

Electronic Supplementary Information

Structure-Antioxidant Activity Relationships in Boldine and Glaucine: A DFT Study

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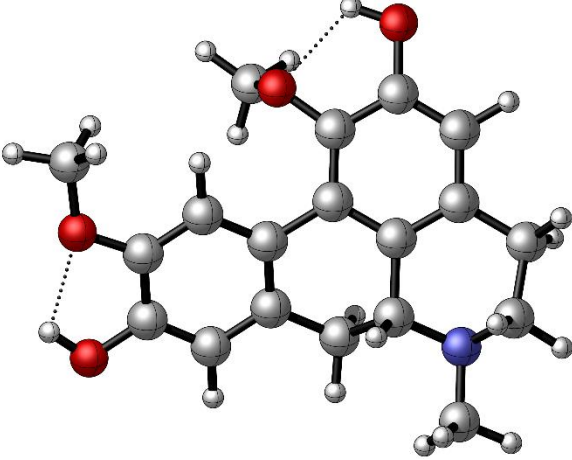
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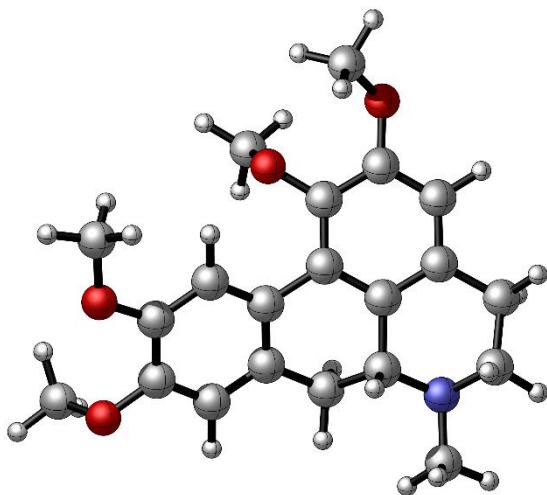
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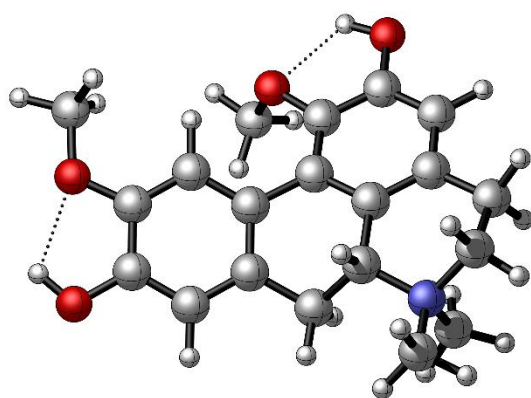
Table S1. Optimized structures at the M08-HX/6-31+G(d,p) level of **B**, **G**, **B-Me⁺** and **G-Me⁺**.

Strucutre	Cartesian coordinates (Å)			
 <p style="text-align: center;">B</p>	C	0.810865000	-0.193568000	0.020250000
	C	0.701801000	-1.510029000	0.493990000
	C	2.067741000	0.285166000	-0.401569000
	C	1.839902000	-2.320001000	0.574282000
	C	3.191943000	-0.523103000	-0.310156000
	C	3.079946000	-1.834397000	0.187082000
	C	-1.679639000	-0.014337000	-0.100010000
	C	-1.699513000	-1.537538000	-0.108867000
	C	-0.421662000	0.635160000	-0.021299000
	C	-0.654227000	-2.034240000	0.892191000
	C	-4.190334000	0.035738000	-0.306629000
	C	-4.008164000	-1.416718000	-0.707460000
	C	-2.857768000	0.734232000	-0.183084000
	N	-3.037342000	-2.075487000	0.171675000
	C	-2.809209000	2.132892000	-0.157304000
	C	-1.586959000	2.776810000	-0.040304000
	C	-0.399205000	2.035576000	0.028153000
	C	-3.062889000	-3.510790000	-0.109144000
	H	-1.382567000	-1.878771000	-1.123834000
	O	-1.535458000	4.143350000	0.007104000
	O	4.185427000	-2.633949000	0.278316000
	O	4.457936000	-0.154052000	-0.673079000
	O	0.762153000	2.781084000	0.126498000
	C	1.305195000	2.816009000	1.454538000
	C	4.642609000	1.199183000	-1.075046000
	H	2.157792000	1.292293000	-0.799770000
	H	1.763897000	-3.344954000	0.940534000
	H	-0.619237000	-3.129636000	0.930099000
	H	-0.927989000	-1.672830000	1.898625000
	H	-4.726301000	0.089479000	0.654102000
	H	-4.814146000	0.556177000	-1.047265000
	H	-3.674658000	-1.484675000	-1.765603000
	H	-4.964183000	-1.951477000	-0.633726000
	H	-3.724862000	2.722486000	-0.224264000
	H	-2.746060000	-3.732000000	-1.148170000
	H	-4.084215000	-3.887770000	0.025604000
	H	-2.412433000	-4.065665000	0.575674000
	H	-0.603116000	4.408794000	0.042199000
	H	4.960643000	-2.144829000	-0.035153000
	H	1.538974000	1.801257000	1.807548000
H	0.591887000	3.291665000	2.143578000	
H	2.224556000	3.409073000	1.404603000	
H	4.086979000	1.413169000	-1.999408000	
H	5.714426000	1.321185000	-1.255864000	
H	4.318945000	1.887696000	-0.279630000	



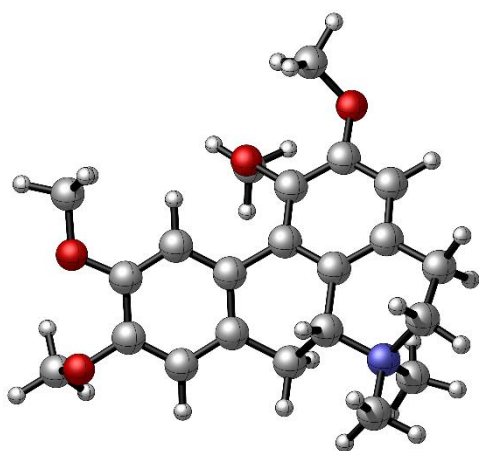
G

C	0.698797000	-0.132012000	-0.036414000
C	0.942627000	-1.447870000	0.389442000
C	1.769253000	0.656500000	-0.501659000
C	2.252637000	-1.937446000	0.393836000
C	3.068834000	0.154988000	-0.504366000
C	3.310117000	-1.149426000	-0.034592000
C	-1.755049000	-0.597876000	-0.089792000
C	-1.383992000	-2.072915000	-0.167373000
C	-0.708285000	0.352479000	-0.008656000
C	-0.219894000	-2.315836000	0.796436000
C	-4.203367000	-1.189170000	-0.216500000
C	-3.668733000	-2.523716000	-0.703389000
C	-3.089006000	-0.179760000	-0.084328000
N	-2.529582000	-2.947035000	0.116335000
C	-3.390037000	1.180554000	0.031332000
C	-2.376855000	2.123065000	0.150287000
C	-1.033975000	1.711394000	0.137820000
C	-2.196244000	-4.327578000	-0.232816000
H	-1.018154000	-2.282219000	-1.201148000
O	-2.740181000	3.433894000	0.338758000
O	4.593530000	-1.657757000	-0.058951000
O	4.158742000	0.840501000	-0.952429000
O	-0.052998000	2.663621000	0.302166000
C	0.144161000	3.014230000	1.675435000
C	3.941529000	2.164233000	-1.428013000
H	1.576109000	1.657077000	-0.875953000
H	2.460029000	-2.957040000	0.724145000
H	0.096267000	-3.365874000	0.790803000
H	-0.551330000	-2.070208000	1.820152000
H	-4.699653000	-1.323174000	0.757517000
H	-4.965836000	-0.810101000	-0.911822000
H	-3.368454000	-2.452140000	-1.771150000
H	-4.450565000	-3.291615000	-0.636785000
H	-4.427188000	1.520433000	0.030712000
H	-1.878624000	-4.419212000	-1.290858000
H	-3.078405000	-4.962085000	-0.082936000
H	-1.394763000	-4.718687000	0.403385000
H	0.462411000	2.132245000	2.252250000
H	-0.780352000	3.424943000	2.110378000
H	0.931733000	3.774851000	1.700913000
H	3.269062000	2.165541000	-2.298162000
H	4.923216000	2.544094000	-1.725887000
H	3.524954000	2.803445000	-0.635855000
C	-2.084591000	4.432862000	-0.452836000
H	-1.219601000	4.853284000	0.076535000
H	-1.762496000	4.016327000	-1.416591000
H	-2.824096000	5.222949000	-0.625977000
C	5.385579000	-1.209907000	1.049369000
H	4.955174000	-1.573336000	1.993831000
H	6.387364000	-1.630721000	0.914539000
H	5.446483000	-0.112377000	1.067940000



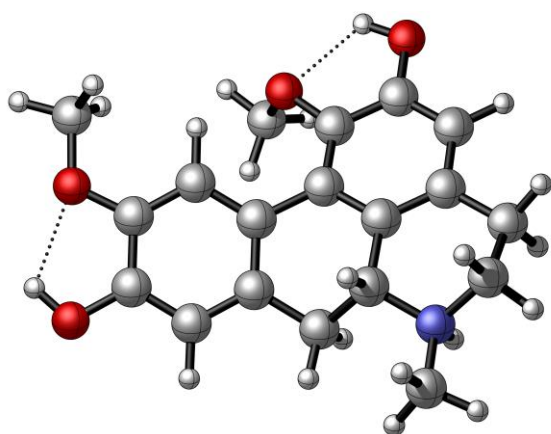
B-Me⁺

C	0.974674000	-0.183888000	-0.010995000
C	0.732256000	-1.498179000	0.412186000
C	2.281536000	0.188553000	-0.384577000
C	1.783225000	-2.416503000	0.494491000
C	3.321093000	-0.726303000	-0.295754000
C	3.072873000	-2.037295000	0.153376000
C	-1.484575000	0.234685000	-0.217365000
C	-1.615214000	-1.281055000	-0.258960000
C	-0.174296000	0.756228000	-0.063961000
C	-0.675692000	-1.898538000	0.775981000
C	-3.967200000	0.535076000	-0.561084000
C	-3.926673000	-0.915368000	-0.991171000
C	-2.580759000	1.090624000	-0.346879000
N	-3.052418000	-1.731061000	-0.072444000
C	-2.404507000	2.476582000	-0.274907000
C	-1.136015000	2.997527000	-0.075078000
C	-0.025931000	2.145060000	0.026922000
C	-3.193326000	-3.162879000	-0.478521000
H	-1.342277000	-1.652581000	-1.261449000
O	-0.960546000	4.346961000	0.017452000
O	4.093310000	-2.940233000	0.243589000
O	4.623816000	-0.469075000	-0.615659000
O	1.191083000	2.773963000	0.198176000
C	1.682693000	2.714067000	1.546752000
C	4.944928000	0.869564000	-0.979767000
H	2.475241000	1.195702000	-0.744081000
H	1.600591000	-3.439899000	0.824748000
H	-0.753775000	-2.992105000	0.798495000
H	-0.923381000	-1.513318000	1.778676000
H	-4.571927000	0.652771000	0.350925000
H	-4.479716000	1.104388000	-1.347910000
H	-3.497708000	-1.029752000	-1.996076000
H	-4.922850000	-1.373221000	-0.972196000
H	-3.256707000	3.150288000	-0.371223000
H	-2.911726000	-3.258615000	-1.532368000
H	-4.240523000	-3.450006000	-0.338312000
H	-2.555216000	-3.790165000	0.149698000
H	-0.011521000	4.524990000	0.113984000
H	4.920481000	-2.520042000	-0.035083000
H	1.806544000	1.670850000	1.870834000
H	0.990039000	3.233019000	2.225080000
H	2.654434000	3.218508000	1.549395000
H	4.432043000	1.155791000	-1.909270000
H	6.027064000	0.892580000	-1.136452000
H	4.671024000	1.566797000	-0.173570000
C	-3.514835000	-1.591608000	1.342998000
H	-4.603228000	-1.714861000	1.353584000
H	-3.049478000	-2.377625000	1.945444000
H	-3.237326000	-0.607081000	1.733633000



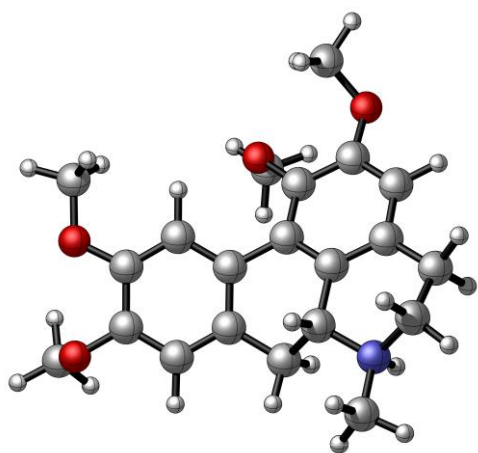
G-Me⁺

C	0.827531000	-0.098987000	-0.067814000
C	0.885543000	-1.445337000	0.323939000
C	2.002352000	0.549426000	-0.493792000
C	2.114214000	-2.110811000	0.337013000
C	3.221565000	-0.124408000	-0.490283000
C	3.275547000	-1.461774000	-0.053421000
C	-1.666758000	-0.225368000	-0.193943000
C	-1.457569000	-1.727829000	-0.308100000
C	-0.502590000	0.569068000	-0.053211000
C	-0.391237000	-2.153559000	0.701653000
C	-4.169369000	-0.472167000	-0.423979000
C	-3.823076000	-1.840177000	-0.970191000
C	-2.931819000	0.365062000	-0.217125000
N	-2.751093000	-2.501868000	-0.141575000
C	-3.053000000	1.748250000	-0.059753000
C	-1.927567000	2.541370000	0.117466000
C	-0.650029000	1.953218000	0.126118000
C	-2.575063000	-3.889317000	-0.671819000
H	-1.116048000	-1.981058000	-1.325957000
O	-2.118652000	3.880061000	0.334195000
O	4.477243000	-2.138360000	-0.072547000
O	4.400880000	0.417453000	-0.901671000
O	0.442707000	2.759127000	0.337575000
C	0.655013000	3.045536000	1.724780000
C	4.373807000	1.769670000	-1.346105000
H	1.952193000	1.576073000	-0.842890000
H	2.175219000	-3.156404000	0.643549000
H	-0.228067000	-3.238298000	0.697303000
H	-0.702438000	-1.855254000	1.716052000
H	-4.738541000	-0.558969000	0.513893000
H	-4.834980000	0.019495000	-1.145787000
H	-3.422589000	-1.778983000	-1.991340000
H	-4.687472000	-2.514836000	-0.962859000
H	-4.035433000	2.222229000	-0.079826000
H	-2.331314000	-3.827214000	-1.737656000
H	-3.517953000	-4.427270000	-0.527879000
H	-1.775139000	-4.394928000	-0.124170000
H	0.854786000	2.115781000	2.278990000
H	-0.221516000	3.552396000	2.157292000
H	1.527379000	3.704774000	1.782373000
H	3.723610000	1.882394000	-2.225660000
H	5.403255000	2.019247000	-1.619084000
H	4.033317000	2.439930000	-0.543520000
C	-1.299845000	4.806511000	-0.393055000
H	-0.413614000	5.092198000	0.187977000
H	-0.991363000	4.379640000	-1.356522000
H	-1.921593000	5.691542000	-0.568593000
C	5.306313000	-1.826579000	1.055833000
H	4.813832000	-2.144421000	1.986245000
H	6.241120000	-2.381172000	0.924772000
H	5.519778000	-0.749155000	1.098588000
C	-3.181459000	-2.585245000	1.288738000
H	-4.211744000	-2.956705000	1.307698000
H	-2.525794000	-3.286589000	1.813352000
H	-3.123690000	-1.596929000	1.756579000



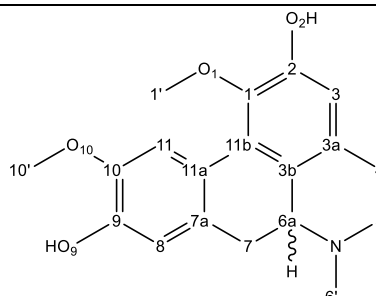
B-H⁺

C	0.831253000	-0.198218000	0.000327000
C	0.701158000	-1.517362000	0.458200000
C	2.099628000	0.267066000	-0.401675000
C	1.825419000	-2.344595000	0.547278000
C	3.211290000	-0.556777000	-0.303057000
C	3.076414000	-1.871206000	0.182633000
C	-1.656632000	0.029299000	-0.128308000
C	-1.676970000	-1.490828000	-0.162014000
C	-0.386262000	0.651759000	-0.041741000
C	-0.662161000	-2.042078000	0.834475000
C	-4.177196000	0.129201000	-0.286699000
C	-4.066160000	-1.312582000	-0.732543000
C	-2.824411000	0.793592000	-0.193780000
N	-3.056674000	-2.020023000	0.121236000
C	-2.753651000	2.189552000	-0.154176000
C	-1.519897000	2.811310000	-0.040245000
C	-0.342751000	2.050147000	0.020287000
C	-3.143241000	-3.494500000	-0.084372000
H	-1.438744000	-1.854859000	-1.176254000
O	-1.447287000	4.172271000	0.016253000
O	4.168910000	-2.684017000	0.282404000
O	4.484848000	-0.202920000	-0.646688000
O	0.828171000	2.774903000	0.122662000
C	1.369418000	2.801203000	1.453227000
C	4.694603000	1.150546000	-1.037299000
H	2.207907000	1.275874000	-0.790407000
H	1.729430000	-3.371706000	0.901954000
H	-0.637023000	-3.137683000	0.823848000
H	-0.944026000	-1.714970000	1.850580000
H	-4.681794000	0.173167000	0.691218000
H	-4.815674000	0.669388000	-0.997549000
H	-3.712802000	-1.408158000	-1.768455000
H	-5.017742000	-1.843437000	-0.626913000
H	-3.660448000	2.793179000	-0.206624000
H	-2.811031000	-3.716155000	-1.104495000
H	-4.185517000	-3.796765000	0.049141000
H	-2.518022000	-4.010716000	0.646863000
H	-0.511672000	4.427254000	0.047114000
H	4.955241000	-2.202401000	-0.015076000
H	1.583253000	1.782572000	1.807231000
H	0.663236000	3.291173000	2.139216000
H	2.299401000	3.377052000	1.403020000
H	4.153877000	1.378098000	-1.967146000
H	5.770288000	1.257304000	-1.203624000
H	4.371051000	1.837924000	-0.240981000
H	-3.278696000	-1.821047000	1.108537000



G-H⁺

C	0.713730000	-0.131553000	-0.051733000
C	0.928111000	-1.454587000	0.364360000
C	1.804136000	0.637811000	-0.501507000
C	2.226393000	-1.973304000	0.378445000
C	3.092345000	0.108476000	-0.497836000
C	3.303256000	-1.204087000	-0.033573000
C	-1.751758000	-0.535365000	-0.120230000
C	-1.389483000	-2.009130000	-0.216711000
C	-0.681384000	0.385760000	-0.029213000
C	-0.248954000	-2.315243000	0.749798000
C	-4.223292000	-1.069105000	-0.210761000
C	-3.763658000	-2.411025000	-0.738995000
C	-3.076581000	-0.092979000	-0.100341000
N	-2.585866000	-2.877044000	0.063672000
C	-3.347334000	1.271254000	0.030071000
C	-2.312737000	2.189924000	0.148336000
C	-0.977997000	1.748941000	0.128649000
C	-2.309667000	-4.317724000	-0.201208000
H	-1.086381000	-2.265278000	-1.246244000
O	-2.647082000	3.503250000	0.344522000
O	4.574062000	-1.739427000	-0.052276000
O	4.197725000	0.771679000	-0.935142000
O	0.022045000	2.676085000	0.298180000
C	0.238174000	3.004132000	1.675442000
C	4.011545000	2.099429000	-1.414165000
H	1.635062000	1.644581000	-0.870438000
H	2.407860000	-2.999876000	0.701400000
H	0.049758000	-3.368437000	0.701209000
H	-0.583677000	-2.098254000	1.779045000
H	-4.695272000	-1.205007000	0.774958000
H	-4.995660000	-0.670093000	-0.880739000
H	-3.424842000	-2.360647000	-1.782788000
H	-4.544894000	-3.172955000	-0.650106000
H	-4.376856000	1.631880000	0.040564000
H	-1.976452000	-4.417340000	-1.239631000
H	-3.237772000	-4.874554000	-0.045448000
H	-1.545084000	-4.684250000	0.487069000
H	0.541726000	2.107498000	2.237103000
H	-0.673857000	3.429310000	2.122394000
H	1.042418000	3.746717000	1.702715000
H	3.342989000	2.112933000	-2.287109000
H	5.002690000	2.456651000	-1.708355000
H	3.605794000	2.748627000	-0.624681000
C	-1.960146000	4.499577000	-0.425716000
H	-1.095265000	4.895872000	0.121561000
H	-1.633695000	4.088859000	-1.390176000
H	-2.683033000	5.304851000	-0.597557000
C	5.376405000	-1.301924000	1.053486000
H	4.938568000	-1.651090000	1.999771000
H	6.368320000	-1.745586000	0.919888000
H	5.461159000	-0.206109000	1.065551000
H	-2.823163000	-2.777361000	1.062492000

Table S2. Comparison of structural parameters of boldine


Parameters	Experimental (Ref. 49)	Calculated M08-HX/6-31+G(d,p)
Bond lengths (Å)		
C1-C2	1.40	1.41
C1-O1	1.38	1.38
O1-C1'	1.43	1.44
C2-C3	1.37	1.39
C2-O2	1.36	1.37
C3-C3a	1.40	1.40
C3a-C4	1.51	1.51
C4-C5	1.51	1.52
C5-N	1.49	1.47
N-C6a	1.51	1.47
C6a-C7	1.52	1.53
C7-C7a	1.51	1.51
C7a-C8	1.39	1.40
C8-C9	1.38	1.39
C9-C10	1.40	1.41
C9-O9	1.37	1.37
C10-C11	1.38	1.39
C10-O10	1.38	1.37
O10-C10'	1.41	1.42
C11-C11a	1.42	1.41
C11a-C11b	1.49	1.48
C11b-C1	1.40	1.40
Bond angles (°)		
C1-C2-C3	120.1	120.4
C1-O1-C1'	115.0	113.4
C3-C2-O2	123.6	120.0
C3b-C3a-C4	121.2	120.0
C3b-C11b-C1	118.2	118.3
C4-C5-N	111.1	110.6
C5-N-C6'	109.7	108.3
N-C6a-C3b	110.6	112.1
C6a-C7-C7a	108.9	109.2
C6a-C3b-C11b	117.3	118.0
C8-C7a-C11a	120.4	119.9
C8-C9-O9	117.8	120.0
C7a-C11a-C11b	118.0	117.9
C10-C11-C11a	120.4	120.3
C10-O10-C10'	117.8	116.8
C11-C10-O10	125.3	125.1
Dihedral angles (°)		
C3-C3a-C4-C5	-174.3	163.9
N-C6a-C7-C7a	179.5	176.6
N-C6a-C3b-C11b	-162.2	164.5
C7-C7a-C8-C9	-178.4	179.0
C10-C11-C11a-C11b	-175.1	178.4
C1-C11b-C11a-C11	27.8	-25.4

Table S3. OH bond dissociation enthalpies (BDEs), proton affinities (PAs), Gibbs free energies of activation and apparent rate constants for HAT and SPLET reactions of Quercetin with HOO[•] at the indicated positions, computed at the level of theory used in ref. 12 and at the one used in this work.

Quercetin OH position	BDE (kcal·mol ⁻¹)		HAT ΔG ^{‡,1M} (kcal·mol ⁻¹)		HAT k _{app} (L·mol ⁻¹ ·s ⁻¹)	
	M05-2X/6-31+G(d,p) ¹	M08-HX/6-31+G(d,p) ²	M05-2X/6-31+G(d,p) ¹	M08-HX/6-31+G(d,p) ²	M05-2X/6-31+G(d,p) ¹	M08-HX/6-31+G(d,p) ²
3-OH	84.2	85.4	16.5	16.8	2.2 × 10 ²	1.6 × 10 ²
4'-OH	83.8	85.3	16.2	17.3	1.2 × 10 ³	2.7 × 10 ²
Quercetin OH position	PA (kcal·mol ⁻¹)		SPLET ΔG ^{‡,1M} (kcal·mol ⁻¹)		SPLET k _{app} (L·mol ⁻¹ ·s ⁻¹)	
	M05-2X/6-31+G(d,p) ¹	M08-HX/6-31+G(d,p) ²	M05-2X/6-31+G(d,p) ¹	M08-HX/6-31+G(d,p) ²	M05-2X/6-31+G(d,p) ¹	M08-HX/6-31+G(d,p) ²
7-OH	23.5	23.7	19.0	17.7	7.5 × 10 ⁻²	6.3 × 10 ⁻¹
4'-OH	23.2	23.3	7.8	7.2	1.2 × 10 ⁷	3.2 × 10 ⁷

¹ Ref. 12

² This work

Table S4. Transition state structures for the HAT reactions between **B**, **G** and their derivatives and the model free radical HOO \cdot , at the indicated positions, optimized at the M08-HX/6-31+G(d,p) level including implicit solvent effects (SMD, solvent: water).

System/position	Coordinates (Å)			Imaginary frequency (cm ⁻¹)	
B/C-6a	C	-0.908596000	-0.090388000	-0.279646000	1023.3i
	C	-0.781421000	-1.369518000	-0.842243000	
	C	-2.158658000	0.314111000	0.233707000	
	C	-1.896605000	-2.209987000	-0.927506000	
	C	-3.258359000	-0.526236000	0.145187000	
	C	-3.130528000	-1.795239000	-0.450707000	
	C	1.578743000	0.171436000	-0.248898000	
	C	1.651938000	-1.318450000	-0.387482000	
	C	0.293738000	0.776945000	-0.222953000	
	C	0.566951000	-1.838398000	-1.326002000	
	C	4.086747000	0.276546000	-0.084822000	
	C	3.947882000	-1.196340000	0.254441000	
	C	2.737372000	0.949786000	-0.104409000	
	N	2.967135000	-1.834740000	-0.628416000	
	C	2.642170000	2.337633000	0.007386000	
	C	1.393252000	2.944952000	-0.026526000	
	C	0.227221000	2.173380000	-0.141387000	
	C	3.035838000	-3.288790000	-0.493910000	
	H	1.318618000	-1.712571000	0.715978000	
	O	1.297291000	4.302491000	0.061184000	
	O	-4.211534000	-2.625023000	-0.544615000	
	O	-4.512593000	-0.232596000	0.601539000	
	O	-0.956587000	2.886542000	-0.142030000	
	C	-1.549521000	3.006799000	-1.444496000	
	C	-4.701229000	1.051958000	1.185438000	
	H	-2.260460000	1.287530000	0.705568000	
	H	-1.804715000	-3.206646000	-1.361499000	
	H	0.567459000	-2.933273000	-1.375352000	
	H	0.769783000	-1.458874000	-2.343351000	
	H	4.570548000	0.385833000	-1.068415000	
	H	4.739344000	0.770353000	0.648233000	
	H	3.636197000	-1.321587000	1.313993000	
	H	4.909228000	-1.709863000	0.131998000	
	H	3.537400000	2.951432000	0.115539000	
	H	2.697710000	-3.619030000	0.507044000	
	H	4.074380000	-3.610358000	-0.631687000	
H	2.428025000	-3.789765000	-1.253863000		
H	0.356988000	4.542431000	0.059009000		
H	-4.983990000	-2.190271000	-0.154052000		
H	-1.758309000	2.015412000	-1.871441000		
H	-0.880049000	3.565054000	-2.114963000		
H	-2.487828000	3.555949000	-1.313664000		
H	-4.081866000	1.166516000	2.086606000		
H	-5.759065000	1.111939000	1.456802000		
H	-4.458490000	1.846717000	0.464196000		
H	2.006978000	-0.561844000	2.854363000		
O	1.066527000	-0.688380000	2.645782000		
O	0.995715000	-1.950921000	2.097744000		
B/2-OH	C	0.865403000	-0.527356000	0.132467000	3539.8i
	C	0.840624000	-1.897517000	0.429834000	
	C	2.083122000	0.081123000	-0.233765000	
	C	2.025877000	-2.639965000	0.399077000	
	C	3.253898000	-0.662786000	-0.257444000	
	C	3.228010000	-2.031770000	0.070302000	
	C	-1.635025000	-0.481250000	0.047363000	
	C	-1.560016000	-1.981658000	-0.172833000	
	C	-0.414480000	0.221280000	0.211858000	
	C	-0.479136000	-2.548544000	0.753433000	
	C	-4.153748000	-0.576472000	-0.168274000	

	C	-3.869000000	-1.935400000	-0.780318000	
	C	-2.878460000	0.195884000	0.056429000	
	N	-2.856322000	-2.644358000	0.007528000	
	C	-2.918284000	1.564268000	0.256701000	
	C	-1.729861000	2.282251000	0.495420000	
	C	-0.477481000	1.594868000	0.466970000	
	C	-2.777583000	-4.024202000	-0.473504000	
	H	-1.215205000	-2.135319000	-1.224614000	
	O	-1.765510000	3.570368000	0.784389000	
	O	4.380477000	-2.764226000	0.050409000	
	O	4.489142000	-0.177674000	-0.583163000	
	O	0.633337000	2.365448000	0.669915000	
	C	1.195043000	2.258975000	1.989598000	
	C	4.586582000	1.219350000	-0.839910000	
	H	2.107020000	1.134349000	-0.501076000	
	H	2.016851000	-3.706493000	0.628275000	
	H	-0.384717000	-3.633921000	0.633504000	
	H	-0.766514000	-2.350182000	1.800009000	
	H	-4.673308000	-0.707808000	0.793588000	
	H	-4.823981000	0.003943000	-0.817157000	
	H	-3.530495000	-1.822656000	-1.832436000	
	H	-4.785167000	-2.539332000	-0.795783000	
	H	-3.864917000	2.106420000	0.256515000	
	H	-2.426712000	-4.074488000	-1.523373000	
	H	-3.773822000	-4.479844000	-0.421780000	
	H	-2.105921000	-4.627654000	0.146307000	
	H	-1.141933000	4.143978000	0.074691000	
	H	5.119614000	-2.189767000	-0.199494000	
	H	1.433968000	1.212792000	2.226953000	
	H	0.487051000	2.659834000	2.728281000	
	H	2.111730000	2.856888000	1.986061000	
	H	3.997804000	1.496365000	-1.726212000	
	H	5.645119000	1.422972000	-1.024934000	
	H	4.243628000	1.798834000	0.030578000	
	O	-0.565254000	4.593204000	-1.001334000	
	O	-0.333134000	3.436322000	-1.702539000	
	H	0.498783000	3.087586000	-1.332433000	
	C	0.401373000	0.178467000	0.287604000	
	C	0.541970000	-1.105837000	0.885675000	
	C	1.540647000	0.909351000	-0.078502000	
	C	1.803454000	-1.615530000	1.130912000	
	C	2.810637000	0.398981000	0.183126000	
	C	2.957228000	-0.881336000	0.804046000	
	C	-2.022708000	-0.268447000	-0.101541000	
	C	-1.693579000	-1.746916000	0.048626000	
	C	-0.973051000	0.673848000	0.049446000	
	C	-0.699658000	-1.892962000	1.204289000	
	C	-4.428176000	-0.839376000	-0.592949000	
	C	-3.868394000	-2.234652000	-0.802056000	
	C	-3.319725000	0.165057000	-0.391603000	
	N	-2.898456000	-2.561476000	0.248149000	
	C	-3.597244000	1.532350000	-0.497347000	
	C	-2.587045000	2.463831000	-0.305067000	
	C	-1.279936000	2.040968000	-0.033952000	
	C	-2.559838000	-3.980378000	0.138151000	
	H	-1.181842000	-2.085083000	-0.883791000	
	O	-2.869127000	3.798423000	-0.379792000	
	O	4.171070000	-1.346273000	1.084193000	
	O	3.965714000	1.015893000	-0.121172000	
	O	-0.348295000	3.045147000	0.136036000	
	C	-0.036729000	3.299778000	1.515764000	
	C	3.890134000	2.252658000	-0.831238000	
	H	1.432156000	1.874242000	-0.565779000	
	H	1.930475000	-2.599879000	1.583312000	
	H	-0.424469000	-2.939997000	1.376166000	
	H	-1.170085000	-1.509895000	2.125827000	
B/9-OH					2854.2i

	H	-5.092277000	-0.834829000	0.285584000	
	H	-5.041519000	-0.544934000	-1.456349000	
	H	-3.390660000	-2.312505000	-1.802366000	
	H	-4.678822000	-2.974467000	-0.770577000	
	H	-4.607953000	1.876890000	-0.722268000	
	H	-2.064916000	-4.211522000	-0.826206000	
	H	-3.477795000	-4.576926000	0.204708000	
	H	-1.898548000	-4.298727000	0.951287000	
	H	-2.041411000	4.292649000	-0.272967000	
	H	4.726557000	-1.442122000	0.181808000	
	H	0.397440000	2.406684000	1.988006000	
	H	-0.944007000	3.601731000	2.058915000	
	H	0.693166000	4.115539000	1.528241000	
	H	3.378506000	2.113483000	-1.794022000	
	H	4.923948000	2.564219000	-1.001204000	
	H	3.367147000	3.011165000	-0.232595000	
	H	3.839635000	-0.550300000	-2.036963000	
	O	3.828050000	-1.477084000	-1.736797000	
	O	5.044876000	-1.679132000	-1.149483000	
B-Me⁺/C-6a	C	-1.058580000	-0.127268000	-0.223873000	<i>1977.7i</i>
	C	-0.796236000	-1.424999000	-0.686134000	
	C	-2.365688000	0.197138000	0.199993000	
	C	-1.825707000	-2.368228000	-0.764248000	
	C	-3.381839000	-0.741111000	0.117224000	
	C	-3.113321000	-2.034148000	-0.376035000	
	C	1.401582000	0.360183000	-0.105759000	
	C	1.594345000	-1.094359000	-0.196805000	
	C	0.056180000	0.845287000	-0.165470000	
	C	0.602329000	-1.801168000	-1.099411000	
	C	3.881916000	0.727897000	0.217955000	
	C	3.895352000	-0.744994000	0.560941000	
	C	2.476230000	1.253583000	0.092489000	
	N	3.019233000	-1.533865000	-0.382345000	
	C	2.247051000	2.622882000	0.148808000	
	C	0.949878000	3.108642000	0.014423000	
	C	-0.136384000	2.228566000	-0.140687000	
	C	3.180969000	-2.980900000	-0.025678000	
	H	1.296697000	-1.500291000	1.011874000	
	O	0.729449000	4.443696000	0.047744000	
	O	-4.110258000	-2.959675000	-0.458951000	
	O	-4.679150000	-0.530055000	0.482946000	
	O	-1.370375000	2.836648000	-0.226352000	
	C	-1.914774000	2.859273000	-1.557031000	
	C	-5.026063000	0.785953000	0.903027000	
	H	-2.575499000	1.185589000	0.598683000	
	H	-1.624496000	-3.378288000	-1.123169000	
	H	0.713823000	-2.890541000	-1.053376000	
	H	0.778232000	-1.490761000	-2.145578000	
	H	4.443472000	0.917567000	-0.709525000	
	H	4.410914000	1.265827000	1.015470000	
	H	3.496903000	-0.932649000	1.568384000	
	H	4.902743000	-1.170739000	0.487589000	
	H	3.071644000	3.321992000	0.290305000	
	H	2.852014000	-3.130711000	1.008078000	
	H	4.242848000	-3.227858000	-0.125037000	
	H	2.599682000	-3.599289000	-0.713658000	
	H	-0.226076000	4.603456000	-0.021213000	
	H	-4.938021000	-2.573656000	-0.135213000	
	H	-2.037835000	1.838594000	-1.945792000	
H	-1.256797000	3.434618000	-2.223732000		
H	-2.892125000	3.347182000	-1.485509000		
H	-4.491648000	1.055436000	1.825263000		
H	-6.102791000	0.771463000	1.093751000		
H	-4.798182000	1.517293000	0.112923000		
H	1.767763000	-0.148018000	2.975312000		
O	0.873003000	-0.408551000	2.699565000		

	O 1.017348000 -1.696709000 2.217570000 C 3.469005000 -1.344881000 -1.801524000 H 4.554688000 -1.488566000 -1.830945000 H 2.977764000 -2.096846000 -2.426332000 H 3.202042000 -0.340666000 -2.145539000	
B-Me⁺/2-OH	C 0.912181000 -0.614621000 0.110393000 C 0.584447000 -1.950459000 0.378274000 C 2.240635000 -0.280039000 -0.221159000 C 1.574901000 -2.936235000 0.353609000 C 3.218563000 -1.263904000 -0.244202000 C 2.886592000 -2.599739000 0.054826000 C -1.514366000 -0.018883000 -0.057991000 C -1.724129000 -1.504405000 -0.299303000 C -0.177570000 0.392103000 0.171559000 C -0.852403000 -2.297399000 0.677278000 C -3.978852000 0.453394000 -0.410543000 C -3.987771000 -0.918849000 -1.047348000 C -2.577726000 0.910060000 -0.092107000 N -3.184807000 -1.900850000 -0.231707000 C -2.331072000 2.248478000 0.159491000 C -1.028511000 2.682555000 0.477401000 C 0.047955000 1.741240000 0.461467000 C -3.372106000 -3.249358000 -0.853733000 H -1.416446000 -1.743726000 -1.332298000 O -0.796623000 3.932320000 0.821060000 O 3.849981000 -3.565122000 0.035200000 O 4.534326000 -1.061114000 -0.544947000 O 1.290725000 2.244047000 0.712762000 C 1.753939000 2.028667000 2.058383000 C 4.938414000 0.278452000 -0.810502000 H 2.497977000 0.747209000 -0.465637000 H 1.327309000 -3.977838000 0.561517000 H -1.003803000 -3.378336000 0.571372000 H -1.101669000 -2.014883000 1.712792000 H -4.598840000 0.465356000 0.498060000 H -4.443958000 1.156670000 -1.113418000 H -3.529816000 -0.908535000 -2.046029000 H -5.003355000 -1.324624000 -1.121256000 H -3.138206000 2.981744000 0.138455000 H -3.066550000 -3.195507000 -1.903810000 H -4.433784000 -3.506583000 -0.779189000 H -2.775476000 -3.990574000 -0.315854000 H -0.060327000 4.401542000 0.104197000 H 4.700910000 -3.162542000 -0.194963000 H 1.760010000 0.955940000 2.298071000 H 1.109055000 2.569029000 2.765290000 H 2.773184000 2.424253000 2.101702000 H 4.426070000 0.671105000 -1.700548000 H 6.015923000 0.241522000 -0.993666000 H 4.730985000 0.924836000 0.055095000 O 0.589721000 4.730650000 -0.926914000 O 0.549187000 3.582880000 -1.675311000 H 1.308010000 3.055703000 -1.363844000 C -3.691537000 -1.949591000 1.175580000 H -4.783358000 -2.029585000 1.136711000 H -3.273563000 -2.830645000 1.671386000 H -3.394667000 -1.043676000 1.714775000	3371.4i
B-Me⁺/9-OH	C 0.576835000 0.227814000 0.265221000 C 0.585664000 -1.088239000 0.805447000 C 1.786404000 0.865850000 -0.039742000 C 1.783846000 -1.731946000 1.044487000 C 2.996686000 0.224676000 0.219969000 C 3.009542000 -1.095973000 0.772503000 C -1.866815000 0.021836000 -0.222093000 C -1.652743000 -1.479373000 -0.099823000	2988.6i

	C	-0.740314000	0.854587000	0.008686000	
	C	-0.733830000	-1.753953000	1.091101000	
	C	-4.290670000	-0.300540000	-0.851520000	
	C	-3.878329000	-1.736275000	-1.092940000	
	C	-3.100571000	0.580098000	-0.562595000	
	N	-2.964905000	-2.231442000	0.000743000	
	C	-3.248716000	1.969369000	-0.630845000	
	C	-2.169419000	2.795461000	-0.357258000	
	C	-0.919595000	2.243849000	-0.039449000	
	C	-2.735923000	-3.690053000	-0.240743000	
	H	-1.184278000	-1.869737000	-1.019141000	
	O	-2.321163000	4.148272000	-0.404038000	
	O	4.163944000	-1.687704000	1.046386000	
	O	4.209790000	0.745614000	-0.023061000	
	O	0.089404000	3.150017000	0.200248000	
	C	0.378205000	3.325800000	1.598280000	
	C	4.272420000	2.036564000	-0.631958000	
	H	1.780334000	1.860022000	-0.477787000	
	H	1.805804000	-2.743231000	1.452060000	
	H	-0.576856000	-2.826074000	1.257443000	
	H	-1.173623000	-1.320542000	2.003984000	
	H	-5.018346000	-0.239305000	-0.028064000	
	H	-4.809228000	0.057075000	-1.750868000	
	H	-3.314774000	-1.847143000	-2.029508000	
	H	-4.743437000	-2.409681000	-1.112142000	
	H	-4.211262000	2.410628000	-0.892732000	
	H	-2.318045000	-3.817236000	-1.244823000	
	H	-3.703236000	-4.197828000	-0.164711000	
	H	-2.053391000	-4.088488000	0.514388000	
	H	-1.457966000	4.562318000	-0.245727000	
	H	4.738841000	-1.786584000	0.144731000	
	H	0.699283000	2.377035000	2.051551000	
	H	-0.510710000	3.705248000	2.122186000	
	H	1.189168000	4.058175000	1.660725000	
	H	3.780110000	2.024287000	-1.614312000	
	H	5.335798000	2.258772000	-0.752175000	
	H	3.805390000	2.791023000	0.015881000	
	H	4.067163000	-0.659123000	-2.011677000	
	O	3.935557000	-1.600117000	-1.795993000	
	O	5.085143000	-1.983088000	-1.161540000	
	C	-3.613234000	-2.063926000	1.338750000	
	H	-4.640807000	-2.435930000	1.263702000	
	H	-3.059642000	-2.653737000	2.075645000	
	H	-3.610018000	-1.007555000	1.627267000	
B-H⁺/C-6a	C	-0.943847000	-0.123518000	-0.244347000	1961.6i
	C	-0.783212000	-1.421639000	-0.752071000	
	C	-2.213378000	0.271713000	0.231583000	
	C	-1.877859000	-2.289858000	-0.824325000	
	C	-3.292754000	-0.592651000	0.154164000	
	C	-3.128236000	-1.883625000	-0.387589000	
	C	1.542035000	0.214438000	-0.238570000	
	C	1.644407000	-1.244894000	-0.359912000	
	C	0.229210000	0.778724000	-0.203963000	
	C	0.572325000	-1.898867000	-1.204165000	
	C	4.059538000	0.421933000	-0.123204000	
	C	4.020423000	-1.047933000	0.231411000	
	C	2.682991000	1.035199000	-0.105296000	
	N	3.022996000	-1.741710000	-0.650376000	
	C	2.543544000	2.412715000	0.004973000	
	C	1.271277000	2.977831000	-0.020346000	
	C	0.125222000	2.170297000	-0.130787000	
	C	3.138916000	-3.224109000	-0.504928000	
	H	1.415043000	-1.667599000	0.853577000	
	O	1.135299000	4.321485000	0.070058000	
	O	-4.187624000	-2.737034000	-0.466223000	
	O	-4.559384000	-0.307123000	0.572199000	

	O -1.071571000 2.854378000 -0.130729000 C -1.668404000 2.966935000 -1.434485000 C -4.796883000 1.011563000 1.055666000 H -2.344801000 1.257560000 0.667629000 H -1.754969000 -3.300591000 -1.215420000 H 0.608081000 -2.991298000 -1.120013000 H 0.748788000 -1.640998000 -2.265598000 H 4.507996000 0.546859000 -1.121741000 H 4.714341000 0.942375000 0.587028000 H 3.692046000 -1.226646000 1.265455000 H 4.989797000 -1.530300000 0.071391000 H 3.417567000 3.057080000 0.102194000 H 2.760799000 -3.505676000 0.484191000 H 4.195599000 -3.489245000 -0.596402000 H 2.570871000 -3.718318000 -1.295495000 H 0.188493000 4.538094000 0.084014000 H -4.976497000 -2.306813000 -0.103642000 H -1.860339000 1.972678000 -1.862122000 H -1.008356000 3.538133000 -2.102845000 H -2.614923000 3.500303000 -1.299654000 H -4.210937000 1.205912000 1.965326000 H -5.864201000 1.063985000 1.288078000 H -4.547128000 1.757073000 0.285639000 H 2.151926000 -0.455281000 2.840915000 O 1.222721000 -0.619583000 2.609124000 O 1.217868000 -1.893992000 2.071524000 H 3.249471000 -1.505902000 -1.630363000	
B-H⁺/2-OH	C 0.881035000 -0.535648000 0.108350000 C 0.829261000 -1.904412000 0.408377000 C 2.116257000 0.047654000 -0.239760000 C 1.999012000 -2.670366000 0.399777000 C 3.272957000 -0.717802000 -0.241817000 C 3.217351000 -2.085433000 0.090182000 C -1.619548000 -0.429267000 0.039365000 C -1.544450000 -1.923843000 -0.215847000 C -0.381634000 0.242104000 0.185875000 C -0.502216000 -2.544630000 0.712183000 C -4.150691000 -0.489877000 -0.046891000 C -3.953527000 -1.810248000 -0.758001000 C -2.851314000 0.260351000 0.104193000 N -2.881369000 -2.593912000 -0.061614000 C -2.865084000 1.626741000 0.316765000 C -1.656653000 2.325383000 0.512605000 C -0.416247000 1.618062000 0.440573000 C -2.859894000 -3.994534000 -0.575902000 H -1.255169000 -2.096317000 -1.267579000 O -1.658562000 3.609299000 0.801992000 O 4.354304000 -2.838453000 0.091743000 O 4.520282000 -0.256904000 -0.548594000 O 0.711815000 2.368237000 0.603586000 C 1.261750000 2.327489000 1.933185000 C 4.648651000 1.137516000 -0.808790000 H 2.164464000 1.098655000 -0.510255000 H 1.964692000 -3.735798000 0.630752000 H -0.423233000 -3.626534000 0.559890000 H -0.800773000 -2.365997000 1.759266000 H -4.589291000 -0.671216000 0.946997000 H -4.871881000 0.115853000 -0.609359000 H -3.618377000 -1.684583000 -1.796631000 H -4.864491000 -2.417272000 -0.744139000 H -3.803727000 2.180196000 0.359742000 H -2.592350000 -3.961604000 -1.637247000 H -3.861074000 -4.415500000 -0.449143000 H -2.137877000 -4.590204000 -0.014346000 H -1.057160000 4.186500000 0.036556000 H 5.108627000 -2.281517000 -0.152864000	3554.7i

	H 1.500405000 1.293606000 2.220217000 H 0.546141000 2.761295000 2.645407000 H 2.176807000 2.927018000 1.908021000 H 4.080854000 1.421333000 -1.706475000 H 5.713964000 1.320024000 -0.975610000 H 4.301267000 1.726311000 0.053633000 O -0.541962000 4.611622000 -1.031875000 O -0.320582000 3.456933000 -1.737152000 H 0.526552000 3.117243000 -1.393020000 H -3.111258000 -2.625399000 0.943345000	
B-H⁺/9-OH	C 0.426150000 0.175881000 0.263979000 C 0.546404000 -1.118175000 0.842896000 C 1.577458000 0.896489000 -0.081215000 C 1.796477000 -1.649201000 1.095287000 C 2.838481000 0.367533000 0.188342000 C 2.963825000 -0.923499000 0.794555000 C -2.008369000 -0.218224000 -0.136259000 C -1.683463000 -1.697154000 -0.008074000 C -0.938818000 0.698617000 0.027250000 C -0.701313000 -1.906871000 1.141263000 C -4.444084000 -0.730451000 -0.588134000 C -3.955137000 -2.140485000 -0.840938000 C -3.299986000 0.238344000 -0.407729000 N -2.935285000 -2.504903000 0.197002000 C -3.553839000 1.610869000 -0.493033000 C -2.525064000 2.520031000 -0.297916000 C -1.222903000 2.070118000 -0.036337000 C -2.666076000 -3.971392000 0.173510000 H -1.248205000 -2.082347000 -0.945430000 O -2.782055000 3.856137000 -0.357160000 O 4.165238000 -1.405407000 1.081393000 O 4.001916000 0.974179000 -0.093458000 O -0.275388000 3.053869000 0.142313000 C 0.043896000 3.291136000 1.524895000 C 3.950867000 2.221582000 -0.788190000 H 1.486143000 1.868833000 -0.556729000 H 1.905003000 -2.642194000 1.532935000 H -0.431293000 -2.962163000 1.257892000 H -1.167887000 -1.560588000 2.079463000 H -5.084289000 -0.718150000 0.307695000 H -5.072530000 -0.418016000 -1.431994000 H -3.454908000 -2.246787000 -1.813155000 H -4.769725000 -2.868968000 -0.773214000 H -4.560389000 1.975198000 -0.702610000 H -2.161084000 -4.211409000 -0.768233000 H -3.624599000 -4.493800000 0.233764000 H -2.045753000 -4.251086000 1.027481000 H -1.946424000 4.337269000 -0.249734000 H 4.733244000 -1.503648000 0.174389000 H 0.453349000 2.383390000 1.990710000 H -0.854844000 3.614756000 2.069262000 H 0.795959000 4.086204000 1.540528000 H 3.450596000 2.100612000 -1.759171000 H 4.990665000 2.521996000 -0.940138000 H 3.429257000 2.977983000 -0.185800000 H 3.893278000 -0.568862000 -2.031944000 O 3.861471000 -1.498360000 -1.741808000 O 5.064687000 -1.724068000 -1.131589000 H -3.322557000 -2.265572000 1.122592000	2835.4i
G/C-6a	C -0.775138000 -0.023030000 -0.200639000 C -0.994562000 -1.315779000 -0.703366000 C -1.850922000 0.692810000 0.361667000 C -2.287119000 -1.849722000 -0.690125000 C -3.131883000 0.147556000 0.380834000 C -3.350636000 -1.130244000 -0.168299000 C 1.695471000 -0.396157000 -0.275676000	1065.2i

	C	1.387964000	-1.862295000	-0.332888000	
	C	0.609818000	0.515889000	-0.239234000	
	C	0.168861000	-2.127709000	-1.211192000	
	C	4.157924000	-0.917366000	-0.232582000	
	C	3.673062000	-2.284403000	0.215009000	
	C	3.017942000	0.069858000	-0.249585000	
	N	2.519511000	-2.701275000	-0.587215000	
	C	3.267334000	1.441508000	-0.243924000	
	C	2.215316000	2.352140000	-0.263013000	
	C	0.887080000	1.892414000	-0.267083000	
	C	2.233293000	-4.118575000	-0.373508000	
	H	1.014159000	-2.111528000	0.800461000	
	O	2.531934000	3.682459000	-0.335528000	
	O	-4.613651000	-1.684236000	-0.127555000	
	O	-4.223047000	0.762319000	0.917093000	
	O	-0.126032000	2.821299000	-0.329181000	
	C	-0.377706000	3.265070000	-1.666609000	
	C	-4.028527000	2.056336000	1.476863000	
	H	-1.673734000	1.670268000	0.799056000	
	H	-2.473549000	-2.852839000	-1.078063000	
	H	-0.107190000	-3.188232000	-1.206581000	
	H	0.418327000	-1.851815000	-2.251215000	
	H	4.600842000	-0.992593000	-1.238284000	
	H	4.950201000	-0.560415000	0.439737000	
	H	3.394902000	-2.263432000	1.290971000	
	H	4.466072000	-3.032300000	0.094486000	
	H	4.290520000	1.820215000	-0.225267000	
	H	1.878649000	-4.307631000	0.657714000	
	H	3.151217000	-4.694716000	-0.535509000	
	H	1.479730000	-4.484936000	-1.077966000	
	H	-0.696813000	2.419660000	-2.295280000	
	H	0.522869000	3.727604000	-2.100000000	
	H	-1.181415000	4.006805000	-1.610074000	
	H	-3.322720000	2.019507000	2.319367000	
	H	-5.009122000	2.381308000	1.836748000	
	H	-3.663507000	2.762584000	0.716903000	
	C	1.836785000	4.596784000	0.523415000	
	H	0.962375000	5.027671000	0.019152000	
	H	1.523700000	4.098050000	1.450232000	
	H	2.550058000	5.394029000	0.760810000	
	C	-5.468013000	-1.191379000	-1.168619000	
	H	-5.063280000	-1.467838000	-2.152993000	
	H	-6.445660000	-1.663204000	-1.026106000	
	H	-5.572999000	-0.098990000	-1.104153000	
	O	0.706669000	-2.198903000	2.196403000	
	O	1.099270000	-0.966632000	2.672732000	
	H	2.050578000	-1.061017000	2.845967000	
G-Me⁺/C-6a	C	-0.900056000	-0.044237000	-0.143581000	2029.9i
	C	-0.922272000	-1.383316000	-0.562126000	
	C	-2.087420000	0.548313000	0.333483000	
	C	-2.127519000	-2.092066000	-0.559943000	
	C	-3.280040000	-0.167696000	0.346439000	
	C	-3.299521000	-1.496162000	-0.124501000	
	C	1.607773000	-0.070699000	-0.122349000	
	C	1.494092000	-1.537451000	-0.142205000	
	C	0.394992000	0.680423000	-0.169128000	
	C	0.353781000	-2.055198000	-0.996276000	
	C	4.125069000	-0.204073000	0.080306000	
	C	3.846908000	-1.619763000	0.533705000	
	C	2.851113000	0.589403000	-0.042705000	
	N	2.790473000	-2.270777000	-0.326750000	
	C	2.899038000	1.976078000	-0.092233000	
	C	1.728075000	2.725108000	-0.204951000	
	C	0.477703000	2.077235000	-0.246635000	
	C	2.666523000	-3.692647000	0.131600000	
	H	1.142593000	-1.818197000	1.094820000	

	O	1.868598000	4.072353000	-0.323361000	
	O	-4.473500000	-2.216180000	-0.089512000	
	O	-4.464636000	0.319618000	0.804276000	
	O	-0.648028000	2.848516000	-0.396112000	
	C	-0.931308000	3.140448000	-1.770092000	
	C	-4.476682000	1.664036000	1.273371000	
	H	-2.065034000	1.565554000	0.710259000	
	H	-2.158034000	-3.132282000	-0.887906000	
	H	0.239771000	-3.142201000	-0.913302000	
	H	0.561294000	-1.820515000	-2.056526000	
	H	4.675692000	-0.197594000	-0.872636000	
	H	4.784796000	0.265398000	0.821749000	
	H	3.456463000	-1.646748000	1.561612000	
	H	4.738135000	-2.254534000	0.469304000	
	H	3.854422000	2.499753000	-0.041441000	
	H	2.377246000	-3.701205000	1.187685000	
	H	3.645792000	-4.165148000	0.002819000	
	H	1.927191000	-4.215607000	-0.479643000	
	H	-1.131068000	2.210612000	-2.324218000	
	H	-0.087310000	3.673956000	-2.234664000	
	H	-1.821937000	3.777230000	-1.781416000	
	H	-3.808220000	1.785082000	2.137945000	
	H	-5.507280000	1.869012000	1.577057000	
	H	-4.182487000	2.360536000	0.474784000	
	C	0.964793000	4.943621000	0.373985000	
	H	0.105488000	5.208368000	-0.254303000	
	H	0.619955000	4.479159000	1.306356000	
	H	1.541381000	5.845785000	0.604950000	
	C	-5.357065000	-1.893248000	-1.173343000	
	H	-4.891262000	-2.161584000	-2.132493000	
	H	-6.266545000	-2.484379000	-1.025945000	
	H	-5.607436000	-0.823161000	-1.168296000	
	C	3.213467000	-2.274024000	-1.766853000	
	H	4.246091000	-2.637177000	-1.811378000	
	H	2.556401000	-2.950650000	-2.321276000	
	H	3.141954000	-1.261738000	-2.177314000	
	O	0.854016000	-1.893138000	2.299752000	
	O	0.988942000	-0.583406000	2.720426000	
	H	1.926841000	-0.498889000	2.961103000	
G-H⁺/C-6a	C	-0.799605000	-0.043169000	-0.179982000	2023.4i
	C	-0.975747000	-1.356406000	-0.643898000	
	C	-1.904829000	0.652827000	0.352755000	
	C	-2.251218000	-1.930589000	-0.631674000	
	C	-3.166469000	0.067744000	0.377018000	
	C	-3.341377000	-1.230982000	-0.142487000	
	C	1.688872000	-0.326876000	-0.261927000	
	C	1.424820000	-1.771215000	-0.311419000	
	C	0.562298000	0.545930000	-0.222680000	
	C	0.205082000	-2.165006000	-1.114982000	
	C	4.183568000	-0.739847000	-0.248567000	
	C	3.797021000	-2.123877000	0.223893000	
	C	2.999804000	0.192616000	-0.237115000	
	N	2.629112000	-2.608335000	-0.586557000	
	C	3.194030000	1.566549000	-0.229794000	
	C	2.104417000	2.438173000	-0.242433000	
	C	0.790949000	1.928817000	-0.250962000	
	C	2.386048000	-4.060270000	-0.332785000	
	H	1.119412000	-2.065278000	0.931694000	
	O	2.381915000	3.767517000	-0.304497000	
	O	-4.584432000	-1.822815000	-0.098021000	
	O	-4.278365000	0.658086000	0.891501000	
	O	-0.250103000	2.820595000	-0.322849000	
	C	-0.539747000	3.212383000	-1.670540000	
	C	-4.130148000	1.969337000	1.426500000	
	H	-1.763935000	1.646328000	0.765194000	
	H	-2.400336000	-2.949884000	-0.991708000	

H	-0.026615000	-3.229958000	-0.999756000
H	0.413894000	-1.982859000	-2.186188000
H	4.599386000	-0.802910000	-1.266935000
H	4.979544000	-0.349326000	0.397812000
H	3.470407000	-2.137531000	1.274083000
H	4.608849000	-2.845167000	0.087476000
H	4.201093000	1.985031000	-0.214696000
H	2.016491000	-4.173714000	0.692123000
H	3.338234000	-4.583770000	-0.453873000
H	1.664191000	-4.447607000	-1.054600000
H	-0.841563000	2.336697000	-2.265066000
H	0.338911000	3.688941000	-2.132825000
H	-1.365718000	3.929424000	-1.621356000
H	-3.429142000	1.971505000	2.273693000
H	-5.123343000	2.268299000	1.773788000
H	-3.783653000	2.671397000	0.654254000
C	1.604433000	4.690614000	0.473946000
H	0.752903000	5.075120000	-0.100719000
H	1.251042000	4.216891000	1.398453000
H	2.282202000	5.515179000	0.719672000
C	-5.456524000	-1.364435000	-1.141436000
H	-5.047198000	-1.640822000	-2.123730000
H	-6.419439000	-1.862393000	-0.989088000
H	-5.591750000	-0.275072000	-1.087928000
O	0.898482000	-2.166044000	2.149810000
O	1.215095000	-0.902824000	2.614562000
H	2.164117000	-0.947844000	2.818517000
H	2.873439000	-2.502370000	-1.585034000

Figure S1. Molar fraction of the neutral, protonated and anionic boldine species as a function of the pH

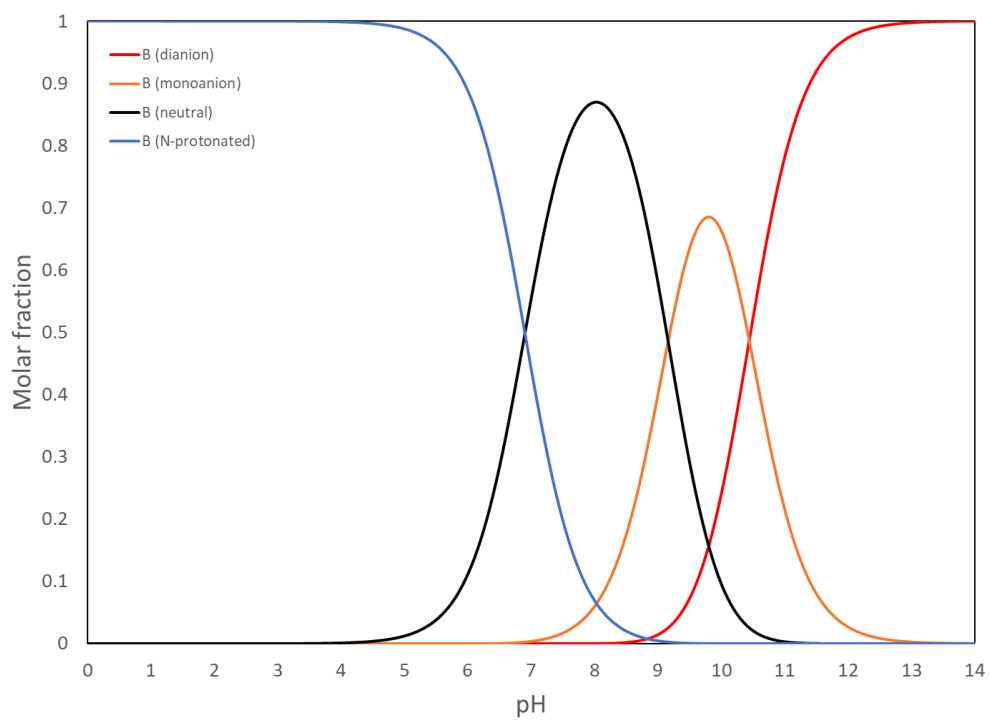


Figure S2. DFT computed spin density plot for the radicals generated from position C-6a in **B**, **G** and their *N*-methylated and *N*-protonated derivatives. Isosurface value = 0.002 a.u.

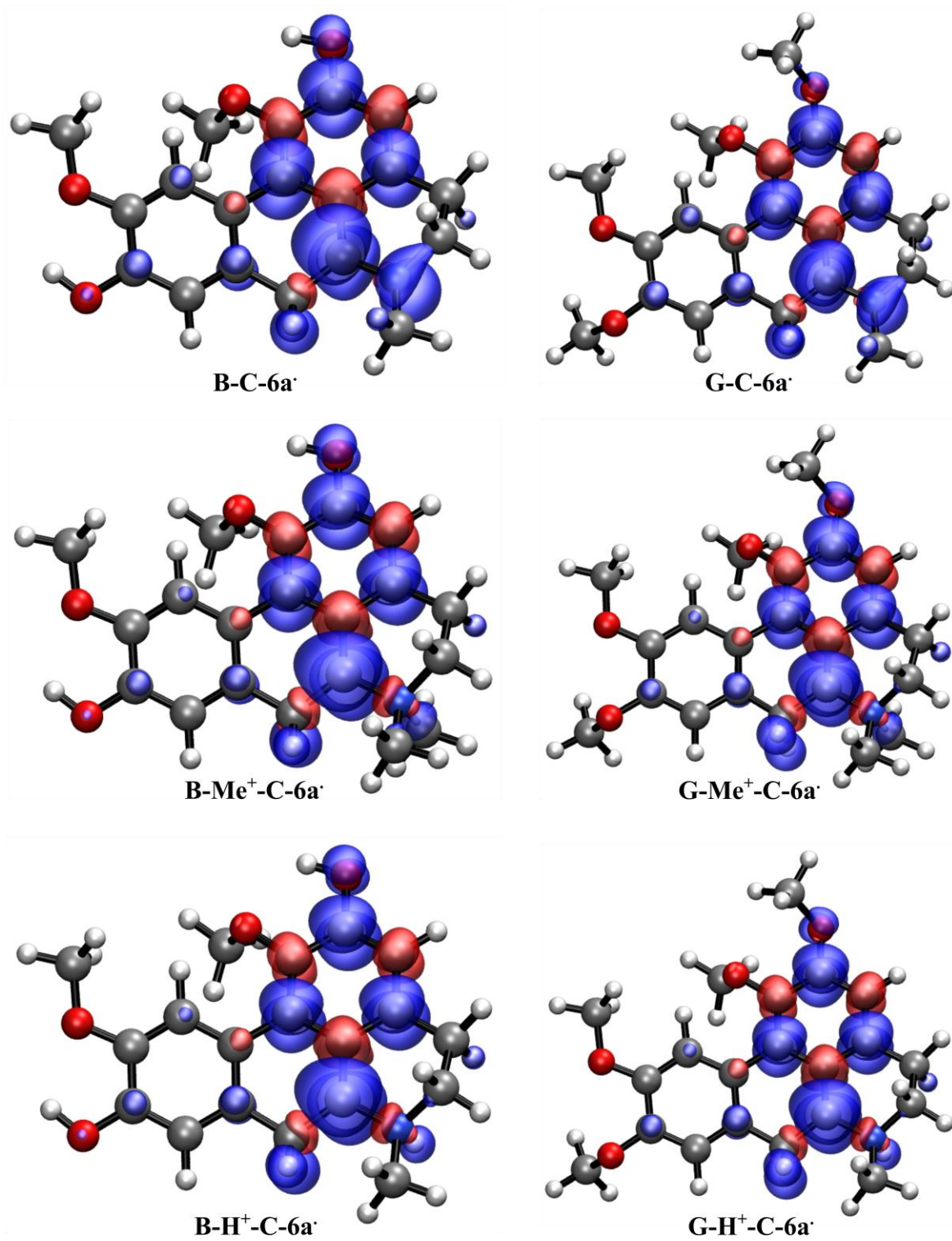


Figure S3. DFT computed spin density plot for the radicals generated from positions C-4 and C-5 in **B**, **G**. Isosurface value = 0.002 a.u.

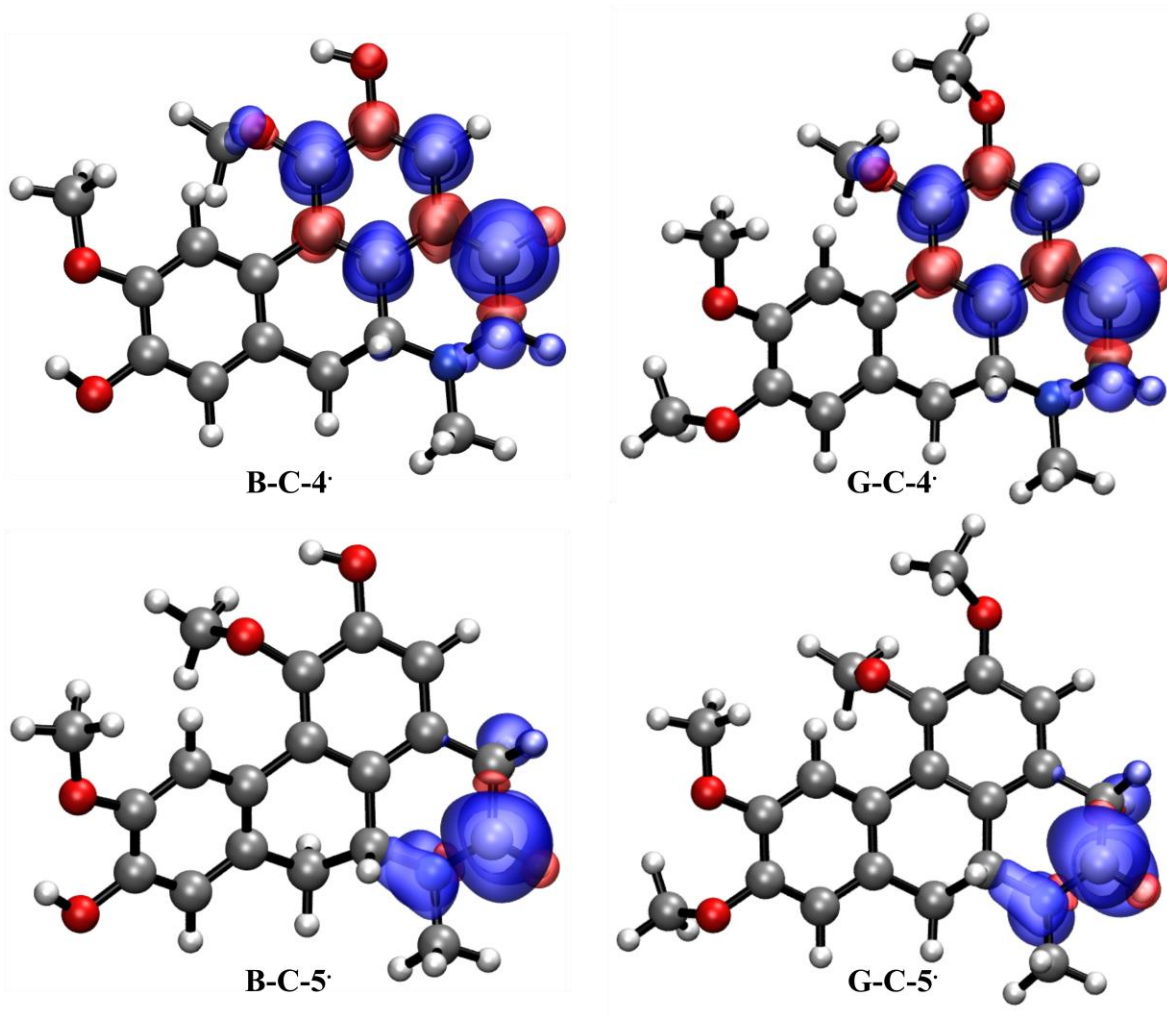


Figure S4. DFT computed spin density plot for the radicals generated from positions 2-OH and 9-OH in **B**, **B-Me⁺** and **B-H⁺**. Isosurface value = 0.002 a.u.

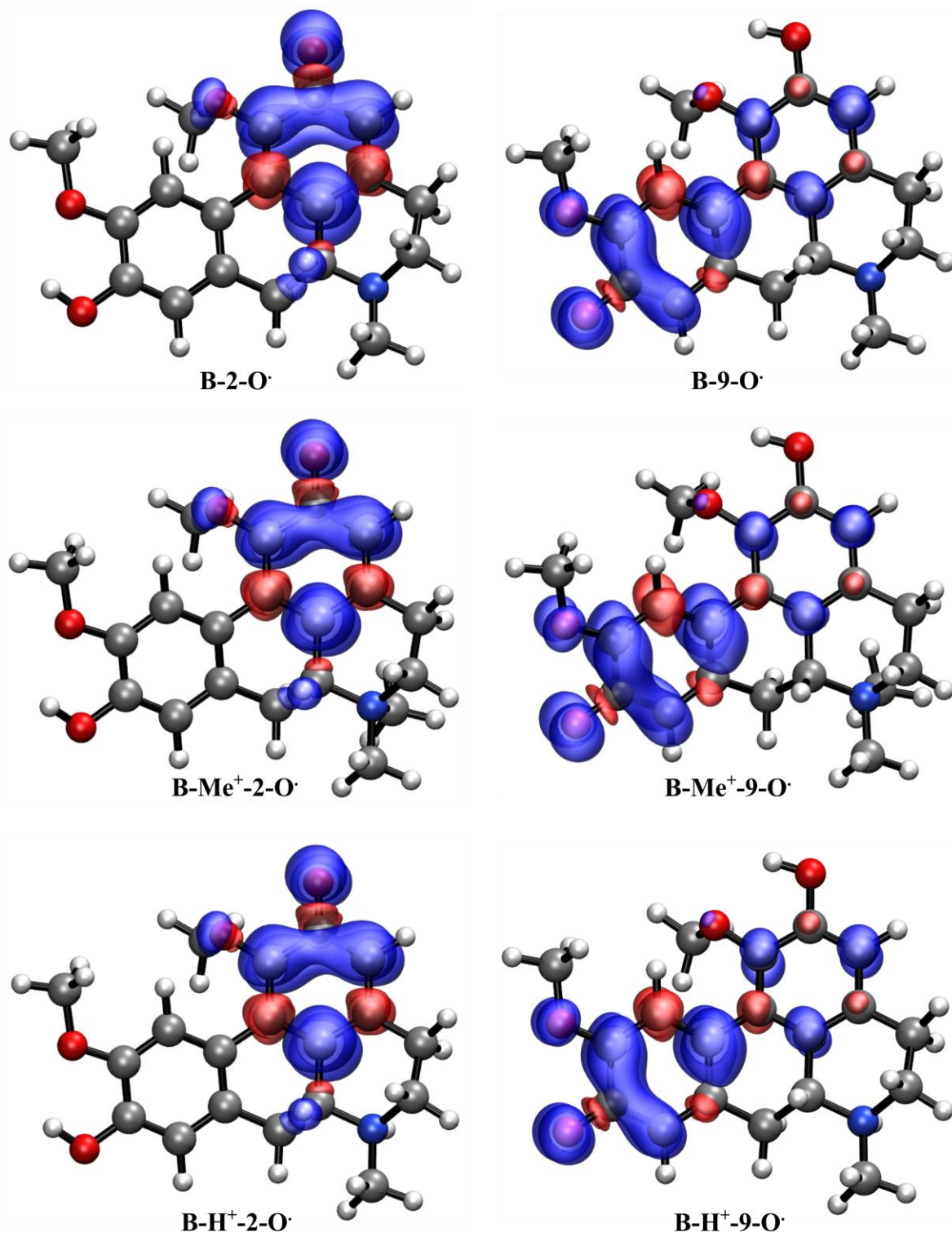


Figure S5. Gibbs free energy profile at 298.15 K for the HAT reaction of **B**, **B-Me⁺** and **B-H⁺** with the HOO[·] radical at the indicated positions. R: reactants, RC: pre-reactive complex, TS: transition state, PC: product complex, P: products.

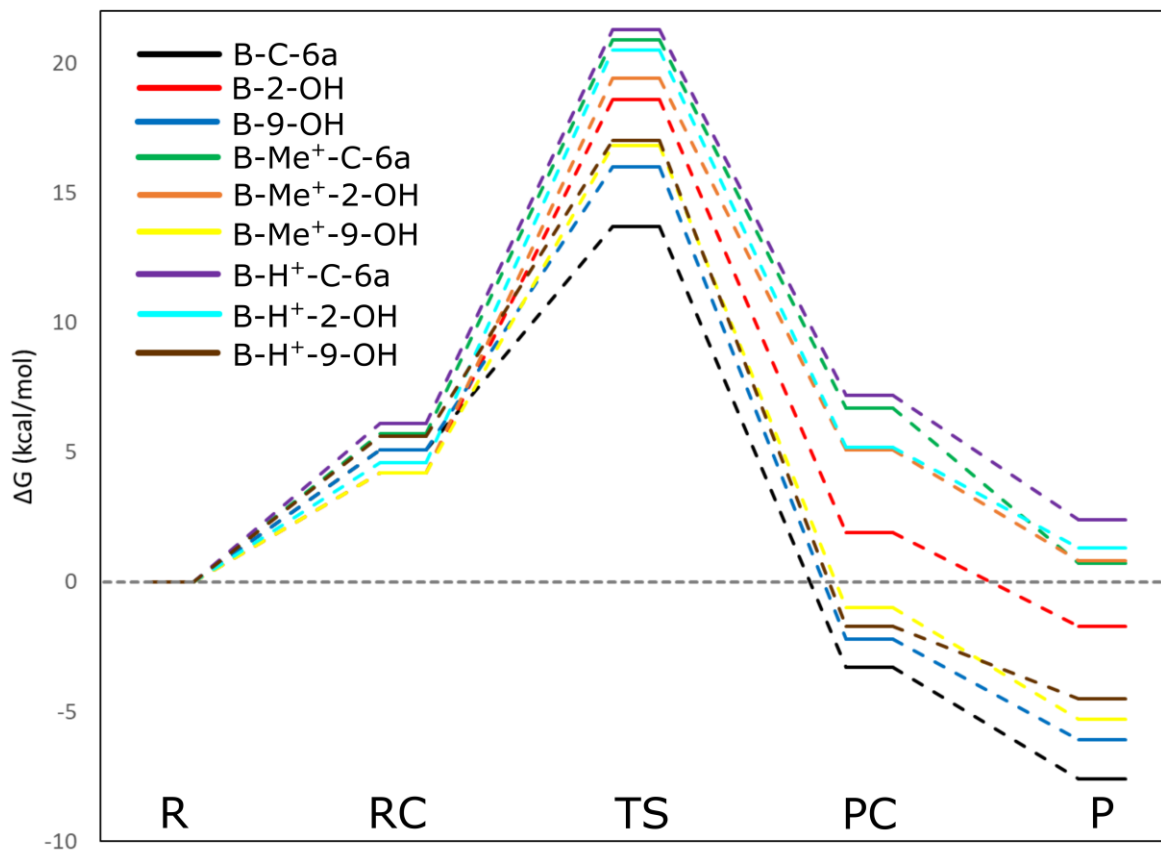


Figure S6. Gibbs free energy profile at 298.15 K for the HAT reaction of **G**, **G-Me⁺** and **G-H⁺** with the HOO[·] radical at the indicated positions. R: reactants, RC: pre-reactive complex, TS: transition state, PC: product complex, P: products.

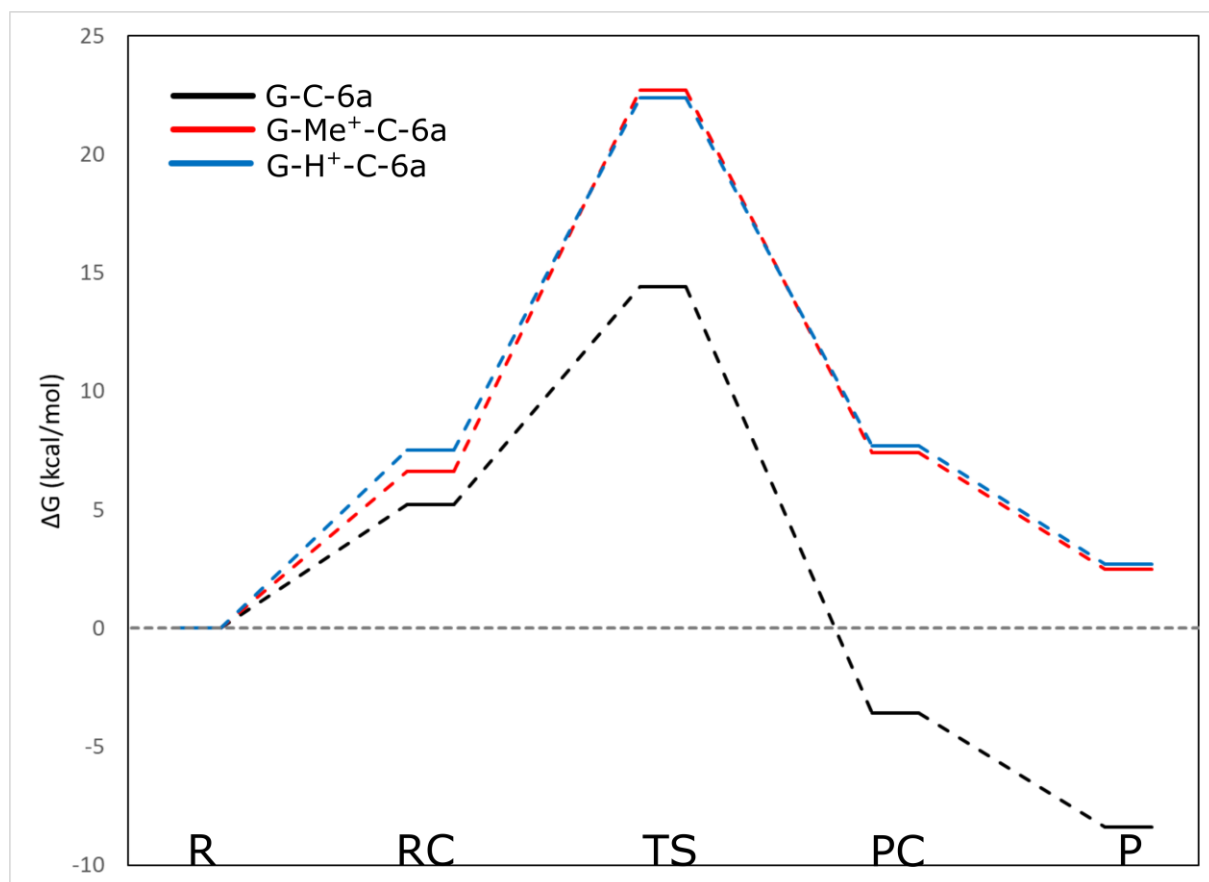


Figure S7. DFT computed spin density plot for the radicals generated from positions 2-OH and 9-OH in **d-B**. Isosurface value = 0.002 a.u.

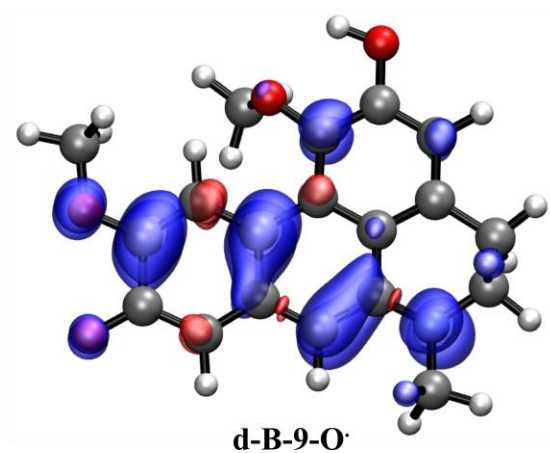
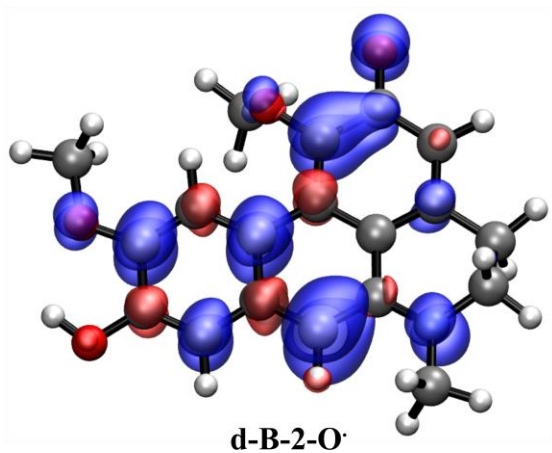


Figure S8. Gibbs free energy profile at 298.15 K for the electron transfer reaction of the conjugate bases of **B**, **B-Me⁺** and **d-B** with the HOO[·] radical.

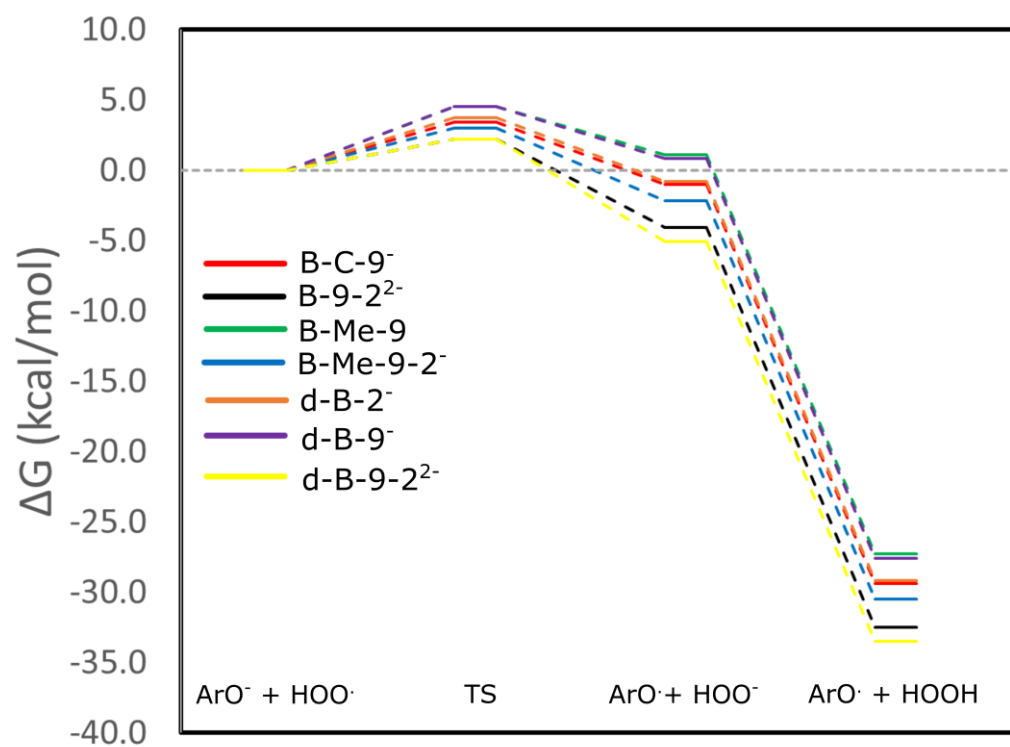


Figure S9. Plot of the logarithm of the rate constant for the HAT (Eq. 12) and SPLET (Eq. 13) reactions of **B** and its protonated and anionic derivatives with HOO^\cdot at 298.15 K as a function of pH.

