A 2+2/4+2 Cyclase

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[#] These authors contributed to this work equally.

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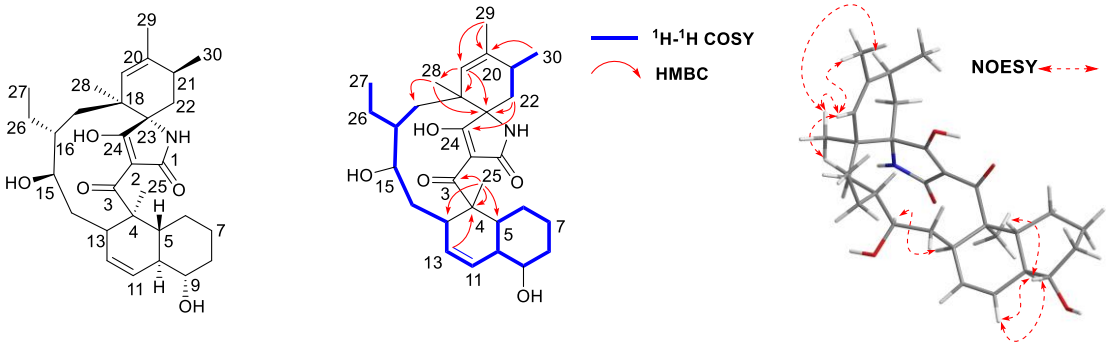
1. Supplementary Text

Physico-Chemical Properties and Structural Elucidation of *endo*-4+2 Product 9.

Compound **9** was isolated as a white amorphous powder: ^{1}H and ^{13}C NMR data (500 and 125 MHz, respectively, recorded in methanol-d_4 and DMSO-d_6) see **Supplementary Tables 3 and 4**. IR (Miro-FTIR) ν_{max} 3381, 2929, 2829, 1674, 1555, 1440, 1376, 1014 cm^{-1}; HR-ESI-MS (positive mode) *m/z* calcd. for $C_{30}H_{44}NO_5$: 498.3214 $[M+H]^+$, found 498.3212. $[\alpha]_D^{20.0}$ -38 (*c* 0.10, MeOH). ECD (*c* 2.0 × 10^{-4}, MeOH) λ_{max} ($\Delta\varepsilon$) = 201 (-0.64), 230 (+0.84), 306 (-0.12), 368 (+0.02) nm.

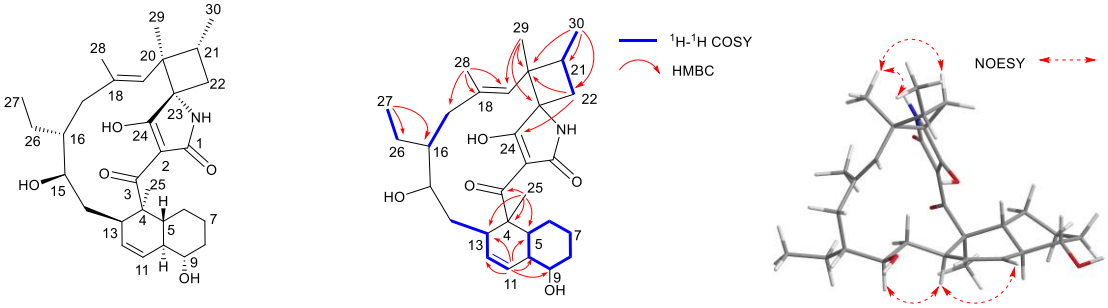


The molecular formula of **9**, which is identical to those of **7** and **8**, was established to be $C_{30}H_{43}NO_5$ by analysis of the HR-ESI-MS data and the ^{13}C and DEPT NMR spectra. The planar structure of **9** was established by comparison of its NMR data with those of substrate **7** and *exo*-4+2 product **8**.[1] Consequently, **9** is highly similar to **8**, with the presence of low field signals [$\delta_{C\text{-}19}$ 125.8 ($\delta_{H\text{-}19}$ 5.13 s) and $\delta_{C\text{-}20}$ 135.7 in methanol-d_4] corresponding to the $\Delta^{19,20}$-alkene group that is also present in *exo*-4+2 product **8**. The HMBC correlations from H_3-28 (δ_H 0.87) to C-17 (δ_C 45.7), C-23 (δ_C 66.0) and from H-19 to C-18 (δ_C 42.4), C-23, C-28 (δ_C 29.0) also supported the proposed structure. The relative configuration of **9**, which was deduced by X-ray diffraction analysis of the complex of PloI4-F124L with **9**, was assigned as (4*R**,5*R**,9*S**,10*S**,13*R**,15*R**,16*R**,18S*,21*S**,23*S**). Compared with the relative configuration of *exo*-4+2 product **8** that was assigned as (4*R**,5*R**,9*S**,10*S**,13*R**,15*R**,16*R**,18*R**,21*R**,23*S**), differences were observed at C18 and C21. The opposite relative configuration at C18 and C21 indicates that **9** is an *endo*-4+2 product. To determine the absolute configuration of **9**, gas-phase and solution DFT conformational analysis and time-dependent density-functional theory (TDDFT)-ECD calculation were carried out, using tools

proved to be effective in the prediction of the stereochemistry of natural products.[2] For comparison, the experimental ECD spectrum of compound **9** was measured at the concentration of 0.20 mM in methanol. The ECD spectrum of **9** in methanol showed a broad intense positive Cotton effect (CE) between 213 nm and 264 nm (accompanied with positive shoulders at 230 nm), and a weak negative CE at 306 nm. Conformational searching of (4*R*,5*R*,9*S*,10*S*,13*R*,15*R*,16*R*,18*S*,21*S*,23*S*)-**9** was undertaken with the CREST code (version 2.8) using the default iMTD-GC procedure.[3] The conformational analysis of (4*R*,5*R*,9*S*,10*S*,13*R*,15*R*,16*R*,18*S*,21*S*,23*S*)-**9** initially gave 30 conformers (energy window < 5 kcal/mol). Re-optimization using the M06-2X/def2-SVP level in vacuo for methanol eventually resulted in 8 conformers. The conformers with a population of over 1% were subjected to subsequent ECD calculations. (**Supplementary Fig. 7**). To obtain the calculated ECD spectrum of compound **9**, TDDFT-ECD theoretical calculations were run at the CAM-B3LYP-SCRF/def2-SVP level in MeOH with polarizable continuum model (PCM) (**Supplementary Fig. 8**). Overall, the Boltzmann-weighted ECD spectrum is in line with the experimentally measured ECD spectrum, allowing assignment of the absolute configuration of **9** as (4*R*,5*R*,9*S*,10*S*,13*R*,15*R*,16*R*,18*S*,21*S*,23*S*). The best consistency was achieved by using the CAM-B3LYP-SCRF/def2-SVP method.

Physico-Chemical Properties and Structural Elucidation of *exo*-2+2 Product 10.

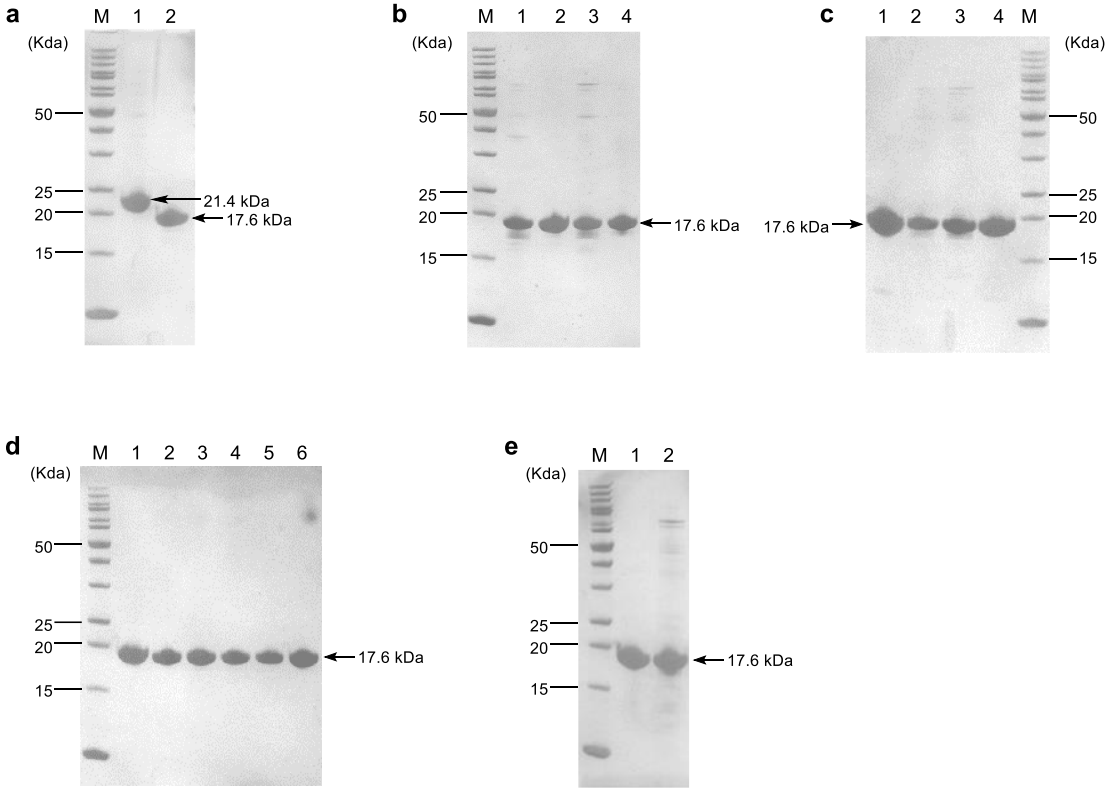
Compound **10** was isolated as a white amorphous powder: ^{1}H and ^{13}C NMR data (500 and 125 MHz, respectively, recorded in methanol-d_4) see **Supplementary Table 5**. IR (KBr) ν_{max} 3362, 2925, 2854, 1667, 1596, 1458, 1378, 1200, 1068, 1034 cm^{-1}; HR-ESI-MS (positive mode) *m/z* calcd. for $C_{30}H_{44}NO_5$: 498.3214 $[M+H]^+$, found 498.3211. $[\alpha]_D^{20.0}$ -50 (*c* 0.70, MeOH). ECD (*c* 2.0 × 10^{-4}, MeOH) λ_{max} ($\Delta\varepsilon$) = 200 (-1.54), 216 (+2.07), 252 (-0.53), 305 (0.18) nm.



The molecular formula of **10**, which are identical to **7**, **8** and **9**, was established to be $C_{30}H_{43}NO_5$ by analysis of the HR-ESI-MS data and the ^{13}C and DEPT NMR spectra. The planar structure of **10** was established by comparison of its NMR data with those of 4+2 products **8** and **9**. Consequently, **10** is similar to **8** and **9**, with the exception of the ^{1}H and ^{13}C NMR signals that correspond to the $\Delta^{19,20}$-alkene unit in 4+2 products **8** and **9** were not observed. In contrast, there are the signals in the low field of ^{1}H and ^{13}C NMR of **10** (δ_C 136.6, C-18 and δ_C 130.2, C-19 δ_H 4.78, H-19), corresponding to the $\Delta^{18,19}$-alkene unit that is also present in substrate **7**. The 2D NMR spectra, including ^{1}H-^{1}H COSY, HMBC and HSQC correlations, further supported that **10** is a 2+2 cycloadduct. The relative configuration of **10**, which was deduced by X-ray diffraction analysis of the complex of PloI4-C16M/D46A/I137V with **10**, was assigned as (4*R**,5*R**,9*S**,10*S**,13*R**,15*R**,16*R**,20*R**,21*R**,23*S**). The presence of the *R** configuration at both C18 and C21 indicates that **10** is an *exo*-2+2 product. To determine the absolute configuration of **10**, gas-phase and solution DFT conformational analysis and TDDFT-ECD calculation were carried out.[2] For comparison, the experimental ECD spectrum of compound **10** was measured at the concentration of 0.20 mM in methanol. The ECD spectrum of **10** in methanol showed a broad intense positive Cotton effect (CE) between 205 nm and 235 nm (accompanied with positive shoulders at 216 nm), and a weak negative CE at 252 nm. Conformational searching of **10** was undertaken with the CREST code (version 2.8) using the default iMTD-GC procedure.[3] The conformational analysis of (4*R*,5*R*,9*S*,10*S*,13*R*,15*R*,16*R*,20*R*,21*R*,23*S*)-**10** initially gave 154 conformers (energy window < 5 kcal/mol). Re-optimization using the B3LYP/TZVP level in vacuo for methanol eventually resulted in 6 conformers. the conformers with a population of over 1% were subjected to subsequent ECD calculations (**Supplementary Fig. 9**). To obtain the calculated ECD spectrum of **10**, TDDFT-ECD theoretical calculations were run at the CAM-B3LYP-SCRF/def2-SVP level in MeOH with polarizable continuum model (PCM) (**Supplementary Fig. 10**). Overall, the Boltzmann-weighted ECD spectrum is in line with the experimentally measured ECD spectrum, allowing assignment of the absolute configuration of **10** as (4*R*,5*R*,9*S*,10*S*,13*R*,15*R*,16*R*,20*R*,21*R*,23*S*). The best consistency was achieved by using the CAM-B3LYP-SCRF/def2-SVP method.

2. Supplementary Figures

Supplementary Figure 1. Coomassie-stained SDS-PAGE analysis of the purified recombinant proteins. Lane M, molecular weight marker. (**a**) Wild-type proteins. Lane 1, PyrI4 (21.4 kDa); Lane 2, PloI4 (17.6 kDa). (**b**) PloI4 variants (17.6 kDa) engineered toward the production of **8**. Lane 1, PloI4-I137F; Lane 2, PloI4-I137Y; Lane 3, PloI4-I137W; and Lane 4, PloI4-I137V. (**c**) PloI4 variants (17.6 kDa) engineered toward the production of **9**. Lane 1, PloI4-F124A; Lane 2, PloI4-F124V; Lane 3, PloI4-F124L; and Lane 4, PloI4-F124I. (**d**) PloI4 variants (17.6 kDa) engineered toward the production of **10**. Lane 1, PloI4-C16M; Lane 2, PloI4-D46A; Lane 3, PloI4-C16M/I137V; Lane 4, PloI4-C16M/D46A/I137V; Lane 5, PloI4-C16M/D46A; and Lane 6, PloI4- D46A/I137V. (**e**) PloI4 variants (17.6 kDa) engineered for the identification of key catalytic residues. Lane 1, PloI4-Q75A; Lane 2, PloI4-Y95A.

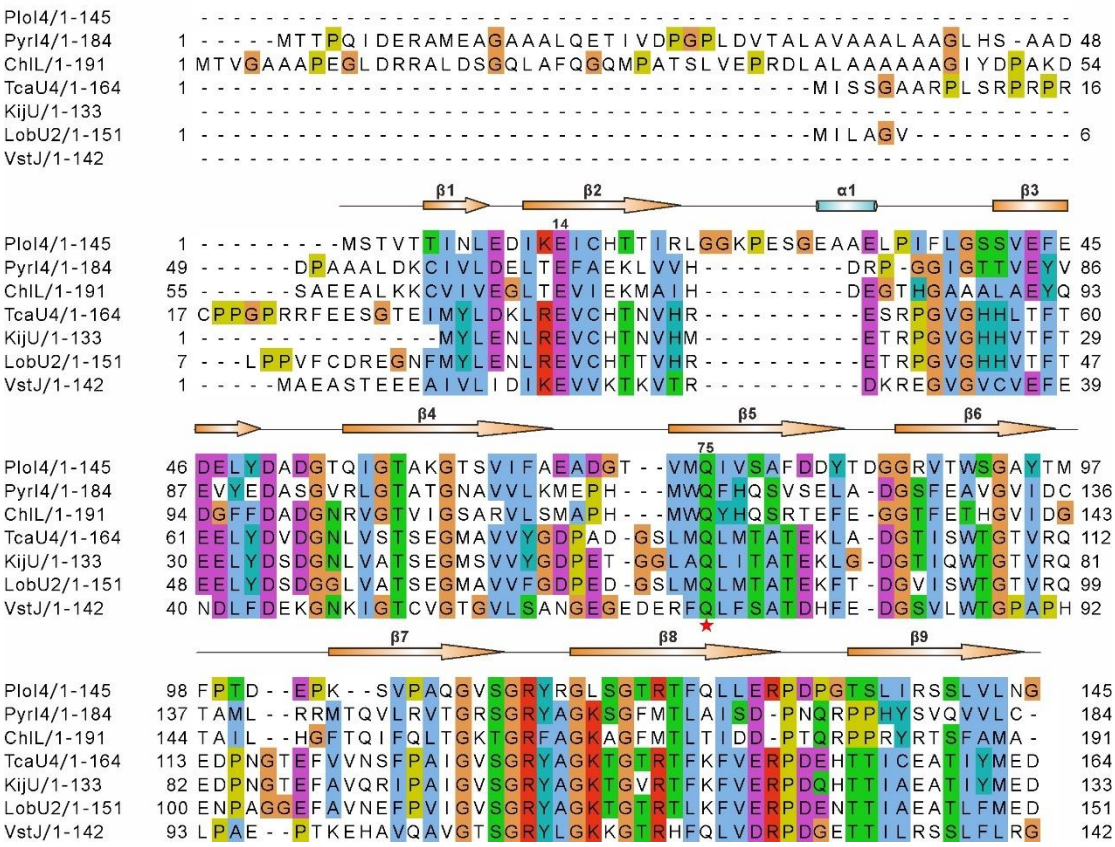


Supplementary Figure 2. Sequence analysis of PloI4 and its homologs. Selected proteins include PyrI4 in pyrroindomycins biosynthesis,[1] ChlL in chlorothricin biosynthesis,[4] TcaU4 in tetracarcin A biosynthesis,[5] KijU in kijanimicin biosynthesis,[6] LobU2 in lobophorins biosynthesis[7] and VstJ in versipelostatin biosynthesis,[8] **(a)** Sequence identity of PloI4 to each of the homologs. **(b)** Multiple sequence alignment of PloI4 with its homologs. The conserved acidic residue glutamine is highlighted with red star. Sequence alignment performed by using ClustalW and colored by using Jalview2.8.1 software (http://www.jalview.org/).

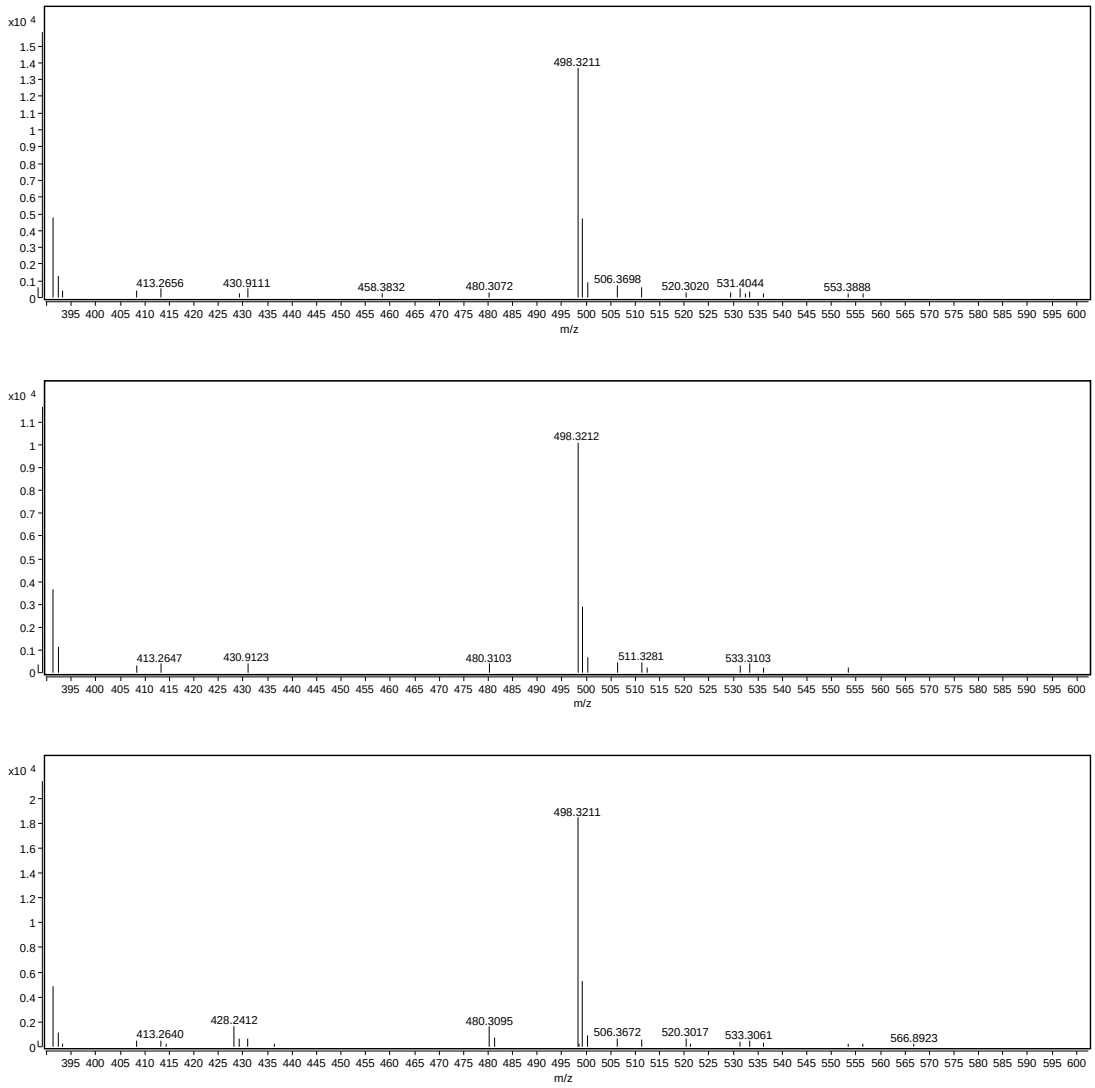
a

Homologs	NCBI accession code	Identity (%)
PyrI4	AFV71338.1	28.1
ChlL	AAZ77701.1	35.7
TcaU4	ACB37739.1	33.6
KijU	WP_157420330.1	32.2
LonU2	AGI99498.1	35.7
VstJ	BAQ21945.1	40.6

b



Supplementary Figure 3. HR-ESI-MS analysis of compounds **8** (top), **9** (middle) and **10** (down).



Supplementary Figure 4. NMR spectra of compound **9** in methanol-d_4. (**a**) ^{1}H NMR spectrum. (**b**) ^{13}C NMR spectrum. (**c**) DEPT-135 NMR spectrum. (**d**) ^{1}H-^{1}H COSY NMR spectrum. (**e**) HSQC NMR spectrum. (**f**) HMBC NMR spectrum. (**g**) NOESY NMR spectrum.

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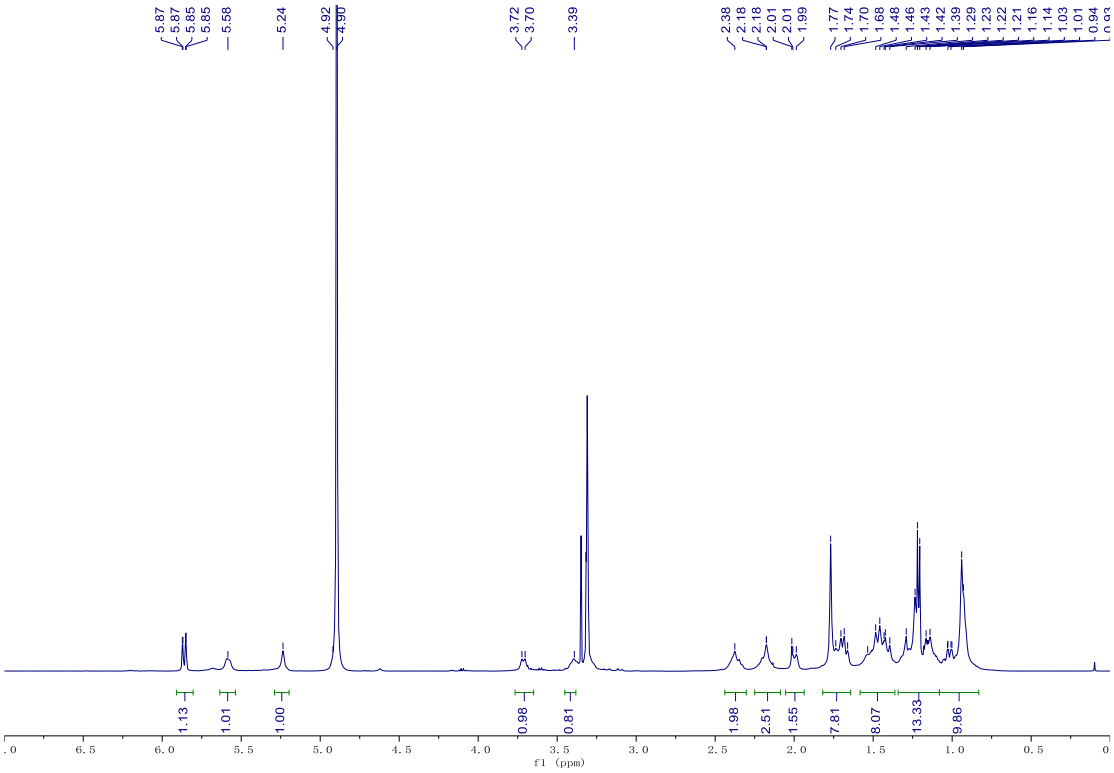

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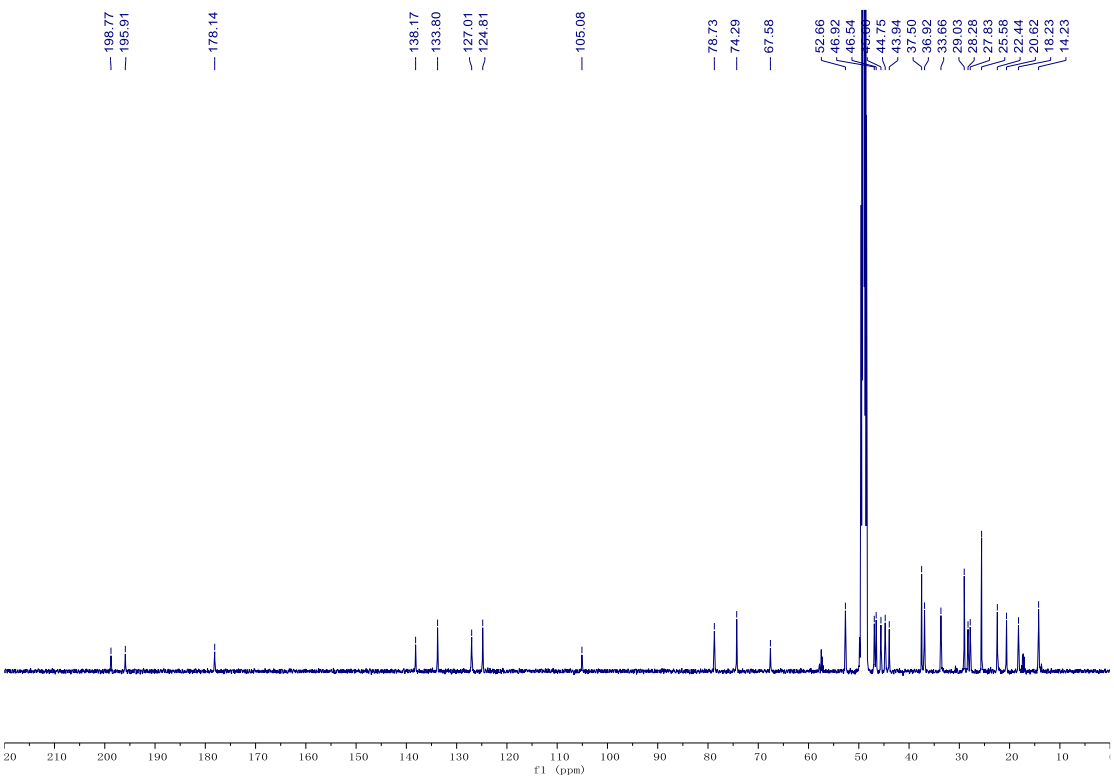
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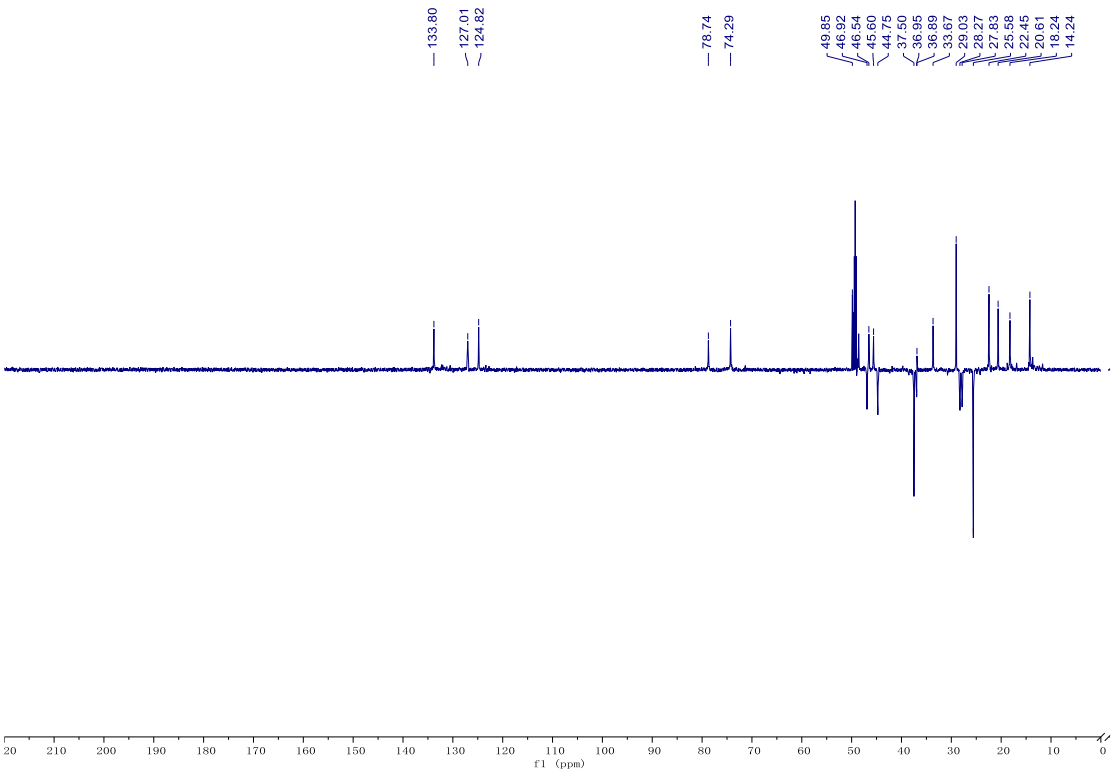
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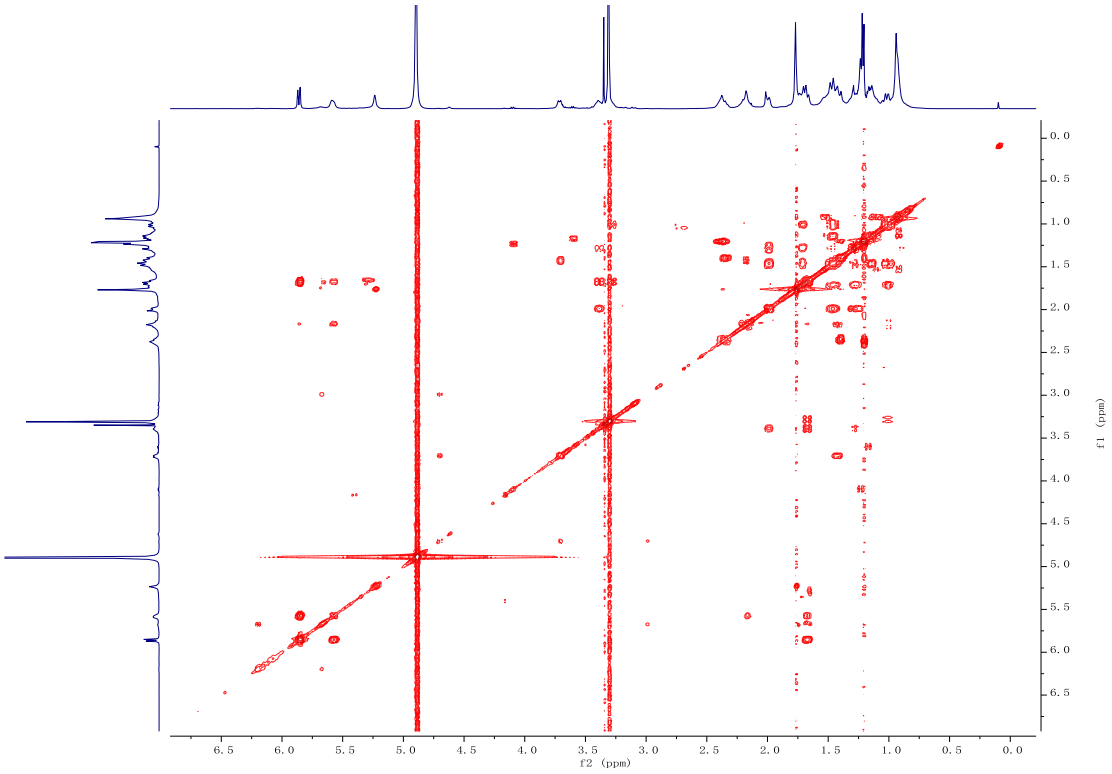

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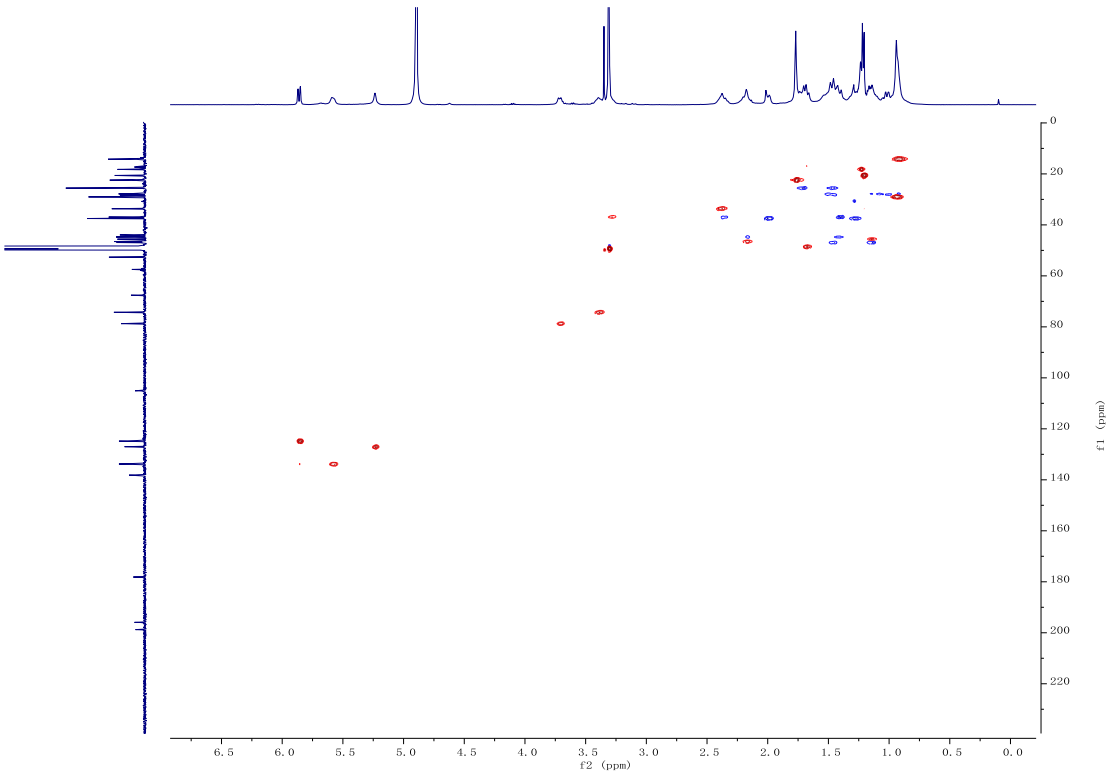

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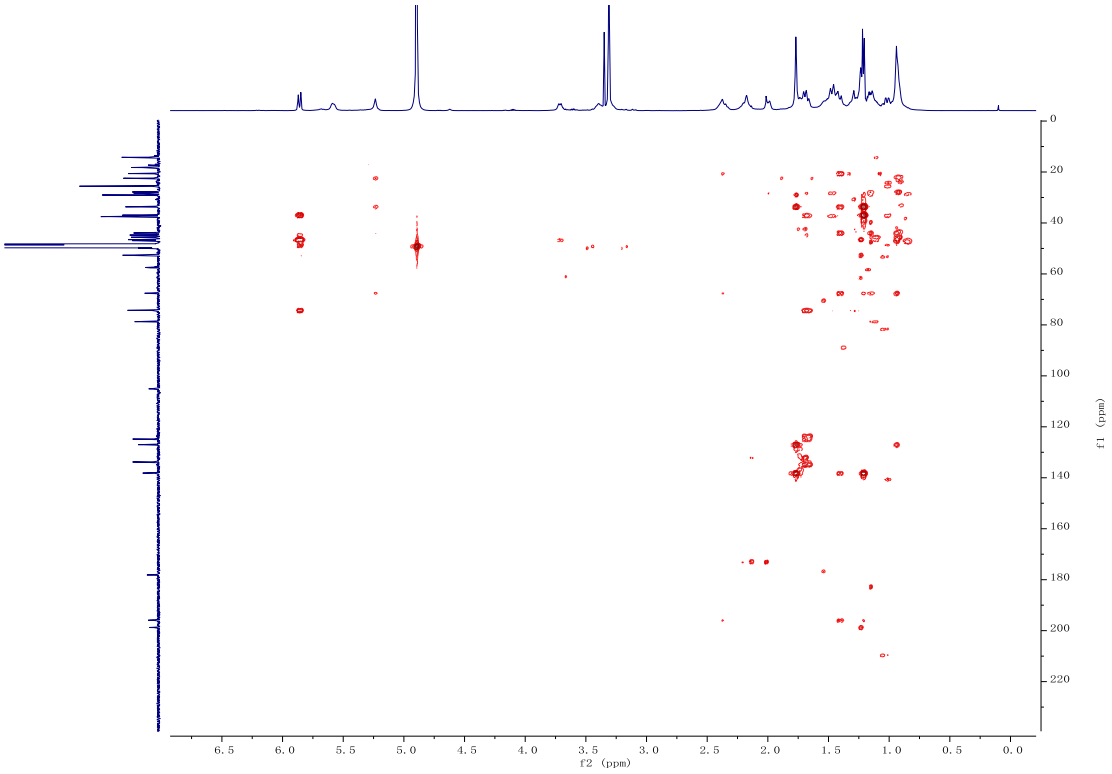

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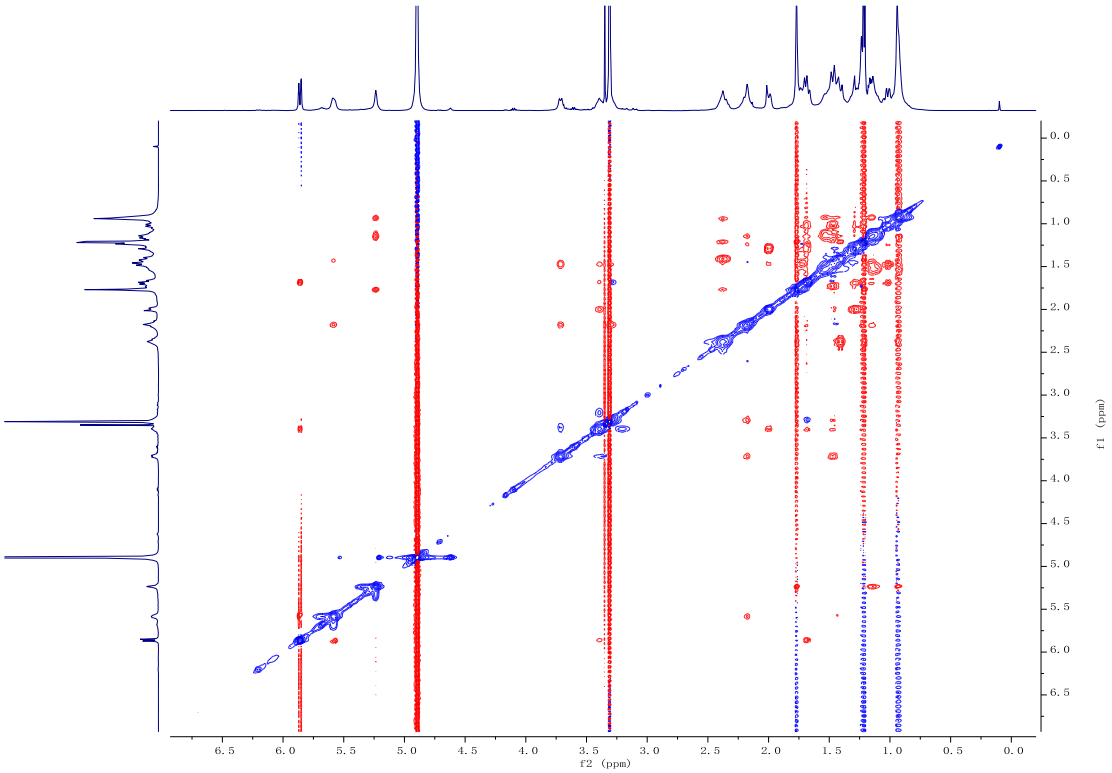

Supplementary Figure 5. NMR spectra of compound **9** in DMSO-d_6. (**a**) ^{1}H NMR spectrum. (**b**) ^{13}C NMR spectrum. (**c**) DEPT-135 NMR spectrum. (**d**) ^{1}H-^{1}H COSY NMR spectrum. (**e**) HSQC NMR spectrum. (**f**) HMBC NMR spectrum. (**g**) NOESY NMR spectrum.

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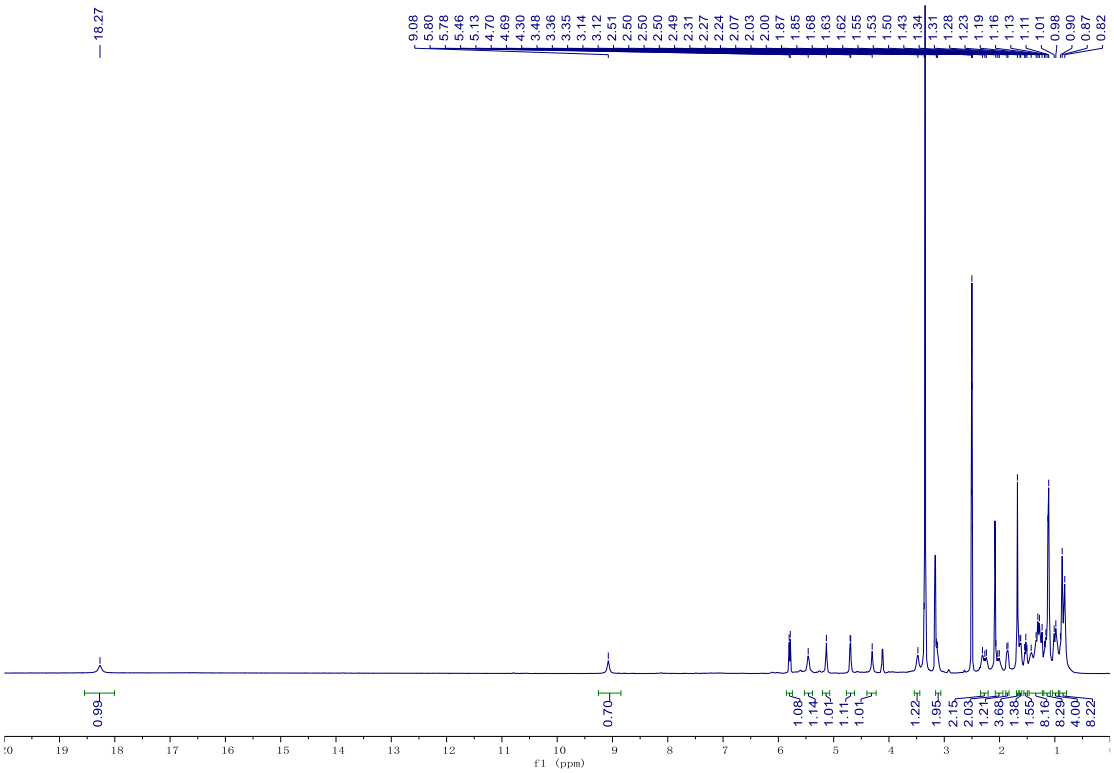

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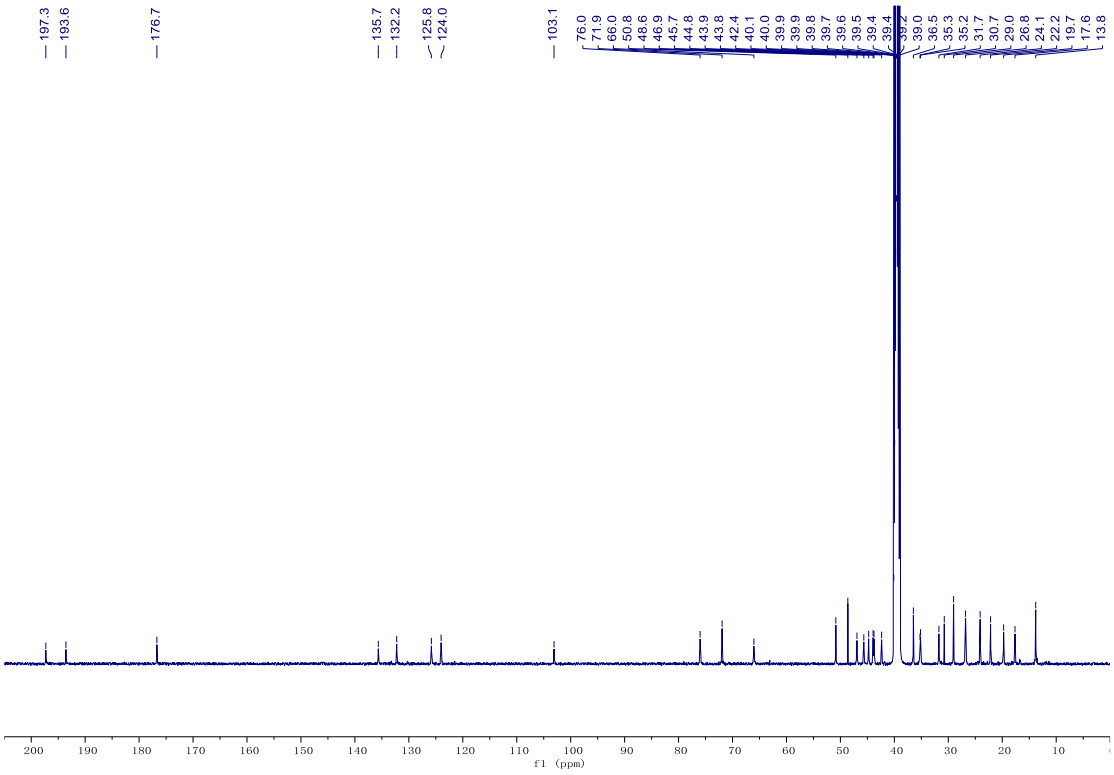
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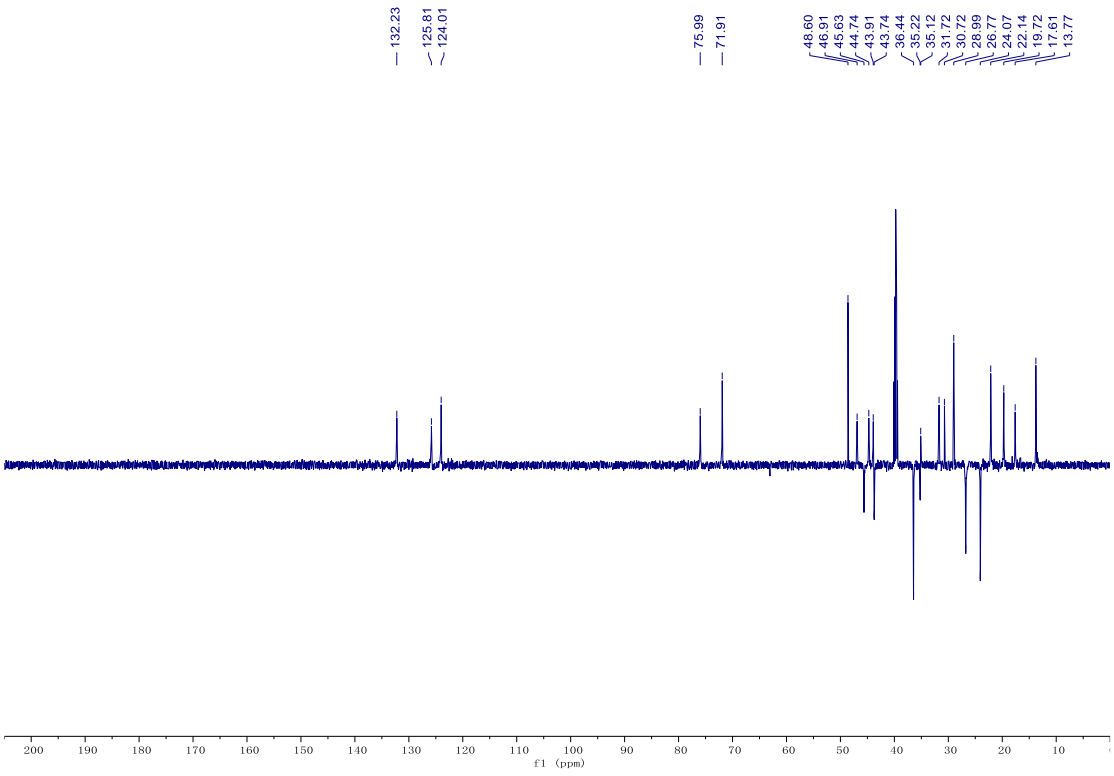
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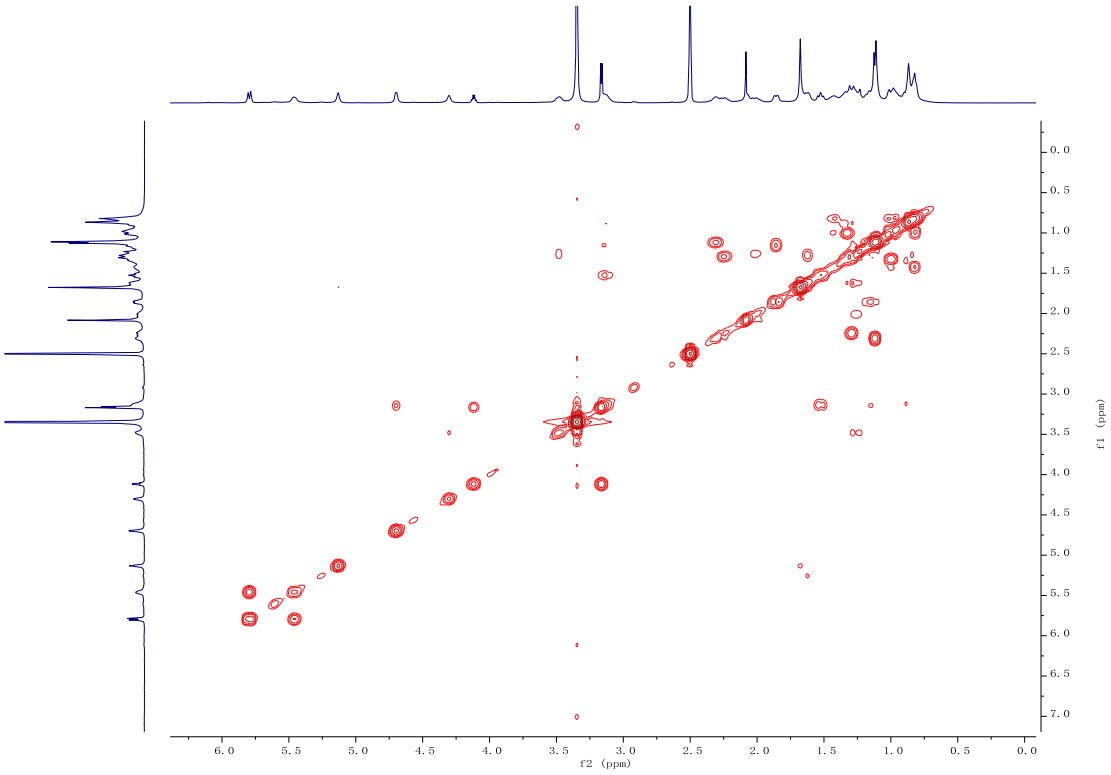

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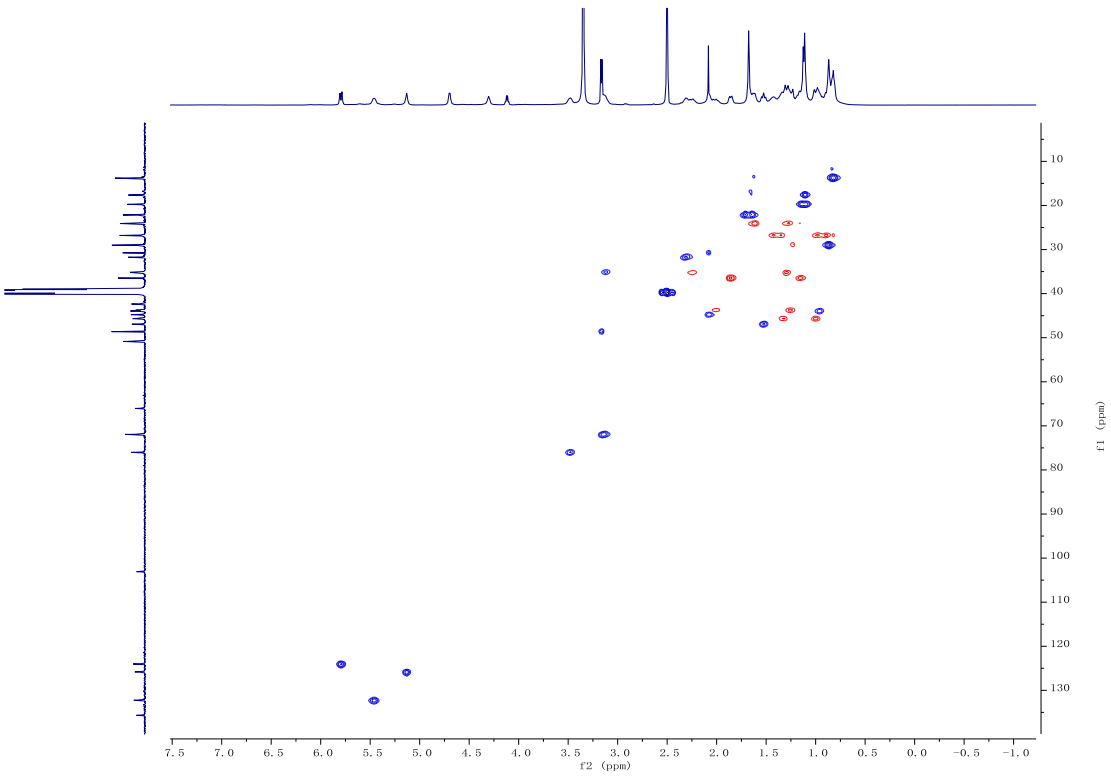

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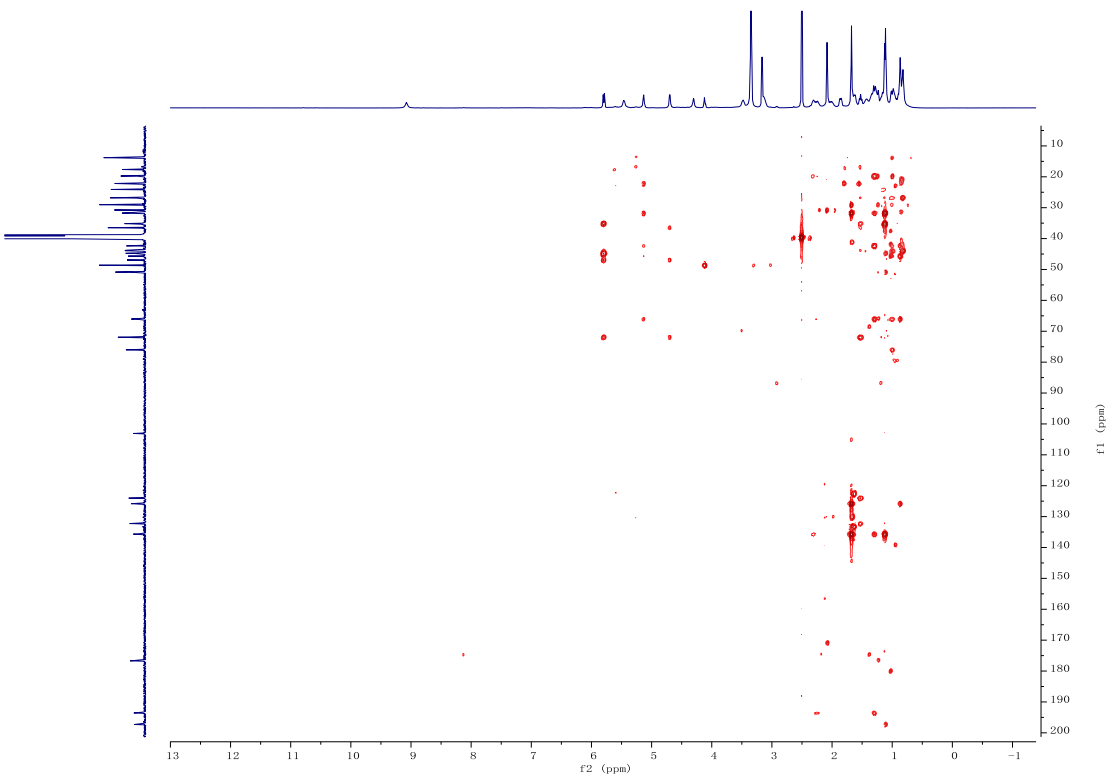

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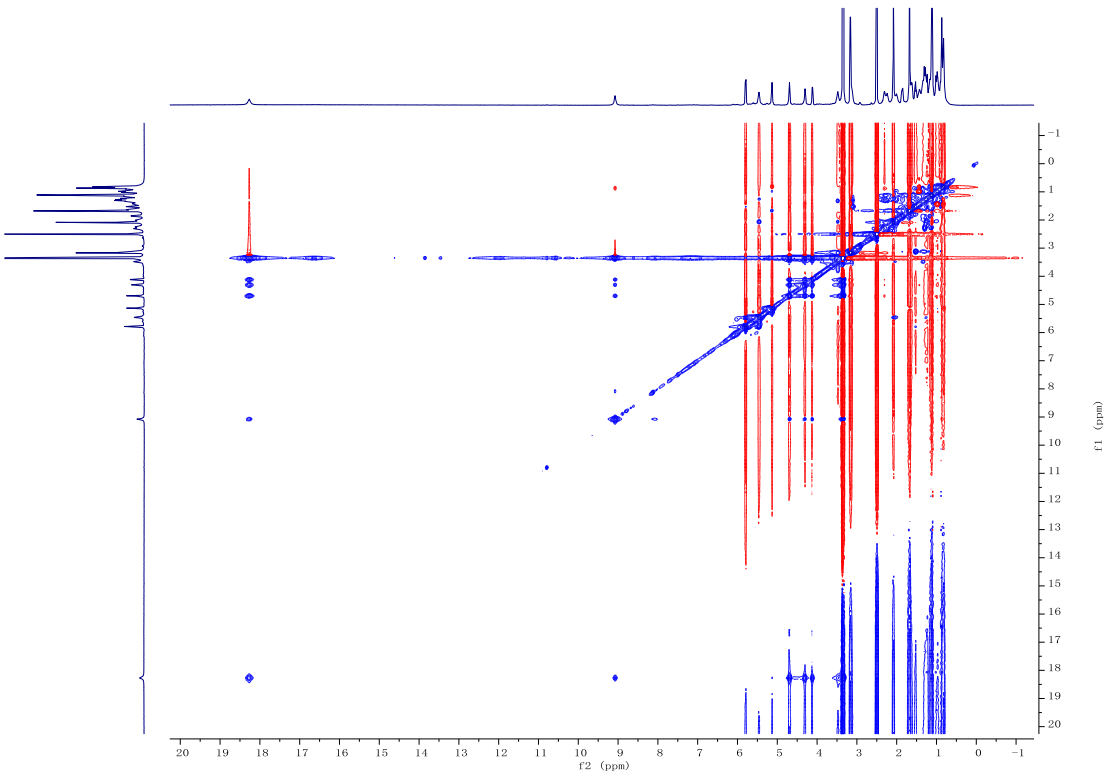

Supplementary Figure 6. NMR spectra of compound **10** in methanol-d_4. (**a**) ^{1}H NMR spectrum. (**b**) ^{13}C NMR spectrum. (**c**) DEPT-135 NMR spectrum. (**d**) ^{1}H-^{1}H COSY NMR spectrum. (**e**) HSQC NMR spectrum. (**f**) HMBC NMR spectrum. (**g**) NOESY NMR spectrum.

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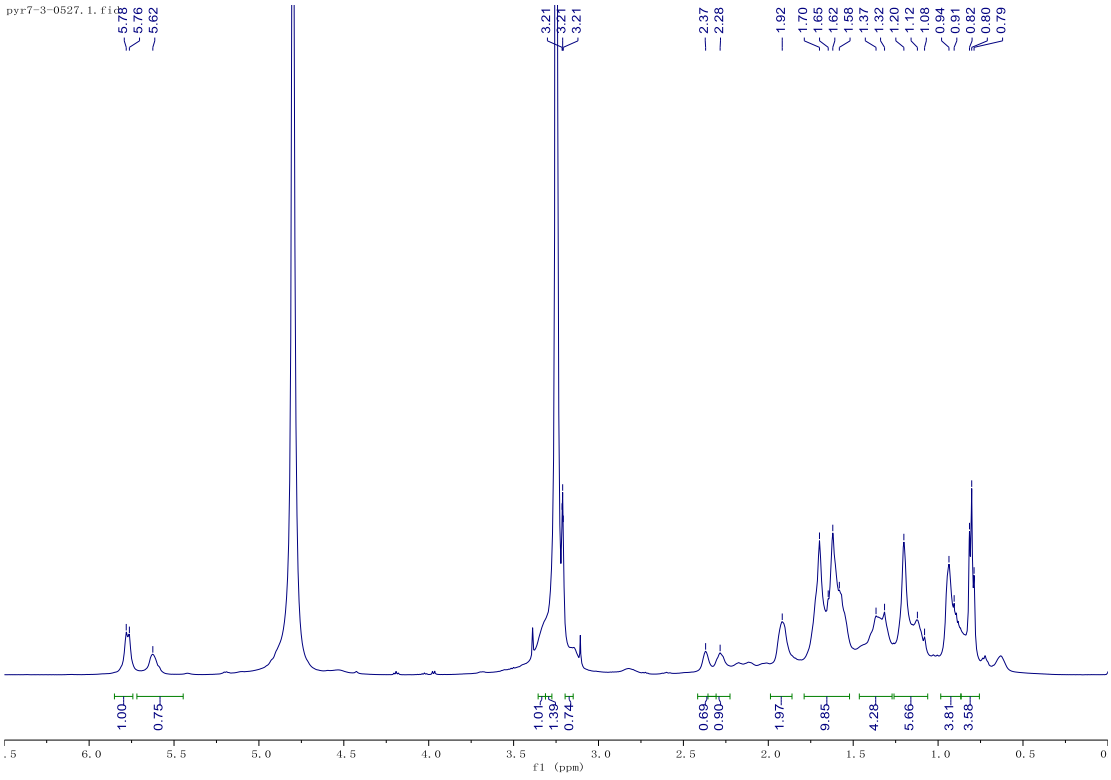

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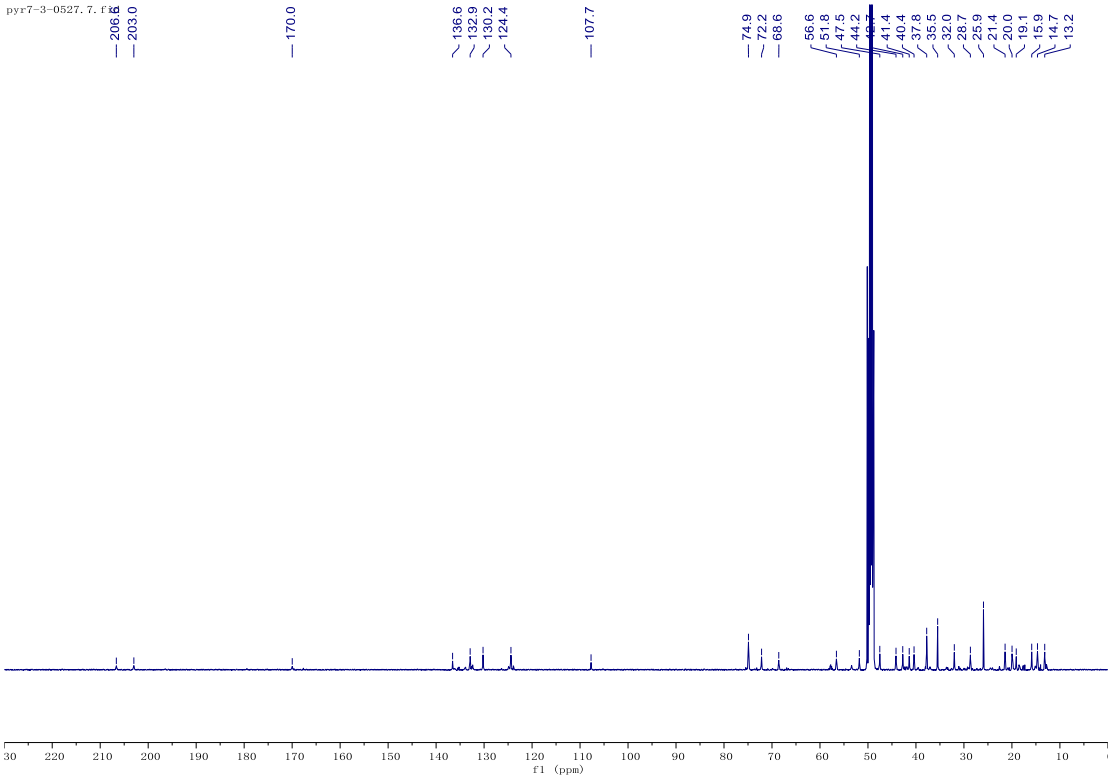
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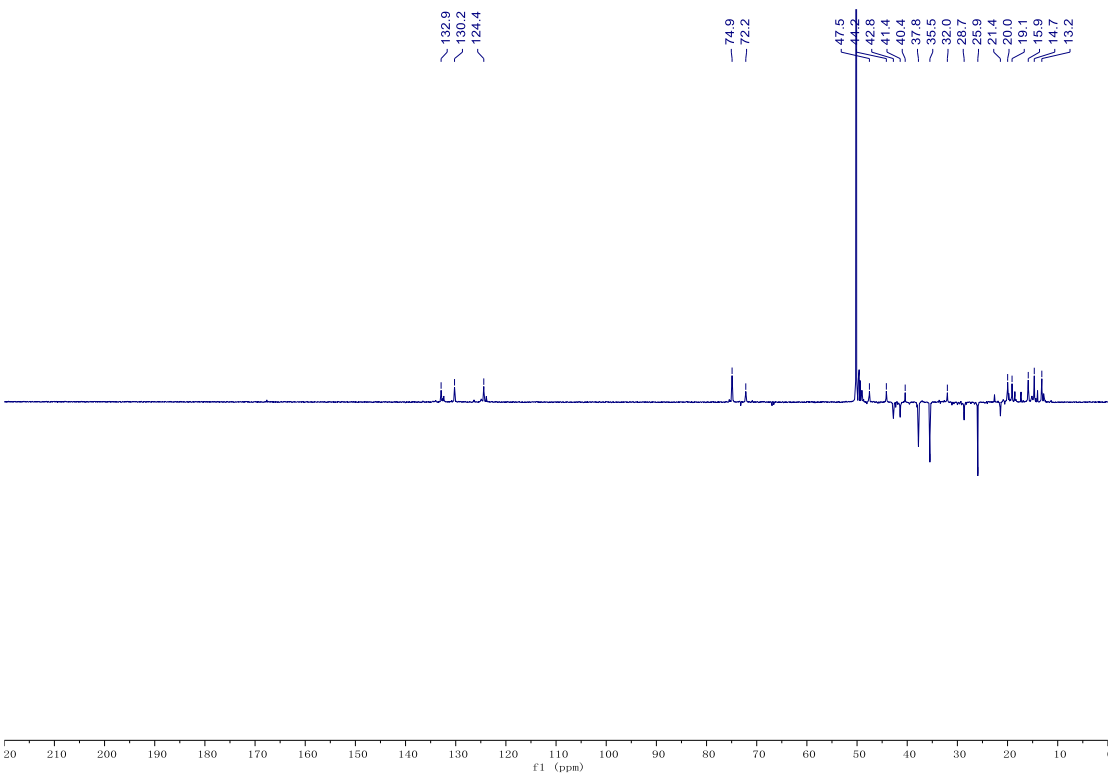
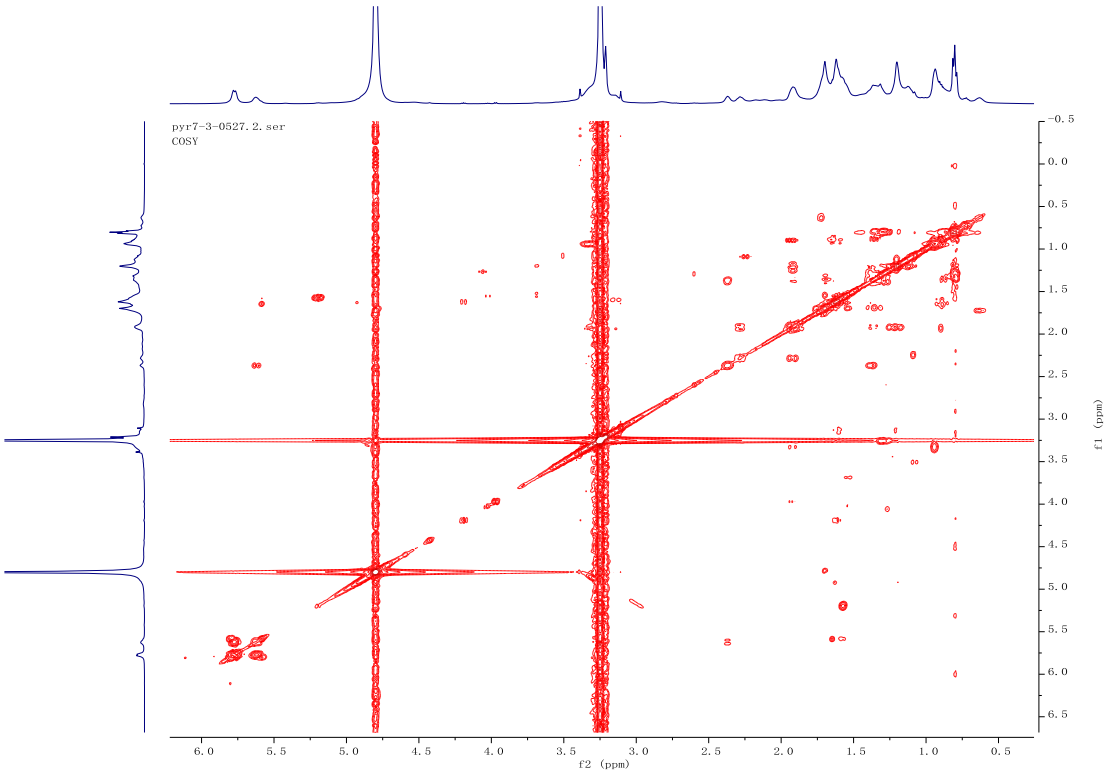
f1 (ppm)

c


132.9
130.2
124.4
74.9
72.2
47.5
44.2
42.8
41.4
40.4
37.8
35.5
32.0
28.7
25.9
21.4
20.0
19.1
15.9
14.7
13.2
f1 (ppm)

d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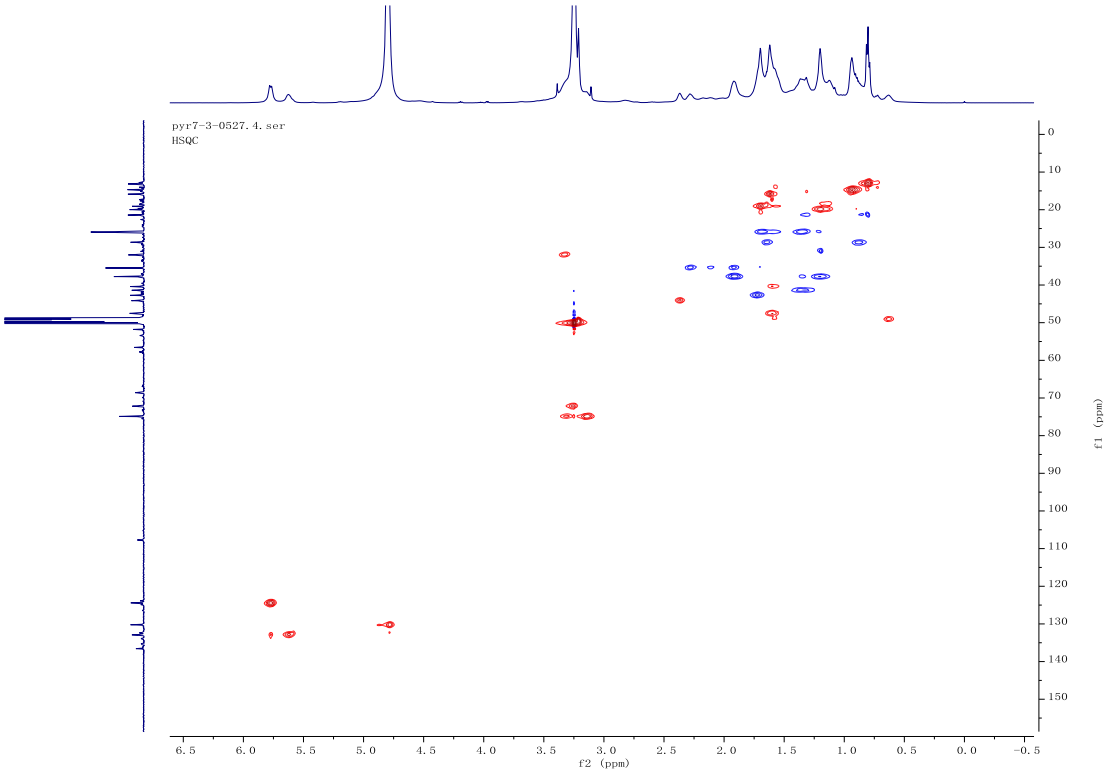
COSY
f2 (ppm)
f1 (ppm)

e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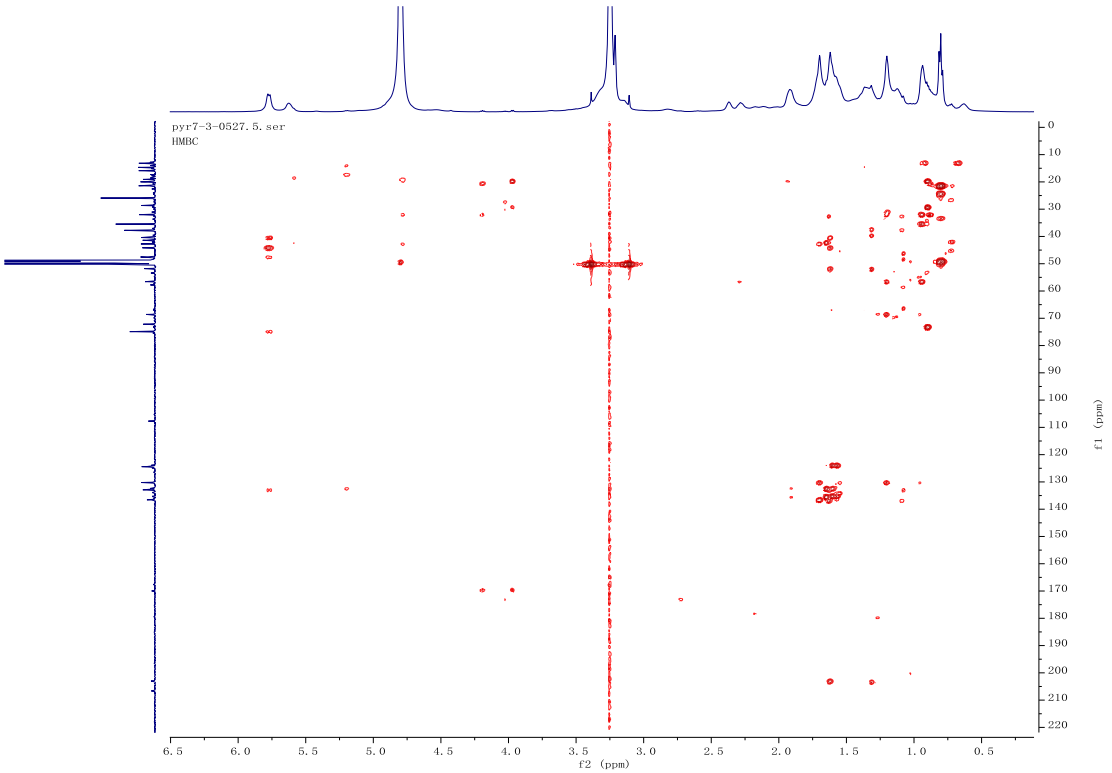
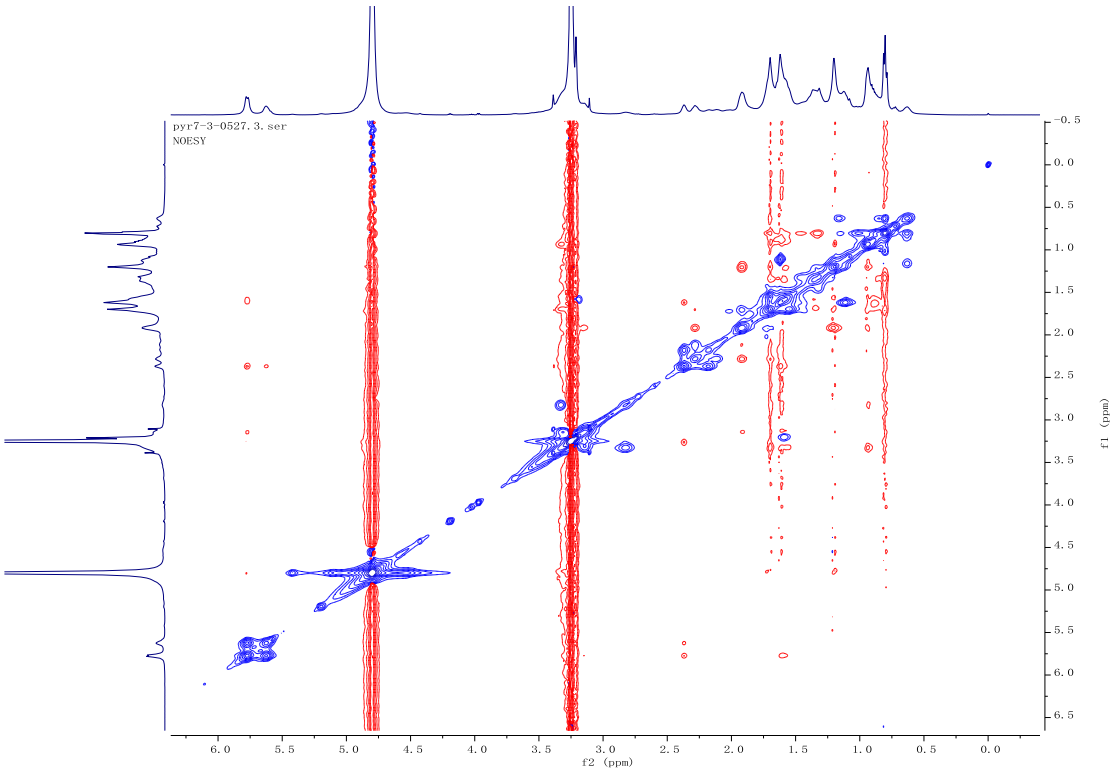
f1 (ppm)

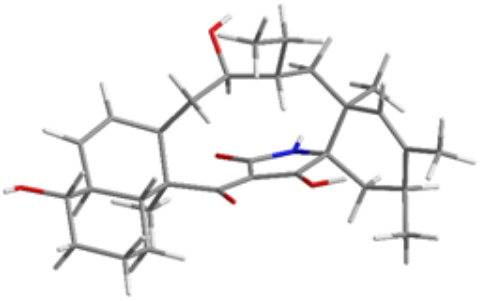
f


pyr7-3-0527.5.ser
HMBC
f2 (ppm)
f1 (ppm)

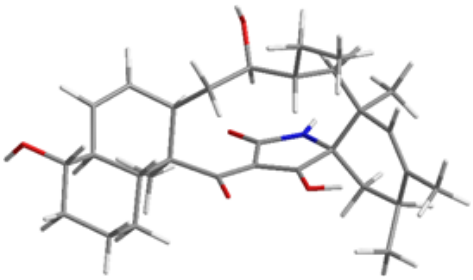
g


pyr7-3-0527.3.ser
NOESY
f2 (ppm)
f1 (ppm)

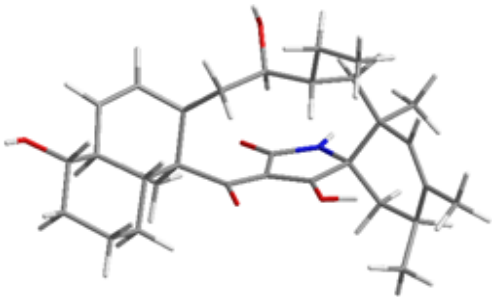
Supplementary Figure 7. Structures and populations of the dominant conformers of (*4R,5R,9S,10S,13R,15R,16R,18S,21S,23S*)-**9**. Re-optimization of the 8 dominant conformers using the M06-2X/def2-SVP method in the gas phase (T=298.15 K).



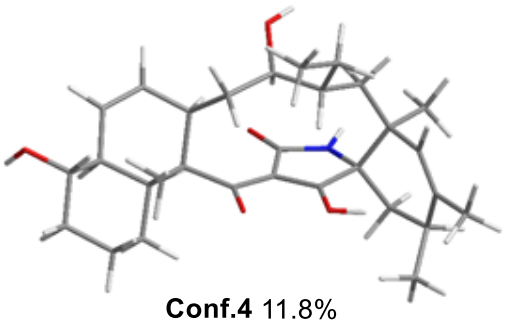
Conf.1 20.9%



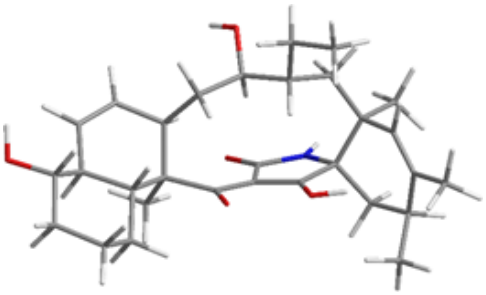
Conf.2 16.7%



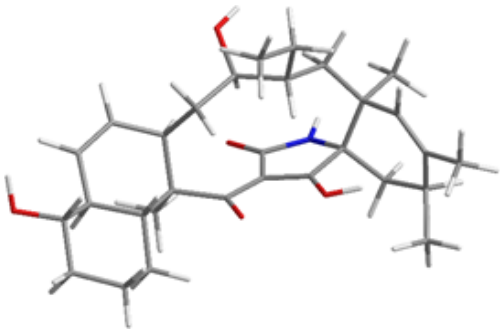
Conf.3 14.1%



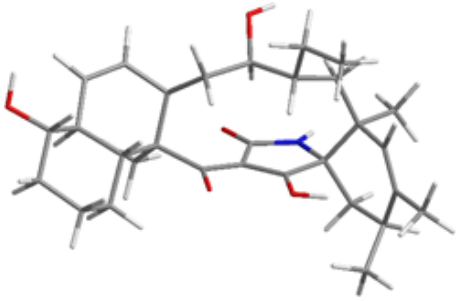
Conf.4 11.8%



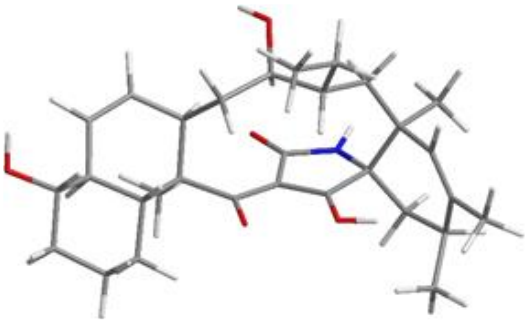
Conf.5 10.6%



Conf.6 9.2%

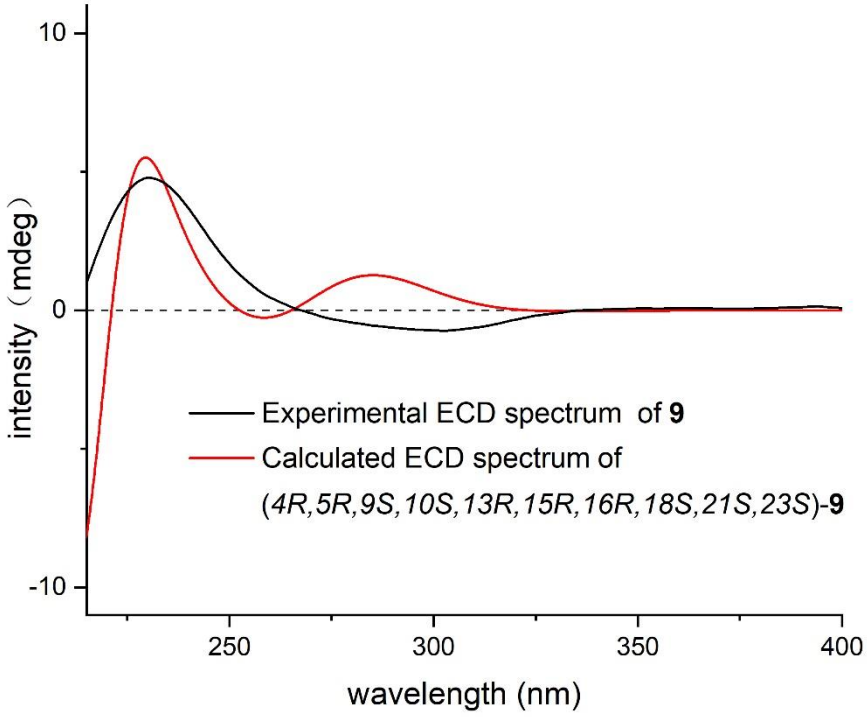


Conf.7 8.1%

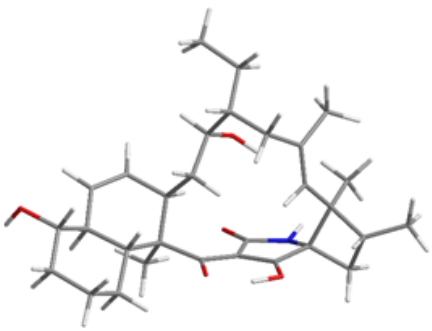


Conf.8 6.5%

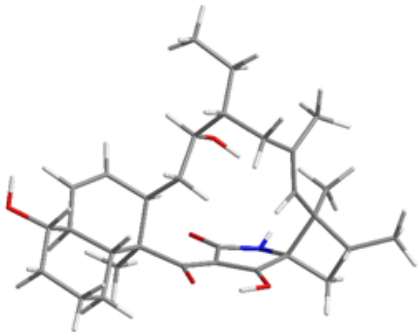
Supplementary Figure 8. Comparison of the experimentally measured ECD spectrum of **9** in methanol with the calculated ECD spectrum of (*4R,5R,9S,10S,13R,15R,16R,18S,21S,23S*)-**9**. TDDFT-ECD theoretical calculations were run at the CAM-B3LYP-SCRF/def2-SVP level in MeOH with polarizable continuum model (PCM).



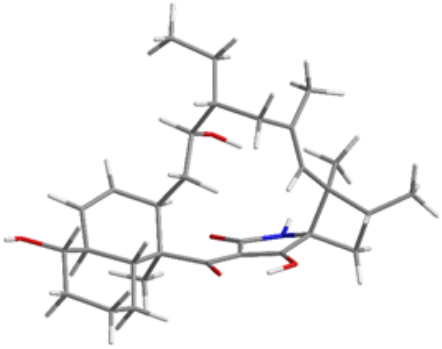
Supplementary Figure 9. Structures and populations of the dominant conformers of (*4R,5R,9S,10S,13R,15R,16R,20R,21R,23S*)-**10**. Re-optimization of the 6 dominant conformers using the B3LYP/TZVP method in the gas phase (T=298.15 K).



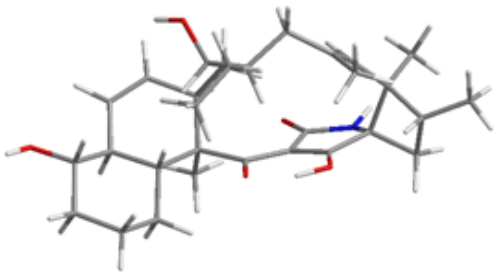
Conf.1 41.5%



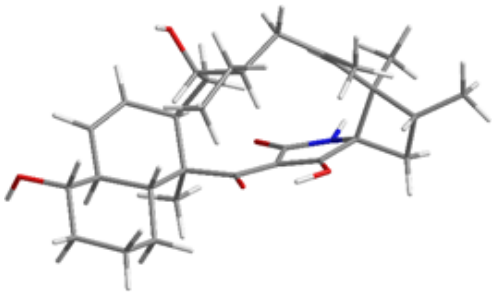
Conf.2 15.1%



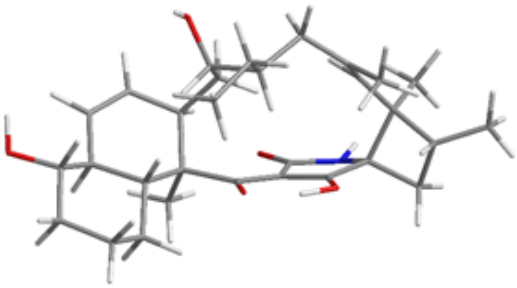
Conf.3 9.3%



Conf.4 5.6%

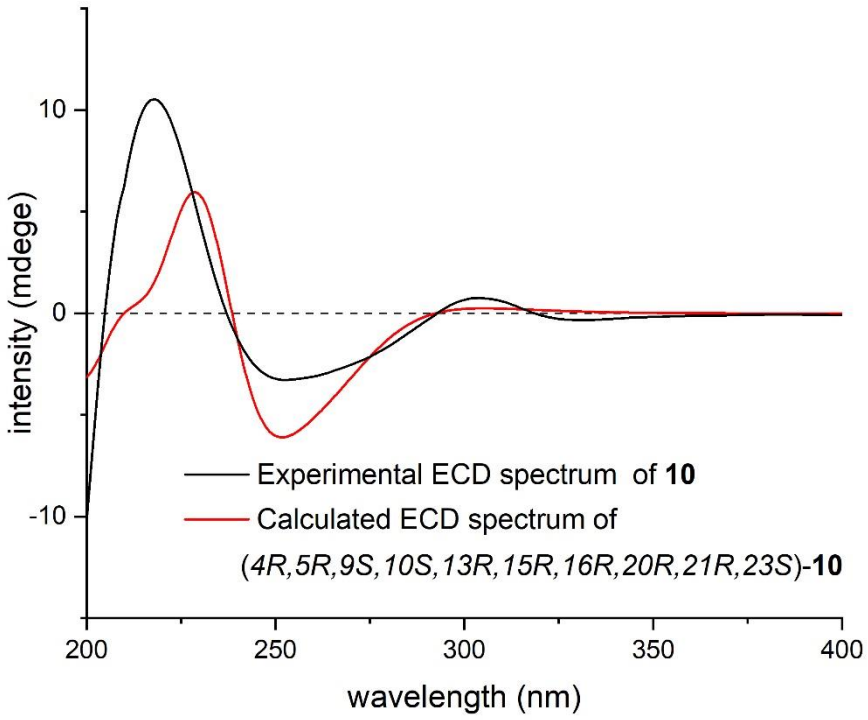


Conf.5 4.3%

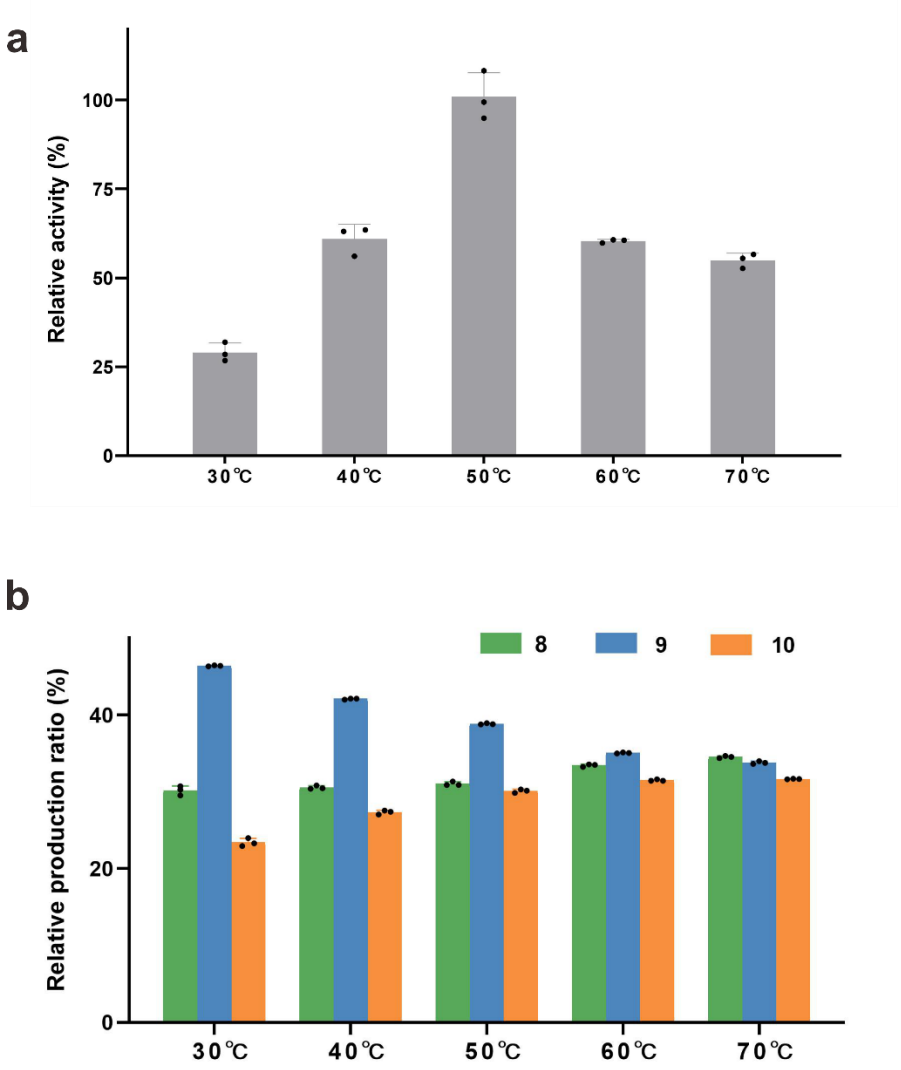


Conf.6 4.2%

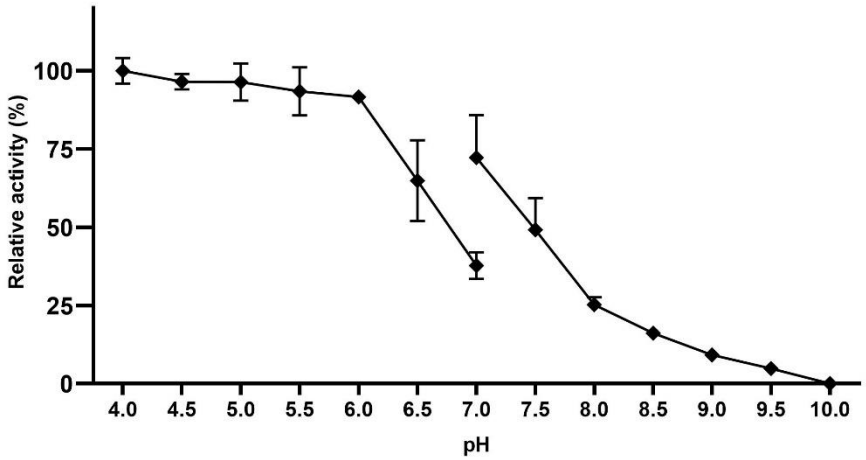
Supplementary Figure 10. Comparison of the experimentally measured ECD spectrum of **10** in methanol with the calculated ECD spectrum of (*4R,5R,9S,10S,13R,15R,16R,20R,21R,23S*)-**10**. TDDFT-ECD theoretical calculations were run at the CAM-B3LYP-SCRF/def2-SVP level in MeOH with polarizable continuum model (PCM).



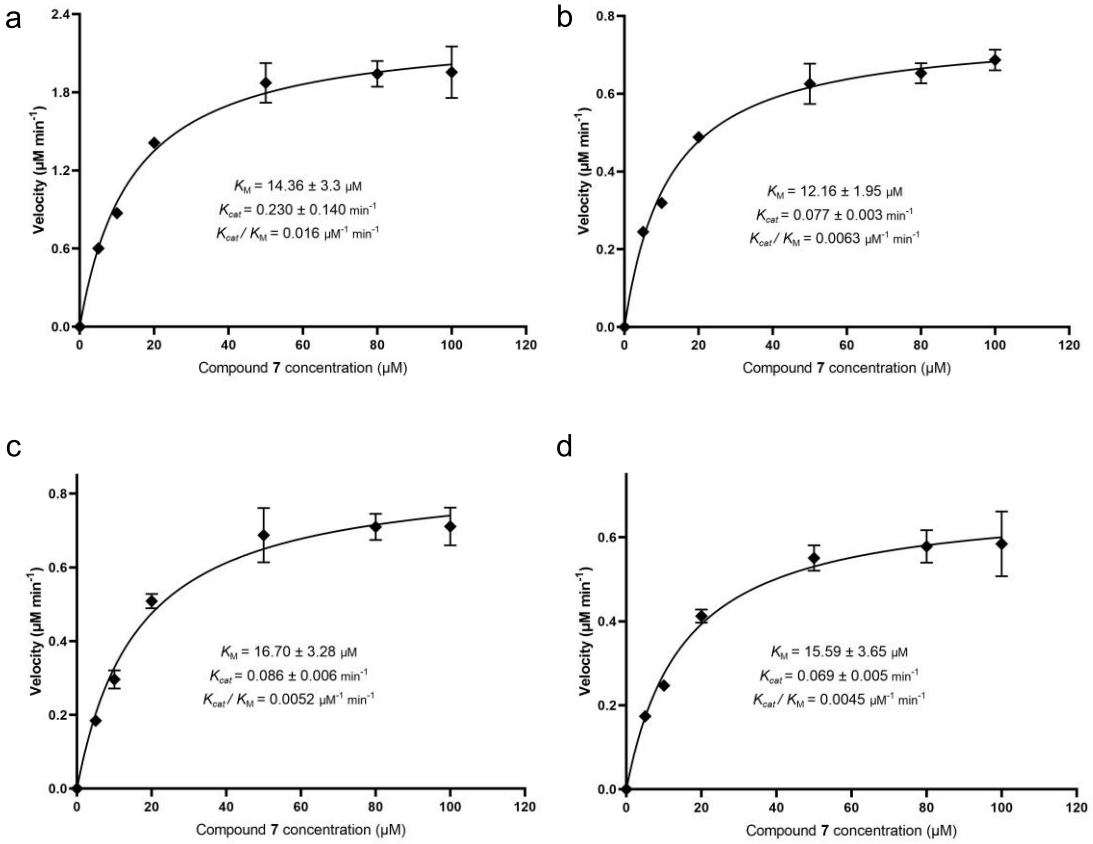
Supplementary Figure 11. Effect of temperature on the activity and selectivity of PloI4. The central value is the mean of three independent replicates with error bars representing the standard deviation. (**a**) Effect of temperature on the activity of PloI4. The activity was quantified by examining the production of all three products, i.e., **8**, **9** and **10**. (**b**) Effect of temperature on the ratio of **8**, **9** and **10**.



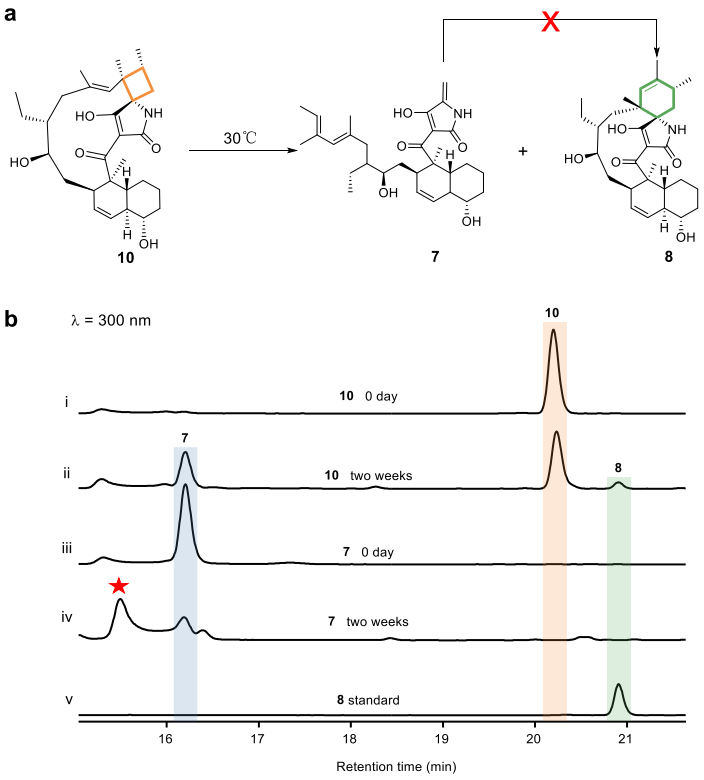
Supplementary Figure 12. Effect of pH value on the activity of PloI4. Reactions were performed by incubating **7** and PloI4 in NaOAc-HOAc (pH in the range of 4.0~7.0) or Tris-HCl (pH in the range of 7.0~10.0) buffer. The activity is quantified by examining the production of all three products, i.e., **8**, **9** and **10**. The central value is the mean of three independent replicates with error bars representing the standard deviation.



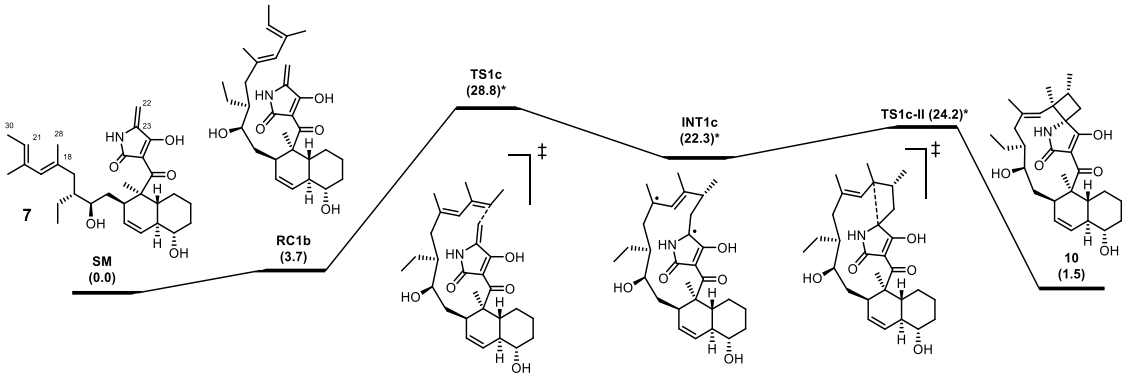
Supplementary Figure 13. Kinetic analysis of PloI4 for compound **7**. The central value is the mean of three independent replicates with error bars representing the standard deviation. (**a**) Analysis the production of all three products, i.e., **8**, **9** and **10**. (**b**) Analysis the production of **8**. (**c**) Analysis the production of **9**. (**d**) Analysis to the production of **10**.



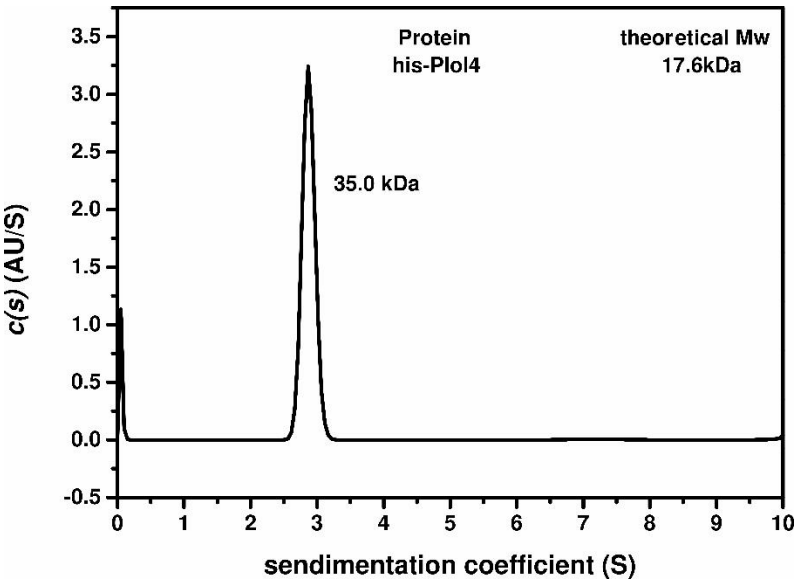
Supplementary Figure 14. Non-enzymatic conversion of compounds **7** and **10** in methanol. (**a**) Reaction profile of the non-enzymatic conversion of **7** and **10** at 30°C. (**b**) HPLC analysis of the non-enzymatic conversion of **10** at days 0 (i) and 14 (ii), and of **7** at days 0 (iii) and 14 (iv). Purified compound **8** was used as a standard (v). **10** was converted spontaneously into **7** and **8** over a 14-day incubation. Compound **7** cannot be converted spontaneously into **8**; instead, it was converted spontaneously into an unknow compound (indicated by red asterisk) that is identical in molecular weight.



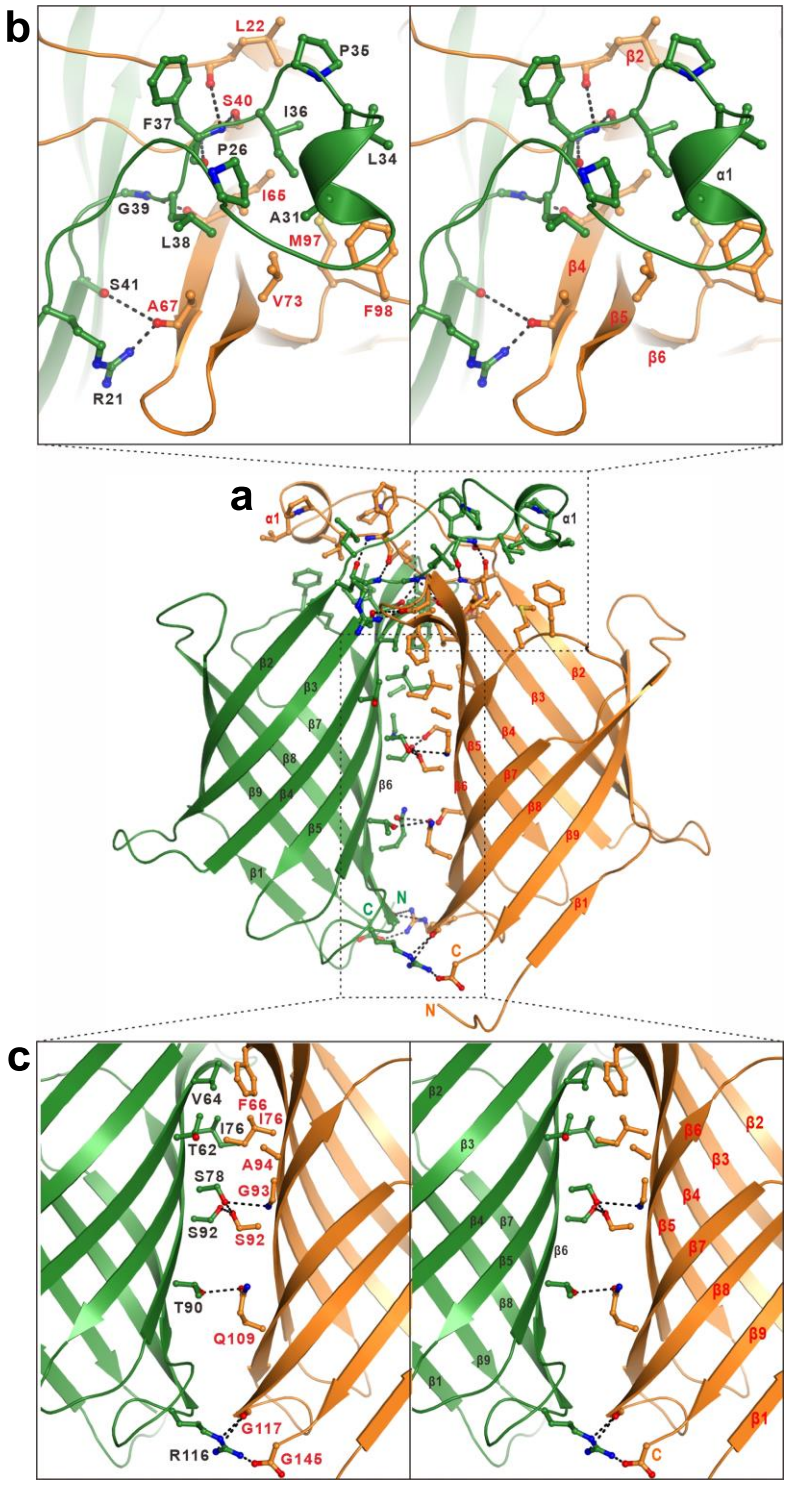
Supplementary Figure 15. Computational analyses of the transition states and energetics in the *s-trans*-path for converting **7** into *exo*-2+2 adduct **10**. Gibbs free energies in kcal/mol are shown. * indicates open-shell energies.



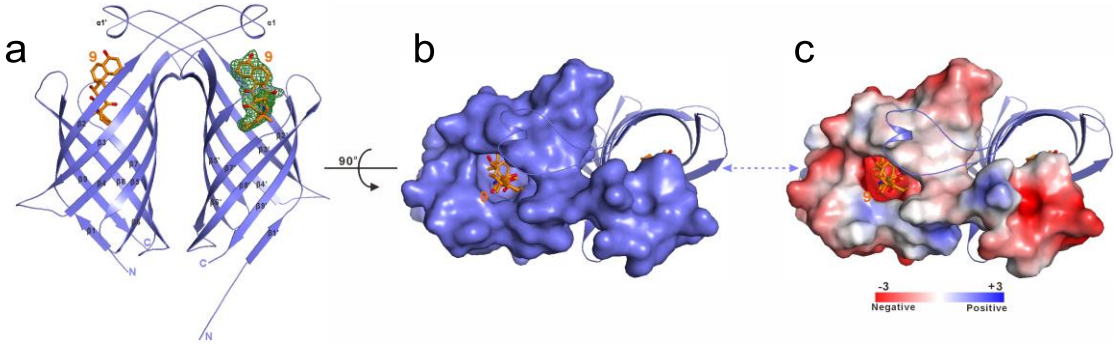
Supplementary Figure 16. Characterization of the dimeric properties of PloI4 in solution by sedimentation velocity analytical ultracentrifugation (SV-AUC).



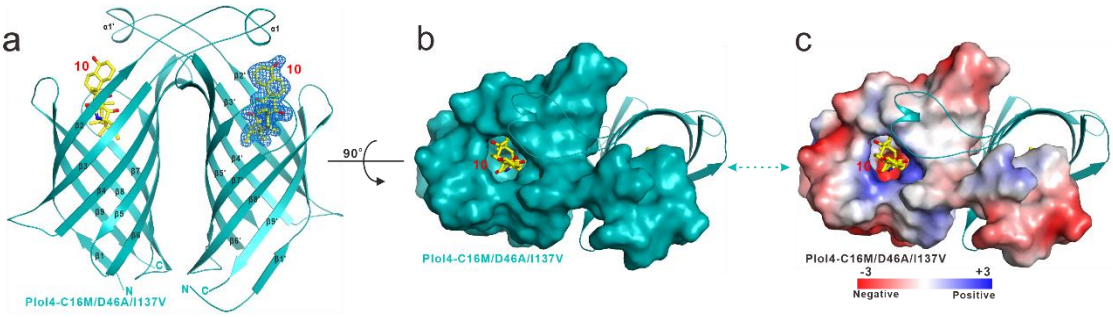
Supplementary Figure 17. Structural analysis of the dimerization interface of PloI4. (**a**) Ribbon-stick representation showing the overall dimer interface. (**b**) Detailed molecular interactions in the symmetric swapped region of PloI4. (**c**) Detailed molecular interactions in the β-barrel core region of PloI4. Hydrogen bonds and salt bridges involved in binding are shown as dotted lines.



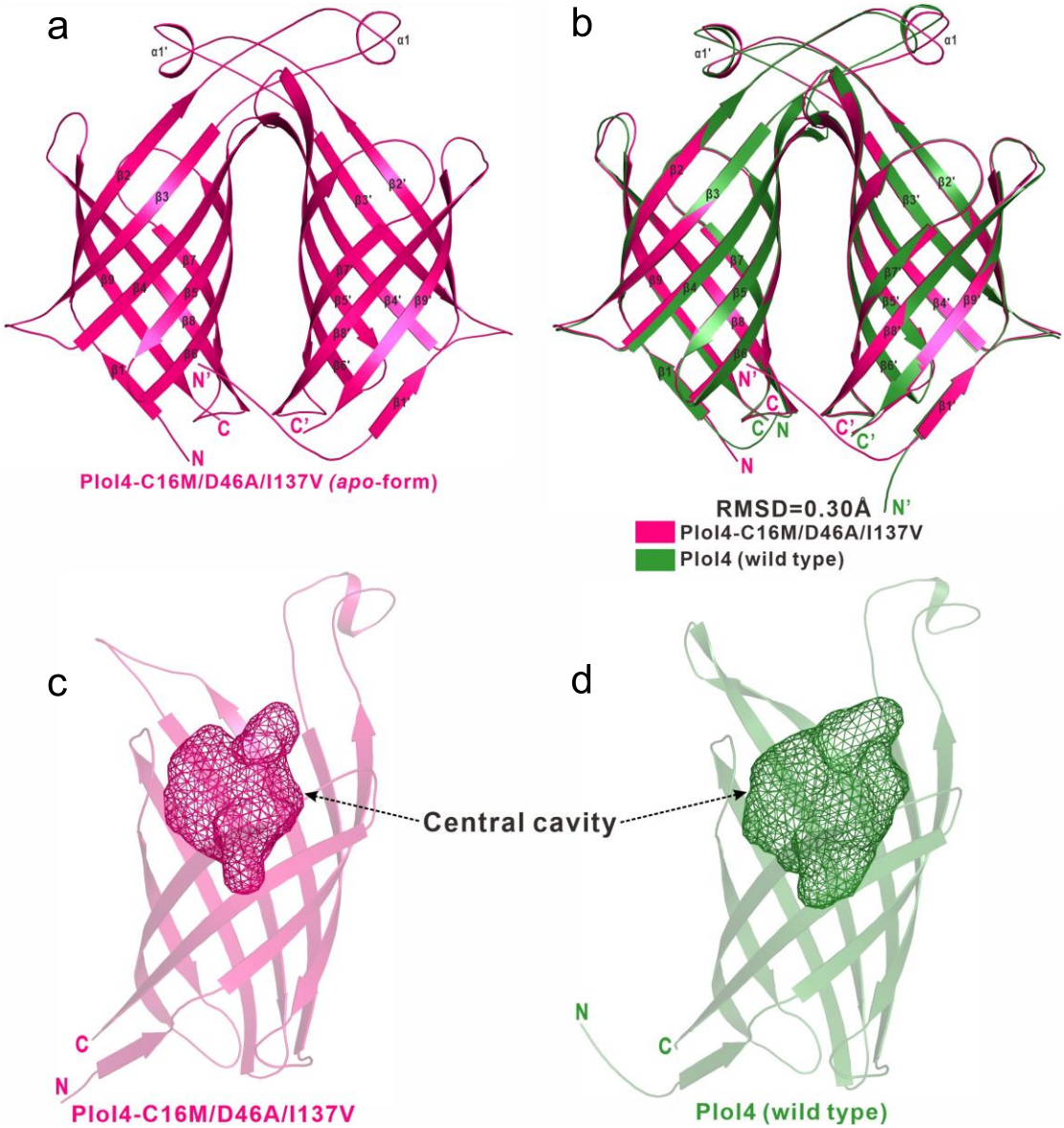
Supplementary Figure 18. Structure of PloI4-F124L in complex with **9**. Ribbon-stick diagram (**a**) and surface representation (**b**) showing the dimer architecture of PloI4-F124L in complex with **9**. Compound **9** (orange) is shown in stick mode. The Fo-Fc map of one of the bound **9** molecules in the dimeric complex is indicated in green, and the electron density map is calculated by omitting **9** from the final PDB file and contoured at 2.0s. (**c**) Surface charge potential representation (contoured at ±3 kT/eV; blue/red) of PloI4-F124L complex, in which the highly acidic cavity is indicated.



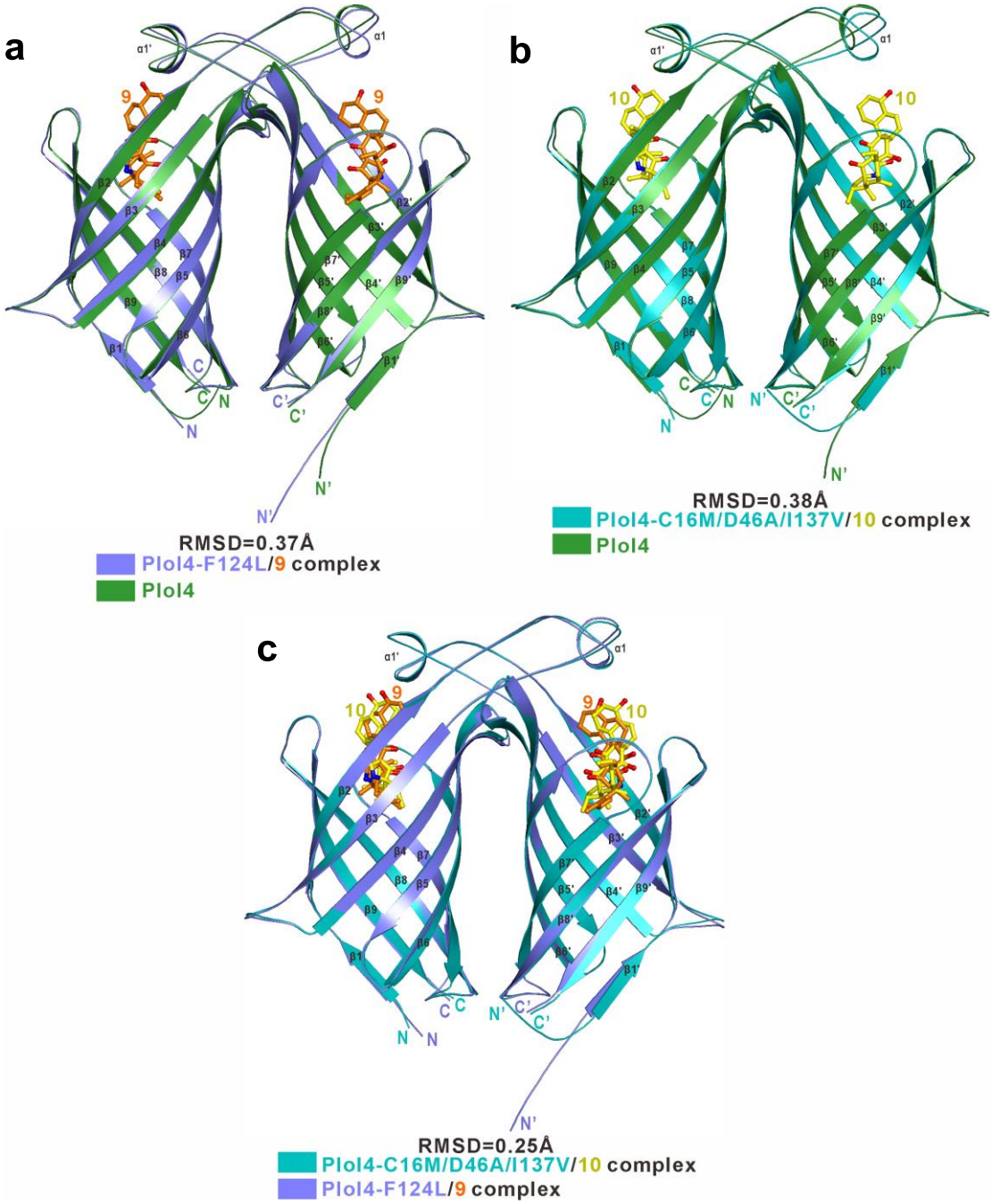
Supplementary Figure 19. Structure of PloI4-C16M/D46A/I137V in complex with **10**. Ribbon-stick diagram (**a**) and surface representation (**b**) showing the dimer architecture of PloI4-C16M/D46A/I137V in complex with **10**. Compound **10** (yellow) is shown in stick mode. The Fo-Fc map of one of the bound **10** molecules in the dimeric complex is indicated in blue, and the electron density map is calculated by omitting **10** from the final PDB file and contoured at 2.0s. (**c**) Surface charge potential representation (contoured at ±3 kT/eV; blue/red) of PloI4-C16M/D46A/I137V complex, in which the highly acidic cavity is indicated.



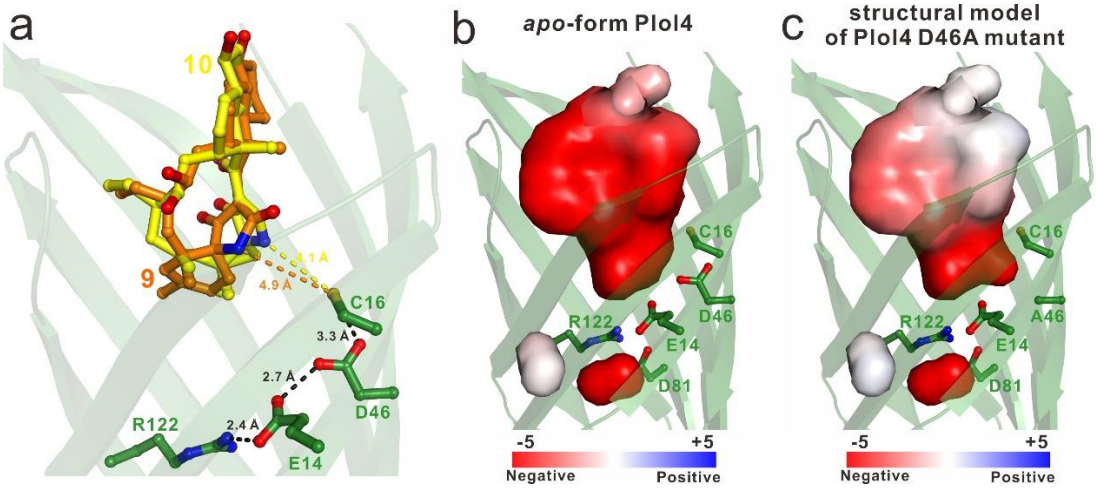
Supplementary Figure 20. Crystal structure alignment of apo-form PloI4 (green) and its variant PloI4-C16M/D46A/I137V (pink). (**a**) Ribbon diagram showing the dimer architecture of PloI4-C16M/D46A/I137V variant. (**b**) Comparison of the conformations of wild-type PloI4 and its PloI4-C16M/D46A/I137V variant. Combination of wireframe diagram and ribbon representation showing the different central cavities of PloI4-C16M/D46A/I137V variant (**c**) and wild-type PloI4 (**d**).



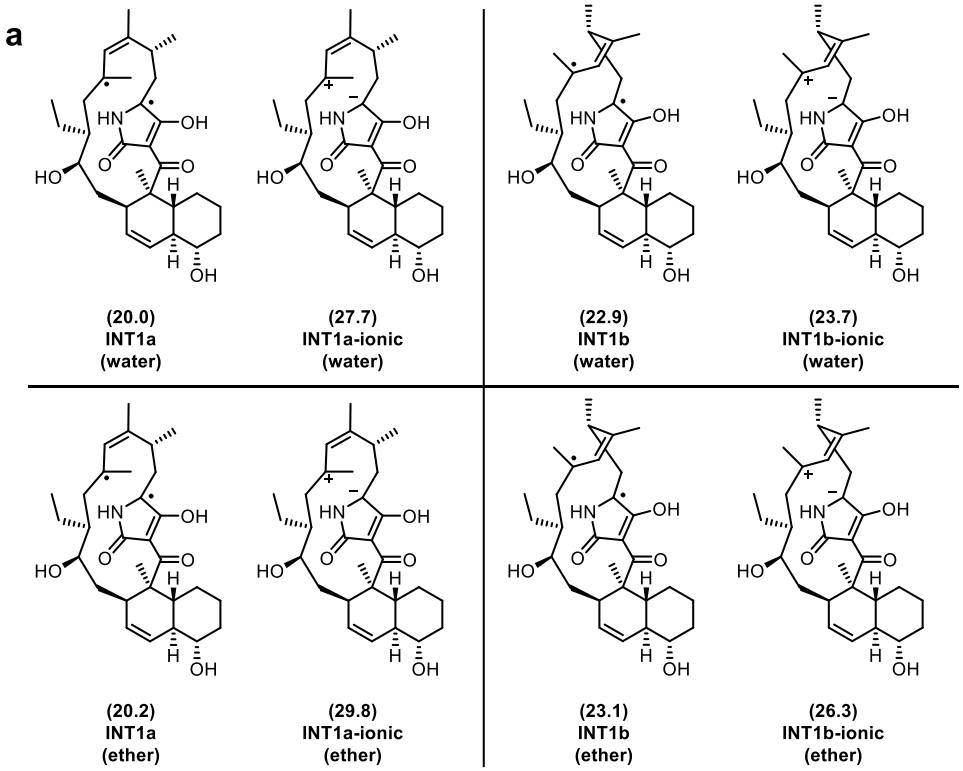
Supplementary Figure 21. Crystal structure alignment of wild-type PloI4 and its variants in complex with their products. (**a**) Wild-type PloI4 and PloI4-F124L/**9** complex. (**b**) Wild-type PloI4 and PloI4-C16M/D46A/I137V/**10** complex. (**c**) PloI4-F124L/**9** complex and PloI4-C16M/D46A/I137V/**10** complex. The structures of wild-type PloI4 (green), PloI4-F124L (purple) and PloI4-C16M/D46A/I137V (blue) are shown in ribbon model, and the products **9** (orange) and **10** (yellow) are shown in stick-ball model.

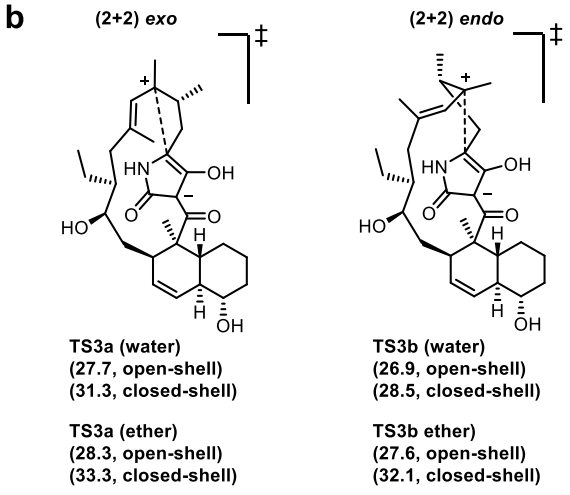


Supplementary Figure 22. Structural analyses and putative hypothesis for the function of D46A mutation. (**a**) Aligned *endo*-4+2 adduct **9** (orange) and *exo*-2+2 adduct **10** (yellow) into the apo-PloI4 (green) structure and the side chains of related residues E14, C16, D46 and R122. Hydrogen bonds among these residues are shown as black dotted lines. The distances from the side chain sulfur of residue C16 to the tetronate amide groups of **9** and **10** are indicated by orange and yellow dashed lines, respectively. (**b**) Surface charge potential of the central cavity of PloI4 (contoured at ±5 kT/eV; blue/red). (**c**) Surface charge potential of the central cavity of the structural model of PloI4-D46A (contoured at ±5 kT/eV; blue/red).

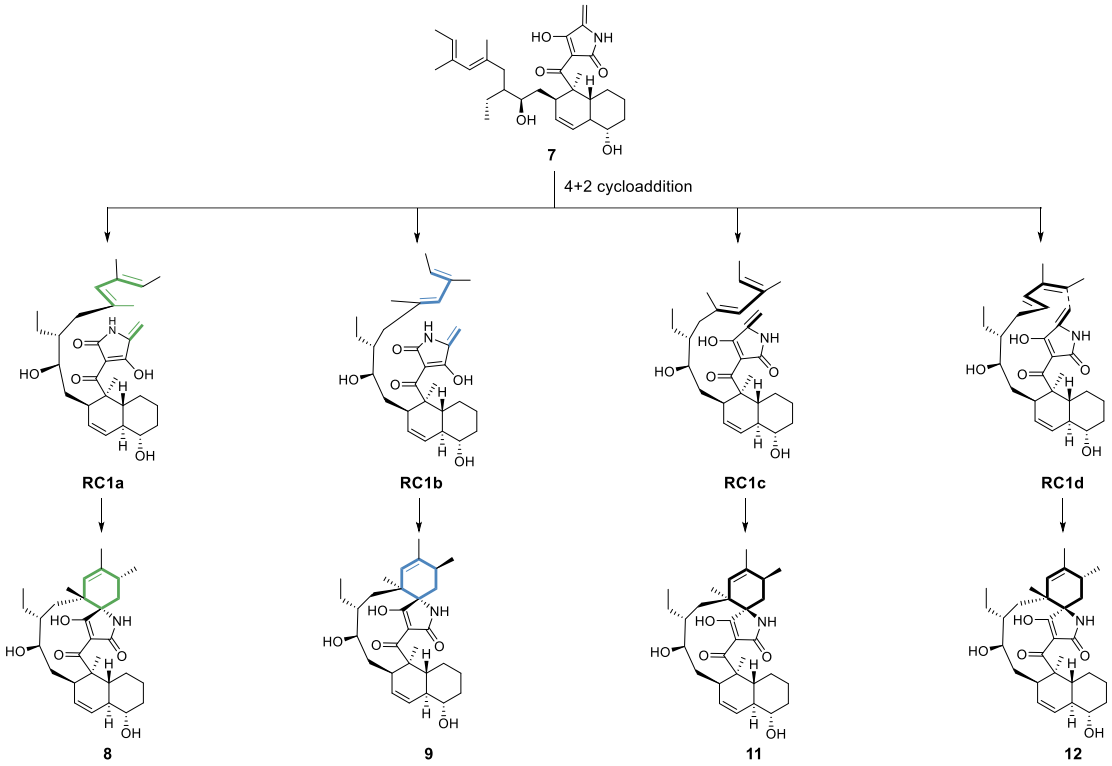


Supplementary Figure 23. Energy comparison of variable intermediate **INT1** and the transition state **TS3** in the *exo* or *endo*-path leading to a 2+2 product. Gibbs free energies in kcal/mol are shown. Density functional M06-2X/6-311++g(2d,p)//M06-2X/6-31g(d,p) was coupled with CPCM solvation of either water or diethyl ether to simulate in-solution and in-enzyme environment, respectively. (**a**) Intermediate **INT1.** (**b**) **TS3**.





Supplementary Figure 24. Four possible 4+2 adducts and corresponding reactive conformers of the **7**. The structures **11** and **12** are unobserved isomers when the reaction is catalyzed by wild-type PloI4.



3. Supplementary Tables

Supplementary Table 1. Bacterial strains and plasmids used in this study.

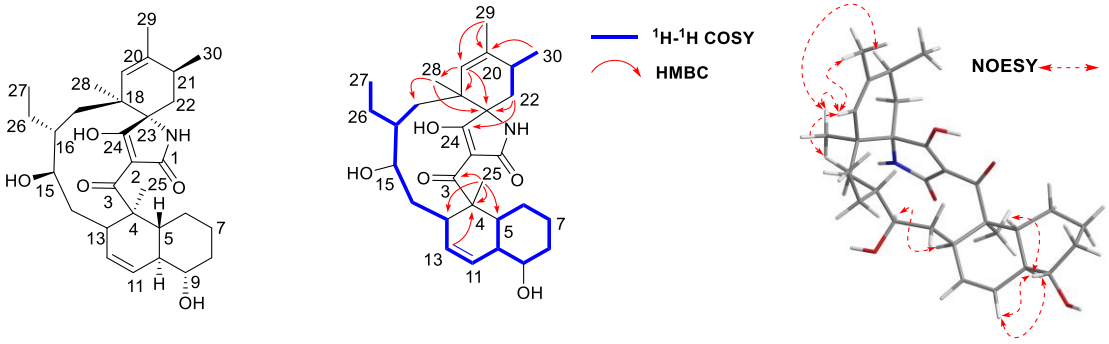
Strain/plasmid	Relevant Characteristics	Source/ Reference
E. coli		
DH5α	Host for general cloning	Invitrogen
BL21 (DE3)	Host for protein expression	NEB
S. raseosporus		
NRRL 21084	Wild type, PYRs producing strain	NRRL
WL2101	*pyrE3* in-frame deletion mutant, PYR non-producing	[1]
***Micromonospora* sp. C39217-R109-7**		
ATCC 53791	Wild type, PLO-A producing strain	ATCC
Plasmids		
pET-28a(+)	Protein expression vector used in *E. coli*, encoding N-terminal 6 × His-tag, kanamycin resistance	Novagen
pWL1022	pET-28a(+) derivative for expressing 6 × His-PyrE3	[1]
pWL1024	pET-28a(+) derivative for expressing 6 × His-PyrI4	[1]
pWL2021	pET-28a(+) derivative for expressing 6 × His-PloI4	This study
pWL2022	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (I137F)	This study
pWL2023	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (I137Y)	This study
pWL2024	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (I137W)	This study
pWL2025	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (I137V)	This study
pWL2026	pET-28a(+) derivative for expressing 6 × His-PloI4	This study

	variant (F124A)	
pWL2027	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (F124V)	This study
pWL2028	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (F124L)	This study
pWL2029	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (F124I)	This study
pWL2030	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (C16M)	This study
pWL2031	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (D46A)	This study
pWL2032	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (C16M/I137V)	This study
pWL2033	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (C16M/D46A/I137V)	This study
pWL2034	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (Q75A)	This study
pWL2035	pET-28a(+) derivative for expressing 6 × His-PloI4 variant (Y95A)	This study

Supplementary Table 2. Oligonucleotide primers used in this study.

Primer	Sequence
PloI4-I137F-For	5’-CCGGGCACTTCTCTGTTCCGTTCTTCTCTG’
PloI4-I137F-Rev	5’-AGTACCAGAGAAGAACGGGACAGAGAAGTG-3’
PloI4-I137Y-For	5’-CCGGGCACTTCTCTGTATCGTTCTTCTCTG-3’
PloI4-I137Y-Rev	5’-AGTACCAGAGAAGAACGATACAGAGAAGTG-3’
PloI4-I137W-For	5’-CCGGGCACTTCTCTGTGGCGTTCTTCTCTG-3’
PloI4-I137W-Rev	5’-AGTACCAGAGAAGAACGCCACAGAGAAGTG-3’
PloI4-I137V-For	5’-CCGGGCACTTCTCTGGTTCGTTCTTCTCTG-3’
PloI4-I137V-Rev	5’- AGTACCAGAGAAGAACGAACCAGAGAAGTG-3’
PloI4-F124A-For	5’-TCTGGCACTCGTACCGCGCAGCTGCTGGAA-3’
PloI4-F124V-Rev	5’-AGGGCGTTCCAGCAGCTGCGCGGTACGAGTG-3’
PloI4-F124V-For	5’-TCTGGCACTCGTACCGTTCAGCTGCTGGAA-3’
PloI4-F124V-Rev	5’-GGGCGTTCCAGCAGCTGAACGGTACGAGTG-3’
PloI4-F124L-For	5’-TCTGGCACTCGTACCCTTCAGCTGCTGGAA-3’
PloI4-F124L-Rev	5’-GGGCGTTCCAGCAGCTGAAGGGTACGAGTG-3’
PloI4-F124I-For	5’-TCTGGCACTCGTACCATTCAGCTGCTGGAA-3’
PloI4-F124I-Rev	5’-GGGCGTTCCAGCAGCTGAATGGTACGAGTG-3’
PloI4-C16M-For	5’-GACATCAAGGAGATCATGCACACCACGATC-3’
PloI4-C16M-Rev	5’-AGACGGATCGTGGTGTGCATGATCTCCTTG-3’
PloI4-D46A-For	5’-TCCGTTGAATTCGAAGCCGAACTGTACGAC-3’
PloI4-D46A-Rev	5’-TCCGCGTCGTACAGTTCGGCTTCGAATTCA-3’
PloI4-Q75A-For	5’-GATGGTACCGTGATGGCAATTGTTAGCGCG-3’
PloI4-Q75A-Rev	5’-TCGAACGCGCTAACAATTGCCATCACGGTA-3’
PloI4-Y95A-For	5’-ACCTGGTCCGGTGCTGCAACCATGTTTCCA-3’
PloI4-Y95A-Rev	5’-TCAGTTGGAAACATGGTTGCAGCACCGGAC-3’

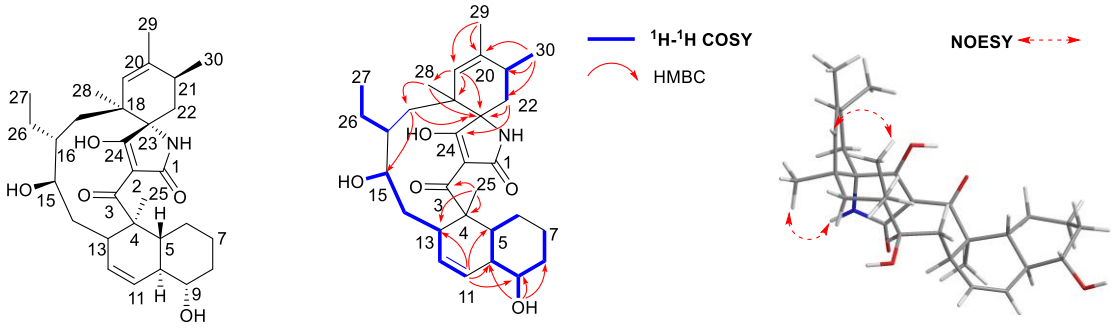
Supplementary Table 3. NMR spectroscopic data for compound **9** recorded in methanol-d_4[a].



No.	δ_C, type	δ_H (type, *J* in Hz)	No.	δ_C, type	δ_H (type, *J* in Hz)
1	178.1, s		**16**	45.6, d	1.16 (m, overlap)
2	105.1, s		**17**	46.9, t	1.46 (m, overlap, H-17a) 1.15 (m, overlap, H-17b)
3	198.8, s		**18**	43.9, s	
4	52.7, s		**19**	127.0, d	5.24 (s)
5	36.9, d	1.48 (m, overlap)	**20**	138.2, s	
6	28.3, t	1.47 (m, overlap, H-6a) 1.02 (m, overlap, H-6b)	**21**	33.7, d	2.38 (br s)
7	25.6, t	1.72 (m, overlap, H-7a) 1.48 (m, overlap, H-7b)	**22**	36.9, t	2.38 (m, H-22a) 1.42 (m, overlap, H-22b)
8	37.5, t	2.00 (m, H-8a) 1.29 (m, H-8b)	**23**	67.6, s	
9	74.3, d	3.39 (m)	**24**	195.9, s	
10	48.5, d	1.69 (m, overlap)	**25**	18.2, q	1.24 (s)
11	124.8, d	5.86 (dd, *J* = 10.1, 1.9 Hz)	**26**	27.8, t	1.52 (m, overlap, H-26a) 1.15 (m, overlap, H-26b)
12	133.8, d	5.58 (br s)	**27**	14.2, q	0.93 (m)
13	46.5. d	2.18 (m, overlap)	**28**	29.0, q	0.94 (s)
14	44.8, t	2.18 (m, overlap, H-14a) 1.42 (m, overlap, H-14b)	**29**	22.4, q	1.77 (s)
15	78.7, d	3.71 (m)	**30**	20.6, q	1.21 (d, *J* = 7.2 Hz)

[a] 500 MHz for ^{1}H and 125 MHz for ^{13}C NMR. Chemical shifts were reported in ppm. ov = overlapped; All signals were determined according to COSY, HSQC, HMBC, and NOESY correlations.

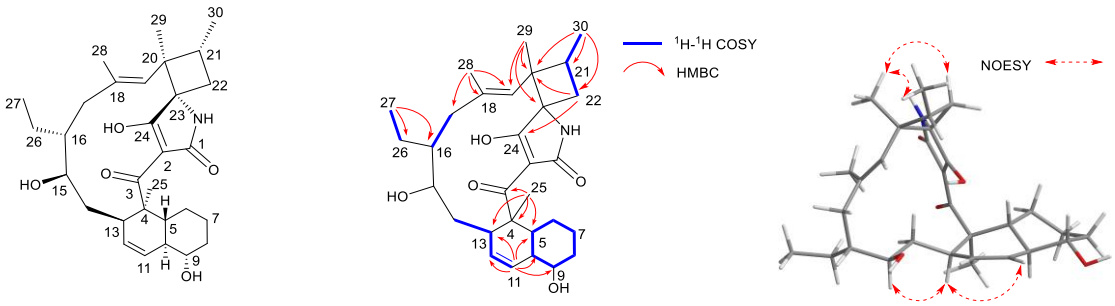
Supplementary Table 4. NMR spectroscopic data for compound **9** recorded in DMSO-d_6[a].



No.	δ_C, type	δ_H (type, *J* in Hz)	No.	δ_C, type	δ_H (type, *J* in Hz)
1	176.7, s		**16**	43.9, d	0.96 (m, overlap)
2	103.1, s		**17**	45.7, t	1.32 (m, overlap, H-17a) 1.00 (m, overlap, H-17b)
3	197.3, s		**18**	42.4, s	
4	50.8, s		**19**	125.8, d	5.13 (s)
5	35.2, d	3.12 (m, overlap)	**20**	135.7, s	
6	26.8, t	1.34 (m, overlap, H-6a) 0.90 (m, overlap, H-6b)	**21**	31.7, d	2.30 (m, overlap)
7	24.1, t	1.62 (m, overlap, H-7a) 1.28 (m, overlap, H-7b)	**22**	35.3, t	2.24 (m, overlap, H-22a) 1.29 (m, overlap, H-22b)
8	36.5, tF	1.86 (d, *J* = 9.5 Hz , H-8a) 1.16 (m, overlap, H-8b)	**23**	66.0, s	
9	71.9, d	3.14 (m, overlap)	**24**	193.6, s	
9-OH		4.70 (d, *J* = 5.5 Hz)	**24-OH**		18.27(s)
10	46.9, d	1.53 (t, *J* = 10.5 Hz)	**25**	17.6, q	1.11 (s)
11	124.0, d	5.79 (d, *J* = 10.1 Hz)	**26**	26.8, t	1.43 (m, overlap, H-26a) 0.98 (m, overlap, H-26b)
12	132.2, d	5.46 (br s)	**27**	13.8, q	0.82 (m)
13	44.8, d	2.07 (m, overlap)	**28**	29.0, q	0.87 (s)
14	43.8, t	2.01 (m, overlap, H-14a) 1.25 (m, overlap, H-14b)	**29**	22.2, q	1.68 (s)
15	76.0, d	3.48 (br s)	**30**	19.7, q	1.12 (d, *J* = 7.2 Hz)
15-OH		4.30 (s)	**NH**		9.08 (s)

[a] 500 MHz for ^{1}H and 125 MHz for ^{13}C NMR. Chemical shifts were reported in ppm. ov = overlapped; All signals were determined according to COSY, HSQC, HMBC, and NOESY correlations.

Supplementary Table 5. NMR spectroscopic data for compound **10** recorded in methanol-d_4[a].



No.	δ_C, type	δ_H (type, *J* in Hz)	No.	δ_C, type	δ_H (type, *J* in Hz)
1	170.0, s		**16**	49.4, d	1.16 (m)
2	107.7, s		**17**	42.7, t	1.91 (m, overlap, H-17a) 1.73 (m, overlap, H-17b)
3	203.0, s		**18**	136.6, s	
4	51.8, s		**19**	130.2, d	4.78 (br s)
5	40.4, d	1.59 (m, overlap)	**20**	56.6, s	
6	28.7, t	1.65 (m, overlap, H-6a); 0.88 (m, H-6b)	**21**	32.0, d	3.33 (br s)
7	25.9, t	1.68 (m, overlap, H-7a) 1.35 (m, overlap, H-7b)	**22**	35.5, t	2.28 (m, H-22a) 1.92 (m, H-22b)
8	37.8, t	1.91 (m, H-8a) 1.21 (m, overlap, H-8b)	**23**	68.6, s	
9	74.9, d	3.14 (m)	**24**	206.6, s	
10	47.5, d	1.60 (m, overlap)	**25**	15.9, q	1.61 (s)
11	124.4, d	5.78 (br s)	**26**	21.4, t	1.32 (m, H-26a) 0.86 (m, H-26b)
12	132.9, d	5.63 (br s)	**27**	13.2, q	0.80 (m)
13	44.2, d	2.37 (br s)	**28**	19.1, q	1.70 (s)
14	41.4, t	1.38 (m, overlap, H-14a) 1.30 (m, H-14b)	**29**	20.0, q	1.20 (s)
15	72.2, d	3.26 (m)	**30**	14.7, q	0.94 (br s)

[a] 500 MHz for ^{1}H and 125 MHz for ^{13}C NMR. Chemical shifts were reported in ppm. ov = overlapped; All signals were determined according to COSY, HSQC, HMBC, and NOESY correlations.

Supplementary Table 6. Comparison of PloI4 and its variants in enzyme activity and selectivity.

		Enzyme activity	Selectivity (**8** vs **9** vs **10**)	Description
PloI4	WT	100%	32:38:40	
	Q75A	n.a.	n.d.	
	Y95A	28%	40:34:26	
	I137F	22%	>95:5	**8** vs **10,** and **9** was not observed
	I137Y	9%	>96:4	**8** vs **10,** and **9** was not observed
	I137W	n.a.	n.d.	
	I137V	71%	15:11:74	
	F124A	68%	>99:1	**9** vs **10,** and **8** was not observed
	F124V	65%	1:95:4	
	F124L	74%	3:95:2	
	F124I	66%	4:93:3	
	C16M	19%	>80:20	**8** vs **10,** and **9** was not observed
	D46A	84%	3:21:76	
	C16M/I137V	7%	>90:10	**8** vs **10,** and **9** was not observed
	C16M/D46A/I137V	101%	>97:3	**8** vs **10,** and **9** was not observed

n.a.: no activity was observed. n.d.: not determined.

Supplementary Table 7. DNA sequences of PloI4 used in this study.

PloI4 from *Micromonospora* sp.C39217-R109-7 (codon optimized for *E. coli*)
ATGAGCACTGTGACCACTATCAACCTGGAGGACATCAAGGAGATCTGCCACACCAC
GATCCGTCTGGGCGGTAAACCGGAGAGCGGTGAAGCAGCAGAACTGCCTATCTTCC
TGGGTAGCTCCGTTGAATTCGAAGACGAACTGTACGACGCGGACGGTACGCAAATT
GGCACCGCTAAAGGTACCTCCGTCATCTTCGCGGAAGCTGATGGTACCGTGATGCAG
ATTGTTAGCGCGTTCGATGATTACACCGATGGTGGTCGCGTTACCTGGTCCGGTGCTT
ACACCATGTTTCCAACTGATGAACCGAAATCCGTACCGGCCCAGGGCGTTTCTGGCC
GTTATCGTGGCCTGTCTGGCACTCGTACCTTTCAGCTGCTGGAACGCCCGGACCCGG
GCACTTCTCTGATTCGTTCTTCTCTGGTACTGAATGGC*

Supplementary Table 8. Statistics of X-ray crystallographic data collection and model refinements.

	PloI4	PloI4-F124L/**9** complex
Data collection		
Wavelength (Å)	0.80000	0.97915
Space group	$P4_322$	$C121$
Unit cell a，b，c (Å)	101.66, 101.66, 234.42	180.98, 88.81, 50.77
Unit cell α，β，γ (°)	90.00, 90.00, 90.00	90.00, 92.73, 90.00
Resolution range (Å)	50.00 - 2.90 (2.95 - 2.90)	90.39 - 2.30 (2.34 - 2.30)
R_{merge} (%)[a]	23.90 (112.70)	29.6 (83.1)
Mean I / σ(I)	12.4 (2.6)	6.8 (2.4)
Completeness (%)	99.9 (100.0)	99.50 (98.1)
Multiplicity	13.8 (13.3)	9.6 (5.8)
Refinement		
Resolution range (Å)	29.73 - 2.90 (2.95 - 2.90)	90.39 - 2.30 (2.37 - 2.30)
Reflections	27906	35402
R_{work} / R_{free} (%)[b]	19.90 (26.70) / 23.34 (30.37)	21.14 (30.45) / 25.45 (36.20)
Number of atoms		
Non-hydrogen atoms	4290	4647
Macromolecules	4286	4341
Ligands	0	144
Solvent	4	162
Wilson B-factor (Å^2)	53.69	56.49
RMSD (bonds) (Å)	0.003	0.003
RMSD (angles) (°)	0.59	0.99
Ramachandran plot[c]		
Favored (%)	96.65	98.59
Allowed (%)	3.35	1.41
Outliers (%)	0.00	0.00

[a] $R_{merge} = \sum|I_i - I_m|/\sum I_i$, where I_i is the intensity of the measured reflection and I_m is the mean intensity of all symmetry related reflections.

[b] $R_{work} = \Sigma||F_{obs}| - |F_{calc}||/\Sigma|F_{obs}|$, where F_{obs} and F_{calc} are observed and calculated structure factors. $R_{free} = \Sigma_T||F_{obs}| - |F_{calc}||/\Sigma_T|F_{obs}|$, where T is a test data set of about 5% of the total reflections randomly chosen and set aside prior to refinement.

[c]Defined by Molprobity.

Numbers in parentheses represent the value for the highest resolution sell.

Supplementary Table 9. Statistics of X-ray crystallographic data collection and model refinements.

	PloI4-C16M/D46A/I137V	PloI4-C16M/D46A/I137V/**10** complex
Data collection		
Wavelength (Å)	0.97853	0.97856
Space group	$C222_1$	$C222_1$
Unit cell a，b，c (Å)	84.96, 174.48, 50.49	84.59, 175.92, 50.69
Unit cell α，β，γ (°)	90.00, 90.00, 90.00	90.00, 90.00, 90.00
Resolution range (Å)	76.39 - 1.97 (2.00 - 1.97)	76.23 - 2.10 (2.14 - 2.10)
R_{merge} (%)[a]	56.3 (137.3)	21.2 (132.1)
Mean I / σ(I)	10.8 (2.2)	10.3 (2.0)
Completeness (%)	97.5 (99.4)	99.9 (100.0)
Multiplicity	13.1 (11.9)	10.7 (10.6)
Refinement		
Resolution range (Å)	76.39 - 1.97 (2.04 - 1.97)	76.23 - 2.10 (2.20 - 2.10)
Reflections	26471	22429
R_{work} / R_{free} (%)[b]	17.20 (21.94) / 21.47 (28.37)	17.68 (21.48) / 21.80 (25.56)
Number of atoms		
Non-hydrogen atoms	2612	2443
Macromolecules	2251	2177
Ligands	48	72
Solvent	313	194
Wilson B-factor (Å^2)	24.93	24.77
RMSD (bonds) (Å)	0.009	0.013
RMSD (angles) (°)	1.13	1.41
Ramachandran plot[c]		
Favored (%)	98.25	98.58
Allowed (%)	1.75	1.42
Outliers (%)	0.00	0.00

[a] $R_{merge} = \sum|I_i - I_m|/\sum I_i$, where I_i is the intensity of the measured reflection and I_m is the mean intensity of all symmetry related reflections.

[b] $R_{work} = \Sigma||F_{obs}| - |F_{calc}||/\Sigma|F_{obs}|$, where F_{obs} and F_{calc} are observed and calculated structure factors. $R_{free} = \Sigma_T||F_{obs}| - |F_{calc}||/\Sigma_T|F_{obs}|$, where T is a test data set of about 5% of the total reflections randomly chosen and set aside prior to refinement.

[c]Defined by Molprobity.

Numbers in parentheses represent the value for the highest resolution sell.

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5. XYZ Coordinates of the DFT Optimized Structure and the Corresponding Energies

SM (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31152936			
Zero-point correction= 0.692496			
Thermal correction to Energy= 0.729761			
Thermal correction to Enthalpy= 0.730705			
Thermal correction to Gibbs Free Energy= 0.624265			
C	1.287511	-1.206885	-0.690317
C	2.482884	-0.572903	0.013794
O	2.824322	-0.959402	1.142082
C	3.268900	0.527648	-0.559149
C	4.378708	0.967751	0.129353
O	4.846962	0.525377	1.263188
H	4.180653	-0.176344	1.537191
C	5.028990	2.073214	-0.592814
C	6.130073	2.718401	-0.208655
H	6.613581	2.425079	0.714632
H	6.554395	3.527818	-0.789797
N	4.228679	2.261830	-1.716411
C	3.140367	1.411282	-1.746592
O	2.278706	1.468595	-2.614779
H	4.337370	3.005322	-2.389952
C	1.731592	-1.695028	-2.081250
H	2.132837	-0.871093	-2.673761
H	0.868707	-2.100183	-2.616764
H	2.490952	-2.477911	-2.004444
C	0.711612	-2.372102	0.154264
C	1.662141	-3.547931	0.436604
H	2.622980	-3.199586	0.815239
C	1.017563	-4.499694	1.449706
C	-0.341493	-5.008010	0.963835
C	-1.267889	-3.868634	0.544151
O	-2.503733	-4.368329	0.057097
H	-2.312144	-4.923591	-0.710361
H	-1.533826	-3.260661	1.420009
C	-0.568877	-2.955513	-0.478526
C	-1.496284	-1.912817	-1.023931
C	-1.133729	-0.647145	-1.213400
C	0.214511	-0.082909	-0.851092
H	0.556251	0.529730	-1.690882
C	0.047083	0.846657	0.375637
H	-0.593884	0.353271	1.113171

H	1.006052	1.053871	0.863141
C	-0.536603	2.203642	-0.033594
H	-1.379972	2.033120	-0.720222
C	-1.062615	3.036201	1.143754
C	0.054415	3.398389	2.130765
C	-0.363297	4.431867	3.175500
H	0.490112	4.736875	3.786747
H	-0.768515	5.328441	2.694611
H	-1.128512	4.041709	3.852282
H	0.904909	3.778751	1.556383
H	0.397495	2.486965	2.638160
H	-1.432766	3.973243	0.701186
C	-2.240653	2.340429	1.860751
C	-3.310955	1.830863	0.924207
C	-3.508282	0.509327	0.783091
C	-4.433010	-0.211744	-0.115283
C	-4.662685	0.199210	-1.373942
C	-5.538776	-0.442083	-2.409148
H	-4.939766	-0.783628	-3.260876
H	-6.260017	0.281058	-2.804699
H	-6.096562	-1.297885	-2.027728
H	-4.133804	1.090066	-1.710803
C	-4.987660	-1.483582	0.479796
H	-4.173011	-2.202074	0.638839
H	-5.441836	-1.287150	1.456154
H	-5.733890	-1.963756	-0.153256
H	-2.914990	-0.148358	1.422432
C	-4.076915	2.900791	0.190679
H	-4.254860	3.754198	0.853851
H	-3.510854	3.282687	-0.668874
H	-5.034621	2.531947	-0.181081
H	-1.854220	1.515364	2.471215
H	-2.688917	3.063376	2.554130
O	0.453479	2.988918	-0.689926
H	0.749919	2.524674	-1.485790
H	-1.865768	0.056098	-1.604558
H	-2.504715	-2.232218	-1.277790
H	-0.268773	-3.614977	-1.313844
H	-0.836083	-5.613489	1.729788
H	-0.191824	-5.655206	0.086589
H	1.679974	-5.347334	1.650903
H	0.888154	-3.967534	2.401084
H	1.852764	-4.093497	-0.497415
H	0.431186	-1.938072	1.126414

RC1a (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31276364			
Zero-point correction= 0.693269			
Thermal correction to Energy= 0.730350			
Thermal correction to Enthalpy= 0.731294			
Thermal correction to Gibbs Free Energy= 0.626297			
C	-18.687912	8.306503	-34.914698
O	-22.228885	8.493513	-31.488024
C	-12.943281	8.146156	-37.312161
C	-12.845065	7.143541	-36.423106
C	-14.946971	5.547673	-38.918873
C	-15.616703	6.494814	-38.263077
C	-15.932979	6.510073	-36.824307
O	-15.496141	5.559218	-36.026034
N	-16.186519	7.672960	-38.750074
C	-16.866079	8.368306	-37.771766
O	-17.421283	9.445954	-37.955245
C	-16.734272	7.577921	-36.530726
C	-17.292294	7.731048	-35.174883
O	-16.619408	7.263673	-34.254202
C	-13.474308	9.470657	-36.932502
C	-13.228942	10.175684	-35.813764
C	-13.872592	11.523338	-35.612057
C	-15.027287	11.510923	-34.586538
C	-15.350576	12.944483	-34.138815
C	-14.334684	13.500768	-33.142279
C	-16.233080	10.799219	-35.215518
C	-17.339535	10.462875	-34.208308
C	-18.606529	9.869391	-34.868581
C	-19.827454	10.458941	-34.209235
C	-20.700213	9.791677	-33.459244
C	-20.588595	8.318539	-33.201615
C	-19.634607	7.896085	-36.056266
C	-19.257306	6.228485	-33.434626
C	-19.597839	5.827651	-31.996454
C	-20.921233	6.448677	-31.549128
C	-20.939014	7.961996	-31.752403
O	-16.734910	11.631778	-36.252302
C	-12.331944	9.719377	-34.691454
C	-12.299307	5.765689	-36.645290
C	-12.561345	8.033137	-38.767627

C	-19.197662	7.760423	-33.552195
H	-22.446207	8.298805	-30.568730
H	-13.221921	7.333791	-35.418582
H	-14.763916	5.609428	-39.984904
H	-14.568832	4.694043	-38.370224
H	-15.704617	5.844246	-35.111038
H	-16.119884	8.003464	-39.701233
H	-14.102217	9.949831	-37.688626
H	-14.288572	11.895659	-36.554292
H	-13.105094	12.235983	-35.286048
H	-14.724118	10.929704	-33.702513
H	-16.344561	12.982584	-33.681227
H	-15.401058	13.582883	-35.028154
H	-14.327345	12.904036	-32.224586
H	-14.573114	14.532201	-32.869588
H	-13.318523	13.494338	-33.548018
H	-15.857168	9.862197	-35.652254
H	-16.948693	9.780834	-33.442225
H	-17.625035	11.383428	-33.689401
H	-18.611216	10.211759	-35.909090
H	-19.953029	11.530316	-34.359631
H	-21.548000	10.303535	-33.012618
H	-21.343728	7.801839	-33.818092
H	-20.636027	8.286334	-35.858699
H	-19.699889	6.809045	-36.156949
H	-19.302561	8.315791	-37.006818
H	-18.312657	5.769058	-33.729637
H	-20.035067	5.841716	-34.106628
H	-18.790149	6.164073	-31.333328
H	-19.647808	4.738228	-31.905601
H	-21.125099	6.214979	-30.497132
H	-21.746879	6.031365	-32.140270
H	-20.191523	8.433367	-31.091874
H	-17.029978	11.048327	-36.967493
H	-11.804307	10.577188	-34.261471
H	-11.601583	8.981163	-35.028935
H	-12.907776	9.261842	-33.878084
H	-11.433223	5.588529	-35.997491
H	-13.052430	5.015923	-36.380835
H	-11.985551	5.590307	-37.675346
H	-11.715261	8.689409	-38.998297
H	-13.398090	8.363948	-39.394482
H	-12.301085	7.017171	-39.065375
H	-18.493635	8.122319	-32.788525

RC1b (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31271367			
Zero-point correction= 0.694238			
Thermal correction to Energy= 0.730853			
Thermal correction to Enthalpy= 0.731797			
Thermal correction to Gibbs Free Energy= 0.629250			
C	-18.812090	8.268109	-34.762534
O	-22.440595	8.855651	-31.478414
C	-12.857010	7.379875	-34.920548
C	-12.301595	6.804899	-35.999355
C	-14.775345	5.323122	-38.383019
C	-15.583752	6.237881	-37.848616
C	-15.939305	6.361845	-36.424223
O	-15.461268	5.514042	-35.540663
N	-16.266294	7.285304	-38.471189
C	-16.961981	8.056488	-37.565295
O	-17.530546	9.104616	-37.852392
C	-16.817588	7.396357	-36.250394
C	-17.414496	7.663485	-34.928481
O	-16.765959	7.289208	-33.949700
C	-13.080087	8.833221	-34.799593
C	-13.527556	9.707141	-35.716130
C	-13.794022	11.139319	-35.294468
C	-15.070193	11.278205	-34.435638
C	-15.354183	12.744756	-34.083771
C	-14.179529	13.465332	-33.422273
C	-16.265183	10.605433	-35.127165
C	-17.498357	10.497424	-34.223514
C	-18.723711	9.828586	-34.888398
C	-19.973651	10.483154	-34.354608
C	-20.865964	9.905126	-33.555268
C	-20.757250	8.475727	-33.115220
C	-19.737346	7.732211	-35.870030
C	-19.424773	6.374277	-33.063197
C	-19.806266	6.147574	-31.597204
C	-21.138282	6.818313	-31.261445
C	-21.146052	8.296645	-31.643363
O	-16.559398	11.336306	-36.310331
C	-13.880043	9.367871	-37.138011
C	-12.039823	5.333922	-36.178590
C	-13.248897	6.608052	-33.682602

C	-19.358297	7.882152	-33.359117
H	-22.685114	8.765320	-30.549792
H	-11.963933	7.456172	-36.802701
H	-14.560204	5.298005	-39.444436
H	-14.322545	4.581529	-37.737407
H	-15.723286	5.846862	-34.656421
H	-16.100192	7.596208	-39.417231
H	-12.922940	9.226432	-33.791570
H	-13.895283	11.780113	-36.178414
H	-12.942581	11.512312	-34.717041
H	-14.893990	10.720866	-33.503001
H	-16.212696	12.789654	-33.405337
H	-15.650630	13.270710	-34.998448
H	-13.799818	12.893506	-32.568310
H	-14.485197	14.448919	-33.056228
H	-13.349655	13.617190	-34.117256
H	-15.938469	9.592143	-35.396567
H	-17.232462	9.967111	-33.299605
H	-17.791750	11.510800	-33.931581
H	-18.675796	10.054291	-35.959575
H	-20.101907	11.525969	-34.640948
H	-21.731418	10.459713	-33.203618
H	-21.496250	7.885120	-33.682914
H	-20.744056	8.133250	-35.731819
H	-19.794784	6.640167	-35.852716
H	-19.393970	8.049049	-36.855248
H	-18.472824	5.884928	-33.274295
H	-20.184085	5.909665	-33.706404
H	-19.014819	6.558979	-30.957173
H	-19.863165	5.076624	-31.379469
H	-21.369788	6.711551	-30.194753
H	-21.950106	6.334158	-31.819777
H	-20.414359	8.843488	-31.024650
H	-16.982973	10.726130	-36.933807
H	-14.811295	9.873548	-37.418899
H	-13.978165	8.291705	-37.293089
H	-13.106246	9.734006	-37.824411
H	-12.851938	4.723535	-35.773314
H	-11.930048	5.088873	-37.237919
H	-11.112990	5.025445	-35.680138
H	-13.203087	5.527451	-33.825614
H	-14.259658	6.884111	-33.362547
H	-12.577687	6.866591	-32.855010
H	-18.674866	8.329568	-32.622860

TS1a (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27872178			
Zero-point correction= 0.694071			
Thermal correction to Energy= 0.729369			
Thermal correction to Enthalpy= 0.730314			
Thermal correction to Gibbs Free Energy= 0.630708			
C	-18.939770	8.149440	-34.741994
O	-22.562683	8.993720	-31.503394
C	-12.600439	8.461488	-37.992420
C	-12.347790	7.171447	-37.485637
C	-13.890431	6.189308	-37.935792
C	-15.111774	6.712990	-37.492594
C	-15.672650	6.624411	-36.209403
O	-15.097614	5.978731	-35.198401
N	-15.922354	7.608217	-38.194501
C	-16.986507	8.051701	-37.436099
O	-17.775984	8.924463	-37.839268
C	-16.874592	7.363104	-36.151922
C	-17.560891	7.500223	-34.887420
O	-16.980171	7.070176	-33.867959
C	-13.242854	9.512900	-37.268348
C	-13.398931	9.708045	-35.920166
C	-13.863446	11.066736	-35.458322
C	-15.063878	11.098867	-34.495913
C	-15.376701	12.542082	-34.073218
C	-14.185968	13.301150	-33.487726
C	-16.259066	10.400808	-35.162881
C	-17.485951	10.302959	-34.243388
C	-18.758260	9.698417	-34.891583
C	-19.958929	10.442109	-34.362280
C	-20.894830	9.930553	-33.566923
C	-20.886017	8.499183	-33.119340
C	-19.875527	7.641583	-35.852518
C	-19.688734	6.318981	-33.034213
C	-20.096596	6.129042	-31.570538
C	-21.389254	6.882595	-31.256352
C	-21.302484	8.354967	-31.651487
O	-16.565214	11.107943	-36.355098
C	-12.966384	8.771464	-34.825940
C	-11.251433	6.325001	-38.106859
C	-12.267046	8.733065	-39.432650

C	-19.524581	7.816049	-33.343410
H	-22.825002	8.916661	-30.578466
H	-12.429625	7.053644	-36.411839
H	-13.748547	6.120554	-39.013857
H	-13.579214	5.293498	-37.403471
H	-15.670577	6.221353	-34.416814
H	-15.790272	7.898917	-39.151382
H	-13.564290	10.348534	-37.887213
H	-14.097033	11.699729	-36.318934
H	-12.997543	11.508853	-34.944872
H	-14.816247	10.521744	-33.592844
H	-16.171951	12.522319	-33.321926
H	-15.777606	13.079497	-34.940519
H	-13.698596	12.717520	-32.698753
H	-14.510849	14.248080	-33.049251
H	-13.433077	13.534059	-34.245317
H	-15.908540	9.392169	-35.416747
H	-17.220659	9.746843	-33.334427
H	-17.736930	11.320078	-33.926720
H	-18.704250	9.899948	-35.966378
H	-20.014656	11.490774	-34.652390
H	-21.722301	10.545386	-33.223339
H	-21.654270	7.954512	-33.694189
H	-20.852233	8.124759	-35.761127
H	-20.018763	6.559390	-35.785764
H	-19.474457	7.885109	-36.836219
H	-18.766385	5.773942	-33.236963
H	-20.471943	5.897282	-33.678349
H	-19.288877	6.498789	-30.925185
H	-20.220841	5.065773	-31.342356
H	-21.640313	6.800590	-30.191614
H	-22.222238	6.443416	-31.820884
H	-20.545744	8.861237	-31.028014
H	-17.024736	10.498628	-36.957135
H	-12.961115	9.289447	-33.864890
H	-11.955513	8.393456	-35.009479
H	-13.631757	7.903887	-34.734106
H	-10.272313	6.777349	-37.924200
H	-11.248115	5.323578	-37.671012
H	-11.375797	6.221374	-39.187967
H	-11.181674	8.727207	-39.585658
H	-12.653860	9.697855	-39.761404
H	-12.676380	7.952527	-40.086993
H	-18.822851	8.226444	-32.602296

TS1b (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27521835			
Zero-point correction= 0.694275			
Thermal correction to Energy= 0.729382			
Thermal correction to Enthalpy= 0.730326			
Thermal correction to Gibbs Free Energy= 0.632006			
C	-19.105845	8.173155	-34.657675
O	-22.885941	9.340324	-31.717049
C	-12.452629	7.256441	-35.544859
C	-12.286726	6.793422	-36.870338
C	-13.892957	5.894330	-37.312599
C	-15.130923	6.511045	-37.057115
C	-15.765087	6.545479	-35.806079
O	-15.222753	6.017330	-34.715541
N	-15.944110	7.272700	-37.906236
C	-17.027403	7.811987	-37.237645
O	-17.773019	8.664672	-37.750756
C	-16.987456	7.245959	-35.888676
C	-17.734848	7.494918	-34.678450
O	-17.209643	7.157074	-33.595320
C	-13.038526	8.506746	-35.186573
C	-13.571704	9.521396	-35.940653
C	-13.874407	10.837699	-35.250476
C	-15.125706	10.884732	-34.346435
C	-15.367704	12.314586	-33.843041
C	-14.148821	12.972568	-33.197160
C	-16.337154	10.289156	-35.076097
C	-17.619966	10.316536	-34.233563
C	-18.871952	9.701662	-34.911644
C	-20.078544	10.512548	-34.510002
C	-21.072416	10.082644	-33.736801
C	-21.126642	8.689830	-33.182409
C	-19.995541	7.603457	-35.775239
C	-19.979582	6.502930	-32.848820
C	-20.479511	6.441157	-31.402712
C	-21.774158	7.236272	-31.232163
C	-21.633187	8.670720	-31.736248
O	-16.531943	10.991533	-36.300092
C	-13.813026	9.559914	-37.416189
C	-11.261053	5.706870	-37.142296
C	-12.038349	6.345018	-34.426458

C	-19.771280	7.966324	-33.270778
H	-23.201746	9.349409	-30.805758
H	-12.276266	7.566356	-37.630541
H	-13.647687	5.715179	-38.358009
H	-13.707115	5.030478	-36.676355
H	-15.836735	6.317481	-33.987164
H	-15.734758	7.523773	-38.860354
H	-13.002999	8.715392	-34.117089
H	-13.987567	11.613776	-36.015258
H	-13.003819	11.100290	-34.640232
H	-14.940808	10.234664	-33.477823
H	-16.177456	12.293264	-33.107148
H	-15.723000	12.923092	-34.683994
H	-13.719467	12.326102	-32.423758
H	-14.426362	13.918214	-32.724901
H	-13.363854	13.188531	-33.926709
H	-16.057507	9.254607	-35.298445
H	-17.438821	9.833731	-33.264303
H	-17.843992	11.367900	-34.026285
H	-18.753469	9.816401	-35.994631
H	-20.088976	11.537442	-34.879313
H	-21.901497	10.740038	-33.489554
H	-21.872541	8.117373	-33.759586
H	-20.959707	8.119257	-35.779728
H	-20.177140	6.534816	-35.629916
H	-19.533794	7.754305	-36.750847
H	-19.054323	5.934127	-32.948134
H	-20.728213	6.036928	-33.503486
H	-19.705731	6.851959	-30.740798
H	-20.637491	5.402335	-31.096199
H	-22.091864	7.243342	-30.182228
H	-22.579132	6.765324	-31.811502
H	-20.904405	9.212546	-31.109373
H	-17.031405	10.404164	-36.892545
H	-14.803861	9.998575	-37.582037
H	-13.768792	8.602941	-37.920869
H	-13.089024	10.246494	-37.875155
H	-11.433595	4.815359	-36.533846
H	-11.292219	5.408171	-38.192595
H	-10.252346	6.071400	-36.925640
H	-12.559001	5.383314	-34.521365
H	-12.284216	6.764817	-33.451006
H	-10.963888	6.133785	-34.462377
H	-19.102614	8.426010	-32.528229

TS1c (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27060978			
Zero-point correction= 0.692213			
Thermal correction to Energy= 0.727974			
Thermal correction to Enthalpy= 0.728918			
Thermal correction to Gibbs Free Energy= 0.628092			
C	2.096860	0.961649	-0.445637
C	0.920546	1.376949	0.442139
O	1.090327	1.473945	1.678244
C	-0.415248	1.595191	-0.064482
C	-1.435977	1.963073	0.840727
O	-1.295711	2.130310	2.143850
H	-0.325325	1.916901	2.295731
C	-2.659769	2.130158	0.155864
N	-2.408907	1.749241	-1.159424
C	-1.060224	1.467106	-1.379363
O	-0.629575	1.165291	-2.491269
H	-3.022026	1.936346	-1.939728
C	-3.924011	2.439803	0.670529
H	-4.624066	2.886464	-0.034506
H	-3.903471	2.933452	1.638904
C	-5.049801	0.979938	1.184342
C	-6.366180	1.711800	1.365335
H	-6.262018	2.519259	2.093822
H	-6.723474	2.149455	0.429694
H	-7.133734	1.023262	1.732012
H	-4.561870	0.721914	2.124592
C	-4.895750	0.000550	0.180577
C	-3.931967	-1.036939	0.410883
C	-3.294606	-1.859118	-0.469323
C	-3.284016	-1.690363	-1.960833
H	-4.043638	-2.326944	-2.433183
H	-3.459667	-0.655898	-2.261003
H	-2.313947	-2.013329	-2.349962
C	-2.491636	-3.014615	0.084259
H	-3.065202	-3.482531	0.889457
H	-2.345060	-3.764940	-0.701307
C	-1.105097	-2.618603	0.635525
H	-1.263635	-1.896480	1.451331
C	-0.364021	-3.834419	1.208119
C	-1.133820	-4.589065	2.291581

H	-1.490293	-3.900345	3.064941
H	-2.000738	-5.116730	1.886296
H	-0.493574	-5.331837	2.773633
H	0.589071	-3.496700	1.628549
H	-0.118449	-4.527909	0.391786
C	-0.292492	-1.884229	-0.441245
H	-0.873269	-1.003894	-0.743395
C	1.080898	-1.407228	0.023100
H	0.988798	-0.931856	1.006893
H	1.728975	-2.279360	0.175141
C	1.732057	-0.447960	-1.015660
C	2.926644	-1.125689	-1.632799
C	4.191443	-0.793515	-1.386768
C	4.572891	0.349800	-0.492808
C	3.405975	0.859019	0.378203
C	3.870743	2.146425	1.078116
C	5.065005	1.843995	1.987963
C	6.221582	1.220943	1.204952
H	7.044904	0.935088	1.867264
C	5.779378	0.003176	0.396691
H	5.485782	-0.806613	1.078156
O	6.859438	-0.523928	-0.359859
H	7.165510	0.176227	-0.951392
H	6.618719	1.964778	0.497741
H	5.404366	2.756258	2.488686
H	4.744413	1.151389	2.777235
H	3.060839	2.587911	1.658274
H	4.177217	2.881695	0.321786
H	3.225298	0.107040	1.162569
H	4.909177	1.185652	-1.133576
H	5.008183	-1.346361	-1.843616
H	2.699783	-1.971945	-2.280430
H	0.995118	-0.281539	-1.809222
O	-0.168668	-2.653815	-1.634681
H	0.432367	-3.388635	-1.455821
H	-3.708085	-1.212731	1.464400
C	-5.729163	0.088254	-1.064608
H	-5.459489	0.966906	-1.668251
H	-6.785511	0.206028	-0.802602
H	-5.635699	-0.796881	-1.689817
C	2.258236	1.970256	-1.596091
H	2.529696	2.958703	-1.214626
H	1.337220	2.052142	-2.172264
H	3.047430	1.634440	-2.274462

INT1a (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.29142871			
Zero-point correction= 0.694817			
Thermal correction to Energy= 0.730460			
Thermal correction to Enthalpy= 0.731404			
Thermal correction to Gibbs Free Energy= 0.631084			
C	-2.140618	-0.430847	0.462989
O	-5.754305	0.394776	3.711138
C	3.850863	-0.120279	-2.845394
C	4.070214	-1.533491	-2.377022
C	2.899139	-2.468326	-2.845114
C	1.599198	-1.954441	-2.375137
C	1.052560	-2.041571	-1.068737
O	1.630586	-2.750196	-0.107058
N	0.817626	-1.083687	-3.057250
C	-0.216688	-0.562817	-2.254897
O	-0.952674	0.340409	-2.654906
C	-0.097743	-1.248053	-0.976056
C	-0.766333	-1.082437	0.311026
O	-0.163188	-1.501861	1.310603
C	3.456214	0.948894	-2.041256
C	3.356699	1.121348	-0.660929
C	2.963385	2.478454	-0.135271
C	1.731795	2.500735	0.793666
C	1.419621	3.932921	1.253622
C	2.604807	4.665223	1.883091
C	0.537865	1.834508	0.093758
C	-0.701672	1.726285	0.993202
C	-1.960098	1.119928	0.321123
C	-3.173089	1.852463	0.839077
C	-4.103770	1.334841	1.636543
C	-4.081903	-0.094255	2.091030
C	-3.082076	-0.935817	-0.644441
C	-2.869754	-2.267032	2.175283
C	-3.272656	-2.456401	3.640604
C	-4.568151	-1.709289	3.958490
C	-4.491343	-0.236876	3.561156
O	0.249843	2.581176	-1.081726
C	3.744409	0.111775	0.387797
C	5.395286	-2.127535	-2.868328
C	4.019263	0.120792	-4.322375

C	-2.717022	-0.769180	1.864167
H	-6.012279	0.322407	4.637679
H	4.055125	-1.575333	-1.288573
H	2.905297	-2.560067	-3.935849
H	3.071186	-3.462000	-2.421372
H	1.136929	-2.505087	0.714195
H	0.994515	-0.738873	-3.991359
H	3.215728	1.851756	-2.604514
H	2.774818	3.166343	-0.965986
H	3.818715	2.874666	0.430480
H	1.953350	1.894967	1.685468
H	0.609191	3.901244	1.988721
H	1.041774	4.499730	0.394448
H	3.068710	4.057441	2.667968
H	2.280001	5.604972	2.337187
H	3.376519	4.906022	1.147601
H	0.876317	0.829667	-0.188902
H	-0.448770	1.165600	1.902799
H	-0.962343	2.739805	1.312966
H	-1.892822	1.330278	-0.751699
H	-3.238281	2.898661	0.543207
H	-4.937957	1.942580	1.976075
H	-4.848892	-0.646719	1.522012
H	-4.061396	-0.462675	-0.537301
H	-3.214687	-2.019956	-0.589571
H	-2.699594	-0.679050	-1.632008
H	-1.944626	-2.808134	1.973303
H	-3.650767	-2.695540	1.533050
H	-2.464600	-2.081809	4.282584
H	-3.390396	-3.519999	3.870059
H	-4.813934	-1.791378	5.024298
H	-5.401131	-2.153745	3.398195
H	-3.735156	0.275088	4.180442
H	-0.190771	1.993739	-1.712900
H	3.809088	0.592889	1.367351
H	4.722034	-0.334750	0.178885
H	3.022052	-0.710013	0.479492
H	6.235961	-1.506513	-2.547793
H	5.536465	-3.134304	-2.465647
H	5.418464	-2.195070	-3.960185
H	5.079236	0.125809	-4.608135
H	3.595498	1.082792	-4.618631
H	3.547677	-0.660598	-4.932512
H	-2.015396	-0.353241	2.602030

INT1b (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28783476			
Zero-point correction= 0.694969			
Thermal correction to Energy= 0.730560			
Thermal correction to Enthalpy= 0.731504			
Thermal correction to Gibbs Free Energy= 0.631622			
C	-19.068625	8.127734	-34.641962
O	-22.904048	9.471414	-31.855055
C	-12.622974	7.277315	-35.651240
C	-12.673812	6.713483	-37.052460
C	-13.798866	5.635953	-37.204141
C	-15.134906	6.200938	-36.920770
C	-15.788022	6.301544	-35.663273
O	-15.302293	5.738835	-34.569751
N	-15.868334	6.940801	-37.789907
C	-16.945866	7.591655	-37.149361
O	-17.612760	8.450639	-37.724195
C	-16.939659	7.090329	-35.781655
C	-17.712108	7.426706	-34.590357
O	-17.213836	7.121950	-33.495669
C	-13.033983	8.546981	-35.267191
C	-13.546740	9.656879	-35.953696
C	-13.823761	10.902373	-35.143644
C	-15.098103	10.869424	-34.264651
C	-15.397938	12.265978	-33.701251
C	-14.208712	12.930378	-33.008028
C	-16.280636	10.268151	-35.037161
C	-17.588881	10.278024	-34.235642
C	-18.807391	9.641481	-34.953198
C	-20.028694	10.471865	-34.645088
C	-21.045500	10.088836	-33.876922
C	-21.123285	8.729110	-33.247881
C	-19.935567	7.517133	-35.756641
C	-20.012446	6.547960	-32.786166
C	-20.544945	6.559647	-31.350394
C	-21.830476	7.380592	-31.244367
C	-21.660096	8.787591	-31.813361
O	-16.444718	10.989069	-36.256110
C	-13.803572	9.739575	-37.433064
C	-11.340554	6.080539	-37.472035
C	-12.071187	6.353921	-34.596751

C	-19.773990	7.988529	-33.266648
H	-23.235922	9.536532	-30.951780
H	-12.906031	7.508474	-37.761862
H	-13.764968	5.236365	-38.223127
H	-13.609750	4.809260	-36.512901
H	-15.862203	6.097838	-33.836216
H	-15.637459	7.115501	-38.759020
H	-12.913038	8.732224	-34.197190
H	-13.905926	11.761142	-35.818847
H	-12.971093	11.096360	-34.481959
H	-14.909241	10.188204	-33.420395
H	-16.218263	12.192628	-32.980063
H	-15.755872	12.901562	-34.521517
H	-13.780655	12.267899	-32.247575
H	-14.517622	13.853531	-32.510929
H	-13.413896	13.185660	-33.713469
H	-15.990155	9.237172	-35.269168
H	-17.432028	9.803476	-33.257945
H	-17.834526	11.326171	-34.039030
H	-18.631318	9.712574	-36.032341
H	-20.023144	11.473676	-35.072504
H	-21.879207	10.760662	-33.692203
H	-21.862634	8.133311	-33.809693
H	-20.899663	8.030443	-35.794438
H	-20.117925	6.453525	-35.579304
H	-19.463576	7.634168	-36.731594
H	-19.095322	5.959604	-32.836081
H	-20.752694	6.063501	-33.436861
H	-19.779029	6.988282	-30.690825
H	-20.725831	5.538259	-31.001381
H	-22.168124	7.442399	-30.202617
H	-22.631054	6.893718	-31.816511
H	-20.937875	9.351056	-31.198375
H	-16.837903	10.384776	-36.902149
H	-14.231957	10.709972	-37.685655
H	-14.512363	8.978456	-37.776389
H	-12.883200	9.609744	-38.016313
H	-11.114818	5.196112	-36.868940
H	-11.377093	5.772044	-38.520545
H	-10.520955	6.793734	-37.350810
H	-12.533924	5.361105	-34.642544
H	-12.246283	6.752378	-33.595419
H	-10.990052	6.206206	-34.714345
H	-19.120622	8.473696	-32.526909

TS2a (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27721922			
Zero-point correction= 0.694704			
Thermal correction to Energy= 0.729154			
Thermal correction to Enthalpy= 0.730098			
Thermal correction to Gibbs Free Energy= 0.633314			
C	-2.265695	-0.710554	-0.630375
O	-6.977501	0.169186	0.550530
C	5.312078	-0.425989	0.297151
C	4.718456	-1.778314	0.513882
C	3.916413	-2.088527	-0.800735
C	2.605163	-1.406604	-0.908249
C	1.467542	-1.709481	-0.133445
O	1.535513	-2.259046	1.072895
N	2.098683	-0.912561	-2.110218
C	0.721255	-0.789224	-2.097739
O	0.101283	-0.224131	-3.014224
C	0.284489	-1.341617	-0.814440
C	-0.942339	-1.227955	-0.053053
O	-0.887584	-1.521212	1.161156
C	4.535069	0.694470	0.219345
C	3.173003	0.898635	0.590968
C	2.611085	2.207752	0.060314
C	1.174480	2.610498	0.415330
C	0.968795	4.123174	0.256730
C	1.580123	4.937008	1.395561
C	0.244509	1.791134	-0.483810
C	-1.196006	1.640073	0.018963
C	-2.098106	0.820750	-0.947689
C	-3.431225	1.511121	-1.073393
C	-4.602906	1.012390	-0.689944
C	-4.742898	-0.351155	-0.083128
C	-2.585254	-1.457794	-1.937340
C	-3.641936	-2.381390	0.837325
C	-4.643617	-2.428907	1.994222
C	-5.966572	-1.771922	1.601471
C	-5.761735	-0.358324	1.062460
O	0.285087	2.357846	-1.784959
C	2.577830	0.398599	1.871460
C	5.725917	-2.892110	0.790911
C	6.749323	-0.348260	-0.131058

C	-3.400514	-0.923454	0.408587
H	-7.617355	0.188106	1.271942
H	3.980956	-1.778317	1.315980
H	4.539536	-1.864490	-1.673307
H	3.742118	-3.171888	-0.799687
H	0.604608	-2.151773	1.423171
H	2.654497	-0.533171	-2.862833
H	4.998973	1.559219	-0.258694
H	2.702844	2.226096	-1.034305
H	3.314453	2.972658	0.424868
H	0.955494	2.348715	1.458808
H	-0.105633	4.332415	0.204335
H	1.385775	4.437667	-0.706049
H	1.128842	4.662988	2.354438
H	1.421621	6.007837	1.244189
H	2.659299	4.774694	1.480549
H	0.697337	0.800826	-0.505614
H	-1.190366	1.182287	1.017483
H	-1.625612	2.641842	0.137695
H	-1.629470	0.870612	-1.935463
H	-3.386332	2.511213	-1.503448
H	-5.515851	1.587306	-0.818750
H	-5.157460	-1.029503	-0.848133
H	-3.500790	-1.051254	-2.377214
H	-2.734715	-2.525916	-1.756991
H	-1.780487	-1.329852	-2.661274
H	-2.710229	-2.864249	1.131464
H	-4.055159	-2.945300	-0.009548
H	-4.214545	-1.906471	2.859430
H	-4.819466	-3.463370	2.305682
H	-6.658446	-1.745726	2.452368
H	-6.450248	-2.356208	0.807716
H	-5.376373	0.291026	1.867205
H	0.196062	1.630770	-2.422926
H	1.509756	0.180365	1.785625
H	2.675088	1.220682	2.596349
H	3.078216	-0.471075	2.286483
H	6.329347	-2.667615	1.674132
H	5.195851	-3.830309	0.972520
H	6.402535	-3.048850	-0.054184
H	7.412199	-0.719297	0.657699
H	7.036194	0.676517	-0.371071
H	6.933736	-0.974516	-1.012439
H	-3.110769	-0.359982	1.308328

TS2b (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27561491			
Zero-point correction= 0.694799			
Thermal correction to Energy= 0.729259			
Thermal correction to Enthalpy= 0.730203			
Thermal correction to Gibbs Free Energy= 0.633252			
C	-19.174421	8.202489	-34.649303
O	-23.096937	9.289453	-31.872220
C	-12.164087	7.463567	-35.638380
C	-12.258219	6.685993	-36.901561
C	-13.729827	6.104967	-37.056736
C	-14.904348	6.974680	-36.813885
C	-15.553723	7.124623	-35.570779
O	-14.989697	6.816798	-34.416210
N	-15.862876	7.286402	-37.765859
C	-17.060244	7.733518	-37.197375
O	-17.969070	8.211482	-37.877491
C	-16.891355	7.554574	-35.754526
C	-17.712322	7.754915	-34.592533
O	-17.168078	7.612385	-33.469076
C	-12.842333	8.644709	-35.478892
C	-13.677678	9.357084	-36.370733
C	-14.290464	10.621579	-35.789958
C	-15.410582	10.502676	-34.725910
C	-15.177754	11.476165	-33.560965
C	-14.005809	11.075487	-32.668411
C	-16.766157	10.759063	-35.400419
C	-17.981422	10.519671	-34.476981
C	-19.138123	9.699571	-35.116118
C	-20.450618	10.389827	-34.846837
C	-21.385559	9.950357	-34.007679
C	-21.257517	8.662951	-33.247273
C	-19.969487	7.353779	-35.653513
C	-19.835218	6.718629	-32.603661
C	-20.332350	6.809900	-31.158134
C	-21.720961	7.446473	-31.092820
C	-21.766724	8.795041	-31.807730
O	-16.742187	12.110015	-35.861246
C	-13.678147	9.393483	-37.871096
C	-11.276106	5.521398	-37.024735
C	-11.511021	6.828024	-34.449974

C	-19.817648	8.116999	-33.240860
H	-23.417429	9.392338	-30.968357
H	-12.084281	7.349090	-37.748373
H	-13.798028	5.680238	-38.062639
H	-13.774924	5.273365	-36.343292
H	-15.708390	7.061530	-33.749661
H	-15.696311	7.364108	-38.758839
H	-12.833797	9.056074	-34.469160
H	-14.672304	11.251649	-36.597685
H	-13.446896	11.173626	-35.352858
H	-15.432739	9.482397	-34.319283
H	-16.085699	11.526833	-32.949609
H	-15.023133	12.482130	-33.966641
H	-14.153583	10.068287	-32.263806
H	-13.897938	11.763866	-31.826236
H	-13.055942	11.079034	-33.213521
H	-16.840089	10.094918	-36.272457
H	-17.667260	10.030964	-33.547919
H	-18.349200	11.508283	-34.183015
H	-18.978881	9.678196	-36.202937
H	-20.595052	11.338041	-35.363856
H	-22.298957	10.518637	-33.854369
H	-21.917748	7.917136	-33.721450
H	-20.994817	7.727723	-35.721711
H	-20.006647	6.307074	-35.338649
H	-19.528255	7.408875	-36.647525
H	-18.842137	6.268541	-32.630720
H	-20.512377	6.066272	-33.170986
H	-19.623508	7.412521	-30.575062
H	-20.356016	5.817321	-30.697446
H	-22.044736	7.570237	-30.052039
H	-22.452973	6.792501	-31.584654
H	-21.120017	9.515854	-31.278770
H	-17.528729	12.248621	-36.402102
H	-14.701814	9.572117	-38.220868
H	-13.296768	8.516391	-38.384015
H	-13.090105	10.265725	-38.188579
H	-11.422311	4.782525	-36.231841
H	-11.415029	5.015447	-37.983721
H	-10.243016	5.874802	-36.976442
H	-12.055196	5.911994	-34.179801
H	-11.525192	7.494326	-33.586115
H	-10.476689	6.533765	-34.653978
H	-19.223397	8.765320	-32.579924

TS3a (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27973957			
Zero-point correction= 0.694182			
Thermal correction to Energy= 0.729281			
Thermal correction to Enthalpy= 0.730226			
Thermal correction to Gibbs Free Energy= 0.631234			
C	1.986929	-0.884810	0.504296
O	6.770884	0.222116	0.181157
C	-4.252436	-0.329124	0.267333
C	-4.646697	-1.201983	-0.916030
C	-4.068700	-2.580093	-0.529643
C	-2.758629	-2.209675	0.106297
C	-1.629779	-1.752625	-0.613186
O	-1.639440	-1.550651	-1.921034
N	-2.325969	-2.392720	1.402214
C	-1.046188	-1.841969	1.591687
O	-0.596234	-1.604364	2.712706
C	-0.535897	-1.565506	0.248778
C	0.712526	-1.078547	-0.307174
O	0.712057	-0.754713	-1.513449
C	-3.588767	0.920389	0.270471
C	-3.079504	1.729955	-0.715301
C	-2.399016	3.004215	-0.285857
C	-0.850554	2.956736	-0.298086
C	-0.272666	4.270195	0.250405
C	-0.832071	5.530842	-0.408162
C	-0.350596	1.717584	0.463868
C	1.178404	1.637477	0.549714
C	1.776620	0.432180	1.326526
C	3.085186	0.889884	1.925318
C	4.288461	0.535857	1.479189
C	4.491633	-0.441004	0.357470
C	2.214898	-2.072515	1.453013
C	3.467679	-1.872149	-1.410181
C	4.580495	-1.485014	-2.389023
C	5.859246	-1.089572	-1.648587
C	5.607027	-0.007982	-0.599222
O	-0.917723	1.739153	1.771461
C	-3.152708	1.463741	-2.195101
C	-6.145322	-1.204418	-1.214125
C	-4.887235	-0.688324	1.588951

C	3.203505	-0.710154	-0.441135
H	7.473142	0.510148	-0.413970
H	-4.102261	-0.868538	-1.801633
H	-4.712831	-3.110562	0.175778
H	-3.921329	-3.232357	-1.396687
H	-0.721559	-1.181869	-2.100893
H	-2.941803	-2.518897	2.194121
H	-3.435273	1.313013	1.275306
H	-2.711598	3.267641	0.729815
H	-2.721986	3.811796	-0.952892
H	-0.514345	2.837043	-1.339628
H	0.812800	4.263828	0.109932
H	-0.449313	4.302766	1.332900
H	-0.763799	5.464801	-1.499706
H	-0.269220	6.412539	-0.091387
H	-1.880151	5.699635	-0.148314
H	-0.744405	0.857578	-0.084496
H	1.604763	1.679639	-0.460524
H	1.516803	2.539600	1.069091
H	1.096708	0.184998	2.152733
H	3.001405	1.602459	2.744488
H	5.185422	0.935128	1.944707
H	4.841522	-1.390911	0.796098
H	3.127435	-1.915517	2.032409
H	2.321435	-3.004528	0.890286
H	1.391587	-2.179498	2.156829
H	2.561812	-2.133174	-1.960175
H	3.780317	-2.759865	-0.844374
H	4.235773	-0.642009	-3.002164
H	4.789759	-2.310129	-3.076933
H	6.625922	-0.747109	-2.354323
H	6.269362	-1.961669	-1.122669
H	5.293169	0.925489	-1.096670
H	-0.896490	0.837772	2.122530
H	-2.782133	2.323693	-2.758164
H	-4.182619	1.271716	-2.515236
H	-2.555620	0.591930	-2.477050
H	-6.488407	-0.201059	-1.482709
H	-6.370195	-1.877390	-2.046409
H	-6.718962	-1.539446	-0.344061
H	-5.793129	-0.086384	1.737845
H	-4.215658	-0.460346	2.422936
H	-5.192487	-1.734454	1.660496
H	3.005282	0.177750	-1.057061

TS3b (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28365226			
Zero-point correction= 0.695306			
Thermal correction to Energy= 0.729877			
Thermal correction to Enthalpy= 0.730821			
Thermal correction to Gibbs Free Energy= 0.633834			
C	-19.010184	8.153204	-34.562167
O	-22.903091	9.387957	-31.786966
C	-13.067856	7.163571	-35.713708
C	-12.731869	6.498457	-37.046290
C	-13.845986	5.457098	-37.246843
C	-15.094576	6.169026	-36.828704
C	-15.827078	6.157392	-35.621090
O	-15.555005	5.353565	-34.597331
N	-15.686247	7.112754	-37.619792
C	-16.757204	7.752020	-36.984504
O	-17.357265	8.695792	-37.517765
C	-16.869586	7.109554	-35.689073
C	-17.675191	7.393419	-34.512261
O	-17.258913	6.956896	-33.425386
C	-13.351322	8.522584	-35.462583
C	-13.659677	9.627706	-36.228208
C	-13.866641	10.939186	-35.491594
C	-15.003147	10.956035	-34.441752
C	-15.215992	12.374689	-33.897532
C	-13.950048	13.035440	-33.353197
C	-16.274768	10.365562	-35.058891
C	-17.472205	10.273328	-34.105831
C	-18.735794	9.680519	-34.786029
C	-19.928553	10.520394	-34.408220
C	-20.971096	10.109694	-33.692181
C	-21.099277	8.705854	-33.182536
C	-19.844008	7.629243	-35.745659
C	-20.068135	6.466841	-32.863934
C	-20.639492	6.381071	-31.445962
C	-21.905368	7.226794	-31.310112
C	-21.679407	8.666716	-31.763968
O	-16.605312	11.134146	-36.211845
C	-13.832963	9.737182	-37.711507
C	-11.323655	5.902424	-37.087359
C	-12.765158	6.330113	-34.497407

C	-19.767605	7.932660	-33.223126
H	-23.263720	9.385280	-30.892452
H	-12.805828	7.233106	-37.848558
H	-13.906486	5.093515	-38.278092
H	-13.692662	4.590373	-36.598007
H	-16.084313	5.721359	-33.849438
H	-15.398357	7.364011	-38.554848
H	-13.361578	8.741106	-34.392965
H	-14.078260	11.728501	-36.220006
H	-12.925662	11.203248	-34.993600
H	-14.719652	10.304768	-33.601872
H	-15.959037	12.333601	-33.094099
H	-15.649381	12.990706	-34.694818
H	-13.450571	12.384376	-32.627247
H	-14.189571	13.975277	-32.849281
H	-13.233454	13.262235	-34.147055
H	-16.011569	9.352755	-35.368782
H	-17.199335	9.688902	-33.216771
H	-17.712636	11.283040	-33.757337
H	-18.600705	9.803450	-35.864830
H	-19.882357	11.553595	-34.750912
H	-21.785742	10.790885	-33.462581
H	-21.834412	8.176377	-33.812335
H	-20.795930	8.165804	-35.790730
H	-20.054017	6.560681	-35.645704
H	-19.323109	7.797563	-36.688970
H	-19.172907	5.849821	-32.939662
H	-20.808435	6.064992	-33.568748
H	-19.881445	6.734737	-30.734738
H	-20.856826	5.340817	-31.183948
H	-22.271934	7.218305	-30.276268
H	-22.701294	6.808308	-31.939995
H	-20.961881	9.159834	-31.086071
H	-16.976184	10.511397	-36.856239
H	-14.874640	10.024730	-37.912429
H	-13.604996	8.836291	-38.273652
H	-13.208306	10.551567	-38.096350
H	-11.203126	5.115754	-36.337214
H	-11.131475	5.462940	-38.069980
H	-10.569023	6.671890	-36.902970
H	-12.970688	5.269101	-34.650355
H	-13.347210	6.661384	-33.635282
H	-11.700063	6.425227	-34.243903
H	-19.123322	8.340593	-32.429789

exo-4+2 adduct **8** (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.35675507			
Zero-point correction= 0.698706			
Thermal correction to Energy= 0.732772			
Thermal correction to Enthalpy= 0.733716			
Thermal correction to Gibbs Free Energy= 0.638223			
C	-18.966264	7.960850	-34.639554
O	-23.073586	8.847664	-32.063320
C	-12.183351	8.404552	-38.251716
C	-12.549012	6.950308	-38.025349
C	-13.397204	6.743666	-36.757621
C	-14.306190	7.945513	-36.429861
C	-15.200952	7.578606	-35.279694
O	-14.698764	7.283262	-34.115936
N	-15.312558	8.135970	-37.462591
C	-16.606215	7.979454	-37.051865
O	-17.577138	8.149540	-37.781171
C	-16.539725	7.613193	-35.609715
C	-17.500586	7.552647	-34.511199
O	-17.038634	7.281248	-33.384503
C	-12.581661	9.387996	-37.438571
C	-13.450264	9.241297	-36.201555
C	-14.280680	10.550033	-36.067254
C	-15.294493	10.679934	-34.900550
C	-15.020525	11.893208	-33.995700
C	-13.754401	11.774513	-33.153832
C	-16.730607	10.756513	-35.450325
C	-17.831400	10.346791	-34.445065
C	-18.960393	9.472670	-35.079561
C	-20.297796	10.121362	-34.835422
C	-21.261442	9.628187	-34.062432
C	-21.139608	8.316718	-33.345512
C	-19.658603	7.107890	-35.716545
C	-19.715259	6.385275	-32.687093
C	-20.291809	6.416235	-31.268941
C	-21.697996	7.014696	-31.261675
C	-21.736678	8.384107	-31.934503
O	-16.926299	12.087543	-35.924205
C	-12.519168	9.117846	-34.980487
C	-13.195765	6.314053	-39.266569
C	-11.304454	8.690464	-39.441762

C	-19.686720	7.807776	-33.273747
H	-23.449414	8.911799	-31.176915
H	-11.599385	6.419823	-37.867643
H	-14.036737	5.862966	-36.879316
H	-12.759889	6.553195	-35.891322
H	-15.530203	7.152001	-33.535443
H	-15.096031	8.505534	-38.377249
H	-12.240874	10.403407	-37.643060
H	-14.804257	10.735448	-37.012444
H	-13.535148	11.351807	-35.986760
H	-15.237449	9.790763	-34.259416
H	-15.881593	12.029214	-33.329185
H	-14.973646	12.790713	-34.620701
H	-13.791099	10.890605	-32.508285
H	-13.631683	12.652058	-32.513383
H	-12.859327	11.694282	-33.777496
H	-16.795729	10.094229	-36.315873
H	-17.396477	9.827250	-33.582374
H	-18.263673	11.269456	-34.044550
H	-18.794789	9.464211	-36.164802
H	-20.438484	11.085787	-35.322415
H	-22.193192	10.171758	-33.932648
H	-21.746957	7.570741	-33.885671
H	-20.672826	7.483417	-35.879563
H	-19.724966	6.061770	-35.406692
H	-19.120908	7.165539	-36.662279
H	-18.719860	5.941789	-32.675617
H	-20.353617	5.747455	-33.312449
H	-19.632626	7.015387	-30.627124
H	-20.314064	5.407657	-30.844896
H	-22.082631	7.096993	-30.238129
H	-22.383015	6.359157	-31.815208
H	-21.142657	9.102210	-31.344161
H	-17.735800	12.096641	-36.449252
H	-13.070416	9.120214	-34.037988
H	-11.836022	9.972581	-34.980951
H	-11.907668	8.214664	-35.022827
H	-12.527849	6.361851	-40.129698
H	-13.416352	5.260860	-39.073391
H	-14.133097	6.809168	-39.534735
H	-10.444909	8.011114	-39.461691
H	-10.934838	9.717690	-39.421056
H	-11.847233	8.545168	-40.381542
H	-19.147413	8.449047	-32.559397

endo-4+2 adduct **9** (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.33878495			
Zero-point correction= 0.699340			
Thermal correction to Energy= 0.733416			
Thermal correction to Enthalpy= 0.734360			
Thermal correction to Gibbs Free Energy= 0.638301			
C	2.148516	0.859328	-0.734476
C	1.738651	-0.651986	-0.875772
C	3.294910	0.976121	0.299149
C	2.951277	-1.527794	-1.070167
H	1.108769	-0.719617	-1.775552
C	0.924488	-1.216413	0.318715
C	4.187226	-1.167804	-0.729394
C	4.530040	0.183986	-0.172417
C	3.739958	2.401932	0.656806
H	2.937383	0.510424	1.229186
C	4.759987	2.354054	1.798692
H	4.206976	2.873000	-0.218104
H	2.884513	3.015105	0.943825
C	5.967668	1.488770	1.433625
H	5.091328	3.364634	2.056644
H	4.274405	1.942640	2.693200
C	5.558649	0.092946	0.967775
H	5.024867	0.764704	-0.972322
O	6.693245	-0.673400	0.594637
H	5.103189	-0.457045	1.802298
H	6.517824	1.968255	0.609911
H	6.661778	1.398768	2.275067
H	2.767758	-2.527323	-1.459947
H	5.015295	-1.859686	-0.859564
C	0.872948	1.518453	-0.218424
C	2.581522	1.426545	-2.094107
H	1.754585	1.434224	-2.802214
H	2.955300	2.448065	-1.983431
H	3.383450	0.810415	-2.508760
O	0.827187	1.922604	0.953417
C	0.253478	-2.580078	0.038394
H	0.156996	-0.516898	0.654250
H	1.604884	-1.351818	1.166415
C	-1.279090	-2.533072	0.287588
O	0.903434	-3.617928	0.756400

H	0.397465	-2.856029	-1.016253
C	-1.909430	-1.689747	-0.855304
H	-1.444717	-2.047043	1.261809
C	-1.826127	-3.968233	0.330195
C	-3.127063	-0.724552	-0.631556
C	-3.723407	-0.748267	0.757409
C	-4.425369	0.250606	1.299271
C	-4.691637	1.563060	0.585590
C	-5.034674	0.104614	2.668893
H	-4.534425	0.752590	3.396411
H	-6.092733	0.391279	2.661431
H	-4.958481	-0.925368	3.023888
H	0.831681	-3.413300	1.697908
C	-3.301594	-4.124175	0.684181
H	-1.637239	-4.421785	-0.653021
H	-1.231962	-4.544990	1.042912
H	-3.953268	-3.565946	0.006339
H	-3.504738	-3.779795	1.703273
H	-3.594760	-5.176009	0.630096
C	-0.410975	1.407740	-0.930867
C	-1.529295	1.228044	-0.152802
C	-0.835933	1.166445	-2.339810
C	-2.728680	0.771080	-0.948286
N	-2.179568	0.909078	-2.283656
O	-1.602405	1.364640	1.146621
H	-2.690413	0.689557	-3.125582
O	-0.197400	1.199733	-3.381893
C	-3.922840	1.721157	-0.747910
C	-4.477013	2.781152	1.497736
H	-3.616039	-1.667111	1.323978
H	-4.597571	1.565079	-1.593790
H	-3.550895	2.746392	-0.846599
H	7.148810	-0.192336	-0.108820
H	-4.715034	3.698808	0.952810
H	-3.437733	2.836168	1.830675
H	-5.122968	2.742071	2.377839
H	-5.763786	1.549765	0.337589
H	-0.697186	1.710279	1.410739
H	-2.192748	-2.402891	-1.639132
H	-1.108826	-1.100881	-1.312381
C	-4.234840	-1.137932	-1.627789
H	-3.875666	-1.111987	-2.662220
H	-5.122245	-0.507701	-1.538283
H	-4.543764	-2.165171	-1.420585

exo-2+2 adduct **10** (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.32914021			
Zero-point correction= 0.698048			
Thermal correction to Energy= 0.732556			
Thermal correction to Enthalpy= 0.733500			
Thermal correction to Gibbs Free Energy= 0.636176			
C	1.987575	-0.849981	0.519782
O	6.799026	0.067035	0.055087
C	-4.002008	-0.628044	0.167198
C	-4.568079	-1.403335	-1.067191
C	-3.911162	-2.697308	-0.515252
C	-2.939144	-1.796575	0.275056
C	-1.686196	-1.487819	-0.485204
O	-1.703210	-1.258514	-1.764424
N	-2.389734	-2.090234	1.580246
C	-1.098291	-1.616584	1.708909
O	-0.571980	-1.354282	2.785394
C	-0.579821	-1.431036	0.334029
C	0.693027	-1.023233	-0.257531
O	0.677875	-0.741988	-1.472973
C	-3.417111	0.762923	0.201439
C	-3.029104	1.663730	-0.712227
C	-2.405981	2.958474	-0.215484
C	-0.858529	3.002026	-0.218011
C	-0.350748	4.325995	0.371454
C	-0.942990	5.575716	-0.279286
C	-0.302300	1.774904	0.519554
C	1.229124	1.699090	0.551220
C	1.841815	0.494325	1.319297
C	3.183834	0.931812	1.855111
C	4.362014	0.521827	1.391313
C	4.501678	-0.498857	0.300101
C	2.192254	-2.021547	1.494133
C	3.385216	-1.938103	-1.402338
C	4.486697	-1.619435	-2.418010
C	5.796987	-1.256139	-1.717950
C	5.610601	-0.137990	-0.693990
O	-0.831610	1.782283	1.842199
C	-3.126794	1.544129	-2.209155
C	-6.060966	-1.381707	-1.340478
C	-4.985353	-0.725144	1.344838

C	3.185623	-0.741189	-0.459795
H	7.498657	0.312644	-0.561778
H	-4.025937	-1.118998	-1.967627
H	-4.573870	-3.252157	0.152417
H	-3.459949	-3.382945	-1.234677
H	-0.732571	-0.999040	-1.964367
H	-2.978652	-2.034596	2.401150
H	-3.218011	1.064925	1.231764
H	-2.736318	3.152244	0.810204
H	-2.775956	3.781088	-0.837772
H	-0.504684	2.927888	-1.257894
H	0.738184	4.365854	0.263163
H	-0.559177	4.328993	1.448323
H	-0.842847	5.533739	-1.369529
H	-0.426452	6.473822	0.069001
H	-2.003848	5.695809	-0.045777
H	-0.701370	0.919440	-0.026008
H	1.619073	1.725412	-0.474462
H	1.594144	2.604032	1.047629
H	1.198540	0.276429	2.181458
H	3.145710	1.674429	2.650484
H	5.283848	0.907808	1.817590
H	4.824591	-1.447414	0.761639
H	3.105432	-1.862952	2.072144
H	2.286995	-2.967475	0.953541
H	1.365239	-2.098743	2.197715
H	2.459640	-2.185793	-1.924738
H	3.681650	-2.819613	-0.818690
H	4.159544	-0.779633	-3.044925
H	4.646192	-2.469889	-3.087976
H	6.559517	-0.962511	-2.449548
H	6.184990	-2.129603	-1.177812
H	5.321713	0.793210	-1.210436
H	-0.730395	0.898338	2.223598
H	-3.606679	2.437215	-2.623654
H	-3.684024	0.670265	-2.539113
H	-2.123556	1.490397	-2.648992
H	-6.397705	-0.365979	-1.571762
H	-6.297435	-2.016962	-2.198643
H	-6.638470	-1.745265	-0.486372
H	-5.836157	-0.063658	1.158630
H	-4.512604	-0.391918	2.273322
H	-5.373338	-1.735514	1.499204
H	3.002373	0.139122	-1.091749

endo-2+2 adduct **13** (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31919882			
Zero-point correction= 0.698356			
Thermal correction to Energy= 0.732622			
Thermal correction to Enthalpy= 0.733566			
Thermal correction to Gibbs Free Energy= 0.637266			
C	-19.063094	8.006617	-34.510513
O	-22.881627	9.601584	-31.825380
C	-13.349944	7.087169	-35.977212
C	-12.728285	6.445171	-37.264250
C	-13.891200	5.417301	-37.264897
C	-14.732235	6.445846	-36.487387
C	-15.748768	6.209685	-35.417516
O	-15.499848	5.428098	-34.404236
N	-15.485770	7.306141	-37.366784
C	-16.680566	7.725024	-36.870052
O	-17.400949	8.546812	-37.439886
C	-16.856881	7.018408	-35.576543
C	-17.793229	7.156870	-34.458392
O	-17.496688	6.545524	-33.416584
C	-13.390897	8.554940	-35.629030
C	-13.632164	9.680425	-36.316192
C	-13.844904	10.973424	-35.533392
C	-14.963775	10.923721	-34.463585
C	-15.236581	12.324426	-33.900178
C	-13.997207	13.027594	-33.347315
C	-16.222052	10.275004	-35.053460
C	-17.360369	10.018033	-34.052572
C	-18.660166	9.504904	-34.744003
C	-19.786074	10.443863	-34.402163
C	-20.869981	10.127846	-33.700549
C	-21.122431	8.744695	-33.180272
C	-19.903624	7.530540	-35.712610
C	-20.317138	6.423747	-32.833563
C	-20.917606	6.400009	-31.425041
C	-22.099115	7.362679	-31.313073
C	-21.730850	8.770849	-31.772772
O	-16.660743	11.073337	-36.147813
C	-13.775151	9.840958	-37.804545
C	-11.293028	5.952918	-37.243228
C	-12.808594	6.355358	-34.738333

C	-19.864298	7.852564	-33.188544
H	-23.264927	9.630168	-30.940784
H	-12.857115	7.118298	-38.116065
H	-14.308812	5.108664	-38.224567
H	-13.662928	4.535546	-36.663564
H	-16.240752	5.649593	-33.751203
H	-15.144578	7.663486	-38.245854
H	-13.323992	8.704487	-34.549706
H	-14.094657	11.776221	-36.236070
H	-12.903773	11.258524	-35.050045
H	-14.629999	10.279345	-33.636538
H	-15.978180	12.246991	-33.098003
H	-15.692638	12.932319	-34.690715
H	-13.474882	12.389327	-32.626142
H	-14.272039	13.953706	-32.835914
H	-13.288355	13.286741	-34.138100
H	-15.896563	9.305598	-35.428799
H	-17.013279	9.310974	-33.286360
H	-17.593943	10.947920	-33.525002
H	-18.505367	9.594896	-35.820671
H	-19.643890	11.464382	-34.755953
H	-21.630546	10.874935	-33.492208
H	-21.887906	8.273367	-33.820057
H	-20.794721	8.158092	-35.802247
H	-20.222348	6.491866	-35.590562
H	-19.337035	7.621058	-36.640288
H	-19.492061	5.715630	-32.895122
H	-21.084427	6.100337	-33.549545
H	-20.141282	6.682117	-30.701717
H	-21.237283	5.386134	-31.164878
H	-22.479671	7.397396	-30.284903
H	-22.921981	7.016902	-31.952309
H	-20.983736	9.201684	-31.084426
H	-17.002822	10.462322	-36.817737
H	-14.819921	10.077846	-38.044040
H	-13.461271	8.970597	-38.379537
H	-13.175580	10.693119	-38.141606
H	-11.133644	5.204271	-36.463125
H	-11.036769	5.496581	-38.203392
H	-10.600259	6.781827	-37.068957
H	-12.835257	5.268329	-34.826354
H	-13.374812	6.627929	-33.846147
H	-11.768852	6.662186	-34.587794
H	-19.202173	8.202595	-32.381057

SM (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31531576			
Zero-point correction= 0.692191			
Thermal correction to Energy= 0.729460			
Thermal correction to Enthalpy= 0.730405			
Thermal correction to Gibbs Free Energy= 0.624108			
C	1.285853	-1.196637	-0.684001
C	2.478732	-0.562080	0.025044
O	2.812431	-0.945780	1.156440
C	3.273581	0.531049	-0.549613
C	4.397061	0.953280	0.128482
O	4.868488	0.505338	1.259363
H	4.195253	-0.182729	1.544230
C	5.060007	2.044135	-0.602758
C	6.178177	2.669319	-0.235179
H	6.669202	2.369970	0.682279
H	6.609621	3.468176	-0.825596
N	4.249606	2.247985	-1.717465
C	3.149597	1.416420	-1.736186
O	2.276544	1.487719	-2.594559
H	4.372240	2.984929	-2.396466
C	1.734513	-1.681053	-2.074755
H	2.134917	-0.854802	-2.664497
H	0.874632	-2.089039	-2.612993
H	2.496572	-2.461107	-1.997635
C	0.712002	-2.366474	0.155785
C	1.667092	-3.539356	0.435067
H	2.626670	-3.188484	0.814757
C	1.025414	-4.497109	1.444239
C	-0.329744	-5.010587	0.953034
C	-1.260969	-3.874319	0.535607
O	-2.492839	-4.379613	0.042262
H	-2.295161	-4.928055	-0.728949
H	-1.532632	-3.271396	1.413349
C	-0.564654	-2.953041	-0.481656
C	-1.495553	-1.910779	-1.021751
C	-1.137658	-0.642857	-1.206028
C	0.209833	-0.075432	-0.845329
H	0.549481	0.536239	-1.686735
C	0.042024	0.857253	0.379234
H	-0.594172	0.363430	1.120688

H	1.001791	1.069853	0.862939
C	-0.549514	2.210256	-0.031311
H	-1.392905	2.034096	-0.716363
C	-1.077671	3.042928	1.145082
C	0.037055	3.408057	2.133658
C	-0.384399	4.440913	3.177577
H	0.467833	4.748556	3.789131
H	-0.792229	5.335988	2.696036
H	-1.148861	4.048539	3.853841
H	0.888047	3.790374	1.561183
H	0.381544	2.497518	2.641546
H	-1.450515	3.978861	0.702126
C	-2.254700	2.345278	1.861896
C	-3.323501	1.833223	0.925017
C	-3.518064	0.510987	0.785444
C	-4.440633	-0.213363	-0.112643
C	-4.673205	0.196676	-1.371201
C	-5.548501	-0.447310	-2.405486
H	-4.949309	-0.786537	-3.257984
H	-6.271722	0.274181	-2.800343
H	-6.103795	-1.304732	-2.024023
H	-4.147790	1.089299	-1.708707
C	-4.990179	-1.487285	0.482980
H	-4.169767	-2.196698	0.652698
H	-5.454484	-1.291567	1.454804
H	-5.726231	-1.976889	-0.154787
H	-2.923063	-0.144317	1.425685
C	-4.090240	2.901264	0.189477
H	-4.267498	3.756528	0.850358
H	-3.525082	3.280271	-0.671889
H	-5.048153	2.531661	-0.181167
H	-1.866641	1.521316	2.472798
H	-2.704485	3.068048	2.554379
O	0.434981	2.999809	-0.692636
H	0.759659	2.517611	-1.467081
H	-1.872627	0.059714	-1.593096
H	-2.503128	-2.232240	-1.276510
H	-0.261413	-3.606749	-1.319934
H	-0.822562	-5.621014	1.716294
H	-0.174952	-5.653711	0.074032
H	1.691369	-5.342295	1.643749
H	0.890927	-3.968780	2.397136
H	1.860363	-4.081075	-0.500464
H	0.427294	-1.936959	1.128744

RC1a (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31696557			
Zero-point correction= 0.692989			
Thermal correction to Energy= 0.730083			
Thermal correction to Enthalpy= 0.731027			
Thermal correction to Gibbs Free Energy= 0.626035			
C	-18.685536	8.316074	-34.918102
O	-22.227434	8.476784	-31.488584
C	-12.943414	8.137722	-37.306367
C	-12.849336	7.133798	-36.418115
C	-14.957344	5.550620	-38.926152
C	-15.625443	6.497383	-38.268186
C	-15.938785	6.513082	-36.829481
O	-15.505870	5.558152	-36.034083
N	-16.192688	7.677919	-38.754933
C	-16.866243	8.373991	-37.776860
O	-17.420751	9.454943	-37.957655
C	-16.733738	7.585910	-36.534839
C	-17.286528	7.747393	-35.178416
O	-16.607069	7.295246	-34.255150
C	-13.471591	9.463503	-36.926485
C	-13.231797	10.166473	-35.805020
C	-13.869617	11.517914	-35.608291
C	-15.028093	11.514869	-34.587154
C	-15.345092	12.951427	-34.144368
C	-14.333121	13.501352	-33.140241
C	-16.234508	10.804080	-35.215536
C	-17.345462	10.477611	-34.210193
C	-18.610953	9.879228	-34.868739
C	-19.832996	10.462309	-34.205342
C	-20.702518	9.788863	-33.456721
C	-20.585663	8.315222	-33.203869
C	-19.630965	7.903260	-36.059561
C	-19.242734	6.232553	-33.442678
C	-19.582416	5.825802	-32.006009
C	-20.909931	6.437823	-31.558456
C	-20.934745	7.951635	-31.755936
O	-16.732475	11.629544	-36.261533
C	-12.346271	9.705805	-34.675334
C	-12.308753	5.754194	-36.642112
C	-12.561186	8.024947	-38.761905

C	-19.192060	7.765022	-33.556307
H	-22.442343	8.276696	-30.569449
H	-13.226797	7.323271	-35.413653
H	-14.775398	5.614660	-39.992208
H	-14.580015	4.695106	-38.379679
H	-15.708667	5.836410	-35.116837
H	-16.127048	8.004485	-39.708039
H	-14.092348	9.945880	-37.686544
H	-14.279075	11.889802	-36.553659
H	-13.099825	12.227438	-35.280669
H	-14.730062	10.935743	-33.700118
H	-16.342542	12.997994	-33.694952
H	-15.381693	13.590048	-35.034522
H	-14.340385	12.907214	-32.220958
H	-14.563973	14.535951	-32.873075
H	-13.313573	13.483100	-33.536980
H	-15.859924	9.863847	-35.645844
H	-16.958203	9.801936	-33.436839
H	-17.631732	11.403115	-33.700189
H	-18.618739	10.223471	-35.908754
H	-19.963230	11.533976	-34.350694
H	-21.550970	10.297616	-33.007446
H	-21.337795	7.797416	-33.823075
H	-20.634417	8.288158	-35.861522
H	-19.690990	6.816209	-36.161702
H	-19.300215	8.325043	-37.009616
H	-18.295204	5.779682	-33.738853
H	-20.017290	5.842930	-34.116586
H	-18.777920	6.164876	-31.340329
H	-19.626484	4.735937	-31.918633
H	-21.114248	6.199833	-30.507800
H	-21.731843	6.017841	-32.153028
H	-20.190053	8.423456	-31.092903
H	-17.023649	11.036625	-36.971426
H	-11.820815	10.561339	-34.238148
H	-11.614602	8.966500	-35.007693
H	-12.930357	9.246991	-33.868595
H	-11.445382	5.571988	-35.992055
H	-13.065787	5.007290	-36.381098
H	-11.993670	5.579422	-37.671769
H	-11.714210	8.680296	-38.992495
H	-13.397409	8.355821	-39.389192
H	-12.301873	7.008831	-39.059625
H	-18.490302	8.129436	-32.791760

RC1b (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.31678867			
Zero-point correction= 0.693908			
Thermal correction to Energy= 0.730550			
Thermal correction to Enthalpy= 0.731494			
Thermal correction to Gibbs Free Energy= 0.628891			
C	-18.809379	8.273956	-34.763991
O	-22.445449	8.848546	-31.483183
C	-12.859628	7.376821	-34.916974
C	-12.306533	6.803431	-35.998064
C	-14.787690	5.314218	-38.383525
C	-15.587715	6.234241	-37.845535
C	-15.941823	6.358893	-36.421516
O	-15.470424	5.505654	-35.539799
N	-16.261350	7.288996	-38.467078
C	-16.953589	8.060227	-37.562736
O	-17.519629	9.112728	-37.847849
C	-16.812951	7.400266	-36.247574
C	-17.409869	7.671888	-34.927337
O	-16.760631	7.305884	-33.945794
C	-13.080529	8.830639	-34.793310
C	-13.525942	9.706376	-35.709537
C	-13.789277	11.139214	-35.287471
C	-15.068048	11.283283	-34.433156
C	-15.348504	12.751073	-34.083614
C	-14.175164	13.467228	-33.414935
C	-16.263409	10.611040	-35.124222
C	-17.496751	10.503134	-34.220665
C	-18.722144	9.834739	-34.886181
C	-19.972127	10.487982	-34.350757
C	-20.865567	9.906740	-33.554691
C	-20.757923	8.475703	-33.119459
C	-19.731687	7.738877	-35.874084
C	-19.422686	6.375529	-33.071084
C	-19.807585	6.143677	-31.606790
C	-21.141757	6.810992	-31.272771
C	-21.149771	8.290567	-31.649000
O	-16.560774	11.338870	-36.309883
C	-13.877276	9.368543	-37.132097
C	-12.048793	5.332533	-36.183015
C	-13.252031	6.602636	-33.680674

C	-19.357863	7.884319	-33.362435
H	-22.690531	8.751677	-30.554941
H	-11.969632	7.455829	-36.800944
H	-14.574367	5.291400	-39.445339
H	-14.340927	4.565968	-37.741237
H	-15.733570	5.830675	-34.653736
H	-16.098056	7.591964	-39.416616
H	-12.923139	9.222366	-33.784637
H	-13.883162	11.780986	-36.171666
H	-12.939221	11.509198	-34.706121
H	-14.895261	10.727863	-33.498777
H	-16.211337	12.799968	-33.410965
H	-15.636259	13.278800	-35.000229
H	-13.803804	12.893902	-32.558415
H	-14.479243	14.452226	-33.051378
H	-13.340107	13.614939	-34.104578
H	-15.937162	9.598052	-35.393937
H	-17.230954	9.971959	-33.297311
H	-17.789737	11.516301	-33.927071
H	-18.674027	10.062731	-35.956907
H	-20.099988	11.532234	-34.632509
H	-21.730705	10.461583	-33.202193
H	-21.494554	7.886581	-33.691765
H	-20.739558	8.137799	-35.737658
H	-19.787362	6.646855	-35.858610
H	-19.385705	8.057097	-36.857922
H	-18.469658	5.888229	-33.282468
H	-20.179613	5.911814	-33.717587
H	-19.019143	6.554497	-30.962659
H	-19.863496	5.072000	-31.392872
H	-21.376754	6.700808	-30.207482
H	-21.950474	6.327195	-31.836015
H	-20.420286	8.835116	-31.026011
H	-16.972030	10.719302	-36.933258
H	-14.806313	9.877014	-37.414994
H	-13.980016	8.292988	-37.287645
H	-13.101097	9.730925	-37.817715
H	-12.859569	4.722597	-35.774770
H	-11.946085	5.090836	-37.243702
H	-11.119484	5.020997	-35.691061
H	-13.202162	5.522449	-33.824643
H	-14.265135	6.873733	-33.363955
H	-12.584839	6.863310	-32.850486
H	-18.676923	8.331191	-32.623499

TS1a (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28432416			
Zero-point correction= 0.693898			
Thermal correction to Energy= 0.729189			
Thermal correction to Enthalpy= 0.730133			
Thermal correction to Gibbs Free Energy= 0.630727			
C	-18.944071	8.151314	-34.736950
O	-22.563592	8.983821	-31.489012
C	-12.582761	8.453089	-37.988629
C	-12.328324	7.171284	-37.473858
C	-13.904301	6.195170	-37.945968
C	-15.119194	6.723189	-37.497475
C	-15.678350	6.627913	-36.215227
O	-15.105787	5.972498	-35.208602
N	-15.935731	7.619149	-38.196170
C	-16.994244	8.059397	-37.435240
O	-17.787152	8.936377	-37.832547
C	-16.881587	7.366980	-36.153105
C	-17.565893	7.500133	-34.887903
O	-16.985799	7.065770	-33.869452
C	-13.237858	9.508097	-37.274957
C	-13.398247	9.712381	-35.930381
C	-13.868630	11.073126	-35.478520
C	-15.064953	11.109272	-34.511247
C	-15.375381	12.553993	-34.091648
C	-14.183731	13.310229	-33.504153
C	-16.264062	10.407595	-35.166613
C	-17.481100	10.298860	-34.234565
C	-18.759202	9.700617	-34.878029
C	-19.955248	10.445238	-34.339804
C	-20.892088	9.930948	-33.546977
C	-20.888224	8.496249	-33.109859
C	-19.882604	7.651111	-35.848444
C	-19.696819	6.312488	-33.039856
C	-20.104178	6.113885	-31.577183
C	-21.395306	6.867839	-31.257935
C	-21.304704	8.342521	-31.642740
O	-16.591909	11.114919	-36.354731
C	-12.966177	8.783896	-34.828873
C	-11.245223	6.308144	-38.091138
C	-12.230149	8.724351	-39.424191

C	-19.528641	7.811042	-33.339776
H	-22.823291	8.902715	-30.563250
H	-12.432134	7.047611	-36.402820
H	-13.751688	6.141116	-39.022514
H	-13.584284	5.302481	-37.414604
H	-15.673711	6.212953	-34.424420
H	-15.791512	7.926100	-39.146750
H	-13.558116	10.337017	-37.903354
H	-14.106128	11.697895	-36.344251
H	-13.002745	11.523364	-34.972694
H	-14.812326	10.536573	-33.606874
H	-16.172682	12.538307	-33.342332
H	-15.771878	13.092503	-34.960435
H	-13.699508	12.724687	-32.714845
H	-14.507296	14.257846	-33.066108
H	-13.428987	13.540942	-34.260421
H	-15.912247	9.401849	-35.428466
H	-17.205784	9.732253	-33.335276
H	-17.729228	11.311652	-33.901947
H	-18.708924	9.907462	-35.951918
H	-20.006826	11.496946	-34.620046
H	-21.715382	10.547805	-33.196598
H	-21.657772	7.957621	-33.688781
H	-20.857748	8.137334	-35.755011
H	-20.030485	6.569371	-35.785173
H	-19.479743	7.896114	-36.831002
H	-18.776460	5.766065	-33.248201
H	-20.481928	5.897287	-33.685847
H	-19.296037	6.477943	-30.929118
H	-20.230733	5.049483	-31.356080
H	-21.646793	6.779801	-30.194151
H	-22.228626	6.433775	-31.826059
H	-20.547126	8.842160	-31.015354
H	-17.037197	10.494473	-36.956865
H	-12.957010	9.309366	-33.871970
H	-11.957551	8.400331	-35.011728
H	-13.634945	7.919821	-34.729799
H	-10.260985	6.750436	-37.910902
H	-11.253457	5.309549	-37.649336
H	-11.370892	6.201025	-39.171634
H	-11.143051	8.708753	-39.561876
H	-12.604959	9.692665	-39.755880
H	-12.638577	7.948550	-40.084110
H	-18.825698	8.215742	-32.596660

TS1b (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28039231			
Zero-point correction= 0.694000			
Thermal correction to Energy= 0.729137			
Thermal correction to Enthalpy= 0.730081			
Thermal correction to Gibbs Free Energy= 0.631694			
C	-19.107615	8.172323	-34.653936
O	-22.892541	9.342775	-31.717958
C	-12.450244	7.257634	-35.551801
C	-12.271188	6.805198	-36.875639
C	-13.897632	5.889334	-37.311215
C	-15.134271	6.502059	-37.050458
C	-15.767227	6.536306	-35.800336
O	-15.228263	6.003176	-34.709873
N	-15.947639	7.267325	-37.899169
C	-17.027395	7.806131	-37.231614
O	-17.775485	8.660761	-37.744886
C	-16.989485	7.240645	-35.882484
C	-17.736919	7.491767	-34.673571
O	-17.214601	7.154499	-33.588479
C	-13.040870	8.506957	-35.187687
C	-13.570048	9.522835	-35.940379
C	-13.873048	10.839209	-35.250122
C	-15.125270	10.887664	-34.347634
C	-15.368018	12.318516	-33.847112
C	-14.149276	12.977517	-33.201925
C	-16.336998	10.288129	-35.073385
C	-17.618195	10.313385	-34.227857
C	-18.870977	9.700445	-34.906438
C	-20.076557	10.513356	-34.506012
C	-21.072758	10.084191	-33.735004
C	-21.130783	8.691032	-33.181585
C	-19.997078	7.603805	-35.772177
C	-19.987812	6.502393	-32.847533
C	-20.489619	6.440484	-31.402074
C	-21.783667	7.236886	-31.233135
C	-21.640009	8.671362	-31.736087
O	-16.541637	10.986526	-36.299420
C	-13.803026	9.560904	-37.417542
C	-11.251838	5.715883	-37.153250
C	-12.036010	6.343891	-34.435127

C	-19.776113	7.965635	-33.268368
H	-23.205589	9.357339	-30.805346
H	-12.274048	7.575173	-37.638402
H	-13.645799	5.719817	-38.356149
H	-13.695354	5.032147	-36.671913
H	-15.837540	6.304707	-33.980441
H	-15.732220	7.520266	-38.851929
H	-13.005383	8.711263	-34.117444
H	-13.981804	11.615583	-36.015320
H	-13.003580	11.100573	-34.638105
H	-14.939322	10.240710	-33.477012
H	-16.178203	12.299346	-33.111576
H	-15.722005	12.926353	-34.689309
H	-13.720843	12.331938	-32.427435
H	-14.427176	13.924095	-32.731684
H	-13.363986	13.191328	-33.931632
H	-16.055965	9.254205	-35.295672
H	-17.435273	9.828405	-33.260111
H	-17.841797	11.364137	-34.016737
H	-18.749413	9.815870	-35.988946
H	-20.084114	11.539328	-34.872758
H	-21.899956	10.744273	-33.488108
H	-21.875943	8.119609	-33.760918
H	-20.960225	8.121701	-35.779229
H	-20.182276	6.535966	-35.625566
H	-19.531826	7.751806	-36.746502
H	-19.063743	5.931638	-32.947288
H	-20.736769	6.038373	-33.503207
H	-19.716819	6.850204	-30.738333
H	-20.649523	5.401770	-31.096476
H	-22.103011	7.244256	-30.184072
H	-22.587707	6.766487	-31.814348
H	-20.912424	9.211837	-31.107110
H	-17.017214	10.382890	-36.895431
H	-14.777789	10.029150	-37.593427
H	-13.784821	8.599411	-37.915177
H	-13.052803	10.218858	-37.876504
H	-11.423894	4.823499	-36.546100
H	-11.287184	5.421024	-38.204291
H	-10.241833	6.078207	-36.938609
H	-12.544652	5.376989	-34.539572
H	-12.291824	6.756092	-33.459065
H	-10.959259	6.144516	-34.466504
H	-19.108691	8.424518	-32.524234

TS1c (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27642832			
Zero-point correction= 0.692115			
Thermal correction to Energy= 0.727815			
Thermal correction to Enthalpy= 0.728759			
Thermal correction to Gibbs Free Energy= 0.628209			
C	2.102969	0.966853	-0.447832
C	0.922444	1.385273	0.435030
O	1.093218	1.483967	1.673450
C	-0.408218	1.598404	-0.075744
C	-1.442580	1.952700	0.830198
O	-1.299837	2.116953	2.137536
H	-0.327193	1.912051	2.283764
C	-2.657795	2.101309	0.144728
N	-2.395717	1.726737	-1.177110
C	-1.046615	1.467671	-1.391980
O	-0.604182	1.179804	-2.508438
H	-3.005319	1.923823	-1.958238
C	-3.933102	2.401249	0.649119
H	-4.627170	2.844386	-0.064582
H	-3.918530	2.911862	1.609250
C	-5.054126	0.978619	1.194591
C	-6.369678	1.711254	1.378305
H	-6.259676	2.518921	2.105466
H	-6.729523	2.148239	0.443564
H	-7.135311	1.023487	1.749478
H	-4.563599	0.720668	2.133334
C	-4.902317	-0.001961	0.191624
C	-3.934286	-1.034163	0.421008
C	-3.299730	-1.853097	-0.465033
C	-3.299451	-1.685667	-1.955158
H	-4.053696	-2.336166	-2.416773
H	-3.491295	-0.655716	-2.258860
H	-2.327970	-2.001505	-2.346586
C	-2.492722	-3.007060	0.082446
H	-3.063895	-3.475969	0.888507
H	-2.347071	-3.754628	-0.705547
C	-1.105790	-2.608815	0.632360
H	-1.265001	-1.889295	1.450149
C	-0.363793	-3.825535	1.202148
C	-1.134846	-4.583771	2.282212

H	-1.495804	-3.897199	3.055379
H	-1.998687	-5.113739	1.873412
H	-0.493223	-5.325140	2.764534
H	0.587441	-3.486668	1.625557
H	-0.114749	-4.516711	0.385121
C	-0.295581	-1.869690	-0.443212
H	-0.875032	-0.985418	-0.736829
C	1.080748	-1.399790	0.020504
H	0.991029	-0.924259	1.004383
H	1.723339	-2.275941	0.170928
C	1.736865	-0.442470	-1.016915
C	2.930530	-1.124288	-1.631237
C	4.195695	-0.794013	-1.383246
C	4.578259	0.348941	-0.489164
C	3.410209	0.862107	0.378598
C	3.877599	2.149337	1.077056
C	5.067983	1.844849	1.991322
C	6.224778	1.216579	1.212690
H	7.044200	0.928699	1.879024
C	5.780171	-0.000924	0.405419
H	5.480185	-0.807741	1.087875
O	6.861496	-0.534835	-0.345972
H	7.171732	0.161611	-0.940210
H	6.627156	1.957457	0.505762
H	5.409331	2.756959	2.490894
H	4.743250	1.154593	2.781073
H	3.066762	2.595004	1.652766
H	4.189430	2.881656	0.320178
H	3.226377	0.111474	1.163530
H	4.919625	1.182910	-1.129236
H	5.011774	-1.348984	-1.838919
H	2.703698	-1.972770	-2.276153
H	1.000943	-0.273271	-1.810685
O	-0.176923	-2.630422	-1.643288
H	0.404250	-3.381971	-1.466453
H	-3.705516	-1.209429	1.472955
C	-5.741460	0.079897	-1.047750
H	-5.473844	0.959394	-1.650677
H	-6.794884	0.200298	-0.776709
H	-5.652134	-0.805879	-1.672025
C	2.271581	1.974782	-1.597689
H	2.546218	2.961881	-1.214877
H	1.350779	2.059887	-2.173762
H	3.061811	1.637592	-2.274455

INT1c (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.29175776			
Zero-point correction= 0.693517			
Thermal correction to Energy= 0.729454			
Thermal correction to Enthalpy= 0.730398			
Thermal correction to Gibbs Free Energy= 0.628918			
C	2.050999	0.983443	-0.453768
C	0.863768	1.413679	0.408550
O	0.990747	1.494673	1.644977
C	-0.460420	1.671714	-0.135554
C	-1.497539	2.050388	0.737375
O	-1.421023	2.205611	2.046926
H	-0.473012	1.972932	2.256852
C	-2.703662	2.244952	0.012324
N	-2.415114	1.961296	-1.278286
C	-1.065038	1.585060	-1.464205
O	-0.644526	1.256768	-2.568094
H	-3.061825	2.012686	-2.054263
C	-4.060456	2.521551	0.540807
H	-4.694283	2.922412	-0.257635
H	-3.995846	3.279040	1.328304
C	-4.714985	1.233619	1.133999
C	-6.119422	1.576026	1.641123
H	-6.062867	2.317770	2.442702
H	-6.744046	1.994831	0.846921
H	-6.614824	0.683646	2.032292
H	-4.099690	0.941528	1.993455
C	-4.660069	0.110738	0.124836
C	-3.780431	-0.941072	0.359134
C	-3.292344	-1.928514	-0.494170
C	-3.392431	-1.891200	-1.992607
H	-4.217027	-2.510165	-2.372755
H	-3.532443	-0.876546	-2.371943
H	-2.468060	-2.294298	-2.419829
C	-2.502171	-3.068140	0.104907
H	-3.065403	-3.502124	0.938157
H	-2.372063	-3.859375	-0.643285
C	-1.104864	-2.663951	0.625537
H	-1.248112	-1.943150	1.445300
C	-0.342868	-3.872464	1.186814
C	-1.086198	-4.622656	2.291934

H	-1.420245	-3.930971	3.072642
H	-1.965567	-5.146653	1.909667
H	-0.436047	-5.366907	2.758498
H	0.620147	-3.533318	1.583444
H	-0.116949	-4.571515	0.369530
C	-0.313624	-1.919211	-0.460346
H	-0.923493	-1.063202	-0.777830
C	1.037008	-1.387549	0.013325
H	0.908783	-0.899192	0.986482
H	1.712703	-2.232363	0.193390
C	1.679128	-0.424061	-1.027053
C	2.874889	-1.097996	-1.647833
C	4.138591	-0.778679	-1.378639
C	4.518087	0.346608	-0.460733
C	3.341633	0.859778	0.395593
C	3.807259	2.134377	1.117550
C	4.981640	1.807522	2.044989
C	6.144475	1.177418	1.276817
H	6.950268	0.874365	1.952838
C	5.701953	-0.026689	0.448452
H	5.383339	-0.838676	1.116074
O	6.789166	-0.561504	-0.292879
H	7.119979	0.140890	-0.868764
H	6.564847	1.922520	0.585033
H	5.323426	2.710698	2.559984
H	4.638590	1.111440	2.821653
H	2.992939	2.579365	1.689334
H	4.134448	2.874886	0.375389
H	3.137967	0.101384	1.167960
H	4.878229	1.186061	-1.082919
H	4.956909	-1.329679	-1.834860
H	2.649568	-1.933546	-2.309244
H	0.939099	-0.256393	-1.817645
O	-0.153543	-2.697523	-1.644448
H	0.440553	-3.431621	-1.439640
H	-3.403230	-0.999441	1.384065
C	-5.521049	0.237087	-1.100535
H	-5.104689	0.919577	-1.855438
H	-6.505047	0.638535	-0.838647
H	-5.675408	-0.727008	-1.585728
C	2.252464	1.992163	-1.597945
H	2.525076	2.976539	-1.207331
H	1.350586	2.089707	-2.200558
H	3.055294	1.648940	-2.255447

TS1c-II (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28685442			
Zero-point correction= 0.693728			
Thermal correction to Energy= 0.728758			
Thermal correction to Enthalpy= 0.729702			
Thermal correction to Gibbs Free Energy= 0.629953			
C	1.926400	0.775572	-0.595562
C	0.672454	0.965652	0.263350
O	0.728855	0.651157	1.473138
C	-0.591263	1.470475	-0.229206
C	-1.620541	1.744244	0.696400
O	-1.581432	1.532577	2.002044
H	-0.684011	1.109515	2.139579
C	-2.737968	2.303732	0.035398
N	-2.387986	2.400709	-1.282864
C	-1.142713	1.798071	-1.545576
O	-0.754810	1.592555	-2.693144
H	-3.019254	2.648241	-2.033006
C	-4.021739	2.755349	0.664207
H	-4.653107	3.240873	-0.085654
H	-3.844675	3.485007	1.461253
C	-4.670729	1.460226	1.191904
C	-6.167820	1.600552	1.466247
H	-6.350769	2.392057	2.198728
H	-6.713604	1.856113	0.552447
H	-6.578359	0.666893	1.860010
H	-4.160014	1.193106	2.123029
C	-4.324763	0.397759	0.156182
C	-3.634442	-0.760433	0.550545
C	-3.204133	-1.844432	-0.191309
C	-3.425058	-2.030437	-1.669585
H	-4.466577	-1.872593	-1.957253
H	-2.810414	-1.334282	-2.255825
H	-3.127154	-3.034565	-1.970812
C	-2.405187	-2.909133	0.518882
H	-2.839795	-3.082992	1.509074
H	-2.474811	-3.851342	-0.037117
C	-0.907506	-2.575144	0.713692
H	-0.836002	-1.756083	1.447472
C	-0.155417	-3.793658	1.268486
C	-0.735586	-4.345714	2.570273

H	-0.841294	-3.549703	3.315091
H	-1.719789	-4.796295	2.419330
H	-0.081993	-5.114221	2.990388
H	0.892008	-3.523067	1.438241
H	-0.153328	-4.589973	0.510747
C	-0.273683	-2.028731	-0.575149
H	-0.802895	-1.102485	-0.829431
C	1.221897	-1.727046	-0.423059
H	1.446915	-1.479957	0.619098
H	1.771623	-2.652389	-0.635772
C	1.746980	-0.592189	-1.342907
C	3.047569	-1.031878	-1.967991
C	4.250515	-0.609443	-1.583526
C	4.452338	0.427150	-0.517098
C	3.181782	0.685054	0.313606
C	3.433703	1.896342	1.222582
C	4.593380	1.595331	2.177142
C	5.863763	1.213808	1.414328
H	6.666698	0.926511	2.100531
C	5.622924	0.080841	0.418180
H	5.375163	-0.842183	0.959537
O	6.806534	-0.220255	-0.306737
H	7.074763	0.585221	-0.769030
H	6.219776	2.086534	0.846869
H	4.792478	2.457460	2.821206
H	4.303676	0.767342	2.837326
H	2.536979	2.146273	1.793001
H	3.690215	2.770500	0.609367
H	3.042917	-0.183518	0.972168
H	4.742635	1.371939	-1.010974
H	5.147622	-1.003267	-2.054517
H	2.962976	-1.795121	-2.740388
H	1.008284	-0.431321	-2.140778
O	-0.499489	-2.878830	-1.696201
H	0.008550	-3.689139	-1.559979
H	-3.351363	-0.780098	1.604726
C	-4.919919	0.589778	-1.211044
H	-4.192561	0.423772	-2.009433
H	-5.327208	1.596640	-1.331543
H	-5.749232	-0.108366	-1.376584
C	2.091273	1.923234	-1.601984
H	2.169740	2.884712	-1.085674
H	1.251977	1.965325	-2.292216
H	3.000152	1.775872	-2.189455

INT1a (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.29550829			
Zero-point correction= 0.694487			
Thermal correction to Energy= 0.730170			
Thermal correction to Enthalpy= 0.731114			
Thermal correction to Gibbs Free Energy= 0.630598			
C	-2.142029	-0.427925	0.465669
O	-5.751099	0.382050	3.725498
C	3.866526	-0.124693	-2.842017
C	4.062815	-1.540979	-2.373263
C	2.886986	-2.460689	-2.860599
C	1.590264	-1.943342	-2.386869
C	1.047352	-2.035044	-1.079125
O	1.627525	-2.749136	-0.122677
N	0.809006	-1.067698	-3.062097
C	-0.223997	-0.552600	-2.256805
O	-0.963510	0.352289	-2.651698
C	-0.102261	-1.240335	-0.979981
C	-0.766400	-1.076747	0.308842
O	-0.159714	-1.494148	1.307346
C	3.468839	0.947392	-2.042203
C	3.351722	1.120681	-0.663573
C	2.960144	2.481016	-0.143683
C	1.727370	2.511688	0.783494
C	1.418901	3.946912	1.236618
C	2.604076	4.675763	1.870224
C	0.531570	1.842998	0.089618
C	-0.702712	1.729245	0.995906
C	-1.963835	1.123404	0.327977
C	-3.175170	1.853820	0.852755
C	-4.103700	1.332195	1.650450
C	-4.080592	-0.098805	2.099115
C	-3.085134	-0.931821	-0.640716
C	-2.865759	-2.270516	2.172906
C	-3.266070	-2.466007	3.638127
C	-4.562376	-1.722270	3.960441
C	-4.487461	-0.248259	3.569458
O	0.230992	2.588147	-1.085308
C	3.725313	0.111569	0.390803
C	5.386818	-2.149805	-2.849037
C	4.066050	0.118513	-4.314600

C	-2.715316	-0.771339	1.866971
H	-6.005820	0.304143	4.652925
H	4.032615	-1.585937	-1.285152
H	2.896730	-2.538122	-3.952008
H	3.050659	-3.460737	-2.448771
H	1.139133	-2.509559	0.702200
H	0.972743	-0.734780	-4.003388
H	3.244377	1.852174	-2.609348
H	2.777128	3.166719	-0.977679
H	3.814943	2.877365	0.422751
H	1.947780	1.910816	1.678752
H	0.604096	3.922070	1.967148
H	1.049046	4.513529	0.373670
H	3.060393	4.067801	2.659258
H	2.281100	5.618434	2.319592
H	3.381021	4.910259	1.138257
H	0.871299	0.839909	-0.196595
H	-0.443341	1.164800	1.901214
H	-0.963064	2.740656	1.322899
H	-1.900407	1.336786	-0.744473
H	-3.241369	2.901705	0.562627
H	-4.936310	1.939599	1.994897
H	-4.847439	-0.649844	1.528461
H	-4.065100	-0.460370	-0.531255
H	-3.216519	-2.016075	-0.587229
H	-2.703690	-0.673829	-1.628322
H	-1.940547	-2.809793	1.966114
H	-3.647355	-2.697424	1.530446
H	-2.458229	-2.092473	4.281026
H	-3.382108	-3.530586	3.863471
H	-4.807167	-1.808394	5.025835
H	-5.394727	-2.166088	3.398572
H	-3.731243	0.261338	4.190288
H	-0.199449	1.992337	-1.716133
H	3.797333	0.597397	1.367619
H	4.695874	-0.350623	0.184088
H	2.991194	-0.699260	0.487658
H	6.230474	-1.538697	-2.517364
H	5.510588	-3.158271	-2.445209
H	5.421948	-2.216733	-3.940457
H	5.132137	0.118733	-4.576831
H	3.653031	1.083076	-4.617436
H	3.603517	-0.659256	-4.935193
H	-2.013267	-0.356586	2.605136

INT1b (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.29191085			
Zero-point correction= 0.694653			
Thermal correction to Energy= 0.730284			
Thermal correction to Enthalpy= 0.731229			
Thermal correction to Gibbs Free Energy= 0.631227			
C	-19.068455	8.129457	-34.640642
O	-22.908686	9.467977	-31.854545
C	-12.622186	7.276884	-35.652097
C	-12.674884	6.712283	-37.052940
C	-13.800468	5.634546	-37.203370
C	-15.134797	6.201807	-36.918214
C	-15.787272	6.302102	-35.660375
O	-15.301784	5.738103	-34.567128
N	-15.866831	6.943507	-37.786034
C	-16.944039	7.592307	-37.146476
O	-17.612428	8.452887	-37.720186
C	-16.938809	7.092168	-35.778367
C	-17.710775	7.429684	-34.588236
O	-17.212714	7.128581	-33.491983
C	-13.033643	8.546546	-35.267211
C	-13.547215	9.656061	-35.953885
C	-13.823662	10.902235	-35.144220
C	-15.098603	10.872679	-34.265952
C	-15.396308	12.270010	-33.703335
C	-14.206294	12.932578	-33.009638
C	-16.282248	10.271203	-35.036339
C	-17.589573	10.280398	-34.233307
C	-18.808022	9.643463	-34.950737
C	-20.029482	10.473427	-34.642240
C	-21.046929	10.088888	-33.875313
C	-21.125361	8.728373	-33.247859
C	-19.934119	7.518086	-35.755739
C	-20.013332	6.547657	-32.787396
C	-20.547223	6.557296	-31.352138
C	-21.833900	7.376552	-31.246795
C	-21.663812	8.784313	-31.813632
O	-16.452505	10.990441	-36.256727
C	-13.802580	9.738557	-37.433606
C	-11.342481	6.078135	-37.473448
C	-12.066939	6.354769	-34.598304

C	-19.775315	7.988847	-33.266170
H	-23.239120	9.532629	-30.950286
H	-12.907616	7.505928	-37.763411
H	-13.768685	5.237451	-38.222960
H	-13.611144	4.807069	-36.513279
H	-15.860810	6.094532	-33.832583
H	-15.639442	7.107749	-38.758385
H	-12.911599	8.732091	-34.197261
H	-13.902549	11.761176	-35.819769
H	-12.971914	11.095336	-34.481127
H	-14.910415	10.192464	-33.420767
H	-16.217374	12.198908	-32.982749
H	-15.752144	12.906648	-34.523897
H	-13.780345	12.269275	-32.248811
H	-14.513999	13.856491	-32.513182
H	-13.410489	13.185718	-33.714716
H	-15.991872	9.240811	-35.269551
H	-17.431725	9.805894	-33.255815
H	-17.835343	11.328451	-34.035693
H	-18.630414	9.715588	-36.029573
H	-20.023992	11.476338	-35.067402
H	-21.880043	10.761641	-33.690553
H	-21.863003	8.132427	-33.811828
H	-20.898481	8.030922	-35.795349
H	-20.116726	6.454754	-35.577499
H	-19.459990	7.633522	-36.729789
H	-19.095904	5.959784	-32.838240
H	-20.752663	6.063538	-33.439287
H	-19.783088	6.986336	-30.690733
H	-20.727611	5.535399	-31.004583
H	-22.173039	7.437253	-30.205769
H	-22.632578	6.888820	-31.820966
H	-20.943262	9.347204	-31.196542
H	-16.821756	10.375419	-36.906937
H	-14.225387	10.711044	-37.687944
H	-14.513554	8.980113	-37.778244
H	-12.882777	9.603896	-38.016340
H	-11.117139	5.193387	-36.870756
H	-11.381638	5.770297	-38.521862
H	-10.522182	6.790799	-37.353276
H	-12.526283	5.360491	-34.645510
H	-12.241309	6.752171	-33.596315
H	-10.985728	6.209739	-34.718151
H	-19.123688	8.474420	-32.525145

TS2a (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28245031			
Zero-point correction= 0.694277			
Thermal correction to Energy= 0.728755			
Thermal correction to Enthalpy= 0.729699			
Thermal correction to Gibbs Free Energy= 0.632847			
C	-2.263018	-0.701543	-0.631468
O	-6.982898	0.154236	0.543458
C	5.303603	-0.432247	0.288801
C	4.715292	-1.778689	0.519258
C	3.915243	-2.092957	-0.803035
C	2.600696	-1.420629	-0.907454
C	1.473474	-1.713321	-0.132455
O	1.535798	-2.268306	1.077217
N	2.089983	-0.923546	-2.114874
C	0.719260	-0.793522	-2.096883
O	0.095773	-0.216727	-3.012897
C	0.282640	-1.342413	-0.814497
C	-0.936455	-1.213070	-0.051661
O	-0.883605	-1.485134	1.169828
C	4.527082	0.692893	0.205722
C	3.179258	0.906636	0.599644
C	2.610374	2.210146	0.068651
C	1.173582	2.610998	0.422123
C	0.968938	4.123638	0.261039
C	1.581970	4.939055	1.397877
C	0.245597	1.787701	-0.475340
C	-1.199560	1.650934	0.018860
C	-2.101065	0.830359	-0.946989
C	-3.436135	1.517479	-1.070248
C	-4.606807	1.013165	-0.689839
C	-4.742913	-0.352569	-0.086584
C	-2.581163	-1.448889	-1.938206
C	-3.632095	-2.377060	0.835876
C	-4.635434	-2.430045	1.991102
C	-5.961678	-1.781622	1.595018
C	-5.764108	-0.366742	1.056983
O	0.296003	2.338416	-1.784303
C	2.583604	0.396330	1.873041
C	5.722188	-2.890374	0.803474
C	6.736065	-0.355089	-0.148536

C	-3.398248	-0.918442	0.406214
H	-7.622322	0.171960	1.265833
H	3.970340	-1.774004	1.313704
H	4.537810	-1.864794	-1.674645
H	3.760435	-3.178775	-0.794995
H	0.612198	-2.140379	1.432399
H	2.648139	-0.528178	-2.857838
H	4.983510	1.545171	-0.299188
H	2.709616	2.227699	-1.024994
H	3.314655	2.972134	0.436948
H	0.954370	2.351227	1.465961
H	-0.105508	4.333585	0.210017
H	1.386701	4.436961	-0.701962
H	1.132789	4.665012	2.357608
H	1.421931	6.009479	1.245297
H	2.661333	4.777730	1.480489
H	0.692120	0.794288	-0.484894
H	-1.203508	1.200857	1.020617
H	-1.623105	2.656690	0.126664
H	-1.631595	0.882758	-1.934298
H	-3.395498	2.520112	-1.495337
H	-5.520937	1.586962	-0.816859
H	-5.152111	-1.031827	-0.853805
H	-3.498103	-1.046056	-2.379123
H	-2.727800	-2.517481	-1.757923
H	-1.774878	-1.317979	-2.659840
H	-2.696910	-2.853076	1.130700
H	-4.040516	-2.944461	-0.011026
H	-4.212100	-1.903906	2.856935
H	-4.805802	-3.465224	2.303081
H	-6.655891	-1.759338	2.443714
H	-6.438818	-2.369609	0.799922
H	-5.385153	0.284208	1.863181
H	0.216278	1.597896	-2.410165
H	1.516966	0.175364	1.781837
H	2.674942	1.222592	2.593823
H	3.089229	-0.468387	2.290509
H	6.326012	-2.659926	1.684752
H	5.189699	-3.825753	0.991685
H	6.396995	-3.054143	-0.041430
H	7.398308	-0.722938	0.642122
H	7.022266	0.667060	-0.398117
H	6.913511	-0.991091	-1.023927
H	-3.112600	-0.352655	1.305643

TS2b (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28083551			
Zero-point correction= 0.694469			
Thermal correction to Energy= 0.728946			
Thermal correction to Enthalpy= 0.729890			
Thermal correction to Gibbs Free Energy= 0.632786			
C	-19.170365	8.206906	-34.650929
O	-23.104146	9.291470	-31.885578
C	-12.157025	7.463929	-35.652778
C	-12.257239	6.688734	-36.913603
C	-13.728316	6.088983	-37.041451
C	-14.905523	6.952188	-36.802789
C	-15.545039	7.123213	-35.564055
O	-14.981692	6.822303	-34.403898
N	-15.866010	7.262013	-37.758082
C	-17.056750	7.719066	-37.192965
O	-17.969548	8.192744	-37.877238
C	-16.886257	7.557258	-35.748966
C	-17.705290	7.765984	-34.590678
O	-17.162512	7.637669	-33.462846
C	-12.836689	8.644422	-35.481126
C	-13.679199	9.357951	-36.362216
C	-14.286960	10.619847	-35.772142
C	-15.417092	10.497831	-34.718449
C	-15.185705	11.461035	-33.544535
C	-14.026104	11.042097	-32.644232
C	-16.766551	10.766609	-35.401102
C	-17.989353	10.529872	-34.486067
C	-19.139383	9.701023	-35.125599
C	-20.455243	10.387864	-34.864041
C	-21.389843	9.949081	-34.023630
C	-21.258514	8.666466	-33.255203
C	-19.961780	7.349053	-35.649966
C	-19.829159	6.731729	-32.598680
C	-20.328760	6.828507	-31.154362
C	-21.720408	7.459009	-31.094963
C	-21.771036	8.803498	-31.817131
O	-16.731690	12.120571	-35.853071
C	-13.709351	9.388918	-37.860770
C	-11.265235	5.534741	-37.052607
C	-11.487149	6.831064	-34.473568

C	-19.816171	8.126594	-33.243403
H	-23.424345	9.399864	-30.981820
H	-12.108765	7.353421	-37.763276
H	-13.797460	5.649041	-38.040315
H	-13.753554	5.268889	-36.314236
H	-15.696415	7.079217	-33.740612
H	-15.696938	7.330215	-38.751661
H	-12.816472	9.052850	-34.470687
H	-14.657315	11.260217	-36.576852
H	-13.442594	11.158710	-35.321453
H	-15.447333	9.475092	-34.319769
H	-16.098748	11.517093	-32.941215
H	-15.015887	12.468218	-33.941177
H	-14.186439	10.032433	-32.250652
H	-13.920825	11.721896	-31.794814
H	-13.071015	11.042478	-33.179930
H	-16.839692	10.107414	-36.277196
H	-17.681232	10.049385	-33.550873
H	-18.362847	11.519638	-34.203565
H	-18.974842	9.675293	-36.211380
H	-20.601550	11.333037	-35.386078
H	-22.305127	10.515963	-33.875340
H	-21.914037	7.914682	-33.726748
H	-20.988841	7.717932	-35.721871
H	-19.995585	6.304318	-35.328124
H	-19.517871	7.399654	-36.642960
H	-18.834081	6.285707	-32.623300
H	-20.502915	6.073507	-33.163260
H	-19.624223	7.437817	-30.572961
H	-20.349024	5.838425	-30.688279
H	-22.046801	7.587393	-30.055897
H	-22.447800	6.798271	-31.584797
H	-21.129491	9.530006	-31.290143
H	-17.512129	12.266553	-36.401237
H	-14.741397	9.558356	-38.190121
H	-13.329436	8.515922	-38.380428
H	-13.137038	10.268224	-38.186933
H	-11.395180	4.790558	-36.261926
H	-11.411462	5.033361	-38.012629
H	-10.235481	5.898764	-37.014886
H	-12.020087	5.907692	-34.205750
H	-11.498084	7.492376	-33.606086
H	-10.453392	6.546132	-34.692242
H	-19.226542	8.781161	-32.584594

TS3a (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28379004			
Zero-point correction= 0.693621			
Thermal correction to Energy= 0.728860			
Thermal correction to Enthalpy= 0.729804			
Thermal correction to Gibbs Free Energy= 0.630208			
C	1.986720	-0.886964	0.504786
O	6.770975	0.226555	0.185963
C	-4.253557	-0.326012	0.270748
C	-4.647929	-1.198806	-0.912190
C	-4.072294	-2.578629	-0.528140
C	-2.757934	-2.216427	0.103292
C	-1.631372	-1.754595	-0.614354
O	-1.641455	-1.547161	-1.921807
N	-2.325297	-2.400571	1.398331
C	-1.044194	-1.858913	1.589821
O	-0.588437	-1.637805	2.713814
C	-0.535506	-1.570462	0.248728
C	0.711302	-1.080450	-0.306034
O	0.710942	-0.749923	-1.511040
C	-3.587801	0.922414	0.272504
C	-3.079822	1.731527	-0.714602
C	-2.397693	3.005580	-0.286828
C	-0.849330	2.955920	-0.299887
C	-0.268559	4.270562	0.242732
C	-0.824644	5.529191	-0.422536
C	-0.349812	1.718456	0.465131
C	1.179026	1.635107	0.548861
C	1.774087	0.429152	1.327503
C	3.080982	0.886083	1.930467
C	4.285162	0.533821	1.484601
C	4.491153	-0.440080	0.360550
C	2.217705	-2.076233	1.450500
C	3.469885	-1.868675	-1.410886
C	4.582763	-1.478080	-2.388281
C	5.860669	-1.083279	-1.646054
C	5.606695	-0.003946	-0.594922
O	-0.910804	1.742383	1.776820
C	-3.156618	1.466315	-2.194325
C	-6.147159	-1.199746	-1.207699
C	-4.883200	-0.686949	1.593693

C	3.203658	-0.709083	-0.439605
H	7.471329	0.519676	-0.409591
H	-4.105166	-0.864862	-1.798562
H	-4.715391	-3.107738	0.178899
H	-3.931218	-3.230223	-1.396595
H	-0.725777	-1.175344	-2.101372
H	-2.939085	-2.548086	2.188437
H	-3.434975	1.315701	1.277282
H	-2.710017	3.271156	0.728430
H	-2.719466	3.812489	-0.955000
H	-0.514434	2.832618	-1.341353
H	0.817024	4.261039	0.103238
H	-0.445938	4.310034	1.325053
H	-0.756237	5.456557	-1.513561
H	-0.259434	6.410980	-0.110192
H	-1.872401	5.701697	-0.163960
H	-0.746959	0.856977	-0.077917
H	1.604308	1.675006	-0.461805
H	1.520169	2.537666	1.065900
H	1.089166	0.183114	2.150008
H	2.996040	1.597611	2.750567
H	5.180533	0.933900	1.952767
H	4.841236	-1.390910	0.797193
H	3.129187	-1.918650	2.031496
H	2.328381	-3.005932	0.884800
H	1.392810	-2.188170	2.151488
H	2.564109	-2.130119	-1.960986
H	3.783409	-2.757197	-0.846911
H	4.238312	-0.633767	-2.999774
H	4.793448	-2.301490	-3.077689
H	6.627520	-0.738410	-2.349932
H	6.270345	-1.956732	-1.121896
H	5.292879	0.929959	-1.091019
H	-0.937899	0.833094	2.105757
H	-2.786434	2.326232	-2.757581
H	-4.187460	1.275281	-2.511750
H	-2.561192	0.594003	-2.477937
H	-6.489220	-0.196148	-1.476610
H	-6.372686	-1.873164	-2.039342
H	-6.719294	-1.534138	-0.336576
H	-5.783317	-0.078028	1.748953
H	-4.205694	-0.467914	2.425215
H	-5.196411	-1.730587	1.662034
H	3.005855	0.180203	-1.053531

TS3b (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28809810			
Zero-point correction= 0.694822			
Thermal correction to Energy= 0.729454			
Thermal correction to Enthalpy= 0.730399			
Thermal correction to Gibbs Free Energy= 0.633261			
C	-19.011659	8.157248	-34.564025
O	-22.907058	9.381723	-31.785299
C	-13.054084	7.165909	-35.704896
C	-12.733565	6.500387	-37.040313
C	-13.850199	5.461673	-37.247178
C	-15.105689	6.165830	-36.839074
C	-15.829918	6.160164	-35.627115
O	-15.554075	5.356204	-34.603541
N	-15.696546	7.109991	-37.628199
C	-16.763914	7.751117	-36.990493
O	-17.366478	8.695836	-37.522890
C	-16.873391	7.112431	-35.693262
C	-17.673970	7.401421	-34.515130
O	-17.252148	6.974902	-33.426217
C	-13.346606	8.521394	-35.454609
C	-13.658612	9.625603	-36.222954
C	-13.866611	10.937798	-35.487956
C	-15.006780	10.958334	-34.442303
C	-15.218375	12.377547	-33.898841
C	-13.952598	13.035047	-33.350068
C	-16.277966	10.367602	-35.059834
C	-17.476852	10.279244	-34.108096
C	-18.740069	9.684940	-34.787505
C	-19.933978	10.522616	-34.408287
C	-20.975527	10.109130	-33.691931
C	-21.101165	8.704784	-33.182650
C	-19.846190	7.631101	-35.745813
C	-20.062598	6.468830	-32.864061
C	-20.633672	6.381517	-31.446043
C	-21.902720	7.222569	-31.310733
C	-21.680966	8.663277	-31.763792
O	-16.611702	11.131510	-36.216586
C	-13.828063	9.733609	-37.706814
C	-11.330096	5.892958	-37.088337
C	-12.749055	6.329728	-34.491571

C	-19.767287	7.935395	-33.224149
H	-23.264547	9.380093	-30.889077
H	-12.803680	7.236473	-37.841076
H	-13.901439	5.101857	-38.279845
H	-13.700043	4.593377	-36.599628
H	-16.074092	5.725182	-33.851416
H	-15.411817	7.354092	-38.566775
H	-13.355751	8.741995	-34.385314
H	-14.071718	11.727427	-36.218080
H	-12.927724	11.200596	-34.985570
H	-14.726339	10.307607	-33.601063
H	-15.964411	12.338933	-33.097983
H	-15.646624	12.995861	-34.697398
H	-13.457821	12.382126	-32.622721
H	-14.191646	13.975450	-32.846916
H	-13.232668	13.259444	-34.141492
H	-16.014853	9.354232	-35.367863
H	-17.205454	9.698279	-33.216473
H	-17.716671	11.290461	-33.763150
H	-18.604461	9.808839	-35.866207
H	-19.890230	11.556758	-34.748909
H	-21.790332	10.789967	-33.461217
H	-21.834477	8.173361	-33.813028
H	-20.799469	8.165394	-35.790577
H	-20.054343	6.562360	-35.644531
H	-19.325914	7.798873	-36.689478
H	-19.165024	5.855119	-32.940618
H	-20.801409	6.063896	-33.568593
H	-19.877623	6.738416	-30.734267
H	-20.847454	5.340656	-31.183874
H	-22.269799	7.213019	-30.277437
H	-22.696227	6.800766	-31.941568
H	-20.965325	9.157783	-31.085266
H	-16.964387	10.500044	-36.863124
H	-14.866148	10.030728	-37.911991
H	-13.608316	8.830298	-38.267687
H	-13.194661	10.541280	-38.091840
H	-11.213353	5.101972	-36.342178
H	-11.146187	5.456734	-38.073856
H	-10.568952	6.655833	-36.903494
H	-12.969106	5.271378	-34.644091
H	-13.316794	6.668693	-33.622844
H	-11.680131	6.409733	-34.249686
H	-19.124174	8.346333	-32.431431

exo-4+2 adduct **8** (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.35675507			
Zero-point correction= 0.698709			
Thermal correction to Energy= 0.732774			
Thermal correction to Enthalpy= 0.733719			
Thermal correction to Gibbs Free Energy= 0.638223			
C	-18.966219	7.961101	-34.639458
O	-23.074047	8.847063	-32.063807
C	-12.183796	8.404715	-38.252041
C	-12.548724	6.950422	-38.025267
C	-13.396964	6.743620	-36.757503
C	-14.306130	7.945293	-36.429938
C	-15.200905	7.578569	-35.279734
O	-14.698722	7.283144	-34.116046
N	-15.312395	8.135491	-37.462759
C	-16.606104	7.979626	-37.051856
O	-17.577031	8.150010	-37.781076
C	-16.539660	7.613608	-35.609677
C	-17.500583	7.552950	-34.511124
O	-17.038694	7.280985	-33.384569
C	-12.581936	9.388083	-37.438730
C	-13.450325	9.241322	-36.201614
C	-14.280749	10.550049	-36.067302
C	-15.294500	10.679897	-34.900559
C	-15.020369	11.893133	-33.995680
C	-13.754242	11.774193	-33.153845
C	-16.730576	10.756645	-35.450184
C	-17.831293	10.346981	-34.444821
C	-18.960343	9.472985	-35.079302
C	-20.297713	10.121676	-34.834963
C	-21.261457	9.628334	-34.062211
C	-21.139659	8.316673	-33.345585
C	-19.658548	7.108347	-35.716603
C	-19.715091	6.385433	-32.686958
C	-20.291897	6.416275	-31.268910
C	-21.698211	7.014417	-31.261910
C	-21.737037	8.383824	-31.934707
O	-16.926220	12.087787	-35.923912
C	-12.519282	9.117795	-34.980550
C	-13.195052	6.313204	-39.266152
C	-11.305426	8.690695	-39.442405

C	-19.686726	7.807911	-33.273652
H	-23.450151	8.910867	-31.177494
H	-11.598697	6.420710	-37.867219
H	-14.036337	5.862829	-36.879330
H	-12.759691	6.553161	-35.891194
H	-15.530278	7.152444	-33.535490
H	-15.095828	8.505404	-38.377279
H	-12.241248	10.403526	-37.643259
H	-14.804322	10.735499	-37.012492
H	-13.535198	11.351801	-35.986814
H	-15.237441	9.790645	-34.259506
H	-15.881391	12.029341	-33.329153
H	-14.973343	12.790645	-34.620675
H	-13.791159	10.890353	-32.508244
H	-13.631203	12.651717	-32.513444
H	-12.859227	11.693648	-33.777544
H	-16.795903	10.094486	-36.315787
H	-17.396268	9.827311	-33.582272
H	-18.263390	11.269643	-34.044129
H	-18.794852	9.464583	-36.164564
H	-20.438216	11.086299	-35.321626
H	-22.193147	10.171960	-33.932301
H	-21.746772	7.570695	-33.885994
H	-20.672547	7.484292	-35.879995
H	-19.725466	6.062285	-35.406722
H	-19.120555	7.165699	-36.662175
H	-18.719609	5.942147	-32.675312
H	-20.353218	5.747468	-33.312399
H	-19.632967	7.015547	-30.626951
H	-20.314025	5.407685	-30.844882
H	-22.083069	7.096610	-30.238440
H	-22.382969	6.358744	-31.815605
H	-21.143338	9.102063	-31.344201
H	-17.735488	12.096903	-36.449325
H	-13.070579	9.120199	-34.038071
H	-11.836021	9.972426	-34.980876
H	-11.907884	8.214562	-35.022778
H	-12.527387	6.361276	-40.129452
H	-13.414701	5.259901	-39.072550
H	-14.132863	6.807450	-39.534218
H	-10.445346	8.012009	-39.462120
H	-10.936562	9.718200	-39.422358
H	-11.848174	8.544395	-40.382031
H	-19.147549	8.449317	-32.559317

endo-4+2 adduct **9** (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.34335097			
Zero-point correction= 0.699134			
Thermal correction to Energy= 0.733242			
Thermal correction to Enthalpy= 0.734186			
Thermal correction to Gibbs Free Energy= 0.638019			
C	2.147026	0.862526	-0.735031
C	1.733229	-0.647987	-0.871874
C	3.296737	0.978223	0.294844
C	2.943423	-1.525657	-1.073597
H	1.097528	-0.716655	-1.767593
C	0.924876	-1.208503	0.328106
C	4.181278	-1.168620	-0.735920
C	4.528784	0.181239	-0.177323
C	3.748111	2.403422	0.646926
H	2.940199	0.516322	1.227051
C	4.768616	2.354860	1.788418
H	4.216569	2.869309	-0.229876
H	2.895510	3.021558	0.932002
C	5.972113	1.482547	1.425763
H	5.105377	3.364701	2.041946
H	4.281881	1.948973	2.684835
C	5.555875	0.087474	0.964140
H	5.026440	0.759445	-0.976916
O	6.687258	-0.686671	0.594333
H	5.096200	-0.457182	1.799993
H	6.525006	1.956451	0.601031
H	6.664655	1.391883	2.268475
H	2.757306	-2.522572	-1.469028
H	5.007954	-1.860754	-0.874160
C	0.874157	1.526741	-0.216147
C	2.578744	1.425442	-2.096581
H	1.750567	1.430569	-2.803184
H	2.950635	2.448079	-1.989723
H	3.382171	0.810043	-2.509357
O	0.832212	1.930672	0.955088
C	0.256263	-2.575217	0.057371
H	0.156831	-0.509346	0.662424
H	1.607664	-1.338028	1.174586
C	-1.276986	-2.530041	0.300059
O	0.906316	-3.605107	0.788744

H	0.404932	-2.860693	-0.994143
C	-1.905548	-1.693810	-0.848944
H	-1.447815	-2.040968	1.271728
C	-1.820004	-3.966953	0.345575
C	-3.125675	-0.729939	-0.632585
C	-3.731840	-0.755425	0.752103
C	-4.434066	0.244004	1.293048
C	-4.689660	1.560863	0.583981
C	-5.054678	0.094294	2.657384
H	-4.557992	0.737044	3.392025
H	-6.111201	0.386097	2.642497
H	-4.985625	-0.937602	3.008361
H	0.811704	-3.401595	1.728864
C	-3.299183	-4.126962	0.681890
H	-1.617940	-4.425442	-0.632825
H	-1.233568	-4.536866	1.070185
H	-3.944019	-3.574255	-0.006894
H	-3.516118	-3.779767	1.697043
H	-3.587137	-5.180275	0.627932
C	-0.412384	1.417233	-0.925819
C	-1.527628	1.220495	-0.147428
C	-0.841954	1.199087	-2.336938
C	-2.725440	0.765381	-0.945465
N	-2.174228	0.902380	-2.280154
O	-1.600513	1.337175	1.154562
H	-2.703901	0.747343	-3.125086
O	-0.210154	1.282005	-3.382832
C	-3.919360	1.717078	-0.748447
C	-4.467303	2.774162	1.500747
H	-3.632764	-1.677055	1.315731
H	-4.593383	1.558972	-1.594325
H	-3.547436	2.742211	-0.848231
H	7.146374	-0.210217	-0.110377
H	-4.698628	3.695060	0.958489
H	-3.428081	2.821552	1.835242
H	-5.114608	2.736003	2.379888
H	-5.761321	1.556739	0.334542
H	-0.705142	1.692038	1.427101
H	-2.185998	-2.411214	-1.629798
H	-1.106029	-1.104620	-1.307946
C	-4.224945	-1.142582	-1.638429
H	-3.855798	-1.115261	-2.669123
H	-5.112677	-0.511848	-1.556578
H	-4.535891	-2.169805	-1.433984

exo-2+2 adduct **10** (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.33256419			
Zero-point correction= 0.697720			
Thermal correction to Energy= 0.732271			
Thermal correction to Enthalpy= 0.733215			
Thermal correction to Gibbs Free Energy= 0.635768			
C	1.982198	-0.855088	0.519487
O	6.799541	0.039660	0.054666
C	-4.007010	-0.616431	0.166882
C	-4.576360	-1.389847	-1.067314
C	-3.923272	-2.685967	-0.515513
C	-2.947599	-1.788540	0.273769
C	-1.694475	-1.482716	-0.486279
O	-1.711415	-1.254255	-1.765376
N	-2.398627	-2.081603	1.579577
C	-1.107324	-1.613641	1.707832
O	-0.578240	-1.355284	2.785809
C	-0.587713	-1.427144	0.333596
C	0.686383	-1.023080	-0.257711
O	0.672501	-0.739292	-1.472379
C	-3.416826	0.772596	0.200970
C	-3.025200	1.672331	-0.712476
C	-2.399074	2.965738	-0.215633
C	-0.851594	3.005871	-0.218083
C	-0.340368	4.331104	0.365502
C	-0.924853	5.579284	-0.295257
C	-0.297088	1.780112	0.522603
C	1.234033	1.696365	0.546589
C	1.841811	0.490635	1.317207
C	3.185184	0.923381	1.853390
C	4.361845	0.507420	1.390423
C	4.498137	-0.515244	0.300447
C	2.182536	-2.027288	1.493763
C	3.375460	-1.950636	-1.401392
C	4.478666	-1.637801	-2.416972
C	5.790500	-1.281021	-1.716520
C	5.609201	-0.160968	-0.693975
O	-0.816995	1.793309	1.850504
C	-3.122015	1.552905	-2.209480
C	-6.069485	-1.364085	-1.338802
C	-4.990008	-0.710367	1.345028

C	3.181073	-0.752156	-0.459772
H	7.498721	0.283894	-0.563892
H	-4.034878	-1.107077	-1.968631
H	-4.587356	-3.237932	0.152957
H	-3.474672	-3.373277	-1.234877
H	-0.742482	-0.996252	-1.968058
H	-2.989072	-2.032861	2.400093
H	-3.219310	1.074212	1.231850
H	-2.729709	3.160865	0.809828
H	-2.766797	3.788987	-0.838253
H	-0.498352	2.927361	-1.257720
H	0.749143	4.365819	0.261478
H	-0.553161	4.342679	1.441606
H	-0.820967	5.529180	-1.384719
H	-0.405358	6.477239	0.049053
H	-1.986023	5.705425	-0.066441
H	-0.703592	0.923667	-0.015219
H	1.618635	1.715795	-0.481158
H	1.607146	2.601620	1.036544
H	1.195616	0.277762	2.178476
H	3.150212	1.668208	2.646969
H	5.284497	0.891534	1.816959
H	4.815635	-1.465085	0.763241
H	3.095408	-1.871802	2.073220
H	2.275668	-2.973092	0.952870
H	1.353482	-2.102624	2.195011
H	2.448523	-2.194949	-1.923037
H	3.667759	-2.833030	-0.817084
H	4.156617	-0.796458	-3.044443
H	4.634214	-2.489482	-3.086188
H	6.554936	-0.991487	-2.447302
H	6.172845	-2.156617	-1.175656
H	5.325792	0.770861	-1.211770
H	-0.747965	0.900559	2.218406
H	-3.682106	0.680814	-2.539280
H	-2.118569	1.495802	-2.648374
H	-3.598496	2.447562	-2.624415
H	-6.403554	-0.347493	-1.570192
H	-6.307767	-1.999017	-2.196667
H	-6.646672	-1.726123	-0.483954
H	-5.838609	-0.046081	1.158539
H	-4.515894	-0.379468	2.273581
H	-5.381474	-1.719201	1.499223
H	3.002713	0.128974	-1.091945

endo-2+2 adduct **13** (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.32276731			
Zero-point correction= 0.697979			
Thermal correction to Energy= 0.732310			
Thermal correction to Enthalpy= 0.733254			
Thermal correction to Gibbs Free Energy= 0.636776			
C	-19.062090	8.009969	-34.509305
O	-22.886938	9.597727	-31.825207
C	-13.351028	7.085258	-35.977204
C	-12.730144	6.446246	-37.266188
C	-13.893048	5.418551	-37.269351
C	-14.734074	6.444385	-36.488677
C	-15.748689	6.209119	-35.417914
O	-15.499022	5.425492	-34.406256
N	-15.485508	7.310159	-37.364830
C	-16.679798	7.725401	-36.869096
O	-17.404288	8.545588	-37.439965
C	-16.855210	7.021263	-35.574260
C	-17.789588	7.163121	-34.455099
O	-17.491860	6.557266	-33.410788
C	-13.395440	8.552149	-35.625849
C	-13.631852	9.678665	-36.313152
C	-13.844537	10.972063	-35.530688
C	-14.964973	10.925938	-34.462496
C	-15.236373	12.327826	-33.901163
C	-13.996698	13.029132	-33.346558
C	-16.223043	10.276254	-35.051441
C	-17.364129	10.025801	-34.052226
C	-18.662529	9.508897	-34.743707
C	-19.790656	10.445580	-34.402719
C	-20.874398	10.127474	-33.701389
C	-21.124520	8.744110	-33.180406
C	-19.901210	7.529586	-35.710490
C	-20.313882	6.425450	-32.832605
C	-20.915101	6.400610	-31.424399
C	-22.099354	7.360058	-31.313676
C	-21.733898	8.768875	-31.773081
O	-16.661970	11.067902	-36.152373
C	-13.766959	9.840013	-37.802141
C	-11.295346	5.952732	-37.245975
C	-12.808108	6.351475	-34.740405

C	-19.863982	7.855139	-33.187773
H	-23.269423	9.624280	-30.939750
H	-12.858418	7.120258	-38.117017
H	-14.310584	5.113015	-38.229876
H	-13.665036	4.535226	-36.670353
H	-16.233471	5.645954	-33.749115
H	-15.153630	7.645885	-38.256365
H	-13.334193	8.699339	-34.545792
H	-14.090328	11.775134	-36.234558
H	-12.904010	11.256206	-35.045696
H	-14.633076	10.283031	-33.633760
H	-15.979784	12.253075	-33.100349
H	-15.688905	12.936868	-34.693149
H	-13.477695	12.390003	-32.623897
H	-14.270793	13.956306	-32.836608
H	-13.285611	13.285493	-34.136206
H	-15.897913	9.305030	-35.421711
H	-17.019263	9.323392	-33.280962
H	-17.598258	10.959042	-33.530600
H	-18.506286	9.598740	-35.820234
H	-19.651164	11.466997	-34.755515
H	-21.635548	10.874345	-33.493626
H	-21.887810	8.270303	-33.821059
H	-20.794686	8.153681	-35.801759
H	-20.216653	6.490241	-35.586551
H	-19.333857	7.619351	-36.637668
H	-19.487206	5.719191	-32.894600
H	-21.080042	6.100196	-33.548881
H	-20.140556	6.685258	-30.700161
H	-21.232566	5.386089	-31.164343
H	-22.480934	7.394676	-30.286213
H	-22.920233	7.011295	-31.953967
H	-20.988823	9.201169	-31.083790
H	-16.988544	10.448792	-36.822960
H	-14.809872	10.079854	-38.046736
H	-13.455331	8.968615	-38.376045
H	-13.162999	10.690220	-38.136364
H	-11.136613	5.201779	-36.467981
H	-11.040427	5.499037	-38.207663
H	-10.601940	6.780757	-37.069894
H	-12.833631	5.264691	-34.831580
H	-13.372636	6.622541	-33.846616
H	-11.768174	6.658243	-34.591268
H	-19.203691	8.207517	-32.379838

SM-A (water)			
E[M06-2X/6-31G(d,p)/CPCM(water)]= -1659.4050429			
Zero-point correction= 0.714143			
Thermal correction to Energy= 0.753208			
Thermal correction to Enthalpy= 0.754152			
Thermal correction to Gibbs Free Energy= 0.643625			
C	-3.626067	-0.219201	0.169053
H	-3.565109	-0.363011	1.258525
C	-3.955135	-1.600991	-0.422990
H	-4.144991	-1.522272	-1.496327
C	-5.201191	-2.167726	0.264485
C	-6.428575	-1.265315	0.081517
C	-6.956118	-1.291802	-1.356335
H	-6.242177	-0.879557	-2.076335
H	-7.888923	-0.727631	-1.444693
H	-7.167966	-2.321317	-1.658479
H	-7.233134	-1.635271	0.729514
C	-6.097573	0.157601	0.560767
H	-5.931179	0.124706	1.646172
C	-4.816792	0.722568	-0.085656
C	-4.551793	2.115163	0.410254
C	-3.337430	2.547718	0.739996
C	-2.076010	1.724714	0.667288
H	-1.303502	2.336159	0.184816
C	-1.575798	1.414946	2.103239
C	-0.078952	1.383061	2.232225
C	0.630600	0.353986	2.690500
C	2.121889	0.366621	2.883098
C	2.835934	-0.726223	2.132583
C	3.994898	-0.539515	1.485550
C	4.794317	-1.598035	0.859541
C	5.878945	-1.337789	0.097422
C	6.374207	-0.021900	-0.351930
C	5.523919	0.901594	-0.831858
C	5.813419	2.298468	-1.299396
C	4.838588	3.292701	-0.656961
H	5.005328	4.307427	-1.026939
H	3.803218	3.014321	-0.879223
H	4.955853	3.300991	0.430793
H	5.696832	2.347624	-2.390153
H	6.843236	2.591818	-1.079540
H	4.471055	0.625845	-0.884480

C	7.872324	0.147044	-0.280320
H	8.216040	0.118920	0.759014
H	8.366602	-0.682473	-0.797960
H	8.216037	1.077754	-0.731998
H	6.477407	-2.191952	-0.224729
C	4.382244	-3.021259	1.132688
H	5.058566	-3.728317	0.648172
H	3.368820	-3.204173	0.754850
H	4.362468	-3.228741	2.207711
H	4.411623	0.465471	1.451320
H	2.380568	-1.716194	2.173133
H	2.328245	0.232564	3.956080
H	2.532468	1.343169	2.602962
H	0.114295	-0.569993	2.957078
H	0.443229	2.295716	1.938071
H	-2.006123	0.472954	2.462941
H	-1.958958	2.201277	2.765634
C	-2.286773	0.461715	-0.243858
C	-1.119439	-0.487059	0.020924
O	-1.267287	-1.490548	0.722816
C	0.214117	-0.312574	-0.583804
C	1.062509	-1.383440	-0.690495
C	2.254590	-0.975249	-1.426958
C	3.257385	-1.719703	-1.877004
H	3.254104	-2.785016	-1.681454
H	4.081215	-1.280462	-2.426153
O	2.156447	0.387101	-1.616633
C	0.955538	0.841718	-1.098930
O	0.718592	2.023776	-1.103361
O	0.905418	-2.611578	-0.261964
H	0.073119	-2.608703	0.268036
C	-2.262535	0.943495	-1.716430
C	-2.356887	-0.126357	-2.809533
H	-1.779994	-1.023743	-2.559716
H	-3.386354	-0.434042	-3.002145
H	-1.957431	0.267635	-3.747604
H	-1.342564	1.512668	-1.856601
H	-3.071072	1.670295	-1.840604
H	-3.210010	3.559997	1.120702
H	-5.412178	2.772511	0.502973
H	-4.999565	0.768217	-1.174060
O	-7.198230	1.038400	0.385542
H	-7.310378	1.184846	-0.562934
H	-5.423965	-3.168593	-0.121307

H	-4.99258	-2.280689	1.336665
H	-3.121828	-2.29179	-0.294943

TS2-A (water)

E[M06-2X/6-31G(d,p)/CPCM(water)]= -1659.3749797

Zero-point correction= 0.714614

Thermal correction to Energy= 0.752006

Thermal correction to Enthalpy= 0.752950

Thermal correction to Gibbs Free Energy= 0.648103

C	3.302987	-0.146545	-0.320567
C	4.583285	-0.462035	0.485969
C	5.831533	-0.049264	-0.319412
C	5.901187	-0.738545	-1.693455
C	4.575338	-0.544290	-2.441580
C	3.362861	-0.982866	-1.613194
C	2.042542	-0.231376	0.592099
C	2.197796	0.838747	1.727725
C	3.524893	0.683524	2.428170
C	4.600967	0.146072	1.859763
O	7.025865	-0.250501	0.423792
C	6.286808	-2.217511	-1.587868
C	1.894241	-1.615347	1.286980
C	0.749380	0.018577	-0.208628
C	2.100120	2.328783	1.320315
C	-0.578911	-0.262429	0.333967
C	0.771396	2.747786	0.769609
C	0.623040	3.526240	-0.299817
C	-0.691372	3.927401	-0.922651
C	-1.867450	3.222940	-0.323843
C	-2.670996	2.408802	-1.024061
C	-3.778224	1.628641	-0.482685
C	-4.509798	0.895307	-1.390786
C	-4.121165	1.799239	0.972612
C	-5.444755	-0.145483	-1.166521
C	-6.183323	-0.690675	-2.358627
O	0.804378	0.334406	-1.406699
C	-1.617565	-0.625143	-0.539702
C	-1.104052	-0.451939	1.670921
O	-2.384111	-0.976985	1.554119
O	-0.666195	-0.219980	2.781951
C	1.590562	-2.816437	0.382539
C	-2.692365	-1.143942	0.213384
C	-3.809596	-1.878308	-0.160072

O	-1.580077	-0.599319	-1.860158
H	3.366461	0.904682	-0.641160
H	4.637536	-1.558566	0.612795
H	5.777111	1.036397	-0.478321
H	6.697495	-0.235973	-2.257044
H	4.458207	0.516575	-2.700121
H	4.609044	-1.096889	-3.387199
H	2.454902	-0.865986	-2.201448
H	3.459151	-2.045535	-1.372085
H	1.391384	0.654822	2.446173
H	3.594463	1.112062	3.426719
H	5.545831	0.107516	2.395312
H	7.059539	-1.181516	0.679990
H	5.573036	-2.798321	-0.995280
H	6.324306	-2.665085	-2.585030
H	7.277159	-2.337888	-1.139683
H	2.807657	-1.809247	1.855491
H	1.103702	-1.518090	2.033662
H	2.900800	2.586620	0.617615
H	2.307119	2.901459	2.235541
H	-0.102636	2.357372	1.291266
H	1.513638	3.898002	-0.807057
H	-0.650406	3.724642	-1.999487
H	-0.817432	5.015216	-0.822325
H	-2.039386	3.383970	0.738371
H	-2.463532	2.262885	-2.083825
H	-4.266050	1.068576	-2.438167
H	-3.506686	1.162855	1.620504
H	-5.171294	1.576231	1.161085
H	-3.948422	2.835138	1.271585
H	-5.887583	-1.727323	-2.565275
H	-5.993379	-0.095659	-3.252472
H	-7.262768	-0.705615	-2.175051
H	2.496048	-3.244609	-0.051655
H	1.105979	-3.606681	0.962149
H	0.917061	-2.557267	-0.441795
H	-4.144056	-2.633164	0.545912
H	-3.859253	-2.175167	-1.202848
H	-0.709000	-0.181691	-2.076754
C	-6.575224	-1.919622	0.255879
C	-6.630970	-2.409059	1.700992
H	-6.412153	-2.763251	-0.427040
H	-7.550215	-1.499025	-0.018643
H	-7.399358	-3.175216	1.823071

H	-5.678144	-2.839816	2.023891
H	-6.865159	-1.581970	2.377104
C	-5.509233	-0.862639	0.037572
H	-5.173208	-0.378052	0.947320

P1-A (water)

E[M06-2X/6-31G(d,p)/CPCM(water)]= -1659.460059

Zero-point correction= 0.719517

Thermal correction to Energy= 0.755909

Thermal correction to Enthalpy= 0.756853

Thermal correction to Gibbs Free Energy= 0.654787

C	-3.128869	0.282017	-0.293063
C	-3.096537	1.782757	-0.617101
H	-2.106817	2.094670	-0.956696
C	-4.134288	2.081066	-1.705176
H	-4.113880	3.143286	-1.972283
H	-3.856907	1.522431	-2.608648
C	-5.560633	1.691362	-1.286382
C	-6.139023	2.670129	-0.259215
H	-6.105408	3.688536	-0.656111
H	-7.185712	2.441884	-0.039088
H	-5.584989	2.668792	0.684614
H	-6.205230	1.735485	-2.173170
C	-5.592386	0.232063	-0.791793
O	-6.888887	-0.140085	-0.347761
H	-7.072324	0.343937	0.468065
H	-5.384979	-0.429254	-1.643673
C	-4.521294	-0.037437	0.283416
C	-4.624580	-1.423813	0.846689
C	-3.567330	-2.204258	1.056358
C	-2.152139	-1.846039	0.675553
H	-1.476115	-2.195858	1.465653
C	-1.794896	-2.619827	-0.626800
C	-0.371009	-3.088026	-0.736453
C	0.415140	-2.929346	-1.800658
C	1.827152	-3.467944	-1.874603
C	2.800708	-2.370759	-1.526282
C	3.273744	-2.209536	-0.292345
C	4.038696	-1.005557	0.217855
C	4.788712	-0.270006	-0.867206
C	4.978401	1.051741	-0.914600
C	5.805408	1.664399	-2.016129
H	6.361560	0.897929	-2.559610

H	5.178758	2.198598	-2.737611
H	6.518586	2.391514	-1.612147
C	4.441595	2.010484	0.135732
C	3.646498	1.300461	1.251827
H	4.297014	1.064689	2.097932
H	2.856016	1.949368	1.642571
C	3.004022	-0.023363	0.831064
C	1.795773	0.156100	-0.056181
C	0.648926	-0.230817	0.588639
C	-0.640427	-0.053934	-0.079697
O	-0.601972	0.292071	-1.273057
C	-1.985410	-0.285088	0.596068
C	-2.029557	0.311379	2.031323
H	-3.083207	0.413835	2.304074
H	-1.604914	-0.412468	2.728225
C	-1.329929	1.659311	2.246564
H	-0.241640	1.560321	2.252967
H	-1.622443	2.073357	3.214986
H	-1.587167	2.395114	1.481662
C	1.066545	-0.786412	1.877059
O	0.445612	-1.340637	2.753808
O	2.418231	-0.625081	1.999242
O	1.873294	0.621649	-1.266907
H	0.914872	0.584724	-1.596187
H	5.333881	2.448623	0.609766
C	3.667152	3.200350	-0.469313
C	3.484773	4.354112	0.515466
H	4.455476	4.724678	0.860078
H	2.955996	5.185803	0.043209
H	2.909240	4.060139	1.397898
H	4.214358	3.576412	-1.338889
H	2.696146	2.853297	-0.836216
H	5.248683	-0.902366	-1.625460
C	5.038885	-1.476250	1.291307
H	5.616294	-0.641626	1.695043
H	4.521942	-1.984042	2.109489
H	5.740854	-2.178991	0.833943
H	3.013244	-2.946681	0.469703
H	3.014509	-1.625628	-2.291899
H	2.027757	-3.866120	-2.874593
H	1.936284	-4.288832	-1.158431
H	0.057092	-2.347393	-2.650347
H	0.012265	-3.650323	0.118904
H	-2.063512	-2.028455	-1.509474

H	-2.436156	-3.510229	-0.654342
H	-3.706266	-3.204299	1.463812
H	-5.621141	-1.772825	1.104090
H	-4.729959	0.667564	1.106219
H	-3.331291	2.362268	0.283972
H	-3.053930	-0.241111	-1.256171

SM-A (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1659.4020085			
Zero-point correction= 0.714421			
Thermal correction to Energy= 0.753474			
Thermal correction to Enthalpy= 0.754418			
Thermal correction to Gibbs Free Energy= 0.643889			
C	-3.625286	-0.222812	0.169041
H	-3.564640	-0.376823	1.257097
C	-3.955856	-1.599060	-0.435024
H	-4.142470	-1.511967	-1.508376
C	-5.204678	-2.168987	0.244736
C	-6.430111	-1.263248	0.066314
C	-6.953213	-1.275845	-1.373342
H	-6.237110	-0.856190	-2.087117
H	-7.886406	-0.711719	-1.458271
H	-7.163754	-2.302133	-1.687195
H	-7.237763	-1.637235	0.707957
C	-6.098751	0.155048	0.559035
H	-5.937697	0.113247	1.644777
C	-4.814203	0.723355	-0.076830
C	-4.548064	2.109448	0.436513
C	-3.333222	2.536154	0.771431
C	-2.072246	1.713641	0.687538
H	-1.300061	2.329966	0.210632
C	-1.570354	1.386337	2.118879
C	-0.073448	1.352361	2.245257
C	0.636047	0.319711	2.695258
C	2.127319	0.332277	2.887923
C	2.844998	-0.751254	2.127568
C	4.002667	-0.553633	1.481725
C	4.807379	-1.602111	0.846174
C	5.887078	-1.328420	0.081929
C	6.369250	-0.005741	-0.361065
C	5.508712	0.914099	-0.829476
C	5.782879	2.316911	-1.287961
C	4.796211	3.295413	-0.639389

H	4.952197	4.314579	-1.001801
H	3.764218	3.007403	-0.864520
H	4.913187	3.297455	0.448461
H	5.665356	2.371309	-2.378371
H	6.809568	2.620160	-1.066348
H	4.457873	0.630900	-0.878421
C	7.866138	0.175533	-0.296161
H	8.215647	0.143689	0.741104
H	8.365318	-0.645782	-0.822246
H	8.198946	1.112219	-0.743651
H	6.491629	-2.175754	-0.247155
C	4.406442	-3.029889	1.111409
H	5.087130	-3.729237	0.621677
H	3.393586	-3.218154	0.734458
H	4.390709	-3.243751	2.185205
H	4.414616	0.453464	1.455738
H	2.394206	-1.743688	2.159620
H	2.334095	0.189542	3.959745
H	2.535723	1.312115	2.616450
H	0.119316	-0.605879	2.955652
H	0.449077	2.266539	1.956606
H	-2.000695	0.440446	2.468268
H	-1.952185	2.164643	2.791461
C	-2.285262	0.461004	-0.237367
C	-1.118676	-0.491501	0.015421
O	-1.267594	-1.504542	0.704052
C	0.215052	-0.310184	-0.585853
C	1.064455	-1.378879	-0.698129
C	2.257396	-0.964049	-1.429883
C	3.260555	-1.705904	-1.883649
H	3.256207	-2.772304	-1.694395
H	4.086150	-1.262528	-2.426699
O	2.159568	0.398618	-1.609385
C	0.957802	0.850403	-1.088567
O	0.719992	2.030924	-1.080717
O	0.905762	-2.610048	-0.277004
H	0.071298	-2.604843	0.250974
C	-2.261075	0.960621	-1.704051
C	-2.362743	-0.095187	-2.809852
H	-1.786454	-0.996799	-2.573974
H	-3.393642	-0.399157	-3.001424
H	-1.967064	0.309513	-3.744953
H	-1.339045	1.527626	-1.839199
H	-3.066090	1.693091	-1.817410

H	-3.205021	3.543177	1.165471
H	-5.408545	2.764955	0.540043
H	-4.993867	0.781881	-1.165428
O	-7.195997	1.039157	0.385840
H	-7.305736	1.189541	-0.561987
H	-5.427820	-3.166729	-0.149075
H	-4.998527	-2.290838	1.316376
H	-3.124459	-2.292486	-0.309356

TS2-A (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1659.3705994			
Zero-point correction= 0.714966			
Thermal correction to Energy= 0.752300			
Thermal correction to Enthalpy= 0.753245			
Thermal correction to Gibbs Free Energy= 0.648534			
C	3.303345	-0.140886	-0.319685
C	4.581019	-0.467104	0.486715
C	5.834352	-0.060319	-0.313850
C	5.901167	-0.741756	-1.691970
C	4.577909	-0.534136	-2.440684
C	3.360808	-0.969532	-1.617526
C	2.041528	-0.224728	0.591805
C	2.200458	0.837856	1.734046
C	3.527426	0.675434	2.432583
C	4.601429	0.135998	1.862641
O	7.024623	-0.276700	0.430279
C	6.276486	-2.223915	-1.594155
C	1.885714	-1.610899	1.281303
C	0.749668	0.030603	-0.209408
C	2.106143	2.330117	1.334098
C	-0.580395	-0.244079	0.334615
C	0.779227	2.748037	0.779876
C	0.634585	3.497939	-0.309930
C	-0.676546	3.889738	-0.944668
C	-1.857021	3.198041	-0.339938
C	-2.669640	2.388811	-1.035337
C	-3.780678	1.618881	-0.489071
C	-4.523556	0.891044	-1.394598
C	-4.123052	1.801620	0.965018
C	-5.455851	-0.147860	-1.164942
C	-6.195114	-0.701452	-2.353258
O	0.803945	0.339532	-1.408863
C	-1.616975	-0.607779	-0.537017

C	-1.107002	-0.424769	1.674271
O	-2.390537	-0.948300	1.557595
O	-0.669158	-0.187139	2.781236
C	1.580370	-2.807495	0.371718
C	-2.695383	-1.121271	0.218992
C	-3.806441	-1.866712	-0.151634
O	-1.579934	-0.586269	-1.857124
H	3.371587	0.911918	-0.634231
H	4.627129	-1.564848	0.609139
H	5.790069	1.026653	-0.465759
H	6.702489	-0.242021	-2.250837
H	4.467946	0.529030	-2.692659
H	4.608969	-1.080481	-3.390117
H	2.455558	-0.842045	-2.207394
H	3.449019	-2.034488	-1.383016
H	1.394456	0.652272	2.452380
H	3.598804	1.100417	3.432442
H	5.546931	0.094169	2.396635
H	7.049982	-1.209925	0.678102
H	5.558822	-2.802787	-1.004159
H	6.310305	-2.667436	-2.593285
H	7.266607	-2.352794	-1.147714
H	2.796361	-1.809549	1.852635
H	1.093614	-1.513478	2.026443
H	2.908972	2.590028	0.634694
H	2.309854	2.898945	2.252304
H	-0.095096	2.375574	1.313986
H	1.527590	3.848388	-0.827817
H	-0.631179	3.666694	-2.017312
H	-0.801803	4.979574	-0.864973
H	-2.025920	3.364870	0.721875
H	-2.464074	2.235297	-2.094375
H	-4.284665	1.064976	-2.443108
H	-3.509732	1.171628	1.620222
H	-5.173809	1.582099	1.154633
H	-3.949725	2.840614	1.253402
H	-5.890121	-1.735423	-2.561077
H	-6.014075	-0.105688	-3.248610
H	-7.273996	-0.726422	-2.167233
H	2.485246	-3.235778	-0.063872
H	1.093673	-3.599069	0.947680
H	0.908355	-2.543693	-0.452390
H	-4.128295	-2.624335	0.557373
H	-3.851570	-2.167687	-1.193543

H	-0.705857	-0.172225	-2.072705
C	-6.566500	-1.929206	0.264827
C	-6.616824	-2.413784	1.711840
H	-6.398682	-2.774549	-0.415114
H	-7.545159	-1.516988	-0.009713
H	-7.377069	-3.187388	1.838320
H	-5.659245	-2.832400	2.036414
H	-6.859032	-1.586613	2.384996
C	-5.506969	-0.866274	0.040552
H	-5.176862	-0.375013	0.949002

P1-A (ether)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1659.4568065			
Zero-point correction= 0.719765			
Thermal correction to Energy= 0.756164			
Thermal correction to Enthalpy= 0.757108			
Thermal correction to Gibbs Free Energy= 0.654963			
C	-3.128013	0.280330	-0.293738
C	-3.095724	1.780775	-0.619080
H	-2.106352	2.091908	-0.960222
C	-4.134436	2.078523	-1.706339
H	-4.113076	3.140300	-1.975466
H	-3.858085	1.518398	-2.609147
C	-5.560518	1.690547	-1.285523
C	-6.136808	2.670788	-0.258568
H	-6.101065	3.689433	-0.654714
H	-7.184237	2.444739	-0.039620
H	-5.582912	2.668321	0.685468
H	-6.206964	1.734381	-2.170888
C	-5.593767	0.231832	-0.788848
O	-6.888715	-0.136333	-0.339699
H	-7.068621	0.351984	0.474007
H	-5.391211	-0.431366	-1.640263
C	-4.519957	-0.039147	0.283232
C	-4.623449	-1.426493	0.844014
C	-3.565930	-2.206303	1.053471
C	-2.150344	-1.847467	0.675033
H	-1.475197	-2.196527	1.466248
C	-1.791430	-2.620567	-0.627094
C	-0.366570	-3.085370	-0.737007
C	0.417075	-2.928768	-1.803213
C	1.830092	-3.464688	-1.877861
C	2.802328	-2.367120	-1.527538

C	3.276011	-2.207995	-0.293683
C	4.039273	-1.003741	0.218039
C	4.788692	-0.266672	-0.866059
C	4.976569	1.055168	-0.912909
C	5.801658	1.669629	-2.014745
H	6.359610	0.904432	-2.558141
H	5.173225	2.201610	-2.736300
H	6.513724	2.398495	-1.611738
C	4.438596	2.012532	0.138129
C	3.644890	1.300229	1.253706
H	4.295395	1.063675	2.099628
H	2.854053	1.947776	1.646121
C	3.003018	-0.023725	0.832233
C	1.795443	0.156227	-0.056098
C	0.649330	-0.231890	0.587741
C	-0.639559	-0.054762	-0.080710
O	-0.601160	0.292999	-1.273809
C	-1.984180	-0.286492	0.595247
C	-2.026908	0.308568	2.031120
H	-3.080291	0.406674	2.306626
H	-1.598125	-0.414128	2.726620
C	-1.330605	1.658240	2.245900
H	-0.242118	1.561258	2.249718
H	-1.620733	2.069959	3.216009
H	-1.591465	2.394753	1.482802
C	1.066301	-0.791337	1.876247
O	0.444650	-1.348974	2.748296
O	2.418702	-0.626574	1.998902
O	1.872635	0.623650	-1.266817
H	0.913270	0.584162	-1.594799
H	5.330227	2.452404	0.612261
C	3.662394	3.201277	-0.466779
C	3.474574	4.353692	0.518548
H	4.443169	4.725652	0.867688
H	2.946561	5.185345	0.045432
H	2.896017	4.058347	1.398501
H	4.210591	3.579730	-1.334768
H	2.693654	2.851783	-0.837143
H	5.249133	-0.897837	-1.625013
C	5.039092	-1.474700	1.291716
H	5.619032	-0.640613	1.692963
H	4.520813	-1.978496	2.111412
H	5.739128	-2.180136	0.835493
H	3.017320	-2.946702	0.467356

H	3.014002	-1.618930	-2.290852
H	2.031474	-3.861844	-2.878168
H	1.940415	-4.286638	-1.163115
H	0.055496	-2.350740	-2.654065
H	0.019711	-3.642967	0.120041
H	-2.061481	-2.030047	-1.509909
H	-2.430701	-3.512394	-0.654931
H	-3.705084	-3.207147	1.458780
H	-5.620506	-1.777040	1.096995
H	-4.726647	0.665151	1.107544
H	-3.329576	2.361164	0.281784
H	-3.053296	-0.243139	-1.256696

TS3a(closed-shell) (ether)

E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27081507

Zero-point correction= 0.695384

Thermal correction to Energy= 0.730114

Thermal correction to Enthalpy= 0.731058

Thermal correction to Gibbs Free Energy= 0.633636

C	1.999915	-0.829147	0.461376
O	6.824475	0.141665	0.133847
C	-4.382959	-0.273232	0.279185
C	-4.692508	-1.170441	-0.902255
C	-4.058856	-2.527445	-0.529337
C	-2.691411	-2.215572	0.012607
C	-1.591966	-1.857834	-0.715363
O	-1.536450	-1.846941	-2.071083
N	-2.303400	-2.145661	1.370153
C	-1.041688	-1.599090	1.503412
O	-0.603828	-1.184080	2.605188
C	-0.503662	-1.523185	0.161113
C	0.731585	-1.033444	-0.379203
O	0.770069	-0.734380	-1.596965
C	-3.677448	0.932114	0.334405
C	-3.018614	1.658236	-0.645412
C	-2.432802	2.967814	-0.238858
C	-0.875936	2.986247	-0.241324
C	-0.388239	4.295434	0.393149
C	-1.014749	5.554498	-0.203661
C	-0.336045	1.725886	0.453097
C	1.195158	1.696648	0.523255
C	1.827171	0.496645	1.274593

C	3.148979	0.964740	1.833711
C	4.345213	0.572828	1.401522
C	4.524207	-0.449726	0.318131
C	2.187278	-2.000905	1.439478
C	3.472098	-1.902469	-1.410481
C	4.597967	-1.575860	-2.395971
C	5.884535	-1.197228	-1.660951
C	5.656692	-0.079836	-0.644771
O	-0.923749	1.655339	1.743449
C	-2.830609	1.253286	-2.067457
C	-6.194547	-1.226268	-1.202029
C	-5.061607	-0.642896	1.562324
C	3.230866	-0.706999	-0.476006
H	7.538899	0.379469	-0.468920
H	-4.162847	-0.813127	-1.784470
H	-4.669867	-3.072187	0.196609
H	-3.991643	-3.157165	-1.422108
H	-0.659629	-1.430306	-2.257773
H	-2.932488	-2.167538	2.158345
H	-3.636702	1.384209	1.321846
H	-2.779283	3.246675	0.758981
H	-2.782797	3.720244	-0.957251
H	-0.529449	2.951409	-1.283552
H	0.696706	4.356255	0.265965
H	-0.578894	4.249734	1.472041
H	-0.911362	5.563908	-1.294264
H	-0.523594	6.449546	0.185497
H	-2.078979	5.637035	0.033971
H	-0.680324	0.880683	-0.151657
H	1.605537	1.762272	-0.492907
H	1.515784	2.600132	1.052708
H	1.175854	0.256061	2.122763
H	3.082518	1.710810	2.625026
H	5.250518	0.975322	1.848221
H	4.843217	-1.394164	0.791135
H	3.092541	-1.851955	2.034431
H	2.281346	-2.948823	0.901608
H	1.343327	-2.065728	2.125777
H	2.561478	-2.156049	-1.954800
H	3.761398	-2.779840	-0.816393
H	4.280151	-0.740183	-3.033478
H	4.785863	-2.425306	-3.060394
H	6.665095	-0.896863	-2.371031
H	6.266134	-2.065662	-1.108034

H	5.372283	0.846910	-1.172066
H	-0.795009	0.755674	2.096803
H	-2.225422	1.986012	-2.602237
H	-3.800914	1.177936	-2.570921
H	-2.351115	0.270566	-2.133070
H	-6.591283	-0.236388	-1.443034
H	-6.363481	-1.880581	-2.060710
H	-6.757102	-1.629818	-0.355452
H	-5.999405	-0.070336	1.600819
H	-4.471327	-0.341992	2.430134
H	-5.327950	-1.696931	1.631349
H	3.055343	0.169008	-1.116642

TS3a(closed-shell) (water)

E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27828380

Zero-point correction= 0.695237

Thermal correction to Energy= 0.729960

Thermal correction to Enthalpy= 0.730904

Thermal correction to Gibbs Free Energy= 0.633481

C	1.998541	-0.834514	0.468922
O	6.820111	0.146922	0.127407
C	-4.350772	-0.291456	0.265101
C	-4.678757	-1.184068	-0.917108
C	-4.059788	-2.541582	-0.525227
C	-2.704985	-2.202282	0.037974
C	-1.604119	-1.838779	-0.690606
O	-1.553709	-1.820985	-2.043914
N	-2.300789	-2.181889	1.392401
C	-1.040319	-1.630533	1.526405
O	-0.596801	-1.232017	2.631788
C	-0.508112	-1.527786	0.182066
C	0.726406	-1.040991	-0.363540
O	0.759736	-0.741594	-1.581690
C	-3.664050	0.930468	0.318679
C	-3.027670	1.671990	-0.658061
C	-2.436776	2.978257	-0.241413
C	-0.880761	2.988983	-0.240783
C	-0.385255	4.295862	0.393522
C	-1.005814	5.557899	-0.203513
C	-0.341365	1.725879	0.450206
C	1.190693	1.691025	0.514897
C	1.822488	0.495320	1.274621

C	3.143487	0.966824	1.832988
C	4.340053	0.575674	1.400107
C	4.520866	-0.449097	0.318741
C	2.193932	-2.002446	1.449563
C	3.468631	-1.908635	-1.404495
C	4.590957	-1.580667	-2.393660
C	5.878305	-1.197491	-1.662372
C	5.650340	-0.078593	-0.647900
O	-0.917018	1.652649	1.747647
C	-2.861518	1.286247	-2.089567
C	-6.180095	-1.216110	-1.218847
C	-5.022316	-0.659267	1.552540
C	3.226453	-0.711871	-0.472092
H	7.529150	0.397302	-0.477295
H	-4.141265	-0.836614	-1.799081
H	-4.679763	-3.077183	0.198569
H	-3.972803	-3.184210	-1.406991
H	-0.676855	-1.402655	-2.231893
H	-2.933832	-2.183779	2.178916
H	-3.624177	1.374284	1.309902
H	-2.784520	3.250496	0.758104
H	-2.782168	3.739339	-0.951963
H	-0.533694	2.953509	-1.282924
H	0.700012	4.352724	0.266705
H	-0.576796	4.253362	1.472590
H	-0.905168	5.564226	-1.294263
H	-0.507786	6.450211	0.183363
H	-2.068807	5.646363	0.036460
H	-0.693289	0.881922	-0.151466
H	1.598117	1.748033	-0.502766
H	1.516293	2.597704	1.035527
H	1.169113	0.259187	2.122788
H	3.076634	1.716433	2.620947
H	5.244400	0.983070	1.844559
H	4.843089	-1.391855	0.793168
H	3.098481	-1.846511	2.043763
H	2.295360	-2.950732	0.913597
H	1.350236	-2.071782	2.135459
H	2.556858	-2.166757	-1.945093
H	3.762365	-2.783924	-0.809531
H	4.269976	-0.746835	-3.031963
H	4.779569	-2.430883	-3.056731
H	6.656166	-0.896203	-2.374367
H	6.262763	-2.064512	-1.109083

H	5.363498	0.846396	-1.176319
H	-0.807762	0.745531	2.084293
H	-2.272614	2.030725	-2.626465
H	-3.840060	1.208576	-2.576194
H	-2.374634	0.309711	-2.175000
H	-6.556210	-0.220289	-1.467627
H	-6.359755	-1.873465	-2.073030
H	-6.750280	-1.601971	-0.369255
H	-5.951009	-0.072189	1.596948
H	-4.424756	-0.364530	2.417670
H	-5.304169	-1.708622	1.624571
H	3.048143	0.162715	-1.113652

TS3b(closed-shell) (ether)

E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27414220

Zero-point correction= 0.695828

Thermal correction to Energy= 0.730155

Thermal correction to Enthalpy= 0.731099

Thermal correction to Gibbs Free Energy= 0.634630

C	-19.084596	8.096687	-34.624313
O	-22.890336	9.556621	-31.836529
C	-12.672592	7.309107	-35.683266
C	-12.722217	6.718944	-37.054030
C	-13.800577	5.581149	-37.093669
C	-15.164472	6.083362	-36.801534
C	-15.838984	6.119088	-35.623294
O	-15.470261	5.492188	-34.476743
N	-15.817117	7.005091	-37.654942
C	-16.927481	7.573599	-37.050315
O	-17.594852	8.477072	-37.621600
C	-16.996254	6.987430	-35.735315
C	-17.759515	7.316202	-34.570827
O	-17.327954	6.958014	-33.446337
C	-13.015293	8.605215	-35.312327
C	-13.521798	9.674951	-36.058878
C	-13.809084	10.923263	-35.294185
C	-15.022129	10.819761	-34.319226
C	-15.349721	12.224405	-33.795256
C	-14.149499	12.979240	-33.226082
C	-16.200872	10.115281	-35.018722
C	-17.498822	10.174692	-34.198745
C	-18.758851	9.601309	-34.899861

C	-19.926976	10.492334	-34.557160
C	-20.971580	10.142344	-33.811043
C	-21.130986	8.766600	-33.235764
C	-19.963054	7.560322	-35.767463
C	-20.149332	6.515569	-32.838242
C	-20.699790	6.504449	-31.409507
C	-21.940705	7.389649	-31.289822
C	-21.685461	8.803271	-31.807626
O	-16.368946	10.709001	-36.298156
C	-13.796139	9.695204	-37.518851
C	-11.347647	6.176125	-37.485016
C	-12.309304	6.386315	-34.572469
C	-19.822309	7.955502	-33.265616
H	-23.240073	9.586105	-30.938164
H	-13.030966	7.467060	-37.778198
H	-13.724133	5.134151	-38.092983
H	-13.538143	4.800271	-36.373037
H	-16.064845	5.904946	-33.798226
H	-15.715304	7.031509	-38.659812
H	-12.894330	8.821739	-34.252565
H	-13.997476	11.745912	-35.985765
H	-12.920809	11.156826	-34.695025
H	-14.726429	10.190337	-33.468583
H	-16.101587	12.129239	-33.006660
H	-15.811196	12.801012	-34.606569
H	-13.625927	12.373944	-32.477970
H	-14.472977	13.902748	-32.740258
H	-13.429247	13.253861	-34.001757
H	-15.900766	9.066178	-35.143865
H	-17.343895	9.683448	-33.228785
H	-17.701512	11.229678	-33.991110
H	-18.598279	9.683752	-35.979062
H	-19.862517	11.508198	-34.946668
H	-21.766826	10.854475	-33.607068
H	-21.892146	8.232508	-33.829815
H	-20.901054	8.121806	-35.813370
H	-20.201951	6.503349	-35.618322
H	-19.453899	7.676897	-36.724298
H	-19.263821	5.883106	-32.902138
H	-20.908113	6.097811	-33.513699
H	-19.921423	6.868211	-30.725641
H	-20.940531	5.482907	-31.098161
H	-22.290646	7.434476	-30.250876
H	-22.757688	6.966729	-31.889183

H	-20.942446	9.303837	-31.163197
H	-16.834572	10.058855	-36.861152
H	-14.168461	10.669394	-37.825070
H	-14.558945	8.939656	-37.751119
H	-12.893987	9.445348	-38.085830
H	-11.057189	5.297524	-36.904908
H	-11.409752	5.878071	-38.534099
H	-10.565307	6.932832	-37.390790
H	-13.260077	5.927355	-34.251623
H	-11.888644	6.917691	-33.718418
H	-11.644107	5.581274	-34.883752
H	-19.154268	8.376709	-32.499876

TS3b(closed-shell) (water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28243435			
Zero-point correction= 0.695306			
Thermal correction to Energy= 0.729891			
Thermal correction to Enthalpy= 0.730836			
Thermal correction to Gibbs Free Energy= 0.633483			
C	-19.110758	8.106421	-34.633631
O	-22.916466	9.550597	-31.838466
C	-12.583215	7.299696	-35.683593
C	-12.665564	6.725067	-37.052946
C	-13.808777	5.633576	-37.098200
C	-15.160672	6.154035	-36.810713
C	-15.821543	6.203879	-35.624051
O	-15.405725	5.627733	-34.468893
N	-15.871471	7.000603	-37.689719
C	-16.975511	7.570177	-37.084551
O	-17.666882	8.452286	-37.662658
C	-17.014789	7.016691	-35.749372
C	-17.775455	7.345701	-34.584392
O	-17.326588	7.015164	-33.457021
C	-12.993901	8.571041	-35.289777
C	-13.529743	9.633393	-36.025056
C	-13.818720	10.883733	-35.259778
C	-15.051407	10.802456	-34.310318
C	-15.365521	12.211254	-33.788542
C	-14.163433	12.943917	-33.194689
C	-16.231546	10.115133	-35.022632
C	-17.536681	10.191722	-34.215356
C	-18.793383	9.611279	-34.916610

C	-19.967258	10.496063	-34.577229
C	-21.006997	10.141799	-33.825562
C	-21.154303	8.768689	-33.239699
C	-19.993756	7.556289	-35.766027
C	-20.147007	6.530013	-32.827808
C	-20.690636	6.525606	-31.396367
C	-21.940749	7.398211	-31.279347
C	-21.702940	8.810438	-31.809207
O	-16.393042	10.709154	-36.304908
C	-13.814981	9.660194	-37.483805
C	-11.342703	6.085506	-37.508568
C	-12.125123	6.390240	-34.594238
C	-19.838578	7.969288	-33.269643
H	-23.253995	9.596885	-30.935701
H	-12.938959	7.489468	-37.773388
H	-13.739211	5.196962	-38.101489
H	-13.564523	4.842434	-36.382291
H	-16.011300	6.027237	-33.792717
H	-15.711999	7.080143	-38.683725
H	-12.861893	8.785122	-34.230866
H	-13.979843	11.709319	-35.955523
H	-12.940527	11.107201	-34.643445
H	-14.781507	10.166762	-33.455615
H	-16.133886	12.127996	-33.014446
H	-15.800592	12.799131	-34.606655
H	-13.663985	12.326353	-32.440384
H	-14.480824	13.870770	-32.711071
H	-13.425009	13.208460	-33.956364
H	-15.939411	9.064592	-35.148111
H	-17.393060	9.718163	-33.235233
H	-17.735575	11.251489	-34.028534
H	-18.630429	9.689653	-35.996262
H	-19.911498	11.510908	-34.970832
H	-21.805799	10.850456	-33.622666
H	-21.913149	8.223579	-33.826876
H	-20.933940	8.114096	-35.812507
H	-20.229932	6.500556	-35.603783
H	-19.490066	7.663901	-36.726573
H	-19.253881	5.907736	-32.891422
H	-20.903896	6.096716	-33.495544
H	-19.913901	6.904414	-30.718845
H	-20.918960	5.504495	-31.074757
H	-22.287226	7.448063	-30.239927
H	-22.754753	6.960746	-31.872404

H	-20.963356	9.323962	-31.171578
H	-16.850533	10.057953	-36.870494
H	-14.213263	10.627986	-37.776817
H	-14.554496	8.888159	-37.730686
H	-12.906833	9.447570	-38.057035
H	-11.139943	5.152339	-36.978459
H	-11.421048	5.853925	-38.573037
H	-10.496762	6.761646	-37.366909
H	-13.021837	5.838848	-34.270134
H	-11.745428	6.942089	-33.734329
H	-11.387569	5.661155	-34.927954
H	-19.171346	8.404609	-32.511441

INT1a(closed-shell)(water)			
E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.27820984			
Zero-point correction= 0.695764			
Thermal correction to Energy= 0.730861			
Thermal correction to Enthalpy= 0.731805			
Thermal correction to Gibbs Free Energy= 0.633774			
C	-19.109345	8.179690	-34.666021
O	-22.874675	9.328458	-31.697238
C	-12.543830	7.212700	-35.502275
C	-12.435582	6.710141	-36.878213
C	-13.822506	5.962813	-37.329029
C	-15.104841	6.599443	-37.045537
C	-15.733000	6.599251	-35.820644
O	-15.179249	6.075496	-34.717549
N	-15.950050	7.305378	-37.911440
C	-17.053925	7.817837	-37.245824
O	-17.812944	8.661112	-37.772715
C	-16.997570	7.261721	-35.903259
C	-17.733669	7.506243	-34.696553
O	-17.199357	7.190012	-33.605767
C	-13.079707	8.459330	-35.158768
C	-13.588431	9.488435	-35.943520
C	-13.870369	10.805806	-35.259984
C	-15.120637	10.867934	-34.348797
C	-15.349896	12.308321	-33.872397
C	-14.124690	12.968303	-33.241293
C	-16.332503	10.261969	-35.070579
C	-17.621492	10.322321	-34.239935
C	-18.877623	9.708957	-34.913107

C	-20.080172	10.519839	-34.498662
C	-21.069918	10.085594	-33.722259
C	-21.121556	8.689236	-33.176076
C	-20.007663	7.616855	-35.779355
C	-19.966765	6.502802	-32.858456
C	-20.459631	6.432991	-31.410349
C	-21.755770	7.223827	-31.230390
C	-21.620532	8.661249	-31.727685
O	-16.508955	10.928442	-36.317105
C	-13.824044	9.538202	-37.412171
C	-11.309908	5.699268	-37.106134
C	-12.094799	6.312032	-34.399399
C	-19.766121	7.967934	-33.276174
H	-23.187086	9.327271	-30.784735
H	-12.296663	7.538031	-37.569554
H	-13.684119	5.773318	-38.396874
H	-13.770460	5.005959	-36.798708
H	-15.800835	6.372572	-33.996915
H	-15.732484	7.585709	-38.855669
H	-13.055883	8.684140	-34.093043
H	-13.979866	11.581469	-36.024112
H	-12.992810	11.051114	-34.651237
H	-14.935283	10.232480	-33.470282
H	-16.158034	12.303082	-33.134659
H	-15.704078	12.903234	-34.723357
H	-13.700326	12.334098	-32.455169
H	-14.393435	13.925708	-32.788380
H	-13.338758	13.163435	-33.975976
H	-16.060163	9.219047	-35.258731
H	-17.452658	9.855183	-33.261056
H	-17.835159	11.380421	-34.055685
H	-18.766536	9.827904	-35.996740
H	-20.093219	11.547300	-34.861146
H	-21.897187	10.742079	-33.466204
H	-21.870253	8.120220	-33.753082
H	-20.972033	8.132892	-35.777050
H	-20.189162	6.547797	-35.636239
H	-19.549593	7.770506	-36.756335
H	-19.037911	5.941165	-32.965323
H	-20.716152	6.035354	-33.511321
H	-19.684126	6.843599	-30.750235
H	-20.613287	5.392526	-31.106925
H	-22.069381	7.224745	-30.179099
H	-22.561850	6.753645	-31.808881

H	-20.889472	9.200929	-31.101487
H	-17.040638	10.342834	-36.886044
H	-14.854439	9.892252	-37.553665
H	-13.696423	8.613760	-37.957728
H	-13.179777	10.318791	-37.837037
H	-11.453630	4.790455	-36.516279
H	-11.285671	5.413038	-38.160327
H	-10.338147	6.128086	-36.848586
H	-12.612150	5.348742	-34.494694
H	-12.317634	6.729037	-33.417754
H	-11.020645	6.107470	-34.470281
H	-19.093359	8.425398	-32.536160

INT1b(closed-shell)(water)

E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28142326

Zero-point correction= 0.695585

Thermal correction to Energy= 0.730859

Thermal correction to Enthalpy= 0.731803

Thermal correction to Gibbs Free Energy= 0.632403

C	-2.159541	-0.445112	0.458557
O	-5.817996	0.434494	3.650225
C	3.866974	-0.071103	-2.845054
C	4.222705	-1.415461	-2.392395
C	2.968259	-2.411158	-2.700786
C	1.672869	-1.957241	-2.224494
C	1.126169	-2.023895	-0.963386
O	1.695458	-2.641796	0.086253
N	0.883384	-1.056007	-2.941877
C	-0.197755	-0.602843	-2.196671
O	-0.979635	0.268719	-2.636077
C	-0.091941	-1.266440	-0.914385
C	-0.775713	-1.097801	0.335932
O	-0.203290	-1.491968	1.380015
C	3.363726	0.950140	-2.027393
C	3.325731	1.076250	-0.644449
C	2.948653	2.422982	-0.101876
C	1.717498	2.448775	0.830356
C	1.396313	3.894253	1.234235
C	2.583917	4.664781	1.809753
C	0.551785	1.736056	0.126202
C	-0.731186	1.722674	0.968222
C	-1.980681	1.101164	0.294048

C	-3.194060	1.848115	0.790353
C	-4.136007	1.344904	1.584225
C	-4.125135	-0.078914	2.055737
C	-3.087304	-0.965340	-0.652577
C	-2.921808	-2.253769	2.182168
C	-3.344354	-2.425615	3.643935
C	-4.641490	-1.670365	3.935875
C	-4.554748	-0.203141	3.521371
O	0.350194	2.374324	-1.124918
C	3.757875	0.073968	0.382761
C	5.452892	-2.020773	-3.074729
C	3.990833	0.213979	-4.308050
C	-2.759498	-0.760845	1.854710
H	-6.090085	0.364650	4.572896
H	4.338030	-1.461611	-1.314087
H	2.976063	-2.577846	-3.783835
H	3.256491	-3.340244	-2.203926
H	1.116845	-2.365719	0.848750
H	0.944646	-0.877278	-3.933344
H	3.020779	1.832531	-2.561997
H	2.776357	3.128244	-0.918098
H	3.821995	2.766934	0.470980
H	1.944820	1.875882	1.740592
H	0.600997	3.876776	1.985316
H	0.993089	4.417821	0.359169
H	3.060893	4.101563	2.619460
H	2.258890	5.624885	2.217969
H	3.344586	4.872756	1.052294
H	0.891986	0.705858	-0.040854
H	-0.532548	1.225508	1.926930
H	-0.978142	2.764294	1.197763
H	-1.901523	1.289919	-0.782033
H	-3.254286	2.891116	0.480894
H	-4.971890	1.960327	1.906002
H	-4.886320	-0.634803	1.482103
H	-4.067973	-0.487761	-0.572708
H	-3.224312	-2.047842	-0.576723
H	-2.679196	-0.728870	-1.635025
H	-1.993675	-2.794946	1.996099
H	-3.696124	-2.687776	1.535332
H	-2.543868	-2.045663	4.292449
H	-3.469128	-3.485953	3.885508
H	-4.902352	-1.738547	4.999350
H	-5.468313	-2.119055	3.369705

H	-3.804922	0.313456	4.144803
H	-0.152217	1.770805	-1.700699
H	3.712737	0.515984	1.379157
H	4.792943	-0.237120	0.203204
H	3.135201	-0.829158	0.380333
H	6.340781	-1.409003	-2.897654
H	5.637256	-3.018649	-2.670112
H	5.310245	-2.118072	-4.153958
H	5.048696	0.345179	-4.569416
H	3.452413	1.117393	-4.594113
H	3.631849	-0.629686	-4.908668
H	-2.066817	-0.340824	2.598538

INT1a(closed-shell)(ether)

E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28484021

Zero-point correction= 0.695642

Thermal correction to Energy= 0.730759

Thermal correction to Enthalpy= 0.731703

Thermal correction to Gibbs Free Energy= 0.633531

C	-19.109098	8.174341	-34.662086
O	-22.882444	9.332900	-31.703720
C	-12.558003	7.211587	-35.503472
C	-12.445382	6.709571	-36.884440
C	-13.813676	5.949255	-37.322611
C	-15.106751	6.573950	-37.028560
C	-15.733679	6.569605	-35.810911
O	-15.188884	6.035332	-34.702686
N	-15.952454	7.285766	-37.896348
C	-17.051405	7.799341	-37.233147
O	-17.809677	8.650431	-37.761785
C	-17.000751	7.241416	-35.893029
C	-17.735344	7.493110	-34.689878
O	-17.207812	7.178078	-33.593850
C	-13.088446	8.457852	-35.152670
C	-13.582710	9.492021	-35.940874
C	-13.860472	10.808907	-35.260082
C	-15.113368	10.868622	-34.350105
C	-15.347473	12.311453	-33.883208
C	-14.123195	12.979574	-33.258964
C	-16.323755	10.250477	-35.064859
C	-17.611105	10.309971	-34.230642
C	-18.869674	9.702550	-34.905076

C	-20.068671	10.519227	-34.491742
C	-21.063865	10.087826	-33.720256
C	-21.125148	8.690239	-33.177845
C	-20.007969	7.617927	-35.778004
C	-19.981361	6.498290	-32.860549
C	-20.479259	6.427550	-31.414211
C	-21.773055	7.222895	-31.237560
C	-21.630147	8.660709	-31.731301
O	-16.512306	10.906049	-36.316463
C	-13.813070	9.538130	-37.408889
C	-11.300075	5.719495	-37.110081
C	-12.099684	6.313365	-34.404782
C	-19.772403	7.963134	-33.275058
H	-23.193137	9.338745	-30.790210
H	-12.312313	7.541442	-37.571846
H	-13.684447	5.761677	-38.392079
H	-13.753637	4.988532	-36.799685
H	-15.802489	6.343622	-33.983929
H	-15.721912	7.578597	-38.834102
H	-13.061802	8.680430	-34.086999
H	-13.965552	11.584585	-36.024544
H	-12.984245	11.050154	-34.648218
H	-14.922851	10.241205	-33.467293
H	-16.153847	12.308322	-33.143561
H	-15.704748	12.900120	-34.737333
H	-13.696194	12.351928	-32.469238
H	-14.394766	13.939393	-32.812913
H	-13.339179	13.171288	-33.996448
H	-16.048838	9.207038	-35.247226
H	-17.441090	9.838864	-33.254019
H	-17.822404	11.367656	-34.041270
H	-18.754393	9.822977	-35.987968
H	-20.074319	11.548698	-34.849146
H	-21.887142	10.749586	-33.464354
H	-21.873733	8.125643	-33.759563
H	-20.969560	8.139531	-35.779169
H	-20.197602	6.550143	-35.635294
H	-19.543533	7.768692	-36.752405
H	-19.054668	5.932865	-32.966862
H	-20.731041	6.035518	-33.516466
H	-19.705068	6.834191	-30.750078
H	-20.638214	5.387219	-31.113270
H	-22.090748	7.223362	-30.187884
H	-22.578169	6.756312	-31.820456

H	-20.900317	9.196137	-31.100495
H	-17.022063	10.299289	-36.884591
H	-14.821859	9.945250	-37.556269
H	-13.727756	8.604347	-37.945422
H	-13.125355	10.281011	-37.834337
H	-11.428250	4.806492	-36.523346
H	-11.270903	5.438227	-38.165310
H	-10.337179	6.166330	-36.850734
H	-12.584559	5.335940	-34.517535
H	-12.339905	6.715133	-33.421264
H	-11.019299	6.142430	-34.472797
H	-19.100843	8.416863	-32.531751

INT1b(closed-shell)(ether)

E[M06-2X/6-31G(d,p)/CPCM(ether)]= -1599.28867094

Zero-point correction= 0.695415

Thermal correction to Energy= 0.730704

Thermal correction to Enthalpy= 0.731648

Thermal correction to Gibbs Free Energy= 0.632258

C	-2.165790	-0.440294	0.461837
O	-5.814135	0.423811	3.672373
C	3.866959	-0.075809	-2.853528
C	4.208488	-1.429966	-2.401318
C	2.957988	-2.398197	-2.727921
C	1.660272	-1.942079	-2.234876
C	1.116509	-2.025344	-0.981077
O	1.679589	-2.663246	0.066689
N	0.854182	-1.046366	-2.949236
C	-0.217126	-0.596484	-2.199809
O	-1.002201	0.285521	-2.630337
C	-0.108392	-1.267253	-0.922956
C	-0.784139	-1.099299	0.328607
O	-0.210939	-1.496648	1.373124
C	3.367355	0.949680	-2.042084
C	3.323226	1.073815	-0.657673
C	2.951541	2.421129	-0.118389
C	1.722884	2.451359	0.818791
C	1.406195	3.900609	1.212811
C	2.597685	4.670975	1.780385
C	0.552858	1.732680	0.127659
C	-0.723229	1.717932	0.981053
C	-1.980411	1.106406	0.311347

C	-3.186884	1.855498	0.821143
C	-4.129741	1.348808	1.612165
C	-4.125936	-0.080131	2.068456
C	-3.101254	-0.945425	-0.649490
C	-2.931828	-2.261128	2.170807
C	-3.351652	-2.445674	3.631826
C	-4.645528	-1.688725	3.933430
C	-4.553329	-0.217892	3.533750
O	0.334900	2.363391	-1.125372
C	3.736206	0.065974	0.369487
C	5.449138	-2.029680	-3.070709
C	4.010549	0.213004	-4.311498
C	-2.763742	-0.765993	1.856787
H	-6.081356	0.349317	4.596543
H	4.316647	-1.475614	-1.322188
H	2.953436	-2.552614	-3.812620
H	3.234421	-3.342387	-2.252381
H	1.110208	-2.380667	0.830777
H	0.943496	-0.825050	-3.930040
H	3.043684	1.837417	-2.578938
H	2.782907	3.126385	-0.935064
H	3.828243	2.759441	0.452646
H	1.955470	1.886958	1.732549
H	0.612705	3.890620	1.965968
H	1.003173	4.420132	0.335159
H	3.074016	4.111201	2.592636
H	2.276183	5.634855	2.182419
H	3.357314	4.870871	1.019810
H	0.891650	0.702044	-0.038348
H	-0.518089	1.212630	1.933969
H	-0.964797	2.758400	1.221613
H	-1.905729	1.303856	-0.763464
H	-3.241295	2.903027	0.525625
H	-4.959675	1.967087	1.944248
H	-4.890546	-0.626729	1.490258
H	-4.078581	-0.461576	-0.563760
H	-3.247019	-2.027293	-0.580217
H	-2.692031	-0.705318	-1.630568
H	-2.006388	-2.803963	1.975828
H	-3.709760	-2.685760	1.522056
H	-2.549086	-2.074633	4.282966
H	-3.480012	-3.507747	3.863422
H	-4.905208	-1.765972	4.996191
H	-5.474366	-2.129153	3.363560

H	-3.800890	0.288945	4.161609
H	-0.160731	1.747497	-1.695743
H	3.681331	0.502122	1.367537
H	4.771987	-0.246693	0.198078
H	3.110399	-0.834229	0.349407
H	6.332569	-1.415342	-2.882031
H	5.629761	-3.026388	-2.661993
H	5.318977	-2.128178	-4.151222
H	5.074787	0.347930	-4.545096
H	3.477618	1.117026	-4.604602
H	3.670095	-0.630636	-4.921402
H	-2.067798	-0.355325	2.602721