Electronic Supplementary Information for: Double-bond delocalization in non-alternant hydrocarbons induces inverted singlet-triplet gaps

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Additional figures

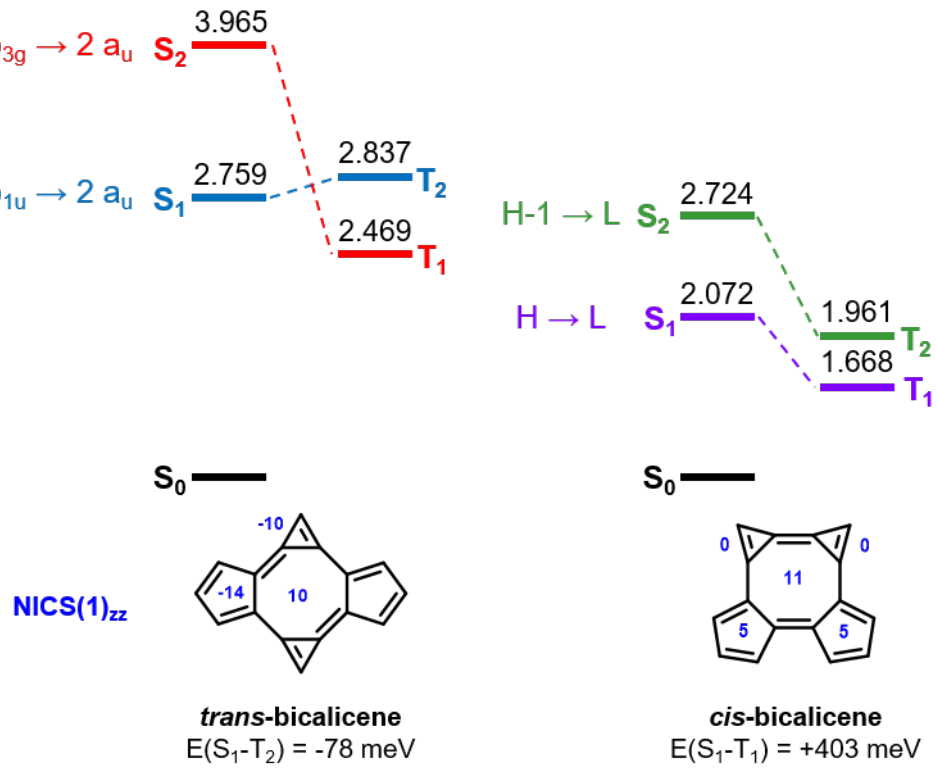

Figure S1: State diagram of the *trans* and *cis* dimers of calicene. The push-pull aromatic *trans*-bicalicene has a Hund's rule violation between the S_1 and T_2 states.[1–3] The hypothetical *cis*-bicalicene is non-planar as it distorts to escape antiaromaticity and has a conventional state ordering that follows Hund's rule. Geometries relaxed at the ωB97X-D/def2-TZVP level; excited state energies computed at the EOM-CCSD/cc-pVDZ level; nucleus-independent chemical shifts evaluated at the B3LYP/6-31G(d)[4,5] level using the out-of-plane components of the magnetic shielding tensor at 1 Å above the centroid of each ring[6] ($NICS(1)_{zz}$, in blue) using the gauge-independent atomic orbital method.[7,8]

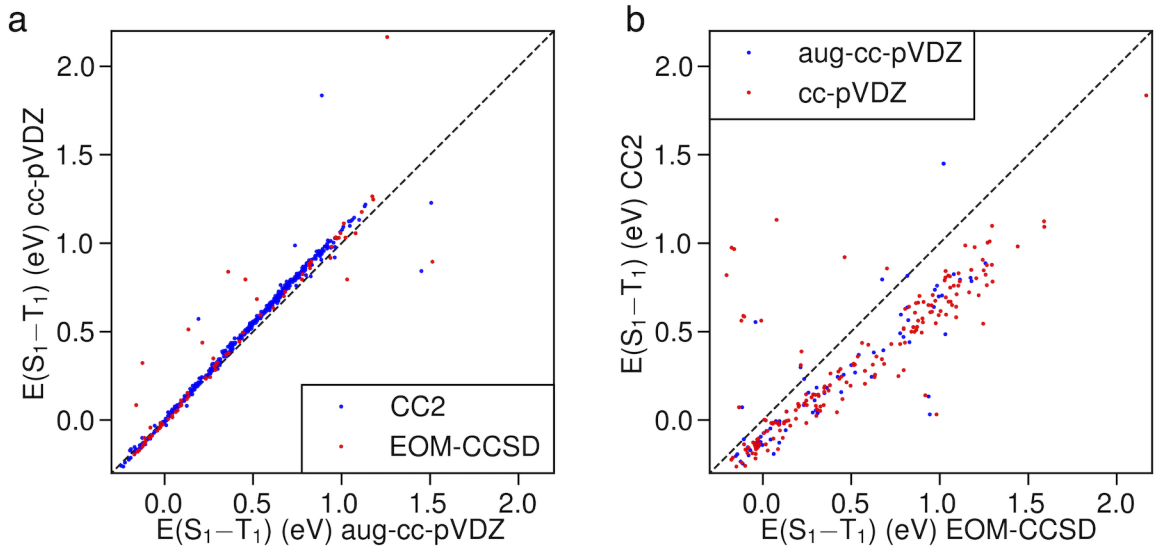

Figure S2: Method comparison of singlet-triplet gap computations based on all three sets of molecules (unsubstituted, constrained, and substituted molecules). a) cc-pVDZ basis plotted against aug-cc-pVDZ basis. b) CC2 plotted against EOM-CCSD. There are several outliers in the two plots where the two methods result in states of different electronic configurations corresponding to S_1 or T_1, thus severely affecting the gap.

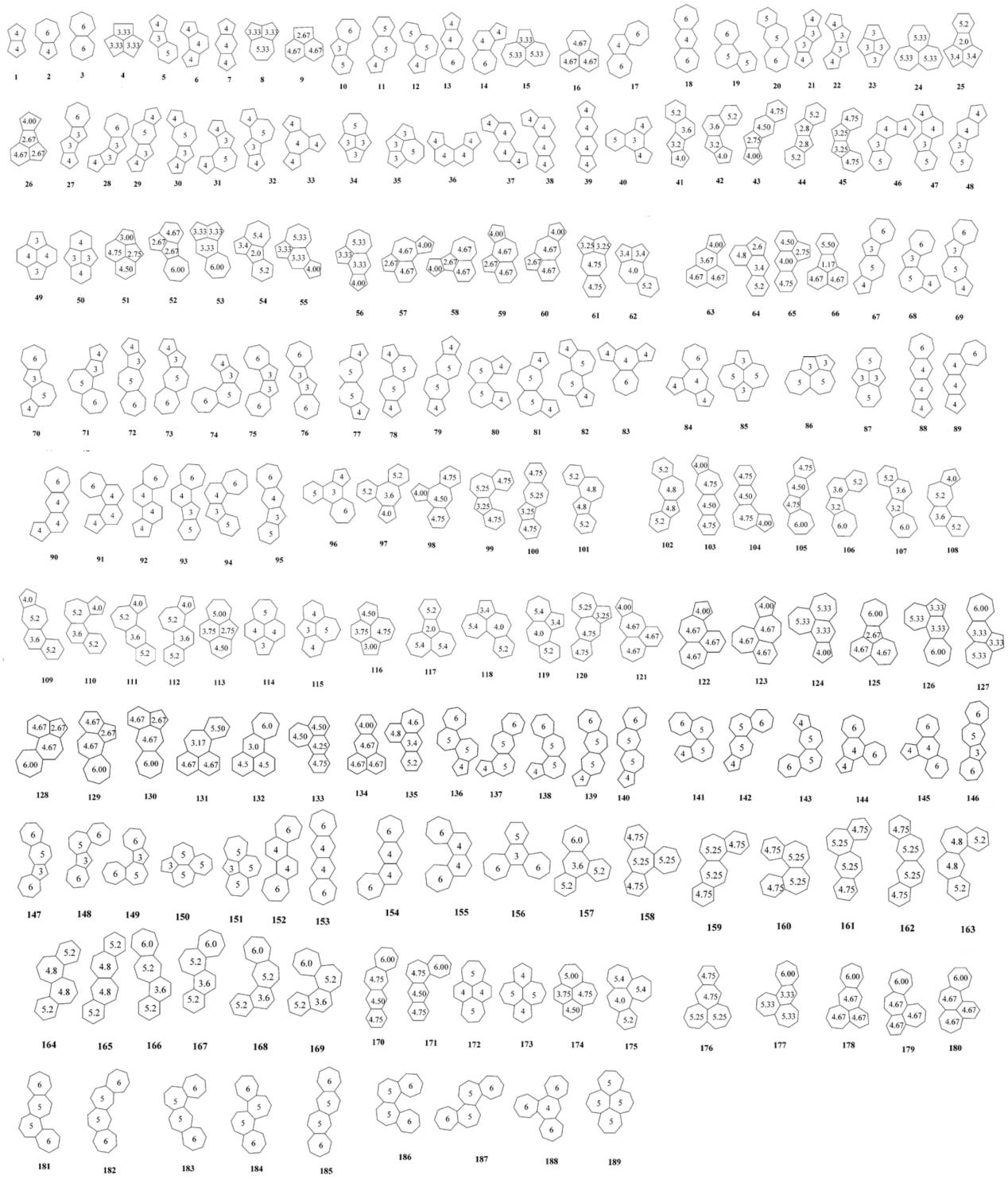

Figure S3: The complete set of 187 fused non-alternant hydrocarbons, with the total number of π-electrons partitioned by each ring. In the original set of 189 molecules, entries 159 and 161 are duplicates, as are entries 184 and 187. Adapted from Balaban & Randic, *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 1701-1707, © 2023 American Chemical Society.

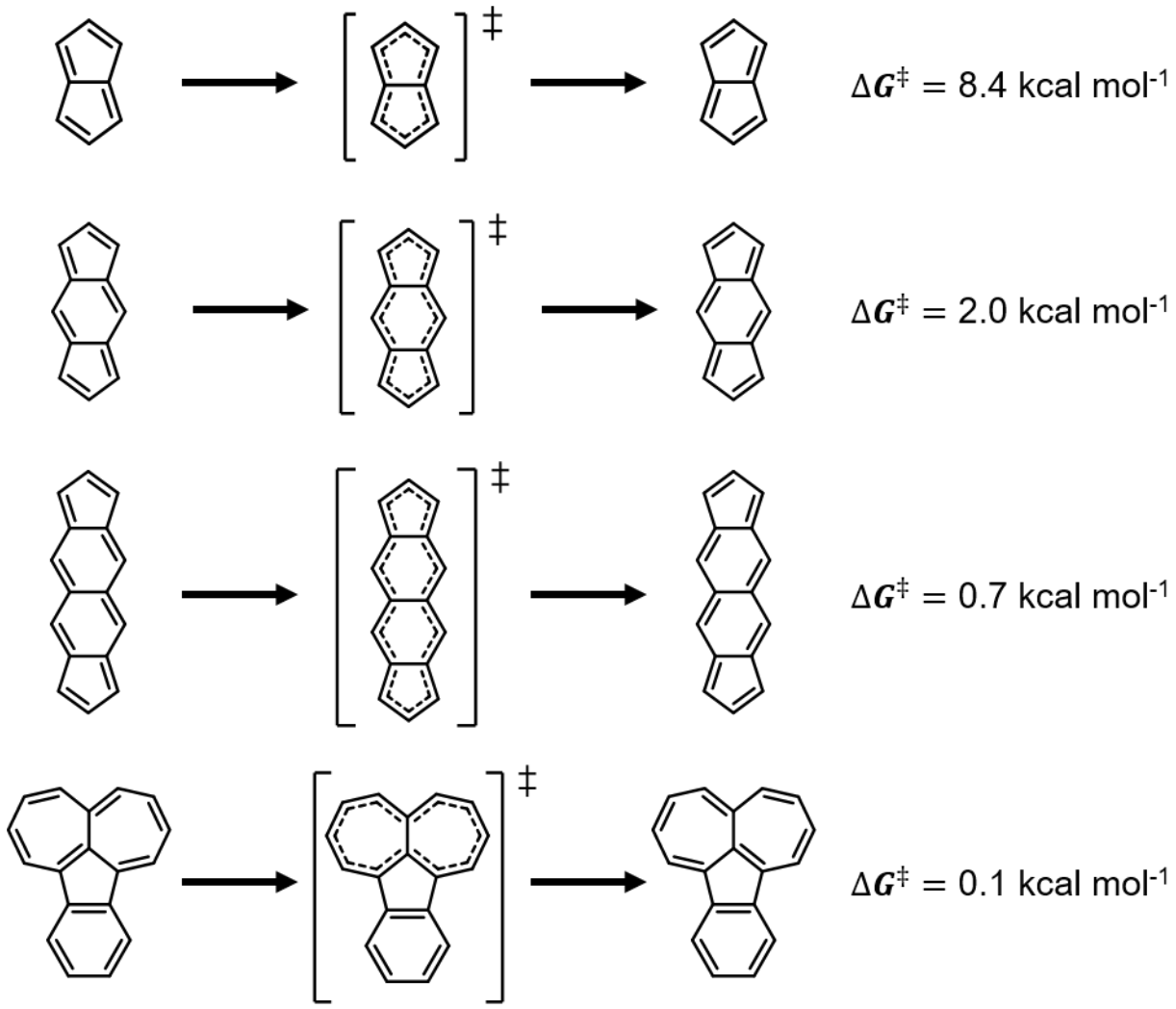

Figure S4: Free energy difference between the double-bond localized ground-state structures and the high-symmetry transition states structures for unsubstituted pentalene, *s*-indacene, dicyclopenta[b, g]naphthalene, and indeno[1,2,3-ef]heptalene. Structures computed at the ωB97X-D/def2-TZVP level. Transition states were confirmed by the presence of a single negative frequency, which in each case corresponded to the expected vibrational mode connecting the (equivalent) left and right bond-localized minima.

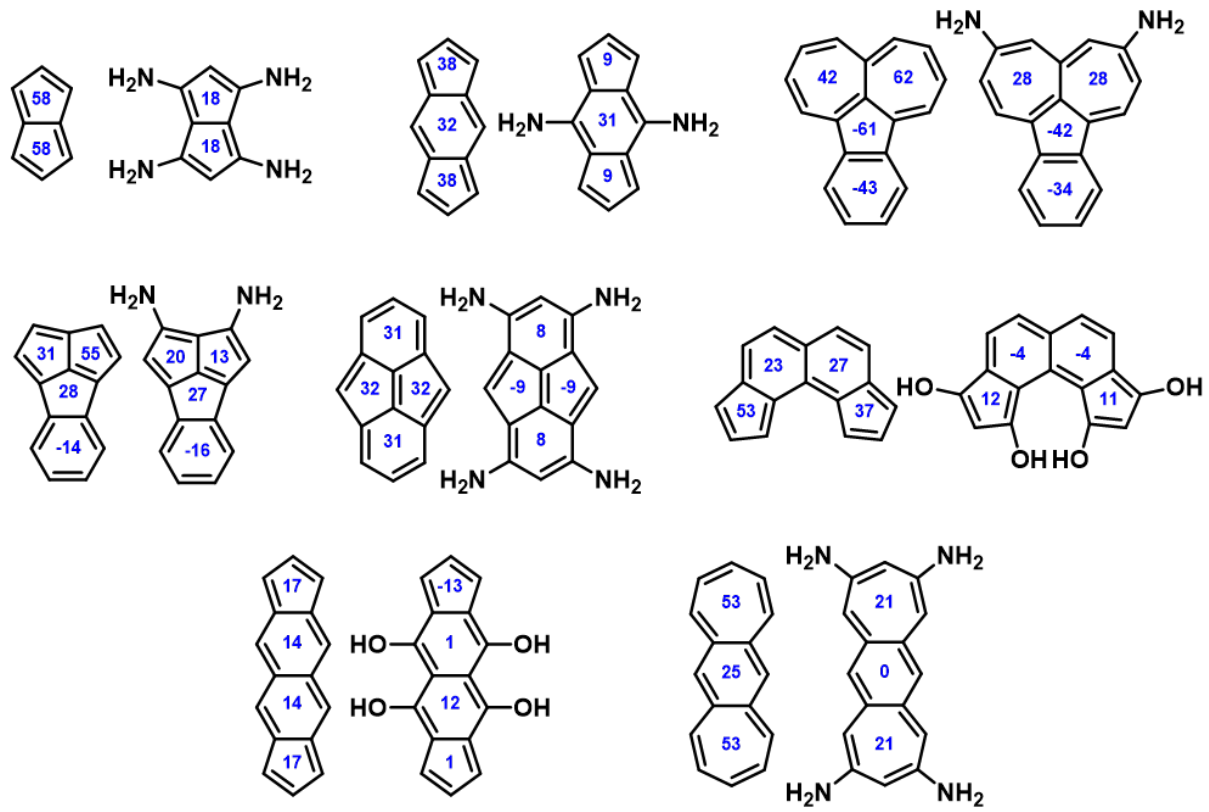

Figure S5: Nucleus-independent chemical shifts for the unconstrained ground-state structures of bare and substituted non-alternant hydrocarbons, computed using the out-of-plane components of the magnetic shielding tensor at 1 Å above the centroid of each ring[6] ($NICS(1)_{zz}$) using the gauge-independent atomic orbital method.[7,8] Geometries relaxed at the ωB97X-D/def2-TZVP level; NICS computed at the B3LYP/6-31G(d)[4,5] level of theory.

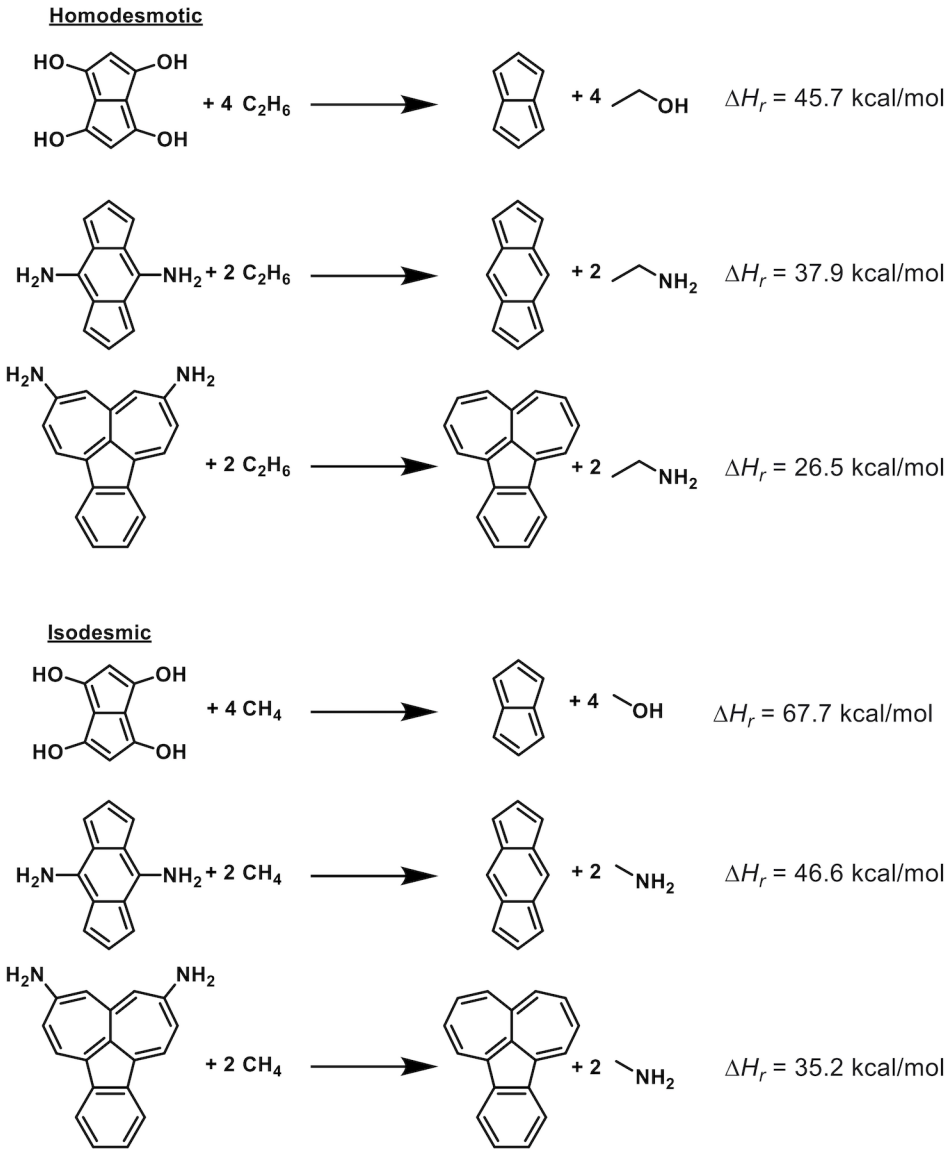

Figure S6: Thermodynamic stabilization of select substituted molecules estimated by homodesmotic and isodesmic reaction equations; computed at the ωB97X-D/def2-TZVP level using the ground-state geometries.[9]

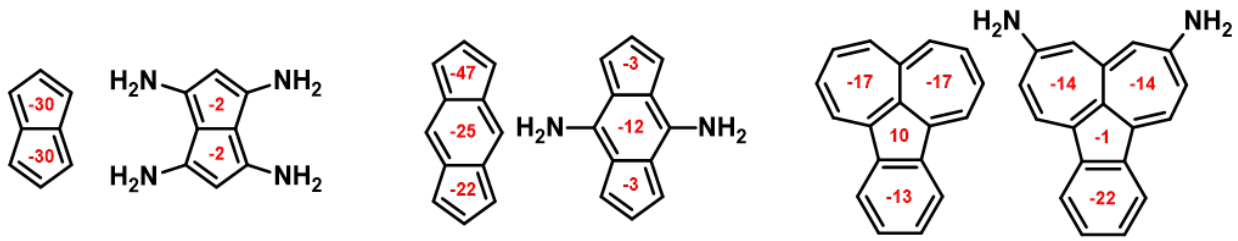

Figure S7: NICS of the optimized T_1 structures of select non-alternant hydrocarbons, computed using the out-of-plane components of the magnetic shielding tensor at 1 Å above the centroid of each ring[6] ($NICS(1)_{zz}$) using the gauge-independent atomic orbital method.[7,8] Geometries were relaxed using unrestricted DFT at the ωB97X-D/def2-TZVP level; NICS computed at the B3LYP/6-31G(d)[4,5] level of theory.

Data tables

Table S1: Singlet-triplet gaps computed for the non-alternant hydrocarbon set; T_x is the triplet state with the same electron configuration as S_1. Energies are given in eV.

	CC2		EOM-CCSD			
	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	cc-pVDZ
Name	S_1-T_1 gap	S_1-T_1 gap	S_1-T_1 gap	S_1-T_x gap	S_1-T_1 gap	S_1-T_x gap
mol1	0.792	0.856	1.019	1.019	1.088	1.088
mol2	-0.005	-0.021	0.073	0.073	0.055	0.055
mol3	0.637	0.702	0.817	0.817	0.886	0.886
mol4	0.759	0.831			1.106	1.106
mol5	0.698	0.752				
mol6	0.699	0.750	0.994	0.994	1.058	1.058
mol7	0.269	0.318	0.521	0.521	0.685	0.555
mol8	-0.023	-0.026	0.093	0.093	0.091	0.091
mol9	0.752	0.805				
mol10	0.342	0.379				
mol11	0.395	0.431	0.681	0.681	0.725	0.725
mol12	0.300	0.328				
mol13	0.190	0.214			0.472	0.472
mol14	0.424	0.462				
mol15	-0.012	-0.017	0.089	0.089	0.081	0.081
mol16	0.705	0.785	1.012	1.012	1.112	1.112
mol17	0.471	0.521				
mol18	0.376	0.437			0.560	0.560
mol19	0.698	0.773				
mol20	0.650	0.712			1.095	1.095
mol21	0.314	0.345			0.673	0.673
mol22	0.544	0.582			1.092	1.092
mol23	0.641	0.694	0.966	0.966	1.033	1.033
mol24	0.591	0.657				
mol25	0.645	0.708			0.960	0.960
mol26	0.605	0.650				
mol27	0.379	0.410				
mol28	0.382	0.411				
mol29	0.297	0.331				
mol30	0.385	0.405				
mol31	0.393	0.430				
mol32	0.438	0.463				
mol33	0.510	0.553			0.904	0.904
mol34	0.181	0.190				
mol35	-0.005	-0.011	0.093	0.093	0.085	0.085
mol36	0.542	0.597			1.035	0.667
mol37	0.511	0.561				
mol38	0.666	0.721				
mol39	0.786	0.848	1.178	0.283	1.248	0.305
mol40	0.586	0.632				
mol41	0.651	0.703				
mol42	0.652	0.705				
mol43	0.687	0.742				
mol44	0.556	0.600				
mol45	0.606	0.650			0.953	0.953
mol46	0.701	0.758				
mol47	0.726	0.788				
mol48	0.649	0.709				
mol49	0.641	0.686				
mol50	0.708	0.761			1.104	1.104
mol51	0.644	0.694				
mol52	0.417	0.463				
mol53	0.070	0.085			0.344	0.344
mol54	0.010	0.007				
mol55	0.287	0.314			0.622	0.622
mol56	0.272	0.301				
mol57	0.306	0.331				
mol58	0.490	0.535				
mol59	0.372	0.403				
mol60	0.572	0.628				
mol61	0.368	0.388			0.218	0.218
mol62	0.077	0.083			0.205	0.205
mol63	0.843	0.913				
mol64	0.878	0.927				
mol65	0.853	0.913				
mol66	0.961	0.921				
mol67	0.108	0.112			0.245	0.245
mol68	0.075	0.077			0.202	0.202
mol69	0.245	0.247	0.422	0.087	0.445	0.120
mol70	0.300	0.290	0.213	0.163	0.438	0.163
mol71	0.573	0.615				
mol72	0.492	0.523				
mol73	0.541	0.576			0.901	0.901
mol74	0.438	0.481				
mol75	0.264	0.275				
mol76	0.057	0.057			0.186	0.186
mol77	0.019	0.045			0.418	0.107
mol78	0.120	0.137				
mol79	0.131	0.134				

	CC2		EOM-CCSD			
	aug-cc-pvdz	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	cc-pVDZ
Name	S_1-T_1 gap	S_1-T_1 gap	S_1-T_1 gap	S_1-T_x gap	S_1-T_1 gap	S_1-T_x gap
mol81	0.129	0.134				
mol82	0.128	0.133				
mol83	0.523	0.563			0.878	0.878
mol84	0.500	0.545				
mol85	-0.047	-0.061	0.042	0.042	0.026	0.026
mol86	0.065	0.064				
mol87	-0.123	-0.132	-0.014	-0.014	-0.021	-0.021
mol88	0.591	0.651			1.069	1.069
mol89	0.659	0.704				
mol90	0.485	0.535				
mol91	0.390	0.432				
mol92	0.380	0.424				
mol93	0.801	0.887				
mol94	0.710	0.779				
mol95	0.512	0.564				
mol96	0.395	0.463				
mol97	0.664	0.723				
mol98	-0.010	-0.016			0.245	0.068
mol99	0.314	0.334				
mol100	0.422	0.451				
mol101	0.494	0.554				
mol102	0.385	0.437				
mol103	0.578	0.628				
mol104	0.458	0.501				
mol105	0.477	0.528			0.872	0.872
mol106	0.135	0.149				
mol107	0.137	0.148				
mol108	0.183	0.190				
mol109	0.190	0.199				
mol110	0.145	0.157				
mol111	0.458	0.501				
mol112	0.140	0.148				
mol113	0.358	0.416				
mol114	0.495	0.535				
mol115	0.203	0.212				
mol116	0.422	0.463				
mol117	0.086	0.091	0.231	0.231	0.239	0.239
mol118	0.023	0.021				
mol119	0.025	0.022				
mol120	0.235	0.251				
mol121	0.482	0.534				
mol122	0.468	0.515				
mol123	0.484	0.526			0.850	0.850
mol124	0.306	0.345				
mol125	0.337	0.365				
mol126	0.268	0.290				
mol127	0.334	0.360			0.642	0.020
mol128	0.673	0.734				
mol129	0.466	0.515				
mol130	0.543	0.597				
mol131	0.922	1.016				
mol132	0.720	0.794				
mol133	0.805	0.890				
mol134	0.805	0.877	1.173	1.173	1.265	1.265
mol135	0.782	0.868				
mol136	0.004	-0.003			0.135	0.135
mol137	0.034	0.029				
mol138	0.028	0.026				
mol139	0.571	0.627				
mol140	0.542	0.594				
mol141	0.010	-0.001			0.146	0.056
mol142	0.042	0.037				
mol143	0.000	-0.011			0.120	0.073
mol144	0.651	0.722				
mol145	0.664	0.728				
mol146	0.111	0.110				
mol147	0.461	0.513				
mol148	0.062	0.059				
mol149	0.072	0.068				
mol150	0.027	0.028				
mol151	-0.009	-0.013			0.066	0.066
mol152	0.790	0.843				
mol153	0.853	0.922			0.462	0.462
mol154	0.696	0.762				
mol155	0.648	0.706			1.219	0.673
mol156	0.454	0.499				
mol157	0.816	0.903				
mol158	1.040	1.124			1.589	1.589
mol159	0.850	0.920				

	CC2		EOM-CCSD			
	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	cc-pVDZ
Name	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_x gap**	**S_1-T_1 gap**	**S_1-T_x gap**
mol160	1.009	1.093			1.591	1.591
mol162	0.762	0.823			1.259	1.259
mol163	0.773	0.842				
mol164	0.754	0.829				
mol165	0.542	0.595			0.993	0.993
mol166	0.613	0.671			1.061	1.061
mol167	0.684	0.752				
mol168	0.613	0.671				
mol169	0.871	0.957				
mol170	0.669	0.731				
mol171	0.711	0.794				
mol172	0.494	0.545			1.245	1.245
mol173	0.852	0.929				
mol174	0.618	0.687				
mol175	0.597	0.665				
mol176	0.638	0.709				
mol177	0.625	0.702				
mol178	0.721	0.797				
mol179	0.665	0.747				
mol180	0.714	0.783				
mol181	0.621	0.682				
mol182	0.563	0.617			1.004	1.004
mol183	0.668	0.734				
mol184	0.680	0.764			1.265	1.265
mol185	0.607	0.670			1.049	1.049
mol186	0.639	0.706				
mol188	0.689	0.784			1.297	1.297
mol189	0.577	0.647				

Table S2: Singlet-triplet gaps computed for the avoided symmetry set; T_x is the triplet state with the same electron configuration as S_1. Energies are given in eV.

		CC2		**EOM-CCSD**			
		aug-cc-pVDZ	**cc-pVDZ**	**aug-cc-pVDZ**	**aug-cc-pVDZ**	**cc-pVDZ**	**cc-pVDZ**
Name	**Description**	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_x gap**	**S_1-T_1 gap**	**S_1-T_x gap**
mol1_d2h	D_{2h} pentalene	-0.234	-0.263	-0.126	-0.126	-0.150	-0.150
mol3_d2h	D_{2h} heptalene	-0.203	-0.223	-0.153	-0.153	-0.178	-0.178
mol3_d2	curved D_2, no BLA	-0.192	-0.211	-0.145	-0.145	-0.170	-0.170
mol4_c2v	planar, BLA in one ring	0.737	0.791	0.971	0.971	1.027	1.027
mol4_d3h	planar	0.246	0.258	0.614	0.614	0.634	0.634
mol7_d2h	D_{2h} indacene	-0.191	-0.163	0.061	-0.161	0.085	-0.184
mol13_c2v	planar, C_{2v}	-0.060	-0.072	0.021	0.021	0.008	0.008
mol18_d2h	planar, D_{2h}	0.039	0.053	0.309	-0.125	0.324	-0.149
mol21_c2h	planar, C_{2h}	-0.008	-0.018	0.125	0.125	0.119	0.119
mol22_c2v	planar, C_{2v}	0.311	0.312	0.500	0.134	0.513	0.113
mol23_c2v	curved, C_{2v}, no BLA	0.471	0.501	0.794	0.358	0.840	0.366
mol23_d2h	planar, D_{2h}	0.184	0.191	0.303	0.275	0.350	0.278
mol24_c2v	planar, C_{2v}, with BLA	0.555	0.611			0.947	0.947
mol24_d3h	planar, D_{3h}		-0.186	-0.041	-0.159	-0.059	-0.180
mol25_c2v	planar, C_{2v}, no BLA	0.073	0.074	-0.117	-0.117	-0.135	-0.135
mol25_cs	curved C_s, no BLA	-0.122	-0.140	-0.030	-0.030	-0.046	-0.046
mol33_c2v	planar, C_{2v}	0.156	0.147	0.258	0.258	0.243	0.243
mol34_c2v	planar, C_{2v}	0.183	0.198	0.361	0.361	0.379	0.379
mol35_c2v	planar, C_{2v}	-0.007	-0.014	0.093	0.093	0.085	0.085
mol36_c2	curved, C_2, no BLA	0.043	0.062	0.282	-0.127	0.306	-0.141
mol36_c2v	planar, C_{2v}, no BLA	0.057	0.078	0.299	-0.122	0.325	-0.136
mol39_d2h	planar, D_{2h}	0.566	0.608	0.822	-0.180	0.859	-0.201
mol45_c2v	planar, C_{2v}, no BLA	0.048	0.048	0.134	0.134	0.132	0.132
mol50_c2h	planar, C_{2h}, with BLA	0.795	0.850	1.114	1.114	1.177	1.177
mol50_c2v	curved, C_{2v}, no BLA	0.795	0.858	0.674	-0.139	0.701	-0.160
mol50_d2h	planar, D_{2h}	0.033	0.033	0.943	-0.140	0.981	-0.162
mol80_c2v	planar, C_{2v}	0.171	0.183			0.347	0.347
mol82_c2h	planar, C_{2h}	0.126	0.129			0.274	0.274
mol83_c2	curved, C_2, no BLA	0.259	0.264			0.382	0.020
mol83_c2v	planar, C_{2v}, no BLA	0.349	0.360			0.536	0.030
mol83_cs	planar, C_s, with BLA	0.383	0.399	0.627	0.1628		
mol88_c2v	planar, C_{2v}, no BLA	-0.073	-0.083	0.004	0.004		
mol117_c2v	planar, C_{2v}, no BLA	-0.093	-0.104	-0.012	-0.012	-0.026	-0.026
mol150_c2v	planar, C_{2v}	0.081	0.086			0.248	0.248
mol153_d2h	planar, D_{2h}	0.642	0.675			0.975	-0.155
mol155_c2	curved, C_2, no BLA	0.110	0.119			0.449	-0.105
mol155_c2v	planar, C_{2v}, no BLA	0.210	0.244			0.631	-0.067
mol158_c2	curved, C_2, no BLA	-0.124	-0.136			-0.107	-0.107
mol158_c2v	planar, C_{2v}, no BLA	-0.139	-0.155			-0.082	-0.115
mol160_c2	curved, C_2, no BLA	0.090	0.093			0.199	0.199
mol160_c2v	planar, C_{2v}, no BLA	0.142	0.144			0.295	0.295
mol162_c2	curved, C_2, no BLA	-0.012	-0.016			0.048	0.048
mol162_c2v	planar, C_{2v}, no BLA	-0.010	-0.015			0.054	0.054
mol182_c2v	planar, C_{2v}, no BLA	0.394	0.431			0.775	0.775
mol184_c2_in	curved, C_2, no BLA	0.020	0.024			0.302	-0.126
mol184_c2_out	curved, C_2, no BLA	0.661	0.722			1.165	1.165
mol184_c2h	planar, C_{2h}	0.461	0.510			0.866	0.866
mol185_c2h	planar, C_{2h}, no BLA	-0.048	-0.058			0.096	-0.049
mol185_cs	plarnar, C_s, with bla	0.400	0.438			0.803	0.803
mol186_cs	curved, C_s, no BLA	0.482	0.548			0.977	0.977
mol188_c2	curved, C_2, no BLA	0.009	-0.001			0.017	-0.015
mol188_c2v	planar, C_{2v}, no BLA	0.015	0.003			0.008	0.008

Table S3: Singlet-triplet gaps computed for the substituted set; T_x is the triplet state with the same electron configuration as S_1. Energies are given in eV.

	CC2		EOM-CCSD			
	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ		cc-pVDZ	
	S_1-T_1 gap	S_1-T_1 gap	S_1-T_1 gap	S_1-T_x gap	S_1-T_1 gap	S_1-T_x gap
mol1_1n_2nme_tbu	-0.080	-0.104			0.060	0.060
mol1_1n_2nme	-0.109	-0.136	0.043	0.043	0.017	0.017
mol1_2n_2nme	0.125	0.082			0.299	-0.069
mol1_1n_2nh2			0.019	0.019		
mol1_2n_4nh2	0.826	0.814	1.079	-0.202	1.057	-0.214
mol1_2n_4nme2	0.944	0.978			1.196	-0.187
mol1_2n_2nh2			0.281	-0.079		
mol1_2n	0.369	0.426	0.542	0.542	0.596	0.596
mol1_2nh	0.888	1.835	1.258	0.029	2.166	2.166
mol1_2nh2_1	-0.147	-0.164	-0.024	-0.024	-0.038	-0.038
mol1_2nh2_2	0.597	0.642	0.779	0.779	0.826	0.826
mol1_2nme2	-0.133	-0.157			-0.031	-0.031
mol1_4nh2	-0.057	-0.031	0.129	-0.112	0.154	-0.120
mol1_2oh_1	0.145	0.147	0.287	0.287	0.285	0.285
mol1_2oh_2	0.761	0.806	0.984	0.984	1.032	1.032
mol1_2ome	0.089	0.095	0.233	0.233	0.235	0.235
mol1_4oh_1	-0.244	-0.258	-0.115	-0.130	-0.100	-0.141
mol1_4oh_1alt	-0.140	-0.141			-0.027	-0.027
mol1_4me	0.605	0.664	0.816	0.816	0.877	0.877
mol1_4ome	-0.224	-0.240	-0.108	-0.108	-0.120	-0.120
mol3_4nh2	0.545	0.613			0.955	0.955
mol3_2cf3	0.622	0.676			1.047	1.047
mol7_1n	0.441	0.496	0.829	0.829	0.897	0.897
mol7_1p	0.158	0.196	0.443	0.443	0.496	0.496
mol7_1p2cl	0.203	0.235			0.432	0.432
mol7_1p2ome	0.278	0.319			0.514	0.514
mol7_2n	0.134	0.141	0.936	0.879	0.918	0.918
mol7_2p	-0.127	-0.100	0.092	-0.121	0.113	-0.146
mol7_2p2cl	0.112	0.136	0.292	0.139	0.316	0.129
mol7_2p2ome	0.269	0.314			0.520	0.305
mol7_2nh	0.153	0.168	0.348	0.348	0.371	0.371
mol7_2cn26	0.175	0.206			0.576	0.430
mol7_2nh2_1	-0.168	-0.185	-0.072	-0.072	-0.088	-0.088
mol7_2nh2_2	0.486	0.515	1.031	1.031	0.796	0.796
mol7_2nme2_1	-0.171	-0.191			-0.037	-0.096
mol7_2oh_1	-0.199	-0.216	-0.081	-0.113	-0.042	-0.130
mol7_2oh_2	0.492	0.520	0.776	0.776	0.810	0.810
mol7_2oh_3	0.257	0.283	0.456	-0.108	0.476	-0.126
mol7_2me	0.251	0.280			0.577	0.521
mol7_2ome	-0.196	-0.172	-0.002	-0.110	0.027	-0.128
mol7_4oh	1.451	0.843	1.022	-0.172	1.033	-0.194
mol7_4nh2	1.046	1.098			1.295	-0.218
mol7_4oh	1.451	0.843	1.021	-0.172	1.033	-0.193
mol7_4ome	0.636	0.662			0.864	-0.176
mol18_4cn_center	0.268	0.311			0.214	0.214
mol18_4nh2_out	0.593	0.629			0.804	-0.305
mol18_diquino	0.737	0.988			1.143	0.359
mol18_tetraquino	0.237	0.250			0.766	0.315
mol24_3nh2	0.450	0.500			0.857	0.857
mol25_2nh2_1	0.149	0.161			0.347	-0.022
mol25_2nh2_2	0.261	0.274			0.426	0.426
mol25_2oh_1	0.006	0.008			0.187	-0.038
mol36_2nh2_2me	0.746	0.802			1.206	0.198
mol36_2nme	0.885	0.907			1.242	0.065
mol36_2nme_2me	0.743	0.761			1.079	-0.022
mol36_2ome	0.832	0.878			1.294	0.421
mol36_4oh	0.892	0.968			1.234	-0.163
mol36_4ome	0.954	1.004			1.270	-0.176
mol36_4nh2	0.931	1.011			1.282	-0.233
mol39_2nh2	0.799	0.819			1.120	-0.205
mol39_2oh	0.939	0.975			1.200	-0.177
mol39_4nh2	1.099	1.133			1.520	0.078
mol39_4oh	0.531	0.587			0.771	-0.105
mol50_2nh2_pent	0.619	0.669			0.908	0.908
mol50_2oh_benz	0.518	0.563			0.654	-0.009
mol50_2oh_pent	0.609	0.651			0.935	0.935
mol50_4nh2_benz	0.521	0.590			0.744	-0.111
mol50_4oh_benz	0.522	0.563			0.676	-0.121
mol117_2cn	-0.116	-0.126			-0.055	-0.055
mol117_2nh2	-0.150	-0.166			-0.095	-0.095
mol117_2oh_benz	-0.099	-0.109			-0.032	-0.032
mol117_2oh	-0.153	-0.166	-0.085	-0.085	-0.099	-0.099
mol117_2ome	-0.118	-0.129			-0.046	-0.046
mol117_4oh_1	-0.170	-0.151			-0.041	-0.041
mol117_4oh_2	0.139	0.145			0.313	0.313
mol158_2nh2	0.905	0.983			1.440	1.440
mol184_4cn	0.592	0.641			1.092	1.092

Table S4: Oscillator strengths for select avoided symmetry molecules computed using Tamm-Dancoff approximated time-dependent density functional theory at the ωB97X-D/def2-TZVP level. Energies are given in eV.

Name	$E(S_1)$	$E(T_1)$	$f(S_1)$
mol1_d2h	0.390	0.153	0.0000
mol3_d2	0.568	0.370	0.0000
mol3_d2h	0.448	0.253	0.0000
mol7_d2h	1.040	0.770	0.0000
mol13_c2v	1.388	1.006	0.0078
mol18_d2h	1.027	0.525	0.0000
mol21_c2h	1.265	0.754	0.0065
mol23_d2h	1.305	0.873	0.0010
mol24_c2v	1.581	0.911	0.0120
mol24_d3h	-0.241	-0.516	0.0003
mol25_c2v	0.225	0.011	0.0001
mol25_cs	1.210	0.976	0.0000
mol35_c2v	1.186	0.832	0.0043
mol36_c2	0.415	-0.051	0.0008
mol36_c2v	0.399	-0.082	0.0007
mol39_d2h	1.434	0.403	0.0000
mol45_c2v	0.404	0.036	0.0006
mol50_c2h	1.339	0.181	0.0397
mol50_c2v	1.023	0.114	0.0000
mol50_d2h	0.684	-0.468	0.0000
mol80_c2v	2.506	1.933	0.0454
mol117_c2v	1.086	0.845	0.0012
mol158_c2	0.621	0.461	0.0022
mol158_c2v	0.473	0.299	0.0020
mol162_c2	0.410	0.124	0.0014
mol162_c2v	0.269	-0.021	0.0011
mol185_c2h	0.628	0.312	0.0040
mol185_cs	1.507	0.935	0.0041
mol188_c2	1.029	0.624	0.0238
mol188_c2v	0.714	0.311	0.0192

Table S5: Oscillator strengths for select substituted molecules computed using Tamm-Dancoff approximated time-dependent density functional theory at the ωB97X-D/def2-TZVP level. Energies are given in eV.

Name	$E(S_1)$	$E(T_1)$	$f(S_1)$
mol1_1n_2nh2	2.324	1.995	0.0061
mol1_1n_2nme	2.549	2.219	0.0067
mol1_1n_2nme_tbu	2.452	2.088	0.0076
mol1_2n	2.331	1.637	0.0000
mol1_2n_2nh2	2.763	2.248	0.0007
mol1_2n_2nme	2.992	2.457	0.0002
mol1_2n_4nh2	3.223	1.835	0.0000
mol1_2n_4nme2	3.083	1.592	0.0000
mol1_2nh	4.340	2.154	0.2936
mol1_2nh2_1	1.759	1.481	0.0000
mol1_2nh2_2	1.763	0.953	0.0000
mol1_2nme2	1.892	1.625	0.0001
mol1_2oh_1	1.778	1.261	0.0023
mol1_2oh_2	1.972	1.065	0.0000
mol1_2ome	1.734	1.266	0.0030
mol1_4me	2.134	1.341	0.0000
mol1_4nh2	2.221	1.789	0.0000
mol1_4oh_1	2.036	1.806	0.0003
mol1_4oh_1alt	2.207	1.905	0.0000
mol1_4ome	1.903	1.672	0.0009
mol7_2nh2_1	1.846	1.604	0.0000
mol7_2nme2_1	1.988	1.765	0.0000
mol7_2oh_1	1.575	1.340	0.0001
mol7_2oh_2	1.661	0.980	0.0001
mol7_2oh_3	1.734	1.040	0.0003
mol7_2ome	1.642	1.413	0.0004
mol7_2p	1.498	1.146	0.0000
mol7_2p2cl	3.477	2.958	0.0000
mol7_2p2ome	4.161	3.492	0.0032
mol7_4nh2	2.270	0.667	0.0000
mol7_4oh	2.098	0.762	0.0000
mol7_4ome	2.137	0.962	0.0000
mol18_4cn_center	1.561	0.881	0.0000
mol18_4nh2_out	1.938	0.846	0.0000
mol25_2nh2_1	2.064	1.438	0.0104
mol25_2nh2_2	1.638	1.030	0.0065
mol25_2oh_1	1.969	1.499	0.0053
mol36_2nh2_2me	1.576	0.274	0.0071
mol36_2nme	1.359	-0.059	0.0051
mol36_2nme_2me	1.467	0.143	0.0025
mol36_2ome	1.487	0.274	0.0136
mol36_4nh2	1.854	0.302	0.1546
mol36_4oh	1.565	0.125	0.0501
mol36_4ome	1.567	0.078	0.0680
mol39_2nh2	2.187	0.814	0.0000
mol39_2oh	1.953	0.524	0.0026
mol39_4nh2	1.868	0.198	0.0000
mol39_4oh	2.249	1.264	0.0029
mol50_2oh_benz	1.546	0.671	0.0098
mol50_4nh2_benz	2.360	1.411	0.0000
mol50_4oh_benz	2.040	1.155	0.0000
mol117_2cn	1.175	0.970	0.0001
mol117_2nh2	1.656	1.471	0.0000
mol117_2oh	1.502	1.320	0.0000
mol117_2oh_benz	1.123	0.887	0.0018
mol117_2ome	1.525	1.332	0.0003
mol117_4oh_1	1.936	1.751	0.0021
mol117_4oh_2	1.211	0.798	0.0058

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