Supporting Information

Photochemical HAT-Mediated Site-Selective C(sp^3)−H Aminoalkylation of Cubanes Catalyzed by TBADT

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1. General Information

Unless otherwise noted, all reagents, catalysts and solvents were purchased from commercial suppliers and used without further purification.

Analytical thin layer chromatography was performed using Qingdao Puke Parting Materials Co. silica gel plates (Silica gel 60 F254). Visualization was by ultraviolet fluorescence (λ = 254 nm) or potassium permanganate ($KMnO_4$). Flash column chromatography was performed using 200-300 mesh silica gel.

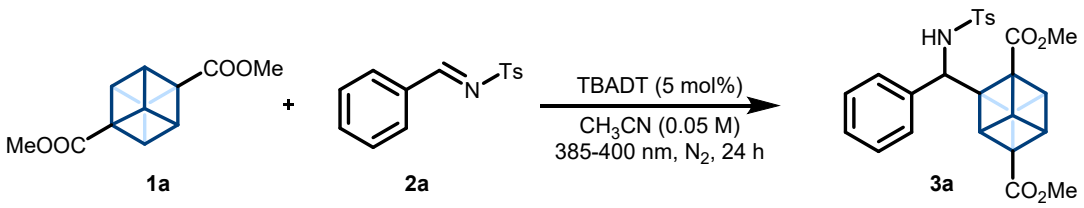
NMR spectra were recorded on Bruker ADVANCE III (400 MHz) spectrometers and JEOL•JNM-ECZL600G. $CDCl_3$ was the solvent used for the NMR analysis, with tetramethylsilane as the internal standard. Chemical shifts were reported up field to TMS (0.00 ppm) for ^{1}H NMR and relative to $CDCl_3$ (77.0 ppm) for ^{13}C NMR.

Melting point was determined using a X-4 made by Peking Taike Apparatus Co. Ltd. HRMS spectra were acquired using an Agilent 6210 ESI/TOF mass spectrometer.

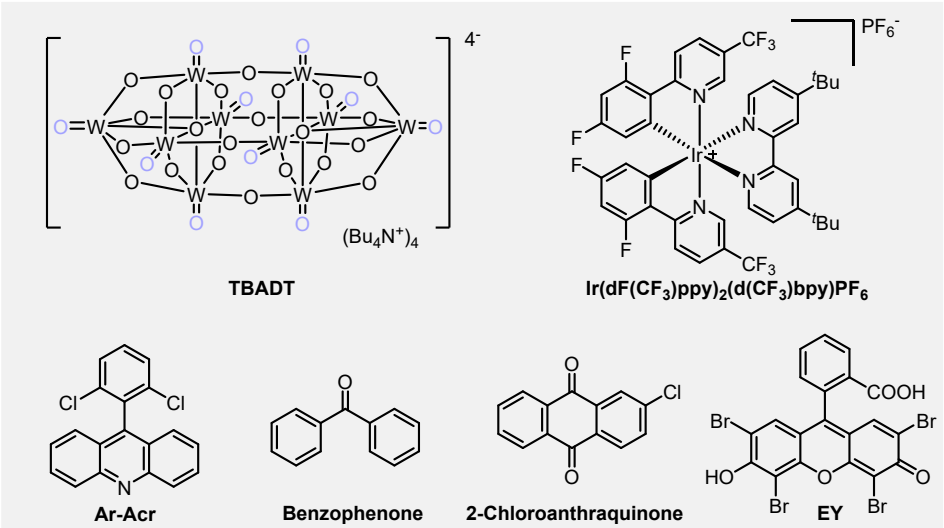
Light Source: Blue LED (Kessil PR160L-390 nm) was bought from Anhui Kemi Machinery Technology Co., Ltd. (http://www.kemiyiqi.com/). Blue LED (HS-385-400nm-72W-8KONG) was bought from Wuhan Geao Chem Technology Co., Ltd (http://www.geaochem.com/).

2. Optimization of reaction conditions

Table S1: Catalysts survey[a]



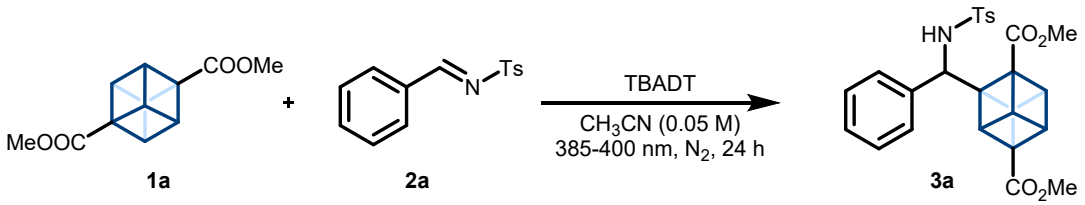
Entry	Cat.	Conv. (%)
1	**TBDAT**	61
2	**Ir(dF(CF$_3$)ppy)$_2$(d(CF$_3$)bpy)PF**	0
3	**Ac-Acr**	<5
4	**Benzophenone**	0
5	**2-Chloroanthraquinone**	10
6	**EY**	0
7	**None**	0
8	**TBDAT** (2.5 mol%)	32



[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.1 mmol), Cat. (5 mol%), in 2.0 mL of CH_3CN under N_2 and irradiated with a 380-400 nm LED for 24 h. Yields were referred to crude ^1H NMR by using 1,3,5-trimethoxybenzene as internal

standard.

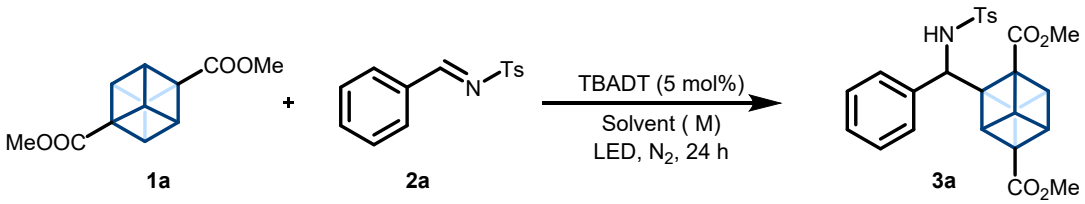
Table S2: Effect of catalyst amount[a]



Entry	TBDAT (mol%)	Conv. (%)
1	5	61
2	2.5	32
3	1	28
4	10	65
5	20	53

[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.1 mmol), TBDAT in CH_3CN (0.05 M) under N_2 and irradiated with a LED for 24 h. Yields were referred to crude ^1H NMR by using 1,3,5-trimethoxybenzene as internal standard.

Table S3: Solvent, concentration and light source survey[a]

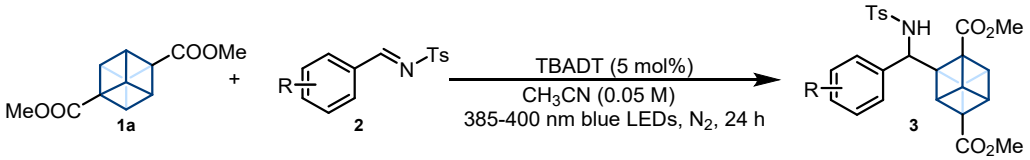


Entry	Solvent	Light source	Conv. (%)
1	Tol (0.05 M)	380-400 nm (70 W)	32
2	Benzene (0.05 M)	380-400 nm (70 W)	35
3	THF (0.05 M)	380-400 nm (70 W)	<5
4	CH_3CN (0.05 M)	380-400 nm (70 W)	61

5	DMF (0.05 M)	380-400 nm (70 W)	<5
6	CH_3CN (0.1 M)	380-400 nm (70 W)	11
8	CH_3CN (0.025 M)	380-400 nm (70 W)	21
9	CH_3CN (0.1 M)	410 nm Kessil lamp	<5
10	CH_3CN (0.1 M)	365 nm Kessil lamp	36
11	CH_3CN (0.1 M)	456 nm Kessil lamp	trace

[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.1 mmol), TBDAT (5 mol%), in solvent under N_2 and irradiated with a LED for 24 h. Yields were referred to crude ^1H NMR by using 1,3,5-trimethoxybenzene as internal standard.

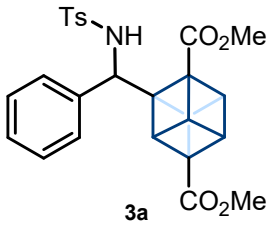
3. General Procedure for the aminoalkylation of cubane



To a 20 mL glass test tube was added TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol) and toluenesulfonyl imine **2** (0.2 mmol) under N_2. Then, degassed MeCN (4 mL, 0.05 M) was added to the test tube under N_2. The vial was capped with flat stopper and irradiated with HS-384-400 nm-72W-8KONG lamps for 24 h with stirring. After the reaction, the stopper was opened and reaction was quenched with air until the blue color disappeared, then the reaction solution was diluted with 10 mL water, extracted with 15 mL ethyl acetate twice, washed with saturated salt water once, the combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by *prep*-HPLC. The corresponding cubane-aryl methylamine product **3** was obtained.

4. Analytical Data of the of cubane-aryl methylamines

dimethyl (2r,3R,4r,5S)-2-(((4-methylphenyl) sulfonamido) (phenyl) methyl) cubane-1,4-dicarboxylate (3a)



Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-benzylidene-4-methylbenzenesulfonamide **2a** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3a** as a white solid (58.4 mg, 61% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

MP: 163-166 °C.

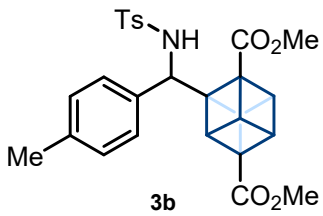
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.16 – 7.08 (m, 3H), 7.05 (d, *J* = 7.6 Hz, 2H), 6.96 – 6.89 (m, 2H), 6.27 (d, *J* = 8.6 Hz, 1H), 4.72 (d, *J* =

8.5 Hz, 1H), 4.17 – 4.06 (m, 3H), 4.00 (dt, *J* = 5.2, 2.5 Hz, 1H), 3.95 (td, *J* = 5.3, 2.5 Hz, 1H), 3.65 (d, *J* = 3.5 Hz, 6H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.21, 171.33, 142.95, 138.17, 136.05, 129.29, 128.38, 127.57, 127.25, 127.13, 60.50, 58.31, 57.08, 52.19, 52.17, 51.85, 48.35, 47.92, 47.45, 44.83, 43.84, 21.55.

HRMS：calculated for $C_{26}H_{25}NO_6S$ [M+Na]$^+$ 502.1295; found 502.1302.

dimethyl (2r,3R,4r,5S)-2-(((4-methylphenyl) sulfonamido) (p-tolyl) methyl) cubane-1,4-dicarboxylate (3b)



3b

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-4-methyl-*N*-(4-methylbenzylidene)benzenesulfonamide **2b** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3b** as a white solid (54.0 mg, 55% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

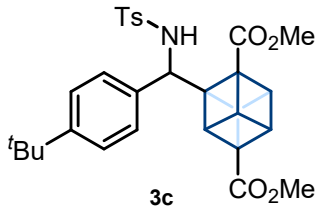
MP: 156-160 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.90 (d, *J* = 7.9 Hz, 2H), 6.80 (d, *J* = 8.1 Hz, 2H), 6.24 (d, *J* = 8.6 Hz, 1H), 4.67 (d, *J* = 8.6 Hz, 1H), 4.15 – 4.04 (m, 3H), 3.97 (ddt, *J* = 15.5, 5.5, 2.7 Hz, 2H), 3.65 (d, *J* = 2.9 Hz, 6H), 2.33 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.16, 171.40, 142.87, 138.23, 137.23, 133.06, 129.24, 129.02, 127.15, 60.54, 58.01, 57.04, 52.18, 52.10, 51.80, 48.29, 47.90, 47.50, 44.77, 43.81, 21.53, 21.13.

HRMS：calculated for $C_{27}H_{27}NO_6S$ [M+Na]$^+$ 516.1452; found 516.1457.

dimethyl (2r,3R,4r,5S)-2-((4-(tert-butyl) phenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3c)



3c

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(4-(*tert*-butyl)benzylidene)-4-methylbenzenesulfonamide **2c** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3c** as a white solid (55.0 mg, 51% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

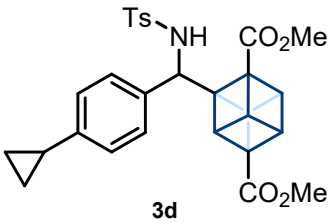
MP: 196-200 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.80 (d, *J* = 8.4 Hz, 2H), 6.28 (d, *J* = 8.8 Hz, 1H), 4.70 (d, *J* = 8.8 Hz, 1H), 4.15 – 4.07 (m, 3H), 3.98 (q, *J* = 2.2 Hz, 2H), 3.65 (d, *J* = 6.0 Hz, 6H), 2.29 (s, 3H), 1.23 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 172.16, 171.42, 150.45, 142.59, 138.34, 132.93, 129.16, 127.17, 126.99, 125.16, 60.46, 58.09, 57.17, 52.28, 52.11, 51.77, 48.39, 47.90, 47.51, 44.83, 43.90, 34.50, 31.42, 21.53.

HRMS：calculated for $C_{30}H_{33}NO_6S$ $[M+Na]^+$ 558.1921; found 558.1927.

dimethyl (2r,3R,4r,5S)-2-((4-cyclopropylphenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3d)



3d

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(4-cyclopropylbenzylidene)-4-methylbenzenesulfonamide **2d** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3d** as a white solid (57.0 mg, 55% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

MP: 191-194 °C.

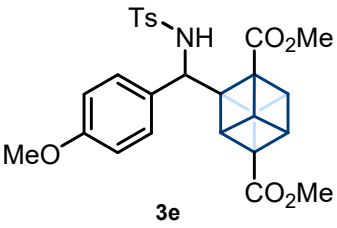
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.3 Hz, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.77 (s, 4H), 6.28 (d, *J* = 8.7 Hz, 1H), 4.66 (d, *J* = 8.7 Hz, 1H), 4.16–4.09 (m,

2H), 4.06 (td, *J* = 5.3, 2.5 Hz, 1H), 3.96 (dtd, *J* = 10.4, 5.6, 2.8 Hz, 2H), 3.65 (s, 6H), 2.32 (s, 3H), 1.28 (d, *J* = 22.0 Hz, 1H), 0.92 (ddd, *J* = 8.4, 3.1, 1.3 Hz, 2H), 0.57 (ddd, *J* = 7.9, 3.9, 2.1 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 172.24, 171.46, 143.43, 142.75, 138.21, 132.96, 129.23, 127.23, 127.14, 125.54, 60.49, 58.09, 57.07, 52.20, 52.14, 51.84, 48.34, 47.90, 47.47, 44.81, 43.84, 21.53, 15.10, 9.43, 9.38.

HRMS：calculated for $C_{29}H_{29}NO_6S$ $[M+Na]^+$ 542.1608; found 542.1613.

dimethyl (2r,3R,4r,5S)-2-((4-methoxyphenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3e)



3e

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(4-methoxybenzylidene)-4-methylbenzenesulfonamide **2e** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3e** as a white solid (51.0 mg, 50% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

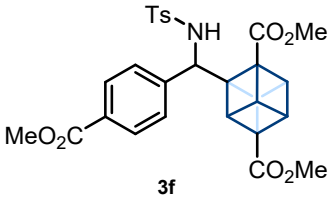
MP: 165-168 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.07 (d, *J* = 8.1 Hz, 2H), 6.85 (d, *J* = 8.6 Hz, 2H), 6.63 (d, *J* = 8.8 Hz, 2H), 6.19 (d, *J* = 8.4 Hz, 1H), 4.67 (d, *J* = 8.2 Hz, 1H), 4.14 (tt, *J* = 4.8, 2.7 Hz, 1H), 4.09 (td, *J* = 5.6, 2.7 Hz, 2H), 3.97 (tt, *J* = 4.9, 2.8 Hz, 2H), 3.73 (s, 3H), 3.66 (d, *J* = 2.2 Hz, 6H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.14, 171.38, 159.02, 142.85, 138.24, 129.27, 128.43, 128.21, 127.15, 113.73, 60.54, 57.69, 57.01, 55.33, 52.19, 52.13, 51.81, 48.20, 47.90, 47.44, 44.69, 43.82, 21.54.

HRMS：calculated for $C_{27}H_{27}NO_7S$ $[M+Na]^+$ 532.1401; found 532.1410.

dimethyl (2r,3R,4r,5S)-2-((4-(methoxycarbonyl) phenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3f)



3f

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), methyl (*E*)-4-((tosylimino)methyl)benzoate **2f** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3f** as a white solid (61.0 mg, 57% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

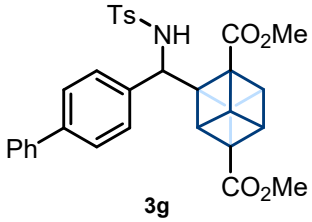
MP: 157-160 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.3 Hz, 2H), 7.04 (t, *J* = 8.8 Hz, 4H), 6.45 (d, *J* = 8.5 Hz, 1H), 4.77 (d, *J* = 8.4 Hz, 1H), 4.18 – 4.07 (m, 3H), 4.00 – 3.92 (m, 2H), 3.89 (s, 3H), 3.68 (s, 3H), 3.65 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 172.17, 171.13, 166.79, 143.31, 141.23, 138.01, 129.65, 129.47, 129.40, 127.38, 127.14, 60.16, 58.12, 57.16, 52.25, 51.85, 48.36, 47.97, 47.33, 44.94, 43.90, 21.49.

HRMS：calculated for $C_{28}H_{27}NO_8S$ $[M+Na]^+$ 560.1350; found 560.1358.

dimethyl (2r,3R,4r,5S)-2-([1,1'-biphenyl]-4-yl((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3g)



3g

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-([1,1'-biphenyl]-4-ylmethylene)-4-methylbenzenesulfonamide **2g** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3g** as a white solid (52.0 mg, 47% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

MP: 187-190 ℃.

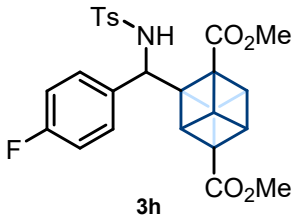
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (t, *J* = 8.2 Hz, 4H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.33 (dd, *J* = 13.3, 7.8 Hz, 3H), 7.01 (dd, *J* = 17.8, 8.1 Hz, 4H), 6.40 (d, *J* = 8.6

Hz, 1H), 4.77 (d, *J* = 8.6 Hz, 1H), 4.15 (dd, *J* = 5.1, 2.6 Hz, 2H), 4.10 (td, *J* = 5.2, 2.5 Hz, 1H), 4.04 (dt, *J* = 5.5, 2.6 Hz, 1H), 3.99 (d, *J* = 5.3 Hz, 1H), 3.66 (d, *J* = 13.0 Hz, 6H), 2.27 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 172.24, 171.33, 142.97, 140.66, 140.48, 138.25, 135.08, 129.30, 128.94, 127.80, 127.56, 127.21, 127.05, 127.02, 60.42, 58.14, 57.18, 52.28, 52.18, 51.83, 48.40, 47.95, 47.48, 44.89, 43.93, 21.51.

HRMS：calculated for $C_{32}H_{29}NO_6S$ $[M+Na]^+$ 578.1608; found 578.1617.

dimethyl (2r,3R,4r,5S)-2-((4-fluorophenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3h)



3h

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(4-fluorobenzylidene)-4-methylbenzenesulfonamide **2h** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3h** as a white solid (46.0 mg, 46% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

MP: 157-160 ℃.

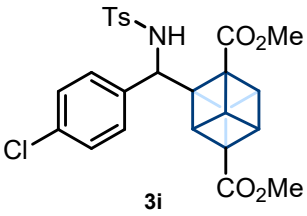
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.96 – 6.90 (m, 2H), 6.80 (t, *J* = 8.7 Hz, 2H), 6.29 (d, *J* = 8.2 Hz, 1H), 4.69 (d, *J* = 8.1 Hz, 1H), 4.15 (ddd, *J* = 7.3, 4.4, 3.0 Hz, 1H), 4.11 – 4.05 (m, 2H), 3.97 (dd, *J* = 2.7, 1.7 Hz, 2H), 3.68 (s, 3H), 3.65 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.18, 171.20,162.25 (d, *J* = 163.0 Hz), 143.20, 138.13, 131.98, 129.36, 129.03 (d, *J* = 5.0 Hz), 127.17, 115.25 (d, *J* = 14.0 Hz), 60.34, 57.69, 57.09, 52.22, 51.85, 48.23, 47.95, 47.33, 44.77, 43.92, 21.54.

^{19}F NMR (377 MHz, $CDCl_3$) δ -114.67.

HRMS：calculated for $C_{26}H_{24}FNO_6S$ $[M+Na]^+$ 520.1201; found 520.1207.

dimethyl (2r,3R,4r,5S)-2-((4-chlorophenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3i)



3i

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(4-chlorobenzylidene)-4-methylbenzenesulfonamide **2i** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3i** as a white solid (44.2 mg, 43% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

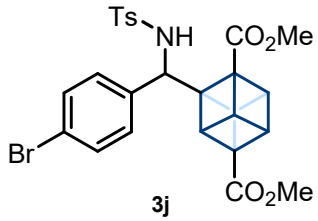
MP: 179-182 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.3 Hz, 2H), 7.08 (dd, *J* = 8.3, 1.9 Hz, 4H), 6.88 (d, *J* = 8.5 Hz, 2H), 6.36 (d, *J* = 8.3 Hz, 1H), 4.68 (d, *J* = 8.2 Hz, 1H), 4.15 (p, *J* = 3.8 Hz, 1H), 4.09 (dd, *J* = 3.7, 2.0 Hz, 2H), 3.96 (dd, *J* = 3.7, 2.1 Hz, 2H), 3.68 (s, 3H), 3.65 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.20, 171.17, 143.32, 138.01, 134.61, 133.56, 129.39, 128.76, 128.51, 127.17, 60.17, 57.80, 57.11, 52.25, 51.86, 48.27, 47.94, 47.29, 44.84, 43.93, 21.55.

HRMS： calculated for $C_{26}H_{24}ClNO_6S$ $[M+Na]^+$ 536.0906; found 536.0914.

dimethyl (2r,3R,4r,5S)-2-((4-bromophenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3j)



3j

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(4-bromobenzylidene)-4-methylbenzenesulfonamide **2j** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3j** as a white solid (61.0 mg, 55% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

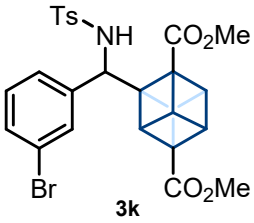
MP: 179-182 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.3 Hz, 2H), 6.37 (d, *J* = 8.2 Hz, 1H), 4.66 (d, *J* = 8.3 Hz, 1H), 4.14 (q, *J* = 3.7 Hz, 1H), 4.11 – 4.07 (m, 2H), 3.96 (dd, *J* = 3.7, 2.0 Hz, 2H), 3.68 (s, 3H), 3.65 (s, 3H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.16, 171.17, 143.34, 137.92, 135.04, 131.44, 129.38, 129.09, 127.15, 121.62, 60.05, 57.83, 57.08, 52.25, 51.87, 48.22, 47.92, 47.25, 44.82, 43.91, 21.57.

HRMS：calculated for $C_{26}H_{24}BrNO_6S$ $[M+Na]^+$ 582.0283; found 582.0389.

dimethyl (2r,3R,4r,5S)-2-((3-bromophenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3k)



3k

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(3-bromobenzylidene)-4-methylbenzenesulfonamide **2k** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3k** as a white solid (54.0 mg, 48% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

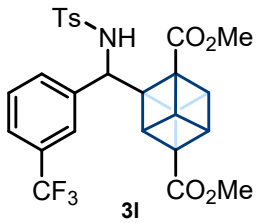
MP: 177-180 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.39 (m, 1H), 7.07 – 7.01 (m, 3H), 7.01 – 6.93 (m, 2H), 6.57 (d, *J* = 8.0 Hz, 1H), 5.31 (d, *J* = 8.1 Hz, 1H), 4.17 – 4.09 (m, 3H), 4.05 (dt, *J* = 4.9, 2.4 Hz, 1H), 3.96 – 3.91 (m, 1H), 3.75 (s, 3H), 3.60 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.29, 171.21, 143.33, 138.04, 137.80, 130.62, 130.32, 129.89, 129.41, 127.01, 126.16, 122.60, 60.14, 57.92, 57.03, 52.38, 52.21, 51.93, 48.26, 47.93, 47.22, 44.85, 43.86, 21.60.

HRMS：calculated for $C_{26}H_{24}BrNO_6S$ $[M+Na]^+$ 582.0380; found 582.0391.

dimethyl (2r,3R,4r,5S)-2-(((4-methylphenyl) sulfonamido) (3-(trifluoromethyl) phenyl) methyl) cubane-1,4-dicarboxylate (3l)



3l

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-4-methyl-*N*-(3-(trifluoromethyl)benzylidene)benzenesulfonamide **2l** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3l** as a white solid (69.0 mg, 63% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

MP: 207-210 ℃.

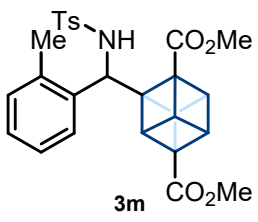
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.08 – 7.01 (m, 3H), 6.49 (d, *J* = 8.2 Hz, 1H), 4.79 (d, *J* = 8.1 Hz, 1H), 4.14 (dtt, *J* = 11.0, 4.4, 2.3 Hz, 3H), 3.99 – 3.93 (m, 2H), 3.69 (s, 3H), 3.64 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.21, 171.12, 143.38, 137.82, 137.00, 131.07,130.72 (d, *J* = 32.0 Hz), 129.40, 128.93, 127.02, 124.18 (dd, *J* = 59.0, 4.0 Hz), 123.88 (d, *J* = 271.0 Hz), 60.05, 58.00, 57.08, 52.28, 51.86, 48.20, 47.95, 47.16, 44.87, 43.90, 21.43.

^{19}F NMR (377 MHz, $CDCl_3$) δ -62.84.

HRMS：calculated for $C_{27}H_{24}F_3NO_6S$ $[M+Na]^+$ 570.1169; found 570.1176.

dimethyl (2r,3R,4r,5S)-2-(((4-methylphenyl) sulfonamido) (o-tolyl) methyl) cubane-1,4-dicarboxylate (3m)



3m

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-4-methyl-*N*-(2-methylbenzylidene)benzenesulfonamide **2m** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC

(0.3% FA) to give compound **3m** as a white solid (45.0 mg, 46% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

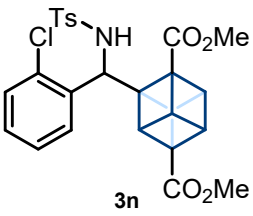
MP: 181-184 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.3 Hz, 2H), 7.03 – 6.96 (m, 4H), 6.89 – 6.82 (m, 2H), 6.37 (d, *J* = 8.3 Hz, 1H), 5.06 (d, *J* = 8.4 Hz, 1H), 4.16 – 4.12 (m, 1H), 4.09 (dd, *J* = 4.5, 1.8 Hz, 2H), 3.98 – 3.93 (m, 1H), 3.87 (dt, *J* = 6.1, 1.9 Hz, 1H), 3.71 (s, 3H), 3.63 (s, 3H), 2.29 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 172.32, 171.31, 142.85, 138.13, 135.63, 134.60, 130.54, 129.19, 127.38, 126.95, 126.29, 126.20, 60.90, 57.60, 53.66, 52.42, 52.24, 51.79, 48.86, 47.84, 47.48, 44.87, 43.94, 21.50, 19.97.

HRMS：calculated for $C_{27}H_{27}NO_6S$ $[M+Na]^+$ 516.1452; found 516.1461.

dimethyl (2r,3R,4r,5S)-2-((2-chlorophenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3n)



3n

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(2-chlorobenzylidene)-4-methylbenzenesulfonamide **2n** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3n** as a white solid (44.0 mg, 43% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

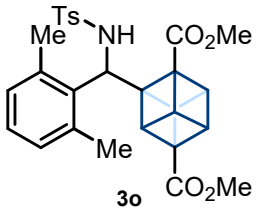
MP: 201-204 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 2H), 7.22 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.09 – 7.00 (m, 4H), 6.96 (td, *J* = 7.4, 1.4 Hz, 1H), 6.52 (d, *J* = 8.1 Hz, 1H), 5.31 (d, *J* = 8.1 Hz, 1H), 4.16 – 4.08 (m, 3H), 4.03 (dt, *J* = 5.2, 2.4 Hz, 1H), 3.94 (ddd, *J* = 7.2, 5.1, 2.7 Hz, 1H), 3.74 (s, 3H), 3.60 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 172.35, 171.15, 143.08, 137.46, 133.74, 133.23, 129.62, 129.30, 128.61, 128.53, 127.22, 126.89, 60.52, 57.53, 54.29, 52.46, 52.31, 51.76, 48.62, 47.89, 47.32, 44.84, 44.05, 21.51.

HRMS：calculated for $C_{26}H_{24}ClNO_6S$ $[M+Na]^+$ 536.0906; found 536.0912.

dimethyl (2r,3R,4r,5S)-2-((2,6-dimethylphenyl) ((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3o)



3o

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-*N*-(2,6-dimethylbenzylidene)-4-methylbenzenesulfonamide **2p** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3o** as a white solid (49.0 mg, 48% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

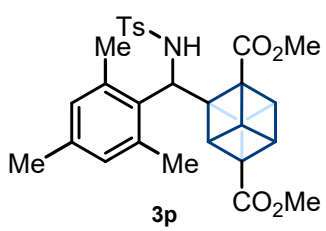
MP: 219-222 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 7.4 Hz, 1H), 6.76 (d, *J* = 7.8 Hz, 1H), 5.41 (d, *J* = 6.2 Hz, 1H), 5.18 (d, *J* = 6.2 Hz, 1H), 4.30 (dd, *J* = 5.7, 2.8 Hz, 1H), 4.18 (td, *J* = 5.4, 2.6 Hz, 1H), 4.12 (tt, *J* = 5.0, 2.3 Hz, 1H), 4.04 (td, *J* = 5.4, 2.7 Hz, 1H), 3.70 (s, 3H), 3.68 (dt, *J* = 5.4, 2.5 Hz, 1H), 3.64 (s, 3H), 2.34 (s, 3H), 2.18 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.44, 170.91, 143.18, 136.17, 133.76, 129.94, 129.26, 128.55, 127.61, 127.07, 60.33, 58.22, 52.90, 52.81, 51.94, 51.76, 49.86, 49.04, 47.31, 44.37, 44.14, 21.58, 21.17, 21.00.

HRMS：calculated for $C_{28}H_{29}NO_6S$ $[M+Na]^+$ 530.1608; found 530.1616.

dimethyl (2r,3R,4r,5S)-2-(mesityl((4-methylphenyl) sulfonamido) methyl) cubane-1,4-dicarboxylate (3p)



3p

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-4-methyl-*N*-(2,4,6-

trimethylbenzylidene)benzenesulfonamide **2p** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3p** as a white solid (44.0 mg, 42% yield).

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

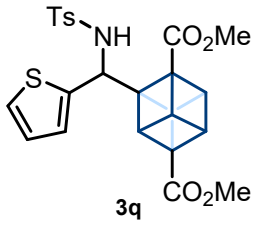
MP: 205-208 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.69 (s, 1H), 6.58 (s, 1H), 5.35 (d, *J* = 6.0 Hz, 1H), 5.10 (d, *J* = 6.1 Hz, 1H), 4.31 (dd, *J* = 5.5, 2.8 Hz, 1H), 4.18 (td, *J* = 5.4, 2.6 Hz, 1H), 4.12 (tt, *J* = 5.1, 2.3 Hz, 1H), 4.03 (td, *J* = 5.2, 2.5 Hz, 1H), 3.70 (s, 4H), 3.65 (s, 3H), 2.35 (s, 3H), 2.17 (s, 3H), 2.12 (s, 3H), 2.07 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.46, 170.92, 143.09, 137.41, 137.14, 137.07, 135.99, 130.97, 130.64, 129.27, 129.21, 127.13, 60.48, 58.26, 52.87, 52.72, 51.86, 51.71, 49.84, 49.12, 47.35, 44.41, 44.16, 21.56, 21.01, 20.87, 20.77.

HRMS：calculated for $C_{29}H_{31}NO_6S$ $[M+Na]^+$ 544.1765; found 544.1772.

dimethyl (2r,3R,4r,5S)-2-(((4-methylphenyl) sulfonamido) (thiophen-2-yl) methyl) cubane-1,4-dicarboxylate (3q)



3q

Following the general procedure using TBADT (0.001 mmol, 5 mol%), 1,4-bis(methoxycarbonyl)cubane **1a** (0.6 mmol), (*E*)-4-methyl-*N*-(thiophen-2-ylmethylene)benzenesulfonamide **2q** (0.2 mmol) and MeCN (4 mL, 0.05 M). The reaction mixture was purified by *prep*-HPLC (0.3% FA) to give compound **3q** as a white solid (32.0 mg, 33% yield).

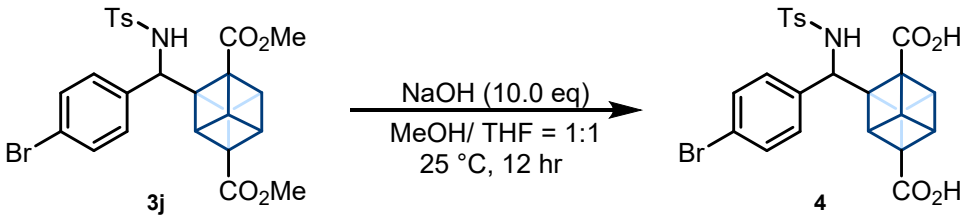
TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.05 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.74 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.59 (d, *J* = 3.5 Hz, 1H), 6.32 (d, *J* = 9.3 Hz, 1H), 5.05 (d, *J* = 9.2 Hz, 1H), 4.23 – 4.15 (m, 2H), 4.12 (dd, *J* = 5.3, 2.3 Hz, 1H), 4.03 (dt, *J* = 5.1, 2.6 Hz, 2H), 3.70 (s, 3H), 3.65 (s, 3H), 2.36 (s, 3H).

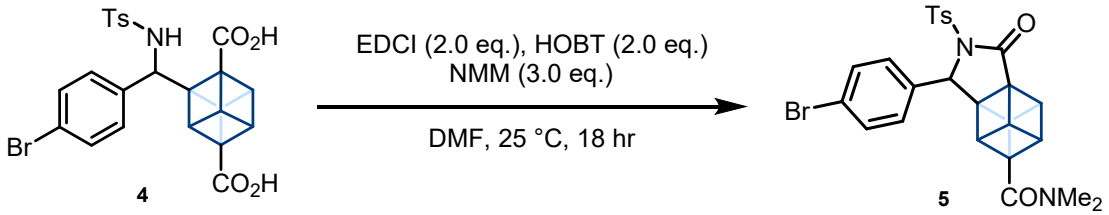
^{13}C NMR (151 MHz, $CDCl_3$) δ 172.05, 171.37, 143.06, 139.71, 138.38, 129.41, 127.07, 126.55, 126.18, 125.33, 60.24, 56.91, 54.08, 52.19, 52.10, 51.90, 48.25, 48.02, 47.71, 44.97, 43.88, 21.61.

HRMS： calculated for $C_{24}H_{23}NO_6S_2$ $[M+Na]^+$ 508.0859; found 508.0867.

5. General Procedure for the amidation ring closure reaction of cubane



To a mixture of compound **3j** (40.0 mg, 0.072 mmol) in MeOH/ THF = 1:1 (6 mL) was added NaOH (28.7 mg, 0.716 mmol) at room temperature under argon atmosphere. The reaction mixture was stirred at room temperature for 12 h. The mixture was diluted with EtOAc (10 mL). The water layers were adjusted to pH = 3 with HCl (1M) and diluted with EtOAc (10 mL*3). The organic layers washed with brine (30 mL) and dried over anhydrous sodium sulfate and concentrated. The crude product **4** was used directly for the next step without further purification.



To a stirred solution of compound **4** (26 mg, 0.049 mmol) in DMF (2 mL) were added NMM (29.8 mg, 0.294 mmol), EDCI (18.8 mg, 0.098 mmol), HOBT (13.3 mg, 0.098 mmol) at room temperature under argon atmosphere. The reaction mixture was stirred at room temperature for 18 h. The mixture was diluted with water (6 mL) and extracted with EtOAc (10 mL*3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered and

concentrated under reduced pressure. The residue was purified by *prep*-HPLC (0.3% FA) to give compound **5** (8.70 mg, 33% yield) as a white solid.

TLC: R_f = 0.25 (Petroleum ether / EtOAc = 3:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.35 (m, 4H), 7.12 (d, *J* = 8.1 Hz, 2H), 6.80 (d, *J* = 8.0 Hz, 2H), 5.61 (s, 1H), 4.47 – 4.43 (m, 2H), 4.33 (dt, *J* = 5.3, 2.8 Hz, 1H), 4.27 (d, *J* = 4.7 Hz, 1H), 3.74 (s, 1H), 2.88 (s, 3H), 2.76 (s, 3H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.72, 169.38, 145.14, 136.43, 135.49, 132.03, 129.26, 128.83, 128.42, 122.43, 67.16, 55.38, 53.06, 50.70, 49.25, 48.64, 47.77, 46.59, 36.15, 35.38, 21.80.

HRMS：calculated for $C_{26}H_{23}BrN_2O_4S$ $[M+Na]^+$ 563.0434; found 563.0443.

6. X-Ray Diffraction Analysis of Product 3f

X-Ray data for compound **3f**

Thermal probability ellipsoids shown at the 50% probability leve.

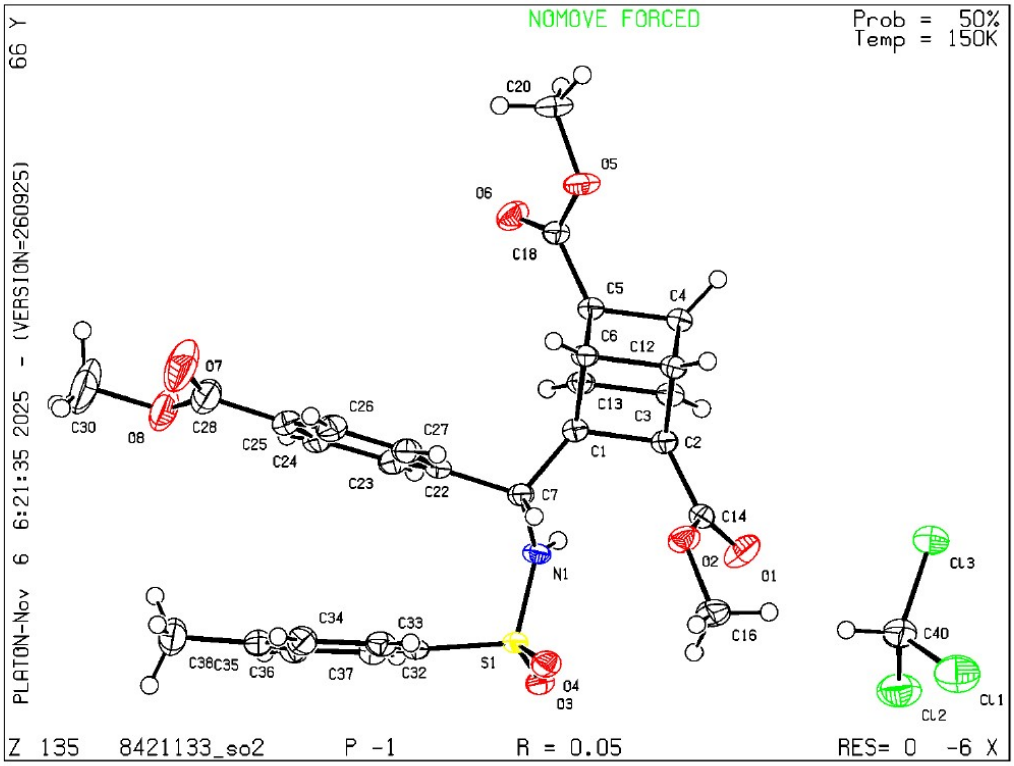
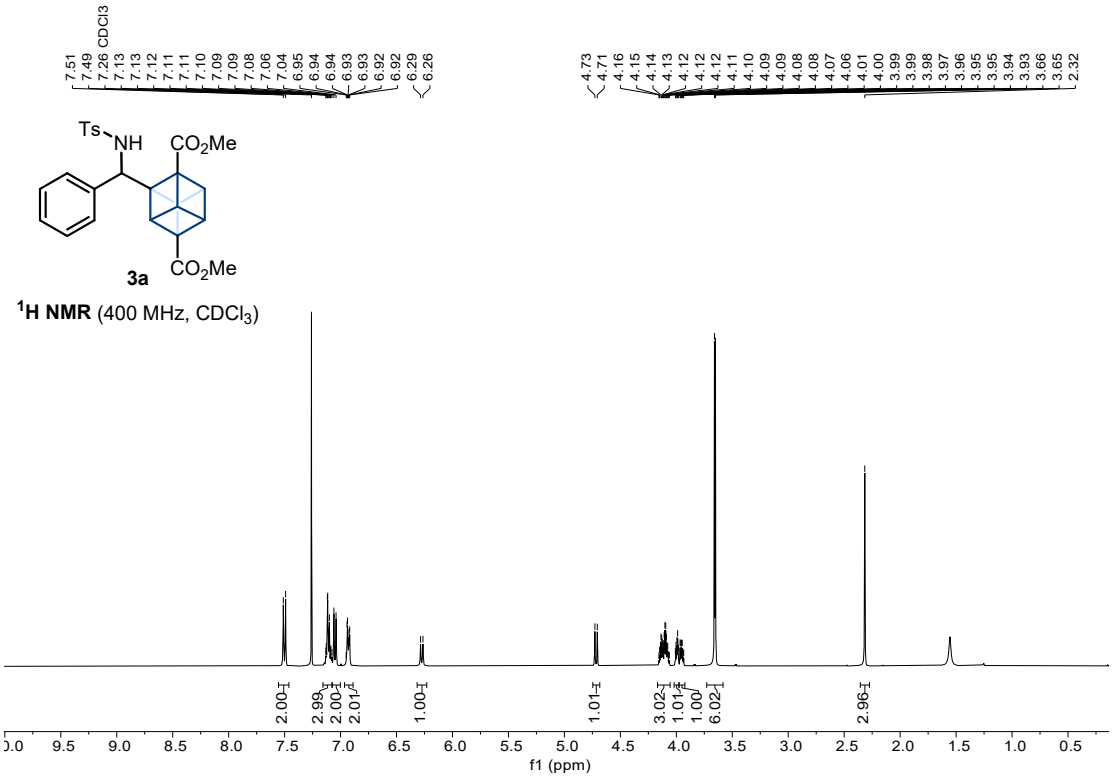


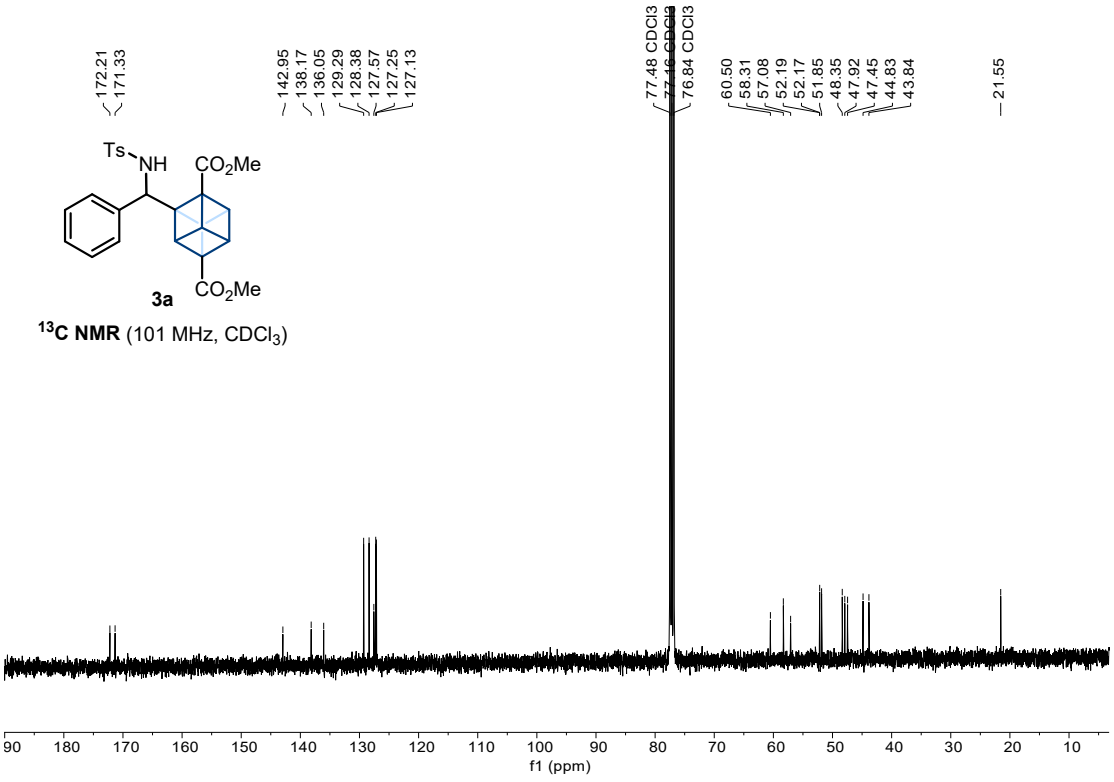
Table S4 Crystal data and structure refinement for 3f.

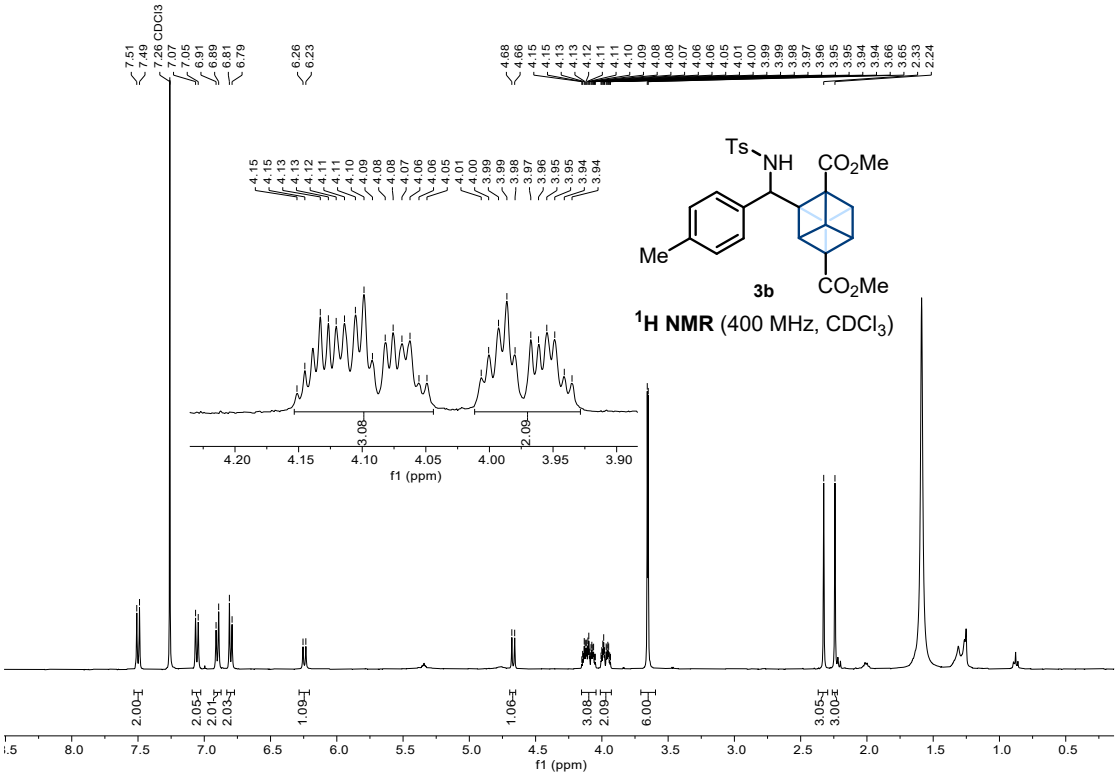
Identification code	2514390
Empirical formula	$C_{29}H_{28}Cl_3NO_8S$
Formula weight	656.93
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.9319(2)
b/Å	12.8338(2)
c/Å	13.0162(2)

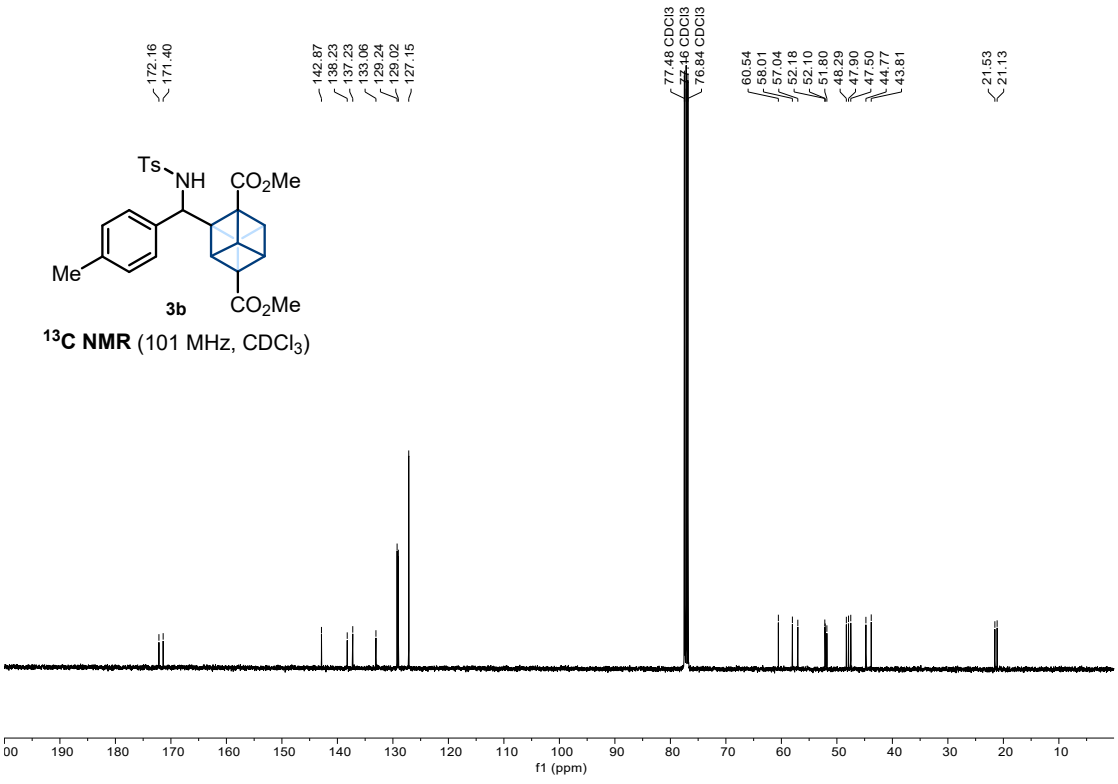
α/°	118.405(2)
β/°	108.271(2)
γ/°	94.0150(10)
Volume/Å^3	1471.87(5)
Z	2
ρ_{calc}g/cm^3	1.482
μ/mm^{-1}	3.930
F(000)	680.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.054 to 146.668
Index ranges	-11 ≤ h ≤ 13, -15 ≤ k ≤ 15, -16 ≤ l ≤ 15
Reflections collected	19887
Independent reflections	5513 [R_{int} = 0.0257, R_{sigma} = 0.0166]
Data/restraints/parameters	5513/0/383
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0505, wR_2 = 0.1368
Final R indexes [all data]	R_1 = 0.0513, wR_2 = 0.1376
Largest diff. peak/hole / e Å^{-3}	1.32/-1.02

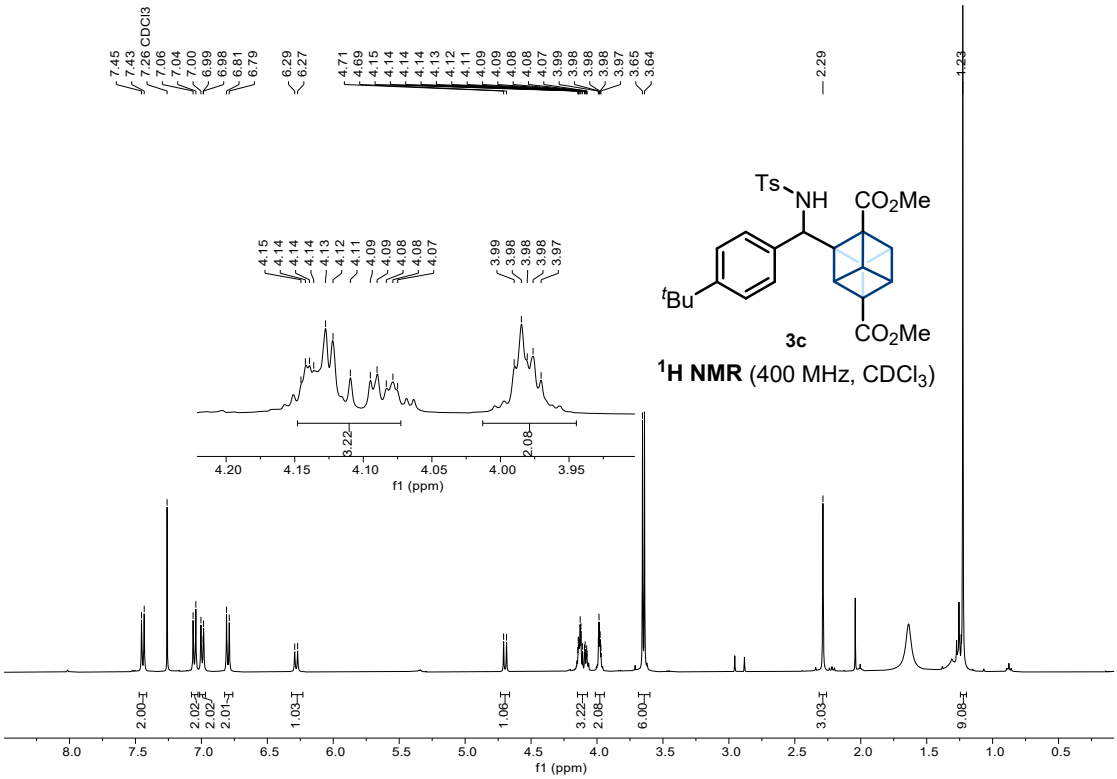
7. NMR Spectra

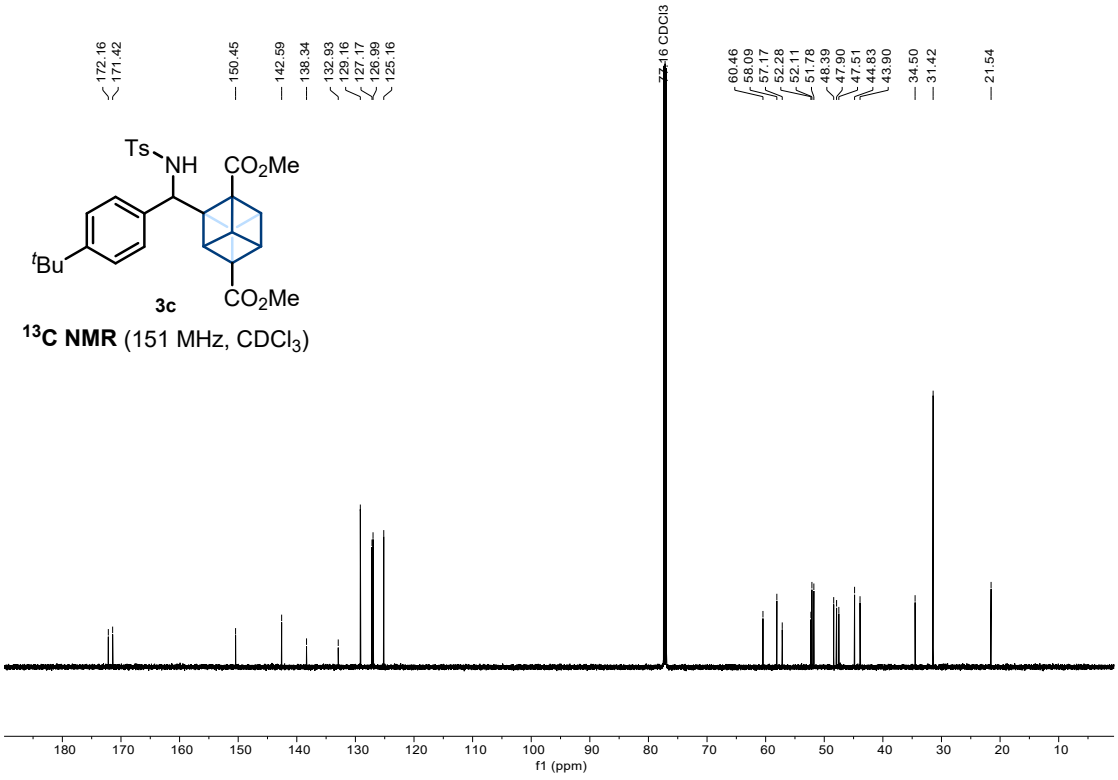


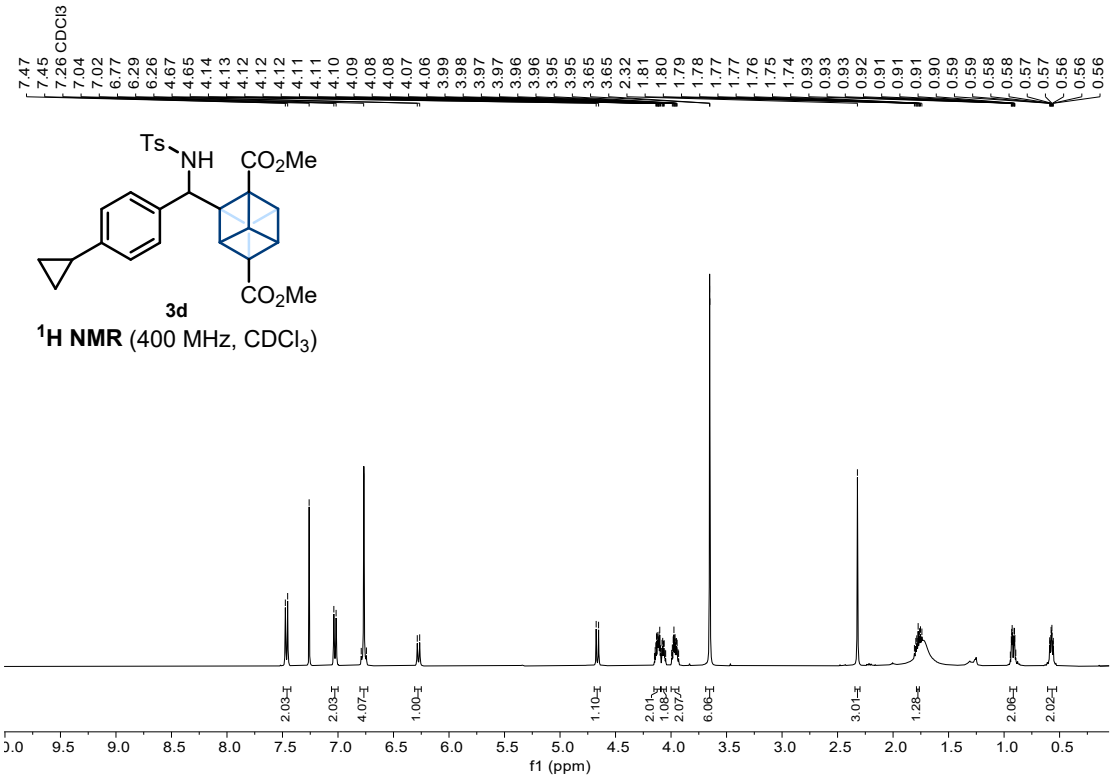


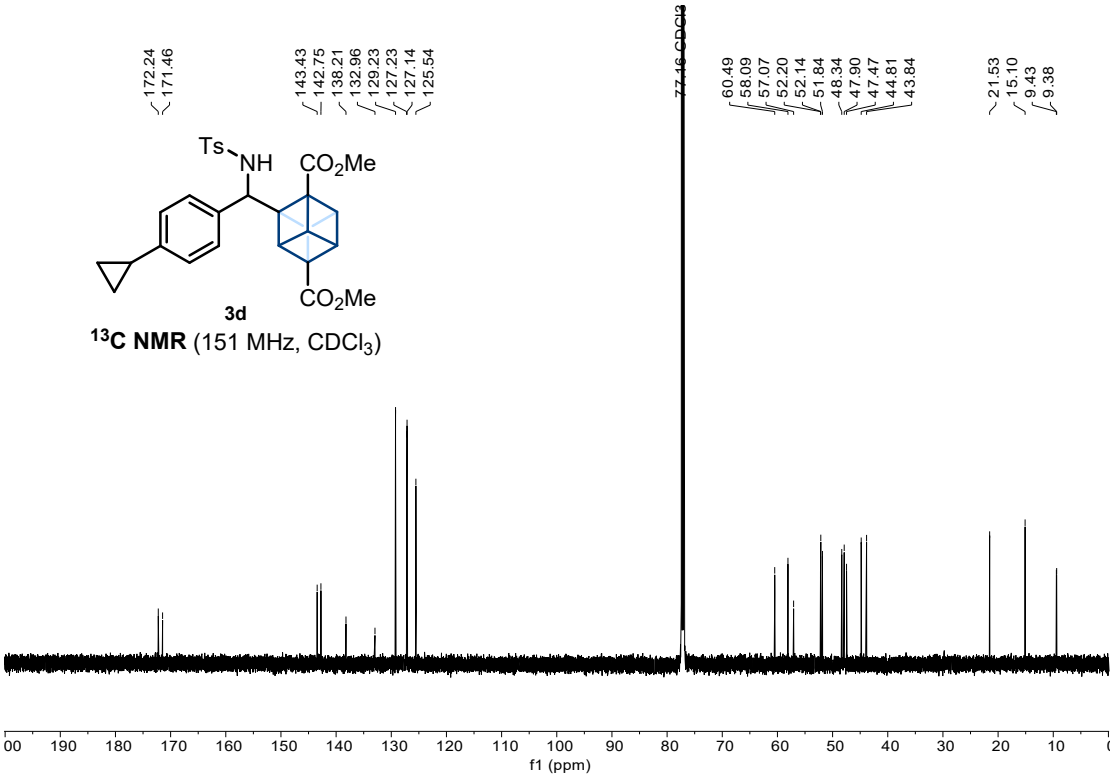

Ts
NH
CO2Me
Me
CO2Me
3b
1H NMR (400 MHz, CDCl3)
f1 (ppm)


Ts
NH
CO2Me
Me
CO2Me
3b
13C NMR (101 MHz, CDCl3)
f1 (ppm)


Ts
NH
CO2Me
tBu
CO2Me
3c
1H NMR (400 MHz, CDCl3)
f1 (ppm)

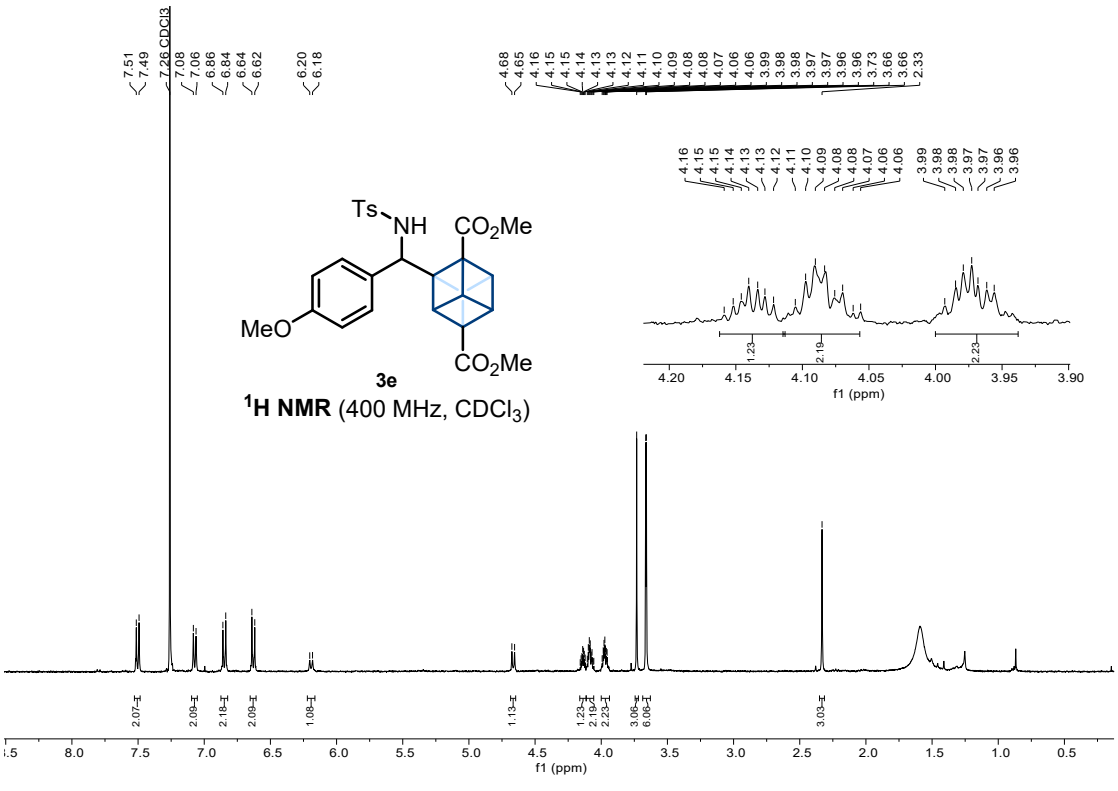

Ts
NH
CO2Me
tBu
CO2Me
3c
13C NMR (151 MHz, CDCl3)
f1 (ppm)


7.47
7.45
7.26 CDCl3
7.04
7.02
6.77
6.29
6.26
4.67
4.65
4.14
4.13
4.12
4.12
4.12
4.11
4.11
4.10
4.09
4.08
4.08
4.07
4.06
3.99
3.98
3.97
3.97
3.96
3.96
3.95
3.95
3.65
2.32
1.81
1.80
1.79
1.78
1.77
1.77
1.76
1.75
1.74
0.93
0.93
0.93
0.92
0.91
0.91
0.91
0.90
0.59
0.59
0.58
0.58
0.57
0.57
0.56
0.56
0.56
Ts
NH
CO2Me
CO2Me
3d
1H NMR (400 MHz, CDCl3)
2.03
2.03
4.07
1.00
1.10
2.01
1.08
2.07
6.06
3.01
1.28
2.06
2.02
f1 (ppm)



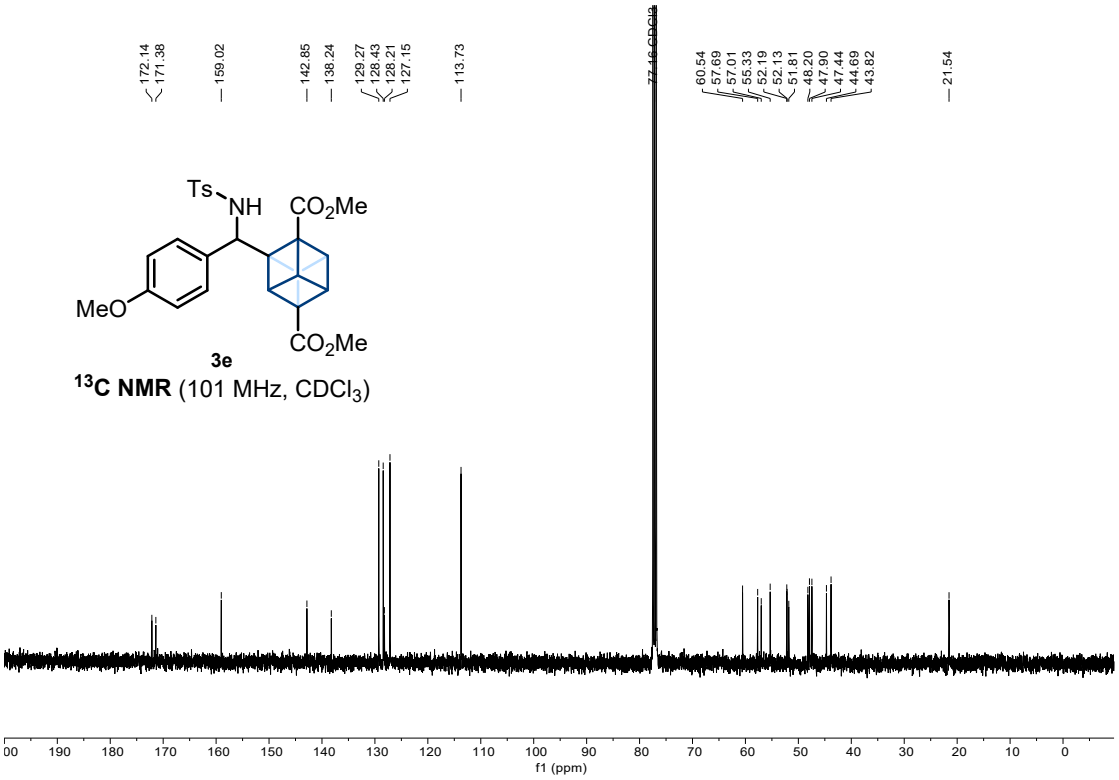
3d

^{13}C NMR (151 MHz, $CDCl_3$)



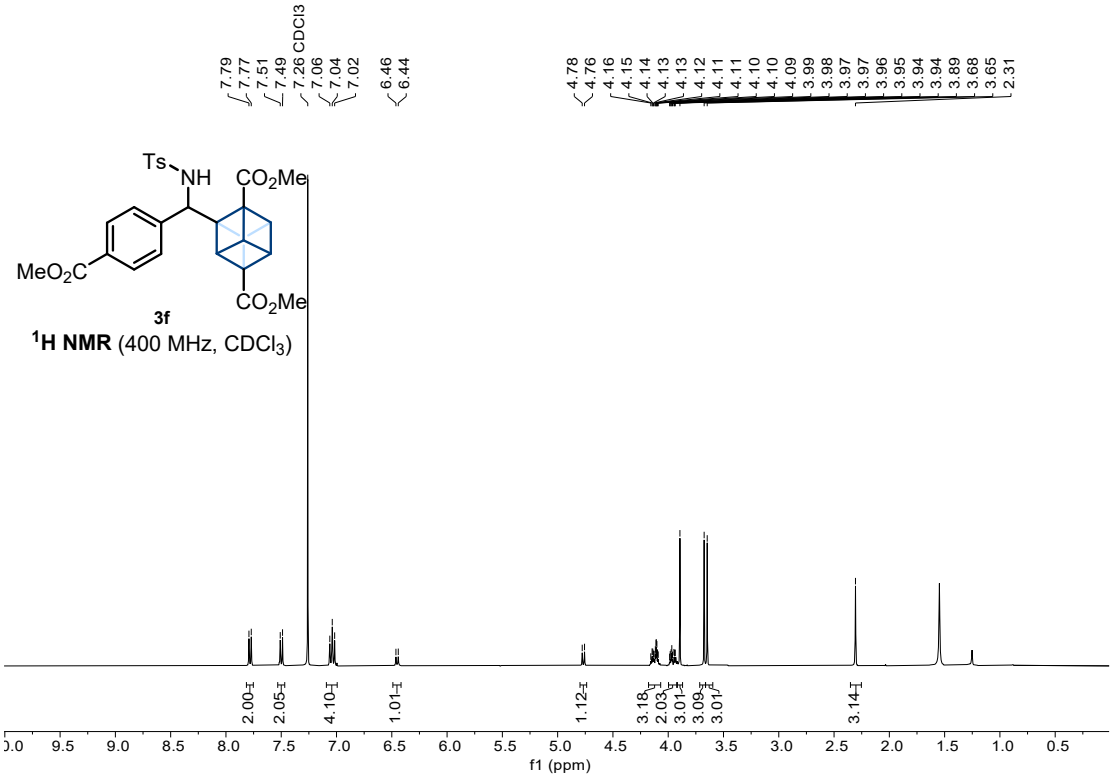
3e

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



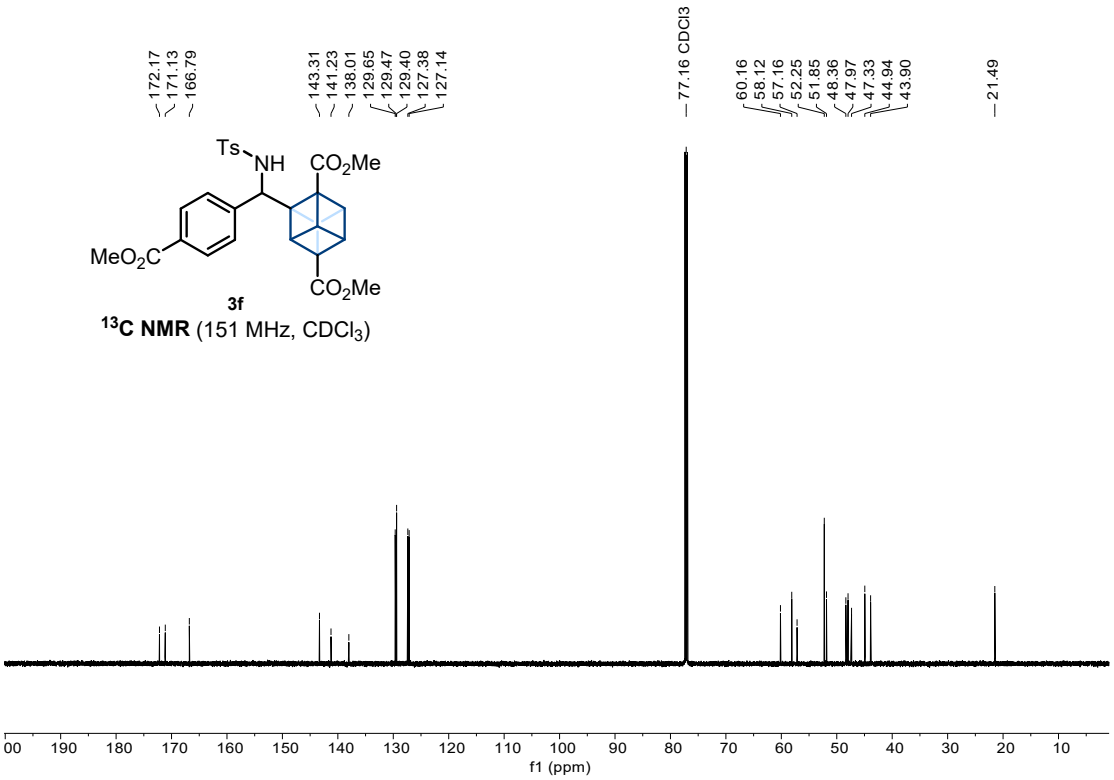
3e

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

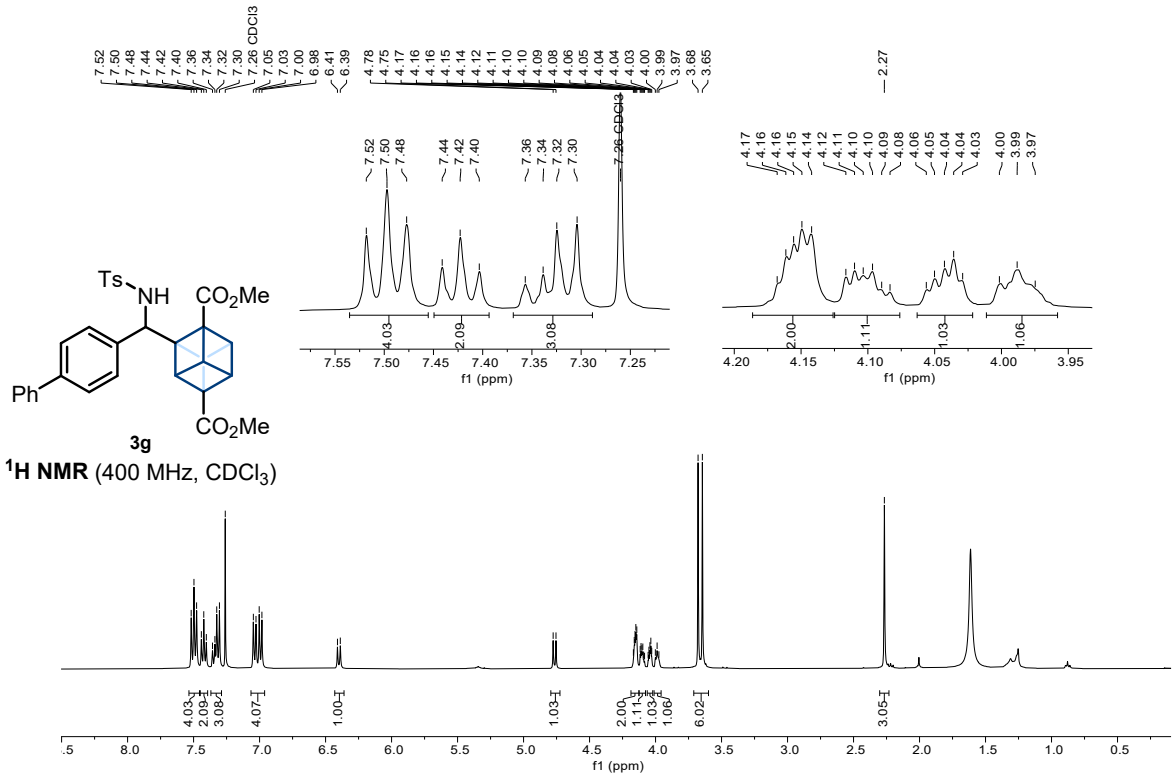


3f

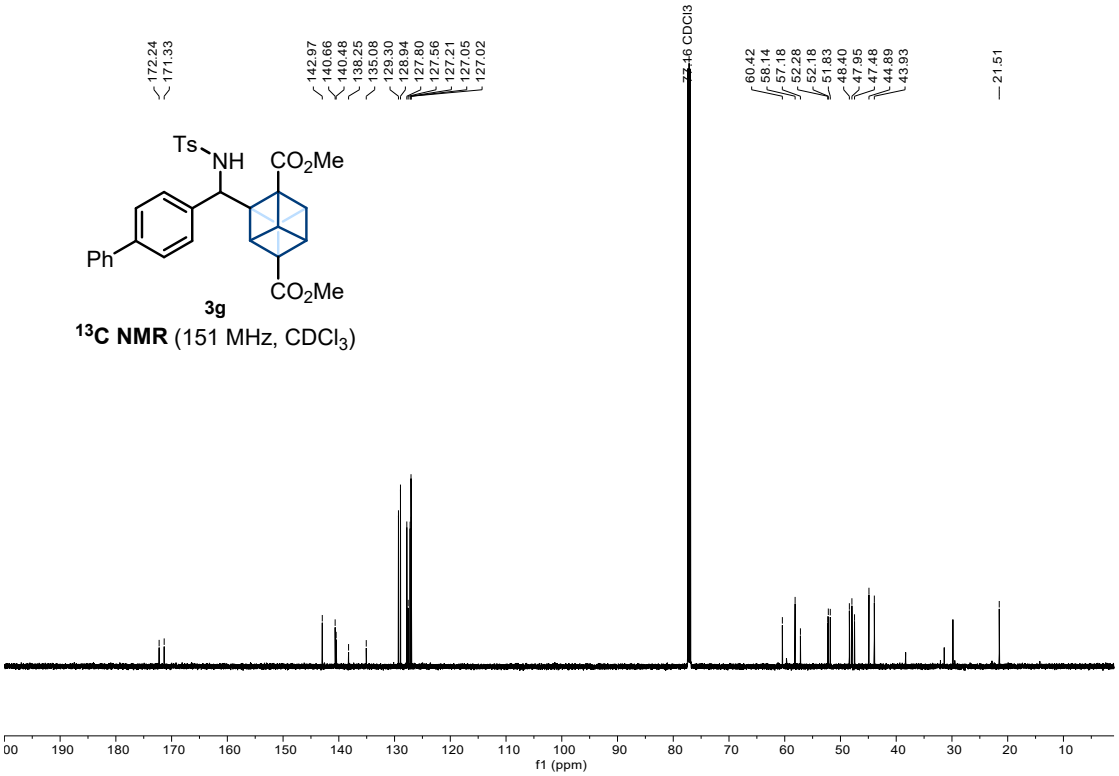
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)

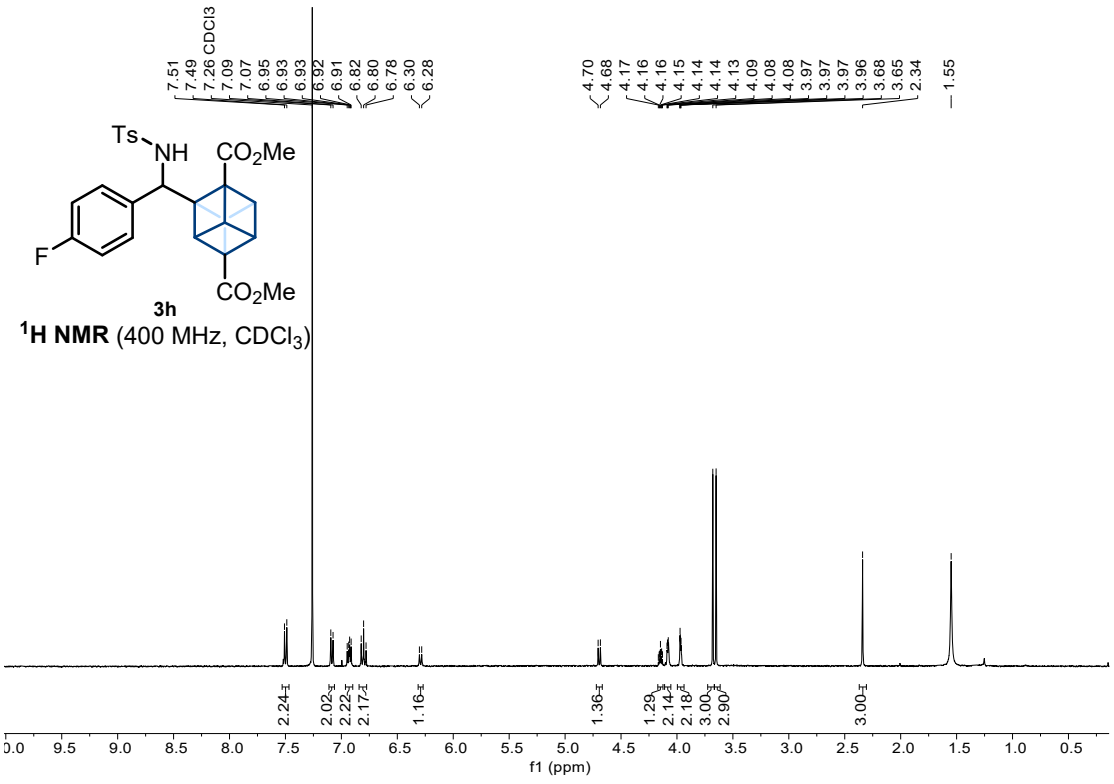


^{1}H NMR (400 MHz, $CDCl_3$)



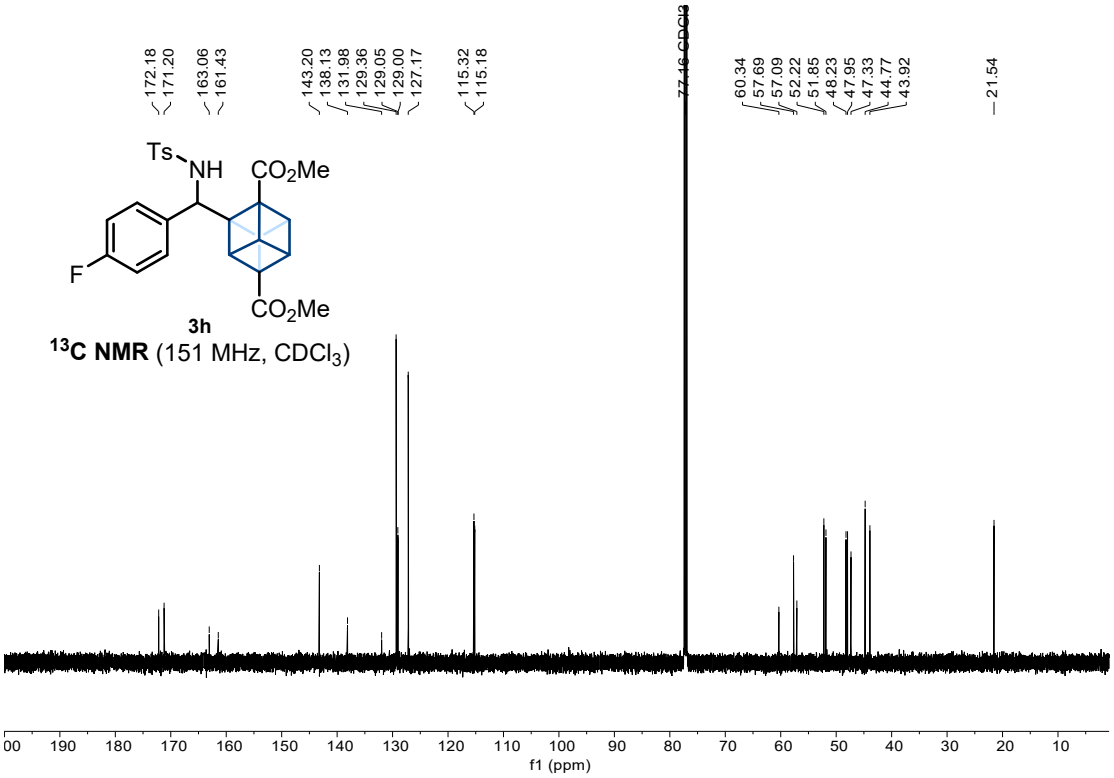
3g

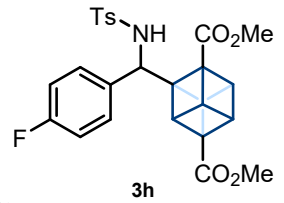
^{13}C NMR (151 MHz, $CDCl_3$)



3h

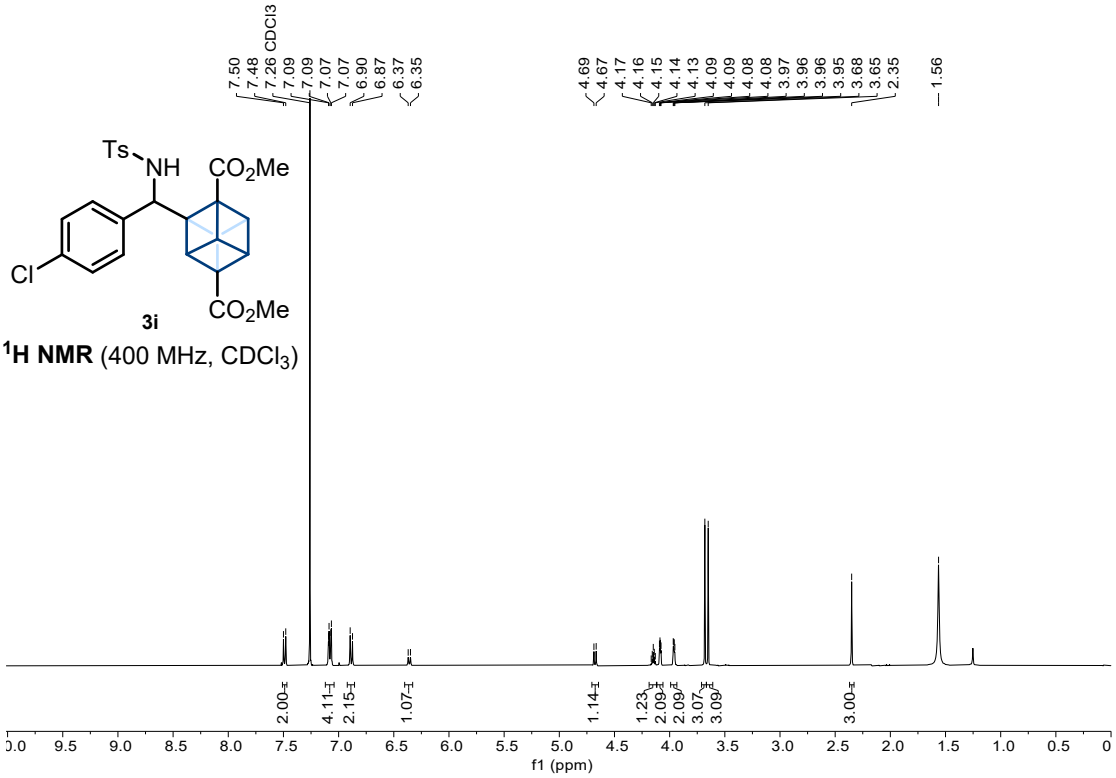
^{1}H NMR (400 MHz, $CDCl_3$)


172.18
171.20
163.06
161.43
143.20
138.13
131.98
129.36
129.05
129.00
127.17
115.32
115.18
77.16 CDCl3
60.34
57.69
57.09
52.22
51.85
48.23
47.95
47.33
44.77
43.92
21.54
Ts
NH
CO2Me
F
CO2Me
3h
13C NMR (151 MHz, CDCl3)
f1 (ppm)

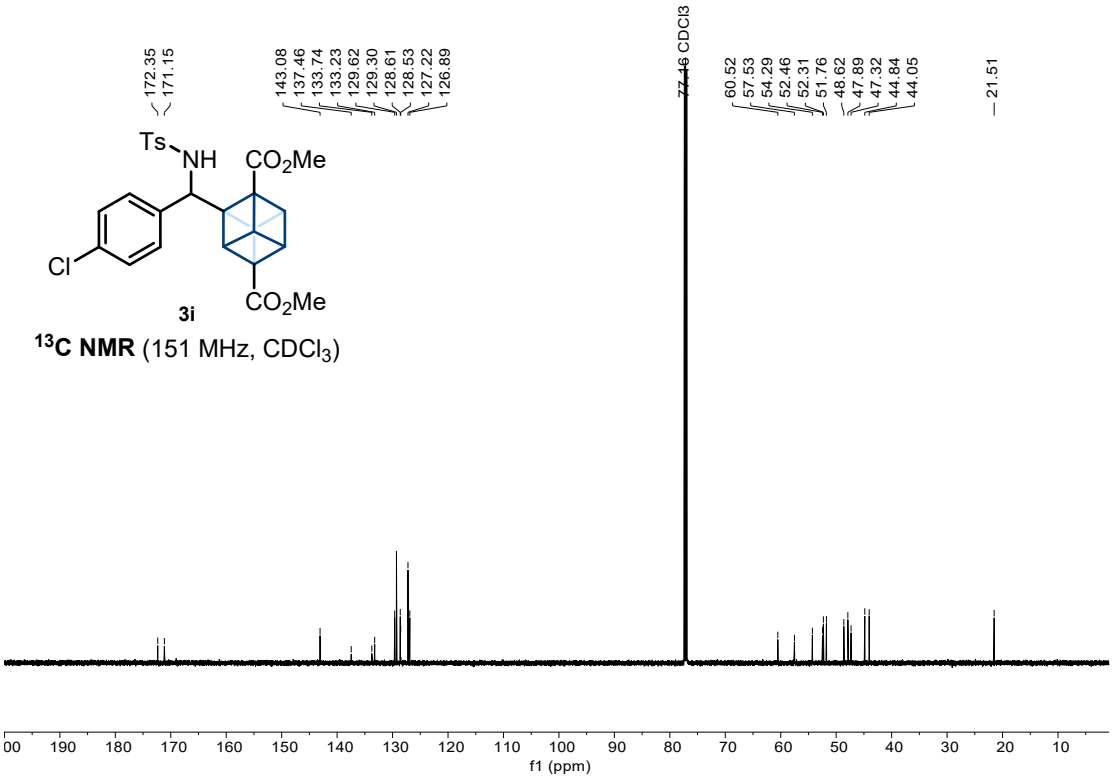


3h

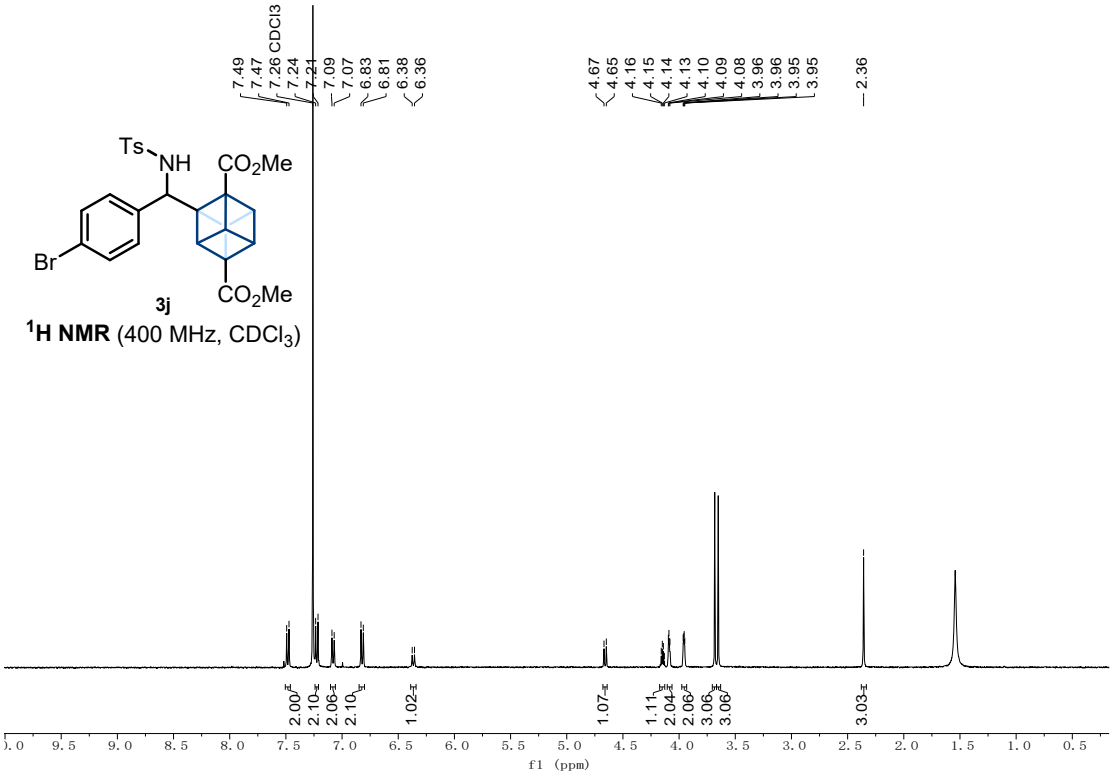
^{19}F NMR (377 MHz, $CDCl_3$)



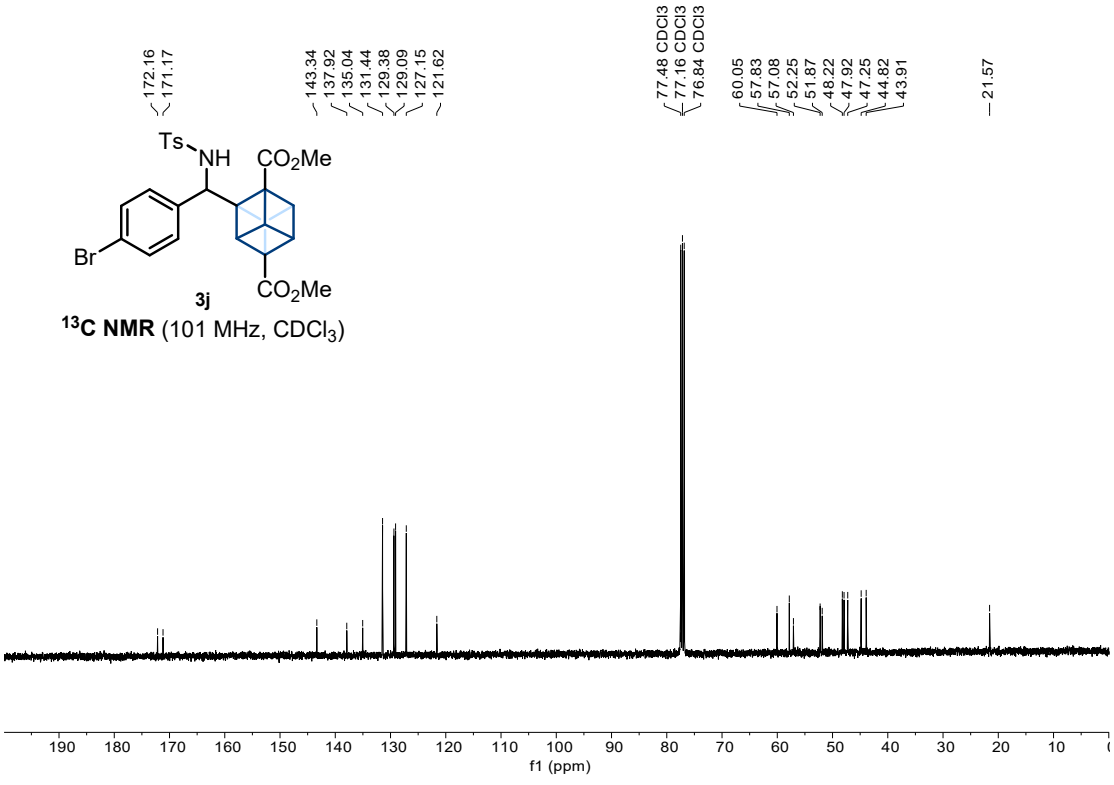
^{1}H NMR (400 MHz, $CDCl_3$)



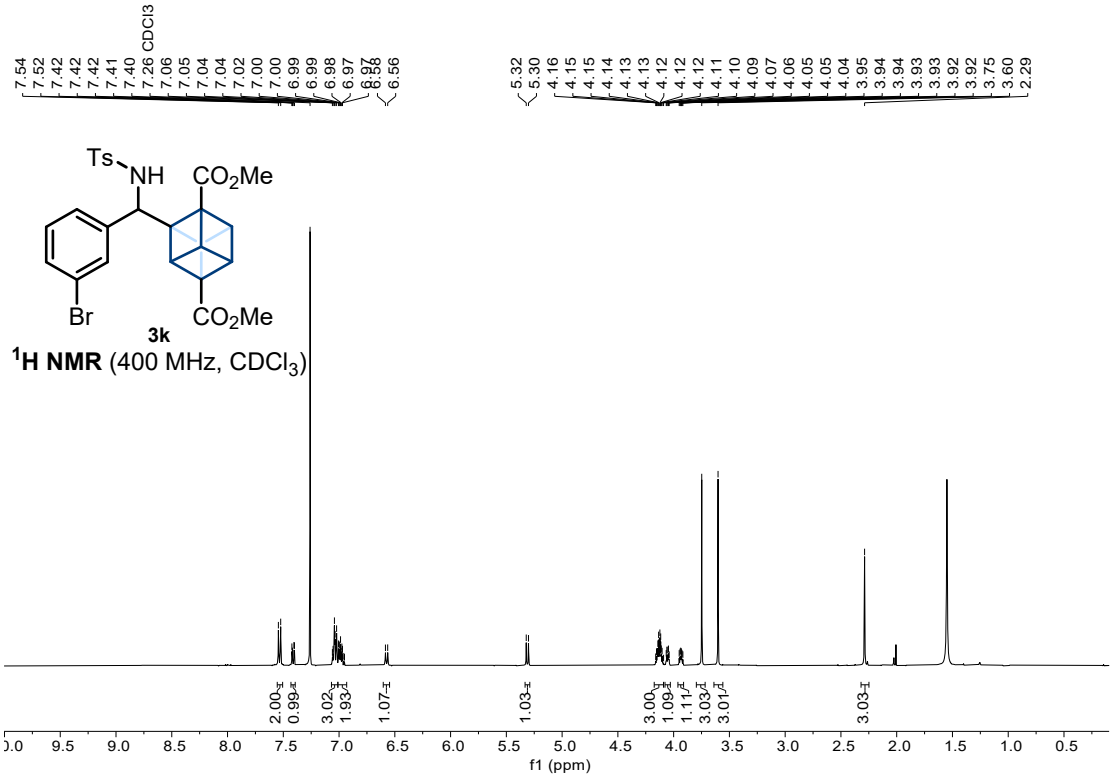
^{13}C NMR (151 MHz, $CDCl_3$)

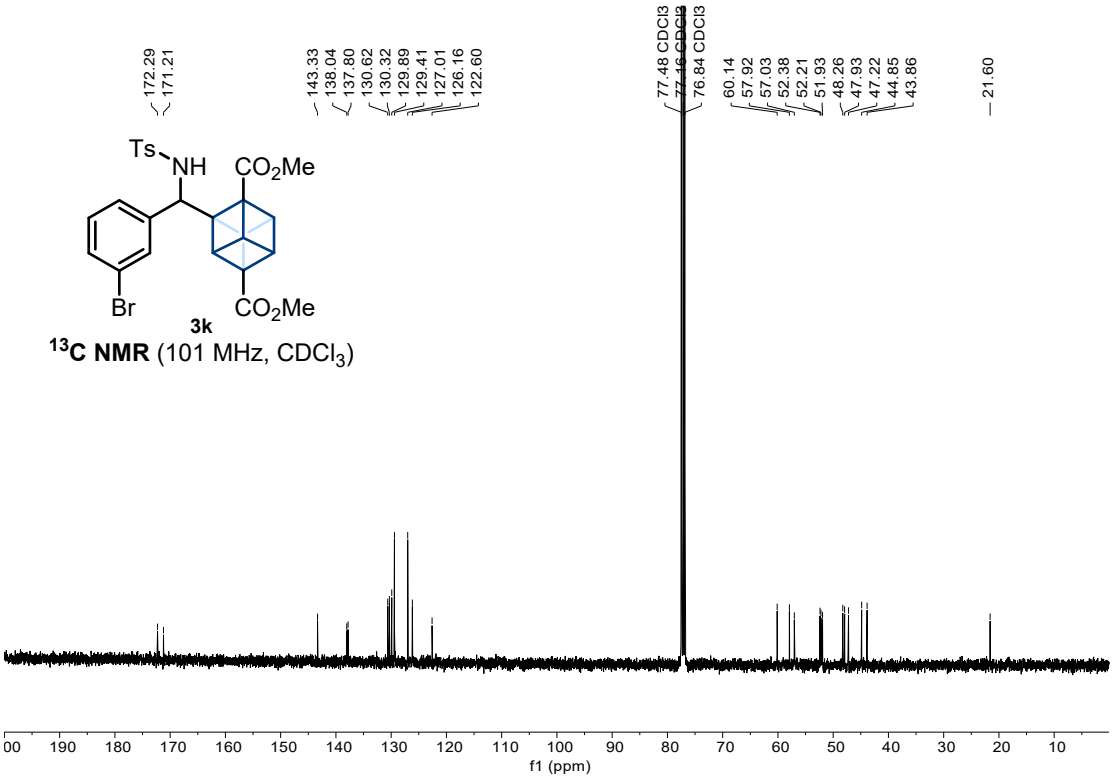


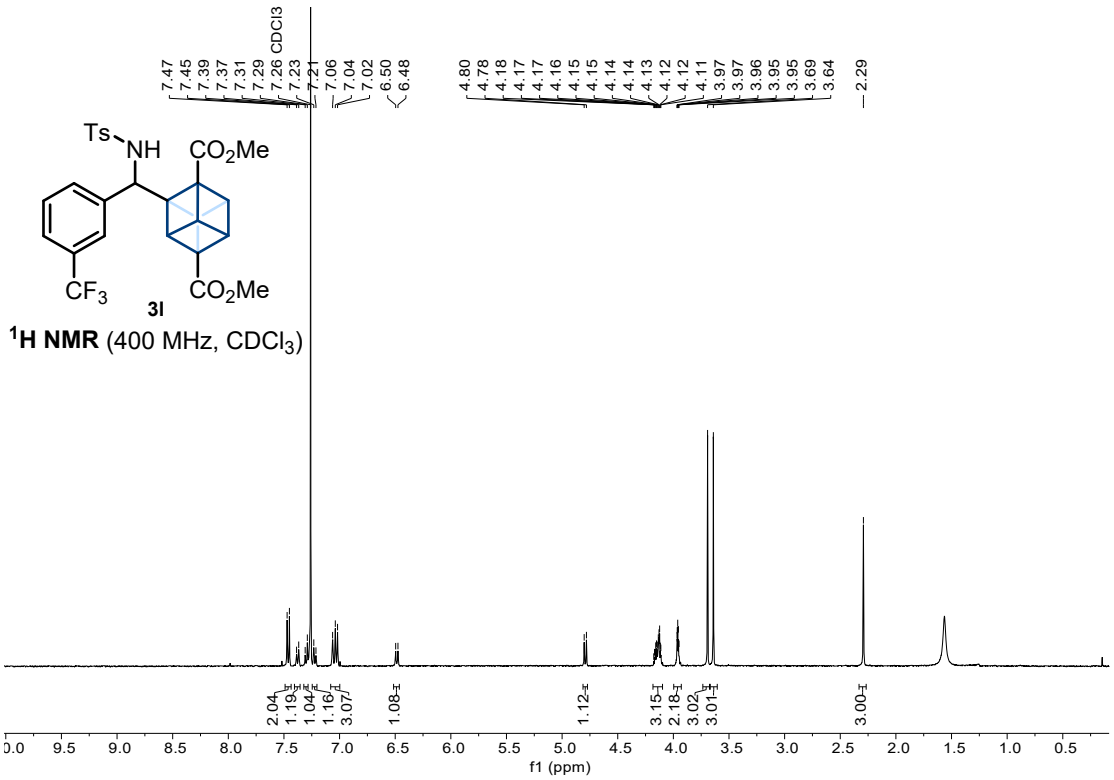
^{1}H NMR (400 MHz, $CDCl_3$)



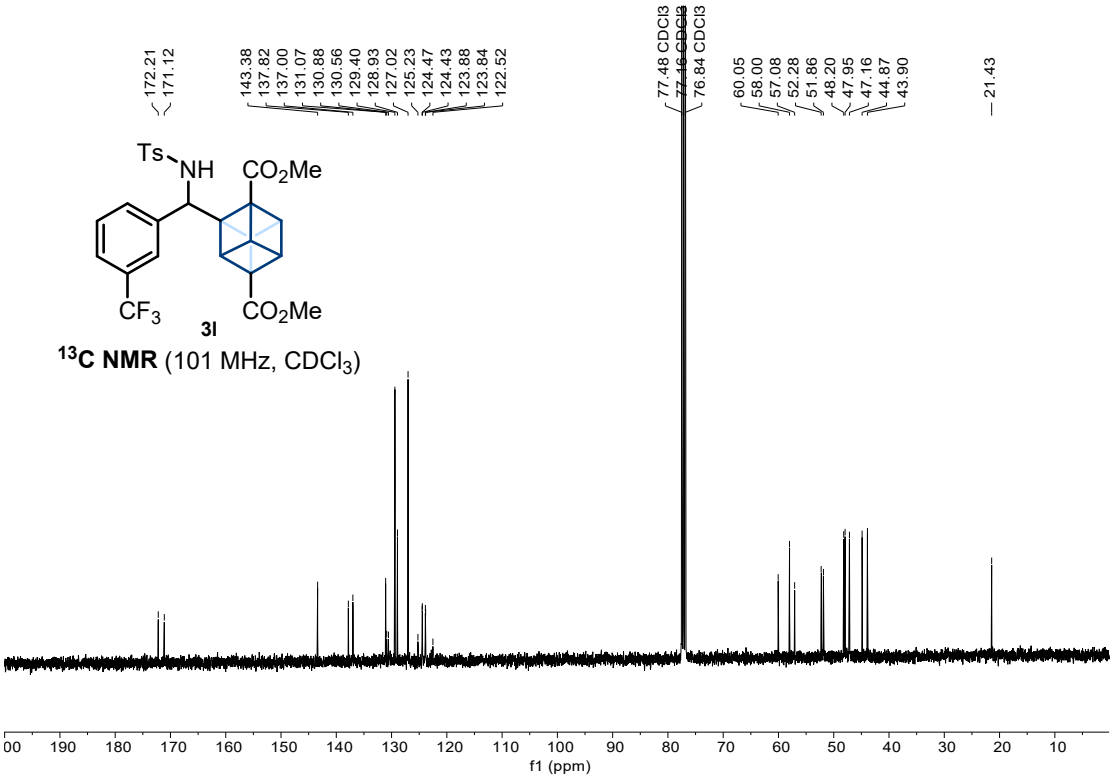
^{13}C NMR (101 MHz, $CDCl_3$)


7.54
7.52
7.42
7.42
7.42
7.41
7.40
7.26 CDCl3
7.06
7.05
7.04
7.04
7.02
7.00
7.00
6.99
6.99
6.98
6.97
6.58
6.56
5.32
5.30
4.16
4.15
4.15
4.14
4.13
4.12
4.12
4.12
4.11
4.10
4.09
4.07
4.06
4.05
4.05
4.04
3.95
3.94
3.94
3.93
3.93
3.92
3.92
3.75
3.60
2.29
Ts
NH
CO2Me
Br
CO2Me
3k
1H NMR (400 MHz, CDCl3)
2.00
0.99
3.02
1.93
1.07
1.03
3.00
1.09
1.11
3.03
3.01
3.03
f1 (ppm)

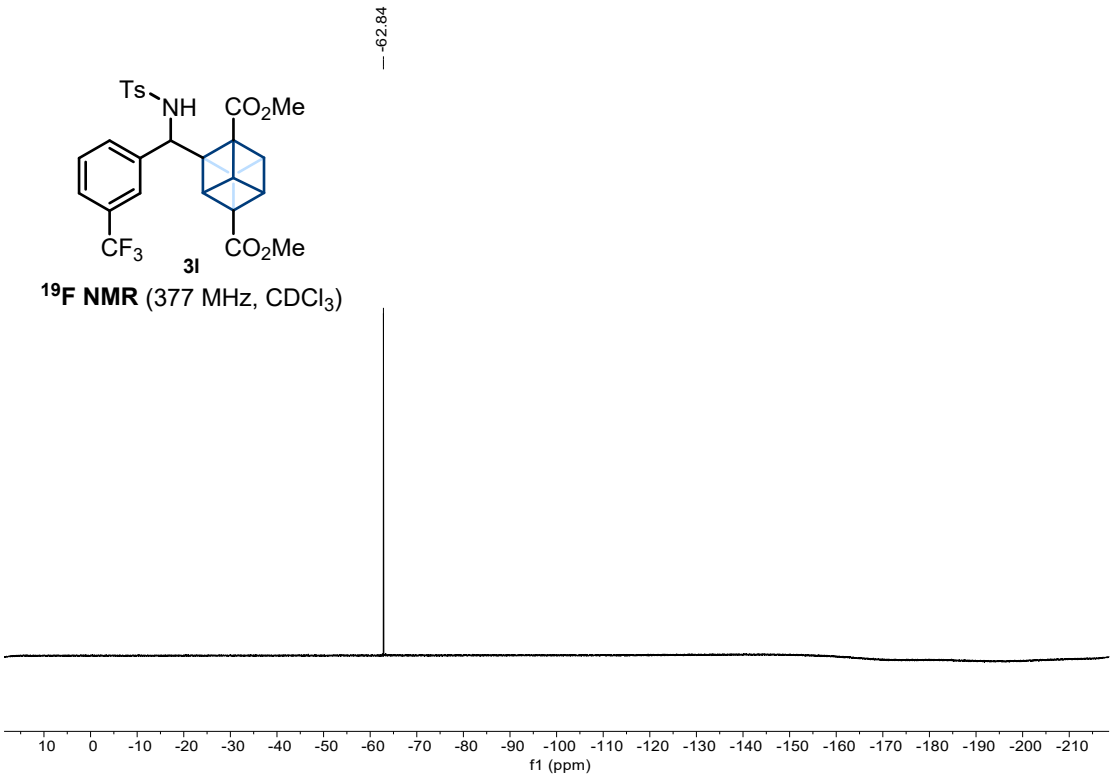

172.29
171.21
143.33
138.04
137.80
130.62
130.32
129.89
129.41
127.01
126.16
122.60
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
60.14
57.92
57.03
52.38
52.21
51.93
48.26
47.93
47.22
44.85
43.86
21.60
Ts
NH
CO2Me
Br
CO2Me
3k
13C NMR (101 MHz, CDCl3)
f1 (ppm)



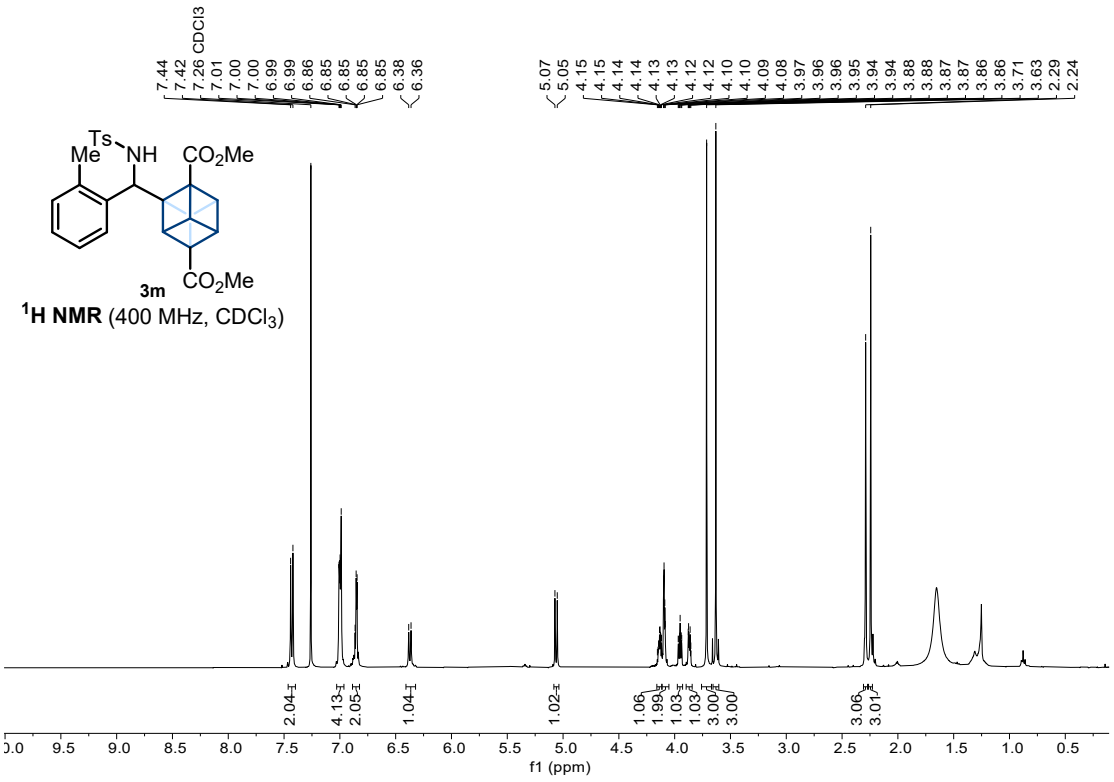
^{1}H NMR (400 MHz, $CDCl_3$)



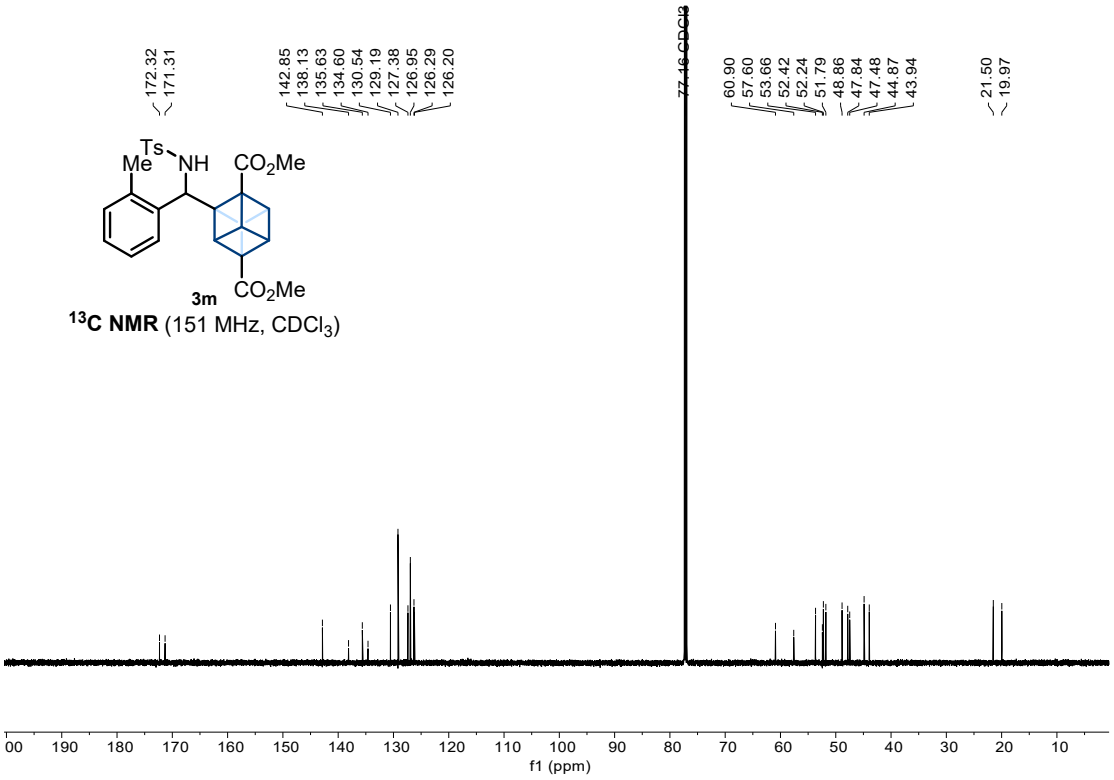
^{13}C NMR (101 MHz, $CDCl_3$)



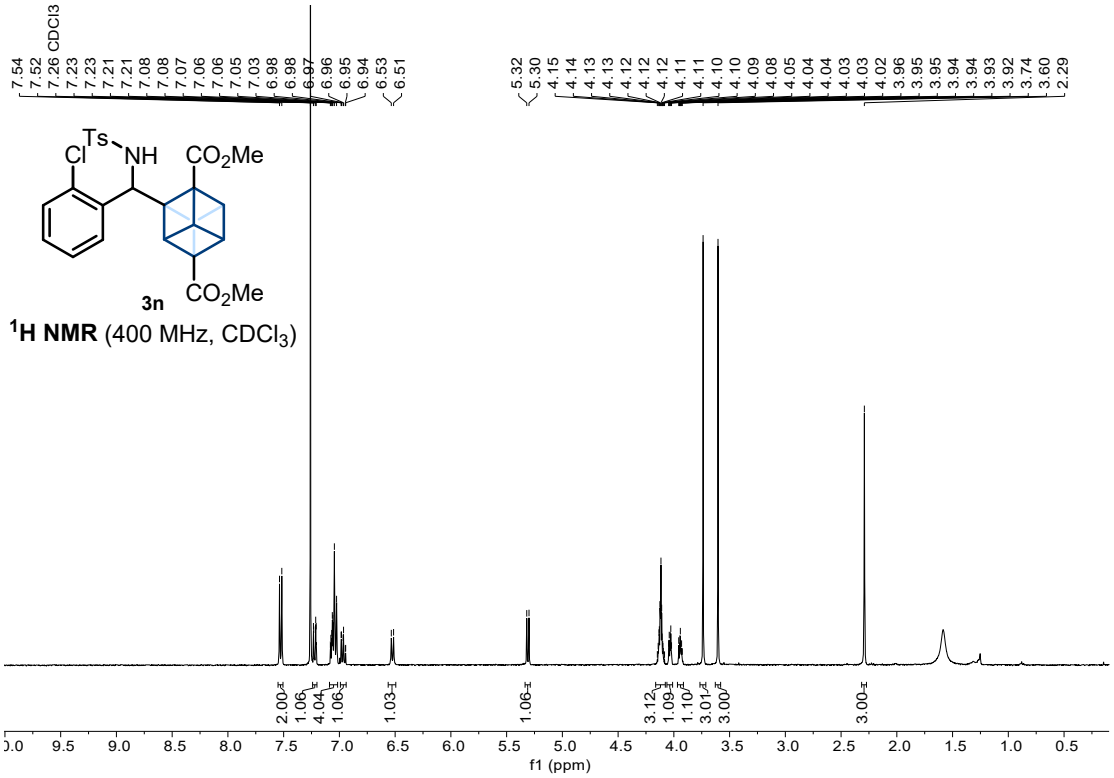
^{19}F NMR (377 MHz, $CDCl_3$)

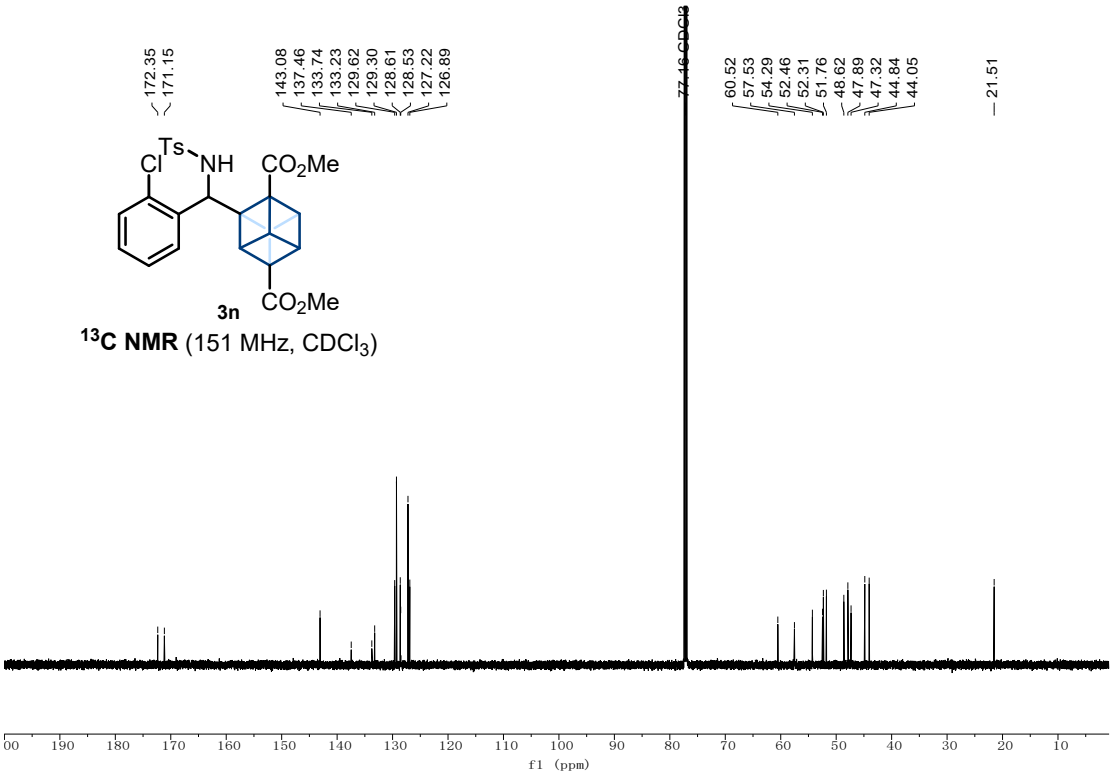


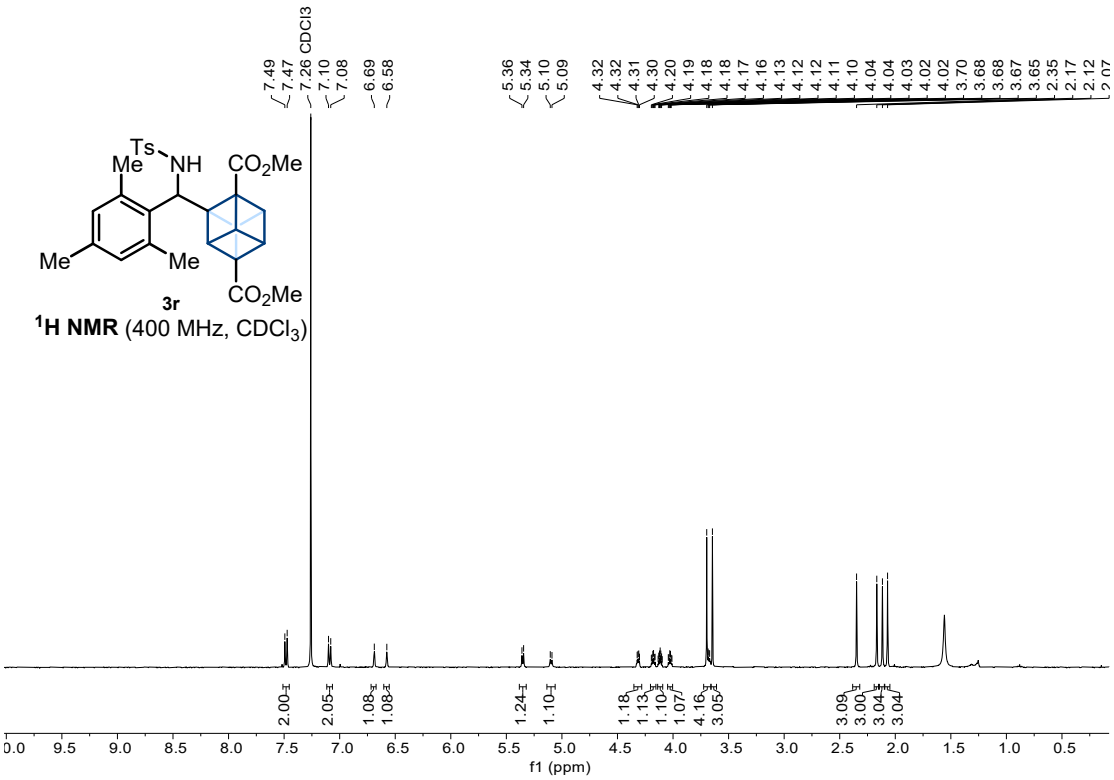
^{1}H NMR (400 MHz, $CDCl_3$)



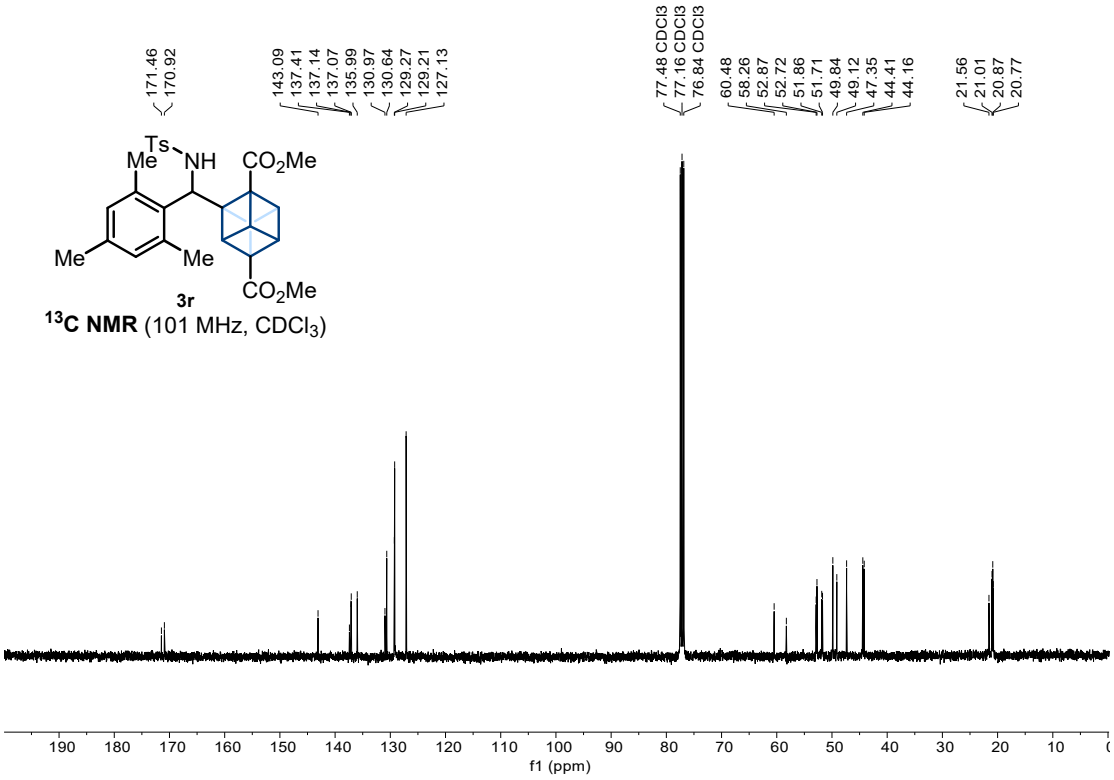
^{13}C NMR (151 MHz, $CDCl_3$)


7.54
7.52
7.26 CDCl3
7.23
7.23
7.21
7.21
7.08
7.08
7.07
7.06
7.06
7.05
7.03
6.98
6.98
6.97
6.96
6.95
6.94
6.53
6.51
5.32
5.30
4.15
4.14
4.13
4.13
4.12
4.12
4.12
4.11
4.11
4.10
4.10
4.09
4.08
4.05
4.04
4.04
4.03
4.03
4.02
3.96
3.95
3.95
3.94
3.94
3.93
3.92
3.74
3.60
2.29
Cl
Ts
NH
CO2Me
CO2Me
3n
1H NMR (400 MHz, CDCl3)
2.00
1.06
4.04
1.06
1.03
1.06
3.12
1.09
1.10
3.01
3.00
3.00
f1 (ppm)

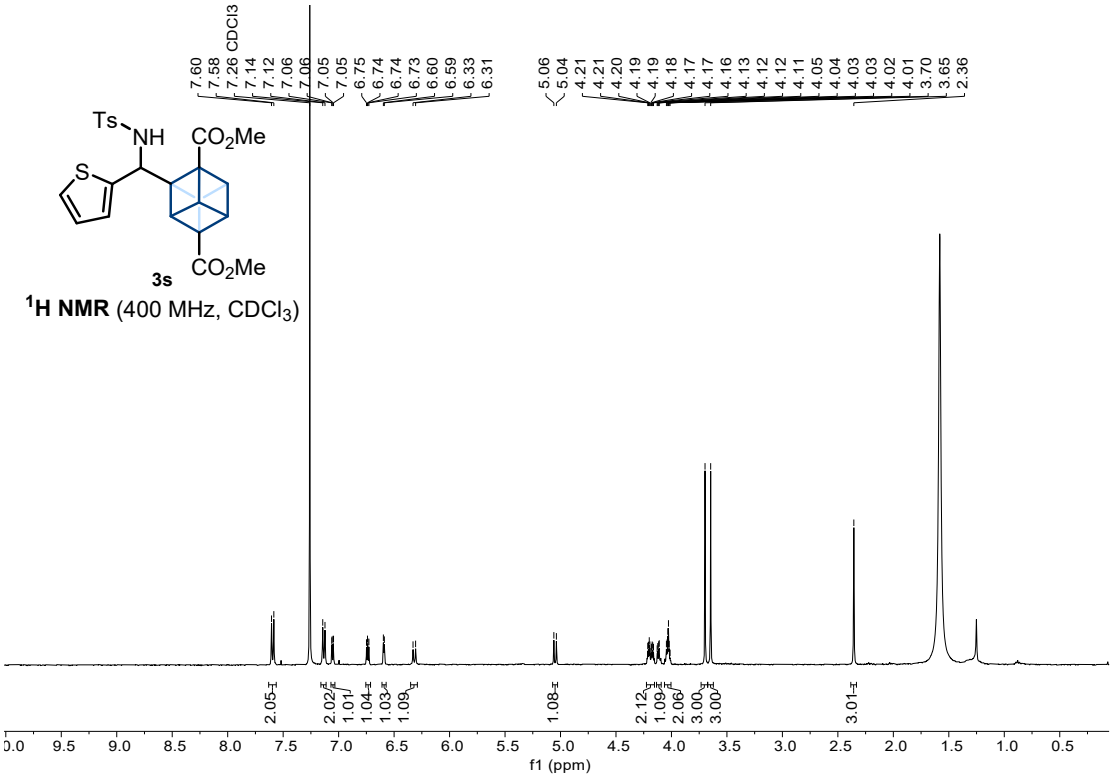

172.35
171.15
143.08
137.46
133.74
133.23
129.62
129.30
128.61
128.53
127.22
126.89
77.46 CDCl3
60.52
57.53
54.29
52.46
52.31
51.76
48.62
47.89
47.32
44.84
44.05
21.51
Cl
Ts
NH
CO2Me
CO2Me
3n
13C NMR (151 MHz, CDCl3)
f1 (ppm)

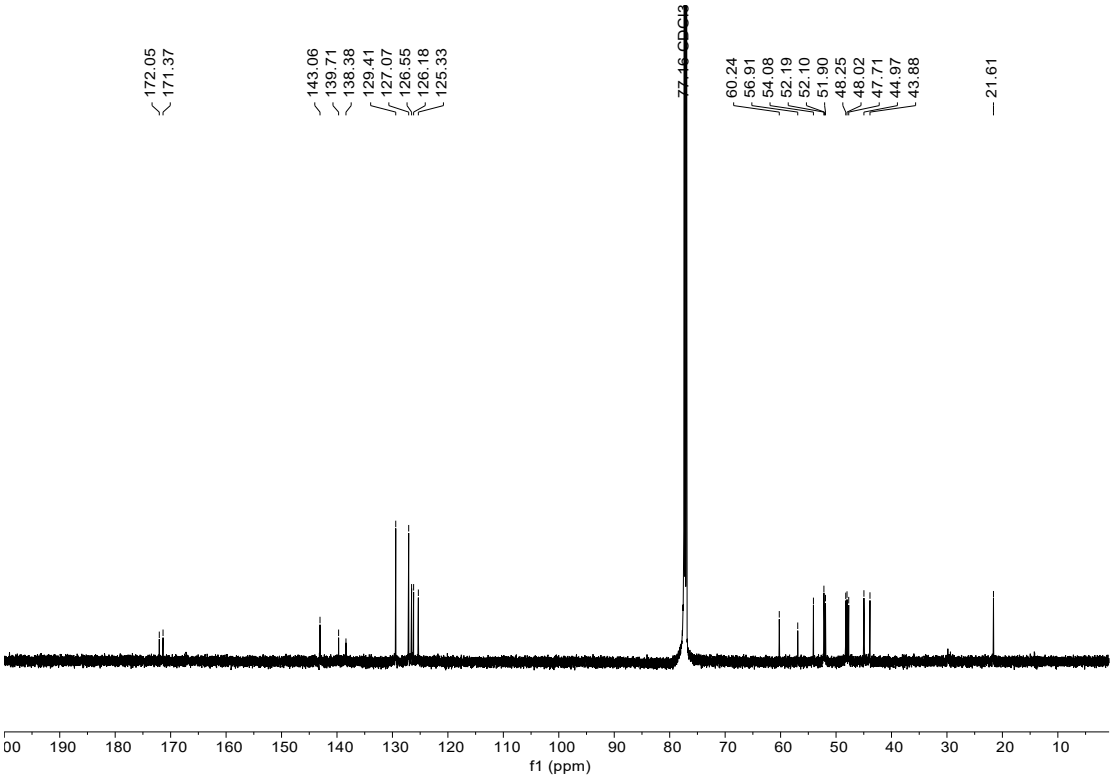


^{1}H NMR (400 MHz, $CDCl_3$)



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


7.60
7.58
CDCl3
7.26
7.14
7.12
7.06
7.06
7.05
7.05
6.75
6.74
6.74
6.73
6.60
6.59
6.33
6.31
5.06
5.04
4.21
4.21
4.20
4.19
4.19
4.18
4.17
4.17
4.16
4.13
4.12
4.12
4.11
4.05
4.04
4.03
4.03
4.02
4.01
3.70
3.65
2.36
Ts
NH
CO2Me
S
CO2Me
3s
1H NMR (400 MHz, CDCl3)
2.05
2.02
1.01
1.04
1.03
1.09
1.08
2.12
1.09
2.06
3.00
3.00
3.01
f1 (ppm)


172.05
171.37
143.06
139.71
138.38
129.41
127.07
126.55
126.18
125.33
77.16
CDCl3
60.24
56.91
54.08
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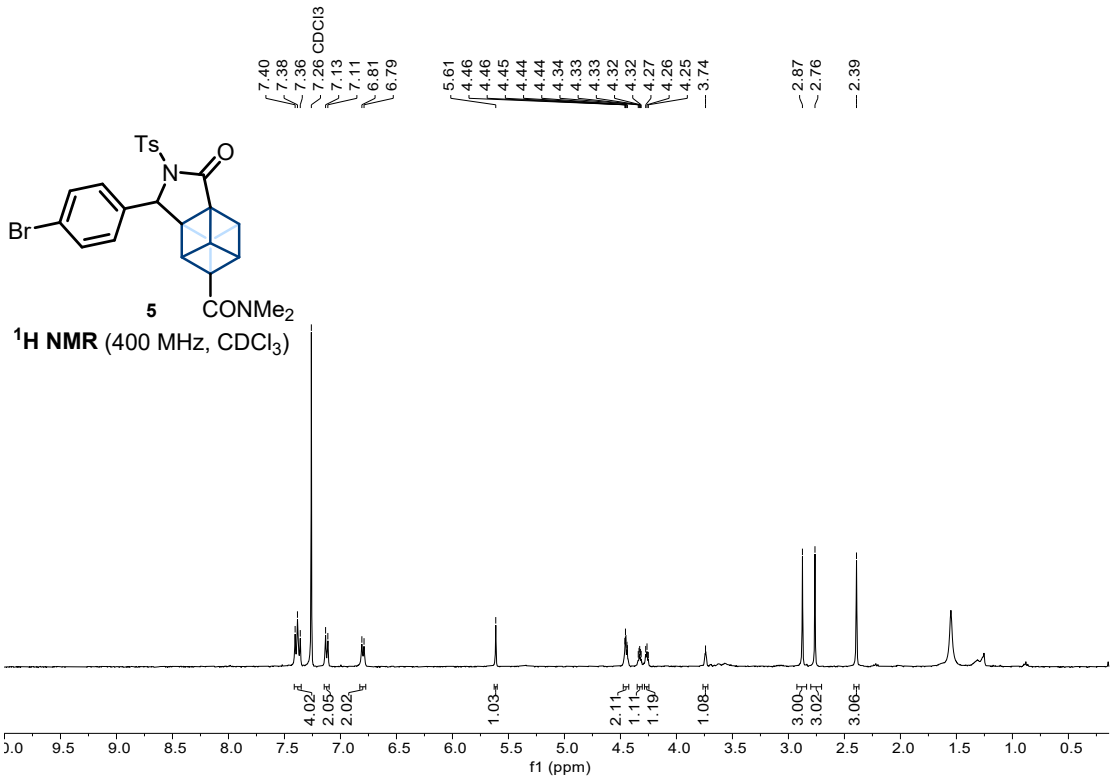
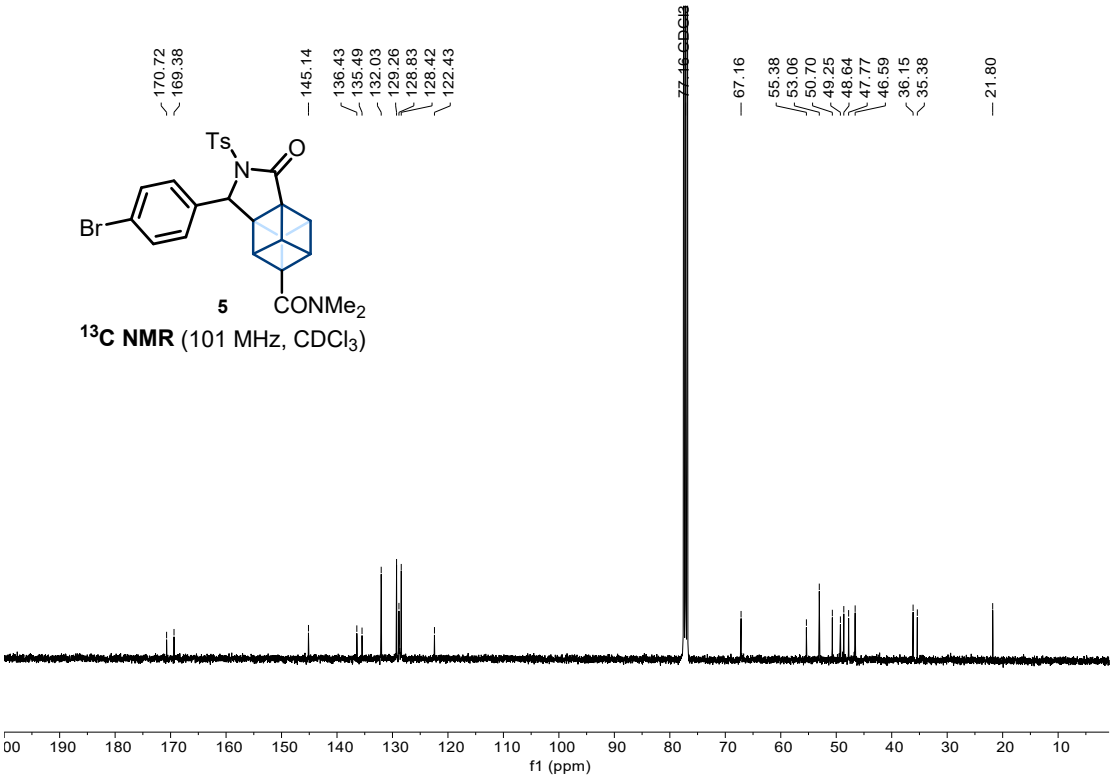
52.10
51.90
48.25
48.02
47.71
44.97
43.88
21.61
f1 (ppm)



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



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