

Supporting Information for

Unveiling the Reactivity of 2H-(Thio)pyran-2-(thi)ones in Cycloaddition Reactions with Strained Alkynes through Density Functional Theory Studies

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1. General materials and methods.

All chemical reagents were of analytical grade, obtained from commercial suppliers, and used without further purification unless otherwise specified. Reactions were monitored by thin layer chromatography on pre-coated glass TLC plates (Analtech UNIPLATE™ silica gel HLF w/ organic binder, 250 μm thickness, with UV254 indicator) or by LC/MS (Agilent 6110 Single Quad, LC-MS, direct-injection mode, ESI). TLC plates were visualized by UV illumination or developed with potassium permanganate stain. NMR spectra (¹H and ¹³C) were obtained using a 400, 500, or 700 MHz Bruker spectrometer and analyzed using MestReNova. ¹H and ¹³C chemical shifts (δ) were referenced to residual solvent peaks. The following residual solvent peaks were chosen: (for ¹H NMR) CDCl₃, 7.26 ppm; (for ¹³C NMR) CDCl₃, 77.16 ppm. The following abbreviations were used to define ¹H NMR peaks: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. High-resolution electrospray ionization (ESI) mass spectra were obtained at CASDA Mass Spectrometry Center at Stony Brook University. The absorption spectrum and kinetics were measured on a Biotek EPOCH 2 microplate reader. On one hand, **exo-BCN** was commercially available and used as received. On the other hand, **PyrS2**¹, **DBCO**², **DMBCN**³, and **Cp-7HT**⁴ were synthesized according to previous reports.

Comment [SL]: Names check

Comment [SL]: Changed:
DBCO-Ac to DBCO in main text and SI

2. Computational details

All calculations were performed using Gaussian 16.⁶ Geometry optimizations of the minima and transition states were carried out using the M06-2X functional⁷ with the 6-311+G(d,p) basis set and SMD model for solvent (50% CH₃CN/H₂O mixture, $\chi = 55.69$ at 25 °C).⁸ Vibrational frequencies were computed at the same level to verify that optimized structures are energy minima or transition structures and to evaluate zero-point vibrational energies (ZPVE) and thermal corrections at 298 K. Intrinsic reaction coordinate (IRC) calculations were performed to verify the expected connections of the first-order saddle points with the local minima found on the potential energy surface.⁹ Distortion/interaction analysis were done at the M06-2X/6-311+G(d,p) level. To this end, the optimized transition state structure is separated into two fragments (distorted BCN and distorted heterocyclic structure), followed by single-point energy calculations on each fragment obtained from the IRC analysis. The energy difference between the distorted fragment and corresponding optimized structure is defined as the distortion energy. The difference between the activation energy and the total distortion energy is the interaction energy.¹⁰ The optimized structures indicated and shown in this study are illustrated using the CYLview program.¹¹

2.1. Supplementary tables.

Table S1. Energetics (in Hartree) of all stationary points.

E: Electronic Energy, **E(ZPE):** Zero Point Corrected Energy, **H:** Enthalpy, **G:** Gibbs energy

Structure	E	E(ZPE)	H	G
1	-464.544920557	-464.324582	-464.313102	-464.360067
2	-343.336211986	-343.255483	-343.249348	-343.284450
3	-666.295373193	-666.218004	-666.211322	-666.248001
4	-666.280184903	-666.201671	-666.195171	-666.231637
5	-989.249134145	-989.173859	-989.166824	-989.204783
RC-2	-807,892719837	-807,590182	-807,571857	-807,636189
RC-3	-1.130,85229857	-1.130,553246	-1.130,534260	-1.130,600672
RC-4	-1.130,83748778	-1.130,537396	-1.130,518567	-1.130,584417
RC-5	-1.453,80619117	-1.453,509603	-1.453,490060	-1.453,558482
TS1-2	-807.867512552	-807.565008	-807.548041	-807.608405
TS1-3	-1130.82080927	-1130.521757	-1130.504129	-1130.565867
TS1-4	-1130.81346697	-1130.513374	-1130.495883	-1130.557890
TS1-5	-1453.77563074	-1453.479090	-1453.460943	-1453.524479
6	-807.947475588	-807.639474	-807.623622	-807.681178
7	-1130.90974296	-1130.605198	-1130.588652	-1130.647759
8	-1130.88236534	-1130.577750	-1130.561104	-1130.621243
9	-1453.85960882	-1453.557642	-1453.540606	-1453.601532
TS2-2	-807.916147927	-807.611080	-807.594932	-807.653287
TS2-3	-1130.87556349	-1130.573641	-1130.556571	-1130.617585
TS2-4	-1130.86609309	-1130.563371	-1130.546758	-1130.606725
TS2-5	-1453.82525959	-1453.526152	-1453.508402	-1453.571600
10	-619.421376131	-619.129578	-619.115444	-619.169195
CO₂	-188.571432072	-188.559701	-188.556144	-188.581037
COS	-511.517209778	-511.508060	-511.504270	-511.530562
CS₂	-834.462963952	-834.456050	-834.452015	-834.479621

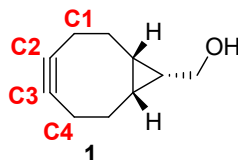
Table S2. Energetics (in Hartree) of all stationary points.E: Electronic Energy, **E(ZPE)**: Zero Point Corrected Energy, **H**: Enthalpy, **G**: Gibbs energy

Structure	E	E(ZPE)	H	G
<i>endo</i> -BCN	-464.544721303	-464.324390	-464.312900	-464.359906
<i>exo</i> -BCN	-464.547800739	-464.327806	-464.316277	-464.363428
DMBCN	-579.076111520	-578.822929	-578.808610	-578.862073
MeCp	-709.455527595	-709.199919	-709.182966	-709.246142
DBCO	-785.454988490	-785.199505	-785.183765	-785.241099
Si7HT	-1136.51189229	-1136.199731	-1136.178392	-1136.247624
PyrS2	-1121.99979941	-1121.835430	-1121.819762	-1121.880024
TS- <i>endo</i> -BCN	-1586.54208636	-1586.156797	-1586.129959	-1586.213547
TS- <i>exo</i> -BCN	-1586.54165981	-1586.156349	-1586.129511	-1586.213093
TS-DMBCN	-1701.07136215	-1700.652355	-1700.622975	-1700.712224
TS-MeCp	-1831.44501715	-1831.022911	-1830.991401	-1831.088427
TS-DBCO	-1907.44003686	-1907.019360	-1906.988372	-1907.081097
TS-Si7HT	-2258.51522839	-2258.037376	-2258.000794	-2258.104949
PROD- <i>endo</i> -BCN	-1586.61197020	-1586.221308	-1586.195525	-1586.277253
PROD - <i>exo</i> -BCN	-1586.61595316	-1586.225556	-1586.199841	-1586.281041
PROD -DMBCN	-1701.14627047	-1700.721588	-1700.693656	-1700.779440
PROD -MeCp	-1831.53004728	-1831.102585	-1831.072089	-1831.167591
PROD -DBCO	-1907.52569243	-1907.100776	-1907.070471	-1907.162000
PROD -Si7HT	-2258.58744853	-2258.105532	-2258.069719	-2258.172473

Table S3. Gibbs activation energies at different levels of theory.

A comparison between M06-2X/6-311+G(d,p), M06-2X/Def2TZVPP and ω B97xD/Def2TZVPP methods was performed for the RDS (**TS1**) to validate the results and all the methods yield very similar results in terms of Gibb activation energies.

M06-2X/6-311+G(d,p)	M06-2X/Def2TZVPP	ω B97xD/Def2TZVPP
ΔG^\ddagger (TS1-2) = 22.7 kcal/mol	ΔG^\ddagger (TS1-2) = 22.4 kcal/mol	ΔG^\ddagger (TS1-2) = 23.5 kcal/mol
ΔG^\ddagger (TS1-3) = 26.5 kcal/mol	ΔG^\ddagger (TS1-3) = 25.8 kcal/mol	ΔG^\ddagger (TS1-3) = 28.2 kcal/mol
ΔG^\ddagger (TS1-4) = 21.2 kcal/mol	ΔG^\ddagger (TS1-4) = 21.1 kcal/mol	ΔG^\ddagger (TS1-4) = 23.4 kcal/mol
ΔG^\ddagger (TS1-5) = 25.3 kcal/mol	ΔG^\ddagger (TS1-5) = 25.7 kcal/mol	ΔG^\ddagger (TS1-5) = 27.4 kcal/mol

Table S4. Geometrical parameters of critical stationary points for *endo*-BCN (**1**).

Structure	Distance (C2-C3)	Angle (C1-C2-C3)	Dihedral angle (C1-C2-C3-C4)
1	1.21 Å	154.6°	-1.1°
TS1-2	1.24 Å	152.7°	-5.6°
TS1-3	1.24 Å	151.7°	-1.7°
TS1-4	1.23 Å	154.6°	-5.3°
TS1-5	1.23 Å	153.0°	-0.9°

2.2. Supplementary figures.

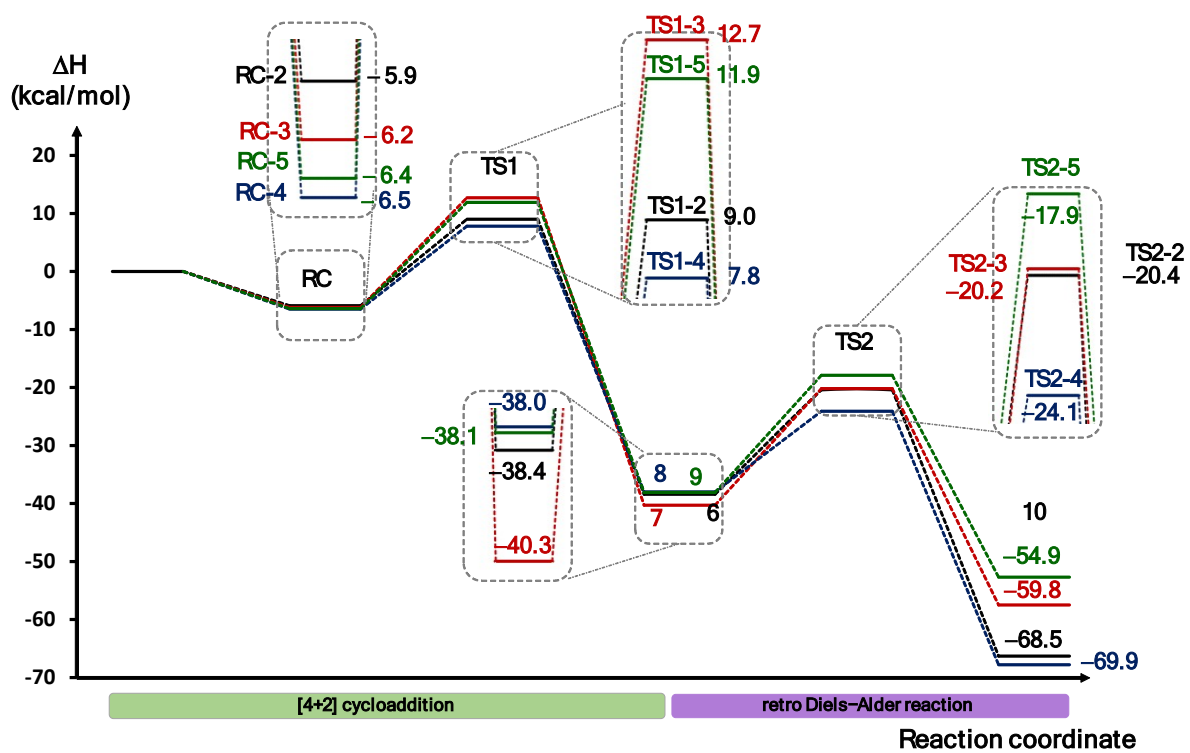
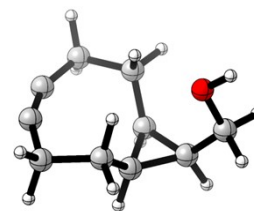


Fig. S1 Enthalpy profile (in kcal/mol) for the cycloaddition of *endo*-BCN (1) with dienes 2, 3, 4 and 5.

2.3. Cartesian coordinates for all the optimized species at the M06-2X/6-311+G(d,p) level of theory in water (SMD).

BCN (1)

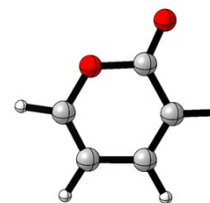
E(electronic) = -464.536915442
 Zero-point correction= 0.219682 (Hartree/Particle)
 Thermal correction to Energy= 0.230274
 Thermal correction to Enthalpy= 0.231219
 Thermal correction to Gibbs Free Energy= 0.184123
 Sum of electronic and zero-point Energies= -464.317234
 Sum of electronic and thermal Energies= -464.306641
 Sum of electronic and thermal Enthalpies= -464.305697
 Sum of electronic and thermal Free Energies= -464.352792



6	2.317376000	0.604186000	-0.262244000	1	-0.365474000	2.604929000	-0.122216000
6	2.317677000	-0.601924000	-0.270967000	6	-0.264359000	0.757264000	0.962867000
6	1.693324000	1.928625000	-0.166874000	6	-0.257933000	-0.766733000	0.959031000
1	1.985387000	2.432510000	0.758539000	6	-1.563080000	-0.011254000	1.022104000
1	1.972702000	2.577722000	-0.998997000	1	-2.028412000	-0.015653000	2.003895000
6	1.694162000	-1.927717000	-0.191916000	1	0.042808000	-1.191302000	1.914178000
1	1.990072000	-2.444502000	0.725127000	1	0.029381000	1.177408000	1.922159000
1	1.970269000	-2.565155000	-1.034047000	6	-2.653081000	-0.024602000	-0.023914000
6	0.168270000	-1.650416000	-0.200247000	1	-3.323833000	0.821135000	0.167176000
1	-0.091153000	-1.194837000	-1.155599000	1	-3.238021000	-0.943649000	0.098980000
1	-0.363531000	-2.605862000	-0.138753000	8	-2.161797000	0.051229000	-1.361040000
6	0.167798000	1.650607000	-0.187228000	1	-2.922441000	-0.012909000	-1.948328000
1	-0.084302000	1.202121000	-1.147462000				

2H-pyran-2-one (2)

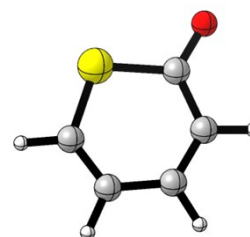
E(electronic) = -343.336211986
 Zero-point correction= 0.080729 (Hartree/Particle)
 Thermal correction to Energy= 0.085920
 Thermal correction to Enthalpy= 0.086864
 Thermal correction to Gibbs Free Energy= 0.051762
 Sum of electronic and zero-point Energies= -343.255483
 Sum of electronic and thermal Energies= -343.250292
 Sum of electronic and thermal Enthalpies= -343.249348
 Sum of electronic and thermal Free Energies= -343.284450



6	-1.770423000	-0.061096000	-0.000007000	8	0.329760000	-1.139496000	-0.000023000
6	-1.023652000	-1.176791000	0.000025000	1	0.810813000	2.183946000	0.000068000
6	1.037866000	0.043080000	-0.000198000	1	-2.848084000	-0.132655000	0.000025000
6	0.259869000	1.253543000	-0.000022000	8	2.251037000	-0.050143000	0.000153000
6	-1.093585000	1.198419000	-0.000006000	1	-1.672709000	2.114561000	0.000049000
1	-1.396840000	-2.191670000	0.000076000				

2H-thiopyranthio-2-one (3)

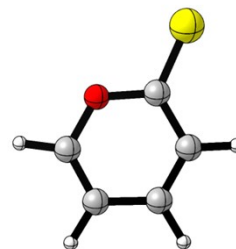
E(electronic) = -666.295373193
 Zero-point correction= 0.077369 (Hartree/Particle)
 Thermal correction to Energy= 0.083107
 Thermal correction to Enthalpy= 0.084051
 Thermal correction to Gibbs Free Energy= 0.047372
 Sum of electronic and zero-point Energies= -666.218004
 Sum of electronic and thermal Energies= -666.212266
 Sum of electronic and thermal Enthalpies= -666.211322
 Sum of electronic and thermal Free Energies= -666.248001



6	-1.905774000	0.239373000	0.000224000	1	-1.649256000	2.377614000	0.000104000
6	-1.355365000	-0.991802000	0.000242000	1	0.761820000	2.421476000	-0.000097000
6	1.100852000	0.314971000	-0.000101000	1	-2.984984000	0.326732000	0.000274000
6	0.239361000	1.471030000	-0.000031000	16	0.341273000	-1.302540000	-0.000085000
6	-1.117717000	1.432315000	0.000082000	8	2.325000000	0.351748000	-0.000207000
1	-1.956101000	-1.894488000	0.000235000				

2H-pyran-2-one (4)

E(electronic) = -666.280184903
Zero-point correction= 0.078513 (Hartree/Particle)
Thermal correction to Energy= 0.084070
Thermal correction to Enthalpy= 0.085014
Thermal correction to Gibbs Free Energy= 0.048548
Sum of electronic and zero-point Energies= -666.201671
Sum of electronic and thermal Energies= -666.196115
Sum of electronic and thermal Enthalpies= -666.195171
Sum of electronic and thermal Free Energies= -666.231637

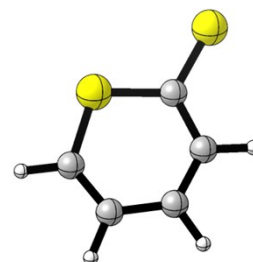


6	2.202761000	-0.081284000	0.000099000
6	1.432712000	-1.184956000	0.000128000
6	-0.598294000	0.059201000	-0.000085000
6	0.186808000	1.247350000	-0.000018000
6	1.546934000	1.181627000	0.000073000
1	3.278975000	-0.173118000	0.000038000

1	1.781946000	-2.208091000	0.000090000
1	-0.337683000	2.192223000	-0.000079000
1	2.133686000	2.092557000	0.000100000
8	0.084456000	-1.118927000	0.000021000
16	-2.259881000	-0.017736000	-0.000093000

2H-thiopyranthio-2-one (5)

E(electronic) = -989.249134145
Zero-point correction= 0.075276 (Hartree/Particle)
Thermal correction to Energy= 0.081366
Thermal correction to Enthalpy= 0.082310
Thermal correction to Gibbs Free Energy= 0.044351
Sum of electronic and zero-point Energies= -989.173859
Sum of electronic and thermal Energies= -989.167768
Sum of electronic and thermal Enthalpies= -989.166824
Sum of electronic and thermal Free Energies= -989.204783

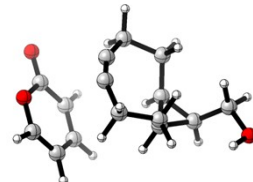


6	-2.275880000	0.371461000	0.000337000
6	-1.812268000	-0.898729000	0.000255000
6	0.718139000	0.195712000	-0.000147000
6	-0.035250000	1.408045000	-0.000302000
6	-1.397619000	1.491877000	-0.000036000
1	-2.470103000	-1.760917000	0.000378000

1	-1.842790000	2.480475000	-0.000169000
16	-0.144859000	-1.316401000	-0.000080000
16	2.390279000	0.129644000	0.000024000
1	0.549234000	2.321025000	-0.000580000
1	-3.345787000	0.537319000	0.000626000

RC-2

E(electronic) = -807.892719837
Zero-point correction= 0.302537 (Hartree/Particle)
Thermal correction to Energy= 0.319918
Thermal correction to Enthalpy= 0.320863
Thermal correction to Gibbs Free Energy= 0.256531
Sum of electronic and zero-point Energies= -807.590182
Sum of electronic and thermal Energies= -807.572802
Sum of electronic and thermal Enthalpies= -807.571857
Sum of electronic and thermal Free Energies= -807.636189

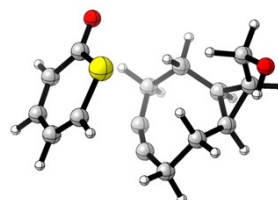


6	-0.481535000	0.930090000	1.433543000
6	-0.306921000	-0.223720000	1.739957000
6	-0.131855000	2.191876000	0.772007000
1	-0.829254000	2.417891000	-0.039673000
1	-0.145797000	3.037524000	1.462249000
6	0.423287000	-1.495667000	1.754662000
1	-0.131688000	-2.272136000	1.222219000
1	0.606063000	-1.854731000	2.769290000
6	1.765665000	-1.196532000	1.039450000
1	2.326849000	-0.488354000	1.653856000
1	2.349073000	-2.122884000	0.993239000
6	1.299450000	1.969919000	0.218934000
1	1.969502000	1.825144000	1.068608000
1	1.620727000	2.878600000	-0.300231000
6	1.370960000	0.796701000	-0.744841000
6	1.572867000	-0.659576000	-0.369381000
6	2.660722000	0.095839000	-1.104646000
1	2.790863000	-0.155322000	-2.152417000

1	1.009514000	-1.345828000	-0.997738000
1	0.698704000	0.926169000	-1.589207000
6	3.955313000	0.433665000	-0.415333000
1	3.792851000	0.774605000	0.609391000
1	4.474284000	1.229334000	-0.953149000
8	4.855808000	-0.681126000	-0.414380000
1	4.416906000	-1.411269000	0.037473000
6	-2.082409000	-1.904227000	-0.906431000
6	-2.900986000	-1.698428000	0.138527000
6	-3.101858000	0.641067000	-0.305909000
6	-2.253217000	0.443490000	-1.452002000
6	-1.755828000	-0.784334000	-1.733214000
1	-3.234719000	-2.450433000	0.840321000
8	-3.417842000	-0.480796000	-0.424333000
1	-1.689975000	-2.892538000	-1.097509000
1	-2.025254000	1.319602000	-2.044182000
8	-3.575307000	1.695184000	0.079099000
1	-1.101849000	-0.922430000	-2.586899000

RC-3

E(electronic) = -1130.85229857
Zero-point correction= 0.299053 (Hartree/Particle)
Thermal correction to Energy= 0.317094
Thermal correction to Enthalpy= 0.318038
Thermal correction to Gibbs Free Energy= 0.251627
Sum of electronic and zero-point Energies= -1130.553246
Sum of electronic and thermal Energies= -1130.535204
Sum of electronic and thermal Enthalpies= -1130.534260



Sum of electronic and thermal Free Energies= -1130.600672

6	-0.330619000	0.580300000	1.918907000	1	3.116724000	1.601744000	1.203428000
6	-0.142971000	1.607413000	1.315347000	1	2.737361000	-0.429544000	2.348666000
6	-0.044093000	-0.807593000	2.293275000	6	3.069197000	-1.036161000	-1.077891000
1	0.332824000	-0.866003000	3.318062000	1	2.005708000	-1.074483000	-1.324775000
1	-0.926998000	-1.448185000	2.231605000	1	3.442575000	-2.061650000	-1.053517000
6	0.557964000	2.486338000	0.375199000	8	3.785006000	-0.391426000	-2.138933000
1	1.068056000	3.296528000	0.903293000	1	3.501245000	0.529743000	-2.167121000
1	-0.120503000	2.939867000	-0.351102000	6	-3.111390000	1.467823000	-0.597491000
6	1.585218000	1.573755000	-0.342249000	6	-2.178988000	1.108737000	-1.503991000
1	1.031322000	0.838368000	-0.930432000	6	-2.228047000	-1.387381000	-0.279679000
1	2.163535000	2.184734000	-1.044328000	6	-3.232263000	-0.734009000	0.522446000
6	1.039959000	-1.272402000	1.288521000	6	-3.627224000	0.556756000	0.376075000
1	0.604633000	-1.251338000	0.287427000	1	-1.796235000	1.797831000	-2.248789000
1	1.303446000	-2.312177000	1.507866000	16	-1.491712000	-0.468696000	-1.619133000
6	2.295024000	-0.416567000	1.356160000	1	-3.484492000	2.484353000	-0.610964000
6	2.541786000	0.887947000	0.619729000	1	-3.666540000	-1.357085000	1.297185000
6	3.315577000	-0.358314000	0.243056000	8	-1.843774000	-2.541006000	-0.124052000
1	4.357294000	-0.385341000	0.546001000	1	-4.387211000	0.931389000	1.053014000

RC-4

E(electronic) = -1130.83748778

Zero-point correction= 0.300092 (Hartree/Particle)

Thermal correction to Energy= 0.317976

Thermal correction to Enthalpy= 0.318921

Thermal correction to Gibbs Free Energy= 0.253071

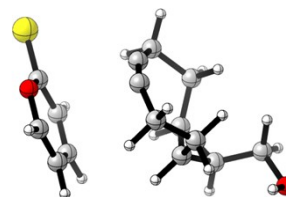
Sum of electronic and zero-point Energies= -1130.537396

Sum of electronic and thermal Energies= -1130.519511

Sum of electronic and thermal Enthalpies= -1130.518567

Sum of electronic and thermal Free Energies= -1130.584417

6	0.327780000	-0.731410000	1.413888000	1	-1.440809000	1.358084000	-0.997689000
6	0.020869000	0.391879000	1.729840000	1	-0.869894000	-0.863523000	-1.592733000
6	0.118544000	-2.025534000	0.755714000	6	-4.154664000	-0.758678000	-0.402460000
1	0.830259000	-2.169350000	-0.062029000	1	-3.949629000	-1.086564000	0.618737000
1	0.237049000	-2.863268000	1.445805000	1	-4.576139000	-1.606555000	-0.945736000
6	-0.851432000	1.570807000	1.752992000	8	-5.182958000	0.238976000	-0.389674000
1	-0.392697000	2.407526000	1.219705000	1	-4.848674000	0.999220000	0.100185000
1	-1.067596000	1.904675000	2.769663000	6	1.504832000	2.128135000	-0.959106000
6	-2.156403000	1.123339000	1.045602000	6	2.349755000	2.080942000	0.088589000
1	-2.631924000	0.357775000	1.663674000	6	2.999764000	-0.162952000	-0.351301000
1	-2.839098000	1.979360000	1.002993000	6	2.116562000	-0.149625000	-1.468609000
6	-1.334268000	-1.968925000	0.218306000	6	1.387668000	0.962197000	-1.765024000
1	-2.006655000	-1.900260000	1.075713000	1	2.539635000	2.880591000	0.791052000
1	-1.556441000	-2.908572000	-0.297668000	8	3.080375000	0.984279000	0.374305000
6	-1.547184000	-0.811808000	-0.743925000	1	0.937007000	3.026247000	-1.155416000
6	-1.914753000	0.611011000	-0.365041000	1	2.045097000	-1.052227000	-2.059395000
6	-2.912043000	-0.265137000	-1.094370000	16	3.940234000	-1.446590000	0.135637000
1	-3.076116000	-0.028765000	-2.140845000	1	0.713378000	0.959562000	-2.613831000



RC-5

E(electronic) = -1453.80619117

Zero-point correction= 0.296588 (Hartree/Particle)

Thermal correction to Energy= 0.315187

Thermal correction to Enthalpy= 0.316131

Thermal correction to Gibbs Free Energy= 0.247709

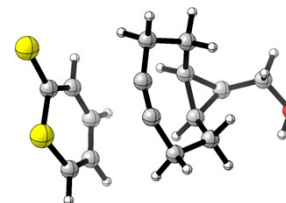
Sum of electronic and zero-point Energies= -1453.509603

Sum of electronic and thermal Energies= -1453.491005

Sum of electronic and thermal Enthalpies= -1453.490060

Sum of electronic and thermal Free Energies= -1453.558482

6	-0.087249000	0.823709000	1.436372000	1	1.575697000	-1.307296000	-1.029803000
6	0.153866000	-0.323024000	1.722349000	1	1.130972000	0.951755000	-1.578062000
6	0.185098000	2.112962000	0.793728000	6	4.390943000	0.642349000	-0.354893000
1	-0.518008000	2.294814000	-0.024697000	1	4.188195000	0.959155000	0.670234000
1	0.102579000	2.949749000	1.490166000	1	4.869396000	1.475924000	-0.872429000
6	0.952803000	-1.552449000	1.714489000	8	5.359359000	-0.413801000	-0.348894000
1	0.446599000	-2.344625000	1.156402000	1	4.964730000	-1.170549000	0.099912000
1	1.144997000	-1.927780000	2.721506000	6	-1.321675000	-2.037649000	-1.164010000
6	2.284946000	-1.162149000	1.023967000	6	-2.205080000	-2.248057000	-0.161140000
1	2.797863000	-0.439787000	1.663816000	6	-2.873448000	0.411562000	-0.409823000
1	2.919337000	-2.053485000	0.963089000	6	-1.906992000	0.342137000	-1.457200000
6	1.635012000	1.995154000	0.258430000	6	-1.191644000	-0.770095000	-1.796800000
1	2.301568000	1.879216000	1.115360000	1	-2.320911000	-3.212151000	0.321794000
1	1.904187000	2.931306000	-0.241339000	16	-3.249457000	-1.040905000	0.470575000
6	1.795404000	0.846524000	-0.724094000	1	-0.699137000	-2.860159000	-1.494233000
6	2.082400000	-0.602216000	-0.374834000	1	-1.732253000	1.266557000	-1.996869000

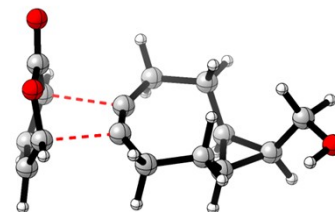


6	3.132938000	0.235378000	-1.074379000
1	3.296992000	0.014599000	-2.124216000

16	-3.684288000	1.809694000	0.026978000
1	-0.471695000	-0.682263000	-2.603297000

TS1-2

E(electronic) = -807.867512552
 Zero-point correction= 0.302505 (Hartree/Particle)
 Thermal correction to Energy= 0.318527
 Thermal correction to Enthalpy= 0.319472
 Thermal correction to Gibbs Free Energy= 0.259107
 Sum of electronic and zero-point Energies= -807.565008
 Sum of electronic and thermal Energies= -807.548985
 Sum of electronic and thermal Enthalpies= -807.548041
 Sum of electronic and thermal Free Energies= -807.608405



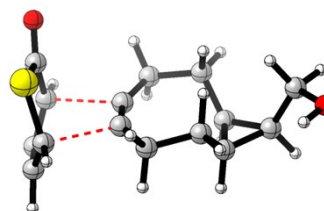
Frequency -414.0642

6	0.701629000	0.489328000	0.130622000
6	0.597786000	-0.721446000	-0.094016000
6	0.143750000	1.841611000	0.301287000
1	0.344863000	2.202888000	1.314670000
1	0.619369000	2.541791000	-0.391044000
6	-0.310683000	-1.868555000	-0.323381000
1	-0.214588000	-2.573132000	0.510281000
1	-0.019414000	-2.409114000	-1.227759000
6	-1.761315000	-1.372638000	-0.449493000
1	-1.833647000	-0.735252000	-1.333992000
1	-2.405374000	-2.241473000	-0.626264000
6	-1.374314000	1.779134000	0.044144000
1	-1.537018000	1.473124000	-0.990865000
1	-1.786983000	2.787010000	0.153613000
6	-2.066451000	0.843763000	1.016569000
6	-2.238101000	-0.642948000	0.790794000
6	-3.443073000	0.273079000	0.773408000
1	-4.091678000	0.217124000	1.641603000

1	-2.145618000	-1.242428000	1.692030000
1	-1.877157000	1.112789000	2.052028000
6	-4.191582000	0.536729000	-0.505155000
1	-3.515754000	0.678420000	-1.351064000
1	-4.799042000	1.438603000	-0.408871000
8	-5.115210000	-0.518900000	-0.799381000
1	-4.610528000	-1.337266000	-0.873396000
6	2.977808000	-1.417330000	1.100602000
6	2.587992000	-1.543524000	-0.223996000
6	3.140589000	0.673502000	-0.767511000
6	3.012280000	0.914589000	0.648693000
6	3.210160000	-0.125173000	1.546469000
1	2.366830000	-2.492617000	-0.694232000
8	3.039129000	-0.630409000	-1.152645000
1	2.908834000	-2.268081000	1.764537000
1	3.055562000	1.952449000	0.953092000
8	3.355393000	1.505266000	-1.636989000
1	3.387996000	0.086790000	2.593538000

TS1-3

E(electronic) = -1130.82080927
 Zero-point correction= 0.299053 (Hartree/Particle)
 Thermal correction to Energy= 0.315736
 Thermal correction to Enthalpy= 0.316680
 Thermal correction to Gibbs Free Energy= 0.254943
 Sum of electronic and zero-point Energies= -1130.521757
 Sum of electronic and thermal Energies= -1130.505073
 Sum of electronic and thermal Enthalpies= -1130.504129
 Sum of electronic and thermal Free Energies= -1130.565867



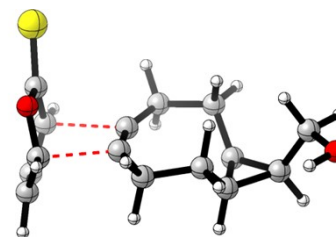
Frequency -411.3972

6	0.499882000	0.543959000	0.269928000
6	0.410441000	-0.682248000	0.151256000
6	-0.097263000	1.891332000	0.302017000
1	0.038494000	2.334860000	1.293630000
1	0.403651000	2.548840000	-0.414497000
6	-0.457634000	-1.862379000	-0.049758000
1	-0.408777000	-2.506994000	0.834531000
1	-0.096667000	-2.457211000	-0.894075000
6	-1.904918000	-1.407590000	-0.308396000
1	-1.928797000	-0.840762000	-1.242054000
1	-2.522530000	-2.300165000	-0.459016000
6	-1.595981000	1.777565000	-0.035318000
1	-1.692034000	1.390819000	-1.051527000
1	-2.030424000	2.782375000	-0.028937000
6	-2.333782000	0.905895000	0.962293000
6	-2.473198000	-0.595849000	0.838833000
6	-3.685830000	0.295709000	0.677436000
1	-4.386368000	0.292332000	1.506241000

1	-2.431603000	-1.124626000	1.786958000
1	-2.213436000	1.255541000	1.983898000
6	-4.357683000	0.456021000	-0.659856000
1	-3.632926000	0.547854000	-1.471604000
1	-4.979123000	1.353557000	-0.664764000
8	-5.251174000	-0.630799000	-0.933049000
1	-4.733946000	-1.444630000	-0.925446000
6	2.821770000	-1.193108000	1.467354000
6	2.444124000	-1.614288000	0.200938000
6	2.974311000	0.875697000	-0.698933000
6	2.757278000	1.102643000	0.719870000
6	2.997831000	0.161037000	1.712070000
1	2.771071000	-1.897769000	2.289131000
1	2.209348000	-2.657661000	0.018779000
1	2.712586000	2.155760000	0.980532000
1	3.130807000	0.509295000	2.729636000
16	3.042116000	-0.811578000	-1.245384000
8	3.141267000	1.770482000	-1.522411000

TS1-4

E(electronic) = -1130.81346697
 Zero-point correction= 0.300093 (Hartree/Particle)
 Thermal correction to Energy= 0.316640
 Thermal correction to Enthalpy= 0.317584
 Thermal correction to Gibbs Free Energy= 0.255577
 Sum of electronic and zero-point Energies= -1130.513374
 Sum of electronic and thermal Energies= -1130.496827
 Sum of electronic and thermal Enthalpies= -1130.495883
 Sum of electronic and thermal Free Energies= -1130.557890

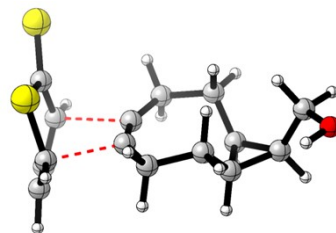


Frequency -402.8919

6	-0.485515000	-0.238745000	0.348463000	1	2.541177000	1.635965000	1.245544000
6	-0.330369000	0.843204000	-0.225786000	1	2.141012000	-0.478554000	2.293528000
6	-0.028235000	-1.517462000	0.909880000	6	4.333312000	-0.864302000	-0.404626000
1	-0.197134000	-1.532680000	1.991058000	1	3.601511000	-1.206197000	-1.139540000
1	-0.591457000	-2.349503000	0.478787000	1	4.896019000	-1.735728000	-0.064663000
6	0.640577000	1.803815000	-0.801432000	8	5.292506000	-0.012324000	-1.043160000
1	0.635965000	2.719263000	-0.199321000	1	4.823762000	0.765812000	-1.366696000
1	0.339949000	2.088798000	-1.812882000	6	-2.566191000	2.058021000	0.809210000
6	2.043625000	1.174666000	-0.824650000	6	-2.246000000	1.731051000	-0.505052000
1	2.022288000	0.307517000	-1.489063000	6	-3.016477000	-0.469134000	-0.315611000
1	2.735124000	1.900972000	-1.266455000	6	-2.834166000	-0.286350000	1.087147000
6	1.475190000	-1.664461000	0.598698000	6	-2.878748000	0.995311000	1.634393000
1	1.601955000	-1.701605000	-0.484755000	1	-1.995072000	2.466134000	-1.258072000
1	1.819180000	-2.623378000	0.998776000	8	-2.831820000	0.628463000	-1.079604000
6	2.284978000	-0.541880000	1.218513000	1	-2.403845000	3.064864000	1.168627000
6	2.539783000	0.795626000	0.557025000	1	-2.929036000	-1.166562000	1.708706000
6	3.679065000	-0.179413000	0.765472000	16	-3.484095000	-1.882946000	-1.073995000
1	4.379895000	0.076325000	1.553493000	1	-3.026244000	1.126903000	2.699106000

TS1-5

E(electronic) = -1453.77563074
 Zero-point correction= 0.296541 (Hartree/Particle)
 Thermal correction to Energy= 0.313743
 Thermal correction to Enthalpy= 0.314687
 Thermal correction to Gibbs Free Energy= 0.251152
 Sum of electronic and zero-point Energies= -1453.479090
 Sum of electronic and thermal Energies= -1453.461888
 Sum of electronic and thermal Enthalpies= -1453.460943
 Sum of electronic and thermal Free Energies= -1453.524479

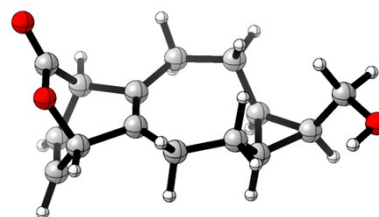


Frequency -406.7439

6	0.302166000	0.267652000	0.451692000	1	-2.782945000	-1.531999000	1.356673000
6	0.148271000	-0.862578000	-0.020630000	1	-2.414362000	0.660759000	2.251769000
6	-0.186959000	1.588403000	0.877647000	6	-4.493613000	0.835910000	-0.555027000
1	-0.063576000	1.700061000	1.959603000	1	-3.730680000	1.102306000	-1.289540000
1	0.391648000	2.384883000	0.401192000	1	-5.051772000	1.741532000	-0.310047000
6	-0.794743000	-1.859551000	-0.575810000	8	-5.446373000	-0.052564000	-1.152481000
1	-0.830854000	-2.733118000	0.084171000	1	-4.984488000	-0.867202000	-1.382782000
1	-0.440774000	-2.212826000	-1.548741000	6	2.405547000	-1.934144000	1.212103000
6	-2.191167000	-1.229754000	-0.718504000	6	2.077137000	-1.920940000	-0.142352000
1	-2.130944000	-0.413536000	-1.442357000	6	2.915936000	0.628034000	-0.238805000
1	-2.865614000	-1.983681000	-1.139922000	6	2.601373000	0.473712000	1.152965000
6	-1.675566000	1.703971000	0.493172000	6	2.674365000	-0.737166000	1.846597000
1	-1.756545000	1.648035000	-0.593897000	1	1.779551000	-2.835929000	-0.644074000
1	-2.034869000	2.693093000	0.794362000	1	2.771473000	-0.705713000	2.925319000
6	-2.514486000	0.637366000	1.170187000	16	2.855053000	-0.791128000	-1.231818000
6	-2.749101000	-0.747342000	0.606062000	16	3.376906000	2.081721000	-0.934801000
6	-3.890920000	0.242836000	0.690163000	1	2.604659000	1.398553000	1.720343000
1	-4.624545000	0.051634000	1.466636000	1	2.254846000	-2.844286000	1.780278000

6

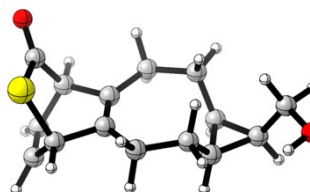
E(electronic) = -807.947475588
 Zero-point correction= 0.308002 (Hartree/Particle)
 Thermal correction to Energy= 0.322910
 Thermal correction to Enthalpy= 0.323854
 Thermal correction to Gibbs Free Energy= 0.266297
 Sum of electronic and zero-point Energies= -807.639474
 Sum of electronic and thermal Energies= -807.624566
 Sum of electronic and thermal Enthalpies= -807.623622
 Sum of electronic and thermal Free Energies= -807.681178



6	0.992342000	0.576918000	0.117297000	1	-2.095764000	-1.196411000	1.670036000
6	0.846501000	-0.738560000	-0.087172000	1	-1.841667000	1.233147000	1.939724000
6	0.123134000	1.808541000	0.109049000	6	-4.250880000	0.502842000	-0.492395000
1	0.282078000	2.299237000	1.078643000	1	-3.618315000	0.640853000	-1.371878000
1	0.559912000	2.491796000	-0.629033000	1	-4.878898000	1.390125000	-0.392492000
6	-0.264290000	-1.719491000	-0.369639000	8	-5.156804000	-0.585133000	-0.715738000
1	-0.193983000	-2.479532000	0.421169000	1	-4.633979000	-1.392966000	-0.779022000
1	0.013593000	-2.246547000	-1.290033000	6	2.822804000	-1.203477000	1.358323000
6	-1.717950000	-1.275609000	-0.482598000	6	2.205102000	-1.455273000	0.002622000
1	-1.844632000	-0.641955000	-1.360636000	6	3.227000000	0.479171000	-0.787826000
1	-2.312042000	-2.176525000	-0.671558000	6	2.468224000	0.948276000	0.433802000
6	-1.375651000	1.699736000	-0.139301000	6	2.989435000	0.094971000	1.577189000
1	-1.557296000	1.299099000	-1.136387000	1	3.094904000	-2.013864000	2.020539000
1	-1.779593000	2.717107000	-0.138698000	1	2.151918000	-2.501101000	-0.280569000
6	-2.062329000	0.887109000	0.934349000	1	2.608793000	2.015366000	0.572934000
6	-2.221681000	-0.600498000	0.771202000	1	3.454594000	0.549949000	2.441307000
6	-3.439870000	0.296242000	0.757798000	8	3.087041000	-0.834658000	-0.996771000
1	-4.046377000	0.263168000	1.657036000	8	3.892941000	1.162748000	-1.533401000

7

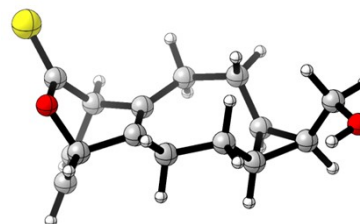
E(electronic) = -1130.90974296
 Zero-point correction= 0.304545 (Hartree/Particle)
 Thermal correction to Energy= 0.320147
 Thermal correction to Enthalpy= 0.321091
 Thermal correction to Gibbs Free Energy= 0.261984
 Sum of electronic and zero-point Energies= -1130.605198
 Sum of electronic and thermal Energies= -1130.589596
 Sum of electronic and thermal Enthalpies= -1130.588652
 Sum of electronic and thermal Free Energies= -1130.647759



6	0.699788000	0.544370000	0.360674000	1	-2.273124000	-1.581822000	1.606031000
6	0.667291000	-0.764053000	0.066388000	1	-2.232153000	0.825493000	2.115615000
6	-0.276603000	1.698077000	0.411014000	6	-4.711087000	0.109126000	-0.294605000
1	-0.180474000	2.128571000	1.416704000	1	-5.379262000	0.926800000	-0.000799000
1	0.127462000	2.465170000	-0.261794000	1	-5.325444000	-0.790800000	-0.416039000
6	-0.369167000	-1.778402000	-0.358260000	8	-4.087922000	0.430905000	-1.536679000
1	-0.293833000	-2.602611000	0.364060000	1	-4.788438000	0.532448000	-2.190033000
1	-0.005602000	-2.201312000	-1.304294000	6	2.730845000	-1.129279000	1.444962000
6	-1.838508000	-1.411658000	-0.522831000	6	2.047953000	-1.436152000	0.140172000
1	-1.962451000	-0.691104000	-1.327664000	6	2.936266000	0.950815000	-0.588965000
1	-2.361692000	-2.318344000	-0.845182000	6	2.119397000	1.048849000	0.707869000
6	-1.758736000	1.515978000	0.106087000	6	2.772945000	0.163871000	1.741603000
1	-1.900451000	1.204602000	-0.925963000	1	3.152553000	-1.926217000	2.044177000
1	-2.225014000	2.503400000	0.191138000	1	1.994280000	-2.500434000	-0.073578000
6	-2.418175000	0.565010000	1.076972000	1	2.110073000	2.097776000	0.995933000
6	-2.446849000	-0.914192000	0.766245000	1	3.242687000	0.595486000	2.615550000
6	-3.732658000	-0.131401000	0.831083000	16	3.082294000	-0.701910000	-1.227398000
1	-4.295113000	-0.311743000	1.743084000	8	3.430806000	1.905278000	-1.143198000

8

E(electronic) = -1130.89052599
 Zero-point correction= 0.305249 (Hartree/Particle)
 Thermal correction to Energy= 0.320693
 Thermal correction to Enthalpy= 0.321637
 Thermal correction to Gibbs Free Energy= 0.262260
 Sum of electronic and zero-point Energies= -1130.585277
 Sum of electronic and thermal Energies= -1130.569833
 Sum of electronic and thermal Enthalpies= -1130.568889
 Sum of electronic and thermal Free Energies= -1130.628266

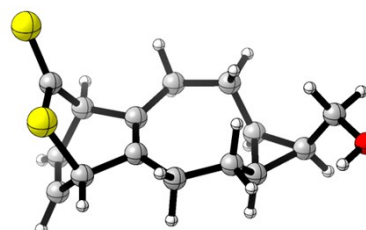


6	-0.753172000	-0.328849000	0.407859000	1	2.530478000	1.573454000	1.242084000
6	-0.545510000	0.858826000	-0.174045000	1	2.149820000	-0.654637000	2.203423000
6	0.038659000	-1.575431000	0.709614000	6	4.430226000	-0.826678000	-0.445277000
1	-0.083810000	-1.762492000	1.784670000	1	3.732914000	-1.170374000	-1.212232000
1	-0.486473000	-2.402228000	0.215888000	1	5.017019000	-1.688101000	-0.120801000
6	0.598502000	1.638613000	-0.774536000	8	5.373411000	0.083153000	-1.025560000
1	0.623373000	2.592356000	-0.229075000	1	4.887638000	0.865472000	-1.311781000
1	0.292237000	1.905202000	-1.792816000	6	-2.414812000	1.854630000	1.145104000
6	2.014831000	1.077265000	-0.823918000	6	-1.852814000	1.662521000	-0.240250000
1	2.051864000	0.218472000	-1.494665000	6	-3.021870000	-0.347001000	-0.402647000
1	2.644373000	1.846980000	-1.283787000	6	-2.226239000	-0.491956000	0.876378000
6	1.521037000	-1.652337000	0.368992000	6	-2.639241000	0.688084000	1.736595000
1	1.657077000	-1.564620000	-0.708708000	1	-2.619344000	2.838293000	1.544784000
1	1.864919000	-2.655313000	0.641100000	1	-1.769546000	2.570380000	-0.827698000
6	2.323520000	-0.623201000	1.131950000	1	-2.407315000	-1.456732000	1.336491000

6	2.559780000	0.742157000	0.544219000	1	-3.094009000	0.531625000	2.705696000
6	3.718920000	-0.211928000	0.729393000	8	-2.825131000	0.824295000	-0.977829000
1	4.384888000	0.027279000	1.552056000	16	-4.017078000	-1.478932000	-1.059632000

9

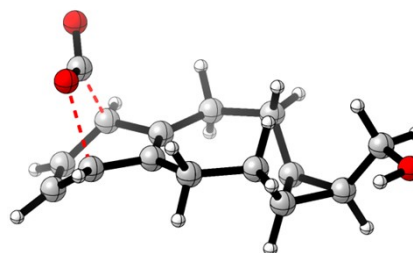
E(electronic) = -1453.85960882
 Zero-point correction= 0.301967 (Hartree/Particle)
 Thermal correction to Energy= 0.318058
 Thermal correction to Enthalpy= 0.319003
 Thermal correction to Gibbs Free Energy= 0.258077
 Sum of electronic and zero-point Energies= -1453.557642
 Sum of electronic and thermal Energies= -1453.541550
 Sum of electronic and thermal Enthalpies= -1453.540606
 Sum of electronic and thermal Free Energies= -1453.601532



6	0.586251000	0.348068000	0.495795000	1	-2.775542000	-1.441409000	1.398875000
6	0.384072000	-0.901925000	0.056597000	1	-2.416392000	0.868885000	2.165095000
6	-0.224399000	1.612883000	0.659008000	6	-4.577975000	0.793934000	-0.590274000
1	-0.132431000	1.897057000	1.715790000	1	-3.845193000	1.059722000	-1.355023000
1	0.316417000	2.393671000	0.109933000	1	-5.175210000	1.682848000	-0.378759000
6	-0.761841000	-1.714194000	-0.501883000	8	-5.497362000	-0.168877000	-1.121554000
1	-0.835141000	-2.605602000	0.135251000	1	-4.999425000	-0.970740000	-1.319217000
1	-0.418149000	-2.091844000	-1.473509000	6	2.321055000	-1.703407000	1.435588000
6	-2.160939000	-1.136852000	-0.677077000	6	1.657094000	-1.761627000	0.088189000
1	-2.146258000	-0.339619000	-1.420489000	6	2.897911000	0.540690000	-0.346666000
1	-2.780623000	-1.935094000	-1.100822000	6	2.051552000	0.609771000	0.928794000
6	-1.696368000	1.679041000	0.271964000	6	2.528995000	-0.468688000	1.875268000
1	-1.807349000	1.504896000	-0.797817000	1	1.479372000	-2.774319000	-0.264114000
1	-2.027615000	2.707426000	0.448931000	1	3.018307000	-0.202444000	-2.803097000
6	-2.542740000	0.735533000	1.094855000	16	2.841378000	-0.996909000	-1.137594000
6	-2.766088000	-0.676921000	0.627933000	16	3.767762000	1.806584000	-0.925018000
6	-3.923389000	0.295811000	0.669843000	1	2.159847000	1.605029000	1.351087000
1	-4.627069000	0.138693000	1.480809000	1	2.605962000	-2.613626000	1.947507000

TS2-2

E(electronic) = -807.916147927
 Zero-point correction= 0.305068 (Hartree/Particle)
 Thermal correction to Energy= 0.320271
 Thermal correction to Enthalpy= 0.321215
 Thermal correction to Gibbs Free Energy= 0.262861
 Sum of electronic and zero-point Energies= -807.611080
 Sum of electronic and thermal Energies= -807.595877
 Sum of electronic and thermal Enthalpies= -807.594932
 Sum of electronic and thermal Free Energies= -807.653287

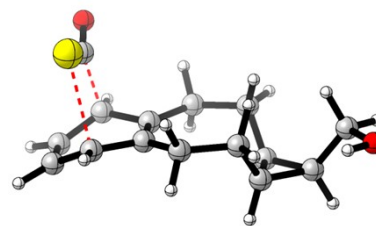


Frequency -422.1890

6	-1.031593000	-0.435382000	0.360577000	1	2.196386000	1.389553000	1.555363000
6	-0.843180000	0.874653000	0.037596000	1	1.879985000	-0.993802000	2.105155000
6	-0.171532000	-1.676782000	0.400389000	6	4.223451000	-0.609948000	-0.470395000
1	-0.315832000	-2.090892000	1.406643000	1	3.559959000	-0.813581000	-1.313670000
1	-0.658248000	-2.396931000	-0.268915000	1	4.823028000	-1.505185000	-0.295261000
6	0.305836000	1.742264000	-0.455672000	8	5.158620000	0.414159000	-0.831937000
1	0.324160000	2.619479000	0.201349000	1	4.664250000	1.233668000	-0.950455000
1	-0.009753000	2.122756000	-1.434170000	6	-3.064625000	1.447713000	1.080132000
6	1.732901000	1.223798000	-0.577238000	6	-2.076602000	1.646271000	0.065634000
1	1.796591000	0.483442000	-1.373731000	6	-3.108933000	-0.657525000	-0.901727000
1	2.345236000	2.071426000	-0.903820000	6	-2.467463000	-0.801045000	0.613649000
6	1.320704000	-1.654790000	0.102304000	6	-3.263973000	0.153380000	1.391288000
1	1.490691000	-1.382000000	-0.938042000	1	-3.674634000	2.269742000	1.429431000
1	1.676624000	-2.684441000	0.207862000	1	-2.073252000	2.594299000	-0.463662000
6	2.074130000	-0.763872000	1.061923000	1	-2.599477000	-1.836964000	0.906306000
6	2.271361000	0.689994000	0.728556000	1	-4.058795000	-0.199276000	2.036784000
6	3.460866000	-0.242887000	0.773697000	8	-3.056405000	0.489262000	-1.389185000
1	4.098961000	-0.131333000	1.644266000	8	-3.556462000	-1.699047000	-1.380841000

TS2-3

E(electronic) = -1130.87556349
 Zero-point correction= 0.301922 (Hartree/Particle)
 Thermal correction to Energy= 0.318048
 Thermal correction to Enthalpy= 0.318993
 Thermal correction to Gibbs Free Energy= 0.257979
 Sum of electronic and zero-point Energies= -1130.573641
 Sum of electronic and thermal Energies= -1130.557515
 Sum of electronic and thermal Enthalpies= -1130.556571
 Sum of electronic and thermal Free Energies= -1130.617585

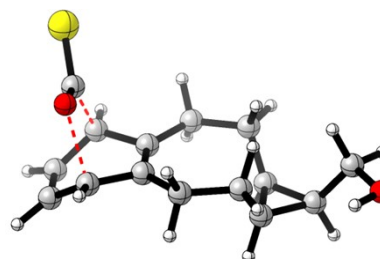


Frequency -462.9724

6	0.833504000	0.496804000	0.541917000	1	-2.493018000	-1.234328000	1.696784000
6	0.669986000	-0.855198000	0.369798000	1	-2.222357000	1.198204000	2.026490000
6	-0.053983000	1.718479000	0.398981000	6	-4.373994000	0.536065000	-0.657319000
1	0.017042000	2.236598000	1.363481000	1	-3.651395000	0.696516000	-1.459936000
1	0.464104000	2.377927000	-0.308391000	1	-5.011667000	1.420311000	-0.603118000
6	-0.454778000	-1.760326000	-0.117940000	8	-5.246320000	-0.545720000	-1.007760000
1	-0.526228000	-2.570325000	0.616137000	1	-4.711259000	-1.345927000	-1.065401000
1	-0.067287000	-2.233658000	-1.029266000	6	2.912054000	-1.253778000	1.445974000
6	-1.869894000	-1.272924000	-0.400293000	6	1.867951000	-1.637781000	0.567704000
1	-1.879181000	-0.619366000	-1.271852000	6	2.948439000	0.832560000	-0.840552000
1	-2.450020000	-2.158221000	-0.683517000	6	2.216216000	0.924819000	0.822471000
6	-1.523677000	1.653215000	0.008926000	6	3.083964000	0.080530000	1.601905000
1	-1.625147000	1.275927000	-1.007069000	1	3.589323000	-1.996205000	1.847781000
1	-1.885332000	2.686156000	-0.014993000	1	1.815520000	-2.683048000	0.278346000
6	-2.341288000	0.860722000	1.001408000	1	2.322504000	1.988209000	1.006528000
6	-2.509314000	-0.620375000	0.801530000	1	3.910108000	0.514257000	2.151966000
6	-3.702492000	0.298779000	0.668372000	16	3.029120000	-0.687440000	-1.545460000
1	-4.400389000	0.265062000	1.498583000	8	3.261644000	1.942144000	-1.191301000

TS2-4

E(electronic) = -1130.86609309
 Zero-point correction= 0.302722 (Hartree/Particle)
 Thermal correction to Energy= 0.318391
 Thermal correction to Enthalpy= 0.319335
 Thermal correction to Gibbs Free Energy= 0.259369
 Sum of electronic and zero-point Energies= -1130.563371
 Sum of electronic and thermal Energies= -1130.547702
 Sum of electronic and thermal Enthalpies= -1130.546758
 Sum of electronic and thermal Free Energies= -1130.606725

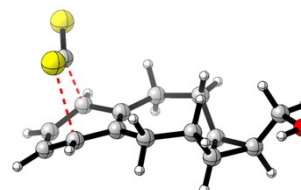


Frequency -367.2682

6	-0.795657000	-0.123359000	0.538593000	1	2.606538000	1.651221000	1.163381000
6	-0.526632000	1.052141000	-0.094149000	1	2.138123000	-0.501367000	2.271269000
6	-0.032822000	-1.393135000	0.838080000	6	4.385852000	-0.928446000	-0.381367000
1	-0.157995000	-1.555619000	1.916267000	1	3.670268000	-1.285257000	-1.125263000
1	-0.603416000	-2.203018000	0.366373000	1	4.938900000	-1.793743000	-0.011309000
6	0.656064000	1.674271000	-0.822338000	8	5.361440000	-0.091257000	-1.014866000
1	0.769151000	2.680085000	-0.401859000	1	4.908485000	0.700193000	-1.328770000
1	0.319611000	1.831082000	-1.853936000	6	-2.630510000	2.048127000	0.869700000
6	2.036202000	1.030209000	-0.855990000	6	-1.691201000	1.920518000	-0.201784000
1	2.014635000	0.123933000	-1.459893000	6	-2.965603000	-0.422475000	-0.554847000
1	2.691229000	1.729386000	-1.387268000	6	-2.235185000	-0.291371000	0.931795000
6	1.440688000	-1.564707000	0.498196000	6	-2.906856000	0.885905000	1.490080000
1	1.578878000	-1.554694000	-0.581779000	1	-3.155779000	2.978522000	1.038741000
1	1.725584000	-2.567600000	0.831470000	1	-1.637881000	2.723114000	-0.931236000
6	2.301855000	-0.539699000	1.198600000	1	-2.429097000	-1.212259000	1.467802000
6	2.591994000	0.773714000	0.524299000	1	-3.686222000	0.764244000	2.232088000
6	3.709315000	-0.217776000	0.759240000	8	-2.829681000	0.561774000	-1.281262000
1	4.391914000	0.042754000	1.561503000	16	-3.772627000	-1.858663000	-0.864200000

TS2-5

E(electronic) = -1453.82525959
 Zero-point correction= 0.299108 (Hartree/Particle)
 Thermal correction to Energy= 0.315913
 Thermal correction to Enthalpy= 0.316858
 Thermal correction to Gibbs Free Energy= 0.253659
 Sum of electronic and zero-point Energies= -1453.526152
 Sum of electronic and thermal Energies= -1453.509346
 Sum of electronic and thermal Enthalpies= -1453.508402



Sum of electronic and thermal Free Energies= -1453.571600

Frequency -447.0591

6	0.635699000	0.133787000	0.693515000	1	-2.852928000	-1.525689000	1.333873000
6	0.369783000	-1.119726000	0.196489000	1	-2.399926000	0.726653000	2.240704000
6	-0.143818000	1.430065000	0.819648000	6	-4.507592000	0.907128000	-0.551816000
1	-0.068284000	1.707881000	1.878198000	1	-3.748609000	1.173377000	-1.290675000
1	0.452386000	2.184744000	0.290950000	1	-5.059656000	1.814609000	-0.300327000
6	-0.803272000	-1.771561000	-0.528591000	8	-5.468193000	0.025376000	-1.146501000
1	-0.965420000	-2.730491000	-0.024787000	1	-5.013807000	-0.795493000	-1.369681000
1	-0.418854000	-2.032408000	-1.522791000	6	2.530402000	-1.956844000	1.182435000
6	-2.166710000	-1.114948000	-0.703344000	6	1.479825000	-2.039902000	0.238599000
1	-2.100596000	-0.273973000	-1.392419000	6	2.870544000	0.601069000	-0.545655000
1	-2.803894000	-1.856494000	-1.197886000	6	2.024674000	0.359366000	1.115329000
6	-1.598654000	1.586019000	0.401031000	6	2.801026000	-0.717575000	1.661824000
1	-1.693226000	1.469459000	-0.677115000	1	3.140729000	-2.824736000	1.396718000
1	-1.875786000	2.622597000	0.617930000	1	1.345521000	-2.984638000	-0.279772000
6	-2.511404000	0.654371000	1.163110000	1	2.203908000	1.329482000	1.560883000
6	-2.791241000	-0.717081000	0.612095000	1	3.644507000	-0.500499000	2.305976000
6	-3.901315000	0.307029000	0.687825000	16	2.801041000	-0.683507000	-1.547781000
1	-4.627113000	0.138663000	1.476741000	16	3.502640000	2.115179000	-0.610311000

10

E(electronic) = -619.421376131

Zero-point correction= 0.291798 (Hartree/Particle)

Thermal correction to Energy= 0.304988

Thermal correction to Enthalpy= 0.305932

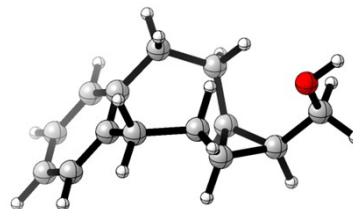
Thermal correction to Gibbs Free Energy= 0.252181

Sum of electronic and zero-point Energies= -619.129578

Sum of electronic and thermal Energies= -619.116389

Sum of electronic and thermal Enthalpies= -619.115444

Sum of electronic and thermal Free Energies= -619.169195



6	-1.441489000	-0.578446000	-0.646687000	1	0.112981000	-0.523393000	-2.109278000
6	-1.498733000	0.806433000	-0.398906000	1	-0.513802000	1.876549000	-1.973482000
6	-0.257027000	-1.202055000	-1.339064000	1	1.474748000	0.813379000	-1.295130000
6	-2.592456000	1.311316000	0.310443000	1	1.602461000	2.377934000	-0.535976000
6	-2.472976000	-1.399104000	-0.185605000	1	2.409737000	-0.020750000	2.395032000
6	-3.558060000	-0.881348000	0.516350000	1	1.837242000	-1.536224000	-0.905635000
6	-0.436728000	1.778000000	-0.884724000	1	0.759052000	-2.611304000	-0.045260000
6	1.031929000	1.444707000	-0.529628000	1	0.632045000	1.325939000	1.609025000
6	0.892170000	-1.571997000	-0.357063000	1	0.349578000	-1.084933000	1.717191000
6	0.972130000	-0.726311000	0.904206000	1	3.747381000	-1.436659000	0.536653000
6	1.132376000	0.770521000	0.819786000	1	4.400469000	0.031326000	1.273714000
6	2.276223000	-0.083398000	1.320345000	1	4.555629000	0.017754000	-1.016683000
6	-3.616597000	0.484915000	0.766840000	1	-4.451552000	0.908278000	1.313490000
6	3.600154000	-0.354490000	0.635032000	1	-2.640213000	2.377459000	0.509261000
8	3.696299000	0.256213000	-0.652362000	1	-2.417946000	-2.465629000	-0.383226000
1	-0.580335000	-2.110566000	-1.851831000	1	-4.347135000	-1.538906000	0.862974000
				1	-0.686229000	2.757590000	-0.469887000

CO₂

E(electronic) = -188.571432072

Zero-point correction= 0.011731 (Hartree/Particle)

Thermal correction to Energy= 0.014344

Thermal correction to Enthalpy= 0.015288

Thermal correction to Gibbs Free Energy= -0.009605

Sum of electronic and zero-point Energies= -188.559701

Sum of electronic and thermal Energies= -188.557088

Sum of electronic and thermal Enthalpies= -188.556144

Sum of electronic and thermal Free Energies= -188.581037



6	0.000000000	0.000000000	0.000018000
8	0.000000000	0.000000000	-1.155116000
8	0.000000000	0.000000000	1.155103000

COS

E(electronic) = -511.517209778

Zero-point correction= 0.009150 (Hartree/Particle)

Thermal correction to Energy= 0.011996

Thermal correction to Enthalpy= 0.012940

Thermal correction to Gibbs Free Energy= -0.013352

Sum of electronic and zero-point Energies= -511.508060

Sum of electronic and thermal Energies= -511.505214

Sum of electronic and thermal Enthalpies= -511.504270

Sum of electronic and thermal Free Energies= -511.530562



6	0.000000000	0.000000000	-0.527079000
8	0.000000000	0.000000000	-1.676933000
16	0.000000000	0.000000000	1.036121000

CS₂

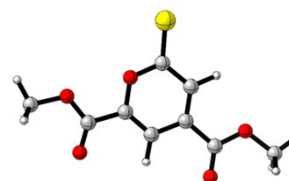
E(electronic) = -834.462963952
 Zero-point correction= 0.006914 (Hartree/Particle)
 Thermal correction to Energy= 0.010005
 Thermal correction to Enthalpy= 0.010949
 Thermal correction to Gibbs Free Energy= -0.016657
 Sum of electronic and zero-point Energies= -834.456050
 Sum of electronic and thermal Energies= -834.452959
 Sum of electronic and thermal Enthalpies= -834.452015
 Sum of electronic and thermal Free Energies= -834.479621



6	0.000000000	0.000000000	0.000069000
16	0.000000000	0.000000000	-1.552032000
16	0.000000000	0.000000000	1.552007000

PyrS2

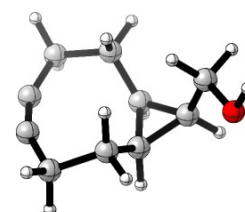
E(electronic) = -1121.99979941
 Zero-point correction= 0.164369 (Hartree/Particle)
 Thermal correction to Energy= 0.179093
 Thermal correction to Enthalpy= 0.180037
 Thermal correction to Gibbs Free Energy= 0.119776
 Sum of electronic and zero-point Energies= -1121.835430
 Sum of electronic and thermal Energies= -1121.820706
 Sum of electronic and thermal Enthalpies= -1121.819762
 Sum of electronic and thermal Free Energies= -1121.880024



6	1.099629000	-0.423318000	0.000408000	1	-5.047089000	-1.305427000	0.894168000
6	-1.159039000	1.110887000	-0.000143000	1	-5.619132000	0.135793000	-0.000054000
6	-0.085951000	-1.052574000	0.000255000	1	-2.029522000	1.751398000	-0.000498000
6	-1.263251000	-0.240927000	-0.000062000	6	2.403219000	-1.152496000	0.000708000
8	1.211831000	0.923824000	0.000359000	8	2.460725000	-2.358717000	0.000094000
6	0.130540000	1.746613000	0.000263000	8	3.440415000	-0.339313000	0.000276000
16	0.386580000	3.373735000	-0.000366000	6	4.735236000	-0.972527000	-0.000233000
6	-2.591408000	-0.936302000	-0.000398000	1	4.844246000	-1.584214000	0.894339000
8	-2.692743000	-2.140333000	-0.000005000	1	4.843534000	-1.584253000	-0.894865000
8	-3.611805000	-0.097456000	-0.000290000	1	5.453055000	-0.158047000	-0.000536000
6	-4.921582000	-0.696266000	-0.000138000	1	-0.134812000	-2.132159000	0.000299000
1	-5.047291000	-1.305417000	-0.894423000				

endo-BCN

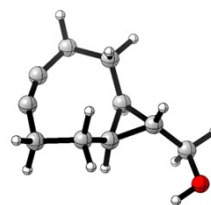
E(electronic) = -464.544721303
 Zero-point correction= 0.220331 (Hartree/Particle)
 Thermal correction to Energy= 0.230877
 Thermal correction to Enthalpy= 0.231822
 Thermal correction to Gibbs Free Energy= 0.184815
 Sum of electronic and zero-point Energies= -464.324390
 Sum of electronic and thermal Energies= -464.313844
 Sum of electronic and thermal Enthalpies= -464.312900
 Sum of electronic and thermal Free Energies= -464.359906



1	-1.448805000	2.670636000	0.900490000	1	-0.372191000	-2.711855000	-0.370603000
6	-1.318051000	2.168089000	-0.061532000	1	-0.369849000	-1.220662000	-1.309872000
1	-1.472811000	2.910939000	-0.846068000	6	1.463320000	-0.528830000	0.774210000
6	-2.214757000	-1.577420000	-0.259816000	6	-2.232290000	1.028638000	-0.184218000
1	-2.677157000	-2.087544000	-1.106723000	1	-2.570515000	-2.061843000	0.653403000
6	0.017040000	-0.965713000	0.809600000	6	-2.514402000	-0.142280000	-0.242571000
1	-0.285277000	-1.388088000	1.764164000	6	2.280461000	-0.633727000	-0.485499000
6	0.367245000	0.508481000	0.900002000	1	2.764142000	-1.610797000	-0.541724000
1	0.257839000	0.910768000	1.903508000	1	1.666231000	-0.513784000	-1.380473000
6	0.102598000	1.557001000	-0.167627000	8	3.346335000	0.323663000	-0.502438000
1	0.837842000	2.363088000	-0.067095000	1	2.042828000	-0.721654000	1.671336000
1	0.216282000	1.135016000	-1.169059000	1	2.953695000	1.202208000	-0.441979000
6	-0.669987000	-1.658528000	-0.355849000				

exo-BCN

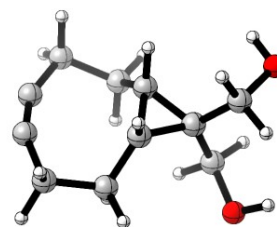
E(electronic) = -464.547800739
 Zero-point correction= 0.219994 (Hartree/Particle)
 Thermal correction to Energy= 0.230579
 Thermal correction to Enthalpy= 0.231524
 Thermal correction to Gibbs Free Energy= 0.184373
 Sum of electronic and zero-point Energies= -464.327806
 Sum of electronic and thermal Energies= -464.317221
 Sum of electronic and thermal Enthalpies= -464.316277
 Sum of electronic and thermal Free Energies= -464.363428



6	2.615455000	-0.248917000	-0.299021000	1	0.561709000	-2.692505000	0.712316000
6	2.391462000	0.935879000	-0.290778000	6	-0.172589000	-0.941622000	-0.272239000
6	2.277703000	-1.663640000	-0.117117000	6	-0.457328000	0.550914000	-0.265022000
1	2.241167000	-2.183432000	-1.078187000	6	-1.429429000	-0.414170000	0.366128000
1	3.000970000	-2.184912000	0.512658000	1	-0.773494000	0.924613000	-1.237471000
6	1.556193000	2.124476000	-0.094743000	1	-0.325313000	-1.394820000	-1.249286000
1	1.331450000	2.605687000	-1.050327000	6	-2.763594000	-0.645425000	-0.282945000
1	2.036191000	2.868082000	0.544106000	1	-2.630817000	-0.750466000	-1.365617000
6	0.259023000	1.596973000	0.568449000	1	-3.233989000	-1.555875000	0.093222000
1	0.513762000	1.184668000	1.548662000	8	-3.687973000	0.411225000	-0.005967000
1	-0.418978000	2.440004000	0.736412000	1	-3.281977000	1.235153000	-0.300725000
6	0.880760000	-1.657661000	0.552649000	1	-1.432884000	-0.418064000	1.453531000
1	0.970047000	-1.188779000	1.536271000				

DMBCN

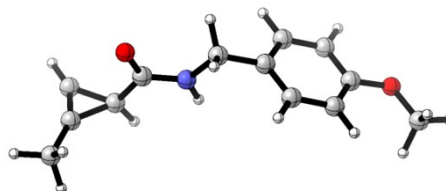
E(electronic) = -579.076111520
 Zero-point correction= 0.253182 (Hartree/Particle)
 Thermal correction to Energy= 0.266557
 Thermal correction to Enthalpy= 0.267501
 Thermal correction to Gibbs Free Energy= 0.214039
 Sum of electronic and zero-point Energies= -578.822929
 Sum of electronic and thermal Energies= -578.809555
 Sum of electronic and thermal Enthalpies= -578.808610
 Sum of electronic and thermal Free Energies= -578.862073



1	-2.217945000	-2.705200000	-0.240467000	6	1.161660000	-0.016940000	-0.156231000
6	-2.245897000	-1.930982000	0.530920000	6	-2.899741000	-0.717327000	0.030575000
1	-2.755639000	-2.349078000	1.400742000	1	-2.368814000	1.926785000	-1.724844000
6	-2.351997000	1.742195000	-0.647418000	6	-2.929827000	0.431730000	-0.333791000
1	-2.890369000	2.559401000	-0.164131000	6	2.297057000	-0.306338000	-1.103370000
6	-0.107481000	0.539905000	-0.762718000	1	2.958597000	0.562120000	-1.185999000
1	-0.071333000	0.624296000	-1.846614000	1	1.895597000	-0.532903000	-2.096004000
6	-0.061362000	-0.899407000	-0.277596000	8	3.035502000	-1.428557000	-0.608273000
1	0.019329000	-1.615041000	-1.093393000	1	3.816363000	-1.539926000	-1.160897000
6	-0.811516000	-1.481950000	0.908470000	6	1.599461000	0.466624000	1.202071000
1	-0.258736000	-2.346390000	1.289895000	1	2.331622000	-0.229881000	1.623197000
1	-0.892710000	-0.759256000	1.722454000	1	0.759137000	0.533053000	1.894372000
6	-0.892837000	1.675159000	-0.129263000	8	2.198609000	1.759040000	1.047558000
1	-0.396475000	2.623506000	-0.356882000	1	2.575432000	2.014804000	1.896313000
1	-0.922060000	1.573847000	0.958087000				

Me-Cp

E(electronic) = -709.455527595
 Zero-point correction= 0.255608 (Hartree/Particle)
 Thermal correction to Energy= 0.271618
 Thermal correction to Enthalpy= 0.272562
 Thermal correction to Gibbs Free Energy= 0.209385
 Sum of electronic and zero-point Energies= -709.199919
 Sum of electronic and thermal Energies= -709.183910
 Sum of electronic and thermal Enthalpies= -709.182966
 Sum of electronic and thermal Free Energies= -709.246142

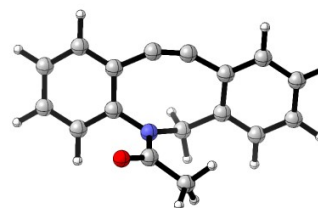


6	3.443615000	1.042506000	1.568636000	6	-2.887840000	-0.593508000	0.789615000
6	3.866294000	0.019793000	0.545662000	6	-3.288998000	0.304572000	-0.197058000
6	3.592004000	1.496245000	0.372910000	1	-0.560030000	0.180257000	-2.206232000
1	4.888397000	-0.354276000	0.521781000	1	-1.328036000	-1.905771000	1.453481000
1	1.594575000	-0.673054000	0.042251000	1	-2.777195000	1.280363000	-2.036121000
1	1.308676000	0.219840000	0.422327000	1	-3.526565000	-0.825950000	1.631098000
6	2.898183000	-0.991044000	0.018534000	8	-4.489752000	0.955144000	-0.195779000
1	3.215308000	1.163147000	2.614331000	6	-5.379550000	0.689749000	0.883726000
8	3.293379000	-2.079045000	-0.429998000	1	-5.655635000	-0.367156000	0.909130000
6	0.570614000	-1.583041000	-0.468633000	1	-4.931508000	0.978935000	1.837494000
1	0.589032000	-2.509238000	0.110500000	1	-6.264203000	1.294326000	0.697187000
1	0.808852000	-1.833990000	-1.505206000	6	3.580032000	2.543357000	-0.663691000

6	-0.787389000	-0.941049000	-0.382583000	1	4.576284000	2.640655000	-1.101412000
6	-1.208478000	-0.035659000	-1.362985000	1	2.893846000	2.261474000	-1.465955000
6	-1.638079000	-1.205456000	0.684757000	1	3.273682000	3.503046000	-0.247847000
6	-2.444067000	0.583023000	-1.276238000				

DBC0

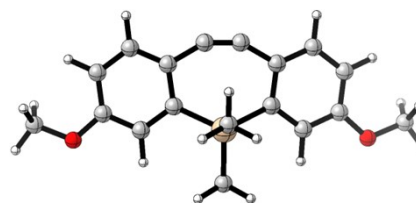
E(electronic) = -785.454988490
 Zero-point correction= 0.255483 (Hartree/Particle)
 Thermal correction to Energy= 0.270280
 Thermal correction to Enthalpy= 0.271224
 Thermal correction to Gibbs Free Energy= 0.213890
 Sum of electronic and zero-point Energies= -785.199505
 Sum of electronic and thermal Energies= -785.184709
 Sum of electronic and thermal Enthalpies= -785.183765
 Sum of electronic and thermal Free Energies= -785.241099



6	-1.971458000	-1.145629000	0.207815000	6	-4.290447000	0.236181000	-0.435113000
6	1.792373000	-1.242781000	0.156095000	1	3.029214000	-2.955540000	0.517995000
6	-0.564432000	0.434235000	-1.228045000	1	5.128262000	-1.787980000	-0.109279000
1	-0.747372000	1.282479000	-1.889697000	1	5.052649000	0.573954000	-0.857975000
6	-1.886987000	0.001713000	-0.615971000	1	2.889881000	1.778045000	-0.963071000
6	1.751150000	0.111099000	-0.254035000	1	-3.236625000	-2.470439000	1.327203000
6	-0.699393000	-1.730716000	0.484262000	1	-5.316051000	-1.239456000	0.748168000
6	0.507112000	-1.788699000	0.443861000	1	-5.194416000	0.778362000	-0.686177000
7	0.504523000	0.816595000	-0.272125000	1	-3.013455000	1.565793000	-1.545596000
6	2.927559000	0.747117000	-0.630458000	6	0.288344000	1.914257000	0.504594000
6	3.011291000	-1.919351000	0.203737000	8	-0.735271000	2.586287000	0.359309000
6	4.140343000	0.065639000	-0.570181000	6	1.309020000	2.271629000	1.552835000
6	4.182589000	-1.261525000	-0.151173000	1	2.099307000	2.878336000	1.105186000
6	-3.200366000	-1.590064000	0.697125000	1	0.807101000	2.864188000	2.315522000
6	-4.359826000	-0.897231000	0.371165000	1	1.765235000	1.390036000	2.002593000
6	-3.062182000	0.680288000	-0.920590000	1	-0.161353000	-0.381206000	-1.830004000

Si7HT

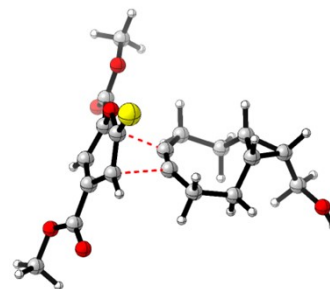
E(electronic) = -1136.51189229
 Zero-point correction= 0.312161 (Hartree/Particle)
 Thermal correction to Energy= 0.332556
 Thermal correction to Enthalpy= 0.333500
 Thermal correction to Gibbs Free Energy= 0.264269
 Sum of electronic and zero-point Energies= -1136.199731
 Sum of electronic and thermal Energies= -1136.179336
 Sum of electronic and thermal Enthalpies= -1136.178392
 Sum of electronic and thermal Free Energies= -1136.247624



6	1.838494000	1.387498000	0.146957000	6	-0.000059000	-0.671666000	2.563014000
6	-1.838401000	1.387323000	0.146816000	1	-0.001389000	0.376241000	2.876132000
14	0.000026000	-0.823109000	0.692606000	1	-0.886762000	-1.155291000	2.983998000
6	1.645759000	-0.023528000	0.115996000	1	0.887889000	-1.153021000	2.983977000
6	-1.645816000	-0.023734000	0.116018000	6	0.000044000	-2.624258000	0.188663000
6	0.605876000	2.095440000	0.328349000	1	-0.000014000	-2.748488000	-0.897860000
6	-0.605656000	2.094831000	0.328183000	1	0.880238000	-3.132690000	0.591945000
6	3.090344000	1.943626000	-0.083560000	1	-0.880180000	-3.132587000	0.592019000
1	3.216220000	3.019884000	-0.060647000	8	4.999508000	-1.135782000	-0.694019000
6	-3.090137000	1.943631000	-0.083884000	6	6.303145000	-0.617727000	-0.928405000
1	-3.215850000	3.019910000	-0.061179000	1	6.311656000	0.043096000	-1.799435000
6	-4.184415000	1.126629000	-0.363072000	1	6.673696000	-0.079082000	-0.052030000
1	-5.151951000	1.576906000	-0.540223000	1	6.937363000	-1.480532000	-1.120480000
6	-4.009093000	-0.255460000	-0.421151000	8	-4.999677000	-1.135665000	-0.693852000
6	-2.744357000	-0.818158000	-0.181181000	6	-6.303298000	-0.617553000	-0.928243000
1	-2.662776000	-1.899707000	-0.226784000	1	-6.673738000	-0.078703000	-0.051949000
6	4.184539000	1.126544000	-0.362851000	1	-6.311825000	0.043091000	-1.799407000
1	5.152156000	1.576708000	-0.539866000	1	-6.937597000	-1.480348000	-1.120090000
6	4.009029000	-0.255501000	-0.421176000	1	2.662529000	-1.899589000	-0.226941000
6	2.744224000	-0.818054000	-0.181255000				

TS-endo-BCN

E(electronic) = -1586.54208636
 Zero-point correction= 0.385289 (Hartree/Particle)
 Thermal correction to Energy= 0.411183
 Thermal correction to Enthalpy= 0.412127
 Thermal correction to Gibbs Free Energy= 0.328539
 Sum of electronic and zero-point Energies= -1586.156797
 Sum of electronic and thermal Energies= -1586.130904
 Sum of electronic and thermal Enthalpies= -1586.129959
 Sum of electronic and thermal Free Energies= -1586.213547

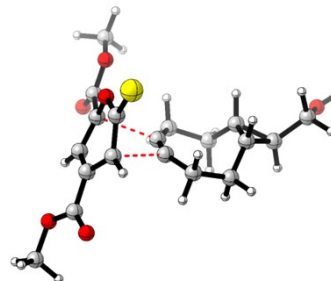


Frequency -339.0705

1	1.466248000	1.918726000	-0.824648000	6	-1.430545000	0.191019000	1.970684000
6	1.201099000	0.986263000	-1.335275000	16	-1.110952000	0.271815000	3.589491000
1	0.641894000	1.255117000	-2.235423000	6	-2.941811000	-2.242765000	-0.496937000
6	0.716698000	-2.220099000	0.634088000	8	-2.701709000	-3.333631000	-0.029184000
1	0.010538000	-3.013063000	0.376019000	8	-3.721961000	-2.043547000	-1.551087000
6	3.117574000	-1.433109000	0.299259000	6	-4.289967000	-3.222472000	-2.149143000
1	3.303258000	-1.318707000	1.364518000	1	-3.494765000	-3.877864000	-2.502610000
6	3.310792000	-0.161047000	-0.499386000	1	-4.912776000	-3.742479000	-1.422121000
1	3.617204000	0.693346000	0.099962000	1	-4.889773000	-2.865046000	-2.980931000
6	2.480648000	0.213040000	-1.707625000	1	-1.469524000	-1.954327000	1.732995000
1	3.077421000	0.845433000	-2.372156000	6	-1.549099000	2.569580000	-0.788454000
1	2.206103000	-0.680116000	-2.274358000	8	-1.776363000	2.696733000	-1.968803000
6	2.081441000	-2.486861000	-0.025587000	8	-1.112387000	3.526245000	0.008530000
1	2.439774000	-3.461072000	0.321162000	6	-0.871257000	4.801887000	-0.616628000
1	1.944553000	-2.563895000	-1.107221000	1	-0.117361000	4.690919000	-1.395652000
6	4.331074000	-1.265350000	-0.575233000	1	-1.798739000	5.187130000	-1.038045000
6	0.376455000	0.141373000	-0.450758000	1	-0.511831000	5.448535000	0.178002000
1	0.812516000	-2.214429000	1.724863000	1	-2.790510000	0.309166000	-1.668201000
6	0.208363000	-0.909272000	0.176687000	1	5.371448000	0.483906000	0.590298000
6	-1.478332000	1.446268000	0.085460000	6	5.171053000	-0.875707000	-1.087684000
6	-1.842029000	-0.929883000	1.142442000	1	5.849348000	-0.287786000	-1.714591000
6	-2.428663000	0.654957000	-0.528478000	1	4.389262000	-1.286675000	-1.729957000
6	-2.644557000	-0.584786000	0.056138000	8	5.897528000	-1.945812000	-0.468380000
8	-1.238922000	1.327276000	1.429388000	1	6.343657000	-2.445402000	-1.160865000

TS-exo-BCN

E(electronic) = -1586.54165981
 Zero-point correction= 0.385310 (Hartree/Particle)
 Thermal correction to Energy= 0.411204
 Thermal correction to Enthalpy= 0.412149
 Thermal correction to Gibbs Free Energy= 0.328567
 Sum of electronic and zero-point Energies= -1586.156349
 Sum of electronic and thermal Energies= -1586.130455
 Sum of electronic and thermal Enthalpies= -1586.129511
 Sum of electronic and thermal Free Energies= -1586.213093

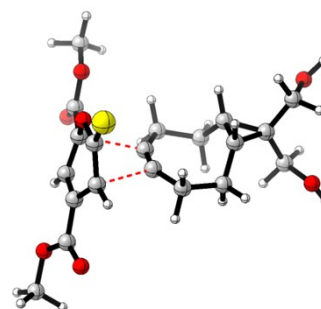


Frequency -339.0674

1	1.466206000	1.919781000	-0.821772000	16	-0.924368000	-0.060659000	3.591827000
6	1.201567000	0.987997000	-1.333925000	6	-3.495075000	-1.632185000	-0.568323000
1	0.642876000	1.258018000	-2.234043000	8	-3.494558000	-2.792192000	-0.220535000
6	0.717218000	-2.220128000	0.632608000	8	-4.250927000	-1.151762000	-1.546838000
1	0.011221000	-3.013092000	0.374043000	6	-5.101276000	-2.101419000	-2.214089000
6	3.117941000	-1.432552000	0.298894000	1	-4.495309000	-2.881001000	-2.674405000
1	3.303179000	-1.319057000	1.364324000	1	-5.799541000	-2.537646000	-1.500663000
6	3.311274000	-0.159702000	-0.498434000	1	-5.632808000	-1.532543000	-2.971189000
1	3.617392000	0.694107000	0.101867000	1	-1.875603000	-1.929252000	1.557100000
6	2.481561000	0.215619000	-1.706567000	6	-1.068020000	2.759626000	-0.487866000
1	3.078569000	0.848918000	-2.370012000	8	-1.329823000	3.072183000	-1.625715000
1	2.207513000	-0.676856000	-2.274613000	8	-0.374166000	3.494220000	0.360942000
6	2.082056000	-2.486180000	-0.027108000	6	0.119749000	4.746630000	-0.152653000
1	2.440523000	-3.460657000	0.318766000	1	0.779541000	4.559709000	-0.999590000
1	1.945326000	-2.562284000	-1.108841000	1	-0.716018000	5.376630000	-0.454104000
6	4.331667000	-1.263772000	-0.575074000	1	0.666076000	5.199557000	0.668975000
6	0.376668000	0.141842000	-0.450913000	1	-2.837572000	0.941681000	-1.487207000
1	0.812981000	-2.215031000	1.723394000	6	5.677806000	-1.073049000	0.053941000
6	0.208653000	-0.909114000	0.175981000	1	6.162126000	-2.038848000	0.231739000
6	-1.479310000	1.446004000	0.085300000	1	5.563699000	-0.561276000	1.015728000
6	-1.840689000	-0.930358000	1.142402000	1	4.325376000	-1.843422000	-1.494881000
6	-2.429108000	0.653890000	-0.528359000	8	6.487955000	-0.284303000	-0.825434000
6	-2.643829000	-0.586044000	0.056345000	1	7.366676000	-0.209532000	-0.437916000
8	-1.239260000	1.327339000	1.429109000	6	-1.341573000	0.114354000	2.003143000

TS-DMBCN

E(electronic) = -1701.07136215
Zero-point correction= 0.419008 (Hartree/Particle)
Thermal correction to Energy= 0.447443
Thermal correction to Enthalpy= 0.448387
Thermal correction to Gibbs Free Energy= 0.359138
Sum of electronic and zero-point Energies= -1700.652355
Sum of electronic and thermal Energies= -1700.623919
Sum of electronic and thermal Enthalpies= -1700.622975
Sum of electronic and thermal Free Energies= -1700.712224

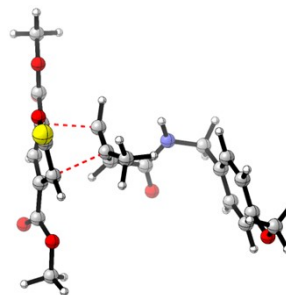


Frequency -339.1906

1	0.834132000	2.138122000	-0.982706000	6	-3.577316000	-2.039828000	-0.442125000
6	0.725369000	1.117508000	-1.365788000	8	-3.430262000	-3.139434000	0.043407000
1	0.175962000	1.179575000	-2.308878000	8	-4.338896000	-1.792330000	-1.499513000
6	0.609103000	-1.838558000	1.012979000	6	-5.004592000	-2.928694000	-2.079022000
1	0.043382000	-2.757015000	0.838876000	1	-4.267496000	-3.653215000	-2.423338000
6	2.867816000	-0.732856000	0.665155000	1	-5.667090000	-3.383962000	-1.343756000
1	2.920081000	-0.436641000	1.710209000	1	-5.574195000	-2.535109000	-2.915690000
6	2.916675000	0.424693000	-0.310890000	1	-2.060151000	-1.847743000	1.768954000
1	3.016217000	1.398443000	0.163789000	6	-1.794289000	2.638199000	-0.804398000
6	2.113873000	0.489122000	-1.594396000	8	-2.033841000	2.776352000	-1.980974000
1	2.648422000	1.098294000	-2.329601000	8	-1.254718000	3.556898000	-0.025714000
1	1.973158000	-0.500376000	-2.032598000	6	-0.909084000	4.799298000	-0.668512000
6	2.036276000	-1.980944000	0.452545000	1	-0.184036000	4.612449000	-1.460275000
1	2.514070000	-2.825766000	0.957450000	1	-1.805067000	5.265106000	-1.076566000
1	1.968635000	-2.237318000	-0.606721000	1	-0.475881000	5.416719000	0.112427000
6	4.129265000	-0.458805000	-0.120967000	1	-3.232395000	0.478912000	-1.644601000
6	-0.012327000	0.284784000	-0.395792000	6	5.275414000	0.148424000	0.647291000
1	0.636092000	-1.674525000	2.095195000	1	5.925912000	-0.632950000	1.058324000
6	-0.056576000	-0.691972000	0.359101000	1	4.885038000	0.738387000	1.482475000
6	-2.052290000	1.354301000	-0.091015000	6	4.548801000	-1.412415000	-1.216847000
6	-2.14223000	-0.909435000	1.236240000	1	3.702373000	-1.714882000	-1.829721000
6	-2.845589000	0.366746000	-0.641147000	1	5.276831000	-0.925226000	-1.872929000
6	-2.919316000	-0.814580000	0.082993000	8	6.028107000	0.985522000	-0.235548000
8	-1.878262000	1.429519000	1.265724000	1	6.807497000	1.297925000	0.236265000
6	-1.843092000	0.289047000	1.980502000	8	5.104156000	-2.625840000	-0.699162000
16	-1.498865000	0.360979000	3.594760000	1	5.954694000	-2.424580000	-0.293925000

TS-Me-Cp

E(electronic) = -1831.44501715
Zero-point correction= 0.422106 (Hartree/Particle)
Thermal correction to Energy= 0.452672
Thermal correction to Enthalpy= 0.453616
Thermal correction to Gibbs Free Energy= 0.356590
Sum of electronic and zero-point Energies= -1831.022911
Sum of electronic and thermal Energies= -1830.992345
Sum of electronic and thermal Enthalpies= -1830.991401
Sum of electronic and thermal Free Energies= -1831.088427



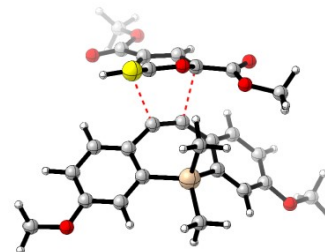
Frequency -386.0312

6	0.996277000	-1.082111000	-0.449343000	6	2.605963000	2.907695000	-0.396150000
6	0.500594000	0.041584000	-1.290105000	8	3.396489000	3.237873000	-1.250070000
6	0.246245000	-0.161953000	0.176346000	8	1.657577000	3.694105000	0.088503000
1	1.195919000	0.821745000	-1.609256000	6	1.590973000	5.021115000	-0.465836000
7	-1.360035000	-1.243156000	-2.169149000	1	2.526688000	5.546291000	-0.277676000
1	-1.120750000	-1.884960000	-1.421848000	1	1.397082000	4.963933000	-1.536313000
6	-0.669464000	-0.085181000	-2.220119000	1	0.767366000	5.508061000	0.047536000
6	3.132618000	-0.732810000	0.163761000	6	-3.695008000	-0.859253000	-1.576541000
6	1.763144000	1.223217000	1.288660000	6	-4.019046000	0.496454000	-1.449715000
6	3.313077000	0.523678000	-0.379803000	6	-4.178961000	-1.749056000	-0.623019000
6	2.599214000	1.550549000	0.225076000	6	-4.796950000	0.944438000	-0.394421000
8	2.827022000	-0.875414000	1.492872000	6	-4.964375000	-1.317038000	0.446024000
6	2.097150000	0.080000000	2.104040000	6	-5.268107000	0.038459000	0.560491000
1	1.121636000	-2.153515000	-0.520218000	1	-3.655378000	1.206291000	-2.184997000
8	-0.972439000	0.848412000	-2.966642000	1	-3.936886000	-2.804161000	-0.705308000
16	1.682186000	-0.123628000	3.687940000	1	-5.053143000	1.992739000	-0.292570000
1	1.104208000	1.958949000	1.728888000	1	-5.326073000	-2.036661000	1.168238000
6	-2.743070000	-1.330217000	-2.648427000	8	-6.025369000	0.570052000	1.565664000
1	-2.940790000	-2.368603000	-2.911924000	6	-6.521900000	-0.323682000	2.556537000
1	-2.827037000	-0.723784000	-3.548400000	1	-7.182096000	-1.071550000	2.110468000

6	3.766658000	-1.938587000	-0.450362000	1	-5.700746000	-0.818945000	3.080435000
8	4.193889000	-1.927070000	-1.580164000	1	-7.084980000	0.289255000	3.256726000
8	3.769695000	-2.980898000	0.356851000	6	-0.922877000	0.011051000	1.081738000
6	4.334843000	-4.192584000	-0.182502000	1	-1.108210000	1.062771000	1.300382000
1	3.771169000	-4.499706000	-1.062516000	1	-1.805970000	-0.391807000	0.571684000
1	5.380368000	-4.027215000	-0.438898000	1	-0.782569000	-0.538006000	2.012857000
1	4.244736000	-4.929230000	0.609904000	1	3.843828000	0.647145000	-1.314291000

TS-Si7HT

E(electronic) = -2258.51522839
 Zero-point correction= 0.477852 (Hartree/Particle)
 Thermal correction to Energy= 0.513490
 Thermal correction to Enthalpy= 0.514434
 Thermal correction to Gibbs Free Energy= 0.410279
 Sum of electronic and zero-point Energies= -2258.037376
 Sum of electronic and thermal Energies= -2258.001738
 Sum of electronic and thermal Enthalpies= -2258.000794
 Sum of electronic and thermal Free Energies= -2258.104949

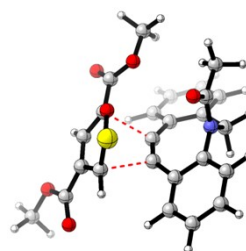


Frequency -327.0985

6	1.639036000	-0.290682000	-0.626998000	1	2.637200000	1.358128000	-1.576925000
6	-1.861947000	-0.784513000	-0.372406000	6	-3.151735000	-0.547747000	-0.841903000
14	0.272200000	-2.471575000	0.701776000	1	-3.456441000	0.459065000	-1.104013000
6	1.686910000	-1.667157000	-0.286288000	6	-4.054340000	-1.593362000	-1.006999000
6	-1.444796000	-2.104583000	-0.047651000	1	-5.048502000	-1.382966000	-1.378098000
6	0.398078000	0.374999000	-0.309352000	6	-3.655775000	-2.894834000	-0.698118000
6	-0.833422000	0.222955000	-0.265306000	6	-2.357652000	-3.137214000	-0.225927000
6	0.799119000	2.227921000	1.016593000	1	-2.094275000	-4.165400000	0.002136000
6	-1.797266000	2.190729000	0.565139000	6	3.829344000	-0.424248000	-1.644809000
6	0.330356000	3.149617000	0.100267000	1	4.639095000	0.062956000	-2.171343000
6	-1.042823000	3.143977000	-0.111437000	6	3.893968000	-1.776835000	-1.307634000
8	0.004043000	1.783640000	2.027092000	6	2.820863000	-2.387068000	-0.640764000
6	-1.326881000	1.686912000	1.829663000	1	2.909264000	-3.444202000	-0.409477000
16	-2.271611000	1.057316000	3.028129000	6	0.336668000	-1.784806000	2.443199000
6	-1.695045000	3.938620000	-1.191931000	1	0.270878000	-0.694396000	2.454151000
8	-2.841683000	3.786343000	-1.532174000	1	-0.483286000	-2.188182000	3.045162000
8	-0.864459000	4.824842000	-1.727459000	1	1.281996000	-2.072981000	2.914616000
6	-1.404376000	5.638512000	-2.781702000	6	0.531800000	-4.323300000	0.723984000
1	-1.721514000	5.010389000	-3.614107000	1	0.502338000	-4.757616000	-0.279184000
1	-2.248123000	6.219967000	-2.410195000	1	1.501260000	-4.561183000	1.171576000
1	-0.594307000	6.295064000	-3.087336000	1	-0.236316000	-4.810370000	1.331526000
1	-2.850595000	2.071104000	0.351250000	8	4.946832000	-2.579145000	-1.585872000
6	2.260835000	2.011974000	1.268296000	6	6.064041000	-2.003333000	-2.252166000
8	3.113033000	2.658853000	0.717284000	1	5.780295000	-1.625959000	-3.238278000
8	2.466936000	1.010995000	2.101684000	1	6.499730000	-1.195354000	-1.658202000
6	3.835673000	0.602854000	2.267834000	1	6.790525000	-2.805279000	-2.364913000
1	4.242990000	0.290356000	1.304735000	8	-4.450312000	-3.981371000	-0.819330000
1	4.425932000	1.421720000	2.678748000	6	-5.779312000	-3.786465000	-1.288764000
1	3.807263000	-0.233361000	2.961020000	1	-6.341279000	-3.136243000	-0.613038000
1	1.027879000	3.707485000	-0.509800000	1	-5.780038000	-3.362755000	-2.296600000
6	2.697757000	0.311260000	-1.301429000	1	-6.236590000	-4.773352000	-1.308482000

TS-DMBCO

E(electronic) = -1907.44003686
 Zero-point correction= 0.420677 (Hartree/Particle)
 Thermal correction to Energy= 0.450720
 Thermal correction to Enthalpy= 0.451664
 Thermal correction to Gibbs Free Energy= 0.358939
 Sum of electronic and zero-point Energies= -1907.019360
 Sum of electronic and thermal Energies= -1906.989317
 Sum of electronic and thermal Enthalpies= -1906.988372
 Sum of electronic and thermal Free Energies= -1907.081097



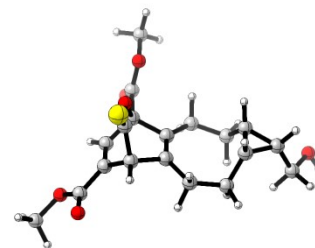
Frequency -413.6878

6	-0.934667000	-1.445799000	-1.182872000	1	-1.693816000	5.667777000	-1.283936000
6	-0.164205000	2.124327000	-0.924051000	1	-3.143975000	3.747054000	-0.669685000
6	-2.764502000	0.330708000	-1.554811000	1	0.544915000	-3.004955000	-1.167655000
1	-3.851430000	0.312367000	-1.656705000	1	-0.988645000	-4.745800000	-2.003511000
6	-2.257365000	-1.099093000	-1.524263000	1	-3.361681000	-4.172498000	-2.484597000
6	-1.543933000	2.330803000	-0.720767000	1	-4.141585000	-1.844259000	-2.209499000
6	-0.062671000	-0.411434000	-0.664841000	6	-2.884836000	1.048721000	0.822359000
6	0.308513000	0.779372000	-0.695911000	8	-2.563953000	1.807228000	1.738305000
6	0.959376000	-1.220362000	1.161597000	6	-3.846419000	-0.087815000	1.038706000

6	2.169965000	1.006361000	0.527692000	1	-4.752657000	0.075719000	0.449261000
1	2.581247000	1.953267000	0.206273000	1	-3.414917000	-1.040672000	0.729772000
6	2.211966000	-1.365723000	0.575269000	1	-4.102172000	-0.126096000	2.095078000
1	2.549715000	-2.342087000	0.253867000	1	-2.373366000	0.806119000	-2.456388000
6	2.854490000	-0.183845000	0.258870000	6	0.094815000	-2.394764000	1.512545000
8	0.691340000	-0.137125000	1.955426000	8	0.469532000	-3.535273000	1.395134000
6	1.294695000	1.039377000	1.675379000	8	-1.101793000	-2.017963000	1.917078000
16	1.032201000	2.342165000	2.644783000	6	-2.046150000	-3.081171000	-2.154591000
7	-2.399457000	1.217654000	-0.438393000	1	-1.637416000	-3.786947000	2.876101000
6	-2.083229000	3.605195000	-0.841824000	1	-2.934299000	-2.598184000	2.550635000
6	0.640841000	3.206333000	-1.292941000	1	-2.263960000	-3.582551000	1.209559000
6	-1.267411000	4.676415000	-1.189605000	6	4.096030000	-0.131661000	-0.556121000
6	0.089572000	4.472372000	-1.430869000	8	4.523663000	0.884425000	-1.057050000
6	-0.488318000	-2.757004000	-1.379539000	8	4.676817000	-1.318196000	-0.670649000
6	-1.350612000	-3.735432000	-1.856550000	6	5.888257000	-1.357052000	-1.446656000
6	-3.114751000	-2.101855000	-1.971131000	1	5.682829000	-1.042827000	-2.469332000
6	-2.674814000	-3.412189000	-2.132375000	1	6.637162000	-0.707512000	-0.994904000
1	1.696970000	3.049301000	-1.476379000	1	6.214583000	-2.392467000	-1.422327000
1	0.720800000	5.303558000	-1.720638000				

PROD-endo-BCN

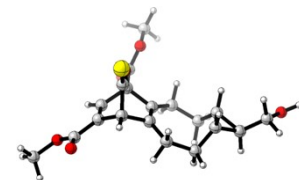
E(electronic) = -1586.61197020
 Zero-point correction= 0.390662 (Hartree/Particle)
 Thermal correction to Energy= 0.415501
 Thermal correction to Enthalpy= 0.416445
 Thermal correction to Gibbs Free Energy= 0.334718
 Sum of electronic and zero-point Energies= -1586.221308
 Sum of electronic and thermal Energies= -1586.196469
 Sum of electronic and thermal Enthalpies= -1586.195525
 Sum of electronic and thermal Free Energies= -1586.277253



1	1.607106000	2.021057000	-0.351985000	16	-1.869625000	-0.218494000	3.366334000
6	1.485045000	1.077927000	-0.900669000	1	5.302925000	-0.637326000	1.271389000
1	1.151254000	1.364298000	-1.904400000	6	-3.396726000	-1.604635000	-0.777495000
6	0.890243000	-2.136070000	0.543967000	8	-3.613941000	-2.663779000	-0.230628000
1	0.342313000	-2.947845000	0.051144000	8	-4.106798000	-1.141661000	-1.800748000
6	3.216087000	-1.252213000	0.937803000	6	-5.190852000	-1.976198000	-2.245054000
1	3.082188000	-1.275052000	2.014969000	1	-4.806176000	-2.939271000	-2.578976000
6	3.455078000	0.103609000	0.330245000	1	-5.906921000	-2.116221000	-1.435939000
1	3.467728000	0.942132000	1.019840000	1	-5.648538000	-1.440741000	-3.071687000
6	2.862341000	0.435732000	-1.017702000	1	-1.539690000	-2.046419000	1.144419000
1	3.502733000	1.163353000	-1.525648000	6	-0.779436000	2.651181000	-0.576427000
1	2.816195000	-0.435026000	-1.671249000	8	-0.914560000	2.980228000	-1.729357000
6	2.369277000	-2.266205000	0.206796000	8	-0.444263000	3.459488000	0.408037000
1	2.672648000	-3.274325000	0.506578000	6	-0.190367000	4.829468000	0.036828000
1	2.508212000	-2.217904000	-0.872495000	1	0.643878000	4.867911000	-0.663212000
6	4.601142000	-0.868479000	0.476816000	1	-1.083768000	5.261436000	-0.4111709000
6	0.335323000	0.341374000	-0.255345000	1	0.059839000	5.337358000	0.963221000
1	0.758969000	-2.318651000	1.619027000	1	-2.616238000	1.017596000	-1.675991000
6	0.108902000	-0.877085000	0.253206000	6	5.253934000	-1.500923000	-0.717960000
6	-0.957397000	1.206883000	-0.135863000	1	5.826591000	-2.380772000	-0.406776000
6	-1.355871000	-1.060705000	0.732507000	1	4.522814000	-1.821247000	-1.462987000
6	-2.081268000	0.524698000	-0.875827000	8	6.139388000	-0.534050000	-1.299167000
6	-2.310421000	-0.685169000	-0.375821000	1	6.605655000	-0.956752000	-2.028377000
8	-1.325978000	1.224739000	1.283405000	6	-1.519449000	0.011577000	1.786189000

PROD-exo-BCN

E(electronic) = -1586.61595316
 Zero-point correction= 0.390397 (Hartree/Particle)
 Thermal correction to Energy= 0.415168
 Thermal correction to Enthalpy= 0.416112
 Thermal correction to Gibbs Free Energy= 0.334912
 Sum of electronic and zero-point Energies= -1586.225556
 Sum of electronic and thermal Energies= -1586.200785
 Sum of electronic and thermal Enthalpies= -1586.199841
 Sum of electronic and thermal Free Energies= -1586.281041



1	1.375338000	2.171598000	-0.648814000	6	-1.227125000	-0.227976000	1.808848000
6	1.176119000	1.279510000	-1.256755000	16	-1.268030000	-0.650168000	3.387800000
1	0.641783000	1.641992000	-2.142503000	6	-3.492442000	-1.647722000	-0.553730000
6	0.983488000	-2.085899000	-0.081338000	8	-3.571447000	-2.770870000	-0.105910000
1	0.391730000	-2.872149000	-0.564928000	8	-4.388183000	-1.116111000	-1.378682000
6	3.320674000	-1.107339000	-0.017504000	6	-5.498943000	-1.958777000	-1.732342000
1	3.435979000	-1.221941000	1.057853000	1	-5.139692000	-2.853633000	-2.239468000

6	3.390460000	0.301438000	-0.541892000	1	-6.058091000	-2.230988000	-0.837753000
1	3.549309000	1.077276000	0.202459000	1	-6.113653000	-1.362299000	-2.400119000
6	2.520924000	0.719098000	-1.701208000	1	-1.301040000	-2.199829000	0.938547000
1	3.023483000	1.515967000	-2.257797000	6	-1.018266000	2.695829000	-0.312619000
1	2.382052000	-0.101485000	-2.406077000	8	-1.390094000	3.152018000	-1.365804000
6	2.389720000	-2.100616000	-0.664857000	8	-0.504527000	3.396397000	0.677650000
1	2.780793000	-3.111172000	-0.509941000	6	-0.354065000	4.809829000	0.435301000
1	2.358190000	-1.953856000	-1.745038000	1	0.314853000	4.964783000	-0.410811000
6	4.546974000	-0.635816000	-0.756367000	1	-1.327800000	5.255505000	0.237271000
6	0.199974000	0.425284000	-0.484876000	1	0.076393000	5.214096000	1.346287000
1	1.043476000	-2.388009000	0.972911000	1	-2.981444000	1.098092000	-1.253609000
6	0.115201000	-0.850835000	-0.087344000	6	5.817478000	-0.425683000	0.016025000
6	-1.072194000	1.203295000	-0.026925000	1	5.593460000	0.086040000	0.958729000
6	-1.229035000	-1.165397000	0.622512000	1	6.523254000	0.188776000	-0.545926000
6	-2.291524000	0.549273000	-0.627239000	1	4.668421000	-1.021589000	-1.765363000
6	-2.384079000	-0.719592000	-0.242337000	8	6.499362000	-1.655360000	0.280277000
8	-1.169562000	1.042220000	1.427452000	1	5.887257000	-2.228256000	0.757285000

PROD-DMBCN

E(electronic) = -1701.14627047

Zero-point correction= 0.424682 (Hartree/Particle)

Thermal correction to Energy= 0.451670

Thermal correction to Enthalpy= 0.452614

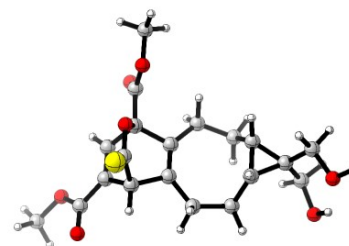
Thermal correction to Gibbs Free Energy= 0.366831

Sum of electronic and zero-point Energies= -1700.721588

Sum of electronic and thermal Energies= -1700.694600

Sum of electronic and thermal Enthalpies= -1700.693656

Sum of electronic and thermal Free Energies= -1700.779440



1	0.818602000	2.318641000	-0.699283000	6	-3.672226000	-1.947347000	-0.496588000
6	0.732878000	1.355512000	-1.219244000	8	-3.673392000	-3.019459000	0.067974000
1	0.231100000	1.575674000	-2.168394000	8	-4.550620000	-1.603592000	-1.432352000
6	0.769624000	-1.870314000	0.315823000	6	-5.541544000	-2.593069000	-1.760967000
1	0.289470000	-2.757436000	-0.113564000	1	-5.057069000	-3.491881000	-2.141138000
6	2.980953000	-0.658643000	0.426200000	1	-6.136551000	-2.829714000	-0.879528000
1	2.984303000	-0.638263000	1.513040000	1	-6.160477000	-2.138990000	-2.529271000
6	2.951604000	0.679747000	-0.262036000	1	-1.562631000	-2.104398000	1.191653000
1	2.940278000	1.552029000	0.386667000	6	-1.654567000	2.630719000	-0.590276000
6	2.140952000	0.861292000	-1.522948000	8	-1.983339000	2.927827000	-1.712482000
1	2.614626000	1.615653000	-2.158336000	8	-1.292799000	3.485133000	0.344657000
1	2.087146000	-0.051423000	-2.115043000	6	-1.268375000	4.872239000	-0.048343000
6	2.214804000	-1.815521000	-0.164987000	1	-0.550537000	5.008802000	-0.856658000
1	2.680945000	-2.754304000	0.148822000	1	-2.262835000	5.182461000	-0.365909000
1	2.251865000	-1.811052000	-1.254238000	1	-0.959584000	5.417423000	0.838304000
6	4.234892000	-0.115101000	-0.221008000	1	-3.376924000	0.748714000	-1.467450000
6	-0.214443000	0.494638000	-0.419681000	6	5.293741000	0.408743000	0.713364000
1	0.774677000	-2.050731000	1.399270000	1	4.831153000	0.874946000	1.588772000
6	-0.205839000	-0.734520000	0.112738000	1	5.911405000	1.154908000	0.201809000
6	-1.586017000	1.180877000	-0.138499000	6	4.798619000	-0.759415000	-1.467547000
6	-1.564770000	-1.108108000	0.764486000	1	4.043557000	-0.896716000	-2.239637000
6	-2.687802000	0.343786000	-0.739030000	1	5.580932000	-0.110066000	-1.879304000
6	-2.687247000	-0.879646000	-0.219692000	8	6.120405000	-0.691576000	1.123161000
8	-1.778804000	1.167522000	1.314798000	1	6.901614000	-0.342542000	1.565894000
6	-1.745931000	-0.054068000	1.833474000	8	5.341839000	-2.058276000	-1.206344000
16	-1.873966000	-0.307490000	3.443346000	1	5.906252000	-1.963333000	-0.426736000

PROD-Me-Cp

E(electronic) = -1831.53004728

Zero-point correction= 0.427463 (Hartree/Particle)

Thermal correction to Energy= 0.457015

Thermal correction to Enthalpy= 0.457959

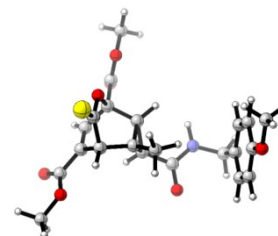
Thermal correction to Gibbs Free Energy= 0.362456

Sum of electronic and zero-point Energies= -1831.102585

Sum of electronic and thermal Energies= -1831.073033

Sum of electronic and thermal Enthalpies= -1831.072089

Sum of electronic and thermal Free Energies= -1831.167591

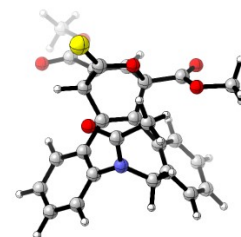


6	-0.688329000	0.837465000	-0.432158000	6	-3.951282000	-1.905572000	-0.376134000
6	-0.529998000	-0.335024000	-1.357268000	8	-4.940140000	-1.755137000	-1.058776000
6	-0.509743000	-0.543041000	0.134964000	8	-3.577109000	-3.068959000	0.139529000
1	-1.390862000	-0.684181000	-1.915014000	6	-4.424166000	-4.193806000	-0.156627000
7	1.499441000	0.447673000	-2.459251000	1	-5.425728000	-4.014988000	0.232903000
1	1.206024000	1.369330000	-2.164601000	1	-4.461000000	-4.355233000	-1.233384000
6	0.762648000	-0.604867000	-2.073318000	1	-3.964649000	-5.041864000	0.342292000
6	-2.085053000	1.354235000	-0.049308000	6	3.761502000	-0.008836000	-1.640601000

6	-1.812158000	-0.972929000	0.865084000	6	4.217413000	-1.301433000	-1.370920000
6	-3.156587000	0.420058000	-0.533656000	6	4.042118000	0.999121000	-0.721661000
6	-3.014439000	-0.806015000	-0.033532000	6	4.927969000	-1.578161000	-0.212143000
8	-2.106614000	1.323172000	1.414756000	6	4.752683000	0.741293000	0.448650000
6	-1.976854000	0.098527000	1.932530000	6	5.192649000	-0.557932000	0.703944000
1	0.110353000	1.561943000	-0.309118000	1	4.008923000	-2.100472000	-2.074390000
8	1.098993000	-1.771674000	-2.289413000	1	3.694745000	2.010001000	-0.913783000
16	-1.987580000	-0.135541000	3.547141000	1	5.282651000	-2.579832000	0.001594000
1	-1.727784000	-1.957494000	1.312699000	1	4.954161000	1.548029000	1.140418000
6	2.902505000	0.284460000	-2.848153000	8	5.893788000	-0.920061000	1.819454000
1	3.210363000	1.210883000	-3.331328000	6	6.170693000	0.094948000	2.778857000
1	2.972247000	-0.522564000	-3.576664000	1	6.784998000	0.886345000	2.342429000
6	-2.273793000	2.785612000	-0.514733000	1	5.244762000	0.519802000	3.174225000
8	-2.659200000	3.032076000	-1.631607000	1	6.719988000	-0.393465000	3.580543000
8	-1.916401000	3.678386000	0.383564000	6	0.769729000	-0.929837000	0.839541000
6	-2.004002000	5.058476000	-0.028406000	1	0.907627000	-2.013312000	0.805826000
1	-1.347483000	5.228189000	-0.880673000	1	1.636952000	-0.456149000	0.371422000
1	-3.034304000	5.298327000	-0.287122000	1	0.739957000	-0.616638000	1.885970000
1	-1.678281000	5.636154000	0.831111000	1	-3.926039000	0.739251000	-1.224635000

PROD-DBCO

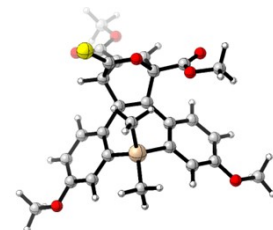
E(electronic) = -1907.52569243
 Zero-point correction= 0.424917 (Hartree/Particle)
 Thermal correction to Energy= 0.454278
 Thermal correction to Enthalpy= 0.455222
 Thermal correction to Gibbs Free Energy= 0.363693
 Sum of electronic and zero-point Energies= -1907.100776
 Sum of electronic and thermal Energies= -1907.071415
 Sum of electronic and thermal Enthalpies= -1907.070471
 Sum of electronic and thermal Free Energies= -1907.162000



6	-1.449176000	-0.872228000	-1.055277000	1	-2.113531000	5.341947000	-1.692521000
6	-0.363133000	2.067550000	-0.582123000	1	-3.297544000	3.742420000	-0.203942000
6	-3.311234000	0.561591000	0.095737000	1	-0.128638000	-2.151720000	-2.182070000
1	-3.861143000	0.031969000	0.872814000	1	-1.875407000	-3.111686000	-3.602658000
6	-2.776615000	-0.438998000	-0.914456000	1	-4.242560000	-2.361673000	-3.326093000
6	-1.664079000	2.361464000	-0.150963000	1	-4.779598000	-0.650941000	-1.636207000
6	-0.265930000	-0.414320000	-0.276082000	6	-1.838154000	1.260572000	1.975444000
6	0.273265000	0.805158000	-0.176017000	8	-0.999139000	2.035737000	2.433400000
6	0.674882000	-1.459237000	0.349408000	6	-2.344956000	0.092132000	2.776434000
6	1.681388000	0.811254000	0.424806000	1	-3.391626000	0.240428000	3.052390000
1	2.124068000	1.799036000	0.488785000	1	-2.268405000	-0.835520000	2.205271000
6	1.998892000	-1.414971000	-0.379056000	1	-1.743763000	0.018943000	3.680313000
1	2.414995000	-2.296097000	-0.848636000	1	-4.040579000	1.193836000	-0.416730000
6	2.539102000	-0.200865000	-0.320910000	6	0.069027000	-2.851213000	0.485598000
8	0.939482000	-1.014872000	1.728722000	8	0.499252000	-3.823670000	-0.080211000
6	1.546635000	0.169649000	1.798890000	8	-0.983599000	-2.829612000	1.275918000
16	2.121846000	0.754801000	3.206172000	6	-1.701566000	-4.071612000	1.415444000
7	-2.332267000	1.437569000	0.716854000	1	-1.047427000	-4.830523000	1.842300000
6	-2.291782000	3.533554000	-0.550390000	1	-2.527636000	-3.853241000	2.085661000
6	0.312713000	2.990118000	-1.382215000	1	-2.068220000	-4.387838000	0.438821000
6	-1.621636000	4.428943000	-1.379264000	6	3.858955000	0.198252000	-0.857349000
6	-0.317969000	4.161300000	-1.787470000	8	4.324436000	1.308397000	-0.723600000
6	-1.157262000	-1.836432000	-2.038845000	8	4.467105000	-0.789247000	-1.503780000
6	-2.139330000	-2.376524000	-2.852174000	6	5.753965000	-0.476758000	-2.066343000
6	-3.755562000	-0.993109000	-1.748934000	1	5.655138000	0.327603000	-2.794501000
6	-3.457325000	-1.954297000	-2.700493000	1	6.443888000	-0.186667000	-1.274688000
1	1.328538000	2.775968000	-1.698657000	1	6.088342000	-1.390351000	-2.549074000
1	0.208445000	4.864650000	-2.421285000				

PROD-Si7HT

E(electronic) = -2258.58744853
 Zero-point correction= 0.481917 (Hartree/Particle)
 Thermal correction to Energy= 0.516785
 Thermal correction to Enthalpy= 0.517730
 Thermal correction to Gibbs Free Energy= 0.414976
 Sum of electronic and zero-point Energies= -2258.105532
 Sum of electronic and thermal Energies= -2258.070663
 Sum of electronic and thermal Enthalpies= -2258.069719
 Sum of electronic and thermal Free Energies= -2258.172473



6	-1.445641000	-0.611527000	-0.485704000	1	-1.224470000	-2.174017000	-1.952599000
6	0.780562000	1.707981000	-0.135225000	6	1.781310000	2.390627000	-0.832418000
14	-1.702761000	1.571655000	1.347912000	1	2.620036000	1.842266000	-1.249766000

6	-2.338793000	0.313357000	0.096411000	6	1.722716000	3.764822000	-1.032867000
6	-0.305578000	2.432807000	0.407796000	1	2.508363000	4.256927000	-1.589819000
6	-0.031214000	-0.706590000	-0.059655000	6	0.648122000	4.478457000	-0.504770000
6	0.908375000	0.249037000	0.029865000	6	-0.350842000	3.810109000	0.209262000
6	0.551231000	-2.075918000	0.352713000	1	-1.164600000	4.405965000	0.610770000
6	2.292719000	-0.312277000	0.403619000	6	-3.239716000	-1.473380000	-1.885769000
6	1.701623000	-2.412620000	-0.559788000	1	-3.561417000	-2.158471000	-2.658519000
6	2.640343000	-1.471245000	-0.506641000	6	-4.124093000	-0.571063000	-1.298442000
8	1.119168000	-1.895453000	1.701829000	6	-3.665557000	0.320128000	-0.324256000
6	2.039235000	-0.939612000	1.763304000	1	-4.380454000	1.020022000	0.097853000
16	2.753766000	-0.523526000	3.170060000	6	-1.103831000	0.727163000	2.909496000
6	3.932671000	-1.483697000	-1.226779000	1	-0.524503000	-0.174955000	2.703602000
8	4.756490000	-0.600192000	-1.133385000	1	-0.487456000	1.406409000	3.505221000
8	4.083673000	-2.559761000	-1.989846000	1	-1.969571000	0.439502000	3.514030000
6	5.310274000	-2.635341000	-2.738172000	6	-3.043320000	2.807845000	1.749172000
1	5.384626000	-1.785106000	-3.415343000	1	-3.416674000	3.316249000	0.856694000
1	6.160130000	-2.650687000	-2.056610000	1	-3.884306000	2.303112000	2.233196000
1	5.251573000	-3.564801000	-3.296819000	1	-2.668280000	3.565098000	2.443623000
1	3.065436000	0.444477000	0.464223000	8	-5.446535000	-0.481662000	-1.616932000
6	-0.493609000	-3.173552000	0.502862000	6	-5.946772000	-1.373700000	-2.609170000
8	-0.558375000	-4.131475000	-0.224980000	1	-5.443980000	-1.211688000	-3.565541000
8	-1.314552000	-2.915627000	1.500876000	1	-5.822917000	-2.412819000	-2.294901000
6	-2.416590000	-3.830644000	1.664103000	1	-7.005346000	-1.145252000	-2.709051000
1	-3.031150000	-3.817985000	0.763490000	8	0.494075000	5.825623000	-0.630040000
1	-2.039461000	-4.834312000	1.855093000	6	1.501476000	6.541939000	-1.339889000
1	-2.975646000	-3.460001000	2.517907000	1	2.472114000	6.432397000	-0.850505000
1	1.716154000	-3.322572000	-1.144265000	1	1.565310000	6.198109000	-2.374816000
6	-1.910530000	-1.483372000	-1.472447000	1	1.195897000	7.585336000	-1.318713000

3. Kinetics determination and cycloadducts characterization details

3.1. 2nd order rate constant determination between PyrS2 and dienophiles

Kinetics between PyrS2 and exo-BCN

Reaction mixtures consisting of PyrS2 (0.4 mM) and exo-BCN (10 mM, 15 mM, and 20 mM) in 50% acetonitrile/water were prepared in separate wells of a 96-well plate at 25 °C. The reaction was monitored by recording the disappearance of the characteristic absorption of pyranthiones (ranging from 390 nm to 440 nm) every 1 or 2 minutes. The pseudo 1st order rate constants were derived from an exponential fitting by plotting the absorbance against the reaction time. The 2nd order rate constants were derived from linear fitting of the pseudo 1st order rates with the concentration of exo-BCN.

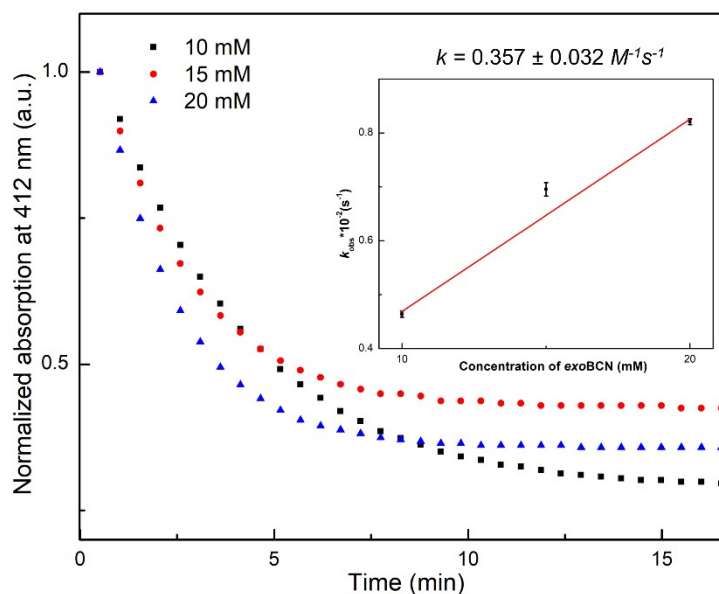


Figure S1 Kinetics evaluation of ligation between **PyrS2** and exo-BCN (10, 20, and 40 mM) in 50% acetonitrile/water.

Kinetics between PyrS2 and DMBCN

Kinetics were determined using PyrS2 (0.4 mM) and DMBCN (4 mM, 6 mM, and 8 mM) in 50% acetonitrile/water using similar protocol as PyrS2 and exo-BCN.

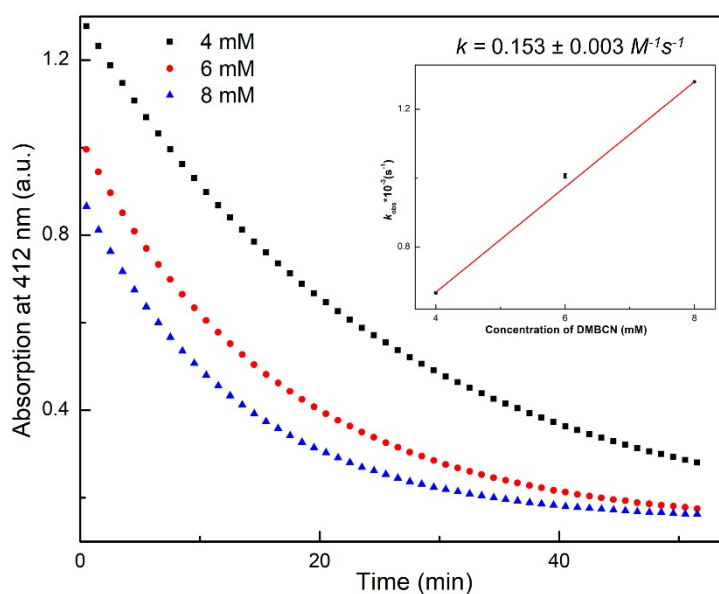


Figure S2 Kinetics evaluation of ligation between **PyrS2** and DMBCN (4, 6, and 8 mM) in 50% acetonitrile/water.

Reactivity tests between PyrS2 and DBCO

Reactivity between PyrS2 (5 mM) and DBCO (5 mM) were mixed in deuterium methanol and the reaction was monitored by ^1H NMR.

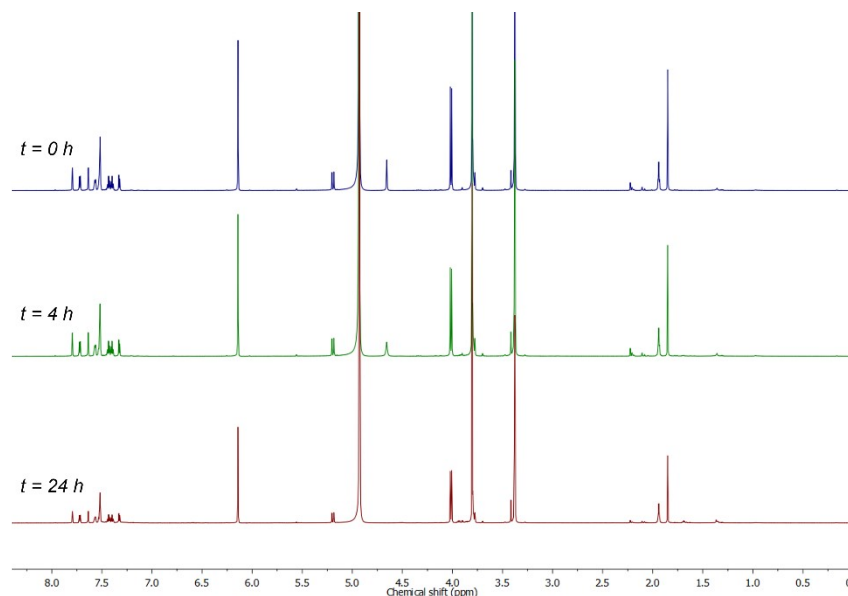


Figure S3 Reactivity evaluation between **PyrS2** and DBCO (5 mM each) in deuterium methanol with different incubation time points.

Kinetics and reactivity determination between PyrS2 and Cp

Reactivity tests between PyrS2 (5 mM) and Cp (5 mM) were analyzed by HPLC. Kinetics were similarly determined using PyrS2 (0.4 mM) and Cp (4 mM, 6 mM, and 8 mM).

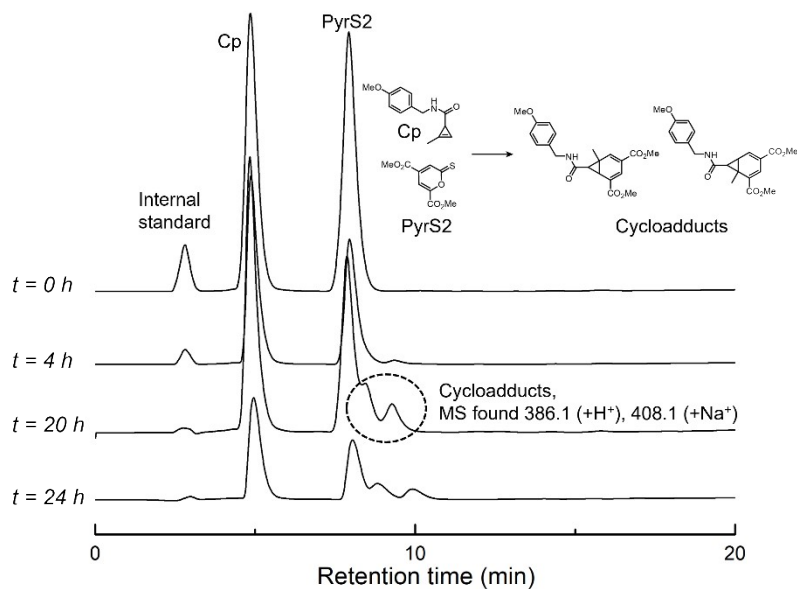


Figure S4 Reaction analysis between **PyrS2** and Cp (5 mM each) in 50% acetonitrile/water using HPLC.

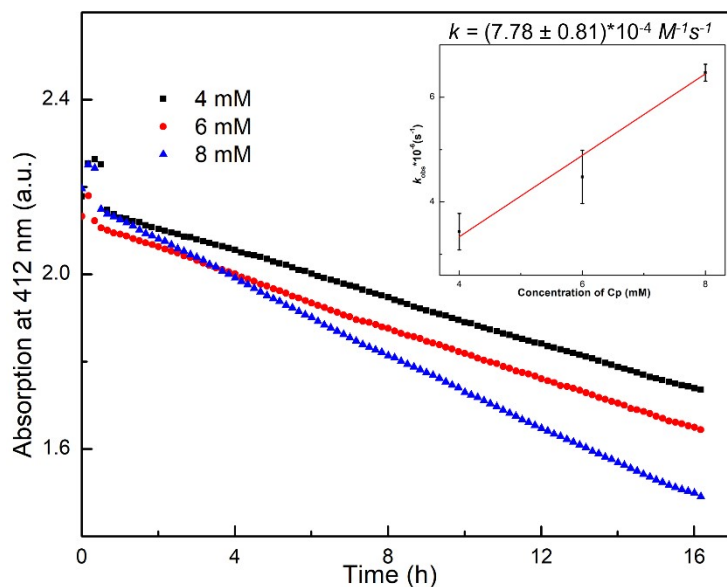


Figure S5 Kinetics evaluation of ligation between **PyrS2** and Cp (4, 6, and 8 mM) in 50% acetonitrile/water.

Kinetics between *PyrS2* and *Si-7HT*

Reaction mixtures consisting of *PyrS2* (0.1 mM) and uncaged Cp-7HT (1 mM, 1.125 mM, and 1.25 mM, illuminated under 365 nm LED for 1 min in quartz test tube) in acetonitrile were prepared in separate wells of a 96-well plate at 25 °C. The reaction was monitored by recording the disappearance of the characteristic absorption of pyranthiones (ranging from 390 nm to 440 nm) every 31 seconds. The pseudo 1st order rate constants were derived from an exponential fitting by plotting the absorbance against the reaction time. The 2nd order rate constants were derived from linear fitting of the pseudo 1st order rates with the concentration of Cp-7HT.

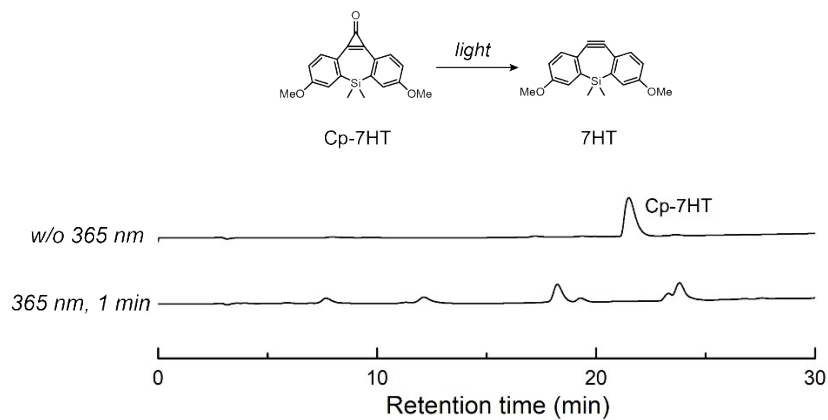


Figure S6 Uncaging analysis of Cp-7HT (2 mM) under illumination of 365 nm LED for 1 min from HPLC in acetonitrile.

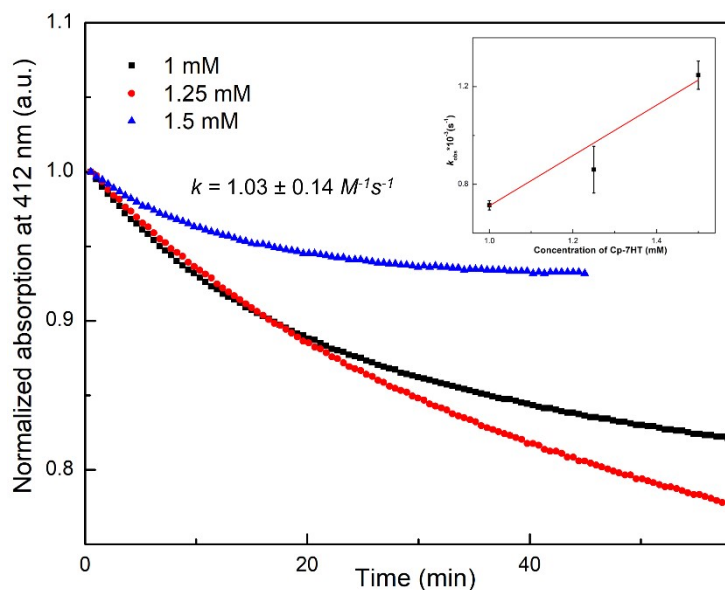
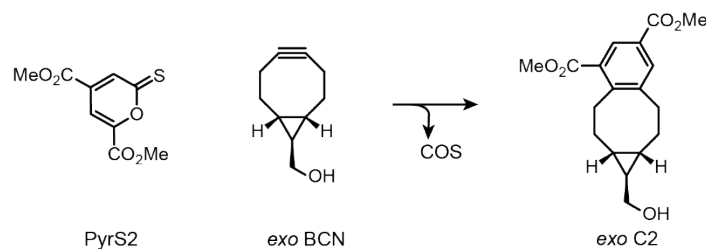


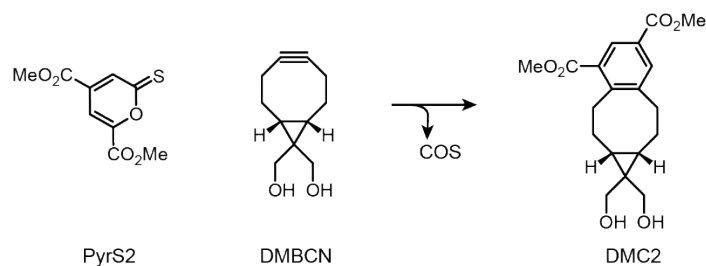
Figure S7 Kinetics evaluation of ligation between **PyrS2** and uncaged Cp-7HT (1, 1.125, and 1.25 mM) in acetonitrile.

3.2. Cycloadducts characterization details

At the end of the kinetics experiments, the reaction mixtures were collected and purified by flash chromatography or preparative TLC for the cycloadducts isolation. For the reaction pairs with relatively slower reaction rates, the reaction was left for at least one week for the completion of the reaction before the cycloadducts isolation. The purified cycloadducts were characterized by ^1H NMR, COSY and HRMS, respectively.

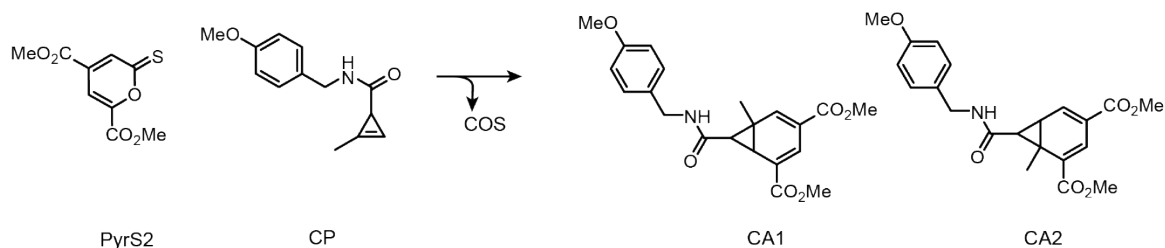


Dimethyl (1*R*,1*aR*,9*aS*)-1-(hydroxymethyl)-1*a*,2,3,8,9,9*a*-hexahydro-1*H*-benzo[*a*]cyclopropa[*e*][8]annulene-4,6-dicarboxylate (exo C2). ^1H NMR (700 MHz, Acetonitrile- d_3) δ = 8.14 (d, J = 1.9 Hz, 1H), 7.89 (d, J = 1.8 Hz, 1H), 3.87 (d, J = 7.8 Hz, 6H), 3.21 (d, J = 11.0 Hz, 2H), 3.12 – 3.05 (m, 2H), 3.02 (br, 1H), 2.93 (dt, J = 14.6, 7.2 Hz, 1H), 2.61 – 2.55 (m, 1H), 2.44 – 2.39 (m, 2H), 1.37 (s, 2H), 0.63 (tt, J = 6.8, 4.5 Hz, 1H), 0.55 (s, 1H), 0.51 (s, 1H). HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{22}\text{NaO}_5$ [$\text{M}+\text{H}$] $^+$: 341.1359, found: 341.1358.

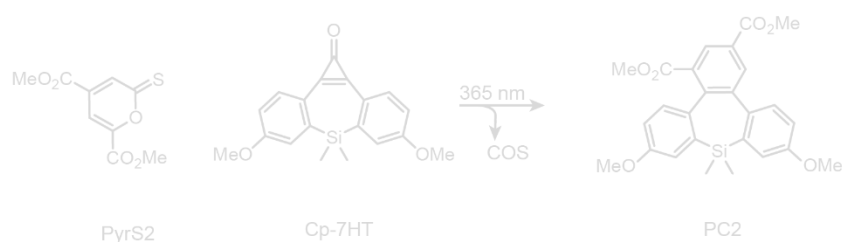


Dimethyl (1*aR*,9*aS*)-1,1-bis(hydroxymethyl)-1*a*,2,3,8,9,9*a*-hexahydro-1*H*-benzo[*a*]cyclopropa[*e*][8]annulene-4,6-dicarboxylate (DMC2). ^1H NMR (700 MHz, Chloroform- d) δ = 8.30 (s, 1H), 7.92 (s, 1H), 3.92 (d, J = 2.4 Hz, 6H), 3.42 (s,

2H), 2.92 (dd, $J = 14.8, 7.4$ Hz, 2H), 2.55 (dt, $J = 15.7, 7.7$ Hz, 2H), 2.35 (t, $J = 7.5$ Hz, 2H), 1.67 – 1.61 (m, 2H), 1.33 (d, $J = 9.0$ Hz, 2H), 0.85 – 0.80 (m, 2H). HRMS (ESI): Calcd for $C_{19}H_{25}O_6$ $[M+H]^+$: 349.1646, found: 349.1642.

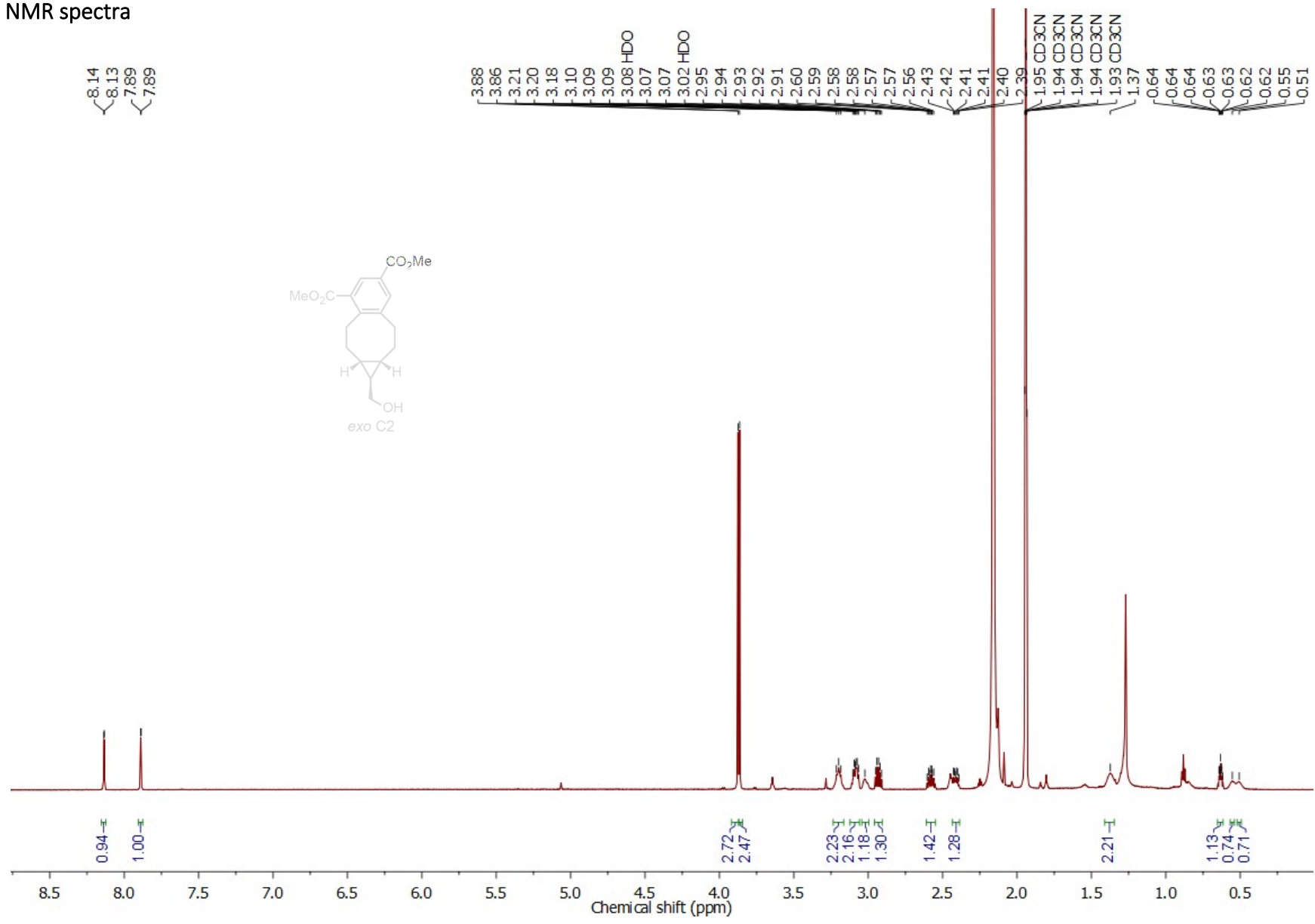


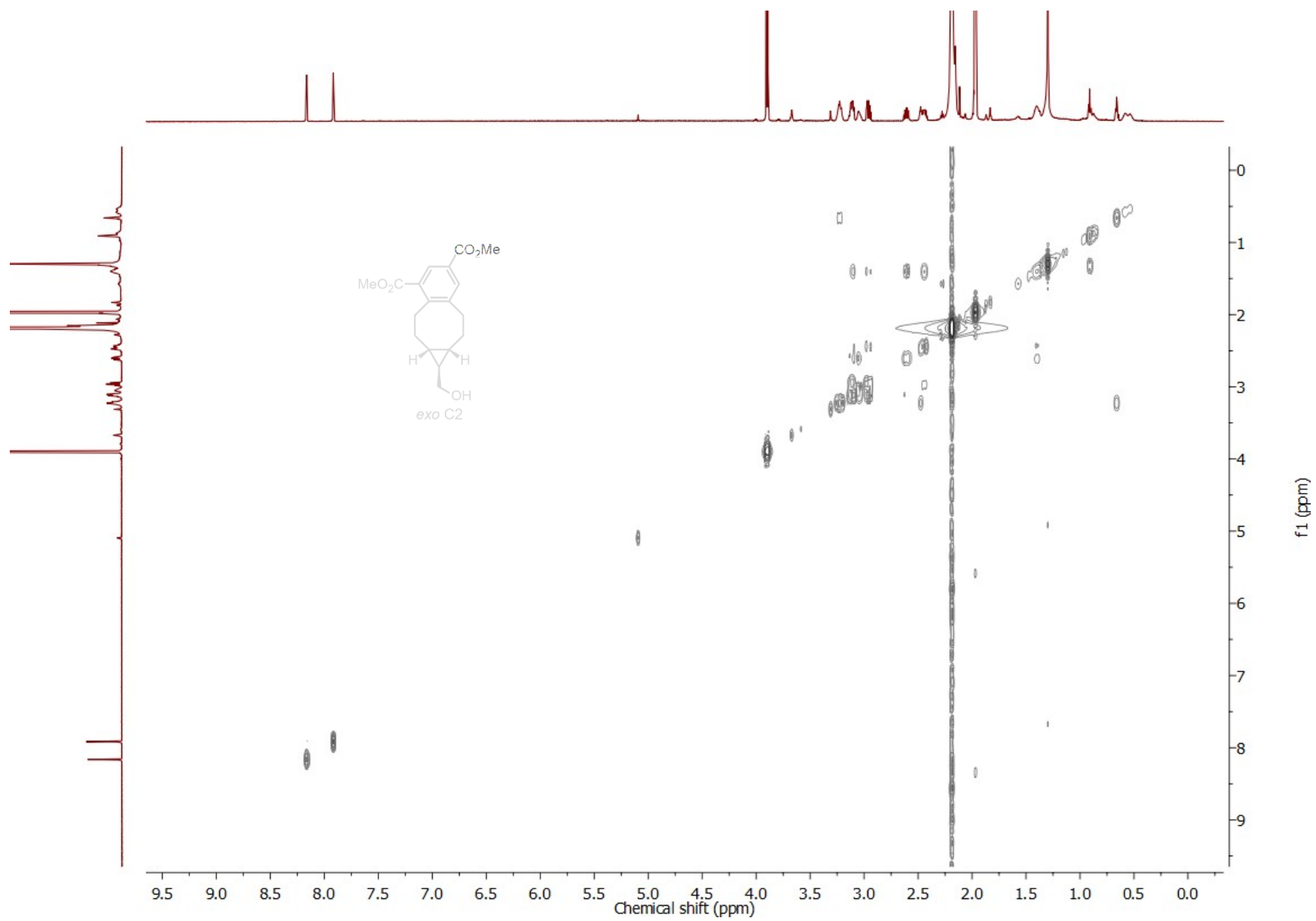
Dimethyl 7-((4-methoxybenzyl)carbamoyl)-1-methylbicyclo[4.1.0]hepta-2,4-diene-2,4-dicarboxylate (CA). 1H NMR (500 MHz, Chloroform- d) $\delta = 7.18 - 7.13$ (m, 2H), 7.05 (d, $J = 7.2$ Hz, 1H), 6.87 – 6.83 (m, 2H), 6.66 (s, 1H), 5.71 (s, 1H), 4.36 (dd, $J = 12.0, 5.6$ Hz, 2H), 3.84 – 3.77 (m, 9H), 2.33 (s, 1H), 2.02 (d, $J = 1.5$ Hz, 1H), 1.25 (s, 3H). HRMS (ESI): Calcd for $C_{21}H_{24}NO_6$ $[M+H]^+$: 386.1598, found: 386.1597.

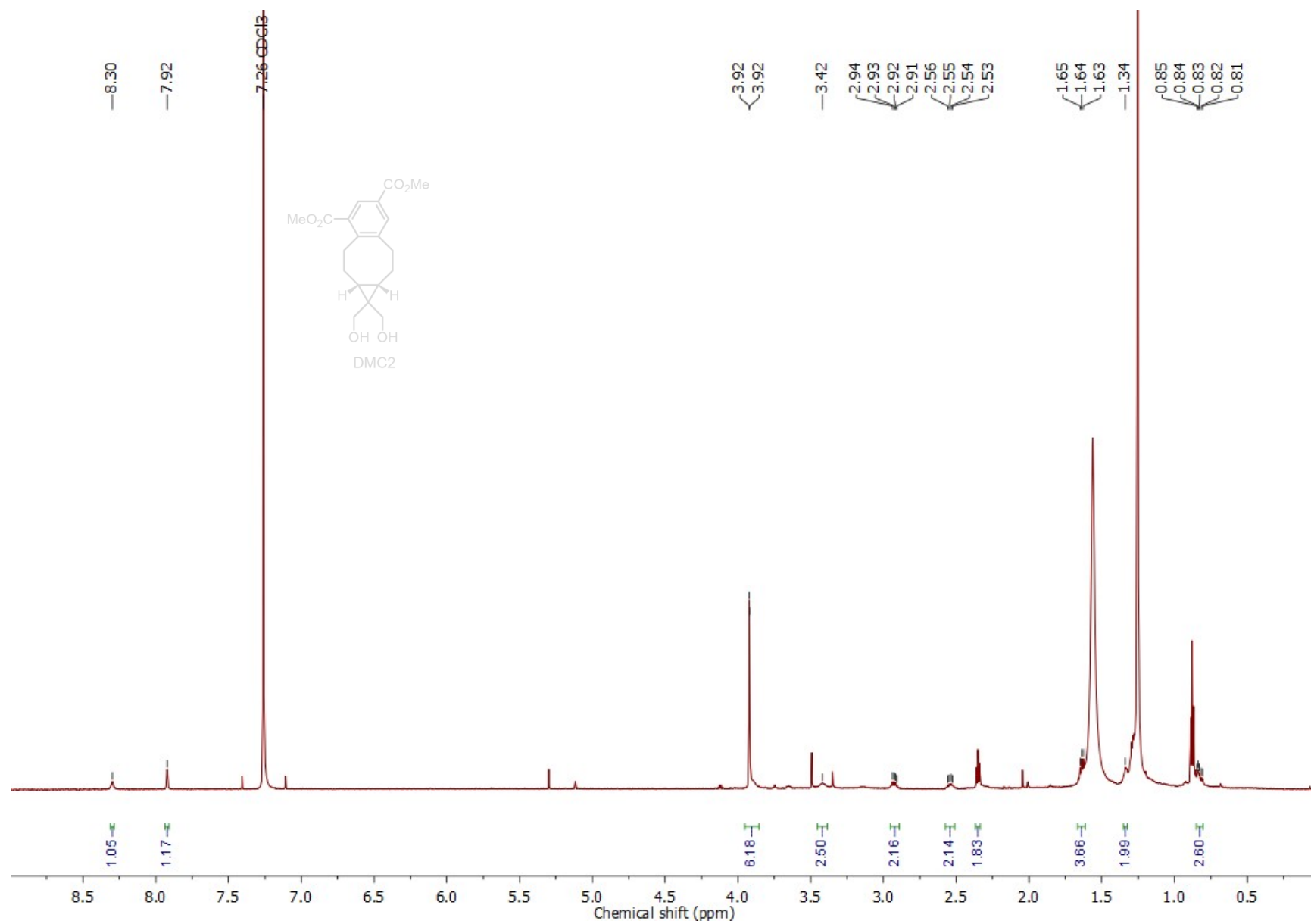


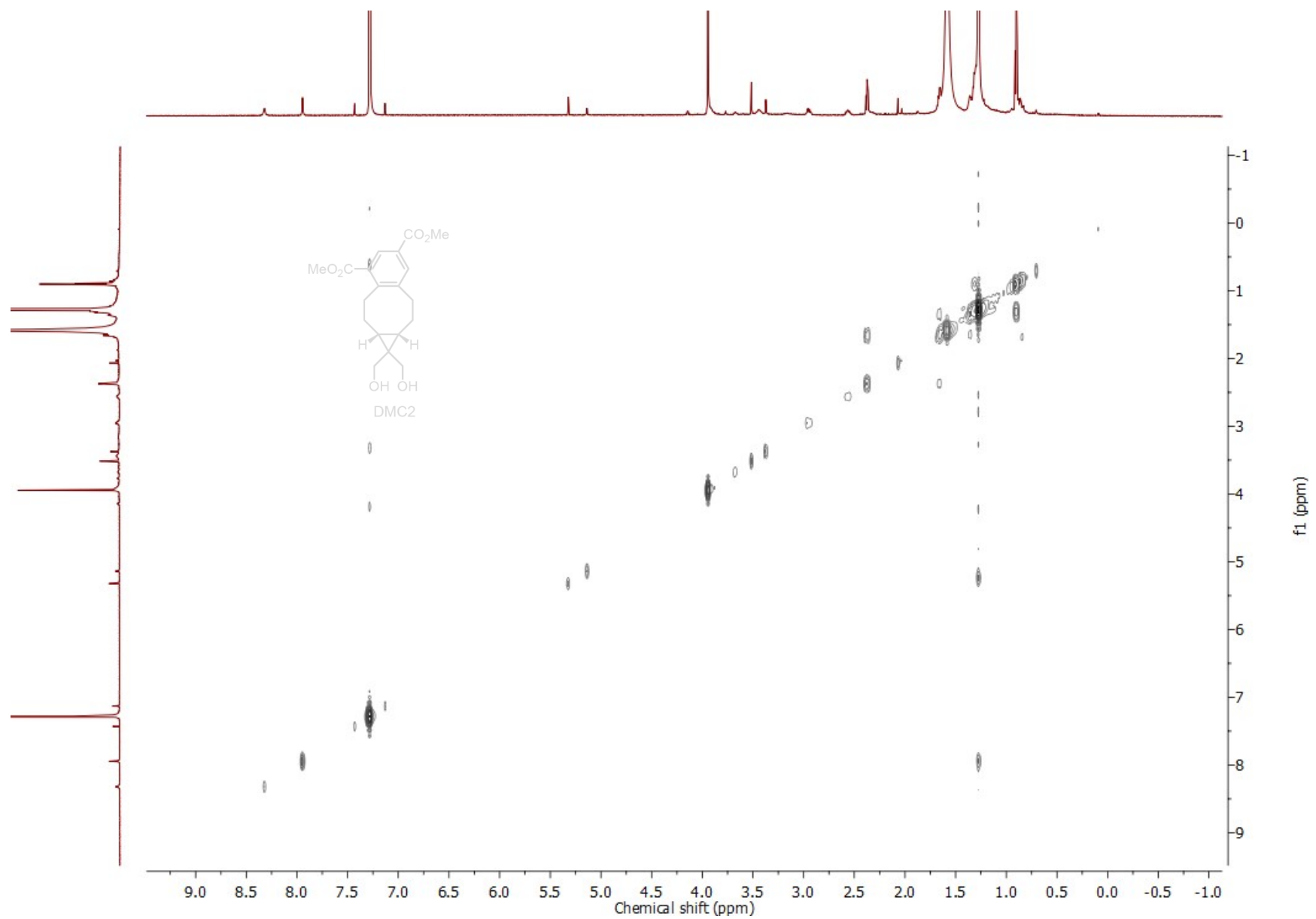
Dimethyl 7,11-dimethoxy-9,9-dimethyl-9H-tribenzo[*b,d,f*]silepine-1,3-dicarboxylate (PC2). 1H NMR (500 MHz, $CDCl_3$) $\delta = 8.27$ (d, $J = 1.9$ Hz, 1H), 8.19 (d, $J = 1.9$ Hz, 1H), 7.41 (d, $J = 8.4$ Hz, 1H), 7.08 – 6.99 (m, 3H), 6.92 (dd, $J = 8.4, 2.8$ Hz, 1H), 6.77 (dd, $J = 8.4, 2.8$ Hz, 1H), 3.96 (s, 3H), 3.80 (d, $J = 11.3$ Hz, 6H), 3.54 (s, 3H), 0.76 (s, 3H), -0.12 (s, 3H). HRMS (ESI): Calcd for $C_{26}H_{27}O_6Si$ $[M+H]^+$: 463.1571, found: 463.1560.

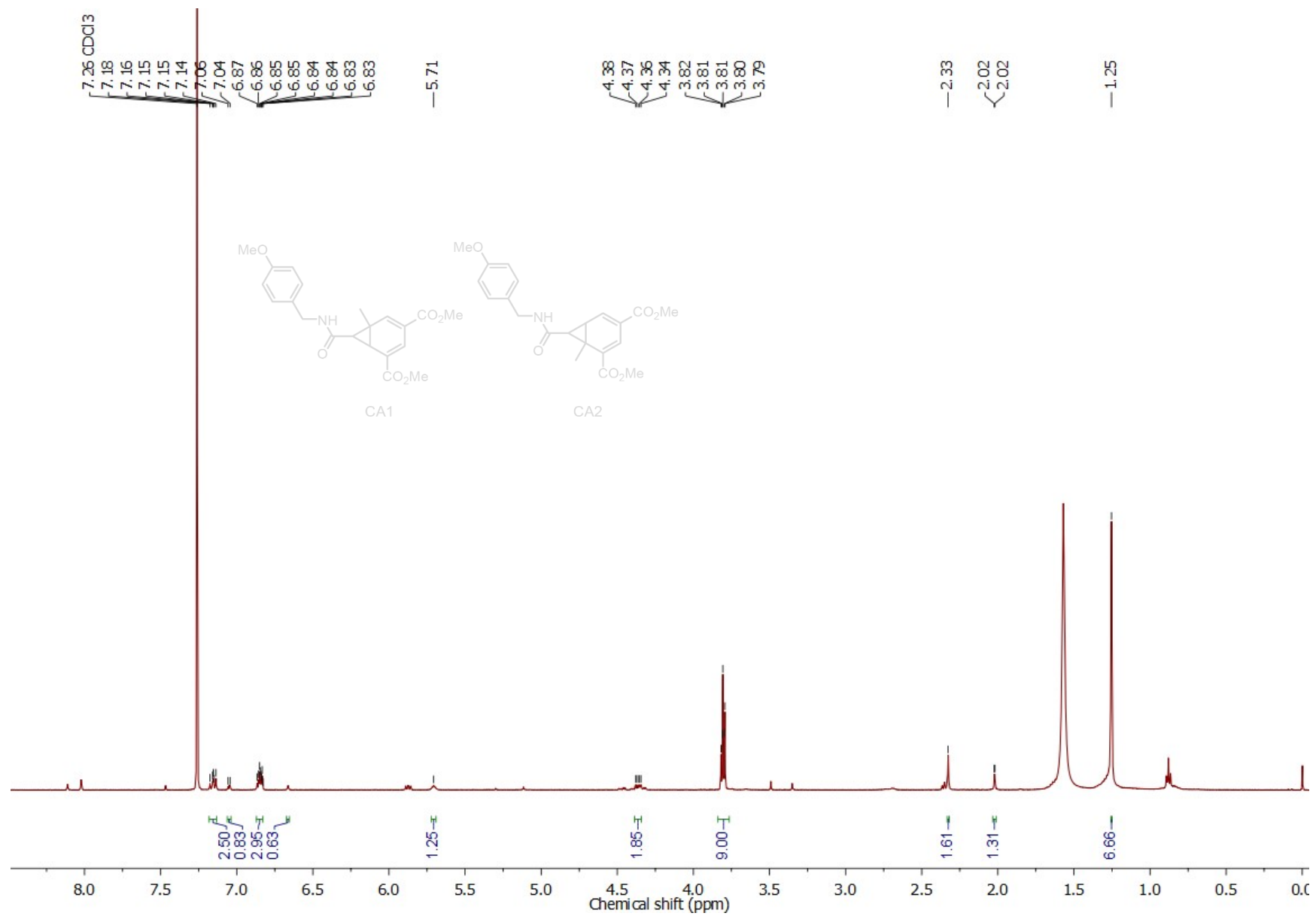
4. NMR spectra

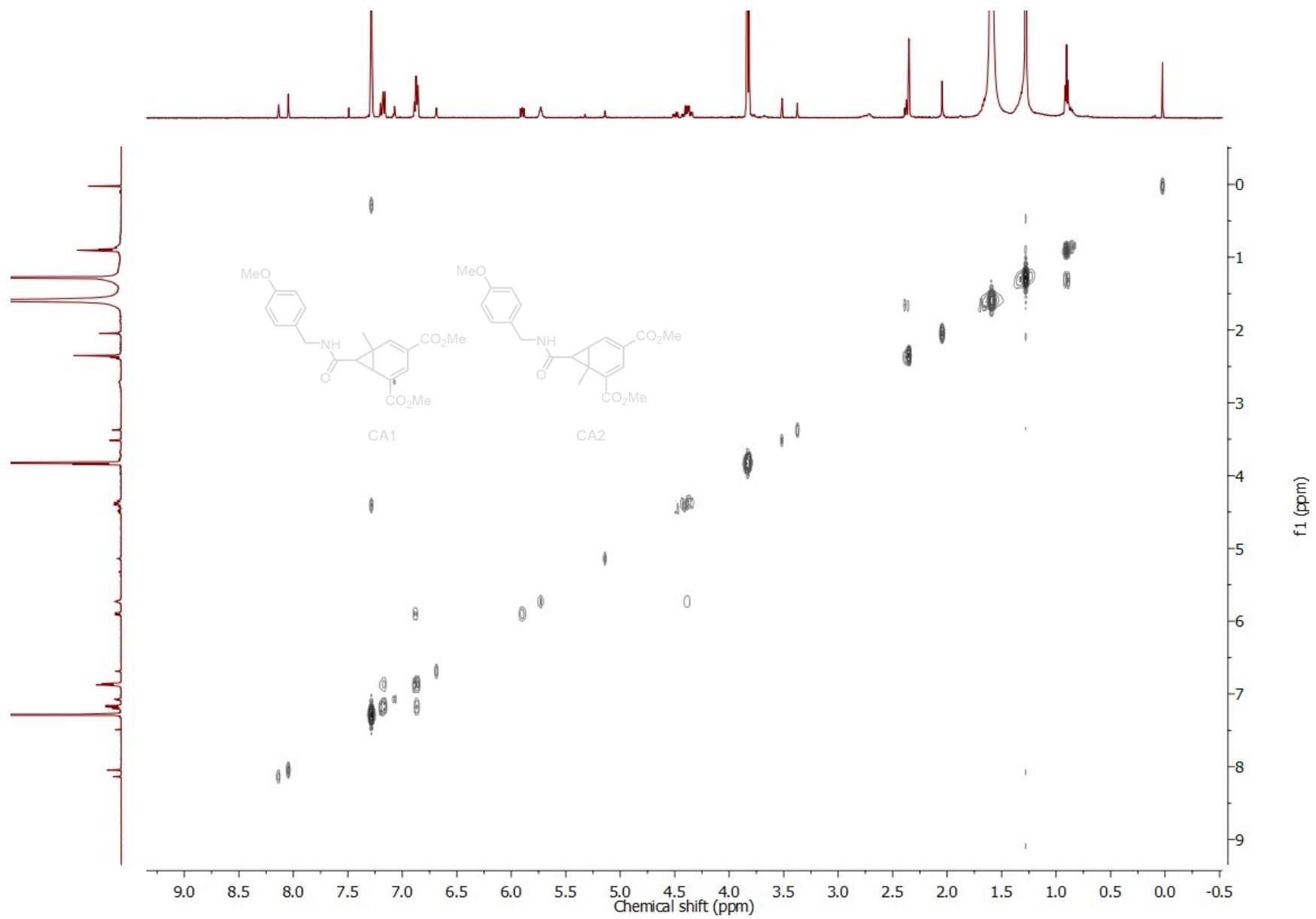


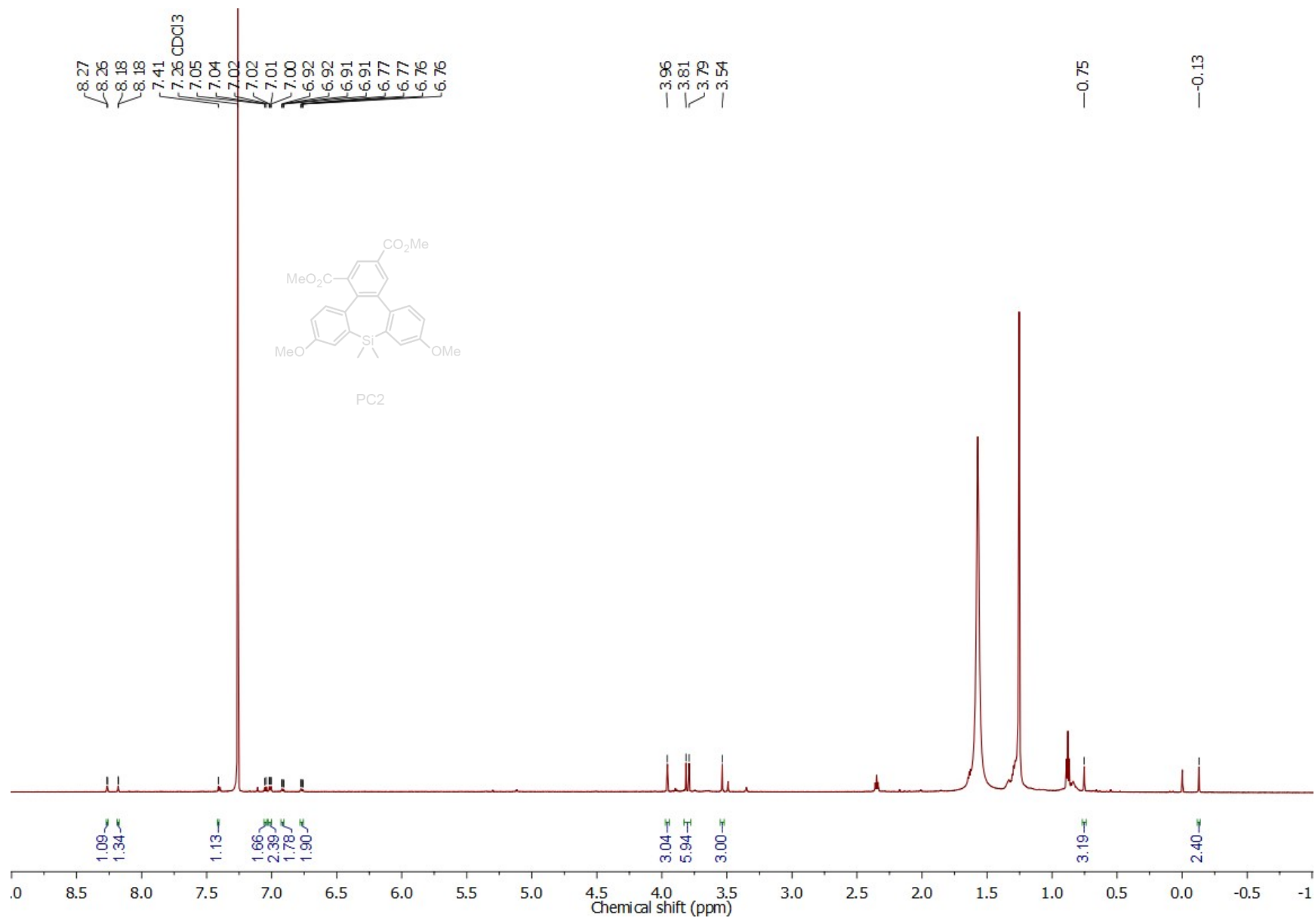


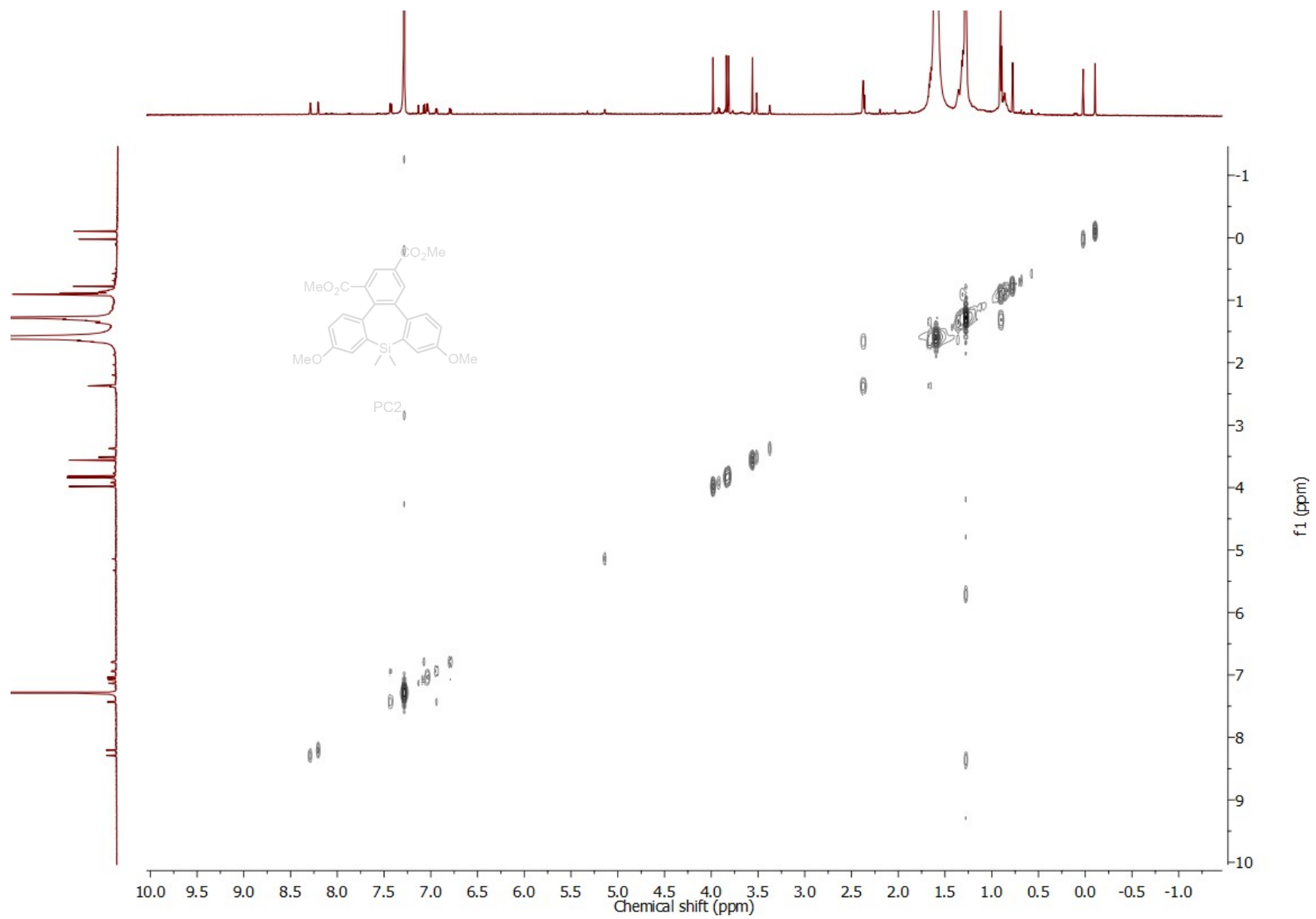












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