

# Supporting information for: Calculating Nuclear Magnetic Resonance Shieldings Using Systematic Fragmentation by Annihilation

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## 1 Coordinates of Molecules

The cartesian coordinates for all molecules in this section are reported in Angstrom. The structures of 12 of these molecules were obtained from the Cambridge Structural Database ([www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk)), and are referred to by the appellations given therein. The remaining 3 molecules—GelA, GelB and glycine—were obtained from Ref. 1.

Table S1: Cartesian coordinates of BAVCAC

Atom Label	x	y	z
C	2.314300	8.878100	0.576100
O	2.000300	9.761500	-0.506700
C	2.672900	9.659400	1.834900
O	3.839000	10.446400	1.484800
C	3.057800	8.710300	2.984000
O	3.539000	9.559600	4.037200
C	1.930300	7.851800	3.496500
O	0.926400	8.639900	4.131000

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Table S1 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	2.467700	6.780200	4.445700
O	3.505100	6.017000	3.827100
C	1.375100	5.882100	4.996500
O	1.952800	5.127900	6.028700
C	1.046800	4.238900	6.663900
C	1.647100	3.897600	8.004400
O	1.987200	5.112100	8.690800
C	2.855800	2.977900	7.878800
O	3.326000	2.541400	9.141200
C	2.519400	1.783800	6.985900
O	3.683500	0.966200	6.763500
C	2.032500	2.289500	5.646100
O	0.827100	3.076500	5.873500
C	1.633900	1.185000	4.709200
O	1.349700	1.673800	3.394800
H	1.492700	8.185700	0.712200
H	2.887100	7.960700	0.519000
H	1.831000	10.174600	2.280600
H	3.884700	8.107500	2.629300
H	1.449800	7.234700	2.747400
H	2.827900	7.280600	5.336100
H	1.260300	5.475600	3.999200
H	0.582900	6.329500	5.583900
H	0.115400	4.688700	6.984700
H	0.979900	3.417000	8.709200
H	3.567500	3.500800	7.251900
H	1.836700	1.269500	7.650900
H	2.835800	2.929900	5.303200
H	0.892900	0.727800	5.353100
H	2.568500	0.685000	4.486900
H	2.736200	10.120000	-1.051000
H	4.236500	11.211000	1.957700
H	4.152000	8.913500	4.453200
H	0.873200	8.847900	5.090300
H	3.480800	6.062900	2.845500
H	1.671300	5.335000	9.594600
H	2.702100	2.415200	9.890300
H	3.668500	0.420200	7.580800

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Table S1 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	1.017600	2.574200	3.182100

Table S2: Cartesian coordinates of BDGPGL

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	1.194700	0.270700	22.537200
C	2.516400	-0.327400	22.986800
C	2.396400	-0.720500	24.463800
C	2.098700	0.572600	25.229500
C	0.742100	1.073800	24.754700
C	0.231200	2.323900	25.421600
O	1.397800	0.736400	21.236000
O	2.849700	-1.456300	22.211200
O	3.627900	-1.313500	24.870100
O	1.996000	0.355000	26.639800
O	0.850100	1.385900	23.350100
O	1.133700	3.428000	25.272500
C	-0.550500	3.838900	22.070200
C	0.678900	3.602200	21.250900
C	0.457300	2.648200	20.065800
C	0.221000	1.209700	20.559400
C	-0.185500	0.217700	19.458500
C	0.933800	-0.203300	18.539000
O	-0.169600	4.663300	23.178200
O	1.070600	4.858000	20.644300
O	1.584000	2.664100	19.213100
O	-0.787700	-0.941600	20.068300
O	0.385700	-1.064500	17.543200
H	0.423600	-0.483600	22.633700
H	3.303100	0.416200	22.954300
H	1.601300	-1.445700	24.585100
H	2.864200	1.310400	25.023400
H	0.004500	0.310200	24.968600
H	0.228600	2.148300	26.490300
H	-0.732300	2.696700	25.096800
H	3.395500	-1.079800	21.485500
H	3.499700	-2.032900	25.527700
H	2.852300	0.013400	26.980900
H	0.845600	3.932000	24.479200

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Table S2 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-1.301200	4.254300	21.409300
H	-0.913100	2.942300	22.557500
H	1.456800	3.231900	21.907000
H	-0.458100	2.893500	19.541600
H	-0.647200	1.186700	21.206300
H	-1.029600	0.640800	18.928100
H	1.724600	-0.679400	19.105400
H	1.358500	0.696000	18.110300
H	-0.932600	5.183400	23.515300
H	1.687900	5.326500	21.249100
H	2.051300	3.528900	19.204300
H	-0.053400	-1.567700	20.255300
H	1.093100	-1.707700	17.314700

Table S3: Cartesian coordinates of BIHYAS10

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	1.474800	0.138500	8.619800
C	2.548600	0.393900	7.663700
C	3.761600	-0.466900	8.041600
O	3.624000	-1.654100	8.314600
C	1.998700	-0.039700	6.305400
C	2.991900	0.232900	5.215200
C	3.680900	-0.704200	4.604700
N	4.966700	0.141700	8.035200
C	6.178500	-0.617200	8.335600
C	6.407100	-0.834000	9.839300
O	7.327100	-1.546800	10.235000
C	7.278400	0.283400	7.754100
C	6.746600	1.684200	8.028700
C	7.467400	0.034300	6.260200
C	5.246200	1.562900	7.742800
N	5.610200	-0.140600	10.653300
C	5.720100	-0.245800	12.100400
C	5.044300	-1.521000	12.573600
O	3.983300	-1.867700	12.027700
C	4.972400	0.997200	12.704500
C	5.598800	2.299200	12.166600
C	4.933600	0.996100	14.235600

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Table S3 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	7.087000	2.369000	12.318500
N	5.583900	-2.197200	13.605700
C	6.884700	-1.829100	14.206500
C	4.803200	-3.306100	14.180700
C	4.131300	-2.765100	15.451800
O	4.818300	-2.633100	16.461200
C	5.627000	-4.559800	14.498900
C	4.677600	-5.686900	14.901000
C	6.477900	-4.975200	13.305300
N	2.823900	-2.400100	15.442100
C	2.285800	-1.982600	16.742200
C	1.872300	-2.581500	14.322800
C	1.168900	-1.254800	13.965900
O	0.315200	-0.770700	14.691100
C	0.848100	-3.652800	14.636100
N	1.501300	-0.740600	12.767500
C	0.873500	0.475500	12.257100
C	0.544800	0.351000	10.767900
C	1.749600	0.519500	9.878000
O	2.818800	0.965000	10.228500
H	2.756500	1.456800	7.672600
H	1.867500	-1.112600	6.373500
H	1.049900	0.456000	6.141200
H	3.136200	1.278900	4.974200
H	3.569700	-1.727900	4.940100
H	4.351200	-0.399600	3.810400
H	6.195400	-1.595700	7.871800
H	8.184000	0.023200	8.287900
H	6.976400	1.918200	9.060800
H	7.325000	2.383200	7.437400
H	7.846400	-0.971800	6.129700
H	6.536900	0.043700	5.706100
H	8.073200	0.799900	5.791300
H	4.673600	2.217900	8.387800
H	4.968700	1.800200	6.723300
H	4.753900	0.252400	10.292200
H	6.778100	-0.289200	12.327800
H	3.954800	0.975600	12.334700

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Table S3 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	5.411200	2.387700	11.103700
H	5.145600	2.989600	12.867200
H	5.883900	1.177900	14.722200
H	4.455500	0.088700	14.583400
H	3.910400	1.197400	14.527800
H	7.641200	1.637400	11.743500
H	7.440900	3.338800	11.991200
H	7.454700	2.190300	13.321300
H	6.814000	-0.817900	14.587800
H	6.952100	-2.453500	15.088800
H	7.667900	-1.789400	13.459500
H	4.149600	-3.583800	13.363000
H	6.310700	-4.377800	15.318800
H	5.182600	-6.644600	14.926500
H	4.162200	-5.374000	15.800700
H	3.986100	-5.907700	14.097300
H	7.131200	-4.160100	13.019400
H	7.073800	-5.829100	13.603200
H	5.810100	-5.323800	12.527200
H	1.256100	-1.729900	16.521500
H	2.457000	-2.764100	17.472200
H	2.908500	-1.243800	17.231600
H	2.427100	-2.954700	13.470800
H	0.304900	-3.369400	15.529200
H	1.404300	-4.572400	14.769900
H	0.300900	-3.851000	13.722800
H	2.378600	-1.102600	12.424900
H	1.433500	1.375400	12.479400
H	-0.048000	0.579500	12.816500
H	0.044100	1.296200	10.598300
H	0.114000	-0.620300	10.558600

Table S4: Cartesian coordinates of DOSLED

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
F	10.498100	-3.859600	-1.088300
F	11.227300	-1.861900	-1.322600
F	9.243600	-2.194900	-0.574200
F	7.021400	-1.081200	5.640900

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Table S4 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
F	7.244100	0.249300	7.313600
F	5.657700	0.555000	5.897400
O	10.660800	-0.375100	1.046900
O	12.317200	-1.224100	2.302100
O	12.188900	-3.563300	0.914300
O	8.566100	1.631400	3.021900
O	6.722000	0.362500	3.227100
O	9.223600	0.837900	5.558700
N	9.039700	3.108100	-0.865900
H	9.263800	3.951200	-0.358800
C	9.933100	1.912000	1.108700
H	10.180100	2.880700	1.525400
C	8.516600	1.575000	1.559500
H	8.253000	0.576000	1.234900
C	7.511300	2.574500	1.028200
H	7.662200	3.528300	1.518400
H	6.510300	2.234000	1.262800
C	7.638100	2.759800	-0.484600
H	7.344900	1.845900	-0.986100
H	6.970300	3.548900	-0.807400
C	9.979900	2.048400	-0.399800
H	10.987500	2.298400	-0.708400
H	9.713400	1.103300	-0.856600
C	10.977100	0.940400	1.588600
H	11.958300	1.253800	1.254200
H	10.980700	0.905400	2.671000
C	11.438600	-1.366200	1.492100
C	11.061300	-2.739800	0.916400
C	10.496800	-2.652700	-0.525600
C	13.322200	-3.129900	0.160000
H	13.236700	-3.489700	-0.858000
H	14.226300	-3.523800	0.607600
H	13.362500	-2.047700	0.159300
C	10.020900	-3.395500	1.835200
C	8.885900	-2.710000	2.256300
H	8.728500	-1.687400	1.936200
C	7.962800	-3.319400	3.075200
H	7.088300	-2.771400	3.403500

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Table S4 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	8.147200	-4.625500	3.479000
H	7.413700	-5.108600	4.112600
C	9.270100	-5.310300	3.071800
H	9.420000	-6.332500	3.396600
C	10.209700	-4.706100	2.250100
H	11.088000	-5.254300	1.932400
C	7.630500	0.968700	3.708700
C	7.885600	1.139000	5.223100
C	6.930500	0.211900	6.012500
C	9.760300	-0.415800	5.114500
H	9.354800	-1.217300	5.719500
H	10.838800	-0.399900	5.211700
H	9.493000	-0.575900	4.077300
C	7.617300	2.587700	5.621600
C	6.482200	3.242400	5.137700
H	5.803700	2.725500	4.470400
C	6.225000	4.545800	5.508400
H	5.344000	5.048100	5.128200
C	7.077300	5.210000	6.355100
H	6.866000	6.230700	6.649000
C	8.203500	4.572600	6.831400
H	8.879300	5.097500	7.495300
C	8.475100	3.268900	6.468800
H	9.362300	2.777300	6.848700
C	9.187300	3.283100	-2.342900
H	8.729400	2.435800	-2.838300
H	10.242300	3.274500	-2.587300
C	8.577800	4.547100	-2.890600
C	9.265700	5.746000	-2.802600
H	10.198800	5.785500	-2.254300
C	8.784300	6.894300	-3.403200
H	9.341200	7.821000	-3.340100
C	7.580800	6.846600	-4.087200
H	7.200400	7.734600	-4.576700
C	6.868700	5.672100	-4.144100
H	5.917100	5.643900	-4.660500
C	7.361100	4.524300	-3.545500
H	6.790600	3.604900	-3.591500

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Table S4 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
F	7.086500	6.868200	3.006600
F	8.309100	8.573100	3.451200
F	7.316100	8.419700	1.552500
O	9.826700	5.161900	0.556100
O	7.709200	5.871400	0.433400
O	9.995600	6.533200	2.987400
C	8.860500	5.921400	0.876900
C	9.233700	7.026900	1.897700
C	7.976100	7.720500	2.470600
C	9.518500	5.356000	3.634100
H	8.462500	5.463900	3.848600
H	10.061300	5.207700	4.559400
H	9.670000	4.501400	2.986300
C	10.086700	8.083800	1.211100
C	9.792400	8.472400	-0.093500
H	8.964400	8.015400	-0.621200
C	10.564100	9.448600	-0.718200
H	10.328800	9.754300	-1.730200
C	11.628500	10.030000	-0.054400
H	12.226600	10.789600	-0.542300
C	11.922200	9.634600	1.229600
H	12.761200	10.079100	1.750400
C	11.153700	8.675600	1.860500
H	11.390400	8.383200	2.876000

Table S5: Cartesian coordinates of GENTBS01

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	3.212300	5.965500	1.411200
C	3.889700	4.975600	2.345900
C	4.896300	4.143400	1.577300
C	4.280900	3.507100	0.349000
C	3.525400	4.556900	-0.465300
C	2.789000	3.939800	-1.630400
O	2.226000	6.665800	2.101600
O	4.521800	5.708500	3.385100
O	5.417100	3.139000	2.456700
O	5.330400	2.957900	-0.465500
O	2.575600	5.221700	0.371500

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Table S5 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	1.858600	2.980300	-1.136300
C	1.518100	2.011600	-2.072800
C	0.463400	1.106900	-1.469100
C	-0.064400	0.138400	-2.523600
C	-0.497700	0.862400	-3.788900
C	0.584500	1.836800	-4.267900
C	0.101600	2.768500	-5.359200
O	1.036900	0.382900	-0.381300
O	-1.173100	-0.569100	-1.982500
O	-0.736000	-0.110100	-4.813700
O	0.975100	2.684900	-3.192100
O	-0.902500	3.668400	-4.895500
H	3.847600	6.763500	1.047100
H	3.106000	4.347100	2.750300
H	5.745100	4.763200	1.316100
H	3.565500	2.741000	0.621300
H	4.221300	5.322200	-0.785900
H	2.193000	4.675700	-2.156000
H	3.585100	3.528700	-2.238700
H	1.716400	7.229800	1.478400
H	5.191600	5.081200	3.737600
H	6.383900	3.310200	2.504800
H	5.170100	2.002300	-0.631200
H	2.400500	1.439900	-2.332500
H	-0.384500	1.705700	-1.160200
H	0.722900	-0.577400	-2.724900
H	-1.419600	1.400900	-3.607200
H	1.448800	1.276500	-4.602500
H	-0.350400	2.192200	-6.157000
H	0.933500	3.382500	-5.681300
H	-0.875100	-1.490600	-1.814300
H	-1.657700	0.109500	-5.075500
H	-0.524100	4.243500	-4.193800
H	0.309700	0.303200	0.275300

Table S6: Cartesian coordinates of GelA

Atom Label	x	y	z
C	-12.220450	1.876231	0.539352
C	-11.084357	1.345636	-0.334529
C	-10.063993	0.516894	0.448114
C	-8.924928	-0.019970	-0.420532
C	-7.904194	-0.848406	0.362077
C	-6.767667	-1.388022	-0.508415
C	-5.743871	-2.213725	0.273133
C	-4.611209	-2.757060	-0.600091
C	-3.581346	-3.576197	0.180465
C	-2.453507	-4.123327	-0.696578
C	-1.414399	-4.931053	0.083533
C	-0.291664	-5.481390	-0.797960
C	0.761383	-6.270372	-0.017385
C	1.857505	-6.851687	-0.916887
C	2.973075	-7.613151	-0.174509
C	4.240813	-6.827541	0.201708
C	4.095725	-5.710971	1.255086
C	3.815516	-4.297436	0.722356
C	5.015655	-3.647781	0.028573
C	4.736380	-2.232889	-0.450985
O	4.467494	-1.418297	0.667595
P	4.137086	0.136126	0.501256
O	4.054035	0.756953	1.828780
O	4.907686	0.735648	-0.609293
O	2.564221	0.053112	-0.053576
C	2.179286	0.622170	-1.251075
C	1.211668	1.790254	-1.066896
N	1.704657	3.045375	-0.363738
C	0.684404	4.115811	-0.710941
C	0.532063	5.443957	0.073136
C	1.750359	6.384633	0.145102
C	2.228311	6.927653	-1.206877
C	3.470272	7.823806	-1.119054
C	3.262001	9.129190	-0.349183
C	1.778826	2.814853	1.117332
C	3.062642	3.412288	-0.878154
C	-0.163103	5.301544	1.448005

Continued on next page

Table S6 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-1.047833	6.501183	1.797341
H	-11.840279	2.516368	1.330758
H	-12.767089	1.062650	1.007974
H	-12.928419	2.456999	-0.044020
H	-11.500073	0.740030	-1.137202
H	-10.577732	2.180659	-0.814356
H	-10.573180	-0.316457	0.929643
H	-9.649556	1.124315	1.251366
H	-8.417074	0.813998	-0.902889
H	-9.341135	-0.626920	-1.222929
H	-8.412133	-1.681027	0.845862
H	-7.486656	-0.240774	1.163411
H	-6.261547	-0.555348	-0.995098
H	-7.186031	-1.997373	-1.307815
H	-6.249925	-3.044404	0.762144
H	-5.322879	-1.603400	1.070636
H	-4.109036	-1.926457	-1.094557
H	-5.032952	-3.371607	-1.393766
H	-4.083429	-4.404260	0.678027
H	-3.155830	-2.960242	0.971034
H	-1.957575	-3.295426	-1.201470
H	-2.879197	-4.746339	-1.481665
H	-1.909129	-5.756492	0.592999
H	-0.984570	-4.305254	0.863517
H	0.192995	-4.656042	-1.317410
H	-0.720158	-6.117559	-1.571337
H	0.276748	-7.087433	0.515132
H	1.194708	-5.628976	0.743341
H	2.293921	-6.061656	-1.524382
H	1.380310	-7.532803	-1.618328
H	2.559100	-8.071352	0.722426
H	3.296076	-8.439226	-0.803640
H	4.953679	-7.556739	0.579396
H	4.687417	-6.427890	-0.705767
H	3.316985	-5.990055	1.961067
H	5.012728	-5.664645	1.838076
H	2.974152	-4.309198	0.034646
H	3.523547	-3.663017	1.551877

Continued on next page

Table S6 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	5.861830	-3.618290	0.709892
H	5.324418	-4.233952	-0.834500
H	3.880038	-2.227444	-1.121377
H	5.585479	-1.833525	-0.990318
H	3.033453	0.904070	-1.847200
H	1.603414	-0.103197	-1.821829
H	0.885843	2.108708	-2.049283
H	0.347981	1.460443	-0.507202
H	0.866172	4.340659	-1.751998
H	-0.273968	3.619119	-0.655176
H	-0.193540	5.945652	-0.567291
H	1.460849	7.223623	0.765899
H	2.572322	5.911778	0.674379
H	2.452037	6.109339	-1.885281
H	1.415461	7.486759	-1.667507
H	3.787980	8.061738	-2.130506
H	4.287748	7.264353	-0.669429
H	3.054018	8.956477	0.701632
H	4.150544	9.749356	-0.404068
H	2.435398	9.700069	-0.763664
H	0.789107	2.573387	1.472573
H	2.465223	2.015753	1.344970
H	2.126224	3.722639	1.579729
H	2.996248	3.552992	-1.947796
H	3.377970	4.326920	-0.409523
H	3.770612	2.628258	-0.658401
H	-0.788323	4.413277	1.455079
H	0.571089	5.165070	2.234198
H	-1.507910	6.359315	2.769355
H	-0.486917	7.428600	1.836748
H	-1.844619	6.625000	1.069694

Table S7: Cartesian coordinates of GelB

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	13.802796	8.768436	-0.660471
H	12.970821	9.420028	-0.912262
H	14.257725	8.439779	-1.590486
H	14.537037	9.362174	-0.125715

Continued on next page

Table S7 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	13.337873	7.578111	0.177430
H	14.197009	6.965331	0.441781
H	12.920264	7.938129	1.115259
C	12.300147	6.712124	-0.539189
H	12.719572	6.352732	-1.477439
H	11.442215	7.327514	-0.805634
C	11.827992	5.519336	0.293999
H	11.407716	5.879319	1.231517
H	12.685980	4.905005	0.561313
C	10.791611	4.653480	-0.424855
H	11.212697	4.291263	-1.361110
H	9.934168	5.268015	-0.694246
C	10.316754	3.462483	0.409647
H	9.893510	3.824057	1.345106
H	11.173334	2.847963	0.680414
C	9.282225	2.596123	-0.311343
H	9.706274	2.231074	-1.245048
H	8.425850	3.210382	-0.584664
C	8.804500	1.407530	0.525120
H	8.377007	1.771053	1.457619
H	9.659313	0.792881	0.800090
C	7.772719	0.540733	-0.199473
H	8.201053	0.171980	-1.129478
H	6.917239	1.153971	-0.477117
C	7.293123	-0.644543	0.641205
H	6.859051	-0.278677	1.568928
H	8.145910	-1.258736	0.920344
C	6.264594	-1.510899	-0.090882
H	6.703705	-1.886661	-1.013683
H	5.405717	-0.904950	-0.369989
C	5.795976	-2.683031	0.762700
H	5.309176	-2.341080	1.664621
H	6.629412	-3.310884	1.052665
N	4.823130	-3.502359	0.015617
C	4.035811	-4.382573	0.603747
H	4.852432	-3.455918	-0.979706
O	3.977464	-4.627520	1.781870
C	3.037805	-5.146958	-0.295900

Continued on next page

Table S7 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	3.436883	-5.379732	-1.273262
C	1.726468	-4.355061	-0.392598
H	1.948528	-3.387177	-0.818541
H	1.311084	-4.205247	0.595307
S	0.506171	-5.232960	-1.444844
S	-1.302654	-4.840272	-0.555811
C	-1.901773	-3.373134	-1.486101
H	-1.572716	-3.452771	-2.514067
H	-1.480507	-2.469423	-1.068790
C	-3.432348	-3.243161	-1.437491
H	-3.724235	-2.410568	-2.062686
C	-3.981735	-3.116882	0.000868
O	-4.343660	-4.141257	0.524089
N	-3.957385	-1.912722	0.540226
H	-3.737918	-1.128202	-0.033647
C	-4.427854	-1.639164	1.911630
H	-4.279333	-2.545182	2.478707
H	-3.773831	-0.877574	2.316733
C	-5.886950	-1.193086	1.967697
H	-6.515487	-1.983713	1.566670
H	-6.147779	-1.097112	3.017641
C	-6.170424	0.129431	1.251041
H	-5.510713	0.901364	1.643745
H	-5.939364	0.035978	0.189306
C	-7.624437	0.584839	1.398479
H	-8.284515	-0.192255	1.017893
H	-7.856718	0.691423	2.455329
C	-7.917835	1.901978	0.677606
H	-7.686626	1.792991	-0.381364
H	-7.252618	2.675199	1.057320
C	-9.368903	2.361490	0.833384
H	-10.033809	1.586768	0.455715
H	-9.598075	2.470209	1.891449
C	-9.664157	3.678495	0.113009
H	-9.434717	3.568947	-0.945884
H	-8.997542	4.451660	0.490797
C	-11.114300	4.139607	0.271178
H	-11.780580	3.365764	-0.106063

Continued on next page

Table S7 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-11.342841	4.248306	1.329705
C	-11.410406	5.456887	-0.448255
H	-11.181268	5.347951	-1.507154
H	-10.743698	6.230179	-0.070555
C	-12.860295	5.918203	-0.289994
H	-13.527520	5.145191	-0.667812
H	-13.089947	6.027096	0.768524
C	-13.157731	7.235763	-1.008218
H	-12.492991	8.009589	-0.630151
H	-12.929530	7.128194	-2.066602
C	-14.607891	7.689506	-0.845934
H	-14.786970	8.625148	-1.365619
H	-15.297162	6.951704	-1.246586
H	-14.857131	7.839860	0.200482
N	2.812289	-6.443420	0.425252
H	3.566788	-7.097980	0.265418
H	2.817098	-6.235061	1.423555
H	1.947822	-6.896191	0.158824
N	-4.099678	-4.474097	-1.984441
H	-5.023806	-4.268016	-2.341186
H	-3.578238	-4.927741	-2.720858
H	-4.226235	-5.119876	-1.204153

Table S8: Cartesian coordinates of HEBLIJ

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
N	-9.495200	12.487000	6.736100
C	-9.615400	12.744800	9.224900
O	-9.978800	13.242100	10.255100
C	-10.048500	13.247100	7.850600
C	-9.819500	14.744200	7.703000
C	-8.328400	15.073000	7.716300
C	-10.490200	15.284500	6.453000
O	-8.810200	11.664100	9.181600
C	-7.208400	10.343900	10.458300
O	-6.658900	10.112500	11.550600
C	-8.503000	11.062700	10.509300
C	-9.609600	10.177000	10.912300
N	-6.708500	9.927500	9.294900

Continued on next page



Table S8 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-4.312100	10.066300	9.060600
O	-4.294000	10.871000	8.125900
C	-5.504600	9.114500	9.227200
C	-5.553200	8.124700	8.057100
C	-4.245300	7.392700	7.922800
C	-6.682800	7.120100	8.280200
N	-3.298000	10.008400	9.958700
C	-2.172300	12.239200	10.207400
O	-1.273600	12.787700	10.849000
C	-2.058700	10.776800	9.740000
C	-1.043700	10.026600	10.612600
C	-1.864100	9.570600	11.769300
C	-3.207300	9.131000	11.137600
N	-3.305600	12.853800	9.889900
C	-4.012500	14.997000	8.913000
O	-4.129900	16.185000	8.884100
C	-3.618500	14.228600	10.160700
C	-4.629800	14.430200	11.289700
C	-5.952000	13.838700	10.952200
C	-4.097400	13.894800	12.620700
O	-4.236700	14.208800	7.838400
C	-5.317600	13.906400	5.673700
O	-5.884300	14.359200	4.653500
C	-4.637400	14.883000	6.592900
C	-3.439200	15.504200	5.906800
N	-5.201200	12.601000	5.901300
C	-7.041500	11.115500	5.379500
O	-7.182700	10.490900	6.427500
C	-5.665800	11.598000	4.931100
C	-4.698400	10.414900	4.816700
C	-5.220300	9.402000	3.856500
C	-3.316100	10.909000	4.437100
N	-8.113800	11.393100	4.595800
C	-10.138200	11.558400	6.080000
O	-11.284900	11.234500	6.363100
C	-9.437900	10.831300	4.930000
C	-10.203000	11.006500	3.608900
C	-9.604900	12.257300	3.019500

Continued on next page

Table S8 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-8.154800	12.111900	3.289200
H	-8.528900	12.710000	6.549900
H	-11.127600	13.200200	7.929900
H	-10.245800	15.149600	8.612200
H	-8.173200	16.143900	7.673200
H	-7.758700	14.390400	8.334700
H	-7.737900	14.734400	6.874000
H	-10.455600	16.366500	6.483200
H	-10.021900	14.697500	5.672600
H	-11.443600	14.834400	6.205300
H	-8.436700	11.940600	11.139900
H	-9.342100	9.808700	11.894900
H	-10.535900	10.709200	10.734100
H	-9.707200	9.534100	10.046200
H	-7.197500	10.169000	8.446000
H	-5.421400	8.563700	10.155900
H	-5.842100	8.701300	7.187000
H	-3.475800	8.117400	7.686900
H	-3.883300	6.898100	8.815600
H	-4.330600	6.688000	7.104900
H	-7.593600	7.594300	8.624200
H	-6.843900	6.743800	7.277600
H	-6.558800	6.835400	9.317800
H	-1.782100	10.661600	8.699300
H	-0.557100	9.312000	9.960300
H	-0.196100	10.662000	10.837900
H	-1.986500	10.533800	12.248900
H	-1.468400	8.710100	12.294600
H	-3.168600	8.091100	10.837600
H	-4.050400	9.334900	11.786100
H	-3.963400	12.322200	9.339600
H	-2.687900	14.676000	10.487200
H	-5.035900	15.430200	11.378300
H	-3.097400	14.265900	12.808000
H	-4.811500	13.914700	13.434700
H	-4.187700	12.843100	12.378600
H	-5.765800	13.614900	9.909100
H	-5.577800	12.825400	10.873300

Continued on next page

Table S8 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-6.669300	14.130200	11.709500
H	-5.419700	15.612000	6.764300
H	-3.728400	15.881100	4.933600
H	-2.843900	16.214900	6.466700
H	-2.674000	14.738800	5.868200
H	-4.820200	12.306500	6.788000
H	-5.781400	12.086700	3.971500
H	-4.682900	10.068600	5.842700
H	-4.555100	8.566600	3.676400
H	-6.128100	8.848600	4.062400
H	-5.183000	10.109000	3.036900
H	-2.556700	10.137600	4.471100
H	-3.461900	11.312200	3.442500
H	-2.766200	11.337100	5.266000
H	-9.323000	9.818400	5.295600
H	-9.925300	10.137600	3.025200
H	-11.270700	11.060400	3.782500
H	-9.719100	12.390600	1.950800
H	-9.970700	13.205800	3.392800
H	-7.635700	13.055100	3.406500
H	-7.781700	11.462300	2.507100

Table S9: Cartesian coordinates of KIVDIC

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
N	-3.101600	6.940900	9.181000
C	-2.885000	6.414700	10.520100
C	-1.426400	6.537700	10.986600
C	-0.485500	5.907600	9.968200
C	-1.231300	5.853400	12.324400
C	-3.851900	7.113700	11.504100
O	-3.416700	7.941800	12.279000
N	-5.140200	6.808500	11.467000
C	-5.828400	6.050900	10.405900
C	-7.181000	5.715600	11.085700
C	-7.421800	6.907000	12.009200
C	-6.053500	7.335300	12.475800
C	-6.118800	6.921700	9.192000
O	-6.141900	8.134300	9.253900

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Table S9 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
N	-6.439100	6.245300	8.077200
C	-7.028200	6.971000	6.970700
C	-8.487800	7.350000	7.274900
C	-3.159000	6.180800	8.077200
O	-3.181400	4.955000	8.096500
H	-3.157800	7.943300	9.080500
H	-3.165600	5.370400	10.459800
H	-1.178700	7.588000	11.079400
H	-0.530200	6.560300	9.105200
H	0.527100	6.233000	10.172200
H	-0.610800	4.835600	9.878300
H	-1.852200	6.263300	13.111400
H	-1.631200	4.850800	12.237200
H	-0.178900	6.030800	12.508300
H	-5.266500	5.190800	10.063200
H	-7.062800	4.939600	11.831900
H	-7.883400	5.470200	10.298800
H	-7.863400	7.675300	11.386700
H	-8.102600	6.610400	12.797500
H	-5.808500	6.943300	13.455100
H	-5.976900	8.412700	12.554600
H	-6.395100	5.250600	7.914000
H	-6.522900	7.863300	6.622500
H	-8.865400	7.785100	6.357800
H	-8.484800	7.877400	8.220800
H	-8.998400	6.438200	7.559100
C	-6.976500	6.180800	5.685300
C	-3.107300	6.971000	6.791800
N	-7.033900	6.940900	4.581600
O	-6.954100	4.955000	5.666000
N	-3.696400	6.245300	5.685300
C	-1.647700	7.350000	6.487700
H	-3.612600	7.863300	7.140100
C	-7.250500	6.414700	3.242500
H	-6.977700	7.943300	4.682000
C	-4.016700	6.921700	4.570500
H	-3.740400	5.250600	5.848600
H	-1.270100	7.785100	7.404800

Continued on next page

Table S9 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-1.650700	7.877400	5.541800
H	-1.137100	6.438200	6.203500
C	-8.709100	6.537700	2.775900
C	-6.283600	7.113700	2.258400
H	-6.969900	5.370400	3.302800
C	-4.307100	6.050900	3.356700
O	-3.993600	8.134300	4.508600
C	-9.650000	5.907600	3.794300
C	-8.904200	5.853400	1.438200
H	-8.956800	7.588000	2.683100
O	-6.718800	7.941800	1.483600
N	-4.995300	6.808500	2.295600
C	-2.954600	5.715600	2.676800
H	-4.869000	5.190800	3.699300
H	-9.605300	6.560300	4.657400
H	-10.662700	6.233000	3.590300
H	-9.524700	4.835600	3.884200
H	-8.283300	6.263300	0.651200
H	-8.504300	4.850800	1.525400
H	-9.956600	6.030800	1.254300
C	-4.082000	7.335300	1.286800
C	-2.713700	6.907000	1.753300
H	-3.072800	4.939600	1.930600
H	-2.252100	5.470200	3.463700
H	-4.327000	6.943300	0.307400
H	-4.158700	8.412700	1.207900
H	-2.272100	7.675300	2.375800
H	-2.032900	6.610400	0.965100

Table S10: Cartesian coordinates of NIYBIG

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	5.588100	7.609400	5.420800
O	3.299000	6.769800	3.949900
O	1.120800	5.846300	5.574600
O	0.711500	7.534500	7.861300
O	4.319400	7.776400	7.308100
O	3.616800	7.026500	9.899700
O	4.976600	9.804500	3.584600

Continued on next page

Table S10 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	4.985600	8.928800	1.521200
O	4.332900	4.776300	3.750600
O	0.161500	7.123300	3.970300
O	0.506900	5.829000	9.328500
O	4.171200	8.071200	11.785400
C	4.295500	7.825400	5.882100
H	3.928500	8.786600	5.544100
C	3.386800	6.705200	5.389300
H	3.761900	5.740000	5.706300
C	1.984400	6.946200	5.934900
H	1.589700	7.861500	5.511400
C	2.011500	7.066400	7.451300
H	2.239500	6.112100	7.909800
C	3.043300	8.126000	7.857000
H	2.739800	9.077000	7.437100
C	3.220300	8.300100	9.345100
H	3.980500	9.045600	9.543000
H	2.292000	8.630000	9.794900
C	6.358100	8.820600	5.265900
H	7.384600	8.636900	5.558100
H	5.956900	9.591300	5.912500
C	6.315300	9.287900	3.832800
H	7.051300	10.065600	3.670300
H	6.530600	8.465000	3.162500
C	4.397900	9.491600	2.405500
C	2.959800	9.910300	2.362100
C	2.380600	10.647200	3.525200
H	1.324800	10.822100	3.359700
H	2.890900	11.596300	3.633200
H	2.512200	10.062900	4.427500
C	2.255700	9.582200	1.279900
H	2.778000	9.003400	0.528200
H	1.215100	9.863200	1.174700
C	3.797000	5.727400	3.242900
C	3.587900	5.923300	1.771600
H	4.383600	6.535500	1.365400
H	2.635900	6.411300	1.602700
H	3.587900	4.959000	1.278700

Continued on next page

Table S10 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	0.241900	6.070400	4.551200
C	-0.582300	4.855800	4.250500
H	-1.633700	5.113000	4.285600
H	-0.372600	4.090700	4.987700
H	-0.336100	4.483400	3.263700
C	0.065300	6.831100	8.835400
C	-1.230800	7.497800	9.181100
H	-1.751900	6.910600	9.927100
H	-1.844200	7.579600	8.292200
H	-1.032200	8.487100	9.574300
C	4.071600	7.049500	11.158300
C	4.446400	5.677500	11.634700
H	4.229300	5.590300	12.692200
H	5.504000	5.514300	11.468400
H	3.876700	4.937600	11.086300

Table S11: Cartesian coordinates of QAZJAC

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	-2.129700	8.873400	2.605700
O	1.193200	9.486900	-0.405800
O	0.617600	5.427300	1.532700
O	3.446900	7.467200	1.619300
O	2.575200	5.397400	-3.270900
O	3.671300	7.307200	-3.814300
O	6.401900	6.846300	2.803400
O	6.512000	6.972200	0.571900
N	-0.405100	9.206300	1.170000
N	0.939900	7.442700	0.538000
N	-0.752500	7.144000	2.103200
N	4.002400	5.548900	0.595100
C	-1.175600	8.443400	2.004800
C	0.611800	8.766700	0.383400
C	0.286900	6.584900	1.414600
C	2.068100	6.880400	-0.210900
C	3.229200	6.644700	0.735400
C	3.855300	4.522600	-0.427800
C	4.764200	4.712500	-1.624100
N	4.552800	5.954400	-2.333300

Continued on next page

Table S11 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	3.524300	6.151700	-3.155300
C	2.666600	7.826800	-4.743100
C	1.442200	8.165000	-3.940000
C	2.426200	6.871900	-5.856100
C	3.312600	9.106000	-5.261600
C	5.042200	5.385700	1.609600
C	6.061900	6.483600	1.568100
C	7.333200	7.975100	2.931200
C	7.235500	8.477600	4.275600
H	4.109800	3.573200	0.026900
H	2.815300	4.547900	-0.728600
H	4.581000	5.378900	2.589500
H	5.523800	4.439700	1.395100
H	4.623800	3.864600	-2.283000
H	2.353000	7.614400	-0.954500
H	1.682300	5.980200	-0.673000
H	5.793000	4.749000	-1.287700
H	-1.326100	6.574900	2.707500
H	-0.712300	10.152000	0.998800
H	2.670800	9.586000	-5.990000
H	0.991900	7.262400	-3.545800
H	1.915800	5.990000	-5.489200
H	0.771100	8.550100	-4.697700
H	1.874600	7.291000	-6.688500
H	3.372400	9.720600	-4.371900
H	4.252600	8.896200	-5.756900
H	7.918600	9.306100	4.416900
H	6.199600	8.770600	4.393400
H	3.417200	6.550000	-6.151600
H	1.562200	8.753500	-3.038800
H	5.315000	6.614400	-2.370200
H	7.600300	7.497400	4.556700
H	8.249200	7.523700	2.570500
H	7.132500	8.816900	2.280000



Table S12: Cartesian coordinates of QEDSAT

Atom Label	x	y	z
F	-5.876100	-0.492000	3.502900
F	-6.959700	-0.874900	1.708700
F	-5.444200	-2.228400	2.342700
O	2.594400	0.160900	-6.096400
O	1.995100	-0.873500	-7.975000
O	-0.477600	0.970600	-6.782000
O	-2.903600	-0.993200	-5.242100
O	-0.402800	-1.642100	-2.319300
O	-1.794500	1.309700	-0.724300
O	-4.708900	-0.470700	0.235600
N	-3.969000	0.682100	2.038000
N	-1.725100	-0.373600	0.758200
N	-2.555800	-1.382800	-1.672400
N	-2.107300	0.416200	-3.681100
N	0.076200	-0.425500	-5.108500
C	3.770300	0.698000	-6.751500
C	4.883700	-0.267200	-6.749200
C	1.836400	-0.650200	-6.811300
C	0.811700	-1.384100	-5.947600
C	-0.128900	-2.179200	-6.830100
C	1.572100	-2.306900	-4.987800
C	-0.622400	0.599600	-5.625300
C	-1.527700	1.361500	-4.639700
C	-2.609500	2.115400	-5.398000
C	-0.665700	2.325500	-3.835800
C	-2.712400	-0.715300	-4.072500
C	-3.178300	-1.692600	-2.956800
C	-4.696300	-1.510400	-2.830200
C	-5.236800	-0.106400	-2.759900
C	-6.728200	-0.062500	-2.430600
C	-7.296600	1.323000	-2.328600
C	-2.830200	-3.129900	-3.403300
C	-3.229500	-4.186900	-2.393100
C	-1.230400	-1.408000	-1.419200
C	-0.765000	-1.196600	-0.003500
C	0.624000	-0.563800	0.043400
C	-0.736300	-2.571400	0.687900

Continued on next page

Table S12 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-2.141600	0.817700	0.336300
C	-3.076900	1.598200	1.286800
C	-3.911900	2.578100	0.487500
C	-2.219400	2.330800	2.304000
C	-4.744100	-0.188800	1.418000
C	-5.771800	-0.946700	2.272400
H	-3.990400	0.731300	2.871300
H	-1.783500	-0.545100	1.500100
H	-3.055800	-1.116900	-1.089900
H	-2.047800	0.571700	-2.953300
H	-0.107800	-0.664800	-4.219000
H	4.044200	1.493100	-6.295700
H	3.551000	0.921400	-7.650400
H	4.603800	-1.066300	-7.165200
H	5.619800	0.105000	-7.227300
H	5.145300	-0.438800	-5.853800
H	0.371200	-2.796100	-7.342200
H	-0.590000	-1.580900	-7.414900
H	-0.755200	-2.635300	-6.288600
H	2.071400	-2.933100	-5.488200
H	2.162800	-1.781700	-4.453400
H	0.952900	-2.752300	-4.427600
H	-2.204600	2.732300	-6.003800
H	-3.146400	1.505100	-5.879600
H	-3.151700	2.602000	-4.782700
H	-0.284300	2.978300	-4.418200
H	0.026800	1.850800	-3.399800
H	-1.203000	2.772200	-3.185300
H	-5.094700	-1.919900	-3.585000
H	-4.970000	-1.950500	-2.039200
H	-4.763000	0.374900	-2.086100
H	-5.098600	0.323100	-3.599000
H	-7.197400	-0.519900	-3.113800
H	-6.862500	-0.493300	-1.598500
H	-6.842300	1.810900	-1.646600
H	-7.188000	1.780300	-3.158400
H	-8.221100	1.277700	-2.116500
H	-1.892300	-3.176400	-3.541600

Continued on next page

Table S12 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-3.280600	-3.301400	-4.221300
H	-2.981700	-5.036500	-2.717700
H	-4.169800	-4.149700	-2.258300
H	-2.786100	-4.011400	-1.569200
H	0.593000	0.305800	-0.355100
H	1.236500	-1.103600	-0.432400
H	0.904900	-0.477300	0.948100
H	-0.121800	-3.131200	0.237900
H	-0.464100	-2.457100	1.592700
H	-1.602900	-2.949100	0.661000
H	-3.338300	3.173800	0.010500
H	-4.458200	2.108700	-0.125400
H	-4.461800	3.087300	1.078200
H	-1.637500	2.939700	1.854000
H	-1.705800	1.709900	2.796200
H	-2.779000	2.825400	2.898200

Table S13: Cartesian coordinates of QEVKOR

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
F	2.178300	0.761600	5.333400
F	2.751300	-1.139600	4.445400
O	2.103300	2.179100	1.066000
O	3.950800	2.722900	-0.020100
O	4.235300	0.121400	2.621700
C	3.293000	2.564900	1.024700
C	4.015600	2.863800	2.330200
N	3.532000	2.097500	3.460900
C	3.699500	0.791300	3.488500
C	3.200600	0.088200	4.765400
N	1.797400	1.138900	-1.494200
C	2.968600	0.314700	-1.876700
C	3.387100	-0.597800	-0.783100
O	2.338500	-1.502400	-0.512900
C	2.742400	-2.453000	0.467300
C	1.586700	-3.295700	0.820200
O	0.656600	-2.538600	1.578900
C	-0.548000	-3.212700	1.886200
C	1.504700	2.238400	-2.454200

Continued on next page

Table S13 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	0.538300	0.255400	2.253900
H	3.849500	3.913600	2.538100
H	5.066900	2.637400	2.202100
H	3.057000	2.591000	4.201800
H	1.962300	1.564000	-0.594000
H	0.993200	0.533600	-1.423700
H	2.632100	-0.228000	-2.751400
H	3.756200	1.020700	-2.109600
H	3.590200	-0.042000	0.124000
H	4.309800	-1.083700	-1.075300
H	3.031200	-1.929300	1.370200
H	3.582300	-3.041900	0.119900
H	1.031300	-3.694900	-0.019500
H	1.915400	-4.174800	1.360600
H	-0.904300	-3.663100	0.968000
H	-0.399000	-4.042800	2.565800
H	0.928600	1.794600	-3.256800
H	2.449300	2.730200	-2.651000
H	1.037900	1.007800	1.866000
H	0.999000	-0.583600	2.030000
C	4.296500	-0.088200	5.831400
F	5.318800	-0.761600	5.263400
F	4.745900	1.139600	6.151500
C	3.797700	-0.791300	7.108400
O	3.261800	-0.121400	7.975200
N	3.965100	-2.097500	7.135900
C	3.481600	-2.863800	8.266600
C	4.204100	-2.564900	9.572100
O	5.393800	-2.179100	9.530800
O	3.546300	-2.722900	10.617000
H	3.647600	-3.913600	8.058700
H	2.430300	-2.637400	8.394700
H	4.440200	-2.591000	6.395000
C	-1.504700	-2.238400	2.454200
N	-1.797400	-1.138900	1.494200
C	-2.968600	-0.314700	1.876700
C	-3.387100	0.597800	0.783100
O	-2.338500	1.502400	0.512900

Continued on next page

Table S13 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-2.742400	2.453000	-0.467300
C	-1.586700	3.295700	-0.820200
O	-0.656600	2.538600	-1.578900
C	0.548000	3.212700	-1.886200
H	0.904300	3.663100	-0.968000
H	0.399000	4.042800	-2.565800
H	-1.031300	3.694900	0.019500
H	-1.915400	4.174800	-1.360600
H	-3.031200	1.929300	-1.370200
H	-3.582300	3.041900	-0.119900
H	-3.590200	0.042000	-0.124000
H	-4.309800	1.083700	1.075300
H	-2.632100	0.228000	2.751400
H	-3.756200	-1.020700	2.109600
H	-1.962300	-1.564000	0.594000
H	-0.993200	-0.533600	1.423700
H	-0.928600	-1.794600	3.256800
H	-2.449300	-2.730200	2.651000

Table S14: Cartesian coordinates of ZEVHIR

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
O	-1.731600	-8.680900	-0.495000
O	-3.666000	-10.409600	-2.830400
O	-5.705300	-11.946000	-0.014700
O	-2.885000	-14.334300	0.291700
O	-4.459500	-16.297800	-2.286900
O	-7.402100	-17.533100	-1.812500
O	-7.248200	-15.663400	-3.021900
N	-2.494200	-7.163800	-1.988600
N	-4.663200	-8.854300	-1.529000
N	-3.732900	-10.844200	0.125900
N	-3.288300	-13.018000	-1.487700
N	-5.530200	-14.631100	-1.217400
C	-1.429900	-6.377100	0.026500
C	-1.899400	-7.509800	-0.827100
C	-2.845900	-8.153100	-3.016700
C	-3.681600	-7.420400	-4.089100
C	-1.593800	-8.813200	-3.628800

Continued on next page

Table S14 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-0.566700	-7.829200	-4.170800
C	-3.751400	-9.247700	-2.448900
C	-5.669300	-9.750700	-0.957500
C	-6.632200	-10.261900	-2.038700
C	-6.446600	-8.940200	0.092100
C	-5.023300	-10.948200	-0.237900
C	-2.985300	-11.969700	0.724700
C	-1.513600	-11.547000	0.799800
C	-3.524900	-12.291800	2.136600
C	-3.060200	-13.224100	-0.171600
C	-3.466100	-14.120200	-2.437800
C	-4.040600	-13.524700	-3.743700
C	-2.145900	-14.831800	-2.720700
C	-4.510100	-15.121600	-1.939200
C	-6.611200	-15.502000	-0.747600
C	-6.120900	-16.401900	0.387400
C	-7.760500	-14.592700	-0.290200
C	-7.104300	-16.373900	-1.906800
C	-7.635400	-16.388300	-4.213600
H	-2.634700	-6.183200	-2.180400
H	-4.663700	-7.885600	-1.246400
H	-3.259300	-9.966700	-0.028900
H	-3.356300	-12.073700	-1.836700
H	-5.544000	-13.640300	-1.027200
H	-1.722800	-6.533600	1.057300
H	-0.351300	-6.349100	-0.066100
H	-1.725800	-5.366400	-0.226000
H	-3.938400	-8.127500	-4.868200
H	-4.577600	-7.041200	-3.613500
H	-3.093400	-6.620700	-4.521800
H	-1.933100	-9.433600	-4.449000
H	-1.127300	-9.443100	-2.881500
H	0.262800	-8.366100	-4.614400
H	-0.999200	-7.220800	-4.955400
H	-0.195800	-7.183600	-3.384300
H	-7.362600	-10.924400	-1.590800
H	-7.168700	-9.460200	-2.531000
H	-6.110000	-10.844000	-2.787800

Continued on next page

Table S14 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-7.230400	-9.546400	0.529200
H	-5.761400	-8.537700	0.827900
H	-6.900600	-8.102900	-0.423300
H	-0.914400	-12.335300	1.238400
H	-1.131100	-11.361800	-0.196300
H	-1.394100	-10.653100	1.399600
H	-2.920300	-13.084200	2.560300
H	-3.441700	-11.393400	2.735700
H	-4.557600	-12.602400	2.037400
H	-4.284300	-14.284900	-4.475400
H	-4.881700	-12.861200	-3.584700
H	-3.136700	-12.990300	-4.008800
H	-1.454000	-14.152000	-3.202500
H	-1.707000	-15.280600	-1.838200
H	-2.355500	-15.594000	-3.460900
H	-6.951600	-16.984400	0.766300
H	-5.319700	-17.049600	0.053600
H	-5.744600	-15.865000	1.249400
H	-8.556600	-15.221000	0.089700
H	-7.450400	-13.981300	0.548300
H	-8.166100	-14.004300	-1.104000
H	-7.792600	-15.694400	-5.030100
H	-6.910400	-17.168100	-4.411200
H	-8.580700	-16.852200	-3.960100

Table S15: Cartesian coordinates of glycine

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-13.131500	-0.172000	2.176700
C	-11.949800	-0.472100	1.288400
O	-10.813700	-0.445200	1.684600
H	-12.805200	0.439900	3.004700
H	-13.519700	-1.105700	2.571900
H	-13.929300	0.328600	1.640800
N	-12.233300	-0.775800	-0.008500
C	-11.228100	-1.400500	-0.844300
C	-10.020700	-0.528100	-1.145400
O	-8.961300	-1.037600	-1.408900
H	-13.186300	-0.932200	-0.250200

Continued on next page

Table S15 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	-10.840300	-2.305600	-0.396900
H	-11.686900	-1.661600	-1.789900
N	-10.195200	0.804500	-1.122800
C	-9.094000	1.701700	-1.379300
C	-7.941500	1.604600	-0.387900
O	-6.850700	2.010300	-0.709200
H	-11.087600	1.169800	-0.884600
H	-8.667600	1.522600	-2.355600
H	-9.465100	2.718300	-1.359300
N	-8.190700	1.070100	0.817000
C	-7.124500	0.891000	1.772200
C	-6.005600	-0.035500	1.315500
O	-4.913700	0.050100	1.824900
H	-9.089800	0.695200	1.030800
H	-6.655000	1.833400	2.013500
H	-7.547700	0.482900	2.680900
N	-6.282700	-0.924500	0.348700
C	-5.249900	-1.784000	-0.173600
C	-4.087300	-1.055500	-0.834100
O	-3.019500	-1.610600	-0.943800
H	-7.186900	-0.953400	-0.070800
H	-4.817700	-2.395500	0.605300
H	-5.694000	-2.441100	-0.910100
N	-4.299200	0.193900	-1.275800
C	-3.219100	0.963100	-1.841200
C	-2.057700	1.225700	-0.891900
O	-0.966500	1.488800	-1.340200
H	-5.181100	0.639300	-1.137700
H	-2.796300	0.469600	-2.704200
H	-3.613400	1.919700	-2.159100
N	-2.297500	1.154300	0.426400
C	-1.225300	1.318500	1.375500
C	-0.113900	0.282900	1.269000
O	0.982600	0.534200	1.711000
H	-3.200100	0.898500	0.766200
H	-0.749100	2.282100	1.266300
H	-1.642600	1.259500	2.372500
N	-0.403300	-0.887700	0.680200

Continued on next page



Table S15 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	0.623000	-1.878700	0.477500
C	1.773700	-1.434700	-0.415700
O	2.839700	-1.999500	-0.342400
H	-1.307100	-1.051200	0.290500
H	1.069100	-2.178400	1.414700
H	0.167900	-2.751100	0.026400
N	1.552200	-0.417700	-1.262600
C	2.620400	0.102200	-2.078400
C	3.791000	0.691200	-1.302200
O	4.870100	0.794000	-1.835900
H	0.671800	0.051900	-1.274400
H	3.037800	-0.665800	-2.713400
H	2.215100	0.880500	-2.712100
N	3.570200	1.079800	-0.036800
C	4.651300	1.575100	0.777600
C	5.768100	0.573900	1.042900
O	6.857400	0.970500	1.378600
H	2.676100	0.949000	0.386300
H	5.121600	2.434700	0.322500
H	4.243800	1.880100	1.732800
N	5.487400	-0.730900	0.892800
C	6.519100	-1.723900	1.051700
C	7.655000	-1.650500	0.038400
O	8.702300	-2.199400	0.283000
H	4.586500	-1.024500	0.581100
H	6.981900	-1.651600	2.025300
H	6.064400	-2.702500	0.967100
N	7.434200	-0.975500	-1.100000
C	8.479200	-0.808000	-2.079300
C	9.650200	0.080800	-1.669700
O	10.647000	0.070800	-2.341800
H	6.563800	-0.512700	-1.251700
H	8.910400	-1.762000	-2.345800
H	8.041600	-0.378500	-2.970800
N	9.492200	0.848100	-0.573800
C	10.568800	1.637400	-0.032200
C	11.399700	0.983100	1.067700
O	12.264300	1.628700	1.606100

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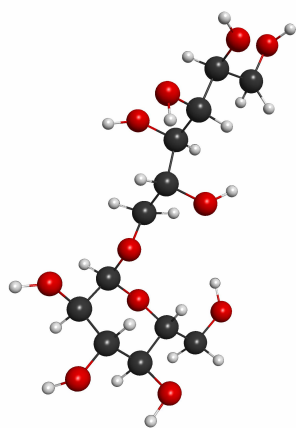
Table S15 – continued from previous page

<b>Atom Label</b>	<b>x</b>	<b>y</b>	<b>z</b>
H	8.632700	0.822100	-0.069300
H	11.249400	1.901000	-0.827500
H	10.172000	2.554000	0.384100
N	11.121600	-0.287200	1.386600
C	11.881600	-0.983400	2.397700
H	10.407800	-0.784100	0.902400
H	11.830400	-0.463200	3.346400
H	11.464400	-1.974500	2.514200
H	12.924600	-1.069400	2.116200

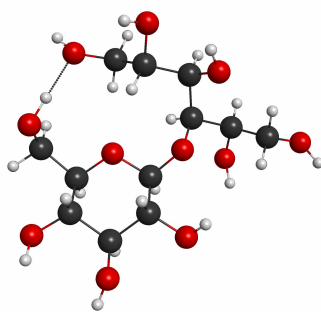


## 2 Molecule Figures

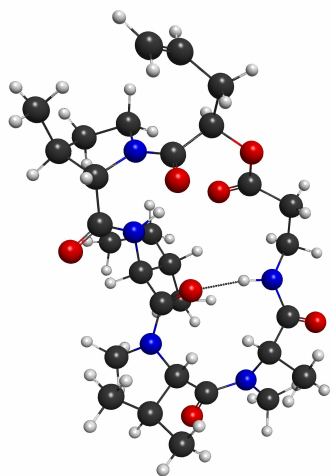
Molecule 1  
BAVCAC



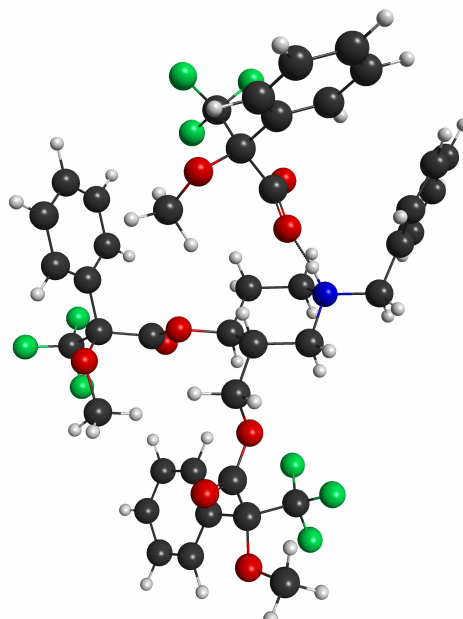
Molecule 2  
BDGPGL



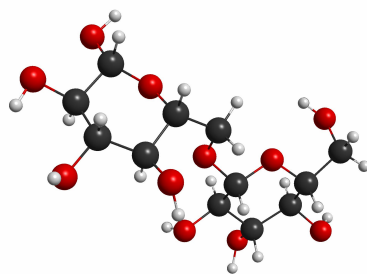
Molecule 3  
BIHYAS10



Molecule 4  
DOSLED

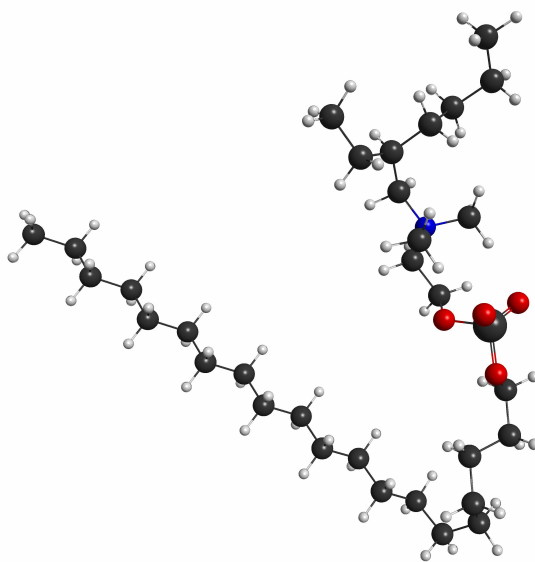


Molecule 5  
GENTBS01

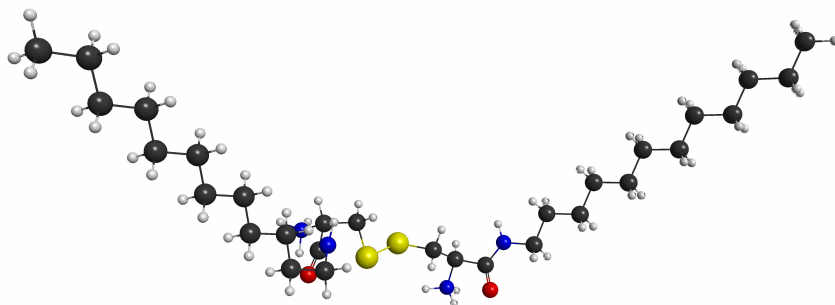




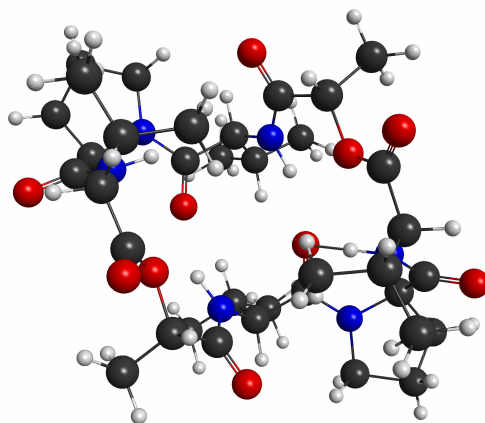
Molecule 6  
GelA



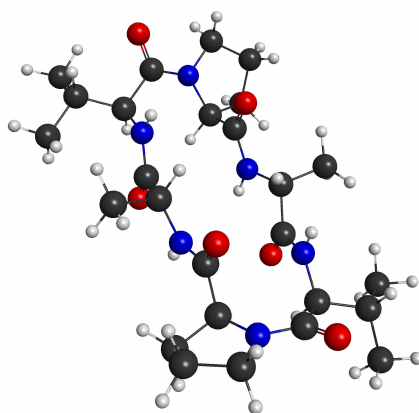
Molecule 7  
GelB



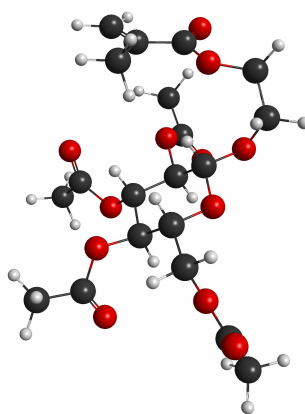
Molecule 8  
HEBLIJ



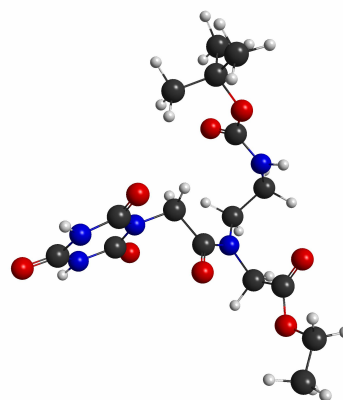
Molecule 9  
KIVDIC



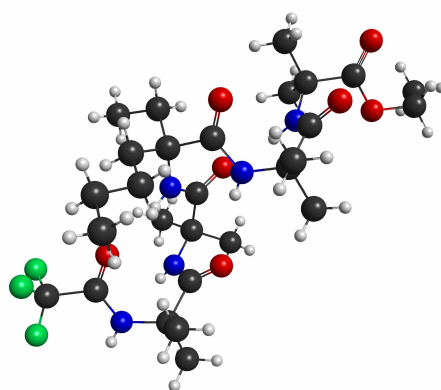
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NIYBIG



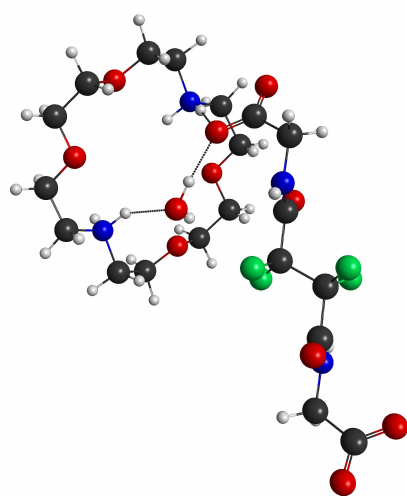
Molecule 11  
QAZJAC



Molecule 12  
QEDSAT

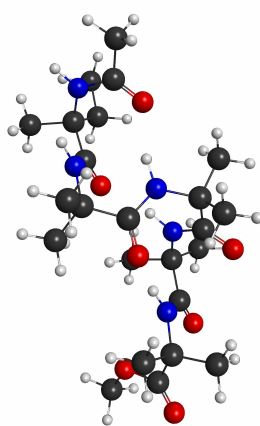


Molecule 13  
QEVKOR

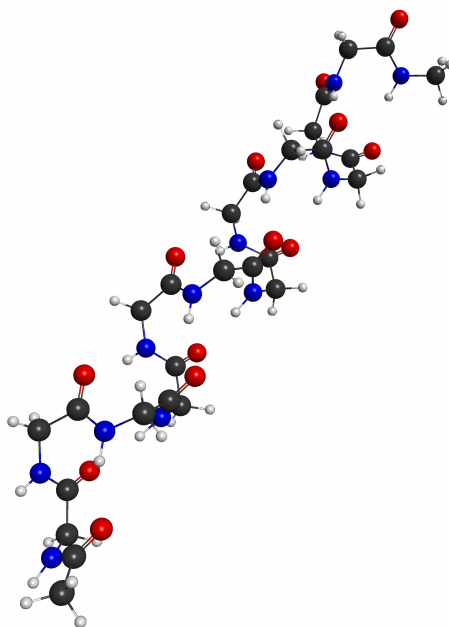




Molecule 14  
ZEVHIR



Molecule 15  
glycine



### 3 CPU Times

This section presents full molecule and Level 4 CPU Times for all molecules in the test set at HF/6-31++G(d,p). In addition, the number of basis functions in the full molecule calculation, as well as the number of fragments and the average number of atoms per fragment at Level 4, are presented as a measure of the expected cost of the calculations.

Table S16: Total CPU Times for the 15 molecules in the test set at Level 4 and for the complete molecule.

	<b>Total Number of Basis Functions</b>	<b>Number of Fragments at Level 4</b>	<b>Average Number of Atoms per Fragment</b>	<b>Level 4 CPU Time</b>	<b>Full Molecule CPU Time</b>
GENTBS01	569	29	18.17	1.321	1.264
BAVCAC	581	25	17.56	0.959	1.312
BDGPGL	581	32	16.96	1.069	1.631
QAJZAC	701	15	16.93	1.176	2.674
NIYBIG	776	39	16.51	1.474	4.353
ZEVHIR	942	13	38.53	15.030	9.284
QEVKOR	957	44	23.47	7.461	7.363
KIVDIC	974	41	23.90	8.841	9.622
BIHYAS10	1092	33	32.69	17.675	16.300
QEDSAT	1105	19	32.36	17.403	14.532
GelB	1114	53	16.71	1.394	4.511
GelA	1134	41	21.02	7.851	7.394
glycine	1265	43	44.65	61.654	9.801
HEBLIJ	1336	55	39.60	58.492	31.615
DOSLED	1430	21	27.04	13.922	31.416

### References

- (1) Hua, W.; Fang, T.; Li, W.; Yu, J.-G.; Li, S. *J. Phys. Chem. A* **2008**, *112*, 10864–10872.