	1.213935000
1	4.243189000	0.559965000	1.304438000
1	3.566321000	-0.890231000	2.086551000

1	1.379281000	-2.569204000	-0.000371000
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8 (RAiii)

6	-2.179008000	0.315619000	-0.049810000
6	-2.564811000	1.658188000	-0.037859000
6	-1.622605000	2.695234000	0.014941000
6	-0.279521000	2.399378000	0.078601000
6	0.160627000	1.061885000	0.045715000
6	-0.777483000	-0.015010000	-0.048207000
6	-0.252254000	-1.389444000	-0.225894000
6	1.181556000	-1.532858000	-0.207545000
6	2.082016000	-0.506690000	-0.056132000
6	1.625670000	0.855472000	0.077280000
1	-3.617454000	1.911291000	-0.039233000
1	-1.962709000	3.727115000	0.027074000
1	0.479154000	3.169779000	0.140112000
8	-0.975709000	-2.407759000	-0.399453000
8	2.420464000	1.828939000	0.203061000
7	-3.182073000	-0.685126000	-0.086963000
6	-4.493143000	-0.316418000	-0.571679000
1	-4.409430000	0.262947000	-1.493337000
1	-5.050405000	-1.233035000	-0.792014000
1	-5.097798000	0.267863000	0.151319000
6	-3.258432000	-1.591894000	1.049088000
1	-3.799857000	-1.126953000	1.896120000
1	-3.788830000	-2.503117000	0.755468000
1	-2.264984000	-1.886082000	1.368557000
7	3.492334000	-0.824037000	-0.048161000
6	4.224392000	-0.270913000	-1.187098000
1	3.721534000	-0.562737000	-2.112638000
1	4.301740000	0.825957000	-1.160044000
1	5.234822000	-0.698429000	-1.202296000
6	4.151324000	-0.529174000	1.223537000
1	5.160923000	-0.958777000	1.209403000
1	4.224614000	0.548174000	1.432450000
1	3.594451000	-1.004855000	2.034951000
1	1.554398000	-2.544702000	-0.328525000