An EDA Complex Directed *N*-centered Radical Generation from Nitrosoarene: A Divergent Synthetic Approach

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Supporting Information

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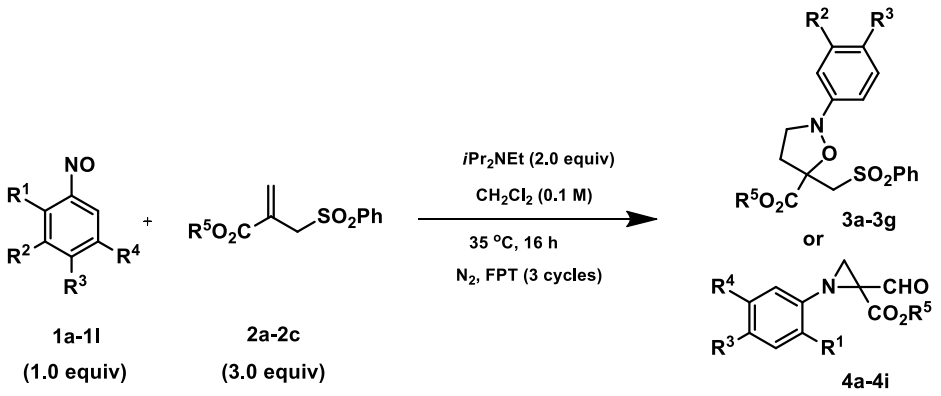
1. General Information

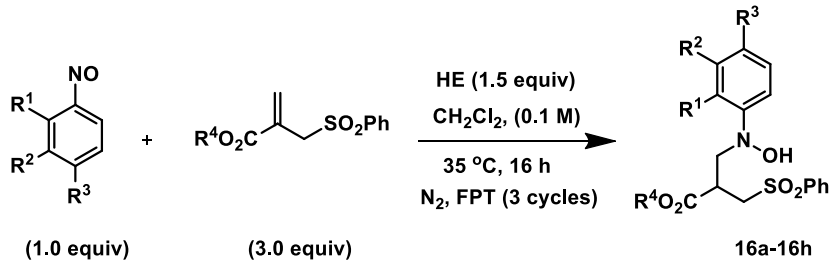
Reactions were performed in flame-dried glassware using conventional Schlenk techniques under a static pressure of nitrogen unless otherwise stated. Liquids and solutions were transferred with syringes. Solvents used were dried and purified by following standard procedures. Technical grade solvents for extraction or chromatography (ethyl acetate, and petroleum ether) were distilled prior to use. $CDCl_3$ was stored over 4Å molecular sieves. Used chemicals were purchased from *Sigma-Aldrich*, *TCI*, *A*lfa-*A*esar and *Sisco Research Laboratories (SRL)* used without further purification. Amines used were purchased from commercial suppliers and used after their respective boiling point distillation. Analytical thin-layer chromatography (TLC) was performed on silica gel 60 F254 glass plates from *Merck*. Flash column chromatography was performed on silica gel 60 (40–63 μm, 230–400 mesh, ASTM) from *Merck* using the indicated solvents. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded in $CDCl_3$ unless otherwise stated on JEOL JNM ECS-400 instrument. Chemical shifts are reported in parts per million (ppm) and are referenced to the residual solvent resonance as the internal standard ($CDCl_3$: δ = 7.26 ppm for **^{1}H NMR** and $CDCl_3$: δ = 77.16 ppm for **^{13}C NMR**;.1,3,5-trimethoxybenzene was used as an internal standard to calculate NMR yields. Data are reported as follows: chemical shift, multiplicity (br = broad singlet, s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, sept = septet, m = multiplet), coupling constants (Hz), and integration. All the HRMS data were recorded on XEVO G2-XS QTOF. All UV data were recorded using UV-2600 (UV-VIS spectrophotometer), SHIMADZU instrument. CV measurements were performed with the three-electrode potentiostat galvanostat PGSTAT302N from Metrohm Autolab using a glassy carbon working electrode, a platinum wire counter electrode, a Ag/AgCl as a reference electrode and tetabutylammonium hexafluorophosphate 0.1 M as supporting electrolyte. The control of the measurement instrument, the acquisition and processing of the cyclic voltammetric data were performed with the software Metrohm Autolab NOVA 1.10.4. Nitrosoarenes,[S1-S8] ethyl 2-((phenylsulfonyl)methyl)acrylate,[S9] tert-butyl 2-((phenylsulfonyl)methyl)acrylate[S10] and 2-isopropyl-5-methylcyclohexyl 2-((phenylsulfonyl)methyl)acrylate[S11] were synthesized according to reported procedure in the literature.

2. General Procedure for the synthesis of isoxazolidine and aziridine derivatives (GP-1)



An oven-dried schlenk tube was charged with nitrosoarene (1.0 equiv) and *i*Pr_2NEt (2.0 equiv) then evacuated and followed by back filled with nitrogen three times. Freshly distilled 0.1 (M) CH_2Cl_2 (with respect to **1**) and allylsulfone (if liquid) [if allylsulfone is solid it was added prior to addition of solvent] were then added via a syringe and the schlenk tube was capped with a stopper.The reaction mixture was degassed via freeze-pump-thaw cycle three times. Finally the reaction mixture was purged with nitrogen for 5 minutes. After that reaction mixture was stirred for 16 h at 35 ^{o}C. The reaction mixture was concentrated directly and then the crude reaction mixture was purified by either flash column chromatography or preparative thin layer chromatography.

3. General Procedure for the synthesis of β-amino acid derivatives (GP-2)

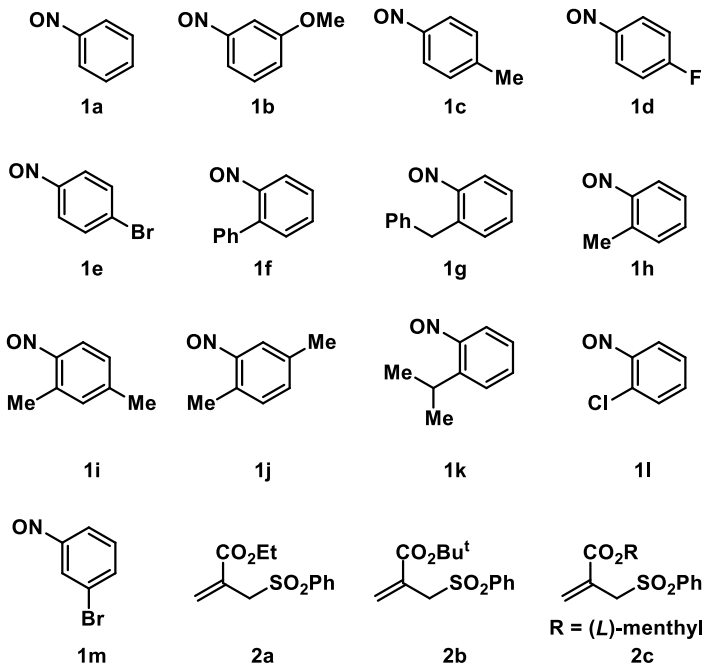


An oven-dried schlenk tube was charged with nitrosoarene (1.0 equiv) and Hantzsch Ester (HE) (1.5 equiv) then evacuated and followed by back filled with nitrogen three times. Freshly distilled 0.1 (M) CH_2Cl_2 (with respect to nitrosoarene) and allylsulfone (if liquid) [if allylsulfone is solid it was added prior to addition of solvent] were then added via a syringe and the schlenk tube was capped with a stopper.The reaction mixture was degassed via freeze-pump-thaw cycle three times. Finally the reaction mixture was purged with nitrogen

for 5 minutes. After that reaction mixture was stirred for 16 h at 35 ^{o}C. The reaction mixture was concentrated directly and then the crude reaction mixture was purified by either flash column chromatography or preparative thin layer chromatography.

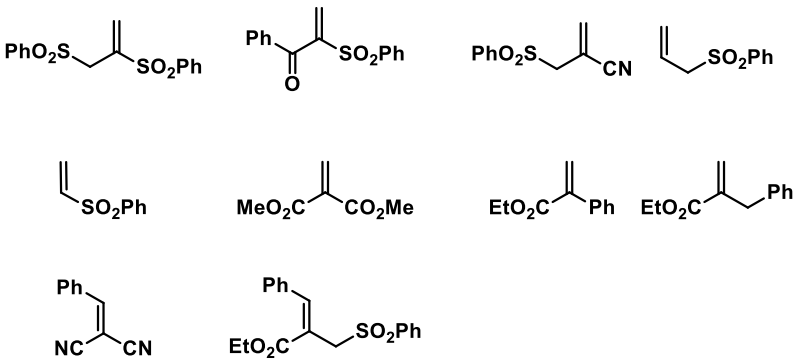
4. List of the substrates used.

The list of the substrates used for GP-1 is given below.



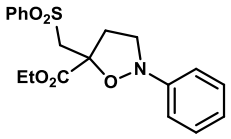
5. List of unreacted substrates

For the following substrates there was neither formation of Isoxazolidine nor aziridine according to GP-1.



6. Experimental details for the synthesized compounds obtained from (GP-1) and (GP-2)

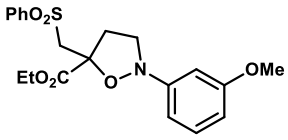
6.1 Ethyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3a)



$C_{19}H_{21}NO_5S$
M = 375.44 g/mol

Prepared according to the GP-1, using **1a** (21.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the Isoxazolidine **3a** (25.0 mg, 33% yield) as greenish yellow oil. **HRMS (ESI):** for $C_{19}H_{22}NO_5S^+$ [$(M+H)^+$]: calculated 376.1219, found 376.1235. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.67 – 7.63 (m, 1H), 7.57 – 7.53 (m, 2H), 7.20 – 7.15 (m, 2H), 6.96 – 6.93(m, 1H), 6.74 – 6.70 (m, 2H), 4.25 – 4.18 (m, 2H), 3.97 (d, *J* = 14.3 Hz, 1H), 3.82 (d, *J* = 14.4 Hz, 1H), 3.58 – 3.47 (m, 2H), 2.91 (ddd, *J* = 12.5, 7.4, 4.9 Hz, 1H), 2.57 (dt, *J* = 12.9, 7.8 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.8, 150.0, 140.4, 134.0, 129.3, 128.7, 128.6, 122.7, 115.8, 81.5, 62.5, 61.8, 53.1, 37.9, 14.1.

6.2 Ethyl 2-(3-methoxyphenyl)-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3b)

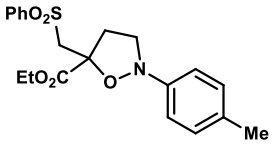


$C_{20}H_{23}NO_6S$
M = 405.46 g/mol

Prepared according to the GP-1, using **1b** (27.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the Isoxazolidine **3b** (23.0 mg, 28% yield) as greenish yellow oil. **HRMS (ESI**): for $C_{20}H_{24}NO_6S^+$ [$(M+H)^+$]: calculated 406.1324, found 406.1328. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 – 7.92 (m, 2H), 7.67 – 7.62 (m, 1H), 7.55 (tt, *J* = 6.7, 1.3 Hz, 2H), 7.09 (t, *J* = 8.2 Hz, 1H), 6.50 (ddd, *J* = 8.2, 2.5, 0.8 Hz, 1H), 6.41 (t, *J* = 2.3 Hz, 1H), 6.33 (ddd, *J* = 8.1, 2.1, 0.8 Hz, 1H), 4.24 – 4.15 (m, 2H), 3.98 (d, *J* = 14.3 Hz, 1H), 3.80 (d, *J* = 14.3 Hz, 1H), 3.76 (s, 3H), 3.60 – 3.48 (m, 2H), 2.92 (ddd, *J* = 12.8, 7.4, 4.8 Hz, 1H), 2.57 (dt, *J* = 13.1, 7.8 Hz,

1H), 1.29 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.7, 160.1, 151.4, 140.2, 134.0, 129.5, 129.3, 128.4, 108.1, 107.7, 102.2, 81.6, 62.5, 61.7, 55.4, 53.2, 37.4, 14.0.

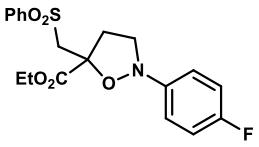
6.3 Ethyl 5-((phenylsulfonyl)methyl)-2-(*p*-tolyl)isoxazolidine-5-carboxylate (3c)



$C_{20}H_{23}NO_5S$
M = 389.47 g/mol

Prepared according to the GP-1, using **1c** (24.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the Isoxazolidine **3c** (20.0 mg, 25% yield) as greenish yellow oil. **HRMS (ESI)**: for $C_{20}H_{24}NO_5S^+$ [$(M+H)^+$]: calculated 390.1375, found 390.1369. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.67 – 7.63 (m, 1H), 7.57 – 7.53 (m, 2H), 6.99 – 6.96 (m, 2H), 6.64 – 6.60 (m, 2H), 4.27 – 4.15 (m, 2H), 3.96 (d, *J* = 14.5 Hz, 1H), 3.82 (d, *J* = 14.3 Hz, 1H), 3.53 – 3.42 (m, 2H), 2.90 (ddd, *J* = 12.4 Hz, 7.3, 4.9 Hz, 1H), 2.54 (dt, *J* = 13.0, 7.7 Hz, 1H), 2.26 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H) **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.8, 147.6, 140.4, 133.9, 132.3, 129.2, 129.2, 128.5, 116.0, 81.5, 62.4, 61.9, 53.3, 37.9, 20.7, 14.1.

6.4 Ethyl 2-(4-fluorophenyl)-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3d)

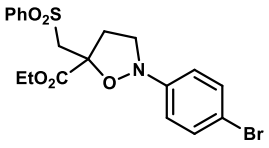


$C_{19}H_{20}FNO_5S$
M = 393.43 g/mol

Prepared according to the GP-1, using **1d** (25.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the Isoxazolidine **3d** (17.0 mg, 21% yield) as greenish yellow oil. **HRMS (ESI)**: for $C_{19}H_{21}FNO_5S^+$ [$(M+H)^+$]: calculated 394.1124, found 394.1121. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 – 7.92 (m, 2H), 7.67 – 7.62 (m, 1H), 7.56 – 7.51 (m, 2H), 6.90 – 6.84 (m, 2H), 6.72 – 6.67 (m, 2H), 4.23 (qd, *J* = 7.1, 4.1 Hz, 2H), 3.94 (d, *J* = 14.4 Hz, 1H), 3.84 (d, *J* = 14.4 Hz,

1H), 3.50 – 3.39 (m, 2H), 2.90 (ddd, *J* = 12.6, 7.4, 5.1 Hz, 1H), 2.59 (ddd, *J* = 13.0, 7.9, 7.2 Hz, 1H), 1.31 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.8, 160.2, 146.0, 140.3, 133.9, 129.3, 128.6, 117.7 (d, *J* = 7.9 Hz), 115.3 (d, *J* = 22.4 Hz), 81.4, 62.6, 61.8, 53.6, 38.3, 14.1. **^{19}F NMR** (376 MHz, $CDCl_3$): δ = –120.9 ppm.

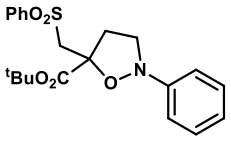
6.5 Ethyl 2-(4-bromophenyl)-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3e)



$C_{19}H_{20}BrNO_5S$
M = 454.33 g/mol

Prepared according to the GP-1, using **1e** (37.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the Isoxazolidine **3e** (27.0 mg, 30% yield) as greenish yellow oil. **HRMS (ESI**): for $C_{19}H_{21}BrNO_5S^+$ [$(M+H)^+$]: calculated 454.0324 , found 454.0307. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.95 – 7.93 (m, 2H), 7.68 – 7.64 (m, 1H), 7.58 – 7.53 (m, 2H), 7.27 (d, *J* = 9.0 Hz, 2H), 6.60 – 6.56 (m, 2H), 4.22 (qd, *J* = 7.1, 4.7 Hz, 2H), 3.93 (d, *J* = 14.4 Hz, 1H), 3.83 (d, *J* = 14.4 Hz, 1H), 3.53 – 3.42 (m, 2H), 2.90 (ddd, *J* = 12.9, 7.5, 4.9 Hz, 1H), 2.58 (dt, *J* = 13.0, 7.7 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H) **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.6, 149.0, 140.4, 134.0, 131.5, 129.3, 128.5, 117.3, 115.2, 81.4, 62.6, 61.6, 52.9, 38.0, 14.1.

6.6 Tert-butyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3f)

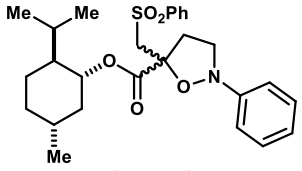


$C_{21}H_{25}NO_5S$
M = 403.49 g/mol

Prepared according to the GP-1, using **1a** (21.0 mg, 0.2 mmol, 1.0 equiv), **2b** (170.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded the Isoxazolidine **3f** (24.0 mg, 30% yield) as greenish yellow oil. **HRMS (ESI**): for $C_{21}H_{26}NO_5S^+$ [$(M+H)^+$]: calculated 404.1532, found 404.1529. **^{1}H NMR** (400 MHz, $CDCl_3$) δ

7.96 – 7.93 (m, 2H), 7.65 – 7.61 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.19 – 7.15 (m, 2H), 6.95 – 6.91 (m, 1H), 6.73 (dd, *J* = 8.7, 1.0 Hz, 2H), 3.95 (d, *J* = 14.3 Hz, 1H), 3.79 (d, *J* = 14.4 Hz, 1H), 3.59 – 3.54 (m, 1H), 3.47 (dt, *J* = 9.3, 7.5 Hz, 1H), 2.85 (ddd, *J* = 12.3, 7.5, 4.6 Hz, 1H), 2.57 (dt, *J* = 12.9, 7.7 Hz, 1H), 1.49 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 168.6, 150.2, 140.7, 133.8, 129.3, 128.7, 128.4, 122.5, 115.7, 83.4, 81.8, 61.7, 53.1, 37.9, 27.9.

6.7 2-Isopropyl-5-methylcyclohexyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3g and 3g')



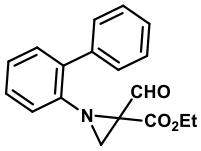
[dr = 2:1]
$C_{27}H_{35}NO_5S$
M = 485.64 g/mol

Prepared according to the GP-1, using **1a** (21.0 mg, 0.2 mmol, 1.0 equiv), **2c** (216.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded the Isoxazolidine **3g** (31.0 mg, 32% yield) as greenish yellow oil. **HRMS (ESI**): for $C_{27}H_{36}NO_5S^+$ [$(M+H)^+$]: calculated 486.2314, found 486.2285. **^{1}H NMR (For major diasteroisomer)** (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.65 – 7.61 (m, 1H), 7.55 – 7.51 (m, 2H), 7.20 – 7.16 (m, 2H), 6.97 – 6.92 (m, 1H), 6.76 (dt, *J* = 8.8, 1.7 Hz, 2H), 4.76 (td, *J* = 10.9, 4.3 Hz, 1H), 3.98 (d, *J* = 14.3 Hz, 1H), 3.81 (d, *J* = 14.3 Hz, 1H), 3.58 – 3.47 (m, 2H), 2.94 (ddd, *J* = 12.4, 7.4, 4.8 Hz, 1H), 2.62 (dt, *J* = 12.9, 7.8 Hz, 1H), 2.08 (dt, *J* = 11.9, 4.5 Hz, 1H), 1.98 – 1.91(m, 1H), 1.70 – 1.64 (m, 2H), 1.53 – 1.46 (m, 1H), 1.45 – 1.37 (m, 1H), 1.09 – 1.00 (m, 1H), 0.97 (d, *J* = 11.3 Hz, 1H), 0.91 (d, *J* = 6.5 Hz, 3H), 0.89 – 0.87 (m, 1H), 0.82 (d, *J* = 7.0 Hz, 3H), 0.72 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.6, 150.0, 140.7, 133.9, 129.3, 128.7, 128.4, 122.6, 115.7, 81.8, 76.8, 61.3, 53.3, 47.2, 40.2, 37.4, 34.3, 31.5, 25.9, 23.2, 22.2, 21.0, 16.0.

^{1}H NMR (For minor diasteroisomer 3g') (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.63 – 7.59 (m, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.17 (t, *J* = 7.9 Hz, 2H), 6.96 – 6.92 (m, 1H), 6.72 – 6.70 (m, 2H), 4.79 (td, *J* = 10.9, 4.3 Hz, 1H), 3.95 (d, *J* = 14.4 Hz, 1H), 3.86 (d, *J* = 14.3 Hz, 1H), 3.62 – 3.56 (m, 1H), 3.46 (m, 1H), 2.88 – 2.81 (m, 1H), 2.69 – 2.62 (m, 1H), 2.15 (d, *J* = 12.3 Hz, 1H), 1.92 (ddp, *J* = 9.7, 7.0, 2.9 Hz, 1H), 1.71 – 1.67 (m, 2H), 1.46 – 1.39 (m, 1H), 1.12 – 1.01 (m, 2H), 0.90 (dd, *J* = 12.2, 6.8 Hz, 6H), 0.85 – 0.80 (m, 2H), 0.77 (d, *J* = 6.9 Hz,

3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.4, 150.0, 140.8, 133.8, 129.2, 128.6, 128.4, 122.6, 115.8, 81.5, 76.8, 61.5, 53.1, 47.1, 40.3, 38.1, 34.3, 31.6, 26.2, 23.2, 22.2, 21.0, 16.1.

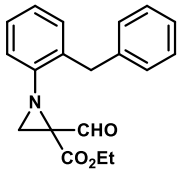
6.8 Ethyl 1-([1,1'-biphenyl]-2-yl)-2-formylaziridine-2-carboxylate (4a)



$C_{18}H_{17}NO_3$
M = 295.33 g/mol

Prepared according to the GP-1, using **1f** (37.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4a** (24.0 mg, 40% yield) as yellowish green oil. **HRMS (ESI**): for $C_{18}H_{18}NO_3^+$ [$(M+H)^+$]: calculated 296.1287, found 296.1280. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 7.39 – 7.34 (m, 5H), 7.33 – 7.31 (m, 1H), 7.22 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.15 (td, *J* = 7.6, 1.2 Hz, 1H), 7.05 (dd, *J* = 7.9, 1.0 Hz, 1H), 4.17 – 4.03 (m, 2H), 2.95 (d, *J* = 3.1 Hz, 1H), 2.92 (d, *J* = 2.9 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 192.2, 167.4, 144.4, 138.3, 133.6, 130.1, 129.8, 128.5, 127.6, 124.1, 120.5, 61.9, 47.4, 42.5, 14.1.

6.9 Ethyl 1-(2-benzylphenyl)-2-formylaziridine-2-carboxylate (4b)

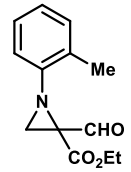


$C_{19}H_{19}NO_3$
M = 309.36 g/mol

Prepared according to the GP-1, using **1g** (39.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4b** (29.0 mg, 46% yield) as yellowish green oil. **HRMS (ESI**) for $C_{19}H_{20}NO_3^+$ [$(M+H)]^+$: calculated 310.1443, found 310.1433. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.57 (s, 1H), 7.30 – 7.26 (m, 2H), 7.23 – 7.19 (m, 2H), 7.12 – 7.09 (m, 2H), 7.04 (td, *J* = 7.4, 1.2 Hz, 1H), 6.96 (td, *J* = 8.2, 1.2 Hz, 2H), 4.19 (qd, *J* = 7.1, 2.0 Hz, 2H), 3.87 (s, 2H), 3.08

(d, *J* = 2.3 Hz, 1H), 3.02 (d, *J* = 2.3 Hz, 1H), 1.18 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.1, 167.1, 144.1, 138.8, 133.2, 130.7, 129.2, 128.6, 127.1, 126.4, 124.5, 120.0, 62.2, 49.3, 39.1, 37.1, 14.0.

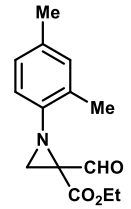
6.10 Ethyl 2-formyl-1-(*o*-tolyl)aziridine-2-carboxylate (4c)



$C_{13}H_{15}NO_3$
M = 233.26 g/mol

Prepared according to the GP-1, using **1h** (24.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4c** (22.0 mg, 47% yield) as yellowish green oil. **HRMS (ESI**) for $C_{13}H_{16}NO_3^+$ $[(M+H)]^+$: calculated 234.1131, found 234.1130. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 7.18 – 7.14 (m, 1H), 7.09 (d, *J* = 7.2 Hz, 1H), 7.00 (td, *J* = 7.4, 1.0 Hz, 1H), 6.90 – 6.88 (m, 1H), 4.23 (q, *J* = 7.0 Hz, 2H), 3.16 (d, *J* = 2.2 Hz, 1H), 3.02 (d, *J* = 2.2 Hz, 1H), 2.12 (s, 3H), 1.19 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 192.9, 167.1, 144.8, 130.6, 130.1, 126.7, 124.3, 119.4, 62.2, 49.1, 39.5, 18.1, 14.1.

6.11 Ethyl 1-(2,4-dimethylphenyl)-2-formylaziridine-2-carboxylate (4d)

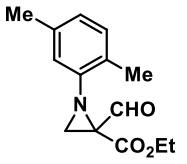


$C_{14}H_{17}NO_3$
M = 247.29 g/mol

Prepared according to the GP-1, using **1i** (27.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4d** (22.0 mg, 44% yield) as yellowish green oil. **HRMS (ESI**) for $C_{14}H_{18}NO_3^+$ $[(M+H)]^+$: calculated 248.1287, found 248.1285. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.91 – 6.89 (m, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 4.27 –

4.22 (m, 2H), 3.14 (d, *J* = 2.0 Hz, 1H), 3.00 (d, *J* = 2.0 Hz, 1H), 2.25 (s, 3H), 2.08 (s, 3H), 1.21 (t, *J* = 6.6 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 192.9, 167.0, 142.2, 133.7, 131.4, 129.9, 127.2, 119.3, 62.2, 49.1, 39.5, 20.8, 17.9, 14.1.

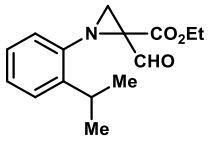
6.12 Ethyl 1-(2,5-dimethylphenyl)-2-formylaziridine-2-carboxylate (4e)



$C_{14}H_{17}NO_3$
M = 247.29 g/mol

Prepared according to the GP-1, using **1j** (27.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4e** (20.0 mg, 40% yield) as yellowish green oil. **HRMS (ESI**) for $C_{14}H_{18}NO_3^+$ $[(M+H)]^+$: calculated 248.1287, found 248.1285. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 1H), 6.69 (s, 1H), 4.24 (q, *J* = 7.1 Hz, 2H), 3.14 (d, *J* = 2.2 Hz, 1H), 3.00 (d, *J* = 2.2 Hz, 1H), 2.30 (s, 3H), 2.07 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 192.9, 167.1, 144.6, 136.3, 130.4, 126.9, 125.0, 120.1, 62.2, 49.1, 39.7, 21.2, 17.6, 14.1.

6.13 Ethyl 2-formyl-1-(2-isopropylphenyl)aziridine-2-carboxylate (4f)

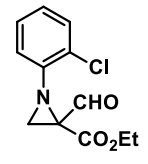


$C_{15}H_{19}NO_3$
M = 261.32 g/mol

Prepared according to the GP-1, using **1k** (30.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4f** (21.0 mg, 40% yield) as yellowish green oil. **HRMS (ESI**) for $C_{15}H_{20}NO_3^+$ $[(M+H)]^+$: calculated 262.1443, found 262.1452. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 7.21 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.14 (td, *J* = 7.5, 1.7 Hz, 1H), 7.08 (td, *J* = 7.4, 1.3 Hz, 1H), 6.88 (dd, *J* = 7.8, 1.3 Hz, 1H), 4.20 (qd, *J* = 10.6, 3.5 Hz, 2H), 3.17 (d, *J* = 2.1

Hz, 1H), 3.01 (d, *J* = 2.2 Hz, 1H), 2.99 – 2.92 (m, 1H), 1.21 – 1.15 (m, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.7, 166.8, 143.1, 140.9, 126.4, 125.9, 124.8, 119.8, 62.2, 50.0, 38.9, 27.7, 22.9, 14.1.

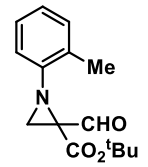
6.14 Synthesis of Ethyl 1-(2-chlorophenyl)-2-formylaziridine-2-carboxylate (4g)



$C_{12}H_{12}ClNO_3$
M = 253.68 g/mol

Prepared according to the GP-1, using **1l** (28.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4g** (12.0 mg, 23% yield) as yellowish green oil. **HRMS (ESI**) for $C_{12}H_{13}ClNO_3^+$ $[(M+H)]^+$: calculated 254.0584, found 254.0592. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 7.29 – 7.26 (m, 1H), 7.23 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.03 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.02 – 6.99 (m, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.08 (d, *J* = 2.5 Hz, 1H), 2.99 (d, *J* = 2.5 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.4, 167.4, 143.6, 129.6, 127.7, 126.1, 124.8, 121.4, 62.4, 48.1, 40.9, 14.2.

6.15 Tert-butyl 2-formyl-1-(*o*-tolyl)aziridine-2-carboxylate (4h)

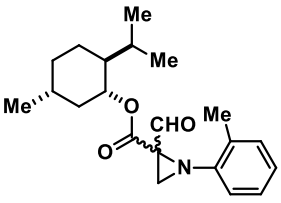


$C_{15}H_{19}NO_3$
M = 261.32 g/mol

Prepared according to the GP-1, using **1h** (24.0 mg, 0.2 mmol, 1.0 equiv), **2b** (170.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4h** (24.0 mg, 46% yield) as yellowish green oil. **HRMS (ESI**) for $C_{15}H_{20}NO_3^+$ $[(M+H)]^+$: calculated 262.1443, found 262.1415. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 7.17 – 7.13 (m, 1H), 7.11 –7.09 (m, 1H), 7.01 – 6.97 (m 1H), 6.87 (d, *J* = 7.7 Hz, 1H), 3.14 (d, *J* = 2.0 Hz, 1H), 2.92 (d, *J* = 2.1 Hz, 1H), 2.15 (s, 3H), 1.30 (s, 9H).**^{13}C**

NMR (101 MHz, $CDCl_3$) δ 194.3, 165.7, 145.2, 130.7, 130.6, 126.6, 124.1, 119.4, 83.5, 49.8, 39.0, 27.8, 18.0.

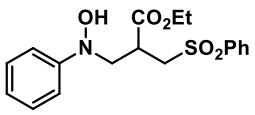
6.16 2-Isopropyl-5-methylcyclohexyl 2-formyl-1-(*o*-tolyl)aziridine-2-carboxylate (4i)



[dr = 1:1]
$C_{21}H_{29}NO_3$
M = 343.46 g/mol

Prepared according to the GP-1, using **1h** (24.0 mg, 0.2 mmol, 1.0 equiv), **2c** (216.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1 v/v) as eluent afforded the aziridine **4i** (23.0 mg, 33% yield) as yellowish green oil. **HRMS (ESI**): for $C_{21}H_{30}NO_3^+$ [$(M+H)^+$]: calculated 344.2226, found 344.2253. **^{1}H NMR (For a mixture of two diasteroisomers)** (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 9.97 (s, 1H), 7.18 – 7.13 (m, 2H), 7.09 (d, *J* = 7.5 Hz, 2H), 7.00 (t, *J* = 7.4 Hz, 2H), 6.88 (d, *J* = 7.9 Hz, 2H), 4.78 (dtd, *J* = 19.6, 11.0, 4.3 Hz, 2H), 3.14 (t, J = 2.4 Hz, 2H), 3.00 – 2.99 (m, 2H), 2.12 (d, *J* = 3.3 Hz, 6H), 1.88 – 1.74 (m, 4H), 1.70 – 1.64 (m, 4H), 1.48 – 1.31 (m, 4H), 1.07 – 0.96 (m, 4H), 0.89 (dd, *J* = 6.8, 1.9 Hz, 6H), 0.85 (dd, *J* = 6.8, 3.1 Hz, 6H), 0.82 – 0.75, (m, 2H), 0.72 (d, *J* = 8.2 Hz, 6H).**^{13}C NMR (For a mixture of two diasteroisomers)** (101 MHz, $CDCl_3$) δ 193.2, 193.1, 166.8, 166.7, 144.9, 144.8, 130.6 (2C), 130.4, 130.3, 126.7 (2C), 124.3, 124.2, 119.4 (2C), 76.6, 76.5, 49.5, 49.0, 46.9, 46.8, 40.6, 40.2, 39.6, 39.2, 34.2, 34.1, 31.5, 31.4, 26.3, 25.9, 23.1 (2C), 22.1, 22.0, 21.0, 20.9, 18.1 (2C), 16.1, 16.0.

6.17 Ethyl 3-(hydroxy(phenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16a)

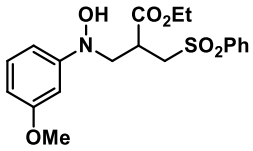


$C_{18}H_{21}NO_5S$
M = 363.43 g/mol

Prepared according to the GP-2, using **1a** (21.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded

the β-amino acid derivative **16a** (57.0 mg, 78% yield) as yellow oil. **HRMS (ESI**): for $C_{18}H_{22}NO_5S^+$ [$(M+H)^+$]: calculated 364.1219, found 364.1284. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 – 7.92 (m, 2H), 7.69 – 7.65 (m, 1H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.29 – 7.25 (m, 2H), 7.12 – 7.10 (m, 2H), 7.00 (t, *J* = 7.3 Hz, 1H), 6.00 (s, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 3.80 (dd, *J* = 14.3, 6.9 Hz, 1H), 3.61 – 3.54 (m, 2H), 3.51 – 3.45 (m, 1H), 3.41 (dd, *J* = 12.2, 7.1 Hz, 1H), 1.21 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.3, 152.3, 138.9, 134.1, 129.5, 128.9, 128.3, 123.0, 116.8, 61.8, 61.1, 54.9, 39.0, 14.1.

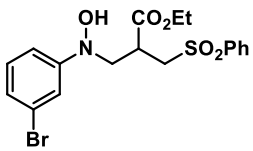
6.18 Ethyl 3-(hydroxy(3-methoxyphenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16b)



$C_{19}H_{23}NO_6S$
M = 393.45 g/mol

Prepared according to the GP-2, using **1b** (27.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16b** (63.0 mg, 80% yield) as yellow oil. **HRMS (ESI**): for $C_{19}H_{24}NO_6S^+$ [$(M+H)^+$]: calculated 394.1324, found 394.1316. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 – 7.92 (m, 2H), 7.69 – 7.65 (m, 1H), 7.57 (t, *J* = 7.7 Hz, 2H), 7.16 (t, *J* = 8.2 Hz, 1H), 6.74 (t, *J* = 2.2 Hz, 1H), 6.63 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.54 (dd, *J* = 8.1, 2.3 Hz, 1H), 6.02 (s, 1H), 4.06 (q, *J* = 7.1 Hz, 2H), 3.85 – 3.76 (m, 4H), 3.59 (t, *J* = 4.4 Hz, 1H), 3.55 (dd, *J* = 4.5, 1.9 Hz, 1H), 3.50 – 3.39 (m, 2H), 1.21 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.3, 160.3, 153.9, 138.9, 134.1, 129.7, 129.5, 128.3, 109.2, 108.3, 102.8, 61.8, 61.0, 55.4, 54.9, 39.0, 14.1.

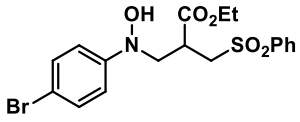
6.19 Ethyl 3-((3-bromophenyl)(hydroxy)amino)-2-((phenylsulfonyl)methyl)propanoate (16c)



$C_{18}H_{20}BrNO_5S$
M = 442.32 g/mol

Prepared according to the GP-2, using **1m** (37.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16c** (55.0 mg, 62% yield) as yellow oil. **HRMS (ESI**): for $C_{18}H_{21}BrNO_5S^+$ [$(M+H)^+$]: calculated 442.0324, found 442.0322. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.71 –7.66 (m,1H), 7.61 –7.57 (m, 2H), 7.31 – 7.30 (m, 1H), 7.15 – 7.10 (m, 2H), 7.01 – 6.98 (m, 1H), 6.08 (s, 1H), 4.08 (q, *J* = 7.1 Hz, 2H), 3.80 (dd, *J* = 14.1, 6.3 Hz, 1H), 3.60 – 3.46 (m, 3H), 3.41 (dd, *J* = 12.3, 7.1 Hz, 1H), 1.22 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.1, 153.6, 138.9, 134.3, 130.3, 129.6, 128.3, 125.7, 122.9, 119.7, 115.3, 62.0, 60.7, 54.9, 38.8, 14.2.

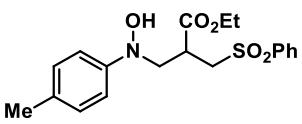
6.20 Ethyl 3-((4-bromophenyl)(hydroxy)amino)-2-((phenylsulfonyl)methyl)propanoate (16d)



$C_{18}H_{20}BrNO_5S$
M = 442.32 g/mol

Prepared according to the GP-2, using **1e** (37.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16d** (69.0 mg, 78% yield) as yellow oil. **HRMS (ESI**): for $C_{18}H_{21}BrNO_5S^+$ [$(M+H)^+$]: calculated 442.0324, found 442.0311. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.4, 1.1 Hz, 2H), 7.71 – 7.67 (m, 1H), 7.61 – 7.57 (m, 2H), 7.40 – 7.36 (m, 2H), 7.02 – 6.98 (m, 2H), 5.92 (s, 1H), 4.08 (q, *J* = 7.1 Hz, 2H), 3.79 (dd, *J* = 14.2, 6.4 Hz, 1H), 3.58 – 3.51 (m, 2H), 3.48 (ddd, *J* = 12.1, 6.4, 4.5 Hz, 1H), 3.39 (dd, *J* = 12.4, 7.2 Hz, 1H), 1.21 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.1, 151.4, 138.9, 134.3, 131.9, 129.6, 128.3, 118.6, 115.6, 61.9, 60.9, 54.9, 38.8, 14.2.

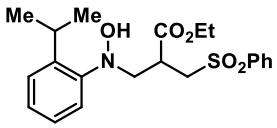
6.21 Ethyl 3-(hydroxy(*p*-tolyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16e)



$C_{19}H_{23}NO_5S$
M = 377.45 g/mol

Prepared according to the GP-2, using **1c** (24.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16e** (49.0 mg, 65% yield) as yellow oil **HRMS (ESI**): for $C_{19}H_{24}NO_5S^+$ [$(M+H)^+$]: calculated 378.1375, found 378.1372. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 2H), 7.70 – 7.66 (m, 1H), 7.61 – 7.56 (m, 2H), 7.08 (t, *J* = 8.9 Hz, 2H), 7.03 – 7.00 (m, 2H), 5.69 (s, 1H), 4.07 (q, *J* = 7.5 Hz, 2H), 3.81 (dd, *J* = 14.3, 7.1 Hz, 1H), 3.59 (dd, *J* = 14.4, 3.9 Hz, 1H), 3.52 – 3.44 (m, 2H), 3.37 – 3.30 (m, 1H), 2.29 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.9, 140.6, 134.1, 130.0, 129.5, 129.2, 129.0, 128.4, 116.7, 60.5, 54.9, 53.9, 39.1, 20.8, 14.2.

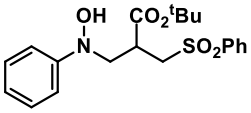
6.22 Ethyl 3-(hydroxy(2-isopropylphenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16f)



$C_{21}H_{27}NO_5S$
M = 405.51 g/mol

Prepared according to the GP-2, using **1k** (30.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16f** (80.0 mg, 99% yield) as white solid. **Melting Point:** 108-109 ^{o}C. **HRMS (ESI**): for $C_{21}H_{28}NO_5S^+$ [$(M+H)^+$]: calculated 406.1688, found 406.1697. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 – 7.95 (m, 2H), 7.71 – 7.67 (m, 1H), 7.62 – 7.58 (m, 2H), 7.50 – 7.47 (m, 1H), 7.26 – 7.22 (m, 1H), 7.21 – 7.18 (m, 2H), 5.72 (s, 1H), 4.06 (qd, *J* = 7.1, 2.9 Hz, 2H), 3.84 (dd, *J* = 14.2, 8.2 Hz, 1H), 3.58 – 3.48 (m, 2H), 3.37 – 3.24 (m, 2H), 3.05 (dd, *J* = 12.4, 7.8 Hz, 1H), 1.25 – 1.16 (m, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.1, 149.0, 142.5, 138.8, 134.1, 129.4, 128.4, 127.0, 126.7, 126.0, 121.2, 62.1, 61.7, 55.3, 39.5, 26.8, 23.8, 14.4.

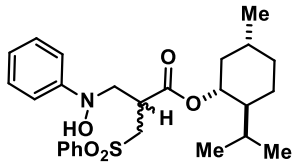
6.23 Tert-butyl 3-(hydroxy(phenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16g)



$C_{20}H_{25}NO_5S$
M = 391.48 g/mol

Prepared according to the GP-2, using **1a** (21.0 mg, 0.2 mmol, 1.0 equiv), **2b** (170.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16g** (50.0 mg, 64% yield) as white solid. **Melting Point:** 95-96 ^{o}C. **HRMS (ESI**): for $C_{20}H_{26}NO_5S^+$ [$(M+H)^+$]: calculated 392.1532, found 392.1527. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.8 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 7.00 (t, *J* = 7.3 Hz, 1H), 6.08 – 6.06, (m, 1H), 3.80 (dd, *J* = 14.5, 6.2 Hz, 1H), 3.58 – 3.49 (m, 2H), 3.38 (q, *J* = 7.3 Hz, 2H), 1.38 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.2, 152.5, 139.0, 134.0, 129.5, 128.9, 128.3, 122.9, 116.8, 82.3, 61.2, 54.8, 39.8, 28.0.

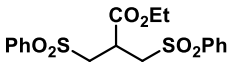
6.24 2-Isopropyl-5-methylcyclohexyl 3-(hydroxy(phenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16h)



[dr = 1:1]
$C_{26}H_{35}NO_5S$
M = 473.62 g/mol

Prepared according to the GP-2, using **1a** (21.0 mg, 0.2 mmol, 1.0 equiv), **2c** (216.0 mg, 0.6 mmol, 3.0 equiv) and HE (76.0 mg, 0.3 mmol, 1.5 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the β-amino acid derivative **16h** (63.0 mg, 67% yield, dr = 1:1) as pale yellow oil. **HRMS (ESI**): for $C_{26}H_{36}NO_5S^+$ [$(M+H)^+$]: calculated 474.2314, found 474.2291. **^{1}H NMR (For a mixture of two diasteroisomers)** (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 4H), 7.70 – 7.66 (m, 2H), 7.60 – 7.56 (m, 4H), 7.32 – 7.27 (m, 4H), 7.14 – 7.10 (m, 4H), 7.03 – 6.99 (m, 2H), 6.02 (s, 1H), 5.94 (s, 1H), 4.69 – 4.59 (m, 2H), 3.90 – 3.82 (m, 2H), 3.64 – 3.59 (m, 2H), 3.58 – 3.50 (m, 2H), 3.49 – 3.42 (m, 2H), 3.41 – 3.35 (m, 2H) 1.91 – 1.66 (m, 8H), 1.48 – 1.30 (m, 4H), 1.06 – 0.94 (m, 2H), 0.91 – 0.82 (m, 16H), 0.66 (dd, *J* = 6.9, 4.6 Hz, 6H). **^{13}C NMR (For a mixture of two diasteroisomers)** (101 MHz, $CDCl_3$) δ 172.0, 171.7, 152.3 (2C), 138.9, 134.1 (2C), 129.5 (2C), 129.1 (2C), 128.9, 128.3, 128.2, 122.9, 116.8 (2C), 116.2, 76.1, 75.9, 60.9, 60.5, 54.9, 54.6, 53.8, 47.2, 46.9 (2C), 40.6, 39.3, 39.0, 34.3, 34.2, 31.4, 31.3, 26.0, 25.9, 23.3, 23.0, 22.1, 21.0, 20.9, 16.2, 15.8.

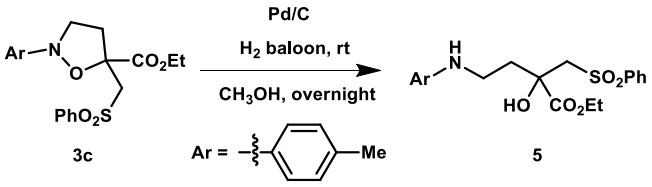
6.25 Ethyl 3-(phenylsulfonyl)-2-((phenylsulfonyl)methyl)propanoate (15)



$C_{18}H_{20}O_6S_2$
M = 396.48 g/mol

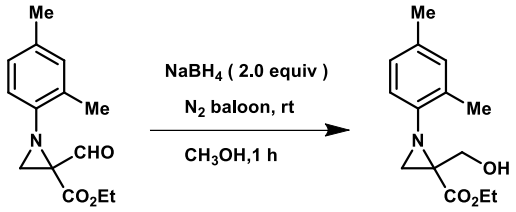
Product **15** was obtained as a side product in GP-1 study. **HRMS (ESI)**: for $C_{18}H_{21}O_6S_2^+$ [$(M+H)^+$]: calculated 397.0780, found 397.0786. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 – 7.85 (m, 4H), 7.72 – 7.68 (m, 2H), 7.61 – 7.56 (m, 4H), 4.09 (q, *J* = 7.3 Hz, 2H), 3.64 (dd, *J* = 6.4, 0.6 Hz, 4H), 3.30 (p, *J* = 6.2 Hz, 1H), 1.24 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.8, 138.7, 134.4, 129.6, 128.3, 62.6, 55.4, 35.8, 14.0.

7. General Procedure for the N-O bond cleavage of isoxazolidine derivative (GP-3)



10% Pd/C was added to a solution of isoxazolidine **3c** in CH_3OH at room temperature under an atmosphere of hydrogen by means of a H_2 balloon. After stirring overnight, the mixture was filtered through celite. The crude reaction mixture was concentrated directly and then it was purified by flash column chromatography [S12]

8. General Procedure for the reduction of aziridine derivative (GP-4)

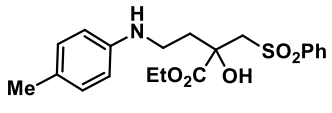


4d **6**

To a stirred mixture of aldehyde **4d** (1.0 equiv) in CH_3OH 0.2 (M) at room temperature was added $NaBH_4$ (2.0 equiv). After 1 h the reaction was quenched by addition of sat. aq. NH_4Cl and the mixture was extracted three times with CH_2Cl_2, dried over Na_2SO_4. The crude reaction mixture was concentrated and then it was purified by flash column chromatography.[S13]

9. Experimental Details for the Synthesized Compounds obtained from (GP-3) and (GP-4)

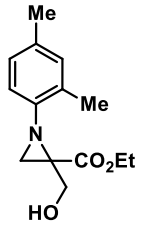
9.1 Ethyl 2-hydroxy-2-((phenylsulfonyl)methyl)-4-(*p*-tolylamino)butanoate (5)



$C_{20}H_{25}NO_5S$
M= 391.48 g/mol

Prepared according to the GP-3, using Pd/C (16.0 mg, 0.005 mmol, 0.1 equiv),and isoxazolidone **3c** (15.0 mg, 0.05 mmol, 1.0 equiv) in CH_3OH (2.5 mL). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the *α*-hydroxy-*γ*-amino acid derivative **5** (14.0 mg, 93% yield) as yellowish orange liquid. **HRMS (ESI**): for $C_{20}H_{26}NO_5S^+$ [$(M+H)^+$]: calculated 392.1532, found 392.1527. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 – 7.88 (m, 2H), 7.67 – 7.63 (m, 1H), 7.58 – 7.53 (m, 2H), 6.97 (d, *J* = 8.1 Hz, 2H), 6.51 (d, *J* = 8.3 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.72 (d, *J* = 14.6 Hz, 1H), 3.60 (d, *J* = 14.6 Hz, 1H), 3.20 (t, *J* = 6.5 Hz, 2H), 2.22 (s, 3H), 2.11 (dt, *J* = 13.8, 6.8 Hz, 1H), 1.98 – 1.91 (m, 1H), 1.66 (s, 1H), 1.24 (t, *J* = 7.2 Hz, 3H), 0.90 – 0.86 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.4, 144.5, 140.7, 134.0, 130.4, 129.9, 129.3, 128.2, 113.7, 74.4, 63.6, 63.2, 39.5, 38.2, 20.5, 14.1.

9.2 Ethyl 1-(2,4-dimethylphenyl)-2-(hydroxymethyl)aziridine-2-carboxylate (6)



$C_{14}H_{19}NO_3$
M= 249.31 g/mol

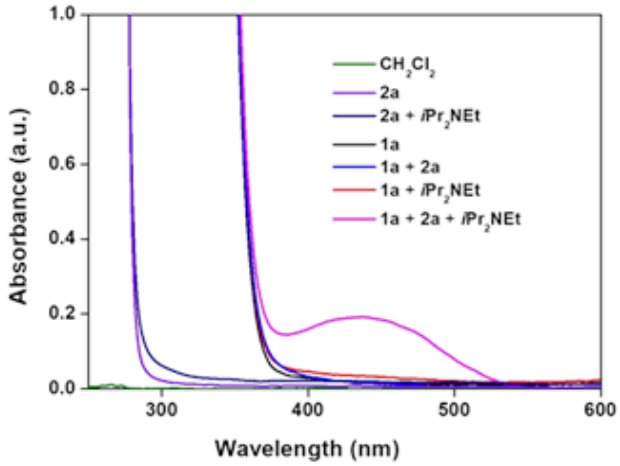
Prepared according to the GP-4, using aldehyde **4d** (25.0 mg, 0.1 mmol, 1.0 equiv) and $NaBH_4$ (7.6 mg, 0.2 mmol, 2.0 equiv). in CH_3OH 0.2 (M). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (10:1 v/v) as eluent afforded **6** (23.0 mg, 92%) as white foam. **HRMS (ESI**): for $C_{14}H_{20}NO_3^+$ [$(M+H)^+$]: calculated 250.1443, found 250.1439 **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.93 – 6.90 (m, 2H), 6.72 (d, *J* = 7.9 Hz, 1H), 4.10 –3.90 (m, 4H), 2.83 (d, *J* = 1.2 Hz, 1H), 2.59 (d, *J* = 1.2 Hz, 1H), 2.38 (dd, *J* =

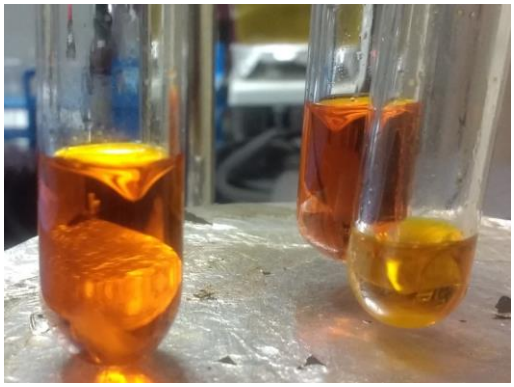
8.6, 4.9 Hz, 1H), 2.25 (s, 3H), 2.17 (s, 3H), 1.02 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.7, 143.5, 132.7, 131.4, 130.3, 127.0, 119.4, 61.5, 61.1, 45.7, 34.9, 20.8, 18.0, 13.9.

10. Mechanistic Evidences

10.1 UV-Vis data

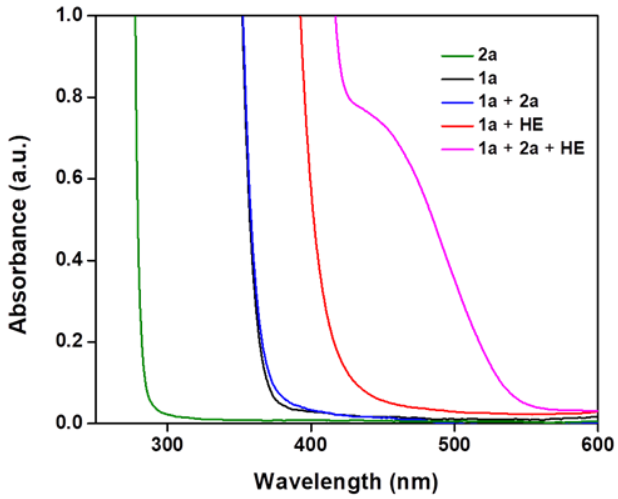
UV data suggests the electron transfer process from *i*Pr_2NEt to the activated complex of nitrosoarene and allylsulfone. Figure S1 represents the generation of a Charge Transfer (CT) band around 550 nm regions in the presence of *i*Pr_2NEt. Similarly in the presence of HE such CT band was also observed, that indicate the SET from HE to the activated complex that is shown in figure S2.





Solution of 1a+2a+*i*Pr_2NEt at the begining (orange colour) and after 16 h (yellow colour)

Figure S1: UV-Vis spectra of 0.1 (M) nitrosobenzene **1a** (0.1 mmol, 1.0 equiv) in freshly distilled CH_2Cl_2 in presence of allylsulfone **2a** (0.3 mmol, 3.0 equiv) and *i*Pr_2NEt (0.2 mmol, 2.0 equiv).



Solution of 1a+2a+HE at the begining (yellow colour) and after 16 h (yellow colour)

Figure S2: UV-Vis spectra of 0.1 (M) nitrosobenzene **1a** (0.1 mmol, 1.0 equiv) in freshly distilled CH_2Cl_2 in presence of allylsulfone **2a** (0.3 mmol, 3.0 equiv) and HE (0.15 mmol, 1.5 equiv)

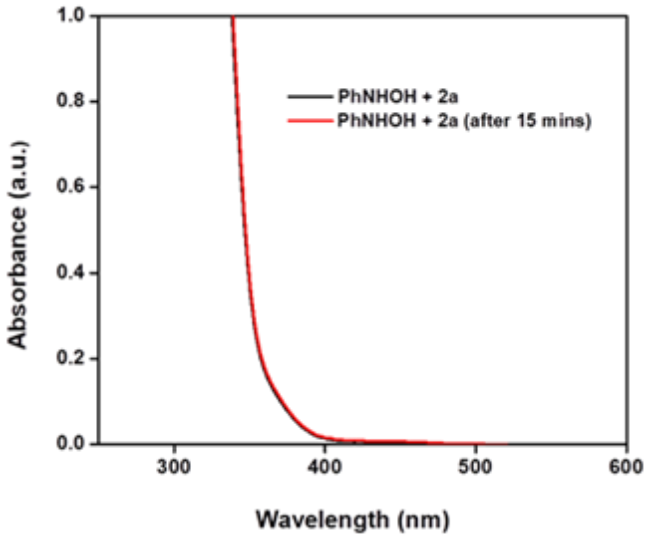


Figure S3 UV-Vis spectra of 0.1 (M) phenylhydroxylamine (0.1 mmol, 1.0 equiv) in freshly distilled CH_2Cl_2 in presence of allylsulfone **2a** (0.3 mmol, 3.0 equiv).

10.2 ^{1}H NMR experiment

The iminium ion side product released in the reaction mixture after SET from *i*Pr_2NEt to the activated adduct was further confirmed by the ^{1}H NMR analysis of the crude reaction mixture.[S14]

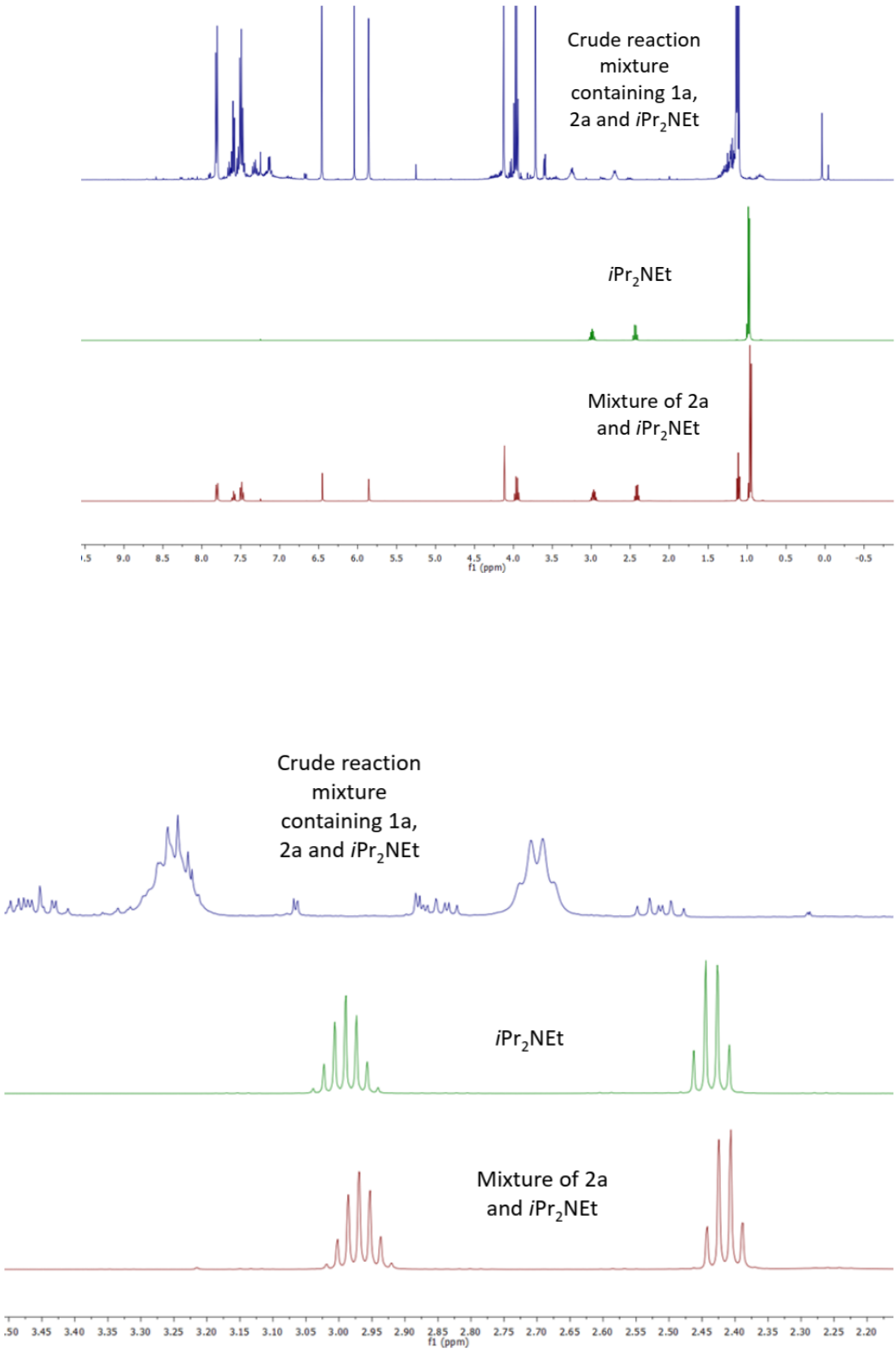


Figure S4 ^{1}H NMR spectra of a mixture of allylsulfone (**2a**, 3.0 equiv) and *i*Pr$_2$NEt (2.0 equiv) (red colour); *i*Pr$_2$NEt (green colour) and a crude reaction mixture of nitrosobenzene (**1a**, 1.0 equiv), *i*Pr$_2$NEt (2.0 equiv) and allylsulfone (**2a**, 3.0 equiv) (blue colour) in $CDCl_3$ after 16 h.

While the allylsulfone signals remain unchanged, the signals of *i*Pr_2NEt (2.40 and 2.98 ppm) shows a broadening, which indicates the formation of radicals or ionic species in the reaction mixture. Downfield shift of signals also suggest the formation of iminium ion.

10.3 Cyclic voltammetric study

The measurements were carried out as follows: a 0.1 (M) solution of tetabutylammonium hexafluorophosphate in acetonitrile was added to the measuring cell and the solution was degassed by argon purge for 5 min. After recording the baseline the electroactive compound was added 0.01 (M) and the solution was again degassed with a stream of argon for 5 min. The cyclic voltammogram was recorded with one to two scans.

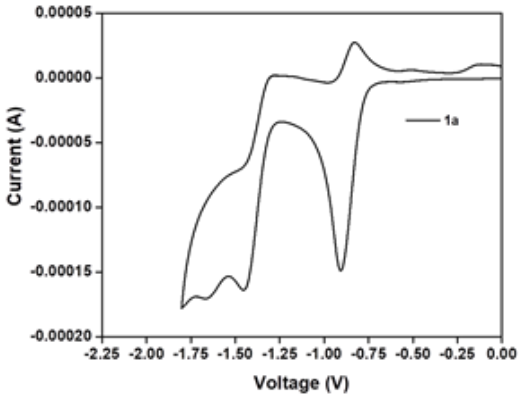


Figure S5a

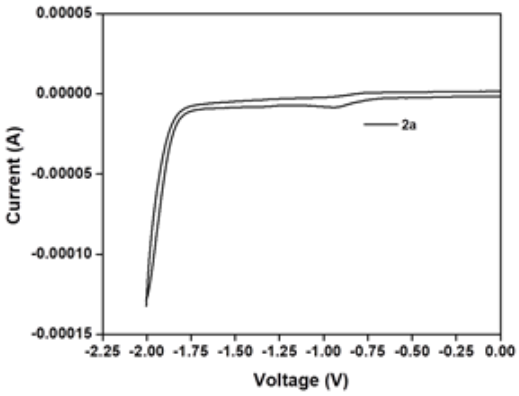
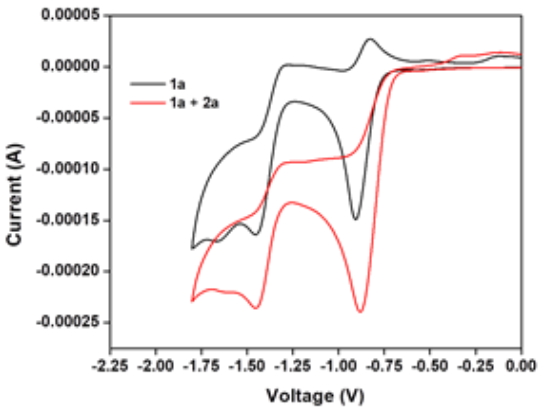


Figure S5b

Figure S5 Cyclic voltammograms of 0.01 (M) solution of nitrosobenzene **1a**, (figure **S5a**) and 0.01 (M) solution of allylsulfone **2a,** (figure **S5b**) under argon. The measurements were performed with a scan rate of 50 mV/s and with tetabutylammonium hexafluorophosphate 0.1 (M) as supporting electrolyte.



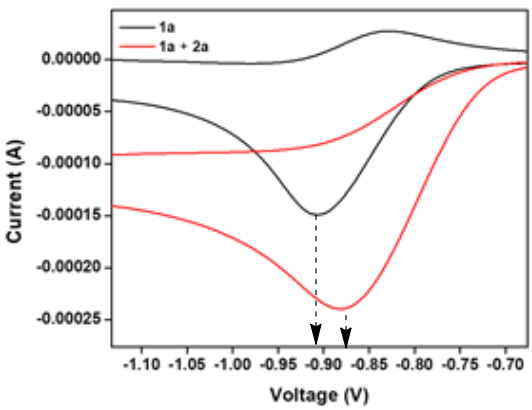


Figure S6 Cyclic voltammogram of nitrosobenzene **1a**, (black colour) and mixture of **1a** (1.0 equiv), and allylsulfone **2a** (3.0 equiv) (red colour) under argon. The peak that corresponds to the reduction of nitrosobenzene **1a** (highlighted by zoomed figure on right side) is shifted to lower potential side (from -0.91 V to -0.88 V) upon addition of allylsulfone. The measurement was performed with a scan rate of 50 mV/s and with tetabutylammonium hexafluorophosphate 0.1 (M) as supporting electrolyte.

10.4 Characterization of intermediates by D-Mass and GC-MS analysis

10.4.1 Characterization of intermediate **10** by D-Mass analysis (figure S7a) and GC-MS analysis (figure S7b).

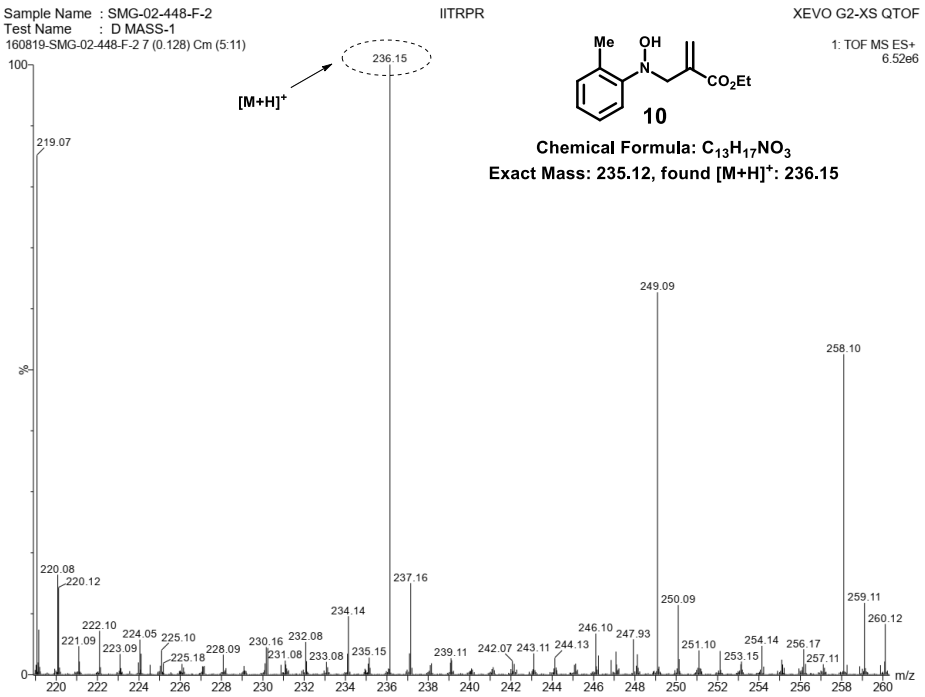


Figure S7a D-Mass data of **10**

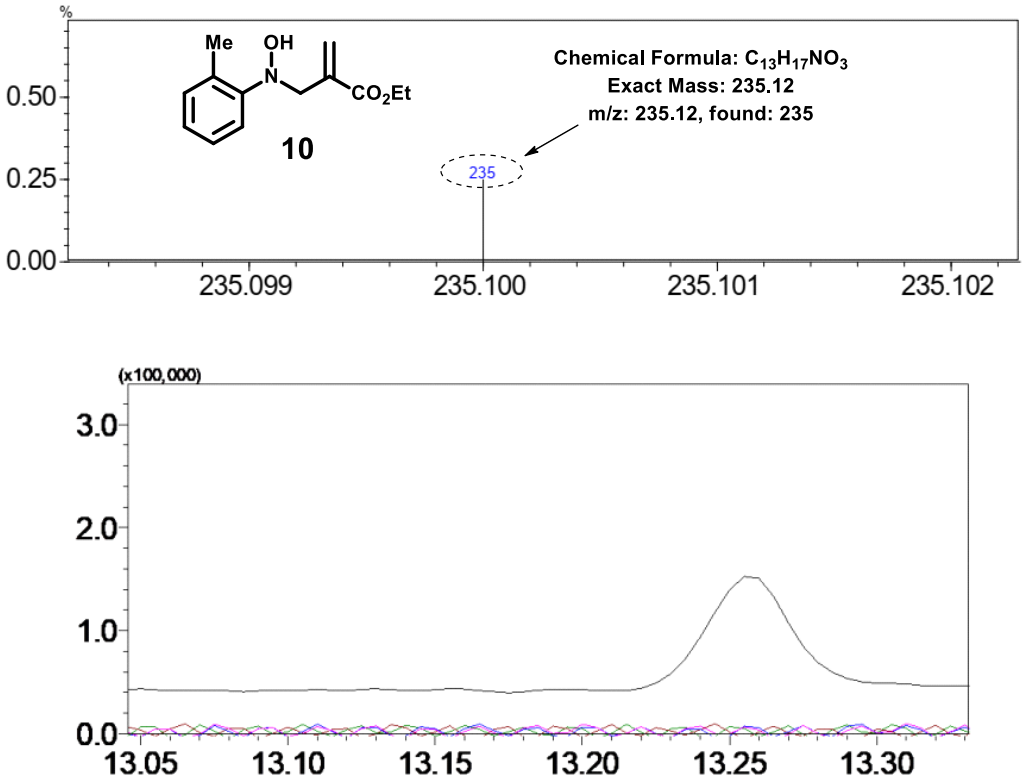


Figure S7b GC-MS data of **10**

10.4.2 Characterization of *N*-(*o*-tolyl)hydroxylamine formed as the side product in the final step of aziridine derivative (**4c**) formation was also done by D-Mass (figure S7c) and GC-MS analysis (figure S7d)

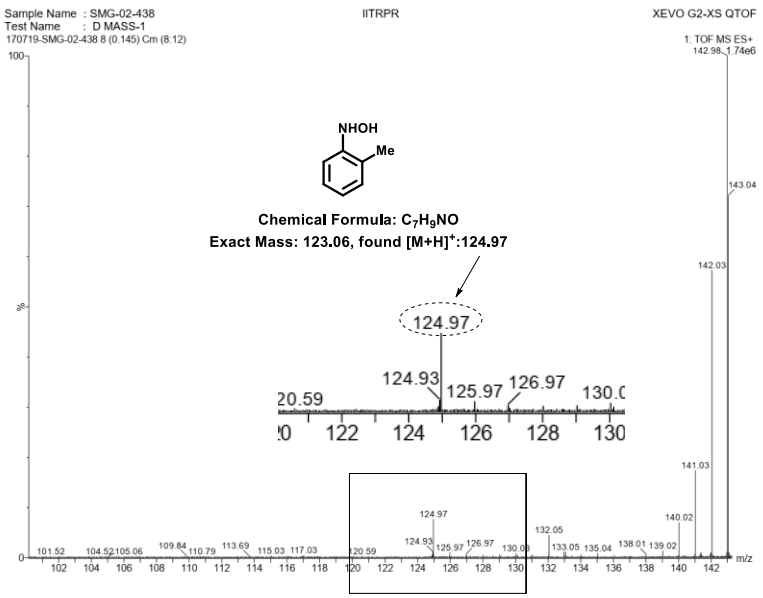


Figure S7c D-Mass data of *N*-(*o*-tolyl)hydroxylamine

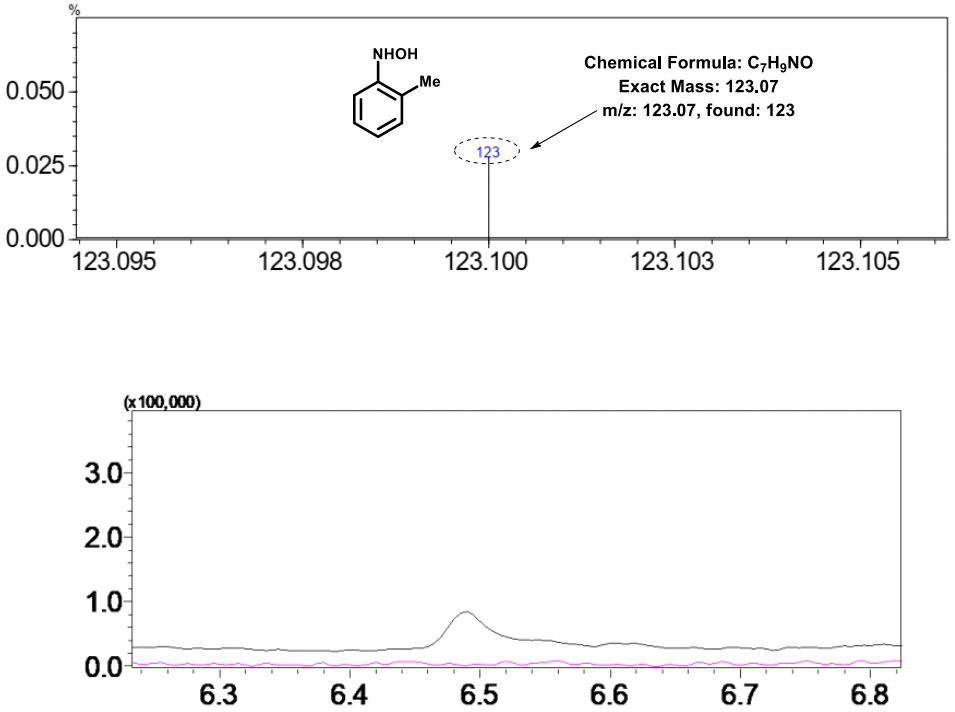


Figure S7d GC-MS data of *N*-(*o*-tolyl)hydroxylamine

10.4.3 Characterization of intermediate **9**˙ by GC-MS analysis (figure S7e).

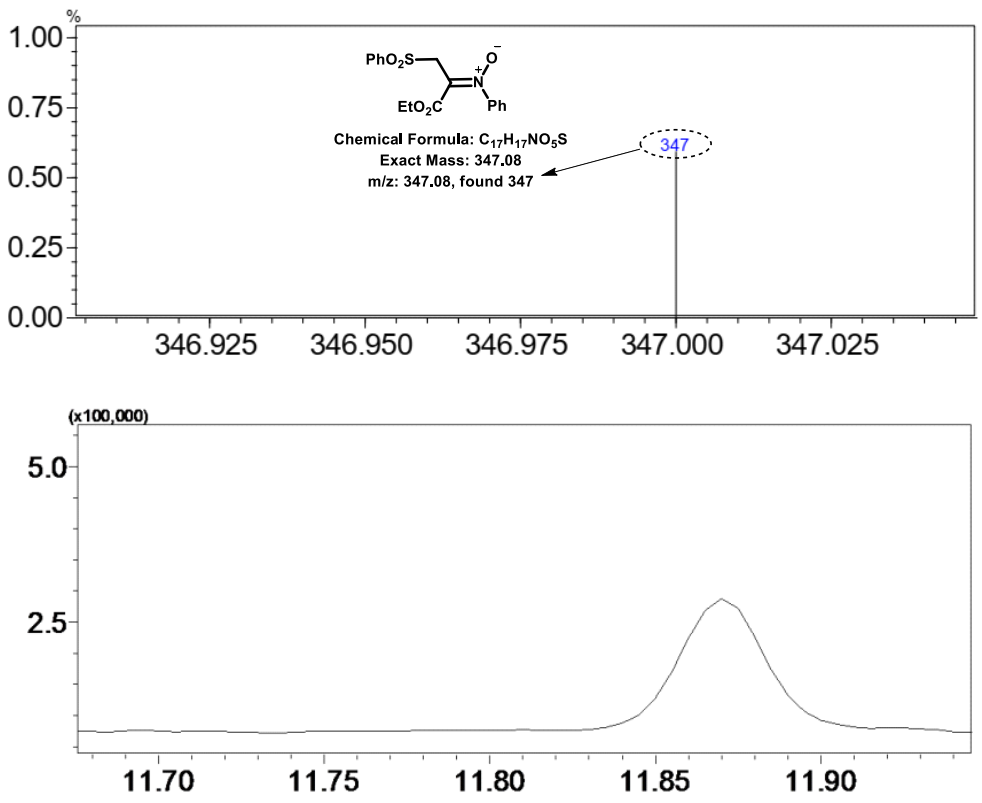
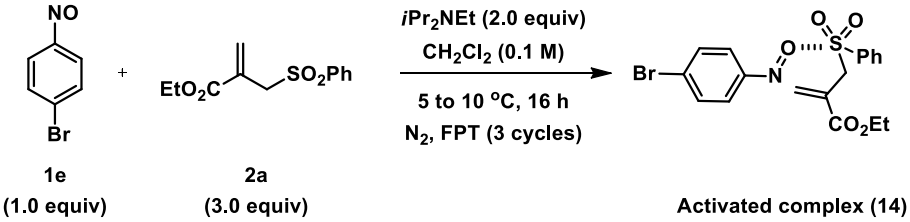


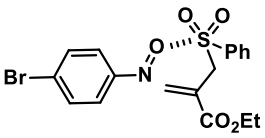
Figure S7e GC-MS data of **9**˙

11. General Procedure for the synthesis of activated complex (GP-5)



An oven-dried schlenk tube was charged with nitrosoarene **1e** (1.0 equiv) and *i*Pr_2NEt (2.0 equiv) then evacuated and followed by back filled with nitrogen three times. Freshly distilled 0.1 (M) CH_2Cl_2 (with respect to **1e**) and allylsulfone **2a** were then added via a syringe and the schlenk tube was capped with a stopper.The reaction mixture was degassed via freeze-pump-thaw cycle three times. Finally the reaction mixture was purged with nitrogen for 5 minutes. After that reaction mixture was stirred for 16 h at 5 to 10 ^{o}C. The reaction mixture was concentrated directly and then the crude reaction mixture was purified by either flash column chromatography or preparative thin layer chromatography.

11.1 Experimental details of activated complex ethyl 2-((phenylsulfonyl)methyl)acrylate compound with 1-bromo-4-nitrosobenzene (1:1) obtained from (GP-5)

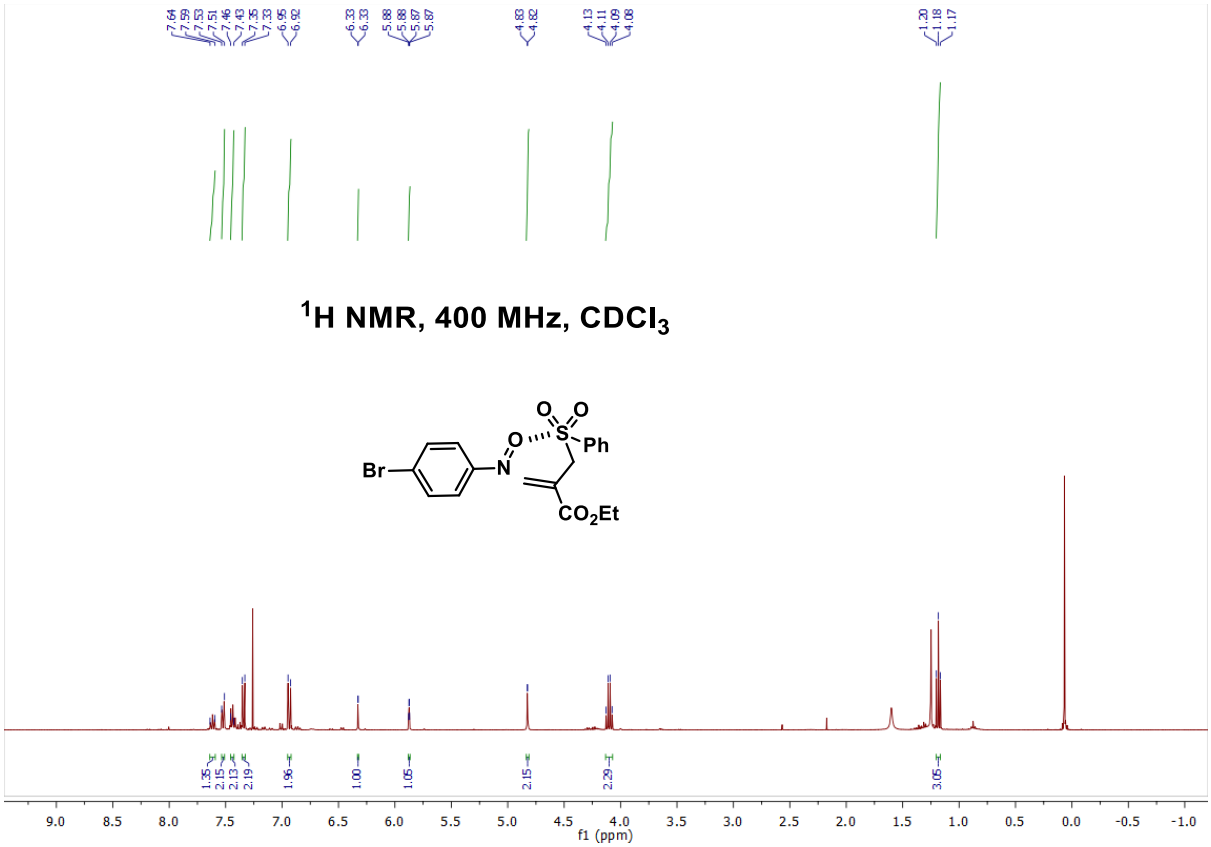


$C_{18}H_{18}BrNO_5S$
M = 440.31 g/mol

Prepared according to the GP-5, using **1e** (37.0 mg, 0.2 mmol, 1.0 equiv), **2a** (152.0 mg, 0.6 mmol, 3.0 equiv) and *i*Pr_2NEt (70.0 µL, 0.4 mmol, 2.0 equiv). Purification by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1 v/v) as eluent afforded the activated complex **14** as greenish yellow oil. **HRMS (ESI)**: for $C_{18}H_{19}BrNO_5S^+$ [$(M+H)^+$]: calculated 440.0167, found 440.0157. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.64 – 7.59 (m, 1H), 7.53 – 7.51 (m, 2H), 7.46 – 7.43 (m, 2H), 7.34 (d, *J* = 9.0 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 6.33 (d, *J* = 1.3 Hz, 1H), 5.87 (q, *J* = 1.1 Hz, 1H), 4.83 (d, *J* = 1.0 Hz, 2H), 4.10 (q, *J* = 7.1 Hz 2H), 1.18 (t, *J* = 7.1 Hz, 3H).

Note: Activated complex **14** is found to be highly unstable, it gets decomposed very quickly.

Ethyl 2-((phenylsulfonyl)methyl)acrylate compound with 1-bromo-4-nitrosobenzene (1:1) (activated complex, 14)



11.2 Experimental evidence for the formation of activated complex (14) of nitrosoarene and allylsulfone.

HRMS data

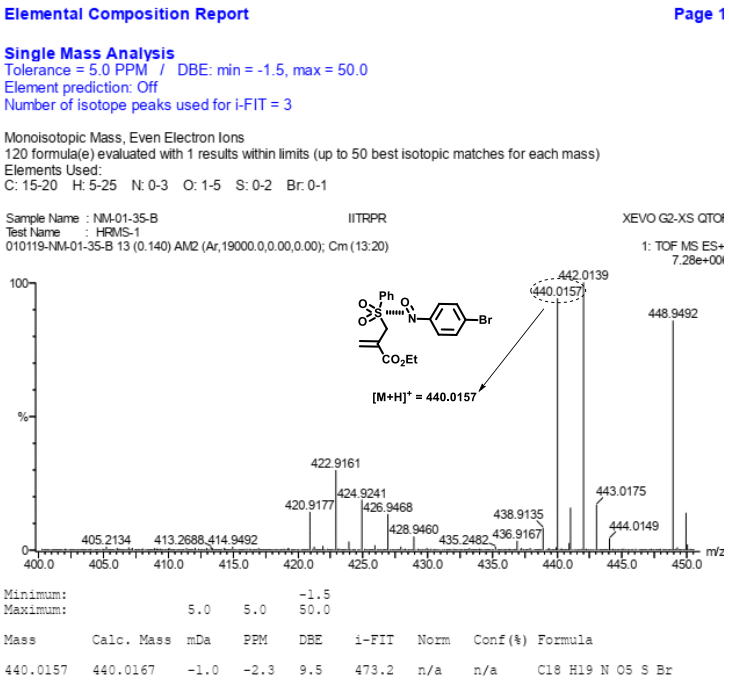


Figure S8 HRMS data of activated complex (**14**)

^{1}H NMR data

In the figure **S9a** (green colour) is used for the allylsulfone (**2a**) and (pink colour) is used for the nitrosoarene (**1e**) allylsulfone activated complex (**14**). In the complex, the chemical shift of the protons of allylsulfone are different from its parent molecule. While the aromatic and olefinic protons show the upfield shift, on other hand the aliphatic protons are shifted towards the downfield region. This is supposed to be due to the SET from *i*Pr$_2$NEt to the complex which changes the electon density, and that leads to a change in chemical shift. It is worth mentioning that in the absence of *i*Pr$_2$NEt such complex formation was not observed.

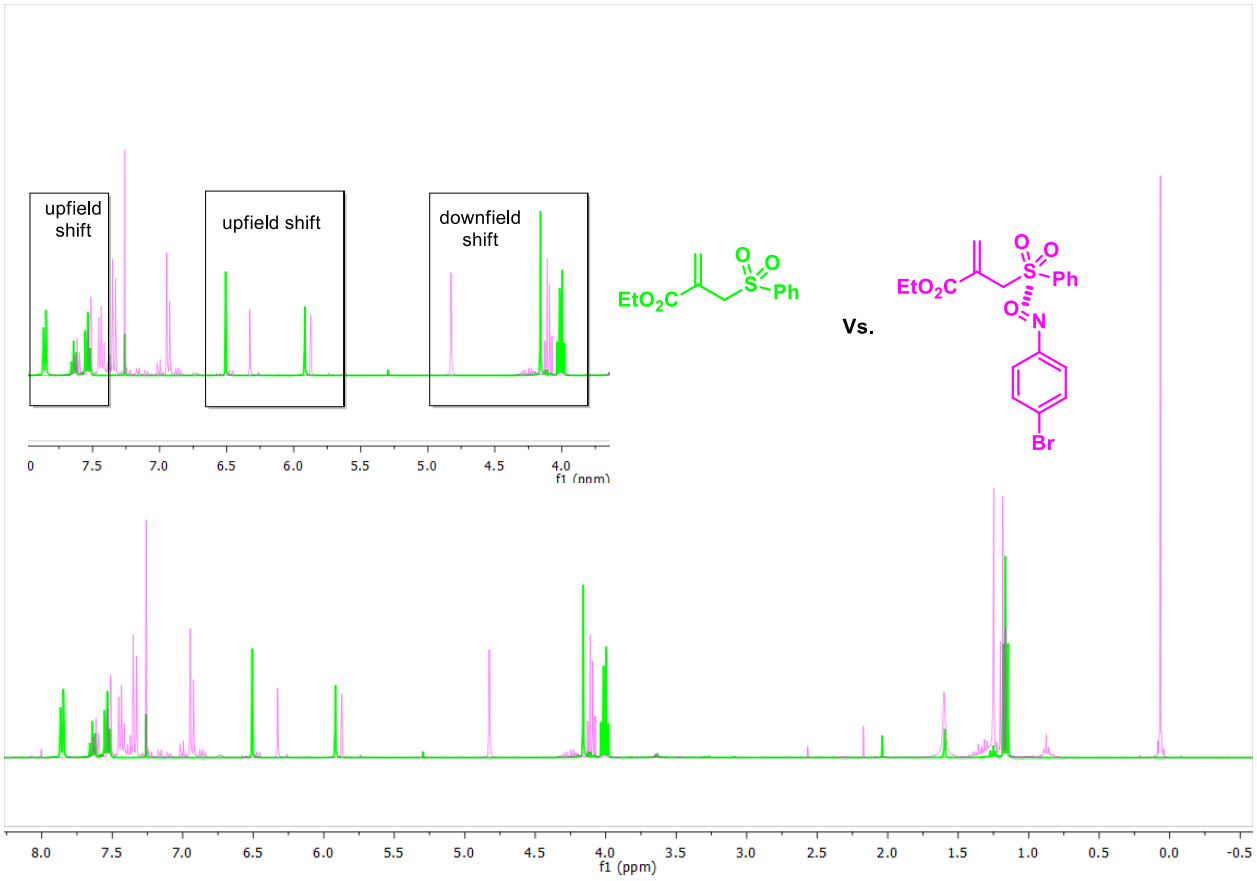


Figure S9a ^{1}H NMR data for activated complex.

In figure **S9b** we have shown the comparison of chemical shifts of **2a** and **1e** with their activated adduct (**14**).The aromatic protons of **1e** show an upfield shift in the complex (**14**) with respect to its parent compound (**1e**). This indicates an increase in electron density in the aromatic ring of **1e**. Therefore we proposed that *i*Pr$_2$NEt transfer an electron to the **1e** of **14**. Where **14** plays a role to activate **1e** in such a way that SET from *i*Pr$_2$NEt becomes easier.

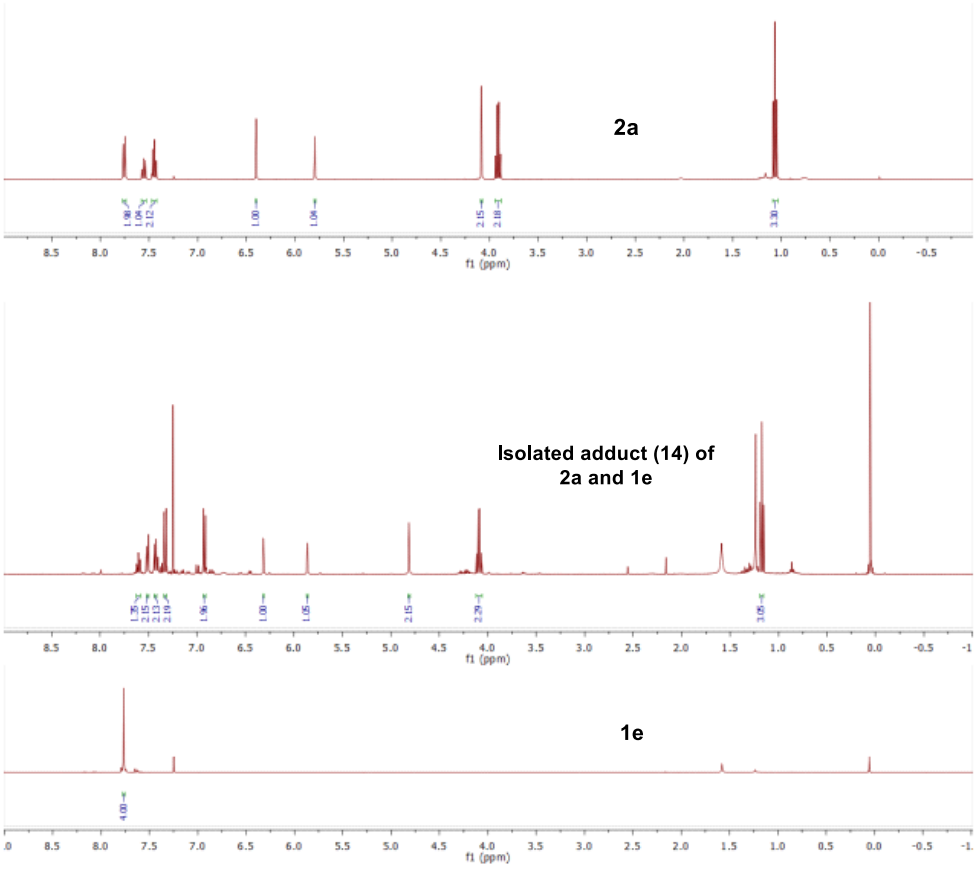


Figure S9b ^{1}H NMR data for activated complex stacked with both **2a** and **1e**.

12. References

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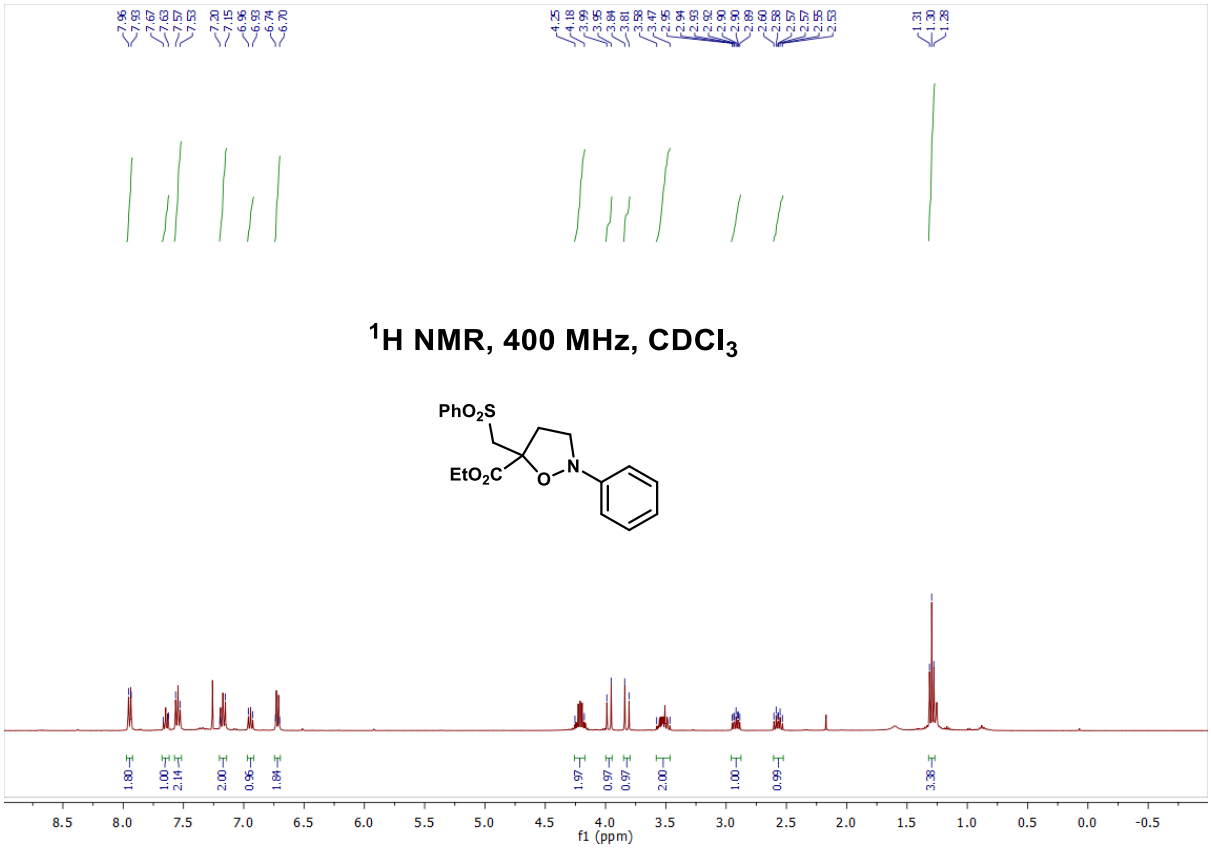
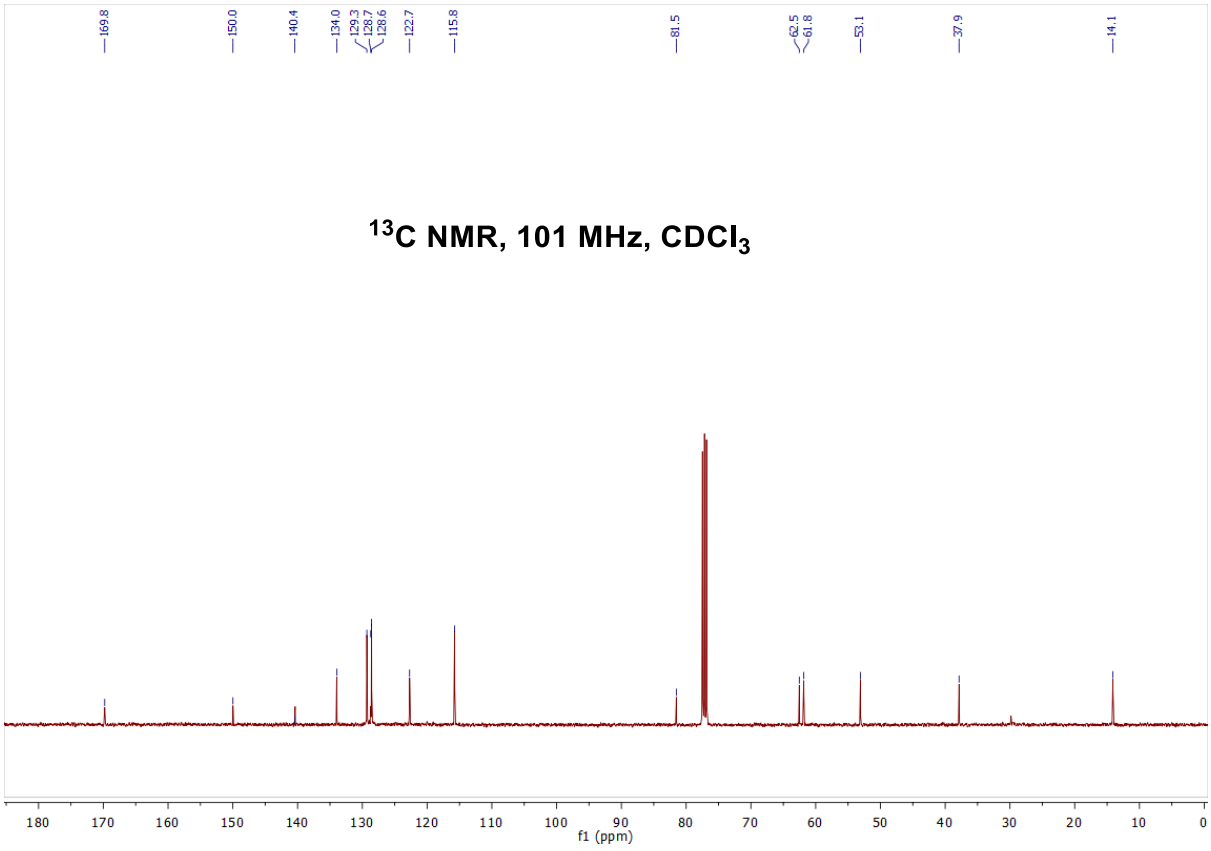
13. Experimental NMR Data

Ethyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3a)

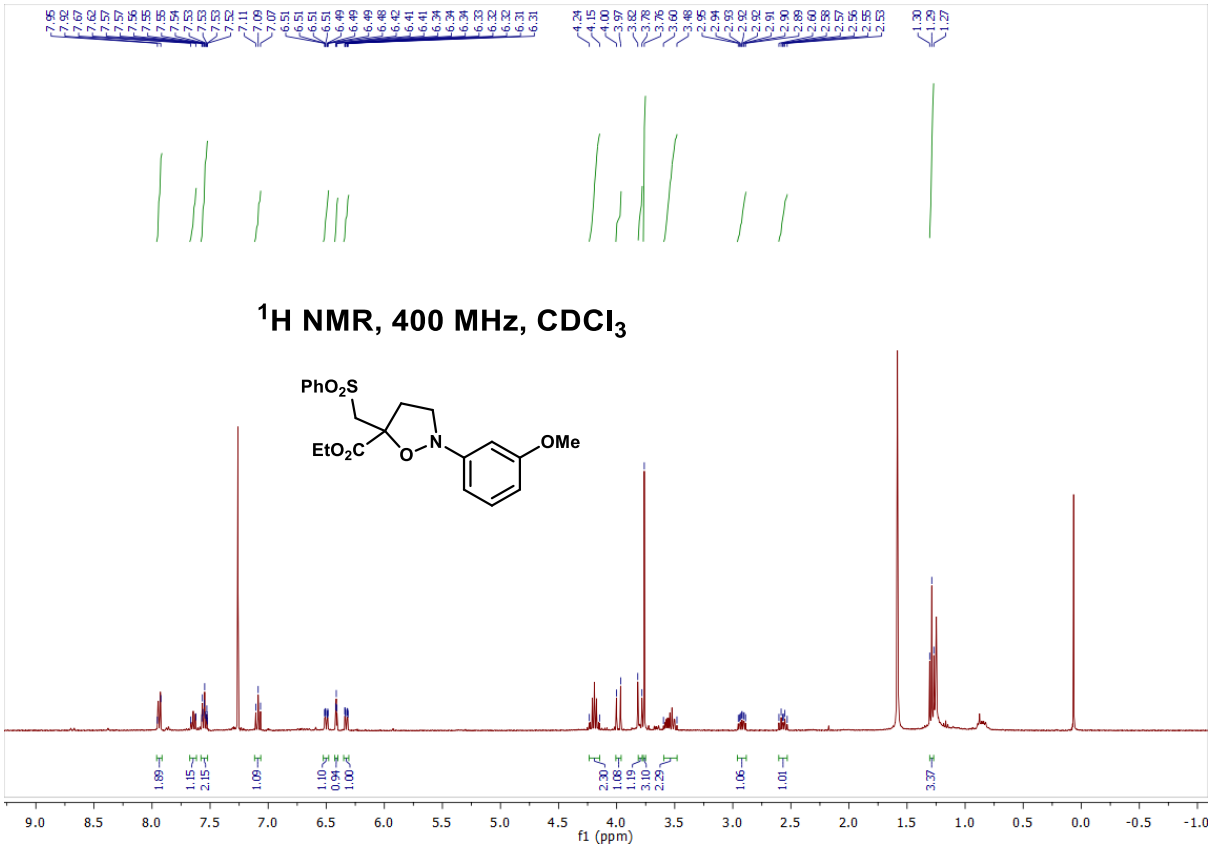


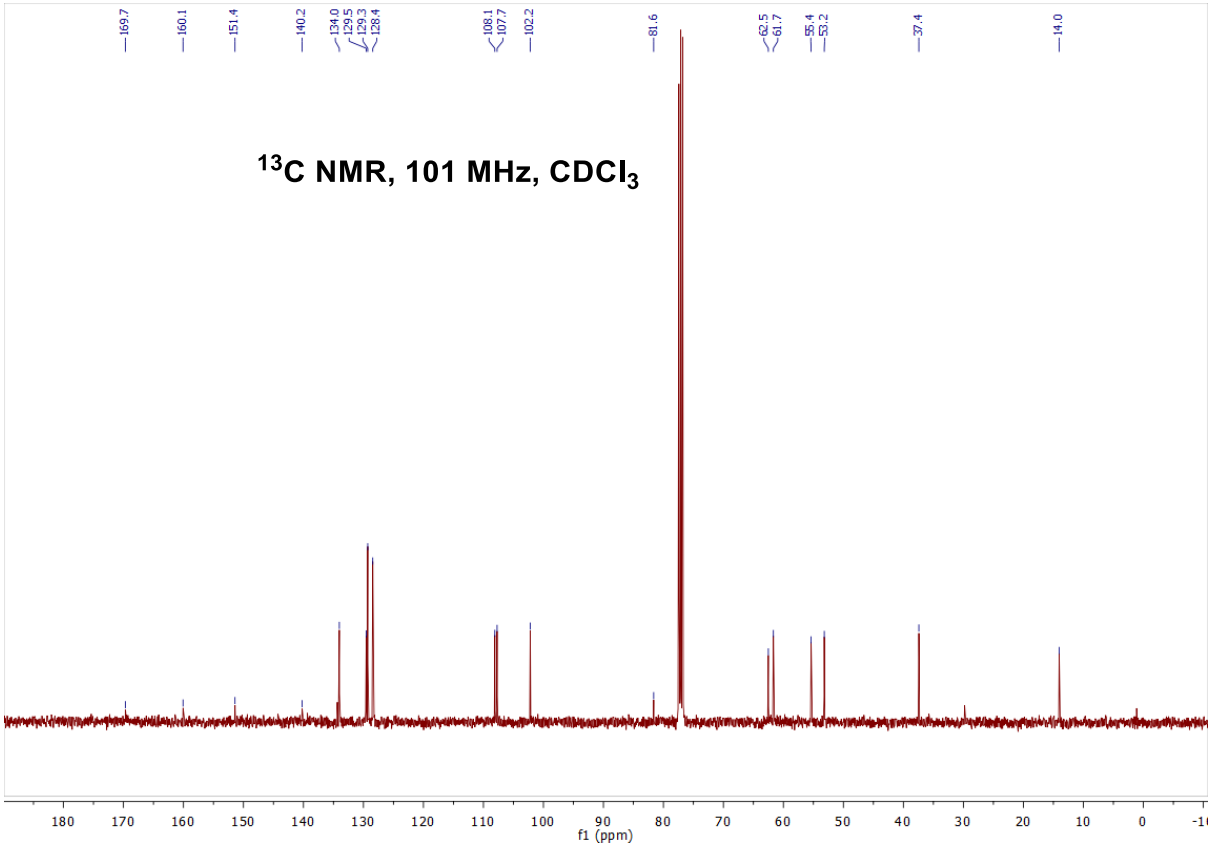
^{1}H NMR, 400 MHz, $CDCl_3$



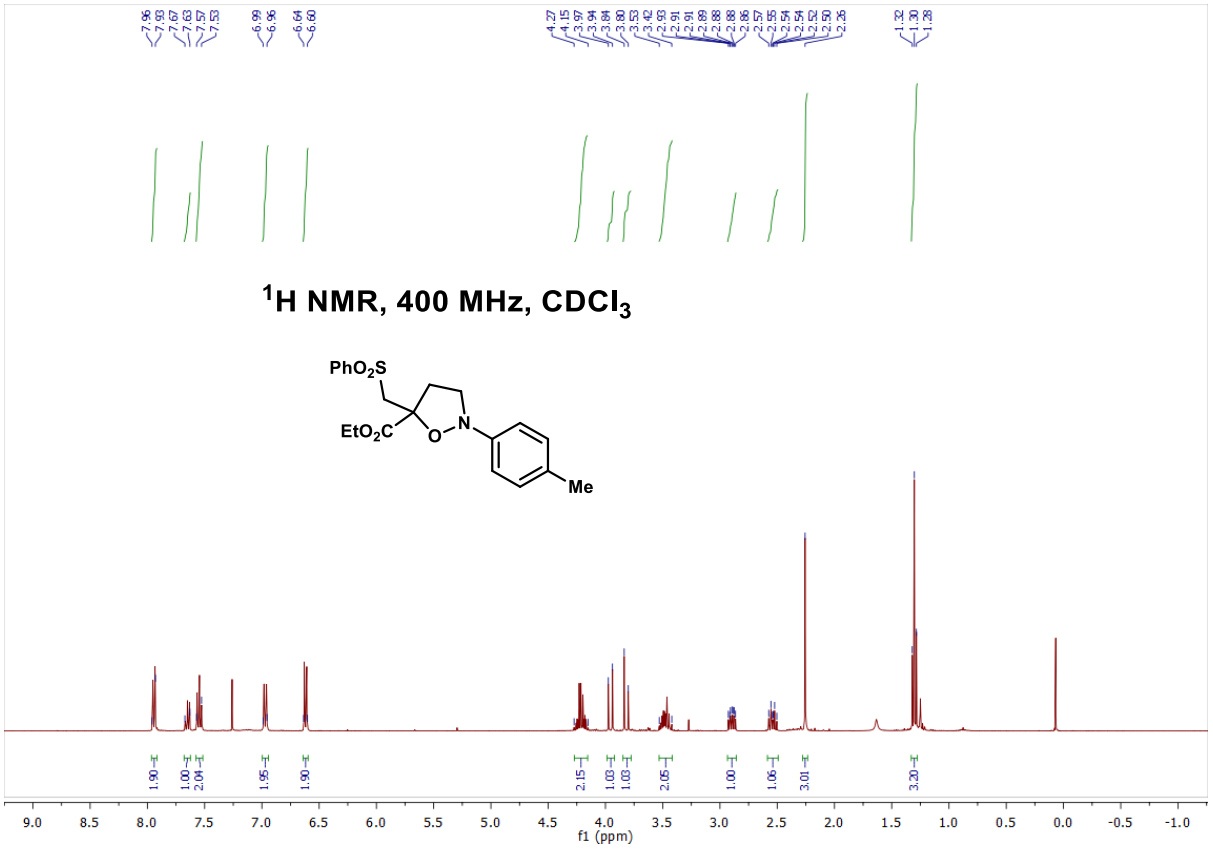
^{13}C NMR, 101 MHz, $CDCl_3$

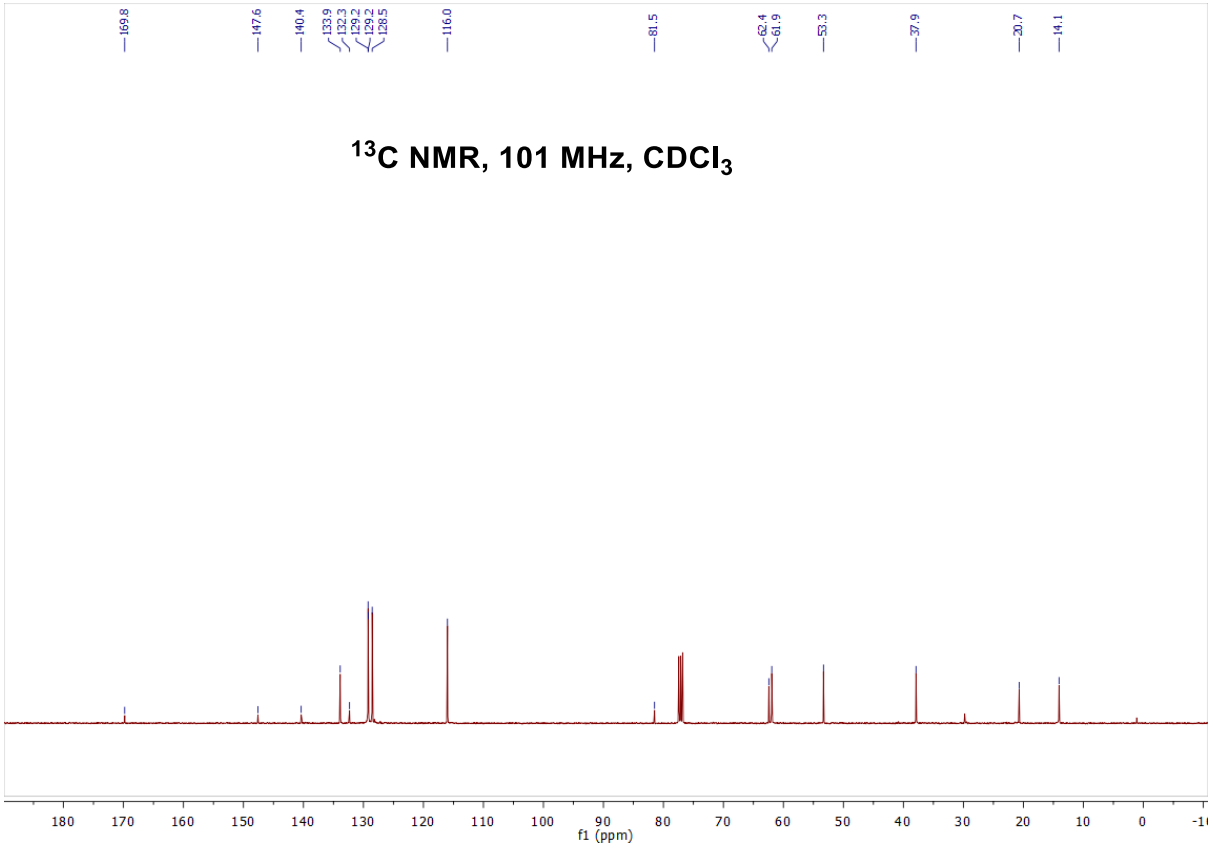
Ethyl 2-(3-methoxyphenyl)-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3b)



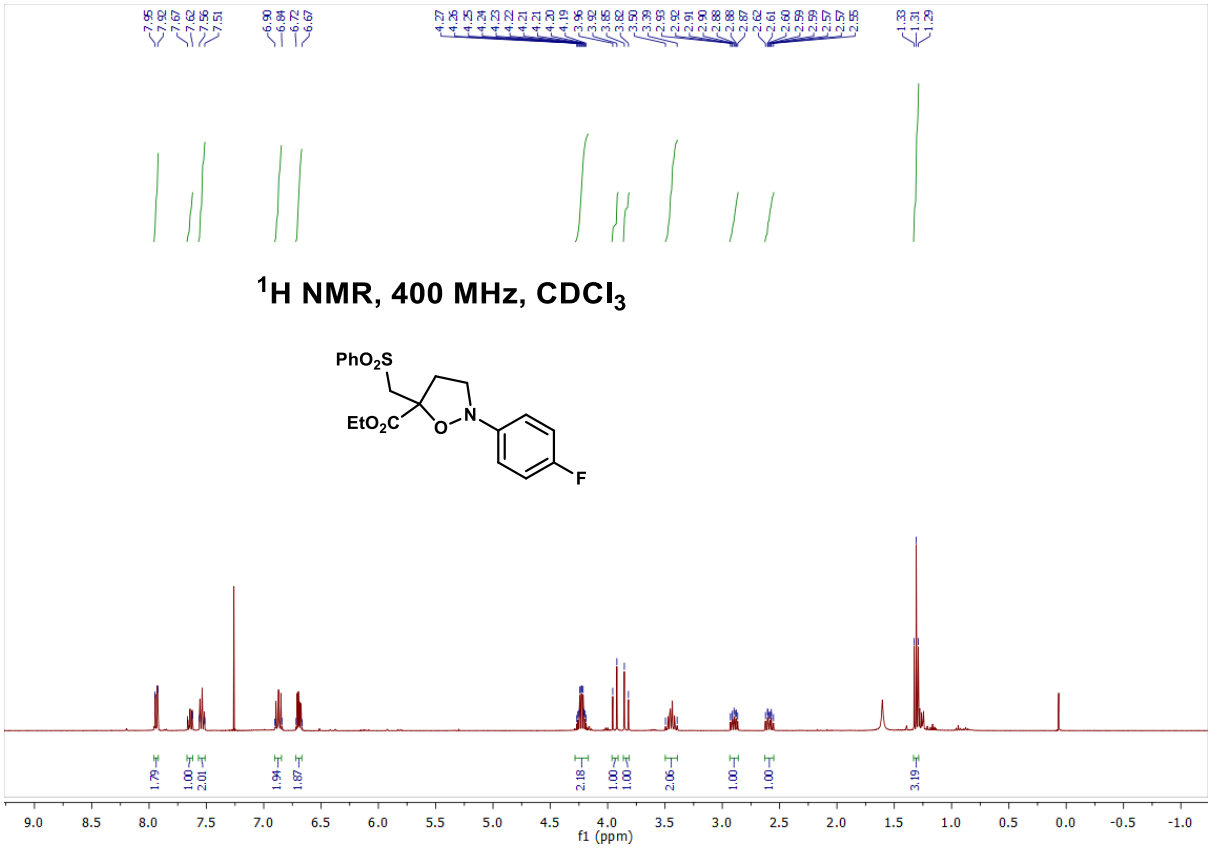


Ethyl 5-((phenylsulfonyl)methyl)-2-(*p*-tolyl)isoxazolidine-5-carboxylate (3c)

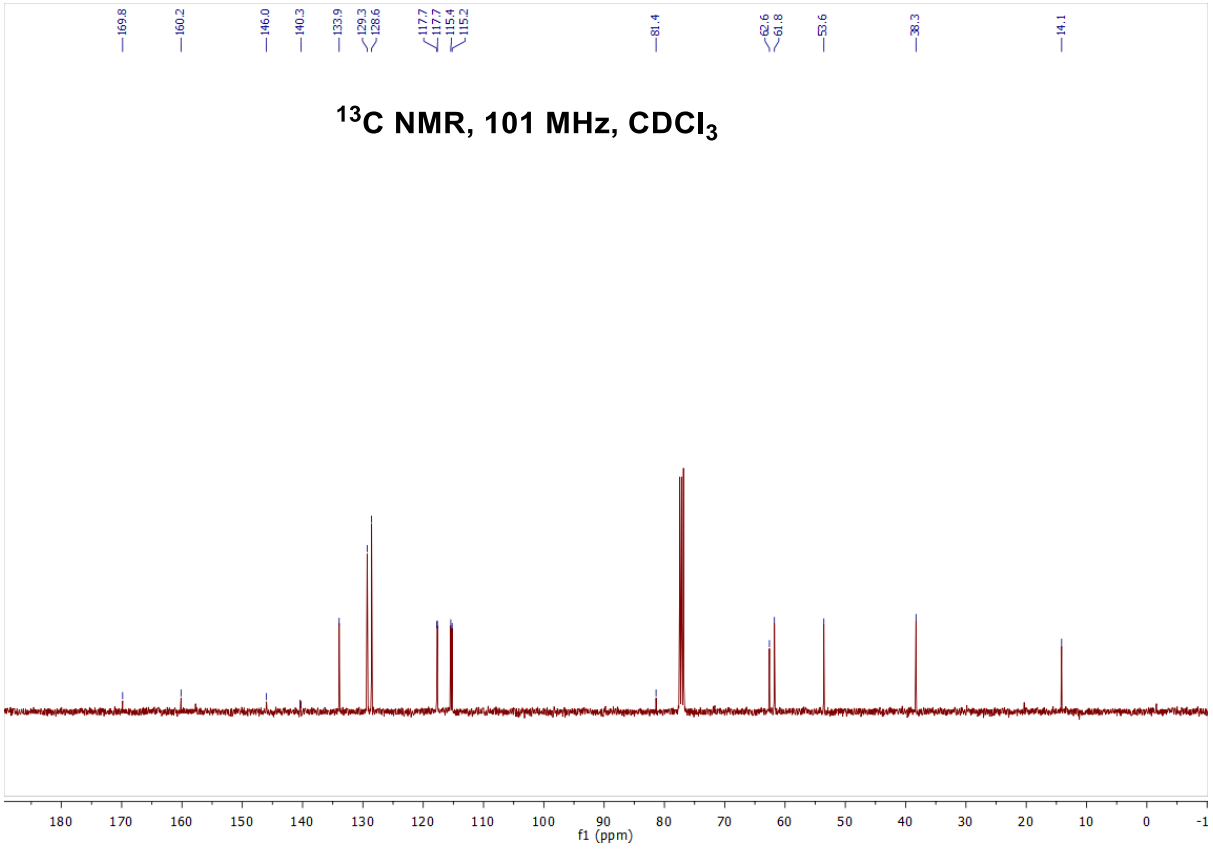




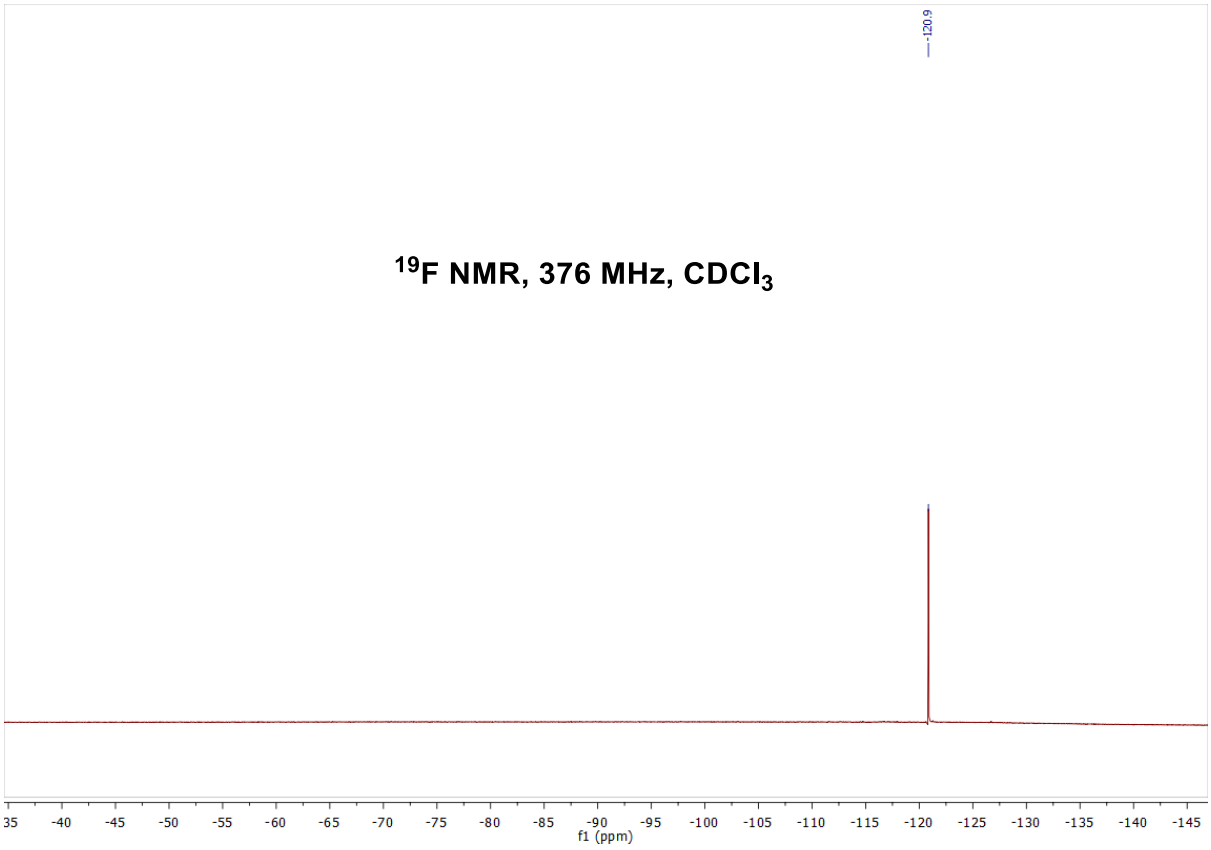
Ethyl 2-(4-fluorophenyl)-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3d)



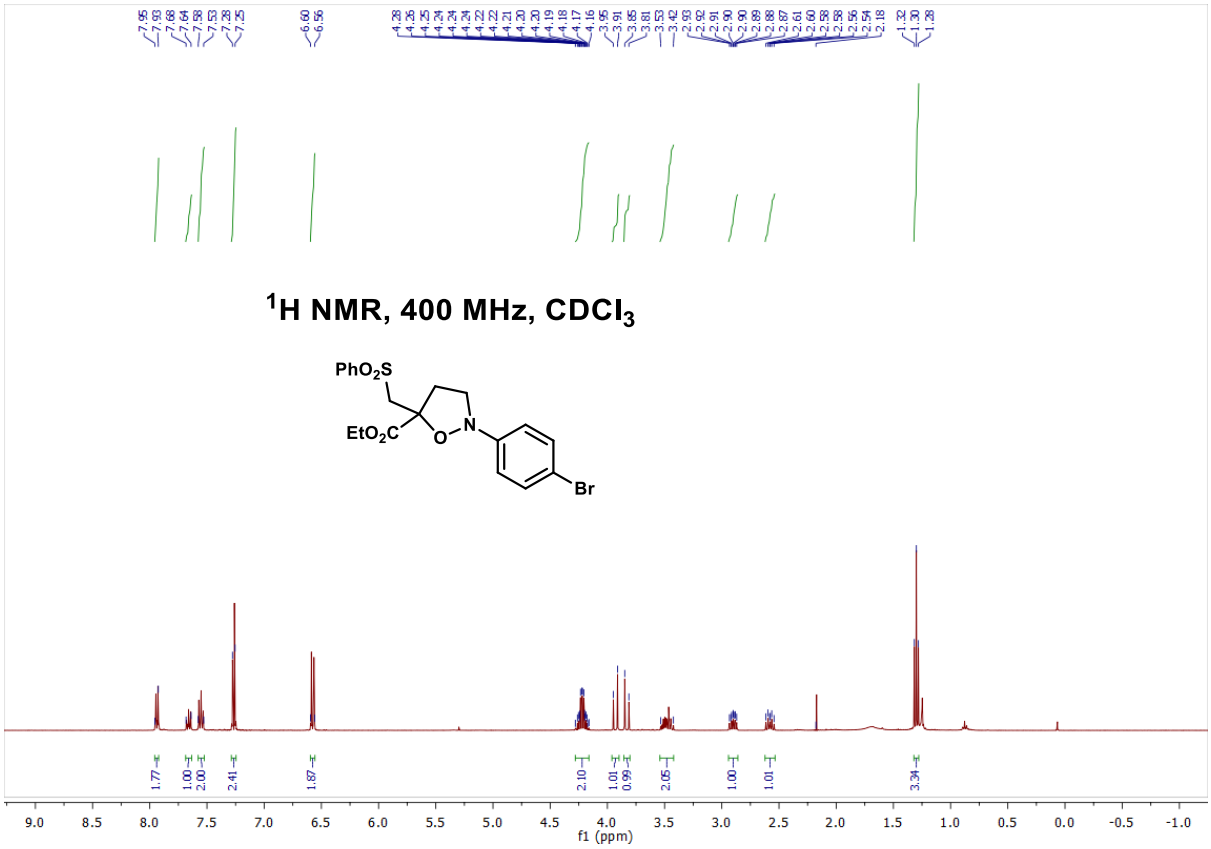
^{1}H NMR, 400 MHz, $CDCl_3$

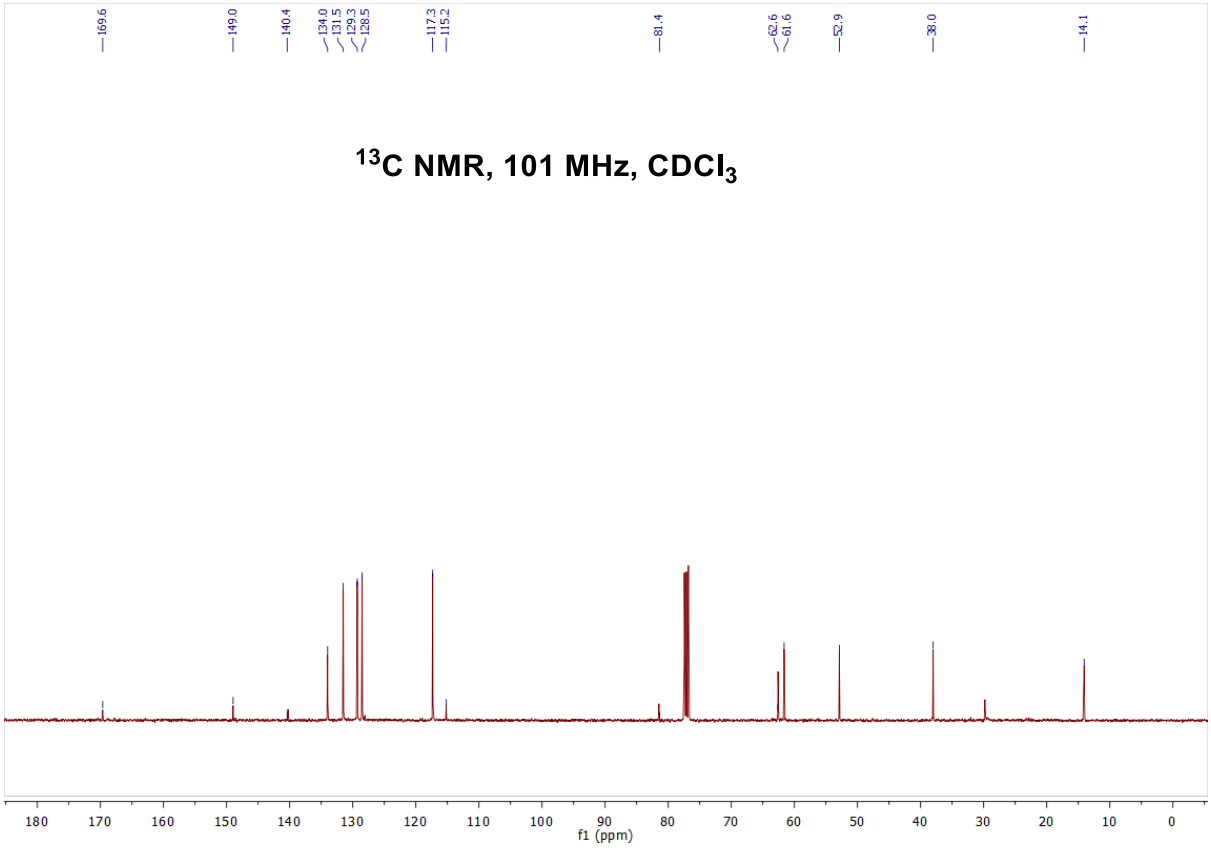


^{13}C NMR, 101 MHz, $CDCl_3$

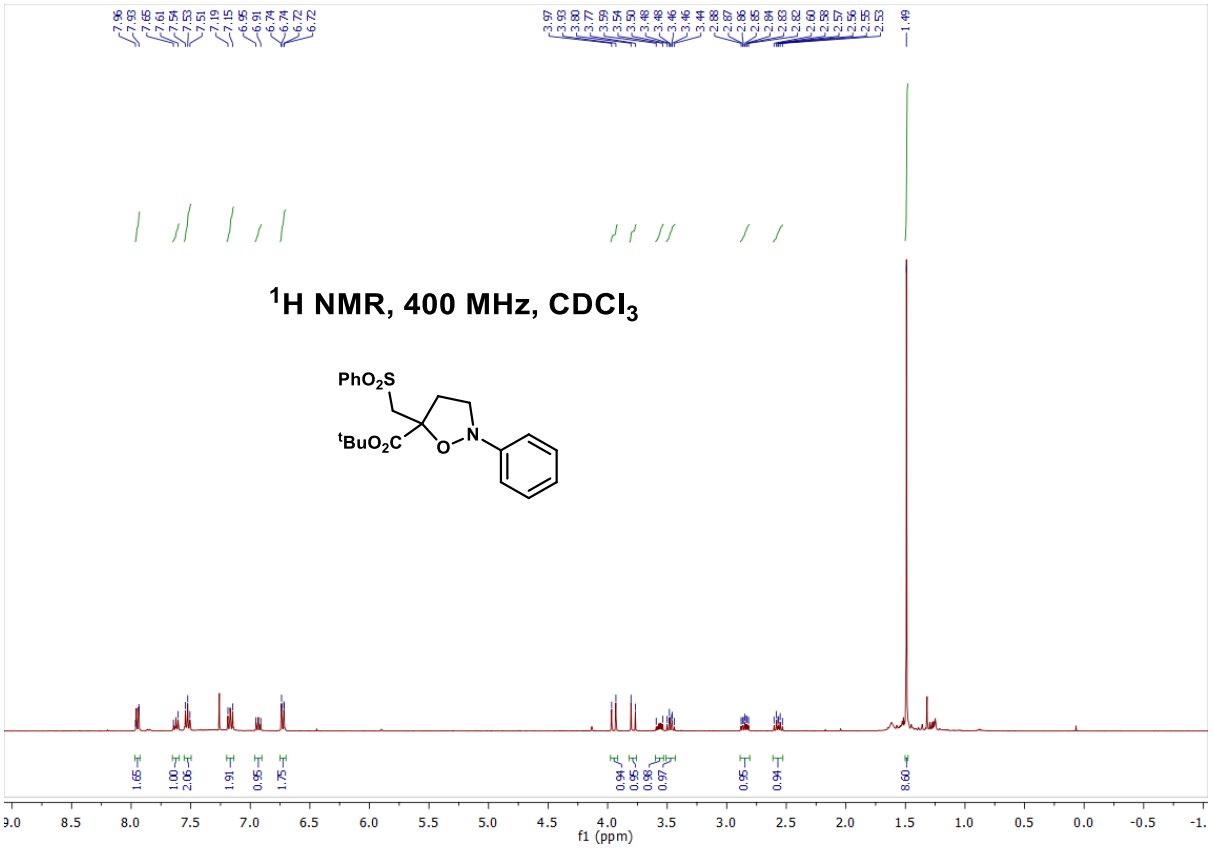

-120.9
^{19}F NMR, 376 MHz, CDCl$_3$
35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145
f1 (ppm)

Ethyl 2-(4-bromophenyl)-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3e)

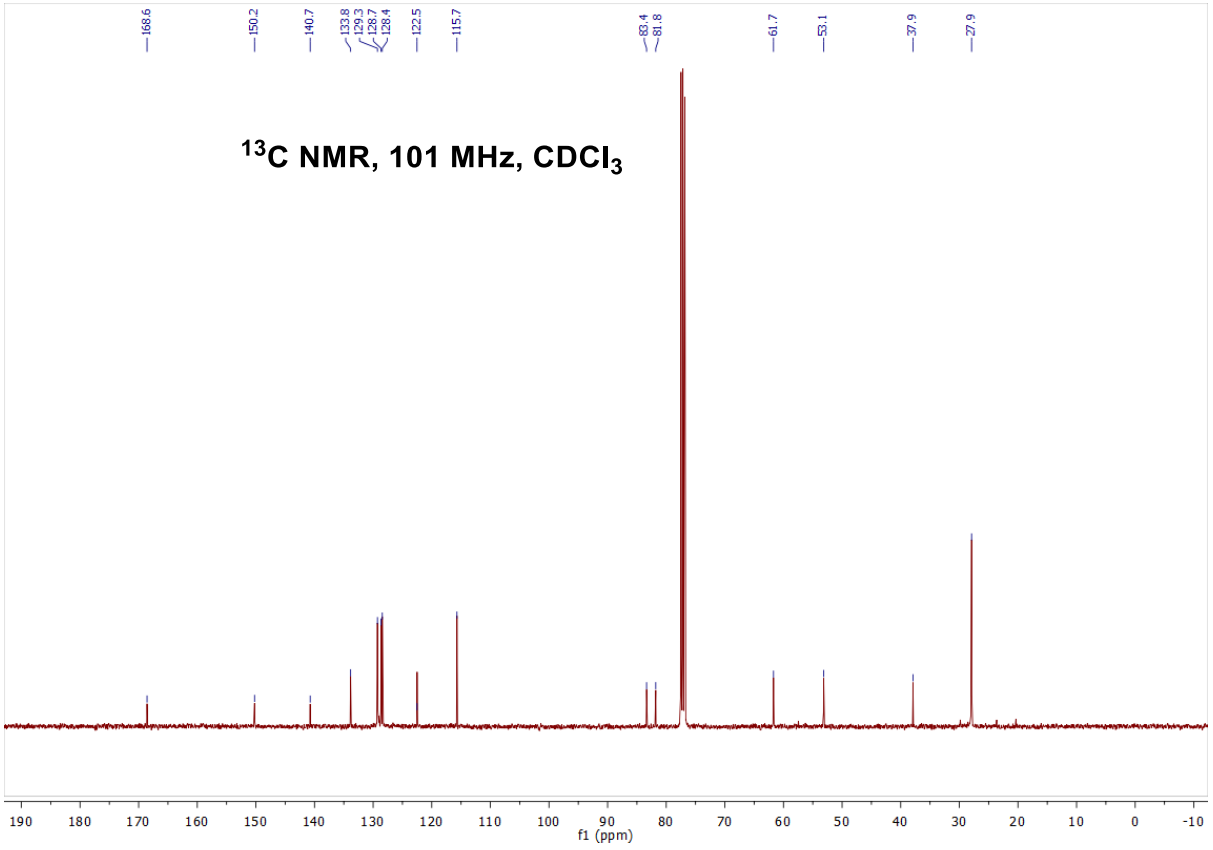




Tert-butyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3f)

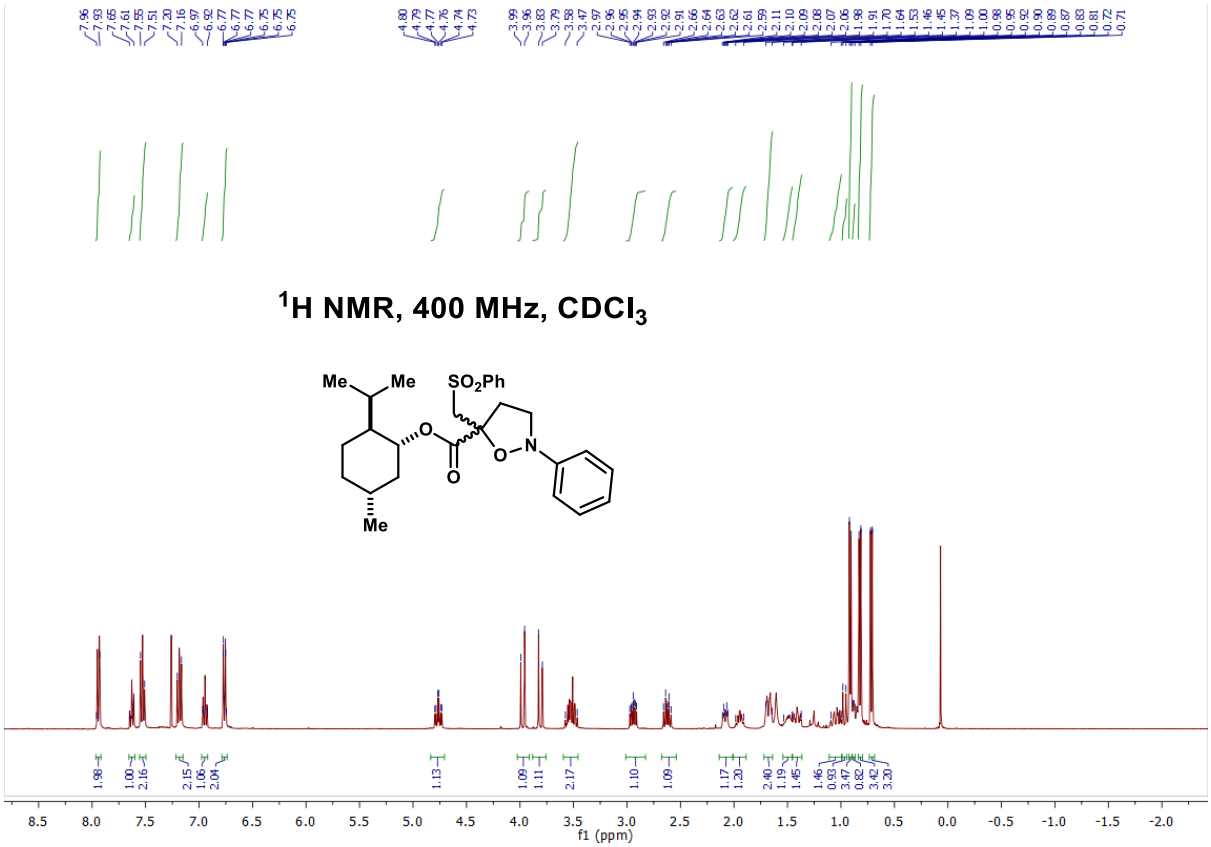


^{1}H NMR, 400 MHz, $CDCl_3$

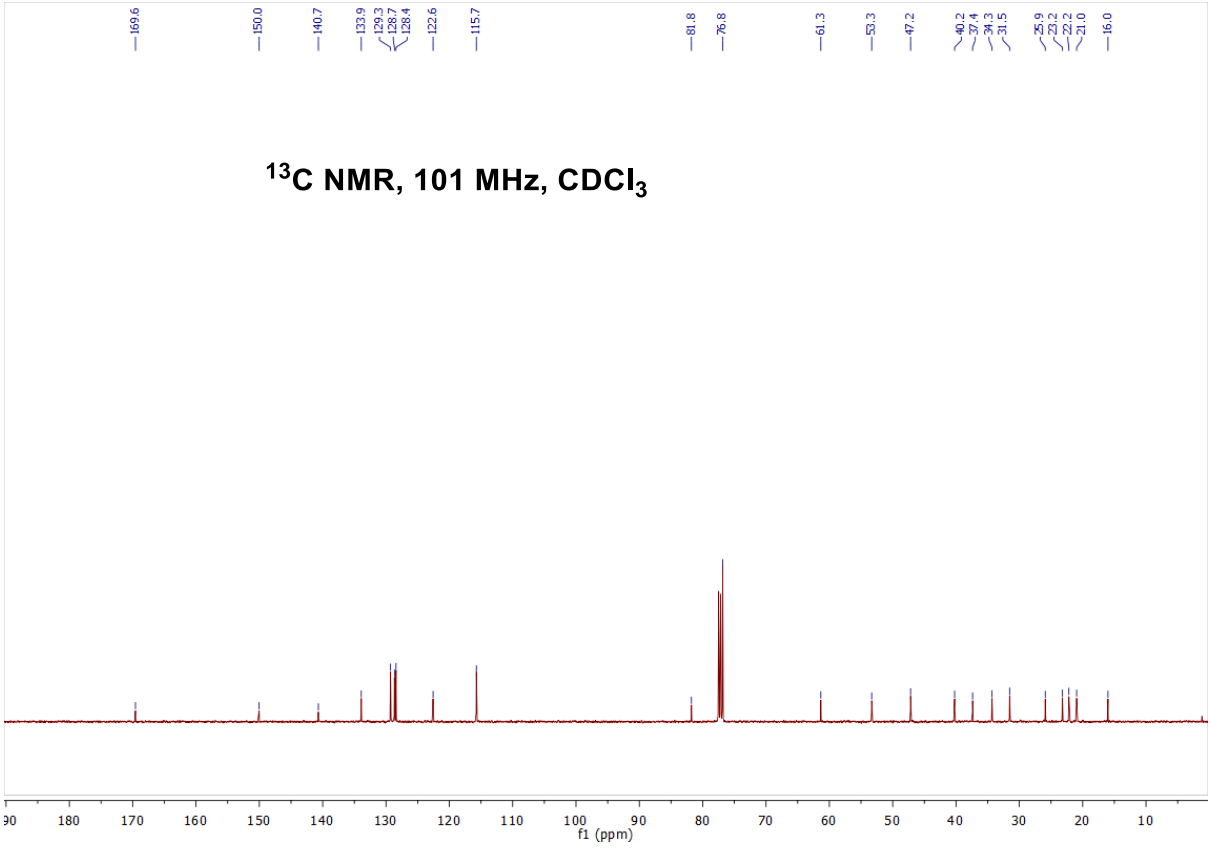


^{13}C NMR, 101 MHz, $CDCl_3$

2-Isopropyl-5-methylcyclohexyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3g)

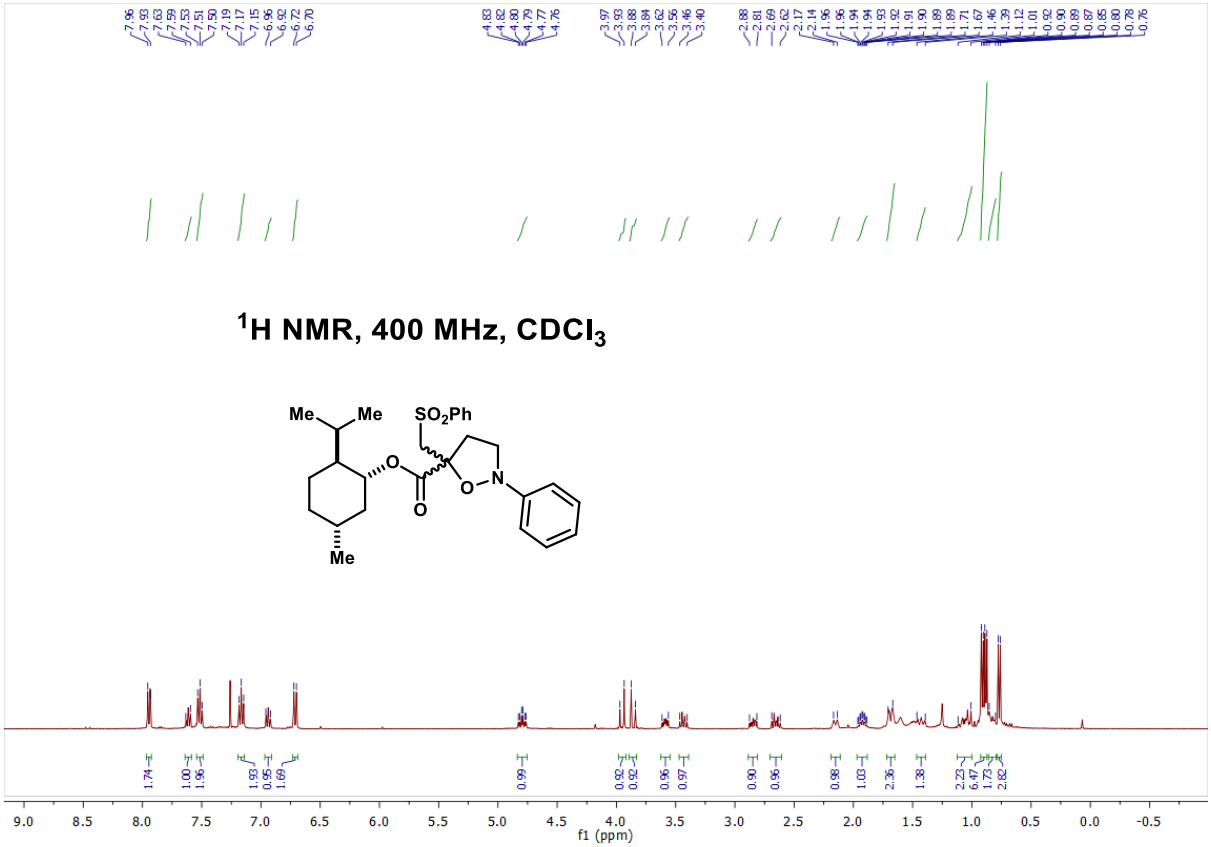


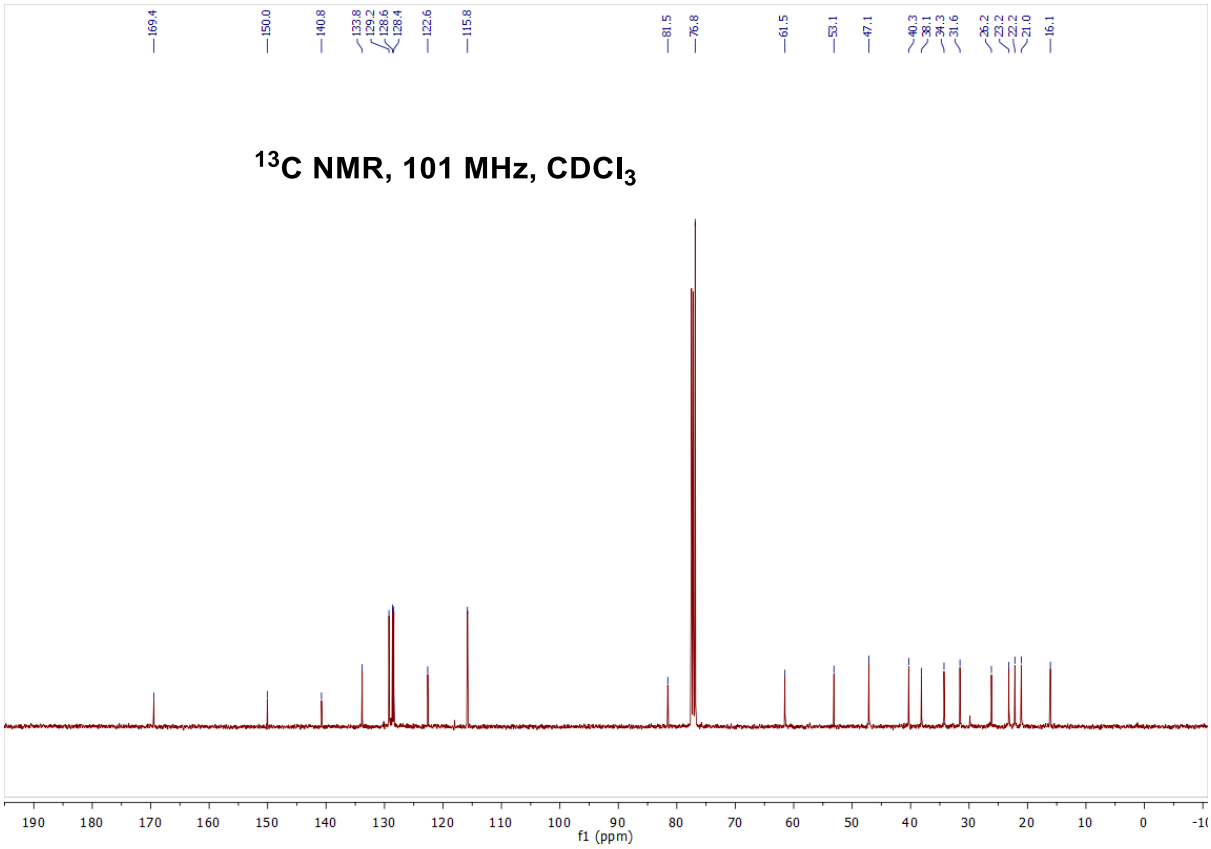
^{1}H NMR, 400 MHz, $CDCl_3$



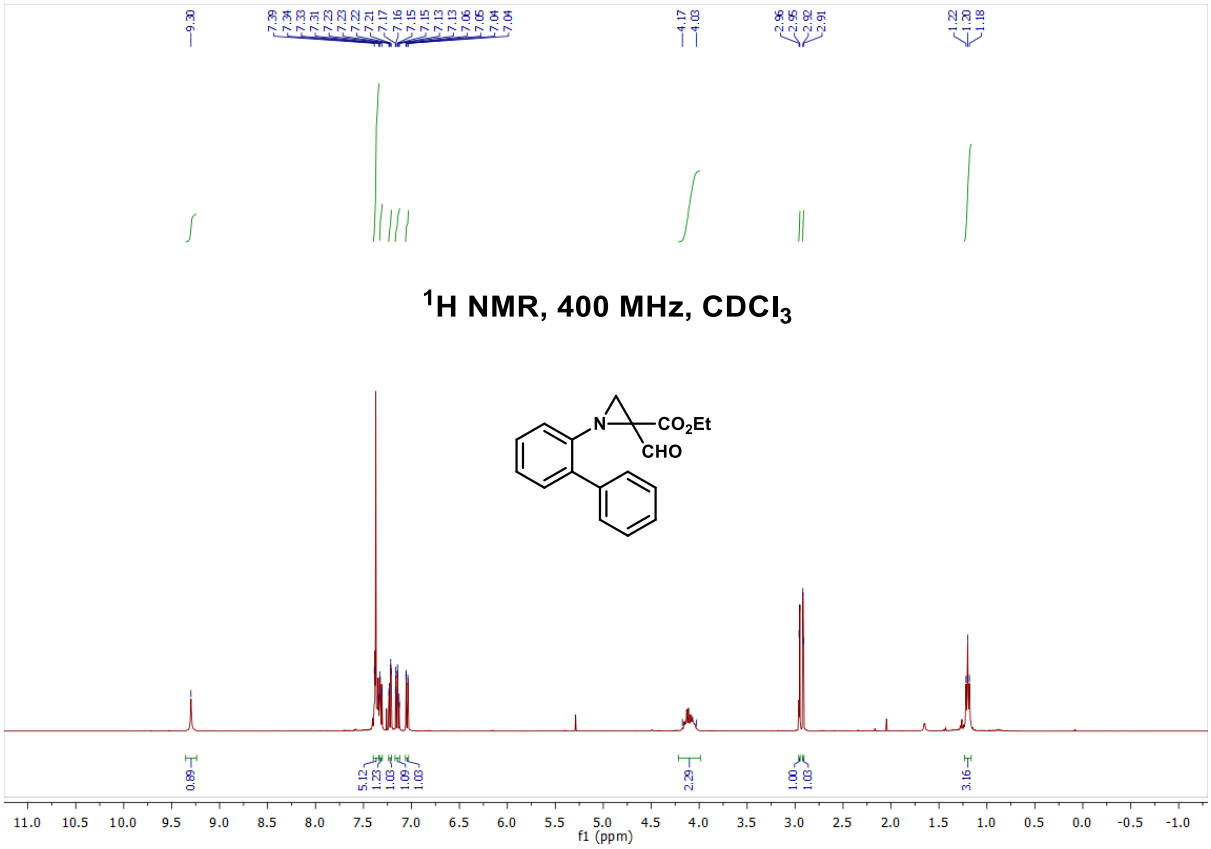
^{13}C NMR, 101 MHz, $CDCl_3$

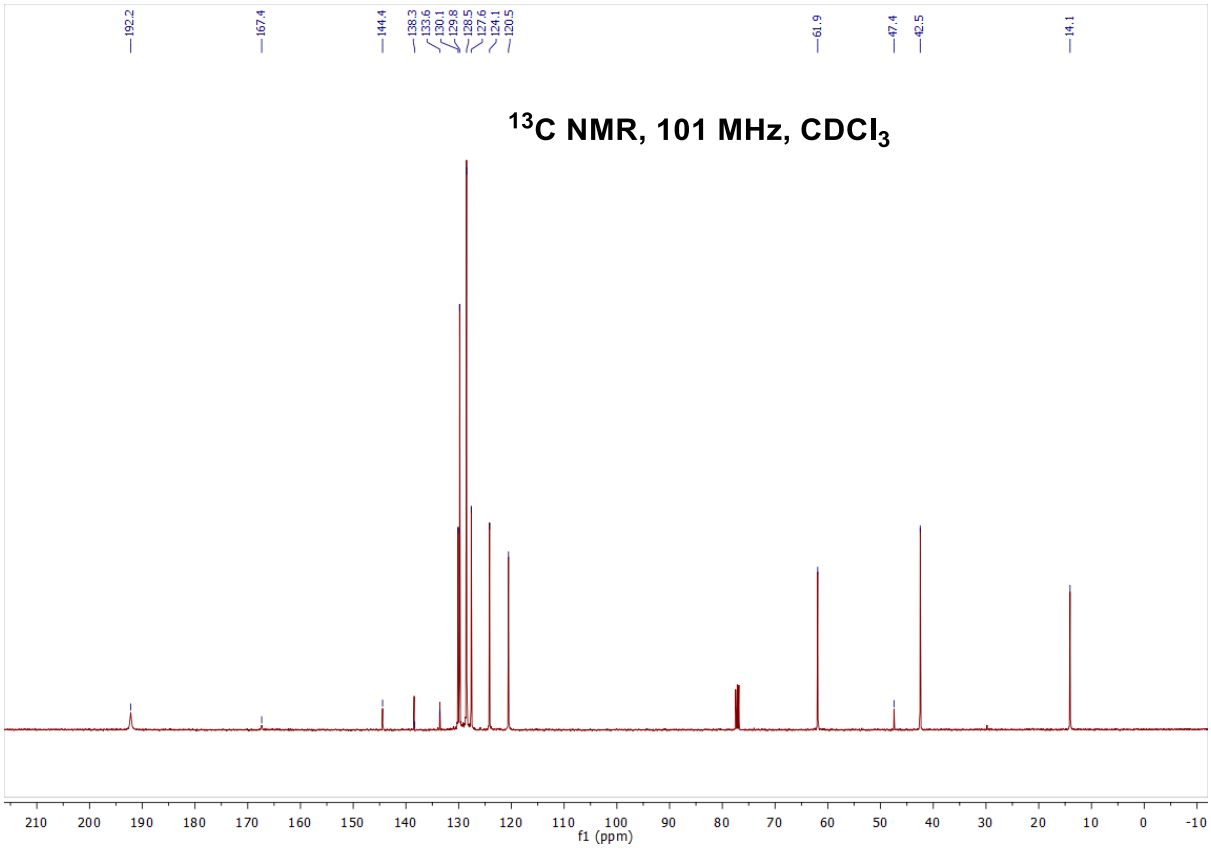
2-Isopropyl-5-methylcyclohexyl 2-phenyl-5-((phenylsulfonyl)methyl)isoxazolidine-5-carboxylate (3g')



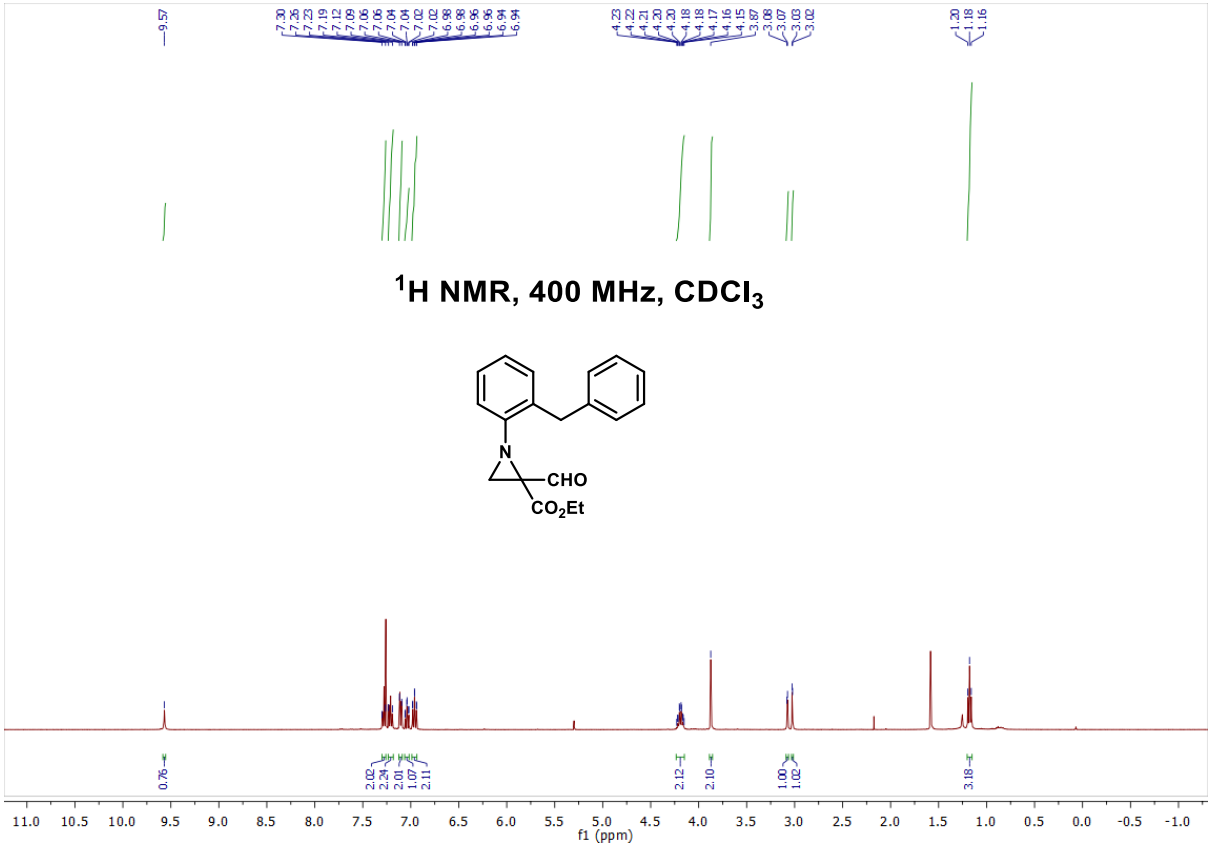


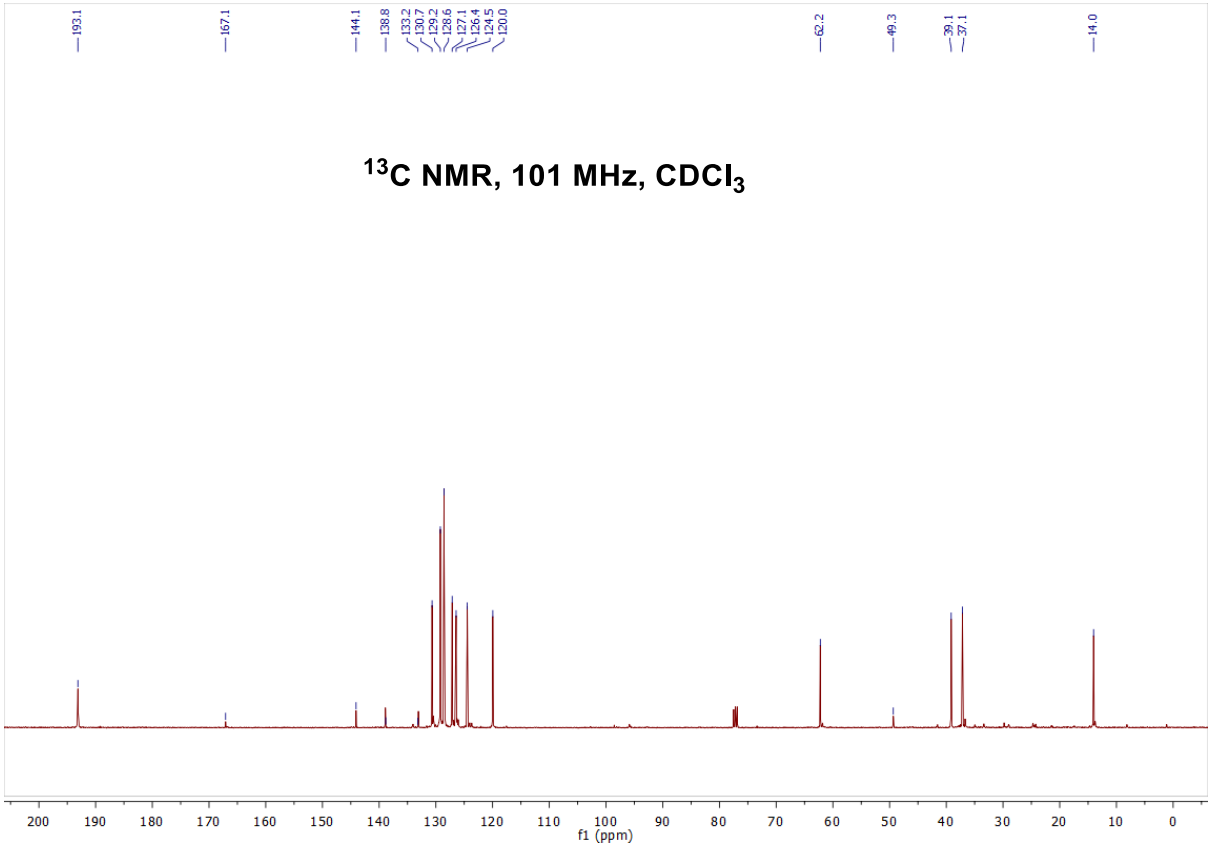
Ethyl 1-([1,1'-biphenyl]-2-yl)-2-formylaziridine-2-carboxylate (4a)



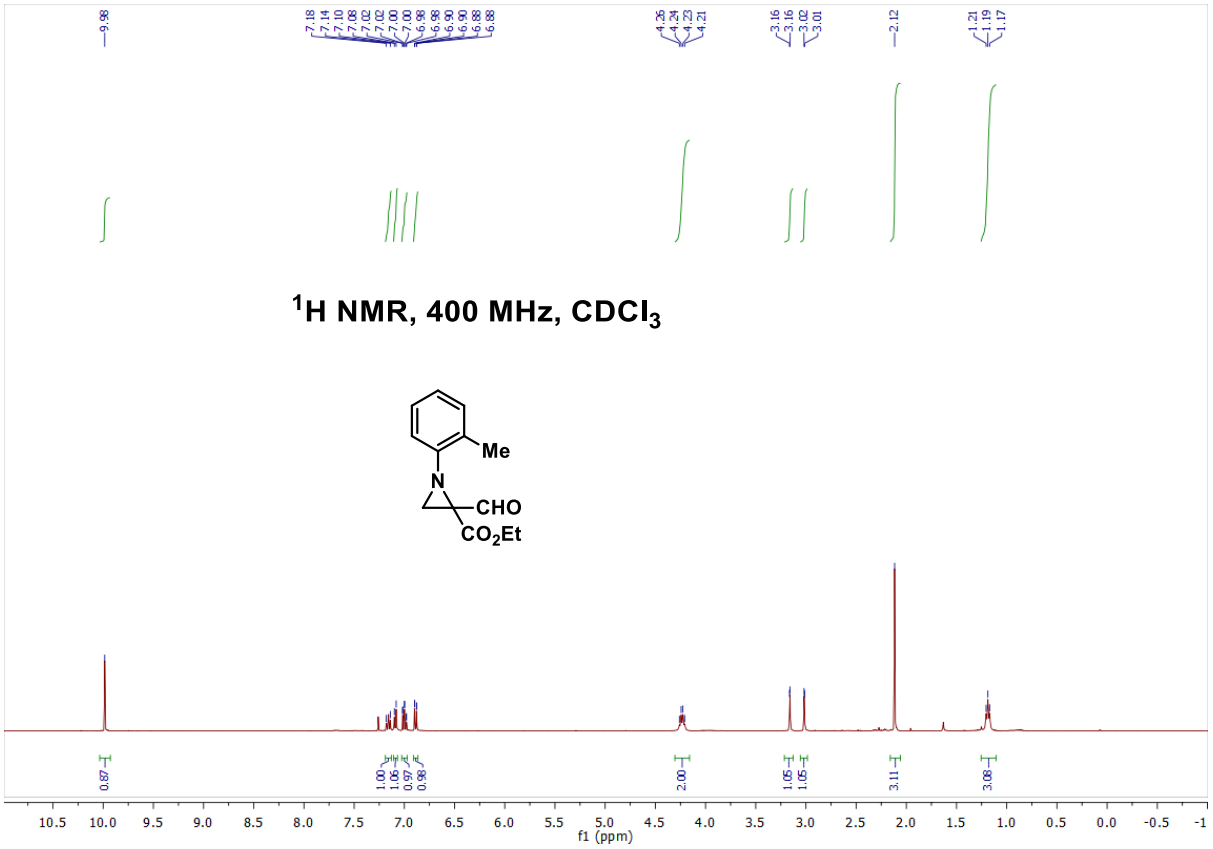


Ethyl 1-(2-benzylphenyl)-2-formylaziridine-2-carboxylate (4b)

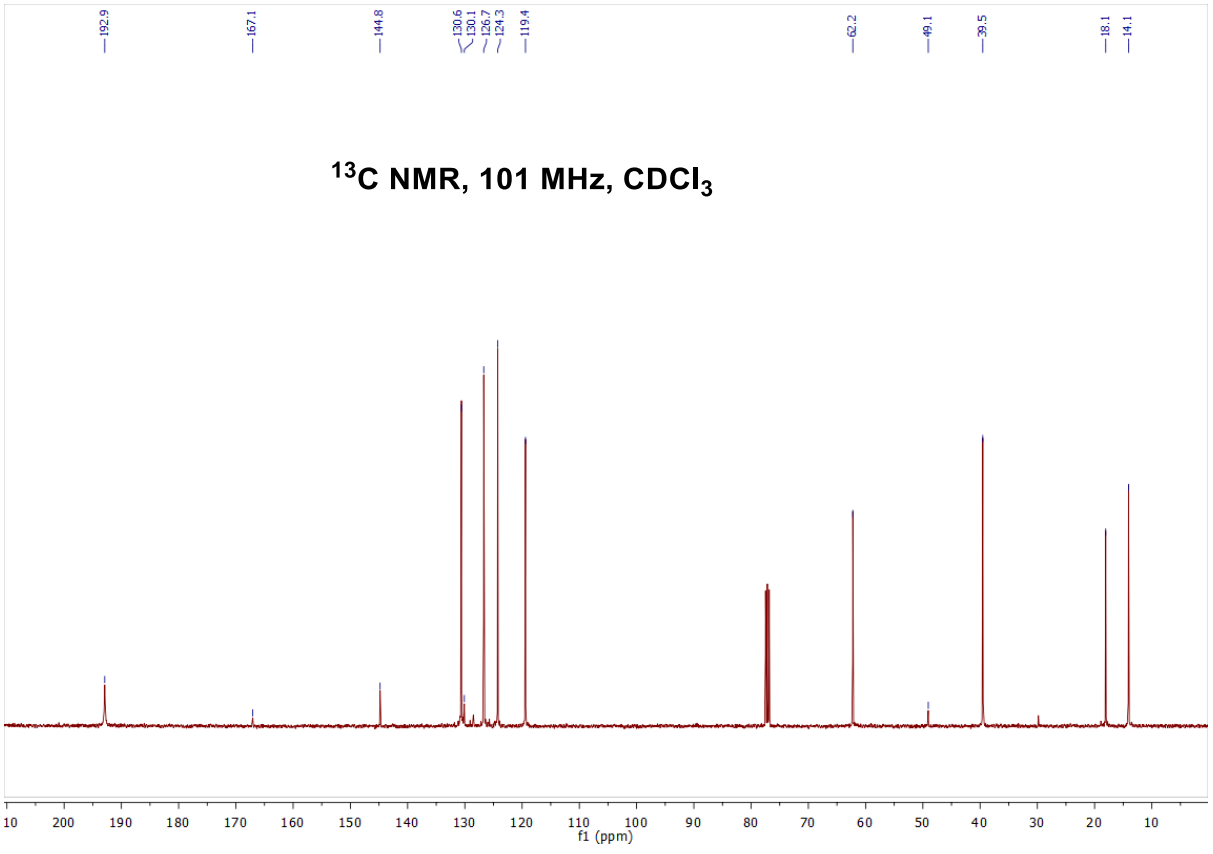




Ethyl 2-formyl-1-(*o*-tolyl)aziridine-2-carboxylate (4c)

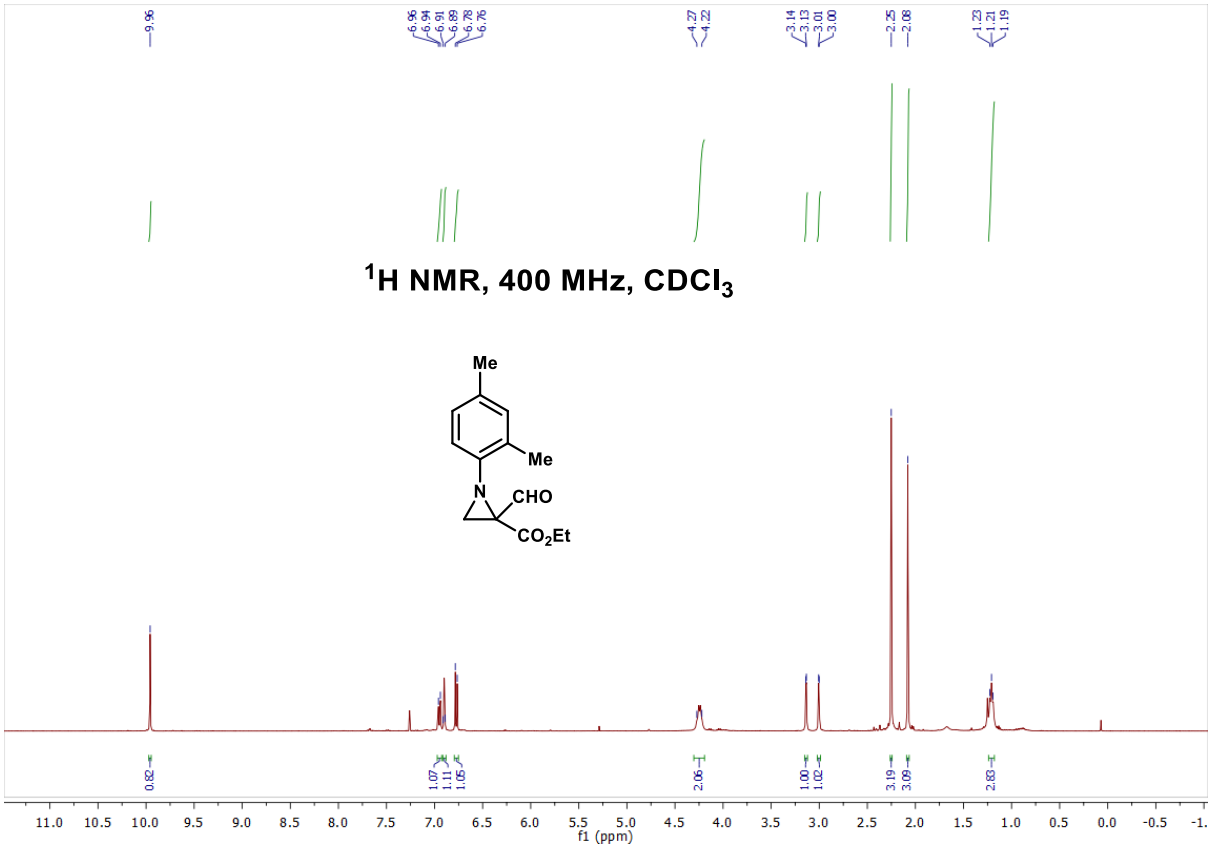


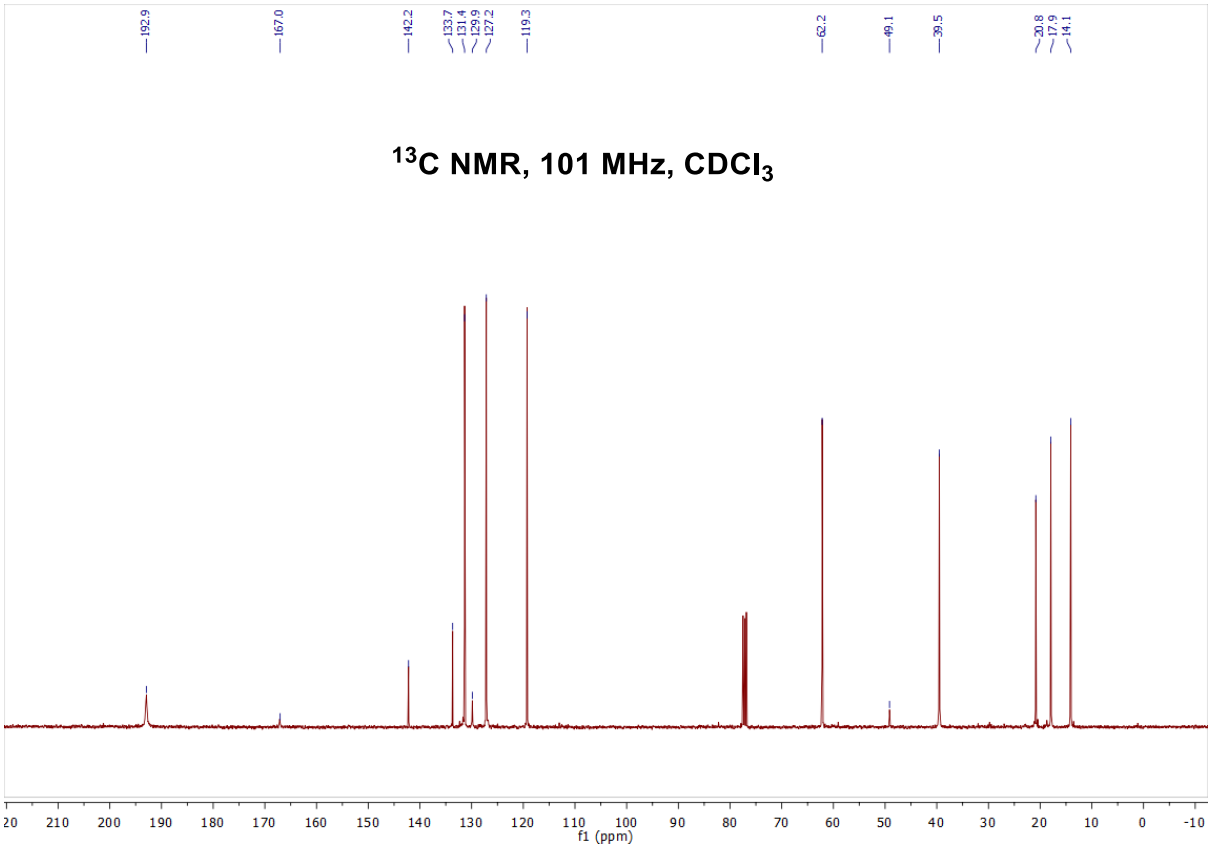
^{1}H NMR, 400 MHz, $CDCl_3$

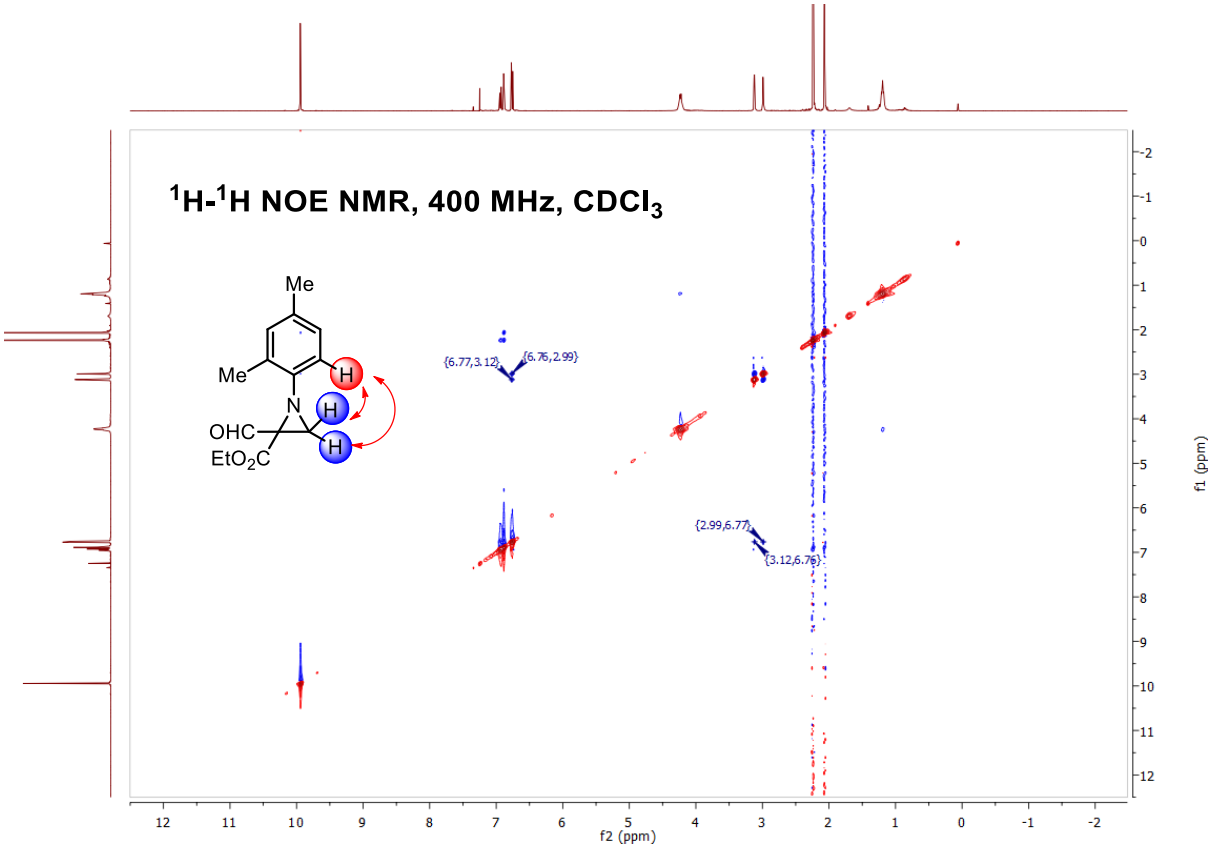


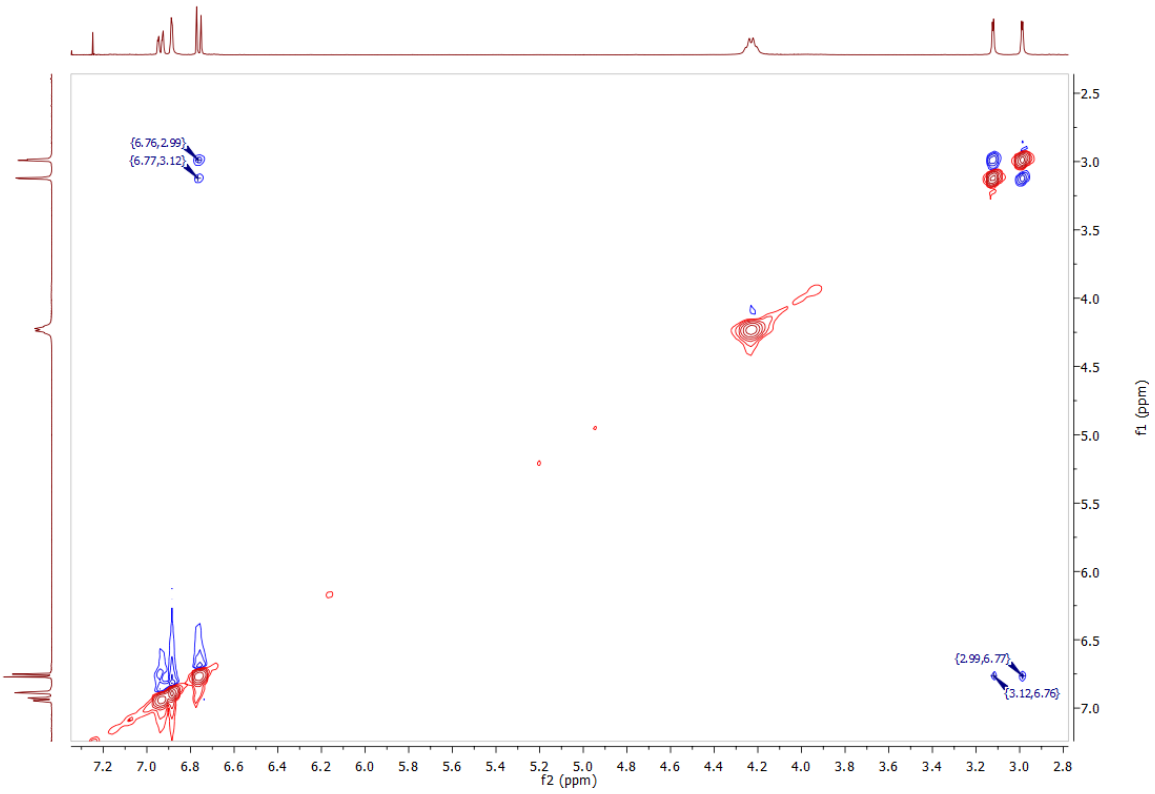
^{13}C NMR, 101 MHz, $CDCl_3$

Ethyl 1-(2,4-dimethylphenyl)-2-formylaziridine-2-carboxylate (4d)

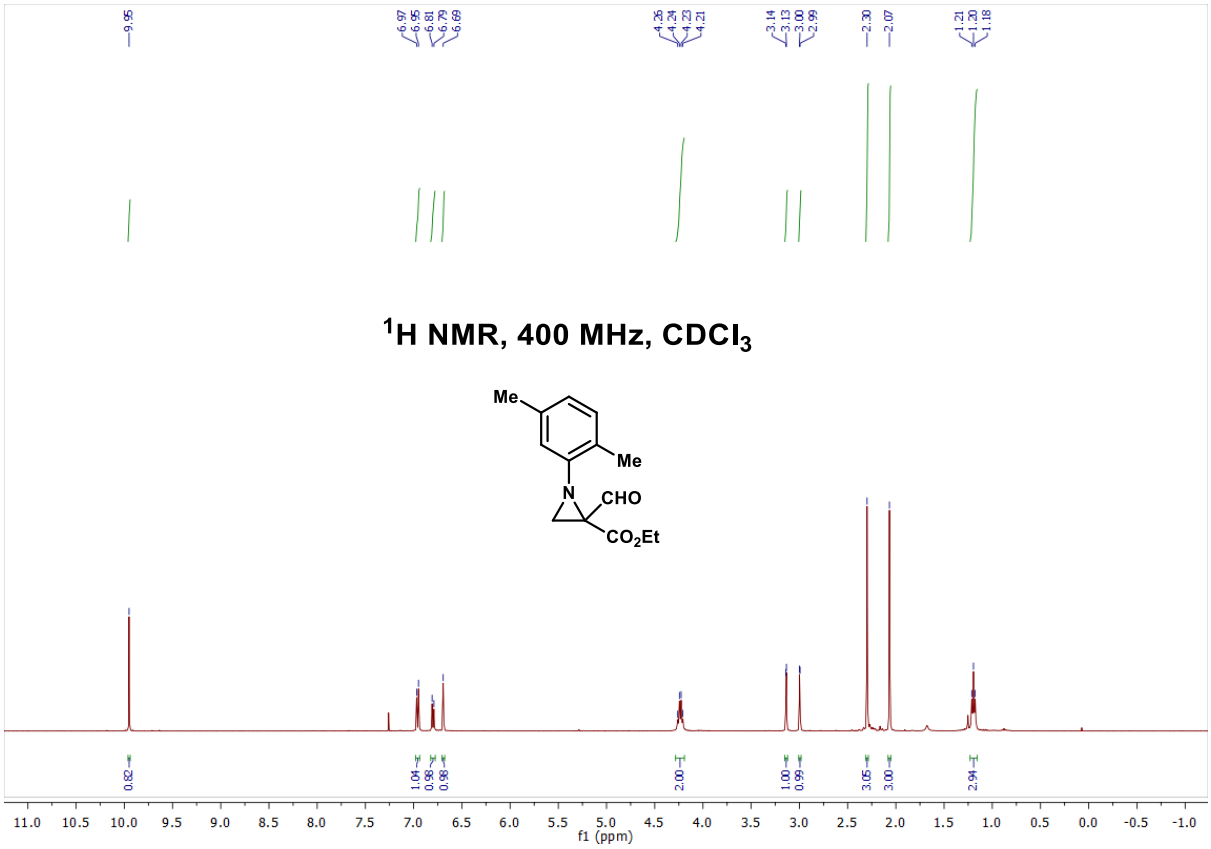


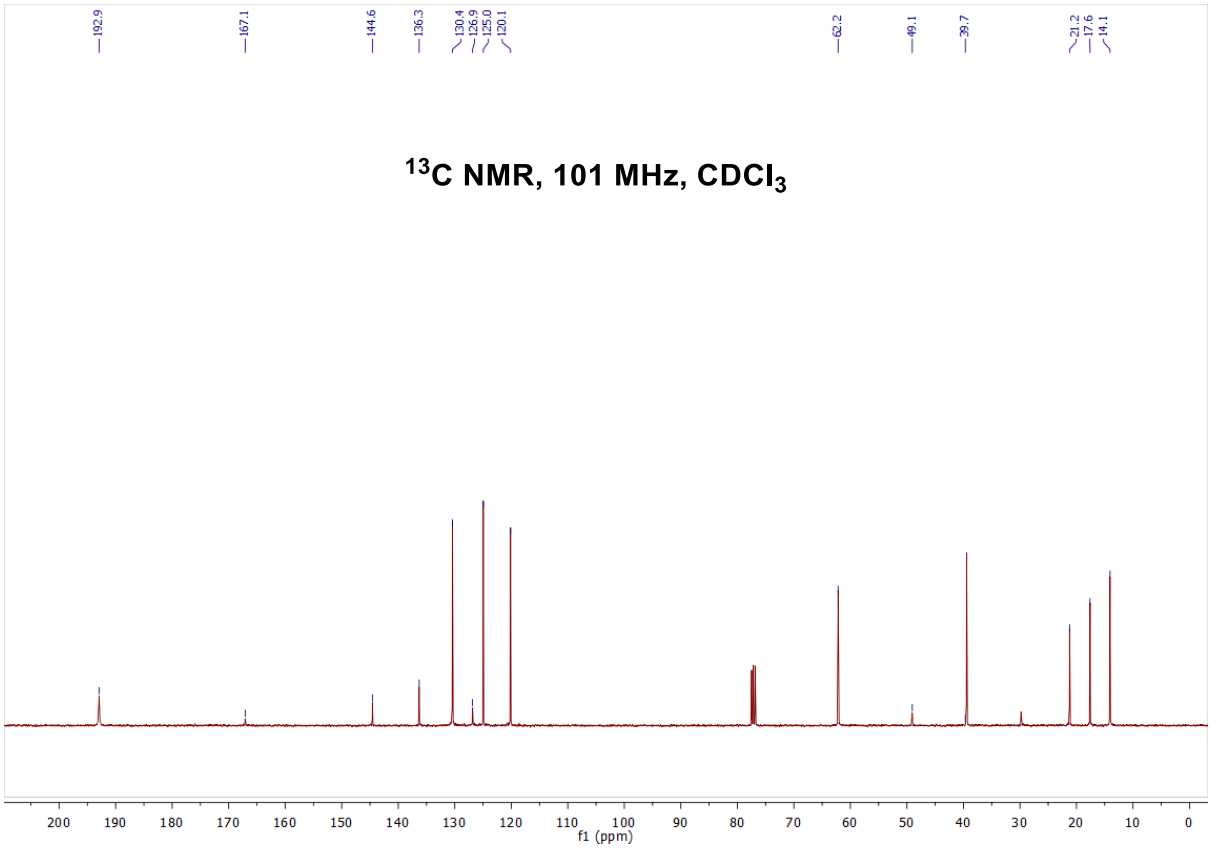



^{1}H-^{1}H NOE NMR, 400 MHz, CDCl$_3$
Me
Me
H
N
H
OHC
EtO$_2$C
H
{6.77,3.12}
{6.76,2.99}
{2.99,6.77}
{3.12,6.76}
f2 (ppm)
f1 (ppm)

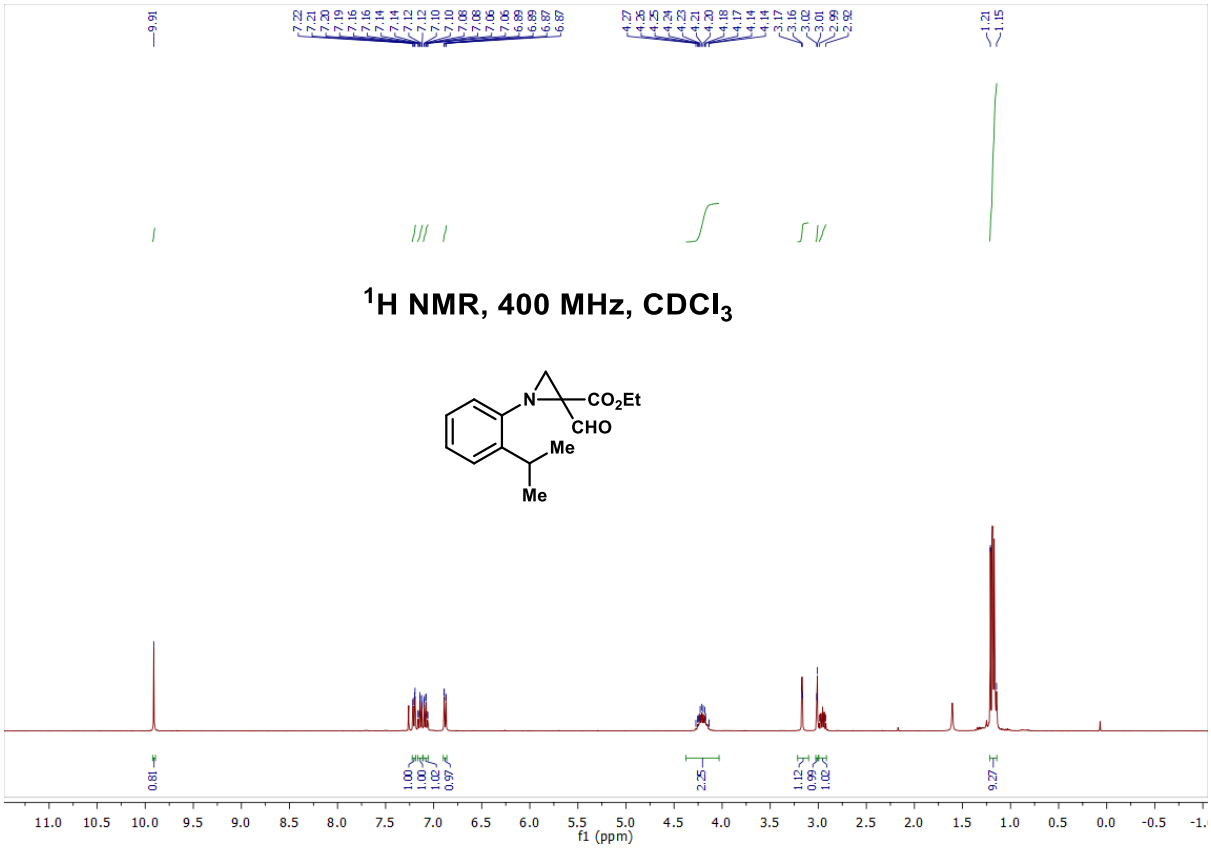

{6.76,2.99}
{6.77,3.12}
{2.99,6.77}
{3.12,6.76}
f2 (ppm)
f1 (ppm)

Ethyl 1-(2,5-dimethylphenyl)-2-formylaziridine-2-carboxylate (4e)

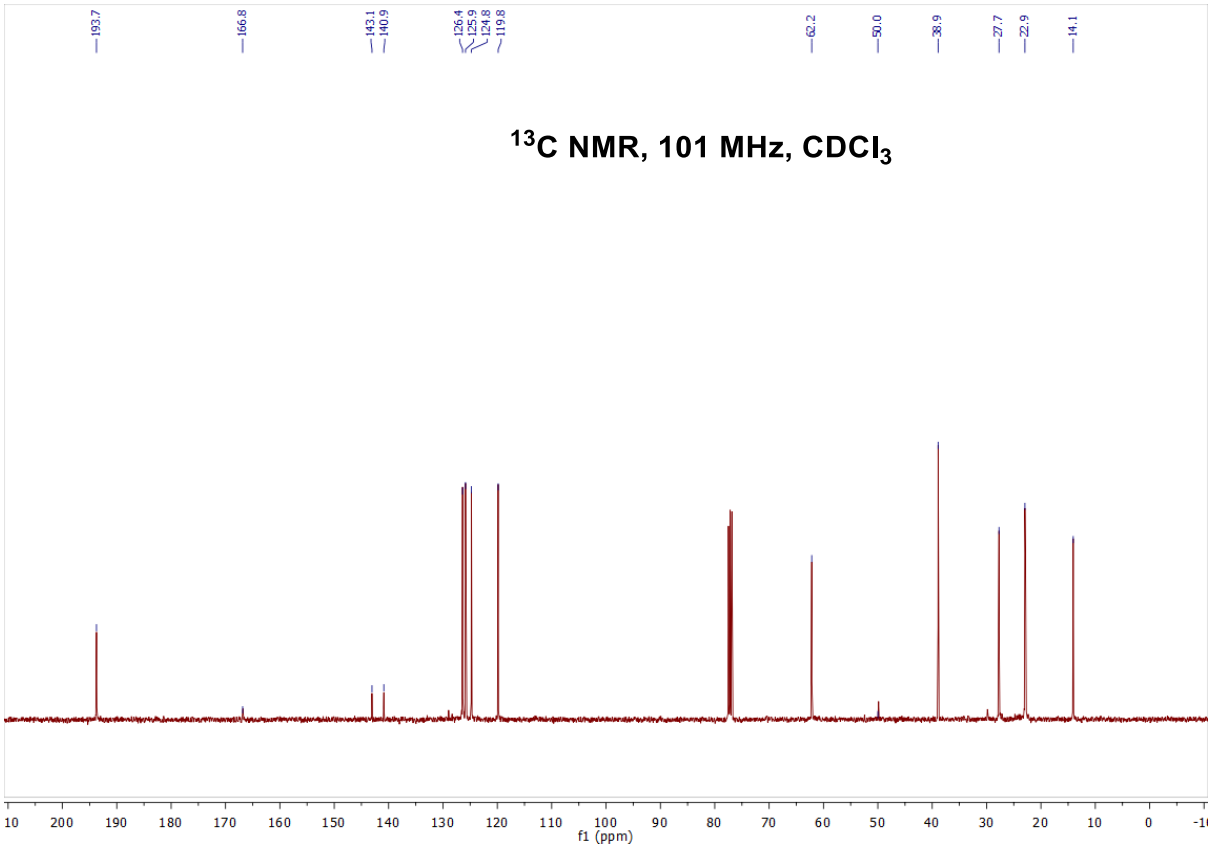




Ethyl 2-formyl-1-(2-isopropylphenyl)aziridine-2-carboxylate (4f)

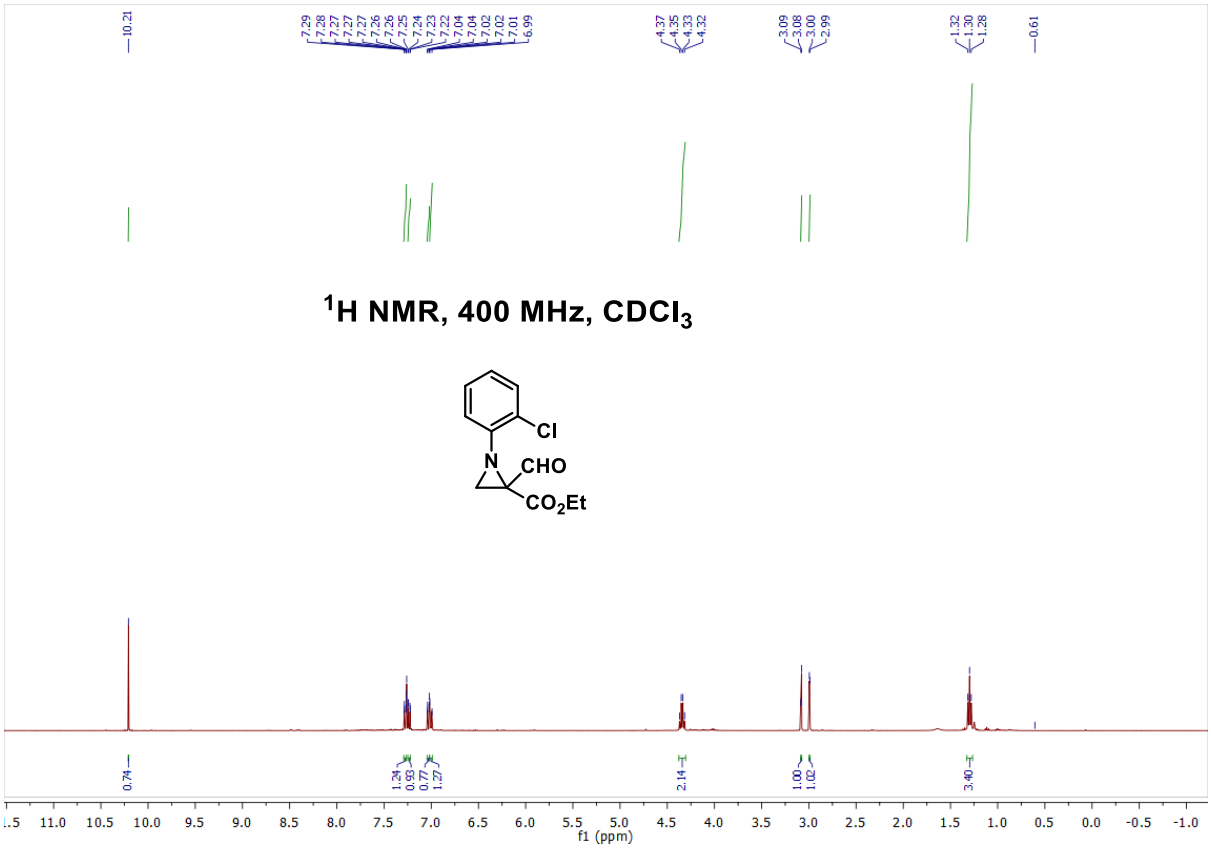


^{1}H NMR, 400 MHz, $CDCl_3$

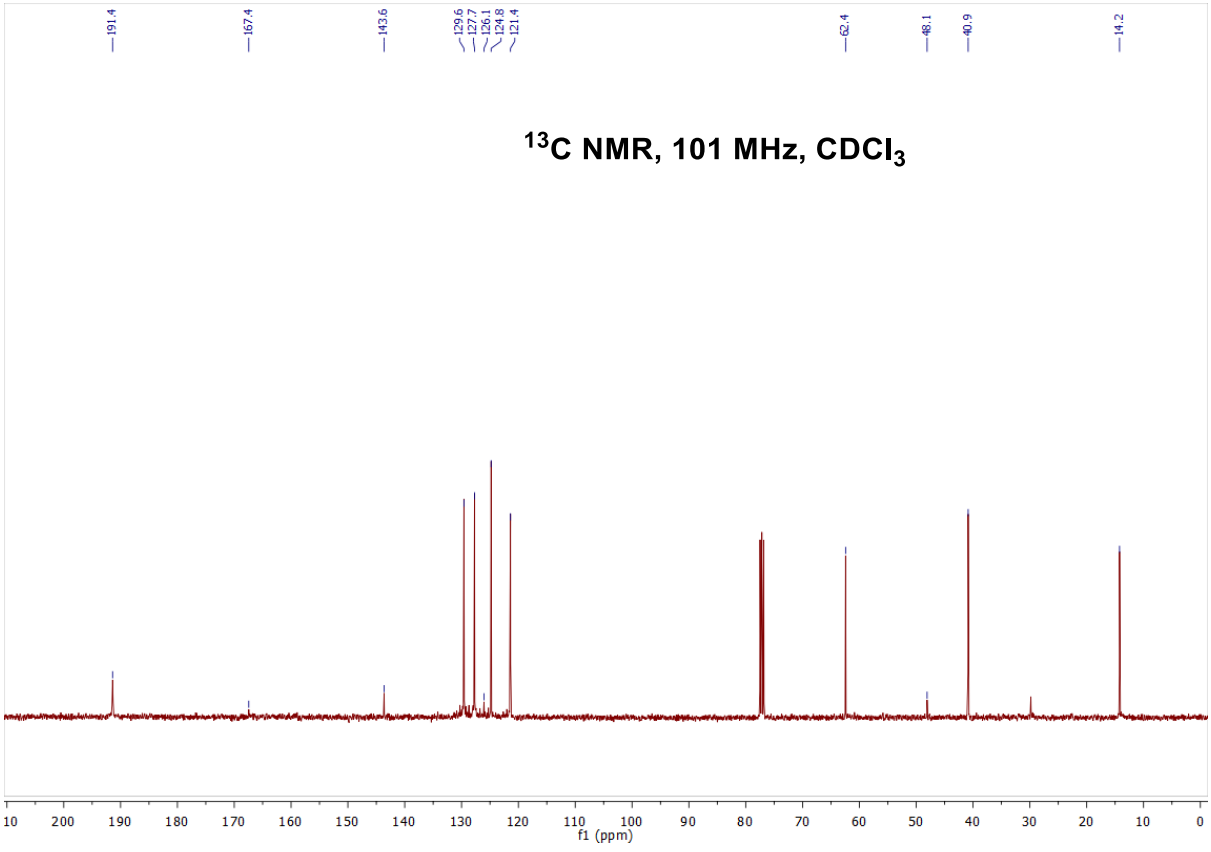


^{13}C NMR, 101 MHz, $CDCl_3$

Synthesis of Ethyl 1-(2-chlorophenyl)-2-formylaziridine-2-carboxylate (4g)

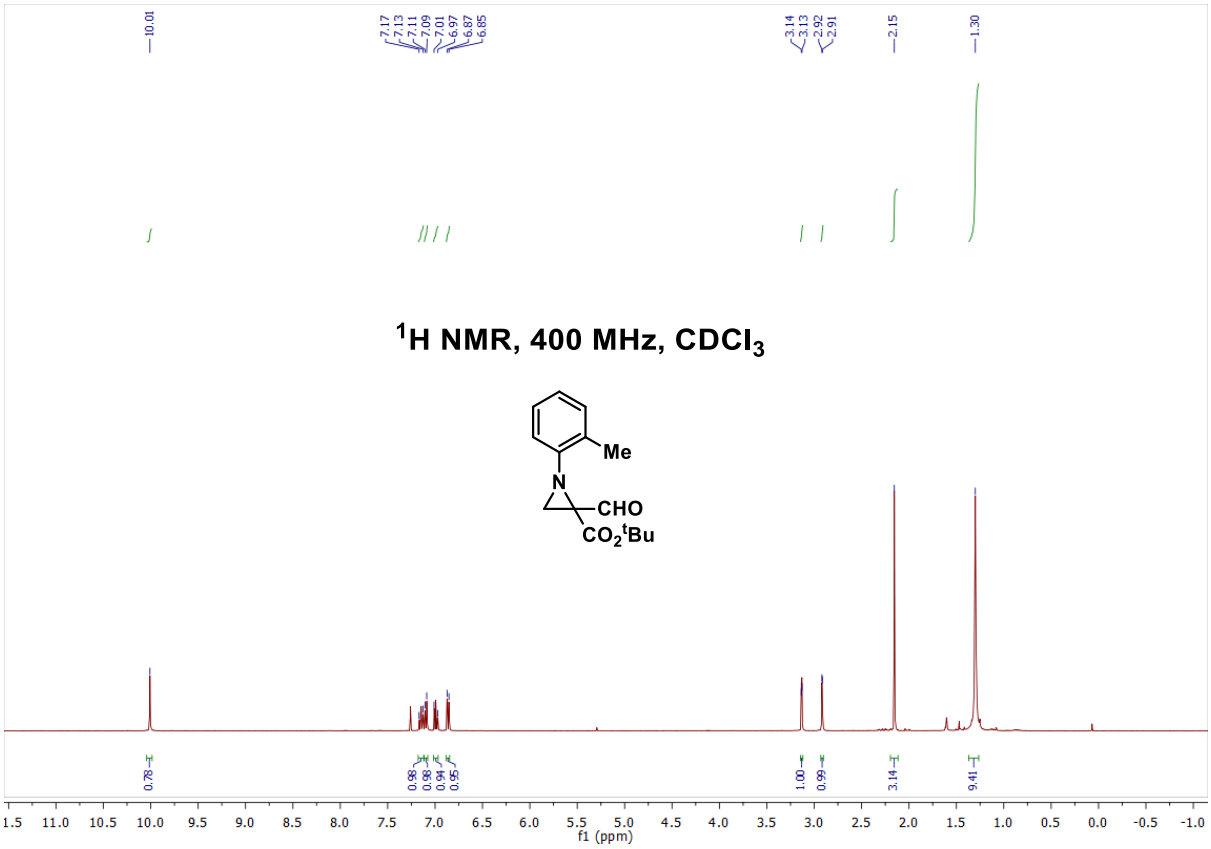


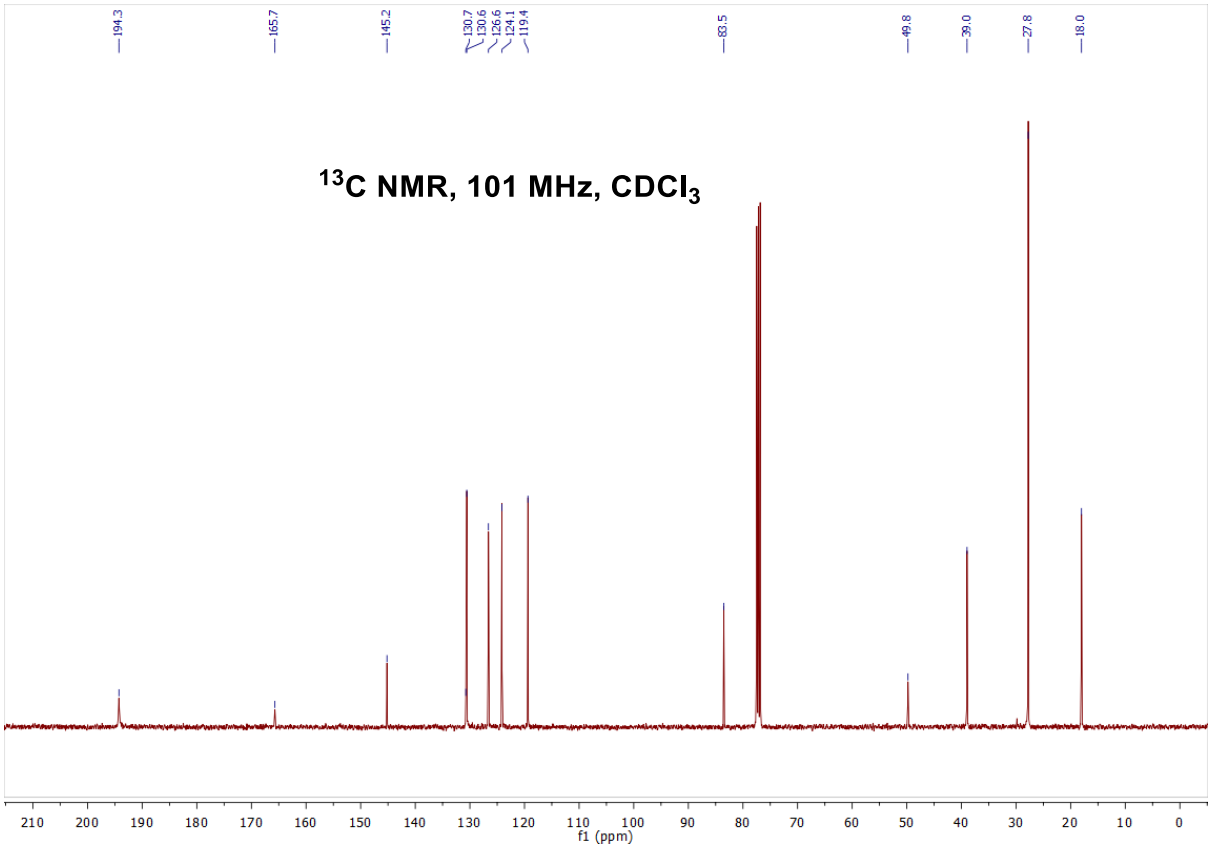
^{1}H NMR, 400 MHz, $CDCl_3$



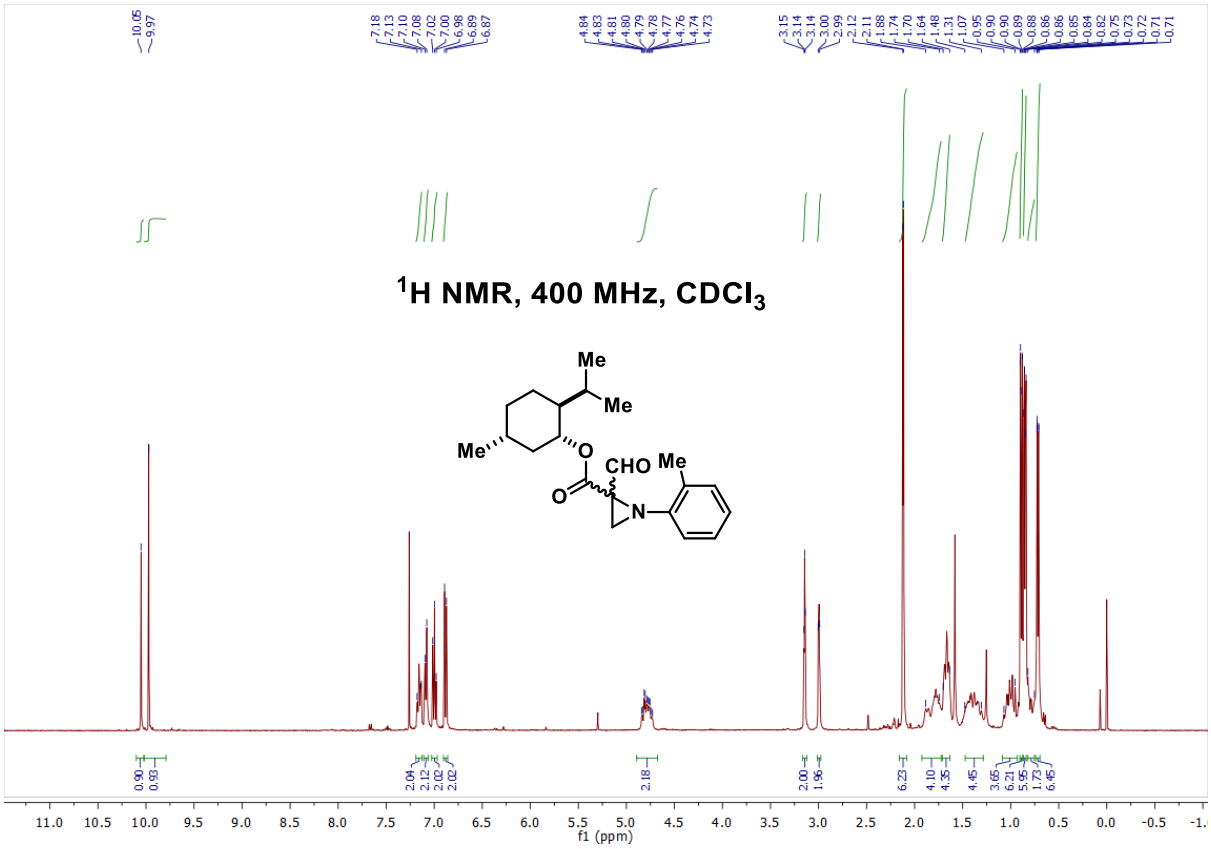
^{13}C NMR, 101 MHz, $CDCl_3$

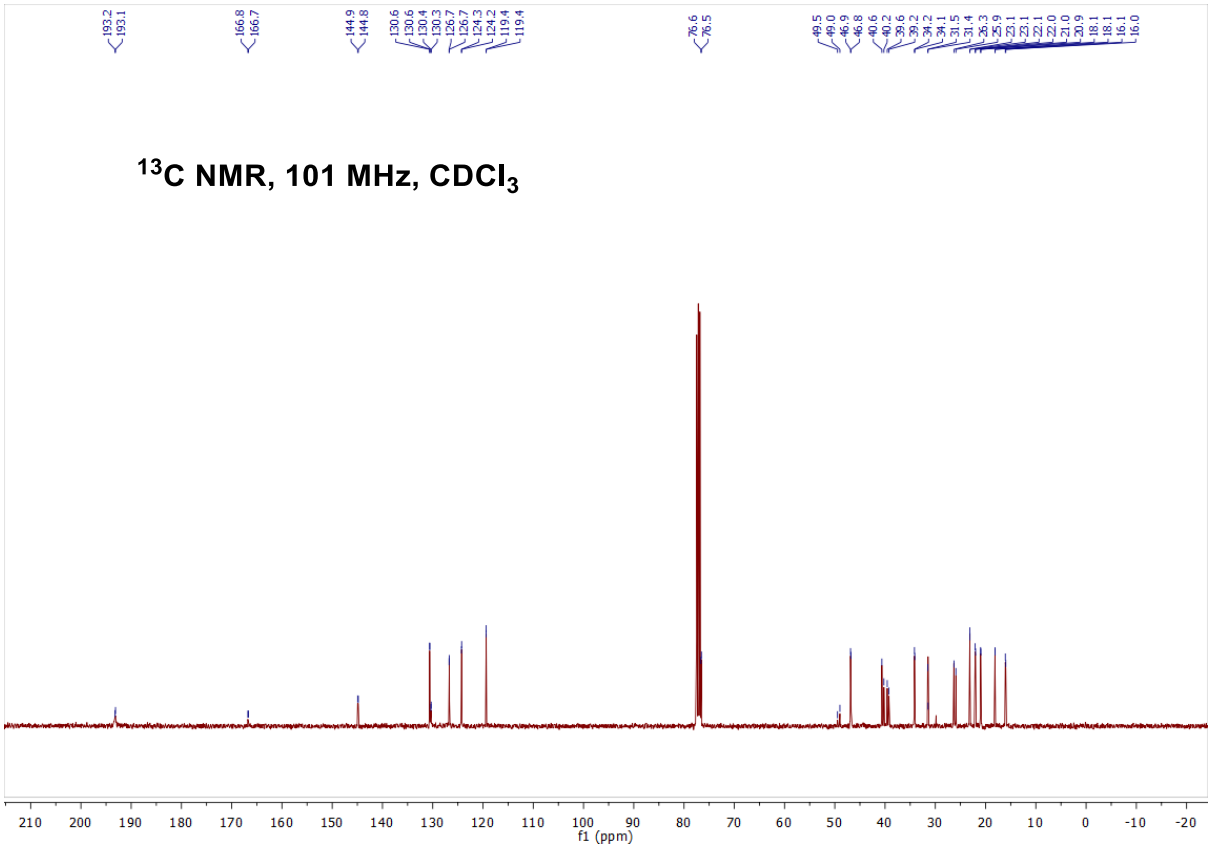
Tert-butyl 2-formyl-1-(*o*-tolyl)aziridine-2-carboxylate (4h)



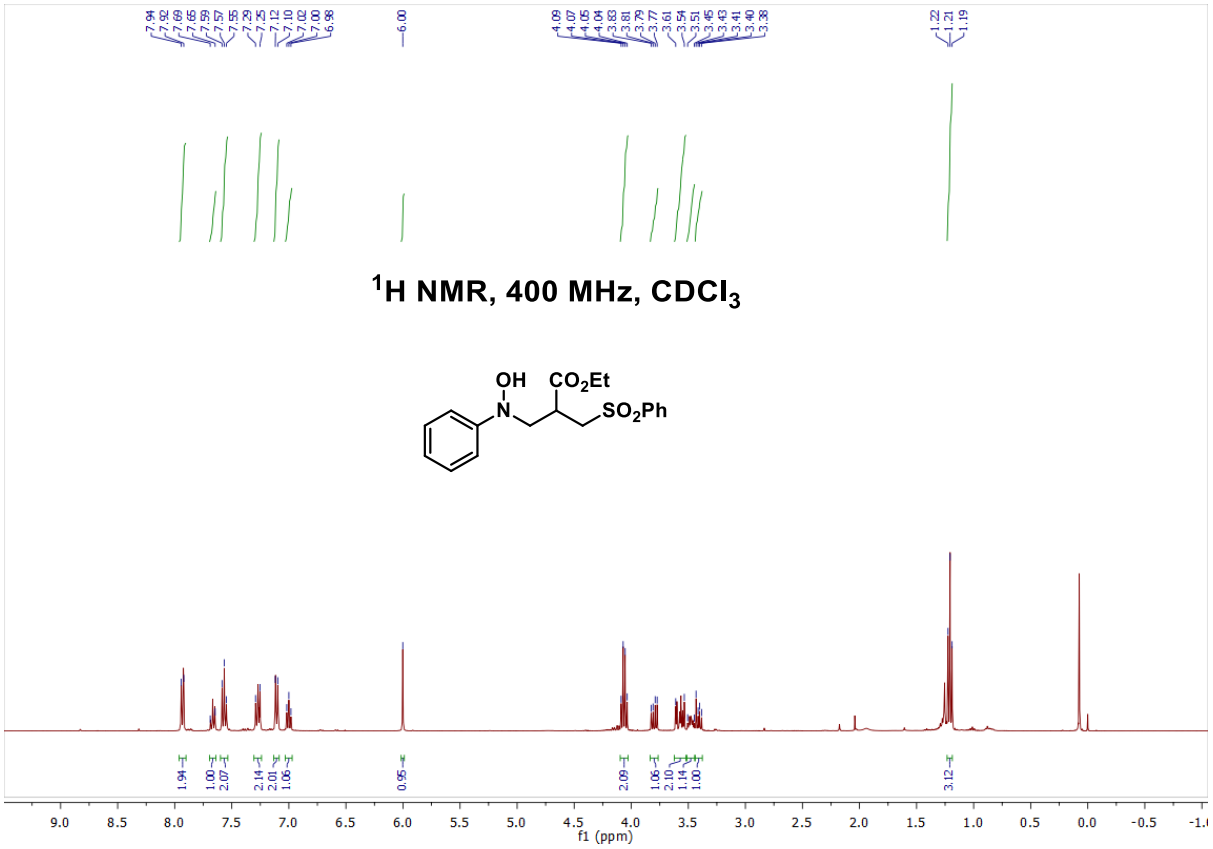


2-Isopropyl-5-methylcyclohexyl 2-formyl-1-(*o*-tolyl)aziridine-2-carboxylate (4i)

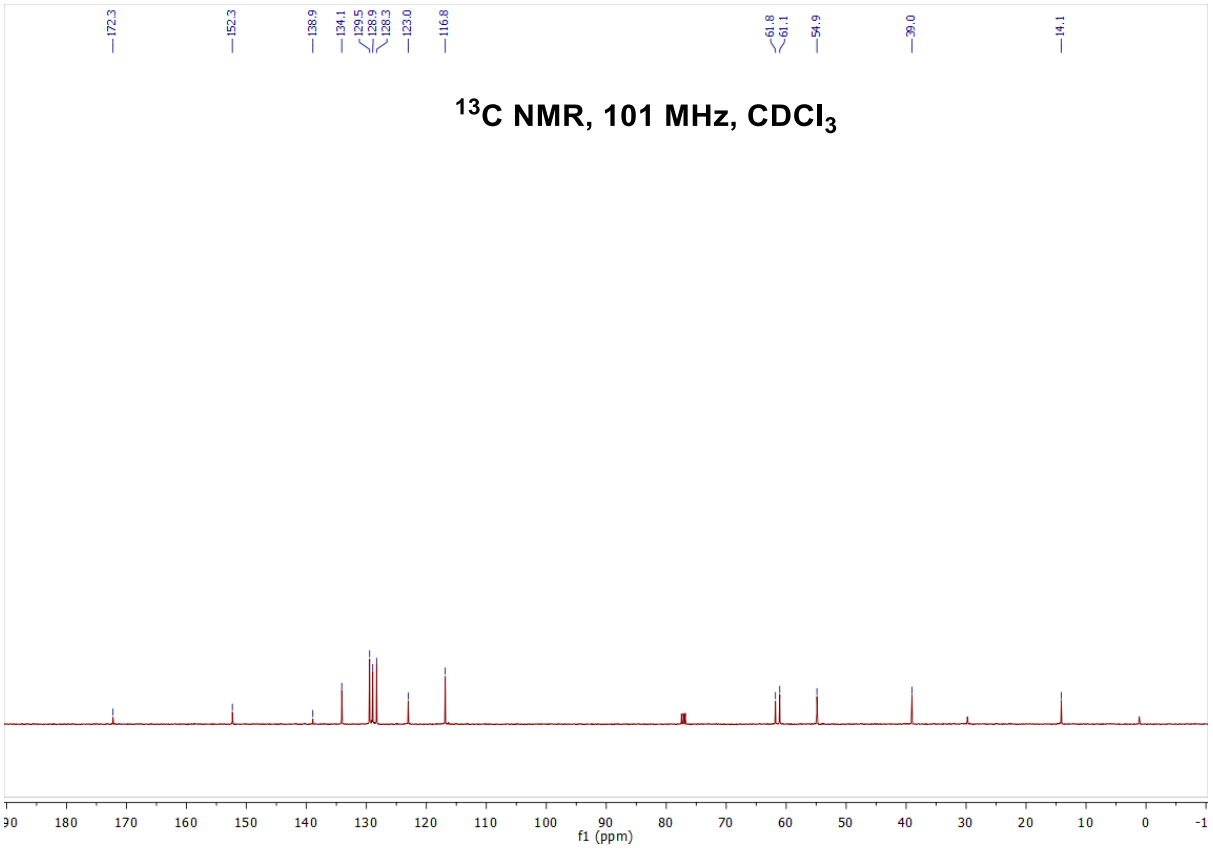




Ethyl 3-(hydroxy(phenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16a)

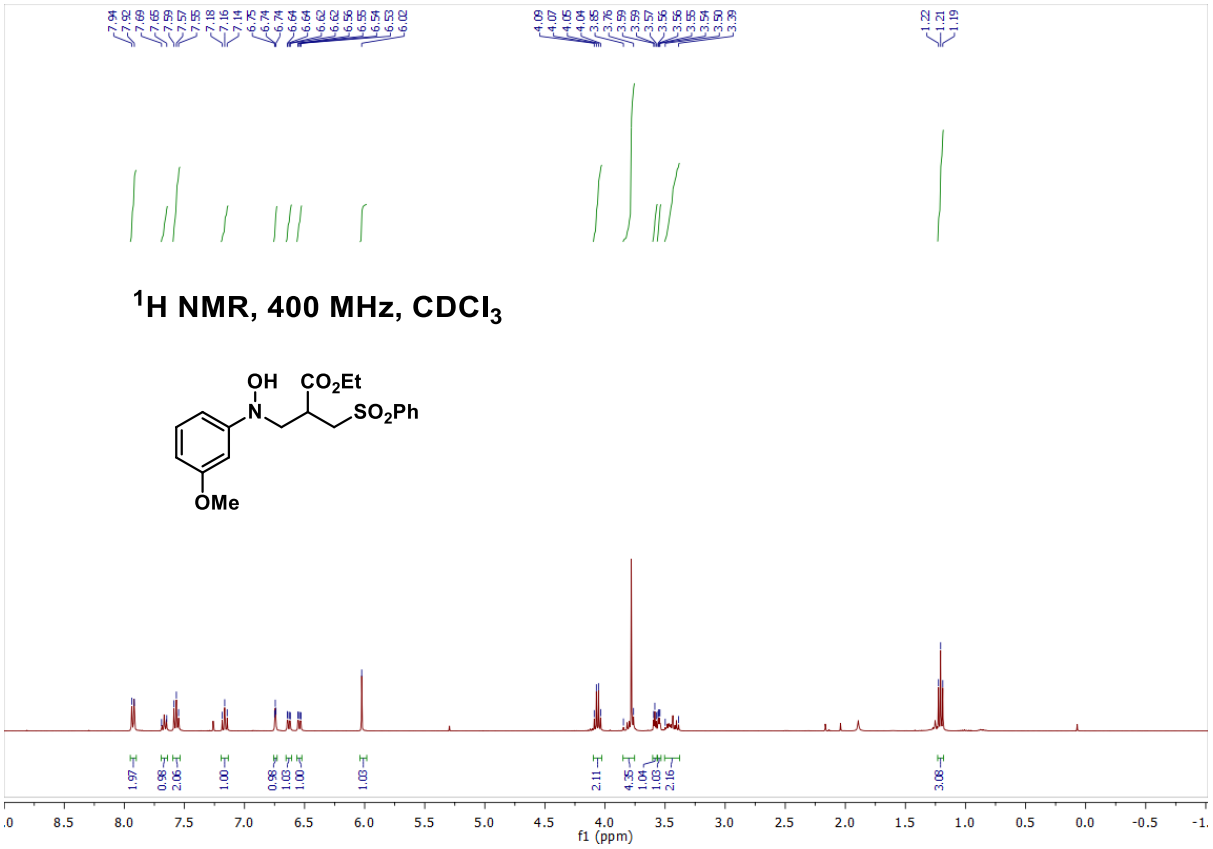


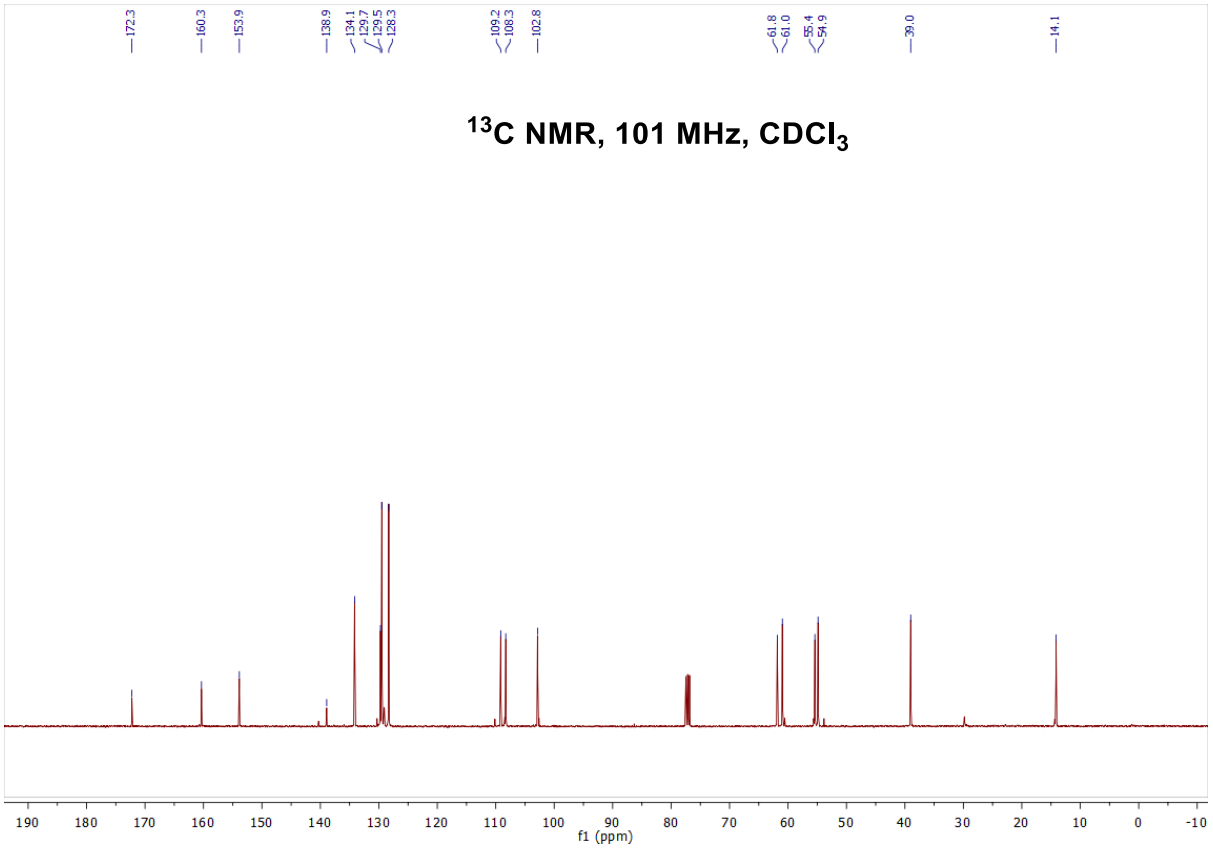
^{1}H NMR, 400 MHz, $CDCl_3$



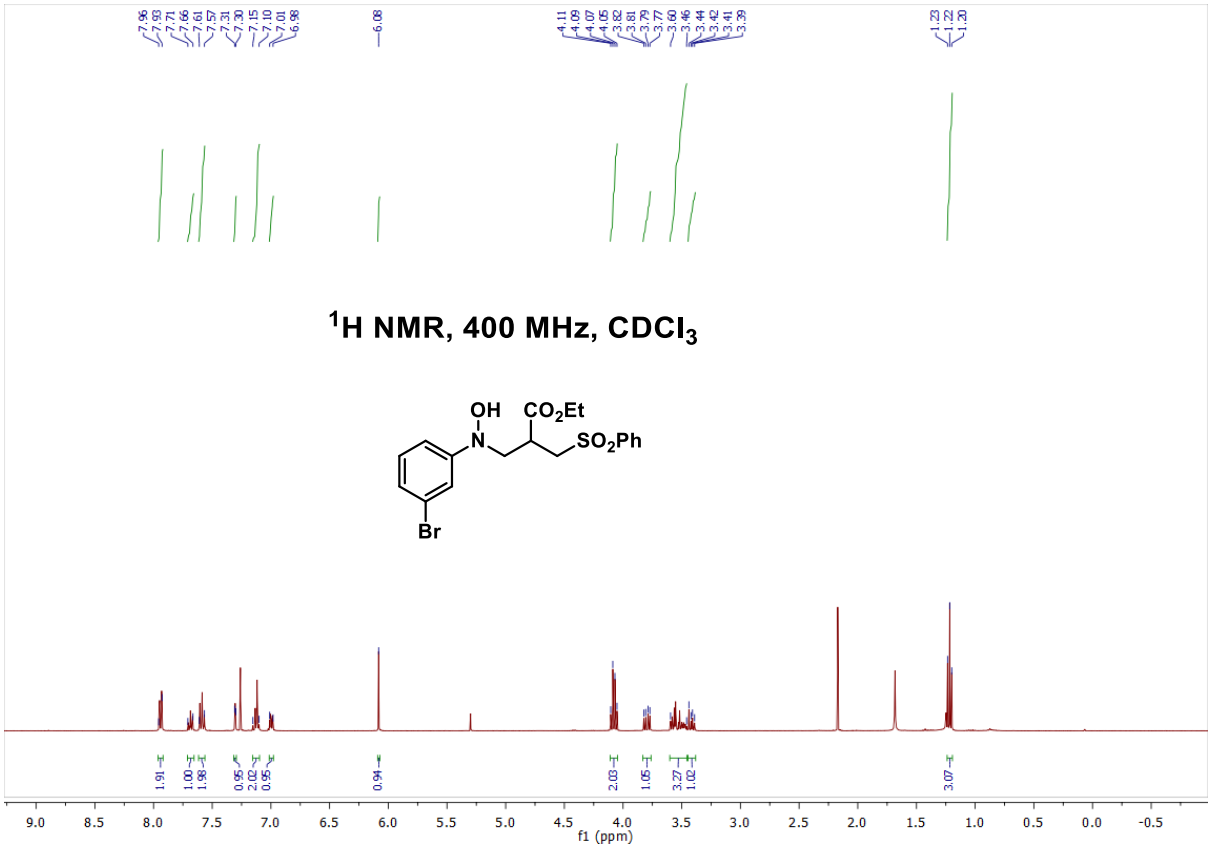
^{13}C NMR, 101 MHz, $CDCl_3$

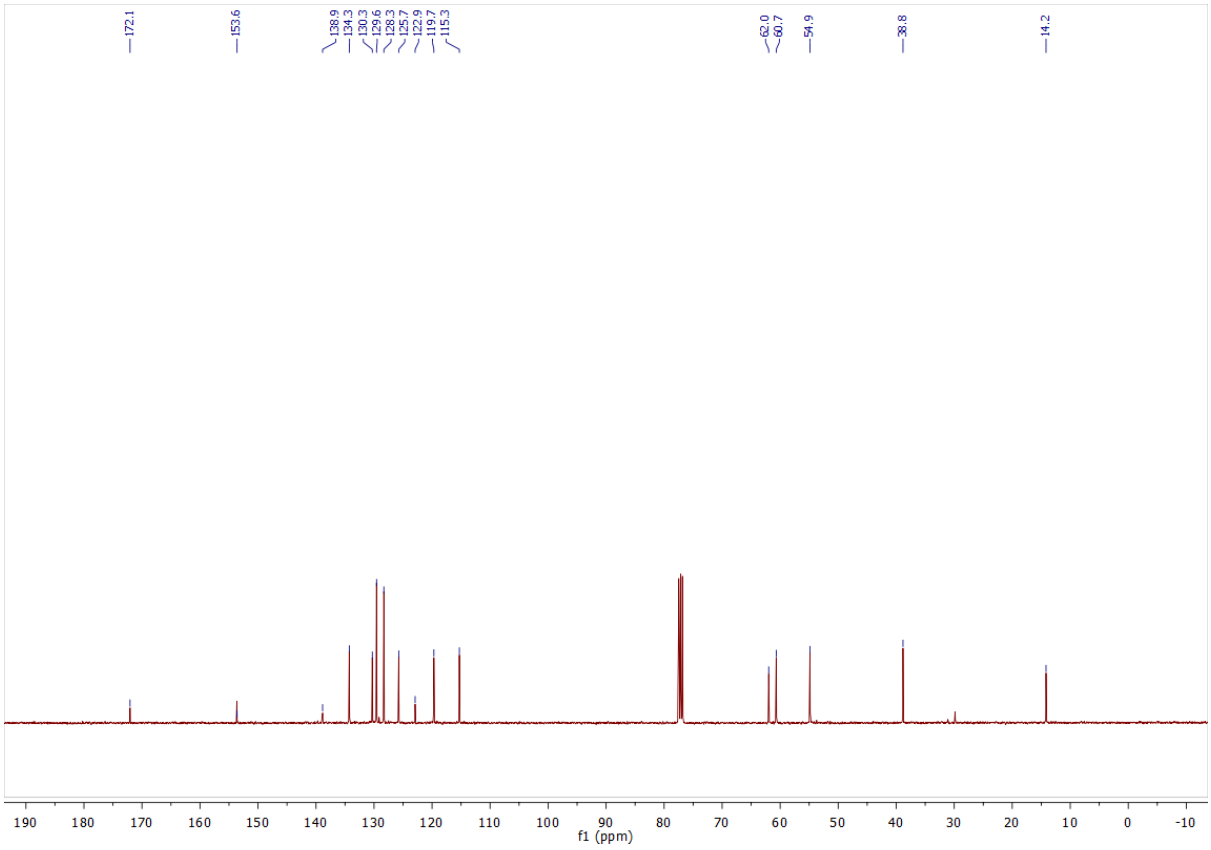
Ethyl 3-(hydroxy(3-methoxyphenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16b)



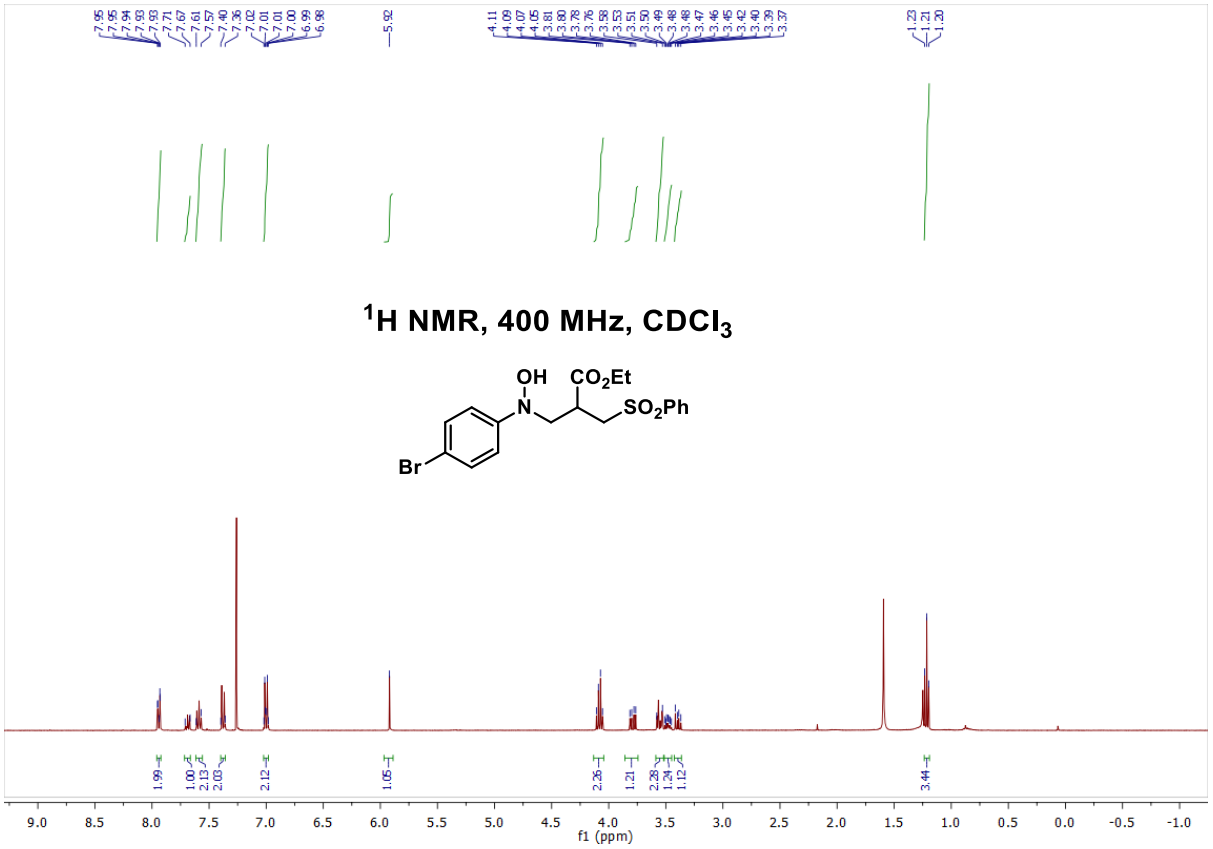


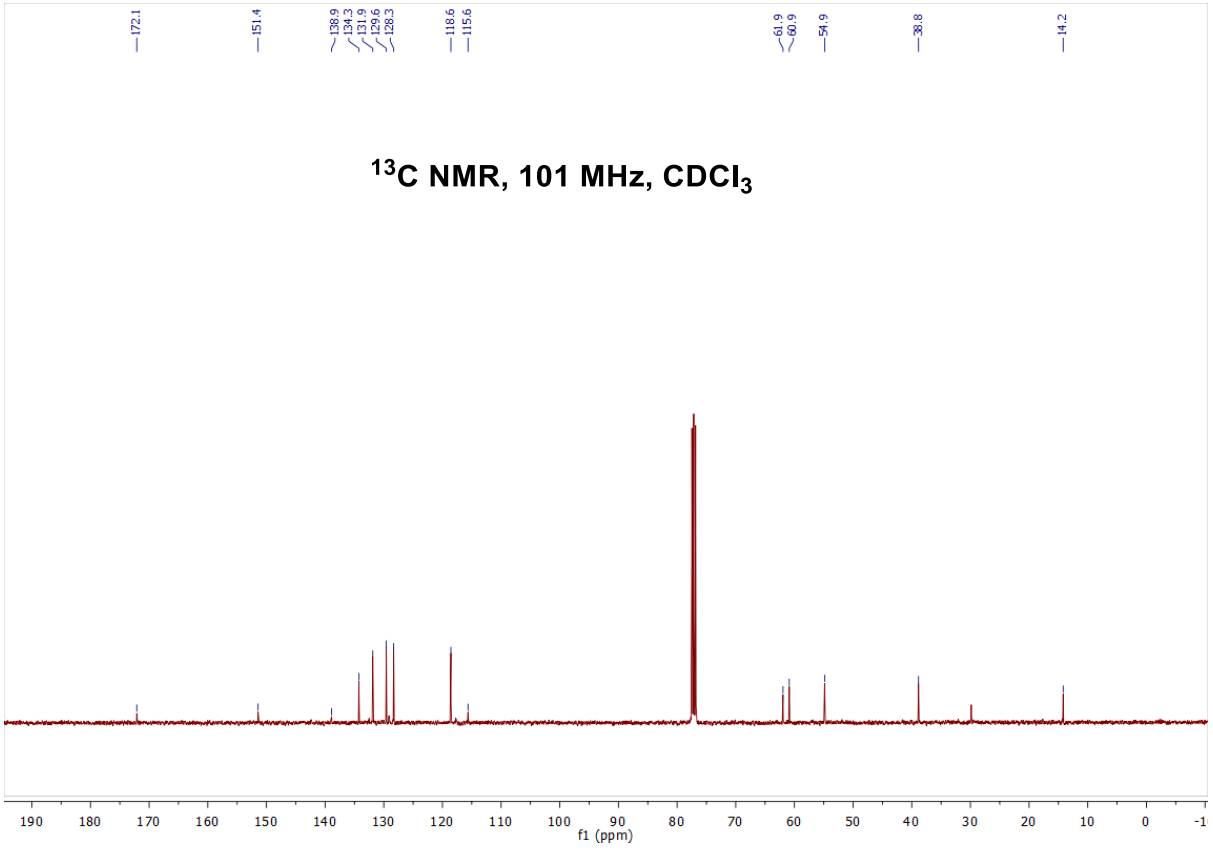
Ethyl 3-((3-bromophenyl)(hydroxy)amino)-2-((phenylsulfonyl)methyl)propanoate (16c)



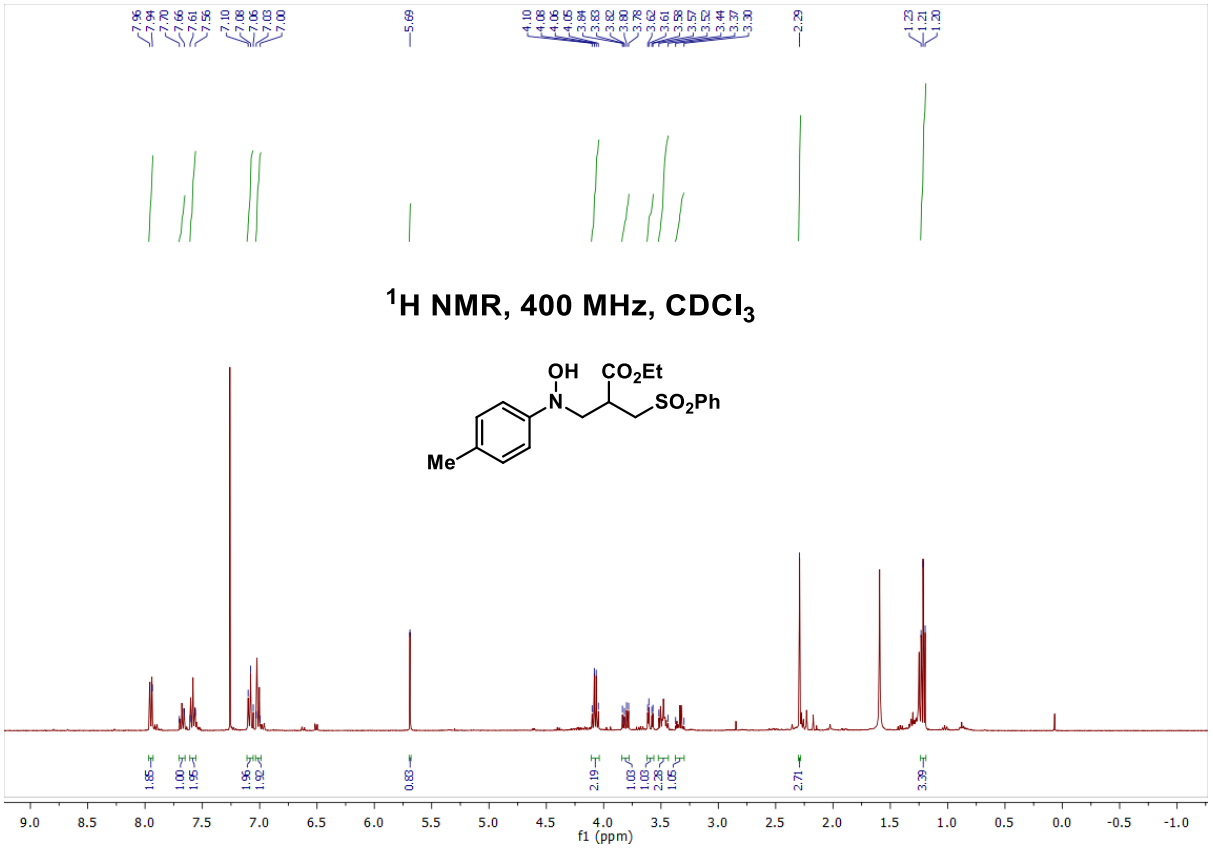


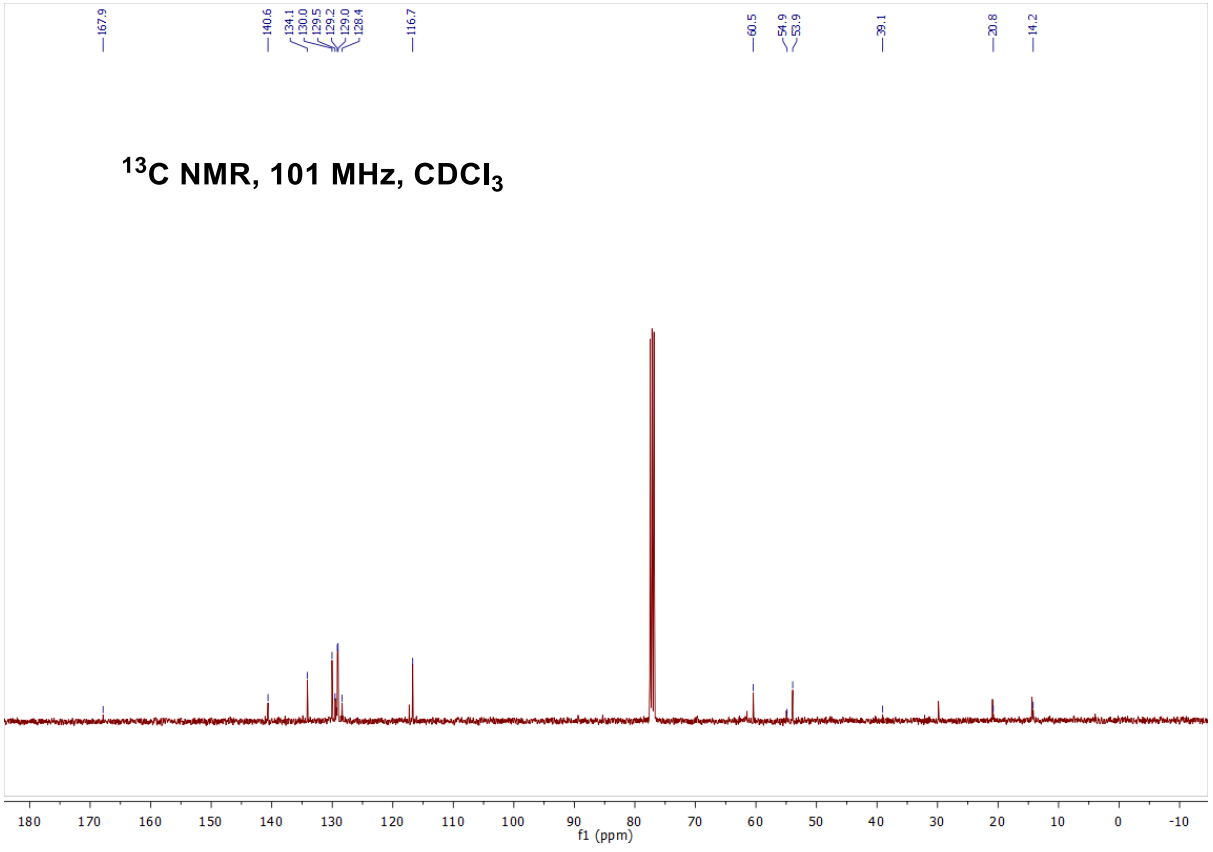
Ethyl 3-((4-bromophenyl)(hydroxy)amino)-2-((phenylsulfonyl)methyl)propanoate (16d)



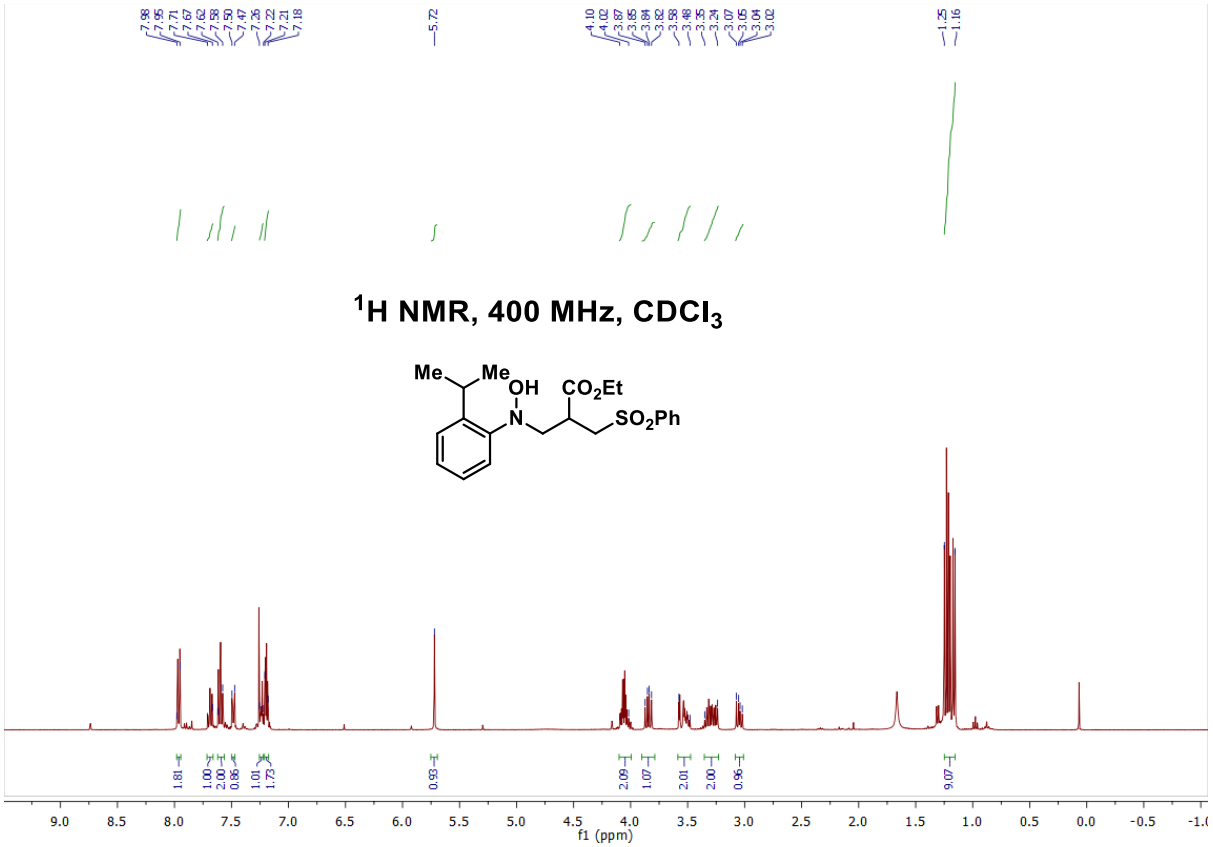


Ethyl 3-(hydroxy(*p*-tolyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16e)

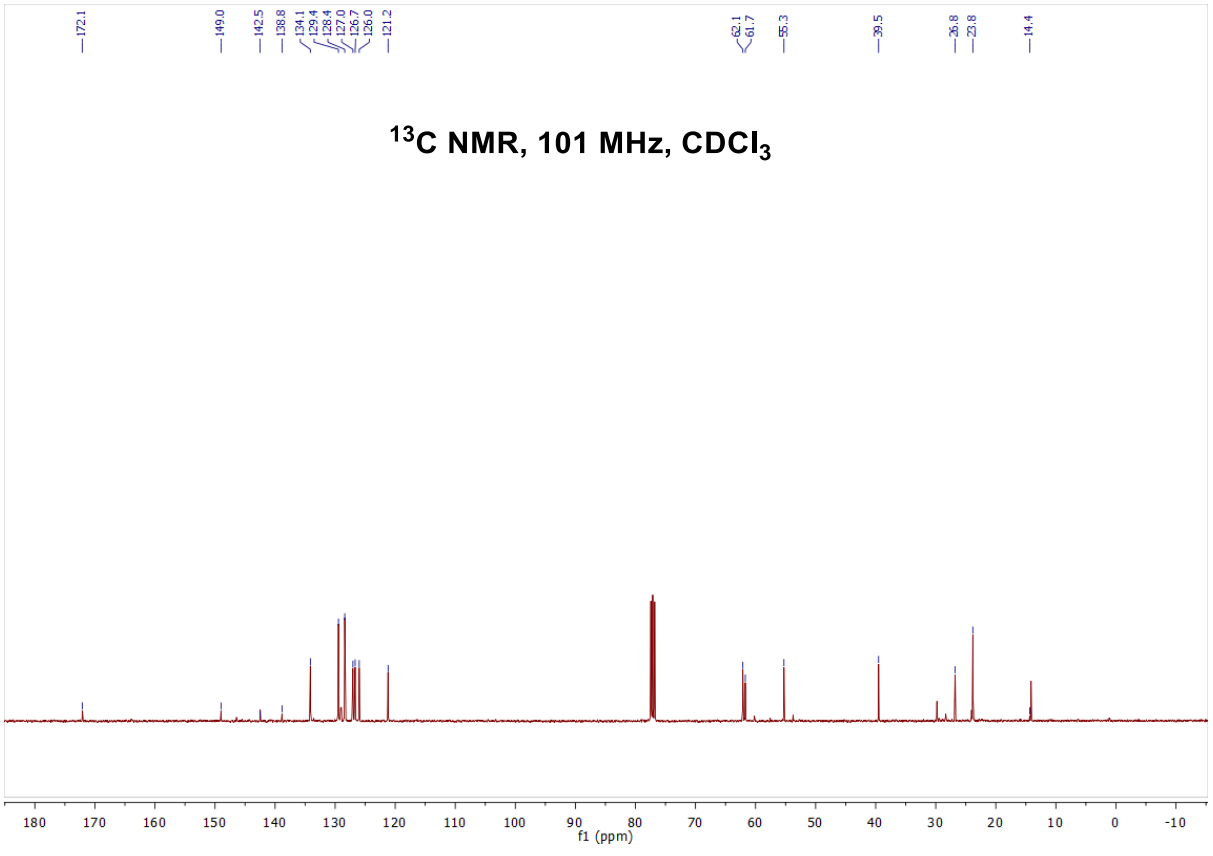




Ethyl 3-(hydroxy(2-isopropylphenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16f)

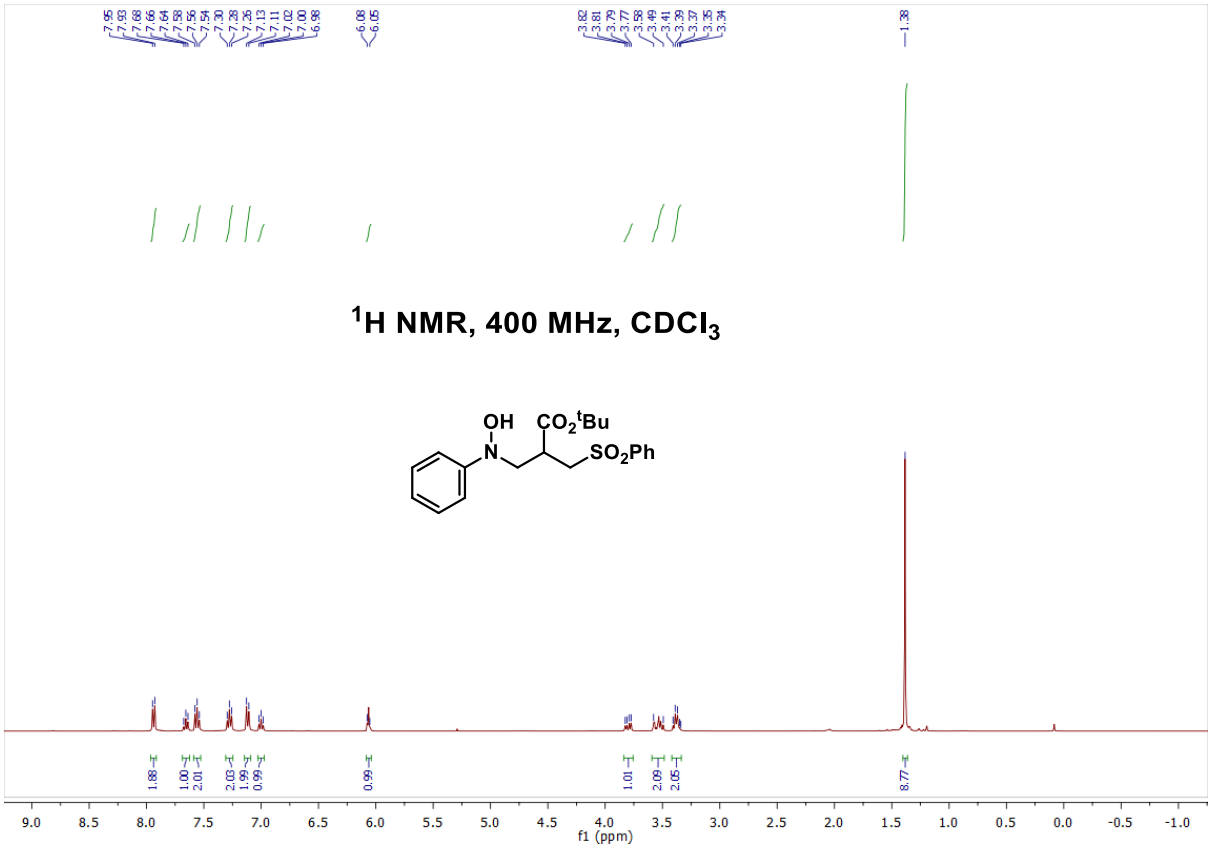


^{1}H NMR, 400 MHz, $CDCl_3$

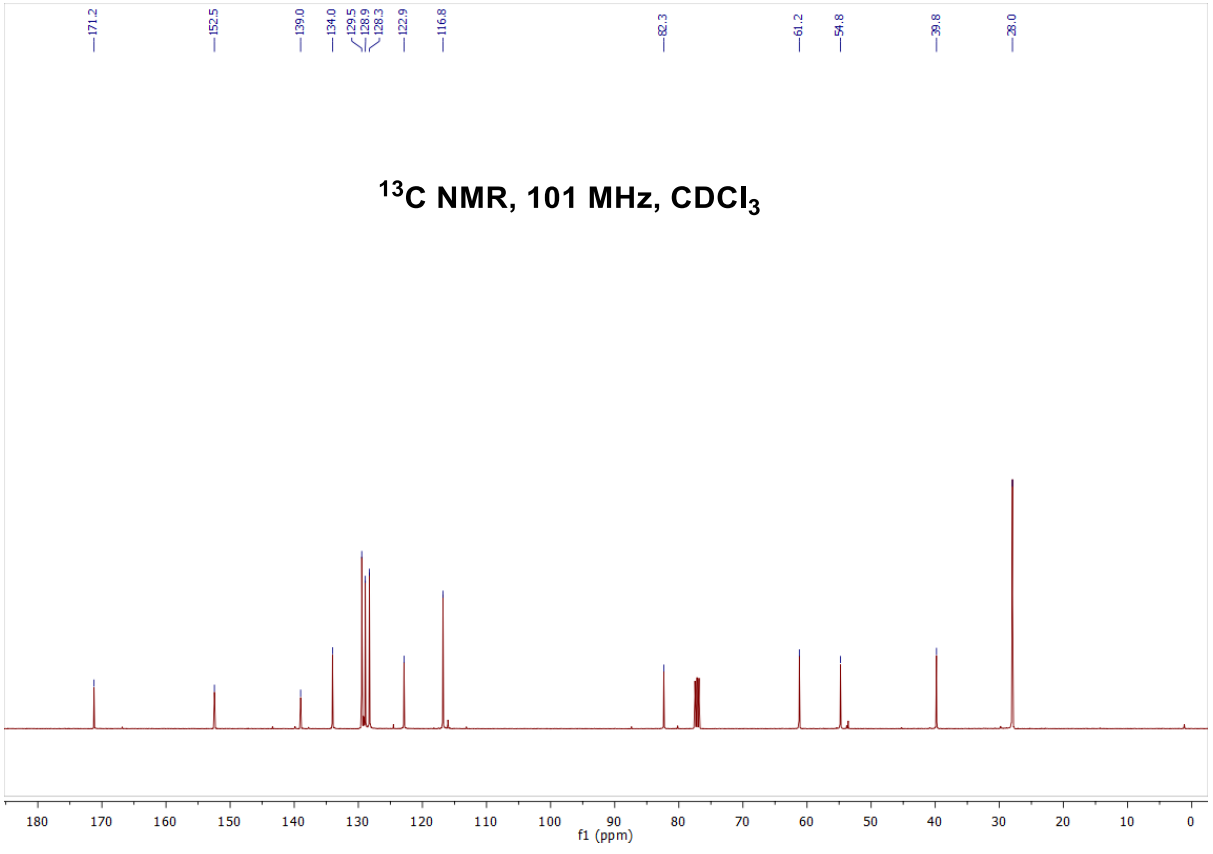


^{13}C NMR, 101 MHz, $CDCl_3$

Tert-butyl 3-(hydroxy(phenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16g)

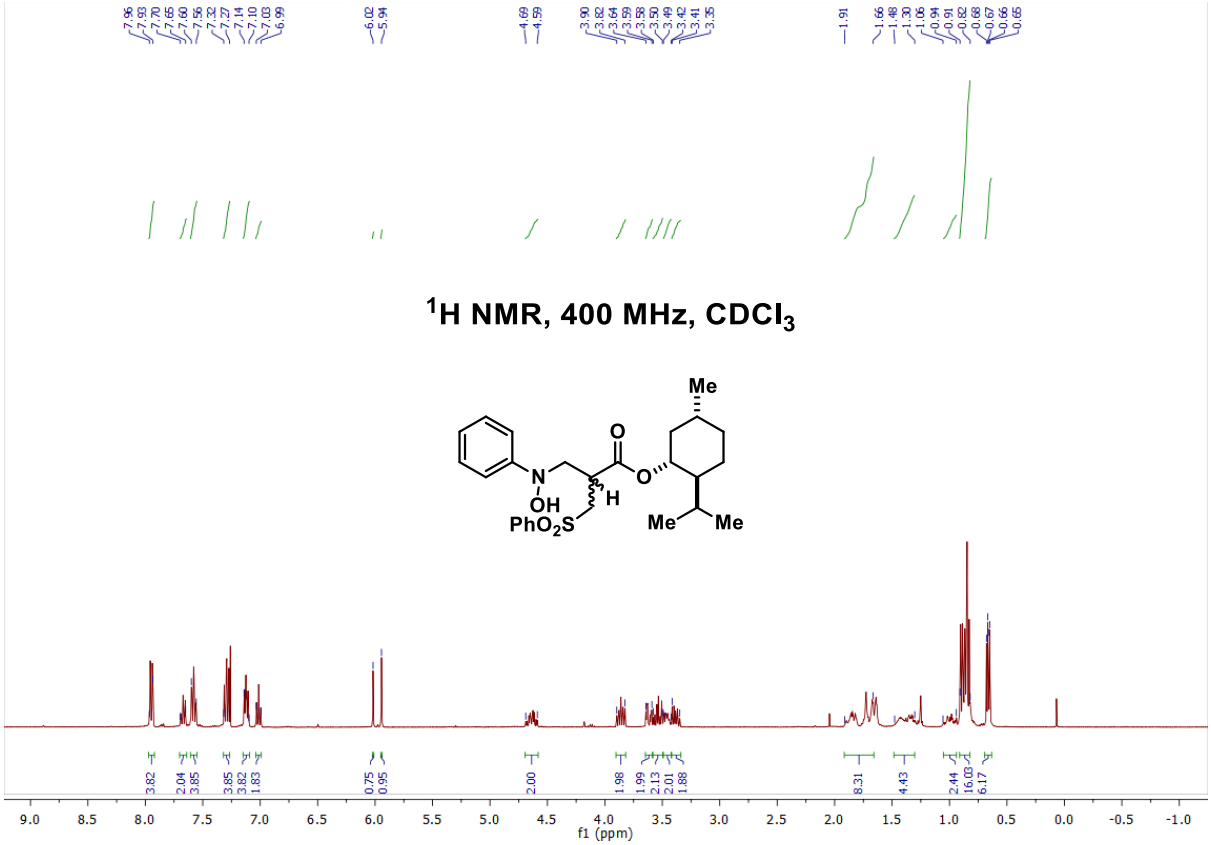


^{1}H NMR, 400 MHz, $CDCl_3$

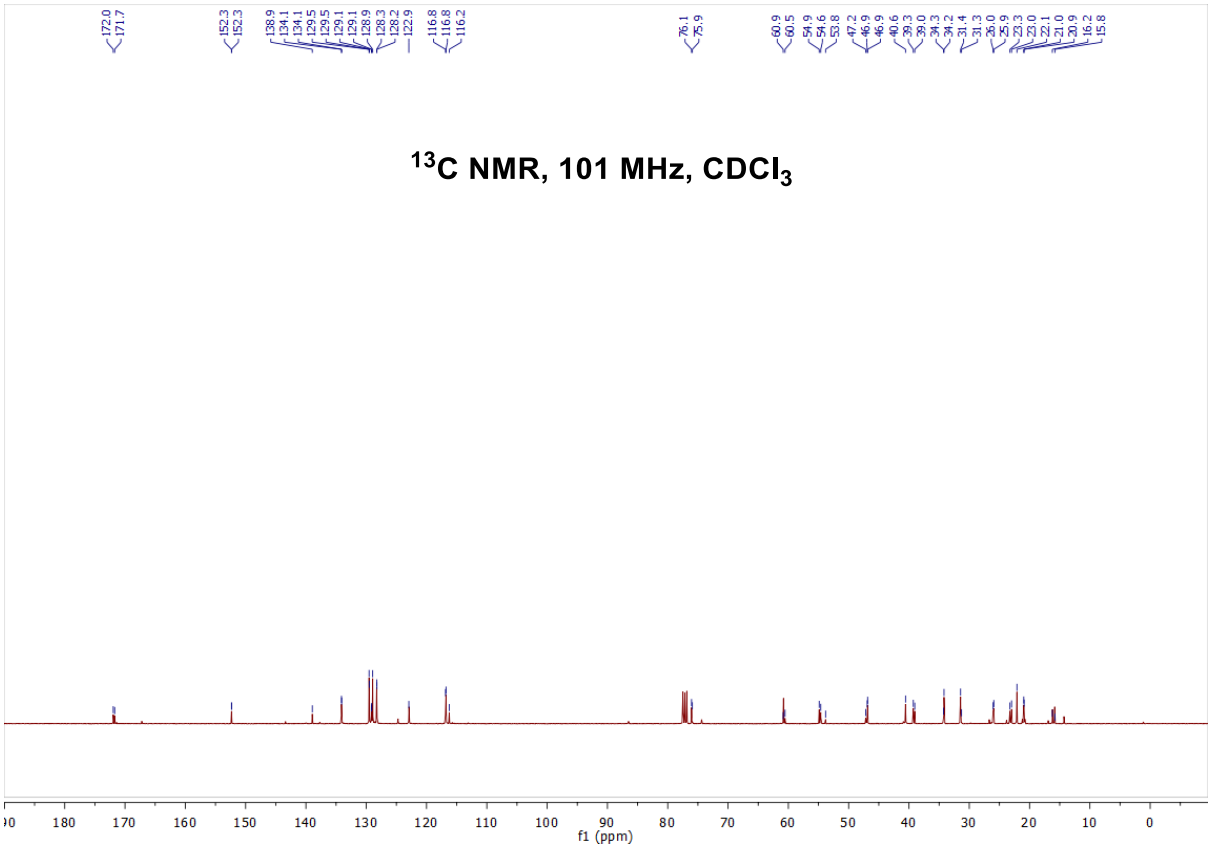


^{13}C NMR, 101 MHz, $CDCl_3$

2-Isopropyl-5-methylcyclohexyl 3-(hydroxy(phenyl)amino)-2-((phenylsulfonyl)methyl)propanoate (16h)

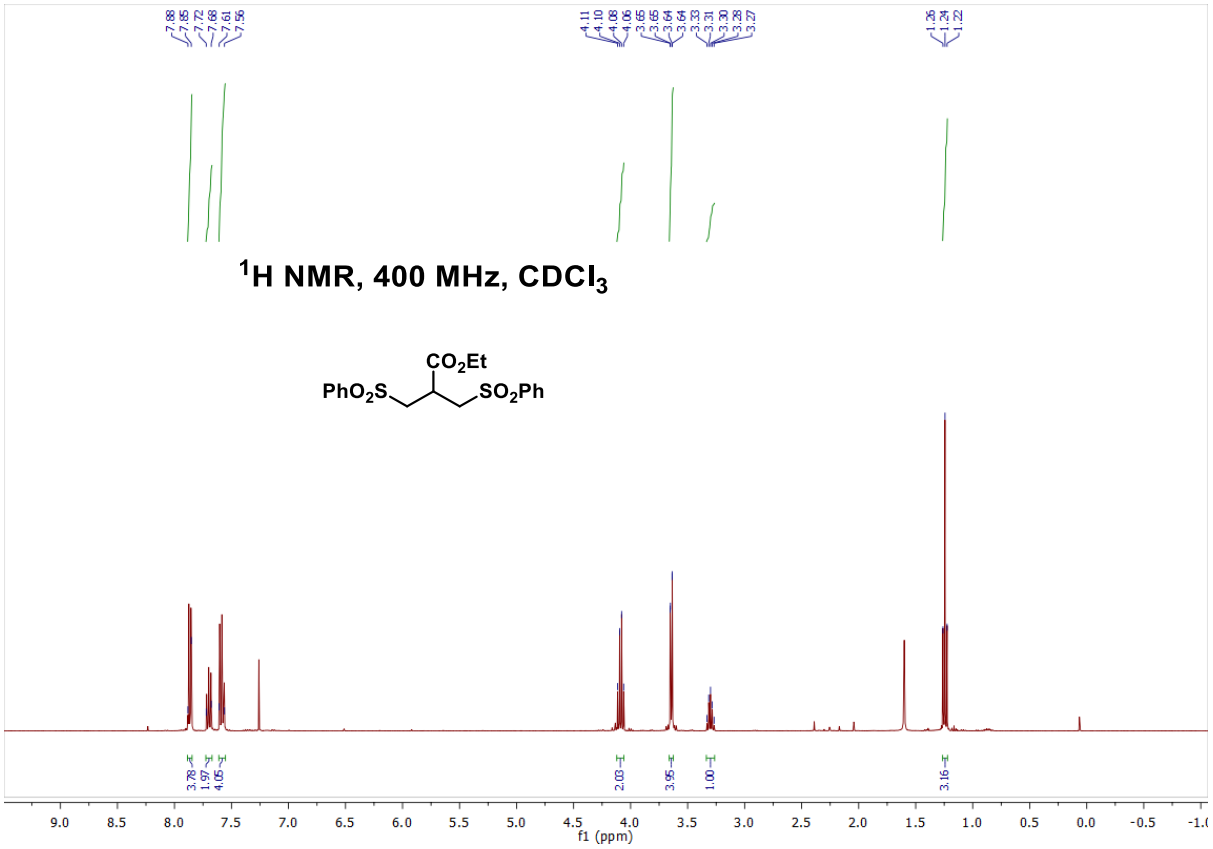


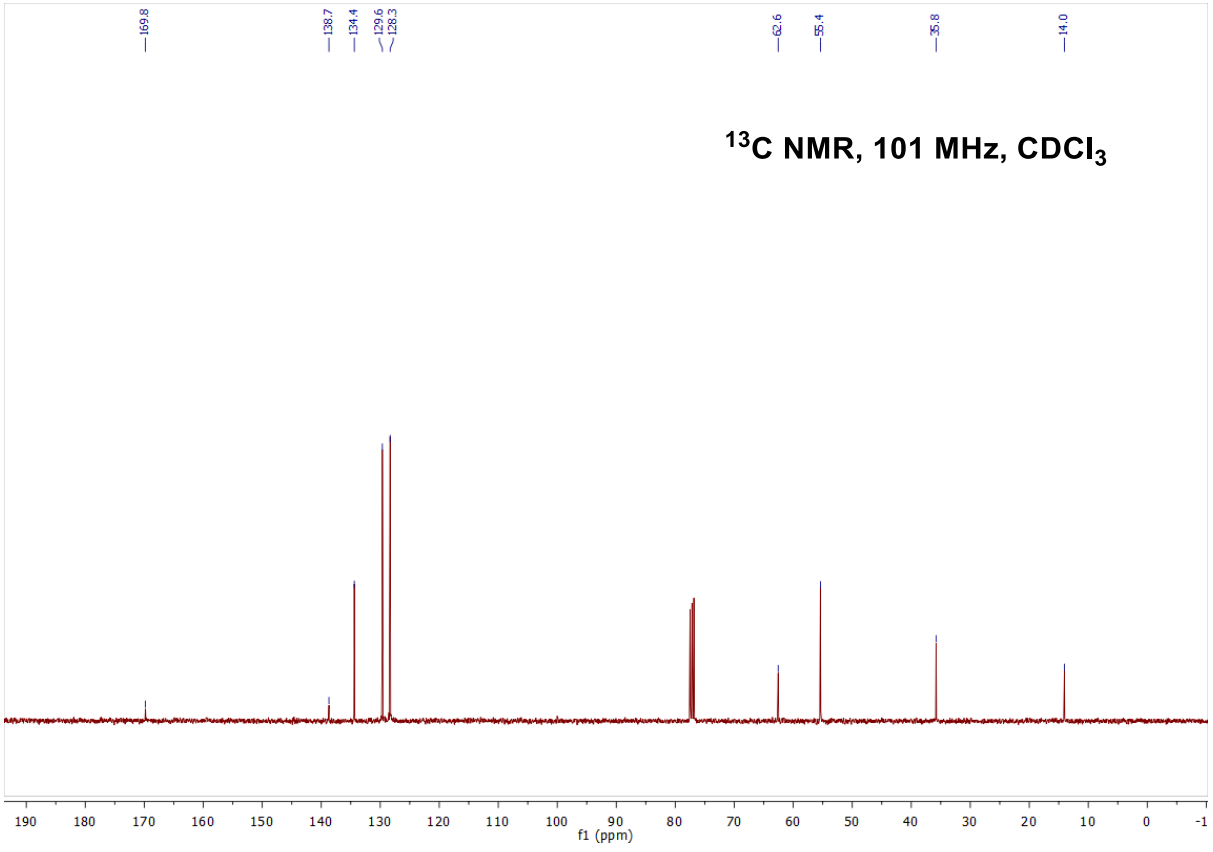
^{1}H NMR, 400 MHz, $CDCl_3$



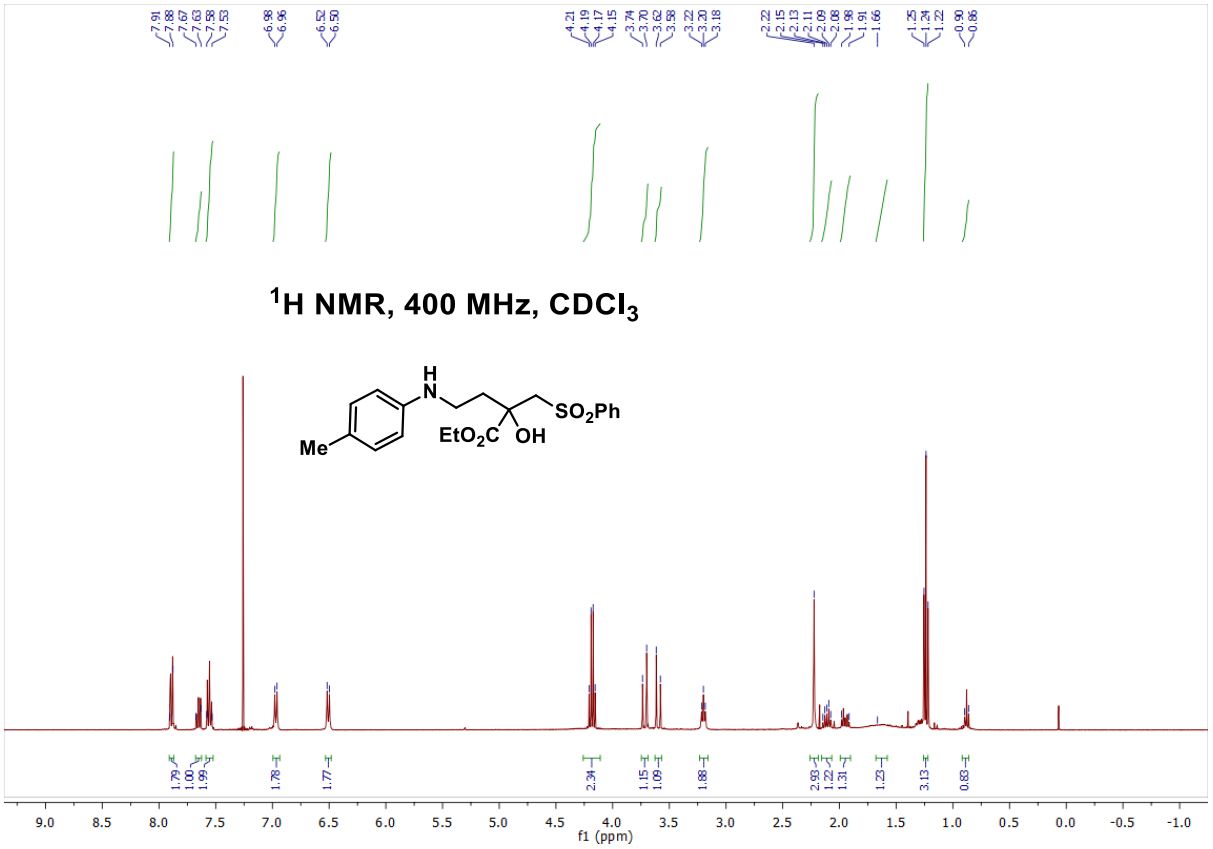
^{13}C NMR, 101 MHz, $CDCl_3$

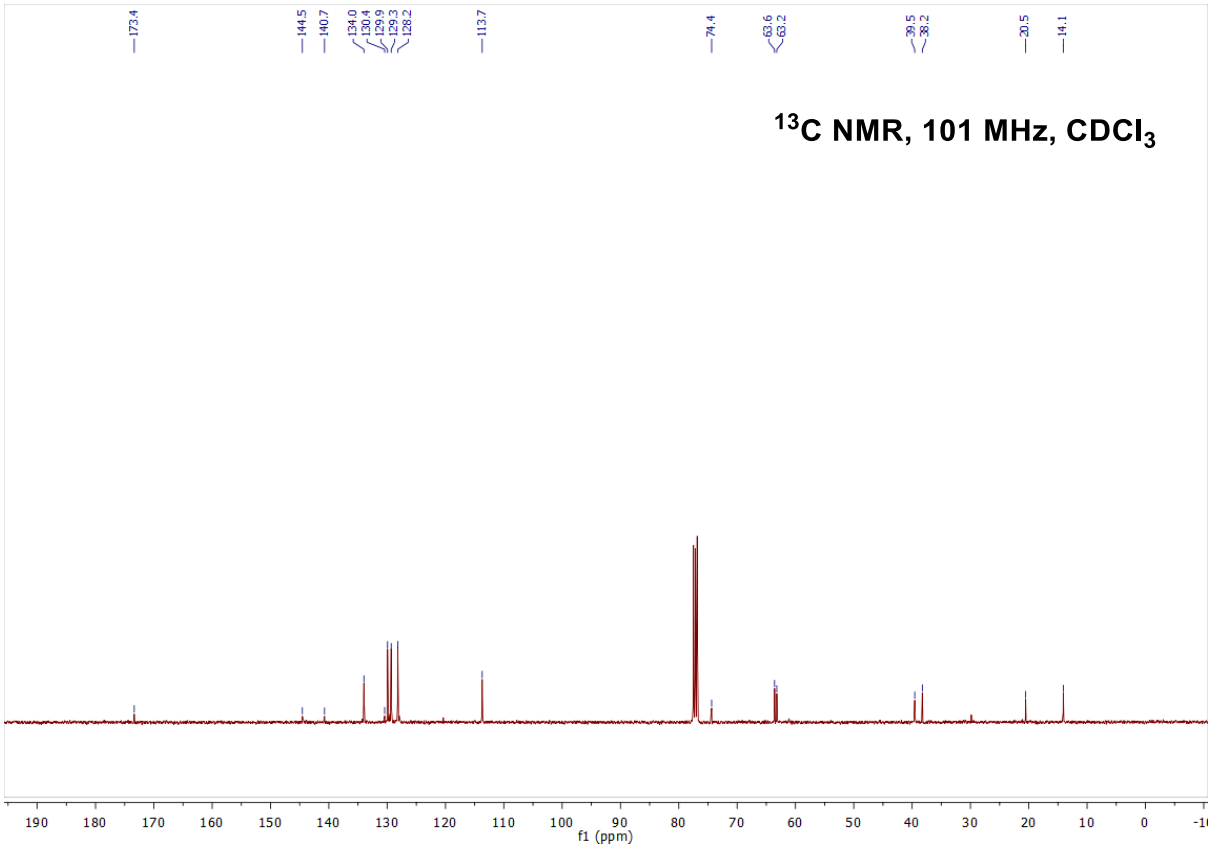
Ethyl 3-(phenylsulfonyl)-2-((phenylsulfonyl)methyl)propanoate (15)





Ethyl 2-hydroxy-2-((phenylsulfonyl)methyl)-4-(*p*-tolylamino)butanoate (5)





Ethyl 1-(2,4-dimethylphenyl)-2-(hydroxymethyl)aziridine-2-carboxylate (6)