Supporting Information

Palladium Catalyzed Stereoselective Intramolecular [3+2] Cycloaddition Reactions of (*E*) & (*Z*)-Ene-Vinylidenecyclopropanes

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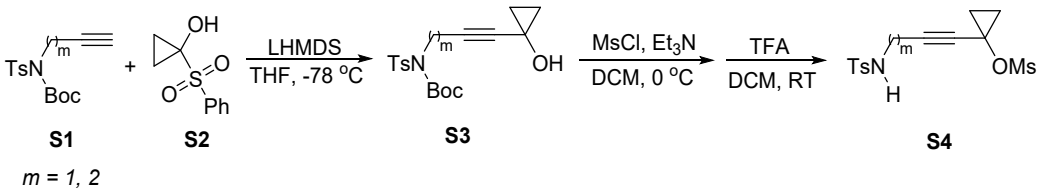
1. General remarks

^{1}H, ^{13}C and ^{19}F NMR spectra were recorded at 400 MHz or 600 MHz, 100 MHz or 150 MHz and 376 MHz, respectively. HRMS spectra were recorded by EI, ESI, FI method. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1}. Mass spectra were recorded by EI, ESI, and HRMS was measured on an Agilent Technologies 6224 TOF LC/MS instrument and a Waters Micromass GCT Permier. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. X-ray structure was determined on a Bruker Smart-1000 X-ray Diffraction meter. The employed solvents were dried up by standard methods when necessary. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC plate analysis with silica gel coated plates (Huanghai GF254). Flash column chromatography was performed by using 300-400 mesh silica gel eluting with ethyl acetate and petroleum ether at increased pressure. Chiral HPLC was performed on a SHIMADZU SPD-10A *vp* series with chiral columns (Chiralpak AD-H columns 4.6 × 250 mm, (Daicel Chemical Ind., Ltd.)).

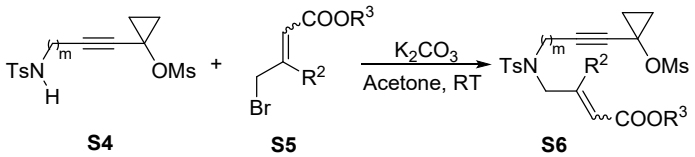
2. General procedures for the synthesis of substrates 1 and 3[1, 2, 3]

Synthesis of substrates **1a-1z** and **3a-3m**

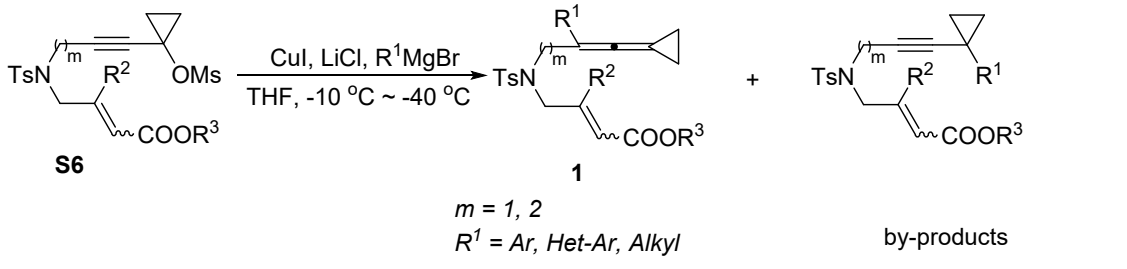


To the solution of compound **S1** (20 mmol) in THF (30 mL) was added LMHDS (22 mmol, 1.0 M in THF) within 20 min at -78 °C under argon. The resulting solution was allowed to stir at -78 °C for 0.5 h before a solution of **S2** (10 mmol) in THF (10 mL) was added into the above mixture. Consequently, the reaction mixture was allowed to warm up to room temperature and was stirred for 8.0 h. Then, saturated NH_4Cl solution was added to quench the reaction. Extracted with ethyl ether, dried over anhydrous Na_2SO_4, filtered, the organic phase was purified by a flash column chromatography on silica gel to give the corresponding product **S3** (PE/EA: 4:1~2:1).

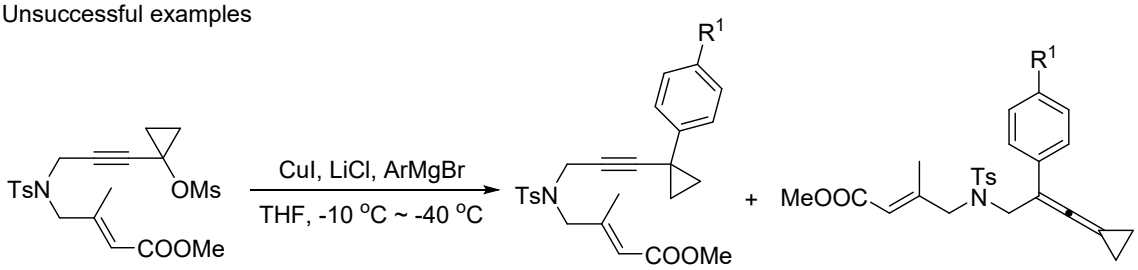
Under argon atmosphere, compound **S3** (4.0 mmol) was dissolved in DCM (10.0 mL) at 0 °C, Et_3N (8.0 mmol) and MsCl (6.0 mmol) was added. After stirring for 1.0 h, the reaction was quenched with H_2O (10.0 mL), extracted with DCM (10 mL x 3), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was transferred into a 50 mL flask with 10 mL DCM. Then, trifluoroacetic acid (TFA, 40 mmol) was added dropwise. After stirring for 12 h, the reaction was quenched with saturated Na_2CO_3 solution, extracted with DCM (10 mL x 3), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO_2) to give the corresponding product **S4** (PE/EA: 4:1~1:1).



To the solution of **S4** (1.5 mmol) and K_2CO_3 (1.8 mmol) in acetone (10 mL) was added **S5** (1.8 mmol). The resulting solution was allowed to stir at room temperature for 8.0 h. Then, H_2O was added to quench the reaction. The reaction mixture was extracted with EA twice, dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO_2) to give the corresponding product **S6** for two steps (PE/EA: 4:1~2:1).



Unsuccessful examples



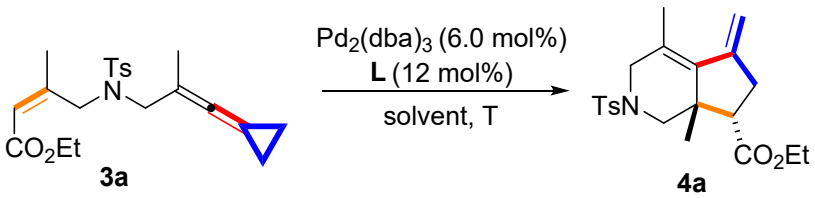
Under argon atmosphere, CuI (2.2 mmol) and LiCl (2.2 mmol) in a three-necked bottle was dried upon heating. Then THF (10 mL) was added. At -5 °C, R^1MgBr (1.0 mol/L in THF, 2.0 mmol, 2.0 mL) was added to the reaction mixture. 10 minutes later, the flask was moved into a -40 °C bath and stirred for a while before a solution of **S6** (1.0 mmol) in THF (10 mL) was added dropwise into the above flask. After stirring at -40 °C for 8.0 h, the reaction was quenched with saturated NH_4Cl solution, extracted with EA (10 mL x 3), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO_2) to give the corresponding product **1** (PE/EA: 10:1). However, during the preparation of some substrates, by-products are inevitably generated. It is difficult to separate this pair of isomers by column chromatography. Fortunately, the by-products do not affect the addition reaction.

Trace of by-products exists in these substrates (**1l**, **1m**, **1o**, **1y**, **1aa**, **3f**, and **3m**), which is difficult to separate. We did not label the byproducts in the spectra. We also attempted to synthesize substrates

bearing electron-withdrawing substituents such as OMe, F, Cl at the benzene ring. However, we only obtained the by-products instead of ene-VDCPs (Unsuccessful examples).

3. Optimization of reaction conditions.

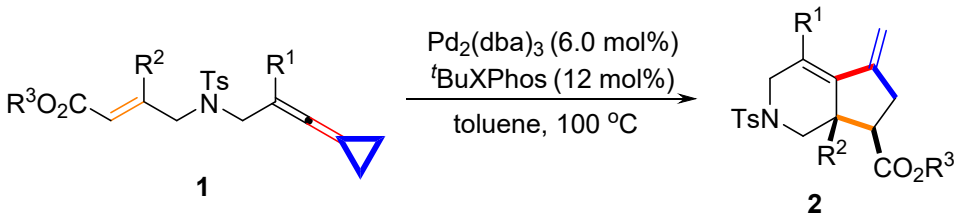
Table S1. Optimization of the palladium-catalyzed [3+2] cycloaddition of (*Z*)-ene-vinylidenecyclopropane **3a** for product **4a**.



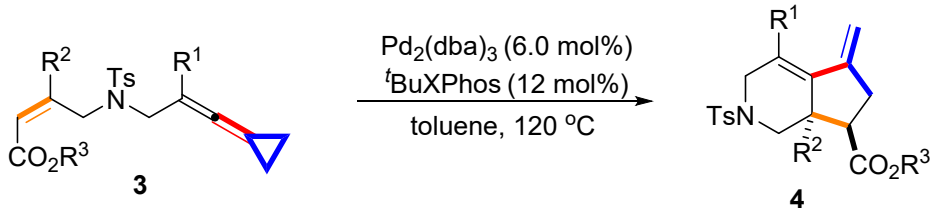
Entry[a]	Catalyst	L	Solvent	T (°C)	Yield/%[b]
1	$Pd_2(dba)_3$	^{t}BuXPhos	toluene	100	-
2	$Pd_2(dba)_3$	^{t}BuXPhos	toluene	110	68
3	**$Pd_2(dba)_3$**	**^{t}BuXPhos**	**toluene**	**120**	**94**
4	$Pd_2(dba)_3$	^{t}BuXPhos	dioxane	120	82
5	$Pd_2(dba)_3$	^{t}BuXPhos	DCE	120	70
6	$Pd_2(dba)_3$	^{t}BuXPhos	PhCl	120	72

[a] Reaction condition: substrate **3a** (0.10 mmol), $Pd_2(dba)_3$ (6 mol%) and **L** (12 mol%) in 1.0 mL anhydrous toluene under argon atmosphere for 8.0 h, [b] Isolated yield.

4. General procedure for the synthesis of 2 and 4.

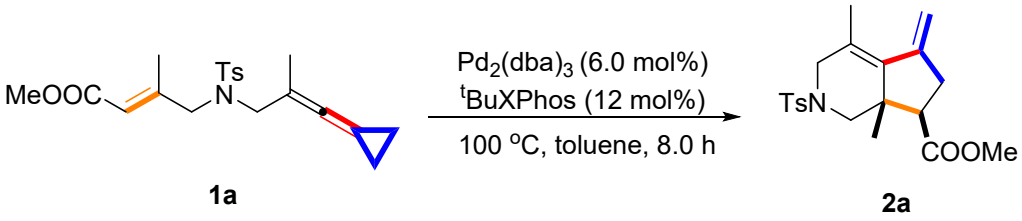


To a 5.0 mL dried tube was charged with **1** (0.1 mmol), Pd_2dba_3 (0.006 mmol) and ^{t}BuXPhos (0.012 mmol). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (2.0 mL) was added into the reaction tube. The reaction mixture was stirred at 100 °C for 8.0 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO_2) to give the corresponding product **2**.



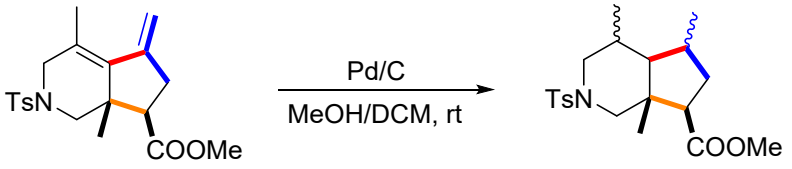
To a 5.0 mL dried tube was charged with **3** (0.1 mmol), Pd_2dba_3 (0.006 mmol) and ^{t}BuXPhos (0.012 mmol). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (2.0 mL) was added into the reaction tube. The reaction mixture was stirred at 120 °C for 8.0 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO_2) to give the corresponding product **4**.

5. Gram scale reaction and synthetic transformations.



1a **2a**

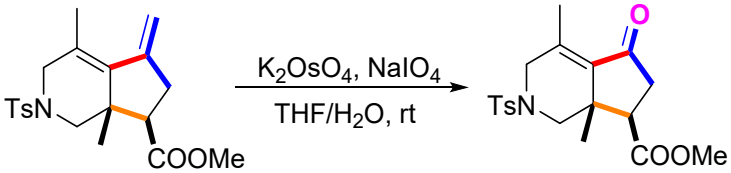
To a 100 mL dried tube was charged with **1a** (1.1 g, 3.0 mmol), Pd_2dba_3 (175.7 mg, 0.18 mmol) and ^{t}BuXPhos (182.2 mg, 0.36 mmol). The reaction tube was evacuated and backfilled with argon (repeated three times). Then, toluene (40.0 mL) was added into the reaction tube. The reaction mixture was stirred at 100 °C for 8.0 h. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO_2) to give the corresponding product **2a** (1.0 g, 92%).



2a
0.1 mmol, 37.5 mg

5
36.7 mg, 98% yield
diastereomeric mixture

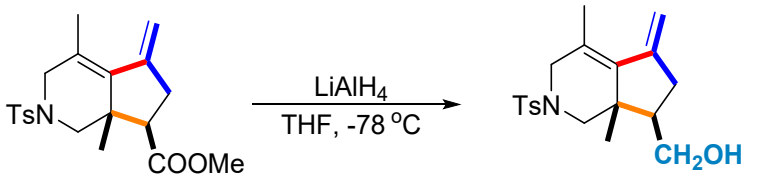
To a solution of **2a** (32.0 mg, 0.1 mmol) in MeOH (5.0 mL) was added Pd/C (7.6 mg, 20% w/w). The reaction system was charged with H_2 balloon and the reaction mixture was stirred at room temperature for 12 h. The reaction mixture was filtered and the volatiles were removed on a rotary evaporator. The residues were passed through a short silica chromatography (PE/EA = 1/1) to afford the desired product **5** (36.7 mg, 98% yield).



2a
0.1 mmol, 37.5 mg

6
36.2 mg, 96% yield

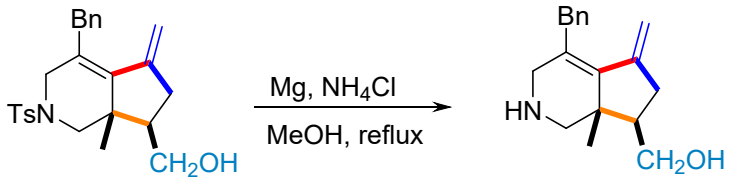
The cycloadduct **2a** (37.5 mg, 0.1 mmol, 1.0 equiv), $K_2OsO_4•2H_2O$ (2.2 mg, 0.006 mmol, 0.06 equiv) and $NaIO_4$ (106.9 mg, 0.5 mmol, 5.0 equiv) were suspended in THF (1.0 mL) and H_2O (1.0 mL). The reaction mixture was stirred for 3.0 h. After being quenched by adding aqueous $Na_2S_2O_3$ solution and extracted by EA, the combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by a flash column chromatography (PE/EA = 4:1) to give the desired product **6** (36.2 mg, 96% yield).



2a
0.1 mmol, 37.5 mg

7
33.3 mg, 96% yield

A solution of **2a** (37.5 mg, 0.1 mmol) in anhydrous THF (2.0 mL) was cooled to -78 °C under nitrogen atmosphere and 1.0 mL (1.0 mmol) of 1.0 M sodium $LiAlH_4$ in THF was added dropwise. The reaction mixture was stirred for 40 min at this temperature. After being stirred for 30 min, the reaction was quenched with saturated NH_4Cl aqueous solution, extracted with ethyl acetate, dried over anhydrous $MgSO_4$, filtered, and evaporated. The residue was chromatographed through a silica gel column (PE/EA = 2/1) to afford product **7** (33.3 mg, 96% yield).



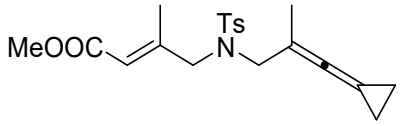
8
44.2 mg, 98% yield

9
15.1 mg, 56% yield

A solution of **9** (44.2 mg, 0.1 mmol), Mg (10.0 eq.) and NH_4Cl (10.0 eq.) in anhydrous MeOH (2.0 mL) was reflux to 80 °C under nitrogen atmosphere. After being stirred for 8 hours, the reaction was quenched with a saturated NH_4Cl aqueous solution, extracted with ethyl acetate, dried over anhydrous $MgSO_4$, filtered, and evaporated under reduced pressure. The residue was chromatographed through

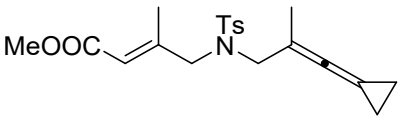
a silica gel column (DCM/MeOH = 2/1) to afford product **9** (15.1 mg, 56% yield).

6. Spectroscopic data.

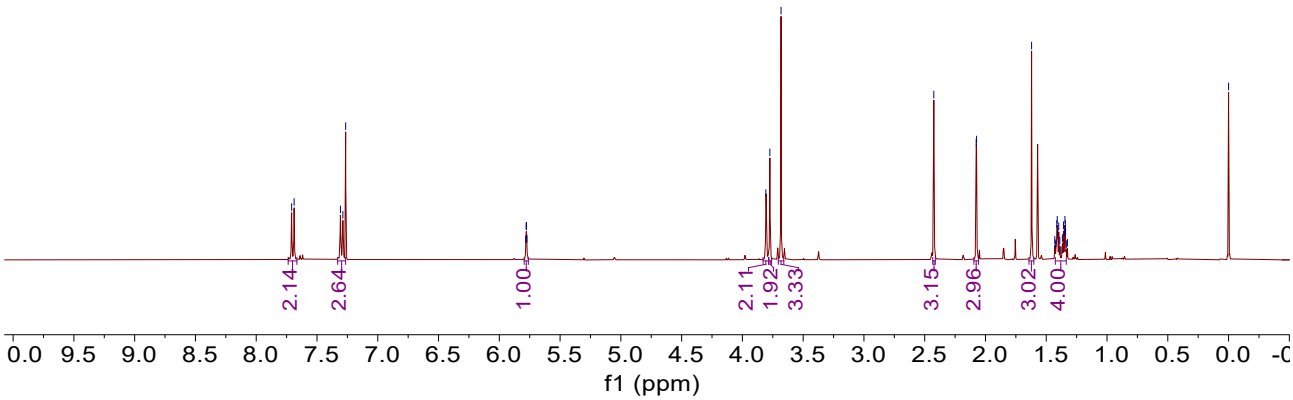


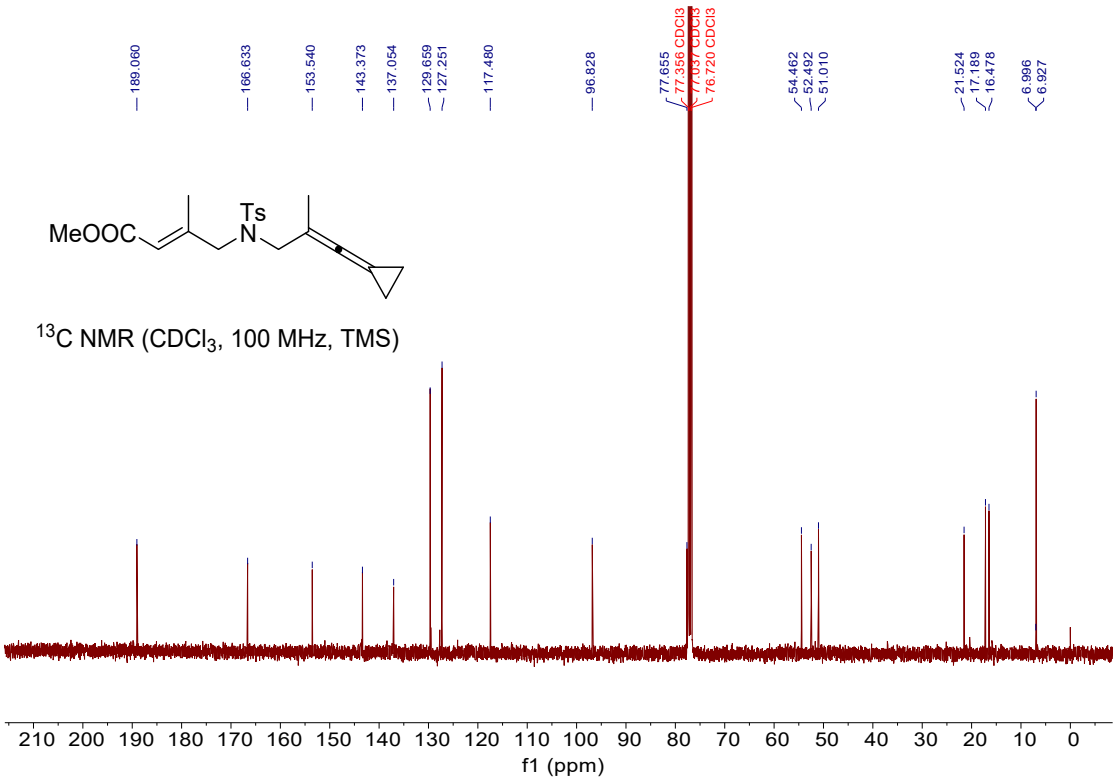
methyl (E)-4-((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1a)

A colorless oil, 90% yield, 338.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.78 (q, *J* = 1.2 Hz, 1H), 3.81 (s, 2H), 3.77 (s, 2H), 3.68 (s, 3H), 2.43 (s, 3H), 2.07 (d, *J* = 1.2 Hz, 3H), 1.62 (s, 3H), 1.45 – 1.32 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.1, 166.6, 153.5, 143.4, 137.1, 129.7, 127.3, 117.5, 96.8, 77.7, 54.5, 52.5, 51.0, 21.5, 17.2, 16.5, 7.0, 6.9. IR (neat) ν 660, 769, 1089, 1216, 1346, 1661, 1719, 2025, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{25}NO_4SNa$ $(M+Na)^+$: 398.1396, Found: 398.1398.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)




189.060
166.633
153.540
143.373
137.054
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127.251
117.480
96.828
77.655
77.356 CDCl3
77.037 CDCl3
76.720 CDCl3
54.462
52.492
51.010
21.524
17.189
16.478
6.996
6.927
MeOOC
Ts
N
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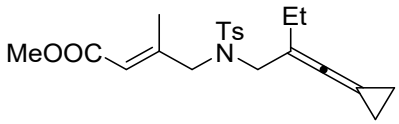
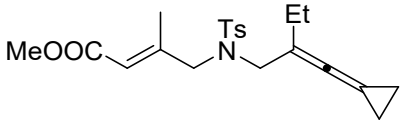
f1 (ppm)

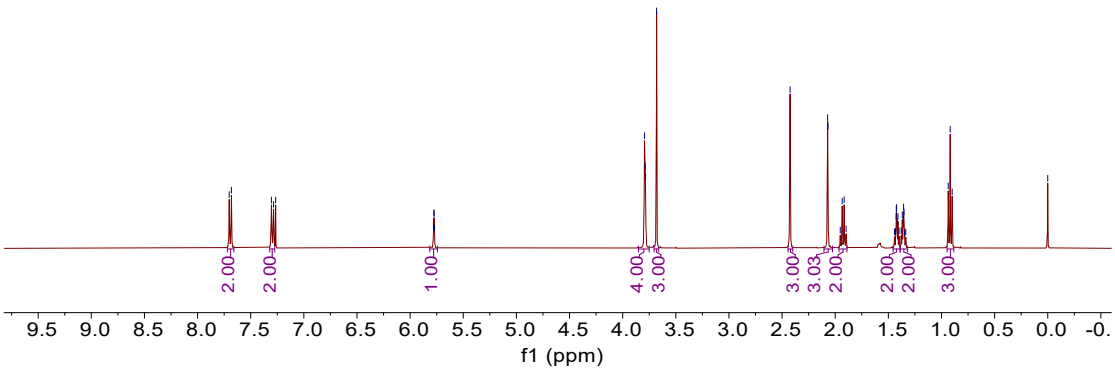


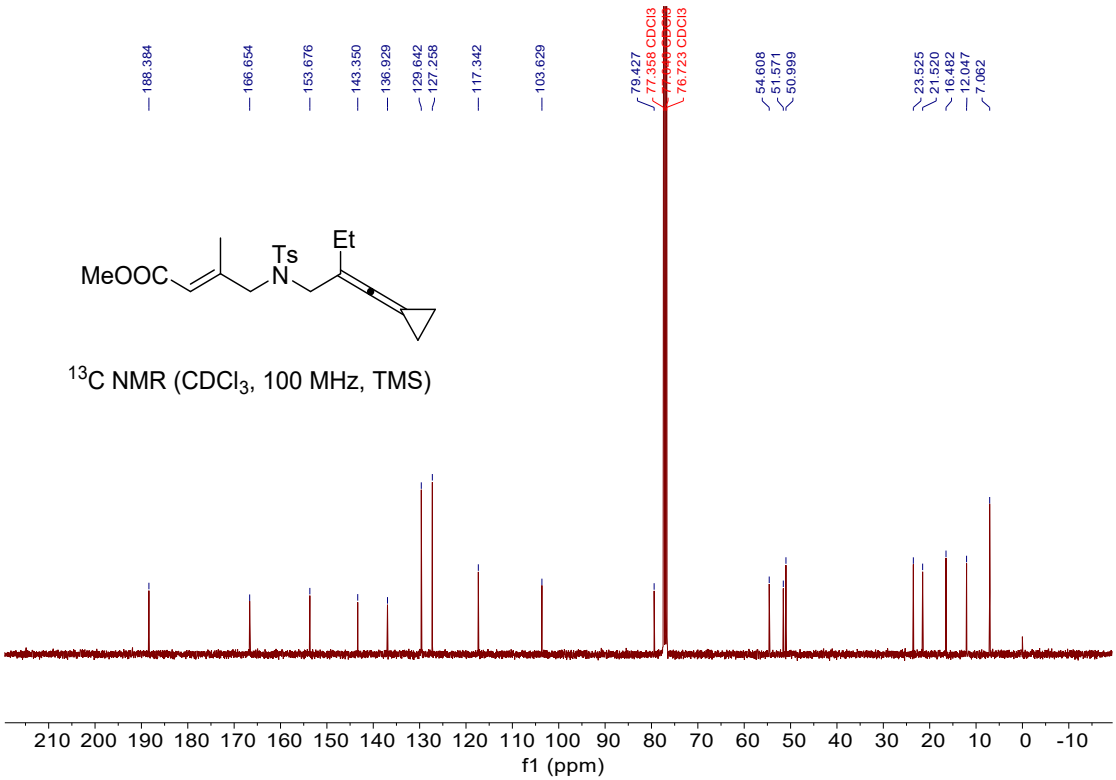
methyl (E)-4-((N-(2-(cyclopropylidene-λ^5-methylene)butyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1b)

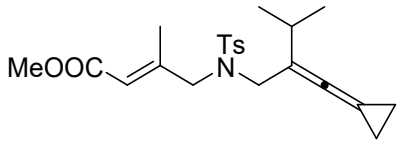
A colorless oil, 90% yield, 351.0 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.78 (q, *J* = 1.2 Hz, 1H), 3.85 – 3.75 (m, 4H), 3.68 (s, 3H), 2.42 (s, 3H), 2.07 (d, *J* = 1.2 Hz, 3H), 1.92 (q, *J* = 7.2 Hz, 2H), 1.45 – 1.39 (m, 2H), 1.39 – 1.32 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.4, 166.7, 153.7, 143.4, 136.9, 129.6, 127.3, 117.3, 103.6, 79.4, 54.6, 51.6, 51.0, 23.5, 21.5, 16.5, 12.0, 7.1. IR (neat) ν 660, 772, 1158, 1446, 1663, 1720, 2020, 2964 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1554.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

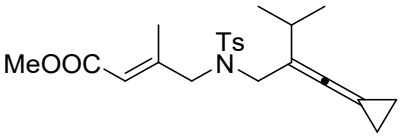



188.384
166.654
153.676
143.350
136.929
129.642
127.258
117.342
103.629
79.427
77.358 CDCl3
76.723 CDCl3
54.608
51.571
50.999
23.525
21.520
16.482
12.047
7.062
MeOOC
Ts
N
Et
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

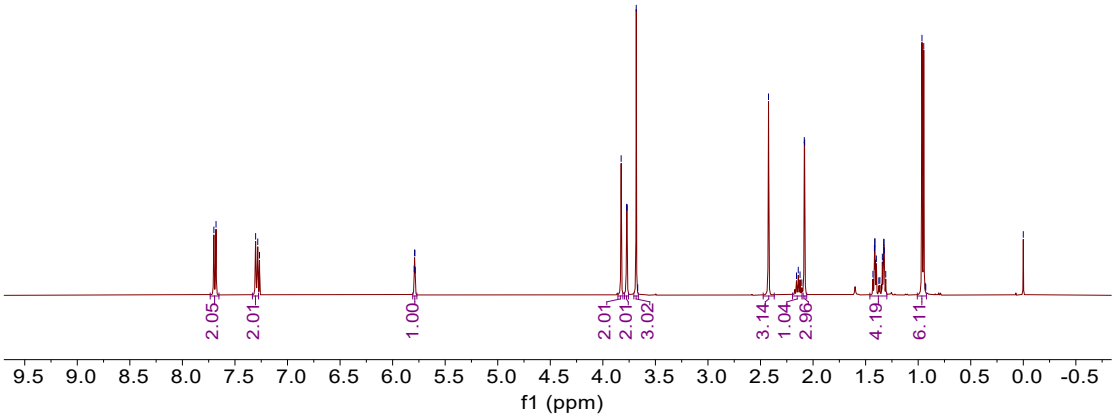


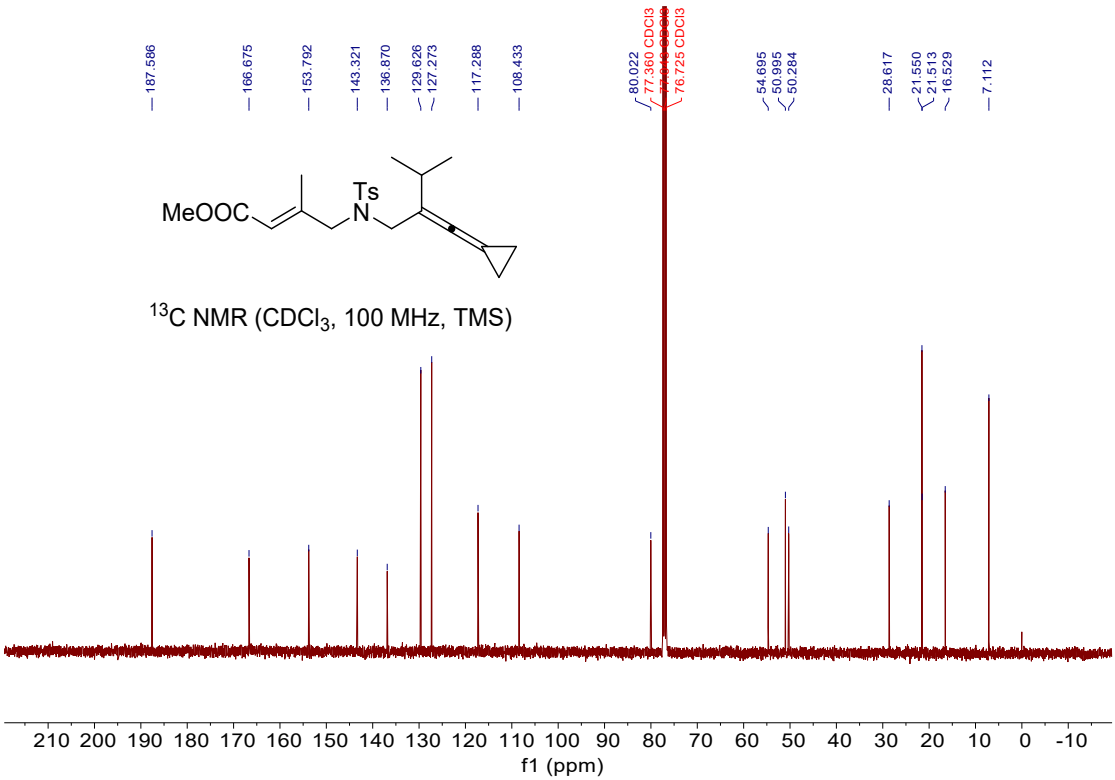
methyl (E)-4-((N-(2-(cyclopropylidene-λ^5-methylene)-3-methylbutyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1c)

A colorless oil, 80% yield, 323.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.79 (q, *J* = 1.2 Hz, 1H), 3.83 (s, 2H), 3.77 (d, *J* = 1.2 Hz, 2H), 3.68 (s, 3H), 2.42 (s, 3H), 2.13 (q, *J* = 6.8 Hz, 1H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.46 – 1.30 (m, 4H), 0.96 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.6, 166.7, 153.8, 143.3, 136.9, 129.6, 127.3, 117.3, 108.4, 80.0, 54.7, 51.0, 50.3, 28.6, 21.5, 21.5, 16.5, 7.1. IR (neat) ν 667, 819, 1221, 1446, 1660, 1721, 2027, 2959 cm^{-1}. HRMS (ESI) calcd. for $C_{22}H_{29}NO_4SNa$ $(M+Na)^+$: 426.1710, Found: 426.1714.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

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143.321
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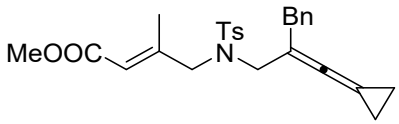
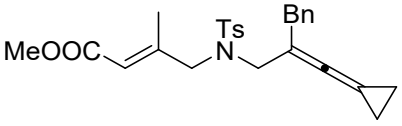
129.626
127.273
117.288
108.433
80.022
77.360 CDCl3
76.725 CDCl3
54.695
50.995
50.284
28.617
21.550
21.513
16.529
7.112
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

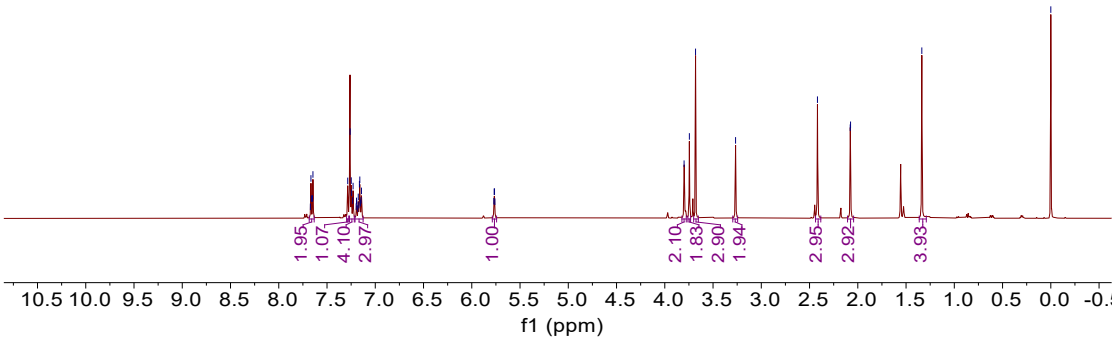


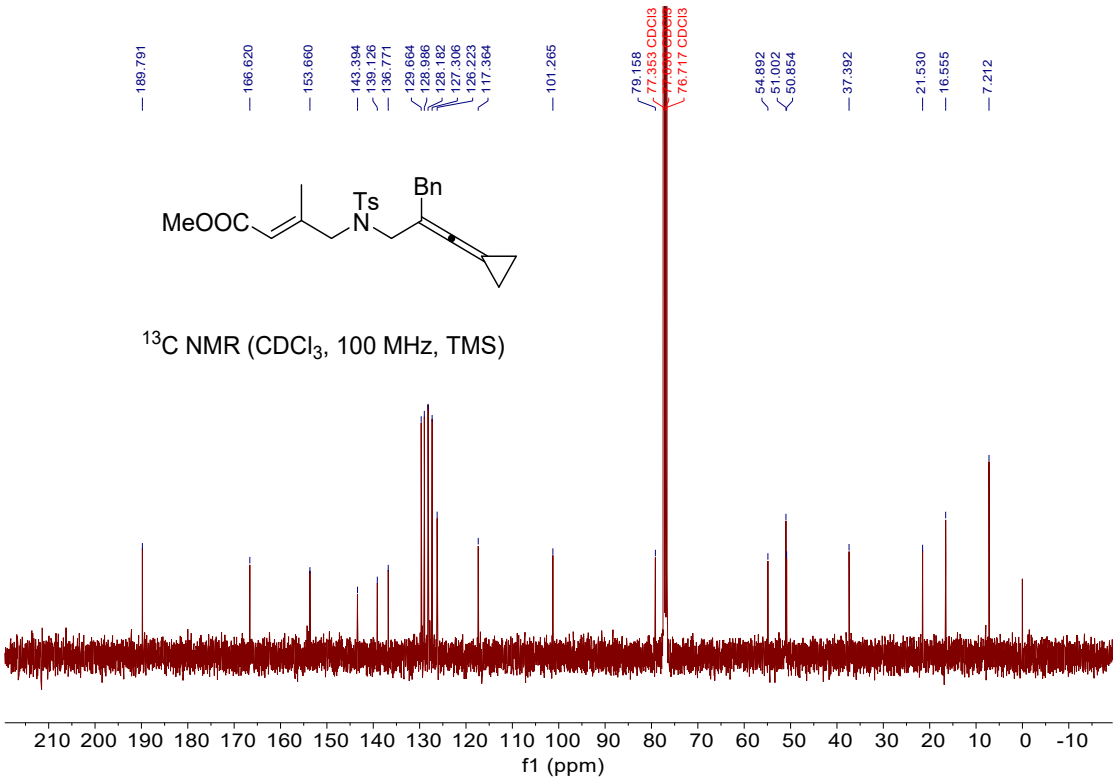
methyl (E)-4-((N-(2-benzyl-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1d)

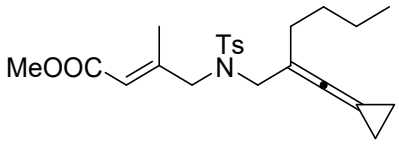
A colorless oil, 90% yield, 408.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.63 (m, 2H), 7.29 (s, 1H), 7.27 – 7.22 (m, 3H), 7.21 – 7.13 (m, 3H), 5.77 (q, *J* = 1.2 Hz, 1H), 3.80 (s, 2H), 3.75 (s, 2H), 3.68 (s, 3H), 3.27 (s, 2H), 2.42 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.32-1.36 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 166.6, 153.7, 143.4, 139.1, 136.8, 129.7, 129.0, 128.2, 127.3, 126.2, 117.4, 101.3, 79.2, 54.9, 51.0, 50.9, 37.4, 21.5, 16.6, 7.2. IR (neat) ν 661, 909, 1216, 1347, 1660, 1722, 2025, 2951 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1707.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

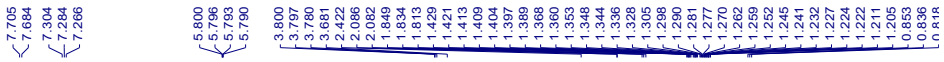


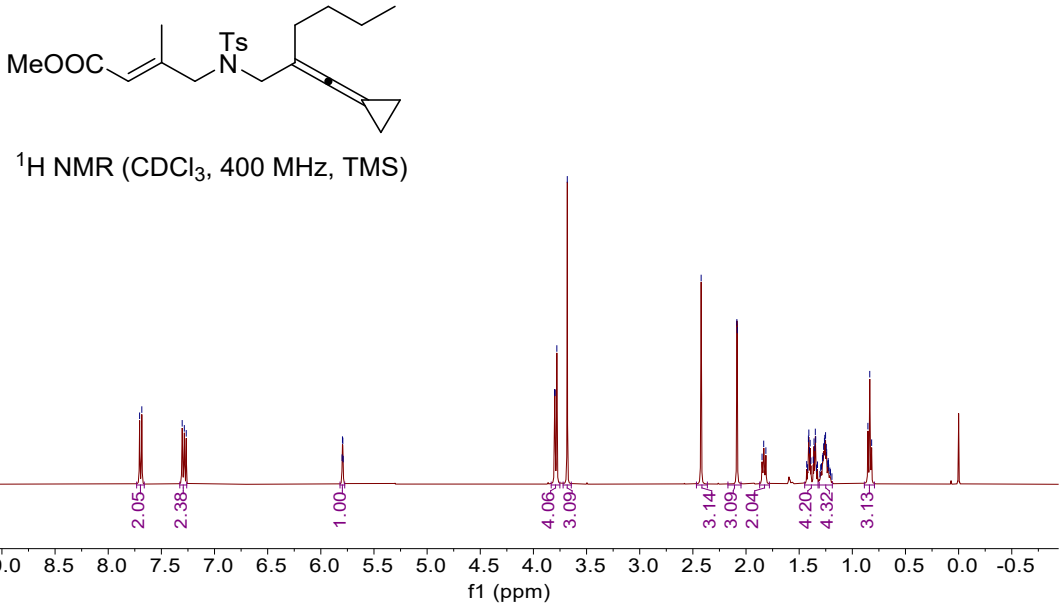

189.791
166.620
153.660
143.394
139.126
136.771
129.664
128.986
128.182
127.306
126.223
117.364
101.265
79.158
77.353 CDCl3
76.717 CDCl3
54.892
51.002
50.854
37.392
21.530
16.555
7.212
MeOOC
Ts
N
Bn
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

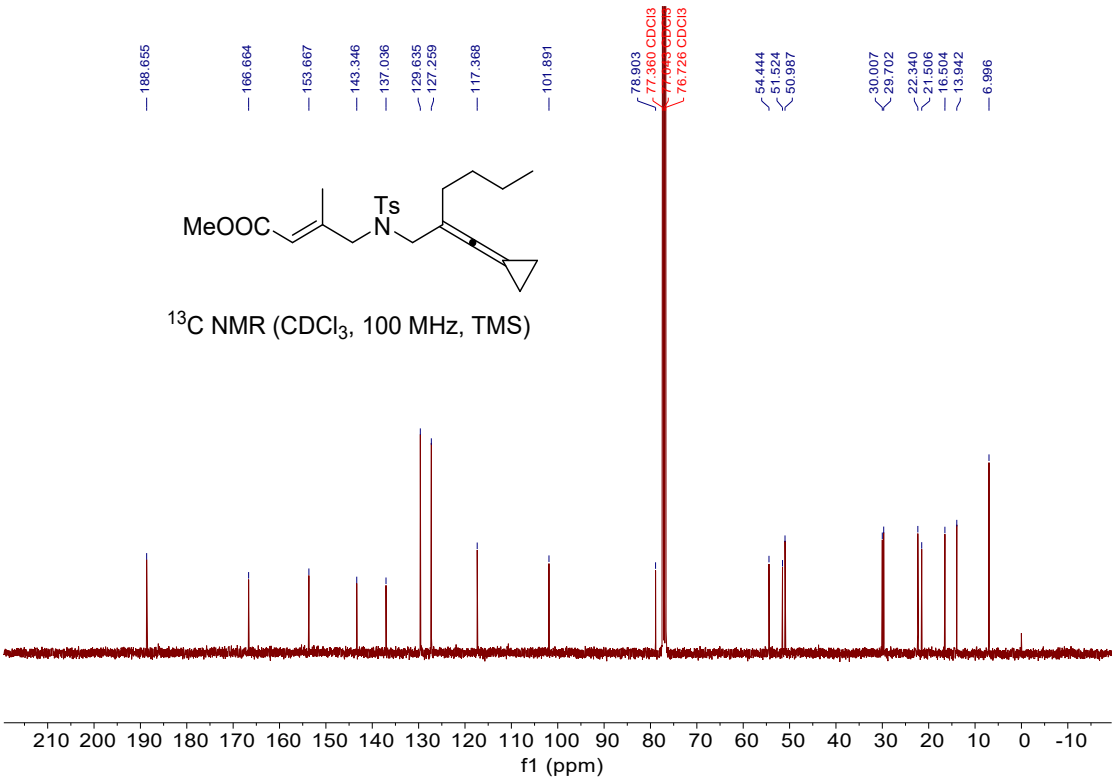


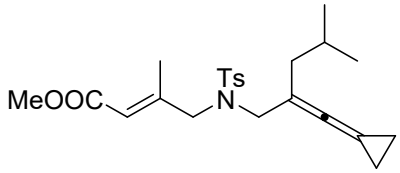
methyl (E)-4-((N-(2-(cyclopropylidene-λ^5-methylene)hexyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1e)

A colorless oil, 90% yield, 375.3 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.79 (q, *J* = 1.2 Hz, 1H), 3.83 – 3.75 (m, 4H), 3.68 (s, 3H), 2.42 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.87 – 1.78 (m, 2H), 1.45 – 1.32 (m, 4H), 1.31 – 1.19 (m, 4H), 0.84 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.7, 166.7, 153.7, 143.3, 137.0, 129.6, 127.3, 117.4, 101.9, 78.9, 54.4, 51.5, 51.0, 30.0, 29.7, 22.3, 21.5, 16.5, 13.9, 7.0. IR (neat) ν 660, 1220, 1358, 1661, 1720, 2020, 2957 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{31}NO_4SNa$ $(M+Na)^+$: 440.1866, Found: 440.1866.



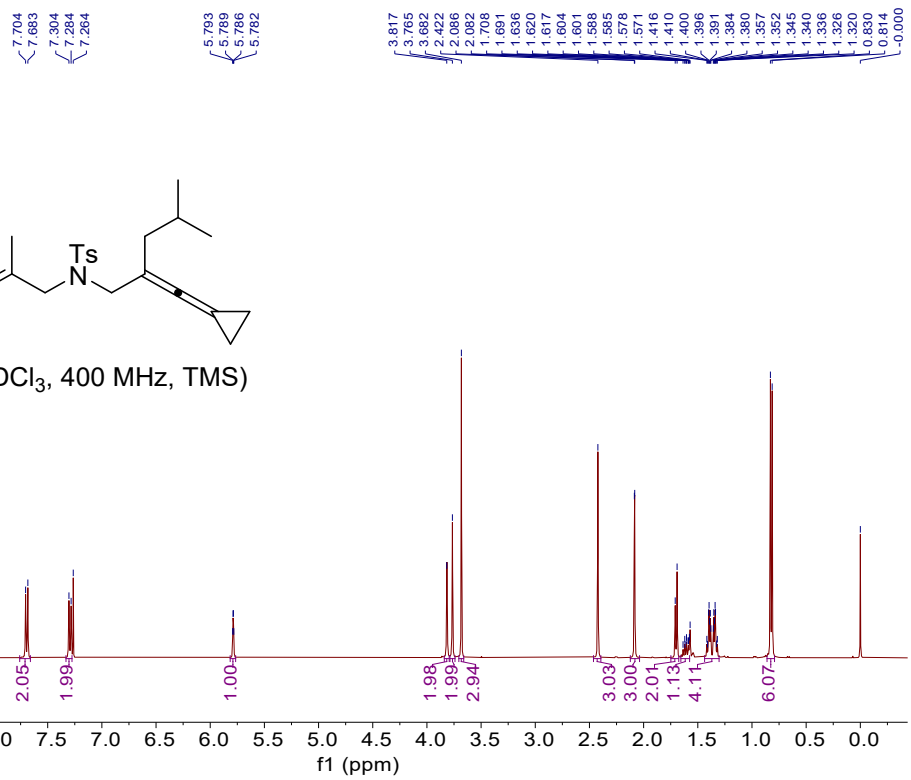


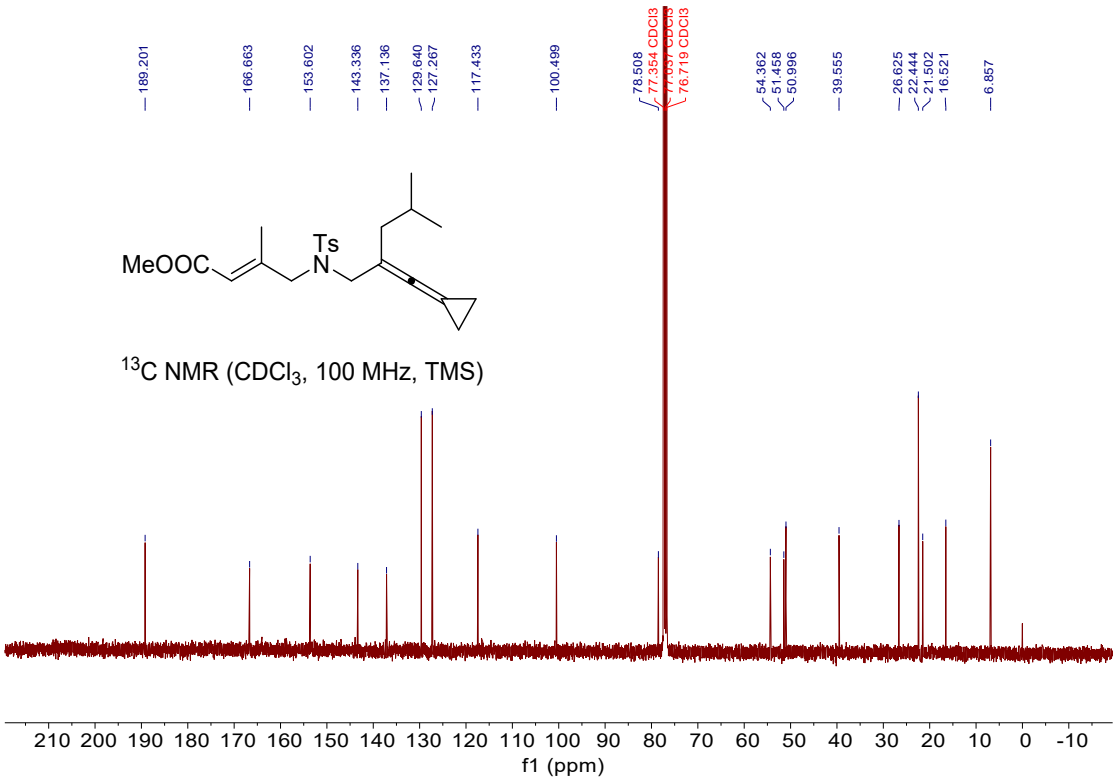

188.655
166.664
153.667
143.346
137.036
129.635
127.259
117.368
101.891
78.903
77.360 CDCl3
76.726 CDCl3
54.444
51.524
50.987
30.007
29.702
22.340
21.506
16.504
13.942
6.996
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

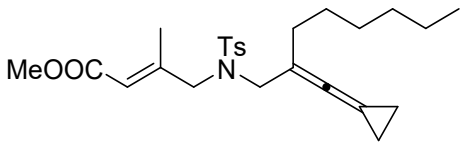


methyl (E)-4-((N-(2-(cyclopropylidene-λ^5-methylene)-4-methylpentyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1f)

A colorless oil, 90% yield, 375.3 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.79 (q, *J* = 1.2 Hz, 1H), 3.82 (s, 2H), 3.76 (s, 2H), 3.68 (s, 3H), 2.42 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.70 (d, *J* = 6.8 Hz, 2H), 1.66 – 1.58 (m, 1H), 1.44 – 1.30 (m, 4H), 0.82 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.2, 166.7, 153.6, 143.3, 137.1, 129.6, 127.3, 117.4, 100.5, 78.5, 54.4, 51.5, 51.0, 39.6, 26.6, 22.4, 21.5, 16.5, 6.9. IR (neat) ν 662, 910, 1659, 1721, 2024, 2952 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{32}NO_4S$ $(M+H)^+$: 418.2047, Found: 418.2043.

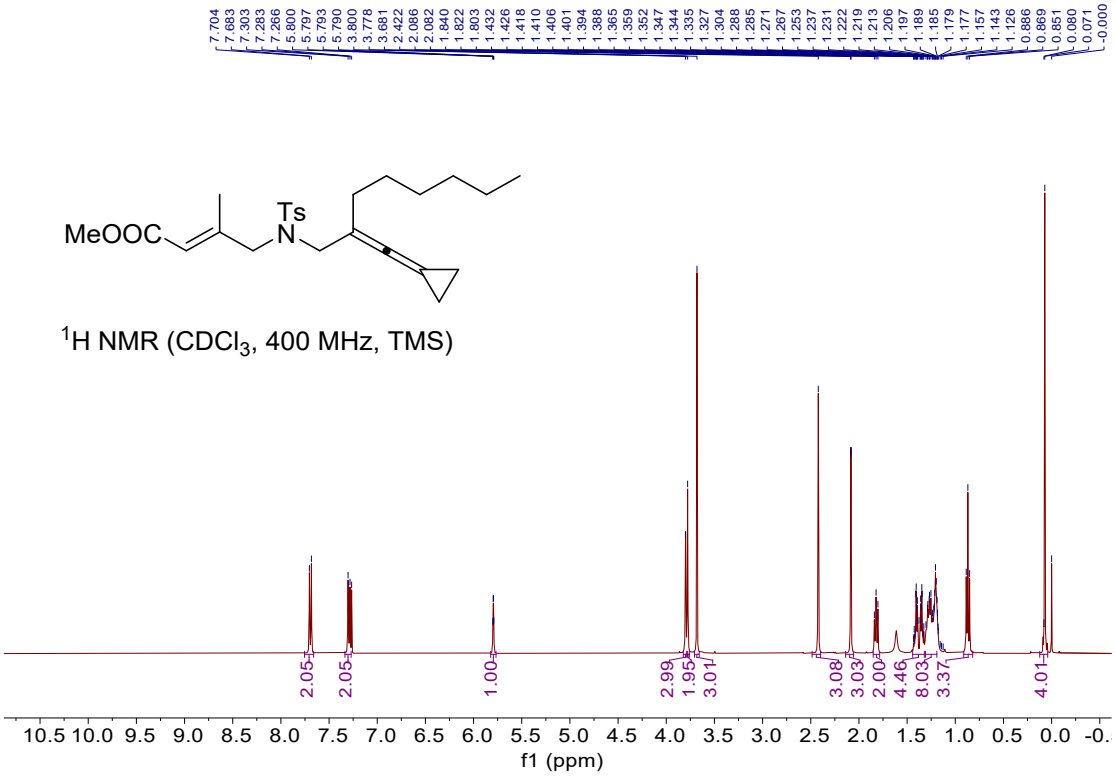


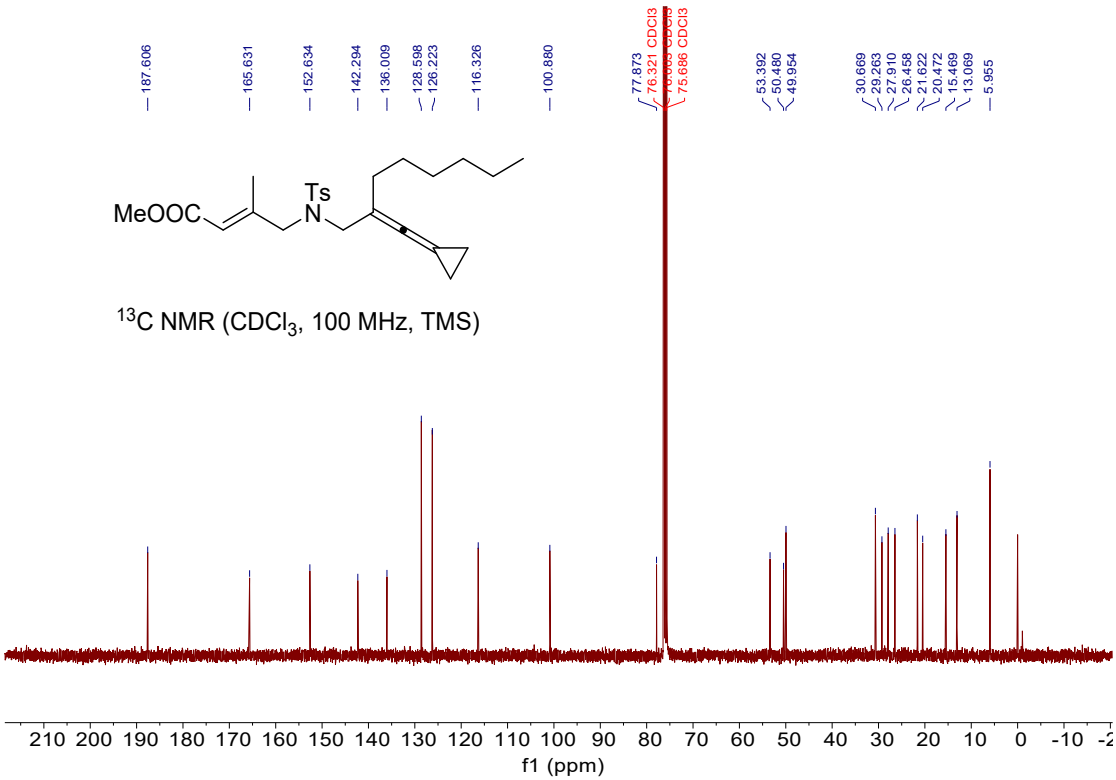

189.201
166.663
153.602
143.336
137.136
129.640
127.267
117.433
100.499
78.508
77.354 CDCl3
77.037 CDCl3
76.719 CDCl3
54.362
51.458
50.996
39.555
26.625
22.444
21.502
16.521
6.857
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

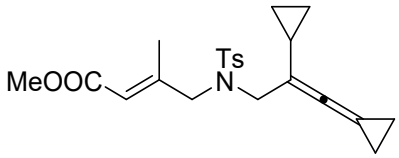


methyl (E)-4-((N-(2-(cyclopropylidene-λ^5-methylene)octyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1g)

A colorless oil, 90% yield, 401.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.79 (q, *J* = 1.2 Hz, 1H), 3.80 (s, 3H), 3.78 (s, 2H), 3.68 (s, 3H), 2.42 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.82 (t, *J* = 7.2 Hz, 2H), 1.44 – 1.32 (m, 4H), 1.31 – 1.12 (m, 8H), 0.87 (t, *J* = 7.2 Hz, 3H), 0.12 – 0.04 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.6, 165.6, 152.6, 142.3, 136.0, 128.6, 126.2, 116.3, 100.9, 77.9, 53.4, 50.5, 50.0, 30.7, 29.3, 27.9, 26.5, 21.6, 20.5, 15.5, 13.1, 6.0. IR (neat) ν 660, 991, 1659, 1721, 2021, 2925 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{35}NO_4SNa$ $(M+Na)^+$: 468.2179, Found: 468.2175.

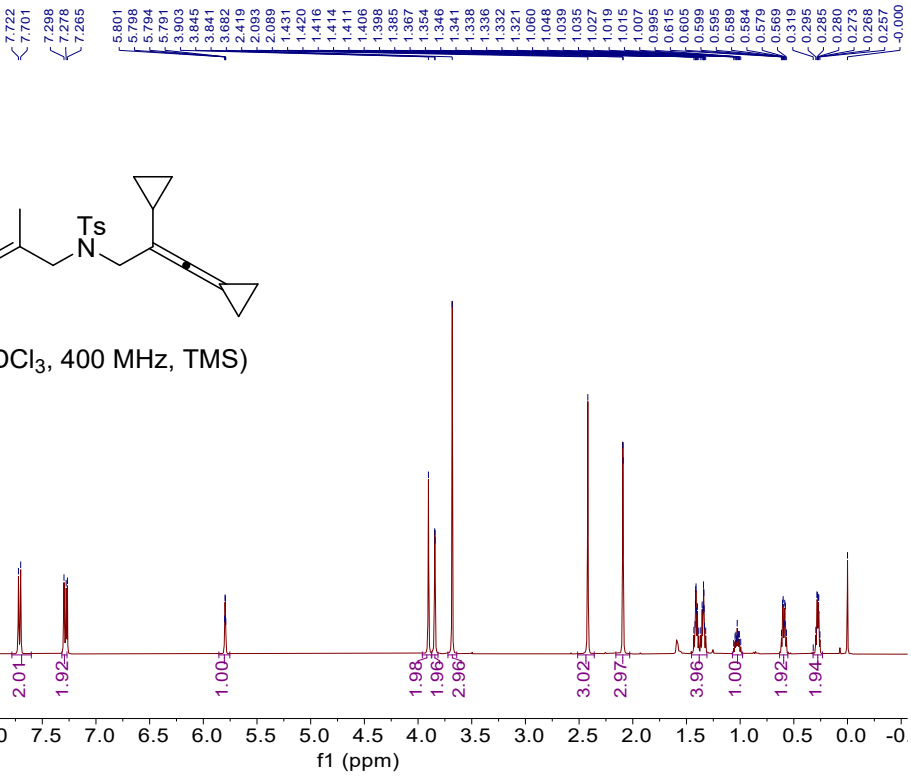


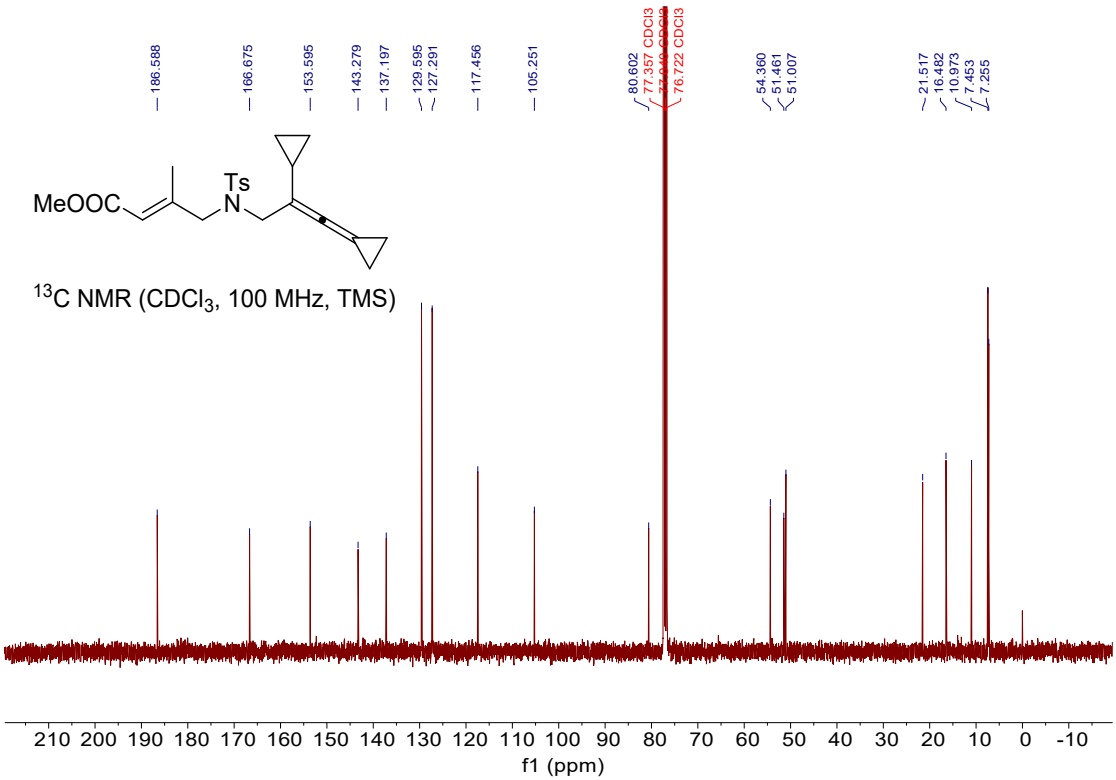

187.606
165.631
152.634
142.294
136.009
128.598
126.223
116.326
100.880
77.873
76.321 CDCl3
75.686 CDCl3
53.392
50.480
49.954
30.669
29.263
27.910
26.458
21.622
20.472
15.469
13.069
5.955
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

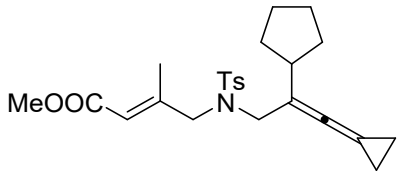


methyl (E)-4-((N-(2-cyclopropyl-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1h)

A colorless oil, 80% yield, 321.6mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.80 (q, *J* = 1.2 Hz, 1H), 3.90 (s, 2H), 3.84 (d, *J* = 1.2 Hz, 2H), 3.68 (s, 3H), 2.42 (s, 3H), 2.09 (d, *J* = 1.2 Hz, 3H), 1.45 – 1.31 (m, 4H), 1.07 – 0.98 (m, 1H), 0.63 – 0.56 (m, 2H), 0.32 – 0.23 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.6, 166.7, 153.6, 143.3, 137.2, 129.6, 127.3, 117.5, 105.3, 80.6, 54.4, 51.5, 51.0, 21.5, 16.5, 11.0, 7.5, 7.3. IR (neat) ν 661, 911, 1346, 1660, 1719, 2020, 2926 cm^{-1}. HRMS (ESI) calcd. for $C_{22}H_{27}NO_4SNa$ $(M+Na)^+$: 424.1553, Found: 424.1558.

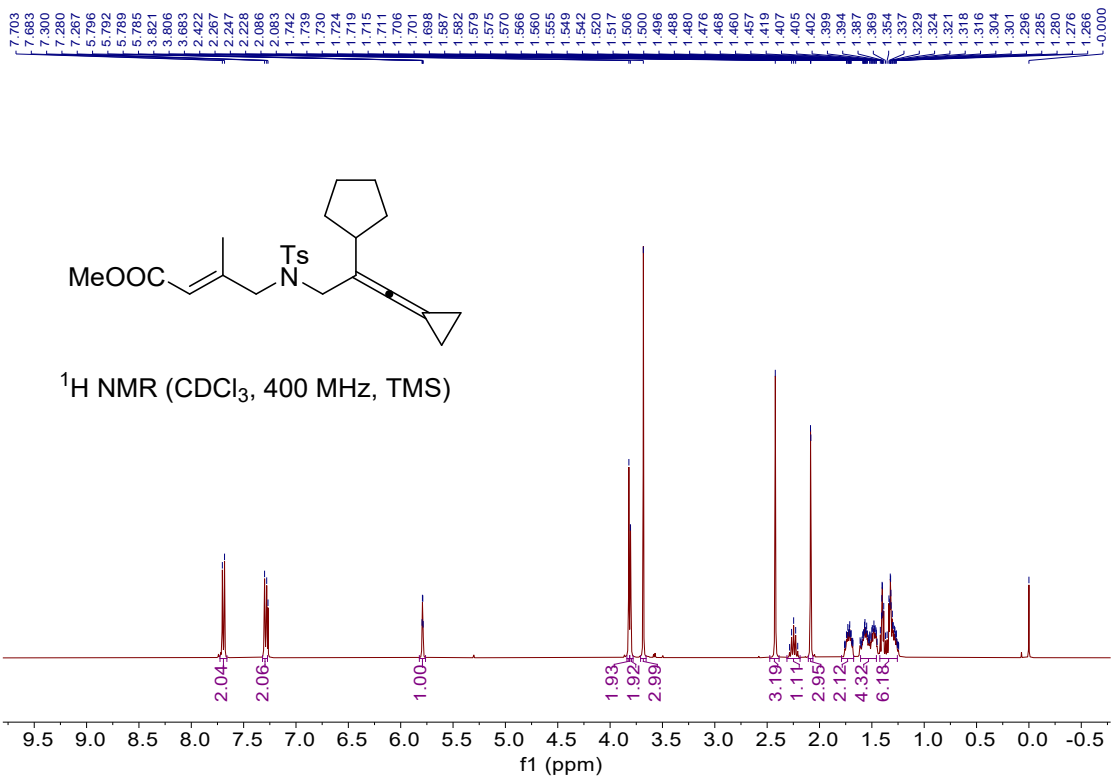


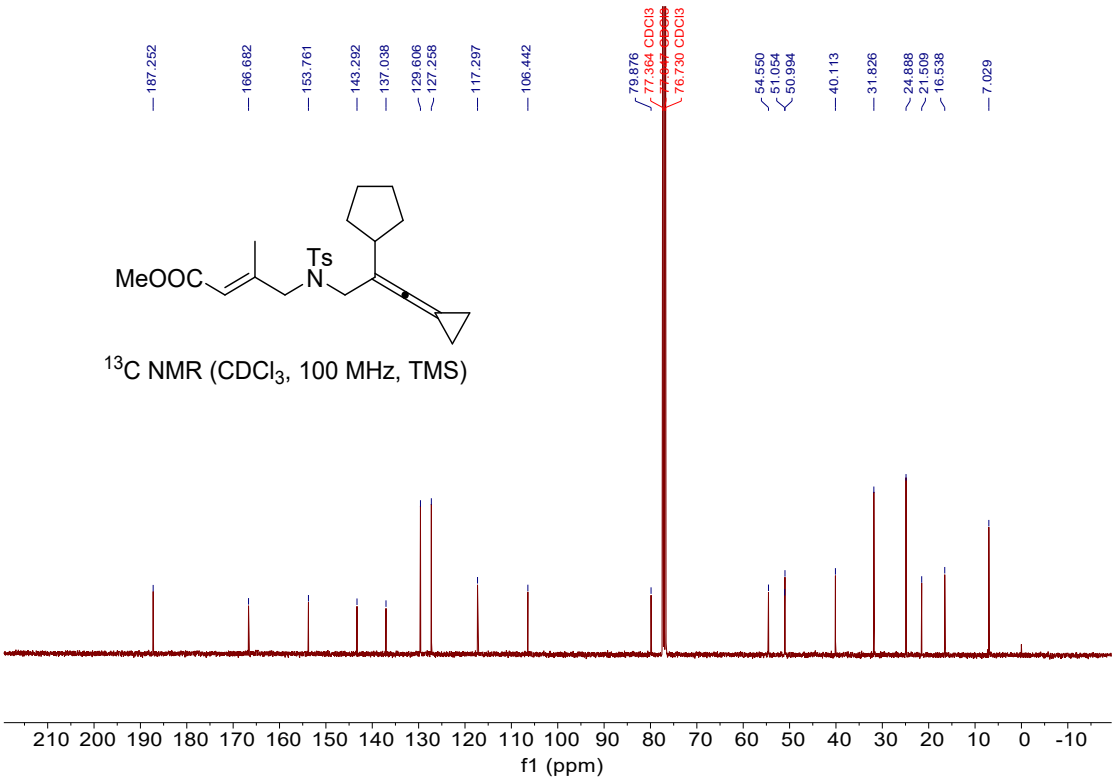

186.588
166.675
153.595
143.279
137.197
129.595
127.291
117.456
105.251
80.602
77.357 CDCl3
76.722 CDCl3
54.360
51.461
51.007
21.517
16.482
10.973
7.453
7.255
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

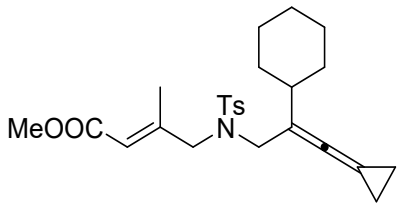


methyl (E)-4-((N-(2-cyclopentyl-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1i)

A colorless oil, 85% yield, 369.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.79 (q, *J* = 1.2 Hz, 1H), 3.82 (s, 2H), 3.81 (s, 2H), 3.68 (s, 3H), 2.42 (s, 3H), 2.25 (p, *J* = 7.8 Hz, 1H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.79 – 1.67 (m, 2H), 1.61 – 1.46 (m, 4H), 1.42 – 1.26 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.3, 166.7, 153.8, 143.3, 137.0, 129.6, 127.3, 117.3, 106.4, 79.9, 54.6, 51.1, 51.0, 40.1, 31.8, 24.9, 21.5, 16.5, 7.0. IR (neat) ν 65, 919, 1346, 1659, 1721, 2022, 2943 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{31}NO_4SNa$ $(M+Na)^+$: 452.1866, Found: 452.1863.

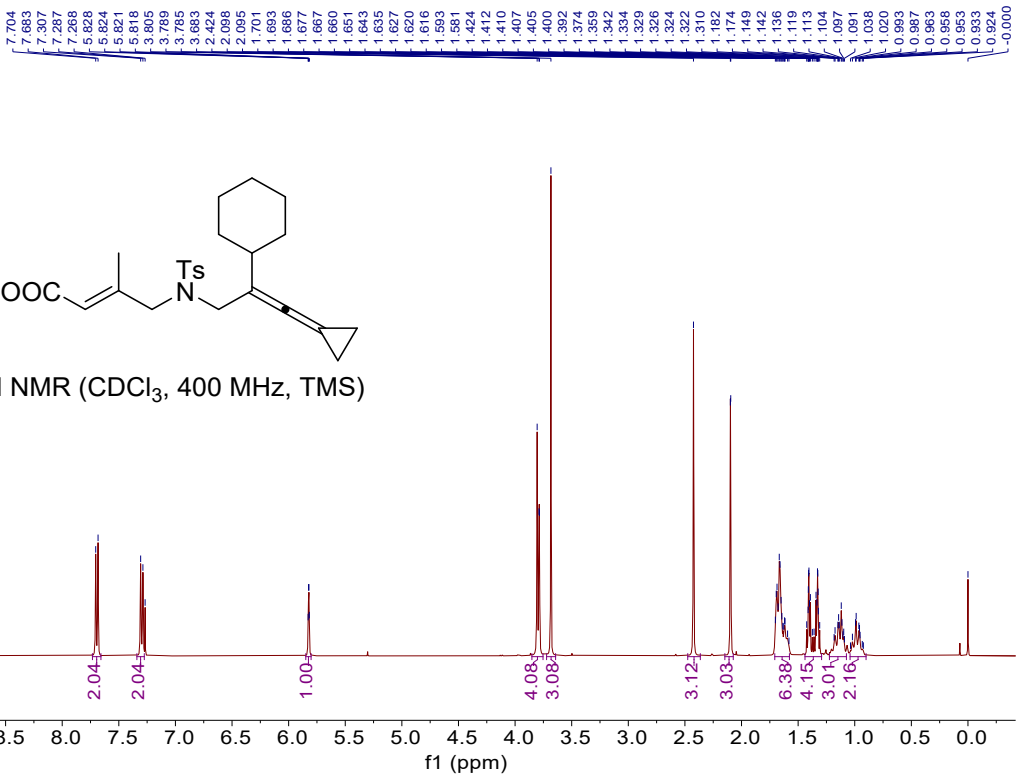


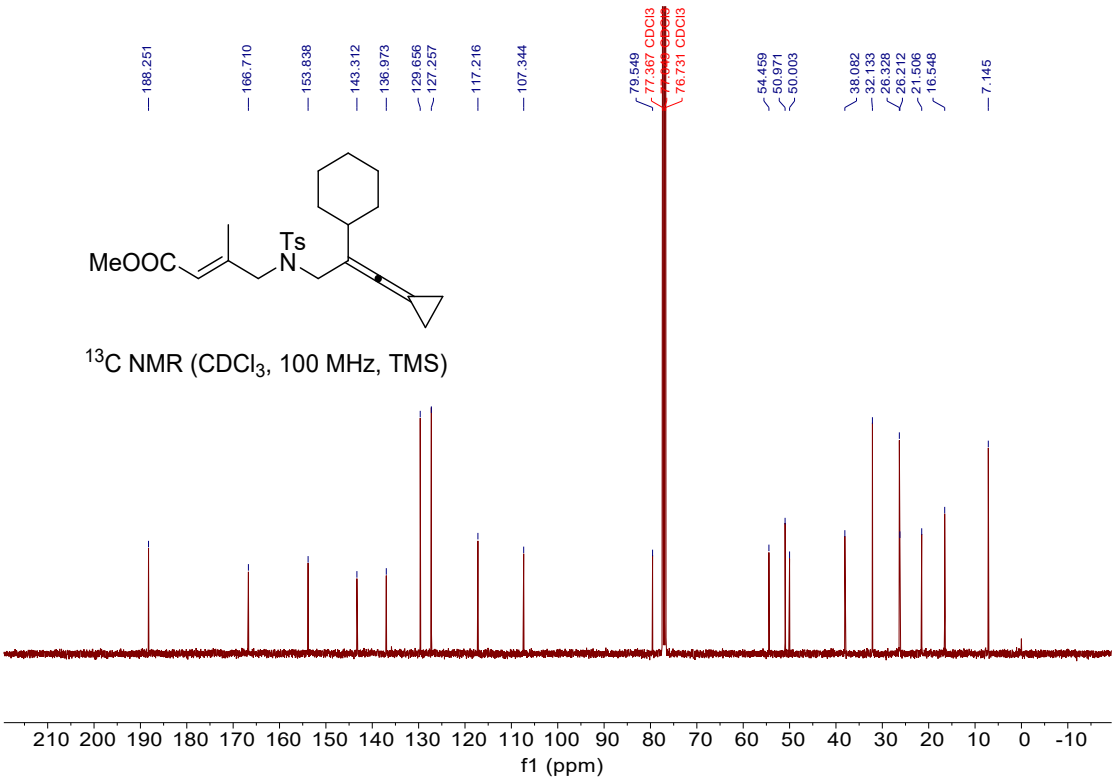

187.252
166.682
153.761
143.292
137.038
129.606
127.258
117.297
106.442
79.876
77.364 CDCl3
76.730 CDCl3
54.550
51.054
50.994
40.113
31.826
24.888
21.509
16.538
7.029
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

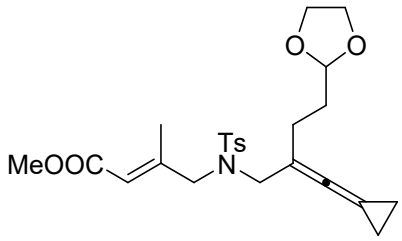


methyl (E)-4-((N-(2-cyclohexyl-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1j)

A colorless oil, 90% yield, 399.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.82 (q, *J* = 1.2 Hz, 1H), 3.85 – 3.75 (m, 4H), 3.68 (s, 3H), 2.42 (s, 3H), 2.10 (d, *J* = 1.2 Hz, 3H), 1.71 – 1.58 (m, 6H), 1.44 – 1.29 (m, 4H), 1.22 – 1.07 (m, 3H), 1.04 – 0.90 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.3, 166.7, 153.8, 143.3, 137.0, 129.7, 127.3, 117.2, 107.3, 79.5, 54.5, 51.0, 50.0, 38.1, 32.1, 26.3, 26.2, 21.5, 16.5, 7.1. IR (neat) ν 660, 769, 1220, 1661, 1723, 2016, 2924 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{33}NO_4SNa$ $(M+Na)^+$: 466.2023, Found: 466.2016.

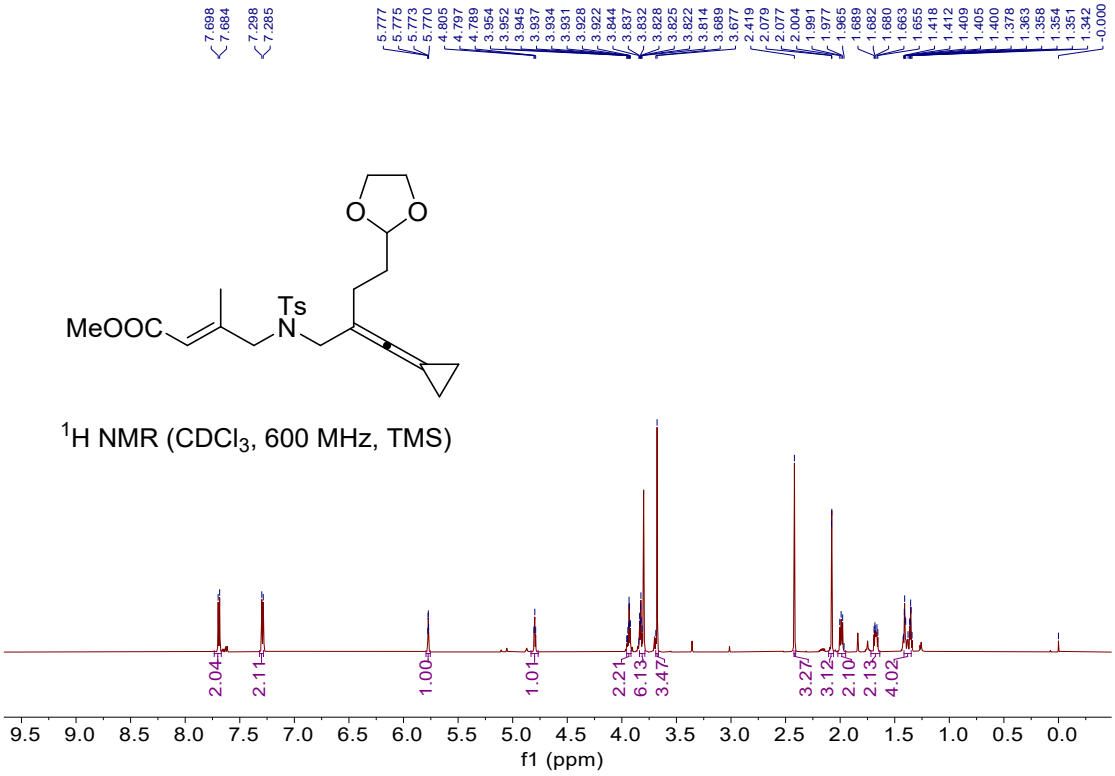


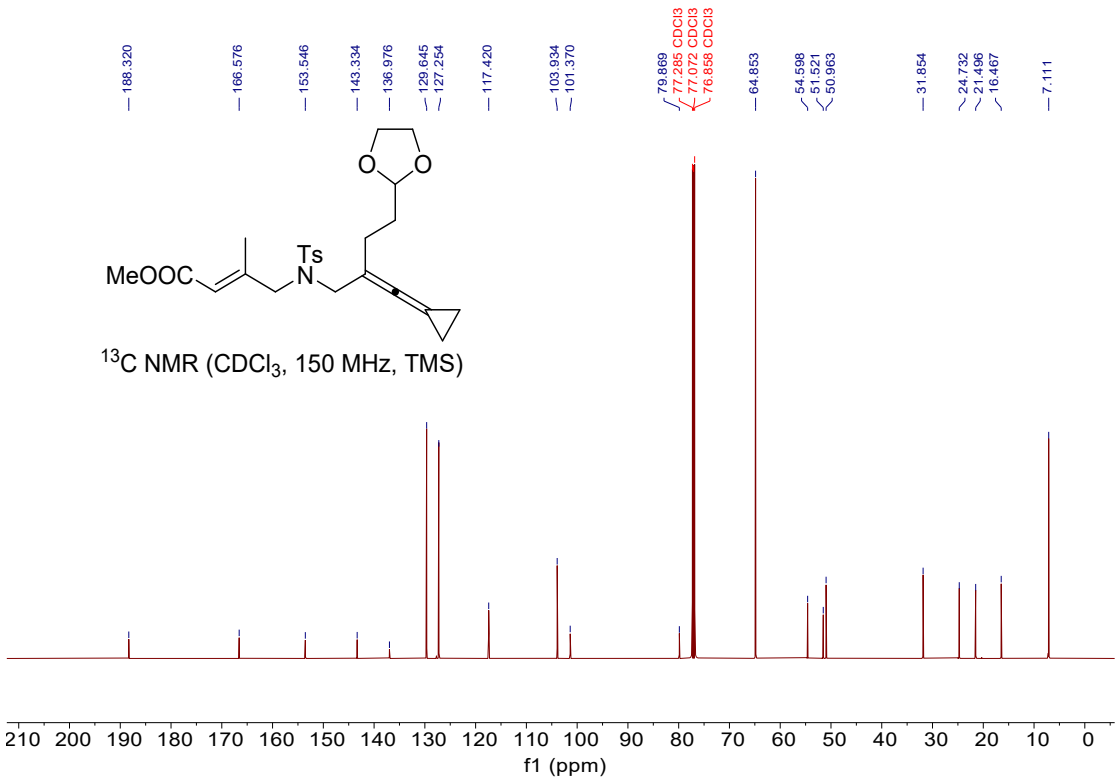

188.251
166.710
153.838
143.312
136.973
129.656
127.257
117.216
107.344
79.549
77.367 CDCl3
76.731 CDCl3
54.459
50.971
50.003
38.082
32.133
26.328
26.212
21.506
16.548
7.145
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

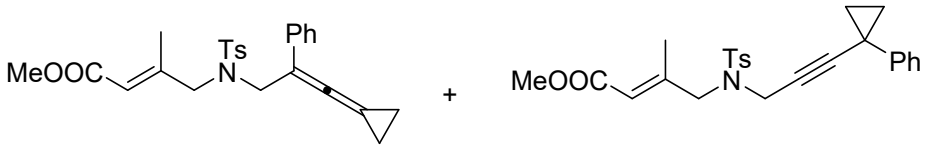


methyl (E)-4-((N-(2-(cyclopropylidene-λ^5-methylene)-4-(1,3-dioxolan-2-yl)butyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1k)

A colorless oil, 80% yield, 368.4 mg. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.77 (q, *J* = 1.2 Hz, 1H), 4.80 (t, *J* = 4.8 Hz, 1H), 3.96 – 3.92 (m, 2H), 3.84 – 3.79 (m, 6H), 3.68 (s, 3H), 2.42 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 2.02 – 1.95 (m, 2H), 1.72 – 1.64 (m, 2H), 1.42 – 1.35 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 188.3, 166.6, 153.5, 143.3, 137.0, 129.6, 127.3, 117.4, 103.9, 101.4, 79.9, 64.9, 54.6, 51.5, 51.0, 31.9, 24.7, 21.5, 16.5, 7.1. IR (neat) ν 661, 1039, 1342, 1661, 1722, 2018, 2982 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{31}NO_4SNa$ $(M+Na)^+$: 484.1764, Found: 484.1770.

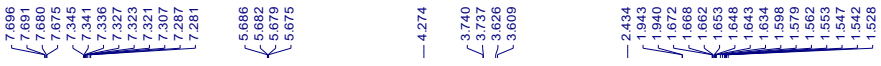


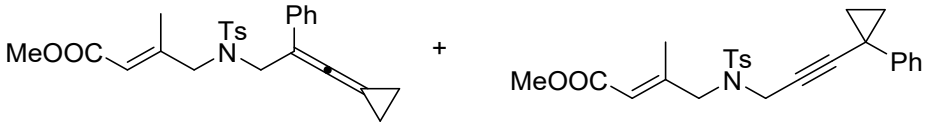

188.320
166.576
153.546
143.334
136.976
129.645
127.254
117.420
103.934
101.370
79.869
77.285 CDCl3
77.072 CDCl3
76.858 CDCl3
64.853
54.598
51.521
50.963
31.854
24.732
21.496
16.467
7.111
O
O
Ts
N
MeOOC
13C NMR (CDCl3, 150 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



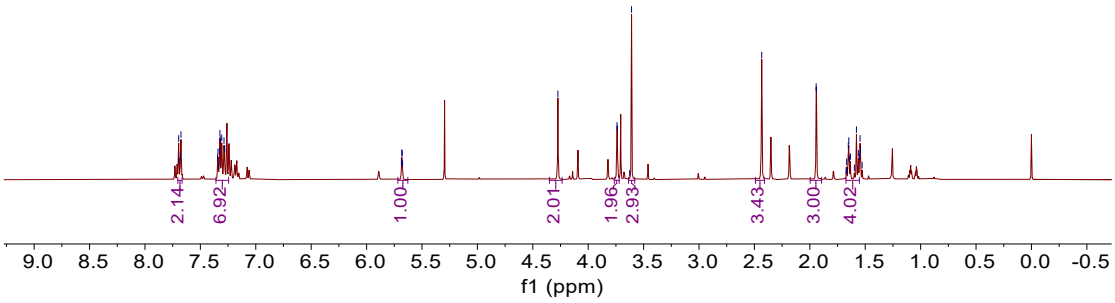
methyl (E)-4-((N-(3-cyclopropylidene-2-phenyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1l)+ methyl (E)-3-methyl-4-((4-methyl-N-(3-(1-phenylcyclopropyl)prop-2-yn-1-yl)phenyl)sulfonamido)but-2-enoate (byproduct 1l') (1l: 1l'=4:1)

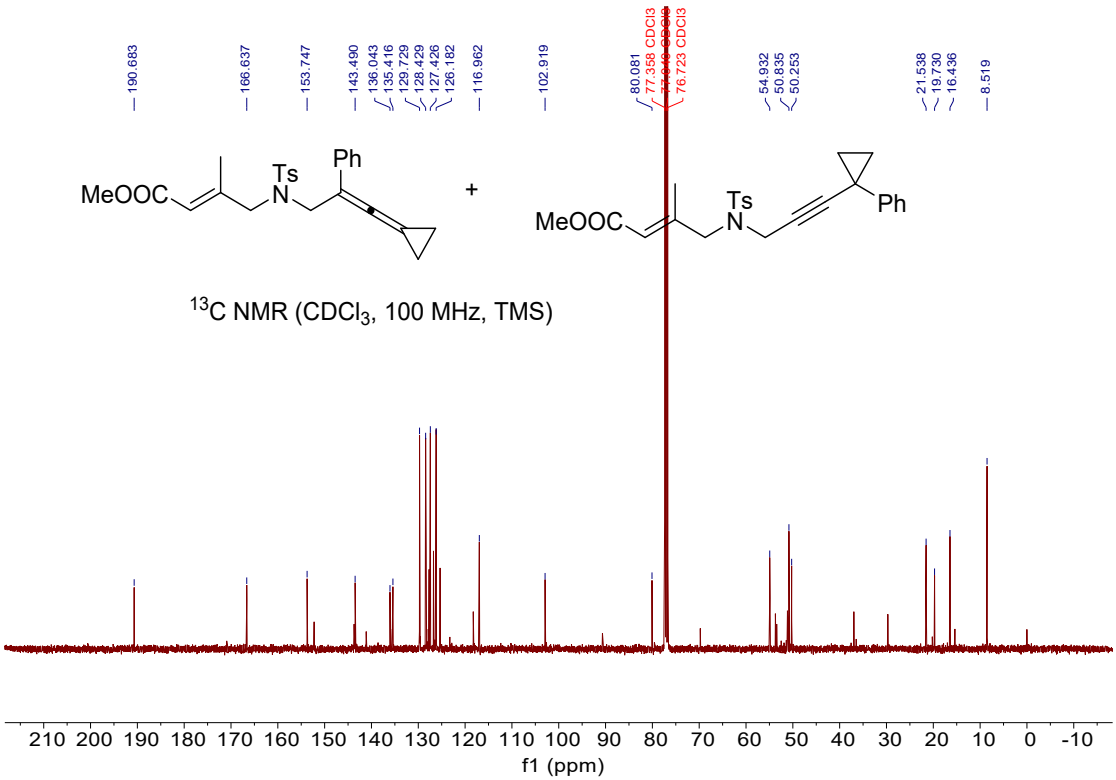
A colorless oil, 90% yield, 338.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.66 (m, 2H), 7.36 – 7.24 (m, 7H), 5.68 (q, *J* = 1.2 Hz, 1H), 4.27 (s, 2H), 3.74 (d, *J* = 1.2 Hz, 2H), 3.61 (s, 3H), 2.43 (s, 3H), 1.94 (d, *J* = 1.2 Hz, 3H), 1.67 – 1.55 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.7, 166.6, 153.7, 143.5, 136.0, 135.4, 129.7, 128.4, 127.4, 126.2, 117.0, 102.9, 80.1, 54.9, 50.8, 50.3, 21.5, 19.7, 16.4, 8.5. IR (neat) ν 652, 769, 1351, 1660, 1722, 2005, 2951 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{27}NO_4SNa$ $(M+Na)^+$: 460.1553, Found: 460.1558.

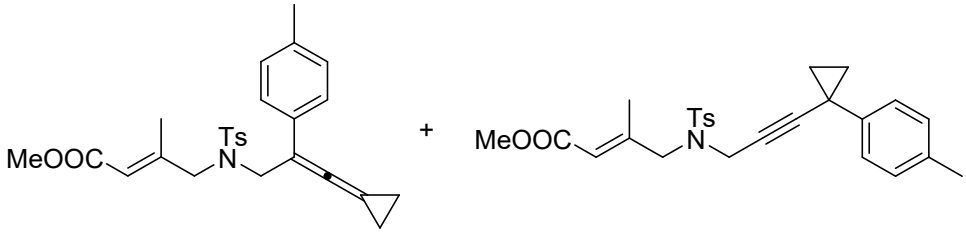




^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

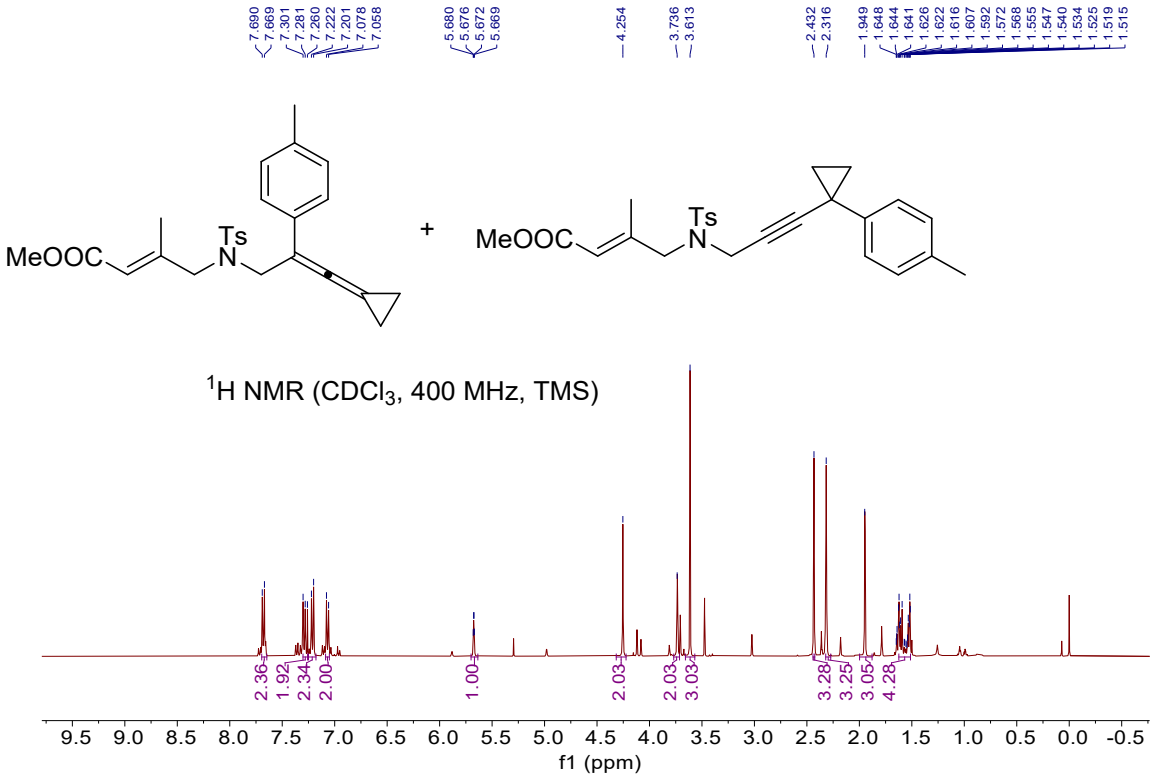


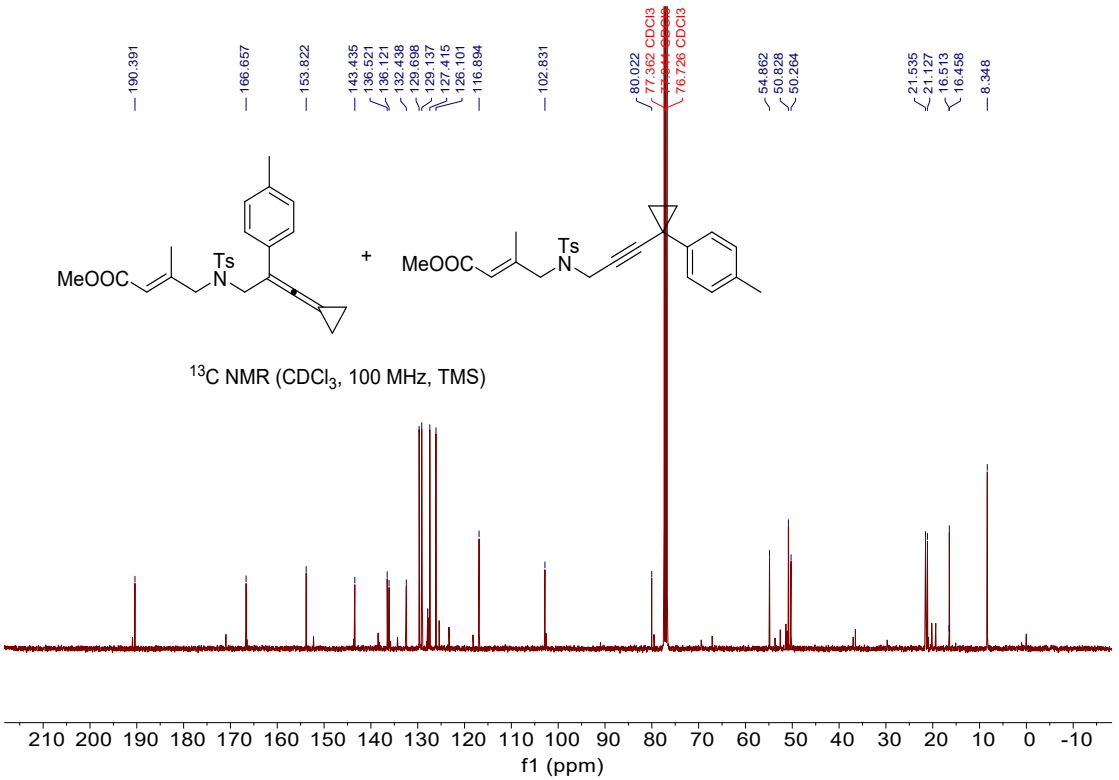

190.683
166.637
153.747
143.490
136.043
135.416
129.729
128.429
127.426
126.182
116.962
102.919
80.081
77.358 CDCl3
76.723 CDCl3
54.932
50.835
50.253
21.538
19.730
16.436
8.519
MeOOC
Ts
N
Ph
+
MeOOC
Ts
N
Ph
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

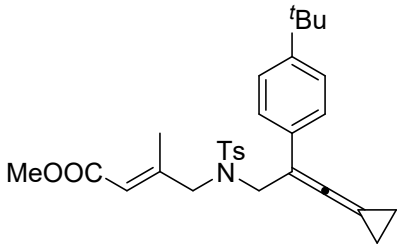


methyl (E)-4-((N-(3-cyclopropylidene-2-(p-tolyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1m)+ methyl (E)-3-methyl-4-((4-methyl-N-(3-(1-(p-tolyl)cyclopropyl)prop-2-yn-1-yl)phenyl)sulfonamido)but-2-enoate (byproduct 1m') (1m: 1m'=5:1)

A colorless oil, 60% yield, 270.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.30 – 7.26 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 5.67 (q, *J* = 1.2 Hz, 1H), 4.25 (s, 2H), 3.74 (s, 2H), 3.61 (s, 3H), 2.43 (s, 3H), 2.32 (s, 3H), 1.95 (s, 3H), 1.62 – 1.51 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 166.7, 153.8, 143.4, 136.5, 136.1, 132.4, 129.7, 129.1, 127.4, 126.1, 116.9, 102.8, 80.0, 54.9, 50.8, 50.3, 21.5, 21.1, 16.5, 16.5, 8.3. IR (neat) ν 662, 1216, 1662, 1720, 2023, 2943 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1714.

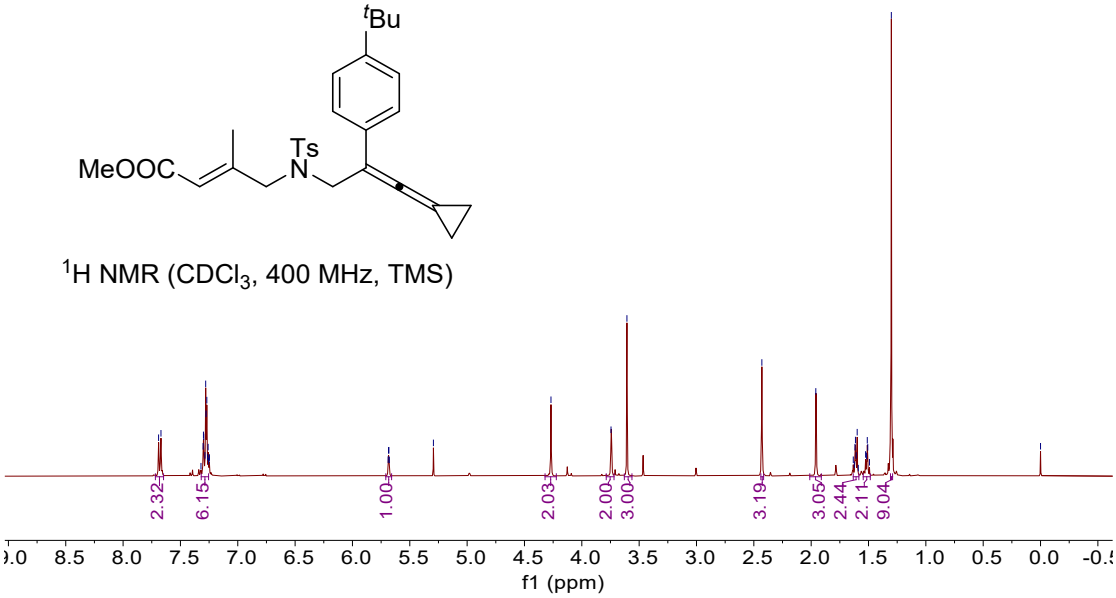


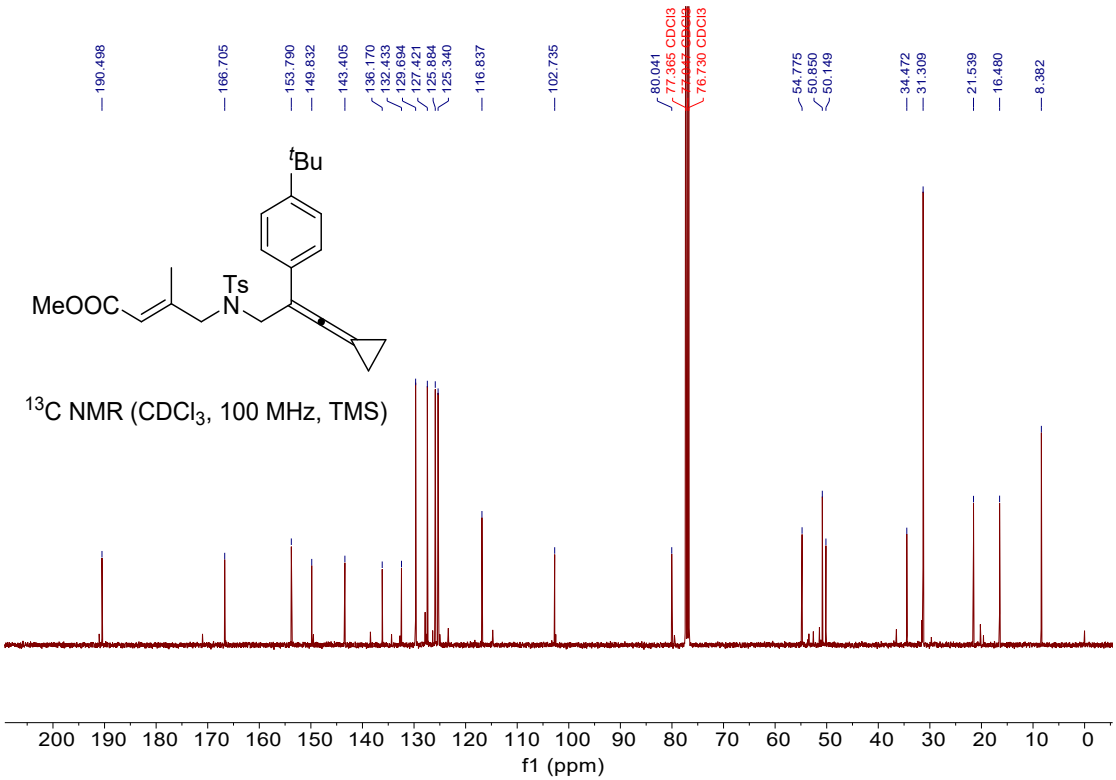

190.391
166.657
153.822
143.435
136.521
136.121
132.438
129.698
129.137
127.415
126.101
116.894
102.831
80.022
77.362 CDCl3
76.726 CDCl3
54.862
50.828
50.264
21.535
21.127
16.513
16.458
8.348
MeOOC
Ts
N
+
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

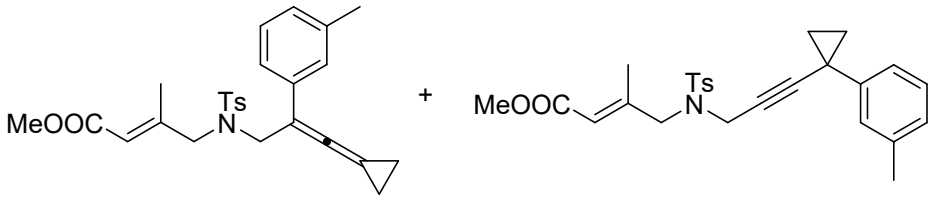


methyl (E)-4-((N-(2-(4-(tert-butyl)phenyl)-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1n)

A colorless oil, 60% yield, 295.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.0 Hz, 2H), 7.32 – 7.25 (m, 6H), 5.68 (q, J = 1.2 Hz, 1H), 4.27 (s, 2H), 3.75 (s, 2H), 3.61 (s, 3H), 2.43 (s, 3H), 1.96 (s, 3H), 1.63 – 1.58 (m, 2H), 1.55 – 1.48 (m, 2H), 1.30 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 166.7, 153.8, 149.8, 143.4, 136.2, 132.4, 129.7, 127.4, 125.9, 125.3, 116.8, 102.7, 80.0, 54.8, 50.8, 50.1, 34.5, 31.3, 21.5, 16.5, 8.4. IR (neat) ν 654, 1094, 1351, 1660, 1722, 2009, 2963 cm^{-1}. HRMS (ESI) calcd. for $C_{29}H_{35}NO_4SNa$ $(M+Na)^+$: 516.2179, Found: 516.2173.

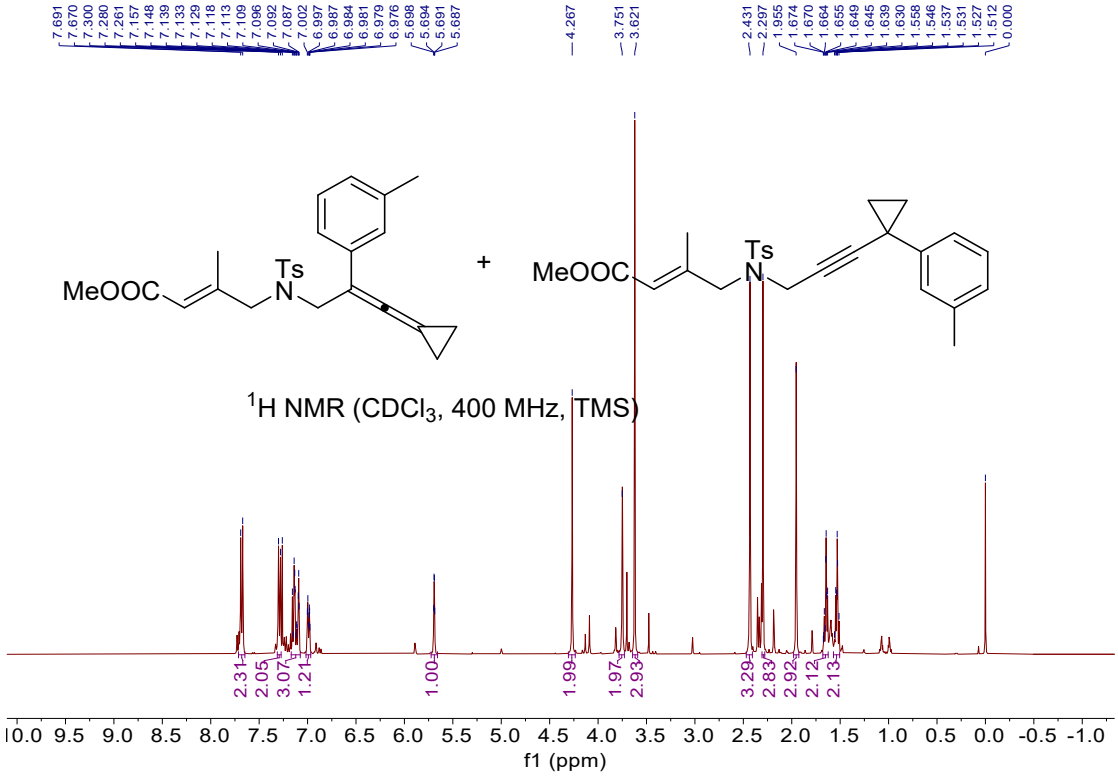


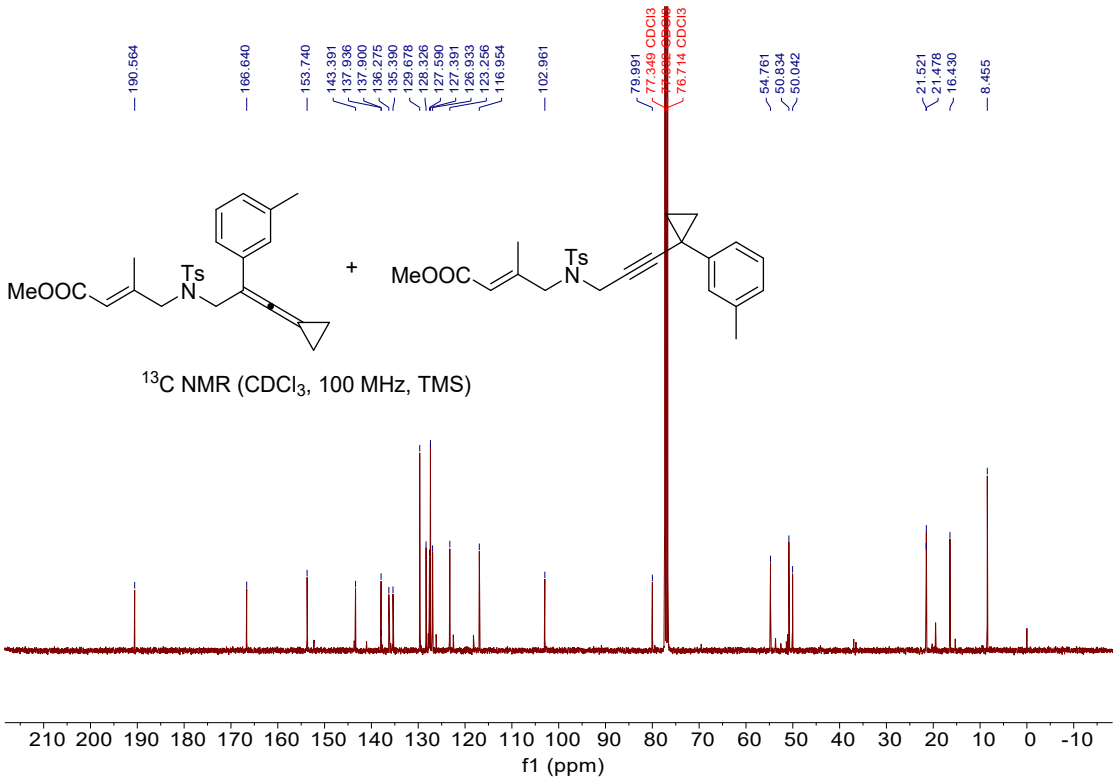

190.498
166.705
153.790
149.832
143.405
136.170
132.433
129.694
127.421
125.884
125.340
116.837
102.735
80.041
77.365 CDCl3
76.730 CDCl3
54.775
50.850
50.149
34.472
31.309
21.539
16.480
8.382
tBu
Ts
N
MeOOC
13C NMR (CDCl3, 100 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

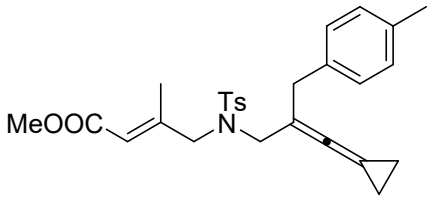


methyl (E)-4-((N-(3-cyclopropylidene-2-(m-tolyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1o) + methyl (E)-3-methyl-4-((4-methyl-N-(3-(1-(m-tolyl)cyclopropyl)prop-2-yn-1-yl)phenyl)sulfonamido)but-2-enoate (byproduct 1o') (1m: 1m'=5:1)

A colorless oil, 60% yield, 270.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.08 (m, 3H), 7.02 – 6.97 (m, 1H), 5.69 (q, *J* = 1.2 Hz, 1H), 4.27 (s, 2H), 3.75 (s, 2H), 3.62 (s, 3H), 2.43 (s, 3H), 2.30 (s, 3H), 1.96 (s, 3H), 1.68 – 1.62 (m, 2H), 1.57 – 1.51 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.6, 166.6, 153.7, 143.4, 137.9, 137.9, 136.3, 135.4, 129.7, 128.3, 127.6, 127.4, 126.9, 123.3, 117.0, 103.0, 80.0, 54.8, 50.8, 50.0, 21.5, 21.5, 16.4, 8.5. IR (neat) ν 677, 1161, 1221, 1653, 1722, 2017, 2962 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1701.

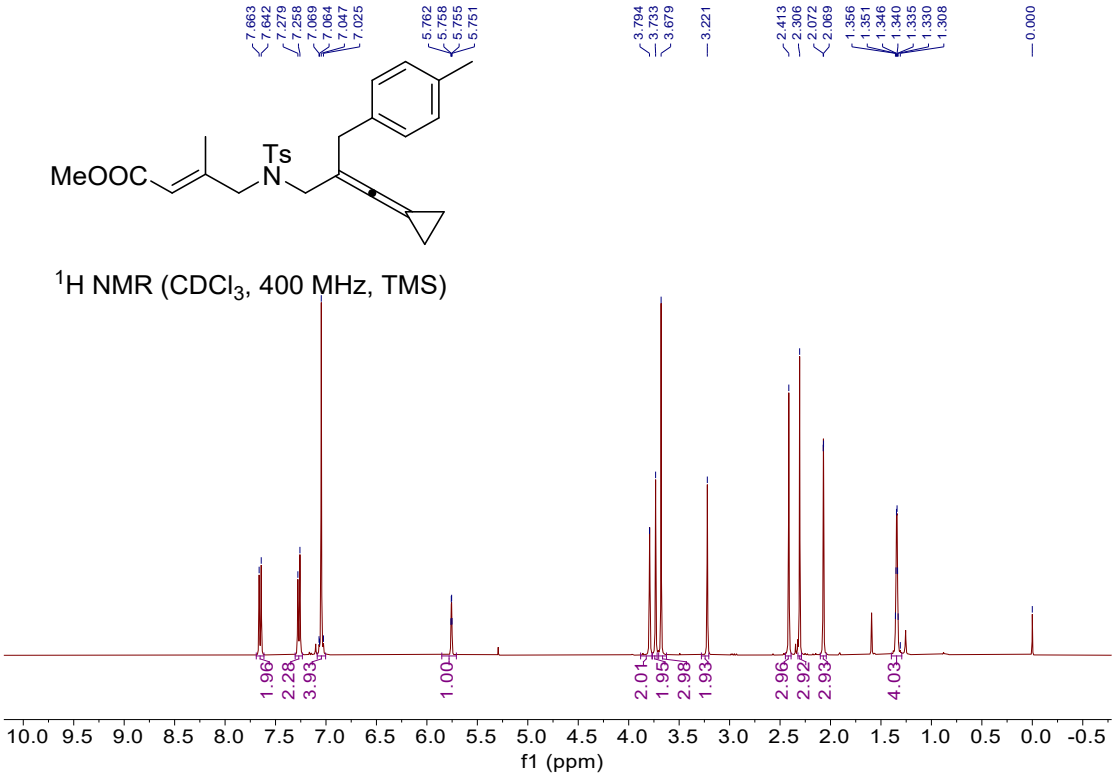


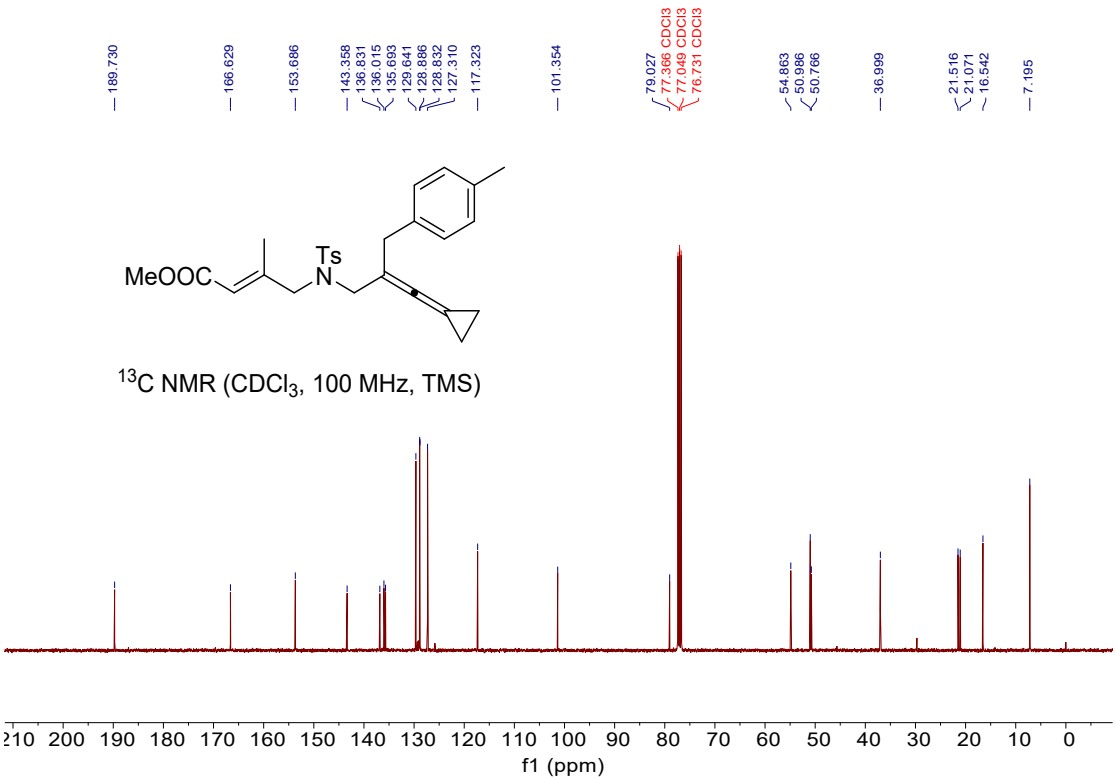

190.564
166.640
153.740
143.391
137.936
137.900
136.275
135.390
129.678
128.326
127.590
127.391
126.933
123.256
116.954
102.961
79.991
77.349 CDCl3
76.714 CDCl3
54.761
50.834
50.042
21.521
21.478
16.430
8.455
MeOOC
Ts
N
+
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

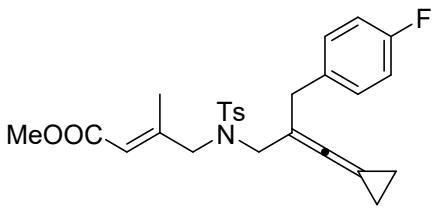


methyl (E)-4-((N-(3-cyclopropylidene-2-(4-methylbenzyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1p)

A colorless oil, 90% yield, 419.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.09 – 7.00 (m, 4H), 5.76 (q, *J* = 1.2 Hz, 1H), 3.79 (s, 2H), 3.73 (s, 2H), 3.68 (s, 3H), 3.22 (s, 2H), 2.41 (s, 3H), 2.31 (s, 3H), 2.07 (d, *J* = 1.2 Hz, 3H), 1.32 - 1.35 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 166.6, 153.7, 143.4, 136.8, 136.0, 135.7, 129.6, 128.9, 128.8, 127.3, 117.3, 101.4, 79.0, 0 54.9, 51.0, 50.8, 37.0, 21.5, 21.1, 16.5, 7.2. IR (neat) ν 661, 71158, 1346, 1134, 1653, 1725, 2021, 2922 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{31}NO_4SNa$ $(M+Na)^+$: 488.1866, Found: 488.1866.

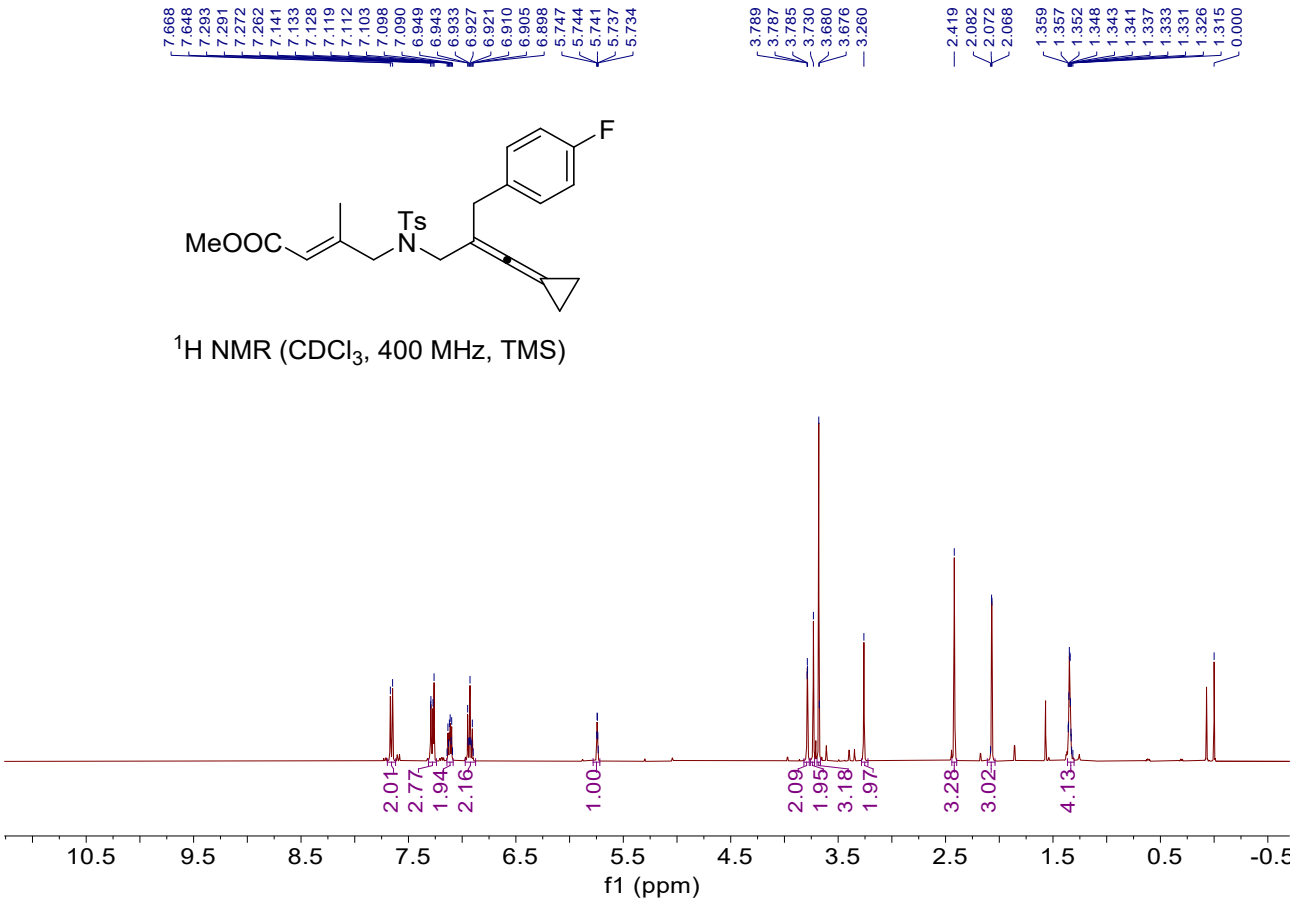


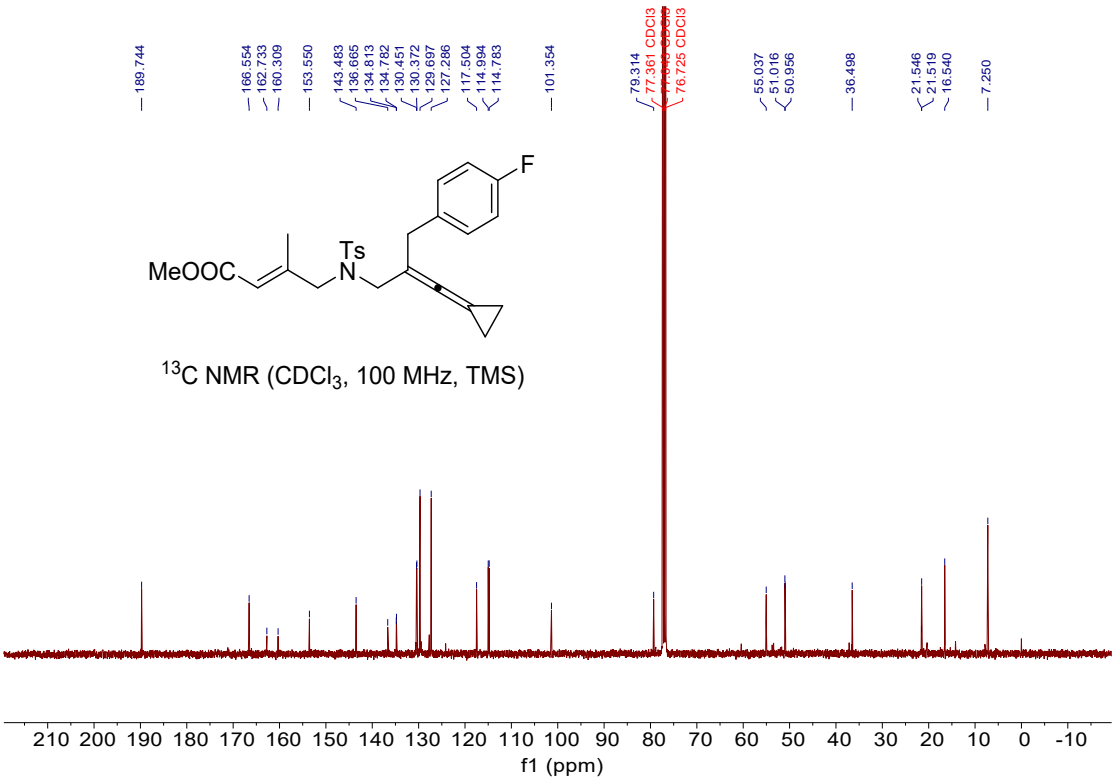

189.730
166.629
153.686
143.358
136.831
136.015
135.693
129.641
128.886
128.832
127.310
117.323
101.354
79.027
77.366 CDCl3
77.049 CDCl3
76.731 CDCl3
54.863
50.986
50.766
36.999
21.516
21.071
16.542
7.195
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



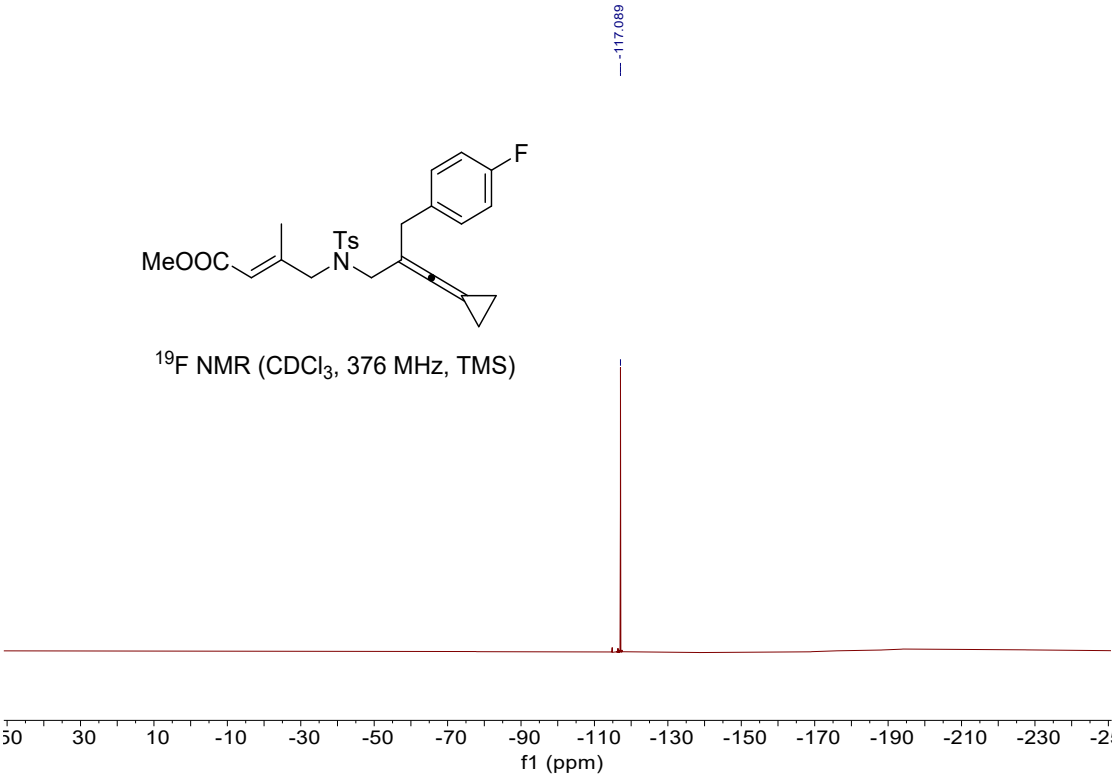
methyl (E)-4-((N-(3-cyclopropylidene-2-(4-fluorobenzyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1q)

A colorless oil, 80% yield, 375.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 8.0 Hz, 2H), 7.31 – 7.24 (m, 3H), 7.14 – 7.08 (m, 2H), 6.97 – 6.88 (m, 2H), 5.78 – 5.72 (m, 1H), 3.82 – 3.77 (m, 2H), 3.73 (s, 2H), 3.68 (s, 3H), 3.26 (s, 2H), 2.42 (s, 3H), 2.07 (d, J = 1.3 Hz, 3H), 1.36 – 1.30 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 166.6, 161.5 (d, $J_{C\text{-}F}$ = 242.4 Hz), 153.6, 143.5, 136.7, 134.78, 134.81, 130.5 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.7, 127.3, 117.5, 114.8 (d, $J_{C\text{-}F}$ = 21.1 Hz), 101.4, 79.3, 55.0, 51.01, 51.00, 36.5, 21.54, 21.52, 16.5, 7.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ 117.1. IR (neat) ν 660, 1092, 1221, 1508, 1662, 1724, 2025, 2949 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{28}NO_4FSNa$ $(M+Na)^+$: 492.1615, Found: 492.1608.

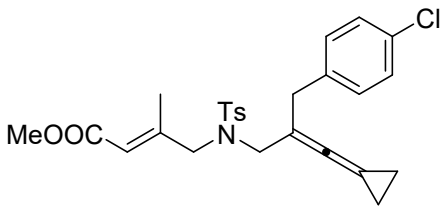




^{13}C NMR ($CDCl_3$, 100 MHz, TMS)

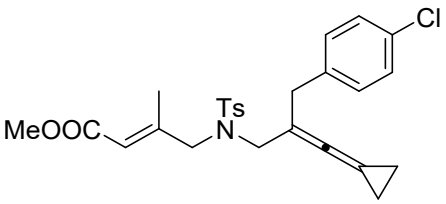


^{19}F NMR ($CDCl_3$, 376 MHz, TMS)

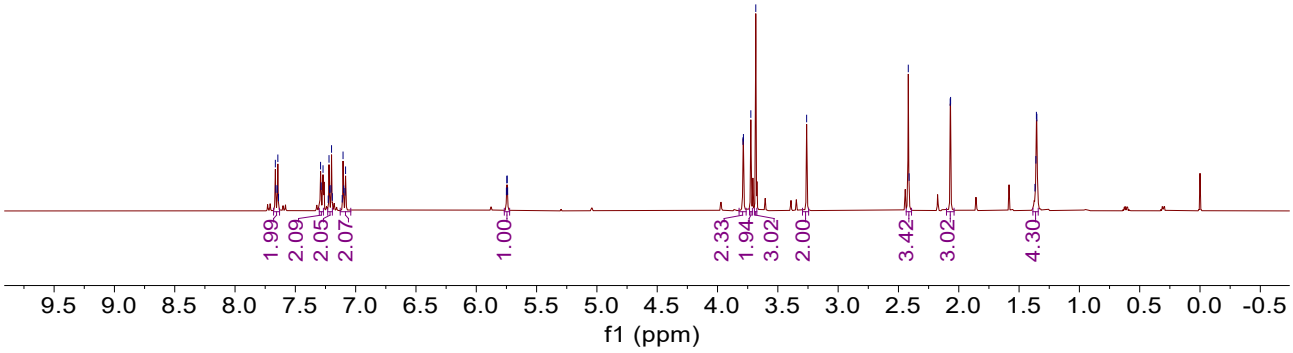


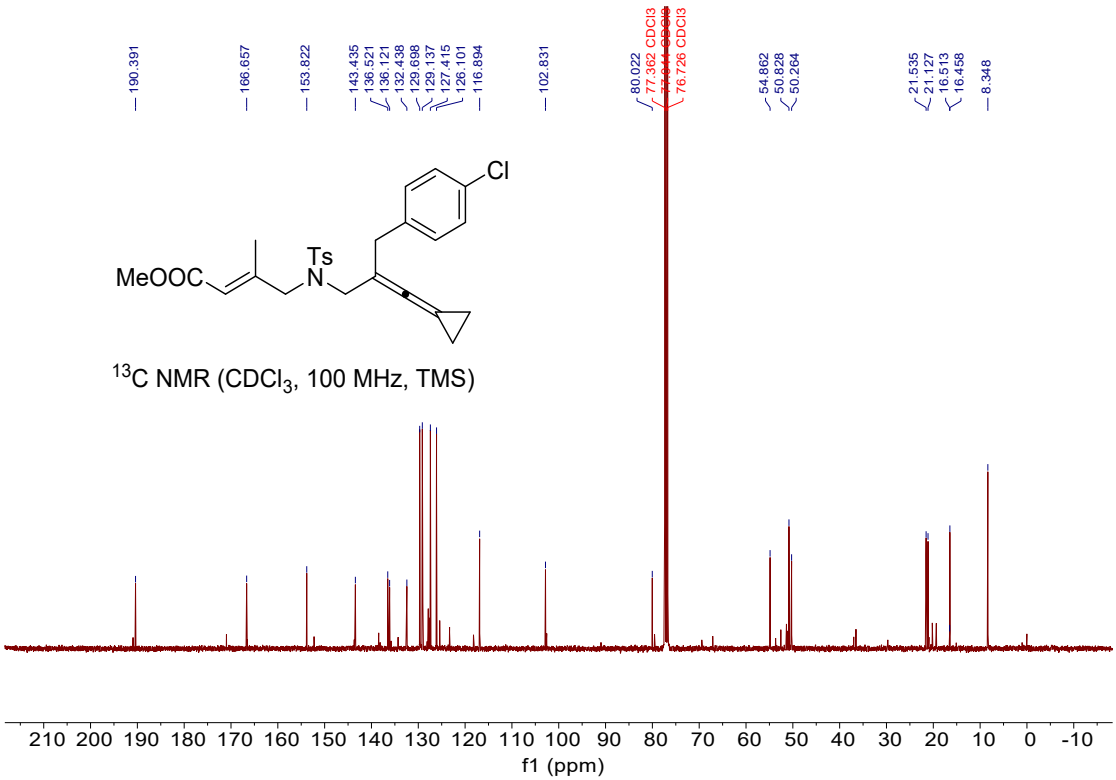
methyl (E)-4-((N-(2-(4-chlorobenzyl)-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1r)

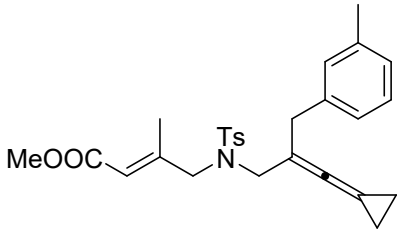
A yellow oil, 80% yield, 388.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.14 – 7.08 (m, 2H), 6.96 – 6.90 (m, 2H), 5.75 (q, *J* = 1.2 Hz, 1H), 3.79 (s, 2H), 3.73 (s, 2H), 3.68 (s, 3H), 3.26 (s, 2H), 2.42 (s, 3H), 2.07 (d, *J* = 1.2 Hz, 3H), 1.37 – 1.32 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 166.7, 153.8, 143.4, 136.5, 136.1, 132.4, 129.7, 129.1, 127.4, 126.1, 116.9, 102.8, 80.0, 54.9, 50.8, 50.3, 21.5, 21.1, 16.5, 16.5, 8.3. IR (neat) ν 657, 908, 1216, 1351, 1661, 1722, 2021, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{28}NO_4SNaCl$ $(M+Na)^+$: 508.1320, Found: 508.1321.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

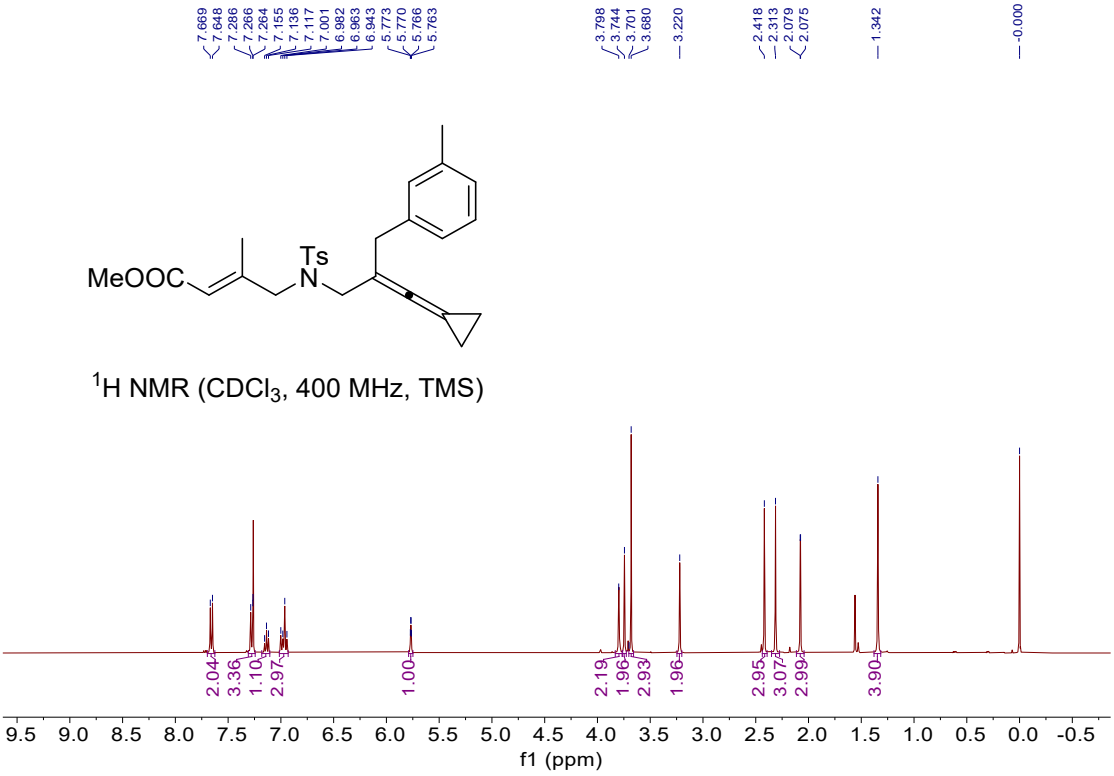


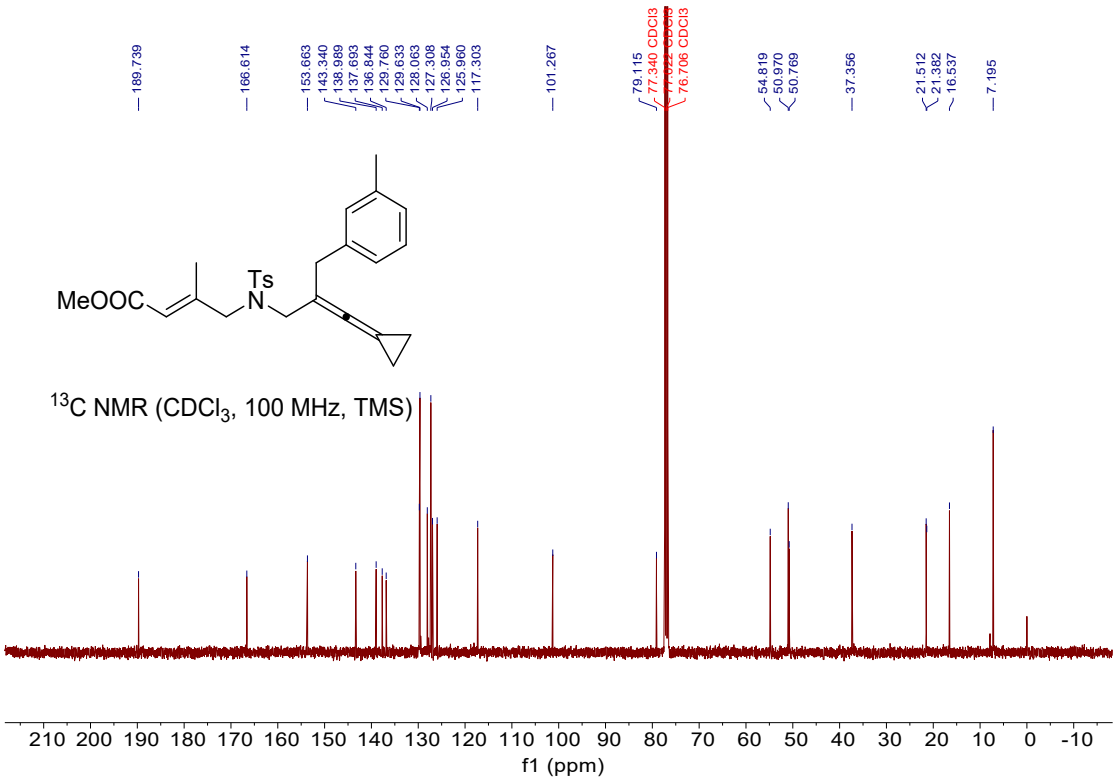

190.391
166.657
153.822
143.435
136.521
136.121
132.438
129.698
129.137
127.415
126.101
116.894
102.831
80.022
77.362 CDCl3
76.726 CDCl3
54.862
50.828
50.264
21.535
21.127
16.513
16.458
8.348
Cl
Ts
N
MeOOC
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

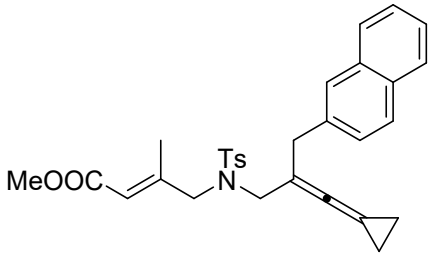


methyl (E)-4-((N-(3-cyclopropylidene-2-(3-methylbenzyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1s)

A colorless oil, 70% yield, 332.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.97 (q, *J* = 7.4 Hz, 3H), 5.77 (q, *J* = 1.2 Hz, 1H), 3.80 (s, 2H), 3.74 (s, 2H), 3.68 (s, 3H), 3.22 (s, 2H), 2.42 (s, 3H), 2.31 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.38 – 1.32 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 166.6, 153.7, 143.3, 139.0, 137.7, 136.8, 129.8, 129.6, 128.1, 127.3, 127.0, 126.0, 117.3, 101.3, 79.1, 54.8, 51.0, 50.8, 37.4, 21.5, 21.4, 16.5, 7.2. IR (neat) ν 662, 910, 1216, 1346, 1659, 1722, 2024, 2953 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{31}NO_4SNa$ $(M+Na)^+$: 488.1866, Found: 488.1861.

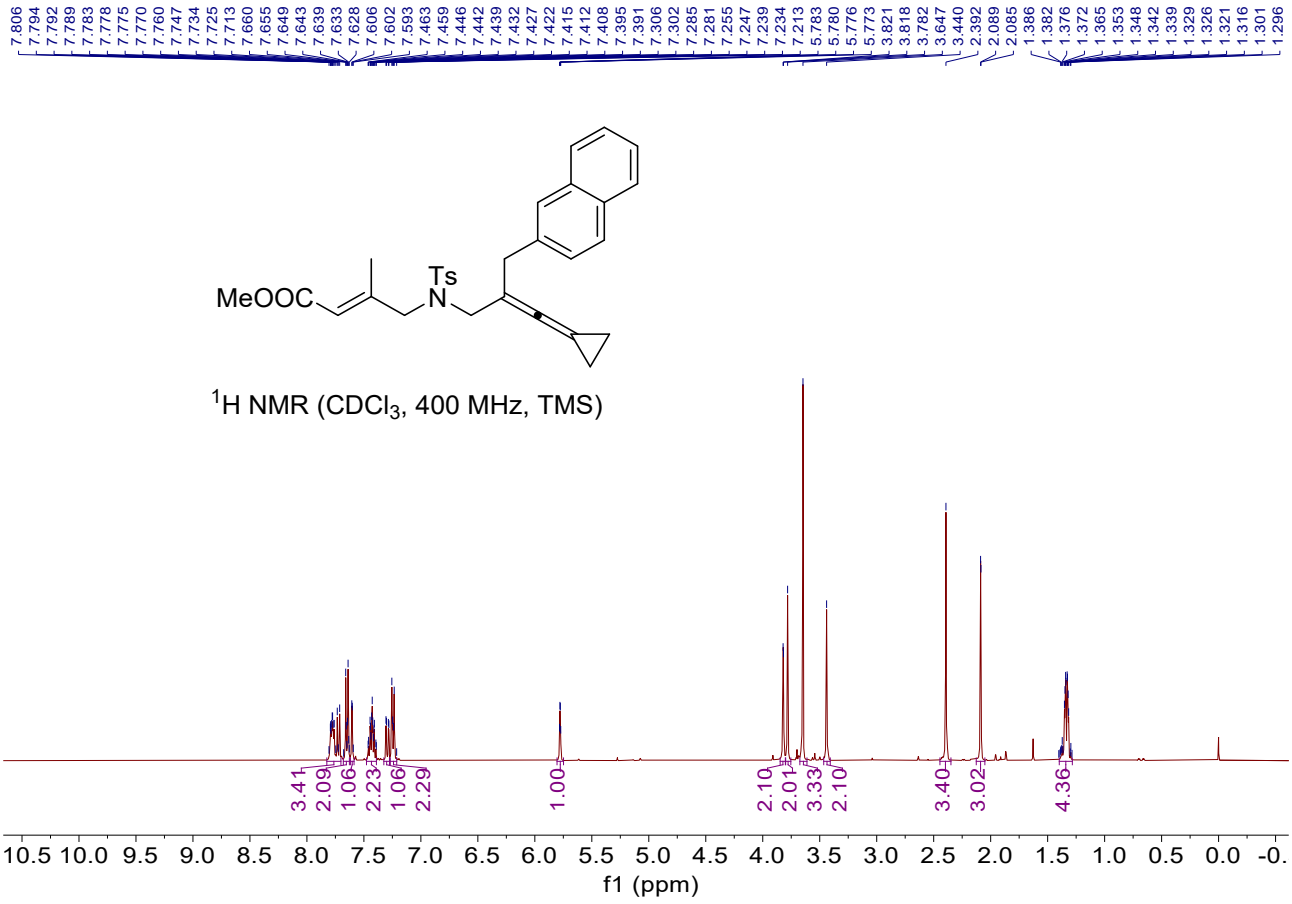


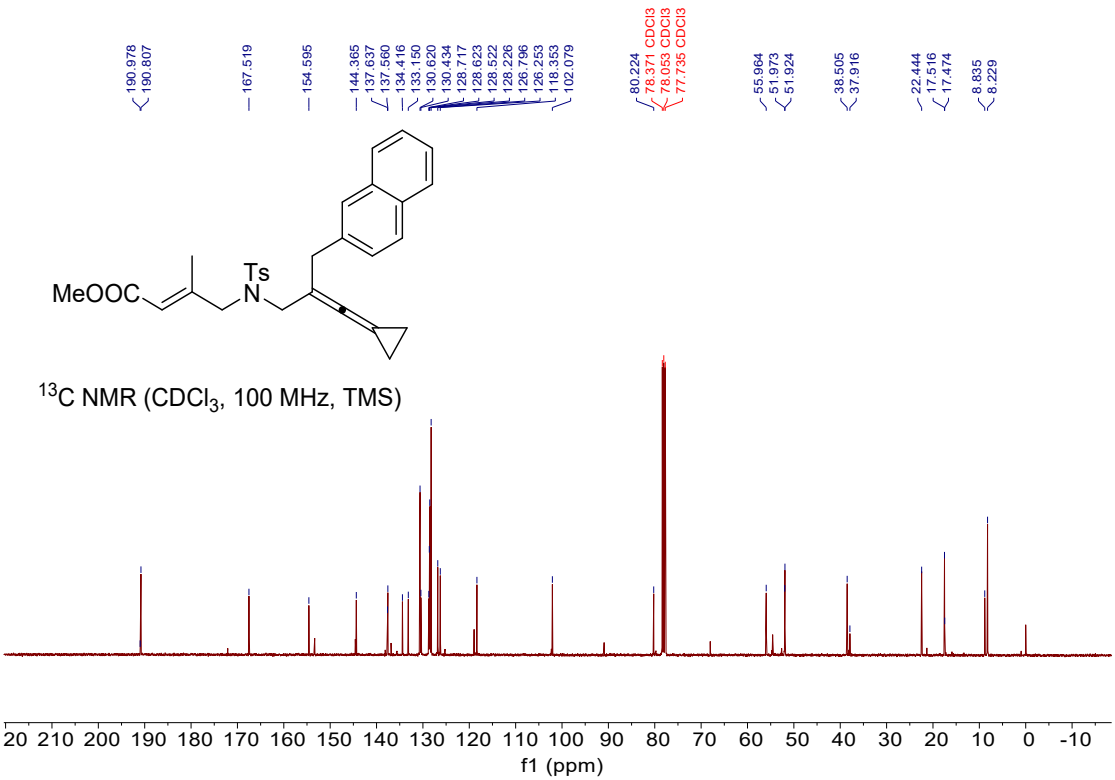

189.739
166.614
153.663
143.340
138.989
137.693
136.844
129.760
129.633
128.063
127.308
126.954
125.960
117.303
101.267
79.115
77.340 CDCl3
76.706 CDCl3
54.819
50.970
50.769
37.356
21.512
21.382
16.537
7.195
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

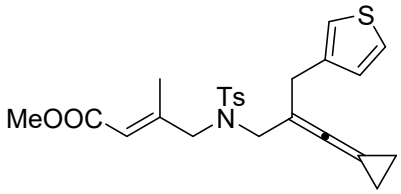


methyl (E)-4-((N-(3-cyclopropylidene-2-(naphthalen-2-ylmethyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1t)

A red oil, 70% yield, 350.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.70 (m, 3H), 7.68 – 7.63 (m, 2H), 7.62 – 7.59 (m, 1H), 7.48 – 7.39 (m, 2H), 7.32 – 7.28 (m, 1H), 7.27 – 7.21 (m, 2H), 5.78 (q, *J* = 1.4 Hz, 1H), 3.82 (d, *J* = 1.4 Hz, 2H), 3.78 (s, 2H), 3.65 (s, 3H), 3.44 (s, 2H), 2.39 (s, 3H), 2.09 (d, *J* = 1.4 Hz, 3H), 1.40 – 1.28 (m, 4H).^{13}C NMR (100 MHz, $CDCl_3$) δ 191.0, 190.8, 167.5, 154.6, 144.4, 137.6, 137.6, 134.4, 133.2, 130.6, 130.4, 128.7, 128.6, 128.5, 128.2, 126.8, 126.3, 118.4, 102.1, 80.2, 56.0, 52.0, 51.9, 38.5, 37.9, 22.4, 17.5, 17.5, 8.8, 8.2. IR (neat) ν 675, 1096, 1346, 1656, 1726, 2031, 2927 cm^{-1}. HRMS (ESI) calcd. for $C_{30}H_{31}NO_4SNa$ $(M+Na)^+$: 524.1866, Found: 524.1873.

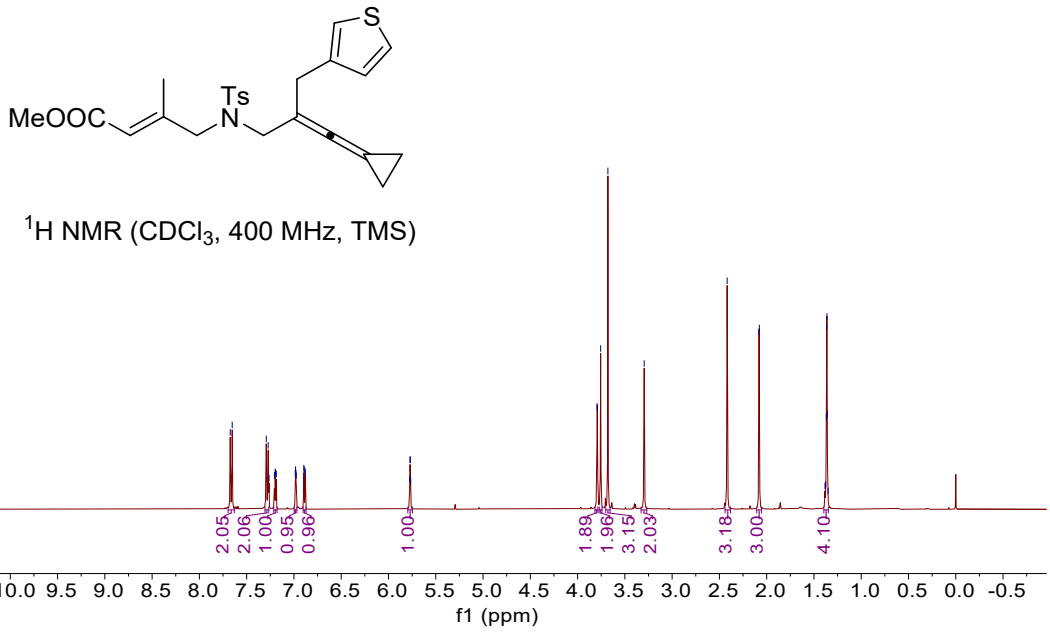


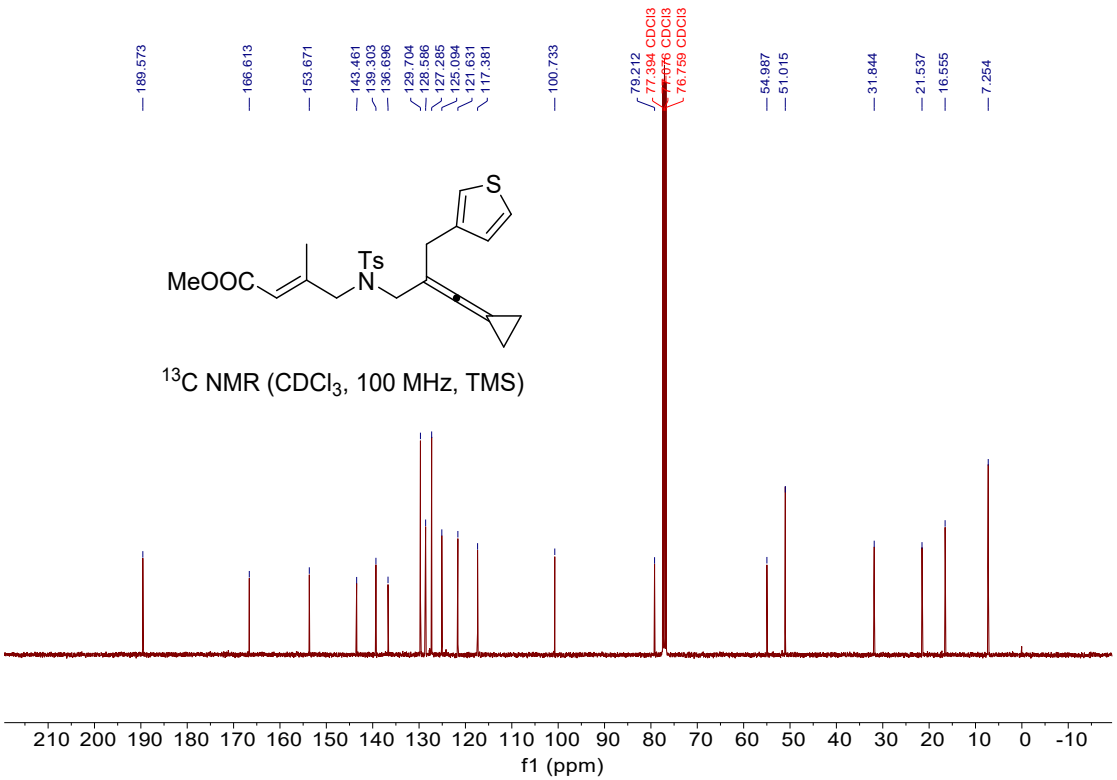

190.978
190.807
167.519
154.595
144.365
137.637
137.560
134.416
133.150
130.620
130.434
128.717
128.623
128.522
128.226
126.796
126.253
118.353
102.079
80.224
78.371 CDCl3
78.053 CDCl3
77.735 CDCl3
55.964
51.973
51.924
38.505
37.916
22.444
17.516
17.474
8.835
8.229
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

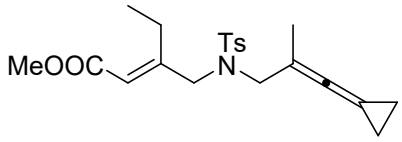


methyl (E)-4-((N-(3-cyclopropylidene-2-(thiophen-3-ylmethyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1u)

A yellow oil, 80% yield, 365.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.20 (dd, *J* = 4.8, 3.2 Hz, 1H), 6.98 (dd, *J* = 2.8, 1.2 Hz, 1H), 6.89 (dd, *J* = 4.8, 1.2 Hz, 1H), 5.77 (q, *J* = 1.2 Hz, 1H), 3.79 (d, *J* = 1.2 Hz, 2H), 3.76 (s, 2H), 3.68 (s, 3H), 3.30 (s, 2H), 2.42 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.39 – 1.35 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.6, 166.6, 153.7, 143.5, 139.3, 136.7, 129.7, 128.6, 127.3, 125.1, 121.6, 117.4, 100.7, 79.2, 55.0, 51.0, 31.8, 21.5, 16.6, 7.3. IR (neat) ν 661, 1089, 1350, 1658, 1722, 2031, 2957 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{27}NO_4S_2Na$ $(M+Na)^+$: 480.1274, Found: 480.1269.

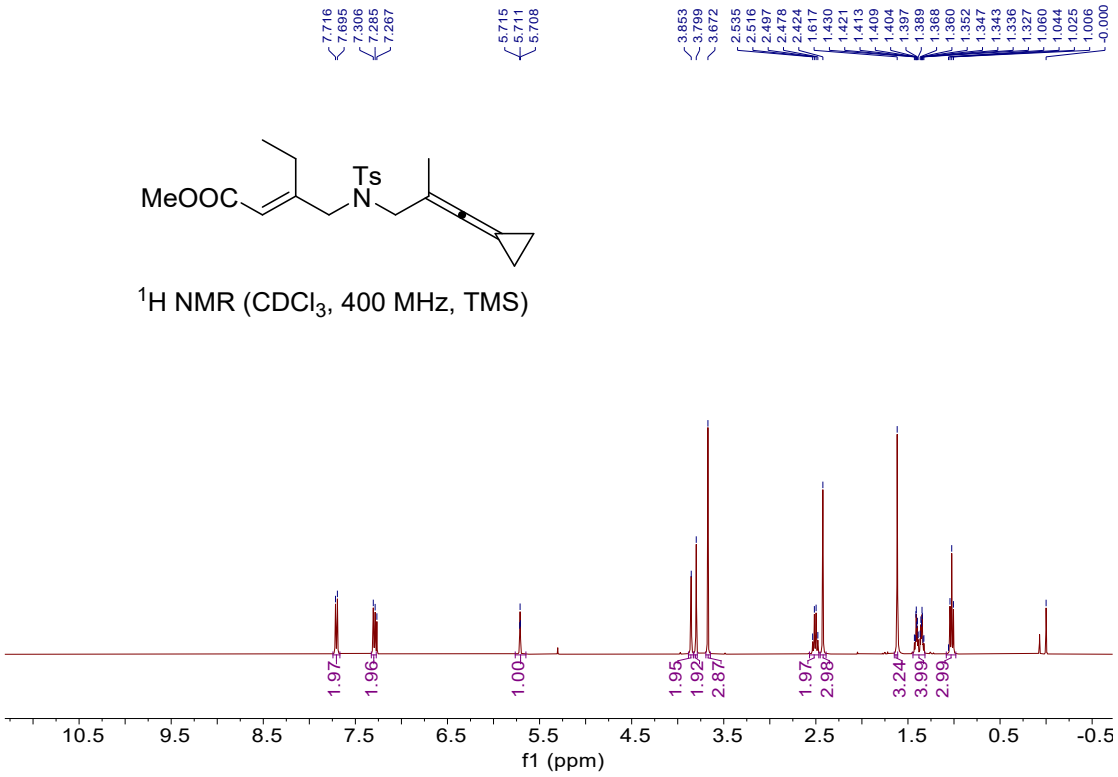


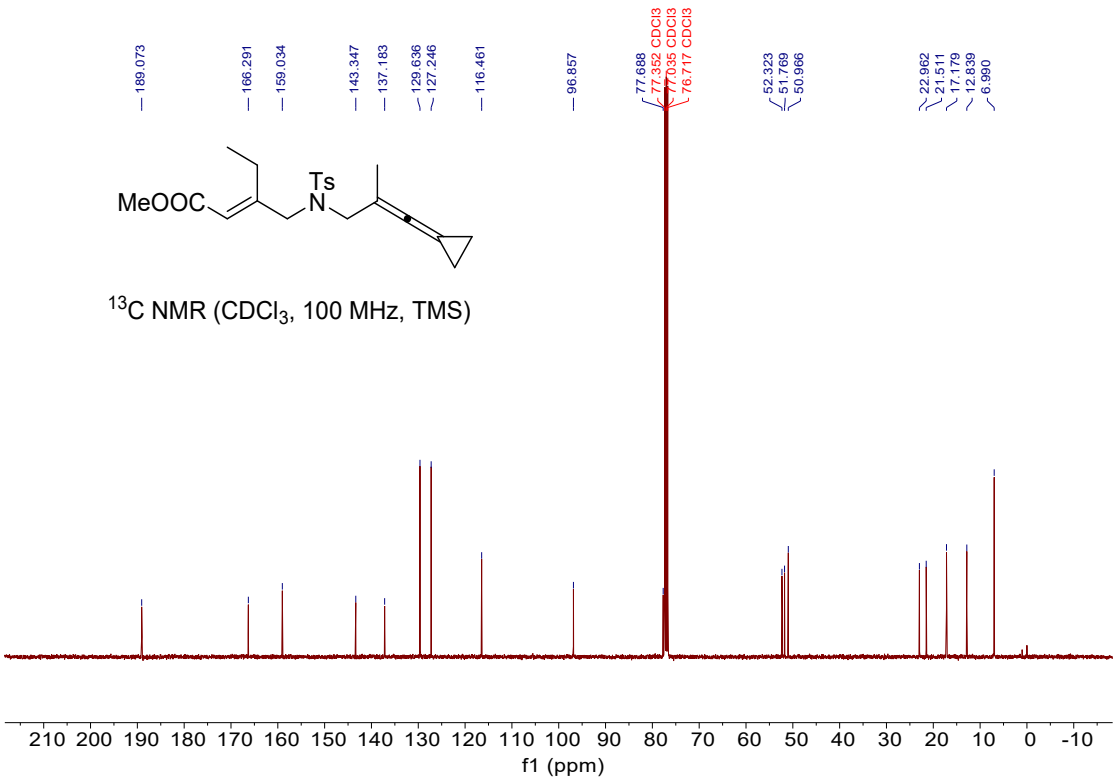

189.573
166.613
153.671
143.461
139.303
136.696
129.704
128.586
127.285
125.094
121.631
117.381
100.733
79.212
77.394 CDCl3
77.076 CDCl3
76.759 CDCl3
54.987
51.015
31.844
21.537
16.555
7.254
S
Ts
N
MeOOC
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

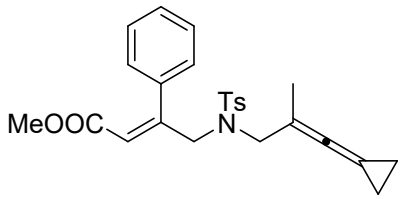


methyl (E)-3-(((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)methyl)pent-2-enoate (1v)

A colorless oil, 80% yield, 311.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.71 (d, *J* = 1.2 Hz, 1H), 3.85 (s, 2H), 3.80 (s, 2H), 3.67 (s, 3H), 2.51 (q, *J* = 7.6 Hz, 2H), 2.42 (s, 3H), 1.61 (s, 3H), 1.45 – 1.32 (m, 4H), 1.02 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.1, 166.3, 159.0, 143.3, 137.2, 129.6, 127.2, 116.5, 96.9, 77.7, 52.3, 51.8, 51.0, 23.0, 21.5, 17.2, 12.8, 7.0. IR (neat) ν 657, 1221, 1661, 1721, 2021, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1551.

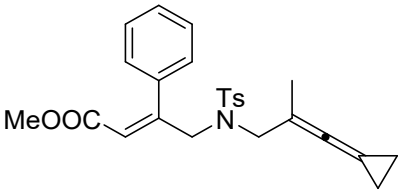



189.073
166.291
159.034
143.347
137.183
129.636
127.246
116.461
96.857
77.688
77.352 CDCl3
77.035 CDCl3
76.717 CDCl3
52.323
51.769
50.966
22.962
21.511
17.179
12.839
6.990
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

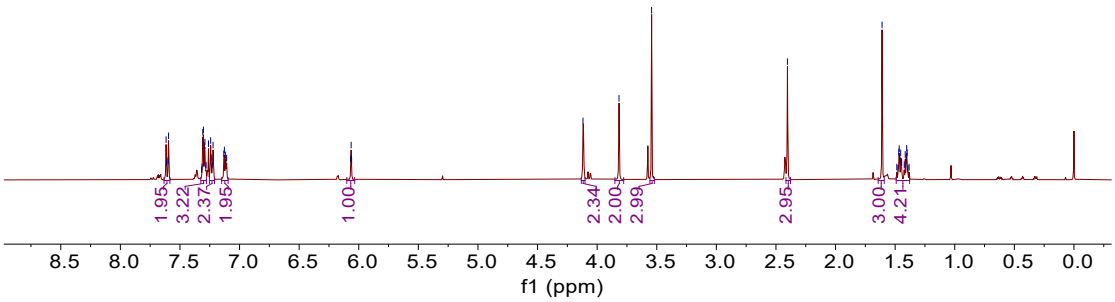


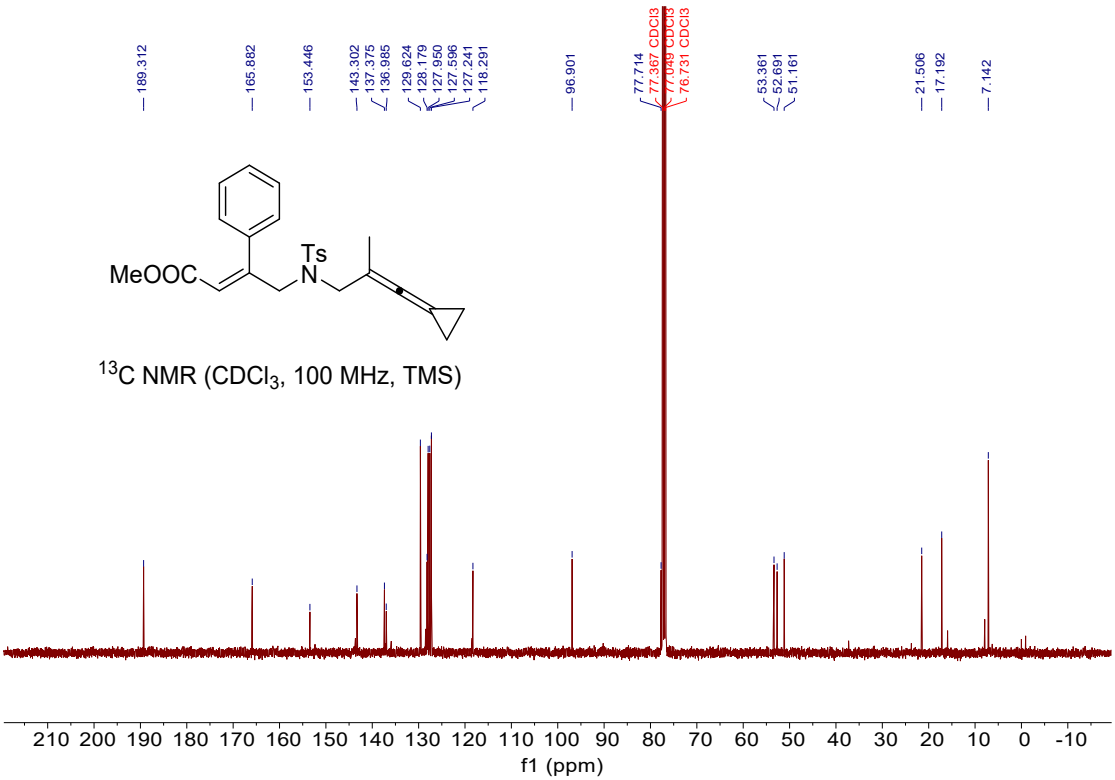
methyl (E)-4-((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-phenylbut-2-enoate (1w)

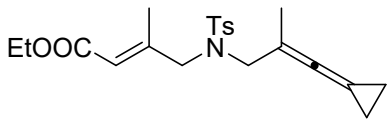
A colorless oil, 90% yield, 338.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 2H), 7.32 – 7.28 (m, 3H), 7.25 – 7.21 (m, 2H), 7.15 – 7.10 (m, 2H), 6.07 (d, *J* = 1.2 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 2H), 3.54 (s, 3H), 2.40 (s, 3H), 1.61 (s, 3H), 1.49 – 1.38 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.3, 165.9, 153.4, 143.3, 137.4, 137.0, 129.6, 128.2, 128.0, 127.6, 127.2, 118.3, 96.9, 77.7, 53.4, 52.7, 51.2, 21.5, 17.2, 7.1. IR (neat) ν 660, 1089, 1446, 1598, 1722, 2022, 2950 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{27}NO_4SNa$ $(M+Na)^+$: 460.1553, Found: 460.1557.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

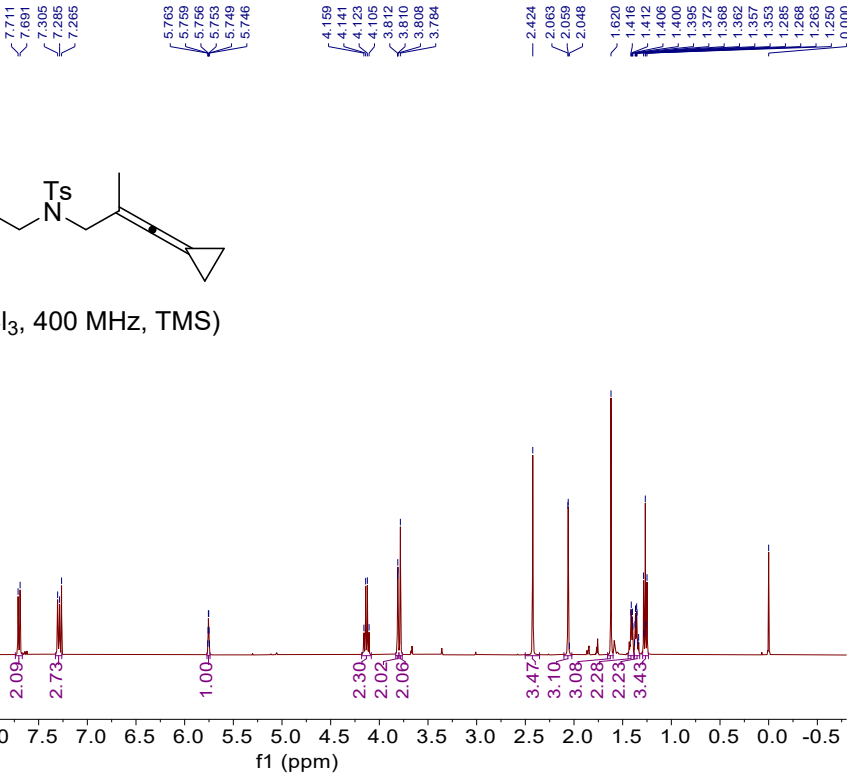


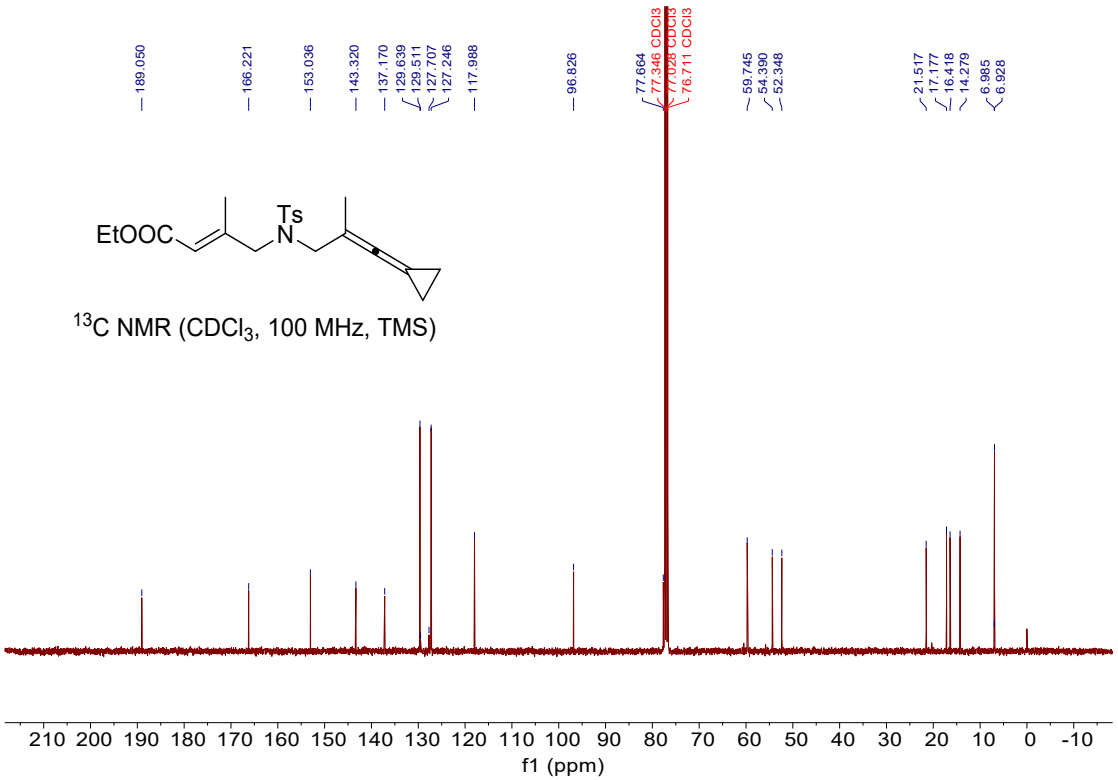

189.312
165.882
153.446
143.302
137.375
136.985
129.624
128.179
127.950
127.596
127.241
118.291
96.901
77.714
77.367 CDCl3
77.049 CDCl3
76.731 CDCl3
53.361
52.691
51.161
21.506
17.192
7.142
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

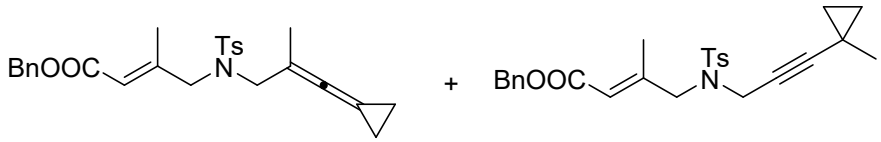


ethyl (E)-4-((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1x)

A colorless oil, 90% yield, 350.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.75 (h, *J* = 1.2 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.83 – 3.80 (m, 2H), 3.78 (s, 2H), 2.42 (s, 3H), 2.06 (d, *J* = 1.2 Hz, 3H), 1.62 (s, 3H), 1.44 – 1.39 (m, 2H), 1.38 – 1.33 (m, 2H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 166.2, 153.0, 143.3, 137.2, 129.6, 129.5, 127.7, 127.2, 118.0, 96.8, 77.7, 59.7, 54.4, 52.3, 21.5, 17.2, 16.4, 14.3, 7.0, 6.9. IR (neat) ν 661, 1042, 1346, 1658, 1721, 2021, 2983 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1556.

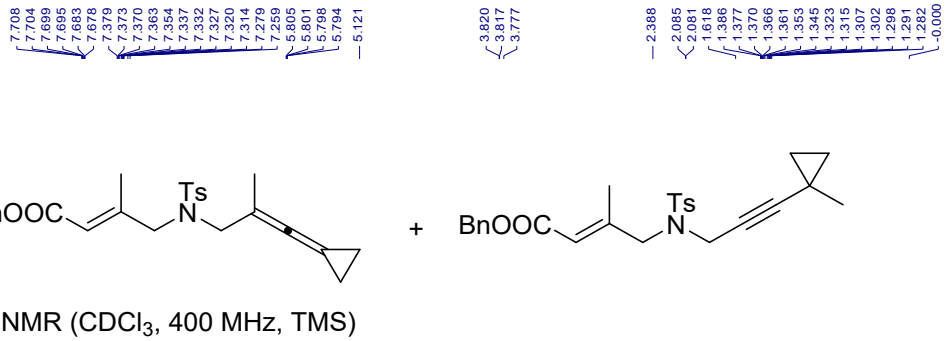



189.050
166.221
153.036
143.320
137.170
129.639
129.511
127.707
127.246
117.988
96.826
77.664
77.346 CDCl3
77.028 CDCl3
76.711 CDCl3
59.745
54.390
52.348
21.517
17.177
16.418
14.279
6.985
6.928
EtOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

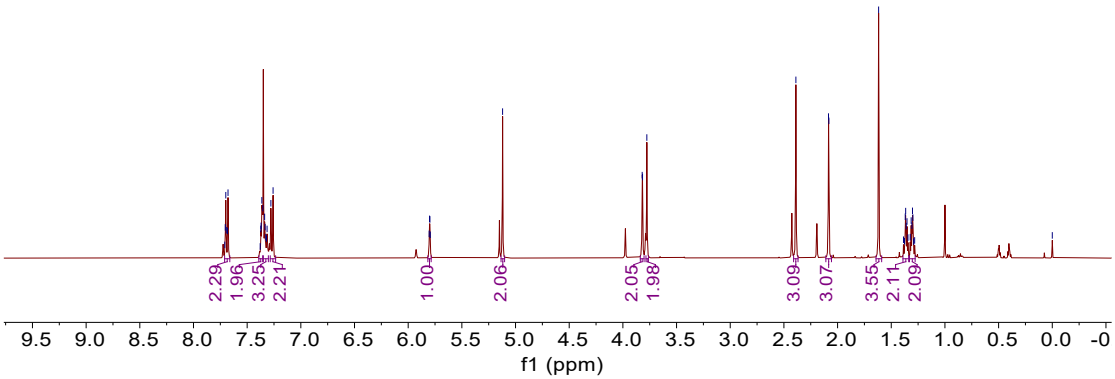


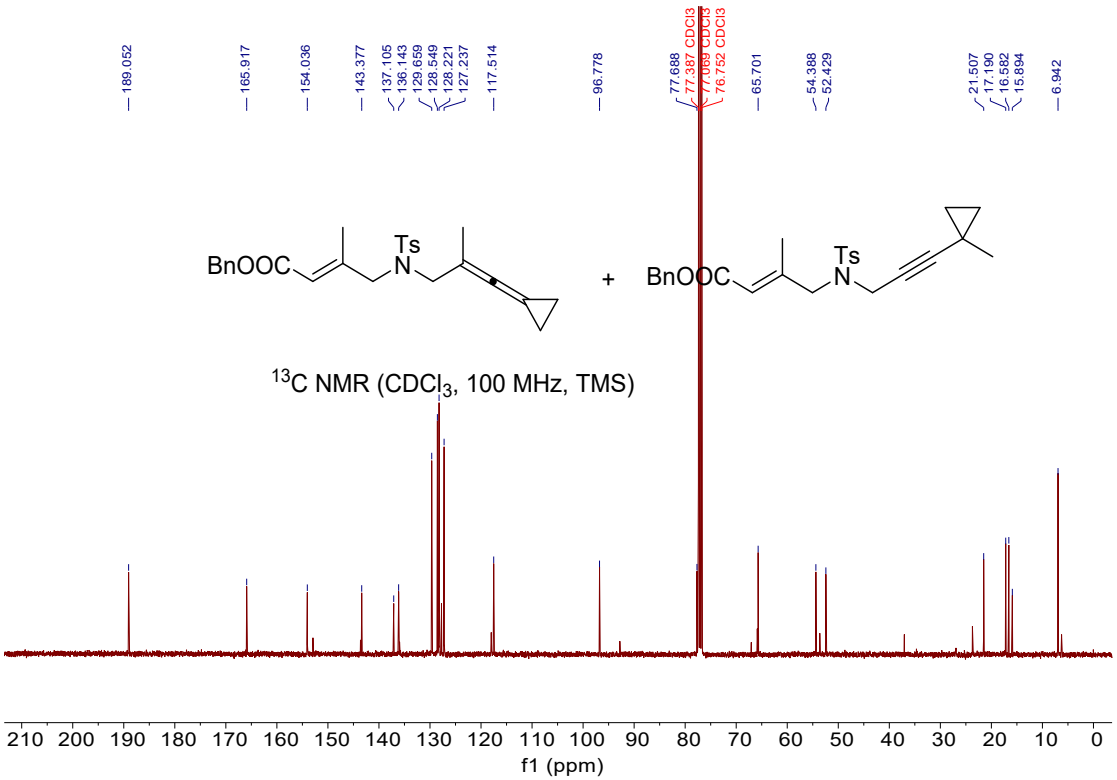
benzyl (E)-4-((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1y) + benzyl (E)-3-methyl-4-((4-methyl-N-(3-(1-methylcyclopropyl)prop-2-yn-1-yl)phenyl)sulfonamido)but-2-enoate (byproduct 1y') (1y: 1y'=5:1)

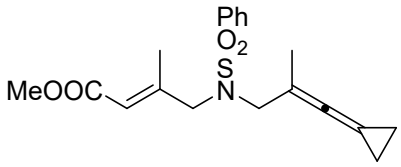
A colorless oil, 90% yield, 405.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.66 (m, 2H), 7.39 – 7.36 (m, 2H), 7.35 – 7.30 (m, 3H), 7.27 (d, *J* = 8.0 Hz, 2H), 5.80 (q, *J* = 1.2 Hz, 1H), 5.12 (s, 2H), 3.82 (d, *J* = 1.2 Hz, 2H), 3.78 (s, 2H), 2.39 (s, 3H), 2.08 (d, *J* = 1.2 Hz, 3H), 1.62 (s, 3H), 1.39 – 1.34 (m, 2H), 1.33 – 1.28 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.1, 165.9, 154.0, 143.4, 137.1, 136.1, 129.7, 128.5, 128.2, 127.2, 117.5, 96.8, 77.7, 65.7, 54.4, 52.4, 21.5, 17.2, 16.6, 15.9, 6.9. IR (neat) ν 660, 1345, 1658, 1722, 2021, 2984 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1707.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

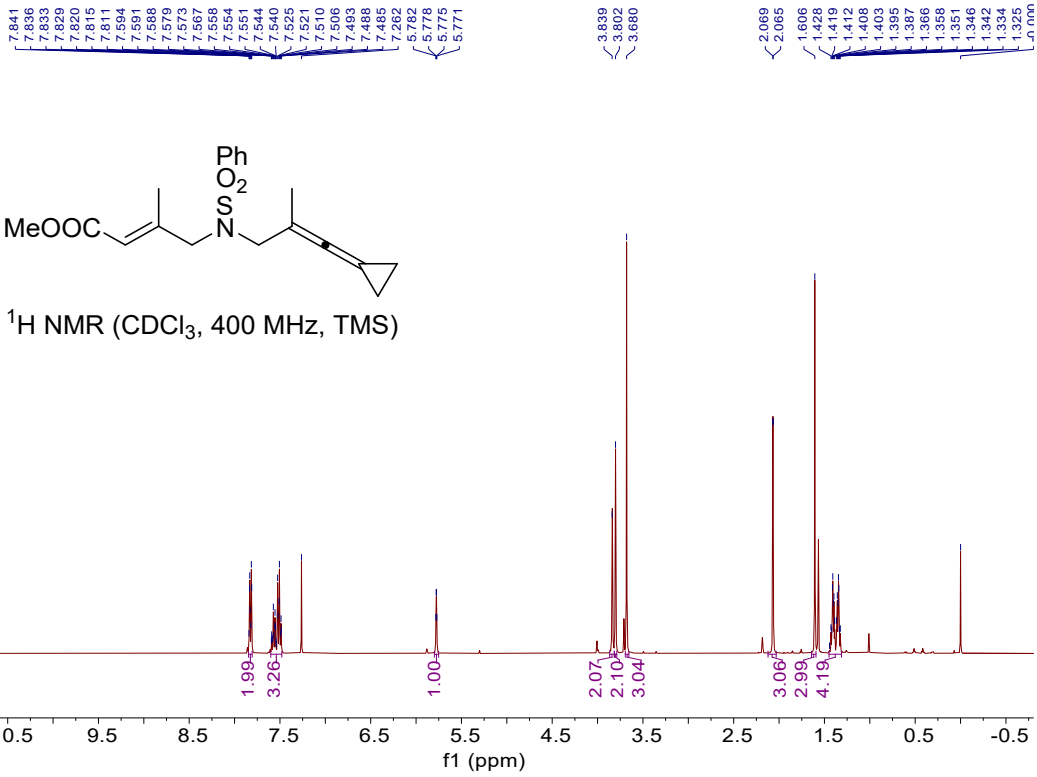


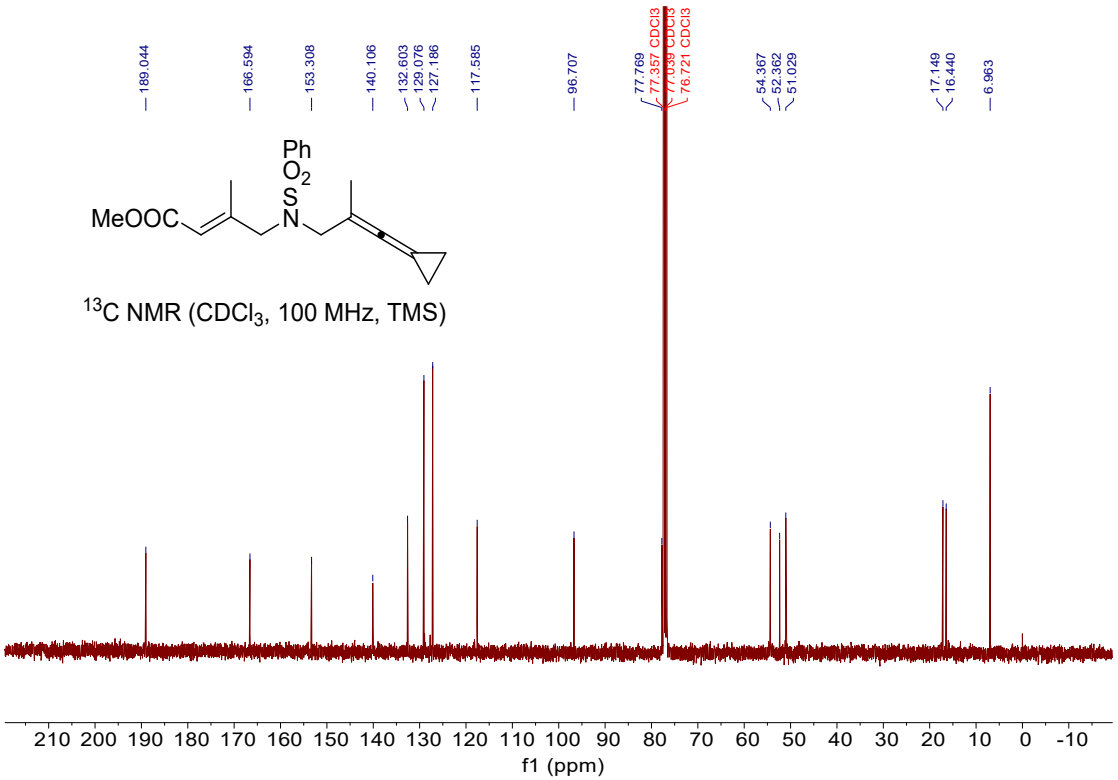

189.052
165.917
154.036
143.377
137.105
136.143
129.659
128.549
128.221
127.237
117.514
96.778
77.688
77.387 CDCl3
77.069 CDCl3
76.752 CDCl3
65.701
54.388
52.429
21.507
17.190
16.582
15.894
6.942
BnOOC
Ts
N
+
BnOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

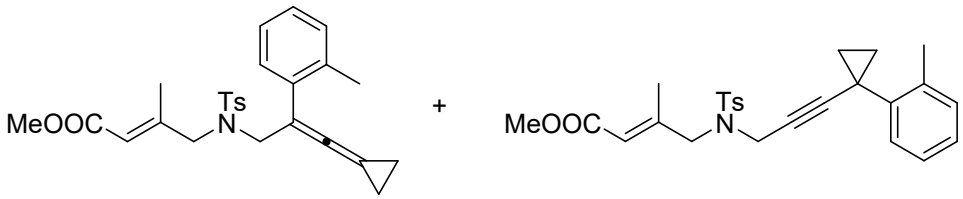


methyl (E)-4-(N-(3-cyclopropylidene-2-methyl-λ^5-allyl)phenylsulfonamido)-3-methylbut-2-enoate (1z)

A colorless oil, 90% yield, 324.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.77 (m, 2H), 7.66 – 7.48 (m, 3H), 5.78 (s, 1H), 3.84 (s, 2H), 3.80 (s, 2H), 3.68 (d, J = 1.2 Hz, 3H), 2.07 (s, 3H), 1.61 (s, 3H), 1.44 – 1.31 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 166.6, 153.3, 140.1, 132.6, 129.1, 127.2, 117.6, 96.7, 77.8, 54.4, 52.4, 51.0, 17.1, 16.4, 7.0. IR (neat) ν 690, 1158, 1356, 1661, 1724, 2023, 2950 cm^{-1}. HRMS (ESI) calcd. for $C_{19}H_{23}NO_4SNa$ $(M+Na)^+$: 384.1240, Found: 384.1239.

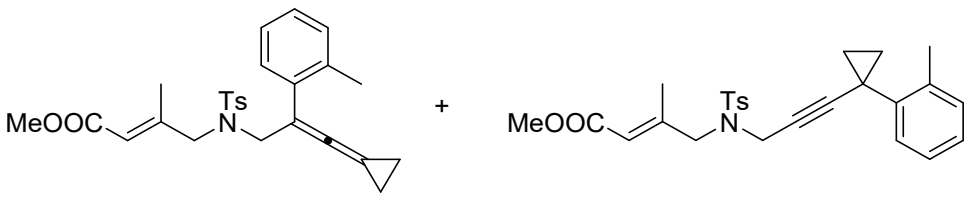


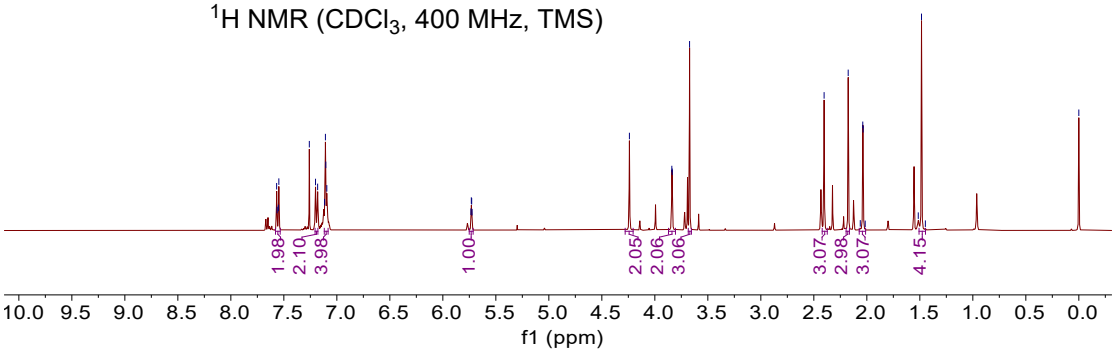

189.044
166.594
153.308
140.106
132.603
129.076
127.186
117.585
96.707
77.769
77.357 CDCl3
77.039 CDCl3
76.721 CDCl3
54.367
52.362
51.029
17.149
16.440
6.963
Ph
O2
S
N
MeOOC
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

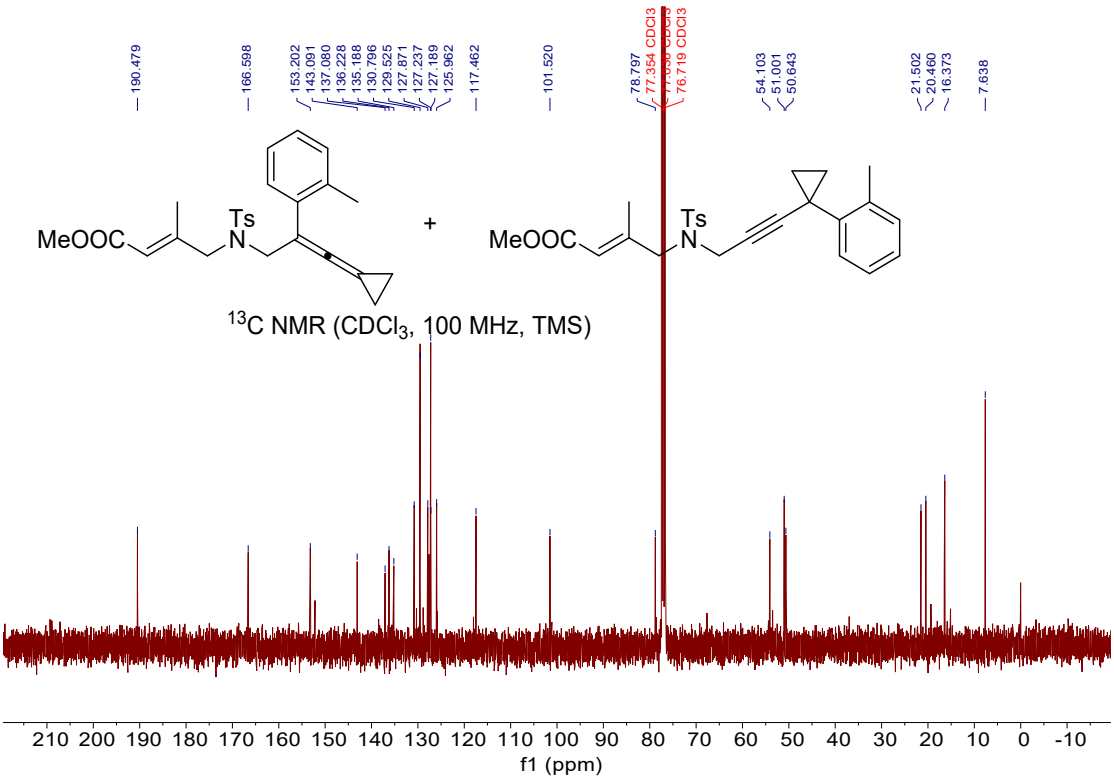


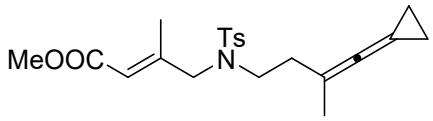
methyl (E)-4-((N-(3-cyclopropylidene-2-(o-tolyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1aa) + methyl (E)-3-methyl-4-((4-methyl-N-(3-(1-(o-tolyl)cyclopropyl)prop-2-yn-1-yl)phenyl)sulfonamido)but-2-enoate (byproduct 1aa') (1m: 1m'=6:1)

A colorless oil, 60% yield, 270.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.53 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 5.2 Hz, 4H), 5.73 (q, *J* = 1.4 Hz, 1H), 4.24 (s, 2H), 3.84 (d, *J* = 1.4 Hz, 2H), 3.67 (s, 3H), 2.40 (s, 3H), 2.18 (s, 3H), 2.04 (d, *J* = 1.3 Hz, 3H), 1.48 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.5, 166.6, 153.2, 143.1, 137.1, 136.2, 135.2, 130.8, 129.5, 127.9, 127.2, 127.2, 126.0, 117.5, 101.5, 78.8, 54.1, 51.0, 50.6, 21.5, 20.5, 16.4, 7.6. IR (neat) ν 662, 1216, 1662, 1720, 2023, 2943 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1712.



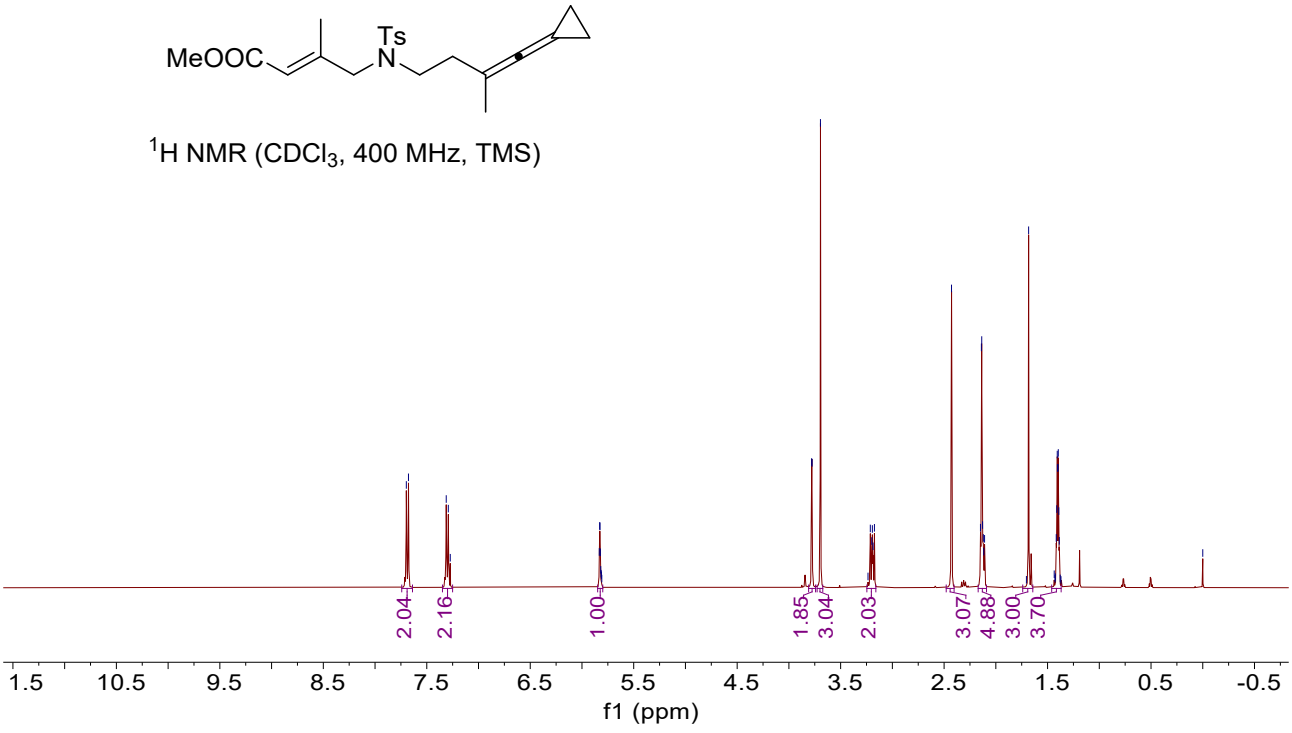


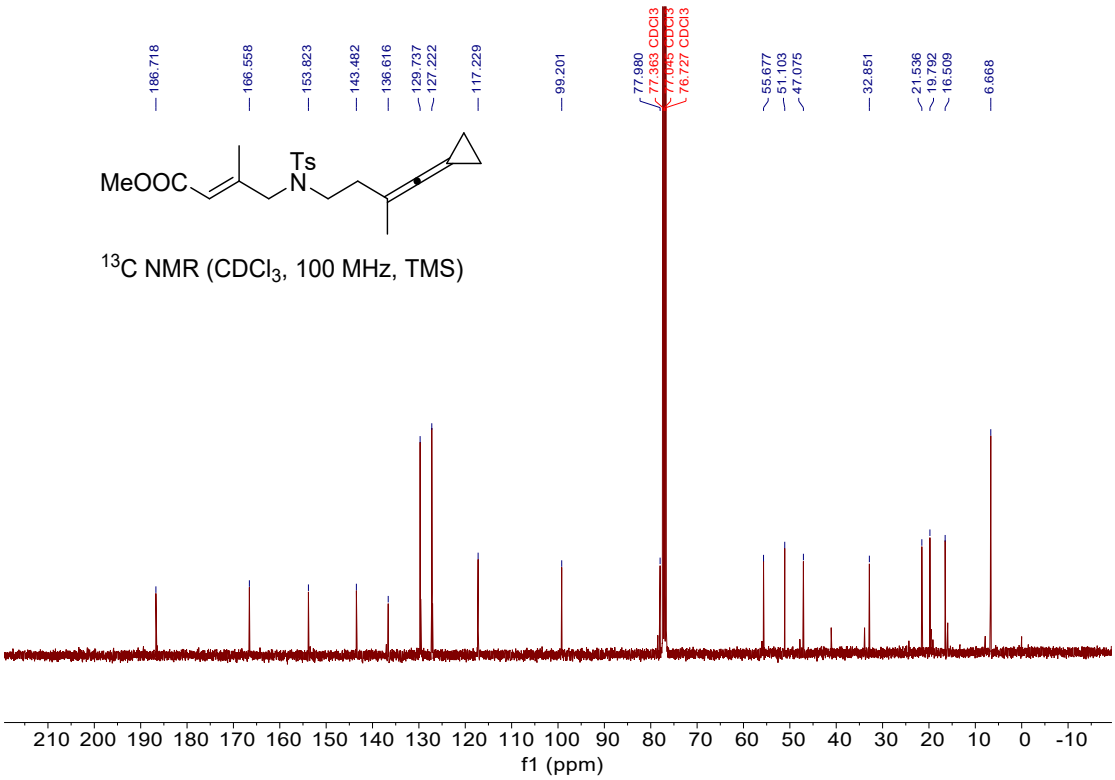

190.479
166.598
153.202
143.091
137.080
136.228
135.188
130.796
129.525
127.871
127.237
127.189
125.962
117.462
101.520
78.797
77.354 CDCl3
76.719 CDCl3
54.103
51.001
50.643
21.502
20.460
16.373
7.638
MeOOC
Ts
N
+
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

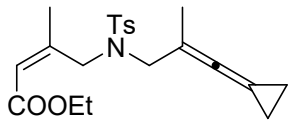


methyl (E)-4-((N-(4-cyclopropylidene-3-methyl-λ^5-but-3-en-1-yl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (1ab)

A colorless oil, 90% yield, 350.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 5.82 (q, J = 1.6 Hz, 1H), 3.78 (s, 2H), 3.70 (s, 3H), 3.23 – 3.15 (m, 2H), 2.43 (s, 3H), 2.17 – 2.08 (m, 5H), 1.68 (s, 3H), 1.44 – 1.34 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.7, 166.6, 153.8, 143.5, 136.6, 129.7, 127.2, 117.2, 99.2, 78.0, 77.4, 77.0, 76.7, 55.7, 51.1, 47.1, 32.9, 21.5, 19.8, 16.5, 6.7. IR (neat) ν 665, 1226, 1661, 1721, 2024, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1560.

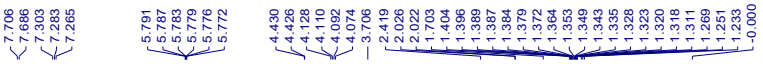


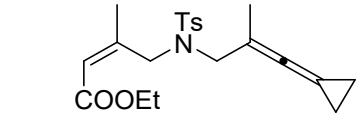

186.718
166.558
153.823
143.482
136.616
129.737
127.222
117.229
99.201
77.980
77.363 CDCl3
77.045 CDCl3
76.727 CDCl3
55.677
51.103
47.075
32.851
21.536
19.792
16.509
6.668
MeOOC
Ts
N
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



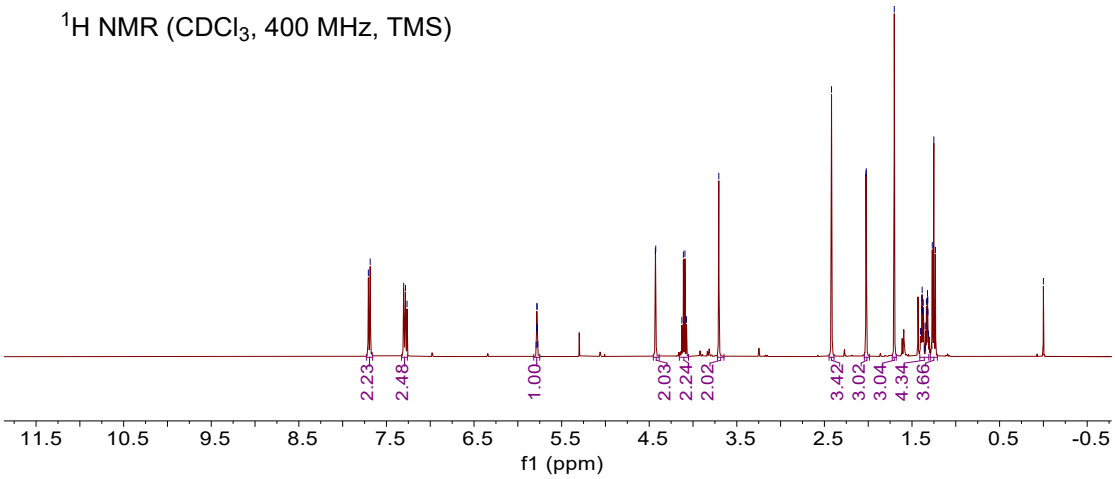
ethyl (Z)-4-((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3a)

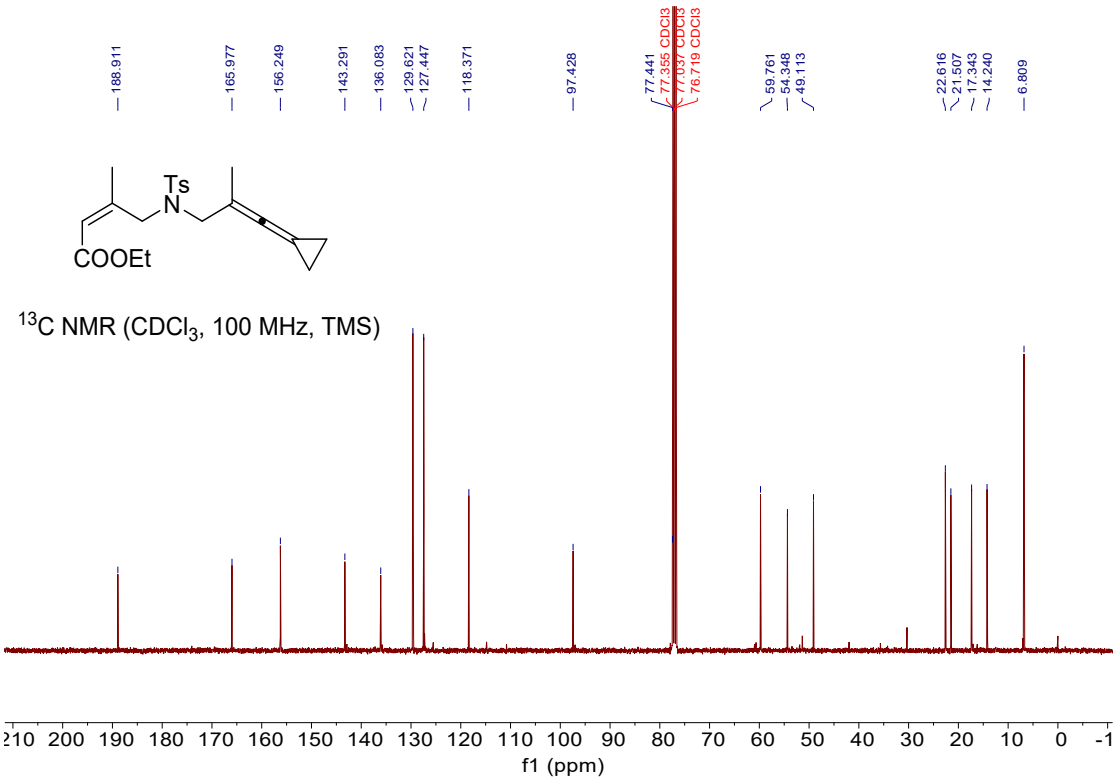
A colorless oil, 90% yield, 350.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.78 (h, *J* = 1.2 Hz, 1H), 4.43 (d, *J* = 1.2 Hz, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.71 (s, 2H), 2.42 (s, 3H), 2.02 (d, *J* = 1.2 Hz, 3H), 1.70 (s, 3H), 1.41 – 1.31 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 166.0, 156.2, 143.3, 136.1, 129.6, 127.4, 118.4, 97.4, 77.4, 59.8, 54.3, 49.1, 22.6, 21.5, 17.3, 14.2, 6.8. IR (neat) ν 660, 1221, 1446, 1651, 1711, 2024, 2983 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1553.

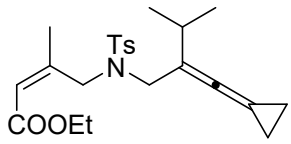




^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

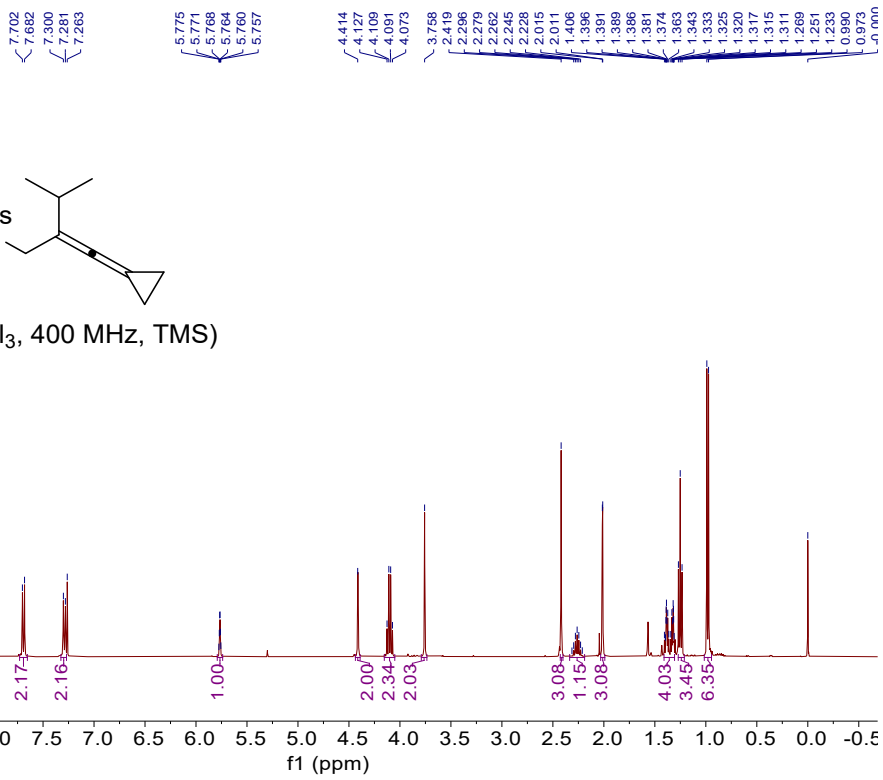


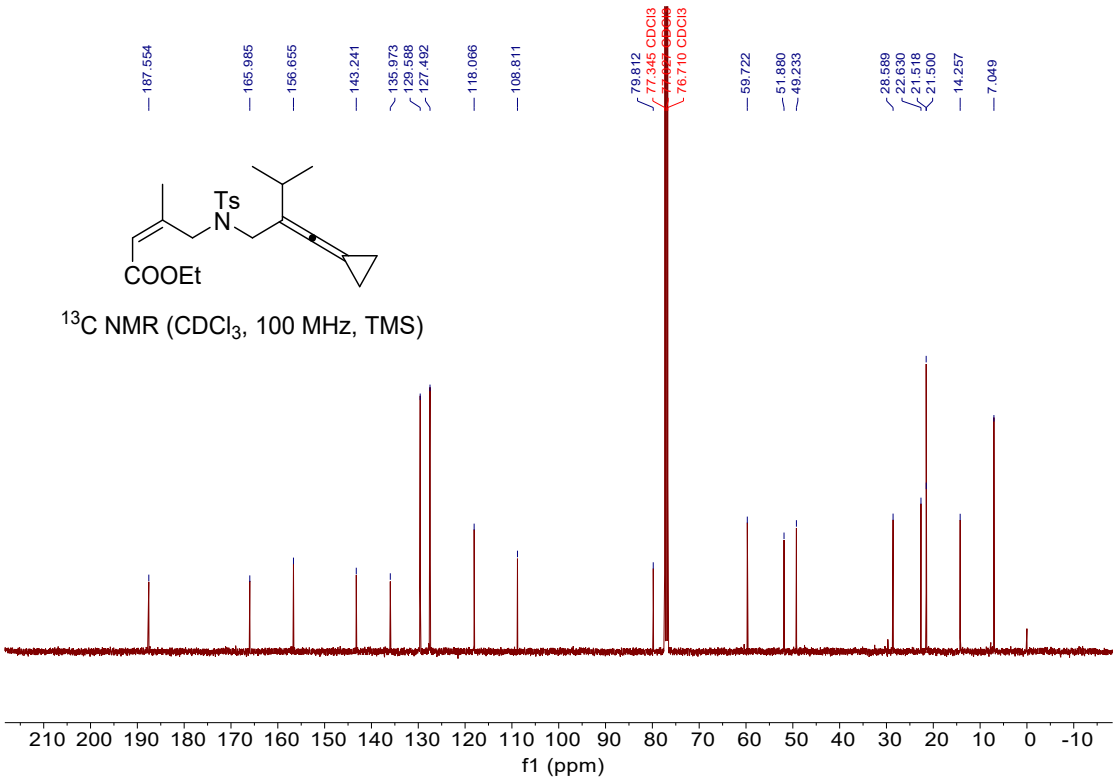

188.911
165.977
156.249
143.291
136.083
129.621
127.447
118.371
97.428
77.441
77.355 CDCl3
77.037 CDCl3
76.719 CDCl3
59.761
54.348
49.113
22.616
21.507
17.343
14.240
6.809
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
f1 (ppm)

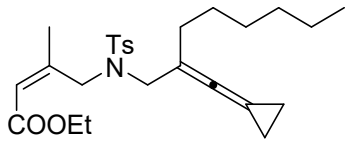


ethyl (Z)-4-((N-(2-(cyclopropylidene-λ^5-methylene)-3-methylbutyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3b)

A colorless oil, 80% yield, 333.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.77 (h, *J* = 1.6 Hz, 1H), 4.41 (s, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.76 (s, 2H), 2.42 (s, 3H), 2.26 (hept, *J* = 6.8 Hz, 1H), 2.01 (d, *J* = 1.6 Hz, 3H), 1.41 – 1.31 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H), 0.98 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.6, 166.0, 156.7, 143.2, 136.0, 129.6, 127.5, 118.1, 108.8, 79.8, 59.7, 51.9, 49.2, 28.6, 22.6, 21.5, 21.5, 14.3, 7.0. IR (neat) ν 665, 1343, 1647, 1711, 2020, 2982 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{31}NO_4SNa$ $(M+Na)^+$: 440.1866, Found: 440.1869.

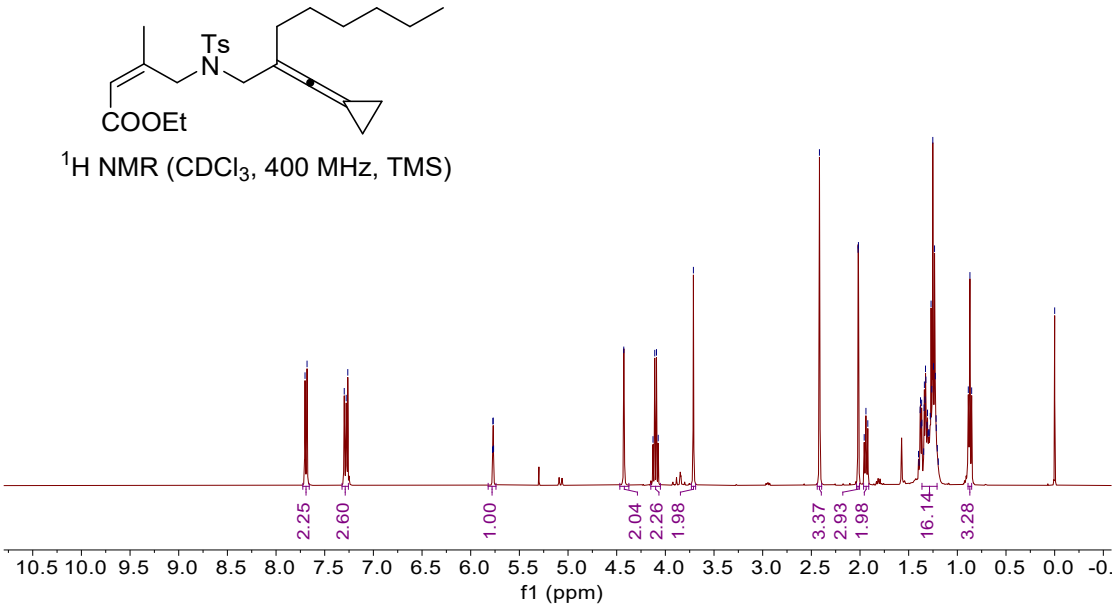


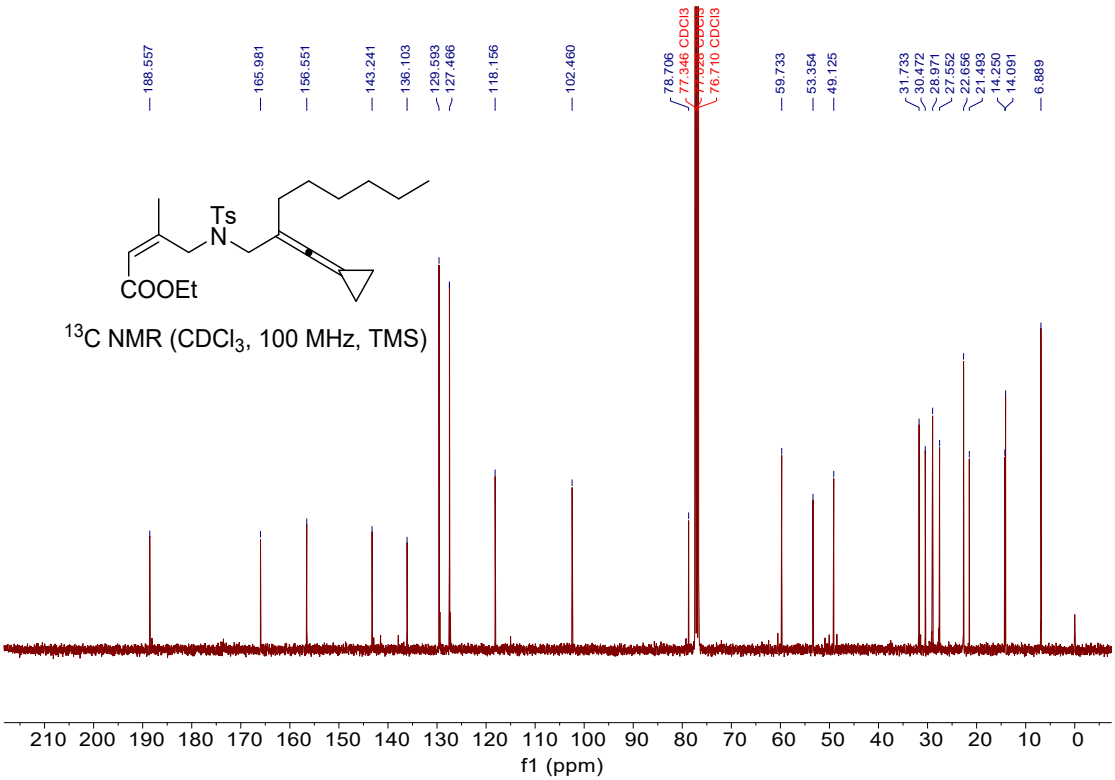

187.554
165.985
156.655
143.241
135.973
129.588
127.492
118.066
108.811
79.812
77.345 CDCl3
76.710 CDCl3
59.722
51.880
49.233
28.589
22.630
21.518
21.500
14.257
7.049
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

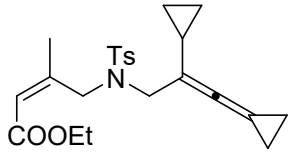


ethyl (Z)-4-((N-(2-(cyclopropylidene-λ^5-methylene)octyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3c)

A colorless oil, 90% yield, 413 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.77 (q, *J* = 1.6 Hz, 1H), 4.43 (s, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.71 (s, 2H), 2.42 (s, 3H), 2.02 (d, *J* = 1.6 Hz, 3H), 1.96 – 1.91 (m, 2H), 1.36 – 1.21 (m, 15H), 0.88 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.6, 166.0, 156.6, 143.2, 136.1, 129.6, 127.5, 118.2, 102.5, 78.7, 59.7, 53.4, 49.1, 31.7, 30.5, 29.0, 27.6, 22.7, 21.5, 14.2, 14.1, 6.9. IR (neat) ν 660, 1216, 1376, 1649, 1712, 2024, 2925 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{37}NO_4SNa$ $(M+Na)^+$: 482.2336, Found: 482.2328.

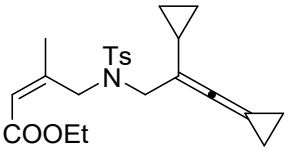



188.557
165.981
156.551
143.241
136.103
129.593
127.466
118.156
102.460
78.706
77.346 CDCl3
76.710 CDCl3
59.733
53.354
49.125
31.733
30.472
28.971
27.552
22.656
21.493
14.250
14.091
6.889
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

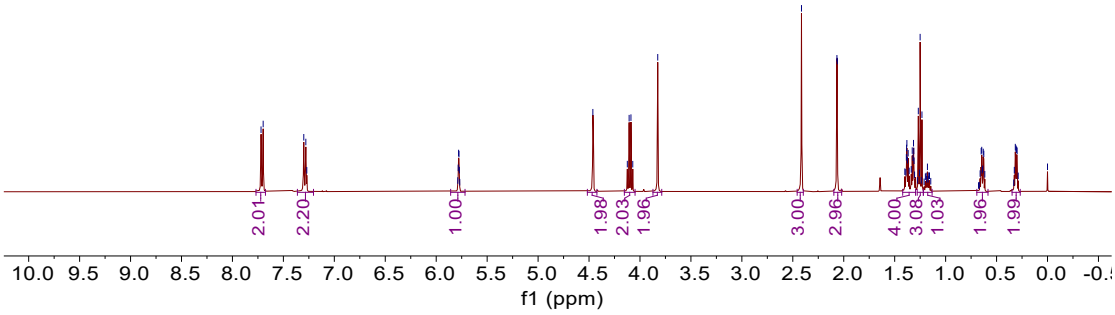


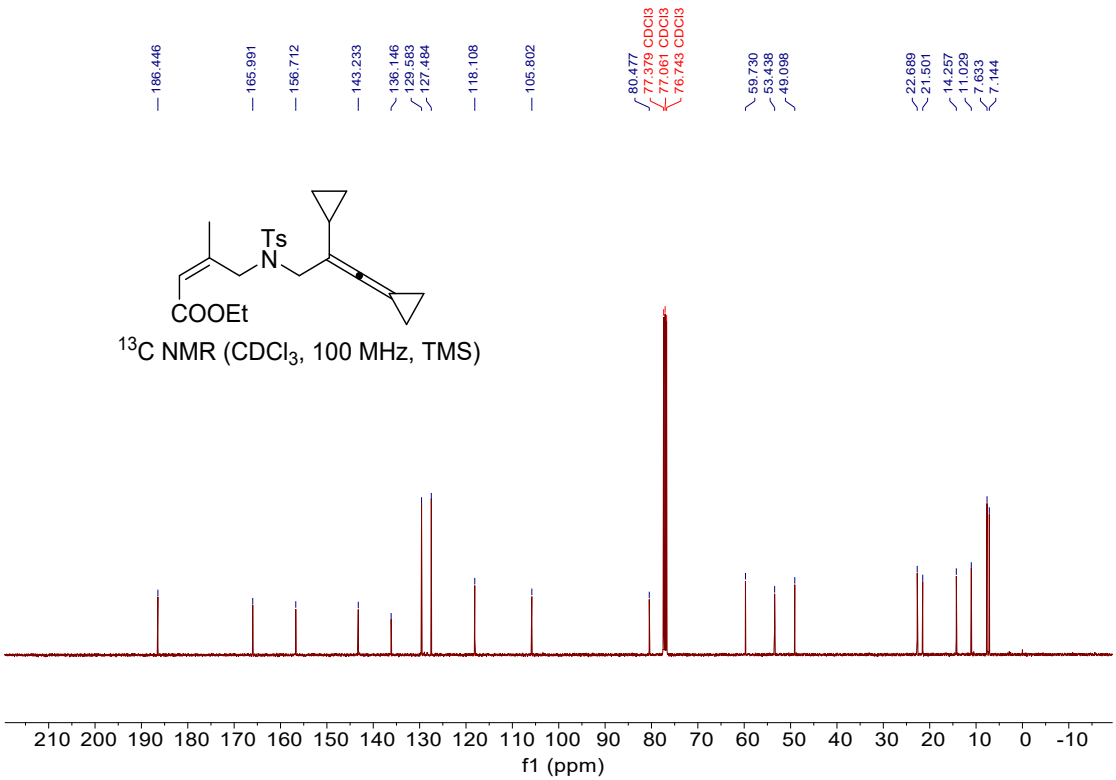
ethyl (Z)-4-((N-(2-(cyclopropylidene-λ^5-methylene)octyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3d)

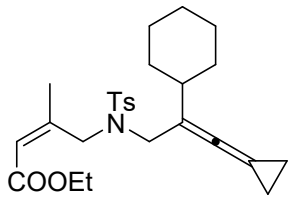
A colorless oil, 80% yield, 332.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.78 (h, *J* = 1.6 Hz, 1H), 4.46 (s, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.83 (s, 2H), 2.41 (s, 3H), 2.07 (d, *J* = 1.6 Hz, 3H), 1.42 – 1.30 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.22 – 1.13 (m, 1H), 0.69 – 0.58 (m, 2H), 0.35 – 0.27 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.4, 166.0, 156.7, 143.2, 136.1, 129.6, 127.5, 118.1, 105.8, 80.5, 59.7, 53.4, 49.1, 22.7, 21.5, 14.3, 11.0, 7.6, 7.1. IR (neat) ν 661, 1348, 1659, 1711, 2024, 2948 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{29}NO_4SNa$ $(M+Na)^+$: 438.1710, Found: 438.1705.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

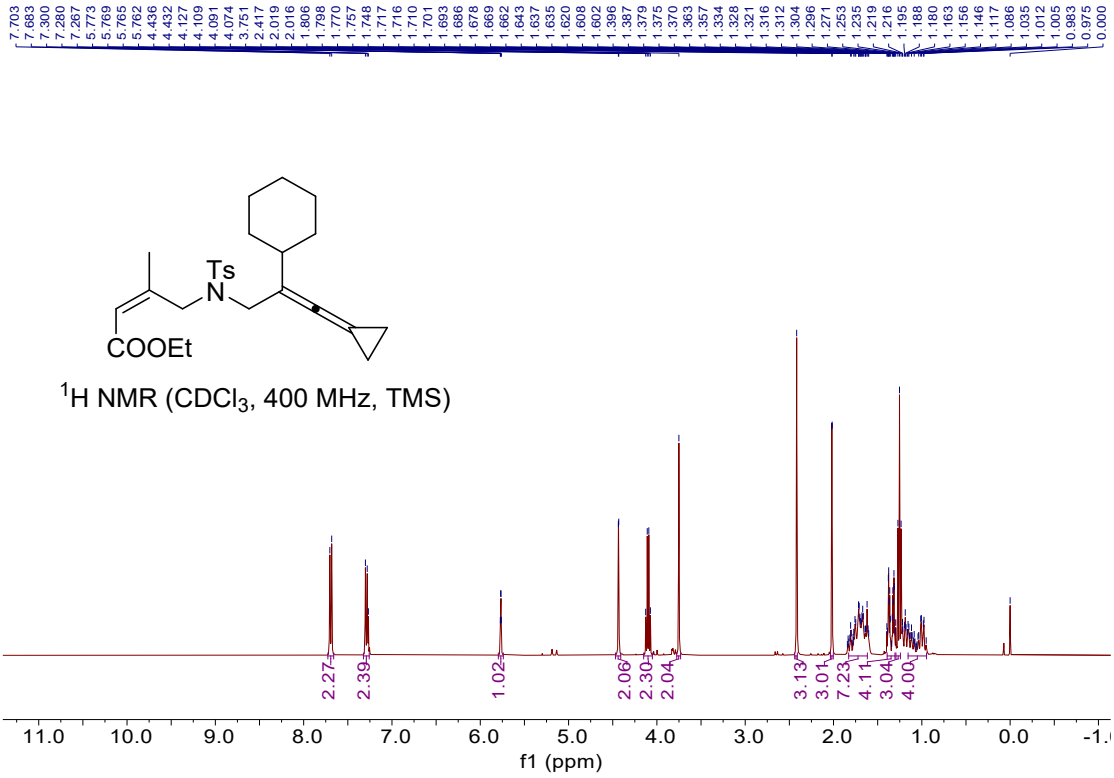


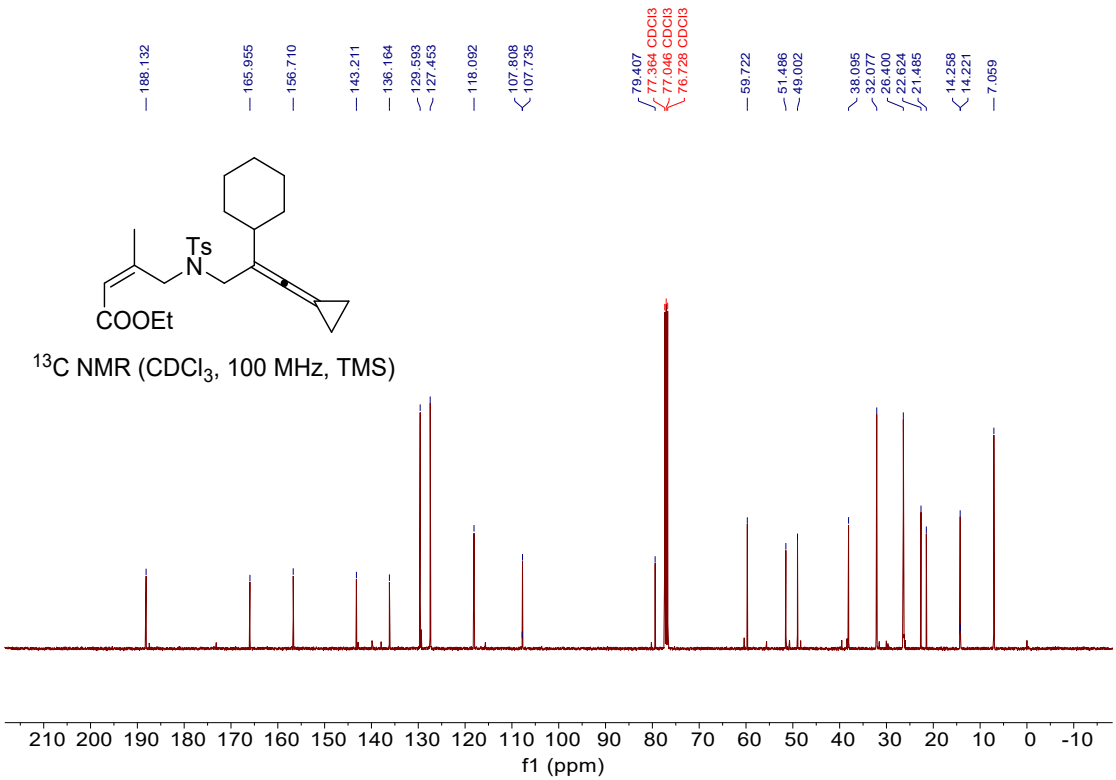

186.446
165.991
156.712
143.233
136.146
129.583
127.484
118.108
105.802
80.477
77.379 CDCl3
77.061 CDCl3
76.743 CDCl3
59.730
53.438
49.098
22.689
21.501
14.257
11.029
7.633
7.144
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

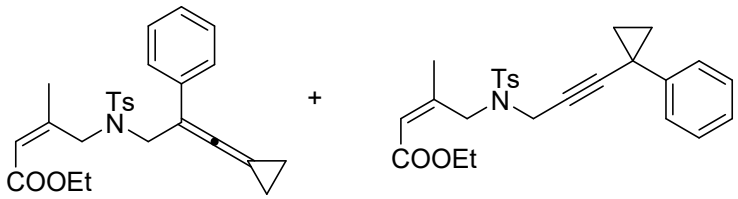


ethyl (Z)-4-((N-(2-cyclohexyl-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3e)

A colorless oil, 90% yield, 365.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.77 (q, *J* = 1.6 Hz, 1H), 4.43 (d, *J* = 1.6 Hz, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.75 (s, 2H), 2.42 (s, 3H), 2.02 (d, *J* = 1.6 Hz, 3H), 1.83 – 1.62 (m, 7H), 1.39 – 1.30 (m, 4H), 1.29 – 1.24 (m, 3H), 1.16 – 0.95 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.1, 166.0, 156.7, 143.2, 136.2, 129.6, 127.5, 118.1, 107.8, 107.7, 79.4, 59.7, 51.5, 49.0, 38.1, 32.1, 26.4, 22.6, 21.5, 14.3, 14.2, 7.1. IR (neat) ν 661, 1343, 1648, 1713, 2025, 2983 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{35}NO_4SNa$ $(M+Na)^+$: 480.2179, Found: 480.2178.

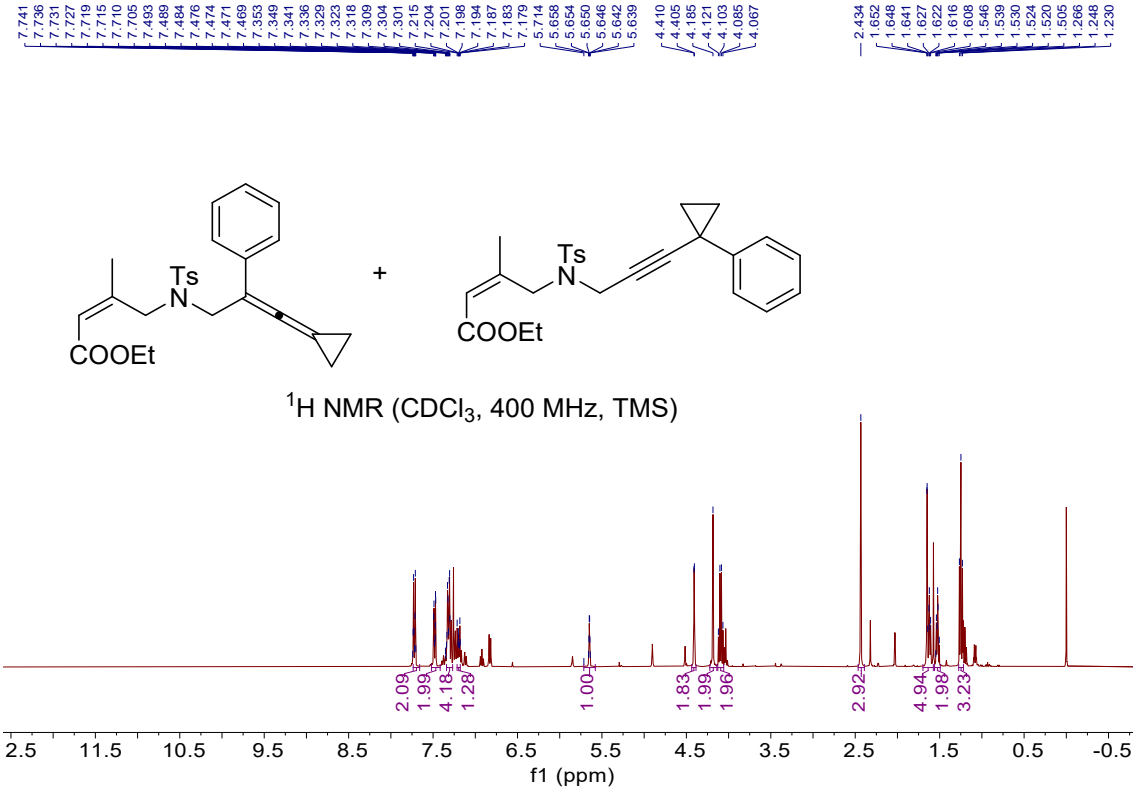


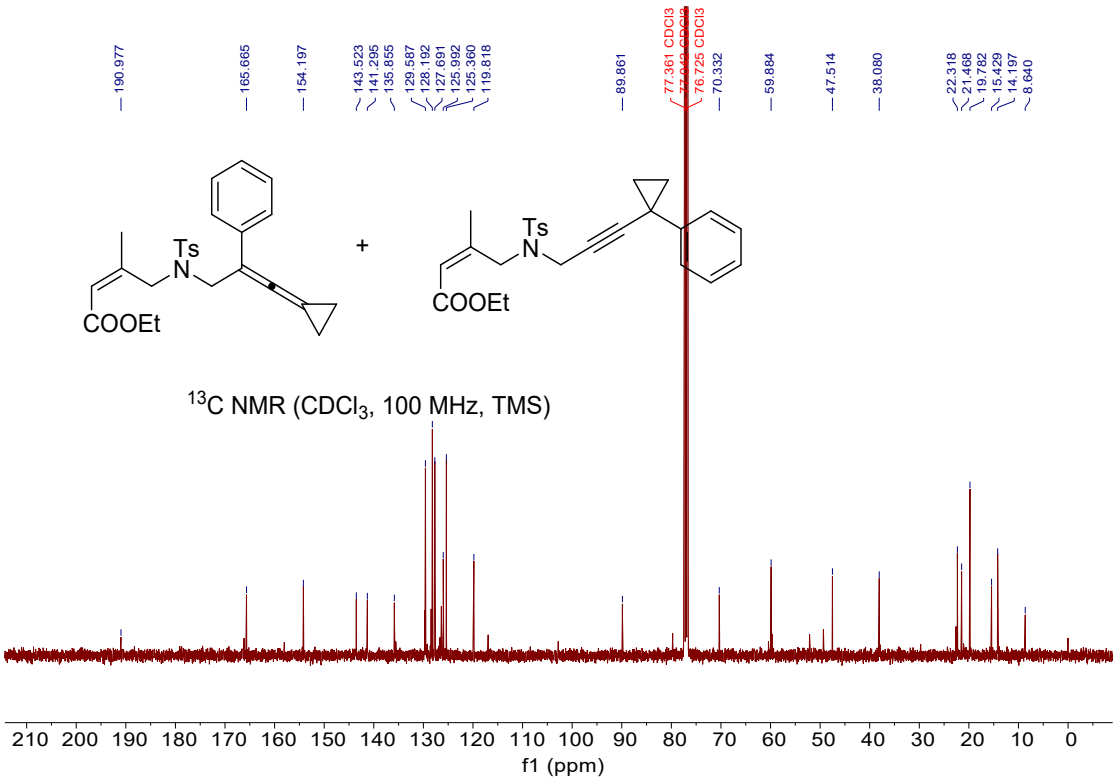

188.132
165.955
156.710
143.211
136.164
129.593
127.453
118.092
107.808
107.735
79.407
77.364 CDCl3
77.046 CDCl3
76.728 CDCl3
59.722
51.486
49.002
38.095
32.077
26.400
22.624
21.485
14.258
14.221
7.059
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

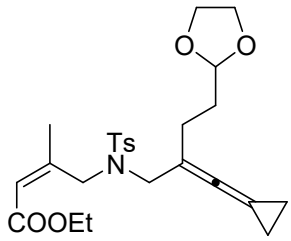


ethyl (Z)-4-((N-(3-cyclopropylidene-2-phenyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3f) + ethyl (Z)-3-methyl-4-((4-methyl-N-(3-(1-phenylcyclopropyl)prop-2-yn-1-yl)phenyl)sulfonamido)but-2-enoate (byproduct 3f') (1m: 1m'=3:1)

A colorless oil, 60% yield, 284.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.66 (m, 2H), 7.52 – 7.42 (m, 2H), 7.32 (dd, *J* = 7.8, 2.0 Hz, 4H), 7.22 – 7.18 (m, 1H), 5.71 – 5.58 (m, 1H), 4.41 (d, *J* = 1.6 Hz, 2H), 4.18 (s, 2H), 4.09 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.70 – 1.57 (m, 5H), 1.56 – 1.49 (m, 2H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.0, 165.7, 154.2, 143.5, 141.3, 135.9, 129.6, 128.2, 127.7, 126.0, 125.4, 119.8, 89.9, 70.3, 59.9, 47.5, 38.1, 22.3, 21.5, 19.8, 15.4, 14.2, 8.6. IR (neat) ν 660, 1043, 1343, 1651, 1712, 2024, 2949 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1716.

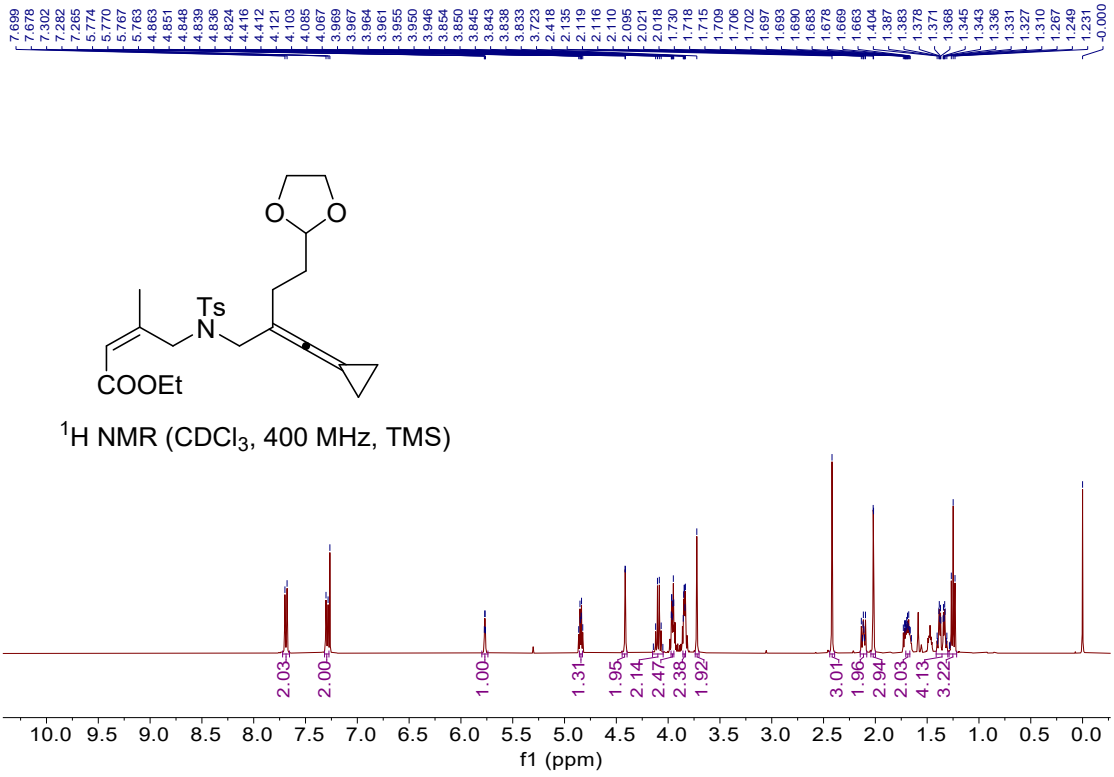


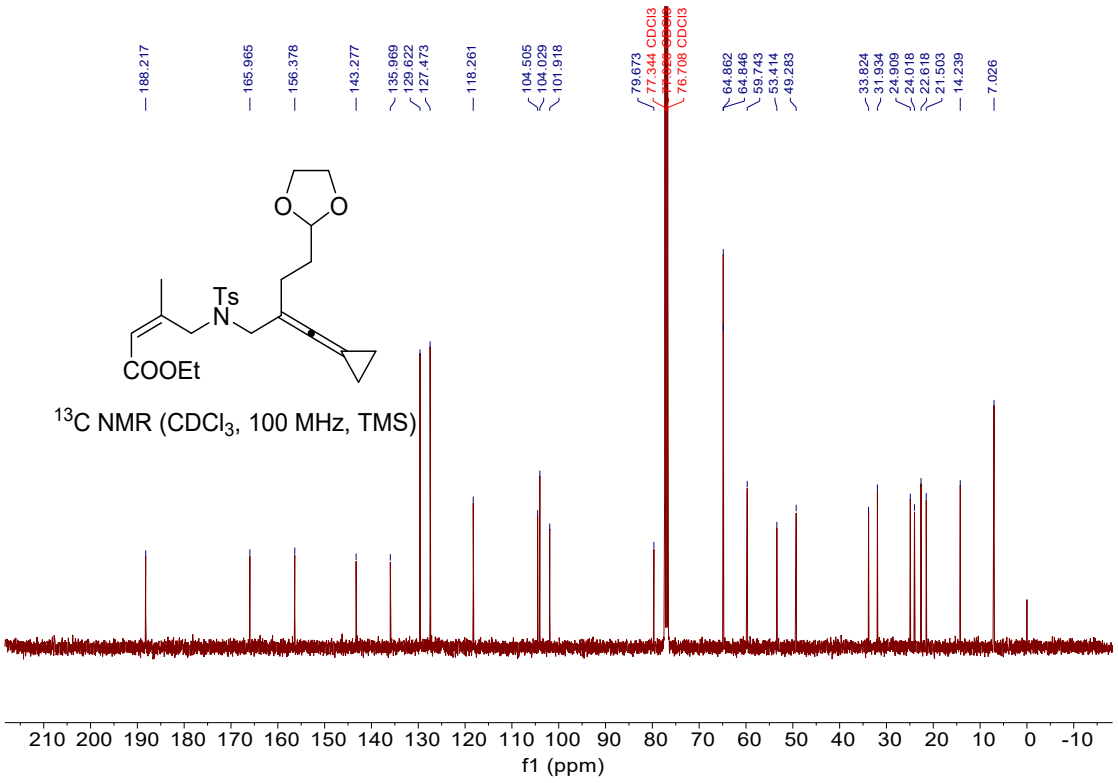

190.977
165.665
154.197
143.523
141.295
135.855
129.587
128.192
127.691
125.992
125.360
119.818
89.861
77.361 CDCl3
76.725 CDCl3
70.332
59.884
47.514
38.080
22.318
21.468
19.782
15.429
14.197
8.640
Ts
N
COOEt
+
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

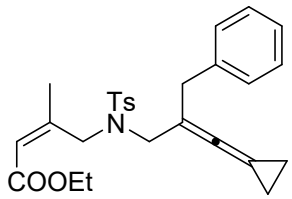


ethyl (Z)-4-((N-(2-(cyclopropylidene-λ^5-methylene)-4-(1,3-dioxolan-2-yl)butyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3g)

A yellow oil, 80% yield, 380.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.77 (q, *J* = 1.6 Hz, 1H), 4.86 – 4.83 (m, 1H), 4.41 (d, *J* = 1.6 Hz, 2H), 4.09 (q, *J* = 7.2 Hz, 2H), 3.97 – 3.94 (m, 2H), 3.86 – 3.83 (m, 2H), 3.72 (s, 2H), 2.42 (s, 3H), 2.15 – 2.08 (m, 2H), 2.02 (d, *J* = 1.6 Hz, 3H), 1.69 (dt, *J* = 8.0, 2.4 Hz, 2H), 1.41 – 1.30 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.2, 166.0, 156.4, 143.3, 136.0, 129.6, 127.5, 118.3, 104.5, 104.0, 101.9, 79.7, 64.9, 64.8, 59.7, 53.4, 49.3, 33.8, 31.9, 24.9, 24.0, 22.6, 21.5, 14.2, 7.0. IR (neat) ν 661, 1043, 1221, 1651, 1712, 2024, 2949 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{33}NO_4SNa$ $(M+Na)^+$: 498.1921, Found: 498.1920.

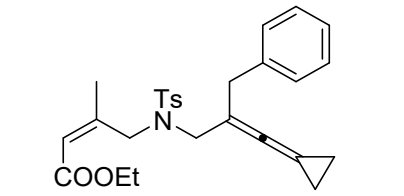



188.217
165.965
156.378
143.277
135.969
129.622
127.473
118.261
104.505
104.029
101.918
79.673
77.344 CDCl3
76.708 CDCl3
64.862
64.846
59.743
53.414
49.283
33.824
31.934
24.909
24.018
22.618
21.503
14.239
7.026
O
O
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

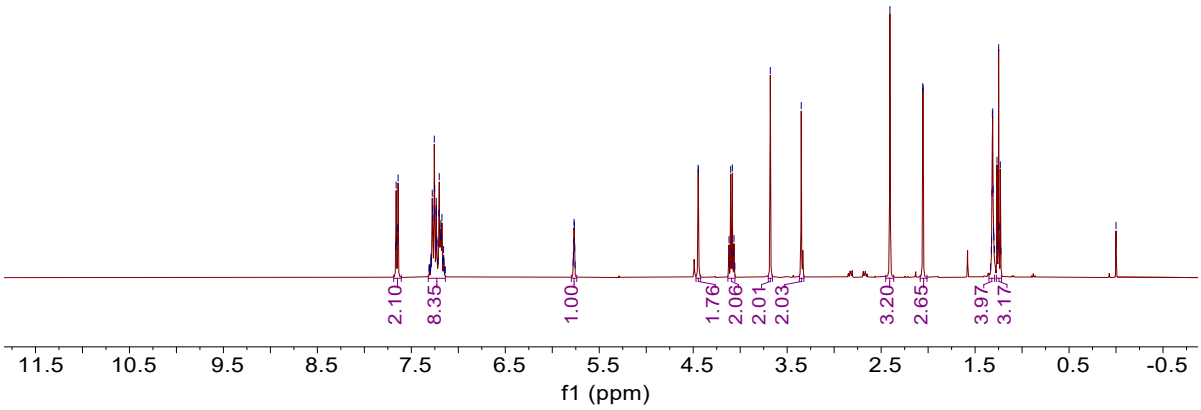


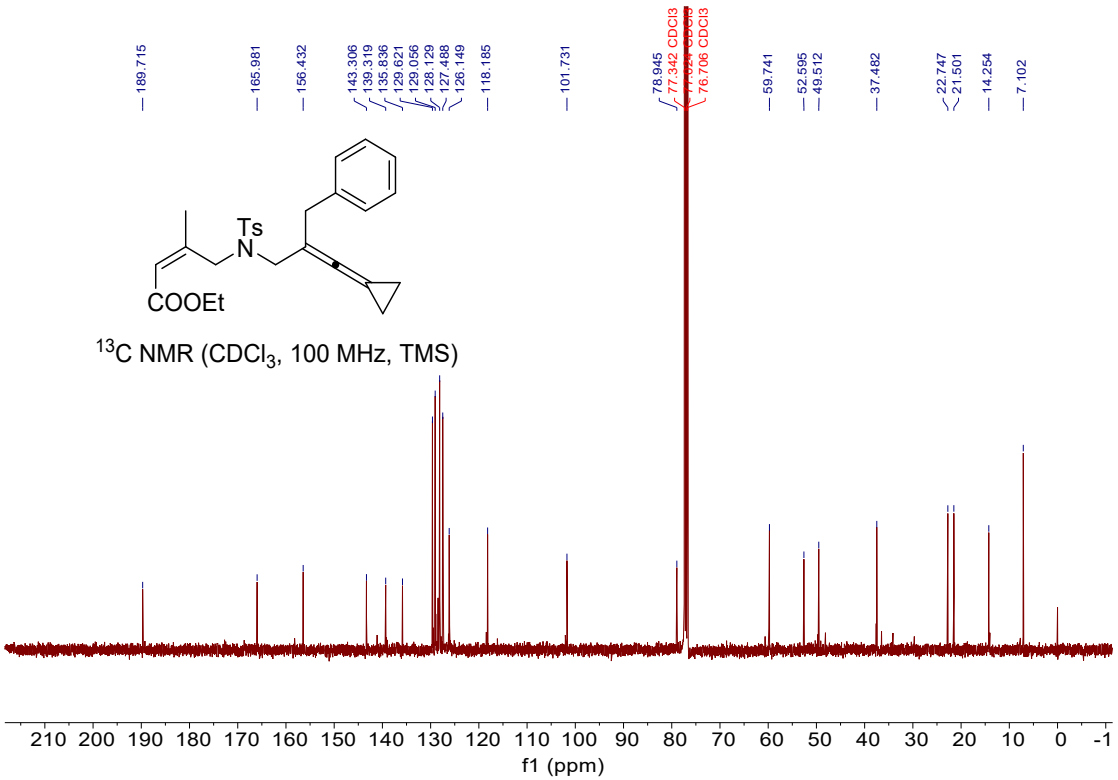
ethyl (Z)-4-((N-(2-benzyl-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3h)

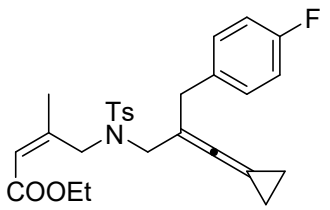
A colorless oil, 90% yield, 418.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.61 (m, 2H), 7.32 – 7.14 (m, 8H), 5.80 – 5.74 (m, 1H), 4.45 (d, *J* = 1.6 Hz, 2H), 4.13 – 4.06 (m, 2H), 3.68 (s, 2H), 3.35 (s, 2H), 2.41 (s, 3H), 2.06 (d, *J* = 1.4 Hz, 3H), 1.31 (q, *J* = 1.6 Hz, 4H), 1.25 (td, *J* = 7.2, 2.4 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 166.0, 156.4, 143.3, 139.3, 135.8, 129.6, 129.1, 128.1, 127.5, 126.1, 118.2, 101.7, 78.9, 59.7, 52.6, 49.5, 37.5, 22.7, 21.5, 14.3, 7.1. IR (neat) ν 662, 1116, 1446, 1649, 1710, 2018, 2924 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{31}NO_4SNa$ $(M+Na)^+$: 488.1866, Found: 488.1861.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

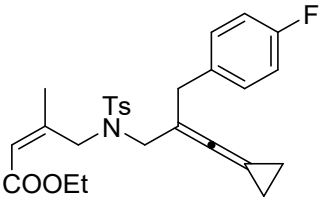



189.715
165.981
156.432
143.306
139.319
135.836
129.621
129.056
128.129
127.488
126.149
118.185
101.731
78.945
77.342 CDCl3
76.706 CDCl3
59.741
52.595
49.512
37.482
22.747
21.501
14.254
7.102
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

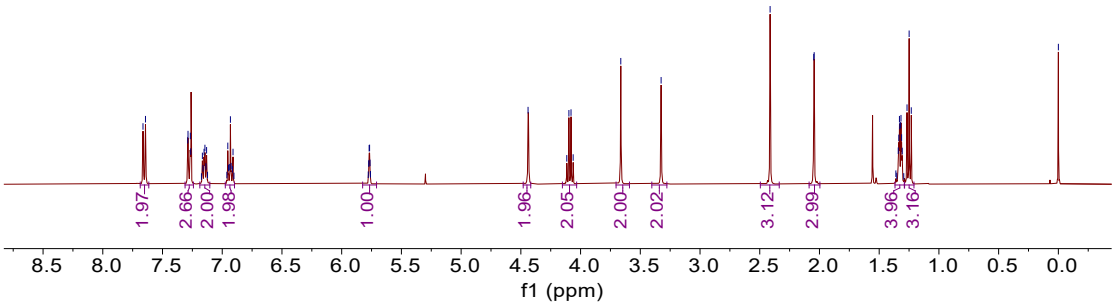


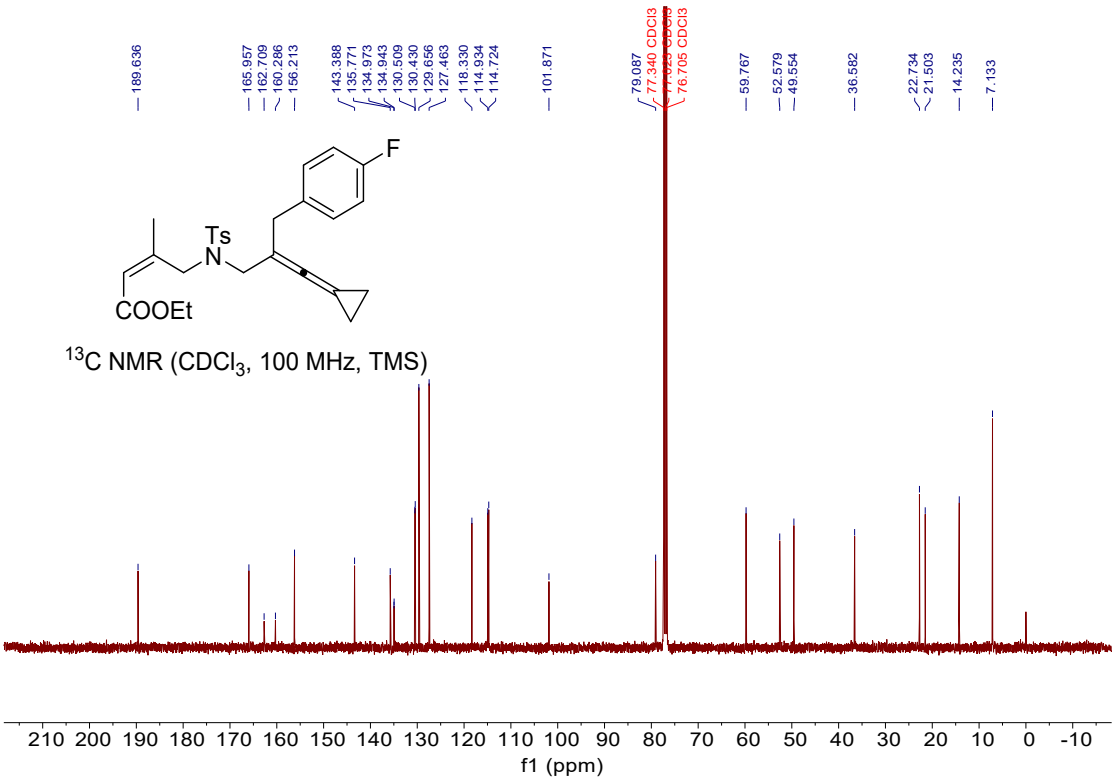
ethyl (Z)-4-((N-(3-cyclopropylidene-2-(4-fluorobenzyl)- λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3i)

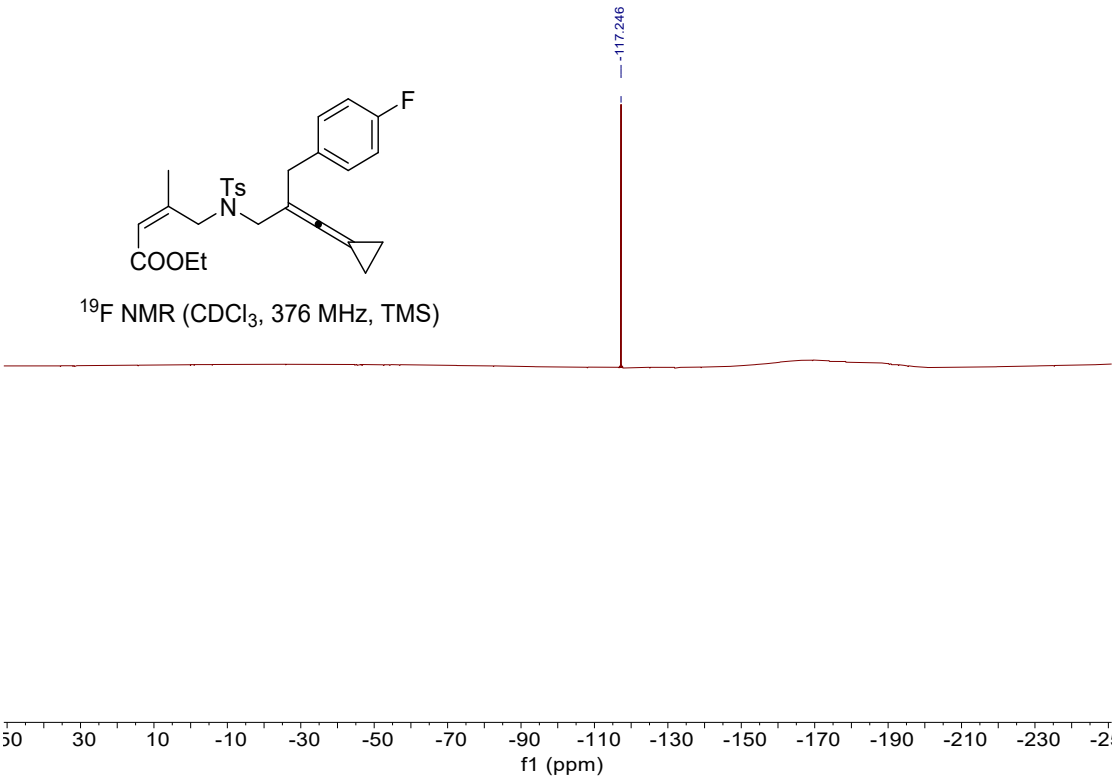
A colorless oil, 70% yield, 338.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.0 Hz, 2H), 7.31 – 7.24 (m, 2H), 7.19 – 7.10 (m, 2H), 6.97 – 6.90 (m, 2H), 5.77 (h, J = 1.6 Hz, 1H), 4.44 (s, 2H), 4.09 (q, J = 7.2 Hz, 2H), 3.66 (s, 2H), 3.33 (s, 2H), 2.41 (s, 3H), 2.05 (d, J = 1.6 Hz, 3H), 1.37 – 1.29 (m, 4H), 1.25 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.6, 166.0, 161.5 (d, $J_{C\text{-}F}$ = 242.3 Hz), 156.2, 143.4, 135.8, 135.0, 134.9, 130.5 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.7, 127.5, 118.3, 114.8 (d, $J_{C\text{-}F}$ = 2.1 Hz), 101.9, 79.1, 59.8, 52.6, 49.6, 36.6, 22.7, 21.5, 14.2, 7.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.25. IR (neat) ν 660, 1049, 1221, 1651, 1712, 2023, 2983 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{30}NO_4FSNa$ $(M+Na)^+$: 506.1772, Found: 506.1764.

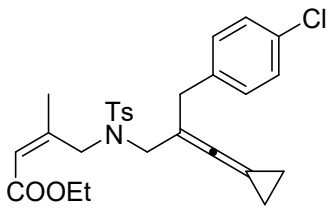


^{1}H NMR ($CDCl_3$, 400 MHz, TMS)



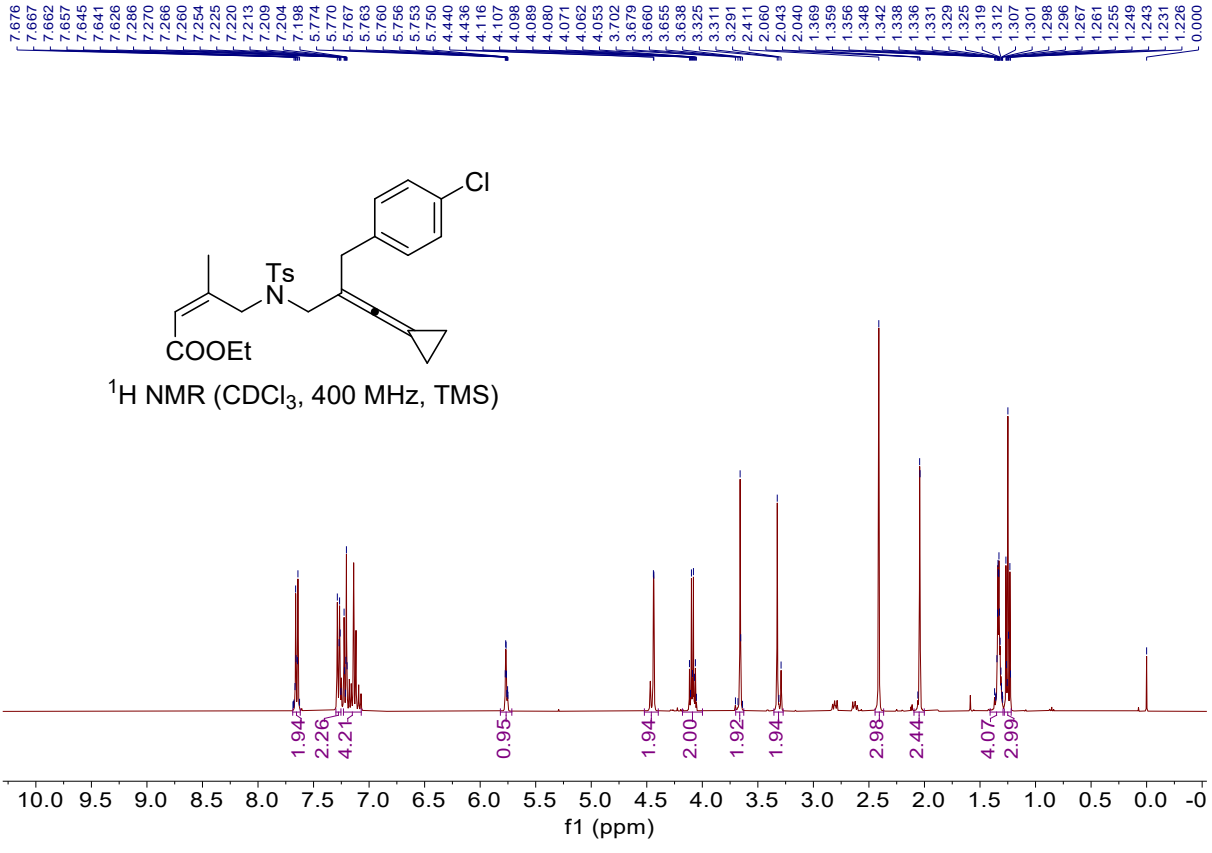

189.636
165.957
162.709
160.286
156.213
143.388
135.771
134.973
134.943
130.509
130.430
129.656
127.463
118.330
114.934
114.724
101.871
79.087
77.340 CDCl3
76.705 CDCl3
59.767
52.579
49.554
36.582
22.734
21.503
14.235
7.133
F
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

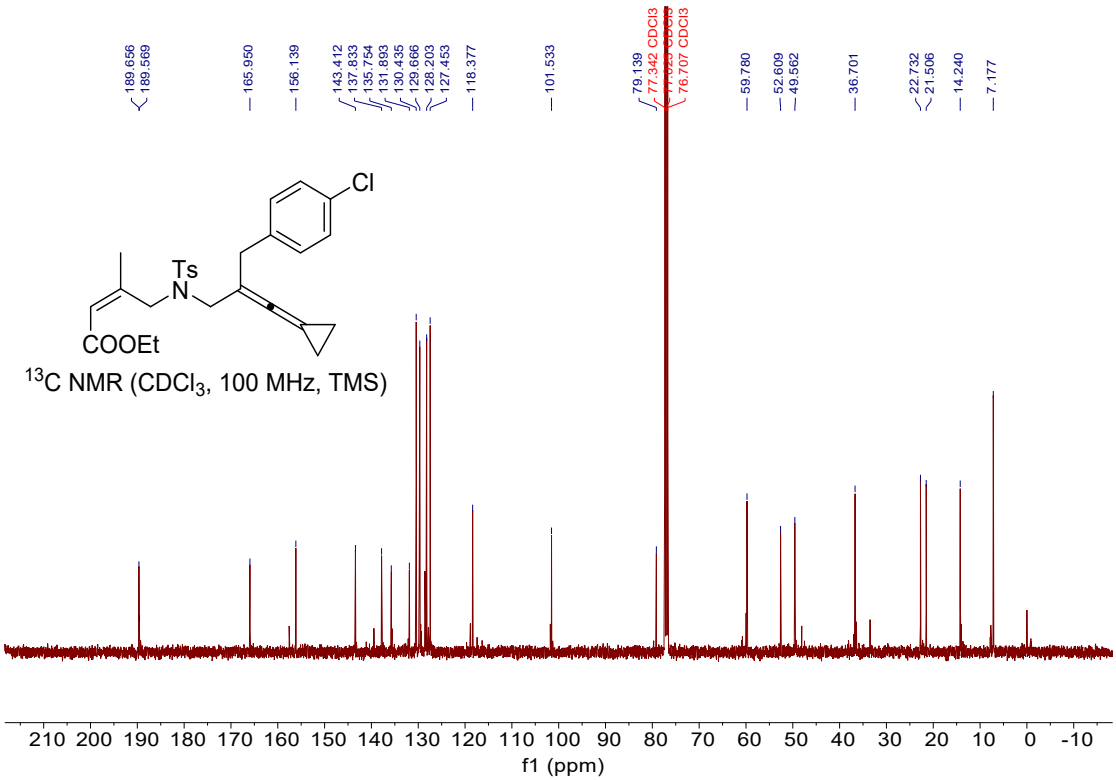

-117.246
F
Ts
N
COOEt
19F NMR (CDCl3, 376 MHz, TMS)
50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

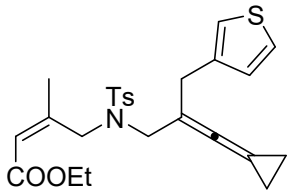


ethyl (Z)-4-((N-(2-(4-chlorobenzyl)-3-cyclopropylidene-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3j)

A yellow oil, 80% yield, 400.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.62 (m, 2H), 7.30 – 7.25 (m, 2H), 7.23 – 7.07 (m, 4H), 5.82 – 5.71 (m, 1H), 4.44 (d, *J* = 1.6 Hz, 2H), 4.18 – 4.00 (m, 2H), 3.66 (d, *J* = 2.1 Hz, 2H), 3.31 (d, *J* = 13.7 Hz, 2H), 2.41 (s, 3H), 2.04 (d, *J* = 1.4 Hz, 2H), 1.41 – 1.29 (m, 4H), 1.28 – 1.22 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 189.6, 166.0, 156.1, 143.4, 137.8, 135.8, 131.9, 130.4, 129.7, 128.2, 127.5, 118.4, 101.5, 79.1, 59.8, 52.6, 49.6, 36.7, 22.7, 21.5, 14.2, 7.2. IR (neat) ν 670, 1221, 1658, 1712, 2016, 2953 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{30}NO_4SClNa$ $(M+Na)^+$: 522.1476, Found: 522.1479.

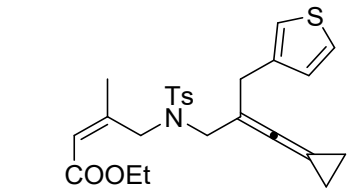



189.656
189.569
165.950
156.139
143.412
137.833
135.754
131.893
130.435
129.666
128.203
127.453
118.377
101.533
79.139
77.342 CDCl3
76.707 CDCl3
59.780
52.609
49.562
36.701
22.732
21.506
14.240
7.177
Cl
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

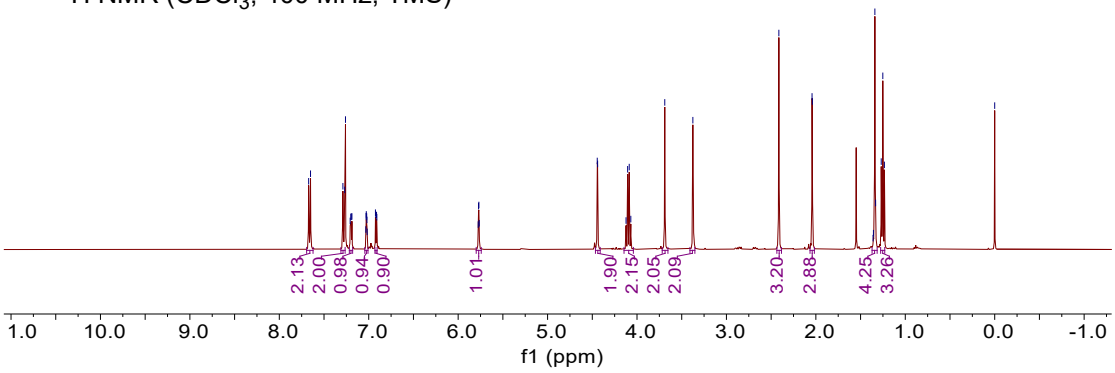


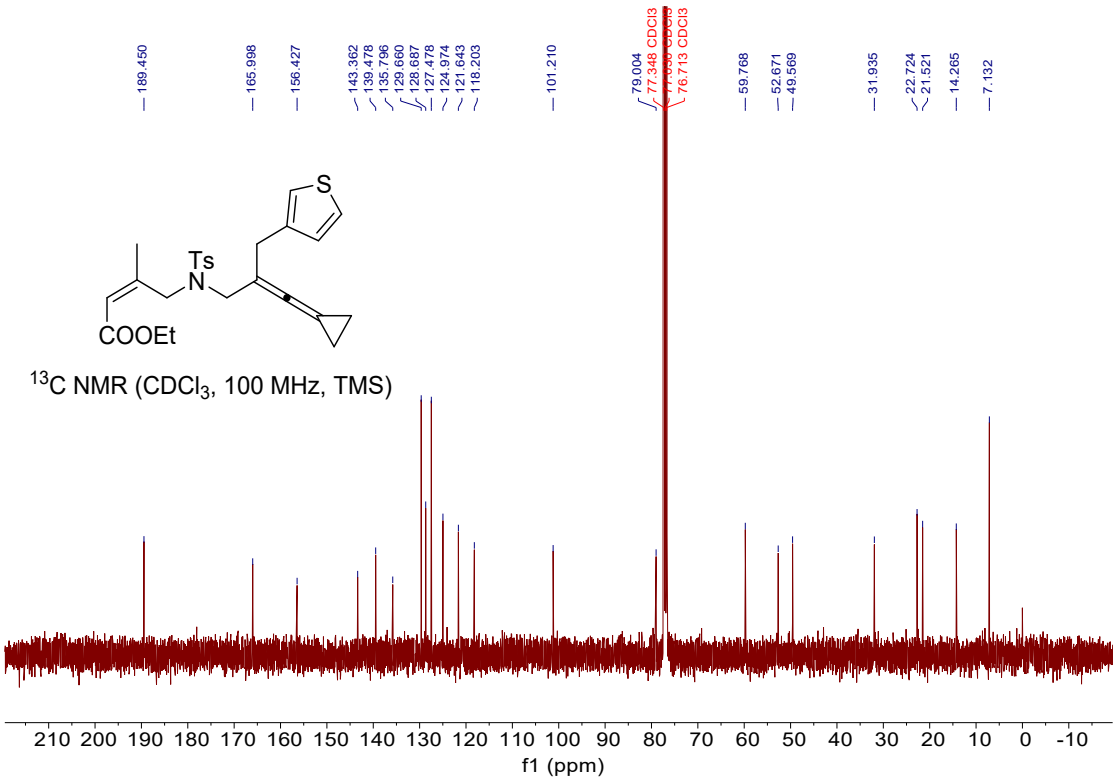
ethyl (Z)-4-((N-(3-cyclopropylidene-2-(thiophen-3-ylmethyl)-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-methylbut-2-enoate (3k)

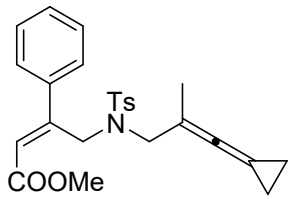
A colorless oil, 82% yield, 378.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.20 (dd, *J* = 4.8, 2.8 Hz, 1H), 7.02 (dd, *J* = 2.8, 1.2 Hz, 1H), 6.92 (dd, *J* = 4.8, 1.2 Hz, 1H), 5.77 (q, *J* = 1.6 Hz, 1H), 4.44 (d, *J* = 1.6 Hz, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.69 (s, 2H), 3.38 (s, 2H), 2.41 (s, 3H), 2.04 (d, *J* = 1.6 Hz, 3H), 1.37 – 1.31 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.5, 166.0, 156.4, 143.4, 139.5, 135.8, 129.7, 128.7, 127.5, 125.0, 121.6, 118.2, 101.2, 79.0, 59.8, 52.7, 49.6, 31.9, 22.7, 21.5, 14.3, 7.1. IR (neat) ν 731, 1346, 1651, 1712, 2022, 2926 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{29}NO_4S_2Na$ $(M+Na)^+$: 494.1430, Found: 494.1428.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

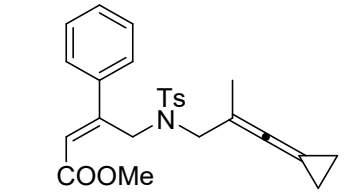



189.450
165.998
156.427
143.362
139.478
135.796
129.660
128.687
127.478
124.974
121.643
118.203
101.210
79.004
77.348 CDCl3
76.713 CDCl3
59.768
52.671
49.569
31.935
22.724
21.521
14.265
7.132
S
Ts
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

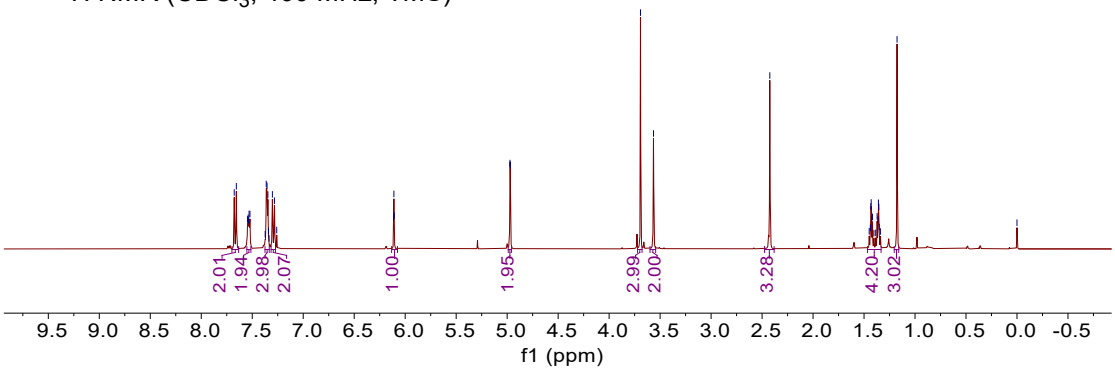


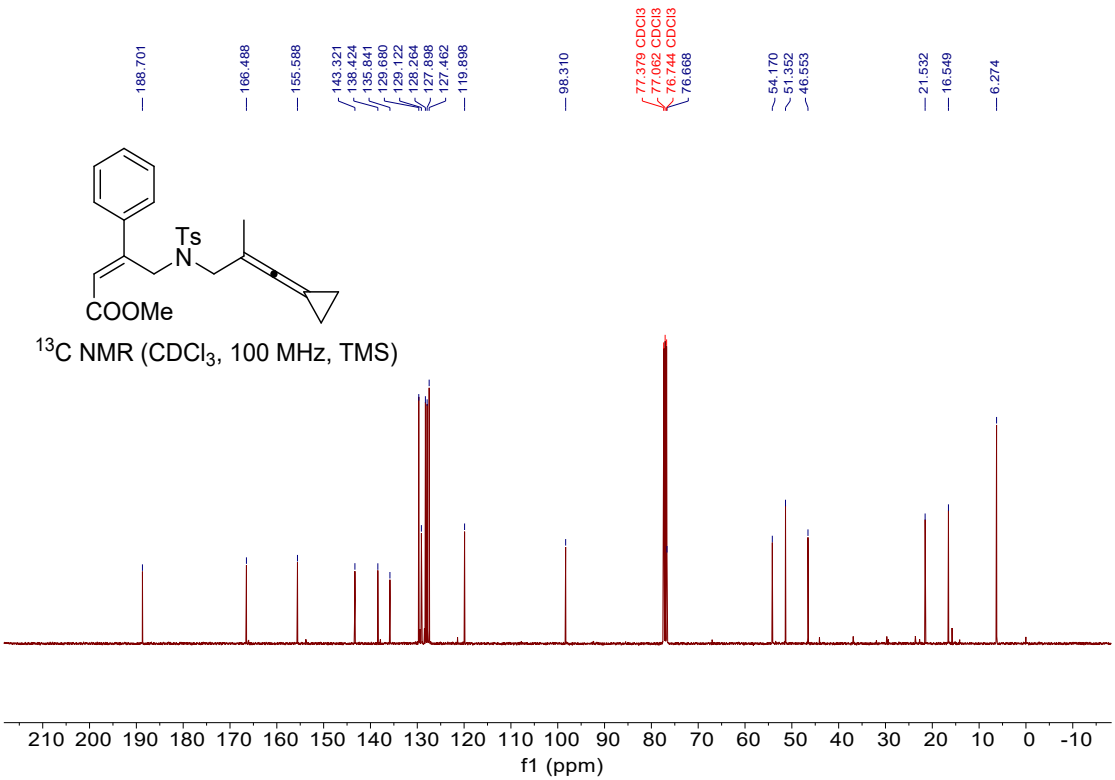
methyl (Z)-4-((N-(3-cyclopropylidene-2-methyl-λ^5-allyl)-4-methylphenyl)sulfonamido)-3-phenylbut-2-enoate (3l)

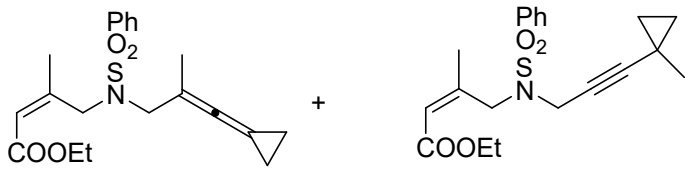
A colorless oil, 80% yield, 368.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 2H), 7.55 – 7.51 (m, 2H), 7.37 – 7.33 (m, 3H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.11 (d, *J* = 1.2 Hz, 1H), 4.97 (d, *J* = 1.2 Hz, 2H), 3.69 (s, 3H), 3.56 (s, 2H), 2.42 (s, 3H), 1.47 – 1.33 (m, 4H), 1.18 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.7, 166.5, 155.6, 143.3, 138.4, 135.8, 129.7, 129.1, 128.3, 127.9, 127.5, 119.9, 98.3, 76.7, 54.2, 51.4, 46.6, 21.5, 16.5, 6.3. IR (neat) ν 663, 1346, 1629, 1721, 2024, 2949 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{27}NO_4SNa$ $(M+Na)^+$: 460.1553, Found: 460.1554.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

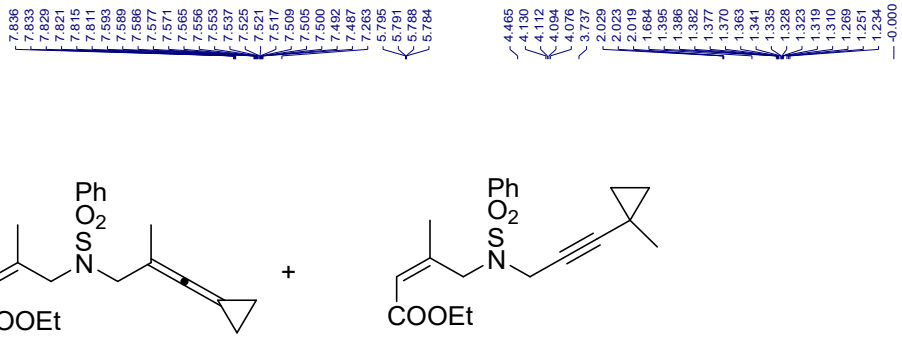


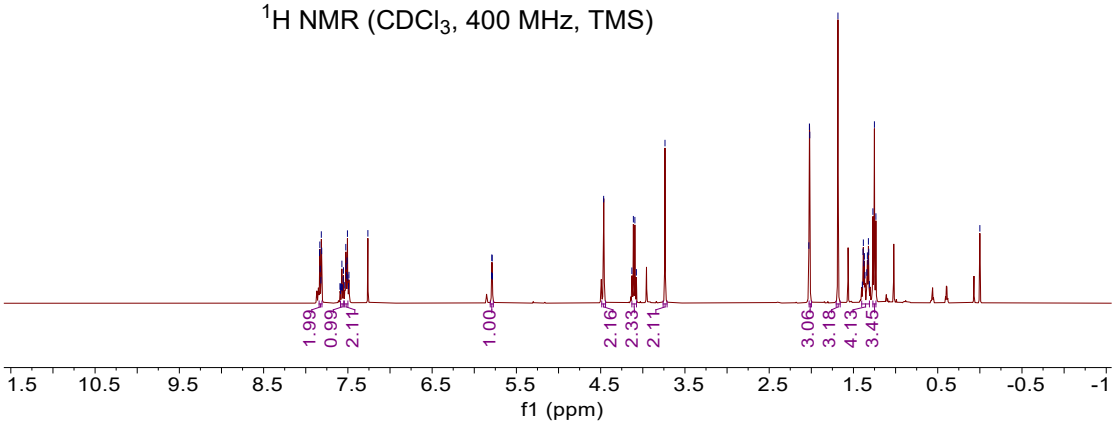

188.701
166.488
155.588
143.321
138.424
135.841
129.680
129.122
128.264
127.898
127.462
119.898
98.310
77.379 CDCl3
77.062 CDCl3
76.744 CDCl3
76.668
54.170
51.352
46.553
21.532
16.549
6.274
Ts
N
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

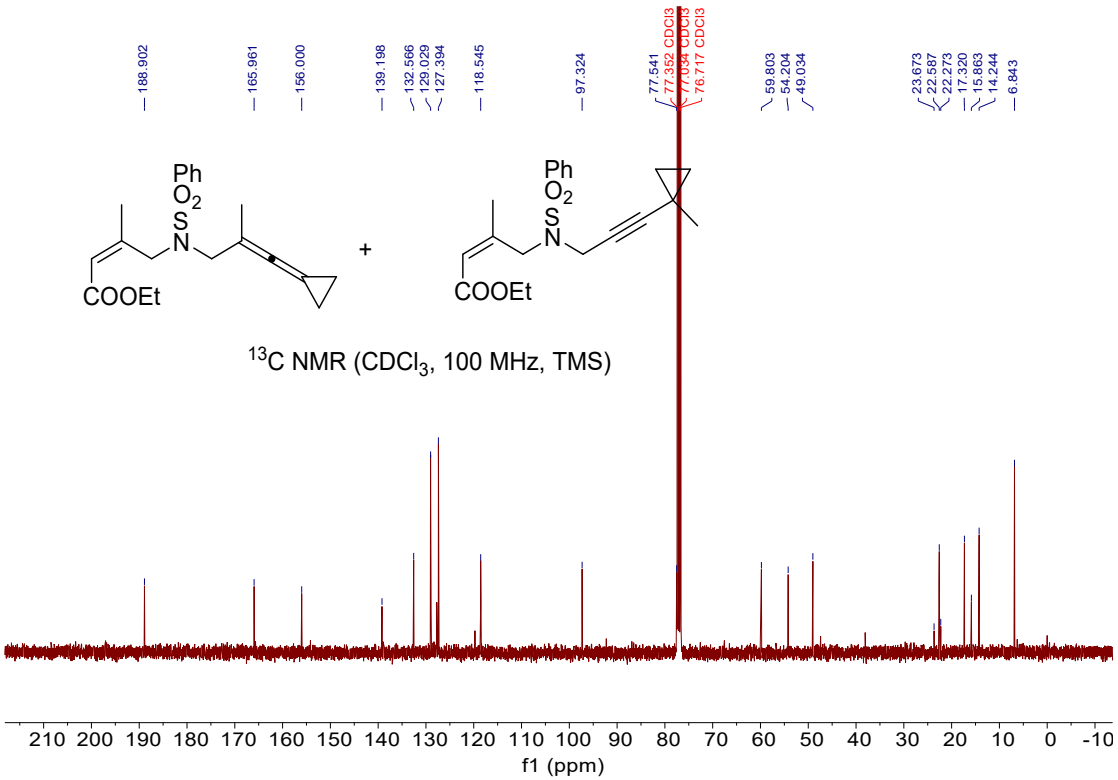


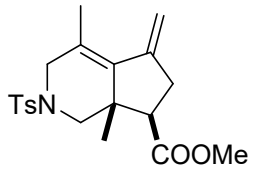
ethyl (Z)-4-(N-(3-cyclopropylidene-2-methyl-λ^5-allyl)phenylsulfonamido)-3-methylbut-2-enoate (3m) + ethyl (Z)-3-methyl-4-(N-(3-(1-methylcyclopropyl)prop-2-yn-1-yl)phenylsulfonamido)but-2-enoate (byproduct 3m') (1m: 1m'=5:1)

A colorless oil, 80% yield, 300.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.81 (m, 2H), 7.59 – 7.55 (m, 1H), 7.54 – 7.50 (m, 2H), 5.79 (q, *J* = 1.6 Hz, 1H), 4.46 (s, 2H), 4.09 (t, *J* = 7.2 Hz, 2H), 3.74 (s, 2H), 2.02 (d, *J* = 1.6 Hz, 3H), 1.68 (s, 3H), 1.40 – 1.31 (m, 4H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 166.0, 156.0, 139.2, 132.6, 129.0, 127.4, 118.5, 97.3, 77.5, 59.8, 54.2, 49.0, 23.7, 22.6, 22.3, 17.3, 15.9, 14.2, 6.8. IR (neat) ν 660, 1344, 1654, 1714, 2025, 2953 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{25}NO_4SNa$ $(M+Na)^+$: 398.1396, Found: 398.1395.



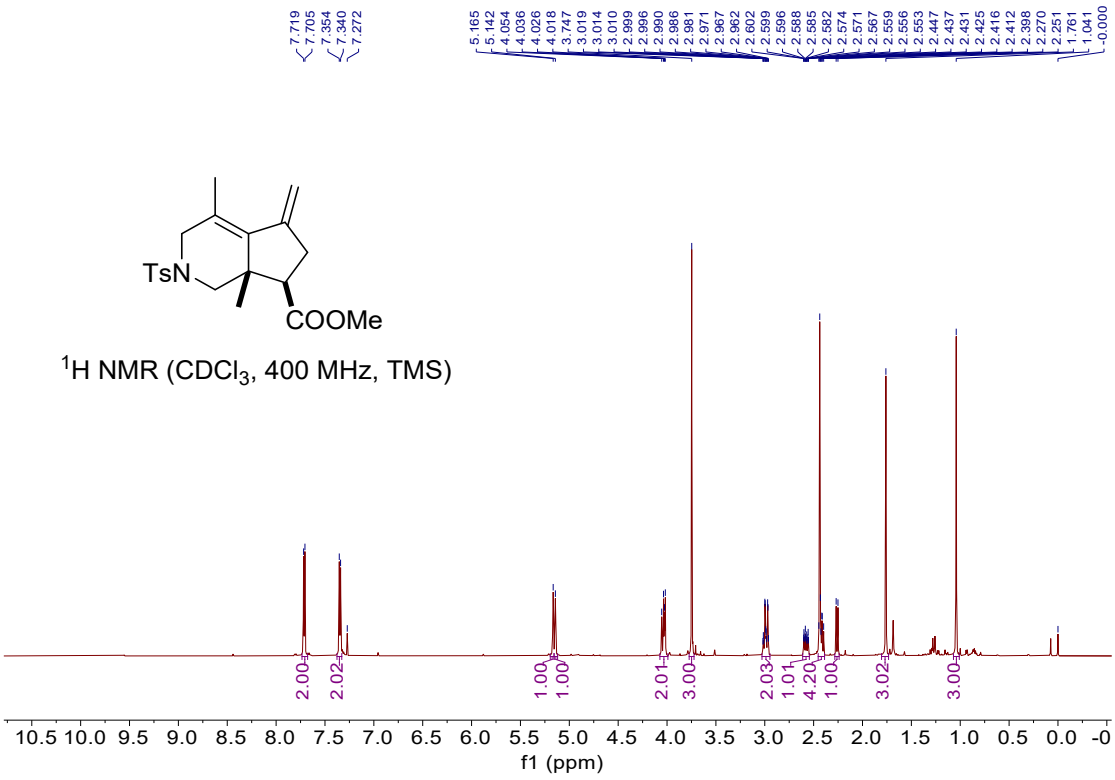


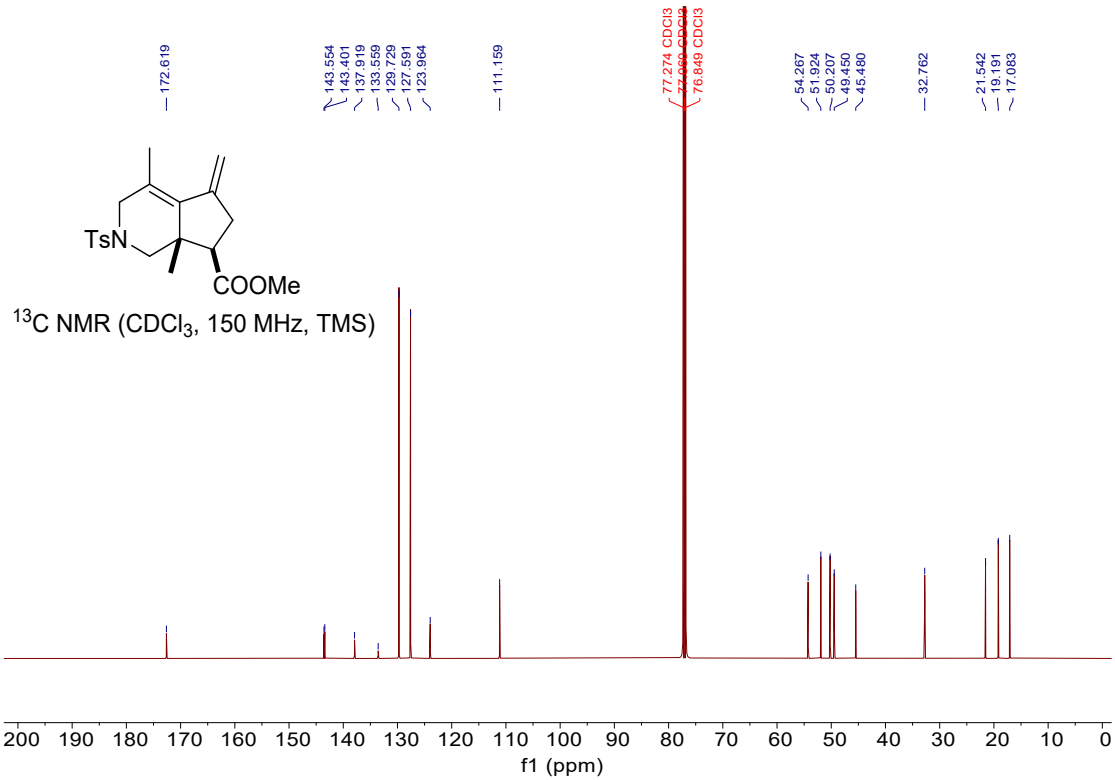

188.902
165.961
156.000
139.198
132.566
129.029
127.394
118.545
97.324
77.541
77.352 CDCl3
77.034 CDCl3
76.717 CDCl3
59.803
54.204
49.034
23.673
22.587
22.273
17.320
15.863
14.244
6.843
Ph
O2
S
N
COOEt
+
Ph
O2
S
N
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

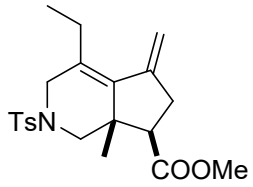


(cis)-methyl-4,7a-dimethyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2a)

A white solid, MP = 121-124 °C, 96% yield, 36.2 mg. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.16 (s, 1H), 5.14 (s, 1H), 4.07 – 3.99 (m, 2H), 3.75 (s, 3H), 3.03 – 2.95 (m, 2H), 2.61 – 2.54 (m, 1H), 2.45 – 2.39 (m, 4H), 2.26 (d, *J* = 11.2 Hz, 1H), 1.76 (s, 3H), 1.04 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.6, 143.6, 143.4, 137.9, 133.6, 129.7, 127.6, 124.0, 111.2, 54.3, 51.9, 50.2, 49.4, 45.5, 32.8, 21.5, 19.2, 17.1. IR (neat) ν 660, 1019, 1220, 1355, 1597, 1709, 2953 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{25}NO_4SNa$ $(M+Na)^+$: 398.1396, Found: 398.1404.

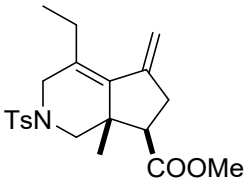



172.619
143.554
143.401
137.919
133.559
129.729
127.591
123.964
111.159
77.274 CDCl3
77.060 CDCl3
76.849 CDCl3
54.267
51.924
50.207
49.450
45.480
32.762
21.542
19.191
17.083
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

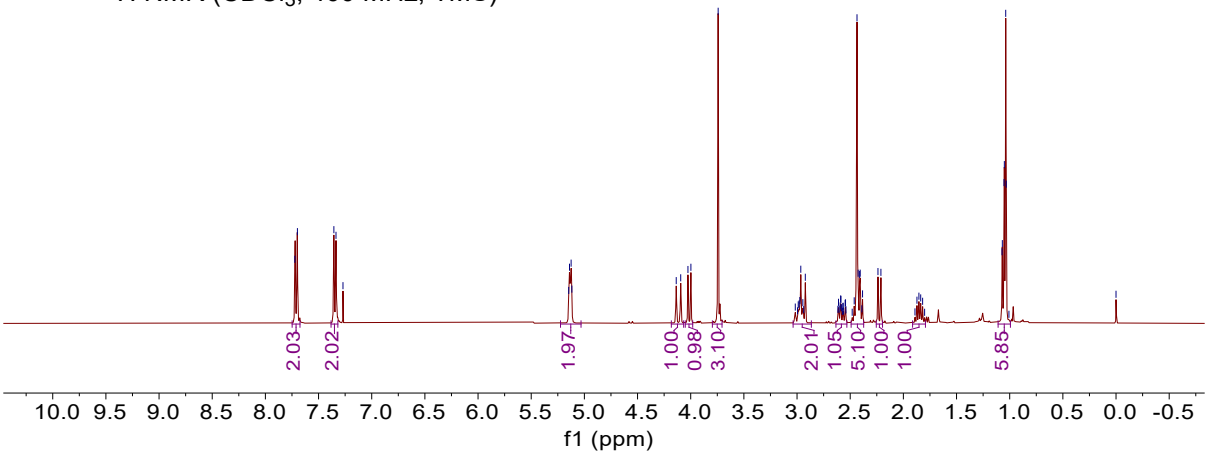


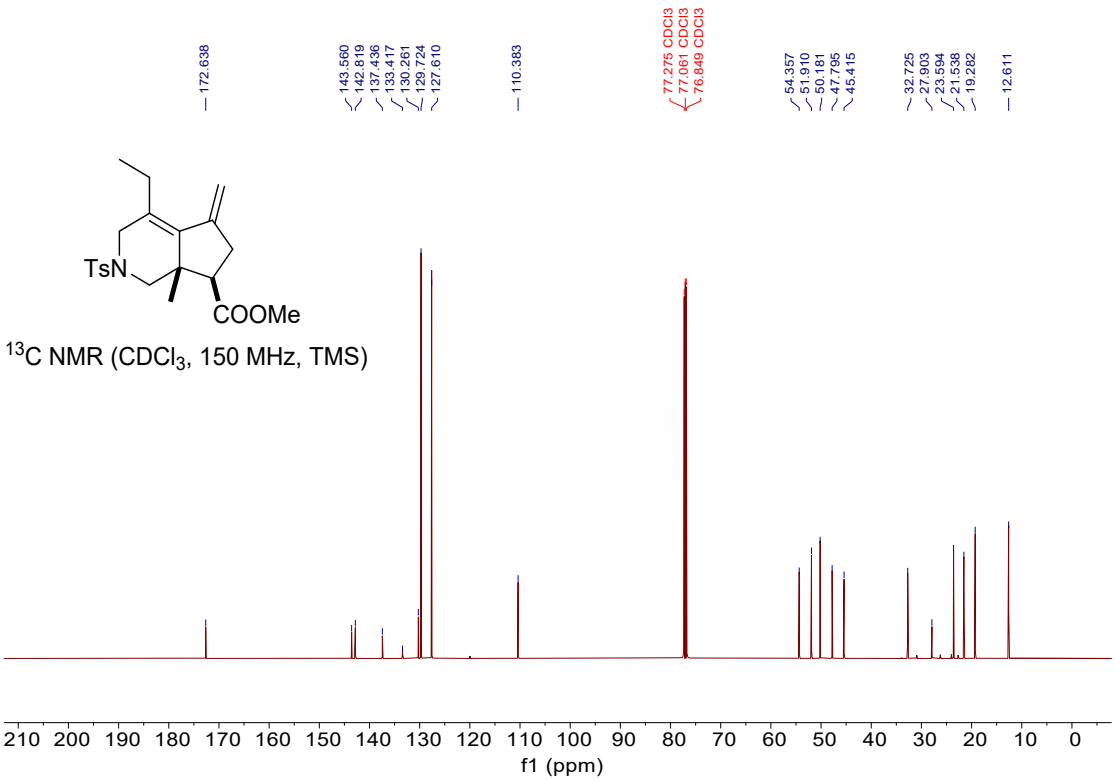
(cis)-methyl-4-ethyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2b)

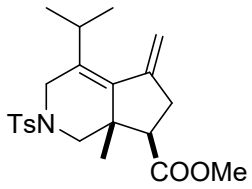
A colorless oil, 94% yield, 36.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.22 – 5.03 (m, 2H), 4.12 (d, *J* = 16.8 Hz, 1H), 4.01 (d, *J* = 11.2 Hz, 1H), 3.74 (s, 3H), 3.04 – 2.87 (m, 2H), 2.63 – 2.53 (m, 1H), 2.49 – 2.37 (m, 5H), 2.23 (d, *J* = 11.2 Hz, 1H), 1.91 – 1.79 (m, 1H), 1.11 – 0.99 (m, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.6, 143.6, 142.8, 137.4, 133.4, 130.3, 129.7, 127.6, 110.4, 54.4, 51.9, 50.2, 47.8, 45.4, 32.7, 27.9, 23.6, 21.5, 19.3, 12.6. IR (neat) ν 662, 1348, 1597, 1736, 2962 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{28}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1541.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

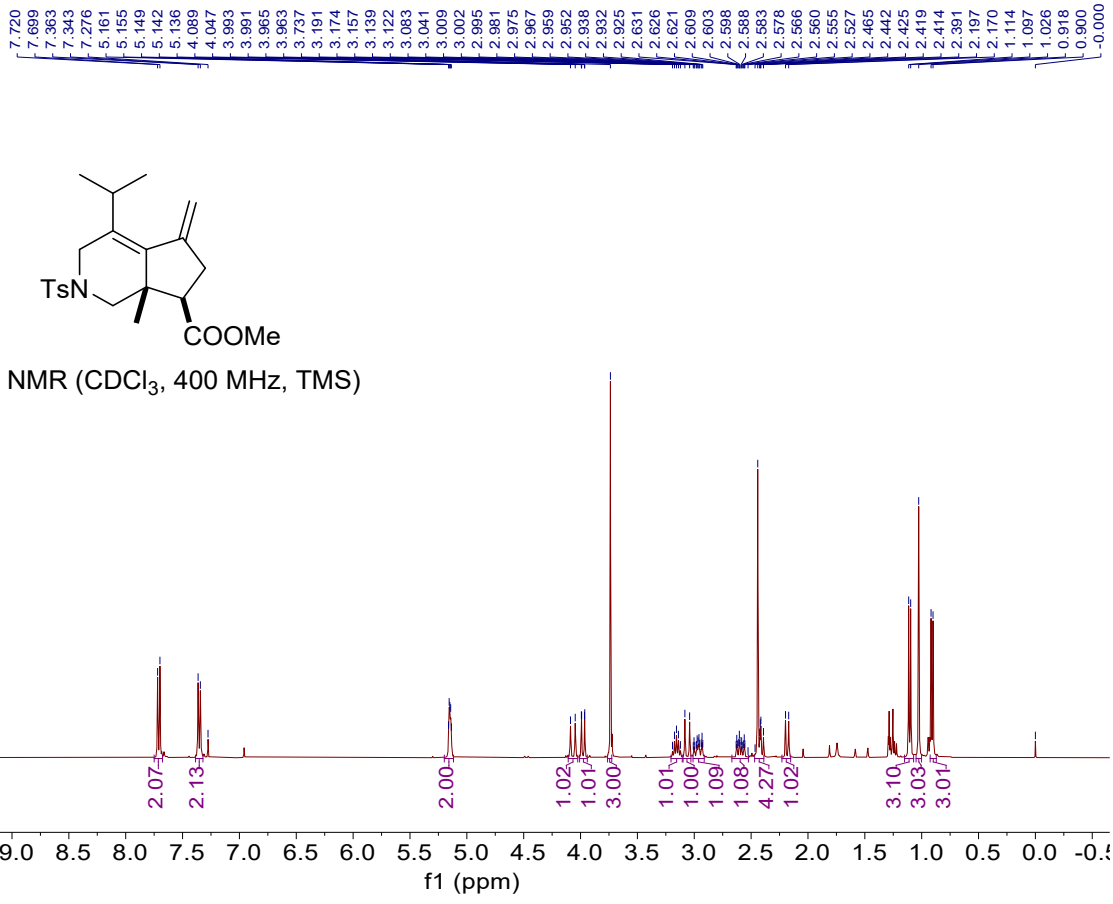


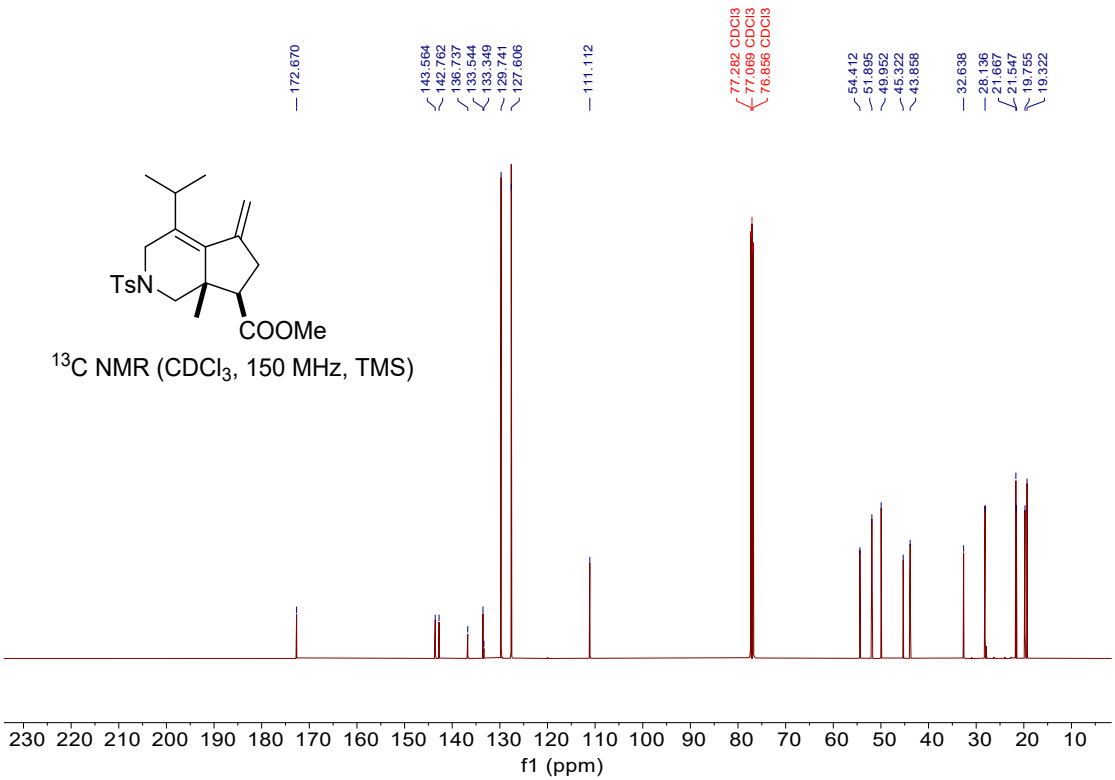

172.638
143.560
142.819
137.436
133.417
130.261
129.724
127.610
110.383
77.275 CDCl3
77.061 CDCl3
76.849 CDCl3
54.357
51.910
50.181
47.795
45.415
32.725
27.903
23.594
21.538
19.282
12.611
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

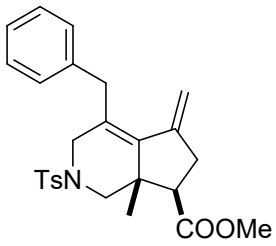


(cis)-methyl-4-isopropyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2c)

A colorless oil, MP = 119-122 ºC, 92% yield, 37.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.20 – 5.12 (m, 2H), 4.07 (d, *J* = 16.8 Hz, 1H), 3.98 (dd, *J* = 11.2, 0.8 Hz, 1H), 3.74 (s, 3H), 3.16 (p, *J* = 7.2 Hz, 1H), 3.06 (d, *J* = 16.8 Hz, 1H), 2.97 (ddt, *J* = 16.8, 11.2, 2.4 Hz, 1H), 2.59 (ddt, *J* = 17.4, 9.2, 2.4 Hz, 1H), 2.47 – 2.39 (m, 4H), 2.18 (d, *J* = 11.2 Hz, 1H), 1.11 (d, *J* = 7.2 Hz, 3H), 1.03 (s, 3H), 0.91 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.7, 143.6, 142.8, 136.7, 133.5, 133.3, 129.7, 127.6, 111.1, 0 54.4, 51.9, 50.0, 45.3, 43.9, 32.6, 28.1, 21.7, 21.5, 19.8, 19.3. IR (neat) ν 662, 1216, 1350, 1651, 1736, 2953 cm^{-1}. HRMS (ESI) calcd. for $C_{22}H_{29}NO_4SNa$ $(M+Na)^+$: 426.1710, Found: 426.1706.

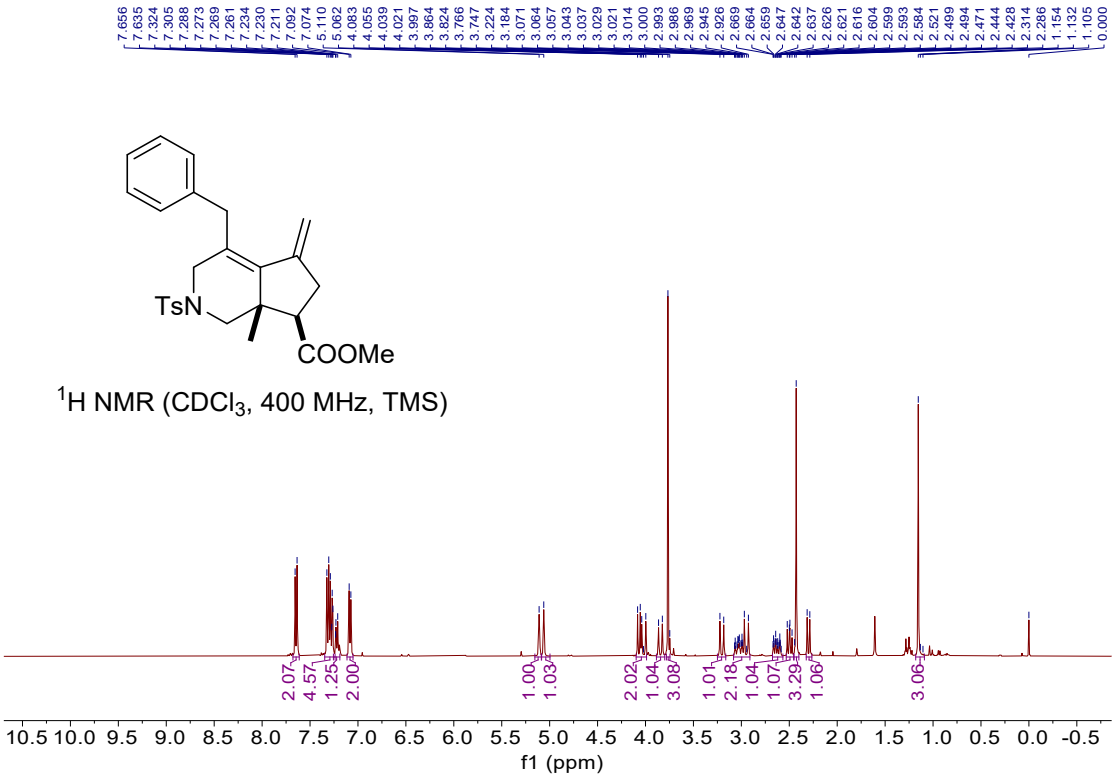


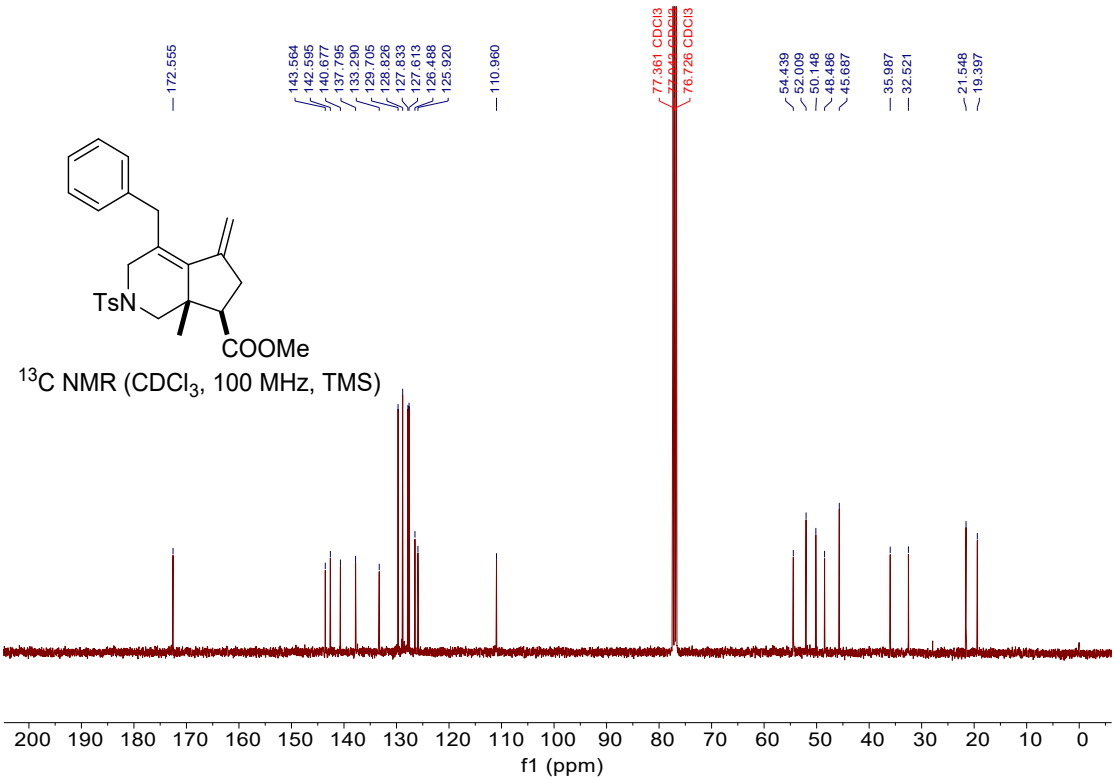

172.670
143.564
142.762
136.737
133.544
133.349
129.741
127.606
111.112
77.282 CDCl3
77.069 CDCl3
76.856 CDCl3
54.412
51.895
49.952
45.322
43.858
32.638
28.136
21.667
21.547
19.755
19.322
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

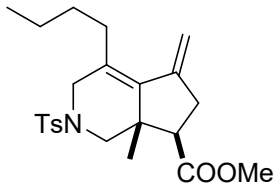


(cis)-methyl-4-benzyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2d)

A colorless oil, 94% yield, 42.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.35 – 7.24 (m, 4H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.08 (d, *J* = 7.2 Hz, 2H), 5.11 (s, 1H), 5.06 (s, 1H), 4.10 – 3.99 (m, 2H), 3.84 (d, *J* = 16.0 Hz, 1H), 3.77 (s, 3H), 3.20 (d, *J* = 16.0 Hz, 1H), 3.08 – 2.91 (m, 2H), 2.63 (ddt, *J* = 17.2, 8.8, 2.0 Hz, 1H), 2.50 (dd, *J* = 11.2, 8.8 Hz, 1H), 2.43 (s, 3H), 2.30 (d, *J* = 11.2 Hz, 1H), 1.15 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 143.6, 142.6, 140.7, 137.8, 133.3, 129.7, 128.8, 127.8, 127.6, 126.5, 125.9, 111.0, 54.4, 52.0, 50.1, 48.5, 45.7, 36.0, 32.5, 21.5, 19.4. IR (neat) ν 659, 1091, 1349, 1654, 1736, 2929 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1714.

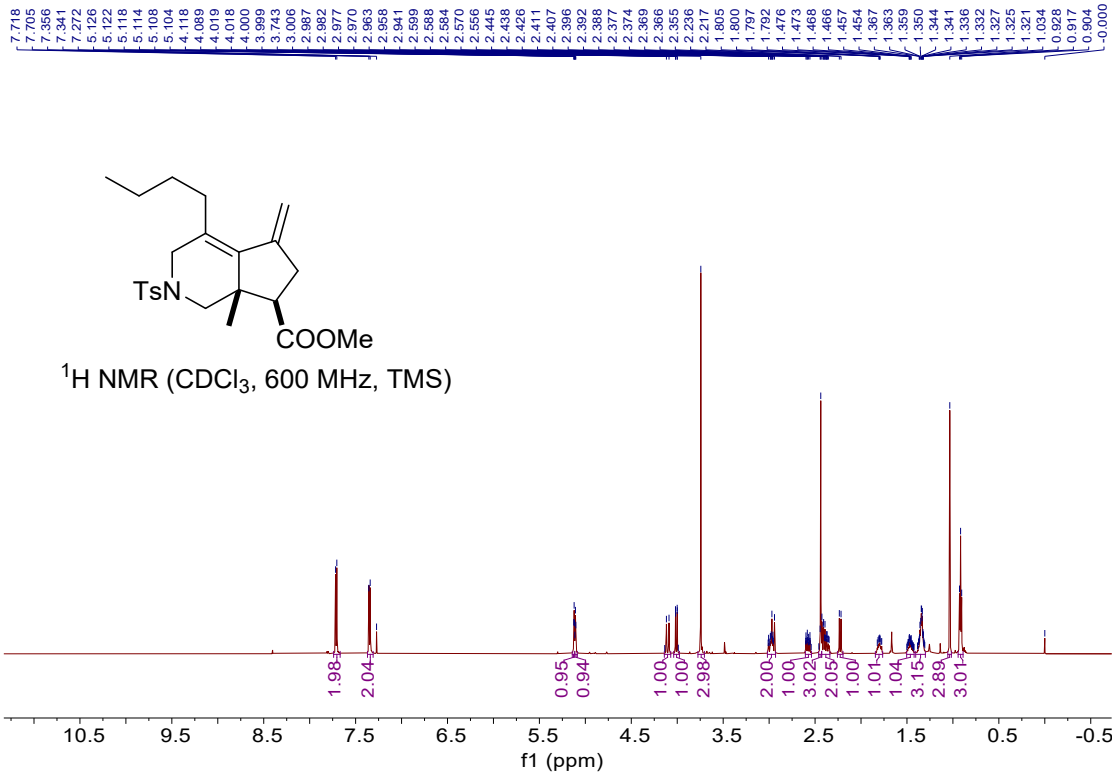


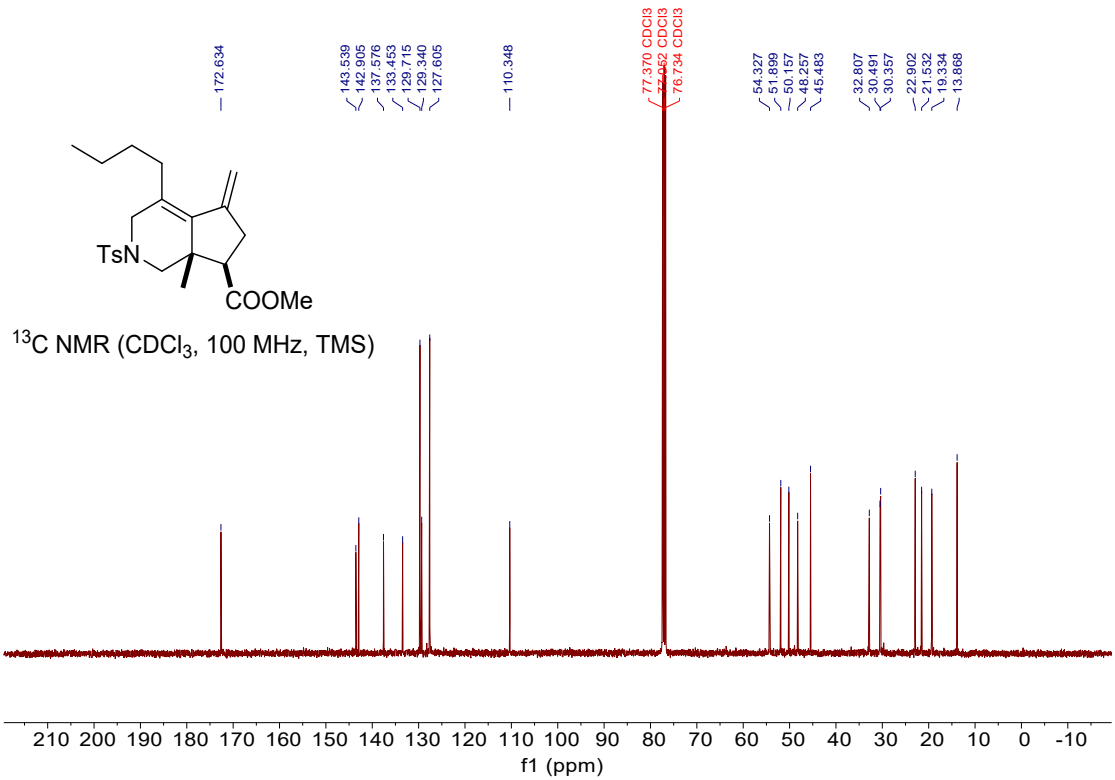

172.555
143.564
142.595
140.677
137.795
133.290
129.705
128.826
127.833
127.613
126.488
125.920
110.960
77.361 CDCl3
77.043 CDCl3
76.726 CDCl3
54.439
52.009
50.148
48.486
45.687
35.987
32.521
21.548
19.397
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

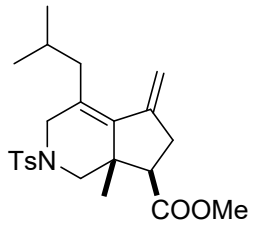


(cis)-methyl-4-butyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2e)

A colorless oil, 92% yield, 38.4 mg. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 5.12 (d, *J* = 2.4 Hz, 1H), 5.11 (d, *J* = 2.4 Hz, 1H), 4.10 (d, *J* = 16.8 Hz, 1H), 4.04 – 3.98 (m, 1H), 3.74 (s, 3H), 3.02 – 2.93 (m, 2H), 2.61 – 2.54 (m, 1H), 2.44 (s, 3H), 2.43 – 2.34 (m, 2H), 2.23 (d, *J* = 11.2 Hz, 1H), 1.84 – 1.76 (m, 1H), 1.50 – 1.42 (m, 1H), 1.40 – 1.30 (m, 3H), 1.03 (s, 3H), 0.92 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 143.5, 142.9, 137.6, 133.5, 129.7, 129.3, 127.6, 110.3, 54.3, 51.9, 50.2, 48.3, 45.5, 32.8, 30.5, 30.4, 22.9, 21.5, 19.3, 13.9. IR (neat) ν 662, 1091, 1356, 1651, 1736, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{31}NO_4SNa$ $(M+Na)^+$: 440.18666, Found: 440.1863.

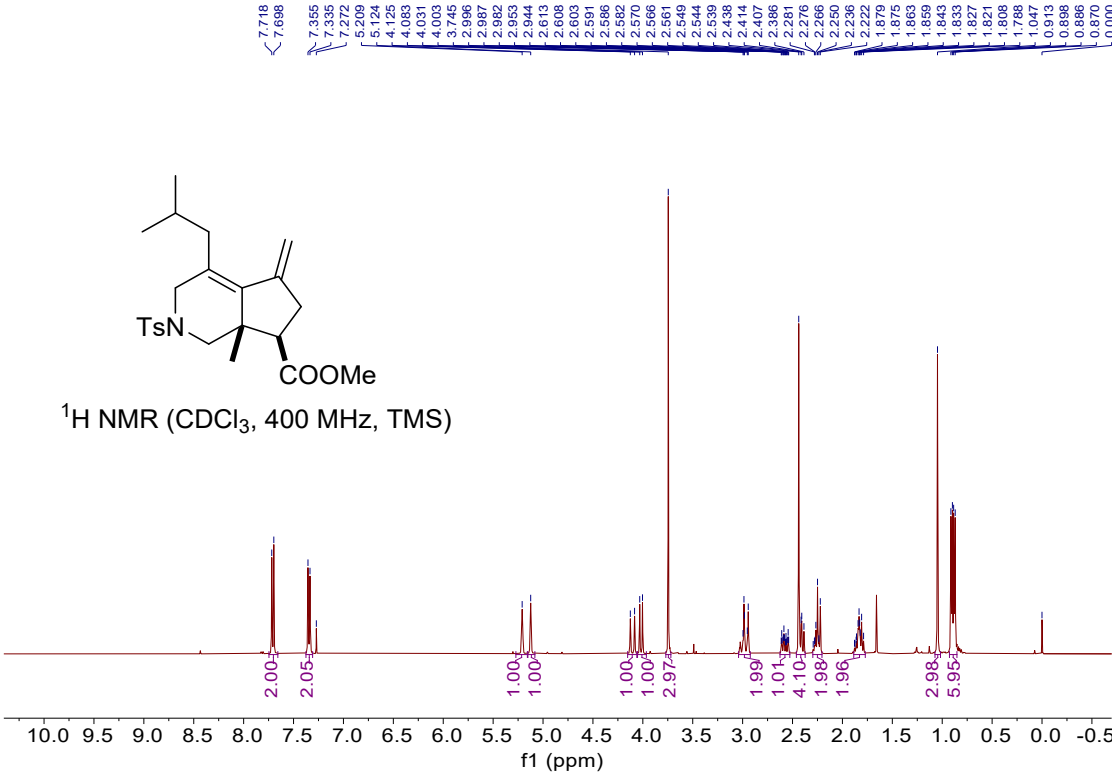


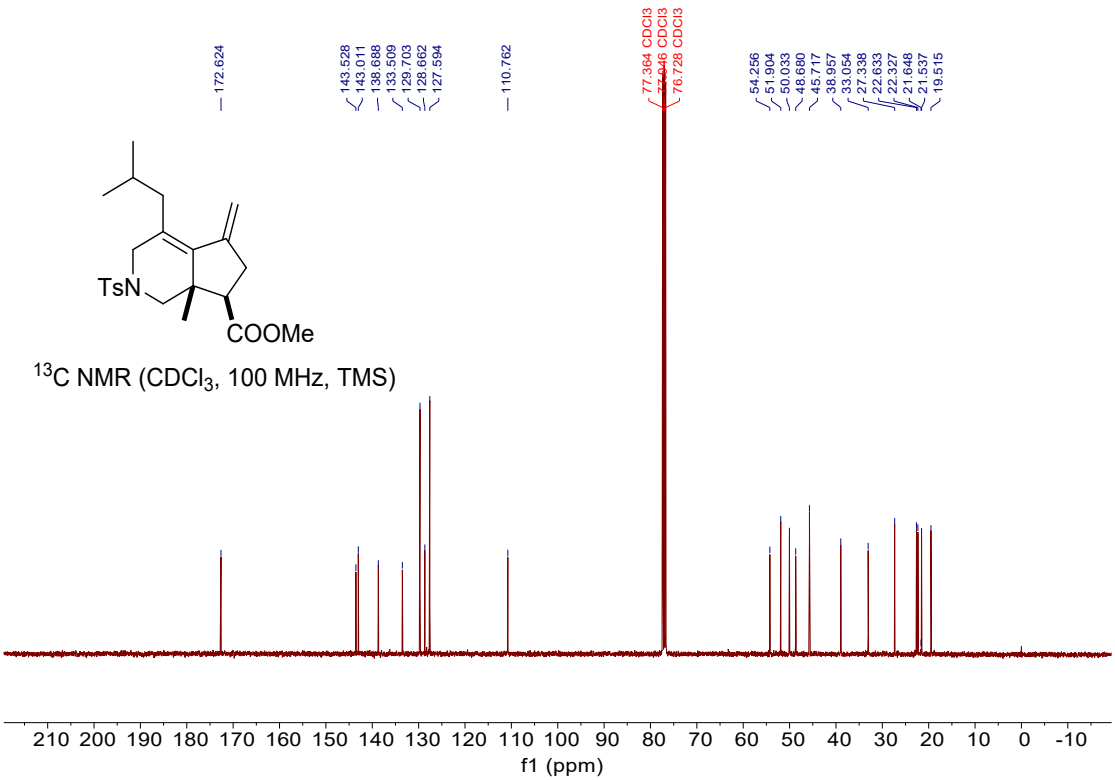

172.634
143.539
142.905
137.576
133.453
129.715
129.340
127.605
110.348
77.370 CDCl3
77.052 CDCl3
76.734 CDCl3
54.327
51.899
50.157
48.257
45.483
32.807
30.491
30.357
22.902
21.532
19.334
13.868
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

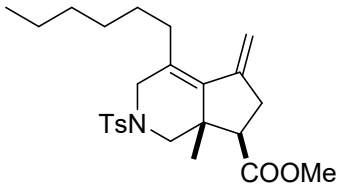


(cis)-methyl-4-isobutyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2f)

A colorless oil, 90% yield, 37.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.21 (s, 1H), 5.12 (s, 1H), 4.10 (d, *J* = 17.2 Hz, 1H), 4.02 (d, *J* = 11.2 Hz, 1H), 3.75 (s, 3H), 3.04 – 2.92 (m, 2H), 2.63 – 2.53 (m, 1H), 2.44 (s, 4H), 2.25 (t, *J* = 8.8 Hz, 2H), 1.89 – 1.77 (m, 2H), 1.05 (s, 3H), 0.93 – 0.85 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 143.5, 143.0, 138.7, 133.5, 129.7, 128.7, 127.6, 110.8, 54.3, 51.9, 50.0, 48.7, 45.7, 39.0, 33.1, 27.3, 22.6, 22.3, 21.6, 21.5, 19.5. IR (neat) ν 661, 1090, 1340, 1655, 1736, 2955 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{31}NO_4SNa$ $(M+Na)^+$: 440.1866, Found: 440.1864.

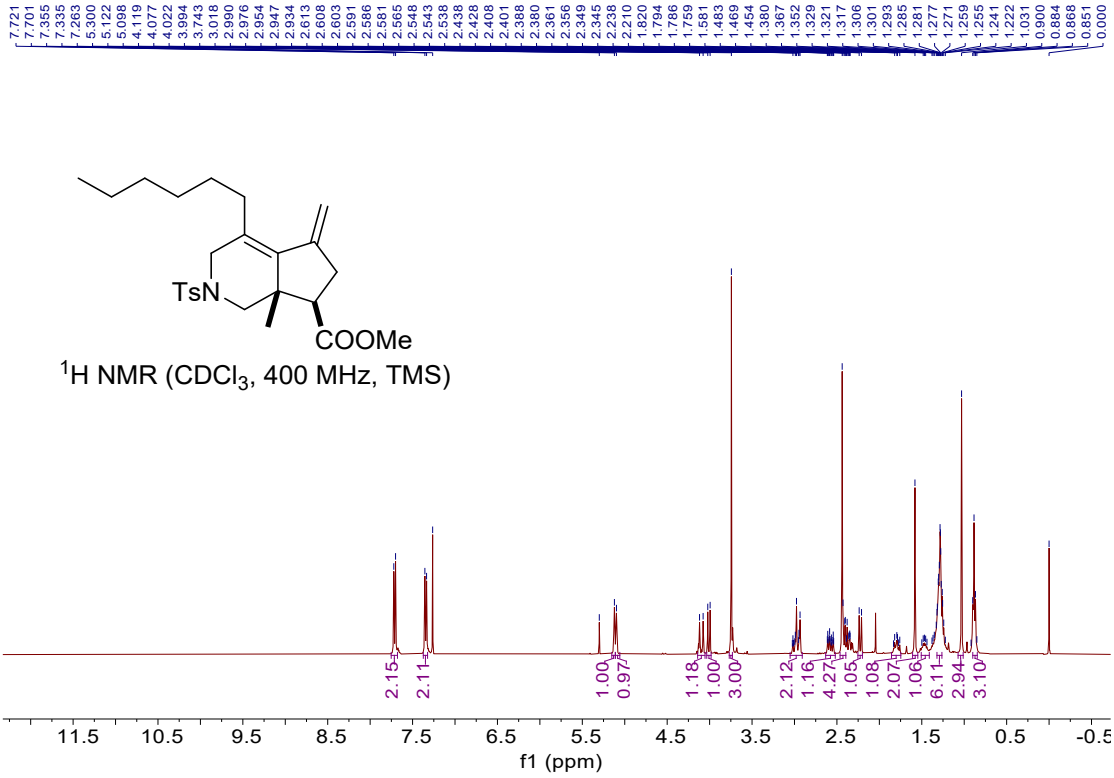


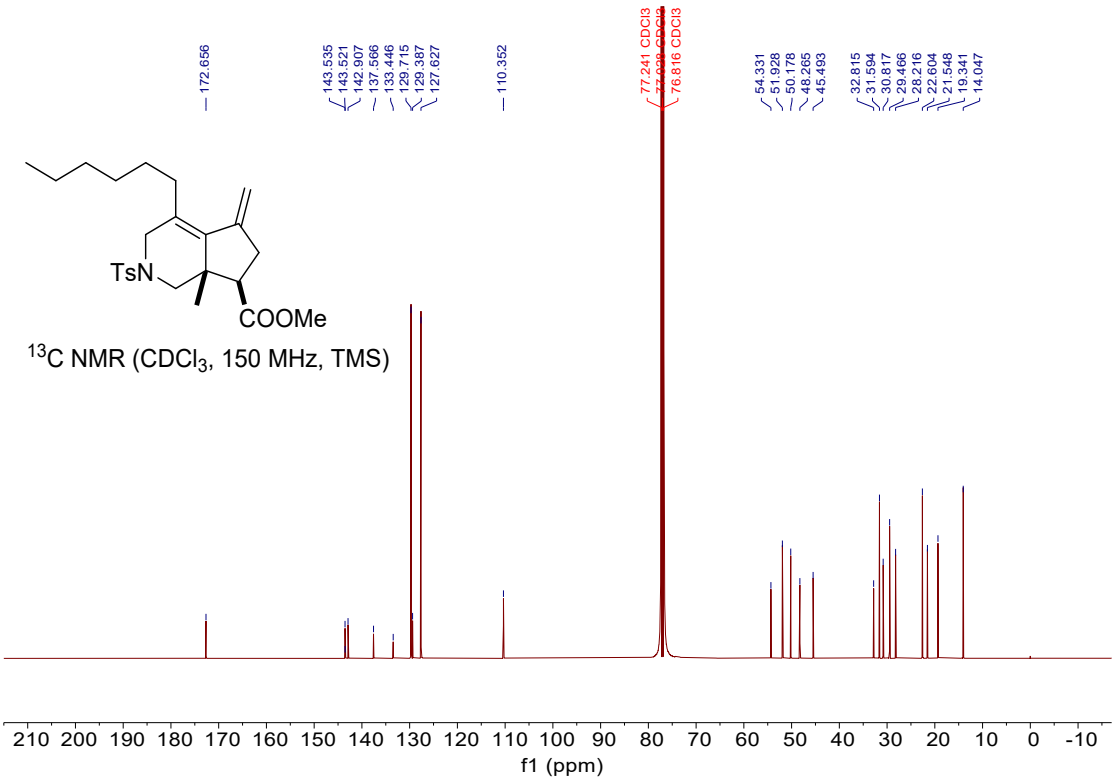

172.624
143.528
143.011
138.688
133.509
129.703
128.662
127.594
110.762
77.364 CDCl3
77.046 CDCl3
76.728 CDCl3
54.256
51.904
50.033
48.680
45.717
38.957
33.054
27.338
22.633
22.327
21.648
21.537
19.515
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

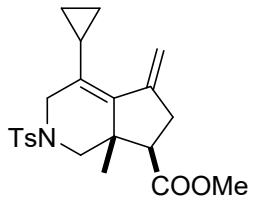


(cis)-methyl-4-hexyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2g)

A colorless oil, 90% yield, 40.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.12 (s, 1H), 5.10 (s, 1H), 4.10 (d, *J* = 16.8 Hz, 1H), 4.01 (d, *J* = 11.2 Hz, 1H), 3.74 (s, 3H), 3.05 – 2.91 (m, 2H), 2.63 – 2.52 (m, 1H), 2.46 – 2.39 (m, 4H), 2.22 (d, *J* = 11.2 Hz, 1H), 1.86 – 1.75 (m, 1H), 1.58 (s, 2H), 1.47 (dt, *J* = 11.8, 6.4 Hz, 1H), 1.32 – 1.26 (m, 6H), 1.03 (s, 3H), 0.88 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.7, 143.5, 143.5, 142.9, 137.6, 133.4, 129.7, 129.4, 127.6, 110.4, 54.3, 51.9, 50.2, 48.3, 45.5, 32.8, 31.6, 30.8, 29.5, 28.2, 22.6, 21.5, 19.3, 14.0. IR (neat) ν 661,1091, 1350, 1655, 1736, 2926 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{35}NO_4SNa$ $(M+Na)^+$: 468.2179, Found: 468.2182.

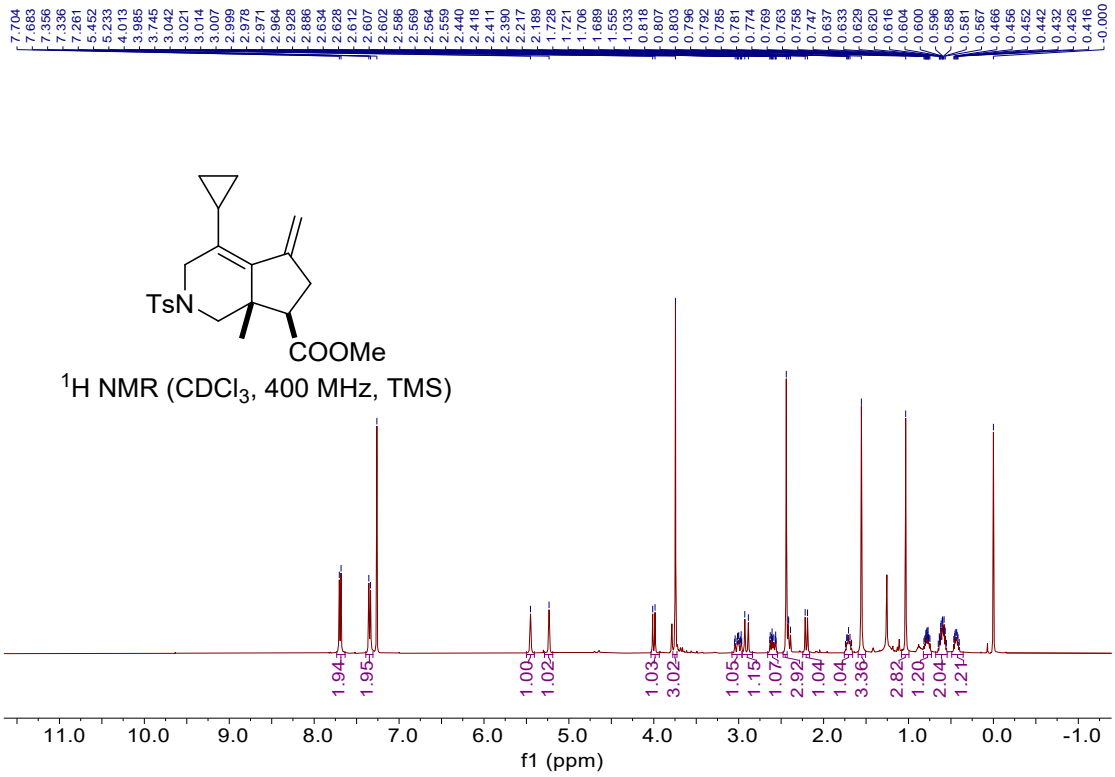


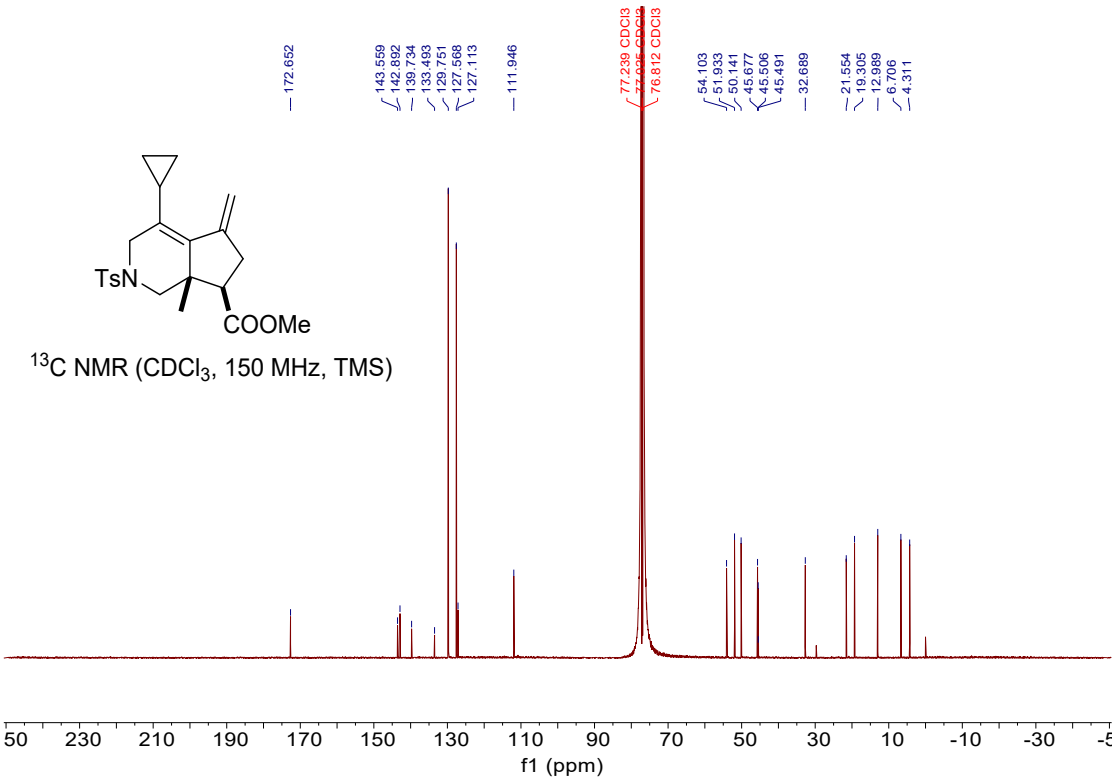

172.656
143.535
143.521
142.907
137.566
133.446
129.715
129.387
127.627
110.352
77.241 CDCl3
77.031 CDCl3
76.816 CDCl3
54.331
51.928
50.178
48.265
45.493
32.815
31.594
30.817
29.466
28.216
22.604
21.548
19.341
14.047
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



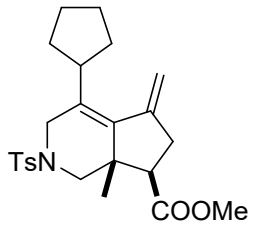
(cis)-methyl-4-cyclopropyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2h)

A colorless oil, 88% yield, 35.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.45 (s, 1H), 5.23 (s, 1H), 4.00 (d, *J* = 11.2 Hz, 1H), 3.74 (s, 3H), 3.01 (ddd, *J* = 17.2, 11.2, 2.8 Hz, 1H), 2.91 (d, *J* = 16.8 Hz, 1H), 2.66 – 2.54 (m, 1H), 2.44 (s, 3H), 2.20 (d, *J* = 11.2 Hz, 1H), 1.71 (h, *J* = 6.4 Hz, 1H), 1.56 (s, 3H), 1.03 (s, 3H), 0.82 – 0.73 (m, 1H), 0.68 – 0.54 (m, 2H), 0.42 – 0.46 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.7, 143.6, 142.9, 139.7, 133.5, 129.8, 127.6, 127.1, 111.9, 0 54.1, 51.9, 50.1, 45.7, 45.5, 45.5, 32.7, 21.6, 19.3, 13.0, 6.7, 4.3. IR (neat) ν 660, 1346, 1651, 1736, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{22}H_{27}NO_4SNa$ $(M+Na)^+$: 424.1553, Found: 424.1554.



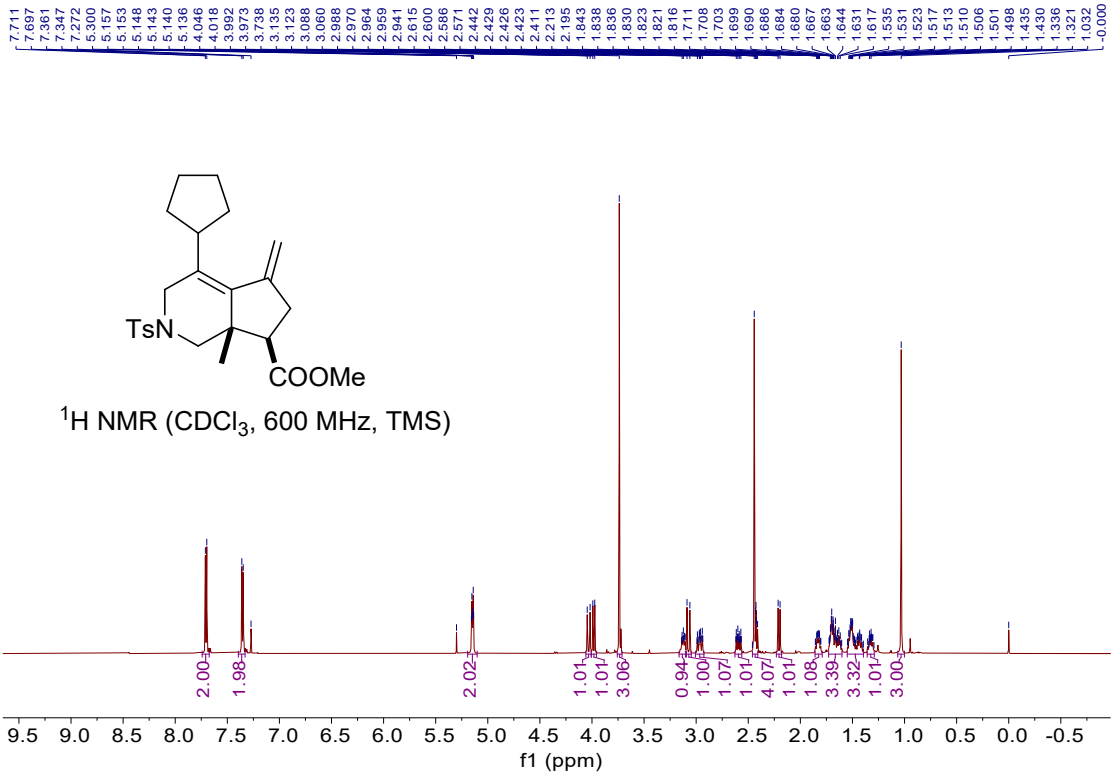


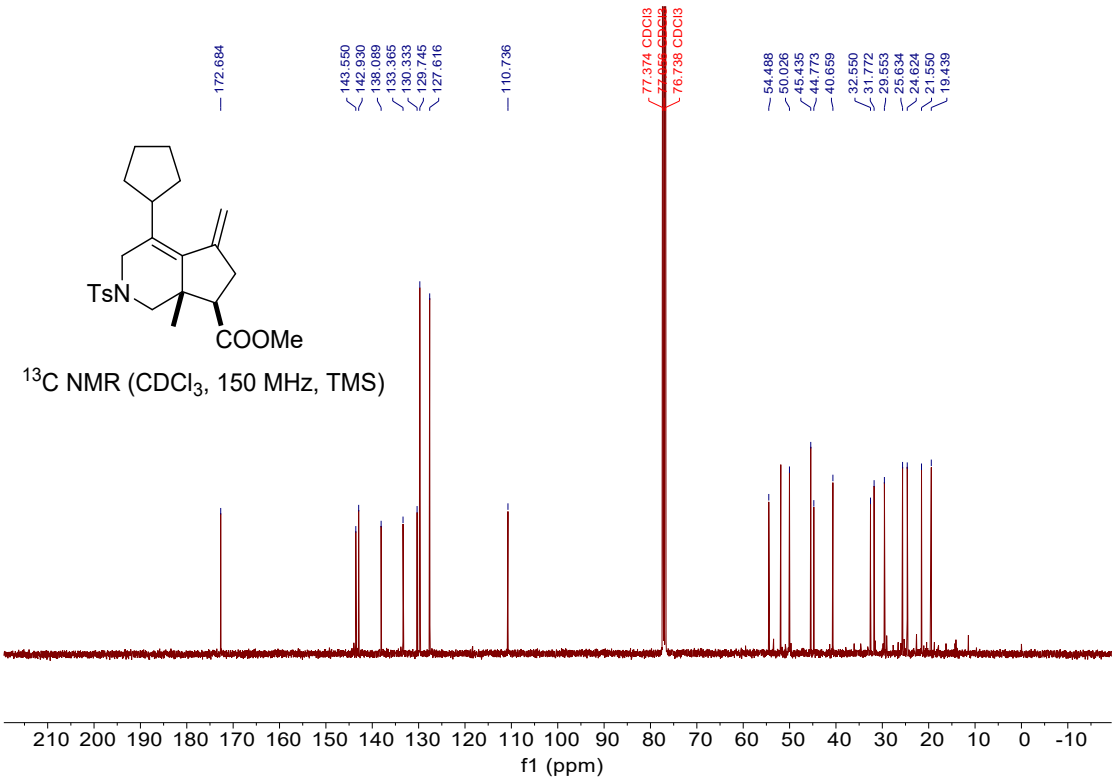
^{13}C NMR ($CDCl_3$, 150 MHz, TMS)

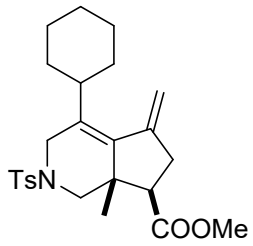


(cis)-methyl-4-cyclopentyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2i)

A colorless oil, 90% yield, 38.6 mg. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.19 – 5.10 (m, 2H), 4.03 (d, *J* = 16.4 Hz, 1H), 3.98 (d, *J* = 11.2 Hz, 1H), 3.74 (s, 3H), 3.16 – 3.10 (m, 1H), 3.07 (d, *J* = 16.4 Hz, 1H), 3.01 – 2.93 (m, 1H), 2.63 – 2.56 (m, 1H), 2.46 – 2.41 (m, 4H), 2.20 (d, *J* = 11.2 Hz, 1H), 1.86 – 1.79 (m, 1H), 1.73 – 1.60 (m, 3H), 1.55 – 1.39 (m, 3H), 1.36 – 1.29 (m, 1H), 1.03 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 143.6, 142.9, 138.1, 133.4, 130.3, 129.7, 127.6, 110.7, 54.5, 50.0, 45.4, 44.8, 40.7, 32.5, 31.8, 29.6, 25.6, 24.6, 21.5, 19.4. IR (neat) ν 662, 1091, 1352, 1597, 1735, 2952 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{31}NO_4SNa$ $(M+Na)^+$: 452.1866, Found: 452.1866.

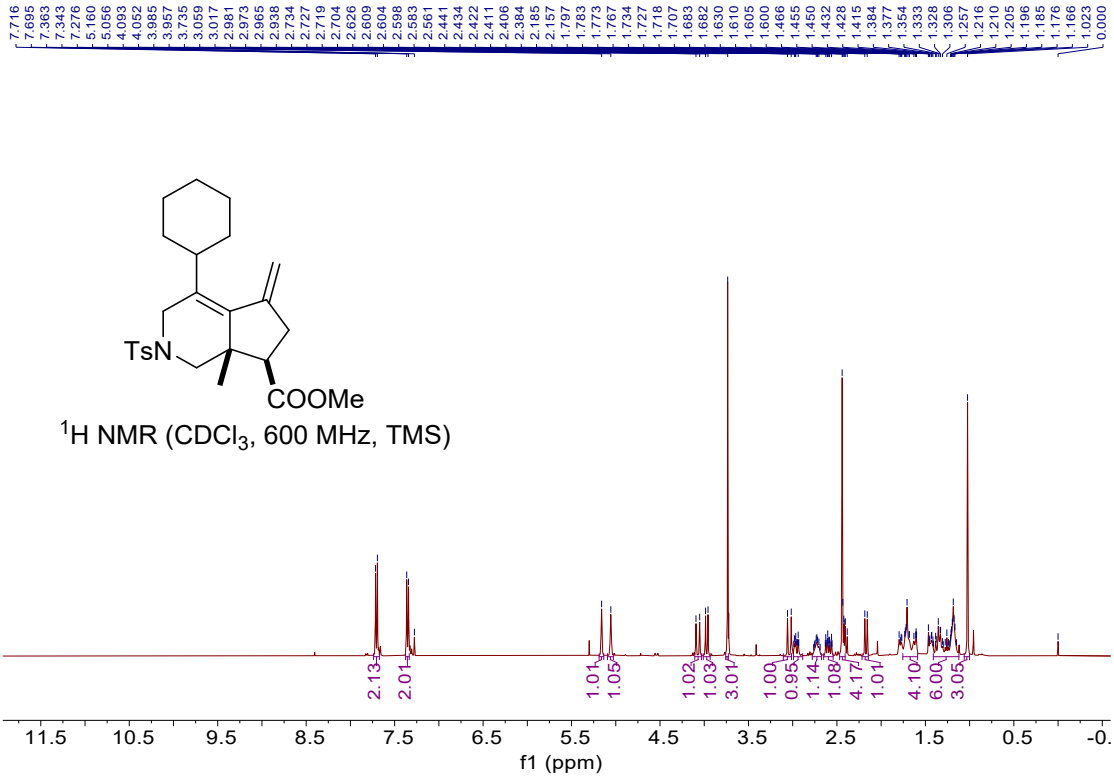


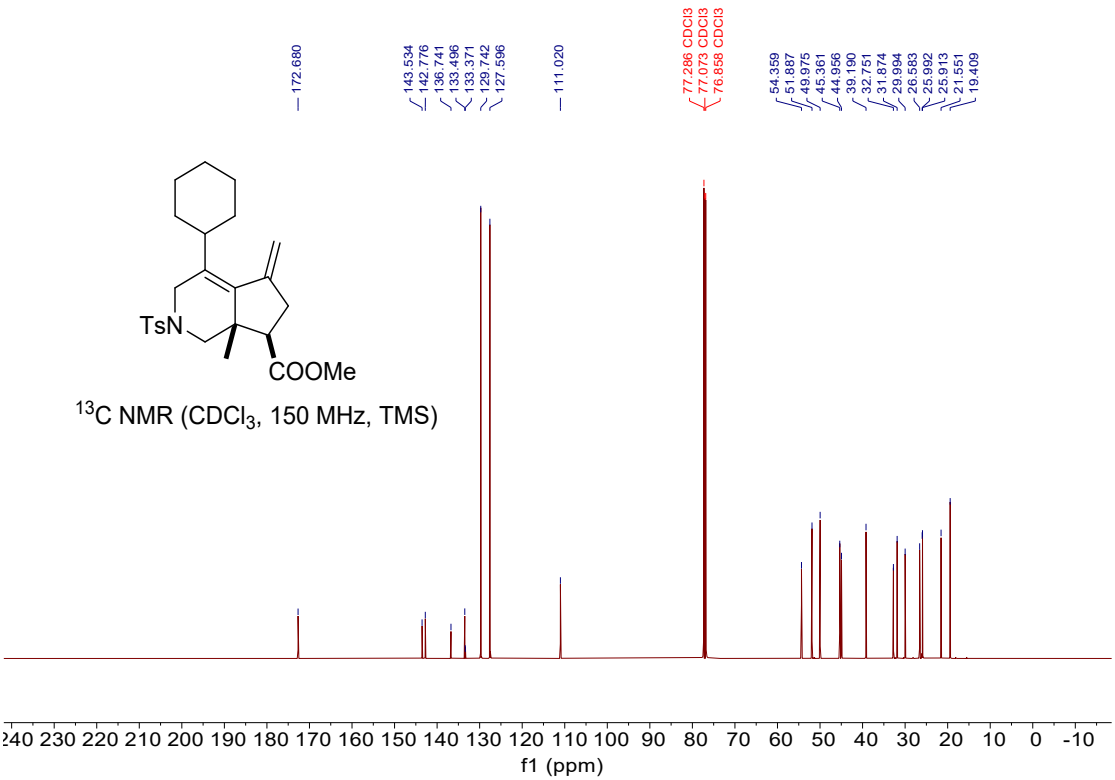

172.684
143.550
142.930
138.089
133.365
130.333
129.745
127.616
110.736
77.374 CDCl3
76.738 CDCl3
54.488
50.026
45.435
44.773
40.659
32.550
31.772
29.553
25.634
24.624
21.550
19.439
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

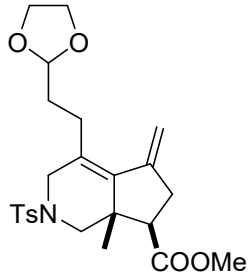


(cis)-methyl-4-cyclopentyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2j)

A colorless oil, 92% yield, 40.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.16 (s, 1H), 5.06 (s, 1H), 4.07 (d, *J* = 16.8 Hz, 1H), 3.97 (d, *J* = 11.2 Hz, 1H), 3.74 (s, 3H), 3.04 (d, *J* = 16.8 Hz, 1H), 2.99 – 2.89 (m, 1H), 2.78 – 2.67 (m, 1H), 2.65 – 2.54 (m, 1H), 2.47 – 2.41 (m, 4H), 2.17 (d, *J* = 11.2 Hz, 1H), 1.83 – 1.59 (m, 4H), 1.49 – 1.12 (m, 6H), 1.02 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.7, 143.5, 142.8, 136.7, 133.5, 133.4, 129.7, 127.6, 111.0, 54.4, 51.9, 50.0, 45.4, 45.0, 39.2, 32.8, 31.9, 30.0, 26.6, 26.0, 25.9, 21.6, 19.4. IR (neat) ν 661, 1089, 1356, 1661, 1736, 2929 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{33}NO_4SNa$ $(M+Na)^+$: 466.2023, Found: 466.2024.

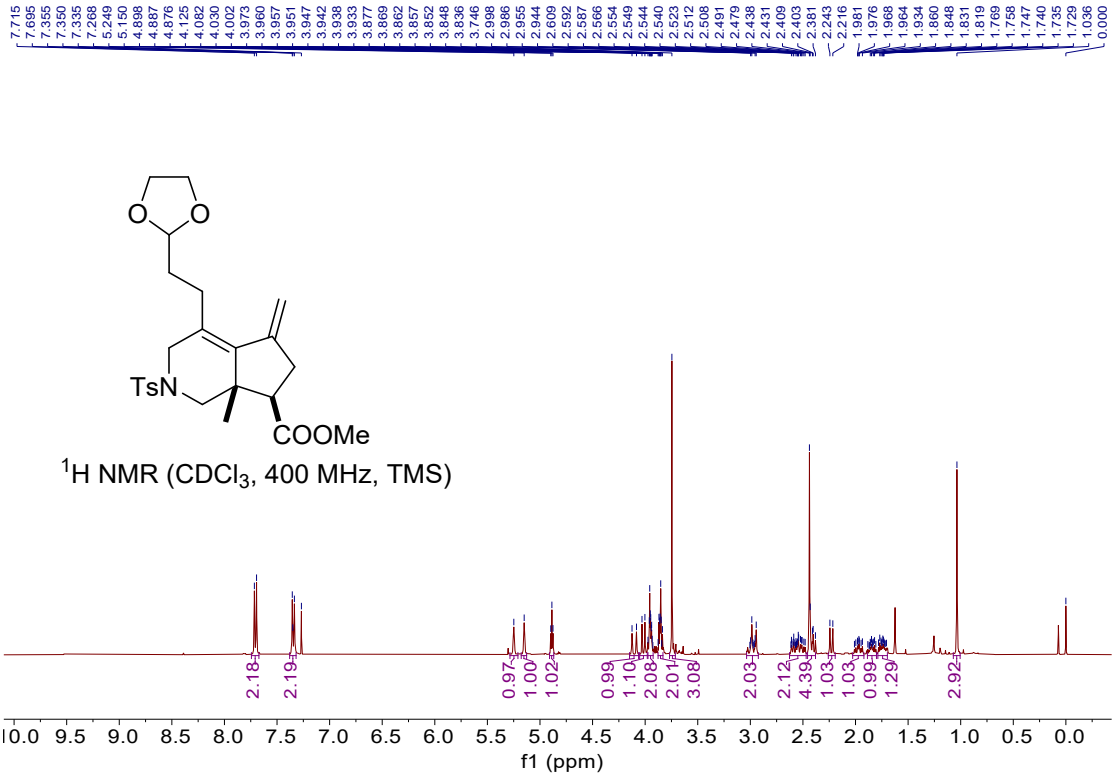


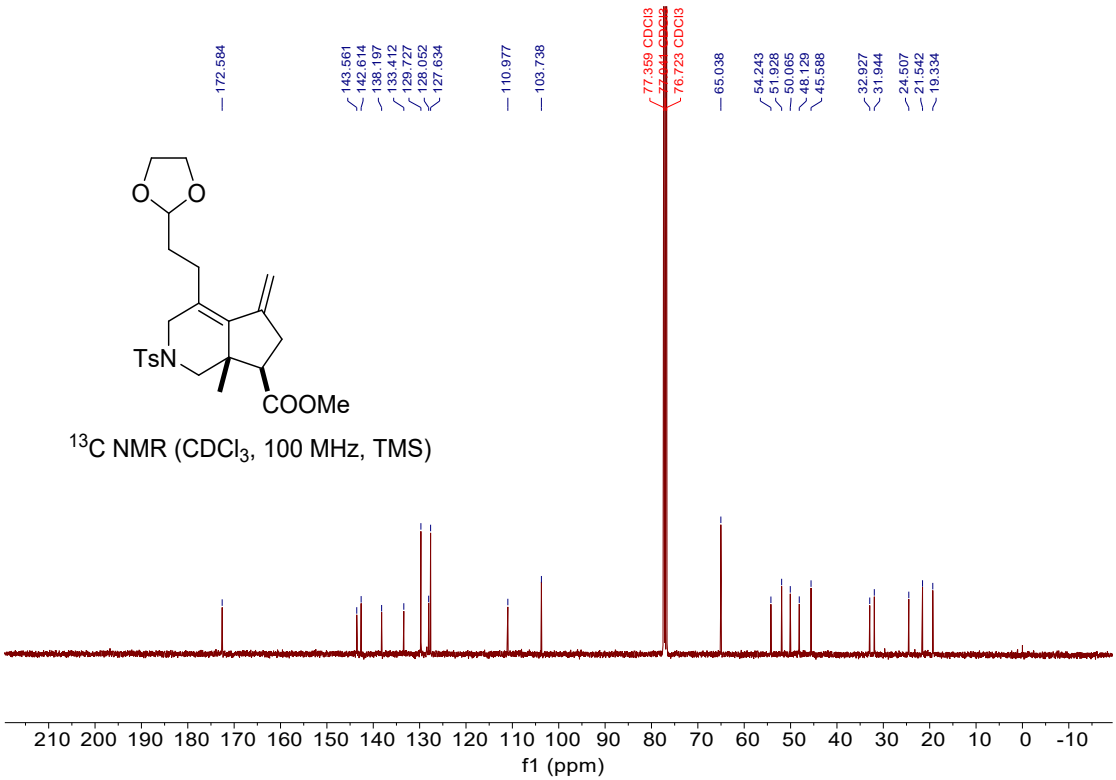

172.680
143.534
142.776
136.741
133.496
133.371
129.742
127.596
111.020
77.286 CDCl3
77.073 CDCl3
76.858 CDCl3
54.359
51.887
49.975
45.361
44.956
39.190
32.751
31.874
29.994
26.583
25.992
25.913
21.551
19.409
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



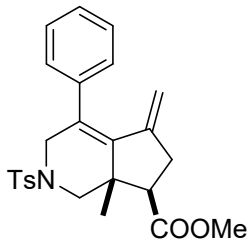
(cis)-methyl-4-(2-(1,3-dioxolan-2-yl)ethyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2k)

A colorless oil, 88% yield, 40.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 5.25 (s, 1H), 5.15 (s, 1H), 4.89 (t, *J* = 4.4 Hz, 1H), 4.10 (d, *J* = 17.2 Hz, 1H), 4.05 – 3.98 (m, 1H), 3.97 – 3.92 (m, 2H), 3.88 – 3.83 (m, 2H), 3.75 (s, 3H), 3.04 – 2.92 (m, 2H), 2.63 – 2.47 (m, 2H), 2.46 – 2.38 (m, 4H), 2.23 (d, *J* = 11.2 Hz, 1H), 2.03 – 1.92 (m, 1H), 1.89 – 1.80 (m, 1H), 1.79 – 1.70 (m, 1H), 1.04 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 143.6, 142.6, 138.2, 133.4, 129.7, 128.1, 127.6, 111.0, 103.7, 65.0, 54.2, 51.9, 50.1, 48.1, 45.6, 32.9, 31.9, 24.5, 21.5, 19.3. IR (neat) ν 664, 965, 1435, 1658, 1736, 2939 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{31}NO_6SNa$ $(M+Na)^+$: 484.1764, Found: 484.1762.



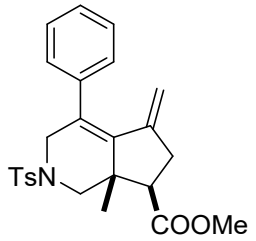


^{13}C NMR ($CDCl_3$, 100 MHz, TMS)

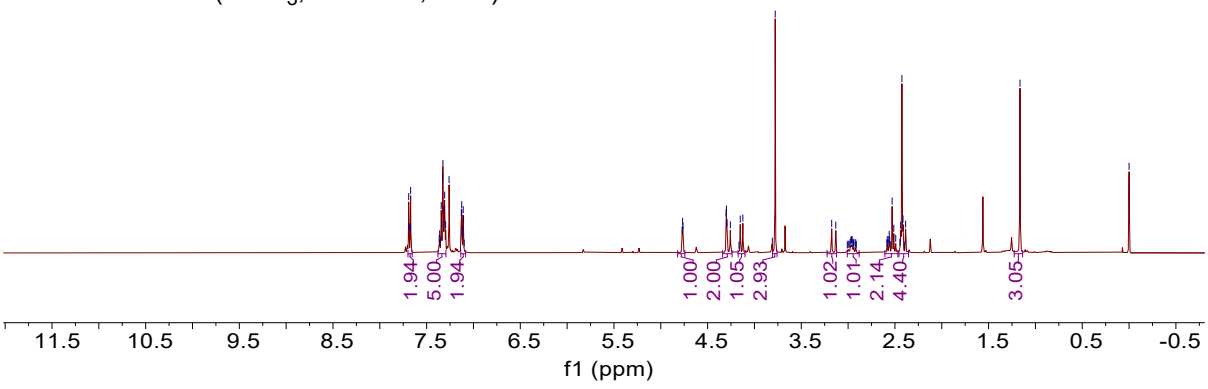


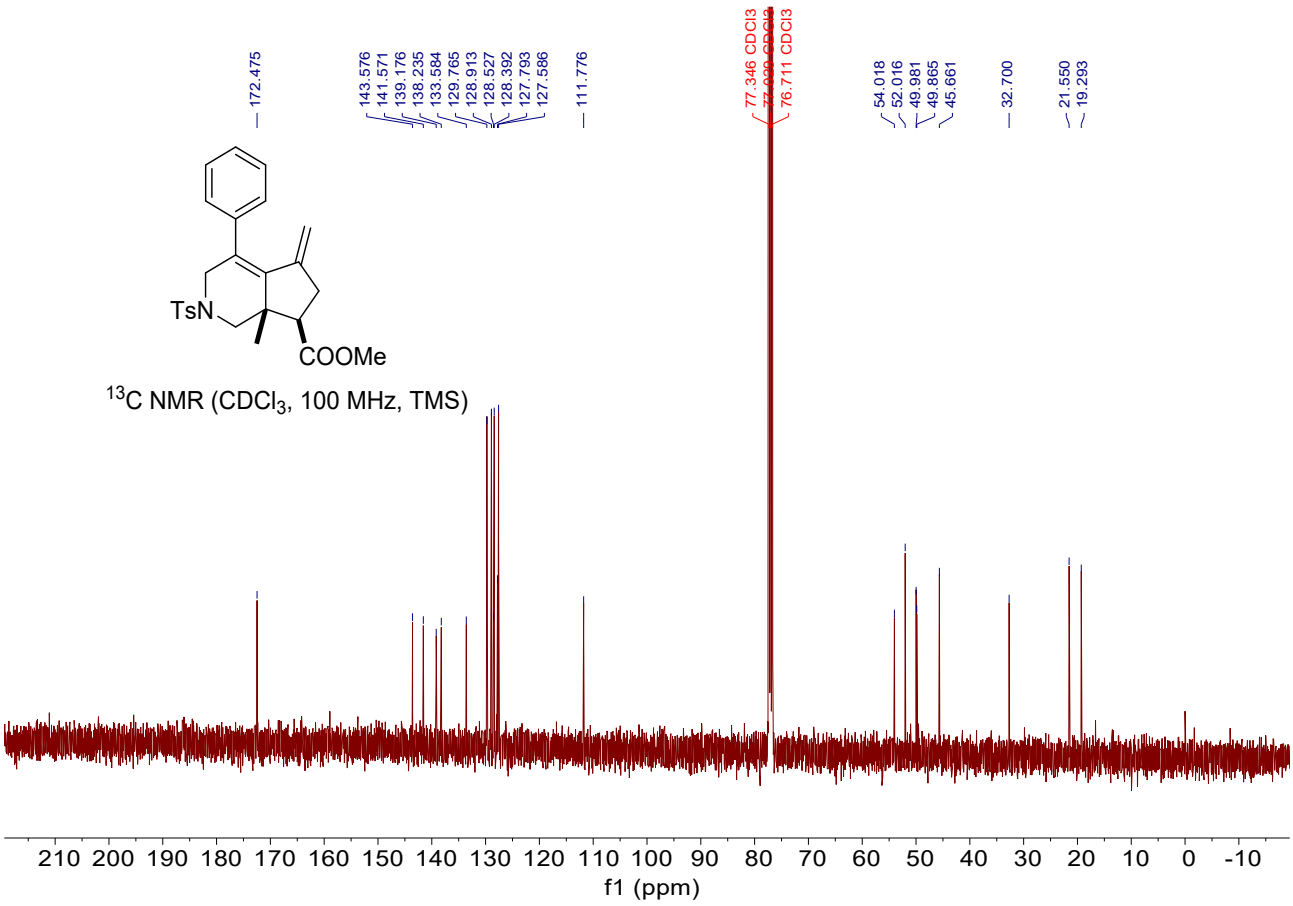
(cis)-methyl-7a-methyl-5-methylene-4-phenyl-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2l)

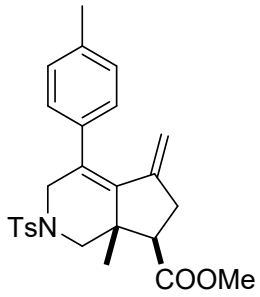
A colorless oil, 80% yield, 35.0 mg. ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.65 (m, 2H), 7.38 – 7.29 (m, 5H), 7.14 – 7.08 (m, 2H), 4.82 – 4.74 (m, 1H), 4.34 – 4.24 (m, 2H), 4.14 (d, *J* = 11.2 Hz, 1H), 3.78 (s, 3H), 3.15 (d, *J* = 17.6 Hz, 1H), 3.01 – 2.88 (m, 1H), 2.61 – 2.47 (m, 2H), 2.46 – 2.35 (m, 4H), 1.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 143.6, 141.6, 139.2, 138.2, 133.6, 129.8, 128.9, 128.5, 128.4, 127.8, 127.6, 111.8, 54.0, 52.0, 50.0, 49.9, 45.7, 32.7, 21.5, 19.3. IR (neat) ν 662, 1208, 1349, 1662, 1734, 2948 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{27}NO_4SNa$ $(M+Na)^+$: 460.1553, Found: 460.1550.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

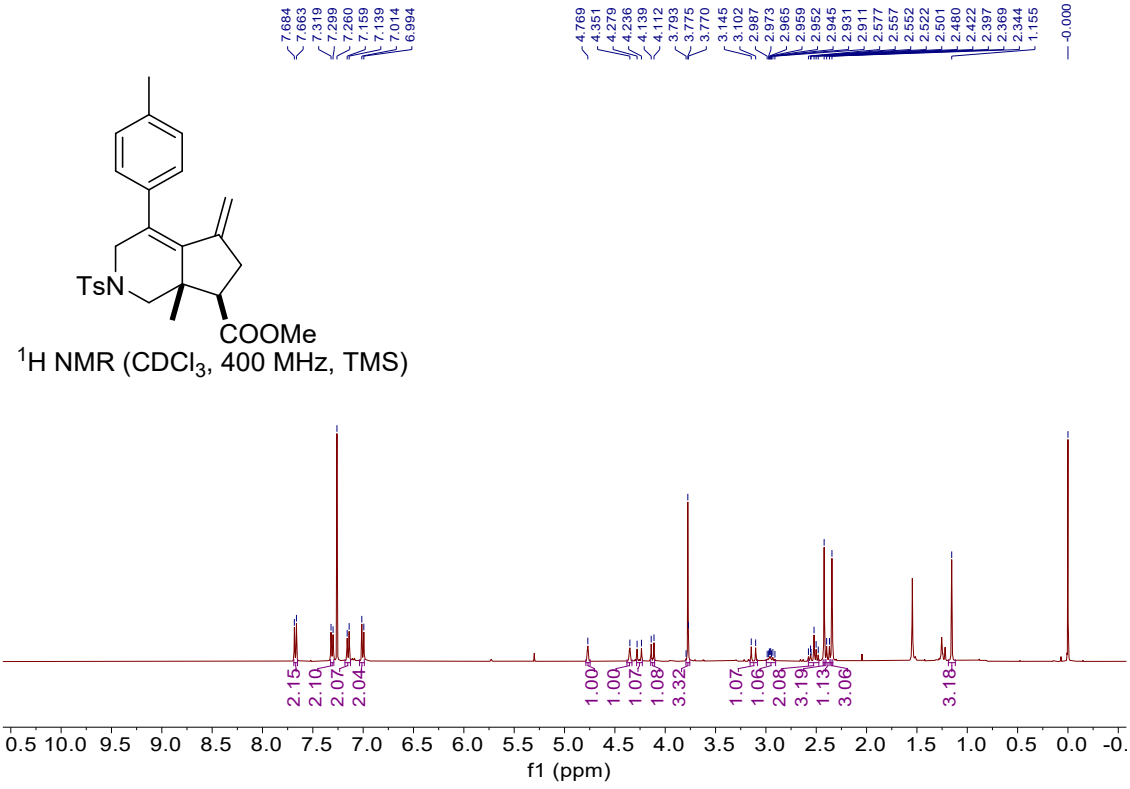


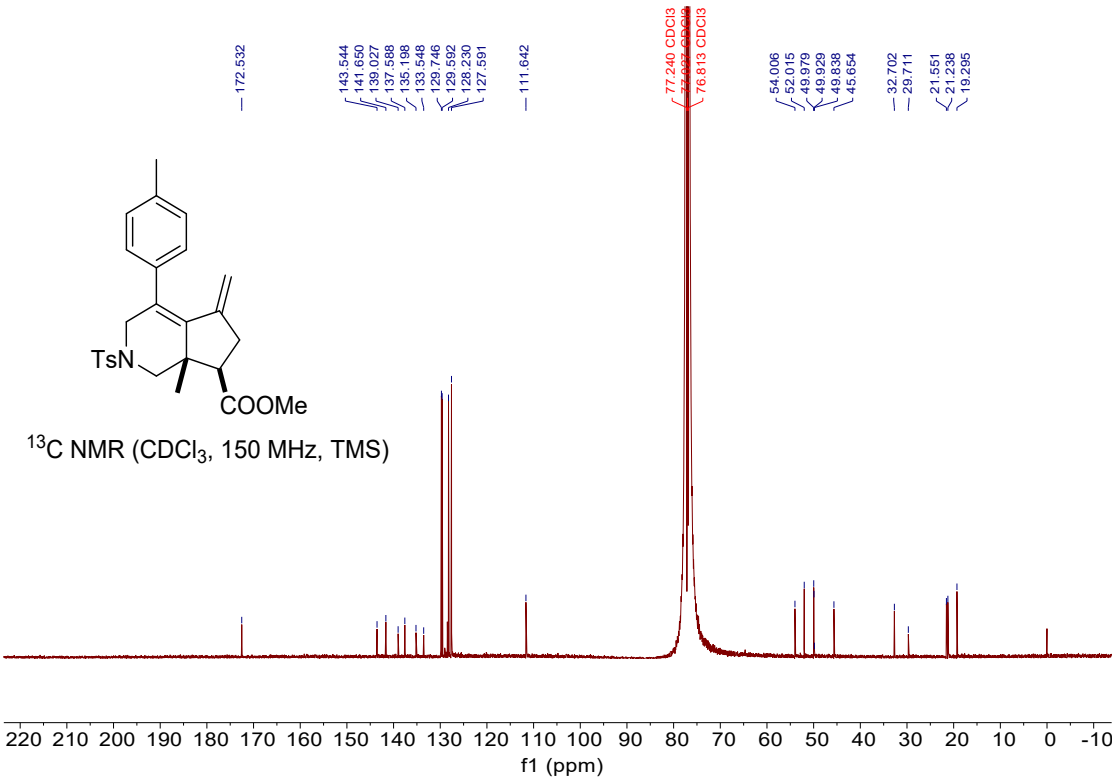

172.475
143.576
141.571
139.176
138.235
133.584
129.765
128.913
128.527
128.392
127.793
127.586
111.776
77.346 CDCl3
77.030 CDCl3
76.711 CDCl3
54.018
52.016
49.981
49.865
45.661
32.700
21.550
19.293
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

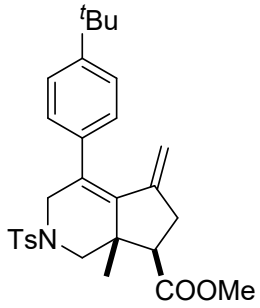


(cis)-methyl-7a-methyl-5-methylene-4-(p-tolyl)-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2m)

A colorless oil, 80% yield, 36.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 4.77 (s, 1H), 4.35 (s, 1H), 4.26 (d, *J* = 17.4 Hz, 1H), 4.13 (d, *J* = 11.2 Hz, 1H), 3.77 (d, *J* = 2.4 Hz, 3H), 3.12 (d, *J* = 17.4 Hz, 1H), 3.00 – 2.90 (m, 1H), 2.58 – 2.47 (m, 2H), 2.42 (s, 3H), 2.38 (d, *J* = 11.2 Hz, 1H), 2.34 (s, 3H), 1.15 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.5, 143.5, 141.7, 139.0, 137.6, 135.2, 133.5, 129.7, 129.6, 128.2, 127.6, 111.6, 0 54.0, 52.0, 50.0, 49.9, 49.8, 45.7, 32.7, 29.7, 21.6, 21.2, 19.3. IR (neat) ν 661, 816, 1093, 1348, 1660, 1736, 2922 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1705.

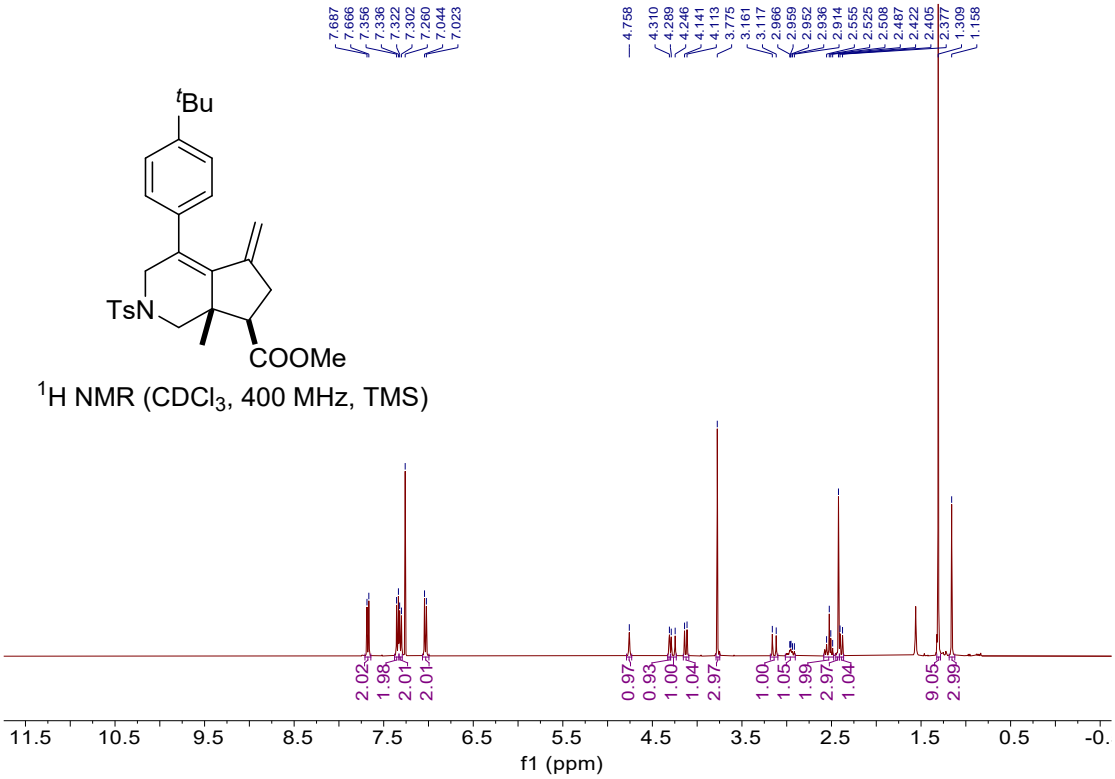


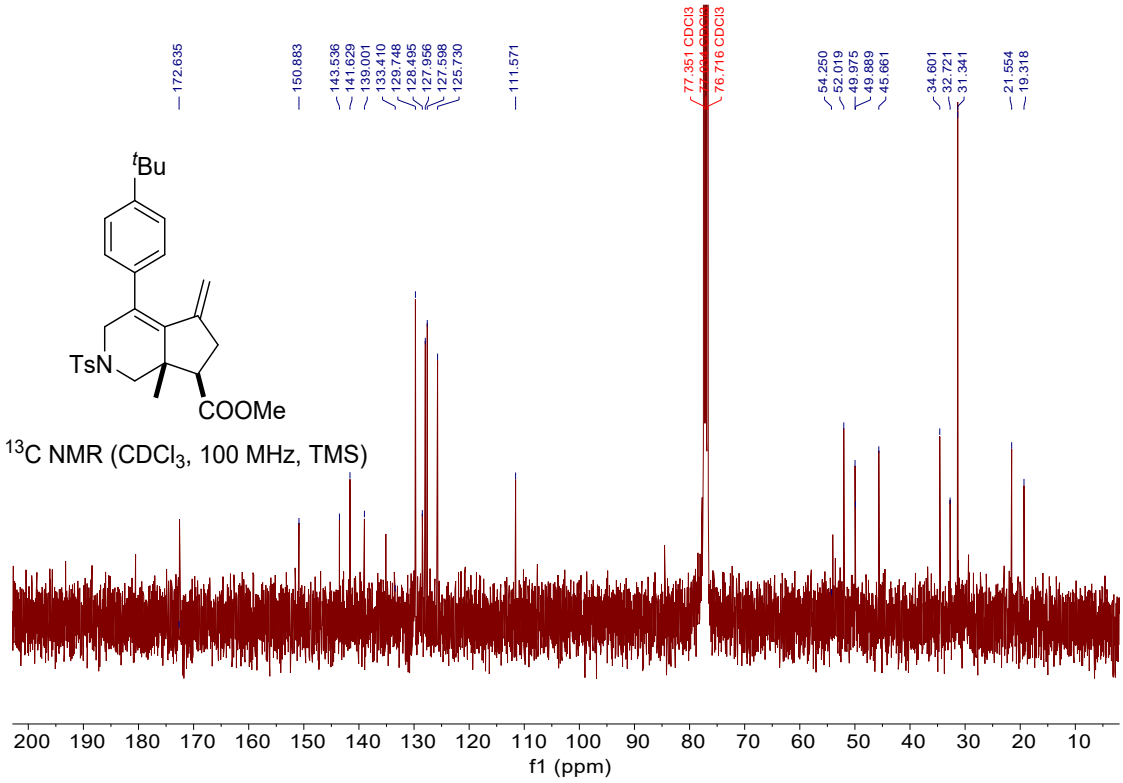

172.532
143.544
141.650
139.027
137.588
135.198
133.548
129.746
129.592
128.230
127.591
111.642
77.240 CDCl3
76.813 CDCl3
54.006
52.015
49.979
49.929
49.838
45.654
32.702
29.711
21.551
21.238
19.295
TsN
COOMe
13C NMR (CDCl3, 150 MHz, TMS)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

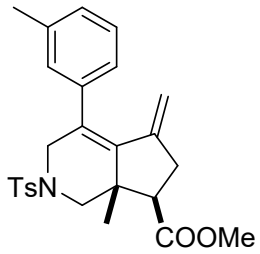


(cis)-methyl-4-(4-(tert-butyl)phenyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2n)

A colorless oil, 82% yield, 40.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 4.76 (s, 1H), 4.31 (s, 1H), 4.27 (d, *J* = 17.4 Hz, 1H), 4.13 (d, *J* = 11.2 Hz, 1H), 3.78 (s, 3H), 3.14 (d, *J* = 17.4 Hz, 1H), 3.02 – 2.90 (m, 1H), 2.59 – 2.48 (m, 2H), 2.42 (s, 3H), 2.39 (d, *J* = 11.2 Hz, 1H), 1.31 (s, 9H), 1.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 150.9, 143.5, 141.6, 139.0, 133.4, 129.7, 128.5, 128.0, 127.6, 125.7, 111.6, 54.3, 52.0, 50.0, 49.9, 45.7, 34.6, 32.7, 31.3, 21.6, 19.3. IR (neat) ν 662, 1091, 1350, 1656, 1734, 2961 cm^{-1}. HRMS (ESI) calcd. for $C_{29}H_{35}NO_4SNa$ $(M+Na)^+$: 516.2179, Found: 516.2171.

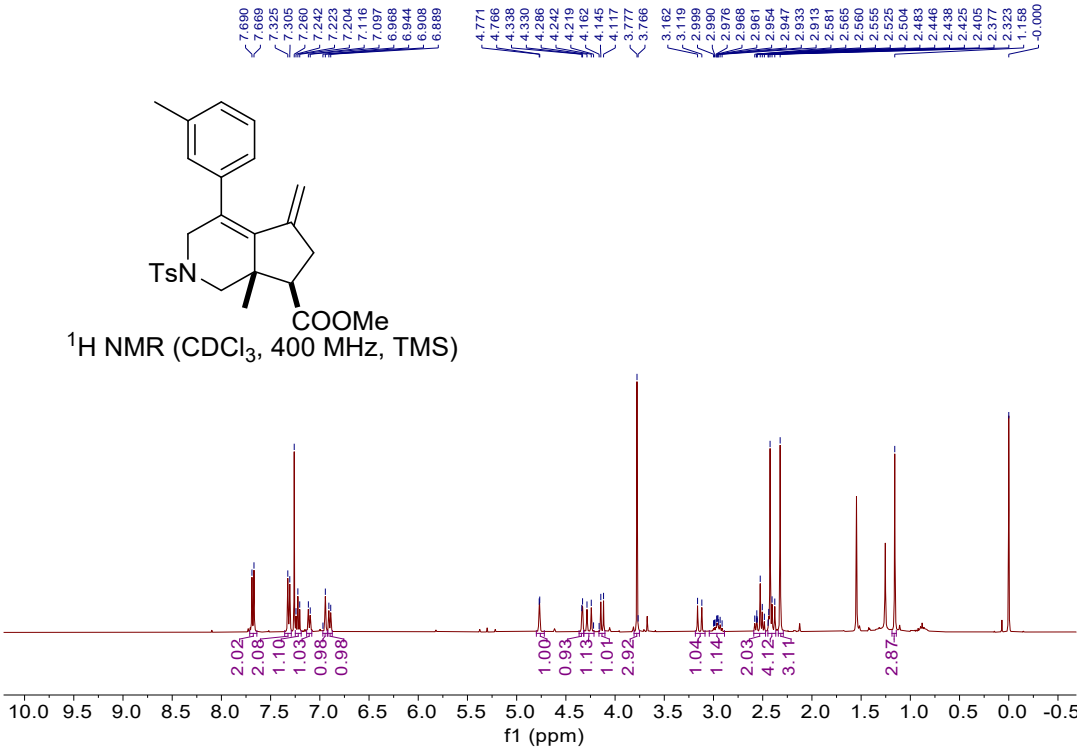


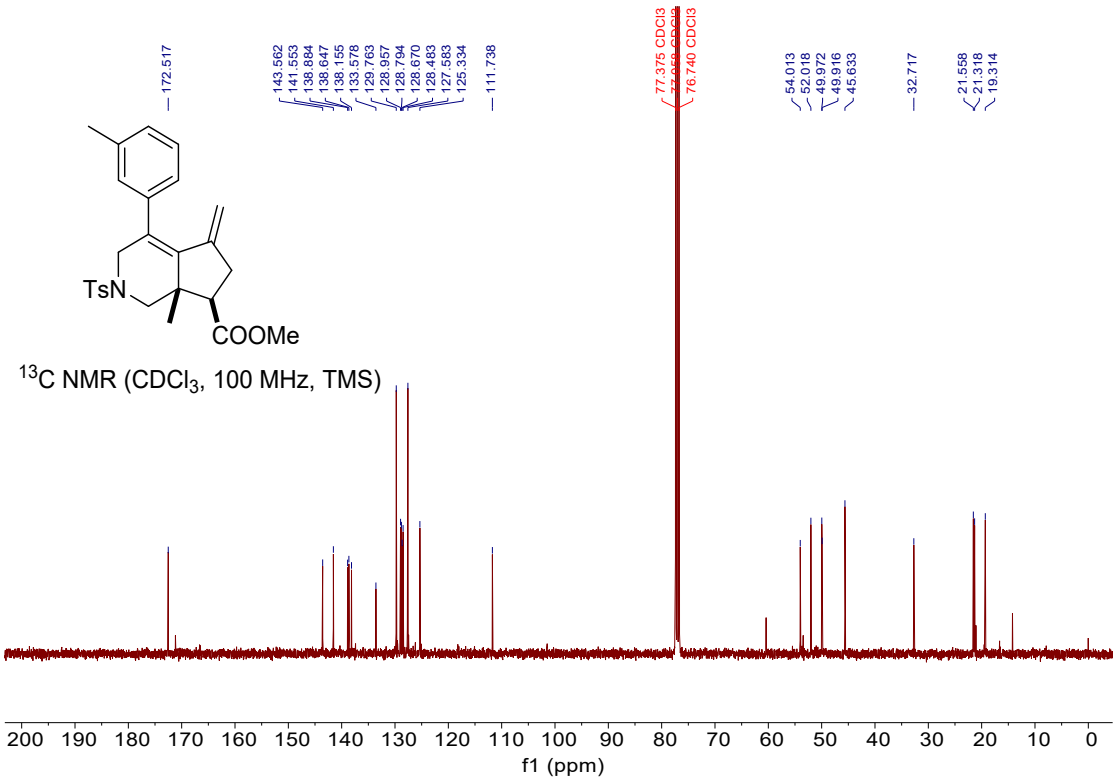

172.635
150.883
143.536
141.629
139.001
133.410
129.748
128.495
127.956
127.598
125.730
111.571
77.351 CDCl3
77.033 CDCl3
76.716 CDCl3
54.250
52.019
49.975
49.889
45.661
34.601
32.721
31.341
21.554
19.318
tBu
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

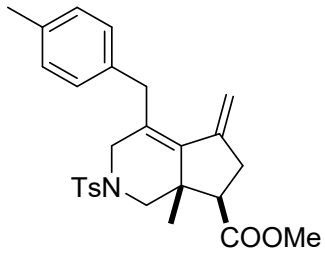


(cis)-methyl-7a-methyl-5-methylene-4-(m-tolyl)-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2o)

A colorless oil, 84% yield, 37.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 6.94 (s, 1H), 6.90 (d, *J* = 7.6 Hz, 1H), 4.80 – 4.72 (m, 1H), 4.33 (d, *J* = 3.1 Hz, 1H), 4.26 (d, *J* = 17.4 Hz, 1H), 4.13 (d, *J* = 11.1 Hz, 1H), 3.78 (s, 3H), 3.14 (d, *J* = 17.4 Hz, 1H), 3.04 – 2.89 (m, 1H), 2.59 – 2.47 (m, 2H), 2.42 (d, *J* = 8.0 Hz, 4H), 2.32 (s, 3H), 1.16 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 143.6, 141.6, 138.9, 138.6, 138.2, 133.6, 129.8, 129.0, 128.8, 128.7, 128.5, 127.6, 125.3, 111.7, 54.0, 52.0, 50.0, 49.9, 45.6, 32.7, 21.6, 21.3, 19.3. IR (neat) ν 668, 1098, 1349, 1659, 1733, 2948 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1704.

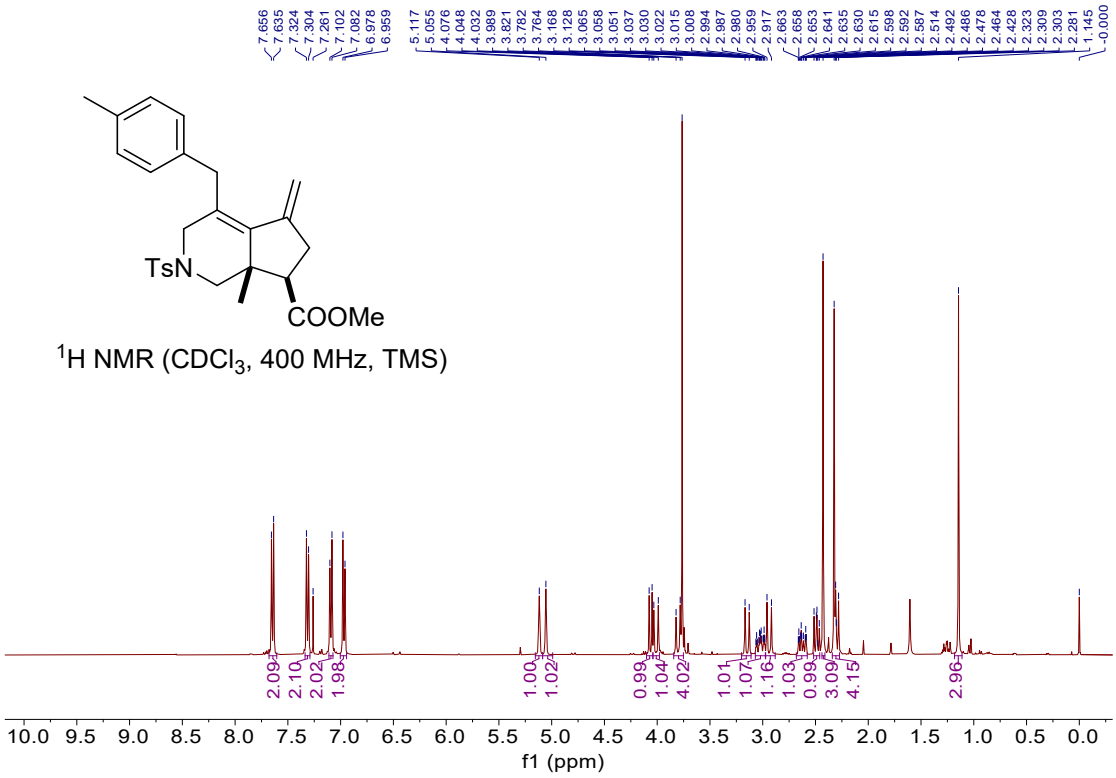


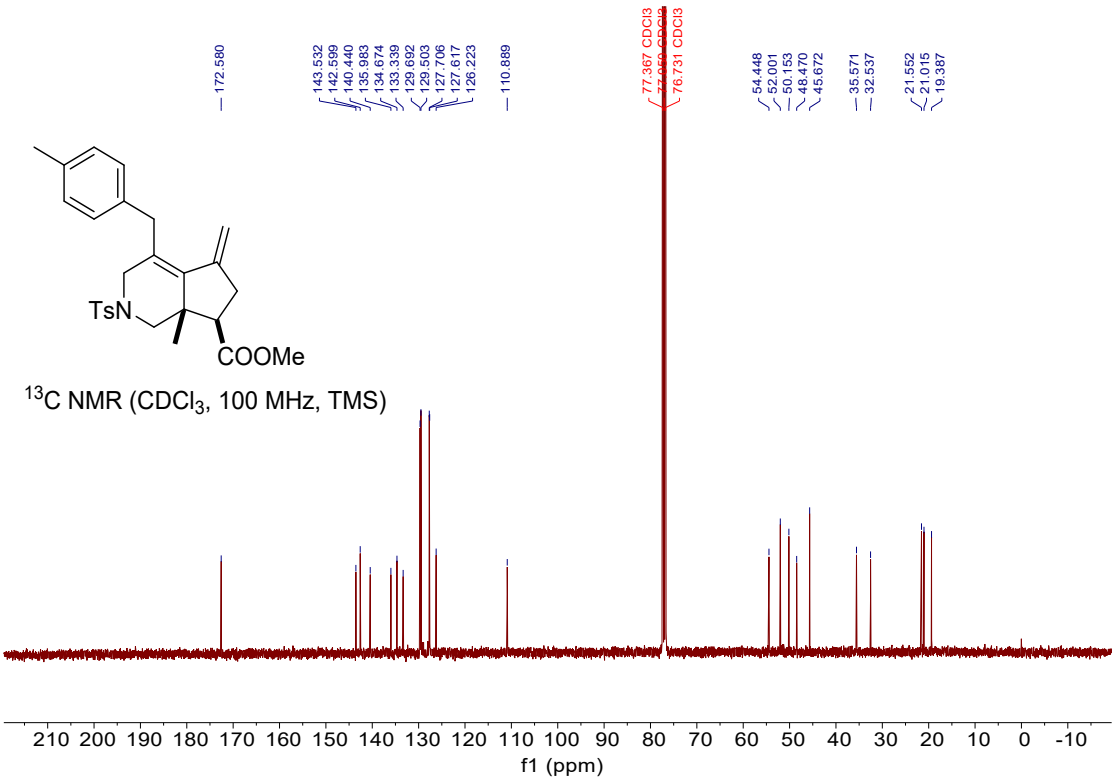

172.517
143.562
141.553
138.884
138.647
138.155
133.578
129.763
128.957
128.794
128.670
128.483
127.583
125.334
111.738
77.375 CDCl3
77.063 CDCl3
76.740 CDCl3
54.013
52.018
49.972
49.916
45.633
32.717
21.558
21.318
19.314
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

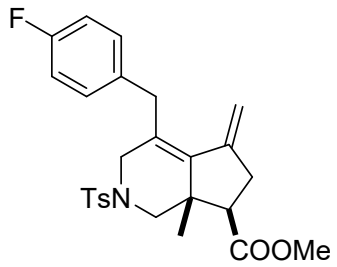


(cis)-methyl-7a-methyl-5-methylene-4-(m-tolyl)-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2p)

A colorless oil, 90% yield, 41.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 5.12 (s, 1H), 5.05 (s, 1H), 4.06 (d, *J* = 11.2 Hz, 1H), 4.01 (d, *J* = 17.2 Hz, 1H), 3.76 (s, 4H), 3.15 (d, *J* = 16.0 Hz, 1H), 3.07 – 2.97 (m, 1H), 2.94 (d, *J* = 17.2 Hz, 1H), 2.68 – 2.58 (m, 1H), 2.52 – 2.46 (m, 1H), 2.43 (s, 3H), 2.34 – 2.27 (m, 4H), 1.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 143.5, 142.6, 140.4, 136.0, 134.7, 133.3, 129.7, 129.5, 127.7, 127.6, 126.2, 110.9, 54.4, 52.0, 50.2, 48.5, 45.7, 35.6, 32.5, 21.6, 21.0, 19.4. IR (neat) ν 661, 1020, 1349, 1597, 1736, 2921 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{31}NO_4SNa$ $(M+Na)^+$: 488.1866, Found: 488.1872.

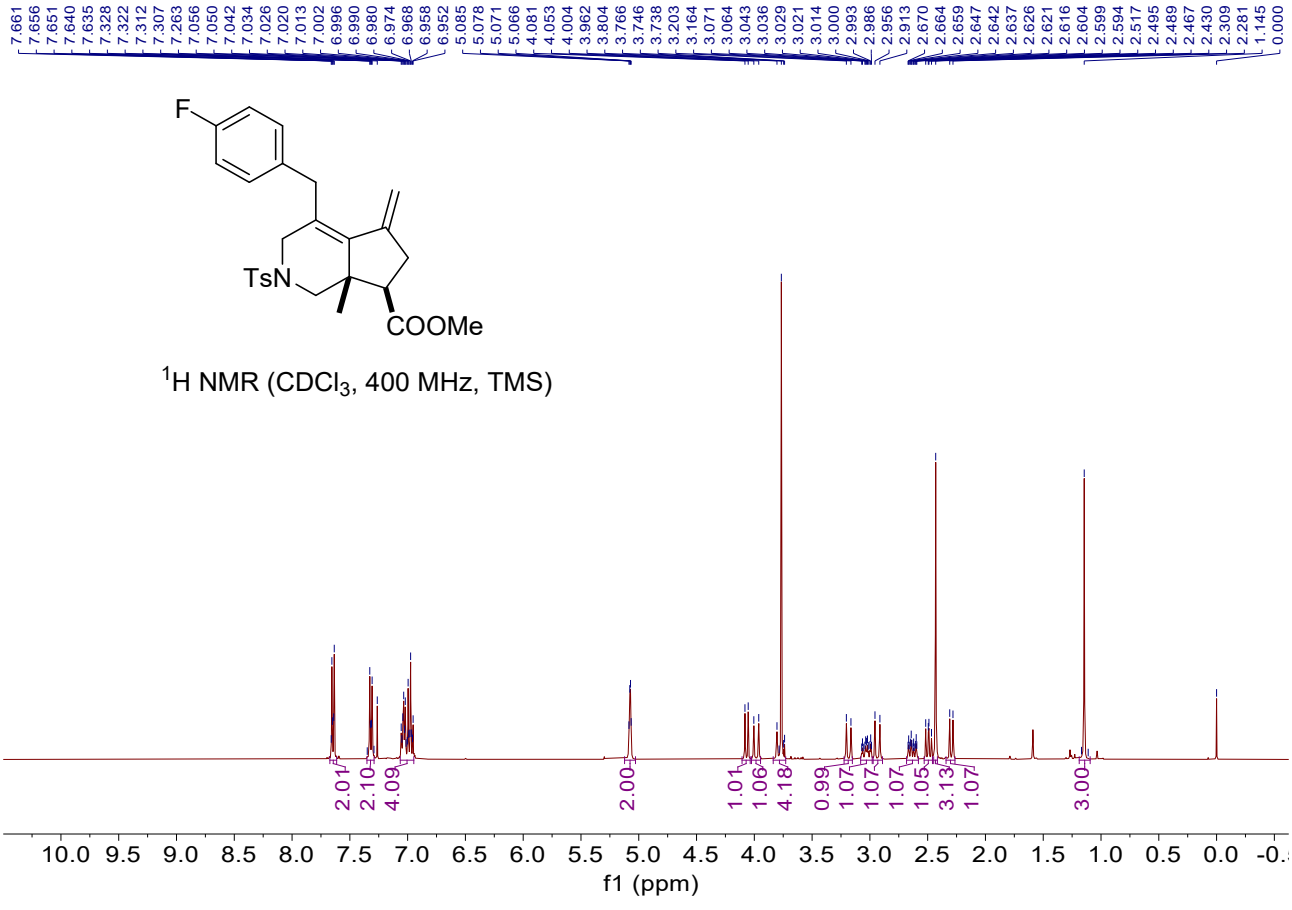


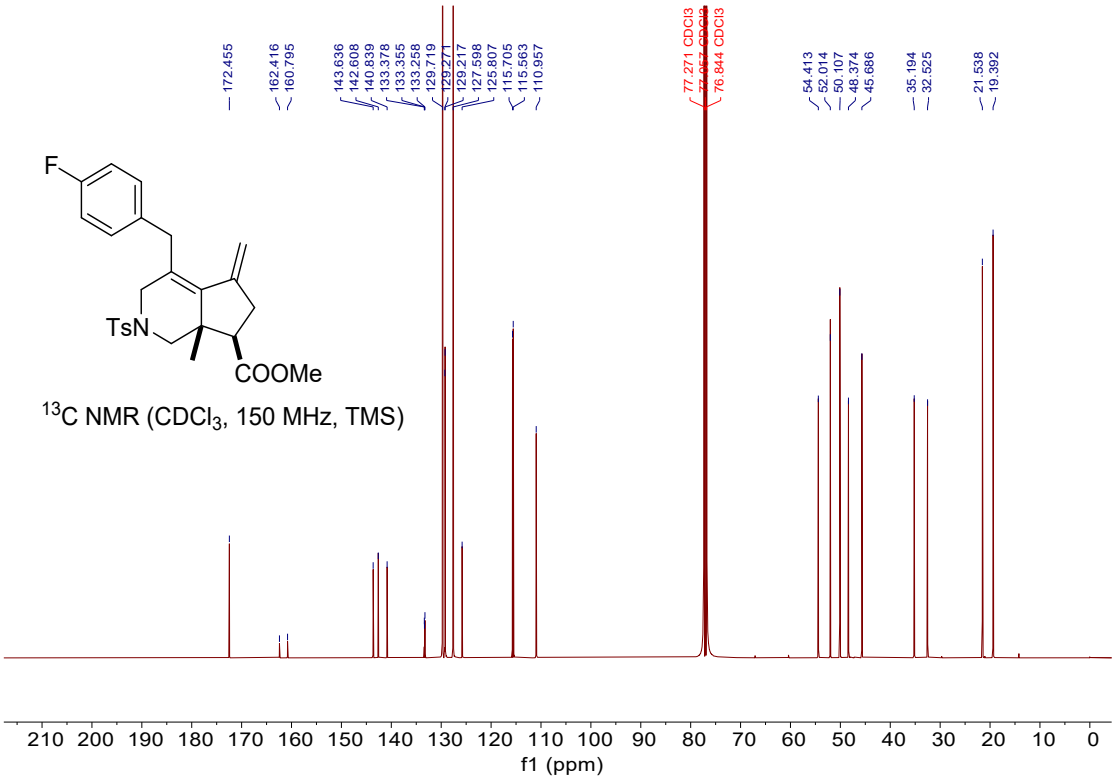

172.580
143.532
142.599
140.440
135.983
134.674
133.339
129.692
129.503
127.706
127.617
126.223
110.889
77.367 CDCl3
77.052 CDCl3
76.731 CDCl3
54.448
52.001
50.153
48.470
45.672
35.571
32.537
21.552
21.015
19.387
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



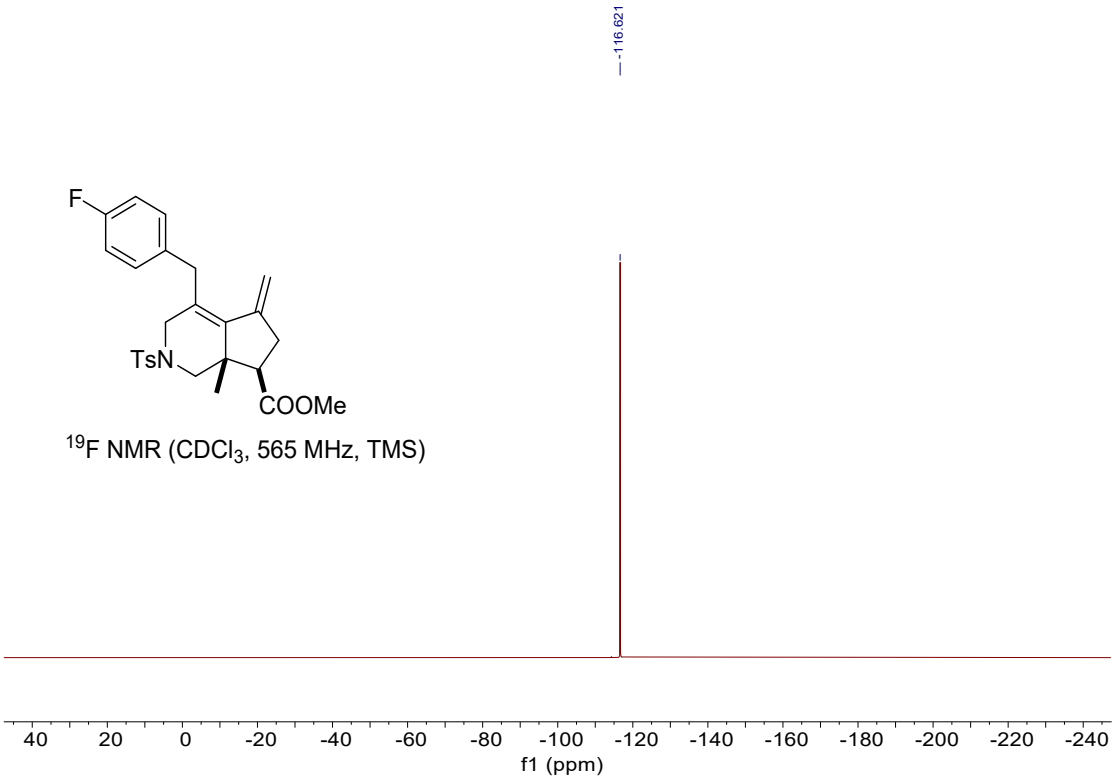
(cis)-methyl-4-(4-fluorobenzyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2q)

A colorless oil, 90% yield, 42.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 7.07 – 6.92 (m, 4H), 5.07 (q, J = 2.4 Hz, 2H), 4.07 (d, J = 11.2 Hz, 1H), 3.98 (d, J = 17.2 Hz, 1H), 3.82 – 3.73 (m, 4H), 3.18 (d, J = 15.8 Hz, 1H), 3.07 – 2.98 (m, 1H), 2.94 (d, J = 17.2 Hz, 1H), 2.68 – 2.57 (m, 1H), 2.49 (dd, J = 11.2, 8.8 Hz, 1H), 2.43 (s, 3H), 2.30 (d, J = 11.2 Hz, 1H), 1.15 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.5, 161.6 (d, $J_{C\text{-}F}$ = 243.2 Hz), 143.6, 142.6, 140.8, 133.4 (d, $J_{C\text{-}F}$ = 3.5 Hz), 133.3, 129.7, 129.3 (d, $J_{C\text{-}F}$ = 8.1 Hz), 127.6, 125.8, 115.7 (d, $J_{C\text{-}F}$ = 21.3 Hz), 111.0, 0 54.4, 52.0, 50.1, 48.4, 45.7, 35.2, 32.5, 21.5, 19.4. ^{19}F NMR (565 MHz, $CDCl_3$) δ -116.62. IR (neat) ν 662, 815, 1091, 1220, 1437, 1661, 1735, 2947 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{28}NO_4FSNa$ $(M+Na)^+$: 492.1615, Found: 492.1618.

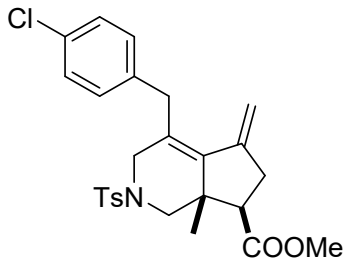




^{13}C NMR ($CDCl_3$, 150 MHz, TMS)

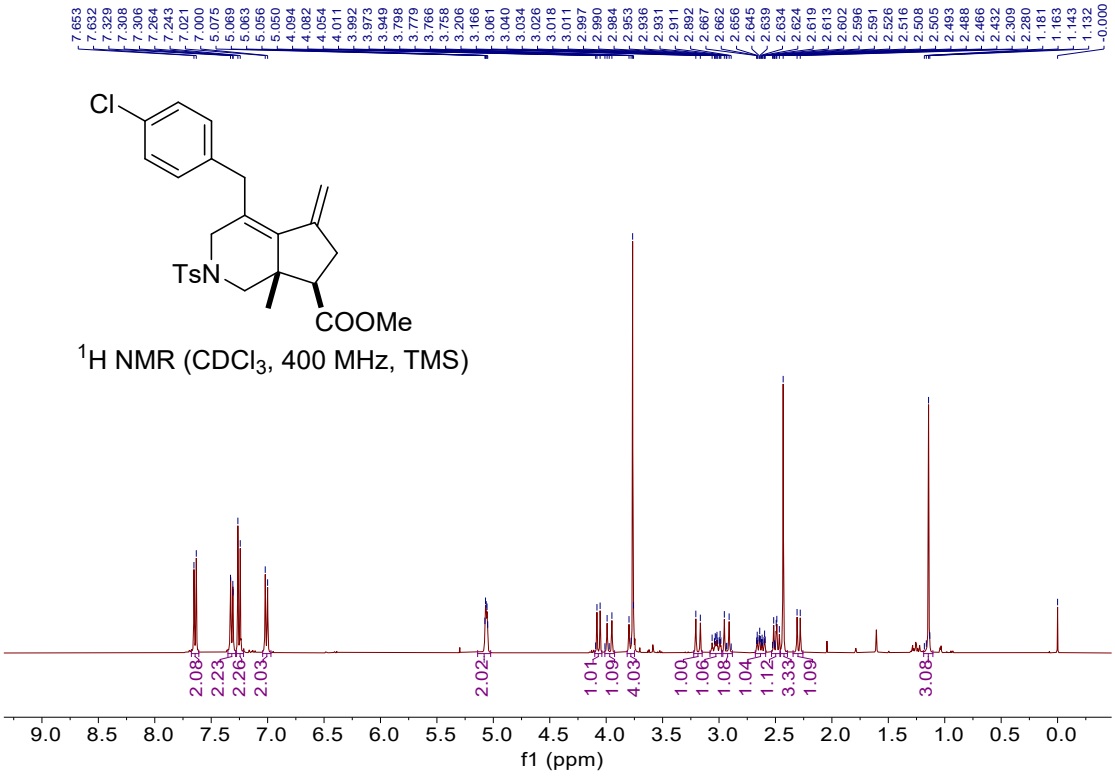


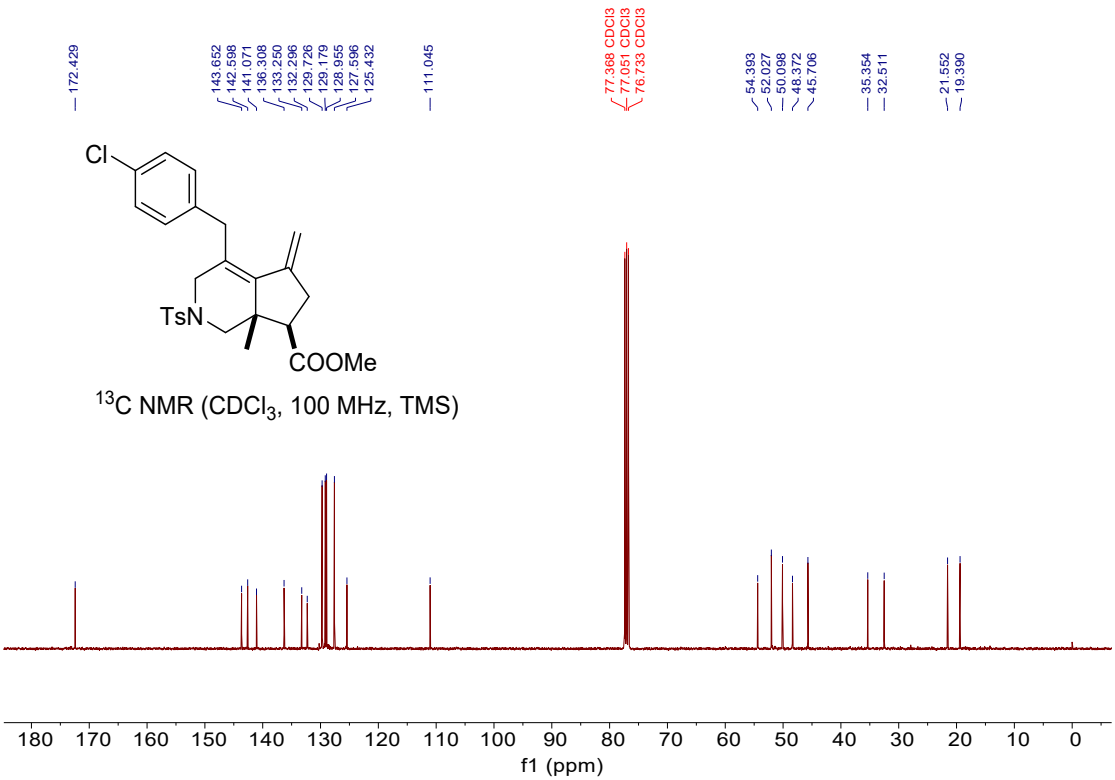
^{19}F NMR ($CDCl_3$, 565 MHz, TMS)

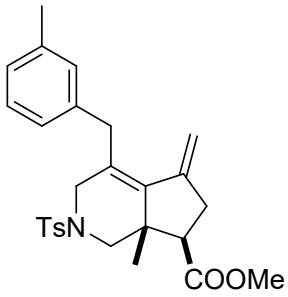


(cis)-methyl-4-(4-chlorobenzyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2r)

A yellow oil, 80% yield, 38.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 5.14 – 5.02 (m, 2H), 4.07 (d, *J* = 11.2 Hz, 1H), 3.97 (d, *J* = 17.2 Hz, 1H), 3.73 – 3.78 (m, 4H), 3.19 (d, *J* = 16.0 Hz, 1H), 3.08 – 2.98 (m, 1H), 2.93 (d, *J* = 17.2 Hz, 1H), 2.68 – 2.59 (m, 1H), 2.54 – 2.46 (m, 1H), 2.43 (s, 3H), 2.29 (d, *J* = 11.2 Hz, 1H), 1.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 143.7, 142.6, 141.1, 136.3, 133.2, 132.3, 129.7, 129.2, 129.0, 127.6, 125.4, 111.0, 54.4, 52.0, 50.1, 48.4, 45.7, 35.4, 32.5, 21.6, 19.4. IR (neat) ν 662, 1091, 1346, 1597, 1733, 2932 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{28}NO_4SClNa$ $(M+Na)^+$: 508.1320, Found: 508.1327.

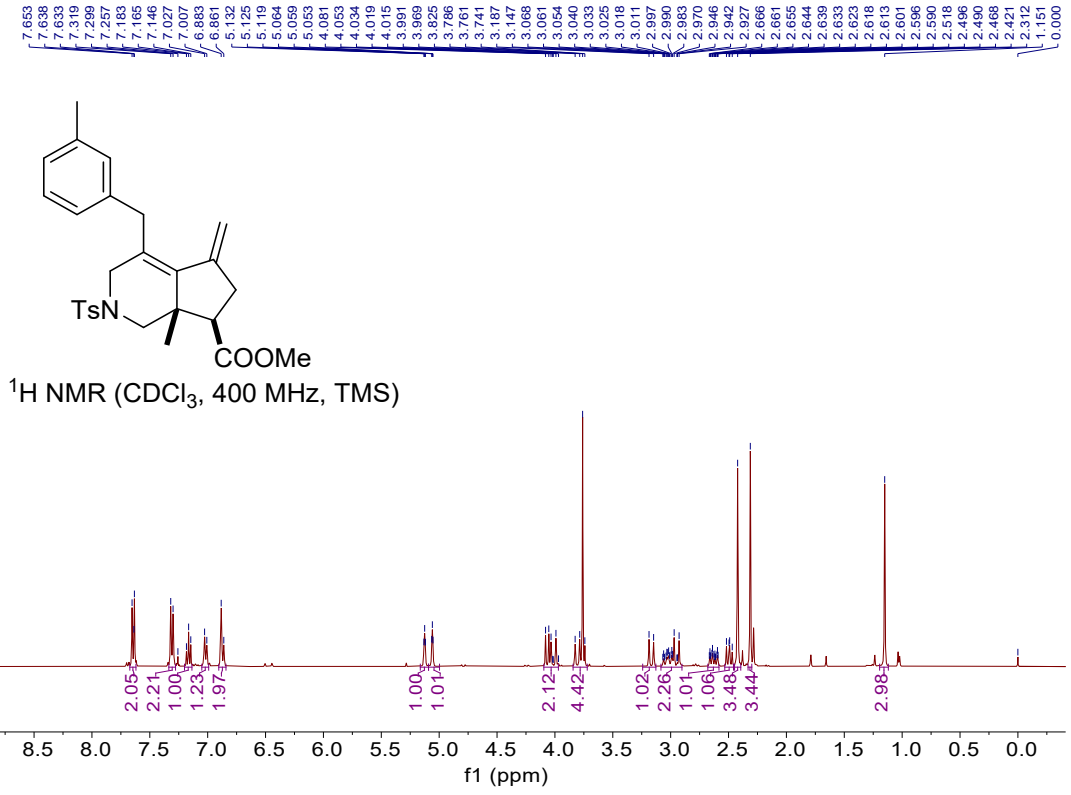


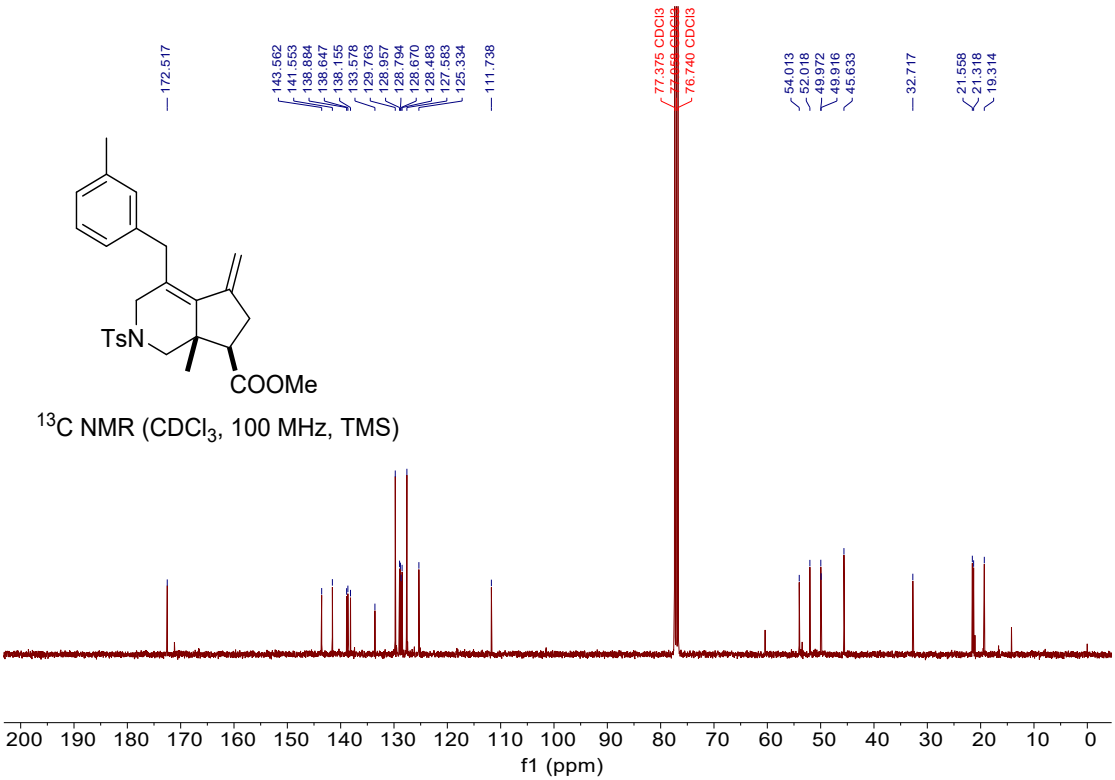

172.429
143.652
142.598
141.071
136.308
133.250
132.296
129.726
129.179
128.955
127.596
125.432
111.045
77.368 CDCl3
77.051 CDCl3
76.733 CDCl3
54.393
52.027
50.098
48.372
45.706
35.354
32.511
21.552
19.390
Cl
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

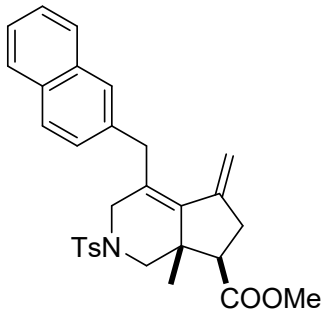


(cis)-methyl-7a-methyl-4-(3-methylbenzyl)-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2s)

A colorless oil, 92% yield, 42.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.16 (t, J = 7.5 Hz, 1H), 7.02 (d, J = 7.7 Hz, 1H), 6.87 (d, J = 9.0 Hz, 2H), 5.13 (d, J = 2.6 Hz, 1H), 5.06 (d, J = 2.2 Hz, 1H), 4.10 – 3.97 (m, 2H), 3.84 – 3.72 (m, 4H), 3.17 (d, J = 15.9 Hz, 1H), 3.08 – 2.90 (m, 2H), 2.68 – 2.58 (m, 1H), 2.49 (dd, J = 11.1, 8.9 Hz, 1H), 2.42 (s, 3H), 2.31 (s, 3H), 1.15 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 143.6, 141.6, 138.9, 138.6, 138.2, 133.6, 129.8, 129.0, 128.8, 128.7, 128.5, 127.6, 125.3, 111.7, 54.0, 52.0, 50.0, 49.9, 45.6, 32.7, 21.6, 21.3, 19.3. IR (neat) ν 662, 1091, 1330, 1598, 1735, 2852, 2924 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{31}NO_4SNa$ $(M+Na)^+$: 488.1866, Found: 488.1862.

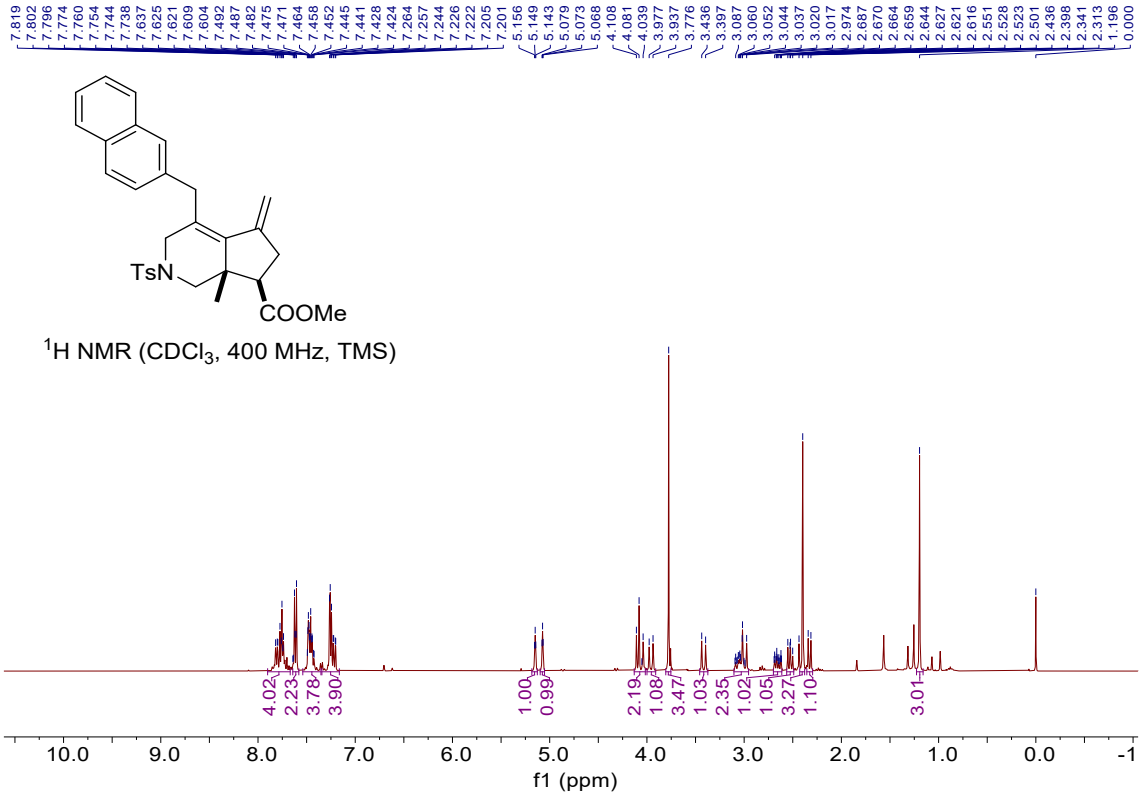


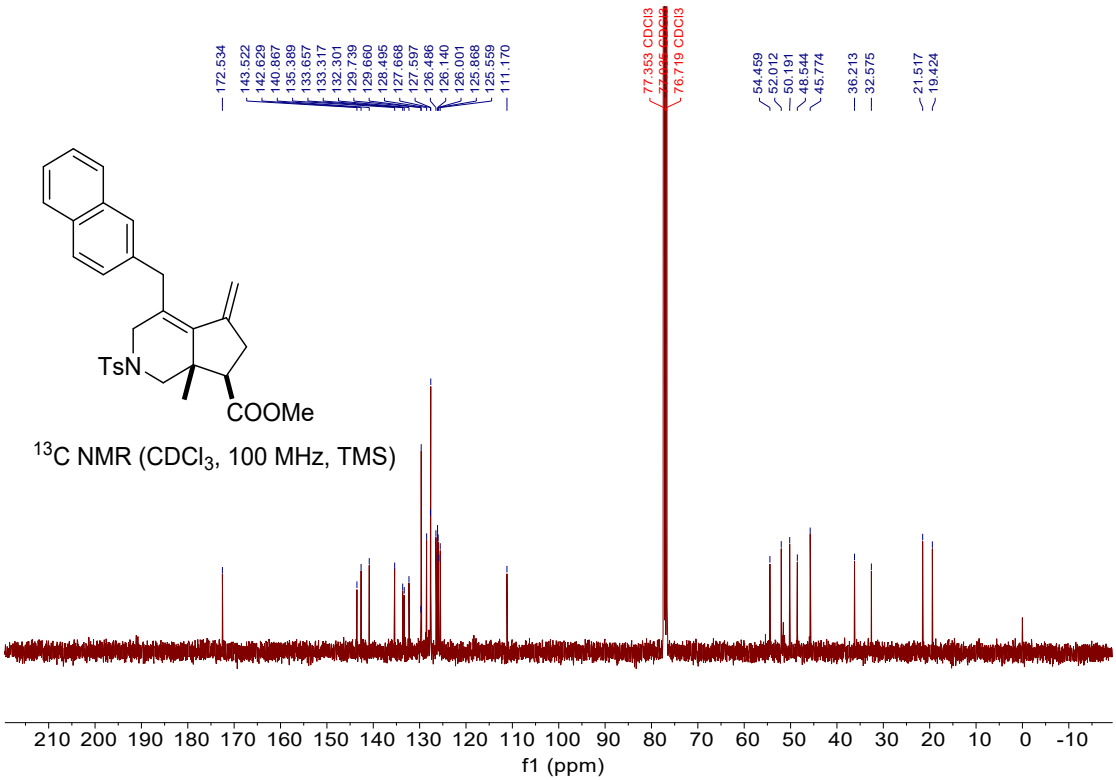

172.517
143.562
141.553
138.884
138.647
138.155
133.578
129.763
128.957
128.794
128.670
128.483
127.583
125.334
111.738
77.375 CDCl3
77.062 CDCl3
76.740 CDCl3
54.013
52.018
49.972
49.916
45.633
32.717
21.558
21.318
19.314
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

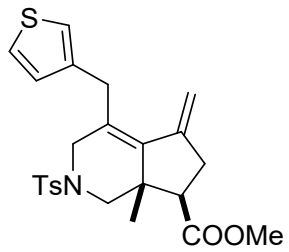


(cis)-methyl-7a-methyl-5-methylene-4-(naphthalen-2-ylmethyl)-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2t)

A colorless oil, 88% yield, 44.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.67 (m, 4H), 7.64 – 7.58 (m, 2H), 7.50 – 7.44 (m, 3H), 7.25 – 7.20 (m, 2H), 5.15 (d, *J* = 2.4 Hz, 1H), 5.08 (d, *J* = 2.4 Hz, 1H), 4.12 – 4.03 (m, 2H), 3.96 (d, *J* = 16.0 Hz, 1H), 3.78 (s, 3H), 3.42 (d, *J* = 16.0 Hz, 1H), 3.09 – 2.96 (m, 2H), 2.71 – 2.60 (m, 1H), 2.56 – 2.49 (m, 1H), 2.42 – 2.32 (m, 4H), 1.20 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 143.5, 142.6, 140.9, 135.4, 133.7, 133.3, 132.3, 129.7, 129.7, 128.5, 127.7, 127.6, 126.5, 126.1, 126.0, 125.9, 125.6, 111.2, 54.5, 52.0, 50.2, 48.5, 45.8, 36.2, 32.6, 21.5, 19.4. IR (neat) ν 661, 1091, 1349, 1598, 1736, 2954 cm^{-1}. HRMS (ESI) calcd. for $C_{30}H_{31}NO_4SNa$ $(M+Na)^+$: 524.1866, Found: 524.1867.

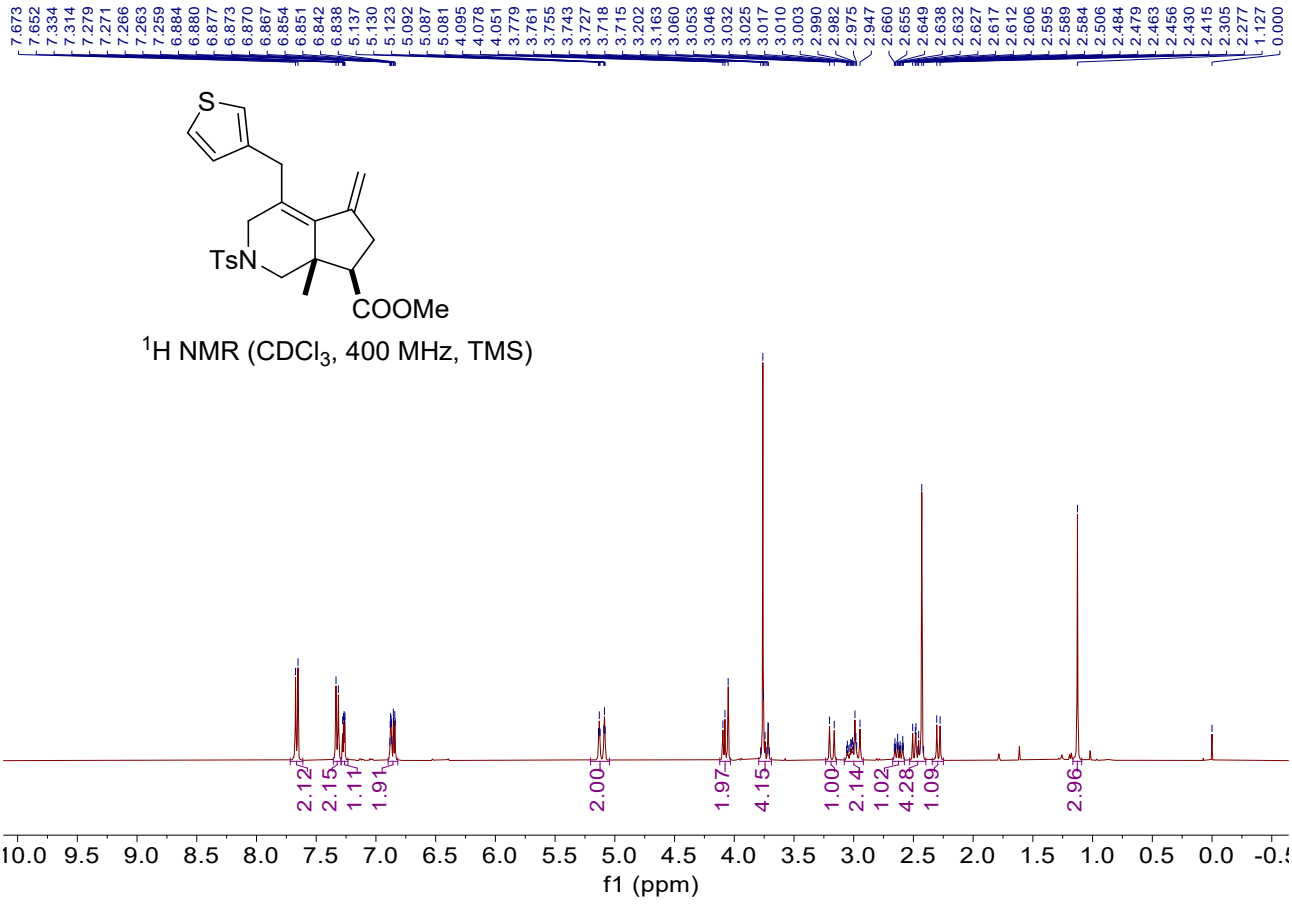


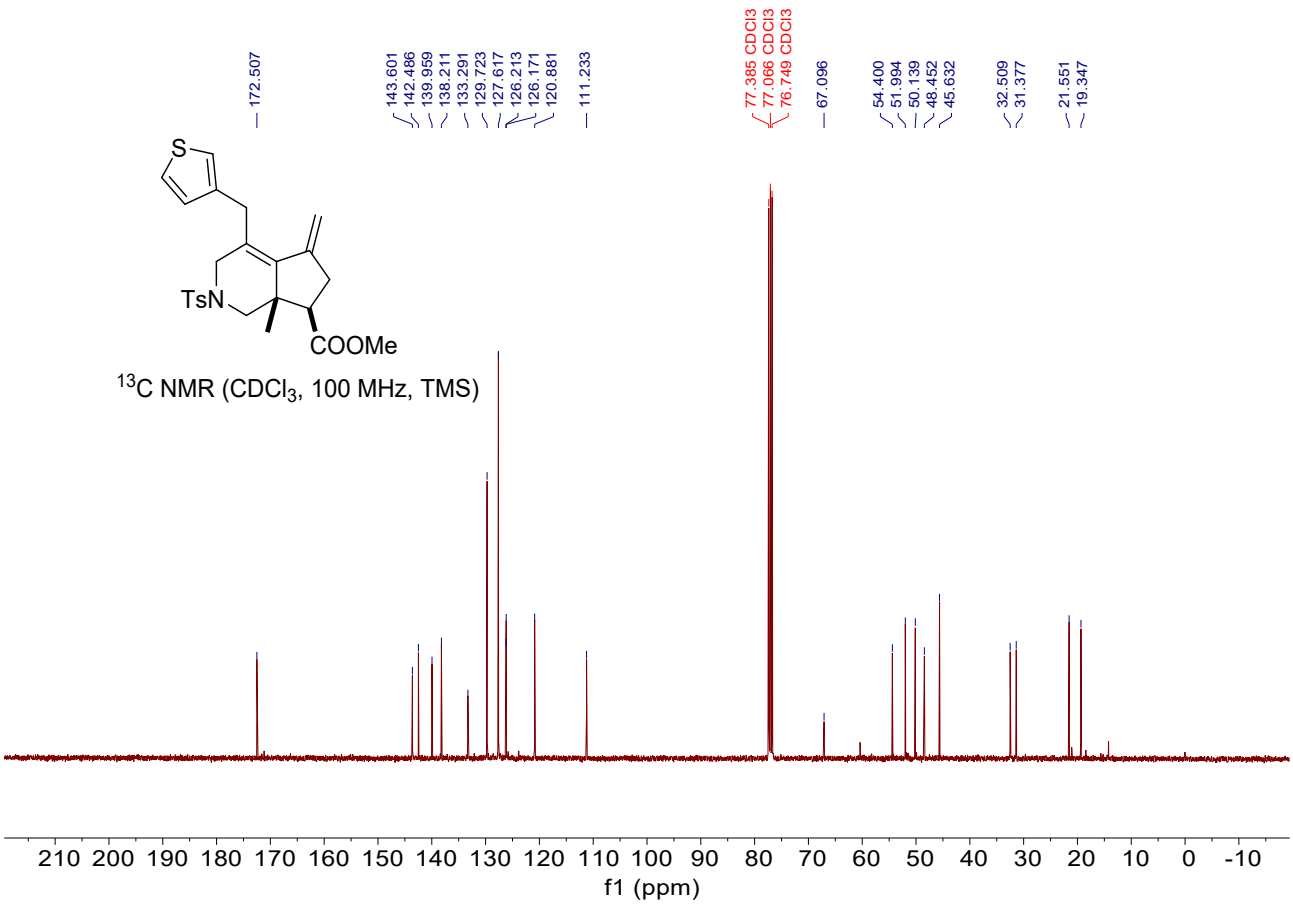

172.534
143.522
142.629
140.867
135.389
133.657
133.317
132.301
129.739
129.660
128.495
127.668
127.597
126.486
126.140
126.001
125.868
125.559
111.170
77.353 CDCl3
77.036 CDCl3
76.719 CDCl3
54.459
52.012
50.191
48.544
45.774
36.213
32.575
21.517
19.424
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



(cis)-methyl-7a-methyl-5-methylene-4-(thiophen-3-ylmethyl)-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2u)

A yellow oil, 90% yield, 41.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.23 (m, 1H), 6.90 – 6.82 (m, 2H), 5.11 (dt, *J* = 16.9, 2.4 Hz, 2H), 4.12 – 4.03 (m, 2H), 3.80 – 3.69 (m, 4H), 3.18 (d, *J* = 15.6 Hz, 1H), 3.08 – 2.92 (m, 2H), 2.62 (d, *J* = 17.2 Hz, 1H), 2.53 – 2.40 (m, 4H), 2.29 (d, *J* = 11.2 Hz, 1H), 1.13 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 143.6, 142.5, 140.0, 138.2, 133.3, 129.7, 127.6, 126.2, 126.2, 120.9, 111.2, 67.1, 54.4, 52.0, 50.1, 48.5, 45.6, 32.5, 31.4, 21.6, 19.3. IR (neat) ν 660, 1091, 1352, 1597, 1733, 2963 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{27}NO_4S_2Na$ $(M+Na)^+$: 480.1274, Found: 480.1273.




172.507
143.601
142.486
139.959
138.211
133.291
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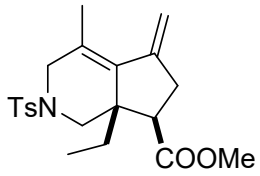
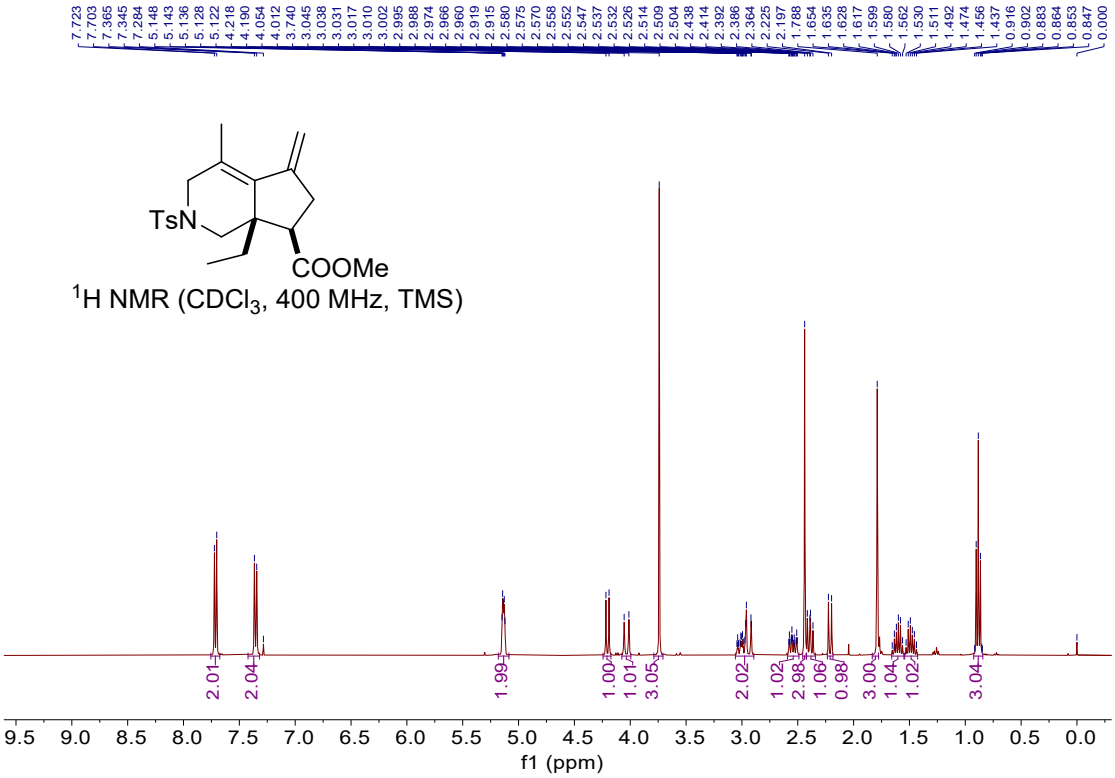
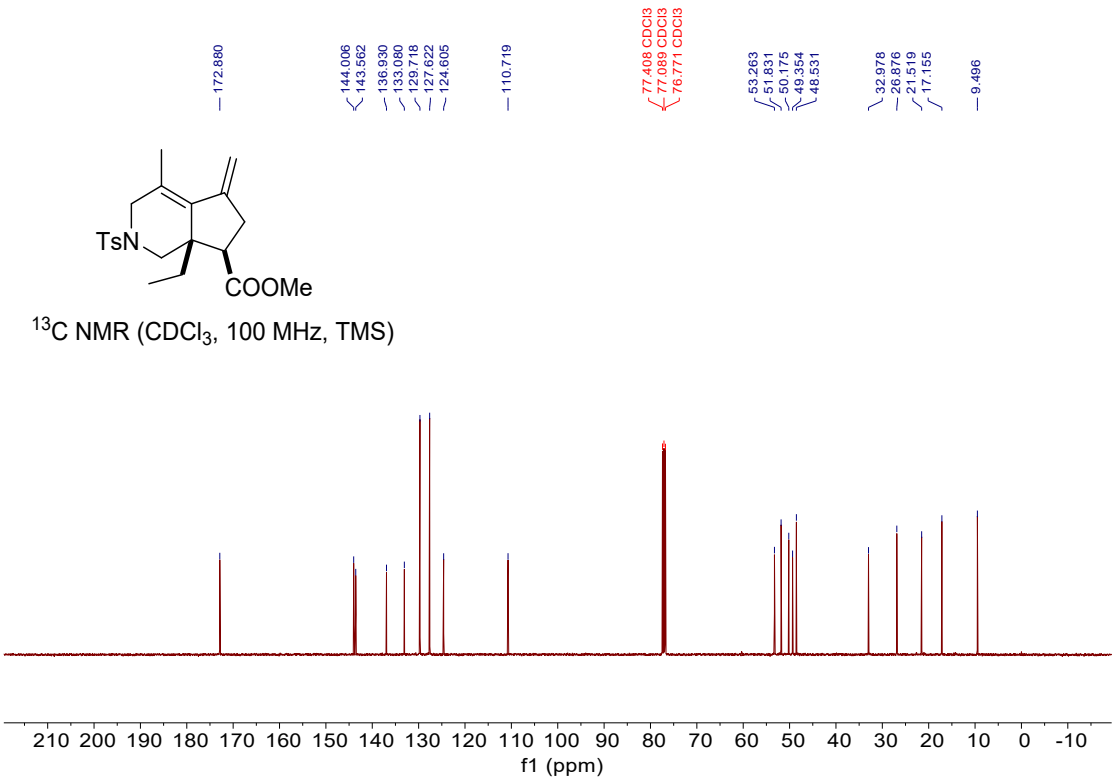
127.617
126.213
126.171
120.881
111.233
77.385 CDCl3
77.066 CDCl3
76.749 CDCl3
67.096
54.400
51.994
50.139
48.452
45.632
32.509
31.377
21.551
19.347
S
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



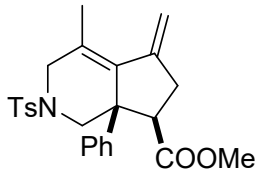
(cis)-methyl-7a-ethyl-4-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2v)

A colorless oil, 92% yield, 36.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.18 – 5.09 (m, 2H), 4.20 (d, *J* = 11.2 Hz, 1H), 4.03 (d, *J* = 17.2 Hz, 1H), 3.74 (s, 3H), 3.06 – 2.89 (m, 2H), 2.59 – 2.49 (m, 1H), 2.44 (s, 3H), 2.42 – 2.34 (m, 1H), 2.21 (d, *J* = 11.2 Hz, 1H), 1.79 (s, 3H), 1.66 – 1.55 (m, 1H), 1.48 (dq, *J* = 14.8, 7.6 Hz, 1H), 0.88 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 144.0, 143.6, 136.9, 133.1, 129.7, 127.6, 124.6, 110.7, 53.3, 51.8, 50.2, 49.4, 48.5, 33.0, 26.9, 21.5, 17.2, 9.5. IR (neat) ν 661, 1091, 1344, 1597, 1734, 2951 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1554.



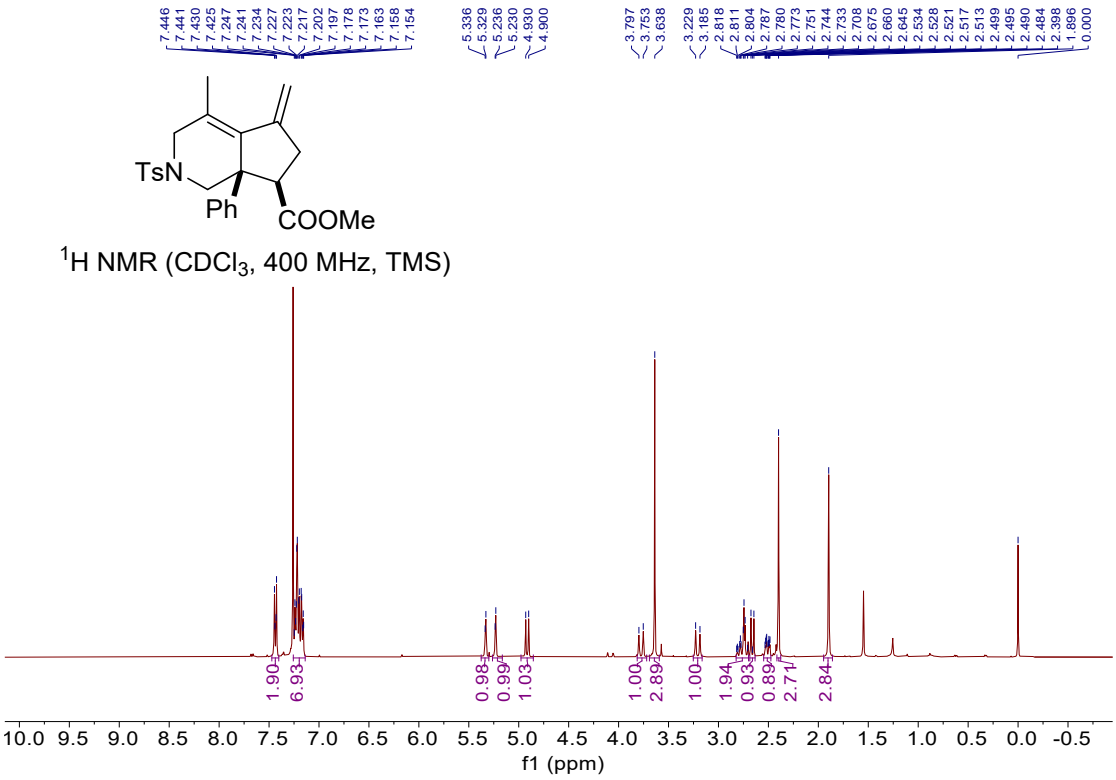


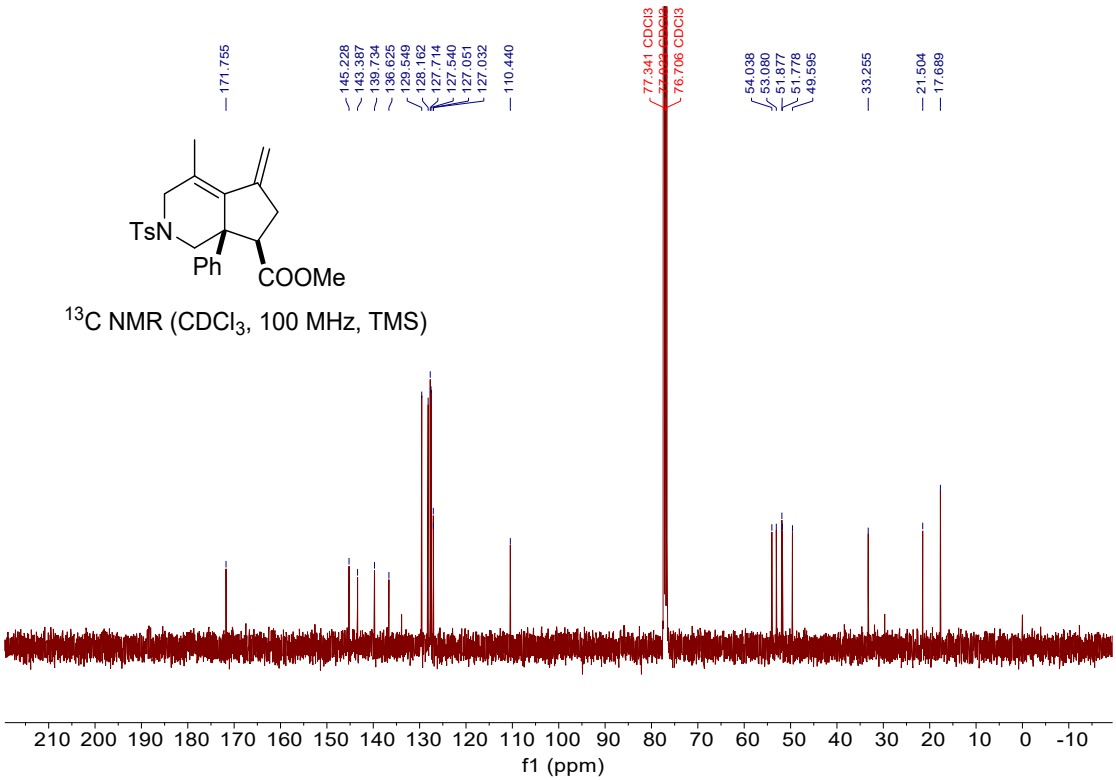
^{13}C NMR ($CDCl_3$, 100 MHz, TMS)

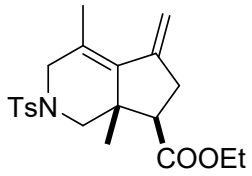


(cis)-methyl-4-methyl-5-methylene-7a-phenyl-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2w)

A colorless oil, 80% yield, 35.0 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.40 (m, 2H), 7.26 – 7.14 (m, 7H), 5.33 (d, *J* = 2.8 Hz, 1H), 5.23 (d, *J* = 2.8 Hz, 1H), 4.92 (d, *J* = 11.6 Hz, 1H), 3.77 (d, *J* = 17.4 Hz, 1H), 3.64 (s, 3H), 3.21 (d, *J* = 17.4 Hz, 1H), 2.82 – 2.70 (m, 2H), 2.66 (d, *J* = 11.6 Hz, 1H), 2.55 – 2.48 (m, 1H), 2.40 (s, 3H), 1.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 145.2, 143.4, 139.7, 136.6, 129.5, 128.2, 127.7, 127.5, 127.1, 127.0, 110.4, 54.0, 53.1, 51.9, 51.8, 49.6, 33.3, 21.5, 17.7. IR (neat) ν 659, 1090, 1350, 1579, 1730, 2948 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{27}NO_4SNa$ $(M+Na)^+$: 460.1553, Found: 460.1545.

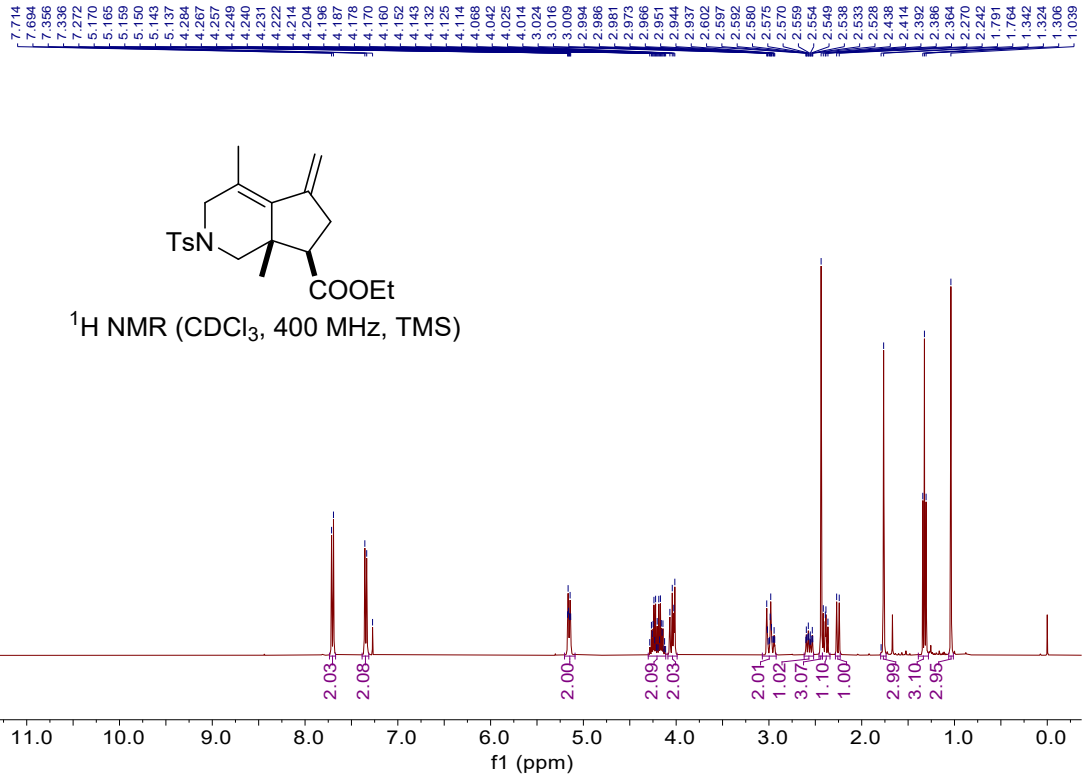


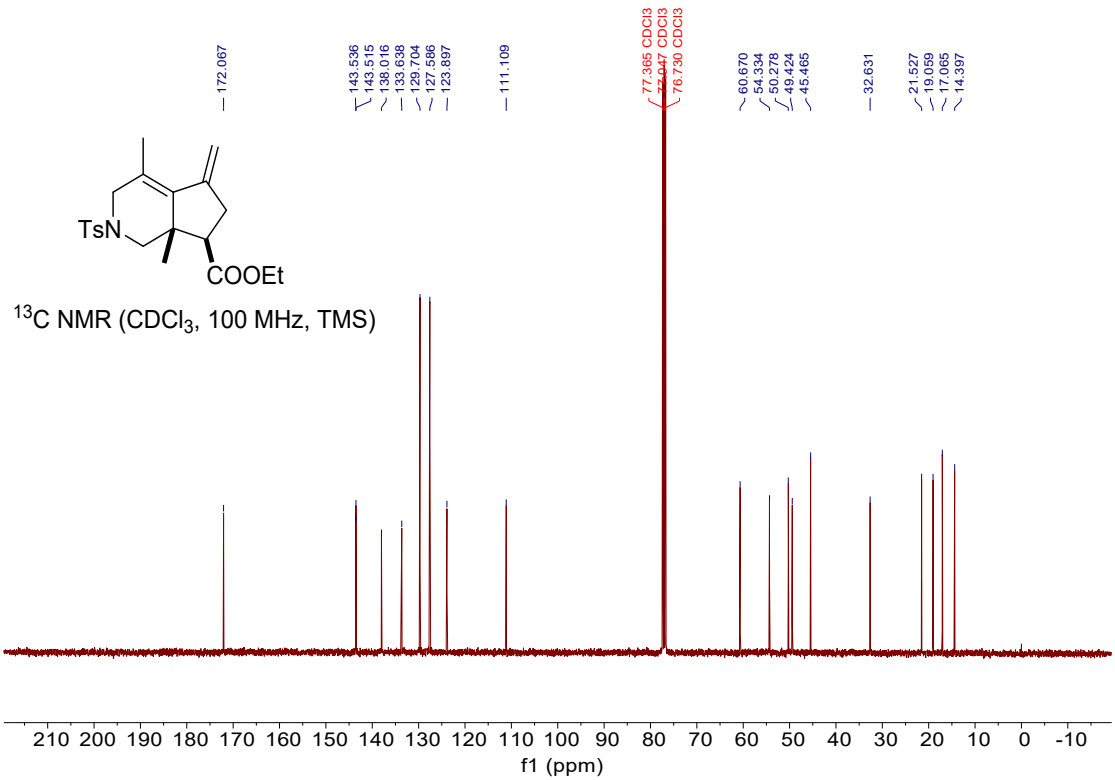

171.755
145.228
143.387
139.734
136.625
129.549
128.162
127.714
127.540
127.051
127.032
110.440
77.341 CDCl3
76.706 CDCl3
54.038
53.080
51.877
51.778
49.595
33.255
21.504
17.689
TsN
Ph
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

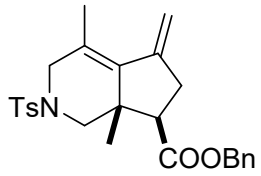


(cis)-ethyl-4,7a-dimethyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2x)

A colorless oil, 90% yield, 35.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.20 – 5.09 (m, 2H), 4.30 – 4.11 (m, 2H), 4.09 – 3.99 (m, 2H), 3.07 – 2.92 (m, 2H), 2.62 – 2.52 (m, 1H), 2.44 (s, 3H), 2.42 – 2.34 (m, 1H), 2.26 (d, *J* = 11.2 Hz, 1H), 1.76 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.04 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 143.5, 143.5, 138.0, 133.6, 129.7, 127.6, 123.9, 111.1, 60.7, 54.3, 50.3, 49.4, 45.5, 32.6, 21.5, 19.1, 17.1, 14.4. IR (neat) ν 661, 1091, 1347, 1597, 1731, 2976 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1547.

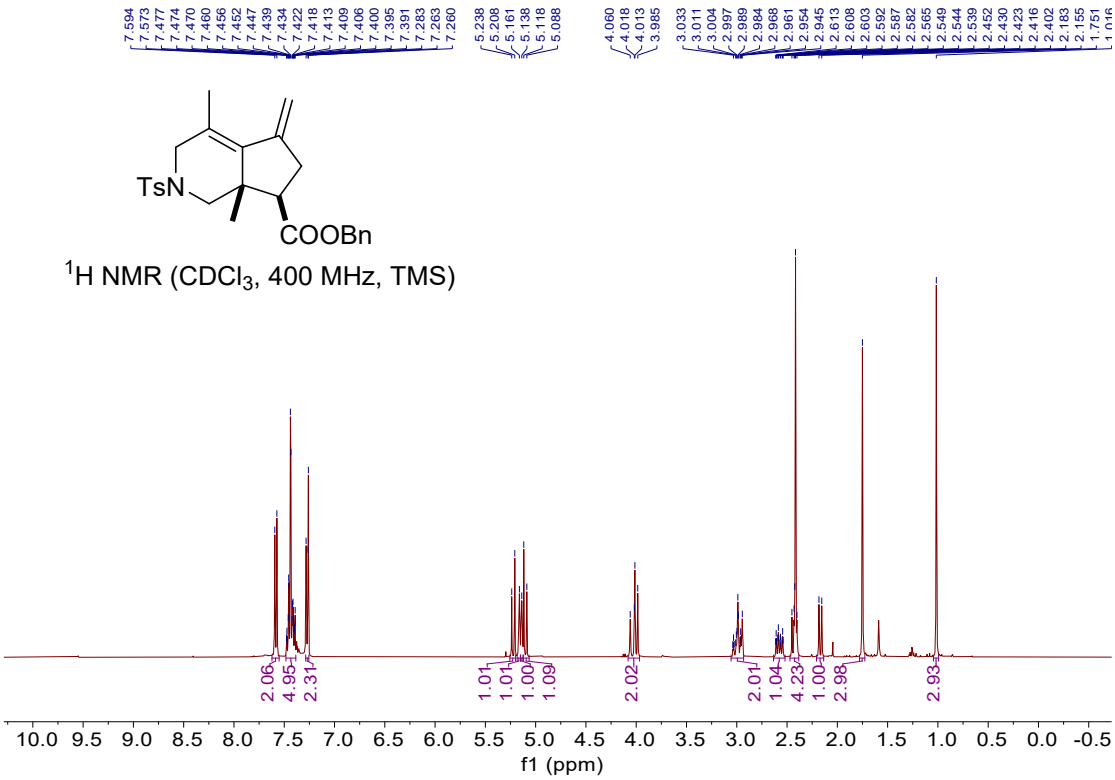


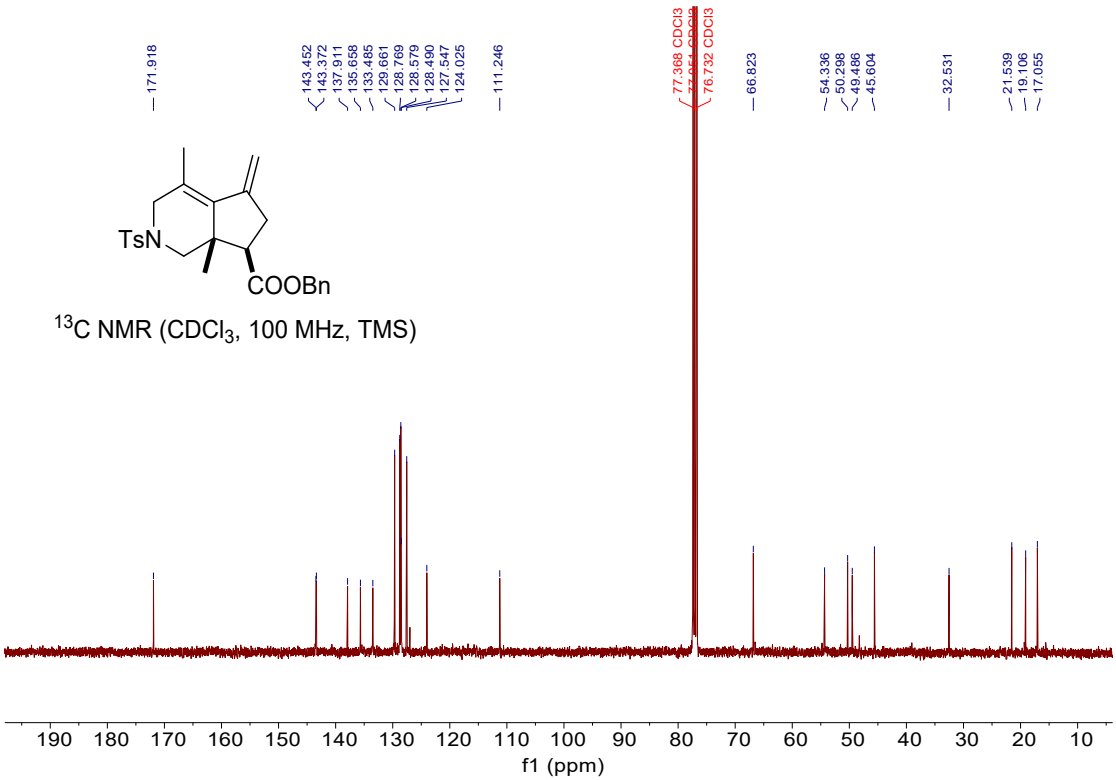

172.067
143.536
143.515
138.016
133.638
129.704
127.586
123.897
111.109
77.365 CDCl3
77.047 CDCl3
76.730 CDCl3
60.670
54.334
50.278
49.424
45.465
32.631
21.527
19.059
17.065
14.397
TsN
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

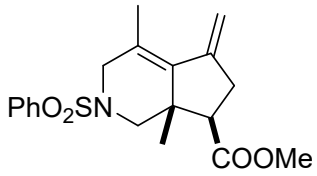


(cis)-benzyl-4,7a-dimethyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2y)

A colorless oil, 90% yield, 40.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.39 (m, 5H), 7.29 – 7.26 (m, 2H), 5.22 (d, *J* = 12.0 Hz, 1H), 5.16 (s, 1H), 5.14 (s, 1H), 5.10 (d, *J* = 12.0 Hz, 1H), 4.08 – 3.97 (m, 2H), 3.06 – 2.93 (m, 2H), 2.63 – 2.52 (m, 1H), 2.47 – 2.38 (m, 4H), 2.17 (d, *J* = 11.2 Hz, 1H), 1.75 (s, 3H), 1.02 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 143.5, 143.4, 137.9, 135.7, 133.5, 129.7, 128.8, 128.6, 128.5, 127.5, 124.0, 111.2, 66.8, 54.3, 50.3, 49.5, 45.6, 32.5, 21.5, 19.1, 17.1. IR (neat) ν 661, 908, 1159, 1355, 1596, 1735, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1714.

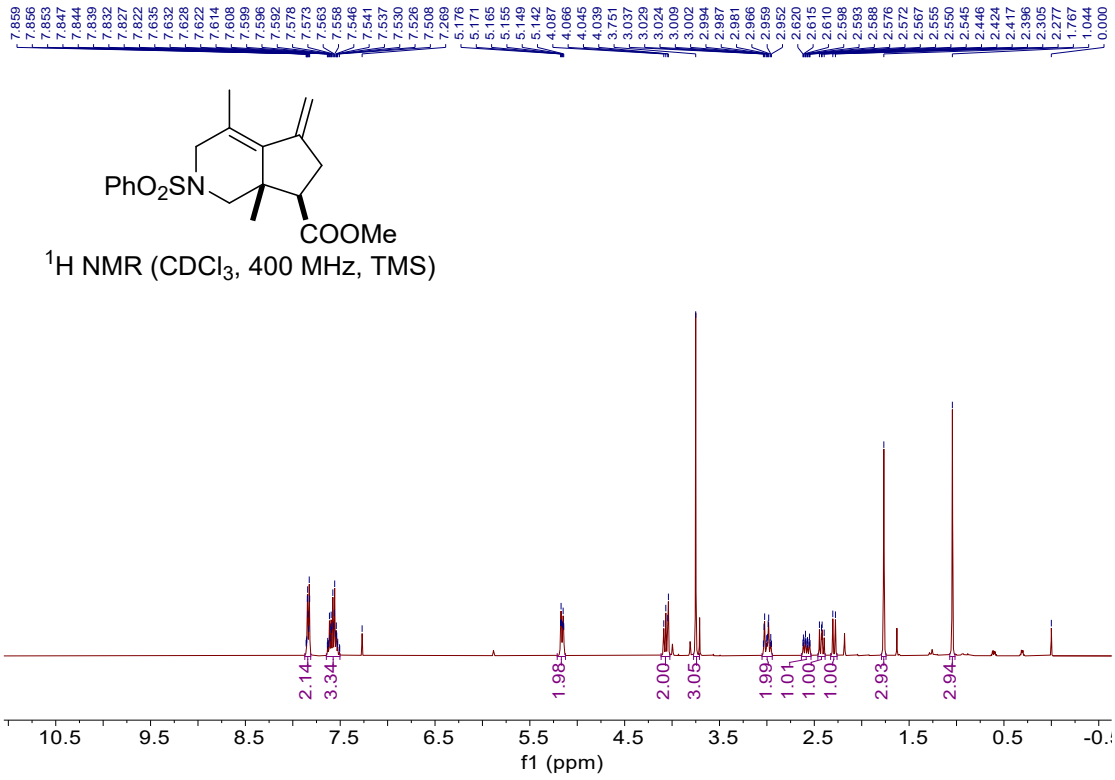


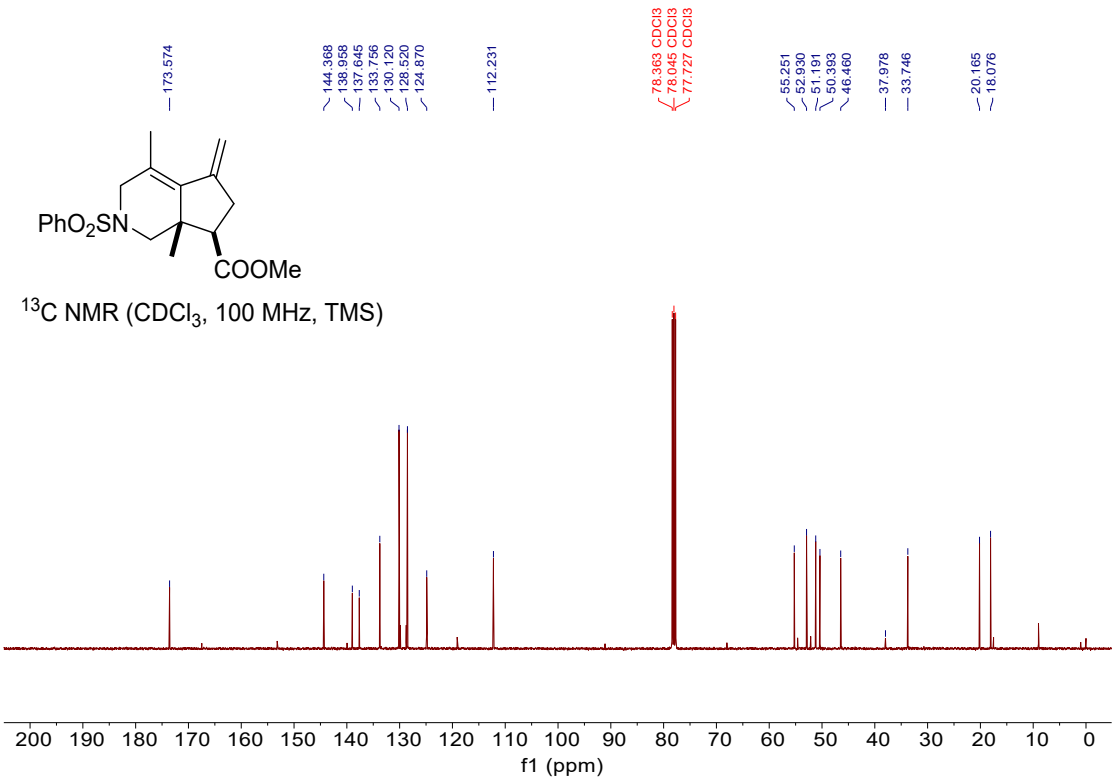

171.918
143.452
143.372
137.911
135.658
133.485
129.661
128.769
128.579
128.490
127.547
124.025
111.246
77.368 CDCl3
77.051 CDCl3
76.732 CDCl3
66.823
54.336
50.298
49.486
45.604
32.531
21.539
19.106
17.055
TsN
COOBn
13C NMR (CDCl3, 100 MHz, TMS)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

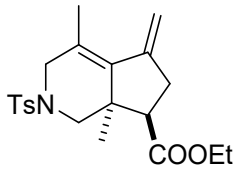


(cis)-methyl-4,7a-dimethyl-5-methylene-2-(phenylsulfonyl)-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (2z)

A colorless oil, 90% yield, 32.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.81 (m, 2H), 7.65 – 7.50 (m, 3H), 5.21 – 5.12 (m, 2H), 4.12 – 4.02 (m, 2H), 3.75 (s, 3H), 3.05 – 2.94 (m, 2H), 2.64 – 2.53 (m, 1H), 2.46 – 2.39 (m, 1H), 2.29 (d, J = 11.2 Hz, 1H), 1.77 (s, 3H), 1.04 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 144.4, 139.0, 137.6, 133.8, 130.1, 128.5, 124.9, 112.2, 55.3, 52.9, 51.2, 50.4, 46.5, 38.0, 33.7, 20.2, 18.1. IR (neat) ν 661, 803, 1091, 1350, 1661, 1717, 2952 cm^{-1}. HRMS (ESI) calcd. for $C_{19}H_{23}NO_4SNa$ $(M+Na)^+$: 384.1240, Found: 384.1231.

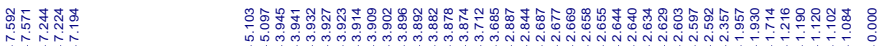


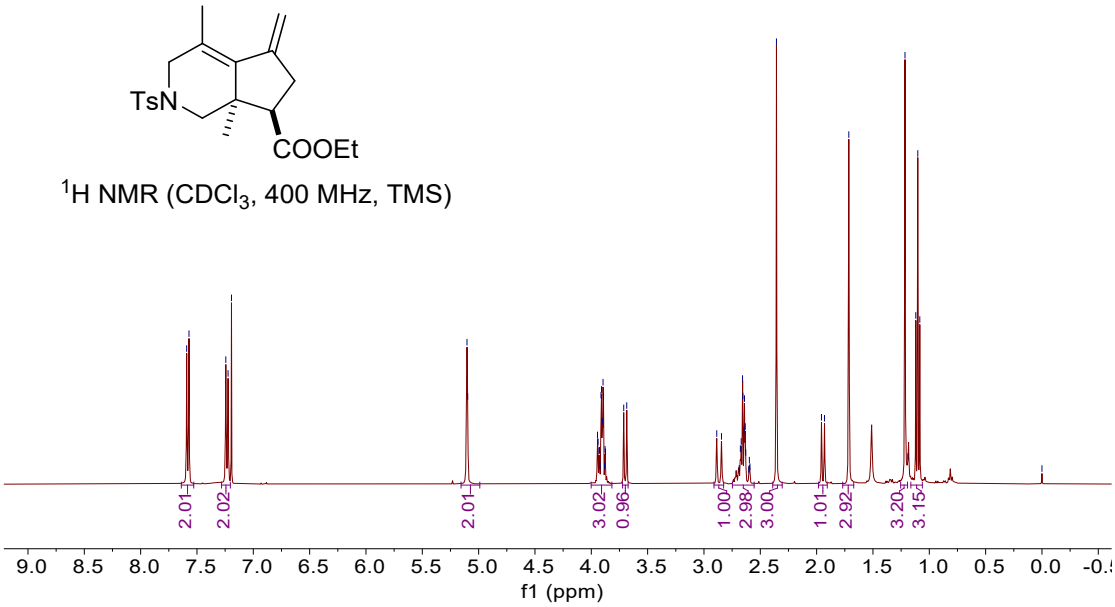

173.574
144.368
138.958
137.645
133.756
130.120
128.520
124.870
112.231
78.363 CDCl3
78.045 CDCl3
77.727 CDCl3
55.251
52.930
51.191
50.393
46.460
37.978
33.746
20.165
18.076
PhO2SN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

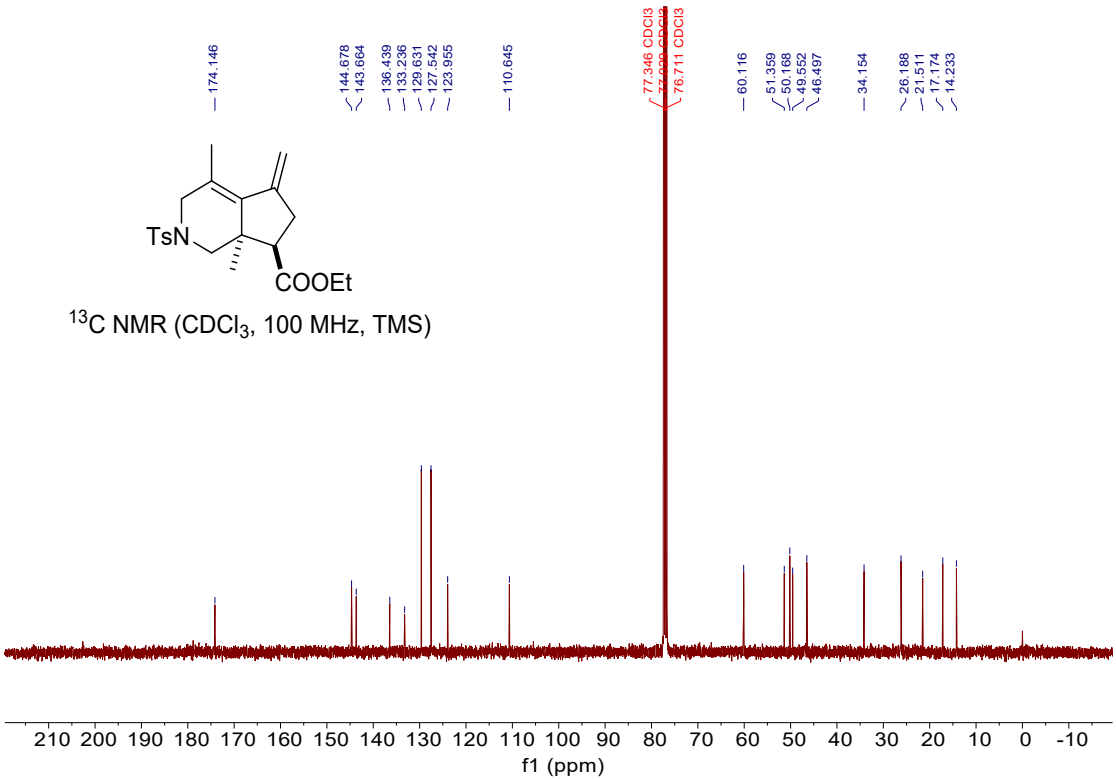


(trans)-ethyl-4,7a-dimethyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4a)

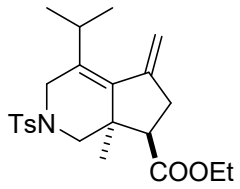
A colorless oil, 94% yield, 36.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 5.16 – 4.99 (m, 2H), 4.00 – 3.82 (m, 3H), 3.70 (d, *J* = 10.8 Hz, 1H), 2.87 (d, *J* = 16.8 Hz, 1H), 2.75 – 2.55 (m, 3H), 2.36 (s, 3H), 1.94 (d, *J* = 10.8 Hz, 1H), 1.71 (s, 3H), 1.22 (s, 3H), 1.10 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 144.7, 143.7, 136.4, 133.2, 129.6, 127.5, 124.0, 110.6, 60.1, 51.4, 50.2, 49.6, 46.5, 34.2, 26.2, 21.5, 17.2, 14.2. IR (neat) ν 660, 817, 1345, 1597, 1731, 2923 cm^{-1}. HRMS (ESI) calcd. for $C_{21}H_{27}NO_4SNa$ $(M+Na)^+$: 412.1553, Found: 412.1550.





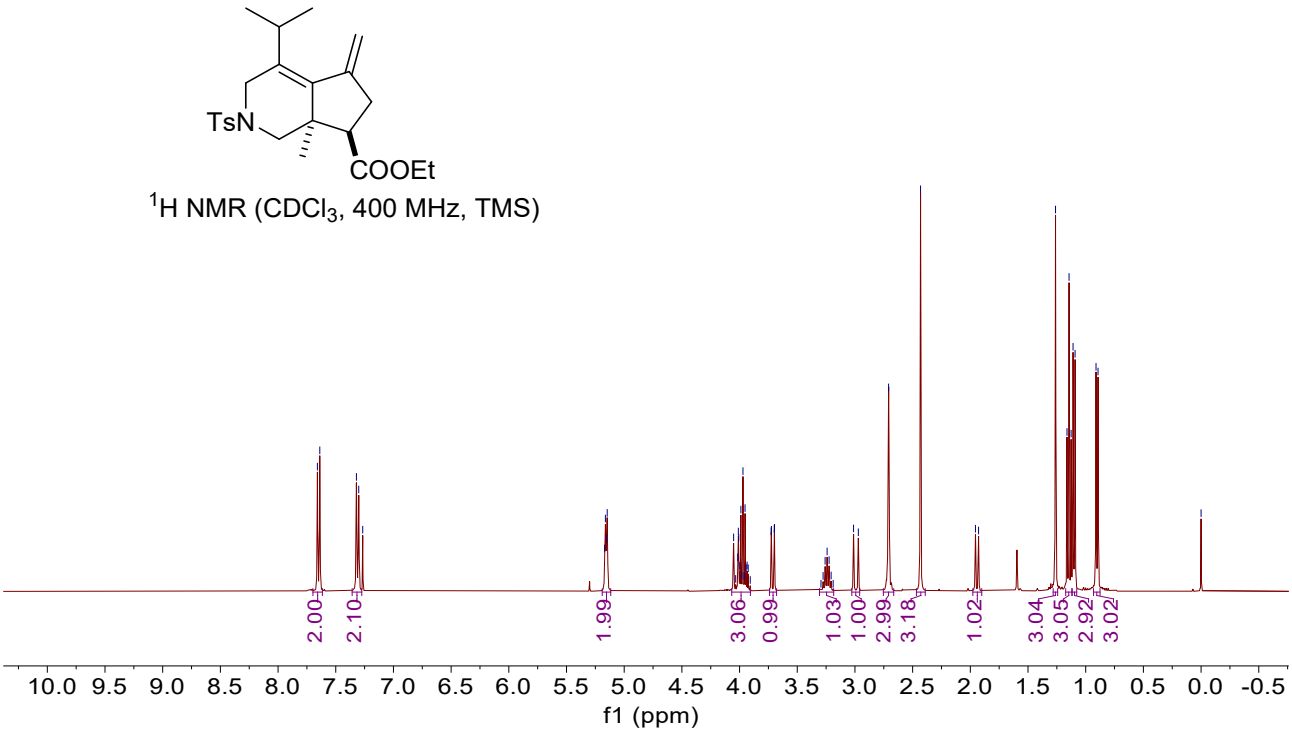


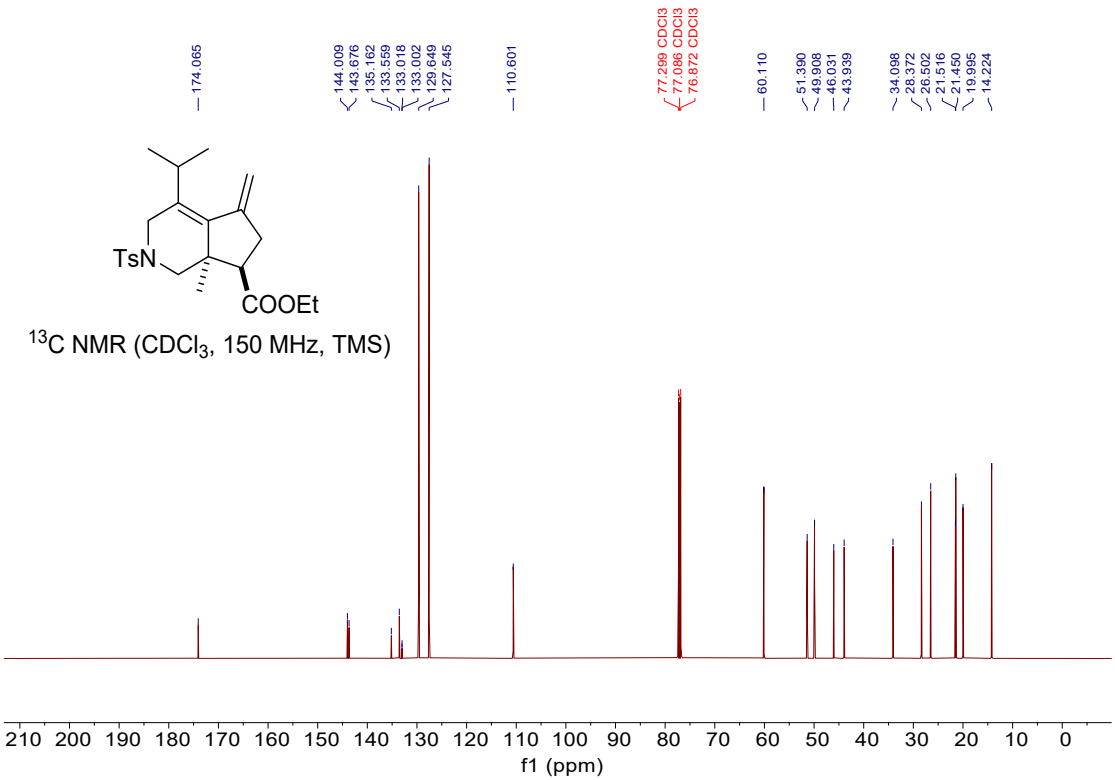
^{13}C NMR ($CDCl_3$, 100 MHz, TMS)

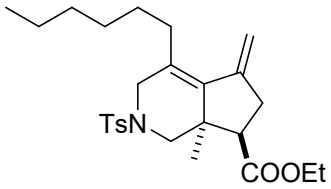


(trans)-ethyl-4-isopropyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4b)

A colorless oil, 90% yield, 37.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.21 – 5.11 (m, 2H), 4.08 – 3.91 (m, 3H), 3.71 (dd, *J* = 10.8, 1.2 Hz, 1H), 3.23 (h, *J* = 7.2 Hz, 1H), 2.99 (d, *J* = 16.4 Hz, 1H), 2.74 – 2.67 (m, 3H), 2.43 (s, 3H), 1.94 (d, *J* = 10.8 Hz, 1H), 1.26 (s, 3H), 1.14 (t, *J* = 7.2 Hz, 3H), 1.10 (d, *J* = 7.2 Hz, 3H), 0.90 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.1, 144.0, 143.7, 135.2, 133.6, 133.0, 133.0, 129.6, 127.5, 110.6, 60.1, 51.4, 49.9, 46.0, 43.9, 34.1, 28.4, 26.5, 21.5, 21.5, 20.0, 14.2. IR (neat) ν 661, 814, 1343, 1597, 1728, 2980 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{31}NO_4SNa$ $(M+Na)^+$: 440.1866, Found: 440.1859.

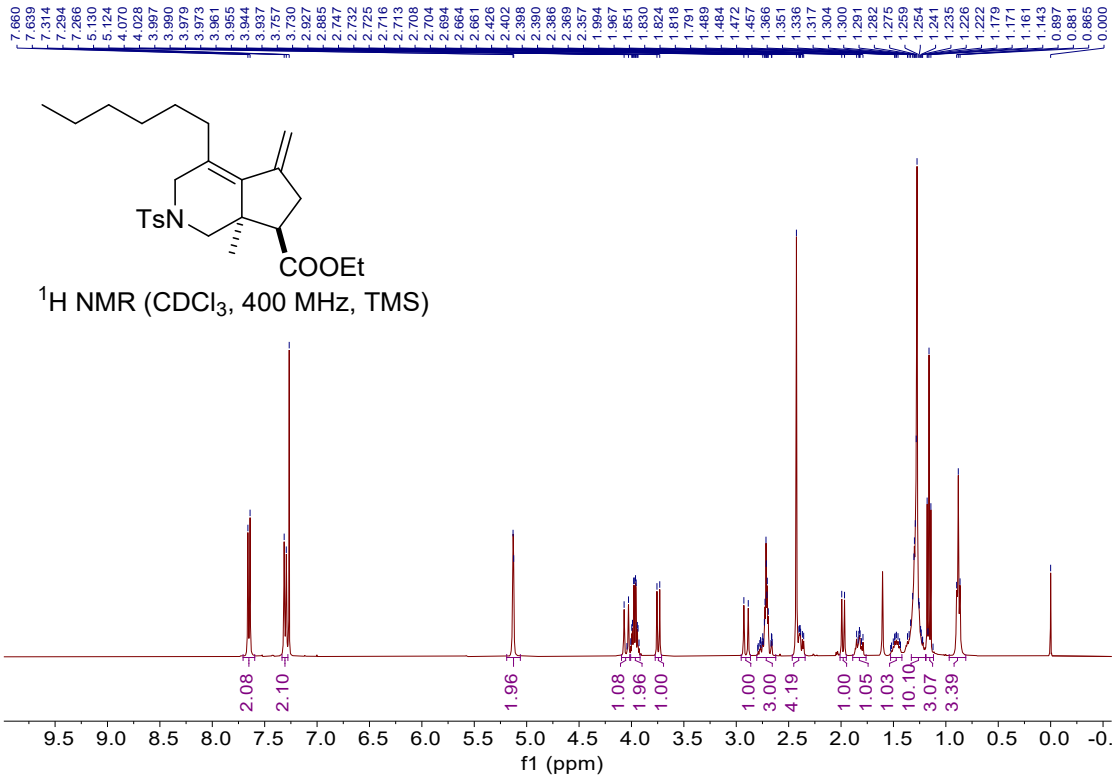


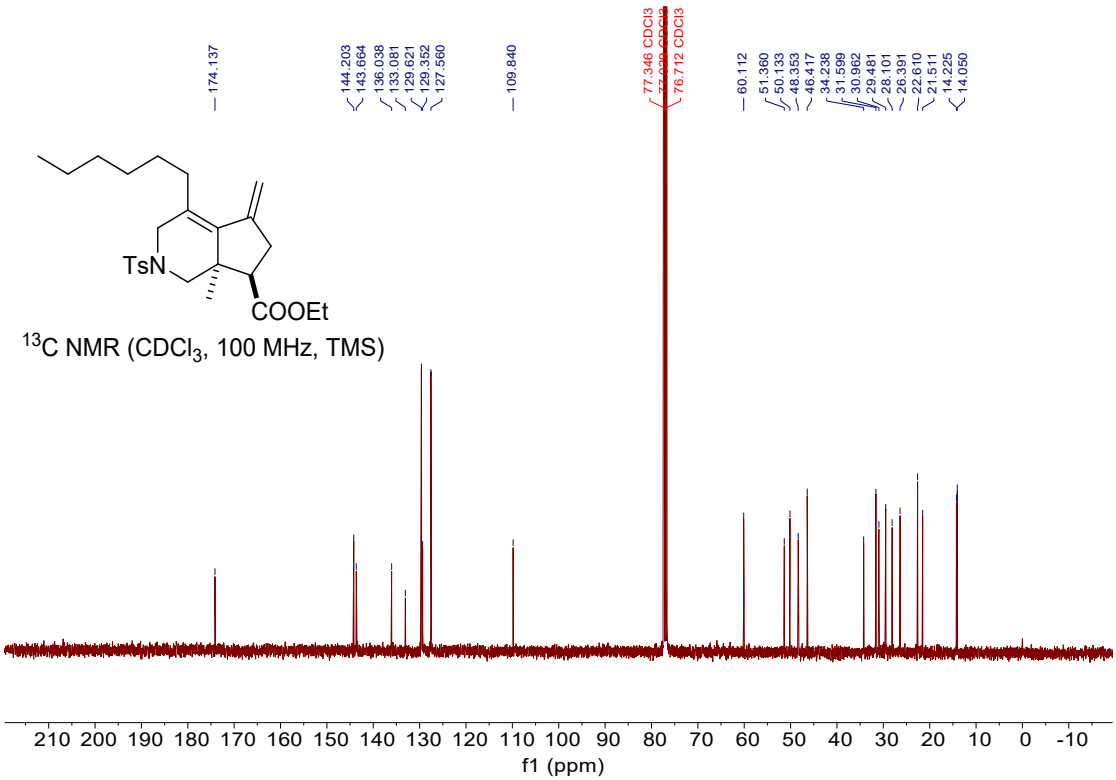

174.065
144.009
143.676
135.162
133.559
133.018
133.002
129.649
127.545
110.601
77.299 CDCl3
77.086 CDCl3
76.872 CDCl3
60.110
51.390
49.908
46.031
43.939
34.098
28.372
26.502
21.516
21.450
19.995
14.224
TsN
COOEt
13C NMR (CDCl3, 150 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



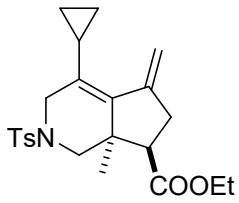
(trans)-ethyl-4-hexyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4c)

A colorless oil, 90% yield, 41.3 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.19 – 5.06 (m, 2H), 4.05 (d, *J* = 16.8 Hz, 1H), 3.97 (qd, *J* = 7.2, 2.8 Hz, 2H), 3.74 (d, *J* = 10.8 Hz, 1H), 2.91 (d, *J* = 16.8 Hz, 1H), 2.80 – 2.62 (m, 3H), 2.43 (s, 4H), 1.98 (d, *J* = 10.8 Hz, 1H), 1.89 – 1.76 (m, 1H), 1.53 – 1.42 (m, 1H), 1.33 – 1.19 (m, 10H), 1.16 (t, *J* = 7.2 Hz, 3H), 0.97 – 0.81 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 144.2, 143.7, 136.0, 133.1, 129.6, 129.4, 127.6, 109.8, 60.1, 51.4, 50.1, 48.4, 46.4, 34.2, 31.6, 31.0, 29.5, 28.1, 26.4, 22.6, 21.5, 14.2, 14.1. IR (neat) ν 661, 813, 1220, 1597, 1712, 2980 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{37}NO_4SNa$ $(M+Na)^+$: 482.2336, Found: 482.2328.



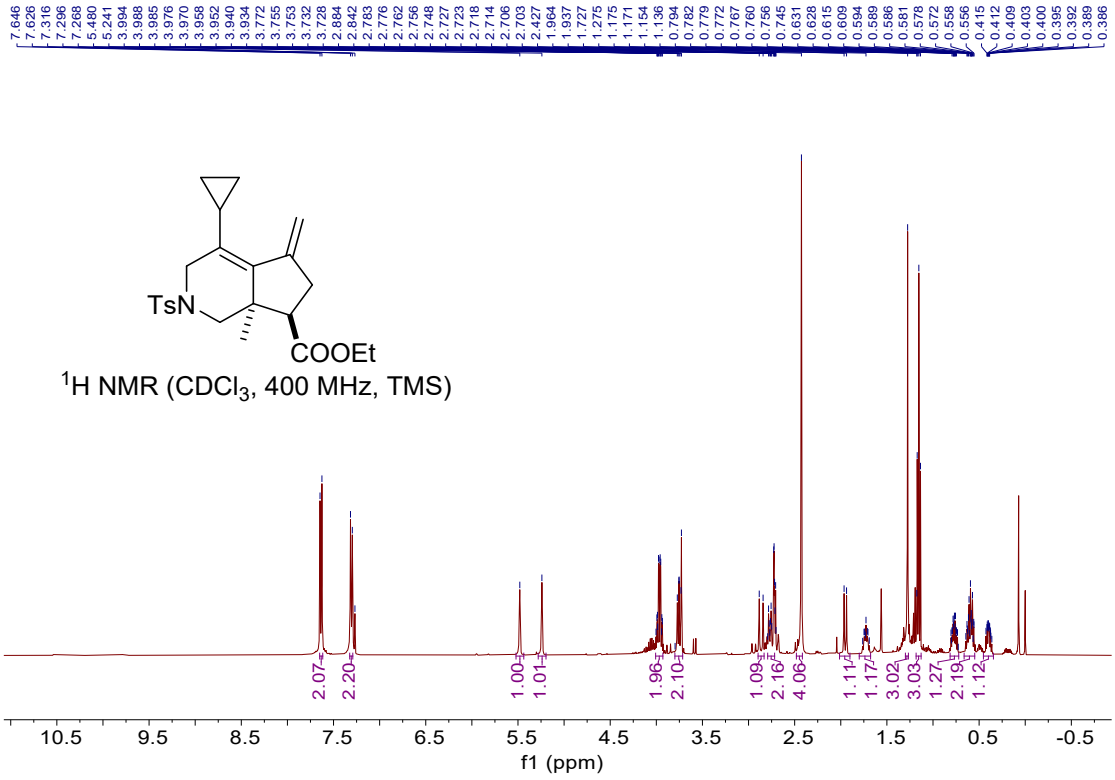


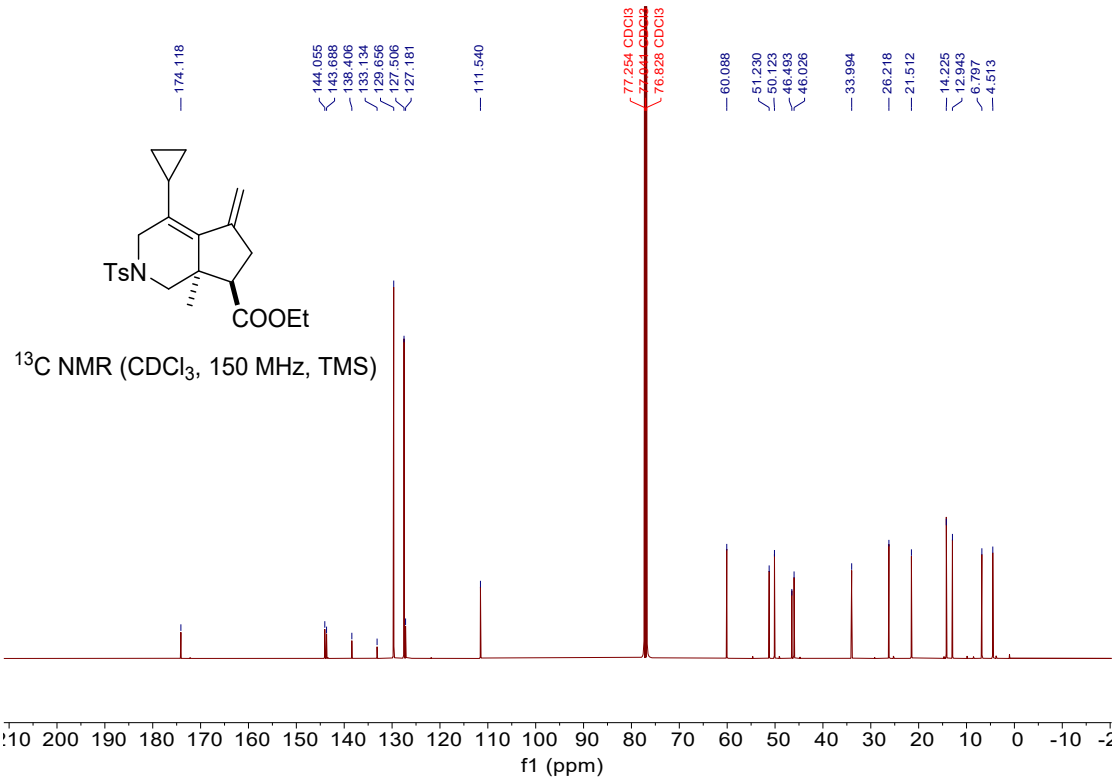
^{13}C NMR ($CDCl_3$, 100 MHz, TMS)

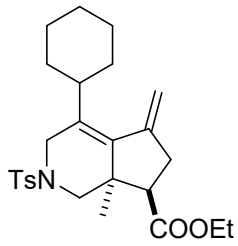


(trans)-ethyl-4-cyclopropyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4d)

A colorless oil, 96% yield, 39.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.48 (s, 1H), 5.24 (s, 1H), 3.96 (qd, *J* = 7.2, 2.4 Hz, 2H), 3.80 – 3.71 (m, 2H), 2.86 (d, *J* = 16.8 Hz, 1H), 2.79 – 2.67 (m, 2H), 2.43 (s, 4H), 1.95 (d, *J* = 10.8 Hz, 1H), 1.80 – 1.68 (m, 1H), 1.28 (s, 3H), 1.15 (t, *J* = 7.2 Hz, 3H), 0.81 – 0.72 (m, 1H), 0.66 – 0.55 (m, 2H), 0.45 – 0.34 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.1, 144.1, 143.7, 138.4, 133.1, 129.7, 127.5, 127.2, 111.5, 60.1, 51.2, 50.1, 46.5, 46.0, 34.0, 26.2, 21.5, 14.2, 12.9, 6.8, 4.5. IR (neat) ν 662, 1093, 1343, 1597, 1710, 2985 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{29}NO_4SNa$ $(M+Na)^+$: 438.1710, Found: 438.1708.

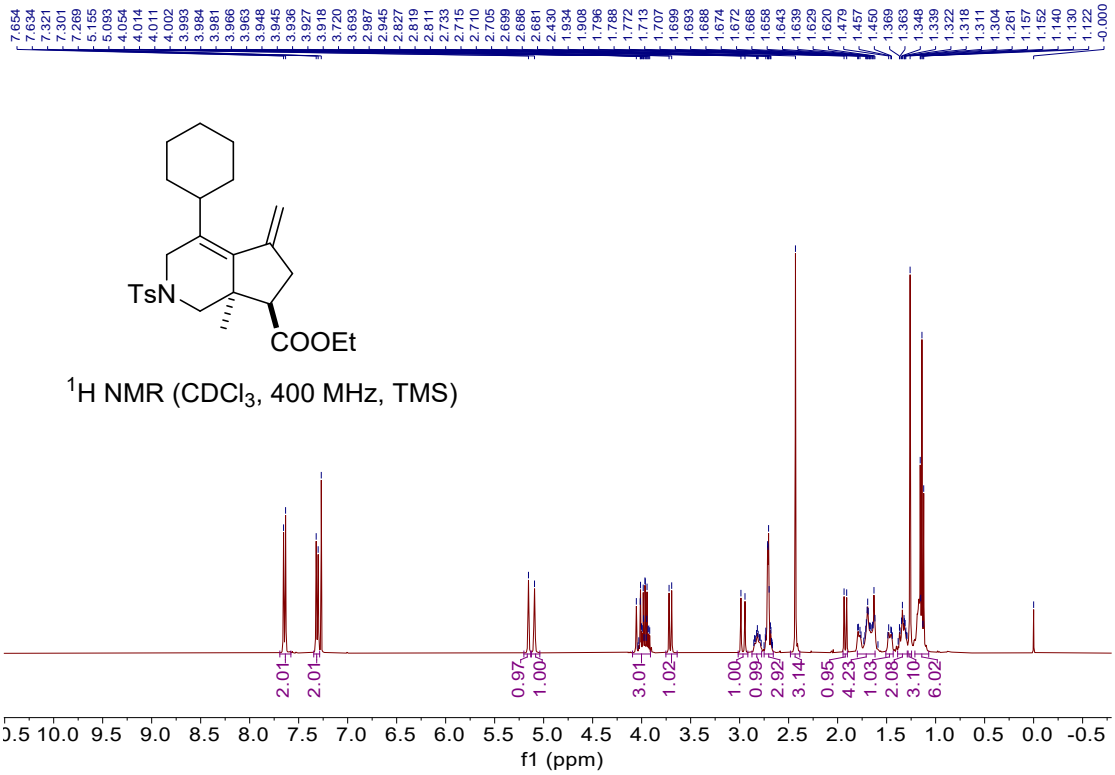


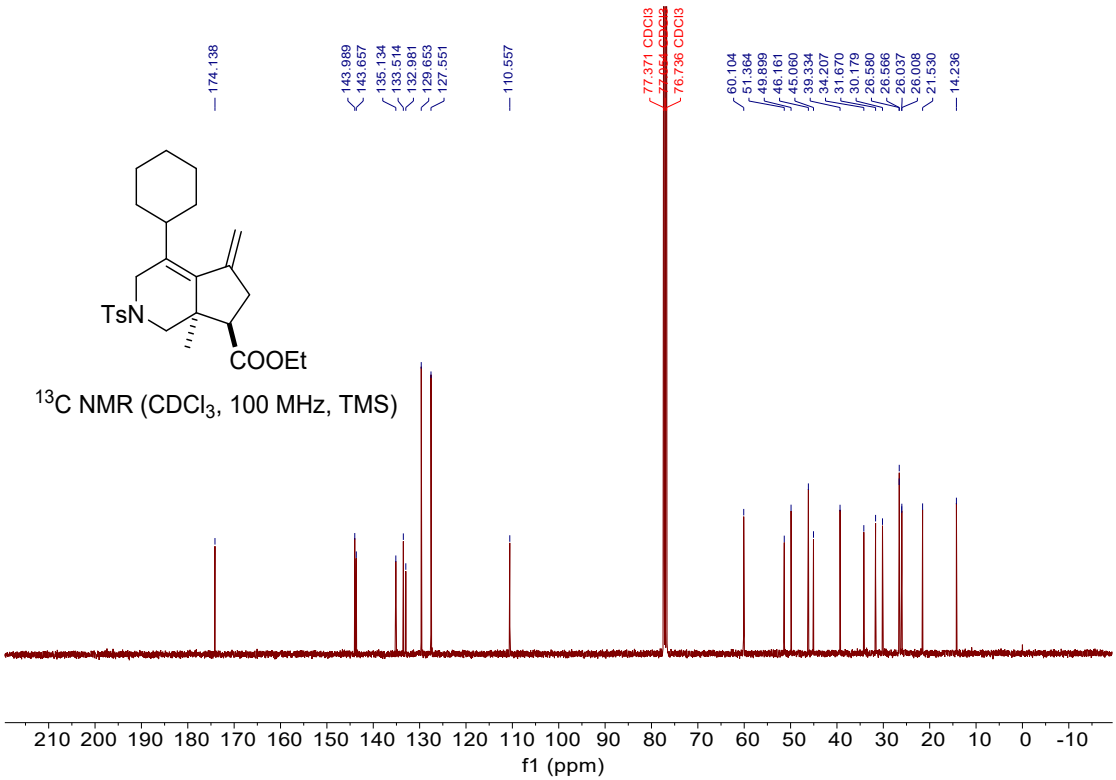

174.118
144.055
143.688
138.406
133.134
129.656
127.506
127.181
111.540
77.254 CDCl3
77.044 CDCl3
76.828 CDCl3
60.088
51.230
50.123
46.493
46.026
33.994
26.218
21.512
14.225
12.943
6.797
4.513
TsN
COOEt
13C NMR (CDCl3, 150 MHz, TMS)
f1 (ppm)

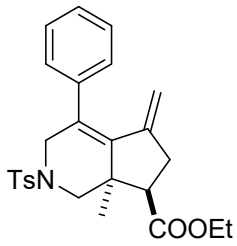


(trans)-ethyl-4-cyclohexyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4e)

A colorless oil, 90% yield, 42.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.15 (s, 1H), 5.09 (s, 1H), 4.09 – 3.91 (m, 3H), 3.71 (d, *J* = 10.8 Hz, 1H), 2.97 (d, *J* = 16.4 Hz, 1H), 2.87 – 2.78 (m, 1H), 2.75 – 2.66 (m, 3H), 2.43 (s, 3H), 1.92 (d, *J* = 10.8 Hz, 1H), 1.80 – 1.62 (m, 4H), 1.51 – 1.43 (m, 1H), 1.39 – 1.29 (m, 2H), 1.26 (s, 3H), 1.14 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 144.0, 143.7, 135.1, 133.5, 133.0, 129.7, 127.6, 110.6, 60.1, 51.4, 49.9, 46.2, 45.1, 39.3, 34.2, 31.7, 30.2, 26.6, 26.6, 26.0, 26.0, 21.5, 14.2. IR (neat) ν 660, 1092, 1376, 1712, 2927 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{35}NO_4SNa$ $(M+Na)^+$: 480.2179, Found: 480.2180.

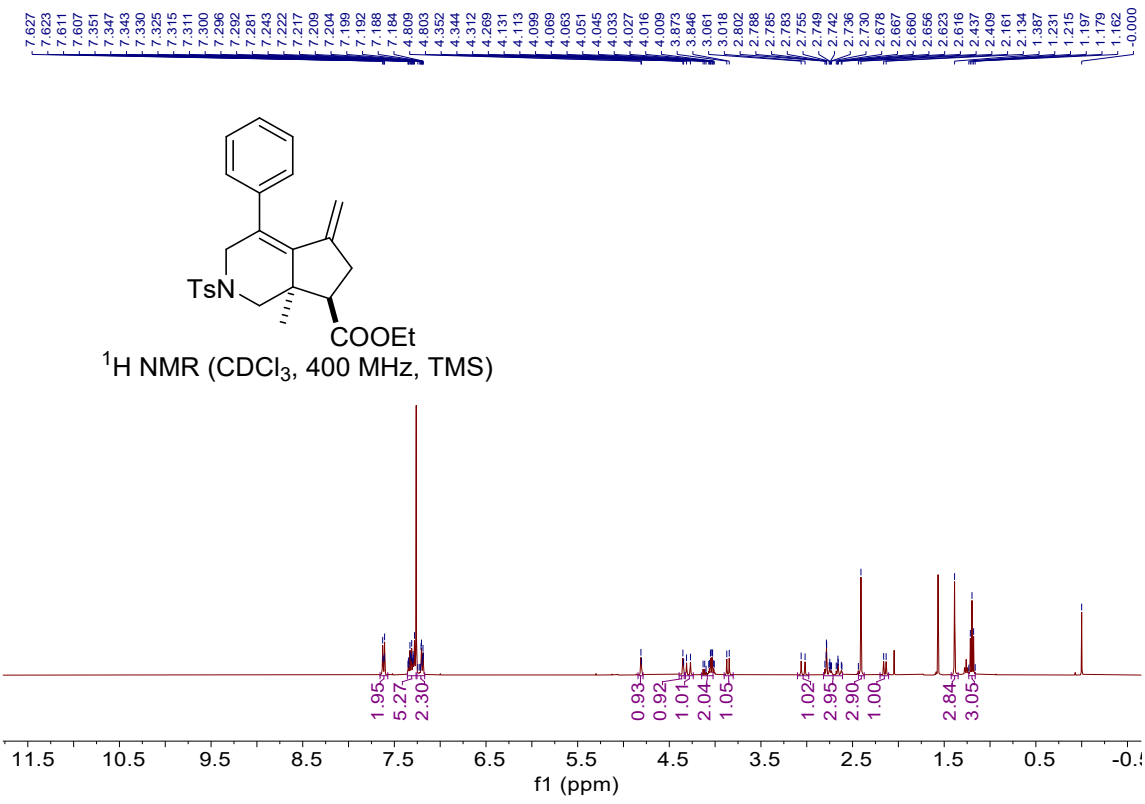


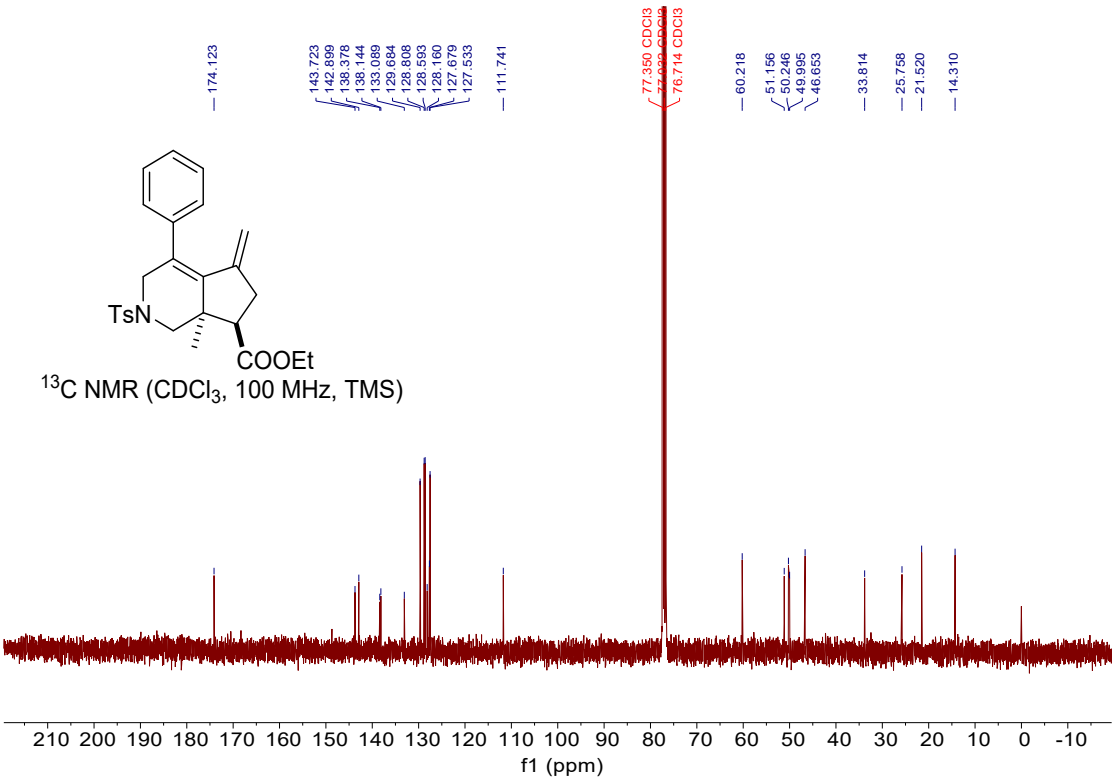

174.138
143.989
143.657
135.134
133.514
132.981
129.653
127.551
110.557
77.371 CDCl3
76.736 CDCl3
60.104
51.364
49.899
46.161
45.060
39.334
34.207
31.670
30.179
26.580
26.566
26.037
26.008
21.530
14.236
TsN
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



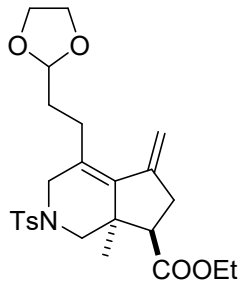
(trans)-ethyl-4-cyclohexyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4f)

A colorless oil, 80% yield, 36.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.57 (m, 2H), 7.36 – 7.26 (m, 5H), 7.25 – 7.17 (m, 2H), 4.81 (d, *J* = 2.8 Hz, 1H), 4.35 (d, *J* = 3.2 Hz, 1H), 4.29 (d, *J* = 17.2 Hz, 1H), 4.04 (qd, *J* = 7.2, 2.4 Hz, 2H), 3.86 (d, *J* = 10.8 Hz, 1H), 3.04 (d, *J* = 17.2 Hz, 1H), 2.82 – 2.61 (m, 3H), 2.41 (s, 3H), 2.15 (d, *J* = 10.8 Hz, 1H), 1.39 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 143.7, 142.9, 138.4, 138.1, 133.1, 129.7, 128.8, 128.6, 128.2, 127.7, 127.5, 111.7, 60.2, 51.2, 50.2, 50.0, 46.7, 33.8, 25.8, 21.5, 14.3. IR (neat) ν 658, 1090, 1348, 1719, 2933 cm^{-1}. HRMS (ESI) calcd. for $C_{26}H_{29}NO_4SNa$ $(M+Na)^+$: 474.1710, Found: 474.1705.



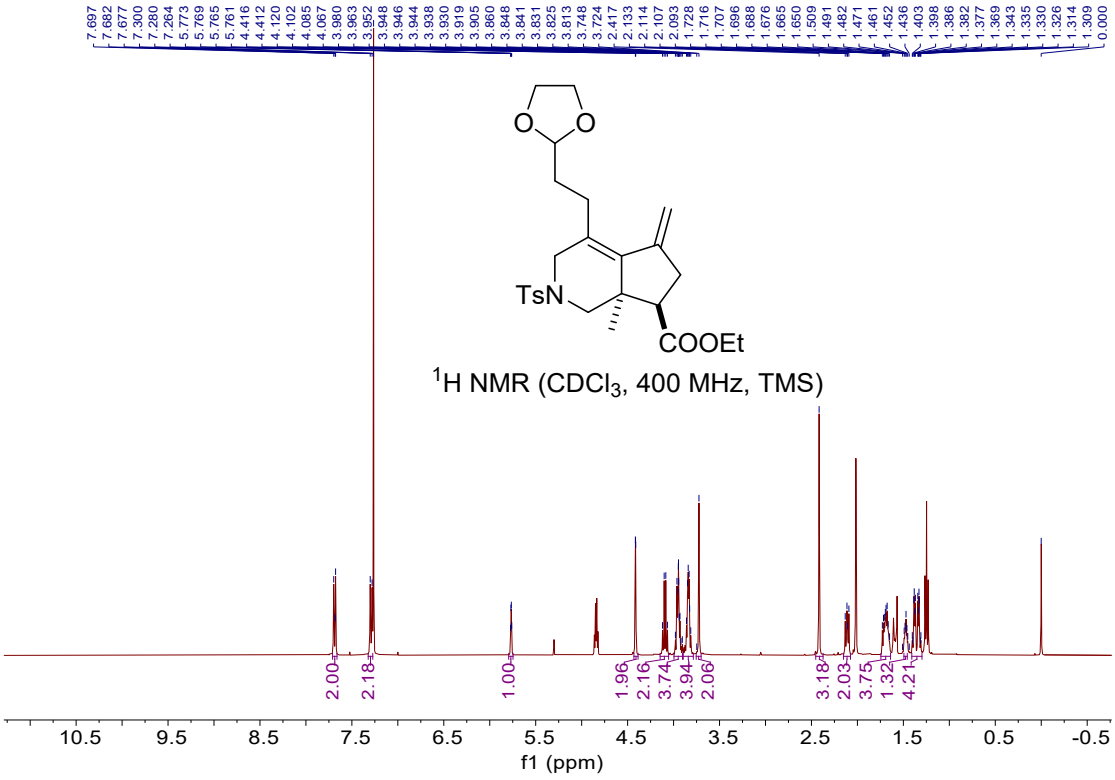


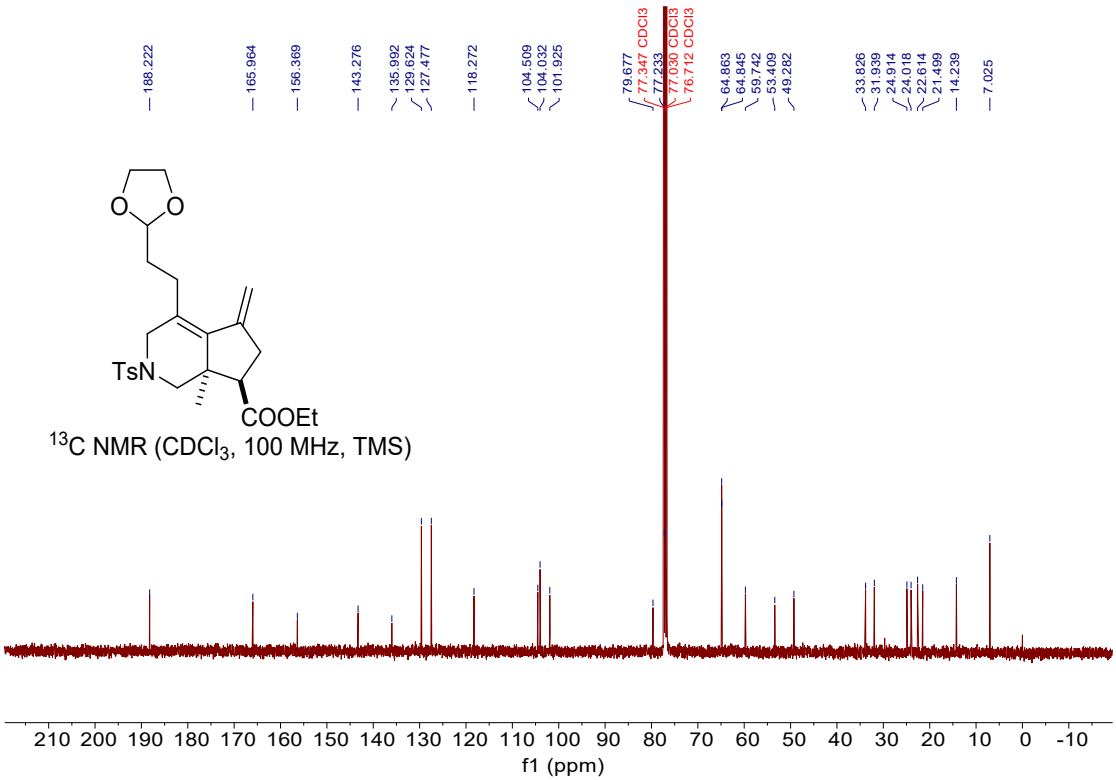
^{13}C NMR ($CDCl_3$, 100 MHz, TMS)



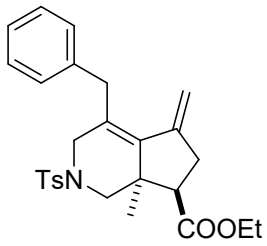
(trans)-ethyl-4-(2-(1,3-dioxolan-2-yl)ethyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4g)

A colorless oil, 70% yield, 33.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.77 (q, *J* = 1.6 Hz, 1H), 4.41 (d, *J* = 1.6 Hz, 2H), 4.09 (q, *J* = 7.2 Hz, 2H), 4.00 – 3.90 (m, 4H), 3.82 – 3.86 (m, 4H), 3.72 (s, 2H), 2.42 (s, 3H), 2.15 – 2.08 (m, 2H), 1.74 – 1.64 (m, 4H), 1.52 – 1.43 (m, 1H), 1.41 – 1.30 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.2, 166.0, 156.4, 143.3, 136.0, 129.6, 127.5, 118.3, 104.5, 104.0, 101.9, 79.7, 77.3, 64.9, 64.8, 59.7, 53.4, 49.3, 33.8, 31.9, 24.9, 24.0, 22.6, 21.5, 14.2, 7.0. IR (neat) ν 664, 1091, 1342, 1455, 1718, 2940 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{33}NO_6SNa$ $(M+Na)^+$: 498.1921, Found: 498.1917.



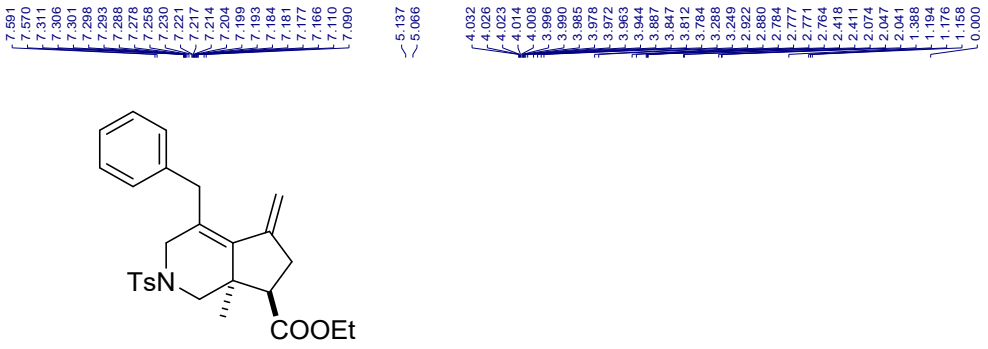


^{13}C NMR ($CDCl_3$, 100 MHz, TMS)

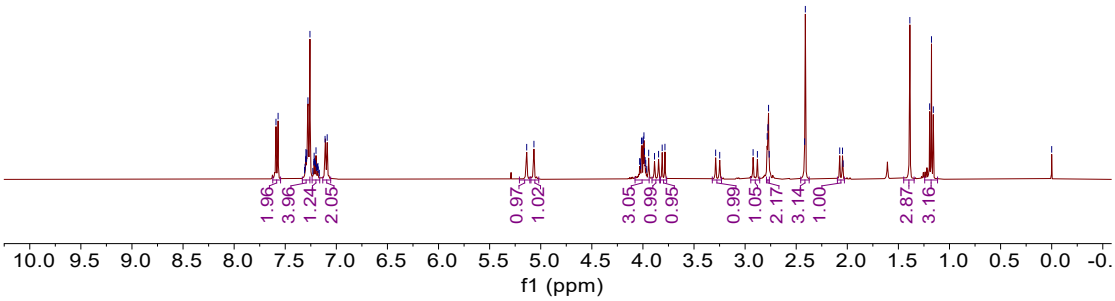


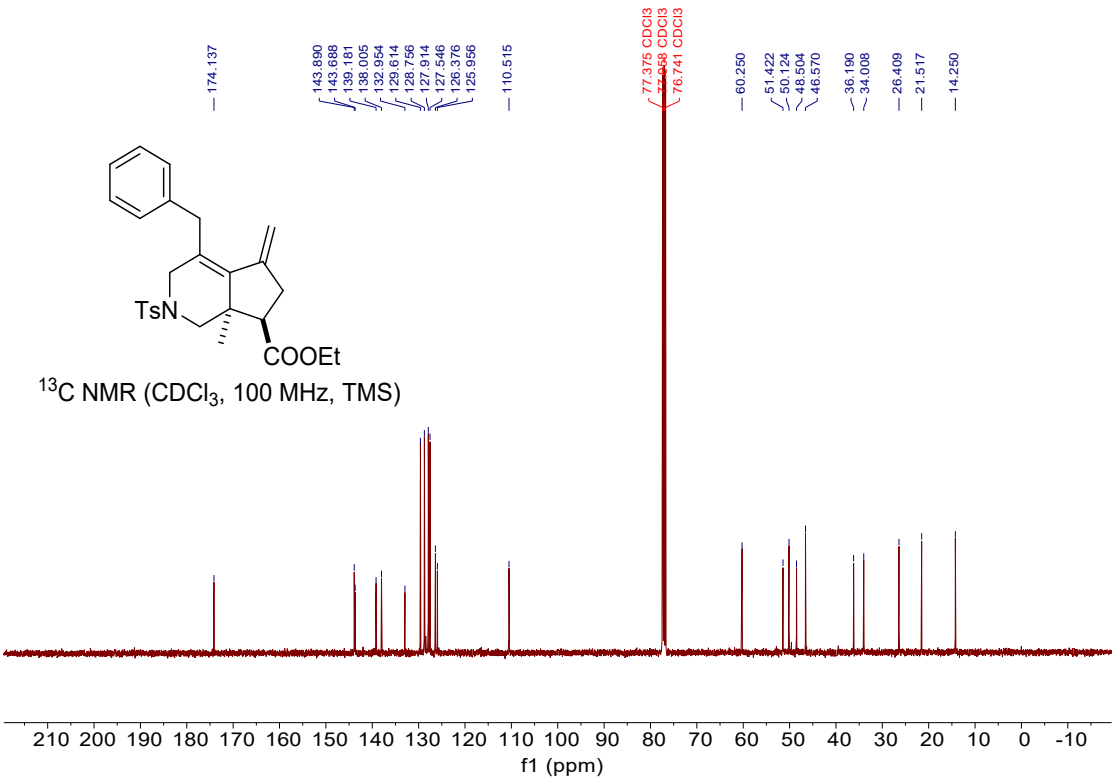
(trans)-ethyl-4-benzyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4h)

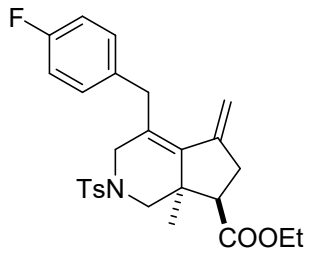
A colorless oil, 90% yield, 41.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 4H), 7.24 – 7.16 (m, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.14 (s, 1H), 5.07 (s, 1H), 4.08 – 3.94 (m, 3H), 3.87 (d, *J* = 16.0 Hz, 1H), 3.80 (d, *J* = 10.8 Hz, 1H), 3.27 (d, *J* = 16.0 Hz, 1H), 2.90 (d, *J* = 16.8 Hz, 1H), 2.79 – 2.76 (m, 2H), 2.41 (s, 3H), 2.06 (d, *J* = 10.8 Hz, 1H), 1.39 (s, 3H), 1.18 (t, *J* = 7.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 143.9, 143.7, 139.2, 138.0, 133.0, 129.6, 128.8, 127.9, 127.5, 126.4, 126.0, 110.5, 60.2, 51.4, 50.1, 48.5, 46.6, 36.2, 34.0, 26.4, 21.5, 14.3. IR (neat) ν 661, 1091, 1356, 1771, 2926 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{31}NO_4SNa$ $(M+Na)^+$: 488.1866, Found: 488.1866.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

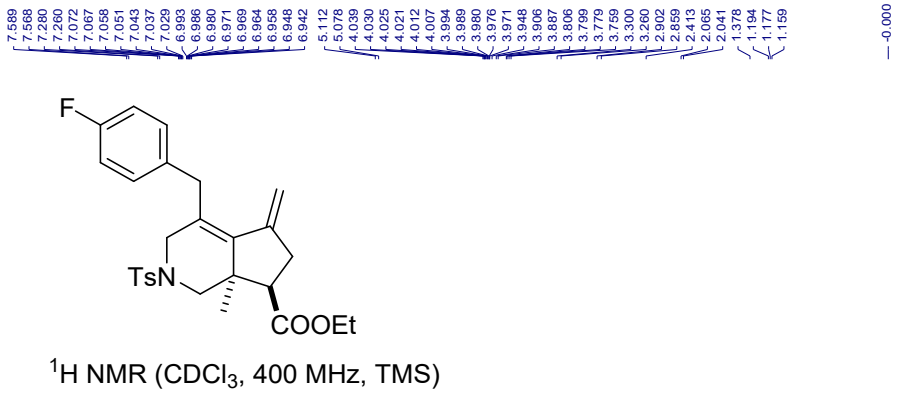



174.137
143.890
143.688
139.181
138.005
132.954
129.614
128.756
127.914
127.546
126.376
125.956
110.515
77.375 CDCl3
77.068 CDCl3
76.741 CDCl3
60.250
51.422
50.124
46.504
46.570
36.190
34.008
26.409
21.517
14.250
TsN
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

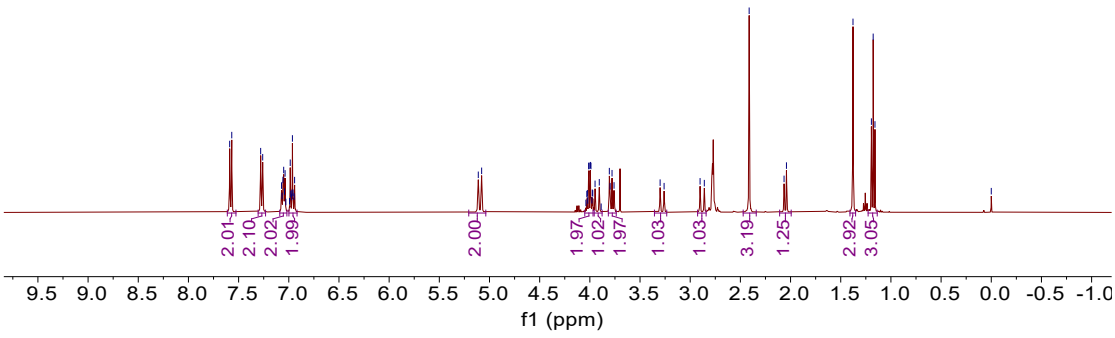


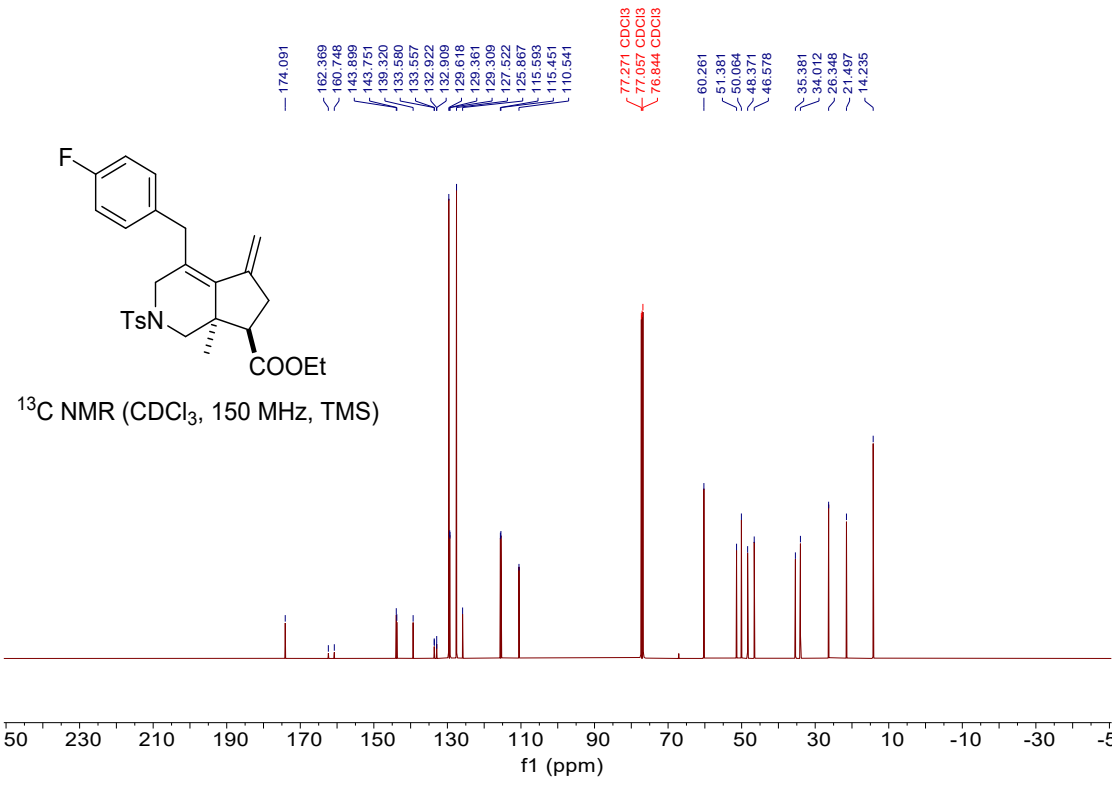
(trans)-ethyl-4-(4-fluorobenzyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4i)

A colorless oil, 90% yield, 43.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 7.09 – 7.02 (m, 2H), 7.00 – 6.92 (m, 2H), 5.09 (d, J = 13.2 Hz, 2H), 4.00 (qd, J = 7.2, 2.0 Hz, 2H), 3.93 (d, J = 16.8 Hz, 1H), 3.82 – 3.74 (m, 2H), 3.28 (d, J = 16.0 Hz, 1H), 2.88 (d, J = 16.8 Hz, 1H), 2.41 (s, 3H), 2.05 (d, J = 9.6 Hz, 1H), 1.38 (s, 3H), 1.18 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 174.1, 162.5 (d, $J_{C\text{-}F}$ = 243.2 Hz), 143.9, 143.8, 139.3, 133.56, 133.58, 132.92, 132.90, 129.5 (d, $J_{C\text{-}F}$ = 7.8 Hz), 129.3, 127.5, 125.9, 115.6 (d, $J_{C\text{-}F}$ = 21.3 Hz), 110.5, 77.3, 77.1, 76.8, 60.3, 51.4, 50.1, 48.4, 46.6, 35.4, 34.0, 26.3, 21.5, 14.2. ^{19}F NMR (565 MHz, $CDCl_3$) δ -116.9. IR (neat) ν 661, 815, 1166, 1355, 1599, 1771, 2978 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{30}NO_4FSNa$ $(M+Na)^+$: 506.1772, Found: 506.1776.

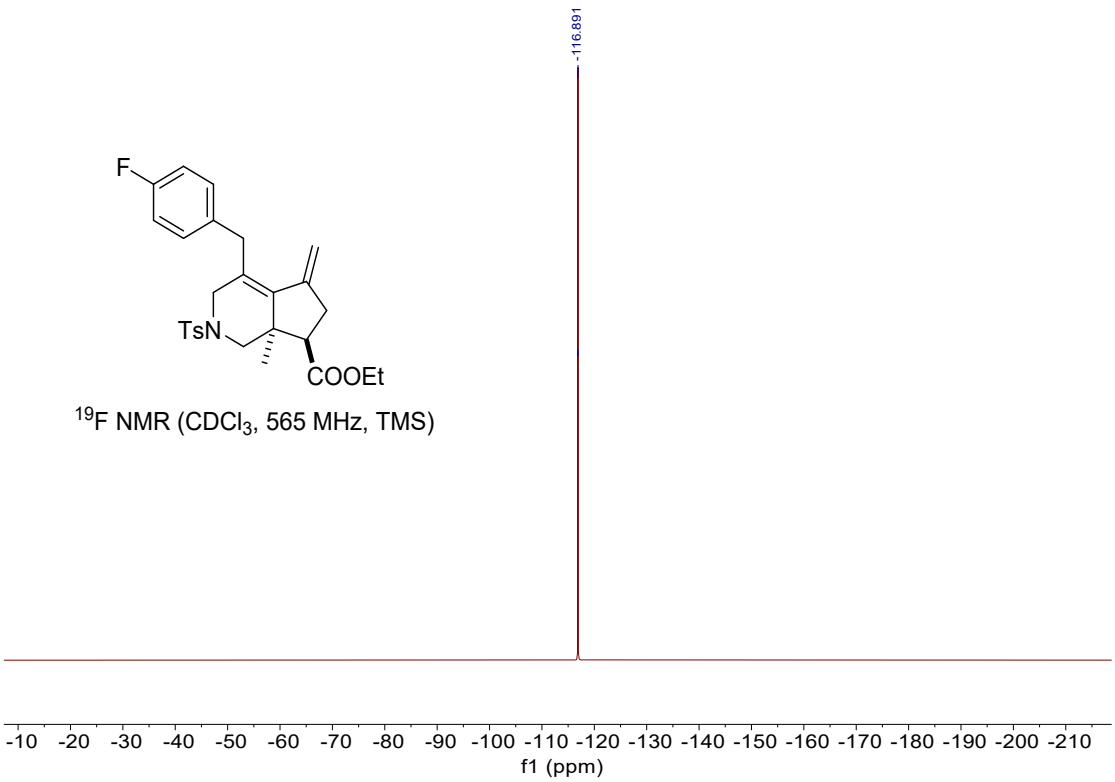


^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

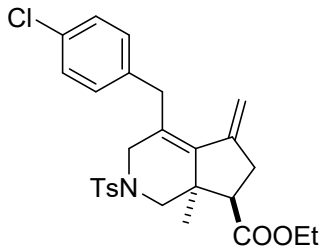




^{13}C NMR ($CDCl_3$, 150 MHz, TMS)

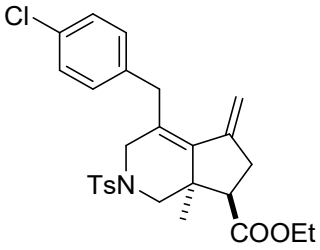


^{19}F NMR ($CDCl_3$, 565 MHz, TMS)

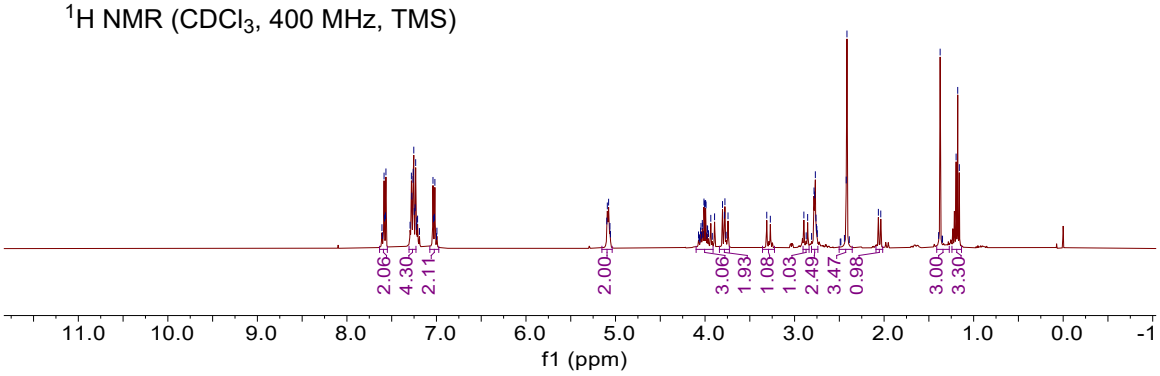


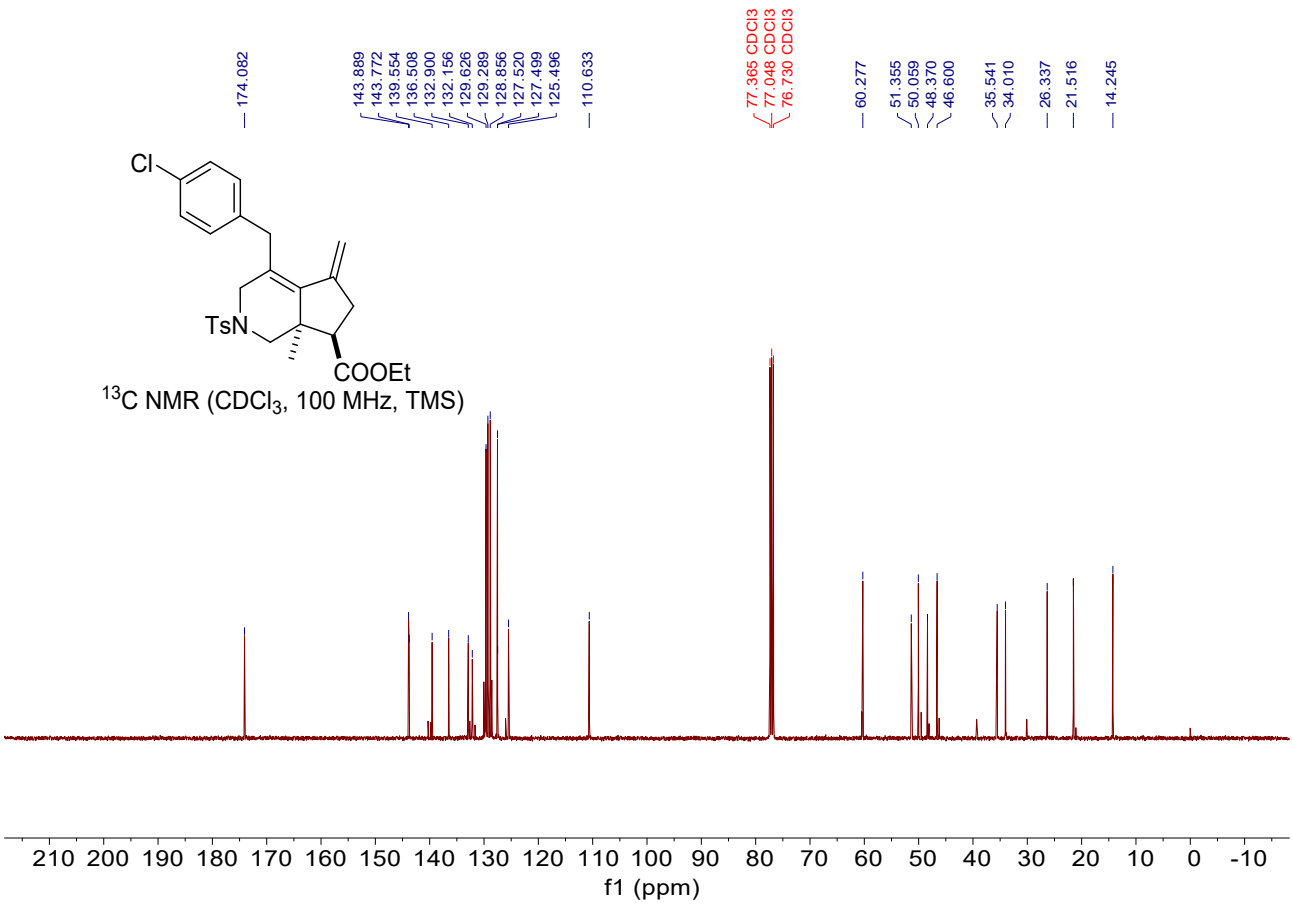
(trans)-ethyl-4-(4-chlorobenzyl)-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4j)

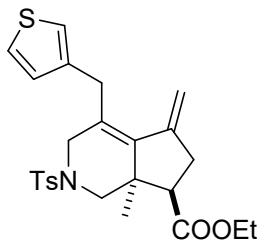
A colorless oil, 88% yield, 44.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.30 – 7.22 (m, 4H), 7.03 (d, *J* = 8.0 Hz, 2H), 5.14 – 5.03 (m, 2H), 4.07 – 3.89 (m, 3H), 3.83 – 3.70 (m, 2H), 3.29 (d, *J* = 16.0 Hz, 1H), 2.93 – 2.84 (m, 1H), 2.80 – 2.72 (m, 3H), 2.42 (d, *J* = 3.2 Hz, 3H), 2.11 – 2.02 (m, 1H), 1.38 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 143.9, 143.8, 139.6, 136.5, 132.9, 132.2, 129.6, 129.3, 128.9, 127.5, 127.5, 125.5, 110.6, 60.3, 51.4, 50.1, 48.4, 46.6, 35.5, 34.0, 26.3, 21.5, 14.2. IR (neat) ν 662, 809, 1091, 1349, 1597, 1735, 2949 cm^{-1}. HRMS (ESI) calcd. for $C_{27}H_{30}NO_4SClNa$ $(M+Na)^+$: 522.1476, Found: 522.1467.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

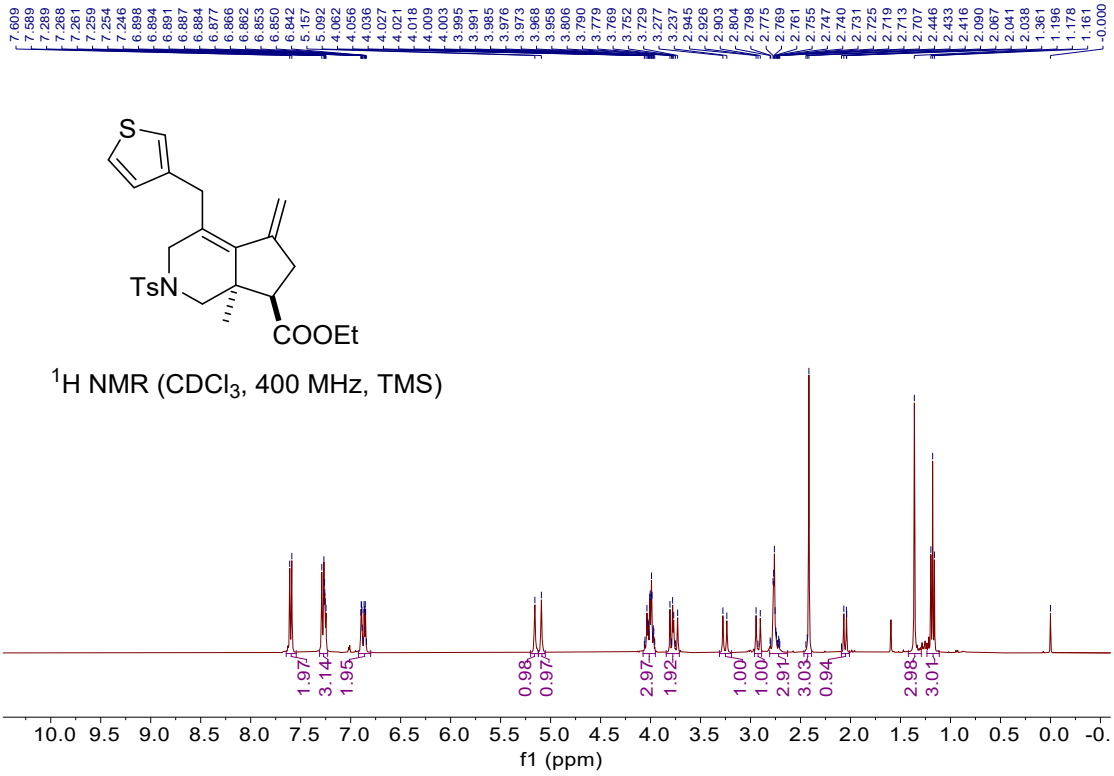


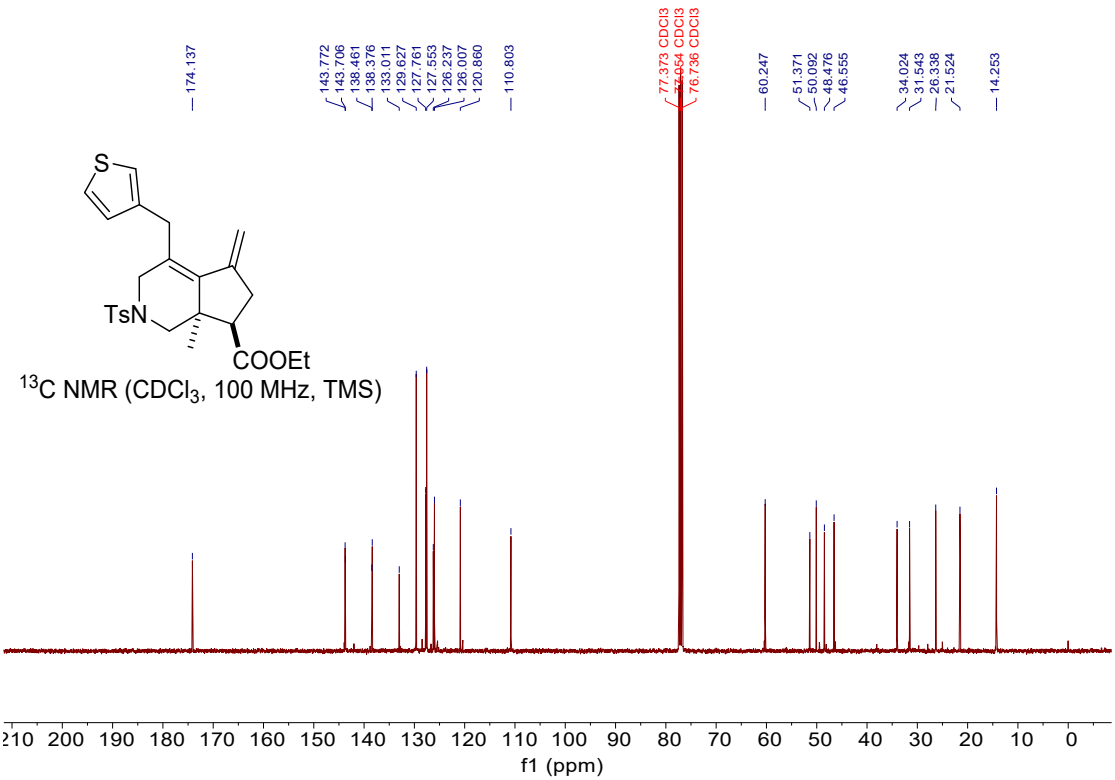

174.082
143.889
143.772
139.554
136.508
132.900
132.156
129.626
129.289
128.856
127.520
127.499
125.496
110.633
77.365 CDCl3
77.048 CDCl3
76.730 CDCl3
60.277
51.355
50.059
48.370
46.600
35.541
34.010
26.337
21.516
14.245
Cl
TsN
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

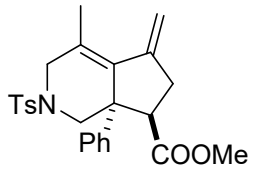


(trans)-ethyl-7a-methyl-5-methylene-4-(thiophen-3-ylmethyl)-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4k)

A colorless oil, 80% yield, 37.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.23 (m, 3H), 6.92 – 6.80 (m, 2H), 5.16 (s, 1H), 5.09 (s, 1H), 4.07 – 3.95 (m, 3H), 3.84 – 3.71 (m, 2H), 3.26 (d, *J* = 16.0 Hz, 1H), 2.92 (d, *J* = 16.8 Hz, 1H), 2.76 (td, *J* = 5.6, 2.4 Hz, 3H), 2.42 (s, 3H), 2.09 – 2.01 (m, 1H), 1.36 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 143.8, 143.7, 138.5, 138.4, 133.0, 129.6, 127.8, 127.6, 126.2, 126.0, 120.9, 110.8, 60.2, 51.4, 50.1, 48.5, 46.6, 34.0, 31.5, 26.3, 21.5, 14.3. IR (neat) ν 660, ,917, 1220, 1418, 1724, 2981 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{29}NO_4S_2Na$ $(M+Na)^+$: 494.1430, Found: 494.1436.

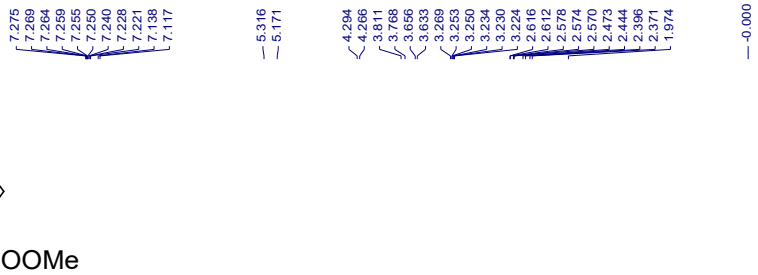


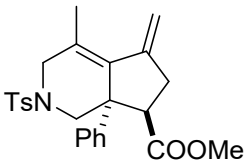

174.137
143.772
143.706
138.461
138.376
133.011
129.627
127.761
127.553
126.237
126.007
120.860
110.803
77.373 CDCl3
77.054 CDCl3
76.736 CDCl3
60.247
51.371
50.092
48.476
46.555
34.024
31.543
26.338
21.524
14.253
S
TsN
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



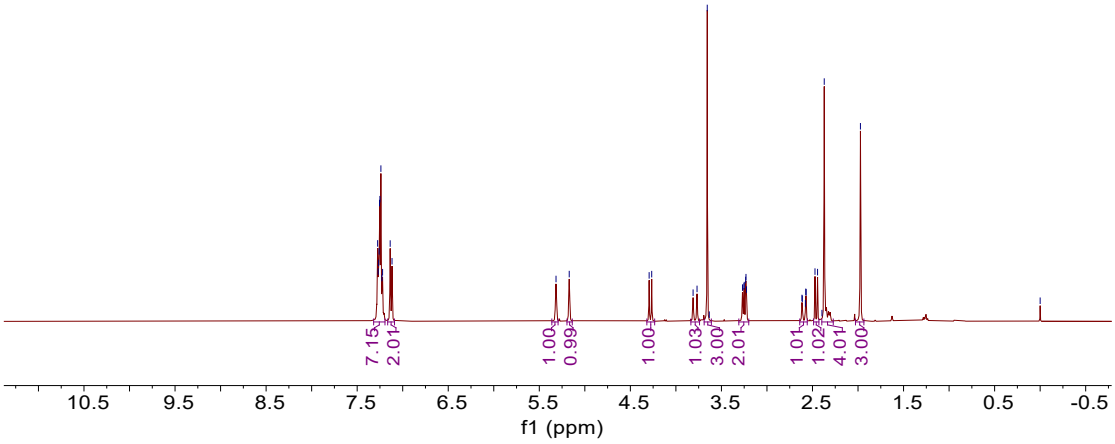
(trans)-ethyl-4-benzyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4l)

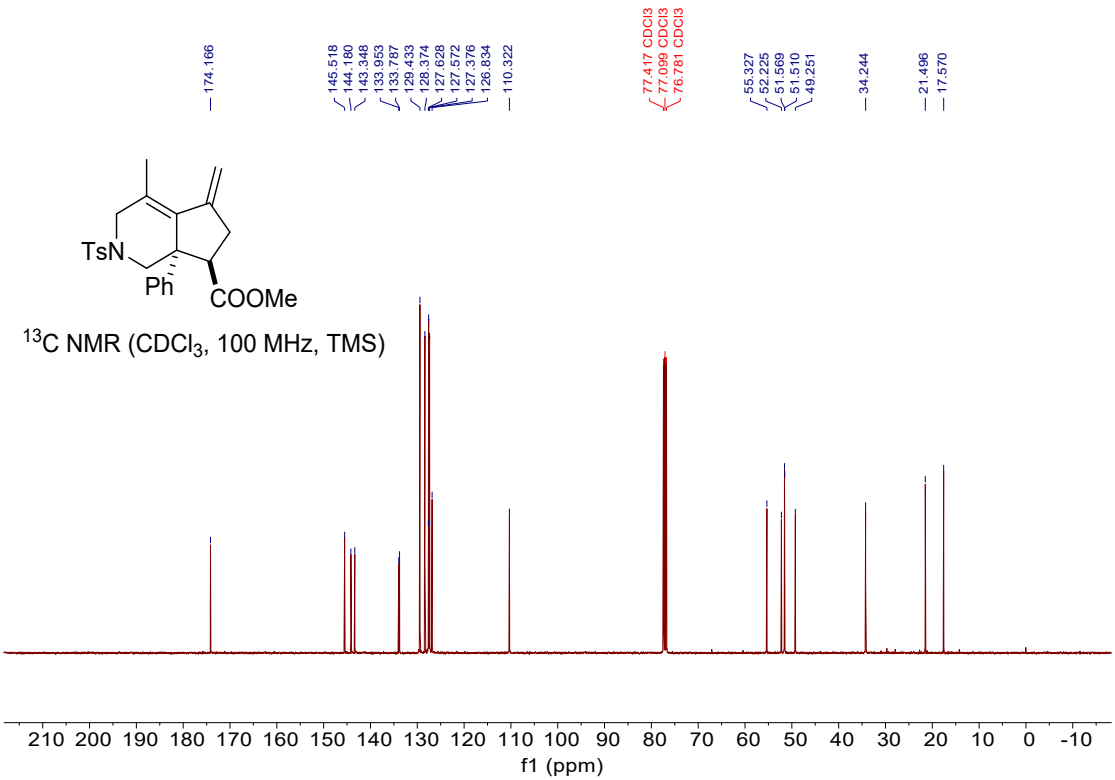
A colorless oil, 70% yield, 30.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.19 (m, 7H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.32 (s, 1H), 5.17 (s, 1H), 4.28 (d, *J* = 11.2 Hz, 1H), 3.79 (d, *J* = 17.2 Hz, 1H), 3.66 (s, 3H), 3.31 – 3.20 (m, 2H), 2.59 (dd, *J* = 16.8, 1.6 Hz, 1H), 2.46 (d, *J* = 11.2 Hz, 1H), 2.37 (s, 4H), 1.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 145.5, 144.2, 143.3, 134.0, 133.8, 129.4, 128.4, 127.6, 127.6, 127.4, 126.8, 110.3, 55.3, 52.2, 51.6, 51.5, 49.3, 34.2, 21.5, 17.6. IR (neat) ν 660, 789, 1106, 1351, 1599, 1735, 2951 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{27}NO_4SNa$ $(M+Na)^+$: 460.1553, Found: 460.1551.

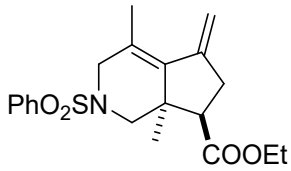




^{1}H NMR ($CDCl_3$, 400 MHz, TMS)

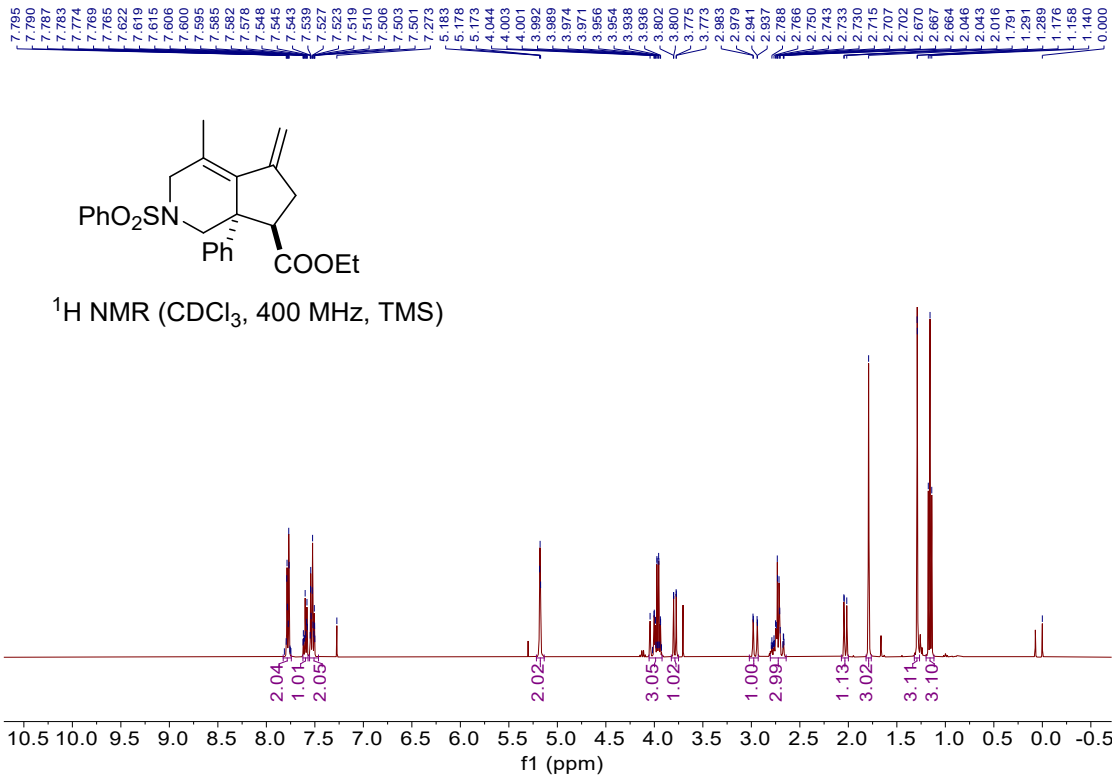


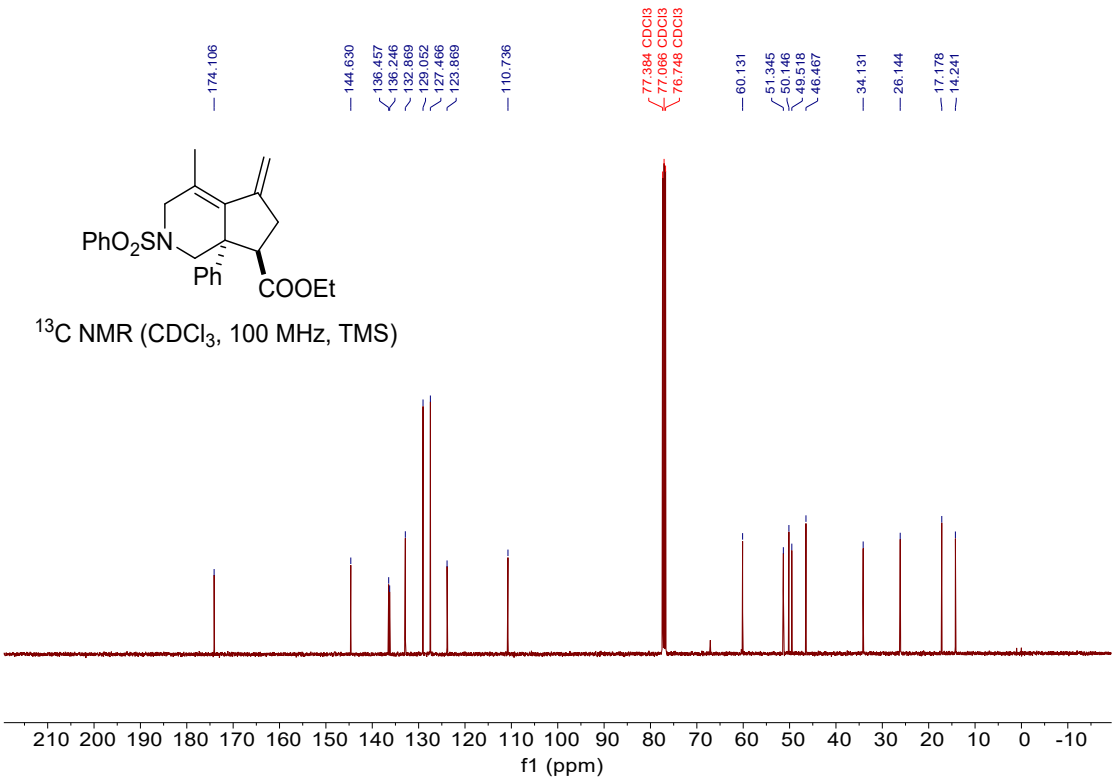

174.166
145.518
144.180
143.348
133.953
133.787
129.433
128.374
127.628
127.572
127.376
126.834
110.322
77.417 CDCl3
77.099 CDCl3
76.781 CDCl3
55.327
52.225
51.569
51.510
49.251
34.244
21.496
17.570
TsN
Ph
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

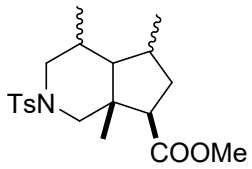


(trans)-ethyl-4-benzyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (4m)

A colorless oil, 90% yield, 33.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.74 (m, 2H), 7.62 – 7.57 (m, 1H), 7.55 – 7.46 (m, 2H), 5.18 (t, *J* = 2.4 Hz, 2H), 4.05 – 3.92 (m, 3H), 3.79 (dd, *J* = 10.8, 0.8 Hz, 1H), 2.96 (dd, *J* = 16.8, 1.6 Hz, 1H), 2.80 – 2.64 (m, 3H), 2.07 – 2.00 (m, 1H), 1.79 (s, 3H), 1.29 (d, *J* = 0.8 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 144.6, 136.5, 136.2, 132.9, 129.1, 127.5, 123.9, 110.7, 60.1, 51.3, 50.1, 49.5, 46.5, 34.1, 26.1, 17.2, 14.2. IR (neat) ν 690, 752, 1150, 1353, 1652, 1713, 2980 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{25}NO_4SNa$ $(M+Na)^+$: 398.1396, Found: 398.1395.

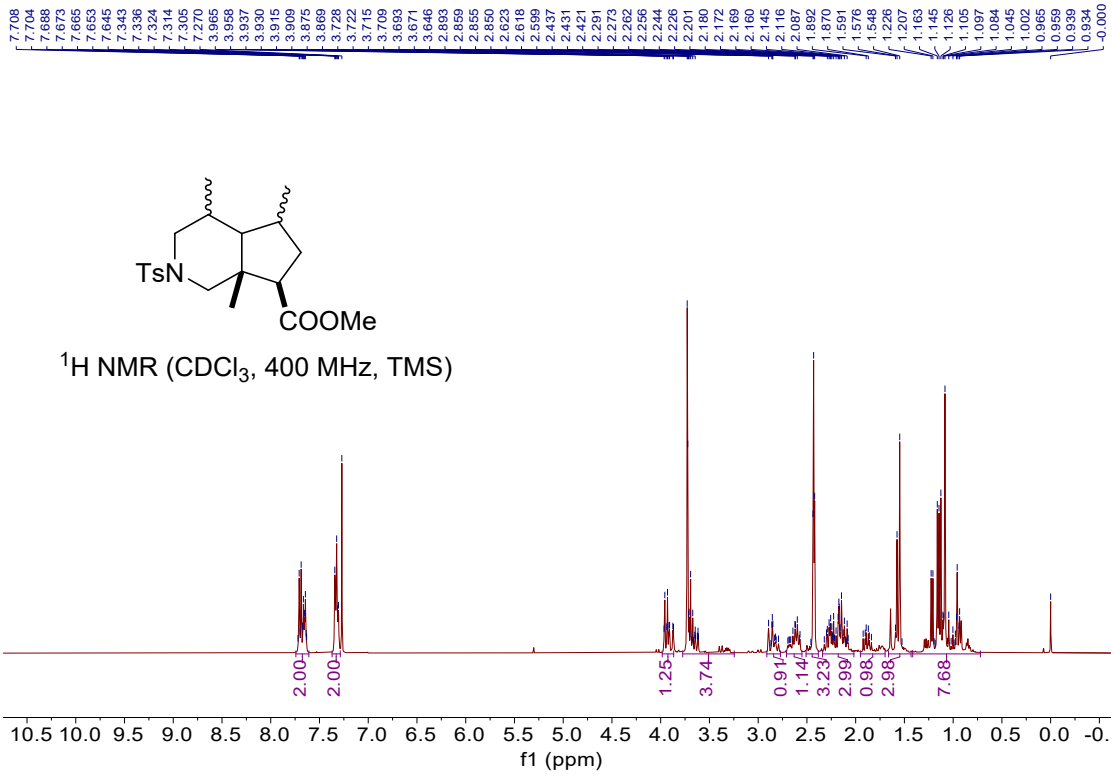


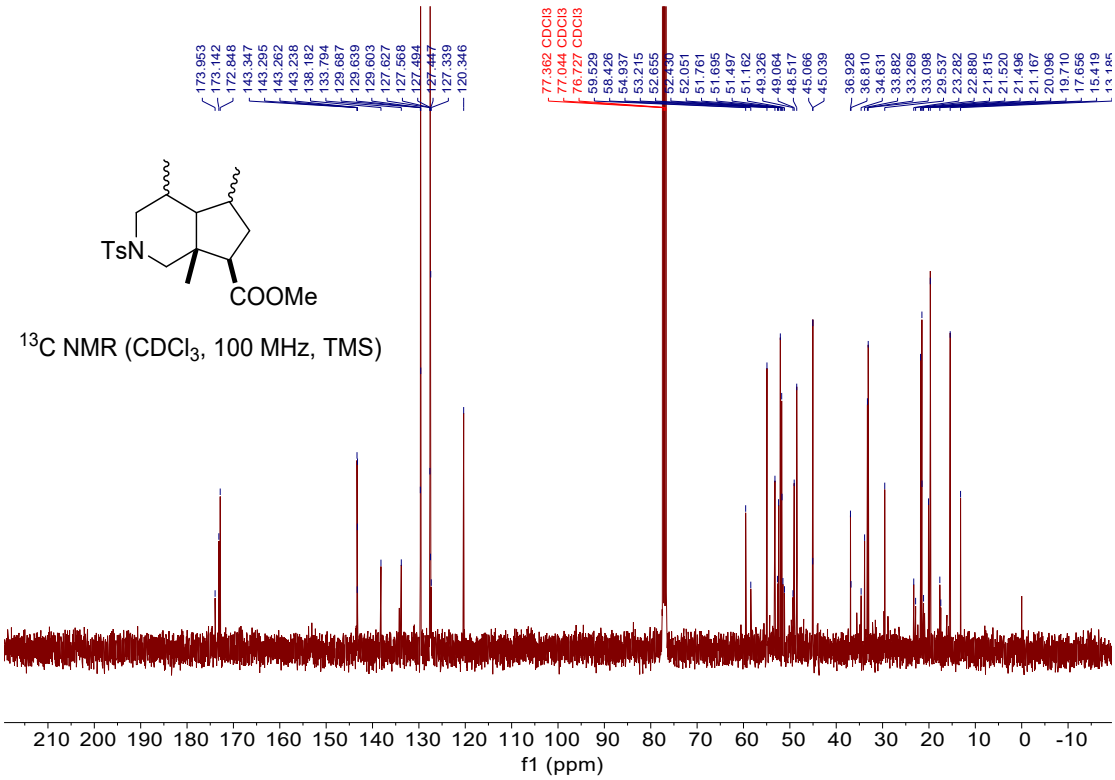

174.106
144.630
136.457
136.246
132.869
129.052
127.466
123.869
110.736
77.384 CDCl3
77.066 CDCl3
76.748 CDCl3
60.131
51.345
50.146
49.518
46.467
34.131
26.144
17.178
14.241
PhO2SN
Ph
COOEt
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

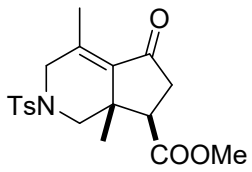


(cis)-methyl-4,5,7a-trimethyl-2-tosyloctahydro-1H-cyclopenta[c]pyridine-7-carboxylate (5)

A yellow oil, 98% yield, 36.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.61 (m, 2H), 7.37 – 7.29 (m, 2H), 3.98 – 3.87 (m, 1H), 3.77 – 3.25 (m, 4H), 2.91 – 2.77 (m, 1H), 2.71 – 2.55 (m, 1H), 2.51 – 2.38 (m, 3H), 2.34 – 2.02 (m, 3H), 1.95 – 1.70 (m, 1H), 1.66 – 1.43 (m, 3H), 1.41 – 0.72 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 173.1, 172.8, 143.3, 143.3, 143.3, 143.2, 138.2, 133.8, 129.7, 129.6, 129.6, 127.6, 127.6, 127.5, 127.4, 127.3, 120.3, 59.5, 58.4, 54.9, 53.2, 52.7, 52.4, 52.1, 51.8, 51.7, 51.5, 51.2, 49.3, 49.1, 48.5, 45.1, 45.0, 36.9, 36.8, 34.6, 33.9, 33.3, 33.1, 29.5, 23.3, 22.9, 21.8, 21.5, 21.5, 21.2, 20.1, 19.7, 17.7, 17.4, 15.4, 13.2. IR (neat) ν 665, 886, 1350, 1715, 2962 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{29}NO_4SNa$ $(M+Na)^+$: 402.1710, Found: 402.1705.

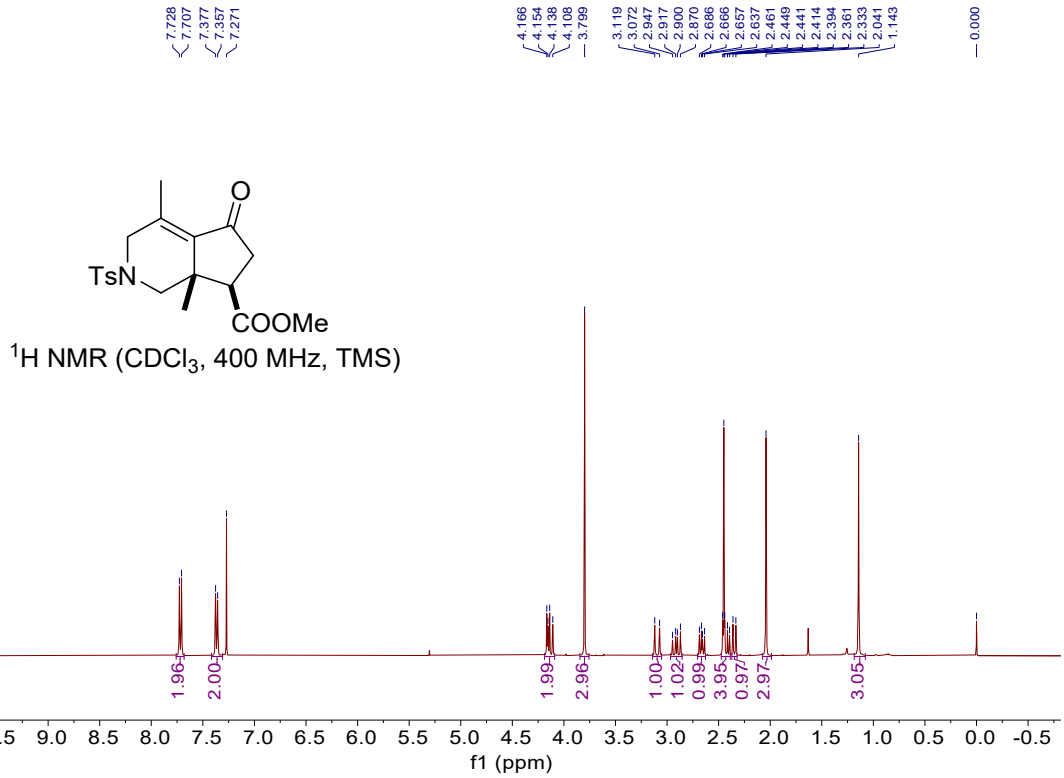


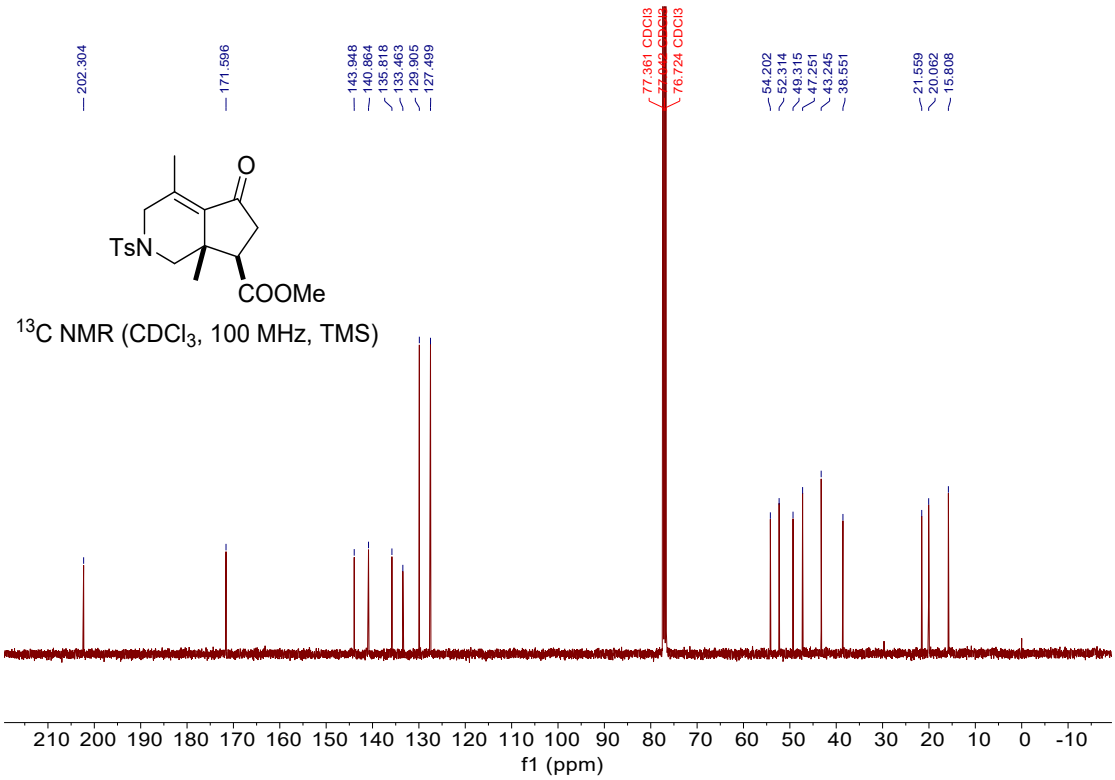

TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
f1 (ppm)

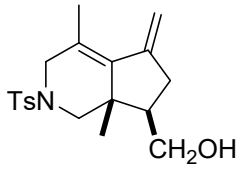


(cis)-methyl-4,7a-dimethyl-5-oxo-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridine-7-carboxylate (6)

A white oil, 96% yield, 36.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 4.19 – 4.09 (m, 2H), 3.80 (s, 3H), 3.10 (d, *J* = 18.8 Hz, 1H), 2.91 (dd, *J* = 18.8, 11.9 Hz, 1H), 2.66 (dd, *J* = 11.6, 8.1 Hz, 1H), 2.47 – 2.39 (m, 4H), 2.35 (d, *J* = 11.6 Hz, 1H), 2.04 (s, 3H), 1.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.3, 171.6, 143.9, 140.9, 135.8, 133.5, 129.9, 127.5, 54.2, 52.3, 49.3, 47.3, 43.2, 38.6, 21.6, 20.1, 15.8. IR (neat) ν 666, 1086, 1350, 1697, 1716, 2962 cm^{-1}. HRMS (ESI) calcd. for $C_{19}H_{23}NO_5SNa$ $(M+Na)^+$: 400.1189, Found: 400.1190.

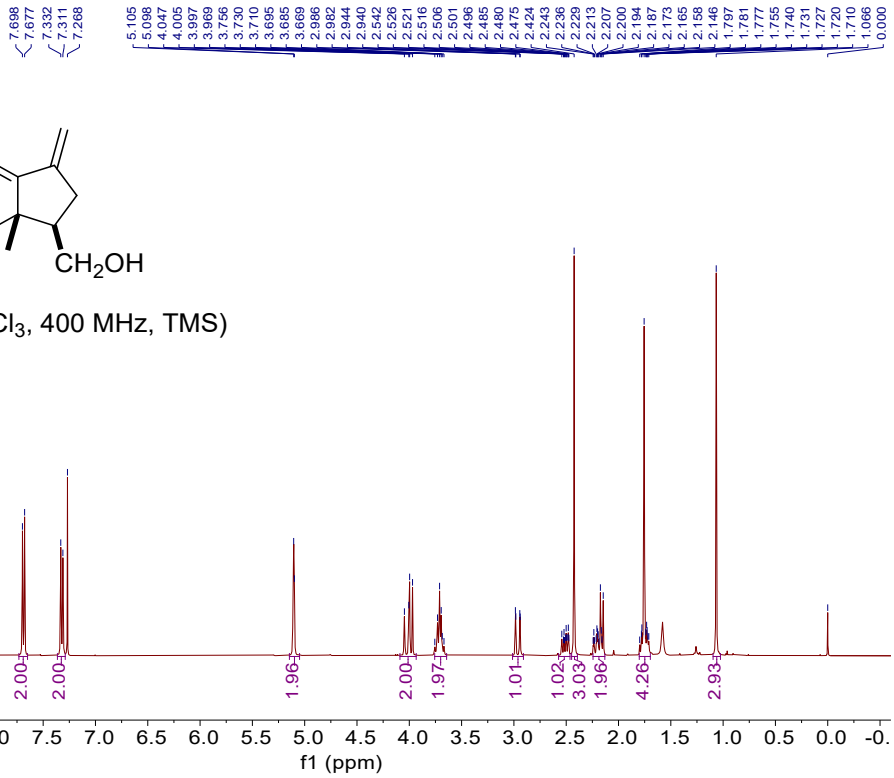


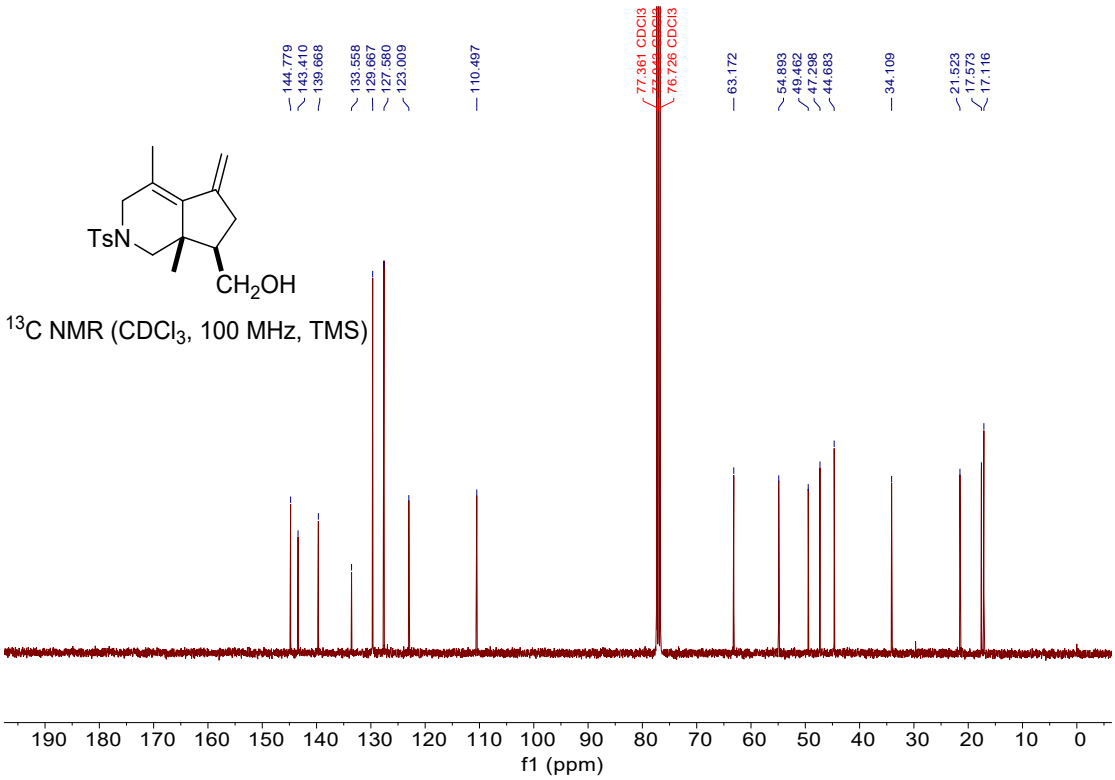

202.304
171.596
143.948
140.864
135.818
133.463
129.905
127.499
77.361 CDCl3
76.724 CDCl3
54.202
52.314
49.315
47.251
43.245
38.551
21.559
20.062
15.808
O
TsN
COOMe
13C NMR (CDCl3, 100 MHz, TMS)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

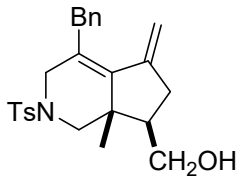


(cis)-4,7a-dimethyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridin-7-yl)methanol (7)

A yellow oil, 96% yield, 33.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 5.15 – 5.05 (m, 2H), 4.09 – 3.93 (m, 2H), 3.76 – 3.64 (m, 2H), 2.96 (dd, *J* = 16.8, 1.4 Hz, 1H), 2.57 – 2.46 (m, 1H), 2.42 (s, 3H), 2.24 – 2.13 (m, 2H), 1.80 – 1.70 (m, 4H), 1.07 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 143.4, 139.7, 133.6, 129.7, 127.6, 123.0, 110.5, 63.2, 54.9, 49.5, 47.3, 44.7, 34.1, 21.5, 17.6, 17.1. IR (neat) ν 665, 1021, 1333, 1597, 2924 cm^{-1}. HRMS (ESI) calcd. for $C_{19}H_{25}NO_3SNa$ $(M+Na)^+$: 370.1447, Found: 370.1442.

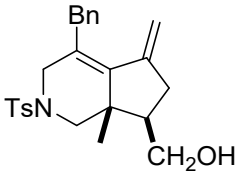


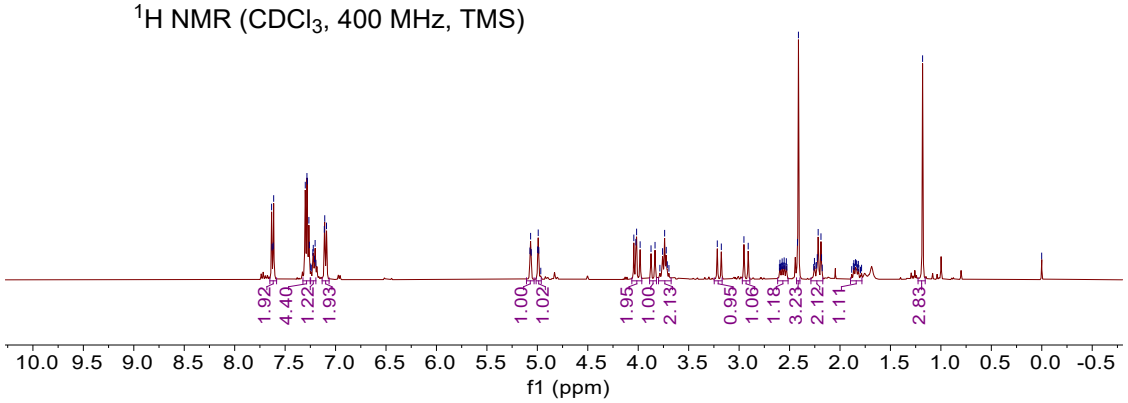

144.779
143.410
139.668
133.558
129.667
127.580
123.009
110.497
77.361 CDCl3
77.044 CDCl3
76.726 CDCl3
63.172
54.893
49.462
47.298
44.683
34.109
21.523
17.573
17.116
TsN
CH2OH
13C NMR (CDCl3, 100 MHz, TMS)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

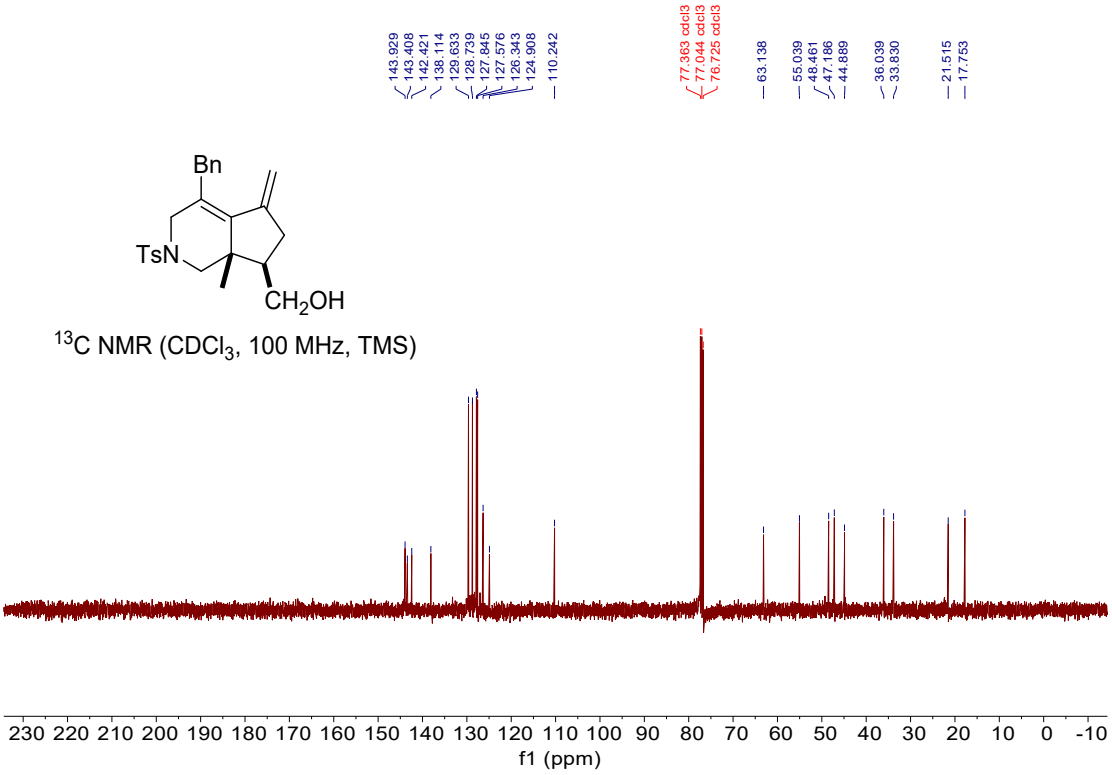


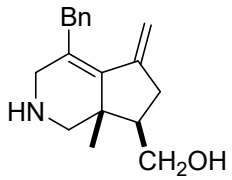
(cis)-4-benzyl-7a-methyl-5-methylene-2-tosyl-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridin-7-yl)methanol (8)

A yellow oil, 98% yield, 44.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.58 (m, 2H), 7.32 – 7.25 (m, 4H), 7.25 – 7.20 (m, 1H), 7.13 – 7.06 (m, 2H), 5.07 (d, *J* = 2.4 Hz, 1H), 4.99 (d, *J* = 2.4 Hz, 1H), 4.06 – 3.96 (m, 2H), 3.85 (d, *J* = 16.0 Hz, 1H), 3.80 – 3.67 (m, 2H), 3.20 (d, *J* = 16.0 Hz, 1H), 2.93 (d, *J* = 16.8 Hz, 1H), 2.62 – 2.51 (m, 1H), 2.41 (s, 3H), 2.29 – 2.17 (m, 2H), 1.90 – 1.78 (m, 1H), 1.18 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 143.4, 142.4, 138.1, 129.6, 128.7, 127.8, 127.6, 126.3, 124.9, 110.2, 63.1, 55.0, 48.5, 47.2, 44.9, 36.0, 33.8, 21.5, 17.8. IR (neat) ν 667, 1022, 1363, 1596, 2924 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{29}NO_3SNa$ $(M+Na)^+$: 446.1760, Found: 446.1760.



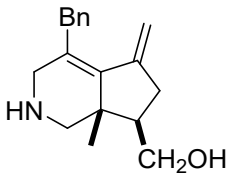



143.929
143.408
142.421
138.114
129.633
128.739
127.845
127.576
126.343
124.908
110.242
77.363 cdcl3
77.044 cdcl3
76.725 cdcl3
63.138
55.039
48.461
47.186
44.889
36.039
33.830
21.515
17.753
Bn
TsN
CH2OH
13C NMR (CDCl3, 100 MHz, TMS)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

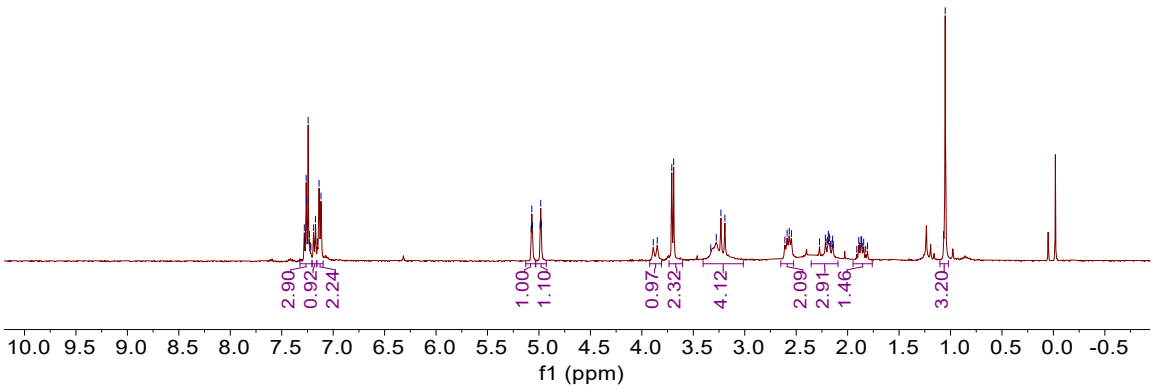


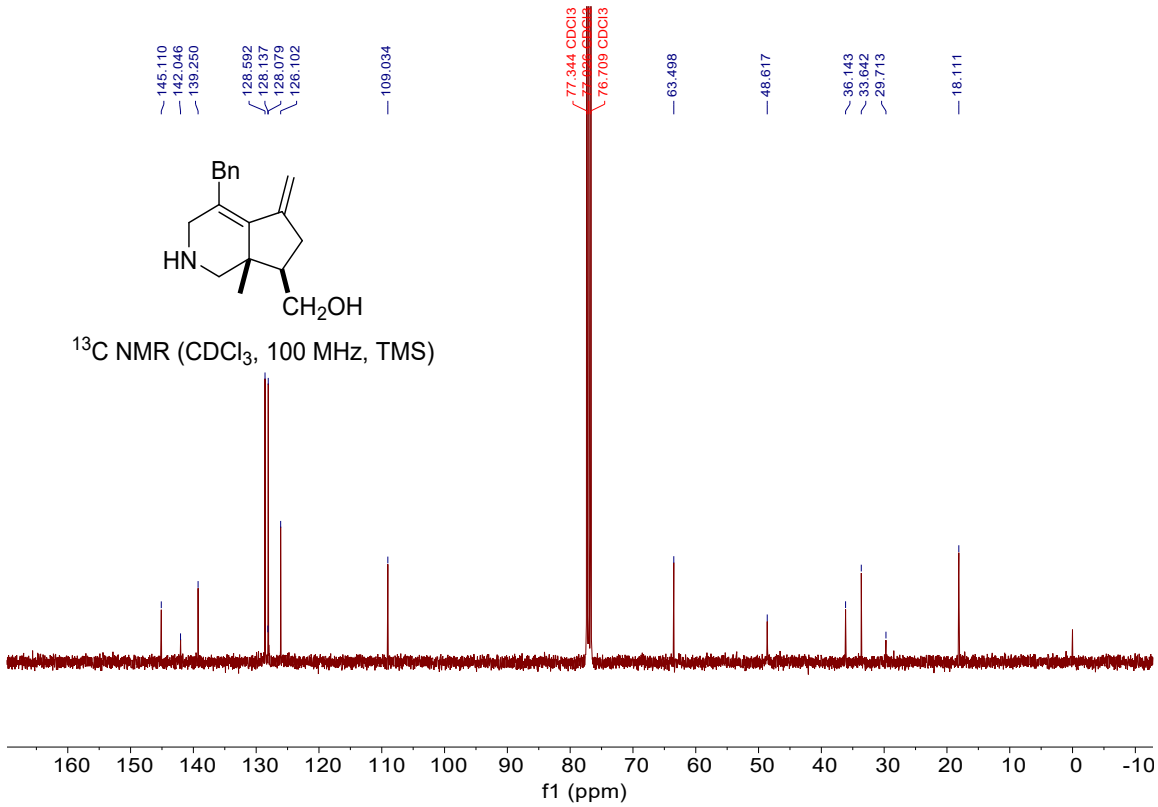
(cis)-4-benzyl-7a-methyl-5-methylene-2,3,5,6,7,7a-hexahydro-1H-cyclopenta[c]pyridin-7-yl)methanol (9)

A yellow oil, 56% yield, 15.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.21 (m, 3H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 2H), 5.07 (t, *J* = 2.4 Hz, 1H), 4.98 (d, *J* = 2.4 Hz, 1H), 3.87 (d, *J* = 15.4 Hz, 1H), 3.70 (d, *J* = 7.2 Hz, 2H), 3.40 – 3.01 (m, 4H), 2.58 (dd, *J* = 16.8, 8.4 Hz, 2H), 2.35 – 2.09 (m, 3H), 1.95 – 1.76 (m, 1H), 1.05 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 142.0, 139.2, 128.6, 128.1, 128.1, 126.1, 109.0, 63.5, 48.6, 36.1, 33.6, 29.7, 18.1. IR (neat) ν 698, 1029, 1541, 2924 cm^{-1}. HRMS (ESI) calcd. for $C_{18}H_{24}NO_3$ $(M+H)^+$: 270.1852, Found: 270.1846.



^{1}H NMR ($CDCl_3$, 400 MHz, TMS)




145.110
142.046
139.250
128.592
128.137
128.079
126.102
109.034
77.344 CDCl3
76.709 CDCl3
63.498
48.617
36.143
33.642
29.713
18.111
Bn
HN
CH2OH
13C NMR (CDCl3, 100 MHz, TMS)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

7. Computational studies

7.1 DFT calculations.

All quantum mechanical calculations have been performed with Gaussian 16.[4] The geometries of all species have been optimized at B3LYP/6-31G(d)/Lanl2dz level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the SMD(toluene)/M06/6-311+G(d,p)/Lanl2dz//B3LYP/6-31G(d)/Lanl2dz level to yield free energy G_{298} at 298.15 K. The solvent effect was estimated by the IEFPCM method with radii and nonelectrostatic terms for SMD salvation model in toluene (ε = 2.3741). All transition states were characterized by only one imaginary frequency pertaining to the desired reaction coordinate. The intrinsic reaction coordinate (IRC) calculations were carried out at the same level of theory to further authenticate the transition states.

Table S2. The total energies, enthalpies and free energies of all species in toluene shown in **Scheme 6**

	E_{tot}	H_{298}	G_{298}
1a	-1530.400171	-1529.9535	-1530.046917
PdL	-1599.719147	-1599.006049	-1599.11262
1a+PdL	-3130.119318	-3128.959549	-3129.159537
2-Int1	-3130.137304	-3128.975995	-3129.160782
2-Ts1	-3130.127365	-3128.968557	-3129.150508
2-Int2	-3130.138826	-3128.978398	-3129.158371
2-Ts2	-3130.109595	-3128.949922	-3129.126309
2-Int3	-3130.129346	-3128.968225	-3129.144583
2-Ts3	-3130.109595	-3128.950568	-3129.119502
2-Int4	-3130.193322	-3129.030167	-3129.197772
2-Ts4	-3130.182306	-3129.020747	-3129.189121
2a	-1530.493307	-1530.044027	-1530.129621
2a+PdL	-3130.212454	-3129.050076	-3129.242241
3a-Me	-1530.398781	-1529.952009	-1530.044963
3a-Me+PdL	-3130.117928	-3128.958058	-3129.157583
4-Int1	-3130.136862	-3128.975368	-3129.15988
4-Ts1	-3130.127724	-3128.96881	-3129.150866
4-Int2	-3130.132701	-3128.972345	-3129.152845
4-Ts2	-3130.095567	-3128.935838	-3129.110807

4-Int3	-3130.132407	-3128.971298	-3129.147608
4-Ts3	-3130.105588	-3128.946306	-3129.116045
4-Int4	-3130.193826	-3129.031092	-3129.199873
4-Ts4	-3130.180548	-3129.019447	-3129.190934
4a-Me	-1530.490918	-1529.041624	-1530.126867

6.2 Archive entries

1a

Zero-point correction= 0.417153 (Hartree/Particle)

Thermal correction to Energy= 0.445727

Thermal correction to Enthalpy= 0.446671

Thermal correction to Gibbs Free Energy= 0.353255

Sum of electronic and zero-point Energies= -1530.433234

Sum of electronic and thermal Energies= -1530.404660

Sum of electronic and thermal Enthalpies= -1530.403716

Sum of electronic and thermal Free Energies= -1530.497133

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -1530.862952

N	7.44804800	0.53864500	0.50003000
C	6.99852100	1.07898000	-0.79294100
H	7.86352800	1.55858400	-1.26140000
H	6.66377500	0.26124700	-1.44713500
C	5.91132900	2.13329500	-0.66789100
C	6.58820100	-0.48920800	1.12760700
H	7.23197400	-1.17262100	1.68929400
H	6.08939900	-1.06505900	0.33907600
C	5.55741000	0.09622800	2.08234300
C	4.27630400	0.02251900	1.79333600
C	3.02191400	-0.04600800	1.49444100
C	1.86607000	0.60532800	0.84711400
C	1.76149300	-0.80766800	1.55317400
H	1.86435700	0.65777200	-0.24099800
H	1.43290300	1.46749700	1.35229800
H	1.24984500	-0.86891200	2.51228900
H	1.67885400	-1.69780300	0.93062100
S	9.11445300	0.44824600	0.77306600
O	9.68668500	1.66799100	0.19534500
O	9.27210400	0.10876800	2.18960400
C	9.73714800	-0.94191100	-0.18047000
C	9.82179300	-2.20464200	0.41171800
C	10.11828200	-0.75303500	-1.51211700
C	10.27231800	-3.28428000	-0.34635100
H	9.56921900	-2.32825500	1.45928700
C	10.56589400	-1.84400200	-2.25415000
H	10.09512300	0.24022400	-1.94753700
C	10.64240200	-3.12586900	-1.68938300
H	10.34848000	-4.26471800	0.11736500
H	10.87280700	-1.69518500	-3.28655900
C	11.10261000	-4.30633700	-2.51122600
H	11.55277500	-5.08151900	-1.88282800
H	10.25989400	-4.76644600	-3.04436500
H	11.83897500	-4.00771000	-3.26462000
C	6.23652900	3.30622300	0.21186500
H	6.24497200	2.98751000	1.26096000
H	7.24896200	3.66942500	-0.00478100
H	5.51370800	4.11128400	0.09235000
C	6.08151300	0.70636600	3.36380900
H	6.57411900	-0.05616100	3.98176000
H	6.84001400	1.46734200	3.14856200
H	5.27626100	1.16062400	3.94670300
C	4.78472800	1.96787400	-1.38886400
C	3.64507300	2.90487500	-1.46757300
O	3.53723200	4.00763300	-0.96342600
O	2.65579100	2.35230700	-2.22468600
C	1.48860300	3.16895500	-2.39575500
H	0.81102700	2.58452600	-3.01874100
H	1.02490800	3.38762100	-1.42991700
H	1.74764300	4.11198600	-2.88534200
H	4.65767400	1.06320700	-1.97723800

PdL

Zero-point correction= 0.675005 (Hartree/Particle)

Thermal correction to Energy= 0.712154

Thermal correction to Enthalpy= 0.713098

Thermal correction to Gibbs Free Energy= 0.606527

Sum of electronic and zero-point Energies= -1599.609148

Sum of electronic and thermal Energies= -1599.572000

Sum of electronic and thermal Enthalpies= -1599.571056

Sum of electronic and thermal Free Energies= -1599.677627

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -1600.040533

Pd	-4.27170700	-0.14773300	0.00313200
P	-2.01657000	-0.23326900	-0.39739100
C	-1.66186200	0.78965400	-1.99273200
C	-1.52478000	-2.08669500	-0.59915000
C	-1.65197000	-2.70119000	0.81129100
H	-0.92868300	-2.28571200	1.51644300
H	-2.65525500	-2.53514800	1.21929600
H	-1.48168500	-3.78420500	0.75131600
C	-2.58704300	-2.76647100	-1.49155800
H	-2.41992600	-3.85222000	-1.47509500
H	-3.60163000	-2.56256600	-1.13066800
H	-2.52375200	-2.44310800	-2.53458900
C	-0.13883200	-2.38593400	-1.19432900
H	0.07239000	-3.45886400	-1.08755900
H	-0.10274500	-2.16373700	-2.26353900

H	0.66685800	-1.83440600	-0.70916600
C	-2.74608600	0.43750300	-3.03551300
H	-2.66126100	1.13260700	-3.88211500
H	-2.62974100	-0.57505000	-3.43257800
H	-3.75225900	0.52443500	-2.60983000
C	-0.28538100	0.60320800	-2.65218600
H	-0.20398000	-0.36829100	-3.14557400
H	-0.15553000	1.36569500	-3.43248900
H	0.54404900	0.69446300	-1.95024000
C	-1.87474000	2.26532500	-1.59288400
H	-2.87315400	2.41353600	-1.16645600
H	-1.14133200	2.61155200	-0.86131500
H	-1.78654400	2.89855000	-2.48551100
C	-1.04206500	0.53342600	1.08290700
C	0.33836800	0.75253400	1.40915400
C	-1.98834100	0.96362900	2.04271800
C	0.64118100	1.36957500	2.64145100
C	-1.65823500	1.57086800	3.25134700
H	-3.04091100	0.80501900	1.81224300
C	-0.32072900	1.77871300	3.55903900
H	1.68857700	1.52909100	2.87691700
H	-2.44655700	1.87286500	3.93565600
H	-0.02067300	2.24890100	4.49193400
C	1.58996000	0.41860200	0.62042700
C	2.29288800	-0.79187200	0.87426500
C	2.19913500	1.40183400	-0.20352100
C	3.47230600	-1.05705400	0.16860900
C	3.38123100	1.08106100	-0.88514200
C	4.01926200	-0.15070700	-0.74315100
H	3.98994400	-1.99396600	0.35325600
H	3.83259600	1.82573500	-1.53556600
C	5.28915400	-0.46725900	-1.52208700
H	5.51354900	0.41151900	-2.14223400
C	5.09038800	-1.66372600	-2.47225800
H	4.87295700	-2.58211400	-1.91390800
H	4.25736700	-1.48768300	-3.16163300
H	5.99491100	-1.84063100	-3.06664500
C	6.49683200	-0.69473500	-0.59283400
H	7.40902300	-0.85999400	-1.17869400
H	6.66233100	0.16891800	0.06061100
H	6.34934400	-1.57367900	0.04596500
C	1.88715100	-1.75373200	1.99686600
H	0.83795900	-1.56598700	2.24139600
C	2.71078000	-1.45476300	3.27025800
H	2.40995000	-2.12455100	4.08516200
H	3.78047900	-1.60804300	3.08365100
H	2.57380200	-0.42550100	3.61313500
C	2.03053700	-3.24762400	1.65050500
H	3.08148600	-3.54248500	1.54898600
H	1.60508300	-3.85537100	2.45757600
H	1.51654600	-3.51032000	0.72313300
C	1.69650200	2.84849000	-0.26389100
H	0.65431100	2.85953600	0.06714800
C	1.75528100	3.49553400	-1.66036500
H	1.26627800	4.47626300	-1.63256400
H	2.78802400	3.66266600	-1.98765300
H	1.25557200	2.89058800	-2.42027500
C	2.49684200	3.72502500	0.72641800
H	3.55999300	3.73952800	0.45796300
H	2.12832900	4.75795300	0.70521300
H	2.41460200	3.35968900	1.75375000

2-Int1

Zero-point correction= 1.108267 (Hartree/Particle)

Thermal correction to Energy= 1.173164

Thermal correction to Enthalpy= 1.174109

Thermal correction to Gibbs Free Energy= 1.006260

Sum of electronic and zero-point Energies= -3129.392785

Sum of electronic and thermal Energies= -3129.327887

Sum of electronic and thermal Enthalpies= -3129.326943

Sum of electronic and thermal Free Energies= -3129.494791

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.160782

N	7.48520821	-11.22022479	-1.67957616
C	6.54741821	-10.81542050	-2.72599123
H	6.74046524	-11.44333173	-3.60085518
H	5.51151938	-10.98685149	-2.39850261
C	6.74957413	-9.37392667	-3.13935640
C	7.23275279	-10.68471146	-0.33261880
H	7.53904729	-11.43493351	0.40245770
H	6.15703926	-10.51100294	-0.21335575
C	8.00816546	-9.40605540	-0.08764876
C	7.36799565	-8.27137563	0.06182212
C	6.71003346	-7.16822874	0.17318464
C	6.12816615	-6.01706379	-0.54575799
C	6.09040718	-6.13395521	1.00579184
H	5.19884923	-6.21551699	-1.07873946
H	6.83032691	-5.33416061	-1.03018758
H	6.75770777	-5.49280388	1.57433871
H	5.12926914	-6.33742604	1.47132530
S	8.15824170	-12.74108944	-1.79849026

O	8.47128447	-12.94494044	-3.20366534	H	1.22439533	-0.66038951	0.51050985
O	9.17658224	-12.82265968	-0.76479025	H	1.45504185	-0.38299873	2.23424054
C	6.85108791	-13.86955999	-1.36050862	H	2.34346384	0.59754893	1.07504140
C	6.71608839	-14.28736284	-0.03933089	C	4.00465431	-1.11397423	2.53115508
C	5.94050830	-14.27573900	-2.33380466	H	4.79812263	-1.85628916	2.64318537
C	5.64929926	-15.10881051	0.30672356	H	4.46576110	-0.12708907	2.42814243
H	7.45525467	-13.99334028	0.69828807	H	3.41294095	-1.11703068	3.45559243
C	4.87998271	-15.09594820	-1.96996687	C	5.45641500	-0.34579000	-0.12290200
H	6.07995327	-13.97482925	-3.36686830	C	5.07777400	1.01834600	-0.11038500
C	4.71365037	-15.51813943	-0.64714725	C	6.82805700	-0.64509100	-0.12065300
H	5.54747369	-15.44478790	1.33516357	C	6.08489900	1.99540200	-0.08558700
H	4.17401049	-15.42274304	-2.72881477	C	7.81070600	0.33545400	-0.09542600
C	3.54241396	-16.38335350	-0.25809178	H	7.14256000	-1.68067300	-0.14971000
H	3.77264592	-16.99722268	0.61763113	C	7.43430400	1.67261200	-0.07461500
H	2.67153509	-15.76514636	-0.00905670	H	5.78301500	3.03908900	-0.08529400
H	3.24999563	-17.04977646	-1.07513318	H	8.85941900	0.05353100	-0.09687500
C	8.13877994	-9.02253601	-3.57870920	H	8.18238800	2.45964600	-0.05760100
H	8.73717999	-8.75933588	-2.70076137	C	3.67831500	1.57890100	-0.15304700
H	8.61781620	-9.88857405	-4.04717315	C	3.09663900	1.91081100	-1.39517500
H	8.14842841	-8.16540811	-4.25123631	C	3.03187600	1.96463200	1.03561800
C	9.50969903	-9.53144323	-0.04402298	C	1.86610200	2.56465100	-1.41401100
H	9.81080365	-10.23070819	0.74493971	C	1.79789900	2.61311900	0.96580000
H	9.88837302	-9.94377306	-0.98614645	C	1.18577700	2.90910700	-0.24707300
H	9.98508935	-8.56551043	0.14090156	H	1.41386800	2.81765200	-2.37165900
Pd	5.18614102	-3.76355308	-0.19819657	H	1.29748500	2.87520300	1.89181000
P	4.21026600	-1.72671100	-0.19430300	C	-0.16275200	3.60441900	-0.33657500
C	3.09225142	-1.46223978	1.34599355	H	-0.70505000	3.13201400	-1.16754500
C	3.19490034	-1.34755778	-1.77001164	C	-1.01918200	3.43972500	0.92025500
C	4.13813159	-1.59844639	-2.95559836	H	-1.11897700	2.38918700	1.21201400
H	4.89632095	-0.81321669	-3.02808854	H	-0.59517100	3.98732100	1.77026400
H	4.65193462	-2.55778422	-2.86701455	H	-2.02174600	3.84579200	0.74722500
H	3.56399795	-1.59177735	-3.89146403	C	0.02076000	5.09040500	-0.67941700
C	2.05493947	-2.37797013	-1.83139952	H	0.59031400	5.21902200	-1.60597100
H	1.57670545	-2.33535854	-2.81874018	H	-0.95042800	5.58406900	-0.80201500
H	2.43379707	-3.39397268	-1.67227011	H	0.56486700	5.60238700	0.12306100
H	1.27835661	-2.18091075	-1.08558727	C	3.65368800	1.72758500	2.40095100
C	2.62045929	0.06481264	-1.96177844	H	4.41975600	0.95778600	2.28376700
H	2.05679725	0.08473159	-2.90388040	C	4.35550900	2.99623300	2.90823600
H	1.93614230	0.37277390	-1.17015045	H	3.64146400	3.82413000	2.99133900
H	3.41357624	0.81267573	-2.04777942	H	4.79324000	2.82372600	3.89844100
C	2.43675145	-2.82361918	1.65174410	H	5.15781800	3.30666000	2.23175500
H	1.83093752	-2.73761775	2.56390744	C	2.63632900	1.23195000	3.43806800
H	1.78173729	-3.16145392	0.84350361	H	1.96453900	0.47885000	3.01727400
H	3.19749652	-3.59613262	1.80307831	H	3.15609300	0.79792000	4.29973600
C	1.97386978	-0.41313436	1.26719445	H	2.01046000	2.04961600	3.81300700

C	3.80909300	1.63308600	-2.70976200
H	4.64027900	0.95364400	-2.50363700
C	2.90722600	0.94916000	-3.74301100
H	2.09553600	1.60587500	-4.07736900
H	3.48827500	0.67140000	-4.62990900
H	2.46179100	0.03961500	-3.32420200
C	4.40882500	2.92815600	-3.27541100
H	4.94926500	2.72983200	-4.20821700
H	3.62302300	3.66322600	-3.48623100
H	5.10929400	3.37885700	-2.56462100
C	5.69132373	-8.55046832	-3.11179336
C	5.69918923	-7.12272399	-3.48325745
O	6.65955320	-6.43199191	-3.75749116
O	4.43986388	-6.64010526	-3.44737712
C	4.30514643	-5.24008587	-3.68085743
H	3.23367947	-5.05050143	-3.74473600
H	4.72852462	-4.67968605	-2.83911678
H	4.80753827	-4.94657791	-4.60565480
H	4.72845897	-8.92281220	-2.77368784

2-Ts1

Zero-point correction= 1.090660 (Hartree/Particle)

Thermal correction to Energy= 1.157864

Thermal correction to Enthalpy= 1.158808

Thermal correction to Gibbs Free Energy= 0.976857

Sum of electronic and zero-point Energies= -3130.027104

Sum of electronic and thermal Energies= -3129.959901

Sum of electronic and thermal Enthalpies= -3129.958956

Sum of electronic and thermal Free Energies= -3130.140907

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.150508

Imaginary frequency is-209.52cm^{-1}

N	-7.16850000	0.54348100	-0.52501200
C	-6.66768000	1.31743900	0.62180900
H	-7.50682900	1.90424500	1.00827700
H	-6.33065000	0.63706000	1.41680000
C	-5.56368300	2.29742100	0.26191200
C	-6.36010600	-0.62182500	-0.94826900
H	-7.04138600	-1.37385800	-1.35739800
H	-5.86848200	-1.05257300	-0.06783600
C	-5.32543100	-0.27963900	-2.01139800
C	-4.04283000	-0.37163000	-1.73668400
C	-2.77978100	-0.46597300	-1.45572700
C	-1.65241600	0.33918600	-0.95098600
C	-1.67060900	-1.43810800	-1.46295800
H	-1.68853600	0.62252300	0.10170600
H	-1.26507400	1.10015100	-1.63026200
H	-1.29145000	-1.73274500	-2.44315200
H	-1.71985500	-2.23363500	-0.71732000
S	-8.84298600	0.46375500	-0.74233700
O	-9.35910200	1.79579300	-0.41214300
O	-9.05079000	-0.14772400	-2.05741600
C	-9.48724300	-0.68047300	0.48485300
C	-9.62737600	-2.03311200	0.16371600
C	-9.82943500	-0.21166000	1.75653300
C	-10.09414400	-2.91923000	1.13329500
H	-9.40447900	-2.37591000	-0.84090900
C	-10.29404000	-1.11223700	2.71280900
H	-9.76322500	0.84774000	1.98009700
C	-10.42595800	-2.47821500	2.42221400
H	-10.21340800	-3.96988300	0.88024600
H	-10.57059500	-0.74594700	3.69849500
C	-10.90384500	-3.45006000	3.47480000
H	-10.06223400	-3.83237200	4.06781400
H	-11.60254600	-2.97520100	4.17143400
H	-11.40440100	-4.31384100	3.02549800
C	-5.88117800	3.26385400	-0.84312400
H	-5.85016400	2.74183300	-1.80703800
H	-6.90484200	3.64153300	-0.73179800
H	-5.17174100	4.08916600	-0.87102600
C	-5.85498100	0.10629800	-3.37583900
H	-6.40126300	-0.73153900	-3.82932100
H	-6.56911400	0.93361100	-3.29620700
H	-5.04444200	0.39864300	-4.04830900
Pd	0.30161900	-0.70584200	-0.75229300
P	2.62118500	-0.91182000	-0.15158700
C	3.22453400	-2.66942900	-0.65952700
C	2.74548600	-0.63519200	1.74902800
C	2.28443800	0.82394700	1.96083700
H	2.95142700	1.54552500	1.48254300
H	1.27748000	0.97447300	1.55631200
H	2.26150700	1.04576900	3.03612500
C	1.69789000	-1.55150200	2.42118700
H	1.58221700	-1.24455100	3.46954800
H	0.72110800	-1.47846400	1.92961600
H	2.00897200	-2.60066000	2.42446000
C	4.09784700	-0.87095700	2.44032800
H	4.02022200	-0.55630600	3.49063600
H	4.37547200	-1.92716400	2.44515000
H	4.91356300	-0.31263200	1.98452200
C	2.09861200	-3.68204600	-0.35157800
H	2.39199200	-4.66644000	-0.74175500

H	1.91642100	-3.79562500	0.72023000
H	1.15669300	-3.38686400	-0.82536000
C	4.51465100	-3.15613200	0.01986500
H	4.33439700	-3.43717800	1.06149700
H	4.88063600	-4.05507800	-0.49440600
H	5.31083000	-2.40965600	0.00700600
C	3.39679300	-2.64203500	-2.19333100
H	2.47482800	-2.31606400	-2.68779500
H	4.20208000	-1.97883300	-2.51637800
H	3.63031900	-3.65498200	-2.54672300
C	3.68320700	0.36032900	-1.12796100
C	5.04069000	0.82340800	-1.09622100
C	2.84905700	0.92581100	-2.12192900
C	5.43030300	1.80165200	-2.03600200
C	3.26783400	1.87929900	-3.04600000
H	1.81349400	0.59342200	-2.15916700
C	4.57994700	2.33044500	-3.00150400
H	6.45487800	2.15708600	-1.99175000
H	2.56509300	2.26314100	-3.78066700
H	4.94399100	3.08182200	-3.69734100
C	6.18137800	0.45010200	-0.16828400
C	6.45673400	1.25959400	0.96526700
C	7.11888800	-0.55513200	-0.53588900
C	7.55930700	0.95089900	1.77338000
C	8.19627400	-0.82604400	0.31596100
C	8.42522500	-0.10396300	1.48979600
H	7.75657000	1.56098900	2.65104400
H	8.89289500	-1.61189600	0.03999800
C	9.59450100	-0.42498600	2.41134200
H	9.56073200	0.29845400	3.23760700
C	9.46489300	-1.83227900	3.02508600
H	8.51633000	-1.94425900	3.56164000
H	9.50406500	-2.60802400	2.25101200
H	10.28209600	-2.02368000	3.73097200
C	10.95297500	-0.25332700	1.70518300
H	11.06278400	0.75755500	1.29737100
H	11.77747900	-0.43055200	2.40617400
H	11.06458700	-0.96214800	0.87605700
C	7.07832000	-1.25736200	-1.89779900
H	6.04580300	-1.23922600	-2.25710300
C	7.93410800	-0.48289100	-2.92637300
H	8.97956600	-0.43583700	-2.59861800
H	7.90713300	-0.98759700	-3.89995000
H	7.57789300	0.54012400	-3.06927800
C	7.54835700	-2.72497900	-1.87986500
H	7.06825900	-3.31055200	-1.09219900
H	7.31775400	-3.19672200	-2.84204000
H	8.63325700	-2.80002500	-1.74122900
C	5.65501600	2.52393100	1.29064400
H	4.70400700	2.46982300	0.75249600
C	5.33905400	2.70128800	2.78837100
H	6.24078600	2.92361900	3.37049700
H	4.65311200	3.54550800	2.92526100
H	4.87192200	1.81214000	3.21973700
C	6.39752700	3.77743700	0.77671300
H	5.81658600	4.68200400	0.99448100
H	7.37422500	3.87743900	1.26523300
H	6.56460900	3.73685600	-0.30345100
C	-4.42897800	2.26546700	0.98841100
C	-3.27334100	3.17516500	0.85219700
O	-3.15147800	4.13662900	0.11535200
O	-2.28674600	2.78618900	1.70788500
C	-1.10194300	3.59384400	1.68007600
H	-0.42577700	3.14738300	2.40996800
H	-0.65032700	3.58329100	0.68428900
H	-1.33399100	4.62758300	1.95182500
H	-4.30839000	1.50407600	1.75424300

2-Int2

Zero-point correction= 1.092391 (Hartree/Particle)

Thermal correction to Energy= 1.159484

Thermal correction to Enthalpy= 1.160428

Thermal correction to Gibbs Free Energy= 0.980456

Sum of electronic and zero-point Energies= -3130.040664

Sum of electronic and thermal Energies= -3129.973571

Sum of electronic and thermal Enthalpies= -3129.972627

Sum of electronic and thermal Free Energies= -3130.152600

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.158371

N	-4.16850152	-10.68328005	-3.60977411
C	-4.87384552	-11.28023197	-2.47754945
H	-5.45285317	-12.12725082	-2.85863913
H	-4.15917884	-11.65533106	-1.72917900
C	-5.84332119	-10.30706642	-1.85053881
C	-3.20715855	-9.61814075	-3.26136985
H	-2.31261996	-9.74198885	-3.88111424
H	-2.90969676	-9.75071665	-2.21545843
C	-3.75708487	-8.22215529	-3.47206602
C	-3.95994054	-7.42789778	-2.44673346
C	-4.17517096	-6.58924027	-1.46420503
C	-5.46193850	-6.13428631	-0.84804264

C	-3.25276853	-5.57132457	-0.88350530	H	-2.13810883	-1.04923634	2.36694160
H	-5.60909720	-6.51052419	0.16944600	C	-1.62970335	-2.16369254	-2.29417082
H	-6.36422709	-6.23015102	-1.45519207	H	-1.10371315	-1.65666945	-3.11315546
H	-2.41918340	-5.24101951	-1.50548375	H	-0.87506182	-2.54233669	-1.60010994
H	-2.92548248	-5.83340832	0.12961186	H	-2.16506141	-3.02208367	-2.71032233
S	-3.77398822	-11.70664468	-4.86296760	C	-1.83173060	0.07333709	-1.18454286
O	-4.93930713	-12.54515227	-5.09859779	H	-1.03690251	-0.15336736	-0.47075246
O	-3.19902333	-10.88316676	-5.91311118	H	-1.35446680	0.52195879	-2.06509550
C	-2.47479305	-12.75081510	-4.22938970	H	-2.48222687	0.83808257	-0.75052722
C	-1.14431085	-12.39103723	-4.42579854	C	-3.60787193	-0.74111198	-2.71586170
C	-2.80389609	-13.88635583	-3.49209770	H	-4.11384196	-1.60499829	-3.14860466
C	-0.13971987	-13.17202803	-3.86580890	H	-4.36056931	-0.04171199	-2.33956603
H	-0.90497506	-11.52480230	-5.03346471	H	-3.06017911	-0.24390513	-3.52613810
C	-1.78749443	-14.65497810	-2.93856535	C	-5.11247900	-1.19105100	0.00847000
H	-3.84340998	-14.17615050	-3.37917785	C	-5.02561300	0.18556700	0.30276700
C	-0.44398765	-14.30719819	-3.10986435	C	-6.37612600	-1.80071000	0.01005500
H	0.89979819	-12.89851707	-4.02623389	C	-6.20838800	0.88899700	0.57698100
H	-2.04147459	-15.54662847	-2.37134222	C	-7.53605700	-1.08836200	0.28202500
C	0.64988877	-15.13076780	-2.47941883	H	-6.45680100	-2.86046200	-0.19983200
H	1.00442666	-15.91132023	-3.15914984	C	-7.45054300	0.27032600	0.56677500
H	1.50974820	-14.50019717	-2.22295919	H	-6.13506900	1.94736300	0.81181500
H	0.30719654	-15.61061342	-1.55763835	H	-8.49750000	-1.59275400	0.27610800
C	-6.88856470	-9.74686908	-2.77197387	H	-8.34507800	0.84532500	0.78652600
H	-6.68135245	-8.68635130	-2.95227487	C	-3.77138000	1.02991300	0.39200700
H	-6.86407096	-10.26184217	-3.73607895	C	-3.22245600	1.31156500	1.67347100
H	-7.88503330	-9.81445464	-2.33145971	C	-3.41767900	1.87712600	-0.68838500
C	-4.01353465	-7.82147938	-4.90573941	C	-2.39538000	2.41554500	1.83687400
H	-3.09786709	-7.88856791	-5.50641951	C	-2.56698600	2.96560300	-0.46945500
H	-4.73795204	-8.50258960	-5.36769331	C	-2.06747800	3.27645800	0.78966900
H	-4.40156547	-6.80105390	-4.96108228	H	-2.02074600	2.63900100	2.83260600
Pd	-4.76519995	-4.17996322	-0.66024055	H	-2.33160600	3.61003600	-1.31014300
P	-3.55607900	-2.13574300	-0.28315200	C	-1.23889300	4.51823500	1.08740500
C	-2.60770886	-1.17341698	-1.63418762	H	-1.79669600	5.07182100	1.85768200
C	-2.03059264	-2.55082319	0.78089956	C	0.13144200	4.15261600	1.67947000
C	-2.46891326	-3.64478462	1.76660495	H	0.04268500	3.49727400	2.55202100
H	-3.20862580	-3.26790288	2.47798458	H	0.74266200	3.65219700	0.92501400
H	-2.89498008	-4.50740411	1.24667277	H	0.66030200	5.05975700	1.99336600
H	-1.59821603	-3.98111851	2.34394644	C	-1.05734400	5.44722600	-0.11416100
C	-0.94843953	-3.15613315	-0.12985185	H	-2.01802100	5.75509600	-0.54253400
H	-0.15535091	-3.58170170	0.49762703	H	-0.52476400	6.35213000	0.19635300
H	-1.34939095	-3.96165911	-0.75188013	H	-0.45324000	4.96366900	-0.88935000
H	-0.48029837	-2.41426287	-0.78187661	C	-4.05716600	1.71981200	-2.05784700
C	-1.43218160	-1.40560248	1.61121057	H	-4.56651800	0.75364700	-2.07222100
H	-0.54990512	-1.78432219	2.14310359	C	-5.12539100	2.79835200	-2.28960300
H	-1.10762595	-0.55390891	1.01030491	H	-4.68364800	3.80066500	-2.24793900

H	-5.58889600	2.67193200	-3.27469400
H	-5.91472200	2.74402900	-1.53339200
C	-3.02581500	1.72797800	-3.19178900
H	-2.18460600	1.06599500	-2.96453800
H	-3.48861900	1.39746600	-4.12843800
H	-2.62882600	2.73552900	-3.36130800
C	-3.59667800	0.50179100	2.90150400
H	-4.20696900	-0.34060600	2.57041300
C	-2.35054700	-0.05765000	3.60001900
H	-1.73681000	0.74331900	4.02670100
H	-2.63661700	-0.72696600	4.41971100
H	-1.72295000	-0.61169700	2.89208400
C	-4.46007500	1.32298900	3.86846800
H	-4.75198600	0.71316300	4.73083600
H	-3.91714300	2.19831600	4.24259200
H	-5.37261200	1.67586600	3.37624700
C	-5.71243542	-10.02566660	-0.54512291
C	-6.62616172	-9.16070609	0.21670397
O	-7.70915719	-8.74560377	-0.14463208
O	-6.12040688	-8.88380317	1.43461900
C	-6.92916007	-8.03210579	2.23830313
H	-6.35095470	-7.83949100	3.14216842
H	-7.13606226	-7.09568591	1.71306511
H	-7.87714510	-8.51868396	2.48599295
H	-4.87932923	-10.43331409	0.01958926

2-Ts2

Zero-point correction= 1.092387 (Hartree/Particle)

Thermal correction to Energy= 1.158729

Thermal correction to Enthalpy= 1.159673

Thermal correction to Gibbs Free Energy= 0.983287

Sum of electronic and zero-point Energies= -3129.991967

Sum of electronic and thermal Energies= -3129.925625

Sum of electronic and thermal Enthalpies= -3129.924681

Sum of electronic and thermal Free Energies= -3130.101068

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.126309

Imaginary frequency is -150.68^{-1}

N	5.98450100	0.27307000	0.61204600
C	5.91109800	1.03714700	-0.64355100
H	6.92679200	1.34175500	-0.91556100
H	5.52191900	0.39457000	-1.44453600
C	5.07194700	2.30011500	-0.52512400
C	4.89497700	-0.70924200	0.86249600
H	5.27886900	-1.40558000	1.61397200
H	4.69635800	-1.27136500	-0.06019900
C	3.60373300	-0.08868600	1.39442200
C	2.43015000	-0.27112600	0.79239500
C	1.98061700	-0.97463700	-0.36433800
C	1.62960100	-2.34121300	-0.42837500
C	1.29957200	-0.15207100	-1.36818300
S	7.52997400	-0.10708200	1.17762800
O	8.34699000	1.09633600	0.97636200
O	7.35513300	-0.70483800	2.50354700
C	8.19799600	-1.38194400	0.09875600
C	7.89869700	-2.72527300	0.34616900
C	8.98496800	-1.02001200	-0.99692400
C	8.38041900	-3.70241400	-0.52176900
H	7.31521900	-2.99873500	1.21864100
C	9.46005000	-2.01199000	-1.85429700
H	9.23940700	0.02213900	-1.15729900
C	9.16536400	-3.36433900	-1.63454700
H	8.14855600	-4.74709500	-0.32820700
H	10.07613300	-1.73028000	-2.70487500
C	9.70679900	-4.43675400	-2.55022600
H	9.96548600	-4.03155300	-3.53369800
H	10.61581800	-4.88950100	-2.13239800
H	8.98070100	-5.24417700	-2.69471000
C	5.57066300	3.32249800	0.46249000
H	6.26486700	2.86121100	1.16820000
H	6.10673000	4.12328000	-0.06368400
H	4.75271500	3.79538700	1.00900000
C	3.75583700	0.66240300	2.70058100
H	4.19196600	0.02033200	3.47982300
H	4.43114200	1.52215700	2.60181000
H	2.78195000	1.02031400	3.04515400
Pd	-0.12287800	-0.46723000	0.11153500
P	-2.12263000	0.73778700	-0.15688600
C	-2.90966800	0.59594900	-1.91116600
C	-2.03689100	2.60837600	0.40121000
C	-1.01331000	2.73970700	1.55057400
H	-1.36794600	2.28121500	2.47725300
H	-0.04469100	2.30035700	1.29122500
H	-0.86364000	3.80732200	1.75873900
C	-1.53154800	3.50085700	-0.75066300
H	-1.38866600	4.51470100	-0.35344600
H	-0.56759000	3.17346100	-1.15189500
H	-2.25147300	3.58311100	-1.56853400
C	-3.39049600	3.13781300	0.90047900
H	-3.27870100	4.19087400	1.19251800
H	-4.17089700	3.08996200	0.13792900

H	-3.73240400	2.58906100	1.78246900
C	-1.85235300	1.08016400	-2.93480400
H	-2.23712400	0.86228600	-3.93949500
H	-1.64719600	2.14853400	-2.89002700
H	-0.90674500	0.54631600	-2.81666700
C	-4.21844600	1.37363300	-2.12598700
H	-4.08477200	2.45252600	-2.00391000
H	-4.56672800	1.20604300	-3.15406900
H	-5.01059700	1.03893900	-1.45440600
C	-3.13132300	-0.89809700	-2.21256100
H	-2.21014500	-1.47140400	-2.06443700
H	-3.92256000	-1.33206700	-1.60481700
H	-3.42857800	-1.00122800	-3.26453800
C	-3.02709600	-0.10031800	1.30143700
C	-4.32242000	-0.65135800	1.54019200
C	-2.09199100	-0.20173900	2.36477600
C	-4.61329500	-1.14118700	2.83051400
C	-2.39634600	-0.72418900	3.61929800
C	-3.68782300	-1.17421300	3.86844000
H	-5.60874300	-1.54068900	2.99953200
H	-1.62543700	-0.76940400	4.38308900
H	1.13535900	-2.74405300	-1.30550700
H	1.89571300	-3.02672200	0.36957900
H	1.51119900	0.91067000	-1.44470500
H	1.00597600	-0.63552100	-2.29980400
C	-5.44214400	-0.88324300	0.55390500
C	-6.47909400	0.07702500	0.39734200
C	-5.56198500	-2.14101900	-0.09260100
C	-7.52665200	-0.17825300	-0.49298200
C	-6.62663700	-2.32563900	-0.99208300
C	-7.60625700	-1.36450000	-1.22676800
H	-8.30700200	0.56804000	-0.61017300
H	-6.69684000	-3.27780500	-1.51560100
C	-4.73131400	-3.42072400	0.15100300
H	-4.76232100	-3.95441400	-0.80868200
C	-5.47378700	-4.31784800	1.16982100
H	-6.51539900	-4.48551000	0.87633300
H	-4.97806000	-5.29298400	1.24825800
H	-5.47204900	-3.86215200	2.16628300
C	-3.24350500	-3.34076100	0.53534200
H	-2.66843400	-2.67770600	-0.11379500
H	-3.09012200	-3.02108900	1.56847400
H	-2.81279000	-4.34520200	0.44000800
H	-1.07328300	0.15534100	2.21629100
H	-3.96751800	-1.57132000	4.84021400
C	-8.73151500	-1.61910600	-2.22064300
H	-8.56447200	-2.61771800	-2.64702800
C	-10.11157000	-1.63558400	-1.53581600
H	-10.35266200	-0.65866200	-1.10000200
H	-10.89843400	-1.87929700	-2.25957100
H	-10.14595900	-2.37804600	-0.73099600
C	-8.70402200	-0.60963500	-3.38418100
H	-8.88041500	0.41241800	-3.02811400
H	-7.73583300	-0.62211200	-3.89674400
H	-9.48287500	-0.84551400	-4.11915800
C	-6.54922600	1.33873800	1.25952300
H	-5.54928700	1.53089100	1.65452800
C	-7.00019900	2.59856600	0.49674300
H	-8.05906700	2.54975500	0.21763500
H	-6.87694200	3.48326000	1.13198800
H	-6.42207000	2.75539700	-0.41928800
C	-7.48031900	1.10843300	2.47021300
H	-7.51923000	2.00515700	3.10072900
H	-8.50101900	0.88300400	2.13880300
H	-7.13774400	0.27493200	3.09105600
C	4.00198900	2.41700900	-1.33521200
H	3.74685600	1.58630600	-1.98634100
C	3.00807700	3.49921400	-1.42093700
O	3.17486333	4.59355169	-0.90092900
O	1.88811910	3.18827848	-2.11403767
C	0.91990094	4.24080452	-2.22238796
H	0.59020470	4.56523700	-1.23166132
H	1.33997095	5.09928596	-2.75391696
H	0.08737824	3.81449361	-2.78334018

2-Int3

Zero-point correction= 1.093462 (Hartree/Particle)

Thermal correction to Energy= 1.160176

Thermal correction to Enthalpy= 1.161121

Thermal correction to Gibbs Free Energy= 0.984763

Sum of electronic and zero-point Energies= -3130.029404

Sum of electronic and thermal Energies= -3129.962690

Sum of electronic and thermal Enthalpies= -3129.961745

Sum of electronic and thermal Free Energies= -3130.138103

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.144583

N	5.12183000	-0.22760000	0.97589800
C	5.16273400	1.00711700	0.16190800
H	6.18050600	1.40777700	0.19620300
H	4.93805900	0.75630600	-0.88018300
C	4.20519400	2.08836400	0.66908500

C	4.30149500	-1.35098900	0.44388000	C	-3.87628000	3.10979100	-1.44747200
H	4.51241900	-2.21638100	1.07748000	H	-4.02037700	4.13352800	-1.81927900
H	4.61486500	-1.58066000	-0.57882400	H	-4.62304700	2.47726500	-1.92853000
C	2.82512600	-1.01412400	0.50645800	H	-4.07579900	3.12403100	-0.37228600
C	2.10119900	-0.77088700	-0.59579400	C	-2.18012600	-0.46879400	-3.67949400
C	2.41021700	-0.75628000	-2.02993900	H	-2.60617200	-1.26912800	-4.29904100
C	3.11622800	-1.60043600	-2.80858000	H	-2.20415300	0.44694700	-4.27095000
C	1.40690500	0.25526700	-2.49583400	H	-1.13768600	-0.72418800	-3.47572700
S	6.54363700	-0.64903100	1.78449700	C	-4.47169500	-0.09163000	-2.71851400
O	7.13031700	0.60647000	2.27426300	H	-4.58134800	0.84691000	-3.26967800
O	6.19342700	-1.73881200	2.69956800	H	-4.85641000	-0.89069400	-3.36722900
C	7.68180700	-1.31288800	0.56311200	H	-5.10741300	-0.05746300	-1.83147300
C	7.61168100	-2.66488000	0.21448300	C	-2.89988500	-1.79747100	-1.74303200
C	8.61464300	-0.46884400	-0.04549000	H	-1.85854800	-2.04742200	-1.50957700
C	8.47043700	-3.16230600	-0.76319500	H	-3.50353700	-1.89770800	-0.84377900
H	6.91360000	-3.32079900	0.72400000	H	-3.26463500	-2.53606800	-2.46941800
C	9.46661200	-0.98460600	-1.02103300	C	-2.65752200	0.85808300	0.64530000
H	8.68983400	0.56713600	0.26734700	C	-3.75732400	0.36486900	1.41100400
C	9.40375500	-2.33239400	-1.40215100	C	-1.64867100	1.55104300	1.35895700
H	8.42181300	-4.21575900	-1.02805900	C	-3.81792400	0.69039300	2.78239800
H	10.19949700	-0.33045000	-1.48735400	C	-1.72547600	1.84387200	2.71857200
C	10.30894000	-2.87595600	-2.48196900	C	-2.84015000	1.42940100	3.43987300
H	10.56487200	-3.92534800	-2.30012300	H	-4.66332500	0.31226000	3.34950700
H	9.82143000	-2.82572000	-3.46499500	H	-0.91567800	2.38556800	3.19947500
H	11.24058500	-2.30459500	-2.55015000	H	3.07457100	-1.52311000	-3.89328700
C	4.34111200	2.35421200	2.14593600	H	3.69168200	-2.42566000	-2.39951900
H	3.85023300	1.57278900	2.73390200	H	1.67143400	1.30893700	-2.36998900
H	5.39451000	2.32249200	2.42135300	H	0.90010700	0.05894700	-3.44317000
H	3.93062800	3.29589000	2.42496300	C	-4.85056700	-0.58305400	0.97817700
C	2.23938600	-1.00845900	1.90002000	C	-6.11204500	-0.09284800	0.54175600
H	2.12546400	-2.03488700	2.28050600	C	-4.68254600	-1.97566300	1.17604500
H	2.89148700	-0.48771800	2.61250900	C	-7.11382700	-0.99833400	0.17729500
H	1.25181500	-0.53603700	1.91738900	C	-5.71904900	-2.83632100	0.77114800
Pd	0.20322500	-0.03203800	-0.82940300	C	-6.92934400	-2.38196000	0.25166600
P	-2.10025100	0.83445300	-1.18109300	H	-8.06879900	-0.61060000	-0.16609100
C	-3.00600900	-0.39443400	-2.37052500	H	-5.57357100	-3.90892500	0.88977700
C	-2.42796100	2.67031800	-1.73372900	C	-3.52699900	-2.67911900	1.91996200
C	-1.51162700	3.68341800	-0.99921600	H	-3.47711300	-3.68198100	1.47485400
H	-0.92693790	3.20169325	-0.20959626	C	-3.92930800	-2.87892200	3.40116100
H	-0.82124395	4.32429529	-1.58790428	H	-4.90622200	-3.36601800	3.49160200
H	-2.20035903	4.37542904	-0.48892466	H	-3.18672600	-3.50064100	3.91658200
C	-2.12635400	2.80166000	-3.23923400	H	-3.98026700	-1.91721300	3.92423200
H	-1.27045291	3.47693847	-3.36417602	C	-2.09667900	-2.11567100	1.85432200
H	-1.85582462	1.84082427	-3.68814972	H	-1.76885800	-1.91254100	0.83266300
H	-2.95976407	3.23587781	-3.79856149	H	-1.97803500	-1.20053400	2.44121400

H	-1.41290900	-2.86425400	2.27354300
H	-0.76009600	1.87360100	0.82365900
H	-2.93752300	1.64621900	4.50018000
C	-8.01282800	-3.36016400	-0.18356200
H	-7.62188900	-4.37212500	-0.00896400
C	-9.29605000	-3.21077500	0.65612600
H	-9.75280900	-2.22368300	0.51531400
H	-10.03793000	-3.96422700	0.36454000
H	-9.08709900	-3.33295700	1.72471100
C	-8.32042300	-3.23689500	-1.68833900
H	-8.73047300	-2.24883700	-1.93043500
H	-7.41626000	-3.37955400	-2.29027200
H	-9.05791100	-3.98843700	-1.99556600
C	-6.45663100	1.39852600	0.57082000
H	-5.51996600	1.96073700	0.59184800
C	-7.26633200	1.88259300	-0.64703100
H	-8.29074700	1.49171300	-0.63781100
H	-7.34034800	2.97623700	-0.63411600
H	-6.80486300	1.58477000	-1.59330700
C	-7.22433200	1.74362300	1.86648000
H	-7.45835400	2.81491000	1.90004000
H	-8.16900300	1.18896900	1.91834000
H	-6.64232200	1.49807700	2.76035000
C	3.44165100	2.68663200	-0.26521200
H	3.54356300	2.26614800	-1.26106400
C	2.25994700	3.60229800	-0.35030200
O	1.45667100	3.43711900	-1.25044200
O	2.03013000	4.69427900	0.43413100
C	2.50588600	4.86609400	1.75552500
H	2.15449500	5.83732600	2.08887300
H	2.09203400	4.09379300	2.42158400
H	3.58584500	4.83032100	1.82256000

2-Ts3

Zero-point correction= 1.092948 (Hartree/Particle)

Thermal correction to Energy= 1.158082

Thermal correction to Enthalpy= 1.159027

Thermal correction to Gibbs Free Energy= 0.990093

Sum of electronic and zero-point Energies= -3130.003441

Sum of electronic and thermal Energies= -3129.938306

Sum of electronic and thermal Enthalpies= -3129.937362

Sum of electronic and thermal Free Energies= -3130.106296

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.119502

Imaginary frequency is -184.14^{-1}

N	-5.47506900	0.33091300	-0.88494000
C	-4.76061200	0.59144400	0.37063500
H	-5.01062300	1.61028600	0.68622800
H	-5.09621300	-0.09404600	1.15873200
C	-3.24837200	0.53719900	0.21016700
C	-5.80307400	-1.06241500	-1.20378300
H	-6.09478500	-1.10064200	-2.25878000
H	-6.68336100	-1.39329300	-0.61893900
C	-4.66662100	-2.03165000	-0.94064500
C	-3.44136400	-1.66780900	-0.55868800
C	-2.37068300	-2.49649600	-0.17496600
C	-2.04406700	-2.72315500	1.19694900
C	-1.19103000	-2.85593400	-0.97644600
S	-6.54280100	1.50279200	-1.44048200
O	-5.93817100	2.80324700	-1.12898600
O	-6.89701400	1.12670800	-2.81167500
C	-8.03872800	1.36638700	-0.45121900
C	-9.04753300	0.48103200	-0.84053500
C	-8.17225900	2.12696600	0.71354800
C	-10.18602600	0.35081900	-0.04647400
H	-8.95116000	-0.07190300	-1.76873700
C	-9.31770900	1.98490900	1.49449700
H	-7.40127400	2.84100300	0.98240000
C	-10.33723300	1.09165400	1.13420700
H	-10.97526700	-0.33060000	-0.35507100
H	-9.42681800	2.58592000	2.39419700
C	-11.56120400	0.92317800	2.00320900
H	-12.43409300	0.62485800	1.41331700
H	-11.40074100	0.14692600	2.76346500
H	-11.80810700	1.84955100	2.53238200
C	-2.73581400	1.22012400	-1.03981600
H	-1.64787300	1.16185000	-1.11733000
H	-3.17881600	0.76844800	-1.92713500
H	-3.03401800	2.27739800	-1.04371300
C	-5.11897100	-3.47167600	-1.14028800
H	-5.95044800	-3.73101800	-0.46768500
H	-5.48498400	-3.63829800	-2.16428400
H	-4.30295600	-4.17542200	-0.95673000
Pd	-0.22518200	-1.68936000	0.49041500
P	2.08476200	-1.40915400	-0.35664800
C	2.19697400	-0.10299100	-1.76629500
C	2.72536600	-3.14087700	-0.98594500
C	2.27500100	-4.22914500	0.01372100
H	2.76355300	-4.12159000	0.98549000
H	1.19288100	-4.22373800	0.16959100
H	2.55868600	-5.21065800	-0.38858200

C	2.10832500	-3.48131700	-2.35775000
H	2.36827900	-4.51839400	-2.60721100
H	1.01877300	-3.40696400	-2.35505700
H	2.49926100	-2.85212700	-3.16122800
C	4.25426000	-3.22375200	-1.09431800
H	4.53479600	-4.21238800	-1.48276900
H	4.67054300	-2.47497200	-1.76926400
H	4.72509000	-3.11130700	-0.11504900
C	0.99812500	-0.34118400	-2.71618400
H	0.99342900	0.46274300	-3.46345600
H	1.04912100	-1.28724600	-3.25694700
H	0.04630700	-0.30370600	-2.17887000
C	3.49741800	-0.09907400	-2.58750500
H	3.64404900	-1.03086800	-3.14169200
H	3.44434400	0.71082800	-3.32756200
H	4.37665300	0.08366700	-1.96802500
C	1.98072000	1.28558300	-1.13474000
H	1.07564100	1.32826800	-0.52324400
H	2.82776400	1.59497800	-0.52564100
H	1.87207000	2.02040200	-1.94391600
C	3.20547100	-1.11691500	1.16094300
C	4.41283900	-0.39857800	1.44188300
C	2.66709900	-1.88595000	2.21845600
C	5.03713900	-0.61393700	2.68775700
C	3.29464300	-2.06183700	3.44850800
H	1.70067100	-2.36091000	2.07711700
C	4.51691400	-1.44126600	3.67748500
H	5.95418500	-0.06818400	2.88759300
H	2.82026900	-2.67024200	4.21334500
H	-1.48322900	-3.61820100	1.46710700
H	-2.66422900	-2.30538600	1.98270500
H	-0.83771600	-3.88111000	-0.85986400
H	-1.14426700	-2.48950300	-2.00045000
H	5.04159800	-1.56265100	4.62125000
C	5.08645300	0.68624700	0.62776400
C	6.19998400	0.39439500	-0.20990600
C	4.72574200	2.04548800	0.83094800
C	6.79553100	1.41928200	-0.95244400
C	5.34538600	3.02444700	0.03397100
C	6.35585500	2.74279800	-0.88055600
H	7.63404200	1.17605300	-1.59852700
H	5.03353800	4.05988400	0.16130500
C	6.97802000	3.84468100	-1.72734500
H	6.46378300	4.77987800	-1.46668500
C	6.75680200	3.59996000	-3.23227200
H	7.25902900	2.68314200	-3.56361600
H	5.69089800	3.49918800	-3.46457900
H	7.15808900	4.43221300	-3.82297900
C	8.47383000	4.03877100	-1.41331500
H	8.88415700	4.87563900	-1.99108600
H	8.63141700	4.24828700	-0.34960900
H	9.05460400	3.14399200	-1.66742500
C	3.83547400	2.64052500	1.94427900
H	3.41864900	3.55710300	1.50441700
C	4.75007600	3.09385300	3.10839300
H	5.56091100	3.74288500	2.76082100
H	4.16533100	3.64385500	3.85572000
H	5.20028400	2.22895000	3.60904800
C	2.63881300	1.86487700	2.51317500
H	1.96055600	1.48421600	1.75186000
H	2.93919200	1.02955600	3.14915900
H	2.05704100	2.55227900	3.13993700
C	6.86355200	-0.98346100	-0.23920700
C	7.28930600	-1.44753600	-1.64564000
H	7.58682000	-2.50222100	-1.61861800
H	6.48413400	-1.34004600	-2.37898700
H	8.15147000	-0.88107200	-2.01615200
C	8.09210600	-1.00388300	0.69746900
H	8.84176000	-0.27270900	0.37236400
H	7.81889500	-0.76588800	1.72994100
H	8.56172500	-1.99533900	0.69255000
H	6.15036500	-1.70977400	0.15354900
C	-2.48383300	0.45641700	1.37095800
H	-2.87886300	-0.12071700	2.20337900
C	-1.08113300	0.77433200	1.52020800
O	-0.47381672	0.70222300	2.73854553
O	-0.30968151	1.10418089	0.58866971
C	-0.93440516	-0.17349940	3.77307123
H	-1.24681770	0.41830331	4.63654815
H	-1.76815820	-0.78580716	3.42327438
H	-0.08846682	-0.80808395	4.05519001

2-Int4

Zero-point correction= 1.097557 (Hartree/Particle)

Thermal correction to Energy= 1.162211

Thermal correction to Enthalpy= 1.163155

Thermal correction to Gibbs Free Energy= 0.995551

Sum of electronic and zero-point Energies= -3130.082350

Sum of electronic and thermal Energies= -3130.017696

Sum of electronic and thermal Enthalpies= -3130.016752

Sum of electronic and thermal Free Energies= -3130.184357

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3130.922961

N	5.47213300	-0.30250500	-1.39843900
C	4.33047700	-0.59889200	-0.52806000
H	4.06426500	-1.64914900	-0.65062800
H	4.55320600	-0.40289000	0.53127900
C	3.13029000	0.28231200	-0.94833800
C	5.94410800	1.08612000	-1.39947900
H	6.40817000	1.28463100	-2.37144100
H	6.73617200	1.23681900	-0.64078700
C	4.85969800	2.10679100	-1.11600800
C	3.58279900	1.75914400	-0.84707600
C	2.53832800	2.71792600	-0.39190100
C	2.79970600	3.67112600	0.52878800
C	1.15551700	2.57994100	-0.91791500
S	6.63961800	-1.48481500	-1.62839700
O	5.93114800	-2.75795200	-1.77849500
O	7.54262000	-0.97238600	-2.66401500
C	7.58574500	-1.57878000	-0.10192000
C	8.75433500	-0.82649700	0.03733000
C	7.12836200	-2.38249000	0.94702600
C	9.45964800	-0.87578800	1.23995200
H	9.11682300	-0.23841900	-0.79896900
C	7.84487100	-2.41888800	2.14094700
H	6.23932800	-2.98966900	0.81400600
C	9.01538700	-1.66353600	2.31021900
H	10.37573400	-0.29924400	1.34444900
H	7.49502100	-3.05212400	2.95295300
C	9.76827100	-1.69202100	3.61958600
H	10.81175400	-1.38775000	3.48921400
H	9.31578000	-1.00778800	4.34984800
H	9.75884500	-2.69252900	4.06567100
C	2.72021000	-0.08434800	-2.39511800
H	1.87089000	0.52157200	-2.72372400
H	3.54283900	0.05058400	-3.10336900
H	2.40933300	-1.13549300	-2.41493300
C	5.41166100	3.51448300	-1.16309000
H	6.02564300	3.74446900	-0.28026200
H	6.06805600	3.63273200	-2.03612200
H	4.62071300	4.26396300	-1.22254500
Pd	0.31651300	0.88426800	-0.07384600
P	-1.96310500	1.46977800	0.19997400
C	-2.88943700	1.55673400	-1.48913500
C	-2.34396800	3.05733300	1.26881000
C	-1.24203600	3.20612400	2.34275300
H	-1.31109900	2.43595200	3.11435000
H	-0.23622000	3.17360500	1.91238200
H	-1.37088300	4.17507500	2.84254200
C	-2.30725300	4.33452400	0.40436800
H	-2.40500300	5.20207400	1.06949700
H	-1.36420000	4.44692900	-0.13848200
H	-3.13095900	4.38574300	-0.31114900
C	-3.70372300	2.98027300	1.98164200
H	-3.85490400	3.89626600	2.56882500
H	-4.53924600	2.89580500	1.28307600
H	-3.74404000	2.13566300	2.67463200
C	-2.15538500	2.59191500	-2.37781000
H	-2.60001600	2.54384900	-3.38002500
H	-2.25140400	3.62072900	-2.03227900
H	-1.09367400	2.35470900	-2.47538500
C	-4.38280800	1.91399200	-1.42535000
H	-4.55591600	2.90920000	-1.00452200
H	-4.79018400	1.92019300	-2.44527700
H	-4.95552000	1.18568000	-0.85042700
C	-2.70178500	0.19956100	-2.19512500
H	-1.64222400	-0.07115400	-2.25880400
H	-3.24766800	-0.60362500	-1.70508200
H	-3.08769000	0.28314900	-3.21959000
C	-2.44240800	0.05604800	1.39527800
C	-3.51303300	-0.88212300	1.51176100
C	-1.41903800	-0.02855300	2.37272600
C	-3.53777700	-1.73108000	2.63780400
C	-1.45602000	-0.89632200	3.46109600
H	-0.54180500	0.60396300	2.27314700
C	-2.54737700	-1.74310300	3.61414900
H	-4.36385900	-2.43117200	2.71652100
H	-0.63223600	-0.90477200	4.16894400
H	2.02823400	4.36648700	0.85246700
H	3.77228000	3.77142000	0.99797800
H	0.52980400	3.43484600	-0.66061400
H	1.10480800	2.37514100	-1.98977700
H	-2.61608700	-2.42620500	4.45618600
C	-4.61352100	-1.18717600	0.52404300
C	-5.89475600	-0.58564500	0.65992200
C	-4.43075900	-2.21608000	-0.43647800
C	-6.91083000	-0.91725400	-0.24174300
C	-5.48429300	-2.48485300	-1.32775900
C	-6.71939200	-1.84437500	-1.26923700
H	-7.88190600	-0.44296300	-0.13303800
H	-5.33064600	-3.24881500	-2.08816300

C	-7.81927000	-2.17131400	-2.27037200
H	-7.41848800	-2.93510500	-2.95063700
C	-8.19513900	-0.94467100	-3.12353400
H	-8.61769100	-0.14426000	-2.50435800
H	-7.31916900	-0.53912600	-3.64169700
H	-8.94417700	-1.21325500	-3.87797000
C	-9.06269000	-2.77062700	-1.58604200
H	-9.81495400	-3.05252600	-2.33230100
H	-8.80475700	-3.66410000	-1.00698500
H	-9.52799700	-2.05119100	-0.90164200
C	-3.24752200	-3.20162600	-0.56261900
H	-3.22883000	-3.47337500	-1.62668800
C	-3.58803700	-4.49852400	0.20975400
H	-4.56464400	-4.89787200	-0.08342100
H	-2.83011300	-5.26622900	0.01320500
H	-3.60651500	-4.31725900	1.29020400
C	-1.81117500	-2.76982300	-0.21823000
H	-1.52095900	-1.83359500	-0.69953600
H	-1.64496600	-2.66772900	0.85636500
H	-1.12542900	-3.54553700	-0.57956100
C	-6.23682400	0.33595200	1.83270000
C	-7.08937000	1.55902800	1.44499500
H	-7.17061400	2.24263000	2.29803500
H	-6.65857800	2.11352100	0.60539000
H	-8.10986900	1.27329800	1.16534100
C	-6.95369000	-0.45827700	2.94674600
H	-7.89690000	-0.87958100	2.57906200
H	-6.33842000	-1.28525000	3.31419100
H	-7.18360100	0.19518700	3.79723500
H	-5.29920900	0.70608600	2.25356800
C	2.11287200	0.00276100	-0.04123600
H	2.66003169	0.20035531	0.85680229
C	2.14761222	-1.50722560	-0.34179144
O	3.32615041	-2.14023590	-0.46778905
O	0.92564043	-2.23569023	-0.48678877
C	1.21859259	-3.60843211	-0.76002632
H	1.78751830	-3.67872888	-1.66350952
H	1.78320801	-4.02071331	0.04999445
H	0.30425331	-4.15301024	-0.87101428

2-Ts4

Zero-point correction= 1.095977 (Hartree/Particle)

Thermal correction to Energy= 1.160615

Thermal correction to Enthalpy= 1.161559

Thermal correction to Gibbs Free Energy= 0.993186

Sum of electronic and zero-point Energies=-3130.063080

Sum of electronic and thermal Energies= -3129.998441

Sum of electronic and thermal Enthalpies= -3129.997497

Sum of electronic and thermal Free Energies= -3130.165871

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3130.903828

Imaginary frequency is -326.78^{-1}

N	5.41457500	0.60348800	1.28846100
C	4.42104700	0.33348000	0.24238500
H	4.04632500	1.28345800	-0.13987900
H	4.84706000	-0.25060900	-0.58650800
C	3.27088400	-0.47242000	0.87892700
C	6.08014400	-0.58175700	1.83762600
H	6.53243500	-0.30140300	2.79451700
H	6.90490500	-0.92041700	1.18153000
C	5.13147700	-1.74641300	2.02812100
C	3.85524600	-1.67925800	1.61213100
C	2.83433900	-2.74364800	1.61859800
C	2.51645600	-3.53120700	2.66218200
C	2.10055600	-2.82796100	0.33459800
S	6.35598100	1.99565100	1.15210200
O	5.44952400	3.07030700	0.74409100
O	7.14690800	2.06765700	2.38366600
C	7.49965700	1.71102500	-0.20389000
C	8.76100700	1.16986300	0.05642300
C	7.10935500	2.01128100	-1.51257800
C	9.62848400	0.91959600	-1.00660400
H	9.06453000	0.98019600	1.08044200
C	7.98883200	1.75374600	-2.56164400
H	6.14236600	2.46667900	-1.69768800
C	9.25656300	1.19898700	-2.32873500
H	10.61494100	0.50966000	-0.80383500
H	7.69006600	1.99705900	-3.57846700
C	10.19028100	0.90072200	-3.47788800
H	9.95114000	-0.06717800	-3.93836600
H	10.11389800	1.66002600	-4.26359100
H	11.23277700	0.85688300	-3.14694800
C	2.43402900	0.41046400	1.81648200
H	1.66973200	-0.18834800	2.32154500
H	3.06815300	0.88779000	2.57065700
H	1.92966900	1.18806100	1.23231700
C	5.78005300	-2.95421900	2.65560200
H	5.18779600	-3.85966000	2.50323800
H	6.78063900	-3.11898100	2.23398200
H	5.91501400	-2.81798000	3.73780900
Pd	0.17049140	-1.35434787	-0.25005599

P	-2.11028260	-1.60766987	-0.47463499
C	-2.90109760	-1.85508387	1.26514701
C	-2.58216060	-3.10220887	-1.63465199
C	-1.62448560	-3.09321487	-2.84680399
H	-1.79280560	-2.23302487	-3.49963399
H	-0.57586860	-3.08432787	-2.53061699
H	-1.80230960	-3.99777487	-3.44420699
C	-2.35822660	-4.43613587	-0.89522699
H	-2.46789160	-5.25945487	-1.61331199
H	-1.35122260	-4.50321487	-0.47002099
H	-3.08653860	-4.60577487	-0.09821199
C	-4.02279860	-3.05228487	-2.16542999
H	-4.20779360	-3.92951587	-2.80094099
H	-4.76702960	-3.06301587	-1.36628299
H	-4.18714060	-2.16291887	-2.77981399
C	-2.04786760	-2.89652687	2.03014001
H	-2.39779160	-2.92538687	3.07070601
H	-2.13228960	-3.90847987	1.63114801
H	-0.99074760	-2.61110187	2.03384601
C	-4.37702860	-2.28106887	1.30989701
H	-4.53876160	-3.26623087	0.86115901
H	-4.70033360	-2.34749787	2.35787201
H	-5.02825260	-1.55929687	0.81458301
C	-2.72079060	-0.52285387	2.01441801
H	-2.98378660	-0.66571087	3.07131801
H	-1.68180760	-0.17743587	1.96637301
H	-1.99550360	3.53943813	1.95683501
C	-2.78900760	-0.12752687	-1.48410299
C	-3.96651560	0.68424813	-1.48539799
C	-1.85122560	0.11851113	-2.51663499
C	-4.16913060	1.55774613	-2.57648699
C	-2.07082160	0.99882213	-3.57174199
H	-0.89728960	-0.39945187	-2.47293899
C	-3.26523660	1.70826413	-3.62219699
H	-5.07074960	2.16293913	-2.57054199
H	-1.30706560	1.12837813	-4.33374199
H	1.72269400	-4.27067300	2.59183900
H	3.03643100	-3.45922900	3.61225100
H	2.66579600	-3.14135700	-0.53735000
H	1.14187100	-3.34229500	0.41069500
H	-3.47805360	2.39795713	-4.43457999
C	-5.00730460	0.88059413	-0.40131699
C	-4.76799460	1.86650713	0.59620501
C	-6.28982360	0.28104313	-0.48241199
C	-5.76767160	2.13099313	1.54047501
C	-7.25167660	0.58654013	0.48892801
C	-7.00882660	1.49317713	1.52195601
H	-5.57927660	2.87151013	2.31297401
H	-8.22658560	0.11109013	0.42336301
C	-8.06131760	1.80434513	2.57813801
H	-7.62586860	2.55165213	3.25558801
C	-8.40707860	0.56292713	3.42258301
H	-9.12037060	0.81993113	4.21500301
H	-8.86153160	-0.22247987	2.80680301
H	-7.51146760	0.14189113	3.89250501
C	-9.33038060	2.42498913	1.96339401
H	-10.04723360	2.69554313	2.74799601
H	-9.09240160	3.32877913	1.39178601
H	-9.82988260	1.72269813	1.28534301
C	-6.70184160	-0.61985387	-1.64774099
H	-5.79424760	-0.91449087	-2.17884699
C	-7.58428560	0.15660013	-2.64906599
H	-7.85878960	-0.48409387	-3.49614999
H	-8.50996660	0.49957413	-2.17158899
H	-7.06721860	1.03596713	-3.04561799
C	-7.42720360	-1.90716387	-1.21081899
H	-8.41775460	-1.69454587	-0.79220599
H	-7.57687360	-2.56490687	-2.07510299
H	-6.86091060	-2.46180987	-0.45624999
C	-3.49339460	2.72140213	0.61950901
H	-2.70070960	2.16510413	0.10947501
C	-3.71580560	4.03580713	-0.16184199
H	-4.51403560	4.62910513	0.30079901
H	-2.80027360	4.63963413	-0.15862399
H	-3.99207460	3.84907413	-1.20293299
C	-2.97945860	3.06277213	2.03197901
H	-3.63907260	3.77071913	2.54750601
H	-2.87586660	2.17693013	2.66501701
H	-3.37121460	0.25165813	1.61599301
C	2.46623291	-1.03638536	-0.26630690
H	3.00522262	-1.18587332	-1.17847106
C	1.71062803	0.27805641	-0.53631446
O	0.35060677	0.29239192	-0.53925921
O	2.43891214	1.48353723	-0.78393968
C	2.24048437	1.89021053	-2.14045848
H	2.31962902	1.03854524	-2.78334445
H	1.26867753	2.32591524	-2.24367117
H	2.98467275	2.61046500	-2.40937696

2a

Zero-point correction= 0.422193 (Hartree/Particle)

Thermal correction to Energy= 0.448298

Thermal correction to Enthalpy= 0.449242

Thermal correction to Gibbs Free Energy= 0.363917

Sum of electronic and zero-point Energies= -1530.520037

Sum of electronic and thermal Energies= -1530.493933

Sum of electronic and thermal Enthalpies= -1530.492989

Sum of electronic and thermal Free Energies= -1530.578313

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -1530.937286

N	0.32863300	-0.80370400	0.43714000
C	0.81615700	-0.56097200	-0.92648800
H	0.48423900	-1.38046500	-1.56534600
H	0.44869000	0.39168700	-1.33563300
C	2.34470300	-0.51284900	-0.84632200
C	0.62165400	0.24627500	1.41975100
H	0.54278900	-0.19692200	2.41805600
H	-0.12749100	1.05937900	1.37301200
C	1.98504400	0.87416700	1.22414200
C	2.77580400	0.50413000	0.20058700
C	4.03297800	1.07980400	-0.29887400
C	5.00860800	1.72882000	0.35076900
C	4.06525800	0.73824700	-1.78645700
S	-1.12825100	-1.63097600	0.63113400
O	-1.11083800	-2.72705600	-0.33919200
O	-1.26546600	-1.86433100	2.07084400
C	-2.43532700	-0.49886800	0.14319100
C	-3.04088600	0.31401300	1.10403400
C	-2.81997300	-0.42403600	-1.19874900
C	-4.02964100	1.21461200	0.70959900
H	-2.76078200	0.21522700	2.14736500
C	-3.80890300	0.48172600	-1.57384000
H	-2.36984500	-1.08855800	-1.92855300
C	-4.42409500	1.31906100	-0.63092600
H	-4.50997400	1.83935900	1.45867700
H	-4.11657700	0.53236300	-2.61554200
C	-5.47720600	2.31442700	-1.05571500
H	-6.11519600	2.60667700	-0.21583100
H	-5.01688500	3.22904500	-1.45240700
H	-6.11819000	1.90700000	-1.84481500
C	2.94701700	-1.90623800	-0.61698900
H	4.02998000	-1.84311900	-0.46581600
H	2.50349300	-2.37974000	0.26319800
H	2.75571100	-2.53713500	-1.49183100
C	2.31424500	1.96073100	2.21387100
H	2.94002200	2.73680700	1.76214500
H	1.40130400	2.43315500	2.59585100
H	2.85617500	1.56400300	3.08348200
H	5.88790100	2.09161800	-0.17661900
H	4.98663400	1.89584400	1.42155300
H	4.10427600	1.63122200	-2.42108300
H	4.93468600	0.10996600	-2.03253500
C	2.84605500	0.04961700	-2.07227200
H	1.84157178	0.33555727	-2.30497700
C	3.53115862	-0.49560021	-3.33914659
O	4.57078952	-1.21716837	-2.99752747
O	3.95723993	0.59646123	-4.15814387
C	5.38624618	0.63910416	-4.19012417
H	5.76354998	-0.30152332	-4.53328852
H	5.70514200	1.41504692	-4.85429153
H	5.75930251	0.83569654	-3.20672170

3a-Me

Zero-point correction= 0.417377 (Hartree/Particle)

Thermal correction to Energy= 0.445828

Thermal correction to Enthalpy= 0.446772

Thermal correction to Gibbs Free Energy= 0.353818

Sum of electronic and zero-point Energies= -1530.434148

Sum of electronic and thermal Energies= -1530.405697

Sum of electronic and thermal Enthalpies= -1530.404753

Sum of electronic and thermal Free Energies= -1530.497707

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -1530.497707

N	0.55046200	0.31040200	-0.70547500
C	-0.06171700	-0.99095400	-0.39554600
H	0.49151100	-1.75132600	-0.95561600
H	0.04488200	-1.21087700	0.67620800
C	-1.51815000	-1.09790700	-0.81512600
C	0.27218300	1.42006700	0.23449600
H	1.14246500	2.08301500	0.24038500
H	0.15302900	1.00786400	1.24346600
C	-0.95468300	2.23363800	-0.14911300
C	-2.03137400	2.19661600	0.60610100
C	-3.08624800	2.14150300	1.34797300
C	-4.39017800	1.50299300	1.64431200
C	-3.86526300	2.65463500	2.49844000
H	-4.38624800	0.49810100	2.06284100
H	-5.22086500	1.70306200	0.96921700
H	-4.34695600	3.62661200	2.40300500
H	-3.51009600	2.43009900	3.50318300
S	2.03703600	0.30677500	-1.51002000
O	1.96463500	-0.78090400	-2.49072500

O	2.28475200	1.69583400	-1.90485500
C	3.30082800	-0.13797000	-0.31055200
C	3.96714600	0.86554800	0.39672300
C	3.59620400	-1.48490000	-0.08313900
C	4.91963300	0.51011600	1.35004400
H	3.76308200	1.90793200	0.17692300
C	4.55104400	-1.82102900	0.87375500
H	3.10799600	-2.25414100	-0.67193800
C	5.22119200	-0.83374700	1.61080400
H	5.44612200	1.29153800	1.89257900
H	4.78895600	-2.86849100	1.04257800
C	6.23434900	-1.21049100	2.66511900
H	6.98054800	-0.42176500	2.80435000
H	5.74855100	-1.37561200	3.63605100
H	6.75989000	-2.13485900	2.40400500
C	-1.80930500	-0.77840000	-2.25314200
H	-1.76033200	0.30673400	-2.40389700
H	-1.03791900	-1.21288900	-2.90023400
H	-2.79670900	-1.12701800	-2.55078900
C	-0.84421400	3.09048800	-1.39105400
H	-0.07811000	3.86636300	-1.25963400
H	-0.53022600	2.48849900	-2.25123100
H	-1.79477900	3.57655800	-1.62469900
C	-2.40968800	-1.52278400	0.10181800
C	-2.11808225	-1.90965673	1.49611472
O	-1.05357876	-1.87426475	2.08474813
O	-3.26492456	-2.34087370	2.09689663
C	-3.12377431	-2.72177641	3.47221389
H	-4.11916473	-3.02942096	3.79517632
H	-2.41426085	-3.54752737	3.57538130
H	-2.76977563	-1.87847034	4.07177410
H	-3.45721715	-1.60766018	-0.17399488

4-Int1

Zero-point correction= 1.092642 (Hartree/Particle)

Thermal correction to Energy= 1.160550

Thermal correction to Enthalpy= 1.161494

Thermal correction to Gibbs Free Energy=0.976982

Sum of electronic and zero-point Energies= -3130.032839

Sum of electronic and thermal Energies= -3129.964932

Sum of electronic and thermal Enthalpies= -3129.963988

Sum of electronic and thermal Free Energies= -3130.148500

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.159880

N	7.44804800	0.53864500	0.50003000
C	6.99852100	1.07898000	-0.79294100
H	7.86352800	1.55858400	-1.26140000
H	6.66377500	0.26124700	-1.44713500
C	5.91132900	2.13329500	-0.66789100
C	6.58820100	-0.48920800	1.12760700
H	7.23197400	-1.17262100	1.68929400
H	6.08939900	-1.06505900	0.33907600
C	5.55741000	0.09622800	2.08234300
C	4.27630400	0.02251900	1.79333600
C	3.02191400	-0.04600800	1.49444100
C	1.86607000	0.60532800	0.84711400
C	1.76149300	-0.80766800	1.55317400
H	1.86435700	0.65777200	-0.24099800
H	1.43290300	1.46749700	1.35229800
H	1.24984500	-0.86891200	2.51228900
H	1.67885400	-1.69780300	0.93062100
S	9.11445300	0.44824600	0.77306600
O	9.68668500	1.66799100	0.19534500
O	9.27210400	0.10876800	2.18960400
C	9.73714800	-0.94191100	-0.18047000
C	9.82179300	-2.20464200	0.41171800
C	10.11828200	-0.75303500	-1.51211700
C	10.27231800	-3.28428000	-0.34635100
H	9.56921900	-2.32825500	1.45928700
C	10.56589400	-1.84400200	-2.25415000
H	10.09512300	0.24022400	-1.94753700
C	10.64240200	-3.12586900	-1.68938300
H	10.34848000	-4.26471800	0.11736500
H	10.87280700	-1.69518500	-3.28655900
C	11.10261000	-4.30633700	-2.51122600
H	11.55277500	-5.08151900	-1.88282800
H	10.25989400	-4.76644600	-3.04436500
H	11.83897500	-4.00771000	-3.26462000
C	6.23652900	3.30622300	0.21186500
H	6.24497200	2.98751000	1.26096000
H	7.24896200	3.66942500	-0.00478100
H	5.51370800	4.11128400	0.09235000
C	6.08151300	0.70636600	3.36380900
H	6.57411900	-0.05616100	3.98176000
H	6.84001400	1.46734200	3.14856200
H	5.27626100	1.16062400	3.94670300
Pd	-0.50560700	-0.22222700	0.52359200
P	-2.71193200	-0.42458500	-0.12648300
C	-3.12672300	-2.30248800	-0.27271600
C	-2.93580100	0.48794300	-1.81055400
C	-2.80898900	1.99108700	-1.48231900

H	-3.62281100	2.35185200	-0.84947900
H	-1.86462100	2.19863200	-0.96676200
H	-2.82582200	2.56958500	-2.41566100
C	-1.73956200	0.11563000	-2.71499300
H	-1.75628600	0.75830700	-3.60648000
H	-0.78576200	0.25791700	-2.19464200
H	-1.78611500	-0.92066900	-3.06207700
C	-4.22906700	0.21775600	-2.59663600
H	-4.29841500	0.93035600	-3.43016800
H	-4.23059100	-0.78185100	-3.03773800
H	-5.13005300	0.31890900	-1.99098800
C	-1.95441900	-2.99318300	-1.00487400
H	-2.08684700	-4.08185700	-0.93746100
H	-1.91711800	-2.73536200	-2.06738600
H	-0.99134100	-2.72825200	-0.55465400
C	-4.42965700	-2.68536300	-0.99324500
H	-4.35528600	-2.52653900	-2.07170900
H	-4.62044800	-3.75719700	-0.84465600
H	-5.29910500	-2.13531800	-0.63234900
C	-3.13626000	-2.83421500	1.17670800
H	-2.18889900	-2.61066700	1.67987500
H	-3.94378200	-2.40563500	1.77454900
H	-3.26784000	-3.92425500	1.16276500
C	-3.87678600	0.38089900	1.18840800
C	-5.29068300	0.57046600	1.34773100
C	-3.05760500	0.89144300	2.22302400
C	-5.74701000	1.24123400	2.50241300
C	-3.53782300	1.54920700	3.35240400
H	-1.98183900	0.75684500	2.12064800
C	-4.90649600	1.72937200	3.49728800
H	-6.81815200	1.37887200	2.61037800
H	-2.84002600	1.91238100	4.10226800
H	-5.32252800	2.23808500	4.36304900
C	-6.43809300	0.15471500	0.44697000
C	-6.98140800	1.07439900	-0.48882600
C	-7.13018100	-1.06471300	0.68766500
C	-8.07315300	0.68076300	-1.27494300
C	-8.21784300	-1.40427000	-0.12533500
C	-8.68801000	-0.56313300	-1.13695100
H	-8.47177300	1.37658800	-2.00862900
H	-8.72587700	-2.34778700	0.05214700
C	-9.85616400	-0.96061100	-2.02971600
H	-10.03715200	-0.12127400	-2.71525200
C	-9.52070700	-2.19432900	-2.88953800
H	-8.62286000	-2.02357200	-3.49359500
H	-9.33909700	-3.07646100	-2.26396300
H	-10.34954800	-2.43082800	-3.56768400
C	-11.15063000	-1.18407600	-1.22467400
H	-11.41104500	-0.29592800	-0.63846400
H	-11.98857500	-1.40876400	-1.89550800
H	-11.04815600	-2.02541200	-0.52895800
C	-6.82186300	-1.95531700	1.89672400
H	-5.80928000	-1.72374000	2.23858000
C	-7.78253800	-1.61701000	3.05947300
H	-8.82251800	-1.81070500	2.77045900
H	-7.55381900	-2.23606800	3.93564900
H	-7.70701300	-0.56839100	3.35990100
C	-6.89106800	-3.46865100	1.61865300
H	-6.27678600	-3.76272300	0.76463400
H	-6.53711100	-4.02099400	2.49693200
H	-7.91805500	-3.80018200	1.42581300
C	-6.51425600	2.53157700	-0.57442300
H	-5.51650800	2.59429100	-0.13117000
C	-6.43296800	3.10082600	-2.00330200
H	-7.42643500	3.21556700	-2.45219900
H	-5.97718300	4.09750900	-1.97731000
H	-5.83471500	2.47295200	-2.66742200
C	-7.44377800	3.43295700	0.26993700
H	-7.10223900	4.47464300	0.23217200
H	-8.46985100	3.39917400	-0.11556700
H	-7.46864000	3.12507300	1.31885400
C	4.78472800	1.96787400	-1.38886400
C	4.44467925	0.80566993	-2.23540286
O	5.06980392	-0.22790539	-2.38643360
O	3.26441703	1.04089571	-2.87484035
C	2.80704749	-0.02129706	-3.72399641
H	1.86469964	0.32733875	-4.14733039
H	3.53132534	-0.21989652	-4.51876100
H	2.65594651	-0.93744721	-3.14611925
H	4.02952915	2.74914441	-1.38251509

4-Ts1

Zero-point correction= 1.090868 (Hartree/Particle)

Thermal correction to Energy= 1.157969

Thermal correction to Enthalpy= 1.158913

Thermal correction to Gibbs Free Energy= 0.976857

Sum of electronic and zero-point Energies= -3130.028108

Sum of electronic and thermal Energies= -3129.961007

Sum of electronic and thermal Enthalpies= -3129.960062

Sum of electronic and thermal Free Energies= -3130.142118

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.150866

Imaginary frequency is -209.71^{-1}

N	7.15586300	-0.91968200	-0.10796800
C	6.80183900	-0.55657600	1.27855000
H	7.70382500	-0.66750900	1.88896800
H	6.47280300	0.48273300	1.33227400
C	5.75784100	-1.48431300	1.87101700
C	6.24498700	-0.42752900	-1.16747400
H	6.84326800	-0.19581800	-2.05405400
H	5.77609700	0.50012600	-0.82217800
C	5.17812400	-1.44332200	-1.55528700
C	3.91323300	-1.21577100	-1.27642800
C	2.66543100	-0.98917500	-1.00143700
C	1.65857900	-1.23436000	0.04844900
C	1.46637700	-0.33777500	-1.56018800
H	1.79083400	-0.69443900	0.98696700
H	1.30310100	-2.26222800	0.14123900
H	0.99855400	-0.83066500	-2.41403700
H	1.48010200	0.75297700	-1.59575400
S	8.79263400	-1.08163500	-0.47925400
O	9.40627400	-1.74982500	0.67348700
O	8.84823400	-1.65401800	-1.82763100
C	9.49072600	0.57142200	-0.57668500
C	9.54471200	1.22695900	-1.80927300
C	9.95689200	1.19708200	0.58327900
C	10.05141500	2.52430100	-1.86999600
H	9.22320800	0.71297900	-2.70863900
C	10.45916400	2.49391800	0.50327200
H	9.95297700	0.66307500	1.52734600
C	10.50699800	3.18144100	-0.71861400
H	10.10266900	3.03090100	-2.83066600
H	10.82951600	2.97732200	1.40401600
C	11.02570800	4.59810400	-0.78773100
H	11.41681500	4.83421600	-1.78259600
H	10.22688600	5.31963800	-0.57023600
H	11.82415800	4.76886600	-0.05791800
C	6.06213500	-2.95479400	1.77534200
H	6.00918700	-3.28732100	0.73293900
H	7.08600800	-3.16022500	2.11150600
H	5.36205800	-3.55132000	2.36704100
C	5.64723000	-2.67490600	-2.30033300
H	6.08057900	-2.39766400	-3.27053300
H	6.44105900	-3.18691700	-1.74496000
H	4.82367500	-3.37264000	-2.47340400
Pd	-0.37296600	-0.41040700	-0.31359400
P	-2.67023800	0.08523100	0.19916400
C	-2.97475400	1.92960800	-0.25939400
C	-2.95324600	-0.24552900	2.07540600
C	-2.98352900	-1.78037800	2.23906300
H	-3.84144800	-2.23979100	1.74341700
H	-2.07511000	-2.23822100	1.83173900
H	-3.03738800	-2.02783800	3.30738800
C	-1.71822200	0.26680300	2.85046500
H	-1.80779000	-0.04103100	3.90148200
H	-0.79048100	-0.14830700	2.44273500
H	-1.63851800	1.35730900	2.83401100
C	-4.20938000	0.38783600	2.69452200
H	-4.37131000	-0.03175100	3.69673600
H	-4.09168700	1.46797900	2.81853500
H	-5.11067800	0.21442100	2.10408000
C	-1.83238400	2.76270700	0.36487100
H	-1.85371500	3.77155000	-0.06922800
H	-1.94703800	2.87426900	1.44741800
H	-0.85099200	2.31871800	0.16331900
C	-4.30984700	2.57067600	0.15162400
H	-4.38169200	2.70367500	1.23335700
H	-4.37818500	3.57148500	-0.29743000
H	-5.17762200	1.99879600	-0.17326400
C	-2.80196300	1.98748100	-1.79342700
H	-1.81606100	1.61258100	-2.08946400
H	-3.55720700	1.39986700	-2.32098700
H	-2.88821300	3.02889100	-2.13033600
C	-3.84326000	-1.07863100	-0.78667100
C	-5.25833000	-1.19574500	-0.99369300
C	-3.03217600	-2.04396400	-1.42960000
C	-5.72466000	-2.24347800	-1.81589800
C	-3.52403500	-3.07444400	-2.22645800
H	-1.95509900	-1.96846900	-1.29218500
C	-4.89367000	-3.17662400	-2.42733400
H	-6.79576200	-2.31443000	-1.97614300
H	-2.83392700	-3.77816700	-2.68423800
H	-5.31780600	-3.96116000	-3.04859800
C	-6.39640200	-0.33602200	-0.47714100
C	-7.10400400	-0.70193300	0.69885000
C	-6.91483500	0.70952100	-1.29045100
C	-8.18920600	0.08389300	1.11116100
C	-8.01061300	1.45140600	-0.83476600
C	-8.64557700	1.17951400	0.37921300
H	-8.71351600	-0.18070200	2.02539200
H	-8.38734300	2.25896900	-1.45594600

C	-9.81867700	2.01546600	0.87376100
H	-10.14144400	1.58246400	1.83059300
C	-9.40431800	3.47458700	1.14429900
H	-8.57516000	3.52482300	1.85854900
H	-9.08123100	3.97300200	0.22252400
H	-10.24523700	4.04598900	1.55549800
C	-11.02026600	1.95208500	-0.08847300
H	-11.34017800	0.91767300	-0.25550000
H	-11.87099900	2.51154200	0.31880100
H	-10.77380500	2.38728700	-1.06430100
C	-6.39228100	0.98523200	-2.70461800
H	-5.40144300	0.53055700	-2.79418200
C	-7.30112900	0.30344300	-3.75177400
H	-8.32091100	0.70330500	-3.69921100
H	-6.91909800	0.48328400	-4.76411900
H	-7.35632700	-0.77831800	-3.60034300
C	-6.25666800	2.48014300	-3.05183300
H	-5.67206400	3.02638400	-2.30734300
H	-5.75818000	2.59080400	-4.02191100
H	-7.23438400	2.96841600	-3.13698600
C	-6.82262800	-2.00338500	1.45788800
H	-5.78943700	-2.29761000	1.25393800
C	-6.99619700	-1.90958300	2.98612800
H	-8.05145900	-1.81744800	3.26842200
H	-6.62000000	-2.82583500	3.45573900
H	-6.45821700	-1.06263300	3.41814000
C	-7.73287900	-3.13600500	0.92980600
H	-7.53083400	-4.06916700	1.46986600
H	-8.78918200	-2.88139600	1.07810300
H	-7.57712400	-3.32449100	-0.13531600
C	4.64377200	-1.05408500	2.49778000
C	4.19086900	0.34400500	2.64235800
O	4.79374100	1.36888500	2.37058100
O	2.92820800	0.36294100	3.14943600
C	2.36478700	1.66770000	3.34569000
H	1.36740400	1.49662300	3.75151200
H	2.97290600	2.24743600	4.04585500
H	2.30382200	2.20845800	2.39737500
H	3.96483700	-1.78757700	2.92299700

4-Int2

Zero-point correction= 1.092332 (Hartree/Particle)

Thermal correction to Energy= 1.159412

Thermal correction to Enthalpy= 1.160356

Thermal correction to Gibbs Free Energy= 0.979856

Sum of electronic and zero-point Energies= -3130.041059

Sum of electronic and thermal Energies= -3129.961007

Sum of electronic and thermal Enthalpies= -3129.973979

Sum of electronic and thermal Free Energies= -3129.973035

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.152845

N	-6.83494900	0.04861500	-0.65339500
C	-6.76150800	1.32921200	0.06700200
H	-7.71084200	1.84843100	-0.09864300
H	-6.65264000	1.14974200	1.14621700
C	-5.65830000	2.24861400	-0.42830200
C	-5.85200200	-0.99352500	-0.26642800
H	-6.32370200	-1.96882100	-0.42059500
H	-5.62731900	-0.88729300	0.80144800
C	-4.56605600	-0.93391800	-1.07909200
C	-3.42713300	-0.61753900	-0.50162200
C	-2.26895100	-0.29888300	0.02620400
C	-1.52458300	1.00872900	0.00260300
C	-1.17577900	-1.19426200	0.51728800
H	-1.54569500	1.54741200	0.95704300
H	-1.73492500	1.66530900	-0.84618800
H	-1.08267600	-2.18111100	0.05971900
H	-1.06009200	-1.21946700	1.60586000
S	-8.35534600	-0.45498700	-1.18349900
O	-9.04192700	0.74861900	-1.66533900
O	-8.12461400	-1.61442500	-2.04912900
C	-9.26012200	-1.04170200	0.25601900
C	-9.19553100	-2.39144300	0.61132100
C	-10.00023800	-0.13899500	1.02485200
C	-9.86444300	-2.82935500	1.75325500
H	-8.64855200	-3.08872700	-0.01399500
C	-10.66235500	-0.59455700	2.16315000
H	-10.07478900	0.89911300	0.71914600
C	-10.60481200	-1.94229900	2.54732800
H	-9.81634300	-3.88035700	2.02794200
H	-11.24064200	0.10733400	2.75931100
C	-11.35370600	-2.43191400	3.76425600
H	-12.38291900	-2.71421800	3.50536700
H	-10.87472200	-3.31372700	4.20215900
H	-11.41412800	-1.65775500	4.53643500
C	-5.63676600	2.51122100	-1.90728900
H	-5.14394300	1.67578000	-2.41902000
H	-6.65924300	2.55903800	-2.29944800
H	-5.08938200	3.42231600	-2.14500400
C	-4.68783700	-1.30177200	-2.54503500
H	-5.00335000	-2.34799400	-2.65990600

H	-5.45326300	-0.69376600	-3.04134000
H	-3.73544800	-1.16707400	-3.06499000
Pd	0.33284500	0.07594100	-0.14303300
P	2.60148300	-0.95022900	-0.37879300
C	2.75092000	-2.13440900	-1.90389100
C	3.13872500	-1.82263900	1.24099800
C	2.80945900	-0.80766100	2.35641800
H	3.38261400	0.11557800	2.25105000
H	1.74670100	-0.54433600	2.35455400
H	3.05570900	-1.24780100	3.33191900
C	2.19880100	-3.03761100	1.42245800
H	2.31896100	-3.41890200	2.44495700
H	1.14645200	-2.77093800	1.28691800
H	2.44268900	-3.85879500	0.74176600
C	4.59170200	-2.30463900	1.39492900
H	4.69129500	-2.79653300	2.37263800
H	4.87464600	-3.03566700	0.63536700
H	5.30755700	-1.48538000	1.36404700
C	1.43009500	-2.93284300	-1.98891400
H	1.46153900	-3.58072300	-2.87531900
H	1.26868500	-3.57487200	-1.11892300
H	0.56777000	-2.26566600	-2.07951100
C	3.93074500	-3.11839400	-1.85209800
H	3.81145700	-3.86133000	-1.05843400
H	3.98690800	-3.66756700	-2.80197300
H	4.88569400	-2.61200200	-1.70538000
C	2.85722000	-1.28655600	-3.18753000
H	2.01856800	-0.59077900	-3.28994600
H	3.78429900	-0.70896600	-3.23745900
H	2.83321100	-1.95996100	-4.05406900
C	3.56027800	0.63669700	-0.81394200
C	4.88838700	1.13149600	-0.63974600
C	2.64530600	1.49841200	-1.47172500
C	5.19427400	2.41039300	-1.15395400
C	2.97168600	2.75759500	-1.96444000
H	1.62143500	1.15634900	-1.64607100
C	4.27264000	3.22100400	-1.80777400
H	6.20919200	2.77186400	-1.02149300
H	2.21354100	3.35710200	-2.45991500
H	4.56991100	4.19795400	-2.17879600
C	6.06280600	0.49437900	0.07010900
C	6.35904300	0.87372700	1.40591200
C	6.98321300	-0.32271100	-0.63896100
C	7.50280300	0.34785000	2.02165700
C	8.10633500	-0.82078400	0.03029500
C	8.38057900	-0.51369500	1.36546600
H	7.72254600	0.62510900	3.04909200
H	8.79778100	-1.45785700	-0.51224000
C	9.60321700	-1.07542900	2.07914400
H	9.59158900	-0.67354900	3.10159700
C	9.54561500	-2.61132200	2.18671500
H	8.62946000	-2.93905900	2.69015500
H	9.56823500	-3.08039600	1.19578200
H	10.40296300	-2.99157400	2.75492100
C	10.91763400	-0.61662000	1.41913100
H	10.97789300	0.47630000	1.37311100
H	11.78214700	-0.98300400	1.98551900
H	11.00517100	-0.99960900	0.39538700
C	6.84105100	-0.59857300	-2.13811200
H	5.77569800	-0.55840300	-2.38727600
C	7.54601800	0.49789800	-2.96788500
H	8.61518000	0.53353300	-2.72665800
H	7.44775300	0.28770900	-4.03998000
H	7.12286200	1.48795600	-2.77973800
C	7.37708300	-1.97508300	-2.57778800
H	7.02690200	-2.78701400	-1.93279100
H	7.05347500	-2.19040000	-3.60238800
H	8.47293000	-1.99984600	-2.57707600
C	5.51985700	1.88900800	2.18905000
H	4.52965100	1.94370600	1.72426000
C	5.32370600	1.51741100	3.67318400
H	6.24620700	1.65261700	4.24939800
H	4.56685900	2.17073800	4.12238500
H	4.99803400	0.48160500	3.80255500
C	6.14372200	3.30003800	2.10682300
H	5.53887700	4.01759800	2.67442400
H	7.15478600	3.30027500	2.53153800
H	6.21123800	3.65925800	1.07648900
C	-4.83998000	2.80298600	0.48785700
C	-4.85672943	2.54873114	1.94081358
O	-5.61438397	1.83357500	2.57301234
O	-3.85759497	3.25523677	2.53889548
C	-3.77230859	3.10551499	3.96024702
H	-2.91803904	3.71000460	4.26860160
H	-4.68698320	3.46365680	4.44186545
H	-3.61852274	2.05723302	4.23220938
H	-4.08501866	3.51558923	0.16763799

4-Ts2

Zero-point correction= 1.092643 (Hartree/Particle)

Thermal correction to Energy= 1.158785

Thermal correction to Enthalpy= 1.159729

Thermal correction to Gibbs Free Energy= 0.984759

Sum of electronic and zero-point Energies= -3129.990161

Sum of electronic and thermal Energies= -3129.924019

Sum of electronic and thermal Enthalpies= -3129.923075

Sum of electronic and thermal Free Energies= -3130.098044

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.110807

Imaginary frequency is -147.82^{-1}

N	5.98450100	0.27307000	0.61204600
C	5.91109800	1.03714700	-0.64355100
H	6.92679200	1.34175500	-0.91556100
H	5.52191900	0.39457000	-1.44453600
C	5.07194700	2.30011500	-0.52512400
C	4.89497700	-0.70924200	0.86249600
H	5.27886900	-1.40558000	1.61397200
H	4.69635800	-1.27136500	-0.06019900
C	3.60373300	-0.08868600	1.39442200
C	2.43015000	-0.27112600	0.79239500
C	1.98061700	-0.97463700	-0.36433800
C	1.62960100	-2.34121300	-0.42837500
C	1.29957200	-0.15207100	-1.36818300
S	7.52997400	-0.10708200	1.17762800
O	8.34699000	1.09633600	0.97636200
O	7.35513300	-0.70483800	2.50354700
C	8.19799600	-1.38194400	0.09875600
C	7.89869700	-2.72527300	0.34616900
C	8.98496800	-1.02001200	-0.99692400
C	8.38041900	-3.70241400	-0.52176900
H	7.31521900	-2.99873500	1.21864100
C	9.46005000	-2.01199000	-1.85429700
H	9.23940700	0.02213900	-1.15729900
C	9.16536400	-3.36433900	-1.63454700
H	8.14855600	-4.74709500	-0.32820700
H	10.07613300	-1.73028000	-2.70487500
C	9.70679900	-4.43675400	-2.55022600
H	9.96548600	-4.03155300	-3.53369800
H	10.61581800	-4.88950100	-2.13239800
H	8.98070100	-5.24417700	-2.69471000
C	5.57066300	3.32249800	0.46249000
H	6.26486700	2.86121100	1.16820000
H	6.10673000	4.12328000	-0.06368400
H	4.75271500	3.79538700	1.00900000
C	3.75583700	0.66240300	2.70058100
H	4.19196600	0.02033200	3.47982300
H	4.43114200	1.52215700	2.60181000
H	2.78195000	1.02031400	3.04515400
Pd	-0.12287800	-0.46723000	0.11153500
P	-2.12263000	0.73778700	-0.15688600
C	-2.90966800	0.59594900	-1.91116600
C	-2.03689100	2.60837600	0.40121000
C	-1.01331000	2.73970700	1.55057400
H	-1.36794600	2.28121500	2.47725300
H	-0.04469100	2.30035700	1.29122500
H	-0.86364000	3.80732200	1.75873900
C	-1.53154800	3.50085700	-0.75066300
H	-1.38866600	4.51470100	-0.35344600
H	-0.56759000	3.17346100	-1.15189500
H	-2.25147300	3.58311100	-1.56853400
C	-3.39049600	3.13781300	0.90047900
H	-3.27870100	4.19087400	1.19251800
H	-4.17089700	3.08996200	0.13792900
H	-3.73240400	2.58906100	1.78246900
C	-1.85235300	1.08016400	-2.93480400
H	-2.23712400	0.86228600	-3.93949500
H	-1.64719600	2.14853400	-2.89002700
H	-0.90674500	0.54631600	-2.81666700
C	-4.21844600	1.37363300	-2.12598700
H	-4.08477200	2.45252600	-2.00391000
H	-4.56672800	1.20604300	-3.15406900
H	-5.01059700	1.03893900	-1.45440600
C	-3.13132300	-0.89809700	-2.21256100
H	-2.21014500	-1.47140400	-2.06443700
H	-3.92256000	-1.33206700	-1.60481700
H	-3.42857800	-1.00122800	-3.26453800
C	-3.02709600	-0.10031800	1.30143700
C	-4.32242000	-0.65135800	1.54019200
C	-2.09199100	-0.20173900	2.36477600
C	-4.61329500	-1.14118700	2.83051400
C	-2.39634600	-0.72418900	3.61929800
C	-3.68782300	-1.17421300	3.86844000
H	-5.60874300	-1.54068900	2.99953200
H	-1.62543700	-0.76940400	4.38308900
H	1.13535900	-2.74405300	-1.30550700
H	1.89571300	-3.02672200	0.36957900
H	1.51119900	0.91067000	-1.44470500
H	1.00597600	-0.63552100	-2.29980400
C	-5.44214400	-0.88324300	0.55390500
C	-6.47909400	0.07702500	0.39734200
C	-5.56198500	-2.14101900	-0.09260100

C	-7.52665200	-0.17825300	-0.49298200
C	-6.62663700	-2.32563900	-0.99208300
C	-7.60625700	-1.36450000	-1.22676800
H	-8.30700200	0.56804000	-0.61017300
H	-6.69684000	-3.27780500	-1.51560100
C	-4.73131400	-3.42072400	0.15100300
H	-4.76232100	-3.95441400	-0.80868200
C	-5.47378700	-4.31784800	1.16982100
H	-6.51539900	-4.48551000	0.87633300
H	-4.97806000	-5.29298400	1.24825800
H	-5.47204900	-3.86215200	2.16628300
C	-3.24350500	-3.34076100	0.53534200
H	-2.66843400	-2.67770600	-0.11379500
H	-3.09012200	-3.02108900	1.56847400
H	-2.81279000	-4.34520200	0.44000800
H	-1.07328300	0.15534100	2.21629100
H	-3.96751800	-1.57132000	4.84021400
C	-8.73151500	-1.61910600	-2.22064300
H	-8.56447200	-2.61771800	-2.64702800
C	-10.11157000	-1.63558400	-1.53581600
H	-10.35266200	-0.65866200	-1.10000200
H	-10.89843400	-1.87929700	-2.25957100
H	-10.14595900	-2.37804600	-0.73099600
C	-8.70402200	-0.60963500	-3.38418100
H	-8.88041500	0.41241800	-3.02811400
H	-7.73583300	-0.62211200	-3.89674400
H	-9.48287500	-0.84551400	-4.11915800
C	-6.54922600	1.33873800	1.25952300
H	-5.54928700	1.53089100	1.65452800
C	-7.00019900	2.59856600	0.49674300
H	-8.05906700	2.54975500	0.21763500
H	-6.87694200	3.48326000	1.13198800
H	-6.42207000	2.75539700	-0.41928800
C	-7.48031900	1.10843300	2.47021300
H	-7.51923000	2.00515700	3.10072900
H	-8.50101900	0.88300400	2.13880300
H	-7.13774400	0.27493200	3.09105600
C	4.00198900	2.41700900	-1.33521200
H	3.38998738	3.31132627	-1.26607487
C	3.55433802	1.53571250	-2.42576351
O	2.74561197	1.88909666	-3.27245282
O	4.10077255	0.29769245	-2.41623520
C	3.68832748	-0.56477718	-3.48536216
H	2.60410458	-0.70533838	-3.47127014
H	3.97804182	-0.14630495	-4.45330785
H	4.20035056	-1.51168035	-3.31012176

4-Int3

Zero-point correction= 1.093603 (Hartree/Particle)

Thermal correction to Energy= 1.160164

Thermal correction to Enthalpy= 1.161108

Thermal correction to Gibbs Free Energy= 0.984798

Sum of electronic and zero-point Energies= -3130.031192

Sum of electronic and thermal Energies= -3129.964632

Sum of electronic and thermal Enthalpies= -3129.963687

Sum of electronic and thermal Free Energies= -3130.139997

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.147608

N	-5.21405100	-0.39007100	-0.66747300
C	-5.55644800	0.96739400	-0.21515000
H	-6.53022000	1.22512100	-0.64449600
H	-5.65536700	0.97651500	0.87782600
C	-4.58082800	2.04550100	-0.65809200
C	-4.33713300	-1.19065500	0.23107000
H	-4.55996600	-2.24700500	0.05076900
H	-4.60738500	-0.95718500	1.26502800
C	-2.85855900	-0.93979700	-0.01157500
C	-2.07568700	-0.38162800	0.92952100
C	-2.31763900	0.12906200	2.28092300
C	-3.02815700	-0.35176200	3.31989700
C	-1.24964400	1.18082000	2.33207800
S	-6.34978100	-1.20684600	-1.60601700
O	-6.96943800	-0.19351400	-2.46976900
O	-5.66427600	-2.37796000	-2.15800800
C	-7.63158800	-1.81530000	-0.50097200
C	-7.50439600	-3.08195400	0.07597700
C	-8.73720200	-1.01109300	-0.21192200
C	-8.48255100	-3.52971100	0.96180800
H	-6.66643400	-3.71616300	-0.19226500
C	-9.70590300	-1.47545700	0.67618300
H	-8.85076500	-0.05055800	-0.70292800
C	-9.59177400	-2.73411700	1.28355200
H	-8.38787700	-4.51905600	1.40289500
H	-10.57148200	-0.85393400	0.89257600
C	-10.63069400	-3.21739600	2.26751000
H	-10.74871900	-4.30522000	2.22406200
H	-10.34601400	-2.96216800	3.29705600
H	-11.60728800	-2.76071700	2.07676600
C	-4.23104000	2.05737400	-2.12070200
H	-3.69177600	1.13778900	-2.37176700
H	-5.13619600	2.05693100	-2.74083800

H	-3.60066200	2.90755100	-2.39208400	C	5.07385100	-0.82191800	-0.89164600
C	-2.34401800	-1.40421500	-1.35385000	C	6.29630800	-0.13829400	-0.64749000
H	-2.34180600	-2.50255900	-1.41552400	C	5.01193600	-2.22317200	-0.67135000
H	-2.98257900	-1.05869900	-2.17594400	C	7.36767700	-0.82494600	-0.06747700
H	-1.32176300	-1.05422600	-1.53019600	C	6.11477700	-2.84941800	-0.06480300
Pd	-0.12341600	0.22944000	0.86184700	C	7.29004800	-2.17944800	0.26485300
P	2.24485700	0.99235200	0.82751600	H	8.29171000	-0.28675200	0.12279200
C	3.20382700	0.18699100	2.29385700	H	6.05169400	-3.91755700	0.13707200
C	2.48914100	2.92277400	0.82118300	C	3.92121400	-3.21367700	-1.13722100
C	1.40321700	3.55818700	-0.07556900	H	3.96958500	-4.03628300	-0.41088900
H	0.39016600	3.27046500	0.21912900	C	4.33495500	-3.81605600	-2.50105400
H	1.47581000	4.64959400	0.01699400	H	5.35368000	-4.21672500	-2.47159600
H	1.54681000	3.31660900	-1.13174500	H	3.65400200	-4.62981500	-2.77857500
C	2.28006000	3.48104400	2.24343700	H	4.29090700	-3.05994000	-3.29258800
H	2.25787200	4.57662900	2.18450200	C	2.44066800	-2.79827100	-1.19483600
H	1.32793500	3.15886600	2.67621600	H	2.09778000	-2.33102300	-0.26958300
H	3.09045000	3.21205600	2.92585200	H	2.22250000	-2.12067300	-2.02290300
C	3.86238200	3.36712300	0.29573100	H	1.83880100	-3.70270500	-1.34696700
H	3.92833600	4.46286700	0.34065900	H	0.79742400	1.24759100	-1.36341900
H	4.69128900	2.96263800	0.88058700	H	2.99801700	0.14940300	-4.86131000
H	3.99923500	3.07499700	-0.74915600	C	8.44795000	-2.91065700	0.93071700
C	2.39750700	0.47570500	3.58563400	H	8.13486500	-3.95526900	1.06402800
H	2.85082300	-0.10298800	4.40112500	C	9.71022600	-2.91742000	0.04741900
H	2.40895900	1.52305800	3.88679100	H	10.09062900	-1.90159200	-0.11331000
H	1.35686400	0.15467400	3.48427700	H	10.50953100	-3.49977900	0.52118700
C	4.66111800	0.62978900	2.49681600	H	9.50423900	-3.35628900	-0.93500800
H	4.74045900	1.69655000	2.72826700	C	8.75457800	-2.33877200	2.32812000
H	5.08678000	0.08249200	3.34912500	H	9.08845800	-1.29608800	2.26615600
H	5.28180200	0.41231600	1.62626900	H	7.86796100	-2.36752000	2.97101300
C	3.13943400	-1.34080700	2.10284600	H	9.54968300	-2.91512800	2.81619600
H	2.10533500	-1.67999500	1.97196500	C	6.52123100	1.30415200	-1.10430300
H	3.73847500	-1.68112900	1.26084700	H	5.54236200	1.76578000	-1.24958100
H	3.53469900	-1.82489400	3.00585100	C	7.30159500	2.16971300	-0.09716600
C	2.77875600	0.49768100	-0.93749300	H	8.35347700	1.86876300	-0.02912000
C	3.91237200	-0.11719400	-1.55226100	H	7.28829300	3.21789300	-0.41746500
C	1.71538900	0.86385600	-1.80001800	H	6.87503200	2.11730900	0.90930500
C	3.94969100	-0.19691600	-2.96003000	C	7.24285000	1.32674300	-2.46978600
C	1.76860900	0.75286600	-3.18720500	H	7.38951600	2.35943000	-2.80937200
C	2.91651500	0.24122700	-3.78173700	H	8.22828600	0.85108600	-2.39721900
H	4.82381400	-0.65607100	-3.41190000	H	6.67097400	0.79767400	-3.23821500
H	0.91508600	1.06044600	-3.78477400	C	-4.12870200	2.92633100	0.25066200
H	-2.93272200	0.08887400	4.31025200	H	-3.19126814	3.44847014	0.06963157
H	-3.65982300	-1.23145300	3.23539800	C	-4.88427907	3.44733020	1.42736666
H	-1.50272000	2.13234700	1.85821100	O	-5.13418745	4.62715842	1.56178516
H	-0.70085500	1.30123600	3.26925900	O	-5.30232953	2.58883944	2.39684553

C	-4.71579198	1.28742074	2.52820054
H	-4.94146948	0.97057043	3.54837572
H	-5.15228382	0.57474610	1.82333304
H	-3.63171775	1.32066700	2.38679448

4-Ts3

Zero-point correction= 1.092997 (Hartree/Particle)

Thermal correction to Energy= 1.158338

Thermal correction to Enthalpy= 1.159282

Thermal correction to Gibbs Free Energy= 0.989543

Sum of electronic and zero-point Energies= -3129.991191

Sum of electronic and thermal Energies= -3129.925850

Sum of electronic and thermal Enthalpies= -3129.924906

Sum of electronic and thermal Free Energies= -3130.094645

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.116045

Imaginary frequency is -280.13^{-1}

N	-5.47506900	0.33091300	-0.88494000
C	-4.76061200	0.59144400	0.37063500
H	-5.01062300	1.61028600	0.68622800
H	-5.09621300	-0.09404600	1.15873200
C	-3.24837200	0.53719900	0.21016700
C	-5.80307400	-1.06241500	-1.20378300
H	-6.09478500	-1.10064200	-2.25878000
H	-6.68336100	-1.39329300	-0.61893900
C	-4.66662100	-2.03165000	-0.94064500
C	-3.44136400	-1.66780900	-0.55868800
C	-2.37068300	-2.49649600	-0.17496600
C	-2.04406700	-2.72315500	1.19694900
C	-1.19103000	-2.85593400	-0.97644600
S	-6.54280100	1.50279200	-1.44048200
O	-5.93817100	2.80324700	-1.12898600
O	-6.89701400	1.12670800	-2.81167500
C	-8.03872800	1.36638700	-0.45121900
C	-9.04753300	0.48103200	-0.84053500
C	-8.17225900	2.12696600	0.71354800
C	-10.18602600	0.35081900	-0.04647400
H	-8.95116000	-0.07190300	-1.76873700
C	-9.31770900	1.98490900	1.49449700
H	-7.40127400	2.84100300	0.98240000
C	-10.33723300	1.09165400	1.13420700
H	-10.97526700	-0.33060000	-0.35507100
H	-9.42681800	2.58592000	2.39419700
C	-11.56120400	0.92317800	2.00320900
H	-12.43409300	0.62485800	1.41331700
H	-11.40074100	0.14692600	2.76346500
H	-11.80810700	1.84955100	2.53238200
C	-2.73581400	1.22012400	-1.03981600
H	-1.64787300	1.16185000	-1.11733000
H	-3.17881600	0.76844800	-1.92713500
H	-3.03401800	2.27739800	-1.04371300
C	-5.11897100	-3.47167600	-1.14028800
H	-5.95044800	-3.73101800	-0.46768500
H	-5.48498400	-3.63829800	-2.16428400
H	-4.30295600	-4.17542200	-0.95673000
Pd	-0.22518200	-1.68936000	0.49041500
P	2.08476200	-1.40915400	-0.35664800
C	2.19697400	-0.10299100	-1.76629500
C	2.72536600	-3.14087700	-0.98594500
C	2.27500100	-4.22914500	0.01372100
H	2.76355300	-4.12159000	0.98549000
H	1.19288100	-4.22373800	0.16959100
H	2.55868600	-5.21065800	-0.38858200
C	2.10832500	-3.48131700	-2.35775000
H	2.36827900	-4.51839400	-2.60721100
H	1.01877300	-3.40696400	-2.35505700
H	2.49926100	-2.85212700	-3.16122800
C	4.25426000	-3.22375200	-1.09431800
H	4.53479600	-4.21238800	-1.48276900
H	4.67054300	-2.47497200	-1.76926400
H	4.72509000	-3.11130700	-0.11504900
C	0.99812500	-0.34118400	-2.71618400
H	0.99342900	0.46274300	-3.46345600
H	1.04912100	-1.28724600	-3.25694700
H	0.04630700	-0.30370600	-2.17887000
C	3.49741800	-0.09907400	-2.58750500
H	3.64404900	-1.03086800	-3.14169200
H	3.44434400	0.71082800	-3.32756200
H	4.37665300	0.08366700	-1.96802500
C	1.98072000	1.28558300	-1.13474000
H	1.07564100	1.32826800	-0.52324400
H	2.82776400	1.59497800	-0.52564100
H	1.87207000	2.02040200	-1.94391600
C	3.20547100	-1.11691500	1.16094300
C	4.41283900	-0.39857800	1.44188300
C	2.66709900	-1.88595000	2.21845600
C	5.03713900	-0.61393700	2.68775700
C	3.29464300	-2.06183700	3.44850800
H	1.70067100	-2.36091000	2.07711700
C	4.51691400	-1.44126600	3.67748500
H	5.95418500	-0.06818400	2.88759300

H	2.82026900	-2.67024200	4.21334500
H	-1.48322900	-3.61820100	1.46710700
H	-2.66422900	-2.30538600	1.98270500
H	-0.83771600	-3.88111000	-0.85986400
H	-1.14426700	-2.48950300	-2.00045000
H	5.04159800	-1.56265100	4.62125000
C	5.08645300	0.68624700	0.62776400
C	6.19998400	0.39439500	-0.20990600
C	4.72574200	2.04548800	0.83094800
C	6.79553100	1.41928200	-0.95244400
C	5.34538600	3.02444700	0.03397100
C	6.35585500	2.74279800	-0.88055600
H	7.63404200	1.17605300	-1.59852700
H	5.03353800	4.05988400	0.16130500
C	6.97802000	3.84468100	-1.72734500
H	6.46378300	4.77987800	-1.46668500
C	6.75680200	3.59996000	-3.23227200
H	7.25902900	2.68314200	-3.56361600
H	5.69089800	3.49918800	-3.46457900
H	7.15808900	4.43221300	-3.82297900
C	8.47383000	4.03877100	-1.41331500
H	8.88415700	4.87563900	-1.99108600
H	8.63141700	4.24828700	-0.34960900
H	9.05460400	3.14399200	-1.66742500
C	3.83547400	2.64052500	1.94427900
H	3.41864900	3.55710300	1.50441700
C	4.75007600	3.09385300	3.10839300
H	5.56091100	3.74288500	2.76082100
H	4.16533100	3.64385500	3.85572000
H	5.20028400	2.22895000	3.60904800
C	2.63881300	1.86487700	2.51317500
H	1.96055600	1.48421600	1.75186000
H	2.93919200	1.02955600	3.14915900
H	2.05704100	2.55227900	3.13993700
C	6.86355200	-0.98346100	-0.23920700
C	7.28930600	-1.44753600	-1.64564000
H	7.58682000	-2.50222100	-1.61861800
H	6.48413400	-1.34004600	-2.37898700
H	8.15147000	-0.88107200	-2.01615200
C	8.09210600	-1.00388300	0.69746900
H	8.84176000	-0.27270900	0.37236400
H	7.81889500	-0.76588800	1.72994100
H	8.56172500	-1.99533900	0.69255000
H	6.15036500	-1.70977400	0.15354900
C	-2.48383300	0.45641700	1.37095800
H	-1.54158739	0.99804422	1.40045790
C	-2.91542559	0.00381077	2.67471727
O	-2.03608199	-0.07616814	3.71334008
O	-4.08840840	-0.31794080	2.97850754
C	-0.87104072	0.75158061	3.79571547
H	0.02219061	0.12283535	3.78017105
H	-0.83776953	1.46177968	2.96690121
H	-0.92350324	1.28362604	4.75074195

4-Int4

Zero-point correction= 1.096969 (Hartree/Particle)

Thermal correction to Energy= 1.161789

Thermal correction to Enthalpy= 1.162733

Thermal correction to Gibbs Free Energy= 0.993953

Sum of electronic and zero-point Energies= -3130.084462

Sum of electronic and thermal Energies= -3130.019641

Sum of electronic and thermal Enthalpies= -3130.018697

Sum of electronic and thermal Free Energies= -3130.187478

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.138454

N	5.73507700	0.10488300	-1.45491500
C	4.68765000	-0.42656400	-0.57857300
H	4.54196800	-1.47900500	-0.81926800
H	4.97189200	-0.33295800	0.48306300
C	3.36823600	0.34897500	-0.83092200
C	6.05378300	1.52264000	-1.28272800
H	6.46572700	1.89394900	-2.22661800
H	6.84441000	1.66662600	-0.52036900
C	4.86883000	2.36705500	-0.86290200
C	3.65162400	1.84671100	-0.58988600
C	2.52694300	2.65587200	-0.04112800
C	2.71015400	3.53339200	0.96910300
C	1.16441500	2.42256500	-0.58384600
S	7.01514500	-0.89811500	-1.87684200
O	6.44474800	-2.21026200	-2.18504000
O	7.81375300	-0.14797100	-2.85138200
C	8.02358700	-1.08899800	-0.40007500
C	9.09768800	-0.22451400	-0.17613300
C	7.70818900	-2.08667600	0.52760800
C	9.85010700	-0.35759900	0.99100000
H	9.35472100	0.51763200	-0.92434600
C	8.47022800	-2.20457200	1.68776800
H	6.89561900	-2.77587500	0.32329600
C	9.54647500	-1.34073800	1.94225400
H	10.69360600	0.30758400	1.15999200
H	8.23257100	-2.98792600	2.40376400

C	10.34863000	-1.46337400	3.21645400	H	-0.93017200	0.06616200	2.36765300
H	11.34401500	-1.02076500	3.10816600	C	-3.33855200	-2.00818200	3.47833200
H	9.84946700	-0.94835600	4.04822300	H	-5.17578300	-2.37853600	2.44662000
H	10.47244400	-2.51068200	3.51280200	H	-1.36412600	-1.48085300	4.18814600
C	2.92796800	0.09426800	-2.29575000	H	1.88100500	4.11694100	1.36323700
H	1.99901300	0.61981500	-2.52874800	H	3.67498100	3.67796100	1.44338000
H	3.70320500	0.42863800	-2.98980600	H	0.47285200	3.20794900	-0.27754600
H	2.76155200	-0.97503100	-2.45102100	H	1.14516200	2.30576200	-1.66919700
C	5.24644300	3.82994100	-0.78917300	H	-3.55748100	-2.71242700	4.27628200
H	5.86571100	4.04862700	0.09274200	C	-5.13211400	-0.98103400	0.33608900
H	5.84739600	4.10675800	-1.66599700	C	-6.32698200	-0.22171600	0.48128600
H	4.37162100	4.48049700	-0.74899500	C	-5.05470600	-1.94215900	-0.70577100
Pd	0.32704900	0.66145200	0.13422800	C	-7.33209200	-0.32294400	-0.48558200
P	-2.09193400	1.27944800	0.32840100	C	-6.08531200	-1.97266600	-1.66175700
C	-2.89756700	1.57221500	-1.39764300	C	-7.21819500	-1.16687500	-1.59271600
C	-2.39146500	2.82382900	1.49131800	H	-8.23278600	0.27217000	-0.36631400
C	-1.33043300	2.79352500	2.61470200	H	-6.00207300	-2.68295900	-2.48278600
H	-1.48640500	1.96188200	3.30618000	C	-8.29726500	-1.23647700	-2.66466300
H	-0.31164500	2.72644800	2.22012500	H	-7.97072200	-1.98235000	-3.40215200
H	-1.41247800	3.71923500	3.19962100	C	-8.45223200	0.10655900	-3.40362100
C	-2.20905600	4.15184400	0.72764900	H	-8.79289000	0.89698900	-2.72412300
H	-2.27733300	4.97464200	1.45114600	H	-7.50148600	0.42965800	-3.84174900
H	-1.23277600	4.22997100	0.24214000	H	-9.18891200	0.02073100	-4.21127000
H	-2.98548800	4.31982300	-0.02216000	C	-9.64696500	-1.71251600	-2.09430200
C	-3.78183200	2.82602500	2.14348600	H	-10.39005600	-1.81152200	-2.89447300
H	-3.87773000	3.71183100	2.78630900	H	-9.54750000	-2.68441300	-1.59863200
H	-4.58608700	2.86625300	1.40606000	H	-10.04349200	-1.00138600	-1.35976300
H	-3.93035200	1.94548100	2.77367800	C	-4.04192600	-3.09700600	-0.86349100
C	-2.00782000	2.57309300	-2.17480600	H	-3.99249200	-3.27857100	-1.94562200
H	-2.40988100	2.65697200	-3.19269800	C	-4.64528900	-4.37559100	-0.23374100
H	-1.99461300	3.57659400	-1.74968300	H	-5.64905800	-4.58040200	-0.61996400
H	-0.97904200	2.21554700	-2.25326800	H	-4.01015500	-5.24272600	-0.45162800
C	-4.34711800	2.08368800	-1.39914400	H	-4.71559900	-4.27767200	0.85557800
H	-4.44039000	3.06760500	-0.92944400	C	-2.58534900	-2.94818500	-0.39671900
H	-4.68649700	2.18948900	-2.43852500	H	-2.10702900	-2.04176700	-0.77194300
H	-5.02919700	1.39446200	-0.90161800	H	-2.49086400	-2.95876300	0.69097100
C	-2.80604700	0.24472900	-2.17578100	H	-2.01691000	-3.80269700	-0.78373500
H	-1.78158400	-0.14461700	-2.18084800	C	-6.60618100	0.63219700	1.71971900
H	-3.47645600	-0.51481700	-1.77917700	C	-7.24954800	1.99694000	1.40656100
H	-3.09656900	0.42758800	-3.21868800	H	-7.26976400	2.61730300	2.31003900
C	-2.83670800	-0.13773000	1.37479200	H	-6.70288800	2.54287200	0.63116500
C	-4.04312500	-0.90728400	1.38347300	H	-8.28644800	1.89046600	1.06778800
C	-1.89783800	-0.42479800	2.39456200	C	-7.50001900	-0.14082800	2.71434500
C	-4.25457400	-1.80385800	2.45202800	H	-8.46848800	-0.38336400	2.26095900
C	-2.12972400	-1.32250100	3.43365300	H	-7.03510000	-1.07923000	3.03190400

H	-7.68783400	0.46298900	3.61064800
H	-5.65484100	0.81991800	2.22123600
C	2.30715600	-0.11997500	0.17640500
C	2.60777738	0.06279366	1.61328024
O	3.61780579	0.47001261	2.15753982
O	1.52192725	-0.36552429	2.36370853
C	1.66162717	-0.20233929	3.78159447
H	2.55884874	-0.70697528	4.14642369
H	1.72630255	0.85998815	4.03635339
H	0.76684263	-0.64597151	4.21903413
H	2.21299642	-1.17450385	0.02147640

4-Ts4

Zero-point correction= 1.095303 (Hartree/Particle)

Thermal correction to Energy= 1.160156

Thermal correction to Enthalpy= 1.161101

Thermal correction to Gibbs Free Energy= 0.989614

Sum of electronic and zero-point Energies= -3130.066892

Sum of electronic and thermal Energies= -3130.002039

Sum of electronic and thermal Enthalpies= -3130.001094

Sum of electronic and thermal Free Energies= -3130.172581

HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -3129.190934

Imaginary frequency is -368.12^{-1}

N	5.22697700	-0.14352900	-1.36472900
C	4.13051500	-0.19978300	-0.39253900
H	3.59336100	-1.13940400	-0.52219000
H	4.52514700	-0.15246800	0.63693600
C	3.17601500	0.98804600	-0.65171200
C	6.09537200	1.02728200	-1.22834000
H	6.69065400	1.11284600	-2.14292700
H	6.81044400	0.90634800	-0.39114400
C	5.30885900	2.30155900	-1.00913000
C	3.98187800	2.27955100	-0.78460100
C	3.09497300	3.44102200	-0.55997200
C	3.09106700	4.55809300	-1.30602000
C	2.10000900	3.22321700	0.54123000
S	5.98183100	-1.59209600	-1.78850900
O	4.91314700	-2.56716500	-2.00988000
O	6.95375400	-1.24873300	-2.83005000
C	6.91024100	-2.13064600	-0.34699400
C	8.24119600	-1.73433000	-0.19245600
C	6.28386600	-2.91685400	0.62462600
C	8.94088400	-2.12370100	0.94914700
H	8.72323400	-1.15139700	-0.96999300
C	6.99865300	-3.29607300	1.75894600
H	5.25973000	-3.24313800	0.47770700
C	8.33428900	-2.90715100	1.94081800
H	9.97812000	-1.81966500	1.06788500
H	6.51355300	-3.91131800	2.51304100
C	9.10913700	-3.35321700	3.15827500
H	9.55563000	-4.34373000	2.99874700
H	9.92532400	-2.66141200	3.39036900
H	8.46343300	-3.42715600	4.03978800
C	2.36865700	0.73939500	-1.94252200
H	1.76384300	1.61614500	-2.19244800
H	3.05987100	0.54836800	-2.76903000
H	1.70837200	-0.12073100	-1.82187400
C	6.16950300	3.53972300	-1.03519700
H	5.66510400	4.39819300	-0.58613500
H	7.10887800	3.36433200	-0.49312300
H	6.44883400	3.81295500	-2.06252100
Pd	0.17970900	2.12893100	0.33142300
P	-2.16548900	1.76792000	0.00692000
C	-2.45542500	1.11706700	-1.78151100
C	-3.14954900	3.43379800	0.27231100
C	-2.59793400	4.14083700	1.53008300
H	-2.82896200	3.59554200	2.44832100
H	-1.51258700	4.27908900	1.47380500
H	-3.06730500	5.13049100	1.61078900
C	-2.90320900	4.38270900	-0.91754200
H	-3.31840700	5.36897400	-0.67181700
H	-1.83501300	4.51472200	-1.12085600
H	-3.39487100	4.04712500	-1.83374600
C	-4.66116200	3.23753700	0.46540400
H	-5.14196300	4.21710900	0.59497600
H	-5.13508100	2.74934300	-0.38852900
H	-4.87238000	2.64821100	1.36192900
C	-1.57781100	1.96484000	-2.73464600
H	-1.59126000	1.48766600	-3.72323400
H	-1.93281400	2.98807100	-2.86218600
H	-0.53964600	2.00144200	-2.39005500
C	-3.90304200	1.11279300	-2.29797200
H	-4.32207200	2.12110500	-2.37244400
H	-3.91957200	0.68148400	-3.30819700
H	-4.55983700	0.50416900	-1.67405100
C	-1.88780300	-0.31374300	-1.82283100
H	-1.81787600	-0.63773900	-2.86994800
H	-0.88816100	-0.37693900	-1.38157000
H	-0.57140600	-3.61090700	0.02375600
C	-2.87558400	0.69430000	1.41626900

C	-3.86341300	-0.33079300	1.54734300
C	-2.25794100	1.13694500	2.61129800
C	-4.23981200	-0.72406700	2.85090000
C	-2.64772400	0.72806200	3.88316600
H	-1.41895600	1.82134100	2.52843900
C	-3.67787700	-0.19755200	4.00862000
H	-4.99419800	-1.50005600	2.93913400
H	-2.13690100	1.12301100	4.75727500
H	2.38415000	5.36276900	-1.11876700
H	3.78164600	4.69612400	-2.13206100
H	2.51415300	3.36269500	1.53991200
H	1.24705900	3.92816700	0.43583800
H	-4.01506700	-0.53749500	4.98416100
C	-4.51400800	-1.19305100	0.48414600
C	-3.85492800	-2.38584000	0.07567900
C	-5.84854000	-0.96368900	0.06295200
C	-4.50766600	-3.24879500	-0.81306700
C	-6.44967300	-1.86237300	-0.82756400
C	-5.79512300	-3.00380200	-1.29286900
H	-3.99744900	-4.15107600	-1.13853000
H	-7.46834900	-1.66929900	-1.15290400
C	-6.45909300	-3.96521200	-2.26999600
H	-5.74428600	-4.77826300	-2.45678400
C	-6.75311500	-3.29014100	-3.62338100
H	-7.17532800	-4.01223800	-4.33263300
H	-7.47480300	-2.47213200	-3.51085300
H	-5.84112300	-2.87226800	-4.06354400
C	-7.73345900	-4.59929900	-1.68053000
H	-8.15834300	-5.33170300	-2.37746100
H	-7.52079600	-5.11079700	-0.73531000
H	-8.50248300	-3.84232600	-1.48520600
C	-6.69860700	0.18399700	0.61092400
H	-6.02998300	0.88279500	1.11849200
C	-7.70171000	-0.33436100	1.66403800
H	-8.29336800	0.49452400	2.07184400
H	-8.39608000	-1.05822600	1.22099000
H	-7.19315700	-0.82748200	2.49844400
C	-7.45367200	0.96878000	-0.47928600
H	-8.24251900	0.36518900	-0.94287800
H	-7.93692800	1.84987600	-0.04086900
H	-6.78573800	1.30915100	-1.27651600
C	-2.48745500	-2.80454800	0.63116600
H	-1.94985100	-1.89951800	0.92925200
C	-2.66144900	-3.68563800	1.88833900
H	-3.21211400	-4.60203000	1.64303700
H	-1.68142600	-3.97907700	2.28463700
H	-3.20546200	-3.16625100	2.68205600
C	-1.58808200	-3.54579800	-0.37747200
H	-1.93675600	-4.56926500	-0.56136100
H	-1.52874200	-3.03026600	-1.33975200
H	-2.54342000	-1.01204500	-1.30918300
C	2.30960300	1.20836200	0.60507800
C	2.75156015	0.49594330	1.86616814
O	3.49155215	-0.47544850	1.95225657
O	2.41049665	1.24245199	2.96271955
C	2.92311436	0.76852060	4.21327695
H	2.48273620	-0.19610886	4.47494798
H	4.01167493	0.66986884	4.17227503
H	2.63568290	1.52122128	4.94927231
H	1.52921454	0.65532418	0.12545000

4a-Me

Zero-point correction= 0.422290 (Hartree/Particle)

Thermal correction to Energy= 0.448350

Thermal correction to Enthalpy= 0.449294

Thermal correction to Gibbs Free Energy= 0.364051

Sum of electronic and zero-point Energies= -1530.516703

Sum of electronic and thermal Energies= -1530.490644

Sum of electronic and thermal Enthalpies= -1530.489699

Sum of electronic and thermal Free Energies= -1530.574942

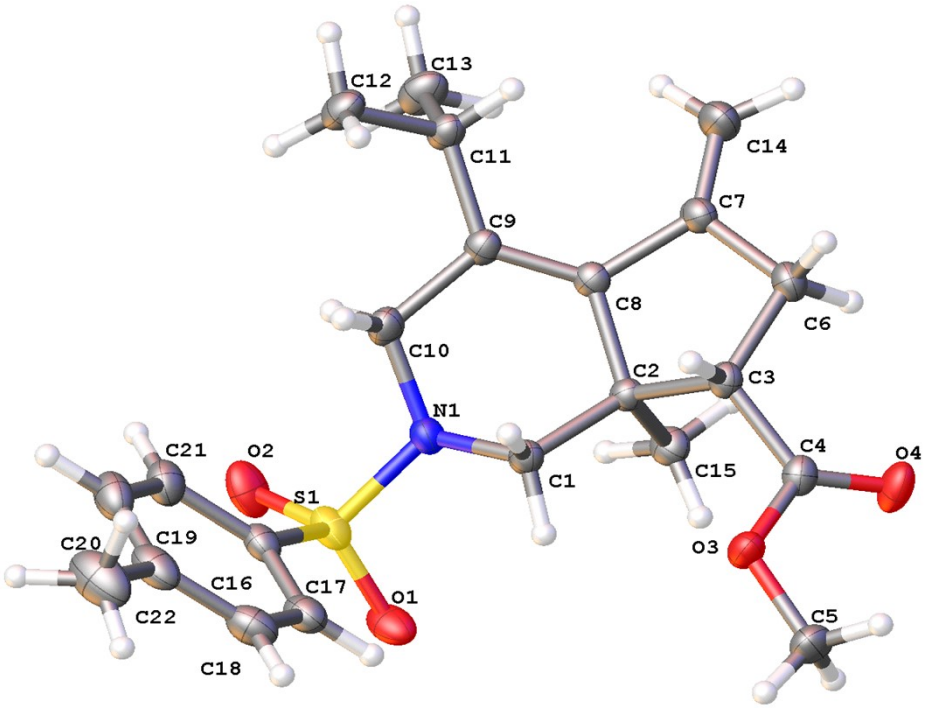
HF(B3LYP/6-311+G(d,p)/Lanl2dz, SMD[toluene])= -1530.126867

N	-0.27959400	0.71174400	0.94495500
C	0.48293400	-0.31321000	0.22231600
H	0.37422800	-1.26217800	0.74764700
H	0.10279700	-0.43497500	-0.80530300
C	1.95170700	0.13164100	0.19091400
C	-0.31561600	2.02628500	0.29822500
H	-0.60680900	2.76424800	1.05312600
H	-1.08627200	2.06340400	-0.49586200
C	1.01069700	2.41456300	-0.32013400
C	2.05575400	1.56345000	-0.33898000
C	3.38553700	1.72434400	-0.96400400
C	4.06284000	2.85413600	-1.21838600
C	3.94505600	0.32956300	-1.23191200
S	-1.67197200	0.23734700	1.76897400
O	-1.34323700	-1.02242700	2.43940500
O	-2.12435200	1.41923400	2.50682900
C	-2.91610800	-0.12465700	0.52319100
C	-3.78845200	0.88239500	0.10337600
C	-2.98626300	-1.40497000	-0.03312400

C	-4.72716800	0.60169500	-0.88842500	H	1.65669900	3.84640200	-1.80859400
H	-3.74903900	1.85930900	0.57329700	H	-0.00834600	4.07868500	-1.23538300
C	-3.93042200	-1.66684500	-1.02309900	H	1.35024700	4.55431600	-0.21748000
H	-2.32962600	-2.18856600	0.32965800	H	5.04616300	2.81962100	-1.68132700
C	-4.80956000	-0.67002000	-1.47172000	H	3.69334800	3.83621200	-0.94773200
H	-5.41446600	1.38173000	-1.20686100	H	4.27911400	0.21121600	-2.26838300
H	-3.99368200	-2.66599600	-1.44750000	H	4.81116100	0.11738000	-0.59600200
C	-5.81093400	-0.95872600	-2.56454100	C	2.79619300	-0.63606400	-0.88489600
H	-6.67691300	-0.29218500	-2.50149700	C	2.29644873	-1.43289869	-2.07416885
H	-5.36182500	-0.81859700	-3.55683600	O	2.85740003	-1.54548144	-3.14261752
H	-6.17148900	-1.99151400	-2.51517000	O	1.11939247	-2.03994844	-1.78735260
C	2.57846400	0.02193300	1.59741200	C	0.57395848	-2.85708430	-2.83826538
H	3.60907900	0.39005900	1.60775300	H	1.26621606	-3.66215338	-3.09762074
H	1.99585600	0.61368900	2.30797500	H	-0.35547371	-3.26434845	-2.43954992
H	2.58510800	-1.01671300	1.94793100	H	0.38000150	-2.25428310	-3.72928182
C	1.00582600	3.79254600	-0.93068700	H	3.40247868	-1.46141894	-0.57488487

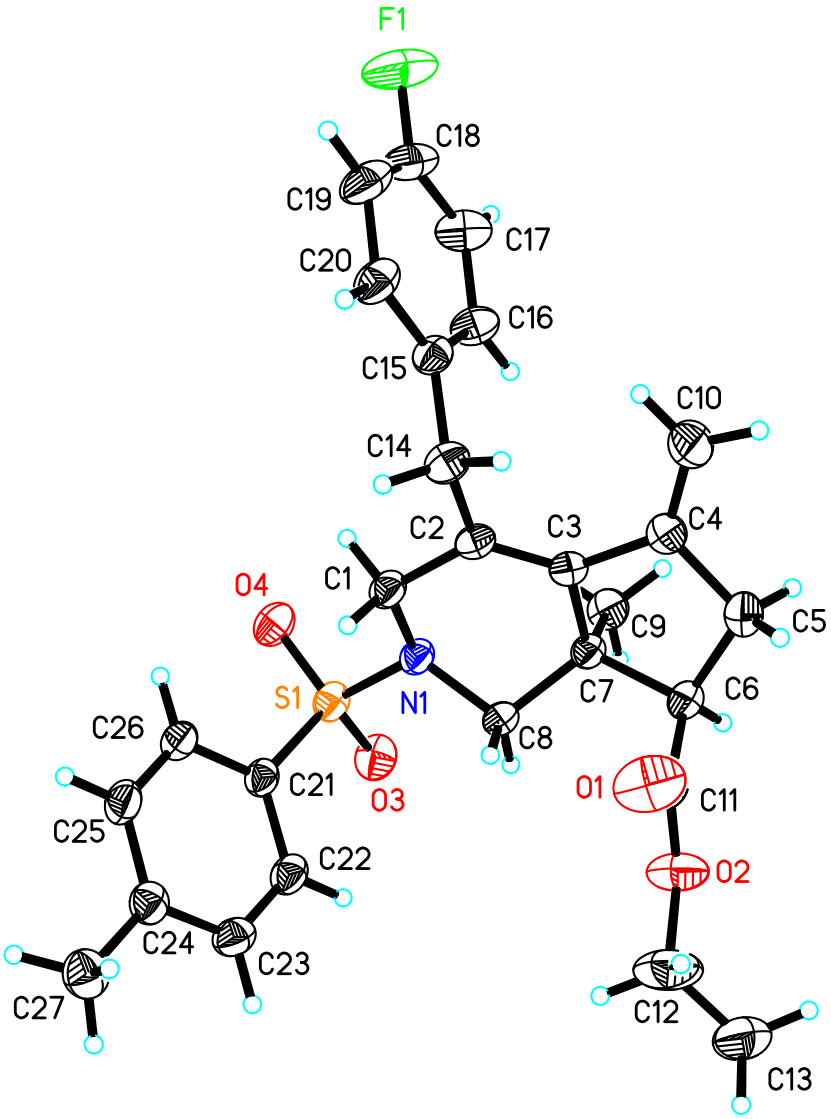
8. X-Ray structures

(a) Product 2c



The crystal data of **2c** have been deposited in CCDC with number 2306250. Empirical Formula: $C_{22}H_{29}NO_4S$; Formula Weight: 403.52; Crystal Color, Habit: colorless; Crystal Dimensions: 0.17 x 0.17 x 0.05 mm^3; Crystal System: Monoclinic; Lattice Parameters: a = 7.6269(2) Å, alpha = 90 deg. b = 12.3105(3) Å, beta = 91.242(2) deg. c = 23.0037(5) Å, gamma = 90 deg.; V = 2159.33(9) $Å^3$; Space group: P 1 21/c 1; Z = 4; D_{calc} = 1.241 g/cm^3; F_{000} = 864; Diffractometer: Rigaku AFC7R; Residuals: R; R_w: 0.0462, 0.1002.

(b) Product 4i



The crystal data of **4i** have been deposited in CCDC with number 2328425. Empirical Formula: $C_{27}H_{30}FNO_4S$; Formula Weight: 483.58; Crystal Color, Habit: colorless; Crystal Dimensions: 0.200 x 0.160 x 0.120 mm^3; Crystal System: Triclinic; Lattice Parameters: a = 8.8399(3) Å, alpha = 71.0650(10) deg. b = 10.9638(5) Å, beta = 82.3880(10) deg. c = 14.6620(6) Å, gamma = 67.8040(10) deg.; V = 1244.45(9) $Å^3$; Space group: P -1; Z = 2; D_{calc} = 1.291 g/cm^3; F_{000} = 512; Diffractometer: Rigaku AFC7R; Residuals: R; R_w: 0.0438, 0.1010.

9. References

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