

Supporting Information

A Computational Challenge of Guanine Quadruplex Involvement in Anticancer Antibiotics

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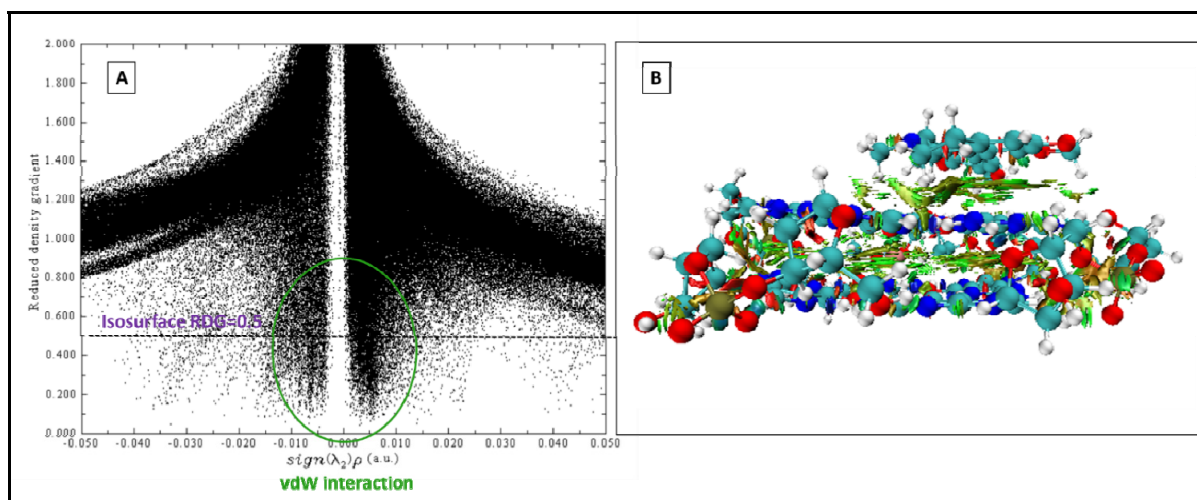


Figure S1. Reduced density gradient (RDG) analysis of dicentrine in complex with a two-layered G-quadruplex (G4). (A) RDG versus $\text{sign}(\lambda_2)\rho$ plot highlighting noncovalent interactions, where negative values indicate attractive interactions (e.g., π - π stacking and hydrogen bonding), values near zero correspond to weak van der Waals interactions, and positive values represent steric repulsion. (B) Three-dimensional RDG isosurface at $\text{RDG} = 0.5$ mapped with a color scale (blue–green–red), where blue denotes strong attractive interactions, green indicates weak dispersive contacts, and red represents repulsive regions. The plots reveal that dicentrine binding to the G4 structure is predominantly stabilized by van der Waals interactions, while also involving attractive interactions such as π - π stacking and hydrogen bonding, along with regions of steric repulsion.

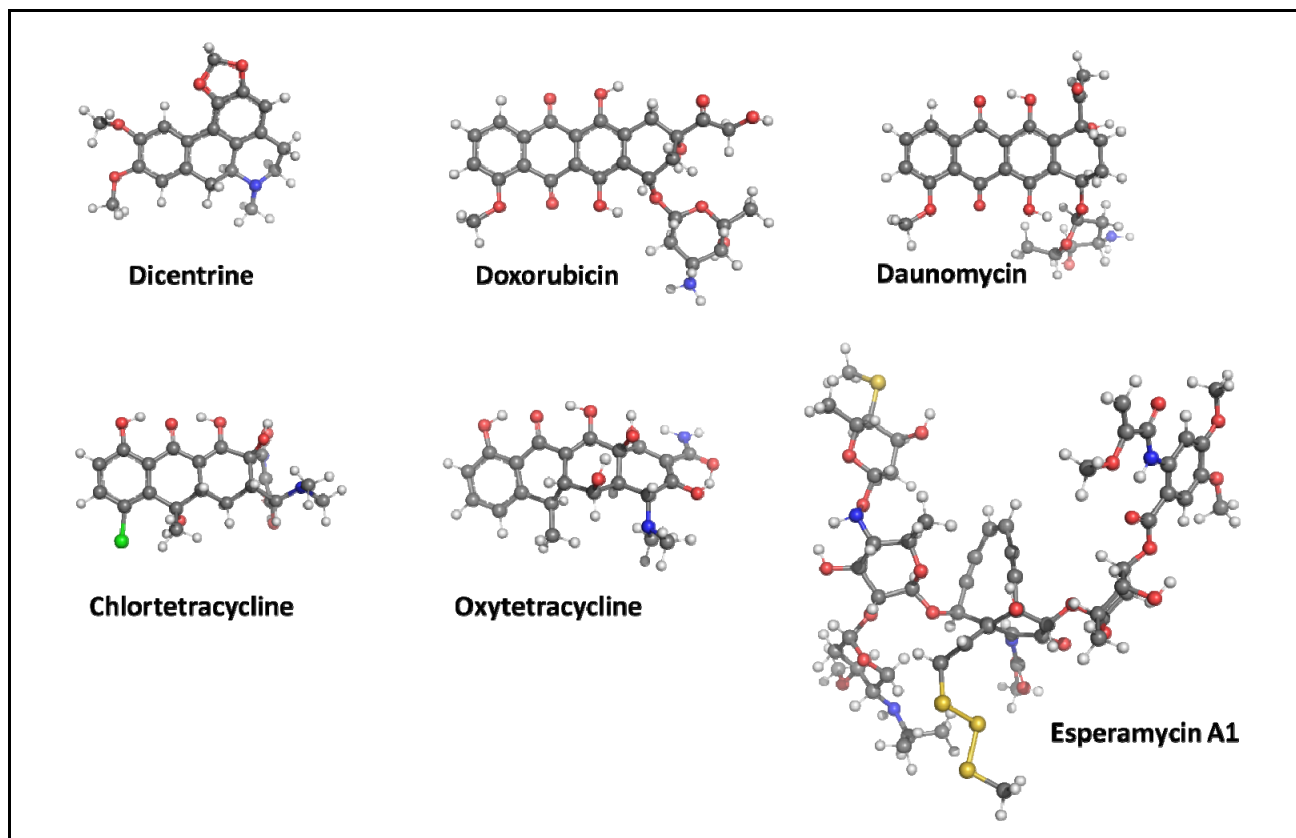


Figure S2. Optimized geometries at the wB97XD/6-31G** level of theory in the gas phase of antibiotics considered in this study. Their chemical structure is presented in Figure 1.

Table S1. Energies of the computed quadruplex Q2K, ligands, and Q2K–ligand complexes (Q2K@Ligand) in n-octanol and water environments, given in Hartree. Complexation energies ΔE ($\Delta E = E(\text{Q2K@Ligand}) - E(\text{Q2K}) - E(\text{Ligand})$) are reported in kcal/mol.

Species	E	ΔE
<i>n-octanol</i>		
Q2K	-4939.512555	-
Dicentrine	-1130.073547	-
Chlortetracycline	-2023.279974	-
Oxytetracycline	-1563.713437	-
Q2K@Dicentrine	-6069.642986	-36.3
Q2K@Chlortetracycline	-6962.857963	-41.7
Q2K@Oxytetracycline	-6503.281943	-35.7
<i>water</i>		
Q2K	-4939.522	-
Dicentrine	-4939.522299	-
Chlortetracycline	-1130.074735	-
Oxytetracycline	-1563.715077	-
Q2K@Dicentrine	-2023.281544	-35.7
Q2K@Chlortetracycline	-6962.868429	-41.1
Q2K@Oxytetracycline	-6503.292329	-35.1

Table S2. Optimized geometries of the ligands and selected Q2K–ligand complexes.

Dicentrine	6	2.983430000	0.597769000	0.414447000
	6	3.279213000	-0.726765000	0.042091000
	6	2.237564000	-1.573283000	-0.326260000
	6	0.916269000	-1.126119000	-0.327005000
	6	0.621154000	0.189299000	0.042732000
	6	1.672996000	1.038789000	0.411018000
	6	-0.211854000	-2.043991000	-0.720337000
	6	-1.429876000	-1.798917000	0.174317000
	6	-1.837397000	-0.336698000	0.042447000
	6	-0.789100000	0.624575000	0.014950000
	7	-2.526891000	-2.713079000	-0.137371000
	6	-3.740750000	-2.315698000	0.563505000
	6	-4.257224000	-1.003284000	0.002555000
	6	-3.174161000	0.045065000	-0.018633000
	6	-3.535564000	1.401213000	-0.115004000
	6	-2.520223000	2.321276000	-0.133830000
	6	-1.185012000	1.945920000	-0.069722000
	8	-2.612066000	3.680811000	-0.255997000
	6	-1.297438000	4.165746000	-0.030433000
	8	-0.401428000	3.070910000	-0.158108000
	1	-1.101724000	-1.955218000	1.226000000
	8	4.588496000	-1.081649000	0.085303000
	6	4.923284000	-2.406681000	-0.258676000
	8	3.974443000	1.445336000	0.830736000
	6	4.811841000	1.919237000	-0.211592000
	6	-2.193793000	-4.092425000	0.174825000
	1	2.438444000	-2.600925000	-0.608567000
	1	1.485572000	2.063688000	0.705268000
	1	-0.510771000	-1.871119000	-1.762464000
	1	0.127416000	-3.079460000	-0.644755000
	1	-4.493615000	-3.097956000	0.426535000
	1	-3.566359000	-2.219586000	1.653547000
	1	-4.622650000	-1.172390000	-1.017365000
	1	-5.108096000	-0.652784000	0.596858000
	1	-4.575027000	1.704446000	-0.172329000
	1	-1.053448000	4.922045000	-0.779402000
	1	-1.226045000	4.581348000	0.985352000
	1	4.435680000	-3.130551000	0.405844000
	1	4.655695000	-2.635142000	-1.298123000
	1	6.003918000	-2.486610000	-0.140709000
	1	5.348312000	1.097974000	-0.697678000
	1	4.228310000	2.468474000	-0.961528000
	1	5.530809000	2.596917000	0.251596000
	1	-1.907284000	-4.237469000	1.233781000
	1	-3.060775000	-4.725468000	-0.031951000
	1	-1.375839000	-4.452091000	-0.452159000
Daunomycin	6	2.335363000	2.355610000	1.924856000
	6	1.568102000	3.629876000	1.532349000
	6	0.847727000	3.551053000	0.166660000
	6	0.036896000	2.258201000	0.106725000
	6	0.643621000	1.093534000	0.574213000

6	2.121285000	1.231238000	0.917509000
6	-1.265594000	2.204584000	-0.416939000
6	-1.974963000	0.991432000	-0.384303000
6	-1.378379000	-0.176162000	0.139513000
6	-0.082778000	-0.121054000	0.660572000
6	-3.367537000	0.974792000	-0.836849000
6	-4.190352000	-0.235352000	-0.577368000
6	-3.596114000	-1.406174000	-0.089069000
6	-2.105278000	-1.479882000	0.030787000
6	-5.562659000	-0.151539000	-0.806986000
6	-6.359513000	-1.247606000	-0.522219000
6	-5.803206000	-2.414651000	-0.009943000
6	-4.424596000	-2.511284000	0.208551000
8	-3.838741000	-3.605550000	0.723991000
6	-4.643060000	-4.710473000	1.073061000
8	-1.514429000	-2.539154000	-0.027562000
8	-3.889582000	1.965043000	-1.365973000
8	0.415430000	-1.222984000	1.244252000
8	-1.789229000	3.311299000	-0.950978000
1	1.280772000	-1.023426000	1.636226000
1	-2.704838000	3.082488000	-1.245398000
6	-0.027545000	4.836725000	0.067046000
8	-0.642236000	5.220890000	1.036106000
6	0.033833000	5.620091000	-1.221238000
8	1.776643000	3.489521000	-0.915030000
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6	3.249057000	-0.807171000	0.453030000
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6	3.394138000	-3.122257000	0.098599000
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6	5.405606000	-1.710548000	-0.473469000
6	4.678412000	-0.454157000	0.049343000
7	6.328614000	-1.360221000	-1.544828000
1	6.725413000	-2.220839000	-1.910666000
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8	5.092835000	-3.840457000	-1.487640000
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	1	0.690945000	-3.627329000	-0.786188000
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	1	4.796910000	-1.991375000	0.203034000
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	8	3.172110000	-2.361474000	0.528986000
	6	3.091593000	-0.083566000	1.185734000
	8	3.737220000	0.840735000	3.258519000
	6	3.537435000	-0.191088000	2.583308000
	7	3.715543000	-1.419015000	3.092878000
	6	3.130964000	1.153777000	0.588314000
	8	3.395592000	2.255522000	1.233670000
	6	2.944023000	1.250853000	-0.909717000
	7	4.127161000	0.694659000	-1.566083000
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	6	4.014478000	0.704857000	-3.017822000
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	6	0.466914000	1.200160000	-0.586616000
	6	-0.857417000	0.508656000	-0.896275000
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	6	0.419103000	-1.604499000	-0.451040000
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	6	1.775492000	-0.995283000	-0.836762000
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	1	3.670616000	-2.220032000	2.475459000
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	1	2.801784000	2.318297000	-1.160694000
	1	5.498183000	1.253291000	-0.065841000
	1	5.336185000	2.454140000	-1.366492000
	1	6.198887000	0.920212000	-1.648548000
	1	4.963989000	0.370638000	-3.442387000
	1	3.794604000	1.709047000	-3.424440000
	1	3.248866000	0.001012000	-3.343881000
	1	1.491743000	0.490301000	-2.325136000
	1	0.582039000	1.238491000	0.499266000
	1	-0.998294000	0.509236000	-1.986886000
	1	-6.630884000	0.775249000	0.659458000
	1	-6.569698000	-1.692413000	0.325830000
	1	-1.408266000	2.888576000	-1.679124000
	1	-2.800724000	1.966096000	-2.270018000
	1	-3.008439000	3.188975000	-1.013178000
	1	0.454173000	2.237081000	-0.934221000
	17	-4.723230000	2.733520000	0.722612000
	8	-1.622281000	1.876882000	0.901679000
	1	-2.310856000	2.467510000	1.224609000
Oxytetracycline	6	1.952726000	-1.589238000	0.322585000
	8	1.583320000	-2.580842000	0.937514000
	6	3.283428000	-1.003987000	0.439178000
	8	5.562496000	-1.239980000	1.052412000
	6	4.406922000	-1.723831000	1.071798000
	7	4.160711000	-2.897626000	1.665739000
	6	3.542743000	0.260956000	-0.064083000
	8	4.740017000	0.773692000	-0.055978000
	6	2.464006000	1.196233000	-0.577043000
	7	2.544132000	2.540387000	-0.024666000
	6	3.388746000	3.463706000	-0.764545000
	6	2.762896000	2.619550000	1.409707000
	6	1.064832000	0.615866000	-0.343850000
	6	-0.013371000	1.404371000	-1.080507000
	8	0.164678000	1.356140000	-2.483577000
	6	-1.409527000	0.904329000	-0.678955000
	6	-2.033062000	1.436184000	0.629037000
	6	-1.872853000	2.943662000	0.817997000
	6	-3.486985000	0.955678000	0.658558000
	6	-4.504507000	1.737356000	1.178835000
	6	-5.821510000	1.262023000	1.216239000
	6	-6.145506000	0.001752000	0.761668000
	6	-5.136724000	-0.820700000	0.244641000

	8	-5.482384000	-2.044286000	-0.158165000
	6	-3.809085000	-0.337923000	0.160291000
	6	-2.770810000	-1.198257000	-0.411170000
	8	-2.981661000	-2.416731000	-0.648544000
	6	-1.468980000	-0.602570000	-0.635465000
	6	-0.380952000	-1.412066000	-0.726430000
	8	-0.444792000	-2.724650000	-0.907503000
	6	1.033026000	-0.874762000	-0.701757000
	8	1.587203000	-1.039389000	-2.012792000
	1	-4.658230000	-2.510433000	-0.418431000
	1	-1.405884000	-2.957609000	-0.931623000
	1	1.474821000	-1.966848000	-2.253505000
	1	4.932304000	-3.378609000	2.097216000
	1	3.207821000	-3.241050000	1.702471000
	1	5.338463000	0.050950000	0.370818000
	1	2.603583000	1.275832000	-1.660302000
	1	3.128917000	3.423931000	-1.825774000
	1	4.463320000	3.257246000	-0.654130000
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6	1.250943000	-5.248283000	2.862787000
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1	-4.081591000	-1.609494000	-4.156971000
1	-5.010181000	3.304668000	-4.927729000
1	0.292467000	1.504102000	-3.743180000
1	-0.338238000	4.887660000	-4.421123000
1	0.937502000	3.734019000	-4.101831000
1	3.699940000	-0.572681000	-2.372072000
1	7.159746000	0.012787000	-2.220547000
1	5.906578000	-1.116689000	-1.761206000
1	3.619409000	5.486099000	-4.535588000
1	7.540489000	-3.259001000	0.044976000

1	-1.998642000	-7.968001000	-0.758784000
1	-6.046667000	0.981950000	-4.703321000
1	5.900403000	4.456188000	-4.014139000
1	6.402695000	-5.434477000	0.755599000
1	-4.117194000	-7.190529000	-1.963784000
8	-0.681544000	1.721781000	-0.900680000
6	-3.274031000	3.333836000	3.449930000
8	-3.026566000	4.437952000	3.916523000
6	-4.546144000	2.638954000	3.629512000
8	-6.860060000	2.728772000	4.138565000
6	-5.757616000	3.324858000	4.116890000
7	-5.650963000	4.592934000	4.532551000
6	-4.659996000	1.294497000	3.316016000
8	-5.801325000	0.666293000	3.370673000
6	-3.476359000	0.418850000	2.957728000
7	-3.452700000	-0.861480000	3.644510000
6	-4.146301000	-1.937025000	2.960985000
6	-3.731646000	-0.823726000	5.068812000
6	-2.149047000	1.162677000	3.150986000
6	-0.988992000	0.348060000	2.579068000
8	-1.231800000	0.007688000	1.235655000
6	0.366839000	1.051378000	2.735732000
6	1.205730000	0.743075000	3.994026000
6	1.282531000	-0.749600000	4.319887000
6	2.580459000	1.392036000	3.804408000
6	3.734709000	0.815501000	4.309970000
6	4.971635000	1.455478000	4.175288000
6	5.086027000	2.677177000	3.546321000
6	3.942686000	3.283102000	3.015383000
8	4.091010000	4.467453000	2.415624000
6	2.687606000	2.636637000	3.125201000
6	1.496960000	3.293734000	2.587896000
8	1.546897000	4.490071000	2.183419000
6	0.257418000	2.551200000	2.579238000
6	-0.914015000	3.235684000	2.438449000
8	-0.980511000	4.516929000	2.108239000
6	-2.265772000	2.569329000	2.552631000
8	-2.815517000	2.472430000	1.242448000
1	3.187038000	4.790564000	2.199305000
1	-0.043829000	4.828909000	2.011261000
1	-2.754413000	3.339000000	0.813214000
1	-6.476872000	5.042225000	4.892149000
1	-4.734348000	5.025017000	4.558462000
1	-6.482136000	1.380622000	3.671085000
1	-3.557789000	0.214602000	1.885385000
1	-3.843105000	-1.951890000	1.911709000
1	-5.243085000	-1.849605000	3.005835000
1	-3.855233000	-2.893849000	3.407081000
1	-3.396876000	-1.760498000	5.524656000
1	-4.800131000	-0.690499000	5.300211000
1	-3.176985000	-0.008894000	5.543734000
1	-1.960015000	1.296665000	4.225529000
1	-0.985556000	-0.606038000	3.104946000

	1	-1.149063000	0.796106000	0.678048000
	1	0.949910000	0.679849000	1.883141000
	1	0.734771000	1.250202000	4.850742000
	1	3.698836000	-0.143685000	4.809219000
	1	5.858855000	0.974730000	4.575172000
	1	6.035617000	3.190695000	3.451351000
	1	0.288167000	-1.158287000	4.509001000
	1	1.726854000	-1.316850000	3.497030000
	1	1.866779000	-0.933208000	5.223806000

Table S3. The Computational Workflow

5.1.File espera_A1.mol - produced by program **ChemSketch** by 3D-optimization from a figure in **ChemDraw**:

ACD/Labs08092508183D

```
170175  0  0  0  0  0  0  0  0  0  1 V2000
 20.5866  -7.9900  -3.3852 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.9130  -6.7013  -3.1978 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.8012  -9.1309  -3.3547 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 22.0899  -7.7327  -3.7128 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.1494  -6.9842  -4.4440 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.3778  -6.4463  -1.9825 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 18.2415  -8.8755  -3.3266 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 20.2852 -10.4172  -3.4879 N   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 22.6668  -8.8529  -4.3945 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 22.1389  -6.4781  -4.5886 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 17.8426  -7.5734  -4.0661 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.1402  -5.7879  -5.1396 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.7771  -7.9543  -5.2701 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.1839  -7.5388  -0.9774 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 17.4461  -9.6189  -2.7985 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.3644 -11.4512  -3.4537 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 23.9720  -9.1450  -3.8678 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 22.0208  -5.4384  -5.2531 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 17.0743  -6.7106  -3.2244 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.5502  -4.8199  -5.6953 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 20.7051  -7.6400   0.0000 S   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.7212 -12.7155  -3.7929 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 18.2181 -11.2172  -3.1400 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 24.3190 -10.6257  -4.0922 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 24.9421  -8.3330  -4.5296 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 21.7106  -4.1603  -6.0244 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 15.6589  -6.9734  -3.0977 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 20.3925  -3.8399  -6.2503 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 22.1546  -7.7347  -1.4120 S   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 19.9283 -12.9798  -5.1702 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 23.3696 -11.4556  -3.4139 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 25.7302 -10.8895  -3.5367 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 26.2641  -8.4828  -4.0010 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 15.3798  -8.5001  -3.0907 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 14.9646  -6.3892  -4.1993 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 22.6025  -5.8329  -1.9422 S   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 23.2240 -12.8181  -3.8390 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 26.7326  -9.9372  -4.1808 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 26.1171 -12.2235  -3.8256 O   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 27.2208  -7.5464  -4.7460 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 13.9991  -8.8011  -3.7074 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 13.5309  -6.3700  -4.0683 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 24.2947  -5.4970  -1.3884 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
 24.5941 -13.5063  -3.8854 C   0  0  0  0  0  0  0  0  0  0  0  0  0  0
```

22.3822	-13.5047	-2.9135	O	0	0	0	0	0	0	0	0	0	0	0
28.0462	-10.1215	-3.5350	N	0	0	0	0	0	0	0	0	0	0	0
13.4848	-10.0237	-3.1767	O	0	0	0	0	0	0	0	0	0	0	0
13.0493	-7.6568	-3.3754	C	0	0	0	0	0	0	0	0	0	0	0
13.1032	-5.1635	-3.2295	C	0	0	0	0	0	0	0	0	0	0	0
24.5814	-14.9217	-3.3045	C	0	0	0	0	0	0	0	0	0	0	0
22.0917	-14.8750	-3.1998	C	0	0	0	0	0	0	0	0	0	0	0
29.0628	-10.4874	-4.5199	O	0	0	0	0	0	0	0	0	0	0	0
12.4291	-10.6829	-3.7504	C	0	0	0	0	0	0	0	0	0	0	0
13.0272	-7.4547	-1.9689	O	0	0	0	0	0	0	0	0	0	0	0
23.3064	-15.6380	-3.7319	C	0	0	0	0	0	0	0	0	0	0	0
25.7141	-15.6436	-3.7856	O	0	0	0	0	0	0	0	0	0	0	0
30.1698	-11.1130	-3.8828	C	0	0	0	0	0	0	0	0	0	0	0
12.3123	-12.1518	-3.5973	C	0	0	0	0	0	0	0	0	0	0	0
11.6156	-10.0750	-4.4097	O	0	0	0	0	0	0	0	0	0	0	0
23.2979	-17.0086	-3.1868	N	0	0	0	0	0	0	0	0	0	0	0
26.9432	-15.1061	-3.3060	C	0	0	0	0	0	0	0	0	0	0	0
30.4346	-12.4788	-4.5287	C	0	0	0	0	0	0	0	0	0	0	0
31.3252	-10.2908	-4.0274	O	0	0	0	0	0	0	0	0	0	0	0
11.0789	-12.7959	-3.5254	C	0	0	0	0	0	0	0	0	0	0	0
13.4814	-12.8932	-3.5298	C	0	0	0	0	0	0	0	0	0	0	0
24.1097	-17.9434	-3.9839	C	0	0	0	0	0	0	0	0	0	0	0
31.6794	-13.1298	-3.9276	C	0	0	0	0	0	0	0	0	0	0	0
32.4691	-10.8242	-3.3585	C	0	0	0	0	0	0	0	0	0	0	0
11.0404	-14.1780	-3.3889	C	0	0	0	0	0	0	0	0	0	0	0
9.8587	-12.0743	-3.5923	N	0	0	0	0	0	0	0	0	0	0	0
13.4351	-14.2714	-3.3923	C	0	0	0	0	0	0	0	0	0	0	0
25.5791	-17.8971	-3.5615	C	0	0	0	0	0	0	0	0	0	0	0
23.5645	-19.3591	-3.7964	C	0	0	0	0	0	0	0	0	0	0	0
32.8626	-12.1588	-4.0096	C	0	0	0	0	0	0	0	0	0	0	0
31.4289	-13.4529	-2.5662	O	0	0	0	0	0	0	0	0	0	0	0
33.6292	-9.8409	-3.4669	C	0	0	0	0	0	0	0	0	0	0	0
12.2107	-14.9150	-3.3234	C	0	0	0	0	0	0	0	0	0	0	0
8.6571	-12.7688	-3.5231	C	0	0	0	0	0	0	0	0	0	0	0
14.5831	-15.0031	-3.3211	O	0	0	0	0	0	0	0	0	0	0	0
34.2850	-12.8700	-3.1421	S	0	0	0	0	0	0	0	0	0	0	0
12.1483	-16.2725	-3.1883	O	0	0	0	0	0	0	0	0	0	0	0
7.3366	-12.1067	-3.5954	C	0	0	0	0	0	0	0	0	0	0	0
8.6914	-13.9722	-3.3974	O	0	0	0	0	0	0	0	0	0	0	0
15.6874	-14.7566	-4.1804	C	0	0	0	0	0	0	0	0	0	0	0
35.7872	-12.2503	-3.9435	C	0	0	0	0	0	0	0	0	0	0	0
12.8082	-17.1374	-4.1012	C	0	0	0	0	0	0	0	0	0	0	0
6.2183	-12.8922	-3.5071	O	0	0	0	0	0	0	0	0	0	0	0
7.2332	-10.7759	-3.7418	C	0	0	0	0	0	0	0	0	0	0	0
4.8775	-12.4200	-3.5808	C	0	0	0	0	0	0	0	0	0	0	0
22.6664	-7.5765	-2.7738	H	0	0	0	0	0	0	0	0	0	0	0
20.1189	-5.9598	-1.3086	H	0	0	0	0	0	0	0	0	0	0	0
17.2111	-7.7736	-4.9635	H	0	0	0	0	0	0	0	0	0	0	0
23.9806	-8.9315	-2.7766	H	0	0	0	0	0	0	0	0	0	0	0
24.2892	-10.8581	-5.1825	H	0	0	0	0	0	0	0	0	0	0	0
15.3001	-6.5311	-2.1413	H	0	0	0	0	0	0	0	0	0	0	0
25.7201	-10.7283	-2.4345	H	0	0	0	0	0	0	0	0	0	0	0
26.2573	-8.2229	-2.9178	H	0	0	0	0	0	0	0	0	0	0	0
22.7698	-12.8408	-4.8558	H	0	0	0	0	0	0	0	0	0	0	0
26.8126	-10.1605	-5.2703	H	0	0	0	0	0	0	0	0	0	0	0
14.0992	-8.9002	-4.8128	H	0	0	0	0	0	0	0	0	0	0	0
13.0756	-6.2991	-5.0832	H	0	0	0	0	0	0	0	0	0	0	0

12.0238	-7.9090	-3.7350	H	0	0	0	0	0	0	0	0	0	0	0
24.6186	-14.8657	-2.1929	H	0	0	0	0	0	0	0	0	0	0	0
23.2624	-15.6778	-4.8454	H	0	0	0	0	0	0	0	0	0	0	0
29.9413	-11.2539	-2.8011	H	0	0	0	0	0	0	0	0	0	0	0
31.9227	-14.0568	-4.4973	H	0	0	0	0	0	0	0	0	0	0	0
32.2250	-10.9886	-2.2834	H	0	0	0	0	0	0	0	0	0	0	0
33.1255	-11.9837	-5.0788	H	0	0	0	0	0	0	0	0	0	0	0
21.2623	-10.5950	-3.6636	H	0	0	0	0	0	0	0	0	0	0	0
19.8708	-7.5195	-6.1202	H	0	0	0	0	0	0	0	0	0	0	0
18.3377	-7.2719	-0.3034	H	0	0	0	0	0	0	0	0	0	0	0
18.9664	-8.5044	-1.4881	H	0	0	0	0	0	0	0	0	0	0	0
22.5278	-3.5014	-6.3858	H	0	0	0	0	0	0	0	0	0	0	0
20.0436	-2.9342	-6.7899	H	0	0	0	0	0	0	0	0	0	0	0
19.0523	-12.6314	-5.7571	H	0	0	0	0	0	0	0	0	0	0	0
20.8348	-12.4330	-5.5045	H	0	0	0	0	0	0	0	0	0	0	0
20.0592	-14.0688	-5.3424	H	0	0	0	0	0	0	0	0	0	0	0
16.1548	-9.0190	-3.6979	H	0	0	0	0	0	0	0	0	0	0	0
15.4203	-8.8772	-2.0448	H	0	0	0	0	0	0	0	0	0	0	0
27.0661	-12.2322	-3.6338	H	0	0	0	0	0	0	0	0	0	0	0
27.1498	-7.7225	-5.8415	H	0	0	0	0	0	0	0	0	0	0	0
26.9383	-6.4949	-4.5223	H	0	0	0	0	0	0	0	0	0	0	0
28.2732	-7.7160	-4.4325	H	0	0	0	0	0	0	0	0	0	0	0
24.9923	-5.4697	-2.2551	H	0	0	0	0	0	0	0	0	0	0	0
24.3107	-4.5087	-0.8789	H	0	0	0	0	0	0	0	0	0	0	0
24.6460	-6.2810	-0.6841	H	0	0	0	0	0	0	0	0	0	0	0
24.9295	-13.5507	-4.9471	H	0	0	0	0	0	0	0	0	0	0	0
25.3004	-12.8962	-3.2920	H	0	0	0	0	0	0	0	0	0	0	0
28.3198	-9.2236	-3.1722	H	0	0	0	0	0	0	0	0	0	0	0
13.0354	-4.2548	-3.8660	H	0	0	0	0	0	0	0	0	0	0	0
12.1079	-5.3763	-2.7826	H	0	0	0	0	0	0	0	0	0	0	0
13.8379	-4.9740	-2.4180	H	0	0	0	0	0	0	0	0	0	0	0
21.7638	-15.3610	-2.2543	H	0	0	0	0	0	0	0	0	0	0	0
21.2715	-14.9348	-3.9459	H	0	0	0	0	0	0	0	0	0	0	0
12.1957	-7.8340	-1.6712	H	0	0	0	0	0	0	0	0	0	0	0
23.7419	-16.9541	-2.2822	H	0	0	0	0	0	0	0	0	0	0	0
27.5135	-14.6532	-4.1457	H	0	0	0	0	0	0	0	0	0	0	0
26.7295	-14.3294	-2.5417	H	0	0	0	0	0	0	0	0	0	0	0
27.5648	-15.9068	-2.8485	H	0	0	0	0	0	0	0	0	0	0	0
29.5578	-13.1403	-4.3435	H	0	0	0	0	0	0	0	0	0	0	0
30.5745	-12.3481	-5.6243	H	0	0	0	0	0	0	0	0	0	0	0
14.4615	-12.3766	-3.5869	H	0	0	0	0	0	0	0	0	0	0	0
24.0329	-17.6406	-5.0537	H	0	0	0	0	0	0	0	0	0	0	0
10.0613	-14.6985	-3.3330	H	0	0	0	0	0	0	0	0	0	0	0
9.8752	-11.0729	-3.6966	H	0	0	0	0	0	0	0	0	0	0	0
26.2376	-18.1327	-4.4252	H	0	0	0	0	0	0	0	0	0	0	0
25.8051	-16.8745	-3.1915	H	0	0	0	0	0	0	0	0	0	0	0
25.7817	-18.6315	-2.7529	H	0	0	0	0	0	0	0	0	0	0	0
23.5305	-19.8936	-4.7694	H	0	0	0	0	0	0	0	0	0	0	0
24.2225	-19.9161	-3.0940	H	0	0	0	0	0	0	0	0	0	0	0
22.5362	-19.3187	-3.3779	H	0	0	0	0	0	0	0	0	0	0	0
31.7471	-14.3548	-2.4569	H	0	0	0	0	0	0	0	0	0	0	0
33.9873	-9.7799	-4.5168	H	0	0	0	0	0	0	0	0	0	0	0
33.2785	-8.8385	-3.1368	H	0	0	0	0	0	0	0	0	0	0	0
34.4674	-10.1647	-2.8157	H	0	0	0	0	0	0	0	0	0	0	0
15.3675	-14.8214	-5.2429	H	0	0	0	0	0	0	0	0	0	0	0
16.0855	-13.7396	-3.9755	H	0	0	0	0	0	0	0	0	0	0	0
16.4858	-15.5077	-3.9996	H	0	0	0	0	0	0	0	0	0	0	0

35.6980	-12.3078	-5.0499	H	0	0	0	0	0	0	0	0	0	0	0	0
35.9501	-11.1926	-3.6449	H	0	0	0	0	0	0	0	0	0	0	0	0
36.6694	-12.8509	-3.6326	H	0	0	0	0	0	0	0	0	0	0	0	0
12.5375	-16.8713	-5.1456	H	0	0	0	0	0	0	0	0	0	0	0	0
13.9063	-17.0320	-3.9654	H	0	0	0	0	0	0	0	0	0	0	0	0
12.5117	-18.1910	-3.9102	H	0	0	0	0	0	0	0	0	0	0	0	0
6.2298	-10.3019	-3.7957	H	0	0	0	0	0	0	0	0	0	0	0	0
8.1424	-10.1445	-3.8096	H	0	0	0	0	0	0	0	0	0	0	0	0
4.6332	-12.1180	-4.6218	H	0	0	0	0	0	0	0	0	0	0	0	0
4.1921	-13.2358	-3.2636	H	0	0	0	0	0	0	0	0	0	0	0	0
4.7398	-11.5447	-2.9099	H	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0								
1	3	2	0	0	0	0	0								
1	4	1	0	0	0	0	0								
2	5	1	0	0	0	0	0								
2	6	2	0	0	0	0	0								
3	7	1	0	0	0	0	0								
3	8	1	0	0	0	0	0								
4	9	1	0	0	0	0	0								
4	10	1	0	0	0	0	0								
5	11	1	0	0	0	0	0								
5	12	1	0	0	0	0	0								
5	13	1	0	0	0	0	0								
6	14	1	0	0	0	0	0								
7	15	2	0	0	0	0	0								
7	11	1	0	0	0	0	0								
8	16	1	0	0	0	0	0								
17	9	1	0	0	0	0	0								
10	18	3	0	0	0	0	0								
11	19	1	0	0	0	0	0								
12	20	3	0	0	0	0	0								
14	21	1	0	0	0	0	0								
16	22	1	0	0	0	0	0								
16	23	2	0	0	0	0	0								
17	24	1	0	0	0	0	0								
17	25	1	0	0	0	0	0								
18	26	1	0	0	0	0	0								
27	19	1	0	0	0	0	0								
20	28	1	0	0	0	0	0								
21	29	1	0	0	0	0	0								
22	30	1	0	0	0	0	0								
24	31	1	0	0	0	0	0								
24	32	1	0	0	0	0	0								
25	33	1	0	0	0	0	0								
26	28	2	0	0	0	0	0								
27	34	1	0	0	0	0	0								
27	35	1	0	0	0	0	0								
29	36	1	0	0	0	0	0								
37	31	1	0	0	0	0	0								
32	38	1	0	0	0	0	0								
32	39	1	0	0	0	0	0								
33	40	1	0	0	0	0	0								
33	38	1	0	0	0	0	0								
34	41	1	0	0	0	0	0								
35	42	1	0	0	0	0	0								
36	43	1	0	0	0	0	0								
37	44	1	0	0	0	0	0								

37	45	1	0	0	0	0
38	46	1	0	0	0	0
41	47	1	0	0	0	0
41	48	1	0	0	0	0
42	49	1	0	0	0	0
42	48	1	0	0	0	0
44	50	1	0	0	0	0
45	51	1	0	0	0	0
46	52	1	0	0	0	0
47	53	1	0	0	0	0
48	54	1	0	0	0	0
50	55	1	0	0	0	0
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51	55	1	0	0	0	0
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53	58	1	0	0	0	0
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57	62	1	0	0	0	0
57	63	1	0	0	0	0
58	64	2	0	0	0	0
58	65	1	0	0	0	0
60	66	1	0	0	0	0
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63	68	1	0	0	0	0
64	69	1	0	0	0	0
64	70	1	0	0	0	0
65	71	2	0	0	0	0
66	72	1	0	0	0	0
66	73	1	0	0	0	0
67	74	1	0	0	0	0
67	75	1	0	0	0	0
68	76	1	0	0	0	0
68	74	1	0	0	0	0
69	77	2	0	0	0	0
70	78	1	0	0	0	0
71	79	1	0	0	0	0
71	77	1	0	0	0	0
74	80	1	0	0	0	0
77	81	1	0	0	0	0
78	82	1	0	0	0	0
78	83	2	0	0	0	0
79	84	1	0	0	0	0
80	85	1	0	0	0	0
81	86	1	0	0	0	0
82	87	1	0	0	0	0
82	88	2	0	0	0	0
87	89	1	0	0	0	0
90	4	1	0	0	0	0
91	6	1	0	0	0	0
92	11	1	0	0	0	0
93	17	1	0	0	0	0
94	24	1	0	0	0	0
95	27	1	0	0	0	0
96	32	1	0	0	0	0
97	33	1	0	0	0	0

98	37	1	0	0	0	0
99	38	1	0	0	0	0
100	41	1	0	0	0	0
101	42	1	0	0	0	0
102	48	1	0	0	0	0
103	50	1	0	0	0	0
104	55	1	0	0	0	0
105	57	1	0	0	0	0
106	67	1	0	0	0	0
107	68	1	0	0	0	0
108	74	1	0	0	0	0
109	8	1	0	0	0	0
110	13	1	0	0	0	0
111	14	1	0	0	0	0
112	14	1	0	0	0	0
113	26	1	0	0	0	0
114	28	1	0	0	0	0
115	30	1	0	0	0	0
116	30	1	0	0	0	0
117	30	1	0	0	0	0
118	34	1	0	0	0	0
119	34	1	0	0	0	0
120	39	1	0	0	0	0
121	40	1	0	0	0	0
122	40	1	0	0	0	0
123	40	1	0	0	0	0
124	43	1	0	0	0	0
125	43	1	0	0	0	0
126	43	1	0	0	0	0
127	44	1	0	0	0	0
128	44	1	0	0	0	0
129	46	1	0	0	0	0
130	49	1	0	0	0	0
131	49	1	0	0	0	0
132	49	1	0	0	0	0
133	51	1	0	0	0	0
134	51	1	0	0	0	0
135	54	1	0	0	0	0
136	60	1	0	0	0	0
137	61	1	0	0	0	0
138	61	1	0	0	0	0
139	61	1	0	0	0	0
140	62	1	0	0	0	0
141	62	1	0	0	0	0
142	65	1	0	0	0	0
143	66	1	0	0	0	0
144	69	1	0	0	0	0
145	70	1	0	0	0	0
146	72	1	0	0	0	0
147	72	1	0	0	0	0
148	72	1	0	0	0	0
149	73	1	0	0	0	0
150	73	1	0	0	0	0
151	73	1	0	0	0	0
152	75	1	0	0	0	0
153	76	1	0	0	0	0
154	76	1	0	0	0	0

```

155 76 1 0 0 0 0
156 84 1 0 0 0 0
157 84 1 0 0 0 0
158 84 1 0 0 0 0
159 85 1 0 0 0 0
160 85 1 0 0 0 0
161 85 1 0 0 0 0
162 86 1 0 0 0 0
163 86 1 0 0 0 0
164 86 1 0 0 0 0
165 88 1 0 0 0 0
166 88 1 0 0 0 0
167 89 1 0 0 0 0
168 89 1 0 0 0 0
169 89 1 0 0 0 0
M END

```

5.2. Edit file espera_A1.mop to obtain input file for MOPAC - remove the bonding part of the .mol file

```

PM7 PRECISE MOZYME XYZ
ChemDraw08051019392D

```

```

C      20.5866   -7.9900   -3.3852
C      19.9130   -6.7013   -3.1978
C      19.8012   -9.1309   -3.3547
C      22.0899   -7.7327   -3.7128
C      19.1494   -6.9842   -4.4440
C      19.3778   -6.4463   -1.9825
C      18.2415   -8.8755   -3.3266
N      20.2852  -10.4172   -3.4879
O      22.6668   -8.8529   -4.3945
C      22.1389   -6.4781   -4.5886
C      17.8426   -7.5734   -4.0661
C      19.1402   -5.7879   -5.1396
O      19.7771   -7.9543   -5.2701
C      19.1839   -7.5388   -0.9774
O      17.4461   -9.6189   -2.7985
C      19.3644  -11.4512   -3.4537
C      23.9720   -9.1450   -3.8678
C      22.0208   -5.4384   -5.2531
O      17.0743   -6.7106   -3.2244
C      19.5502   -4.8199   -5.6953
S      20.7051   -7.6400    0.0000
O      19.7212  -12.7155   -3.7929
O      18.2181  -11.2172   -3.1400
C      24.3190  -10.6257   -4.0922
O      24.9421   -8.3330   -4.5296
C      21.7106   -4.1603   -6.0244
C      15.6589   -6.9734   -3.0977
C      20.3925   -3.8399   -6.2503
S      22.1546   -7.7347   -1.4120
C      19.9283  -12.9798   -5.1702
O      23.3696  -11.4556   -3.4139
C      25.7302  -10.8895   -3.5367

```

C	26.2641	-8.4828	-4.0010
C	15.3798	-8.5001	-3.0907
O	14.9646	-6.3892	-4.1993
S	22.6025	-5.8329	-1.9422
C	23.2240	-12.8181	-3.8390
C	26.7326	-9.9372	-4.1808
O	26.1171	-12.2235	-3.8256
C	27.2208	-7.5464	-4.7460
C	13.9991	-8.8011	-3.7074
C	13.5309	-6.3700	-4.0683
C	24.2947	-5.4970	-1.3884
C	24.5941	-13.5063	-3.8854
O	22.3822	-13.5047	-2.9135
N	28.0462	-10.1215	-3.5350
O	13.4848	-10.0237	-3.1767
C	13.0493	-7.6568	-3.3754
C	13.1032	-5.1635	-3.2295
C	24.5814	-14.9217	-3.3045
C	22.0917	-14.8750	-3.1998
O	29.0628	-10.4874	-4.5199
C	12.4291	-10.6829	-3.7504
O	13.0272	-7.4547	-1.9689
C	23.3064	-15.6380	-3.7319
O	25.7141	-15.6436	-3.7856
C	30.1698	-11.1130	-3.8828
C	12.3123	-12.1518	-3.5973
O	11.6156	-10.0750	-4.4097
N	23.2979	-17.0086	-3.1868
C	26.9432	-15.1061	-3.3060
C	30.4346	-12.4788	-4.5287
O	31.3252	-10.2908	-4.0274
C	11.0789	-12.7959	-3.5254
C	13.4814	-12.8932	-3.5298
C	24.1097	-17.9434	-3.9839
C	31.6794	-13.1298	-3.9276
C	32.4691	-10.8242	-3.3585
C	11.0404	-14.1780	-3.3889
N	9.8587	-12.0743	-3.5923
C	13.4351	-14.2714	-3.3923
C	25.5791	-17.8971	-3.5615
C	23.5645	-19.3591	-3.7964
C	32.8626	-12.1588	-4.0096
O	31.4289	-13.4529	-2.5662
C	33.6292	-9.8409	-3.4669
C	12.2107	-14.9150	-3.3234
C	8.6571	-12.7688	-3.5231
O	14.5831	-15.0031	-3.3211
S	34.2850	-12.8700	-3.1421
O	12.1483	-16.2725	-3.1883
C	7.3366	-12.1067	-3.5954
O	8.6914	-13.9722	-3.3974
C	15.6874	-14.7566	-4.1804
C	35.7872	-12.2503	-3.9435
C	12.8082	-17.1374	-4.1012
O	6.2183	-12.8922	-3.5071
C	7.2332	-10.7759	-3.7418
C	4.8775	-12.4200	-3.5808

H	22.6664	-7.5765	-2.7738
H	20.1189	-5.9598	-1.3086
H	17.2111	-7.7736	-4.9635
H	23.9806	-8.9315	-2.7766
H	24.2892	-10.8581	-5.1825
H	15.3001	-6.5311	-2.1413
H	25.7201	-10.7283	-2.4345
H	26.2573	-8.2229	-2.9178
H	22.7698	-12.8408	-4.8558
H	26.8126	-10.1605	-5.2703
H	14.0992	-8.9002	-4.8128
H	13.0756	-6.2991	-5.0832
H	12.0238	-7.9090	-3.7350
H	24.6186	-14.8657	-2.1929
H	23.2624	-15.6778	-4.8454
H	29.9413	-11.2539	-2.8011
H	31.9227	-14.0568	-4.4973
H	32.2250	-10.9886	-2.2834
H	33.1255	-11.9837	-5.0788
H	21.2623	-10.5950	-3.6636
H	19.8708	-7.5195	-6.1202
H	18.3377	-7.2719	-0.3034
H	18.9664	-8.5044	-1.4881
H	22.5278	-3.5014	-6.3858
H	20.0436	-2.9342	-6.7899
H	19.0523	-12.6314	-5.7571
H	20.8348	-12.4330	-5.5045
H	20.0592	-14.0688	-5.3424
H	16.1548	-9.0190	-3.6979
H	15.4203	-8.8772	-2.0448
H	27.0661	-12.2322	-3.6338
H	27.1498	-7.7225	-5.8415
H	26.9383	-6.4949	-4.5223
H	28.2732	-7.7160	-4.4325
H	24.9923	-5.4697	-2.2551
H	24.3107	-4.5087	-0.8789
H	24.6460	-6.2810	-0.6841
H	24.9295	-13.5507	-4.9471
H	25.3004	-12.8962	-3.2920
H	28.3198	-9.2236	-3.1722
H	13.0354	-4.2548	-3.8660
H	12.1079	-5.3763	-2.7826
H	13.8379	-4.9740	-2.4180
H	21.7638	-15.3610	-2.2543
H	21.2715	-14.9348	-3.9459
H	12.1957	-7.8340	-1.6712
H	23.7419	-16.9541	-2.2822
H	27.5135	-14.6532	-4.1457
H	26.7295	-14.3294	-2.5417
H	27.5648	-15.9068	-2.8485
H	29.5578	-13.1403	-4.3435
H	30.5745	-12.3481	-5.6243
H	14.4615	-12.3766	-3.5869
H	24.0329	-17.6406	-5.0537
H	10.0613	-14.6985	-3.3330
H	9.8752	-11.0729	-3.6966
H	26.2376	-18.1327	-4.4252

H	25.8051	-16.8745	-3.1915
H	25.7817	-18.6315	-2.7529
H	23.5305	-19.8936	-4.7694
H	24.2225	-19.9161	-3.0940
H	22.5362	-19.3187	-3.3779
H	31.7471	-14.3548	-2.4569
H	33.9873	-9.7799	-4.5168
H	33.2785	-8.8385	-3.1368
H	34.4674	-10.1647	-2.8157
H	15.3675	-14.8214	-5.2429
H	16.0855	-13.7396	-3.9755
H	16.4858	-15.5077	-3.9996
H	35.6980	-12.3078	-5.0499
H	35.9501	-11.1926	-3.6449
H	36.6694	-12.8509	-3.6326
H	12.5375	-16.8713	-5.1456
H	13.9063	-17.0320	-3.9654
H	12.5117	-18.1910	-3.9102
H	6.2298	-10.3019	-3.7957
H	8.1424	-10.1445	-3.8096
H	4.6332	-12.1180	-4.6218
H	4.1921	-13.2358	-3.2636
H	4.7398	-11.5447	-2.9099

5.3 MOPAC produces the file **espera_A1.arc** with semiempirical QM energies

SUMMARY OF PM7 CALCULATION

MOPAC v22.0.6 Linux
Tue Mar 31 20:27:53

2026

Empirical Formula: C59 H80 N4 O22 S4 = 169 atoms

PM7 PRECISE MOZYME XYZ
ChemDraw08051019392D

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

KJ/MOL	HEAT OF FORMATION	=	-690.03154 KCAL/MOL	=	-2887.09198
	GRADIENT NORM	=	9.55810	=	0.73524
PER ATOM	DIPOLE	=	14.49085 DEBYE	POINT GROUP:	C1
	NO. OF FILLED LEVELS	=	246		
	MOLECULAR WEIGHT	=	1325.5346		

MOLECULAR DIMENSIONS (Angstroms)

Atom		Atom		Distance
H	169	H	161	30.70403
H	114	H	164	16.64079
S	29	H	116	9.09656

SCF CALCULATIONS = 671

WALL-CLOCK TIME = 5 MINUTES AND 14.148 SECONDS

COMPUTATION TIME = 19 MINUTES AND 58.133 SECONDS

FINAL GEOMETRY OBTAINED
 PM7 PRECISE MOZYME XYZ
 ChemDraw08051019392D

C	20.76707048	+1	-8.34525320	+1	-3.00118239	+1
C	19.77560203	+1	-7.29192006	+1	-2.82253994	+1
C	20.24489522	+1	-9.48198832	+1	-3.52629324	+1
C	22.19193354	+1	-7.86938616	+1	-2.88755112	+1
C	19.09060264	+1	-7.10268667	+1	-4.19364308	+1
C	19.39741487	+1	-6.64270312	+1	-1.71957430	+1
C	18.72531339	+1	-9.51834107	+1	-3.71139554	+1
N	20.96969612	+1	-10.60809621	+1	-3.90328432	+1
O	22.89643508	+1	-8.64936950	+1	-3.85385801	+1
C	22.23626095	+1	-6.46295643	+1	-3.24879986	+1
C	18.00935085	+1	-8.20875474	+1	-4.18671719	+1
C	19.04450086	+1	-5.67750705	+1	-4.37880694	+1
O	19.88312544	+1	-7.56837355	+1	-5.28820998	+1
C	20.00226771	+1	-6.85351687	+1	-0.38397185	+1
O	18.09131090	+1	-10.48217950	+1	-3.39747819	+1
C	20.52551213	+1	-11.37574254	+1	-4.97342368	+1
C	24.27717294	+1	-8.75156405	+1	-3.64963838	+1
C	22.11548197	+1	-5.29565864	+1	-3.57090006	+1
O	17.11487045	+1	-7.87944501	+1	-3.15418012	+1
C	19.61835226	+1	-4.60295501	+1	-4.42405831	+1
S	20.63768727	+1	-5.22865092	+1	0.19696052	+1
O	21.49400605	+1	-12.28933143	+1	-5.29646806	+1
O	19.47167646	+1	-11.26723891	+1	-5.55515811	+1
C	24.62112513	+1	-10.13329542	+1	-4.25060122	+1
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C	21.83271027	+1	-3.96254770	+1	-3.93239351	+1
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C	20.59198172	+1	-3.59282305	+1	-4.34199210	+1
S	22.50216930	+1	-5.34830779	+1	0.83137112	+1
C	21.13984129	+1	-13.15881533	+1	-6.36996302	+1
O	24.29108447	+1	-10.98565783	+1	-3.16927541	+1
C	26.12306536	+1	-10.26829566	+1	-4.52822499	+1
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O	15.31342843	+1	-7.25888048	+1	-4.39491768	+1
S	24.01601901	+1	-4.73699070	+1	-0.28577003	+1
C	24.10181216	+1	-12.35035216	+1	-3.51106287	+1
C	26.75065839	+1	-9.00198220	+1	-5.15346455	+1
O	26.20721017	+1	-11.33370094	+1	-5.45318152	+1
C	26.64010077	+1	-6.44445236	+1	-5.15326150	+1
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C	25.34249840	+1	-13.13161319	+1	-3.07022896	+1
O	23.00406434	+1	-12.68808678	+1	-2.67411729	+1
N	28.21776298	+1	-9.07678716	+1	-4.93127409	+1
O	13.47127692	+1	-10.78116862	+1	-3.76630032	+1
C	13.16614051	+1	-8.36234009	+1	-3.96105911	+1
C	13.54022698	+1	-5.87721517	+1	-3.54153595	+1
C	24.95307917	+1	-14.51191322	+1	-2.53176095	+1
C	22.51877785	+1	-13.99495022	+1	-2.90506327	+1
O	28.67889502	+1	-10.24069902	+1	-5.60561317	+1
C	12.30286527	+1	-11.29748424	+1	-4.22066625	+1
O	13.04515422	+1	-8.29900478	+1	-2.55289779	+1
C	23.64786769	+1	-15.01728552	+1	-3.20274263	+1
O	25.92199252	+1	-15.47714206	+1	-2.91452574	+1
C	29.44283955	+1	-11.00461010	+1	-4.67224151	+1
C	12.16500039	+1	-12.68943372	+1	-3.79924668	+1
O	11.52216625	+1	-10.63136190	+1	-4.86578510	+1
N	23.15550524	+1	-16.30115597	+1	-2.67772324	+1
C	27.17908711	+1	-15.32580468	+1	-2.28385689	+1
C	29.56204826	+1	-12.38833209	+1	-5.32436723	+1
O	30.70858231	+1	-10.36818348	+1	-4.62934283	+1
C	10.90263118	+1	-13.30891845	+1	-3.67242641	+1
C	13.33593545	+1	-13.42254650	+1	-3.54069793	+1
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O	29.97799551	+1	-13.35866296	+1	-3.26188739	+1
C	32.83299744	+1	-10.10490773	+1	-3.75787573	+1
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C	8.46563424	+1	-12.87332907	+1	-3.51358109	+1
O	14.35056664	+1	-15.55230233	+1	-2.92245251	+1
S	33.14540664	+1	-13.38396105	+1	-3.46395672	+1
O	11.75321821	+1	-16.66373208	+1	-2.72225903	+1
C	7.44995540	+1	-11.80894485	+1	-3.85272344	+1
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C	15.62297612	+1	-14.91624692	+1	-2.90889558	+1
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C	12.84881843	+1	-17.53043109	+1	-2.45168369	+1
O	6.69896635	+1	-12.27856349	+1	-4.87699306	+1
C	7.35567896	+1	-10.64795516	+1	-3.20685069	+1
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H	22.61093543	+1	-8.06361849	+1	-1.86640439	+1
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H	20.77754318	+1	-7.64272962	+1	-0.38004972	+1
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H	20.33692120	+1	-2.56828364	+1	-4.60772351	+1
H	20.28054991	+1	-13.77576697	+1	-6.08647689	+1
H	20.91474613	+1	-12.58012212	+1	-7.27294454	+1
H	22.04783393	+1	-13.76065914	+1	-6.49643884	+1
H	16.14253751	+1	-9.95181569	+1	-4.51011729	+1
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5.4. The **MOPAC** archive file has the coordinates to be input to **GAUSSIAN** or **ORCA** --- the job-input file has to be given the extension **.gjf** (Gaussian Job File) under Windows, or **.com** -- under Linux for **GAUSSIAN**, or the extension **.inp** for **ORCA**. The **espera_A1.gjf** has the form

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# opt=loose freq oniom(wb97xd/6-31g(d,p):pm7) iop(1/8=1,5/7=26144)
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esperamicin_A1.mol ---- ChemDraw08051019392D, Chemical Book

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H	26.11790313	-5.58147647	-4.71216136
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H	25.91078386	-5.93561581	-1.12637143
H	24.68416929	-7.08979944	-0.59121242
H	24.48898482	-6.23661911	-2.14794322
H	26.03988989	-13.23452494	-3.92781750
H	25.88820665	-12.55752786	-2.29705658
H	28.71986706	-8.33382291	-5.41941307
H	14.13585127	-4.99963736	-3.82399200
H	12.47928632	-5.62442748	-3.63371950
H	13.73478395	-6.06978855	-2.47673582
H	21.99439786	-14.22399170	-1.95685793
H	21.78364838	-13.95868100	-3.72683334
H	12.79725752	-9.18508075	-2.20784588
H	23.57801521	-16.53096127	-1.78256334
H	27.67385676	-14.40072145	-2.60543164
H	27.08412371	-15.36218952	-1.19525762
H	27.74066146	-16.19590016	-2.64677394
H	28.58289586	-12.90863878	-5.31355903
H	29.86873202	-12.29645131	-6.38231083
H	14.30316652	-12.92010949	-3.64298737

H	23.07452605	-17.05989454	-4.66235309
H	9.87437937	-15.17165243	-3.19476454
H	9.90098859	-11.66634112	-4.44861740
H	25.41797988	-17.49726786	-3.76625756
H	24.76022968	-18.60921216	-2.56446785
H	24.62708374	-18.99411047	-4.28179937
H	22.05533001	-19.24970500	-3.94559573
H	22.19252336	-18.78899570	-2.24153104
H	21.12235575	-17.88052129	-3.30672411
H	30.47620159	-13.97169829	-2.68758901
H	33.33658757	-10.05783864	-4.72963226
H	32.49833662	-9.08010300	-3.53163946
H	33.56233344	-10.38867761	-2.99236836
H	15.87854723	-14.52575172	-3.89971056
H	15.66728164	-14.12971726	-2.14788219
H	16.29060497	-15.74547009	-2.64177621
H	34.63425403	-13.54237750	-5.40641107
H	34.92577195	-12.04655415	-4.48772047
H	35.50207708	-13.60239181	-3.86097212
H	13.48821404	-17.63961019	-3.33414848
H	13.42077011	-17.17985529	-1.58611687
H	12.33586421	-18.47499747	-2.22366441
H	6.61378782	-9.89551932	-3.40578311
H	8.02062014	-10.36012336	-2.40769759
H	5.91943740	-10.51302344	-5.65767293
H	5.13746082	-12.08844394	-6.06278376
H	4.88595313	-11.35298922	-4.43588756

The last file will contain energies, orbitals, charges, etc. produced by GAUSSIAN (Espera.log) or ORCA (Espera.OUT)

5.5. FILE `espera.log` ----- follows with final coordinates and Gaussian archive

```
%nproc=24
%Mem=48GB
%chk=espr
# OPT FREQ ONIOM(wB97XD/6-31G**:PM7)
```

```
ESPERAMYCIN -- ONIOM
```

```
0,1
```

1	1	0	3.635420	-7.624491	4.362382
2	8	0	3.014602	-7.805933	3.629431
3	6	0	3.712085	-8.113620	2.440012
4	1	0	2.891190	-8.386602	1.743789
5	1	0	4.355697	-8.992821	2.613478
6	6	0	4.511063	-6.929984	1.893798

7	1	0	5.304108	-7.262139	1.186417
8	8	0	3.619085	-6.153289	1.083991
9	6	0	3.577501	-4.826263	1.592065
10	1	0	4.308723	-4.221762	0.983054
11	7	0	2.241214	-4.313153	1.379834
12	6	0	1.016784	-4.908472	1.619205
13	1	0	0.935349	-5.942078	1.932534
14	7	0	0.024280	-4.082878	1.408370
15	6	0	0.622218	-2.897499	1.023827
16	6	0	0.056974	-1.619273	0.756212
17	8	0	-1.132007	-1.293959	0.792411
18	7	0	1.034445	-0.665543	0.469735
19	1	0	0.689629	0.289068	0.305092
20	6	0	2.383747	-0.895802	0.503472
21	7	0	3.214412	0.155006	0.283060
22	1	0	2.868885	1.116187	0.283528
23	1	0	4.109216	0.031004	0.742565
24	7	0	2.918440	-2.070704	0.738436
25	6	0	1.998333	-3.012202	1.001926
26	6	0	5.082588	-5.978140	2.998109
27	1	0	5.273109	-6.487533	3.960622
28	6	0	3.958982	-4.916707	3.076591
29	1	0	3.124646	-5.270140	3.702859
30	1	0	4.287265	-3.954849	3.499598
31	8	0	6.259527	-5.496761	2.392236
32	15	0	7.343201	-4.464498	3.073837
33	8	0	8.302554	-4.308193	1.961150
34	8	0	7.614231	-4.775250	4.486372
35	8	0	6.378089	-3.128302	3.212707
36	6	0	6.169158	-2.180845	2.188411
37	1	0	5.064807	-2.088529	2.091532
38	1	0	6.561131	-2.439924	1.185890
39	6	0	6.798955	-0.863865	2.690644
40	1	0	7.775114	-0.655630	2.200178
41	8	0	5.941505	0.206884	2.261505
42	6	0	5.466351	0.972078	3.346752
43	1	0	5.577975	2.040995	3.029442
44	7	0	4.052283	0.656174	3.502010
45	6	0	3.507800	-0.613071	3.670528
46	1	0	4.134027	-1.491459	3.802898
47	7	0	2.207514	-0.598309	3.633697
48	6	0	1.873789	0.726229	3.425719
49	6	0	0.594304	1.316382	3.231298
50	8	0	-0.502199	0.752692	3.207089
51	7	0	0.681377	2.693809	3.043629
52	1	0	-0.220001	3.168913	2.877873
53	6	0	1.849695	3.411807	3.039288
54	7	0	1.737178	4.739116	2.867072
55	1	0	0.839550	5.223163	2.936909
56	1	0	2.575456	5.281053	3.021220
57	7	0	3.048558	2.864206	3.160549
58	6	0	2.993053	1.533979	3.335241
59	6	0	6.934612	-0.758395	4.225658
60	1	0	6.502706	-1.618134	4.782604
61	6	0	6.269692	0.582551	4.591338
62	1	0	5.655522	0.510310	5.501084
63	1	0	7.051257	1.336013	4.817693

64	8	0	8.292515	-0.618242	4.580846
65	1	0	8.749434	-1.487797	4.518964
66	1	0	4.514611	4.554335	2.463982
67	8	0	4.592540	5.415119	2.945778
68	6	0	5.607487	6.220353	2.405840
69	1	0	6.432891	5.591012	2.022879
70	1	0	5.963005	6.807192	3.278952
71	6	0	5.067700	7.158314	1.322377
72	1	0	5.830258	7.928235	1.054259
73	8	0	4.893196	6.403840	0.120250
74	6	0	3.590271	6.543778	-0.407334
75	1	0	3.745593	6.781663	-1.490412
76	7	0	2.930948	5.246417	-0.295417
77	6	0	3.565708	4.036681	-0.064045
78	1	0	4.645627	3.961111	0.035850
79	7	0	2.715673	3.046091	-0.047161
80	6	0	1.481263	3.620164	-0.265437
81	6	0	0.185197	3.024991	-0.292216
82	8	0	-0.102116	1.841349	-0.080758
83	7	0	-0.810463	3.955361	-0.567689
84	1	0	-1.777591	3.573648	-0.647171
85	6	0	-0.602618	5.298000	-0.723441
86	7	0	-1.686312	6.064501	-0.933569
87	1	0	-2.575932	5.691976	-1.298982
88	1	0	-1.492354	7.038075	-1.094070
89	7	0	0.589362	5.873842	-0.648792
90	6	0	1.574916	4.990256	-0.422874
91	6	0	3.710184	7.817052	1.664310
92	1	0	3.239915	7.349871	2.559010
93	6	0	2.867540	7.638156	0.385854
94	1	0	1.816269	7.377399	0.616431
95	1	0	2.834027	8.573017	-0.205134
96	8	0	3.980903	9.219524	1.753508
97	15	0	3.533333	10.154155	2.967334
98	8	0	4.136402	11.446534	2.694047
99	8	0	3.131941	9.471216	4.185468
100	8	0	1.864871	10.571540	2.450484
101	6	0	0.998651	10.246478	1.642994
102	1	0	1.126656	9.518967	0.828250
103	6	0	-0.351759	10.911590	1.789794
104	1	0	-0.369786	11.886070	1.240760
105	8	0	-1.296231	10.093462	1.124214
106	6	0	-2.237350	9.536875	2.040218
107	1	0	-3.217741	9.603446	1.493096
108	7	0	-1.889164	8.156132	2.260318
109	6	0	-0.695555	7.661499	2.785783
110	1	0	0.100698	8.307845	3.122769
111	7	0	-0.689651	6.365232	2.842049
112	6	0	-1.913459	5.972073	2.345169
113	6	0	-2.449005	4.661378	2.166929
114	8	0	-1.890577	3.586762	2.409065
115	7	0	-3.745118	4.693588	1.662539
116	1	0	-4.214000	3.770423	1.587372
117	6	0	-4.420729	5.833371	1.306456
118	7	0	-5.649114	5.692493	0.814898
119	1	0	-6.164378	4.796650	0.769938
120	1	0	-6.112228	6.541255	0.538397

121	7	0	-3.911073	7.062084	1.438450
122	6	0	-2.686690	7.053928	1.960848
123	6	0	-0.808740	11.097647	3.260209
124	1	0	-0.070141	10.727400	4.002357
125	6	0	-2.159388	10.373405	3.329187
126	1	0	-2.268790	9.762581	4.241593
127	1	0	-2.985645	11.114130	3.370237
128	8	0	-1.069981	12.461363	3.490508
129	1	0	-0.262912	12.924837	3.799940
130	1	0	-10.158143	-1.086766	1.205905
131	8	0	-10.405603	-1.506526	0.342127
132	6	0	-10.477127	-0.512772	-0.661127
133	1	0	-10.842394	-1.047418	-1.557978
134	1	0	-9.454445	-0.125559	-0.827924
135	6	0	-11.445467	0.589106	-0.240052
136	1	0	-12.498507	0.249226	-0.216121
137	8	0	-11.129151	0.907671	1.131165
138	6	0	-10.784352	2.256875	1.264257
139	1	0	-11.145493	2.544274	2.278902
140	7	0	-9.312323	2.391284	1.232916
141	6	0	-8.646633	3.521602	0.786835
142	1	0	-9.165797	4.371545	0.366108
143	7	0	-7.356573	3.433629	0.932476
144	6	0	-7.153605	2.187896	1.482377
145	6	0	-5.938378	1.595540	1.908163
146	8	0	-4.813272	2.117665	1.876402
147	7	0	-6.118624	0.317419	2.408067
148	1	0	-5.260651	-0.145957	2.751258
149	6	0	-7.342835	-0.309485	2.506659
150	7	0	-7.344905	-1.558679	2.979815
151	1	0	-6.515542	-2.028182	3.367836
152	1	0	-8.248254	-1.994728	3.079740
153	7	0	-8.490147	0.262310	2.164443
154	6	0	-8.344692	1.497370	1.668552
155	6	0	-11.254739	1.903962	-1.052966
156	1	0	-10.217293	1.945577	-1.466492
157	6	0	-11.416308	2.980632	0.076033
158	1	0	-10.983685	3.942169	-0.208889
159	1	0	-12.491469	3.173372	0.245548
160	8	0	-12.306420	2.056115	-1.945090
161	15	0	-12.063894	2.452362	-3.537643
162	8	0	-13.001592	3.566882	-3.754635
163	8	0	-11.991119	1.192955	-4.308195
164	8	0	-10.479351	2.885154	-3.566223
165	6	0	-9.914192	4.074569	-3.032647
166	1	0	-9.120142	3.717101	-2.339153
167	1	0	-10.593364	4.749215	-2.485717
168	6	0	-9.281907	4.802719	-4.231371
169	1	0	-10.005672	5.462380	-4.753102
170	8	0	-8.284754	5.703933	-3.713237
171	6	0	-7.039465	5.509355	-4.332638
172	1	0	-6.756063	6.510603	-4.738650
173	7	0	-6.061477	5.143301	-3.303916
174	6	0	-4.908429	5.852538	-3.010914
175	1	0	-4.716679	6.830461	-3.425139
176	7	0	-4.115088	5.207634	-2.201457
177	6	0	-4.764494	4.016500	-1.944871

178	6	0	-4.317820	2.867222	-1.242709
179	8	0	-3.220131	2.720688	-0.676551
180	7	0	-5.246104	1.842954	-1.250990
181	1	0	-4.933903	0.944783	-0.850084
182	6	0	-6.476041	1.917306	-1.866086
183	7	0	-7.306785	0.879066	-1.749327
184	1	0	-7.043034	-0.013563	-1.313467
185	1	0	-8.020328	0.858883	-2.471745
186	7	0	-6.875449	2.967462	-2.564736
187	6	0	-5.985697	3.949198	-2.602488
188	6	0	-8.586999	3.840361	-5.214834
189	1	0	-8.582921	2.777266	-4.878341
190	6	0	-7.171737	4.412990	-5.401267
191	1	0	-6.413293	3.609745	-5.300643
192	1	0	-7.054133	4.815811	-6.421990
193	8	0	-9.216202	3.929798	-6.479092
194	1	0	-10.060536	3.426981	-6.459640
195	1	0	-11.291752	-3.446504	0.522482
196	8	0	-11.876691	-4.234160	0.621204
197	6	0	-11.402423	-5.309606	-0.154291
198	1	0	-11.265041	-4.980837	-1.200635
199	1	0	-12.235789	-6.035791	-0.100364
200	6	0	-10.116269	-5.913072	0.407111
201	1	0	-10.006447	-6.983602	0.118734
202	8	0	-9.018376	-5.246121	-0.237067
203	6	0	-8.073137	-4.889050	0.767455
204	1	0	-7.364352	-5.754481	0.895291
205	7	0	-7.348096	-3.733815	0.277503
206	6	0	-7.849949	-2.621825	-0.365199
207	1	0	-8.892139	-2.566256	-0.664359
208	7	0	-6.933832	-1.712415	-0.563725
209	6	0	-5.779403	-2.249769	-0.025041
210	6	0	-4.477075	-1.704949	0.088442
211	8	0	-4.095679	-0.573692	-0.255442
212	7	0	-3.581718	-2.601507	0.667674
213	1	0	-2.617789	-2.252514	0.767642
214	6	0	-3.921708	-3.845039	1.155443
215	7	0	-2.943878	-4.591560	1.696355
216	1	0	-1.975003	-4.292280	1.782112
217	1	0	-3.243235	-5.440648	2.155703
218	7	0	-5.139198	-4.337778	1.094954
219	6	0	-6.007298	-3.510294	0.499899
220	6	0	-9.941298	-5.735984	1.954857
221	1	0	-10.891146	-5.488980	2.469667
222	6	0	-8.900401	-4.593183	2.026983
223	1	0	-9.401168	-3.613804	1.980642
224	1	0	-8.293821	-4.611172	2.948283
225	8	0	-9.451501	-7.010403	2.312714
226	15	0	-8.920382	-7.464708	3.793350
227	8	0	-8.715230	-8.913847	3.591415
228	8	0	-9.634823	-6.798427	4.901247
229	8	0	-7.472313	-6.654578	3.857434
230	6	0	-6.305864	-7.031751	3.159292
231	1	0	-5.925229	-6.079529	2.720663
232	1	0	-6.451530	-7.743417	2.322952
233	6	0	-5.278675	-7.607215	4.161439
234	1	0	-5.012897	-8.658137	3.919440

235	8	0	-4.041462	-6.895836	3.956885
236	6	0	-3.651292	-6.188448	5.101740
237	1	0	-2.540172	-6.309083	5.166537
238	7	0	-3.963959	-4.769660	4.862855
239	6	0	-5.198714	-4.245824	4.545891
240	1	0	-6.110949	-4.838626	4.611381
241	7	0	-5.129084	-3.002717	4.160979
242	6	0	-3.780245	-2.693988	4.209767
243	6	0	-3.090612	-1.546481	3.746943
244	8	0	-3.569905	-0.522601	3.238849
245	7	0	-1.711162	-1.675159	3.891335
246	1	0	-1.155870	-0.859227	3.603537
247	6	0	-1.070430	-2.796003	4.359611
248	7	0	0.270776	-2.739004	4.452341
249	1	0	0.836457	-1.980294	4.071218
250	1	0	0.722268	-3.608150	4.681102
251	7	0	-1.700202	-3.892586	4.734741
252	6	0	-3.037909	-3.787172	4.625724
253	6	0	-5.640215	-7.466328	5.655342
254	1	0	-6.600641	-6.941655	5.854216
255	6	0	-4.438924	-6.740271	6.294019
256	1	0	-4.751852	-5.964879	7.007888
257	1	0	-3.832272	-7.462133	6.873907
258	8	0	-5.687768	-8.745997	6.254571
259	1	0	-6.530820	-9.192424	6.012789
260	19	0	-2.457873	0.994568	1.252193
261	6	0	5.178807	-3.548036	-3.257903
262	6	0	4.969279	-4.902331	-2.657282
263	6	0	4.076954	-2.785425	-3.427618
264	6	0	6.503599	-3.072942	-3.853084
265	6	0	3.771683	-5.656514	-3.312840
266	6	0	5.618493	-5.558377	-1.682682
267	6	0	2.765841	-3.304277	-2.950912
268	7	0	4.014941	-1.570778	-4.177252
269	8	0	7.564999	-3.239480	-2.878244
270	6	0	6.761083	-3.825042	-5.082504
271	6	0	2.488016	-4.726478	-3.394989
272	6	0	4.213191	-6.034365	-4.669304
273	8	0	3.439838	-6.835261	-2.586873
274	6	0	6.776212	-5.146672	-0.845578
275	8	0	1.947017	-2.598188	-2.354200
276	6	0	3.209704	-1.618808	-5.293523
277	6	0	8.457335	-2.127796	-2.647641
278	6	0	6.784018	-4.515368	-6.081065
279	8	0	1.439959	-5.332706	-2.643362
280	6	0	4.704079	-6.274353	-5.752611
281	16	0	7.874808	-6.591694	-0.316318
282	8	0	3.128756	-0.506668	-6.082229
283	8	0	2.571516	-2.625961	-5.619039
284	6	0	7.850029	-1.167512	-1.615519
285	8	0	9.689618	-2.661152	-2.220657
286	6	0	6.527682	-5.477032	-7.098996
287	6	0	0.173676	-5.573948	-3.369925
288	6	0	5.493285	-6.339842	-6.933024
289	16	0	8.311629	-7.634215	-2.215242
290	6	0	3.869695	0.701219	-5.794938
291	8	0	6.915185	-0.382743	-2.394118

292	6	0	8.966440	-0.296965	-1.032330
293	6	0	9.903761	-2.648885	-0.763093
294	6	0	-0.574461	-4.246477	-3.502256
295	8	0	-0.527044	-6.546912	-2.647259
296	16	0	10.266923	-6.868299	-2.915402
297	6	0	5.769765	0.252214	-1.783574
298	6	0	10.043424	-1.174011	-0.325876
299	8	0	9.569567	0.428660	-2.114581
300	6	0	11.080277	-3.555042	-0.476671
301	6	0	-0.903987	-3.799910	-2.087233
302	6	0	-1.042939	-6.136584	-1.328539
303	6	0	9.716848	-5.498849	-4.079710
304	6	0	6.101391	1.306297	-0.737519
305	8	0	5.097836	0.844769	-2.906202
306	7	0	11.418913	-0.728341	-0.580826
307	8	0	-1.320043	-2.387136	-2.045232
308	6	0	-1.823781	-4.817863	-1.419517
309	6	0	-1.891358	-7.286128	-0.831549
310	6	0	6.991658	2.439669	-1.258088
311	6	0	5.336922	2.273292	-3.125177
312	8	0	11.618530	0.688995	-0.224010
313	6	0	-2.434728	-1.852268	-2.577273
314	8	0	-3.034246	-5.078158	-2.132051
315	6	0	6.768414	2.674484	-2.773873
316	8	0	6.618453	3.603430	-0.480561
317	6	0	11.810155	0.870178	1.177413
318	6	0	-2.267571	-0.451965	-2.971318
319	8	0	-3.490590	-2.513410	-2.734077
320	7	0	7.770612	1.965214	-3.582028
321	6	0	7.545843	4.709550	-0.538062
322	6	0	12.723872	2.091384	1.351432
323	8	0	10.548249	1.094956	1.835867
324	6	0	-3.307725	0.287293	-3.587419
325	6	0	-0.994576	0.123670	-2.827629
326	6	0	8.677339	2.756163	-4.435150
327	6	0	12.058868	3.167262	2.216859
328	6	0	9.843369	2.289351	1.371483
329	6	0	-3.012151	1.565060	-4.085059
330	7	0	-4.581600	-0.283276	-3.699897
331	6	0	-0.714354	1.383790	-3.318897
332	6	0	9.678642	3.520610	-3.560094
333	6	0	9.398486	1.789389	-5.378926
334	6	0	10.721010	3.564625	1.600638
335	8	0	12.893171	4.352419	2.245762
336	6	0	8.506276	2.246669	2.082592
337	6	0	-1.733488	2.097056	-3.978193
338	6	0	-5.665805	0.199989	-4.389476
339	8	0	0.538990	1.972688	-3.244820
340	16	0	9.835272	4.896202	2.609215
341	8	0	-1.496492	3.279100	-4.649858
342	6	0	-6.843755	-0.732796	-4.410803
343	8	0	-5.702487	1.307356	-4.953480
344	6	0	1.637577	1.153816	-2.786633
345	6	0	10.633330	6.415808	1.871202
346	6	0	-0.962438	4.415780	-3.918264
347	8	0	-8.013520	-0.016379	-4.451294
348	6	0	-6.740649	-2.067717	-4.418721

349	6	0	-9.258287	-0.728320	-4.629352
350	1	0	6.407870	-2.008045	-4.079360
351	1	0	5.186829	-6.528503	-1.439003
352	1	0	4.397772	-0.698951	-3.812700
353	1	0	2.203230	-4.624060	-4.448285
354	1	0	2.529710	-6.712403	-2.228510
355	1	0	7.386287	-4.381008	-1.307331
356	1	0	6.419200	-4.790608	0.140625
357	1	0	8.631214	-1.591185	-3.580240
358	1	0	7.312627	-1.733387	-0.838628
359	1	0	7.140541	-5.509738	-7.989036
360	1	0	0.412765	-6.016874	-4.337856
361	1	0	5.267971	-7.077223	-7.692294
362	1	0	3.738430	1.326599	-6.673001
363	1	0	3.451369	1.198480	-4.917572
364	1	0	4.931665	0.486828	-5.638036
365	1	0	8.558623	0.396371	-0.288820
366	1	0	9.013222	-3.078373	-0.271061
367	1	0	0.048923	-3.508974	-4.012431
368	1	0	-1.487096	-4.415231	-4.078745
369	1	0	5.094943	-0.513325	-1.384964
370	1	0	9.880287	-1.126765	0.756626
371	1	0	8.886997	0.971222	-2.607242
372	1	0	11.257091	-3.582965	0.604580
373	1	0	11.985153	-3.209577	-0.970246
374	1	0	10.838765	-4.567792	-0.810970
375	1	0	0.023244	-3.740651	-1.517497
376	1	0	-0.177071	-5.974067	-0.675392
377	1	0	9.146479	-4.756152	-3.523682
378	1	0	9.125769	-5.924022	-4.887647
379	1	0	10.635233	-5.052446	-4.461117
380	1	0	5.147914	1.745671	-0.428010
381	1	0	6.531327	0.842615	0.160159
382	1	0	11.578415	-0.684866	-1.586303
383	1	0	-2.020959	-4.497870	-0.394126
384	1	0	-1.304763	-8.206480	-0.806749
385	1	0	-2.754506	-7.412028	-1.484996
386	1	0	-2.252585	-7.061726	0.180292
387	1	0	8.055901	2.240207	-1.102505
388	1	0	4.629498	2.845967	-2.514604
389	1	0	5.125464	2.446573	-4.178946
390	1	0	-3.482442	-4.228328	-2.334790
391	1	0	6.854018	3.749067	-2.973319
392	1	0	12.196652	-0.049231	1.617822
393	1	0	7.382844	1.147860	-4.041834
394	1	0	7.205516	5.428545	0.205928
395	1	0	7.544898	5.189286	-1.522782
396	1	0	8.560366	4.381643	-0.289006
397	1	0	12.930569	2.520739	0.367499
398	1	0	13.679229	1.790484	1.789126
399	1	0	-0.228224	-0.475314	-2.356025
400	1	0	8.101770	3.482005	-5.036418
401	1	0	11.889137	2.798080	3.235550
402	1	0	9.704758	2.178489	0.288951
403	1	0	-3.769853	2.136971	-4.597095
404	1	0	-4.671933	-1.184727	-3.237665
405	1	0	10.366045	4.100598	-4.180576

406	1	0	10.253946	2.813078	-2.952378
407	1	0	9.169666	4.218130	-2.885006
408	1	0	8.686809	1.260655	-6.023667
409	1	0	10.100722	2.327020	-6.018864
410	1	0	9.956389	1.049416	-4.793542
411	1	0	10.936276	4.031645	0.633123
412	1	0	13.641341	4.232844	2.849226
413	1	0	7.810922	2.992976	1.698608
414	1	0	8.627477	2.378473	3.160994
415	1	0	8.070077	1.248656	1.924184
416	1	0	2.513366	1.796656	-2.816698
417	1	0	1.481121	0.819513	-1.760135
418	1	0	1.773987	0.278835	-3.430549
419	1	0	11.711946	6.310367	1.948343
420	1	0	10.282612	7.269247	2.450518
421	1	0	10.331137	6.528912	0.827470
422	1	0	-0.730128	5.159528	-4.677363
423	1	0	-1.730741	4.803467	-3.244867
424	1	0	-0.061236	4.139427	-3.368889
425	1	0	-5.776825	-2.555679	-4.406767
426	1	0	-7.607594	-2.716863	-4.441447
427	1	0	-9.461274	-1.383391	-3.773706
428	1	0	-9.245978	-1.312470	-5.551012
429	1	0	-10.022771	0.052838	-4.688883

Rotational constants (GHZ): 0.0042784 0.0026709
0.0020978

.5. Test job not archived.

1\1\GINC-SL054\FOpt\ONIOM(wB97XD/6-31G(d,p):wB97XD/6-31G:PM7)\Mixed\C1
39H175K1N44062P4S4(2-)\ROOT\17-Oct-2025\0\#\# opt=loose oniom(wb97xd/6-
31g(d,p):wb97xd/6-31g:pm7) iop(1/8=1,5/7=6144)\ONIOM-separation of th
e antiparallel stem-Q2: coordinates from Sponer, JACS 2013, 135, 9785-
9796 + esperamycin\ -2,1\H,1.5305624852,-8.9455178525,2.4761479613\O,0
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LAWS OF PROGRAMMING DEFINITION: A WORKING PROGRAM
IS ONE THAT HAS
ONLY UNOBSERVED
BUGS.