Supporting Information

Kinetic, Thermodynamic, and Dynamic Control in Normal vs. Cross [2 + 2] Cycloadditions of Ene-Keteniminium Ions: Computational Understanding, Prediction, and Experimental Verification

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Table of Contents

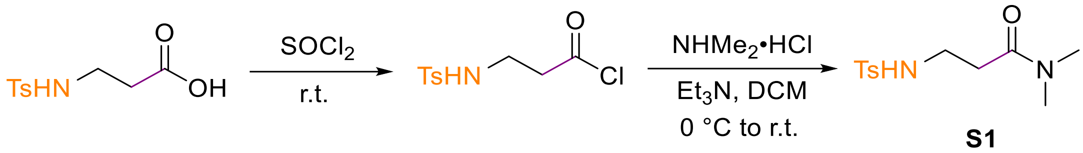
S1. General Information

All reactions were carried out in oven-dried glassware. All chemicals were used as received without further purification. DCE (with molecular sieves, water ≤30 ppm) was purchased from J&K. Flash column chromatographies were performed using silica gel (200−300 mesh). Analytical thin layer chromatographies (TLCs) were performed with 0.2−0.3 mm silica gel HSGF254 plates. Melting points (**M.P.**, uncorrected) were determined in open glass capillaries. Nuclear magnetic resonance (NMR) spectra were measured on Bruker AVANCE III 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz), Bruker AVANCE III HD 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz) and Bruker AVANCE NEO 600 (^{1}H at 600 MHz; ^{13}C at 151 MHz) NMR spectrometers. Data for ^{1}H NMR spectra are reported as follows: chemical shift *δ* (ppm) referenced to either tetramethylsilane (TMS, 0.00 ppm) or $CHDCl_2$ (5.32 ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, dp = doublet of pentets, ddd = doublet of doublet of doublets, dtt = doublet of triplet of triplets), coupling constant *J* (Hz), and integration. Data for ^{13}C NMR spectra are reported in terms of chemical shift *δ* (ppm) referenced to either $CDCl_3$ (77.16 ppm) or CD_2Cl_2 (53.84 ppm). High-resolution mass spectrometry (HRMS) data were recorded on Bruker Apex IV and Bruker Solarix XR fourier transform ion cyclotron resonance (FTICR) mass spectrometers (electrospray ionization, ESI). Single crystal X-ray diffraction data were collected on a XtaLAB PRO 007HF(Mo): Kappa single diffractometer at 180 K.

Abbreviations:

collidine = 2,4,6-trimethylpyridine
DBU = 1,8-diazabicyclo[5.4.0]undecane-7-ene
DCE = 1,2-dichloroethane
DCM = dichloromethane
DIAD = diisopropyl azodicarboxylate
DMF = *N*,*N*-dimethylformamide
EA = ethyl acetate
h = hour(s)
Ms = methanesulfonyl
PE = petroleum ether
r.t. = room temperature
Tf = trifluoromethanesulfonyl
Tf_2O = trifluoromethanesulfonic anhydride
TFA = trifluoroacetic acid
THF = tetrahydrofuran
Ts = 4-toluenesulfonyl

S2. Syntheses of Substrates

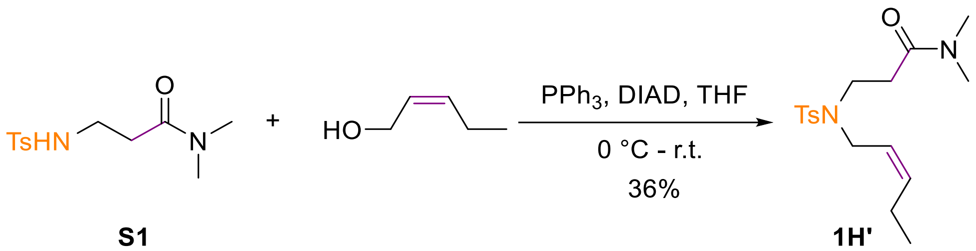


***N*,*N*-dimethyl-3-((4-methylphenyl)sulfonamido)propenamide (S1)**

To 3-((4-methylphenyl)sulfonamido)propanoic acid (2.0 g, 8.2 mmol) was added sulfurous dichloride (10 mL, 138.8 mmol, 16.9 equiv) and the mixture was stirred for 24 h. Then the mixture was concentrated to give crude product 3-((4-methylphenyl)sulfonamido)propanoyl chloride, which was used directly in the next step.

To a solution of above crude 3-((4-methylphenyl)sulfonamido)propanoyl chloride and $NHMe_2$•HCl (1.648 g, 20.3 mmol, 2.5 equiv) in DCM (20 mL) was added triethylamine (5.5 mL, 39.6 mmol, 4.8 equiv) in 0 °C ice bath. The reaction mixture was then warmed up to r.t. and stirred for 24 h. After quenched by water, the mixture was extracted by DCM and the organic phase was washed by water, dried over sodium sulfate and concentrated to give crude solid. The crude solid was recrystallized to give the previously reported **S1**[1] (1.184 g, 4.4 mmol, 53% yield for 2 steps) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 3.18 (t, J = 5.6 Hz, 2H), 2.93 (s, 6H), 2.55 (t, J = 5.7 Hz, 2H), 2.42 (s, 3H).



(*Z*)-*N*,*N*-dimethyl-3-((4-methyl-*N*-(pent-2-en-1-yl)phenyl)sulfonamido)propenamide (1H')

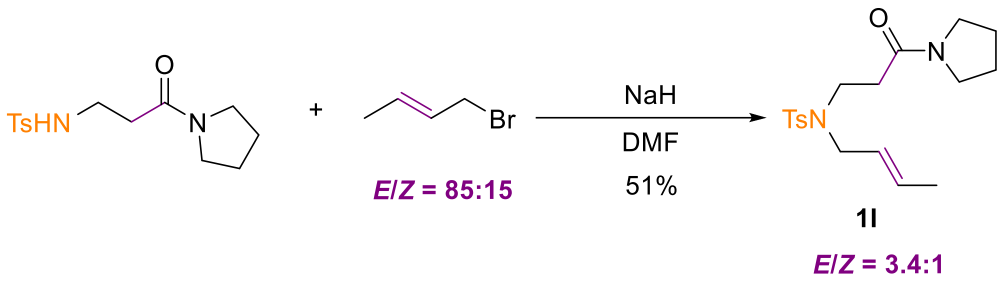
To a solution of **S1** (270.9 mg, 1.0 mmol), (*Z*)-pent-2-en-1-ol (95.0 mg, 1.1 mmol, 1.1 equiv) and PPh_3 (314.5 mg, 1.2 mmol, 1.2 equiv) in THF (10 mL) was added DIAD (0.24 mL, 1.2 mmol, 1.2 equiv) under an argon atmosphere at 0 °C. The mixture was warmed up naturally and stirred for 24 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA = 1:1) afforded the product **1H'** (121.8 mg, 0.36 mmol, 36%) as a colorless oil.

TLC (1:2 PE/EA, R_f): 0.6.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 5.57 – 5.48 (m, 1H), 5.25 – 5.16 (m, 1H), 3.92 – 3.80 (m, 2H), 3.45 – 3.24 (m, 2H), 3.01 (s, 3H), 2.92 (s, 3H), 2.78 – 2.61 (m, 2H), 2.43 (s, 3H), 2.11 – 1.95 (m, 2H), 0.95 (t, J = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 143.4, 136.5, 136.4, 129.8, 127.4, 123.4, 46.1, 44.5, 37.3, 35.3, 34.2, 21.6, 20.7, 14.1.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{17}H_{27}N_2O_3S^+$: 339.1737; found: 339.1739.



(*E*)-*N*-(but-2-en-1-yl)-4-methyl-*N*-(3-oxo-3-(pyrrolidin-1-yl)propyl)benzenesulfonamide (1l)

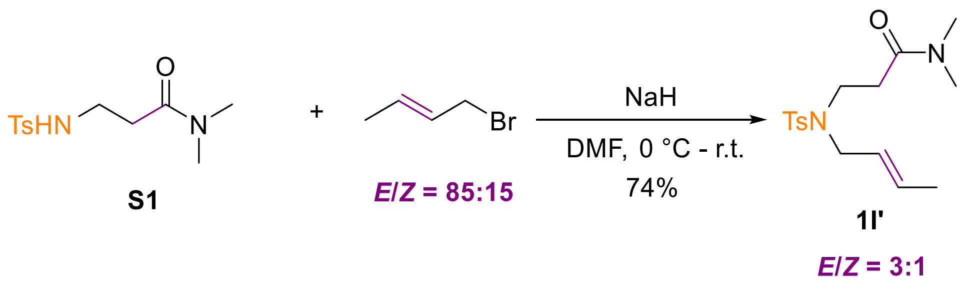
To a solution of 4-methyl-*N*-(3-oxo-3-(pyrrolidin-1-yl)propyl)benzenesulfonamide[2] (300.0 mg, 1 mmol) in DMF (3 mL) was added NaH (60.0 mg, 60 wt % in mineral oil, 1.5 mmol, 1.5 equiv) at room temperature under argon atmosphere. Then a solution of (*E*)-crotyl bromide (162.0 mg, *E*/*Z*=85%:15%, as purchased, 1.2 mmol, 1.2 equiv) in DMF (2 mL) was added after the reaction mixture was stirred to become a clean solution. The mixture was stirred for another 13 h and then quenched with saturated aqueous ammonium chloride solution and water. This was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 5:1 to 1:1) to give **1l** (181.0 mg, 0.52 mmol, 51%) as a yellow oil. The *E*/*Z* was determined to be 3.4:1 by ^{1}H NMR (δ 3.76 vs 3.86).

TLC (1:2 PE/EA, R_f): 0.7.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 5.67 – 5.55 (m, 1H), 5.35 – 5.20 (m, 1H), 3.76 (d, J = 6.8 Hz, 2H), 3.52 – 3.40 (m, 6H), 2.72 (q, J = 8.4, 7.2 Hz, 2H), 2.45 (s, 3H), 2.05 – 1.95 (m, 2H), 1.95 – 1.84 (m, 2H), 1.70 – 1.62 (m, 3H).

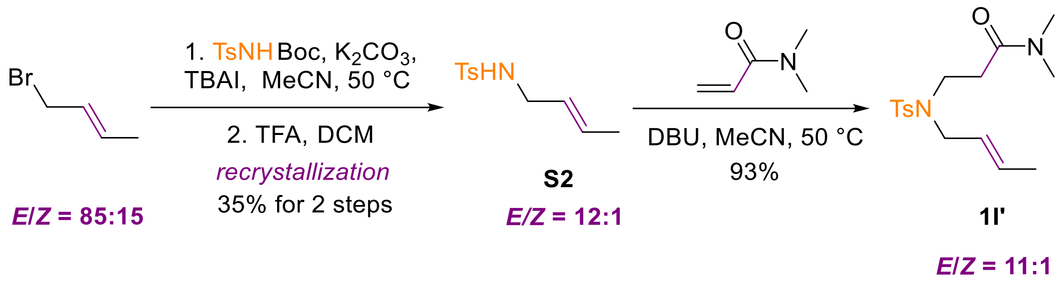
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 143.3, 136.8, 130.8, 129.8, 127.4, 125.7, 51.5, 46.8, 45.7, 43.7, 34.6, 26.2, 24.5, 21.6, 17.8.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{18}H_{27}N_2O_3S^+$: 351.1737; found: 351.1734.



(*E*)-3-((*N*-(but-2-en-1-yl)-4-methylphenyl)sulfonamido)-*N*,*N*-dimethylpropanamide (1l')

To a suspension of NaH (60.0 mg, 60 wt % in mineral oil, 1.5 mmol, 1.5 equiv) in DMF (2 mL) was added a solution of **S1** (270.8 mg, 1 mmol) in DMF (2 mL) at 0 °C under argon atmosphere. After stirred for 10 min, the reaction solution was added (*E*)-crotyl bromide (202.5 mg, *E*/*Z*=85%:15%, as purchased, 1.5 mmol, 1.5 equiv). The mixture was stirred for another 12 h at r.t. and then quenched with saturated aqueous ammonium chloride solution and water. This was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 5:1 to 1:1) to give **1l'** (238.6 mg, 0.74 mmol, 74%) as a colorless oil. The *E*/*Z* was determined to be 3:1 by ^{1}H NMR (δ 3.73 vs 3.85).



(*E*)-*N*-(but-2-en-1-yl)-4-methylbenzenesulfonamide (S2)

To a solution of *tert*-butyl tosylcarbamate (1.4 g, 5.2 mmol) and potassium carbonate (1.0 g, 7.2 mmol, 1.4 equiv) and tetrabutylammonium iodide (396.4 mg, 1.1 mmol, 0.2 equiv) in acetonitrile (15 mL) was added a solution (*E*)-crotyl bromide (877.6 mg, *E*/*Z*=85%:15%, as purchased, 6.5 mmol, 1.25 equiv) in acetonitrile (2 mL) and the mixture was stirred at 50 °C for 18 h. Then, saturated ammonium chloride aq. was added and the aqueous layer was extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude residue was dissolved in DCM (17 mL) and TFA (3.9 mL, 50 mmol) was added. The mixture was stirred for 3 h at room temperature and the reaction was quenched by saturated aq. $NaHCO_3$. The aqueous layer was extracted with DCM. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography (PE/EA = 10:1 to 5:1) to afford **S2** (1.068 g, 4.7 mmol) as a colorless oil, which was recrystallized to give previously reported compound **S2**[3] (408.0 mg, 1.8 mmol, 35% for 2 steps) as a colorless crystal. The *E*/*Z* was determined to be 12:1 by ^{1}H NMR.

TLC (5:1 PE/EA, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 5.65 – 5.49 (m, 1H), 5.43 – 5.25 (m, 1H), 4.46 (brs, 1H), 3.50 (d, J = 5.8 Hz, 2H), 2.43 (s, 3H), 1.61 (d, J = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5, 137.2, 129.9, 129.8, 127.3, 125.8, 45.5, 21.6, 17.7.

(*E*)-3-((*N*-(but-2-en-1-yl)-4-methylphenyl)sulfonamido)-*N*,*N*-dimethylpropanamide (1l')

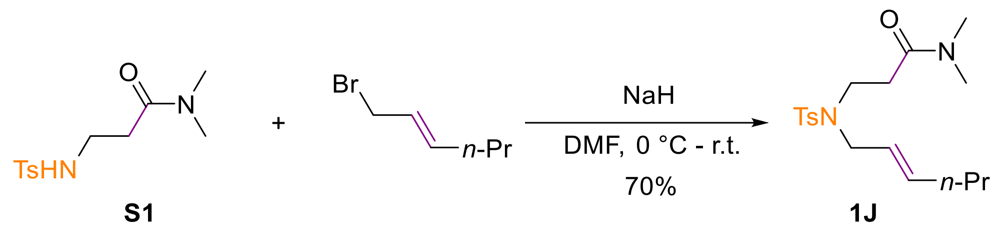
To a solution of **S2** (226.2 mg, 1.0 mmol) and 1,8-diazabicyclo[5.4.0]undec-7-ene (76.1 mg, 0.5 mmol, 0.5 equiv) in acetonitrile (1 mL) was added a solution of *N*,*N*-dimethylacrylamide (207.3 mg, 2.09 mmol, 2.1 equiv) in acetonitrile (1 mL). The mixture was heated to 50 °C and stirred for 24 h. After quenched by water, the mixture was extracted by EA and the organic phase was washed by water for several times. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by flash column chromatography (PE/EA = 2:1 to 1:1) to afford **1l'** (302.8 mg, 0.93 mmol, 93%) as a colorless oil. The *E*/*Z* was determined to be 11:1 by ^{1}H NMR.

TLC (1:2 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 5.65 – 5.55 (m, 1H), 5.34 – 5.17 (m, 1H), 3.73 (d, J = 6.8 Hz, 2H), 3.37 (dd, J = 8.5, 6.7 Hz, 2H), 3.02 (s, 3H), 2.94 (s, 3H), 2.81 – 2.67 (m, 2H), 2.42 (s, 3H), 1.62 (d, J = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 143.4, 136.6, 131.0, 129.8, 127.4, 125.7, 51.6, 44.1, 37.4, 35.4, 34.0, 21.6, 17.8.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{16}H_{25}N_2O_3S^+$: 325.1581; found: 325.1580.



(*E*)-3-((*N*-(hex-2-en-1-yl)-4-methylphenyl)sulfonamido)-*N*,*N*-dimethylpropanamide (1J)

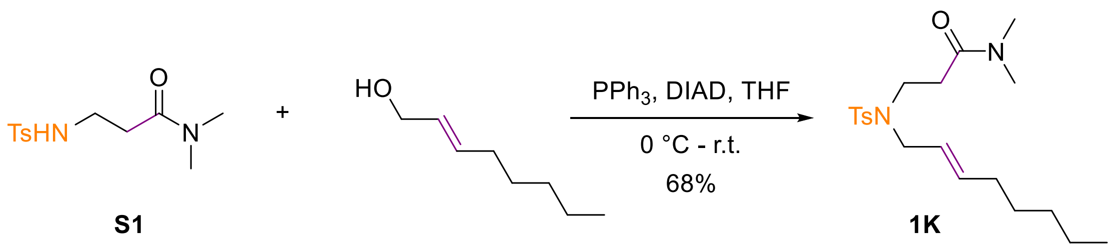
To a solution of **S1** (271.0 mg, 1.0 mmol) in DMF (5 mL) was added NaH (61 mg, 60 wt % in mineral oil, 1.5 mmol, 1.5 equiv). After the reaction mixture was stirred for 5 min. (*E*)-1-bromohex-2-ene (262 mg, 1.6 mmol, 1.6 equiv) was added. The mixture was stirred for another 10 h and 50 min and then quenched with saturated aqueous ammonium chloride solution and water. This mixture was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 1:1) to give **1J** (246.0 mg, 0.7 mmol, 70%) as a colorless oil.

TLC (1:2 PE/EA, R_f): 0.6.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 5.64 – 5.50 (m, 1H), 5.63 – 5.54 (m, 1H), 3.75 (dd, J = 6.7, 1.3 Hz, 2H), 3.47 – 3.26 (m, 2H), 3.03 (s, 3H), 2.95 (s, 3H), 2.84 – 2.68 (m, 2H), 2.42 (s, 3H), 2.00 – 1.85 (m, 2H), 1.32 (h, J = 7.4 Hz, 2H), 0.84 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 143.4, 136.7, 136.0, 129.8, 127.3, 124.6, 51.6, 44.1, 37.3, 35.3, 34.3, 34.1, 22.2, 21.6, 13.7.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{18}H_{29}N_2O_3S^+$: 353.1893; found: 353.1888.



(*E*)-*N*,*N*-dimethyl-3-((4-methyl-*N*-(oct-2-en-1-yl)phenyl)sulfonamido)propenamide (1K)

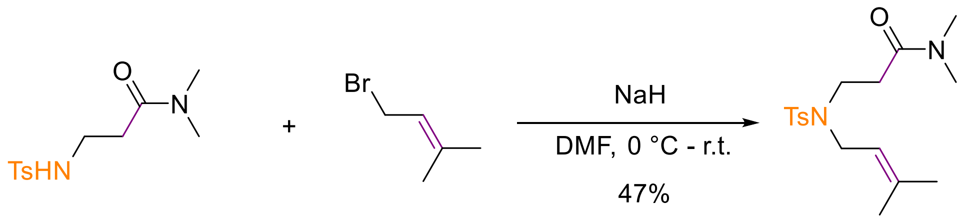
To a solution of **S1** (274.3 mg, 1.01 mmol), (*E*)-oct-2-en-1-ol (0.23 mL, 1.51 mmol, 1.5 equiv) and PPh_3 (524.0 mg, 2.0 mmol, 2 equiv) in THF (10 mL) was added DIAD (0.4 mL, 2.0 mmol, 2 equiv) under an argon atmosphere at 0 °C. The mixture was warmed up naturally and stirred for 24 h, which was then concentrated in vacuo. Purification of the residue through column chromatography on silica gel (PE/EA = 1:1) afforded the product **1K** (261.8 mg, 0.69 mmol, 68%) as a colorless oil.

TLC (1:2 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 5.58 (dt, J = 13.6, 6.7 Hz, 1H), 5.32 – 5.18 (m, 1H), 3.75 (d, J = 6.7 Hz, 2H), 3.37 (dd, J = 8.6, 6.8 Hz, 2H), 3.01 (s, 3H), 2.93 (s, 3H), 2.79 – 2.66 (m, 2H), 2.42 (s, 3H), 1.95 (q, J = 6.8 Hz, 2H), 1.39 – 1.11 (m, 6H), 0.86 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 143.4, 136.6, 136.4, 129.8, 127.4, 124.3, 51.6, 44.2, 37.3, 35.4, 34.1, 32.2, 31.4, 28.7, 22.6, 21.6, 14.1.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{20}H_{33}N_2O_3S^+$: 381.2206; found: 381.2209.



S1 **1L**

***N*,*N*-dimethyl-3-((4-methyl-*N*-(3-methylbut-2-en-1-yl)phenyl)sulfonamido)propenamide (1L)**

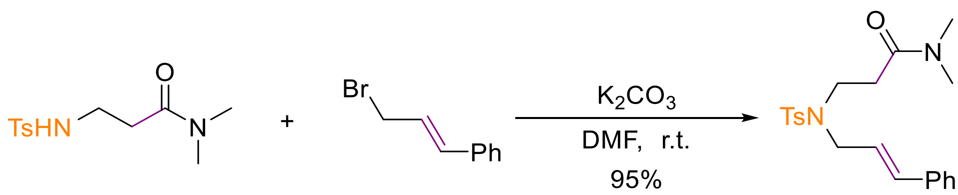
To a solution of NaH (74.0 mg, 60 wt % in mineral oil, 1.85 mmol, 1.5 equiv) in DMF (5 mL) was added a solution of **S1** (334.0 mg, 1.24 mmol) in DMF (3 mL) in 0 °C ice bath under argon atmosphere. Then 1-bromo-3-methylbut-2-ene (0.22 mL, 1.90 mmol, 1.5 equiv) was added after the reaction mixture was stirred to be a clean solution. The mixture was warmed up to r.t., stirred for another 12 h, and then quenched with saturated aqueous ammonium chloride solution and water. This was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 1:1) to give **1L** (197.1 mg, 0.58 mmol, 47%) as a colorless oil.

TLC (1:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.1 Hz, 2H), 5.00 (t, J = 7.0 Hz, 1H), 3.80 (d, J = 7.0 Hz, 2H), 3.48 – 3.27 (m, 2H), 3.01 (s, 3H), 2.93 (s, 3H), 2.78 – 2.65 (m, 2H), 2.42 (s, 3H), 1.65 (s, 3H), 1.62 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 143.3, 137.4, 136.6, 129.7, 127.4, 119.1, 47.1, 44.4, 37.3, 35.3, 34.2, 25.9, 21.6, 18.0.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{17}H_{27}N_2O_3S^+$: 339.1737; found: 339.1739.



S1 **1M**

3-((*N*-cinnamyl-4-methylphenyl)sulfonamido)-*N*,*N*-dimethylpropanamide (1M)

The mixture of **S1** (354.8 mg, 1.31 mmol), (*E*)-(3-bromoprop-1-en-1-yl)benzene (392.2 mg, 1.99 mmol, 1.5 equiv) and potassium carbonate (362.8 mg, 2.63 mmol, 2 equiv) in DMF (6 mL) was stirred at r.t. for 12 h under argon atmosphere. The mixture was quenched by adding water and extracted with EA several times. The combined organic phase was washed successively with deionized water and brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/EA = 1:1) to yield **1M** (481.8 mg, 1.25 mmol, 95%) as a white solid.

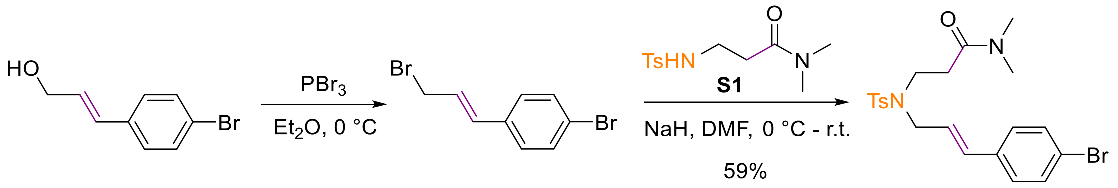
TLC (1:2 PE/EA, R_f): 0.4.

M. P. 116.0-117.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.69 (m, 2H), 7.34 – 7.21 (m, 7H), 6.46 (d, J = 15.8 Hz, 1H), 5.98 (dt, J = 16.5, 6.7 Hz, 1H), 3.98 (d, J = 6.7 Hz, 2H), 3.53 – 3.36 (m, 2H), 2.96 (s, 3H), 2.89 (s, 3H), 2.73 (t, J = 7.5 Hz, 2H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 143.5, 136.6, 136.3, 134.0, 129.9, 128.7, 128.0, 127.4, 126.6, 124.2, 51.9, 44.6, 37.3, 35.3, 34.2, 21.6.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{21}H_{27}N_2O_3S^+$: 387.1737; found: 387.1736.



1N

(*E*)-3-((*N*-(3-(4-bromophenyl)allyl)-4-methylphenyl)sulfonamido)-*N*,*N*-dimethylpropanamide (1N)

To a solution of (*E*)-3-(4-bromophenyl)prop-2-en-1-ol[4] (426.1 mg, 2 mmol) in ethyl ether (10 mL) was added PBr_3 (0.38 mL, 4 mmol, 2 equiv) in 0 °C ice bath. The mixture was then warmed up to r.t. and stirred for 2 h. Subsequently, the mixture was quenched by saturated $NaHCO_3$, diluted by water and extracted by ethyl ether. The organic phase was washed by water, brine and dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by column chromatography (PE) and used directly for the next step.

The mixture of **S1** (270.3 mg, 1.0 mmol) and NaH (60 mg, 60 wt % in mineral oil, 1.5 mmol, 1.5 equiv) was added DMF (3 mL) under argon atmosphere. (*E*)-1-bromo-4-(3-bromoprop-1-en-1-yl)benzene (the above residue, < 2 mmol, < 2 equiv) was added to the solution in 0 °C ice bath. The resulted mixture was warmed up and stirred for 18 h. After quenched by with saturated aqueous ammonium chloride solution and water, the mixture was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 2:1 to 1:1) to give **1N** (275.4 mg, 0.59 mmol, 59% yield based on **S1**) as a yellow solid.

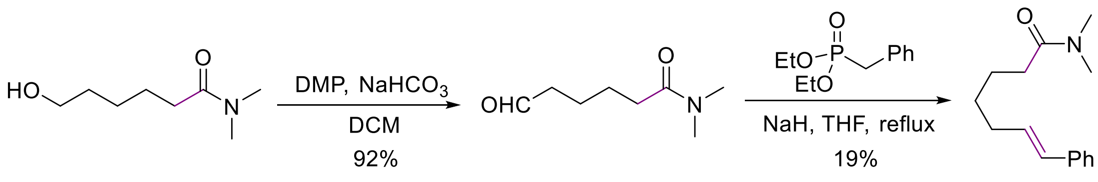
TLC (1:2 PE/EA, R_f): 0.7.

M. P. 89.5-92.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.4 Hz, 2H), 6.39 (d, J = 15.9 Hz, 1H), 5.97 (dt, J = 15.8, 6.6 Hz, 1H), 3.97 (d, J = 6.5 Hz, 2H), 3.49 – 3.40 (m, 2H), 2.96 (s, 3H), 2.89 (s, 3H), 2.77 – 2.63 (m, 2H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 143.6, 136.7, 135.3, 132.7, 131.8, 129.9, 128.1, 127.4, 125.2, 121.8, 51.7, 44.7, 37.3, 35.4, 34.2, 21.6.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{21}H_{26}BrN_2O_3S^+$: 465.0842; found: 465.0842.



1O

(*E*)-*N*,*N*-dimethyl-7-phenylhept-6-enamide (1O)

To a solution of Dess–Martin periodinane (2.56 g, 6.04 mmol, 1.2 equiv) and sodium bicarbonate (1.27 g, 15.09 mmol, 3 equiv) in DCM (5 mL) was added a solution of 6-hydroxy-*N*,*N*-dimethylhexanamide[5] (0.8 g, 5.03 mmol) in DCM (5 mL) in 0 °C ice bath. The mixture was stirred for 2 h at r.t. After quenched by saturated sodium bicarbonate (a.q.), the reaction mixture was added by $Na_2S_2O_3$ until no new white precipitation formed. The mixture was extracted by DCM, and the organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, concentrated to give *N*,*N*-dimethyl-6-oxohexanamide (0.726 g, 4.62 mmol, 92%) as a light yellow oil.

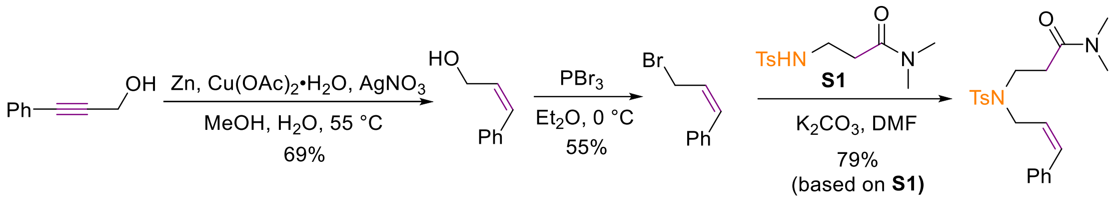
To a suspension of NaH (0.222 g, 60 wt % in mineral oil, 5.55 mmol, 1.2 equiv) in THF (5 mL) was added a solution of diethyl benzylphosphonate (1.265 g, 5.55 mmol, 1.2 equiv) in THF (3 mL) under argon atmosphere. The mixture was stirred for 20 min at rt. Subsequently, the reaction was added by a solution of *N*,*N*-dimethyl-6-oxohexanamide (0.726 g, 4.62 mmol). The reaction mixture was heated to reflux for 3 h. After quenched by aqueous ammonium chloride solution and water, the mixture was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 20:1 to 10:1 to 5:1) to give **1O** (0.207 g, 0.89 mmol, 19%) as a yellow oil.

TLC (1:2 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.35 (d, J = 7.3 Hz, 2H), 7.32 – 7.26 (m, 2H), 7.22 – 7.16 (m, 1H), 6.41 (d, J = 15.9 Hz, 1H), 6.26 (dt, J = 15.8, 6.8 Hz, 1H), 2.97 (s, 3H), 2.89 (s, 3H), 2.36 – 2.29 (m, 2H), 2.29 – 2.20 (m, 2H), 1.66 (dt, J = 15.1, 7.3 Hz, 2H), 1.52 (apparent p, J = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 173.2, 138.5, 131.4, 130.4, 129.0, 127.3, 126.4, 37.6, 35.5, 33.6, 33.4, 29.7, 25.3.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{15}H_{22}NO^+$: 232.1696; found: 232.1691.



1P

(*Z*)-*N*,*N*-dimethyl-3-((4-methyl-*N*-(3-phenylallyl)phenyl)sulfonamido)propenamide (1P)

Zinc powder (4.8480 g, 74.1 mmol, 12.4 equiv) was added to a round bottom flask and treated with 3 M HCl. The liquid was decanted and freshly activated Zinc powder was washed with lots of water to neutral. To the above slurry of zinc in water (10 mL) was added $Cu(OAc)_2$•H_2O (1.2058 g, 6.0 mmol, 1 equiv) at 0 °C. After stirred for 15 min, $AgNO_3$ (1.3370 g, 7.9 mmol, 1.3 equiv) was added. The reaction mixture was stirred for another 10 min and then filtered, washed with water. The solid was transferred to a 100 mL round bottom flask, and then 3-phenylprop-2-yn-1-ol (793.0 mg, 6.0 mmol), water (24 mL), MeOH (20 mL) were added. The reaction mixture was stirred for 24 h at 55 °C and filtered through celite by washing with EA. The reaction mixture was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 10:1 to 5:1) to give (*Z*)-3-phenylprop-2-en-1-ol (552.2 mg, 4.1 mmol, 69%) as a yellow oil.

To a solution of (*Z*)-3-phenylprop-2-en-1-ol (362.3 mg, 2.7 mmol) in Et_2O was added phosphorus tribromide (0.1 mL, 1.1 mmol, 0.4 equiv) in 0 °C ice bath. The mixture was stirred for 5 min and then warmed up to r.t. and stirred for 25 min. Subsequently, the mixture was quenched by saturated $NaHCO_3$, diluted by water and extracted by EA. The organic phase was washed by water, brine and dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum to afford (*Z*)-(3-bromoprop-1-en-1-yl)benzene (291.3 mg, 1.5 mmol, 55%) as a colorless oil. The *Z*/*E* was determined to be 10:1 by ^{1}H NMR.

The mixture of **S1** (365.0 mg, 1.35 mmol) and K_2CO_3 (373.1 mg 2.7 mmol, 2.0 equiv) was added DMF (6 mL) under argon atmosphere. (*Z*)-(3-bromoprop-1-en-1-yl)benzene (291.3 mg, 1.5 mmol, 1.1 equiv) was added to the solution. The resulted mixture was stirred for 18 h. After quenched by water, the mixture was then extracted with EA. The combined organic layer was washed with water and brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (PE/EA = 5:1 to 2:1 to 1:1) to give **1P** (411.9 mg, 1.07 mmol, 79% yield based on **S1**) as a yellow solid. The *Z*/*E* was determined to be 13:1 by ^{1}H NMR.

TLC (1:2 PE/EA, R_f): 0.5.

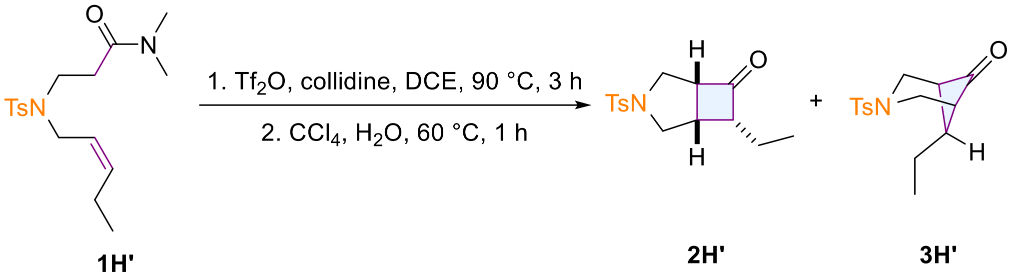
M. P. 101.0-102.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.3 Hz, 2H), 7.39 – 7.21 (m, 5H), 7.15 (dd, J = 7.1, 1.8 Hz, 2H), 6.55 (dd, J = 11.7, 2.0 Hz, 1H), 5.50 (dt, J = 11.6, 6.5 Hz, 1H), 4.13 (dd, J = 6.5, 1.9 Hz, 2H), 3.42 – 3.30 (m, 2H), 2.90 (s, 3H), 2.88 (s, 3H), 2.60 – 2.53 (m, 2H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6, 143.5, 136.5, 136.1, 132.7, 129.9, 128.9, 128.5, 127.5, 127.4, 127.3, 46.7, 44.5, 37.2, 35.3, 33.5, 21.6.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{21}H_{27}N_2O_3S^+$: 387.1737; found: 387.1741.

S3. Experimental Validation



Under argon atmosphere, to a solution of **1H'** (61.0 mg, 0.18 mmol) in DCE (2 mL) in a dried reaction tube with stir bar was added trifluoromethanesulfonic anhydride (60 μL, 0.36 mmol, 2.0 equiv) and collidine (40 μL, 0.20 mmol, 1.1 equiv). After addition was completed, the reaction mixture was heated at 90 °C for 3 h. After cooling to room temperature, the reaction mixture was hydrolyzed in a two phases system H_2O-$CC1_4$ (1 mL+1 mL) at 60 °C for 1 h. The reaction mixture was decanted and the aqueous layers was extracted with Et_2O. The organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by column chromatography (PE/EA = 10:1 to 5:1) to give **2H'** (5.8 mg, 11%) as an off-white solid and **3H'** (16.1 mg, 30%) as a colorless oil.

Run 2: **1H'** (61.0 mg, 0.18 mmol), Tf_2O (60 μL, 0.36 mmol, 2.0 equiv), collidine (40 μL, 0.20 mmol, 1.1 equiv), **2H'** (6.8 mg, 13%), **3H'** (17.9 mg, 34%).

The average yield of **2H'** is 12%. The average yield of **3H'** is 32%.

(±)-(1*S*,5*R*,7*R*)-7-ethyl-3-tosyl-3-azabicyclo[3.2.0]heptan-6-one (2H')

TLC (3:1 PE/EA, R_f): 0.3.

M. P. 116.0-118.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 3.77 (d, J = 9.7 Hz, 1H), 3.67 (d, J = 10.3 Hz, 1H), 3.58 (ddd, J = 7.2, 7.2, 3.2 Hz, 1H), 3.33 – 3.20 (m, 1H), 3.07 – 2.99 (m, 1H), 2.76 (dd, J = 10.3, 6.9 Hz, 1H), 2.59 (dd, J = 9.7, 6.9 Hz, 1H), 2.44 (s, 3H), 1.78 (apparent dt, J = 13.8, 7.4 Hz, 1H), 1.50 (apparent dt, J = 13.7, 7.5 Hz, 1H), 0.98 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 211.8, 144.2, 131.4, 129.8, 128.3, 63.0, 60.6, 49.5, 48.3, 32.9, 21.7, 17.0, 12.3.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{15}H_{20}NO_3S^+$: 294.1158; found: 294.1166.

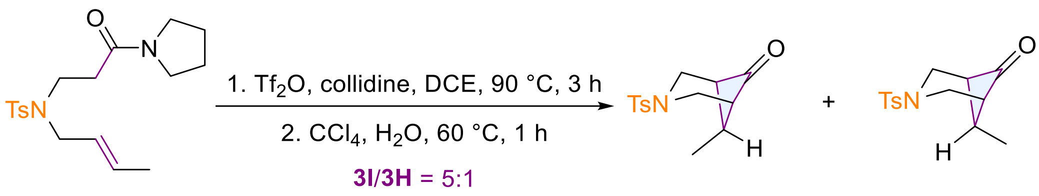
(1*R*,5*S*,7*s*)-7-ethyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3H')

TLC (3:1 PE/EA, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.3 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 3.90 (dt, J = 10.5, 1.9 Hz, 2H), 3.77 (d, J = 10.1 Hz, 2H), 3.03 – 2.95 (m, 2H), 2.45 (s, 3H), 2.13 (apparent p, J = 7.0 Hz, 1H), 1.32 (apparent p, J = 7.4 Hz, 2H), 0.87 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 205.7, 144.1, 134.2, 129.9, 127.3, 55.6, 48.2, 32.0, 21.7, 15.9, 12.5.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{15}H_{20}NO_3S^+$: 294.1158; found: 294.1166.



E/*Z* = 3.4:1
1I **3H** **3I**

Under argon atmosphere, to a solution of **1I** (70.9 mg, *E*/*Z* = 3.4:1, 0.2 mmol) in DCE (2 mL) in a dried reaction tube with stir bar was added trifluoromethanesulfonic anhydride (80 μL, 0.48 mmol, 2.4 equiv) and collidine (45 μL, 0.22 mmol, 1.1 equiv). After addition was completed, the reaction mixture was heated at 90 °C for 3 h. After cooling to room temperature, the reaction mixture was hydrolyzed in a two phases system H_2O-CCl_4 (1 mL+1 mL) at 60 °C for 1 h. The reaction mixture was decanted and the aqueous layer was extracted with Et_2O. The organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by preparative thin layer chromatography (PE/EA = 3:1) to give the **3H** (4.1 mg, 7%) as colorless oil and **3I** (26.7 mg, 48%) as off-white solid. The total yield of **3H** and **3I** is 55%. **3I**/**3H** was determined to be 5:1 by ^{1}H NMR of crude products.
Run 2: **1I** (70.9 mg, *E*/*Z* = 3.4:1, 0.2 mmol), Tf_2O (80 μL, 0.48 mmol, 2.4 equiv), collidine (45 μL, 0.22 mmol, 1.1 equiv), **3H** (4.1 mg, 7%) and **3I** (29.1 mg, 52%). The total yield of **3H** and **3I** is 59%. Purified by column chromatography (PE/EA = 5:1).
The average total yield is 57%.

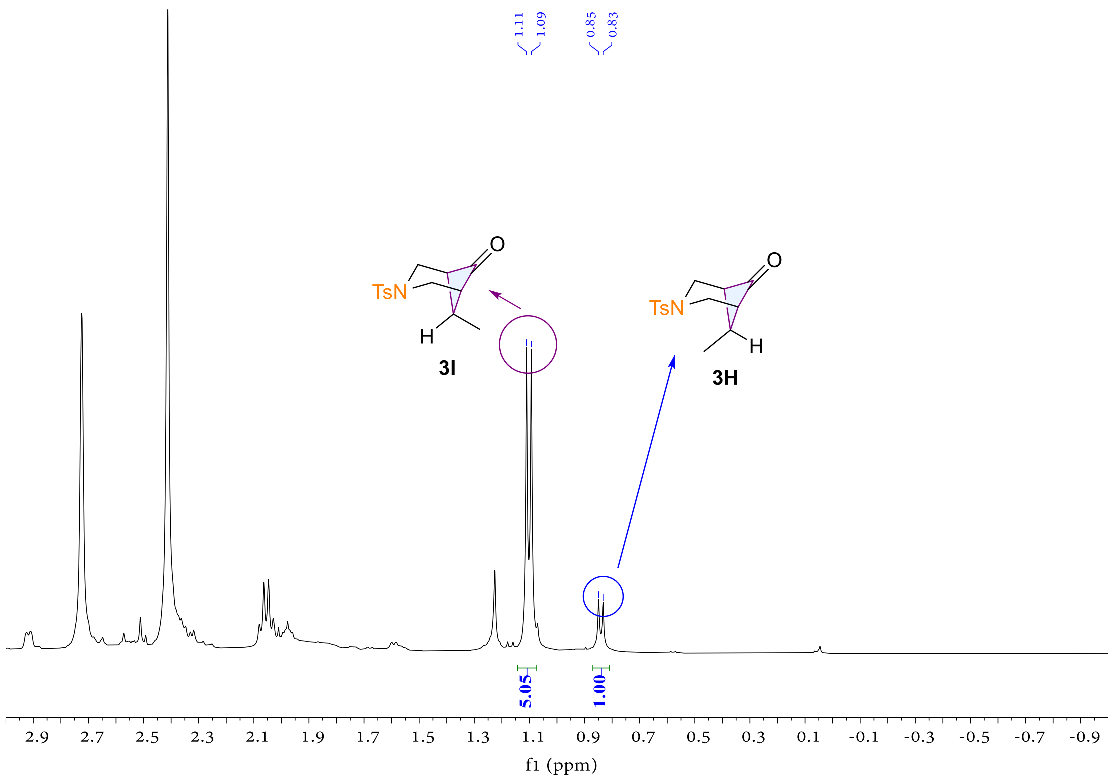


Figure S1. Part of the ^{1}H NMR spectrum of the crude products for reaction of **1I** (*E*/*Z* = 3.4:1).

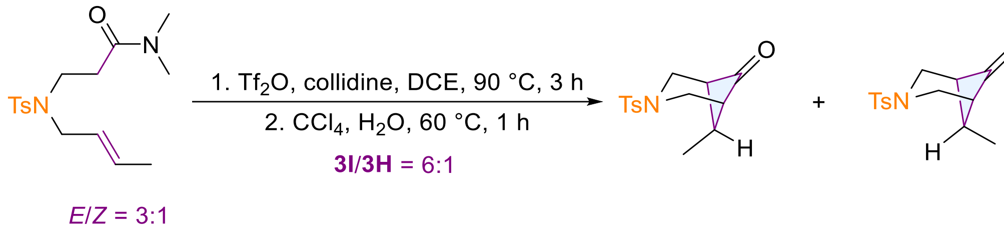
(1*R*,5*S*,7*s*)-7-methyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3H)

TLC (3:1 PE/EA, R_f): 0.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.2 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 3.94 (d, J = 10.4 Hz,

2H), 3.78 (d, J = 10.4 Hz, 2H), 2.95 (d, J = 6.2 Hz, 2H), 2.45 (s, 3H), 2.38 (q, J = 6.6 Hz, 1H), 0.93 (d, J = 6.8 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 206.1, 144.1, 134.2, 130.0, 127.4, 56.6, 48.1, 25.0, 21.7, 7.1.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{14}H_{18}NO_3S^+$: 280.1002; found: 280.1007.

(1*R*,5*S*,7*r*)-7-methyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3I)
TLC (3:1 PE/EA, R_f): 0.4.
M. P. 88.5-90.2 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.1 Hz, 2H), 3.94 (d, J = 9.8 Hz, 2H), 3.83 (d, J = 10.0 Hz, 2H), 2.76 (s, 2H), 2.44 (s, 3H), 2.13 (q, J = 6.8 Hz, 1H), 1.14 (d, J = 6.9 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 207.2, 144.0, 134.1, 129.9, 127.4, 60.6, 53.1, 30.2, 21.6, 16.9.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{14}H_{18}NO_3S^+$: 280.1002; found: 280.1002.



1I' **3H** **3I**

Under argon atmosphere, to a solution of **1I'** (64.9 mg, E/Z = 3:1, 0.2 mmol) in DCE (2 mL) in a dried reaction tube with stir bar was added trifluoromethanesulfonic anhydride (80 μL, 0.48 mmol, 2.4 equiv) and collidine (45 μL, 0.22 mmol, 1.1 equiv). After addition was completed, the reaction mixture was heated at 90 °C for 3 h. After cooling to room temperature, the reaction mixture was hydrolyzed in a two phases system H_2O-CCl_4 (1 mL+1 mL) at 60 °C for 1 h. The reaction mixture was decanted and the aqueous layer was extracted with Et_2O. The organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by preparative thin layer chromatography (PE/EA = 3:1) to give the **3H** (11.3 mg, 20%) as colorless oil and **3I** (33.9 mg, 61%) as off-white solid. The total yield of **3H** and **3I** is 81%. **3I**/**3H** was determined to be 6:1 by ^{1}H NMR of crude products.
Run 2: **1I'** (64.9 mg, E/Z = 3:1, 0.2 mmol), Tf_2O (80 μL, 0.48 mmol, 2.4 equiv), collidine (45 μL, 0.22 mmol, 1.1 equiv), **3H** (10.3 mg, 18%) and **3I** (32.8 mg, 59%). Purified by column chromatography (PE/EA = 5:1). The total yield of **3H** and **3I** is 77%.
The average total yield is 79%.

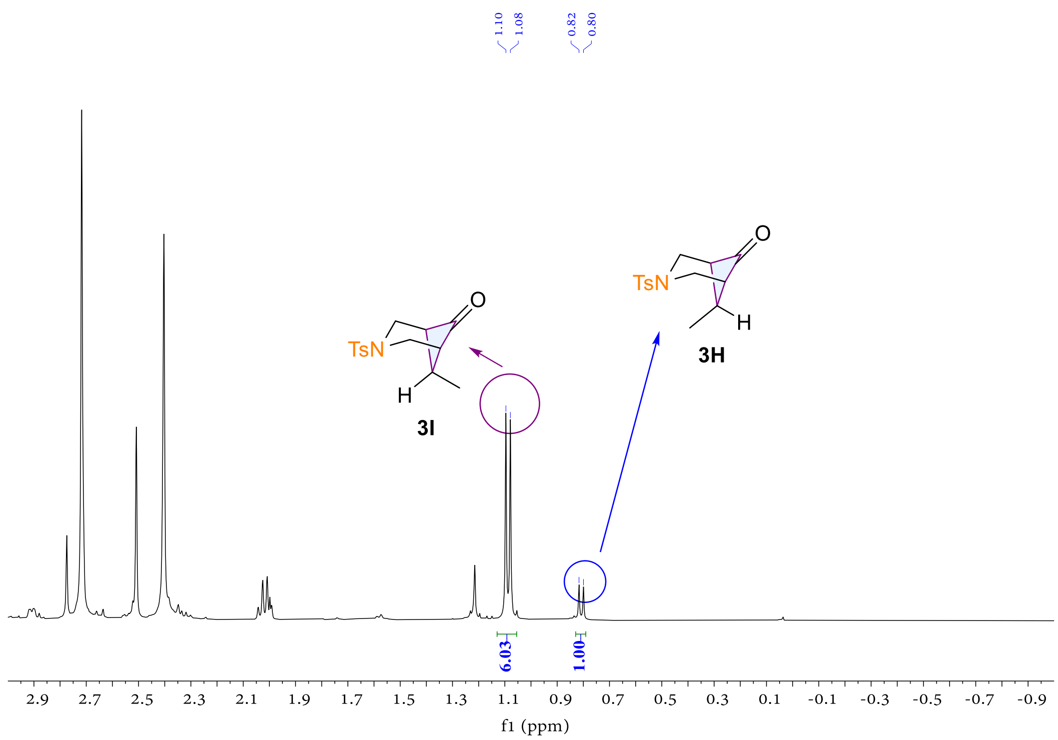
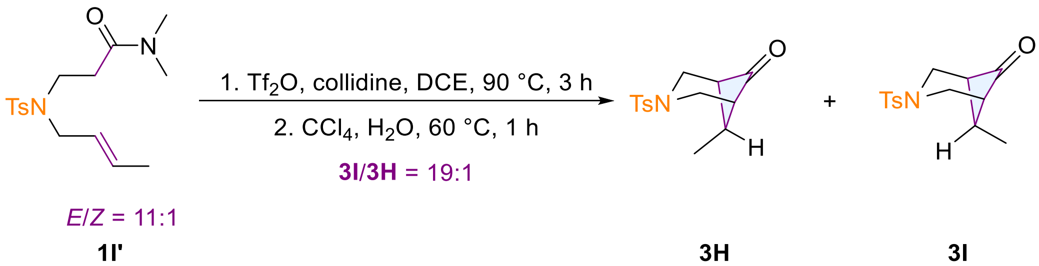


Figure S2. Part of the ^{1}H NMR spectrum of the crude products for reaction of **1I'** (E/Z = 3:1).



Under argon atmosphere, to a solution of **1I'** (64.9 mg, E/Z = 11:1, 0.2 mmol) in DCE (2 mL) in a dried reaction tube with stir bar was added trifluoromethanesulfonic anhydride (80 μL, 0.48 mmol, 2.4 equiv) and collidine (45 μL, 0.22 mmol, 1.1 equiv). After addition was completed, the reaction mixture was heated at 90 °C for 3 h. After cooling to room temperature, the reaction mixture was hydrolyzed in a two phases system H_2O-CCl_4 (1 mL+1 mL) at 60 °C for 1 h. The reaction mixture was decanted and the aqueous layer is extracted with DCM. The organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by column chromatography (PE/EA = 10.1 to 5:1) to give **3I** (36.7 mg, 66%). According to the ^{1}H NMR of crude products, **3I**/**3H** = 19:1. **3H** was not isolated, considering the amount is very little.

Run 2: **1I'** (65.0 mg, E/Z = 11:1, 0.2 mmol), Tf_2O (80 μL, 0.48 mmol), collidine (45 μL, 0.22 mmol), **3I** (36.0 mg, 64%).

The average yield of **3I** is 65%.

Another commonly used procedure[2] was also tested: A solution of **1I'** (64.9 mg, E/Z = 11:1, 0.2 mmol) in DCE (2 mL) was added over 3 min to a solution of trifluoromethanesulfonic anhydride (51 μL, 0.3 mmol, 1.5 equiv) in 2 mL of DCE. A solution of collidine (45 μL, 0.22 mmol, 1.1 equiv) in DCE (2 mL) was then added slowly over 4 min. After addition was completed the reaction mixture was heated at 90 °C for 2 h. After cooling to room temperature, the reaction mixture was concentrated under vacuum.

The residue was hydrolyzed in a two phases system H_2O-CCl_4 (2 mL+2 mL) at reflux for 2 h. The reaction mixture was decanted and the aqueous layer was extracted with DCM. The organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. According to the ^1H NMR of crude products, **3I**/**3H** = 22:1 (no normal product observed), similar to the above result.

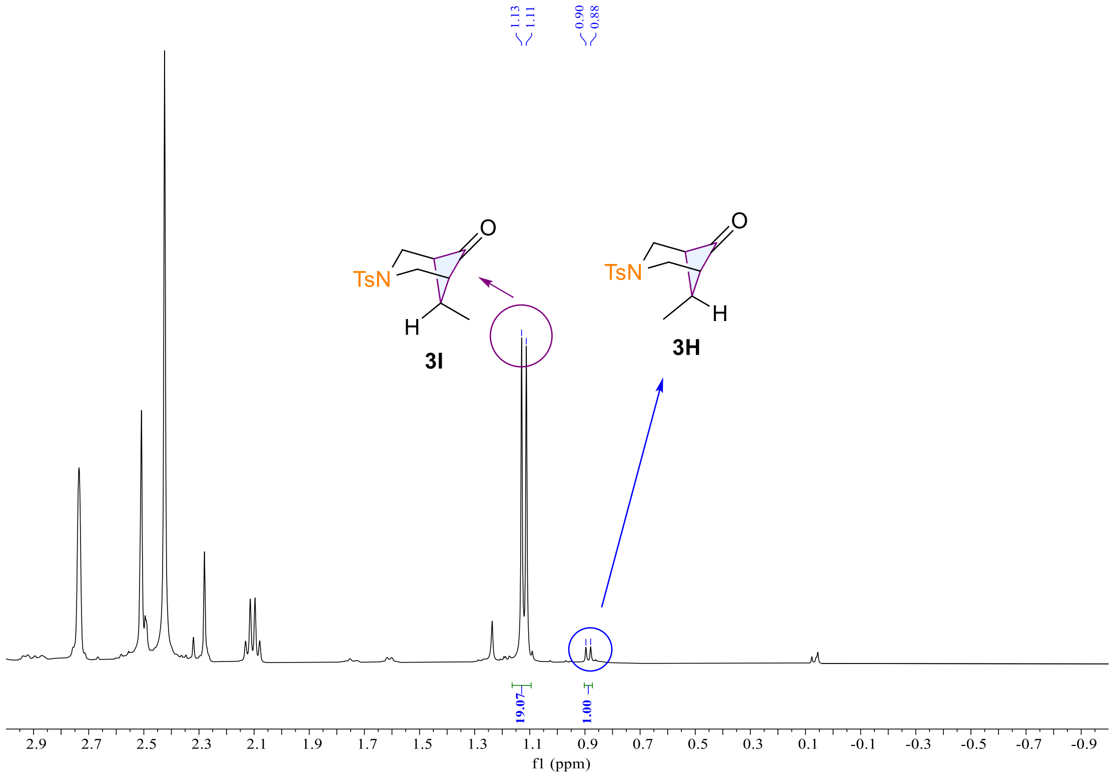
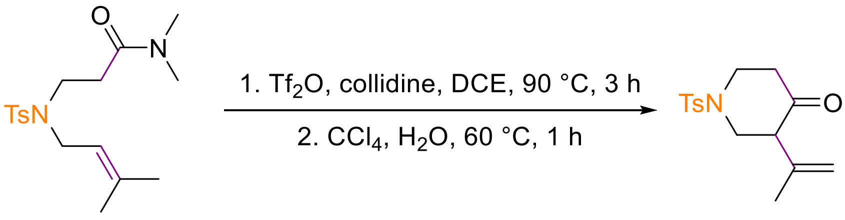


Figure S3. Part of the ^1H NMR spectrum of the crude products for reaction of **1I'** (E/Z = 11:1).



1L **4L**

3-(prop-1-en-2-yl)-1-tosylpiperidin-4-one (4L)

Under argon atmosphere, to a solution of **1L** (67.7 mg, 0.2 mmol) in DCE (2 mL) in a dried reaction tube with stir bar was added trifluoromethanesulfonic anhydride (80 µL, 0.48 mmol, 2.4 equiv) and collidine (45 µL, 0.22 mmol, 1.1 equiv). After addition was completed, the reaction mixture was heated at 90 °C for 3 h. After cooling to room temperature, the reaction mixture was hydrolyzed in a two phases system H_2O-CCl_4 (1 mL+1 mL) at 60 °C for 1 h. The reaction mixture was decanted and the aqueous layer was extracted with DCM. The organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by column chromatography (PE/EA = 10.1 to 5:1) to give **4L** (22.8 mg, 39%) as a yellow solid.

Run 2: **1L** (67.7 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **4L** (21.3 mg, 36%).

The average yield is 38%.

TLC (3:1 PE/EA, R_f): 0.5.

M. P. 84.5-86.5 °C.

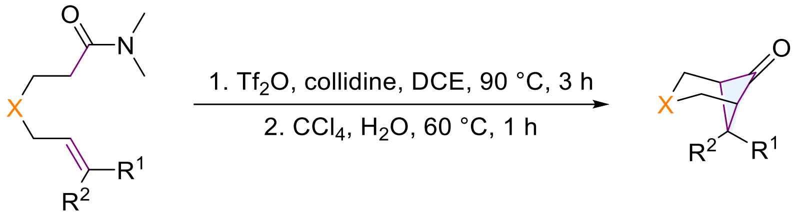
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.3 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 5.05 (s, 1H), 4.90 (s, 1H), 3.74 – 3.62 (m, 2H), 3.25 – 3.06 (m, 3H), 2.63 – 2.55 (m, 2H), 2.45 (s, 3H), 1.73 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 205.5, 144.3, 139.8, 133.3, 130.1, 127.7, 115.3, 56.6, 49.8, 46.5, 40.1, 21.8, 21.7.

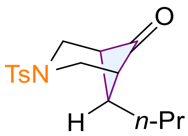
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{15}H_{20}NO_3S^+$: 294.1158; found: 294.1164.

S4. Cross [2 + 2] Cycloadditions

General procedure:



Under argon atmosphere, to a solution of amide **1** (0.2 mmol) in DCE (2 mL) in a dried reaction tube with stir bar was added trifluoromethanesulfonic anhydride (80 μL, 0.48 mmol, 2.4 equiv) and collidine (45 μL, 0.22 mmol, 1.1 equiv). After addition was completed, the reaction mixture was heated at 90 °C for 3 h. After cooling to room temperature, the reaction mixture was hydrolyzed in a two phases system H_2O-$CC1_4$ (1 mL+1 mL) at 60 °C for 1 h. The reaction mixture was decanted and the aqueous layer was extracted with Et_2O or DCM. The organic layers were washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was purified by column chromatography (PE/EA = 10:1 to 5:1) to give the corresponding product **3**.



3J

(1*R*,5*S*,7*r*)-7-propyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3J)

Eluted with PE/EA 10:1, 5:1, yellow oil.

Run 1: **1J** (69.9 mg, 0.2 mmol), Tf_2O (80 μL, 0.48 mmol), collidine (45 μL, 0.22 mmol), **3J** (36.5 mg, 60%).

Run 2: **1J** (70.7 mg, 0.2 mmol), Tf_2O (80 μL, 0.48 mmol), collidine (45 μL, 0.22 mmol), **3J** (37.9 mg, 61%).

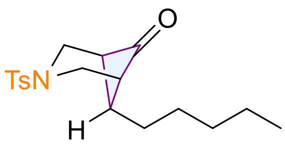
TLC (3:1 PE/EA, R_f): 0.7.

The average yield is 61%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 3.94 (d, J = 9.9 Hz, 2H), 3.82 (d, J = 10.1 Hz, 2H), 2.80 (s, 2H), 2.44 (s, 3H), 1.99 (t, J = 7.4 Hz, 1H), 1.50 – 1.20 (m, 4H), 0.89 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 207.2, 144.0, 134.1, 129.9, 127.3, 58.9, 53.2, 35.3, 33.3, 21.6, 20.9, 13.9.

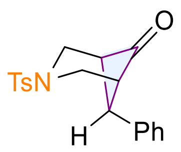
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{16}H_{22}NO_3S^+$: 308.1315; found: 308.1323.



3K

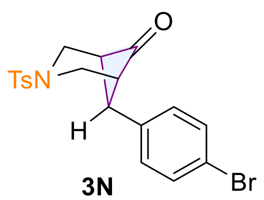
(1*R*,5*S*,7*r*)-7-pentyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3K)

Eluted with PE/EA 10:1, 5:1, yellow oil.
TLC (2:1 PE/EA, R_f): 0.7.
Run 1: **1K** (76.1 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45µL, 0.22 mmol), **3K** (47.0 mg, 70%).
Run 2: **1K** (76.1 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45µL, 0.22 mmol), **3K** (50.5 mg, 75%).
The average yield is 73%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 3.94 (dd, J = 11.6, 1.6 Hz, 2H), 3.82 (d, J = 10.1 Hz, 2H), 2.80 (s, 2H), 2.44 (s, 3H), 1.97 (t, J = 7.7 Hz, 1H), 1.46 – 1.33 (m, 2H), 1.32 – 1.16 (m, 6H), 0.87 (t, J = 6.8 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 207.2, 144.0, 134.1, 130.0, 127.4, 58.9, 53.3, 35.5, 31.5, 31.1, 27.4, 22.6, 21.6, 14.0.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{18}H_{26}NO_3S^+$: 336.1628; found: 336.1626.



3M

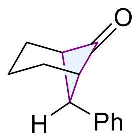
(1*R*,5*S*,7*r*)-7-phenyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3M)
Eluted with PE/EA 10:1, 5:1, white solid.
Run 1: **1M** (77.3 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3M** (58.2 mg, 85%).
Run 2: **1M** (77.3 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3M** (59.4 mg, 87%).
The average yield is 86%.
TLC (2:1 PE/EA, R_f): 0.7.
M. P. 171.0-172.5 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.2 Hz, 2H), 7.36 (d, J = 8.1 Hz, 2H), 7.33 – 7.19 (m, 3H), 7.13 (d, J = 7.2 Hz, 2H), 4.18 (d, J = 10.0 Hz, 2H), 3.93 (d, J = 10.1 Hz, 2H), 3.29 (s, 1H), 3.21 (s, 2H), 2.46 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 206.9, 144.2, 139.1, 134.1, 130.1, 129.1, 127.5, 127.4, 126.8, 60.8, 54.1, 40.1, 21.7.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{19}H_{20}NO_3S^+$: 342.1158; found: 342.1170.



3N

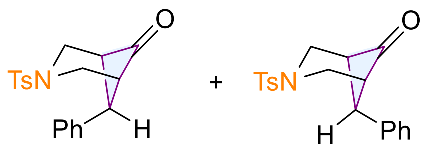
(1*R*,5*S*,7*r*)-7-(4-bromophenyl)-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3N)
Eluted with PE/EA 5:1, yellow solid.
Run 1: **1N** (93.1 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3N** (56.1 mg, 67%).

Run 2: **1N** (93.1 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3N** (59.8 mg, 71%).
The average yield is 69%.
TLC (2:1 PE/EA, R_f): 0.6.
M. P. 150.3-152.2 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.1 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.3 Hz, 2H), 4.17 (d, J = 10.0 Hz, 2H), 3.91 (d, J = 10.3 Hz, 2H), 3.27 (s, 1H), 3.19 (s, 2H), 2.45 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 206.3, 144.3, 138.1, 134.1, 132.2, 130.1, 128.5, 127.4, 121.4, 60.9, 53.9, 39.6, 21.7.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{19}H_{19}BrNO_3S^+$: 420.0264; found: 420.0284.



3O

(1*R*,5*S*,7*s*)-7-phenylbicyclo[3.1.1]heptan-6-one (3O)
Eluted with PE/EA 20:1, colorless oil.
Run 1: **1O** (46.2 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3O** (26.9 mg, 72%).
Run 2: **1O** (46.2 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3O** (25.8 mg, 69%).
The average yield is 71%.
TLC (10:1 PE/EA, R_f): 0.5.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 2H), 7.24 – 7.16 (m, 3H), 3.20 – 3.12 (m, 2H), 3.09 (s, 1H), 2.64 – 2.39 (m, 4H), 1.86 (dtt, J = 15.0, 7.5, 4.0 Hz, 1H), 1.69 (dp, J = 14.4, 8.4 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 213.4, 141.9, 128.8, 126.81, 126.78, 63.3, 43.9, 35.2, 17.7.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{13}H_{15}O^+$: 187.1117; found: 187.1118.



3P **3M**

(1*R*,5*S*,7*s*)-7-phenyl-3-tosyl-3-azabicyclo[3.1.1]heptan-6-one (3P)
Eluted with PE/EA 10:1, 5:1, yellow solid (**3P**). No distinct signal of the normal product was observed by crude ^{1}H NMR and TLC.
Run 1: **1P** (77.3 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3P** (24.5 mg, 36%) and **3M** (8.3 mg, 12%).
Run 2: **1P** (77.3 mg, 0.2 mmol), Tf_2O (80 µL, 0.48 mmol), collidine (45 µL, 0.22 mmol), **3P** (24.6 mg, 36%) and **3M** (8.8 mg, 13%).
The average yield for **3P** is 36%, the average yield for **3M** is 13%.
TLC (3:1 PE/EA, R_f): 0.3.

M. P. 168.0-170.0 °C.

^{1}H NMR of **3P** (400 MHz, $CDCl_3$) δ 7.28 (d, J = 8.2 Hz, 2H), 7.22 – 7.16 (m, 3H), 7.06 (d, J = 8.0 Hz, 2H), 6.99 – 6.93 (m, 2H), 3.97 – 3.91 (m, 4H), 3.64 (t, J = 6.3 Hz, 1H), 3.48 (dt, J = 6.2, 1.6 Hz, 2H), 2.38 (s, 3H).

^{13}C NMR of **3P** (101 MHz, $CDCl_3$) δ 204.7, 143.4, 133.8, 133.6, 129.7, 129.1, 127.7, 127.0, 126.8, 56.0, 48.0, 33.4, 21.6.

HRMS of **3P** (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{19}H_{20}NO_3S^+$: 342.1158; found: 342.1152.

S5. Additional Computational Results

S5.1 Gibbs Energy Profile of 1b and 1d

Similar to **1a**, substrate **1b** undergoes cyclopropanation first to give **IN-1b** via **TS1-1b** with an activation free energy of 11.3 kcal/mol (Figure S4). This process is exergonic by 10.7 kcal/mol. Subsequently, rearrangements of **IN-1b** give rise to the normal product (**NP-1b**) and cross product (**CP-1b**) via **TS2-1b** and **TS3-1b**, respectively. The normal pathway is kinetically favored since **TS2-1b** is energetically lower by 1.4 kcal/mol compared to **TS3-1b**. Transition state (TS) **TS2-1b** possesses a secondary carbocation, while **TS3-1b** resembles a less stable primary carbocation. Thus, **TS2-1b** is more favored. The reaction selectivity is kinetically controlled and generation of normal [2 + 2] product is preferred, which is in consistent with the experimental result.

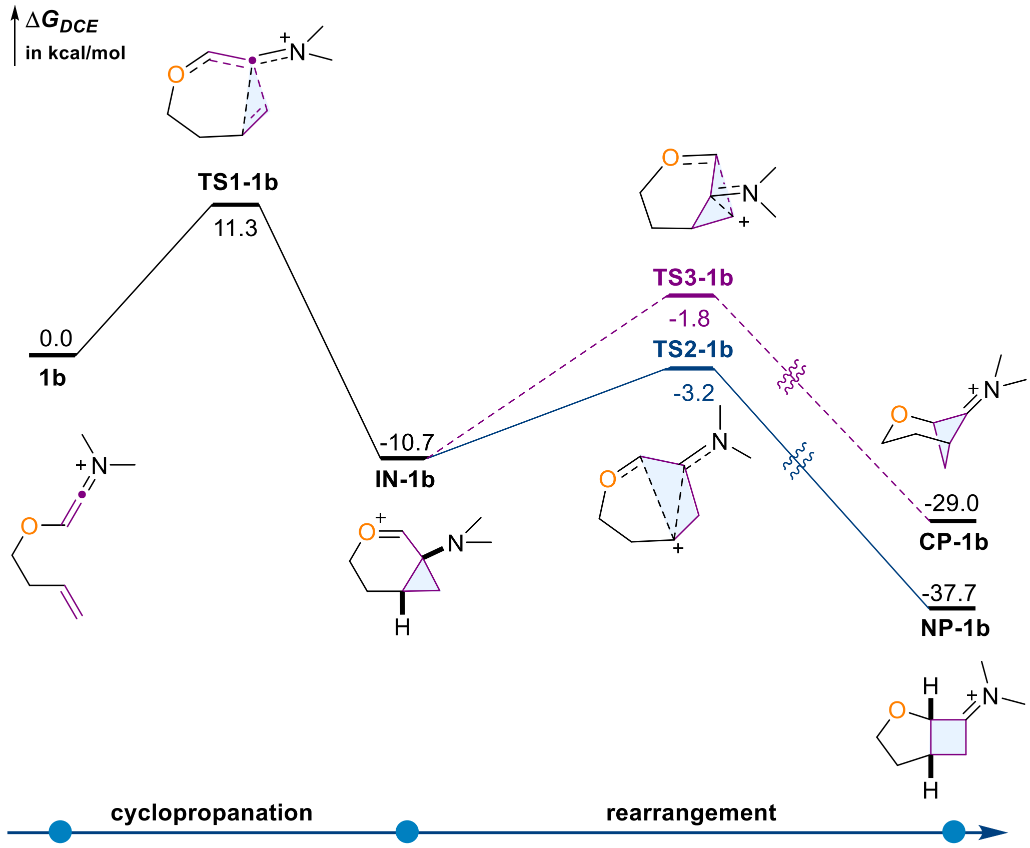


Figure S4. Gibbs energy profile for [2 + 2] cycloaddition of **1b**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//*ω*B97X-D/def2-SVP level.

As shown in Figure S5, ene-keteniminium **1d** with a *E* alkene undergoes cyclopropanation reaction to form **IN-1d** with an activation free energy of 10.7 kcal/mol. After **IN-1d** is generated, there are three reaction pathways, giving respectively to normal [2 + 2] product **NP-1d**, cross [2 + 2] product **CP-1d** and Friedel-Crafts (F-C) product **FC-1d** (this is different from **IN-1c**, which has two reaction pathways after the first cyclopropanation step). The first pathway in these three competing pathways involves a 1,2-rearrangement process via **TS2-1d**, giving rise to **NP-1d**, with an activation free energy of 14.6

kcal/mol. The second pathway also involves a 1,2-rearrangement process via **TS3-1d**, affording **CP-1d**, with an activation free energy of 7.7 kcal/mol. Similar to **1c**, **TS3-1d** experiencing less distortion is more favored than **TS2-1d**. The third pathway for intermediate **IN-1d** to undertake is the proton abstraction process by the nitrogen atom (a 1,5-proton shift process) to form **FC-1d**, with an activation free energy of 12.9 kcal/mol. Consequently, formation of cross [2 + 2] cycloaddition product is the most favored and **CP-1d** is the kinetic product. **CP-1d** could isomerize to a more stable F-C product **FC-1d**, with an activation free energy of 29.4 kcal/mol. Transformation from **CP-1d** to **NP-1d** is not feasible due to this higher activation free energy. It should be noted that isomerization of **CP-1d** to **NP-1d** is still possible if there is no F-C pathway, considering that the activation free energy for this is 31.1 kcal/mol, very close to that for the reaction of **1c**. Therefore, the selectivity between **NP-1d** and **CP-1d** can be viewed as thermodynamic control.

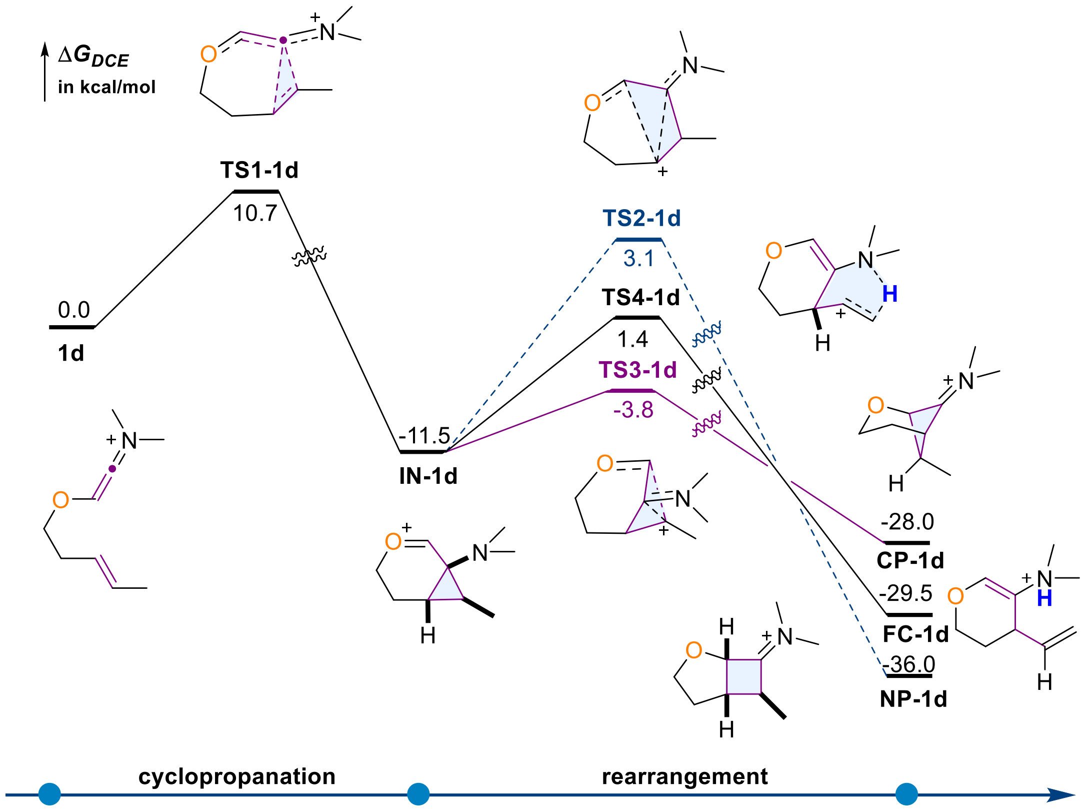


Figure S5. Gibbs energy profile for [2 + 2] cycloaddition and F-C pathway of **1d**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//*ω*B97X-D/def2-SVP level.

S5.2 More Discussions on [2 + 2] Cycloaddition for 1e

In addition to the concerted rearrangement pathway from **NP-1e** to **CP-1e**, there is a stepwise pathway shown in Figure S6 featuring generation of a carbocation at the first stage, which is also highly disfavored. The potential energy surface of [2 + 2] cycloaddition for **1e** is shown in Figure S7, which clearly shows that **TS1-1e** is not ambimodal. After passing through **TS1-1e**, the reaction leads to **NP-1e** directly.

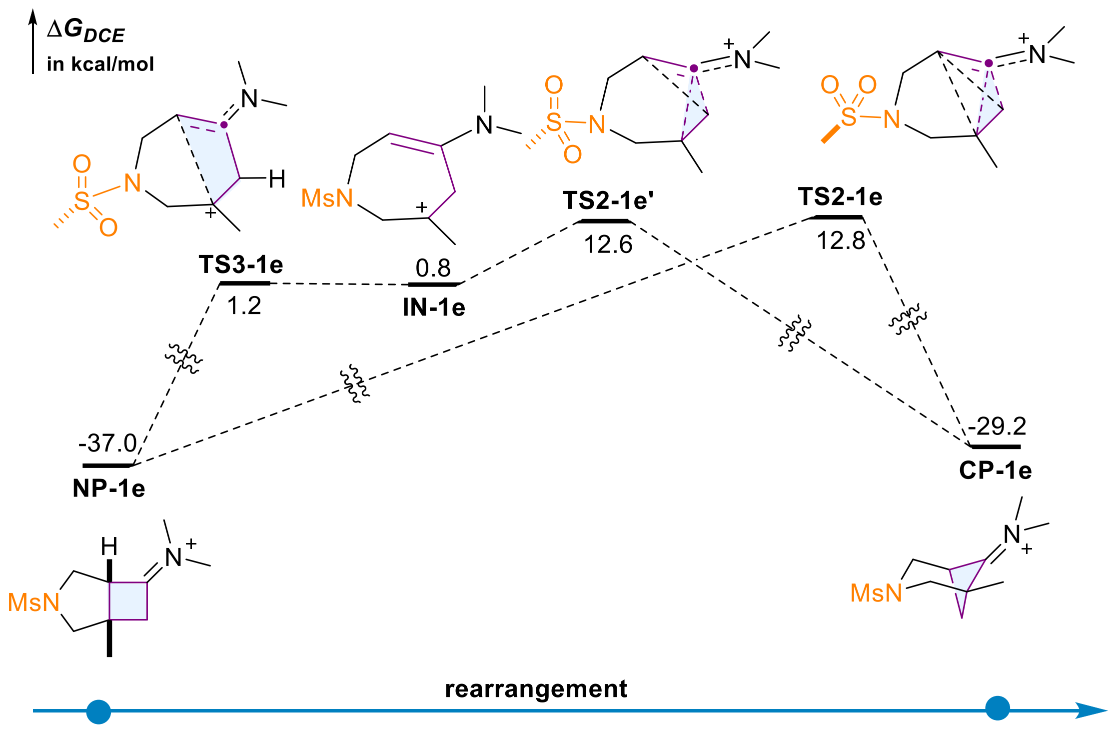


Figure S6. The stepwise rearrangement pathway from **NP-1e** to **CP-1e**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//ωB97X-D/def2-SVP level.

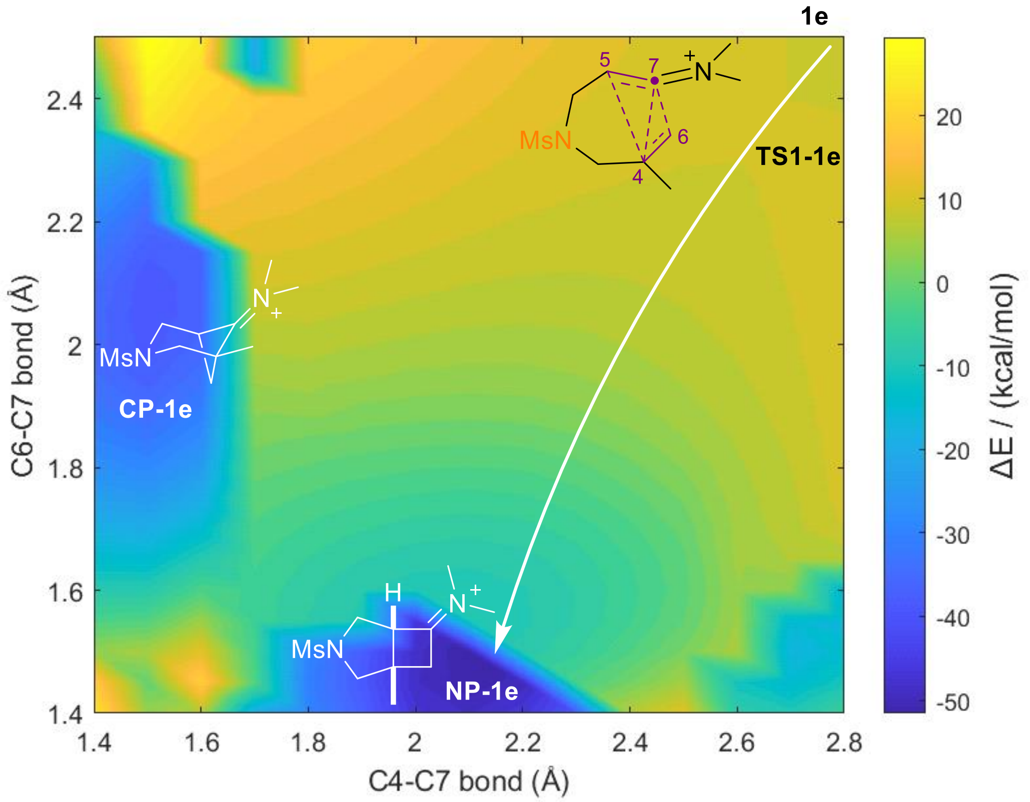


Figure S7. Potential energy surface of [2 + 2] cycloaddition for **1e**. Computed at ωB97X-D/def2-SVP level.

Table S1. Relaxed Potential Energy Surface Scan for [2 + 2] Cycloaddition of 1e

C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)
2.8	2.5	-1049.454498	2.7	2.5	-1049.453634	2.6	2.5	-1049.452967
2.8	2.45	-1049.453993	2.7	2.45	-1049.453633	2.6	2.45	-1049.453152
2.8	2.4	-1049.453727	2.7	2.4	-1049.453595	2.6	2.4	-1049.453313
2.8	2.35	-1049.453437	2.7	2.35	-1049.453527	2.6	2.35	-1049.453453
2.8	2.3	-1049.453117	2.7	2.3	-1049.453437	2.6	2.3	-1049.453586
2.8	2.25	-1049.452802	2.7	2.25	-1049.453368	2.6	2.25	-1049.453754
2.8	2.2	-1049.452509	2.7	2.2	-1049.453338	2.6	2.2	-1049.453975
2.8	2.15	-1049.452238	2.7	2.15	-1049.453354	2.6	2.15	-1049.45425
2.8	2.1	-1049.452022	2.7	2.1	-1049.453455	2.6	2.1	-1049.454624
2.8	2.05	-1049.451885	2.7	2.05	-1049.45366	2.6	2.05	-1049.455118
2.8	2	-1049.45183	2.7	2	-1049.453975	2.6	2	-1049.455739
2.8	1.95	-1049.451856	2.7	1.95	-1049.454409	2.6	1.95	-1049.456496
2.8	1.9	-1049.451959	2.7	1.9	-1049.454939	2.6	1.9	-1049.457365
2.8	1.85	-1049.452126	2.7	1.85	-1049.455537	2.6	1.85	-1049.458305
2.8	1.8	-1049.45231	2.7	1.8	-1049.456148	2.6	1.8	-1049.459239
2.8	1.75	-1049.452437	2.7	1.75	-1049.456691	2.6	1.75	-1049.460058
2.8	1.7	-1049.45352	2.7	1.7	-1049.457039	2.6	1.7	-1049.460633
2.8	1.65	-1049.458296	2.7	1.65	-1049.458519	2.6	1.65	-1049.460755
2.8	1.6	-1049.492929	2.7	1.6	-1049.464095	2.6	1.6	-1049.461506
2.8	1.55	-1049.493419	2.7	1.55	-1049.492207	2.6	1.55	-1049.461109
2.8	1.5	-1049.491151	2.7	1.5	-1049.495545	2.6	1.5	-1049.459193
2.8	1.45	-1049.48549	2.7	1.45	-1049.491652	2.6	1.45	-1049.486134
2.8	1.4	-1049.475649	2.7	1.4	-1049.483455	2.6	1.4	-1049.480133
2.5	2.5	-1049.452103	2.4	2.5	-1049.45089	2.3	2.5	-1049.449221
2.5	2.45	-1049.452474	2.4	2.45	-1049.45149	2.3	2.45	-1049.450075
2.5	2.4	-1049.452836	2.4	2.4	-1049.452066	2.3	2.4	-1049.450906
2.5	2.35	-1049.453186	2.4	2.35	-1049.452637	2.3	2.35	-1049.451731
2.5	2.3	-1049.453539	2.4	2.3	-1049.453219	2.3	2.3	-1049.452579
2.5	2.25	-1049.453938	2.4	2.25	-1049.453858	2.3	2.25	-1049.453461
2.5	2.2	-1049.454397	2.4	2.2	-1049.454566	2.3	2.2	-1049.454417
2.5	2.15	-1049.454922	2.4	2.15	-1049.455353	2.3	2.15	-1049.455456
2.5	2.1	-1049.455559	2.4	2.1	-1049.456262	2.3	2.1	-1049.456633
2.5	2.05	-1049.456329	2.4	2.05	-1049.457325	2.3	2.05	-1049.457981
2.5	2	-1049.457254	2.4	2	-1049.458568	2.3	2	-1049.459536
2.5	1.95	-1049.458352	2.4	1.95	-1049.460029	2.3	1.95	-1049.461378
2.5	1.9	-1049.459636	2.4	1.9	-1049.461961	2.3	1.9	-1049.463828
2.5	1.85	-1049.461471	2.4	1.85	-1049.464503	2.3	1.85	-1049.466742
2.5	1.8	-1049.463795	2.4	1.8	-1049.467246	2.3	1.8	-1049.469838
2.5	1.75	-1049.466124	2.4	1.75	-1049.469958	2.3	1.75	-1049.472916

2.5	1.7	-1049.468181	2.4	1.7	-1049.472393	2.3	1.7	-1049.475728
2.5	1.65	-1049.469636	2.4	1.65	-1049.474228	2.3	1.65	-1049.477975
2.5	1.6	-1049.470092	2.4	1.6	-1049.475095	2.3	1.6	-1049.479293
2.5	1.55	-1049.469071	2.4	1.55	-1049.474518	2.3	1.55	-1049.479217
2.5	1.5	-1049.465981	2.4	1.5	-1049.471913	2.3	1.5	-1049.477166
2.5	1.45	-1049.460111	2.4	1.45	-1049.466553	2.3	1.45	-1049.472436
2.5	1.4	-1049.450412	2.4	1.4	-1049.457549	2.3	1.4	-1049.53077
2.2	2.5	-1049.447157	2.1	2.5	-1049.444744	2	2.5	-1049.442242
2.2	2.45	-1049.448281	2.1	2.45	-1049.446153	2	2.45	-1049.443888
2.2	2.4	-1049.449374	2.1	2.4	-1049.447511	2	2.4	-1049.445496
2.2	2.35	-1049.450461	2.1	2.35	-1049.448847	2	2.35	-1049.447072
2.2	2.3	-1049.451556	2.1	2.3	-1049.450187	2	2.3	-1049.448643
2.2	2.25	-1049.452684	2.1	2.25	-1049.451551	2	2.25	-1049.450226
2.2	2.2	-1049.45388	2.1	2.2	-1049.452966	2	2.2	-1049.451846
2.2	2.15	-1049.455165	2.1	2.15	-1049.454474	2	2.15	-1049.453534
2.2	2.1	-1049.456582	2.1	2.1	-1049.456108	2	2.1	-1049.455331
2.2	2.05	-1049.458181	2.1	2.05	-1049.457908	2	2.05	-1049.457273
2.2	2	-1049.460002	2.1	2	-1049.459911	2	2	-1049.459393
2.2	1.95	-1049.46212	2.1	1.95	-1049.462191	2	1.95	-1049.46189
2.2	1.9	-1049.46483	2.1	1.9	-1049.465072	2	1.9	-1049.464818
2.2	1.85	-1049.467968	2.1	1.85	-1049.468297	2	1.85	-1049.467998
2.2	1.8	-1049.471315	2.1	1.8	-1049.471732	2	1.8	-1049.471356
2.2	1.75	-1049.474672	2.1	1.75	-1049.475217	2	1.75	-1049.474765
2.2	1.7	-1049.477801	2.1	1.7	-1049.478532	2	1.7	-1049.478053
2.2	1.65	-1049.480426	2.1	1.65	-1049.481412	2	1.65	-1049.48099
2.2	1.6	-1049.482183	2.1	1.6	-1049.483524	2	1.6	-1049.483268
2.2	1.55	-1049.482626	2.1	1.55	-1049.484451	2	1.55	-1049.542216
2.2	1.5	-1049.481197	2.1	1.5	-1049.551544	2	1.5	-1049.545562
2.2	1.45	-1049.54781	2.1	1.45	-1049.550888	2	1.45	-1049.546124
2.2	1.4	-1049.542277	2.1	1.4	-1049.546594	2	1.4	-1049.543073
1.9	2.5	-1049.440068	1.8	2.5	-1049.438422	1.7	2.5	-1049.502216
1.9	2.45	-1049.441777	1.8	2.45	-1049.440058	1.7	2.45	-1049.50051
1.9	2.4	-1049.443525	1.8	2.4	-1049.4418	1.7	2.4	-1049.4399
1.9	2.35	-1049.445287	1.8	2.35	-1049.443609	1.7	2.35	-1049.441658
1.9	2.3	-1049.44706	1.8	2.3	-1049.445503	1.7	2.3	-1049.443556
1.9	2.25	-1049.448842	1.8	2.25	-1049.447442	1.7	2.25	-1049.445992
1.9	2.2	-1049.450644	1.8	2.2	-1049.449407	1.7	2.2	-1049.448392
1.9	2.15	-1049.452487	1.8	2.15	-1049.451393	1.7	2.15	-1049.45078
1.9	2.1	-1049.4544	1.8	2.1	-1049.453413	1.7	2.1	-1049.453208
1.9	2.05	-1049.456425	1.8	2.05	-1049.455489	1.7	2.05	-1049.45569
1.9	2	-1049.458598	1.8	2	-1049.457646	1.7	2	-1049.458187
1.9	1.95	-1049.460949	1.8	1.95	-1049.459919	1.7	1.95	-1049.460677
1.9	1.9	-1049.464335	1.8	1.9	-1049.462327	1.7	1.9	-1049.463144

1.9	1.85	-1049.467371	1.8	1.85	-1049.466551	1.7	1.85	-1049.465577
1.9	1.8	-1049.470504	1.8	1.8	-1049.469363	1.7	1.8	-1049.467931
1.9	1.75	-1049.473651	1.8	1.75	-1049.472118	1.7	1.75	-1049.470157
1.9	1.7	-1049.476682	1.8	1.7	-1049.474704	1.7	1.7	-1049.472156
1.9	1.65	-1049.479402	1.8	1.65	-1049.476969	1.7	1.65	-1049.473793
1.9	1.6	-1049.481542	1.8	1.6	-1049.478683	1.7	1.6	-1049.474867
1.9	1.55	-1049.482779	1.8	1.55	-1049.479525	1.7	1.55	-1049.475079
1.9	1.5	-1049.528249	1.8	1.5	-1049.515316	1.7	1.5	-1049.474026
1.9	1.45	-1049.529406	1.8	1.45	-1049.516991	1.7	1.45	-1049.47122
1.9	1.4	-1049.527169	1.8	1.4	-1049.515313	1.7	1.4	-1049.500442
1.6	2.5	-1049.428767	1.5	2.5	-1049.420076	1.4	2.5	-1049.456828
1.6	2.45	-1049.432102	1.5	2.45	-1049.424071	1.4	2.45	-1049.469173
1.6	2.4	-1049.435249	1.5	2.4	-1049.427818	1.4	2.4	-1049.480676
1.6	2.35	-1049.438254	1.5	2.35	-1049.431394	1.4	2.35	-1049.491157
1.6	2.3	-1049.441165	1.5	2.3	-1049.511943	1.4	2.3	-1049.500453
1.6	2.25	-1049.444023	1.5	2.25	-1049.518868	1.4	2.25	-1049.508408
1.6	2.2	-1049.446864	1.5	2.2	-1049.524258	1.4	2.2	-1049.514881
1.6	2.15	-1049.525813	1.5	2.15	-1049.528046	1.4	2.15	-1049.519757
1.6	2.1	-1049.526957	1.5	2.1	-1049.530184	1.4	2.1	-1049.522954
1.6	2.05	-1049.526611	1.5	2.05	-1049.530704	1.4	2.05	-1049.524441
1.6	2	-1049.524899	1.5	2	-1049.529715	1.4	2	-1049.524283
1.6	1.95	-1049.521981	1.5	1.95	-1049.527381	1.4	1.95	-1049.522627
1.6	1.9	-1049.51796	1.5	1.9	-1049.523879	1.4	1.9	-1049.519696
1.6	1.85	-1049.512865	1.5	1.85	-1049.519299	1.4	1.85	-1049.515664
1.6	1.8	-1049.506691	1.5	1.8	-1049.513659	1.4	1.8	-1049.510623
1.6	1.75	-1049.499472	1.5	1.75	-1049.507042	1.4	1.75	-1049.504763
1.6	1.7	-1049.491372	1.5	1.7	-1049.499555	1.4	1.7	-1049.498032
1.6	1.65	-1049.482277	1.5	1.65	-1049.491064	1.4	1.65	-1049.490359
1.6	1.6	-1049.472274	1.5	1.6	-1049.481616	1.4	1.6	-1049.481778
1.6	1.55	-1049.461339	1.5	1.55	-1049.471178	1.4	1.55	-1049.472306
1.6	1.5	-1049.44933	1.5	1.5	-1049.459689	1.4	1.5	-1049.462004
1.6	1.45	-1049.437657	1.5	1.45	-1049.468761	1.4	1.45	-1049.438595
1.6	1.4	-1049.457555	1.5	1.4	-1049.462127	1.4	1.4	-1049.429835

S5.3 More Discussions on [2 + 2] Cycloaddition of 1h

To understand the bifurcation potential energy surface (PES) more directly, we also did the relaxed potential energy surface scan for the [2 + 2] cycloaddition of **1h**. The calculated results were drawn as a 3D surface (Figure S8a) and 2D contour (Figure S8b). After passing through **TS1-1h**, the PES bifurcates to give **NP-1h** and **CP-1h**, which is connected by rearrangement transition state, **TS3-1h**. Intermediate **IN1-1h** can easily afford **NP-1h** in an almost barrierless manner. The lifetime of trajectories is correlated with the shape of PES. If the PES in which the trajectories pass through is steep, the trajectories could be relatively short-lived. While the trajectories would be relatively long-lived, if the PES is flat. In the case of **1h**, the trajectories leading to **NP-1h** are usually long-lived since they have to pass through **IN1-1h**. While the trajectories leading to **CP-1h** are relatively short-lived since there is no stable intermediate on the path from **TS1-1h** to **CP-1h**. But the lifetimes of some trajectories are even longer if they firstly surf the **TS3-1h** area and then afford the product (either **NP-1h** or **CP-1h**).

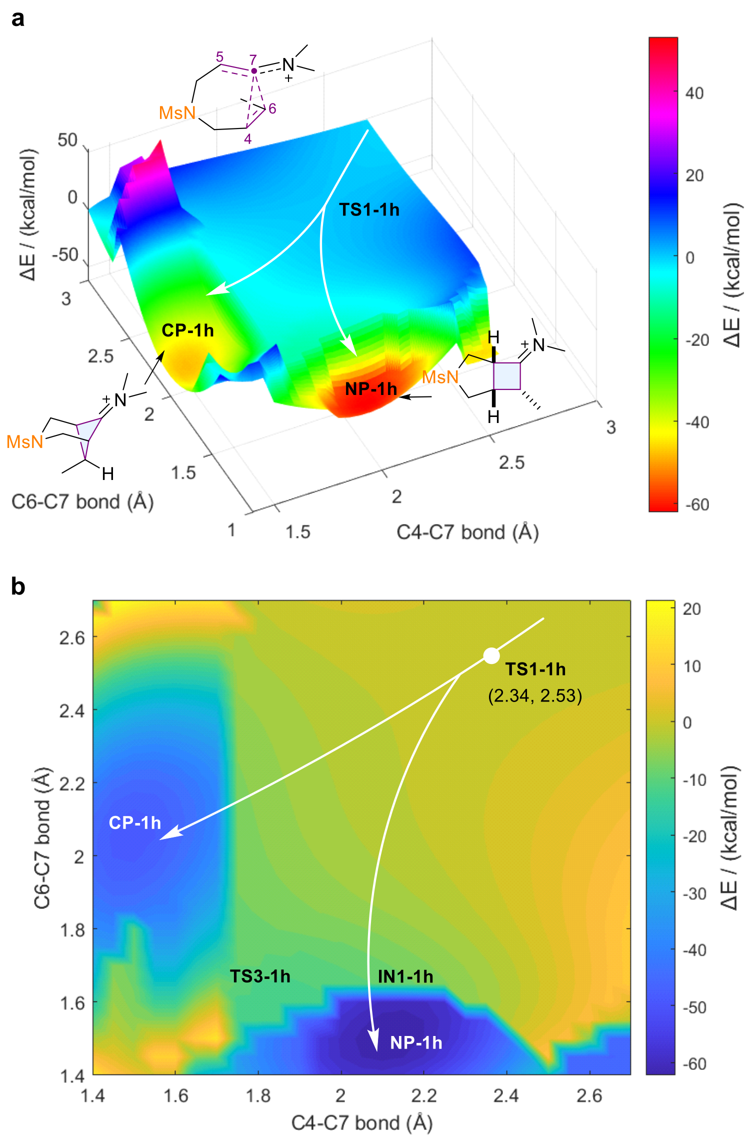


Figure S8. 3D (a) and 2D (b) potential energy surfaces of [2 + 2] cycloaddition for **1h**. Computed at ωB97X-D/def2-SVP level.

As mentioned in the main text, there are *endo* and *exo* carbocation regions on the PES, which make lifetime of trajectories passing through them longer. The *endo* cation is a real intermediate which can be located, while the *exo* one could not be located. We can call it as an entropic intermediate, according to previous work by Singleton and Houk.[6-8] To further support the hypothesis that there is a hidden "intermediate" between **TS1-1h** to **CP-1h**, we calculated the free energy profile along the IRC of **TS1-1h** based on variational transition state theory. And indeed, there is an intermediate region resembling an *exo* carbocation on the free energy profile, which is regarded as an entropic intermediate (Figure S9).

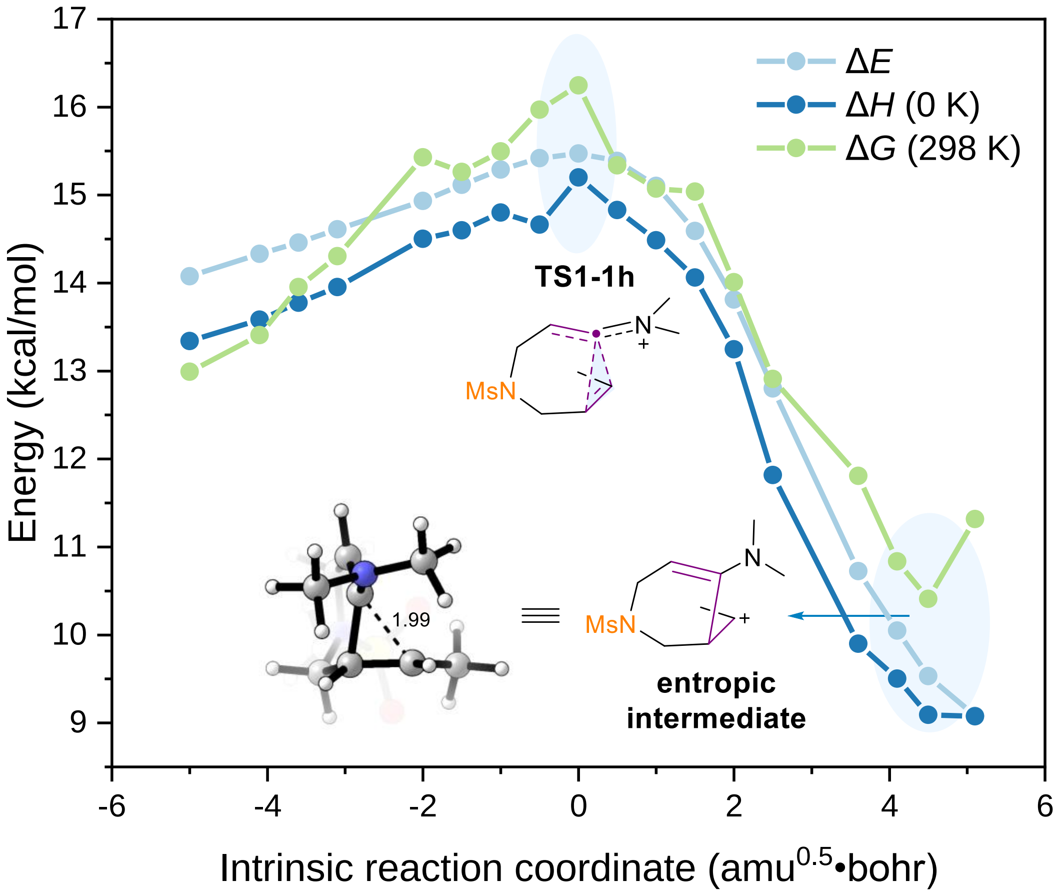


Figure S9. Energy profiles along the IRC through **TS1-1h**. The free-energy profile is based on generalized free energies of activation obtained from KiSThelP.[9] The bong length is reported in Å.

We also analyzed the time gap between the formations of the two bonds, as shown in Figure S10. The time gaps for most normal [2 + 2] trajectories are longer than 300 fs. While a half of cross [2 + 2] trajectories have time gaps shorter than 300 fs. It should be noted that almost all the trajectories are dynamically stepwise, since the time gaps between the formations of the two bonds are longer than 60 fs, a time criterion defined by Houk et al.[8]

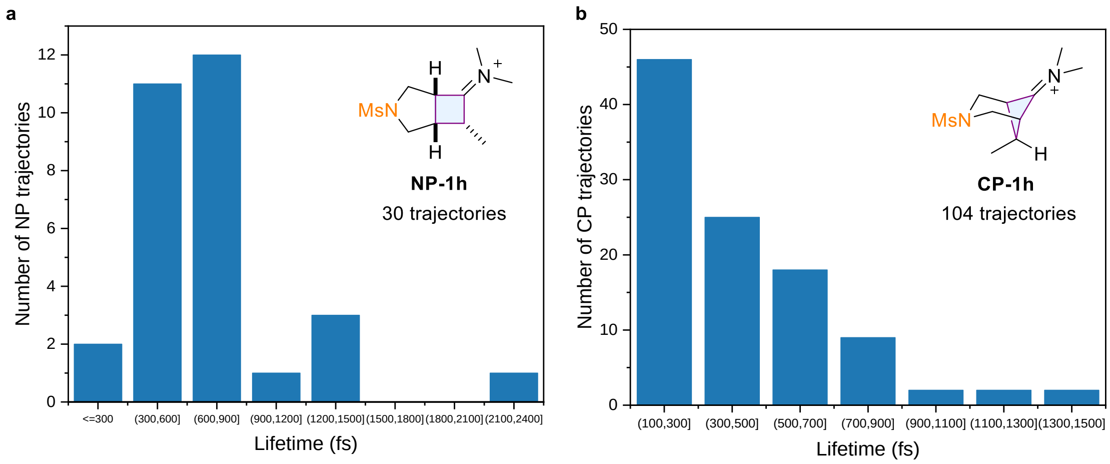


Figure S10. The time gap between formations of the first bond and the second bond for normal [2 + 2] and cross [2 + 2] trajectories.

Table S2. Relaxed Potential Energy Surface Scan for [2 + 2] Cycloaddition of 1h

C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)
2.7	2.7	-1049.448738	2.65	2.7	-1049.448546	2.6	2.7	-1049.448351
2.7	2.65	-1049.448334	2.65	2.65	-1049.448232	2.6	2.65	-1049.448123
2.7	2.6	-1049.447814	2.65	2.6	-1049.447805	2.6	2.6	-1049.447791
2.7	2.55	-1049.44718	2.65	2.55	-1049.447271	2.6	2.55	-1049.447359
2.7	2.5	-1049.446425	2.65	2.5	-1049.446637	2.6	2.5	-1049.446832
2.7	2.45	-1049.44555	2.65	2.45	-1049.445892	2.6	2.45	-1049.446201
2.7	2.4	-1049.444565	2.65	2.4	-1049.445048	2.6	2.4	-1049.445486
2.7	2.35	-1049.443473	2.65	2.35	-1049.444107	2.6	2.35	-1049.444684
2.7	2.3	-1049.44228	2.65	2.3	-1049.443082	2.6	2.3	-1049.443807
2.7	2.25	-1049.441027	2.65	2.25	-1049.442011	2.6	2.25	-1049.442901
2.7	2.2	-1049.439739	2.65	2.2	-1049.440913	2.6	2.2	-1049.441981
2.7	2.15	-1049.438432	2.65	2.15	-1049.439806	2.6	2.15	-1049.441062
2.7	2.1	-1049.437139	2.65	2.1	-1049.438733	2.6	2.1	-1049.440186
2.7	2.05	-1049.435901	2.65	2.05	-1049.437729	2.6	2.05	-1049.439391
2.7	2	-1049.434742	2.65	2	-1049.436817	2.6	2	-1049.438705
2.7	1.95	-1049.433692	2.65	1.95	-1049.436021	2.6	1.95	-1049.438153
2.7	1.9	-1049.432768	2.65	1.9	-1049.435353	2.6	1.9	-1049.437748
2.7	1.85	-1049.43196	2.65	1.85	-1049.434835	2.6	1.85	-1049.43752
2.7	1.8	-1049.431254	2.65	1.8	-1049.434546	2.6	1.8	-1049.437575
2.7	1.75	-1049.431067	2.65	1.75	-1049.434651	2.6	1.75	-1049.43793
2.7	1.7	-1049.431027	2.65	1.7	-1049.434788	2.6	1.7	-1049.438269
2.7	1.65	-1049.431185	2.65	1.65	-1049.434749	2.6	1.65	-1049.438263
2.7	1.6	-1049.441363	2.65	1.6	-1049.434242	2.6	1.6	-1049.437651
2.7	1.55	-1049.448809	2.65	1.55	-1049.4456	2.6	1.55	-1049.435914
2.7	1.5	-1049.519528	2.65	1.5	-1049.519478	2.6	1.5	-1049.457351
2.7	1.45	-1049.520217	2.65	1.45	-1049.520775	2.6	1.45	-1049.520373
2.7	1.4	-1049.517477	2.65	1.4	-1049.518702	2.6	1.4	-1049.51891
2.55	2.7	-1049.448134	2.5	2.7	-1049.447889	2.45	2.7	-1049.447614
2.55	2.65	-1049.447993	2.5	2.65	-1049.447838	2.45	2.65	-1049.447665
2.55	2.6	-1049.447752	2.5	2.6	-1049.447693	2.45	2.6	-1049.447619
2.55	2.55	-1049.447416	2.5	2.55	-1049.447457	2.45	2.55	-1049.447482
2.55	2.5	-1049.446994	2.5	2.5	-1049.447137	2.45	2.5	-1049.44726
2.55	2.45	-1049.446477	2.5	2.45	-1049.446732	2.45	2.45	-1049.446958
2.55	2.4	-1049.44588	2.5	2.4	-1049.44625	2.45	2.4	-1049.446582
2.55	2.35	-1049.445215	2.5	2.35	-1049.445702	2.45	2.35	-1049.446145
2.55	2.3	-1049.444484	2.5	2.3	-1049.445102	2.45	2.3	-1049.445662
2.55	2.25	-1049.443734	2.5	2.25	-1049.444491	2.45	2.25	-1049.445177
2.55	2.2	-1049.442979	2.5	2.2	-1049.443889	2.45	2.2	-1049.444712
2.55	2.15	-1049.442232	2.5	2.15	-1049.443301	2.45	2.15	-1049.444274

2.55	2.1	-1049.441539	2.5	2.1	-1049.442777	2.45	2.1	-1049.443905
2.55	2.05	-1049.440936	2.5	2.05	-1049.442355	2.45	2.05	-1049.443646
2.55	2	-1049.440449	2.5	2	-1049.44206	2.45	2	-1049.44353
2.55	1.95	-1049.440113	2.5	1.95	-1049.441924	2.45	1.95	-1049.443581
2.55	1.9	-1049.439962	2.5	1.9	-1049.441988	2.45	1.9	-1049.443833
2.55	1.85	-1049.440006	2.5	1.85	-1049.44227	2.45	1.85	-1049.444314
2.55	1.8	-1049.44034	2.5	1.8	-1049.442839	2.45	1.8	-1049.445102
2.55	1.75	-1049.440923	2.5	1.75	-1049.443663	2.45	1.75	-1049.446144
2.55	1.7	-1049.441479	2.5	1.7	-1049.444427	2.45	1.7	-1049.447126
2.55	1.65	-1049.44166	2.5	1.65	-1049.444825	2.45	1.65	-1049.447745
2.55	1.6	-1049.441058	2.5	1.6	-1049.444442	2.45	1.6	-1049.447612
2.55	1.55	-1049.439287	2.5	1.55	-1049.442758	2.45	1.55	-1049.446224
2.55	1.5	-1049.435683	2.5	1.5	-1049.43916	2.45	1.5	-1049.442998
2.55	1.45	-1049.519022	2.5	1.45	-1049.432904	2.45	1.45	-1049.502897
2.55	1.4	-1049.51813	2.5	1.4	-1049.48253	2.45	1.4	-1049.494269
2.4	2.7	-1049.447307	2.35	2.7	-1049.446959	2.3	2.7	-1049.446576
2.4	2.65	-1049.447462	2.35	2.65	-1049.447223	2.3	2.65	-1049.446955
2.4	2.6	-1049.447517	2.35	2.6	-1049.447383	2.3	2.6	-1049.447226
2.4	2.55	-1049.447477	2.35	2.55	-1049.447446	2.3	2.55	-1049.447396
2.4	2.5	-1049.447351	2.35	2.5	-1049.447419	2.3	2.5	-1049.447472
2.4	2.45	-1049.447148	2.35	2.45	-1049.447312	2.3	2.45	-1049.447466
2.4	2.4	-1049.446872	2.35	2.4	-1049.447135	2.3	2.4	-1049.447389
2.4	2.35	-1049.446542	2.35	2.35	-1049.446909	2.3	2.35	-1049.447264
2.4	2.3	-1049.446175	2.35	2.3	-1049.446654	2.3	2.3	-1049.447114
2.4	2.25	-1049.445808	2.35	2.25	-1049.4464	2.3	2.25	-1049.446962
2.4	2.2	-1049.445467	2.35	2.2	-1049.44617	2.3	2.2	-1049.446831
2.4	2.15	-1049.445163	2.35	2.15	-1049.44598	2.3	2.15	-1049.44674
2.4	2.1	-1049.444934	2.35	2.1	-1049.445877	2.3	2.1	-1049.446743
2.4	2.05	-1049.444823	2.35	2.05	-1049.445895	2.3	2.05	-1049.446876
2.4	2	-1049.444866	2.35	2	-1049.446075	2.3	2	-1049.447171
2.4	1.95	-1049.445083	2.35	1.95	-1049.446441	2.3	1.95	-1049.447665
2.4	1.9	-1049.445505	2.35	1.9	-1049.447011	2.3	1.9	-1049.448368
2.4	1.85	-1049.446154	2.35	1.85	-1049.447817	2.3	1.85	-1049.449316
2.4	1.8	-1049.447157	2.35	1.8	-1049.449012	2.3	1.8	-1049.450679
2.4	1.75	-1049.448381	2.35	1.75	-1049.450409	2.3	1.75	-1049.452238
2.4	1.7	-1049.449573	2.35	1.7	-1049.45178	2.3	1.7	-1049.453769
2.4	1.65	-1049.450423	2.35	1.65	-1049.45285	2.3	1.65	-1049.455033
2.4	1.6	-1049.450554	2.35	1.6	-1049.453263	2.3	1.6	-1049.455736
2.4	1.55	-1049.449508	2.35	1.55	-1049.528898	2.3	1.55	-1049.53578
2.4	1.5	-1049.51832	2.35	1.5	-1049.527179	2.3	1.5	-1049.534606
2.4	1.45	-1049.513414	2.35	1.45	-1049.522732	2.3	1.45	-1049.530675
2.4	1.4	-1049.505087	2.35	1.4	-1049.514796	2.3	1.4	-1049.523207
2.25	2.7	-1049.446201	2.2	2.7	-1049.445853	2.15	2.7	-1049.445546

2.25	2.65	-1049.446697	2.2	2.65	-1049.446468	2.15	2.65	-1049.446282
2.25	2.6	-1049.447081	2.2	2.6	-1049.446964	2.15	2.6	-1049.446887
2.25	2.55	-1049.44736	2.2	2.55	-1049.44735	2.15	2.55	-1049.447377
2.25	2.5	-1049.447539	2.2	2.5	-1049.447634	2.15	2.5	-1049.447761
2.25	2.45	-1049.447632	2.2	2.45	-1049.447825	2.15	2.45	-1049.448049
2.25	2.4	-1049.447654	2.2	2.4	-1049.447939	2.15	2.4	-1049.448254
2.25	2.35	-1049.447621	2.2	2.35	-1049.447996	2.15	2.35	-1049.448398
2.25	2.3	-1049.447562	2.2	2.3	-1049.448018	2.15	2.3	-1049.448503
2.25	2.25	-1049.447499	2.2	2.25	-1049.448037	2.15	2.25	-1049.448592
2.25	2.2	-1049.447457	2.2	2.2	-1049.448074	2.15	2.2	-1049.448698
2.25	2.15	-1049.447457	2.2	2.15	-1049.448155	2.15	2.15	-1049.448849
2.25	2.1	-1049.447549	2.2	2.1	-1049.448325	2.15	2.1	-1049.449087
2.25	2.05	-1049.447781	2.2	2.05	-1049.448633	2.15	2.05	-1049.449455
2.25	2	-1049.448178	2.2	2	-1049.449111	2.15	2	-1049.449996
2.25	1.95	-1049.448774	2.2	1.95	-1049.44979	2.15	1.95	-1049.450736
2.25	1.9	-1049.449589	2.2	1.9	-1049.450691	2.15	1.9	-1049.451697
2.25	1.85	-1049.450665	2.2	1.85	-1049.451881	2.15	1.85	-1049.452982
2.25	1.8	-1049.452174	2.2	1.8	-1049.453517	2.15	1.8	-1049.454723
2.25	1.75	-1049.453871	2.2	1.75	-1049.455327	2.15	1.75	-1049.456637
2.25	1.7	-1049.455555	2.2	1.7	-1049.457139	2.15	1.7	-1049.458527
2.25	1.65	-1049.45699	2.2	1.65	-1049.458715	2.15	1.65	-1049.460198
2.25	1.6	-1049.539483	2.2	1.6	-1049.542399	2.15	1.6	-1049.543464
2.25	1.55	-1049.541045	2.2	1.55	-1049.544573	2.15	1.55	-1049.546257
2.25	1.5	-1049.540458	2.2	1.5	-1049.544592	2.15	1.5	-1049.546895
2.25	1.45	-1049.537085	2.2	1.45	-1049.541815	2.15	1.45	-1049.544732
2.25	1.4	-1049.530141	2.2	1.4	-1049.535447	2.15	1.4	-1049.538966
2.1	2.7	-1049.445334	2.05	2.7	-1049.445251	2	2.7	-1049.445319
2.1	2.65	-1049.446188	2.05	2.65	-1049.446223	2	2.65	-1049.446408
2.1	2.6	-1049.446902	2.05	2.6	-1049.447043	2	2.6	-1049.447331
2.1	2.55	-1049.447492	2.05	2.55	-1049.44773	2	2.55	-1049.448112
2.1	2.5	-1049.44797	2.05	2.5	-1049.448298	2	2.5	-1049.448765
2.1	2.45	-1049.448347	2.05	2.45	-1049.44876	2	2.45	-1049.449307
2.1	2.4	-1049.448639	2.05	2.4	-1049.449133	2	2.4	-1049.449754
2.1	2.35	-1049.448864	2.05	2.35	-1049.449432	2	2.35	-1049.450124
2.1	2.3	-1049.449043	2.05	2.3	-1049.449679	2	2.3	-1049.450433
2.1	2.25	-1049.449198	2.05	2.25	-1049.449895	2	2.25	-1049.450704
2.1	2.2	-1049.449363	2.05	2.2	-1049.45011	2	2.2	-1049.450963
2.1	2.15	-1049.449574	2.05	2.15	-1049.450364	2	2.15	-1049.451246
2.1	2.1	-1049.449869	2.05	2.1	-1049.450695	2	2.1	-1049.451595
2.1	2.05	-1049.450285	2.05	2.05	-1049.451142	2	2.05	-1049.452054
2.1	2	-1049.450866	2.05	2	-1049.451745	2	2	-1049.452661
2.1	1.95	-1049.451641	2.05	1.95	-1049.452535	2	1.95	-1049.453445
2.1	1.9	-1049.452631	2.05	1.9	-1049.453531	2	1.9	-1049.454422

2.1	1.85	-1049.45399	2.05	1.85	-1049.454745	2	1.85	-1049.4556
2.1	1.8	-1049.455841	2.05	1.8	-1049.456904	2	1.8	-1049.457926
2.1	1.75	-1049.457823	2.05	1.75	-1049.458912	2	1.75	-1049.459909
2.1	1.7	-1049.459759	2.05	1.7	-1049.460854	2	1.7	-1049.461817
2.1	1.65	-1049.461456	2.05	1.65	-1049.462538	2	1.65	-1049.463458
2.1	1.6	-1049.542598	2.05	1.6	-1049.539761	2	1.6	-1049.535933
2.1	1.55	-1049.545991	2.05	1.55	-1049.543728	2	1.55	-1049.540276
2.1	1.5	-1049.547243	2.05	1.5	-1049.545574	2	1.5	-1049.542533
2.1	1.45	-1049.545704	2.05	1.45	-1049.544643	2	1.45	-1049.542063
2.1	1.4	-1049.54056	2.05	1.4	-1049.540112	2	1.4	-1049.538063
1.95	2.7	-1049.445558	1.9	2.7	-1049.445997	1.85	2.7	-1049.446747
1.95	2.65	-1049.446764	1.9	2.65	-1049.447296	1.85	2.65	-1049.448053
1.95	2.6	-1049.447785	1.9	2.6	-1049.448406	1.85	2.6	-1049.44918
1.95	2.55	-1049.448655	1.9	2.55	-1049.44936	1.85	2.55	-1049.450197
1.95	2.5	-1049.449393	1.9	2.5	-1049.45018	1.85	2.5	-1049.451094
1.95	2.45	-1049.450013	1.9	2.45	-1049.450877	1.85	2.45	-1049.451873
1.95	2.4	-1049.450529	1.9	2.4	-1049.451465	1.85	2.4	-1049.452538
1.95	2.35	-1049.450963	1.9	2.35	-1049.451961	1.85	2.35	-1049.453105
1.95	2.3	-1049.451328	1.9	2.3	-1049.45238	1.85	2.3	-1049.453583
1.95	2.25	-1049.451647	1.9	2.25	-1049.452742	1.85	2.25	-1049.45399
1.95	2.2	-1049.451945	1.9	2.2	-1049.453072	1.85	2.2	-1049.454353
1.95	2.15	-1049.45225	1.9	2.15	-1049.453396	1.85	2.15	-1049.454692
1.95	2.1	-1049.452605	1.9	2.1	-1049.453748	1.85	2.1	-1049.455034
1.95	2.05	-1049.453054	1.9	2.05	-1049.454168	1.85	2.05	-1049.455413
1.95	2	-1049.45364	1.9	2	-1049.454706	1.85	2	-1049.455876
1.95	1.95	-1049.454399	1.9	1.95	-1049.455406	1.85	1.95	-1049.456478
1.95	1.9	-1049.455333	1.9	1.9	-1049.456278	1.85	1.9	-1049.45725
1.95	1.85	-1049.456448	1.9	1.85	-1049.457313	1.85	1.85	-1049.458182
1.95	1.8	-1049.457735	1.9	1.8	-1049.458485	1.85	1.8	-1049.459233
1.95	1.75	-1049.460826	1.9	1.75	-1049.461681	1.85	1.75	-1049.460344
1.95	1.7	-1049.462656	1.9	1.7	-1049.463381	1.85	1.7	-1049.463998
1.95	1.65	-1049.464219	1.9	1.65	-1049.464818	1.85	1.65	-1049.46526
1.95	1.6	-1049.465271	1.9	1.6	-1049.465736	1.85	1.6	-1049.466006
1.95	1.55	-1049.523321	1.9	1.55	-1049.517544	1.85	1.55	-1049.465914
1.95	1.5	-1049.537325	1.9	1.5	-1049.520363	1.85	1.5	-1049.514257
1.95	1.45	-1049.537413	1.9	1.45	-1049.520646	1.85	1.45	-1049.51467
1.95	1.4	-1049.533979	1.9	1.4	-1049.517574	1.85	1.4	-1049.511718
1.8	2.7	-1049.447979	1.75	2.7	-1049.449606	1.7	2.7	-1049.421546
1.8	2.65	-1049.449271	1.75	2.65	-1049.433793	1.7	2.65	-1049.434882
1.8	2.6	-1049.4502	1.75	2.6	-1049.451931	1.7	2.6	-1049.447472
1.8	2.55	-1049.451114	1.75	2.55	-1049.452322	1.7	2.55	-1049.459184
1.8	2.5	-1049.452061	1.75	2.5	-1049.452977	1.7	2.5	-1049.469894
1.8	2.45	-1049.452927	1.75	2.45	-1049.453911	1.7	2.45	-1049.479506

1.8	2.4	-1049.453686	1.75	2.4	-1049.454786	1.7	2.4	-1049.487906
1.8	2.35	-1049.454337	1.75	2.35	-1049.455553	1.7	2.35	-1049.495026
1.8	2.3	-1049.454894	1.75	2.3	-1049.456213	1.7	2.3	-1049.500806
1.8	2.25	-1049.45536	1.75	2.25	-1049.45677	1.7	2.25	-1049.505192
1.8	2.2	-1049.455761	1.75	2.2	-1049.457235	1.7	2.2	-1049.508153
1.8	2.15	-1049.456123	1.75	2.15	-1049.457631	1.7	2.15	-1049.50969
1.8	2.1	-1049.456458	1.75	2.1	-1049.457975	1.7	2.1	-1049.509856
1.8	2.05	-1049.456792	1.75	2.05	-1049.458276	1.7	2.05	-1049.50876
1.8	2	-1049.457169	1.75	2	-1049.458574	1.7	2	-1049.506479
1.8	1.95	-1049.45764	1.75	1.95	-1049.458896	1.7	1.95	-1049.503062
1.8	1.9	-1049.458255	1.75	1.9	-1049.4593	1.7	1.9	-1049.498505
1.8	1.85	-1049.459038	1.75	1.85	-1049.459862	1.7	1.85	-1049.492772
1.8	1.8	-1049.459938	1.75	1.8	-1049.460564	1.7	1.8	-1049.48584
1.8	1.75	-1049.460886	1.75	1.75	-1049.461321	1.7	1.75	-1049.477753
1.8	1.7	-1049.461762	1.75	1.7	-1049.461994	1.7	1.7	-1049.468563
1.8	1.65	-1049.465533	1.75	1.65	-1049.462414	1.7	1.65	-1049.458368
1.8	1.6	-1049.466067	1.75	1.6	-1049.465886	1.7	1.6	-1049.447239
1.8	1.55	-1049.465758	1.75	1.55	-1049.465332	1.7	1.55	-1049.43514
1.8	1.5	-1049.507588	1.75	1.5	-1049.463514	1.7	1.5	-1049.422016
1.8	1.45	-1049.508217	1.75	1.45	-1049.501138	1.7	1.45	-1049.458573
1.8	1.4	-1049.505493	1.75	1.4	-1049.498707	1.7	1.4	-1049.491216
1.65	2.7	-1049.421693	1.6	2.7	-1049.421036	1.55	2.7	-1049.419388
1.65	2.65	-1049.435309	1.6	2.65	-1049.434824	1.55	2.65	-1049.433214
1.65	2.6	-1049.448241	1.6	2.6	-1049.448034	1.55	2.6	-1049.446577
1.65	2.55	-1049.460356	1.6	2.55	-1049.460504	1.55	2.55	-1049.4593
1.65	2.5	-1049.47154	1.6	2.5	-1049.472102	1.55	2.5	-1049.471246
1.65	2.45	-1049.481648	1.6	2.45	-1049.482678	1.55	2.45	-1049.482241
1.65	2.4	-1049.490572	1.6	2.4	-1049.492109	1.55	2.4	-1049.492147
1.65	2.35	-1049.498224	1.6	2.35	-1049.500293	1.55	2.35	-1049.500846
1.65	2.3	-1049.50454	1.6	2.3	-1049.507146	1.55	2.3	-1049.508236
1.65	2.25	-1049.509449	1.6	2.25	-1049.512591	1.55	2.25	-1049.514224
1.65	2.2	-1049.512914	1.6	2.2	-1049.516574	1.55	2.2	-1049.518738
1.65	2.15	-1049.514921	1.6	2.15	-1049.51907	1.55	2.15	-1049.521745
1.65	2.1	-1049.515505	1.6	2.1	-1049.5201	1.55	2.1	-1049.523247
1.65	2.05	-1049.514767	1.6	2.05	-1049.519741	1.55	2.05	-1049.523298
1.65	2	-1049.512803	1.6	2	-1049.518113	1.55	2	-1049.522021
1.65	1.95	-1049.509676	1.6	1.95	-1049.515294	1.55	1.95	-1049.519524
1.65	1.9	-1049.505399	1.6	1.9	-1049.51131	1.55	1.9	-1049.515851
1.65	1.85	-1049.499944	1.6	1.85	-1049.511001	1.55	1.85	-1049.511001
1.65	1.8	-1049.493284	1.6	1.8	-1049.50494	1.55	1.8	-1049.50494
1.65	1.75	-1049.485422	1.6	1.75	-1049.497658	1.55	1.75	-1049.497658
1.65	1.7	-1049.476439	1.6	1.7	-1049.489187	1.55	1.7	-1049.489187
1.65	1.65	-1049.466392	1.6	1.65	-1049.47958	1.55	1.65	-1049.47958

1.65	1.6	-1049.455334	1.6	1.6	-1049.468843	1.55	1.6	-1049.468843
1.65	1.55	-1049.443262	1.6	1.55	-1049.4569	1.55	1.55	-1049.4569
1.65	1.5	-1049.430097	1.6	1.5	-1049.443577	1.55	1.5	-1049.443577
1.65	1.45	-1049.456801	1.6	1.45	-1049.428466	1.55	1.45	-1049.428466
1.65	1.4	-1049.482862	1.6	1.4	-1049.443986	1.55	1.4	-1049.443986
1.5	2.7	-1049.416284	1.45	2.7	-1049.411336	1.4	2.7	-1049.473798
1.5	2.65	-1049.430006	1.45	2.65	-1049.424762	1.4	2.65	-1049.416908
1.5	2.6	-1049.44342	1.45	2.6	-1049.438076	1.4	2.6	-1049.429912
1.5	2.55	-1049.456319	1.45	2.55	-1049.451031	1.4	2.55	-1049.442768
1.5	2.5	-1049.468538	1.45	2.5	-1049.463427	1.4	2.5	-1049.455223
1.5	2.45	-1049.479897	1.45	2.45	-1049.475075	1.4	2.45	-1049.467061
1.5	2.4	-1049.490236	1.45	2.4	-1049.485792	1.4	2.4	-1049.478076
1.5	2.35	-1049.499419	1.45	2.35	-1049.495422	1.4	2.35	-1049.488091
1.5	2.3	-1049.507325	1.45	2.3	-1049.503819	1.4	2.3	-1049.496944
1.5	2.25	-1049.513849	1.45	2.25	-1049.510862	1.4	2.25	-1049.504487
1.5	2.2	-1049.518903	1.45	2.2	-1049.516454	1.4	2.2	-1049.510607
1.5	2.15	-1049.522439	1.45	2.15	-1049.520521	1.4	2.15	-1049.515205
1.5	2.1	-1049.524436	1.45	2.1	-1049.523027	1.4	2.1	-1049.51823
1.5	2.05	-1049.524926	1.45	2.05	-1049.523985	1.4	2.05	-1049.519673
1.5	2	-1049.524028	1.45	2	-1049.523492	1.4	2	-1049.519605
1.5	1.95	-1049.521872	1.45	1.95	-1049.521695	1.4	1.95	-1049.518188
1.5	1.9	-1049.518526	1.45	1.9	-1049.518696	1.4	1.9	-1049.515553
1.5	1.85	-1049.514005	1.45	1.85	-1049.514523	1.4	1.85	-1049.51175
1.5	1.8	-1049.463212	1.45	1.8	-1049.50916	1.4	1.8	-1049.506772
1.5	1.75	-1049.462176	1.45	1.75	-1049.502589	1.4	1.75	-1049.500607
1.5	1.7	-1049.461084	1.45	1.7	-1049.457608	1.4	1.7	-1049.493268
1.5	1.65	-1049.45995	1.45	1.65	-1049.455891	1.4	1.65	-1049.48476
1.5	1.6	-1049.458437	1.45	1.6	-1049.453904	1.4	1.6	-1049.474995
1.5	1.55	-1049.45618	1.45	1.55	-1049.451252	1.4	1.55	-1049.463882
1.5	1.5	-1049.452735	1.45	1.5	-1049.447456	1.4	1.5	-1049.451162
1.5	1.45	-1049.447495	1.45	1.45	-1049.441914	1.4	1.45	-1049.436425
1.5	1.4	-1049.439653	1.45	1.4	-1049.433814	1.4	1.4	-1049.419055

S5.4 More Discussions on [2 + 2] Cycloaddition of 1i

The F-C pathway was also considered for **1i**, which is shown in Figure S11. Compared to cross [2 + 2] pathway via **TS3-1i**, the F-C pathway is disfavored by 2.7 kcal/mol. Thus, the cross [2 + 2] cycloaddition product is the favored product, which is supported by the experimental result.

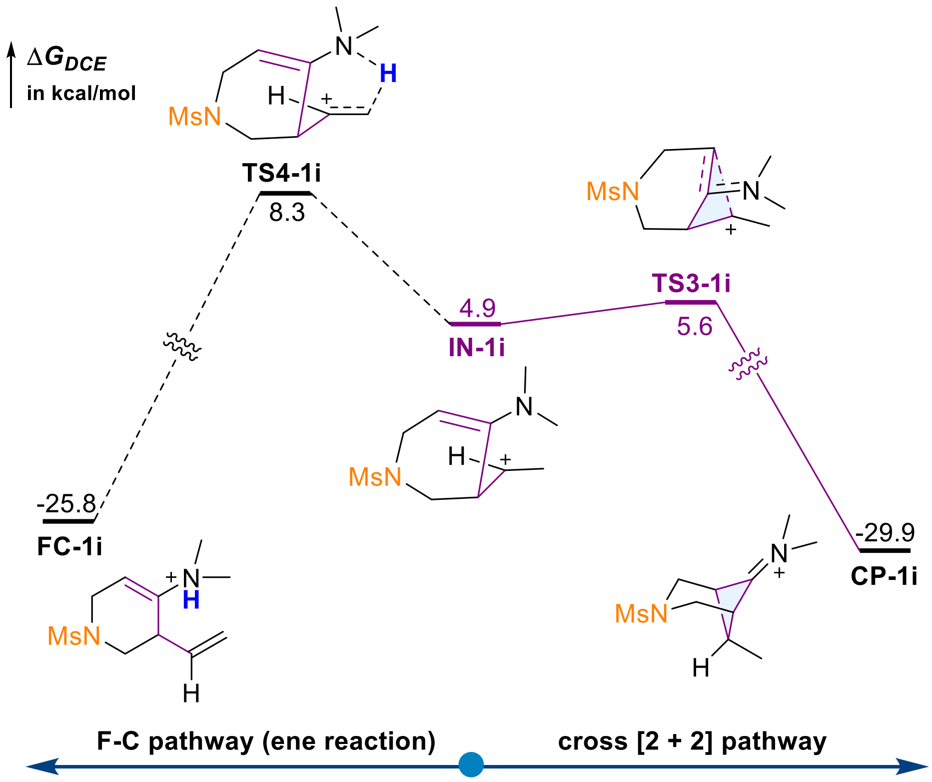


Figure S11. Comparison of F-C pathway and cross [2 + 2] pathway of **IN-1i.** Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//ωB97X-D/def2-SVP level.

We also tried to locate the *endo* carbocation for **1i**, but such a structure finally turns into an *exo* carbocation during optimization (Figure S12) both in the gas phase and solution phase. This means the *exo* carbocation is relatively more stable than the *endo* carbocation.

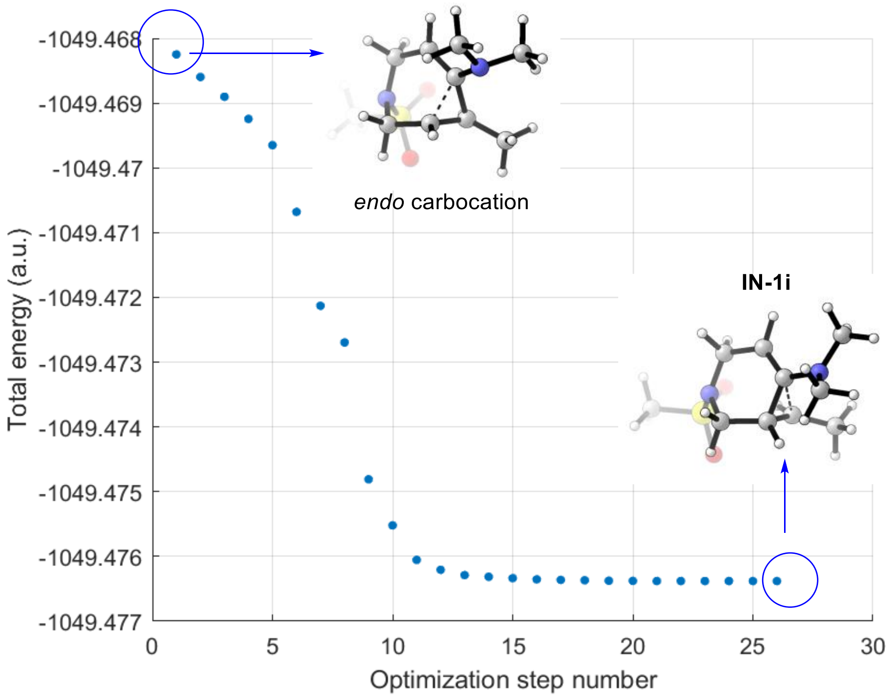


Figure S12. Optimization process for *endo* carbocation for **1i**. Computed at ωB97X-D/def2-SVP level.

S5.5 More Discussions on [2 + 2] Cycloadditions of 1g and 1f

The scans of potential energy surfaces of **1g** and **1f** are shown in Figure S13. It can be seen clearly that the potential energy surface bifurcates after **TS1-1g** while it doesn't for **TS1-1f**. Calculations showed that, the isomerization process from **NP-1g** to **CP-1g** has an activation free energy of 47.5 kcal/mol (Figure S15). Thus, the selectivity of [2 + 2] cycloaddition of **1g** is controlled by dynamics. Non-covalent interaction (NCI) analysis was also performed for **TS1-1g** (Figure S15), finding that there is weak hydrogen bonding between the oxygen in the Ms group and H on the alkene.

The isomerization process from **NP-1f** to **CP-1f** has an activation free energy of 43.1 kcal/mol (Figure S14), suggesting that this process is impossible under experimental conditions. Therefore, only the normal [2 + 2] product could be isolated, consistent with the experiment.

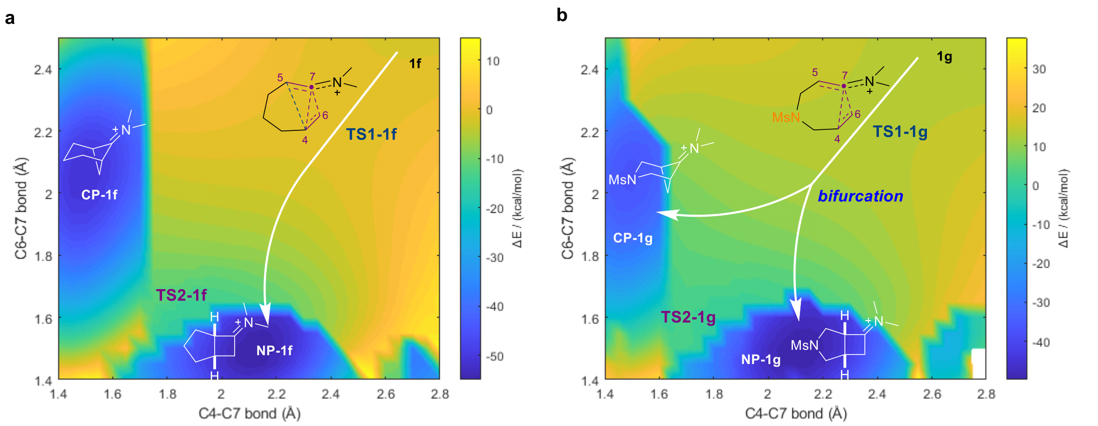


Figure S13. 2D potential energy surfaces of [2 + 2] cycloadditions of **1f** (a) and **1g** (b). Computed at *ω*B97X-D/def2-SVP level.

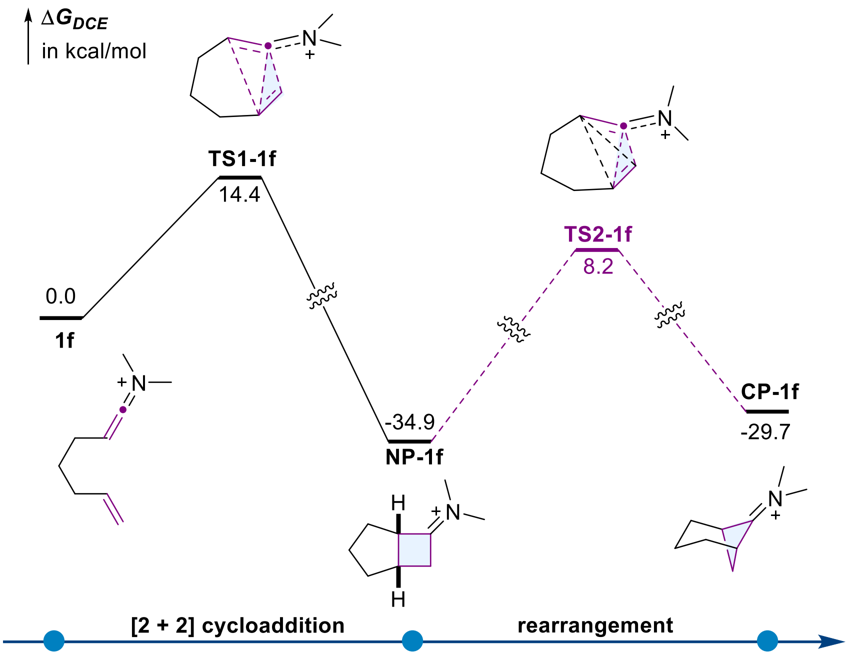


Figure S14. Gibbs energy profile for [2 + 2] cycloaddition of **1f**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//*ω*B97X-D/def2-SVP level.

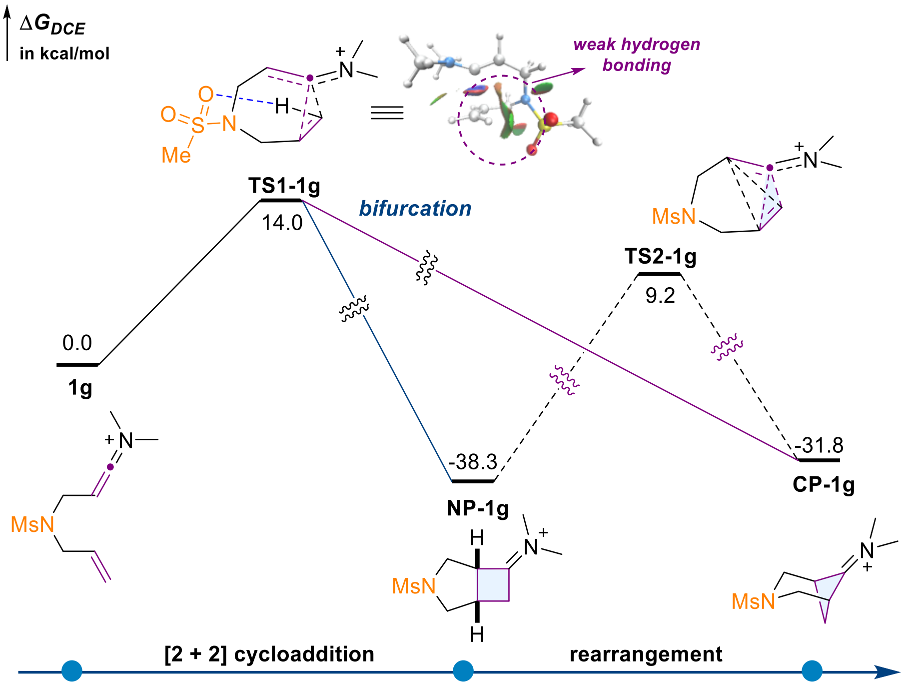


Figure S15. Gibbs energy profile for [2 + 2] cycloaddition of **1g**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//ωB97X-D/def2-SVP level.

Table S3. Relaxed Potential Energy Surface Scan for [2 + 2] Cycloaddition of 1f

C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)
2.8	2.5	-406.605261	2.75	2.5	-406.605288	2.7	2.5	-406.605249
2.8	2.45	-406.604599	2.75	2.45	-406.604716	2.7	2.45	-406.604763
2.8	2.4	-406.603852	2.75	2.4	-406.60407	2.7	2.4	-406.604215
2.8	2.35	-406.603023	2.75	2.35	-406.603353	2.7	2.35	-406.603608
2.8	2.3	-406.602114	2.75	2.3	-406.602569	2.7	2.3	-406.602944
2.8	2.25	-406.601148	2.75	2.25	-406.601743	2.7	2.25	-406.602252
2.8	2.2	-406.600136	2.75	2.2	-406.600884	2.7	2.2	-406.601542
2.8	2.15	-406.599073	2.75	2.15	-406.599991	2.7	2.15	-406.600813
2.8	2.1	-406.597995	2.75	2.1	-406.599098	2.7	2.1	-406.600098
2.8	2.05	-406.596924	2.75	2.05	-406.598231	2.7	2.05	-406.599423
2.8	2	-406.595865	2.75	2	-406.597389	2.7	2	-406.598792
2.8	1.95	-406.594827	2.75	1.95	-406.59658	2.7	1.95	-406.598209
2.8	1.9	-406.593809	2.75	1.9	-406.595797	2.7	1.9	-406.59766
2.8	1.85	-406.592787	2.75	1.85	-406.595008	2.7	1.85	-406.597107
2.8	1.8	-406.591716	2.75	1.8	-406.594161	2.7	1.8	-406.596479
2.8	1.75	-406.590543	2.75	1.75	-406.593184	2.7	1.75	-406.595675
2.8	1.7	-406.589202	2.75	1.7	-406.591994	2.7	1.7	-406.59458
2.8	1.65	-406.587645	2.75	1.65	-406.590539	2.7	1.65	-406.593105
2.8	1.6	-406.58839	2.75	1.6	-406.588843	2.7	1.6	-406.591249

2.8	1.55	-406.587358	2.75	1.55	-406.58693	2.7	1.55	-406.589227
2.8	1.5	-406.582015	2.75	1.5	-406.617454	2.7	1.5	-406.662009
2.8	1.45	-406.613643	2.75	1.45	-406.660293	2.7	1.45	-406.66247
2.8	1.4	-406.653462	2.75	1.4	-406.656776	2.7	1.4	-406.659626
2.65	2.5	-406.605144	2.6	2.5	-406.604972	2.55	2.5	-406.604727
2.65	2.45	-406.604743	2.6	2.45	-406.604654	2.55	2.45	-406.604491
2.65	2.4	-406.604289	2.6	2.4	-406.604293	2.55	2.4	-406.604222
2.65	2.35	-406.603788	2.6	2.35	-406.603895	2.55	2.35	-406.603924
2.65	2.3	-406.603241	2.6	2.3	-406.60346	2.55	2.3	-406.603601
2.65	2.25	-406.602678	2.6	2.25	-406.603023	2.55	2.25	-406.603285
2.65	2.2	-406.602113	2.6	2.2	-406.602595	2.55	2.2	-406.602991
2.65	2.15	-406.601541	2.6	2.15	-406.602175	2.55	2.15	-406.602718
2.65	2.1	-406.600999	2.6	2.1	-406.6018	2.55	2.1	-406.602502
2.65	2.05	-406.600512	2.6	2.05	-406.601496	2.55	2.05	-406.602374
2.65	2	-406.600085	2.6	2	-406.601271	2.55	2	-406.602343
2.65	1.95	-406.599726	2.6	1.95	-406.601137	2.55	1.95	-406.602426
2.65	1.9	-406.599424	2.6	1.9	-406.601087	2.55	1.9	-406.60262
2.65	1.85	-406.599141	2.6	1.85	-406.601086	2.55	1.85	-406.602896
2.65	1.8	-406.5988	2.6	1.8	-406.601074	2.55	1.8	-406.603204
2.65	1.75	-406.598291	2.6	1.75	-406.600962	2.55	1.75	-406.603525
2.65	1.7	-406.597757	2.6	1.7	-406.600935	2.55	1.7	-406.603893
2.65	1.65	-406.597042	2.6	1.65	-406.600513	2.55	1.65	-406.603821
2.65	1.6	-406.595516	2.6	1.6	-406.599227	2.55	1.6	-406.602883
2.65	1.55	-406.593245	2.6	1.55	-406.596546	2.55	1.55	-406.600535
2.65	1.5	-406.612103	2.6	1.5	-406.591621	2.55	1.5	-406.596166
2.65	1.45	-406.617632	2.6	1.45	-406.616038	2.55	1.45	-406.589028
2.65	1.4	-406.619471	2.6	1.4	-406.619004	2.55	1.4	-406.577965
2.5	2.5	-406.604406	2.45	2.5	-406.603993	2.4	2.5	-406.603484
2.5	2.45	-406.604259	2.45	2.45	-406.603938	2.4	2.45	-406.603524
2.5	2.4	-406.604078	2.45	2.4	-406.603851	2.4	2.4	-406.603532
2.5	2.35	-406.603876	2.45	2.35	-406.603749	2.4	2.35	-406.603533
2.5	2.3	-406.603663	2.45	2.3	-406.603644	2.4	2.3	-406.603541
2.5	2.25	-406.603466	2.45	2.25	-406.603564	2.4	2.25	-406.603576
2.5	2.2	-406.603302	2.45	2.2	-406.603526	2.4	2.2	-406.603662
2.5	2.15	-406.603169	2.45	2.15	-406.60353	2.4	2.15	-406.603798
2.5	2.1	-406.603107	2.45	2.1	-406.603616	2.4	2.1	-406.604026
2.5	2.05	-406.603145	2.45	2.05	-406.603815	2.4	2.05	-406.604378
2.5	2	-406.603301	2.45	2	-406.604145	2.4	2	-406.604874
2.5	1.95	-406.60359	2.45	1.95	-406.604631	2.4	1.95	-406.605544
2.5	1.9	-406.604016	2.45	1.9	-406.605272	2.4	1.9	-406.606385
2.5	1.85	-406.604555	2.45	1.85	-406.606054	2.4	1.85	-406.607391
2.5	1.8	-406.605164	2.45	1.8	-406.606944	2.4	1.8	-406.608542
2.5	1.75	-406.60589	2.45	1.75	-406.608044	2.4	1.75	-406.609986

2.5	1.7	-406.606628	2.45	1.7	-406.609131	2.4	1.7	-406.611397
2.5	1.65	-406.60693	2.45	1.65	-406.609805	2.4	1.65	-406.612428
2.5	1.6	-406.606377	2.45	1.6	-406.609654	2.4	1.6	-406.61268
2.5	1.55	-406.604458	2.45	1.55	-406.608199	2.4	1.55	-406.611707
2.5	1.5	-406.600566	2.45	1.5	-406.604886	2.4	1.5	-406.66326
2.5	1.45	-406.585872	2.45	1.45	-406.648278	2.4	1.45	-406.658767
2.5	1.4	-406.628018	2.45	1.4	-406.639864	2.4	1.4	-406.650737
2.35	2.5	-406.602866	2.3	2.5	-406.60214	2.25	2.5	-406.601323
2.35	2.45	-406.603008	2.3	2.45	-406.602395	2.25	2.45	-406.601701
2.35	2.4	-406.603124	2.3	2.4	-406.602626	2.25	2.4	-406.602056
2.35	2.35	-406.603236	2.3	2.35	-406.602855	2.25	2.35	-406.602405
2.35	2.3	-406.603359	2.3	2.3	-406.603098	2.25	2.3	-406.602765
2.35	2.25	-406.60351	2.3	2.25	-406.603366	2.25	2.25	-406.603148
2.35	2.2	-406.603714	2.3	2.2	-406.603686	2.25	2.2	-406.603583
2.35	2.15	-406.603977	2.3	2.15	-406.604071	2.25	2.15	-406.604088
2.35	2.1	-406.60434	2.3	2.1	-406.604564	2.25	2.1	-406.604704
2.35	2.05	-406.604838	2.3	2.05	-406.6052	2.25	2.05	-406.60547
2.35	2	-406.605491	2.3	2	-406.605999	2.25	2	-406.606406
2.35	1.95	-406.606329	2.3	1.95	-406.606993	2.25	1.95	-406.607543
2.35	1.9	-406.607356	2.3	1.9	-406.608193	2.25	1.9	-406.6089
2.35	1.85	-406.608568	2.3	1.85	-406.609591	2.25	1.85	-406.610463
2.35	1.8	-406.609978	2.3	1.8	-406.611246	2.25	1.8	-406.612342
2.35	1.75	-406.61172	2.3	1.75	-406.613247	2.25	1.75	-406.614578
2.35	1.7	-406.61343	2.3	1.7	-406.61523	2.25	1.7	-406.616807
2.35	1.65	-406.61479	2.3	1.65	-406.616895	2.25	1.65	-406.618741
2.35	1.6	-406.615429	2.3	1.6	-406.617909	2.25	1.6	-406.682648
2.35	1.55	-406.673173	2.3	1.55	-406.679845	2.25	1.55	-406.684879
2.35	1.5	-406.671989	2.3	1.5	-406.679254	2.25	1.5	-406.684909
2.35	1.45	-406.668008	2.3	1.45	-406.675837	2.25	1.45	-406.682097
2.35	1.4	-406.660444	2.3	1.4	-406.668802	2.25	1.4	-406.675642
2.2	2.5	-406.600425	2.15	2.5	-406.599438	2.1	2.5	-406.5984
2.2	2.45	-406.60093	2.15	2.45	-406.600079	2.1	2.45	-406.599181
2.2	2.4	-406.601411	2.15	2.4	-406.600691	2.1	2.4	-406.599931
2.2	2.35	-406.601883	2.15	2.35	-406.60129	2.1	2.35	-406.600664
2.2	2.3	-406.602363	2.15	2.3	-406.601893	2.1	2.3	-406.601396
2.2	2.25	-406.602864	2.15	2.25	-406.602518	2.1	2.25	-406.602146
2.2	2.2	-406.603416	2.15	2.2	-406.603192	2.1	2.2	-406.602943
2.2	2.15	-406.604041	2.15	2.15	-406.603939	2.1	2.15	-406.60381
2.2	2.1	-406.604776	2.15	2.1	-406.604794	2.1	2.1	-406.604779
2.2	2.05	-406.605662	2.15	2.05	-406.605794	2.1	2.05	-406.605884
2.2	2	-406.606722	2.15	2	-406.606965	2.1	2	-406.607157
2.2	1.95	-406.607989	2.15	1.95	-406.608345	2.1	1.95	-406.608634
2.2	1.9	-406.609483	2.15	1.9	-406.609955	2.1	1.9	-406.610337

2.2	1.85	-406.611195	2.15	1.85	-406.611794	2.1	1.85	-406.612272
2.2	1.8	-406.613271	2.15	1.8	-406.614056	2.1	1.8	-406.614742
2.2	1.75	-406.615725	2.15	1.75	-406.61671	2.1	1.75	-406.617543
2.2	1.7	-406.618167	2.15	1.7	-406.619324	2.1	1.7	-406.620286
2.2	1.65	-406.620327	2.15	1.65	-406.621658	2.1	1.65	-406.622743
2.2	1.6	-406.685286	2.15	1.6	-406.686059	2.1	1.6	-406.684899
2.2	1.55	-406.688153	2.15	1.55	-406.689561	2.1	1.55	-406.689016
2.2	1.5	-406.688821	2.15	1.5	-406.690872	2.1	1.5	-406.690958
2.2	1.45	-406.68664	2.15	1.45	-406.689335	2.1	1.45	-406.690062
2.2	1.4	-406.680801	2.15	1.4	-406.684132	2.1	1.4	-406.685504
2.05	2.5	-406.59735	2	2.5	-406.59631	1.95	2.5	-406.595315
2.05	2.45	-406.598274	2	2.45	-406.597373	1.95	2.45	-406.596517
2.05	2.4	-406.599164	2	2.4	-406.598404	1.95	2.4	-406.597688
2.05	2.35	-406.600033	2	2.35	-406.599415	1.95	2.35	-406.59884
2.05	2.3	-406.600899	2	2.3	-406.600419	1.95	2.3	-406.599983
2.05	2.25	-406.601779	2	2.25	-406.601431	1.95	2.25	-406.601127
2.05	2.2	-406.602696	2	2.2	-406.602469	1.95	2.2	-406.602291
2.05	2.15	-406.603679	2	2.15	-406.603563	1.95	2.15	-406.603496
2.05	2.1	-406.604758	2	2.1	-406.604744	1.95	2.1	-406.604771
2.05	2.05	-406.60596	2	2.05	-406.606042	1.95	2.05	-406.60615
2.05	2	-406.607319	2	2	-406.607482	1.95	2	-406.607666
2.05	1.95	-406.608875	2	1.95	-406.609098	1.95	1.95	-406.609338
2.05	1.9	-406.610654	2	1.9	-406.610927	1.95	1.9	-406.611189
2.05	1.85	-406.612652	2	1.85	-406.612965	1.95	1.85	-406.613244
2.05	1.8	-406.614867	2	1.8	-406.615203	1.95	1.8	-406.61547
2.05	1.75	-406.618236	2	1.75	-406.618794	1.95	1.75	-406.619234
2.05	1.7	-406.621063	2	1.7	-406.621663	1.95	1.7	-406.622097
2.05	1.65	-406.623595	2	1.65	-406.624231	1.95	1.65	-406.624659
2.05	1.6	-406.681819	2	1.6	-406.677351	1.95	1.6	-406.626672
2.05	1.55	-406.686489	2	1.55	-406.682311	1.95	1.55	-406.677533
2.05	1.5	-406.68902	2	1.5	-406.685234	1.95	1.5	-406.680629
2.05	1.45	-406.688739	2	1.45	-406.685436	1.95	1.45	-406.681069
2.05	1.4	-406.684813	2	1.4	-406.682068	1.95	1.4	-406.678017
1.9	2.5	-406.594379	1.85	2.5	-406.593485	1.8	2.5	-406.592571
1.9	2.45	-406.595729	1.85	2.45	-406.594994	1.8	2.45	-406.59426
1.9	2.4	-406.597044	1.85	2.4	-406.596465	1.8	2.4	-406.595906
1.9	2.35	-406.598336	1.85	2.35	-406.597906	1.8	2.35	-406.597517
1.9	2.3	-406.599619	1.85	2.3	-406.599334	1.8	2.3	-406.599103
1.9	2.25	-406.600899	1.85	2.25	-406.600752	1.8	2.25	-406.600673
1.9	2.2	-406.602189	1.85	2.2	-406.602175	1.8	2.2	-406.602238
1.9	2.15	-406.603507	1.85	2.15	-406.603609	1.8	2.15	-406.603798
1.9	2.1	-406.604874	1.85	2.1	-406.605071	1.8	2.1	-406.605363
1.9	2.05	-406.606322	1.85	2.05	-406.606586	1.8	2.05	-406.606946

1.9	2	-406.607887	1.85	2	-406.608186	1.8	2	-406.60857
1.9	1.95	-406.609599	1.85	1.95	-406.6099	1.8	1.95	-406.61027
1.9	1.9	-406.611468	1.85	1.9	-406.611755	1.8	1.9	-406.612076
1.9	1.85	-406.613501	1.85	1.85	-406.613759	1.8	1.85	-406.613997
1.9	1.8	-406.615697	1.85	1.8	-406.615888	1.8	1.8	-406.616034
1.9	1.75	-406.617985	1.85	1.75	-406.618086	1.8	1.75	-406.618124
1.9	1.7	-406.622375	1.85	1.7	-406.620248	1.8	1.7	-406.62014
1.9	1.65	-406.624881	1.85	1.65	-406.6249	1.8	1.65	-406.621922
1.9	1.6	-406.626822	1.85	1.6	-406.626733	1.8	1.6	-406.62639
1.9	1.55	-406.672403	1.85	1.55	-406.627699	1.8	1.55	-406.627176
1.9	1.5	-406.675694	1.85	1.5	-406.670237	1.8	1.5	-406.664095
1.9	1.45	-406.676374	1.85	1.45	-406.671181	1.8	1.45	-406.665334
1.9	1.4	-406.673612	1.85	1.4	-406.668731	1.8	1.4	-406.663207
1.75	2.5	-406.591529	1.7	2.5	-406.627315	1.65	2.5	-406.62891
1.75	2.45	-406.593427	1.7	2.45	-406.637325	1.65	2.45	-406.639414
1.75	2.4	-406.595278	1.7	2.4	-406.646112	1.65	2.4	-406.64872
1.75	2.35	-406.597086	1.7	2.35	-406.653589	1.65	2.35	-406.65673
1.75	2.3	-406.598858	1.7	2.3	-406.65967	1.65	2.3	-406.66335
1.75	2.25	-406.600606	1.7	2.25	-406.664297	1.65	2.25	-406.668508
1.75	2.2	-406.602333	1.7	2.2	-406.667433	1.65	2.2	-406.672154
1.75	2.15	-406.604037	1.7	2.15	-406.669073	1.65	2.15	-406.674276
1.75	2.1	-406.60572	1.7	2.1	-406.669268	1.65	2.1	-406.674899
1.75	2.05	-406.607386	1.7	2.05	-406.66813	1.65	2.05	-406.674119
1.75	2	-406.609044	1.7	2	-406.665839	1.65	2	-406.672114
1.75	1.95	-406.610716	1.7	1.95	-406.662518	1.65	1.95	-406.669046
1.75	1.9	-406.612433	1.7	1.9	-406.658192	1.65	1.9	-406.664968
1.75	1.85	-406.614229	1.7	1.85	-406.652838	1.65	1.85	-406.659862
1.75	1.8	-406.616116	1.7	1.8	-406.646441	1.65	1.8	-406.653713
1.75	1.75	-406.618052	1.7	1.75	-406.639022	1.65	1.75	-406.646535
1.75	1.7	-406.619911	1.7	1.7	-406.630656	1.65	1.7	-406.638386
1.75	1.65	-406.621497	1.7	1.65	-406.621456	1.65	1.65	-406.629362
1.75	1.6	-406.622575	1.7	1.6	-406.611534	1.65	1.6	-406.61954
1.75	1.55	-406.626354	1.7	1.55	-406.601013	1.65	1.55	-406.608963
1.75	1.5	-406.625632	1.7	1.5	-406.624187	1.65	1.5	-406.597346
1.75	1.45	-406.658696	1.7	1.45	-406.6512	1.65	1.45	-406.619153
1.75	1.4	-406.656919	1.7	1.4	-406.649785	1.65	1.4	-406.641701
1.6	2.5	-406.629431	1.55	2.5	-406.628531	1.5	2.5	-406.625767
1.6	2.45	-406.640399	1.55	2.45	-406.639923	1.5	2.45	-406.637528
1.6	2.4	-406.650205	1.55	2.4	-406.650203	1.5	2.4	-406.648243
1.6	2.35	-406.658742	1.55	2.35	-406.659248	1.5	2.35	-406.657772
1.6	2.3	-406.665906	1.55	2.3	-406.666945	1.5	2.3	-406.665988
1.6	2.25	-406.671605	1.55	2.25	-406.673186	1.5	2.25	-406.672768
1.6	2.2	-406.675777	1.55	2.2	-406.677898	1.5	2.2	-406.678022

1.6	2.15	-406.678394	1.55	2.15	-406.681031	1.5	2.15	-406.681685
1.6	2.1	-406.679468	1.55	2.1	-406.682582	1.5	2.1	-406.683735
1.6	2.05	-406.679078	1.55	2.05	-406.682613	1.5	2.05	-406.68421
1.6	2	-406.677387	1.55	2	-406.681266	1.5	2	-406.68324
1.6	1.95	-406.674579	1.55	1.95	-406.678739	1.5	1.95	-406.68102
1.6	1.9	-406.670757	1.55	1.9	-406.675177	1.5	1.9	-406.677734
1.6	1.85	-406.665913	1.55	1.85	-406.67061	1.5	1.85	-406.673457
1.6	1.8	-406.660031	1.55	1.8	-406.665012	1.5	1.8	-406.668163
1.6	1.75	-406.653122	1.55	1.75	-406.658395	1.5	1.75	-406.661863
1.6	1.7	-406.645226	1.55	1.7	-406.650787	1.5	1.7	-406.654585
1.6	1.65	-406.636421	1.55	1.65	-406.642248	1.5	1.65	-406.646359
1.6	1.6	-406.626755	1.55	1.6	-406.6328	1.5	1.6	-406.637188
1.6	1.55	-406.616218	1.55	1.55	-406.622397	1.5	1.55	-406.626997
1.6	1.5	-406.604757	1.55	1.5	-406.610889	1.5	1.5	-406.615588
1.6	1.45	-406.616371	1.55	1.45	-406.59796	1.5	1.45	-406.602634
1.6	1.4	-406.610328	1.55	1.4	-406.582072	1.5	1.4	-406.582216
1.45	2.5	-406.620574	1.4	2.5	-406.612233			
1.45	2.45	-406.632643	1.4	2.45	-406.624529			
1.45	2.4	-406.643743	1.4	2.4	-406.635949			
1.45	2.35	-406.653714	1.4	2.35	-406.646319			
1.45	2.3	-406.662418	1.4	2.3	-406.65548			
1.45	2.25	-406.669724	1.4	2.25	-406.663286			
1.45	2.2	-406.675519	1.4	2.2	-406.669604			
1.45	2.15	-406.679725	1.4	2.15	-406.674345			
1.45	2.1	-406.682293	1.4	2.1	-406.677441			
1.45	2.05	-406.683238	1.4	2.05	-406.678883			
1.45	2	-406.68267	1.4	2	-406.678743			
1.45	1.95	-406.680778	1.4	1.95	-406.677207			
1.45	1.9	-406.677783	1.4	1.9	-406.674519			
1.45	1.85	-406.673806	1.4	1.85	-406.67085			
1.45	1.8	-406.668837	1.4	1.8	-406.666224			
1.45	1.75	-406.662886	1.4	1.75	-406.660652			
1.45	1.7	-406.655982	1.4	1.7	-406.654162			
1.45	1.65	-406.648124	1.4	1.65	-406.646722			
1.45	1.6	-406.639286	1.4	1.6	-406.638276			
1.45	1.55	-406.62938	1.4	1.55	-406.628719			
1.45	1.5	-406.618171	1.4	1.5	-406.617793			
1.45	1.45	-406.605255	1.4	1.45	-406.605085			
1.45	1.4	-406.588141	1.4	1.4	-406.590012			

Table S4. Relaxed Potential Energy Surface Scan for [2 + 2] Cycloaddition of 1g

C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)
2.8	2.5	-1010.169277	2.75	2.5	-1010.168892	2.7	2.5	-1010.168637
2.8	2.45	-1010.168656	2.75	2.45	-1010.168454	2.7	2.45	-1010.16827
2.8	2.4	-1010.16804	2.75	2.4	-1010.167934	2.7	2.4	-1010.167852
2.8	2.35	-1010.16734	2.75	2.35	-1010.16734	2.7	2.35	-1010.167354
2.8	2.3	-1010.166557	2.75	2.3	-1010.166679	2.7	2.3	-1010.166789
2.8	2.25	-1010.165714	2.75	2.25	-1010.165963	2.7	2.25	-1010.166196
2.8	2.2	-1010.164819	2.75	2.2	-1010.165203	2.7	2.2	-1010.16558
2.8	2.15	-1010.163864	2.75	2.15	-1010.164405	2.7	2.15	-1010.164929
2.8	2.1	-1010.162881	2.75	2.1	-1010.163601	2.7	2.1	-1010.164285
2.8	2.05	-1010.161895	2.75	2.05	-1010.162809	2.7	2.05	-1010.163669
2.8	2	-1010.160904	2.75	2	-1010.162028	2.7	2	-1010.163087
2.8	1.95	-1010.159921	2.75	1.95	-1010.161273	2.7	1.95	-1010.16254
2.8	1.9	-1010.158935	2.75	1.9	-1010.160531	2.7	1.9	-1010.162018
2.8	1.85	-1010.157915	2.75	1.85	-1010.159776	2.7	1.85	-1010.161486
2.8	1.8	-1010.15681	2.75	1.8	-1010.158947	2.7	1.8	-1010.160883
2.8	1.75	-1010.155547	2.75	1.75	-1010.157962	2.7	1.75	-1010.160118
2.8	1.7	-1010.154065	2.75	1.7	-1010.156728	2.7	1.7	-1010.159071
2.8	1.65	-1010.152936	2.75	1.65	-1010.155189	2.7	1.65	-1010.157633
2.8	1.6	-1010.190551	2.75	1.6	-1010.195166	2.7	1.6	-1010.209327
2.8	1.55	-1010.188913	2.75	1.55	-1010.195414	2.7	1.55	-1010.211061
2.8	1.5	-1010.18375	2.75	1.5	-1010.19217	2.7	1.5	-1010.210104
2.8	1.45	--	2.75	1.45	-1010.145739	2.7	1.45	-1010.205748
2.8	1.4	--	2.75	1.4	-1010.161432	2.7	1.4	-1010.197158
2.65	2.5	-1010.168383	2.6	2.5	-1010.168107	2.55	2.5	-1010.167806
2.65	2.45	-1010.1681	2.6	2.45	-1010.167909	2.55	2.45	-1010.16768
2.65	2.4	-1010.167761	2.6	2.4	-1010.16765	2.55	2.4	-1010.167517
2.65	2.35	-1010.167355	2.6	2.35	-1010.16735	2.55	2.35	-1010.167299
2.65	2.3	-1010.166902	2.6	2.3	-1010.166988	2.55	2.3	-1010.167048
2.65	2.25	-1010.166417	2.6	2.25	-1010.166618	2.55	2.25	-1010.166791
2.65	2.2	-1010.165927	2.6	2.2	-1010.166249	2.55	2.2	-1010.166535
2.65	2.15	-1010.165423	2.6	2.15	-1010.165881	2.55	2.15	-1010.166298
2.65	2.1	-1010.164937	2.6	2.1	-1010.165545	2.55	2.1	-1010.166105
2.65	2.05	-1010.164491	2.6	2.05	-1010.165265	2.55	2.05	-1010.165983
2.65	2	-1010.164091	2.6	2	-1010.165048	2.55	2	-1010.16594
2.65	1.95	-1010.163747	2.6	1.95	-1010.1649	2.55	1.95	-1010.165992
2.65	1.9	-1010.163444	2.6	1.9	-1010.16482	2.55	1.9	-1010.166131
2.65	1.85	-1010.16314	2.6	1.85	-1010.164777	2.55	1.85	-1010.166351
2.65	1.8	-1010.162759	2.6	1.8	-1010.164713	2.55	1.8	-1010.16661
2.65	1.75	-1010.162195	2.6	1.75	-1010.164654	2.55	1.75	-1010.167016
2.65	1.7	-1010.161286	2.6	1.7	-1010.164764	2.55	1.7	-1010.167493
2.65	1.65	-1010.159888	2.6	1.65	-1010.164466	2.55	1.65	-1010.167538

2.65	1.6	-1010.157945	2.6	1.6	-1010.163296	2.55	1.6	-1010.166731
2.65	1.55	-1010.211303	2.6	1.55	-1010.1607	2.55	1.55	-1010.164526
2.65	1.5	-1010.211173	2.6	1.5	-1010.210015	2.55	1.5	-1010.160298
2.65	1.45	-1010.207716	2.6	1.45	-1010.207654	2.55	1.45	-1010.153296
2.65	1.4	-1010.200044	2.6	1.4	-1010.201082	2.55	1.4	-1010.127243
2.5	2.5	-1010.167489	2.45	2.5	-1010.167105	2.4	2.5	-1010.166676
2.5	2.45	-1010.167435	2.45	2.45	-1010.167156	2.4	2.45	-1010.166809
2.5	2.4	-1010.167342	2.45	2.4	-1010.167149	2.4	2.4	-1010.166897
2.5	2.35	-1010.167227	2.45	2.35	-1010.167104	2.4	2.35	-1010.166959
2.5	2.3	-1010.167068	2.45	2.3	-1010.167053	2.4	2.3	-1010.166996
2.5	2.25	-1010.166918	2.45	2.25	-1010.16701	2.4	2.25	-1010.167049
2.5	2.2	-1010.166792	2.45	2.2	-1010.166988	2.4	2.2	-1010.167153
2.5	2.15	-1010.166674	2.45	2.15	-1010.167001	2.4	2.15	-1010.167273
2.5	2.1	-1010.166612	2.45	2.1	-1010.167077	2.4	2.1	-1010.167469
2.5	2.05	-1010.166642	2.45	2.05	-1010.167239	2.4	2.05	-1010.167769
2.5	2	-1010.166762	2.45	2	-1010.167514	2.4	2	-1010.168194
2.5	1.95	-1010.167001	2.45	1.95	-1010.167928	2.4	1.95	-1010.168774
2.5	1.9	-1010.167358	2.45	1.9	-1010.168479	2.4	1.9	-1010.169507
2.5	1.85	-1010.167822	2.45	1.85	-1010.169175	2.4	1.85	-1010.17039
2.5	1.8	-1010.168373	2.45	1.8	-1010.169975	2.4	1.8	-1010.171441
2.5	1.75	-1010.169168	2.45	1.75	-1010.171112	2.4	1.75	-1010.172874
2.5	1.7	-1010.169976	2.45	1.7	-1010.17225	2.4	1.7	-1010.174301
2.5	1.65	-1010.17039	2.45	1.65	-1010.173002	2.4	1.65	-1010.175392
2.5	1.6	-1010.169965	2.45	1.6	-1010.172967	2.4	1.6	-1010.175752
2.5	1.55	-1010.168184	2.45	1.55	-1010.171653	2.4	1.55	-1010.24295
2.5	1.5	-1010.164472	2.45	1.5	-1010.231109	2.4	1.5	-1010.241272
2.5	1.45	-1010.214443	2.45	1.45	-1010.226176	2.4	1.45	-1010.236806
2.5	1.4	-1010.205688	2.45	1.4	-1010.217737	2.4	1.4	-1010.228777
2.35	2.5	-1010.166184	2.3	2.5	-1010.165644	2.25	2.5	-1010.165068
2.35	2.45	-1010.166411	2.3	2.45	-1010.16597	2.25	2.45	-1010.165503
2.35	2.4	-1010.166598	2.3	2.4	-1010.166259	2.25	2.4	-1010.165901
2.35	2.35	-1010.166761	2.3	2.35	-1010.166525	2.25	2.35	-1010.166271
2.35	2.3	-1010.166913	2.3	2.3	-1010.16679	2.25	2.3	-1010.166638
2.35	2.25	-1010.167071	2.3	2.25	-1010.167057	2.25	2.25	-1010.16701
2.35	2.2	-1010.16726	2.3	2.2	-1010.167352	2.25	2.2	-1010.167405
2.35	2.15	-1010.167498	2.3	2.15	-1010.167693	2.25	2.15	-1010.167849
2.35	2.1	-1010.167818	2.3	2.1	-1010.16812	2.25	2.1	-1010.16838
2.35	2.05	-1010.168249	2.3	2.05	-1010.168668	2.25	2.05	-1010.169023
2.35	2	-1010.16881	2.3	2	-1010.169355	2.25	2	-1010.169832
2.35	1.95	-1010.169533	2.3	1.95	-1010.170201	2.25	1.95	-1010.170803
2.35	1.9	-1010.17042	2.3	1.9	-1010.17124	2.25	1.9	-1010.17197
2.35	1.85	-1010.171491	2.3	1.85	-1010.172474	2.25	1.85	-1010.173339
2.35	1.8	-1010.172773	2.3	1.8	-1010.173962	2.25	1.8	-1010.175017

2.35	1.75	-1010.174459	2.3	1.75	-1010.175878	2.25	1.75	-1010.177132
2.35	1.7	-1010.176158	2.3	1.7	-1010.177817	2.25	1.7	-1010.179288
2.35	1.65	-1010.177561	2.3	1.65	-1010.179514	2.25	1.65	-1010.181253
2.35	1.6	-1010.178336	2.3	1.6	-1010.256286	2.25	1.6	-1010.260758
2.35	1.55	-1010.251216	2.3	1.55	-1010.257963	2.25	1.55	-1010.263062
2.35	1.5	-1010.250099	2.3	1.5	-1010.257444	2.25	1.5	-1010.263165
2.35	1.45	-1010.246164	2.3	1.45	-1010.254089	2.25	1.45	-1010.260428
2.35	1.4	-1010.238622	2.3	1.4	-1010.247096	2.25	1.4	-1010.254033
2.2	2.5	-1010.164462	2.15	2.5	-1010.163827	2.1	2.5	-1010.163201
2.2	2.45	-1010.165013	2.15	2.45	-1010.164496	2.1	2.45	-1010.163991
2.2	2.4	-1010.165521	2.15	2.4	-1010.165121	2.1	2.4	-1010.164733
2.2	2.35	-1010.165998	2.15	2.35	-1010.165708	2.1	2.35	-1010.165433
2.2	2.3	-1010.166463	2.15	2.3	-1010.166278	2.1	2.3	-1010.166112
2.2	2.25	-1010.166937	2.15	2.25	-1010.166851	2.1	2.25	-1010.16679
2.2	2.2	-1010.167434	2.15	2.2	-1010.167449	2.1	2.2	-1010.167489
2.2	2.15	-1010.167976	2.15	2.15	-1010.168093	2.1	2.15	-1010.168232
2.2	2.1	-1010.168595	2.15	2.1	-1010.168815	2.1	2.1	-1010.169046
2.2	2.05	-1010.169354	2.15	2.05	-1010.169662	2.1	2.05	-1010.169974
2.2	2	-1010.170254	2.15	2	-1010.170649	2.1	2	-1010.171038
2.2	1.95	-1010.171341	2.15	1.95	-1010.17182	2.1	1.95	-1010.17227
2.2	1.9	-1010.172615	2.15	1.9	-1010.17319	2.1	1.9	-1010.173712
2.2	1.85	-1010.174101	2.15	1.85	-1010.174771	2.1	1.85	-1010.175361
2.2	1.8	-1010.17594	2.15	1.8	-1010.176735	2.1	1.8	-1010.177224
2.2	1.75	-1010.178229	2.15	1.75	-1010.179186	2.1	1.75	-1010.180032
2.2	1.7	-1010.180568	2.15	1.7	-1010.181666	2.1	1.7	-1010.1826
2.2	1.65	-1010.182765	2.15	1.65	-1010.259291	2.1	1.65	-1010.257914
2.2	1.6	-1010.263474	2.15	1.6	-1010.264434	2.1	1.6	-1010.263647
2.2	1.55	-1010.266406	2.15	1.55	-1010.267929	2.1	1.55	-1010.267731
2.2	1.5	-1010.267141	2.15	1.5	-1010.269276	2.1	1.5	-1010.269643
2.2	1.45	-1010.265038	2.15	1.45	-1010.267806	2.1	1.45	-1010.268738
2.2	1.4	-1010.259272	2.15	1.4	-1010.262681	2.1	1.4	-1010.253219
2.05	2.5	-1010.16262	2	2.5	-1010.162106	1.95	2.5	-1010.161691
2.05	2.45	-1010.163531	2	2.45	-1010.163134	1.95	2.45	-1010.162829
2.05	2.4	-1010.164389	2	2.4	-1010.164107	1.95	2.4	-1010.163919
2.05	2.35	-1010.165204	2	2.35	-1010.165039	1.95	2.35	-1010.164968
2.05	2.3	-1010.165995	2	2.3	-1010.165946	1.95	2.3	-1010.165987
2.05	2.25	-1010.166779	2	2.25	-1010.166836	1.95	2.25	-1010.16698
2.05	2.2	-1010.167574	2	2.2	-1010.167725	1.95	2.2	-1010.167966
2.05	2.15	-1010.168408	2	2.15	-1010.168641	1.95	2.15	-1010.168965
2.05	2.1	-1010.169308	2	2.1	-1010.169617	1.95	2.1	-1010.170008
2.05	2.05	-1010.170307	2	2.05	-1010.170682	1.95	2.05	-1010.171125
2.05	2	-1010.171438	2	2	-1010.171861	1.95	2	-1010.172348
2.05	1.95	-1010.172718	2	1.95	-1010.173189	1.95	1.95	-1010.173705

2.05	1.9	-1010.174207	2	1.9	-1010.174699	1.95	1.9	-1010.175206
2.05	1.85	-1010.175889	2	1.85	-1010.176388	1.95	1.85	-1010.176884
2.05	1.8	-1010.177788	2	1.8	-1010.178279	1.95	1.8	-1010.178734
2.05	1.75	-1010.180777	2	1.75	-1010.181434	1.95	1.75	-1010.182012
2.05	1.7	-1010.183388	2	1.7	-1010.184043	1.95	1.7	-1010.184575
2.05	1.65	-1010.185805	2	1.65	-1010.186419	1.95	1.65	-1010.186881
2.05	1.6	-1010.260893	2	1.6	-1010.2561	1.95	1.6	-1010.249264
2.05	1.55	-1010.265561	2	1.55	-1010.261326	1.95	1.55	-1010.255006
2.05	1.5	-1010.268068	2	1.5	-1010.264413	1.95	1.5	-1010.258629
2.05	1.45	-1010.267775	2	1.45	-1010.264708	1.95	1.45	-1010.259489
2.05	1.4	-1010.263857	2	1.4	-1010.261395	1.95	1.4	-1010.256806
1.9	2.5	-1010.161401	1.85	2.5	-1010.161196	1.8	2.5	-1010.161012
1.9	2.45	-1010.162633	1.85	2.45	-1010.162535	1.8	2.45	-1010.162495
1.9	2.4	-1010.163842	1.85	2.4	-1010.16386	1.8	2.4	-1010.163921
1.9	2.35	-1010.165007	1.85	2.35	-1010.165141	1.8	2.35	-1010.165329
1.9	2.3	-1010.166132	1.85	2.3	-1010.166381	1.8	2.3	-1010.166701
1.9	2.25	-1010.167231	1.85	2.25	-1010.16759	1.8	2.25	-1010.168029
1.9	2.2	-1010.168315	1.85	2.2	-1010.168776	1.8	2.2	-1010.16933
1.9	2.15	-1010.169401	1.85	2.15	-1010.169954	1.8	2.15	-1010.170606
1.9	2.1	-1010.170511	1.85	2.1	-1010.17113	1.8	2.1	-1010.17186
1.9	2.05	-1010.17167	1.85	2.05	-1010.172326	1.8	2.05	-1010.173102
1.9	2	-1010.172909	1.85	2	-1010.173576	1.8	2	-1010.174354
1.9	1.95	-1010.174269	1.85	1.95	-1010.174912	1.8	1.95	-1010.175643
1.9	1.9	-1010.175752	1.85	1.9	-1010.176351	1.8	1.9	-1010.177002
1.9	1.85	-1010.177393	1.85	1.85	-1010.17792	1.8	1.85	-1010.178456
1.9	1.8	-1010.179174	1.85	1.8	-1010.179607	1.8	1.8	-1010.180017
1.9	1.75	-1010.181062	1.85	1.75	-1010.18137	1.8	1.75	-1010.181638
1.9	1.7	-1010.184987	1.85	1.7	-1010.183122	1.8	1.7	-1010.183208
1.9	1.65	-1010.187186	1.85	1.65	-1010.187325	1.8	1.65	-1010.187287
1.9	1.6	-1010.188904	1.85	1.6	-1010.18886	1.8	1.6	-1010.188614
1.9	1.55	-1010.242286	1.85	1.55	-1010.235703	1.8	1.55	-1010.189114
1.9	1.5	-1010.245988	1.85	1.5	-1010.239533	1.8	1.5	-1010.232684
1.9	1.45	-1010.252139	1.85	1.45	-1010.24081	1.8	1.45	-1010.234172
1.9	1.4	-1010.250005	1.85	1.4	-1010.238694	1.8	1.4	-1010.232308
1.75	2.5	-1010.160726	1.7	2.5	-1010.160172	1.65	2.5	-1010.158441
1.75	2.45	-1010.162374	1.7	2.45	-1010.161995	1.65	2.45	-1010.160834
1.75	2.4	-1010.163956	1.7	2.4	-1010.163779	1.65	2.4	-1010.163037
1.75	2.35	-1010.165492	1.7	2.35	-1010.165498	1.65	2.35	-1010.165089
1.75	2.3	-1010.16701	1.7	2.3	-1010.167172	1.65	2.3	-1010.167029
1.75	2.25	-1010.168483	1.7	2.25	-1010.168825	1.65	2.25	-1010.168902
1.75	2.2	-1010.169918	1.7	2.2	-1010.170425	1.65	2.2	-1010.170751
1.75	2.15	-1010.171314	1.7	2.15	-1010.171966	1.65	2.15	-1010.172594
1.75	2.1	-1010.172663	1.7	2.1	-1010.173437	1.65	2.1	-1010.174364

1.75	2.05	-1010.173966	1.7	2.05	-1010.174827	1.65	2.05	-1010.176036
1.75	2	-1010.175229	1.7	2	-1010.176133	1.65	2	-1010.177585
1.75	1.95	-1010.176473	1.7	1.95	-1010.177358	1.65	1.95	-1010.178993
1.75	1.9	-1010.177728	1.7	1.9	-1010.178521	1.65	1.9	-1010.180249
1.75	1.85	-1010.179016	1.7	1.85	-1010.179633	1.65	1.85	-1010.181347
1.75	1.8	-1010.180388	1.7	1.8	-1010.180722	1.65	1.8	-1010.1824
1.75	1.75	-1010.18182	1.7	1.75	-1010.181866	1.65	1.75	-1010.183684
1.75	1.7	-1010.1832	1.7	1.7	-1010.18302	1.65	1.7	-1010.184909
1.75	1.65	-1010.184337	1.7	1.65	-1010.183924	1.65	1.65	-1010.185854
1.75	1.6	-1010.188134	1.7	1.6	-1010.184319	1.65	1.6	-1010.186285
1.75	1.55	-1010.188364	1.7	1.55	-1010.183899	1.65	1.55	-1010.185871
1.75	1.5	-1010.187375	1.7	1.5	-1010.185964	1.65	1.5	-1010.184186
1.75	1.45	-1010.226935	1.7	1.45	-1010.218933	1.65	1.45	-1010.180691
1.75	1.4	-1010.22536	1.7	1.4	-1010.21769	1.65	1.4	-1010.209141
1.6	2.5	-1010.157423	1.55	2.5	-1010.154621	1.5	2.5	-1010.151091
1.6	2.45	-1010.160122	1.55	2.45	-1010.158233	1.5	2.45	-1010.154548
1.6	2.4	-1010.162599	1.55	2.4	-1010.161026	1.5	2.4	-1010.157698
1.6	2.35	-1010.164899	1.55	2.35	-1010.163613	1.5	2.35	-1010.160615
1.6	2.3	-1010.16707	1.55	2.3	-1010.166061	1.5	2.3	-1010.163405
1.6	2.25	-1010.169159	1.55	2.25	-1010.16846	1.5	2.25	-1010.23682
1.6	2.2	-1010.171224	1.55	2.2	-1010.241775	1.5	2.2	-1010.242074
1.6	2.15	-1010.242095	1.55	2.15	-1010.244901	1.5	2.15	-1010.245739
1.6	2.1	-1010.243156	1.55	2.1	-1010.246445	1.5	2.1	-1010.24779
1.6	2.05	-1010.242773	1.55	2.05	-1010.246478	1.5	2.05	-1010.248266
1.6	2	-1010.24109	1.55	2	-1010.245144	1.5	2	-1010.247307
1.6	1.95	-1010.238281	1.55	1.95	-1010.24262	1.5	1.95	-1010.245091
1.6	1.9	-1010.234425	1.55	1.9	-1010.239037	1.5	1.9	-1010.241791
1.6	1.85	-1010.22952	1.55	1.85	-1010.234413	1.5	1.85	-1010.237461
1.6	1.8	-1010.22356	1.55	1.8	-1010.228738	1.5	1.8	-1010.232093
1.6	1.75	-1010.216575	1.55	1.75	-1010.222033	1.5	1.75	-1010.2257
1.6	1.7	-1010.208638	1.55	1.7	-1010.214361	1.5	1.7	-1010.218336
1.6	1.65	-1010.199853	1.55	1.65	-1010.205816	1.5	1.65	-1010.210074
1.6	1.6	-1010.190264	1.55	1.6	-1010.196409	1.5	1.6	-1010.200907
1.6	1.55	-1010.179874	1.55	1.55	-1010.186119	1.5	1.55	-1010.190779
1.6	1.5	-1010.168538	1.55	1.5	-1010.174748	1.5	1.5	-1010.179463
1.6	1.45	-1010.156055	1.55	1.45	-1010.161996	1.5	1.45	-1010.166594
1.6	1.4	-1010.142076	1.55	1.4	-1010.147478	1.5	1.4	-1010.151683
1.45	2.5	-1010.182834	1.4	2.5	-1010.176295			
1.45	2.45	-1010.19669	1.4	2.45	-1010.188695			
1.45	2.4	-1010.207852	1.4	2.4	-1010.200199			
1.45	2.35	-1010.217868	1.4	2.35	-1010.210635			
1.45	2.3	-1010.226626	1.4	2.3	-1010.21986			
1.45	2.25	-1010.233959	1.4	2.25	-1010.227718			

1.45	2.2	-1010.239766	1.4	2.2	-1010.234069			
1.45	2.15	-1010.243976	1.4	2.15	-1010.238825			
1.45	2.1	-1010.24655	1.4	2.1	-1010.241932			
1.45	2.05	-1010.247497	1.4	2.05	-1010.243371			
1.45	2	-1010.246937	1.4	2	-1010.243233			
1.45	1.95	-1010.245056	1.4	1.95	-1010.241709			
1.45	1.9	-1010.242052	1.4	1.9	-1010.239016			
1.45	1.85	-1010.238026	1.4	1.85	-1010.235307			
1.45	1.8	-1010.232984	1.4	1.8	-1010.23061			
1.45	1.75	-1010.226933	1.4	1.75	-1010.224933			
1.45	1.7	-1010.219923	1.4	1.7	-1010.21802			
1.45	1.65	-1010.211992	1.4	1.65	-1010.210757			
1.45	1.6	-1010.20312	1.4	1.6	-1010.202231			
1.45	1.55	-1010.17371	1.4	1.55	-1010.192611			
1.45	1.5	-1010.170153	1.4	1.5	-1010.181647			
1.45	1.45	-1010.164835	1.4	1.45	-1010.157169			
1.45	1.4	-1010.156952	1.4	1.4	-1010.148712			

S5.6 Gibbs Energy Profile of 1l

Interestingly, **1l** with the terminal position of the alkene part substituted by two alkyl group undergoes nucleophilic addition to form **IN-1l** via **TS1-1l**, which is not an ambimodal transition state (Figure S16). Subsequently, **IN-1l** could undergo three different isomerization processes. Compared to cycloaddition to form **NP-1l** via **TS2-1l**, cycloaddition to form the cross [2 + 2] product **CP-1l** via **TS3-1l** is 7.6 kcal/mol more favored. Therefore, the cross [2 + 2] product is predicted to be the product which can be observed for **1l**, considering that the isomerization process (from **CP-1l** to **NP-1l**) with a free energy barrier of 42.4 kcal/mol can be ruled out. This also indicates the selectivity between NP and CP is again controlled by kinetics for substrate **1l**. In addition to the normal and cross cycloaddition pathways, there is the third pathway, which is the F-C pathway (ene reaction pathway) via **TS4-1l** leading to **FC-1l**. Calculations found that the 1,5-proton shift step (could be also viewed as a stepwise ene reaction from **1l** to **FC-1l**) in the F-C pathway is nearly barrierless, which means F-C product should be dominant. Indeed, we isolated F-C product in a yield of 38% with no significant amount of cross [2 + 2] product experimentally (Figure 4 in the main text), which again supported our hypothesis.

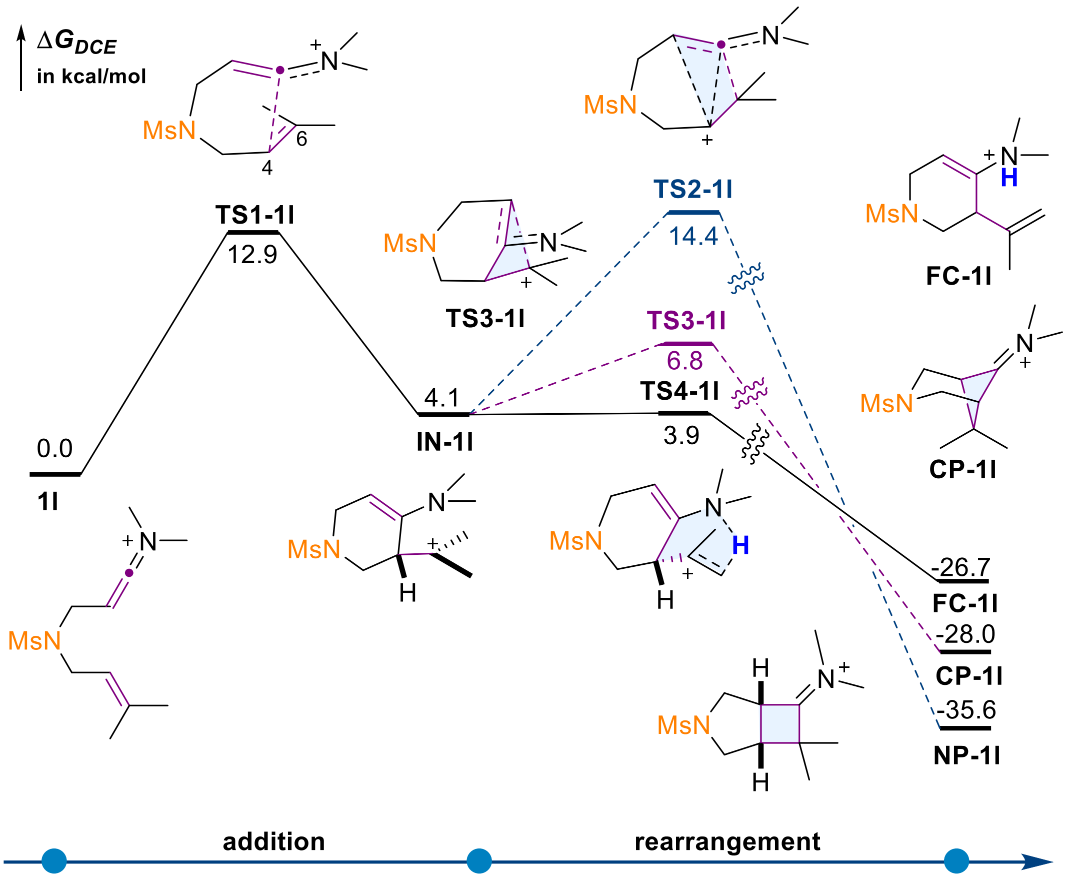


Figure S16. Gibbs energy profile for [2 + 2] cycloaddition and F-C pathway of **1l**. Computed at SMD(DCE)/DLPNO-CCSD(T)/cc-pVTZ//ωB97X-D/def2-SVP level.

S5.7 The Differences between the Mechanism for [2 + 2] Cycloaddition of Ene-Keteniminium Ions and Ene-Ketenes

In our previous study,[10] the [2 + 2] cycloaddition of ene-ketenes with *α*-O tethers is concerted and asynchronous. While it becomes stepwise for the [2 + 2] cycloaddition of ene-keteneiminium ions with *α*-O tethers and a cyclopropanation intermediate is formed first. This can be understood by the model shown in Figure S17a. After the C6−C7 bond formation for ene-ketene **1a-O**, the ketene oxygen is negatively charged and can donate electrons strongly. Consequently, C5 is more nucleophilic and can attack the formal carbocation at C4 position, giving the [2 + 2] product directly. But for **1a**, it is different. After the formation of the C6−C7 bond, the dimethyl amino group is perpendicular to the alkene plane, reducing the electron donating ability of nitrogen. However, the *α*-O can donate electrons to the double bond, helping C7 attacks the carbocation at C4 position, giving a cyclopropane intermediate.

Scheme 3 (in the main text) describes the kinetic, thermodynamic, and dynamic control in normal vs. cross [2 + 2] cycloadditions for ene-keteniminium ions. The dynamic nature of some [2 + 2] reactions is due to the fact that both *endo* and *exo* carbocations have similar stabilities and two forming bonds (C4−C7 and C6−C7) are close, as exemplified by the transition state structure of **TS1-1h** shown in Figure 3a (in the main text). Surprisingly, our previous study showed that, almost all the intramolecular [2 + 2] cycloaddition transition states for ene-ketenes are kinetically controlled. For example, model substrate **1h-O** has similar tether and substituents, but the regiochemistry is kinetically controlled. Why?

We attributed this difference to the high reactivity of keteniminium ions with respect to that of ketenes. For ketenes, both the normal and cross [2 + 2] cycloadditions of **1h-O** (the ketene analogue of **1h**) have an activation free energy up to 32~33 kcal/mol, much higher than that of [2 + 2] cycloaddition of **1h** (16.0 kcal/mol) and their corresponding transition states are late and much more like the products (see **TS-NP** and **TS-CP** in Figure 17b). As a result, *endo* and *exo* carbocations in ene-ketenes are distinguishably generated in the transition states and their relative stabilities determine that their [2 + 2] reactions are kinetically controlled, not dynamically controlled.

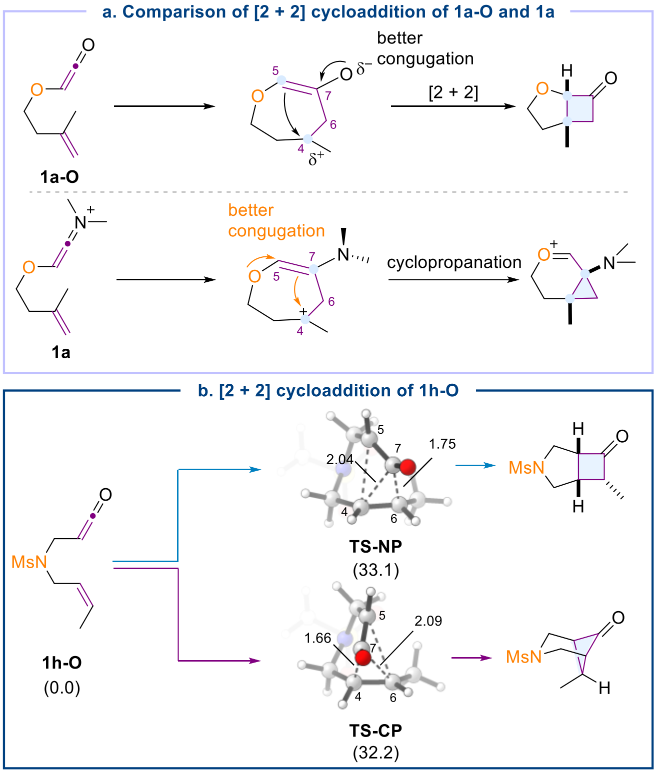


Figure S17. Comparison of intramolecular [2 + 2] cycloadditions of ene-ketenes and ene-keteniminium ions. The bond lengths are reported in Å. Gibbs energies in parentheses are reported in kcal/mol. Computed at the DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//ωB97X-D/def2-SVP level.

S5.8 Computational Results for 1m

For phenyl substituted ene-keteniminium **1m**, the Gibbs energy profile is a little different from that of **1i**. The electrophilic addition transition state **TS1-1m** is not ambimodal (Figures S18 and S19a) and has an activation free energy of 12.9 kcal/mol. After that, the rearrangement to afford the normal product **NP-1m** is energetically disfavored because **TS2-1m** is 10.5 kcal/mol higher than rearrangement transition state **TS3-1m**. Thus, generation of the cross product is preferred, which was validated by the experiment (Figure 7 in the main text).

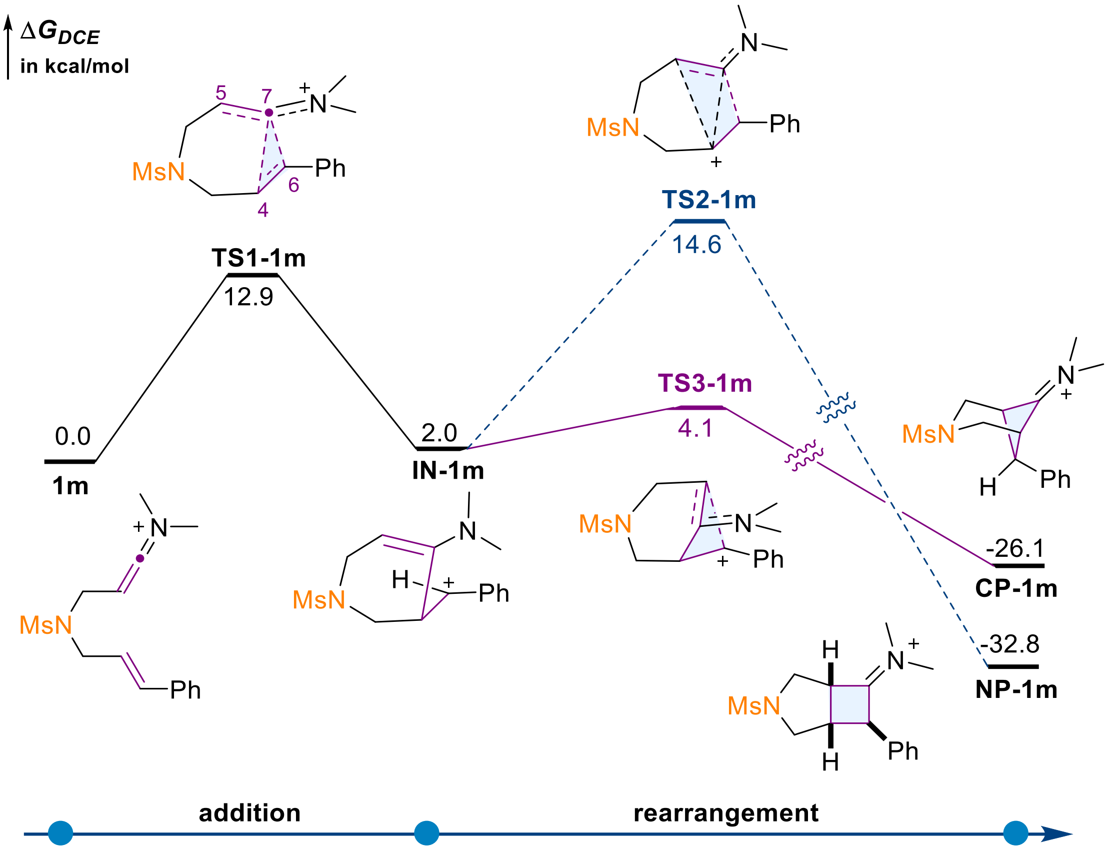


Figure S18. Gibbs energy profile for [2 + 2] cycloaddition of **1m**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//ωB97X-D/def2-SVP level.

We also tried to locate the *endo* carbocation, finding that **IN-1m** is connected to **NP-1m** directly via **TS2-1m** and optimization of an *endo* carbocation structure directly leads to the *exo* carbocation. In addition, **IN-1m** is much more stable than **TS2-1m** with *endo* carbocation characters (Figure S19b), which can explain why **TS1-1m** is not ambimodal.

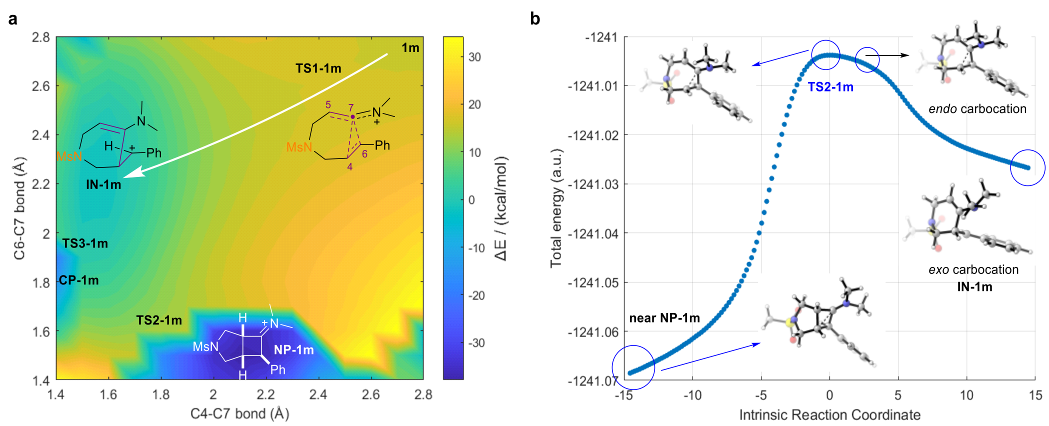


Figure S19. Potential energy surface for [2 + 2] cycloaddition of **1m** (a) and IRC for **TS2-1m** (b). Computed at ωB97X-D/def2-SVP level.

Table S5. Relaxed Potential Energy Surface Scan for [2 + 2] Cycloaddition of 1m

C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)	C4-C7 (Å)	C6-C7 (Å)	*E* (a.u.)
2.8	2.8	-1241.000976	2.7	2.8	-1241.00079	2.6	2.8	-1241.000433
2.8	2.7	-1241.000494	2.7	2.7	-1241.000416	2.6	2.7	-1241.000252
2.8	2.6	-1240.999561	2.7	2.6	-1240.999718	2.6	2.6	-1240.999817
2.8	2.5	-1240.998088	2.7	2.5	-1240.998535	2.6	2.5	-1240.998924
2.8	2.4	-1240.996019	2.7	2.4	-1240.996817	2.6	2.4	-1240.997525
2.8	2.3	-1240.99335	2.7	2.3	-1240.994554	2.6	2.3	-1240.995637
2.8	2.2	-1240.990159	2.7	2.2	-1240.991863	2.6	2.2	-1240.993355
2.8	2.1	-1240.986556	2.7	2.1	-1240.988851	2.6	2.1	-1240.990813
2.8	2	-1240.982715	2.7	2	-1240.985726	2.6	2	-1240.988252
2.8	1.9	-1240.97873	2.7	1.9	-1240.982633	2.6	1.9	-1240.985848
2.8	1.8	-1240.974784	2.7	1.8	-1240.979509	2.6	1.8	-1240.983682
2.8	1.7	-1240.970211	2.7	1.7	-1240.975903	2.6	1.7	-1240.981494
2.8	1.6	-1241.03426	2.7	1.6	-1240.970904	2.6	1.6	-1240.978203
2.8	1.5	-1241.03074	2.7	1.5	-1241.015794	2.6	1.5	-1240.970365
2.8	1.4	-1241.014605	2.7	1.4	-1241.011052	2.6	1.4	-1241.036593
2.5	2.8	-1240.999876	2.4	2.8	-1240.999104	2.3	2.8	-1240.998184
2.5	2.7	-1241.000014	2.4	2.7	-1240.999732	2.3	2.7	-1240.999448
2.5	2.6	-1240.999891	2.4	2.6	-1240.999989	2.3	2.6	-1241.000183
2.5	2.5	-1240.999319	2.4	2.5	-1240.999792	2.3	2.5	-1241.000434
2.5	2.4	-1240.998238	2.4	2.4	-1240.999058	2.3	2.4	-1241.000093
2.5	2.3	-1240.996676	2.4	2.3	-1240.997808	2.3	2.3	-1240.999192
2.5	2.2	-1240.994752	2.4	2.2	-1240.996188	2.3	2.2	-1240.997852
2.5	2.1	-1240.992589	2.4	2.1	-1240.994326	2.3	2.1	-1240.996219
2.5	2	-1240.990426	2.4	2	-1240.992468	2.3	2	-1240.994564
2.5	1.9	-1240.988508	2.4	1.9	-1240.990864	2.3	1.9	-1240.99316
2.5	1.8	-1240.987039	2.4	1.8	-1240.989854	2.3	1.8	-1240.992426
2.5	1.7	-1240.986068	2.4	1.7	-1240.989857	2.3	1.7	-1240.993086
2.5	1.6	-1240.984331	2.4	1.6	-1240.98947	2.3	1.6	-1241.074875
2.5	1.5	-1240.978131	2.4	1.5	-1241.058694	2.3	1.5	-1241.074986
2.5	1.4	-1241.037762	2.4	1.4	-1241.045548	2.3	1.4	-1241.063804
2.2	2.8	-1240.997371	2.1	2.8	-1240.997097	2	2.8	-1240.998078
2.2	2.7	-1240.999407	2.1	2.7	-1240.999963	2	2.7	-1241.001697
2.2	2.6	-1241.000709	2.1	2.6	-1241.001887	2	2.6	-1241.004248
2.2	2.5	-1241.001475	2.1	2.5	-1241.003152	2	2.5	-1241.005901
2.2	2.4	-1241.001566	2.1	2.4	-1241.003694	2	2.4	-1241.006858
2.2	2.3	-1241.001006	2.1	2.3	-1241.003477	2	2.3	-1241.006966
2.2	2.2	-1240.999915	2.1	2.2	-1241.002605	2	2.2	-1241.006282
2.2	2.1	-1240.998466	2.1	2.1	-1241.001284	2	2.1	-1241.004985
2.2	2	-1240.996932	2.1	2	-1240.999776	2	2	-1241.003372
2.2	1.9	-1240.995592	2.1	1.9	-1240.998375	2	1.9	-1241.001732
2.2	1.8	-1240.99502	2.1	1.8	-1240.997831	2	1.8	-1241.001055

2.2	1.7	-1240.995982	2.1	1.7	-1240.998736	2	1.7	-1241.001522
2.2	1.6	-1241.082367	2.1	1.6	-1241.082361	2	1.6	-1241.074706
2.2	1.5	-1241.084925	2.1	1.5	-1241.087434	2	1.5	-1241.081792
2.2	1.4	-1241.076106	2.1	1.4	-1241.081171	2	1.4	-1241.077811
1.9	2.8	-1241.000802	1.8	2.8	-1241.005039	1.7	2.8	-1241.00905
1.9	2.7	-1241.005131	1.8	2.7	-1241.010049	1.7	2.7	-1241.014871
1.9	2.6	-1241.008249	1.8	2.6	-1241.013706	1.7	2.6	-1241.019204
1.9	2.5	-1241.010249	1.8	2.5	-1241.016112	1.7	2.5	-1241.022131
1.9	2.4	-1241.011459	1.8	2.4	-1241.017473	1.7	2.4	-1241.023797
1.9	2.3	-1241.011825	1.8	2.3	-1241.018074	1.7	2.3	-1241.024635
1.9	2.2	-1241.011285	1.8	2.2	-1241.017677	1.7	2.2	-1241.024456
1.9	2.1	-1241.009947	1.8	2.1	-1241.016345	1.7	2.1	-1241.02323
1.9	2	-1241.008081	1.8	2	-1241.014246	1.7	2	-1241.02102
1.9	1.9	-1241.006168	1.8	1.9	-1241.011808	1.7	1.9	-1241.018014
1.9	1.8	-1241.004996	1.8	1.8	-1241.009711	1.7	1.8	-1241.014749
1.9	1.7	-1241.004525	1.8	1.7	-1241.007941	1.7	1.7	-1241.011524
1.9	1.6	-1241.003952	1.8	1.6	-1241.005794	1.7	1.6	-1241.007567
1.9	1.5	-1241.066633	1.8	1.5	-1241.052427	1.7	1.5	-1241.001224
1.9	1.4	-1241.06673	1.8	1.4	-1241.05062	1.7	1.4	-1241.03513
1.6	2.8	-1241.010178	1.5	2.8	-1241.033499	1.4	2.8	-1241.017933
1.6	2.7	-1241.016928	1.5	2.7	-1241.012799	1.4	2.7	-1241.025994
1.6	2.6	-1241.022124	1.5	2.6	-1241.018867	1.4	2.6	-1241.004476
1.6	2.5	-1241.025797	1.5	2.5	-1241.023481	1.4	2.5	-1241.009933
1.6	2.4	-1241.02804	1.5	2.4	-1241.02654	1.4	2.4	-1241.014012
1.6	2.3	-1241.029211	1.5	2.3	-1241.028229	1.4	2.3	-1241.016544
1.6	2.2	-1241.029422	1.5	2.2	-1241.029064	1.4	2.2	-1241.018102
1.6	2.1	-1241.028474	1.5	2.1	-1241.02865	1.4	2.1	-1241.018469
1.6	2	-1241.026421	1.5	2	-1241.027069	1.4	2	-1241.017661
1.6	1.9	-1241.023242	1.5	1.9	-1241.024273	1.4	1.9	-1241.05716
1.6	1.8	-1241.019074	1.5	1.8	-1241.020063	1.4	1.8	-1241.05018
1.6	1.7	-1241.014332	1.5	1.7	-1241.014354	1.4	1.7	-1241.038224
1.6	1.6	-1241.008574	1.5	1.6	-1241.007032	1.4	1.6	-1241.021747
1.6	1.5	-1241.00004	1.5	1.5	-1240.996451	1.4	1.5	-1241.000646
1.6	1.4	-1240.985322	1.5	1.4	-1240.979199	1.4	1.4	-1240.972235

S5.9 Computational Results for 1p

Figure S20 is the computed surfaces (geometry optimizations were carried out in the gas phase and then single point energy calculations in DCE were performed). The first electrophilic addition step via the ambimodal transition state **TS1-1p** has an activation free energy of 13.5 kcal/mol, and then both the *exo* carbocation **IN1-1p** and *endo* carbocation **IN2-1p** are formed. These two intermediates are connected by a rearrangement transition state **TS4-1p**. The normal and cross [2 + 2] pathways via **TS2-1p** and **TS3-1p** have quite low free energies of activations, meaning that the selectivity is dynamically controlled.

CP-1p is predicted to be the main product according to the carbocation model. Importantly, there is another pathway involving the C–C bond rotation: the *exo*-Z cation **IN1-1p** could isomerize to the *exo*-E cation **IN-1m**. This stepwise process is disfavored by 3.5 kcal/mol with respect to the cross [2 + 2] process to form **CP-1p**. Consequently, the **CP-1p** is the dominant product, while **CP-1m** will not be formed. This is not consistent with experiments.

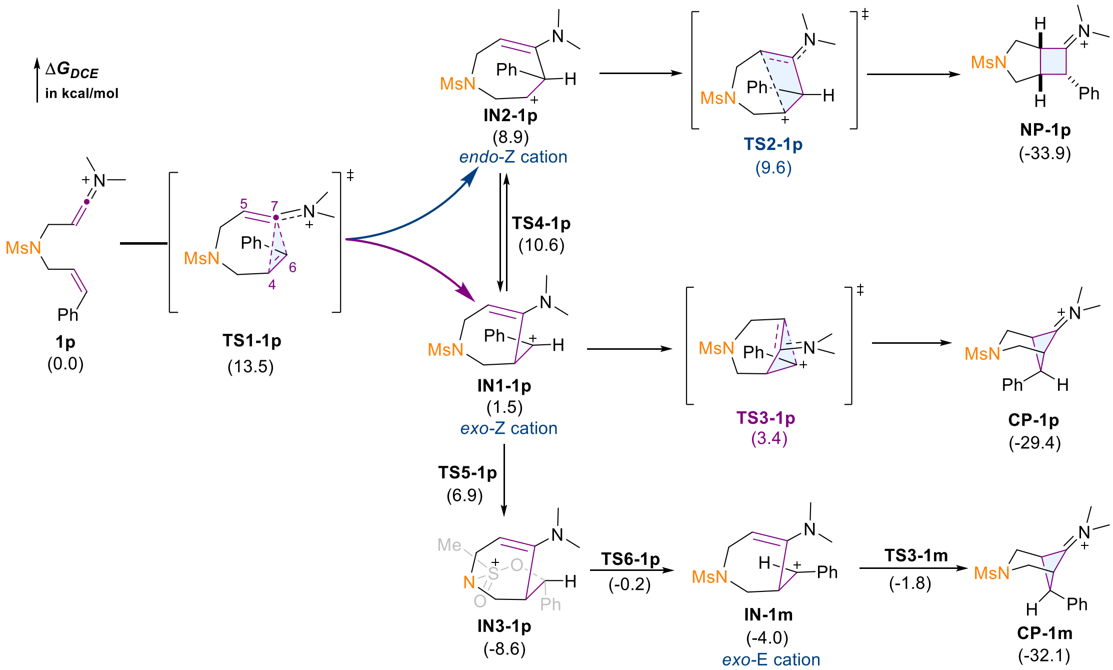


Figure S20. Gibbs energy profile for [2 + 2] cycloaddition of **1p**. Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//*ω*B97X-D/def2-SVP level.

We then calculated the profile with structures optimized in solution (Figure S21) and the Gibbs energy profile is similar. In this case, C–C bond rotation is easier than direct formation of the cross [2 + 2] product. This means that **CP-1m** should be the major product while **CP-1p** is the minor product. This disagrees with experiments shown in Figure 7 (in the main text). Because the activation free energies for these two processes are very low, 0.7 and 2.1 kcal/mol, respectively, we hypothesized that dynamics plays a role in forming two products. In this case, the three products are all dynamically controlled. This has been well described by the previous report[11] and we also did quasiclassical trajectories (QCTs) molecular dynamics simulation to elucidate it (Figure S22).

We were pleased to find that most trajectories (77 out of 100) lead to cross [2 + 2] product **CP-1p**, and a small number of trajectories (16 out of 100) lead to normal [2 + 2] product **NP-1p**, which is consistent with experiments. We hypothesized that the amount of formed normal [2 + 2] product was very low and it was not detected by ^{1}H NMR. Interestingly, there are 2 (out of 100) trajectories leading to *E*-*exo* cation **IN-1m**. This means **CP-1m** could be observed, consistent with the experimental results, although the ratio for **IN-1m** was underestimated here. We attribute this underestimation for the long propagation time for trajectories leading to **IN-1m**, which is difficult for the program (many trajectories terminated after a long time of propagation). The other 5 out of the 100 trajectories recross to give back the starting material.

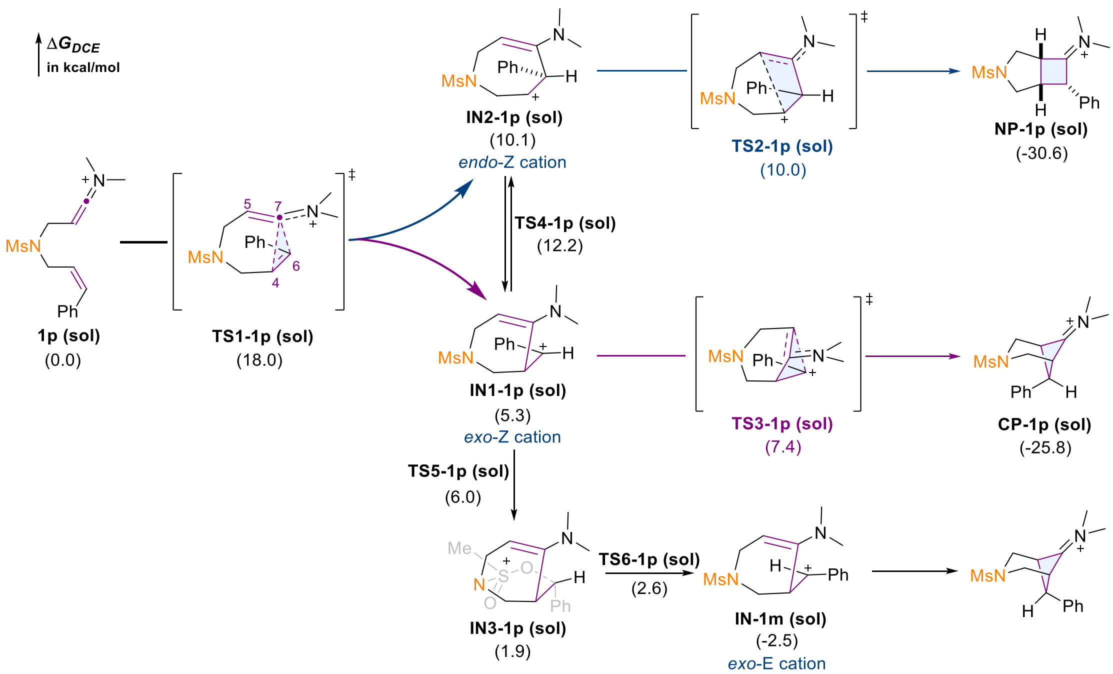


Figure S21. Gibbs energy profile for [2 + 2] cycloaddition of **1p** (structure optimized in solution phase). Computed at DLPNO-CCSD(T)/cc-pVTZ:SMD(DCE)//SMD(DCE)/ωB97X-D/def2-SVP level.

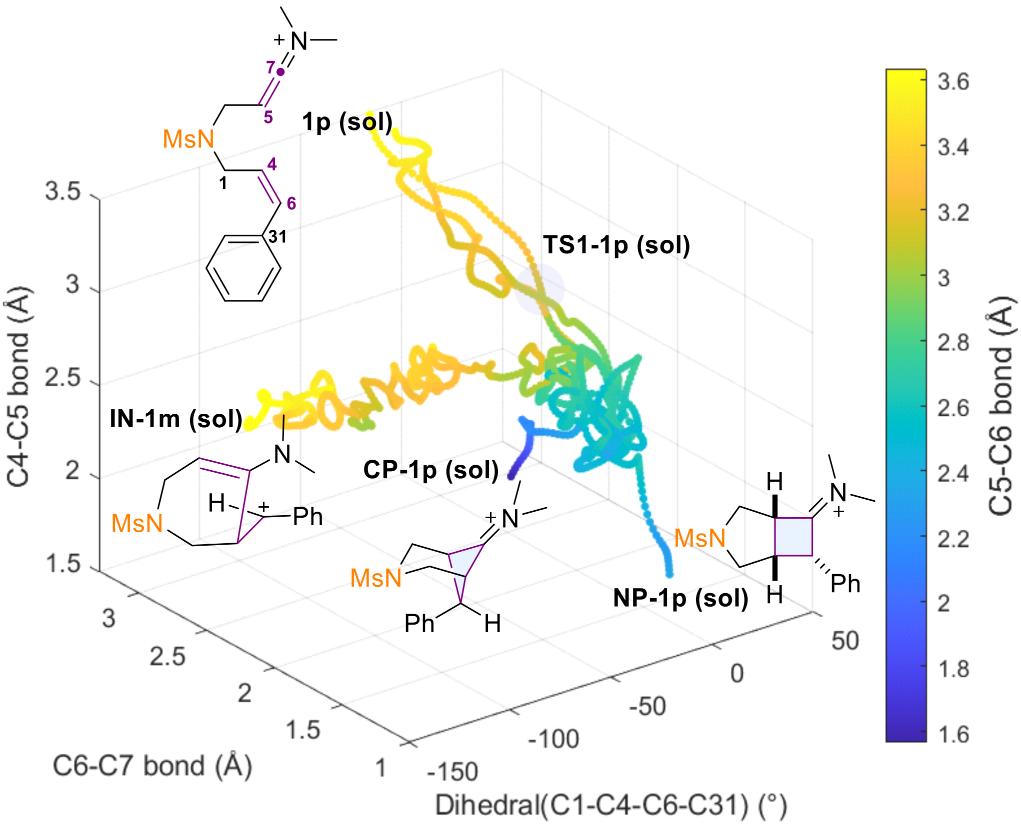


Figure S22. Representative trajectories leading to **CP-1p**, **NP-1p** and **IN-1m** for **1p**. Molecular dynamics simulations were performed at SMD(DCE)/ωB97X-D/def2-SVP level of theory and the temperature was set to be 363.15 K. Quasiclassical trajectories (QCTs) were initiated in the region of the potential energy surface near **TS1-1p (sol)** and propagated forward and backward until either one of the products is formed (the forming C−C bond shorter than 1.6 Å for **NP-1p (sol)** and **CP-1p (sol)**; the dihedral of C1−C4−C6−C31 is smaller than -120° or larger than 120° for **IN-1m (sol)** or the reactants are generated. QM-like gaussian distribution of displacements were used. The classical equations of motion were integrated with a velocity-Verlet algorithm using Singleton's program Progdyn,[12-15] with the energies and derivatives computed on the fly with SMD(DCE)/ωB97X-D/def2-SVP using Gaussian 09. The step length for integration was 1 fs.

S5.10 Solution Phase Optimization and QCT Molecular Dynamics Simulation Results for Selected Examples

The Gibbs energy profile for [2 + 2] cycloaddition of **1a** calculated by the solution phase optimized structures is shown in Figure S23, which is similar with that from the gas phase calculations (in the main text).

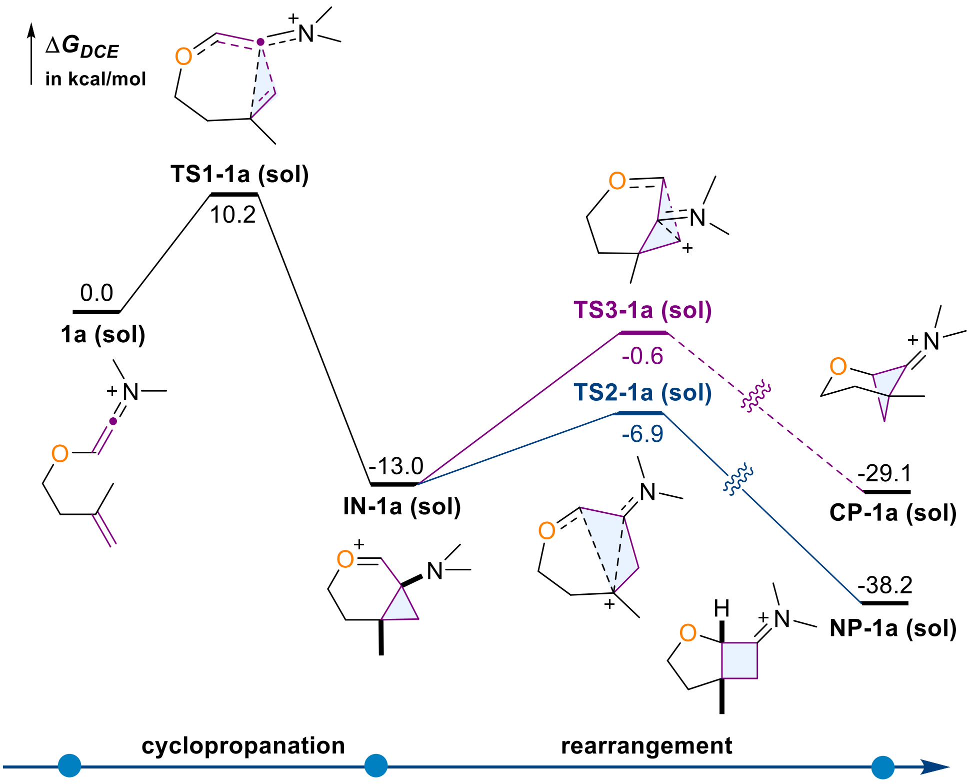


Figure S23. Gibbs energy profile based on solution phase geometry optimization for [2 + 2] cycloaddition of **1a**. Computed at DLPNO-CCSD(T)/cc-pVTZ: SMD(DCE)//SMD(DCE)/ωB97X-D/def2-SVP level.

We also calculated the Gibbs energy profile with the structures optimized in solution phase of the dynamically controlled case (**1h**), finding that the reaction pathway is almost the same as that from the gas phase optimized result (Figure S24). The difference is that a new transition state **TS4-1h (sol)** and intermediate, namely the *exo* carbocation intermediate **IN2-1h (sol)**, appeared. This intermediate is also proposed in our cation model. It's an entropic intermediate in the gas phase, while it turns into a real intermediate in solution phase simulation, which gives further support for our cation model. Solution phase QCT molecular dynamics simulation was also carried out through initiating trajectories from **TS1-**

1h (sol) region (Table S6). We found that the predicted NP/CP ratio is 1:3.4, close to the gas phase result, 1:3.5.

Thus, the above results suggest that there is no distinct difference between structure optimizations of stationary points in the gas phase and solution.

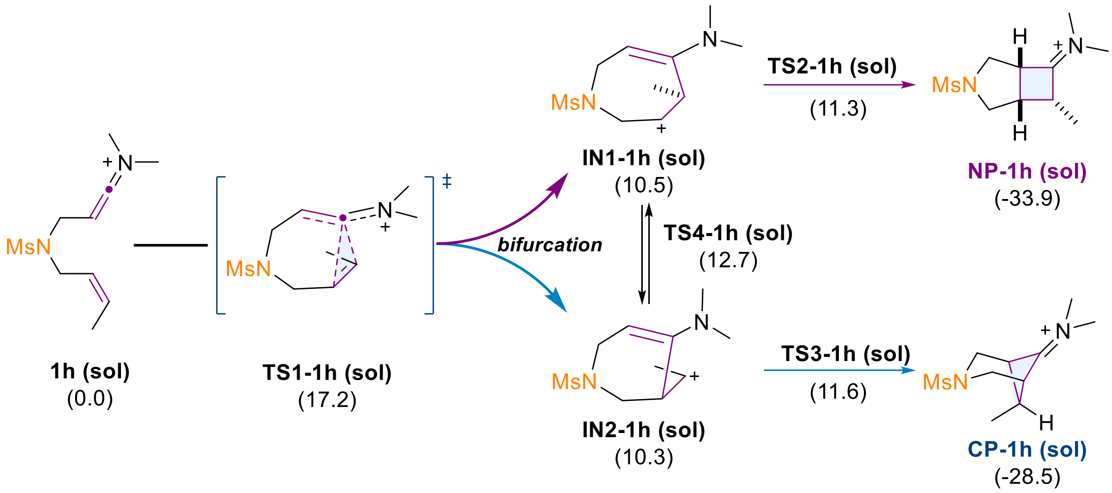


Figure S24. Gibbs energy profile based on solution phase geometry for [2 + 2] cycloaddition of **1h**. Computed at DLPNO-CCSD(T)/cc-pVTZ: SMD(DCE)//SMD(DCE)/ωB97X-D/def2-SVP level.

Table S6. Comparison of Gas and Solution Phase QCT Molecular Dynamics Simulation Results for [2 + 2] Cycloaddition of 1h

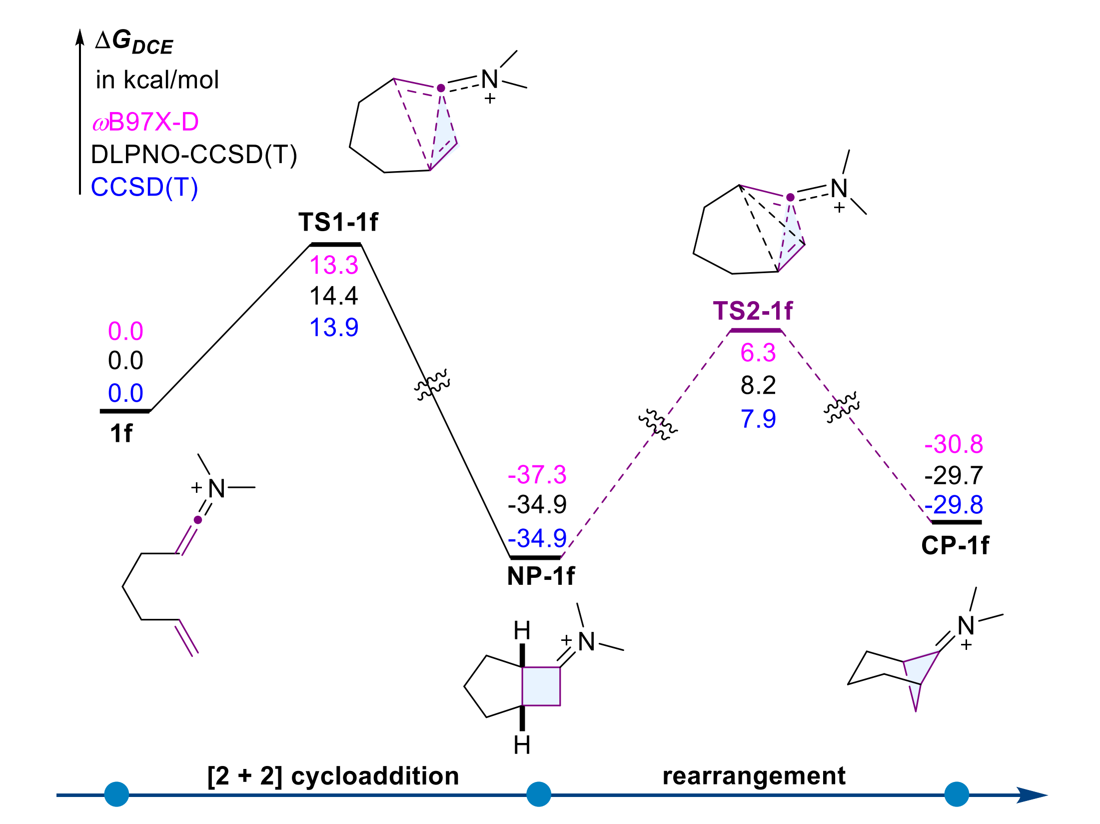
Phase	NP trajectories	CP trajectories	Recross trajectories
gas	30	104	9
DCE[a]	44	148	5

[a]Molecular dynamics simulations were performed at SMD(DCE)/*ω*B97X-D/def2-SVP level of theory and the temperature was set to be 363.15 K. Quasiclassical trajectories (QCTs) were initiated in the region of the potential energy surface near **TS1-1h(sol)** and propagated forward and backward until either one of the products is formed (the forming C−C bond shorter than 1.6 Å) or the reactants are generated. QM-like gaussian distribution of displacements were used. The classical equations of motion were integrated with a velocity-Verlet algorithm using Singleton's program Progdyn, with the energies and derivatives computed on the fly with SMD(DCE)/*ω*B97X-D/def2-SVP using Gaussian 09. The step length for integration was 1 fs.

S5.11 Evaluation of Functionals by Further Benchmark Study

To further support that *ω*B97X-D[16] is a good functional for our system, we did a benchmark study by using single point energies obtained at CCSD(T)[17]/cc-pVTZ[18] level (Table S7) based on the structures optimized at *ω*B97X-D/def2-SVP[19] level as reference using Gaussian 09 software package.[20] Pruned integration grids with 99 radial shells and 590 angular points per shell were used. Except for DLPNO-CCSD(T)[21,22] (the settings for calculations are the same as that mentioned in the main text), several other popular methods were tested, including *ω*B97X-D, M06-2X,[23] B3LYP,[24,25] B3LYP-D3BJ,[24–26] BMK,[27] M06,[23] M06-D3,[23,26] PBE0,[28] and PBE0-D3BJ.[26,28] The [2 + 2] reaction of **1f** was used as the model reaction. Among all the methods, DLPNO-CCSD(T) showed the best performance, with a small MAD (mean absolute deviation) of 0.2 kcal/mol. It was found that *ω*B97X-D and M06-2X also gave a relative smaller MAD compared with other popular functionals. Unfortunately, functionals like B3LYP, B3LYP-D3BJ and PBE0-D3BJ performs poor for the current reaction system. Consequently, it's appropriate to choose *ω*B97X-D as the functional to optimize the structures and DLPNO-CCSD(T) for single point energy refinement.

Table S7. Benchmark Study with CCSD(T)/cc-pVTZ as the Reference[a]

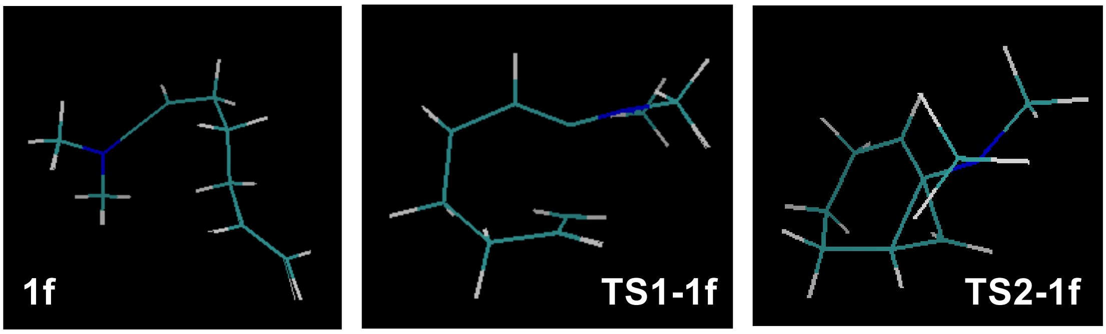


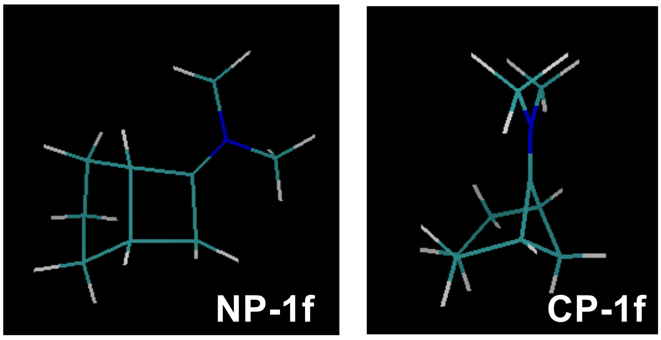
	DLPNO-CCSD(T)	*ω*B97X-D	M06-2X	B3LYP	B3LYP-D3BJ	BMK	M06	M06-D3	PBE0	PBE0-D3BJ
TS1-1f	0.5	-0.6	-0.9	1.5	-2.6	0.8	-1.5	-1.7	-2.3	-4.4
NP-1f	0.0	-2.4	1.3	9.8	6.8	-6.0	1.2	1.3	-3.9	-5.3
TS2-1f	0.2	-1.6	-1.9	7.3	3.7	-2.3	-3.2	-3.3	-4.9	-6.6
CP-1f	0.1	-1.0	1.8	11.4	8.2	-5.1	2.6	2.5	-2.9	-4.5
MAD	0.2	1.4	1.5	7.5	5.3	3.5	2.1	2.2	3.5	5.2

[a]The unit is kcal/mol. The basis set is cc-pVTZ for each functionals. The Gibbs energy of **1f** was set to be 0 kcal/mol.

S5.12 Evaluation of Basis Sets on Structure Optimization

To evaluate the size effect of the basis sets during structure optimization, we also did a comparison of the structures optimized by a larger basis set (6-311G(d,p)) and the used basis set (def2-SVP). As shown in Figure S25, the RMSD (root mean square displacement/deviation) between the two level is quite small, which indicates it's propriate to use *ω*B97X-D/def2-SVP level for all structure optimization, with the consideration of both accuracy and efficiency.





Structure	RMSD
1f	0.0631
TS1-1f	0.0325
TS2-1f	0.0239
NP-1f	0.0102
CP-1f	0.0079

Figure S25. The alignment of structures optimized at ωB97X-D/def2-SVP and ωB97X-D/6-311G(d,p) level. Visualized and computed (RMSD) by VMD software package.[29]

S6. Computed Energies of the Stationary Points

Table S8. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

Stationary point	TCG^{a,b} (a.u.)	SPE^{a,b} (a.u.)	SPE^{c} (a.u.)	SPE^{d} (a.u.)
1a	0.195229	-481.733656	-481.818760	-481.384102
TS1-1a	0.200219	-481.734176	-481.812758	-481.379260
IN-1a	0.206781	-481.779902	-481.861643	-481.417379
TS2-1a	0.206643	-481.768871	-481.848873	-481.409243
NP-1a	0.206707	-481.815763	-481.899135	-481.456099
TS3-1a	0.206821	-481.758074	-481.838750	-481.399030
CP-1a	0.208034	-481.799080	-481.883630	-481.440271
1b	0.170064	-442.452904	-442.537658	-442.139455
TS1-1b	0.174195	-442.449585	-442.528825	-442.131137
NP-1b	0.180714	-442.534185	-442.618853	-442.210279
TS2-1b	0.180107	-442.479997	-442.561739	-442.157628
IN-1b	0.180038	-442.494190	-442.577666	-442.167732
TS3-1b	0.179260	-442.477520	-442.559952	-442.153772
CP-1b	0.181598	-442.516790	-442.603117	-442.195565
1c	0.195791	-481.732958	-481.817470	-481.382503
TS1-1c	0.200832	-481.730789	-481.809158	-481.374239
IN-1c	0.205540	-481.766041	-481.848321	-481.402541
TS2-1c	0.206150	-481.753901	-481.833476	-481.393946
NP-1c	0.208075	-481.813851	-481.896896	-481.453114
TS3-1c	0.206586	-481.760203	-481.839946	-481.399742
CP-1c	0.208264	-481.798185	-481.882942	-481.440076
1d	0.195969	-481.734428	-481.819131	-481.384014
TS1-1d	0.200996	-481.733587	-481.812471	-481.377738
IN-1d	0.206813	-481.778424	-481.860611	-481.415622
TS2-1d	0.207951	-481.754597	-481.834868	-481.395551
NP-1d	0.207154	-481.814198	-481.897227	-481.454301
TS3-1d	0.206028	-481.765526	-481.845517	-481.404896
CP-1d	0.207713	-481.798178	-481.883036	-481.440271
TS4-1d	0.204681	-481.754904	-481.835081	-481.394983
FC-1d	0.208686	-481.792505	-481.879088	-481.441799
1e	0.244084	-1049.473932	-1049.556202	-1048.754995
TS1-1e	0.244731	-1049.453519	-1049.540175	-1048.731375
NP-1e	0.250508	-1049.532601	-1049.628257	-1048.806995
TS2-1e	0.250826	-1049.464196	-1049.550815	-1048.7369130
TS2-1e’	0.249071	-1049.455508	-1049.548191	-1048.729436

CP-1e	0.250647	-1049.522513	-1049.617021	-1048.795862
TS3-1e	0.249399	-1049.477258	-1049.566782	-1048.751165
IN-1e	0.248208	-1049.477322	-1049.566831	-1048.750684
1f	0.194080	-406.609992	-406.695876	-406.275925
TS1-1f	0.198409	-406.603581	-406.682190	-406.264505
NP-1f	0.204212	-406.691192	-406.774472	-406.344315
TS2-1f	0.202809	-406.618652	-406.702012	-406.274159
CP-1f	0.206050	-406.684261	-406.766546	-406.338872
1g	0.218680	-1010.191262	-1010.272951	-1009.508835
TS1-1g	0.218808	-1010.167029	-1010.254127	-1009.481197
NP-1g	0.224522	-1010.250148	-1010.347287	-1009.560318
TS2-1g	0.221336	-1010.174505	-1010.268978	-1009.484041
CP-1g	0.223771	-1010.240458	-1010.336953	-1009.549809
1h	0.244724	-1049.472101	-1049.553725	-1048.751933
TS-1h	0.245961	-1049.447444	-1049.534607	-1048.722060
NP-1h	0.252192	-1049.530493	-1049.626210	-1048.803579
TS2-1h	0.249896	-1049.464162	-1049.551739	-1048.732243
CP-1h	0.252717	-1049.524976	-1049.617131	-1048.794338
IN1-1h	0.249878	-1049.466111	-1049.553465	-1048.735237
TS3-1h	0.250559	-1049.465916	-1049.553047	-1048.735744
1i	0.244630	-1049.474022	-1049.555764	-1048.754326
TS1-1i	0.245201	-1049.451706	-1049.538916	-1048.728365
IN-1i	0.248243	-1049.476380	-1049.560953	-1048.747299
TS2-1i	0.250098	-1049.458261	-1049.549319	-1048.733151
NP-1i	0.251352	-1049.530207	-1049.625857	-1048.804449
TS3-1i	0.249476	-1049.476370	-1049.560966	-1048.747449
CP-1i	0.250793	-1049.521868	-1049.616927	-1048.794850
TS4-1i	0.247797	-1049.468940	-1049.554140	-1048.740763
FC-1i	0.251085	-1049.499322	-1049.599188	-1048.783763
1l	0.272054	-1088.754426	-1088.835591	-1087.998192
TS1-1l	0.272096	-1088.730284	-1088.819272	-1087.969839
IN-1l	0.275110	-1088.761999	-1088.846115	-1087.991708
TS2-1l	0.276272	-1088.731751	-1088.822114	-1087.970303
NP-1l	0.279038	-1088.810708	-1088.904762	-1088.049008
TS3-1l	0.276784	-1088.754317	-1088.839079	-1087.988489
CP-1l	0.278765	-1088.804505	-1088.896062	-1088.039116
TS4-1l	0.275135	-1088.759348	-1088.843772	-1087.991808
FC-1l	0.278690	-1088.792492	-1088.881433	-1088.039537

1m	0.293405	-1241.015893	-1241.101526	-1240.133586
TS1-1m	0.296345	-1240.999954	-1241.087607	-1240.114014
IN-1m	0.299301	-1241.030197	-1241.112226	-1240.139960
TS2-1m	0.299065	-1241.003819	-1241.091858	-1240.113519
NP-1m	0.299176	-1241.068835	-1241.165897	-1240.180220
TS3-1m	0.300870	-1241.025020	-1241.109946	-1240.135158
CP-1m	0.300723	-1241.065314	-1241.159356	-1240.174118
1p	0.296099	-1241.012121	-1241.095914	-1240.128622
TS1-1p	0.294762	-1240.983016	-1241.075937	-1240.096577
IN1-1p	0.298639	-1241.016195	-1241.100338	-1240.128486
IN2-1p	0.298380	-1241.003414	-1241.094067	-1240.109899
TS2-1p	0.299824	-1241.003119	-1241.093473	-1240.110475
NP-1p	0.303982	-1241.083140	-1241.169477	-1240.187997
TS3-1p	0.298905	-1241.013528	-1241.099003	-1240.124300
CP-1p	0.303472	-1241.073192	-1241.158596	-1240.181249
TS4-1p	0.298903	-1241.002655	-1241.093105	-1240.107823
TS5-1p	0.300913	-1241.013676	-1241.095270	-1240.124690
IN3-1p	0.303142	-1241.041285	-1241.123280	-1240.151142
TS6-1p	0.300956	-1241.023227	-1241.104825	-1240.135957
1h-O	0.165353	-990.417595	-990.434386	-989.7848925
TS-NP	0.171067	-990.368725	-990.391758	-989.7316507
TS-CP	0.171199	-990.369493	-990.392681	-989.7329623

[a]Computed at the ωB97X-D/def2-SVP level.

[b]A standard state at 1 atm and 298.15 K was used.

[c]Computed at the SMD(DCE)/ωB97X-D/def2-SVP//ωB97X-D/def2-SVP level.

[d]Computed at the DLPNO-CCSD(T)/cc-pVTZ//ωB97X-D/def2-SVP level.

Table S9. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs) of Stationary Points Optimized in Solution Phase

Stationary point	TCG[a,b] (a.u.)	SPE[a,b] (a.u.)	SPE[c] (a.u.)	SPE[d] (a.u.)
1a (sol)	0.197707	-481.819330	-481.733219	-481.384071
TS1-1a (sol)	0.201584	-481.812805	-481.734110	-481.379087
IN-1a (sol)	0.206591	-481.861882	-481.779658	-481.417542
TS2-1a (sol)	0.206120	-481.849104	-481.768604	-481.409109
NP-1a (sol)	0.206762	-481.899442	-481.815466	-481.456082
TS3-1a (sol)	0.207096	-481.839102	-481.757704	-481.399129
CP-1a (sol)	0.207839	-481.884011	-481.800042	-481.442726
1h (sol)	0.242300	-1049.555226	-1049.469289	-1048.749623
TS1-1h (sol)	0.245997	-1049.535903	-1049.445732	-1048.721722
TS4-1h (sol)	0.250148	-1049.553548	-1049.462033	-1048.731613

IN1-1h (sol)	0.250133	-1049.555329	-1049.463958	-1048.735237
TS2-1h (sol)	0.251076	-1049.554814	-1049.463802	-1048.735341
IN2-1h (sol)	0.247797	-1049.553901	-1049.463032	-1048.733813
TS3-1h (sol)	0.249956	-1049.553829	-1049.463279	-1048.734219
NP-1h (sol)	0.252753	-1049.627792	-1049.528661	-1048.800961
CP-1h (sol)	0.252566	-1049.619810	-1049.521275	-1048.792777
1p (sol)	0.293183	-1241.098107	-1241.006345	-1240.124622
TS1-1p (sol)	0.295991	-1241.076186	-1240.982547	-1240.096798
IN1-1p (sol)	0.299935	-1241.101535	-1241.014906	-1240.128092
TS4-1p (sol)	0.298516	-1241.094754	-1241.001149	-1240.108679
IN2-1p (sol)	0.298351	-1241.096360	-1241.000391	-1240.109478
TS2-1p (sol)	0.298460	-1241.095607	-1241.000325	-1240.110496
NP-1p (sol)	0.303541	-1241.170627	-1241.081630	-1240.186561
TS3-1p (sol)	0.299630	-1241.099889	-1241.012337	-1240.123485
CP-1p (sol)	0.303645	-1241.159737	-1241.071352	-1240.179530
TS5-1p (sol)	0.300099	-1241.098618	-1241.010784	-1240.125942
IN3-1p (sol)	0.299688	-1241.106975	-1241.023133	-1240.136022
TS6-1p (sol)	0.299639	-1241.105998	-1241.021785	-1240.134418
IN-1m (sol)	0.297078	-1241.113857	-1241.026719	-1240.137172

[a]Computed at the SMD(DCE)/ωB97X-D/def2-SVP level.

[b]A standard state at 1 atm and 298.15 K was used.

[c]Computed at the ωB97X-D/def2-SVP//SMD(DCE)/ωB97X-D/def2-SVP level.

[d]Computed at the DLPNO-CCSD(T)/cc-pVTZ//SMD(DCE)/ωB97X-D/def2-SVP level.

Table S10. Single-Point Energies (SPEs) Calculated by Different Methods[a]

Stationary point	CCSD(T)	ωB97X-D	M06-2X	B3LYP	B3LYP-D3BJ
1f	-406.279628	-407.038356	-406.972901	-407.180466	-407.219937
TS1-1f	-406.269062	-407.028720	-406.963803	-407.167564	-407.213491
NP-1f	-406.347963	-407.110502	-407.039086	-407.233229	-407.277401
TS2-1f	-406.278222	-407.039553	-406.974490	-407.167490	-407.212592
CP-1f	-406.342711	-407.103000	-407.033118	-407.225428	-407.270031
Stationary point	BMK	M06	M06-D3	PBE0	PBE0-D3BJ
1f	-406.863192	-406.836969	-406.840395	-406.662435	-406.683336
TS1-1f	-406.851296	-406.828794	-406.832566	-406.655479	-406.679736
NP-1f	-406.941161	-406.903361	-406.906711	-406.737022	-406.760144
TS2-1f	-406.865384	-406.840666	-406.844229	-406.668843	-406.692470
CP-1f	-406.934331	-406.895944	-406.899459	-406.730167	-406.753564

[a]Computed at Method/cc-pVTZ//ωB97X-D/def2-SVP level. The unit is a.u..

S7. Cartesian Coordinates of the Stationary Points

1a

C	-2.146294	-0.527069	1.076833
H	-2.416818	-1.592858	1.108807
H	-2.272234	-0.135207	2.101058
C	-3.048467	0.222607	0.121237
C	0.763193	-0.892273	-1.046376
C	-3.936811	-0.429914	-0.632109
C	1.828201	-0.319184	-0.509779
H	-4.034393	-1.517942	-0.590266
H	0.893871	-1.339874	-2.040633
H	-4.608820	0.102648	-1.309831
C	-0.671406	-0.412865	0.748696
O	-0.439324	-0.984211	-0.548613
H	-0.337296	0.641112	0.722232
H	-0.054524	-0.962905	1.481089
N	2.901203	0.167689	-0.071478
C	3.281983	1.573867	-0.313784
H	3.396106	2.078546	0.654993
H	4.241467	1.588955	-0.848004
H	2.505527	2.062512	-0.911085
C	3.860389	-0.627674	0.721624
H	3.981495	-0.153222	1.704702
H	3.481077	-1.648491	0.833296
H	4.825903	-0.633524	0.198187
C	-2.900911	1.720404	0.089416
H	-1.907841	2.028286	-0.281069
H	-3.649965	2.183134	-0.566229
H	-3.016642	2.151291	1.097460

TS1-1a

C	-2.271992	0.532667	-0.120403
H	-2.390345	0.610670	-1.212920
H	-3.136951	1.064744	0.310841
C	-1.008652	1.236762	0.318420
C	-0.211674	-1.650218	-0.565481
C	-0.377228	0.921523	1.468149
C	0.696530	-0.781939	-0.137300
H	-0.751917	0.173561	2.169289
H	0.499762	1.488481	1.791974
H	0.249975	-2.479419	-1.121982
C	-2.368883	-0.925173	0.280272
O	-1.510352	-1.778046	-0.482890
N	1.900258	-0.358794	-0.103664
C	2.442961	0.532204	-1.135433
H	2.590188	1.536871	-0.712954
H	3.413052	0.139569	-1.469971
H	1.747940	0.580849	-1.980049
C	2.754036	-0.583161	1.067339
H	3.734658	-0.947064	0.731774
H	2.889026	0.366378	1.607342
H	2.285913	-1.322338	1.725839
H	-2.163088	-1.086100	1.349135
H	-3.370453	-1.316690	0.070983
C	-0.558798	2.368763	-0.557220
H	0.350701	2.855667	-0.181127
H	-0.392007	2.030961	-1.592327
H	-1.353253	3.131219	-0.607141

IN-1a

C	-2.059619	0.678363	-0.333017
H	-2.070026	0.796209	-1.427758
H	-2.800944	1.385350	0.071039
C	-0.688379	1.041099	0.199351
C	-0.255623	-1.414803	-0.249725
C	-0.261208	0.497036	1.480599
C	0.343334	-0.223564	0.239277
H	-0.934772	-0.076199	2.119464
H	0.521254	1.035837	2.019764
H	0.381025	-2.196491	-0.684999
C	-2.503858	-0.720027	0.042813
O	-1.495500	-1.687980	-0.346928
N	1.711349	-0.011279	-0.018342
C	2.126376	-0.052350	-1.410934
H	3.088675	0.467426	-1.521742
H	2.260211	-1.079693	-1.805055
H	1.390676	0.470366	-2.038413
C	2.641336	-0.630908	0.910163
H	2.718680	-1.729034	0.777153
H	3.643173	-0.203904	0.764241
H	2.340506	-0.432640	1.948351
C	-0.103341	2.330311	-0.316007
H	0.947684	2.434994	-0.021976
H	-0.179473	2.393059	-1.410620
H	-0.672784	3.169466	0.111713

H	-3.406505	-1.033172	-0.491777
H	-2.676924	-0.849733	1.119310

TS2-1a

C	2.267087	0.686440	0.229968
H	2.609937	0.650443	1.274089
H	2.808934	1.502585	-0.277872
C	0.800624	0.978996	0.167653
C	0.387426	-1.205868	0.261869
C	0.137038	0.813491	-1.160507
C	-0.491064	-0.356699	-0.450689
H	0.783498	0.582802	-2.010521
H	-0.579696	1.595672	-1.422110
H	-0.047876	-1.841843	1.036638
C	2.559339	-0.626820	-0.484836
O	1.636669	-1.568736	0.034513
N	-1.799159	-0.296679	-0.124456
C	-2.337313	-1.058805	0.995451
H	-3.379213	-0.762463	1.157769
H	-2.317599	-2.144165	0.805331
H	-1.784117	-0.845124	1.923505
C	-2.745661	0.470277	-0.931223
H	-3.703463	-0.064440	-0.951676
H	-2.922050	1.480075	-0.525355
H	-2.404676	0.548939	-1.970017
H	3.560276	-1.013984	-0.263776
H	2.458401	-0.546462	-1.577263
C	0.160065	1.839085	1.205764
H	-0.934174	1.726731	1.205915
H	0.548881	1.620402	2.209026
H	0.378456	2.896894	0.980701

NP-1a

C	2.007266	0.448537	0.968594
H	3.011001	0.762257	0.649020
H	2.095192	0.033132	1.982147
C	1.454494	-0.562376	-0.052755
C	0.458235	0.339942	-0.859549
C	0.249309	-1.422529	0.458185
C	-0.669116	-0.441108	-0.188417
H	0.123443	-1.534406	1.547135
H	0.195590	-2.423309	-0.001887
H	0.468579	0.266972	-1.958325
C	1.044690	1.638004	0.897301
O	0.566319	1.653767	-0.447497
N	-1.922892	-0.198746	-0.075136
C	-2.543150	0.952943	-0.742329
H	-3.170210	1.480776	-0.012038
H	-1.766482	1.631375	-1.110187
H	-3.175165	0.594115	-1.566339
C	-2.814309	-1.044643	0.720213
H	-3.205802	-0.461800	1.565461
H	-3.653285	-1.365050	0.087936
H	-2.277023	-1.924554	1.088650
C	2.513047	-1.321642	-0.830503
H	3.108534	-1.955361	-0.156536
H	2.063634	-1.970685	-1.597154
H	3.198090	-0.623623	-1.333085
H	1.515588	2.607445	1.098386
H	0.195209	1.521032	1.598313

TS3-1a

C	-2.010308	0.816900	-0.282111
H	-2.144842	1.578570	-1.064128
H	-2.745175	1.034584	0.506875
C	-0.600664	0.932339	0.312016
C	-0.375780	-1.455811	0.151404
C	-0.395112	0.057164	1.523552
C	0.323865	-0.227646	-0.018828
H	-1.257250	-0.451475	1.962347
H	0.437474	0.274818	2.197903
H	0.132009	-2.379703	0.445472
C	-2.247479	-0.549042	-0.904355
O	-1.641683	-1.602593	-0.121885
H	-1.800137	-0.607056	-1.908973
H	-3.308310	-0.809998	-0.971955
N	1.685199	-0.111767	-0.086264
C	2.498457	-1.249128	0.300139
H	3.545699	-0.928354	0.369493
H	2.202957	-1.617708	1.294471
H	2.446081	-2.083145	-0.425145
C	2.263974	0.751747	-1.112221
H	3.133503	1.291124	-0.709914
H	2.588897	0.159233	-1.984248
H	1.531570	1.486564	-1.461192
C	-0.058733	2.343939	0.381453
H	-0.026257	2.810463	-0.612871
H	-0.732524	2.945991	1.007881

H	0.944053	2.376442	0.826613

CP-1a

C	-1.452286	0.565114	-1.075792
H	-0.800899	0.678007	-1.956967
H	-2.273389	1.289539	-1.188283
C	-0.647924	0.939751	0.208037
C	-0.526265	-1.102557	0.847906
C	-1.264472	0.139362	1.400621
C	0.449117	-0.097686	0.254393
H	-2.357945	0.098791	1.477774
H	-0.840566	0.450175	2.365879
H	-0.166760	-1.873561	1.541178
C	-2.023062	-0.856255	-0.964738
O	-1.164346	-1.722078	-0.231510
N	1.692873	-0.164304	-0.052774
C	2.467051	-1.397159	0.134231
H	3.257840	-1.218592	0.875532
H	1.815792	-2.211309	0.464902
H	2.926929	-1.669883	-0.824767
C	2.435958	0.950990	-0.645785
H	3.302932	1.180470	-0.011807
H	2.790205	0.649346	-1.640853
H	1.797993	1.833148	-0.732392
C	-0.396993	2.427806	0.355799
H	-0.038627	2.887033	-0.577333
H	-1.347048	2.918878	0.611408
H	0.317986	2.644202	1.162706
H	-2.154508	-1.313794	-1.952883
H	-3.012022	-0.831897	-0.480626

1b

C	2.469482	0.596438	0.931677
H	2.851050	1.526595	0.482830
H	2.562651	0.708788	2.024995
C	3.263078	-0.590576	0.461505
C	-0.398015	0.276578	-1.255167
C	4.223172	-0.540208	-0.459097
C	-1.507496	0.049147	-0.571389
H	4.502803	0.399392	-0.945477
H	3.018511	-1.551481	0.931576
H	-0.489474	0.288132	-2.349480
H	4.776344	-1.435067	-0.752735
C	0.989575	0.478497	0.628798
O	0.805947	0.481942	-0.795676
H	0.572655	-0.466588	1.025900
H	0.420377	1.326381	1.049107
N	-2.616021	-0.152308	-0.013745
C	-3.093876	-1.510336	0.316097
H	-3.250386	-1.573310	1.401365
H	-4.048242	-1.679723	-0.200338
H	-2.349886	-2.245564	-0.006950
C	-3.522911	0.953067	0.356842
H	-3.685950	0.924271	1.442571
H	-3.072927	1.906587	0.062346
H	-4.481018	0.806561	-0.159679

TS1-1b

C	2.136203	0.775624	0.703116
H	2.109407	0.371075	1.726201
H	2.940936	1.529914	0.699490
C	0.833776	1.446870	0.370380
C	0.385234	-1.475130	-0.090411
C	0.366235	1.650242	-0.877160
C	-0.568465	-0.546029	-0.120031
H	0.912713	1.351547	-1.774921
H	-0.562433	2.201723	-1.041480
H	0.260867	1.845936	1.214956
H	-0.028900	-2.490338	-0.008052
C	2.517271	-0.324378	-0.268700
O	1.690408	-1.485086	-0.153946
N	-1.807843	-0.270447	0.058078
C	-2.355526	-0.020472	1.394945
H	-2.531092	1.058432	1.526942
H	-3.312133	-0.550827	1.496991
H	-1.650810	-0.378745	2.153106
C	-2.693176	0.028021	-1.070321
H	-3.620176	-0.552113	-0.964172
H	-2.943277	1.100290	-1.070913
H	-2.194825	-0.239309	-2.008189
H	2.496203	0.016163	-1.314939
H	3.525855	-0.698418	-0.060900

IN-1b

C	-1.874622	0.926240	-0.745309
H	-1.850878	0.640767	-1.807741
H	-2.471429	1.848000	-0.672001
C	-0.468928	1.177643	-0.256538

C	-0.487603	-1.280832	0.228171
C	-0.111505	1.079416	1.150915
C	0.326933	-0.101680	0.224402
H	-0.860684	0.870833	1.917435
H	0.747831	1.647075	1.512277
H	0.154169	1.810919	-0.893595
H	0.008255	-2.260423	0.204028
C	-2.576090	-0.142887	0.069325
O	-1.752405	-1.341143	0.170182
N	1.677647	-0.338582	-0.094948
C	2.063636	-0.146127	-1.481576
H	2.241818	0.916293	-1.741872
H	2.991527	-0.698755	-1.685124
H	1.289499	-0.542610	-2.154494
C	2.693365	-0.010671	0.887547
H	3.614662	-0.560955	0.650936
H	2.948787	1.067400	0.914883
H	2.372481	-0.324031	1.890519
H	-2.795989	0.169416	1.098893
H	-3.505451	-0.491323	-0.392580
H	3.589893	-0.602195	-0.413027
H	2.520426	0.473627	-1.341891

TS2-1b

C	2.230061	0.594471	0.833358
H	2.523567	0.024855	1.725783
H	2.777247	1.552535	0.843712
C	0.766640	0.867889	0.828000
C	0.408890	-1.075437	-0.219779
C	0.131213	1.403989	-0.399445
C	-0.473726	0.025068	-0.363652
H	0.793519	1.630152	-1.238558
H	-0.601546	2.199769	-0.252236
H	0.218602	0.956018	1.769584
H	-0.032020	-2.031079	0.076803
C	2.588269	-0.159818	-0.445762
O	1.673314	-1.241818	-0.530414
N	-1.786120	-0.113862	-0.072521
C	-2.296906	-1.318522	0.567692
H	-3.329879	-1.140920	0.886077
H	-2.298417	-2.185134	-0.113037
H	-1.711764	-1.567571	1.467902
C	-2.739589	0.954484	-0.355599
H	-3.710134	0.502945	-0.595271
H	-2.877859	1.633693	0.502465
H	-2.434418	1.532152	-1.236232

NP-1b

C	-2.389975	0.392616	0.541836
H	-3.390358	0.186324	0.137558
H	-2.505825	1.094767	1.378902
C	-1.496969	0.929234	-0.581684
C	-0.660667	-0.332837	-0.962756
C	-0.193874	1.678021	-0.171796
C	0.546851	0.395369	-0.370391
H	-0.143172	2.096752	0.846174
H	0.113028	2.460674	-0.884420
H	-2.057278	1.408628	-1.391606
H	-0.552571	-0.593183	-2.026674
C	-1.712011	-0.918203	0.959129
O	-1.094999	-1.418121	-0.227507
N	1.700225	-0.025557	-0.003308
C	2.110987	-1.418748	-0.221322
H	2.880460	-1.448039	-1.005040
H	2.535470	-1.805563	0.714230
H	1.241687	-2.022483	-0.501796
C	2.678551	0.844582	0.651875
H	2.855106	0.482627	1.674198
H	3.620834	0.801157	0.089282
H	2.314832	1.876935	0.677197
H	-0.945443	-0.750852	1.740493
H	-2.405717	-1.684078	1.325376

TS3-1b

C	-1.839198	1.143887	-0.545461
H	-1.657422	1.300613	-1.618241
H	-2.476352	1.970762	-0.201590
C	-0.493323	1.174852	0.165045
C	-0.429290	-1.202563	0.063340
C	-0.342974	0.411853	1.449870
C	0.346991	-0.023327	-0.107624
H	-1.209977	-0.028392	1.949824
H	0.500950	0.646689	2.103150
H	0.021079	2.136486	0.112165
H	0.044039	-2.171524	0.247085
C	-2.576201	-0.165354	-0.295233
O	-1.709208	-1.310120	-0.126778
N	1.690444	-0.032877	-0.314411

C	2.419680	-1.278155	-0.137350
H	3.460238	-1.129532	-0.446252
H	2.419150	-1.622792	0.913369
H	2.004013	-2.072206	-0.775822
C	2.444101	1.209975	-0.238243
H	2.592622	1.561672	0.798734
H	3.432418	1.046940	-0.683941
H	1.955659	1.999562	-0.822630
H	-3.170144	-0.125118	0.628534
H	-3.254439	-0.429071	-1.115353

CP-1b

C	-1.666470	1.181945	-0.571386
H	-1.402910	1.935510	-1.327625
H	-2.612325	1.495841	-0.106993
C	-0.591158	1.122601	0.539618
C	-0.626576	-1.023992	0.632860
C	-1.080397	0.096337	1.609809
C	0.379074	0.037688	0.186360
H	-2.156910	0.102520	1.826185
H	-0.493908	0.120158	2.537845
H	-0.222540	2.108182	0.849976
H	-0.264272	-1.978654	1.035072
C	-1.779840	-0.192225	-1.245005
O	-1.586314	-1.269398	-0.340258
H	-1.017471	-0.267421	-2.044727
H	-2.761477	-0.339572	-1.710404
N	1.634837	0.004030	-0.079748
C	2.364777	-1.259439	-0.233452
H	2.877367	-1.252605	-1.204348
H	3.112193	-1.345301	0.567212
H	1.672912	-2.106290	-0.194846
C	2.433165	1.220653	-0.257560
H	3.240301	1.231453	0.487577
H	2.873767	1.212277	-1.263496
H	1.806483	2.109462	-0.138589

1c

C	2.100229	1.014240	0.256246
H	2.497813	1.137656	-0.760981
H	2.173463	1.994289	0.753643
C	2.866007	-0.020784	1.037291
C	-1.370227	1.507071	-0.679868
C	3.698776	-0.940766	0.537571
C	-2.110164	0.475491	-0.307882
H	2.711979	-0.004367	2.122121
H	-1.887890	2.325213	-1.197865
H	4.178239	-1.614702	1.256490
C	0.636446	0.632951	0.165226
O	-0.086826	1.677102	-0.508524
H	0.506557	-0.304170	-0.406512
H	0.192542	0.500254	1.169284
N	-2.890201	-0.456651	0.012443
C	-3.157315	-1.600471	-0.882820
H	-2.854330	-2.523944	-0.371322
H	-4.234813	-1.635940	-1.092394
H	-2.591927	-1.474424	-1.811705
C	-3.592952	-0.482232	1.311236
H	-3.296081	-1.390622	1.852472
H	-3.326095	0.410237	1.886283
H	-4.674642	-0.506760	1.122751
C	4.083357	-1.158208	-0.892461
H	3.575441	-0.480129	-1.591758
H	5.169017	-1.023434	-1.019513
H	3.861801	-2.193163	-1.197138

TS1-1c

C	2.041066	-0.168578	1.048614
H	2.071937	-0.958209	1.812227
H	2.875103	0.516341	1.274764
C	0.730989	0.570836	1.118705
C	0.085359	-1.586086	-0.669315
C	0.409118	1.658590	0.369007
C	-0.691188	-0.581842	-0.260871
H	-0.569300	2.113533	0.561499
H	0.056275	0.301912	1.937283
H	-0.475620	-2.421709	-1.109157
C	2.309155	-0.783219	-0.318253
O	1.377314	-1.799002	-0.668894
N	-1.929210	-0.253075	-0.086442
C	-2.643075	-0.593208	1.145316
H	-2.720203	0.292920	1.795684
H	-3.657082	-0.933324	0.893643
H	-2.109512	-1.393089	1.670706
C	-2.600233	0.681281	-0.988510
H	-3.591472	0.285484	-1.250131
H	-2.731625	1.657646	-0.494607
H	-2.003518	0.804820	-1.898893

H	2.296937	-0.023773	-1.114686
H	3.282981	-1.285287	-0.336507
C	1.254935	2.375842	-0.628082
H	1.186181	3.458291	-0.442004
H	2.313359	2.089644	-0.589262
H	0.884751	2.216648	-1.653971

IN-1c

C	-2.003725	-0.349747	-0.993810
H	-2.323188	-0.871640	-1.906650
H	-2.728748	0.461089	-0.835698
C	-0.605345	0.224172	-1.201060
C	-0.112702	-0.482787	1.162383
C	-0.230177	1.455653	-0.477340
C	0.402845	0.079029	-0.050860
H	0.569856	2.030974	-0.953962
H	-0.143530	0.073888	-2.179284
H	0.504728	-0.520265	2.071491
C	-2.082502	-1.354470	0.136039
O	-1.253152	-1.008868	1.305627
H	-1.710546	-2.348219	-0.152026
H	-3.089158	-1.460531	0.551933
N	1.783728	-0.090483	-0.310435
C	2.707811	0.711150	0.470672
H	2.831057	0.358134	1.514644
H	3.699393	0.685780	-0.002313
H	2.376736	1.758911	0.497298
C	2.208526	-1.457896	-0.561488
H	3.186843	-1.449346	-1.062486
H	2.308873	-2.070552	0.357031
H	1.494919	-1.951319	-1.237694
C	-1.157642	2.263146	0.390386
H	-1.872420	1.654595	0.961893
H	-0.587863	2.877773	1.100397
H	-1.740357	2.945556	-0.246088

TS2-1c

C	2.125614	-0.160298	1.130445
H	2.293376	-0.994376	1.825590
H	2.745331	0.687990	1.467791
C	0.693570	0.246348	1.152830
C	0.236167	-1.163115	-0.493389
C	0.115688	1.249908	0.213266
C	-0.566437	-0.018308	-0.253745
H	-0.616788	1.867015	0.741828
H	0.114969	0.052403	2.060193
H	-0.294082	-2.117502	-0.564544
C	2.539891	-0.532126	-0.290747
O	1.496633	-1.335158	-0.825427
N	-1.896610	-0.162234	-0.052226
C	-2.511182	-1.471834	0.112090
H	-3.537751	-1.339129	0.471412
H	-2.554901	-2.037504	-0.832844
H	-1.973312	-2.070028	0.865302
C	-2.773345	1.001277	0.022862
H	-3.741571	0.741303	-0.423517
H	-2.949036	1.330235	1.061047
H	-2.370114	1.836614	-0.562238
C	0.922518	2.113404	-0.747450
H	0.272251	2.902268	-1.148409
H	1.314400	1.557570	-1.606763
H	1.755138	2.607121	-0.226684
H	3.445442	-1.149108	-0.317948
H	2.704950	0.350489	-0.918194

NP-1c

C	-2.400001	0.159336	0.342261
H	-3.376268	-0.180630	-0.029296
H	-2.578968	1.026254	0.992196
C	-1.493286	0.459165	-0.856103
C	-0.603682	-0.816810	-0.916837
C	-0.223560	1.349530	-0.626481
C	0.564369	0.073489	-0.498870
H	0.054390	1.839765	-1.576858
H	-2.053463	0.711718	-1.763043
H	-0.459502	-1.315794	-1.887158
C	-1.688483	-0.986914	1.068453
O	-1.016655	-1.720477	0.045484
N	1.726617	-0.229133	-0.049558
C	2.152282	-1.629974	0.079955
H	2.897477	-1.852496	-0.696264
H	2.612628	-1.760290	1.068068
H	1.284546	-2.291982	-0.006006
C	2.711866	0.776801	0.354703
H	2.787747	0.795577	1.450837
H	3.685594	0.495610	-0.066842
H	2.425788	1.763292	-0.020509
C	-0.220736	2.366634	0.509131

H	0.685638	2.986210	0.514886
H	-0.317884	1.883551	1.492209
H	-1.076179	3.044180	0.379972
H	-2.364114	-1.676377	1.588291
H	-0.953113	-0.608367	1.805272

TS3-1c

C	-1.685504	-1.281515	-0.593484
H	-1.608445	-2.349361	-0.840539
H	-2.539596	-0.887158	-1.161913
C	-0.412455	-0.557193	-1.025186
C	-0.221030	0.463835	1.151999
C	-0.474941	0.934694	-1.036463
C	0.505815	-0.099755	0.083891
H	0.364838	1.423261	-1.539479
H	0.107831	-1.010913	-1.872954
H	0.205276	1.197458	1.842904
C	-1.905528	-1.153868	0.908120
O	-1.444543	0.116330	1.434141
H	-1.346730	-1.928322	1.455430
H	-2.961146	-1.212793	1.192108
N	1.857230	-0.008977	-0.078252
C	2.598457	0.895485	0.779296
H	3.627882	0.976417	0.409002
H	2.158884	1.904730	0.749176
H	2.641244	0.553057	1.830187
C	2.600052	-1.131884	-0.634994
H	3.459719	-0.759424	-1.209150
H	2.970761	-1.806210	0.155779
H	1.972820	-1.720411	-1.314976
C	-1.726495	1.744667	-0.932554
H	-1.498965	2.802241	-0.748976
H	-2.429918	1.389701	-0.168672
H	-2.238943	1.673128	-1.907043

CP-1c

C	-1.211515	-0.597814	1.471974
H	-0.764736	-0.975730	2.403004
H	-2.230415	-1.004045	1.414160
C	-0.413932	-1.106207	0.251820
C	-0.444886	0.797014	-0.745916
C	-1.101332	-0.586339	-1.064725
C	0.616126	-0.075645	-0.085105
H	-0.598725	-1.036271	-1.935228
H	-0.125801	-2.162422	0.327737
H	-0.166365	1.464378	-1.571842
C	-1.191973	0.937550	1.489301
O	-1.185432	1.510057	0.188233
H	-0.285524	1.282682	2.023282
H	-2.061315	1.352854	2.012982
N	1.900492	-0.063757	-0.107248
C	2.661092	1.064612	-0.654975
H	3.218380	0.729543	-1.540553
H	1.987383	1.884106	-0.922719
H	3.371917	1.411981	0.106318
C	2.705274	-1.170550	0.417759
H	3.328924	-1.575322	-0.390998
H	3.356374	-0.789441	1.215866
H	2.058223	-1.957408	0.816414
C	-2.607220	-0.643937	-1.225424
H	-2.887502	-0.262821	-2.217076
H	-3.123860	-0.028623	-0.477807
H	-2.966739	-1.679716	-1.146930

1d

C	1.836812	-1.323515	-0.695614
H	2.150563	-2.056817	0.063634
H	1.851004	-1.847797	-1.666109
C	2.768072	-0.144701	-0.719093
C	-0.852265	0.106432	1.261167
C	3.749782	0.059131	0.161849
C	-1.966556	0.198335	0.553482
H	3.894469	-0.679893	0.960851
H	2.614831	0.581124	-1.528922
H	-0.884413	0.508725	2.282484
C	0.395291	-0.938224	-0.430574
O	0.294927	-0.395519	0.896277
H	0.050137	-0.164856	-1.142990
H	-0.278849	-1.810887	-0.492907
N	-3.076068	0.308767	-0.027320
C	-3.424674	1.494722	-0.835432
H	-3.632153	1.170007	-1.863916
H	-4.326294	1.955100	-0.409563
H	-2.590414	2.203353	-0.818669
C	-4.112784	-0.740335	0.049851
H	-4.329005	-1.095645	-0.966628
H	-3.750856	-1.563554	0.674126
H	-5.021556	-0.302136	0.483854

C	4.698375	1.214785	0.150140
H	5.736850	0.863366	0.044972
H	4.486397	1.911540	-0.673236
H	4.650026	1.771367	1.099386

TS1-1d

C	2.206058	0.597447	0.814003
H	2.315598	-0.015194	1.721225
H	2.935517	1.417879	0.915267
C	0.814717	1.171313	0.724952
C	0.672953	-1.681646	-0.300353
C	0.306392	1.772350	-0.369199
C	-0.382576	-0.898079	-0.113414
H	0.911931	1.823517	-1.282122
H	0.231131	1.197529	1.653286
H	0.387387	-2.741761	-0.369780
C	2.603777	-0.232693	-0.392160
O	1.961725	-1.509798	-0.423581
N	-1.636240	-0.751018	0.075187
C	-2.217838	-0.742150	1.422350
H	-2.591987	0.265699	1.654570
H	-3.058003	-1.449990	1.452660
H	-1.456643	-1.036794	2.152463
C	-2.576162	-0.540593	-1.034712
H	-3.219437	-1.428233	-1.124513
H	-3.203738	0.335663	-0.826072
H	-2.017254	-0.393222	-1.964795
H	2.394905	0.283904	-1.342057
H	3.671206	-0.478494	-0.368770
C	-1.010108	2.472333	-0.427228
H	-1.579185	2.196138	-1.326858
H	-1.621080	2.289223	0.468531
H	-0.843757	3.559954	-0.496135

IN-1d

C	2.050911	0.166138	1.063798
H	2.051516	-0.660249	1.790402
H	2.712467	0.949149	1.463419
C	0.644428	0.698195	0.908817
C	0.449953	-1.082783	-0.828267
C	0.213495	1.418357	-0.283491
C	-0.259441	-0.104262	-0.077120
H	0.105666	0.918812	1.835180
H	-0.096239	-1.889948	-1.335173
C	2.632264	-0.300747	-0.256770
O	1.710054	-1.186673	-0.957065
N	-1.611789	-0.342925	0.244047
C	-1.840796	-1.368335	1.248652
H	-2.874454	-1.296338	1.614794
H	-1.690296	-2.399361	0.868360
H	-1.172649	-1.214164	2.108049
C	-2.540314	-0.373646	-0.873426
H	-2.492395	-1.313836	-1.460277
H	-3.568551	-0.274476	-0.498369
H	-2.347482	0.468216	-1.551642
H	0.938665	1.539824	-1.093640
C	-0.854589	2.475477	-0.240418
H	-1.642072	2.219129	0.478987
H	-0.388370	3.422319	0.070882
H	-1.302928	2.633612	-1.229979
H	3.540064	-0.900848	-0.133990
H	2.853691	0.521657	-0.949453

TS2-1d

C	2.299870	0.412234	0.851608
H	2.639280	-0.212130	1.689594
H	2.764722	1.406885	0.955125
C	0.813330	0.568774	0.869315
C	0.565951	-1.230037	-0.279873
C	0.131709	1.217927	-0.289423
C	-0.410632	-0.202532	-0.335877
H	0.276721	0.567475	1.822958
H	0.207543	-2.225416	-0.000276
C	2.698332	-0.196641	-0.487626
O	1.819655	-1.298108	-0.677947
N	-1.687579	-0.469297	0.030101
C	-2.053509	-1.711098	0.694254
H	-3.046674	-1.583833	1.143228
H	-2.100652	-2.570412	0.003257
H	-1.351470	-1.939071	1.509782
C	-2.806234	0.277056	-0.543003
H	-3.373994	0.819240	0.227881
H	-2.460203	0.982373	-1.303860
H	-3.483388	-0.430794	-1.043956
H	0.815133	1.427603	-1.118522
C	-0.753313	2.415082	0.002552
H	-1.299154	2.751699	-0.887311
H	-1.467567	2.216299	0.811499

H	-0.105686	3.243793	0.321023
H	3.715339	-0.604543	-0.488770
H	2.612836	0.516175	-1.320350

NP-1d

C	-2.393447	0.099418	0.684279
H	-3.406898	0.058618	0.262457
H	-2.459648	0.585007	1.667764
C	-1.470750	0.834520	-0.293207
C	-0.707853	-0.344864	-0.970687
C	-0.126008	1.408975	0.255106
C	0.531699	0.147994	-0.227470
H	-2.004087	1.519915	-0.962742
H	-0.608418	-0.347216	-2.066655
C	-1.800345	-1.313200	0.763435
O	-1.210846	-1.548337	-0.515187
N	1.642477	-0.431000	0.046487
C	1.966856	-1.759655	-0.488528
H	2.765532	-1.660034	-1.236435
H	2.323714	-2.389602	0.336659
H	1.071972	-2.211965	-0.927989
C	2.656100	0.183947	0.905236
H	2.819372	-0.456902	1.782413
H	3.595832	0.265422	0.342253
H	2.332643	1.179015	1.226077
H	-0.082464	1.507533	1.353891
C	0.349637	2.699426	-0.415989
H	1.365725	2.975240	-0.101106
H	0.338201	2.608948	-1.511911
H	-0.327464	3.518019	-0.136530
H	-1.028098	-1.386675	1.553592
H	-2.541820	-2.100990	0.941298

TS3-1d

C	2.046636	0.195851	1.139578
H	2.178574	-0.181859	2.163366
H	2.696686	1.076063	1.033490
C	0.597732	0.621596	0.913789
C	0.502449	-0.630465	-1.130969
C	0.332506	1.396903	-0.337134
C	-0.233305	-0.265476	0.020832
H	0.072462	0.983043	1.802406
H	0.031108	-0.897122	-2.081826
C	2.437626	-0.905313	0.164296
O	1.802339	-0.743421	-1.127491
H	2.125893	-1.892289	0.539249
H	3.511549	-0.929147	-0.045460
N	-1.575723	-0.442624	0.182238
C	-2.358195	-0.874479	-0.960557
H	-3.423768	-0.817918	-0.706470
H	-2.190604	-0.207535	-1.820265
H	-2.134941	-1.914766	-1.262843
C	-2.114911	-0.760006	1.498238
H	-3.114356	-0.316252	1.607658
H	-2.195520	-1.849702	1.651113
H	-1.477506	-0.352302	2.291513
H	1.188496	1.541631	-1.002572
C	-0.788537	2.369494	-0.466767
H	-1.038867	2.559111	-1.518851
H	-1.684602	2.030018	0.070232
H	-0.465269	3.326123	-0.024315

CP-1d

C	1.604132	-0.864269	1.229900
H	1.307152	-1.550867	2.036023
H	2.572128	-0.424256	1.509485
C	0.582340	0.287122	1.088731
C	0.616548	0.223737	-1.058020
C	1.116618	1.270400	-0.012527
C	-0.404415	-0.094045	0.031662
H	0.229648	0.688460	2.047832
H	0.270654	0.575800	-2.039316
C	1.682017	-1.640267	-0.091602
O	1.530434	-0.806816	-1.230838
H	0.882145	-2.405984	-0.109621
H	2.640000	-2.161431	-0.203936
N	-1.674593	-0.285045	0.016003
C	-2.417524	-0.480377	-1.233430
H	-2.991479	-1.413403	-1.159333
H	-3.112476	0.358567	-1.376276
H	-1.727949	-0.545390	-2.080438
C	-2.477722	-0.324604	1.241210
H	-3.234170	0.471007	1.199733
H	-2.983757	-1.297292	1.303824
H	-1.840990	-0.185104	2.119752
H	2.212960	1.353768	-0.021404
C	0.439696	2.627058	-0.069347
H	0.755900	3.178152	-0.966119

H	-0.659894	2.549455	-0.094188
H	0.708668	3.229826	0.809212

TS4-1d

C	2.031013	0.675285	0.859686
H	2.112899	0.197143	1.846886
H	2.592870	1.618215	0.909239
C	0.555870	0.944812	0.576050
C	0.622251	-1.422419	-0.247199
C	0.195550	1.670792	-0.648186
C	-0.141995	-0.366894	0.147552
H	0.060639	1.363280	1.464926
H	0.178555	-2.395701	-0.475426
C	2.652798	-0.226185	-0.190604
O	1.929030	-1.448362	-0.339521
N	-1.547431	-0.364591	0.094596
C	-2.248493	-0.282380	1.383630
H	-3.297389	-0.009128	1.207617
H	-2.209386	-1.246737	1.913499
H	-1.792045	0.486166	2.019570
C	-2.187902	-1.285336	-0.850355
H	-2.138787	-2.329145	-0.499903
H	-3.245200	-1.009901	-0.953175
H	-1.702242	-1.204289	-1.831591
H	0.870394	1.606095	-1.509432
C	-1.113671	2.143643	-0.806161
H	-1.618592	1.010863	-0.576606
H	-1.565499	2.638879	0.066345
H	-1.404342	2.567414	-1.771145
H	3.674384	-0.517072	0.078580
H	2.690992	0.255037	-1.181867

FC-1d

C	2.023974	0.463398	0.766511
H	2.101958	0.044534	1.781238
H	2.660794	1.358410	0.735677
C	0.559024	0.840110	0.485814
C	0.428294	-1.583340	-0.194509
C	0.359239	1.900687	-0.570115
C	-0.176512	-0.414744	0.080937
H	0.127264	1.218567	1.429991
H	-0.108140	-2.508239	-0.422747
C	2.533858	-0.561637	-0.230025
O	1.739235	-1.749289	-0.217860
N	-1.640462	-0.263028	-0.001627
C	-2.315949	-0.431156	1.321362
H	-3.373828	-0.156433	1.226301
H	-2.218512	-1.479589	1.626342
H	-1.825587	0.214484	2.057935
C	-2.309376	-1.065687	-1.065422
H	-2.284823	-2.126607	-0.792571
H	-3.353071	-0.739136	-1.145615
H	-1.783448	-0.904242	-2.012882
H	0.883158	1.745026	-1.521151
C	-0.442750	2.958911	-0.422803
H	-1.755014	0.726637	-0.281358
H	-0.957438	3.161793	0.523521
H	-0.580145	3.688199	-1.224421
H	2.522693	-0.162852	-1.259209
H	3.554672	-0.884288	0.002712

1e

C	-1.467373	-0.786243	-0.428670
H	-1.269054	-0.501216	-1.474756
H	-1.129679	-1.837225	-0.353607
C	-2.954641	-0.718762	-0.153936
C	0.974529	-1.283893	1.799431
C	-3.483563	0.122685	0.737644
C	1.852130	-1.195727	0.849401
H	-2.863329	0.805795	1.323255
H	1.169185	-1.936004	2.658093
N	2.620400	-1.011518	-0.124068
C	-0.294416	-0.435744	1.751778
H	-0.149037	0.401191	2.451867
H	-1.134593	-1.035348	2.132145
C	3.611654	0.082728	-0.126104
H	3.349012	0.753842	-0.954478
H	3.549784	0.628960	0.819830
H	4.608523	-0.351049	-0.277186
C	2.484081	-1.779188	-1.375090
H	2.079004	-1.090102	-2.129176
H	3.474168	-2.145201	-1.674203
H	1.798970	-2.618375	-1.215671
N	-0.638551	0.042903	0.435645
S	0.183710	1.342701	-0.213919
O	1.127571	1.755369	0.816837
O	0.686017	0.954197	-1.527846
C	-1.037165	2.604050	-0.443660

H	-1.843365	2.207026	-1.073050
H	-1.413525	2.905363	0.540556
H	-0.530974	3.439939	-0.943692
H	-4.561175	0.156785	0.911471
C	-3.771299	-1.672842	-0.978890
H	-3.609352	-1.501859	-2.055680
H	-3.485166	-2.717393	-0.773431
H	-4.844025	-1.566963	-0.773973

TS1-1e

C	-0.633569	1.525526	-0.660488
H	-0.396365	1.880584	-1.678310
H	-1.365743	2.235142	-0.243189
C	0.603015	1.577908	0.209839
C	0.847888	-1.141361	-1.265324
C	0.803052	0.662805	1.186387
C	1.763974	-0.731856	-0.423055
H	0.058707	-0.092938	1.445094
H	1.242305	-1.934447	-1.917092
N	2.972943	-0.827899	0.012426
C	-0.586277	-0.780082	-1.562121
H	-0.610004	-0.478049	-2.625838
H	-1.154363	-1.720165	-1.498844
H	1.651251	0.770886	1.867103
C	4.026838	0.061563	-0.474942
H	4.231342	0.844235	0.271931
H	4.941733	-0.524374	-0.637488
H	3.713763	0.523244	-1.417959
C	3.272168	-1.623174	1.204859
H	4.160402	-2.239116	1.008744
H	3.477822	-0.956680	2.057008
H	2.419000	-2.269166	1.440363
N	-1.232248	0.214615	-0.753091
S	-2.369495	-0.278788	0.392879
O	-1.977465	-1.612368	0.819374
O	-2.486445	0.820079	1.330407
C	-3.888127	-0.411890	-0.516020
H	-4.144376	0.575763	-0.916278
H	-3.773167	-1.154688	-1.314402
H	-4.647088	-0.745462	0.203837
C	1.522961	2.731878	-0.035470
H	2.361263	2.757756	0.672507
H	1.916166	2.714780	-1.064827
H	0.964151	3.676701	0.065990

NP-1e

C	-0.742710	-1.492680	-0.321115
H	-1.369503	-2.130155	0.328219
H	-1.020652	-1.695514	-1.366094
C	0.742663	-1.751240	-0.051252
C	1.124734	-0.638070	0.999549
C	1.679163	-1.055932	-1.092068
C	1.995725	-0.030979	-0.057649
H	1.195307	-0.650991	-1.995250
H	1.649960	-0.949005	1.915372
N	2.743111	1.014202	-0.067349
C	-0.165867	0.143971	1.259970
H	-0.677591	-0.295493	2.135886
H	-0.028685	1.216016	1.448548
H	2.555878	-1.652128	-1.394627
C	2.891969	1.876455	1.107318
H	3.961453	2.009730	1.317216
H	2.441532	2.856080	0.895214
H	2.402189	1.425856	1.976066
C	3.486050	1.424362	-1.259904
H	3.181727	2.442772	-1.537302
H	4.561053	1.420181	-1.033569
H	3.281609	0.740503	-2.089824
N	-0.899773	-0.075100	0.010122
S	-2.487170	0.548603	0.019586
O	-3.404140	-0.515117	0.380589
O	-2.397819	1.772847	0.792233
C	-2.740801	0.953494	-1.689503
H	-2.004532	1.707481	-1.987956
H	-2.670812	0.043230	-2.296970
H	-3.758840	1.360697	-1.748148
C	1.080988	-3.190492	0.279324
H	0.507584	-3.534236	1.152293
H	0.836641	-3.850365	-0.566635
H	2.151217	-3.311201	0.504176

IN-1e

C	-0.569632	1.231843	-0.501804
H	-0.606539	1.407826	-1.594054
H	-1.149885	2.051838	-0.035275
C	0.825289	1.343919	0.002271
C	1.010771	-1.127154	-0.620694
C	1.200453	0.603070	1.200896

C	1.822900	-0.431508	0.239448
H	0.367349	0.209834	1.787388
H	1.503226	-1.833276	-1.295059
N	3.187430	-0.414269	0.134792
C	-0.476445	-1.146016	-0.758044
H	-0.725283	-1.185545	-1.837344
H	-0.846435	-2.100274	-0.344411
H	1.967446	1.089189	1.808579
C	3.822029	-0.922558	-1.070079
H	3.839055	-2.026455	-1.112285
H	3.307530	-0.538037	-1.962479
H	4.861588	-0.570279	-1.097538
C	4.023975	-0.487336	1.328192
H	4.327516	-1.527938	1.531548
H	4.930191	0.119278	1.190057
H	3.494861	-0.119959	2.214861
N	-1.131709	-0.033894	-0.095613
S	-2.841626	-0.104623	-0.000875
O	-3.264432	1.279681	0.083135
O	-3.302842	-0.998037	-1.042391
C	-3.109777	-0.885218	1.569658
H	-2.640068	-1.876152	1.569733
H	-2.709432	-0.239993	2.359502
H	-4.198589	-0.988539	1.669194
C	1.761582	2.312453	-0.601791
H	2.796200	1.938798	-0.528033
H	1.507675	2.560570	-1.639631
H	1.720878	3.238089	0.000724

TS2-1e

C	0.353579	1.077553	0.866687
H	-0.013351	1.202910	1.898185
H	0.973237	1.947507	0.618543
C	-0.849619	1.038878	-0.088067
C	-0.937978	-1.370679	0.382631
C	-0.692642	0.175969	-1.262252
C	-1.693376	-0.242010	0.093807
H	0.238986	-0.351668	-1.487477
H	-1.443472	-2.342788	0.412347
N	-3.060916	-0.242243	-0.148597
C	0.474710	-1.378853	0.852988
H	0.383468	-1.730747	1.903963
H	1.046612	-2.158028	0.325113
H	-1.409910	0.257912	-2.083060
C	-3.885097	0.406033	0.867502
H	-4.092632	-0.269298	1.718285
H	-3.392775	1.304103	1.256774
H	-4.843766	0.709137	0.423997
C	-3.646163	-1.457115	-0.687052
H	-3.749600	-2.265534	0.063052
H	-4.651604	-1.229287	-1.065895
H	-3.046576	-1.829190	-1.531067
N	1.167388	-0.118506	0.767144
S	2.546415	-0.053716	-0.238877
O	2.498377	-1.249909	-1.067481
O	2.547020	1.267540	-0.835369
C	3.910516	-0.190686	0.880204
H	3.880806	0.658891	1.572178
H	3.842787	-1.148391	1.409506
H	4.817820	-0.156189	0.262552
C	-1.566708	2.362475	-0.253854
H	-2.489616	2.254510	-0.837048
H	-1.806978	2.805197	0.722645
H	-0.897879	3.055221	-0.783155

TS2-1e'

C	-0.367878	1.074595	-0.350363
H	-0.240051	1.198705	-1.440386
H	-0.931341	1.949003	0.002602
C	1.013384	1.064918	0.306008
C	0.998479	-1.375094	-0.031407
C	1.116010	0.265603	1.532588
C	1.794627	-0.235461	0.034961
H	0.224721	-0.206657	1.952004
H	1.490829	-2.352855	-0.085843
N	3.184304	-0.235987	-0.021139
C	-0.466347	-1.397382	-0.209670
H	-0.566881	-1.788469	-1.250618
H	-0.930463	-2.181528	0.409985
H	1.982782	0.378567	2.188340
C	3.757743	0.301834	-1.252644
H	3.755624	-0.445862	-2.067422
H	3.198199	1.180246	-1.593541
H	4.795947	0.610671	-1.067992
C	3.871980	-1.415291	0.474087
H	3.808810	-2.282720	-0.211950
H	4.936153	-1.177332	0.605128
H	3.471624	-1.708382	1.456076

N	-1.109544	-0.126555	-0.001978
S	-2.804583	-0.096489	-0.235058
O	-3.089955	1.080292	-1.026438
O	-3.152961	-1.436937	-0.660589
C	-3.437955	0.161874	1.403280
H	-3.143442	-0.681333	2.038762
H	-3.061963	1.117550	1.787437
H	-4.531012	0.199521	1.302475
C	1.758921	2.381037	0.222314
H	2.785820	2.287722	0.596360
H	1.783190	2.752455	-0.811268
H	1.231005	3.125672	0.833890

CP-1e

C	0.233949	-1.181885	-0.480014
H	0.251473	-1.053339	-1.573534
H	0.743313	-2.134745	-0.258537
C	-1.227414	-1.298253	-0.005091
C	-1.044377	0.104416	1.621798
C	-1.212955	-1.432651	1.548234
C	-1.704566	0.112987	0.274569
H	-0.396477	-2.033050	1.972110
H	-1.503127	0.655538	2.452372
N	-2.506499	0.941866	-0.293862
C	0.432173	0.471219	1.444062
H	0.556772	1.564278	1.475192
H	1.003391	0.055986	2.290221
H	-2.179233	-1.772724	1.943536
C	-3.108494	0.699595	-1.607831
H	-4.198948	0.621835	-1.498964
H	-2.874206	1.549449	-2.262370
H	-2.712491	-0.218461	-2.046789
C	-2.865055	2.222958	0.322194
H	-2.543692	3.038470	-0.339633
H	-3.955717	2.269548	0.444590
H	-2.379241	2.331049	1.296202
N	0.885596	-0.030158	0.145618
S	2.548325	0.135374	-0.169859
O	3.154263	0.597766	1.062444
O	2.964468	-1.081693	-0.837531
C	2.611821	1.462140	-1.350079
H	2.058100	1.168089	-2.249437
H	2.198780	2.368211	-0.891569
H	3.673659	1.607783	-1.589276

C	-2.025140	-2.312409	-0.803635
H	-3.089240	-2.297690	-0.527999
H	-1.931606	-2.169475	-1.889683
H	-1.637873	-3.315974	-0.575529

TS3-1e

C	-0.581755	1.243939	-0.472653
H	-0.657232	1.446604	-1.557830
H	-1.125901	2.059039	0.040928
C	0.835578	1.310746	-0.019801
C	1.011540	-1.060541	-0.665416
C	1.214533	0.589072	1.200190
C	1.835924	-0.439775	0.249596
H	0.377496	0.206816	1.788772
H	1.498628	-1.709051	-1.398678
N	3.193653	-0.449980	0.150531
C	-0.479939	-1.120620	-0.760714
H	-0.757137	-1.159663	-1.832052
H	-0.811984	-2.085422	-0.338966
H	1.969973	1.095888	1.805530
C	3.837146	-0.963252	-1.047766
H	3.821300	-2.066032	-1.100520
H	3.355614	-0.553551	-1.947504
H	4.886299	-0.640741	-1.049416
C	4.044210	-0.428377	1.336086
H	4.466806	-1.429024	1.521457
H	4.873893	0.280990	1.201432
H	3.480654	-0.143595	2.231140
N	-1.141900	-0.026344	-0.074323
S	-2.852815	-0.103691	0.003672
O	-3.281583	1.276269	0.117486
O	-3.302681	-0.972683	-1.063567
C	-3.129471	-0.924342	1.552055
H	-2.657255	-1.913836	1.530269
H	-2.736097	-0.298226	2.360521
H	-4.218675	-1.032701	1.641259
C	1.770826	2.273331	-0.640479
H	2.810727	1.922869	-0.546689
H	1.525035	2.484923	-1.688509
H	1.703200	3.218264	-0.071295

1f

C	1.674056	0.065451	-0.376056
H	0.797219	-0.406592	-0.858811

H	2.259536	0.516364	-1.193672
C	2.484027	-1.001197	0.305435
C	-1.059685	1.783565	-0.433148
C	3.741877	-1.314499	0.000827
C	-1.561908	0.604479	-0.232640
H	4.283199	-0.801498	-0.800241
H	1.984954	-1.539068	1.122234
H	-1.730361	2.507235	-0.917186
H	4.279940	-2.097331	0.539913
C	1.215774	1.163205	0.591536
H	0.699269	0.715383	1.459803
H	2.105600	1.661180	1.004254
N	-2.040237	-0.544697	-0.050251
C	-1.905579	-1.609620	-1.063243
H	-1.321828	-2.432498	-0.629182
H	-2.908619	-1.967617	-1.330226
H	-1.397859	-1.210815	-1.947710
C	-2.746366	-0.903379	1.194945
H	-2.215511	-1.740200	1.668009
H	-2.765857	-0.038267	1.865938
H	-3.769477	-1.211548	0.942037
C	0.325311	2.231734	-0.036056
H	0.183548	3.078917	0.655065
H	0.792863	2.660805	-0.938084

1f (Optimized at *ω*B97X-D/6-311G(d,p) level)

C	1.662087	0.102484	-0.396193
H	0.805828	-0.333737	-0.929467
H	2.286495	0.573527	-1.161611
C	2.427471	-0.997825	0.280720
C	-1.089125	1.787620	-0.424671
C	3.690701	-1.305933	0.024470
C	-1.558702	0.602544	-0.233109
H	4.266359	-0.768843	-0.723460
H	1.888717	-1.557401	1.045065
H	-1.763088	2.500122	-0.897910
H	4.196548	-2.106253	0.551391
C	1.181120	1.167911	0.597835
H	0.655676	0.693857	1.437046
H	2.055545	1.656139	1.033852
N	-1.995087	-0.556979	-0.053783
C	-1.827482	-1.616423	-1.072740
H	-1.210431	-2.407956	-0.646071
H	-2.812562	-2.008036	-1.326621
H	-1.348237	-1.195643	-1.953112
C	-2.682842	-0.945849	1.196683
H	-2.122884	-1.761183	1.655448
H	-2.723710	-0.089390	1.864878
H	-3.689145	-1.282273	0.946482
C	0.292493	2.244542	-0.020231
H	0.146406	3.076226	0.676305
H	0.759764	2.675282	-0.912311

TS1-1f

C	2.130117	0.959582	0.629832
H	2.105776	0.660813	1.690517
H	2.829420	1.812784	0.584121
C	0.781642	1.467353	0.225651
C	0.345056	-1.443990	0.016836
C	0.248902	1.356348	-1.015700
C	-0.584656	-0.512798	-0.070053
H	0.797256	0.922479	-1.854228
H	-0.692130	1.853387	-1.260275
H	0.209466	2.009729	0.987805
H	-0.119040	-2.422620	0.209081
C	2.630813	-0.186100	-0.243143
N	-1.850426	-0.275228	0.091169
C	-2.375281	0.111283	1.400112
H	-2.523915	1.202461	1.444584
H	-3.342772	-0.383749	1.560884
H	-1.675476	-0.197609	2.184841
C	-2.736679	-0.093966	-1.056112
H	-3.662911	-0.660685	-0.888069
H	-2.991932	0.971023	-1.179215
H	-2.247619	-0.463728	-1.964390
H	2.635742	0.111233	-1.302187
H	3.680476	-0.398909	0.001942
C	1.841598	-1.478037	-0.044370
H	2.115175	-2.214909	-0.817255
H	2.146396	-1.953145	0.905337

TS1-1f (Optimized at *ω*B97X-D/6-311G(d,p) level)

C	-2.100725	-0.978515	0.623035
H	-2.069657	-0.687153	1.677886
H	-2.777238	-1.839687	0.572927
C	-0.746055	-1.449140	0.198027
C	-0.355274	1.433090	0.039869

C	-0.232586	-1.308276	-1.045063
C	0.568210	0.505052	-0.066187
H	-0.795275	-0.878042	-1.863980
H	0.705383	-1.782793	-1.308229
H	-0.160241	-1.989214	0.939020
H	0.098884	2.401874	0.256522
C	-2.630873	0.165784	-0.235042
N	1.838548	0.292152	0.099697
C	2.352467	-0.144408	1.399572
H	2.471733	-1.232793	1.413606
H	3.324591	0.319908	1.569198
H	1.663829	0.161419	2.184617
C	2.728888	0.123298	-1.049064
H	3.654171	0.669498	-0.861382
H	2.966306	-0.935483	-1.194546
H	2.251356	0.520484	-1.942432
H	-2.643857	-0.119892	-1.288997
H	-3.671637	0.361289	0.028380
C	-1.851229	1.463846	-0.030553
H	-2.122023	2.192589	-0.801449
H	-2.163090	1.928544	0.913419

NP-1f

C	2.573372	-0.535799	0.131284
H	3.418608	-0.194143	-0.485720
H	2.915393	-1.421290	0.686491
C	1.382123	-0.837766	-0.778209
C	0.540811	0.486963	-0.844305
C	0.175585	-1.555493	-0.103290
C	-0.592967	-0.282611	-0.241524
H	0.328568	-1.877328	0.940646
H	-0.260676	-2.398065	-0.662986
H	1.657008	-1.276073	-1.744831
H	0.311332	0.914187	-1.832604
C	2.091312	0.604887	1.035897
N	-1.812097	0.029764	0.025644
C	-2.349498	1.364020	-0.246836
H	-3.224499	1.269666	-0.904112
H	-2.660389	1.827415	0.699545
H	-1.591611	1.987762	-0.730916
C	-2.746751	-0.928471	0.617497
H	-3.128211	-0.519721	1.563082
H	-3.588519	-1.083685	-0.071306
H	-2.244798	-1.882698	0.806764
C	1.245589	1.484111	0.106856
H	0.548342	2.147672	0.638976
H	1.894364	2.122872	-0.510427
H	1.475459	0.214537	1.864601
H	2.916863	1.161497	1.499068

NP-1f (Optimized at ωB97X-D/6-311G(d,p) level)

C	2.571643	-0.531883	0.130718
H	3.412320	-0.184624	-0.475963
H	2.907122	-1.412933	0.681254
C	1.385187	-0.833478	-0.783413
C	0.539944	0.490465	-0.847826
C	0.180371	-1.554028	-0.104214
C	-0.591735	-0.282209	-0.244384
H	0.338712	-1.866932	0.932701
H	-0.249330	-2.392074	-0.659108
H	1.658630	-1.268215	-1.742222
H	0.314033	0.917096	-1.827106
C	2.081158	0.602404	1.040762
N	-1.806680	0.026930	0.024184
C	-2.348902	1.362346	-0.248942
H	-3.216458	1.262494	-0.902294
H	-2.657296	1.818236	0.692889
H	-1.595157	1.980958	-0.728753
C	-2.741002	-0.933438	0.620271
H	-3.115396	-0.524018	1.559349
H	-3.576044	-1.086930	-0.064650
H	-2.237665	-1.878760	0.806488
C	1.236240	1.484307	0.111999
H	0.537291	2.133721	0.643111
H	1.882974	2.123578	-0.493270
H	1.466629	0.206750	1.857357
H	2.898972	1.156228	1.501105

TS2-1f

C	1.856997	-1.212370	-0.325071
H	1.651508	-1.463458	-1.377067
H	2.462647	-2.033815	0.083110
C	0.531439	-1.155886	0.414961
C	0.294262	1.207120	-0.285723
C	0.391222	-0.279868	1.564466
C	-0.377733	0.040165	0.056592
H	1.211576	0.351487	1.909976
H	-0.444704	-0.413338	2.253604

H	-0.052039	-2.080259	0.450771
H	-0.308870	2.091073	-0.525303
C	2.622439	0.107247	-0.209772
N	-1.758026	-0.123986	0.078206
C	-2.565742	1.064726	0.277186
H	-3.588449	0.763225	0.540331
H	-2.167808	1.659712	1.113105
H	-2.629371	1.709181	-0.621640
C	-2.316620	-1.078905	-0.871594
H	-1.711016	-1.993442	-0.914099
H	-3.325965	-1.364639	-0.545810
H	-2.385647	-0.661817	-1.893516
C	1.752596	1.334252	-0.508753
H	1.788132	1.599848	-1.586352
H	2.135694	2.244271	-0.016619
H	3.484337	0.102893	-0.890233
H	3.053004	0.198096	0.798548

TS2-1f (Optimized at ωB97X-D/6-311G(d,p) level)

C	1.851611	-1.211120	-0.327905
H	1.637082	-1.460432	-1.370496
H	2.458622	-2.023311	0.076278
C	0.533919	-1.151490	0.425110
C	0.283110	1.201956	-0.279690
C	0.410256	-0.270321	1.572223
C	-0.379667	0.037143	0.057054
H	1.226372	0.361102	1.897447
H	-0.417345	-0.391563	2.259712
H	-0.043224	-2.068733	0.476350
H	-0.317826	2.079980	-0.509968
C	2.617551	0.110257	-0.224791
N	-1.760132	-0.140954	0.105230
C	-2.569058	1.058389	0.269446
H	-3.586145	0.759597	0.523035
H	-2.182163	1.661937	1.094110
H	-2.616934	1.677252	-0.639056
C	-2.303708	-1.075537	-0.881582
H	-1.705269	-1.985722	-0.925206
H	-3.313943	-1.354663	-0.581441
H	-2.344420	-0.635424	-1.887148
C	1.741040	1.337503	-0.512089
H	1.777628	1.607705	-1.580307
H	2.119133	2.233149	-0.007338
H	3.458424	0.104442	-0.918871
H	3.060601	0.200680	0.769636

CP-1f

C	-1.440703	1.283809	-0.623515
H	-0.805162	1.609492	-1.462616
H	-2.135631	2.110943	-0.420607
C	-0.549143	1.071361	0.629610
C	-0.549091	-1.071320	0.629697
C	-1.172333	0.000045	1.577015
C	0.434308	0.000000	0.291986
H	-2.263222	-0.000027	1.688410
H	-0.699350	0.000128	2.566931
H	-0.177797	2.016654	1.047200
H	-0.177774	-2.016667	1.047191
C	-2.217539	-0.000030	-0.962101
N	1.672770	0.000001	-0.058121
C	2.422306	-1.239583	-0.273871
H	2.804584	-1.251552	-1.303536
H	3.270289	-1.275660	0.423683
H	1.776756	-2.108599	-0.114396
C	2.422335	1.239563	-0.273828
H	1.777190	2.108605	-0.112858
H	3.271140	1.274858	0.422760
H	2.803408	1.252261	-1.303935
C	-1.440729	-1.283830	-0.623410
H	-0.805217	-1.609577	-1.462505
H	-2.135672	-2.110913	-0.420382
H	-3.159903	0.000038	-0.396847
H	-2.509495	-0.000073	-2.021141

CP-1f (Optimized at ωB97X-D/6-311G(d,p) level)

C	1.436875	-1.284514	-0.624112
H	0.805231	-1.604496	-1.458389
H	2.129507	-2.103109	-0.421054
C	0.547780	-1.072320	0.630927
C	0.547762	1.072340	0.630889
C	1.178180	0.000032	1.575005
C	-0.434821	-0.000003	0.291720
H	2.262049	0.000045	1.673035
H	0.714622	0.000044	2.560621
H	0.179944	-2.008333	1.048983
H	0.179910	2.008365	1.048905
C	2.214344	-0.000011	-0.963709

N	-1.669459	-0.000009	-0.056162
C	-2.421097	1.241382	-0.273081
H	-2.799958	1.248342	-1.295815
H	-3.260602	1.274936	0.422612
H	-1.777071	2.102413	-0.116596
C	-2.421103	-1.241391	-0.273092
H	-1.777344	-2.102444	-0.115636
H	-3.261172	-1.274465	0.421939
H	-2.799141	-1.248806	-1.296130
C	1.436860	1.284494	-0.624160
H	0.805214	1.604437	-1.458450
H	2.129480	2.103105	-0.421129
H	3.151466	0.000004	-0.404474
H	2.495401	-0.000028	-2.017617

1g

C	1.680409	1.483602	-0.260465
H	2.336042	2.102415	0.372340
H	2.306348	1.113532	-1.086482
C	0.548283	2.302430	-0.815489
C	-0.868805	0.695330	1.857603
C	0.271309	3.548447	-0.433834
C	-1.635648	0.220220	0.928605
H	0.869230	4.062872	0.325826
H	-0.042791	1.812588	-1.596505
H	-1.338253	1.162493	2.731292
N	-2.303667	-0.270220	-0.012684
C	0.650003	0.546600	1.828969
H	0.891377	-0.279645	2.516097
H	1.086353	1.461540	2.254917
C	-2.673576	-1.698478	-0.028121
H	-2.178462	-2.152557	-0.896638
H	-2.312809	-2.176386	0.887270
H	-3.764533	-1.775853	-0.120517
C	-2.636413	0.510223	-1.216930
H	-2.015483	0.122569	-2.036706
H	-3.701764	0.372570	-1.440420
H	-2.415345	1.567229	-1.036779
N	1.258323	0.325585	0.538826
S	1.004668	-1.134770	-0.232015
O	0.319588	-1.973854	0.744118
O	0.372790	-0.880384	-1.521956
C	2.623174	-1.793151	-0.523461
H	3.189440	-1.105635	-1.162783
H	3.115237	-1.944693	0.443949
H	2.472794	-2.749576	-1.040898
H	-0.546095	4.117854	-0.883273

TS1-1g

C	-0.504213	1.063966	-1.327689
H	-0.199330	0.874633	-2.370086
H	-1.240530	1.882898	-1.356799
C	0.669978	1.525813	-0.508002
C	1.046397	-1.401897	-0.575898
C	0.819779	1.238785	0.805327
C	1.915316	-0.525039	-0.121012
H	0.072437	0.676146	1.371022
H	1.394550	2.180637	-1.005749
H	1.521472	-2.373445	-0.770681
N	3.165882	-0.313122	0.145328
C	-0.419322	-1.372543	-0.918031
H	-0.490141	-1.750161	-1.955624
H	-0.905571	-2.126661	-0.279868
H	1.637000	1.683515	1.377250
C	4.054111	0.264966	-0.861818
H	4.172741	1.346828	-0.688004
H	5.039333	-0.215302	-0.789671
H	3.640142	0.094897	-1.862174
C	3.653845	-0.345498	1.523575
H	4.592656	-0.915147	1.557980
H	3.845877	0.677951	1.883648
H	2.911203	-0.829859	2.167720
N	-1.122564	-0.124902	-0.786341
S	-2.323780	0.021667	0.394025
O	-1.970810	-0.896664	1.464759
O	-2.467075	1.444877	0.628240
C	-3.794923	-0.580943	-0.392167
H	-4.016128	0.055550	-1.256605
H	-3.646781	-1.626909	-0.686237
H	-4.594395	-0.507452	0.356866

NP-1g

C	0.791713	1.702783	0.026386
H	1.448467	2.162079	0.786077
H	1.091344	2.087277	-0.959487
C	-0.674613	1.974029	0.343785
C	-1.132611	0.726590	1.179267
C	-1.679526	1.581421	-0.776465

C	-2.063911	0.398840	0.049173
H	-1.242258	1.327169	-1.755354
H	-0.850675	2.959189	0.789334
H	-1.621252	0.891200	2.150855
N	-2.891736	-0.565022	-0.139174
C	0.101706	-0.180853	1.256099
H	0.638380	0.030371	2.199128
H	-0.113117	-1.256126	1.220425
H	-2.509453	2.289450	-0.931454
C	-3.093428	-1.623808	0.853048
H	-4.166458	-1.706767	1.070761
H	-2.734426	-2.577007	0.440789
H	-2.549929	-1.392536	1.774338
C	-3.681758	-0.678986	-1.366425
H	-3.463130	-1.644305	-1.842901
H	-4.749608	-0.637836	-1.111781
H	-3.435491	0.135432	-2.055143
N	0.855822	0.238746	0.071427
S	2.398802	-0.476633	-0.059494
O	3.382634	0.434856	0.490976
O	2.226980	-1.819457	0.460933
C	2.627677	-0.556555	-1.817418
H	1.843656	-1.188306	-2.248538
H	2.619511	0.457110	-2.235606
H	3.616614	-1.010293	-1.965277

TS2-1g

C	-0.293217	1.245316	-0.289787
H	-0.149275	1.442249	-1.366590
H	-0.901468	2.068690	0.106879
C	1.058753	1.219521	0.403233
C	1.179900	-1.166427	-0.233850
C	1.189329	0.420230	1.598759
C	1.911789	-0.031780	0.083391
H	0.333302	-0.146654	1.970754
H	1.658423	2.131702	0.336941
H	1.716546	-2.081523	-0.507971
N	3.296181	0.073039	0.066020
C	-0.284661	-1.224569	-0.391638
H	-0.400610	-1.499614	-1.467261
H	-0.705786	-2.095539	0.139015
H	2.050278	0.545811	2.257494
C	3.874650	0.965689	-0.932016
H	4.906502	1.207896	-0.644234
H	3.890956	0.511894	-1.940230
H	3.317190	1.909669	-0.988956
C	4.052967	-1.145232	0.291454
H	4.071370	-1.819044	-0.587428
H	5.092731	-0.883292	0.528728
H	3.641397	-1.693851	1.151902
N	-0.976751	-0.013542	-0.030364
S	-2.679900	-0.038962	-0.213095
O	-3.040399	1.211371	-0.844530
O	-2.981109	-1.332355	-0.791906
C	-3.271498	-0.014994	1.460503
H	-2.915260	-0.911814	1.980651
H	-2.932135	0.906604	1.948101
H	-4.367782	-0.024929	1.393332

CP-1g

C	-0.231145	0.642870	-1.275411
H	-0.261710	-0.172101	-2.014461
H	-0.812919	1.480479	-1.693193
C	1.216216	1.106756	-1.071759
C	1.216348	1.107659	1.070774
C	1.249797	2.233874	-0.000951
C	1.840344	0.262739	-0.000176
H	0.395226	2.923665	-0.001218
H	1.737337	1.248265	-2.026981
H	1.737646	1.249996	2.025778
N	2.725770	-0.668358	0.000196
C	-0.230947	0.643893	1.275084
H	-0.261427	-0.170471	2.014786
H	-0.812633	1.481847	1.692294
H	2.192904	2.794017	-0.001248
C	3.258933	-1.239683	-1.239401
H	4.344023	-1.072299	-1.276232
H	3.062099	-2.320110	-1.246476
H	2.782935	-0.776485	-2.108923
C	3.259178	-1.238413	1.240280
H	3.064815	-2.319278	1.247204
H	4.343858	-1.068547	1.278072
H	2.781318	-0.776318	2.109368
N	-0.764127	0.157747	0.000053
S	-2.416448	-0.248621	0.000335
O	-2.947210	0.197568	1.272518
O	-2.948462	0.199901	-1.270512
C	-2.401934	-2.025247	-0.001301

H	-1.901962	-2.378248	-0.910842
H	-1.900816	-2.379816	0.906998
H	-3.454376	-2.338822	-0.000916

1h

C	1.331604	-1.484138	-0.459210
H	2.070334	-2.074021	0.102355
H	0.962345	-2.145245	-1.257064
C	1.944743	-0.257812	-1.078277
C	0.465722	0.906076	1.805088
C	3.121863	0.291721	-0.755808
C	-0.143491	1.633264	0.923989
H	1.352631	0.190735	-1.881925
H	0.931879	1.403335	2.663487
N	-0.761804	2.253103	0.026300
C	0.474258	-0.618980	1.740352
H	-0.262377	-0.961690	2.483986
H	1.461459	-0.966053	2.077690
C	-2.220350	2.462147	0.103325
H	-2.669227	1.921119	-0.740232
H	-2.596911	2.047343	1.042858
H	-2.423583	3.537990	0.026591
C	-0.098581	2.685525	-1.215640
H	-0.490196	2.056705	-2.027238
H	-0.340532	3.741020	-1.392994
H	0.982493	2.546304	-1.115664
N	0.209107	-1.216171	0.453921
S	-1.333074	-1.113393	-0.178152
O	-2.152211	-0.544353	0.885806
O	-1.270016	-0.436681	-1.468945
C	-1.832506	-2.790752	-0.454497
H	-1.146446	-3.264586	-1.166435
H	-1.840921	-3.313549	0.508597
H	-2.842269	-2.740520	-0.882122
H	3.431716	1.173660	-1.329802
C	4.099888	-0.155415	0.285514
H	3.775810	-1.044907	0.842687
H	5.071066	-0.387069	-0.178585
H	4.289711	0.653656	1.008769

TS1-1h

C	0.426908	-0.175018	1.551209
H	0.242696	-1.075080	2.162956
H	1.133371	0.457820	2.110527
C	-0.862566	0.585755	1.361249
C	-1.068564	-1.427345	-0.724457
C	-1.076165	1.595971	0.476005
C	-2.008685	-0.628480	-0.275498
H	-1.634067	0.406356	2.118173
H	-1.488883	-2.222088	-1.356810
N	-3.274934	-0.371700	-0.238952
C	0.413912	-1.544882	-0.521011
C	-4.105486	-0.852535	0.864975
H	-5.064163	-1.208494	0.463819
H	-3.597072	-1.676679	1.377972
H	-4.298787	-0.034468	1.577076
C	-3.863181	0.629414	-1.127419
H	-4.780694	0.219609	-1.572018
H	-4.119035	1.537301	-0.558477
H	-3.152617	0.880578	-1.922941
N	1.034842	-0.537532	0.290202
S	2.522277	0.086329	-0.177222
O	2.494972	0.139544	-1.627106
O	2.729174	1.269201	0.637897
C	3.727728	-1.126500	0.305713
H	3.693241	-1.248826	1.394861
H	3.521930	-2.068782	-0.216692
H	4.704325	-0.730826	-0.002964
H	-2.055969	2.080804	0.559462
C	-0.144355	2.187698	-0.531966
H	-0.591017	3.075406	-0.995276
H	0.808328	2.472847	-0.060842
H	0.117703	1.477507	-1.330687
H	0.571695	-2.564634	-0.112681
H	0.882797	-1.529433	-1.517796

NP-1h

C	-0.829898	1.321319	-0.949174
H	-1.498316	1.351206	-1.827522
H	-1.086274	2.174314	-0.305094
C	0.628793	1.318615	-1.391408
C	1.015215	-0.197758	-1.454546
C	1.701368	1.543171	-0.271864
C	2.000667	0.072803	-0.357391
H	0.799397	1.909244	-2.298416
H	1.461142	-0.589922	-2.380435
N	2.828532	-0.697121	0.254951
C	-0.243375	-0.957778	-1.016562

H	-0.054156	-1.857175	-0.417498
H	-0.806238	-1.260162	-1.918375
C	2.926448	-2.128632	-0.042590
H	2.684970	-2.699707	0.864428
H	2.233920	-2.403128	-0.843651
H	3.955017	-2.359993	-0.350376
C	3.731024	-0.206276	1.299261
H	3.375752	-0.550192	2.280730
H	4.733800	-0.613512	1.117621
H	3.776298	0.886434	1.280874
N	-0.950289	0.052605	-0.224995
S	-2.517034	-0.417499	0.258479
O	-3.476482	0.116544	-0.688301
O	-2.412304	-1.840425	0.518103
C	-2.708253	0.444622	1.798060
H	-1.952151	0.082320	2.503054
H	-2.630987	1.525026	1.626440
H	-3.717892	0.196999	2.151722
H	2.567365	2.097839	-0.677189
C	1.267378	2.147984	1.059206
H	2.103672	2.243018	1.764365
H	0.875237	3.159037	0.882322
H	0.478365	1.542570	1.525270

TS2-1h

C	0.330122	-0.729418	1.299439
H	0.084725	-1.771961	1.564213
H	0.996877	-0.329563	2.075997
C	-0.950143	0.082809	1.296514
C	-1.180251	-0.650160	-1.081402
C	-1.083669	1.358979	0.663220
C	-1.841018	-0.102539	-0.015947
H	-1.608804	-0.086563	2.155734
H	-1.783703	-1.026621	-1.916048
N	-3.236437	-0.062482	0.130339
C	0.268254	-0.931834	-1.174982
C	-3.828088	-1.321064	0.561699
H	-3.840440	-2.087829	-0.238232
H	-3.275699	-1.726788	1.421636
H	-4.863555	-1.145566	0.884063
C	-3.964051	0.617675	-0.928736
H	-3.990820	0.048730	-1.879669
H	-5.002258	0.780075	-0.608734
H	-3.513253	1.601250	-1.125568
N	1.012904	-0.658565	0.025718
S	2.539649	0.057887	-0.082827
O	2.607709	0.613904	-1.423958
O	2.684086	0.884734	1.099839
C	3.692607	-1.283703	0.027124
H	3.564419	-1.782921	0.994943
H	3.522954	-1.969389	-0.811402
H	4.692653	-0.835196	-0.041688
H	-2.005915	1.872242	0.956630
C	-0.098309	2.218202	-0.057451
H	-0.612844	3.058284	-0.538358
H	0.592269	2.619972	0.703894
H	0.528311	1.714380	-0.798415
H	0.334462	-1.994809	-1.492206
H	0.703879	-0.359369	-2.017865

IN1-1h

C	0.472913	-0.393370	1.530473
H	0.364879	-1.321390	2.117750
H	1.106248	0.301374	2.111155
C	-0.853906	0.280782	1.378243
C	-1.139886	-1.068288	-0.699810
C	-1.182119	1.280353	0.399254
C	-1.862146	-0.057914	-0.106058
H	-1.576767	0.132619	2.186955
H	-1.731318	-1.836117	-1.210011
N	-3.233951	-0.124968	0.073973
C	0.320144	-1.364672	-0.707706
C	-3.863519	-1.431789	0.138973
H	-4.022961	-1.891471	-0.854843
H	-3.256411	-2.113907	0.752319
H	-4.847554	-1.329489	0.616796
C	-4.074267	0.904059	-0.528239
H	-4.325238	0.660964	-1.576133
H	-5.009871	0.994551	0.040764
H	-3.578092	1.882375	-0.520757
N	1.091434	-0.623918	0.253172
S	2.546416	0.113142	-0.168596
O	2.486979	0.294542	-1.607513
O	2.701150	1.222645	0.752906
C	3.804214	-1.085645	0.186736
H	3.785964	-1.313856	1.259009
H	3.628894	-1.979192	-0.424237
H	4.759512	-0.618778	-0.087957

H	-2.016039	1.894105	0.753123
C	-0.233619	2.045158	-0.499653
H	-0.812850	2.765324	-1.091758
H	0.490715	2.599593	0.112748
H	0.333292	1.417272	-1.193348
H	0.427370	-2.460235	-0.578184
H	0.703322	-1.141350	-1.722295

TS3-1h

C	0.524649	-0.335600	1.567578
H	0.481184	-1.228802	2.214291
H	1.128759	0.431676	2.087377
C	-0.835906	0.251627	1.392845
C	-1.139388	-1.151326	-0.553740
C	-1.205570	1.225273	0.378636
C	-1.893628	-0.066981	-0.144282
H	-1.563715	0.082336	2.193587
H	-1.714536	-2.000555	-0.936113
N	-3.255198	-0.128055	-0.006865
C	0.334286	-1.406398	-0.609727
C	-3.926201	-1.413956	0.040848
H	-4.048181	-1.877043	-0.955453
H	-3.375974	-2.108486	0.692811
H	-4.928262	-1.273484	0.467766
C	-4.095169	0.974839	-0.461887
H	-4.525508	0.755128	-1.453206
H	-4.919029	1.142191	0.246898
H	-3.522004	1.904774	-0.552663
N	1.119932	-0.601535	0.288183
S	2.558578	0.124868	-0.194894
O	2.462627	0.262582	-1.636146
O	2.732176	1.261887	0.689501
C	3.831384	-1.057452	0.163449
H	3.844167	-1.251085	1.242571
H	3.643235	-1.970838	-0.413507
H	4.776584	-0.596580	-0.153029
H	-2.008771	1.861735	0.762437
C	-0.249553	1.997625	-0.512272
H	-0.824036	2.743484	-1.077162
H	0.497518	2.524532	0.096285
H	0.287886	1.373826	-1.233310
H	0.479299	-2.488879	-0.430375
H	0.673154	-1.216338	-1.645667

CP-1h

C	-0.105606	-0.173802	-1.266538
H	0.219199	-1.118945	-1.737845
H	-0.797497	0.322487	-1.961040
C	1.129511	0.728786	-1.066580
C	1.129542	0.728847	1.066594
C	0.864712	1.845586	-0.000031
C	1.972421	0.113800	0.000030
H	1.583807	0.987958	-2.032026
H	1.583735	0.987950	2.032106
N	3.072930	-0.553293	0.000010
C	-0.105622	-0.173760	1.266504
H	0.219139	-1.118877	1.737881
H	-0.797508	0.322617	1.960951
C	3.740967	-0.959905	-1.238819
H	4.744471	-0.513881	-1.270591
H	3.834825	-2.054153	-1.251809
H	3.164141	-0.632973	-2.109150
C	3.741068	-0.959838	1.238806
H	3.834241	-2.054141	1.252231
H	4.744861	-0.514433	1.270090
H	3.164725	-0.632157	2.109175
N	-0.787060	-0.399534	-0.000016
S	-2.483853	-0.355996	-0.000012
O	-2.883233	0.228017	1.266621
O	-2.883278	0.227740	-1.266755
C	-2.965124	-2.063273	0.000189
H	-2.579236	-2.541676	-0.907626
H	-2.579697	-2.541331	0.908383
H	-4.063107	-2.073056	-0.000098
H	1.736634	2.518015	-0.000097
C	-0.400500	2.682810	-0.000017
H	-0.412275	3.332088	-0.886669
H	-1.324279	2.095879	0.000476
H	-0.411766	3.332785	0.886128

1i

C	0.582458	-2.030737	-0.103482
H	0.904199	-2.825070	0.588293
H	0.120555	-2.540316	-0.962542
C	1.758231	-1.218277	-0.564821
C	0.404062	0.639993	2.000066
C	2.972769	-1.281307	-0.012163
C	0.345070	1.498947	1.033159

H	3.128740	-1.965072	0.833529
H	1.573101	-0.565527	-1.425318
H	0.857630	0.951071	2.948343
N	0.233389	2.266984	0.048197
C	-0.220032	-0.749323	1.903646
H	-1.155991	-0.704087	2.482554
H	0.447060	-1.455726	2.418737
C	-0.987733	3.067058	-0.166558
H	-1.448467	2.709003	-1.096838
H	-1.677988	2.905355	0.666496
H	-0.702601	4.123159	-0.255532
C	1.247936	2.313979	-1.017934
H	0.798400	1.864863	-1.914422
H	1.512512	3.362597	-1.203906
H	2.128129	1.742367	-0.706679
N	-0.470319	-1.261731	0.578586
S	-1.673919	-0.558040	-0.340801
O	-2.361362	0.362853	0.556884
O	-1.086374	-0.045127	-1.573847
C	-2.772246	-1.884162	-0.757869
H	-2.229412	-2.641998	-1.334968
H	-3.183074	-2.298977	0.169534
H	-3.564871	-1.439399	-1.373453
C	4.171673	-0.510399	-0.463922
H	4.564046	0.123995	0.347188
H	4.987941	-1.193713	-0.745130
H	3.950065	0.122890	-1.335575

TS1-1i

C	0.584321	0.069584	1.651886
H	0.294576	-0.682379	2.404078
H	1.291592	0.753540	2.145213
C	-0.618120	0.865755	1.204191
C	-0.846492	-1.760524	-0.194740
C	-0.709981	1.465379	-0.002902
C	-1.799892	-0.869380	-0.074502
H	0.087816	1.306764	-0.735724
H	-1.372496	1.084371	1.970421
H	-1.262615	-2.741510	-0.467321
N	-3.042621	-0.558085	-0.171472
C	0.644794	-1.778241	0.005992
H	0.844180	-2.660010	0.644243
H	1.096166	-1.991096	-0.976246
C	-3.902659	-0.500850	1.011599
H	-4.163050	0.545268	1.232037
H	-4.824553	-1.064491	0.811450
H	-3.382778	-0.942386	1.868917
C	-3.648441	-0.180016	-1.453815
H	-4.381048	-0.949242	-1.739401
H	-4.161783	0.785292	-1.352225
H	-2.870966	-0.110826	-2.222540
N	1.250787	-0.598496	0.555091
S	2.468269	0.184252	-0.307203
O	2.216542	-0.078592	-1.714552
O	2.520056	1.534707	0.218157
C	3.960554	-0.658178	0.154080
H	4.109221	-0.544542	1.234147
H	3.884548	-1.713172	-0.135500
H	4.773440	-0.170833	-0.400140
C	-1.779331	2.425832	-0.395888
H	-2.126397	2.255255	-1.424399
H	-2.634034	2.420278	0.295755
H	-1.352590	3.442667	-0.387099

NP-1i

C	-0.762640	-1.620334	0.288172
H	-1.401943	-2.057375	1.075335
H	-0.953244	-2.166717	-0.647293
C	0.705218	-1.653061	0.699621
C	0.961840	-0.249867	1.348817
C	1.732037	-1.321293	-0.426187
C	1.879967	0.035762	0.197651
H	1.281117	-1.260097	-1.432014
H	0.969109	-2.531880	1.299977
H	1.431881	-0.209192	2.342431
N	2.527845	1.091683	-0.143111
C	-0.379692	0.486248	1.266482
H	-0.930516	0.331070	2.212312
H	-0.305703	1.566224	1.089143
C	2.519087	2.308161	0.673575
H	3.554194	2.646904	0.812586
H	1.950296	3.091095	0.152677
H	2.066779	2.109566	1.650209
C	3.307247	1.163251	-1.380744
H	3.029970	2.079701	-1.918117
H	4.377925	1.200044	-1.136169
H	3.099342	0.294388	-2.012735
N	-1.013591	-0.184337	0.127340

S	-2.624690	0.297181	-0.153906
O	-3.514309	-0.646924	0.493870
O	-2.647997	1.711331	0.168030
C	-2.774742	0.096333	-1.910811
H	-2.054364	0.756466	-2.405694
H	-2.620547	-0.956708	-2.174947
H	-3.803621	0.392562	-2.154376
C	2.992713	-2.186407	-0.444405
H	3.730209	-1.829524	-1.176377
H	3.470909	-2.217084	0.545524
H	2.715704	-3.213777	-0.717796

TS2-1i

C	0.592731	0.264873	1.348161
H	0.698421	-0.506232	2.133102
H	1.084679	1.179204	1.723799
C	-0.839091	0.600442	1.104149
C	-0.946112	-1.258270	-0.345433
C	-1.269583	1.250308	-0.124933
C	-1.829176	-0.195900	-0.252057
H	-0.439935	1.413495	-0.819633
H	-1.535576	0.579027	1.949511
H	-1.409052	-2.250069	-0.380631
N	-3.174598	-0.387438	-0.031831
C	0.541509	-1.315171	-0.423565
H	0.881226	-2.220819	0.115790
H	0.809681	-1.490129	-1.481647
C	-3.634401	-1.614459	0.594346
H	-4.649559	-1.451531	0.981709
H	-3.678481	-2.472088	-0.102768
H	-2.987463	-1.877369	1.443999
C	-4.134075	0.189733	-0.971146
H	-4.501291	-0.583772	-1.666957
H	-4.995835	0.613060	-0.434432
H	-3.672643	0.978149	-1.573251
N	1.176033	-0.111654	0.076115
S	2.890578	-0.067749	-0.016597
O	3.302511	0.772467	1.088633
O	3.347139	-1.433231	-0.173085
C	3.169247	0.798256	-1.539053
H	2.713003	0.239494	-2.364959
H	2.759657	1.810631	-1.450792
H	4.259469	0.831724	-1.667688
C	-2.225432	2.423532	-0.023033
H	-2.583439	2.736703	-1.011216
H	-3.085495	2.202917	0.621638
H	-1.677565	3.271276	0.410994

IN-1i

C	0.420138	-0.080999	1.537875
H	0.093620	-0.832607	2.273411
H	1.041319	0.660093	2.053534
C	-0.810624	0.608692	0.944643
C	-0.964081	-1.317630	-0.568701
C	-0.670245	1.196553	-0.373305
C	-1.680579	-0.363761	0.114856
H	0.223202	0.963522	-0.961356
H	-1.409060	1.184285	1.658030
H	-1.506240	-2.055705	-1.167383
N	-3.041028	-0.181132	0.044912
C	0.490741	-1.610243	-0.393827
H	0.521927	-2.652221	-0.015634
H	0.995490	-1.630212	-1.373079
C	-3.811764	-0.089424	1.278059
H	-4.739680	0.467901	1.089020
H	-4.078352	-1.086514	1.671243
H	-3.256553	0.445318	2.058408
C	-3.752071	-0.770439	-1.074617
H	-3.892841	-1.862899	-0.971292
H	-4.746565	-0.310851	-1.149292
H	-3.215128	-0.568260	-2.012972
N	1.200549	-0.712834	0.492354
S	2.522395	0.150288	-0.141116
O	2.426504	0.046391	-1.589865
O	2.503371	1.447953	0.509783
C	3.943935	-0.753565	0.401009
H	3.957734	-0.759078	1.497034
H	3.895877	-1.769184	-0.009171
H	4.817608	-0.219468	0.004608
C	-1.560296	2.234512	-0.921257
H	-1.686729	2.133634	-2.007399
H	-2.532164	2.278215	-0.415721
H	-1.028359	3.190260	-0.752747

TS3-1i

C	0.417231	-0.065167	1.532727
H	0.093559	-0.809559	2.276830
H	1.036453	0.683376	2.039803

C	-0.816419	0.613183	0.931170
C	-0.962565	-1.290382	-0.590734
C	-0.673609	1.173361	-0.404906
C	-1.689642	-0.365488	0.126349
H	0.231075	0.945600	-0.977449
H	-1.402441	1.213212	1.634359
H	-1.495014	-2.011765	-1.217668
N	-3.048204	-0.195676	0.063788
C	0.489770	-1.594539	-0.399507
H	0.504318	-2.636315	-0.019275
H	1.004394	-1.621055	-1.372858
C	-3.816523	-0.042945	1.292360
H	-4.723306	0.543556	1.088813
H	-4.119331	-1.019710	1.708428
H	-3.241525	0.487841	2.060519
C	-3.768547	-0.804189	-1.039366
H	-3.893048	-1.896978	-0.923139
H	-4.769471	-0.357450	-1.102461
H	-3.249873	-0.603637	-1.988388
N	1.200271	-0.704770	0.493405
S	2.532026	0.149731	-0.132802
O	2.441811	0.049914	-1.582268
O	2.521584	1.445818	0.520933
C	3.943306	-0.767854	0.413229
H	3.952437	-0.775587	1.509287
H	3.887970	-1.782256	0.000969
H	4.823352	-0.240843	0.021498
C	-1.565370	2.199605	-0.974242
H	-1.667116	2.095675	-2.062502
H	-2.548912	2.230143	-0.490062
H	-1.053363	3.163801	-0.794020

CP-1i

C	0.338712	-0.498015	-1.275813
H	0.490851	0.297184	-2.021001
H	0.789090	-1.416173	-1.686688
C	-1.159778	-0.740920	-1.068345
C	-1.156056	-0.733296	1.073370
C	-1.368945	-1.854781	0.006917
C	-1.654737	0.185663	0.000009
H	-0.572330	-2.613303	0.008284
H	-1.700302	-0.811151	-2.021538
H	-1.692909	-0.796668	2.029106
N	-2.409398	1.226031	-0.002695
C	0.343437	-0.489340	1.272605
H	0.497204	0.311510	2.012000
H	0.796784	-1.404276	1.687395
C	-2.865073	1.856731	-1.243989
H	-3.962675	1.828789	-1.281213
H	-2.532520	2.903347	-1.254750
H	-2.451634	1.333954	-2.111663
C	-2.862037	1.865810	1.234993
H	-2.527600	2.911883	1.238389
H	-3.959635	1.840181	1.273916
H	-2.448565	1.347882	2.105556
N	0.938637	-0.087205	-0.003830
S	2.631450	0.076962	-0.006730
O	3.103807	-0.486087	1.242079
O	3.083730	-0.397460	-1.299067
C	2.873114	1.836190	0.054460
H	2.426060	2.289246	-0.838049
H	2.430814	2.226793	0.978474
H	3.959688	1.995181	0.058165
C	-2.745432	-2.492665	0.011559
H	-2.877765	-3.122681	0.902312
H	-3.551161	-1.739871	0.010280
H	-2.880786	-3.128895	-0.874303

TS4-1i

C	0.489656	0.297431	1.528678
H	0.262662	-0.257518	2.453147
H	1.084306	1.177168	1.801111
C	-0.835822	0.742703	0.897640
C	-0.871947	-1.588681	-0.029498
C	-0.757359	1.587608	-0.299437
C	-1.567619	-0.474860	0.252530
H	0.126530	1.485060	-0.940634
H	-1.488227	1.186683	1.665373
H	-1.395943	-2.464223	-0.422570
N	-2.901736	-0.240282	-0.132616
C	0.591711	-1.770813	0.217622
H	0.718421	-2.571034	0.971639
H	1.066784	-2.132940	-0.706581
C	-3.870833	-0.054098	0.953844
H	-4.797118	0.368719	0.542964
H	-4.101147	-1.012533	1.445969
H	-3.481699	0.640660	1.708654
C	-3.426769	-1.049514	-1.234128

H	-3.618619	-2.089915	-0.922975
H	-4.374973	-0.613558	-1.574095
H	-2.714173	-1.045755	-2.069220
N	1.247216	-0.552482	0.638429
S	2.472589	0.107942	-0.310703
O	2.442749	-0.589647	-1.581894
O	2.299199	1.553568	-0.244344
C	3.973707	-0.306656	0.534385
H	3.949689	0.133317	1.538196
H	4.063643	-1.398611	0.573533
H	4.791710	0.126141	-0.056383
C	-1.902936	2.258115	-0.743104
H	-1.863867	2.781393	-1.701943
H	-2.553161	1.204338	-0.762553
H	-2.520906	2.746113	0.025631

FC-1i

C	-0.399953	0.570341	-1.120746
H	-0.349034	0.060301	-2.101153
H	-0.945026	1.509017	-1.273202
C	1.024529	0.851510	-0.627482
C	0.928816	-1.531398	0.179809
C	1.112965	1.893667	0.460101
C	1.625008	-0.435247	-0.110576
H	0.438505	1.741376	1.310621
H	1.609012	1.200469	-1.497810
H	1.406010	-2.444113	0.544021
N	3.087532	-0.344018	0.112212
C	-0.561410	-1.577027	0.030831
H	-0.822096	-2.250717	-0.809478
H	-0.993333	-2.044340	0.928054
C	3.864389	-0.622553	-1.134427
H	4.923489	-0.400879	-0.955261
H	3.733187	-1.680036	-1.391768
H	3.482377	0.005988	-1.946241
C	3.607381	-1.123207	1.271086
H	3.551119	-2.193866	1.045905
H	4.654538	-0.843011	1.436400
H	3.004385	-0.887277	2.154927
N	-1.098884	-0.239821	-0.139185
S	-2.792653	-0.102938	-0.060394
O	-3.168774	0.930748	-1.004021
O	-3.328192	-1.448831	-0.127096
C	-3.067391	0.517803	1.581828
H	-2.660652	-0.194531	2.309272
H	-2.597273	1.503906	1.670267
H	-4.155991	0.599332	1.699833
C	1.965719	2.921455	0.447165
H	2.005451	3.640499	1.268590
H	2.624918	3.112547	-0.407622
H	3.227740	0.651815	0.353157

1l

C	0.729934	-1.796316	-0.392052
H	1.236465	-2.581841	0.186808
H	0.293694	-2.303687	-1.264915
C	1.685699	-0.736938	-0.865151
C	0.251915	0.609736	1.959400
C	2.902219	-0.464782	-0.365336
C	-0.063319	1.510840	1.084818
H	1.330362	-0.157983	-1.724045
H	0.738091	0.926570	2.889141
N	-0.419956	2.307550	0.184658
C	-0.120120	-0.860796	1.782754
H	-0.997551	-1.033363	2.425659
H	0.702393	-1.468360	2.186035
C	-1.782249	2.873437	0.156724
H	-2.268179	2.499920	-0.754372
H	-2.337482	2.526955	1.033171
H	-1.705202	3.968060	0.134765
C	0.443683	2.613567	-0.968048
H	-0.005814	2.127909	-1.845332
H	0.476853	3.702155	-1.101554
H	1.445755	2.213365	-0.786575
N	-0.385377	-1.306986	0.437177
S	-1.779228	-0.787432	-0.319989
O	-2.544278	-0.089362	0.707113
O	-1.419009	-0.079525	-1.543925
C	-2.639748	-2.269386	-0.770453
H	-2.017633	-2.860958	-1.452397
H	-2.877592	-2.824246	0.144127
H	-3.555395	-1.945691	-1.282077
C	3.759200	0.611469	-0.975988
H	3.991755	1.397239	-0.237351
H	4.727261	0.197278	-1.299620
H	3.286104	1.074446	-1.853447
C	3.530276	-1.170288	0.805616
H	3.744501	-0.451463	1.613863

H	2.917851	-1.980297	1.221570
H	4.500102	-1.603199	0.514318

TS1-1l

C	0.614388	0.217640	1.524799
H	0.543934	-0.485320	2.373556
H	1.298772	1.023301	1.831582
C	-0.748693	0.803967	1.235360
C	-0.770158	-1.864464	-0.252427
C	-1.058308	1.641731	0.214164
C	-1.823418	-1.105722	-0.117656
H	-1.496265	0.668436	2.025751
H	-1.069169	-2.867681	-0.593819
N	-3.072032	-0.855062	-0.198459
C	0.706285	-1.737772	-0.007062
C	-3.959341	-1.017882	0.957729
H	-4.384352	-0.043182	1.235317
H	-4.774908	-1.702188	0.684468
H	-3.394668	-1.432158	1.799852
C	-3.684822	-0.398325	-1.454013
H	-4.265172	-1.227143	-1.885468
H	-4.356694	0.443734	-1.246725
H	-2.901314	-0.089467	-2.154626
N	1.199919	-0.449890	0.376409
S	2.678365	0.039222	-0.257149
O	2.659915	-0.355669	-1.652808
O	2.860484	1.417021	0.157740
C	3.910812	-0.938432	0.574272
H	3.869511	-0.724853	1.649211
H	3.739029	-2.001107	0.363373
H	4.879771	-0.627224	0.162280
C	-2.404398	2.303769	0.176365
H	-2.857090	2.244843	-0.824872
H	-3.102523	1.910548	0.928443
H	-2.272375	3.379751	0.379743
C	-0.108796	2.041885	-0.882330
H	0.123387	1.197303	-1.549039
H	-0.533892	2.848962	-1.493181
H	0.855456	2.380170	-0.477788
H	0.939539	-2.518913	0.747233
H	1.205481	-2.039881	-0.941201

IN-1l

C	0.399440	0.011723	1.392113
H	0.184765	-0.724109	2.186312
H	0.982041	0.827565	1.837848
C	-0.950041	0.532460	0.886899
C	-0.931876	-1.527304	-0.510806
C	-0.978651	1.643258	-0.085973
C	-1.685859	-0.579770	0.079298
H	-1.576414	0.791111	1.752954
H	-1.430028	-2.363540	-1.007717
N	-3.070239	-0.478419	-0.026151
C	0.558556	-1.624593	-0.470874
H	0.809824	-2.634319	-0.090278
H	0.964525	-1.572369	-1.495520
C	-3.842376	-0.562435	1.209751
H	-4.871267	-0.229083	1.018687
H	-3.874435	-1.593537	1.604136
H	-3.422712	0.088203	1.988781
C	-3.704166	-1.148990	-1.151848
H	-3.749939	-2.246083	-1.021572
H	-4.733543	-0.780638	-1.256640
H	-3.157749	-0.924694	-2.078000
N	1.169399	-0.581572	0.327028
S	2.685806	-0.000100	-0.079948
O	2.794291	-0.121382	-1.522862
O	2.807371	1.292147	0.579754
C	3.849516	-1.112070	0.663938
H	3.716080	-1.088710	1.751881
H	3.690934	-2.117592	0.255577
H	4.847353	-0.744879	0.390105
C	-2.234721	2.368399	-0.169258
H	-2.253674	3.188485	-0.893791
H	-2.958482	1.548800	-0.452529
H	-2.604962	2.681278	0.819809
C	0.121545	1.967940	-1.002010
H	0.994351	2.274436	-0.387639
H	0.495121	1.092385	-1.553226
H	-0.140290	2.770994	-1.698663

TS2-1l

C	0.640714	0.077047	1.377703
H	0.764865	-0.737806	2.114682
H	1.094574	0.980485	1.821682
C	-0.803980	0.375056	1.168241
C	-0.884895	-1.268759	-0.467884
C	-1.373480	1.189612	0.088440

C	-1.826922	-0.276085	-0.239501
H	-1.462197	0.198178	2.026079
H	-1.315406	-2.264498	-0.617753
N	-3.148784	-0.595670	-0.042393
C	0.604565	-1.302307	-0.569510
H	0.944158	-2.281182	-0.180389
H	0.861566	-1.314513	-1.645510
C	-3.530300	-1.923517	0.402739
H	-4.545799	-1.874607	0.819422
H	-3.540330	-2.672970	-0.410506
H	-2.856254	-2.269616	1.199891
C	-4.164439	0.079320	-0.846955
H	-4.559328	-0.609907	-1.611906
H	-5.001457	0.423090	-0.221107
H	-3.739712	0.939045	-1.375287
N	1.254954	-0.196031	0.097854
S	2.964553	-0.172141	0.045002
O	3.369827	0.488488	1.268700
O	3.401200	-1.507909	-0.305833
C	3.295266	0.903179	-1.326674
H	2.854253	0.478430	-2.236567
H	2.894194	1.897613	-1.101440
H	4.388688	0.939606	-1.423161
C	-2.468127	2.127500	0.604119
H	-3.028441	2.587902	-0.217985
H	-3.171910	1.625933	1.279431
H	-1.975938	2.939791	1.158108
C	-0.500855	1.886716	-0.950477
H	0.131345	2.641054	-0.459999
H	0.148513	1.208993	-1.508841
H	-1.154919	2.409944	-1.661502

NP-1l

C	-0.820167	-1.443741	0.662634
H	-1.451942	-1.724669	1.523627
H	-0.999591	-2.177848	-0.135058
C	0.641529	-1.354926	1.087684
C	0.852392	0.154893	1.433999
C	1.725736	-1.251340	-0.047616
C	1.804161	0.224742	0.278501
H	0.895482	-2.081129	1.869023
H	1.294872	0.410477	2.408088
N	2.452405	1.219451	-0.215909
C	-0.500869	0.828967	1.180818
H	-1.061999	0.871356	2.132105
H	-0.442111	1.846623	0.775801
C	2.357551	2.566743	0.354543
H	3.372101	2.957186	0.508092
H	1.822970	3.220971	-0.348296
H	1.828840	2.543392	1.312057
C	3.330514	1.102385	-1.381512
H	2.983695	1.795984	-2.159442
H	4.352799	1.375957	-1.087129
H	3.319514	0.081585	-1.769444
N	-1.111401	-0.081057	0.207987
S	-2.735391	0.283924	-0.160072
O	-3.598069	-0.532031	0.672240
O	-2.803024	1.732566	-0.138474
C	-2.875101	-0.281510	-1.836794
H	-2.187129	0.296124	-2.463674
H	-2.670148	-1.357953	-1.880220
H	-3.916766	-0.090607	-2.126986
C	3.025950	-1.962109	0.360957
H	3.845266	-1.747430	-0.340198
H	3.350986	-1.679089	1.373183
H	2.849792	-3.047494	0.355643
C	1.277475	-1.639642	-1.455403
H	0.971912	-2.696054	-1.449255
H	0.424799	-1.032431	-1.788355
H	2.089587	-1.547540	-2.189941

TS3-1l

C	0.376234	-0.308520	1.312270
H	0.181267	-1.233618	1.882095
H	0.966233	0.360525	1.952819
C	-0.968807	0.330355	0.984467
C	-1.011091	-0.748118	-1.135881
C	-0.980851	1.444999	-0.017057
C	-1.764151	-0.500995	-0.002005
H	-1.522078	0.577597	1.898768
H	-1.491354	-1.152400	-2.030275
N	-3.094127	-0.677759	0.098386
C	0.471288	-0.936214	-1.129013
H	0.623015	-2.008997	-1.365731
H	0.934127	-0.391449	-1.971397
C	-3.790914	-0.755113	1.375336
H	-4.648960	-0.066113	1.393614
H	-4.161883	-1.778269	1.541813

H	-3.126600	-0.508853	2.209807
C	-3.857624	-1.084471	-1.071667
H	-3.640113	-2.124760	-1.366287
H	-4.927185	-1.010395	-0.841977
H	-3.647777	-0.419011	-1.922194
N	1.133842	-0.559907	0.102080
S	2.747616	-0.074233	0.026136
O	3.003870	0.262533	-1.362358
O	2.933814	0.898321	1.090025
C	3.686180	-1.522773	0.432654
H	3.422069	-1.843457	1.447338
H	3.474276	-2.302358	-0.308711
H	4.743181	-1.229076	0.386623
C	-2.236522	2.233617	-0.148585
H	-2.320554	2.698757	-1.139820
H	-3.146328	1.669962	0.088495
H	-2.156132	3.057097	0.585679
C	0.240933	2.090858	-0.583219
H	1.020593	2.177966	0.189832
H	0.708228	1.541624	-1.413664
H	-0.013397	3.088030	-0.963398

CP-1l

C	-0.278352	-0.210747	-1.274205
H	-0.100272	-1.165123	-1.801335
H	-0.906150	0.412472	-1.926604
C	1.072357	0.494133	-1.065028
C	1.072333	0.494150	1.064992
C	0.985642	1.650391	-0.000017
C	1.806295	-0.249939	-0.000006
H	1.565012	0.686228	-2.028108
H	1.564944	0.686277	2.028092
N	2.773133	-1.098394	0.000016
C	-0.278398	-0.210678	1.274175
H	-0.100382	-1.165023	1.801377
H	-0.906190	0.412637	1.926492
C	3.362414	-1.610470	-1.239129
H	4.426886	-1.340236	-1.270727
H	3.270223	-2.704820	-1.254312
H	2.848931	-1.188720	-2.108393
C	3.362332	-1.610558	1.239158
H	3.268797	-2.704789	1.254956
H	4.427147	-1.341617	1.270103
H	2.849787	-1.187678	2.108425
N	-0.959148	-0.417127	-0.000020
S	-2.651045	-0.285436	-0.000026
O	-3.019962	0.317247	1.266997
O	-3.019965	0.316945	-1.267197
C	-3.218541	-1.966296	0.000187
H	-2.858092	-2.463738	-0.907854
H	-2.858047	-2.463487	0.908348
H	-4.315598	-1.920307	0.000220
C	2.275558	2.473700	0.000040
H	2.316535	3.120099	0.888629
H	3.185733	1.851050	0.000196
H	2.316747	3.119964	-0.888636
C	-0.225228	2.572655	0.000014
H	-0.193026	3.222755	-0.886338
H	-1.189761	2.055936	-0.000406
H	-0.193449	3.222141	0.886837

TS4-1l

C	0.451290	0.097155	1.460856
H	0.296167	-0.567499	2.328207
H	1.018750	0.969274	1.808090
C	-0.934463	0.521257	0.959911
C	-0.859335	-1.633446	-0.322808
C	-1.068792	1.672276	0.018234
C	-1.598547	-0.626249	0.156616
H	-1.560730	0.717447	1.844741
H	-1.346517	-2.461116	-0.844868
N	-2.981771	-0.443805	-0.105728
C	0.624482	-1.754456	-0.169696
H	0.838547	-2.673624	0.411074
H	1.072344	-1.896752	-1.166178
C	-3.868248	-0.668233	1.042719
H	-4.871225	-0.288297	0.806656
H	-3.937054	-1.740954	1.284986
H	-3.496489	-0.134639	1.927208
C	-3.497686	-1.030562	-1.343595
H	-3.572577	-2.128861	-1.278197
H	-4.501978	-0.630382	-1.535084
H	-2.840745	-0.762916	-2.181209
N	1.211782	-0.582554	0.440622
S	2.644600	0.043003	-0.154796
O	2.626417	-0.165559	-1.592298
O	2.763378	1.376076	0.415413
C	3.928455	-0.969835	0.533371

H	3.902077	-0.879223	1.625544
H	3.779569	-2.006593	0.207690
H	4.875549	-0.581620	0.136299
C	-2.357058	2.229377	-0.040107
H	-2.559008	3.008266	-0.780867
H	-2.852181	1.110468	-0.316444
H	-2.898628	2.345096	0.909037
C	-0.025204	2.014573	-0.968000
H	0.858356	2.391080	-0.418570
H	0.347312	1.132342	-1.509604
H	-0.362927	2.779680	-1.675940

FC-1l

C	0.409759	1.547258	-0.363251
C	-0.776435	0.822172	0.308347
C	-0.323987	-1.001249	-1.392467
C	-2.076181	1.613079	0.332536
C	-1.016463	-0.508454	-0.369520
H	-0.477294	0.614087	1.348036
H	-0.560499	-1.966957	-1.845879
N	-2.068336	-1.295425	0.309582
C	0.895357	-0.265592	-1.888668
C	-1.458200	-2.197086	1.337694
H	-2.247944	-2.579836	1.995647
H	-0.957560	-3.021082	0.815847
H	-0.711759	-1.630535	1.907876
C	-3.014782	-2.008711	-0.588685
H	-2.483655	-2.804114	-1.123025
H	-3.810557	-2.451140	0.022571
H	-3.435374	-1.290147	-1.301318
N	1.418838	0.622605	-0.862038
S	2.379963	-0.136790	0.322524
O	1.719010	0.004639	1.616479
O	2.706013	-1.456685	-0.186450
C	3.842270	0.862733	0.339854
H	4.309045	0.809335	-0.650037
H	3.569967	1.892117	0.600980
H	4.498707	0.433611	1.107951
C	-2.740171	1.760661	1.488756
H	-3.693338	2.293883	1.535731
H	-2.624131	-0.578504	0.809841
H	-2.326032	1.401359	2.436351
C	-2.589365	2.161700	-0.971610
H	-2.020983	3.057333	-1.268613
H	-2.485926	1.432504	-1.791460
H	-3.643815	2.457474	-0.896541
H	0.071394	2.137409	-1.227490
H	0.854113	2.252405	0.350992
H	1.666053	-0.992987	-2.170504
H	0.665669	0.329464	-2.788307

1m

C	-0.931923	-2.089790	-0.067257
H	-0.794563	-2.919125	0.643729
H	-1.375803	-2.531764	-0.972164
C	0.380966	-1.443301	-0.400233
C	-0.951149	0.499235	2.152018
C	1.502001	-1.617557	0.310622
C	-0.613482	1.334167	1.222007
H	1.472256	-2.266181	1.195769
H	0.367831	-0.780350	-1.271232
H	-0.698123	0.752919	3.188354
N	-0.363369	2.122299	0.279450
C	-1.772446	-0.757877	1.894229
H	-2.758195	-0.568475	2.347704
H	-1.314911	-1.587141	2.453960
C	-1.363020	3.109348	-0.173988
H	-1.609625	2.863343	-1.215405
H	-2.263758	3.019326	0.440951
H	-0.921610	4.111780	-0.104657
C	0.890089	2.046546	-0.490245
H	0.636335	1.723272	-1.508832
H	1.341742	3.046469	-0.515138
H	1.572648	1.328044	-0.024040
N	-1.923608	-1.175656	0.521606
S	-2.849835	-0.232126	-0.503260
O	-3.467709	0.778161	0.346239
O	-2.022363	0.187120	-1.628505
C	-4.108581	-1.319791	-1.113594
H	-3.642418	-2.152065	-1.654050
H	-4.705312	-1.672074	-0.264642
H	-4.720194	-0.720826	-1.800771
C	2.794754	-0.964767	0.034112
C	3.160693	-0.559237	-1.259795
C	3.675579	-0.704083	1.094242
C	4.359176	0.114084	-1.478380
H	2.513157	-0.797610	-2.107004
C	4.873134	-0.026131	0.875507

H	3.417468	-1.034983	2.103858
C	5.215424	0.388885	-0.410640
H	4.637331	0.411138	-2.491681
H	5.546876	0.170519	1.711809
H	6.158371	0.910662	-0.585250

TS1-1m

C	-1.582440	0.581707	1.621280
H	-1.714245	1.564886	2.101406
H	-2.013061	-0.166138	2.304403
C	-0.114385	0.280917	1.428985
C	-0.769319	2.192454	-0.756468
C	0.338270	-0.618445	0.521840
C	0.432322	1.850788	-0.360560
H	-0.382833	-1.066085	-0.167854
H	0.566311	0.698926	2.178351
H	-0.739227	3.104090	-1.371246
N	1.704002	2.021041	-0.397288
C	-2.164871	1.679455	-0.520323
H	-2.746587	2.553822	-0.170836
H	-2.571382	1.403806	-1.506060
C	2.406077	2.753277	0.658969
H	3.190720	2.113741	1.085357
H	2.868123	3.652255	0.225332
H	1.696705	3.048504	1.439931
C	2.525521	1.513568	-1.504285
H	2.947627	2.372328	-2.047500
H	3.339671	0.891892	-1.106753
H	1.902698	0.915954	-2.177625
N	-2.320008	0.568809	0.375707
S	-3.042980	-0.845784	-0.178895
O	-2.759555	-0.931073	-1.602011
O	-2.633101	-1.889013	0.741424
C	-4.785223	-0.572125	0.021564
H	-4.996513	-0.415310	1.085678
H	-5.087445	0.291844	-0.582500
H	-5.284161	-1.480583	-0.340503
C	1.722794	-1.047819	0.332264
C	2.757355	-0.706729	1.220039
C	2.034265	-1.804752	-0.808901
C	4.071136	-1.071654	0.947125
H	2.535631	-0.168855	2.144536
C	3.348808	-2.170453	-1.082695
H	1.232856	-2.100429	-1.491041
C	4.371237	-1.793871	-0.211472
H	4.866630	-0.809276	1.647484
H	3.577235	-2.756294	-1.974868
H	5.402939	-2.082732	-0.421774

IN-1m

C	1.467628	0.938101	-1.377849
H	1.625784	1.974569	-1.715260
H	1.792923	0.260384	-2.175145
C	-0.025847	0.741776	-1.083232
C	0.484433	1.871668	1.061440
C	-0.353349	-0.511372	-0.405811
C	-0.452593	1.636470	0.112071
H	0.454577	-1.004570	0.144598
H	-0.645491	0.952984	-1.963214
H	0.234314	2.530347	1.897738
N	-1.776095	2.014361	0.179102
C	1.917990	1.444392	1.000734
H	2.530696	2.363920	1.065056
H	2.163930	0.843098	1.890540
C	-2.310048	2.856076	-0.879485
H	-3.401037	2.730737	-0.940457
H	-2.093253	3.925084	-0.703513
H	-1.881856	2.587873	-1.854939
C	-2.365948	2.239524	1.484872
H	-2.089724	3.218594	1.919553
H	-3.461013	2.209831	1.395151
H	-2.054593	1.443564	2.175364
N	2.255235	0.684207	-0.189342
S	2.995151	-0.819460	-0.005410
O	2.609313	-1.338245	1.300333
O	2.683864	-1.569429	-1.209973
C	4.729751	-0.463357	0.028372
H	5.009678	-0.004508	-0.926769
H	4.940175	0.202486	0.873990
H	5.241200	-1.425238	0.163859
C	-1.628150	-1.089151	-0.265372
C	-2.778575	-0.593159	-0.935408
C	-1.762881	-2.193929	0.621231
C	-4.014939	-1.172236	-0.706584
H	-2.689182	0.220324	-1.653971
C	-3.001746	-2.764726	0.841383
H	-0.875268	-2.578851	1.129595
C	-4.124654	-2.248822	0.180952

H	-4.900095	-0.801396	-1.225305
H	-3.106808	-3.610888	1.521654
H	-5.103195	-2.703092	0.352950

TS2-1m

C	-1.507150	0.495746	1.676279
H	-1.787446	1.284226	2.391996
H	-1.602752	-0.479112	2.185486
C	-0.066575	0.607734	1.273124
C	-0.731887	2.152510	-0.401902
C	0.444605	-0.044870	0.082600
C	0.468592	1.478802	-0.284418
H	-0.318348	-0.559969	-0.506718
H	0.651426	0.968649	2.016315
H	-0.649480	3.218876	-0.638331
N	1.680793	2.124609	-0.283331
C	-2.153785	1.689320	-0.303905
H	-2.757305	2.536817	0.064888
H	-2.495624	1.480727	-1.334122
C	1.745244	3.523440	0.097288
H	2.783708	3.768186	0.359845
H	1.436774	4.212255	-0.711594
H	1.119083	3.709776	0.982329
C	2.697761	1.730743	-1.258675
H	2.682696	2.418666	-2.121575
H	3.695845	1.758815	-0.798712
H	2.521102	0.715748	-1.627179
N	-2.364344	0.520415	0.518527
S	-2.849953	-0.939234	-0.198757
O	-2.550855	-0.823904	-1.617296
O	-2.262530	-1.988769	0.612768
C	-4.607955	-0.959415	0.007732
H	-4.834234	-0.947622	1.080026
H	-5.037650	-0.092312	-0.507651
H	-4.959619	-1.891843	-0.453371
C	1.729662	-0.826096	0.112261
C	1.850053	-1.894449	-0.781082
C	2.775997	-0.546482	0.997173
C	3.011799	-2.664111	-0.803266
H	1.028898	-2.130761	-1.462521
C	3.935423	-1.315940	0.972345
H	2.709163	0.287226	1.699245
C	4.057064	-2.373662	0.070404
H	3.095972	-3.496670	-1.503907
H	4.748896	-1.090978	1.664557
H	4.966996	-2.976371	0.055208

NP-1m

C	1.269383	-1.234705	-0.925574
H	1.775092	-1.510067	-1.867811
H	1.141272	-2.149162	-0.327673
C	-0.047954	-0.524916	-1.200280
C	0.313956	0.997103	-1.245784
C	-0.945209	-0.272815	0.057738
C	-0.642935	1.190553	-0.111228
H	-0.446448	-0.635716	0.973643
H	-0.601665	-0.921102	-2.059356
H	0.074012	1.570118	-2.153467
N	-1.094041	2.247553	0.463319
C	1.802904	1.066262	-0.867878
H	2.394331	1.153811	-1.797005
H	2.072144	1.906222	-0.214978
C	-0.654496	3.588621	0.073500
H	-1.532943	4.183615	-0.210758
H	-0.159414	4.066485	0.929903
H	0.043020	3.534560	-0.768045
C	-2.071815	2.191395	1.552964
H	-1.647035	2.692811	2.433014
H	-2.983715	2.718284	1.240485
H	-2.319000	1.152801	1.792151
N	2.015546	-0.212806	-0.185060
S	3.642817	-0.551159	0.185865
O	4.175840	-1.440803	-0.827523
O	4.240128	0.742787	0.455666
C	3.501494	-1.455910	1.706323
H	3.039149	-0.810027	2.460554
H	2.922733	-2.371484	1.535181
H	4.529145	-1.714656	1.993658
C	-2.391666	-0.701211	0.030466
C	-2.886118	-1.584329	0.993938
C	-3.251547	-0.224029	-0.967421
C	-4.221632	-1.985454	0.961422
H	-2.224072	-1.968695	1.774357
C	-4.585189	-0.621969	-0.997068
H	-2.880730	0.459443	-1.738034
C	-5.072163	-1.503889	-0.031325
H	-4.597009	-2.680294	1.714942
H	-5.247288	-0.247120	-1.779852

H	-6.117002	-1.818625	-0.056483

TS3-1m

C	1.493626	1.159404	-1.217764
H	1.648775	2.233971	-1.403365
H	1.872704	0.603194	-2.083081
C	-0.007033	0.893508	-1.040201
C	0.184244	1.306080	1.287055
C	-0.316881	-0.341898	-0.265373
C	-0.587277	1.597450	0.170800
H	0.523353	-0.888021	0.173059
H	-0.571908	1.032445	-1.966661
H	-0.203637	1.529516	2.284731
N	-1.845575	2.073490	0.193925
C	1.680554	1.118660	1.247707
H	2.102133	2.087430	1.581104
H	1.975674	0.372922	1.999553
C	-2.422532	2.787638	-0.934877
H	-3.440093	2.424717	-1.141720
H	-2.474417	3.867013	-0.720009
H	-1.813808	2.660318	-1.837187
C	-2.552285	2.191957	1.458568
H	-2.180724	3.031407	2.070834
H	-3.616447	2.361468	1.253864
H	-2.465949	1.257090	2.031152
N	2.226389	0.736975	-0.038913
S	3.095122	-0.719725	-0.116180
O	2.634280	-1.551596	0.989025
O	2.988093	-1.185129	-1.485121
C	4.769276	-0.243055	0.209899
H	5.093442	0.445685	-0.578559
H	4.822887	0.222177	1.201412
H	5.362324	-1.166726	0.189043
C	-1.590355	-1.011242	-0.203303
C	-2.698890	-0.627745	-0.984011
C	-1.714910	-2.108179	0.676337
C	-3.902731	-1.311620	-0.871107
H	-2.612359	0.180245	-1.710806
C	-2.920234	-2.784136	0.788203
H	-0.851609	-2.420173	1.269676
C	-4.015865	-2.381502	0.018848
H	-4.754953	-1.021518	-1.487893
H	-3.010690	-3.631673	1.469354
H	-4.963582	-2.917260	0.103376

CP-1m

C	1.414287	1.052582	-1.159506
H	1.573477	2.130704	-1.327233
H	1.809971	0.506873	-2.024800
C	-0.117856	0.764875	-1.052903
C	-0.141393	0.528197	1.063045
C	-0.340926	-0.476554	-0.132040
C	-0.655814	1.537312	0.099353
H	0.448166	-1.237156	-0.202849
H	-0.601999	0.831455	-2.035029
H	-0.673978	0.358332	2.006998
N	-1.414988	2.572613	0.210254
C	1.380774	0.787230	1.281739
H	1.531701	1.803707	1.681996
H	1.751041	0.066934	2.021301
C	-1.881708	3.324352	-0.954807
H	-2.977274	3.257652	-1.011061
H	-1.592348	4.378040	-0.843857
H	-1.440576	2.921563	-1.871676
C	-1.915997	3.036321	1.504861
H	-1.658050	4.096160	1.631513
H	-3.009084	2.925229	1.527980
H	-1.472018	2.453500	2.317284
N	2.098872	0.604287	0.036144
S	3.085986	-0.785980	-0.096290
O	2.765819	-1.643641	1.032129
O	2.953277	-1.262921	-1.460356
C	4.724519	-0.150150	0.128118
H	4.933420	0.571862	-0.669584
H	4.792880	0.311395	1.120094
H	5.401067	-1.011956	0.057393
C	-1.702844	-1.123515	-0.151859
C	-1.865939	-2.321385	0.555399
C	-2.809592	-0.570989	-0.804631
C	-3.108082	-2.945872	0.616191
H	-1.005394	-2.773487	1.056092
C	-4.055469	-1.197270	-0.745222
H	-2.716405	0.346280	-1.391865
C	-4.208056	-2.383186	-0.032341
H	-3.217041	-3.882546	1.166096
H	-4.907632	-0.760378	-1.269599
H	-5.181066	-2.875973	0.010107

1h-O

C	0.226428	0.805821	-1.023640
H	0.950158	0.254390	-1.652679
H	-0.682320	0.957134	-1.624399
C	0.818011	2.140858	-0.631256
C	1.946487	-1.295214	0.604213
C	0.167858	3.100091	0.036476
C	3.094357	-0.885903	0.099933
H	1.858779	2.317899	-0.920520
H	1.799039	-2.377095	0.647813
C	0.874586	-0.345434	1.104465
H	1.324865	0.601393	1.437337
H	0.376042	-0.788298	1.974280
N	-0.153812	-0.003311	0.132816
S	-1.518164	-0.938332	0.024637
O	-1.724248	-1.543660	1.328707
O	-2.550516	-0.131851	-0.607737
C	-1.134030	-2.255643	-1.119673
H	-0.307600	-2.849998	-0.712999
H	-2.040712	-2.866788	-1.212756
H	-0.867724	-1.821088	-2.091033
H	0.722977	4.018795	0.260632
C	-1.250054	3.057188	0.514862
H	-1.282303	3.107809	1.615712
H	-1.802374	3.935931	0.145631
H	-1.783832	2.150146	0.204130
O	4.104822	-0.516280	-0.334386

TS-NP

C	-0.167620	-0.046359	1.538468
H	-0.195229	-0.851800	2.293009
H	0.417562	0.790297	1.956399
C	-1.550514	0.442986	1.256987
C	-1.727287	-1.433870	-0.353827
C	-1.944054	1.151317	0.103310
C	-2.660847	-0.406796	-0.234218
O	-3.871942	-0.403803	-0.199102
H	-2.284729	0.341854	2.061331
H	-2.188837	-2.397882	-0.596123
C	-0.237542	-1.433594	-0.523764
H	0.051901	-1.229596	-1.569369
H	0.103840	-2.462386	-0.302038
N	0.469788	-0.467805	0.314699
S	1.933072	0.148732	-0.150129
C	3.144626	-1.009358	0.456376
H	4.128000	-0.632941	0.146989
H	3.077247	-1.052996	1.550110
H	2.953620	-1.990405	0.004418
O	1.989172	0.101375	-1.601026
O	2.127415	1.394299	0.575910
H	-2.875131	1.705139	0.238920
C	-1.023202	1.759470	-0.936918
H	-0.238734	2.367920	-0.462347
H	-0.515076	1.021296	-1.567905
H	-1.610632	2.408694	-1.598969

TS-CP

C	-0.354268	-0.130235	1.373141
H	-0.471763	-1.030319	2.002900
H	0.224360	0.609337	1.944167
C	-1.723466	0.412885	1.027394
C	-1.752300	-1.137077	-0.922996
C	-1.861458	1.345359	-0.042996
C	-2.592139	-0.605662	0.052169
O	-3.788569	-0.699601	0.256813
H	-2.400459	0.534691	1.878730
H	-2.211015	-1.884046	-1.580486
H	-2.887825	1.697601	-0.186451
C	-0.805963	2.026083	-0.847290
H	-0.430322	1.409634	-1.679203
H	-1.221060	2.942432	-1.288082
H	0.068950	2.277417	-0.229348
C	-0.256252	-1.174941	-0.921971
H	0.057336	-2.239530	-0.888337
H	0.130634	-0.781059	-1.879659
N	0.374139	-0.419026	0.150611
S	1.941538	0.083777	-0.027587
O	2.201362	0.202408	-1.452045
O	2.143951	1.212302	0.869095
C	2.941472	-1.258582	0.583832
H	3.989466	-0.954830	0.466579
H	2.705719	-1.422214	1.642366
H	2.734688	-2.154226	-0.014664

1p

C	-0.040399	-1.631555	0.946423
H	-0.920586	-2.193717	0.611085
H	0.588962	-2.349383	1.490974

C	-0.418158	-0.500150	1.874554
C	-0.121590	0.923760	-1.324925
C	-1.546218	0.222227	1.828033
C	0.744981	1.643369	-0.686996
H	0.330753	-0.245788	2.630701
H	-0.909064	1.421639	-1.901129
N	1.626320	2.250967	-0.032560
C	-0.045010	-0.599693	-1.350897
H	0.397622	-0.873526	-2.321441
H	-1.075889	-0.982132	-1.334861
C	2.938201	2.572160	-0.624488
H	3.695632	2.008612	-0.063931
H	2.951102	2.256735	-1.671669
H	3.109930	3.651955	-0.527941
C	1.460229	2.550172	1.400003
H	2.148070	1.892381	1.949057
H	1.709833	3.604925	1.570697
H	0.427393	2.340619	1.694331
N	0.679788	-1.225251	-0.268037
S	2.339180	-1.075493	-0.205203
O	2.716985	-0.390950	-1.436472
O	2.708789	-0.495161	1.080608
C	2.960622	-2.734580	-0.262203
H	2.586616	-3.296325	0.601840
H	2.646994	-3.190724	-1.208023
H	4.054005	-2.651808	-0.211282
H	-1.652245	1.040301	2.551140
C	-2.653489	0.089571	0.850908
C	-3.294666	-1.130704	0.594462
C	-3.076862	1.228234	0.148795
C	-4.292501	-1.219009	-0.375026
H	-3.033581	-2.014193	1.181496
C	-4.070792	1.140267	-0.823769
H	-2.621106	2.197442	0.371213
C	-4.673587	-0.087974	-1.096365
H	-4.787435	-2.175189	-0.556587
H	-4.389230	2.036697	-1.360260
H	-5.458174	-0.158322	-1.852137

TS1-1p

C	0.072491	1.521473	-1.094680
H	-0.326624	2.549557	-1.016477
H	0.792567	1.534030	-1.928672
C	-1.078758	0.616080	-1.445752
C	-1.285422	0.979318	1.455521
C	-1.240720	-0.724405	-1.282277
C	-2.285657	0.837002	0.623331
H	-1.863971	1.127809	-2.012922
H	-1.634178	1.309150	2.444468
N	-3.532874	0.858311	0.328156
C	0.184157	0.697010	1.329206
H	0.313021	-0.395298	1.452244
H	0.679388	1.157379	2.195584
C	-4.129570	2.004376	-0.361583
H	-5.074494	2.266455	0.133270
H	-3.443516	2.857611	-0.319263
H	-4.333813	1.740665	-1.410673
C	-4.351254	-0.351660	0.443972
H	-5.298499	-0.095657	0.937775
H	-4.564355	-0.752755	-0.558681
H	-3.815462	-1.100221	1.037850
N	0.807553	1.160048	0.100354
S	2.486783	1.158271	0.073064
O	2.904454	0.240184	1.114487
O	2.886594	0.991429	-1.313630
C	2.957169	2.800675	0.566494
H	2.566234	3.518696	-0.164394
H	2.574063	2.998613	1.574770
H	4.054892	2.821043	0.569445
H	-2.207440	-1.120268	-1.618159
C	-0.338629	-1.733794	-0.719490
C	-0.889860	-2.779932	0.041781
C	1.046175	-1.708034	-0.939769
C	-0.068423	-3.736442	0.626859
H	-1.973255	-2.838901	0.179938
C	1.865409	-2.671321	-0.358967
H	1.492490	-0.943030	-1.575417
C	1.313511	-3.676340	0.433635
H	-0.503793	-4.537293	1.227329
H	2.942773	-2.628444	-0.524693
H	1.960593	-4.426943	0.891529

IN1-1p

C	0.143822	-1.106817	-1.215219
H	0.593052	-2.041186	-1.601027
H	-0.590257	-0.769914	-1.957318
C	1.275370	-0.101593	-1.045509
C	1.701771	-1.246452	1.098020

C	1.025522	1.281401	-0.584838
C	2.239245	-0.565956	0.064409
H	1.839498	-0.030494	-1.991337
H	2.350986	-1.612320	1.896400
N	3.548594	-0.117873	-0.015042
C	0.269836	-1.659044	1.222774
H	-0.190432	-1.205820	2.115607
H	0.265911	-2.753834	1.399324
C	4.324176	-0.452965	-1.201570
H	5.199758	0.207519	-1.263578
H	4.678619	-1.499832	-1.183037
H	3.742380	-0.310247	-2.121789
C	4.331664	-0.124243	1.206485
H	4.641322	-1.141332	1.514083
H	5.241934	0.471269	1.053369
H	3.755548	0.329266	2.025119
N	-0.527409	-1.297466	0.056759
S	-2.145835	-1.723338	0.081805
O	-2.619076	-1.432096	1.417812
O	-2.735791	-1.094712	-1.093865
C	-2.216477	-3.482785	-0.169615
H	-1.773392	-3.726378	-1.142944
H	-1.699704	-3.990853	0.653486
H	-3.281651	-3.748313	-0.161228
H	1.982671	1.781882	-0.387776
C	-0.098259	2.065392	-0.309363
C	0.160969	3.351842	0.266788
C	-1.451100	1.696394	-0.574793
C	-0.873657	4.207477	0.579126
H	1.194226	3.647751	0.463067
C	-2.477032	2.564243	-0.259073
H	-1.709532	0.737065	-1.017505
C	-2.192759	3.808678	0.318976
H	-0.671717	5.182962	1.023187
H	-3.508777	2.270968	-0.457146
H	-3.014985	4.483646	0.568974

IN2-1p

C	-0.014499	-1.667643	1.234247
H	-0.328006	-2.720924	1.345126
H	0.694053	-1.443319	2.051847
C	-1.192595	-0.764789	1.424826
C	-1.554906	-1.022064	-1.041635
C	-1.295072	0.589511	0.954595
C	-2.147484	-0.294219	-0.036858
H	-1.964741	-1.104156	2.122200
H	-2.222622	-1.381518	-1.831876
N	-3.523263	-0.201898	0.126054
C	-0.143662	-1.452245	-1.213487
H	-0.158011	-2.456587	-1.682171
H	0.309812	-0.766564	-1.959380
C	-4.343538	-1.304114	-0.342871
H	-5.325627	-1.251835	0.147083
H	-4.517023	-1.288221	-1.435996
H	-3.878087	-2.263220	-0.071852
C	-4.147856	1.106534	-0.034677
H	-4.355867	1.330016	-1.096939
H	-5.097834	1.131323	0.516817
H	-3.506455	1.906662	0.356072
N	0.645751	-1.405386	-0.013415
S	2.287071	-1.031133	-0.087051
O	2.443277	-0.115944	-1.198428
O	2.671570	-0.706475	1.273177
C	3.081557	-2.558780	-0.526307
H	2.890022	-3.300810	0.257810
H	2.710298	-2.891608	-1.503298
H	4.155629	-2.339175	-0.589017
H	-2.038315	1.153686	1.530377
C	-0.177740	1.440842	0.428940
C	-0.223646	1.993276	-0.853806
C	0.870683	1.774001	1.289772
C	0.786331	2.850612	-1.280798
H	-1.050984	1.755212	-1.528135
C	1.879748	2.630515	0.858176
H	0.912547	1.356647	2.298110
C	1.840805	3.166753	-0.426458
H	0.750836	3.271600	-2.287008
H	2.705236	2.870524	1.530014
H	2.637047	3.831596	-0.765386

TS2-1p

C	0.087648	-1.640160	1.300049
H	-0.135113	-2.706099	1.485639
H	0.773995	-1.297664	2.097739
C	-1.153393	-0.824804	1.424558
C	-1.549468	-1.204402	-0.933946
C	-1.331060	0.525509	0.908361
C	-2.171330	-0.306568	-0.087539

H	-1.932991	-1.195218	2.098410
H	-2.209256	-1.730765	-1.630460
N	-3.531471	-0.214875	0.035735
C	-0.108400	-1.546609	-1.137730
H	-0.071750	-2.573446	-1.548552
H	0.282367	-0.872232	-1.925800
C	-4.379257	-1.284287	-0.455847
H	-5.370586	-1.190622	0.007462
H	-4.517315	-1.258684	-1.552428
H	-3.964525	-2.262618	-0.171115
C	-4.179172	1.091063	0.108727
H	-4.627907	1.355177	-0.863312
H	-4.974055	1.082864	0.868767
H	-3.461184	1.880739	0.359744
N	0.713379	-1.393611	0.034902
S	2.335723	-0.965044	-0.089051
O	2.439910	-0.092009	-1.239020
O	2.731191	-0.570841	1.249821
C	3.179194	-2.479555	-0.481238
H	3.031172	-3.195036	0.336297
H	2.802252	-2.866274	-1.435983
H	4.242783	-2.223232	-0.575203
H	-2.042624	1.076878	1.534269
C	-0.228313	1.409377	0.394786
C	-0.252809	1.910089	-0.909299
C	0.776327	1.818962	1.274478
C	0.734222	2.794213	-1.336574
H	-1.043916	1.609613	-1.601876
C	1.764521	2.698583	0.842382
H	0.800069	1.444684	2.300623
C	1.745918	3.185480	-0.462780
H	0.715274	3.174692	-2.359178
H	2.556846	2.998268	1.529988
H	2.524959	3.870533	-0.801426

NP-1p

C	-0.509286	-0.808916	1.916209
H	-0.791598	-1.216652	2.898021
H	0.217965	-1.496149	1.462508
C	0.022415	0.628052	2.088870
C	-1.083331	1.539702	1.469043
C	1.042610	1.162067	1.021930
C	-0.133729	1.778352	0.318914
H	0.317501	0.831815	3.124019
H	-1.326554	2.466597	2.010904
N	-0.301585	2.311904	-0.835387
C	-2.289320	0.624969	1.232361
H	-2.934386	0.653395	2.125068
H	-2.897850	0.897305	0.361638
C	-1.614245	2.786704	-1.278429
H	-1.478066	3.686617	-1.889590
H	-2.080202	1.987614	-1.872669
H	-2.241208	3.030412	-0.414304
C	0.769615	2.406178	-1.829178
H	0.509939	1.763598	-2.682142
H	0.843375	3.449048	-2.164314
H	1.721699	2.080428	-1.401433
N	-1.707313	-0.699156	1.074201
S	-1.764936	-1.413463	-0.438654
O	-1.755062	-0.350320	-1.450497
O	-0.749814	-2.446243	-0.466120
C	-3.366964	-2.169442	-0.476682
H	-3.403375	-2.929820	0.311621
H	-4.137828	-1.403207	-0.331713
H	-3.466760	-2.628377	-1.468897
H	1.570468	2.015414	1.488498
C	2.052885	0.256168	0.371181
C	3.326875	0.156176	0.944025
C	1.741699	-0.528929	-0.743488
C	4.270443	-0.719677	0.414091
H	3.585098	0.766298	1.813848
C	2.686565	-1.405387	-1.272331
H	0.754818	-0.472244	-1.204906
C	3.950804	-1.502992	-0.694982
H	5.260513	-0.789800	0.868301
H	2.424568	-2.020608	-2.134674
H	4.689956	-2.191160	-1.109291

TS3-1p

C	0.254375	-1.320198	-1.136822
H	0.713852	-2.309881	-1.308307
H	-0.430996	-1.141553	-1.976275
C	1.385202	-0.302028	-1.141227
C	1.491580	-0.316576	1.234320
C	1.133909	1.106433	-0.699052
C	2.260027	-0.441587	0.089282
H	1.938252	-0.353883	-2.086284
H	1.969577	-0.144142	2.200969

N	3.599676	-0.337001	0.036073
C	0.043773	-0.661220	1.319832
H	-0.543953	0.243466	1.580652
H	-0.068382	-1.339875	2.183927
C	4.390769	-0.746534	-1.115839
H	5.029522	0.078671	-1.465110
H	5.035075	-1.597515	-0.846516
H	3.753906	-1.072291	-1.944220
C	4.343370	-0.020250	1.245007
H	4.309585	-0.843895	1.977565
H	5.391947	0.161712	0.982093
H	3.949770	0.892922	1.716779
N	-0.487189	-1.275979	0.111436
S	-2.122361	-1.656744	0.102270
O	-2.734913	-0.867815	1.153584
O	-2.562065	-1.557889	-1.280928
C	-2.196803	-3.366745	0.573725
H	-1.655102	-3.964535	-0.168834
H	-1.768181	-3.479206	1.576724
H	-3.260187	-3.639773	0.582295
H	2.052558	1.702327	-0.685916
C	-0.061796	1.849969	-0.442198
C	0.082099	3.077080	0.255794
C	-1.350428	1.462068	-0.874038
C	-1.021600	3.858084	0.546203
H	1.075962	3.396691	0.578805
C	-2.451093	2.256422	-0.587679
H	-1.507847	0.557898	-1.457412
C	-2.292022	3.442816	0.128764
H	-0.902753	4.793798	1.094473
H	-3.439935	1.939452	-0.921019
H	-3.164654	4.057597	0.359057

CP-1p

C	-0.025904	0.540155	-1.227833
H	-0.710502	0.734051	-2.060477
H	0.936271	1.025910	-1.441504
C	0.198888	-0.993126	-1.069180
C	0.198881	-0.993106	1.069201
C	1.305117	-1.288932	0.000018
C	-0.753076	-1.437493	0.000008
H	0.227777	-1.514218	-2.034497
H	0.227792	-1.514254	2.034487
N	-1.907625	-1.992167	0.000017
C	-0.025887	0.540150	1.227860
H	0.936303	1.025893	1.441502
H	-0.710461	0.734083	2.060516
C	-2.638405	-2.263185	-1.240541
H	-3.470313	-1.549004	-1.307945
H	-1.981624	-2.124445	-2.104175
H	-3.015231	-3.293383	-1.215696
C	-2.638508	-2.263053	1.240540
H	-3.470815	-1.549295	1.307486
H	-3.014827	-3.293451	1.216039
H	-1.981985	-2.123648	2.104258
N	-0.595614	1.093095	0.000023
S	-2.263094	1.400448	0.000014
O	-2.801195	0.897393	-1.258067
O	-2.801087	0.897816	1.258297
C	-2.374667	3.165944	-0.000294
H	-1.887924	3.545855	0.905476
H	-1.888201	3.545585	-0.906323
H	-3.444598	3.411545	-0.000153
H	1.509034	-2.372257	0.000018
C	2.611713	-0.542700	0.000001
C	3.249246	-0.227956	-1.205016
C	3.249230	-0.227897	1.205022
C	4.490311	0.406066	-1.205611
H	2.781382	-0.487553	-2.158800
C	4.490274	0.406127	1.205610
H	2.781325	-0.487477	2.158794
C	5.111349	0.728094	-0.000008
H	4.976379	0.645307	-2.153346
H	4.976337	0.645440	2.153330
H	6.082950	1.225446	0.000007

TS4-1p

C	-0.182293	-1.647703	1.098742
H	-0.610660	-2.665617	1.095308
H	0.532330	-1.587750	1.932506
C	-1.309535	-0.663360	1.342200
C	-1.575531	-0.679817	-1.154866
C	-1.241619	0.730859	1.018635
C	-2.169325	-0.312595	0.025136
H	-2.024531	-0.950804	2.119817
H	-2.208021	-0.727020	-2.049451
N	-3.551898	-0.114542	0.186139
C	-0.178857	-1.097909	-1.341853

C	-4.346744	-1.331792	0.117239
H	-4.446883	-1.730445	-0.911981
H	-3.898021	-2.111327	0.749916
H	-5.355804	-1.129682	0.502025
C	-4.109380	1.017298	-0.535411
H	-4.136792	0.864832	-1.633489
H	-5.138704	1.194642	-0.195723
H	-3.526012	1.926543	-0.327786
N	0.535526	-1.357352	-0.121910
S	2.215286	-1.190108	-0.129143
O	2.510584	-0.223245	-1.168464
O	2.611025	-1.008914	1.253839
C	2.823131	-2.771001	-0.664319
H	2.515156	-3.535417	0.058878
H	2.442307	-2.983728	-1.670564
H	3.917761	-2.687011	-0.687132
H	-2.065259	1.320860	1.439786
H	-0.195357	-1.960573	-2.040301
H	0.334507	-0.280839	-1.896922
C	-0.084278	1.512030	0.520205
C	1.055639	1.593366	1.326619
C	-0.156569	2.261988	-0.660470
C	2.120612	2.403642	0.941748
H	1.120392	1.022053	2.253834
C	0.917558	3.055260	-1.048062
H	-1.054507	2.217428	-1.283766
C	2.056971	3.126699	-0.245726
H	3.011073	2.452349	1.570059
H	0.865175	3.624252	-1.977865
H	2.900323	3.747717	-0.552350

TS5-1p

C	-0.502933	-1.011753	1.382416
H	-1.160875	-1.738864	1.887011
H	0.311903	-0.789546	2.077568
C	-1.356999	0.213237	1.026966
C	-2.131962	-1.167321	-0.868805
C	-0.721171	1.340851	0.294445
C	-2.440648	-0.202769	0.023347
H	-1.832007	0.610297	1.941629
H	-2.876336	-1.486930	-1.600781
N	-3.570470	0.595196	-0.022858
C	-0.842990	-1.929714	-0.912222
H	-0.331894	-1.736330	-1.871259
H	-1.086607	-3.010122	-0.893511
C	-4.344790	0.800786	1.192801
H	-4.977298	1.691375	1.076647
H	-4.996952	-0.062335	1.418216
H	-3.698943	0.969974	2.064038
C	-4.381881	0.549371	-1.224681
H	-4.972592	-0.382396	-1.308518
H	-5.084544	1.393523	-1.216407
H	-3.742978	0.640307	-2.114267
N	0.056175	-1.578705	0.173714
S	1.701321	-1.668293	-0.079667
O	2.028462	-0.935643	-1.291702
O	2.322779	-1.307689	1.187935
C	2.011488	-3.390735	-0.380254
H	1.716663	-3.960824	0.508276
H	1.459866	-3.712519	-1.271806
H	3.091053	-3.478016	-0.558342
H	-1.452654	1.893685	-0.308809
C	0.596738	1.780612	0.176233
C	0.891468	2.637953	-0.932983
C	1.646616	1.447033	1.083299
C	2.179367	3.067633	-1.162326
H	0.086341	2.918188	-1.615830
C	2.925016	1.915606	0.862376
H	1.442688	0.854616	1.970718
C	3.193460	2.700900	-0.264764
H	2.410487	3.692458	-2.025690
H	3.724799	1.659471	1.557386
H	4.214208	3.047754	-0.442552

IN3-1p

C	-1.067561	-0.393436	1.682015
H	-1.531185	0.096468	2.547517
H	-0.475163	-1.237760	2.059870
C	-0.237444	0.593221	0.868244
C	-2.465852	1.497042	0.220232
C	0.491750	-0.118112	-0.308209
C	-1.130202	1.697869	0.318422
H	0.521595	1.020116	1.535528
H	-3.127544	2.282580	-0.142878
N	-0.471692	2.805378	-0.179620
C	-3.143215	0.197713	0.549620
H	-3.801127	-0.127426	-0.268844
H	-3.775728	0.265394	1.449994

C	0.768891	3.266094	0.426032
H	1.173494	4.083446	-0.183257
H	0.632469	3.648600	1.454415
H	1.538385	2.481040	0.439534
C	-1.268310	3.818399	-0.840057
H	-1.932162	4.364956	-0.143728
H	-0.604912	4.546347	-1.323091
H	-1.891755	3.359268	-1.621624
N	-2.168700	-0.877598	0.828969
S	-1.625981	-1.729479	-0.459163
O	-2.336547	-1.454678	-1.677154
O	-0.070913	-1.500276	-0.462743
C	-1.672732	-3.437668	-0.041186
H	-1.170042	-3.588036	0.921139
H	-2.734924	-3.709482	0.009890
H	-1.163882	-3.978237	-0.850150
H	0.267046	0.397784	-1.250789
C	1.971945	-0.298300	-0.166768
C	2.807227	0.038316	-1.235375
C	2.533091	-0.792675	1.017742
C	4.188725	-0.109510	-1.121115
H	2.376633	0.423978	-2.163007
C	3.910694	-0.947773	1.128435
H	1.896680	-1.061358	1.864982
C	4.739831	-0.603829	0.058760
H	4.835123	0.161102	-1.957816
H	4.342664	-1.334927	2.053004
H	5.821427	-0.721106	0.148907

TS6-1p

C	1.248708	0.249586	-1.639076
H	1.548708	1.021825	-2.363440
H	1.066501	-0.684230	-2.180891
C	-0.055841	0.752422	-0.964996
C	1.521242	2.196437	0.311023
C	-0.621998	-0.214692	-0.010684
C	0.253838	1.980717	-0.092665
H	0.030010	-0.470083	0.832672
H	-0.761546	0.998380	-1.767131
H	1.757703	3.086318	0.896491
N	-0.860911	2.693014	0.356283
C	2.694598	1.303647	0.013417
H	3.433837	1.855905	-0.593407
H	3.197107	1.033190	0.953740

C	-1.806803	3.197058	-0.625821
H	-2.734589	3.493318	-0.117183
H	-1.418599	4.076006	-1.174704
H	-2.075342	2.431247	-1.364400
C	-0.654573	3.605314	1.463126
H	-0.085623	4.512243	1.179518
H	-1.631430	3.928902	1.847699
H	-0.116442	3.095645	2.274781
N	2.320733	0.080328	-0.689834
S	2.365904	-1.373669	0.157659
O	2.264455	-1.096617	1.584156
O	1.361489	-2.226397	-0.473134
C	3.977116	-2.022554	-0.177847
H	4.070354	-2.180779	-1.258130
H	4.725047	-1.309984	0.190582
H	4.051105	-2.971751	0.368518
C	-1.898883	-0.781607	0.013538
C	-2.883089	-0.536575	-0.987535
C	-2.199793	-1.674775	1.082948
C	-4.111855	-1.157831	-0.910662
H	-2.668736	0.138669	-1.816747
C	-3.434272	-2.292687	1.149402
H	-1.436172	-1.872009	1.838980
C	-4.384085	-2.030861	0.155573
H	-4.870998	-0.976747	-1.672667
H	-3.667060	-2.979536	1.964002
H	-5.360478	-2.518709	0.207406

1p (sol)

C	-0.185430	-1.218800	0.623899
H	-1.035864	-1.659540	0.086420
H	0.138819	-1.960497	1.369219
C	-0.549278	0.068191	1.309261
C	0.822077	0.963880	-1.853751
C	-1.726627	0.707999	1.283536
C	1.364835	1.719216	-0.953794
H	0.286907	0.540018	1.836974
H	0.551918	1.419392	-2.814103
N	1.937889	2.400491	-0.071738
C	0.607555	-0.522275	-1.664816
H	1.217378	-1.029242	-2.429264
H	-0.442014	-0.751816	-1.900368
C	3.406642	2.474521	0.002003
H	3.710430	2.085147	0.982337

H	3.839725	1.862571	-0.794619
H	3.704354	3.526435	-0.094339
C	1.188441	3.149792	0.947403
H	1.489726	2.779608	1.936087
H	1.453567	4.210821	0.852582
H	0.114820	3.004970	0.791647
N	0.899113	-1.026823	-0.342455
S	2.460386	-1.365282	0.096997
O	3.320387	-0.684280	-0.866571
O	2.593774	-1.076018	1.519097
C	2.653568	-3.111650	-0.129818
H	1.932689	-3.635277	0.510946
H	2.487797	-3.348906	-1.188427
H	3.681093	-3.362961	0.166591
H	-1.775146	1.685632	1.777626
C	-2.977613	0.276240	0.620097
C	-3.476262	-1.031661	0.722995
C	-3.710133	1.214088	-0.126123
C	-4.653545	-1.398198	0.070666
H	-2.952187	-1.763621	1.341875
C	-4.883143	0.846740	-0.781290
H	-3.347189	2.243217	-0.196927
C	-5.356641	-0.463402	-0.688669
H	-5.028455	-2.420044	0.165676
H	-5.434428	1.588518	-1.364091
H	-6.279088	-0.751308	-1.198256

TS1-1p (sol)

C	0.227799	-1.516314	1.103268
H	-0.028762	-2.586170	1.006912
H	0.908975	-1.425863	1.962097
C	-1.030832	-0.747545	1.391379
C	-1.214986	-1.198763	-1.378028
C	-1.299820	0.578898	1.197177
C	-2.146747	-0.951926	-0.482013
H	-1.770243	-1.310979	1.969175
H	-1.639831	-1.547053	-2.328011
N	-3.429197	-0.973193	-0.284453
C	0.276034	-1.141022	-1.377420
H	0.575364	-0.287501	-2.007141
H	0.604172	-2.052884	-1.911074
C	-4.050787	-2.087043	0.423634
H	-4.988504	-2.352317	-0.083803
H	-3.375002	-2.950184	0.419212
H	-4.275847	-1.797369	1.462534
C	-4.236078	0.225903	-0.475179
H	-5.195678	-0.062180	-0.925773
H	-4.429632	0.715270	0.493357
H	-3.712360	0.920066	-1.142500
N	0.911976	-1.020880	-0.075667
S	2.576726	-0.975376	-0.077655
O	2.968118	-0.133404	-1.197461
O	2.997524	-0.641216	1.278004
C	3.119005	-2.631443	-0.414004
H	2.752143	-3.294755	0.379761
H	2.746414	-2.943511	-1.398050
H	4.217235	-2.609813	-0.415989
H	-2.305753	0.889489	1.502074
C	-0.488168	1.674173	0.647677
C	-1.131114	2.643206	-0.141431
C	0.876902	1.824911	0.929486
C	-0.414114	3.707488	-0.680119
H	-2.201048	2.548081	-0.343872
C	1.588585	2.898924	0.402973
H	1.389373	1.106875	1.568909
C	0.949644	3.835035	-0.410731
H	-0.921668	4.444413	-1.306355
H	2.652878	2.998880	0.626155
H	1.513621	4.672086	-0.828659

IN1-1p (sol)

C	0.060627	-1.038227	-1.185533
H	0.454937	-1.988751	-1.587174
H	-0.653801	-0.642937	-1.916940
C	1.240356	-0.096413	-1.011945
C	1.638931	-1.310152	1.095649
C	1.063772	1.300040	-0.570792
C	2.193543	-0.627105	0.074353
H	1.787747	-0.045868	-1.969061
H	2.274689	-1.728883	1.878621
N	3.525869	-0.248373	-0.008877
C	0.188616	-1.642350	1.242674
H	-0.221452	-1.167778	2.148066
H	0.121703	-2.735058	1.408268
C	4.258240	-0.554856	-1.227263
H	5.179656	0.043575	-1.256613
H	4.537298	-1.624160	-1.286219
H	3.677356	-0.305333	-2.124795

C	4.327757	-0.374462	1.190195
H	4.569700	-1.426456	1.438588
H	5.275284	0.163723	1.045807
H	3.802083	0.072480	2.046129
N	-0.614766	-1.223036	0.092554
S	-2.191920	-1.751219	0.070338
O	-2.695646	-1.621311	1.428411
O	-2.853746	-1.047001	-1.025486
C	-2.153378	-3.474548	-0.351494
H	-1.698494	-3.590229	-1.343674
H	-1.590240	-4.025237	0.412649
H	-3.197576	-3.814805	-0.369273
H	2.040137	1.771306	-0.403167
C	-0.023492	2.134977	-0.290480
C	0.306638	3.427724	0.225800
C	-1.397735	1.809601	-0.493720
C	-0.683261	4.338958	0.534842
H	1.357810	3.683990	0.376509
C	-2.375712	2.732135	-0.183953
H	-1.701317	0.841540	-0.883621
C	-2.022559	3.987678	0.331314
H	-0.426340	5.321273	0.933355
H	-3.426142	2.480146	-0.336594
H	-2.808968	4.705323	0.576715

TS4-1p (sol)

C	-0.064916	-1.562478	1.087778
H	-0.419025	-2.605311	1.014906
H	0.611949	-1.491630	1.948887
C	-1.268434	-0.674718	1.320694
C	-1.484000	-0.650673	-1.167170
C	-1.289047	0.732862	1.021554
C	-2.129657	-0.434615	0.023389
H	-1.938016	-1.010079	2.118252
H	-2.074497	-0.683289	-2.088748
N	-3.524121	-0.333878	0.171254
C	-0.047921	-0.901575	-1.335035
C	-4.196397	-1.617992	0.282449
H	-4.216008	-2.174679	-0.675777
H	-3.698489	-2.245063	1.036839
H	-5.234411	-1.458194	0.608301
C	-4.176975	0.610188	-0.716715
H	-4.221676	0.266138	-1.769226
H	-5.208433	0.776070	-0.374191

H	-3.647076	1.573921	-0.688338
N	0.658857	-1.142110	-0.098119
S	2.318313	-1.250588	-0.155800
O	2.751575	-0.355824	-1.218126
O	2.806901	-1.081542	1.205127
C	2.666892	-2.914636	-0.657249
H	2.257204	-3.603356	0.092769
H	2.223775	-3.091979	-1.645762
H	3.759906	-3.010935	-0.708750
H	-2.181448	1.251963	1.387250
H	0.033982	-1.735026	-2.061881
H	0.378850	-0.017577	-1.853116
C	-0.205752	1.625068	0.554673
C	1.038333	1.614021	1.195515
C	-0.456571	2.563070	-0.455927
C	2.024600	2.520769	0.816945
H	1.240417	0.894946	1.990375
C	0.537542	3.456843	-0.842662
H	-1.431940	2.575843	-0.949589
C	1.779617	3.436638	-0.205370
H	2.995137	2.499522	1.316407
H	0.341949	4.174246	-1.642358
H	2.559991	4.138089	-0.508621

IN2-1p (sol)

C	0.088284	-1.547366	1.257494
H	-0.136733	-2.625258	1.333491
H	0.760952	-1.279841	2.088372
C	-1.159626	-0.745362	1.439771
C	-1.499921	-1.067691	-1.009223
C	-1.340964	0.597828	0.963355
C	-2.122484	-0.362685	-0.005003
H	-1.895106	-1.131748	2.149765
H	-2.148675	-1.490324	-1.783242
N	-3.509548	-0.343695	0.155802
C	-0.076558	-1.430887	-1.172604
H	-0.047267	-2.487697	-1.506349
H	0.312728	-0.830536	-2.016634
C	-4.245074	-1.514717	-0.281626
H	-5.240674	-1.505178	0.185068
H	-4.389523	-1.556432	-1.378576
H	-3.721887	-2.427570	0.039041
C	-4.180652	0.911318	-0.148024
H	-4.278818	1.072671	-1.238641

H	-5.188373	0.900233	0.291013
H	-3.636914	1.766303	0.275358
N	0.714687	-1.190290	0.006714
S	2.369361	-1.057715	-0.122893
O	2.626254	-0.285740	-1.327810
O	2.850890	-0.608799	1.174222
C	2.963632	-2.706930	-0.389495
H	2.696139	-3.325615	0.476898
H	2.523444	-3.101437	-1.314230
H	4.055664	-2.639504	-0.488725
H	-2.121399	1.123970	1.523874
C	-0.275435	1.514137	0.438732
C	-0.375530	2.089857	-0.830612
C	0.781929	1.875102	1.278264
C	0.583931	3.004215	-1.262693
H	-1.204259	1.818656	-1.489940
C	1.740390	2.787417	0.843519
H	0.863206	1.432770	2.273328
C	1.645008	3.353058	-0.427685
H	0.501624	3.444102	-2.259048
H	2.571267	3.051987	1.501031
H	2.400141	4.064331	-0.769502

TS2-1p (sol)

C	0.165355	-1.474233	1.343045
H	0.038568	-2.553792	1.534245
H	0.798671	-1.053793	2.143508
C	-1.141608	-0.767593	1.425308
C	-1.508907	-1.271549	-0.864306
C	-1.383971	0.563482	0.876206
C	-2.170081	-0.336475	-0.088903
H	-1.895597	-1.168958	2.107866
H	-2.143973	-1.900711	-1.494448
N	-3.534825	-0.311451	0.036071
C	-0.058791	-1.552818	-1.067271
H	0.033413	-2.626831	-1.315319
H	0.266985	-0.987258	-1.958894
C	-4.318968	-1.449104	-0.398523
H	-5.324288	-1.368369	0.037325
H	-4.429139	-1.504717	-1.497435
H	-3.865460	-2.384985	-0.039877
C	-4.240745	0.961045	0.003511
H	-4.626970	1.168655	-1.009601
H	-5.090070	0.939309	0.702332
H	-3.583440	1.792946	0.283409
N	0.757543	-1.178644	0.063593
S	2.402226	-1.005341	-0.110160
O	2.614405	-0.303278	-1.365084
O	2.891220	-0.462424	1.147790
C	3.044187	-2.649345	-0.287373
H	2.809003	-3.223834	0.617942
H	2.604138	-3.112170	-1.180077
H	4.132033	-2.554054	-0.408007
H	-2.115901	1.100126	1.489272
C	-0.305394	1.481627	0.369978
C	-0.290543	1.932728	-0.951821
C	0.650716	1.959943	1.270541
C	0.680386	2.840973	-1.371751
H	-1.036290	1.569309	-1.663319
C	1.620984	2.865257	0.848930
H	0.640478	1.616080	2.307682
C	1.638767	3.308023	-0.473768
H	0.687796	3.183116	-2.408981
H	2.370146	3.224234	1.557949
H	2.401937	4.015668	-0.805133

NP-1p (sol)

C	-0.501971	-0.823529	1.912258
H	-0.816790	-1.224712	2.886809
H	0.252374	-1.502826	1.494719
C	-0.003749	0.620277	2.090857
C	-1.119975	1.511890	1.463251
C	1.014309	1.174244	1.034784
C	-0.158045	1.810094	0.342762
H	0.278375	0.828677	3.127803
H	-1.409867	2.418989	2.012917
N	-0.304531	2.419850	-0.774336
C	-2.292287	0.573665	1.170833
H	-2.971501	0.574608	2.036918
H	-2.872474	0.843470	0.280154
C	-1.603951	2.932399	-1.207563
H	-1.450550	3.899462	-1.701039
H	-2.037704	2.217605	-1.920636
H	-2.271111	3.063640	-0.349735
C	0.794573	2.616029	-1.717028
H	0.577263	2.053294	-2.635339
H	0.855363	3.686338	-1.953421
H	1.739622	2.278601	-1.283446

N	-1.671345	-0.738892	1.028172
S	-1.707572	-1.481513	-0.456625
O	-1.627884	-0.473409	-1.520652
O	-0.723796	-2.554591	-0.427644
C	-3.329636	-2.183880	-0.520556
H	-3.421075	-2.914732	0.291919
H	-4.075049	-1.384645	-0.421318
H	-3.422736	-2.671799	-1.500356
H	1.556046	2.011374	1.510625
C	2.008381	0.258911	0.369834
C	3.246910	0.062081	0.994612
C	1.722915	-0.441600	-0.806347
C	4.180157	-0.820179	0.455339
H	3.480722	0.606898	1.913157
C	2.659482	-1.321698	-1.348159
H	0.762095	-0.312778	-1.308006
C	3.888259	-1.514692	-0.719845
H	5.141826	-0.963757	0.953237
H	2.418970	-1.864278	-2.265037
H	4.619685	-2.206002	-1.144584

TS3-1p (sol)

C	0.173535	-1.297558	-1.152470
H	0.579646	-2.316228	-1.274124
H	-0.481145	-1.101429	-2.011145
C	1.350351	-0.339989	-1.160741
C	1.459166	-0.433864	1.244437
C	1.173152	1.077428	-0.763081
C	2.206872	-0.490808	0.089747
H	1.931925	-0.447627	-2.082823
H	1.953428	-0.365489	2.215679
N	3.553688	-0.389261	0.024656
C	-0.009569	-0.657449	1.318540
H	-0.513542	0.283269	1.622016
H	-0.177797	-1.367768	2.146602
C	4.326148	-0.980113	-1.054765
H	5.096811	-0.275551	-1.401225
H	4.824894	-1.902276	-0.712353
H	3.691034	-1.245485	-1.906962
C	4.301861	-0.047995	1.218725
H	4.353742	-0.886308	1.935863
H	5.326133	0.220624	0.929732
H	3.849766	0.820191	1.720805
N	-0.591741	-1.156120	0.077868
S	-2.175038	-1.640022	0.110833
O	-2.821826	-0.911733	1.193120
O	-2.687496	-1.533983	-1.251285
C	-2.139721	-3.358350	0.544540
H	-1.585646	-3.906673	-0.227974
H	-1.663234	-3.467171	1.527303
H	-3.182328	-3.701788	0.585678
H	2.116643	1.632091	-0.758228
C	0.017670	1.874562	-0.468547
C	0.241269	3.080057	0.240547
C	-1.296595	1.561392	-0.882098
C	-0.814277	3.917168	0.562735
H	1.259027	3.335219	0.545402
C	-2.345914	2.414657	-0.570772
H	-1.503314	0.672813	-1.474132
C	-2.110591	3.581109	0.159665
H	-0.633345	4.836364	1.122708
H	-3.356804	2.164683	-0.897105
H	-2.944487	4.240817	0.409840

CP-1p (sol)

C	-0.072501	0.466988	-1.237636
H	-0.783174	0.628964	-2.054691
H	0.865018	0.983071	-1.486924
C	0.196401	-1.052167	-1.070657
C	0.196406	-1.051988	1.070557
C	1.304628	-1.316663	-0.000034
C	-0.748126	-1.507595	-0.000011
H	0.235259	-1.576801	-2.032221
H	0.235213	-1.576609	2.032134
N	-1.906343	-2.048451	0.000075
C	-0.072354	0.467183	1.237382
H	0.865234	0.983252	1.486456
H	-0.782893	0.629333	2.054521
C	-2.624824	-2.345051	-1.236915
H	-3.535268	-1.732114	-1.259562
H	-2.000744	-2.109595	-2.104010
H	-2.894602	-3.409067	-1.241826
C	-2.625218	-2.343974	1.237095
H	-3.537073	-1.733078	1.257506
H	-2.892590	-3.408596	1.244182
H	-2.002590	-2.105014	2.104288
N	-0.632701	1.012447	-0.000138
S	-2.243292	1.487090	-0.000063

O	-2.845776	1.053162	-1.257289
O	-2.845919	1.052537	1.256881
C	-2.168901	3.253033	0.000416
H	-1.641277	3.579026	0.905593
H	-1.641232	3.579527	-0.904551
H	-3.204597	3.618716	0.000502
H	1.531398	-2.394229	0.000064
C	2.599905	-0.550368	-0.000022
C	3.234610	-0.224086	-1.204717
C	3.234596	-0.224296	1.204742
C	4.469636	0.423551	-1.205415
H	2.761082	-0.480199	-2.156145
C	4.469621	0.423332	1.205580
H	2.761047	-0.480574	2.156115
C	5.090154	0.750992	0.000115
H	4.950292	0.671939	-2.154533
H	4.950264	0.671539	2.154752
H	6.056575	1.260159	0.000169

TS5-1p (sol)

C	-0.337163	0.819509	-1.227213
H	-0.946159	1.444046	-1.903723
H	0.595081	0.587182	-1.746813
C	-1.146725	-0.429087	-0.869395
C	-2.365239	1.130570	0.624068
C	-0.470666	-1.465587	-0.047804
C	-2.390058	-0.017927	-0.080212
H	-1.439348	-0.930522	-1.812568
H	-3.244211	1.448141	1.188148
N	-3.398851	-0.973402	-0.002941
C	-1.198065	2.068821	0.701065
H	-0.928538	2.249720	1.751606
H	-1.494532	3.047241	0.270286
C	-3.950535	-1.513927	-1.234635
H	-4.497959	-2.440765	-1.011464
H	-4.650122	-0.807837	-1.721350
H	-3.163964	-1.764016	-1.957481
C	-4.389158	-0.814092	1.040852
H	-5.092809	0.018525	0.844426
H	-4.977251	-1.739254	1.121489
H	-3.896557	-0.630899	2.006588
N	-0.039814	1.515722	0.012215
S	1.430846	2.256452	0.200960
O	1.550749	2.598000	1.610411
O	2.419907	1.389002	-0.428359
C	1.363189	3.766772	-0.729683
H	1.183239	3.526325	-1.785637
H	0.564960	4.402520	-0.325379
H	2.337474	4.259986	-0.610569
H	-1.143472	-1.943003	0.675134
C	0.835400	-1.950586	-0.030554
C	1.154779	-2.868742	1.020299
C	1.845371	-1.618554	-0.985030
C	2.425500	-3.393367	1.132052
H	0.376950	-3.139127	1.737742
C	3.104336	-2.167701	-0.873703
H	1.618185	-0.963697	-1.822272
C	3.395988	-3.038862	0.186580
H	2.672447	-4.081610	1.941190
H	3.874949	-1.924296	-1.605926
H	4.401779	-3.457592	0.269770

IN3-1p (sol)

C	0.950151	-0.169662	-1.652966
H	1.225545	0.357230	-2.577838
H	0.474468	-1.116905	-1.927520
C	-0.055342	0.751447	-0.898475
C	2.002633	1.928749	-0.115074
C	-0.797700	0.017106	0.146967
C	0.660476	1.901354	-0.208072
H	-0.249636	-0.180696	1.075625
H	-0.742598	1.119106	-1.670391
H	2.505505	2.762671	0.376703
N	-0.206451	2.778558	0.455848
C	2.900882	0.829664	-0.617502
H	3.427365	1.136633	-1.537769
H	3.680555	0.616367	0.127184
C	-1.345127	3.321121	-0.268969
H	-2.033728	3.790800	0.447126
H	-1.043823	4.086026	-1.010297
H	-1.908504	2.539101	-0.792898
C	0.392835	3.731594	1.364692
H	0.967328	4.522456	0.843130
H	-0.400890	4.219095	1.947557
H	1.068972	3.217371	2.062913
N	2.165924	-0.399107	-0.909495
S	2.134610	-1.579748	0.280382
O	2.333010	-0.980269	1.596822

O	0.919304	-2.360186	0.046313
C	3.546437	-2.574063	-0.092411
H	3.417600	-2.999501	-1.094865
H	4.443699	-1.944062	-0.041606
H	3.589980	-3.363684	0.670208
C	-2.105405	-0.461336	0.083717
C	-2.955713	-0.245994	-1.041955
C	-2.588355	-1.220208	1.191061
C	-4.227415	-0.779153	-1.049973
H	-2.608856	0.343063	-1.892039
C	-3.863106	-1.749691	1.168107
H	-1.928537	-1.383699	2.045681
C	-4.676073	-1.527375	0.050024
H	-4.886606	-0.619792	-1.904260
H	-4.235465	-2.335522	2.009453
H	-5.686011	-1.943926	0.033212

TS6-1p (sol)

C	1.220886	0.246294	-1.599645
H	1.489418	1.003707	-2.351344
H	1.096233	-0.713892	-2.110594
C	-0.111893	0.698869	-0.960848
C	1.367139	2.241722	0.326538
C	-0.655958	-0.295222	-0.020665
C	0.118300	1.944029	-0.087095
H	0.010976	-0.571466	0.805295
H	-0.807478	0.917081	-1.778329
H	1.548105	3.149283	0.905189
N	-1.035146	2.604281	0.342684
C	2.594106	1.420713	0.045623
H	3.298253	2.006971	-0.571461
H	3.115602	1.199987	0.988402
C	-2.033737	2.990433	-0.640069
H	-2.972476	3.236036	-0.123346
H	-1.722194	3.875986	-1.227772
H	-2.254209	2.178551	-1.342183
C	-0.875960	3.579924	1.398510
H	-0.353649	4.499384	1.066220
H	-1.868780	3.872823	1.768248
H	-0.310057	3.145853	2.235749
N	2.290090	0.167496	-0.633245
S	2.575023	-1.273826	0.154922
O	2.451487	-1.076790	1.597656
O	1.724085	-2.271095	-0.489649

C	4.267247	-1.635240	-0.203976
H	4.377473	-1.739235	-1.290142
H	4.892213	-0.819456	0.181597
H	4.509084	-2.576504	0.308120
C	-1.924318	-0.870836	0.004023
C	-2.896873	-0.655404	-1.018125
C	-2.241758	-1.724027	1.103842
C	-4.130828	-1.262810	-0.927721
H	-2.661742	-0.022262	-1.874528
C	-3.484734	-2.319136	1.185332
H	-1.488288	-1.891605	1.876777
C	-4.422694	-2.085428	0.172281
H	-4.879796	-1.108634	-1.705511
H	-3.735854	-2.966470	2.026411
H	-5.405944	-2.557575	0.236306

IN-1m (sol)

C	-1.439151	-0.722237	-1.281937
H	-1.683631	-1.742621	-1.619956
H	-1.759369	-0.012065	-2.053308
C	0.070519	-0.616331	-1.066243
C	-0.398029	-1.716743	1.113021
C	0.477911	0.638494	-0.441644
C	0.503946	-1.518971	0.122843
H	0.632708	-0.883178	-1.969260
H	-0.139628	-2.382940	1.940556
N	1.812670	-1.945941	0.146157
C	-1.809033	-1.231336	1.118579
H	-2.007113	-0.653912	2.033770
H	-2.460494	-2.126533	1.165258
C	2.284418	-2.803011	-0.927001
H	3.378981	-2.728022	-1.005650
H	2.018912	-3.861340	-0.748922
H	1.852937	-2.505712	-1.892285
C	2.444632	-2.179325	1.428197
H	2.155827	-3.148020	1.878387
H	3.536306	-2.180811	1.294136
H	2.181184	-1.373121	2.127021
N	-2.108804	-0.408463	-0.035608
S	-3.288360	0.752484	0.035315
O	-3.418299	1.135768	1.434286
O	-2.954403	1.758342	-0.965901
C	-4.788530	-0.046082	-0.465072
H	-4.663461	-0.425185	-1.487461

H	-5.002975	-0.862509	0.236179
H	-5.586063	0.708722	-0.430790
H	-0.312105	1.205410	0.062810
C	1.793168	1.120369	-0.308328
C	2.025529	2.201215	0.586957
C	2.896188	0.517431	-0.969418
C	3.312714	2.636414	0.834132
H	1.173948	2.666240	1.088999
C	4.183603	0.964636	-0.713784
H	2.734858	-0.260814	-1.713554
C	4.389489	2.010688	0.189348
H	3.493491	3.458852	1.527996
H	5.032862	0.507822	-1.224304
H	5.406921	2.356684	0.386519

1a (sol)

C	-2.106765	-0.562341	1.049453
H	-2.374898	-1.629580	1.054090
H	-2.204850	-0.199423	2.087359
C	-3.051754	0.212934	0.158739
C	0.775977	-0.824484	-1.132373
C	-4.062183	-0.396529	-0.470218
C	1.841765	-0.326252	-0.541106
H	-4.222447	-1.475579	-0.381059
H	0.902841	-1.207467	-2.152517
H	-4.766521	0.163619	-1.093243
C	-0.642854	-0.421796	0.689359
O	-0.441568	-0.923378	-0.637126
H	-0.311717	0.631563	0.721589
H	-0.013042	-1.002940	1.384744
N	2.892876	0.150938	-0.052837
C	3.247860	1.571238	-0.204317
H	3.335447	2.011216	0.797700
H	4.216235	1.629974	-0.718115
H	2.470019	2.078569	-0.783541
C	3.842490	-0.670483	0.714741
H	3.916734	-0.253723	1.727738
H	3.484712	-1.704315	0.747061
H	4.821313	-0.613490	0.220900
C	-2.806578	1.692697	0.039644
H	-1.872150	1.899925	-0.508621
H	-3.624590	2.195298	-0.495135
H	-2.702428	2.156901	1.034386

TS1-1a (sol)

C	-2.225820	0.626107	-0.183516
H	-2.280538	0.694376	-1.281671
H	-3.074408	1.217085	0.200196
C	-0.940139	1.246345	0.305275
C	-0.269955	-1.642917	-0.479826
C	-0.368889	0.886280	1.475633
C	0.638735	-0.777329	-0.047929
H	-0.820523	0.170237	2.164627
H	0.542327	1.383012	1.820291
H	0.193241	-2.508150	-0.974658
C	-2.435917	-0.812438	0.237510
O	-1.580581	-1.736704	-0.441110
N	1.857032	-0.392073	-0.082054
C	2.415490	0.335943	-1.222806
H	2.642646	1.369554	-0.925392
H	3.346529	-0.160867	-1.529973
H	1.696519	0.330421	-2.048766
C	2.725565	-0.515860	1.086682
H	3.663978	-0.999558	0.781831
H	2.950337	0.487052	1.479761
H	2.226698	-1.116251	1.854876
H	-2.315961	-0.954079	1.321829
H	-3.445294	-1.143683	-0.032303
C	-0.366679	2.325961	-0.561172
H	0.564014	2.738919	-0.149559
H	-0.179365	1.952565	-1.580040
H	-1.099129	3.144957	-0.656899

IN-1a (sol)

C	-2.047255	0.666999	-0.348954
H	-2.030880	0.785159	-1.443340
H	-2.801887	1.363608	0.046280
C	-0.687453	1.032630	0.209551
C	-0.233488	-1.415068	-0.247079
C	-0.273542	0.476143	1.493230
C	0.337123	-0.201938	0.233750
H	-0.950712	-0.116766	2.109446
H	0.502733	1.009375	2.046652
H	0.421096	-2.201068	-0.645674
C	-2.490632	-0.731340	0.013349
O	-1.466742	-1.700886	-0.352203
N	1.713398	0.020570	-0.010349
C	2.118095	0.004190	-1.404687

H	3.095770	0.498722	-1.508144
H	2.215422	-1.017337	-1.824846
H	1.391355	0.561106	-2.012912
C	2.620986	-0.675913	0.880448
H	2.655986	-1.769587	0.695982
H	3.638948	-0.280133	0.749316
H	2.326511	-0.515101	1.927582
H	-3.376665	-1.046149	-0.546990
H	-2.685857	-0.866954	1.084639
C	-0.123373	2.345022	-0.268654
H	0.914970	2.475943	0.059212
H	-0.168498	2.416917	-1.364799
H	-0.730911	3.161014	0.151935

TS2-1a (sol)

C	2.236594	0.714129	0.267047
H	2.549377	0.666056	1.319883
H	2.771022	1.548020	-0.218137
C	0.769877	0.982167	0.167844
C	0.401218	-1.224247	0.234710
C	0.137508	0.811411	-1.169697
C	-0.474306	-0.371091	-0.467797
H	0.806495	0.591351	-2.004016
H	-0.592864	1.577630	-1.438618
H	-0.032549	-1.881208	0.992456
C	2.574625	-0.574182	-0.463265
O	1.665981	-1.555652	0.018949
N	-1.786424	-0.328146	-0.144363
C	-2.306907	-1.068253	0.993675
H	-3.349840	-0.775692	1.157372
H	-2.277139	-2.157649	0.827427
H	-1.742876	-0.833569	1.910965
C	-2.730250	0.468560	-0.917093
H	-3.703698	-0.038087	-0.906769
H	-2.861728	1.482954	-0.504283
H	-2.417146	0.543815	-1.965186
H	3.581161	-0.936734	-0.225091
H	2.493350	-0.474437	-1.554996
C	0.090093	1.810433	1.203164
H	-1.002629	1.692773	1.164387
H	0.453049	1.571249	2.211648
H	0.312428	2.872215	1.000386

TS3-1a (sol)

C	-2.012767	0.798292	-0.289886
H	-2.148358	1.559147	-1.072035
H	-2.757269	0.992337	0.495522
C	-0.612684	0.930802	0.315533
C	-0.355659	-1.445097	0.177439
C	-0.400446	0.041016	1.517438
C	0.325088	-0.213641	-0.005567
H	-1.266193	-0.468453	1.947255
H	0.424290	0.257612	2.200980
H	0.162675	-2.356488	0.489163
C	-2.213812	-0.565908	-0.921710
O	-1.618120	-1.615174	-0.124409
H	-1.735188	-0.611380	-1.912132
H	-3.270388	-0.835514	-1.018910
N	1.691525	-0.070317	-0.057654
C	2.505045	-1.212320	0.307703
H	3.552046	-0.889557	0.381926
H	2.202166	-1.601244	1.291378
H	2.448119	-2.032947	-0.433290
C	2.228155	0.730625	-1.150910
H	3.170393	1.202719	-0.836444
H	2.427615	0.108176	-2.041950
H	1.527256	1.520927	-1.440662
C	-0.084385	2.343605	0.396155
H	-0.051465	2.810219	-0.598263
H	-0.768928	2.934408	1.022357
H	0.916300	2.379407	0.846798

CP-1a (sol)

C	-1.476138	0.612307	-1.046393
H	-0.845686	0.710377	-1.943642
H	-2.278398	1.361956	-1.121458
C	-0.619685	0.937765	0.210233
C	-0.534316	-1.116698	0.817148
C	-1.212458	0.137110	1.413004
C	0.449491	-0.128120	0.214810
H	-2.303836	0.128704	1.527203
H	-0.735718	0.420514	2.361322
H	-0.170748	-1.908118	1.483375
C	-2.093619	-0.786159	-0.933905
O	-1.251171	-1.701438	-0.239344
N	1.692986	-0.197089	-0.080212
C	2.474282	-1.418557	0.118843
H	3.327714	-1.184699	0.768992

H	1.861477	-2.202327	0.572217
H	2.845835	-1.756039	-0.857677
C	2.443141	0.920864	-0.653101
H	3.179824	1.269827	0.082968
H	2.969259	0.557392	-1.545226
H	1.771821	1.735710	-0.931479
C	-0.319944	2.412318	0.381076
H	0.013175	2.879518	-0.557095
H	-1.244177	2.920534	0.694153
H	0.442772	2.579680	1.155419
H	-2.274365	-1.219992	-1.926039
H	-3.065007	-0.726895	-0.417094

1h (sol)

C	0.651159	-1.749873	-0.504692
H	1.063118	-2.602932	0.053470
H	0.097650	-2.168492	-1.357657
C	1.727048	-0.832264	-1.012989
C	0.506777	0.708845	1.922426
C	3.023634	-0.856721	-0.682018
C	0.483120	1.594238	0.978579
H	1.375731	-0.065858	-1.712628
H	0.824558	1.026647	2.922708
N	0.385596	2.424937	0.045184
C	0.051233	-0.720308	1.718740
H	-0.787720	-0.886539	2.412293
H	0.861503	-1.391105	2.041416
C	-0.876634	3.138519	-0.211642
H	-1.167126	2.936810	-1.250611
H	-1.645796	2.766301	0.471892
H	-0.701886	4.213093	-0.071810
C	1.510837	2.732557	-0.849194
H	1.200565	2.512779	-1.878870
H	1.739028	3.802139	-0.752019
H	2.377684	2.125865	-0.568847
N	-0.312288	-1.063937	0.363658
S	-1.789976	-0.624228	-0.242690
O	-2.366048	0.317124	0.714051
O	-1.607959	-0.219334	-1.631208
C	-2.770150	-2.099849	-0.225668
H	-2.288179	-2.857557	-0.856606
H	-2.860611	-2.447381	0.811119
H	-3.755109	-1.835506	-0.633953
H	3.670567	-0.104078	-1.149683
C	3.717321	-1.791129	0.259199
H	3.045597	-2.532886	0.712156
H	4.522763	-2.333701	-0.261844
H	4.200095	-1.223368	1.071429

TS1-1h (sol)

C	0.389499	-0.171997	1.410918
H	0.245981	-1.138817	1.922619
H	1.057852	0.436558	2.037713
C	-0.933284	0.534318	1.272776
C	-1.070580	-1.300984	-0.857387
C	-1.173416	1.600081	0.456184
C	-1.997291	-0.559962	-0.285683
H	-1.685248	0.287180	2.028700
H	-1.498386	-2.083998	-1.496281
N	-3.288147	-0.423437	-0.196035
C	0.418781	-1.348986	-0.763337
C	-4.012464	-0.990641	0.934852
H	-4.981206	-1.370615	0.582673
H	-3.433637	-1.814102	1.369449
H	-4.189221	-0.217928	1.700847
C	-3.993125	0.561692	-1.005725
H	-4.923616	0.113258	-1.381285
H	-4.245856	1.446360	-0.398536
H	-3.365854	0.863389	-1.852673
N	1.006770	-0.361841	0.110937
S	2.596081	0.057992	-0.127837
O	2.799235	0.125330	-1.567452
O	2.847077	1.230691	0.701698
C	3.567678	-1.280983	0.509236
H	3.348747	-1.401422	1.578223
H	3.327578	-2.193381	-0.052015
H	4.622272	-1.011120	0.362159
H	-2.176785	2.032873	0.530513
C	-0.244914	2.286630	-0.487870
H	-0.584108	3.319200	-0.647643
H	0.790434	2.294054	-0.125101
H	-0.246530	1.787967	-1.471054
H	0.667926	-2.382229	-0.447985
H	0.826204	-1.221338	-1.777020

IN1-1h (sol)

C	0.467911	-0.316489	1.494237
H	0.407653	-1.276494	2.033032

H	1.076896	0.376096	2.098202
C	-0.884858	0.305368	1.372987
C	-1.145712	-1.036664	-0.702478
C	-1.241070	1.308609	0.409209
C	-1.878396	-0.048952	-0.086853
H	-1.584632	0.126930	2.193955
H	-1.717730	-1.828392	-1.196593
N	-3.255042	-0.149020	0.106608
C	0.317901	-1.279297	-0.737016
C	-3.836968	-1.475236	0.176855
H	-3.957194	-1.953901	-0.814330
H	-3.215975	-2.127086	0.809129
H	-4.834308	-1.400975	0.633774
C	-4.095965	0.818540	-0.581678
H	-4.250751	0.546810	-1.642973
H	-5.078360	0.863503	-0.090079
H	-3.655443	1.823422	-0.549285
N	1.057867	-0.458523	0.186027
S	2.584703	0.089724	-0.162830
O	2.627792	0.295827	-1.604072
O	2.845366	1.192669	0.751097
C	3.684607	-1.238030	0.238817
H	3.590180	-1.461950	1.309168
H	3.425466	-2.109680	-0.375920
H	4.701728	-0.894334	0.005906
H	-2.091004	1.898690	0.763077
C	-0.303750	2.098536	-0.479599
H	-0.885883	2.861096	-1.013856
H	0.450497	2.606621	0.137592
H	0.224379	1.492121	-1.221664
H	0.470739	-2.361444	-0.555500
H	0.661246	-1.090079	-1.769878

IN2-1h (sol)

C	-0.278780	-0.302840	-1.296518
H	-0.100683	-1.314042	-1.699285
H	-0.894217	0.251884	-2.016400
C	1.056401	0.396366	-1.129712
C	1.180874	-0.646169	1.099370
C	1.130935	1.583942	-0.300547
C	1.895094	-0.179760	0.029741
H	1.650975	0.435098	-2.048582
H	1.710443	-1.097326	1.942157
N	3.271904	-0.145490	-0.058938
C	-0.292356	-0.736574	1.184632
C	3.902643	-0.780450	-1.205320
H	3.953321	-1.879625	-1.094384
H	3.365626	-0.553798	-2.135320
H	4.926725	-0.396018	-1.312161
C	4.023746	-0.257107	1.174787
H	4.036310	-1.286542	1.581879
H	5.063750	0.044425	0.987636
H	3.602624	0.416510	1.935339
N	-0.978820	-0.332255	-0.023614
S	-2.617513	-0.065299	0.030996
O	-2.939742	0.238332	1.417692
O	-2.932695	0.894627	-1.019977
C	-3.365826	-1.612107	-0.397444
H	-3.045982	-1.890695	-1.410049
H	-3.058693	-2.366082	0.338422
H	-4.453996	-1.464885	-0.366360
H	2.115813	2.060153	-0.300207
C	0.044859	2.320530	0.385008
H	-0.168454	1.923095	1.391236
H	0.367173	3.361219	0.522624
H	-0.892988	2.276599	-0.185258
H	-0.508133	-1.785959	1.469272
H	-0.647026	-0.123669	2.035660

TS2-1h (sol)

C	0.526116	-0.238090	1.531424
H	0.543111	-1.153538	2.145902
H	1.089672	0.546925	2.064576
C	-0.863576	0.275810	1.378025
C	-1.139144	-1.134409	-0.522856
C	-1.269982	1.246147	0.371535
C	-1.919540	-0.059080	-0.140502
H	-1.569061	0.075186	2.189633
H	-1.685630	-2.024589	-0.847207
N	-3.280382	-0.160246	0.013836
C	0.338216	-1.329317	-0.620074
C	-3.905624	-1.466232	0.048565
H	-3.982899	-1.935411	-0.950089
H	-3.346819	-2.140263	0.714570
H	-4.922769	-1.357284	0.449376
C	-4.143735	0.905114	-0.473620
H	-4.508821	0.683455	-1.491912
H	-5.013273	1.015827	0.190881

H	-3.615452	1.865125	-0.511345
N	1.090572	-0.431646	0.221235
S	2.604281	0.103389	-0.189949
O	2.609795	0.252284	-1.638646
O	2.883847	1.242428	0.673188
C	3.721744	-1.203365	0.232827
H	3.655344	-1.389196	1.312476
H	3.453967	-2.098186	-0.343850
H	4.730629	-0.862922	-0.037736
H	-2.080630	1.865955	0.764215
C	-0.329771	2.040844	-0.515935
H	-0.916125	2.800541	-1.050511
H	0.425354	2.554448	0.094930
H	0.194260	1.431056	-1.258818
H	0.542243	-2.389223	-0.379687
H	0.629714	-1.181113	-1.674380

TS3-1h (sol)

C	-0.270052	-0.272769	-1.292735
H	-0.095790	-1.273082	-1.723171
H	-0.876999	0.305261	-2.001294
C	1.069025	0.412710	-1.097515
C	1.178852	-0.591774	1.126232
C	1.125824	1.578526	-0.219388
C	1.903853	-0.206794	0.025489
H	1.645446	0.505247	-2.023882
H	1.696841	-0.993128	2.000689
N	3.270499	-0.195540	-0.056898
C	-0.295671	-0.704687	1.194204
C	3.927353	-0.675343	-1.261560
H	4.066305	-1.771292	-1.242415
H	3.354231	-0.420704	-2.161150
H	4.915580	-0.202267	-1.350322
C	4.032636	-0.363524	1.163641
H	4.020451	-1.404812	1.536644
H	5.077244	-0.083299	0.971809
H	3.641005	0.297471	1.950884
N	-0.980175	-0.332309	-0.025666
S	-2.621818	-0.079587	0.016864
O	-2.959915	0.214891	1.401865
O	-2.939062	0.882497	-1.031876
C	-3.352041	-1.630847	-0.425858
H	-3.020325	-1.901039	-1.436899
H	-3.044672	-2.385697	0.308964
H	-4.441722	-1.493329	-0.404141
H	2.114390	2.044561	-0.167982
C	0.015631	2.324189	0.416949
H	-0.211551	1.964702	1.434809
H	0.330913	3.371225	0.525586
H	-0.910458	2.257709	-0.168637
H	-0.490976	-1.755520	1.488844
H	-0.673731	-0.090893	2.033118

TS4-1h (sol)

C	-0.312599	-0.634301	-1.275562
H	-0.118818	-1.699308	-1.484946
H	-0.955886	-0.237757	-2.071526
C	1.000671	0.117840	-1.282443
C	1.188858	-0.564335	1.111048
C	1.139011	1.399042	-0.651432
C	1.863842	-0.090033	0.018645
H	1.639695	-0.069753	-2.151760
H	1.765058	-0.926055	1.969243
N	3.262533	-0.079210	-0.118657
C	-0.267882	-0.753437	1.213382
C	3.808754	-1.301537	-0.684584
H	3.774038	-2.152244	0.025215
H	3.252493	-1.584078	-1.589999
H	4.857364	-1.134593	-0.970563
C	4.001776	0.428658	1.021795
H	4.015487	-0.269204	1.882830
H	5.044588	0.610681	0.724155
H	3.567632	1.383248	1.353406
N	-0.983865	-0.452816	-0.001822
S	-2.578150	0.014872	0.071023
O	-2.770074	0.616051	1.383995
O	-2.854357	0.783149	-1.135271
C	-3.518013	-1.483108	-0.001662
H	-3.296794	-1.990617	-0.949365
H	-3.249011	-2.109939	0.858269
H	-4.578808	-1.201119	0.045310
H	2.078531	1.902481	-0.896006
C	0.105553	2.255440	0.010560
H	-0.281465	1.861745	0.957415
H	0.530769	3.247021	0.206406
H	-0.758415	2.356681	-0.664655
H	-0.397672	-1.803885	1.548736
H	-0.653429	-0.136062	2.046530

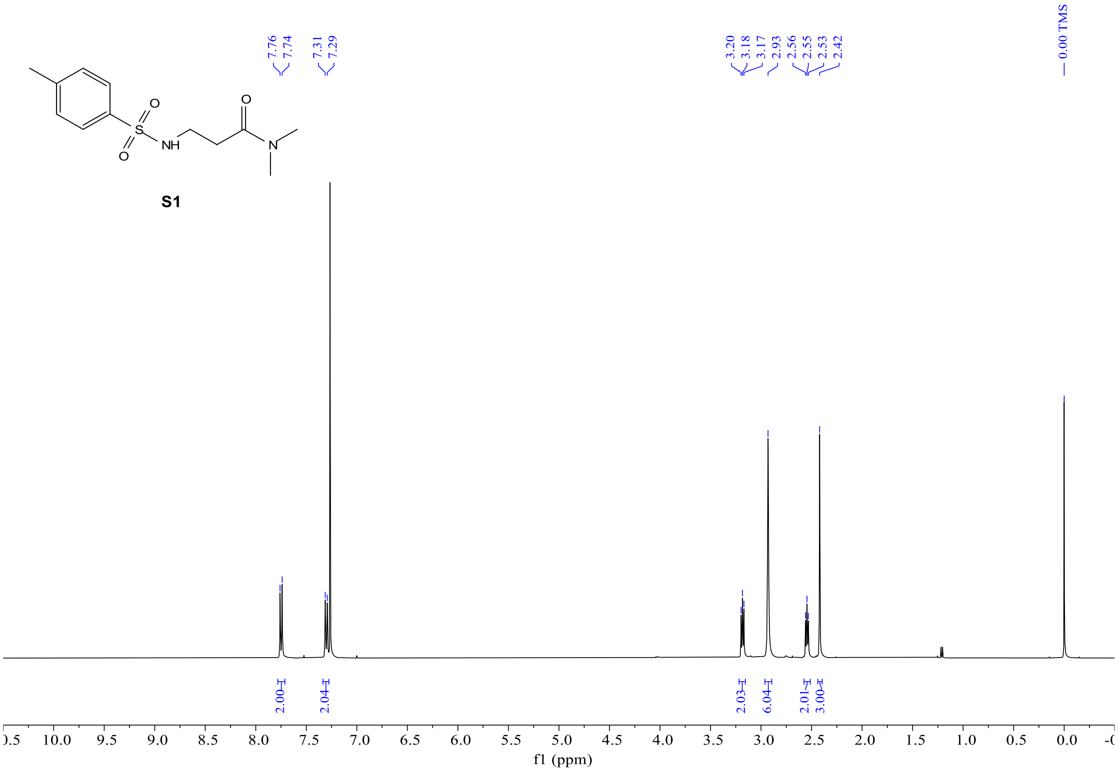
NP-1h (sol)

C	-0.855979	1.251120	-1.062379
H	-1.487004	1.249362	-1.967694
H	-1.138167	2.117149	-0.447110
C	0.616708	1.241926	-1.447905
C	1.028474	-0.267591	-1.436593
C	1.645871	1.530267	-0.305041
C	1.998748	0.070767	-0.344282
H	0.813082	1.794229	-2.372816
H	1.495729	-0.695368	-2.333926
N	2.862910	-0.642348	0.278747
C	-0.219332	-1.039241	-0.989942
H	-0.002899	-1.871691	-0.309158
H	-0.732942	-1.433357	-1.883540
C	3.026160	-2.071484	0.017367
H	2.832484	-2.622231	0.947818
H	2.335893	-2.404371	-0.763282
H	4.061655	-2.251530	-0.300461
C	3.741310	-0.083500	1.305821
H	3.349570	-0.349478	2.297345
H	4.739628	-0.520724	1.182113
H	3.805734	1.004274	1.204064
N	-0.997321	0.000559	-0.311171
S	-2.505338	-0.406363	0.280125
O	-3.548410	0.080297	-0.616708
O	-2.446733	-1.827014	0.602502
C	-2.593052	0.530300	1.780133
H	-1.808041	0.178949	2.460117
H	-2.478195	1.597025	1.548425
H	-3.589162	0.343317	2.204353
H	2.505387	2.107723	-0.687291
C	1.148295	2.139116	0.999856
H	1.963999	2.254276	1.726187
H	0.736693	3.138045	0.796762
H	0.360758	1.522389	1.454503

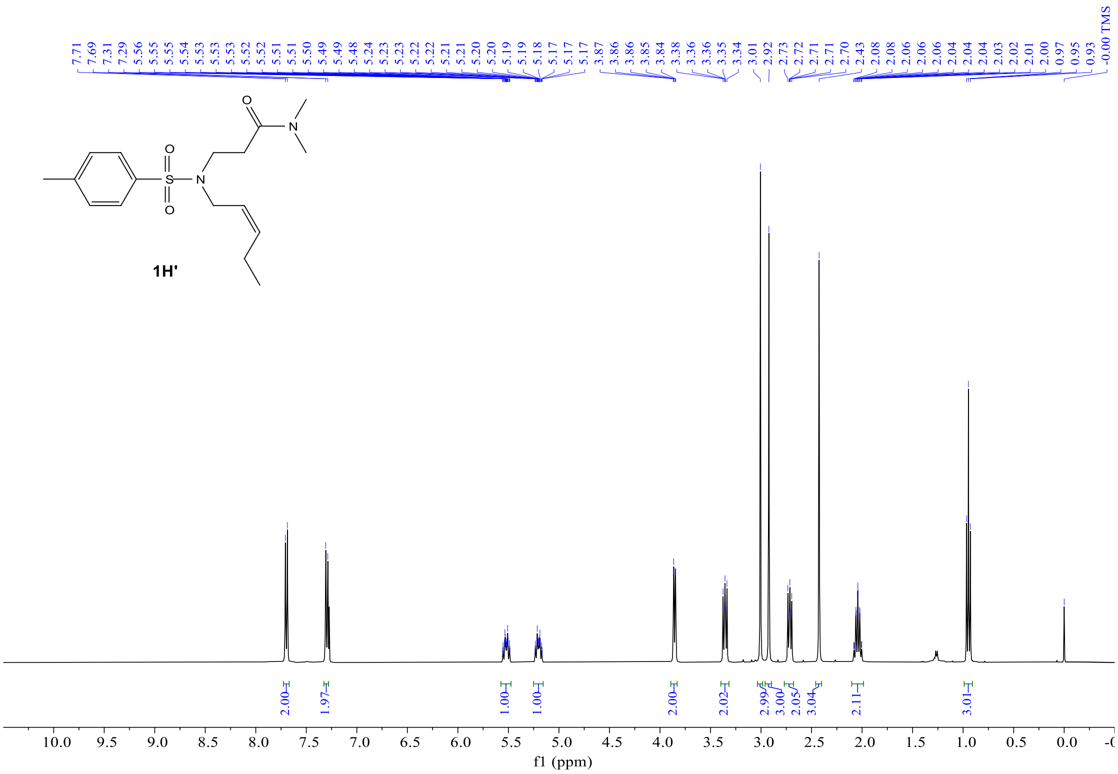
CP-1h (sol)

C	0.180353	0.219542	1.290374
H	0.048052	-0.721334	1.850754
H	0.789696	0.897353	1.904697
C	-1.188908	0.864132	1.068753
C	-1.188966	0.864270	-1.068615
C	-1.105300	2.001810	0.000139
C	-1.896864	0.095107	0.000039
H	-1.694256	1.043122	2.025533
H	-1.694354	1.043387	-2.025350
N	-2.838841	-0.772589	0.000013
C	0.180282	0.219692	-1.290382
H	0.047940	-0.721116	-1.850864
H	0.789595	0.897570	-1.904662
C	-3.405859	-1.307289	1.236591
H	-4.480710	-1.083450	1.257926
H	-3.263116	-2.396017	1.243356
H	-2.913123	-0.863888	2.106845
C	-3.406005	-1.307061	-1.236595
H	-3.263222	-2.395781	-1.243608
H	-4.480867	-1.083258	-1.257735
H	-2.913405	-0.863461	-2.106823
N	0.833715	-0.014966	-0.000035
S	2.431351	-0.450834	-0.000088
O	3.004520	-0.004974	-1.263154
O	3.004647	-0.004861	1.262880
C	2.422463	-2.224194	0.000003
H	1.911788	-2.575558	0.905855
H	1.911731	-2.575652	-0.905781
H	3.470437	-2.552992	-0.000011
H	-2.060965	2.544788	0.000197
C	0.048993	2.983836	0.000172
H	-0.008409	3.629901	0.888647
H	1.031424	2.492228	0.000126
H	-0.008444	3.630001	-0.888227

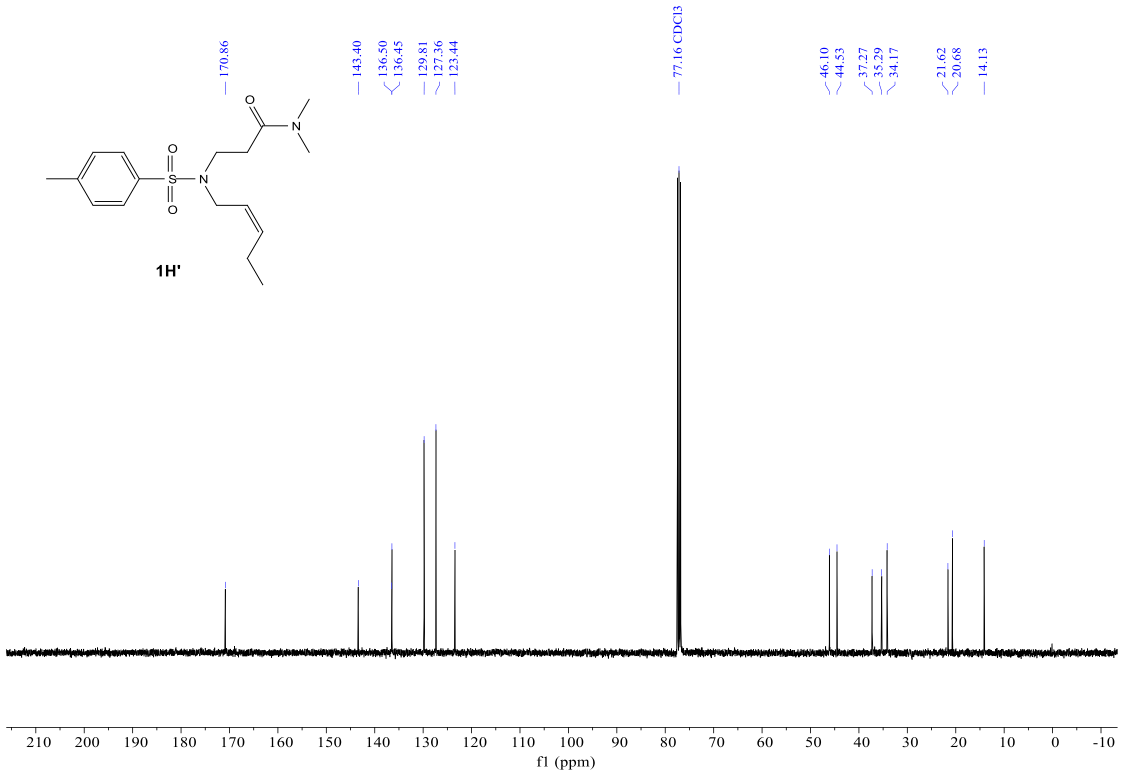
S8. Copies of NMR Spectra



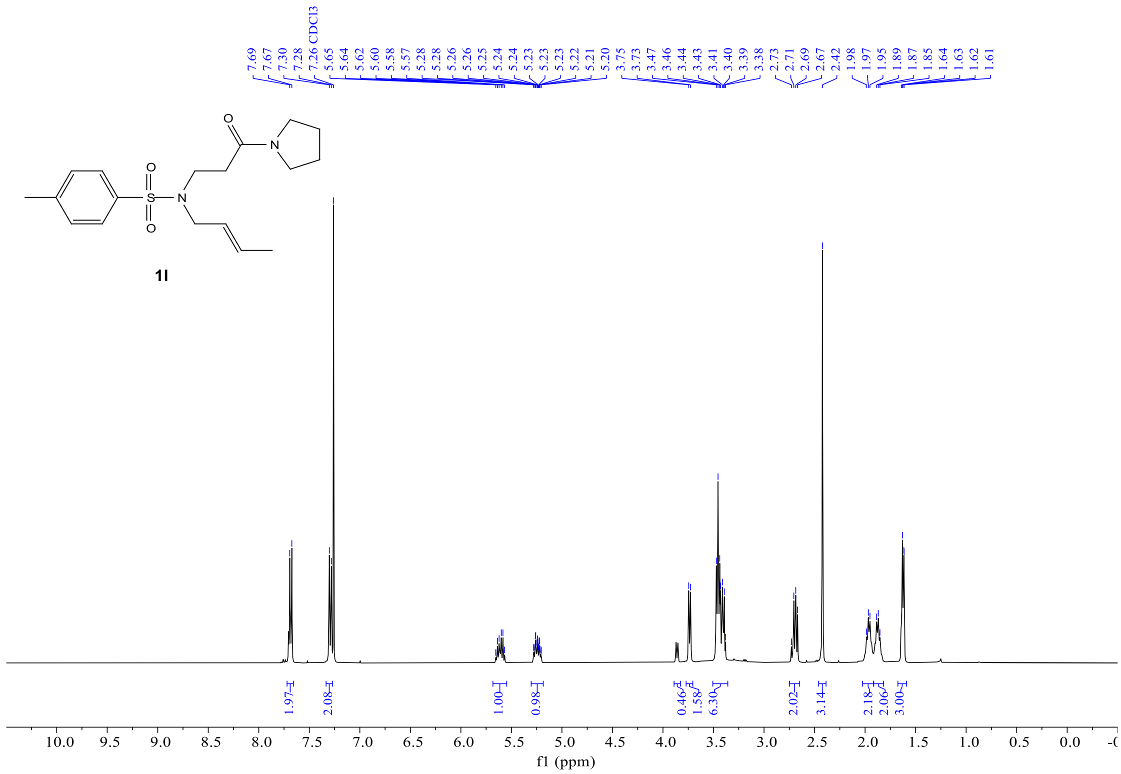
^{1}H NMR of compound **S1** (400 MHz, $CDCl_3$)



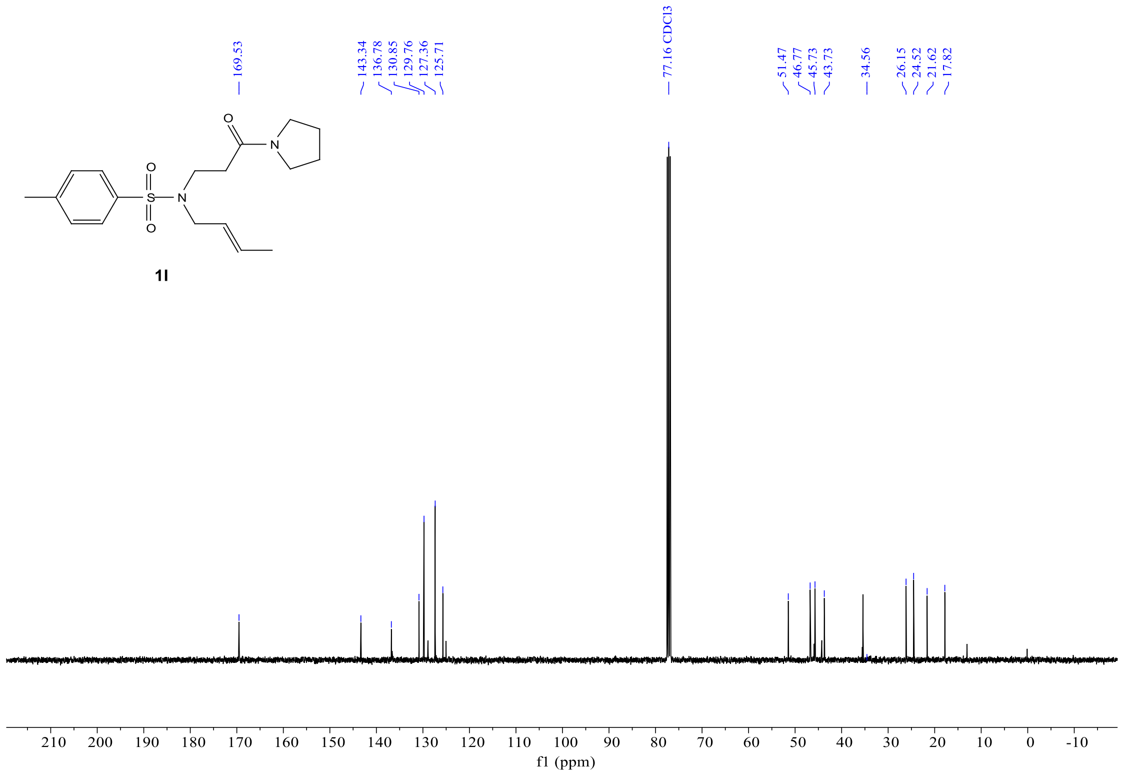
^{1}H NMR of compound **1H'** (400 MHz, $CDCl_3$)



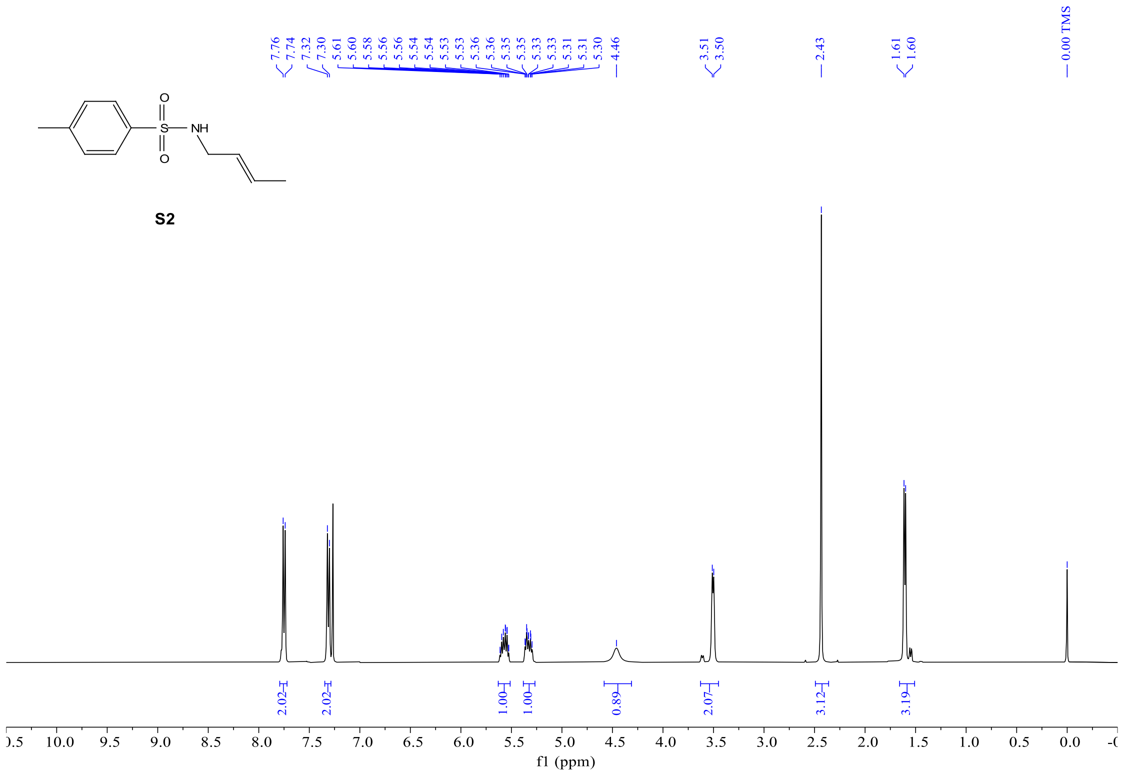
^{13}C NMR of compound **1H'** (101 MHz, $CDCl_3$)



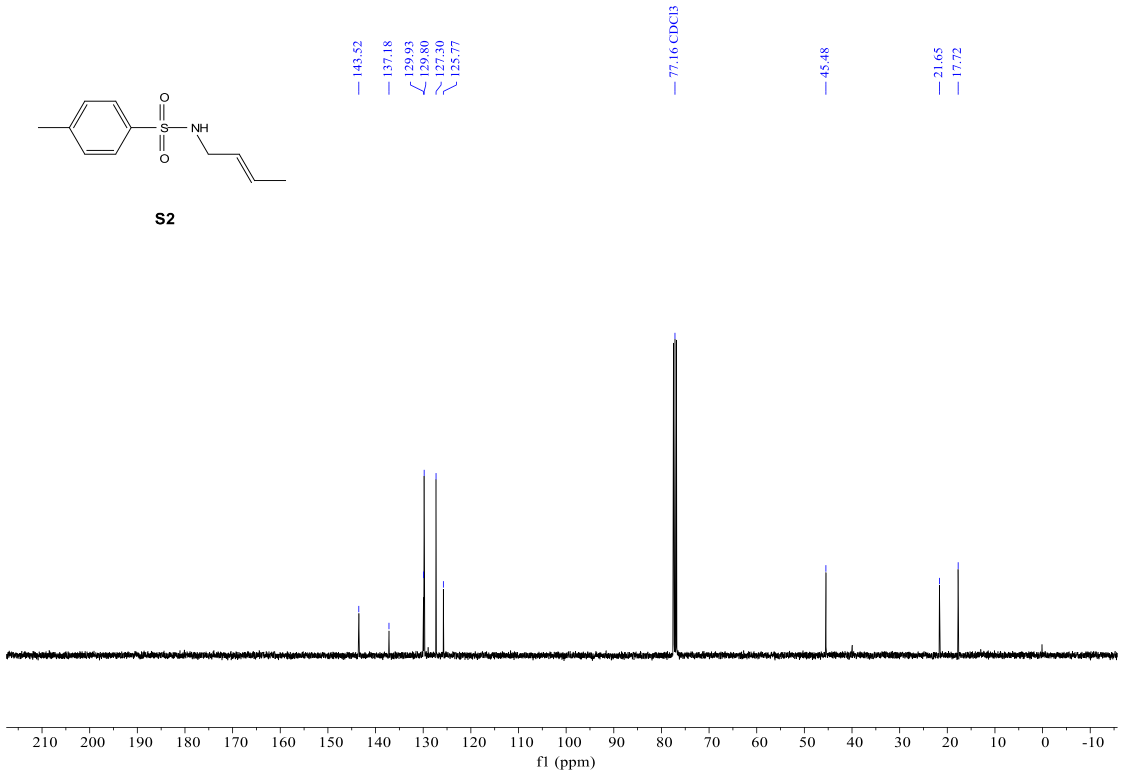
^{1}H NMR of compound **1I** (400 MHz, $CDCl_3$)



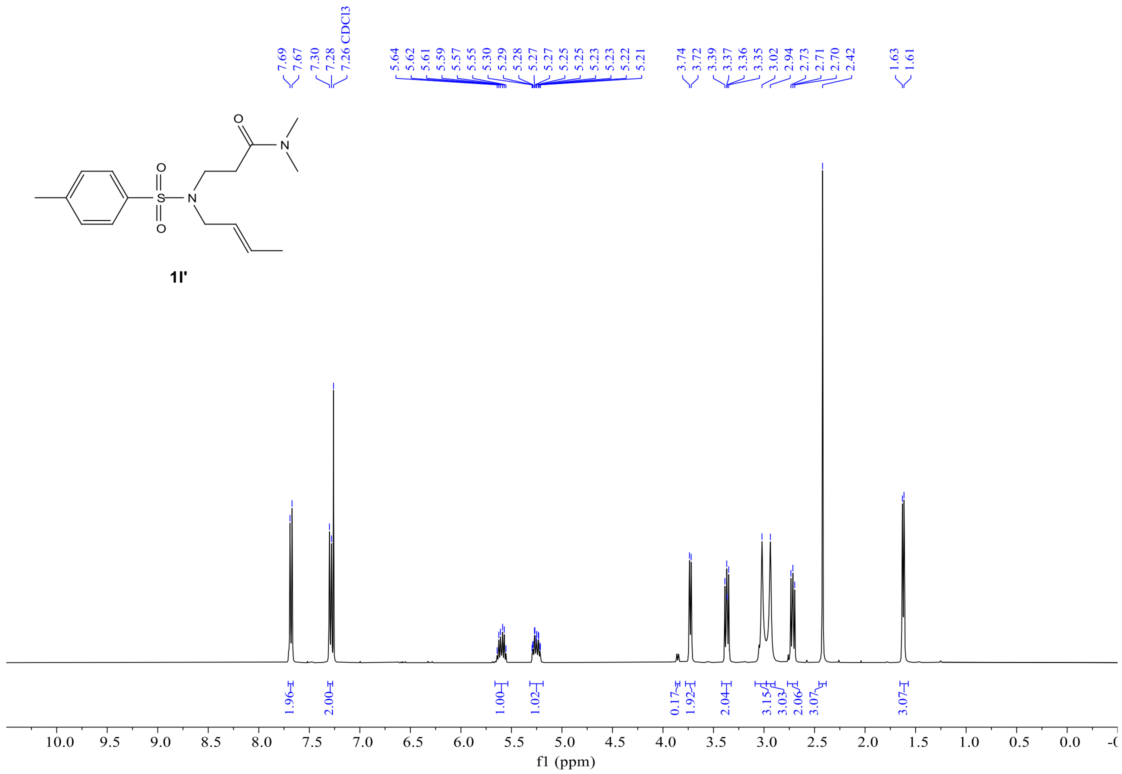
^{13}C NMR of compound **1l** (101 MHz, $CDCl_3$)



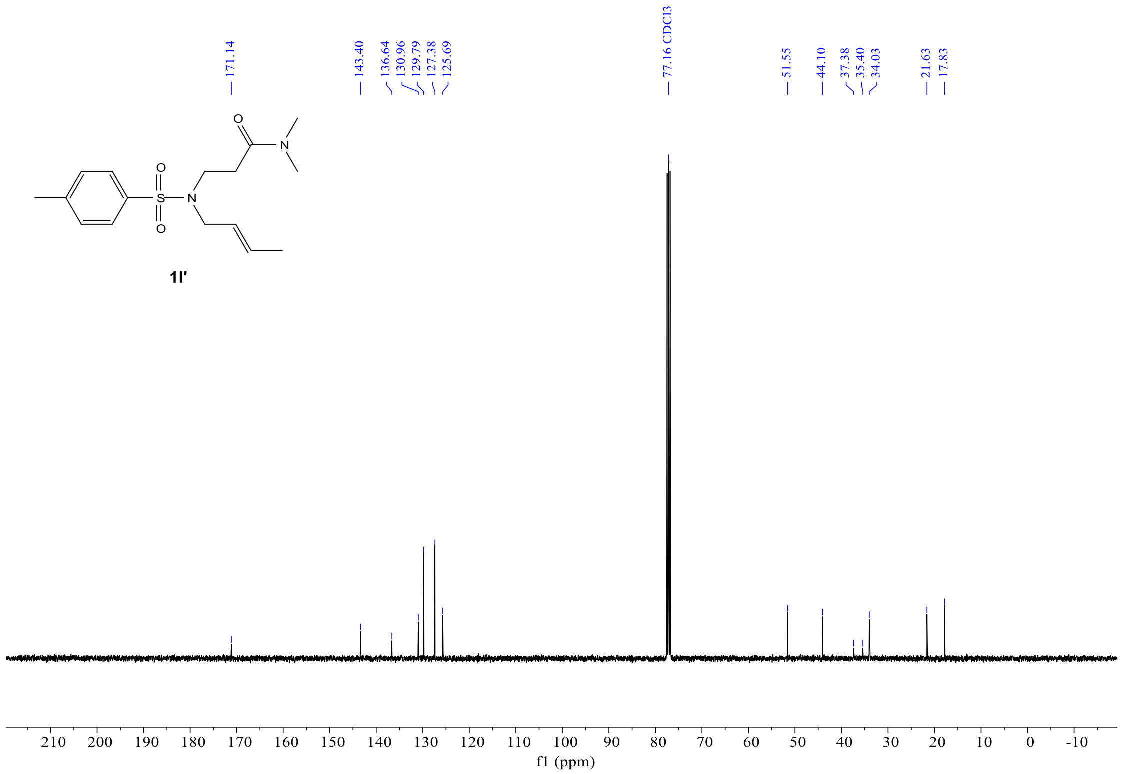
^{1}H NMR of compound **S2** (400 MHz, $CDCl_3$)



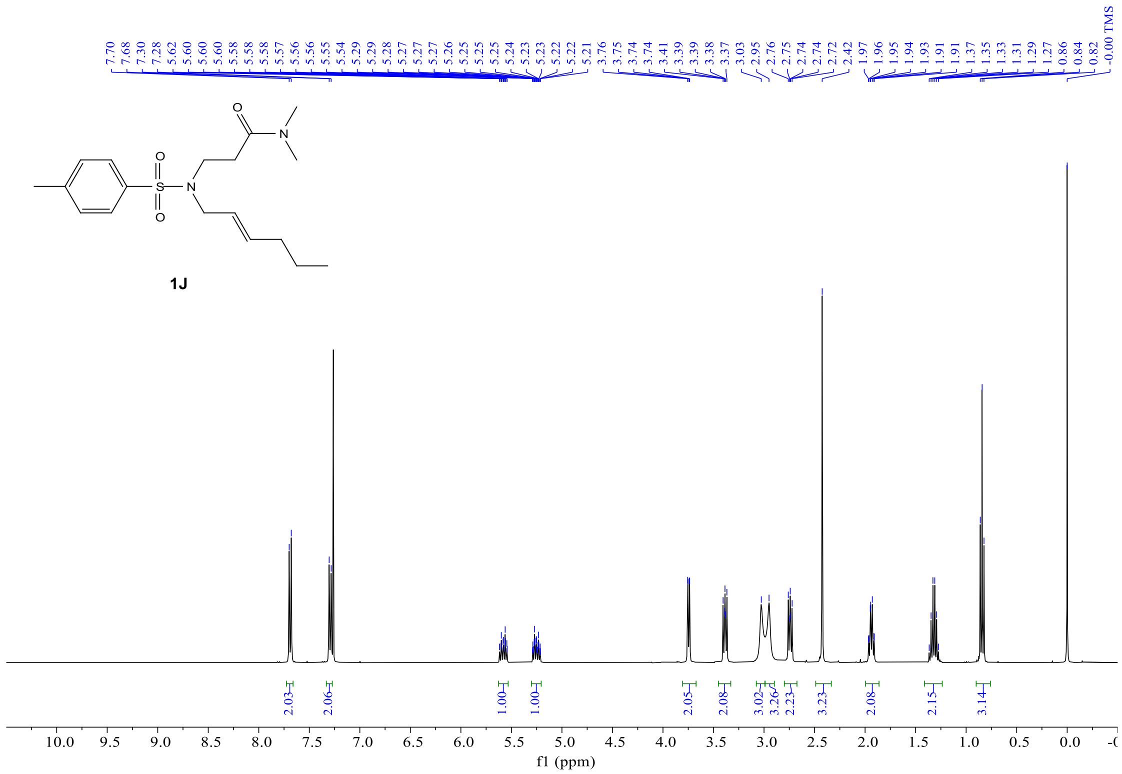
^{13}C NMR of compound **S2** (101 MHz, $CDCl_3$)



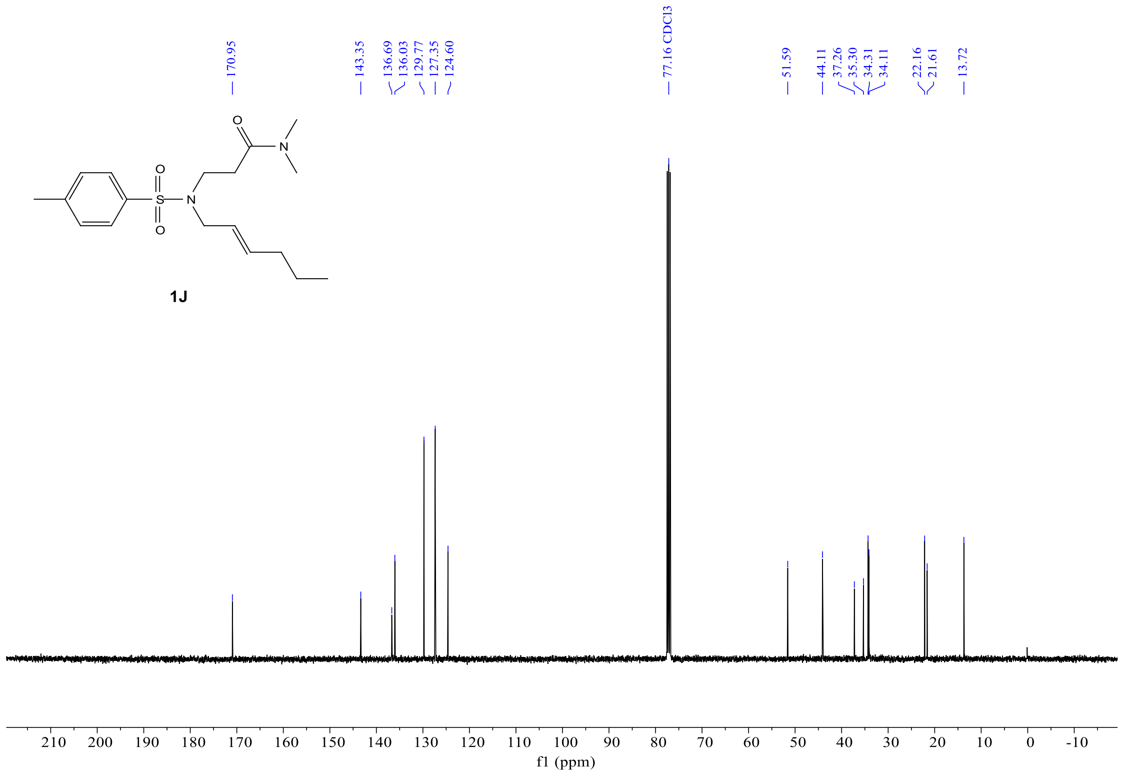
^{1}H NMR of compound **1l’** (400 MHz, $CDCl_3$)



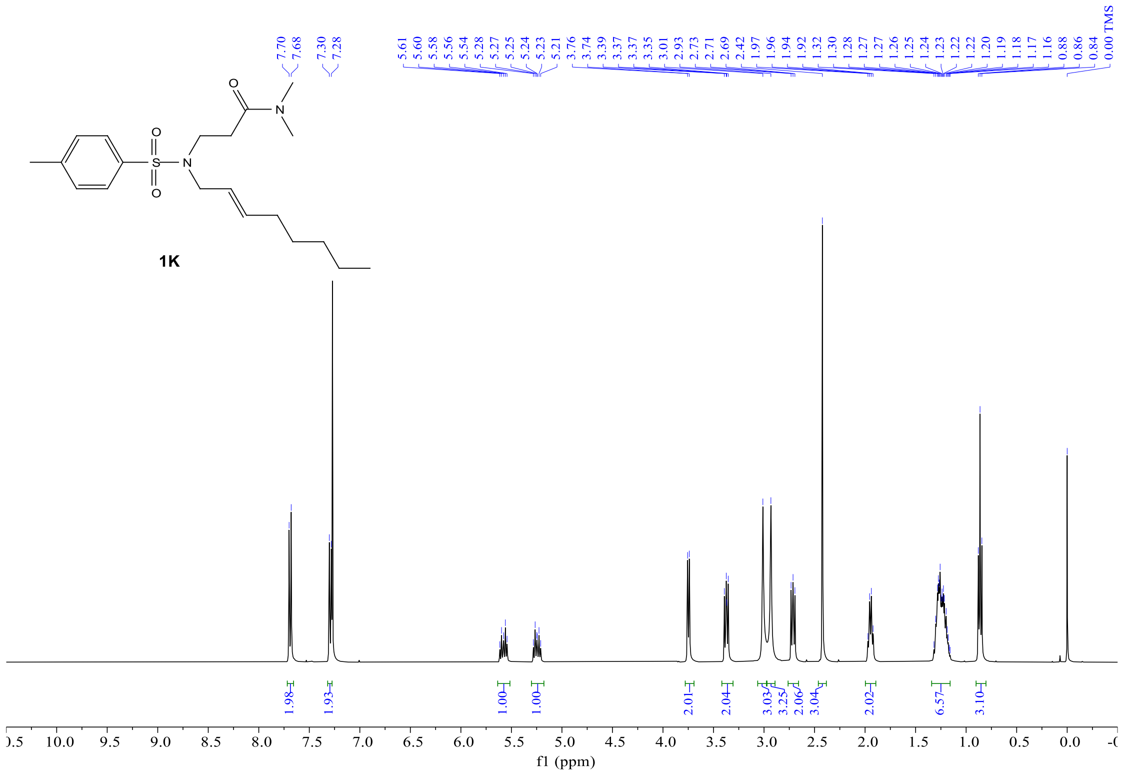
^{13}C NMR of compound **1I’** (101 MHz, $CDCl_3$)



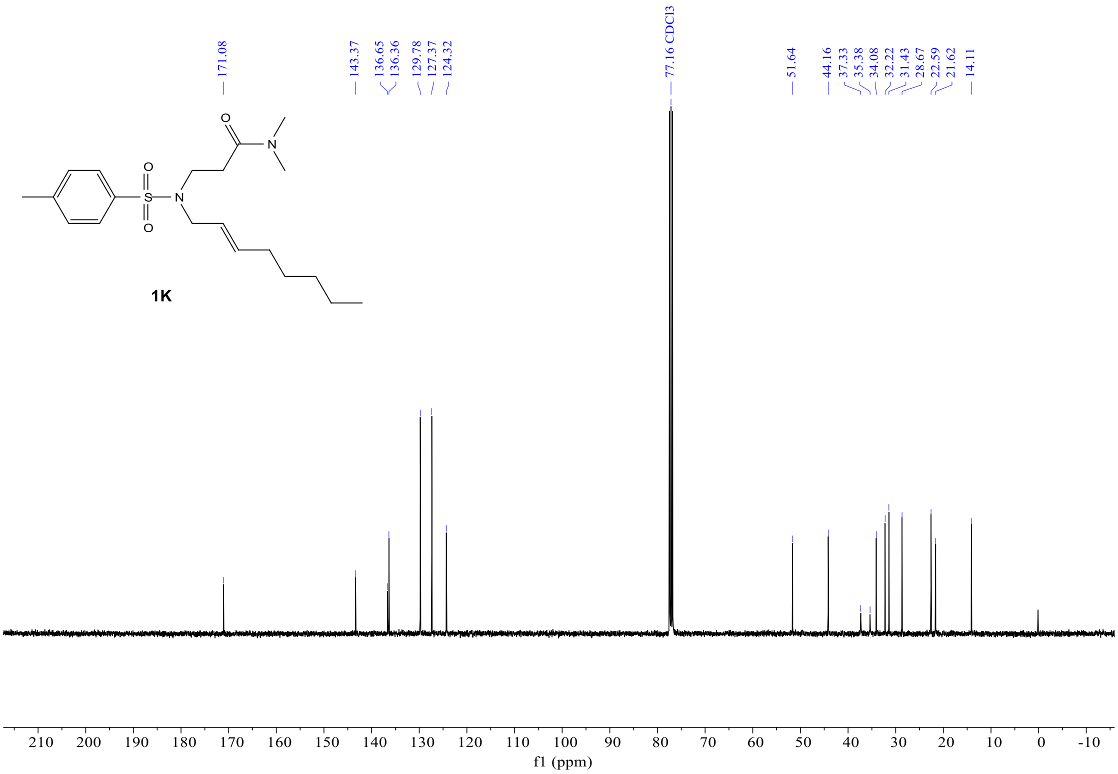
^{1}H NMR of compound **1J** (400 MHz, $CDCl_3$)



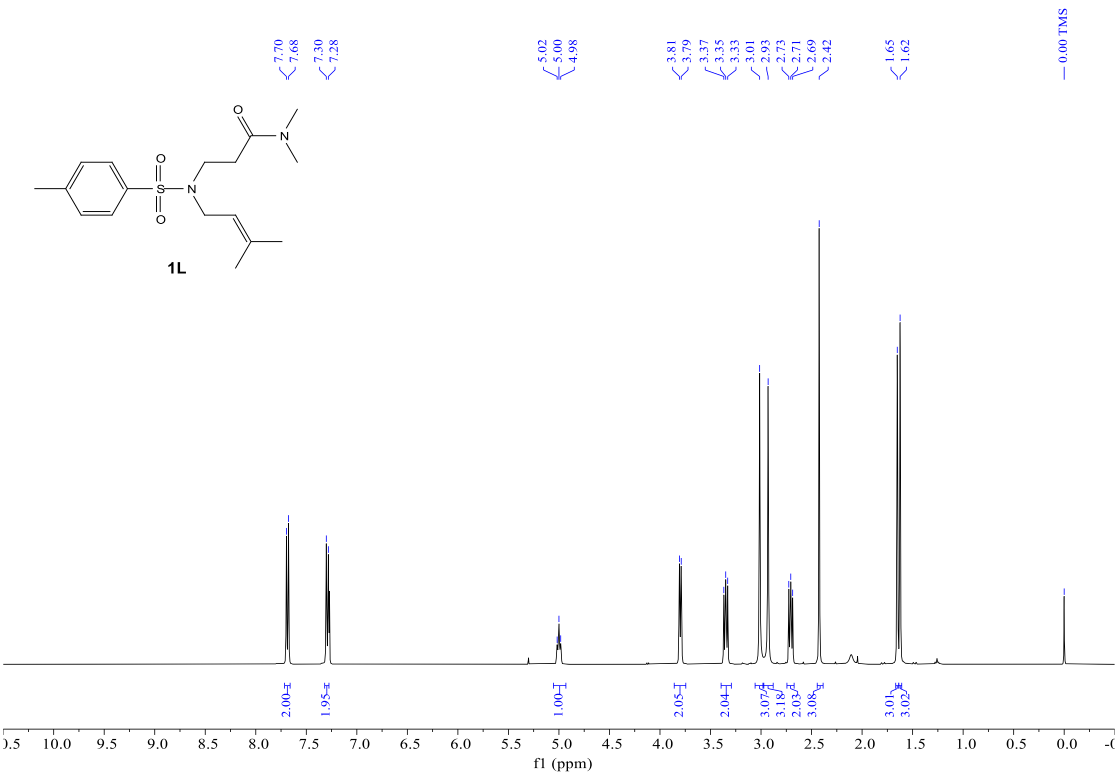
^{13}C NMR of compound **1J** (101 MHz, $CDCl_3$)



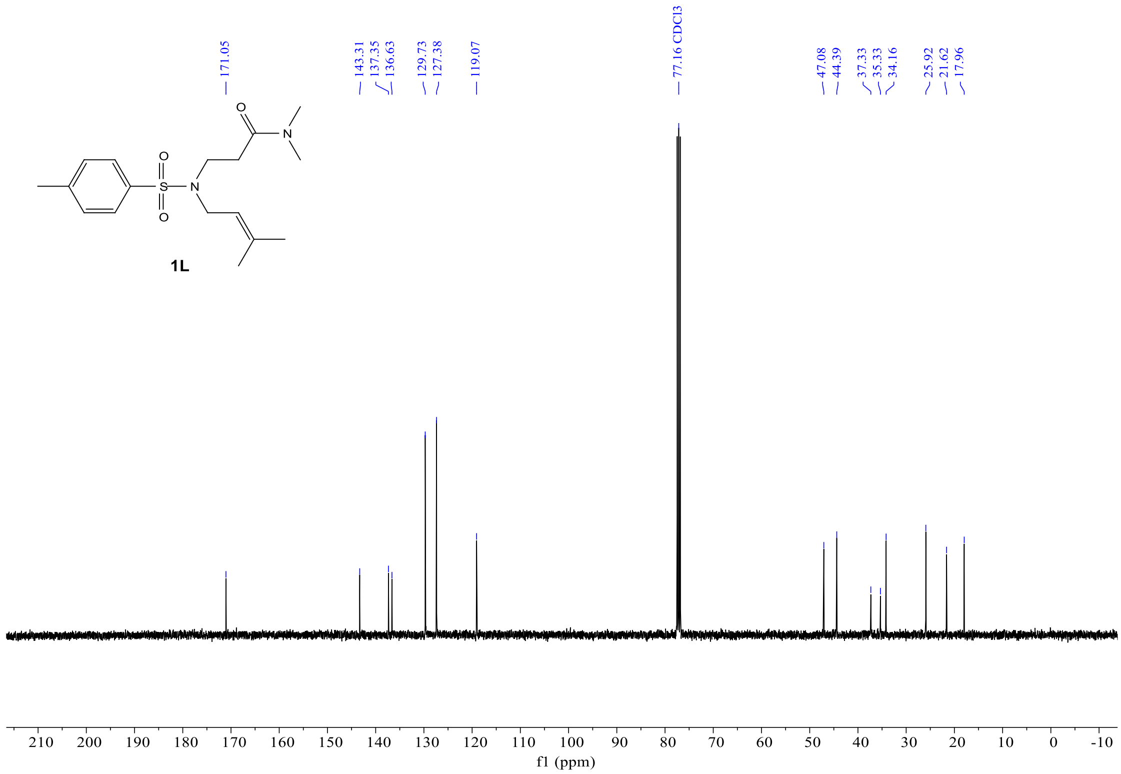
^{1}H NMR of compound **1K** (400 MHz, $CDCl_3$)



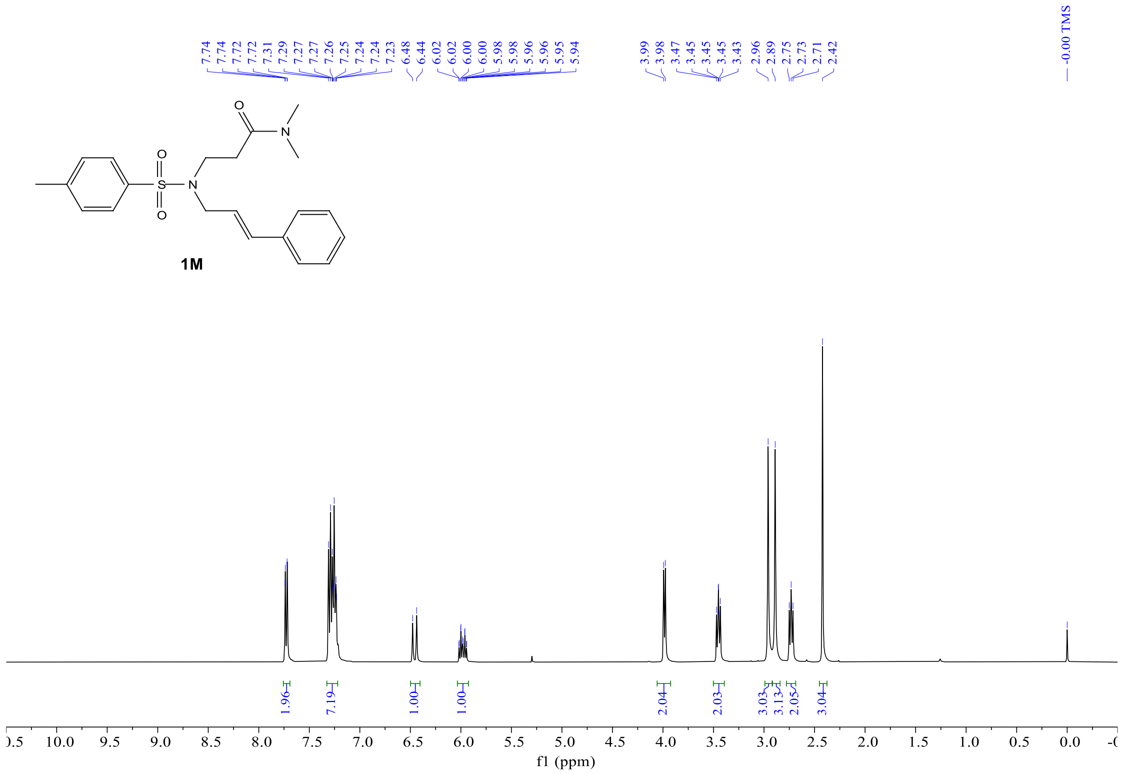
^{13}C NMR of compound **1K** (101 MHz, $CDCl_3$)



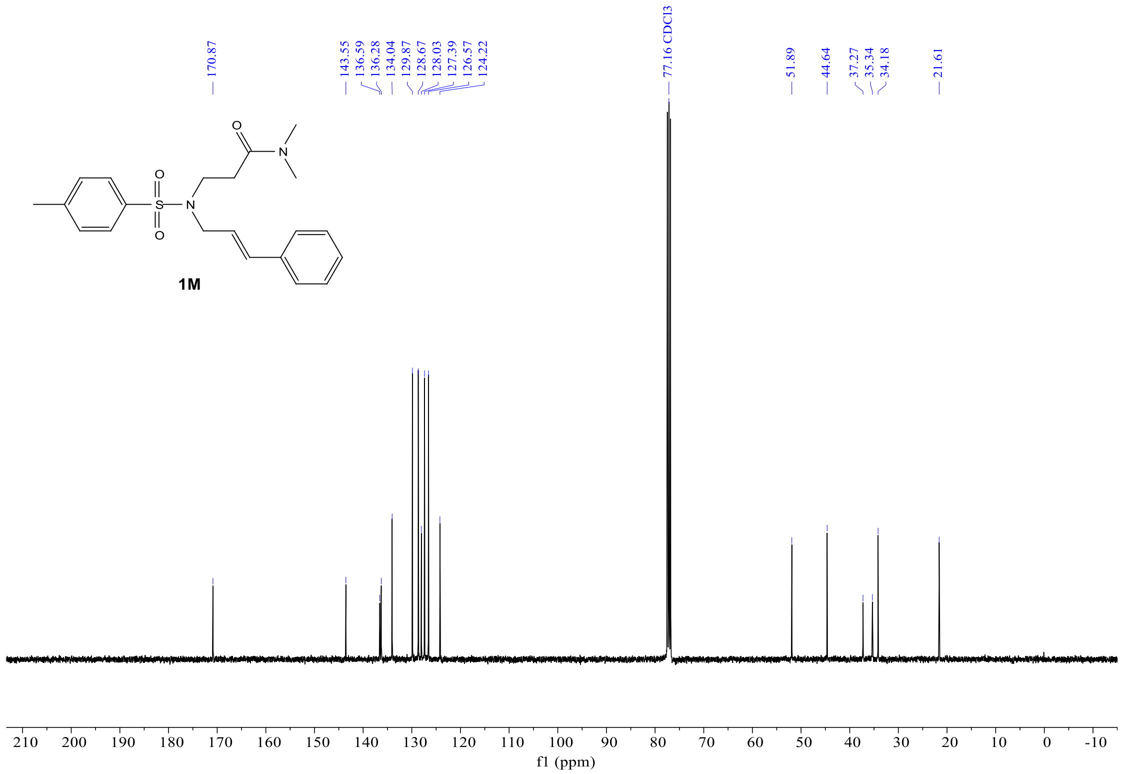
^{1}H NMR of compound **1L** (400 MHz, $CDCl_3$)



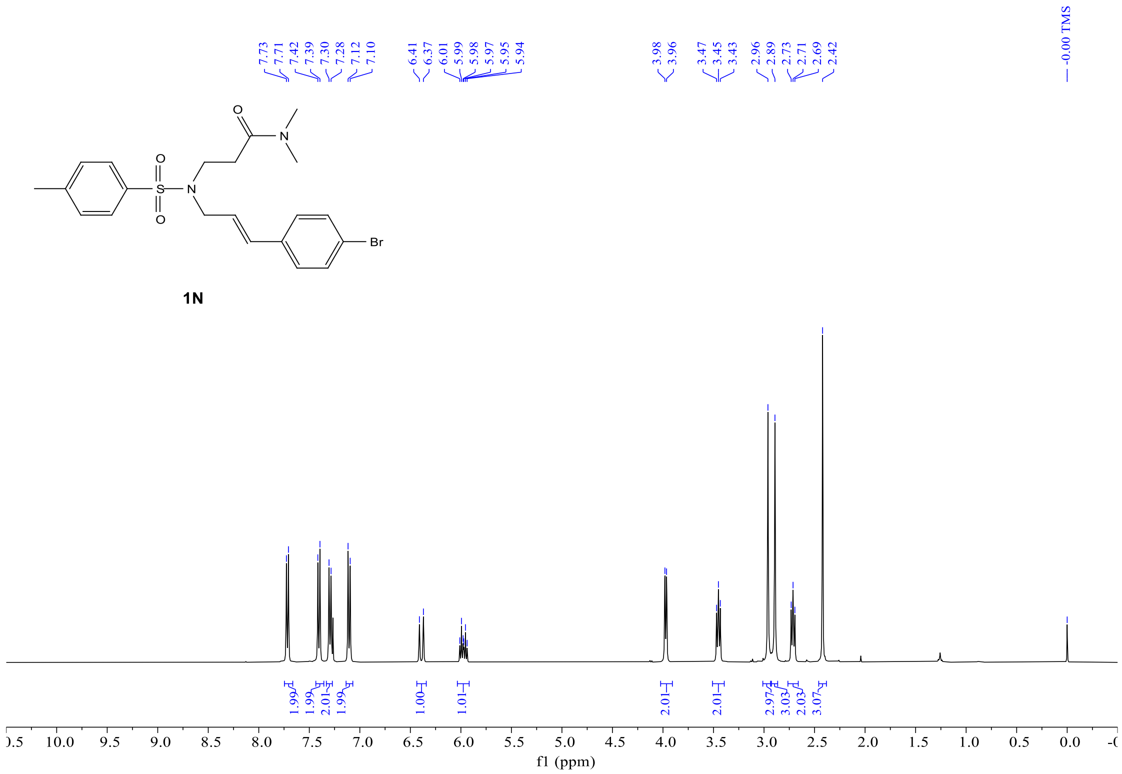
^{13}C NMR of compound **1L** (101 MHz, $CDCl_3$)



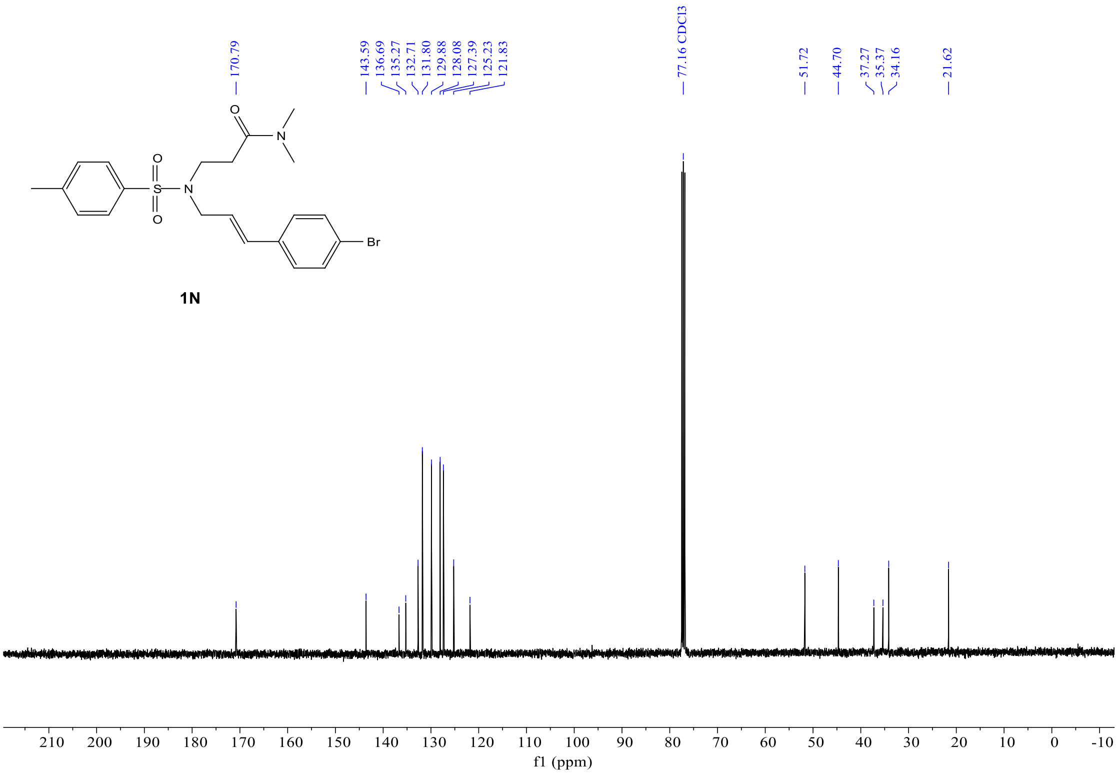
^{1}H NMR of compound **1M** (400 MHz, $CDCl_3$)



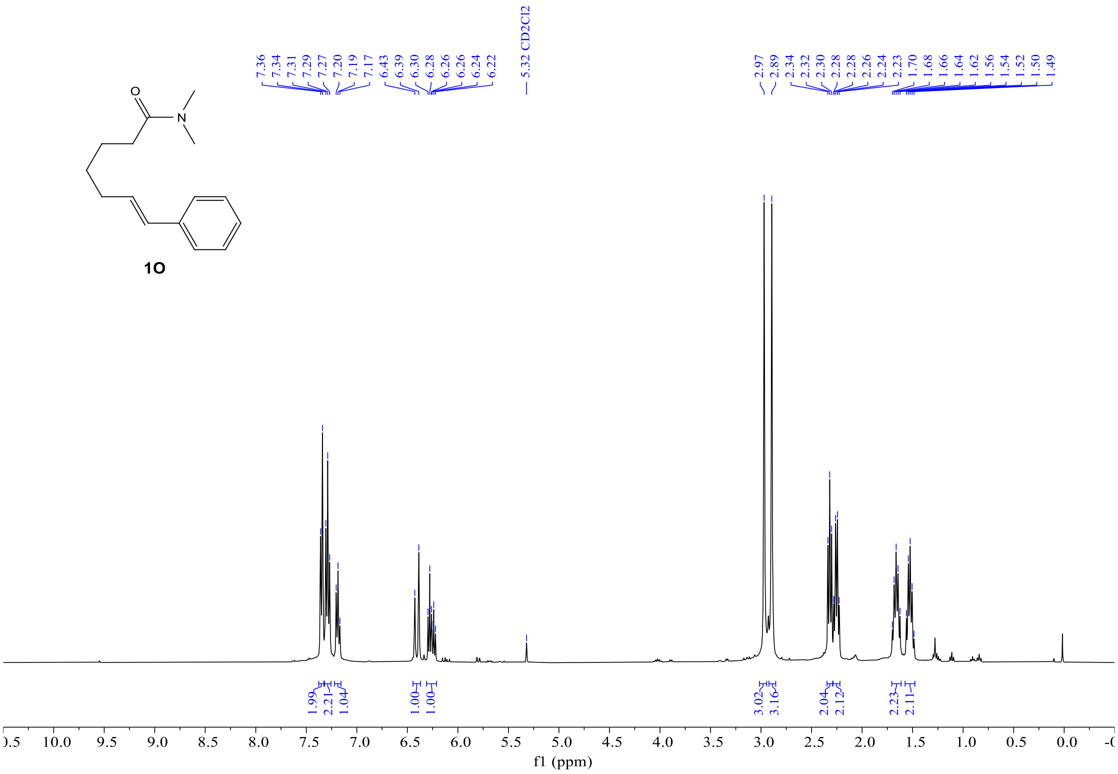
^{13}C NMR of compound **1M** (101 MHz, $CDCl_3$)



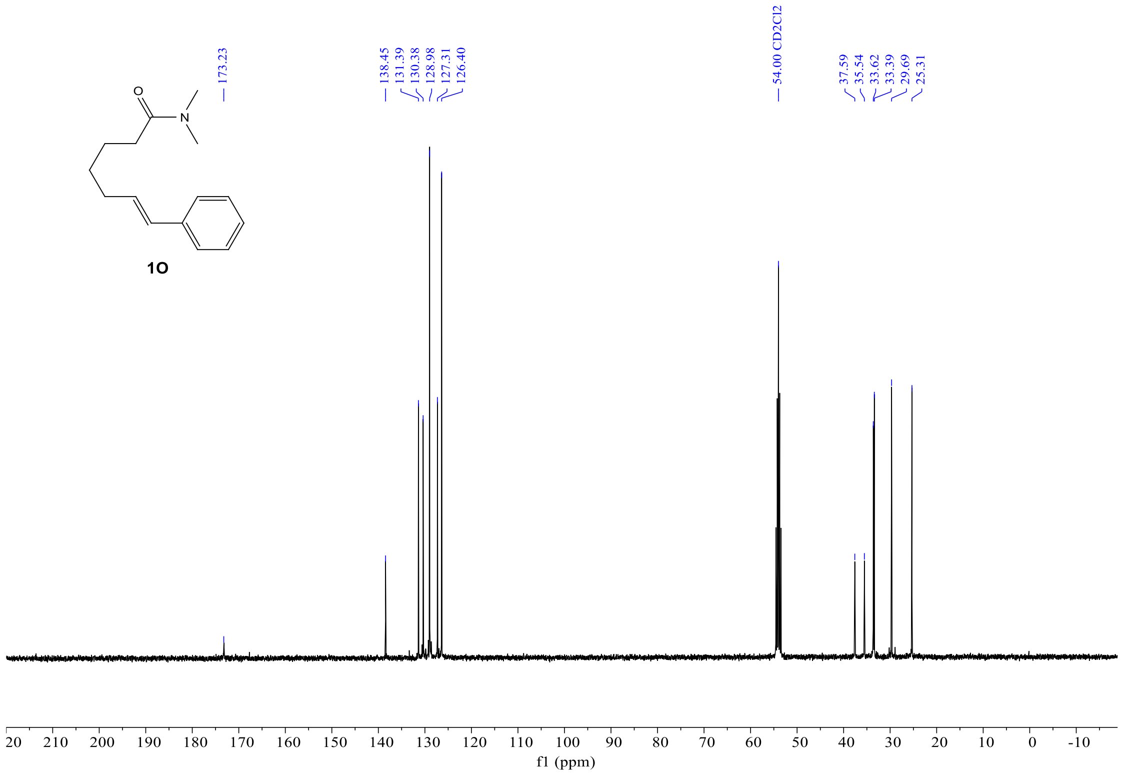
^{1}H NMR of compound **1N** (400 MHz, $CDCl_3$)



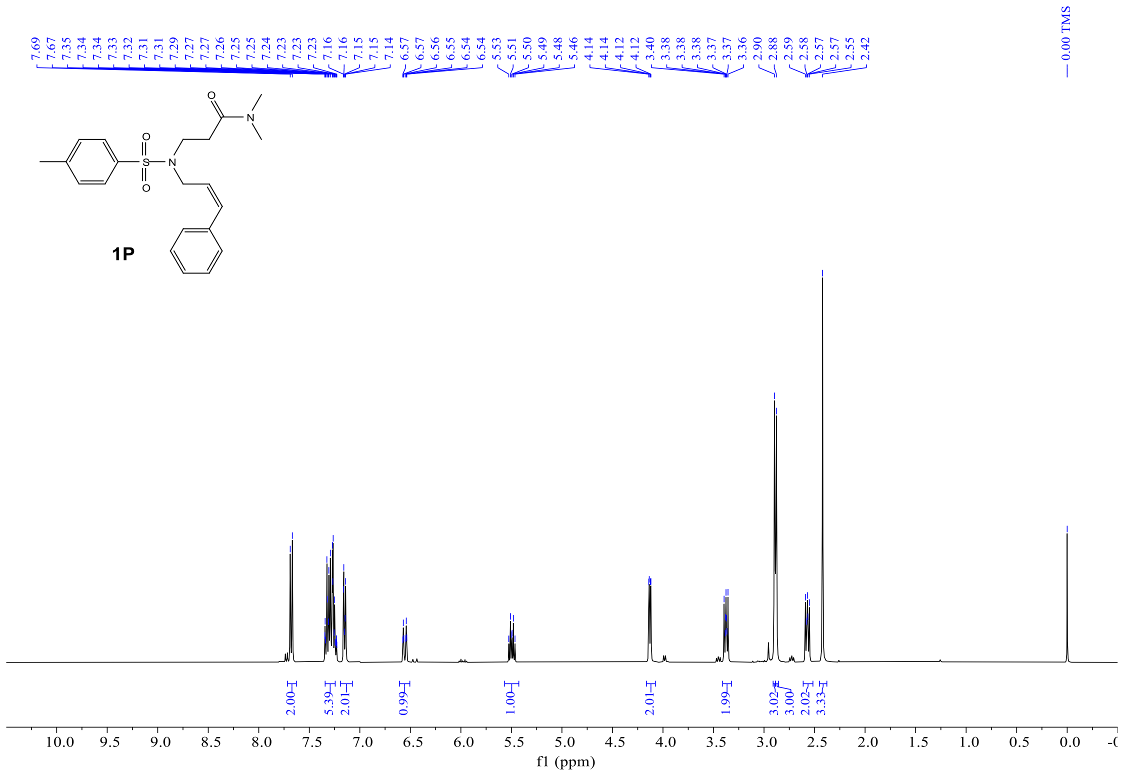
^{13}C NMR of compound **1N** (101 MHz, $CDCl_3$)



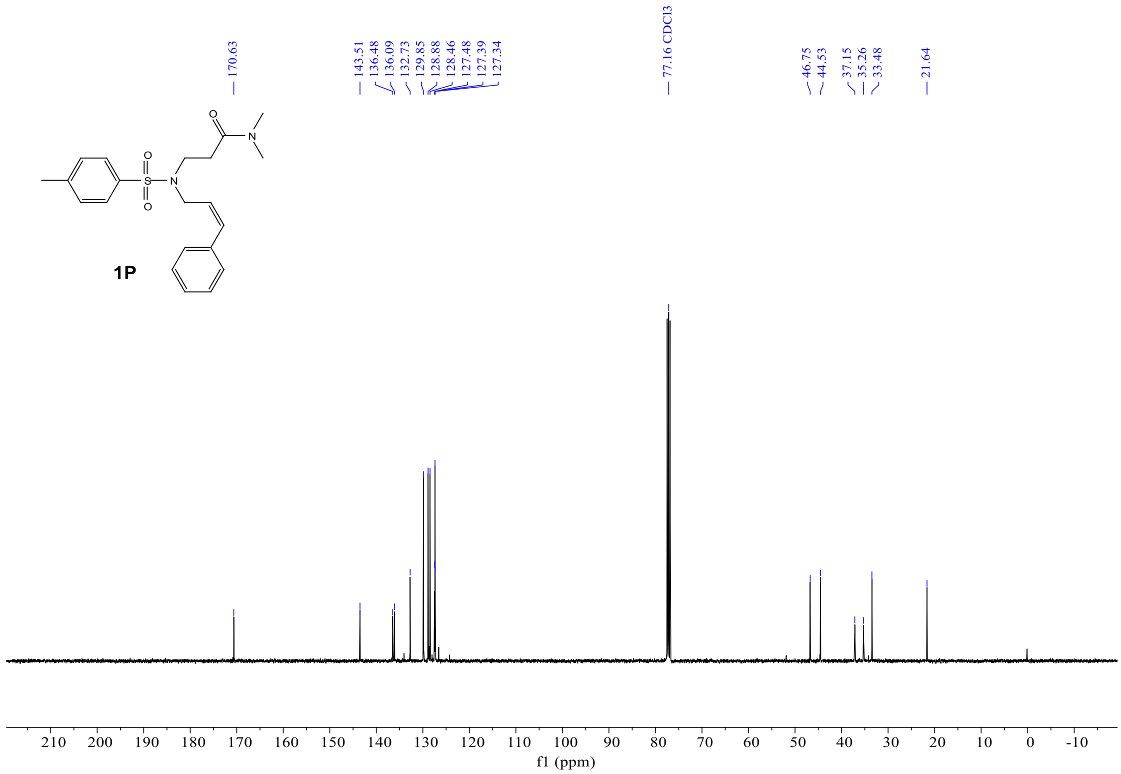
^{1}H NMR of compound **1O** (400 MHz, CD_2Cl_2)



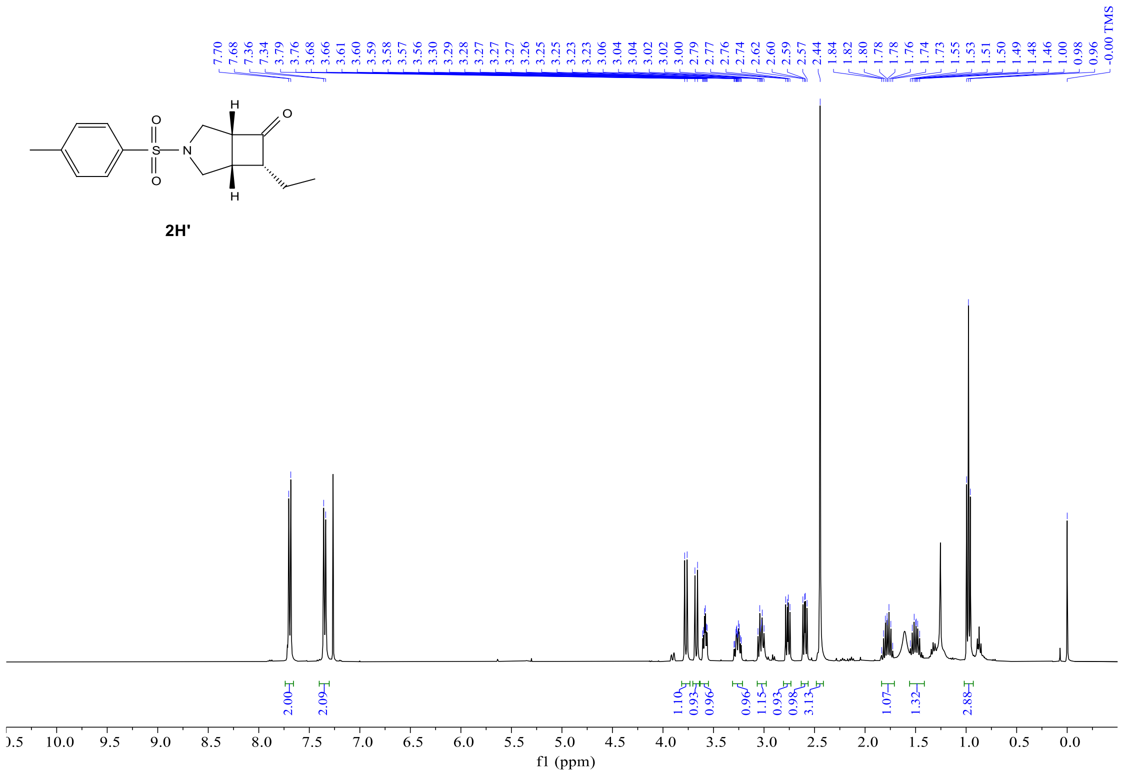
^{13}C NMR of compound **1O** (101 MHz, CD_2Cl_2)



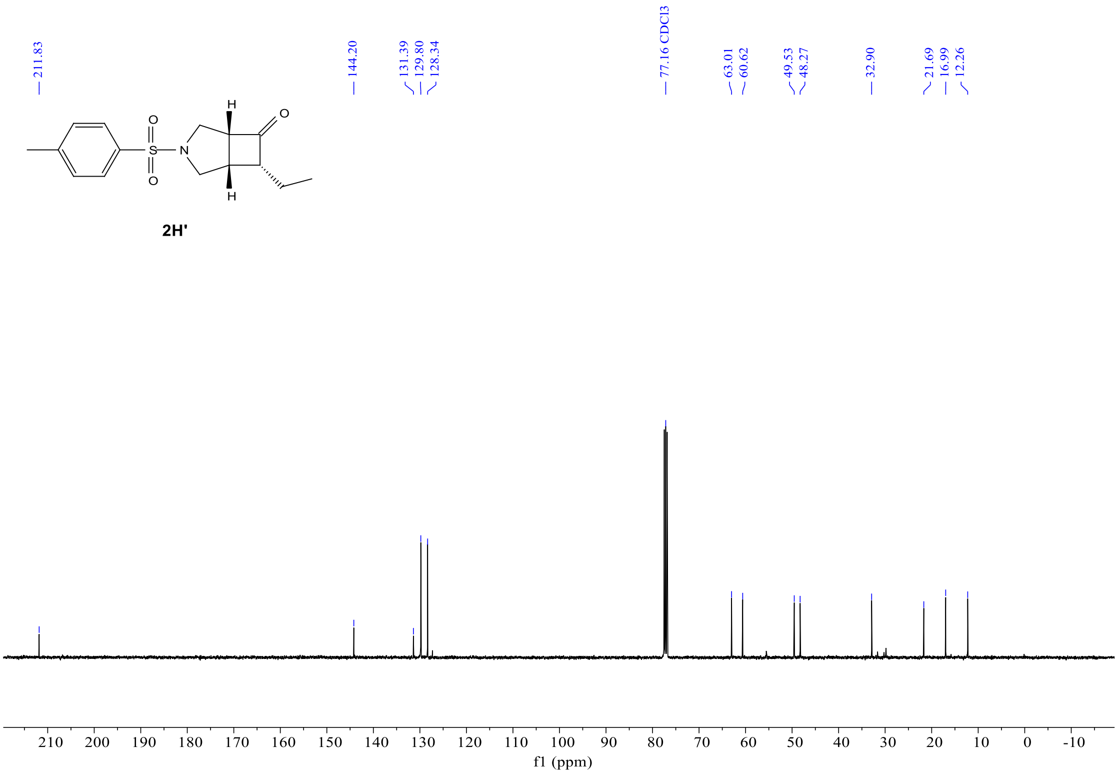
^{1}H NMR of compound **1P** (400 MHz, $CDCl_3$)



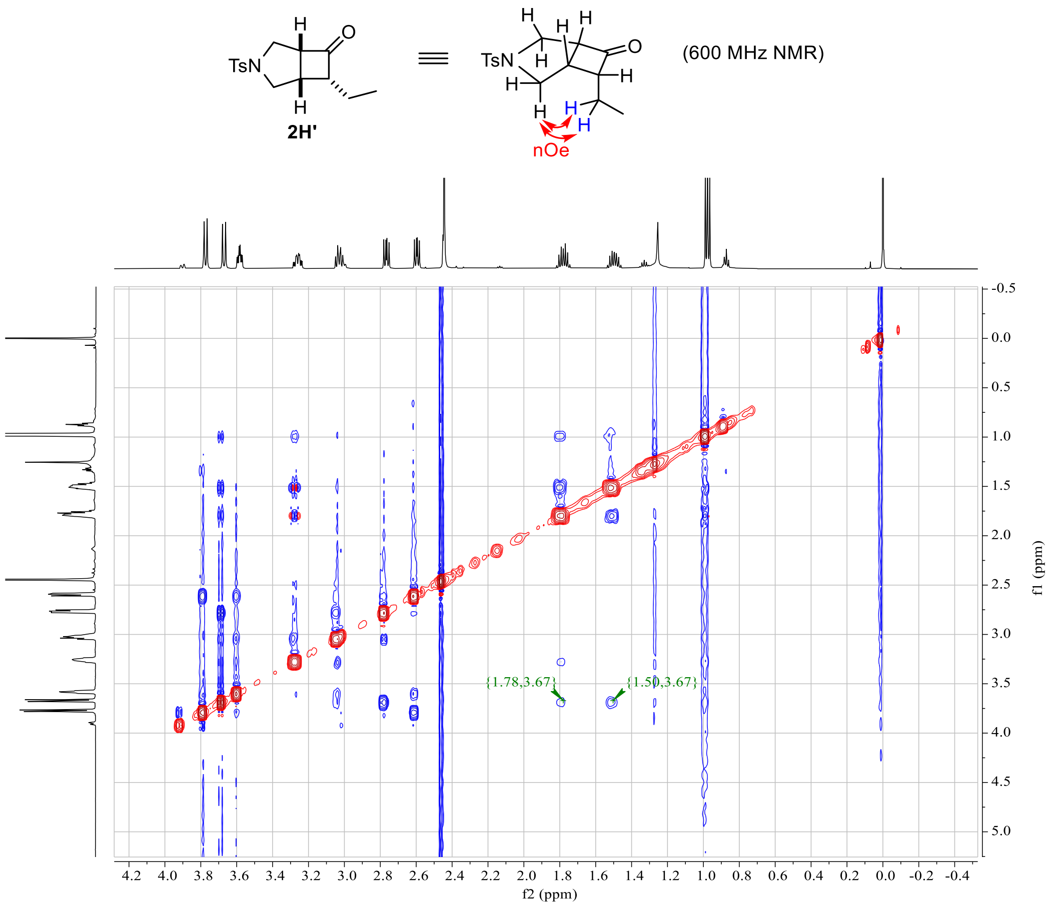
^{13}C NMR of compound **1P** (101 MHz, $CDCl_3$)



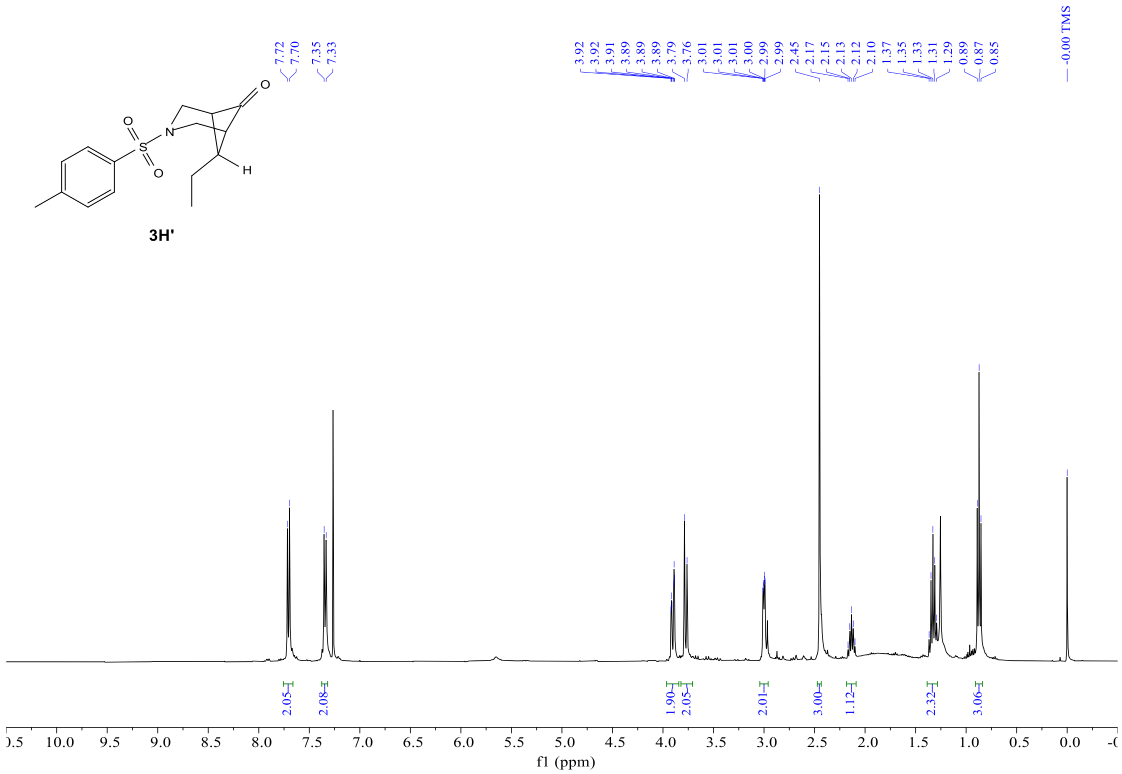
^{1}H NMR of compound **2H'** (400 MHz, $CDCl_3$)



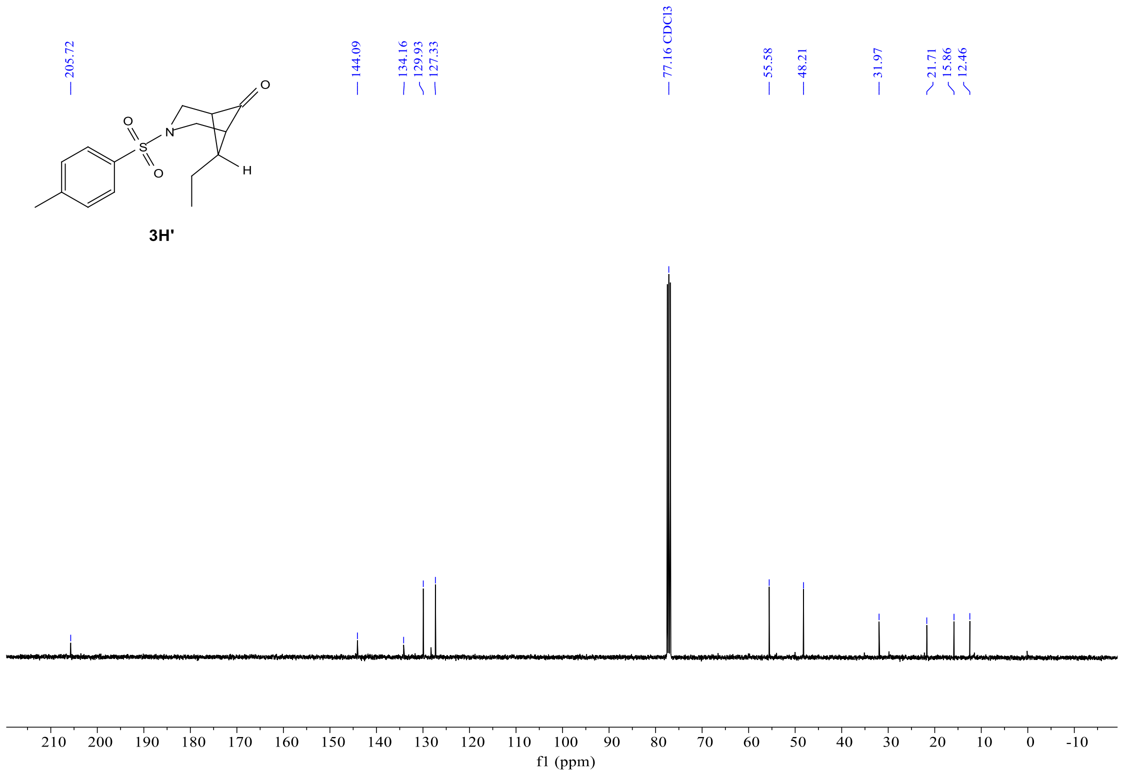
^{13}C NMR of compound **2H’** (101 MHz, $CDCl_3$)



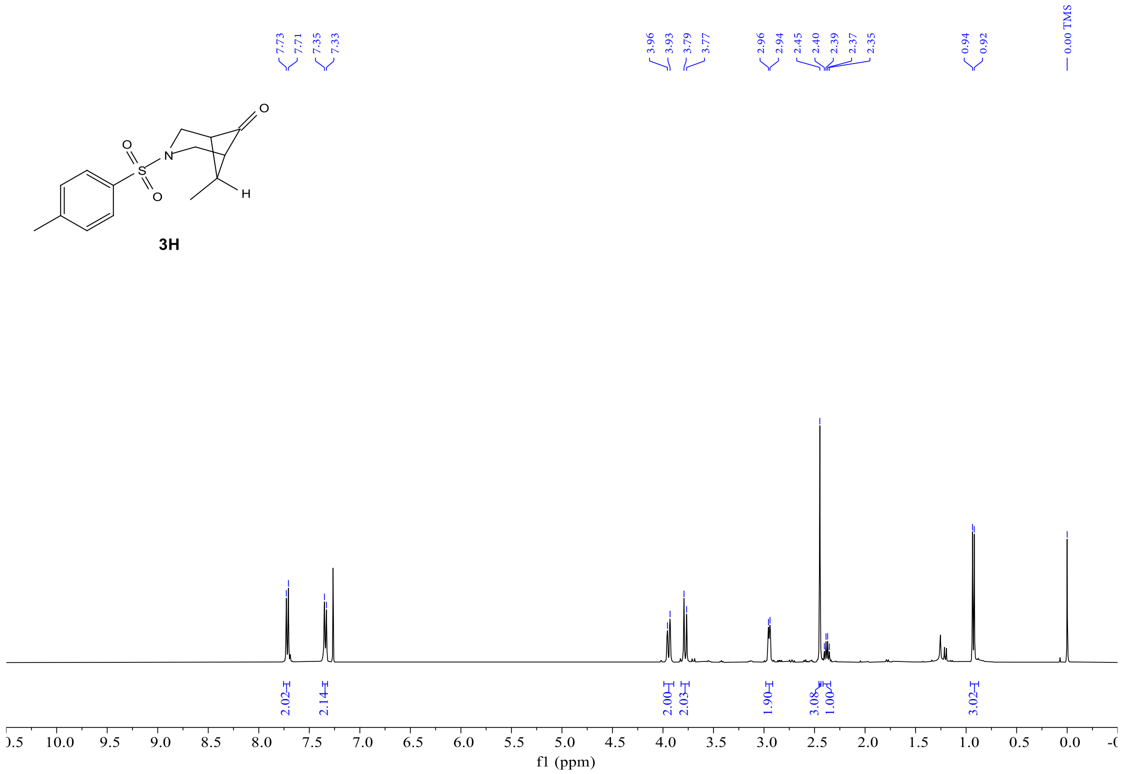
NOESY NMR of compound **2H’** (600 MHz, $CDCl_3$)



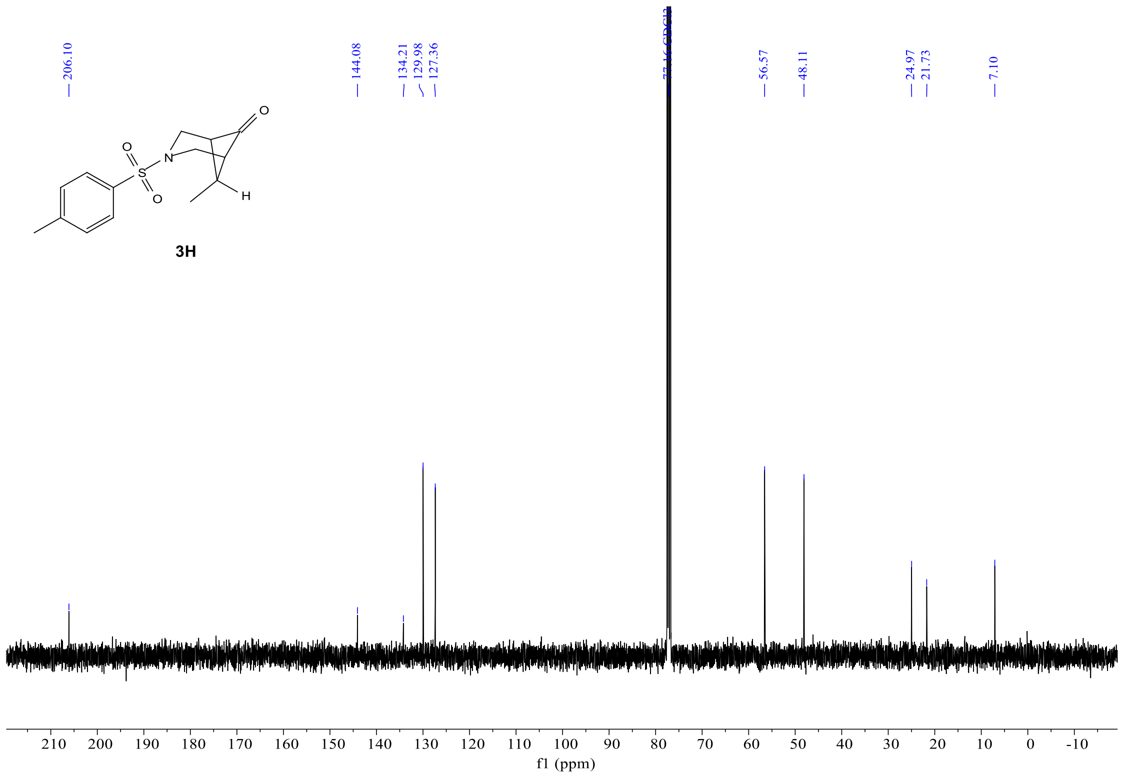
^{1}H NMR of compound **3H'** (400 MHz, $CDCl_3$)



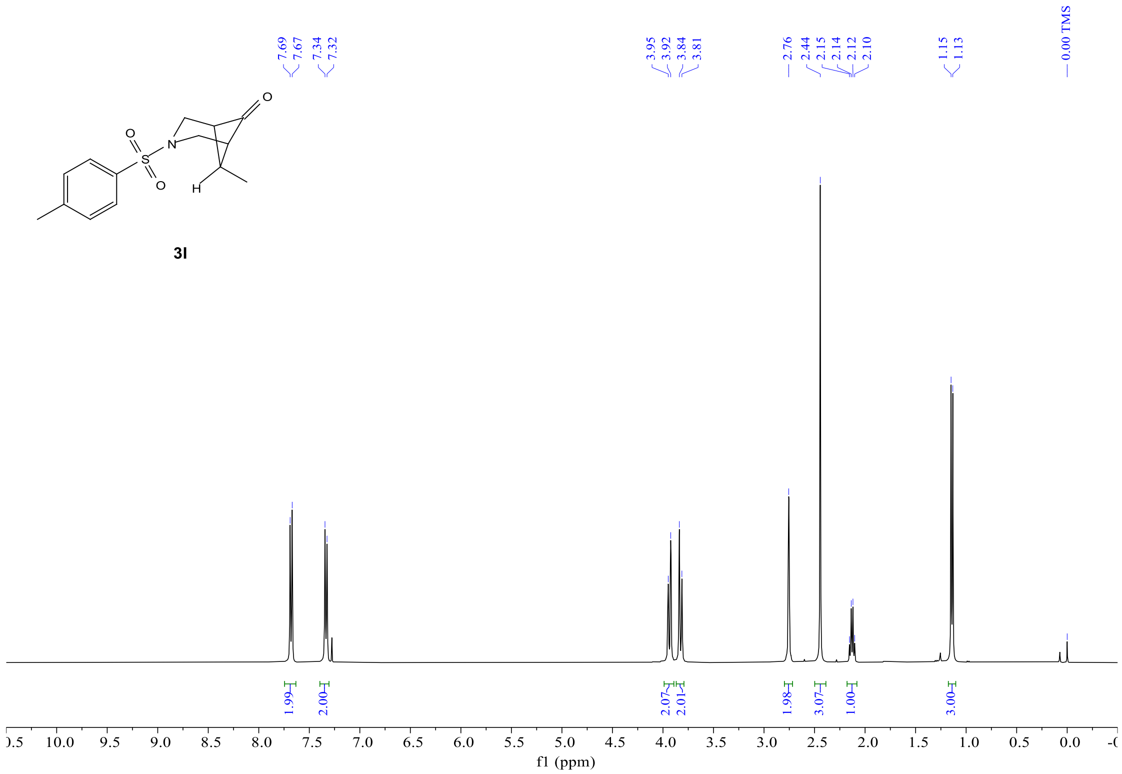
^{13}C NMR of compound **3H'** (101 MHz, $CDCl_3$)



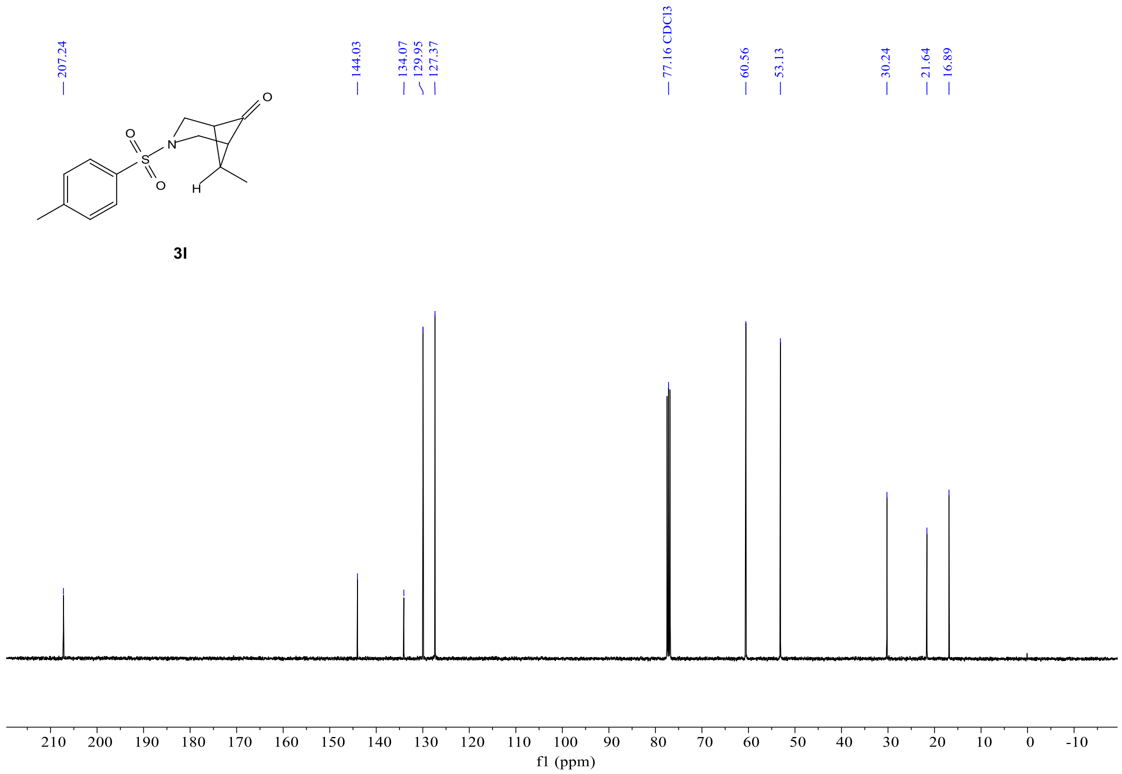
^{1}H NMR of compound **3H** (400 MHz, $CDCl_3$)



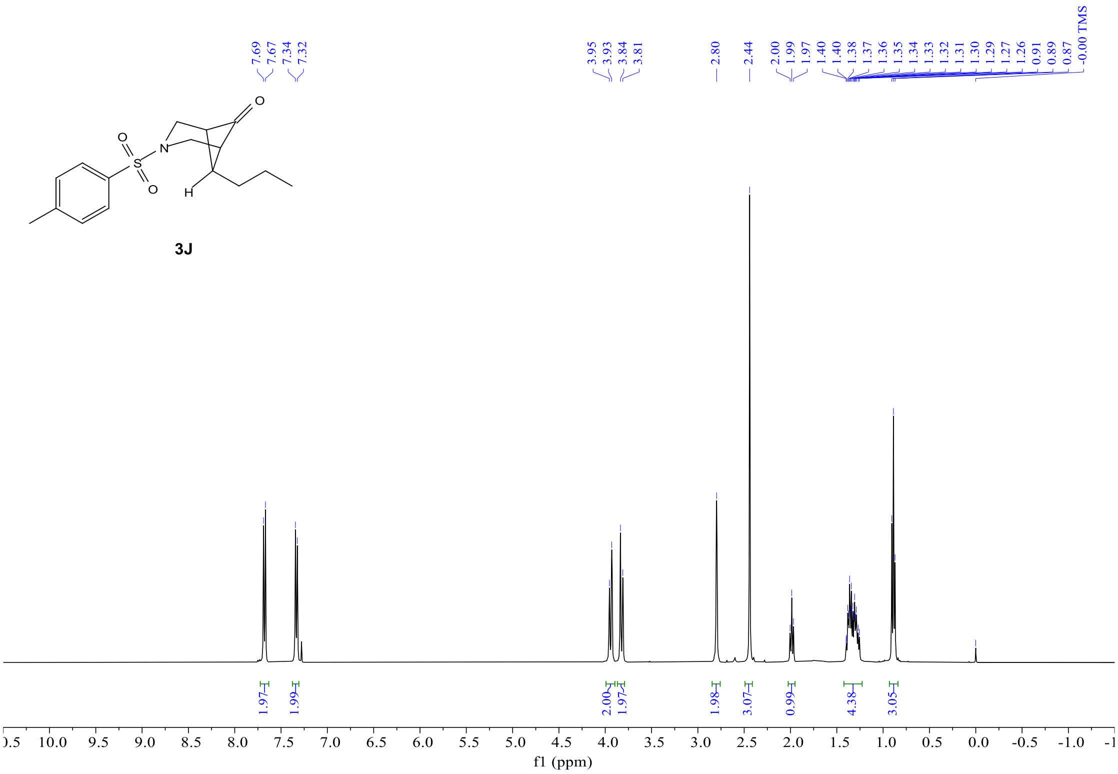
^{13}C NMR of compound **3H** (101 MHz, $CDCl_3$)



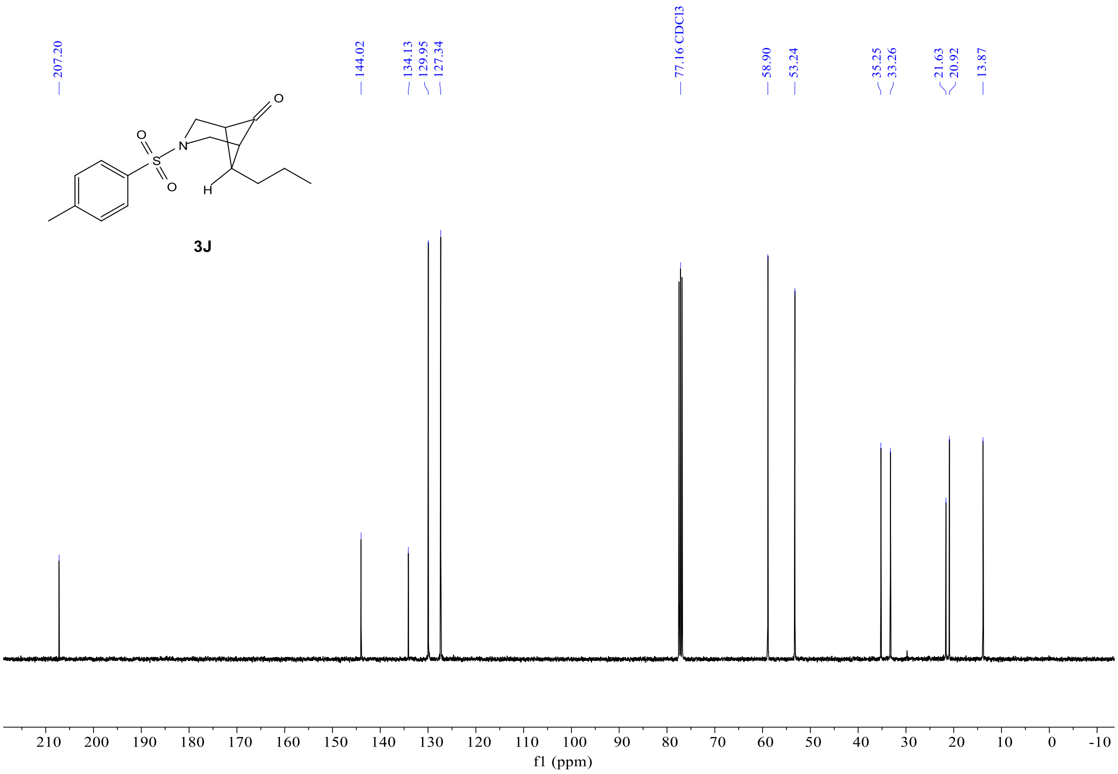
[1]H NMR of compound **3l** (400 MHz, $CDCl_3$)



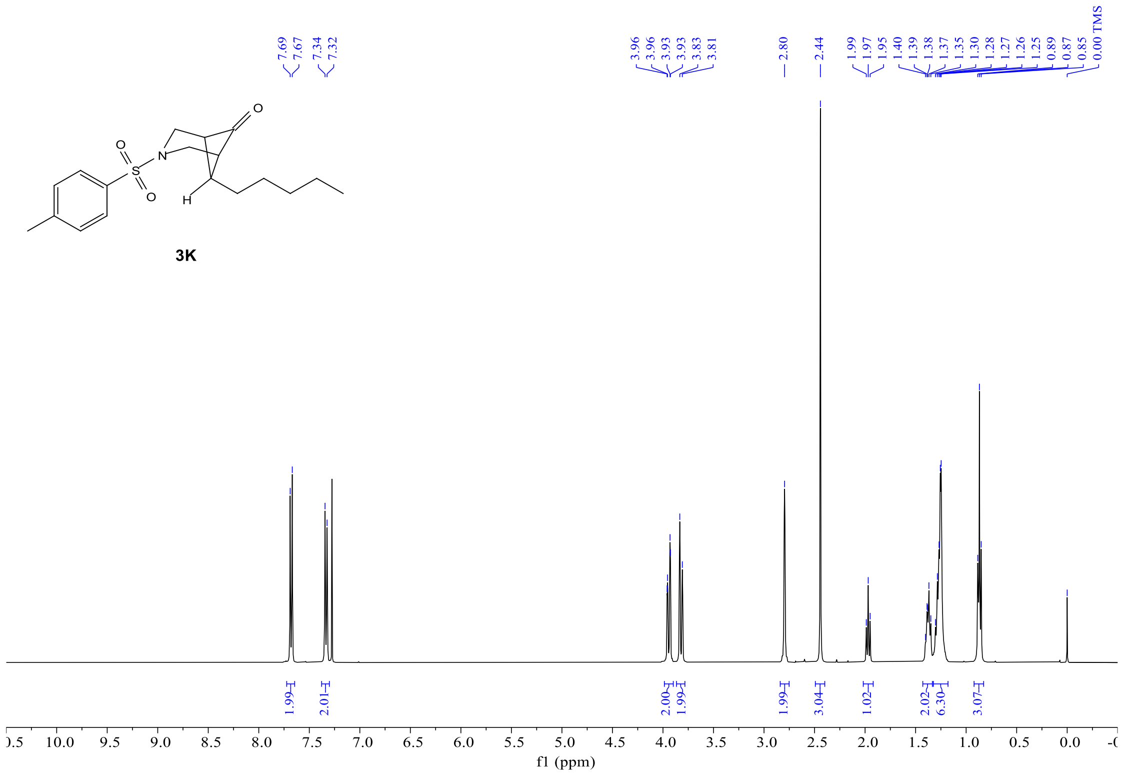
[13]C NMR of compound **3l** (101 MHz, $CDCl_3$)



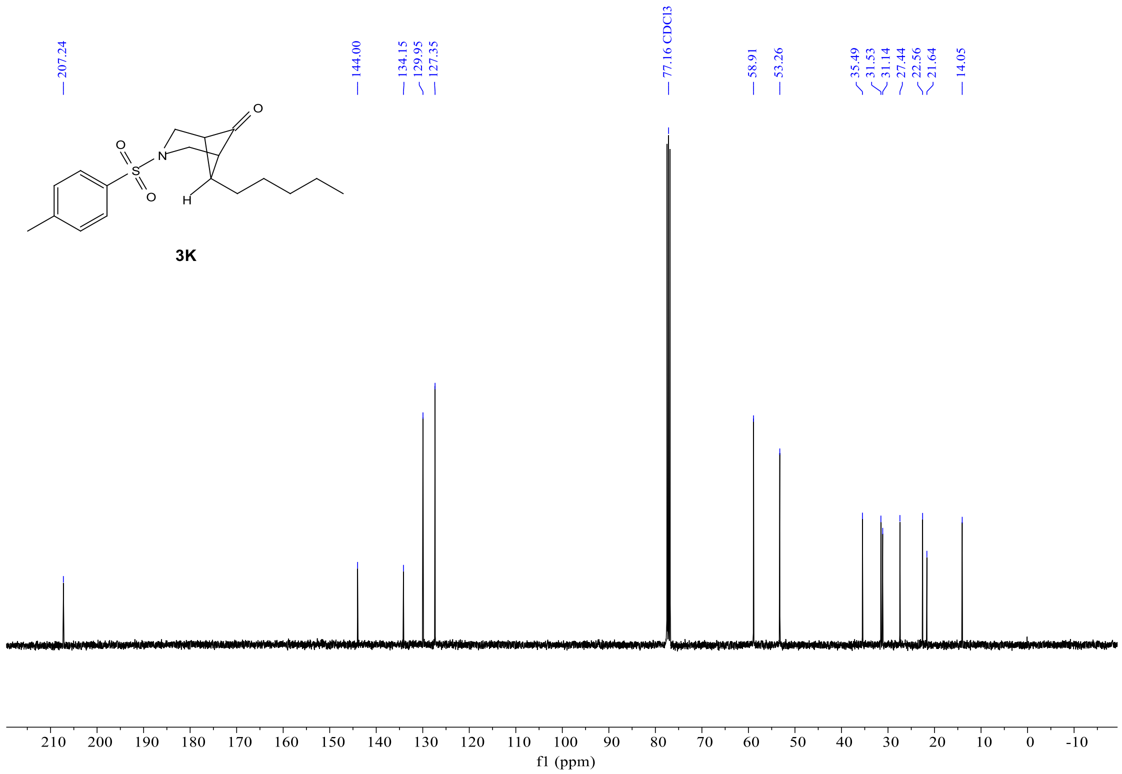
[1]H NMR of compound **3J** (400 MHz, $CDCl_3$)



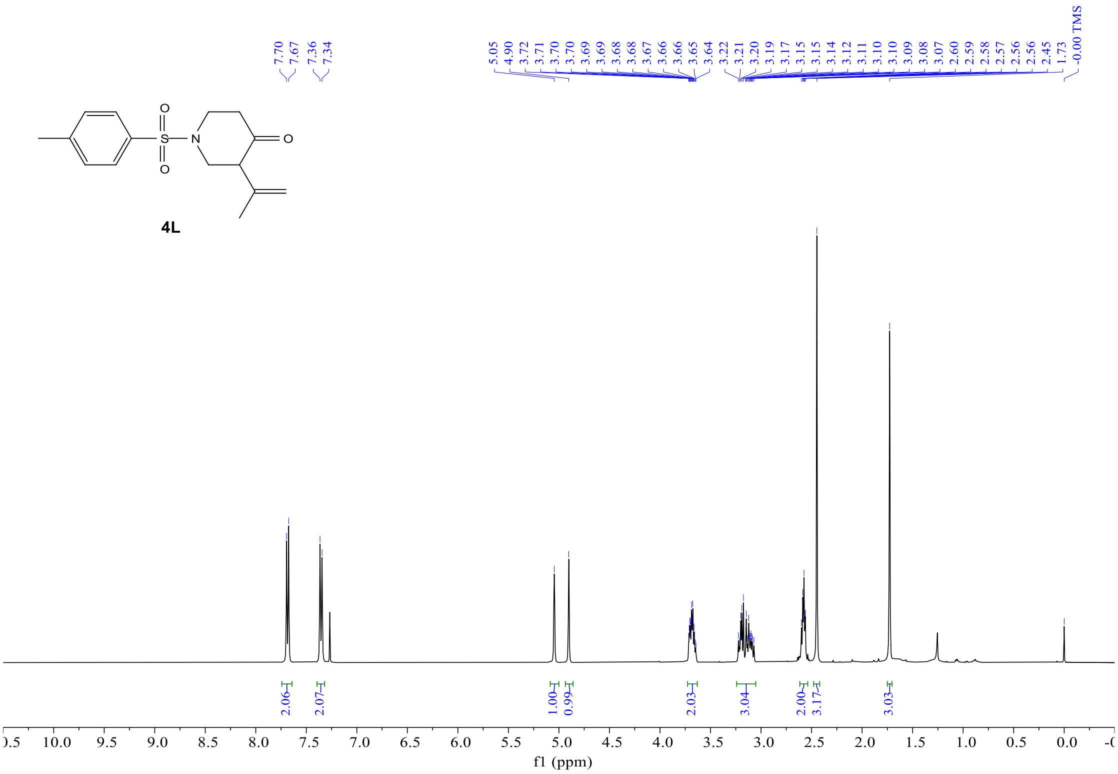
[13]C NMR of compound **3J** (101 MHz, $CDCl_3$)



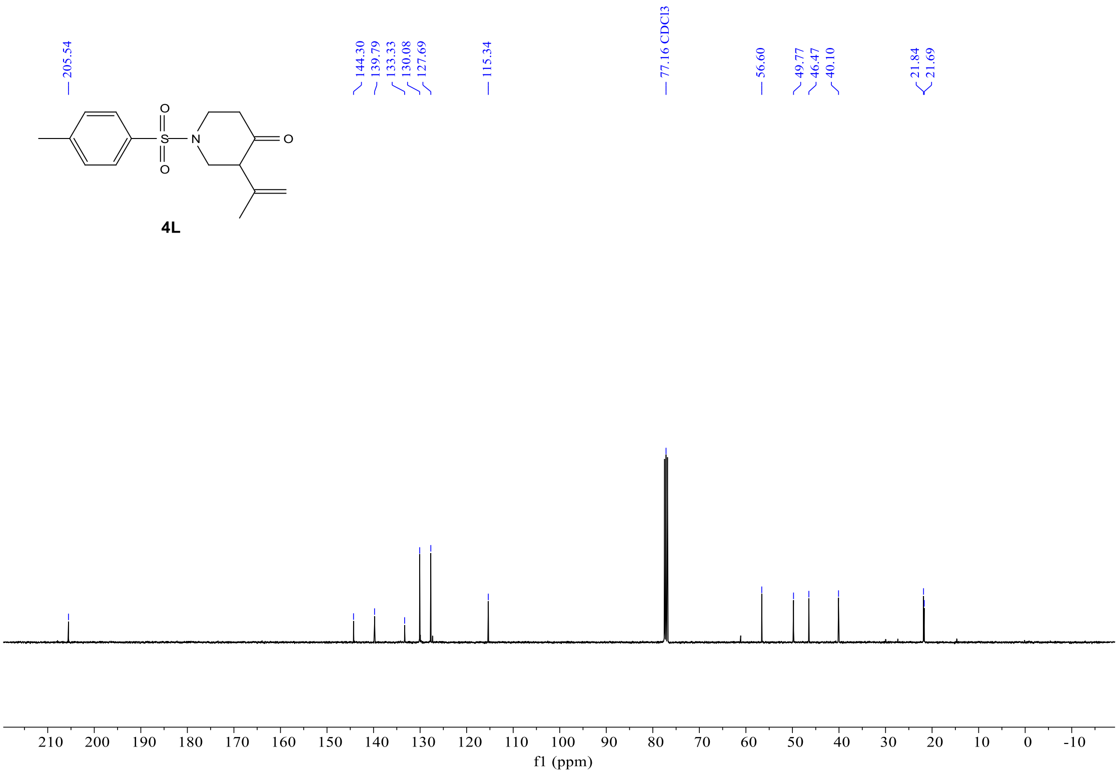
^{1}H NMR of compound **3K** (400 MHz, $CDCl_3$)



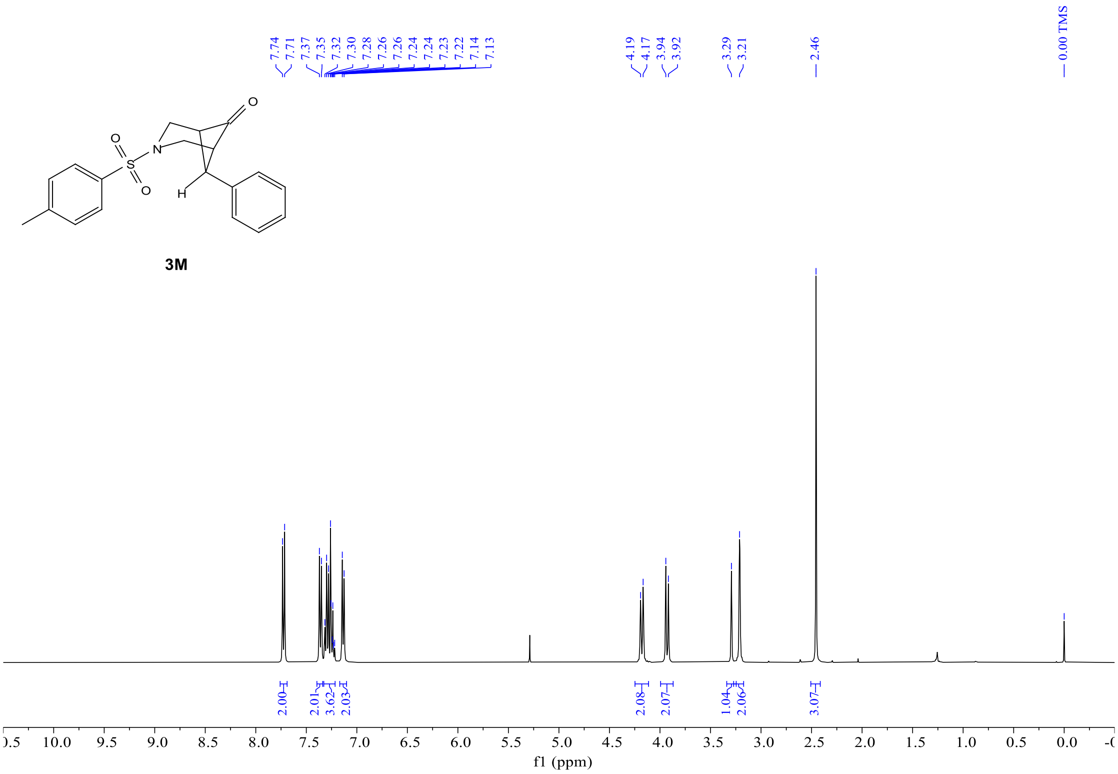
^{13}C NMR of compound **3K** (101 MHz, $CDCl_3$)



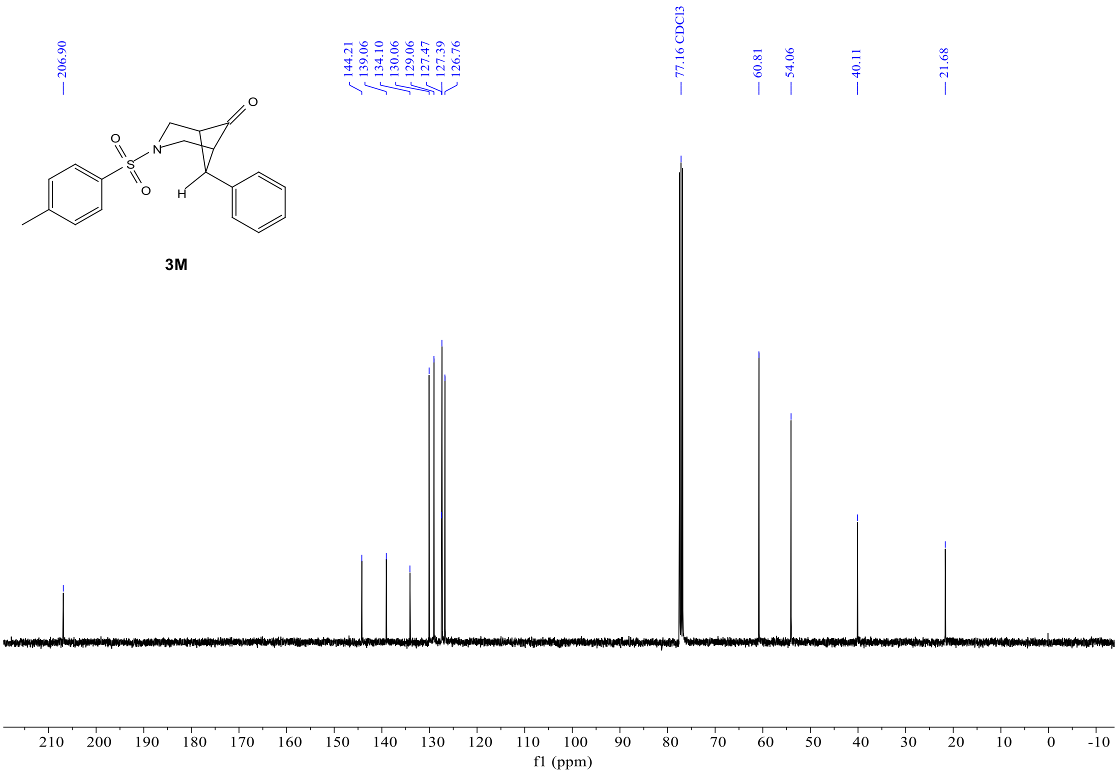
^{1}H NMR of compound **4L** (400 MHz, $CDCl_3$)



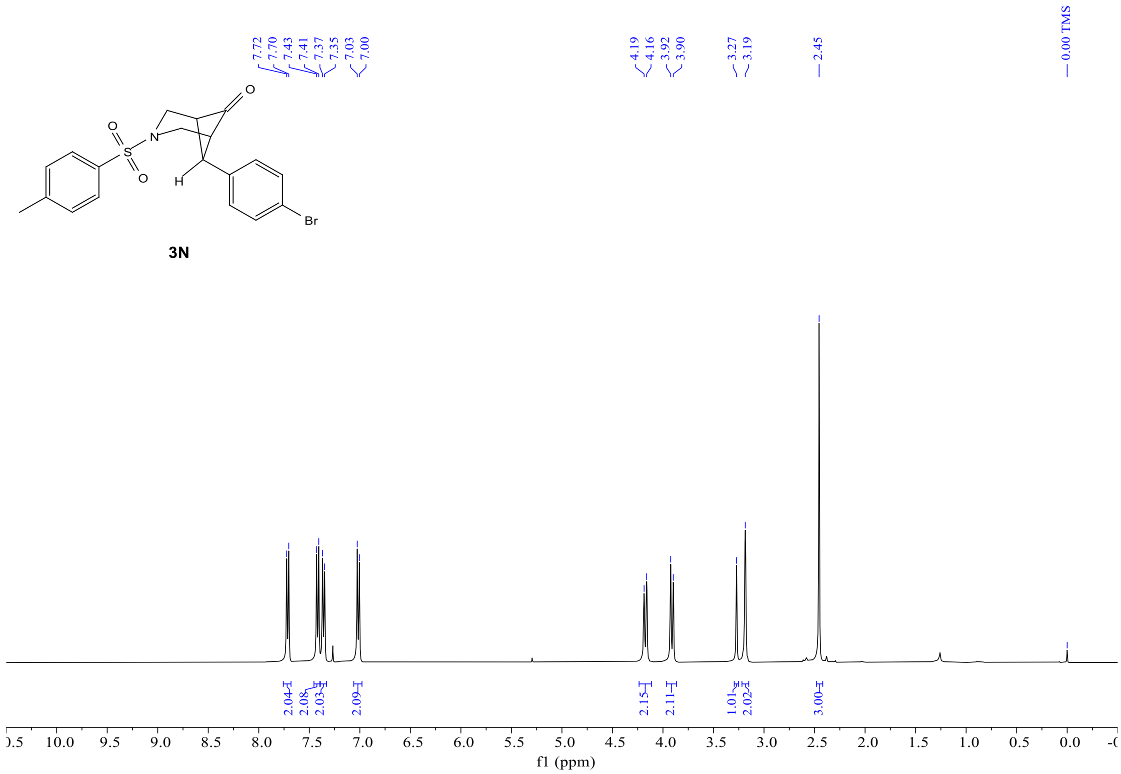
^{13}C NMR of compound **4L** (101 MHz, $CDCl_3$)



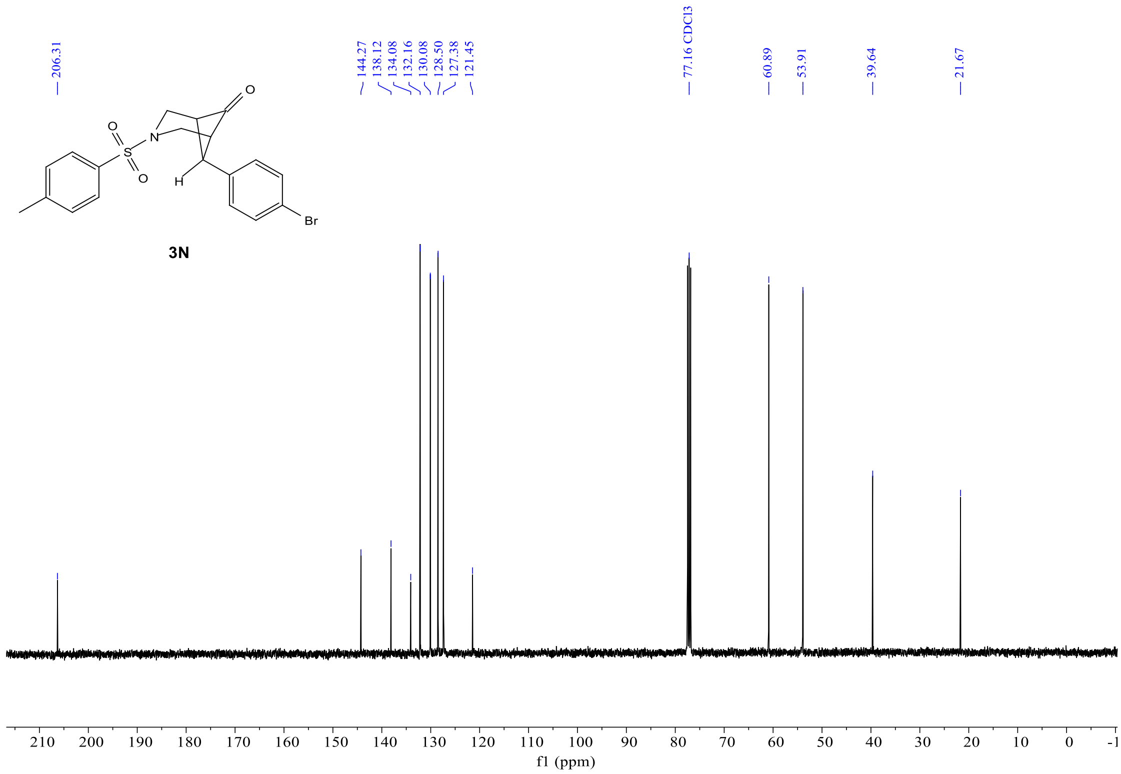
[1]H NMR of compound **3M** (400 MHz, $CDCl_3$)



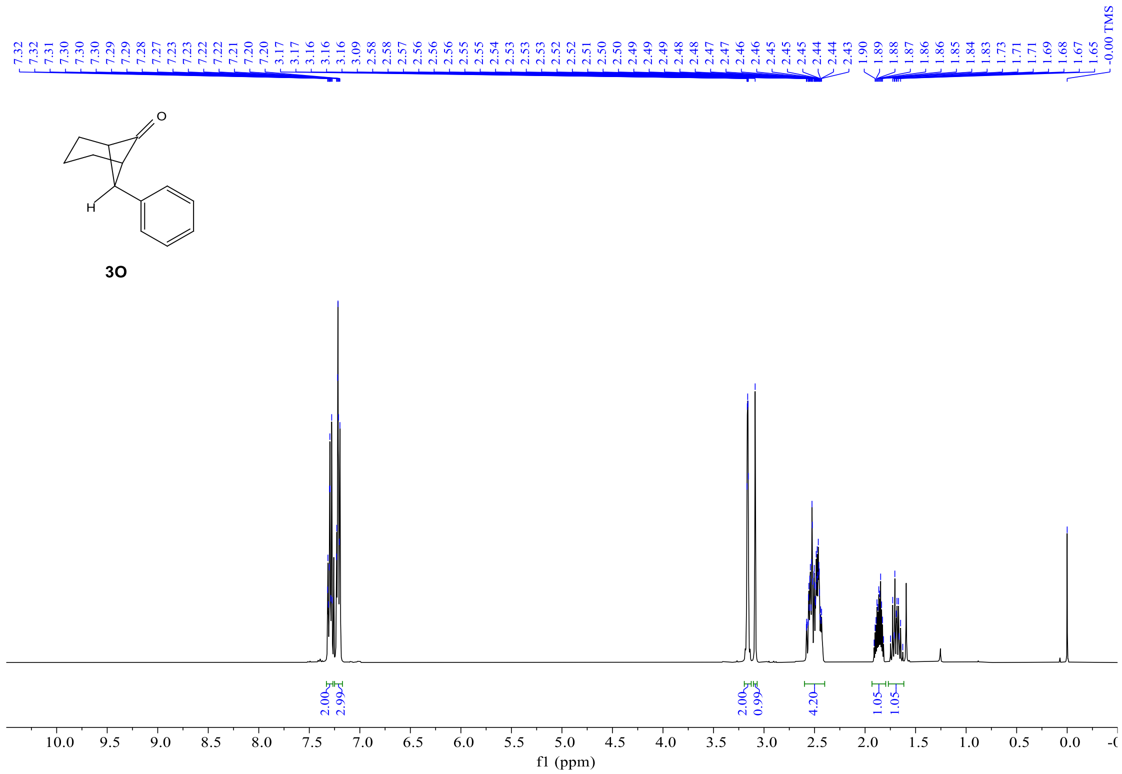
[13]C NMR of compound **3M** (101 MHz, $CDCl_3$)



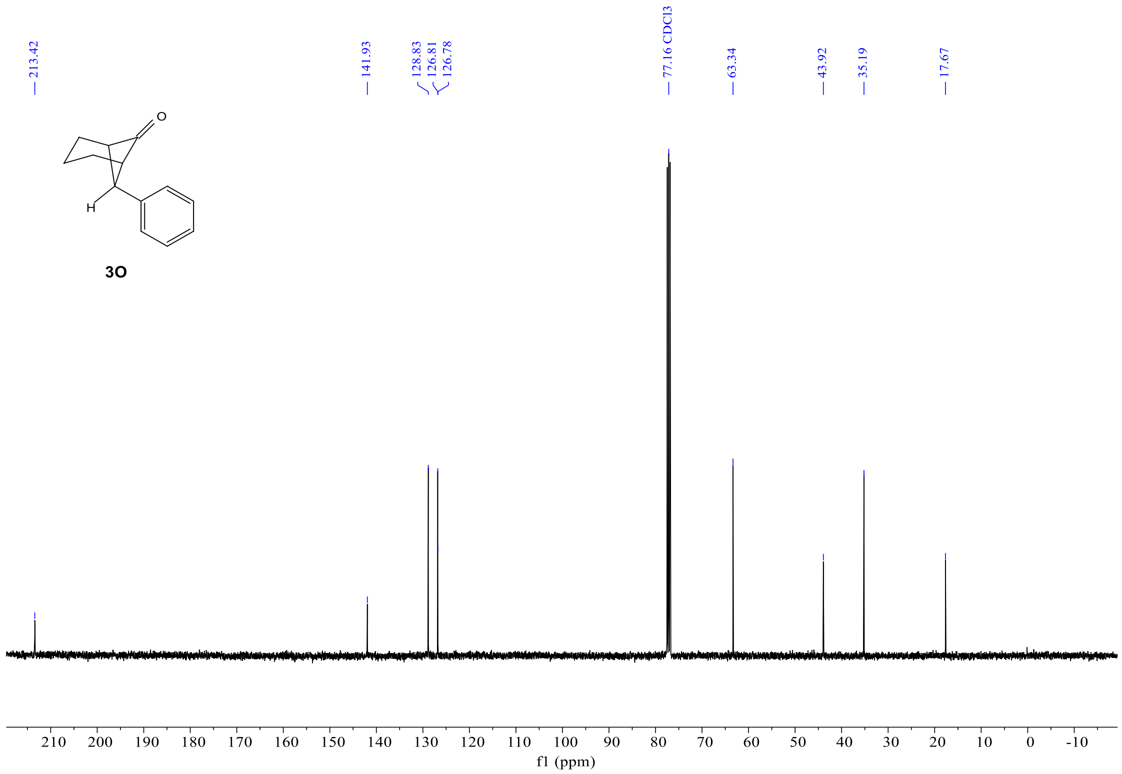
^{1}H NMR of compound **3N** (400 MHz, $CDCl_3$)



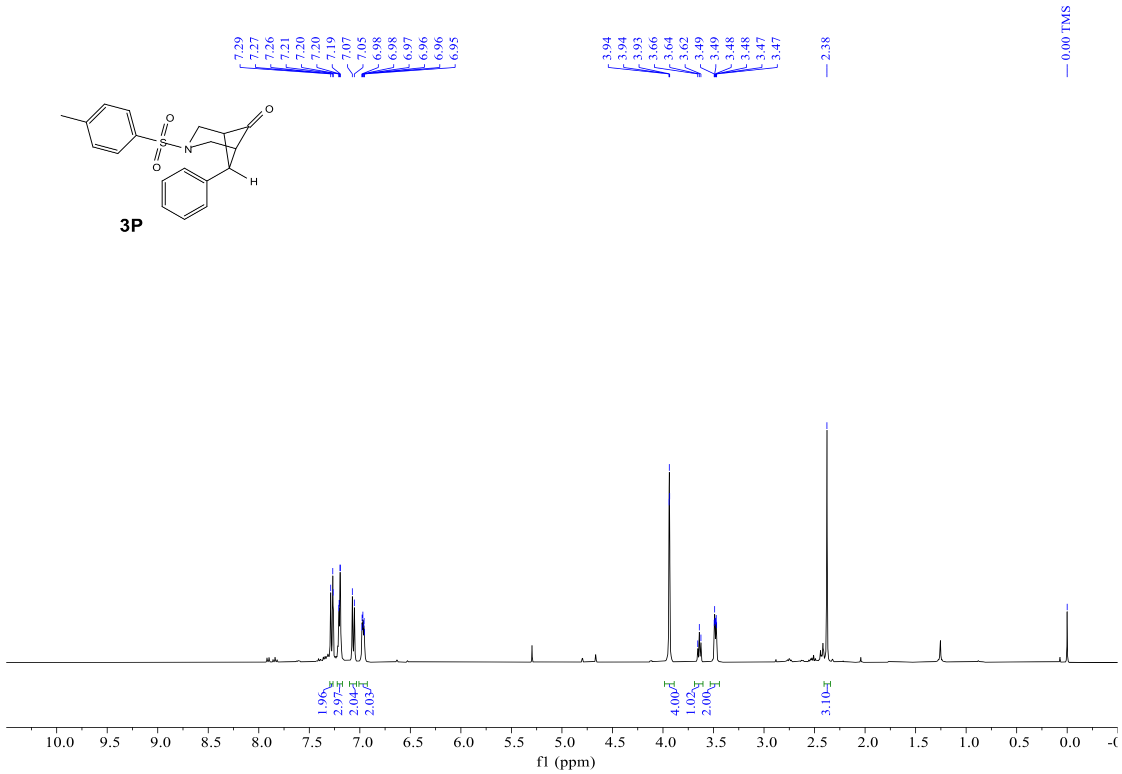
^{13}C NMR of compound **3N** (101 MHz, $CDCl_3$)



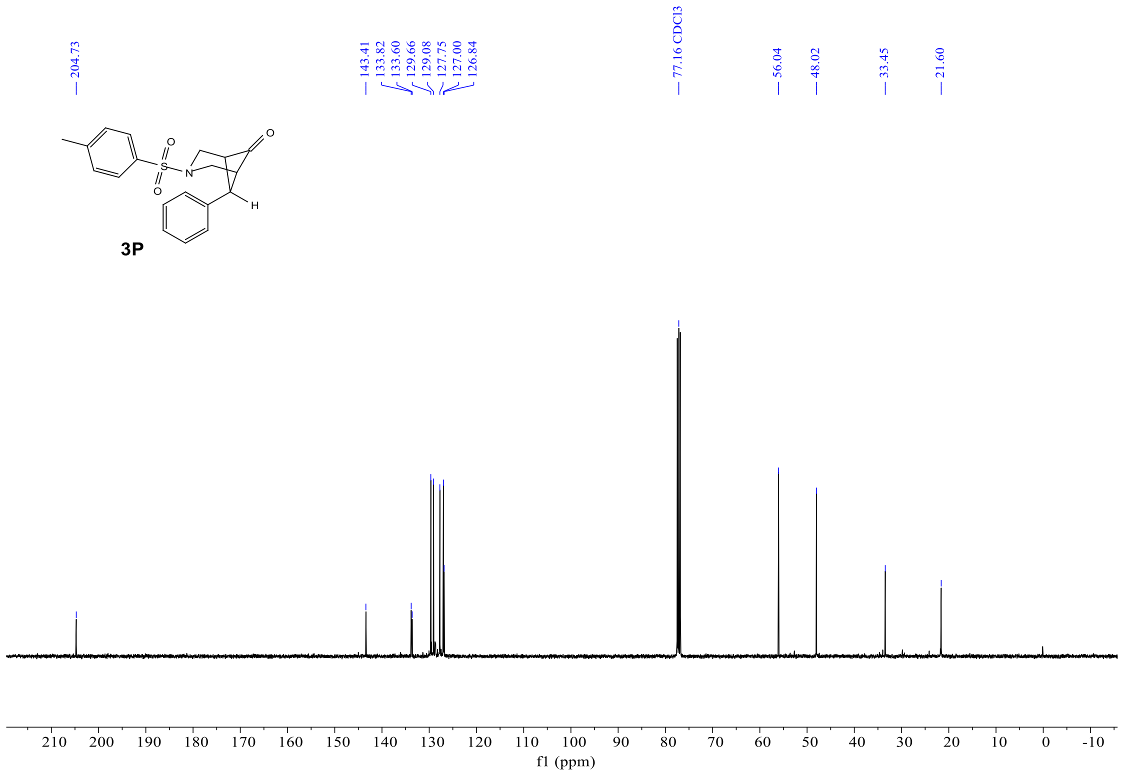
^{1}H NMR of compound **3O** (400 MHz, $CDCl_3$)



^{13}C NMR of compound **3O** (101 MHz, $CDCl_3$)

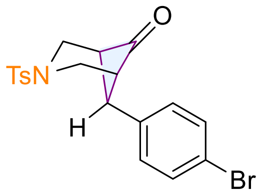


[1]H NMR of compound **3P** (400 MHz, $CDCl_3$)



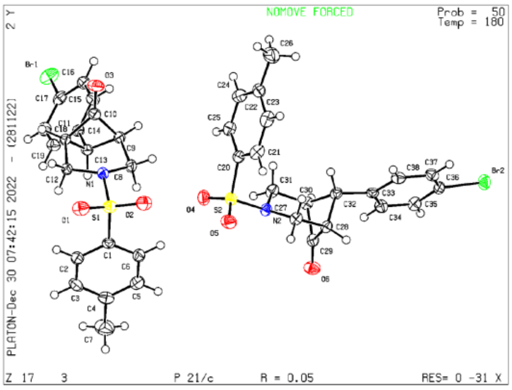
[13]C NMR of compound **3P** (101 MHz, $CDCl_3$)

S9. X-ray Data

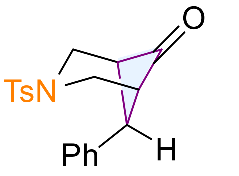


3N
CCDC: 2233622

≡

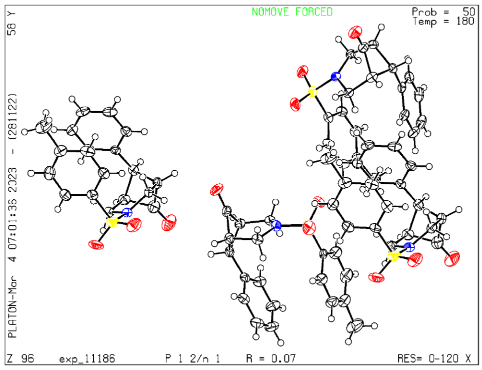


Crystal data	
Chemical formula	$C_{19}H_{18}BrNO_3S$
M_r	420.31
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	180
a, b, c (Å)	23.6009 (6), 9.9527 (3), 16.2181 (5)
β (°)	109.259 (3)
V (Å^3)	3596.32 (19)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.42
Crystal size (mm)	0.27 × 0.15 × 0.09
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.093, 1.04
No. of reflections	9445
No. of parameters	453
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.39



3P

CCDC: 2246406



Crystal data	
Chemical formula	$C_{19}H_{19}NO_3S$
M_r	341.41
Crystal system, space group	Monoclinic, $P2/n$
Temperature (K)	180
a, b, c (Å)	25.6057 (7), 10.0984 (3), 26.4319 (8)
β (°)	99.980 (3)
V (Å^3)	6731.2 (3)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.13 × 0.13 × 0.1
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.200, 1.04
No. of reflections	11889
No. of parameters	869
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.42, −0.40

S10. References

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