Supplementary Information for:

Preparation and Characterization of a Small Library of Thermally-Labile End-Caps for Variable-Temperature Triggering of Self-Immolative Polymers

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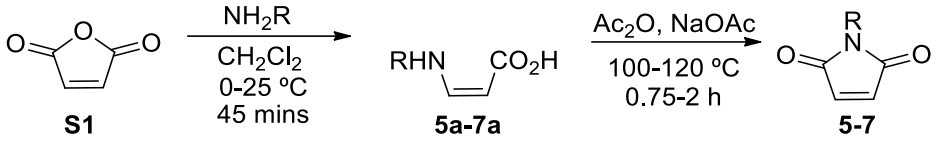
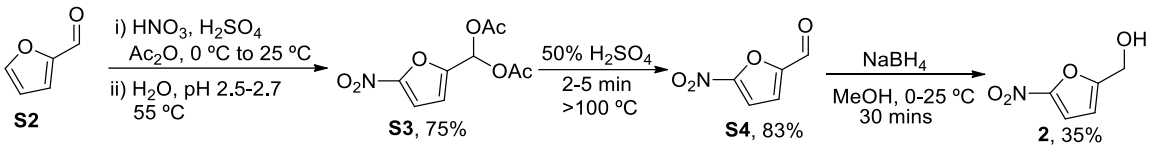
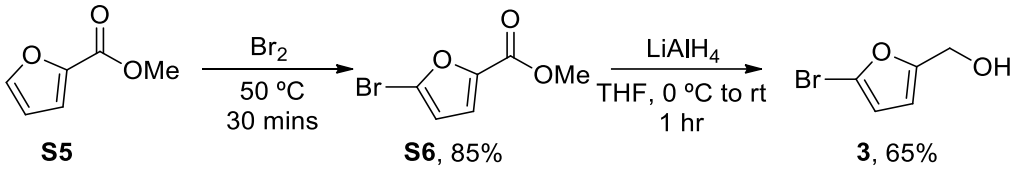
1. Schemes for the synthesis of starting materials not referenced in the main text.



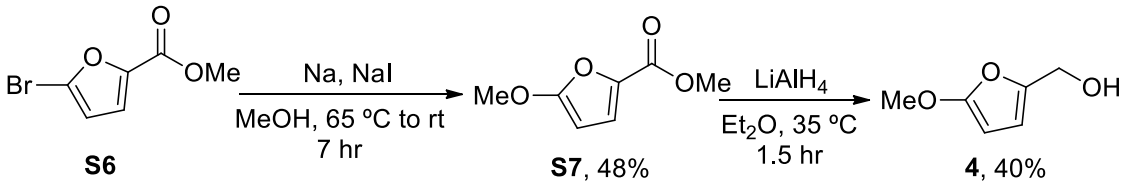
Scheme S1. Synthesis of maleimides from maleic anhydride.



Scheme S2. Synthesis of 5-nitro-2-furanmethanol **2**



Scheme S3. Synthesis of 5-Bromo-2-furanmethanol **3**



Scheme S4. Synthesis of 5-methoxy-2-furanmethanol **4**

2. Additional computational and experimental figures

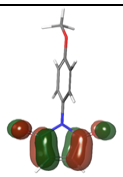
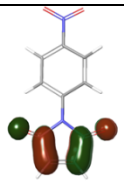
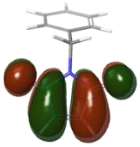
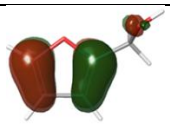
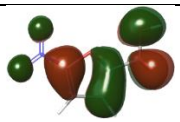
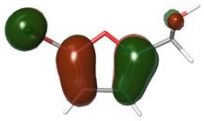
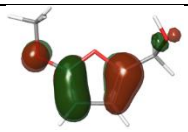
	 LUMO **5** = -0.09802	 LUMO **6** = -0.1061	 LUMO **7** = -0.0981
 HOMO **1** = -0.2281	HOMO- LUMO gap (Eg) **15** = 0.13	HOMO- LUMO gap (Eg) **16** = 0.12	HOMO- LUMO gap (Eg) **17** = 0.13
 HOMO **2** = -0.2587	HOMO- LUMO gap (Eg) **25** = 0.16	HOMO- LUMO gap (Eg) **26** = 0.15	HOMO- LUMO gap (Eg) **27** = 0.16
 HOMO **3** = -0.2311	HOMO- LUMO gap (Eg) **35** = 0.13	HOMO- LUMO gap (Eg) **36** = 0.12	HOMO- LUMO gap (Eg) **37** = 0.13
 HOMO **4** = -0.2019	HOMO- LUMO gap (Eg) **45** = 0.10	HOMO- LUMO gap (Eg) **46** = 0.09	-

Figure S1. B3LYP/6-311++G(d,p) calculated HOMO of the dienes, and LUMO of the dienophiles as well as calculated $HOMO_{(diene)}$- $LUMO_{(dienophile)}$ gap for each pair of cycloadducts. As the Diels-Alder reaction forming **47** was not useful in this study, it has been excluded from our computational analyses.

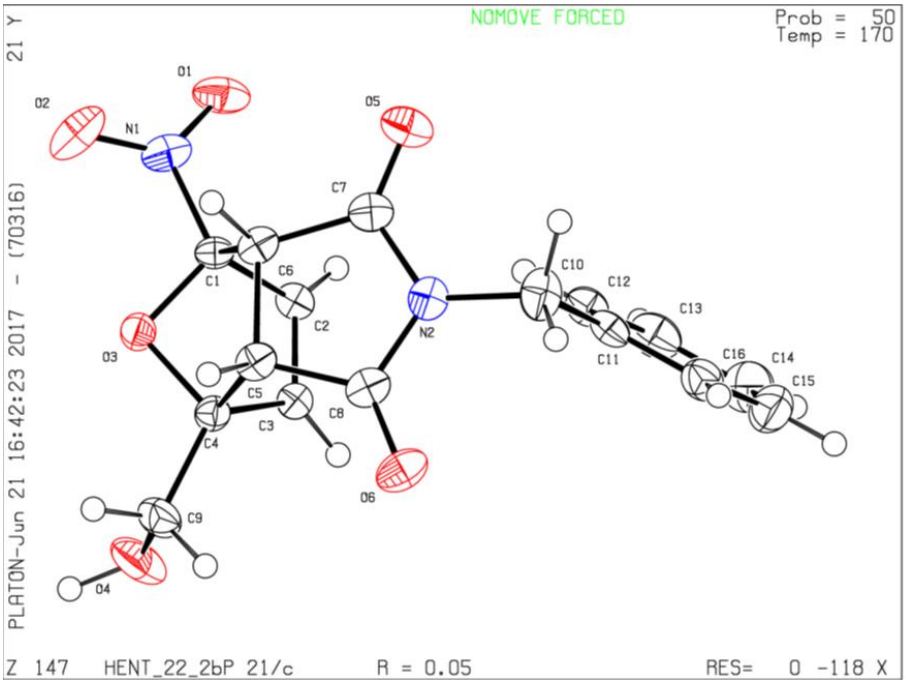


Figure S2. Ellipsoid plot of the **27$_{endo}$** crystal structure prepared with PLATON. CCDC # 1814084

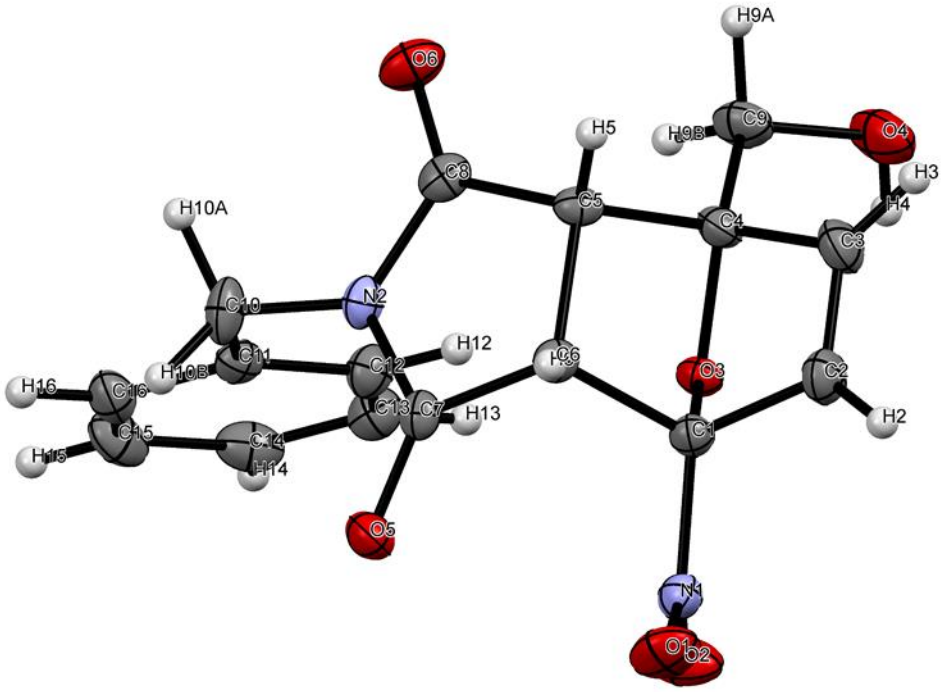


Figure S3. Ellipsoid plot of the **27$_{exo}$** crystal structure prepared with Mercury (v 3.10). CCDC # 1814083

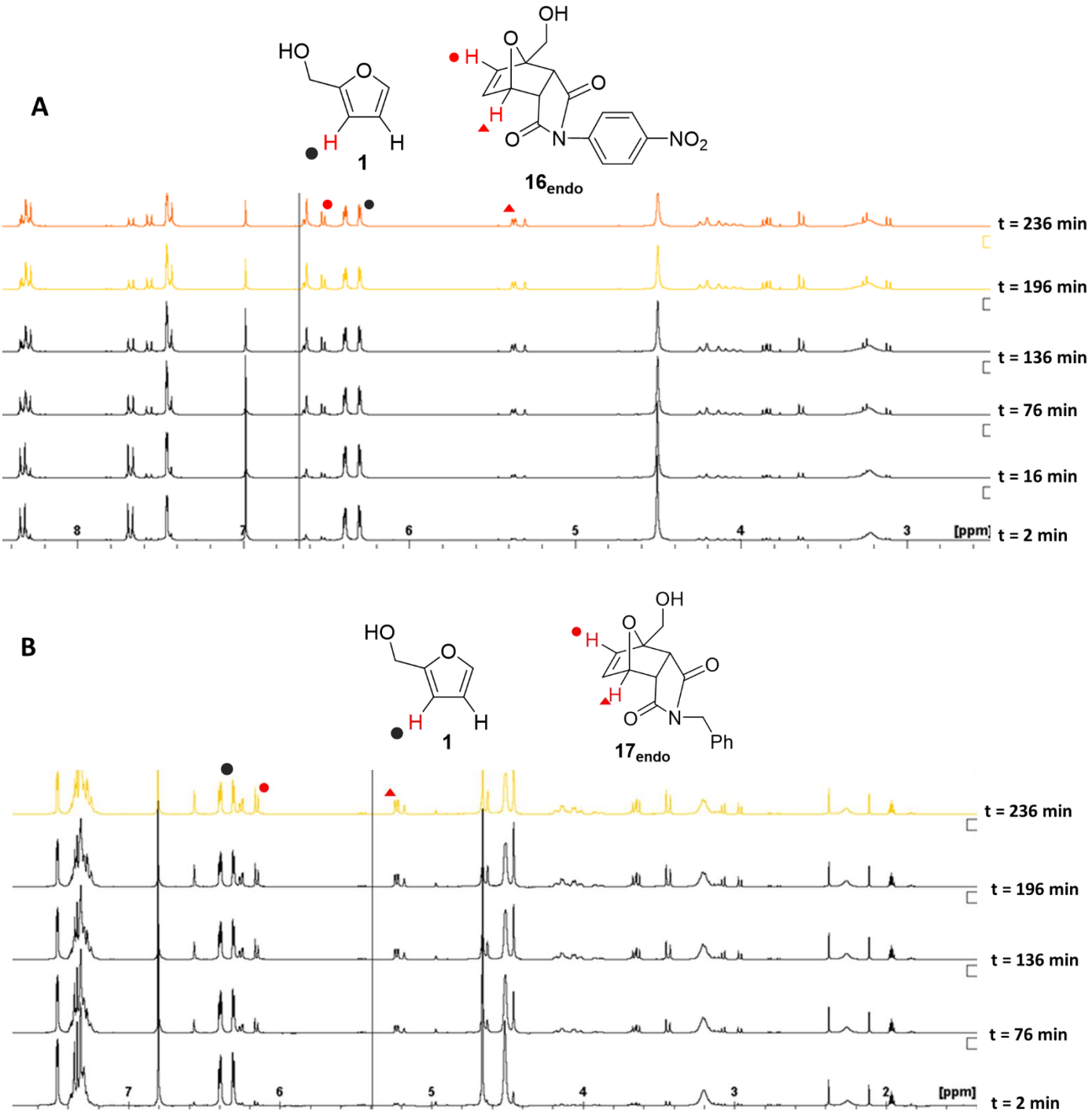


Figure S4. Sample kinetic experiment with selected spectra showing the cycloaddition of α-furfuryl alcohol **1** with (a) N-(p-nitro)-maleimide **6** and (b) Bz-maleimide **7** at 40 °C. Selected timepoints shown only. The ratio of starting material (●) to the *endo* (●) product (*exo* product is not observable) was determined using the relative integrations of the identified signals.

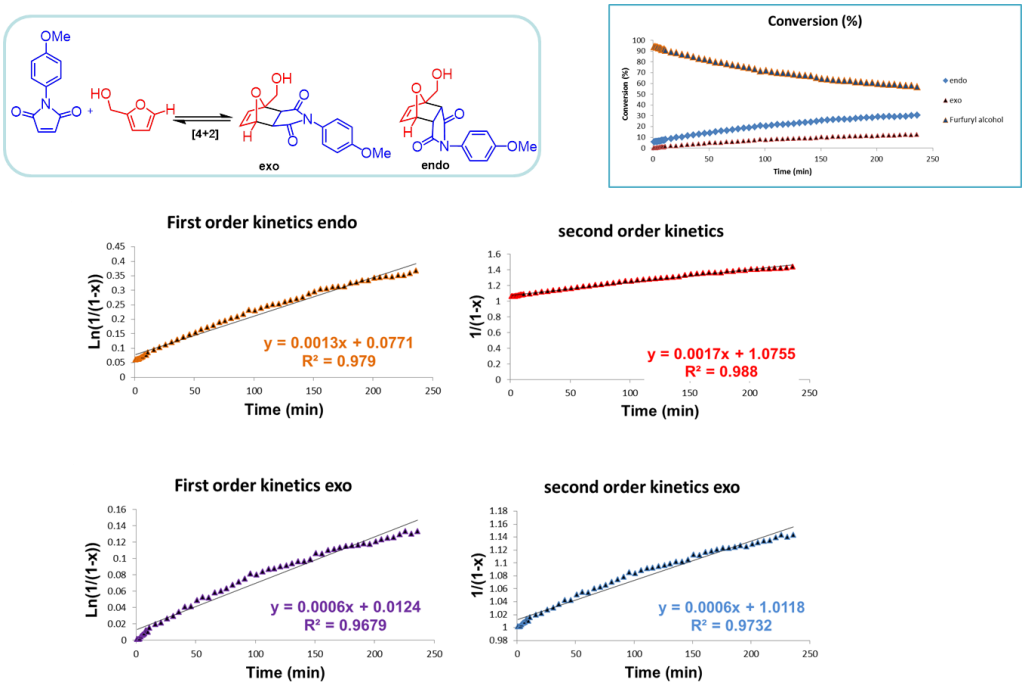
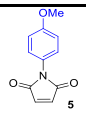
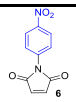
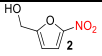
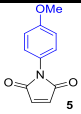
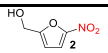
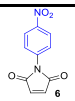
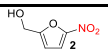


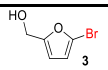
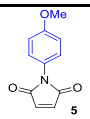
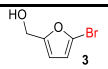
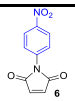
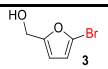
Figure S5. Forward kinetic profiles of the Diels-Alder reaction between α-furfuryl alcohol **1** and maleimide **5** at 40 °C showing the conversion over time and the approximate second-order kinetics profile of the reaction.

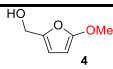
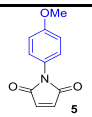
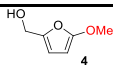
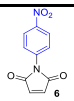
Table S1. M06-2X/6-311+G** calculated activation barriers for the forward ($\Delta G^{\ddagger}_{(DA)}$) and reverse ($\Delta G^{\ddagger}_{(rDA)}$) reactions, and the reaction free energies of the processes (ΔG).

Cycloadduct			M06-2X/6-311+G** $\Delta G^{\ddagger}_{(DA)}$ (kcal/mol)	M06-2X/6-311+G** ΔG (kcal/mol)	M06-2X/6-311+G** $\Delta G^{\ddagger}_{(rDA)}$ (kcal/mol)
15$_{endo}$ **15**$_{exo}$			9.5 10.1 $\Delta\Delta G^{\ddagger}$ = 0.6	-19.4 -20.6	20.7 22.3
16$_{endo}$ **16**$_{exo}$			8.9 12.0 $\Delta\Delta G^{\ddagger}$ = 3.1	-18.7 -19.7	20.3 20.6
17$_{endo}$ **17**$_{exo}$			9.6 10.7 $\Delta\Delta G^{\ddagger}$ = 1.1	-19.7 -21.2	22.8 28.6

Cycloadduct			M06-2X/6-311+G** $\Delta G^{\ddagger}_{(DA)}$ (kcal/mol)	M06-2X/6-311+G** ΔG (kcal/mol)	M06-2X/6-311+G** $\Delta G^{\ddagger}_{(rDA)}$ (kcal/mol)
25$_{endo}$ **25**$_{exo}$			11.8 12.7 $\Delta\Delta G^{\ddagger}$ = 0.9	-18.4 -20.5	22.1 23.7

26$_{endo}$ **26**$_{exo}$			12.0 13.1 $\Delta\Delta G^{\ddagger}$ = 1.1	-17.3 -19.2	22.0 23.3
27$_{endo}$ **27**$_{exo}$			11.9 12.1 $\Delta\Delta G^{\ddagger}$ = 0.2	-18.9 -20.7	22.6 23.5

Cycloadduct			**M06-2X/6-311+G**** $\Delta G^{\ddagger}_{(DA)}$ **(kcal/mol)**	**M06-2X/6-311+G**** ΔG **(kcal/mol)**	**M06-2X/6-311+G**** $\Delta G^{\ddagger}_{(rDA)}$ **(kcal/mol)**
35$_{endo}$ **35**$_{exo}$			10.5 11.4 $\Delta\Delta G^{\ddagger}$ = 0.9	-21.6 -21.9	24.0 24.5
36$_{endo}$ **36**$_{exo}$			11.1 11.3 $\Delta\Delta G^{\ddagger}$ = 0.2	-19.4 -20.7	23.0 24.0
37$_{endo}$ **37**$_{exo}$			10.0 11.6 $\Delta\Delta G^{\ddagger}$ = 1.6	-22.1 -22.5	24.1 25.1

Cycloadduct			**M06-2X/6-311+G**** $\Delta G^{\ddagger}_{(DA)}$ **(kcal/mol)**	**M06-2X/6-311+G**** ΔG **(kcal/mol)**	**M06-2X/6-311+G**** $\Delta G^{\ddagger}_{(rDA)}$ **(kcal/mol)**
45$_{endo}$ **45**$_{exo}$			7.1 9.7 $\Delta\Delta G^{\ddagger}$ = 2.6	-20.6 -20.1	16.5 18.4
46$_{endo}$ **46**$_{exo}$			6.2 8.9 $\Delta\Delta G^{\ddagger}$ = 2.7	-22.8 -19.5	17.9 16.1

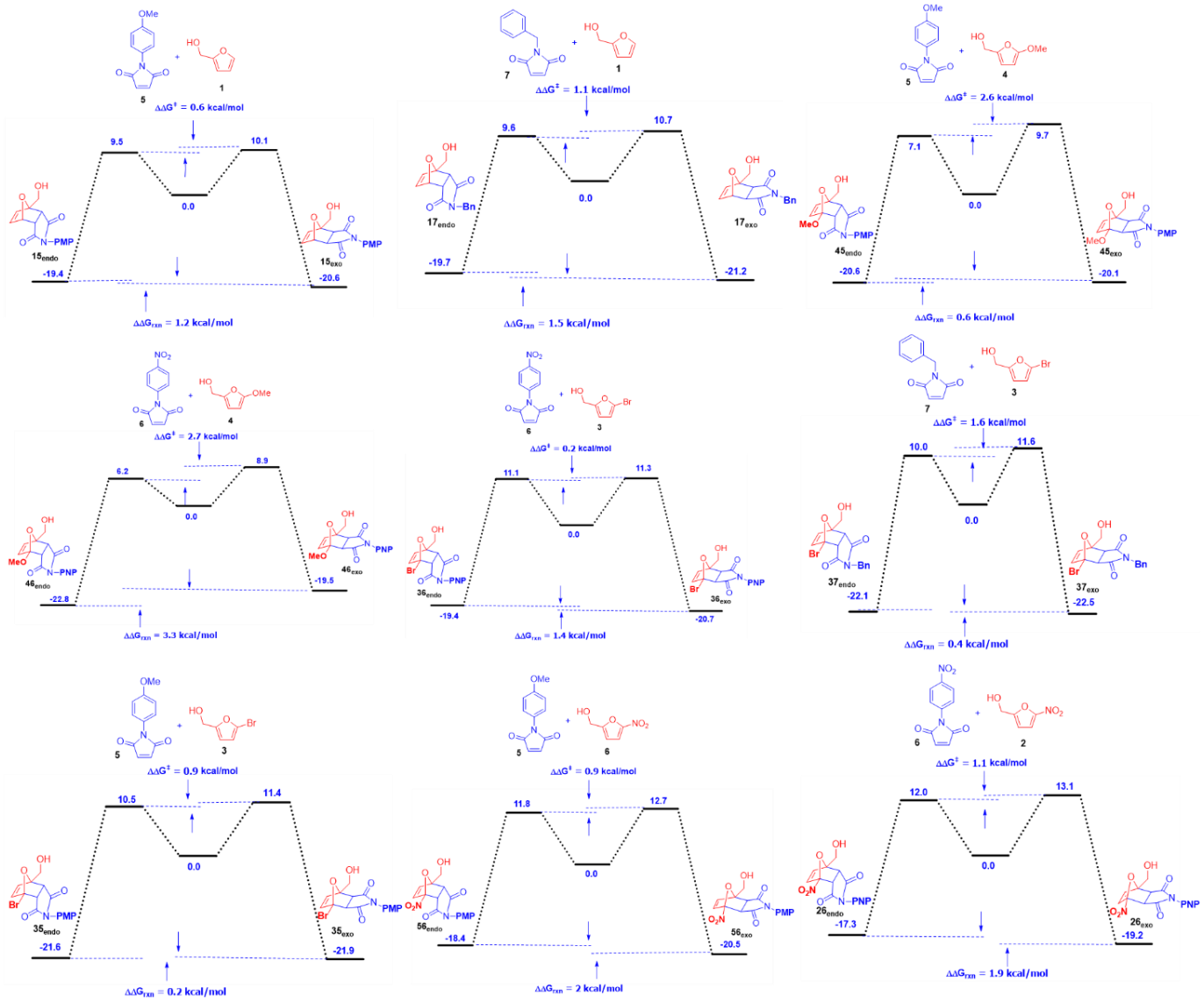
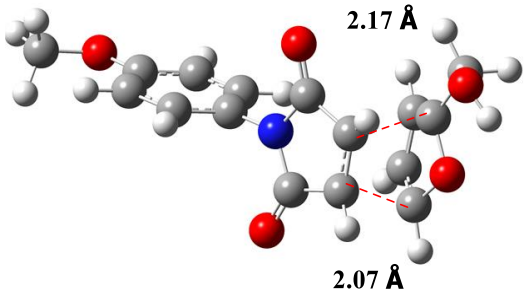


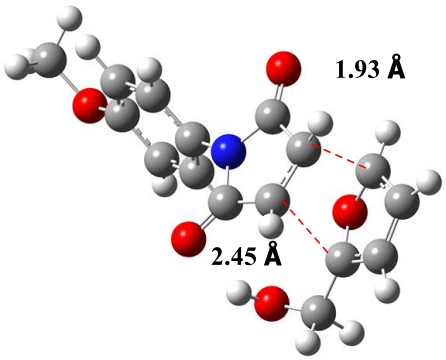
Figure S6. M06-2X/6-311+G** calculated potential energy surfaces of the forward and reverse Diels-Alder reactions between the different substituted α-furfuryl alcohols (**1-4)** and maleimide derivatives (**5-7**) not provided in the main text.

asynchronous TS



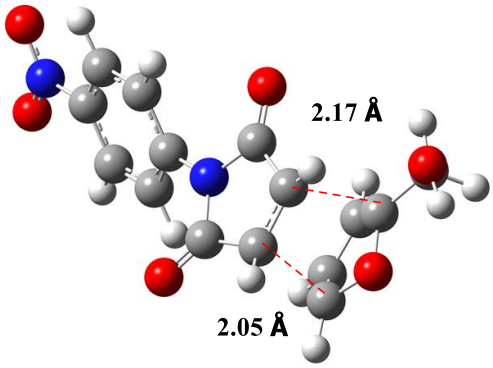
Endo-TS15; 9.5 kcal/mol

highly asynchronous TS



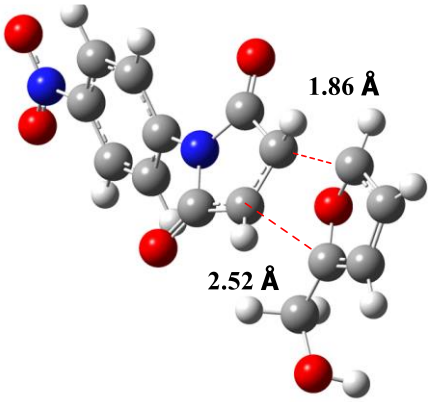
Exo-TS15; 10.1 kcal/mol

asynchronous TS



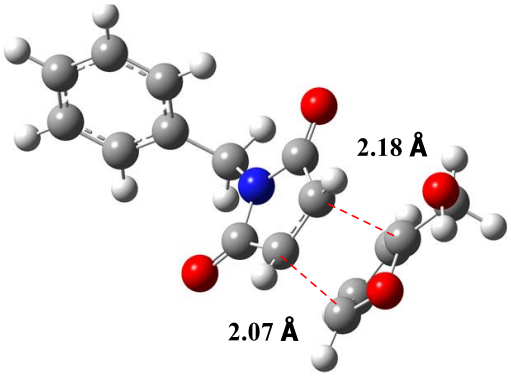
Endo-TS16; 8.9 kcal/mol

highly asynchronous TS



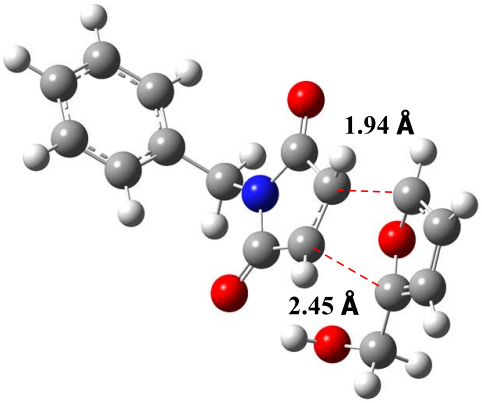
Exo-TS16; 12.0 kcal/mol

asynchronous TS



Endo-TS17; 9.6 kcal/mol

highly asynchronous TS



Exo-TS17; 10.7 kcal/mol

Figure S7. Illustration of the degree of asymmetry in the transition states (**TS15-17**) of the asynchronous ***Endo*** pathways compared with the highly asynchronous ***Exo*** pathways leading to products **15**, **16**, and **17**.

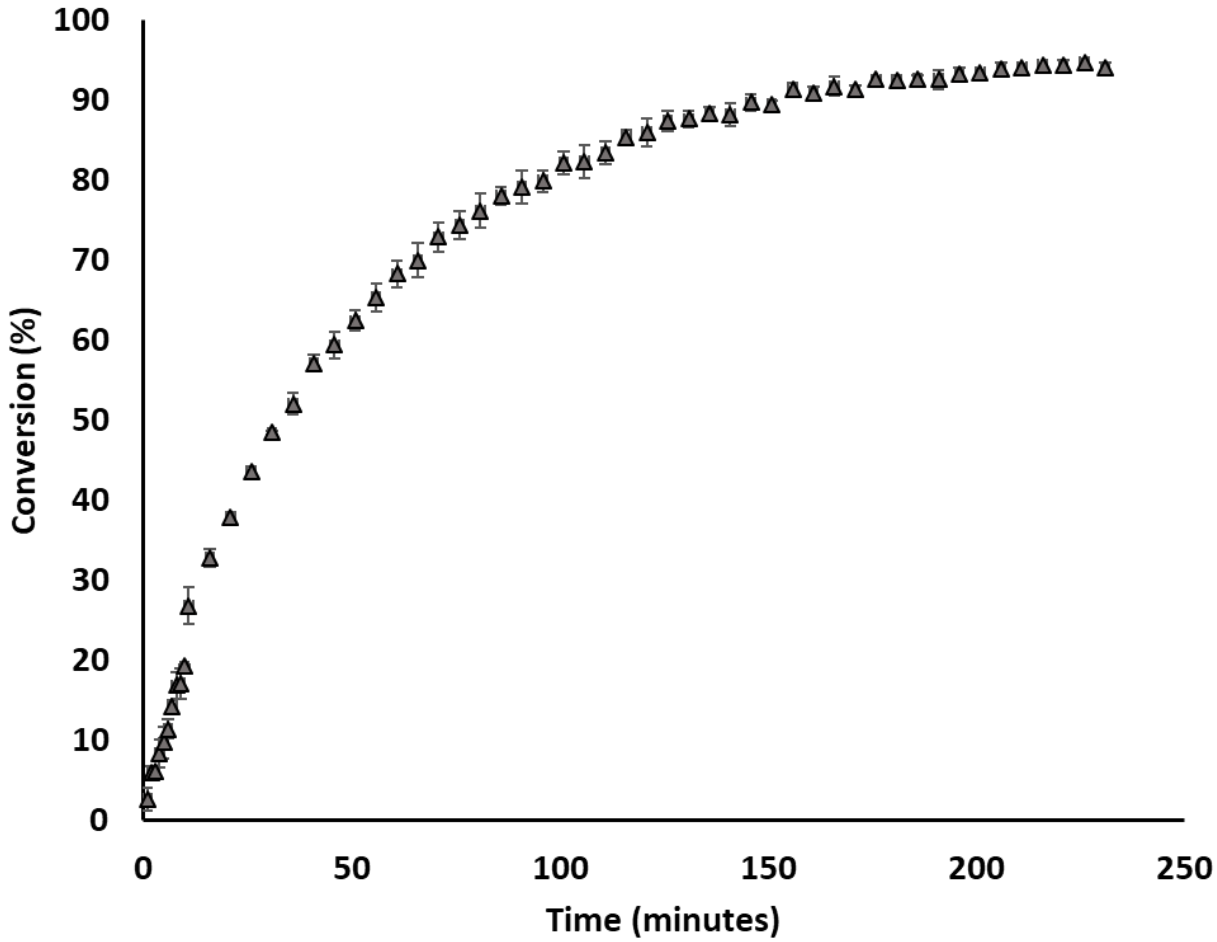
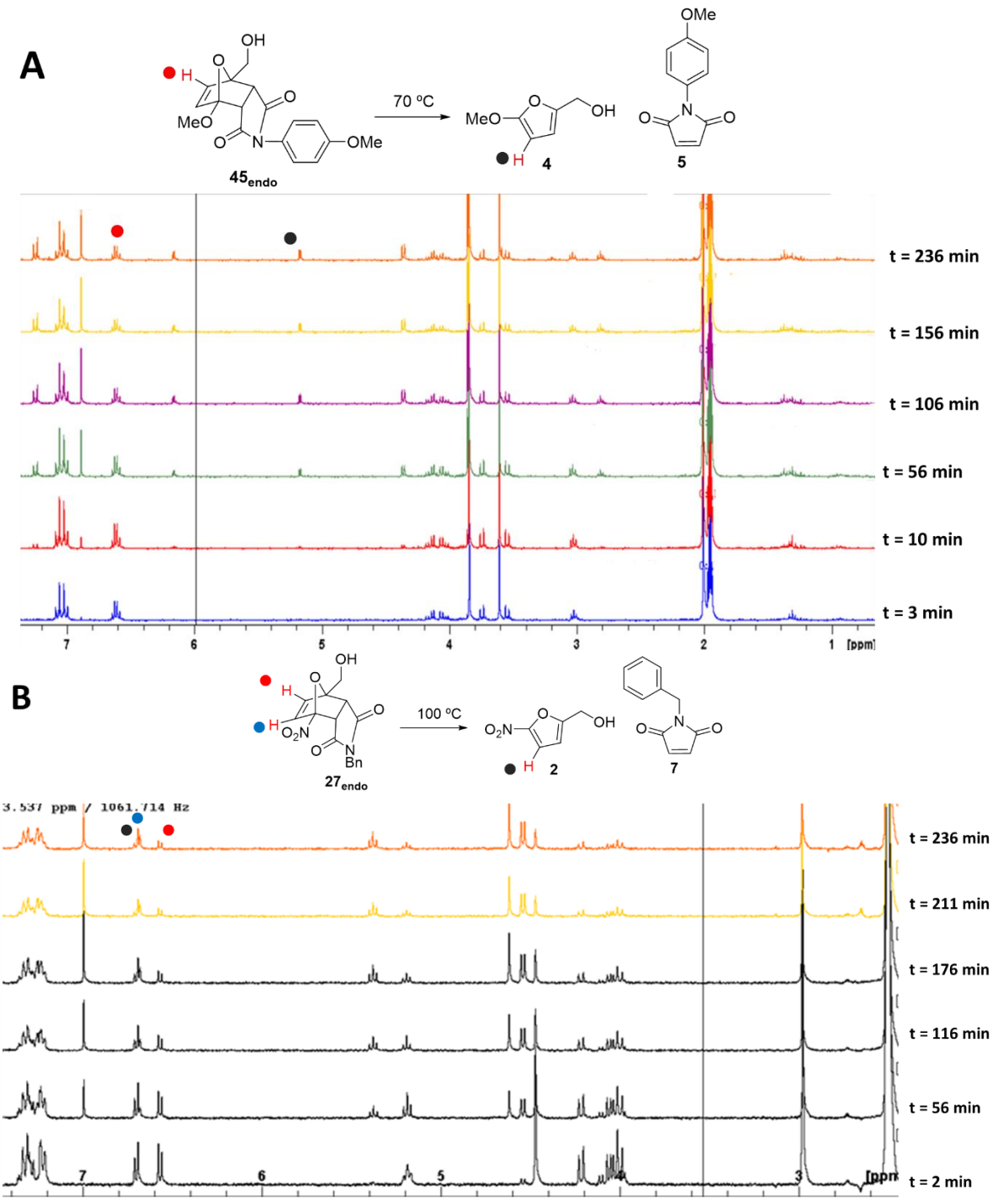


Figure S8. Mean conversion as a function of time for the cycloreversion reaction of **15** as determined by the formation.


A
70 °C
45endo
4
5
t = 236 min
t = 156 min
t = 106 min
t = 56 min
t = 10 min
t = 3 min
[ppm]
B
100 °C
27endo
2
7
t = 236 min
t = 211 min
t = 176 min
t = 116 min
t = 56 min
t = 2 min
[ppm]

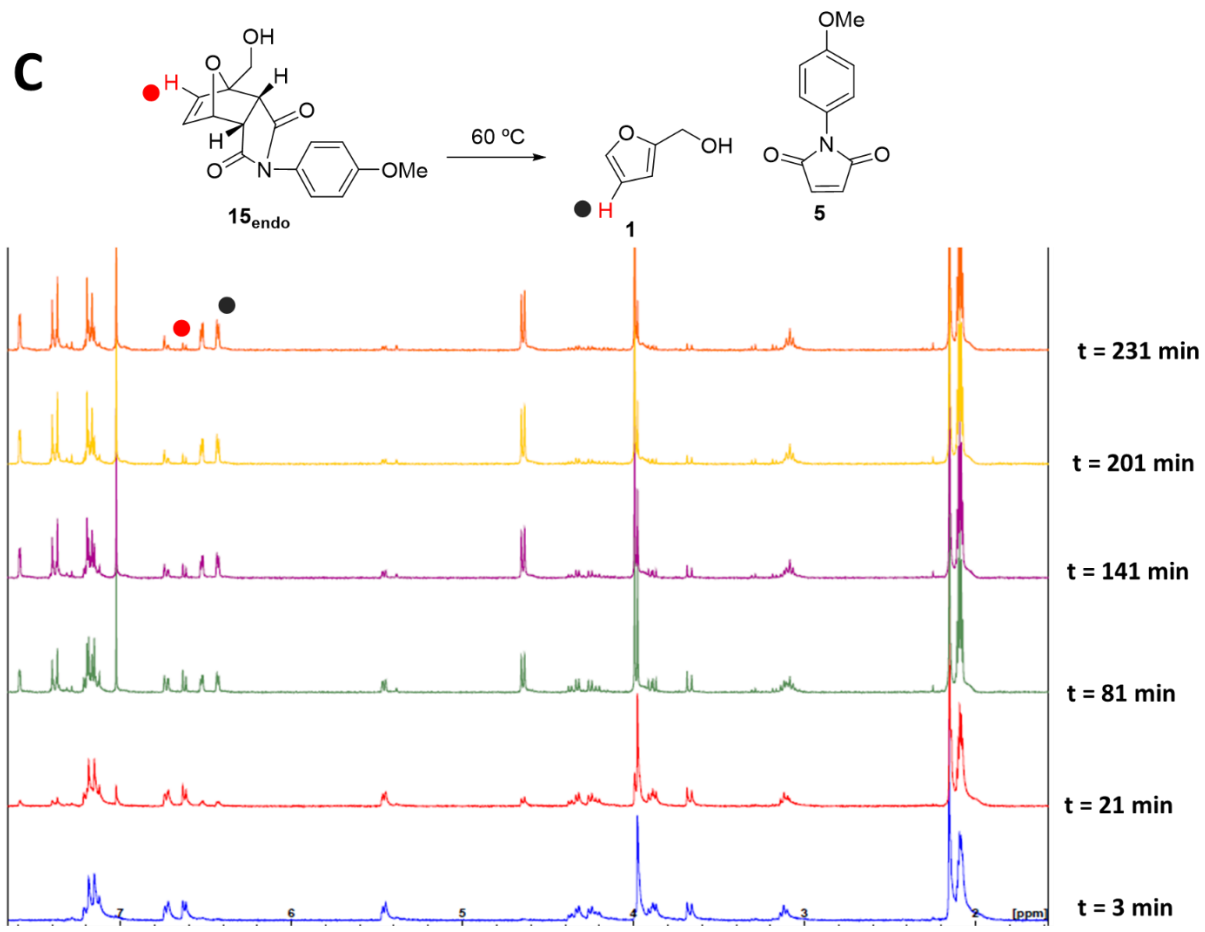


Figure S9. Sample kinetic experiment with selected spectra showing the cycloreversion of (**a**) methoxy-substituted furfuryl alcohol **45**$_{endo}$ at 70°C**;** (**b**) **27**$_{endo}$ at 100°C; (**c**) **15**$_{endo}$ at 60°C**.** Selected timepoints shown only. B is an example of the most complicated case where no clear integration could be determined. The Integration of the new olefinic peak overlaps with that of the cycloadduct. So, the integration of the red resonance was subtracted from the blue/black resonance to provide an estimate of the amount of product.

3. ^{1}H spectra for the known compounds

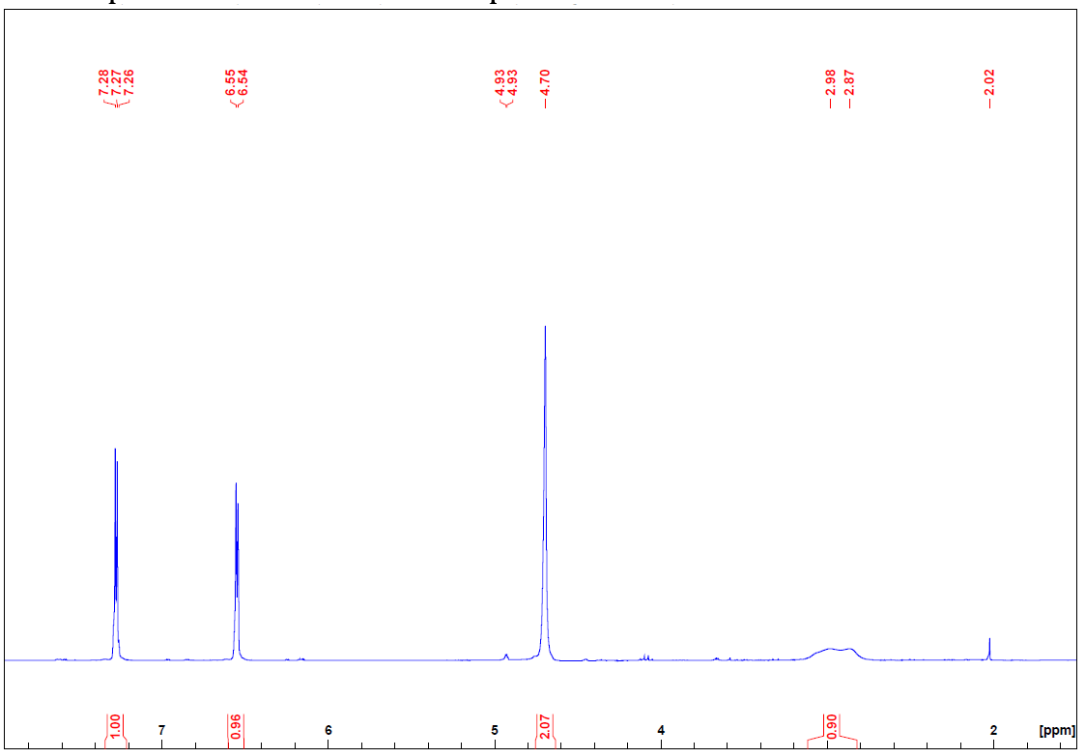


Figure S10. ^{1}H NMR of **2**

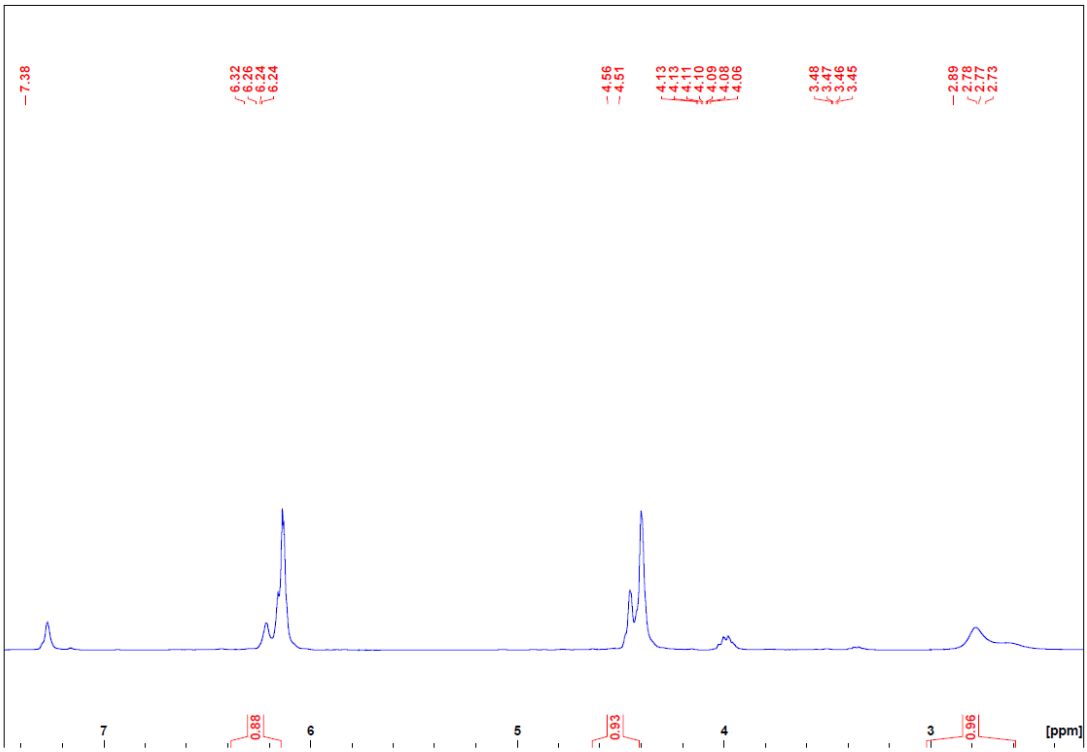


Figure S11. ^{1}H NMR of **3**

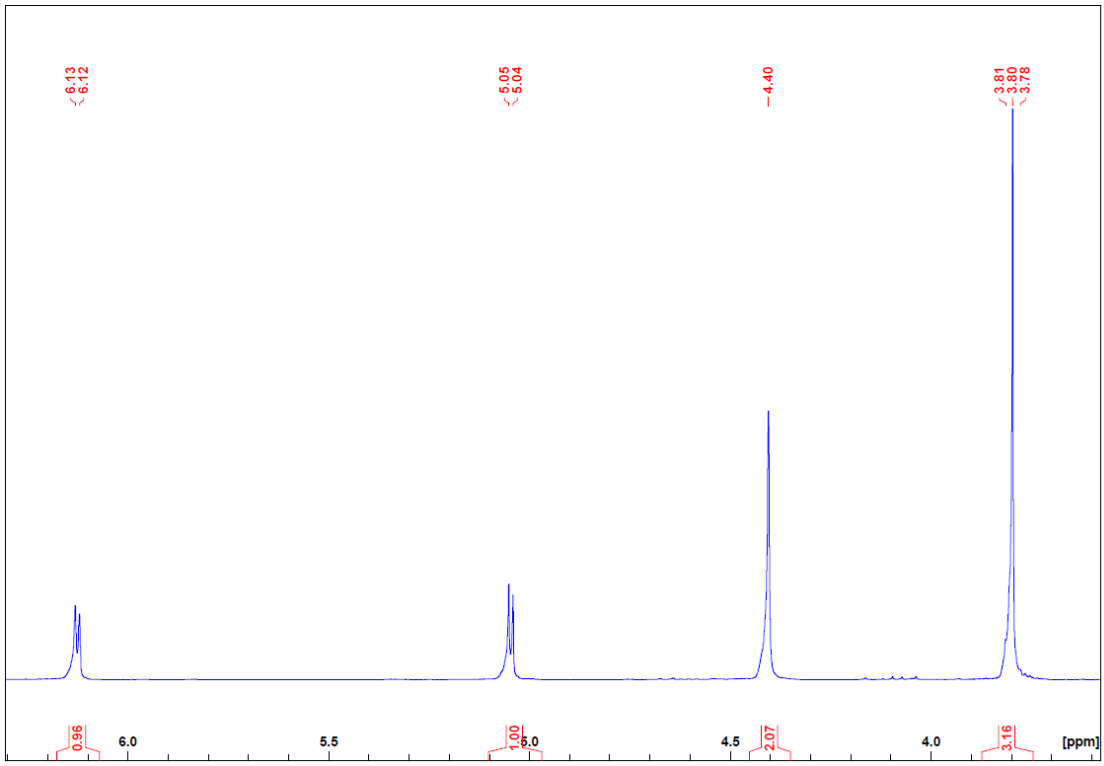


Figure S12. ^{1}H NMR of **4**

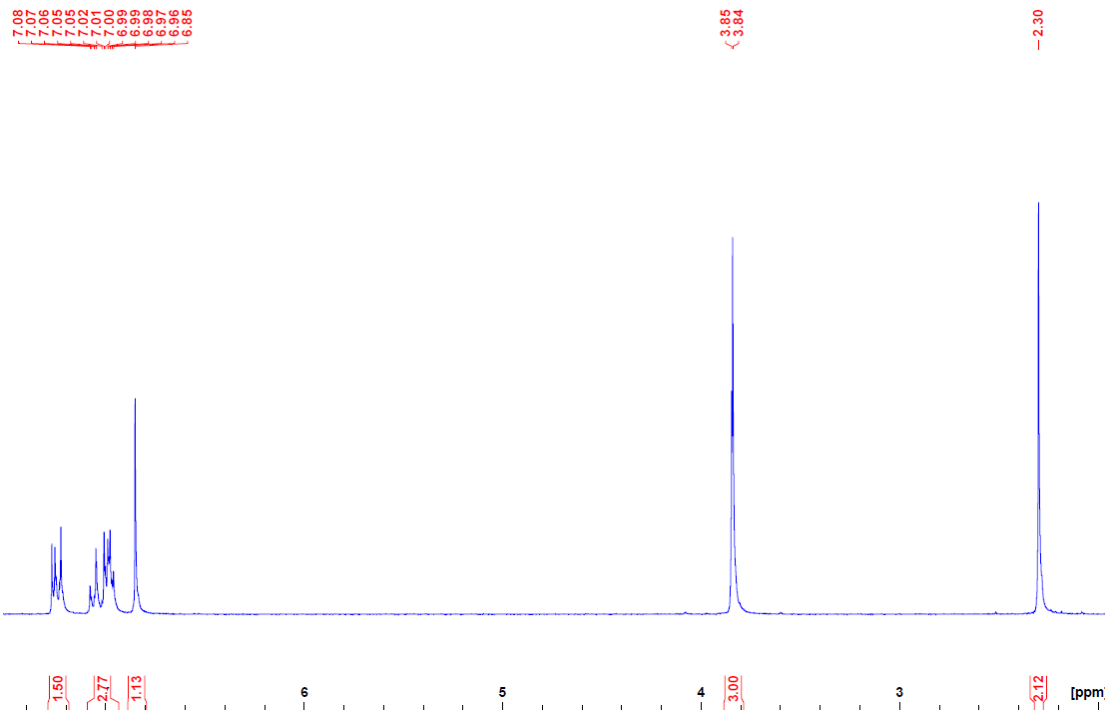


Figure S13. ^{1}H NMR of **5**

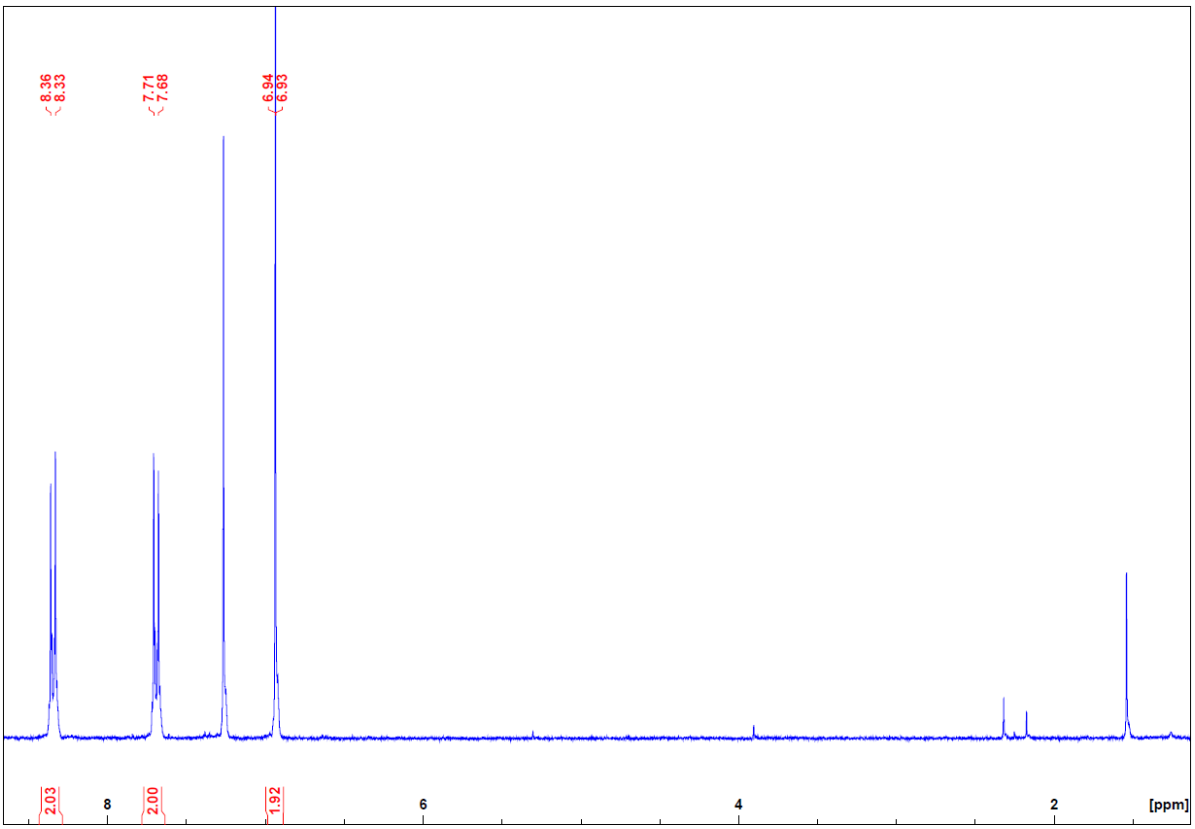


Figure S14. ^{1}H NMR of **6**

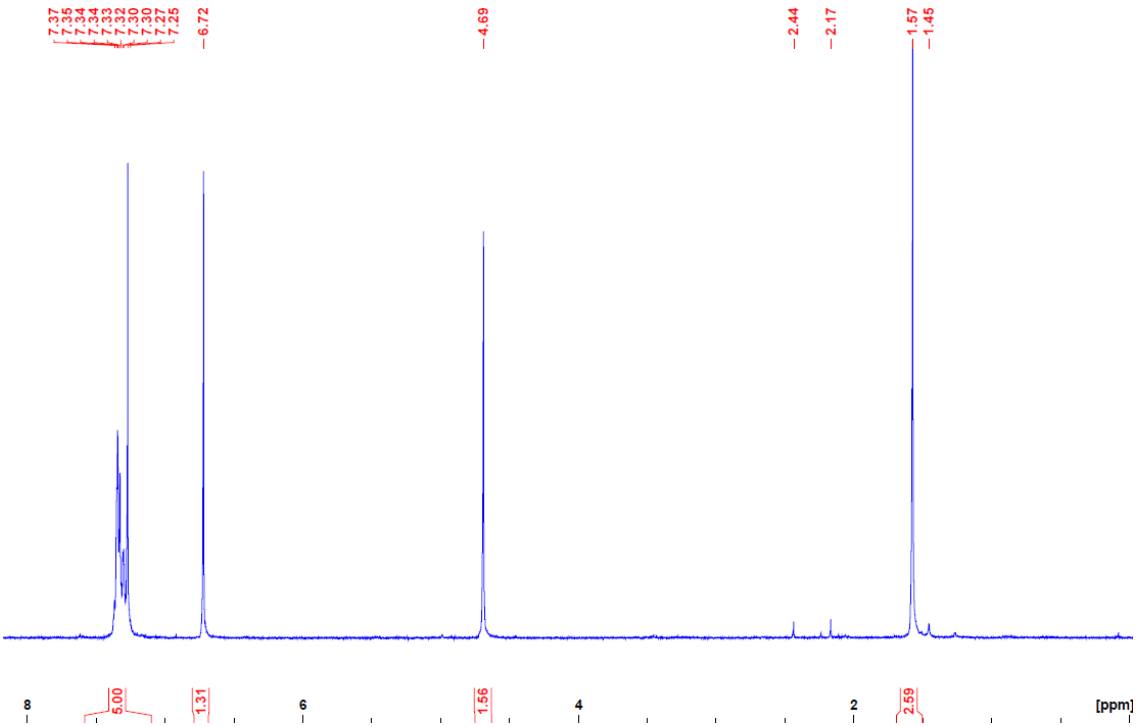


Figure S15. ^{1}H NMR of **7**

4. ^{1}H and ^{13}C NMR spectra for new compounds

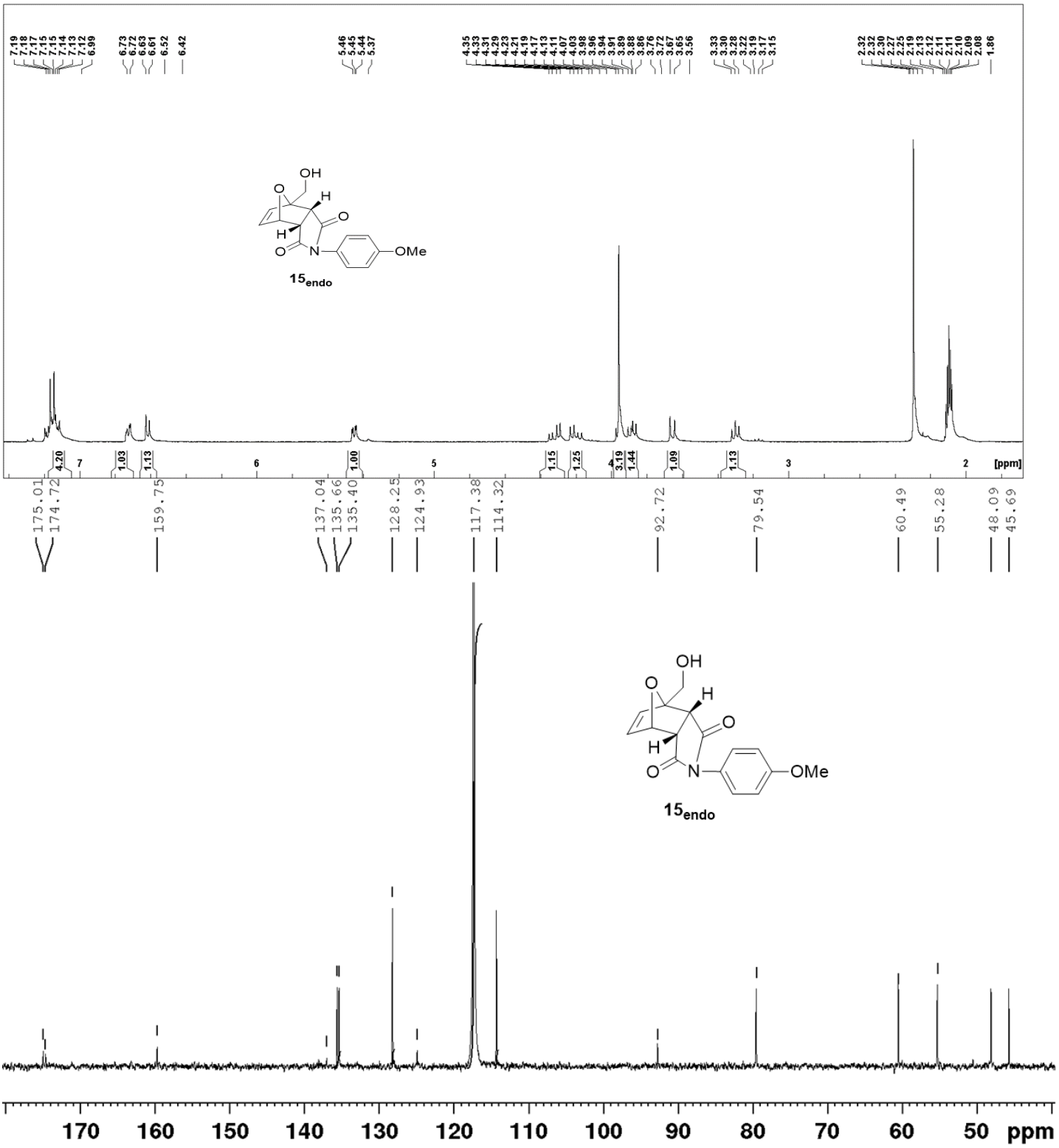


Figure S16. ^{1}H and ^{13}C NMR of **15$_{endo}$**

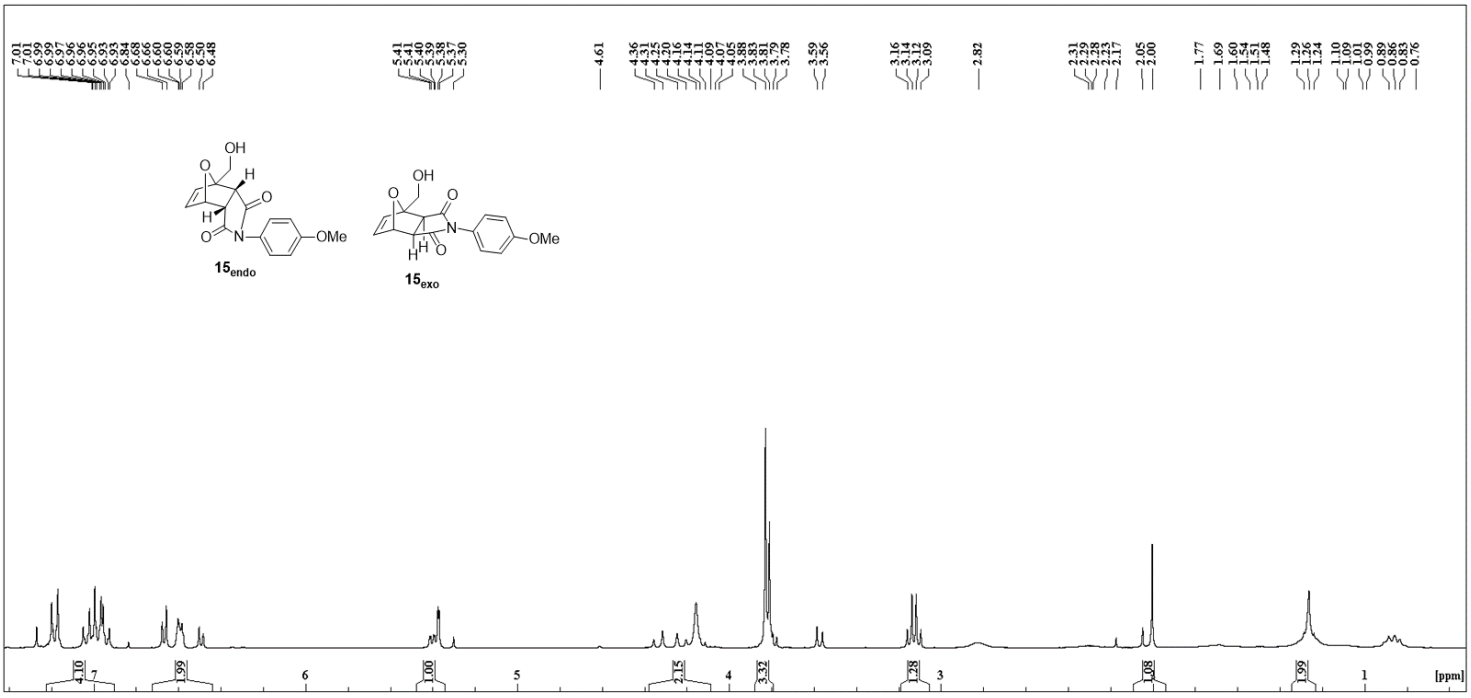


Figure S17. ^{1}H NMR of **15$_{endo}$** and **15$_{exo}$** mixture.

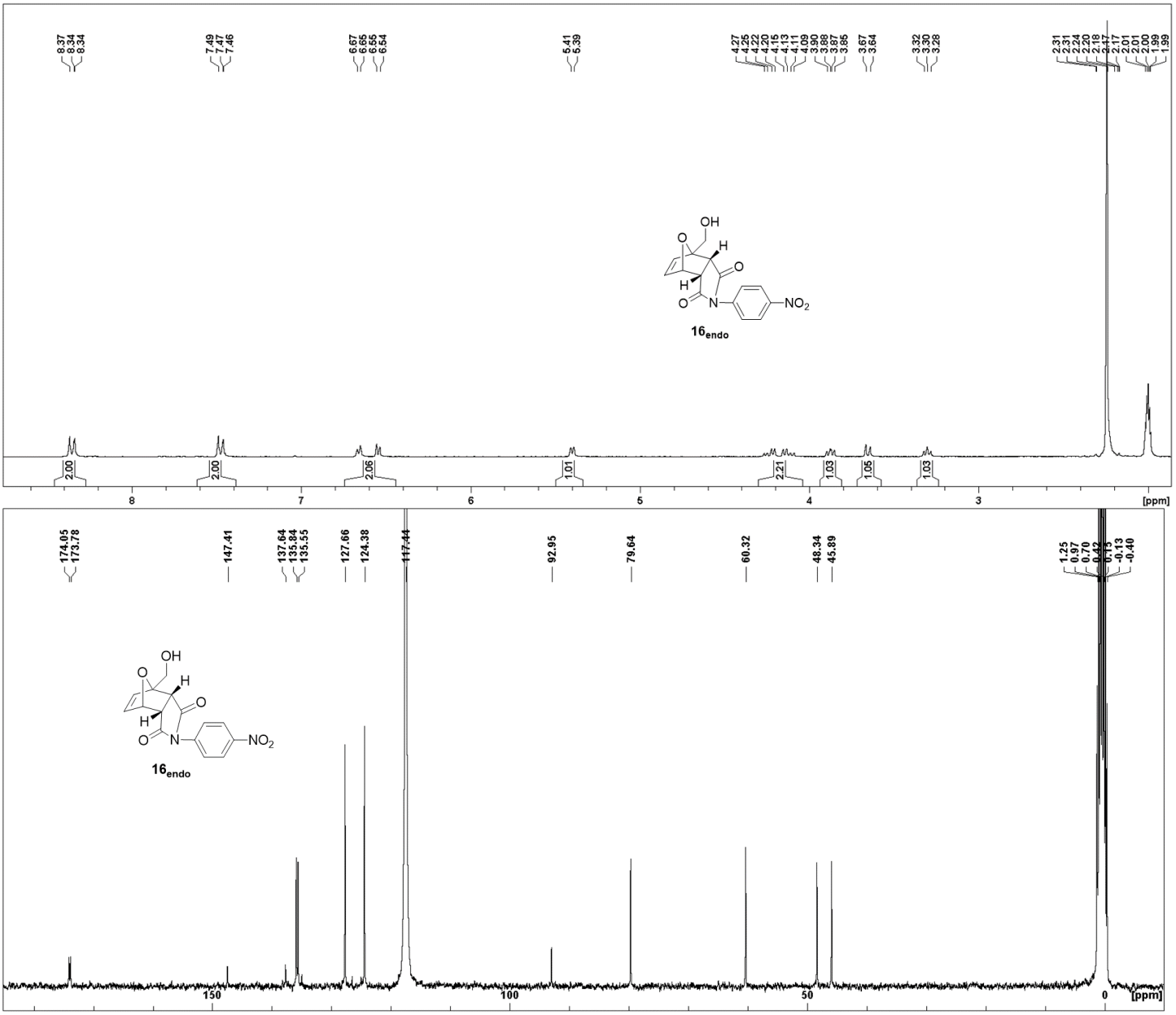


Figure S18. ^{1}H and ^{13}C NMR of **16$_{endo}$**.

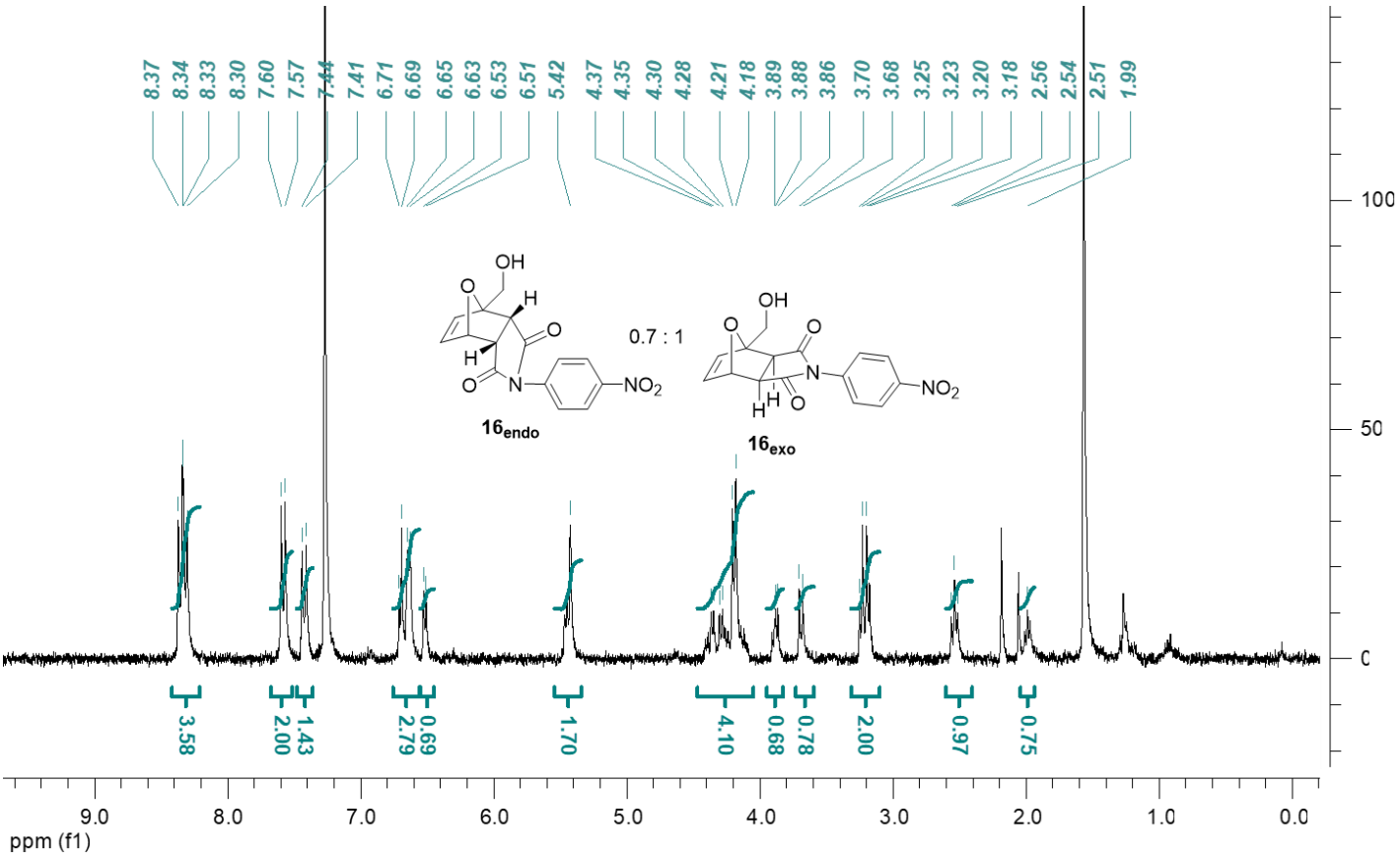


Figure S19. ^{1}H NMR of **16$_{endo}$** and **16$_{exo}$** mixture.

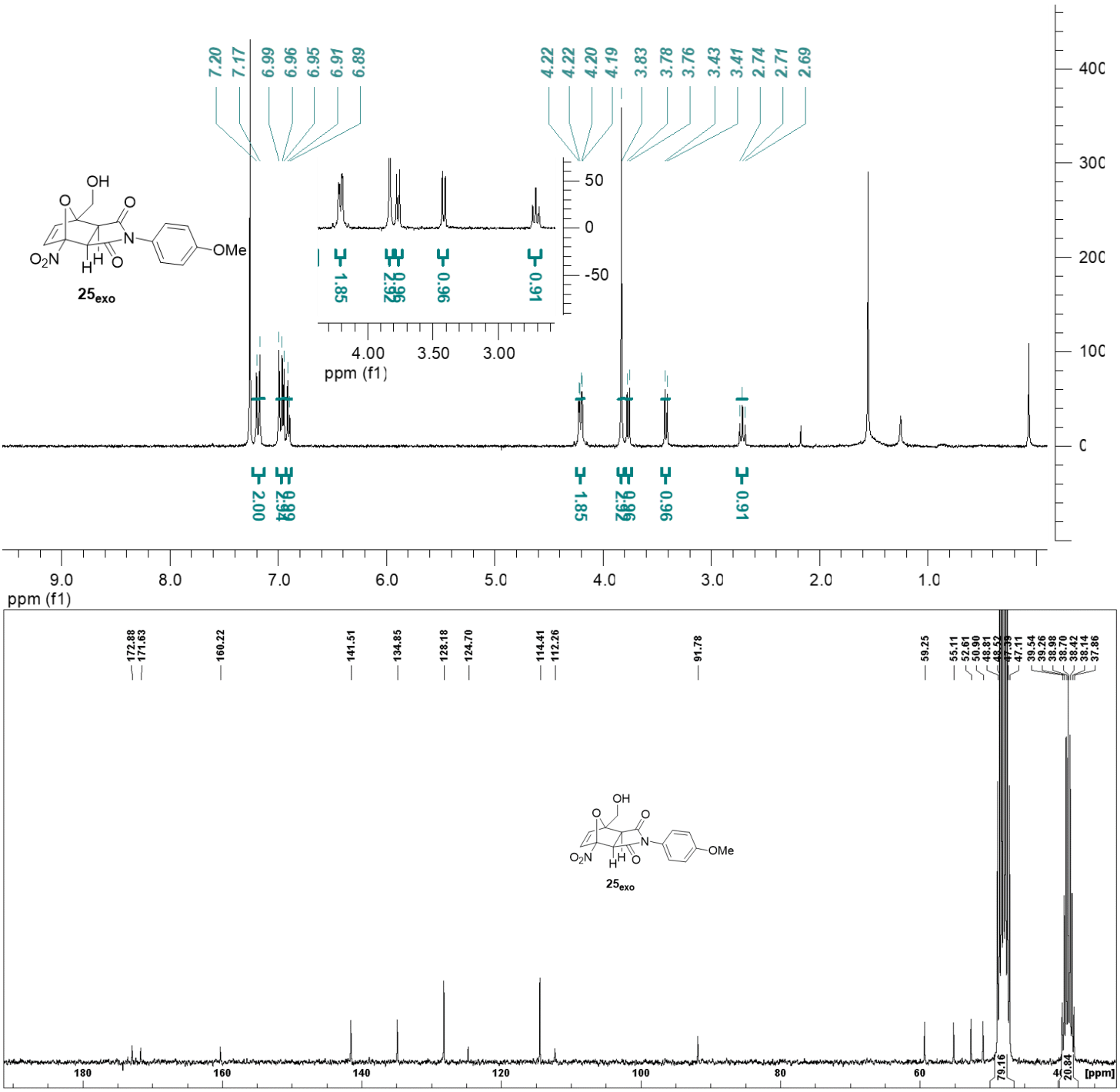


Figure S20. ^{1}H and ^{13}C NMR of **25_{exo}**.

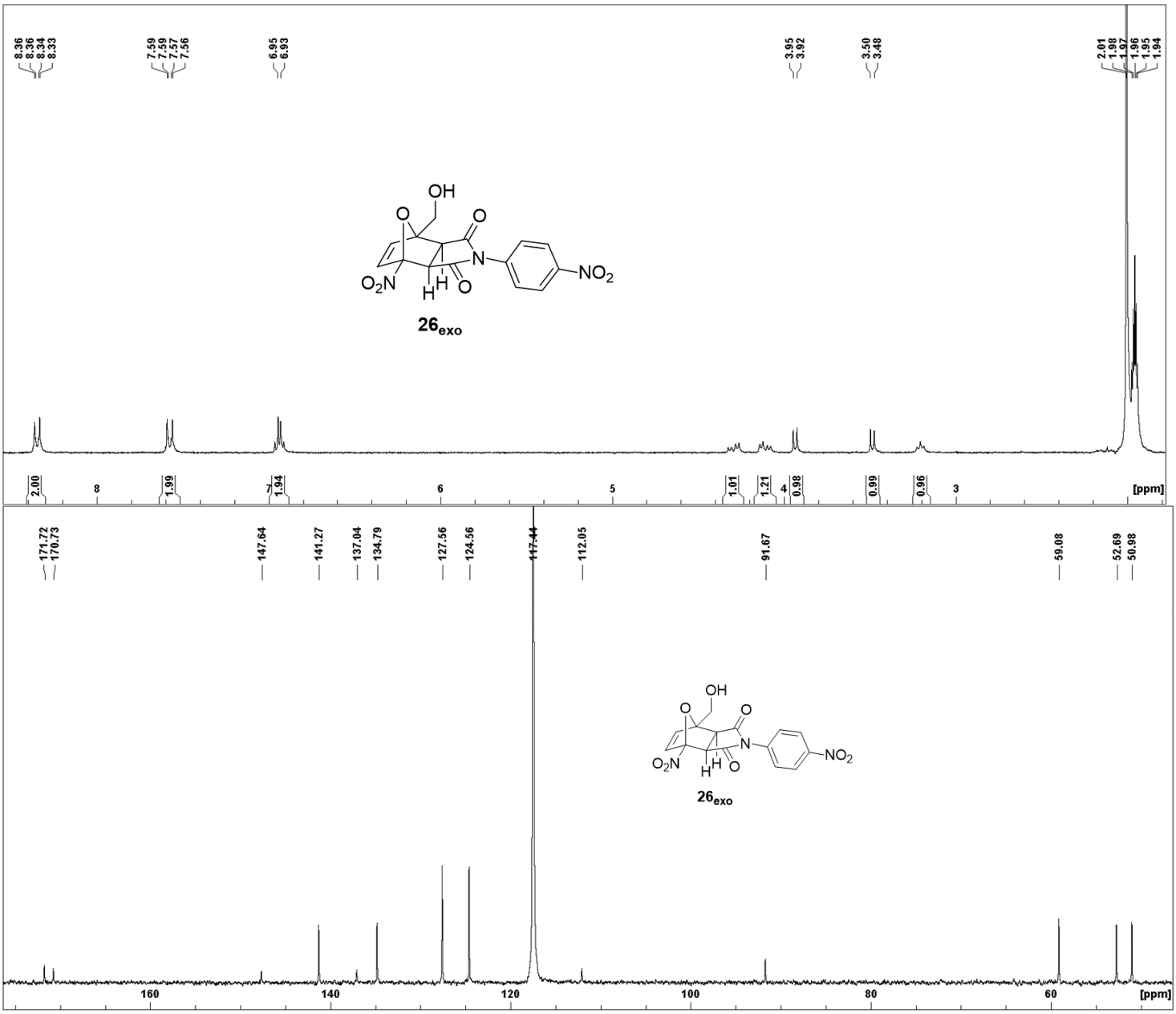


Figure S21. ^{1}H and ^{13}C NMR of **26_{exo}**.

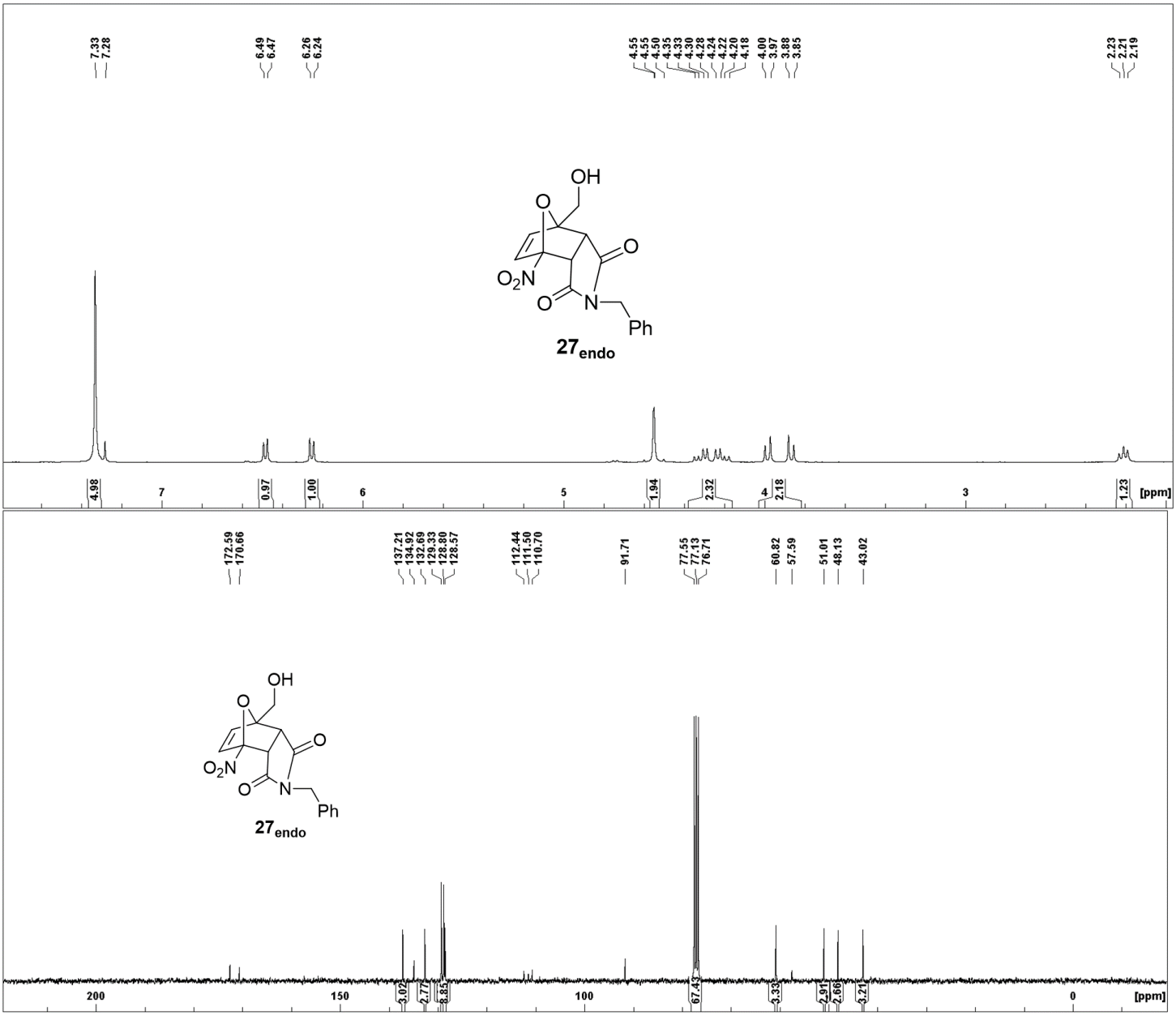


Figure S22. ^{1}H and ^{13}C NMR of **27**$_{endo}$.

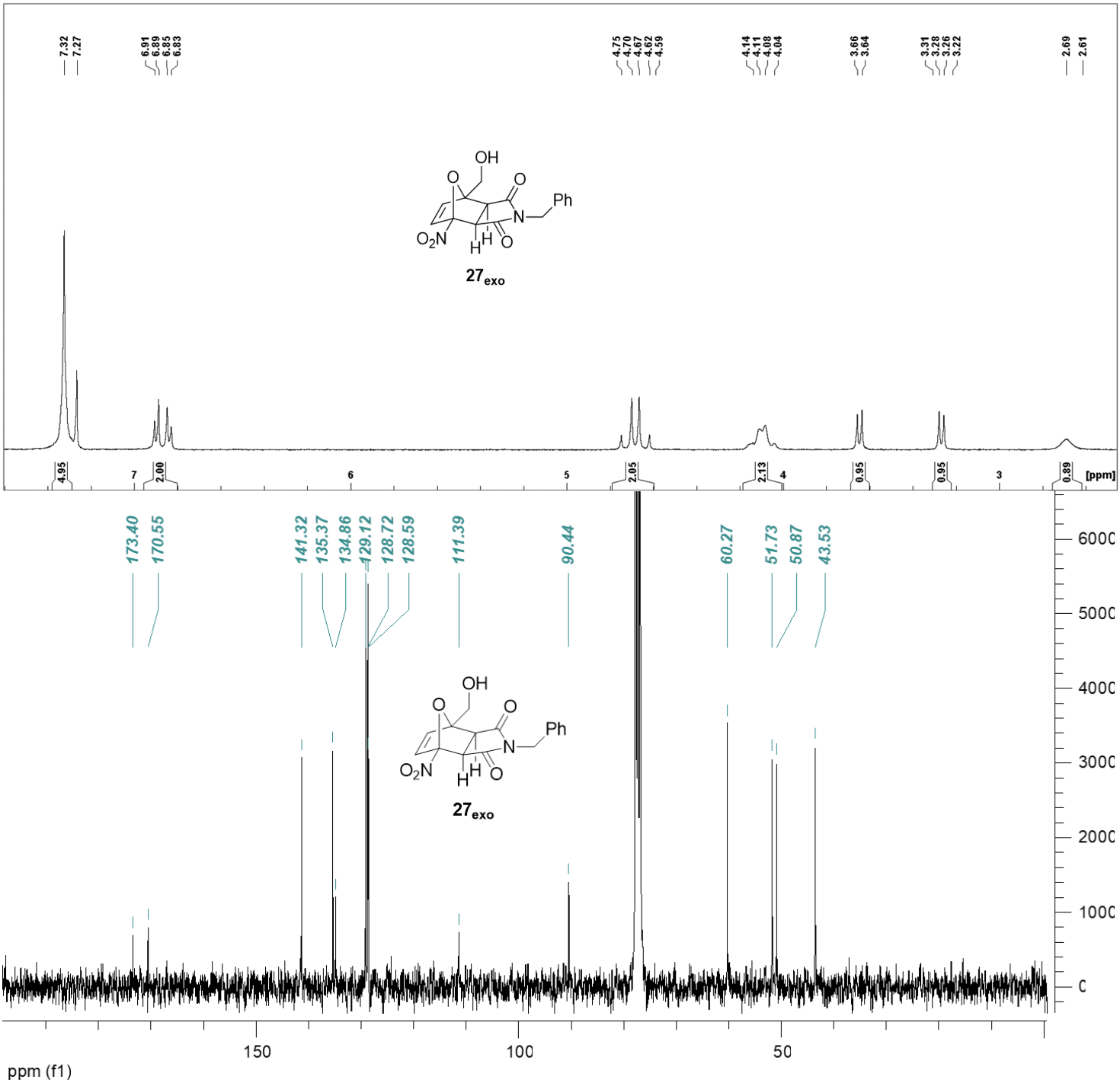


Figure S23. ^{1}H and ^{13}C NMR of **27_{exo}**.

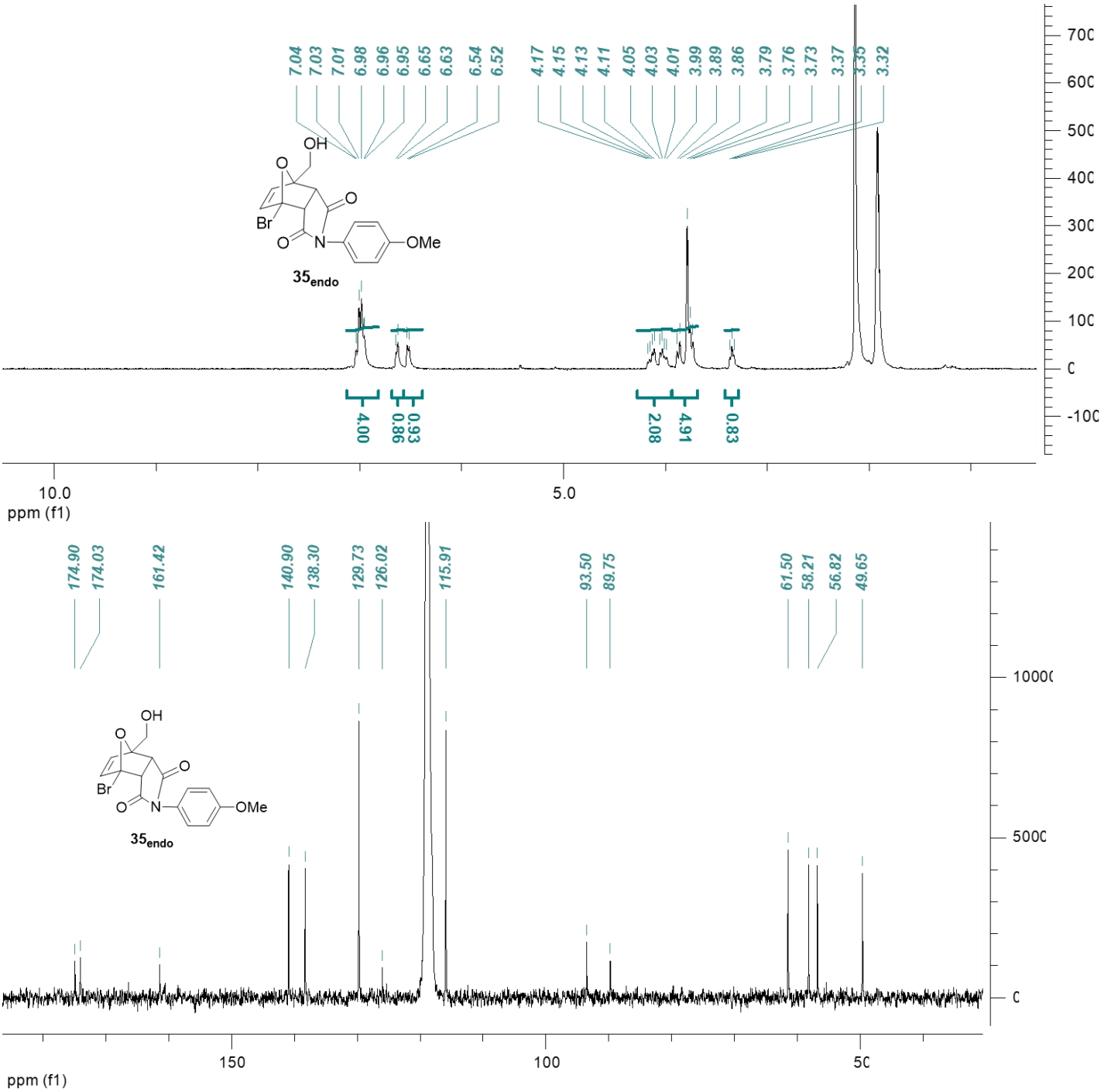


Figure S24. ^{1}H and ^{13}C NMR of **35$_{endo}$**.

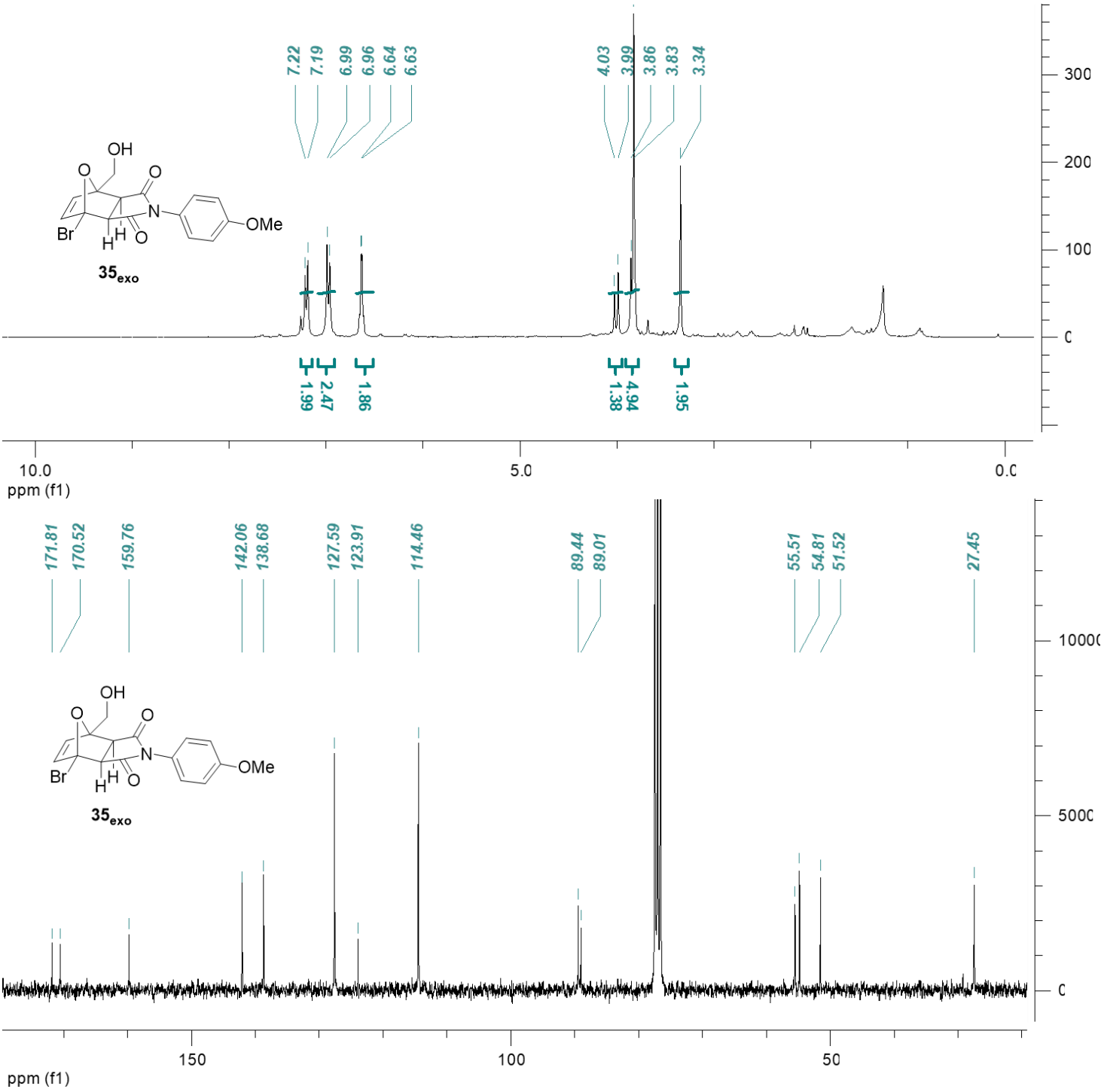


Figure S25. ^{1}H NMR of **35$_{exo}$**.

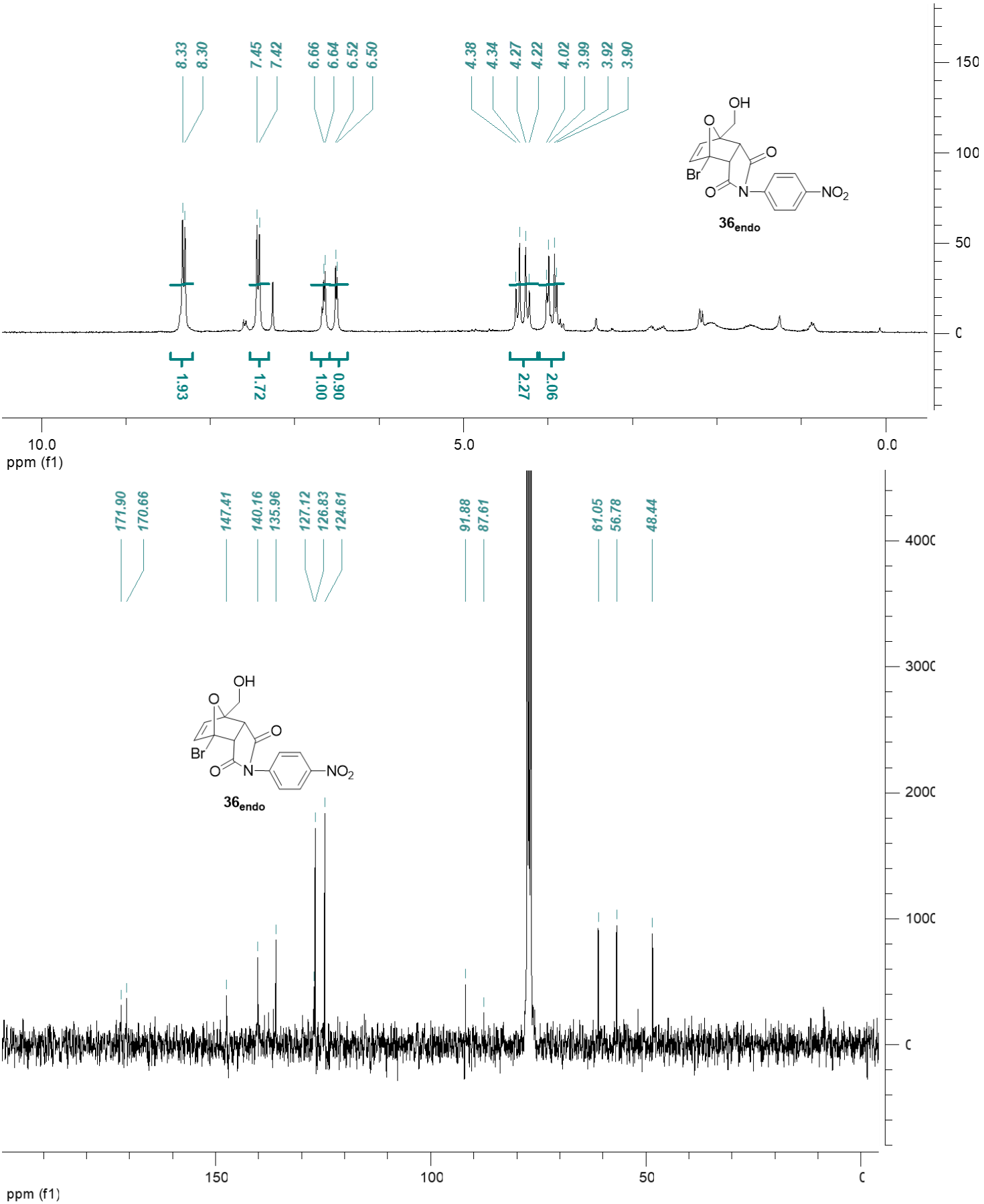


Figure S26. ^{1}H and ^{13}C NMR of **36_{endo}**.

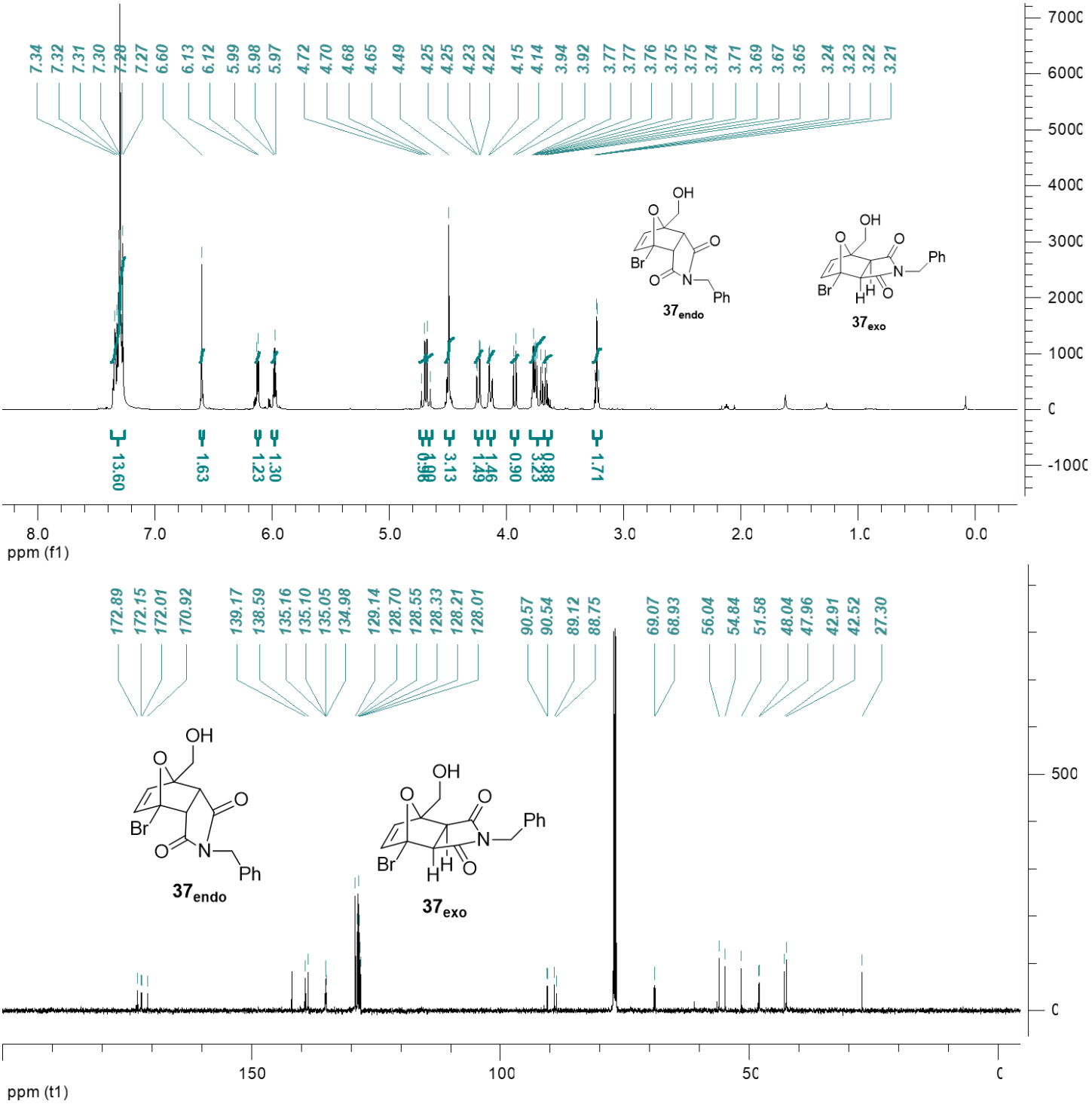


Figure S27. ^{1}H NMR of **37$_{endo}$** and **37$_{exo}$** mixture.

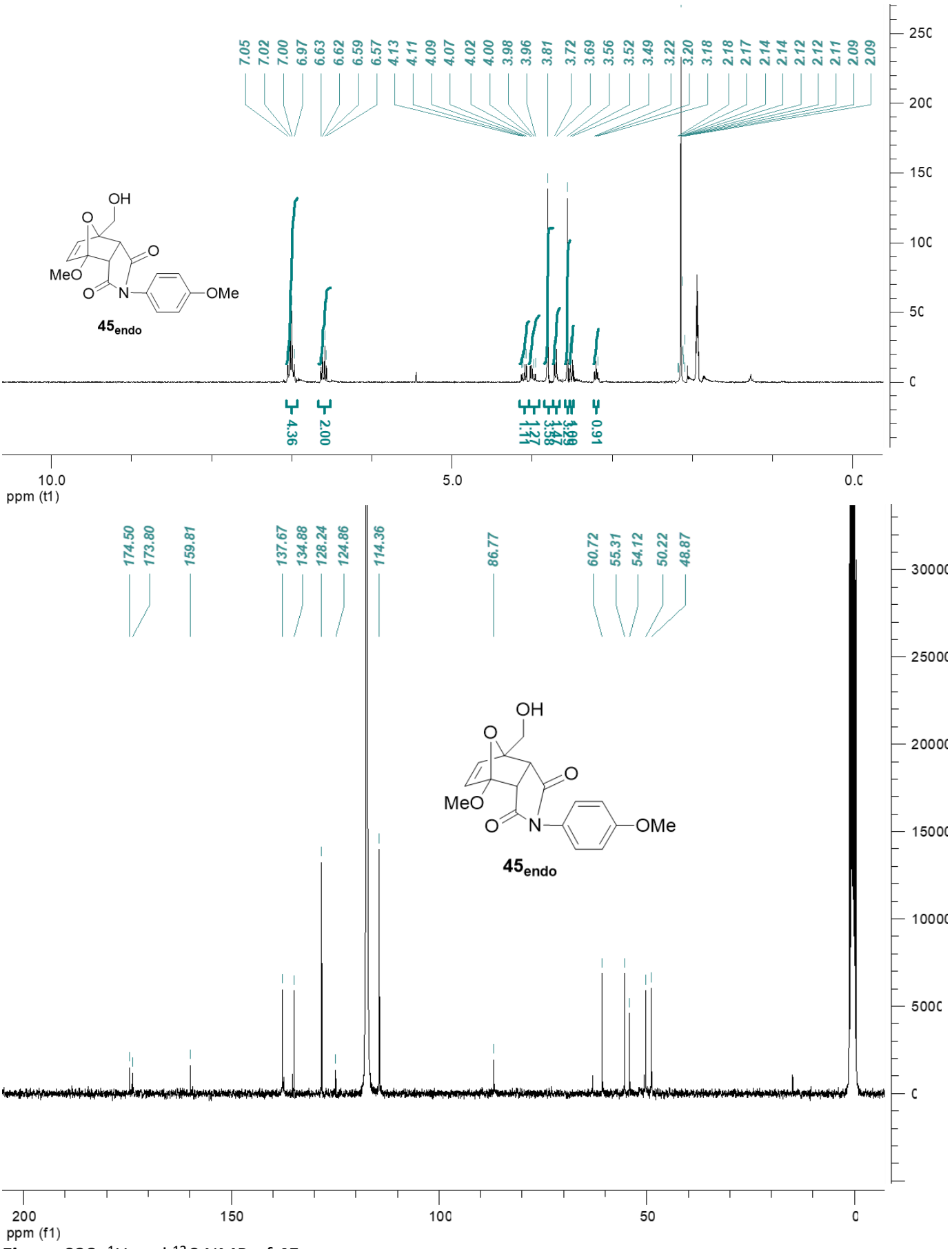


Figure S28. ^{1}H and ^{13}C NMR of **45**$_{endo}$

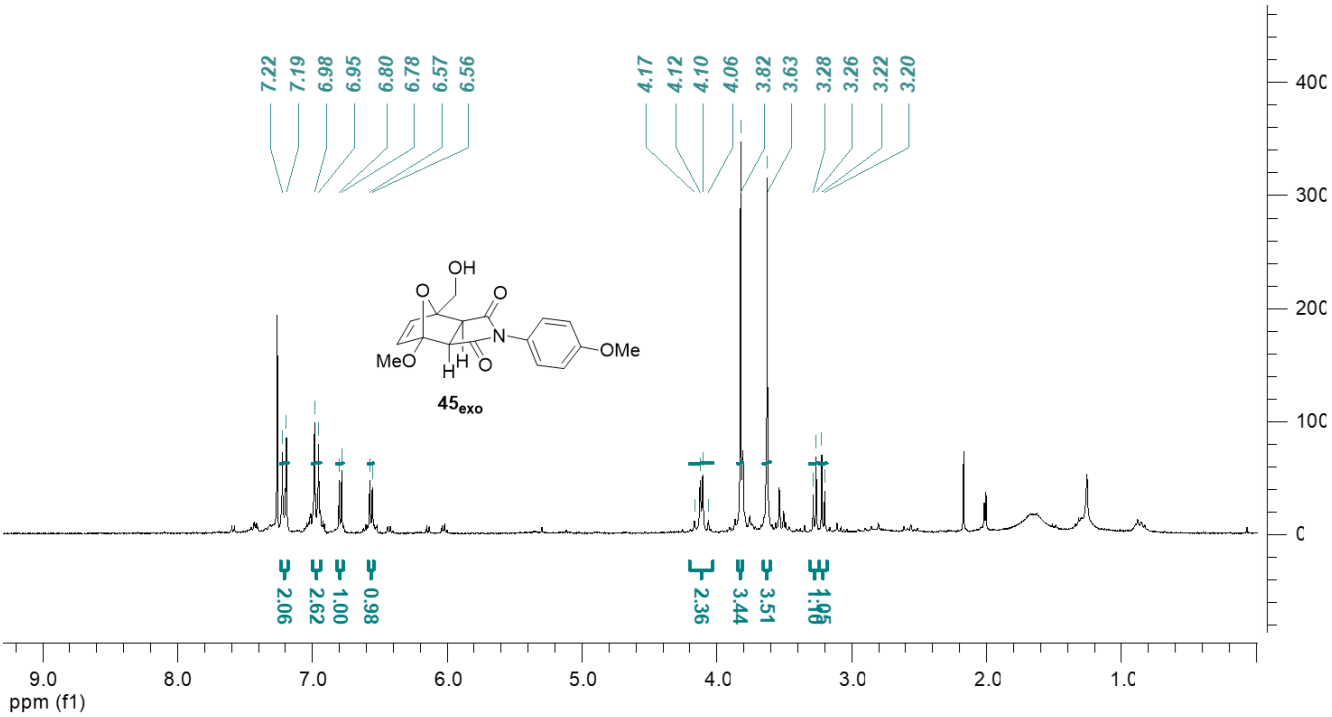


Figure S29. ^{1}H NMR of **45$_{exo}$**.

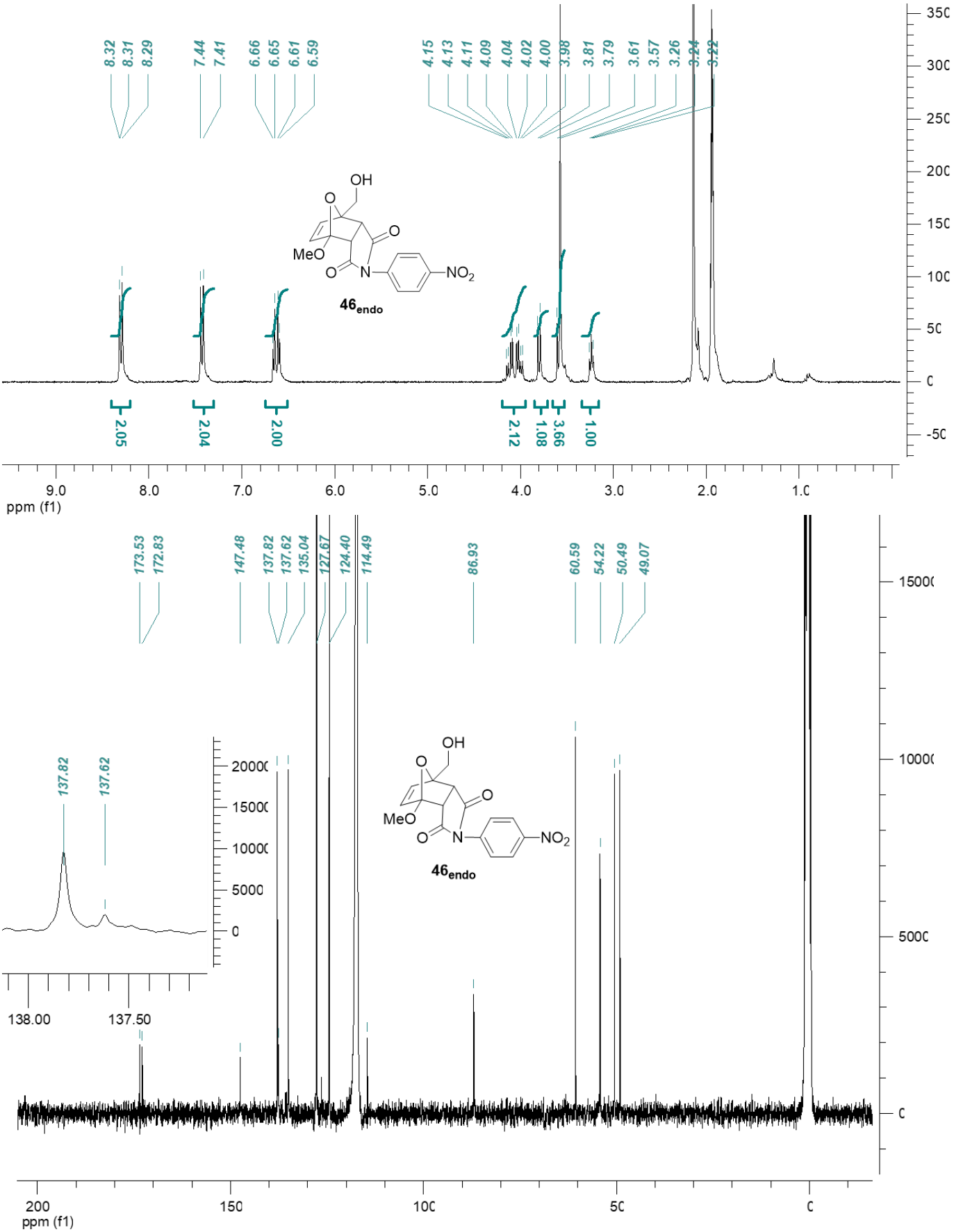


Figure S30. ^{1}H and ^{13}C NMR of **46$_{endo}$**

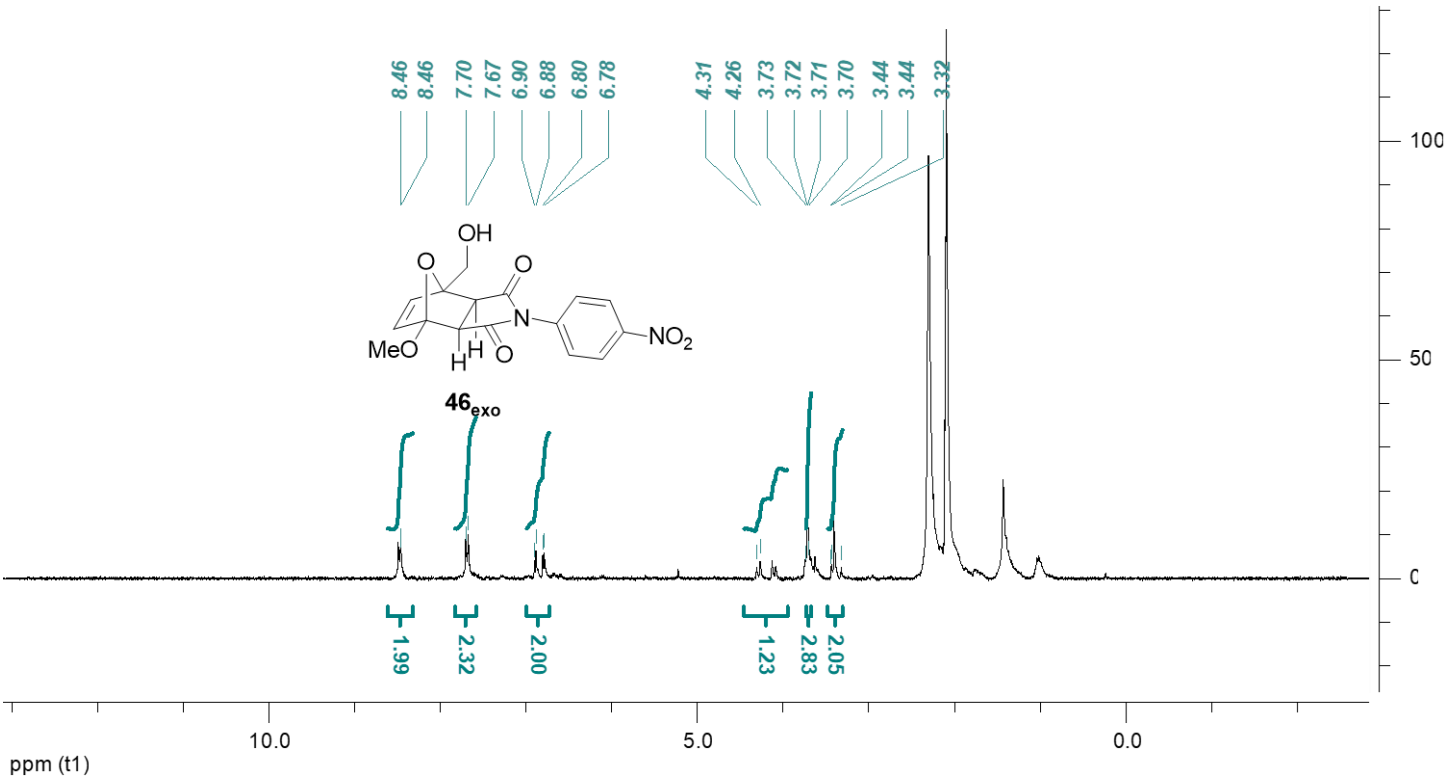


Figure S31. ^{1}H NMR of **46$_{exo}$**.

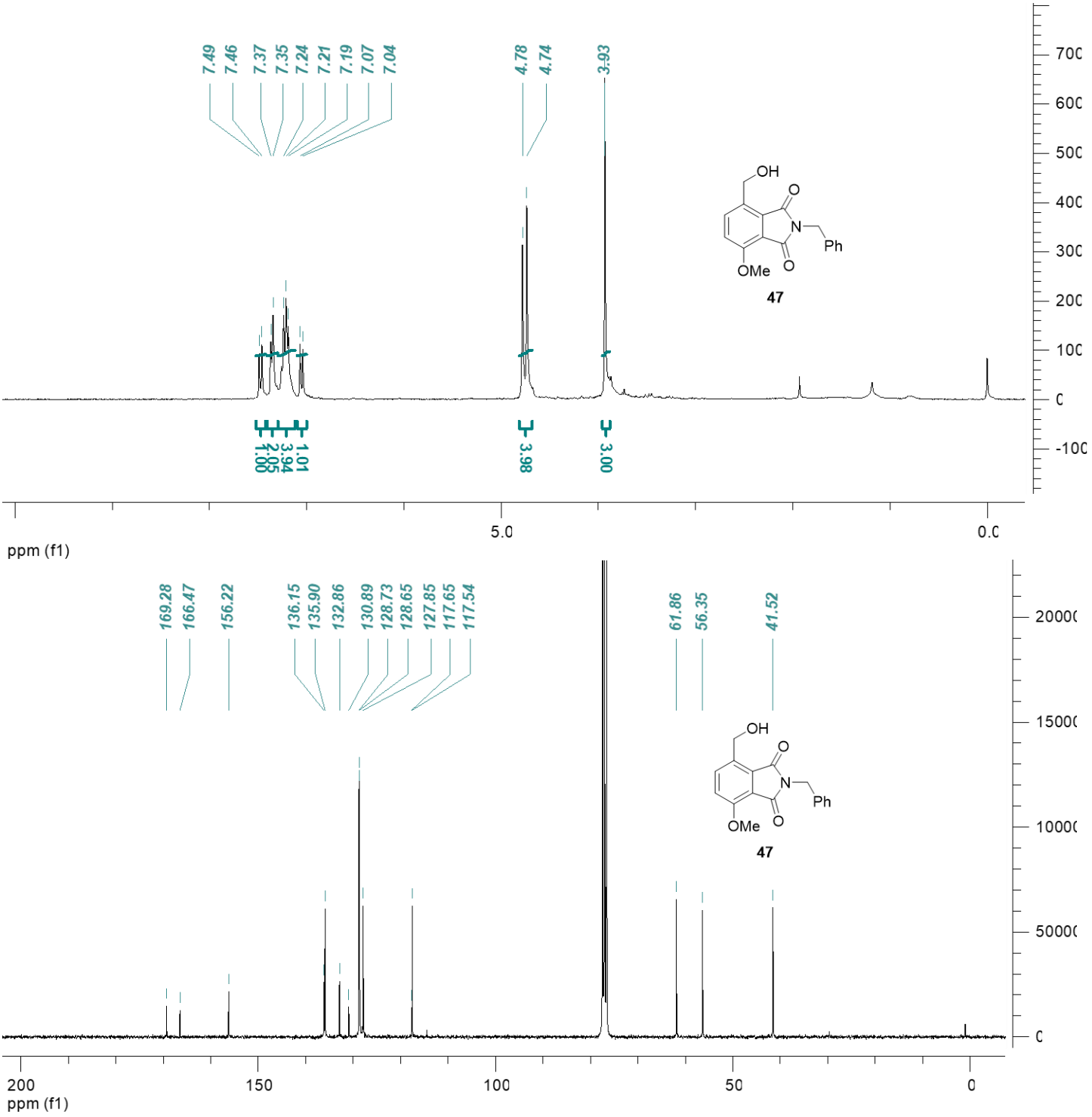


Figure S32. ^{1}H and ^{13}C NMR of **47**

5. Coordinates of the reported computational structures.

DA reaction of α-furfuryl alcohols **1** and N-(p-methoxyphenyl)-maleimide **5**

Pre-complex of Endo-TS15

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geom=connectivity temperature=308
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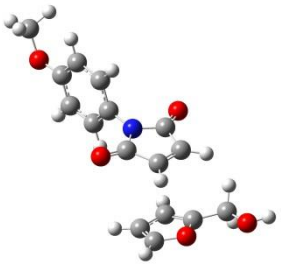
Endo-TS15



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 H                  1.42094600    1.88282600    2.10348400
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 C                  0.47332300    1.42906900   -0.88833800
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H	-3.58119300	-0.07971200	2.48733800
H	-4.55142800	-0.31802200	-1.69611100
O	-5.51251900	-0.34333200	0.86458800
C	-6.54438000	-0.48971800	-0.11551600
H	-7.47292700	-0.57670600	0.44464800
H	-6.59311700	0.38515400	-0.76985400
H	-6.39336300	-1.39208300	-0.71449700
H	3.29293000	2.75000100	0.30583100

Product of Endo-TS15

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C	2.94684500	1.72983700	0.10825200
H	2.19733100	-0.49275800	2.49260300
H	1.87196300	2.14736900	2.12090000
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C	1.95618400	1.14387500	-0.97307600
C	0.76159600	-0.89490900	-0.41821500
C	0.47958800	1.40402300	-0.75746500
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H	2.24776600	1.48785900	-1.96517300
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O	0.45020900	-2.03809300	-0.16487200
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C	-3.80518100	-0.25289100	-0.94433000
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H	-3.71478600	0.03806000	2.44061000
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H	-6.57014200	0.35541500	-0.97030700
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Pre-complex of Exo-TS15

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C	4.66250400	2.17033100	-1.18980500
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H	3.39802700	3.80206200	-0.49312600
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C	-1.08400800	-4.10873100	-0.44759600
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H	-2.78744800	2.19874500	-1.79317300
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H	-4.52279800	3.69638000	-1.26896000
H	-4.32631700	5.00542000	-0.07648900
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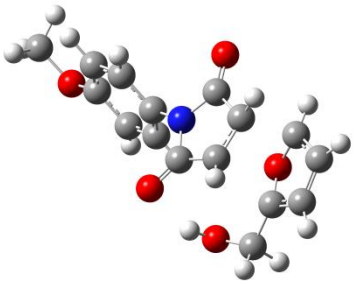
Exo-TS15



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.284985 (Hartree/Particle)
Thermal correction to Energy= 0.304971
Thermal correction to Enthalpy= 0.305946
Thermal correction to Gibbs Free Energy= 0.234668
Sum of electronic and zero-point Energies= -1049.555323
Sum of electronic and thermal Energies= -1049.535337
Sum of electronic and thermal Enthalpies= -1049.534362
Sum of electronic and thermal Free Energies= -1049.605640

0 1

C	-4.48235700	0.21644400	-0.15976600
C	-4.35166300	-1.02013200	-0.73704400
C	-3.24973400	0.88944400	-0.35645600
C	-2.98998300	-1.11113600	-1.17294500
H	-5.31709600	0.60496200	0.40340700
H	-5.05149200	-1.84156800	-0.71554800
C	-2.17189600	-0.52506300	1.33069000
C	-2.10881300	-1.64180200	0.45806700
H	-2.88674200	-0.36631800	2.12172700
H	-2.60863300	-2.57999400	0.66130600
C	-0.66733600	-1.75295700	0.01538900
C	-0.85561600	0.09039200	1.39480500
O	-0.48208400	1.06866700	2.03414200
O	-0.17299600	-2.61224800	-0.68445900
O	-2.50038700	0.19010000	-1.23824800
N	0.00527100	-0.65347600	0.54833000
C	-2.97796600	2.35723400	-0.17459600

H	-3.39538200	2.88533000	-1.03887700
H	-3.53126900	2.69186100	0.70909200
O	-1.60939800	2.71386000	-0.11242800
H	-1.24399100	2.40854500	0.73164600
C	1.36164000	-0.30692100	0.25674400
C	2.40255400	-1.09998700	0.72792000
C	1.64582200	0.82881600	-0.50773200
C	3.72846300	-0.77687100	0.43700000
H	2.18380400	-1.97661700	1.32562600
C	2.96081800	1.16449200	-0.79140000
H	0.83496100	1.44579500	-0.87624400
C	4.01149200	0.36162500	-0.32439500
H	4.51938400	-1.41175800	0.81139100
H	3.19411500	2.04333700	-1.38041400
O	5.26616600	0.76950900	-0.66185300
C	6.38240200	-0.01081400	-0.22473800
H	6.33731700	-1.02497900	-0.63157800
H	7.26511900	0.49593200	-0.60899400
H	6.43164300	-0.05220200	0.86698400
H	-2.60599700	-1.76368200	-1.94433900

Product of Exo-TS15

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.288747 (Hartree/Particle)
Thermal correction to Energy= 0.308031
Thermal correction to Enthalpy= 0.309006
Thermal correction to Gibbs Free Energy= 0.239033
Sum of electronic and zero-point Energies= -1049.591434
Sum of electronic and thermal Energies= -1049.572150
Sum of electronic and thermal Enthalpies= -1049.571175
Sum of electronic and thermal Free Energies= -1049.641148

0 1

C	-4.54608500	-0.07887600	0.30617900
C	-4.43834800	-1.31220100	-0.18531900
C	-3.21893300	0.62092200	-0.00265100
C	-3.03807700	-1.39408100	-0.77066700
H	-5.34966000	0.35585700	0.88455600
H	-5.13115500	-2.13834300	-0.10883600
C	-2.18021700	-0.01888600	1.01353300
C	-2.06792400	-1.45950500	0.46088500
H	-2.52322100	0.06160200	2.04440800
H	-2.33808100	-2.25093100	1.15893900
C	-0.61473900	-1.62258100	0.06082100
C	-0.76674200	0.53295900	0.92443500
O	-0.39095800	1.63589200	1.27549800
O	-0.09872000	-2.59385100	-0.44230300
O	-2.81787000	-0.04361500	-1.22112400
N	0.06476900	-0.43665800	0.37520500
C	-3.32694700	2.13163500	-0.15249400
H	-4.11603000	2.33461300	-0.87943600
H	-3.64754300	2.54502200	0.81146000

```
 O                -2.16323900    2.78703600   -0.63391500
 H                -1.48907300    2.75574800    0.05964100
 C                 1.46559500   -0.23361600    0.12605000
 C                 2.39201200   -0.47848100    1.13220200
 C                 1.89114700    0.20850200   -1.12838500
 C                 3.75324100   -0.28280800    0.89902000
 H                 2.05679300   -0.82252900    2.10350700
 C                 3.24225800    0.40292800   -1.36943400
 H                 1.16494100    0.39917000   -1.90952100
 C                 4.18236300    0.15961800   -0.35711200
 H                 4.45743900   -0.47751000    1.69574500
 H                 3.58969800    0.74494400   -2.33671600
 O                 5.48182000    0.38174600   -0.69041200
 C                 6.49391300    0.15782500    0.29628300
 H                 6.50534200   -0.88709500    0.61820000
 H                 7.43692700    0.39889900   -0.18948500
 H                 6.35102400    0.81106900    1.16146100
 H                -2.84414700   -2.11169000   -1.56236400
```

DA reaction of α-furfuryl alcohols **1** and N-(p-nitro)-maleimide **6**

Pre-complex of Endo-TS16

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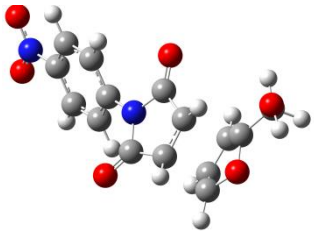
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.253230 (Hartree/Particle)
 Thermal correction to Energy=                    0.275744
 Thermal correction to Enthalpy=                  0.276719
 Thermal correction to Gibbs Free Energy=         0.192015
 Sum of electronic and zero-point Energies=          -1139.630824
 Sum of electronic and thermal Energies=             -1139.608311
 Sum of electronic and thermal Enthalpies=           -1139.607336
 Sum of electronic and thermal Free Energies=        -1139.692039

0 1
 C                -4.68554500    1.92325600    0.42845000
 C                -5.43119700    2.05963100    1.64723400
 C                -5.30194400    0.95315800   -0.30227700
 C                -6.44599000    1.15913500    1.57300100
 H                -3.80578200    2.47477200    0.13479700
 H                -5.23542300    2.73643900    2.46424600
 C                -1.39006500   -1.54982600   -0.40457100
 C                -0.91128300   -2.58427400    0.28704600
 C                -0.28407100   -0.57044000   -0.63088400
 C                 0.53963800   -2.36442600    0.56212500
 H                -2.39499200   -1.37226100   -0.76856300
 H                -1.42261100   -3.47369100    0.62431200
 O                 1.30779500   -3.08912000    1.14923400
 O                -0.33468200    0.49271600   -1.20288600
 O                -6.38853700    0.47762100    0.39101000
 C                -5.02484200    0.32801100   -1.62293300
 H                -5.93284900    0.31086300   -2.23559100
 H                -4.27292200    0.92173400   -2.14223500
```

O	-4.48187500	-1.00362300	-1.52450500
H	-5.16940900	-1.58969700	-1.18669800
N	0.86732300	-1.12000800	-0.02209100
C	2.15157200	-0.52035500	-0.00641900
C	2.87763000	-0.46341000	1.18847200
C	2.68430600	0.00947500	-1.18696500
C	4.13732900	0.11779800	1.20465600
H	2.45771800	-0.86665500	2.09918100
C	3.93780200	0.60380900	-1.17379000
H	2.12430400	-0.04770800	-2.10970000
C	4.64920400	0.64749200	0.02272600
H	4.71104700	0.17253300	2.11869000
H	4.36537100	1.01625800	-2.07642000
N	5.97897100	1.27023600	0.03839300
O	6.40399400	1.75665400	-1.00637600
O	6.60454000	1.27573700	1.09535400
H	-7.25364200	0.89171300	2.23400100

Endo-TS16



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.254304 (Hartree/Particle)
Thermal correction to Energy= 0.274574
Thermal correction to Enthalpy= 0.275549
Thermal correction to Gibbs Free Energy= 0.202611
Sum of electronic and zero-point Energies= -1139.593993
Sum of electronic and thermal Energies= -1139.573723
Sum of electronic and thermal Enthalpies= -1139.572748
Sum of electronic and thermal Free Energies= -1139.645687

0 1

C	2.45100200	-0.29182300	-1.70597500
C	2.25233500	-1.59186200	-1.32014900
C	3.48438200	0.22406200	-0.86875500
C	3.14207800	-1.81998800	-0.22825300
H	1.88231900	0.28614400	-2.41849200
H	1.49085400	-2.27755100	-1.65831600
C	2.34001600	0.48682300	0.96162400
C	2.18657400	-0.87385100	1.32000500
C	1.01541100	1.02560400	0.60748800
C	0.73988800	-1.20277300	1.22982300
H	3.08632800	1.15527200	1.36414700
H	2.75774400	-1.35698000	2.10077900
O	0.17244500	-2.22460400	1.55227400
O	0.70743200	2.15699400	0.29272500

O	4.11283500	-0.84096800	-0.27410900
C	4.32343000	1.44974200	-1.09718900
H	5.00310800	1.25765000	-1.93703500
H	3.66678500	2.27213600	-1.38268800
O	5.04911200	1.87011300	0.05010100
H	5.74643600	1.22866700	0.22860100
N	0.09599000	-0.06009300	0.69396400
C	-1.28722600	0.01532700	0.40042400
C	-1.90751600	-1.03008700	-0.29606600
C	-2.03432000	1.12581900	0.81425400
C	-3.26449700	-0.97106200	-0.57496100
H	-1.33084700	-1.88442400	-0.62024000
C	-3.38987000	1.19571300	0.52729200
H	-1.55755300	1.92649800	1.35988800
C	-3.98951800	0.14467400	-0.16216200
H	-3.75485700	-1.76987000	-1.11273700
H	-3.97894000	2.04475800	0.84338600
N	-5.42419100	0.21193300	-0.45798800
O	-6.04063000	1.22018000	-0.12102900
O	-5.94536800	-0.74336600	-1.02905900
H	3.46640500	-2.76988800	0.16925200

Product of Endo-TS16

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---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.257953 (Hartree/Particle)
 Thermal correction to Energy=                    0.277576
 Thermal correction to Enthalpy=                  0.278551
 Thermal correction to Gibbs Free Energy=         0.206551
 Sum of electronic and zero-point Energies=          -1139.626671
 Sum of electronic and thermal Energies=             -1139.607048
 Sum of electronic and thermal Enthalpies=           -1139.606072
 Sum of electronic and thermal Free Energies=        -1139.678072
0 1
```

C	2.65029600	0.42078200	1.67547100
C	2.50256400	1.67717000	1.25134700
C	3.39631900	-0.30993100	0.56325000
C	3.15134900	1.72881400	-0.12249500
H	2.25818200	-0.04244000	2.57029000
H	1.96247300	2.48863600	1.71856100
C	2.38751000	-0.49471800	-0.64648600
C	2.22382000	0.95202000	-1.13989300
C	0.99476900	-0.96234200	-0.29125200
C	0.74146600	1.24383900	-1.06123200
H	2.82843200	-1.16934800	-1.37980800
H	2.57470600	1.11668700	-2.15804700
O	0.17124900	2.26492400	-1.36836000
O	0.66641700	-2.03669900	0.15612300
O	4.20621100	0.75785300	0.01424700
C	4.24135100	-1.50864600	0.93964500
H	4.94220400	-1.21155800	1.72767500
H	3.59405400	-2.29273000	1.33615300
O	4.93112100	-2.07026900	-0.17227000

H	5.56986100	-1.42144000	-0.49085800
N	0.09960000	0.09203400	-0.56527800
C	-1.30619100	0.01100100	-0.33395400
C	-1.92452100	0.94957800	0.49505500
C	-2.04545700	-1.00682600	-0.94036900
C	-3.29261500	0.87533400	0.71863900
H	-1.34029900	1.72851100	0.96553600
C	-3.41268900	-1.09250000	-0.71506600
H	-1.55716800	-1.72277000	-1.58734700
C	-4.01543100	-0.14731900	0.11051300
H	-3.79131000	1.58969800	1.35774700
H	-4.00434100	-1.87077400	-1.17518800
N	-5.46535500	-0.23170700	0.34783100
O	-6.08539100	-1.15006300	-0.17991400
O	-5.98513200	0.62018100	1.06235800
H	3.53244700	2.68027900	-0.47908200

Pre-complex of Exo-TS16

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

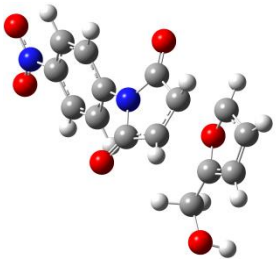
Zero-point correction= 0.253762 (Hartree/Particle)
Thermal correction to Energy= 0.275925
Thermal correction to Enthalpy= 0.276900
Thermal correction to Gibbs Free Energy= 0.193752
Sum of electronic and zero-point Energies= -1139.632955
Sum of electronic and thermal Energies= -1139.610793
Sum of electronic and thermal Enthalpies= -1139.609817
Sum of electronic and thermal Free Energies= -1139.692966

0 1

C	1.23003700	-3.39704500	-1.03775500
C	0.39863200	-3.35128300	-2.20649800
C	0.39527300	-3.40984900	0.03909600
C	-0.88316000	-3.33653900	-1.75648800
H	2.30823500	-3.41837300	-1.00245500
H	0.71494000	-3.33292200	-3.23757300
C	3.97604400	1.18485700	0.40549800
C	3.90253600	2.21732800	-0.43314400
H	4.84775500	0.70003100	0.81872300
H	4.69929400	2.79685800	-0.87476800
C	2.46466900	2.51342900	-0.71283600
C	2.59296100	0.72539600	0.73129100
O	2.27189800	-0.19831600	1.44728300
O	2.00042100	3.38016700	-1.41151400
O	-0.90738900	-3.37436900	-0.39243000
N	1.71582300	1.56667600	0.02825100
C	0.62908200	-3.44298800	1.50984400
H	0.00766000	-4.21315500	1.97244200
H	1.67778300	-3.70621700	1.68304300
O	0.28886100	-2.22105000	2.17735400
H	0.88834900	-1.52395300	1.86867300

H	-1.84250800	-3.30367500	-2.24533000
C	0.29734200	1.49286800	0.05886800
C	-0.41915300	1.47670700	-1.14148600
C	-0.36761100	1.44309500	1.28755400
C	-1.80517100	1.41571800	-1.11624500
H	0.10335100	1.50636100	-2.08748800
C	-1.75292300	1.36692800	1.31912700
H	0.19241600	1.47122000	2.21219500
C	-2.45210300	1.35728200	0.11532700
H	-2.37688300	1.40119900	-2.03302500
H	-2.28513700	1.32789300	2.25866700
N	-3.92014600	1.28519100	0.14536400
O	-4.52306400	1.31011400	-0.92388900
O	-4.47369400	1.20298300	1.23803100

Exo-TS16



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.254225 (Hartree/Particle)
Thermal correction to Energy= 0.274523
Thermal correction to Enthalpy= 0.275499
Thermal correction to Gibbs Free Energy= 0.202067
Sum of electronic and zero-point Energies= -1139.593364
Sum of electronic and thermal Energies= -1139.573066
Sum of electronic and thermal Enthalpies= -1139.572091
Sum of electronic and thermal Free Energies= -1139.645522

0 1

C	-4.41763800	1.09853600	0.75765900
C	-3.26904000	-0.80257700	0.52394800
C	-3.04005700	1.28225800	1.12548500
O	-2.50715700	-0.00351800	1.29527700
H	-5.14920500	1.88930500	0.69088700
C	-2.29586200	0.58125200	-1.34156200
C	-2.22430200	1.72123100	-0.49061200
N	-0.10984600	0.72349700	-0.58139800
C	-1.00939800	-0.05918500	-1.40247100
C	-0.76724700	1.85597300	-0.09759200
O	-0.64695600	-1.05643300	-2.00673000
O	-0.26414700	2.75253600	0.54581800
H	-3.05440700	0.37031500	-2.07723800
H	-2.71332600	2.65687000	-0.73410300

C	-4.52704300	-0.19043400	0.30358600
H	-5.36690300	-0.66041400	-0.18241800
C	1.24533400	0.40306500	-0.33989500
C	2.22864600	1.39730100	-0.43301100
C	1.60356000	-0.91136000	-0.01136900
C	3.55816800	1.08400800	-0.19274400
H	1.95290900	2.40801400	-0.69627300
C	2.93249900	-1.23239400	0.21963800
H	0.84461100	-1.67604300	0.06684600
C	3.89518400	-0.22903400	0.12872700
H	4.32669500	1.84031600	-0.26471800
H	3.22171900	-2.24113900	0.47769400
C	-2.85889500	-2.24101000	0.39658800
H	-2.47166600	-2.57653000	1.36636300
H	-2.04933600	-2.33846100	-0.33118300
O	-3.91846300	-3.06313500	-0.06583800
H	-4.55061600	-3.19635100	0.65001900
N	5.30008700	-0.56445500	0.37615900
O	6.13412800	0.33601100	0.30849600
O	5.58195700	-1.73150900	0.63989900
H	-2.68051100	1.99343200	1.85716200

Product of Exo-TS16

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.258571 (Hartree/Particle)
Thermal correction to Energy= 0.277830
Thermal correction to Enthalpy= 0.278805
Thermal correction to Gibbs Free Energy= 0.208172
Sum of electronic and zero-point Energies= -1139.627966
Sum of electronic and thermal Energies= -1139.608707
Sum of electronic and thermal Enthalpies= -1139.607732
Sum of electronic and thermal Free Energies= -1139.678365

0 1

C	-4.76445900	0.01845800	0.17019800
C	-4.65841000	-1.28883500	-0.06156400
C	-3.41296200	0.63095600	-0.20922300
C	-3.23549100	-1.49823600	-0.55259700
H	-5.58501900	0.56752500	0.61099700
H	-5.36910100	-2.07674700	0.14399400
C	-2.43143400	0.19587500	0.96240100
C	-2.32174600	-1.32518400	0.71310700
H	-2.81765500	0.48294800	1.93982800
H	-2.63597800	-1.95971700	1.54071700
C	-0.85904300	-1.58404700	0.41934600
C	-1.00839200	0.70997300	0.83459400
O	-0.62783900	1.85398400	0.97960000
O	-0.34013600	-2.64079600	0.15178600
O	-2.96944500	-0.26687200	-1.25015300
N	-0.16719800	-0.36050000	0.51917500
C	-3.48644400	2.08264500	-0.66054300
H	-4.24219600	2.14414000	-1.44614400

H	-3.83725200	2.68376100	0.18683300
O	-2.29231600	2.61582800	-1.21358300
H	-1.65357700	2.73921200	-0.49802000
H	-3.01887000	-2.36114900	-1.17522100
C	1.23986700	-0.22817300	0.30953800
C	1.79789200	-0.65200200	-0.89794700
C	2.03635400	0.31934900	1.31691400
C	3.16615900	-0.53275900	-1.10139600
H	1.16868800	-1.06629500	-1.67375000
C	3.40379300	0.45083700	1.11648200
H	1.59246200	0.63572500	2.25094300
C	3.94739400	0.01957500	-0.09030800
H	3.62059800	-0.85308100	-2.02788400
H	4.04017100	0.87074400	1.88204000
N	5.39805000	0.15129700	-0.30366800
O	5.86835100	-0.27106700	-1.35547000
O	6.06679700	0.67726900	0.58070800

DA reaction of α-furfuryl alcohols **1** and *N*-benzyl-maleimide **7**

Pre-complex of Endo-TS17

---

opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

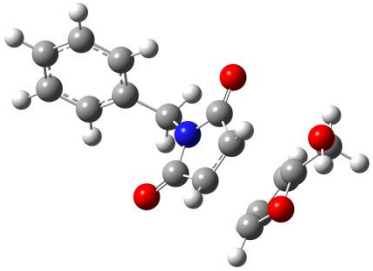
Zero-point correction= 0.279880 (Hartree/Particle)
Thermal correction to Energy= 0.301149
Thermal correction to Enthalpy= 0.302124
Thermal correction to Gibbs Free Energy= 0.219293
Sum of electronic and zero-point Energies= -974.364461
Sum of electronic and thermal Energies= -974.343193
Sum of electronic and thermal Enthalpies= -974.342217
Sum of electronic and thermal Free Energies= -974.425048

0 1

C	5.02205800	-0.45496100	-1.24244100
C	5.99393000	-1.44816700	-0.88491500
C	5.10463500	0.52995600	-0.30575800
C	6.59594000	-0.99880200	0.24686400
H	4.34999700	-0.47143800	-2.08626400
H	6.21184800	-2.36909000	-1.40240000
C	0.52229700	0.08871500	0.66501500
C	0.06223400	-0.91262300	1.41604600
C	-0.46308800	0.34132500	-0.43771600
C	-1.24428700	-1.37949000	0.84961500
H	1.43599600	0.66104200	0.76766600
H	0.50267300	-1.36755700	2.29106600
O	-1.94997100	-2.28597700	1.23819500
O	-0.39344800	1.16171500	-1.32853700
O	6.07203800	0.20716500	0.61461900
C	4.37459100	1.80759200	-0.09053300
H	5.08196700	2.62595500	0.08166400
H	3.79773600	2.03781800	-0.98565100
O	3.42352000	1.75255800	0.99074900

H	3.90844900	1.66034000	1.81910700
N	-1.50818500	-0.56707800	-0.25461600
C	-2.66460700	-0.70987800	-1.13553100
H	-2.79074400	-1.76952300	-1.36251100
H	-2.40116700	-0.19973900	-2.06477300
C	-3.95393400	-0.14291000	-0.56872400
C	-3.99513000	1.12947800	0.01175200
C	-5.13659300	-0.88122300	-0.66264200
C	-5.19593800	1.65080600	0.49002900
H	-3.08795200	1.71835000	0.09247500
C	-6.34118900	-0.35915000	-0.18982000
H	-5.11660600	-1.87255900	-1.10352500
C	-6.37370800	0.90844300	0.38915200
H	-5.21267100	2.63791300	0.93836000
H	-7.24955300	-0.94598300	-0.26770800
H	-7.30737500	1.31470000	0.76132400
H	7.37432300	-1.38903700	0.88092200

Endo-TS17



---

opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction=	0.281005 (Hartree/Particle)
Thermal correction to Energy=	0.299980
Thermal correction to Enthalpy=	0.300955
Thermal correction to Gibbs Free Energy=	0.230529
Sum of electronic and zero-point Energies=	-974.326817
Sum of electronic and thermal Energies=	-974.307842
Sum of electronic and thermal Enthalpies=	-974.306867
Sum of electronic and thermal Free Energies=	-974.377293

0 1

C	-2.65372300	-0.58894800	1.43513600
C	-2.32901300	-1.82534300	0.93707500
C	-3.24850400	0.13512400	0.36138500
C	-2.70344200	-1.80698300	-0.43723800
H	-2.41441200	-0.17843200	2.40437300
H	-1.77140100	-2.61167300	1.42220100
C	-1.44805800	0.59094300	-0.77330900
C	-1.16900100	-0.69915300	-1.27944200
C	-0.38207200	0.93702700	0.19304500
C	0.10190800	-1.15816200	-0.64695600
H	-1.94908200	1.37915400	-1.31512500

```
 H                -1.37622200   -1.01007000   -2.29404400
 O                 0.72783300   -2.18263400   -0.84993600
 O                -0.21726400    1.96945700    0.82003900
 O                -3.59409900   -0.76923300   -0.61282000
 C                -4.09649800    1.37216000    0.45043800
 H                -5.06394400    1.10495900    0.89441000
 H                -3.60787400    2.08054300    1.12010200
 O                -4.28322000    2.03254700   -0.79490400
 H                -4.84081800    1.48208200   -1.35677700
 N                 0.46896700   -0.17716900    0.27670500
 C                 1.61099700   -0.28335700    1.18404700
 H                 1.62344500   -1.29534700    1.59037400
 H                 1.41410100    0.40928300    2.00456400
 C                 2.94857700    0.03310800    0.53842300
 C                 3.18117600    1.27928700   -0.05663900
 C                 3.98004300   -0.90909600    0.55648900
 C                 4.41901700    1.57232400   -0.62546700
 H                 2.39236100    2.02342500   -0.07086100
 C                 5.22267800   -0.61596100   -0.00781800
 H                 3.81147200   -1.87984000    1.01096600
 C                 5.44452000    0.62508700   -0.60214700
 H                 4.58548400    2.54157200   -1.08236400
 H                 6.01247100   -1.35859800    0.01342400
 H                 6.40798100    0.85420600   -1.04342400
 H                -2.84396700   -2.65053700   -1.09591800
```

Product of Endo-TS17

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.284867 (Hartree/Particle)
 Thermal correction to Energy=                    0.303077
 Thermal correction to Enthalpy=                  0.304052
 Thermal correction to Gibbs Free Energy=         0.233191
 Sum of electronic and zero-point Energies=           -974.361977
 Sum of electronic and thermal Energies=              -974.343768
 Sum of electronic and thermal Enthalpies=            -974.342793
 Sum of electronic and thermal Free Energies=         -974.413653


0 1
 C                -2.80901100   -0.65369000    1.33566700
 C                -2.53110200   -1.85564100    0.82745100
 C                -2.98907200    0.27465200    0.13800700
 C                -2.53369100   -1.67712900   -0.68239300
 H                -2.81983000   -0.34325600    2.37133800
 H                -2.26287200   -2.76359400    1.34916700
 C                -1.56022900    0.51829000   -0.49929500
 C                -1.23993200   -0.86834600   -1.08665300
 C                -0.42784100    0.81263200    0.46150100
 C                 0.05840900   -1.28666800   -0.42618100
 H                -1.63257500    1.31212400   -1.24211700
 H                -1.12193300   -0.87395100   -2.16997900
```

```
 O                  0.66578000   -2.32625800   -0.57784300
 O                 -0.28457100    1.79821500    1.15588200
 O                 -3.52087100   -0.64058200   -0.85252400
 C                 -3.88309400    1.48546700    0.30489200
 H                 -4.85866400    1.15431400    0.67822300
 H                 -3.44403700    2.15665300    1.04505000
 O                 -4.02537200    2.23743200   -0.89621100
 H                 -4.47225400    1.68320500   -1.54702200
 N                  0.46414300   -0.25946700    0.42448700
 C                  1.66723000   -0.34188700    1.26293600
 H                  1.73228500   -1.36199800    1.64101200
 H                  1.49649900    0.32940100    2.10570600
 C                  2.94281000    0.02995500    0.53088900
 C                  3.12440700    1.32136400    0.02049100
 C                  3.96701200   -0.90800700    0.37838800
 C                  4.30543300    1.66318900   -0.63486600
 H                  2.34197300    2.06295800    0.13989400
 C                  5.15339500   -0.56570200   -0.27243800
 H                  3.83709500   -1.91196300    0.76822700
 C                  5.32427100    0.72002300   -0.78244800
 H                  4.43367300    2.66682600   -1.02464100
 H                  5.93937300   -1.30436900   -0.38278900
 H                  6.24415500    0.98743200   -1.29005900
 H                 -2.75559900   -2.53897400   -1.30351800
```

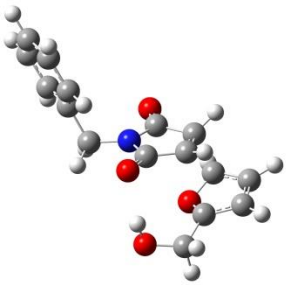
Pre-complex of Exo-TS17

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.280707 (Hartree/Particle)
 Thermal correction to Energy=                    0.301418
 Thermal correction to Enthalpy=                  0.302393
 Thermal correction to Gibbs Free Energy=         0.222527
 Sum of electronic and zero-point Energies=           -974.367616
 Sum of electronic and thermal Energies=              -974.346905
 Sum of electronic and thermal Enthalpies=            -974.345930
 Sum of electronic and thermal Free Energies=         -974.425796

0 1
 C                 -3.75137700    0.58601000    1.49610800
 C                 -4.58944000   -0.53401700    1.81702800
 C                 -4.09409100    0.98746800    0.23977000
 C                 -5.38052900   -0.73568800    0.73112700
 H                 -2.99359200    1.03543100    2.11897300
 H                 -4.59947700   -1.10657800    2.73109400
 C                 -0.80300400   -1.63467900    0.03635500
 C                 -0.01905100   -2.65036200    0.39620100
 H                 -1.85783200   -1.48567100    0.21340600
 H                 -0.27020800   -3.54939700    0.93903400
 C                  1.37304100   -2.37170000   -0.08786600
 C                  0.03125200   -0.63190800   -0.70163500
 O                 -0.32582600    0.42180500   -1.19672000
 O                  2.35951800   -3.06405100    0.02703300
 O                 -5.09706800    0.18183700   -0.23888000
```

```
 N                  1.32596400   -1.13010200   -0.73172300
 C                 -3.59709200    2.06851600   -0.65730500
 H                 -4.43747400    2.64508900   -1.05107400
 H                 -2.97417500    2.74478800   -0.06230100
 O                 -2.88685000    1.58671200   -1.80348800
 H                 -2.06324500    1.16262700   -1.50753100
 C                  2.47047000   -0.47778800   -1.37891700
 H                  2.06312600    0.13448900   -2.18424800
 H                 -6.15576000   -1.44624400    0.49759500
 C                  3.30433800    0.36438300   -0.43243500
 C                  2.84468700    1.61353600    0.00260600
 C                  4.54849500   -0.09164900    0.01222500
 C                  3.61281400    2.38689100    0.87086900
 H                  1.88513900    1.98323500   -0.34258200
 C                  5.32035700    0.68267400    0.87945900
 H                  4.91669700   -1.05595800   -0.32103700
 C                  4.85323600    1.92280400    1.31205700
 H                  3.24680500    3.35373300    1.19784400
 H                  6.28451900    0.31695900    1.21442500
 H                  5.45213800    2.52613800    1.98487000
 H                  3.07874800   -1.26531600   -1.82385700
```

Exo-TS17



```
---------------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=253
 ---------------------------------------------------------------------
Zero-point correction=                           0.281424 (Hartree/Particle)
 Thermal correction to Energy=                    0.294501
 Thermal correction to Enthalpy=                  0.295302
 Thermal correction to Gibbs Free Energy=         0.242425
 Sum of electronic and zero-point Energies=           -974.327259
 Sum of electronic and thermal Energies=              -974.314183
 Sum of electronic and thermal Enthalpies=            -974.313381
 Sum of electronic and thermal Free Energies=         -974.366258


0 1
 C                 -4.16706000   -0.38307100    0.71337500
 C                 -3.81303300   -1.69925100    0.56392200
 C                 -3.32674400    0.36445500   -0.15012000
 C                 -2.67857900   -1.70666000   -0.30975800
 H                 -4.88655000    0.04077300    1.39715500
 H                 -4.17394400   -2.55220400    1.11818100
 C                 -1.41544900    0.01815400    1.34364100
```

C	-1.24587400	-1.32998100	0.93698900
H	-1.88898400	0.36467600	2.24781500
H	-1.34219800	-2.17061900	1.61156700
C	-0.03199400	-1.34655400	0.03368400
C	-0.40287900	0.82902300	0.68072700
O	-0.20522700	2.04059000	0.74496900
O	0.49007700	-2.30804100	-0.49608500
O	-2.67382700	-0.48509600	-0.97528700
N	0.37823200	-0.03079700	-0.11666000
C	-3.50657000	1.79635400	-0.57258900
H	-4.31048800	1.82876500	-1.31610700
H	-3.84967200	2.36064600	0.30104500
O	-2.37673400	2.39238200	-1.18152400
H	-1.69212100	2.52603500	-0.50843300
C	1.43522100	0.40644000	-1.02805900
H	1.23445700	1.45678500	-1.24721200
H	-2.33548400	-2.53656000	-0.91115600
C	2.83750100	0.24249300	-0.46900400
C	3.21107000	0.86857400	0.72640900
C	3.78627300	-0.51560600	-1.15969300
C	4.50669500	0.73361300	1.22115300
H	2.48668600	1.46594000	1.26926700
C	5.08625700	-0.64828300	-0.66865200
H	3.50780900	-1.00835700	-2.08539600
C	5.44902900	-0.02520500	0.52410700
H	4.78281500	1.22399400	2.14804200
H	5.81064400	-1.24144500	-1.21557400
H	6.45729400	-0.12890100	0.90893600
H	1.33463000	-0.15959600	-1.95487900

Product of Exo-TS17

```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.285681 (Hartree/Particle)
 Thermal correction to Energy=                    0.303432
 Thermal correction to Enthalpy=                  0.304407
 Thermal correction to Gibbs Free Energy=         0.237574
 Sum of electronic and zero-point Energies=           -974.363724
 Sum of electronic and thermal Energies=              -974.345973
 Sum of electronic and thermal Enthalpies=            -974.344998
 Sum of electronic and thermal Free Energies=         -974.411831

0 1
```

C	-3.91431100	-0.41506200	1.16852600
C	-3.70241200	-1.70445000	0.91031300
C	-2.96712400	0.36552700	0.25172400
C	-2.60319900	-1.73175700	-0.13943600
H	-4.55119800	0.03349300	1.91845200
H	-4.12142300	-2.57381100	1.39710200
C	-1.52922600	0.16386900	0.89203100
C	-1.28565200	-1.33914100	0.61526700
H	-1.50996400	0.45597200	1.94164100
H	-1.11273000	-1.95529700	1.49691500

C	-0.05841100	-1.38225900	-0.27471800
C	-0.39160500	0.86700100	0.16771800
O	-0.18379700	2.06808200	0.12410800
O	0.45516300	-2.36106400	-0.77054400
O	-2.86290600	-0.52451300	-0.88194700
N	0.40566600	-0.07856300	-0.45122400
C	-3.46222800	1.75562300	-0.12083000
H	-4.47477700	1.65001500	-0.51564400
H	-3.52389700	2.34946600	0.79931600
O	-2.71249100	2.42951100	-1.12031400
H	-1.84943000	2.65970700	-0.74693900
C	1.58006000	0.25562700	-1.27392800
H	1.40620100	1.25791000	-1.66555600
H	-2.53096700	-2.59250600	-0.79766800
C	2.88611500	0.19505500	-0.50583600
C	3.22955600	1.21269500	0.39283200
C	3.77040000	-0.87143600	-0.69273000
C	4.43178200	1.15950500	1.09538800
H	2.55463300	2.04888700	0.53833000
C	4.97624300	-0.92410300	0.00758500
H	3.51673800	-1.66297200	-1.38943700
C	5.30835500	0.09006200	0.90467200
H	4.68739000	1.95497200	1.78641900
H	5.65389500	-1.75582600	-0.14907200
H	6.24517900	0.05055500	1.44892300
H	1.59288300	-0.44727100	-2.10612200

DA reaction of nitro-substituted α-furfuryl alcohols **2** and N-(p-methoxyphenyl)-maleimide **5**

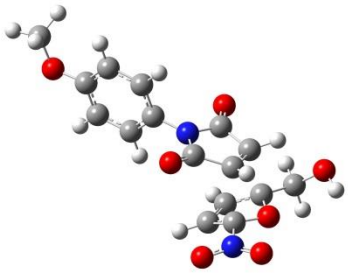
Pre-complex of Endo-TS25

```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.285662 (Hartree/Particle)
 Thermal correction to Energy=                    0.310981
 Thermal correction to Enthalpy=                  0.311957
 Thermal correction to Gibbs Free Energy=         0.219503
 Sum of electronic and zero-point Energies=          -1254.154344
 Sum of electronic and thermal Energies=             -1254.129025
 Sum of electronic and thermal Enthalpies=           -1254.128049
 Sum of electronic and thermal Free Energies=        -1254.220503
0 1
```

C	3.49484500	-1.02774300	-1.56479800
C	4.14746200	-1.89616500	-0.65256800
C	4.06340900	0.21037300	-1.41312600
C	5.06533300	-1.11217700	-0.01080300
H	2.70099400	-1.28022700	-2.24910700
H	3.97129100	-2.94532700	-0.48431900
C	0.20073500	1.82083500	0.28758900
C	-0.23756100	2.19245100	1.49056400
C	-0.86348800	0.99831100	-0.37341700
C	-1.61382400	1.64045900	1.69900800
H	1.14608900	2.03465500	-0.19484200
H	0.25765900	2.78908000	2.24258200

O	-2.33006900	1.76702000	2.66728900
O	-0.83399300	0.48414900	-1.46961700
O	5.03588600	0.16403200	-0.45768200
C	3.81342600	1.53426000	-2.05325500
H	4.74856300	1.93786000	-2.45429200
H	3.11974900	1.39014500	-2.88072700
O	3.20108500	2.47220500	-1.16059400
H	3.86987800	2.80676600	-0.55151000
N	-1.93272900	0.92832600	0.53278400
C	-3.16303800	0.23261700	0.30330400
C	-3.28540400	-1.11067400	0.66900700
C	-4.23808200	0.89148200	-0.28328600
C	-4.47608700	-1.78505800	0.44691900
H	-2.44716900	-1.62268300	1.12663100
C	-5.44052400	0.22207200	-0.51051700
H	-4.14097800	1.93311400	-0.56588500
C	-5.56201900	-1.12282800	-0.14440900
H	-4.58511600	-2.82619200	0.72545600
H	-6.26266400	0.75506500	-0.96728200
O	-6.68607800	-1.86830000	-0.32084500
C	-7.83393600	-1.25273800	-0.91341500
H	-8.59700600	-2.02718000	-0.95075100
H	-8.19045900	-0.41739200	-0.30455000
H	-7.61551800	-0.90584400	-1.92712500
N	6.00066300	-1.42272400	1.00770600
O	6.72678100	-0.52473100	1.43527800
O	6.02659500	-2.59111300	1.40510700

Endo-TS25



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.286283 (Hartree/Particle)
Thermal correction to Energy= 0.309443
Thermal correction to Enthalpy= 0.310419
Thermal correction to Gibbs Free Energy= 0.230800
Sum of electronic and zero-point Energies= -1254.109690
Sum of electronic and thermal Energies= -1254.086530
Sum of electronic and thermal Enthalpies= -1254.085554
Sum of electronic and thermal Free Energies= -1254.165172

0 1

C	-1.87174800	0.68724900	1.67986800
C	-1.88531500	-0.67515700	1.57298000
C	-2.74572200	1.19364000	0.66016300
C	-2.74316900	-0.93808500	0.46616700
H	-1.25206700	1.29357100	2.32269300
H	-1.29175100	-1.40567300	2.09769200
C	-1.52551800	0.98766200	-1.02692500
C	-1.54497600	-0.40878800	-1.22237700
C	-0.12878600	1.36696500	-0.65947400
C	-0.16723900	-0.92792600	-0.97968400
H	-2.12205400	1.68755700	-1.59577100
H	-2.17875900	-0.91914500	-1.93465300
O	0.24436700	-2.06013000	-1.11438400
O	0.32738500	2.47584500	-0.48174900
O	-3.53966400	0.14269100	0.24216200
C	-3.38736400	2.55504600	0.61845200
H	-4.11727400	2.61740300	1.43441700
H	-2.61491000	3.30247800	0.80321000
O	-3.98706800	2.86270700	-0.62860700
H	-4.80900300	2.36601700	-0.71471400
N	0.60471200	0.16955600	-0.56139300
C	1.99519800	0.09817500	-0.22048900
C	2.39248800	0.10140000	1.11889000
C	2.95286700	0.02804300	-1.22683200
C	3.73896900	0.03799100	1.44358100
H	1.64796500	0.15320500	1.90380700
C	4.30920900	-0.04245800	-0.91011200
H	2.64407300	0.02873600	-2.26543600
C	4.70661400	-0.03656400	0.43128300
H	4.06094500	0.04102000	2.47787500
H	5.03482500	-0.09839800	-1.70950000
O	5.99948400	-0.09971700	0.84940700
C	7.03652900	-0.18433200	-0.13306000
H	7.96876200	-0.22891600	0.42583000
H	6.93061500	-1.08781000	-0.73983400
H	7.03972300	0.69787300	-0.77915800
N	-3.34389300	-2.22719500	0.15960900
O	-4.37290600	-2.24256700	-0.50207100
O	-2.74147900	-3.21653000	0.56167300

Product of Endo-TS25

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.289625 (Hartree/Particle)
Thermal correction to Energy= 0.312259
Thermal correction to Enthalpy= 0.313234
Thermal correction to Gibbs Free Energy= 0.234593
Sum of electronic and zero-point Energies= -1254.145382
Sum of electronic and thermal Energies= -1254.122747
Sum of electronic and thermal Enthalpies= -1254.121772
Sum of electronic and thermal Free Energies= -1254.200414

0 1

C	2.02165600	-0.62256100	1.73484600
C	2.07148700	0.69894100	1.56842500

C	2.61087200	-1.23896100	0.47025100
C	2.68199100	0.87463400	0.19095800
H	1.57396100	-1.17864900	2.54636800
H	1.67968900	1.49448600	2.18297700
C	1.57165200	-1.03033800	-0.70533100
C	1.62472100	0.49312400	-0.91921900
C	0.12118400	-1.33538000	-0.38595100
C	0.19854500	0.98213300	-0.71754900
H	1.89587900	-1.60699000	-1.57059800
H	1.99318000	0.79211400	-1.90005100
O	-0.20253700	2.11898100	-0.80303600
O	-0.35988800	-2.41673100	-0.13847400
O	3.57631500	-0.21076800	0.08598300
C	3.26962400	-2.59888500	0.57763900
H	4.04075300	-2.55669200	1.35383400
H	2.51539100	-3.32566200	0.88488800
O	3.80299400	-3.05409200	-0.65801300
H	4.58601800	-2.53184100	-0.86837000
N	-0.59665300	-0.13122100	-0.42618400
C	-2.00772100	-0.04496700	-0.16640800
C	-2.46210800	0.25308000	1.12010500
C	-2.91523000	-0.26032600	-1.19638800
C	-3.82304300	0.33503900	1.36906000
H	-1.75105900	0.41901200	1.92050200
C	-4.28633500	-0.18202800	-0.95388900
H	-2.55722100	-0.49046400	-2.19284200
C	-4.74447600	0.11735900	0.33389600
H	-4.19284400	0.56558700	2.36069200
H	-4.97620000	-0.35357000	-1.76817100
O	-6.05568400	0.21788000	0.67818100
C	-7.05089500	0.00462100	-0.32818000
H	-8.00785700	0.13535000	0.17226600
H	-6.95734200	0.73654300	-1.13508600
H	-6.98695200	-1.00790300	-0.73611100
N	3.39240100	2.17984200	-0.07884600
O	4.37258300	2.15485800	-0.79983000
O	2.90157100	3.17679900	0.42660400

Pre-complex of Exo-TS25

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

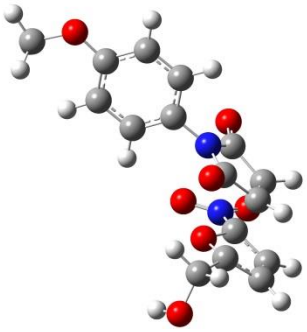
Zero-point correction= 0.285816 (Hartree/Particle)
Thermal correction to Energy= 0.310945
Thermal correction to Enthalpy= 0.311921
Thermal correction to Gibbs Free Energy= 0.222179
Sum of electronic and zero-point Energies= -1254.154602
Sum of electronic and thermal Energies= -1254.129472
Sum of electronic and thermal Enthalpies= -1254.128497
Sum of electronic and thermal Free Energies= -1254.218238

0 1

C	4.32800700	-1.21084300	0.21820900
C	2.39893400	-1.35808100	1.35147500

C	3.31311800	-0.60753900	-0.47191200
O	2.13999100	-0.68094200	0.19663800
H	5.35602500	-1.29018800	-0.09330100
C	-0.03244700	3.81328400	1.14194700
C	-0.51672400	4.24232000	-0.02278800
N	-1.24635300	2.05258000	0.23732700
C	-0.47616800	2.39887100	1.35654200
C	-1.31350500	3.13888500	-0.64932200
O	-0.23149600	1.67610200	2.29717500
O	-1.90687500	3.15381700	-1.70391600
H	0.58159900	4.33557300	1.86062400
H	-0.39997100	5.20486500	-0.49840300
C	3.72583500	-1.70105700	1.40538400
H	4.20758100	-2.24300600	2.20326100
C	-1.86915200	0.78045900	0.02887600
C	-3.10287600	0.50049800	0.62278900
C	-1.24719300	-0.17732500	-0.76512100
C	-3.70620600	-0.73163500	0.42434100
H	-3.58648700	1.24934200	1.23877400
C	-1.84908200	-1.42049100	-0.97353500
H	-0.28790600	0.03935700	-1.22042700
C	-3.08495500	-1.70079300	-0.37717900
H	-4.66177400	-0.96192100	0.87944800
H	-1.35375400	-2.14653800	-1.60332800
O	-3.75578400	-2.87372300	-0.51717100
C	-3.17898700	-3.90584900	-1.32458700
H	-2.21401600	-4.22619900	-0.92248600
H	-3.88193300	-4.73514900	-1.28756900
H	-3.05886300	-3.57430500	-2.35951300
C	1.24143600	-1.58103300	2.26644800
H	0.78515400	-0.61985900	2.52334700
H	1.61246300	-2.04594800	3.17951000
O	0.26769600	-2.47143200	1.71213200
H	-0.26070100	-1.99107700	1.06115000
N	3.30153800	0.04759100	-1.72708600
O	4.37716100	0.12637900	-2.32799400
O	2.23381600	0.49802900	-2.14713600

Exo-TS25



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.286456 (Hartree/Particle)

```
 Thermal correction to Energy=                    0.309628
 Thermal correction to Enthalpy=                  0.310603
 Thermal correction to Gibbs Free Energy=         0.230856
 Sum of electronic and zero-point Energies=          -1254.108860
 Sum of electronic and thermal Energies=             -1254.085688
 Sum of electronic and thermal Enthalpies=           -1254.084713
 Sum of electronic and thermal Free Energies=        -1254.164460


0 1
 C                  4.06242500    0.50767200    0.05208400
 C                  2.70328500   -1.25882000   -0.26322700
 C                  2.74542800    0.88062800   -0.35570800
 O                  2.12239700   -0.18948800   -0.91355500
 H                  4.84122400    1.18887900    0.35360400
 C                  1.72013900   -0.74818600    1.58671400
 C                  1.74034200    0.66086600    1.50178100
 N                 -0.42738900   -0.03654300    1.02220700
 C                  0.31233400   -1.18729500    1.34614300
 C                  0.35013200    1.11709800    1.18716700
 O                 -0.14651100   -2.30740000    1.41705400
 O                 -0.05544700    2.25589800    1.09398400
 H                  2.32690600   -1.33033400    2.26403700
 H                  2.36873200    1.31141900    2.09211600
 C                  4.02045500   -0.85335600    0.13494700
 H                  4.77756600   -1.51872300    0.52067100
 C                 -1.80825000   -0.03673400    0.63830100
 C                 -2.80593500   -0.02763400    1.61663200
 C                 -2.15578400   -0.04307100   -0.70794600
 C                 -4.14142200   -0.02501600    1.24477500
 H                 -2.53285300   -0.02160800    2.66514500
 C                 -3.49663300   -0.03806800   -1.09189200
 H                 -1.37987500   -0.05072900   -1.46412200
 C                 -4.49572000   -0.02912300   -0.11244500
 H                 -4.92591700   -0.01781200    1.99170300
 H                 -3.74305800   -0.04146300   -2.14445600
 O                 -5.82995500   -0.02352900   -0.37664000
 C                 -6.26091700   -0.02192200   -1.74124000
 H                 -5.91798100   -0.91950200   -2.26315400
 H                 -7.34818200   -0.01435300   -1.70671900
 H                 -5.90552600    0.86982500   -2.26479900
 C                  2.27935000   -2.62527100   -0.72229000
 H                  1.20131800   -2.64692100   -0.89272600
 H                  2.51845900   -3.34455400    0.06074300
 O                  2.99715000   -3.03804000   -1.88556900
 H                  2.66915200   -2.54357600   -2.64601500
 N                  2.38876200    2.17597200   -0.91915400
 O                  3.01777800    3.13873300   -0.49383000
 O                  1.48271800    2.22293000   -1.73771700
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Product of Exo-TS25

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 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
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Zero-point correction= 0.289877 (Hartree/Particle)
Thermal correction to Energy= 0.312415
Thermal correction to Enthalpy= 0.313390
Thermal correction to Gibbs Free Energy= 0.235501
Sum of electronic and zero-point Energies= -1254.147939
Sum of electronic and thermal Energies= -1254.125401
Sum of electronic and thermal Enthalpies= -1254.124426
Sum of electronic and thermal Free Energies= -1254.202315

0 1

C	4.08793400	-0.45041400	-0.42678400
C	2.63355000	1.27070800	0.00006100
C	2.70146100	-0.86035600	0.04419000
O	2.32218100	0.17540300	0.91973000
H	4.85306100	-1.13444100	-0.76058300
C	1.67649100	0.89292800	-1.20387100
C	1.70893200	-0.65338400	-1.15609800
N	-0.50863500	0.07882400	-0.76128500
C	0.21526600	1.25617200	-0.97624400
C	0.27717900	-1.07007200	-0.83613700
O	-0.26215400	2.36651300	-0.98340600
O	-0.12103800	-2.20034000	-0.67723800
H	2.01455600	1.33297300	-2.14042300
H	2.04737800	-1.15083200	-2.06244600
C	4.03640800	0.87860300	-0.45707900
H	4.77814900	1.57559700	-0.81918100
C	-1.92104600	0.05426900	-0.49441700
C	-2.82712900	0.01051000	-1.55597600
C	-2.37853000	0.07278300	0.81733400
C	-4.18877300	-0.01372200	-1.29868000
H	-2.46490400	-0.00473600	-2.57701700
C	-3.74703300	0.04720100	1.08466600
H	-1.67010200	0.10584600	1.63647900
C	-4.65796500	0.00407800	0.02332000
H	-4.90602700	-0.04769500	-2.10957700
H	-4.08362500	0.06132600	2.11171000
O	-6.00876200	-0.02330100	0.17147800
C	-6.55834500	-0.01353800	1.49316700
H	-6.27800500	0.89734300	2.02913000
H	-7.63793300	-0.04101500	1.36265900
H	-6.23607800	-0.89163000	2.05940300
C	2.45699400	2.61355900	0.67830500
H	1.44587500	2.69429700	1.08617500
H	2.58732900	3.40344100	-0.06295800
O	3.43842400	2.83085900	1.68530000
H	3.29222200	2.19717000	2.39763400
N	2.61629900	-2.21350300	0.70548900
O	3.05041400	-3.14468700	0.04432100
O	2.13244500	-2.29080100	1.81794300

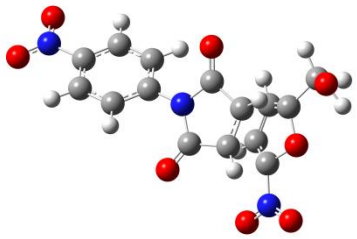
DA reaction of nitro-substituted α-furfuryl alcohols **2** and N-(p-nitro)-maleimide **6**

Pre-complex of Endo-TS26

```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.255599 (Hartree/Particle)
 Thermal correction to Energy=                    0.280808
 Thermal correction to Enthalpy=                  0.281783
 Thermal correction to Gibbs Free Energy=         0.189068
 Sum of electronic and zero-point Energies=          -1344.192159
 Sum of electronic and thermal Energies=             -1344.166950
 Sum of electronic and thermal Enthalpies=           -1344.165974
 Sum of electronic and thermal Free Energies=        -1344.258689

0 1
 C                 -3.95267700    1.34509400   -1.22855800
 C                 -4.75777300    2.04981400   -0.29701200
 C                 -4.41666800    0.05562200   -1.26100900
 C                 -5.65174200    1.12677700    0.16950300
 H                 -3.12991700    1.73641600   -1.80496800
 H                 -4.69371300    3.08435300   -0.00428100
 C                 -0.23410300   -2.01924200   -0.00624700
 C                  0.38466200   -2.88758200    0.79390700
 C                  0.73050000   -0.94245800   -0.38511500
 C                  1.79518900   -2.44509700    1.00365300
 H                 -1.25352900   -2.02758900   -0.37117800
 H                 -0.00284700   -3.78219400    1.25840700
 O                  2.65070100   -2.96941100    1.67656000
 O                  0.54095000    0.00777400   -1.10695900
 O                 -5.46724300   -0.08482400   -0.40220400
 C                 -3.99697200   -1.16371000   -2.00989700
 H                 -4.85748100   -1.59713400   -2.52947800
 H                 -3.25703300   -0.87327300   -2.75455000
 O                 -3.37186900   -2.14033400   -1.16911100
 H                 -4.04784700   -2.57207800   -0.63356100
 N                  1.94952400   -1.25320100    0.25980600
 C                  3.14190000   -0.49174700    0.16998200
 C                  3.09083100    0.89872600    0.31907300
 C                  4.36141100   -1.13570800   -0.06749200
 C                  4.25500400    1.64727000    0.22439600
 H                  2.14815400    1.39072700    0.51223600
 C                  5.53067900   -0.39345500   -0.14923100
 H                  4.39464500   -2.20873100   -0.19242800
 C                  5.46104500    0.98998900   -0.00530400
 H                  4.23396200    2.72158200    0.33835800
 H                  6.48055100   -0.87436300   -0.33401500
 N                 -6.69555700    1.24457300    1.12108600
 O                 -7.36921500    0.24780200    1.38397500
 O                 -6.86310200    2.35596700    1.63130100
 N                  6.69552500    1.77954200   -0.09945500
 O                  7.75451100    1.18214900   -0.27321800
 O                  6.61162700    3.00089100   -0.00015700
```

Endo-TS26



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.256446 (Hartree/Particle)
Thermal correction to Energy= 0.279434
Thermal correction to Enthalpy= 0.280409
Thermal correction to Gibbs Free Energy= 0.200927
Sum of electronic and zero-point Energies= -1344.147074
Sum of electronic and thermal Energies= -1344.124086
Sum of electronic and thermal Enthalpies= -1344.123111
Sum of electronic and thermal Free Energies= -1344.202592

0 1

C	1.95909100	-0.85627600	1.61352800
C	1.97486800	0.50916200	1.64893600
C	2.89510700	-1.25773600	0.60093800
C	2.89631400	0.88204600	0.62603300
H	1.30725100	-1.52511400	2.15466100
H	1.35080400	1.18396800	2.21168400
C	1.78109500	-0.86653400	-1.12860600
C	1.81148900	0.54362400	-1.16751000
C	0.37194700	-1.28106900	-0.89033100
C	0.42573100	1.04563700	-0.95501600
H	2.41155100	-1.50301000	-1.73395600
H	2.48205700	1.12297500	-1.78731300
O	0.02871500	2.18822100	-0.98139900
O	-0.09417400	-2.39707900	-0.87170200
O	3.70890700	-0.17248600	0.34249600
C	3.53801000	-2.61096300	0.45238200
H	4.21889000	-2.76335200	1.29811300
H	2.75555200	-3.36828900	0.51333100
O	4.20762200	-2.78862800	-0.78380600
H	5.04163100	-2.30500500	-0.76532900
N	-0.37700300	-0.09081400	-0.70173500
C	-1.76821300	-0.05596300	-0.41645200
C	-2.28528400	-0.85557700	0.60877000
C	-2.61239200	0.77041700	-1.16633400
C	-3.64445200	-0.83213100	0.88566700
H	-1.63102200	-1.49030600	1.18922300
C	-3.97126300	0.80520300	-0.88714200
H	-2.21040000	1.37861300	-1.96347500
C	-4.46916000	0.00207300	0.13529800
H	-4.05991200	-1.44170400	1.67519800
H	-4.63781200	1.43593800	-1.45766000
N	3.51477600	2.19491600	0.49655800
O	4.58894100	2.27241300	-0.08249200
O	2.88028500	3.13913400	0.95236400

```
 N                -5.90815600    0.03335000    0.42952800
 O                -6.61915100    0.78434000   -0.23264800
 O                -6.33279800   -0.69321000    1.32395000
```

Product of Endo-TS26

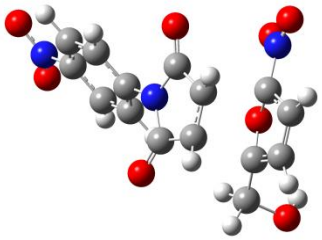
```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.259389 (Hartree/Particle)
 Thermal correction to Energy=                    0.281992
 Thermal correction to Enthalpy=                  0.282967
 Thermal correction to Gibbs Free Energy=         0.203312
 Sum of electronic and zero-point Energies=          -1344.181607
 Sum of electronic and thermal Energies=             -1344.159004
 Sum of electronic and thermal Enthalpies=           -1344.158029
 Sum of electronic and thermal Free Energies=        -1344.237684
0 1
 C                 2.16846500   -0.82590600    1.66498800
 C                 2.20730300    0.50635700    1.66891900
 C                 2.81135600   -1.27181800    0.35542800
 C                 2.86617400    0.86031600    0.34898100
 H                 1.70032900   -1.48421300    2.38318900
 H                 1.78487100    1.21533200    2.36405600
 C                 1.81373400   -0.92345500   -0.82475900
 C                 1.85351900    0.61447400   -0.84066700
 C                 0.35984200   -1.28611100   -0.60630500
 C                 0.41704800    1.06472000   -0.63196400
 H                 2.17873700   -1.38288800   -1.74234800
 H                 2.25075500    1.03998500   -1.76196100
 O                 0.00316900    2.19661100   -0.58155700
 O                -0.11655800   -2.39267800   -0.53186700
 O                 3.77556400   -0.19565900    0.13971200
 C                 3.48340500   -2.62880300    0.31027000
 H                 4.22358200   -2.68174500    1.11527900
 H                 2.72823200   -3.39632400    0.48954900
 O                 4.06925300   -2.91135200   -0.95245600
 H                 4.85040700   -2.35641700   -1.06181700
 N                -0.37667100   -0.08890600   -0.51197500
 C                -1.79126000   -0.05001800   -0.31113100
 C                -2.34626100   -0.68224700    0.80255500
 C                -2.59645100    0.61783300   -1.23540300
 C                -3.72112000   -0.65249400    0.99445900
 H                -1.71063400   -1.18883500    1.51586100
 C                -3.97102900    0.65955000   -1.04488400
 H                -2.15424100    1.09609300   -2.09871900
 C                -4.51149100    0.02050900    0.06731100
 H                -4.17385300   -1.13412900    1.84913300
 H                -4.61437600    1.16959500   -1.74729400
 N                 3.56752600    2.19551000    0.27876500
 O                 4.61075100    2.26005200   -0.34381300
 O                 3.00725000    3.12545500    0.83689300
 N                -5.96975200    0.05768400    0.27009600
 O                -6.65045800    0.67465300   -0.54316200
 O                -6.43283900   -0.53007000    1.24251100
```

Pre-complex of Exo-TS26

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.255450 (Hartree/Particle)
 Thermal correction to Energy=                    0.280771
 Thermal correction to Enthalpy=                  0.281746
 Thermal correction to Gibbs Free Energy=         0.189186
 Sum of electronic and zero-point Energies=          -1344.191378
 Sum of electronic and thermal Energies=             -1344.166058
 Sum of electronic and thermal Enthalpies=           -1344.165082
 Sum of electronic and thermal Free Energies=        -1344.257642

0 1
 C                  4.65123900   -0.43366600    0.42076400
 C                  3.97751700    1.49367400   -0.50429700
 C                  3.45212600   -0.03786100    0.94478500
 O                  3.02306100    1.12209300    0.39681400
 H                  5.20485500   -1.31907400    0.68472100
 C                  1.13382400   -2.33128400   -1.64363900
 C                  0.67988400   -3.27551900   -0.82082000
 N                 -0.85729300   -1.53126800   -0.74655600
 C                  0.18046200   -1.18077600   -1.63865900
 C                 -0.60428700   -2.81458500   -0.21142700
 O                  0.24958600   -0.15295400   -2.26942700
 O                 -1.29991100   -3.39358200    0.58801000
 H                  2.02565000   -2.32695800   -2.25223200
 H                  1.11134700   -4.23518500   -0.57837400
 C                  4.99093400    0.57044700   -0.52184800
 H                  5.87446500    0.61187600   -1.13826500
 C                 -1.98458700   -0.72506500   -0.44543300
 C                 -3.26365200   -1.29232700   -0.44506900
 C                 -1.80905100    0.63179500   -0.15283500
 C                 -4.36768400   -0.50686700   -0.14683600
 H                 -3.39498400   -2.33870800   -0.68151800
 C                 -2.91089600    1.42465800    0.13358800
 H                 -0.81813500    1.06284300   -0.14441100
 C                 -4.17628100    0.84334400    0.13544000
 H                 -5.36286500   -0.92779700   -0.14419800
 H                 -2.79372200    2.47385000    0.36389700
 C                  3.74537400    2.77197300   -1.23723200
 H                  2.76370400    2.74936000   -1.72160400
 H                  4.50664900    2.86694800   -2.01070800
 O                  3.86952600    3.92183600   -0.39523900
 H                  3.08592900    3.98504400    0.16310200
 N                 -5.34362500    1.67951900    0.44350000
 O                 -6.44992900    1.14648100    0.46265300
 O                 -5.15918500    2.87290700    0.66743000
 N                  2.62708200   -0.63507000    1.92996600
 O                  1.57881900   -0.06940500    2.24286600
 O                  3.01858500   -1.70014300    2.41593200
```

Exo-TS26



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.256486 (Hartree/Particle)
Thermal correction to Energy= 0.279563
Thermal correction to Enthalpy= 0.280539
Thermal correction to Gibbs Free Energy= 0.200530
Sum of electronic and zero-point Energies= -1344.146120
Sum of electronic and thermal Energies= -1344.123042
Sum of electronic and thermal Enthalpies= -1344.122067
Sum of electronic and thermal Free Energies= -1344.202076

0 1

C	4.28006100	0.54530700	0.07549400
C	2.95101600	-1.26495700	-0.07114800
C	2.97623000	0.84679700	-0.42761700
O	2.38734500	-0.29464600	-0.87200400
H	5.03998600	1.26982000	0.31871000
C	1.88397700	-0.52495500	1.66069300
C	1.90813000	0.86045900	1.38671200
N	-0.24926900	0.09823800	0.93832800
C	0.49163900	-1.00243500	1.43808600
C	0.53256200	1.27044700	0.97218500
O	0.02790300	-2.09910600	1.65399600
O	0.13934700	2.38391200	0.70781700
H	2.46508400	-1.00860900	2.43134800
H	2.50882200	1.58643700	1.91444100
C	4.24534900	-0.79381200	0.32983300
H	4.99099100	-1.39548600	0.82663200
C	-1.61492800	0.04078300	0.55145000
C	-2.51580500	0.99508400	1.03633700
C	-2.04990700	-0.97525800	-0.30600800
C	-3.84970600	0.94062300	0.65757600
H	-2.17777100	1.77161400	1.70708800
C	-3.38471200	-1.04218100	-0.67784700
H	-1.35014300	-1.70676100	-0.68427200
C	-4.26655400	-0.07966600	-0.19307000
H	-4.55953800	1.66873800	1.02306500
H	-3.73732000	-1.81941100	-1.34053100
C	2.56077900	-2.68587400	-0.36497000
H	1.49585900	-2.74417800	-0.59627800
H	2.75444500	-3.29049900	0.52079100
O	3.35092900	-3.24149800	-1.41547200
H	3.06908400	-2.85896800	-2.25496700
N	-5.67963100	-0.14370800	-0.59004500
O	-6.43791700	0.72934300	-0.17685800

```
 O                -6.03632800   -1.06752800   -1.31632200
 N                 2.64116200    2.05374700   -1.17684700
 O                 1.76831300    1.98301600   -2.02815800
 O                 3.25364100    3.06740600   -0.86204000
```

Product of Exo-TS26

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
 Zero-point correction=                           0.259750 (Hartree/Particle)
 Thermal correction to Energy=                    0.282228
 Thermal correction to Enthalpy=                  0.283203
 Thermal correction to Gibbs Free Energy=         0.204328
 Sum of electronic and zero-point Energies=          -1344.183866
 Sum of electronic and thermal Energies=             -1344.161388
 Sum of electronic and thermal Enthalpies=           -1344.160413
 Sum of electronic and thermal Free Energies=        -1344.239288

0 1
 C                 4.29126400   -0.52361900   -0.42852100
 C                 2.85585200    1.24661300   -0.17248400
 C                 2.91495600   -0.86489000    0.11929100
 O                 2.55975400    0.26880800    0.87472200
 H                 5.04488100   -1.24799700   -0.69685600
 C                 1.86832700    0.73751800   -1.30233000
 C                 1.89543300   -0.79218600   -1.07557500
 N                -0.31006600   -0.00407700   -0.71635100
 C                 0.41709300    1.13927800   -1.08657700
 C                 0.47268100   -1.16368000   -0.67702100
 O                -0.05827400    2.24054500   -1.21809200
 O                 0.07365700   -2.26184700   -0.37476900
 H                 2.18552700    1.06381700   -2.29124000
 H                 2.21116200   -1.39380600   -1.92520800
 C                 4.24508300    0.79291600   -0.61387200
 H                 4.98091500    1.43710700   -1.07276600
 C                -1.70887500    0.01307300   -0.41752100
 C                -2.58184700   -0.76570600   -1.17806000
 C                -2.17666500    0.80923300    0.62851600
 C                -3.93991200   -0.75373900   -0.88889500
 H                -2.20574200   -1.37139000   -1.99157600
 C                -3.53448000    0.83242400    0.91816700
 H                -1.48641400    1.40099700    1.21451000
 C                -4.39376700    0.04771100    0.15457100
 H                -4.63628800   -1.34715000   -1.46357800
 H                -3.92133100    1.43968600    1.72372500
 C                 2.70373400    2.66191000    0.34622000
 H                 1.70417000    2.79950200    0.76737200
 H                 2.81953100    3.35688200   -0.48702900
 O                 3.71179600    2.98765200    1.29521600
 H                 3.57708800    2.44798000    2.08323700
 N                -5.83485100    0.06640300    0.46106100
 O                -6.57713100   -0.64253400   -0.21082500
 O                -6.22174900    0.79002500    1.37304400
 N                 2.83628000   -2.13080200    0.93581300
 O                 2.37181300   -2.07312000    2.05752100
```

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 O                  3.25434500   -3.13545900    0.38072000
```

DA reaction of nitro-substituted α-furfuryl alcohols **2** and N-(benzyl)-maleimide **7**

Pre-complex of Endo-TS27

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.282273 (Hartree/Particle)
 Thermal correction to Energy=                    0.306200
 Thermal correction to Enthalpy=                  0.307176
 Thermal correction to Gibbs Free Energy=         0.216119
 Sum of electronic and zero-point Energies=          -1178.925711
 Sum of electronic and thermal Energies=             -1178.901784
 Sum of electronic and thermal Enthalpies=           -1178.900808
 Sum of electronic and thermal Free Energies=        -1178.991865

0 1
 C                 -3.63633500    0.92868700    1.59546400
 C                 -4.36895800   -0.28345400    1.67623600
 C                 -3.85556400    1.44423300    0.34428000
 C                 -4.97672000   -0.41297300    0.45850700
 H                 -3.02074100    1.36963600    2.36289700
 H                 -4.44128000   -0.96825200    2.50445400
 C                  0.24693400    0.37099800   -0.87848600
 C                  0.63182000   -0.67700600   -1.60752400
 C                  1.19375100    0.51529200    0.27644400
 C                  1.84550900   -1.28551500   -0.97230700
 H                 -0.58890300    1.04223000   -1.02864400
 H                  0.19148500   -1.08189500   -2.50683700
 O                  2.46445000   -2.26678400   -1.32521000
 O                  1.16808000    1.34137200    1.16448500
 O                 -4.68425300    0.62224200   -0.36122400
 C                 -3.36830700    2.66792500   -0.35590400
 H                 -4.21839400    3.25001100   -0.72563100
 H                 -2.82189300    3.27842300    0.36195100
 O                 -2.45995500    2.36957100   -1.42196700
 H                 -2.96372400    2.06118600   -2.18433100
 N                  2.13798200   -0.50515100    0.14741800
 C                  3.22382800   -0.77420800    1.08962400
 H                  3.23406400   -1.84544700    1.29463200
 H                  2.95649000   -0.25879600    2.01435300
 C                  4.58954300   -0.32303800    0.60505200
 C                  5.65711200   -1.22388300    0.58137200
 C                  4.81206000    1.00107600    0.20903300
 C                  6.92604800   -0.81291000    0.17023200
 H                  5.49693800   -2.25388000    0.88254600
 C                  6.07660400    1.41247900   -0.20692300
 H                  3.99601900    1.71552800    0.22677100
 C                  7.13838900    0.50608200   -0.22657900
 H                  7.74388300   -1.52459600    0.15547300
 H                  6.23467800    2.44099700   -0.51154100
 H                  8.12232500    0.82687900   -0.54950100
 N                 -5.82966800   -1.42369000   -0.05068700
```

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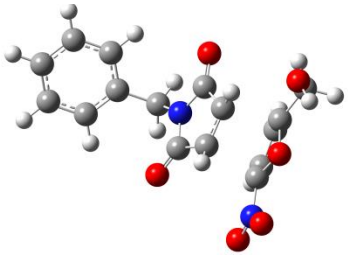
 O                -6.25010600   -1.31504900   -1.20310900
 O                -6.09989400   -2.36045900    0.70642000
```

Endo-TS27



```
---------------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.283010 (Hartree/Particle)
 Thermal correction to Energy=                    0.304715
 Thermal correction to Enthalpy=                  0.305690
 Thermal correction to Gibbs Free Energy=         0.228980
 Sum of electronic and zero-point Energies=          -1178.881488
 Sum of electronic and thermal Energies=             -1178.859783
 Sum of electronic and thermal Enthalpies=           -1178.858807
 Sum of electronic and thermal Free Energies=        -1178.935518

0 1
 C                -2.13013500    0.68612200    1.66558500
 C                -2.16148000   -0.67449400    1.54110600
 C                -2.59343200    1.22867200    0.41976800
 C                -2.61319100   -0.90137300    0.20930400
 H                -1.73526900    1.26620800    2.48567000
 H                -1.80672600   -1.42947100    2.22336900
 C                -0.89133500    0.97891800   -0.76329900
 C                -0.88477000   -0.41524600   -0.97274400
 C                 0.30118200    1.30507500    0.07673100
 C                 0.30320200   -0.97769300   -0.26408400
 H                -1.23389500    1.70076900   -1.49179700
 H                -1.25292500   -0.90631500   -1.86286900
 O                 0.69287100   -2.12747700   -0.23576800
 O                 0.69289800    2.39658300    0.43781900
 O                -3.24403000    0.21182100   -0.25327000
 C                -3.13089000    2.61568200    0.18720800
 H                -4.08434000    2.71082000    0.72021500
 H                -2.43103300    3.32915900    0.62370200
 O                -3.27640500    2.94611200   -1.18367800
 H                -4.04730000    2.48844500   -1.53878800
 N                 0.91621500    0.09022000    0.39638800
 C                 2.08916400   -0.04298400    1.26861400
 H                 1.96925200   -0.96879500    1.83120200
 H                 2.04904700    0.79227500    1.96861500
 C                 3.40921800   -0.04904900    0.51960400
 C                 3.92548600    1.13399200   -0.02362200
 C                 4.13494000   -1.23460200    0.37340200
 C                 5.14120700    1.12792600   -0.70495700
 H                 3.37369600    2.06048700    0.09062700
```

C	5.35410000	-1.24184400	-0.30559700
H	3.74537000	-2.15613000	0.79200700
C	5.85873300	-0.06092100	-0.84805700
H	5.53128900	2.05110300	-1.11885600
H	5.90714100	-2.16860400	-0.40985800
H	6.80584800	-0.06502500	-1.37571100
N	-3.12774100	-2.16235900	-0.29967400
O	-3.87406600	-2.13306600	-1.26899400
O	-2.73895300	-3.17760200	0.26785400

Product of Endo-TS27

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.286493 (Hartree/Particle)
Thermal correction to Energy= 0.307635
Thermal correction to Enthalpy= 0.308610
Thermal correction to Gibbs Free Energy= 0.232708
Sum of electronic and zero-point Energies= -1178.917726
Sum of electronic and thermal Energies= -1178.896584
Sum of electronic and thermal Enthalpies= -1178.895609
Sum of electronic and thermal Free Energies= -1178.971511

0 1

C	-2.23096900	0.87911700	1.60046800
C	-2.37410100	-0.44474800	1.54521900
C	-2.26822400	1.37713300	0.15903000
C	-2.48606900	-0.74231200	0.06103600
H	-2.03032600	1.49538200	2.46546400
H	-2.31520000	-1.18659200	2.32660600
C	-0.91905800	0.94330800	-0.54403300
C	-1.07237600	-0.58700100	-0.62690200
C	0.35685300	1.16646700	0.24517200
C	0.13206400	-1.15120900	0.11297900
H	-0.85289600	1.43109800	-1.51569900
H	-1.10785000	-0.97628600	-1.64406800
O	0.40511900	-2.31813200	0.28587000
O	0.84305100	2.22771800	0.56855800
O	-3.15524200	0.38781900	-0.45159100
C	-2.75865900	2.78691500	-0.09881900
H	-3.75080500	2.90340400	0.34945400
H	-2.07805300	3.48543700	0.39129700
O	-2.77184800	3.12336100	-1.47919200
H	-3.47956200	2.63040200	-1.91071300
N	0.90002500	-0.07938100	0.55786500
C	2.13585800	-0.24229800	1.34119200
H	2.04995500	-1.20183200	1.85154000
H	2.14544000	0.55009400	2.08888600
C	3.39289300	-0.19081900	0.49468700
C	3.72186800	-1.25309000	-0.35663600
C	4.24740200	0.91298200	0.56349400
C	4.88017600	-1.20641900	-1.12951800
H	3.07183800	-2.11945800	-0.41061500
C	5.41044800	0.95865000	-0.20631000

H	4.00362000	1.73995000	1.22145300
C	5.72787200	-0.09972900	-1.05605400
H	5.12477100	-2.03576000	-1.78367700
H	6.06548100	1.82015300	-0.14149400
H	6.63094500	-0.06539900	-1.65492500
N	-3.20676900	-2.01330900	-0.31864700
O	-3.94809700	-1.98551200	-1.28313900
O	-2.96123500	-2.99318700	0.36723700

Pre-complex of Exo-TS27

---

opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

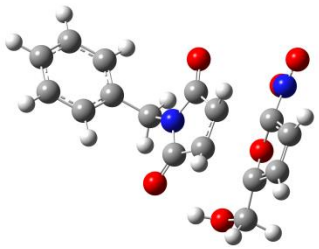
Zero-point correction= 0.283154 (Hartree/Particle)
Thermal correction to Energy= 0.306463
Thermal correction to Enthalpy= 0.307438
Thermal correction to Gibbs Free Energy= 0.220085
Sum of electronic and zero-point Energies= -1178.929963
Sum of electronic and thermal Energies= -1178.906655
Sum of electronic and thermal Enthalpies= -1178.905680
Sum of electronic and thermal Free Energies= -1178.993032

0 1

C	2.08937700	-1.78077600	-0.14504400
C	2.85088800	-1.49556500	1.01656700
C	2.59866000	-1.00758400	-1.15768500
C	3.76873800	-0.56335700	0.61795700
H	1.26369700	-2.46891200	-0.22913500
H	2.74453800	-1.90796900	2.00587400
C	-0.33924800	2.64094500	-0.16412700
C	-1.11070100	3.24950900	0.73593500
H	0.69178200	2.83196100	-0.42173600
H	-0.87131100	4.06326800	1.40399900
C	-2.46902200	2.61430900	0.70554800
C	-1.14953500	1.57591100	-0.83797900
O	-0.80498800	0.81995000	-1.72904000
O	-3.44242800	2.89434300	1.36818600
O	3.63658400	-0.25615500	-0.69232300
N	-2.41069500	1.60446300	-0.26346900
C	2.22985300	-0.84291700	-2.59575200
H	3.11110600	-1.01014600	-3.21937500
H	1.48936400	-1.61007100	-2.84303400
O	1.76002500	0.46534100	-2.90202100
H	0.89267200	0.59668600	-2.47706000
C	-3.53023600	0.74123000	-0.65030300
H	-3.55349000	0.69269400	-1.73929000
C	-3.45832400	-0.65558700	-0.06246500
C	-3.40817400	-1.77057500	-0.90253000
C	-3.46824400	-0.85078500	1.32391100
C	-3.36861100	-3.06036800	-0.37026000
H	-3.39867400	-1.63172200	-1.97844500
C	-3.42381600	-2.13698100	1.85748400
H	-3.51571100	0.00428000	1.98988100
C	-3.37442900	-3.24626900	1.01090600

H	-3.33009900	-3.91613100	-1.03488600
H	-3.43344400	-2.27422700	2.93294500
H	-3.34236200	-4.24708600	1.42639300
H	-4.43406600	1.25371000	-0.31641600
N	4.78904000	0.10051800	1.34173000
O	5.49504900	0.91942500	0.75136200
O	4.90757200	-0.19015900	2.53627000

Exo-TS27



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.283542 (Hartree/Particle)
Thermal correction to Energy= 0.304928
Thermal correction to Enthalpy= 0.305904
Thermal correction to Gibbs Free Energy= 0.229834
Sum of electronic and zero-point Energies= -1178.880081
Sum of electronic and thermal Energies= -1178.858694
Sum of electronic and thermal Enthalpies= -1178.857718
Sum of electronic and thermal Free Energies= -1178.933788

0 1

C	-3.72762600	-0.79908400	-1.05694000
C	-3.67310100	0.56216600	-1.10513000
C	-2.80432800	-1.22077400	-0.04347300
C	-2.65080900	0.91160700	-0.16622900
H	-4.28154900	-1.46416500	-1.70194500
H	-4.15592000	1.24263100	-1.78737000
C	-1.00240200	-0.91929200	-1.29806800
C	-0.97535600	0.49304000	-1.31309100
H	-1.29136600	-1.54475200	-2.12891100
H	-1.21134800	1.10680300	-2.17030700
C	0.17092700	0.92422800	-0.44285000
C	0.10973400	-1.37083400	-0.41921600
O	0.45171400	-2.51526000	-0.16159700
O	0.55835300	2.05186800	-0.22319200
O	-2.47225500	-0.12224200	0.70540300
N	0.72885500	-0.23458500	0.09654300
C	-2.82996300	-2.56196700	0.64906100
H	-3.78156100	-2.62869900	1.18602900
H	-2.83705900	-3.33760300	-0.12384300
O	-1.81004800	-2.76195300	1.60369800
H	-0.98661000	-2.96636200	1.13701200
C	1.80598400	-0.24629700	1.09206100

H	1.73295200	-1.20468800	1.60838000
C	3.19042200	-0.06388900	0.49784700
C	3.70827900	-0.99436900	-0.41138000
C	3.97929700	1.02594600	0.87410500
C	4.98826100	-0.83190500	-0.93728900
H	3.11086600	-1.85063400	-0.70521100
C	5.26393000	1.18734900	0.35285600
H	3.58799900	1.75434600	1.57634300
C	5.77041200	0.25996200	-0.55589100
H	5.37774300	-1.55999000	-1.64006200
H	5.86425100	2.03839500	0.65435700
H	6.76724500	0.38449200	-0.96353000
H	1.59695400	0.54519900	1.81206600
N	-2.49839500	2.24028600	0.41703000
O	-2.08088700	2.32920300	1.56146600
O	-2.77784800	3.18210700	-0.31656100

Product of Exo-TS27

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.287229 (Hartree/Particle)
Thermal correction to Energy= 0.307899
Thermal correction to Enthalpy= 0.308874
Thermal correction to Gibbs Free Energy= 0.235070
Sum of electronic and zero-point Energies= -1178.919137
Sum of electronic and thermal Energies= -1178.898467
Sum of electronic and thermal Enthalpies= -1178.897492
Sum of electronic and thermal Free Energies= -1178.971296

0 1

C	-3.51334300	-0.75131800	-1.37201100
C	-3.47839100	0.57816200	-1.36000000
C	-2.51129100	-1.22488100	-0.31722600
C	-2.42702800	0.90496200	-0.31155400
H	-4.05735200	-1.40534400	-2.03877700
H	-3.96086000	1.30138800	-1.99950200
C	-1.08585200	-0.95414000	-0.95690200
C	-1.02456600	0.59231000	-0.94486800
H	-0.99702300	-1.41012000	-1.94199200
H	-0.89604500	1.07008900	-1.91371500
C	0.15222800	0.93213400	-0.03762000
C	0.10406300	-1.38291700	-0.10769200
O	0.45180000	-2.52450800	0.12779300
O	0.51613200	2.03697600	0.29296100
O	-2.56610700	-0.12326300	0.63938600
N	0.75646100	-0.25542000	0.35989700
C	-2.84263900	-2.56594000	0.32206900
H	-3.87460400	-2.51457200	0.67423400
H	-2.79470800	-3.33078800	-0.46200500
O	-2.05053600	-2.91511400	1.44303700
H	-1.16815300	-3.16034600	1.13107700
C	1.93308900	-0.30067400	1.24562600
H	1.91139200	-1.27883300	1.72614300
C	3.24258100	-0.08429100	0.51322100

```
 C                  3.73833400   -1.05776900   -0.36288900
 C                  3.98131700    1.08372500    0.71854600
 C                  4.94757100   -0.86053600   -1.02634600
 H                  3.18020700   -1.97425900   -0.52138700
 C                  5.19539000    1.28002500    0.05908500
 H                  3.60718600    1.84297400    1.39653000
 C                  5.67940200    0.30965000   -0.81661100
 H                  5.32208200   -1.62214900   -1.70101300
 H                  5.75929100    2.19023700    0.22907300
 H                  6.62183500    0.46121100   -1.33059300
 H                  1.78884100    0.46424200    2.00809200
 N                 -2.54165200    2.27080200    0.31852300
 O                 -2.59205800    2.35340600    1.53004600
 O                 -2.57059800    3.20595200   -0.46748300
```

DA reaction of bromo-substituted α-furfuryl alcohols **3** and N-(p-methoxyphenyl)-maleimide **5**

Pre-complex of Endo-TS35

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---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.272983 (Hartree/Particle)
 Thermal correction to Energy=                    0.297193
 Thermal correction to Enthalpy=                  0.298169
 Thermal correction to Gibbs Free Energy=         0.207927
 Sum of electronic and zero-point Energies=          -3623.140613
 Sum of electronic and thermal Energies=             -3623.116402
 Sum of electronic and thermal Enthalpies=           -3623.115427
 Sum of electronic and thermal Free Energies=        -3623.205669

0 1
 C                 -3.56288700    1.19753800    1.87055700
 C                 -4.14722100   -0.11133600    1.92853300
 C                 -3.86303100    1.71942500    0.65072700
 C                 -4.75799200   -0.28106900    0.72719200
 H                 -2.99108100    1.68542800    2.64448800
 H                 -4.11621800   -0.81735400    2.74165100
 C                  0.08322800    0.75743200   -1.15632600
 C                  0.24356000   -0.34154600   -1.89411700
 C                  1.34740100    1.00360600   -0.38985000
 C                  1.61868800   -0.88684500   -1.66354900
 H                 -0.77696400    1.41001400   -1.07292800
 H                 -0.45325800   -0.81785300   -2.56814500
 O                  2.12535100   -1.86921200   -2.15867400
 O                  1.58484800    1.90207200    0.38687700
 O                 -4.60912100    0.80588400   -0.06725400
 C                 -3.55865900    3.00942800   -0.01210000
 H                 -4.47100600    3.43437400   -0.44424800
 H                 -3.17855000    3.70155000    0.74530700
 O                 -2.57958600    2.79993100   -1.04772600
 H                 -2.49704100    3.61808500   -1.55185200
 N                  2.23405000   -0.02551600   -0.74269000
 C                  3.56505900   -0.17484700   -0.23721000
 C                  3.80423600   -0.98903000    0.87323700
```
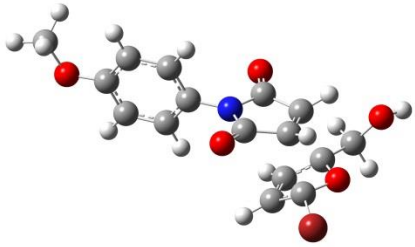

C	4.62217400	0.49106900	-0.84793600
C	5.09270900	-1.13383800	1.36379800
H	2.97922200	-1.50565400	1.34927400
C	5.92169500	0.35518300	-0.35966200
H	4.43497500	1.12099500	-1.70959200
C	6.16038500	-0.46163500	0.75092400
H	5.29245000	-1.76226400	2.22323200
H	6.72702200	0.88423600	-0.84976500
Br	-5.73761000	-1.71309100	0.01321300
O	7.38565300	-0.66480700	1.30611000
C	8.51777100	-0.00015000	0.73698900
H	9.37097100	-0.30287100	1.34021400
H	8.67573500	-0.30918800	-0.29999600
H	8.40189600	1.08604900	0.78683200

Endo-TS35



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---------------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.273537 (Hartree/Particle)
 Thermal correction to Energy=                    0.295675
 Thermal correction to Enthalpy=                  0.296651
 Thermal correction to Gibbs Free Energy=         0.218692
 Sum of electronic and zero-point Energies=          -3623.101118
 Sum of electronic and thermal Energies=             -3623.078979
 Sum of electronic and thermal Enthalpies=           -3623.078004
 Sum of electronic and thermal Free Energies=        -3623.155963

0 1
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C	-1.56176600	0.94347000	1.63976400
C	-1.68398000	-0.41466400	1.50516000
C	-2.40714000	1.53513100	0.65431500
C	-2.57840900	-0.60574200	0.41327600
H	-0.87650600	1.48474900	2.27440700
H	-1.12724500	-1.19355200	2.00114000
C	-1.18721700	1.24295200	-1.08015200
C	-1.32320900	-0.14964300	-1.24691200
C	0.22459100	1.51843200	-0.70438000
C	0.00426400	-0.77088500	-0.98967600
H	-1.73585300	1.98914400	-1.63544400
H	-1.98702900	-0.62052300	-1.95744000
O	0.33295800	-1.93465000	-1.10322300
O	0.77175700	2.59036500	-0.53772700
O	-3.27607000	0.55639600	0.21435800

C	-2.91832600	2.94228500	0.65239900
H	-3.71685100	3.02083600	1.40070100
H	-2.09700300	3.59813300	0.96070100
O	-3.40823300	3.28413700	-0.63973200
H	-3.85026500	4.13800400	-0.57901900
N	0.86124200	0.26794300	-0.57938700
C	2.23670800	0.09306300	-0.22179600
C	2.61910500	0.07357600	1.12204200
C	3.19994000	-0.05106600	-1.21505600
C	3.95380300	-0.08403500	1.46384500
H	1.87055700	0.18266500	1.89735600
C	4.54429600	-0.21660400	-0.88199600
H	2.90413000	-0.03372200	-2.25734000
C	4.92574400	-0.23103900	0.46384100
H	4.26292500	-0.09823000	2.50203500
H	5.27309500	-0.32855700	-1.67258000
Br	-3.55191500	-2.19883300	0.06717300
O	6.20687500	-0.38129000	0.89804500
C	7.24750200	-0.53404900	-0.07188700
H	8.16883200	-0.63509000	0.49772900
H	7.09248100	-1.43111000	-0.67774400
H	7.31333300	0.34405400	-0.72033900

Product of Endo-TS35

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---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.277244 (Hartree/Particle)
 Thermal correction to Energy=                    0.298617
 Thermal correction to Enthalpy=                  0.299593
 Thermal correction to Gibbs Free Energy=         0.223654
 Sum of electronic and zero-point Energies=          -3623.140551
 Sum of electronic and thermal Energies=             -3623.119177
 Sum of electronic and thermal Enthalpies=           -3623.118202
 Sum of electronic and thermal Free Energies=        -3623.194141

0 1
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C	-1.73914100	0.93977800	1.72014000
C	-1.87152800	-0.37772300	1.56584400
C	-2.28297200	1.57379300	0.44343900
C	-2.49087000	-0.55052400	0.18952100
H	-1.25654800	1.47688300	2.52486100
H	-1.53068300	-1.18358900	2.19854200
C	-1.25018500	1.28199000	-0.71902600
C	-1.41219000	-0.23742100	-0.91337500
C	0.21482600	1.48792000	-0.39121800
C	-0.02579000	-0.82123800	-0.70315100
H	-1.52238500	1.87011900	-1.59477600
H	-1.79291700	-0.51985600	-1.89364200
O	0.29952100	-1.98432400	-0.77118700
O	0.77169400	2.53442200	-0.14741100

O	-3.31192100	0.60955400	0.07209000
C	-2.84950800	2.97610000	0.52856900
H	-3.61971300	2.99825500	1.30684900
H	-2.04998500	3.65984200	0.81928700
O	-3.35884200	3.44368300	-0.71387300
H	-4.15143200	2.93834600	-0.92996900
N	0.84694000	0.23679800	-0.41933900
C	2.24740100	0.05496300	-0.15595400
C	2.67673800	-0.30642700	1.12285800
C	3.17222900	0.24081500	-1.17630500
C	4.02877600	-0.48189800	1.37326100
H	1.95290200	-0.44924300	1.91622600
C	4.53479300	0.07018500	-0.93234300
H	2.83389800	0.51980800	-2.16715700
C	4.96712900	-0.29405700	0.34755700
H	4.37861200	-0.76314300	2.35907800
H	5.23737400	0.22104700	-1.73987600
Br	-3.53124300	-2.17122700	-0.09325300
O	6.26802000	-0.48789300	0.69256400
C	7.27879800	-0.31237800	-0.30531800
H	8.22360600	-0.51625000	0.19380100
H	7.14253300	-1.01588500	-1.13128000
H	7.28086200	0.71224000	-0.68717600

Pre-complex of Exo-TS35

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

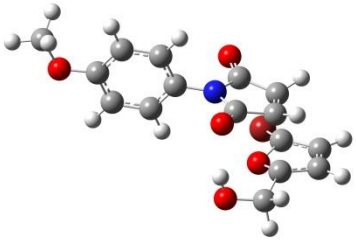
Zero-point correction= 0.273825 (Hartree/Particle)
Thermal correction to Energy= 0.297504
Thermal correction to Enthalpy= 0.298479
Thermal correction to Gibbs Free Energy= 0.209209
Sum of electronic and zero-point Energies= -3623.144420
Sum of electronic and thermal Energies= -3623.120742
Sum of electronic and thermal Enthalpies= -3623.119767
Sum of electronic and thermal Free Energies= -3623.209037

0 1

C	2.55661900	-1.93834800	0.79268000
C	3.53913900	-1.19156800	1.52541000
C	2.84979800	-1.80479100	-0.52967600
C	4.35572800	-0.65780100	0.58081700
H	1.73521600	-2.50390000	1.20451700
H	3.62322700	-1.07173000	2.59276500
C	0.11984800	2.06347800	-0.83352300
C	-0.46526200	3.12958900	-0.28931500
H	1.12271600	1.95769300	-1.21952300
H	-0.06191800	4.11647500	-0.11766200
C	-1.86859100	2.76672600	0.08903100
C	-0.86243300	0.93401600	-0.84729300
O	-0.69824700	-0.19515800	-1.26735500
O	-2.70851300	3.46633100	0.60467900
O	3.97076600	-1.01014500	-0.66981300
N	-2.03863500	1.41816300	-0.27636300

C	2.22055800	-2.31633400	-1.77913900
H	2.97634700	-2.78048100	-2.41688900
H	1.49693500	-3.08874200	-1.49734000
O	1.60898900	-1.29828800	-2.57572100
H	0.85571200	-0.92588100	-2.08478400
C	-3.24549200	0.66515500	-0.10272100
C	-4.21379400	0.65751000	-1.11018700
C	-3.45645100	-0.05223800	1.06949800
C	-5.38444700	-0.06486800	-0.94030600
H	-4.04732900	1.21792300	-2.02246700
C	-4.63129300	-0.78215300	1.24965500
H	-2.70373900	-0.04369600	1.84892700
C	-5.60141600	-0.78923300	0.24129300
H	-6.14459100	-0.08010900	-1.71182500
H	-4.77442400	-1.33230400	2.16910900
Br	5.87094000	0.44220900	0.71300300
O	-6.77967900	-1.46405800	0.31310500
C	-7.07037600	-2.22047600	1.49262500
H	-8.04939900	-2.66373000	1.32401600
H	-6.33196700	-3.01258000	1.64405100
H	-7.10854900	-1.57484400	2.37429600

Exo-TS35



---

opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.274401 (Hartree/Particle)
Thermal correction to Energy= 0.296072
Thermal correction to Enthalpy= 0.297047
Thermal correction to Gibbs Free Energy= 0.219748
Sum of electronic and zero-point Energies= -3623.099344
Sum of electronic and thermal Energies= -3623.077673
Sum of electronic and thermal Enthalpies= -3623.076698
Sum of electronic and thermal Free Energies= -3623.153997

0 1

C	-3.85794200	1.39969700	0.18804300
C	-3.99016400	0.05812600	0.41139800
C	-2.59074600	1.59482400	-0.44649300
C	-2.77485900	-0.52657100	-0.05650800
H	-4.51060100	2.19311600	0.52018200
H	-4.76089000	-0.46430600	0.95567100
C	-1.42890800	1.42364500	1.38132500
C	-1.58578100	0.04628500	1.65574300
H	-1.90088500	2.22286500	1.93295900
H	-2.21924600	-0.36394700	2.42714600

C	-0.27753900	-0.61546000	1.40718500
C	-0.02452400	1.62520500	0.93144300
O	0.53197900	2.67545700	0.64617000
O	0.04355300	-1.76551900	1.61659000
O	-2.15504200	0.36580300	-0.88608400
N	0.58470700	0.37150100	0.88206400
C	-2.22671400	2.80262500	-1.28081100
H	-2.90448200	2.82602400	-2.13930900
H	-2.42998300	3.69522100	-0.67885400
O	-0.91544000	2.80166100	-1.80795500
H	-0.29499300	2.99544700	-1.08948900
C	1.91710200	0.12644800	0.41689700
C	3.00117700	0.33931200	1.26133600
C	2.12975900	-0.32775400	-0.88757100
C	4.30246100	0.10620700	0.81607800
H	2.83442100	0.68981800	2.27298300
C	3.41891000	-0.56739000	-1.33772200
H	1.28498300	-0.49062400	-1.54607500
C	4.51431400	-0.35049600	-0.48921200
H	5.12980300	0.28134300	1.48950000
H	3.59831400	-0.92050800	-2.34599700
Br	-2.57267500	-2.34955400	-0.53760800
O	5.73838100	-0.61082300	-1.02335000
C	6.90000500	-0.41138100	-0.21215200
H	6.88031900	-1.05799500	0.66952400
H	7.74713900	-0.67886300	-0.84010700
H	6.99003400	0.63374100	0.09683900

Product of Exo-TS35

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.277793 (Hartree/Particle)
 Thermal correction to Energy=                    0.298790
 Thermal correction to Enthalpy=                  0.299766
 Thermal correction to Gibbs Free Energy=         0.224808
 Sum of electronic and zero-point Energies=          -3623.140100
 Sum of electronic and thermal Energies=             -3623.119103
 Sum of electronic and thermal Enthalpies=           -3623.118128
 Sum of electronic and thermal Free Energies=        -3623.193085

0 1
 C                 -3.83006500    1.42562200    0.61715900
 C                 -3.97314800    0.10945100    0.74594700
 C                 -2.47258700    1.64874500   -0.05313300
 C                 -2.68905600   -0.47709100    0.18149200
 H                 -4.47212000    2.21565600    0.98115900
 H                 -4.74613600   -0.46044700    1.23946000
 C                 -1.40458800    1.33651300    1.07105500
 C                 -1.57655800   -0.19390800    1.25972500
 H                 -1.57756300    1.92891700    1.96931300
 H                 -1.90090500   -0.50838300    2.24997800
 C                 -0.20241000   -0.78305200    0.98014100
```

C	0.04638600	1.50805800	0.64630500
O	0.60717100	2.55570800	0.38830100
O	0.13279700	-1.93800900	1.08120800
O	-2.34531500	0.44038900	-0.85152100
N	0.65820500	0.26285200	0.61451400
C	-2.38732600	2.91936700	-0.88848700
H	-3.24540200	2.92485600	-1.56334700
H	-2.49261500	3.77272900	-0.20743300
O	-1.23544100	3.04279200	-1.70423000
H	-0.47128100	3.19692800	-1.13029500
C	2.03875800	0.06398000	0.26634900
C	3.03094200	0.26782800	1.21731400
C	2.37597800	-0.33683000	-1.02804800
C	4.37210600	0.07669300	0.88608000
H	2.76343200	0.57581600	2.22106400
C	3.70622700	-0.53337500	-1.36386500
H	1.59859200	-0.49269900	-1.76632100
C	4.71344000	-0.32725400	-0.40941200
H	5.12921600	0.24255600	1.63941400
H	3.98581100	-0.84512400	-2.36280300
Br	-2.83601800	-2.28527000	-0.52573000
O	5.98587600	-0.54476900	-0.83558700
C	7.06387300	-0.35649800	0.08700600
H	6.97487400	-1.03523400	0.93966800
H	7.97005800	-0.58747800	-0.46871000
H	7.10467100	0.67801800	0.43867500

DA reaction of bromo-substituted α-furfuryl alcohols **3** and N-(p-nitro)-maleimide **6**

Pre-complex of Endo-TS36

```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
```

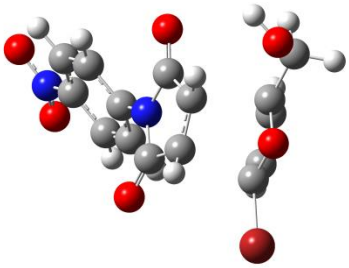
```
Zero-point correction=                           0.243242 (Hartree/Particle)
 Thermal correction to Energy=                    0.267191
 Thermal correction to Enthalpy=                  0.268166
 Thermal correction to Gibbs Free Energy=         0.178155
 Sum of electronic and zero-point Energies=          -3713.179154
 Sum of electronic and thermal Energies=             -3713.155205
 Sum of electronic and thermal Enthalpies=           -3713.154230
 Sum of electronic and thermal Free Energies=        -3713.244241
```

0 1

C	5.95064300	0.38799600	-1.11947300
C	5.74879900	-1.02159100	-0.94598400
C	4.94194700	1.02401200	-0.46280100
C	4.62312200	-1.12937100	-0.19347000
H	6.74985900	0.86440100	-1.66580400
H	6.35115400	-1.83060900	-1.32440900
C	0.41296200	2.12727600	0.29338200
C	0.02151400	2.33020800	1.55154000
C	-0.68543500	1.43375700	-0.44554700
C	-1.35830300	1.78977500	1.73187800
H	1.35237600	2.38125000	-0.18241700

```
 H                  0.55421700    2.80341000    2.36307100
 O                 -2.04222500    1.80342100    2.72786100
 O                 -0.69643500    1.07290400   -1.59853100
 O                  4.11183200    0.08588100    0.11820200
 C                  4.57979700    2.45379900   -0.28081700
 H                  4.36013500    2.66429800    0.76735000
 H                  5.43494100    3.06629300   -0.58111400
 O                  3.39620700    2.84279500   -1.00012100
 H                  3.55628400    2.71334900   -1.94293000
 N                 -1.73891000    1.25443900    0.48049300
 C                 -2.97870100    0.62733900    0.19994800
 C                 -3.49168700   -0.32576100    1.08701700
 C                 -3.68012400    0.96389000   -0.96326300
 C                 -4.70650100   -0.93874400    0.81687100
 H                 -2.94192900   -0.58986500    1.97926900
 C                 -4.88847600    0.34352500   -1.24561800
 H                 -3.28560000    1.70851400   -1.63999700
 C                 -5.38755700   -0.59825500   -0.34928300
 H                 -5.11585900   -1.67818200    1.49013100
 H                 -5.44332600    0.59227300   -2.13885200
 Br                 3.69514000   -2.62295300    0.46050300
 N                 -6.66933900   -1.25168900   -0.64251500
 O                 -7.10959500   -2.05754000    0.17327900
 O                 -7.24183400   -0.96223100   -1.68994100
```

Endo-TS36



```
---------------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.243620 (Hartree/Particle)
 Thermal correction to Energy=                    0.265685
 Thermal correction to Enthalpy=                  0.266660
 Thermal correction to Gibbs Free Energy=         0.188492
 Sum of electronic and zero-point Energies=          -3713.138218
 Sum of electronic and thermal Energies=             -3713.116153
 Sum of electronic and thermal Enthalpies=           -3713.115178
 Sum of electronic and thermal Free Energies=        -3713.193346

0 1
 C                 -1.63602600    0.75244000    1.71865300
 C                 -1.77874400   -0.58172700    1.44647100
 C                 -2.53312200    1.45227200    0.85268800
 C                 -2.74441300   -0.65284500    0.40113500
```

H	-0.90889800	1.21856800	2.36644000
H	-1.20514300	-1.41324900	1.82353700
C	-1.44483200	1.35465200	-0.96596100
C	-1.57234100	-0.01429100	-1.27693100
C	-0.02051400	1.62438700	-0.64905300
C	-0.23365900	-0.63806200	-1.16149900
H	-2.03028400	2.13363000	-1.43070500
H	-2.26900500	-0.41739000	-1.99710700
O	0.10619000	-1.77043600	-1.42692200
O	0.51049300	2.68353500	-0.39237600
O	-3.43635800	0.52519500	0.36524000
C	-3.06121300	2.84636000	1.07462000
H	-3.82681500	2.78903700	1.85477400
H	-2.24332100	3.46189000	1.45584000
O	-3.67335300	3.42575800	-0.07027100
H	-3.05599300	4.03780700	-0.48361600
N	0.64480600	0.37336500	-0.68624500
C	2.01826800	0.17102300	-0.39960300
C	2.41055800	-0.92819400	0.37396300
C	2.97643500	1.06231600	-0.89765200
C	3.75361800	-1.14011100	0.64751400
H	1.66980500	-1.61230500	0.76260600
C	4.32051000	0.86136800	-0.61795300
H	2.67219800	1.90372400	-1.50266900
C	4.69231800	-0.23932600	0.14980600
H	4.07130300	-1.98269200	1.24483800
H	5.07219900	1.53860100	-0.99745300
Br	-3.74343400	-2.19578800	-0.06455600
N	6.11406600	-0.45776100	0.44094100
O	6.42700400	-1.44916900	1.09554800
O	6.92614600	0.36063700	0.01664700

Product of Endo-TS36

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.246871 (Hartree/Particle)
Thermal correction to Energy= 0.268369
Thermal correction to Enthalpy= 0.269345
Thermal correction to Gibbs Free Energy= 0.192187
Sum of electronic and zero-point Energies= -3713.175344
Sum of electronic and thermal Energies= -3713.153846
Sum of electronic and thermal Enthalpies= -3713.152871
Sum of electronic and thermal Free Energies= -3713.230029

0 1

C	-1.87055400	0.80287000	1.78089900
C	-1.99744300	-0.50191800	1.54084800
C	-2.48291000	1.52043200	0.57958600
C	-2.67848500	-0.58366700	0.18592300
H	-1.35630200	1.28871600	2.59855700
H	-1.62079900	-1.34599200	2.09904500
C	-1.50135300	1.32518700	-0.64868000
C	-1.65011300	-0.17940900	-0.93720500

```
 C                 -0.02846000    1.54123800   -0.37582200
 C                 -0.25254900   -0.75726800   -0.81880800
 H                 -1.82330000    1.95715100   -1.47570800
 H                 -2.06407400   -0.40288200   -1.91901600
 O                  0.08605100   -1.90547600   -0.97545500
 O                  0.52220000    2.57833600   -0.09154200
 O                 -3.51367800    0.57011500    0.18545500
 C                 -3.04767600    2.90806200    0.81908500
 H                 -3.85871400    2.82001500    1.54556900
 H                 -2.26454500    3.53119400    1.26028300
 O                 -3.58882100    3.50576900   -0.35372200
 H                 -2.92876300    4.08170300   -0.75292900
 N                  0.62272000    0.29889400   -0.50185500
 C                  2.02639100    0.12423700   -0.30306200
 C                  2.47965200   -0.78234800    0.65700200
 C                  2.92518600    0.86409100   -1.07375300
 C                  3.84378300   -0.95593300    0.84861000
 H                  1.77348200   -1.34433400    1.25277700
 C                  4.29061600    0.70228500   -0.88158200
 H                  2.56112300    1.55574600   -1.82126600
 C                  4.72803800   -0.20774900    0.07668300
 H                  4.21774000   -1.65095900    1.58650300
 H                  5.00486600    1.26304500   -1.46711800
 Br                -3.71075800   -2.19392700   -0.16951200
 N                  6.17546500   -0.38512600    0.28020300
 O                  6.54586300   -1.21052200    1.10924100
 O                  6.94135600    0.30140100   -0.38904800
```

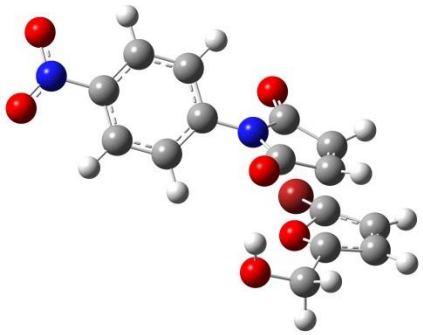
Pre-complex of Exo-TS36

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.243876 (Hartree/Particle)
 Thermal correction to Energy=                    0.267431
 Thermal correction to Enthalpy=                  0.268407
 Thermal correction to Gibbs Free Energy=         0.180677
 Sum of electronic and zero-point Energies=          -3713.181328
 Sum of electronic and thermal Energies=             -3713.157773
 Sum of electronic and thermal Enthalpies=           -3713.156798
 Sum of electronic and thermal Free Energies=        -3713.244527

0 1
 C                  3.23947500   -0.74634500    1.82312300
 C                  4.31290500    0.17907000    1.59715200
 C                  3.25515100   -1.64264700    0.79884800
 C                  4.89733000   -0.23089800    0.44180600
 H                  2.54541900   -0.74168000    2.64921100
 H                  4.60402600    1.02061800    2.20353400
 C                  0.47600700    1.45596700   -0.27441100
 C                 -0.03816800    2.68393800   -0.22288400
 H                  1.50969400    1.14886300   -0.32603100
 H                  0.46831600    3.63742800   -0.23183000
 C                 -1.52763500    2.58459200   -0.15117700
 C                 -0.63905400    0.46368300   -0.23623500
```

O	-0.56543200	-0.74674000	-0.25120000
O	-2.33612300	3.47836800	-0.10517600
O	4.28614000	-1.32917000	-0.06494300
N	-1.83121700	1.20107000	-0.16221400
C	2.41153600	-2.81863600	0.44726400
H	3.04429000	-3.67951400	0.22004200
H	1.80209700	-3.06913900	1.32191400
O	1.59677900	-2.61677900	-0.71146000
H	0.92718900	-1.94242600	-0.50875400
C	-3.13856300	0.64823400	-0.11527300
C	-3.50187500	-0.34984700	-1.02496800
C	-4.05069700	1.10889200	0.83931500
C	-4.77641900	-0.89605100	-0.97686300
H	-2.79550600	-0.69384000	-1.76731100
C	-5.33116100	0.57570300	0.88325700
H	-3.76042200	1.87380600	1.54578900
C	-5.67483400	-0.42285400	-0.02413600
H	-5.07547900	-1.66712700	-1.67222200
H	-6.04925000	0.91740400	1.61480800
N	-7.02769100	-0.99512200	0.02487500
O	-7.81301700	-0.55497300	0.85980800
O	-7.30850300	-1.88661800	-0.77132100
Br	6.35512100	0.44127000	-0.53035300

Exo-TS36



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.244466 (Hartree/Particle)
Thermal correction to Energy= 0.266005
Thermal correction to Enthalpy= 0.266980
Thermal correction to Gibbs Free Energy= 0.190187
Sum of electronic and zero-point Energies= -3713.137104
Sum of electronic and thermal Energies= -3713.115565
Sum of electronic and thermal Enthalpies= -3713.114590
Sum of electronic and thermal Free Energies= -3713.191383

0 1

C	-4.08949000	1.24399300	0.17349800
C	-4.16790100	-0.11825800	0.22371700

C	-2.79377500	1.57016500	-0.34177300
C	-2.89656700	-0.58937000	-0.22618900
H	-4.80205000	1.96225100	0.55039000
H	-4.94511100	-0.73658500	0.64408000
C	-1.74318400	1.22996800	1.51409800
C	-1.86214500	-0.17534000	1.62636600
H	-2.27402600	1.94433100	2.12540700
H	-2.53207100	-0.68840600	2.29888200
C	-0.52264400	-0.76908800	1.40612800
C	-0.32490900	1.52756200	1.18872500
O	0.21350500	2.61600700	1.07873100
O	-0.17692500	-1.92421600	1.50872300
O	-2.27018200	0.42322500	-0.89610600
N	0.33977200	0.29919500	1.03875200
C	-2.45453700	2.88401300	-1.00932900
H	-3.05918700	2.95316900	-1.91845500
H	-2.77599100	3.68880500	-0.33971300
O	-1.10763000	3.03265300	-1.41229400
H	-0.57147000	3.22190800	-0.62888700
C	1.69020600	0.15221300	0.62740200
C	2.13432100	0.80190200	-0.52932500
C	2.56532500	-0.63988000	1.37783900
C	3.45392300	0.66749500	-0.93509400
H	1.44847300	1.39973800	-1.11366800
C	3.88368700	-0.78871900	0.97008100
H	2.21824000	-1.13201300	2.27497400
C	4.31081300	-0.12960600	-0.17964000
H	3.81317200	1.15969900	-1.82744100
H	4.57459700	-1.39530000	1.53783000
N	5.70729900	-0.28004200	-0.60933500
O	6.44210500	-1.00949300	0.05126300
O	6.07537100	0.33089600	-1.60919100
Br	-2.56950700	-2.32761500	-0.90563900

Product of Exo-TS36

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.247724 (Hartree/Particle)
Thermal correction to Energy= 0.268655
Thermal correction to Enthalpy= 0.269630
Thermal correction to Gibbs Free Energy= 0.194234
Sum of electronic and zero-point Energies= -3713.176129
Sum of electronic and thermal Energies= -3713.155198
Sum of electronic and thermal Enthalpies= -3713.154223
Sum of electronic and thermal Free Energies= -3713.229620

0 1

C	-4.06803200	1.31075800	0.62282700
C	-4.19106000	-0.01360000	0.62046000
C	-2.68502200	1.61642400	0.04440300
C	-2.87126900	-0.52543100	0.06615600
H	-4.74210700	2.05339500	1.02646500
H	-4.97576800	-0.63938700	1.01828800

C	-1.66761100	1.21386200	1.18968000
C	-1.81394700	-0.32935300	1.21789000
H	-1.90079800	1.71157400	2.13049900
H	-2.17232100	-0.74655600	2.15732700
C	-0.41930700	-0.86783400	0.94282200
C	-0.20350900	1.45821300	0.86432100
O	0.34953500	2.53338700	0.75900600
O	-0.06561400	-2.01951700	0.92948600
O	-2.49518600	0.49202100	-0.85624400
N	0.43872400	0.22854400	0.72914300
C	-2.58179100	2.96138200	-0.66239900
H	-3.40192100	3.01495900	-1.38089900
H	-2.74189100	3.74659800	0.08606500
O	-1.38963900	3.17767300	-1.39766900
H	-0.66711200	3.32535500	-0.77190600
C	1.83231900	0.09299500	0.43590600
C	2.33668800	0.62380000	-0.75192200
C	2.66347100	-0.56775400	1.34121200
C	3.68940800	0.49865200	-1.03914800
H	1.67742600	1.12438800	-1.44826000
C	4.01571200	-0.70452900	1.05638200
H	2.25980100	-0.96730700	2.26166000
C	4.50671100	-0.16616100	-0.12947300
H	4.10374500	0.90021900	-1.95265100
H	4.67988700	-1.21158900	1.74130500
N	5.94151500	-0.30569800	-0.43301400
O	6.64406800	-0.91607700	0.36640000
O	6.36368400	0.19524000	-1.47031500
Br	-2.95119900	-2.25948400	-0.81430900

DA reaction of bromo-substituted α-furfuryl alcohols **3** and N-(benzyl)-maleimide **7**

Pre-complex of Endo-TS37

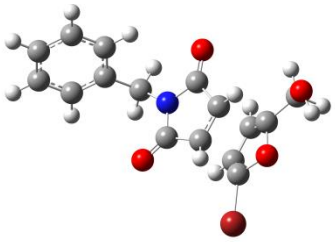
```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.269728 (Hartree/Particle)
 Thermal correction to Energy=                    0.292503
 Thermal correction to Enthalpy=                  0.293478
 Thermal correction to Gibbs Free Energy=         0.205514
 Sum of electronic and zero-point Energies=          -3547.912379
 Sum of electronic and thermal Energies=             -3547.889604
 Sum of electronic and thermal Enthalpies=           -3547.888628
 Sum of electronic and thermal Free Energies=        -3547.976592

0 1
```

C	-3.36899500	0.88470500	1.41252000
C	-4.53844400	0.09176500	1.66241200
C	-3.42741600	1.29255800	0.11598500
C	-5.21775300	0.07771800	0.48639900
H	-2.58488600	1.11978400	2.11533100
H	-4.82846800	-0.39287000	2.57982700
C	1.06903100	-0.27849700	-0.88700600
C	1.60751500	-1.37039300	-1.43134500

C	1.96563500	0.18515600	0.22340000
C	2.88170400	-1.69030400	-0.71006500
H	0.15287500	0.23782800	-1.14523300
H	1.24311700	-1.97643700	-2.24776400
O	3.63879400	-2.61872300	-0.89915000
O	1.81233000	1.13663100	0.96018900
O	-4.57751400	0.79651300	-0.46782800
C	-2.53586300	2.10542900	-0.75269700
H	-3.11554600	2.86444100	-1.28827100
H	-1.80835600	2.61444200	-0.12106500
O	-1.77179700	1.32239300	-1.68744800
H	-2.36974100	0.96862400	-2.35562400
N	3.04212300	-0.70328500	0.26355500
C	4.14061000	-0.65469100	1.22691300
H	4.29834000	-1.66345100	1.61091900
H	3.79060300	-0.03368400	2.05427800
C	5.43714300	-0.10426300	0.66111200
C	5.46921800	1.12625400	-0.00539900
C	6.63041500	-0.80985400	0.83432300
C	6.67093100	1.63689200	-0.49184600
H	4.55351700	1.69057700	-0.14531000
C	7.83636000	-0.29778600	0.35311100
H	6.61862600	-1.76684300	1.34547500
C	7.85934000	0.92640200	-0.31280600
H	6.68061500	2.59066400	-1.00745300
H	8.75351200	-0.85869900	0.49374100
H	8.79416700	1.32421200	-0.69113800
Br	-6.83326600	-0.73190400	-0.01710800

Endo-TS37



---

opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.270415 (Hartree/Particle)
Thermal correction to Energy= 0.291028
Thermal correction to Enthalpy= 0.292003
Thermal correction to Gibbs Free Energy= 0.216692
Sum of electronic and zero-point Energies= -3547.873428
Sum of electronic and thermal Energies= -3547.852815
Sum of electronic and thermal Enthalpies= -3547.851839
Sum of electronic and thermal Free Energies= -3547.927150

0 1

C	-1.80830100	1.01101700	1.67985100

C	-1.89210200	-0.35230000	1.56123100
C	-2.30159700	1.56262500	0.46012800
C	-2.40754500	-0.58781400	0.25543900
H	-1.34644100	1.57632200	2.47517900
H	-1.52009600	-1.11045700	2.23178200
C	-0.60760000	1.22352300	-0.79345600
C	-0.68228200	-0.17374900	-0.95288600
C	0.60648800	1.51847900	0.01537400
C	0.48605200	-0.77135100	-0.25012800
H	-0.94950900	1.94934000	-1.51684400
H	-1.09074200	-0.67633900	-1.81733900
O	0.82275900	-1.93856400	-0.18384600
O	1.06369800	2.59996500	0.33676200
O	-2.99873300	0.56462200	-0.19209100
C	-2.78990400	2.96633100	0.22359800
H	-3.73541000	3.10421200	0.76194200
H	-2.06044900	3.65792200	0.64653100
O	-2.93918900	3.29809400	-1.14926900
H	-3.71166500	2.83927300	-1.49911900
N	1.16748300	0.28462300	0.36605000
C	2.32773200	0.11743400	1.24202000
H	2.12853900	-0.72917700	1.89981100
H	2.37872900	1.01890700	1.85545200
C	3.63784500	-0.09494600	0.50455300
C	4.12512800	0.86861800	-0.38707400
C	4.39325000	-1.24803800	0.73164500
C	5.34078600	0.67737000	-1.04091100
H	3.55421300	1.77312000	-0.56628400
C	5.61392000	-1.43925400	0.08227300
H	4.02534700	-2.00324000	1.41822800
C	6.08960700	-0.47766300	-0.80744400
H	5.70648800	1.43191000	-1.72849300
H	6.18782200	-2.34011300	0.26873300
H	7.03607300	-0.62507200	-1.31529000
Br	-3.23292600	-2.19581700	-0.32326700

Product of Endo-TS37

```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.274121 (Hartree/Particle)
 Thermal correction to Energy=                    0.293986
 Thermal correction to Enthalpy=                  0.294961
 Thermal correction to Gibbs Free Energy=         0.221433
 Sum of electronic and zero-point Energies=          -3547.912840
 Sum of electronic and thermal Energies=             -3547.892975
 Sum of electronic and thermal Enthalpies=           -3547.892000
 Sum of electronic and thermal Free Energies=        -3547.965528
0 1
```

C	-1.98705600	1.14047100	1.62807100
C	-2.12400300	-0.18427100	1.56981200
C	-2.02493600	1.63616600	0.18565800
C	-2.23635500	-0.50073000	0.08797200
H	-1.78509300	1.75797500	2.49225900

```
 H                -2.06266600   -0.91895500    2.35874200
 C                -0.67217700    1.20695500   -0.51249200
 C                -0.82831300   -0.32408600   -0.59101900
 C                 0.60287600    1.43310500    0.27507200
 C                 0.36862000   -0.88440300    0.15961900
 H                -0.60307400    1.69441000   -1.48434000
 H                -0.85292700   -0.71438100   -1.60731100
 O                 0.63375400   -2.04962300    0.36106100
 O                 1.09592000    2.49626700    0.58726900
 O                -2.90925400    0.64855000   -0.42302700
 C                -2.51643100    3.04597200   -0.07054500
 H                -3.50721500    3.16196200    0.38155400
 H                -1.83510400    3.74754800    0.41424200
 O                -2.53811100    3.38264300   -1.45186400
 H                -3.22516100    2.86142500   -1.88366300
 N                 1.14206900    0.18804300    0.59701800
 C                 2.37545000    0.01955100    1.38284400
 H                 2.22631000   -0.84775800    2.02524600
 H                 2.46493200    0.90735200    2.00863900
 C                 3.60970000   -0.16062200    0.52068800
 C                 4.23378400    0.94645700   -0.06696000
 C                 4.14261300   -1.43480500    0.30271300
 C                 5.36497400    0.77987500   -0.86400200
 H                 3.83337200    1.93992000    0.10275700
 C                 5.27643000   -1.60263900   -0.49268400
 H                 3.66842100   -2.29805900    0.75634800
 C                 5.88855900   -0.49577300   -1.07949100
 H                 5.84082300    1.64524200   -1.31158200
 H                 5.68057300   -2.59608500   -0.65171500
 H                 6.77022200   -0.62482600   -1.69710000
 Br               -3.19168000   -2.13091700   -0.37949300
```

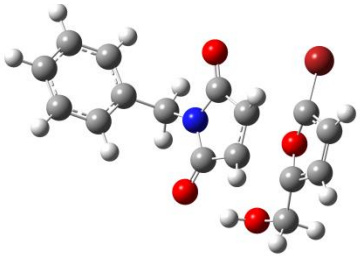
Pre-complex of Exo-TS37

```
---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.270470 (Hartree/Particle)
 Thermal correction to Energy=                    0.292754
 Thermal correction to Enthalpy=                  0.293730
 Thermal correction to Gibbs Free Energy=         0.207496
 Sum of electronic and zero-point Energies=          -3547.915207
 Sum of electronic and thermal Energies=             -3547.892923
 Sum of electronic and thermal Enthalpies=           -3547.891948
 Sum of electronic and thermal Free Energies=        -3547.978181

0 1
 C                -2.94997000   -2.06224100    0.35528800
 C                -3.57693500   -1.27880600   -0.67079100
 C                -2.62188700   -1.21448800    1.36834700
 C                -3.57678700   -0.00667900   -0.19548600
 H                -2.76832500   -3.12563500    0.33625900
 H                -3.96748500   -1.61327400   -1.61755900
 C                 2.48927000   -3.33044200   -0.70882200
 C                 3.08053400   -2.85933200   -1.80592500
```

H	2.45689500	-4.33977100	-0.32666700
H	3.65516900	-3.38548900	-2.55349700
C	2.82089600	-1.38502700	-1.88818100
C	1.81330500	-2.19246200	-0.00643100
O	1.16488700	-2.24408300	1.02220500
O	3.16734700	-0.60850100	-2.74938000
O	-3.01104800	0.06773700	1.03357000
N	2.06388900	-1.05172000	-0.75763900
C	-1.95090700	-1.39631400	2.68534600
H	-2.53444800	-0.91568500	3.47371400
H	-1.91411500	-2.46973400	2.89907600
O	-0.64725700	-0.80987400	2.75316000
H	-0.05990500	-1.28434800	2.14221000
Br	-4.20636300	1.60304400	-0.92759700
C	1.56632500	0.29379900	-0.46494400
H	0.74995900	0.17048300	0.24885000
H	1.14329400	0.70242600	-1.38340700
C	2.62079500	1.23438700	0.08863800
C	3.39682700	0.87766800	1.19724100
C	2.80420900	2.49324300	-0.48855700
C	4.33961700	1.76335400	1.71512200
H	3.26618800	-0.09410600	1.66115300
C	3.74391100	3.38422900	0.03173200
H	2.21257000	2.77910500	-1.35197700
C	4.51514700	3.02055400	1.13418300
H	4.93418600	1.47415600	2.57444100
H	3.87584000	4.35697700	-0.42854400
H	5.24813700	3.70950800	1.53833700

Exo-TS37



```
---------------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.271141 (Hartree/Particle)
 Thermal correction to Energy=                    0.291340
 Thermal correction to Enthalpy=                  0.292316
 Thermal correction to Gibbs Free Energy=         0.218398
 Sum of electronic and zero-point Energies=          -3547.870868
 Sum of electronic and thermal Energies=             -3547.850669
 Sum of electronic and thermal Enthalpies=           -3547.849694
 Sum of electronic and thermal Free Energies=        -3547.923612

0 1
 C                 -3.38882300    1.33307600    1.15367800
```

C	-3.45911400	-0.02684000	1.26901600
C	-2.48042600	1.61588000	0.08550100
C	-2.55462800	-0.53800300	0.29081200
H	-3.82842600	2.07553700	1.80271600
H	-3.95991100	-0.61700900	2.02002700
C	-0.68156600	1.27142800	1.25026800
C	-0.75589600	-0.12687800	1.43729400
H	-0.86234300	2.00992100	2.01687400
H	-1.04492500	-0.61778300	2.35372300
C	0.32343400	-0.74616500	0.62212000
C	0.42921200	1.52222300	0.28784100
O	0.84979400	2.59900400	-0.11734900
O	0.65929200	-1.91107100	0.55938600
O	-2.29472400	0.44762000	-0.61891600
N	0.93705800	0.29119600	-0.09841900
C	-2.45579500	2.91204500	-0.69368200
H	-3.42093200	3.01058400	-1.19946100
H	-2.38042600	3.73144000	0.02994100
O	-1.46765500	2.99728100	-1.69997700
H	-0.60488700	3.11173100	-1.27281000
Br	-2.61364800	-2.29431200	-0.42092900
C	1.98123300	0.09193900	-1.10587900
H	1.95630100	0.97178600	-1.75119900
H	1.70168700	-0.77552100	-1.70430500
C	3.37018100	-0.10066500	-0.52390300
C	3.96174100	0.89422300	0.26422400
C	4.08973100	-1.26779500	-0.79179200
C	5.24515900	0.71991700	0.77800100
H	3.41800100	1.80912500	0.47283100
C	5.37768600	-1.44212700	-0.28284200
H	3.64100100	-2.04688900	-1.39889600
C	5.95750400	-0.44949900	0.50523800
H	5.69169000	1.49835200	1.38660700
H	5.92318000	-2.35398300	-0.49875500
H	6.95682000	-0.58396500	0.90363200

Product of Exo-TS37

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.274900 (Hartree/Particle)
Thermal correction to Energy= 0.294309
Thermal correction to Enthalpy= 0.295284
Thermal correction to Gibbs Free Energy= 0.223582
Sum of electronic and zero-point Energies= -3547.912314
Sum of electronic and thermal Energies= -3547.892904
Sum of electronic and thermal Enthalpies= -3547.891929
Sum of electronic and thermal Free Energies= -3547.963631

0 1

C	-3.02509900	1.44154700	1.51805600
C	-3.25858400	0.13226500	1.50445600
C	-2.00748900	1.71061800	0.40690600
C	-2.36113400	-0.41004200	0.40347600

H	-3.38644600	2.18682000	2.21292400
H	-3.84746300	-0.47558200	2.17492000
C	-0.63655300	1.15280700	0.96268400
C	-0.89817500	-0.37705300	0.98278600
H	-0.38684500	1.58471000	1.93166600
H	-0.85336700	-0.84505600	1.96459900
C	0.19254300	-0.97025300	0.10214400
C	0.55674000	1.31840600	0.03194100
O	1.09059300	2.36584500	-0.28908900
O	0.39991500	-2.14007800	-0.12234600
O	-2.33379900	0.65620000	-0.54051200
N	0.97028800	0.07413500	-0.39837700
C	-2.10047800	3.10366500	-0.20144600
H	-3.14270900	3.27021400	-0.48046500
H	-1.84614000	3.82569000	0.58439900
O	-1.33222400	3.31743300	-1.37243400
H	-0.39576600	3.31356800	-1.12505000
Br	-2.97244700	-2.05765300	-0.43595000
C	2.12057700	-0.13379500	-1.29661200
H	2.14567600	0.71877200	-1.97434200
H	1.90333600	-1.03295200	-1.87207000
C	3.43575000	-0.27093300	-0.55476000
C	4.24241000	0.84988400	-0.33055500
C	3.86067600	-1.51906700	-0.08531500
C	5.45058700	0.72720300	0.35519600
H	3.92283100	1.81991900	-0.69447000
C	5.06802200	-1.64254300	0.60123100
H	3.24520100	-2.39459800	-0.25939500
C	5.86495700	-0.51930800	0.82423800
H	6.06816900	1.60308300	0.51932200
H	5.38791400	-2.61536800	0.95741000
H	6.80485300	-0.61590800	1.35592600

DA reaction of methoxy-substituted α-furfuryl alcohols **4** and N-(p-methoxyphenyl)-maleimide **5**

Pre-complex of Endo-TS45

---

opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

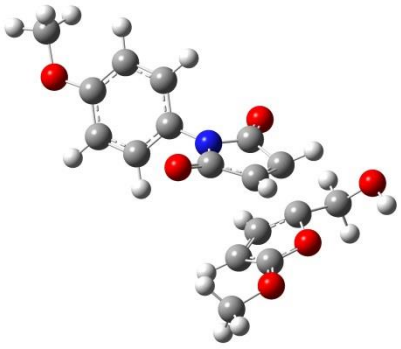
Zero-point correction= 0.315566 (Hartree/Particle)
Thermal correction to Energy= 0.341085
Thermal correction to Enthalpy= 0.342060
Thermal correction to Gibbs Free Energy= 0.250085
Sum of electronic and zero-point Energies= -1164.120095
Sum of electronic and thermal Energies= -1164.094576
Sum of electronic and thermal Enthalpies= -1164.093601
Sum of electronic and thermal Free Energies= -1164.185576

0 1

C	4.58307600	-1.56527500	0.11093200
C	5.85678300	-1.60134000	0.77871100
C	4.62820800	-0.56566000	-0.80652000
C	6.58545700	-0.59961600	0.20619100
H	3.73889000	-2.21142000	0.29730200

H	6.17285900	-2.27295300	1.55860300
C	-0.01647800	1.57232000	-0.17929800
C	-0.57249100	2.56940100	0.50964100
C	-1.05526800	0.51632000	-0.40838800
C	-2.00754500	2.23652500	0.77645000
H	0.99813200	1.47106600	-0.54472300
H	-0.12778500	3.49222200	0.85232200
O	-2.82959900	2.89786600	1.37127600
O	-0.93023200	-0.53728700	-0.99247600
O	5.87966300	0.04056900	-0.75277000
C	3.66299200	-0.00756200	-1.78327000
H	4.13409500	0.11237700	-2.76496800
H	2.83074100	-0.70341400	-1.88726400
O	3.07538000	1.24794500	-1.37681600
H	3.76619500	1.92054600	-1.36856200
N	-2.23500300	0.98079300	0.19349000
C	-3.48351500	0.28032300	0.21080600
C	-3.78209900	-0.59189700	1.26118800
C	-4.40235100	0.46739600	-0.81612400
C	-4.99190800	-1.26863800	1.27955800
H	-3.06519300	-0.73703400	2.06070300
C	-5.62226600	-0.20886200	-0.80704100
H	-4.16922700	1.14437800	-1.62956100
C	-5.92054900	-1.08150200	0.24508000
H	-5.23641600	-1.94732600	2.08765700
H	-6.32080200	-0.04656100	-1.61596100
O	-7.07766500	-1.78874700	0.35183800
C	-8.07075900	-1.64053900	-0.66765800
H	-8.89228600	-2.29099100	-0.37537600
H	-8.42493000	-0.60751500	-0.72462600
H	-7.68493900	-1.95425400	-1.64151600
O	7.81768500	-0.11323300	0.36653500
C	8.60841700	-0.75945300	1.37830800
H	8.74644200	-1.81600500	1.13621900
H	9.56775600	-0.24866000	1.37704200
H	8.13141100	-0.65854200	2.35619300

Endo-TS45



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 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308
```

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 ---------------------------------------------------------------------
Zero-point correction=                           0.315991 (Hartree/Particle)
 Thermal correction to Energy=                    0.339463
 Thermal correction to Enthalpy=                  0.340438
 Thermal correction to Gibbs Free Energy=         0.260357
 Sum of electronic and zero-point Energies=          -1164.087072
 Sum of electronic and thermal Energies=             -1164.063600
 Sum of electronic and thermal Enthalpies=           -1164.062625
 Sum of electronic and thermal Free Energies=        -1164.142706

0 1
 C                 -1.92190900    0.20726900    1.56293500
 C                 -2.22478600   -1.10998100    1.32069100
 C                 -2.67409800    1.00260100    0.62824800
 C                 -3.28673100   -1.09461700    0.38690300
 H                 -1.14546400    0.58816900    2.20843200
 H                 -1.76083800   -1.99022000    1.73398400
 C                 -1.64112600    1.03740700   -0.91493100
 C                 -1.58689700   -0.25571900   -1.50860300
 C                 -0.22895100    1.34459900   -0.45677700
 C                 -0.27200400   -0.80131400   -1.35789600
 H                 -2.16348700    1.85827300   -1.39596100
 H                 -2.31337200   -0.68652600   -2.17912400
 O                  0.22419000   -1.85192800   -1.75230000
 O                  0.18426000    2.39576300    0.00256100
 O                 -3.71328200    0.14483100    0.15725700
 C                 -3.17267200    2.39698300    0.94964300
 H                 -3.86565300    2.34697700    1.79540200
 H                 -2.31159800    2.99748600    1.24626700
 O                 -3.77852000    3.05324200   -0.15710100
 H                 -4.65208000    2.67269900   -0.30362600
 N                  0.50275300    0.18460700   -0.63320700
 C                  1.87583100    0.02441600   -0.27775900
 C                  2.23662500   -0.86338500    0.74054200
 C                  2.86565600    0.74249400   -0.94218100
 C                  3.56980300   -1.02907500    1.08474800
 H                  1.46903100   -1.42282400    1.26162800
 C                  4.20915600    0.59275500   -0.59553500
 H                  2.59216500    1.42526400   -1.73762000
 C                  4.56561800   -0.29848100    0.42144300
 H                  3.85891800   -1.71627700    1.87088800
 H                  4.95711000    1.16625400   -1.12534600
 O                  5.84442300   -0.52336700    0.83560600
 C                  6.90552100    0.19937200    0.20577100
 H                  7.81955700   -0.13317400    0.69332200
 H                  6.95848800   -0.02807200   -0.86264500
 H                  6.78686700    1.27721800    0.34842300
 O                 -4.04421200   -2.03593100   -0.11215400
 C                 -3.66860600   -3.41000100    0.16061800
 H                 -3.70369700   -3.59975300    1.23357100
 H                 -4.40911400   -4.01473500   -0.35370100
 H                 -2.67356900   -3.60582600   -0.23955200
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Product of Endo-TS45

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```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------

 Zero-point correction=                           0.319619 (Hartree/Particle)
 Thermal correction to Energy=                    0.342296
 Thermal correction to Enthalpy=                  0.343272
 Thermal correction to Gibbs Free Energy=         0.265260
 Sum of electronic and zero-point Energies=          -1164.114653
 Sum of electronic and thermal Energies=             -1164.091976
 Sum of electronic and thermal Enthalpies=           -1164.091000
 Sum of electronic and thermal Free Energies=        -1164.169012

0 1
 C                 -2.22550700   -0.43790700   -1.69054700
 C                 -2.24648900    0.88240500   -1.50757200
 C                 -2.82143000   -1.05273400   -0.42895600
 C                 -2.84706200    1.09026000   -0.11591800
 H                 -1.79529600   -0.99717400   -2.51020900
 H                 -1.83320400    1.65482600   -2.13985300
 C                 -1.76466700   -0.89994100    0.73777800
 C                 -1.75959700    0.62173000    0.95870100
 C                 -0.33553400   -1.26790000    0.40252300
 C                 -0.31710700    1.04570200    0.75324400
 H                 -2.10377200   -1.47442600    1.59936300
 H                 -2.10047400    0.93189500    1.94675600
 O                  0.14797600    2.16060300    0.84544400
 O                  0.09986300   -2.36766900    0.14109200
 O                 -3.74819100   -0.01794600   -0.02242600
 C                 -3.51339700   -2.39445800   -0.55620100
 H                 -4.27380700   -2.32651900   -1.34190800
 H                 -2.77923500   -3.14480700   -0.85477700
 O                 -4.08282600   -2.84304900    0.66876100
 H                 -4.80371800   -2.24716300    0.90452000
 N                  0.43242800   -0.09693500    0.44268600
 C                  1.84143900   -0.06563700    0.16554200
 C                  2.29141800    0.17989400   -1.13365600
 C                  2.75486600   -0.28057700    1.19053300
 C                  3.65133900    0.20986800   -1.40039300
 H                  1.57634200    0.34587100   -1.93049000
 C                  4.12513900   -0.25354400    0.93124100
 H                  2.40159200   -0.47059300    2.19714700
 C                  4.57754200   -0.00673700   -0.36946100
 H                  4.01650100    0.39915800   -2.40248900
 H                  4.81862900   -0.42351100    1.74282100
 O                  5.88782600    0.04180600   -0.73081300
 C                  6.88698800   -0.17036700    0.27150400
 H                  7.84203000   -0.08466000   -0.24226000
 H                  6.82465800    0.58880400    1.05598300
 H                  6.79715400   -1.16722200    0.71191900
 O                 -3.56494700    2.22969100    0.17372700
 C                 -2.86567300    3.47678900    0.04368500
 H                 -2.58316400    3.66357900   -0.99608900
 H                 -3.56727500    4.24314000    0.36680800
 H                 -1.97517700    3.49879400    0.67538900
```

Pre-complex of Exo-TS45

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---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.315385 (Hartree/Particle)
 Thermal correction to Energy=                    0.341012
 Thermal correction to Enthalpy=                  0.341987
 Thermal correction to Gibbs Free Energy=         0.250303
 Sum of electronic and zero-point Energies=          -1164.116579
 Sum of electronic and thermal Energies=             -1164.090952
 Sum of electronic and thermal Enthalpies=           -1164.089977
 Sum of electronic and thermal Free Energies=        -1164.181660

0 1
 C                  3.95509500   -0.62242300   -0.90164500
 C                  2.74753500   -1.31851000    0.87049000
 C                  2.71707500   -1.01455300   -1.31112300
 O                  1.96455500   -1.44446100   -0.26667800
 H                  4.75703400   -0.24902500   -1.51564500
 C                  1.22108500    2.93393300    1.12378300
 C                  1.09191200    3.29218500   -0.15298900
 N                 -0.61010500    1.77486500    0.28868400
 C                  0.14128600    1.95127400    1.45973500
 C                 -0.08108900    2.56840600   -0.74025800
 O                 -0.06380300    1.40409900    2.52043600
 O                 -0.50747900    2.63628200   -1.87132000
 H                  1.95144500    3.25280800    1.85260700
 H                  1.68991500    3.97865900   -0.73391800
 C                  3.96207900   -0.82349100    0.52761200
 H                  4.77688400   -0.61912200    1.20403000
 C                 -1.75271600    0.91974600    0.16511300
 C                 -3.03764500    1.44424700    0.32926100
 C                 -1.58453100   -0.43181600   -0.11582700
 C                 -4.14461900    0.61830900    0.20975800
 H                 -3.16583900    2.49729900    0.55033600
 C                 -2.69261900   -1.27125500   -0.23345800
 H                 -0.58663500   -0.83484600   -0.24302700
 C                 -3.97907300   -0.74588400   -0.07138000
 H                 -5.14665300    1.01080800    0.33355900
 H                 -2.53934500   -2.31904800   -0.45098700
 O                 -5.12406800   -1.47464000   -0.16644600
 C                 -5.02729600   -2.87410100   -0.44852600
 H                 -4.47234000   -3.39636400    0.33572900
 H                 -6.05123300   -3.24062600   -0.47486500
 H                 -4.55177000   -3.04838800   -1.41765700
 C                  2.10388600   -1.72330700    2.15887800
 H                  1.46325400   -2.59706900    1.98607000
 H                  1.46735500   -0.92372400    2.54872000
 O                  3.06814600   -1.97574400    3.17848000
 H                  3.63730100   -2.69787300    2.88640700
 O                  2.07528300   -1.08182900   -2.48104600
 C                  2.82075400   -0.61126000   -3.61557300
 H                  3.72116400   -1.21432000   -3.75701400
```
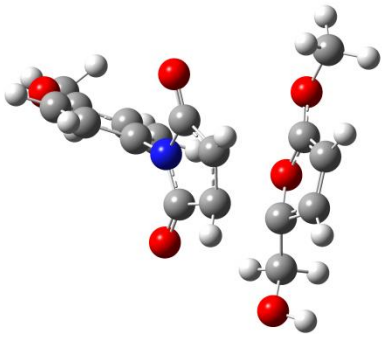

H	2.16078400	-0.72107700	-4.47220600
H	3.09162900	0.43920600	-3.48343600

Exo-TS45



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.316290 (Hartree/Particle)
Thermal correction to Energy= 0.339717
Thermal correction to Enthalpy= 0.340693
Thermal correction to Gibbs Free Energy= 0.261050
Sum of electronic and zero-point Energies= -1164.082966
Sum of electronic and thermal Energies= -1164.059539
Sum of electronic and thermal Enthalpies= -1164.058563
Sum of electronic and thermal Free Energies= -1164.138206

0 1

C	3.89503200	1.07438800	-0.21287800
C	2.80338500	-0.89460900	-0.48327200
C	2.60299900	1.27399800	-0.75870600
O	2.06076900	0.12025100	-1.14357800
H	4.57555400	1.85015300	0.09763100
C	1.86859000	-0.89750900	1.16563000
C	1.75141700	0.44026400	1.64154800
N	-0.34357300	-0.18766100	0.90601500
C	0.44898700	-1.31383300	0.80480800
C	0.40507700	0.90217800	1.48247200
O	0.06839600	-2.42741900	0.48711100
O	-0.11705600	1.97712500	1.75932600
H	2.43793800	-1.65680400	1.68962400
H	2.46865900	0.98101400	2.23726700
C	4.05785700	-0.28433800	-0.13182100
H	4.90030100	-0.81118700	0.28957100
C	-1.72895300	-0.13329600	0.56702400
C	-2.69778400	-0.06889400	1.57358800
C	-2.12671400	-0.14614300	-0.76630700
C	-4.04424700	-0.01524700	1.24564800
H	-2.39243100	-0.06205800	2.61298600
C	-3.47934600	-0.10418200	-1.10747300
H	-1.37860400	-0.18887300	-1.54901600

```
 C                 -4.44454800   -0.03525100   -0.09781400
 H                 -4.80214400    0.03704900    2.01812100
 H                 -3.76031400   -0.11943400   -2.15144200
 O                 -5.78842300    0.01583500   -0.31828300
 C                 -6.26340600   -0.00076800   -1.66695200
 H                 -5.97036500   -0.92277600   -2.17703300
 H                 -7.34820600    0.04724900   -1.59855900
 H                 -5.89444500    0.86391600   -2.22576500
 C                  2.70300300   -2.24117400   -1.18287300
 H                  3.09500500   -2.14611400   -2.20000900
 H                  1.66230600   -2.55557800   -1.24161400
 O                  3.40300500   -3.24028500   -0.45020500
 H                  4.33241100   -3.22485100   -0.70294600
 O                  1.96035600    2.34183200   -1.15720300
 C                  2.54536200    3.62790400   -0.83322100
 H                  3.51295100    3.73116100   -1.32504300
 H                  1.84625600    4.36412300   -1.21777000
 H                  2.64350600    3.72700100    0.24814900
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Product of Exo-TS45

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---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.319849 (Hartree/Particle)
 Thermal correction to Energy=                    0.342498
 Thermal correction to Enthalpy=                  0.343473
 Thermal correction to Gibbs Free Energy=         0.265715
 Sum of electronic and zero-point Energies=          -1164.113445
 Sum of electronic and thermal Energies=             -1164.090796
 Sum of electronic and thermal Enthalpies=           -1164.089821
 Sum of electronic and thermal Free Energies=        -1164.167579

0 1
 C                  4.15403900    0.72868400    0.05192200
 C                  2.76956900   -1.05034700   -0.34939400
 C                  2.72589600    1.11266300   -0.34172300
 O                  2.35735300    0.03614100   -1.20905900
 H                  4.92686800    1.41717600    0.36143600
 C                  1.85133000   -0.76827100    0.90882300
 C                  1.83052400    0.77788000    0.93501500
 N                 -0.37426500   -0.01058200    0.60168600
 C                  0.39822500   -1.17080900    0.70464100
 C                  0.37300600    1.16052300    0.76468600
 O                 -0.04713600   -2.29543100    0.64483000
 O                 -0.09673200    2.27628800    0.77906300
 H                  2.23207500   -1.24578100    1.81012700
 H                  2.22265700    1.23343000    1.84244600
 C                  4.17140800   -0.60193400    0.05845000
 H                  4.96784300   -1.26208300    0.37349100
 C                 -1.79724100   -0.02216600    0.40867000
 C                 -2.64815900   -0.15290900    1.50852500
 C                 -2.32529400    0.09603600   -0.87121600
 C                 -4.02169600   -0.16586600    1.32224800
 H                 -2.23303900   -0.24381500    2.50529500
```

C	-3.70621000	0.08556200	-1.06799700
H	-1.66121400	0.19670400	-1.72147300
C	-4.55997100	-0.04671400	0.03243700
H	-4.69524500	-0.26724700	2.16452300
H	-4.09637100	0.17897600	-2.07172100
O	-5.91762900	-0.07052900	-0.04750300
C	-6.53316800	0.03839300	-1.33475800
H	-6.23847200	-0.79136200	-1.98319400
H	-7.60487500	-0.00506700	-1.15313900
H	-6.28177500	0.98941500	-1.81228600
C	2.63811300	-2.38548000	-1.06781000
H	3.23186900	-2.34807200	-1.98582400
H	1.59767700	-2.56202300	-1.33969300
O	3.04060400	-3.46953300	-0.23293200
H	3.99527700	-3.57856400	-0.29558600
O	2.49545600	2.29262000	-1.01391100
C	2.82790000	3.49401700	-0.30256700
H	3.89071100	3.52392700	-0.04897700
H	2.59900600	4.31295600	-0.98154500
H	2.22190400	3.59347800	0.60070000

DA reaction of methoxy-substituted α-furfuryl alcohols **4** and N-(p-nitro)-maleimide **6**

Pre-complex of Endo-TS46

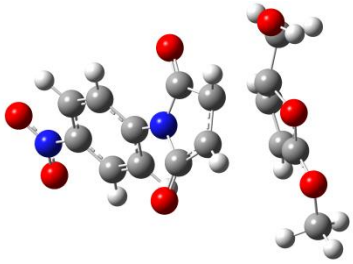
```
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.285521 (Hartree/Particle)
 Thermal correction to Energy=                    0.310906
 Thermal correction to Enthalpy=                  0.311881
 Thermal correction to Gibbs Free Energy=         0.219712
 Sum of electronic and zero-point Energies=          -1254.157871
 Sum of electronic and thermal Energies=             -1254.132486
 Sum of electronic and thermal Enthalpies=           -1254.131511
 Sum of electronic and thermal Free Energies=        -1254.223680

0 1
```

C	4.38389600	0.31528400	-1.61311000
C	5.31144500	-0.78230300	-1.68567400
C	4.78584100	1.12650500	-0.60163900
C	6.21614700	-0.54788100	-0.69144300
H	3.52256100	0.47433600	-2.24377700
H	5.29998900	-1.60951700	-2.37484700
C	0.55945800	0.36923200	1.35785000
C	0.20449200	-0.57210100	2.23120000
C	-0.62141000	0.70847300	0.50990300
C	-1.23237400	-0.91450500	2.02332200
H	1.51712300	0.85289800	1.22382200
H	0.79683900	-1.05133900	2.99632200
O	-1.89538600	-1.69849100	2.62527900
O	-0.68222200	1.49222500	-0.38618000
O	5.93302500	0.59276100	-0.02280300
C	4.27163300	2.38773700	-0.01579100

H	5.07407000	3.12906800	0.06887600
H	3.50587500	2.78947600	-0.67902600
O	3.63332000	2.22247900	1.26860200
H	4.30568100	1.96280900	1.90899800
N	-1.68444300	-0.10358500	0.96091300
C	-2.99770300	-0.10821400	0.42605700
C	-3.63639900	-1.32527100	0.16327900
C	-3.64589600	1.10417700	0.16489900
C	-4.92394200	-1.33281600	-0.35287500
H	-3.12814100	-2.25927200	0.35610600
C	-4.92794500	1.10230700	-0.36494300
H	-3.15335200	2.04189400	0.37928800
C	-5.55218900	-0.11752300	-0.61326900
H	-5.43088400	-2.26370300	-0.56287200
H	-5.44345700	2.02949800	-0.57042800
O	7.30260800	-1.17224400	-0.23256300
C	7.63690200	-2.39876600	-0.90371400
H	7.84392200	-2.21044300	-1.95998200
H	8.52978600	-2.77377500	-0.41039900
H	6.82259000	-3.12058000	-0.80456300
N	-6.91277100	-0.12240500	-1.16487900
O	-7.43521500	0.95698600	-1.42930000
O	-7.46536100	-1.20564500	-1.33604400

Endo-TS46



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 # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p)
scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.286105 (Hartree/Particle)
 Thermal correction to Energy=                    0.309438
 Thermal correction to Enthalpy=                  0.310414
 Thermal correction to Gibbs Free Energy=         0.230403
 Sum of electronic and zero-point Energies=          -1254.127362
 Sum of electronic and thermal Energies=             -1254.104030
 Sum of electronic and thermal Enthalpies=           -1254.103054
 Sum of electronic and thermal Free Energies=        -1254.183065
0 1
```

C	-2.03029400	-0.16918300	-1.57082700
C	-2.29676700	1.15901400	-1.34678400
C	-2.86690700	-0.93749900	-0.68851600
C	-3.41604400	1.18431600	-0.48268900
H	-1.23452800	-0.57898100	-2.17415000
H	-1.77919000	2.02027100	-1.73551900
C	-1.91682300	-1.04295700	0.91234900
C	-1.83098100	0.23111000	1.53904600

C	-0.50381400	-1.41585300	0.52366300
C	-0.50038800	0.73034900	1.46178400
H	-2.50516300	-1.84623300	1.34411600
H	-2.57672200	0.68867500	2.16924000
O	0.02245400	1.74530000	1.90494800
O	-0.12542800	-2.47739600	0.06621300
O	-3.88894700	-0.03704800	-0.26168000
C	-3.41263700	-2.30456600	-1.05153600
H	-4.06501700	-2.21129900	-1.92525500
H	-2.56742900	-2.93940800	-1.32086000
O	-4.09370600	-2.94592000	0.01874500
H	-4.96236200	-2.54107900	0.12301400
N	0.28042900	-0.28720100	0.74936700
C	1.65047700	-0.16708200	0.43978800
C	2.14305400	1.04813100	-0.06033400
C	2.52265900	-1.24970000	0.62889700
C	3.48781400	1.18228800	-0.36659800
H	1.47141800	1.88050600	-0.21053900
C	3.86740800	-1.12308300	0.31503500
H	2.14841800	-2.18308500	1.02200400
C	4.33702000	0.09265700	-0.17816800
H	3.87643700	2.11207500	-0.75703500
H	4.54861500	-1.94937100	0.46039700
O	-4.15552200	2.15244900	-0.01802200
C	-3.72248500	3.51375200	-0.27913100
H	-3.70657000	3.69761700	-1.35328300
H	-4.46405100	4.14383400	0.20176000
H	-2.73955600	3.67684500	0.16277300
N	5.75645700	0.22940200	-0.50530900
O	6.15790000	1.31665000	-0.91743700
O	6.48696700	-0.74852600	-0.35413500

Product of Endo-TS46

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 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.289478 (Hartree/Particle)
 Thermal correction to Energy=                    0.312055
 Thermal correction to Enthalpy=                  0.313031
 Thermal correction to Gibbs Free Energy=         0.234749
 Sum of electronic and zero-point Energies=          -1254.156791
 Sum of electronic and thermal Energies=             -1254.134214
 Sum of electronic and thermal Enthalpies=           -1254.133239
 Sum of electronic and thermal Free Energies=        -1254.211520

0 1
```

C	-2.28599700	0.55100800	1.60366800
C	-2.28781000	-0.77875300	1.52169600
C	-2.94636700	1.05439400	0.32365200
C	-2.92799700	-1.11222100	0.17299200
H	-1.82485000	1.18022500	2.35283000
H	-1.82438300	-1.49855300	2.18161300
C	-1.92415900	0.81729600	-0.86861600
C	-1.91952100	-0.71386200	-0.96998000

```
 C                 -0.48730300    1.21257800   -0.61392500
 C                 -0.47774000   -1.13293300   -0.77209600
 H                 -2.29486300    1.32482700   -1.75844000
 H                 -2.29640300   -1.10631600   -1.91434200
 O                 -0.02642200   -2.25376200   -0.76976300
 O                 -0.04215500    2.32768800   -0.47215500
 O                 -3.87190800   -0.01443200    0.03493100
 C                 -3.64243500    2.39911400    0.36652100
 H                 -4.37208700    2.39134700    1.18373600
 H                 -2.90501300    3.17660600    0.57397100
 O                 -4.26154100    2.74044300   -0.86871100
 H                 -4.97923100    2.11646700   -1.03007500
 N                  0.28667600    0.03488400   -0.57619000
 C                  1.69343200    0.02385600   -0.33812800
 C                  2.20604700    0.65506400    0.79743900
 C                  2.54026400   -0.61853400   -1.24428200
 C                  3.57459700    0.64958100    1.02971200
 H                  1.54069200    1.14258500    1.49646900
 C                  3.90902000   -0.63659900   -1.01330500
 H                  2.13385200   -1.09647700   -2.12502000
 C                  4.40543300    0.00068600    0.12052100
 H                  3.99207600    1.13057100    1.90254300
 H                  4.58231000   -1.12714800   -1.70140900
 N                  5.85616400   -0.01237700    0.36658000
 O                  6.57217400   -0.61521600   -0.42733500
 O                  6.28061100    0.57991500    1.35429400
 O                 -3.49033800   -2.33709000   -0.04937400
 C                 -4.43362300   -2.78347200    0.94294000
 H                 -5.28806700   -2.10633800    0.99401900
 H                 -4.76117600   -3.76878600    0.61823700
 H                 -3.96114700   -2.86013500    1.92522200
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Pre-complex of Exo-TS46

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---------------------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile)
geom=connectivity temperature=308
 ---------------------------------------------------------------------
Zero-point correction=                           0.284913 (Hartree/Particle)
 Thermal correction to Energy=                    0.310648
 Thermal correction to Enthalpy=                  0.311624
 Thermal correction to Gibbs Free Energy=         0.217937
 Sum of electronic and zero-point Energies=          -1254.154556
 Sum of electronic and thermal Energies=             -1254.128820
 Sum of electronic and thermal Enthalpies=           -1254.127845
 Sum of electronic and thermal Free Energies=        -1254.221532

0 1
 C                 -3.97152400   -0.04392500    1.63239500
 C                 -3.72048800   -0.90085700   -0.43817100
 C                 -2.77073400   -0.67932600    1.54376200
 O                 -2.58566800   -1.20448900    0.30237700
 H                 -4.36322800    0.45832500    2.50144600
 C                 -1.58038900    2.72752600   -1.16365700
 C                 -1.40372800    3.13554800    0.09215000
 N                  0.36991100    1.71411800   -0.40212500
```
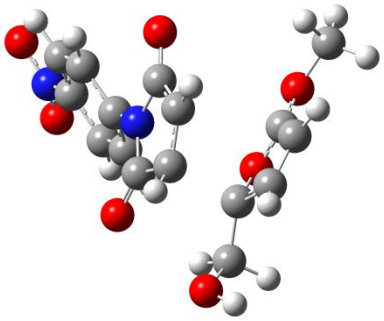

C	-0.46375600	1.80892200	-1.53936100
C	-0.15864600	2.51471200	0.63601600
O	-0.27708600	1.25629100	-2.59706900
O	0.31741600	2.64173800	1.73860200
H	-2.36723200	2.97874500	-1.85900200
H	-2.01380000	3.79850200	0.68718900
C	-4.57891600	-0.18906700	0.33945700
H	-5.54498100	0.18138900	0.03222000
C	1.55672600	0.94276000	-0.31816900
C	2.71218600	1.50401900	0.23682400
C	1.56360400	-0.37455400	-0.79001400
C	3.87204300	0.74835000	0.32830900
H	2.70529500	2.52511000	0.59071000
C	2.72478300	-1.12986700	-0.71412400
H	0.66611600	-0.80692800	-1.20871900
C	3.86361400	-0.55885500	-0.15172100
H	4.77340600	1.16643300	0.75307000
H	2.74721000	-2.14908700	-1.07233300
C	-3.77784200	-1.43667300	-1.82057900
H	-2.83325700	-1.25070500	-2.34333700
H	-4.57278100	-0.92147100	-2.35963200
O	-4.10222900	-2.84075500	-1.89184800
H	-3.36630400	-3.34067600	-1.52046900
N	5.09167400	-1.35899000	-0.06219400
O	6.07931800	-0.84926200	0.46049200
O	5.07396900	-2.50096100	-0.51405200
O	-1.77046500	-0.77947500	2.42387100
C	-1.07544900	-2.04644200	2.48225200
H	-0.55678900	-2.24508400	1.54404800
H	-0.35563400	-1.94708100	3.29107100
H	-1.78006200	-2.85167600	2.70275500

Exo-TS46



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opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.286408 (Hartree/Particle)
Thermal correction to Energy= 0.309701
Thermal correction to Enthalpy= 0.310677
Thermal correction to Gibbs Free Energy= 0.230830
Sum of electronic and zero-point Energies= -1254.123206
Sum of electronic and thermal Energies= -1254.099912
Sum of electronic and thermal Enthalpies= -1254.098937
Sum of electronic and thermal Free Energies= -1254.178784

0 1

C	4.08275800	1.11817200	-0.29121300
C	3.04053200	-0.89669300	-0.37022000
C	2.80698900	1.22705900	-0.89404300
O	2.28205900	0.03036900	-1.13608900
H	4.74318400	1.93744800	-0.05961800
C	2.07248800	-0.79197500	1.25925400
C	1.92840100	0.56810200	1.65354800
N	-0.14611500	-0.12181800	0.90515400
C	0.67076700	-1.24913400	0.89798100
C	0.59745000	1.01970600	1.43124500
O	0.30796400	-2.38488100	0.66114300
O	0.07066300	2.11172800	1.60879000
H	2.63994700	-1.51295200	1.83664700
H	2.64885500	1.17071500	2.18174000
C	4.26880300	-0.22023500	-0.05646300
H	5.11399600	-0.67922200	0.43350700
C	-1.50472100	-0.10933800	0.53196000
C	-2.44079000	0.60169100	1.29811100
C	-1.92494200	-0.81222800	-0.60778400
C	-3.77646400	0.61685000	0.92670900
H	-2.11998100	1.13679700	2.17901900
C	-3.26055900	-0.80982400	-0.97644000
H	-1.20522900	-1.35345400	-1.20500500
C	-4.17397200	-0.09143500	-0.20586200
H	-4.50639400	1.15769900	1.51209600
H	-3.59326700	-1.34426800	-1.85484200
C	2.99133200	-2.30551800	-0.94352400
H	3.43235500	-2.30052100	-1.94460600
H	1.95804200	-2.63918200	-1.02466900
O	3.66430200	-3.21745700	-0.08441700
H	4.60081300	-3.23396100	-0.30865800
O	2.14430900	2.23010700	-1.40036100
C	2.70733700	3.55815200	-1.23406900
H	3.67353200	3.61562900	-1.73533300
H	1.99544600	4.22825400	-1.70563800
H	2.80061300	3.78844600	-0.17277600
N	-5.58370200	-0.08179500	-0.59510000
O	-6.37015400	0.58445000	0.07645000
O	-5.92235100	-0.74009600	-1.57768800

Product of Exo-TS46

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opt=calcfc freq=noraman b3lyp/6-311++g(d,p) scrf=(iefpcm,solvent=acetonitrile) geom=connectivity temperature=308

Zero-point correction= 0.289824 (Hartree/Particle)
Thermal correction to Energy= 0.312352
Thermal correction to Enthalpy= 0.313328
Thermal correction to Gibbs Free Energy= 0.235614
Sum of electronic and zero-point Energies= -1254.150164
Sum of electronic and thermal Energies= -1254.127635
Sum of electronic and thermal Enthalpies= -1254.126660
Sum of electronic and thermal Free Energies= -1254.204373

0 1

C	-4.36503800	0.73610700	-0.01971300
C	-2.98457200	-1.07651100	0.20665300
C	-2.94394300	1.07464300	0.43416600
O	-2.58435300	-0.08974000	1.18287900
H	-5.13348500	1.45396100	-0.26661100
C	-2.04839600	-0.66085100	-1.00255300
C	-2.03049700	0.87753100	-0.86215900
N	0.17126300	0.05922300	-0.57207400
C	-0.60146600	-1.08717900	-0.81963900
C	-0.58106400	1.24573600	-0.62540000
O	-0.15333800	-2.20809900	-0.88420900
O	-0.11653500	2.35453100	-0.50351500
H	-2.41455200	-1.04044500	-1.95478100
H	-2.40993200	1.42901700	-1.72029600
C	-4.37954900	-0.58580100	-0.17248000
H	-5.16872600	-1.20719200	-0.57265500
C	1.57856100	0.02447500	-0.33626200
C	2.43779700	0.74433100	-1.16884100
C	2.07637900	-0.73147300	0.72693900
C	3.80613300	0.71528500	-0.93486100
H	2.04159600	1.31867300	-1.99503800
C	3.44393600	-0.77339600	0.96123700
H	1.39930300	-1.27795700	1.36923600
C	4.28782600	-0.04570600	0.12664800
H	4.49001800	1.26415200	-1.56613700
H	3.85075000	-1.35050000	1.77908200
C	-2.86272700	-2.48211800	0.77760100
H	-3.47879000	-2.54662700	1.67899200
H	-1.82856700	-2.68451900	1.05621500
O	-3.23901000	-3.46768600	-0.18160700
H	-4.19182900	-3.60105900	-0.14043100
O	-2.71715100	2.17395100	1.23006500
C	-3.07940500	3.44365700	0.66731700
H	-4.15235500	3.49592700	0.46590300
H	-2.81980000	4.18536000	1.41983500
H	-2.51461700	3.64379300	-0.24618800
N	5.73798500	-0.08196500	0.37531600
O	6.46531500	0.59640800	-0.34379400
O	6.15037100	-0.78883700	1.28996400