Metal-Free C(sp^3)−H Functionalization of Sulfonamides via Strain-Release Rearrangement

(Supporting Information)

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1. General Information

Unless otherwise mentioed, all reactions were performed under an argon atmosphere using flame-dried glasswares. All new compounds were fully characterized. NMR-spectra were recorded on Bruker ARX-400 MHz or Jeol ECX-400 MHz. Chemical shifts (δ values) were reported in ppm with $CDCl_3$. Coupling constants were reported in Hz, and multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); q (quartet); quint (quintet); m (multiplet);dd (doubletof doublets); ddd (doublet of doublet of doublets); dddd (doublet of doublet of doublet of doublets); dt (doublet of triplets); td (triplet of doublets); ddt (doublet of doublet of triplets); dq (doubletof quartets); app (apparent); br (broad). Mass spectra were conducted at Micromass Q-Tof instrument (ESI) and Agilent Technologies 5973N (EI). For the React IR kinetic experiments, the reaction spectra were recorded using an IC 10 and IC 15 from Mettler-Toledo Auto Chem. Data manipulation was carried out using the iC IR software, version 4.2. All reactions were carried out in flame-dried reaction vessels (10 ML) with Teflon screw caps under argon. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. 1,4-Diazabicyclo[2.2.2]octane (DABCO) and *N,N*-dimethylformamide (DMF) were purchased from Sigma-Aldrich. DMF was dried over CaH_2. All arylimine substrates are synthesized according to the reported literature[1] (Note: After the reaction, the mixture was filtered through a short pad of silica gel and concentrated in rotary evaporator evaporation. The excess of aldehyde was removed under vacuum. Then the products were obtained by recrystallization with DCM/petroleum ether. Due to the instability of these compounds, they were used directly without further purification.).

2. Preparation of *N*-fluorosulfonamide

General Procedure A:[2]

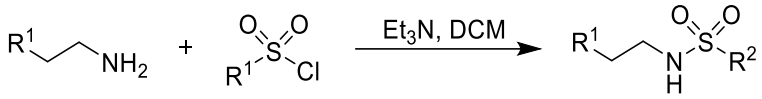


Fig. S1

Aliphatic amine (1 equiv.) was added dropwise to a solution of sulfonyl chloride (1 equiv.) and DCM (0.2 M). Then triethyl amine (3 equiv.) was added to the reaction mixture dropwise. The reaction was stirred at 30 ºC for 12 h. After the reaction, the mixture washed with 1 N aq. HCl (50 mL/20 mmol), saturated $NaHCO_3$ (50 mL/20mmol) and brine solution (50 mL/20 mmol) respectively. Organic portion was dried over anhyd. $MgSO_4$ and concentrated in rotary evaporator evaporation. the crude product waas used directly without further purification.

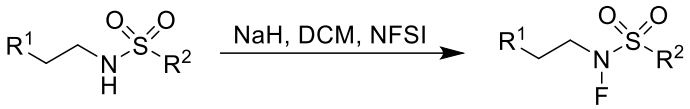


Fig. S2

Sodium hydride (10 mmol, 2 equiv.) was washed with pentane (2 times) and dried under vacuum and filled with nitrogen. In an oven dried round bottom flask with stir bar, the cleaning sodium hydride (10 mmol, 2 equiv.) and dry DCM (40 mL) was added under argon atmosphere. Subsequently, a solution of sulfonamide (1 equiv.) in dry DCM (0.5 M) was added dropwise to the NaH suspension in DCM. The mixture was stirred at 30 ºC for 1.0 h. A solution of NFSI (3 equiv.) in dry DCM (0.5 M) was added to dropwise to the reaction mixture at 30 ºC. The reaction was stirred for overnight at 30 ºC. The reaction was quenched with 50 mL of ice water. The organic part was washed with 30 mL $NaHCO_3$, and 30 mL brine solution respectively. The organic part was dried over anhyd. Na_2SO_4, filtrated, and then concentrated in vacuo. The corresponding *N*-fluorosulfonamides were obtained by silica gel flash column chromatography using petroleum ether (PE)/ethyl acetate mixture as eluent.

General Procedure B:[3]

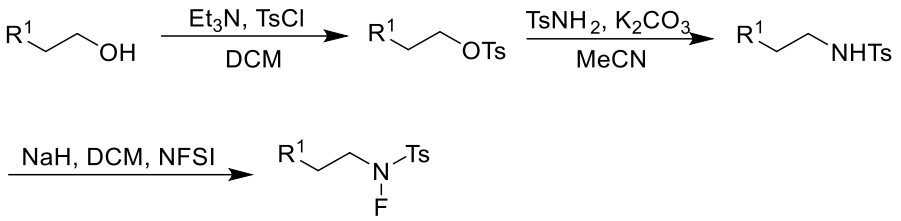


Fig. S3

To a stirred solution of alkyl alcohols (1 equiv.) and trimethylamine (1.5 equiv.) in DCM (0.25 M) at 0 °C was added dropwise tosyl chloride (1.2 equiv.). The mixture was slowly warmed to room temperature with continue stirring for 10 h, and then diluted with saturated sodium bicarbonate (10 mL), extracted with DCM (2 × 20 mL). The combined organic layer was washed with brine (2 × 10 mL), dried over $MgSO_4$ and then concentrated under reduced pressure. The crude products were used directly without further purification.

Ts-Protected hydroxyl compound was dissolved in MeCN (0.2 M) and treated with $TsNH_2$ (2.0 eq) and K_2CO_3 (2.0 eq) at rt. The reaction mixture was refluxed at 95 °C for 12 h. It was then concentrated under reduced pressure and the residue was suspended in AcOEt (5 mL/mmol). The resulting mixture was washed with H_2O (5 mL/mmol) and the organic phase was dried over $MgSO_4$. The solvent was then removed under reduced pressure and the crude product was purified by flash column chromatography using petroleum ether/ethyl acetate mixture as eluent.

Sodium hydride (10 mmol, 2 equiv.) was washed with pentane (2 times) and dried under vacuum and filled with nitrogen. In an oven dried round bottom flask with stir bar, the cleaning sodium hydride (10 mmol, 2 equiv.) and dry DCM (40 mL) was added under argon atmosphere. Subsequently, a solution of sulfonamide (1 equiv.) in dry DCM (0.5 M) was added dropwise to the NaH suspension in DCM. The mixture was stirred at 30 ºC for 1.0 h. A solution of NFSI (3 equiv.) in dry DCM (0.5 M) was added to dropwise to the reaction mixture at 30 ºC. The reaction was stirred for overnight at 30 ºC. The reaction was quenched with 50 mL of ice water. The organic part was washed with 30 mL $NaHCO_3$, and 30 mL brine solution respectively. The organic part was dried

over anhyd. Na_2SO_4, filtrated, and then concentrated in vacuo. The corresponding *N*-fluorosulfonamides were obtained by silica gel flash column chromatography using petroleum ether/ethyl acetate mixture as eluent.

General Procedure C:[2]

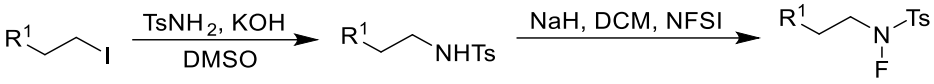
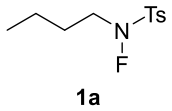


Fig. S4

Sulfonamide (2 equiv.) and KOH (1.3 equiv.) and DMSO (0.5 M) were added into an oven dried round bottom flask was stir bar. The reaction mixture was stirred at 60° C for 2 h. Then iodide (1 equiv.) was added. The mixture was stirred for overnight at 60 °C. After the reaction, 10 % aq. LiCl solution (0.25 M) and ethyl acetate (0.25M) were added. The organic part was dried over anhyd. Na_2SO_4 and concentrated in rotary evaporator. The corresponding product was purified by flash column chromatography using ethyl acetate/petroleum ether mixture as eluent.

Sodium hydride (10 mmol, 2 equiv.) was washed with pentane (2 times) and dried under vacuum and filled with nitrogen. In an oven dried round bottom flask with stir bar, the cleaning sodium hydride (10 mmol, 2 equiv.) and dry DCM (40 mL) was added under argon atmosphere. Subsequently, a solution of sulfonamide (1 equiv.) in dry DCM (0.5 M) was added dropwise to the NaH suspension in DCM. The mixture was stirred at 30 °C for 1.0 h. A solution of NFSI (3 equiv.) in dry DCM (0.5 M) was added to dropwise to the reaction mixture at 30 °C. The reaction was stirred for overnight at 30 °C. The reaction was quenched with 50 mL of ice water. The organic part was washed with 30 mL $NaHCO_3$, and 30 mL brine solution respectively. The organic part was dried over anhyd. Na_2SO_4, filtrated, and then concentrated in vacuo. The corresponding *N*-fluorosulfonamides were obtained by silica gel flash column chromatography using petroleum ether/ethyl acetate mixture as eluent.

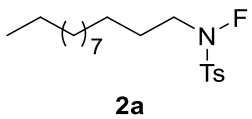
***N*-Butyl-*N*-fluoro-4-methylbenzenesulfonamide (1a)**



1a

General procedure **A**, with 5.0 mmol scale, **1a** was prepared from commercially available primary amine to obtain a yellow oil (0.91 g, 74%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 7.4 Hz, 2H), 7.40 (d, *J* = 7.4 Hz, 2H), 3.24 (t, *J* = 6.6 Hz, 1H), 3.14 (t, *J* = 6.6 Hz, 1H), 2.47 (s, 3H), 1.72 – 1.65 (m, 2H), 1.42 (q, *J* = 7.4 Hz, 2H), 0.94 – 0.89 (m, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 129.9, 129.89, 128.8, 53.47 (d, *J* = 12.1 Hz), 28.2, 21.8, 19.7, 13.6; **HRMS m/z (ESI):** calcd for $C_{11}H_{17}FNO_2S^+$ $[M+H]^+$: 246.0959, found 246.0961.

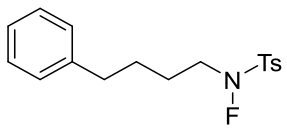
_N_-Dodecyl-_N_-fluoro-4-methylbenzenesulfonamide (2a)



2a

General procedure **A**, with 5.0 mmol scale, **2a** was prepared from commercially available primary amine to obtain a colorless oil (1.18 g, 66%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 3.24 (t, *J* = 7.0 Hz, 1H), 3.14 (t, *J* = 7.0 Hz, 1H), 2.48 (s, 3H), 1.70 (q, *J* = 7.2 Hz, 2H), 1.42 – 1.34 (m, 2H), 1.31 – 1.21 (m, 16H), 0.87 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 129.94, 129.90, 128.8, 53.7 (d, *J* = 12.1 Hz), 31.9, 29.6, 29.5, 29.4, 29.3, 29.1, 26.5, 26.3, 22.7, 21.8, 14.1; **HRMS m/z (ESI):** calcd for $C_{19}H_{32}FNNaO_2S^+$ $[M+Na]^+$: 380.2030, found 380.2034.

_N_-Fluoro-4-methyl-_N_-(4-phenylbutyl)benzenesulfonamide (3a)

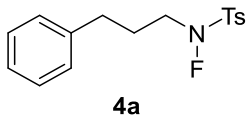


3a

General procedure **A**, with 5.0 mmol scale, **3a** was prepared from commercially available primary amine to obtain a colorless oil (1.03 g, 64%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.24 (t, *J* = 7.2 Hz, 2H), 7.19 – 7.09 (m, 3H), 3.24 (d, *J* = 5.6 Hz, 1H), 3.13 (t, *J* = 5.6 Hz, 1H), 2.60 (t, *J* = 6.3 Hz, 2H), 2.45 (s, 3H), 1.76 – 1.68 (m, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 141.7, 129.92, 129.90, 128.8, 128.3, 126.4,

125.9, 53.5 (d, J = 13.1 Hz), 35.3, 28.3, 25.8, 21.8; **HRMS m/z (ESI):** calcd for $C_{17}H_{20}FNNaO_2S^+$ $[M+Na]^+$: 344.1091, found 344.1096.

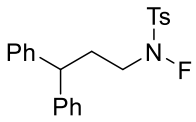
***N*-Fluoro-4-methyl-*N*-(3-phenylpropyl)benzenesulfonamide (4a)**



4a

General procedure **A**, with 5.0 mmol scale, **4a** was prepared from commercially available primary amine to obtain a white solid (0.94 g, 61%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.28 (t, J = 7.6 Hz, 2H), 7.17 (t, J = 6.9 Hz, 3H), 3.26 (t, J = 6.7 Hz, 1H), 3.16 (t, J = 6.7 Hz, 1H), 2.74 (t, J = 7.6 Hz, 2H), 2.47 (s, 3H), 2.05 – 1.98 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.3, 140.6, 129.9, 129.3, 128.54, 128.45, 126.1, 52.9 (d, J = 12.1 Hz), 32.4, 27.9, 21.7; **HRMS m/z (ESI):** calcd for $C_{16}H_{18}FNNaO_2S^+$ $[M+Na]^+$: 330.0934, found 330.0937.

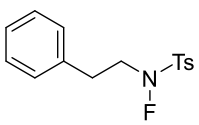
***N*-(3,3-Diphenylpropyl)-*N*-fluoro-4-methylbenzenesulfonamide (5a)**



5a

General procedure **A**, with 5.0 mmol scale, **5a** was prepared from commercially available primary amine to obtain a yellow solid (0.98 g, 51%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.73 (d, J = 7.3 Hz, 2H), 7.33 (d, J = 7.3 Hz, 2H), 7.27 – 7.16 (m, 10H), 4.13 (t, J = 7.8 Hz, 1H), 3.21 (t, J = 6.6 Hz, 1H), 3.11 (t, J = 6.6 Hz, 1H), 2.48 – 2.42 (m, 2H), 2.42 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 143.4, 129.8, 128.6, 127.7, 126.5, 52.0 (d, J = 12.1 Hz), 47.7, 31.8, 21.7; **HRMS m/z (ESI):** calcd for $C_{22}H_{22}FNNaO_2S^+$ $[M+Na]^+$: 406.1247, found 406.1249.

***N*-Fluoro-4-methyl-N-phenethylbenzenesulfonamide (6a)**

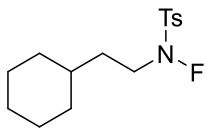


6a

General procedure **A**, with 5.0 mmol scale, **6a** was prepared from commercially available primary amine to obtain a yellow solid (0.95 g, 65%) by flash chromatography on silica gel (50:1–20:1,

PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.37 (m, 2H), 7.34 – 7.28 (m, 2H), 7.27 – 7.24 (m, 1H), 7.22 – 7.17 (m, 2H), 3.53 – 3.45 (m, 1H), 3.43 – 3.35 (m, 1H), 3.04 (dd, *J* = 8.8, 6.5 Hz, 2H), 2.48 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.3, 137.3, 129.99, 129.95, 128.8, 128.64, 128.59, 126.8, 55.1 (d, *J* = 12.1 Hz), 32.8, 21.8; **HRMS m/z (ESI):** calcd for $C_{15}H_{16}FNNaO_2S^+$ $[M+Na]^+$: 316.0778, found 316.0782.

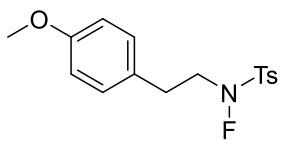
***N*-(2-Cyclohexylethyl)-*N*-fluoro-4-methylbenzenesulfonamide (7a)**



7a

General procedure **A**, with 5.0 mmol scale, **7a** was prepared from commercially available primary amine to obtain a colorless oil (0.93 g, 62%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 3.27 (dd, *J* = 7.7, 6.7 Hz, 1H), 3.17 (dd, *J* = 7.7, 6.7 Hz, 1H), 2.47 (s, 3H), 1.71 – 1.57 (m, 7H), 1.46 – 1.33 (m, 1H), 1.28 – 1.10 (m, 3H), 0.89 (q, *J* = 11.7 Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 129.9, 128.6, 51.7 (d, *J* = 13.1 Hz), 34.8, 33.4, 32.9, 26.3, 26.0, 21.7; **HRMS m/z (ESI):** calcd for $C_{15}H_{22}FNNaO_2S^+$ $[M+Na]^+$: 322.1247, found 322.1252.

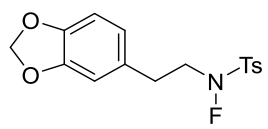
***N*-Fluoro-*N*-(4-methoxyphenethyl)-4-methylbenzenesulfonamide (8a)**



8a

General procedure **A**, with 5.0 mmol scale, **8a** was prepared from commercially available primary amine to obtain a yellow oil (0.90 g, 56%) by flash chromatography on silica gel (40:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.36 (m, 2H), 7.11 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 3.78 (s, 3H), 3.52 – 3.39 (m, 1H), 3.39 – 3.29 (m, 1H), 2.98 (dd, *J* = 8.7, 6.5 Hz, 2H), 2.47 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.4, 146.3, 129.94, 129.88, 129.8, 129.2, 128.5, 114.0, 55.3 (d, *J* = 12.1 Hz), 55.2, 31.9, 21.7; **HRMS m/z (ESI):** calcd for $C_{16}H_{18}FNNaO_3S^+$ $[M+Na]^+$: 346.0884, found 346.0887.

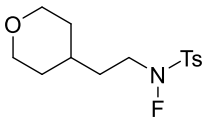
***N*-(2-(Denzo[*d*][1,3]dioxol-5-yl)ethyl)-*N*-fluoro-4-methylbenzenesulfonamide (9a)**



9a

General procedure **A**, with 5.0 mmol scale, **9a** was prepared from commercially available primary amine to obtain a yellow solid (0.91 g, 54%) by flash chromatography on silica gel (30:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.36 (m, 2H), 6.72 (d, *J* = 7.9 Hz, 1H), 6.68 – 6.60 (m, 2H), 5.91 (s, 2H), 3.49 – 3.37 (m, 1H), 3.37 – 3.26 (m, 1H), 2.93 (dd, *J* = 8.6, 6.5 Hz, 2H), 2.46 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 147.7, 146.3, 130.9, 130.0, 129.9, 128.5, 121.8, 109.2, 108.3, 100.9, 55.3 (d, *J* = 13.1 Hz), 32.5, 21.7; **HRMS m/z (ESI):** calcd for $C_{16}H_{16}FNNaO_4S^+$ $[M+Na]^+$: 360.0676, found 360.0680.

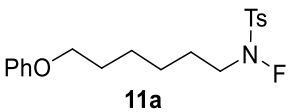
***N*-Fluoro-4-methyl-*N*-(2-(tetrahydro-2*H*-pyran-4-yl)ethyl)benzenesulfonamide (10a)**



10a

General procedure **A**, with 5.0 mmol scale, **10a** was prepared from commercially available primary amine to obtain a white solid (0.80 g, 53%) by flash chromatography on silica gel (30:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 3.94 (dd, *J* = 11.2, 4.0 Hz, 2H), 3.37 (td, *J* = 11.9, 1.8 Hz, 2H), 3.30 (t, *J* = 6.8 Hz, 1H), 3.20 (t, *J* = 6.8 Hz, 1H), 2.48 (s, 3H), 1.80 – 1.68 (m, 1H), 1.67 – 1.58 (m, 4H), 1.33 – 1.24 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.3, 129.96, 129.92, 128.6, 67.8, 50.9 (d, *J* = 12.1 Hz), 32.9, 32.6, 32.0, 21.8; **HRMS m/z (ESI):** calcd for $C_{14}H_{20}FNNaO_3S^+$ $[M+Na]^+$: 324.1040, found 324.1043.

***N*-Fluoro-4-methyl-*N*-(6-phenoxyhexyl)benzenesulfonamide (11a)**

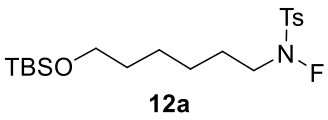


11a

General procedure **A**, with 5.0 mmol scale, **11a** was prepared from commercially available primary amine to obtain a white solid (0.89 g, 49%) by flash chromatography on silica gel

(40:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.25 (m, 2H), 6.97 – 6.90 (m, 1H), 6.90 – 6.86 (m, 2H), 3.94 (t, *J* = 6.9 Hz, 2H), 3.27 (t, *J* = 6.9 Hz, 1H), 3.17 (t, *J* = 6.9 Hz, 1H), 2.48 (s, 3H), 1.84 – 1.70 (m, 4H), 1.52 – 1.43 (m, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.9, 146.2, 129.9, 129.4, 128.7, 120.5, 114.4, 67.5, 53.6 (d, *J* = 12.1 Hz), 29.0, 26.3, 26.2, 25.6, 21.8; **HRMS m/z (ESI):** calcd for $C_{19}H_{24}FNNaO_3S^+$ $[M+Na]^+$: 388.1353, found 388.1357.

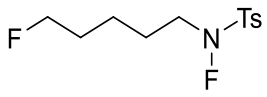
_N_-(6-((_tert_-Butyldimethylsilyl)oxy)hexyl)-_N_-fluoro-4-methylbenzenesulfonamide (12a)



12a

General procedure **A**, with 5.0 mmol scale, **12a** was prepared from commercially available primary amine to obtain a yellow oil (1.03 g, 51%) by flash chromatography on silica gel (30:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 3.58 (t, *J* = 6.5 Hz, 2H), 3.24 (t, *J* = 7.0 Hz, 1H), 3.14 (t, *J* = 7.0 Hz, 1H), 2.48 (s, 3H), 1.71 (p, *J* = 7.2 Hz, 2H), 1.54 – 1.45 (m, 2H), 1.43 – 1.30 (m, 4H), 0.88 (s, 9H), 0.03 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 129.93, 129.90, 128.8, 63.0, 53.7 (d, *J* = 13.1 Hz), 32.6, 26.4, 26.3, 25.9, 25.3, 21.8, 18.3, -5.3; **HRMS m/z (ESI):** calcd for $C_{19}H_{34}FNNaO_3SSi^+$ $[M+Na]^+$: 426.1905, found 426.1909.

_N_-Fluoro-_N_-(5-fluoropentyl)-4-methylbenzenesulfonamide (13a)

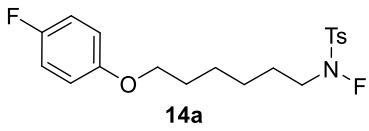


13a

General procedure **B**, with 5.0 mmol scale, **13a** was prepared from commercially available primary amine to obtain a colorless oil (0.85 g, 61%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 4.49 (t, *J* = 6.0 Hz, 1H), 4.37 (t, *J* = 6.0 Hz, 1H), 3.25 (t, *J* = 6.8 Hz, 1H), 3.15 (t, *J* = 6.8 Hz, 1H), 2.47 (s, 3H), 1.78 – 1.65 (m, 4H), 1.57 – 1.48 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.3, 129.91, 129.85, 128.5, 83.7 (d, *J* = 165.6

Hz), 53.5 (d, *J* = 12.1 Hz), 29.8 (d, *J* = 20.2 Hz), 25.8, 22.3 (d, *J* = 5.1 Hz), 21.7; **HRMS m/z (ESI):** calcd for $C_{12}H_{17}F_2NNaO_2S^+$ $[M+Na]^+$: 300.0840, found 300.0845.

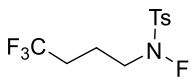
_N_-Fluoro-_N_-(6-(4-fluorophenoxy)hexyl)-4-methylbenzenesulfonamide (14a)



14a

General procedure **A**, with 5.0 mmol scale, **14a** was prepared from commercially available primary amine to obtain a yellow solid (0.92 g, 48%) by flash chromatography on silica gel (40:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.40 (d, J = 8.3 Hz, 2H), 6.99 – 6.92 (m, 2H), 6.84 – 6.78 (m, 2H), 3.90 (t, *J* = 6.4 Hz, 2H), 3.27 (t, *J* = 6.9 Hz, 1H), 3.16 (t, *J* = 6.9 Hz, 1H), 2.48 (s, 3H), 1.75 (qt, *J* = 9.7, 4.2 Hz, 4H), 1.48 (p, *J* = 3.6 Hz, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.3, 155.9, 155.1, 146.2, 129.9, 128.7, 115.7 (d, *J* = 22.2 Hz), 115.3 (d, *J* = 8.1 Hz), 68.2, 53.6 (d, *J* = 12.1 Hz), 29.0, 26.3, 26.2, 25.6, 21.8; **HRMS m/z (ESI):** calcd for $C_{19}H_{23}F_2NNaO_3S^+$ $[M+Na]^+$: 406.1259, found 406.1263.

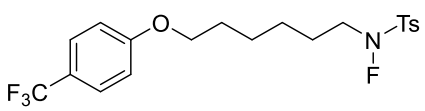
_N_-Fluoro-4-methyl-_N_-(4,4,4-trifluorobutyl)benzenesulfonamide (15a)



15a

General procedure **A**, with 5.0 mmol scale, **15a** was prepared from commercially available primary amine to obtain a yellow oil (0.90 g, 60%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 3.34 (t, *J* = 6.5 Hz, 1H), 3.24 (t, *J* = 6.5 Hz, 1H), 2.48 (s, 3H), 2.33 – 2.19 (m, 2H), 2.04 – 1.92 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.6, 130.0, 129.9, 128.3, 52.3 (d, *J* = 12.1 Hz), 30.8 (q, *J* = 58.6, 29.3 Hz), 21.71, 19.2 (d, *J* = 3.0 Hz); **HRMS m/z (ESI):** calcd for $C_{11}H_{13}F_4NNaO_2S^+$ $[M+Na]^+$: 322.0495, found 322.0499.

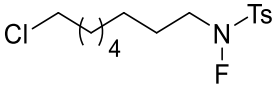
_N_-Fluoro-4-methyl-_N_-(6-(4-(trifluoromethyl)phenoxy)hexyl)benzenesulfonamide (16a)



16a

General procedure **A**, with 5.0 mmol scale, **16a** was prepared from commercially available primary amine to obtain a white solid (0.89 g, 41%) by flash chromatography on silica gel (40:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 3.98 (t, *J* = 6.4 Hz, 2H), 3.27 (t, *J* = 6.8 Hz, 1H), 3.17 (t, *J* = 6.8 Hz, 1H), 2.48 (s, 3H), 1.86 – 1.68 (m, 4H), 1.54 – 1.45 (m, 4H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 161.4, 146.3, 129.9, 128.7, 126.8 (q, *J* = 6.1, 3.0 Hz), 114.3, 67.8, 53.5 (d, *J* = 13.1 Hz), 28.8, 26.2, 26.1, 25.5, 21.8; **HRMS m/z (ESI):** calcd for $C_{20}H_{23}F_4NNaO_3S^+$ $[M+Na]^+$: 456.1227, found 456.1232.

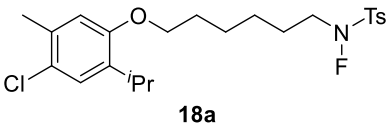
_N_-(8-Chlorooctyl)-_N_-fluoro-4-methylbenzenesulfonamide (17a)



17a

General procedure **A**, with 5.0 mmol scale, **17a** was prepared from commercially available primary amine to obtain a yellow oil (0.99 g, 59%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 3.51 (t, *J* = 6.7 Hz, 2H), 3.22 (t, *J* = 6.9 Hz, 1H), 3.12 (t, *J* = 7.0 Hz, 1H), 2.47 (s, 3H), 1.78 – 1.63 (m, 4H), 1.44 – 1.34 (m, 4H), 1.33 – 1.25 (m, 4H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 146.2, 129.9, 129.8, 128.6, 53.7 (d, *J* = 12.1 Hz), 45.0, 32.4, 28.8, 28.5, 26.6, 26.3, 26.1, 21.7; **HRMS m/z (ESI):** calcd for $C_{15}H_{23}ClFNNaO_2S^+$ $[M+Na]^+$: 358.1014, found 358.1017.

_N_-(6-(4-Chloro-2-isopropyl-5-methylphenoxy)hexyl)-_N_-fluoro-4-methylbenzenesulfonamide (18a)

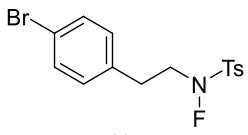


18a

General procedure **A**, with 5.0 mmol scale, **18a** was prepared from commercially available primary amine to obtain a colorless oil (0.96 g, 42%) by flash chromatography on silica gel (30:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ

7.82 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.12 (s, 1H), 6.66 (s, 1H), 3.91 (t, J = 6.2 Hz, 2H), 3.29 – 3.14 (m, 3H), 2.48 (s, 3H), 2.32 (s, 3H), 1.85 – 1.70 (m, 4H), 1.56 – 1.47 (m, 4H), 1.18 (s, 3H), 1.17 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 154.6, 146.2, 136.2, 133.4, 129.9, 128.6, 126.4, 125.2, 113.6, 67.8, 53.6 (d, *J* = 12.1 Hz), 29.1, 26.6, 26.23, 26.19, 25.7, 22.5, 21.8, 20.0; **HRMS m/z (ESI):** calcd for $C_{23}H_{31}ClFNNaO_3S^+$ $[M+Na]^+$: 478.1589, found 478.1593.

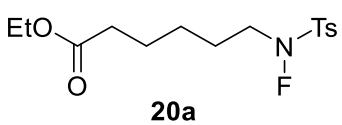
_N_-(4-Bromophenethyl)-_N_-fluoro-4-methylbenzenesulfonamide (19a)



19a

General procedure **A**, with 5.0 mmol scale, **19a** was prepared from commercially available primary amine to obtain a yellow solid (0.98 g, 53%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.41 (dd, *J* = 8.0, 5.7 Hz, 4H), 7.07 (d, *J* = 8.3 Hz, 2H), 3.47 (dd, *J* = 8.2, 6.6 Hz, 1H), 3.37 (dd, *J* = 8.3, 6.6 Hz, 1H), 3.07 – 2.91 (m, 2H), 2.48 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.4, 136.3, 131.7, 130.6, 130.0, 129.9, 128.5, 120.7, 54.7 (d, *J* = 12.1 Hz), 32.1, 21.8; **HRMS m/z (ESI):** calcd for $C_{15}H_{15}BrFNNaO_2S^+$ $[M+Na]^+$: 393.9883, found 393.9886.

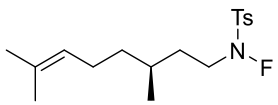
Ethyl 6-((_N_-fluoro-4-methylphenyl)sulfonamido)hexanoate (20a)



20a

General procedure **B**, with 5.0 mmol scale, **20a** was prepared from commercially available primary amine to obtain a colorless oil (0.79 g, 48%) by flash chromatography on silica gel (30:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 4.11 (q, *J* = 7.1 Hz, 2H), 3.24 (t, *J* = 6.9 Hz, 1H), 3.13 (t, *J* = 6.9 Hz, 1H), 2.47 (s, 3H), 2.29 (t, *J* = 7.4 Hz, 2H), 1.75 – 1.68 (m, 2H), 1.66 – 1.59 (m, 2H), 1.47 – 1.39 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.4, 146.2, 129.9, 128.6, 60.3, 53.5 (d, *J* = 12.1 Hz), 34.0, 26.03, 25.95, 24.4, 21.8, 14.2; **HRMS m/z (ESI):** calcd for $C_{15}H_{22}FNNaO_4S^+$ $[M+Na]^+$: 354.1146, found 354.1149.

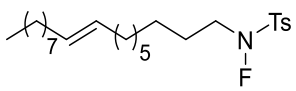
(*S*)-*N*-(3,7-Dimethyloct-6-en-1-yl)-*N*-fluoro-4-methylbenzenesulfonamide (21a)



21a

General procedure **B**, with 5.0 mmol scale, **21a** was prepared from commercially available primary amine to obtain a yellow oil (0.83 g, 51%) by flash chromatography on silica gel (40:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.83 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 5.06 (tt, *J* = 7.1, 1.3 Hz, 1H), 3.29 (t, *J* = 7.2 Hz, 1H), 3.19 (t, *J* = 7.2 Hz, 1H), 2.48 (s, 3H), 1.96 (tt, *J* = 14.6, 7.3 Hz, 2H), 1.78 – 1.71 (m, 1H), 1.68 – 1.65 (m, 3H), 1.58 (s, 3H), 1.51 (dd, *J* = 13.7, 7.3 Hz, 1H), 1.35 – 1.28 (m, 1H), 1.21 – 1.12 (m, 1H), 0.89 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 131.5, 129.92, 129.90, 128.9, 124.3, 51.8 (d, *J* = 13.1 Hz), 36.8, 33.0, 29.9, 25.7, 25.3, 21.8, 19.2, 17.6; **HRMS m/z (ESI):** calcd for $C_{17}H_{26}FNNaO_2S^+$ $[M+Na]^+$: 350.1560, found 350.1563.

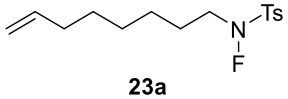
(*E*)-*N*-Fluoro-4-methyl-*N*-(octadec-9-en-1-yl)benzenesulfonamide (22a)



22a

General procedure **A**, with 5.0 mmol scale, **22a** was prepared from commercially available primary amine to obtain a colorless oil (1.12 g, 51%) by flash chromatography on silica gel (40:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 5.35 (ddd, J = 12.0, 5.7, 3.2 Hz, 2H), 3.24 (t, *J* = 7.0 Hz, 1H), 3.13 (t, *J* = 7.0 Hz, 1H), 2.48 (s, 3H), 2.00 (d, *J* = 6.2 Hz, 2H), 1.69 (p, *J* = 7.2 Hz, 2H), 1.44 – 1.16 (m, 24H), 0.87 (t, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.1, 129.9, 129.89, 129.87, 129.7, 128.7, 53.7 (d, *J* = 13.1 Hz), 32.6, 32.5, 31.9, 29.71, 29.65, 29.5, 29.28, 29.27, 29.10, 29.05, 27.2, 27.1, 26.5, 26.2, 22.7, 14.1; **HRMS m/z (ESI):** calcd for $C_{25}H_{42}FNNaO_2S^+$ $[M+Na]^+$: 462.2812, found 462.2815.

***N*-Fluoro-4-methyl-*N*-(oct-7-en-1-yl)benzenesulfonamide (23a)**

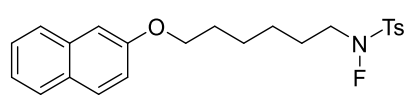


23a

General procedure **B**, with 5.0 mmol scale, **23a** was prepared from commercially available primary amine to obtain a

yellow oil (0.81 g, 54%) by flash chromatography on silica gel (40:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 5.78 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 4.97 (dq, *J* = 17.2, 1.6 Hz, 1H), 4.92 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 1H), 3.23 (t, *J* = 7.0 Hz, 1H), 3.13 (t, *J* = 7.0 Hz, 1H), 2.47 (s, 3H), 2.02 (q, J = 6.9 Hz, 2H), 1.73 – 1.65 (m, 2H), 1.42 – 1.29 (m, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.2, 138.8, 129.9, 128.6, 114.3, 53.7 (d, *J* = 12.1 Hz), 33.5, 28.5, 28.5, 26.3, 26.1, 21.7; **HRMS m/z (ESI):** calcd for $C_{15}H_{22}FNNaO_2S^+$ $[M+Na]^+$: 322.1247, found 322.1251.

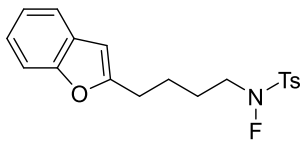
_N_-Fluoro-4-methyl-_N_-(6-(naphthalen-2-yloxy)hexyl)benzenesulfonamide (24a)



24a

General procedure **A**, with 5.0 mmol scale, **24a** was prepared from commercially available primary amine to obtain a yellow solid (0.89 g, 43%) by flash chromatography on silica gel (40:1–10:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.78 – 7.70 (m, 3H), 7.42 (dd, *J* = 17.8, 8.1 Hz, 3H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.16 – 7.10 (m, 2H), 4.06 (t, *J* = 6.4 Hz, 2H), 3.28 (t, *J* = 6.9 Hz, 1H), 3.18 (t, *J* = 6.9 Hz, 1H), 2.48 (s, 3H), 1.91 – 1.81 (m, 2H), 1.80 – 1.73 (m, 2H), 1.57 – 1.48 (m, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 156.9, 146.2, 134.5, 129.9, 129.9, 129.3, 128.84, 128.79, 127.6, 126.7, 126.3, 123.5, 118.9, 106.5, 67.6, 53.6 (d, *J* = 12.1 Hz), 29.0, 26.3, 26.2, 25.7, 21.7; **HRMS m/z (ESI):** calcd for $C_{23}H_{26}FNNaO_3S^+$ $[M+Na]^+$: 438.1510, found 438.1514.

_N_-(4-(Benzofuran-2-yl)butyl)-_N_-fluoro-4-methylbenzenesulfonamide (25a)

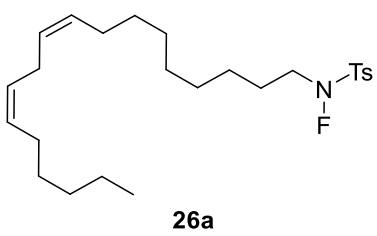


25a

General procedure **C**, with 5.0 mmol scale, **25a** was prepared from commercially available primary amine to obtain a yellow oil (0.72 g, 40%) by flash chromatography on silica gel (30:1–8:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.53 – 7.46 (m, 1H), 7.40 (t, *J* = 8.6 Hz, 3H), 7.25 – 7.17 (m,

2H), 6.40 (s, 1H), 3.30 (t, J = 6.5 Hz, 1H), 3.20 (t, J = 6.5 Hz, 1H), 2.81 (t, J = 7.1 Hz, 2H), 2.48 (s, 3H), 1.94 – 1.79 (m, 4H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 158.4, 154.5, 146.3, 129.9, 129.8, 128.7, 128.5, 123.2, 122.4, 120.2, 110.6, 102.2, 53.4, 53.3, 27.8, 25.6, 24.6, 21.7; **HRMS m/z (ESI):** calcd for $C_{19}H_{20}FNNaO_3S^+$ $[M+Na]^+$: 384.1040, found 384.1042.

_N_-Fluoro-4-methyl-_N_-((9_Z_,12_Z_)-octadeca-9,12-dien-1-yl)benzenesulfonamide (26a)



26a

General procedure **B**, with 5.0 mmol scale, **26a** was prepared from commercially available primary amine to obtain a yellow oil (0.90 g, 41%) by flash chromatography on silica gel (40:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.81 (d, J = 8.1 Hz, 2H), 7.40 (d, J = 8.1 Hz, 2H), 5.35 (tt, J = 11.0, 4.5 Hz, 4H), 3.23 (t, J = 7.0 Hz, 1H), 3.13 (t, J = 7.0 Hz, 1H), 2.76 (t, J = 6.3 Hz, 2H), 2.47 (s, 3H), 2.03 (t, J = 6.8 Hz, 4H), 1.69 (p, J = 7.1 Hz, 2H), 1.37 – 1.25 (m, 16H), 0.88 (t, J = 6.6 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 146.1, 130.1, 130.0, 129.86, 129.85, 128.8, 127.9, 127.8, 53.7 (d, J = 12.1 Hz), 31.4, 29.5, 29.3, 29.2, 29.1, 29.0, 27.12, 27.11, 26.5, 26.2, 25.6, 22.5, 21.7, 14.0; **HRMS m/z (ESI)**: calcd for $C_{25}H_{41}FNO_2S^+$ $[M+H]^+$: 438.2837, found 438.2841.

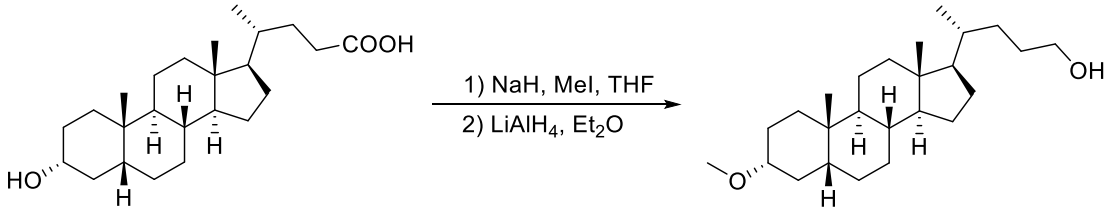


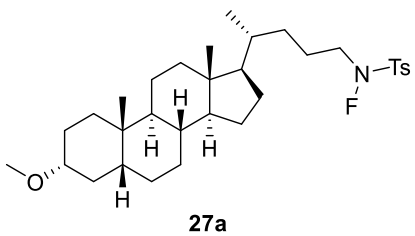
Fig. S5

To a solution of hyodeoxycholic acid (10 mmol, 1.0 equiv) in THF (100 mL, 0.1 M) at 0 °C was added NaH (60 mmol, 6.0 equiv, 60 % dispersion in mineral oil). The reaction mixture to stir for 1 h at room temperature, it was cooled to 0 °C. MeI (100 mmol, 10 equiv) was slowly added to the mixture and it was allowed to stir at 40 °C for

24 hours by TLC monitor. A second portion of NaH (60 mmol, 6.0 equiv, 60 % dispersion in mineral oil) and MeI (47 mmol, 4.7 equiv) were added to the reaction mixture, and the reaction was allowed to stir at 40 °C for by TLC monitor. A third portion of NaH (60 mmol, 6.0 equiv, 60 % dispersion in mineral oil) and MeI (47 mmol, 4.7 equiv) were added to the reaction mixture and the reaction was allowed to stir at 40 °C for another 24 h. The reaction mixture was quenched with sat. aq. NH_4Cl at 0 °C. the aqueous layer was extracted three times with EtOAc and separated organic layer was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (PE:EtOAc = 10:1).

To a solution of acid (7.0 mmol, 1.0 equiv) in Et_2O (30 mL) at 0 °C was added $LiAlH_4$ (9.1 mmol, 1.3 equiv) slowly and the mixture was allowed to warm to room temperature and stirred for 4.0 h. The reaction mixture was quenched with aq. 1 M NaOH and was filtered through Celite. The aqueous layer was extracted three times with EtOAc and separated organic layer was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The corresponding alcohol was purified by flash column chromatography (PE:EtOAc = 3:1).

_N_-Fluoro-_N_-((_R_)-4-((3_R_,5_R_,8_R_,9_S_,10_S_,13_R_,14_S_,17_R_)-3-methoxy-10,13-dimethylhexadecahydro-1_H_-cyclopenta[a]phenanthren-17-yl)pentyl)-4-methylbenzenesulfonamide (27a)



27a

General procedure **B**, with 3.0 mmol scale, **27a** was prepared from the corresponding alcohol to obtain a colorless oil (0.64 g, 39%) by flash chromatography on silica gel (20:1–8:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 3.33 (s, 3H), 3.23 – 3.06 (m, 3H), 2.47 (s, 3H), 1.96 – 1.88 (m, 1H), 1.86 – 1.71 (m, 5H), 1.70 – 1.61 (m, 1H), 1.57 – 1.50 (m, 2H), 1.48 – 1.25 (m, 8H), 1.27 –

1.17 (m, 4H), 1.14 – 0.91 (m, 7H), 0.90 – 0.87 (m, 6H), 0.61 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.1, 129.94, 129.89, 128.9, 80.4, 56.4, 55.9, 55.5, 54.2 (d, *J* = 13.1 Hz), 42.7, 41.99, 40.3, 40.1, 35.8, 35.4, 35.3, 34.9, 32.7, 28.2, 27.3, 26.7, 26.4, 24.2, 23.4, 23.0, 21.79, 20.75, 18.5, 12.0; **HRMS m/z (ESI)**: calcd for $C_{32}H_{51}FNO_3S^+$ $[M+H]^+$: 548.3568, found 548.3570.

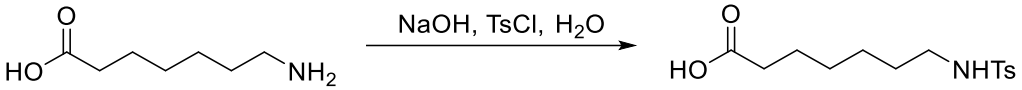


Fig. S6

To a solution of 7-aminoheptanoic acid (8.5 mmol, 1.0 equiv) in water (11 mL), was added 10 N NaOH (2 mL) followed by tosyl chloride (8.5 mmol, 1.0 equiv) into 3 portions over 15 min. The reaction mixture was then heated at reflux temperature for 3 h. After cooling to rt, the reaction mixture was extracted with Et_2O (2 × 15 mL) and acidified to pH = 1 with 4 N HCl. The acidic phase was extracted with DCM (3 × 15 mL), dried and concentrated in vacuo. The product was purified by flash column chromatography (5:1–2:1, PE/EtOAc).

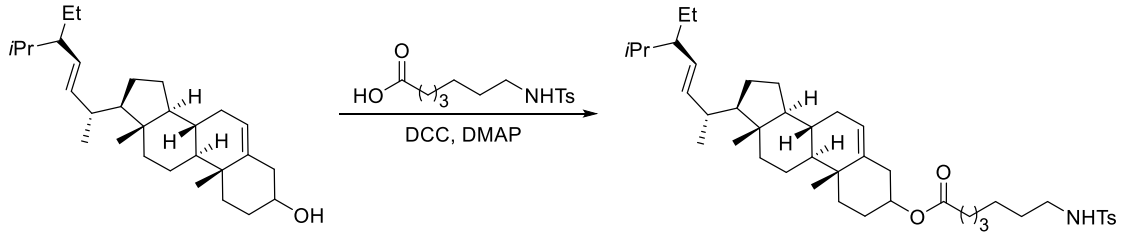
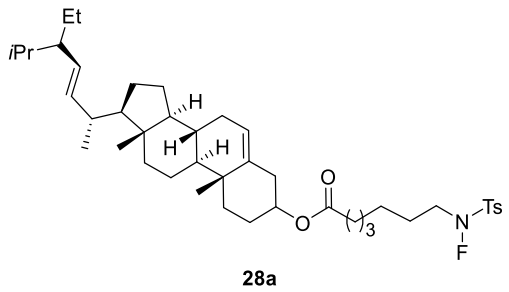


Fig. S7

To a solution of acid (5.00 mmol, 1.0 equiv) in DCM (25 mL) at 23 °C was added the desired alcohol (5.50 mmol, 1.1 equiv), followed by 4-DMAP (0.050 mmol, 0.1 equiv) and DCC (5.50 mmol, 1.1 equiv). The reaction mixture was stirred at 23 °C overnight. Upon completion, the reaction mixture was filtered through Celite and the filter cake was washed with DCM (3 × 5 mL). The resultant filtrate was concentrated and purified by flash column chromatography (8:1–3:1, PE/EtOAc) to afford the corresponding esters.

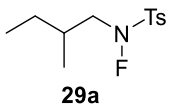
(8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((2*R*,5*S*,*E*)-5-Ethyl-6-methylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-yl 7-((*N*-fluoro-4-methylphenyl)sulfonamido)heptanoate (28a)



28a

General procedure **A**, with 3.0 mmol scale, **28a** was prepared from the corresponding amide to obtain a colorless oil (0.75 g, 35%) by flash chromatography on silica gel (20:1–5:1, PE/EtOAc).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.39 (m, 2H), 5.37 (d, *J* = 4.5 Hz, 1H), 5.15 (dd, *J* = 15.1, 8.6 Hz, 1H), 5.01 (dd, *J* = 15.1, 8.6 Hz, 1H), 4.71 – 4.53 (m, 1H), 3.24 (t, *J* = 6.9 Hz, 1H), 3.14 (t, *J* = 6.9 Hz, 1H), 2.48 (s, 3H), 2.28 (dd, *J* = 10.9, 7.9 Hz, 4H), 2.06 – 1.94 (m, 3H), 1.88 – 1.81 (m, 2H), 1.74 – 1.67 (m, 3H), 1.54 (ddd, *J* = 16.0, 12.5, 6.9 Hz, 8H), 1.45 – 1.40 (m, 4H), 1.36 – 1.31 (m, 2H), 1.28 – 1.21 (m, 2H), 1.19 – 1.10 (m, 4H), 1.02 (d, *J* = 3.5 Hz, 6H), 0.98 – 0.89 (m, 2H), 0.86 – 0.78 (m, 10H), 0.69 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.0, 146.2, 139.6, 138.3, 129.9, 129.2, 128.7, 122.6, 73.7, 56.7, 55.8, 53.6 (d, *J* = 13.1 Hz), 51.2, 50.0, 42.1, 40.5, 39.6, 38.1, 36.9, 36.5, 34.4, 31.8, 28.9, 28.5, 27.7, 26.2, 26.1, 25.4, 24.7, 24.3, 21.8, 21.2, 21.1, 21.0, 19.3, 18.9, 12.3, 12.0; **HRMS m/z (ESI)**: calcd for $C_{43}H_{67}FNO_4S^+$ $[M+H]^+$: 712.4769, found 712.4771.

***N*-Fluoro-4-methyl-*N*-(2-methylbutyl)benzenesulfonamide (29a)**

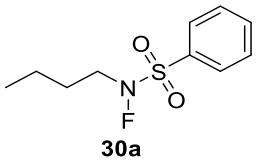


29a

General procedure **C**, with 5.0 mmol scale, **29a** was prepared from commercially available primary amine to obtain a yellow oil (0.87 g, 67%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 3.10 (td, *J* = 13.8, 6.8 Hz, 1H), 2.96 (td, *J* = 13.8, 6.8 Hz, 1H), 2.48 (s, 3H), 1.81 (dt, *J* = 13.1, 6.6 Hz, 1H), 1.49 (dq, *J* = 13.9, 7.1, 6.6 Hz, 1H), 1.22 (dt, *J* = 14.2, 7.3 Hz, 1H),

0.98 (d, J = 6.7 Hz, 3H), 0.88 (t, J = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.1, 129.90, 129.88, 128.9, 59.2 (d, J = 12.1 Hz), 32.3, 26.9, 21.8, 17.1, 10.9; **HRMS m/z (ESI):** calcd for $C_{12}H_{19}FNO_2S^+$ $[M+H]^+$: 246.0959, found 246.0961.

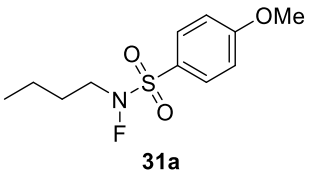
N-Butyl-N-fluorobenzenesulfonamide (30a)



30a

General procedure **A**, with 5.0 mmol scale, **30a** was prepared from commercially available primary amine to obtain a colorless oil (0.68 g, 59%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 (d, J = 8.0 Hz, 2H), 7.75 (t, J = 7.2 Hz, 1H), 7.62 (t, J = 7.7 Hz, 2H), 3.27 (t, J = 6.9 Hz, 1H), 3.17 (t, J = 6.9 Hz, 1H), 1.69 (p, J = 7.1 Hz, 2H), 1.43 (h, J = 7.4 Hz, 2H), 0.92 (t, J = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 134.9, 131.8, 129.8, 129.2, 53.4 (d, J = 13.1 Hz), 28.2, 19.7, 13.5; **HRMS m/z (ESI)**: calcd for $C_{10}H_{15}FNO_2S^+$ $[M+H]^+$: 232.0802, found 232.0803.

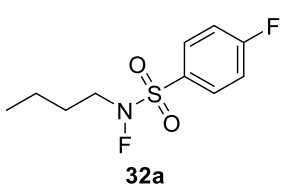
N-Butyl-N-fluoro-4-methoxybenzenesulfonamide (31a)



31a

General procedure **A**, with 5.0 mmol scale, **31a** was prepared from commercially available primary amine to obtain a colorless oil (0.80 g, 61%) by flash chromatography on silica gel (40:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.87 (d, J = 8.9 Hz, 2H), 7.06 (d, J = 8.9 Hz, 2H), 3.91 (s, 3H), 3.26 (t, J = 7.0 Hz, 1H), 3.15 (t, J = 7.0 Hz, 1H), 1.72 – 1.66 (m, 2H), 1.43 (q, J = 7.4 Hz, 2H), 0.92 (t, J = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.7, 132.2, 123.1, 114.5, 55.8, 53.4 (d, J = 12.1 Hz), 28.3, 19.8, 13.6; **HRMS m/z (ESI):** calcd for $C_{11}H_{17}FNO_3S^+$ $[M+H]^+$: 262.0908, found 262.0907.

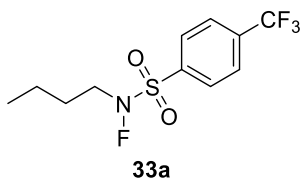
N-Butyl-N,4-difluorobenzenesulfonamide (32a)



32a

General procedure **A**, with 5.0 mmol scale, **32a** was prepared from commercially available primary amine to obtain a yellow oil (0.65 g, 52%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.97 (dd, *J* = 8.8, 5.0 Hz, 2H), 7.32 – 7.26 (m, 2H), 3.29 (t, *J* = 7.0 Hz, 1H), 3.19 (t, *J* = 7.0 Hz, 1H), 1.71 (q, *J* = 7.2 Hz, 2H), 1.44 (dt, *J* = 15.0, 7.4 Hz, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 166.5 (d, *J* = 259.6 Hz), 132.8 (d, *J* = 10.1 Hz), 128.0 (d, *J* = 3.0 Hz), 116.7 (d, *J* = 22.2 Hz), 53.20 (d, *J* = 12.1 Hz), 28.2, 19.7, 13.5; **HRMS m/z (ESI)**: calcd for $C_{10}H_{14}F_2NO_2S^+$ $[M+H]^+$: 250.0708, found 250.0712.

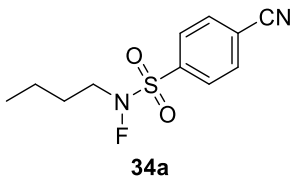
_N_-Butyl-_N_-fluoro-4-(trifluoromethyl)benzenesulfonamide (33a)



33a

General procedure **A**, with 5.0 mmol scale, **33a** was prepared from commercially available primary amine to obtain a yellow oil (0.84 g, 56%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.09 (d, *J* = 8.3 Hz, 2H), 7.89 (d, *J* = 8.3 Hz, 2H), 3.27 (dt, *J* = 40.4, 7.0 Hz, 2H), 1.75 – 1.67 (m, 2H), 1.48 – 1.40 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 136.4 (d, *J* = 33.3 Hz), 135.8, 130.5, 126.4 (d, *J* = 4.0 Hz), 122.9 (q, *J* = 279.8 Hz), 53.1 (d, *J* = 13.1 Hz), 28.1, 19.7, 13.5; **HRMS m/z (ESI):** calcd for $C_{11}H_{14}F_4NO_2S^+$ $[M+H]^+$: 300.0676, found 300.0675.

_N_-Butyl-4-cyano-_N_-fluorobenzenesulfonamide (34a)

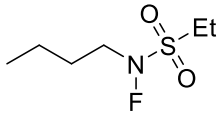


34a

General procedure **A**, with 5.0 mmol scale, **34a** was prepared from commercially available primary amine to obtain a yellow solid (0.76 g, 59%) by flash chromatography on silica gel (10:1–7:1, PE/EtOAc). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.07 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 2H), 3.28 (dt, *J* = 40.2, 7.0 Hz, 2H), 1.72 (q, *J* = 7.2 Hz, 2H), 1.42 (dt, *J* = 14.7, 7.4 Hz, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR**

(101 MHz, $CDCl_3$) δ 136.5, 132.9, 130.4, 118.5, 116.8, 53.0 (d, *J* = 12.1 Hz), 28.1, 19.7, 13.5; **HRMS m/z (ESI)**: calcd for $C_{11}H_{14}FN_2O_2S^+$ $[M+H]^+$: 257.0755, found 257.0753.

***N*-Butyl-*N*-fluoroethanesulfonamide (35a)**



35a

General procedure **A**, with 5.0 mmol scale, **35a** was prepared from commercially available primary amine to obtain a yellow oil (0.59 g, 65%) by flash chromatography on silica gel (50:1–20:1, PE/EtOAc). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 3.52 (t, *J* = 7.1 Hz, 1H), 3.42 (t, *J* = 7.1 Hz, 1H), 3.32 (q, *J* = 7.5 Hz, 2H), 1.76 (p, *J* = 7.2 Hz, 2H), 1.46 (q, *J* = 7.8 Hz, 5H), 0.96 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 49.8, 49.6, 44.2, 28.0, 19.8, 13.6, 7.3; **HRMS m/z (ESI):** calcd for $C_6H_{15}FNO_2S^+$ $[M+H]^+$: 184.0802, found 184.0798.

3. Experimental Procedures and Characterization of Products

General Procedure D:

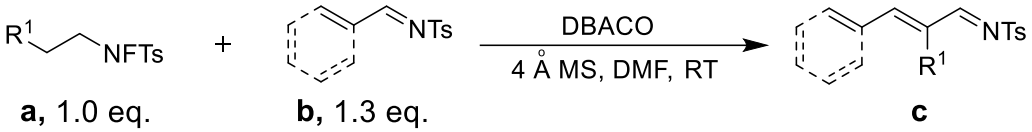
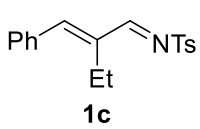


Fig. S8

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-fluorosulfonamides (0.2 mmol, 1.0 equiv), imines (**1b**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. After the reaction, DCM (15 mL) was added into reaction mixture, and then washed by 20 mL water. The organic part was concentrated in vacuo. The residue was purified by flash column chromatography using petroleum ether/ethyl acetate mixture as eluent to afford the corresponding products.

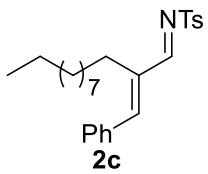
***N*-((*Z*)-2-((*E*)-Benzylidene)butylidene)-4-methylbenzenesulfonamide (1c)**



1c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 50.7 mg (81%) of **1c** as a yellow oil: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.65 (s, 1H), 7.86 (*d*, *J* = 8.2 Hz, 2H), 7.49 – 7.38 (m, 5H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.23 (s, 1H), 2.65 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.2, 150.9, 144.2, 140.8, 135.7, 134.8, 129.88, 129.87, 129.7, 128.8, 127.8, 21.6, 19.5, 12.8; **IR (film)**: 3054, 2987, 2305, 2254, 1422, 1265, 1090, 910, 741, 706, 651, 538 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{18}H_{20}NO_2S^+$ $[M+H]^+$: 314.1209, found 314.1213.

***N*-((*E*)-2-((*E*)-Benzylidene)dodecylidene)-4-methylbenzenesulfonamide (2c)**

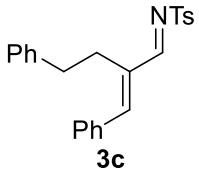


2c

General procedure **D**, with 0.2 mmol scale, the *N*-dodecyl-*N*-fluoro-4-methylbenzenesulfonamide (**2a**, 71.4 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 68.9 mg (81%) of **2c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.65 (s, 1H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.47 – 7.39 (m, 5H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.23 (s, 1H), 2.66 – 2.51 (m, 2H), 2.44 (s, 3H), 1.48 (p, *J* = 7.5 Hz, 2H), 1.35 – 1.15 (m, 14H), 0.89 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.5, 151.0, 144.1, 139.8, 135.8, 134.9, 129.9, 129.8, 129.6, 128.79, 127.8, 31.9, 29.7, 29.6, 29.4, 29.3, 29.2, 28.0, 26.0, 22.7, 21.6, 14.1; **IR (film)**: 3054, 2928, 2855,

1567, 1422, 1319, 1265, 1158, 1090, 896, 740, 705, 587, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{26}H_{36}NO_2S^+$ $[M+H]^+$: 426.2461, found 426.2463.

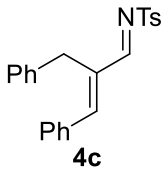
***N*-((*E*)-2-((*E*)-Benzylidene)-4-phenylbutylidene)-4-methylbenzenesulfonamide (3c)**



3c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(4-phenylbutyl)benzenesulfonamide (**3a**, 64.2 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 58.4 mg (75%) of **3c** as a colorless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.39 – 7.35 (m, 5H), 7.32 – 7.29 (m, 2H), 7.23 – 7.12 (m, 3H), 7.13 – 7.03 (m, 3H), 2.90 (dd, *J* = 10.0, 6.2 Hz, 2H), 2.75 (dd, *J* = 10.0, 6.2 Hz, 2H), 2.40 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.0, 151.8, 144.3, 141.0, 138.4, 135.6, 134.7, 129.9, 129.72, 129.67, 128.8, 128.34, 128.27, 127.8, 126.1, 33.8, 28.0, 21.6; **IR (film)**: 3055, 2987, 2305, 1681, 1598, 1568, 1496, 1454, 1422, 1320, 1305, 1266, 1210, 1184, 1158, 1090, 1002, 896, 856, 812, 746, 705, 587, 556 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{24}H_{24}NO_2S^+$ $[M+H]^+$: 390.1522, found 390.1520.

***N*-((1*E*,2*E*)-2-Benzyl-3-phenylallylidene)-4-methylbenzenesulfonamide (4c)**

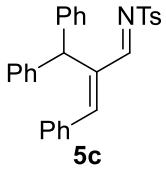


4c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(4-phenylbutyl)benzenesulfonamide (**4a**, 61.4 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column

chromatography (PE:EA = 10:1) to afford 51.8 mg (69%) of **4c** as a colorless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.79 (s, 1H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.52 (s, 1H), 7.46 – 7.42 (m, 2H), 7.39 – 7.35 (m, 3H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.12 (m, 3H), 7.05 (dd, *J* = 7.8, 1.7 Hz, 2H), 4.04 (s, 2H), 2.40 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.3, 152.6, 144.0, 138.1, 136.9, 135.7, 134.5, 130.2, 130.0, 129.5, 128.84, 128.4, 128.0, 127.5, 126.1, 31.9, 21.6; **IR (film)**: 3750, 3649, 3055, 1716, 1567, 1319, 1265, 1158, 1090, 849, 789, 739, 704, 588, 558, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{23}H_{22}NO_2S^+$ $[M+H]^+$: 376.1366, found 376.1369.

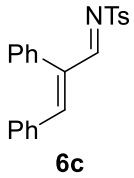
***N*-((1*E*,2*E*)-2-Benzhydryl-3-phenylallylidene)-4-methylbenzenesulfonamide (5c)**



5c

General procedure **D**, with 0.2 mmol scale, the *N*-(3,3-diphenylpropyl)-*N*-fluoro-4-methylbenzenesulfonamide (**5a**, 76.6 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 59.6 mg (66%) of **5c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.07 – 8.86 (m, 1H), 7.42 – 7.38 (m, 5H), 7.25 – 7.19 (m, 6H), 7.18 (t, *J* = 1.6 Hz, 1H), 7.16 (d, *J* = 1.6 Hz, 2H), 7.13 – 7.09 (m, 6H), 5.77 (s, 1H), 2.39 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.1, 150.2, 143.7, 141.3, 140.4, 135.3, 134.3, 129.8, 129.6, 129.4, 129.2, 128.7, 128.4, 127.2, 126.5, 52.0, 21.6; **IR (film)**: 3735, 3401, 3054, 1598, 1421, 1318, 1265, 1158, 1089, 896, 831, 764, 749, 704, 584, 419, 405 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{29}H_{26}NO_2S^+$ $[M+H]^+$: 452.1679, found 452.1681.

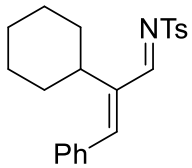
***N*-((1*E*,2*E*)-2,3-Diphenylallylidene)-4-methylbenzenesulfonamide (6c)**



6c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-phenethylbenzenesulfonamide (**6a**, 58.6 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 44.8 mg (62%) of **6c** as a white solid: **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.89 (s, 1H), 7.82 – 7.74 (m, 2H), 7.44 (s, 1H), 7.39 – 7.34 (m, 3H), 7.32 – 7.26 (m, 3H), 7.22 – 7.13 (m, 4H), 7.12 – 7.07 (m, 2H), 2.42 (s, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 173.5, 151.0, 144.2, 138.2, 135.5, 134.2, 133.9, 131.1, 130.5, 129.6, 129.5, 128.8, 128.4, 127.9, 126.5, 21.6; **IR (film)**: 3054, 2987, 2306, 1563, 1422, 1265, 1158, 1090, 896, 746, 705, 567 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{20}NO_2S^+$ $[M+H]^+$: 362.1209, found 362.1212.

***N*-((1*E*,2*E*)-2-Cyclohexyl-3-phenylallylidene)-4-methylbenzenesulfonamide (7c)**

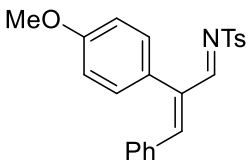


7c

General procedure **D**, with 0.2 mmol scale, the *N*-(2-cyclohexylethyl)-*N*-fluoro-4-methylbenzenesulfonamide (**7a**, 59.8 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 43.3 mg (59%) of **7c** as a colorless oil: **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.79 (s, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.44 (s, 1H), 7.39 – 7.35 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.14 (dd, *J* = 6.3, 2.7 Hz, 2H), 2.84 – 2.73 (m, 1H), 2.43 (s, 3H), 1.86 – 1.68 (m, 5H), 1.40 – 1.30 (m, 2H), 1.28 – 1.16 (m, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 169.3, 146.0, 144.3, 143.1, 135.1, 134.8, 129.8, 129.7, 129.1, 128.6, 128.0, 38.5, 32.6, 26.59, 26.2, 21.6; **IR (film)**: 3649, 2926, 2852, 1670, 1597, 1564, 1494, 1447, 1319, 1305, 1224, 1183, 1158, 1089, 1019,

929, 876, 826, 812, 778, 748, 701, 679, 661, 594, 560, 539, 524, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{26}NO_2S^+$ $[M+H]^+$: 368.1679, found 368.1680.

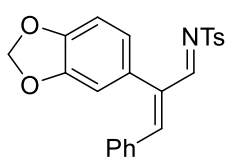
***N*-((1*E*,2*E*)-2-(4-Methoxyphenyl)-3-phenylallylidene)-4-methylbenzenesulfonamide (8c)**



8c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-*N*-(4-methoxyphenethyl)-4-methylbenzenesulfonamide (**8a**, 64.6 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 50.1 mg (64%) of **8c** as a colorless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.87 (s, 1H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.39 (s, 1H), 7.33 – 7.26 (m, 3H), 7.21 (t, *J* = 7.5 Hz, 2H), 7.14 (d, *J* = 7.4 Hz, 2H), 7.11 – 7.03 (m, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 3.83 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.8, 159.6, 150.9, 144.2, 137.8, 135.5, 134.4, 131.0, 130.8, 130.3, 129.6, 128.5, 127.9, 125.8, 114.2, 55.2, 21.6; **IR (film)**: 3400, 3054, 2986, 1567, 1514, 1421, 1320, 1265, 1158, 1089, 1032, 896, 809, 739, 705, 595, 563 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{23}H_{22}NO_3S^+$ $[M+H]^+$: 392.1315, found 392.1320.

***N*-((1*E*,2*E*)-2-(Benzo[d][1,3]dioxol-5-yl)-3-phenylallylidene)-4-methylbenzenesulfonamide (9c)**

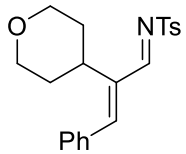


9c

General procedure **D**, with 0.2 mmol scale, the *N*-(2-(Denzo[*d*][1,3]dioxol-5-yl)ethyl)-*N*-fluoro-4-methylbenzenesulfonamide (**9a**, 67.4 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into

a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 48.6 mg (60%) of **9c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.85 (s, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.39 (s, 1H), 7.30 (t, *J* = 7.5 Hz, 3H), 7.23 (d, *J* = 7.1 Hz, 2H), 7.17 (d, *J* = 7.3 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, 1H), 6.62 (d, *J* = 7.3 Hz, 2H), 5.99 (s, 2H), 2.43 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.6, 151.2, 148.0, 147.7, 144.2, 137.7, 135.5, 134.1, 131.1, 130.5, 129.7, 128.5, 127.9, 123.1, 109.9, 108.9, 101.2, 21.6; **IR (film)**: 2254, 1791, 1569, 1506, 1386, 1265, 1241, 1157, 1090, 910, 804, 734, 651, 547 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{23}H_{20}NO_4S^+$ $[M+H]^+$: 406.1108, found 406.1109.

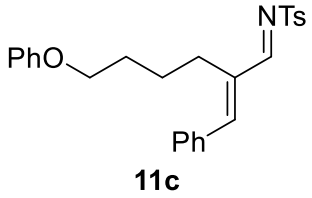
4-Methyl-*N*-((1*E*,2*E*)-3-phenyl-2-(tetrahydro-2*H*-pyran-4-yl)allylidene)benzenesulfonamide (10c)



10c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(2-(tetrahydro-2*H*-pyran-4-yl)ethyl)benzenesulfonamide (**10a**, 60.2 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 39.1 mg (53%) of **10c** as a colorless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.82 (s, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.47 (s, 1H), 7.42 – 7.38 (m, 3H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.19 – 7.13 (m, 2H), 4.01 (d, *J* = 11.3 Hz, 2H), 3.50 (t, *J* = 11.5 Hz, 2H), 3.08 – 3.03 (m, 1H), 2.44 (s, 3H), 1.76 – 1.63 (m, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.8, 146.5, 144.5, 141.0, 134.8, 134.4, 129.84, 129.80, 129.4, 128.7, 128.0, 68.1, 35.9, 32.1, 21.7; **IR (film)**:3406, 1611, 1384, 1265, 1159, 744, 705, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{21}H_{24}NO_3S^+$ $[M+H]^+$: 370.1471, found 370.1474.

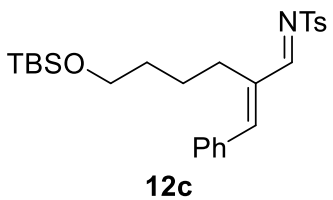
***N*-((*E*)-2-((*E*)-Benzylidene)-6-phenoxyhexylidene)-4-methylbenzenesulfonamide (11c)**



11c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(6-phenoxyhexyl)benzenesulfonamide (**11a**, 73.0 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 63.2 mg (73%) of **11c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.49 – 7.43 (m, 2H), 7.38 – 7.26 (m, 8H), 6.95 (d, *J* = 7.3 Hz, 1H), 6.85 (dd, *J* = 8.7, 1.0 Hz, 2H), 3.92 (t, *J* = 6.1 Hz, 2H), 2.76 – 2.66 (m, 2H), 2.43 (s, 3H), 1.81 (q, *J* = 6.3 Hz, 2H), 1.74 – 1.66 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 158.9, 151.5, 144.3, 139.2, 135.6, 134.8, 130.0, 129.9, 129.7, 129.4, 128.9, 127.8, 120.6, 114.4, 66.8, 29.0, 25.6, 24.4, 21.6; **IR (film)**: 3944, 3692, 3054, 2987, 2686, 2306, 1599, 1568, 1497, 1422, 1266, 1158, 1089, 896, 749, 706, 588, 558 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{26}H_{28}NO_3S^+$ $[M+H]^+$: 434.1784, found 434.1787.

***N*-((*E*)-2-((*E*)-Benzylidene)-6-((*tert*-butyldimethylsilyl)oxy)hexylidene)-4-methylbenzenesulfonamide (12c)**

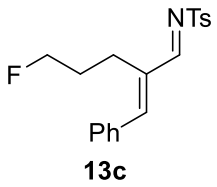


12c

General procedure **D**, with 0.2 mmol scale, the *N*-(6-((*tert*-butyldimethylsilyl)oxy)hexyl)-*N*-fluoro-4-methylbenzenesulfonamide (**12a**, 80.6 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 70.7 mg (75%) of **12c** as a colorless oil: **^{1}H**

NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.47 – 7.39 (m, 5H), 7.34 – 7.31 (m, 2H), 7.24 (s, 1H), 3.55 (t, *J* = 5.7 Hz, 2H), 2.63 (t, *J* = 7.4 Hz, 2H), 2.43 (s, 3H), 1.57 – 1.51 (m, 4H), 0.85 (s, 9H), 0.00 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 151.3, 144.1, 139.5, 135.7, 134.8, 129.9, 129.6, 128.8, 127.8, 62.6, 32.8, 25.9, 25.8, 24.4, 21.6, 18.2, -5.4; **IR (film)**: 3054, 2986, 2956, 2858, 2305, 2254, 1567, 1422, 1319, 1265, 1158, 1090, 910, 838, 742, 706, 651, 587, 557 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{26}H_{38}NO_3SSi^+$ $[M+H]^+$: 472.2336, found 472.2344.

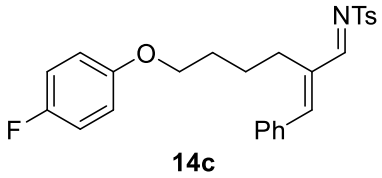
***N*-*((E)*-2-*((E)*-Benzylidene)-5-fluoropentylidene)-4-methylbenzenesulfonamide (13c)**



13c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-*N*-(5-fluoropentyl)-4-methylbenzenesulfonamide (**13a**, 55.4 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 49 mg (71%) of **13c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.50 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.47 – 7.41 (m, 3H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.30 (s, 1H), 4.51 (t, *J* = 5.7 Hz, 1H), 4.39 (t, *J* = 5.7 Hz, 1H), 2.83 – 2.74 (m, 2H), 2.44 (s, 3H), 1.98 – 1.87 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.2, 152.0, 144.4, 138.0, 135.4, 134.5, 130.2, 130.0, 129.7, 128.9, 127.8, 83.3 (d, *J* = 165.6 Hz), , 28.8 (d, *J* = 19.2 Hz), 22.2 (d, *J* = 4.0 Hz), 21.6; **IR (film)**: 2961, 2925, 1676, 1598, 1566, 1493, 1448, 1400, 1319, 1291, 1210, 1184, 1156, 1088, 1036, 1000, 927, 903, 841, 805, 755, 683, 604, 586, 557 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{21}FNO_2S^+$ $[M+H]^+$: 346.1272, found 346.1274.

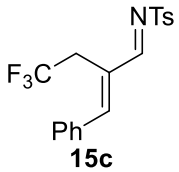
***N*-*((E)*-2-*((E)*-Benzylidene)-6-(4-fluorophenoxy)hexylidene)-4-methylbenzenesulfonamide (14c)**



14c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-*N*-(6-(4-fluorophenoxy)hexyl)-4-methylbenzenesulfonamide (**14a**, 76.6 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 71.3 mg (79%) of **14c** as a colorless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.37 (p, *J* = 2.9 Hz, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 2.3 Hz, 1H), 6.98 – 6.93 (m, 2H), 6.80 – 6.75 (m, 2H), 3.87 (t, *J* = 6.1 Hz, 2H), 2.76 – 2.64 (m, 2H), 2.43 (s, 3H), 1.79 (q, *J* = 6.2 Hz, 2H), 1.74 – 1.68 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.3, 157.1 (d, *J* = 239.4 Hz), 155.0, 151.5, 144.3, 139.1, 135.6, 134.7, 130.0, 129.9, 129.7, 128.9, 127.8, 115.7 (d, *J* = 23.2 Hz), 115.3 (d, *J* = 8.1 Hz), 67.58, 29.0, 25.5, 24.3, 21.6; **IR (film)**: 3055, 2927, 2871, 1598, 1563, 1505, 1472, 1398, 1318, 1305, 1291, 1266, 1248, 1208, 1184, 1155, 1089, 1064, 1030, 1019, 1000, 927, 828, 788, 754, 737, 683, 653, 586, 557, 514, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{26}H_{27}FNO_3S^+$ $[M+H]^+$: 452.1690, found 452.1692.

***N*-*((E)*-2-*((E)*-Benzylidene)-4,4,4-trifluorobutylidene)-4-methylbenzenesulfonamide (15c)**

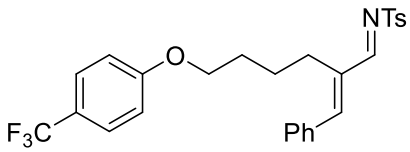


15c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(4,4,4-trifluorobutyl)benzenesulfonamide (**15a**, 59.8 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 52.1 mg (71%) of **15c** as a white solid: **^{1}H**

NMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.61 (s, 1H), 7.54 – 7.50 (m, 2H), 7.49 – 7.45 (m, 3H), 7.34 (d, *J* = 8.3 Hz, 2H), 3.57 (q, *J* = 10.1 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 172.8, 155.7, 144.5, 135.2, 133.5, 130.9, 129.7, 129.1, 127.8, 30.7 (q, *J* = 31.3 Hz), 21.7; **IR (film)**: 3389, 3057, 2927, 1572, 1495, 1322, 1266, 1252, 1215, 1185, 1159, 1141, 1088, 1030, 896, 854, 833, 790, 748, 697, 680, 591, 565, 420, 413 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{18}H_{17}F_3NO_2S^+$ $[M+H]^+$: 368.0927, found 368.0930.

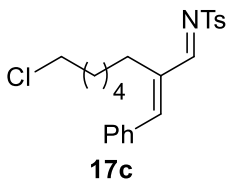
***N*-*((E)*-2-*((E)*-Benzylidene)-6-(4-(trifluoromethyl)phenoxy)hexylidene)-4-methylbenzenesulfonamide (16c)**



16c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(6-(4-(trifluoromethyl)phenoxy)hexyl)benzenesulfonamide (**16a**, 86.6 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamid e (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 76.2 mg (76%) of **16c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.54 – 7.51 (m, 2H), 7.48 – 7.43 (m, 2H), 7.40 – 7.36 (m, 3H), 7.33 – 7.27 (m, 3H), 6.89 (d, *J* = 8.3 Hz, 2H), 3.95 (t, *J* = 6.1 Hz, 2H), 2.76 – 2.66 (m, 2H), 2.42 (s, 3H), 1.82 (q, *J* = 6.4 Hz, 2H), 1.76 – 1.68 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.3, 161.4 (q, *J* = 2.0 Hz), 151.6, 144.3, 139.0, 135.5, 134.7, 130.0, 129.8, 129.7, 128.9, 127.8, 126.8 (q, *J* = 4.0 Hz), 122.6 (q, *J* = 32.3 Hz), 114.36, 67.3, 28.8, 25.5, 24.3, 21.6; **IR (film)**: 3054, 2986, 2305, 1615, 1566, 1519, 1422, 1328, 1265, 1209, 1158, 1113, 1089, 1069, 1010, 896, 839, 813, 745, 705, 638, 587, 558, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{27}H_{27}F_3NO_3S^+$ $[M+H]^+$: 502.1658, found 502.1661.

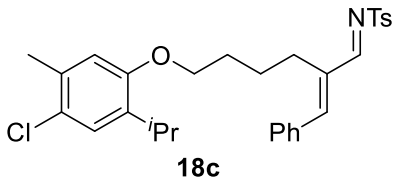
***N*-((*E*)-2-((*E*)-Benzylidene)-8-chlorooctylidene)-4-methylbenzenesulfonamide (17c)**



17c

General procedure **D**, with 0.2 mmol scale, the *N*-(8-chlorooctyl)-*N*-fluoro-4-methylbenzenesulfonamide (**17a**, 67.0 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamid e (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 64.5 mg (80%) of **17c** as a colorless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.43 (m, 4H), 7.42 – 7.38 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.23 (s, 1H), 3.45 (t, *J* = 6.7 Hz, 2H), 2.68 – 2.55 (m, 2H), 2.43 (s, 3H), 1.66 (p, *J* = 6.7 Hz, 2H), 1.54 – 1.44 (m, 2H), 1.39 – 1.27 (m, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 151.2, 144.3, 139.5, 135.6, 134.8, 129.9, 129.9, 129.7, 128.9, 127.8, 45.0, 32.3, 28.8, 27.8, 26.4, 25.8, 21.6; **IR (film)**: 3393, 3054, 2987, 2306, 1567, 1422, 1266, 1158, 1090, 896, 749, 706, 587 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{27}ClNO_2S^+$ $[M+H]^+$: 404.1446, found 404.1449.

***N*-((*E*)-2-((*E*)-Benzylidene)-6-(4-chloro-2-isopropyl-5-methylphenoxy)hexylidene)-4-methylbenzenesulfonamide (18c)**

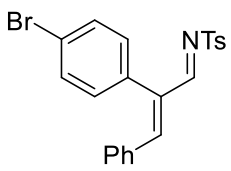


18c

General procedure **D**, with 0.2 mmol scale, the *N*-(6-(4-chloro-2-isopropyl-5-methylphenoxy)hexyl)-*N*-fluoro-4-methylbenzenesulfonamide (**18a**, 91.0 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamid e (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 76.4 mg (73%) of **18c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.84 (d, *J* = 8.2 Hz,

2H), 7.50 – 7.43 (m, 2H), 7.40 – 7.34 (m, 3H), 7.33 – 7.27 (m, 3H), 7.11 (s, 1H), 6.63 (s, 1H), 3.88 (t, *J* = 5.9 Hz, 2H), 3.16 (p, *J* = 6.9 Hz, 1H), 2.78 – 2.62 (m, 2H), 2.43 (s, 3H), 2.32 (s, 3H), 1.88 – 1.79 (m, 2H), 1.78 – 1.70 (m, 2H), 1.11 (d, *J* = 6.9 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 154.6, 151.5, 144.3, 139.2, 136.2, 135.6, 134.8, 133.5, 130.0, 129.9, 129.7, 128.9, 127.8, 126.5, 125.3, 113.6, 67.3, 29.3, 26.6, 25.6, 24.6, 22.5, 21.6, 20.0; **IR (film)**: 3054, 2987, 2306, 1567, 1496, 1422, 1319, 1265, 1158, 1090, 896, 748, 705, 587, 558, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{30}H_{35}ClNO_3S^+$ $[M+H]^+$: 524.2021, found 524.2026.

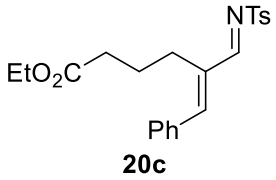
***N*-((1*E*,2*E*)-2-(4-Bromophenyl)-3-phenylallylidene)-4-methylbenzenesulfonamide (19c)**



19c

General procedure **D**, with 0.2 mmol scale, the *N*-(4-bromophenethyl)-*N*-fluoro-4-methylbenzenesulfonamide (**19a**, 74.2 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 49.2 mg (56%) of **19c** as a yellow solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.87 (s, 1H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.44 (s, 1H), 7.31 (d, *J* = 8.2 Hz, 3H), 7.23 (d, *J* = 7.2 Hz, 2H), 7.12 (d, *J* = 7.4 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 2.43 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 172.9, 151.5, 144.3, 137.0, 135.3, 133.8, 132.6, 132.0, 131.3, 131.0, 130.7, 129.7, 128.7, 127.9, 122.7, 21.6; **IR (film)**: 3420, 3054, 2987, 2306, 1568, 1422, 1265, 1159, 1090, 896, 804, 741, 705, 548, 425, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{19}BrNO_2S^+$ $[M+H]^+$: 440.0314, found 440.0312.

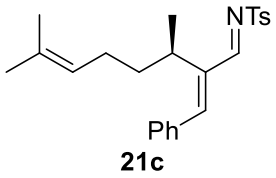
Ethyl (*E*)-6-phenyl-5-((E)-(tosylimino)methyl)hex-5-enoate (20c)



20c

General procedure **D**, with 0.2 mmol scale, the *ethyl* 6-((*N*-fluoro-4-methylphenyl)sulfonamido)hexanoate (**20a**, 66.2 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 61.5 mg (77%) of **20c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.65 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.51 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.28 (s, 1H), 4.12 – 4.06 (m, 2H), 2.72 – 2.63 (m, 2H), 2.44 (s, 3H), 2.33 (t, *J* = 7.1 Hz, 2H), 1.87 – 1.79 (m, 2H), 1.22 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.3, 173.1, 151.9, 144.3, 138.4, 135.5, 134.6, 130.1, 130.0, 129.7, 128.9, 127.8, 60.3, 34.0, 25.5, 23.1, 21.6, 14.2; **IR (film)**: 3839, 3735, 3649, 3420, 3055, 2985, 2306, 1731, 1567, 1456, 1376, 1319, 1266, 1185, 1158, 1090, 1029, 896, 813, 745, 704, 588, 558, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{26}NO_4S^+$ $[M+H]^+$: 400.1577, found 400.1580.

_N_-((_R_,_E_)-2-((_E_)-Benzylidene)-3,7-dimethyloct-6-en-1-ylidene)-4-methylbenzenesulfonamide (21c)

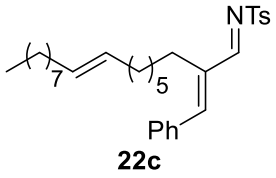


21c

General procedure **D**, with 0.2 mmol scale, the *(S)*-*N*-(3,7-dimethyloct-6-en-1-yl)-*N*-fluoro-4-methylbenzenesulfonamide (**21a**, 65.4 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 43.5 mg (55%) of **21c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.86 (s, 1H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.45 (s, 1H), 7.41 – 7.37 (m, 3H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.19 – 7.14 (m, 2H), 5.00 (t, *J* = 7.0 Hz, 1H), 3.01 (q, *J* = 6.9 Hz, 1H), 2.43 (s,

3H), 1.90 (p, *J* = 7.1 Hz, 2H), 1.62 (s, 3H), 1.59 (s, 1H), 1.49 (s, 3H), 1.48 – 1.38 (m, 1H), 1.14 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.3, 146.4, 144.3, 142.8, 135.3, 134.7, 131.6, 129.8, 129.7, 129.2, 128.6, 127.9, 124.1, 36.2, 33.9, 25.9, 25.6, 21.6, 20.1, 17.6; **IR (film)**: 3421, 1650, 1385, 1266, 1158, 1044, 764, 749, 419, 406 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{24}H_{30}NO_2S^+$ $[M+H]^+$: 396.1992, found 396.1991.

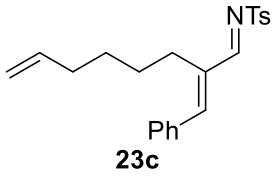
***N*-((1*E*,8*E*)-2-((*E*)-Benzylidene)heptadec-8-en-1-ylidene)-4-methylbenzenesulfonamide (22c)**



22c

General procedure **D**, with 0.2 mmol scale, the (*E*)-*N*-fluoro-4-methyl-*N*-(octadec-9-en-1-yl)benzenesulfonamide (**22a**, 87.9 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 81.3 mg (78%) of **22c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.65 (s, 1H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.48 – 7.39 (m, 5H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.23 (s, 1H), 5.43 – 5.26 (m, 2H), 2.67 – 2.57 (m, 2H), 2.44 (s, 3H), 1.99 (dd, *J* = 12.1, 6.0 Hz, 3H), 1.56 – 1.45 (m, 2H), 1.37 – 1.19 (m, 19H), 0.87 (t, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.5, 151.0, 144.1, 139.8, 135.8, 134.9, 130.0, 129.9, 129.8, 129.6, 128.8, 127.8, 31.9, 29.7, 29.54, 29.53, 29.48, 29.29, 29.27, 28.8, 28.0, 27.2, 27.1, 26.0, 22.6, 21.6, 14.1; **IR (film)**: 2925, 2854, 1598, 1567, 1495, 1463, 1402, 1321, 1305, 1291, 1265, 1209, 1184, 1158, 1090, 1019, 1000, 969, 926, 846, 812, 787, 739, 684, 587, 557, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{32}H_{46}NO_2S^+$ $[M+H]^+$: 508.3244, found 508.3249.

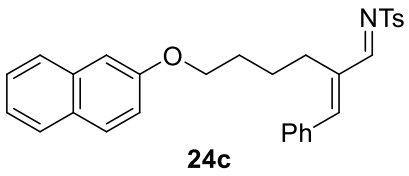
***N*-((*E*)-2-((*E*)-Benzylidene)oct-7-en-1-ylidene)-4-methylbenzenesulfonamide (23c)**



23c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(oct-7-en-1-yl)benzenesulfonamide (**23a**, 59.8 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 46.3 mg (63%) of **23c** as a yellow oil: **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.65 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.48 – 7.38 (m, 5H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.24 (s, 1H), 5.72 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.00 – 4.84 (m, 2H), 2.67 – 2.58 (m, 2H), 2.44 (s, 3H), 2.01 (q, *J* = 6.9 Hz, 2H), 1.57 – 1.47 (m, 2H), 1.41 (p, *J* = 8.2, 7.6 Hz, 2H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 174.4, 151.1, 144.2, 139.6, 138.5, 135.7, 134.8, 129.9, 129.6, 128.8, 127.8, 114.4, 33.2, 28.8, 27.4, 25.9, 21.6; **IR (film)**: 3054, 2986, 2929, 2305, 1598, 1567, 1422, 1319, 1305, 1265, 1209, 1158, 1090, 896, 847, 806, 742, 705, 587, 558 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{26}NO_2S^+$ $[M+H]^+$: 368.1679, found 368.1684.

_N_-((_E_)-2-((_E_)-Benzylidene)-6-(naphthalen-2-yloxy)hexylidene)-4-methylbenzenesulfonamide (24c)

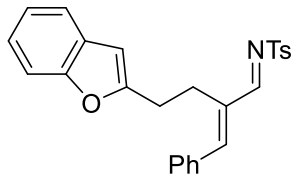


24c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-(6-(naphthalen-2-yloxy)hexyl)benzenesulfonamide (**24a**, 83.0 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 71.5 mg (74%) of **24c** as a white solid: **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.69 (s, 1H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.79 – 7.71 (m, 3H), 7.47 (dt, *J* = 8.0, 3.8 Hz, 3H), 7.38 – 7.31 (m, 4H), 7.31 –

7.27 (m, 3H), 7.13 – 7.07 (m, 2H), 4.04 (t, *J* = 6.1 Hz, 2H), 2.84 – 2.69 (m, 2H), 2.40 (s, 3H), 1.88 (q, *J* = 6.4 Hz, 2H), 1.80 – 1.73 (m, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 151.5, 144.2, 139.2, 135.6, 134.5, 130.0, 129.9, 129.8, 129.7, 129.7, 129.3, 128.9, 127.9, 127.7, 127.6, 126.7, 126.3, 123.5, 118.9, 106.5, 67.0, 28.9, 25.5, 24.4, 21.6; **IR (film)**: 3054, 2987, 2305, 1629, 1600, 1567, 1510, 1465, 1421, 1390, 1319, 1305, 1265, 1217, 1183, 1158, 1120, 1090, 896, 841, 813, 746, 705, 587, 559, 475 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{30}H_{30}NO_3S^+$ $[M+H]^+$: 484.1941, found 484.1944.

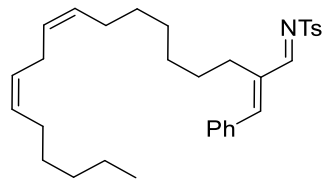
***N*-((*E*)-4-(Benzofuran-2-yl)-2-((*E*)-benzylidene)butylidene)-4-methylbenzenesulfonamide (25c)**



25c

General procedure **D**, with 0.2 mmol scale, the *N*-(4-(benzofuran-2-yl)butyl)-*N*-fluoro-4-methylbenzenesulfonamide (**25a**, 72.2 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 67.8 mg (79%) of **25c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.69 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.36 (m, 6H), 7.35 – 7.30 (m, 4H), 7.20 – 7.13 (m, 2H), 6.28 (s, 1H), 3.09 (dd, *J* = 8.7, 6.3 Hz, 2H), 3.01 – 2.95 (m, 2H), 2.44 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.9, 157.6, 154.6, 152.5, 144.4, 137.5, 135.5, 134.4, 130.0, 129.8, 129.7, 128.9, 128.6, 127.8, 123.3, 122.4, 120.3, 110.7, 102.6, 26.5, 24.5, 21.7; **IR (film)**: 3054, 2987, 2306, 1570, 1422, 1265, 1158, 1090, 896, 741, 705 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{28}H_{28}NO_3S^+$ $[M+H]^+$: 458.1784, found 458.1788.

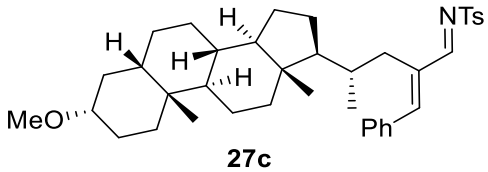
***N*-((1*E*,9*Z*,12*Z*)-2-((*E*)-Benzylidene)octadeca-9,12-dien-1-ylidene)-4-methylbenzenesulfonamide (26c)**



26c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-4-methyl-*N*-((9*Z*,12Z)-octadeca-9,12-dien-1-yl)benzenesulfonamide (**26a**, 79.0 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 20:1) to afford 62.1 mg (67%) of **26c** as a yellow oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.65 (s, 1H), 7.90 – 7.83 (m, 2H), 7.44 (dd, *J* = 7.0, 1.8 Hz, 4H), 7.42 – 7.40 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.23 (s, 1H), 5.41 – 5.31 (m, 4H), 2.76 (t, *J* = 6.0 Hz, 2H), 2.68 – 2.58 (m, 2H), 2.44 (s, 3H), 2.08 – 1.98 (m, 4H), 1.53 – 1.45 (m, 2H), 1.36 – 1.26 (m, 12H), 0.90 – 0.86 (m, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.5, 151.1, 144.2, 139.7, 135.7, 134.9, 130.2, 130.0, 129.9, 129.7, 128.8, 128.0, 127.81, 127.76, 53.4, 31.5, 29.6, 29.4, 29.3, 28.8, 28.0, 27.2, 26.0, 25.6, 22.5, 21.6, 14.1; **IR (film)**: 3054, 2987, 2930, 2858, 2306, 1567, 1422, 1265, 1158, 1090, 896, 742, 705, 588, 558 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{29}H_{38}NO_2S^+$ $[M+H]^+$: 464.2618, found 464.2620.

_N_-((_R_,_E_)-2-((_E_)-Benzylidene)-4-((3_R_,5_R_,8_R_,9_S_,10_S_,13_R_,14_S_,17_R_)-3-methoxy-10,13-dimethylhexadecahydro-1_H_-cyclopenta[_a_]phenanthren-17-yl)pentylidene)-4-methylbenzenesulfonamide (27c)

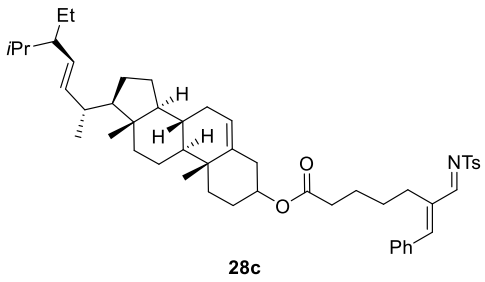


27c

General procedure **D**, with 0.2 mmol scale, the *N*-fluoro-*N*-((*R*)-4-((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-methoxy-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentyl)-4-methylbenzenesulfonamide (**27a**, 109.5 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL

Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 76.3 mg (62%) of **27c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.43 – 7.36 (m, 3H), 7.33 – 7.30 (m, 3H), 3.34 (s, 3H), 3.20 – 3.08 (m, 1H), 2.73 (dd, *J* = 13.2, 2.9 Hz, 1H), 2.47 (d, *J* = 11.3 Hz, 1H), 2.43 (s, 3H), 1.88 – 1.68 (m, 6H), 1.65 – 1.54 (m, 3H), 1.43 – 1.18 (m, 9H), 1.13 – 0.92 (m, 6H), 0.89 (s, 3H), 0.60 (d, *J* = 6.6 Hz, 3H), 0.39 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.6, 151.9, 144.0, 139.1, 135.9, 135.2, 129.7, 129.58, 129.55, 128.6, 127.6, 80.3, 57.3, 56.3, 55.5, 42.8, 41.9, 40.2, 39.9, 35.8, 35.2, 34.9, 34.8, 32.7, 32.1, 27.8, 27.2, 26.7, 26.3, 24.2, 23.3, 21.6, 20.7, 18.4, 11.7; **IR (film)**: 3054, 2985, 2939, 2867, 2305, 1567, 1422, 1318, 1265, 1158, 1091, 909, 746, 705, 651, 587, 560, 419 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{39}H_{54}NO_3S^+$ $[M+H]^+$: 616.3819, found 616.3822.

(8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((2*R*,5*S*,*E*)-5-Ethyl-6-methylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl (*E*)-7-phenyl-6-((*E*)-(tosylimino)methyl)hept-6-enoate (28c)

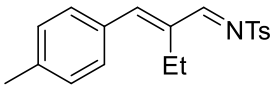


28c

General procedure **D**, with 0.2 mmol scale, the (8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((2*R*,5*S*,*E*)-5-ethyl-6-methylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 7-((*N*-fluoro-4-methylphenyl)sulfonamido)heptanoate (**28a**, 142.4 mg, 0.2 mmol), *N*-benzylidene-4-methylbenzenesulfonamide (**1b**, 67.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 94.7 mg (63%) of **28c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 7.85 (d,

J = 8.3 Hz, 2H), 7.46 – 7.43 (m, 4H), 7.42 – 7.38 (m, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.25 (s, 1H), 5.35 (d, *J* = 4.2 Hz, 1H), 5.15 (dd, *J* = 15.1, 8.6 Hz, 1H), 5.01 (dd, *J* = 15.1, 8.7 Hz, 1H), 4.65 – 4.53 (m, 1H), 2.67 – 2.60 (m, 2H), 2.44 (s, 3H), 2.29 – 2.23 (m, 4H), 2.05 – 1.92 (m, 3H), 1.87 – 1.80 (m, 2H), 1.70 (dd, *J* = 9.2, 5.3 Hz, 2H), 1.56 – 1.50 (m, 7H), 1.42 – 1.37 (m, 2H), 1.27 – 1.06 (m, 8H), 1.01 (s, 6H), 0.97 – 0.91 (m, 2H), 0.87 – 0.81 (m, 4H), 0.8 (s, 3H), 0.78 (s, 3H), 0.69 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.3, 172.8, 151.4, 144.2, 139.6, 139.1, 138.3, 135.6, 134.7, 130.0, 129.9, 129.7, 129.2, 128.9, 127.8, 122.6, 73.8, 56.7, 55.8, 51.2, 50.0, 42.1, 40.5, 39.6, 38.1, 36.9, 36.5, 34.2, 31.84, 31.78, 28.9, 27.7, 27.5, 26.9, 25.8, 25.4, 25.0, 24.3, 21.7, 21.2, 21.1, 21.0, 19.3, 18.9, 12.2, 12.0; **IR (film)**: 3054, 2957, 2870, 2306, 1723, 1568, 1422, 1319, 1265, 1158, 1090, 896, 848, 747, 705, 587, 558 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{50}H_{70}NO_4S^+$ $[M+H]^+$: 780.5020, found 780.5023.

4-Methyl-*N*-((*Z*)-2-((*E*)-4-methylbenzylidene)butylidene)benzenesulfonamide (29c)

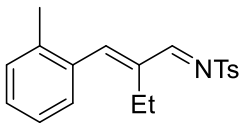


29c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), (*E*)-4-methyl-*N*-(4-methylbenzylidene)benzenesulfonamide (**2b**, 71.1 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 52.3 mg (80%) of **29c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.63 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.23 (m, 2H), 7.19 (s, 1H), 2.66 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 2.40 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 151.1, 144.1, 140.6, 140.1, 136.0, 132.2, 130.1, 129.7, 129.6, 127.8, 21.6, 21.5, 19.5, 12.7; **IR (film)**: 2967, 2930, 1677, 1559, 1466, 1405, 1318, 1201, 1171, 1127,

1084, 1021, 908, 834, 814, 786, 705, 681, 631, 609, 563, 477 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{22}NO_2S^+$ $[M+H]^+$: 328.1366, found 328.1371.

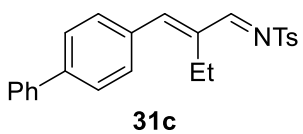
4-Methyl-*N*-((*Z*)-2-((*E*)-2-methylbenzylidene)butylidene)benzenesulfonamide (30c)



30c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-methyl-*N*-(2-methylbenzylidene)benzenesulfonamide (**3b**, 71.1 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 49.8 mg (76%) of **30c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.71 (s, 1H), 7.88 (d, *J* = 8.3 Hz, 2H), 7.40 (s, 1H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.30 – 7.23 (m, 4H), 2.50 (q, *J* = 7.5 Hz, 2H), 2.45 (s, 3H), 2.31 (s, 3H), 1.05 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.8, 150.0, 144.2, 141.5, 137.1, 135.8, 134.1, 130.5, 129.7, 129.4, 128.3, 127.8, 125.9, 21.6, 20.0, 19.5, 13.2; **IR (film)**: 2965, 2925, 1677, 1559, 1466, 1405, 1318, 1201, 1184, 1156, 1127, 1089, 1018, 908, 834, 814, 788, 705, 681, 622, 609, 563, 477 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{22}NO_2S^+$ $[M+H]^+$: 328.1366, found 328.1370.

***N*-((1*Z*,2*E*)-2-([1,1'-Biphenyl]-4-ylmethylene)butylidene)-4-methylbenzenesulfonamide (31c)**

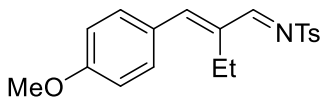


31c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-([1,1'-biphenyl]-4-ylmethylene)-4-methylbenzenesulfonamide (**4b**, 87.2 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was

purified by flash column chromatography (PE:EA = 10:1) to afford 63.1 mg (81%) of **31c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.88 (d, *J* = 8.3 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.64 – 7.61 (m, 2H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.41 – 7.37 (m, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.26 (d, *J* = 1.8 Hz, 1H), 2.71 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.17 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.2, 150.5, 144.2, 142.7, 140.7, 139.8, 135.7, 133.8, 130.6, 129.7, 128.9, 128.0, 127.8, 127.4, 127.0, 21.6, 19.6, 12.8; **IR (film)**: 3030, 2963, 2925, 1679, 1598, 1564, 1487, 1466, 1400, 1319, 1290, 1194, 1157, 1090, 1077, 1019, 1006, 876, 828, 778, 765, 737, 683, 610, 591, 559 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{24}H_{24}NO_2S^+$ $[M+H]^+$: 390.1522, found 390.1522.

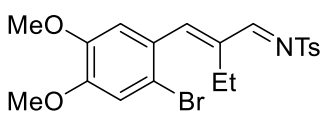
***N*-((*Z*)-2-((*E*)-4-Methoxybenzylidene)butylidene)-4-methylbenzenesulfonamide (32c)**



32c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(4-methoxybenzylidene)-4-methylbenzenesulfonamide (**5b**, 75.2 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 8:1) to afford 53.6 mg (78%) of **32c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.61 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.9 Hz, 2H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.14 (s, 1H), 6.96 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 2.66 (q, *J* = 7.5 Hz, 2H), 2.42 (s, 3H), 1.12 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.5, 161.1, 151.1, 144.0, 138.5, 136.0, 132.2, 129.6, 127.7, 127.6, 114.4, 55.4, 21.6, 19.4, 12.5; **IR (film)**: 3266, 2967, 2935, 2840, 1675, 1601, 1557, 1510, 1466, 1406, 1305, 1259, 1205, 1177, 1156, 1118, 1089, 1077, 1029, 879, 830, 786, 757, 721, 705, 683, 620, 570, 557, 482 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{22}NO_3S^+$ $[M+H]^+$: 344.1315, found 344.1319.

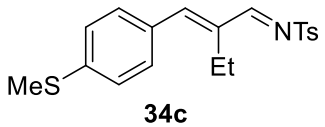
***N*-((*Z*)-2-((*E*)-2-Bromo-4,5-dimethoxybenzylidene)butylidene)-4-methylbenzenesulfonamide (33c)**



33c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(2-bromo-4,5-dimethoxybenzylidene)-4-methylbenzenesulfonamide (**6b**, 103.6 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 5:1) to afford 67.0 mg (74%) of **33c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.67 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.46 (s, 1H), 7.36 – 7.31 (m, 2H), 7.14 (s, 1H), 6.98 (s, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 2.59 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.14 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.1, 152.3, 149.8, 145.2, 144.2, 140.6, 135.7, 129.7, 127.8, 123.4, 116.4, 114.4, 112.9, 56.8, 56.3, 21.6, 19.8, 12.9; **IR (film)**: 2960, 2926, 1677, 1596, 1560, 1488, 1464, 1390, 1319, 1288, 1219, 1183, 1157, 1090, 1075, 1051, 1031, 830, 782, 750, 709, 686, 665, 587, 554 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{23}BrNO_4S^+$ $[M+H]^+$: 452.0526, found 452.0528.

4-Methyl-*N*-((*Z*)-2-((*E*)-4-(methylthio)benzylidene)butylidene)benzenesulfonamide (34c)

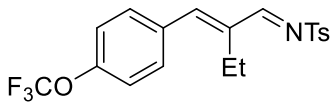


34c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), (*E*)-4-methyl-*N*-(4-(methylthio)benzylidene)benzenesulfonamide (**7b**, 79.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 8:1) to afford 53.9 mg

(75%) of **34c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.61 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.14 (s, 1H), 2.65 (q, *J* = 7.5 Hz, 2H), 2.51 (s, 3H), 2.43 (s, 3H), 1.12 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.2, 150.4, 144.1, 142.2, 139.9, 135.8, 131.1, 130.5, 129.6, 127.7, 125.7, 21.6, 19.5, 14.9, 12.6; **IR (film)**: 2966, 2923, 1595, 1558, 1492, 1466, 1399, 1317, 1283, 1259, 1192, 1156, 1089, 1012, 874, 834, 813, 775, 718, 674, 638, 613, 557 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{22}NO_2S_2^+$ $[M+H]^+$: 360.1086, found 360.1086.

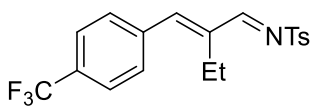
4-Methyl-*N*-((*Z*)-2-((*E*)-4-(trifluoromethoxy)benzylidene)butylidene)benzenesulfonamide (35c)



35c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-methyl-*N*-(4-(trifluoromethoxy)benzylidene)benzenesulfonamide (**8b**, 89.3 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 61.2 mg (77%) of **35c** as a colorless oil: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.20 (s, 1H), 2.62 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.12 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.8, 149.9, 148.6, 144.4, 141.5, 135.5, 133.3, 131.4, 129.7, 127.8, 121.0, 120.3 (q, *J* = 207.1 Hz), 21.6, 19.4, 12.8; **IR (film)**: 2968, 2926, 1683, 1568, 1507, 1468, 1401, 1320, 1259, 1204, 1158, 1090, 1077, 1018, 874, 831, 814, 766, 750, 705, 683, 598, 557 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{19}F_3NO_3S^+$ $[M+H]^+$: 398.1032, found 398.1033.

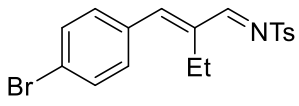
4-Methyl-*N*-((*Z*)-2-((*E*)-4-(trifluoromethyl)benzylidene)butylidene)benzenesulfonamide (36c)



36c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-methyl-*N*-(4-(trifluoromethyl)benzylidene)benzenesulfonamide (**9b**, 85.1 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 15:1) to afford 55.7 mg (73%) of **36c** as a colorless oil: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.66 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.25 (s, 1H), 2.62 (q, *J* = 7.5 Hz, 2H), 2.45 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.4, 148.2, 144.5, 142.8, 138.2, 131.2 (q, *J* = 32.8 Hz), 135.3, 129.8 (d, *J* = 2.5 Hz), 127.9, 125.7 (q, *J* = 3.8 Hz), 125.6 (q, *J* = 207.9 Hz), 21.7, 19.6, 12.9; **IR (film)**: 2926, 1615, 1571, 1467, 1399, 1323, 1159, 1127, 1090, 1068, 1015, 873, 827, 780, 686, 664, 636, 617, 598, 556 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{19}F_3NO_2S^+$ $[M+H]^+$: 382.1083, found 382.1083.

***N*-((*Z*)-2-((*E*)-4-Bromobenzylidene)butylidene)-4-methylbenzenesulfonamide (37c)**

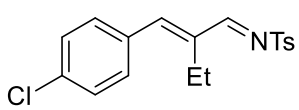


37c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(4-bromobenzylidene)-4-methylbenzenesulfonamide (**10b**, 87.9 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 15:1) to afford 58.1 mg (74%) of **37c** as a colorless oil: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.62 (s, 1H), 7.85 (d, *J* = 7.9 Hz, 2H), 7.60 – 7.52 (m, 2H),

7.33 (dd, *J* = 8.1, 5.5 Hz, 4H), 7.15 (s, 1H), 2.61 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.11 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.8, 149.1, 144.3, 141.4, 135.5, 133.6, 132.1, 131.2, 129.7, 127.8, 124.3, 21.6, 19.5, 12.7; **IR (film)**: 2961, 2925, 1565, 1487, 1466, 1393, 1318, 1304, 1288, 1201, 1184, 1157, 1090, 1077, 1008, 872, 836, 815, 775, 714, 686, 670, 632, 598, 556, 518 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{18}H_{19}BrNO_2S^+$ $[M+H]^+$: 392.0314, found 392.0317.

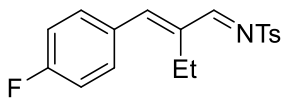
_N_-((_Z_)-2-((_E_)-4-Chlorobenzylidene)butylidene)-4-methylbenzenesulfonamide (38c)



38c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(4-chlorobenzylidene)-4-methylbenzenesulfonamide (**11b**, 76.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 15:1) to afford 55.0 mg (79%) of **38c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.63 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.38 (m, 4H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.17 (s, 1H), 2.62 (q, *J* = 7.5 Hz, 2H), 1.11 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.8, 149.0, 144.3, 141.2, 135.9, 135.5, 133.2, 131.1, 129.7, 129.1, 127.8, 21.6, 19.4, 12.7; **IR (film)**: 2968, 2925, 1565, 1490, 1467, 1396, 1319, 1305, 1289, 1201, 1184, 1157, 1090, 1012, 898, 873, 837, 816, 776, 721, 705, 676, 637, 614, 556, 523 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{18}H_{19}ClNO_2S^+$ $[M+H]^+$: 348.0820, found 348.0820.

_N_-((_Z_)-2-((_E_)-4-Fluorobenzylidene)butylidene)-4-methylbenzenesulfonamide (39c)

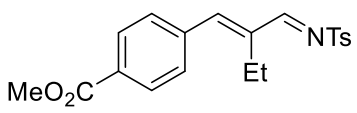


39c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol),

N-(4-fluorobenzylidene)-4-methylbenzenesulfonamide (**12b**, 72.1 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 15:1) to afford 47.7 mg (72%) of **39c** as a colorless oil: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.63 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.18 (s, 1H), 7.13 (t, *J* = 8.6 Hz, 2H), 2.63 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.12 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.0, 164.35 (d, *J* = 253.3 Hz), 149.4, 144.3, 140.5 (d, *J* = 1.26 Hz), 135.6, 132.0 (d, *J* = 8.8 Hz), 131.0 (d, *J* = 2.5 Hz), 129.7, 127.8, 116.1 (d, *J* = 21.4 Hz), 21.6, 19.4, 12.7; **IR (film)**: 2965, 2925, 1597, 1564, 1508, 1467, 1400, 1319, 1304, 1232, 1202, 1184, 1157, 1090, 1077, 1019, 878, 829, 814, 788, 764, 713, 682, 646, 619, 562 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{18}H_{19}FNO_2S^+$ $[M+H]^+$: 332.1115, found 332.1116.

Methyl 4-((*E*)-2-((*Z*)-(tosylimino)methyl)but-1-en-1-yl)benzoate (40c)

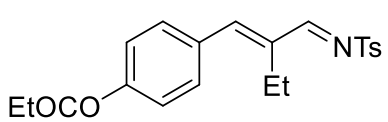


40c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), methyl 4-((tosylimino)methyl)benzoate (**13b**, 82.5 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 6:1) to afford 55.0 mg (74%) of **40c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.65 (s, 1H), 8.08 (d, *J* = 8.4 Hz, 2H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.50 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.25 (s, 1H), 3.93 (s, 3H), 2.63 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.12 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.6, 166.3, 148.9, 144.4, 142.6, 139.0, 135.3, 130.8, 129.9, 129.7, 129.5, 127.8, 52.3, 21.6, 19.6, 12.9; **IR (film)**: 2953, 1722, 1683, 1606, 1568, 1436, 1400, 1317, 1282,

1184, 1158, 1110, 1090, 1017, 902, 874, 831, 776, 764, 707, 685, 671, 636, 603, 557 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{22}NO_4S^+$ $[M+H]^+$: 372.1264, found 372.1264.

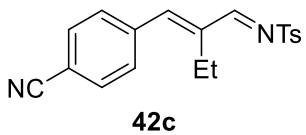
4-((*E*)-2-((*Z*)-(Tosylimino)methyl)but-1-en-1-yl)phenyl propionate (41c)



41c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-((tosylimino)methyl)phenyl propionate (**14b**, 86.2 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 5:1) to afford 54.0 mg (70%) of **41c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.63 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 6.5 Hz, 2H), 7.17 (s, 1H), 2.68 – 2.58 (m, 4H), 2.44 (s, 3H), 1.27 (t, *J* = 7.5 Hz, 3H), 1.13 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.1, 172.6, 151.7, 149.7, 144.2, 140.7, 135.6, 132.3, 131.1, 129.7, 127.8, 122.1, 27.7, 21.6, 19.4, 12.7, 8.9; **IR (film)**: 2970, 1761, 1597, 1563, 1505, 1463, 1400, 1354, 1319, 1305, 1276, 1260, 1214, 1157, 1090, 1076, 1016, 982, 904, 877, 831, 788, 765, 750, 683, 580, 556 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{21}H_{24}NO_4S^+$ $[M+H]^+$: 386.1421, found 386.1422.

***N*-((*Z*)-2-((*E*)-4-Cyanobenzylidene)butylidene)-4-methylbenzenesulfonamide (42c)**

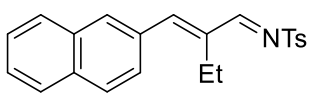


42c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(4-cyanobenzylidene)-4-methylbenzenesulfonamide (**15b**, 73.9 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was

purified by flash column chromatography (PE:EA = 3:1) to afford 45.3 mg (67%) of **42c** as a white solid: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.66 (s, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.21 (s, 1H), 2.61 (q, *J* = 7.5 Hz, 2H), 2.45 (s, 3H), 1.12 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 174.4, 151.1, 144.1 140.6, 140.0, 136.0, 132.2, 130.1, 129.7, 129.6, 127.8, 21.6, 21.5, 19.5, 12.7; **IR (film)**: 2957, 2925, 2228, 1683, 1570, 1466, 1398, 1319, 1290, 1199, 1157, 1089, 1018, 872, 825, 779, 680, 620, 559 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{19}H_{19}N_2O_2S^+$ $[M+H]^+$: 339.1162, found 339.1165.

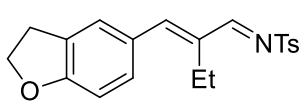
4-Methyl-*N*-((1*Z*,2*E*)-2-(naphthalen-2-ylmethylene)butylidene)benzenesulfonamide (43c)



43c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-methyl-*N*-(naphthalen-2-ylmethylene)benzenesulfonamide (**16b**, 80.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 53.1 mg (73%) of **43c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.70 (s, 1H), 7.94 (s, 1H), 7.92 – 7.82 (m, 5H), 7.60 – 7.51 (m, 3H), 7.40 – 7.31 (m, 3H), 2.75 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.20 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.3, 151.0, 144.2, 140.9, 135.7, 133.6, 133.0, 132.4, 130.6, 129.7, 128.7, 128.5, 127.8, 127.7, 127.6, 126.8, 126.4, 21.6, 19.6, 12.9; **IR (film)**: 2965, 2925, 1677, 1559, 1466, 1405, 1318, 1201, 1184, 1156, 1127, 1089, 1018, 908, 834, 814, 788, 705, 681, 622, 609, 563, 477 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{22}H_{22}NO_2S^+$ $[M+H]^+$: 364.1366, found 364.1371.

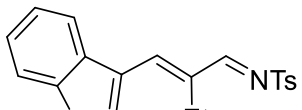
***N*-((1*Z*,2*E*)-2-((2,3-Dihydrobenzofuran-5-yl)methylene)butylidene)-4-methylbenzenesulfonamide (44c)**



44c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-((2,3-dihydrobenzofuran-5-yl)methylene)-4-methylbenzenesulfonamide (**17b**, 78.4 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 8:1) to afford 49.1 mg (69%) of **44c** as a white solid: **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.60 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.38 (s, 1H), 7.35 – 7.30 (m, 3H), 7.13 (s, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 4.65 (t, *J* = 8.6 Hz, 2H), 3.26 (t, *J* = 8.6 Hz, 2H), 2.67 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 174.7, 162.1, 151.7, 143.9, 137.9, 136.1, 132.0, 129.6, 128.2, 127.71, 127.65, 127.1, 109.9, 72.0, 29.3, 21.6, 19.4, 12.5; **IR (film)**: 2959, 2924, 2854, 1671, 1599, 1550, 1492, 1467, 1407, 1364, 1315, 1276, 1250, 1202, 1155, 1104, 1089, 981, 935, 815, 789, 764, 750, 684, 593, 562 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{22}NO_3S^+$ $[M+H]^+$: 356.1315, found 356.1316.

_N_-((1_Z_,2_E_)-2-(Benzofuran-3-ylmethylene)butylidene)-4-methylbenzenesulfonamide (45c)

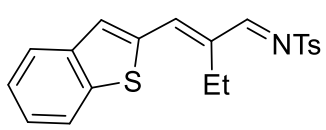


45c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(benzofuran-3-ylmethylene)-4-methylbenzenesulfonamide (**18b**, 77.8 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 8:1) to afford 50.9 mg (72%) of **45c** as a white solid: **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.62 (s, 1H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.29 – 7.26 (m, 1H), 7.08 (s, 1H), 7.03 (s, 1H),

2.90 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.14 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.7, 156.0, 152.5, 144.2, 140.5, 135.6, 129.7, 127.8, 127.0, 123.6, 122.0, 113.9, 111.5, 21.6, 20.0, 13.0; **IR (film)**: 2967, 2926, 2876, 1680, 1610, 1597, 1563, 1523, 1453, 1393, 1349, 1318, 1293, 1258, 1196, 1158, 1130, 1089, 1079, 1019, 949, 888, 858, 831, 814, 784, 751, 705, 678, 622, 611, 559, 450 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{20}NO_3S^+$ $[M+H]^+$: 354.1158, found 354.1159.

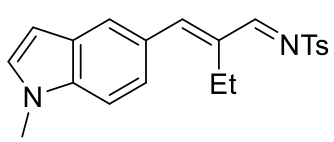
_N_-((1_Z_,2_E_)-2-(Benzo[_b_]thiophen-2-ylmethylene)butylidene)-4-methylbenzenesulfonamide (46c)



46c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-(benzo[*b*]thiophen-3-ylmethylene)-4-methylbenzenesulfonamide (**19b**, 82.0 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 8:1) to afford 54.7 mg (74%) of **46c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 7.92 – 7.80 (m, 4H), 7.56 (s, 1H), 7.44 – 7.37 (m, 3H), 7.33 (d, *J* = 8.1 Hz, 2H), 2.81 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.14 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.2, 144.2, 143.0, 142.3, 139.5, 138.3, 137.7, 135.7, 131.3, 129.7, 127.7, 126.5, 125.1, 124.7, 122.2, 21.6, 20.0, 12.6; **IR (film)**: 2967, 2926, 2876, 1680, 1597, 1563, 1523, 1453, 1349, 1318, 1258, 1196, 1130, 1089, 1019, 949, 858, 831, 814, 784, 751, 705, 678, 622, 559, 450 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{20}NO_2S_2$ $[M+H]^+$: 370.0930, found 370.0932.

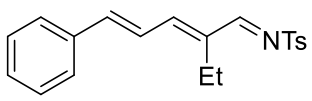
4-Methyl-_N_-((1_Z_,2_E_)-2-((1-methyl-1_H_-indol-5-yl)methylene)butylidene)benzenesulfonamide (47c)



47c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-methyl-*N*-((1-methyl-1*H*-indol-5-yl)methylene)benzenesulfonamide (**20b**, 81.2 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 5:1) to afford 46.9 mg (64%) of **47c** as a white solid: **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.67 (s, 1H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.65 (d, *J* = 8.3 Hz, 1H), 7.49 (s, 1H), 7.38 (s, 1H), 7.35 – 7.29 (m, 3H), 7.19 (d, *J* = 3.0 Hz, 1H), 6.52 (d, *J* = 2.6 Hz, 1H), 3.84 (s, 3H), 2.78 (q, *J* = 7.5 Hz, 2H), 2.44 (s, 3H), 1.20 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 174.8, 153.5, 143.9, 138.5, 136.6, 136.2, 131.8, 130.1, 129.6, 128.3, 127.7, 121.7, 121.2, 112.0, 101.5, 32.9, 21.6, 19.7, 12.6; **IR (film)**: 2948, 2920, 2866, 1672, 1581, 1532, 1481, 1427, 1349, 1318, 1258, 1181, 1123, 1064, 1019, 868, 841, 772, 742, 678, 562, 477 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{21}H_{23}N_2O_2S$ $[M+H]^+$: 367.1475, found 367.1475.

***N*-((1*Z*,2*E*,4*E*)-2-Ethyl-5-phenylpenta-2,4-dien-1-ylidene)-4-methylbenzenesulfonamide (48c)**

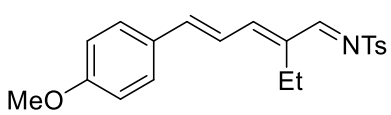


48c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), 4-methyl-*N*-((1*E*,2*E*)-3-phenylallylidene)benzenesulfonamide (**21b**, 74.2 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 41.4 mg (61%) of **48c** as a colorless oil: **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.54 (s, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.55 – 7.50 (m, 2H), 7.42 – 7.34 (m, 3H), 7.32 (d, *J* = 8.1 Hz, 2H),

7.20 (dd, *J* = 15.3, 11.5 Hz, 1H), 7.02 – 6.95 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.05 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.6, 150.2, 144.0, 142.7, 140.5, 135.9, 135.8, 129.7, 129.6, 128.9, 127.7, 127.6, 123.2, 21.6, 19.2, 13.7; **IR (film)**: 2925, 1572, 1547, 1493, 1449, 1397, 1318, 1280, 1199, 1155, 1089, 969, 863, 828, 782, 765, 751, 680, 554 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{22}NO_2S^+$ $[M+H]^+$: 340.1366, found 340.1370.

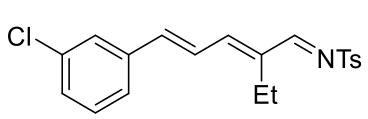
***N*-((1*Z*,2*E*,4*E*)-2-Ethyl-5-(4-methoxyphenyl)penta-2,4-dien-1-ylidene)-4-methylbenzenesulfonamide (49c)**



49c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-((1*E*,2*E*)-3-(4-methoxyphenyl)allylidene)-4-methylbenzenesulfonamide (**22b**, 82.0 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 8:1) to afford 46.6 mg (63%) of **49c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.52 (s, 1H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.07 (dd, *J* = 15.4, 11.0 Hz, 1H), 6.97 – 6.90 (m, 4H), 3.85 (s, 3H), 2.55 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.04 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.7, 161.1, 151.1, 143.9, 142.8, 139.3, 136.2, 129.6, 129.3, 128.7, 127.7, 121.2, 114.5, 55.4, 21.6, 19.2, 13.7; **IR (film)**: 3854, 3744, 3727, 3704, 3628, 3199, 3006, 2957, 2924, 2350, 1728, 1568, 1545, 1509, 1463, 1304, 1247, 1155, 1089, 906, 857, 765, 578 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{21}H_{24}NO_3S^+$ $[M+H]^+$: 370.1471, found 370.1476.

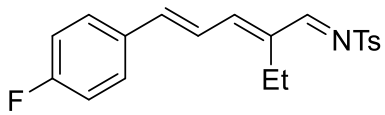
***N*-((1*Z*,2*E*,4*E*)-5-(3-Chlorophenyl)-2-ethylpenta-2,4-dien-1-ylidene)-4-methylbenzenesulfonamide (50c)**



50c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-((1*E*,2*E*)-3-(3-chlorophenyl)allylidene)-4-methylbenzenesulfonamide (**23b**, 83.1 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 41.1 mg (55%) of **50c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.54 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.49 (s, 1H), 7.39 – 7.30 (m, 5H), 7.21 – 7.15 (m, 1H), 6.98 – 6.87 (m, 2H), 2.57 (q, *J* = 7.6 Hz, 2H), 2.43 (s, 3H), 1.05 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.4, 149.2, 144.2, 141.4, 140.7, 137.7, 135.8, 134.9, 130.2, 129.7, 129.5, 127.8, 127.1, 125.9, 124.4, 21.6, 19.2, 13.8; **IR (film)**: 3266, 2961, 2925, 1700, 1595, 1551, 1464, 1394, 1319, 1277, 1258, 1196, 1157, 1089, 1019, 968, 892, 833, 814, 782, 765, 750, 706, 697, 679, 629, 555 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{21}ClNO_2S^+$ $[M+H]^+$: 374.0976, found 374.0978.

_N_-((1_Z_,2_E_,4_E_)-2-Ethyl-5-(4-fluorophenyl)penta-2,4-dien-1-ylidene)-4-methylbenzenesulfonamide (51c)



51c

General procedure **D**, with 0.2 mmol scale, the *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 49.1 mg, 0.2 mmol), *N*-((1*E*,2*E*)-3-(4-fluorophenyl)allylidene)-4-methylbenzenesulfonamide (**24b**, 78.9 mg, 0.26 mmol), 4Å molecular sieve (150 mg) and DABCO (22.4 mg, 0.2 mol) was added into a 10.0 mL Schlenk tube with a stirring bar. The mixture was stirred at room temperature under Ar for 24 h. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford 42.2 mg (59%) of **51c** as a colorless oil: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.54 (s, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.56 – 7.46 (m, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.05 (m, 3H), 6.99 – 6.92 (m,

2H), 2.56 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.04 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.6, 163.5 (d, *J* = 252.0 Hz), 149.9, 144.1, 141.3, 140.5, 135.9, 132.1 (d, *J* = 2.5 Hz), 129.7, 129.4 (d, *J* = 8.8 Hz), 127.7, 123.0 (d, *J* = 2.5 Hz), 116.1 (d, *J* = 22.7 Hz), 21.6, 19.2, 13.7; **IR (film)**: 2973, 2921, 1584, 1548, 1506, 1453, 1412, 1303, 1217, 1202, 1171, 1141, 1072, 1012, 862, 821, 812, 788, 764, 713, 682, 646, 619, 562 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{20}H_{21}FNO_2S$ $[M+H]^+$: 358.1272, found 358.1274.

4. Synthetic Utility of the Imine Products.

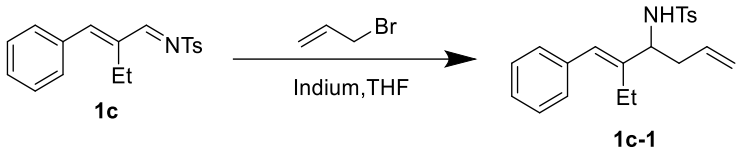


Fig. S9

***(E)-N-(5*-Benzylidenehept-1-en-4-yl)-4methylbenzenesulfonamide (1c-1)**[4]

To a stirred mixture of the imine **1c** (1.0 eq.**,** 0.4 mmol) and allyl bromide (3.0 eq., 1.2 mmol) in THF (4 mL) was added indium (3.0 eq., 1.2 mmol) powder. The reaction was stirred overnight, quenched by adding 1 N HCl (2 mL), and extracted with ether (2 × 15 mL). The combined organic phase was washed with saturated $NaHCO_3$ solution and brine and dried over anhydrous Na_2SO_4. The crude product, after evaporation of ether, was purified by flash column chromatography (silica gel, PE:EA (10:1→5:1) to afford 113.8 mg (80%) of **4c-1** as a colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** 7.74 (d, *J* = 8.3 Hz, 2H), 7.28 – 7.16 (m, 5H), 7.00 (dd, *J* = 7.3, 1.6 Hz, 2H), 6.23 (s, 1H), 5.74 – 5.53 (m, 1H), 5.14 – 5.10 (m, 1H), 5.09 – 5.02 (m, 2H), 4.02 – 3.92 (m, 1H), 2.42 – 2.35 (m, 2H), 2.35 (s, 3H), 2.14 (dt, *J* = 15.1, 7.5 Hz, 1H), 2.05 – 1.93 (m, 1H), 0.93 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 143.1, 141.6, 137.9, 137.1, 133.4, 129.4, 128.4, 128.0, 127.3, 127.1, 126.4, 118.9, 58.0, 39.0, 21.8, 21.4, 13.1.

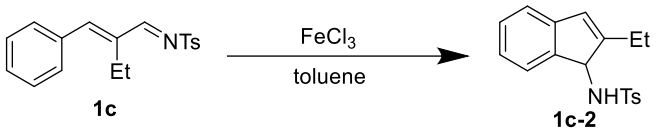


Fig. S10

***N*-(2-Ethyl-1*H*-inden-1-yl)-4-methylbenzenesulfonamide (1c-2)**[5]

To a stirred solution of the imine **1c** (0.40 mmol) in toluene (6 mL) was added $FeCl_3$ (20 mol %). The resulting mixture was stirred at 40 °C. After the imine was completely consumed (monitored by TLC), the reaction was quenched by addition of H_2O (3 mL) and then extracted with ethyl acetate (2 × 5 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The crude product was purified by column chromatography (silica gel, PE:EA (10:1→5:1) to afford 92.8 mg (74%) of **1c-2** as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 7.7 Hz, 2H), 7.22 – 7.14 (m, 1H), 7.10 (d, *J* = 7.3 Hz, 1H), 6.95 (td, *J* = 7.4, 1.2 Hz, 1H), 6.74 (d, *J* = 7.4 Hz, 1H), 6.34 (s, 1H), 4.77 (d, *J* = 9.7 Hz, 1H), 4.49 (d, *J* = 9.7 Hz, 1H), 2.48 (s, 3H), 2.44 – 2.33 (m, 1H), 2.26 – 2.12 (m, 1H), 1.10 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 152.3, 143.6, 143.4, 143.1, 138.5, 129.8, 128.4, 127.2, 125.9, 124.9, 123.4, 120.4, 61.4, 21.6, 21.1, 12.4.

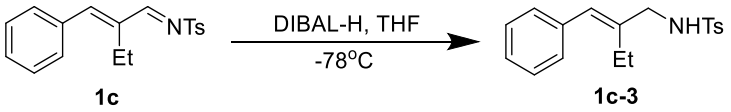


Fig. S11

(*E*)-*N*-(2-Benzylidenebutyl)-4-methylbenzenesulfonamide (1c-3)[6]

To a stirred solution of the imine **1c** (1.0 eq., 0.4 mmol) in THF (4 mL) at -78 °C was added DIBAL-H (1.0 M in toluene, 1.4 eq., 0.56 mmol). The resulting mixture was warmed to room temperature and stirred for 16 h before it was cooled to at 0 °C and sequentially quenched with water (2.8 mL), NaOH (10% aq., 2.8 mL) and water (7.0 mL). The resulting mixture was warmed to room temperature and stirred for 15 min,

filtered through a short pad of Celite and eluted with Et_2O (10 mL), and concentrated under reduced pressure. The resulting residue was purified by flash column chromatography (silica gel, PE:EA (10:1→5:1) to afford **1c-3** (107.2mg, 85%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.31 – 7.24 (m, 4H), 7.22 – 7.17 (m, 1H), 7.09 (d, *J* = 7.2 Hz, 2H), 6.31 (s, 1H), 5.01 (t, *J* = 6.4 Hz, 1H), 3.66 (dd, *J* = 6.4, 1.3 Hz, 2H), 2.39 (s, 3H), 2.20 (q, *J* = 7.5 Hz, 2H), 1.00 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 143.3, 138.9, 137.0, 136.9, 129.6, 128.4, 128.1, 127.5, 127.1, 126.6, 48.5, 21.8, 21.4, 12.6.

(*E*)-4-Chloro-2-(1-phenylbut-1-en-2-yl)tetrahydro-2*H*-pyran (1c-4)[7]

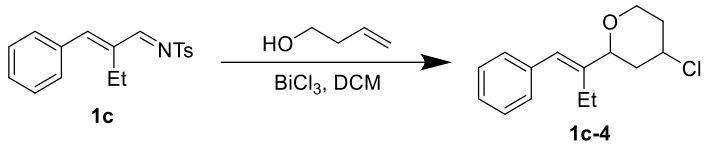


Fig. S12

A mixture of the imine **1c** (1.0 eq., 0.40 mmol), homoallyl alcohol (1.2 eq., 0.48 mmol), $BiCl_3$ (0.4 eq., 0.160 mmol) and CH_2Cl_2 (2.0 mL) was stirred at room temperature. When the reaction did not proceed further as indicated by TLC, the reaction mixture was directly purified by flash column chromatography (silica gel, PE:EA (30:1→10:1) to afford 62.2 mg (62%) of **1c-4** as a colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.36 (t, *J* = 7.4 Hz, 2H), 7.31 – 7.22 (m, 3H), 6.59 (s, 1H), 4.28 – 4.02 (m, 2H), 3.90 (d, *J* = 11.1 Hz, 1H), 3.55 (td, *J* = 12.2, 2.2 Hz, 1H), 2.53 – 2.36 (m, 2H), 2.33 – 2.22 (m, 1H), 2.21 – 2.11 (m, 1H), 2.07 – 1.92 (m, 1H), 1.91 – 1.75 (m, 1H), 1.13 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 143.2, 137.4, 128.6, 128.1, 126.5, 125.7, 80.1, 67.2, 56.0, 42.4, 37.0, 21.7, 13.7.

5. Mechanistic Studies

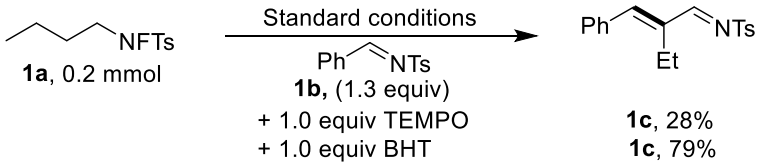


Fig. S13

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 0.2 mmol, 1.0 equiv), imines (**1b**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg), TEMPO or BHT (0.2 mmol, 1.0 equiv) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. The reaction was monitored by TLC and GC-Ms. The residue was purified by flash column chromatography on silica gel (PE:EA = 20:1) to afford 17.6 mg (28%) of **1c**.

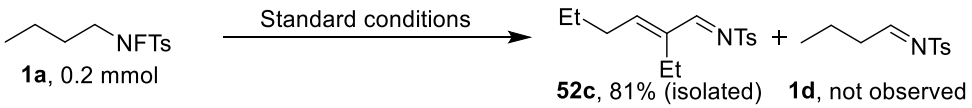


Fig. S14

When removing imine **1b**, the reaction was proceeded under the standard conditions. The reaction was detected by GC-Ms and TLC. The residue was purified by flash column chromatography on silica gel (PE:EA = 20:1) to afford 45.3 mg (81%) of **52c** as a colourless oil: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.46 (s, 1H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 6.47 (t, *J* = 7.5 Hz, 1H), 2.43 (s, 3H), 2.38 – 2.30 (m, 4H), 1.52 (q, *J* = 7.4 Hz, 2H), 0.95 (q, *J* = 7.4 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 173.6, 156.9, 144.1, 141.2, 135.7, 129.6, 127.7, 31.4, 21.9, 21.6, 18.7, 13.9, 13. 2; **IR (film)**: 3734, 3054, 2986, 2254, 1748, 1574, 1423, 1265, 1158, 1089, 910, 741, 705, 538 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{15}H_{22}NO_2S^+$ $[M+H]^+$: 280.1366, found 280.1371.

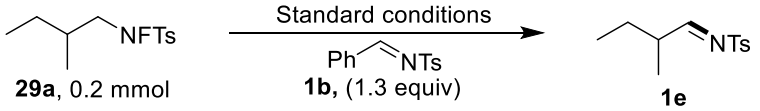


Fig. S15

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-fluoro-4-methyl-*N*-(2-methylbutyl)benzenesulfonamide (**29a**, 0.2 mmol, 1.0 equiv), imines (**1b**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. The reaction was monitored by TLC and GC-Ms. The yield of products (44%) was determined by GC-Ms using dodecane as internal standard.

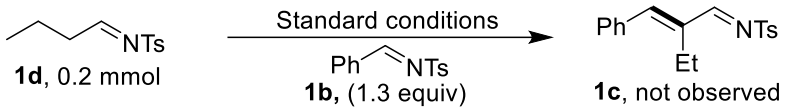


Fig. S16

When using **1d** as starting materials, the reaction was proceeded under the standard conditions. The reaction was monitored by TLC and GC-Ms. No desired products were detected.

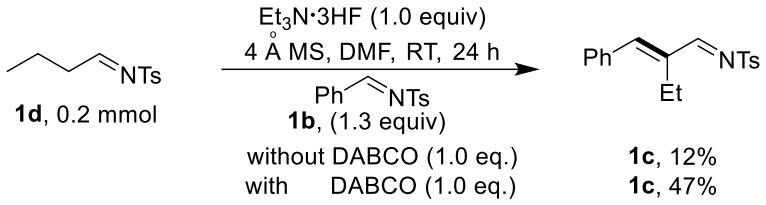
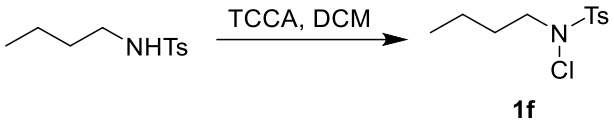


Fig. S17

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-butylidene-4-methylbenzenesulfonamide (**1d**, 0.2 mmol, 1.0 equiv), imine (**1b**, 0.26 mmol, 1.3 equiv), $Et_3N·3HF$ (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. The reaction was monitored by TLC and GC-Ms. The yield of products (12%) was determined by GC-Ms using dodecane as internal standard. When adding DABCO (0.2 mmol, 1.0 eq.) into the reaction, its yield increased to 47%.



1f

Fig. S18

According to literature, to an ice-cooled solution of sulfonamide (5.0 mmol, 1.0 equiv.) in CH_2Cl_2 (50 mL) was added trichloroisocyanuric acid (TCCA) (5.5 mmol, 1.1 equiv.). The resulting mixture was stirred at room temperature for 4.0 h. The mixture was poured into a separatory funnel containing 50 mL of H_2O. The layer was separated and the aqueous layer was extracted with CH_2Cl_2 (20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The crude product was purified by flash chromatography on silica gel (PE: EtOAc =5:1) to afford 1.1 g (83%) of **1f**: **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 3.22 (t, *J* = 6.8 Hz, 2H), 2.47 (s, 3H), 1.65 (p, *J* = 7.0 Hz, 2H), 1.39 (dt, *J* = 14.7, 7.4 Hz, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 145.3, 129.8, 129.6, 129.5, 56.3, 29.0, 21.7, 19.2, 13.6.

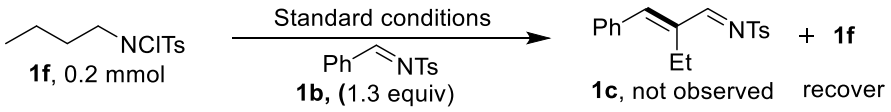


Fig. S19

When using **1f** as starting materials, the reaction was proceeded under the standard conditions. The desired product was not detected by GC-Ms and TLC.

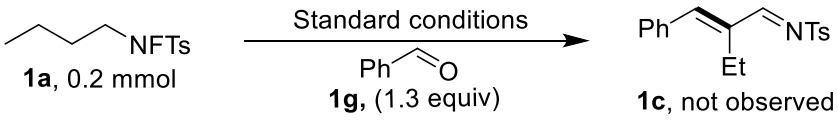


Fig. S20

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 0.2 mmol, 1.0 equiv), benzaldehyde (**1b**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for

24 h. The reaction was monitored by TLC and GC-Ms. No desired products were detected.

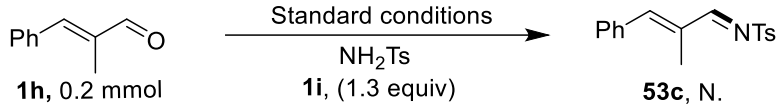
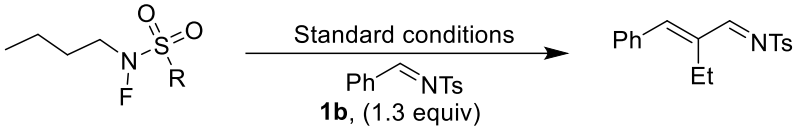


Fig. S21

A 10.0 mL Schlenk tube with a stirring bar was added with *(E)*-2-methyl-3-phenylacrylaldehyde (**1a**, 0.2 mmol, 1.0 equiv), 4-methylbenzenesulfonamide (**1i**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. The product **53c** was not detected by TLC and GC-Ms.



30a, R = C_6H_5 — **1c**, 75%
31a, R = 4-$OCH_3C_6H_4$ — **1c**, 67%
32a, R = 4-FC_6H_4 — **1c**, 74%
33a, R = 4-$CF_3C_6H_4$ — **1c**, 72%
34a, R = 4-CNC_6H_4 — **1c**, 70%
35a, R = CH_2CH_3 — **1c**, 46%

Fig. S22

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-fluorosulfonamides (**30a-35a**, 0.2 mmol, 1.0 equiv), imine (**1b**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. The reaction was monitored by TLC, NMR^H and GC-Ms. The residue was isolated by flash column chromatography on silica gel (PE: EtOAc =20:1).

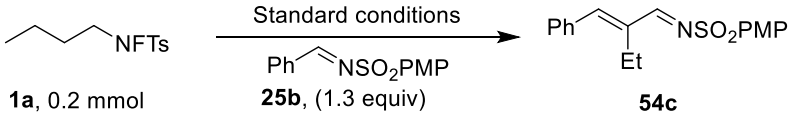
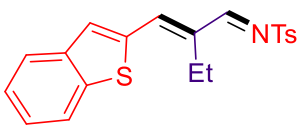


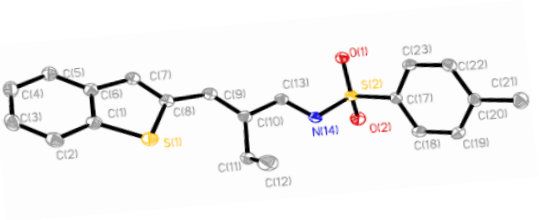
Fig. S23

A 10.0 mL Schlenk tube with a stirring bar was added with *N*-butyl-*N*-fluoro-4-methylbenzenesulfonamide (**1a**, 0.2 mmol, 1.0 equiv), imine (**25b**, 0.26 mmol, 1.3 equiv), DABCO (0.2 mol, 1.0 equiv), 4Å molecular sieve (150 mg) and DMF (1.0 mL) under argon. The resulting mixture was stirred at room temperature under Ar for 24 h. The reaction was monitored by TLC, NMR and GC-Ms. The residue was purified by flash column chromatography on silica gel (PE:EA = 20:1) to afford 46.8 mg (71%) of **54c** as a white solid: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.62 (s, 1H), 7.91 (d, *J* = 8.9 Hz, 2H), 7.49 – 7.38 (m, 5H), 7.22 (s, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 3.88 (s, 3H), 2.65 (q, *J* = 7.5 Hz, 2H), 1.13 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.7, 163.4, 150.6, 140.9, 134.9, 130.1, 130.0, 129.87, 129.85, 128.8, 114.3, 55.6, 19.5, 12.8; **IR (film)**: 3246, 2962, 2927, 2831, 1672, 1601, 1556, 1507, 1462, 1406, 1302, 1249, 1203, 1171, 1151, 1115, 1078, 1021, 871, 830, 784, 753, 716, 703, 681, 578, 577 cm^{-1}; **HRMS m/z (ESI)**: calcd for $C_{18}H_{20}NO_3S$ $[M+H]^+$: 330.1158, found 330.1158.

6. Crystallographic Data



46c



46c, X-ray crystallographic

S(1)–C(8)	1.748(3)	C(2)–C(3)–C(4)	121.4(3)
S(2)–O(1)	1.4347(18)	C(2)–C(3)–H(3)	119.300
S(2)–O(2)	1.4357(19)	C(4)–C(3)–H(3)	C119.300
S(2)–N(14)	1.651(2)	C(5)–C(4)–C(3)	121.0(3)
S(2)–C(17)	1.757(3)	C(5)–C(4)–H(4)	119.500
N(14)–C(13)	1.278(3)	C(3)–C(4)–H(4)	119.500
N(14)–H(14)	0.880	C(4)–C(5)–C(6)	119.2(3)
S(1)–C(1)	1.736(3)	C(4)–C(5)–H(5)	120.400
C(1)–C(2)	1.390(4)	C(6)–C(5)–H(5)	120.400
C(1)–C(6)	1.405(4)	C(5)–C(6)–C(1)	118.9(3)
C(2)–C(3)	1.371(4)	C(5)–C(6)–C(7)	129.5(3)
C(2)–H(2)	0.950	C(1)–C(6)–C(7)	111.5(2)
C(3)–C(4)	1.386(4)	C(8)–C(7)–C(6)	114.2(2)
C(3)–H(3)	0.950	C(8)–C(7)–H(7)	122.900
C(4)–C(5)	1.368(4)	C(6)–C(7)–H(7)	122.900
C(4)–H(4)	0.950	C(7)–C(8)–C(9)	123.1(2)
C(5)–C(6)	1.398(4)	C(7)–C(8)–S(1)	111.2(2)
C(5)–H(5)	0.950	C(9)–C(8)–S(1)	125.69(19)
C(6)–C(7)	1.424(4)	C(10)–C(9)–C(8)	131.0(2)
C(7)–C(8)	1.361(4)	C(10)–C(9)–H(9)	114.500
C(7)–H(7)	0.950	C(8)–C(9)–H(9)	114.500
C(8)–C(9)	1.435(4)	C(9)–C(10)–C(13)	115.5(2)
C(9)–C(10)	1.356(3)	C(9)–C(10)–C(11)	125.7(2)
C(9)–H(9)	0.950	C(13)–C(10) –C(11)	118.8(2)
C(10)–C(13)	1.442(4)	C(10)–C(11)–C(12)	113.6(2)
C(10)–C(11)	1.501(4)	C(10)–C(11)–H(11A)	108.800
C(11)–C(12)	1.520(4)	C(12)–C(11)–H(11A)	108.800
C(11)–H(11A)	0.99	C(10)–C(11)–H(11B)	108.800
C(11)–H(11B)	0.99	C(12)–C(11)–H(11B)	108.800
C(12)–H(12A)	0.980	H(11A)–C(11)–H(11B)	107.700

C(12)–H(12B)	0.980	C(11)–C(12)–H(12A)	109.500
C(12)–H(12C)	0.980	C(11)–C(12)–H(12B)	109.500
C(13)–H(13)	0.950	H(12A)–C(12)–H(12B)	109.500
C(17)–C(23)	1.382(3)	C(11)–C(12)–H(12C)	109.500
C(17)–C(18)	1.386(4)	H(12A)–C(12)–H(12C)	109.500
C(18)–C(19)	1.382(4)	H(12B)–C(12)–H(12C)	109.500
C(18)–H(18)	0.950	N(14)–C(13)–C(10)	122.3(2)
C(19)–C(20)	1.390(4)	N(14)–C(13)–H(13)	118.900
C(19)–H(19)	0.950	C(10)–C(13)–H(13)	118.900
C(20)–C(22)	1.390(4)	C(23)–C(17)–C(18)	120.6(2)
C(20)–C(21)	1.502(4)	C(23)–C(17)–S(2)	119.47(19)
C(21)–H(21A)	0.98	C(18)–C(17)–S(2)	119.85(19)
C(21)–H(21B)	0.980	C(19)–C(18)–C(17)	119.1(2)
C(21)–H(21C)	0.980	C(19)–C(18)–H(18)	120.400
C(22)–C(23)	1.378(4)	C(17)–C(18)–H(18)	120.400
C(22)–H(22)	0.950	C(18)–C(19)–C(20)	121.3(2)
C(23)–H(23)	0.950	C(18)–C(19)–H(19)	119.400
C(1)–S(1)–C(8)	91.68(13)	C(20)–C(19)–H(19)	119.400
O(1)–S(2)–O(2)	117.98(12)	C(19)–C(20)–C(22)	118.3(2)
O(1)–S(2)–N(14)	112.13(11)	C(19)–C(20)–C(21)	121.5(2)
O(2)–S(2)–N(14)	106.31(11)	C(22)–C(20)–C(21)	120.2(2)
O(1)–S(2)–C(17)	108.61(11)	C(20)–C(21)–H(21A)	109.500
O(2)–S(2)–C(17)	108.65(12)	C(20)–C(21)–H(21B)	109.500
N(14)–S(2)–C(17)	101.93(12)	H(21A)–C(21)–H(21B)	109.500
C(13)–N(14)–S(2)	117.57(19)	C(20)–C(21)–H(21C)	109.500
C(13)–N(14)–H(14)	121.200	H(21A)–C(21)–H(21C)	109.500
S(2)–N(14)–H(14)	121.200	H(21B)–C(21)–H(21C)	109.500
C(2)–C(1)–C(6)	121.4(3)	C(23)–C(22)–C(20)	121.1(2)
C(2)–C(1)–S(1)	127.3(2)	C(23)–C(22)–H(22)	119.400
C(6)–C(1)–S(1)	111.3(2)	C(20)–C(22)–H(22)	119.400
C(3)–C(2)–C(1)	118.0(3)	C(22)–C(23)–C(17)	119.5(2)
C(3)–C(2)–H(2)	121.000	C(22)–C(23)–H(23)	120.200
C(1)–C(2)–H(2)	121.000	C(17)–C(23)–H(23)	120.200

7. Computational details

All the calculations were performed with the Gaussian 09 package.[8] Geometry optimization was performed with the B3LYP-D3[9]-[11] functional and 6-31+G(d) basis set in dimethylformamide (DMF) solvent (using the SMD[12]-[14] solvent model). Frequency analysis was carried out at the same level to verify the stationary points as an intermediate or transition state and to obtain the thermodynamic energy corrections. Intrinsic reaction coordinates (IRC)[15] were calculated to confirm the connection between the transition state and the correct reactant/product. Single-point calculations were carried out with the M11[16] functional and 6-311+G(d,p) basis set in DMF solvent (using the SMD solvent model). All of the three-dimensional molecular diagrams of the molecules were generated with CYLview.[17]

Absolute calculated electronic energies, correction of enthalpies, and free energies.

Geometry	$E_{(elec\text{-}B3\text{-}D3)}$[1]	$G_{(corr\text{-}B3\text{-}D3)}$[2]	$H_{(corr\text{-}B3\text{-}D3)}$[3]	$E_{(M11)}$[4]	IF[5]
DABCO	-345.381118	0.154167	0.191669	-345.228342	
$HDABCO^+$	-345.855115	0.1695	0.207542	-345.700586	
HF	-100.452028	-0.007807	0.011955	-100.469847	
DABCOHF	-445.876305	0.166322	0.207334	-445.734095	
H_2F_2	-200.907328	-0.003268	0.02394	-200.942145	
FHF^-	-200.487309	-0.011906	0.012913	-200.516749	
NH_2Ts	-875.563563	0.116967	0.166567	-875.398338	
1a	-1132.006975	0.211605	0.27729	-1131.749201	
1b	-1144.747284	0.192982	0.258169	-1144.431014	
1c	-1300.805644	0.278376	0.354128	-1300.396708	
55-ts	-1477.379677	0.381443	0.466671	-1476.956772	-567.34
1d	-1031.617622	0.198945	0.261474	-1031.353167	
56-ts	-1031.353167	0.368604	0.450538	-1376.568171	-1512.27
57	-1377.009809	0.375788	0.45716	-1376.596713	
58-ts	-2622.241036	0.611515	0.731671	-2621.513447	-252.13
59	-2622.274916	0.617459	0.736988	-2621.560928	
60-ts	-2622.247339	0.613998	0.731956	-2621.536214	-252.58
61	-2622.250234	0.61634	0.734586	-2621.542102	
62	-2176.38092	0.425704	0.524233	-2175.813961	
63	-2377.313774	0.446116	0.553479	-2376.767714	
64-ts	-2377.289961	0.43878	0.550209	-2376.740052	-99.67
65	-1301.214433	0.293212	0.366423	-1300.804789	
66-ts	-1646.594956	0.462998	0.555779	-1646.026217	-984.33
67	-1646.643336	0.472435	0.562123	-1646.082153	
68-ts	-1646.61981	0.468016	0.560934	-1646.044223	-166.72
69-ts	-1477.375517	0.381901	0.466572	-1476.950769	-454.34
70-ts	-1131.9457	0.204393	0.270551	-1131.67718	-1298.29
71-ts	-1376.984534	0.36855	0.450394	-1376.5645	-1548.13
72	-1377.011054	0.375054	0.455728	-1376.595744	
73-ts	-2622.234276	0.608377	0.729969	-2621.507895	-212.81
74	-2622.275641	0.61553	0.736182	-2621.556168	
75-ts	-2622.247708	0.610262	0.732509	-2621.527381	-236
76	-2622.252005	0.609291	0.732865	-2621.538506	
77	-2176.387415	0.422846	0.524545	-2175.817653	
78	-2377.321637	0.442591	0.552962	-2376.774329	

79-ts	-2377.295976	0.441958	0.550717	-2376.744497	-115.67
80-ts	-2176.308602	0.417425	0.515829	-2175.734843	-1183.3
81	-1300.7727	0.27972	0.353024	-1300.373176	
82-ts	-1300.7454	0.276285	0.351036	-1300.329581	-198.97
83-ts	-2276.793852	0.423628	0.531857	-2276.233443	-1074.89
84	-2522.253655	0.617341	0.735039	-2521.519211	
85-ts	-2522.195423	0.611837	0.729396	-2521.458993	-127.77
86-ts	-1301.195679	0.290764	0.364872	-1300.774235	-257.24
87	-1301.207262	0.289528	0.365933	-1300.785747	
88-ts	-1501.692316	0.291515	0.378119	-1501.302089	-164.05
quinuclidine	-329.359633	0.164494	0.202925	-329.194799	
TS- quinuclidine	-1461.359226	0.395325	0.477054	-1460.92491	-565.61
$C_7H_{13}NHF$	-429.857209	0.17782	0.219245	-429.70279	

1. The electronic energy calculated by B3-D3/6-31+g(d) in DMF. 2. The thermal correction to Gibbs free energy calculated by B3-D3/6-31+g(d) in DMF. 3. The thermal correction to enthalpy calculated by B3-D3/6-31+g(d) in DMF. 4. The electronic energy calculated by M11/6-311+G(d,p) in DMF. 5.The B3-D3 calculated imaginary frequencies for the transition states.

The diastereoselectivity for the ring-closure process.

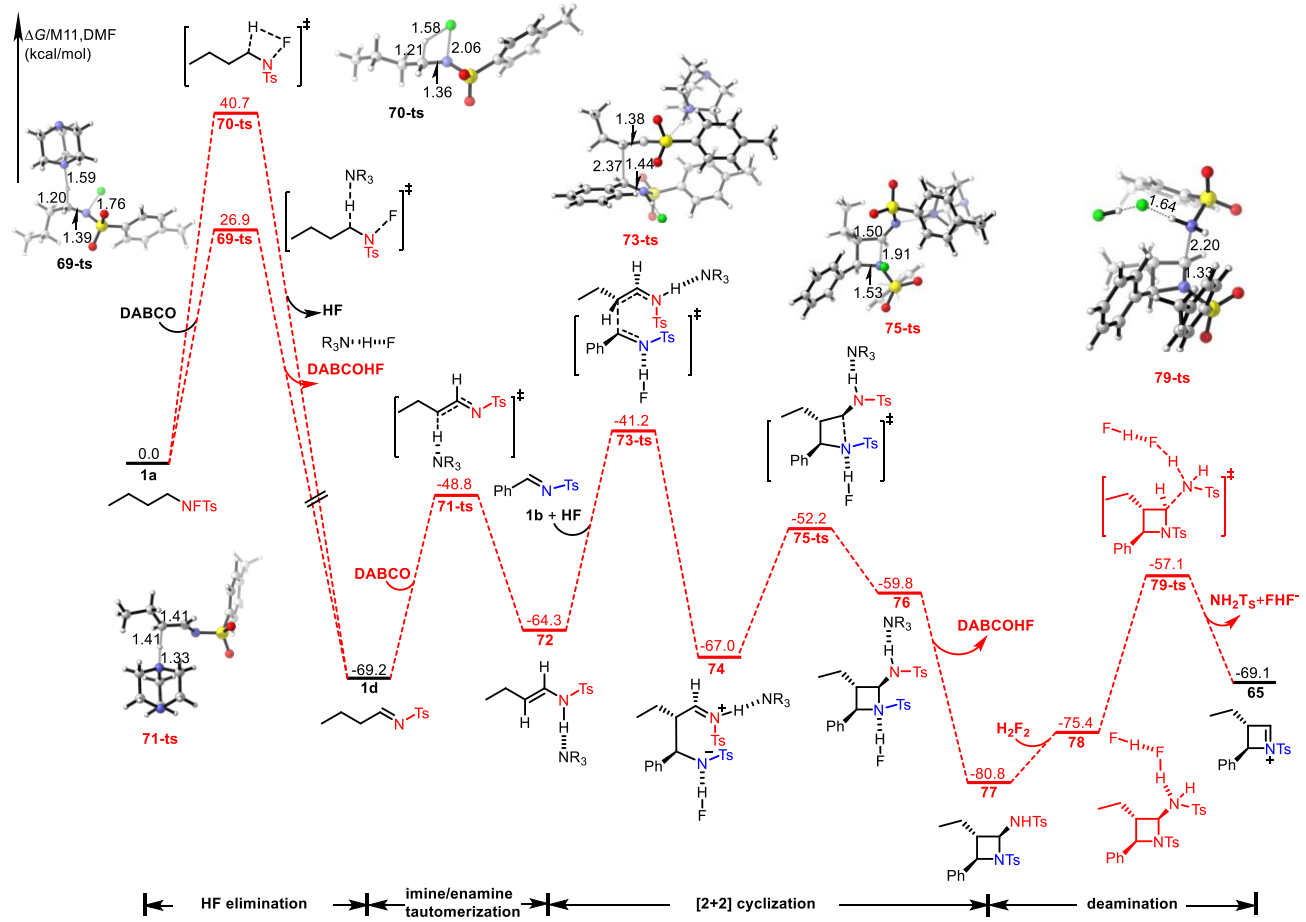


Fig. S24 Energy profiles for the unfavored paths for HF elimination, imine/enamine tautomerization, [2+2] cyclization and deamination steps calculated by the M11/(6-311+G(d,p), SMD)//B3LYP-D3/(6-31+G(d), SMD) level of theory. The energies are in kcal/mol and represent the relative free energies calculated with the DFT/M11 method in DMF. The bond distances are in angstrom.

Two possible pathways for HF elimination were considered by calculations and the results are shown in Figure S24. HF direct elimination in the absence of base was considered at the beginning and the relative energy of corresponding transition state **70-ts** was calculated to be higher than that of **55-ts** by 17.8 kcal/mol. Another *cis* base-assisted HF elimination transition state **69-ts** was also calculated and 4.0 kcal/mol higher than that of **55-ts**. Therefore, the favored path for HF elimination is through transition state **55-ts**.

The diastereoselectivity arises from the imine/enamine tautomerization step. As shown in Figure S24, the (*Z*)-enamine **72** can be generated via transition state **71-ts** with an energy barrier of 20.4 kcal/mol in the presence of DABCO to afford a hydrogen bond, which is higher that of **56-ts** by 2.3 kcal/mol.

In the subsequent intermolecular nucleophilic attack process, (*Z*)-enamine **72** plays as a nucleophile and reacts with imine **1b** via transition state **73-ts** to form zwitterionic intermediate **74** followed by intramolecular nucleophilic addition via transition state **75-ts** to achieve the stepwise [2+2] cycloaddition. After release of DABCO and HF, an azetidine intermediate **77** is generated reversibly. The relative free energies of transition states **73-ts** and **75-ts** are calculated to be -41.2 and -52.2

kcal/mol respectively, which are higher than those of **58-ts** and **60-ts**.

Followed, Brønsted acid assisted deamination can occur via transition state **79-ts** with an energy barrier of 23.7 kcal/mol in the presence of HF and generates iminium intermediate **65**. So, we can exclude this path based on above calculation results.

The other paths for the deamination step.

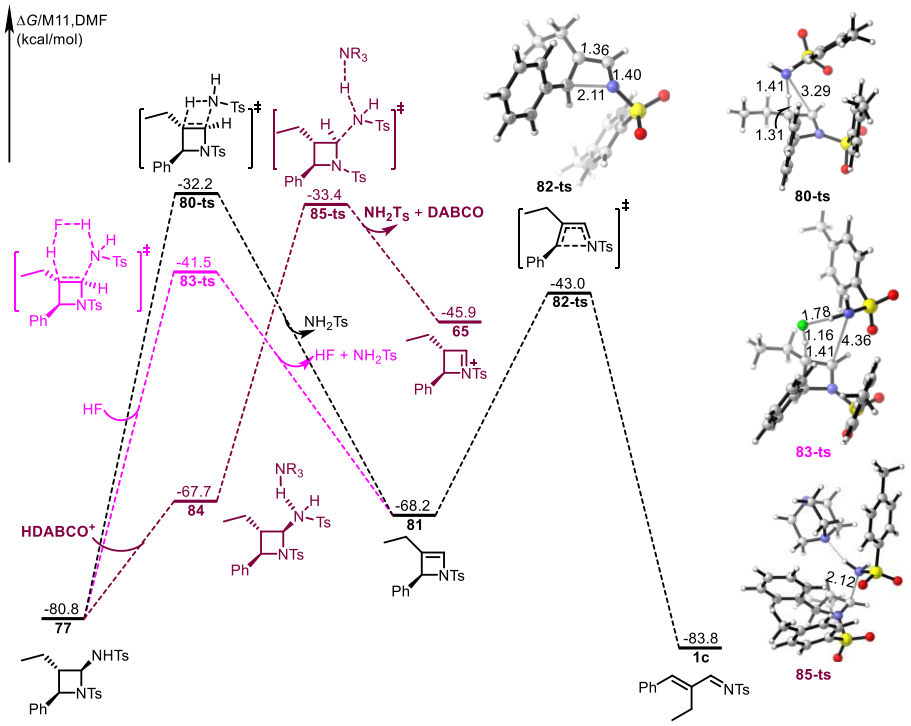


Fig. S25 Energy profiles for the unfavored paths of NH_2TS elimination step calculated by the M11/(6-311+G(d,p), SMD)//B3LYP-D3/(6-31+G(d), SMD) level of theory. The energies are in kcal/mol and represent the relative free energies calculated with the DFT/M11 method in DMF. The bond distances are in angstrom.

In *N*-((*2S,3S,4R*)-3-ethyl-4-phenyl-1-tosylazetidin-2-yl)-4-methylbenzenesulfonamide **77**, proton neighboring to NHTs group locates conductively to afford deamination transition state **80-ts** and finish NH_2Ts elimination process followed by ring-opening via **82-ts** (black lines in Figure S25). The high relative free energies of **80-ts** and **82-ts** made this path excluded. When we used HF as proton-shuttle to assist NH_2T_S elimination, the barrier was decreased compared with the one-step NH_2T_S elimination path. However, the relative free energy of **83-ts** is still higher than that of **64-ts** by 14.8 kcal/mol. It concludes that the one-step NH_2T_S elimination paths are unfavored and can be ruled out. The plausible path for NH_2T_S elimination goes through Brønsted acid assisted deamination.

As $DABCOH^+$ can be used as acid to prompt NH_2T_S elimination, the path through transition state **85-ts** was also considered (Figure S25, brown path). The barrier was calculated to be 47.4 kcal/mol, so this path was also ruled out.

Another path for the ring-opening step.

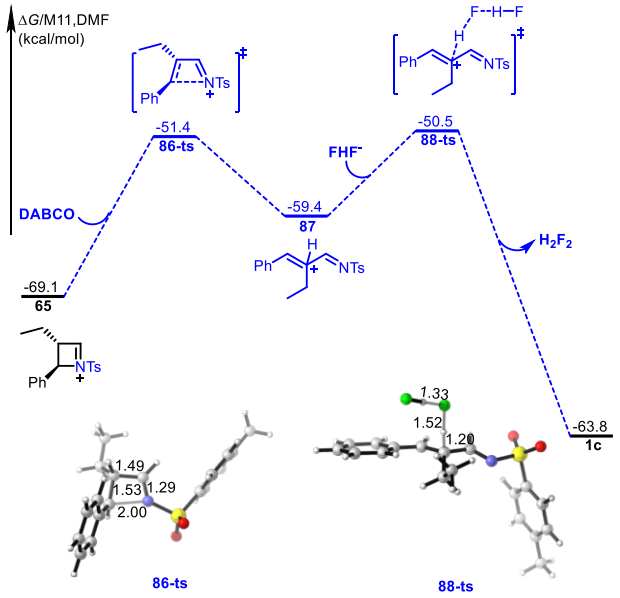


Fig. S26 Energy profile for the ring-opening step without DABCO calculated by the M11/(6-311+G(d,p), SMD)//B3LYP-D3/(6-31+G(d), SMD) level of theory. The energies are in kcal/mol and represent the relative free energies calculated with the DFT/M11 method in DMF. The bond distances are in angstrom.

For the ring-opening step, the iminium intermediate **65** can be deprotonated by FHF^-. As shown in Figure S26, this alternative path goes through ring-opening via transition state **86-ts** followed by deprotonation via **88-ts** to achieve product **1c**. The calculated barrier for ring-opening is 17.7 kcal/mol and 18.6 kcal/mol for deprotonation, which is a bit higher than the path with DABCO via transition states **66-ts** and **68-ts** by 4.4 kcal/mol. Therefore, we can preclude this path.

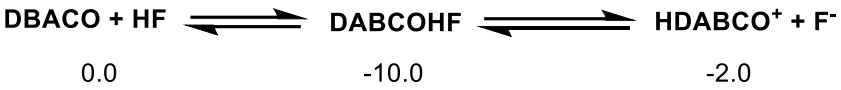


Fig. S27 The relative Gibbs free energies of species (kcal/mol).

According to the doubt of the removed species in the first step, we calculated the relative Gibbs free energies of DABCO, HF, protonated $HDABCO^+$, F^- and hydrogen bonded DABCOHF at the M11/6-311+G(d,p)/SMD//B3LYP-D3/6-31+G(d)/SMD level of theory. As shown in Figure S27, the compound DABCOHF is more stable than separated DABCO and HF or protonated $HDABCO^+$. There is strong hydrogen bond between DABCO and HF, which makes energies drop by 10.0 kcal/mol. The energies of protonated $HDABCO^+$ and F^- are also higher than DABCOHF by 8.0 kcal/mol. So, the fluoride is not removed as a fluoride anion in this reaction. The removed species in the first step and the cyclization step is hydrogen bonded compound DABCOHF.

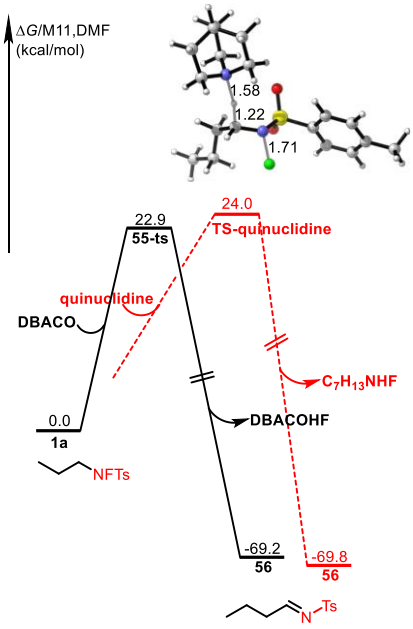


Fig. S28 Energy profiles for the HF elimination step with DBACO or quinuclidine as base at the M11/6-311+G(d,p)/SMD//B3LYP-D3/6-31+G(d)/SMD level of theory.

In order to see whether quinuclidine offers a similar energetics as DBACO in the first step, we calculated the first step with quinuclidine as base and the results are shown in figure S28. As you proposed, the barrier is 24.0 kcal/mol, which is only 1.1 kcal/mol higher that of DBACO path with transition state **55-ts**. The relative energy of generated (*E*)-imine **1d** is also similar.

Optimized geometries for all the intermediates and transition states calculated by B3-D3/6-31+g(d) in DMF.

DABCO

C	0.78051600	-0.38225900	-1.33238100
C	-0.78007600	-0.38229300	-1.33262600
H	1.17779400	0.33009800	-2.06434700
H	1.17745600	-1.37461100	-1.57488300
H	-1.17716200	0.32981800	-2.06493500
H	-1.17689000	-1.37474000	-1.57494300
C	0.78037300	1.34526300	0.33547800
H	1.17710200	1.62265100	1.31874400
H	1.17777600	2.05163200	-0.40226100
C	-0.78018400	1.34550000	0.33496600
H	-1.17747800	1.62328600	1.31789100
H	-1.17688800	2.05178500	-0.40323100
C	-0.78052000	-0.96298500	0.99716200
H	-1.17732600	-0.67682500	1.97785300
H	-1.17771000	-1.95303100	0.74584800
C	0.77989200	-0.96333000	0.99731600
H	1.17663300	-0.67764400	1.97817200
H	1.17668800	-1.95347700	0.74578100
N	-1.28891400	0.00027300	-0.00019600
N	1.28891500	-0.00003300	0.00031500

$HDABCO^+$

H	2.24372400	-0.00169600	-0.00203600
C	0.73593500	-0.87846300	-1.12822100
C	-0.81461400	-0.90428900	-1.05159100
H	1.11051400	-0.43661100	-2.05293100
H	1.18822800	-1.86071300	-0.98265100
H	-1.24264700	-0.59224200	-2.00761100
H	-1.16695800	-1.91423700	-0.82667000
C	0.73852800	1.41523500	-0.19689500
H	1.11460000	1.99390100	0.64841800
H	1.19112400	1.78053100	-1.12005400
C	-0.81224400	1.36451000	-0.25681800
H	-1.23845100	2.03733000	0.49168400
H	-1.16460700	1.67518600	-1.24378400
C	-0.81233000	-0.45829500	1.31023500
H	-1.16336700	0.24144200	2.07297400
H	-1.24005400	-1.44237200	1.51829700
C	0.73813600	-0.53818200	1.32340500
H	1.19223400	0.07739100	2.10141600
H	1.11198400	-1.56028600	1.40208500
N	-1.30224900	0.00089800	0.00102900
N	1.21985100	-0.00100000	-0.00100500

HF

F	0.00000000	0.00000000	0.09474100
H	0.00000000	0.00000000	-0.85267000

DABCOHF

H	-1.85562300	0.00449700	0.00518100
F	-3.27783800	-0.00018000	0.00010200
C	-0.27200900	0.51826800	-1.31640000
C	1.28140600	0.50284000	-1.29345100
H	-0.68845400	-0.13112900	-2.08919600
H	-0.68167500	1.52318700	-1.43840600
H	1.66958700	-0.14071000	-2.08785600
H	1.67605500	1.51159300	-1.44392700
C	-0.27234000	-1.39902800	0.21332900
H	-0.68458800	-1.74256000	1.16454800
H	-0.68662200	-2.00656800	-0.59436100
C	1.28126500	-1.37260700	0.20728400
H	1.67367700	-1.73911900	1.15997800
H	1.67150500	-2.00778500	-0.59293700
C	1.28829800	0.86470200	1.08080300
H	1.68245200	0.48925800	2.02936600
H	1.68119000	1.87235800	0.91927600
C	-0.26516400	0.88542400	1.10784700
H	-0.67572100	0.49348800	2.04091400
H	-0.67595300	1.88140600	0.92950100
N	1.77946800	-0.00279600	-0.00304100
N	-0.75861300	0.00224000	0.00311700

H_2F_2

F	0.00000000	0.00000000	-1.29066500
H	0.00000000	0.00000000	0.53179100
H	0.00000000	0.00000000	-2.23934900
F	0.00000000	0.00000000	1.48039400

FHF^-

F	0.00000000	0.00000000	1.15054400
H	0.00000000	0.00000000	-0.00018300
F	0.00000000	0.00000000	-1.15052400

NH_2Ts

S	-1.89835800	0.05511700	-0.11869800
O	-2.33909500	1.46022300	-0.22784500
O	-2.38452100	-0.91164200	-1.12130000
C	-0.11632100	0.03488000	-0.05671100
C	0.58452400	1.23867800	0.00095600
C	1.98111400	1.20561800	0.03666400
C	2.67819300	-0.00982600	0.01457200
C	1.94138900	-1.20754200	-0.04400000
C	0.55085200	-1.19574600	-0.08084600
H	0.05272600	2.18376100	0.01695100
H	2.53386100	2.14019800	0.08181800
H	2.46758500	-2.15871100	-0.06139000
H	-0.00610100	-2.12632100	-0.12365800
C	4.18378100	-0.04614500	0.04592000
H	4.58237200	-0.47431200	-0.88291500
H	4.60469000	0.95681600	0.16711000
H	4.54397000	-0.67427000	0.87000500

N	-2.28907900	-0.62356000	1.37524200
H	-2.14686800	0.05134400	2.13049900
H	-3.26720700	-0.92360500	1.36788100

1a

S	0.00134000	1.28655200	0.19686500
O	-0.26529500	1.76772000	1.56065600
O	-0.13157400	2.20232200	-0.94533100
C	1.55786400	0.44393000	0.11881400
C	1.98445600	-0.28858300	1.23300600
C	2.32080400	0.52031700	-1.04713100
C	3.20459600	-0.95293000	1.16508400
H	1.37735000	-0.33819600	2.13097200
C	3.54319600	-0.15096300	-1.09038400
H	1.97044500	1.09026100	-1.90070800
C	4.00194600	-0.89446300	0.00709800
H	3.54798600	-1.52464400	2.02339600
H	4.14721300	-0.09616600	-1.99176100
C	5.32240300	-1.61632500	-0.03940800
H	5.80264600	-1.51028500	-1.01693300
H	6.00629300	-1.22369300	0.72387700
H	5.19007500	-2.68566900	0.16700500
N	-1.12059000	-0.08115600	0.05718100
C	-2.53066100	0.34484700	-0.00236900
H	-2.67944500	0.93961200	0.90584700
C	-3.45815600	-0.86857300	0.00239500
C	-4.93054500	-0.44350500	0.03553800
H	-3.22760400	-1.48994800	0.87738300
H	-3.27138700	-1.47685500	-0.89076900
C	-5.88015300	-1.64407600	0.03226900
H	-5.11183500	0.16836400	0.93027300
H	-5.14398000	0.19708500	-0.83144400
H	-6.92817900	-1.32080200	0.05833200
H	-5.73949300	-2.25524300	-0.86880700
H	-5.70522700	-2.28775400	0.90422400
H	-2.70418700	0.98541400	-0.87558300
F	-0.81639300	-0.62740100	-1.25638600

1b

S	-0.64589300	1.72538700	-0.16146800
O	-0.87982400	2.55401500	-1.35794100
O	-0.48521300	2.39756700	1.14573300
C	-1.93396400	0.50300700	-0.02839700
C	-2.51112200	-0.00855600	-1.19574300
C	-2.32326300	0.05227800	1.23366000
C	-3.49651300	-0.98604900	-1.08518700
H	-2.19859100	0.35304400	-2.16991700
C	-3.31482900	-0.92614100	1.32256000
H	-1.86602100	0.45918600	2.12930600
C	-3.91410900	-1.45906900	0.17165000
H	-3.95224600	-1.38792900	-1.98669400
H	-3.62759300	-1.27846600	2.30190400
C	-4.98850000	-2.51045500	0.26892500
H	-5.15409900	-2.81831500	1.30596000
H	-5.93860800	-2.13419700	-0.13171500
H	-4.72197400	-3.39886600	-0.31684600
N	0.69642300	0.74148800	-0.54186300
C	1.64221200	0.69861700	0.33498600
H	1.57187500	1.26006000	1.27196400
C	2.85141200	-0.09212000	0.13904600
C	3.82589700	-0.07796200	1.15306000
C	3.06427800	-0.85845300	-1.02358700
C	4.99868400	-0.82006800	1.00987700
H	3.65641400	0.51634300	2.04732200
C	4.23535300	-1.59678400	-1.16206200
H	2.31064600	-0.86609300	-1.80490500
C	5.20344000	-1.57865400	-0.14678500
H	5.74911800	-0.80675200	1.79517200
H	4.40047100	-2.18784500	-2.05851500
H	6.11636400	-2.15698300	-0.26086100

1c

S	-2.00136300	-1.49822600	-0.82074600
O	-2.47570600	-2.80355400	-0.32416700
O	-1.73744800	-1.34847700	-2.26934100
C	-3.14815600	-0.23136400	-0.31388500
C	-3.94954600	-0.44353200	0.81196200
C	-4.81971700	0.56562900	1.21847600
C	-4.89995100	1.78193800	0.51860000
C	-4.07936300	1.96537900	-0.60510700
C	-3.20146800	0.96683700	-1.02848100
H	-3.89620800	-1.38055000	1.35621400
H	-5.44862700	0.40752100	2.09106300
H	-4.12939800	2.89951700	-1.15831400
H	-2.57210300	1.11798300	-1.89944600
C	-5.86006200	2.85395700	0.96408100
H	-5.69829500	3.78811000	0.41730200
H	-6.89831900	2.53846100	0.79643200
H	-5.75450300	3.05669400	2.03658700
N	-0.64141100	-1.10705600	0.12074900
C	0.42008900	-0.73228600	-0.52283000
H	0.42217500	-0.67387900	-1.61533500
C	1.64743200	-0.37734000	0.16672500
C	2.67638500	-0.00991000	-0.65208400
H	2.44861900	0.02183600	-1.71743000
C	1.65677400	-0.43124700	1.67419000
C	1.88969800	-1.84876400	2.22441600
H	0.68496300	-0.07303700	2.03334900
H	2.41275100	0.25423600	2.06736500
H	1.88793200	-1.83605900	3.32100100
H	1.10005800	-2.53112200	1.89077300
H	2.85059500	-2.25632900	1.88948300
C	4.04327400	0.40170500	-0.34255700

C	4.71428000	1.17851900	-1.31322800
C	4.74346200	0.05503400	0.83282500
C	6.01564300	1.62979000	-1.10221000
H	4.19597000	1.43307700	-2.23451100
C	6.05102400	0.49644300	1.03530800
H	4.28787200	-0.58926900	1.57332900
C	6.68892400	1.29231200	0.07721400
H	6.50709400	2.23598400	-1.85842900
H	6.57701500	0.21077500	1.94237500
H	7.70698000	1.63471500	0.24246600

55-ts

S	-1.11711700	0.56374500	-0.75553800
O	-0.19614800	-0.38798800	-1.40826300
O	-1.41810600	1.83279600	-1.43410400
C	-2.63517800	-0.27025800	-0.35330800
C	-2.57599000	-1.58214300	0.12848100
C	-3.85104800	0.38044200	-0.55355900
C	-3.76596900	-2.24323700	0.41730200
H	-1.62067700	-2.07535800	0.27654300
C	-5.03385500	-0.30310800	-0.26436400
H	-3.87495000	1.39903600	-0.92490400
C	-5.01106300	-1.61689900	0.22499700
H	-3.73179500	-3.26235400	0.79421100
H	-5.98722200	0.19485900	-0.41978800
C	-6.28687900	-2.35180900	0.54350600
H	-7.16651300	-1.74139900	0.31727200
H	-6.35614100	-3.28309900	-0.03243200
H	-6.32377000	-2.62663300	1.60534100
N	-0.42033500	0.73447000	0.83644300
C	0.83386400	1.31873100	0.93078100
H	1.55489900	0.40844500	0.55947400
F	-1.62031500	1.79756800	1.47422800
C	2.16375400	-1.95727000	0.44912900
C	3.29583900	-3.00240100	0.20033100
H	1.78784500	-2.00158500	1.47621900
H	1.32307300	-2.09263100	-0.23476300
H	3.49246000	-3.58796900	1.10424500
H	3.01603900	-3.69282100	-0.60187200
C	3.82750200	-0.35447600	1.15884800
H	4.18309400	0.66710900	0.99430600
H	3.43622800	-0.42616100	2.17830100
C	4.94856200	-1.40720100	0.89300000
H	5.88115700	-0.91605600	0.59716500
H	5.14438500	-2.00242400	1.79076400
C	4.30251800	-1.53795800	-1.41463500
H	5.24169600	-1.05510500	-1.70357900
H	4.01325900	-2.22954600	-2.21262400
C	3.18470800	-0.47636500	-1.16771600
H	3.55803900	0.54296600	-1.30336900
H	2.32626000	-0.62312600	-1.82693900
N	4.54536400	-2.32315000	-0.18967800
N	2.70973500	-0.60260500	0.22535100
C	1.26947100	2.55730200	0.15064300
C	0.60007100	3.87027500	0.57872100
H	1.12210600	2.40045800	-0.92404500
H	2.35430900	2.64249200	0.30312100
C	1.19505900	5.07728300	-0.15099500
H	-0.47455700	3.80606200	0.38048200
H	0.71614400	3.99828400	1.66407600
H	0.70597100	6.00982200	0.15806400
H	2.26912200	5.17765300	0.05524600
H	1.07209500	4.98011500	-1.23806200
H	1.09664100	1.36604200	1.99524700

1d

S	-0.12968500	-1.71355600	0.12312600
O	0.14869600	-2.83900000	-0.78679800
O	-0.45934700	-2.00367500	1.53484400
C	1.22548900	-0.55959100	0.06991900
C	1.99173200	-0.46031400	-1.09592500
C	1.47881300	0.24888300	1.17909600
C	3.03157000	0.46504800	-1.13916200
H	1.78215800	-1.09697500	-1.94911600
C	2.52636900	1.16886800	1.11557500
H	0.87480900	0.16020000	2.07597000
C	3.31565600	1.29164800	-0.03781100
H	3.63537500	0.54631600	-2.03959300
H	2.73449100	1.79814400	1.97673400
C	4.44733200	2.28360400	-0.10397900
H	4.53906800	2.84741500	0.82943800
H	5.40128300	1.77568200	-0.29407200
H	4.29436600	2.99730000	-0.92336300
N	-1.36648300	-0.79800500	-0.65032600
C	-2.37118100	-0.46987500	0.07767400
H	-2.42330500	-0.75096100	1.13554500
C	-3.49521800	0.33882800	-0.47157200
C	-3.59055200	1.70493600	0.24063600
H	-4.42702000	-0.21814900	-0.29620400
H	-3.36887900	0.47244600	-1.55109600
C	-4.78031400	2.52276300	-0.26482700
H	-3.67976500	1.54476200	1.32303900
H	-2.65755600	2.25886000	0.07522300
H	-4.83169400	3.49237400	0.24523100
H	-4.70014700	2.71276200	-1.34273800
H	-5.72581600	1.99535900	-0.08484700

56-ts

S	-1.58862800	-1.25830500	0.12377000
O	-1.47805600	-2.07860300	1.35103700
O	-1.30239100	-1.92595700	-1.17317400
C	-3.26524000	-0.62759700	0.04368700
C	-4.05362100	-0.59833600	1.19329900

C	-3.74894400	-0.13274000	-1.17223300
C	-5.34455000	-0.06714000	1.12063700
H	-3.66841700	-0.98791200	2.12977500
C	-5.03709600	0.39389800	-1.22717100
H	-3.12871600	-0.16183200	-2.06262300
C	-5.85530400	0.43620300	-0.08384100
H	-5.96267000	-0.04725000	2.01464200
H	-5.41728100	0.77578700	-2.17181100
C	-7.24605500	1.01217700	-0.16381100
H	-7.84952300	0.48071700	-0.91046900
H	-7.76089400	0.94834500	0.80013100
H	-7.21649300	2.06682000	-0.46623900
N	-0.68089000	0.11227800	0.35880700
C	0.01572200	0.55719100	-0.68010500
C	0.92970900	1.62978600	-0.59859600
C	0.88245700	2.59287600	0.58130100
H	1.14109100	2.08934000	-1.56988600
H	2.11223400	0.92281700	-0.40738300
C	1.93368700	3.70093900	0.46809500
H	-0.11693800	3.04857100	0.66338600
H	1.03374100	2.03700100	1.51638000
H	1.89106000	4.37943600	1.32930500
H	2.94741800	3.28489600	0.41736000
H	1.77603300	4.30022200	-0.43854300
C	3.66079000	0.32746900	1.23849700
C	4.95645400	-0.52129100	1.41562800
H	3.81853800	1.37804600	1.49375800
H	2.83022600	-0.05839400	1.83486100
H	5.77075000	0.09445700	1.80983600
H	4.78452000	-1.34904500	2.11047600
C	4.32220600	0.83857500	-1.04457500
H	3.97303200	0.79138100	-2.07995400
H	4.44332500	1.88800100	-0.76390800
C	5.62610000	0.01595200	-0.82557600
H	5.97702300	-0.41233700	-1.76955900
H	6.42031500	0.65029900	-0.42018700
C	4.31697100	-1.95105100	-0.40494300
H	4.64831100	-2.35752700	-1.36530300
H	4.17284100	-2.78439400	0.28946800
C	2.99621800	-1.14367000	-0.57328800
H	2.63807000	-1.14530100	-1.60674300
H	2.19727300	-1.51777200	0.07186300
N	5.38701600	-1.08613300	0.12366600
N	3.25393600	0.26691500	-0.18820300
H	-0.05070100	0.02411200	-1.63378800
57			
S	-1.02566500	-1.02701100	-0.78606000
O	-0.50399600	-2.14749400	0.03780200
O	-1.14717400	-1.27280500	-2.25219300
C	-2.69960100	-0.69130300	-0.21013200
C	-3.05515700	-1.00332100	1.10335400
C	-3.60758600	-0.04296500	-1.05404200
C	-4.33021000	-0.67195800	1.56814600
H	-2.34503500	-1.50469700	1.75331200
C	-4.87586100	0.28580700	-0.57496500
H	-3.32943300	0.19258300	-2.07611800
C	-5.25904100	-0.02291800	0.74099200
H	-4.60787100	-0.92408400	2.58884900
H	-5.58180600	0.78603400	-1.23440700
C	-6.63766000	0.33052600	1.23995900
H	-7.41114000	-0.19722400	0.66697600
H	-6.75909800	0.06667800	2.29560400
H	-6.83409500	1.40463400	1.13104900
N	-0.15026200	0.27721800	-0.41707100
C	-0.30953900	1.39327900	-1.24630400
C	0.01026500	2.65954800	-0.89796600
C	0.52914000	3.11610500	0.43844300
H	-0.11648600	3.42741100	-1.66174000
H	1.44603200	-0.15679600	0.02735900
C	1.85040400	3.89527300	0.33794000
H	-0.21638700	3.77155800	0.91711000
H	0.65226500	2.25326800	1.10205600
H	2.18868200	4.23098200	1.32694700
H	2.64515500	3.27977900	-0.10126900
H	1.73198800	4.78421700	-0.29538500
C	2.94538700	0.30542500	1.43795600
C	4.44027200	-0.06253300	1.64119100
H	2.79228800	1.37642100	1.30811000
H	2.30490900	-0.05388100	2.24578100
H	5.03779400	0.84439700	1.76823400
H	4.56505600	-0.68557700	2.53111800
C	3.22732700	0.18909100	-1.00482200
H	2.87029200	-0.35486100	-1.88151900
H	2.95093500	1.23939700	-1.10050900
C	4.74301300	-0.01658000	-0.74134200
H	5.20610300	-0.53881700	-1.58301900
H	5.24430000	0.94710000	-0.61530500
C	4.22921600	-2.08451300	0.36523800
H	4.59085600	-2.60299200	-0.52721500
H	4.46113400	-2.70019600	1.23879200
C	2.69888100	-1.84213800	0.27164300
H	2.24827600	-2.29263900	-0.61286200
H	2.15884600	-2.18526600	1.15464600
N	4.95691400	-0.80942100	0.48168900
N	2.48206400	-0.36038600	0.17659100
H	-0.69007500	1.21429700	-2.25469100
58-ts			
C	-1.88929000	-1.42570600	0.29198300
C	-0.36711100	-0.81047300	-1.91003400
C	-0.66273800	-2.10357000	-1.47343500

H	-1.48182900	-0.41944400	0.31650000
H	-1.17825200	-0.23287600	-2.35201300
H	-1.58533200	-2.51662900	-1.86999000
C	0.42567900	-3.08699800	-1.11960800
C	-0.02897400	-4.54274300	-1.25580600
H	0.78963900	-2.91352500	-0.09937200
H	1.29098600	-2.91122800	-1.77359100
H	0.77204600	-5.23365500	-0.96521100
H	-0.89723400	-4.74694700	-0.62027800
H	-0.31166100	-4.76895600	-2.29210800
N	-3.19171500	-1.56516400	-0.05909200
S	-3.94344400	-0.31730100	-0.86668300
O	-5.38771500	-0.50057200	-0.61394100
O	-3.51095500	-0.25320400	-2.28256600
C	-3.38765900	1.18149000	-0.06021000
C	-2.63150100	2.11137900	-0.77102500
C	-3.71472200	1.38896700	1.28546600
C	-2.21520200	3.27915700	-0.12658900
H	-2.35097500	1.92529000	-1.80092200
C	-3.28579500	2.55550800	1.91122900
H	-4.29018600	0.64955900	1.83426100
C	-2.53571900	3.52123500	1.21435000
H	-1.61504900	4.00120000	-0.67304400
H	-3.53374700	2.72227600	2.95677800
C	-2.08988700	4.78195100	1.90736200
H	-2.95406100	5.40876900	2.16456000
H	-1.56779200	4.55398600	2.84371600
H	-1.42030600	5.36987800	1.27321000
S	0.97745900	1.32606900	-2.31634200
O	-0.22682600	1.79805800	-3.04590100
O	2.26957700	1.43245000	-3.03293200
C	1.13271700	2.28042800	-0.80526300
C	0.77412100	1.73378200	0.42364800
C	1.60625500	3.59394300	-0.89302000
C	0.90137600	2.50327500	1.58148800
H	0.40680400	0.71891100	0.47935200
C	1.72040800	4.35216900	0.26979200
H	1.88671500	4.01850900	-1.85234500
C	1.37652700	3.81905900	1.52545100
H	0.61904800	2.07267700	2.53872100
H	2.08577100	5.37432500	0.20523400
C	1.52266100	4.65150600	2.77272900
H	1.11157100	4.13647000	3.64644800
H	2.57973200	4.86988300	2.97385300
H	1.00989300	5.61476000	2.66680500
N	0.83713700	-0.23650800	-1.77966800
C	-1.31188000	-2.31025800	1.31793900
C	-0.18399800	-1.85501800	2.02265700
C	-1.85011000	-3.56879900	1.64108700
C	0.39642200	-2.63370300	3.02439300
H	0.23698200	-0.88421300	1.78436300
C	-1.26818300	-4.34640700	2.64113500
H	-2.71777400	-3.94230800	1.10989200
C	-0.14293100	-3.88499800	3.33598500
H	1.26859700	-2.26388700	3.55683300
H	-1.69376500	-5.31759800	2.87958900
H	0.30644900	-4.49604100	4.11421900
H	2.43236300	-0.69883600	-0.90349600
C	3.12894600	-1.20901000	1.00370300
C	4.51691800	-1.45947700	1.65202100
H	2.59078800	-0.37606100	1.45741600
H	2.49422500	-2.09349900	1.01244400
H	4.66061800	-0.79306100	2.50675800
H	4.58989300	-2.49230600	2.00324800
C	4.16704300	0.42131100	-0.52220300
H	4.28059900	0.65280700	-1.58073900
H	3.57981100	1.20658700	-0.04669400
C	5.51737800	0.16667800	0.19897600
H	6.35098700	0.34552000	-0.48537400
H	5.62288400	0.83899800	1.05470800
C	5.45776400	-2.14120300	-0.45248300
H	6.26528800	-1.93951100	-1.16118400
H	5.56704300	-3.16567900	-0.08662500
C	4.07715100	-1.96399800	-1.14024700
H	4.15604700	-1.68041400	-2.19120700
H	3.44763900	-2.84948700	-1.05172900
N	5.60127900	-1.21940200	0.68625800
N	3.35889100	-0.84671900	-0.43633300
H	-3.79195700	-2.83729700	-0.40484000
F	-4.20916800	-3.75371200	-0.69600100

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C	1.87054900	-1.22057300	-0.27119600
C	0.74735600	-0.10090000	-2.13724200
C	2.09432800	-0.58239000	-1.67728100
H	1.55289800	-0.41339300	0.39233900
H	0.17156900	-0.74481500	-2.80619300
H	2.39909400	-1.37691000	-2.36637300
C	3.16970400	0.52881400	-1.64990500
C	4.56033500	0.03832700	-2.06042400
H	3.20953600	0.96883100	-0.64803700
H	2.86473500	1.33411500	-2.32687900
H	5.27779700	0.86792500	-2.03346700
H	4.93129600	-0.74897500	-1.39734200
H	4.54567200	-0.36056000	-3.08256400
N	0.74175700	-2.16005700	-0.40006600
S	-0.00074600	-2.67606900	0.97918200
O	0.28920500	-1.69250500	2.04800700
O	0.28785700	-4.09786700	1.27572500
C	-1.74629100	-2.56008900	0.59024100
C	-2.20249600	-2.18818800	-0.67231500

C	-2.64454100	-2.80514900	1.63505800
C	-3.57529100	-2.03806200	-0.88164100
H	-1.50120700	-1.99534900	-1.47446300
C	-4.00873000	-2.64201900	1.41106100
H	-2.28579800	-3.09784600	2.61741800
C	-4.49513600	-2.24125300	0.15448800
H	-3.93026600	-1.73066900	-1.86150200
H	-4.70731400	-2.81446700	2.22593300
C	-5.96510700	-1.98759400	-0.05094800
H	-6.23798100	-0.99739300	0.33891000
H	-6.23091000	-2.01009600	-1.11287800
H	-6.57736400	-2.72604300	0.47907300
S	-1.27686000	1.45626700	-2.33789100
O	-1.75713300	0.49429000	-3.35078200
O	-1.16081000	2.87142300	-2.73726100
C	-2.28257800	1.32137500	-0.87009500
C	-1.76914500	0.82985800	0.33055500
C	-3.62513500	1.69470100	-0.98752600
C	-2.61917500	0.71551700	1.42926800
H	-0.73246700	0.53054200	0.41408800
C	-4.46020500	1.55921200	0.11890500
H	-4.01874900	2.07627700	-1.92493500
C	-3.97400300	1.06253300	1.34011300
H	-2.22331800	0.32622900	2.36251700
H	-5.50705800	1.83746600	0.03153100
C	-4.89767400	0.85912800	2.51046500
H	-5.75697400	1.53634200	2.46580700
H	-5.28448800	-0.16899400	2.51145600
H	-4.37696700	1.01242400	3.46186000
N	0.27417500	1.02571300	-1.74070700
C	3.13748000	-1.83673800	0.28698000
C	3.84390300	-1.18234300	1.30218900
C	3.63622200	-3.04249600	-0.22453600
C	5.04006100	-1.71412700	1.79442000
H	3.45524800	-0.25305300	1.71086600
C	4.82857900	-3.57797700	0.26615100
H	3.08853100	-3.56007700	-1.00770500
C	5.53713700	-2.91311000	1.27470100
H	5.57835600	-1.19564700	2.58389200
H	5.20672000	-4.51356000	-0.13832200
H	6.46577100	-3.33060400	1.65536700
H	0.95440800	2.38325700	-0.53838000
C	1.45289400	2.45014100	1.48134300
C	1.92360500	3.55221500	2.46669200
H	0.51959200	1.97868200	1.79066800
H	2.20627500	1.68127700	1.30772800
H	1.33882900	3.50323300	3.38894100
H	2.97889900	3.41660500	2.71832000
C	0.02203900	4.06575400	0.29065600
H	-0.10084700	4.54961000	-0.67876300
H	-0.86220600	3.46767400	0.50976300
C	0.36793100	5.06132900	1.42943500
H	0.23303700	6.08889400	1.08162100
H	-0.28645800	4.89903200	2.29006900
C	2.65498100	5.01654200	0.70790900
H	2.47076300	5.98725700	0.23981600
H	3.69147000	4.99043500	1.05430500
C	2.40595500	3.86669300	-0.30390000
H	2.19938500	4.22164200	-1.31494000
H	3.22610100	3.14970800	-0.33225200
N	1.76142800	4.88954300	1.87137800
N	1.18502900	3.11697700	0.15999900
H	0.83803100	-2.91544800	-1.15103700
F	0.94256300	-3.88660900	-2.33537200

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C	-2.18660100	-1.21676300	0.35828600
C	-0.62648700	-0.31589600	1.71139700
C	-2.11481800	-0.70377900	1.80003600
H	-2.35022700	-0.36174100	-0.30285200
H	0.03508400	-0.81645700	2.41895800
H	-2.18979700	-1.55052100	2.49092600
C	-3.09110000	0.38384600	2.22608200
C	-4.53794400	-0.11374700	2.29395900
H	-3.02358800	1.22724500	1.53391500
H	-2.78238000	0.76098500	3.21021300
H	-5.20166300	0.67752000	2.66352600
H	-4.90258700	-0.42281000	1.30771800
H	-4.63091100	-0.97476300	2.96821200
N	-0.71029000	-1.55946400	0.33940400
S	-0.02067100	-1.40985300	-1.19039800
O	-0.11050400	-0.00493900	-1.65375400
O	-0.62013000	-2.41601900	-2.09493500
C	1.69172900	-1.84935400	-0.92495800
C	2.26639200	-1.93090900	0.34434000
C	2.45254500	-2.07861700	-2.07450000
C	3.61636200	-2.25524100	0.45431100
H	1.68815200	-1.74999500	1.23918200
C	3.80519400	-2.39224100	-1.94347700
H	2.00237700	-2.01289800	-3.06044800
C	4.40711800	-2.48803100	-0.68045300
H	4.06512000	-2.31466600	1.44214000
H	4.39994100	-2.56421800	-2.83668200
C	5.86721300	-2.82506300	-0.53117200
H	6.37318300	-2.09264300	0.10883300
H	5.99436900	-3.80802700	-0.05881700
H	6.37506700	-2.84703800	-1.50028900
S	0.98956500	1.64715200	2.07610200
O	1.22180700	1.10657800	3.44040500
O	0.75830900	3.10912900	1.95417400
C	2.48435500	1.30319200	1.13878700

C	2.45590300	1.33104900	-0.25703800
C	3.68305900	1.10494900	1.82460200
C	3.64091000	1.16064500	-0.96666000
H	1.51748100	1.43710400	-0.78405900
C	4.86359300	0.93343900	1.09735500
H	3.69368100	1.07343200	2.90885500
C	4.86306400	0.96142000	-0.30405000
H	3.61428900	1.16090800	-2.05365200
H	5.79718100	0.76523800	1.62856000
C	6.13159100	0.76644600	-1.09269300
H	6.98654800	0.57835600	-0.43597000
H	6.03618000	-0.07997300	-1.78353800
H	6.35630100	1.65328900	-1.69940200
N	-0.31528400	0.95562300	1.36037200
C	-3.15822000	-2.30673300	-0.00918800
C	-3.97770000	-2.13623900	-1.13292200
C	-3.30184700	-3.46816300	0.76269700
C	-4.91971100	-3.10571500	-1.48703800
H	-3.87377100	-1.23688500	-1.73534500
C	-4.23972100	-4.44179400	0.41051100
H	-2.68008700	-3.61685700	1.63938100
C	-5.05189800	-4.26452500	-0.71542700
H	-5.54656600	-2.95710400	-2.36264200
H	-4.33850400	-5.33823900	1.01750700
H	-5.78259200	-5.02221200	-0.98660600
H	-1.09807700	2.05116500	0.15458900
C	-2.58810400	2.21911500	-1.32780000
C	-3.09993800	3.34748600	-2.26339400
H	-2.14868200	1.38205700	-1.87014400
H	-3.36289300	1.84735700	-0.65606100
H	-2.86375100	3.11541700	-3.30557200
H	-4.18443300	3.45102500	-2.17017600
C	-0.41429200	3.36276800	-1.33783400
H	0.39605600	3.67276100	-0.67798500
H	-0.07126500	2.54793900	-1.97532100
C	-1.02056500	4.54007800	-2.14750200
H	-0.56573200	5.48709600	-1.84468400
H	-0.83822500	4.39436000	-3.21576800
C	-2.72543300	4.94350400	-0.50845400
H	-2.32295000	5.93646100	-0.28989300
H	-3.80739500	4.96718000	-0.35151400
C	-2.06366800	3.88441400	0.41193800
H	-1.22749900	4.27695000	0.99016300
H	-2.77491100	3.41210800	1.09057800
N	-2.47301800	4.63629700	-1.92621500
N	-1.50275200	2.80098600	-0.46704100
H	-0.41319900	-2.80025500	0.93783700
F	-0.16710800	-3.71053100	1.43820700

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C	-2.34316500	-1.09379200	0.36957900
C	-0.62406200	-0.44183600	1.54413700
C	-2.14623700	-0.62116800	1.82307900
H	-2.50588300	-0.22576200	-0.27408100
H	0.02276600	-0.93328600	2.27335100
H	-2.27569900	-1.46617300	2.50656800
C	-2.95337200	0.56763300	2.30991000
C	-4.45491100	0.27130200	2.36886500
H	-2.77164900	1.42393500	1.65601400
H	-2.58802800	0.85260900	3.30589400
H	-5.00649900	1.13341000	2.76361900
H	-4.85540600	0.04666000	1.37283000
H	-4.66772600	-0.59009400	3.01478900
N	-0.85556300	-1.44318800	0.34001200
S	-0.14191100	-1.32965800	-1.21604900
O	-0.17199700	0.05234300	-1.73301000
O	-0.83569300	-2.34458600	-2.03184700
C	1.55199200	-1.84068400	-0.97046800
C	2.11374000	-2.05335000	0.28881300
C	2.30658600	-2.00981200	-2.13518100
C	3.44790900	-2.44369600	0.37396900
H	1.54467100	-1.92044700	1.19758600
C	3.64112600	-2.39802300	-2.02742300
H	1.86736000	-1.83938000	-3.11366500
C	4.23241700	-2.62074200	-0.77491600
H	3.88876900	-2.59916600	1.35485000
H	4.23187200	-2.52392000	-2.93077200
C	5.67453800	-3.03559900	-0.65142800
H	6.21112900	-2.37807600	0.04246100
H	5.75287800	-4.05648900	-0.25516100
H	6.18457800	-3.00768100	-1.61915400
S	1.01874400	1.49149800	2.02356700
O	1.17103800	0.91412800	3.38994400
O	0.87471800	2.97251100	1.93677500
C	2.57431000	1.14165500	1.17822200
C	2.62626800	1.20290700	-0.21720200
C	3.72809000	0.88611600	1.91815400
C	3.84290500	1.01701600	-0.86688100
H	1.71905400	1.35664500	-0.78805000
C	4.94254100	0.69251700	1.25210600
H	3.67686300	0.82644500	3.00032300
C	5.02087300	0.75965700	-0.14522100
H	3.87774000	1.04907300	-1.95331800
H	5.83950900	0.47869300	1.82866600
C	6.32467100	0.54841900	-0.87068400
H	7.12546600	0.26358300	-0.18103700
H	6.22873500	-0.23757700	-1.62936700
H	6.63611800	1.46295100	-1.39257300
N	-0.20566000	0.86432900	1.20030800
C	-3.33171300	-2.16644100	0.01313500
C	-4.10907900	-2.01237900	-1.14298000

C	-3.53237000	-3.29578600	0.81874400
C	-5.06406000	-2.96869100	-1.49633500
H	-3.95919200	-1.13765100	-1.77118100
C	-4.48333500	-4.25688200	0.46699400
H	-2.94779200	-3.42873800	1.72305500
C	-5.25135900	-4.09737000	-0.69188000
H	-5.65777900	-2.83412700	-2.39687000
H	-4.62693600	-5.12886400	1.09990100
H	-5.99226400	-4.84507900	-0.96292500
H	-0.94147400	2.06397600	0.14475100
C	-2.48335800	2.35669100	-1.26766500
C	-2.93859700	3.51239300	-2.19941100
H	-2.14140500	1.48034800	-1.81739900
H	-3.25748800	2.06067300	-0.55835900
H	-2.75625200	3.25363400	-3.24622400
H	-4.00829800	3.70049400	-2.07224800
C	-0.22688700	3.32770500	-1.37495100
H	0.62680900	3.58038400	-0.74581500
H	0.03376200	2.48608500	-2.01585800
C	-0.77137400	4.54342400	-2.17093500
H	-0.23550800	5.45519600	-1.89278100
H	-0.64011500	4.38010400	-3.24424500
C	-2.37813500	5.08170700	-0.47349800
H	-1.89751000	6.04404600	-0.27622500
H	-3.44896400	5.18494200	-0.27668800
C	-1.76089500	3.98094000	0.42904900
H	-0.87663000	4.31038800	0.97265300
H	-2.48003300	3.57029400	1.13919100
N	-2.20325800	4.75194300	-1.89791700
N	-1.31921900	2.85299400	-0.45978500
H	-0.60677000	-2.88281200	0.88194300
F	-0.40234100	-3.79548300	1.26398500

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C	-0.81181800	0.88990100	-0.53661500
C	0.73223300	-0.26945700	0.43175300
C	0.53461000	1.25839500	0.14764700
N	-0.73613000	-0.41023000	0.19743700
S	-1.46833300	-1.80357900	-0.40838900
O	-1.03238100	-2.91633300	0.45342700
O	-1.29488800	-1.92203700	-1.87135400
C	-3.17639600	-1.40843800	-0.08406100
C	-3.67346200	-1.57051700	1.21183200
C	-3.95835300	-0.85341400	-1.09728600
C	-4.97515100	-1.16152700	1.48995100
H	-3.05052900	-1.99836200	1.99077200
C	-5.25659300	-0.44114400	-0.79765100
H	-3.55623600	-0.73050900	-2.09674000
C	-5.78061000	-0.57907000	0.49616600
H	-5.36970400	-1.28413500	2.49542900
H	-5.86756000	0.00277400	-1.57918500
C	-7.16191100	-0.07742500	0.82500600
H	-7.63604900	-0.68933100	1.59994700
H	-7.11199500	0.95261900	1.20476000
H	-7.80628200	-0.07029800	-0.06030700
S	2.90864900	-1.84912000	-0.08885000
O	3.21317400	-2.69777400	-1.25315200
O	2.66251600	-2.44640400	1.23141300
C	4.23748300	-0.66763000	0.08775700
C	4.75315500	-0.04964400	-1.05699400
C	4.73042100	-0.36654200	1.35653600
C	5.77389600	0.88490500	-0.91597400
H	4.36381700	-0.29205100	-2.04101700
C	5.76002400	0.57065400	1.47679000
H	4.32070400	-0.85410500	2.23435500
C	6.29345100	1.21060900	0.35028600
H	6.17728200	1.37117000	-1.80077600
H	6.15063200	0.80659400	2.46320000
C	7.39149700	2.23384100	0.48047800
H	7.74688700	2.30950400	1.51288900
H	8.24439700	1.98010700	-0.16090200
H	7.03762800	3.22509900	0.16828700
N	1.53142700	-1.01788600	-0.51492800
H	1.03120000	-0.56358000	1.43588200
H	1.54330800	-0.69994300	-1.48169100
C	1.54830400	2.05474300	-0.65829100
H	1.01043200	2.88346200	-1.13888200
H	1.95322700	1.44109700	-1.47291500
C	2.68483900	2.61481300	0.20005400
H	3.40813300	3.16317900	-0.41424700
H	2.29129200	3.30594000	0.95655300
H	3.22376200	1.81853500	0.72195800
H	0.32757000	1.75791100	1.09920100
C	-2.03344100	1.72660500	-0.28976400
C	-2.61508500	1.79870500	0.98352100
C	-2.61040700	2.44379700	-1.34479700
C	-3.76100400	2.56641700	1.19367400
H	-2.18205500	1.23053600	1.80161700
C	-3.75273400	3.22263300	-1.13512500
H	-2.17249200	2.37655800	-2.33813400
C	-4.33481000	3.28047600	0.13430800
H	-4.21440300	2.60003900	2.18100600
H	-4.19469300	3.76890000	-1.96448100
H	-5.23213100	3.87156700	0.29822600
H	-0.66445400	0.74697700	-1.61443000

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C	-1.27716700	-2.38552800	0.14994200
C	0.58773800	-1.40792900	-0.32165000
C	-0.20946800	-2.57142200	-0.97257400
H	0.51053100	-0.46259200	-0.86052400
H	-0.57144300	-2.30789200	-1.96697500

C	0.43816200	-3.95123700	-1.00187000
C	-0.54080500	-5.01021100	-1.51759500
H	0.77927200	-4.23081500	0.00485100
H	1.31892900	-3.92970600	-1.65732000
H	-0.06540000	-5.99741500	-1.53553400
H	-1.42945700	-5.07645300	-0.87863900
H	-0.87250200	-4.77273200	-2.53588700
N	-0.26975800	-1.50049800	0.84909000
S	-0.56289100	-0.24985900	1.93463300
O	0.76651400	0.32937100	2.17924200
O	-1.34502600	-0.85551800	3.02256000
C	-1.55895600	1.00786000	1.16200700
C	-0.95196900	1.86035200	0.23742800
C	-2.91163000	1.12929100	1.48498100
C	-1.72233700	2.83842900	-0.38755600
H	0.10328400	1.76899800	0.01594100
C	-3.66244500	2.12131500	0.85890800
H	-3.36664000	0.45880900	2.20463000
C	-3.08694700	2.98192300	-0.09048300
H	-1.25391600	3.50359500	-1.10823400
H	-4.71665400	2.22286700	1.10309400
C	-3.92785700	4.01574300	-0.79199800
H	-3.30698900	4.78992400	-1.25422600
H	-4.52583800	3.54795900	-1.58619200
H	-4.62873800	4.49545000	-0.09956000
S	3.17867900	-0.83242500	-1.21244200
O	2.75822200	-1.33881300	-2.51884900
O	4.49846900	-1.13702400	-0.66728500
C	2.75797200	0.86933200	-1.03797000
C	2.06802200	1.49865300	-2.08022100
C	3.14122300	1.55099100	0.12383700
C	1.75795000	2.84980300	-1.94562900
H	1.78091400	0.94870400	-2.96942600
C	2.81099100	2.89665200	0.23299500
H	3.67159600	1.04923600	0.92592300
C	2.11507900	3.56430300	-0.79133500
H	1.22198400	3.35280100	-2.74518100
H	3.09022800	3.43846600	1.13246400
C	1.73281500	5.00916400	-0.62733000
H	2.60033900	5.61480300	-0.33944900
H	1.30893500	5.41900300	-1.54870000
H	0.98610300	5.11558800	0.17041300
N	2.03991500	-1.64946800	-0.02744400
H	2.38250000	-1.44550000	1.00815100
C	-2.58786900	-1.76200300	-0.25854500
C	-3.76004400	-2.14982700	0.40204500
C	-2.67138700	-0.80689000	-1.28436000
C	-4.99590400	-1.60008900	0.04666600
H	-3.70246900	-2.88687100	1.19940400
C	-3.90207700	-0.25657500	-1.64004000
H	-1.77755600	-0.47595300	-1.80408800
C	-5.06925600	-0.65245300	-0.97690000
H	-5.89621400	-1.91192400	0.56960000
H	-3.95005700	0.48692200	-2.43100100
H	-6.02688500	-0.21978800	-1.25422400
H	-1.45931700	-3.27981400	0.74907100
H	2.25157600	-2.65433400	-0.12580700
F	4.33108500	0.22690200	3.04548200
H	3.76156200	-0.55878200	2.69644400
F	3.07671100	-1.61115400	2.24924700

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C	-1.04696300	1.05494200	-0.37898000
C	-0.17947900	0.04487500	1.26674700
C	-0.28216100	1.51772400	0.91453400
H	-0.04848000	-0.49187500	2.19721400
H	-0.99461600	1.94643000	1.62989800
C	0.91606200	2.44296900	0.77577200
C	0.47717300	3.82587800	0.28642800
H	1.63730900	2.01605600	0.07600300
H	1.40799500	2.52404000	1.75043600
H	1.34312600	4.49324400	0.20844400
H	0.00830600	3.76752200	-0.70359400
H	-0.24425400	4.28320500	0.97492700
N	-0.96828100	-0.31671900	0.26092600
S	-1.67543000	-1.85272700	-0.13161600
O	-1.08481500	-2.76799500	0.84890100
O	-1.48500800	-2.02621000	-1.57077100
C	-3.39039400	-1.58484500	0.20967900
C	-3.81740600	-1.54310500	1.53913600
C	-4.27045700	-1.38111200	-0.85724900
C	-5.16163000	-1.28471400	1.79707500
H	-3.11896900	-1.69823100	2.35522900
C	-5.60939300	-1.13168700	-0.57394700
H	-3.91447500	-1.40654800	-1.88062900
C	-6.07390800	-1.07324300	0.75081100
H	-5.50689500	-1.24325100	2.82628500
H	-6.30363300	-0.96630600	-1.39334600
C	-7.52098300	-0.77068000	1.03255700
H	-7.79455300	0.21249300	0.62874200
H	-8.17570700	-1.50874800	0.55271800
H	-7.72871200	-0.77110600	2.10678400
S	2.44479200	-0.84889900	-0.68938300
O	1.94460800	0.26182400	-1.51100100
O	2.06089400	-2.23001700	-1.00924900
C	4.21539400	-0.72436300	-0.57061100
C	4.84271200	0.47705200	-0.90197000
C	4.94123800	-1.82916900	-0.11119900
C	6.22958300	0.56560700	-0.77499200
H	4.26422000	1.32458100	-1.25272900
C	6.32292800	-1.71784400	0.00928200

H	4.43794300	-2.75639000	0.14357500
C	6.98786100	-0.52232800	-0.31878500
H	6.72788000	1.49597500	-1.03346800
H	6.89723800	-2.57113400	0.36108000
C	8.48336600	-0.42171100	-0.17315300
H	8.77875100	-0.53079300	0.87838100
H	8.98661500	-1.21943000	-0.73323700
H	8.85575800	0.54190400	-0.53392400
N	1.87760300	-0.56636800	0.90395200
H	2.48554200	0.12213100	1.42000800
C	-2.42697600	1.56041500	-0.67502500
C	-2.77954700	1.82767900	-2.00358500
C	-3.37898800	1.74544700	0.33869100
C	-4.06458000	2.27938600	-2.31874300
H	-2.04504600	1.67745900	-2.79091300
C	-4.66117600	2.19371900	0.02546100
H	-3.13073400	1.51905700	1.37121500
C	-5.00714000	2.46292600	-1.30412300
H	-4.32717200	2.48289500	-3.35339300
H	-5.39430300	2.32361000	0.81659600
H	-6.00901900	2.80767800	-1.54597000
H	-0.41158900	1.06949200	-1.26518100
H	1.91849600	-1.45406000	1.41391600
F	4.36574600	2.97388600	1.59002200
H	3.97101100	2.05869600	1.94218500
F	3.50055300	0.95670500	2.39316300

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C	1.42694200	0.63532900	-0.56734400
C	2.78962100	-0.42107400	0.62360900
C	2.87512200	0.93015600	-0.02045700
H	3.43748700	-1.06548800	1.21237900
C	3.98264400	1.12252900	-1.06228300
C	5.36711000	1.24079200	-0.42465700
H	3.73724500	2.03416400	-1.62007000
H	3.95527200	0.28963700	-1.77517200
H	6.12824000	1.40033100	-1.19696400
H	5.40946900	2.08543200	0.27368200
H	5.63361000	0.33039900	0.12618400
N	1.59562400	-0.68127500	0.19536600
S	0.63849600	-2.20912900	0.30132200
O	0.87050900	-2.67036500	1.66831400
O	1.07963000	-2.99141900	-0.85134200
C	-0.97993500	-1.57693900	0.06139600
C	-1.65726500	-1.01680500	1.15257500
C	-1.52204100	-1.59046300	-1.22748600
C	-2.90847400	-0.45707600	0.93113400
H	-1.21408900	-1.00894500	2.14231100
C	-2.78025500	-1.02583200	-1.41857100
H	-0.97631600	-2.02394800	-2.05819100
C	-3.48457600	-0.44556000	-0.35232800
H	-3.44458700	-0.00925300	1.76297200
H	-3.21629800	-1.02493300	-2.41327100
C	-4.82201600	0.20496200	-0.56923100
H	-5.57379400	-0.20757600	0.11444100
H	-4.75744200	1.28163300	-0.36507300
H	-5.17170900	0.07004900	-1.59687700
C	0.27589300	1.48800400	-0.13548700
C	-0.66516100	1.90127900	-1.08558100
C	0.12784900	1.88390400	1.20272700
C	-1.74085800	2.70898800	-0.70634400
H	-0.55802200	1.58423400	-2.11925500
C	-0.94665600	2.68749300	1.58098500
H	0.84419200	1.55591200	1.95149300
C	-1.88302200	3.10256200	0.62636300
H	-2.46907300	3.02074400	-1.44973600
H	-1.05771400	2.98560500	2.61989300
H	-2.72263400	3.72513000	0.92362900
H	1.41007700	0.42090100	-1.63654500
H	2.89013400	1.73172100	0.72556900

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C	-0.05612700	0.91486300	1.25515300
C	0.72098700	-0.83133800	0.46832200
C	-0.39111900	-0.62831300	1.33416900
H	1.27557200	-1.67293800	0.06412500
C	-0.61211500	-1.36102900	2.65393400
C	-0.17953200	-2.82856900	2.59933800
H	-1.67163600	-1.28762700	2.92627400
H	-0.04722200	-0.84398900	3.44028700
H	-0.44487800	-3.33840800	3.53271800
H	-0.66235000	-3.36416600	1.77517600
H	0.90586400	-2.91345500	2.46577600
N	0.98030300	0.46740300	0.25924800
S	2.05145700	1.27980200	-0.83108500
O	2.12978600	2.63770900	-0.28709000
O	1.57718400	1.05045200	-2.20026100
C	3.55349900	0.38232200	-0.56138900
C	4.28361100	0.63087800	0.60736700
C	3.95801200	-0.57217500	-1.49591100
C	5.44641500	-0.09739700	0.83066900
H	3.94967000	1.37334800	1.32496100
C	5.12952500	-1.28919800	-1.24966600
H	3.37625700	-0.75027700	-2.39363300
C	5.88792500	-1.06530600	-0.09138200
H	6.02440800	0.08660000	1.73246400
H	5.45770500	-2.03261900	-1.97063800
C	7.15779600	-1.83129400	0.16530400
H	7.30026900	-2.62780300	-0.57122900
H	8.02711400	-1.16247300	0.11819900
H	7.15015100	-2.27868700	1.16648500
C	-1.08390200	1.90670900	0.80882700

C	-1.85239100	2.54307000	1.79379700
C	-1.33984700	2.17545800	-0.54030700
C	-2.87716100	3.42025200	1.43267400
H	-1.65004100	2.34448100	2.84372300
C	-2.35506800	3.06433000	-0.90180500
H	-0.75635300	1.69134700	-1.31574900
C	-3.13122100	3.68394000	0.08216800
H	-3.47085200	3.90249700	2.20462200
H	-2.54159700	3.26598600	-1.95325400
H	-3.92415800	4.37123800	-0.20014400
H	0.45030100	1.23645000	2.16758200
C	-3.65009000	-1.60999400	-2.26125200
C	-2.40706600	-1.10227400	-1.47007900
H	-3.40958700	-2.51272100	-2.83114800
H	-3.99518600	-0.84300000	-2.96155900
H	-1.50882000	-1.68960000	-1.68732000
H	-2.19636200	-0.05288200	-1.68083200
C	-4.32215800	-3.02493500	-0.44887200
H	-5.13152700	-3.22847000	0.25902900
H	-4.16113000	-3.92224400	-1.05447800
C	-3.01695000	-2.63000100	0.30574800
H	-3.13300000	-2.70641400	1.38939100
H	-2.16822800	-3.24721000	-0.00010500
C	-3.82256400	-0.34606600	0.35260600
H	-4.01136500	-0.48705500	1.42011200
H	-3.52548700	0.68901900	0.18384400
C	-5.05441500	-0.74270500	-0.51729900
H	-5.91801100	-0.96853700	0.11598600
H	-5.32787900	0.07462200	-1.19191600
N	-2.68494400	-1.22104300	-0.01928500
N	-4.75231100	-1.93057600	-1.33662700
H	-1.45832000	-0.86499900	0.64140100

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C	1.81792000	-1.77448800	-0.23912000
C	0.46619600	-1.81574700	1.31786500
C	1.75621700	-2.17280400	1.22944700
H	-0.32442300	-1.81014700	2.05802100
C	2.77022700	-2.73935300	2.15944600
C	2.23460300	-2.93270400	3.58057700
H	3.65971200	-2.09545800	2.17433800
H	3.11388100	-3.70076600	1.74943800
H	3.00817400	-3.36304900	4.22622200
H	1.92155700	-1.97633700	4.01715400
H	1.37086000	-3.60856000	3.58997900
N	0.34788600	-1.28669600	-0.04085400
S	-0.78257600	-2.06800200	-1.10408300
O	-0.87302100	-3.50771800	-0.79049000
O	-0.39334700	-1.65319700	-2.46310700
C	-2.31567200	-1.27900700	-0.66308500
C	-2.94883600	-1.62315300	0.53419600
C	-2.87440200	-0.34682000	-1.54102700
C	-4.15052900	-0.99658900	0.86210500
H	-2.52214600	-2.36784900	1.19772300
C	-4.08613300	0.25154500	-1.20395200
H	-2.37173300	-0.09765200	-2.46940800
C	-4.73784200	-0.05511100	0.00208700
H	-4.64609000	-1.25291400	1.79453600
H	-4.52952300	0.97428000	-1.88425000
C	-6.04392700	0.60819000	0.35192200
H	-5.94092800	1.70036200	0.34981400
H	-6.81758300	0.35666500	-0.38466100
H	-6.39827900	0.29699200	1.33942400
C	2.74140500	-0.69242300	-0.72251200
C	2.84498100	-0.44589000	-2.09978700
C	3.48356400	0.09413900	0.16774300
C	3.66572400	0.57723300	-2.57725500
H	2.27035100	-1.05261500	-2.79405300
C	4.31477400	1.11247000	-0.30924700
H	3.41631400	-0.08054100	1.23610200
C	4.40477000	1.35944900	-1.68176600
H	3.73160700	0.76246800	-3.64617200
H	4.88522300	1.71444900	0.39310600
H	5.04680200	2.15409000	-2.05259500
H	1.83651100	-2.63283000	-0.91702100
H	0.10458000	0.60170900	0.10589400
C	-1.42336300	3.50496300	0.90147800
C	-1.39480700	2.03584300	0.40409000
H	-1.82830200	3.56082700	1.91549500
H	-2.05480200	4.10804700	0.24360300
H	-1.90812900	1.34399800	1.07344800
H	-1.79540200	1.92725000	-0.60229300
C	0.74258400	3.36633200	1.92323200
H	1.76914300	3.73712200	1.85910000
H	0.35262100	3.59631800	2.91829800
C	0.70255000	1.83556900	1.67714100
H	1.69382700	1.38726600	1.63239400
H	0.09679200	1.30272800	2.41228900
C	0.75628400	2.40034400	-0.73066300
H	1.80300000	2.10237000	-0.70215500
H	0.32012500	2.10318400	-1.68575400
C	0.55101900	3.90406100	-0.40921500
H	1.51378400	4.42199300	-0.42025400
H	-0.10117200	4.37156500	-1.15175800
N	0.04806400	1.61547600	0.33991000
N	-0.06566800	4.07609200	0.91750300

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C	1.28148200	-2.19255100	-0.39407300
C	-0.64092900	-1.78597700	0.63013900
C	0.45007800	-2.57089300	0.76771100
H	-1.59543400	-1.81108200	1.14886800

C	0.79406600	-3.60087600	1.80728800
C	-0.35702400	-3.86753700	2.78050300
H	1.68411600	-3.28887800	2.36876700
H	1.07665400	-4.53368000	1.29984600
H	-0.06673300	-4.63277900	3.50901900
H	-0.62853100	-2.95948000	3.33269900
H	-1.25038500	-4.22309000	2.25332100
N	-0.32655300	-0.80300200	-0.33687200
S	-1.41782200	-0.59868500	-1.60853900
O	-1.61219200	-1.87175900	-2.34121100
O	-0.91607900	0.57125200	-2.36116600
C	-2.96694400	-0.17112100	-0.82779500
C	-3.83852600	-1.18905900	-0.43055100
C	-3.27041400	1.17357800	-0.58703400
C	-5.02285700	-0.84864300	0.22549200
H	-3.60358900	-2.22777800	-0.63680100
C	-4.45903600	1.49314300	0.06380900
H	-2.59834200	1.95529200	-0.92057800
C	-5.35000100	0.49036700	0.48560500
H	-5.70449800	-1.63647300	0.53504200
H	-4.70406100	2.53723500	0.24310300
C	-6.62847600	0.85695700	1.19294200
H	-6.41801800	1.38547600	2.13156600
H	-7.23869000	1.52853800	0.57609900
H	-7.22394300	-0.03106000	1.42620800
C	2.65282600	-1.76375700	-0.37139800
C	3.35182600	-1.65186500	-1.59618000
C	3.30246300	-1.39573800	0.82948400
C	4.66537200	-1.19619200	-1.61754600
H	2.84497300	-1.91959900	-2.51959700
C	4.61768000	-0.94734000	0.80376600
H	2.76625700	-1.45227300	1.77008800
C	5.29842300	-0.84512300	-0.41789400
H	5.19742800	-1.10955600	-2.56025100
H	5.11413300	-0.66539000	1.72762500
H	6.32376900	-0.48605500	-0.43430400
H	0.90804300	-2.49460300	-1.36822100
H	0.51189600	0.75344500	0.03415900
C	0.72230200	4.10698500	0.44616900
C	0.01221300	2.78949800	0.03430200
H	0.23755800	4.54634900	1.32220000
H	0.67671200	4.83005400	-0.37255800
H	-0.86516600	2.57127700	0.64463900
H	-0.26837200	2.76711100	-1.01873000
C	2.21071600	2.96540500	1.94468900
H	3.26435000	2.75183700	2.14458900
H	1.79288900	3.48451900	2.81139000
C	1.43141000	1.64855800	1.68324000
H	2.04597100	0.76011700	1.82228700
H	0.52864800	1.56078700	2.29054600
C	2.16931300	1.82804700	-0.66504100
H	2.85179400	1.00771900	-0.45021500
H	1.80016100	1.73173500	-1.68702300
C	2.79638200	3.21688200	-0.37134500
H	3.86072800	3.10743200	-0.14614600
H	2.69217200	3.87566000	-1.23754900
N	0.98645700	1.66525300	0.24819300
N	2.13506200	3.85828400	0.77694200

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S	-1.52351900	0.68292300	1.24764000
O	-1.92944000	2.05795200	1.60089300
O	-0.96269100	-0.17425600	2.30402200
C	-2.87574400	-0.14405700	0.44690300
C	-3.63007900	0.55679600	-0.49973100
C	-3.17765900	-1.45938600	0.79456600
C	-4.70221700	-0.08765400	-1.10993500
H	-3.38313300	1.58150600	-0.75765600
C	-4.26284100	-2.08397200	0.17714500
H	-2.57707400	-1.98593000	1.52815500
C	-5.03664500	-1.41402800	-0.78149800
H	-5.29279300	0.44590900	-1.85050600
H	-4.50797400	-3.10860400	0.44344200
C	-6.20502400	-2.09015800	-1.45023000
H	-7.13732600	-1.54671200	-1.25067800
H	-6.07239700	-2.11244100	-2.53921600
H	-6.32621500	-3.11920200	-1.09781000
N	-0.42113000	0.96995800	-0.06300200
C	0.84312700	1.40852700	0.32280900
H	1.61297000	0.50481000	0.16378700
F	-0.26037200	-0.71261700	-0.55791200
C	2.48948200	-1.76040200	0.72769600
C	3.63826000	-2.79345600	0.49777800
H	2.39362300	-1.49145300	1.78405700
H	1.52525200	-2.13235400	0.37112800
H	4.07001100	-3.11041500	1.45263400
H	3.26525400	-3.68158000	-0.02231300
C	4.05040700	0.06785700	0.49334200
H	4.25328700	0.97304100	-0.08560900
H	3.88705500	0.35029400	1.53789900
C	5.20159900	-0.97981700	0.34797100
H	6.02493200	-0.56891900	-0.24503600
H	5.59367700	-1.26630300	1.32899900
C	4.14664900	-1.82715700	-1.63495300
H	4.94311800	-1.37024700	-2.23097400
H	3.82027300	-2.74186600	-2.14008900
C	2.95110800	-0.83626000	-1.45629800
H	3.12455700	0.10466300	-1.98665800
H	2.00795700	-1.26697400	-1.80345600
N	4.70666400	-2.19569500	-0.32243100
N	2.80354700	-0.53027500	-0.02158400

C	1.36571500	2.54795500	-0.55829000
C	0.64793400	3.88206800	-0.33023700
H	1.27471900	2.24721800	-1.61036300
H	2.43781400	2.66276500	-0.35158200
C	1.21507000	5.00565300	-1.20083100
H	-0.42264000	3.75287900	-0.53763200
H	0.72850900	4.15740400	0.73089500
H	0.68869900	5.95205500	-1.02360000
H	2.28023700	5.17066900	-0.99029900
H	1.12005100	4.76417100	-2.26790100
H	0.94587600	1.58987000	1.40190500

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S	0.03475400	1.24687900	-0.14599100
O	0.30689800	1.81177000	-1.48363700
O	0.24732400	2.06625900	1.04835800
C	-1.53642500	0.45089100	-0.10940200
C	-1.99072800	-0.18935900	-1.26866700
C	-2.29069500	0.48181500	1.06459200
C	-3.23369800	-0.81211900	-1.23640300
H	-1.38901600	-0.20234700	-2.17131500
C	-3.53640400	-0.14358900	1.06856300
H	-1.91484000	0.97733700	1.95267900
C	-4.02468200	-0.79853000	-0.07281500
H	-3.60007800	-1.31430400	-2.12785700
H	-4.13639800	-0.12425500	1.97389400
C	-5.36886400	-1.47560100	-0.06478100
H	-6.02749500	-1.04009100	-0.82674800
H	-5.26752500	-2.54268000	-0.29942500
H	-5.85917000	-1.38173300	0.90888400
N	1.17437800	-0.08190800	-0.27822000
C	2.43110900	0.14971100	0.19462100
H	2.64489500	1.14340700	0.61111600
C	3.57589700	-0.58309800	-0.49350800
C	4.81937600	-0.65668600	0.39710800
H	3.80414800	-0.03368400	-1.41765500
H	3.24199600	-1.58658400	-0.78113700
C	5.99694600	-1.31934400	-0.31997400
H	5.10075300	0.35740000	0.71208500
H	4.57588300	-1.21541400	1.31089600
H	6.87880500	-1.36341500	0.33062900
H	5.74926000	-2.34537600	-0.62140400
H	6.27387200	-0.76141900	-1.22398700
H	2.07619900	-0.48423700	1.15784000
F	0.62080600	-1.01201100	1.48012500

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S	-1.49428700	-1.00367400	-0.59847200
O	-1.26475100	-2.36981400	-0.07521000
O	-1.31259400	-0.79190400	-2.05849800
C	-3.18124100	-0.54982100	-0.19623800
C	-3.85210500	-1.21205300	0.83139500
C	-3.79351000	0.49421500	-0.89758500
C	-5.15365000	-0.82161000	1.15821200
H	-3.36808300	-2.02258700	1.36614900
C	-5.09132300	0.87063000	-0.55958100
H	-3.26420700	1.00240400	-1.69750800
C	-5.79253600	0.22046700	0.47170200
H	-5.67892300	-1.33827000	1.95759700
H	-5.57087300	1.67976500	-1.10550600
C	-7.20027000	0.63534000	0.81577300
H	-7.25609700	1.71232900	1.01656300
H	-7.88400100	0.42744500	-0.01765100
H	-7.56905800	0.10155900	1.69745200
N	-0.59510500	0.04181500	0.32467800
C	0.06030100	1.00522300	-0.31140700
C	0.98141000	1.87092600	0.31676500
H	2.13561700	1.05844400	0.23415100
C	4.47662400	0.87194500	0.21024400
C	5.58362000	-0.22428700	0.19493100
H	4.51884800	1.51089400	-0.67540400
H	4.53507300	1.50240200	1.10095400
H	6.22530200	-0.11159300	-0.68430100
H	6.21024700	-0.15374000	1.08928300
C	2.99600000	-0.61829700	-1.00917500
H	2.00639200	-1.07891800	-0.97398100
H	3.03550000	0.05951200	-1.86655000
C	4.13360700	-1.68103400	-1.04154800
H	3.71549500	-2.69163600	-1.07557500
H	4.76813300	-1.54196700	-1.92214300
C	4.14355800	-1.75013300	1.35961000
H	3.70150400	-2.75035000	1.32027800
H	4.79024400	-1.69502700	2.24074100
C	3.03315700	-0.66074600	1.42173600
H	2.02941300	-1.09162100	1.41964300
H	3.13432800	-0.01577000	2.29881800
N	4.98100900	-1.56837000	0.15935100
N	3.15169600	0.20384300	0.21838600
H	-0.04592600	1.08839900	-1.39924800
C	1.30284700	3.20037600	-0.36515400
C	2.44272700	3.96225300	0.31745200
H	0.41382900	3.85020600	-0.37777500
H	1.56100800	3.01709600	-1.41806400
H	2.61458800	4.93116000	-0.16828800
H	2.20636200	4.15600500	1.37232100
H	3.38157200	3.39899700	0.28595200
H	0.88257300	1.92601800	1.40760700

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S	1.25487800	1.10989800	1.79795300
O	0.92482500	0.24184800	2.93997600
O	2.04463800	2.33626700	2.01746700
C	2.07867900	0.10941900	0.56571800

C	2.23673100	-1.25988300	0.77920200
C	2.49513700	0.70672900	-0.63061000
C	2.81793600	-2.04084300	-0.22235100
H	1.90848000	-1.70956100	1.70943300
C	3.06377300	-0.09015000	-1.62076200
H	2.37882600	1.77339400	-0.79077700
C	3.23321400	-1.47387100	-1.43510500
H	2.94439400	-3.10785500	-0.05804100
H	3.38446700	0.36801200	-2.55322200
C	3.85913900	-2.31568400	-2.51674200
H	4.90669800	-2.02915800	-2.67707600
H	3.83380100	-3.37919900	-2.25945300
H	3.33846300	-2.17877400	-3.47247400
N	-0.20661700	1.57660500	1.12639100
C	-0.20839800	2.61955400	0.17080100
C	-1.01921400	2.66772200	-0.89584100
H	-0.79807600	0.73064600	0.88441400
C	-1.16938800	-1.17585300	-0.91931400
C	-1.89384700	-2.48050100	-1.36708500
H	-1.33074800	-0.36281500	-1.63379300
H	-0.09129800	-1.32863200	-0.81639300
H	-2.37356800	-2.35008800	-2.34334700
H	-1.18888400	-3.31563700	-1.44335000
C	-3.14235300	-0.45520600	0.26062500
H	-3.51171600	-0.14090300	1.24265000
H	-3.26562200	0.38204700	-0.43361000
C	-3.88266500	-1.72894700	-0.24948000
H	-4.67239600	-2.03149600	0.44682800
H	-4.34238200	-1.55177300	-1.22802600
C	-2.29175100	-3.09157600	0.91933600
H	-3.07459100	-3.35459900	1.63921400
H	-1.62088600	-3.95180500	0.81799200
C	-1.50886700	-1.82412900	1.37724000
H	-1.85892800	-1.46206800	2.34930200
H	-0.43769600	-2.02411900	1.45502300
N	-2.93457200	-2.85163100	-0.38734500
N	-1.69686800	-0.73696100	0.39161400
H	0.47684500	3.43200200	0.39743700
C	-1.08615000	3.84222900	-1.83204900
C	-2.45898800	4.53357900	-1.81827300
H	-0.87614600	3.50124200	-2.85699800
H	-0.30388700	4.56736800	-1.57206400
H	-2.48997200	5.35991400	-2.53981100
H	-3.25759500	3.82736700	-2.07984400
H	-2.68209600	4.93952200	-0.82356500
H	-1.70076900	1.84205200	-1.09371800

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C	3.35066700	0.14715100	-0.73382300
C	0.99339500	-1.40368400	-0.68543600
C	2.24010200	-1.91832900	-0.38194200
H	3.51672500	-0.24463100	-1.73096800
H	0.71615800	-1.37754700	-1.74087500
H	2.53161900	-2.01385600	0.66031200
C	2.95648500	-2.80374700	-1.36703600
C	2.65428600	-4.29464500	-1.14106200
H	4.04071900	-2.65559500	-1.28779500
H	2.66949100	-2.52360600	-2.38990600
H	3.22044600	-4.92077800	-1.84324600
H	2.92661400	-4.59871200	-0.12214800
H	1.58624000	-4.50465100	-1.27926000
N	2.56070400	1.22775000	-0.63451700
S	1.90341600	1.85920500	-2.07685500
O	1.86802200	0.77391600	-3.07325700
O	2.65902800	3.08494400	-2.39047100
C	0.23892800	2.33053800	-1.66386500
C	0.01953700	3.44768600	-0.85466100
C	-0.82010400	1.63033100	-2.24491400
C	-1.29296700	3.85264700	-0.61247500
H	0.85273600	3.98339400	-0.41394400
C	-2.12087300	2.06799000	-2.00948500
H	-0.62853500	0.77008800	-2.87586900
C	-2.37955100	3.17452700	-1.18488200
H	-1.47380000	4.71027100	0.02965200
H	-2.95035300	1.54280700	-2.47512800
C	-3.79788600	3.60166900	-0.91578900
H	-4.33258700	3.80309500	-1.85236800
H	-4.34803700	2.80789500	-0.39478800
H	-3.83407600	4.50336100	-0.29698700
S	0.16481800	-0.97818900	1.74279200
O	1.32257900	-0.24638100	2.31292500
O	0.01944300	-2.39235100	2.17867500
C	-1.33087500	-0.11066100	2.20332600
C	-1.52086700	1.20425900	1.76732600
C	-2.27195200	-0.74318000	3.01253700
C	-2.67603900	1.88189100	2.14473300
H	-0.78208700	1.68682500	1.13724700
C	-3.42671400	-0.04730400	3.38384900
H	-2.11192600	-1.76531900	3.33861400
C	-3.64822300	1.26821400	2.95521700
H	-2.83007700	2.90176900	1.80396400
H	-4.16677800	-0.53903800	4.01007800
C	-4.89903300	2.01552000	3.34019400
H	-5.52559700	1.42365400	4.01497300
H	-4.65482500	2.96188700	3.83865200
H	-5.49473400	2.26479900	2.45252400
N	0.05754500	-0.82648600	0.09509500
C	4.39280400	-0.12710900	0.25752600
C	5.55989700	-0.78196800	-0.18218600
C	4.28729500	0.26047300	1.60601200
C	6.60036600	-1.04594200	0.70896000

H	5.65624200	-1.06116300	-1.22708000
C	5.32843700	-0.00996300	2.49137600
H	3.38429900	0.74269300	1.95486700
C	6.48591100	-0.66397600	2.04942200
H	7.49894400	-1.54461200	0.35597300
H	5.23665200	0.28711700	3.53280900
H	7.29403300	-0.87119500	2.74593600
H	-1.61941300	-1.17831600	-0.49490500
C	-3.69633300	-0.81771900	-0.39805000
C	-4.96184900	-1.50499600	-0.97555100
H	-3.69205600	-0.79086100	0.69103700
H	-3.54384800	0.18927900	-0.78229900
H	-5.69205700	-1.67503900	-0.17966500
H	-5.42563400	-0.87603400	-1.74032000
C	-2.57898000	-2.99728400	-0.17631600
H	-1.71122800	-3.55658200	-0.52960900
H	-2.49394900	-2.85082200	0.90047800
C	-3.92713100	-3.64023400	-0.59860400
H	-3.75329300	-4.62673300	-1.03671900
H	-4.58223700	-3.75794600	0.26873600
C	-3.73163600	-2.57342300	-2.73991600
H	-3.45169200	-3.54644100	-3.15263700
H	-4.28156300	-2.01896300	-3.50513200
C	-2.46844200	-1.78037300	-2.31104400
H	-1.53817900	-2.29461900	-2.55837600
H	-2.44535400	-0.77344600	-2.72601600
N	-4.62132800	-2.80007900	-1.58924100
N	-2.50912100	-1.63824700	-0.81572300
H	2.60076400	2.00216200	0.22866100
F	2.64681900	2.96415600	1.10484700

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C	-2.91346600	-0.10450600	-0.70252900
C	-1.05091600	1.37257300	-1.19520000
C	-2.47320400	1.38001100	-0.71735200
H	-2.86593900	-0.47000300	-1.73217800
H	-0.86851600	0.70004200	-2.03856600
H	-2.54646200	1.80015700	0.28615000
C	-3.34096000	2.21322000	-1.69089900
C	-2.99890000	3.70333700	-1.71684700
H	-4.38396300	2.08103100	-1.38271100
H	-3.25284800	1.78673500	-2.69929400
H	-3.68682200	4.23583200	-2.38444200
H	-3.08315800	4.14723700	-0.71876800
H	-1.98079200	3.88462100	-2.08155800
N	-1.87196000	-0.83052800	0.05805200
S	-1.72587100	-2.46387000	-0.23588400
O	-1.88468100	-2.67216000	-1.69192700
O	-2.57247000	-3.28399500	0.66047900
C	-0.01778800	-2.76927400	0.20676300
C	0.43463100	-2.45332500	1.49238700
C	0.81508200	-3.39071400	-0.72318600
C	1.74888400	-2.76320600	1.83403700
H	-0.21974800	-1.95153600	2.20052500
C	2.12569300	-3.70480100	-0.35418800
H	0.44822600	-3.62733300	-1.71620200
C	2.61339200	-3.39232400	0.92168200
H	2.11381400	-2.50837200	2.82551700
H	2.77913100	-4.18956400	-1.07452400
C	4.04228300	-3.68063200	1.30238000
H	4.61869400	-2.74835100	1.37056800
H	4.10182600	-4.16876400	2.28239600
H	4.53114700	-4.32394100	0.56390400
S	0.07558000	3.16892700	0.43832400
O	-1.16340800	3.27909400	1.22970800
O	0.62175400	4.38774100	-0.18306300
C	1.34093800	2.38505000	1.41744300
C	1.00206900	1.26538600	2.18494600
C	2.64097200	2.89015900	1.38441900
C	2.00308900	0.65038500	2.93218900
H	-0.01305800	0.86878300	2.21017900
C	3.62596100	2.25640700	2.14532800
H	2.88002100	3.75736600	0.77842700
C	3.32542200	1.12783500	2.92217500
H	1.75423400	-0.22058200	3.53176400
H	4.64231200	2.64077700	2.12717400
C	4.39345500	0.42074300	3.71435700
H	5.33493100	0.97870800	3.70351800
H	4.08416900	0.28051700	4.75705200
H	4.58438000	-0.57743500	3.29859500
N	-0.00397100	2.02876000	-0.84281300
C	-4.32683000	-0.29612800	-0.18886000
C	-5.33087900	-0.73435600	-1.06072200
C	-4.65585200	-0.02253000	1.14694600
C	-6.64563000	-0.89732800	-0.61123300
H	-5.08156200	-0.95049600	-2.09712900
C	-5.96747100	-0.18407800	1.59820600
H	-3.87875100	0.29633700	1.83630000
C	-6.96754700	-0.62105100	0.72066100
H	-7.41375900	-1.24119000	-1.29943500
H	-6.20964300	0.02826400	2.63666300
H	-7.98761700	-0.74747000	1.07440000
H	1.56554200	1.21659000	-1.38434100
C	2.96267400	-0.17312300	-0.68073100
C	4.20176500	-0.88818000	-1.28109000
H	3.21632700	0.49381800	0.14068300
H	2.18630200	-0.86540200	-0.35759600
H	5.11834200	-0.52675800	-0.80729400
H	4.12944500	-1.96463800	-1.11851200
C	3.38170400	1.63649000	-2.30490300
H	2.86566600	2.28850400	-3.01207500

H	3.72764100	2.22679200	-1.45448600
C	4.51219700	0.80048900	-2.96221800
H	4.53782600	0.97292300	-4.04154900
H	5.48134900	1.08338400	-2.54277300
C	3.04877300	-1.06048800	-3.38020000
H	3.15947600	-0.94563800	-4.46171000
H	2.88893100	-2.11882400	-3.15830700
C	1.84970500	-0.21531500	-2.87250400
H	1.43541600	0.44088900	-3.64017600
H	1.05083100	-0.82365300	-2.44594600
N	4.29996100	-0.63747900	-2.72919200
N	2.36323800	0.66983100	-1.77082400
H	-1.84619800	-0.61901800	1.10239200
F	-1.70093200	-0.30057200	2.62985000

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C	-2.75476700	-0.29363800	0.49485800
C	-0.57865200	0.02950800	0.99219400
C	-1.83699900	-0.44554500	1.72030200
H	-3.09991400	0.74487800	0.44909000
H	-0.60849000	1.10178000	0.79662300
H	-1.73781200	-1.49665300	1.99013300
C	-2.20616200	0.38644200	2.94695400
C	-1.20288600	0.24824000	4.09546300
H	-3.20203600	0.06853700	3.28431700
H	-2.29461700	1.44127500	2.65127600
H	-1.53212600	0.81847300	4.97267900
H	-1.09077700	-0.80092800	4.39689000
H	-0.21195800	0.61903300	3.80741200
N	-1.64853000	-0.50083900	-0.50332400
S	-1.68393000	0.40521300	-1.90545100
O	-2.90977500	0.10635700	-2.67954000
O	-0.37054300	0.18451000	-2.54914500
C	-1.77645700	2.12634500	-1.42043200
C	-0.59654900	2.82502700	-1.15839100
C	-3.02320200	2.74126100	-1.26904300
C	-0.66897400	4.15286200	-0.73755900
H	0.36386000	2.33958300	-1.28684800
C	-3.07825500	4.06836000	-0.84549300
H	-3.93372600	2.19282000	-1.48527000
C	-1.90639200	4.79360800	-0.57159800
H	0.24924500	4.69821900	-0.53490100
H	-4.04597600	4.54935200	-0.72585000
C	-1.98223200	6.23402700	-0.13614300
H	-2.24722600	6.88080000	-0.98330300
H	-2.75175400	6.37612500	0.63156700
H	-1.02380100	6.58085900	0.26325400
S	1.12598900	-1.91864500	1.54510600
O	0.00725900	-2.88897300	1.63227500
O	1.99890500	-1.81845200	2.74012800
C	2.18484400	-2.37788900	0.16949400
C	1.86949300	-1.96891300	-1.12631000
C	3.30611800	-3.17398000	0.42013500
C	2.69541200	-2.36284600	-2.18109800
H	1.01066700	-1.33565400	-1.31876000
C	4.11937100	-3.55782300	-0.64520000
H	3.54836400	-3.47509400	1.43430800
C	3.82864300	-3.15893900	-1.96113800
H	2.45629700	-2.03788300	-3.19070600
H	4.99683000	-4.17083500	-0.45253400
C	4.72274900	-3.57585600	-3.10097200
H	4.35066300	-3.19700600	-4.05820000
H	5.74397700	-3.19990300	-2.95807600
H	4.78944600	-4.66912600	-3.16824900
N	0.68435700	-0.39687800	1.09465200
C	-3.95100800	-1.20127700	0.38005800
C	-5.20115800	-0.65794700	0.05455300
C	-3.85283100	-2.58178800	0.61016000
C	-6.33250100	-1.47323700	-0.04759100
H	-5.28473600	0.41154200	-0.12363500
C	-4.97990600	-3.40005000	0.50687600
H	-2.89382800	-3.02101500	0.86619500
C	-6.22376700	-2.84900000	0.17696600
H	-7.29433100	-1.03493700	-0.30182000
H	-4.88774700	-4.46840500	0.68592100
H	-7.10025500	-3.48715300	0.09872900
H	2.06451500	0.59341500	0.69650000
C	3.27776000	1.37045900	-0.84805800
C	4.55080200	2.25662500	-0.91694400
H	3.43624900	0.36611500	-1.24198700
H	2.42346300	1.82141600	-1.35361100
H	5.39658700	1.68108700	-1.30282300
H	4.38170900	3.10906000	-1.58042100
C	4.05305700	0.62078000	1.35897500
H	3.70113400	0.42968500	2.37321300
H	4.28299100	-0.33105400	0.87755400
C	5.23343600	1.62751800	1.29790300
H	5.45554300	2.01909000	2.29435800
H	6.13015400	1.13388400	0.91371900
C	3.76515200	3.50226300	0.98023000
H	4.06655700	3.94080400	1.93530600
H	3.51152600	4.31354700	0.29241100
C	2.54779100	2.56093800	1.18165300
H	2.31027200	2.39157900	2.23380500
H	1.65347400	2.90698700	0.66293000
N	4.90845300	2.76310000	0.41852900
N	2.90739600	1.22495800	0.59823200
H	-1.46478200	-1.92902800	-0.99088400
F	-1.38562800	-2.86150200	-1.41288700

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C	2.68209300	0.80666000	0.51515200

C	0.65615200	0.04485100	0.54886600
C	1.64056100	0.55059300	1.63458600
H	3.37497700	-0.03615800	0.46262400
H	0.67550100	-1.04626400	0.49997200
H	1.30557600	1.48576000	2.08395700
C	2.02583600	-0.46344500	2.70368200
C	0.85123600	-0.83356200	3.61226600
H	2.84825800	-0.04675200	3.30025900
H	2.41397800	-1.36558300	2.21120300
H	1.16055100	-1.56466000	4.36889500
H	0.45602200	0.04832400	4.12937700
H	0.02876800	-1.27438300	3.03606400
N	1.57299200	0.63407500	-0.51555400
S	1.91882000	-0.32948400	-1.90495700
O	2.95053800	0.40945700	-2.64782800
O	0.61234200	-0.61742100	-2.51547900
C	2.63030100	-1.84922000	-1.30684600
C	1.78882500	-2.91869400	-0.98194500
C	4.01372700	-1.93487000	-1.12565300
C	2.34687400	-4.08199200	-0.45955400
H	0.72064100	-2.84721900	-1.14605400
C	4.55310600	-3.10987600	-0.60241300
H	4.65772100	-1.10408700	-1.39264900
C	3.73322800	-4.19544200	-0.25750400
H	1.69723500	-4.91636200	-0.20743600
H	5.62789600	-3.18361800	-0.46044700
C	4.31856200	-5.46641400	0.29879700
H	3.80897500	-5.76082800	1.22415600
H	4.19614100	-6.29279000	-0.41349100
H	5.38652700	-5.35553800	0.51016500
S	-1.36196700	1.74695500	1.24026200
O	-0.43238400	2.88130400	1.05891900
O	-1.77989700	1.44485100	2.62543700
C	-2.83533400	1.98438600	0.26225900
C	-2.71242100	2.17404100	-1.11860300
C	-4.08067900	1.98245400	0.88714000
C	-3.86483500	2.35792700	-1.87565700
H	-1.73505600	2.16925300	-1.59017300
C	-5.22660300	2.16952800	0.10966600
H	-4.15552200	1.82720600	1.95774600
C	-5.13826800	2.35561100	-1.27654100
H	-3.77920800	2.50064000	-2.95014600
H	-6.20195100	2.16352100	0.58901700
C	-6.37324100	2.54452400	-2.11831200
H	-7.27838300	2.55226100	-1.50306800
H	-6.32715700	3.48840000	-2.67581100
H	-6.46841100	1.73898900	-2.85776600
N	-0.71944700	0.42540500	0.46082200
C	3.45443300	2.09070800	0.45307800
C	4.84027600	2.04639100	0.24795200
C	2.82700300	3.33524100	0.61436100
C	5.59237700	3.22417000	0.20394300
H	5.33011800	1.08374100	0.12129500
C	3.57646000	4.51236300	0.56655600
H	1.75426900	3.38179000	0.77270700
C	4.96056700	4.46114900	0.36194800
H	6.66643000	3.17473200	0.04449800
H	3.07981200	5.47143000	0.69048900
H	5.54117800	5.37938700	0.32716800
H	-1.41217200	-0.37752600	0.41600200
C	-3.54184900	-1.41675000	-0.76412900
C	-4.55833100	-2.59513600	-0.84846200
H	-4.04476400	-0.46991400	-0.55452900
H	-2.97477900	-1.30281000	-1.69370800
H	-5.58819900	-2.23034400	-0.76867100
H	-4.46083200	-3.13451100	-1.79683500
C	-3.30896600	-1.73845200	1.61516500
H	-2.57857700	-1.95195600	2.40240400
H	-3.74183200	-0.75382900	1.81150000
C	-4.40747100	-2.83965600	1.53586800
H	-4.29321100	-3.57040400	2.34395100
H	-5.40867300	-2.40186000	1.61217600
C	-2.96303600	-4.11438100	0.10558300
H	-2.78800900	-4.79661000	0.94453300
H	-2.92496800	-4.69781400	-0.82081500
C	-1.90891400	-2.96666200	0.08665200
H	-1.14387100	-3.10787100	0.85715100
H	-1.41125600	-2.90167500	-0.88515900
N	-4.32154200	-3.55599700	0.24778700
N	-2.57822700	-1.67085300	0.33067200
H	0.98949800	2.02658600	-1.27409400
F	0.68620700	2.76106800	-1.85480100

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C	0.60894900	0.77917600	0.79117600
C	-0.84270900	-0.75866600	0.36903500
C	-0.90550600	0.79234000	0.42627700
H	-1.25362400	-1.24259100	1.25867200
H	-1.05507400	1.19509800	-0.58137000
C	-1.85039300	1.44141100	1.42464000
C	-1.67614900	2.96102600	1.48275200
H	-1.67444000	1.00491100	2.41735100
H	-2.88187800	1.19866900	1.14976200
H	-2.38042300	3.40741500	2.19511400
H	-0.66160600	3.23668800	1.79483000
H	-1.85860100	3.41364700	0.49950700
N	0.63741900	-0.65498400	0.35699600
S	1.62639600	-1.75636500	1.17444100
O	1.25296400	-3.09706000	0.69163100
O	1.61846000	-1.50779700	2.63162800
C	3.21246500	-1.27296200	0.52626000

C	3.57910900	-1.70078400	-0.75409900
C	4.02024900	-0.40878900	1.26365900
C	4.77845200	-1.24863100	-1.29443100
H	2.93405500	-2.36635700	-1.31864900
C	5.21761400	0.03819200	0.70178800
H	3.71615900	-0.08019900	2.25133700
C	5.61190600	-0.36801300	-0.58038100
H	5.07222400	-1.57469100	-2.28914800
H	5.84846400	0.71911700	1.26689100
C	6.89276700	0.13022000	-1.19650500
H	7.54256700	-0.70624600	-1.48246300
H	6.68641900	0.70418600	-2.10906800
H	7.44476300	0.77463800	-0.50534000
S	-2.87870300	-2.07760500	-0.83334000
O	-3.00188800	-2.99124400	0.31221000
O	-3.05996600	-2.58141600	-2.20569000
C	-3.99059500	-0.70473400	-0.56473700
C	-4.82537100	-0.69771400	0.55117900
C	-3.97298400	0.36549900	-1.46672600
C	-5.65803100	0.40397700	0.76471000
H	-4.81963000	-1.53073600	1.24569400
C	-4.80185900	1.45740900	-1.23179500
H	-3.31402600	0.35509600	-2.32998000
C	-5.65649600	1.49518600	-0.11430500
H	-6.31097700	0.41597400	1.63349200
H	-4.78622000	2.29686300	-1.92250500
C	-6.54400500	2.68912000	0.12190400
H	-7.24595900	2.82502000	-0.71065000
H	-7.12336200	2.57883900	1.04370900
H	-5.95067000	3.60904600	0.19596000
N	-1.32300200	-1.45605900	-0.81022000
H	-1.11816500	-0.95965200	-1.67875600
C	1.57688500	1.67898200	0.07688600
C	2.21033600	2.71616000	0.77235000
C	1.86209500	1.49500200	-1.28260500
C	3.11149500	3.56298400	0.12039600
H	2.00513800	2.85173200	1.83180700
C	2.76757400	2.33393100	-1.93504800
H	1.38993400	0.67799100	-1.82082500
C	3.39527600	3.37144000	-1.23541500
H	3.60047300	4.36093800	0.67336400
H	2.99051900	2.17369500	-2.98691400
H	4.10456800	4.02058000	-1.74237600
H	0.73235700	0.87070300	1.87547500

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C	-0.65417500	0.75896700	-1.22577800
C	0.74783700	-0.78196900	-0.70922600
C	0.85122500	0.76230900	-0.79286800
H	1.20187600	-1.32296300	-1.54282100
H	0.95967400	1.19668300	0.20308300
C	1.84408100	1.36587800	-1.77000200
C	1.64283400	2.87586200	-1.91956800
H	1.73758600	0.87171800	-2.74495500
H	2.85832300	1.16261200	-1.41587800
H	2.38607000	3.29879700	-2.60567300
H	0.64752500	3.11144200	-2.31504500
H	1.74806200	3.38241800	-0.95186700
N	-0.70012200	-0.65123600	-0.73937900
S	-1.72318100	-1.85466500	-1.32165600
O	-1.15146700	-3.09336800	-0.74907800
O	-1.91964300	-1.76647400	-2.77867100
C	-3.22669600	-1.39629500	-0.49788000
C	-3.38385100	-1.72849400	0.85088800
C	-4.15669600	-0.60319200	-1.17103800
C	-4.50003000	-1.25047400	1.53056500
H	-2.64406900	-2.33699900	1.36096200
C	-5.26308500	-0.12727500	-0.46842000
H	-4.01195600	-0.34778300	-2.21491000
C	-5.44722400	-0.43374700	0.88800400
H	-4.63346000	-1.50283600	2.57930500
H	-5.98817200	0.49970900	-0.98002200
C	-6.61206000	0.13365600	1.65424400
H	-6.98576400	-0.57779200	2.39871000
H	-6.30449500	1.04022800	2.19362800
H	-7.43456100	0.40897300	0.98638600
S	2.81272400	-2.19703500	0.64814100
O	2.87172200	-3.11806600	-0.48570200
O	2.87753900	-2.68205000	2.02513900
C	3.84579200	-0.79814400	0.37841300
C	4.62833900	-0.75706100	-0.77861900
C	3.86891500	0.22475800	1.33525900
C	5.45763400	0.34564700	-0.97432200
H	4.59054200	-1.56022700	-1.50606500
C	4.68646600	1.32314300	1.10131900
H	3.25842600	0.17109200	2.23013300
C	5.49242600	1.40099800	-0.05011600
H	6.07757800	0.39063100	-1.86508700
H	4.70521500	2.13313000	1.82523600
C	6.35768000	2.60836500	-0.28562900
H	6.93968800	2.85541000	0.60986200
H	7.04674500	2.44984100	-1.12033400
H	5.73577400	3.48301000	-0.51792700
N	1.13715800	-1.46858400	0.57251100
H	0.97887200	-0.82609900	1.45242700
C	-1.66105000	1.67220300	-0.58881900
C	-2.36245100	2.59403300	-1.37453600
C	-1.94041700	1.58466900	0.78171500
C	-3.33027200	3.42372400	-0.80014700
H	-2.15902900	2.65136300	-2.44134100
C	-2.91263600	2.40452800	1.35502700

H	-1.40964800	0.86075200	1.39225300
C	-3.61124500	3.32635900	0.56578100
H	-3.87227100	4.13267600	-1.42069700
H	-3.13240600	2.31923500	2.41606700
H	-4.37296600	3.95957400	1.01324700
H	-0.72942800	0.80601100	-2.31737800
H	0.50402200	-2.27752400	0.69051300
F	1.17901100	2.26172900	2.63138000
H	0.98543000	1.25826400	2.62998900
F	0.73561200	-0.07466400	2.66012200

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C	-0.54445100	1.33642000	-1.28655300
C	0.68346000	-0.38582500	-1.14387400
C	0.95178800	1.07721700	-0.84972600
H	1.29010100	-1.20370500	-1.50938100
H	1.11655500	1.27397100	0.21041800
C	2.02886500	1.73325000	-1.70890600
C	2.09547700	3.24079000	-1.45896200
H	1.82385300	1.52933500	-2.76796100
H	2.98895100	1.26704600	-1.46766900
H	2.87264400	3.69890200	-2.08152000
H	1.14174100	3.72808900	-1.69605200
H	2.33131900	3.45122100	-0.40885000
N	-0.57994400	-0.16209900	-1.48380900
S	-1.77764300	-1.20628400	-2.18785600
O	-1.11799300	-2.51197100	-2.26780000
O	-2.24390100	-0.50613400	-3.38596100
C	-3.03133200	-1.18916600	-0.94457600
C	-2.90498400	-2.03873700	0.15793800
C	-4.07630400	-0.26615800	-1.05289000
C	-3.84811500	-1.94562900	1.17830500
H	-2.09508000	-2.75857800	0.21905000
C	-5.00867200	-0.19671300	-0.02300400
H	-4.15270900	0.38661200	-1.91470300
C	-4.90411300	-1.02234700	1.10907300
H	-3.76267600	-2.59948700	2.04170100
H	-5.82436400	0.51750800	-0.09253200
C	-5.89083400	-0.89221000	2.23706900
H	-6.91184400	-0.76878000	1.85907400
H	-5.86223000	-1.76452800	2.89732500
H	-5.65886900	-0.00455000	2.84148700
S	2.22945200	-2.31096100	0.97224500
O	2.13903400	-3.33862600	-0.07793000
O	2.40002500	-2.73176400	2.37259900
C	3.47588000	-1.11835900	0.53664500
C	4.20519900	-1.29979300	-0.63934700
C	3.70425600	-0.02673400	1.38173700
C	5.18447200	-0.36238200	-0.97118500
H	4.01449600	-2.15259600	-1.28185300
C	4.67368000	0.90444500	1.02135600
H	3.13033500	0.10100600	2.29348100
C	5.42674500	0.75306300	-0.15624600
H	5.76111400	-0.49653800	-1.88241300
H	4.85015100	1.76306000	1.66377000
C	6.44377300	1.79138500	-0.54869700
H	6.98909200	2.16492800	0.32500900
H	7.16476100	1.39263900	-1.26945800
H	5.94662000	2.65301700	-1.01510800
N	0.81124600	-1.36434900	0.81733500
H	0.76270600	-0.66322200	1.60128800
C	-1.57158700	1.89962300	-0.35507400
C	-2.43506100	2.89994400	-0.81904900
C	-1.71708400	1.41753000	0.95292300
C	-3.43130900	3.41682300	0.01440200
H	-2.33091600	3.26603500	-1.83753600
C	-2.71242100	1.92938800	1.78366500
H	-1.05497600	0.64555300	1.32737500
C	-3.57368800	2.92916800	1.31614400
H	-4.09828600	4.19065100	-0.35606900
H	-2.82021900	1.54402300	2.79387300
H	-4.35298200	3.32239500	1.96364400
H	-0.59305900	1.81634000	-2.26564400
H	-0.00157700	-1.98657300	0.87837400
F	1.33843200	2.57564200	2.53187500
H	1.06165000	1.57068800	2.68768500
F	0.73562200	0.34375400	2.89523900

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C	-2.88280500	0.41240700	0.51301000
C	-2.35579700	1.59460700	-1.10896200
C	-2.45040000	1.90016700	0.27676900
H	-2.14827000	2.13017500	-2.02698500
H	-1.19745800	2.15123900	0.57942100
C	-3.19045600	3.07885300	0.88848200
C	-3.08676300	3.07639000	2.41663500
H	-4.24681300	3.05289700	0.58914700
H	-2.76334800	4.00349700	0.47975700
H	-3.62093000	3.93446600	2.84118700
H	-3.52659200	2.16454100	2.83940500
H	-2.04278000	3.12832100	2.74724000
N	-2.61680400	0.28549800	-0.98396300
S	-2.32259500	-1.03188400	-2.04879000
O	-2.09980000	-0.38830400	-3.34922900
O	-3.44046000	-1.95739200	-1.84459500
C	-0.82713600	-1.76434700	-1.44650200
C	0.37417400	-1.06417800	-1.59792200
C	-0.88553600	-3.00429200	-0.80712000
C	1.53979100	-1.63668900	-1.10049900
H	0.40034400	-0.08370600	-2.06163600
C	0.29718800	-3.55574800	-0.31747800
H	-1.83113500	-3.52066900	-0.68846900

C	1.52083500	-2.88197800	-0.44966000
H	2.47834300	-1.10424500	-1.20944900
H	0.26496000	-4.51785100	0.18633700
C	2.78549700	-3.45283500	0.13369400
H	3.65100900	-3.23578900	-0.50083000
H	2.98442900	-3.00603000	1.11701500
H	2.70959200	-4.53646600	0.26990300
S	1.07910000	2.78234600	-0.32708800
O	1.65839400	4.14948800	-0.43800800
O	0.40328800	2.25695600	-1.55021400
C	2.46252300	1.66448300	-0.03376800
C	3.42045000	1.50701600	-1.04282800
C	2.58275100	0.97133500	1.16859400
C	4.49309800	0.64224300	-0.83920900
H	3.32397500	2.04392300	-1.98189200
C	3.66232000	0.10234000	1.35726400
H	1.83586400	1.10101800	1.94362300
C	4.63052700	-0.07723400	0.36196300
H	5.23256000	0.51448600	-1.62653900
H	3.74587700	-0.44703400	2.29170700
C	5.79072800	-1.01871300	0.55995400
H	5.85868000	-1.74026800	-0.26320400
H	6.74126700	-0.46977100	0.58538800
H	5.69668600	-1.57512400	1.49777900
N	0.08443600	2.61415800	0.92083500
H	0.11888800	3.42239500	1.54180100
C	-2.16665000	-0.55320800	1.40945800
C	-2.90375000	-1.58584100	2.00598200
C	-0.78425900	-0.48364700	1.63133900
C	-2.27118400	-2.53522600	2.81387800
H	-3.97556100	-1.64661500	1.83288300
C	-0.15226200	-1.42936600	2.43797400
H	-0.20652000	0.31231800	1.18244600
C	-0.89264300	-2.45807200	3.03096400
H	-2.85359100	-3.33132900	3.27003800
H	0.92059900	-1.36652300	2.59707400
H	-0.39672900	-3.19669600	3.65542800
H	-3.96366600	0.33705600	0.65167500

81

C	-1.35616600	0.24450400	0.55122500
C	-2.77054300	-0.80168200	-0.52070900
C	-2.86955100	0.22392400	0.34393700
H	-3.42257800	-1.42488500	-1.12130200
C	-3.94225600	1.11963600	0.84986400
C	-5.33088700	0.75990100	0.31471300
H	-3.68896400	2.15630100	0.58084100
H	-3.94150700	1.09337200	1.94958900
H	-6.08694700	1.44480500	0.71498100
H	-5.36023600	0.82415900	-0.77989800
H	-5.61273000	-0.26074600	0.60108500
N	-1.31981800	-0.82422100	-0.55419400
S	-0.44467600	-2.25244900	-0.24323100
O	-0.56997200	-3.07408600	-1.46392200
O	-0.79615000	-2.88715500	1.04651400
C	1.17689400	-1.52696300	-0.10850400
C	1.71048500	-0.85170900	-1.21274500
C	1.85054000	-1.57221600	1.11073400
C	2.93566300	-0.20775000	-1.07744300
H	1.16962900	-0.81390700	-2.15255300
C	3.08390100	-0.92653300	1.22359000
H	1.41464500	-2.08800700	1.95956600
C	3.63856600	-0.23032900	0.14107400
H	3.35177500	0.33045000	-1.92536500
H	3.61355600	-0.95328400	2.17213900
C	4.95109600	0.49643600	0.27152200
H	5.68119000	0.12304900	-0.45750300
H	4.82054200	1.56855800	0.07658300
H	5.37485800	0.37950000	1.27380200
C	-0.53709700	1.45916800	0.22699300
C	0.50688500	1.84480700	1.07536000
C	-0.77242400	2.18726100	-0.94822400
C	1.31502700	2.93953200	0.75283500
H	0.69800200	1.27378800	1.98002400
C	0.03244100	3.28017500	-1.27249700
H	-1.57840500	1.88797600	-1.61365900
C	1.08077400	3.65748500	-0.42302600
H	2.12996400	3.22293600	1.41380700
H	-0.15345700	3.83629600	-2.18777100
H	1.71028000	4.50586200	-0.67888700
H	-1.05719000	-0.18143800	1.51265200

82-ts

C	1.23545000	0.10243500	-0.36032400
C	0.21068100	-1.47569000	-1.52316700
C	1.04784200	-0.42754800	-1.72251100
H	-0.35965100	-2.06504600	-2.23768400
C	1.67387800	0.10149000	-2.98144100
C	1.40041500	1.59743300	-3.19873200
H	1.28174300	-0.48025600	-3.82458000
H	2.75928900	-0.06386900	-2.96710500
H	1.87045700	1.94570200	-4.12640800
H	0.32344400	1.79474900	-3.26430500
H	1.80317100	2.19427500	-2.37104600
N	0.21524400	-1.73400100	-0.14490000
S	-1.27899500	-2.06602500	0.55606200
O	-1.01993800	-2.35990200	1.97939700
O	-1.99009500	-3.08196300	-0.25936300
C	-2.20302700	-0.53401400	0.46503300
C	-2.18657600	0.34698100	1.54989500
C	-2.84920200	-0.19557600	-0.72692000
C	-2.83929500	1.57424100	1.43734700

H	-1.67036500	0.07635600	2.46504300
C	-3.49340700	1.03843600	-0.82283500
H	-2.85542600	-0.88384500	-1.56581900
C	-3.50192200	1.93917200	0.25381700
H	-2.83368400	2.25997600	2.28115900
H	-3.99806100	1.30467400	-1.74820900
C	-4.22892100	3.25530400	0.15376300
H	-5.24925200	3.16374500	0.55097100
H	-3.72242000	4.03514200	0.73291600
H	-4.30939500	3.58864900	-0.88624000
C	2.49438000	0.37827500	0.28643100
C	2.51528500	1.23088500	1.41325700
C	3.70102300	-0.20650900	-0.15861200
C	3.71459900	1.51500500	2.05925300
H	1.58317700	1.66678300	1.76336100
C	4.89691300	0.07720400	0.49239000
H	3.68733900	-0.88965200	-1.00172200
C	4.90572200	0.94016300	1.59741500
H	3.72669000	2.17721100	2.92017200
H	5.82301400	-0.37447500	0.14869400
H	5.84215600	1.15814300	2.10391000
H	0.37222200	0.57493400	0.09955800

83-ts

C	1.41561300	2.31325700	0.44074500
C	-0.12509500	1.40289000	1.48151900
C	-0.14957600	2.29275300	0.38914600
H	-0.84454200	0.91907400	2.13181300
H	-0.64654700	1.49315600	-0.65612800
C	-1.00295300	3.54426000	0.25296000
C	-0.73668900	4.28876000	-1.05835800
H	-0.80121500	4.21593100	1.09926100
H	-2.05963800	3.25651000	0.31998200
H	-1.35529100	5.19202900	-1.11839600
H	0.31382900	4.59729700	-1.12804700
H	-0.96175500	3.66123000	-1.92794900
N	1.21829900	1.29518900	1.55094300
S	2.24951000	0.19929000	2.36488100
O	1.39256700	-0.40358700	3.39266200
O	3.43104500	0.98703100	2.73082800
C	2.70555600	-1.00641800	1.14934500
C	1.73332000	-1.89843500	0.69204200
C	4.00960600	-1.01027200	0.64689900
C	2.08546400	-2.81255200	-0.29857100
H	0.71967800	-1.86545300	1.07838000
C	4.33950000	-1.94005900	-0.33480000
H	4.74212800	-0.29705600	1.00739600
C	3.38629300	-2.84840100	-0.82558500
H	1.33470600	-3.50289100	-0.67282800
H	5.34897400	-1.95220600	-0.73741200
C	3.75712500	-3.82055800	-1.91380900
H	2.93605200	-4.51026500	-2.13205100
H	4.00913900	-3.28571600	-2.83887400
H	4.63906300	-4.40893300	-1.63248700
S	-2.31390300	-1.97880000	0.19580100
O	-1.52032400	-1.35806400	1.27283100
O	-2.66173300	-3.40784600	0.27826300
C	-3.82405800	-1.03585000	0.02278700
C	-3.86464700	0.28741100	0.47292700
C	-4.92603000	-1.62033100	-0.60405300
C	-5.03051800	1.02742900	0.28999900
H	-3.00289600	0.73076000	0.95825500
C	-6.08514200	-0.86241800	-0.77867100
H	-4.88535300	-2.64941200	-0.94628400
C	-6.15671300	0.46742200	-0.33704200
H	-5.06797600	2.05603700	0.64025000
H	-6.94746400	-1.31336200	-1.26268100
C	-7.41174800	1.28138900	-0.51734000
H	-7.85688200	1.53190200	0.45436200
H	-7.19616400	2.22878900	-1.02639600
H	-8.15930100	0.73715500	-1.10299200
N	-1.41875700	-1.78775900	-1.19987700
H	-1.89625400	-2.21826900	-1.99458800
C	2.28563000	1.89214900	-0.70730600
C	3.44671000	2.62640300	-0.98219100
C	1.98746300	0.76693000	-1.48994700
C	4.29532100	2.24989200	-2.02827000
H	3.68702200	3.49406800	-0.37240600
C	2.83261300	0.38964500	-2.53206700
H	1.10416100	0.17660500	-1.27980100
C	3.98881900	1.12996700	-2.80561400
H	5.19262300	2.82848500	-2.23123800
H	2.59374600	-0.48841300	-3.12570000
H	4.64775100	0.83147100	-3.61683000
H	1.78582400	3.23566800	0.89334700
H	-1.25200000	-0.78422300	-1.38492500
F	-1.17283900	0.98203600	-1.55206300

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C	-3.11632000	-0.32096900	-0.71228600
C	-1.12398900	-0.32571600	-1.53211200
C	-2.22581800	0.75022200	-1.41900500
H	-1.08052400	-0.77352600	-2.52971300
H	-1.93989500	1.51105700	-0.69093100
C	-2.73011700	1.38861900	-2.70049600
C	-3.91841200	2.32176400	-2.45509300
H	-3.01060600	0.59972000	-3.41111300
H	-1.90294300	1.94901800	-3.15770900
H	-4.24325300	2.79558900	-3.38901000
H	-4.77362700	1.77479100	-2.04067700
H	-3.65507700	3.11717900	-1.74612300
N	-1.87056400	-1.13824000	-0.55404400

S	-1.91955400	-2.82405200	-0.58039700
O	-1.81234500	-3.35732200	-1.95138800
O	-3.10596600	-3.18019800	0.22077100
C	-0.43392300	-3.23140300	0.31719000
C	0.51431000	-4.07704200	-0.25859900
C	-0.26355500	-2.71388800	1.60460300
C	1.65274500	-4.40785900	0.47483000
H	0.37232600	-4.45206300	-1.26505800
C	0.88324600	-3.05323400	2.32008600
H	-1.00659800	-2.05151300	2.03740100
C	1.85754700	-3.90130700	1.76782700
H	2.40252100	-5.05654100	0.02878400
H	1.02900000	-2.64803300	3.31792200
C	3.10794300	-4.24815300	2.53271400
H	3.15530100	-5.32566400	2.73619600
H	4.00347600	-3.99054700	1.95412200
H	3.15067400	-3.71828000	3.48925900
S	1.51039400	-0.49626000	-2.08018800
O	1.50652700	0.40441900	-3.24470500
O	1.41797700	-1.94476300	-2.33056100
C	2.90502400	-0.14650600	-1.03412500
C	3.87651800	0.74959000	-1.47509300
C	3.01406200	-0.80064700	0.19848100
C	4.97914300	0.99771600	-0.65522100
H	3.77259400	1.24984300	-2.43182300
C	4.11222500	-0.52717200	1.00647500
H	2.26093600	-1.50899900	0.52601700
C	5.11185200	0.37308600	0.59285500
H	5.74290700	1.69454200	-0.98959300
H	4.20140000	-1.02553400	1.96841000
C	6.29786300	0.64733700	1.47911700
H	6.86949100	-0.27192600	1.65922100
H	6.96876700	1.38631400	1.03057400
H	5.97547100	1.02247300	2.45844900
N	0.22658800	0.03046800	-1.06844900
H	0.45894000	1.92860700	-0.48988900
C	-3.79977400	0.05391600	0.57123200
C	-5.18918400	0.22209500	0.60202100
C	-3.05711500	0.29218700	1.73590100
C	-5.82861000	0.63482700	1.77547400
H	-5.77120900	0.02787800	-0.29590300
C	-3.69292700	0.69871000	2.91065200
H	-1.98143800	0.14651300	1.72083100
C	-5.08166000	0.87534100	2.93312600
H	-6.90810400	0.76160700	1.78644900
H	-3.10631800	0.87695400	3.80852200
H	-5.57736300	1.19149400	3.84729100
H	-3.82260800	-0.77026900	-1.41765800
C	-0.07703000	2.68831700	1.36969200
C	0.10326100	4.04142300	2.11045300
H	-1.12388100	2.44138700	1.19346300
H	0.41085200	1.85441900	1.87733100
H	-0.87156100	4.48425800	2.33048400
H	0.63627200	3.88887200	3.05246200
C	-0.06623700	3.92934300	-0.76497300
H	0.40939600	3.93869900	-1.74705600
H	-1.11942900	3.66804100	-0.87448000
C	0.14887600	5.24584700	0.03071800
H	0.73012600	5.95679100	-0.56213300
H	-0.81480200	5.70211900	0.27164400
C	2.19168800	4.41638000	0.98788700
H	2.76483400	5.14619600	0.41019900
H	2.71220400	4.23578300	1.93205200
C	2.05131500	3.09240900	0.18988300
H	2.47603100	3.15329600	-0.81189700
H	2.47500100	2.23243600	0.70954900
N	0.87033400	4.99010400	1.28779400
N	0.57985600	2.82315900	0.02236700
H	0.36655100	-0.32488600	-0.11838100

85-ts

C	-2.08818100	1.63113600	-0.91578300
C	-1.03492800	0.54345700	-2.38674500
C	-0.92454900	1.98396700	-1.92473900
H	-0.85360000	0.06176300	-3.33989400
H	0.01537800	2.23288200	-1.43745200
C	-1.28155200	3.00916300	-3.00118500
C	-1.37315300	4.42029000	-2.41649100
H	-2.23290900	2.72912900	-3.47139700
H	-0.51023400	2.96961900	-3.78011400
H	-1.62547300	5.14358800	-3.20027100
H	-2.14611400	4.48027400	-1.64097000
H	-0.41912900	4.72260900	-1.96774700
N	-2.06247900	0.28350600	-1.57693400
S	-3.34035400	-0.89953900	-1.71784900
O	-2.76050800	-1.99644600	-2.49220600
O	-4.49013100	-0.14397700	-2.22574600
C	-3.61669200	-1.33797400	-0.03147200
C	-2.96087500	-2.44851100	0.50249400
C	-4.42500000	-0.50540400	0.75226100
C	-3.11175000	-2.71652600	1.86134300
H	-2.33372000	-3.07175100	-0.12208100
C	-4.55488300	-0.79150800	2.10657600
H	-4.93012200	0.35043600	0.31831100
C	-3.89351300	-1.88992900	2.68352300
H	-2.60613700	-3.57685200	2.29108000
H	-5.17220400	-0.14921200	2.72869300
C	-4.00179200	-2.14947300	4.16166800
H	-3.34843800	-1.46059300	4.71461000
H	-5.02404000	-1.98461500	4.51989100
H	-3.70026700	-3.17118100	4.41260800

S	0.94417600	-1.88515000	-1.47006300
O	0.90371900	-2.45149500	-2.82566800
O	-0.09060400	-2.22702600	-0.48707400
C	2.53783200	-2.17177100	-0.73621400
C	3.69201400	-1.85342200	-1.46107700
C	2.60432000	-2.68203400	0.55994600
C	4.93120500	-2.04295300	-0.85891700
H	3.62716600	-1.45688600	-2.46980600
C	3.85888600	-2.87750100	1.13945900
H	1.69737800	-2.91170500	1.10825800
C	5.03504300	-2.55498400	0.44795900
H	5.83446100	-1.79047500	-1.40838500
H	3.92137500	-3.27509900	2.14871900
C	6.38775200	-2.73997700	1.08264700
H	7.02848800	-3.37715200	0.46077000
H	6.90021100	-1.77541000	1.19040900
H	6.30493400	-3.19549900	2.07410900
N	0.83012100	-0.19137600	-1.68544200
C	-1.82518300	1.61954200	0.56187500
C	-2.23506600	2.71651000	1.32944800
C	-1.17921400	0.54556500	1.18571600
C	-1.99554900	2.74303000	2.70593100
H	-2.74631600	3.54717500	0.84880500
C	-0.95484600	0.56430900	2.56272400
H	-0.86943400	-0.31760200	0.60807300
C	-1.35861700	1.66352600	3.32721600
H	-2.31653600	3.59962700	3.29269500
H	-0.46641200	-0.28232500	3.03748400
H	-1.18230200	1.67716400	4.39950200
H	-3.01182000	2.16041100	-1.15941500
H	1.43634500	0.08923200	-2.46298300
H	1.13097800	0.37383900	-0.83720500
C	4.31236300	2.72448600	-0.06282200
C	3.16827800	1.95557000	-0.78808900
H	4.49352700	3.69627600	-0.53487200
H	5.24693300	2.15366800	-0.09049700
H	2.68829700	2.57531100	-1.55349500
H	3.54447700	1.04754500	-1.27028500
C	2.66858700	3.66335100	1.40789000
H	2.44583100	3.89295300	2.45571600
H	2.78045500	4.61075100	0.86938300
C	1.54173900	2.79016600	0.77950000
H	0.81033700	2.48474800	1.52992200
H	1.01511500	3.33879900	-0.00668100
C	2.76125100	0.77404000	1.27009800
H	1.97287200	0.41728100	1.93981200
H	3.23619200	-0.09263500	0.80939100
C	3.80744600	1.64743700	2.02206000
H	3.49844800	1.83403100	3.05627200
H	4.78455400	1.15231200	2.04366400
N	2.12498900	1.56220800	0.18864000
N	3.96055000	2.95318600	1.35183800

86-ts

C	2.09812000	0.87403800	0.62074600
C	-0.02463200	1.09560300	-0.06336000
C	1.21534600	1.92578700	-0.05963500
H	-1.03280800	1.37938900	-0.36455000
C	1.12631400	3.24850300	0.72650200
C	0.25297200	4.28354400	0.01700500
H	2.14807800	3.62926100	0.84222400
H	0.74147600	3.04053300	1.73218900
H	0.23294200	5.21740700	0.59020200
H	0.64104300	4.50818700	-0.98389800
H	-0.78055900	3.93303600	-0.08937900
N	0.34221300	-0.04706500	0.39742200
S	-0.66467200	-1.43816200	0.68485200
O	-0.59999300	-1.63774400	2.13608600
O	-0.14539700	-2.46344400	-0.22528900
C	-2.28392700	-0.92493800	0.19302100
C	-3.11156500	-0.29932700	1.13070200
C	-2.67748200	-1.09869900	-1.13990300
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C	-3.93663200	-0.64975800	-1.52474900
H	-2.01598200	-1.57592300	-1.85521800
C	-4.79954700	-0.02651700	-0.60514100
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H	-4.25769300	-0.78456600	-2.55422100
C	-6.16340000	0.43695400	-1.03983600
H	-6.64985200	1.03268700	-0.26168600
H	-6.10078500	1.03860200	-1.95430300
H	-6.80779800	-0.42338000	-1.26360900
C	3.20279200	0.18471600	0.03546000
C	4.06837000	-0.53518700	0.89560900
C	3.44974100	0.18834000	-1.35893400
C	5.15853900	-1.22162800	0.37664100
H	3.86789100	-0.54020100	1.96338700
C	4.54042400	-0.50169800	-1.86969500
H	2.78603000	0.72248200	-2.03026800
C	5.39294600	-1.20471300	-1.00477200
H	5.82443200	-1.76891400	1.03669600
H	4.73296100	-0.49972500	-2.93814800
H	6.24448600	-1.74283800	-1.41198300
H	2.06882200	0.89470600	1.70747300
H	1.52759700	2.13195100	-1.08914400

87

S	-1.72195200	1.84443200	-0.05218300
O	-1.86717800	2.78955900	-1.17053800
O	-1.58139300	2.36882300	1.32105800
C	-3.03398300	0.64546700	-0.09631300

C	-3.67957600	0.38635800	-1.30839200
C	-4.67200700	-0.59124000	-1.34300600
C	-5.02304100	-1.31169500	-0.18903700
C	-4.34968900	-1.03088700	1.01114500
C	-3.35506400	-0.05591900	1.06878900
H	-3.41311800	0.93699800	-2.20447800
H	-5.18179800	-0.79926900	-2.28018000
H	-4.60716900	-1.58193000	1.91177700
H	-2.83955600	0.15230200	2.00047600
C	-6.11749100	-2.34489900	-0.23641800
H	-6.02081500	-3.06699700	0.58076800
H	-7.10134400	-1.86533200	-0.14128600
H	-6.11064600	-2.88765900	-1.18795900
N	-0.38251700	0.83583600	-0.47855900
C	0.49603300	0.65616200	0.42959600
H	0.43282800	1.12201500	1.41891400
C	1.63599200	-0.28972200	0.18248500
C	2.91958700	0.28815200	0.61267800
H	2.88337600	0.97439200	1.45961400
C	1.40953400	-1.58327600	1.08067600
C	0.09428800	-2.28135200	0.73784300
H	1.43672100	-1.29437700	2.13647500
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H	-0.77864700	-1.67585900	1.00162400
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C	4.38631100	-0.91380700	-0.98601300
C	6.59181400	0.30071300	0.30879700
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C	5.66966100	-1.19570400	-1.40622000
H	3.53689700	-1.37355000	-1.47784300
C	6.76701000	-0.59048800	-0.76241300
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88-ts

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C	-5.28118500	1.70196500	0.63797400
C	-4.48301600	1.95841900	-0.49114600
C	-3.59246100	1.00421200	-0.97537900
H	-4.19260200	-1.47184600	1.30648200
H	-5.77396200	0.24316000	2.14868400
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H	-2.98177400	1.21004100	-1.84845700
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H	-5.73092300	3.69629900	1.32613400
H	-7.02610000	2.94291300	0.39354900
H	-6.73135800	2.42721100	2.06610300
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C	0.07621500	-0.63578500	-0.62844300
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C	2.17590500	0.58968500	-0.72397300
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C	1.22632900	-0.08230900	1.60051300
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H	0.20599100	0.27431800	1.77667500
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C	3.95737200	2.09821700	-1.34489200
C	4.20175100	0.80828400	0.73252400
C	5.17513000	2.71502100	-1.10628600
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H	6.87041600	2.84365100	0.21939700
H	1.98980800	-1.29447400	-0.10599500
F	2.71559800	-2.60360200	-0.34429700
H	3.92877100	-2.63582300	0.19489500
F	4.87708100	-2.67825700	0.60311500

Quinuclidine

C	-0.79687400	-0.69321400	1.20407800
C	0.76097500	-0.72465700	1.25047900
H	-1.20611900	-0.17562400	2.07914800
H	-1.21057700	-1.70810400	1.19754800
H	1.13385200	-0.23004200	2.15640500
H	1.12889200	-1.75846300	1.26857200
C	-0.79531000	1.39037800	-0.00111300
H	-1.20478100	1.88934200	-0.88685100
H	-1.20794500	1.89268500	0.88127000
C	0.76240100	1.44472100	0.00145200
H	1.13483000	1.98083000	-0.88069400
H	1.13201500	1.97736200	0.88690000
C	0.76054300	-0.72194600	-1.25237900
H	1.12985200	-0.22251900	-2.15713000
H	1.13157400	-1.75452700	-1.27529700

C	-0.79735300	-0.69537800	-1.20256800
H	-1.21026400	-0.18216300	-2.07848300
H	-1.20772300	-1.71155700	-1.19141500
N	-1.29434500	0.00126400	0.00027500
C	1.29351900	-0.00063700	-0.00019200
H	2.38940800	-0.00166300	-0.00043100

TS-quinuclidine

S	1.12651000	0.54525900	0.77086400
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C	2.64544400	-0.28464300	0.36151900
C	2.58805300	-1.58719600	-0.14524400
C	3.86066600	0.36244200	0.57686500
C	3.77901100	-2.24207600	-0.44402500
H	1.63363100	-2.07796700	-0.30627400
C	5.04451300	-0.31480600	0.27729500
H	3.88335700	1.37442800	0.96604400
C	5.02344500	-1.61884100	-0.23745200
H	3.74614900	-3.25370700	-0.84077800
H	5.99702900	0.18158600	0.44288700
C	6.30039800	-2.34633400	-0.56844200
H	6.38645900	-3.27178500	0.01490200
H	6.32476400	-2.63082000	-1.62788000
H	7.17792800	-1.72680900	-0.35946500
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C	-0.82421800	1.31139500	-0.91479300
H	-1.54975900	0.40925200	-0.53443100
F	1.62412100	1.77091500	-1.45679800
C	-2.18365000	-1.95082000	-0.43922700
C	-3.31666600	-3.00852900	-0.31204100
H	-1.72835800	-1.96187000	-1.43488000
H	-1.39191600	-2.11179500	0.29581600
H	-3.50120100	-3.49477600	-1.27756500
H	-3.02889800	-3.79086800	0.40003100
C	-3.81823200	-0.31177500	-1.15782000
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H	-3.41394700	-0.43549800	-2.16736500
C	-5.01712800	-1.26750900	-0.89960400
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H	-5.30650700	-1.77758900	-1.82574500
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C	-1.24616900	2.56262600	-0.14689600
C	-0.57591600	3.86592300	-0.60262300
H	-1.08797400	2.42052400	0.92829700
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H	-0.66271200	6.01244600	-0.21538400
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H	-1.00204000	5.00899100	1.20570100
H	-1.08664900	1.35373800	-1.97955400
C	-4.59544400	-2.29541300	0.16739000
H	-5.39696600	-3.02423800	0.32782200

$C_7H_{13}NHF$

H	-1.84924000	-0.00020000	0.00027900
F	-3.29833100	-0.00010600	0.00006400
C	-0.28186600	-1.42014600	-0.05926200
C	1.26472900	-1.44559300	-0.05542400
H	-0.71264400	-1.93095000	0.80460300
H	-0.70681200	-1.85432900	-0.96687200
H	1.63002500	-2.00977300	0.80919400
H	1.63497900	-1.94458800	-0.95721500
C	-0.28178600	0.65892600	1.25927600
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C	1.26500700	0.67469200	1.27939300
H	1.63006300	1.70567100	1.33606500
H	1.63503700	0.14330500	2.16257700
C	1.26462400	0.77089100	-1.22405500
H	1.63474000	1.80139100	-1.20474100
H	1.62958500	0.30497900	-2.14551500
C	-0.28208900	0.76155200	-1.19990100
H	-0.70675700	1.76462000	-1.12184800
H	-0.71290400	0.26908900	-2.07427800
N	-0.76035300	-0.00024800	0.00007300
C	1.79063000	-0.00030500	-0.00025500
H	2.88497300	-0.00036400	-0.00053600

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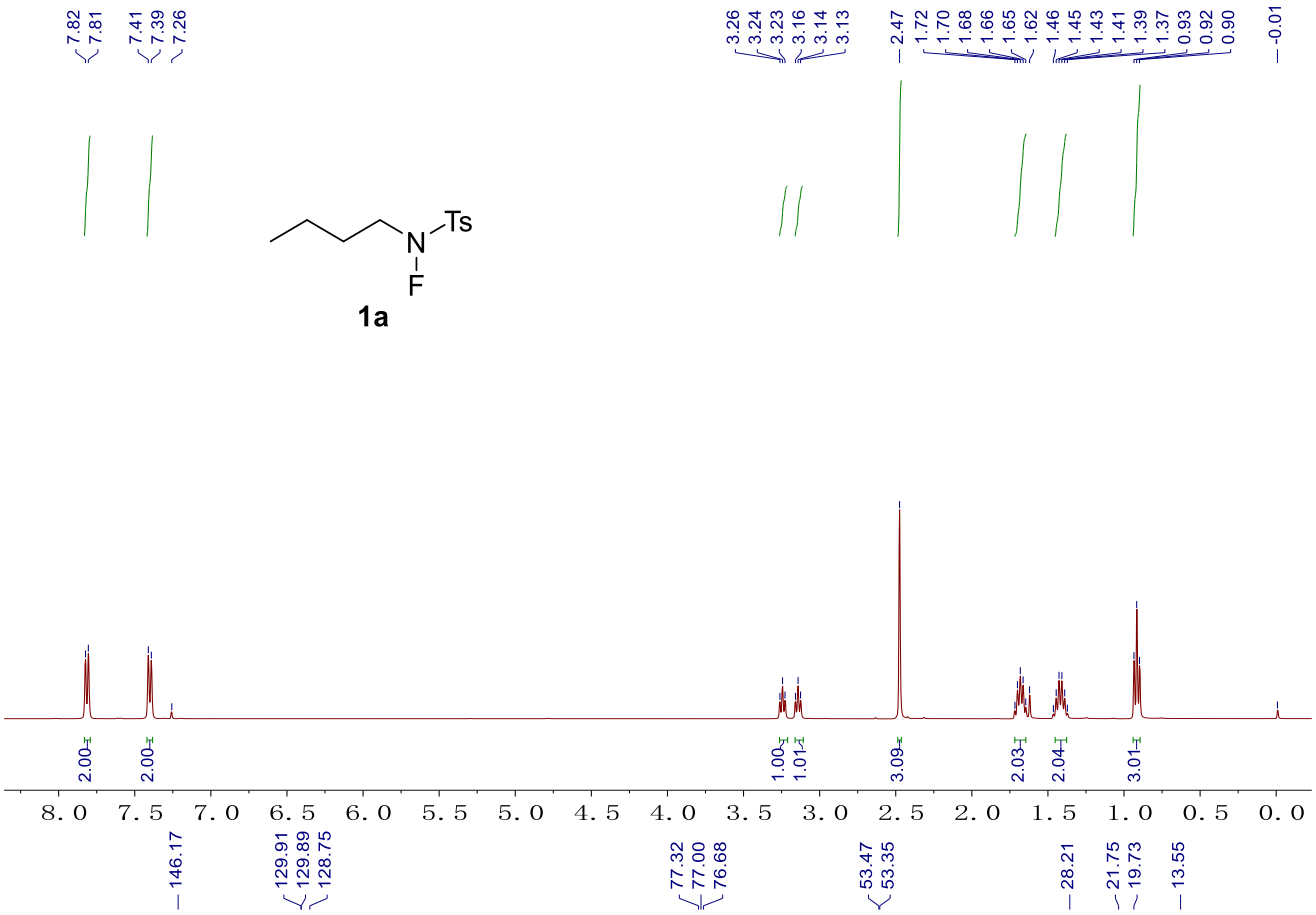
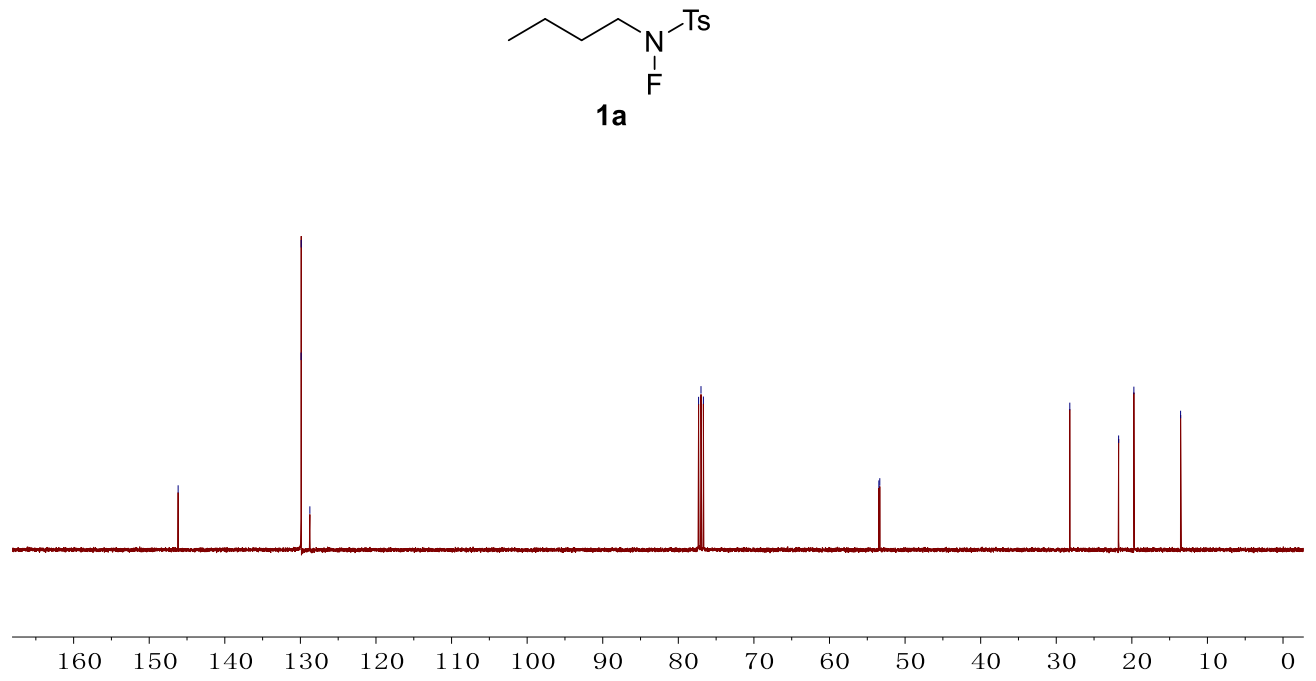
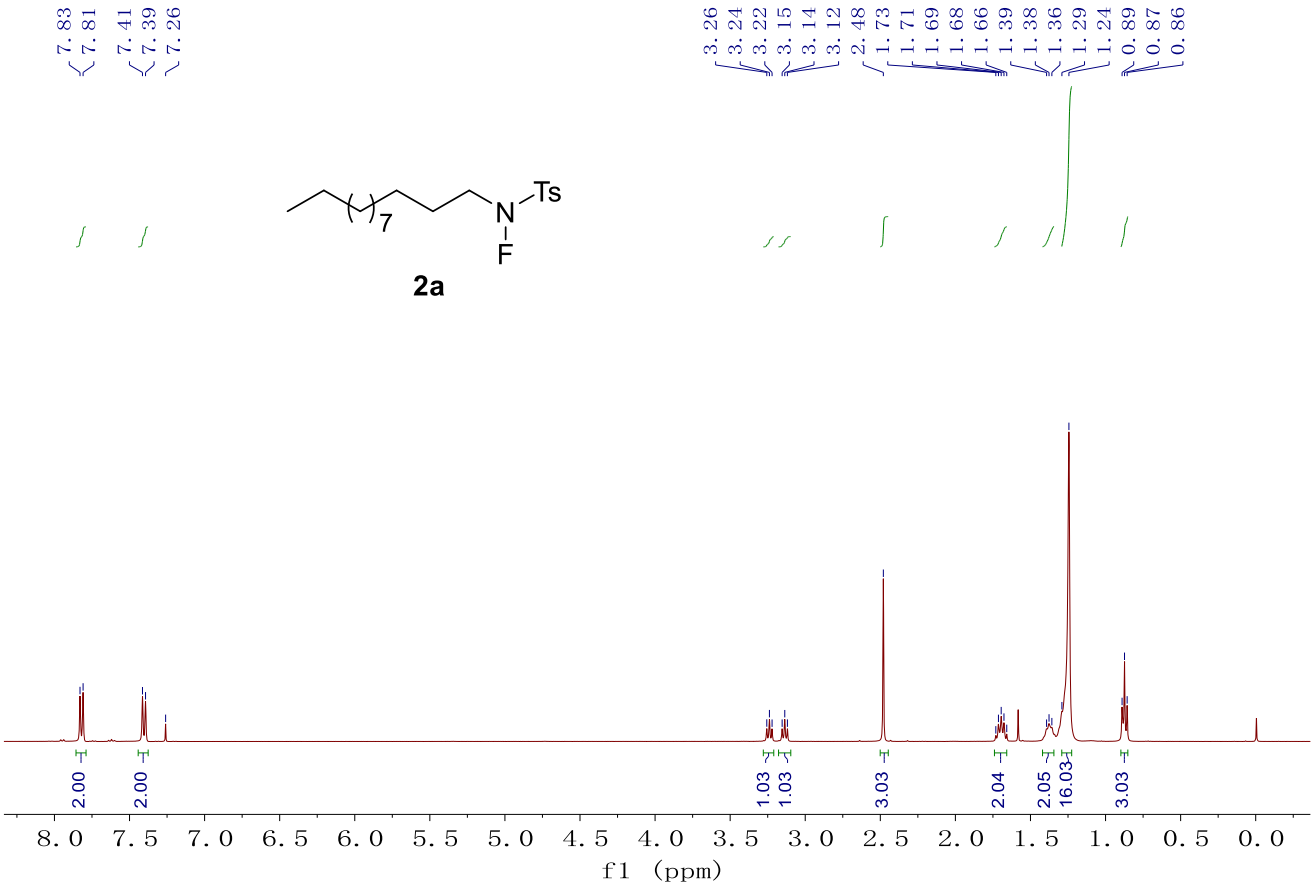
9. Copies of NMR Spectra



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1.29
1.24
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Ts
N
F
7
2a
2.00
2.00
1.03
1.03
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16.03
3.03
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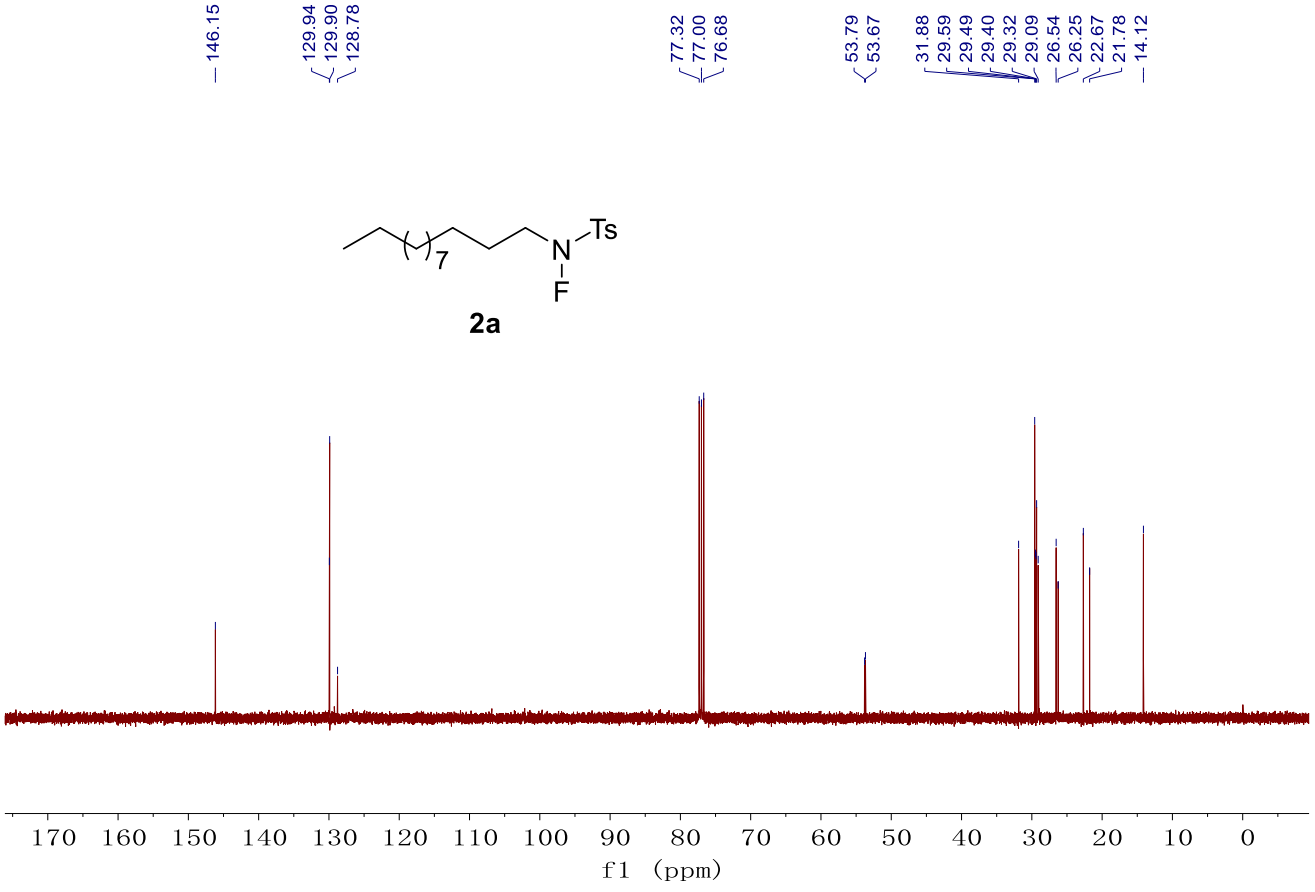
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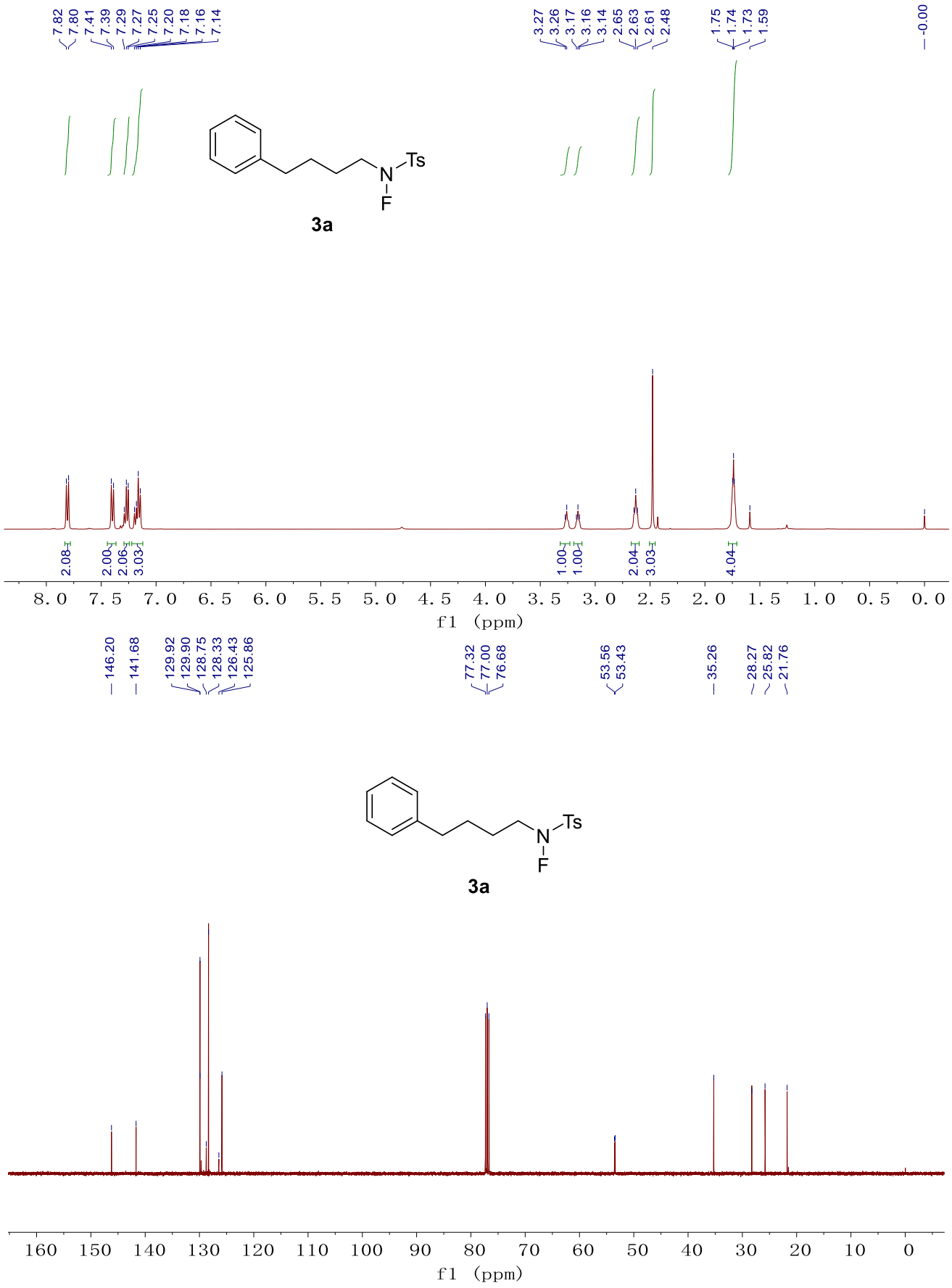
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f1 (ppm)
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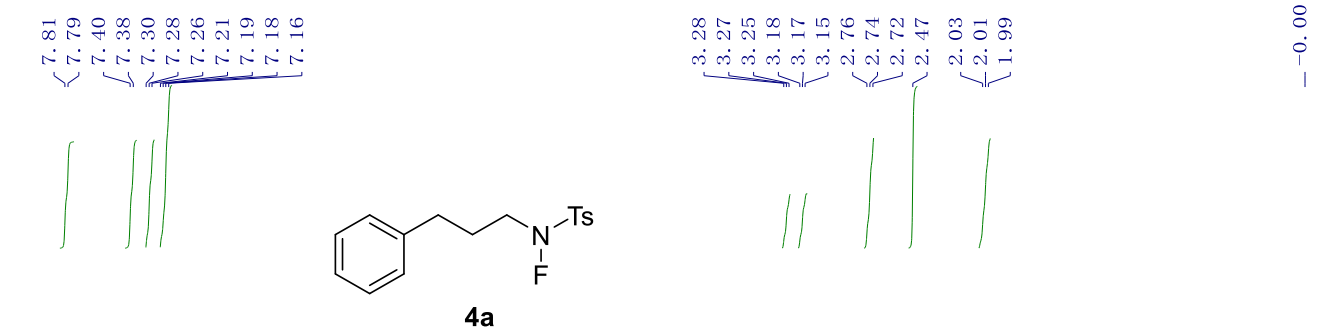
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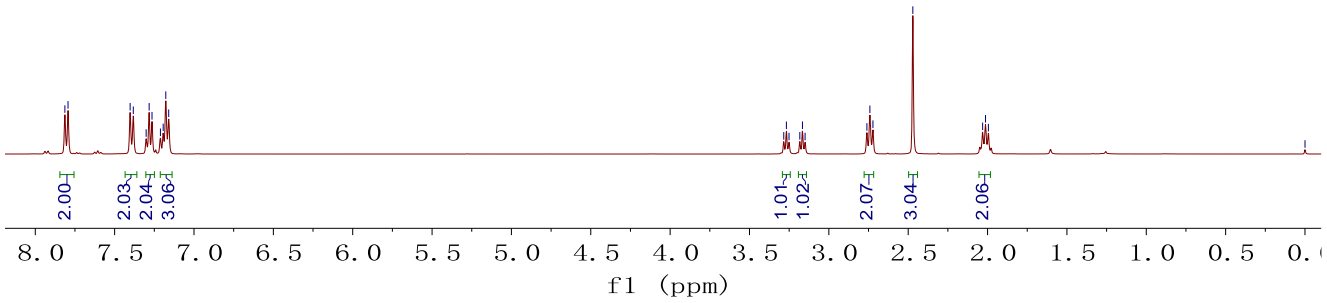
4a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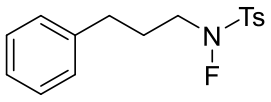
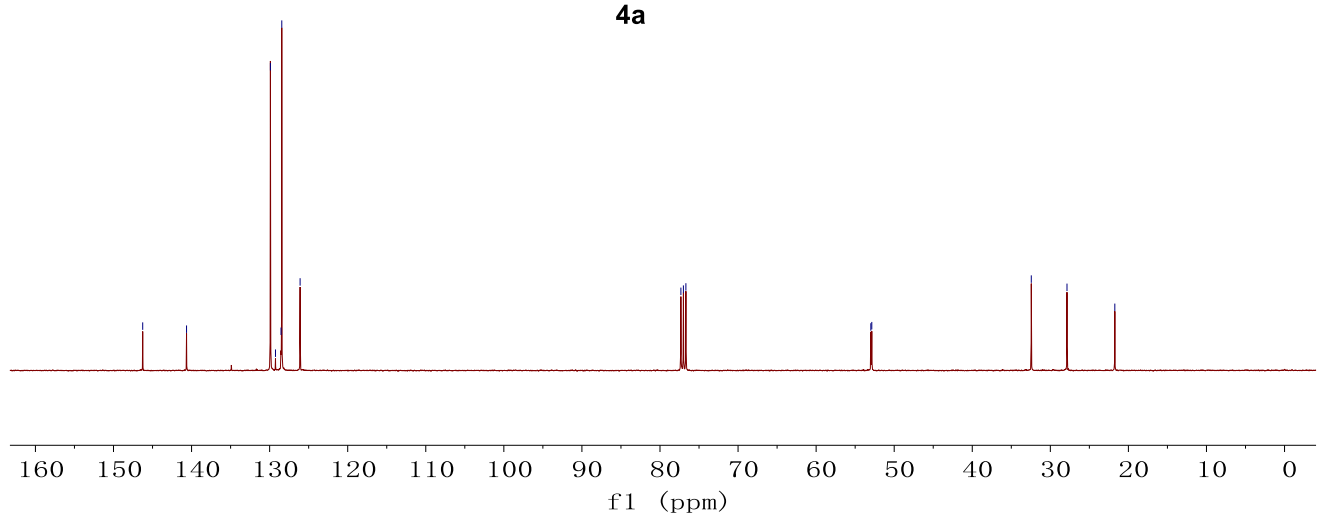
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


146.26
140.64
129.90
129.25
128.54
128.45
126.10
77.32
77.00
76.68
52.99
52.87
32.44
27.87
21.74


Ts
N
F

4a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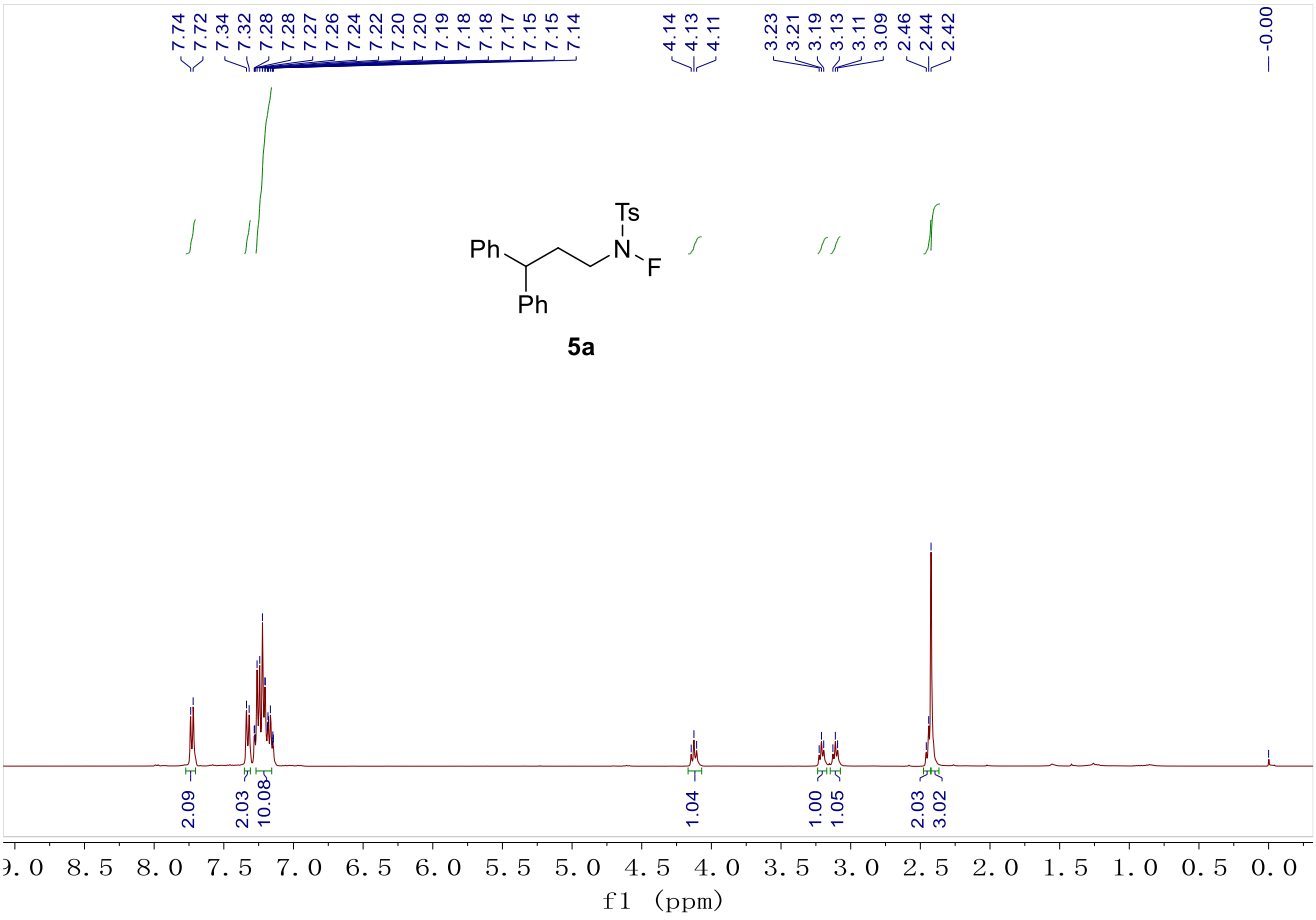
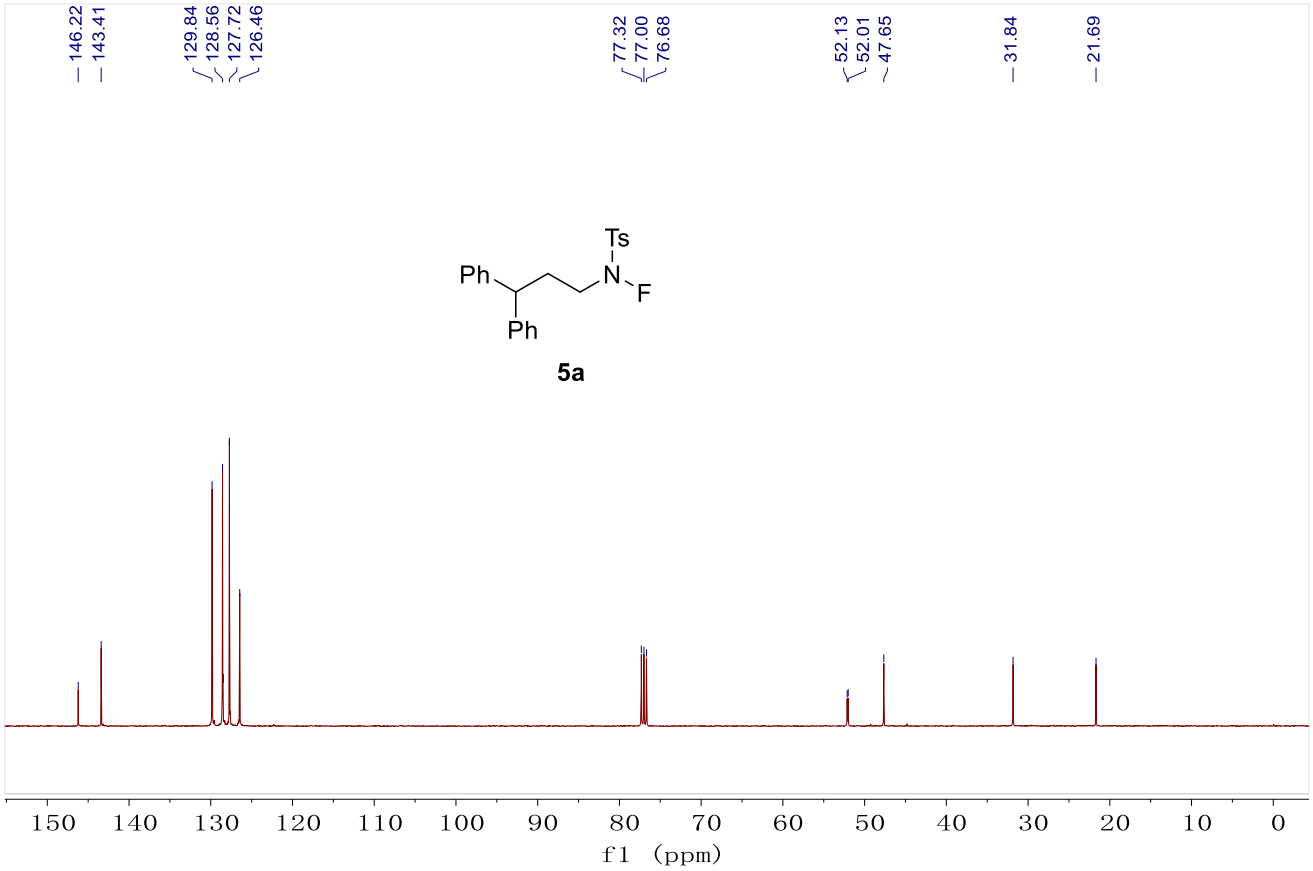
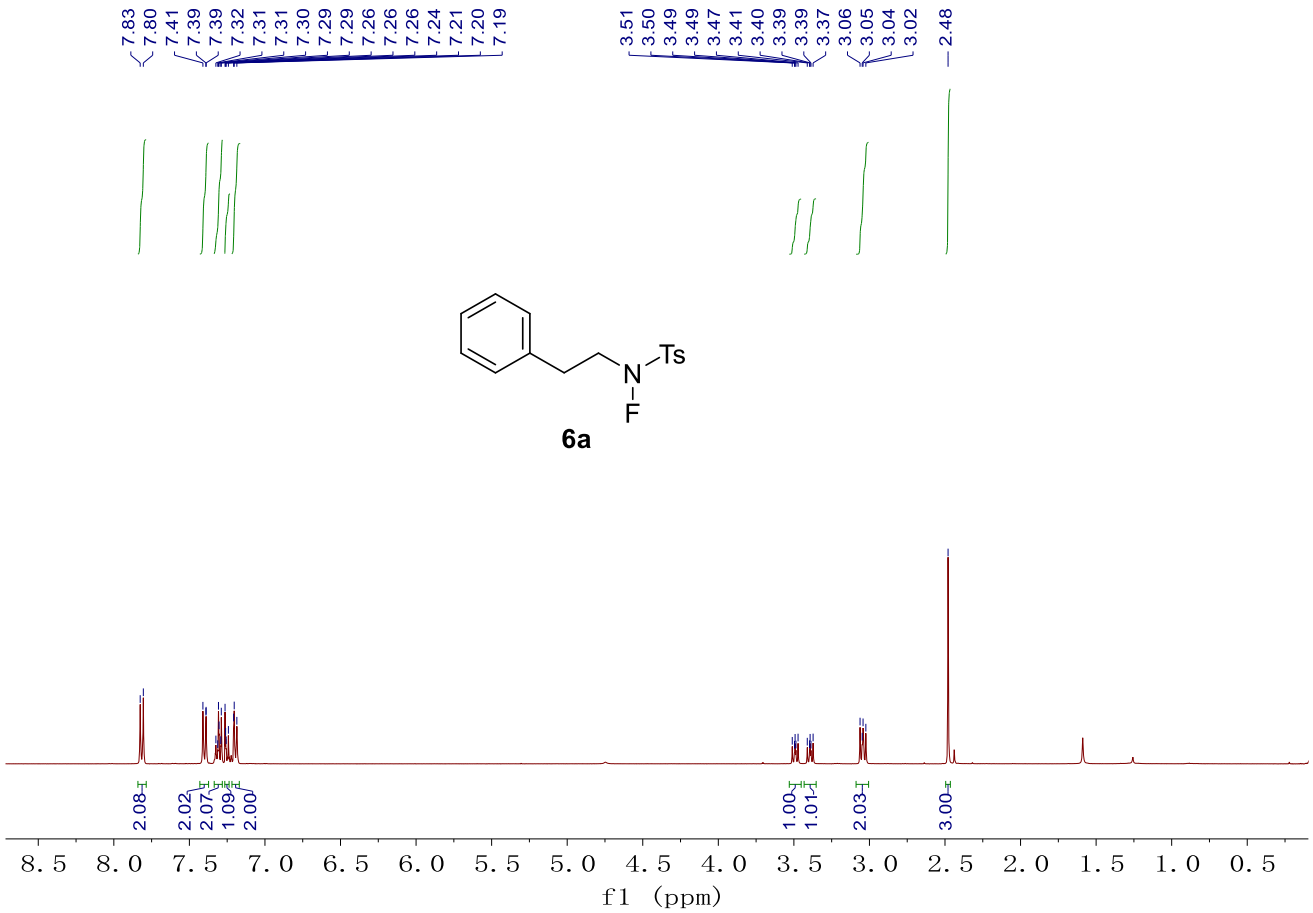
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.74
7.72
7.34
7.32
7.28
7.28
7.27
7.26
7.24
7.22
7.20
7.20
7.19
7.18
7.18
7.17
7.15
7.15
7.14
4.14
4.13
4.11
3.23
3.21
3.19
3.13
3.11
3.09
2.46
2.44
2.42
-0.00
Ts
N
F
Ph
Ph
2.09
2.03
10.08
1.04
1.00
1.05
2.03
3.02
f1 (ppm)

5a


146.22
143.41
129.84
128.56
127.72
126.46
77.32
77.00
76.68
52.13
52.01
47.65
31.84
21.69
Ts
N
F
Ph
Ph
f1 (ppm)

5a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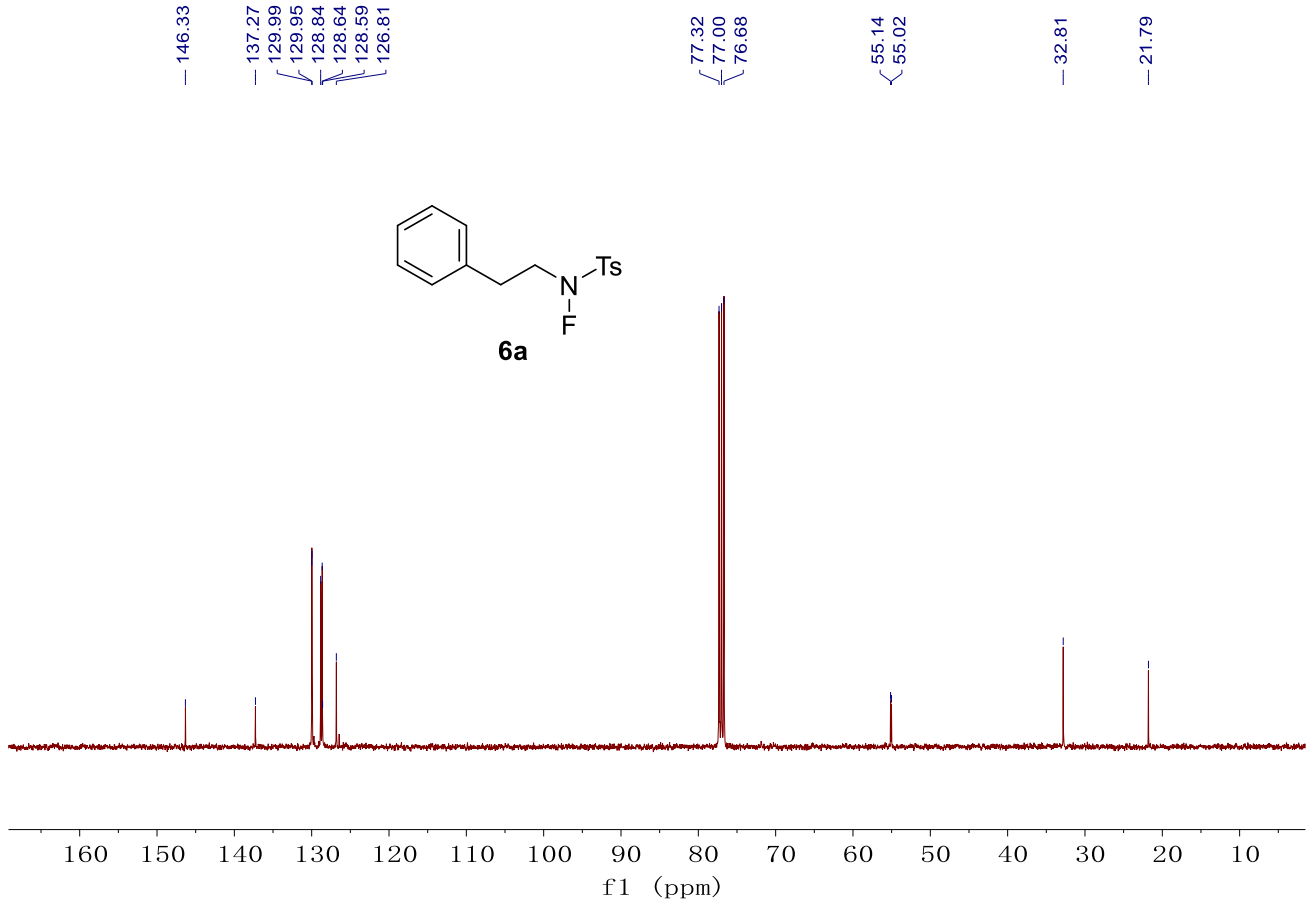
7.80
7.41
7.39
7.39
7.32
7.31
7.31
7.30
7.29
7.29
7.26
7.26
7.26
7.24
7.21
7.20
7.19
3.51
3.50
3.49
3.49
3.47
3.41
3.40
3.39
3.39
3.37
3.06
3.05
3.04
3.02
2.48
Ts
N
F
6a
2.08
2.02
2.07
1.09
2.00
1.00
1.01
2.03
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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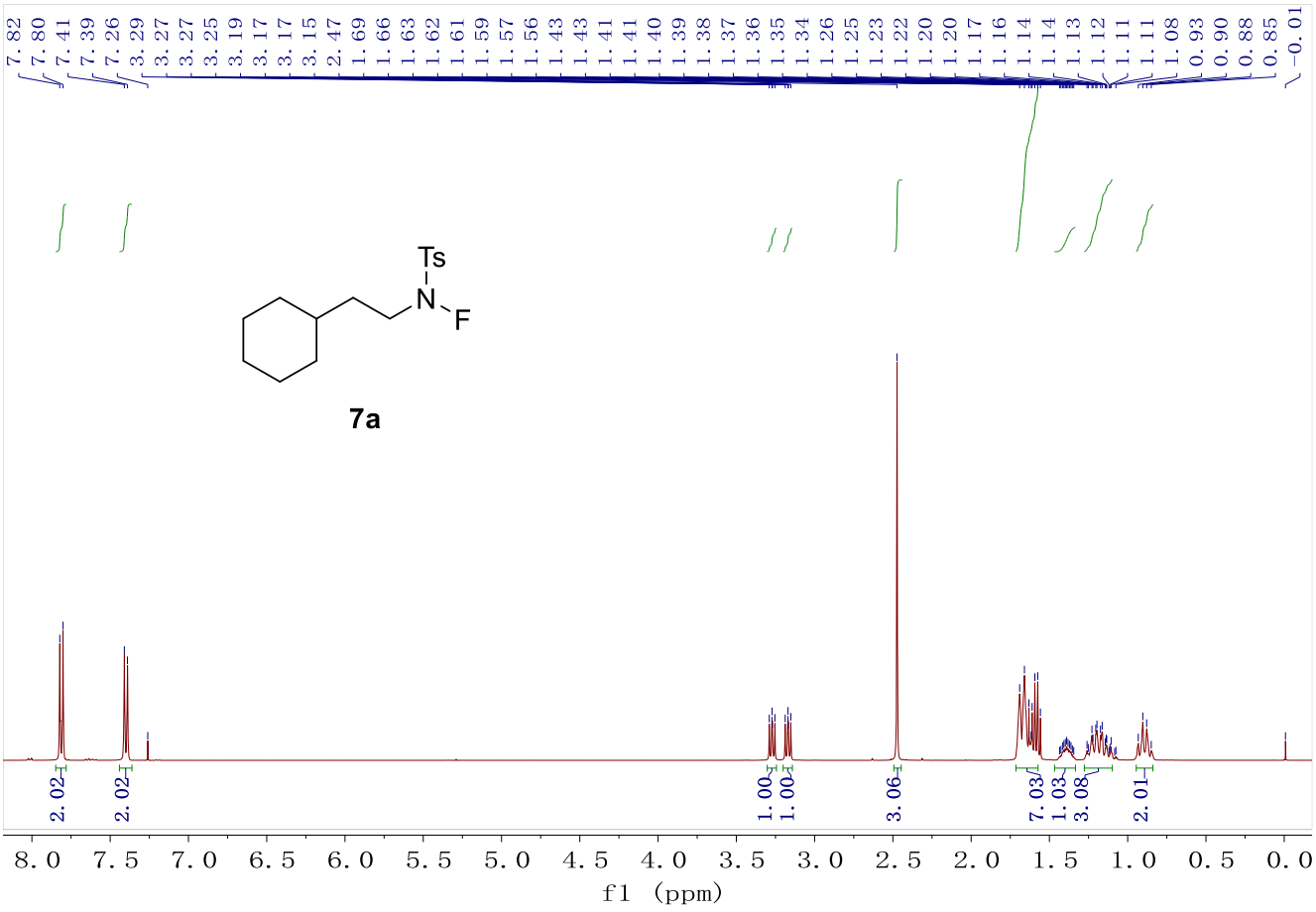
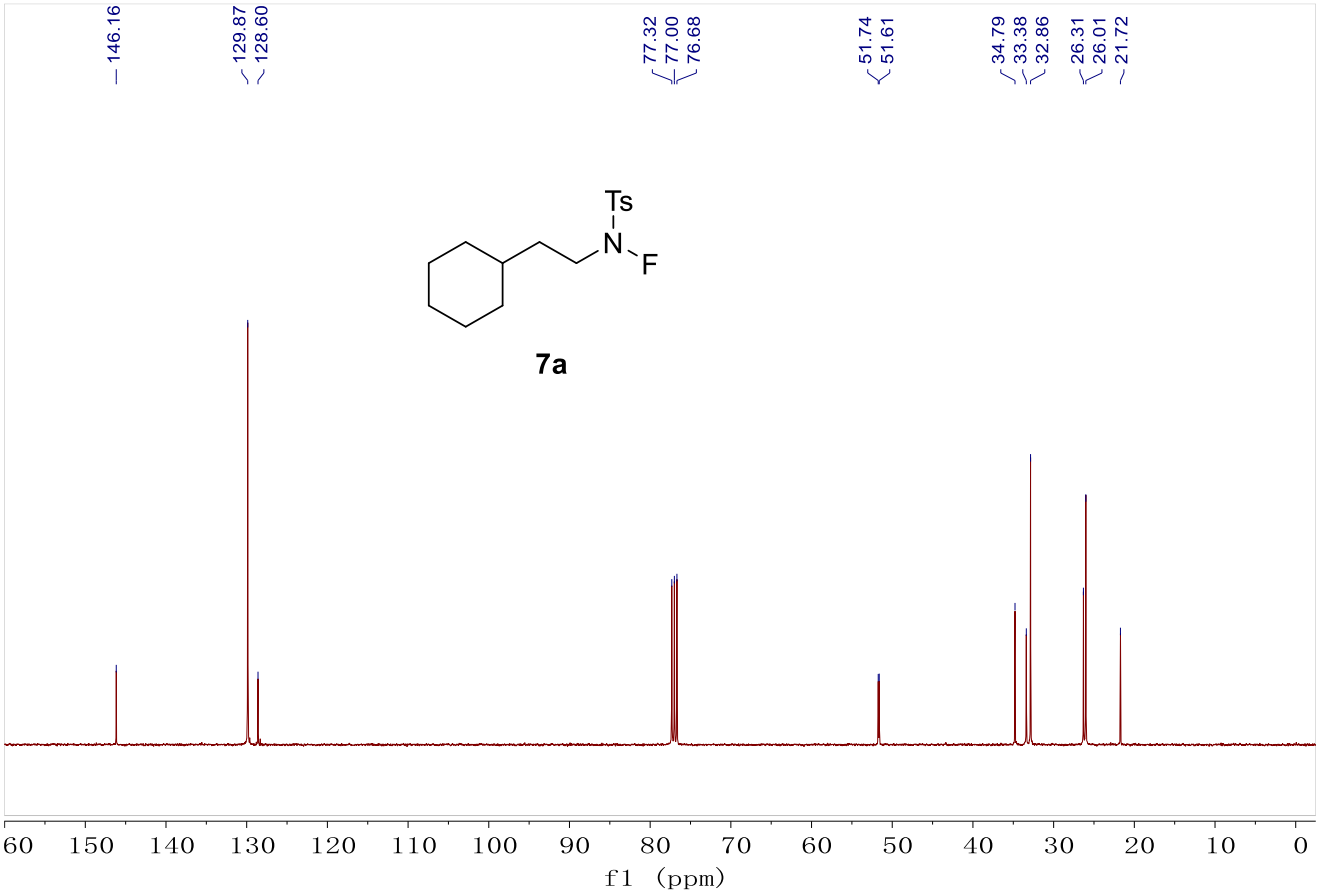
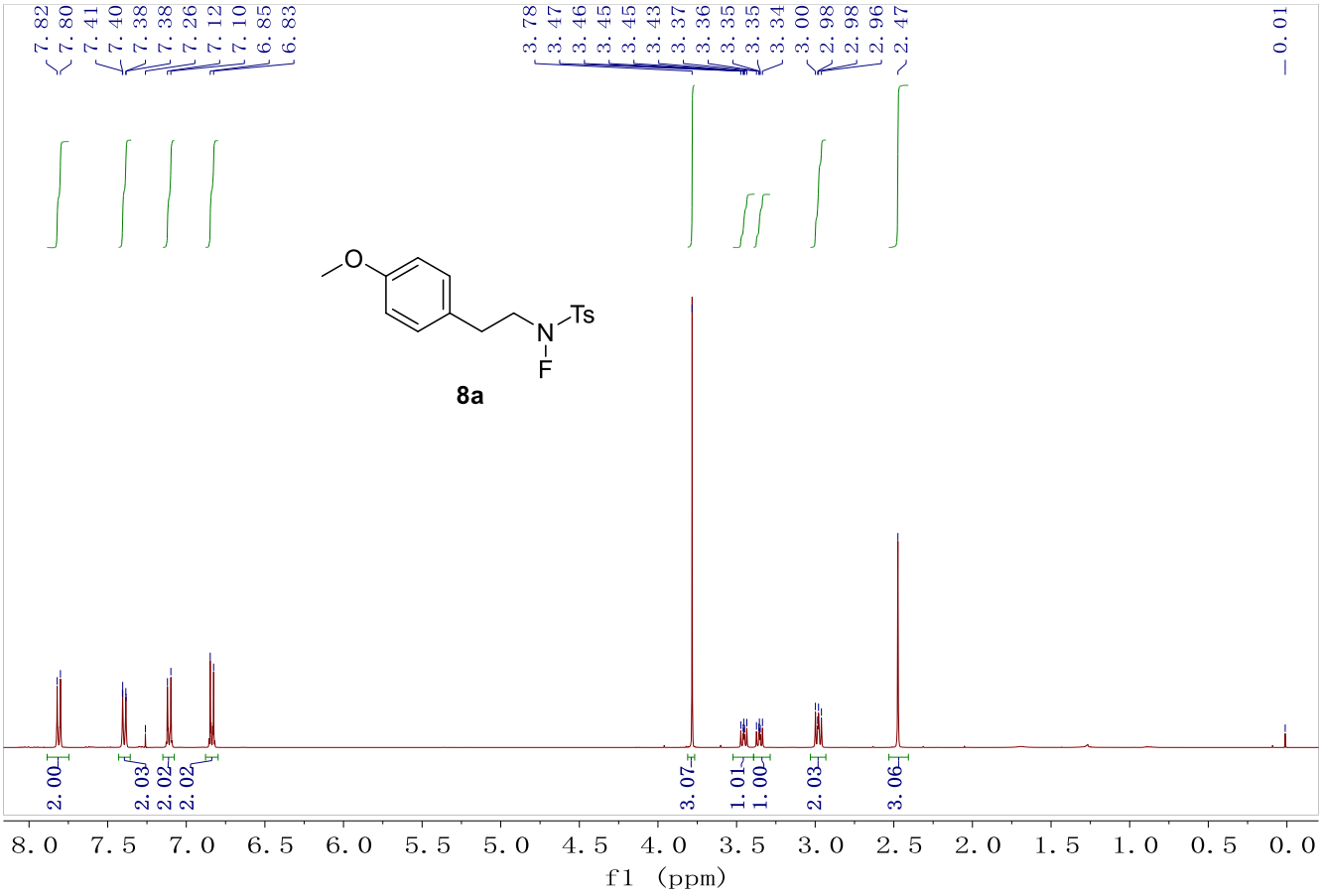
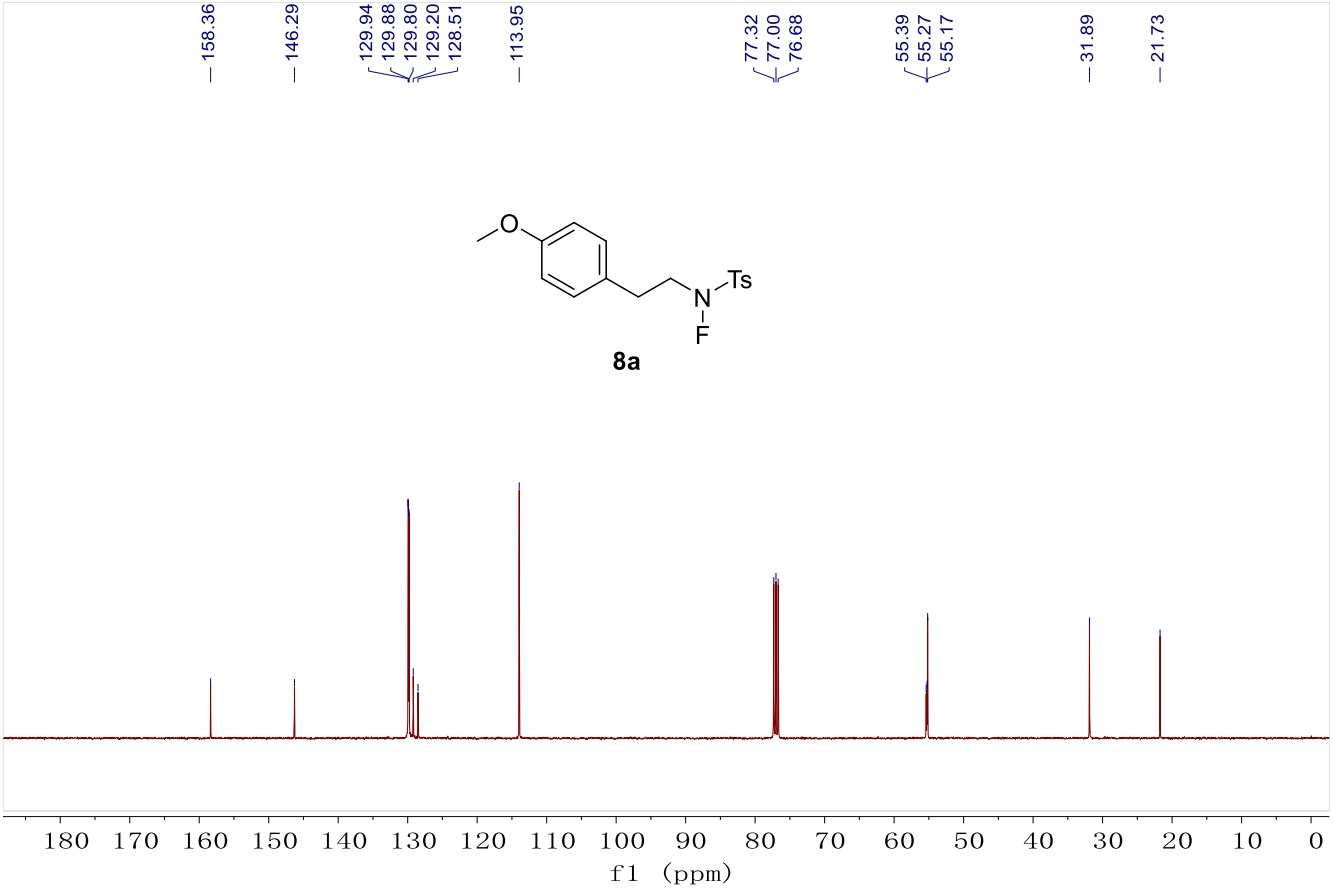
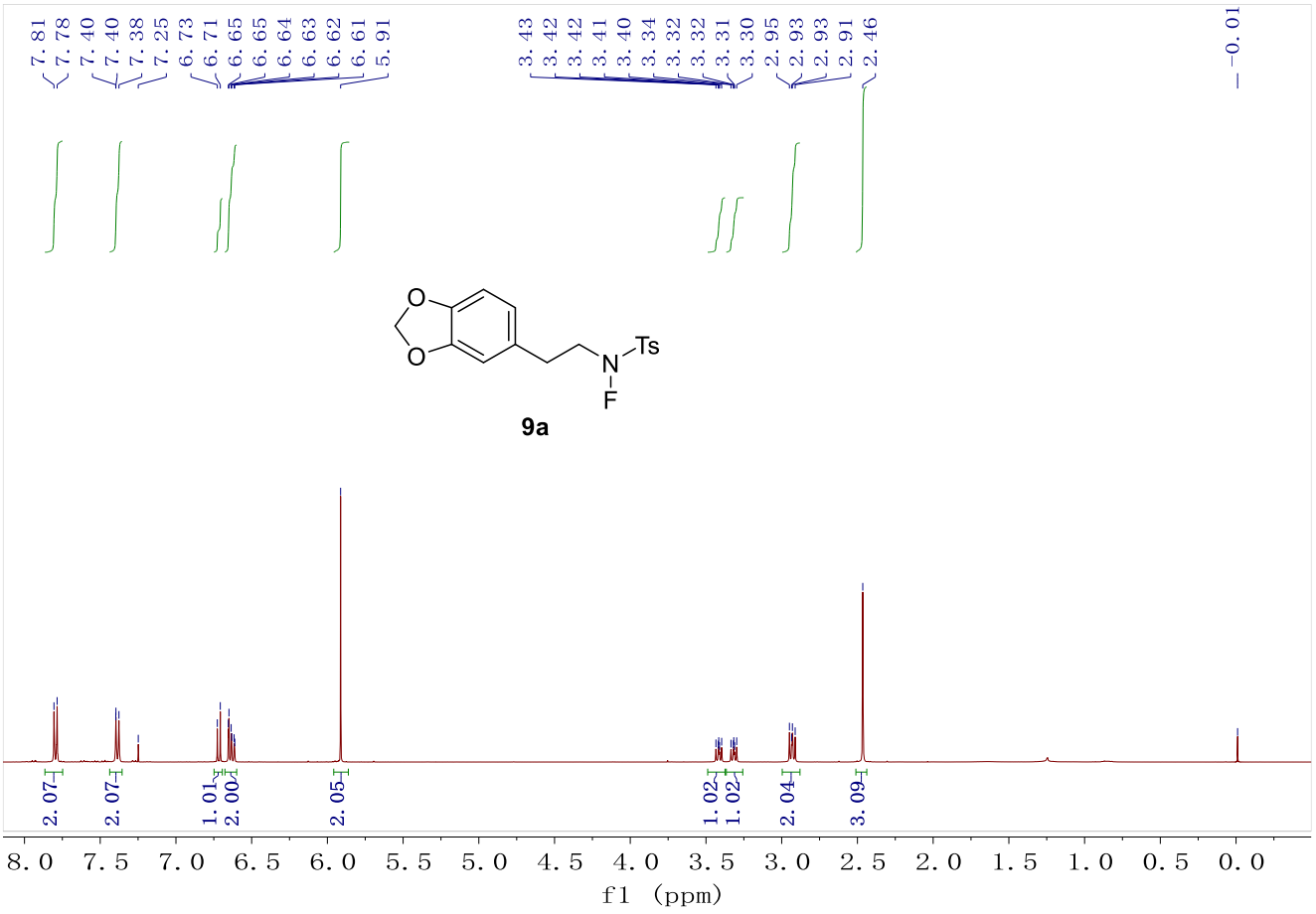
137.27
129.99
129.95
128.84
128.64
128.59
126.81
77.32
77.00
76.68
55.14
55.02
32.81
21.79
Ts
N
F
6a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

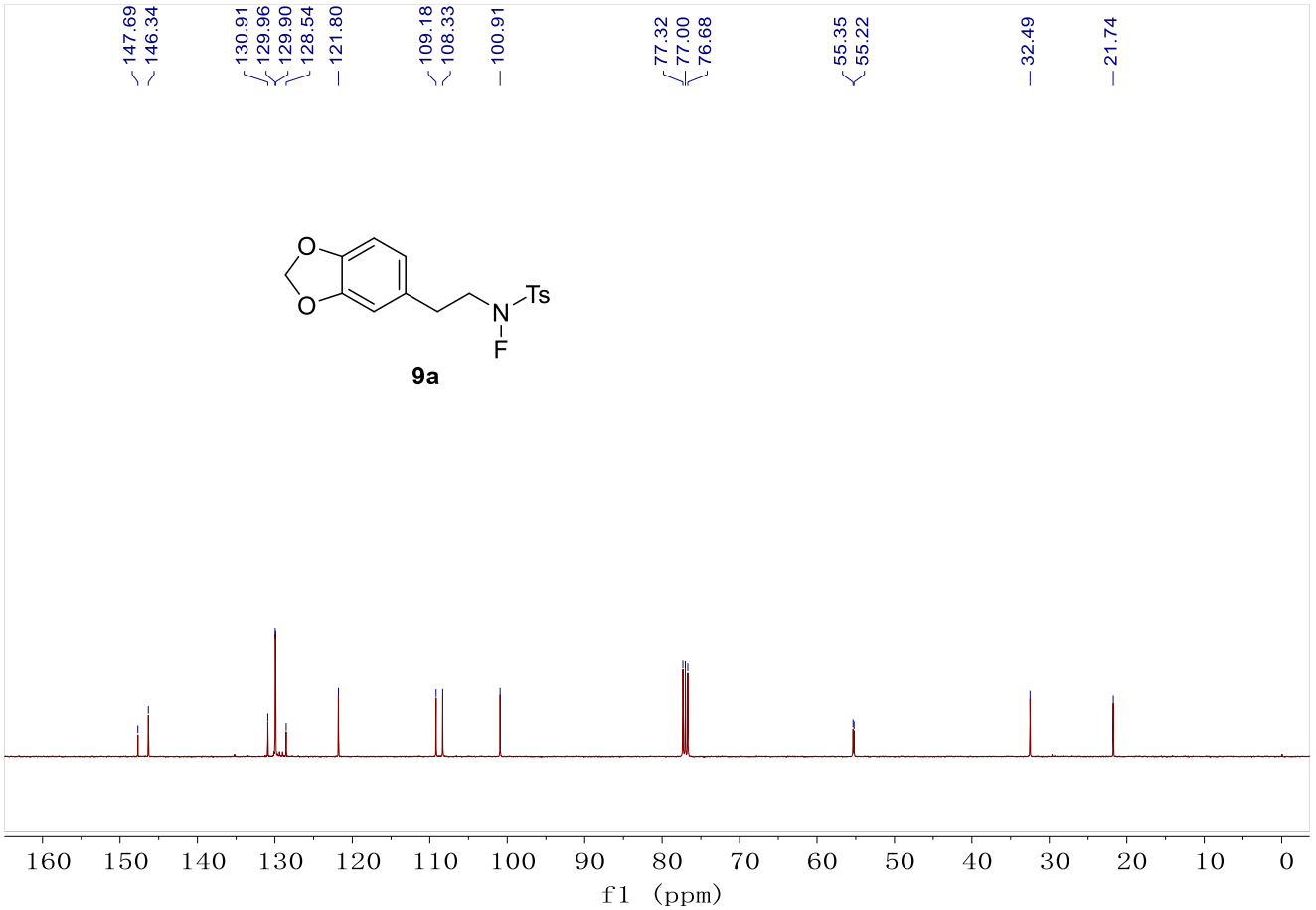

7.82
7.80
7.41
7.39
7.26
3.29
3.27
3.27
3.25
3.19
3.17
3.17
3.15
2.47
1.69
1.66
1.63
1.62
1.61
1.59
1.57
1.56
1.43
1.43
1.41
1.41
1.40
1.39
1.38
1.37
1.36
1.35
1.34
1.26
1.25
1.23
1.22
1.20
1.20
1.17
1.16
1.14
1.14
1.13
1.12
1.11
1.11
1.08
0.93
0.90
0.88
0.85
-0.01
Ts
N
F
7a
2.02
2.02
1.00
1.00
3.06
7.03
1.03
3.08
2.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


146.16
129.87
128.60
77.32
77.00
76.68
51.74
51.61
34.79
33.38
32.86
26.31
26.01
21.72
Ts
N
F
7a
60 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.82
7.80
7.41
7.40
7.38
7.38
7.26
7.12
7.10
6.85
6.83
3.78
3.47
3.46
3.45
3.45
3.43
3.37
3.36
3.35
3.35
3.34
3.00
2.98
2.98
2.96
2.47
0.01
O
Ts
N
F
8a
2.00
2.03
2.02
2.02
3.07
1.01
1.00
2.03
3.06
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


158.36
146.29
129.94
129.88
129.80
129.20
128.51
113.95
77.32
77.00
76.68
55.39
55.27
55.17
31.89
21.73
O
Ts
N
F
8a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.81
7.78
7.40
7.40
7.38
7.25
6.73
6.71
6.65
6.65
6.64
6.63
6.62
6.61
5.91
3.43
3.42
3.42
3.41
3.40
3.34
3.32
3.32
3.31
3.30
2.95
2.93
2.93
2.91
2.46
0.01
O
O
N
Ts
F
9a
2.07
2.07
1.01
2.00
2.05
1.02
1.02
2.04
3.09
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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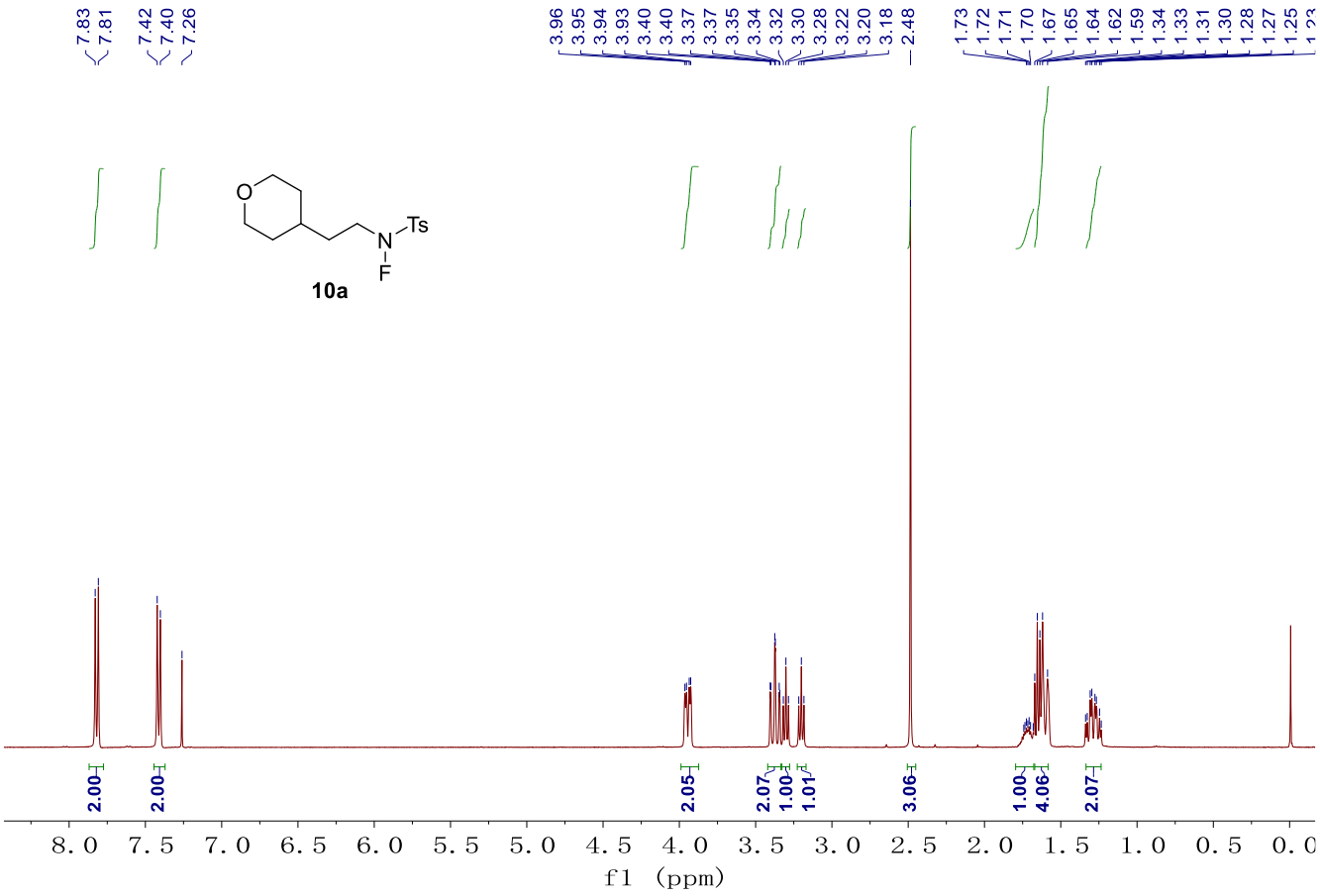
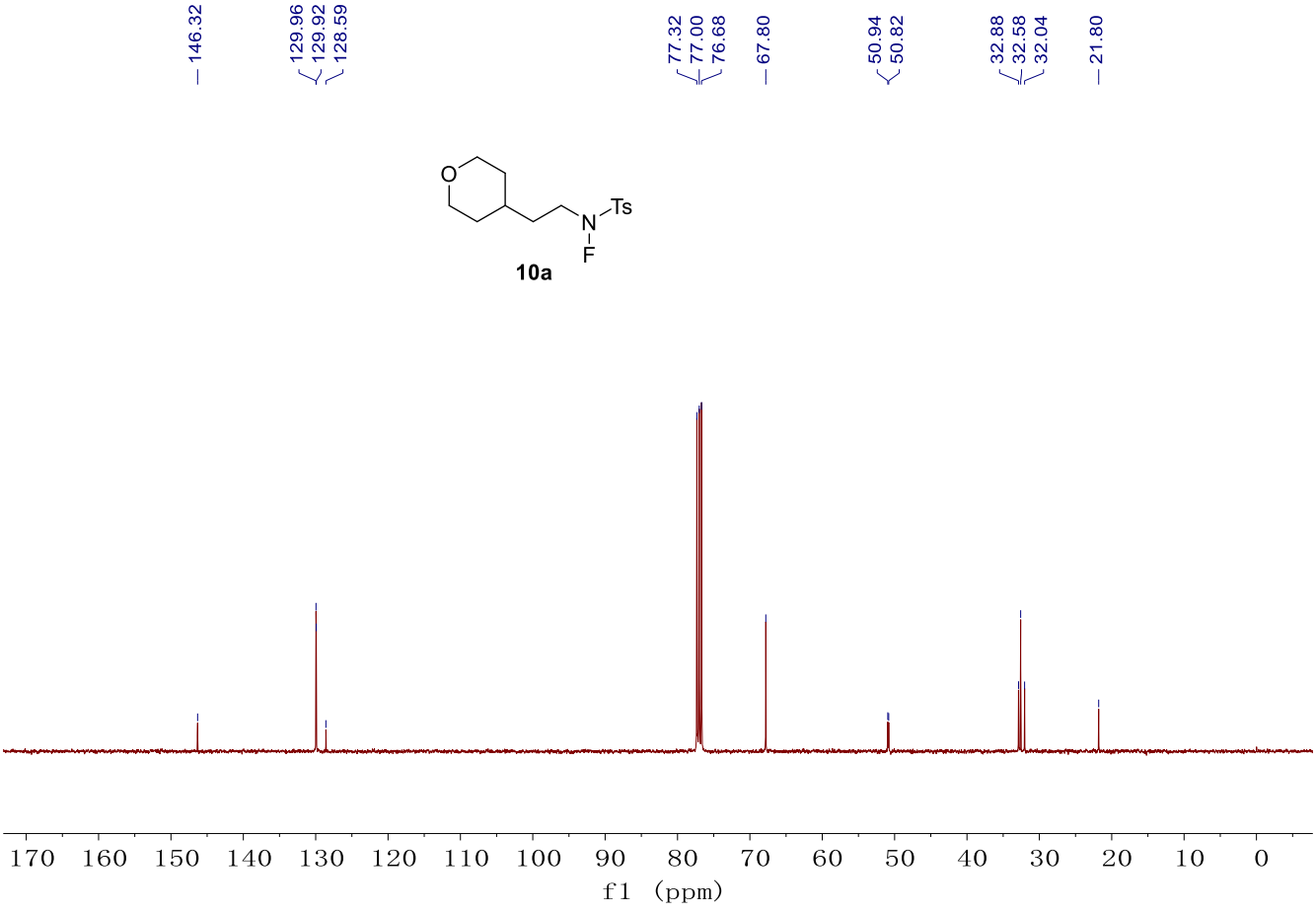
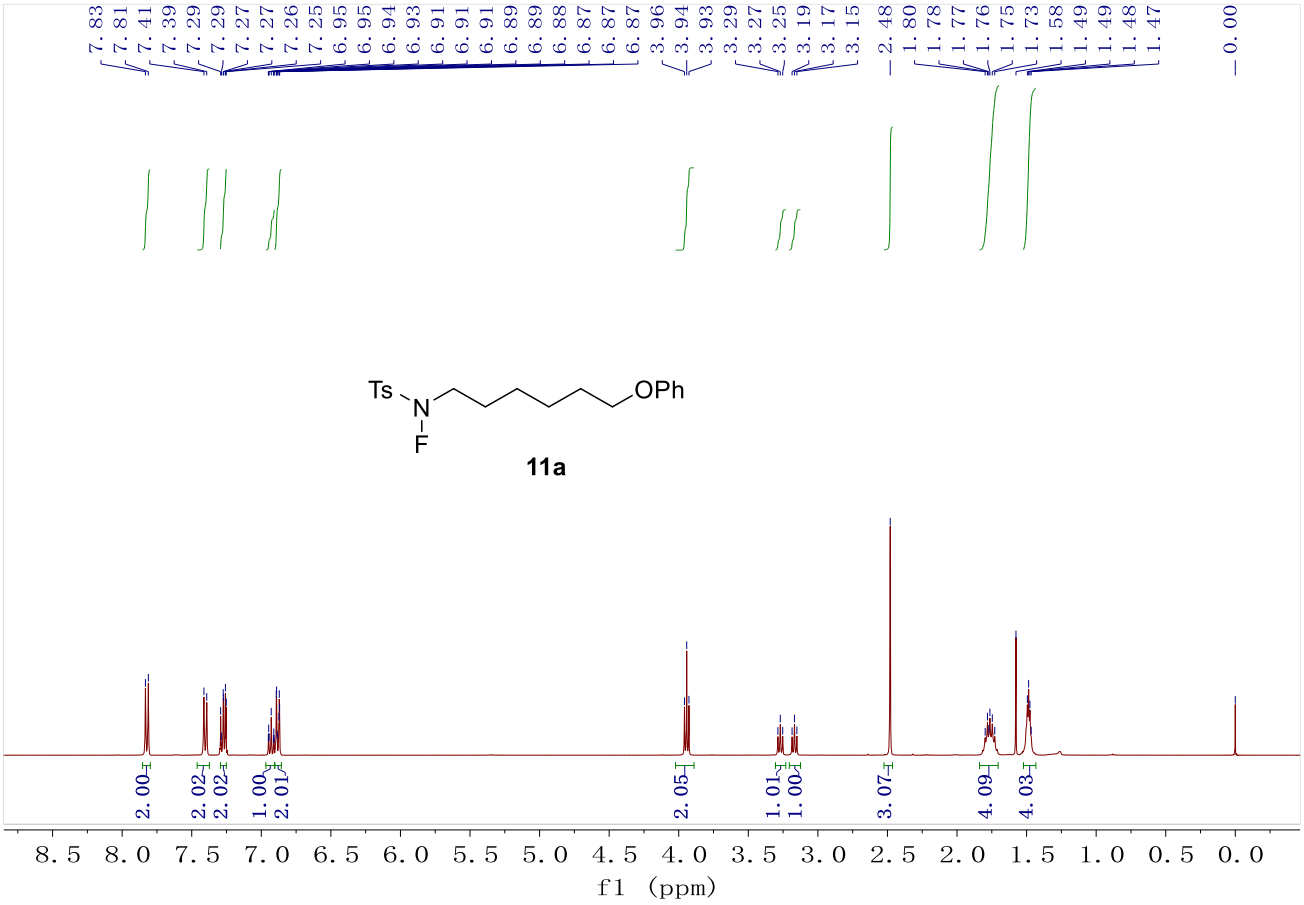
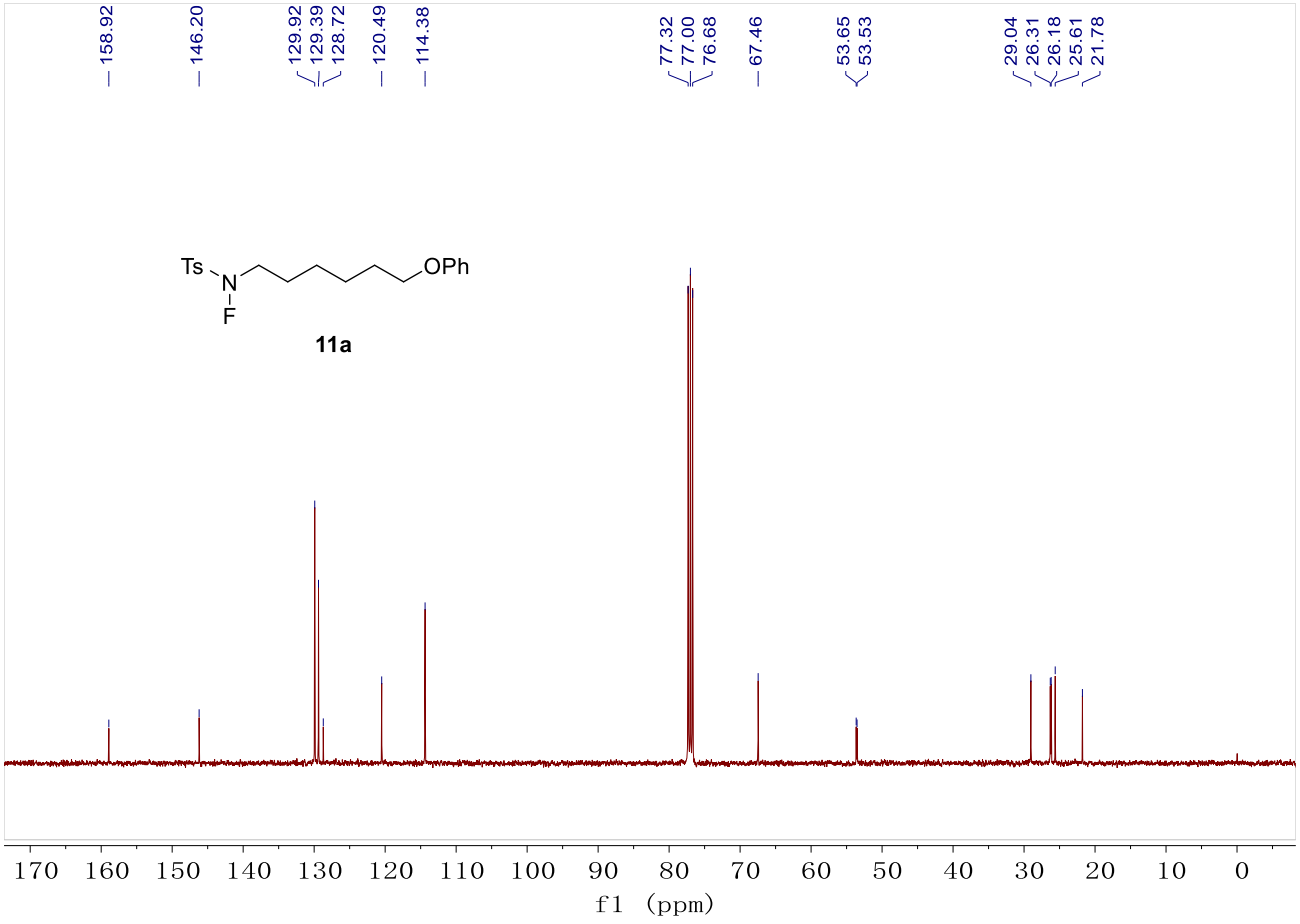
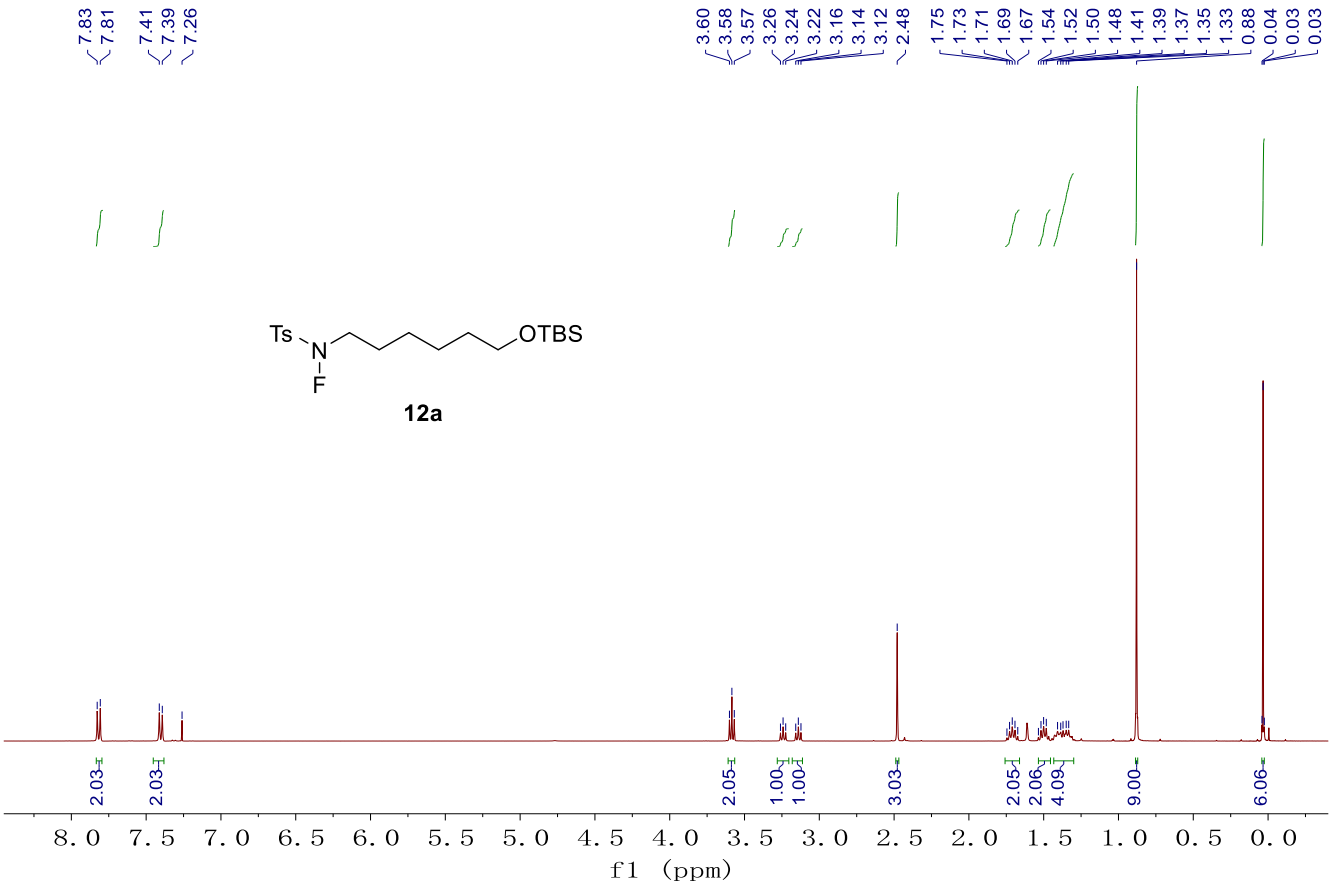
146.34
130.91
129.96
129.90
128.54
121.80
109.18
108.33
100.91
77.32
77.00
76.68
55.35
55.22
32.49
21.74
O
O
N
Ts
F
9a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

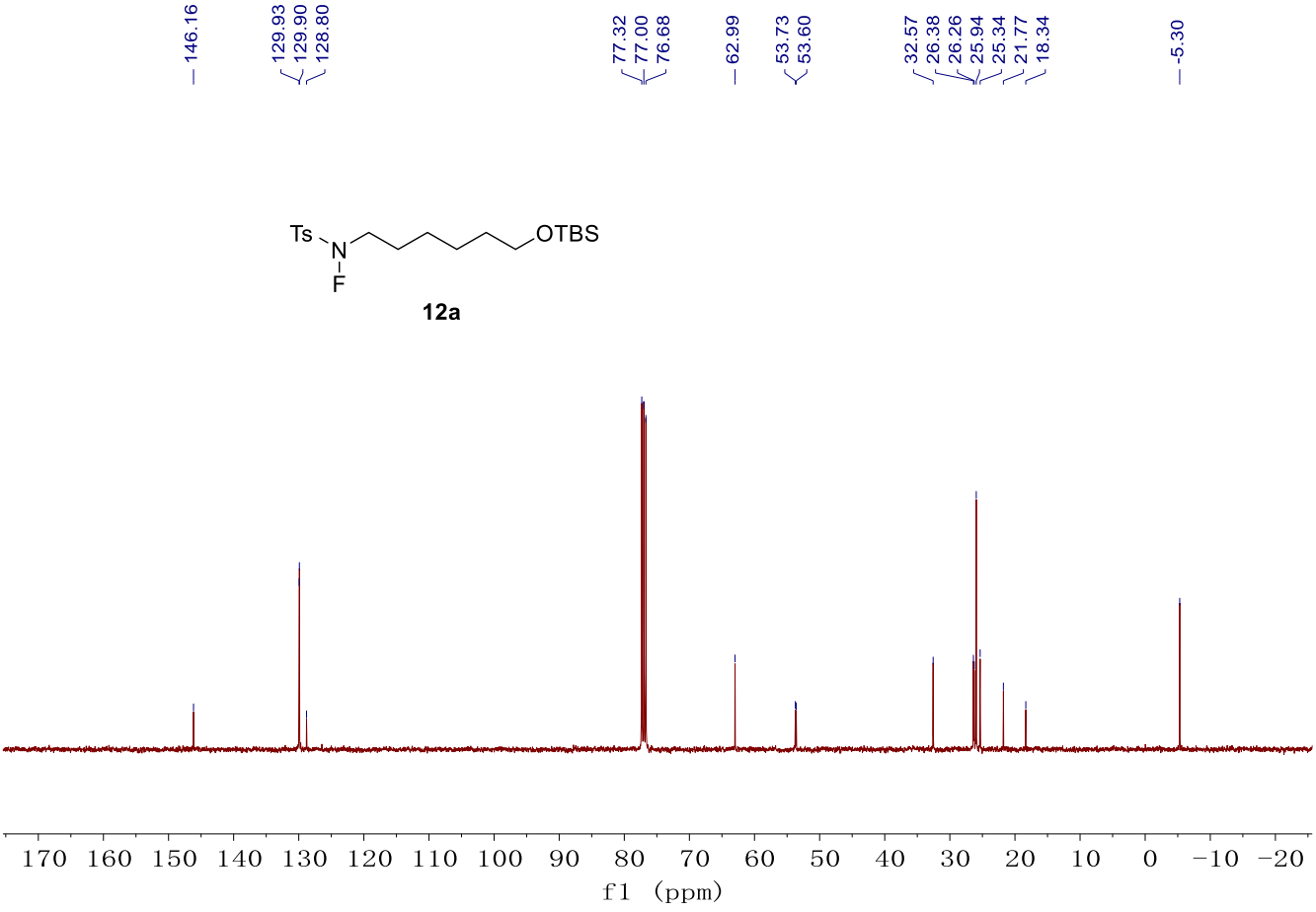

7.83
7.81
7.42
7.40
7.26
3.96
3.95
3.94
3.93
3.40
3.40
3.37
3.37
3.35
3.34
3.32
3.30
3.28
3.22
3.20
3.18
2.48
1.73
1.72
1.71
1.70
1.67
1.65
1.64
1.62
1.59
1.34
1.33
1.31
1.30
1.28
1.27
1.25
O
N
Ts
F
10a
2.00
2.00
2.05
2.07
1.00
1.01
3.06
1.00
4.06
2.07
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


146.32
129.96
129.92
128.59
77.32
77.00
76.68
67.80
50.94
50.82
32.88
32.58
32.04
21.80
O
N
Ts
F
10a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.83 7.81 7.41 7.39 7.29 7.29 7.27 7.27 7.26 7.25 6.95 6.95 6.94 6.93 6.91 6.91 6.89 6.89 6.88 6.87 6.87 6.87 3.96 3.94 3.93 3.29 3.27 3.25 3.19 3.17 3.15 2.48 1.80 1.78 1.77 1.76 1.75 1.73 1.58 1.49 1.49 1.48 1.47 0.00
Ts
N
F
OPh
11a
2.00 2.02 2.02 1.00 2.01 2.05 1.01 1.00 3.07 4.09 4.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


158.92 146.20 129.92 129.39 128.72 120.49 114.38 77.32 77.00 76.68 67.46 53.65 53.53 29.04 26.31 26.18 25.61 21.78
Ts
N
F
OPh
11a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.83
7.81
7.41
7.39
7.26
3.60
3.58
3.57
3.26
3.24
3.22
3.16
3.14
3.12
2.48
1.75
1.73
1.71
1.69
1.67
1.54
1.52
1.50
1.48
1.41
1.39
1.37
1.35
1.33
0.88
0.04
0.03
0.03
Ts
N
F
OTBS
12a
2.03
2.03
2.05
1.00
1.00
3.03
2.05
2.06
4.09
9.00
6.06
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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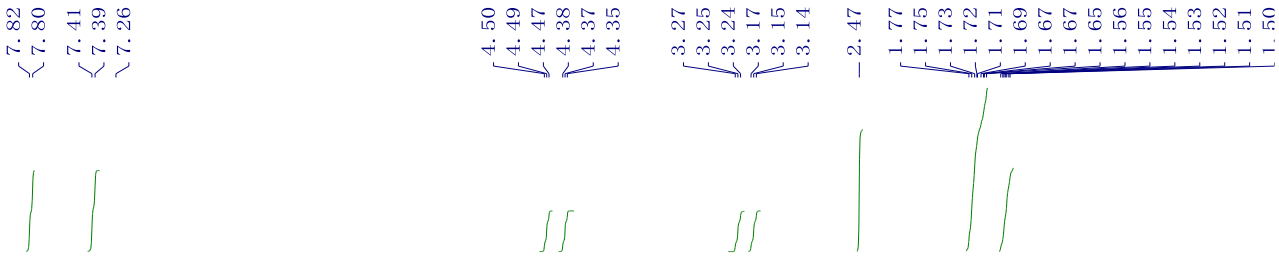
129.93
129.90
128.80
77.32
77.00
76.68
62.99
53.73
53.60
32.57
26.38
26.26
25.94
25.34
21.77
18.34
-5.30
Ts
N
F
OTBS
12a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.82
7.80
7.41
7.39
7.26
4.50
4.49
4.47
4.38
4.37
4.35
3.27
3.25
3.24
3.17
3.15
3.14
2.47
1.77
1.75
1.73
1.72
1.71
1.69
1.67
1.67
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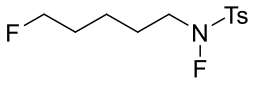
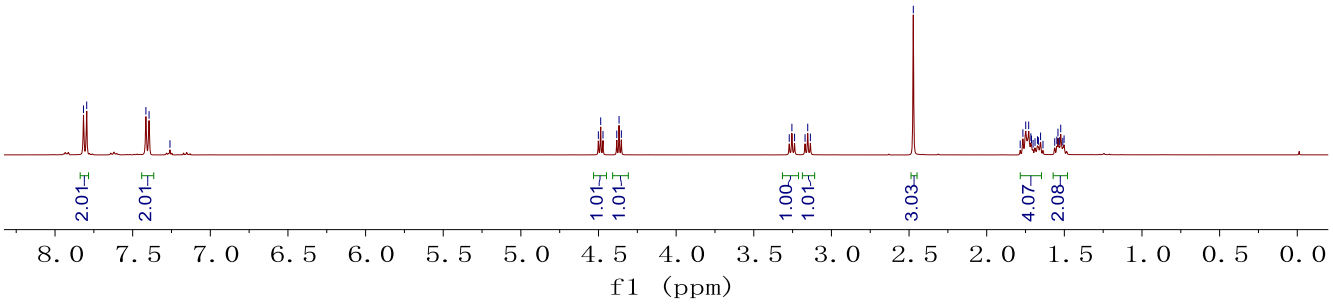
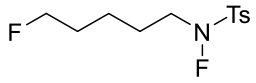
1.56
1.55
1.54
1.53
1.52
1.51


F
N
Ts
F

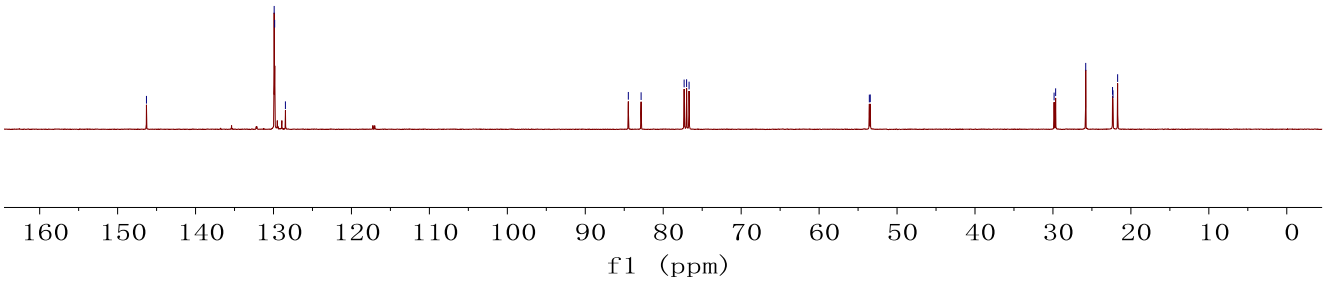
13a

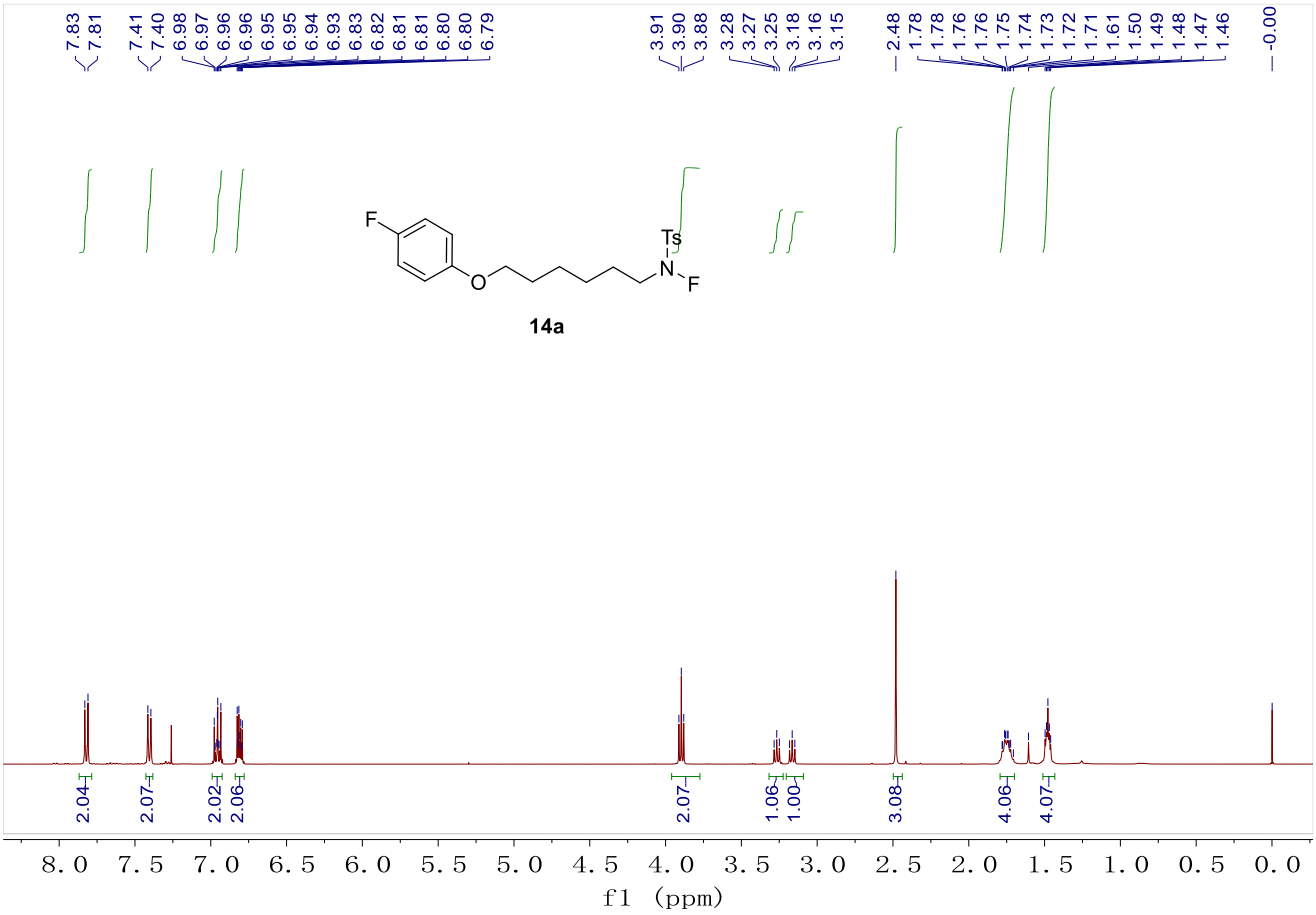

2.01
2.01
1.01
1.01
1.00
1.01
3.03
4.07
2.08
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

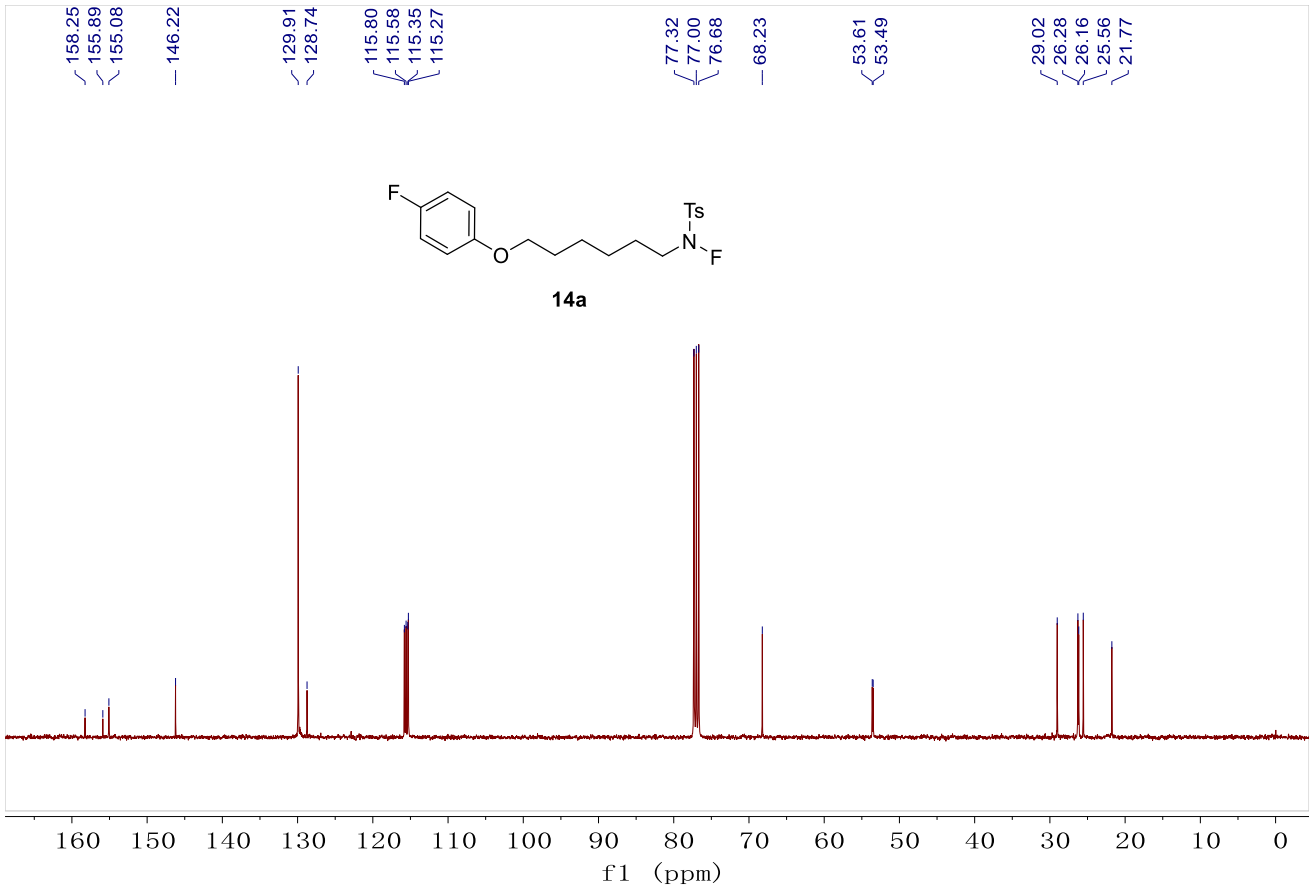

146.30
129.91
129.85
128.47
84.48
82.84
77.32
77.00
76.68
53.56
53.44
29.85
29.65
25.80
22.35
22.30
21.70

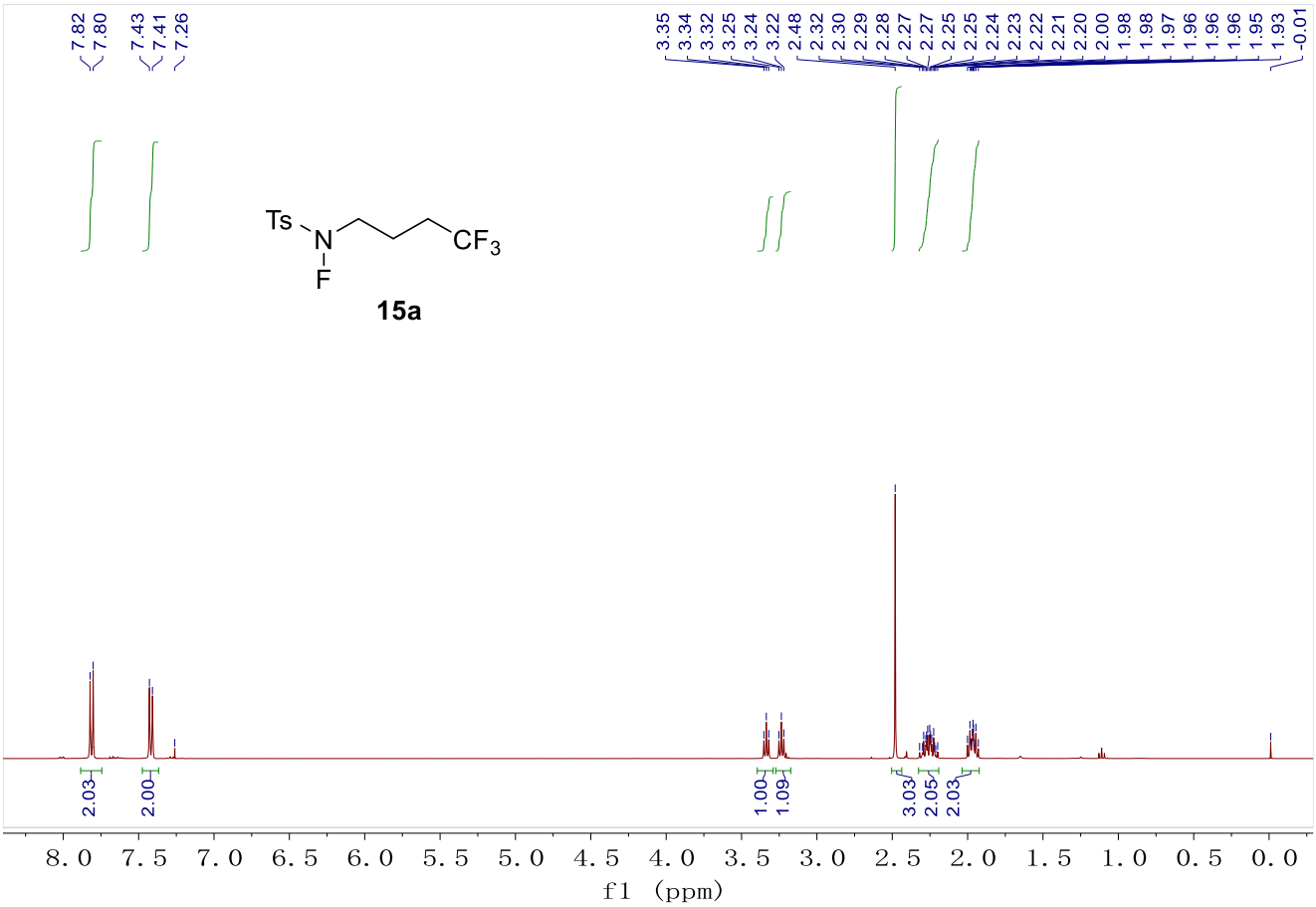

F
N
Ts
F

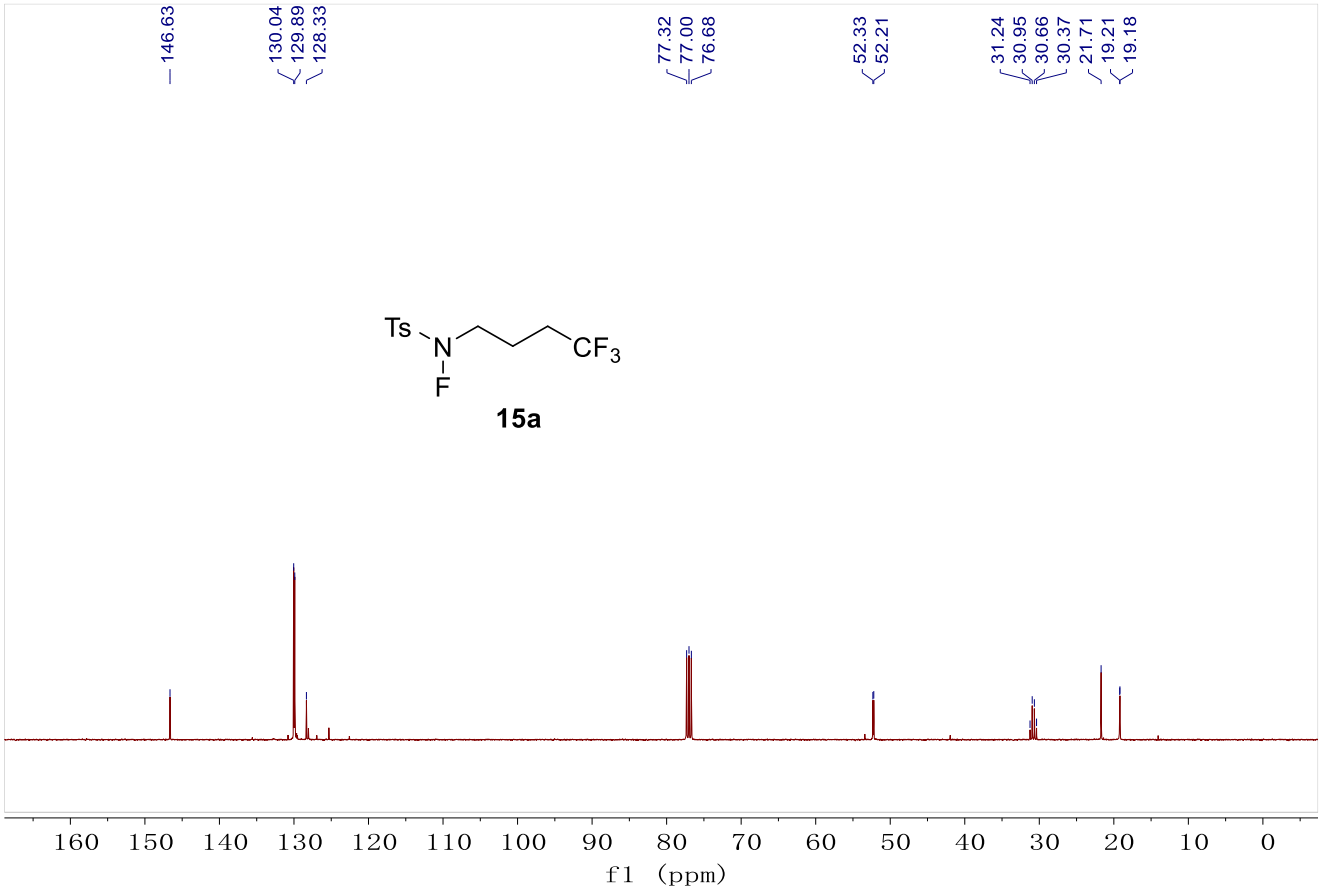
13a


160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.83 7.81 7.41 7.40 6.98 6.97 6.96 6.96 6.95 6.95 6.94 6.93 6.83 6.82 6.81 6.81 6.80 6.80 6.79
3.91 3.90 3.88 3.28 3.27 3.25 3.18 3.16 3.15
2.48 1.78 1.78 1.76 1.76 1.75 1.74 1.73 1.72 1.71 1.61 1.50 1.49 1.48 1.47 1.46
-0.00
F
O
Ts
N
F
14a
2.04 2.07 2.02 2.06 2.07 1.06 1.00 3.08 4.06 4.07
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


158.25 155.89 155.08 146.22 129.91 128.74 115.80 115.58 115.35 115.27
77.32 77.00 76.68 68.23 53.61 53.49 29.02 26.28 26.16 25.56 21.77
F
O
Ts
N
F
14a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.82
7.80
7.43
7.41
7.26
3.35
3.34
3.32
3.25
3.24
3.22
2.48
2.32
2.30
2.29
2.28
2.27
2.27
2.25
2.25
2.24
2.23
2.22
2.21
2.20
2.00
1.98
1.98
1.97
1.96
1.96
1.96
1.95
1.93
-0.01
Ts
N
F
CF3
15a
2.03
2.00
1.00
1.09
3.03
2.05
2.03
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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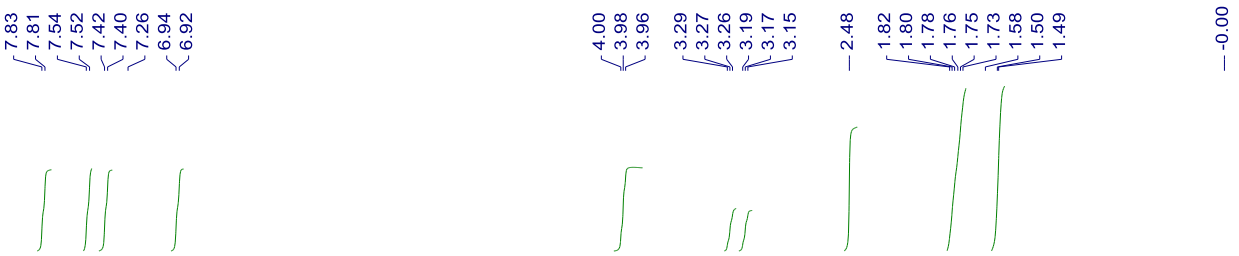
130.04
129.89
128.33
77.32
77.00
76.68
52.33
52.21
31.24
30.95
30.66
30.37
21.71
19.21
19.18
Ts
N
F
CF3
15a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.81
7.54
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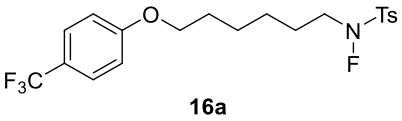
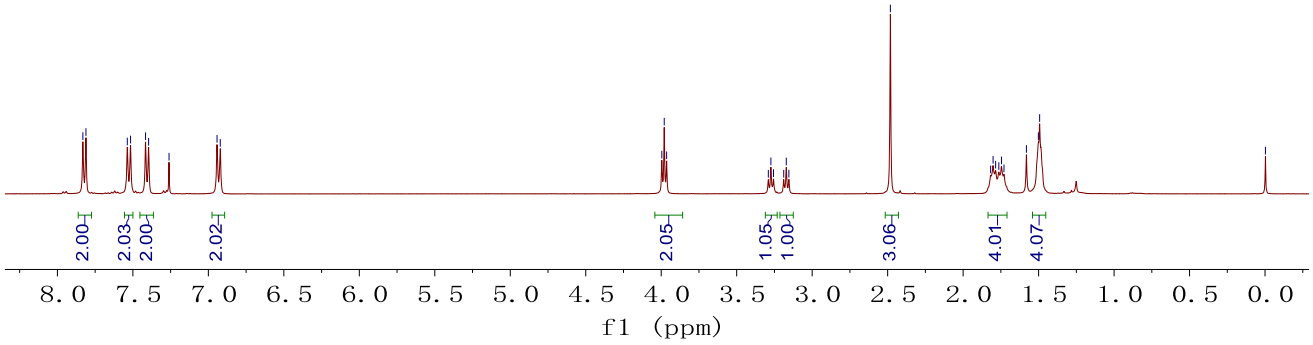
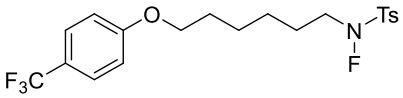
7.26
6.94
6.92
4.00
3.98
3.96
3.29
3.27
3.26
3.19
3.17
3.15
2.48
1.82
1.80
1.78
1.76
1.75
1.73
1.58
1.50
1.49
0.00


O
Ts
N
F
F3C

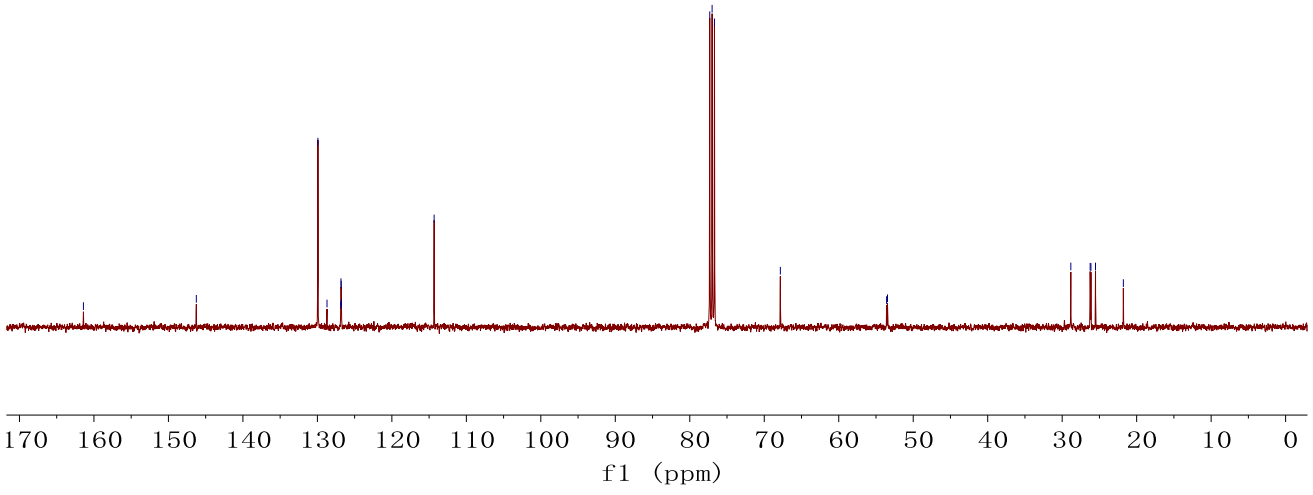
16a


2.00
2.03
2.00
2.02
2.05
1.05
1.00
3.06
4.01
4.07
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.41
146.25
129.93
128.71
126.86
126.83
126.80
126.76
114.33
77.32
77.00
76.68
67.84
53.58
53.45
28.84
26.24
26.14
25.53
21.79


O
Ts
N
F
F3C

16a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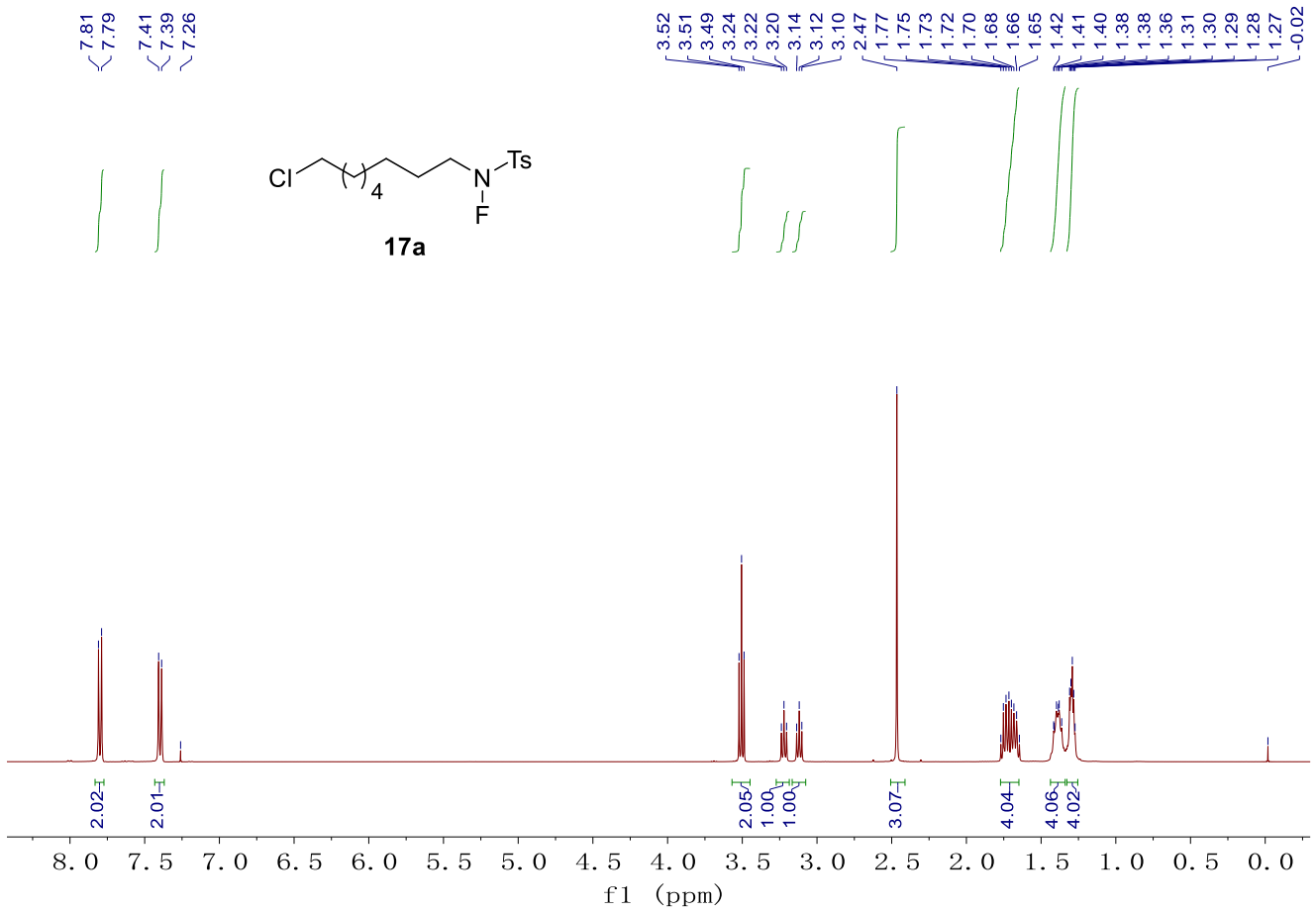
f1 (ppm)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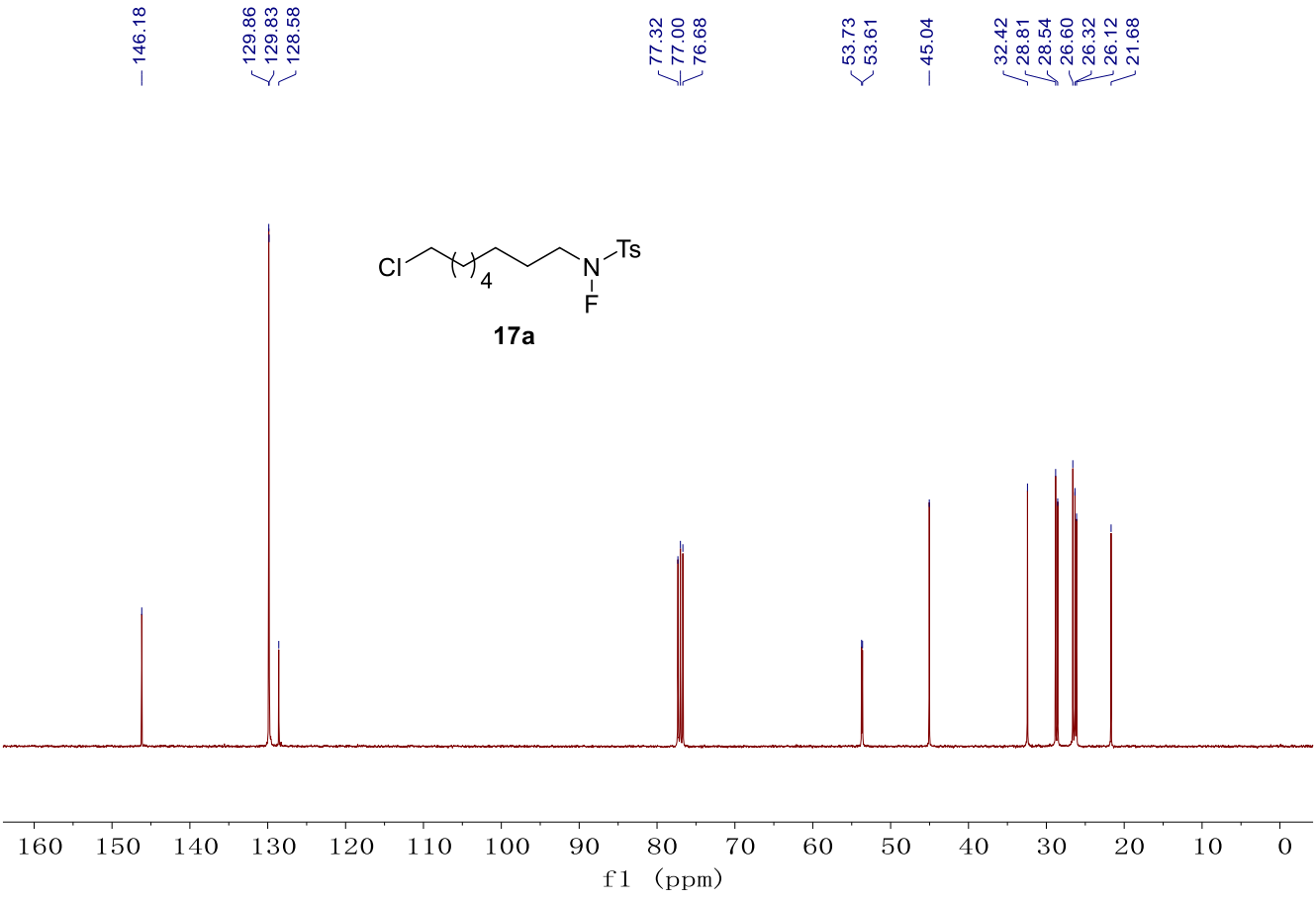
3.51
3.49
3.24
3.22
3.20
3.14
3.12
3.10
2.47
1.77
1.75
1.73
1.72
1.70
1.68
1.66
1.65
1.42
1.41
1.40
1.38
1.38
1.36
1.31
1.30
1.29
1.28
1.27
-0.02
Cl
4
N
Ts
F
17a
2.02
2.01
2.05
1.00
1.00
3.07
4.04
4.06
4.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.86
129.83
128.58
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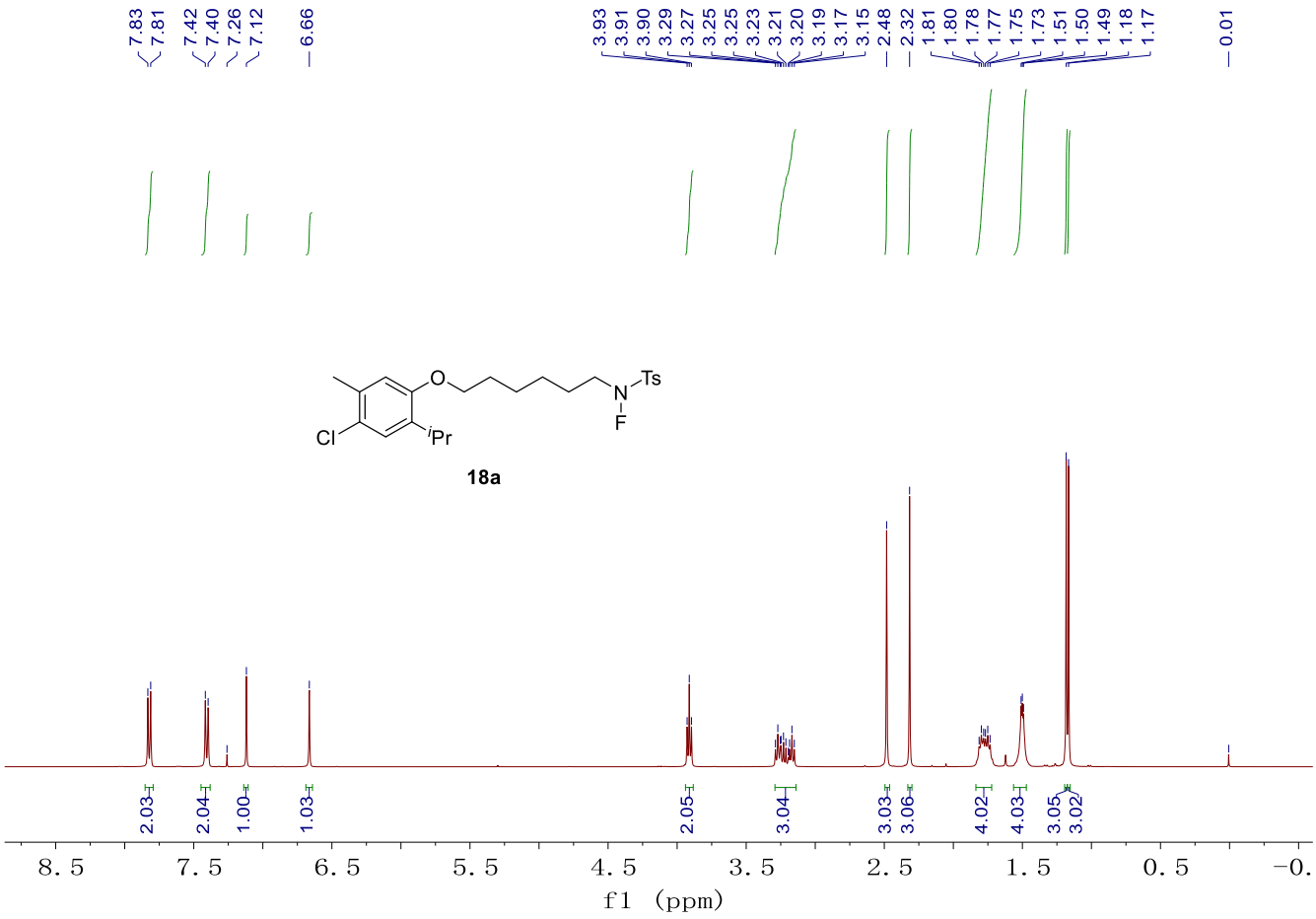
77.00
76.68
53.73
53.61
45.04
32.42
28.81
28.54
26.60
26.32
26.12
21.68
Cl
4
N
Ts
F
17a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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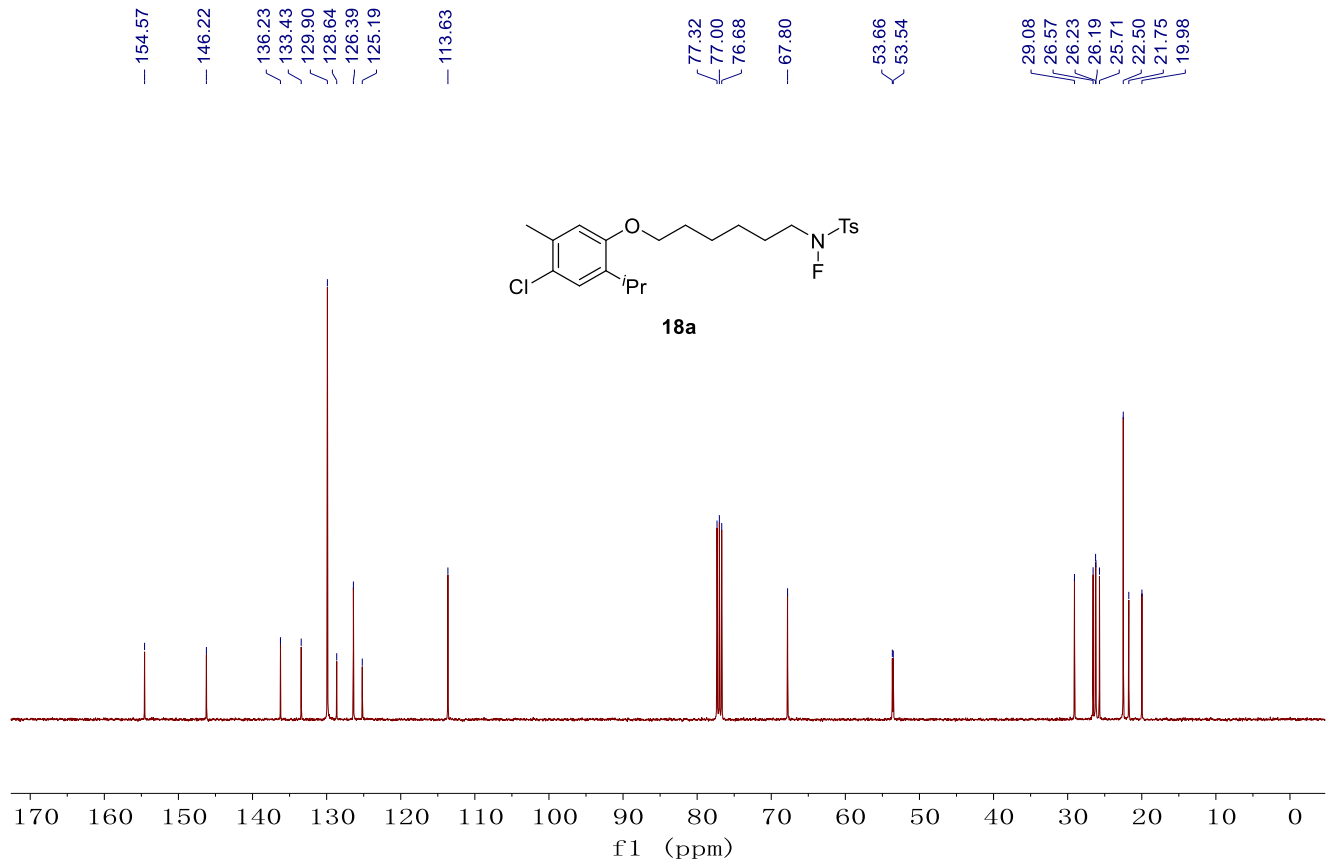
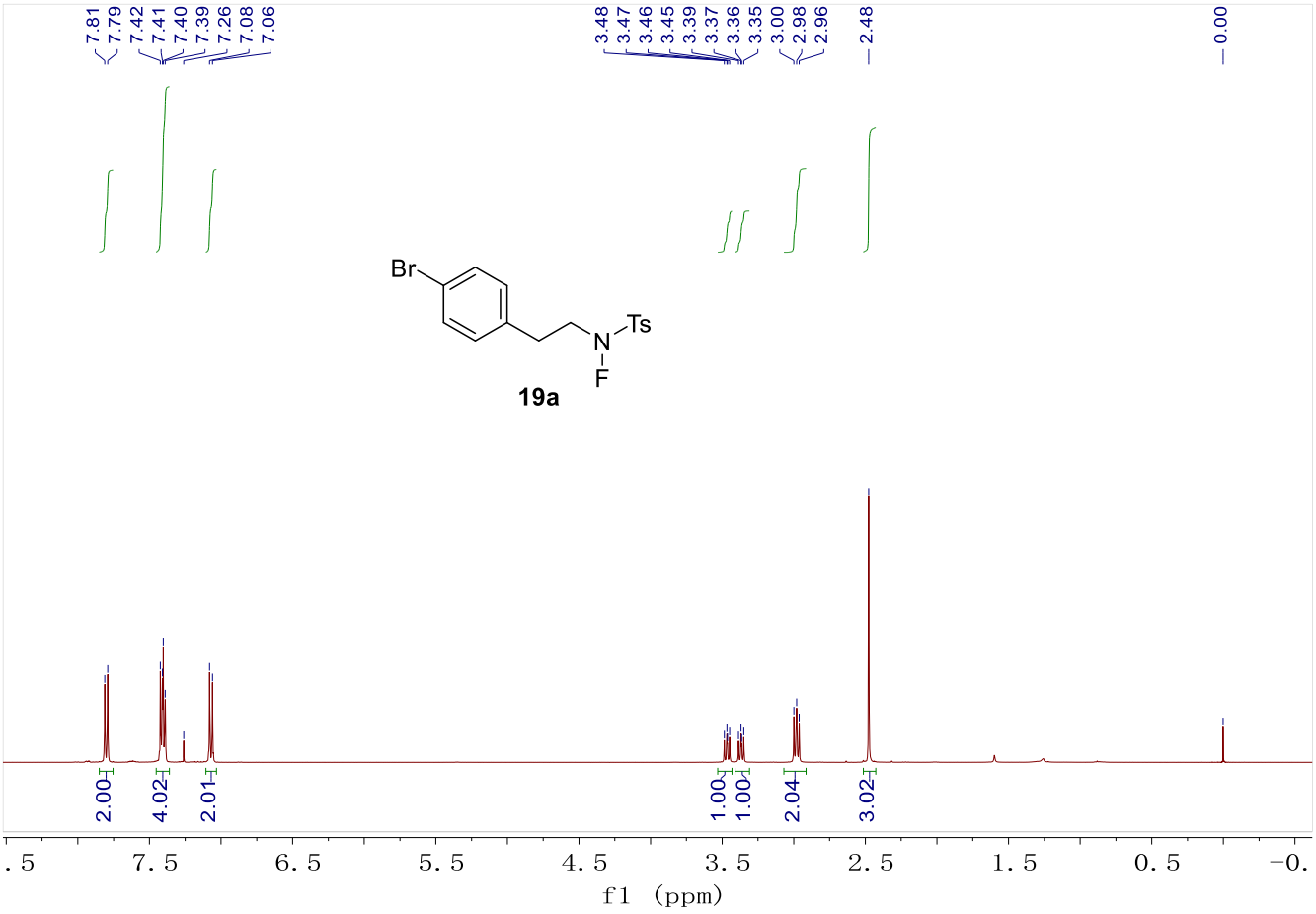
7.81
7.42
7.40
7.26
7.12
6.66
3.93
3.91
3.90
3.29
3.27
3.25
3.25
3.23
3.21
3.20
3.19
3.17
3.15
2.48
2.32
1.81
1.80
1.78
1.77
1.75
1.73
1.51
1.50
1.49
1.18
1.17
0.01
O
Ts
N
F
Cl
iPr
18a
2.03
2.04
1.00
1.03
2.05
3.04
3.03
3.06
4.02
4.03
3.05
3.02
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.
f1 (ppm)


154.57
146.22
136.23
133.43
129.90
128.64
126.39
125.19
113.63
77.32
77.00
76.68
67.80
53.66
53.54
29.08
26.57
26.23
26.19
25.71
22.50
21.75
19.98
O
Ts
N
F
Cl
iPr
18a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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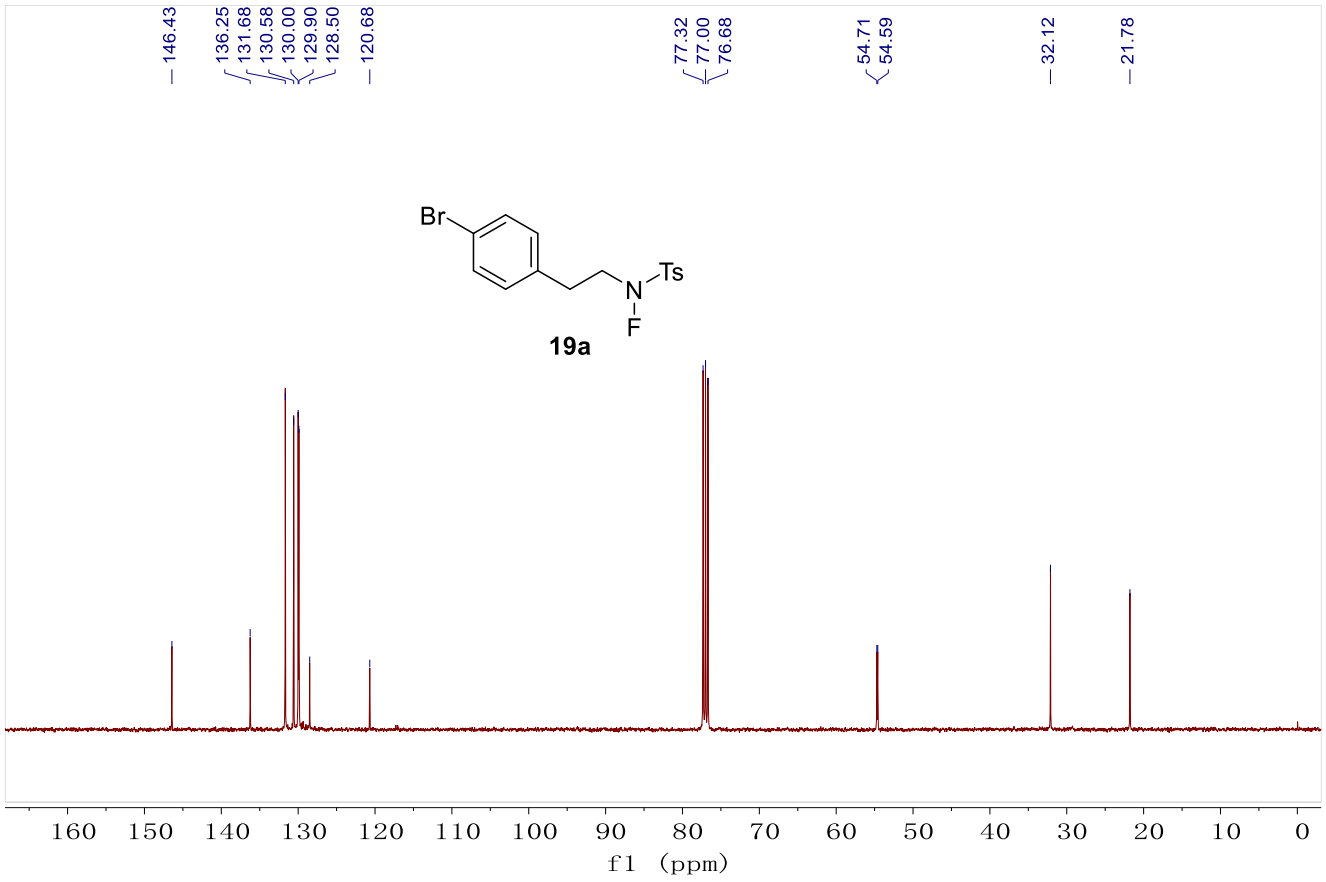
7.79
7.42
7.41
7.40
7.39
7.26
7.08
7.06
3.48
3.47
3.46
3.45
3.39
3.37
3.36
3.35
3.00
2.98
2.96
2.48
0.00
Br
N
Ts
F
19a
2.00
4.02
2.01
1.00
1.00
2.04
3.02
f1 (ppm)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131.68
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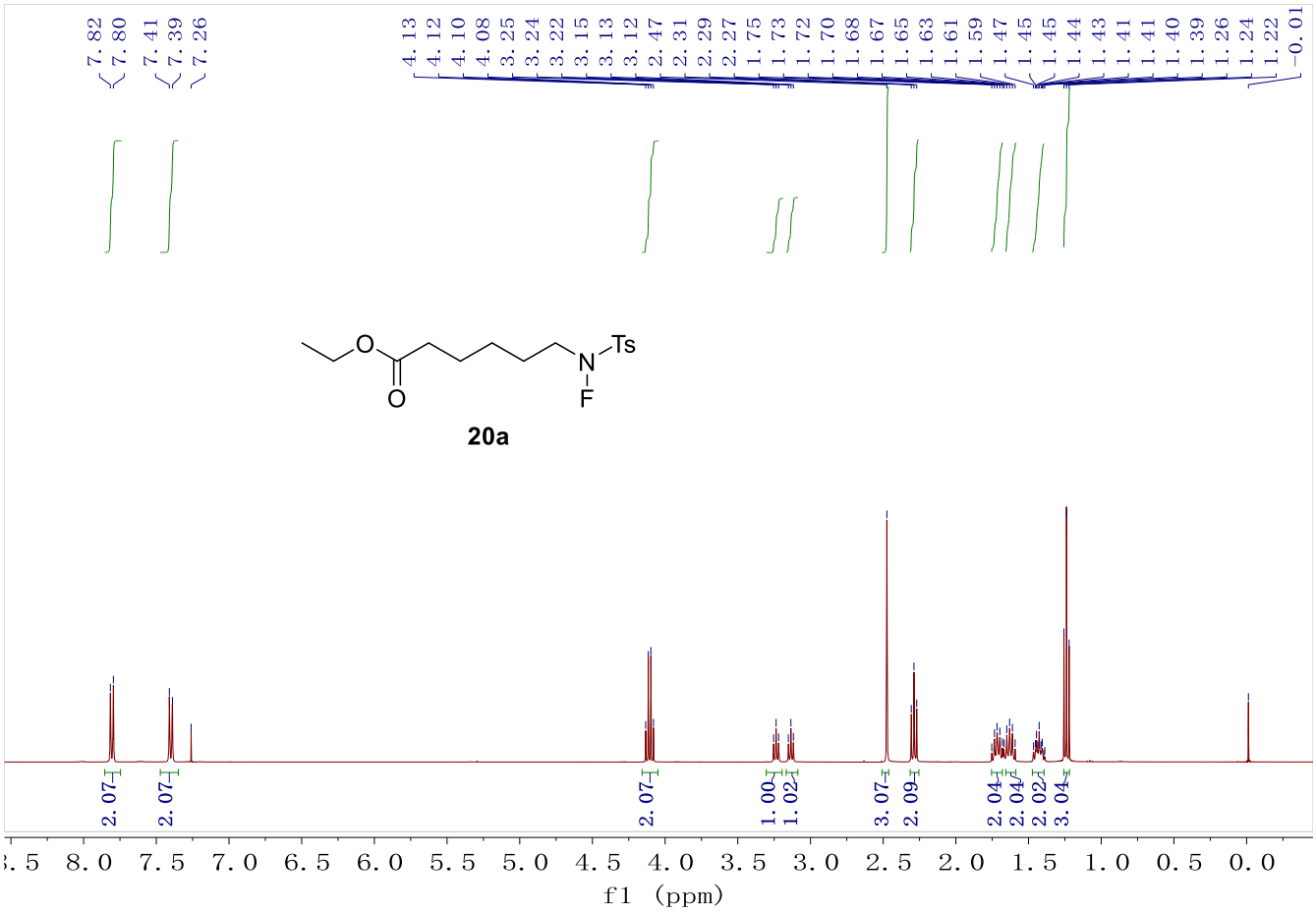
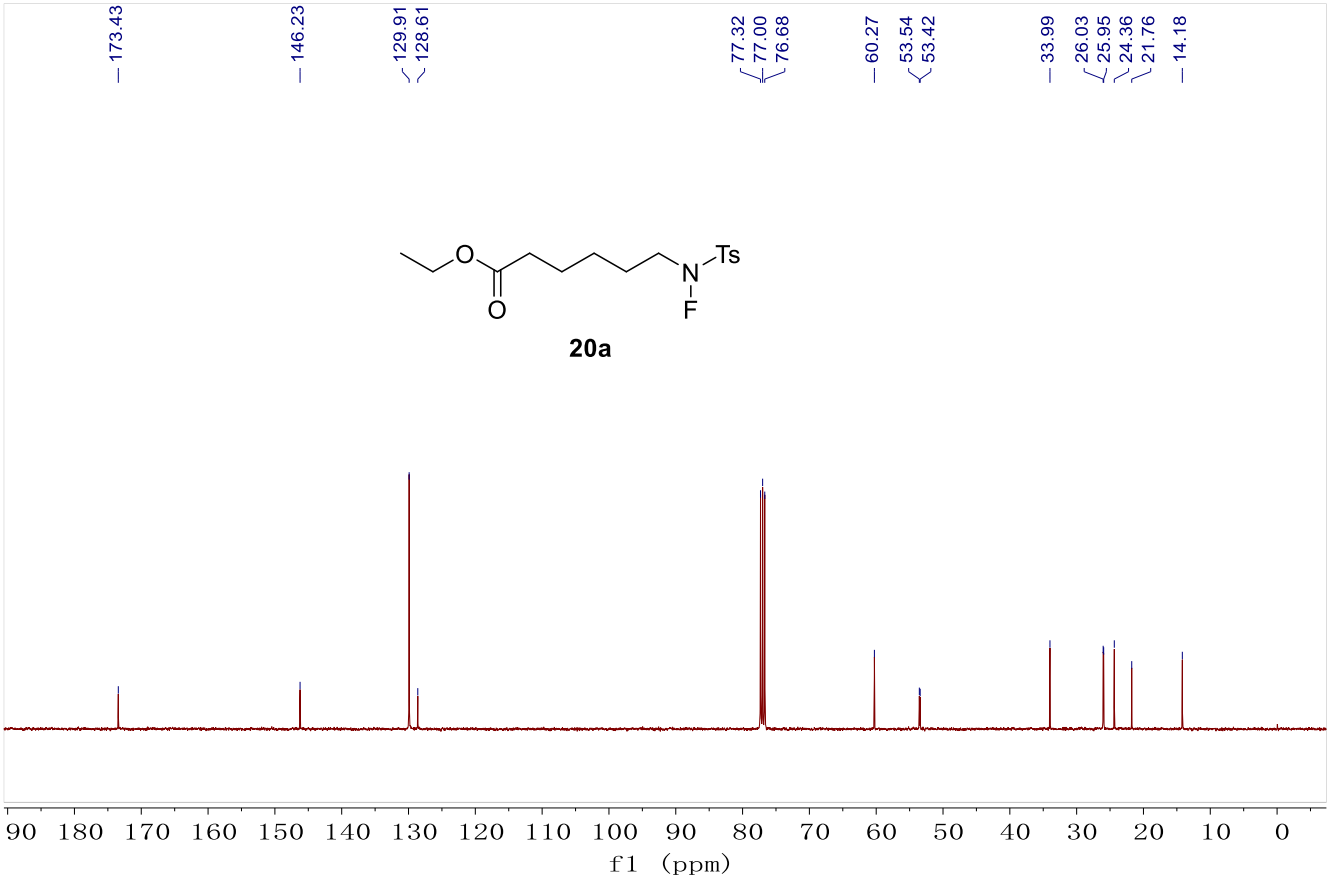
129.90
128.50
120.68
77.32
77.00
76.68
54.71
54.59
32.12
21.78
Br
N
Ts
F
19a
f1 (ppm)


7.82
7.80
7.41
7.39
7.26
4.13
4.12
4.10
4.08
3.25
3.24
3.22
3.15
3.13
3.12
2.47
2.31
2.29
2.27
1.75
1.73
1.72
1.70
1.68
1.67
1.65
1.63
1.61
1.59
1.47
1.45
1.45
1.44
1.43
1.41
1.41
1.40
1.39
1.26
1.24
1.22
-0.01
O
O
N
Ts
F
20a
2.07
2.07
2.07
1.00
1.02
3.07
2.09
2.04
2.04
2.02
3.04
f1 (ppm)


173.43
146.23
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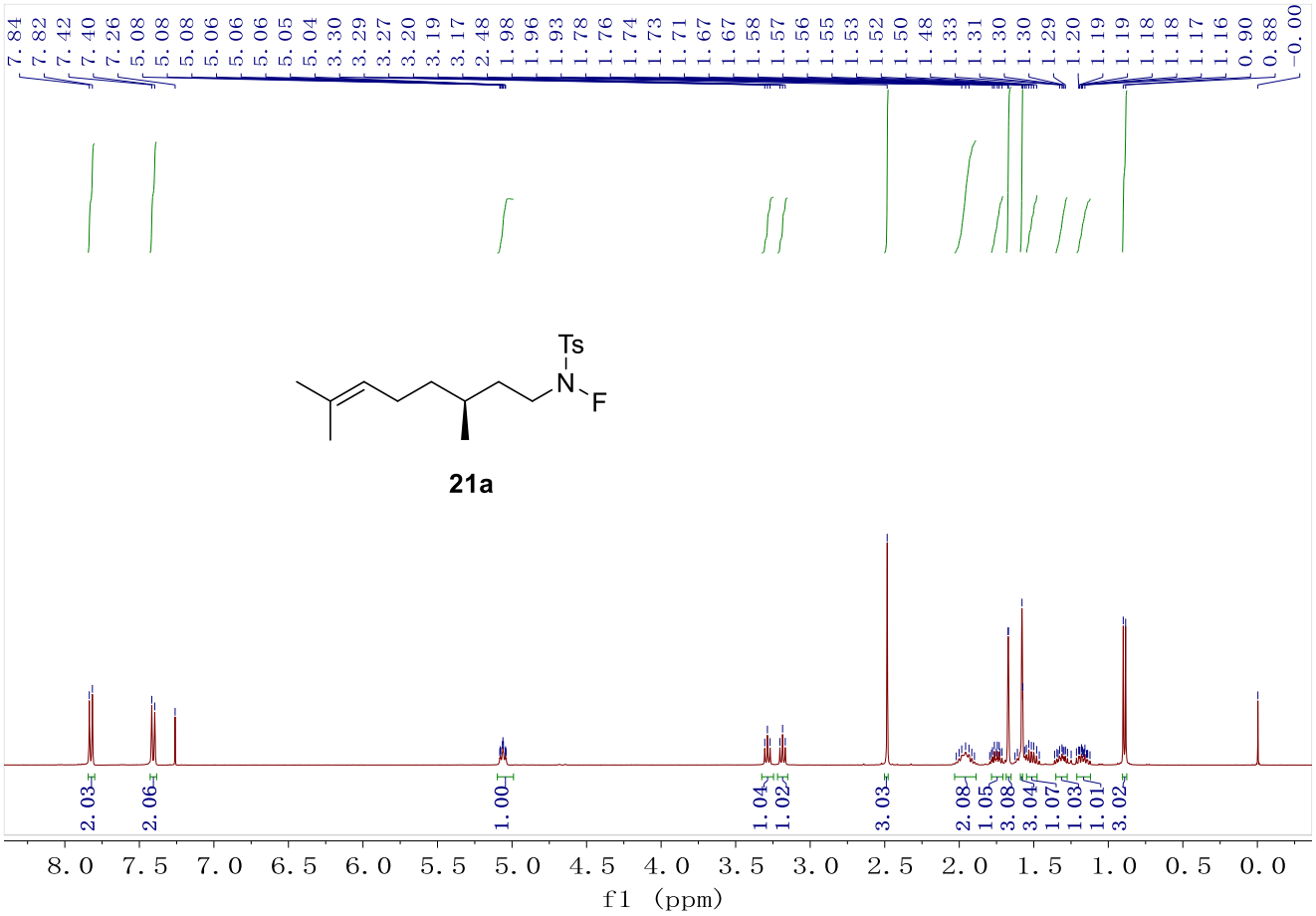
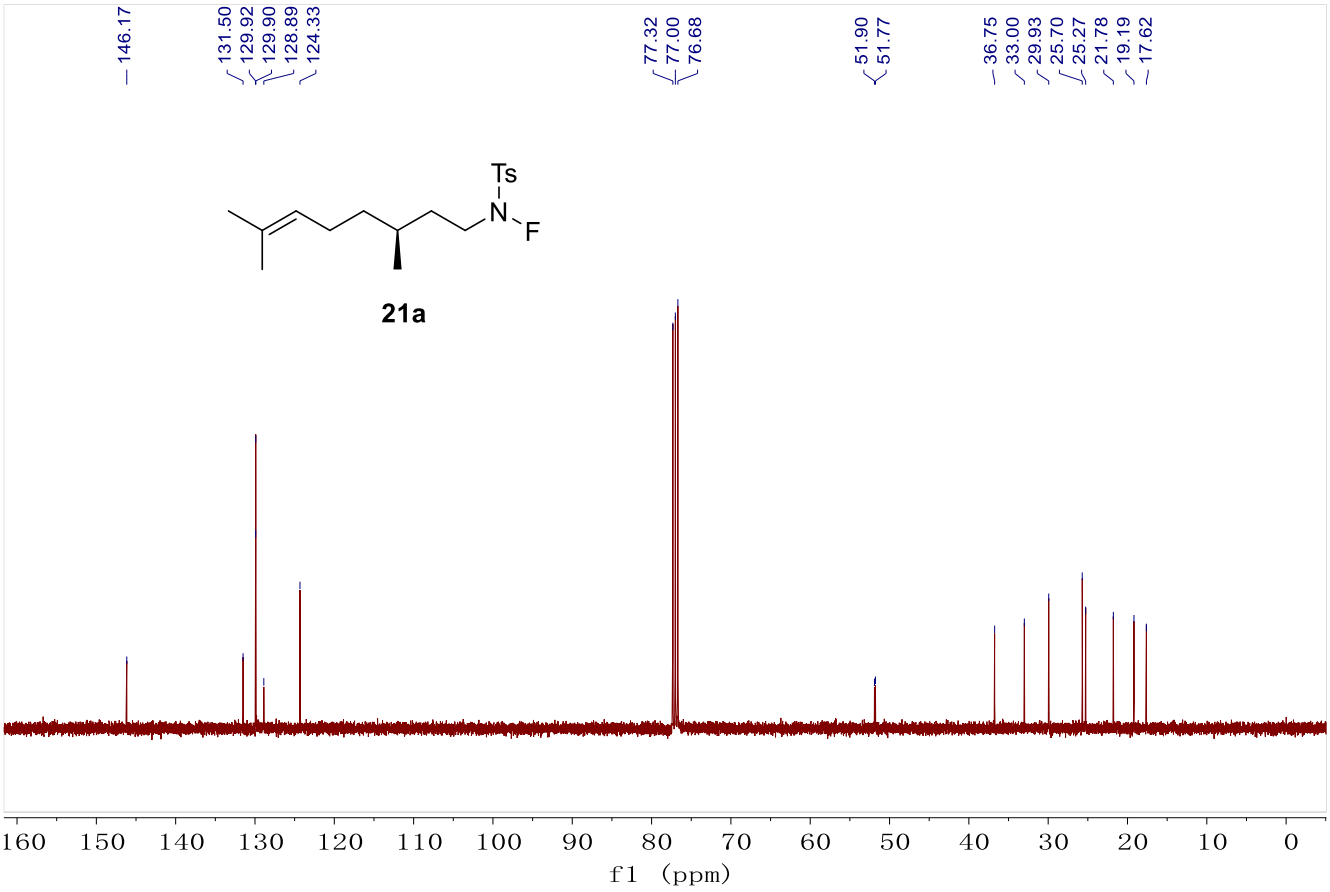
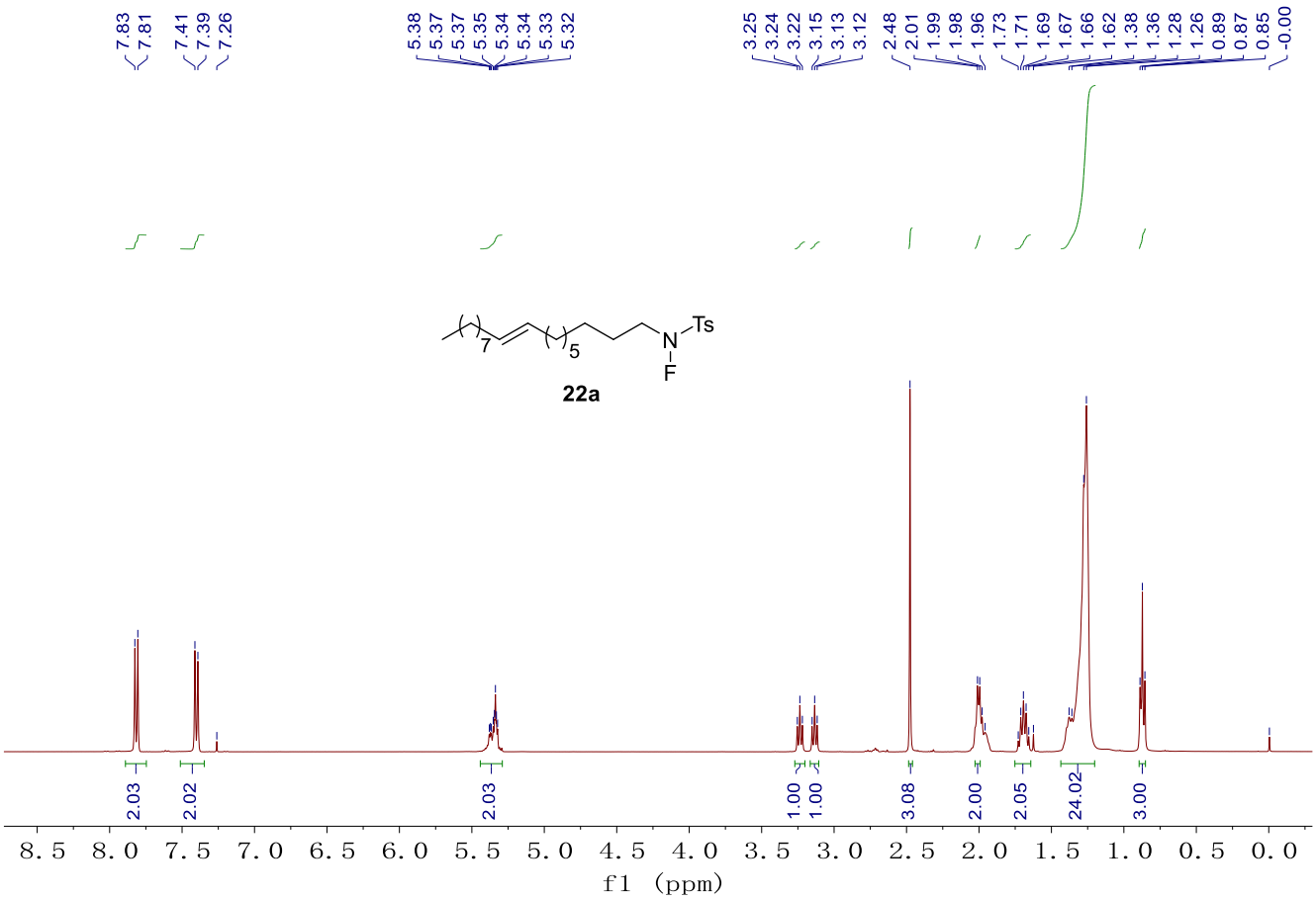
128.61
77.32
77.00
76.68
60.27
53.54
53.42
33.99
26.03
25.95
24.36
21.76
14.18
O
O
N
Ts
F
20a
f1 (ppm)


7.84 7.82 7.42 7.40 7.26 5.08 5.08 5.08 5.06 5.06 5.06 5.05 5.04 3.30 3.29 3.27 3.20 3.19 3.17 2.48 1.98 1.96 1.93 1.78 1.76 1.74 1.73 1.71 1.67 1.67 1.58 1.57 1.56 1.55 1.53 1.52 1.50 1.48 1.33 1.31 1.30 1.30 1.29 1.20 1.19 1.19 1.18 1.18 1.17 1.16 0.90 0.88 -0.00
Ts
N
F
21a
2.03 2.06 1.00 1.04 1.02 3.03 2.08 1.05 3.08 3.04 1.07 1.03 1.01 3.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


146.17
131.50 129.92 129.90 128.89 124.33
77.32 77.00 76.68
51.90 51.77
36.75 33.00 29.93 25.70 25.27 21.78 19.19 17.62
Ts
N
F
21a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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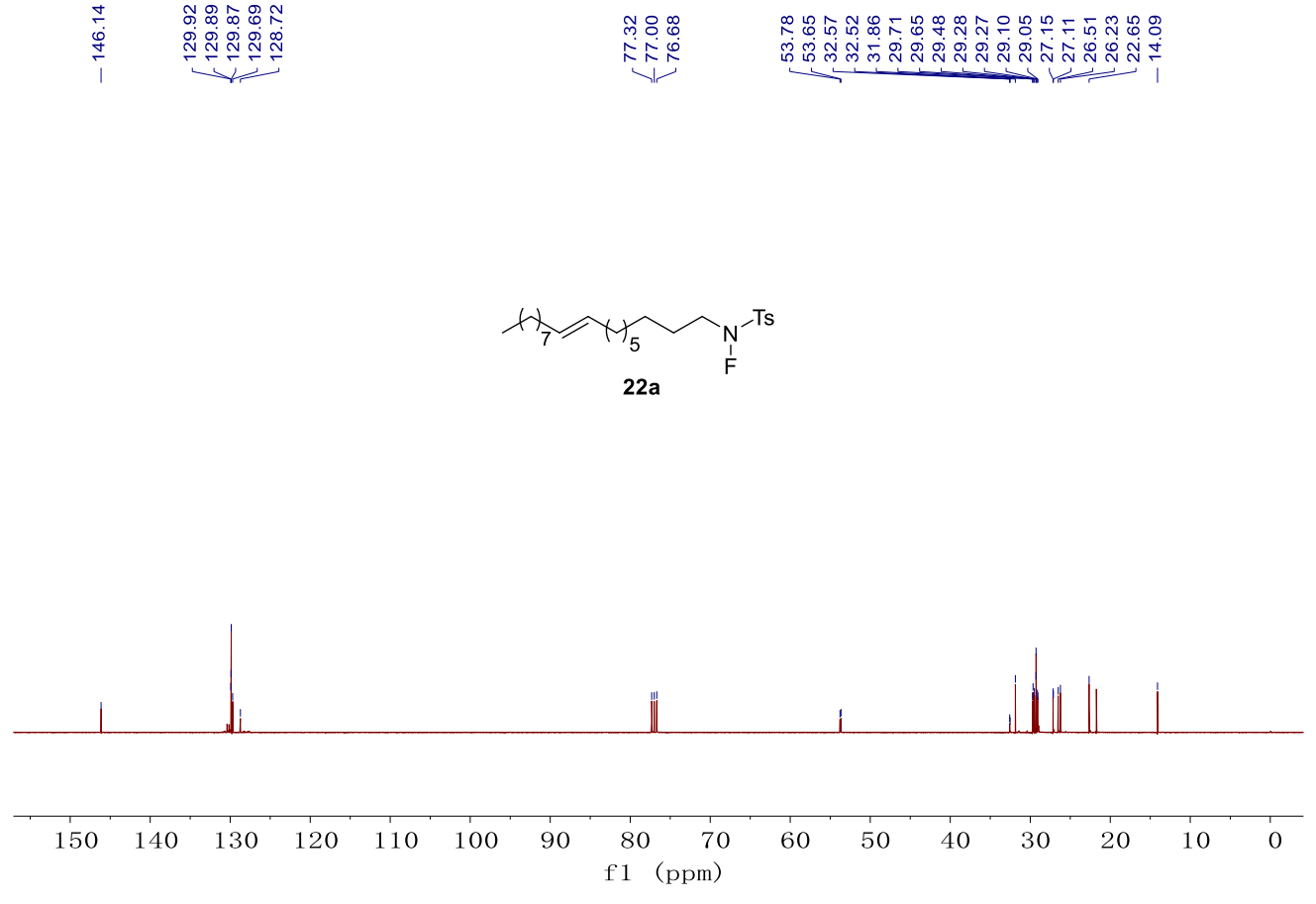
7.41
7.39
7.26
5.38
5.37
5.37
5.35
5.34
5.34
5.33
5.32
3.25
3.24
3.22
3.15
3.13
3.12
2.48
2.01
1.99
1.98
1.96
1.73
1.71
1.69
1.67
1.66
1.62
1.38
1.36
1.28
1.26
0.89
0.87
0.85
-0.00
Ts
N
F
22a
2.03
2.02
2.03
1.00
1.00
3.08
2.00
2.05
24.02
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.72
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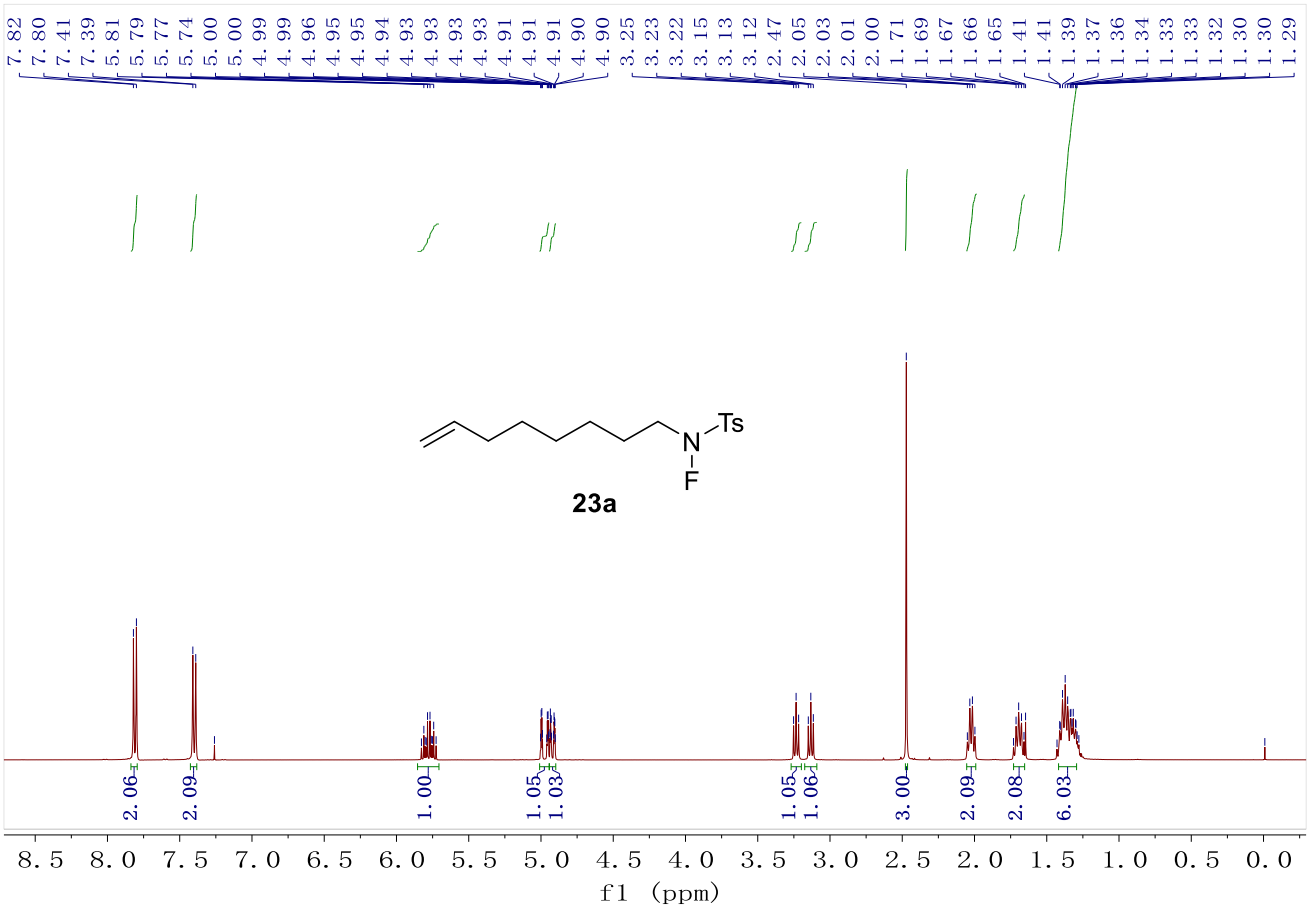
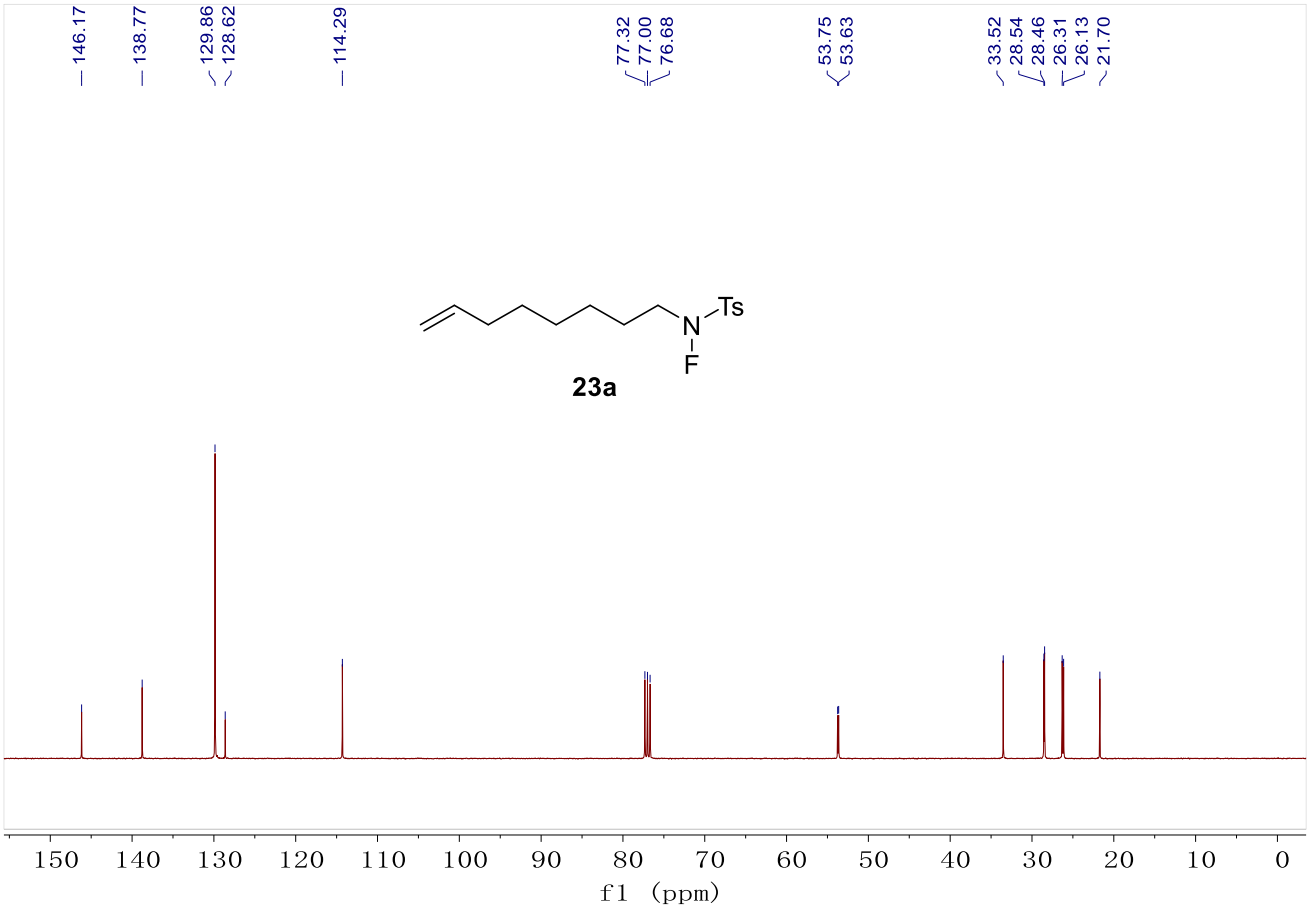
77.00
76.68
53.78
53.65
32.57
32.52
31.86
29.71
29.65
29.48
29.28
29.27
29.10
29.05
27.15
27.11
26.51
26.23
22.65
14.09
Ts
N
F
22a
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.82 7.80 7.41 7.39 5.81 5.79 5.77 5.74 5.00 5.00 4.99 4.99 4.96 4.95 4.95 4.94 4.93 4.93 4.93 4.93 4.91 4.91 4.90 4.90
3.25 3.23 3.22 3.15 3.13 3.12 2.47 2.05 2.03 2.01 2.00 1.71 1.69 1.67 1.66 1.65 1.41 1.41 1.39 1.37 1.36 1.34 1.33 1.33 1.32 1.30 1.30 1.29
Ts
N
F
23a
2.06 2.09 1.00 1.05 1.03 1.05 1.06 3.00 2.09 2.08 6.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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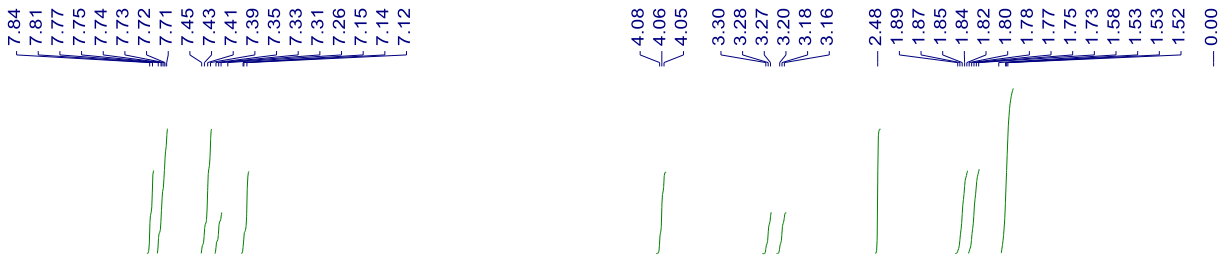
Ts
N
F
23a
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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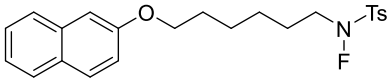
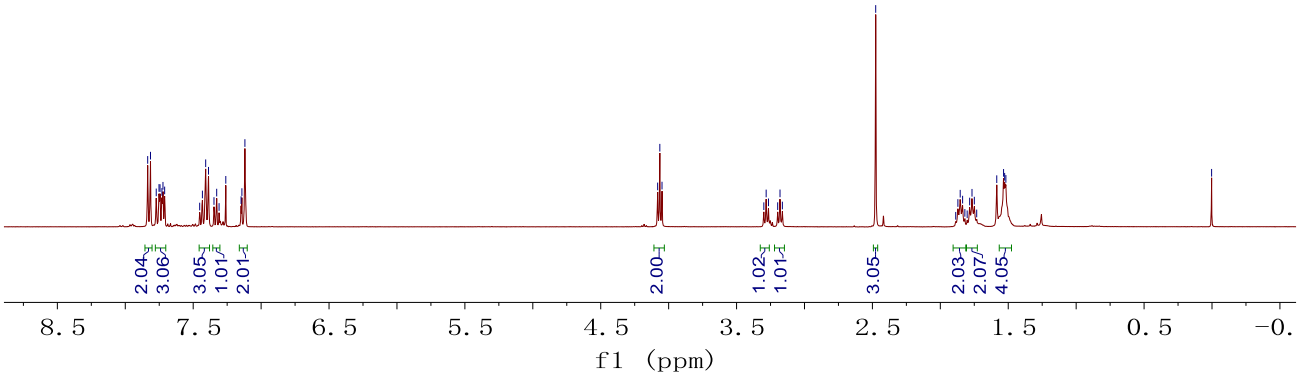
7.43
7.41
7.39
7.35
7.33
7.31
7.26
7.15
7.14
7.12
4.08
4.06
4.05
3.30
3.28
3.27
3.20
3.18
3.16
2.48
1.89
1.87
1.85
1.84
1.82
1.80
1.78
1.77
1.75
1.73
1.58
1.53
1.53
1.52
0.00


O
N
Ts
F

24a


2.04
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3.05
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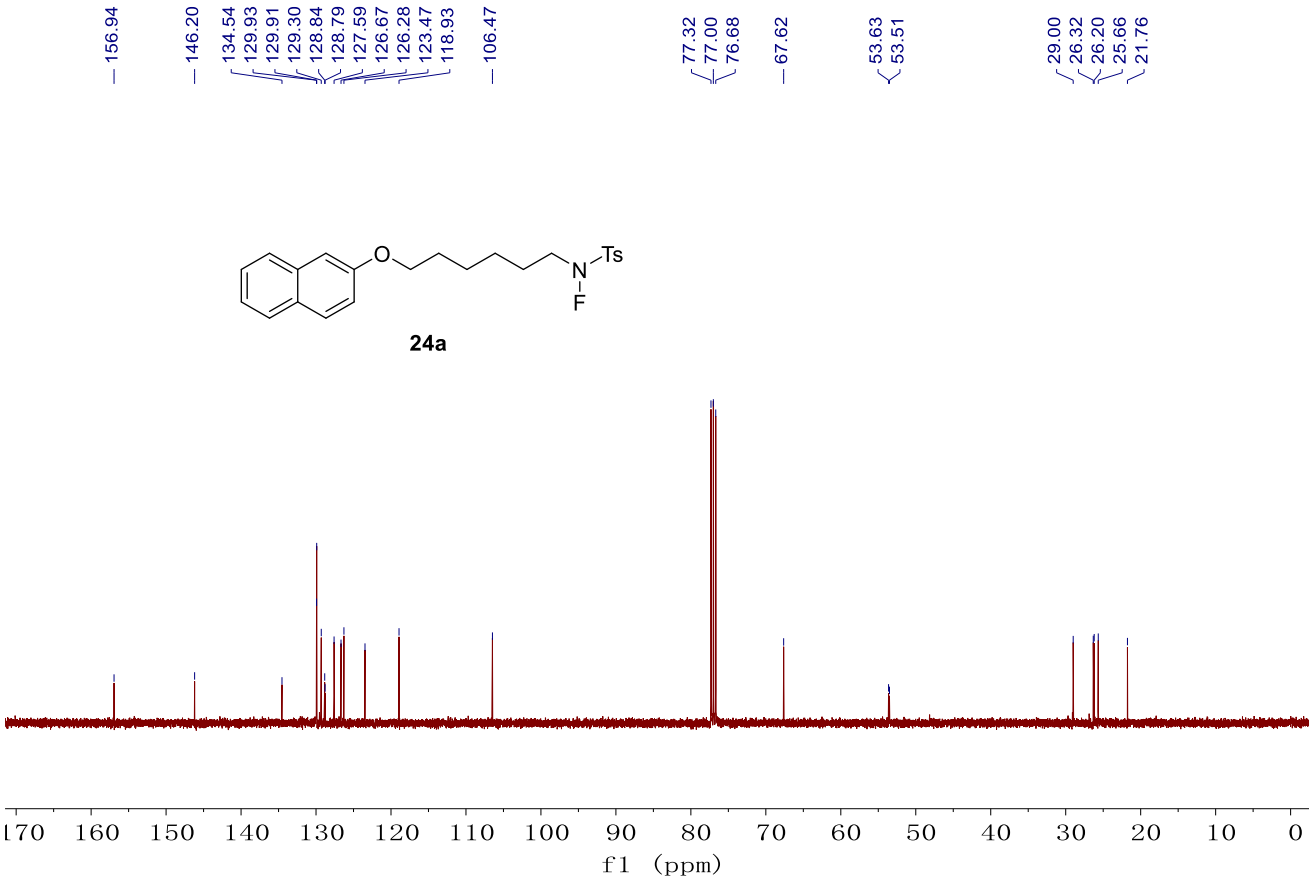
2.00
1.02
1.01
3.05
2.03
2.07
4.05
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.
f1 (ppm)

O
N
Ts
F

24a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129.30
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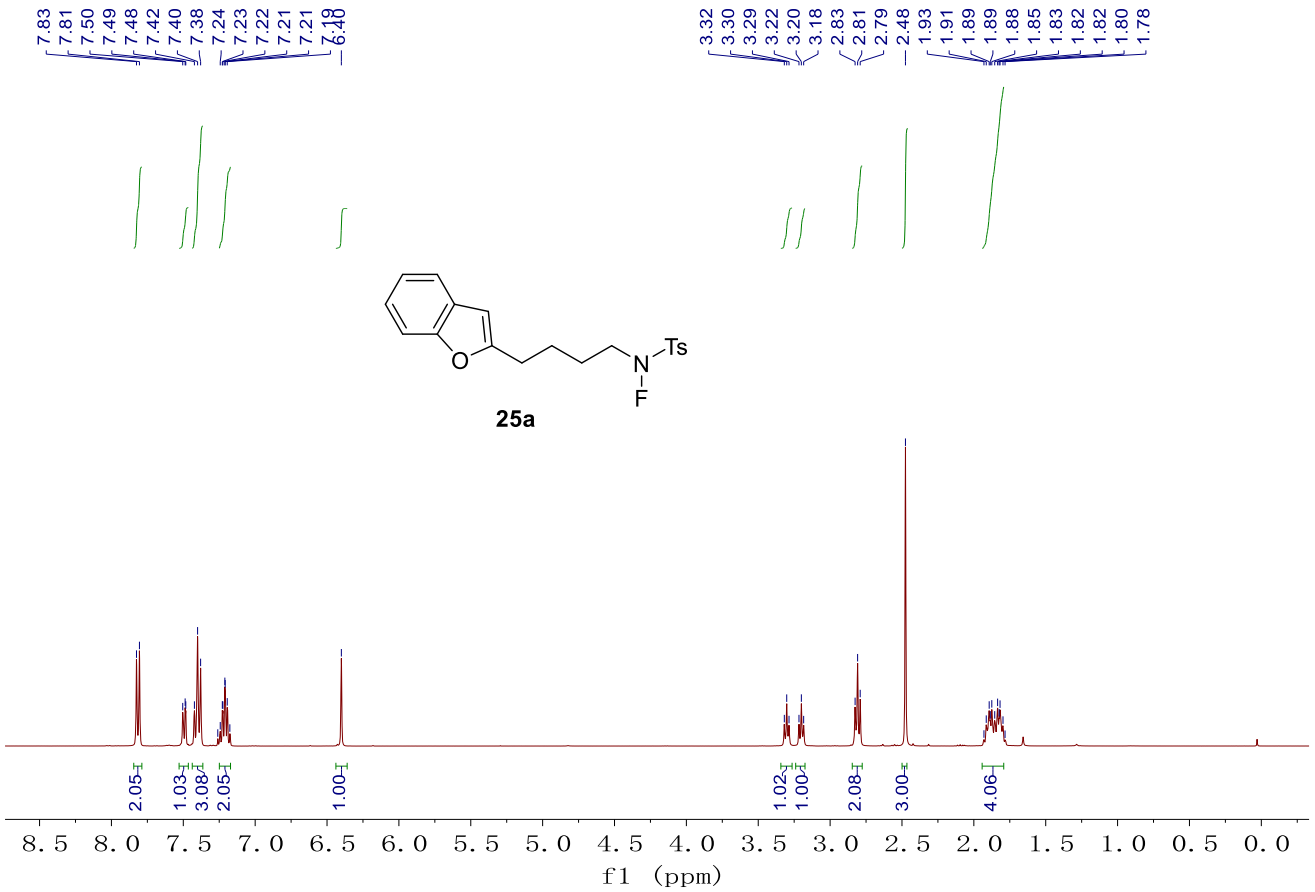
128.79
127.59
126.67
126.28
123.47
118.93
106.47
77.32
77.00
76.68
67.62
53.63
53.51
29.00
26.32
26.20
25.66
21.76
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.83
7.81
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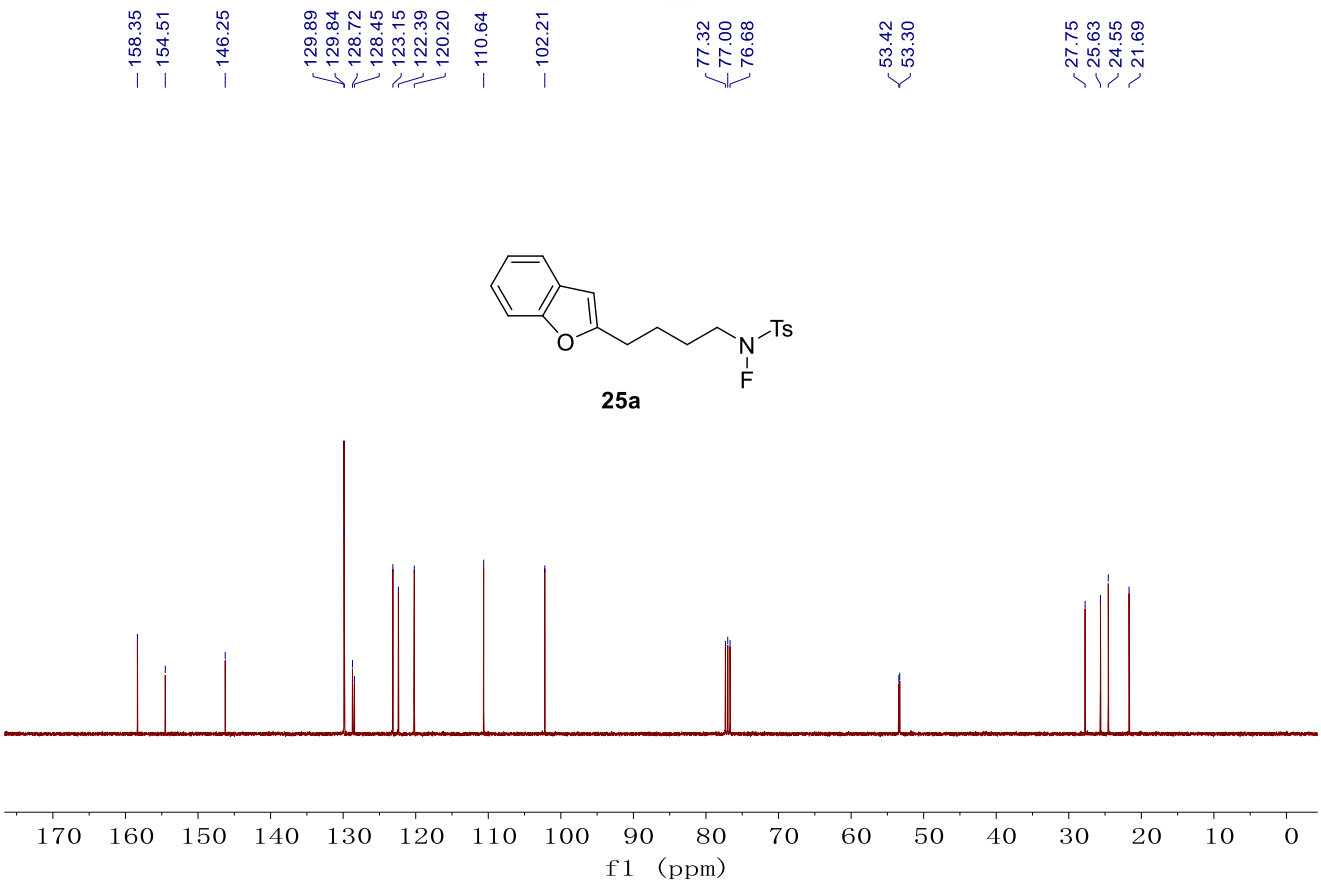
7.49
7.48
7.42
7.40
7.38
7.24
7.23
7.22
7.21
7.21
7.19
6.40
3.32
3.30
3.29
3.22
3.20
3.18
2.83
2.81
2.79
2.48
1.93
1.91
1.89
1.89
1.88
1.85
1.83
1.82
1.82
1.80
1.78
Ts
N
F
O
25a
2.05
1.03
3.08
2.05
1.00
1.02
1.00
2.08
3.00
4.06
f1 (ppm)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128.72
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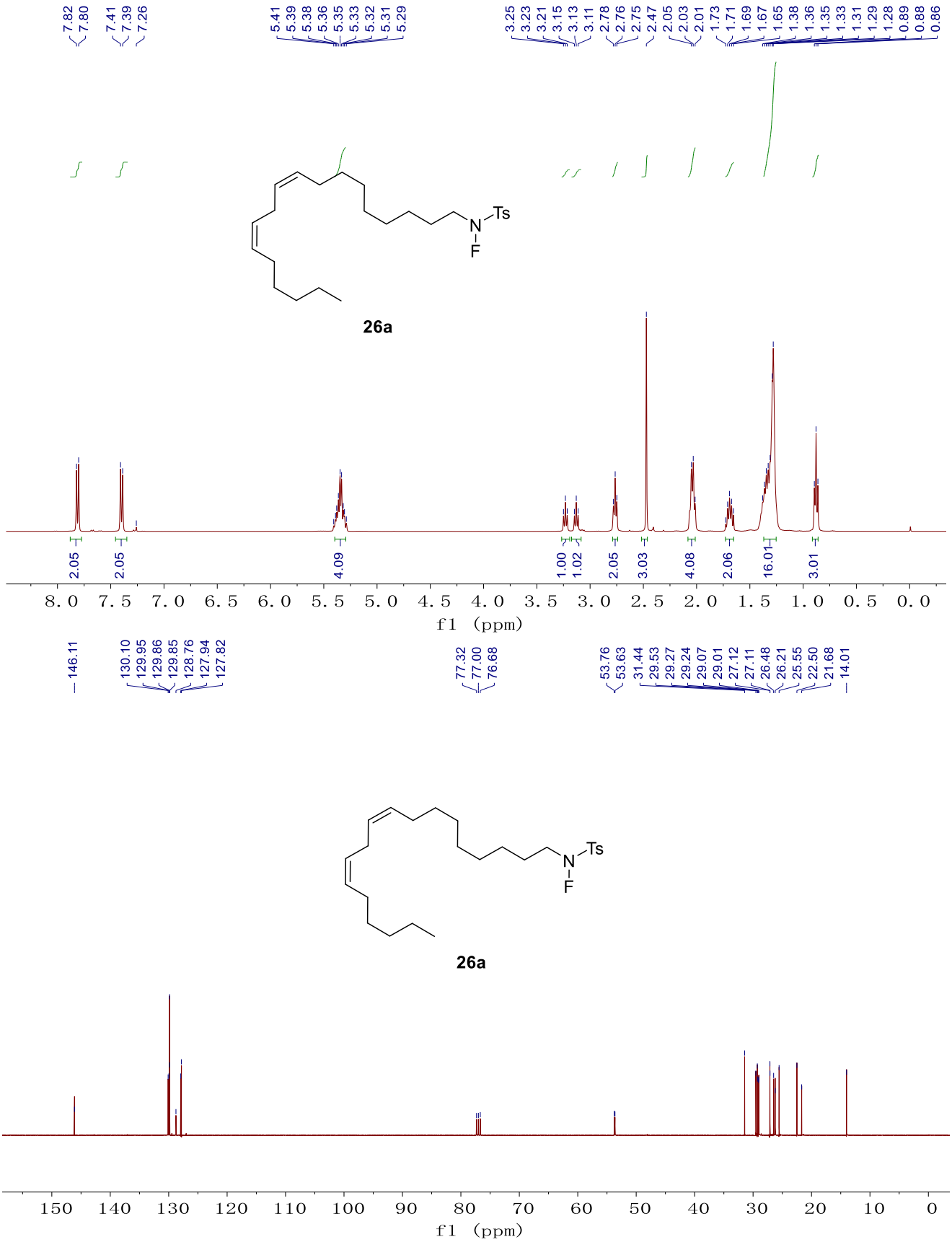
123.15
122.39
120.20
110.64
102.21
77.32
77.00
76.68
53.42
53.30
27.75
25.63
24.55
21.69
Ts
N
F
O
25a
f1 (ppm)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7.39
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5.41
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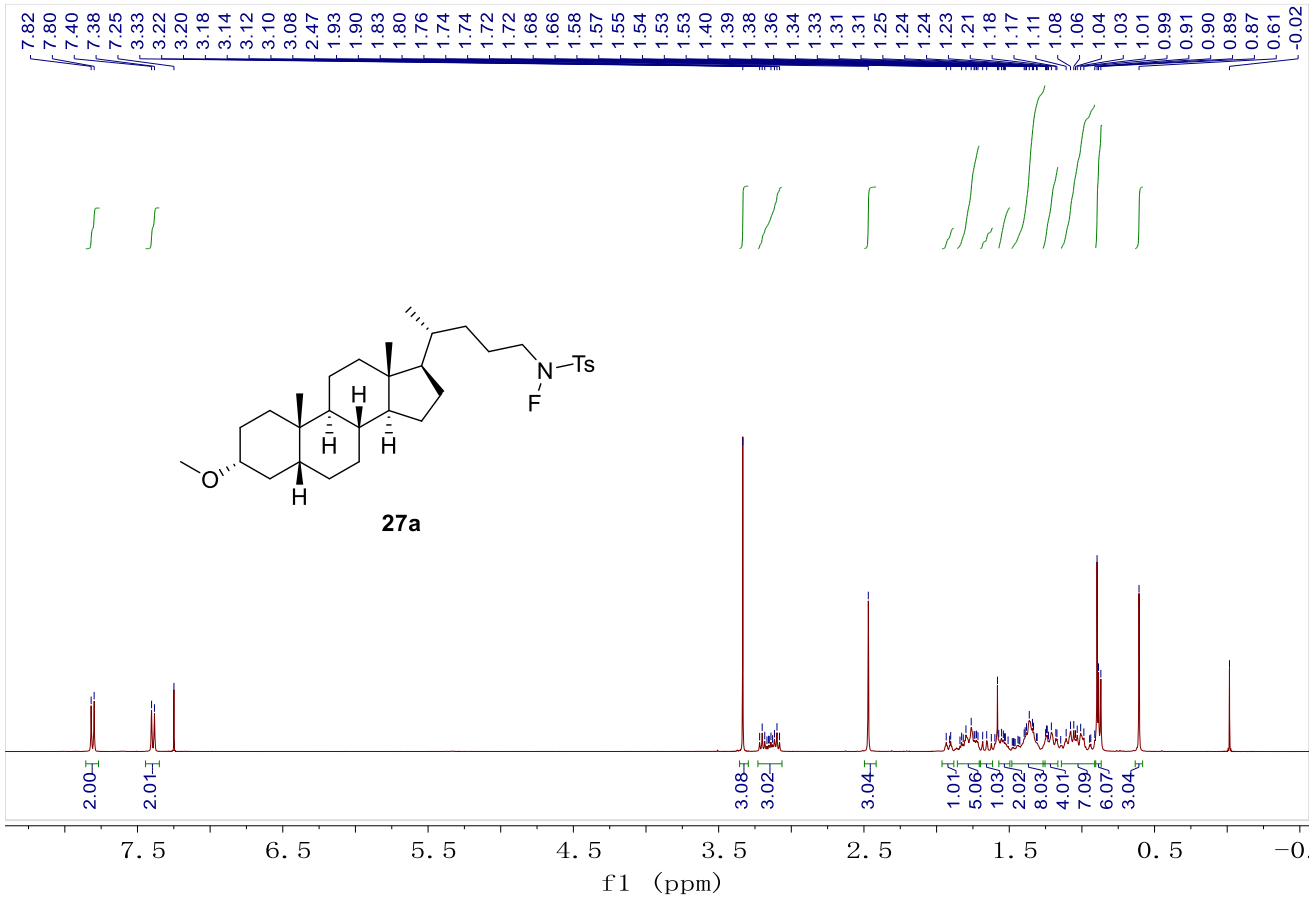
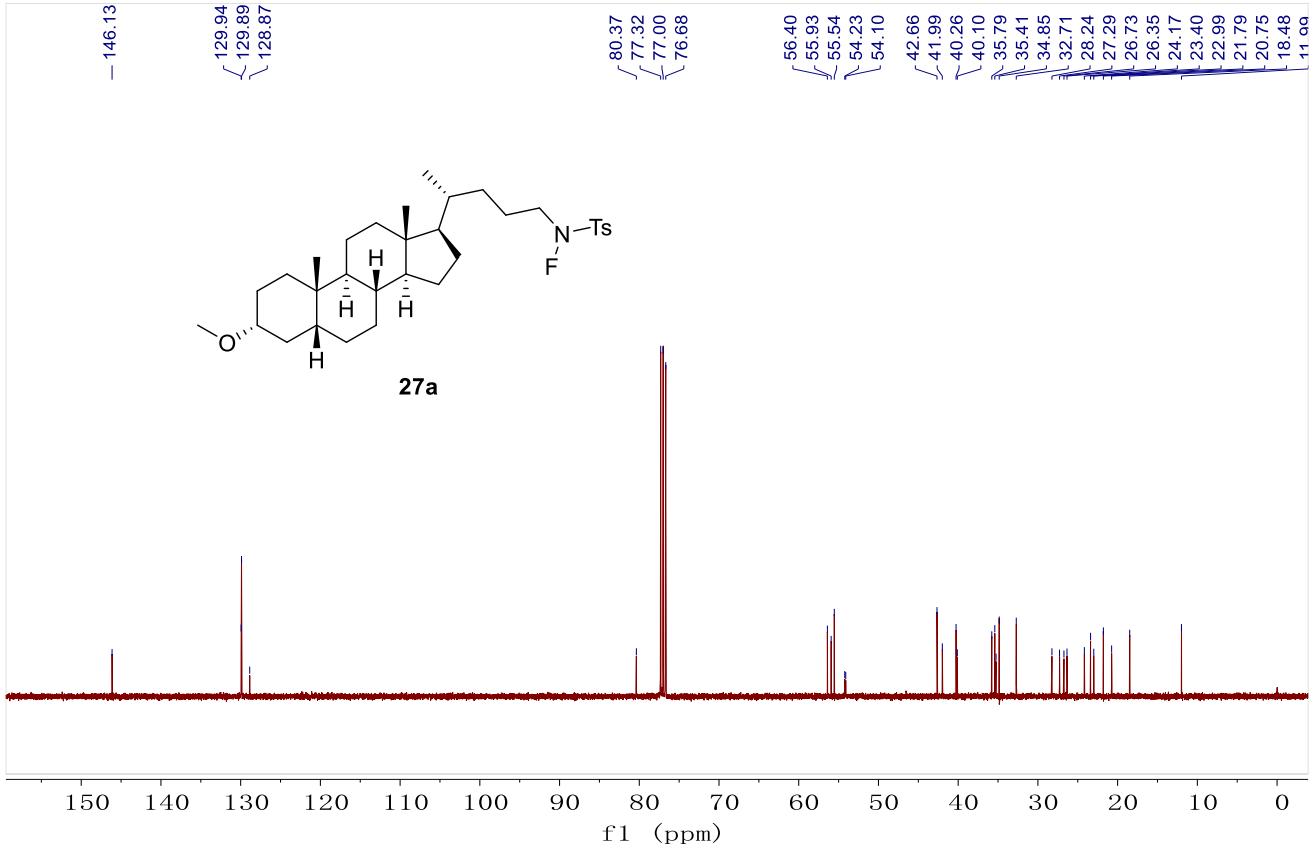
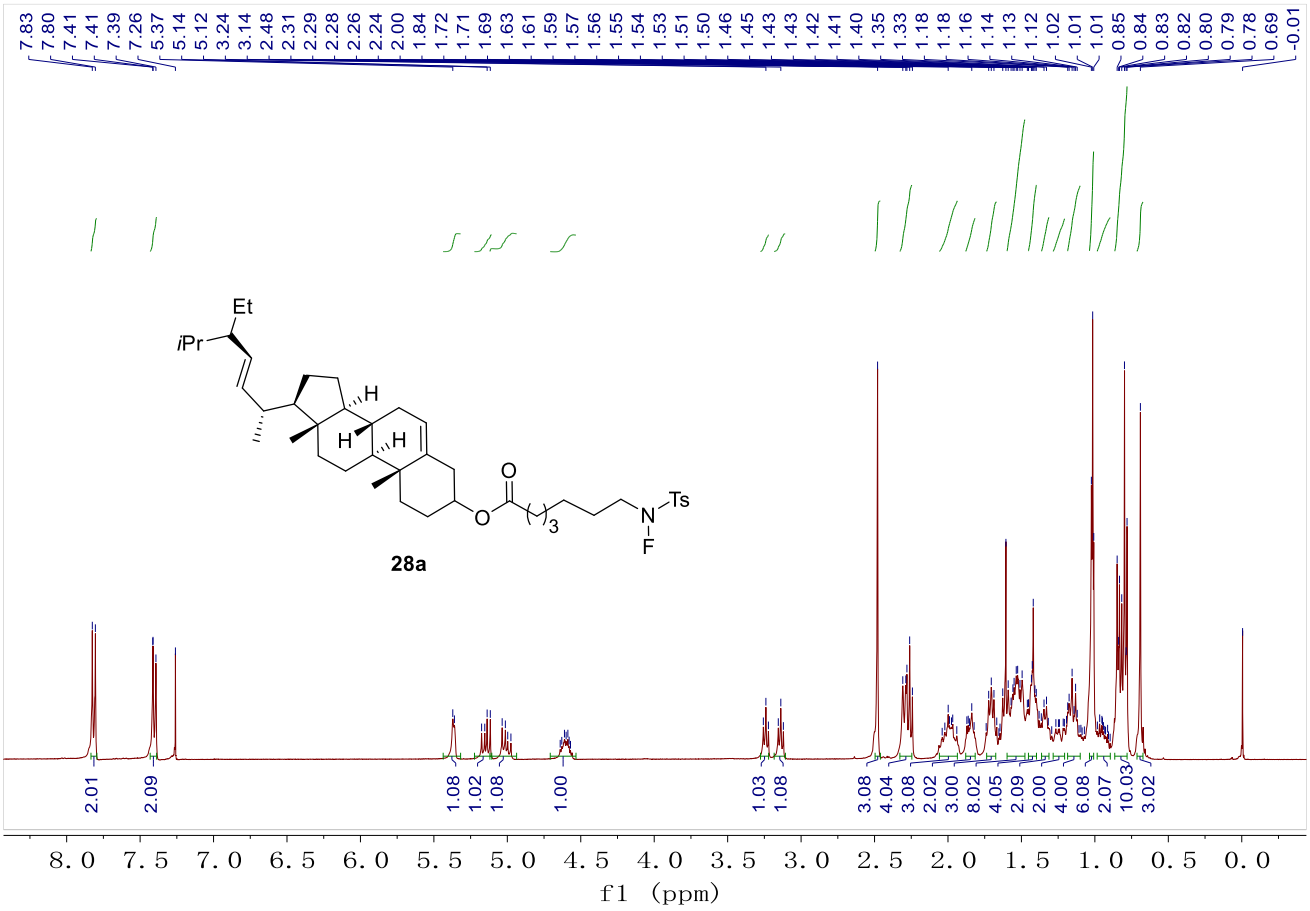
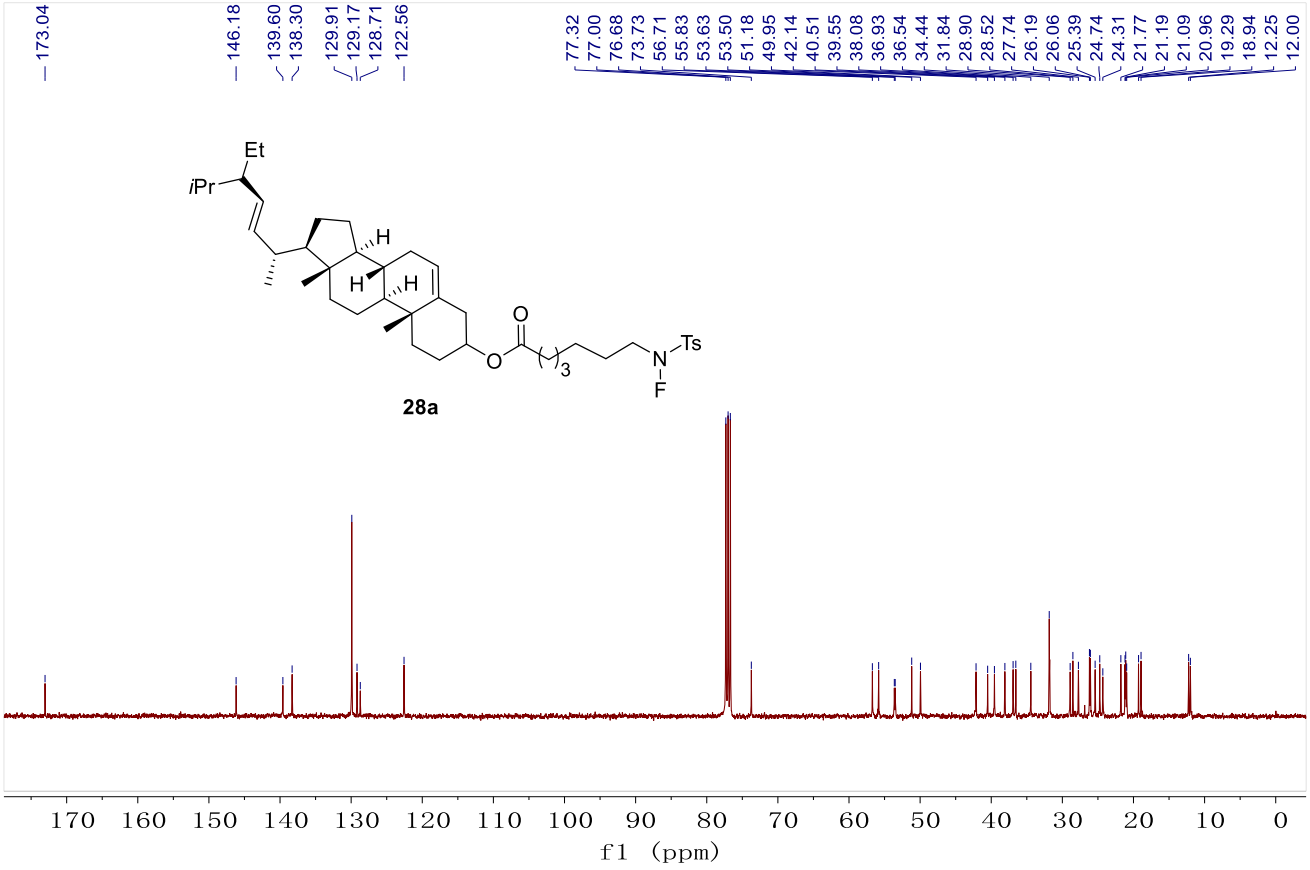
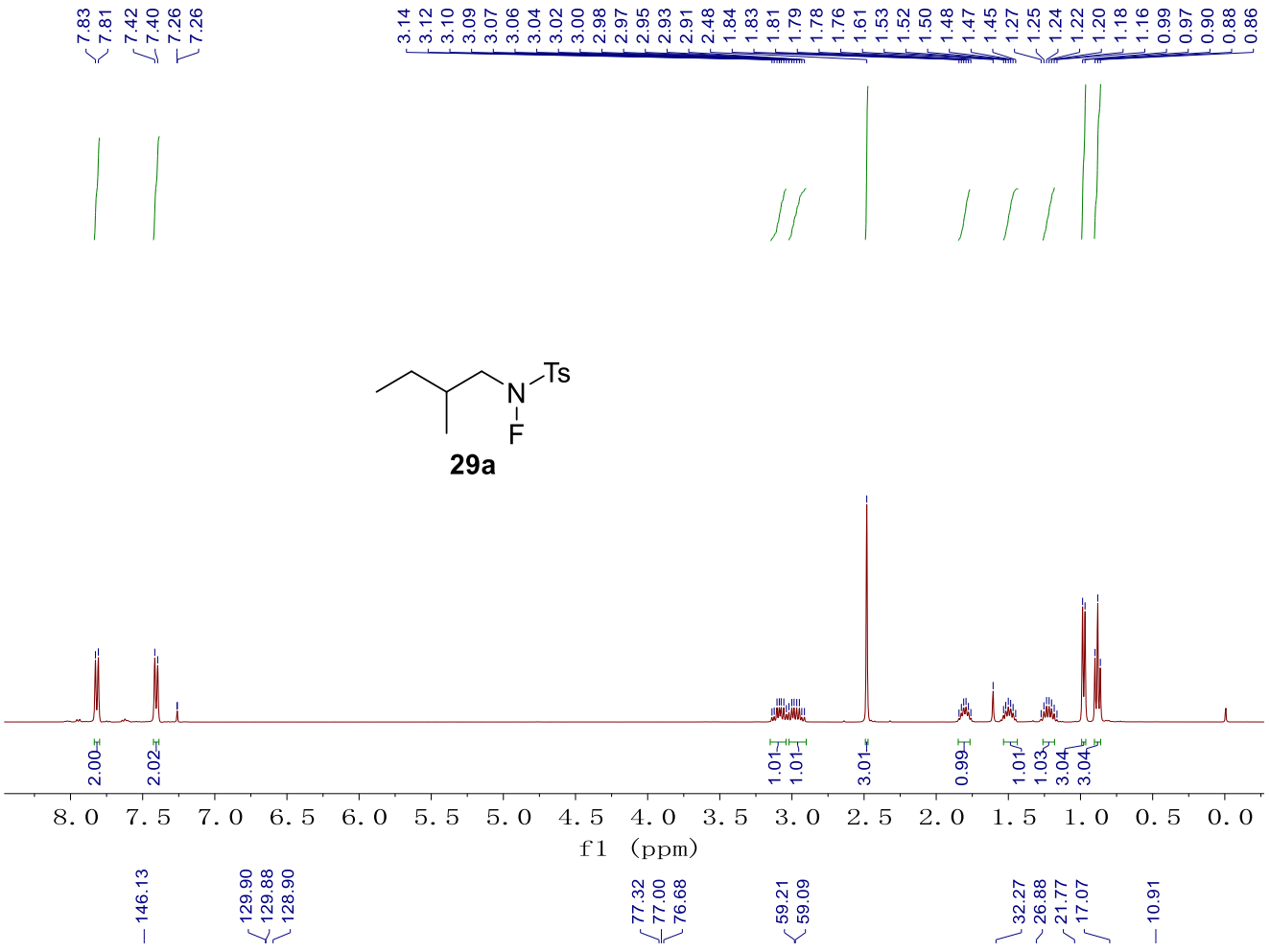
5.38
5.36
5.35
5.33
5.32
5.31
5.29
3.25
3.23
3.21
3.15
3.13
3.11
2.78
2.76
2.75
2.47
2.05
2.03
2.01
1.73
1.71
1.69
1.67
1.65
1.38
1.36
1.35
1.33
1.31
1.29
1.28
0.89
0.88
0.86
Ts
N
F
26a
2.05
2.05
4.09
1.00
1.02
2.05
3.03
4.08
2.06
16.01
3.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
146.11
130.10
129.95
129.86
129.85
128.76
127.94
127.82
77.32
77.00
76.68
53.76
53.63
31.44
29.53
29.27
29.24
29.07
29.01
27.12
27.11
26.48
26.21
25.55
22.50
21.68
14.01
Ts
N
F
26a
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

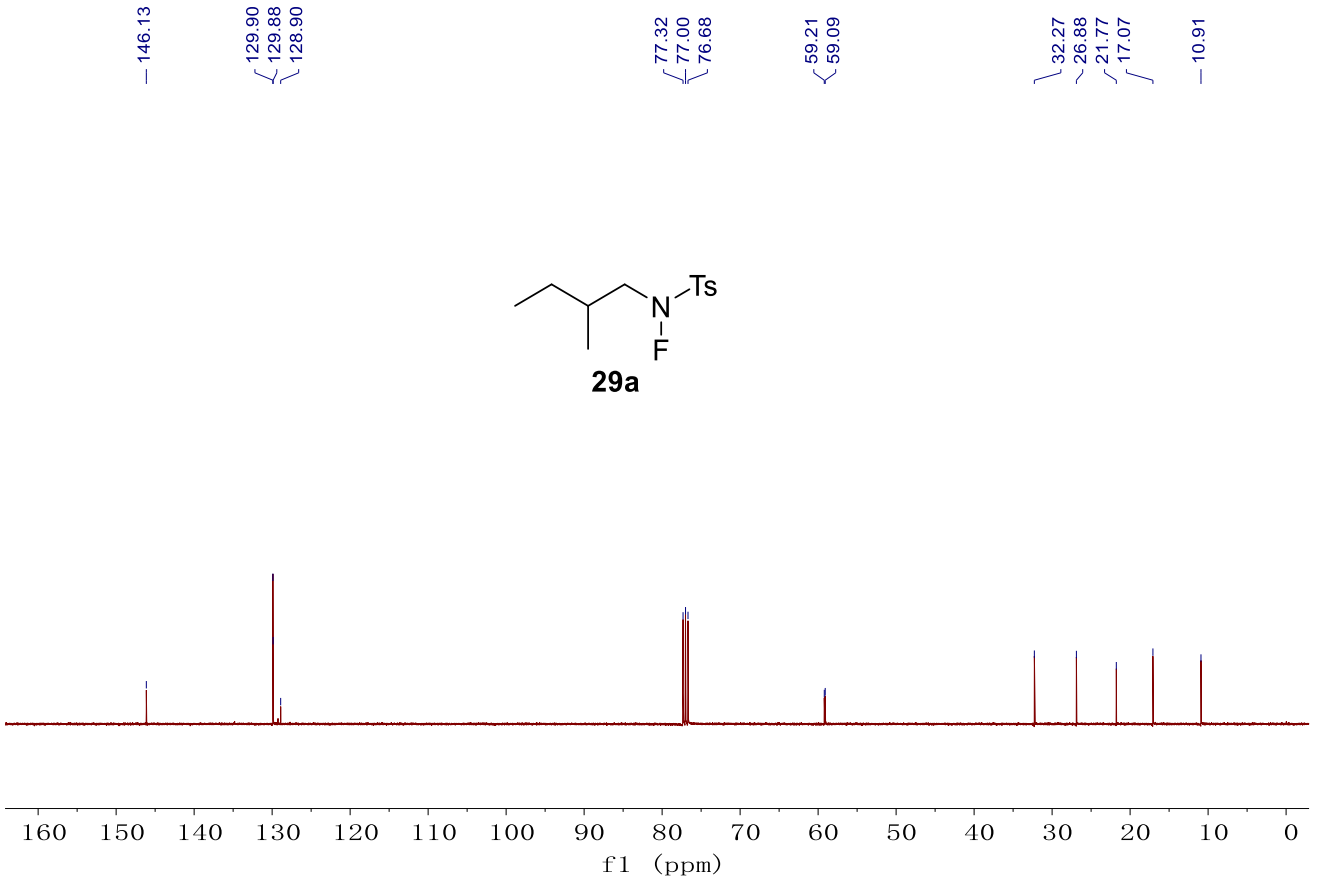

7.82 7.80 7.40 7.38 7.25 3.33 3.22 3.20 3.18 3.14 3.12 3.10 3.08 2.47 1.93 1.90 1.83 1.80 1.76 1.74 1.74 1.72 1.72 1.68 1.66 1.58 1.57 1.55 1.54 1.53 1.53 1.40 1.39 1.38 1.36 1.34 1.33 1.31 1.31 1.25 1.24 1.24 1.23 1.21 1.18 1.17 1.11 1.08 1.06 1.04 1.03 1.01 0.99 0.91 0.90 0.89 0.87 0.61 -0.02
N
Ts
F
H
H
H
H
O
27a
2.00 2.01 3.08 3.02 3.04 1.01 5.06 1.03 2.02 8.03 4.01 7.09 6.07 3.04
7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

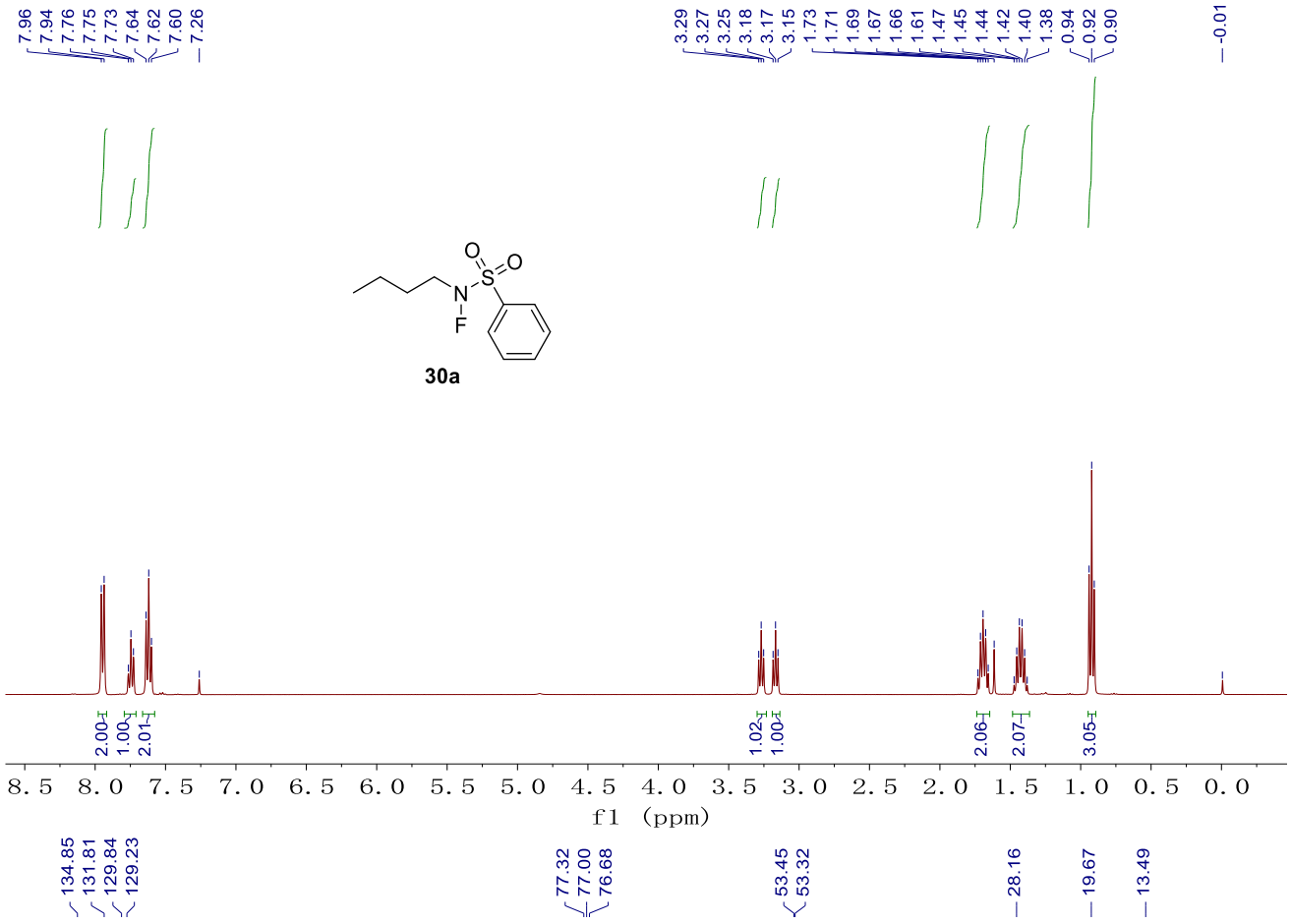

146.13
129.94 129.89 128.87
80.37 77.32 77.00 76.68
56.40 55.93 55.54 54.23 54.10 42.66 41.99 40.26 40.10 35.79 35.41 34.85 32.71 28.24 27.29 26.73 26.35 24.17 23.40 22.99 21.79 20.75 18.48
N
Ts
F
H
H
H
H
O
27a
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Et
iPr
H
H
H
O
O
3
N
Ts
F
28a
f1 (ppm)

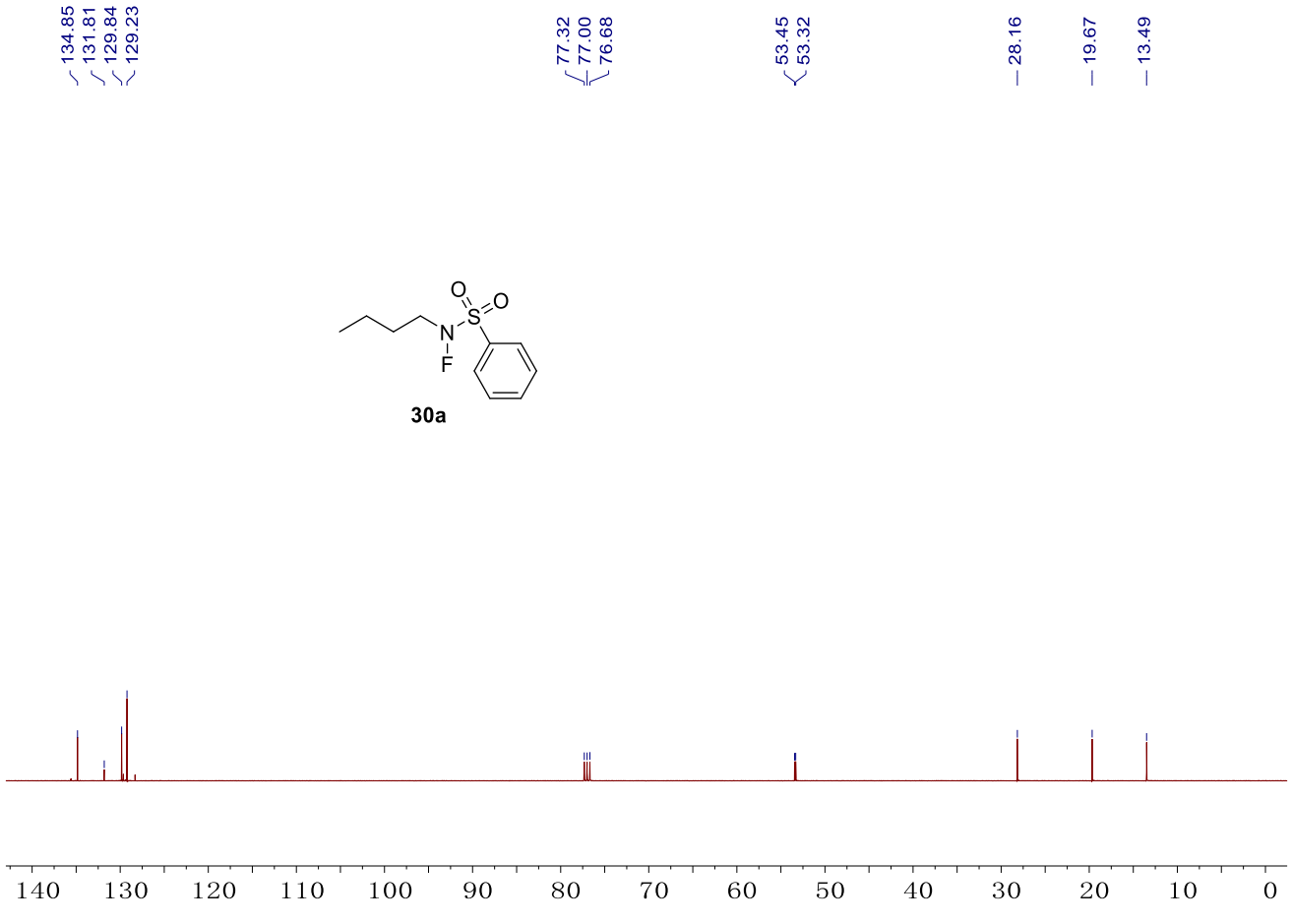

Et
iPr
H
H
H
O
O
3
N
Ts
F
28a
f1 (ppm)


7.83
7.81
7.42
7.40
7.26
7.26
3.14
3.12
3.10
3.09
3.07
3.06
3.04
3.02
3.00
2.98
2.97
2.95
2.93
2.91
2.48
1.84
1.83
1.81
1.79
1.78
1.76
1.61
1.53
1.52
1.50
1.48
1.47
1.45
1.27
1.25
1.24
1.22
1.20
1.18
1.16
0.99
0.97
0.90
0.88
0.86
Ts
N
F
29a
2.00
2.02
1.01
1.01
3.01
0.99
1.01
1.03
3.04
3.04
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

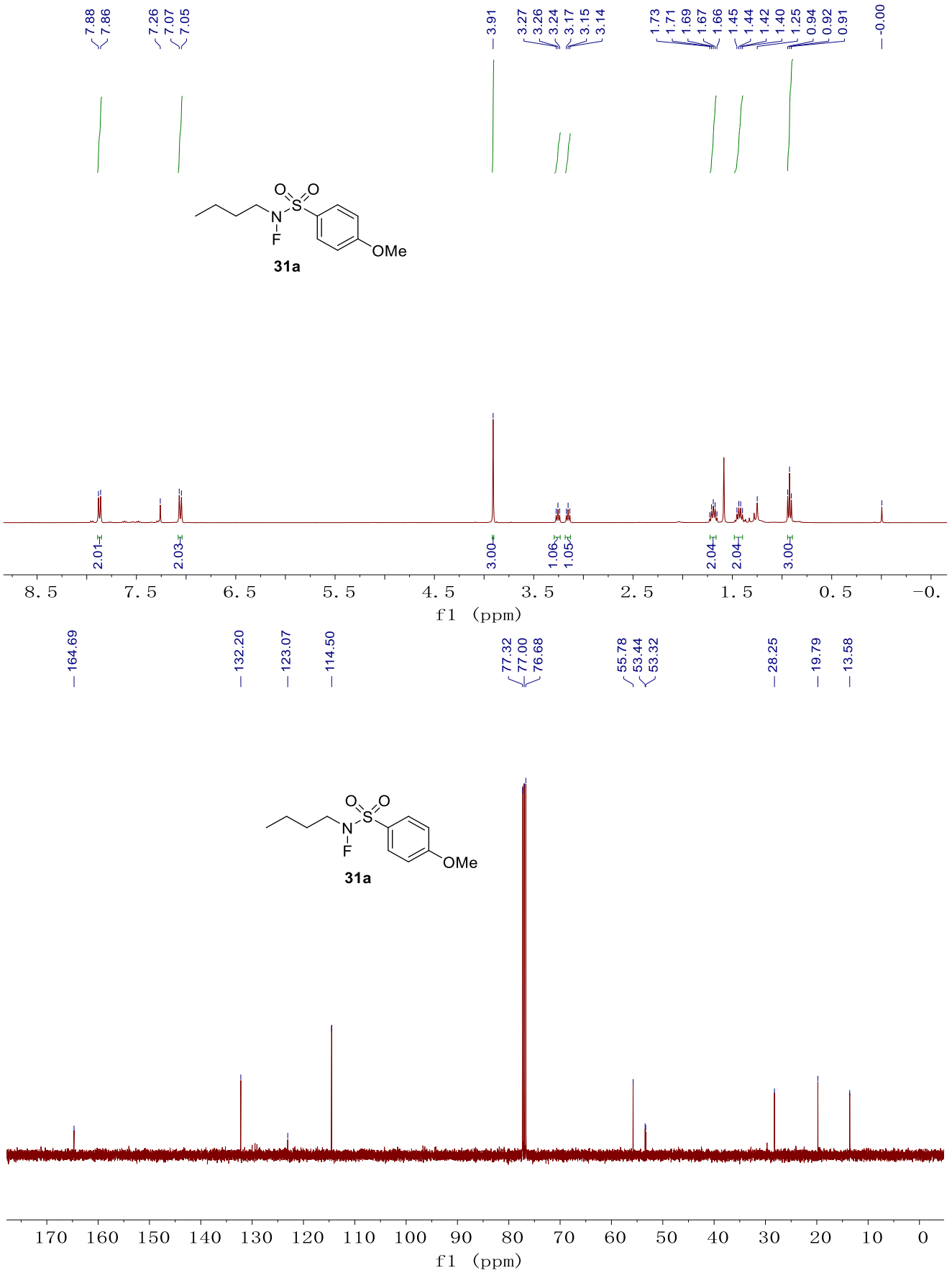

146.13
129.90
129.88
128.90
77.32
77.00
76.68
59.21
59.09
32.27
26.88
21.77
17.07
10.91
Ts
N
F
29a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

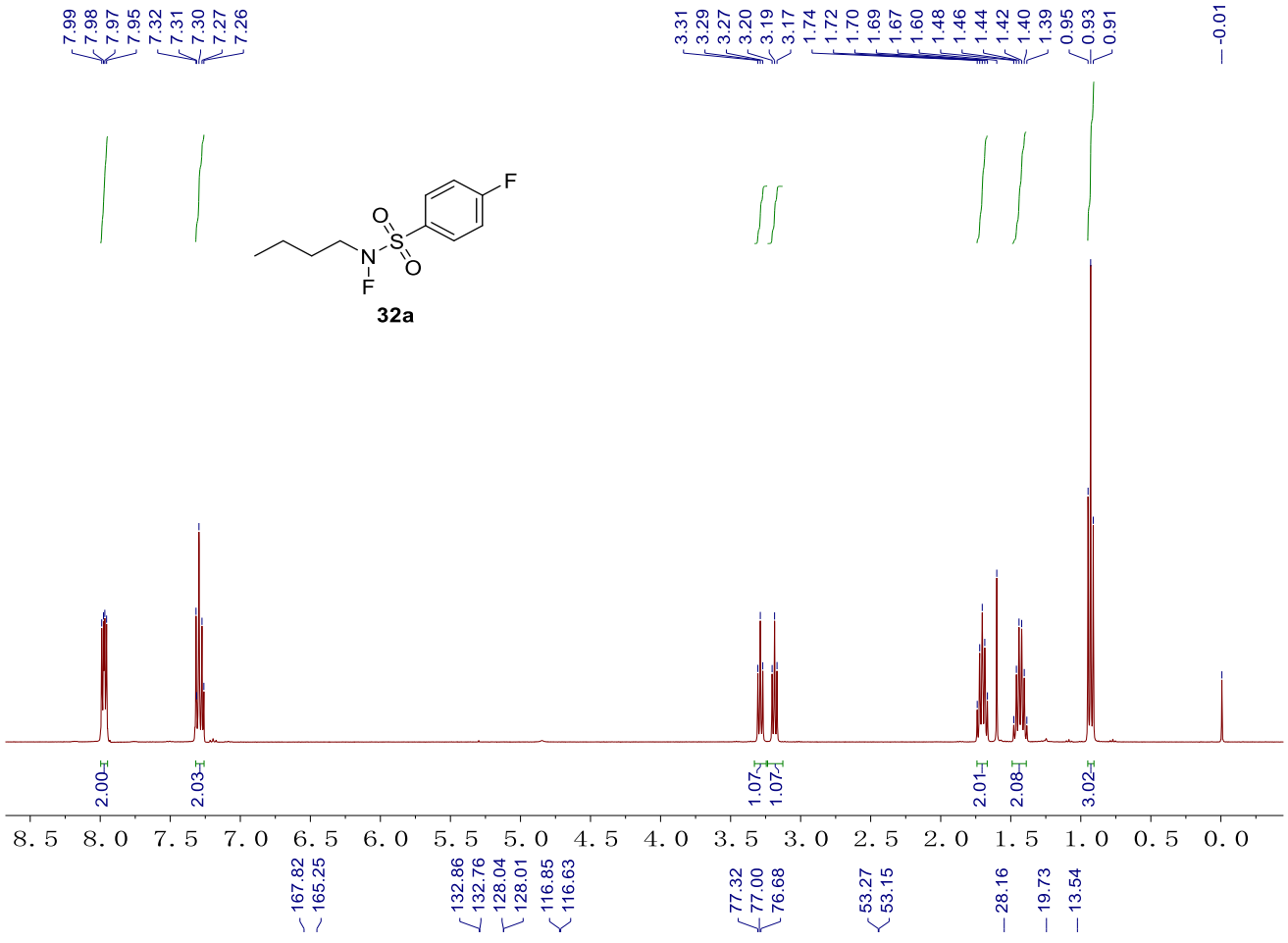

7.96
7.94
7.76
7.75
7.73
7.64
7.62
7.60
7.26
3.29
3.27
3.25
3.18
3.17
3.15
1.73
1.71
1.69
1.67
1.66
1.61
1.47
1.45
1.44
1.42
1.40
1.38
0.94
0.92
0.90
-0.01
O
S
O
N
F
2.00
1.00
2.01
1.02
1.00
2.06
2.07
3.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

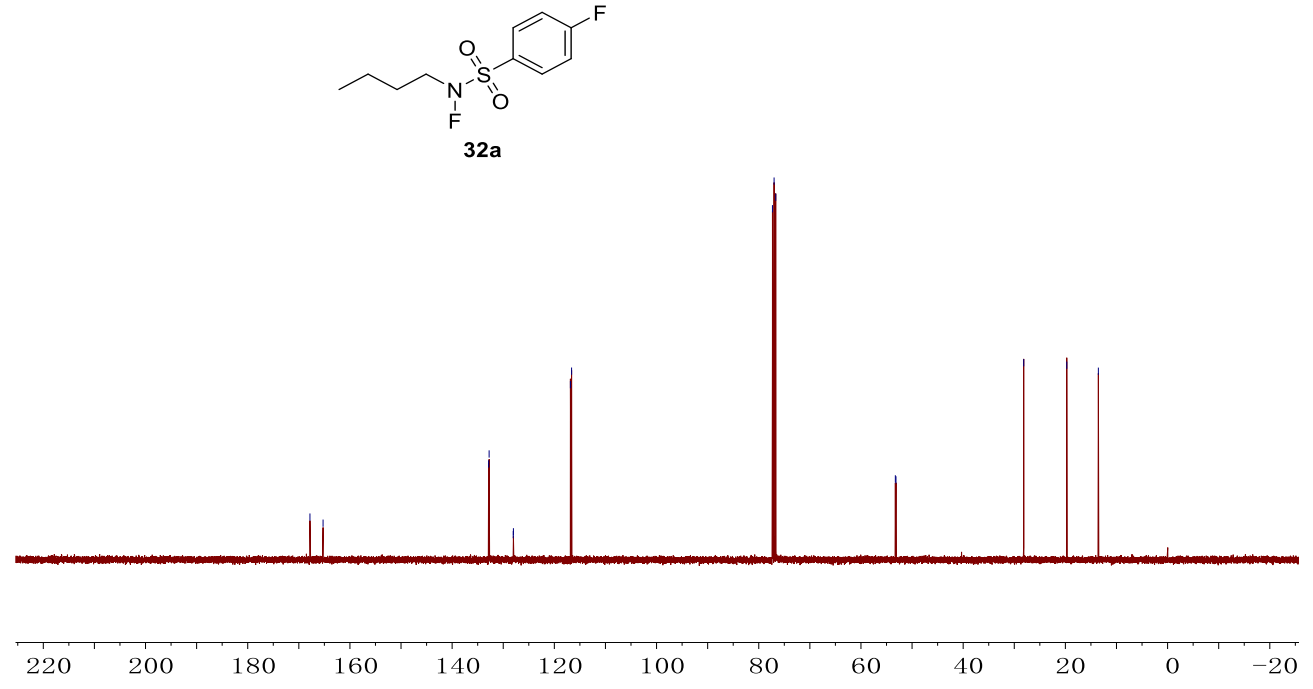
30a

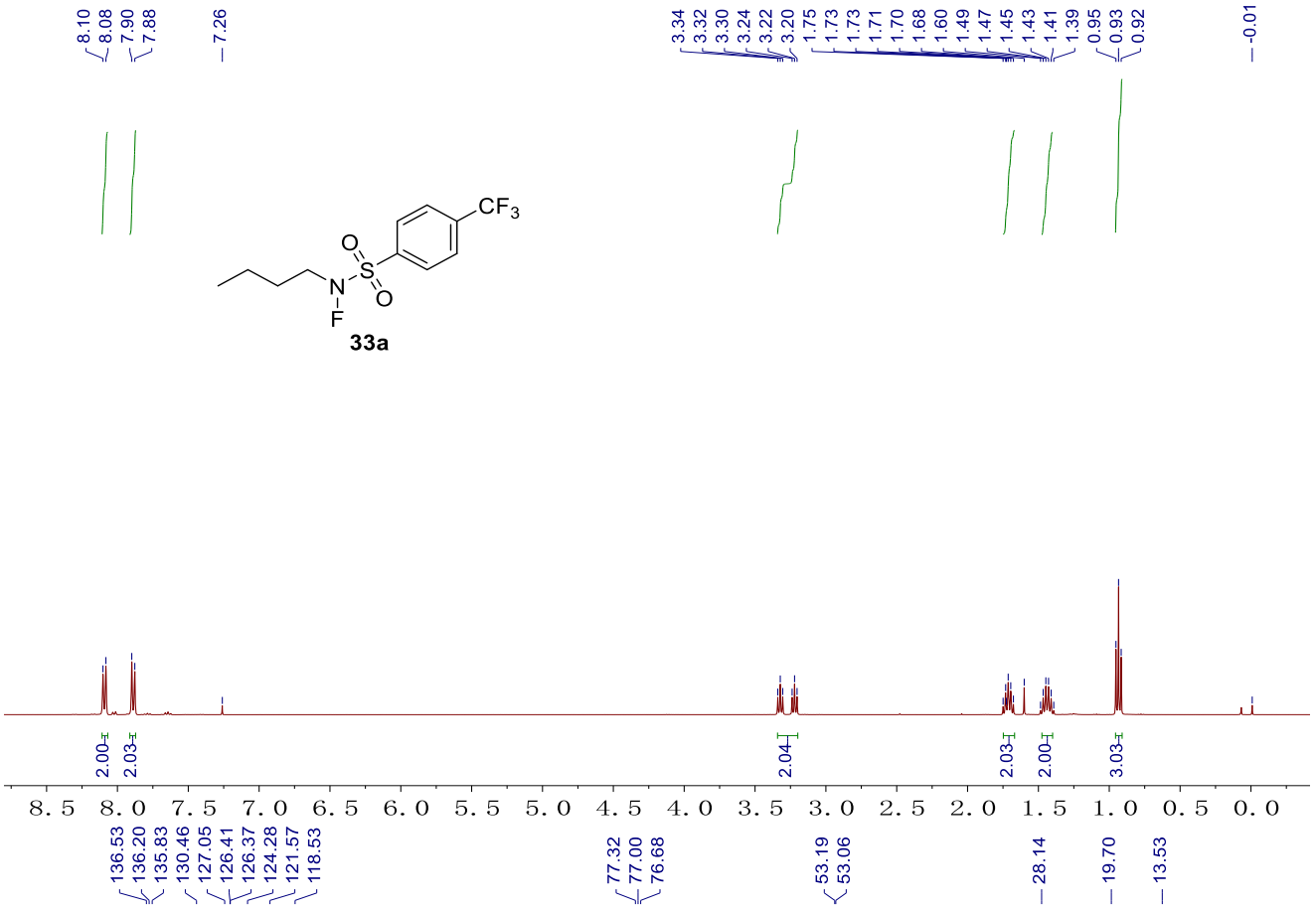

134.85
131.81
129.84
129.23
77.32
77.00
76.68
53.45
53.32
28.16
19.67
13.49
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

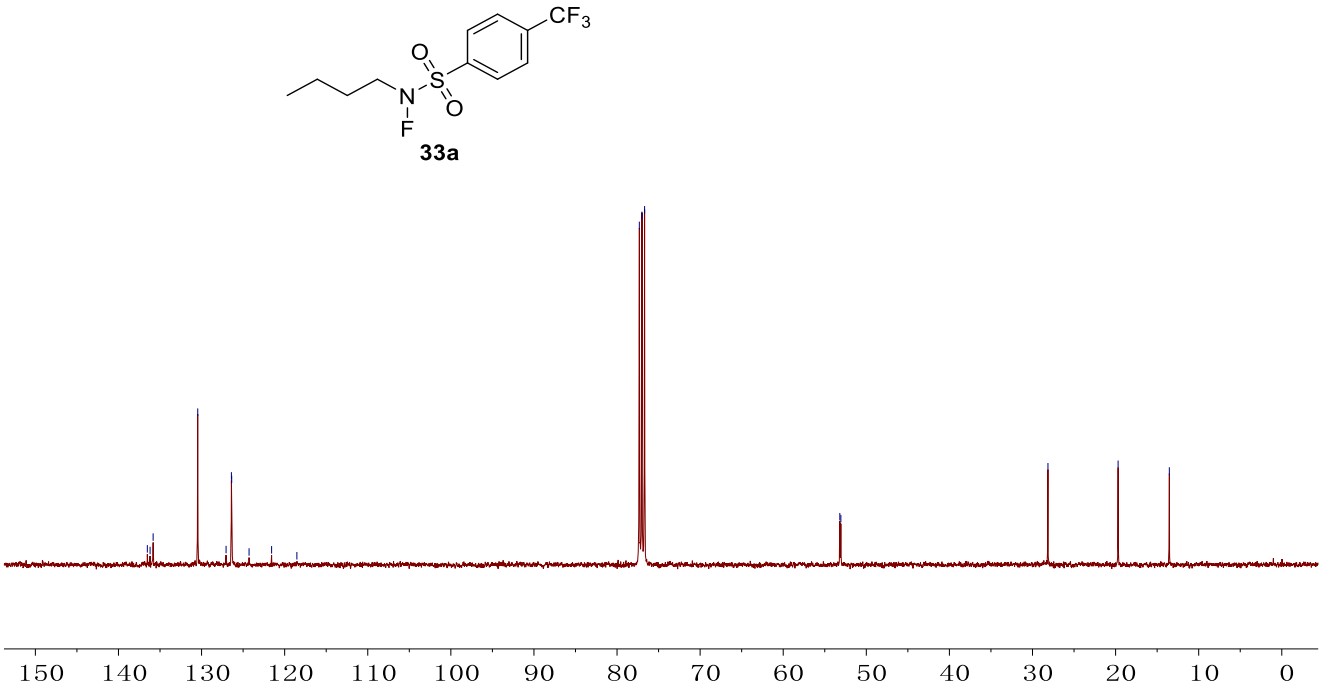
30a

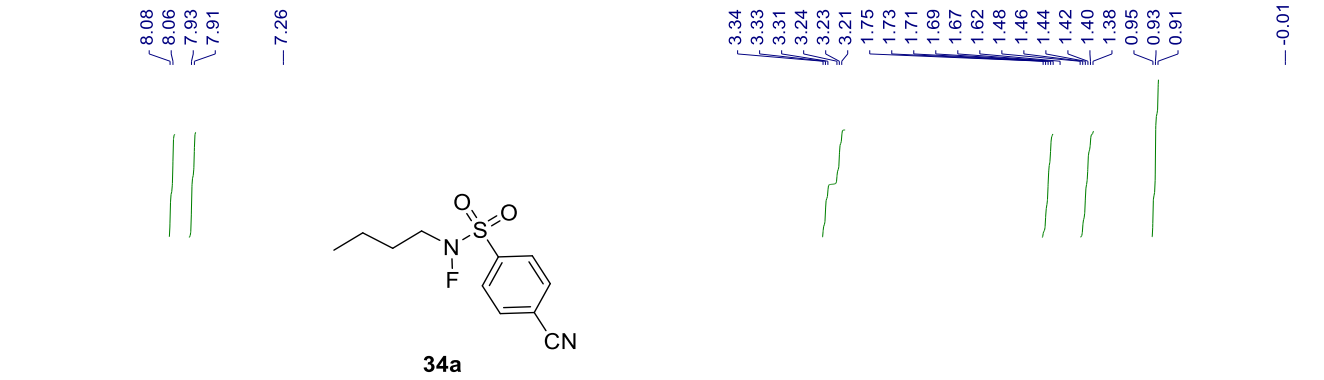

7.88
7.86
7.26
7.07
7.05
3.91
3.27
3.26
3.24
3.17
3.15
3.14
1.73
1.71
1.69
1.67
1.66
1.45
1.44
1.42
1.40
1.25
0.94
0.92
0.91
-0.00
O
O
S
N
F
OMe
31a
2.01
2.03
3.00
1.06
1.05
2.04
2.04
3.00
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
f1 (ppm)
164.69
132.20
123.07
114.50
77.32
77.00
76.68
55.78
53.44
53.32
28.25
19.79
13.58
O
O
S
N
F
OMe
31a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.99
7.98
7.97
7.95
7.32
7.31
7.30
7.27
7.26
3.31
3.29
3.27
3.20
3.19
3.17
1.74
1.72
1.70
1.69
1.67
1.60
1.48
1.46
1.44
1.42
1.40
1.39
0.95
0.93
0.91
-0.01
F
O
S
O
N
F
32a
2.00
2.03
1.07
1.07
2.01
2.08
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
167.82
165.25
132.86
132.76
128.04
128.01
116.85
116.63
77.32
77.00
76.68
53.27
53.15
28.16
19.73
13.54

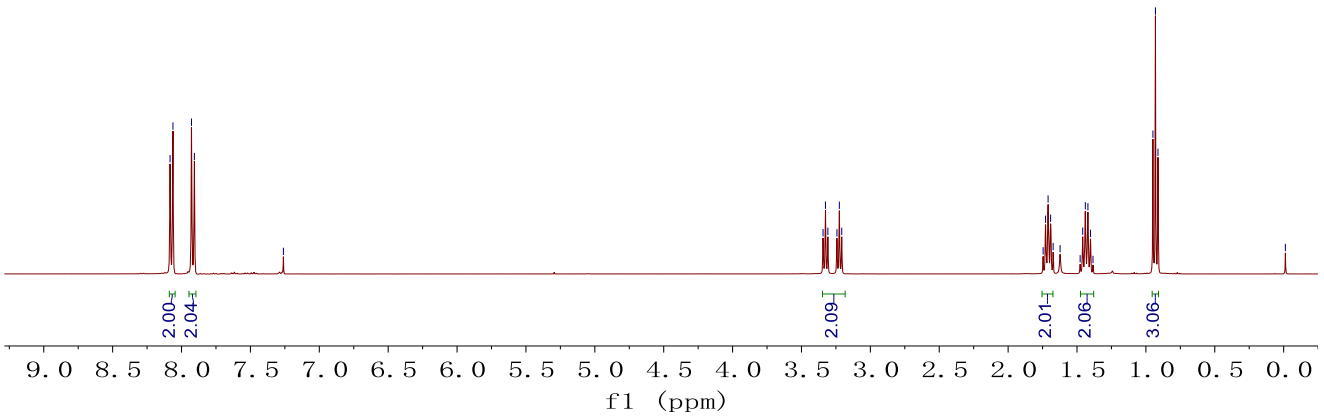

F
O
S
O
N
F
32a
220 200 180 160 140 120 100 80 60 40 20 0 -20

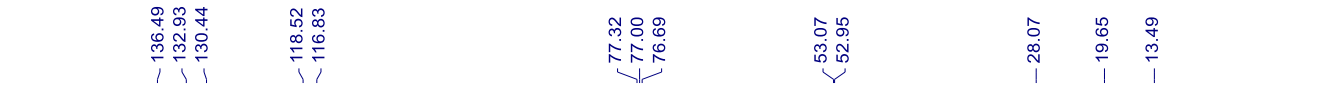

8.10
8.08
7.90
7.88
7.26
3.34
3.32
3.30
3.24
3.22
3.20
1.75
1.73
1.73
1.71
1.70
1.68
1.60
1.49
1.47
1.45
1.43
1.41
1.39
0.95
0.93
0.92
-0.01
CF3
O
S
O
N
F
33a
2.00
2.03
2.04
2.03
2.00
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
136.53
136.20
135.83
130.46
127.05
126.41
126.37
124.28
121.57
118.53
77.32
77.00
76.68
53.19
53.06
28.14
19.70
13.53

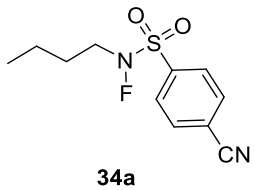

CF3
O
S
O
N
F
33a
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


8.08
8.06
7.93
7.91
7.26
3.34
3.33
3.31
3.24
3.23
3.21
1.75
1.73
1.71
1.69
1.67
1.62
1.48
1.46
1.44
1.42
1.40
1.38
0.95
0.93
0.91
-0.01
O
O
S
N
F
CN

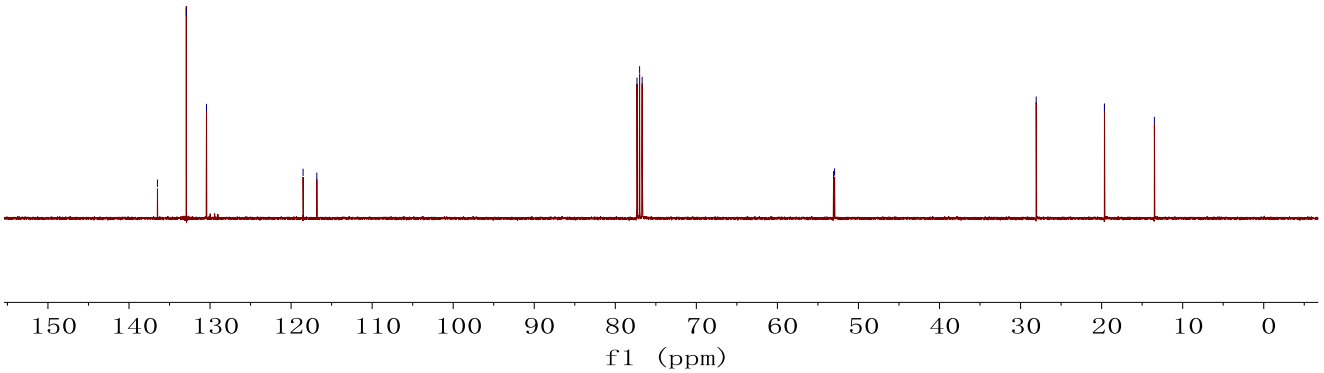
34a

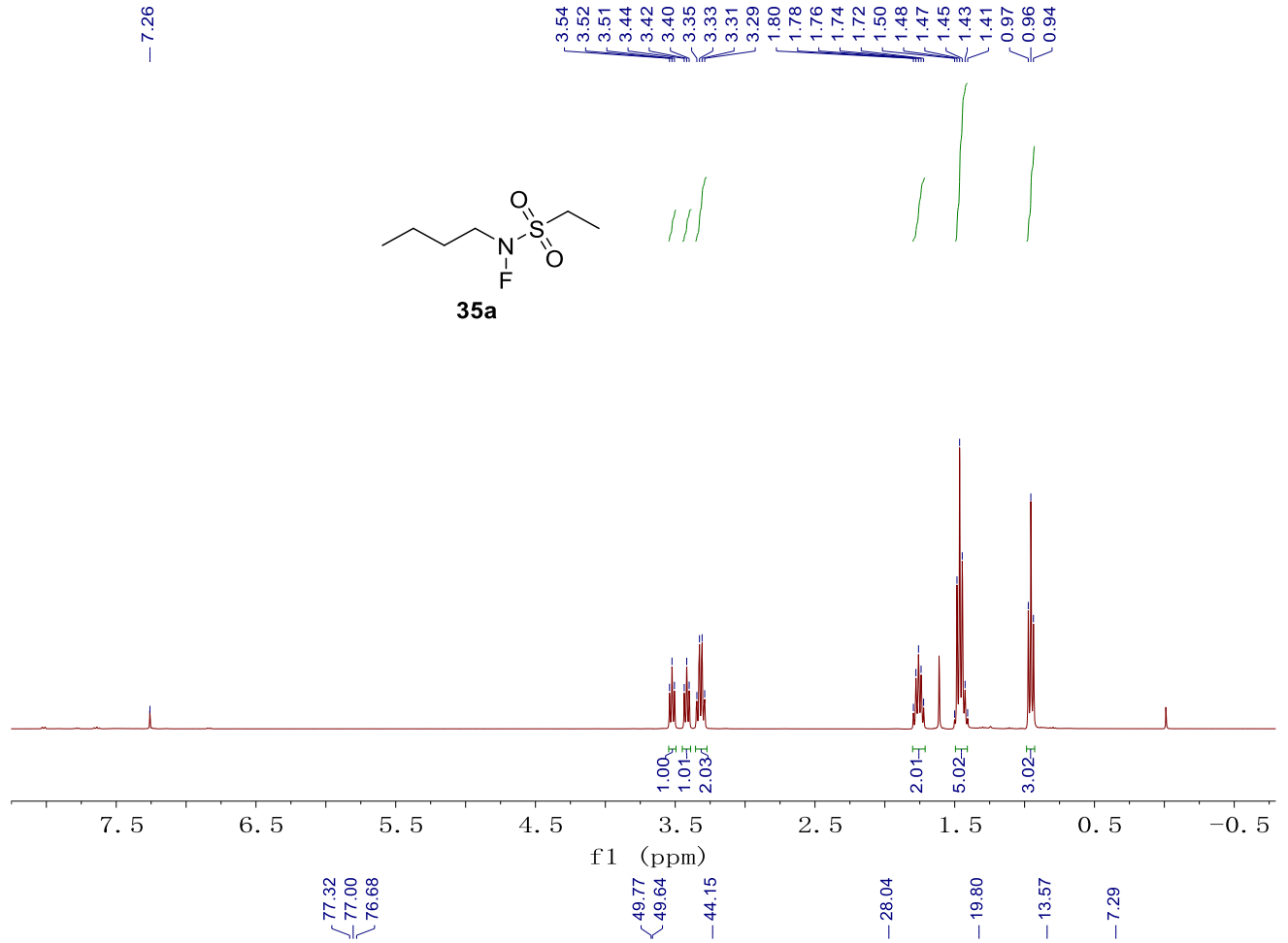

2.00
2.04
2.09
2.01
2.06
3.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


136.49
132.93
130.44
118.52
116.83
77.32
77.00
76.69
53.07
52.95
28.07
19.65
13.49


O
O
S
N
F
CN

34a


150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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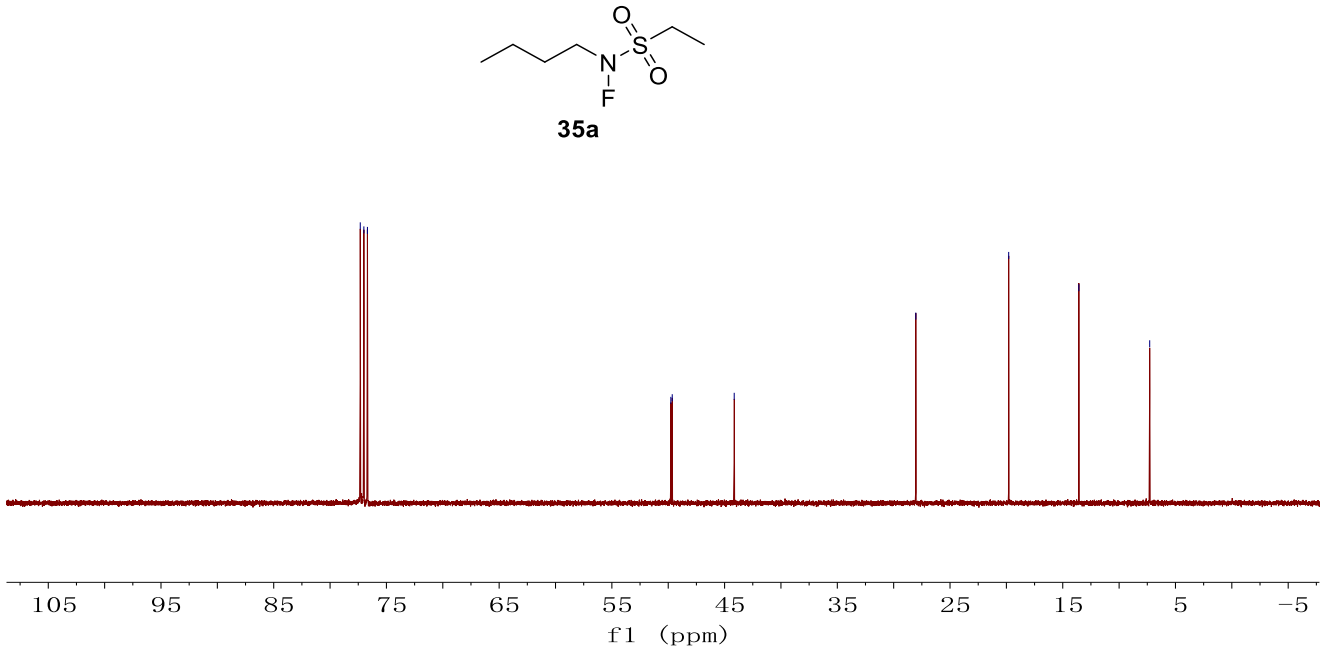
3.35
3.33
3.31
3.29
1.80
1.78
1.76
1.74
1.72
1.50
1.48
1.47
1.45
1.43
1.41
0.97
0.96
0.94
35a
1.00
1.01
2.03
2.01
5.02
3.02
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)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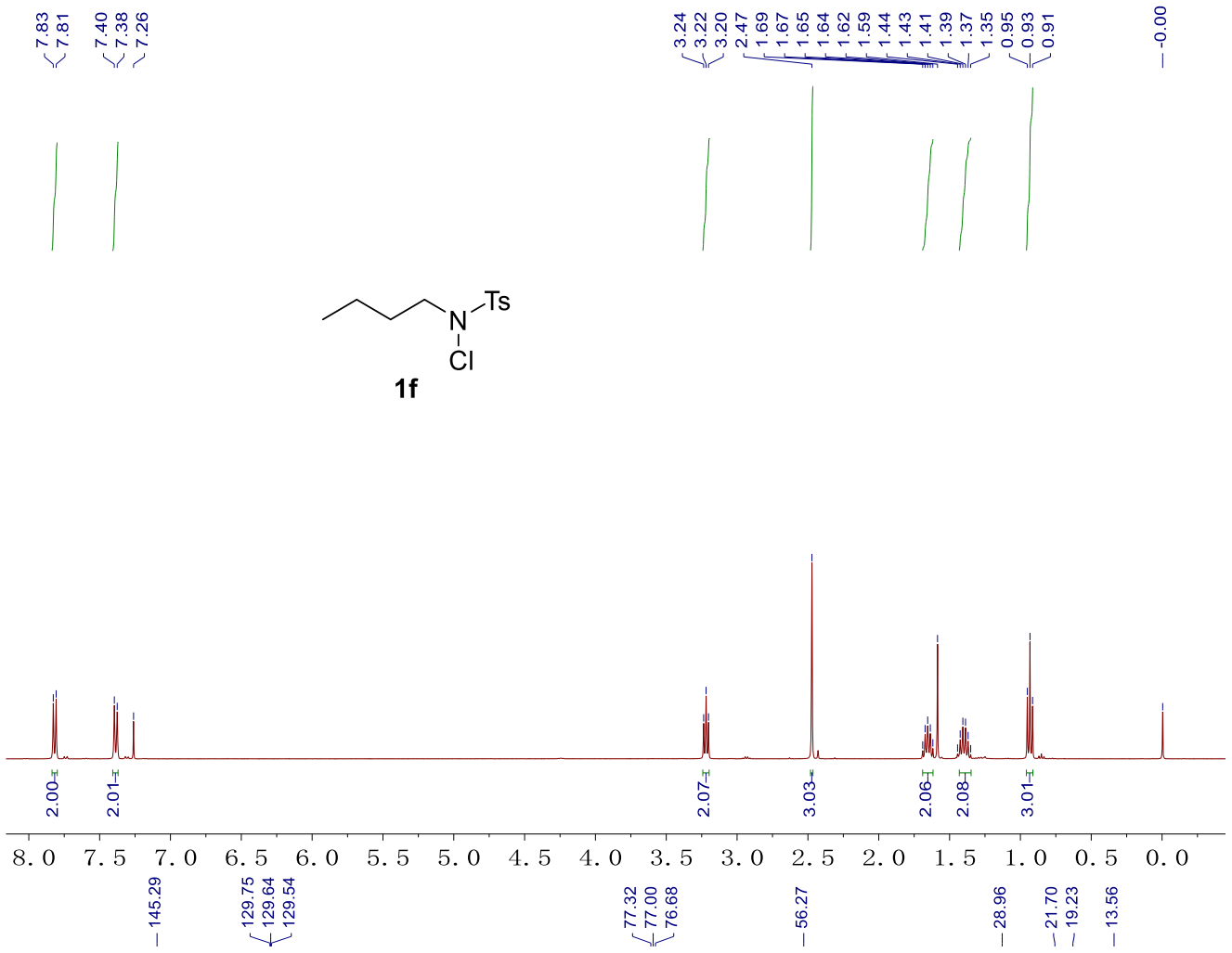
77.00
76.68
49.77
49.64
44.15
28.04
19.80
13.57
7.29
35a
105
95
85
75
65
55
45
35
25
15
5
−5
f1 (ppm)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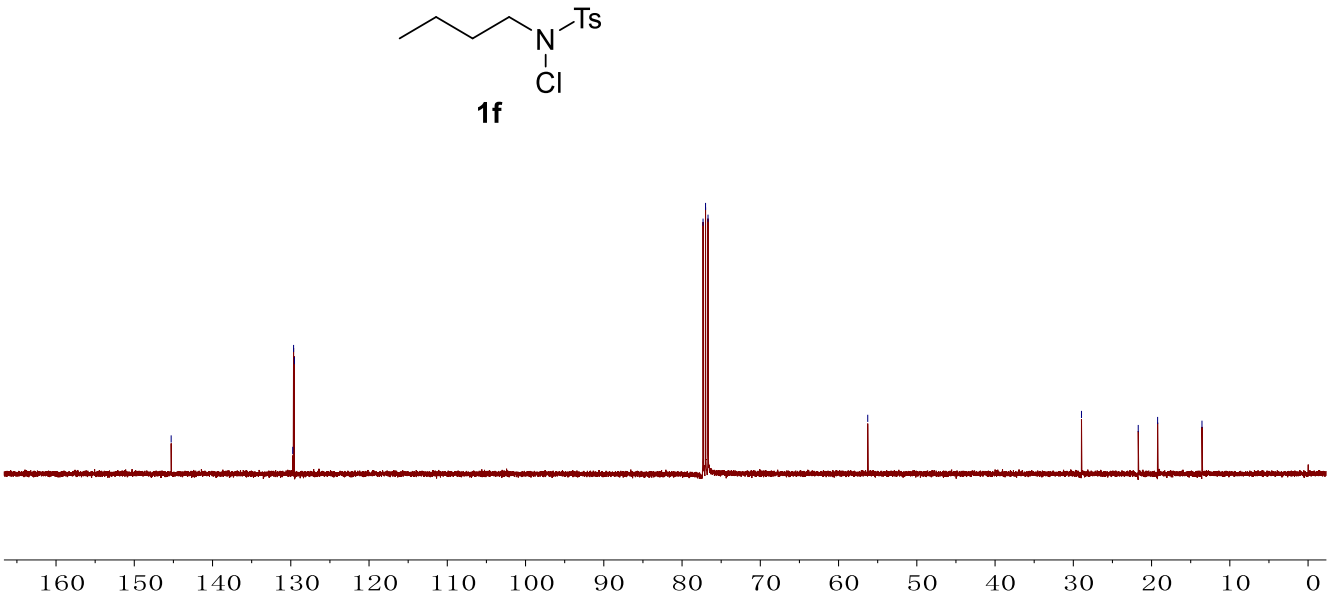
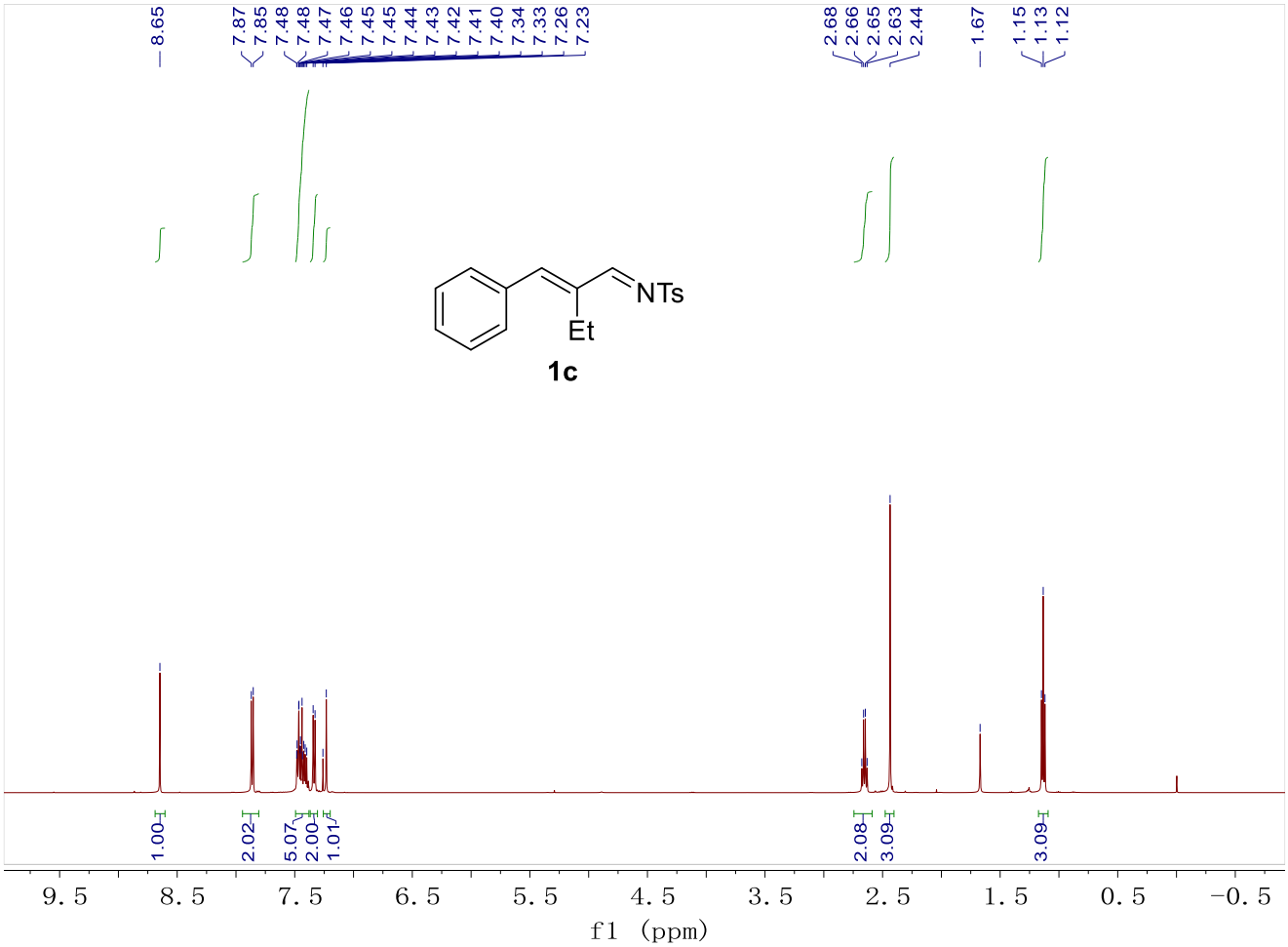
7.40
7.38
7.26
3.24
3.22
3.20
2.47
1.69
1.67
1.65
1.64
1.62
1.59
1.44
1.43
1.41
1.39
1.37
1.35
0.95
0.93
0.91
-0.00
Ts
N
Cl
1f
2.00
2.01
2.07
3.03
2.06
2.08
3.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


145.29
129.75
129.64
129.54
77.32
77.00
76.68
56.27
28.96
21.70
19.23
13.56
Ts
N
Cl
1f
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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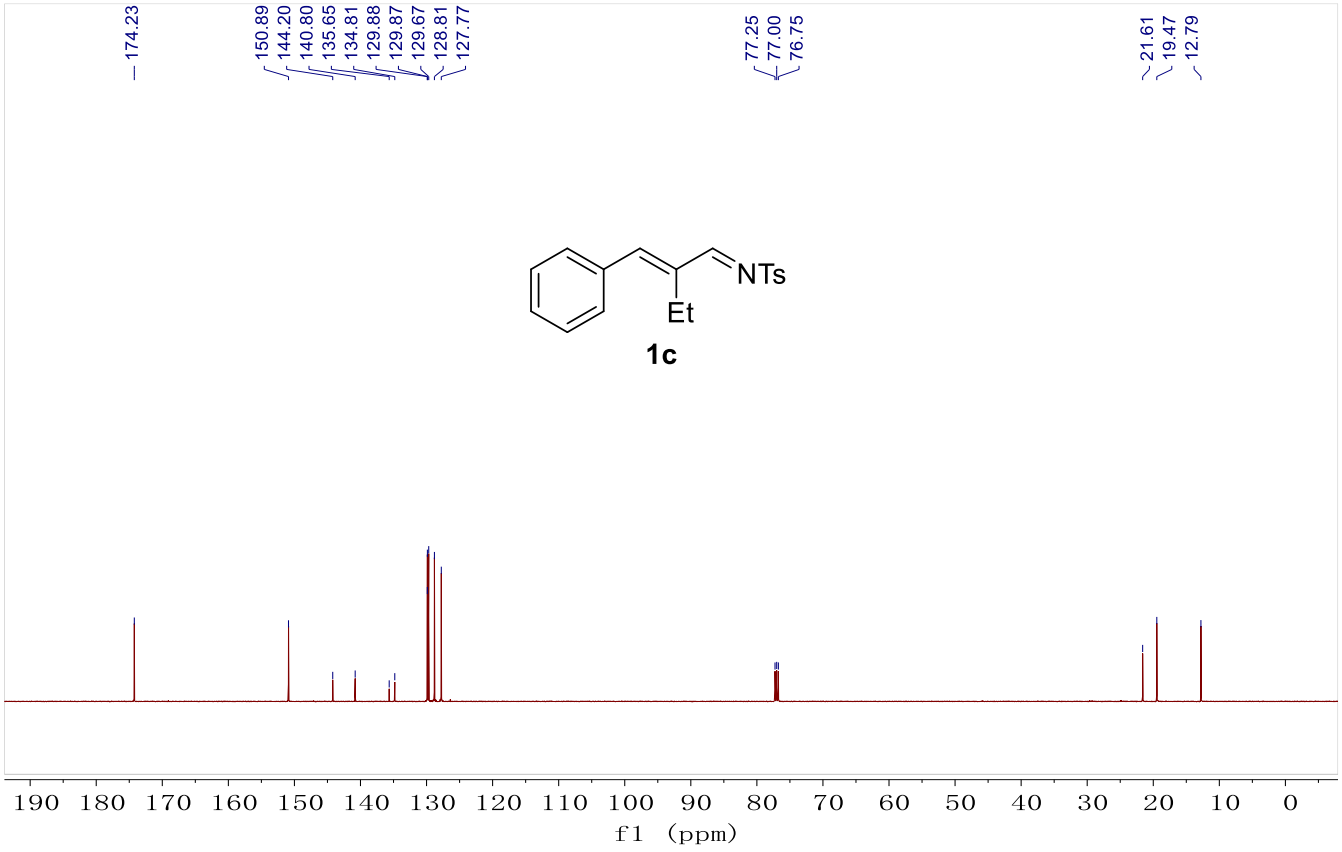
7.48
7.47
7.46
7.45
7.45
7.44
7.43
7.42
7.41
7.40
7.34
7.33
7.26
7.23
2.68
2.66
2.65
2.63
2.44
1.67
1.15
1.13
1.12
NTs
Et
1c
1.00
2.02
5.07
2.00
1.01
2.08
3.09
3.09
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)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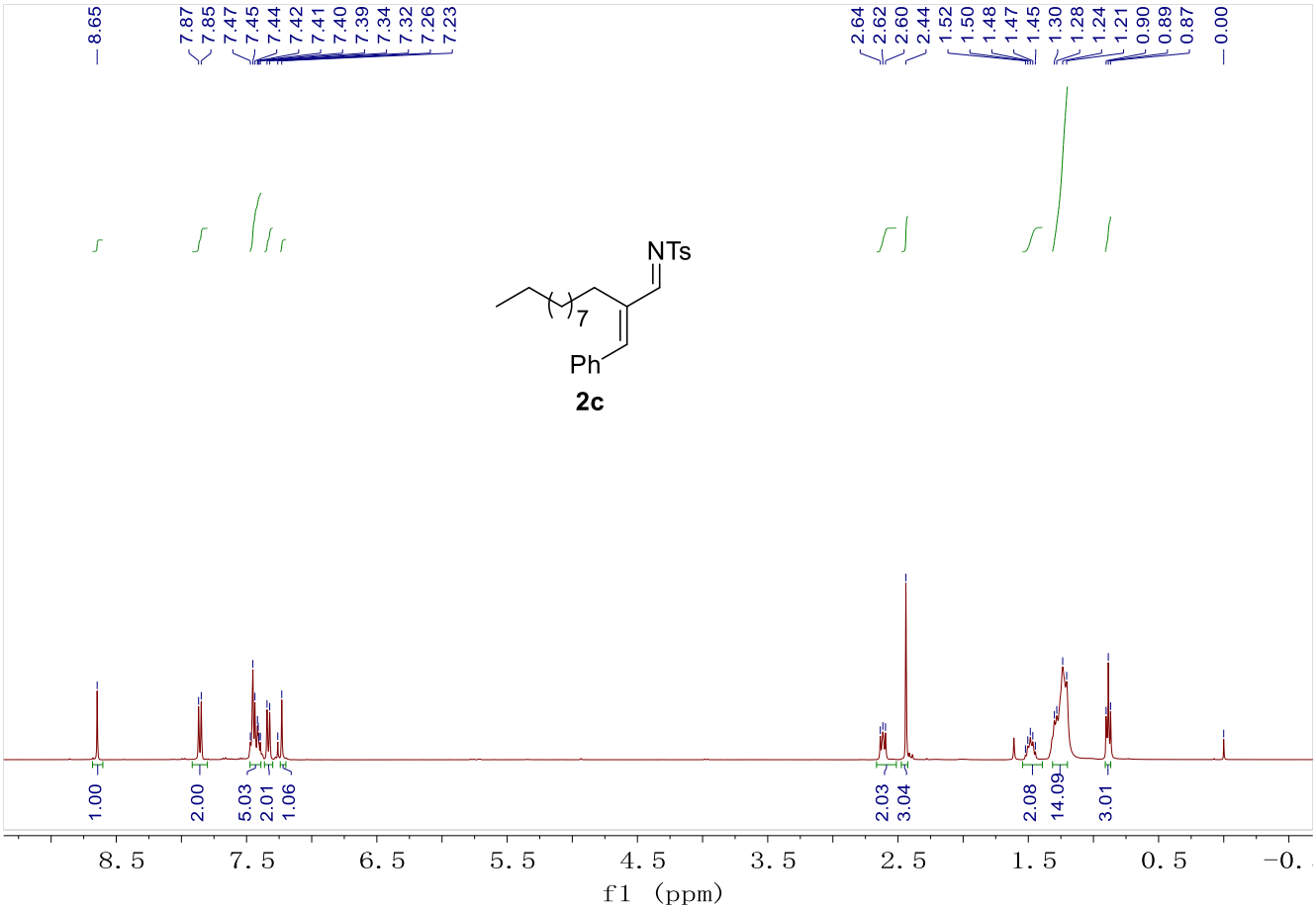
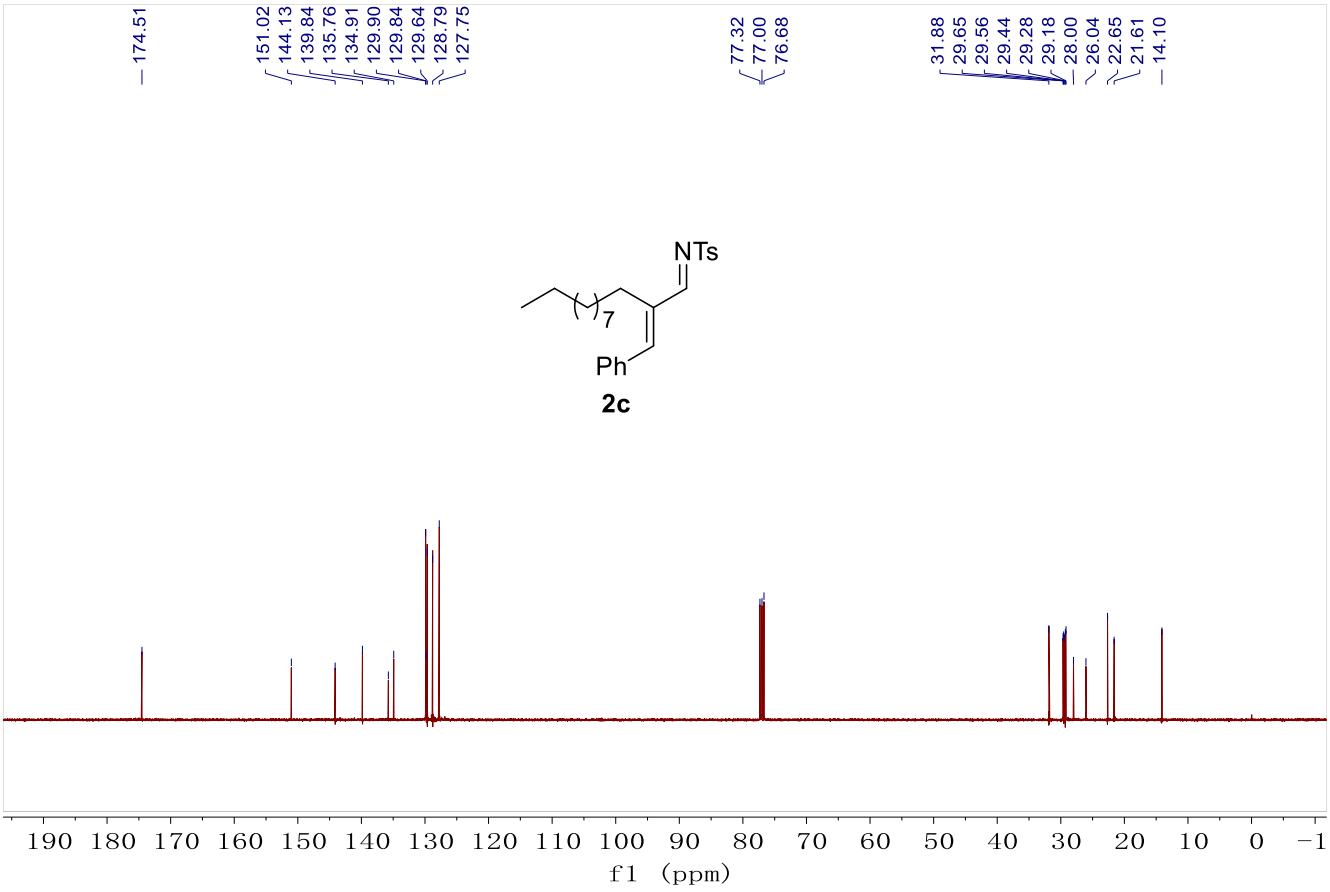
144.20
140.80
135.65
134.81
129.88
129.87
129.67
128.81
127.77
77.25
77.00
76.75
21.61
19.47
12.79
NTs
Et
1c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.65
7.87
7.85
7.47
7.45
7.44
7.42
7.41
7.40
7.39
7.34
7.32
7.26
7.23
2.64
2.62
2.60
2.44
1.52
1.50
1.48
1.47
1.45
1.30
1.28
1.24
1.21
0.90
0.89
0.87
0.00
NTs
7
Ph
2c
1.00
2.00
5.03
2.01
1.06
2.03
3.04
2.08
14.09
3.01
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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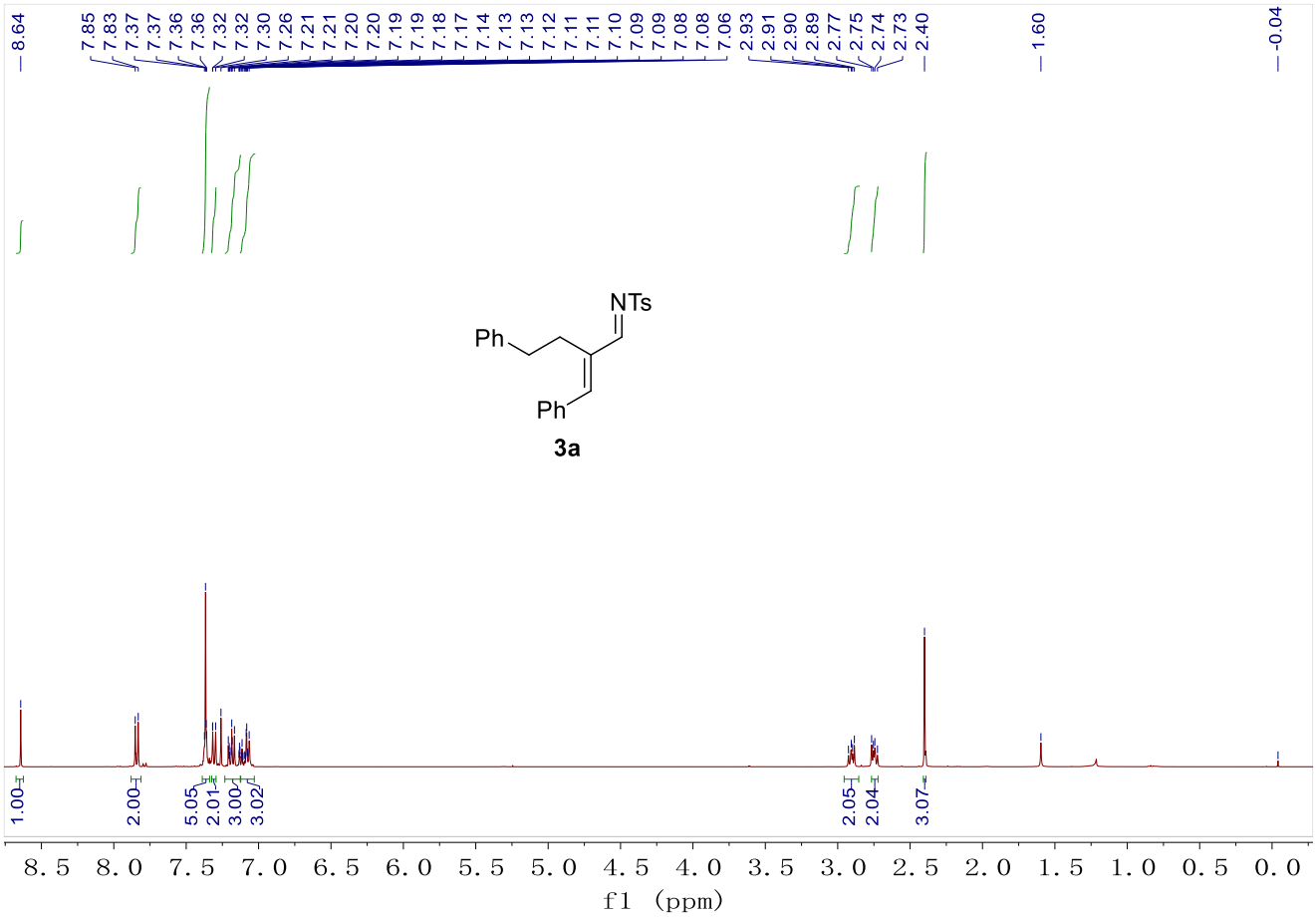
151.02
144.13
139.84
135.76
134.91
129.90
129.84
129.64
128.79
127.75
77.32
77.00
76.68
31.88
29.65
29.56
29.44
29.28
29.18
28.00
26.04
22.65
21.61
14.10
NTs
7
Ph
2c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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7.37
7.37
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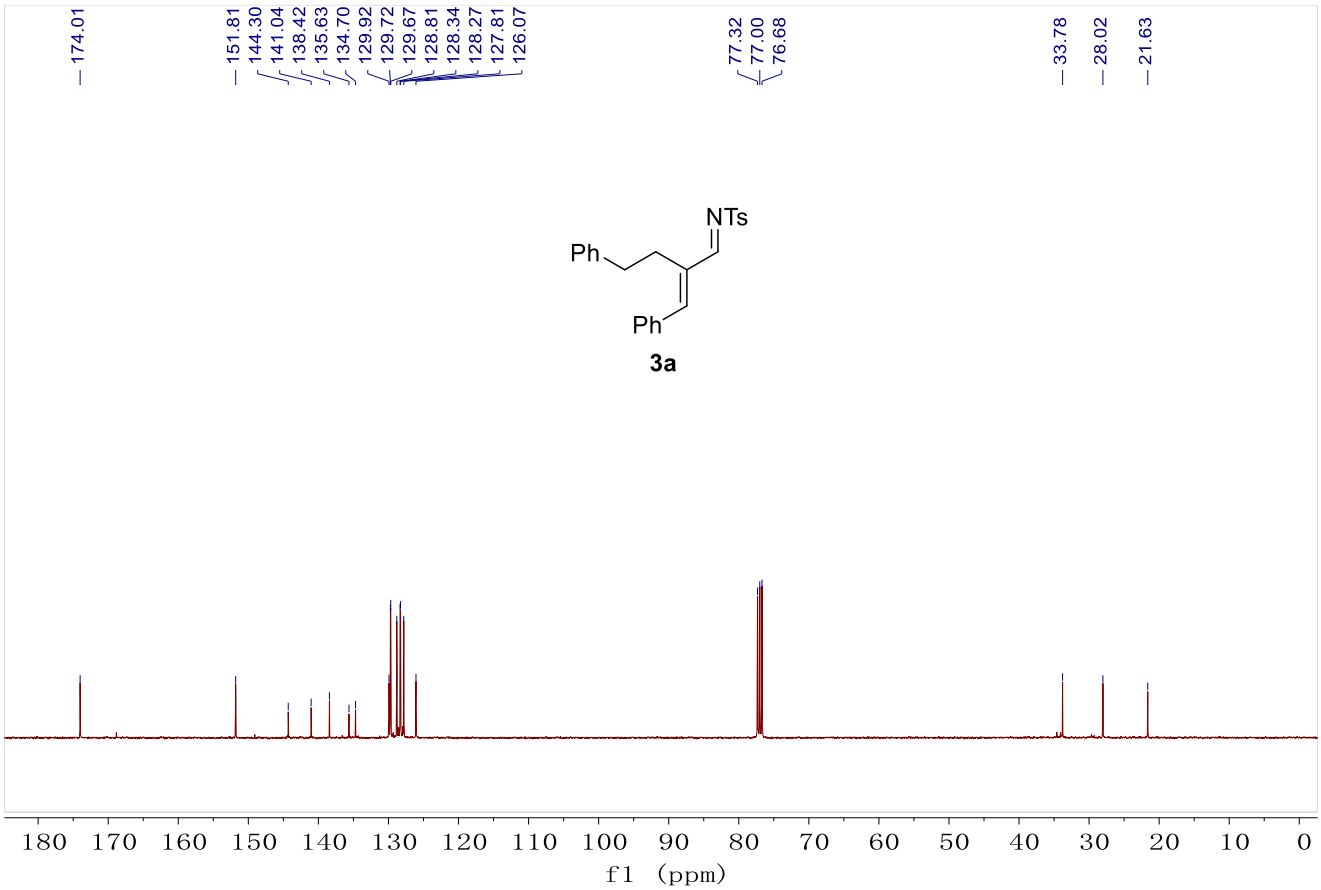
7.36
7.32
7.32
7.30
7.26
7.21
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.14
7.13
7.13
7.12
7.11
7.11
7.10
7.09
7.09
7.08
7.08
7.06
2.93
2.91
2.90
2.89
2.77
2.75
2.74
2.73
2.40
1.60
-0.04
NTs
Ph
Ph
3a
1.00
2.00
5.05
2.01
3.00
3.02
2.05
2.04
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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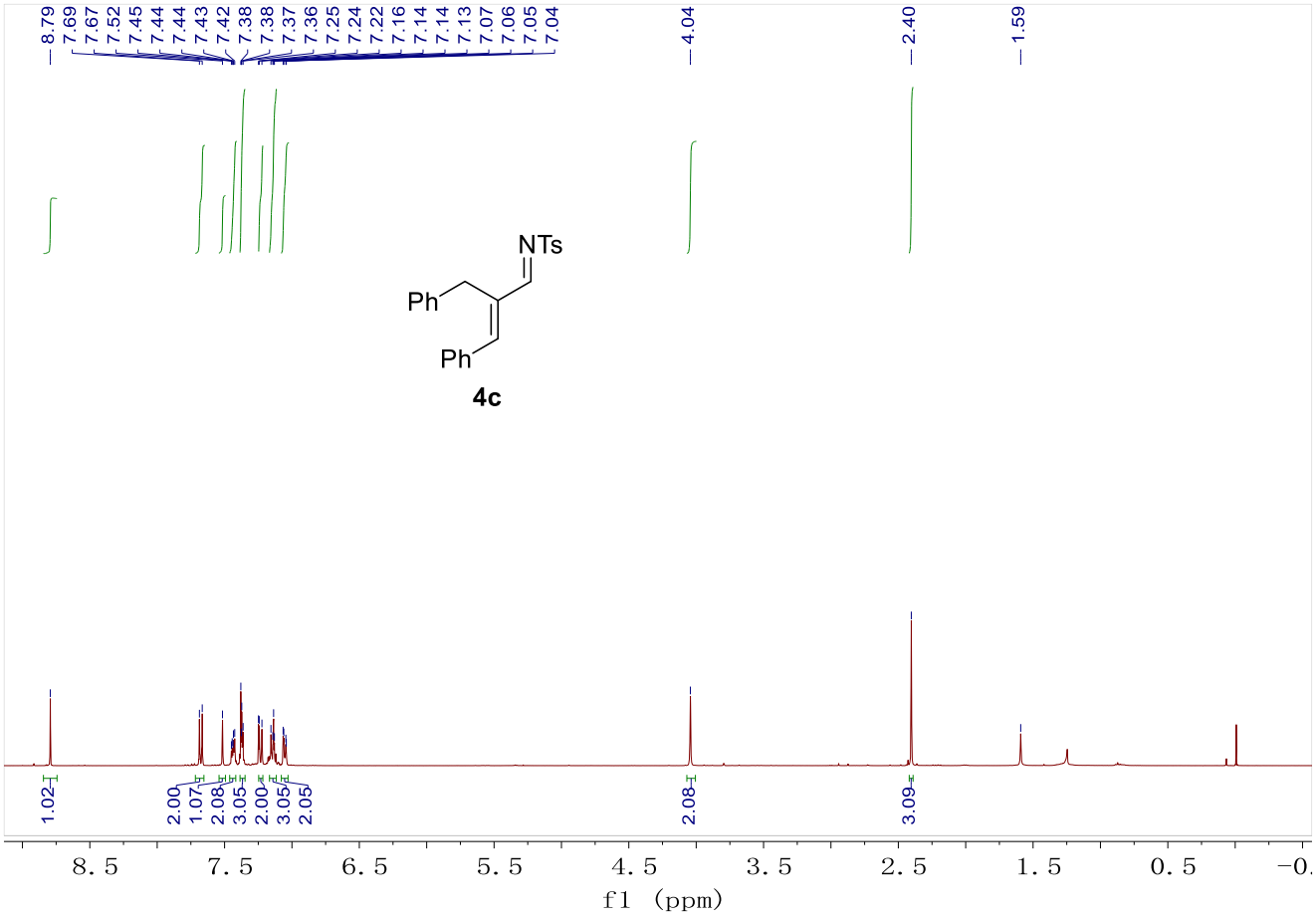
134.70
129.92
129.72
129.67
128.81
128.34
128.27
127.81
126.07
77.32
77.00
76.68
33.78
28.02
21.63
NTs
Ph
Ph
3a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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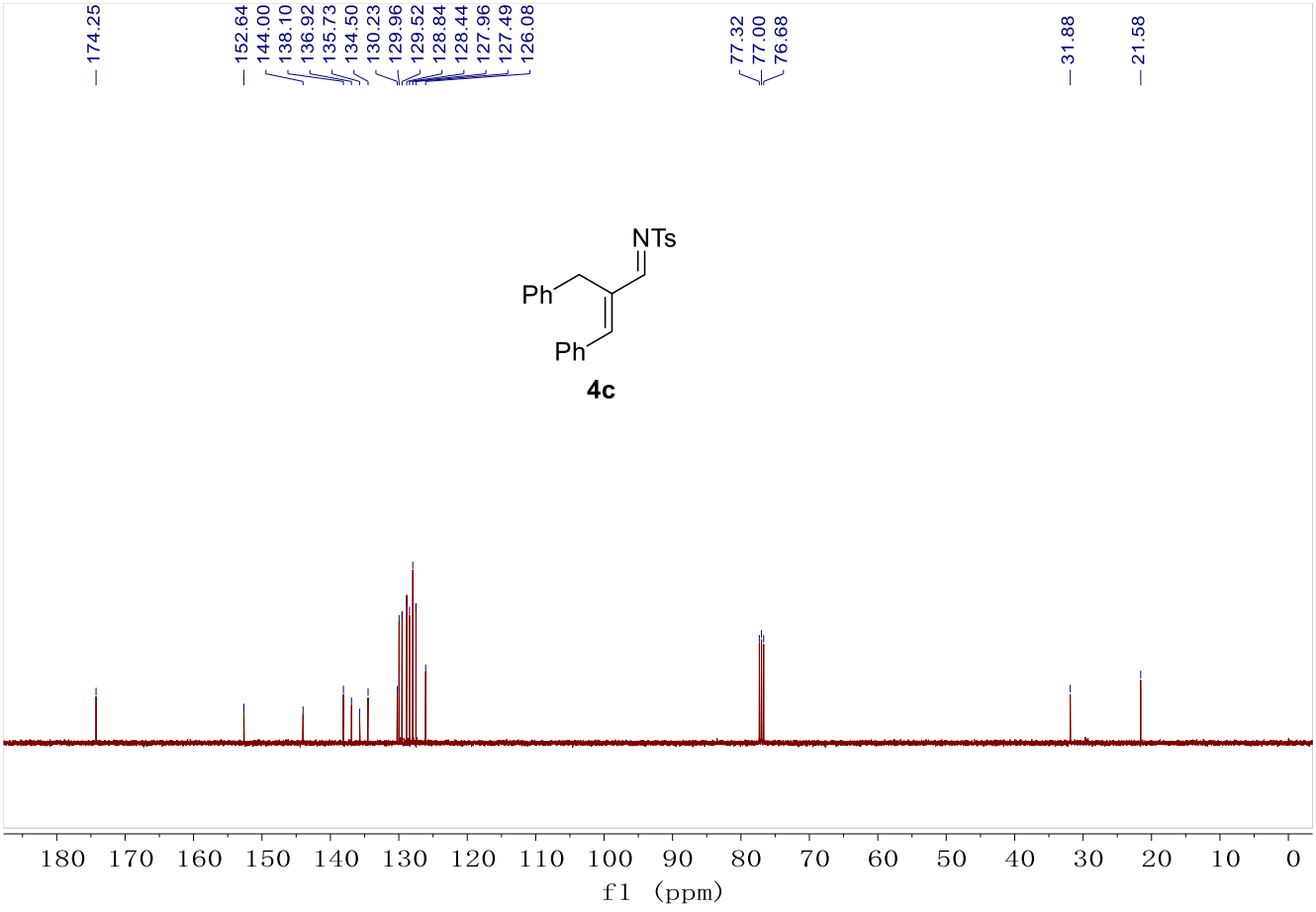
7.38
7.37
7.36
7.25
7.24
7.22
7.16
7.14
7.14
7.13
7.07
7.06
7.05
7.04
4.04
2.40
1.59
NTs
Ph
Ph
4c
1.02
2.00
1.07
2.08
3.05
2.00
3.05
2.05
2.08
3.09
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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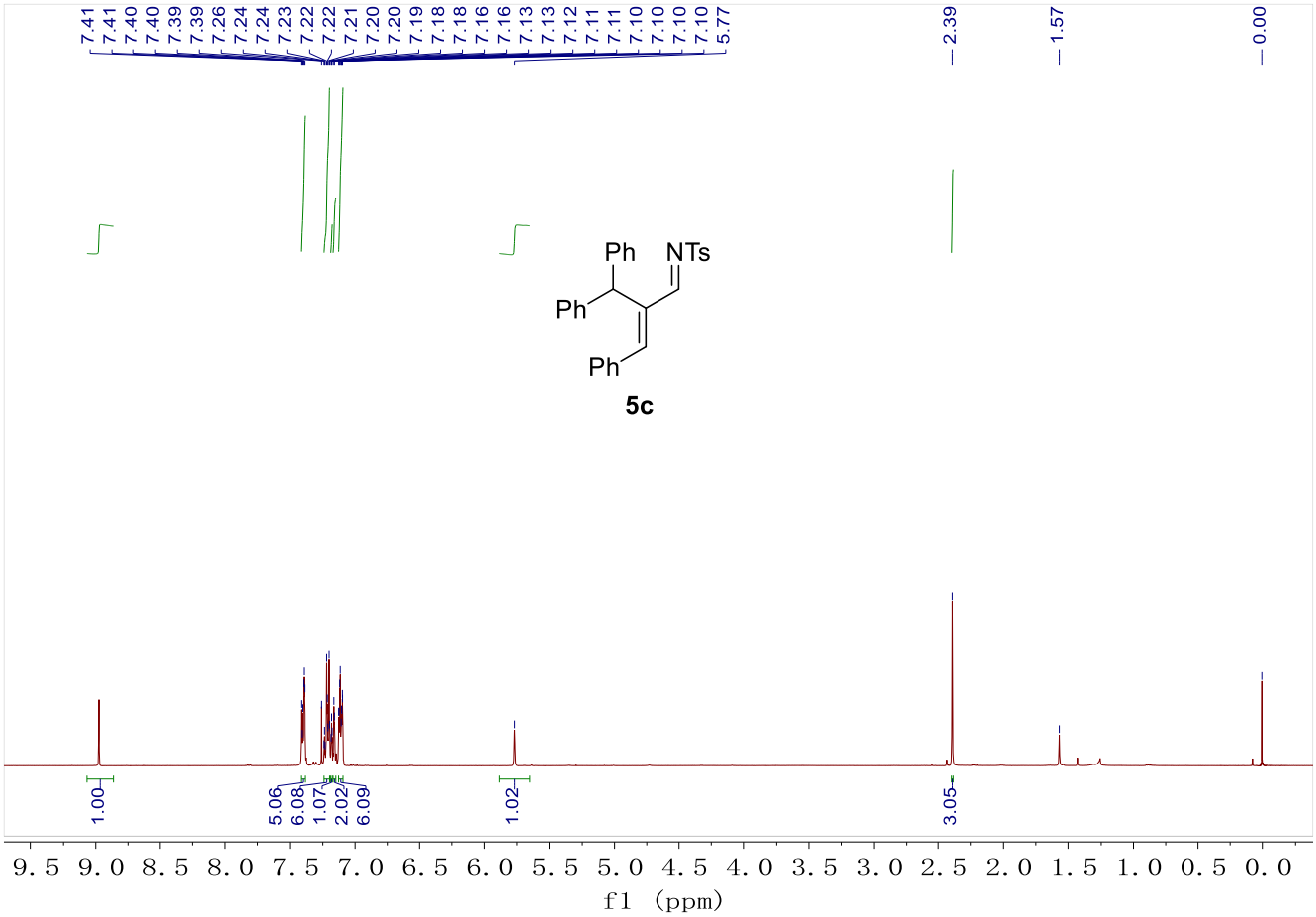
134.50
130.23
129.96
129.52
128.84
128.44
127.96
127.49
126.08
77.32
77.00
76.68
31.88
21.58
NTs
Ph
Ph
4c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.21
7.20
7.20
7.19
7.18
7.18
7.16
7.16
7.13
7.13
7.12
7.11
7.11
7.10
7.10
7.10
7.10
5.77
2.39
1.57
0.00
Ph
NTs
Ph
Ph
5c
1.00
5.06
6.08
1.07
2.02
6.09
1.02
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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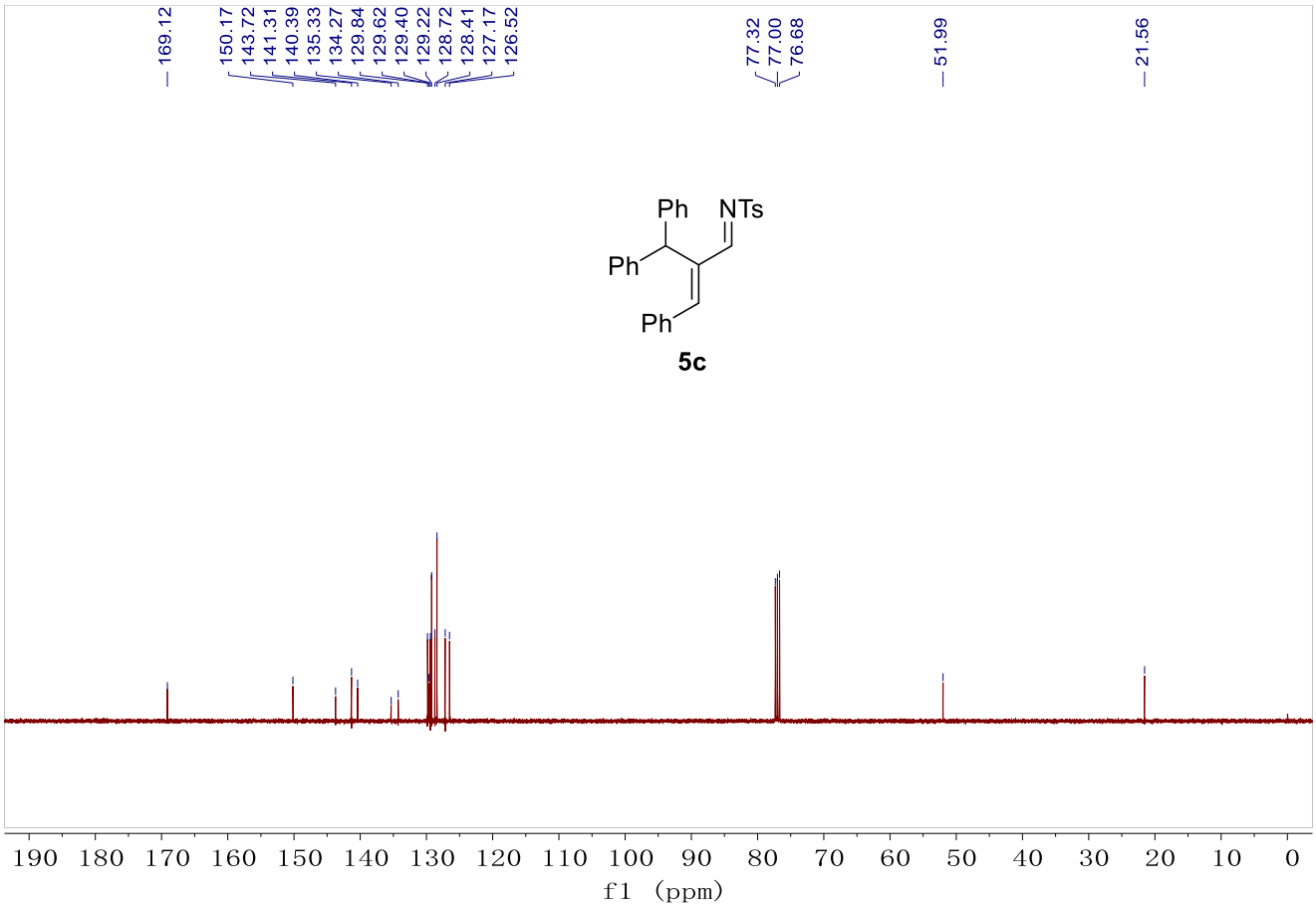
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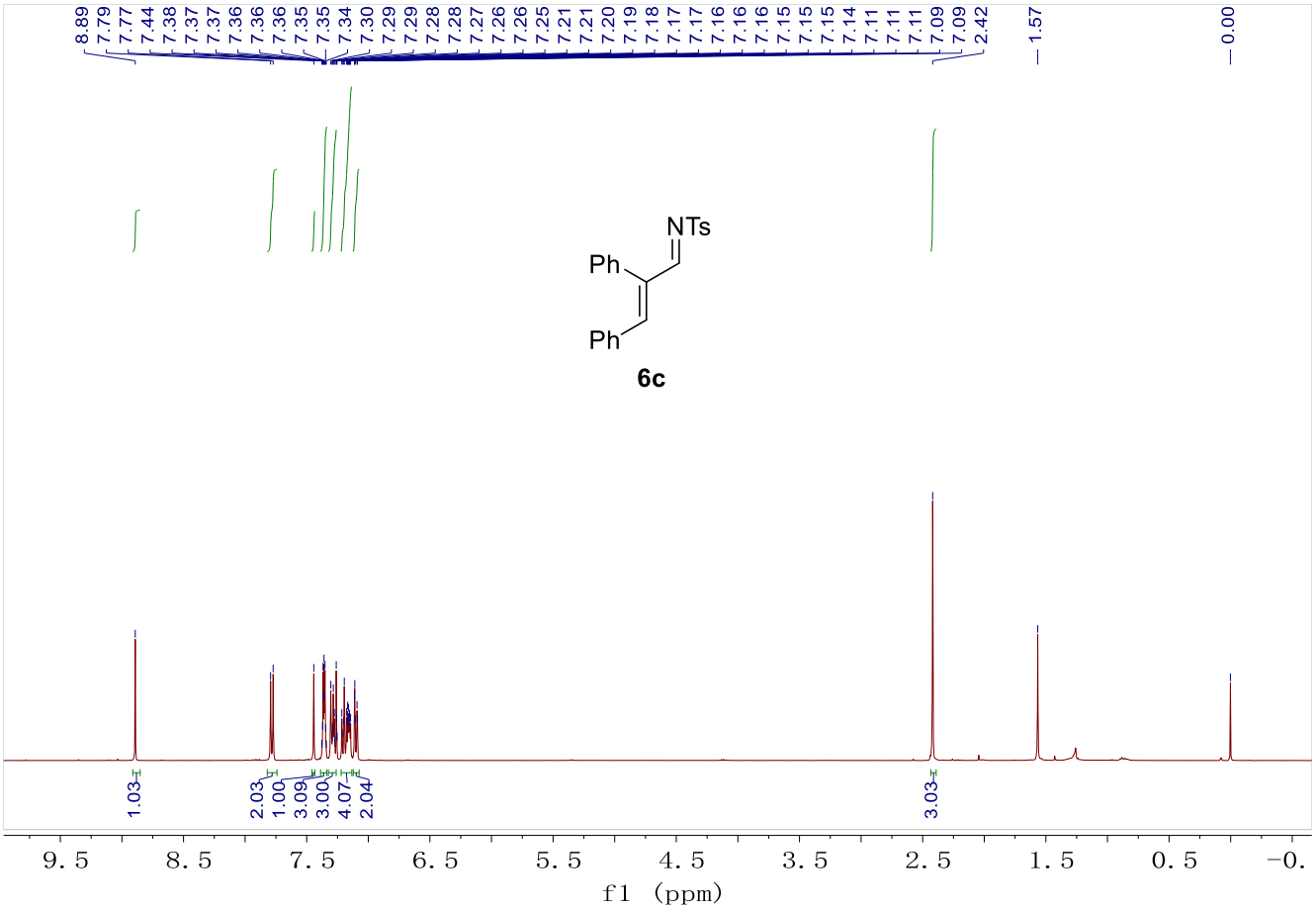
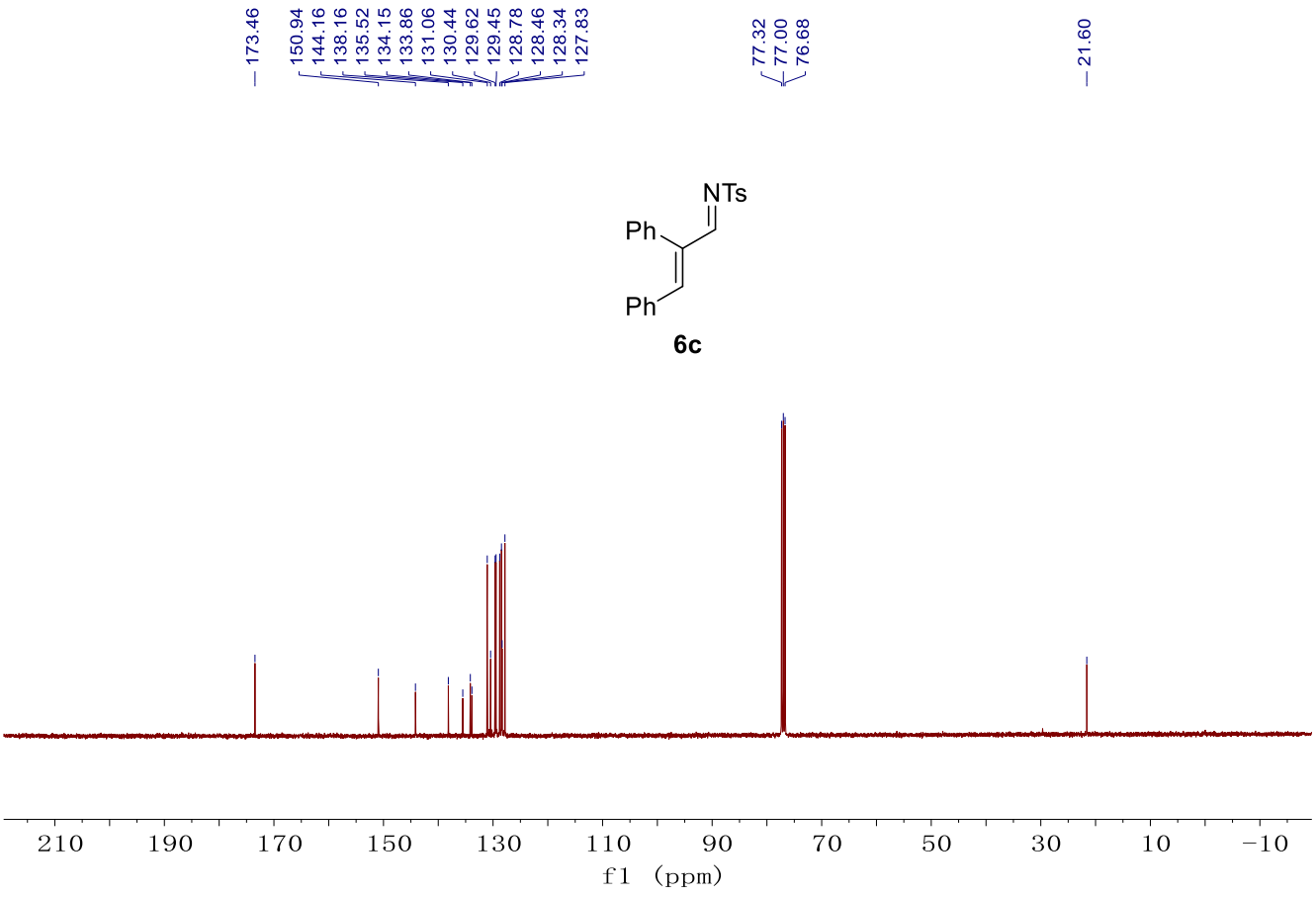
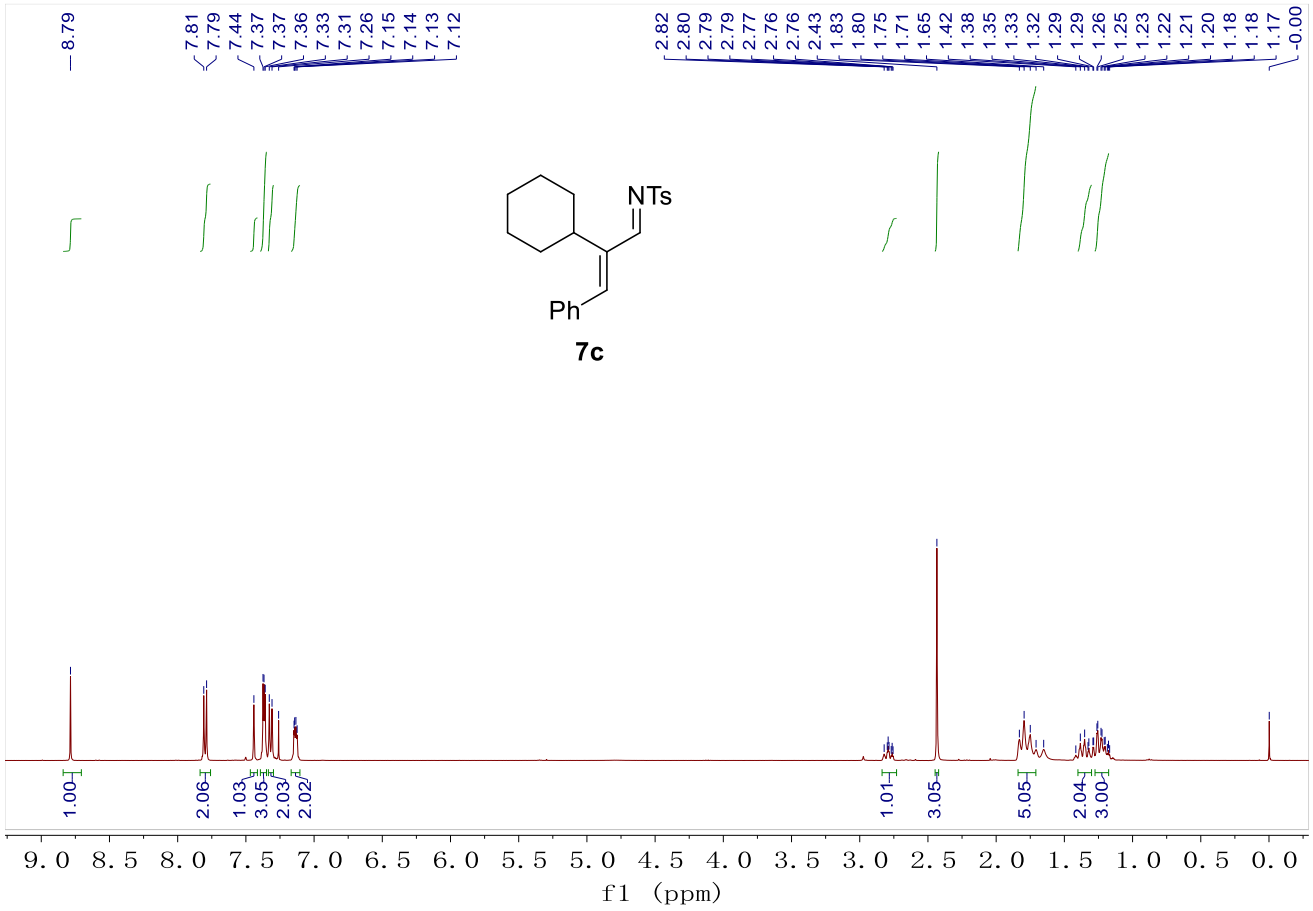
150.17
143.72
141.31
140.39
135.33
134.27
129.84
129.62
129.40
129.22
128.72
128.41
127.17
126.52
77.32
77.00
76.68
51.99
21.56
Ph
NTs
Ph
Ph
5c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.89 7.79 7.77 7.44 7.38 7.37 7.37 7.36 7.36 7.36 7.35 7.35 7.34 7.30 7.29 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.21 7.21 7.20 7.19 7.18 7.17 7.17 7.16 7.16 7.16 7.15 7.15 7.15 7.14 7.11 7.11 7.11 7.09 7.09 2.42 1.57 0.00
NTs
Ph
Ph
6c
1.03 2.03 1.00 3.09 3.00 4.07 2.04 3.03
9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0.
f1 (ppm)


173.46 150.94 144.16 138.16 135.52 134.15 133.86 131.06 130.44 129.62 129.45 128.78 128.46 128.34 127.83
77.32 77.00 76.68
21.60
NTs
Ph
Ph
6c
210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)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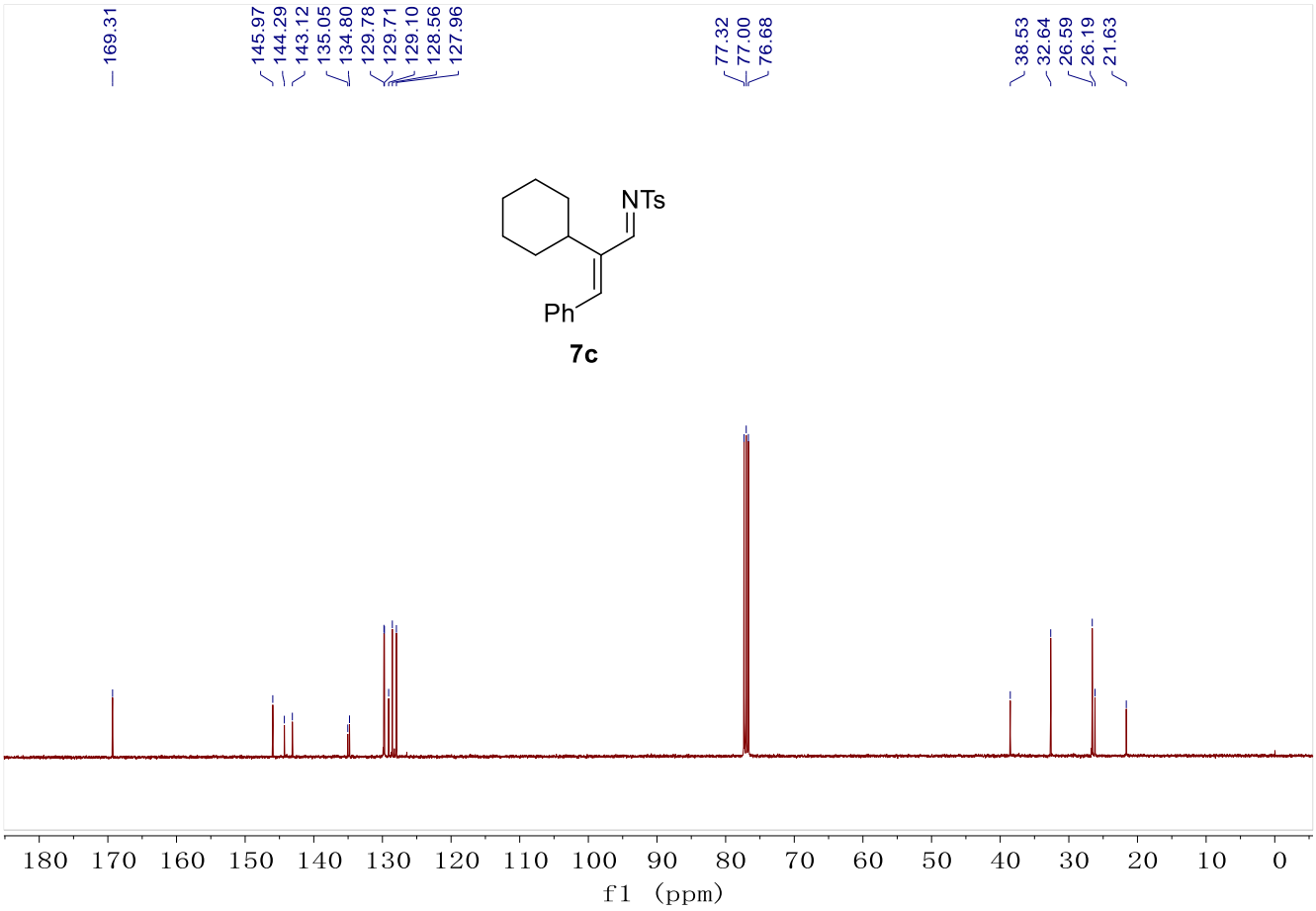
7.81
7.79
7.44
7.37
7.37
7.36
7.33
7.31
7.26
7.15
7.14
7.13
7.12
2.82
2.80
2.79
2.79
2.77
2.76
2.76
2.43
1.83
1.80
1.75
1.71
1.65
1.42
1.38
1.35
1.33
1.32
1.29
1.29
1.26
1.25
1.23
1.22
1.21
1.20
1.18
1.18
1.17
0.00
NTs
Ph
7c
1.00
2.06
1.03
3.05
2.03
2.02
1.01
3.05
5.05
2.04
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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145.97
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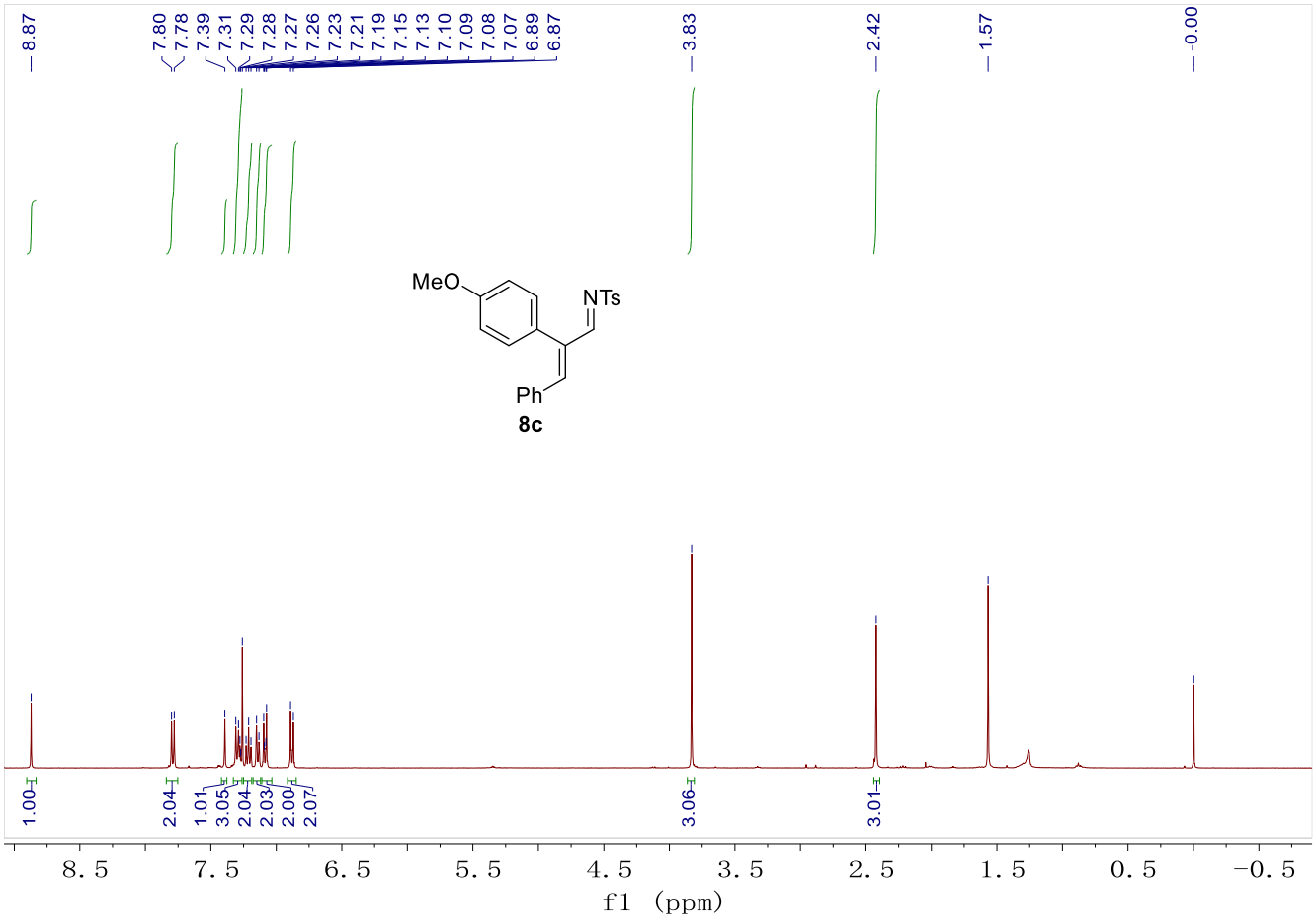
143.12
135.05
134.80
129.78
129.71
129.10
128.56
127.96
77.32
77.00
76.68
38.53
32.64
26.59
26.19
21.63
NTs
Ph
7c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.80
7.78
7.39
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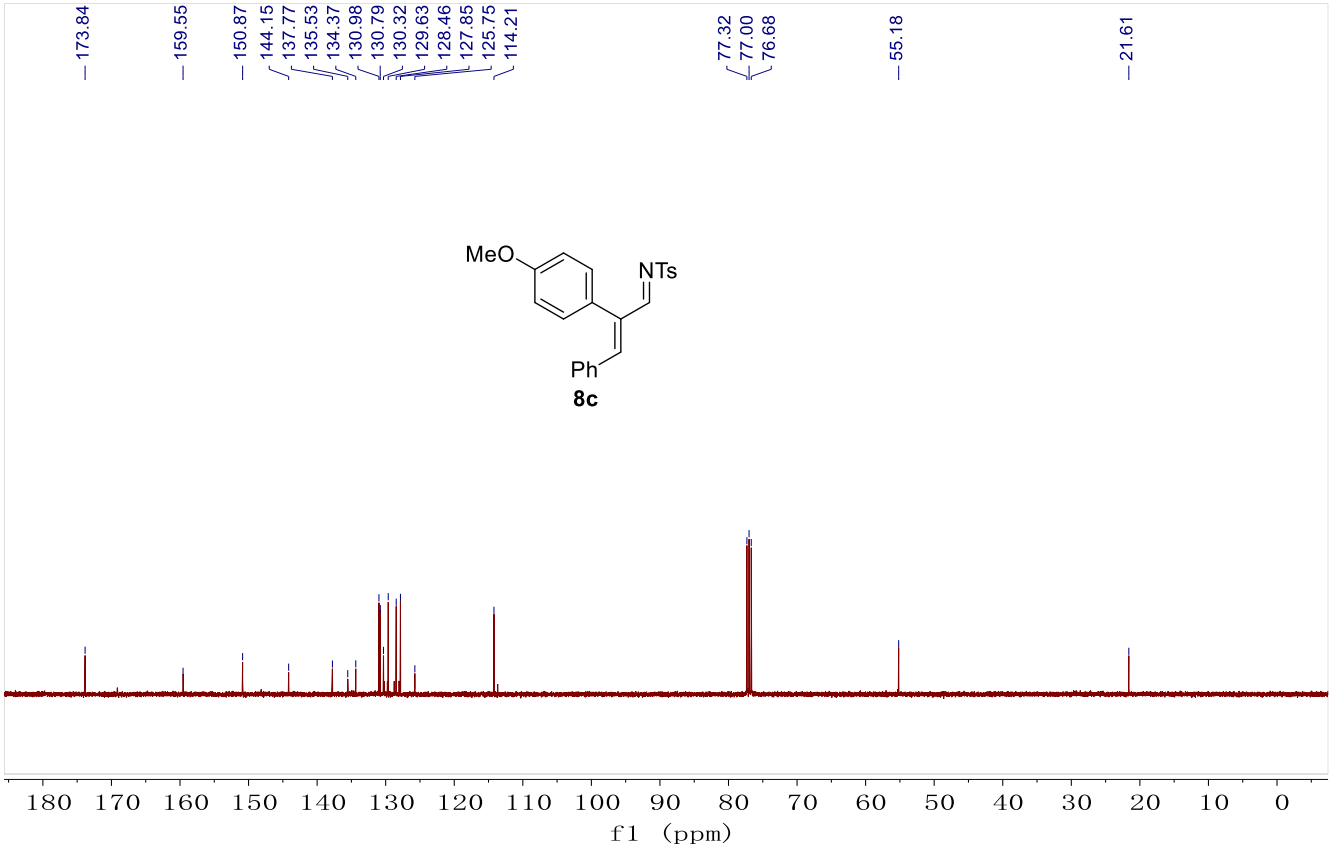
7.29
7.28
7.27
7.26
7.23
7.21
7.19
7.15
7.13
7.10
7.09
7.08
7.07
6.89
6.87
3.83
2.42
1.57
-0.00
MeO
NTs
Ph
8c
1.00
2.04
1.01
3.05
2.04
2.03
2.00
2.07
3.06
3.01
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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159.55
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144.15
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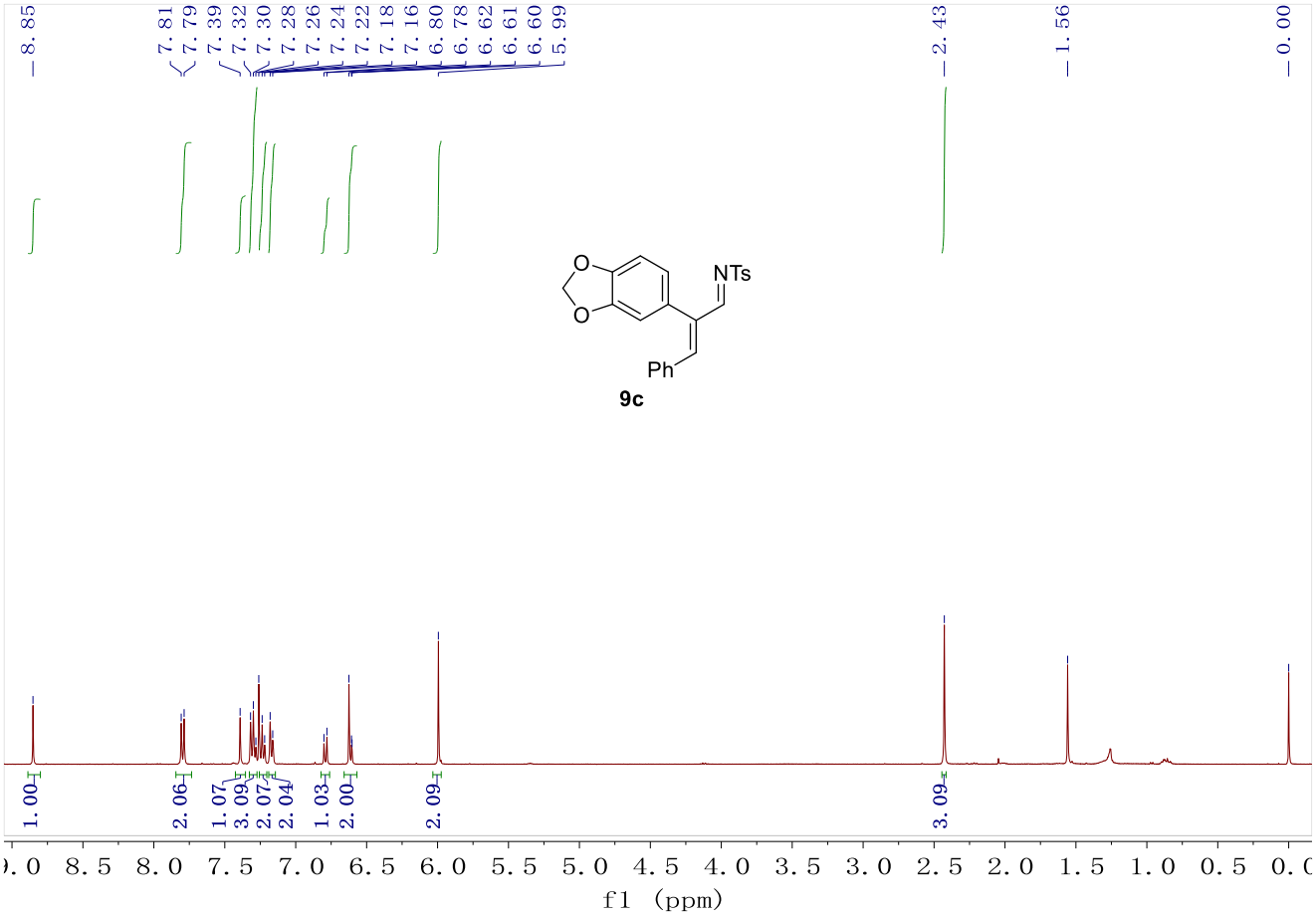
135.53
134.37
130.98
130.79
130.32
129.63
128.46
127.85
125.75
114.21
77.32
77.00
76.68
55.18
21.61
MeO
NTs
Ph
8c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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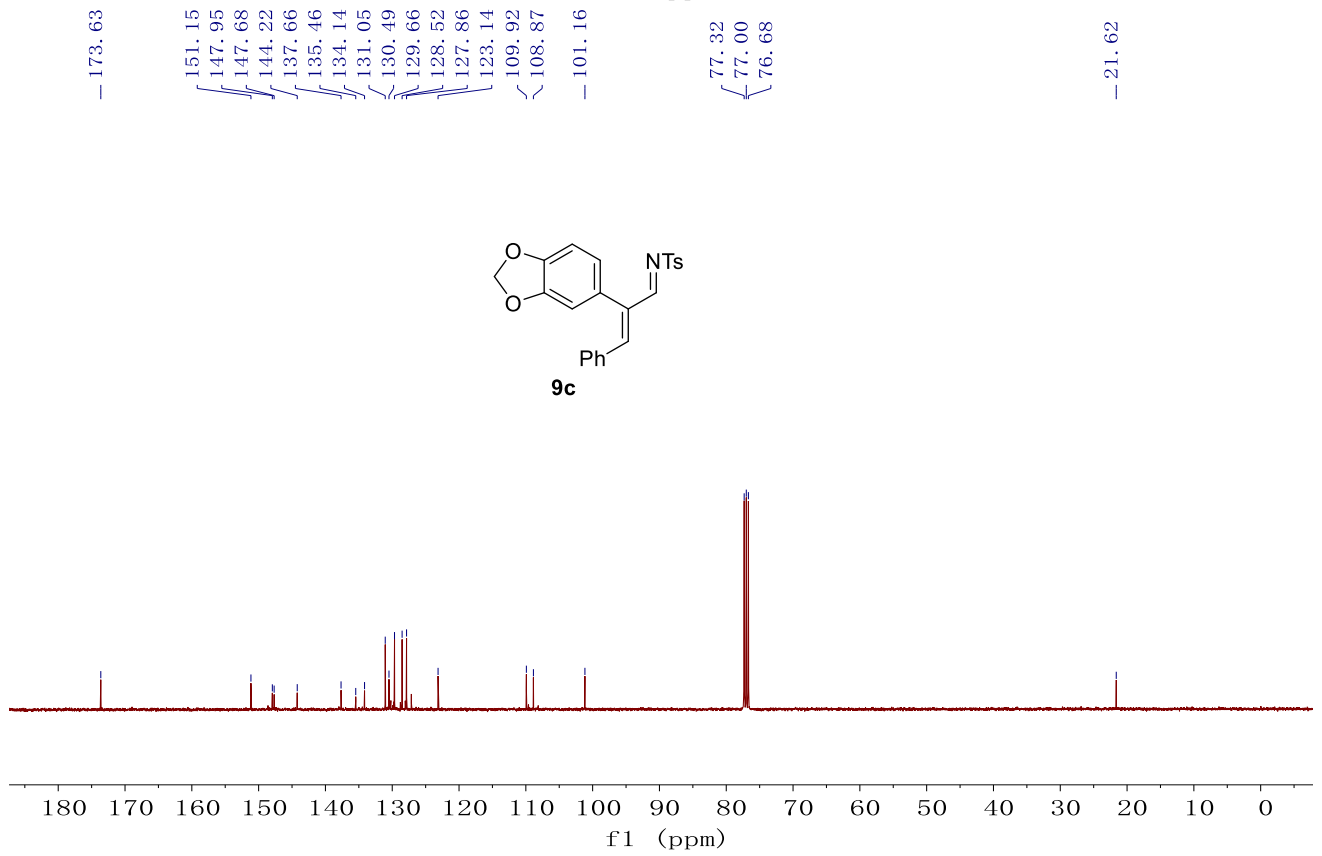
7.30
7.28
7.26
7.24
7.22
7.18
7.16
6.80
6.78
6.62
6.61
6.60
5.99
2.43
1.56
0.00
NTs
O
O
Ph
9c
1.00
2.06
1.07
3.09
2.07
2.04
1.03
2.00
2.09
3.09
f1 (ppm)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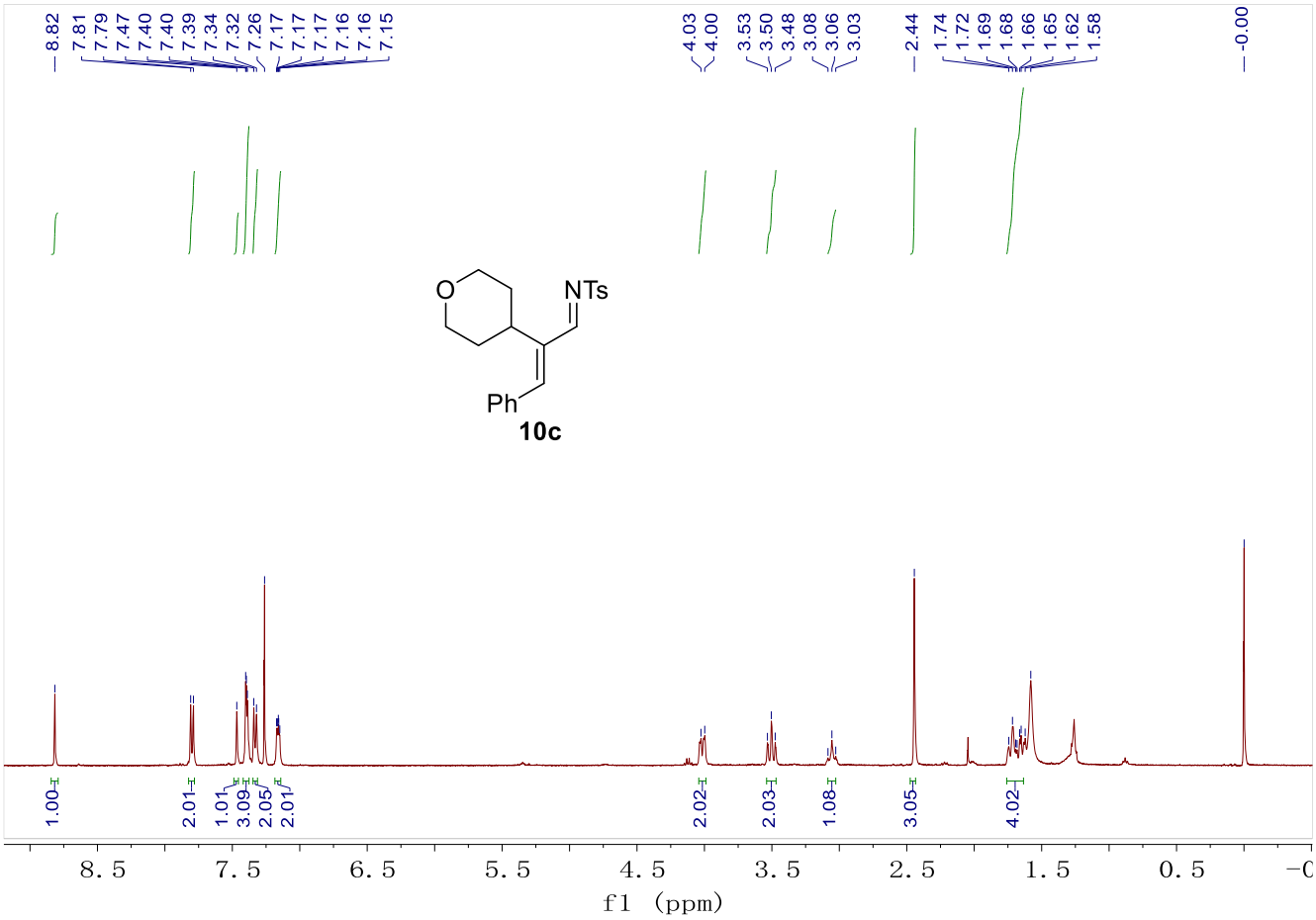
135.46
134.14
131.05
130.49
129.66
128.52
127.86
123.14
109.92
108.87
101.16
77.32
77.00
76.68
21.62
NTs
O
O
Ph
9c
f1 (ppm)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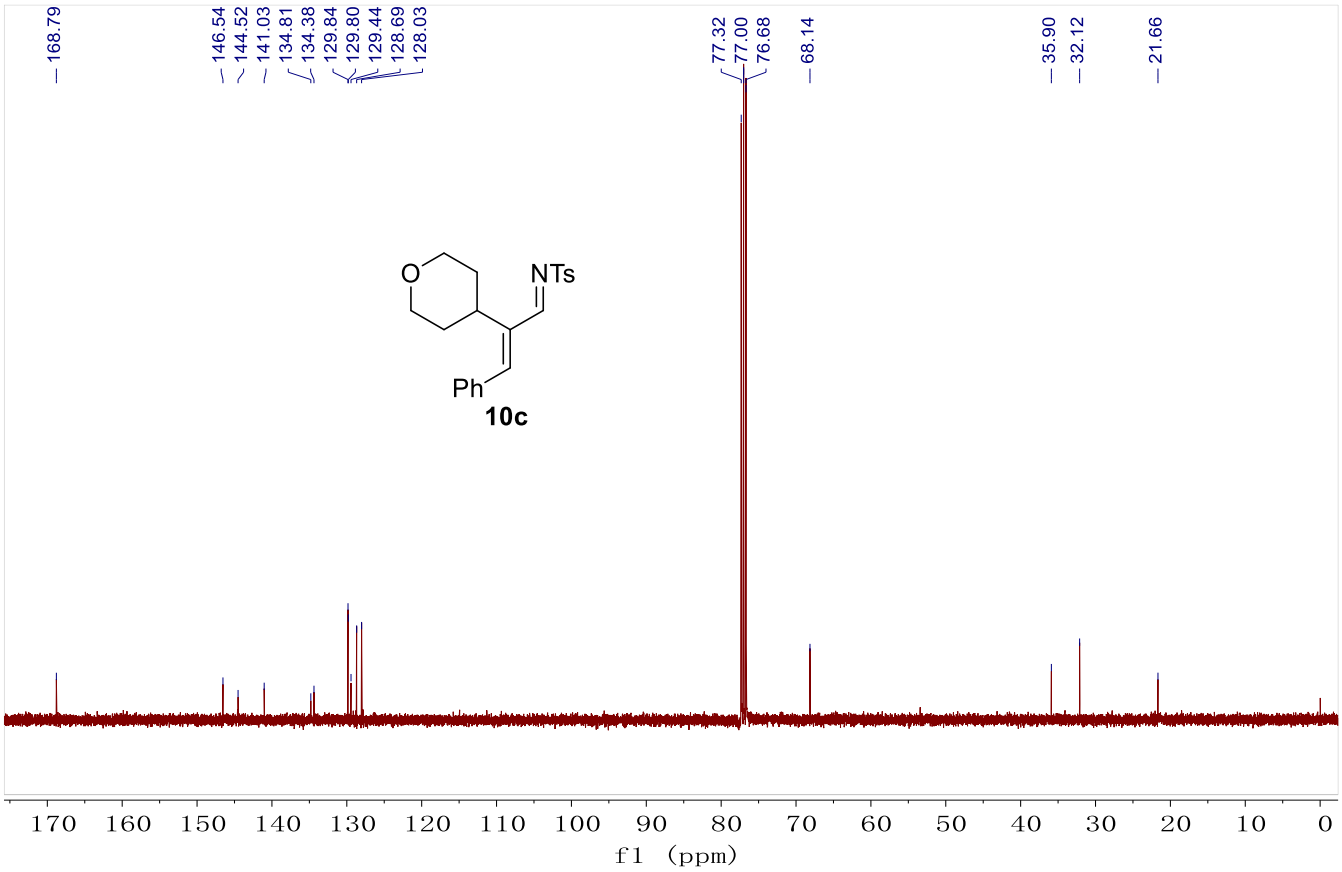
7.26
7.17
7.17
7.17
7.16
7.16
7.15
4.03
4.00
3.53
3.50
3.48
3.08
3.06
3.03
2.44
1.74
1.72
1.69
1.68
1.66
1.65
1.62
1.58
-0.00
O
NTs
Ph
10c
1.00
2.01
1.01
3.09
2.05
2.01
2.02
2.03
1.08
3.05
4.02
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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134.38
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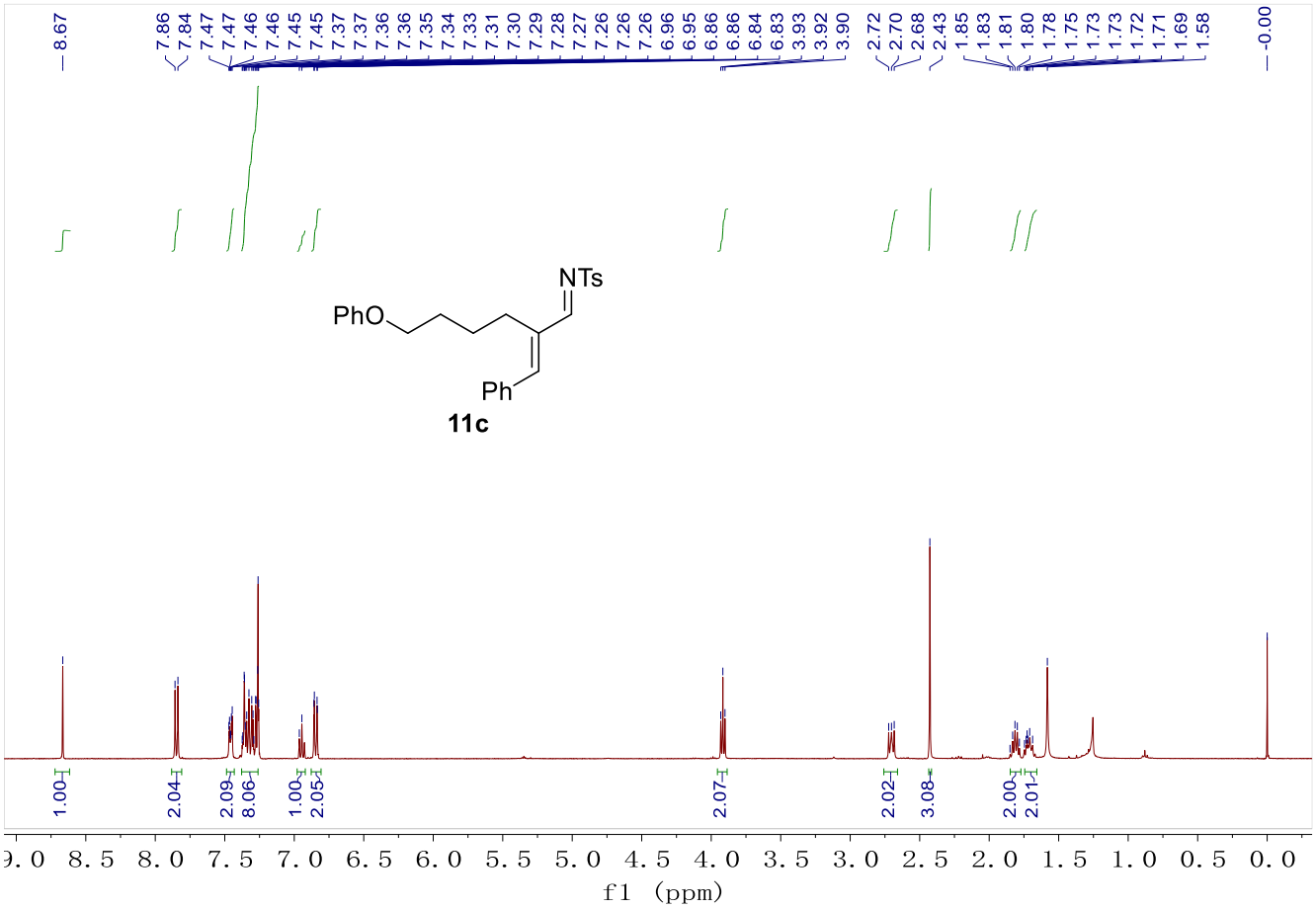
129.80
129.44
128.69
128.03
77.32
77.00
76.68
68.14
35.90
32.12
21.66
O
NTs
Ph
10c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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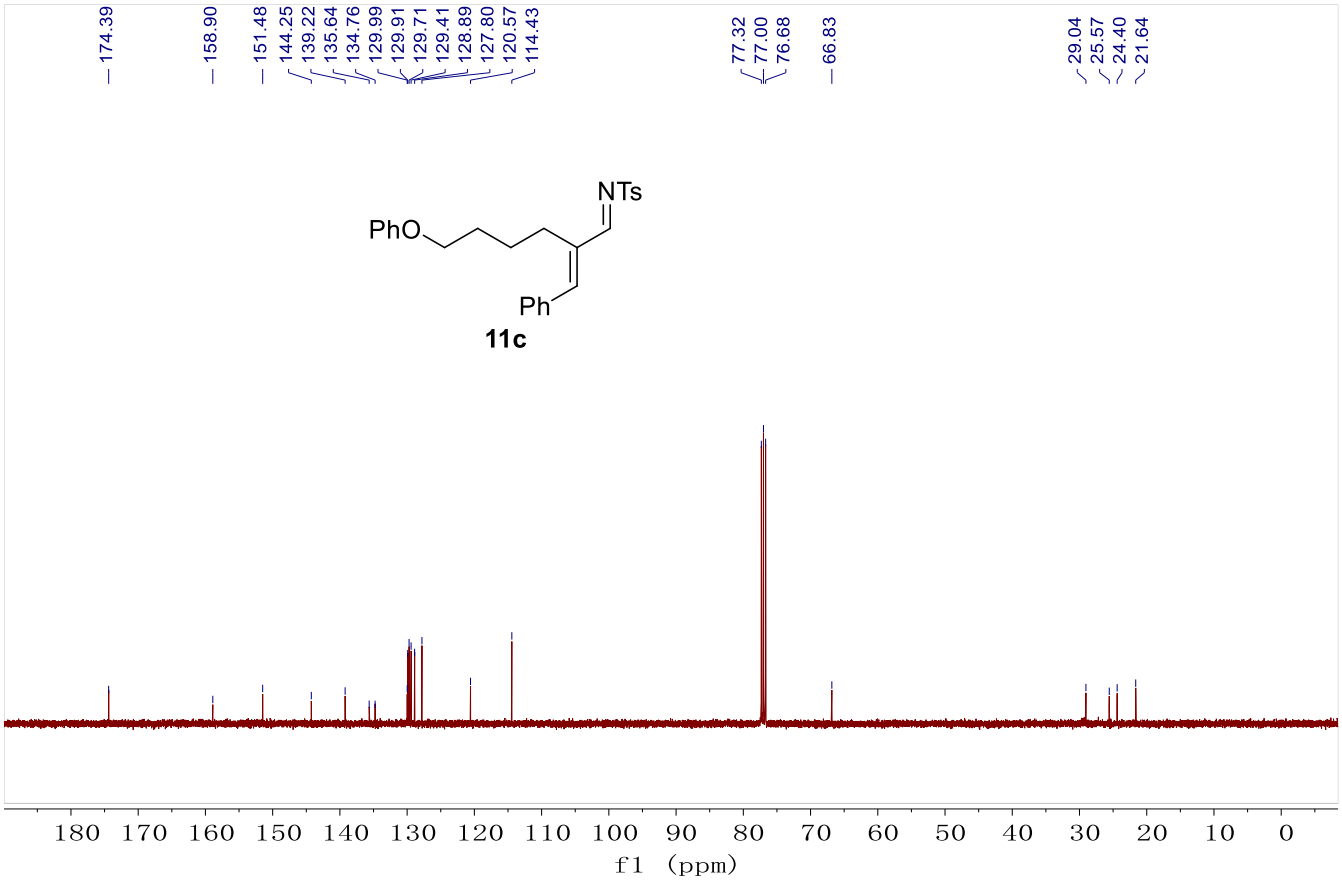
7.37
7.37
7.36
7.36
7.35
7.34
7.33
7.31
7.30
7.29
7.28
7.27
7.26
7.26
7.26
6.96
6.95
6.86
6.86
6.84
6.83
3.93
3.92
3.90
2.72
2.70
2.68
2.43
1.85
1.83
1.81
1.80
1.78
1.75
1.73
1.73
1.72
1.71
1.69
1.58
0.00
NTs
PhO
Ph
11c
1.00
2.04
2.09
8.06
1.00
2.05
2.07
2.02
3.08
2.00
2.01
f1 (ppm)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129.41
128.89
127.80
120.57
114.43
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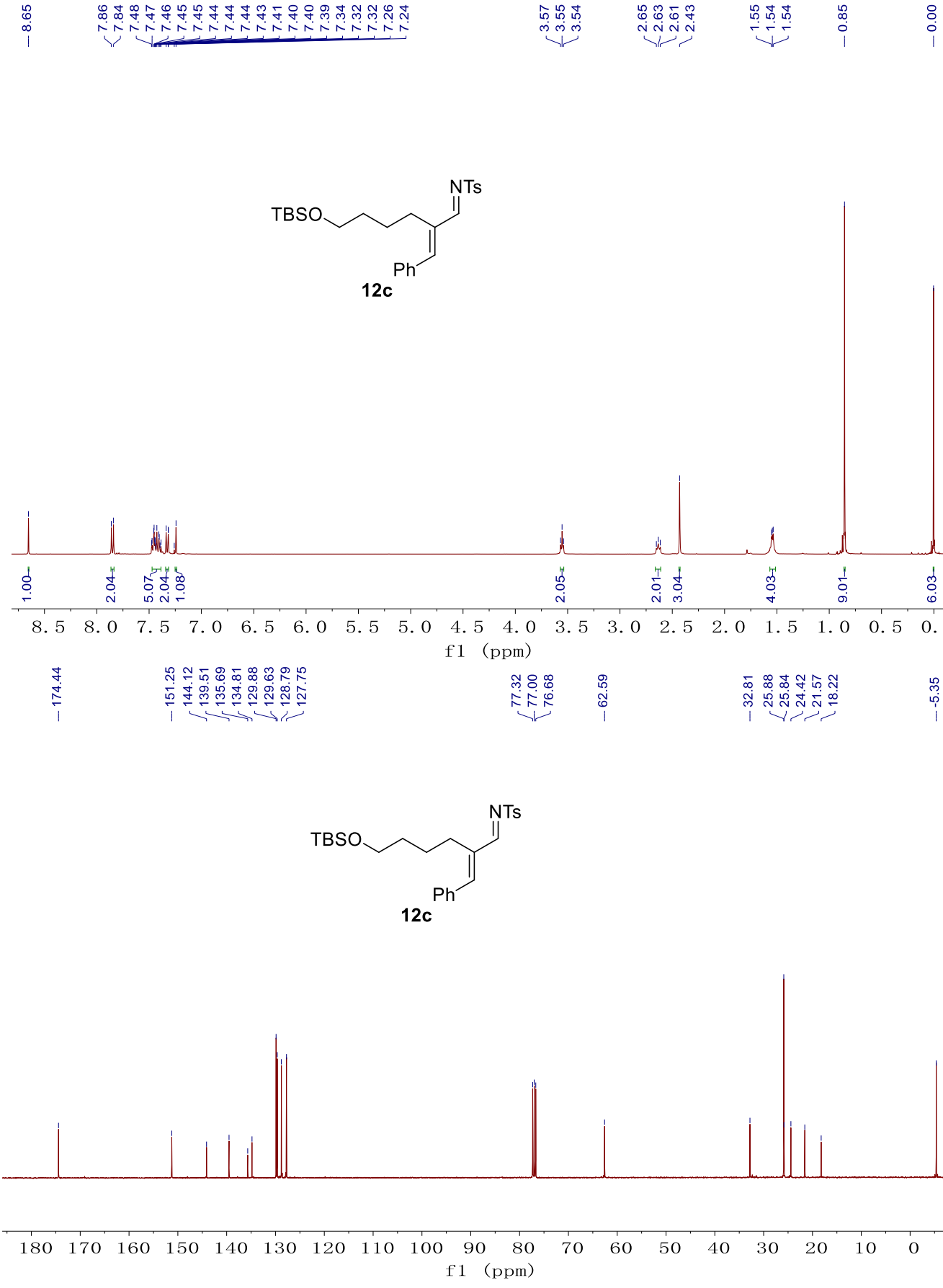
66.83
29.04
25.57
24.40
21.64
NTs
PhO
Ph
11c
f1 (ppm)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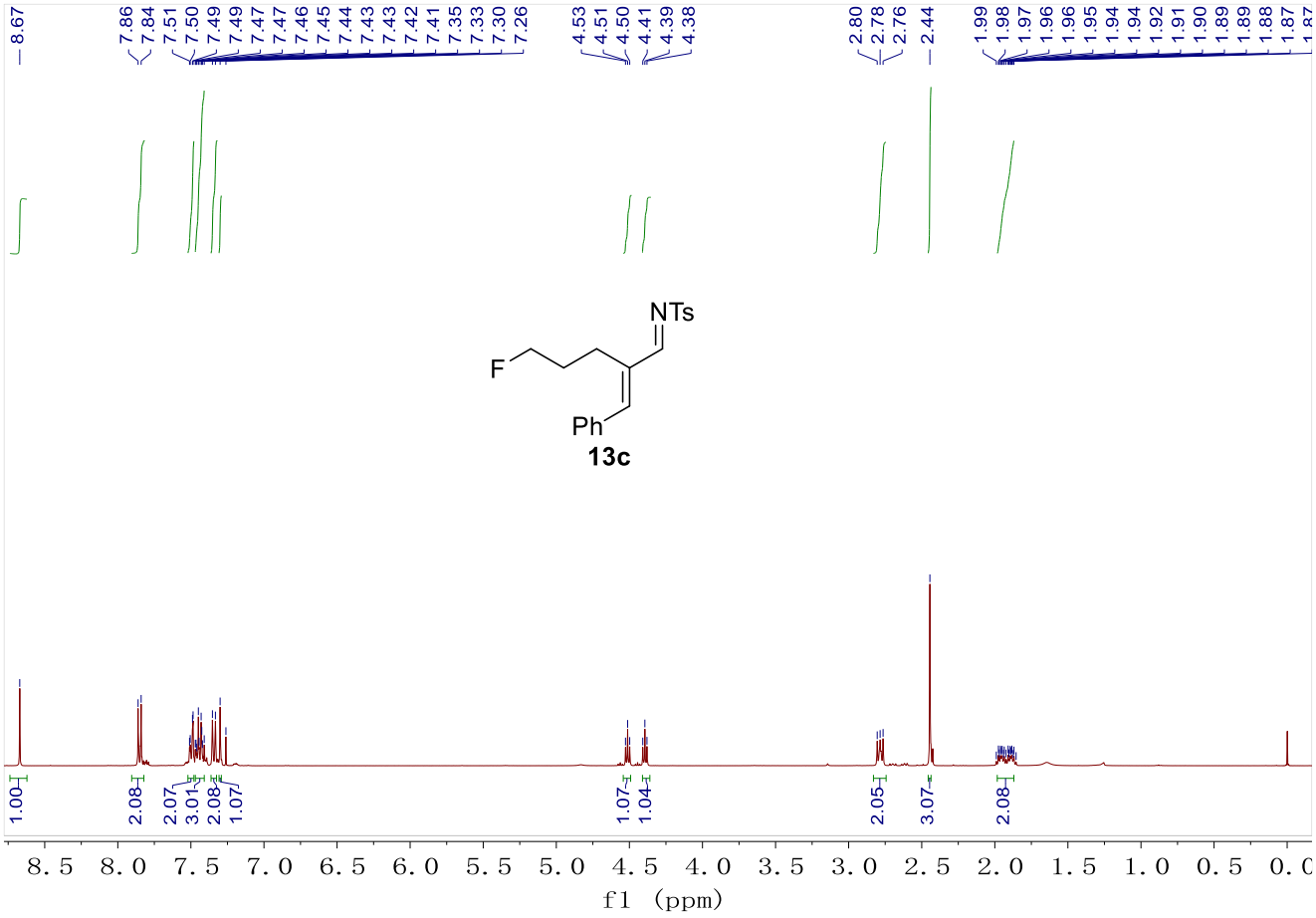
7.48
7.47
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.41
7.40
7.40
7.39
7.34
7.32
7.32
7.26
7.24
3.57
3.55
3.54
2.65
2.63
2.61
2.43
1.55
1.54
1.54
0.85
0.00
NTs
TBSO
Ph
12c
1.00
2.04
5.07
2.04
1.08
2.05
2.01
3.04
4.03
9.01
6.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
174.44
151.25
144.12
139.51
135.69
134.81
129.88
129.63
128.79
127.75
77.32
77.00
76.68
62.59
32.81
25.88
25.84
24.42
21.57
18.22
-5.35
NTs
TBSO
Ph
12c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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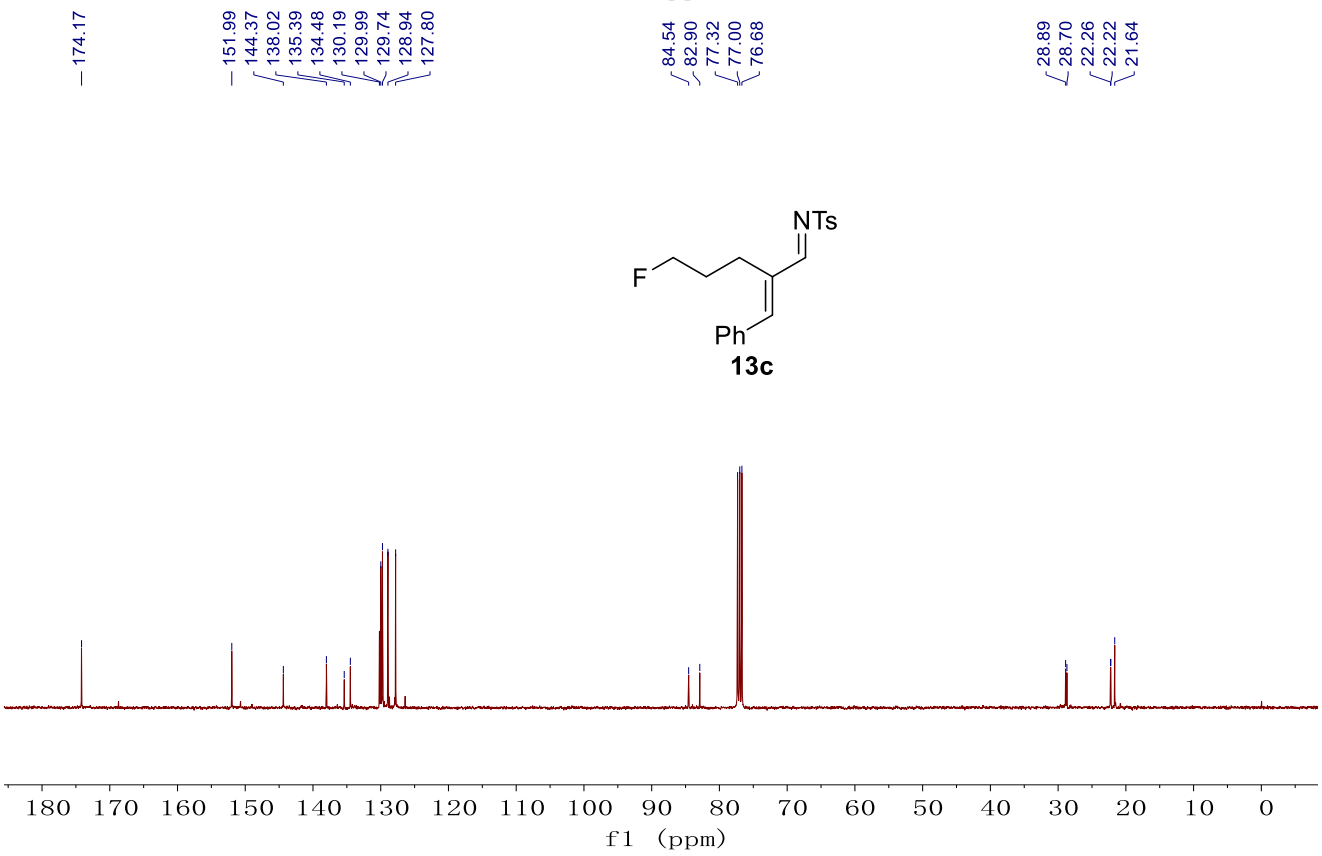
7.46
7.45
7.44
7.43
7.43
7.42
7.41
7.35
7.33
7.30
7.26
4.53
4.51
4.50
4.41
4.39
4.38
2.80
2.78
2.76
2.44
1.99
1.98
1.97
1.96
1.96
1.95
1.94
1.94
1.92
1.91
1.90
1.89
1.89
1.88
1.87
NTs
F
Ph
13c
1.00
2.08
2.07
3.01
2.08
1.07
1.07
1.04
2.05
3.07
2.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.48
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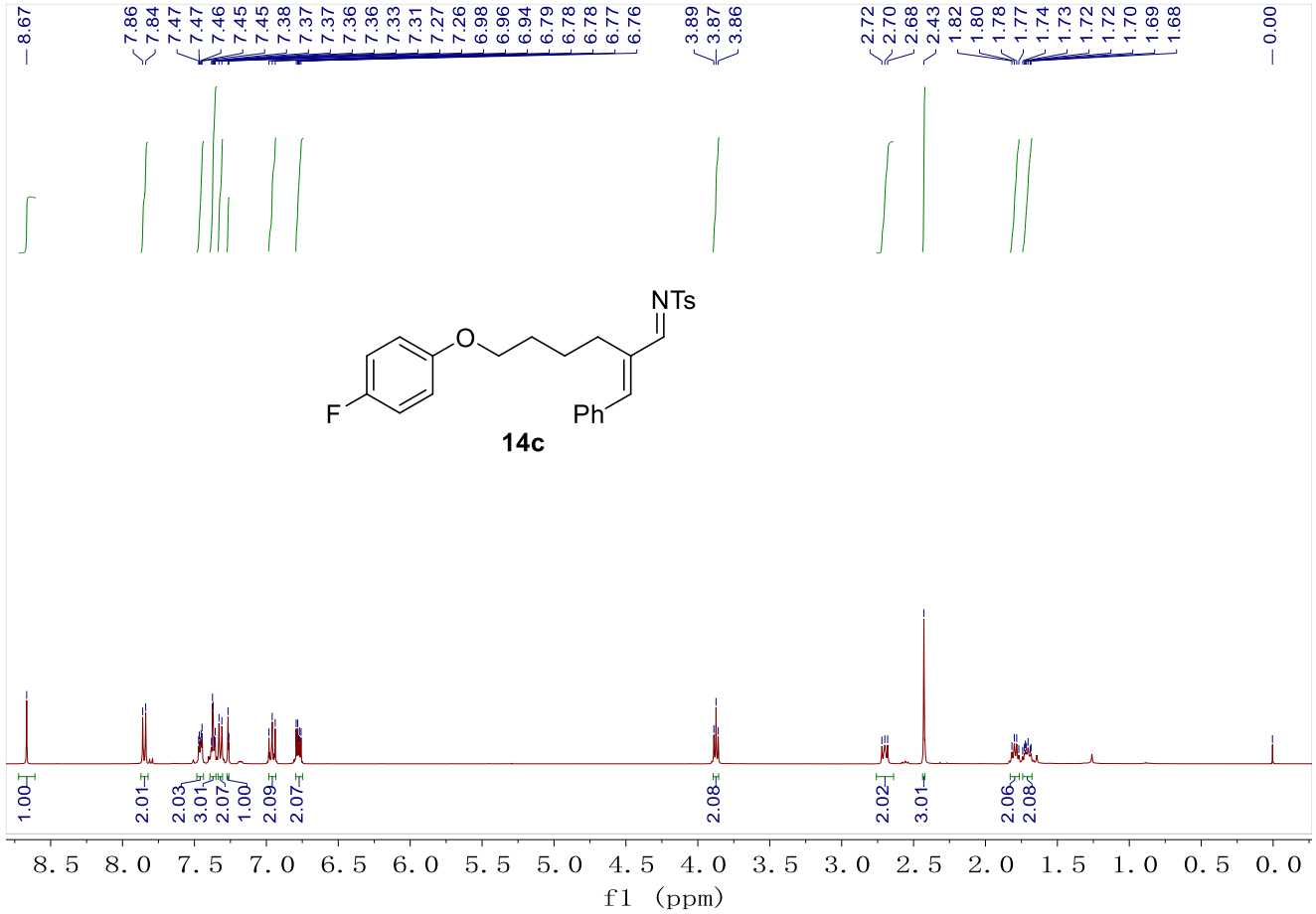
129.99
129.74
128.94
127.80
84.54
82.90
77.32
77.00
76.68
28.89
28.70
22.26
22.22
21.64
NTs
F
Ph
13c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.47
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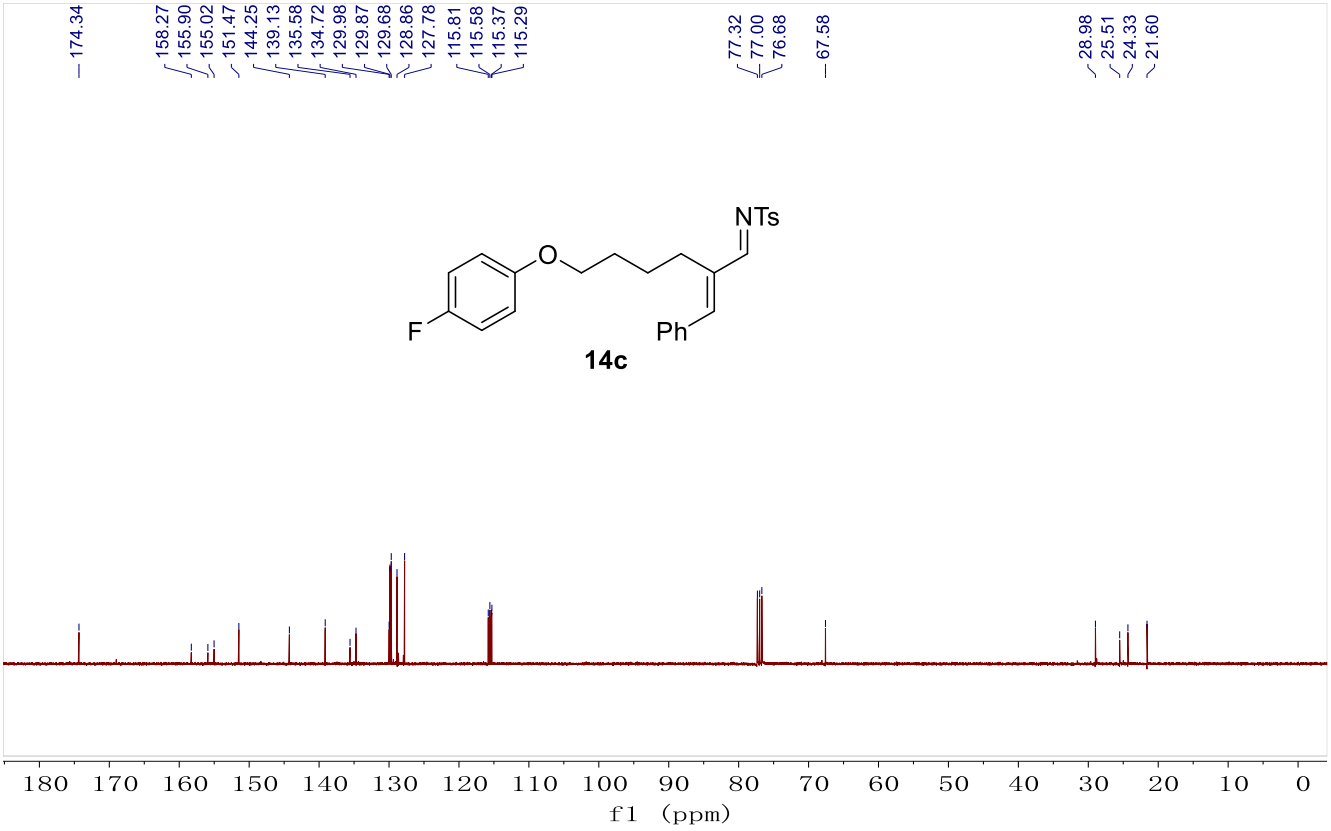
7.33
7.31
7.27
7.26
6.98
6.96
6.94
6.79
6.78
6.78
6.77
6.76
3.89
3.87
3.86
2.72
2.70
2.68
2.43
1.82
1.80
1.78
1.77
1.74
1.73
1.72
1.72
1.70
1.69
1.68
0.00
NTs
O
F
Ph
14c
1.00
2.01
2.03
3.01
2.07
1.00
2.09
2.07
2.08
2.02
3.01
2.06
2.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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139.13
135.58
134.72
129.98
129.87
129.68
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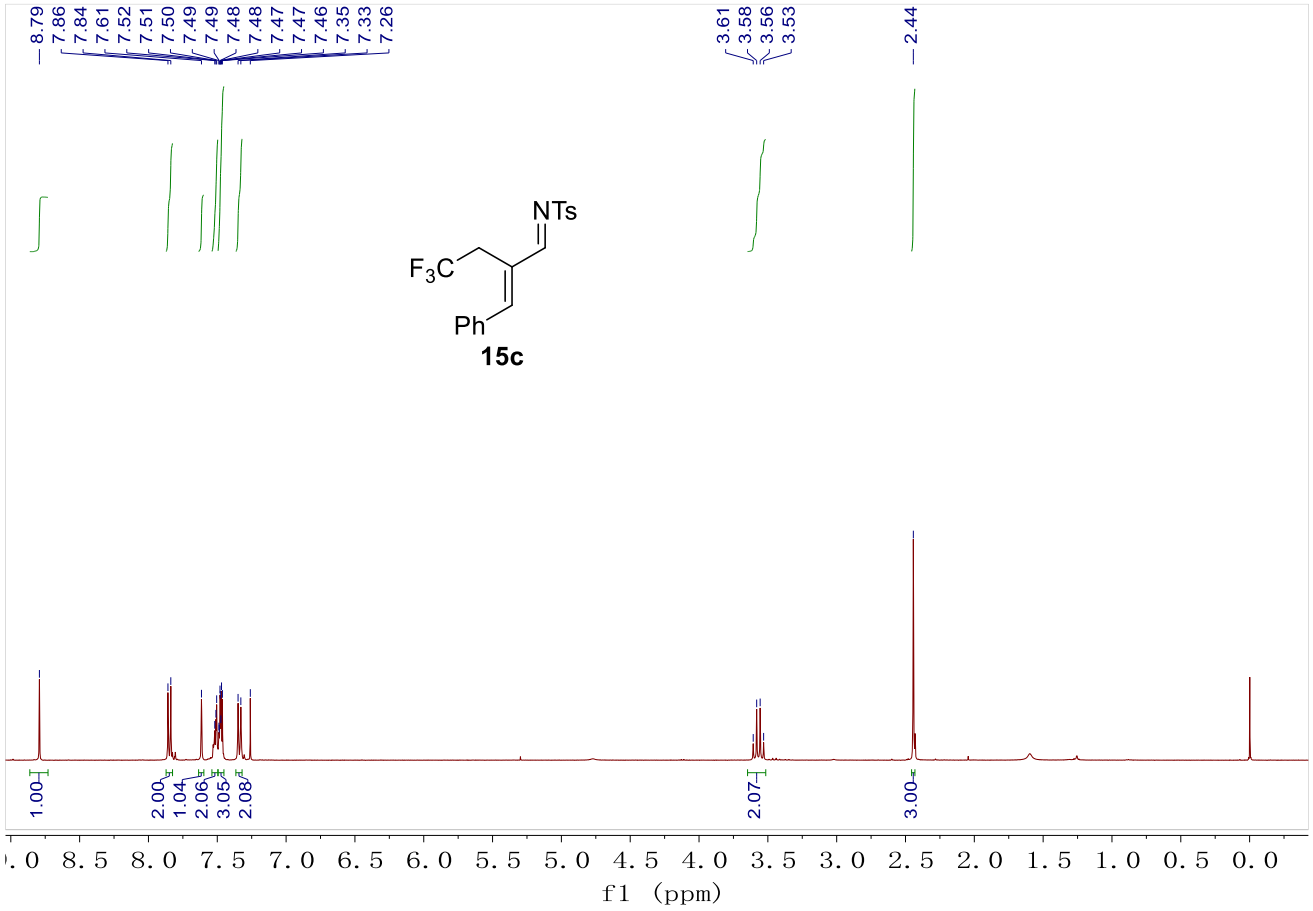
127.78
115.81
115.58
115.37
115.29
77.32
77.00
76.68
67.58
28.98
25.51
24.33
21.60
NTs
O
F
Ph
14c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.86
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7.51
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.35
7.33
7.26
3.61
3.58
3.56
3.53
2.44
NTs
F3C
Ph
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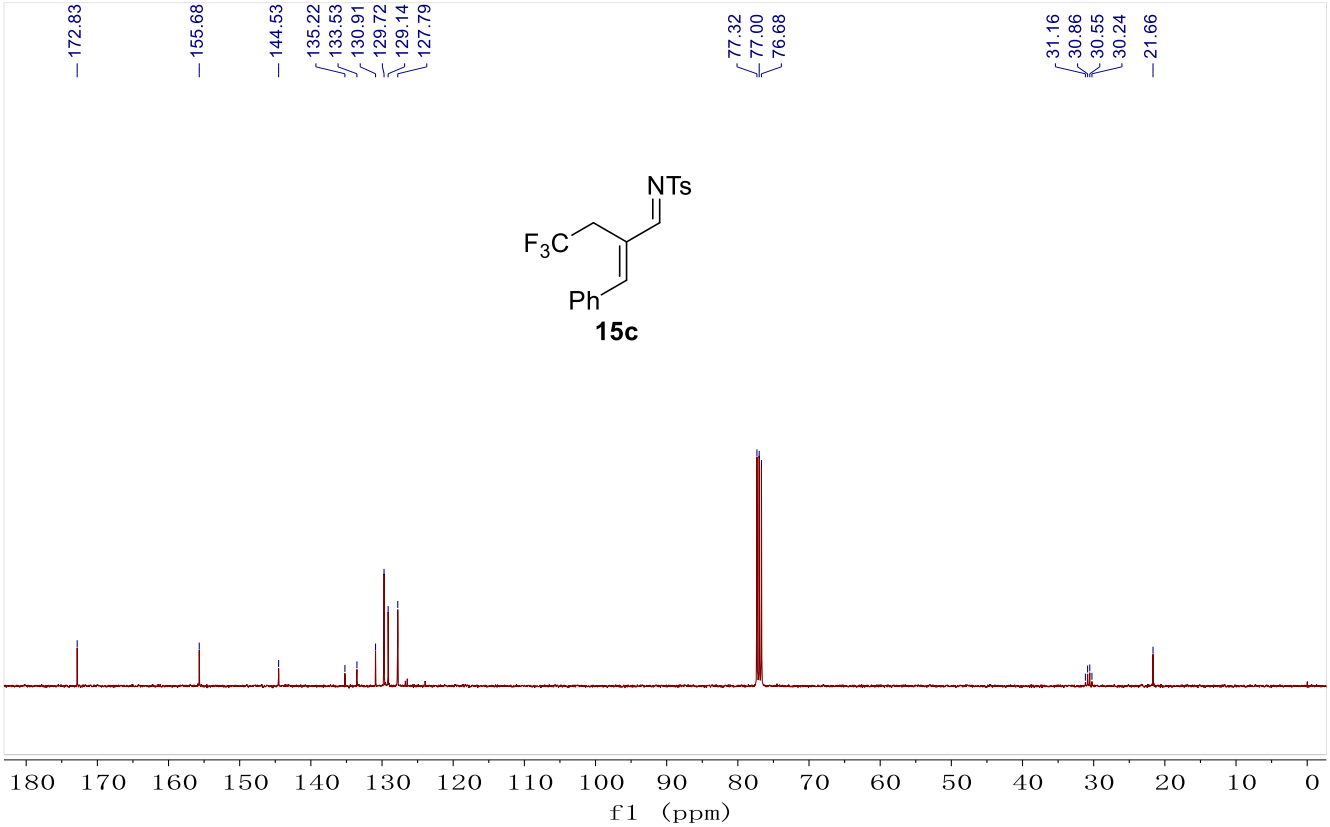
2.00
1.04
2.06
3.05
2.08
2.07
3.00
f1 (ppm)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133.53
130.91
129.72
129.14
127.79
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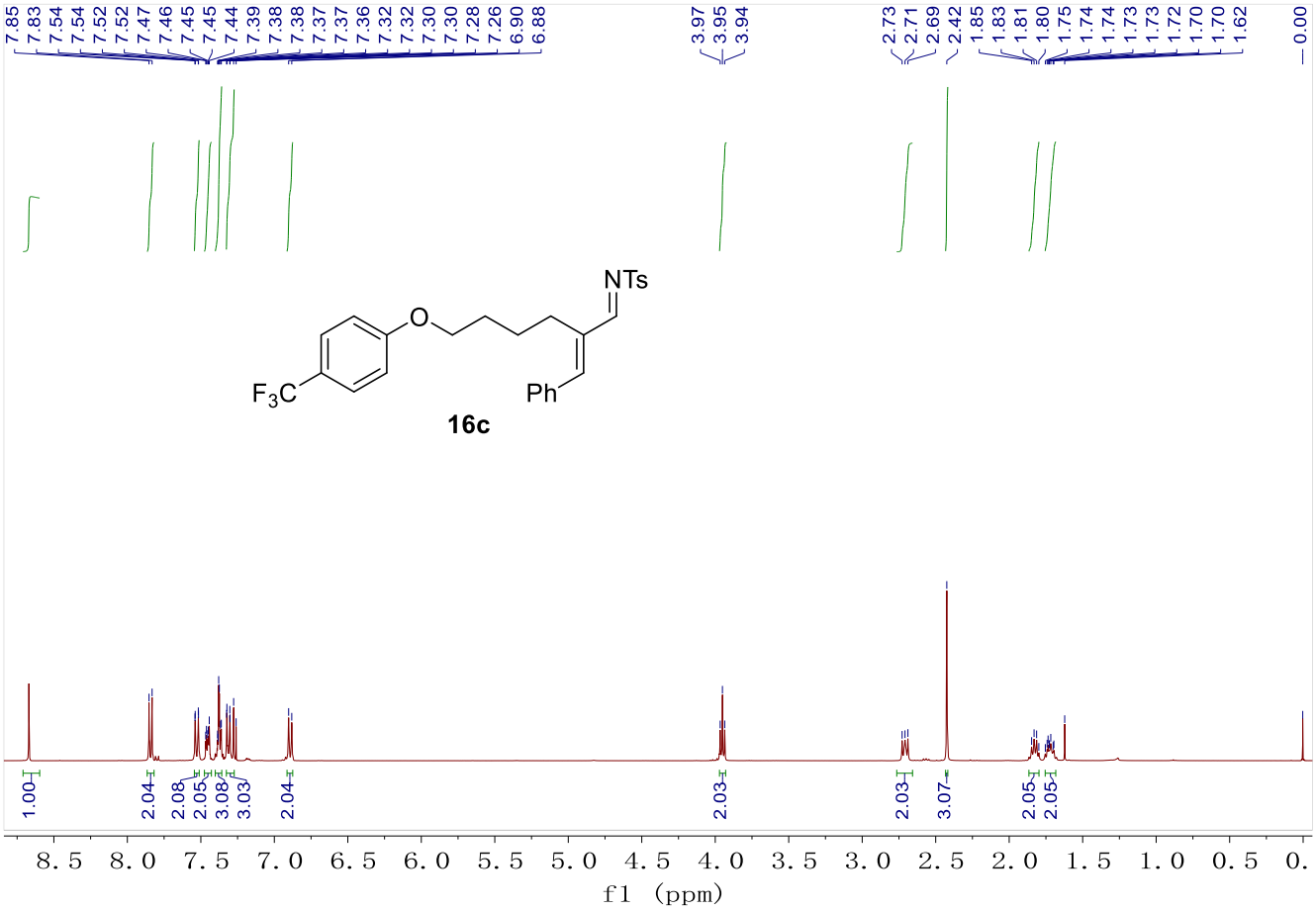
76.68
31.16
30.86
30.55
30.24
21.66
NTs
F3C
Ph
15c
f1 (ppm)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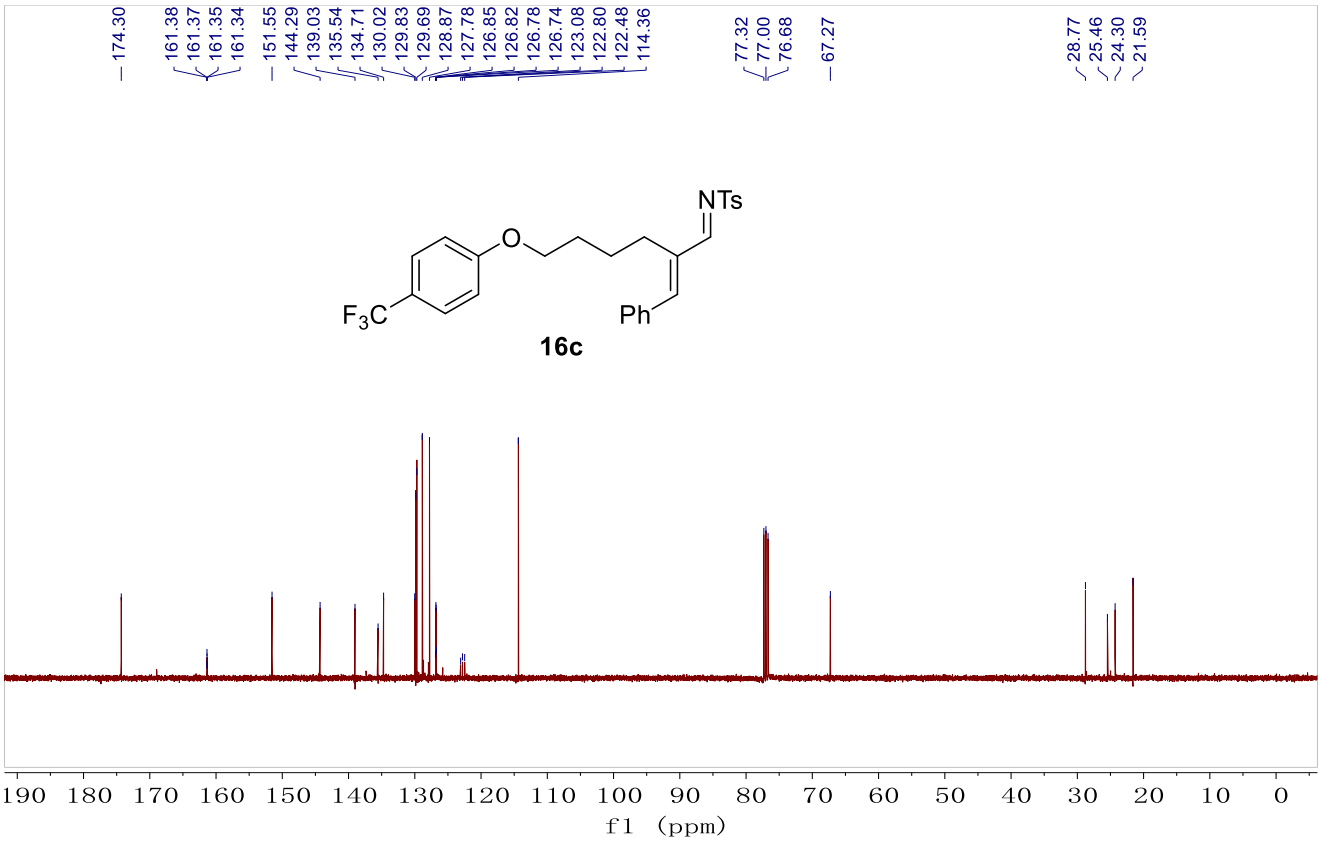
3.97 3.95 3.94
2.73 2.71 2.69 2.42 1.85 1.83 1.81 1.80 1.75 1.74 1.74 1.73 1.73 1.72 1.70 1.70 1.62
0.00
NTs
O
F3C
Ph
16c
1.00 2.04 2.08 2.05 3.08 3.03 2.04 2.03 2.03 3.07 2.05 2.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)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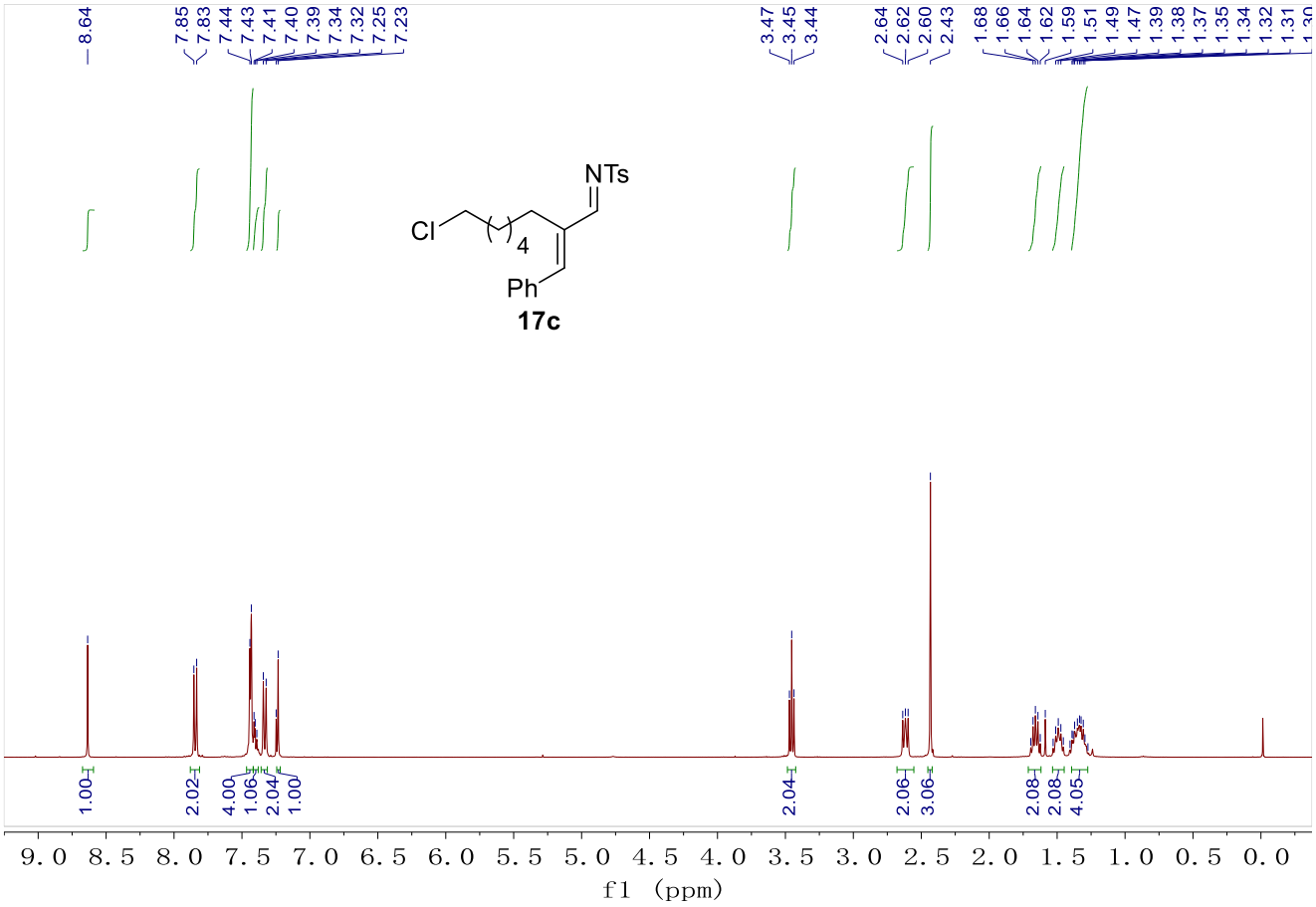
161.38 161.37 161.35 161.34
151.55 144.29 139.03 135.54 134.71 130.02 129.83 129.69 128.87 127.78 126.85 126.82 126.78 126.74 123.08 122.80 122.48 114.36
77.32 77.00 76.68
67.27
28.77 25.46 24.30 21.59
NTs
O
F3C
Ph
16c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.32
7.25
7.23
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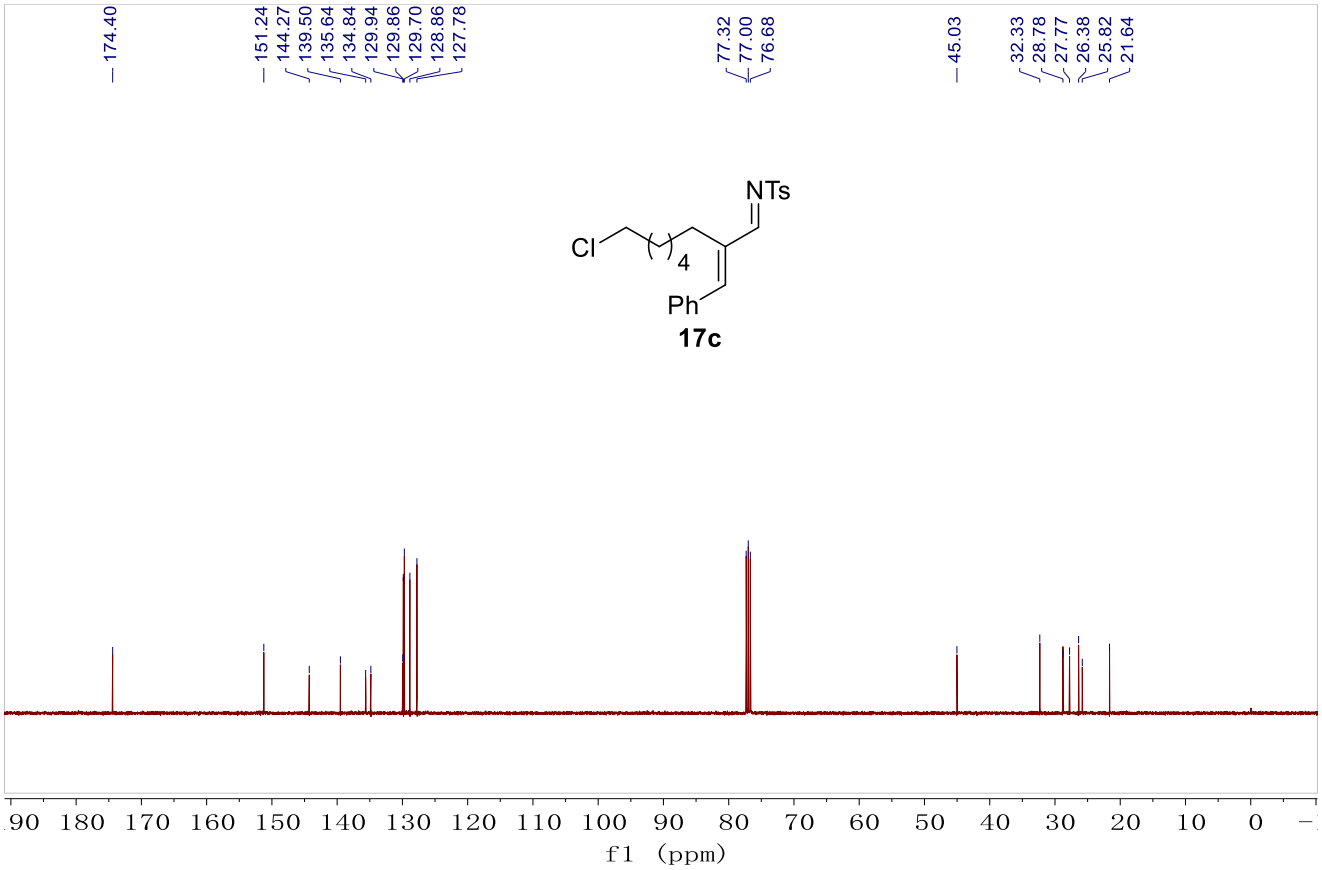
3.45
3.44
2.64
2.62
2.60
2.43
1.68
1.66
1.64
1.62
1.59
1.51
1.49
1.47
1.39
1.38
1.37
1.35
1.34
1.32
1.31
NTs
Cl
4
Ph
17c
1.00
2.02
4.00
1.06
2.04
1.00
2.04
2.06
3.06
2.08
2.08
4.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.86
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128.86
127.78
77.32
77.00
76.68
45.03
32.33
28.78
27.77
26.38
25.82
21.64
NTs
Cl
4
Ph
17c
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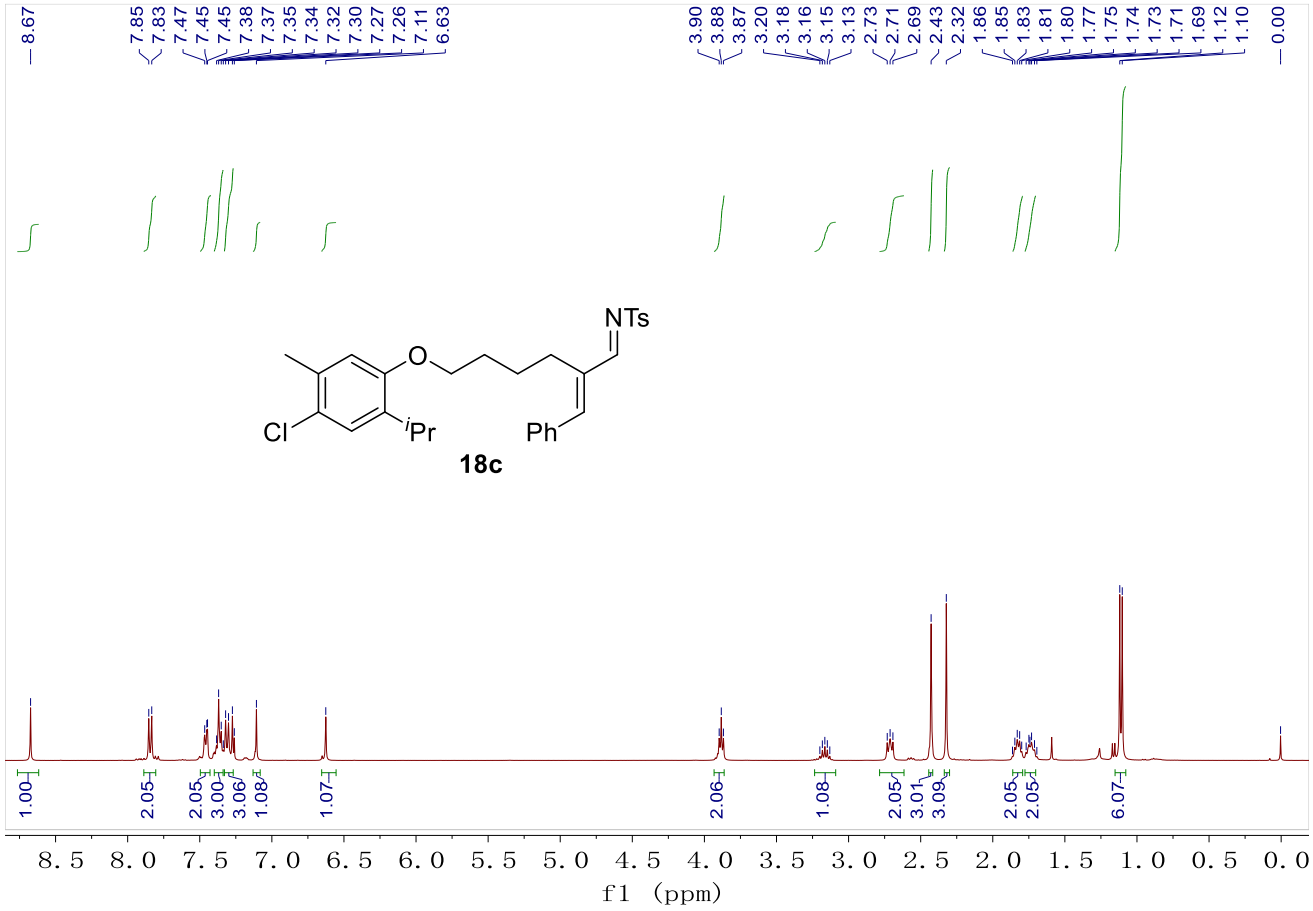
f1 (ppm)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7.45
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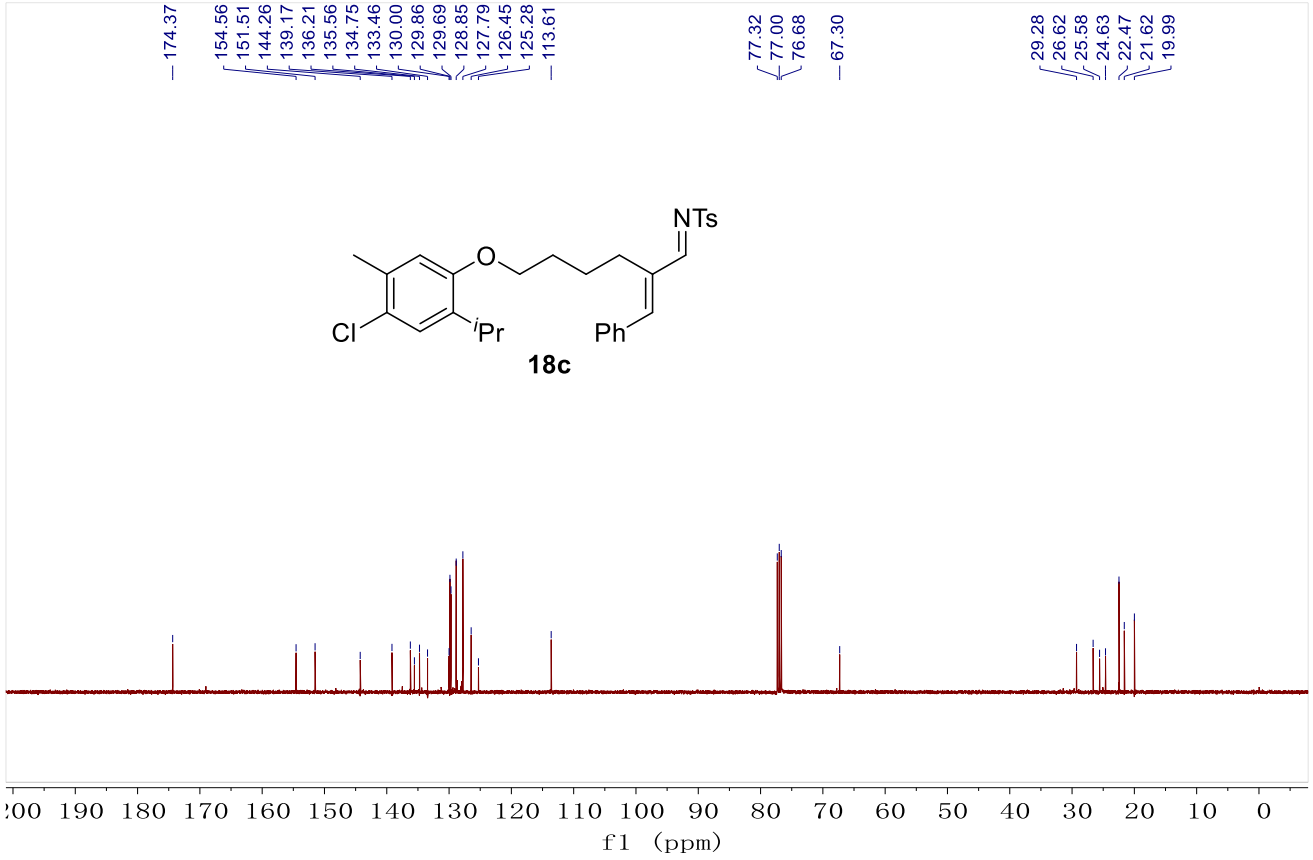
7.34
7.32
7.30
7.27
7.26
7.11
6.63
3.90
3.88
3.87
3.20
3.18
3.16
3.15
3.13
2.73
2.71
2.69
2.43
2.32
1.86
1.85
1.83
1.81
1.80
1.77
1.75
1.74
1.73
1.71
1.69
1.12
1.10
0.00
NTs
O
Cl
iPr
Ph
18c
1.00
2.05
2.05
3.00
3.06
1.08
1.07
2.06
1.08
2.05
3.01
3.09
2.05
2.05
6.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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144.26
139.17
136.21
135.56
134.75
133.46
130.00
129.86
129.69
128.85
127.79
126.45
125.28
113.61
77.32
77.00
76.68
67.30
29.28
26.62
25.58
24.63
22.47
21.62
19.99
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O
Cl
iPr
Ph
18c
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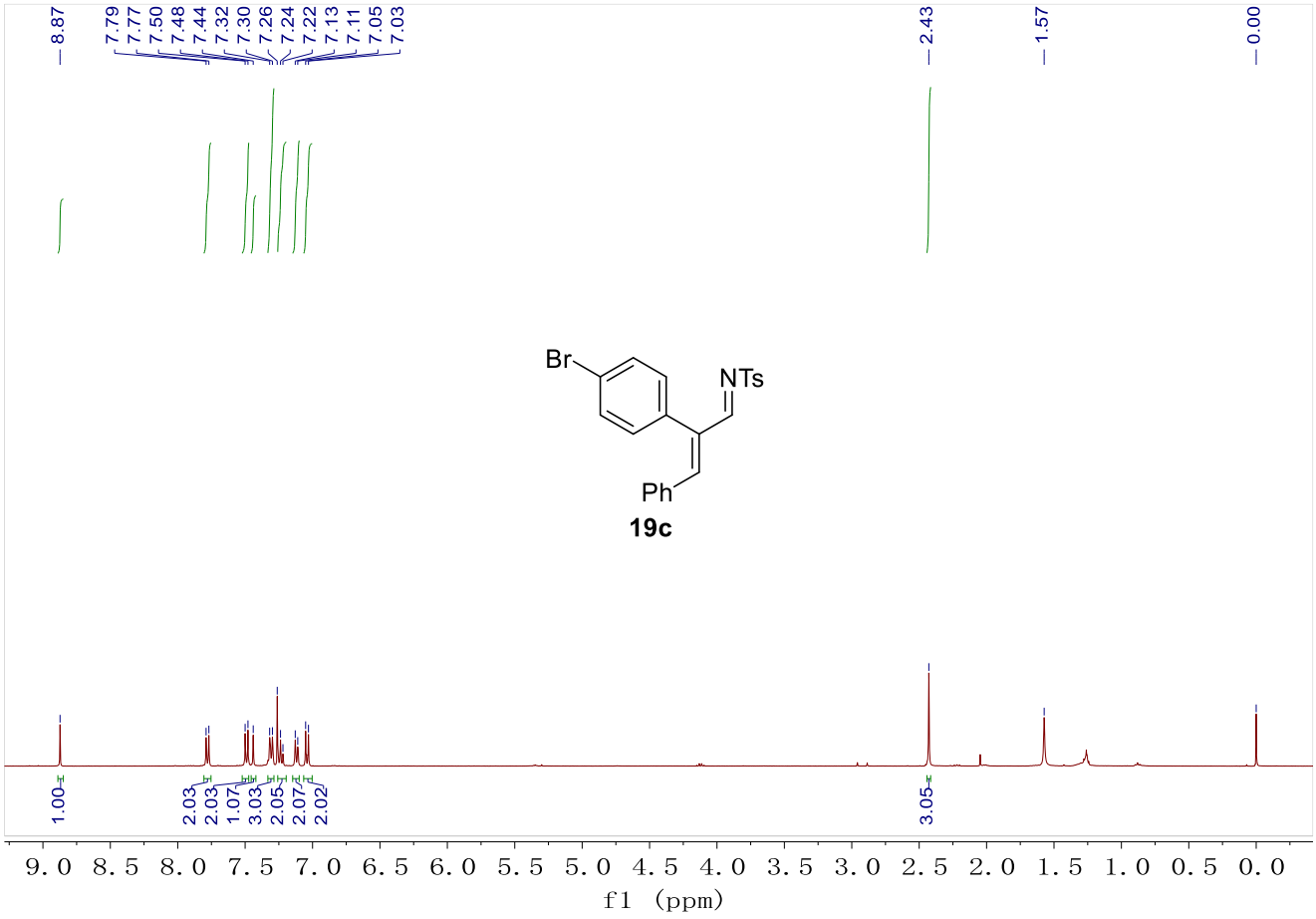
f1 (ppm)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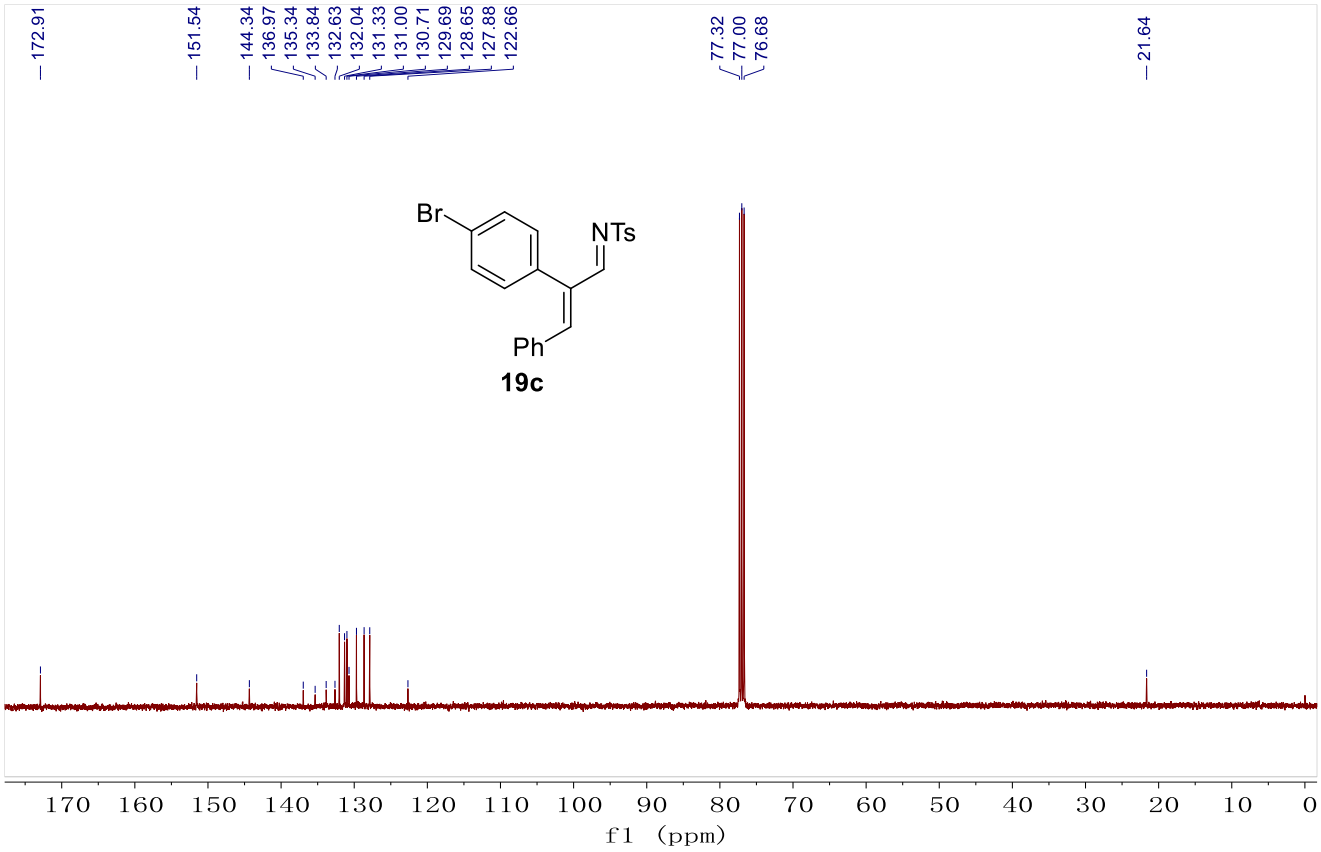
7.48
7.44
7.32
7.30
7.26
7.24
7.22
7.13
7.11
7.05
7.03
2.43
1.57
0.00
Br
NTs
Ph
19c
1.00
2.03
2.03
1.07
3.03
2.05
2.07
2.02
3.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.00
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129.69
128.65
127.88
122.66
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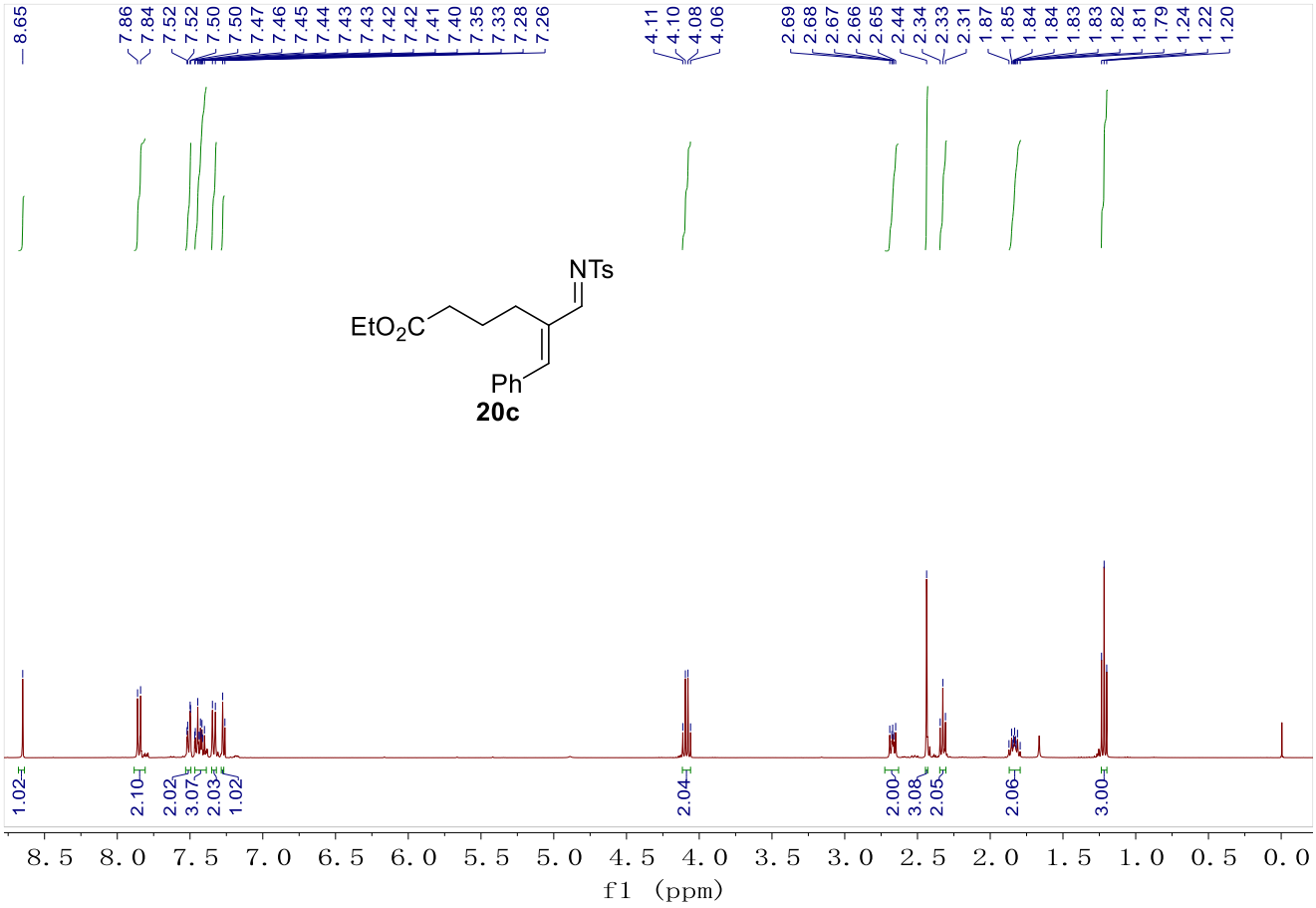
21.64
Br
NTs
Ph
19c
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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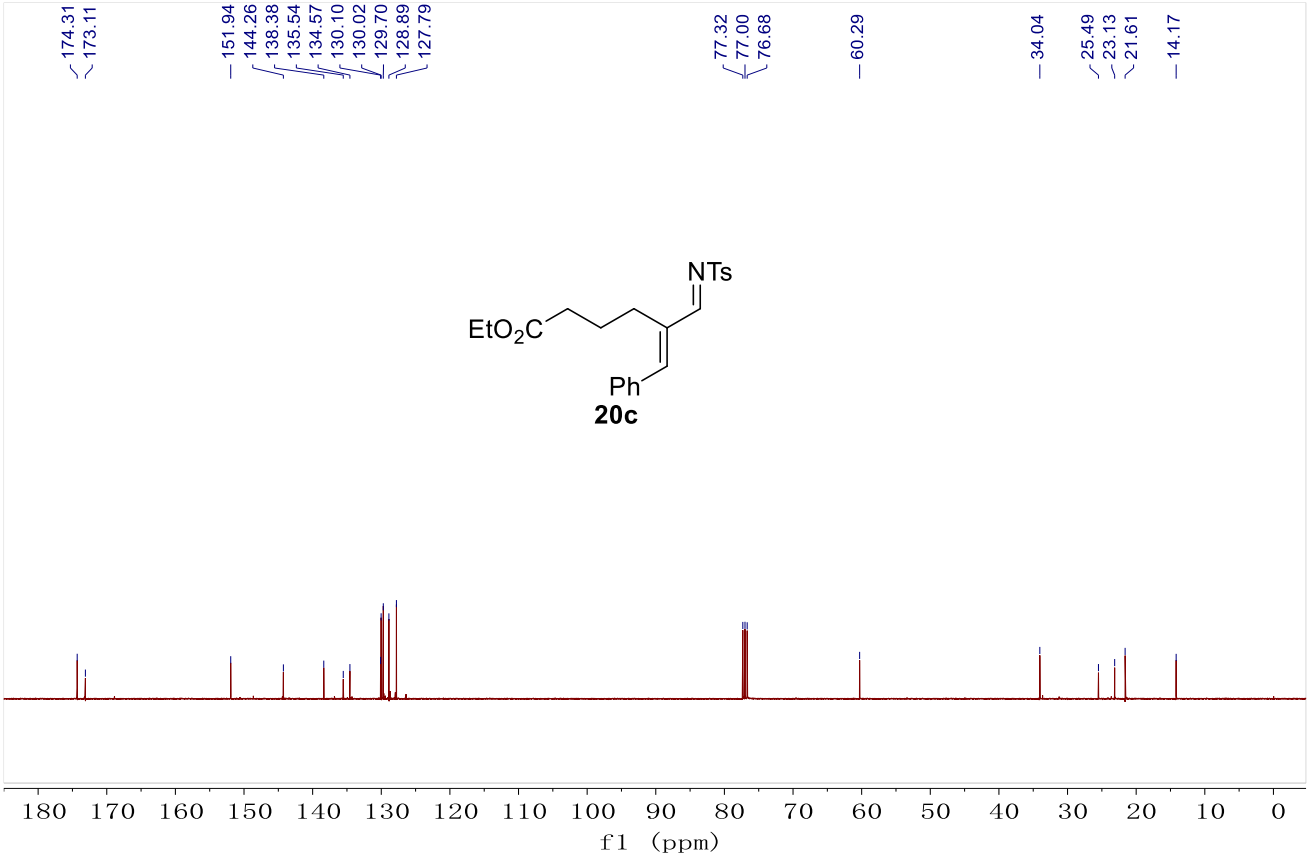
7.84
7.52
7.52
7.50
7.50
7.47
7.46
7.45
7.44
7.43
7.43
7.42
7.42
7.41
7.40
7.35
7.33
7.28
7.26
4.11
4.10
4.08
4.06
2.69
2.68
2.67
2.66
2.65
2.44
2.34
2.33
2.31
1.87
1.85
1.84
1.84
1.83
1.83
1.82
1.81
1.79
1.24
1.22
1.20
NTs
EtO2C
Ph
20c
1.02
2.10
2.02
3.07
2.03
1.02
2.04
2.00
3.08
2.05
2.06
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.54
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130.10
130.02
129.70
128.89
127.79
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77.00
76.68
60.29
34.04
25.49
23.13
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14.17
NTs
EtO2C
Ph
20c
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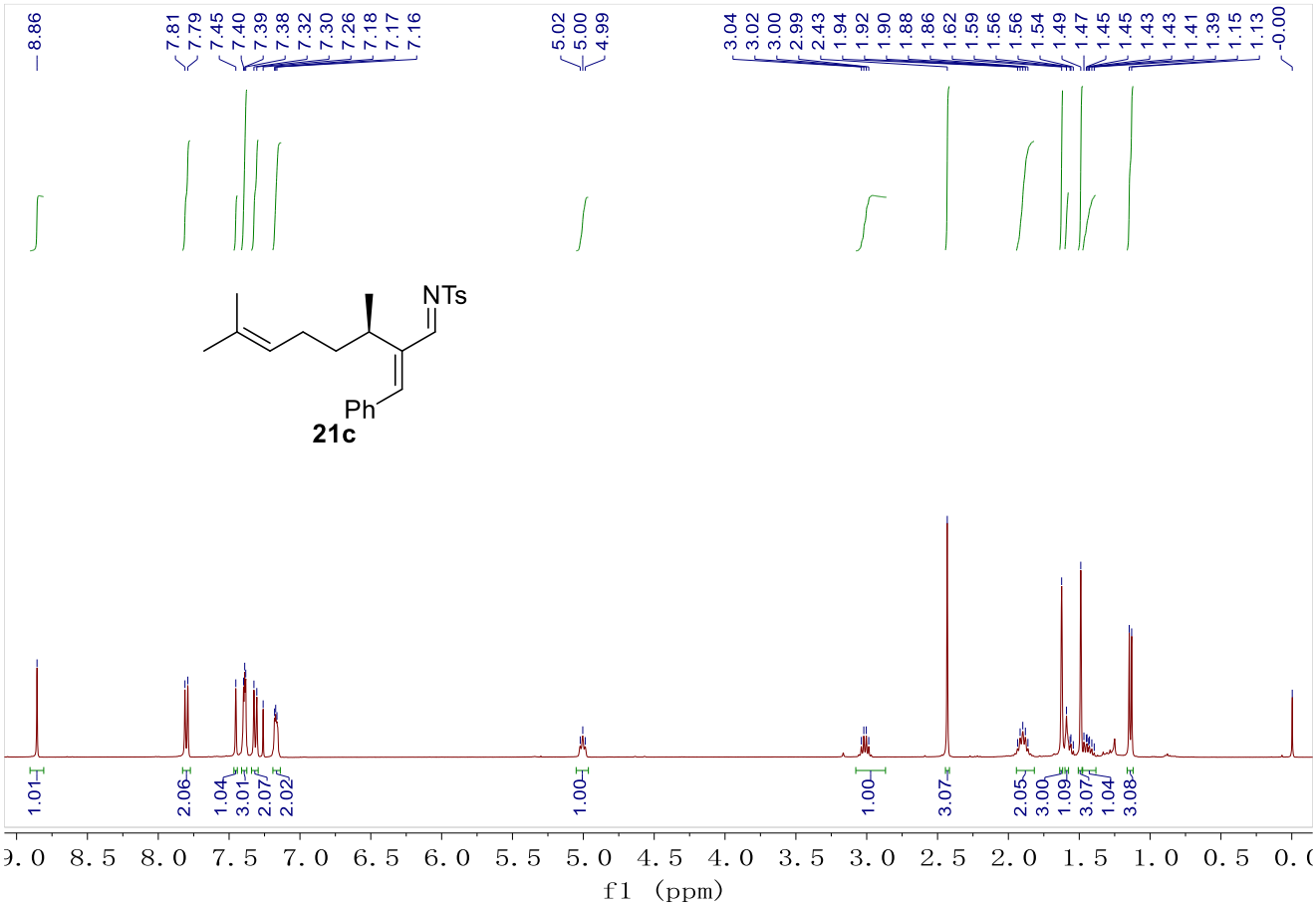
f1 (ppm)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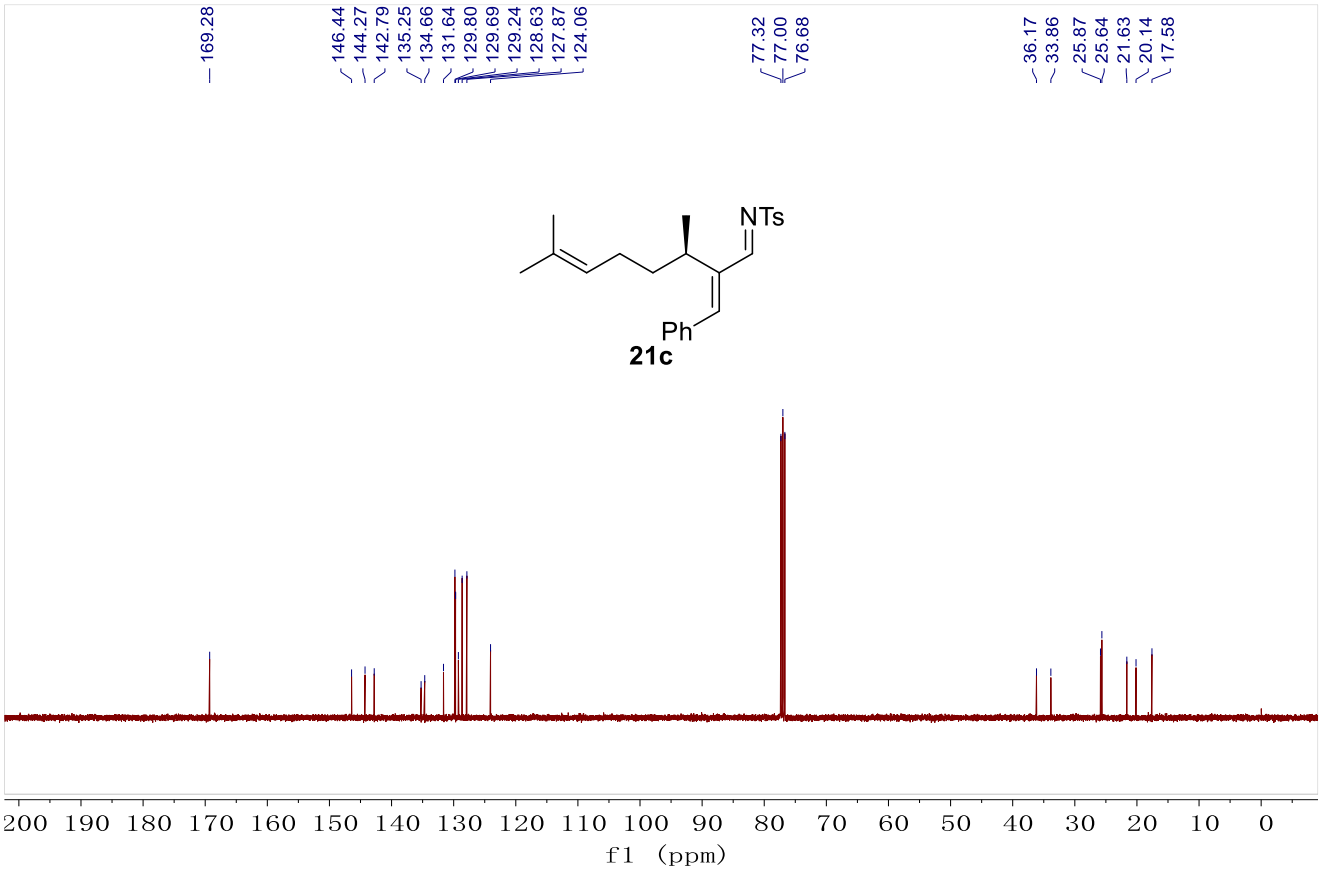
7.32
7.30
7.26
7.18
7.17
7.16
5.02
5.00
4.99
3.04
3.02
3.00
2.99
2.43
1.94
1.92
1.90
1.88
1.86
1.62
1.59
1.56
1.56
1.54
1.49
1.47
1.45
1.45
1.43
1.43
1.41
1.39
1.15
1.13
-0.00
NTs
Ph
21c
1.01
2.06
1.04
3.01
2.07
2.02
1.00
1.00
3.07
2.05
3.00
1.09
3.07
1.04
3.08
f1 (ppm)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131.64
129.80
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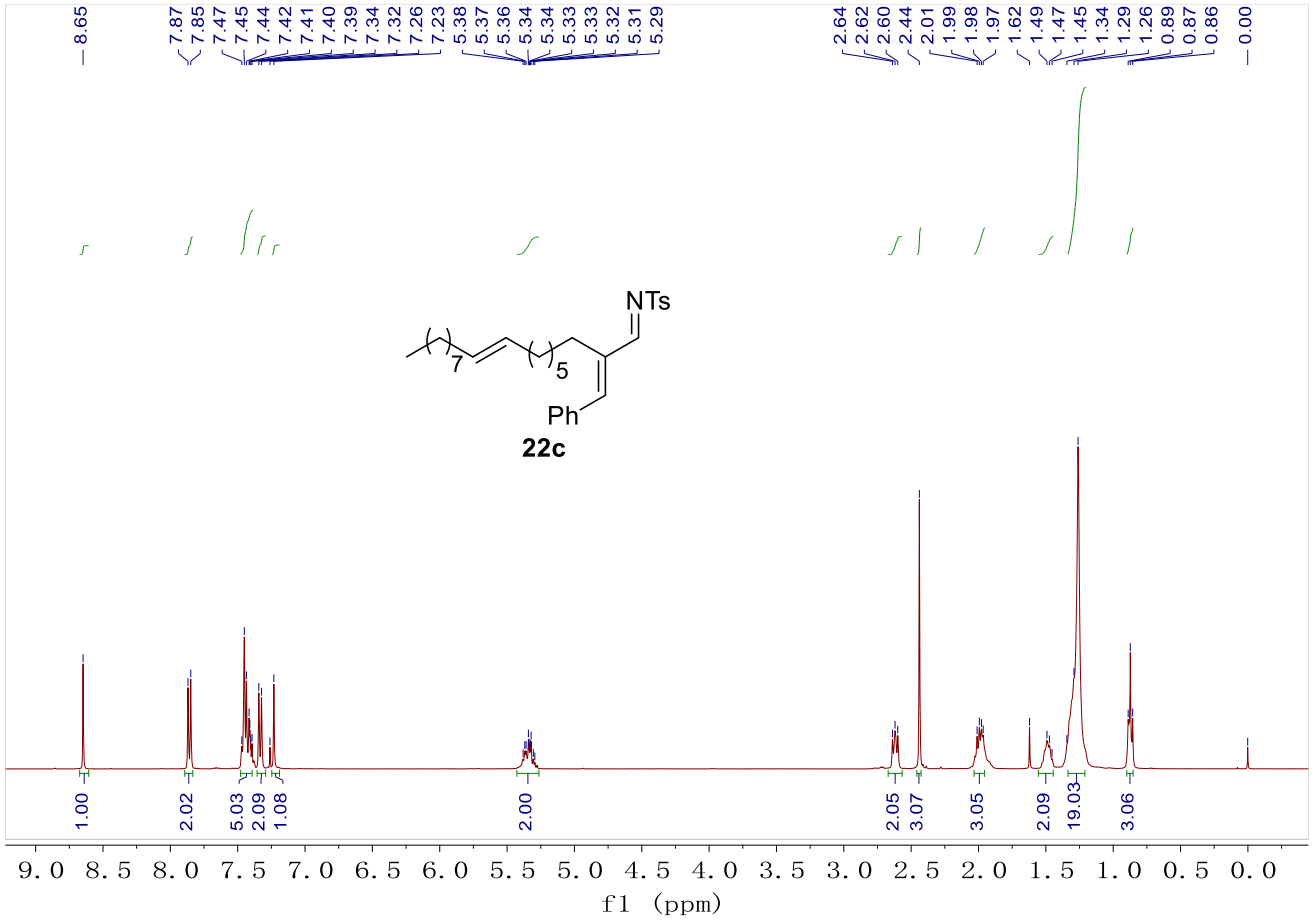
129.24
128.63
127.87
124.06
77.32
77.00
76.68
36.17
33.86
25.87
25.64
21.63
20.14
17.58
NTs
Ph
21c
f1 (ppm)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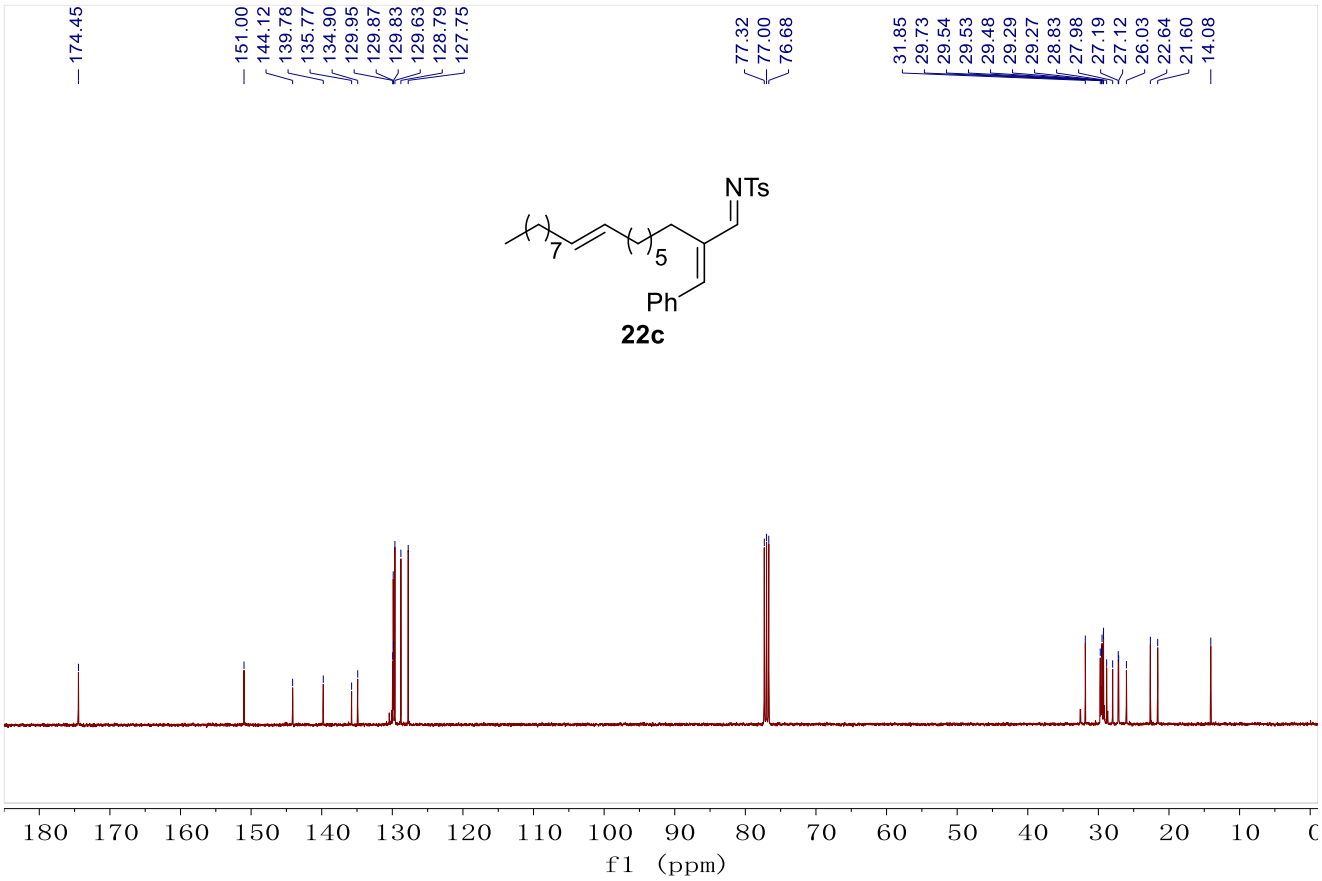
7.39
7.34
7.32
7.26
7.23
5.38
5.37
5.36
5.34
5.34
5.33
5.33
5.32
5.31
5.29
2.64
2.62
2.60
2.44
2.01
1.99
1.98
1.97
1.62
1.49
1.47
1.45
1.34
1.29
1.26
0.89
0.87
0.86
0.00
NTs
7
5
Ph
22c
1.00
2.02
5.03
2.09
1.08
2.00
2.05
3.07
3.05
2.09
19.03
3.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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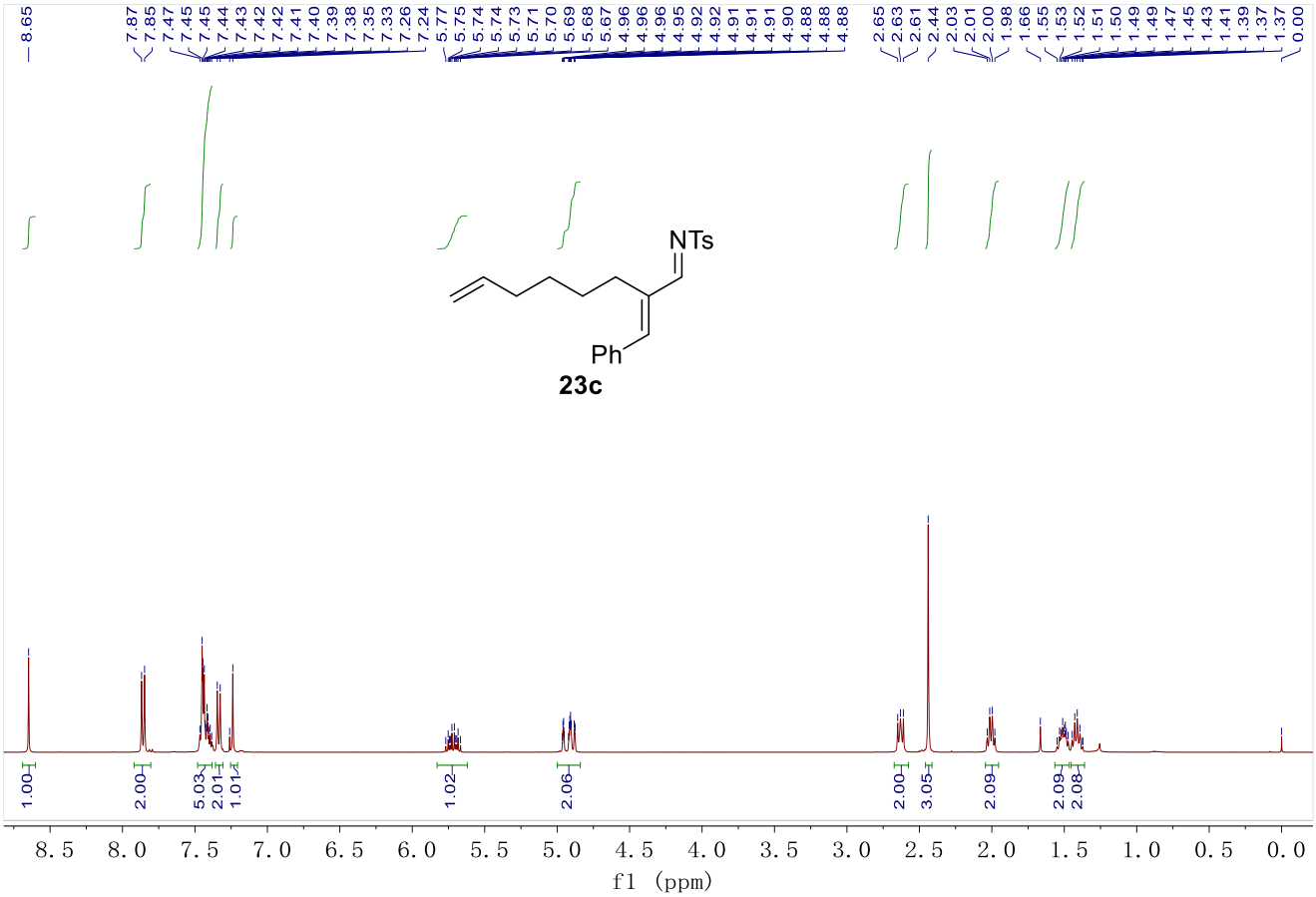
128.79
127.75
77.32
77.00
76.68
31.85
29.73
29.54
29.53
29.48
29.29
29.27
28.83
27.98
27.19
27.12
26.03
22.64
21.60
14.08
NTs
7
5
Ph
22c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.87 7.85 7.47 7.45 7.45 7.44 7.43 7.42 7.42 7.41 7.40 7.39 7.38 7.35 7.33 7.26 7.24
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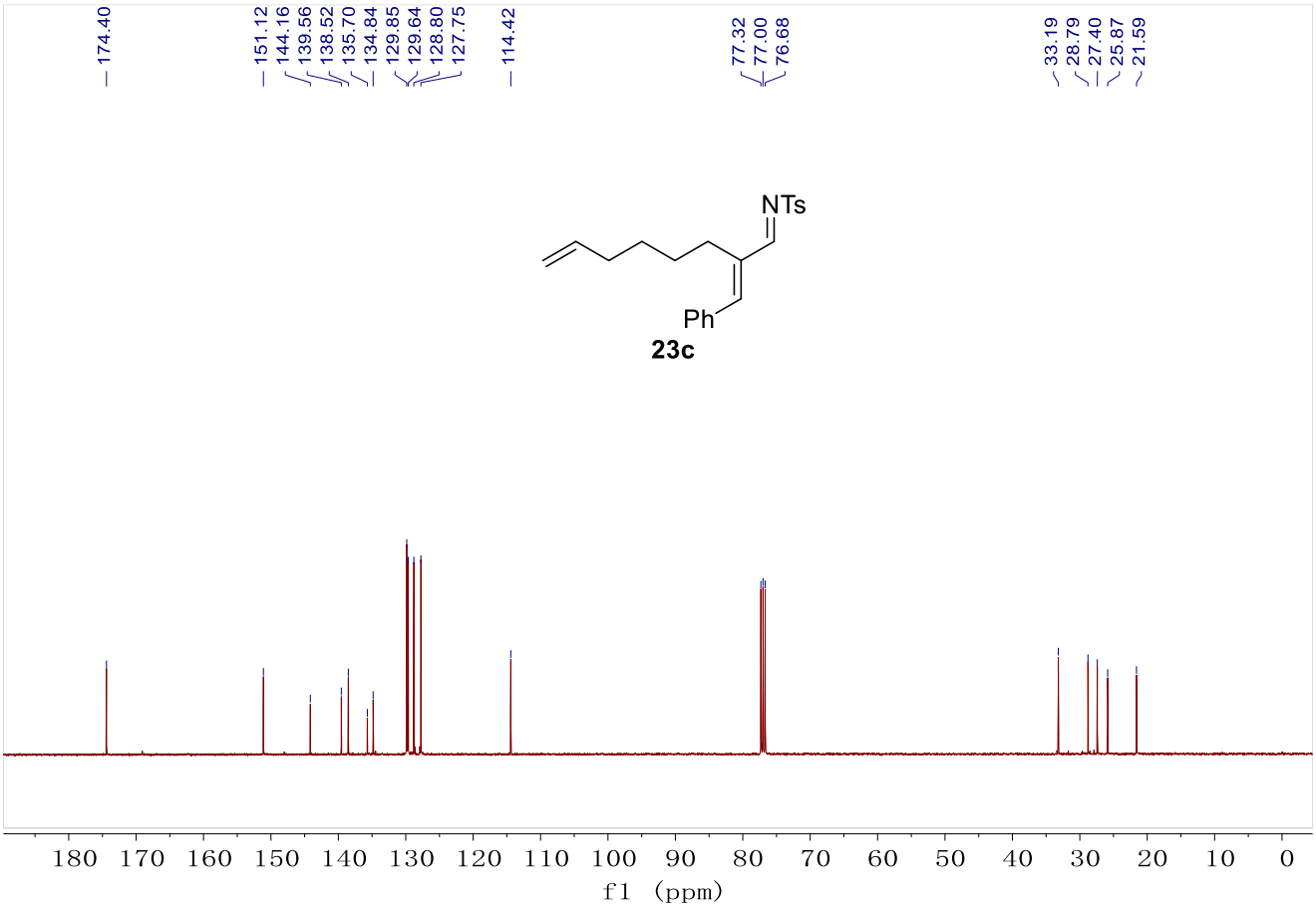
2.65 2.63 2.61 2.44 2.03 2.01 2.00 1.98 1.66 1.55 1.53 1.52 1.51 1.50 1.49 1.49 1.47 1.45 1.43 1.41 1.39 1.37 1.37 0.00
NTs
Ph
23c
1.00 2.00 5.03 2.01 1.01 1.02 2.06 2.00 3.05 2.09 2.09 2.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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114.42
77.32 77.00 76.68
33.19 28.79 27.40 25.87 21.59
NTs
Ph
23c
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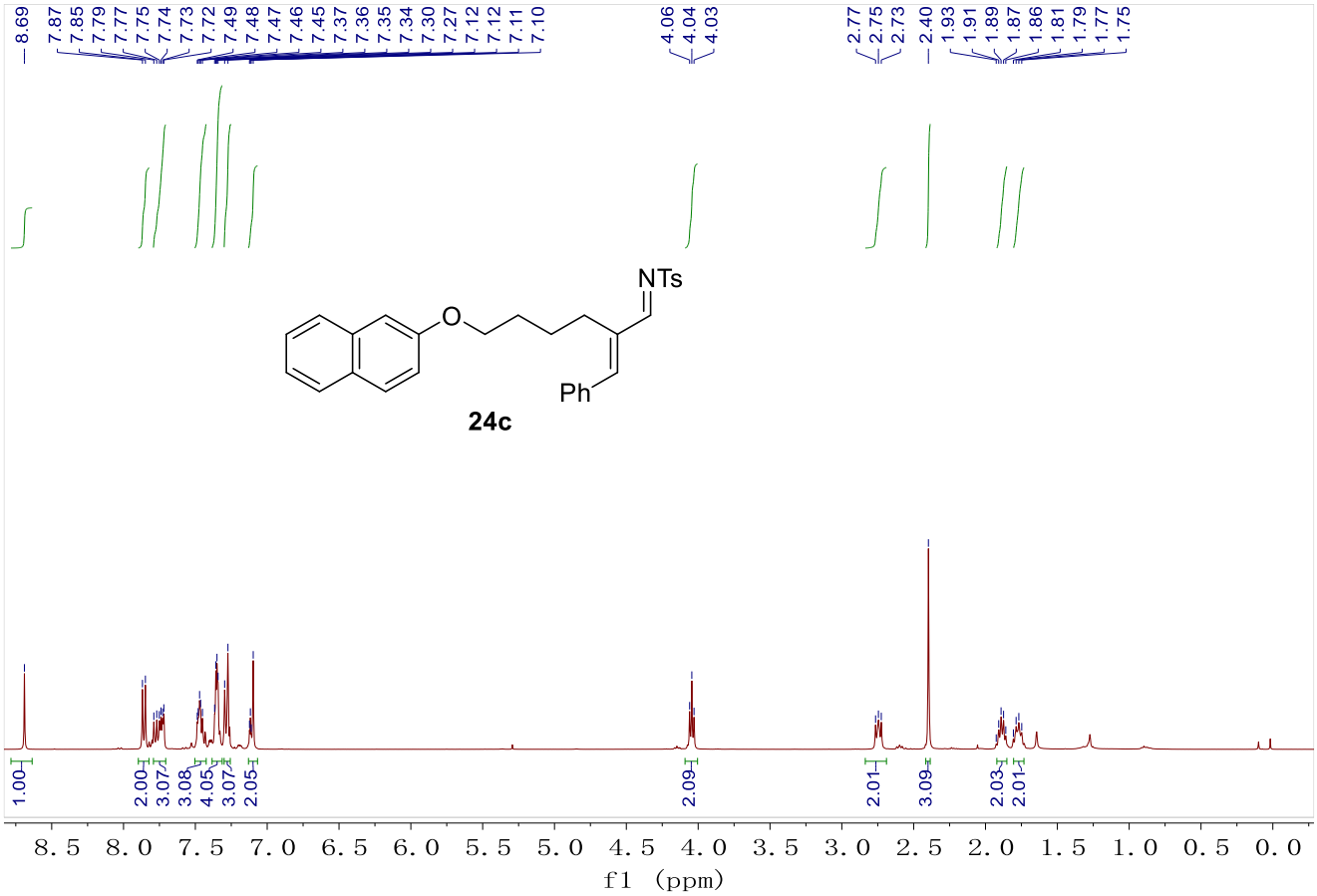
f1 (ppm)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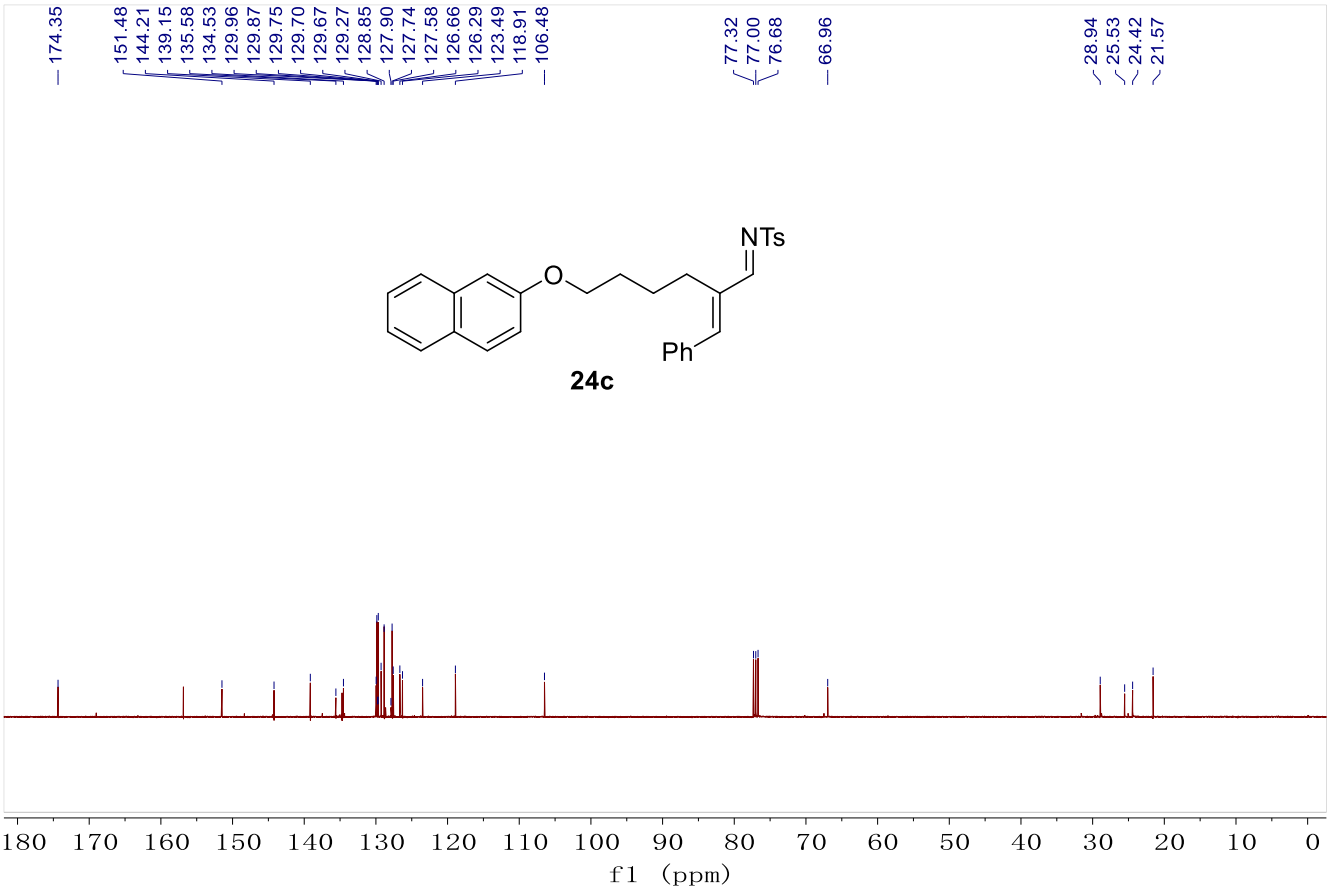
7.30
7.27
7.12
7.11
7.10
4.06
4.04
4.03
2.77
2.75
2.73
2.40
1.93
1.91
1.89
1.87
1.86
1.81
1.79
1.77
1.75
NTs
O
Ph
24c
1.00
2.00
3.07
3.08
4.05
3.07
2.05
2.09
2.01
3.09
2.03
2.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.85
127.90
127.74
127.58
126.66
126.29
123.49
118.91
106.48
77.32
77.00
76.68
66.96
28.94
25.53
24.42
21.57
NTs
O
Ph
24c
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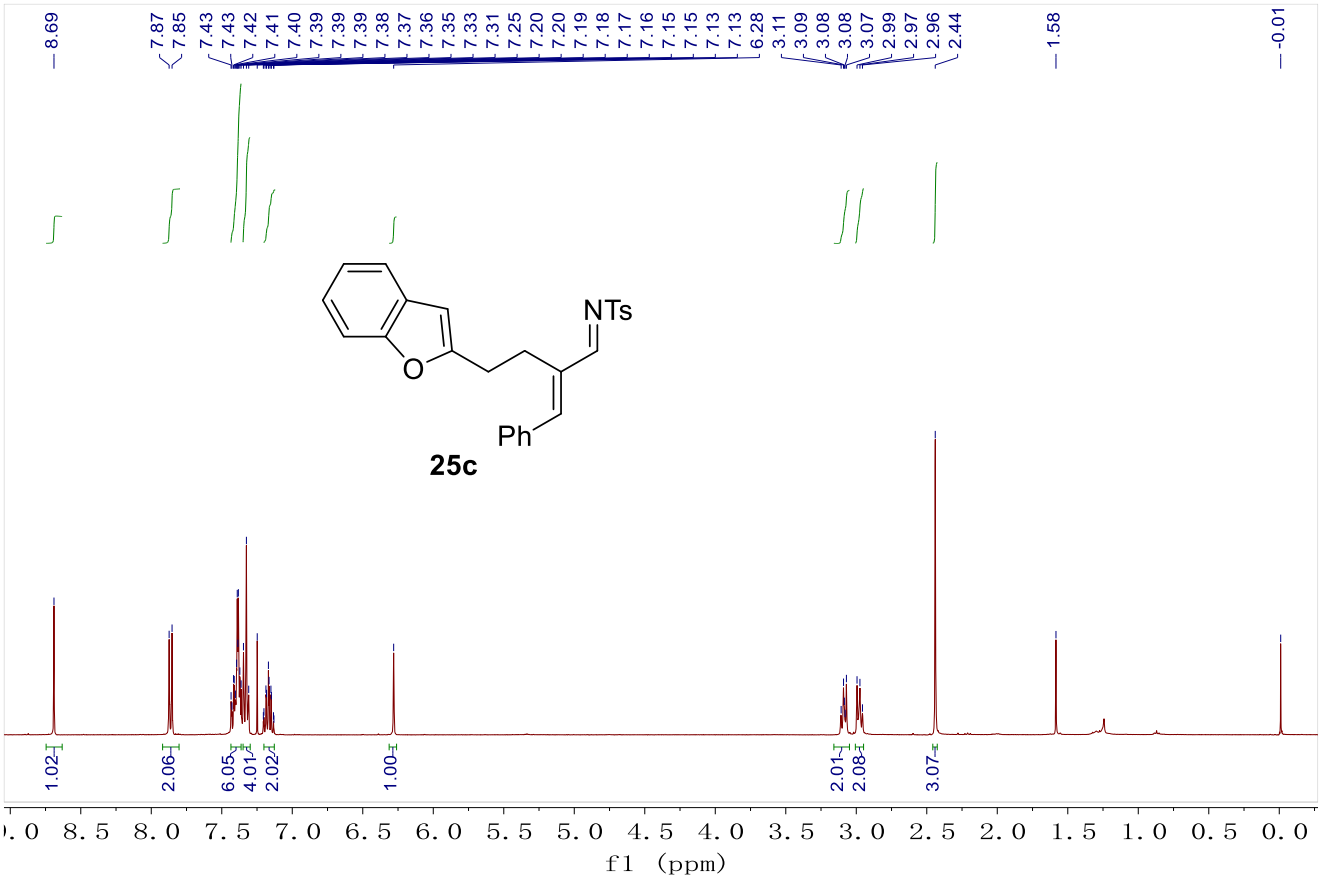
f1 (ppm)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7.36
7.35
7.33
7.31
7.25
7.20
7.20
7.19
7.18
7.17
7.16
7.15
7.15
7.13
7.13
6.28
3.11
3.09
3.08
3.08
3.07
2.99
2.97
2.96
2.44
1.58
-0.01
NTs
O
Ph
25c
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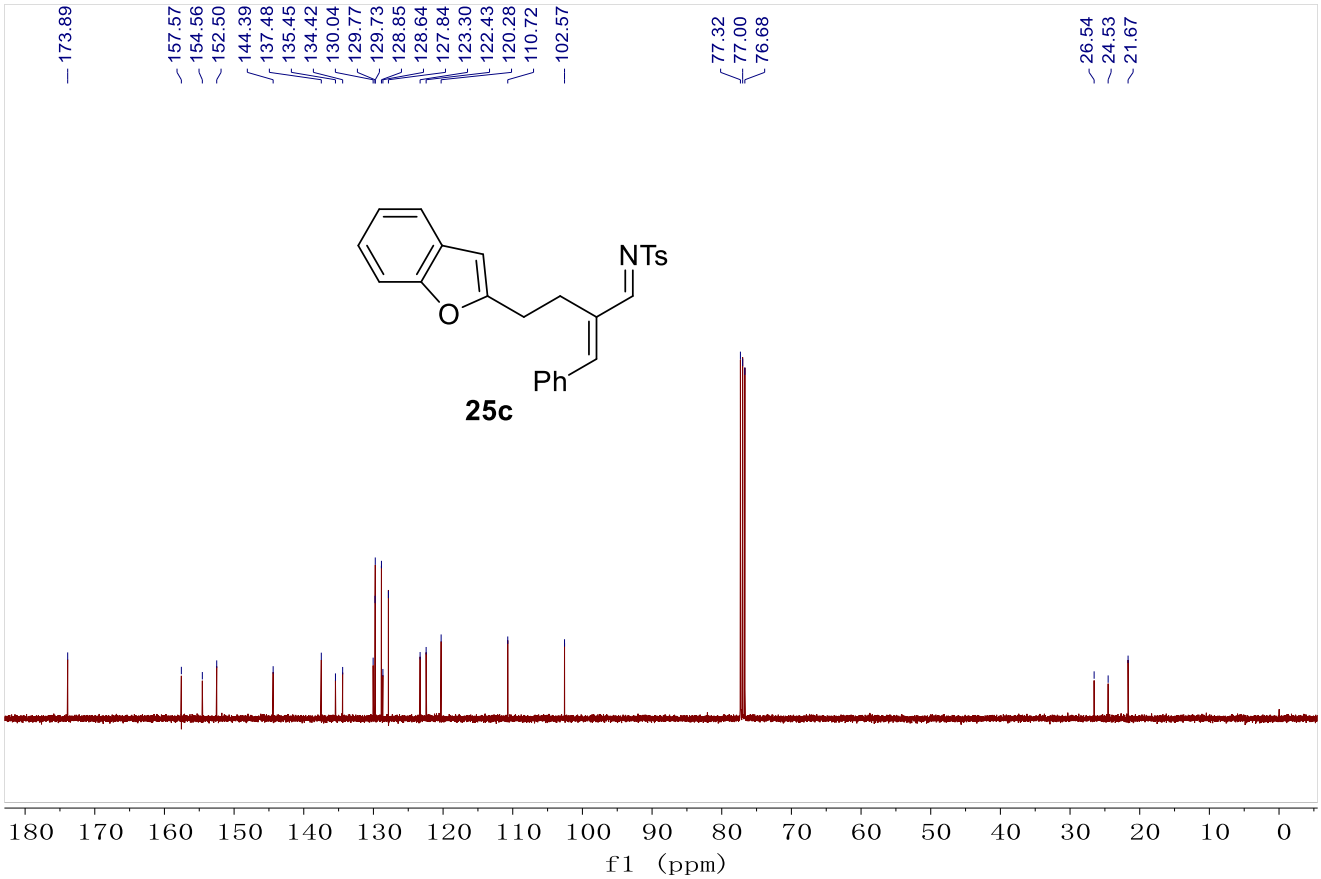
2.06
6.05
4.01
2.02
1.00
2.01
2.08
3.07
f1 (ppm)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134.42
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128.64
127.84
123.30
122.43
120.28
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26.54
24.53
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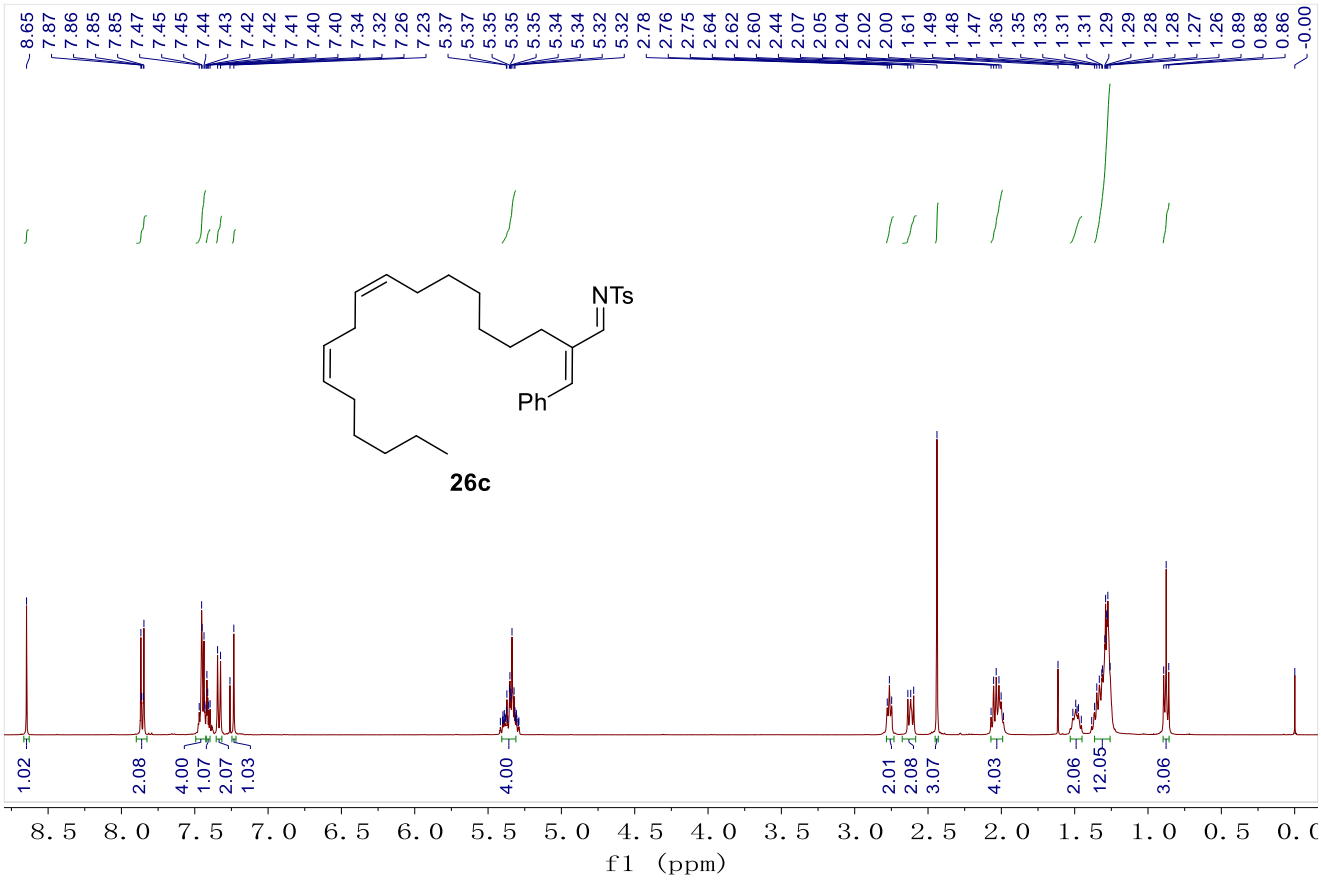
NTs
O
Ph
25c
f1 (ppm)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NTs
Ph
26c
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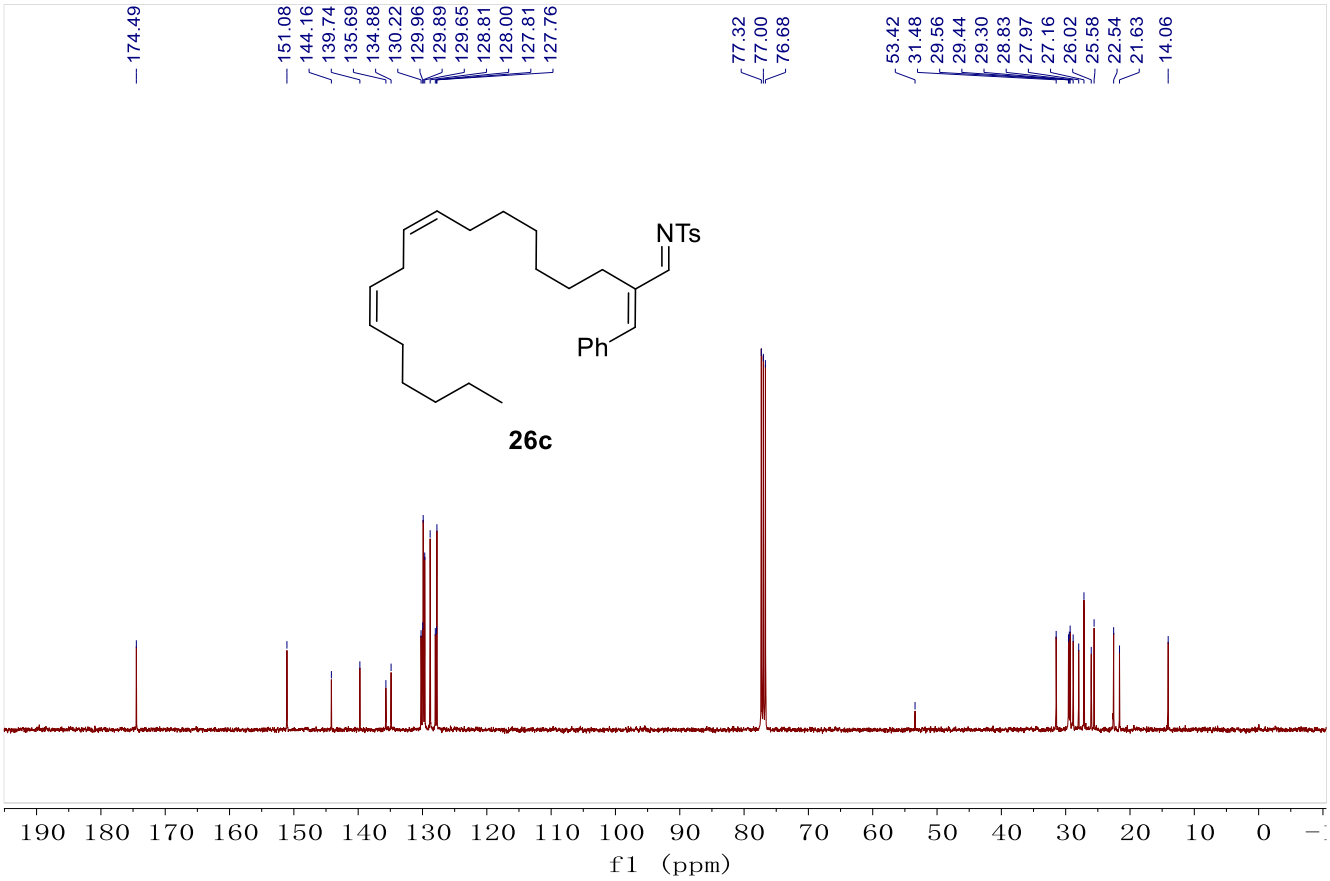
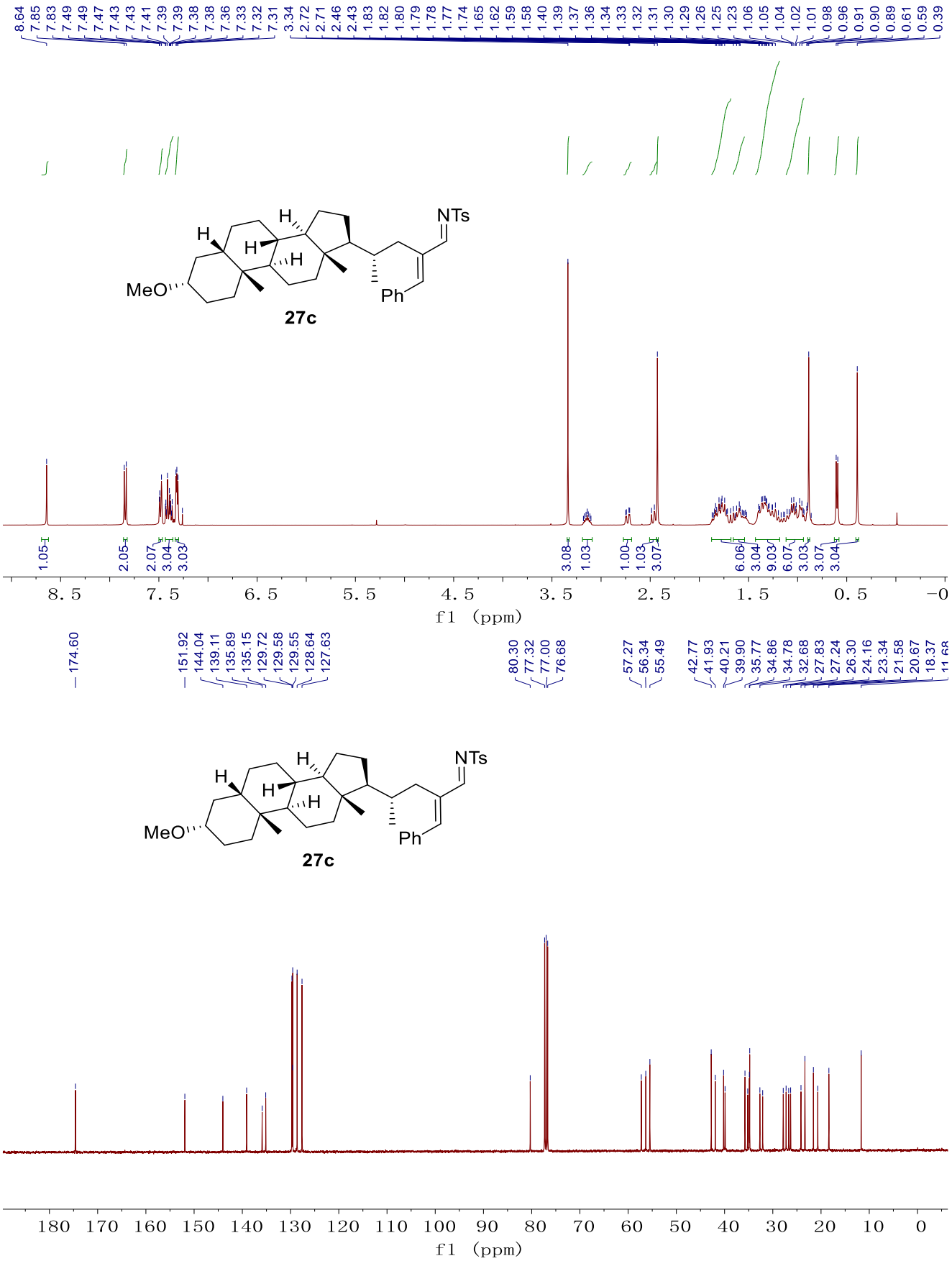
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


174.49
151.08 144.16 139.74 135.69 134.88 130.22 129.96 129.89 129.65 128.81 128.00 127.81 127.76
77.32 77.00 76.68
53.42 31.48 29.56 29.44 29.30 28.83 27.97 27.16 26.02 25.58 22.54 21.63 14.06
NTs
Ph
26c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.64 7.85 7.83 7.49 7.49 7.47 7.43 7.43 7.41 7.39 7.39 7.38 7.38 7.36 7.33 7.32 7.31
3.34 2.72 2.71 2.46 2.43 1.83 1.82 1.80 1.79 1.78 1.77 1.74 1.65 1.62 1.59 1.58 1.40 1.39 1.37 1.36 1.34 1.33 1.32 1.31 1.30 1.29 1.26 1.25 1.23 1.06 1.05 1.04 1.02 1.01 0.98 0.96 0.91 0.90 0.89 0.61 0.59 0.39
H
H
H
H
NTs
MeO
Ph
27c
1.05 2.05 2.07 3.04 3.03 3.08 1.03 1.00 1.03 3.07 6.06 3.04 9.03 6.07 3.03 3.07 3.04
8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 −0
f1 (ppm)
174.60 151.92 144.04 139.11 135.89 135.15 129.72 129.58 129.55 128.64 127.63 80.30 77.32 77.00 76.68 57.27 56.34 55.49 42.77 41.93 40.21 39.90 35.77 34.86 34.78 32.68 27.83 27.24 26.30 24.16 23.34 21.58 20.67 18.37
H
H
H
H
NTs
MeO
Ph
27c
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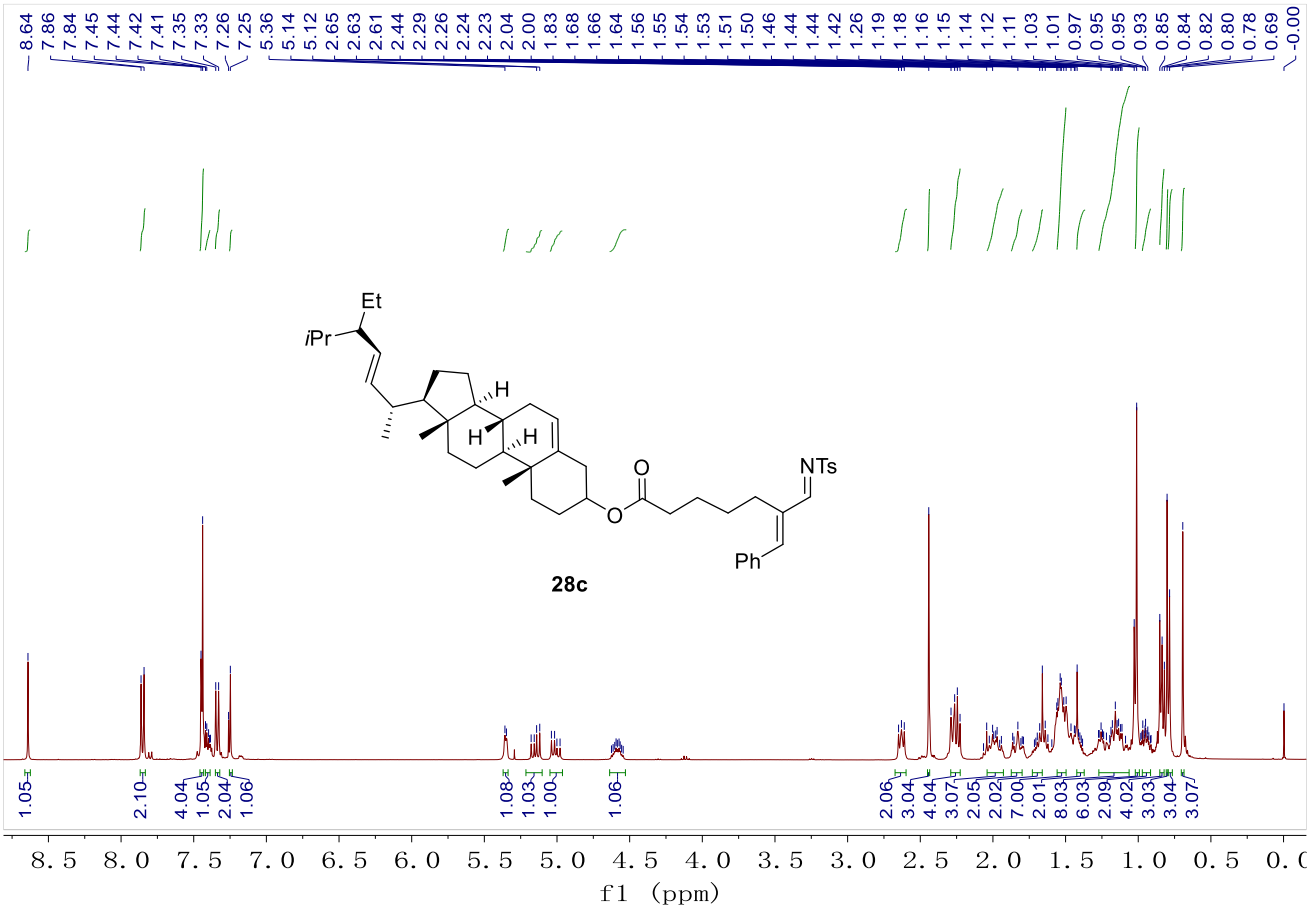
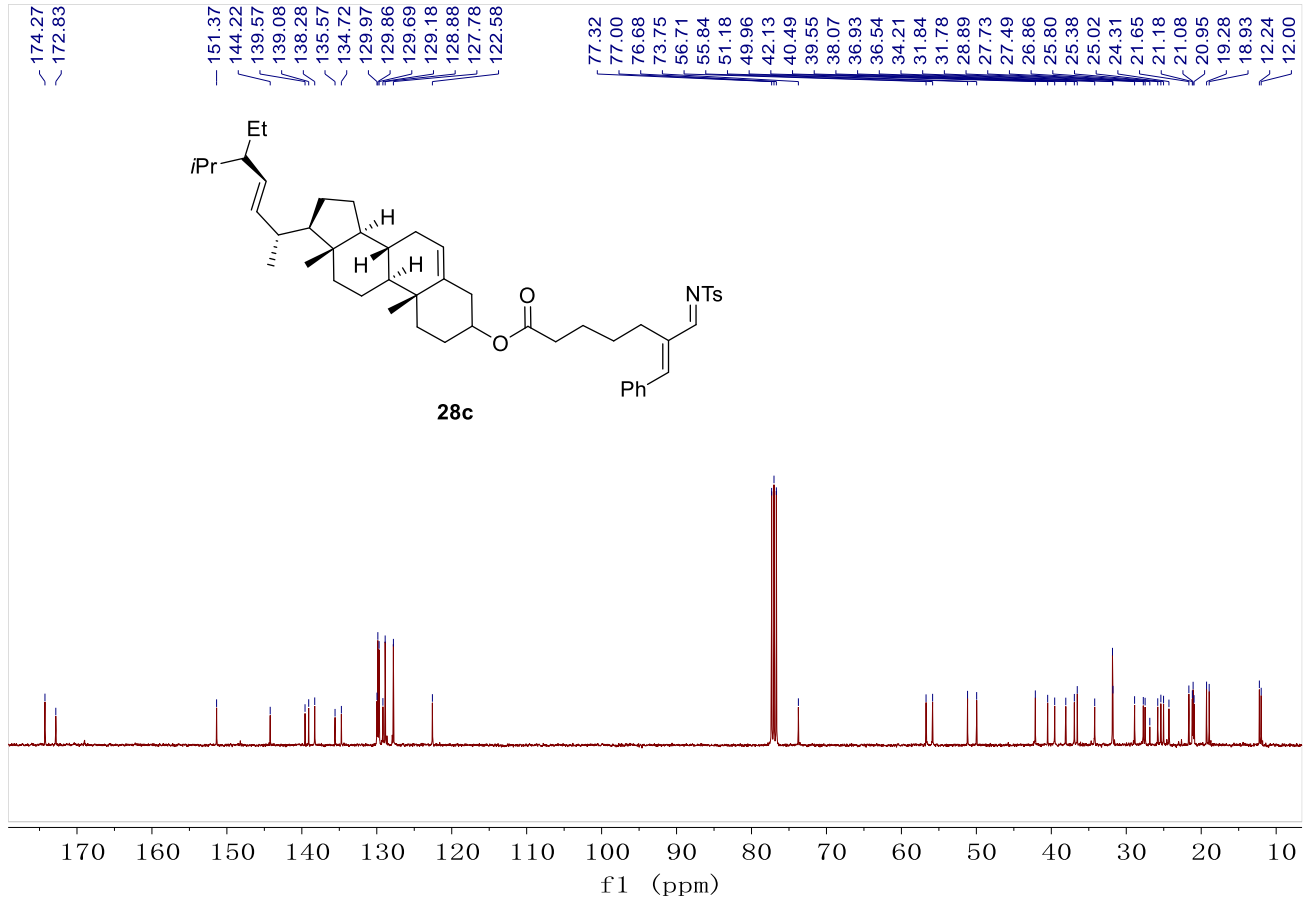
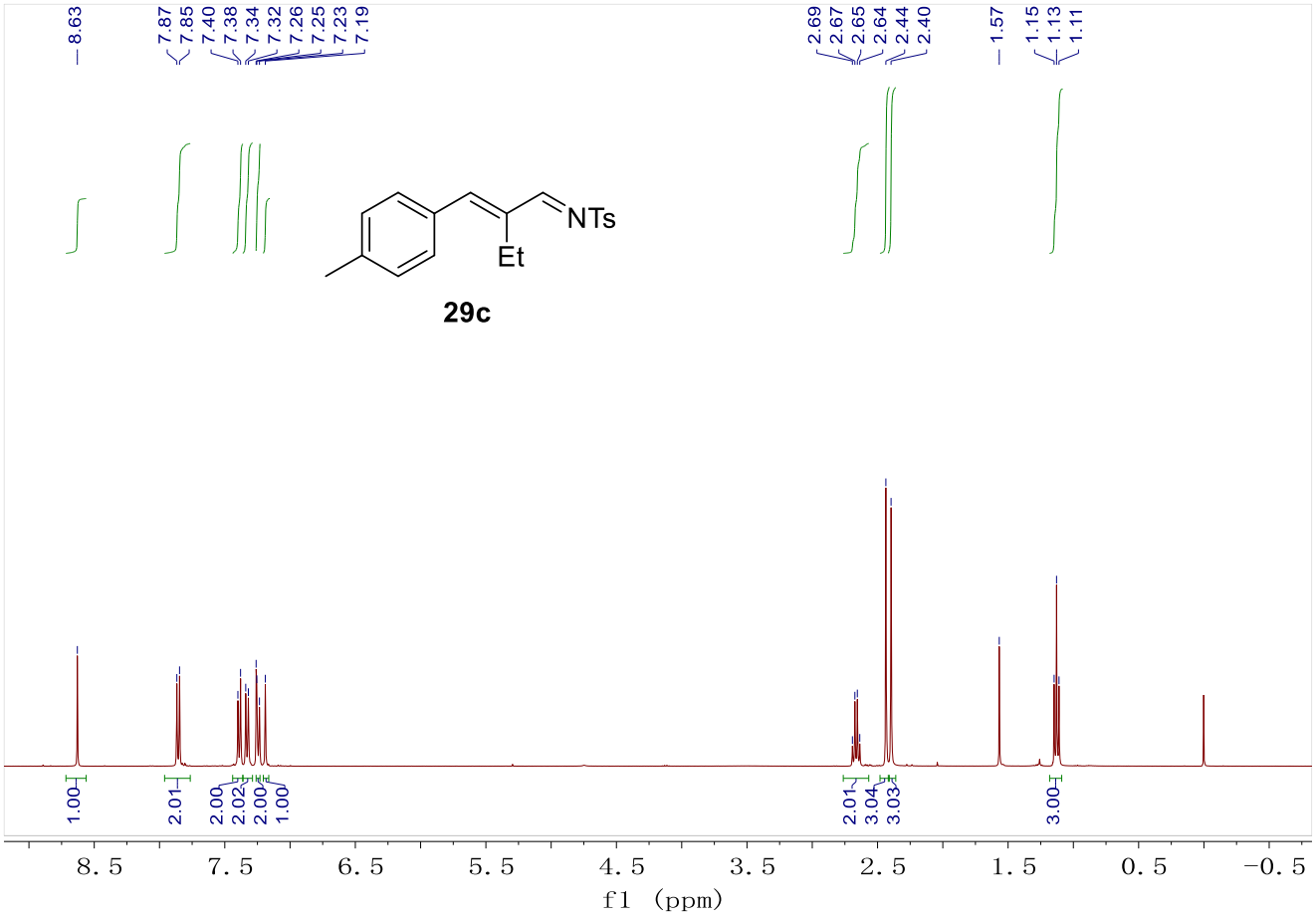
f1 (ppm)


Et
iPr
H
H
H
O
O
NTs
Ph
28c


Et
iPr
H
H
H
O
O
NTs
Ph
28c
f1 (ppm)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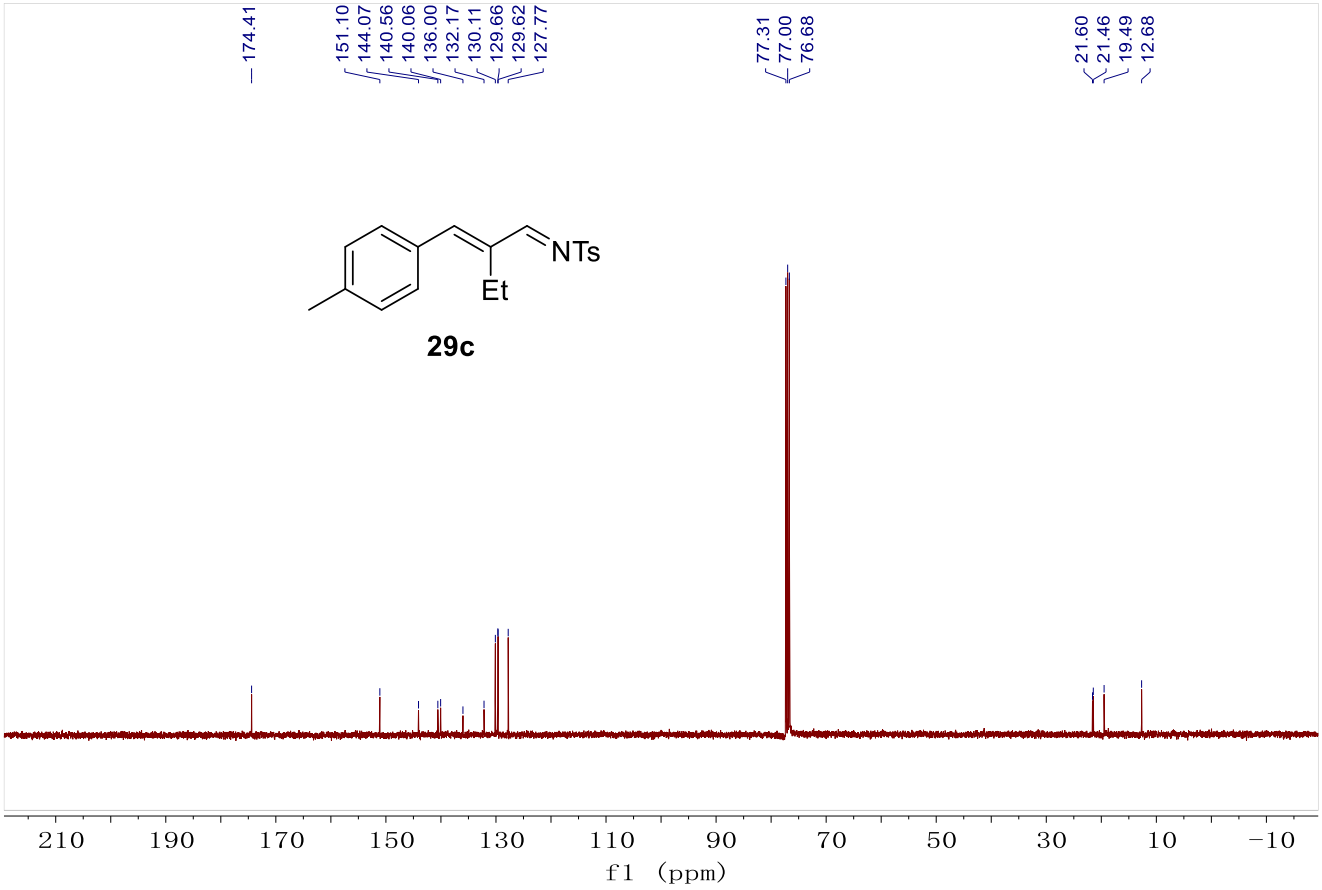
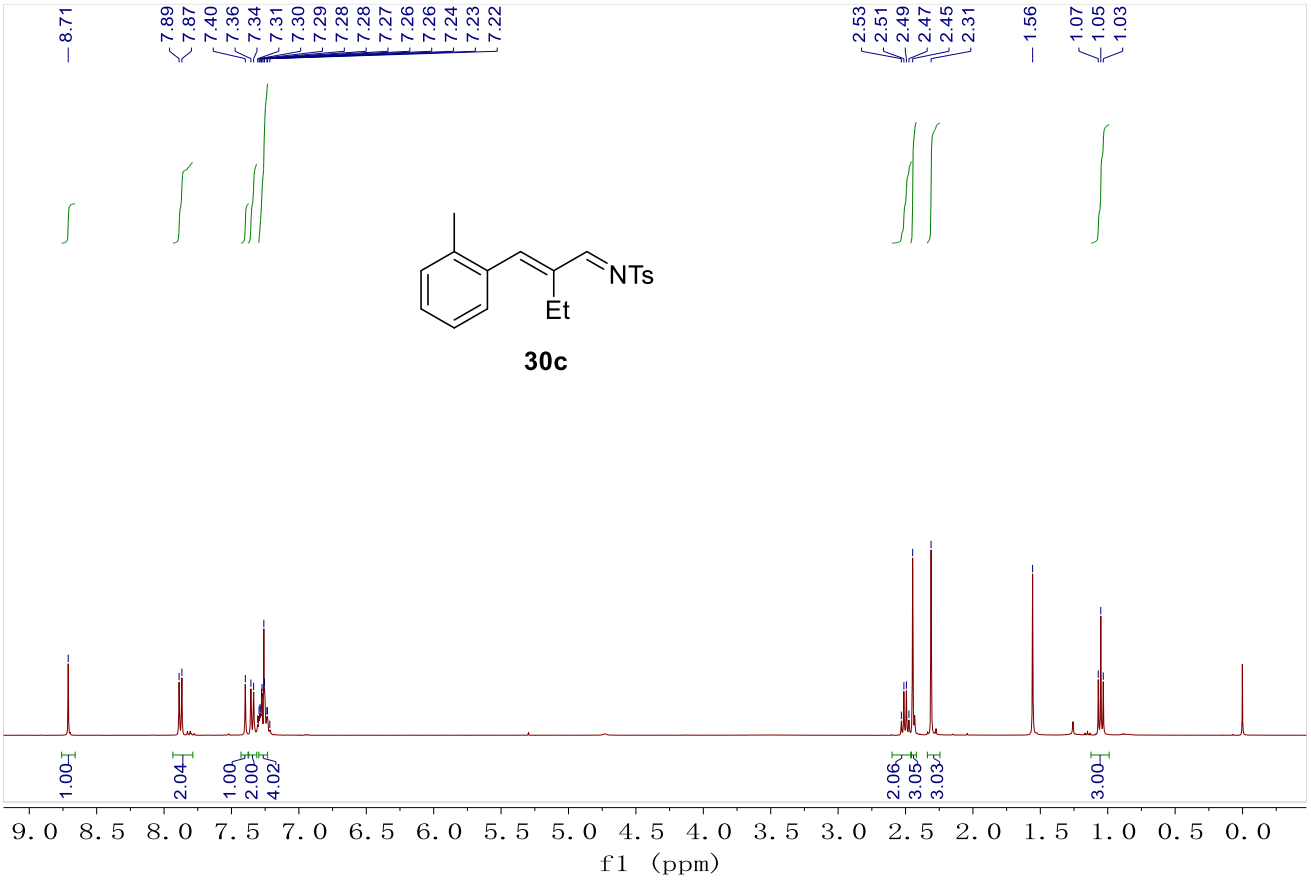
7.38
7.34
7.32
7.26
7.25
7.23
7.19
2.69
2.67
2.65
2.64
2.44
2.40
1.57
1.15
1.13
1.11
NTs
Et
1.00
2.01
2.00
2.02
2.00
1.00
2.01
3.04
3.03
3.00
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)

29c


174.41
151.10
144.07
140.56
140.06
136.00
132.17
130.11
129.66
129.62
127.77
77.31
77.00
76.68
21.60
21.46
19.49
12.68
NTs
Et
210
190
170
150
130
110
90
70
50
30
10
−10
f1 (ppm)

29c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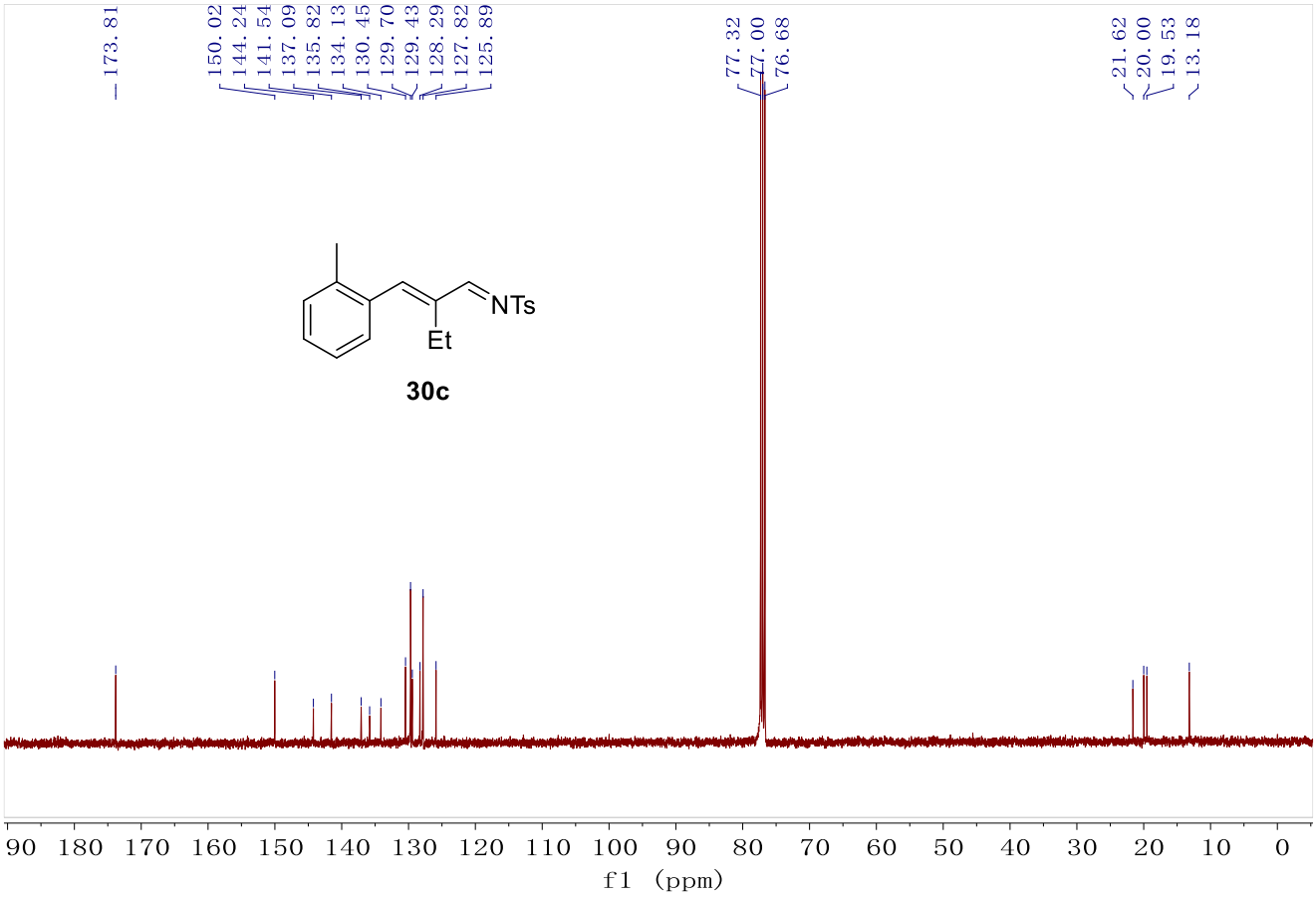
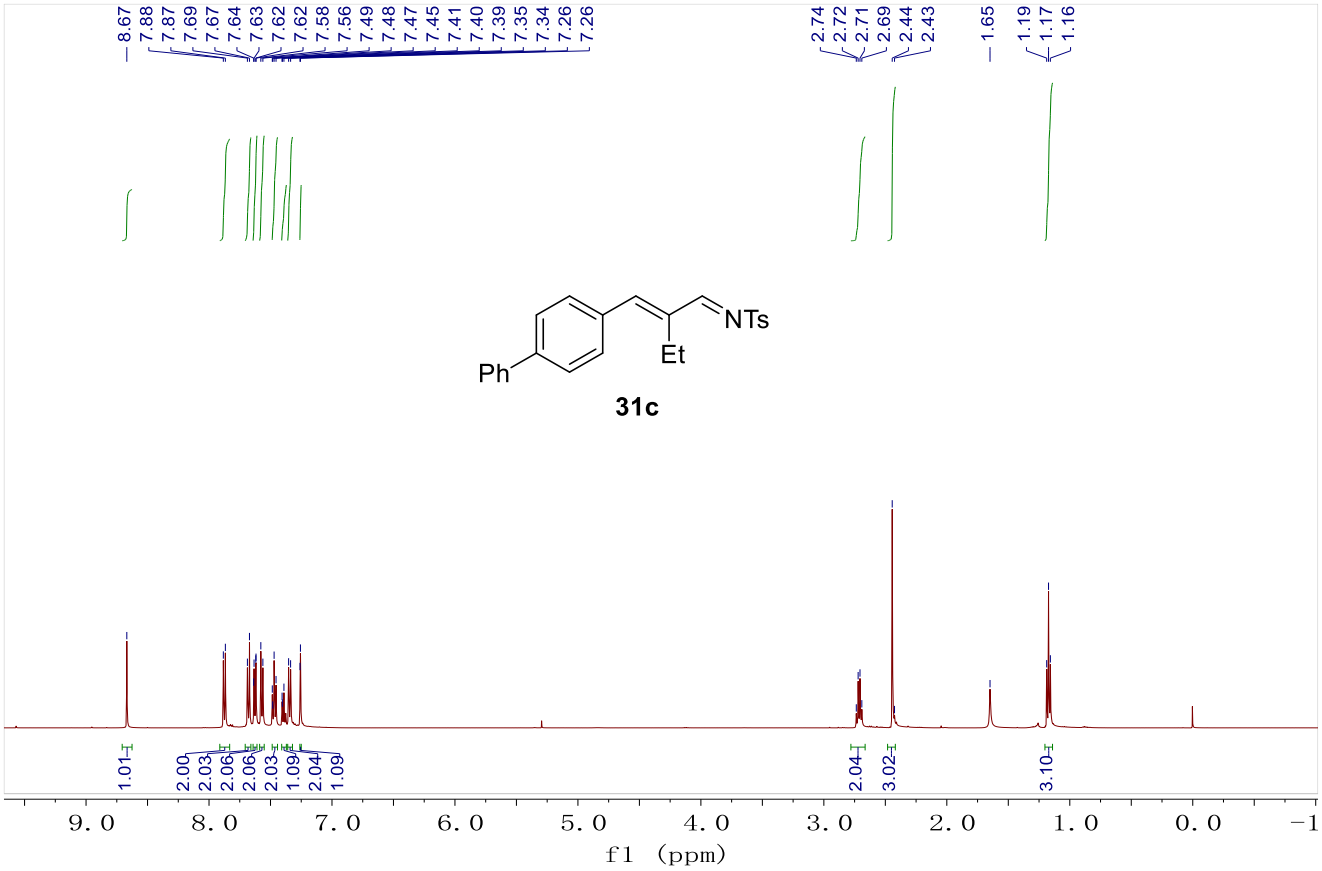
7.28
7.28
7.27
7.26
7.26
7.24
7.23
7.22
2.53
2.51
2.49
2.47
2.45
2.31
1.56
1.07
1.05
1.03
NTs
Et
30c
1.00
2.04
1.00
2.00
4.02
2.06
3.05
3.03
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


173.81
150.02
144.24
141.54
137.09
135.82
134.13
130.45
129.70
129.43
128.29
127.82
125.89
77.32
77.00
76.68
21.62
20.00
19.53
13.18
NTs
Et
30c
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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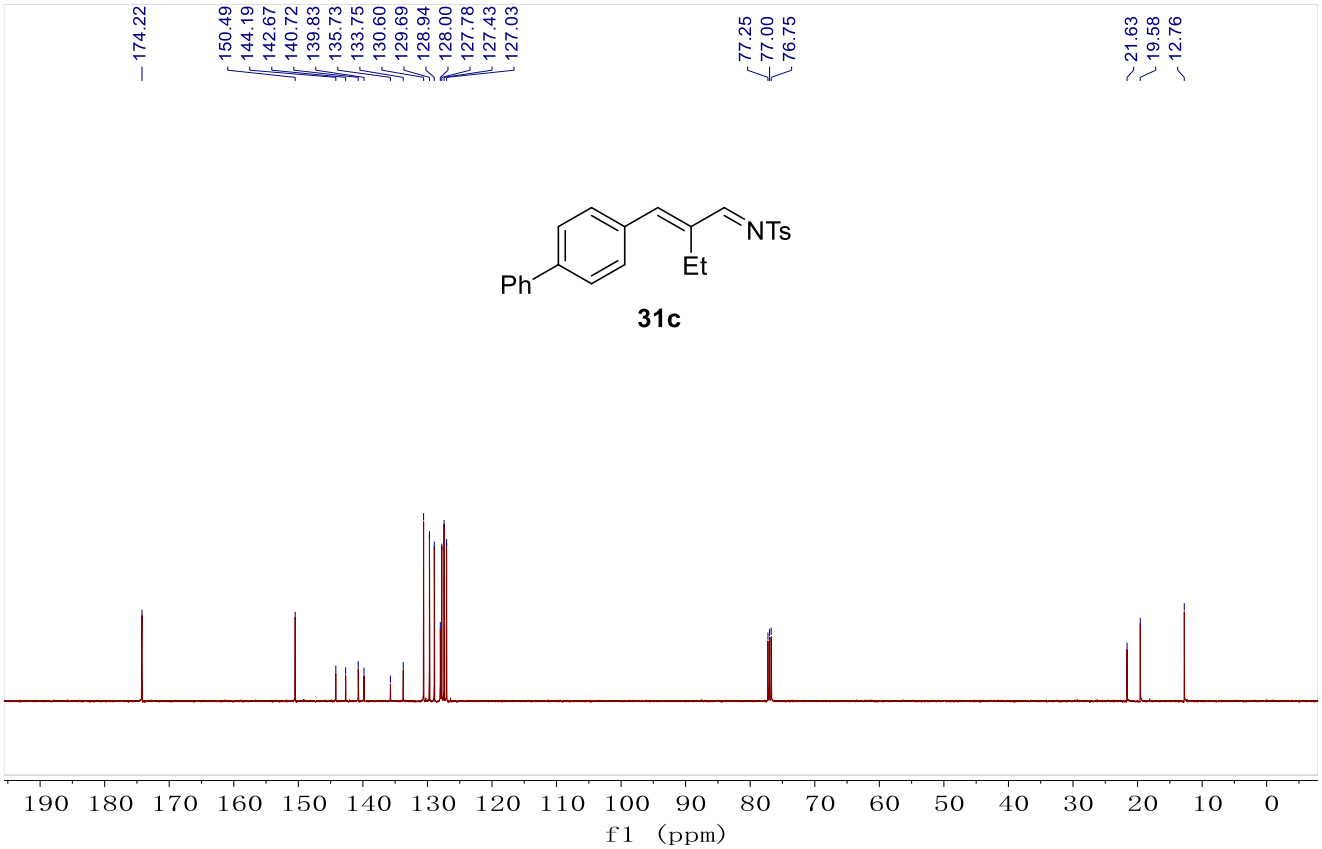
7.88
7.87
7.69
7.67
7.64
7.63
7.62
7.62
7.58
7.56
7.49
7.48
7.47
7.45
7.41
7.40
7.39
7.35
7.34
7.26
7.26
2.74
2.72
2.71
2.69
2.44
2.43
1.65
1.19
1.17
1.16
NTs
Et
Ph
31c
1.01
2.00
2.03
2.06
2.06
2.03
1.09
2.04
1.09
2.04
3.02
3.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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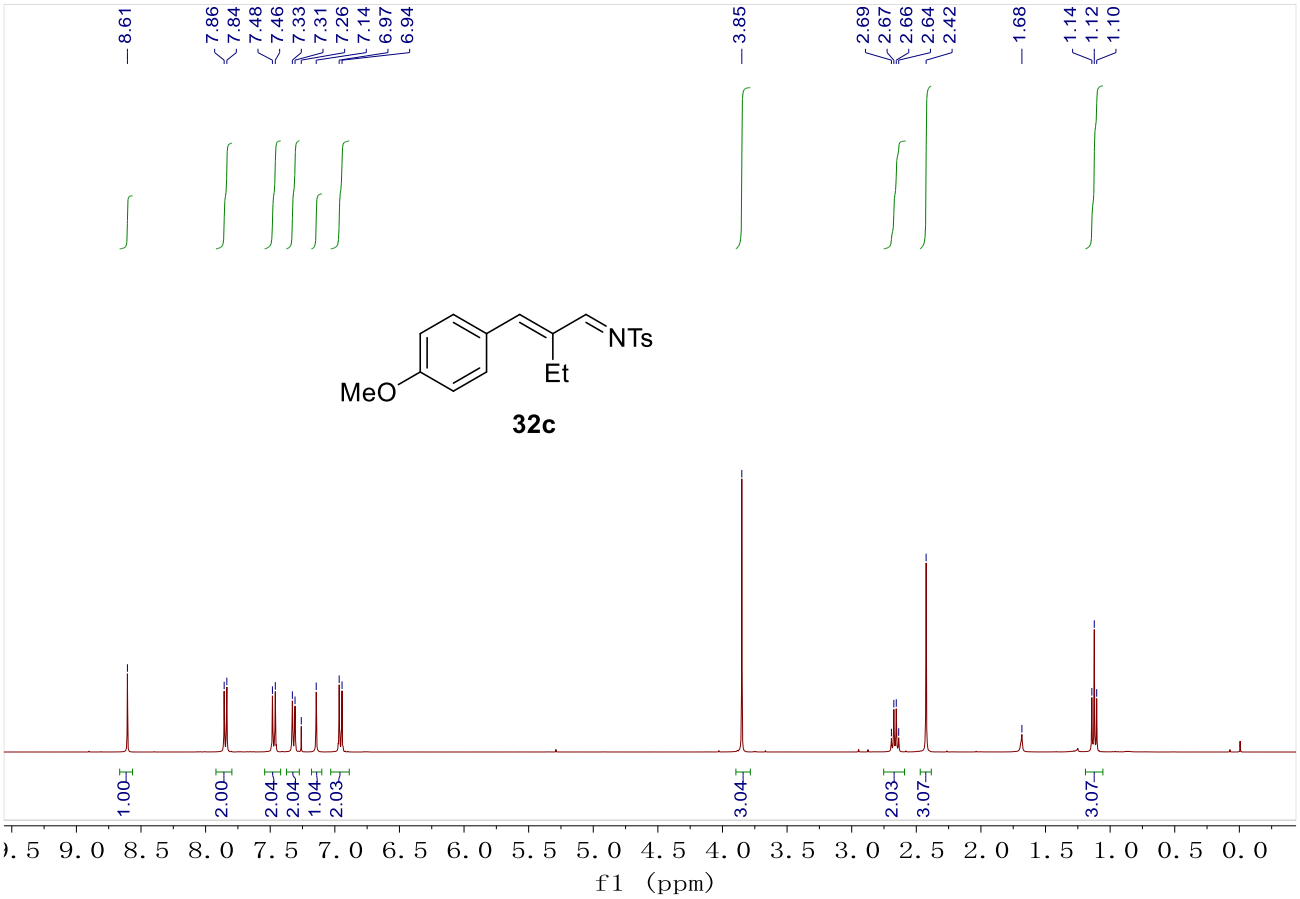
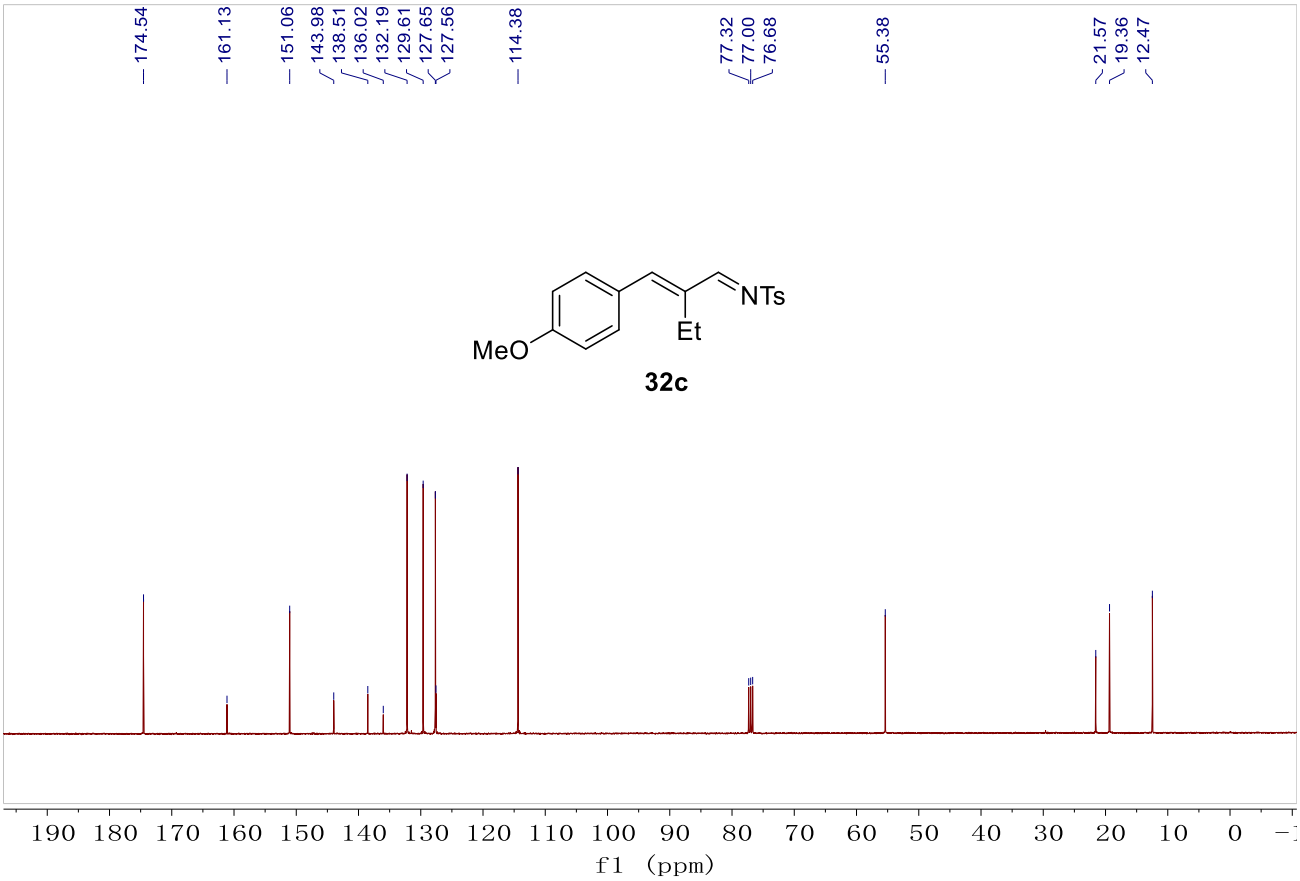
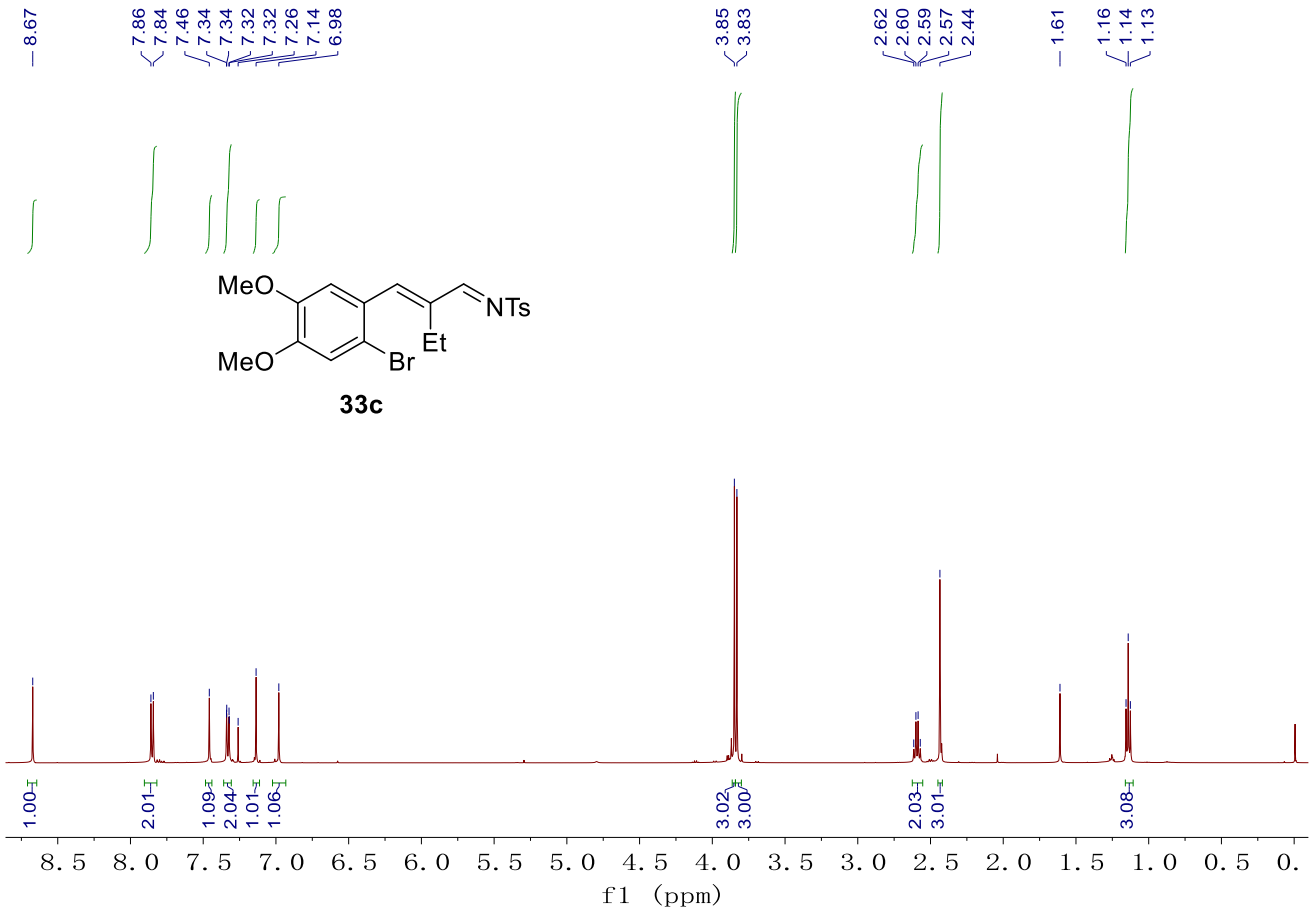
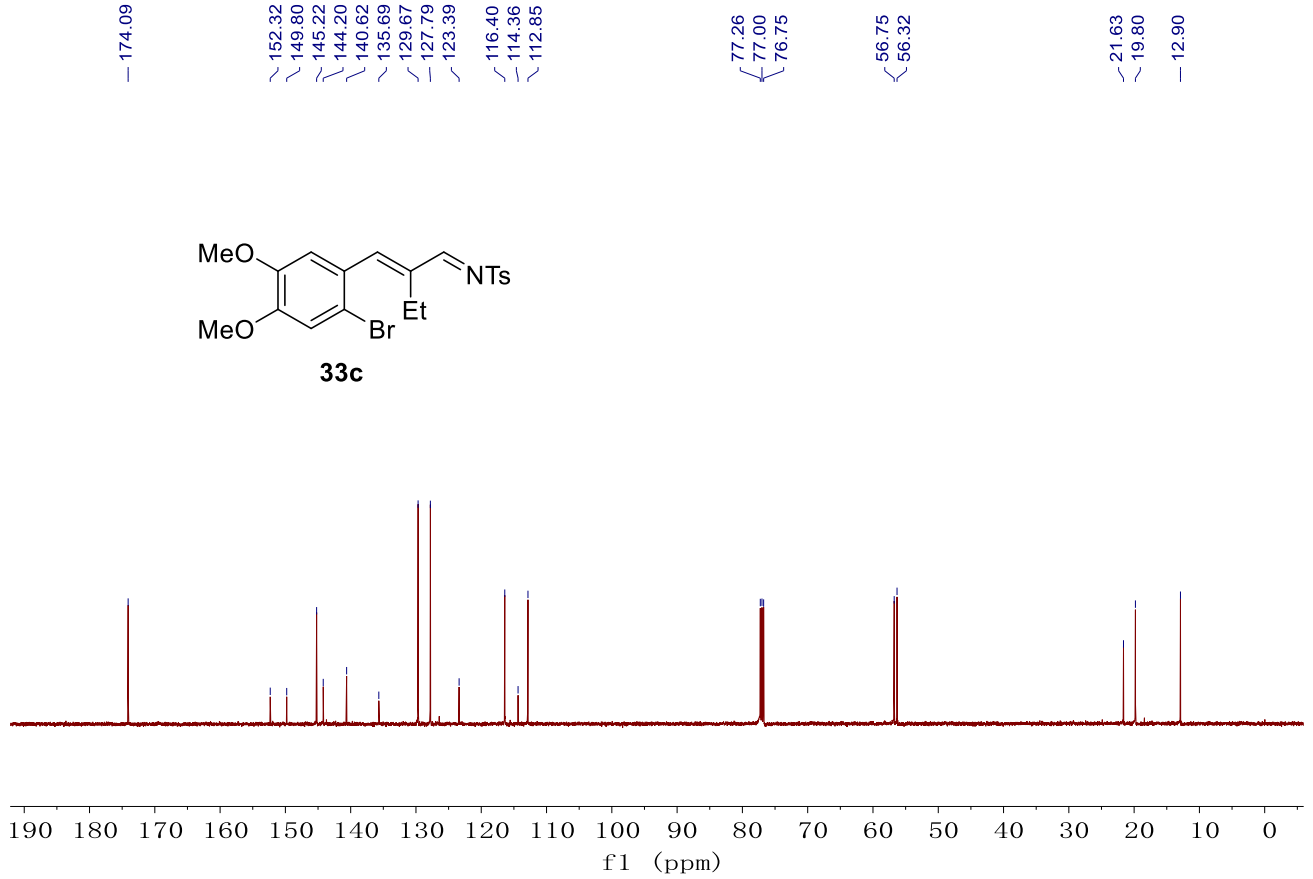
150.49
144.19
142.67
140.72
139.83
135.73
133.75
130.60
129.69
128.94
128.00
127.78
127.43
127.03
77.25
77.00
76.75
21.63
19.58
12.76
NTs
Et
Ph
31c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.61
7.86
7.84
7.48
7.46
7.33
7.31
7.26
7.14
6.97
6.94
3.85
2.69
2.67
2.66
2.64
2.42
1.68
1.14
1.12
1.10
NTs
Et
MeO
32c
1.00
2.00
2.04
2.04
1.04
2.03
3.04
2.03
3.07
3.07
f1 (ppm)


174.54
161.13
151.06
143.98
138.51
136.02
132.19
129.61
127.65
127.56
114.38
77.32
77.00
76.68
55.38
21.57
19.36
12.47
NTs
Et
MeO
32c
f1 (ppm)


8.67
7.86
7.84
7.46
7.34
7.34
7.32
7.32
7.26
7.14
6.98
3.85
3.83
2.62
2.60
2.59
2.57
2.44
1.61
1.16
1.14
1.13
MeO
MeO
Br
Et
NTs
1.00
2.01
1.09
2.04
1.01
1.06
3.02
3.00
2.03
3.01
3.08
f1 (ppm)

33c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152.32
149.80
145.22
144.20
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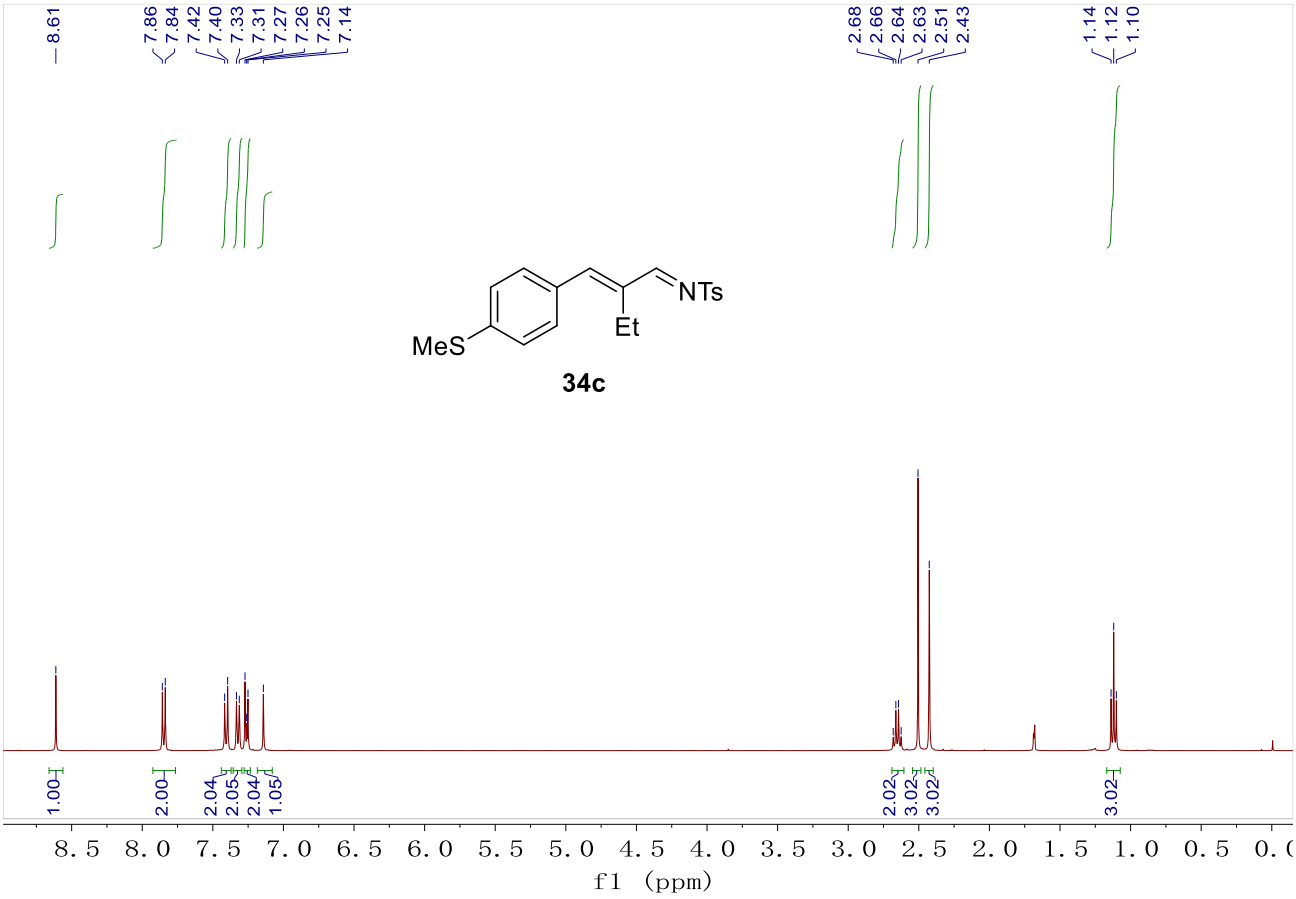
135.69
129.67
127.79
123.39
116.40
114.36
112.85
77.26
77.00
76.75
56.75
56.32
21.63
19.80
12.90
MeO
MeO
Br
Et
NTs
f1 (ppm)

33c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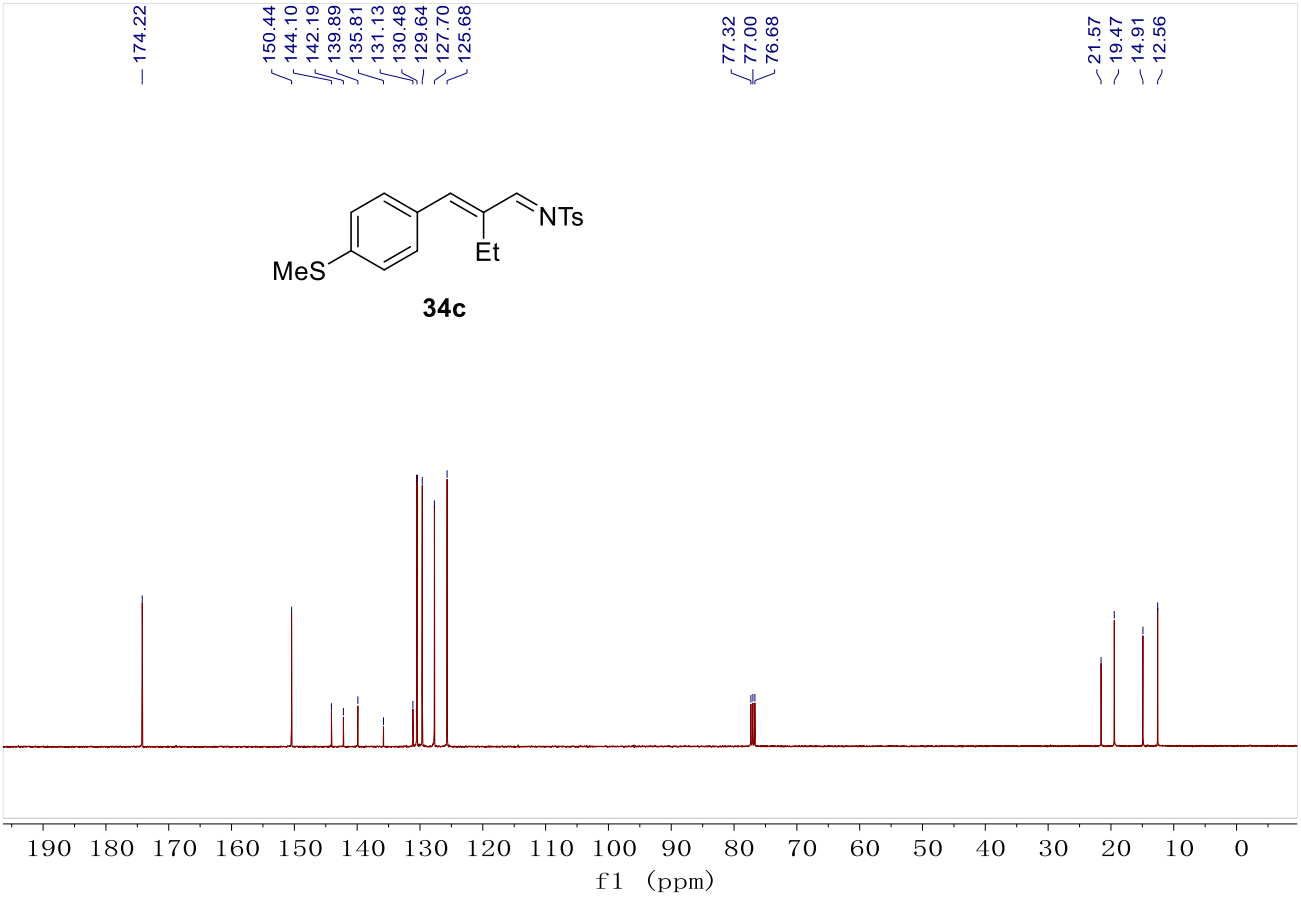
7.86
7.84
7.42
7.40
7.33
7.31
7.27
7.26
7.25
7.14
2.68
2.66
2.64
2.63
2.51
2.43
1.14
1.12
1.10
NTs
Et
MeS
34c
1.00
2.00
2.04
2.05
2.04
1.05
2.02
3.02
3.02
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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150.44
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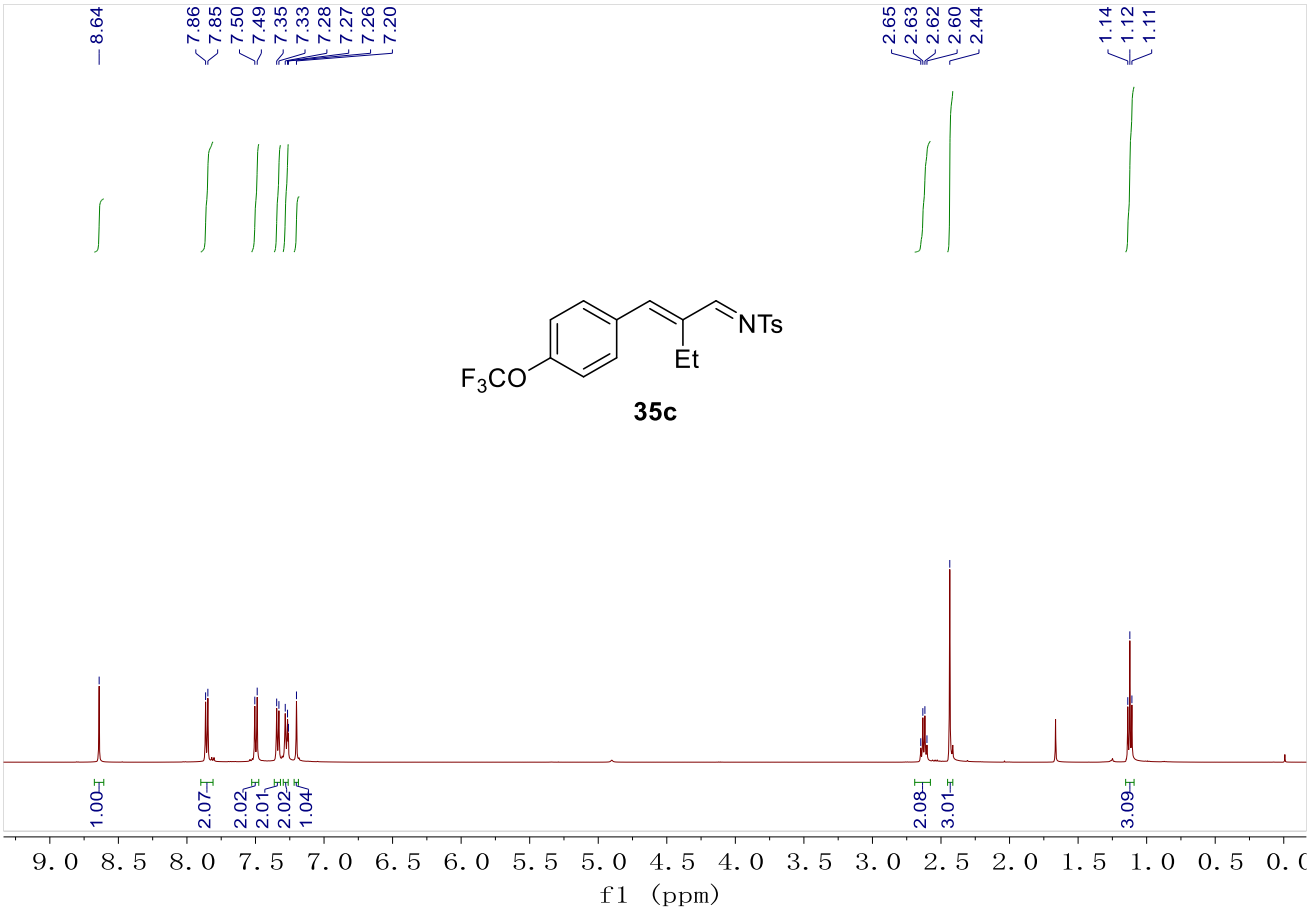
142.19
139.89
135.81
131.13
130.48
129.64
127.70
125.68
77.32
77.00
76.68
21.57
19.47
14.91
12.56
NTs
Et
MeS
34c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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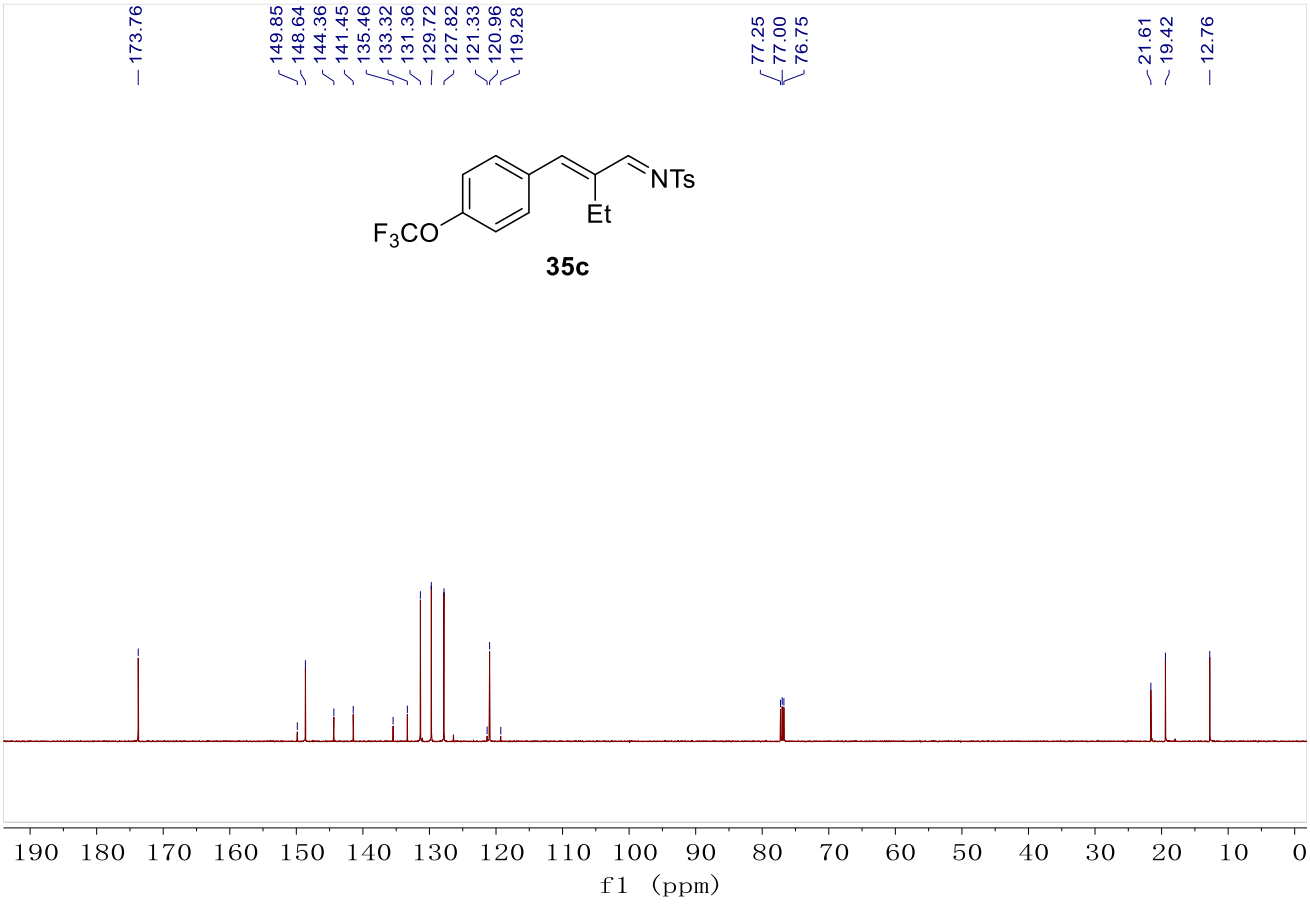
7.86
7.85
7.50
7.49
7.35
7.33
7.28
7.27
7.26
7.20
2.65
2.63
2.62
2.60
2.44
1.14
1.12
1.11
NTs
Et
F3CO
35c
1.00
2.07
2.02
2.01
2.02
1.04
2.08
3.01
3.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.36
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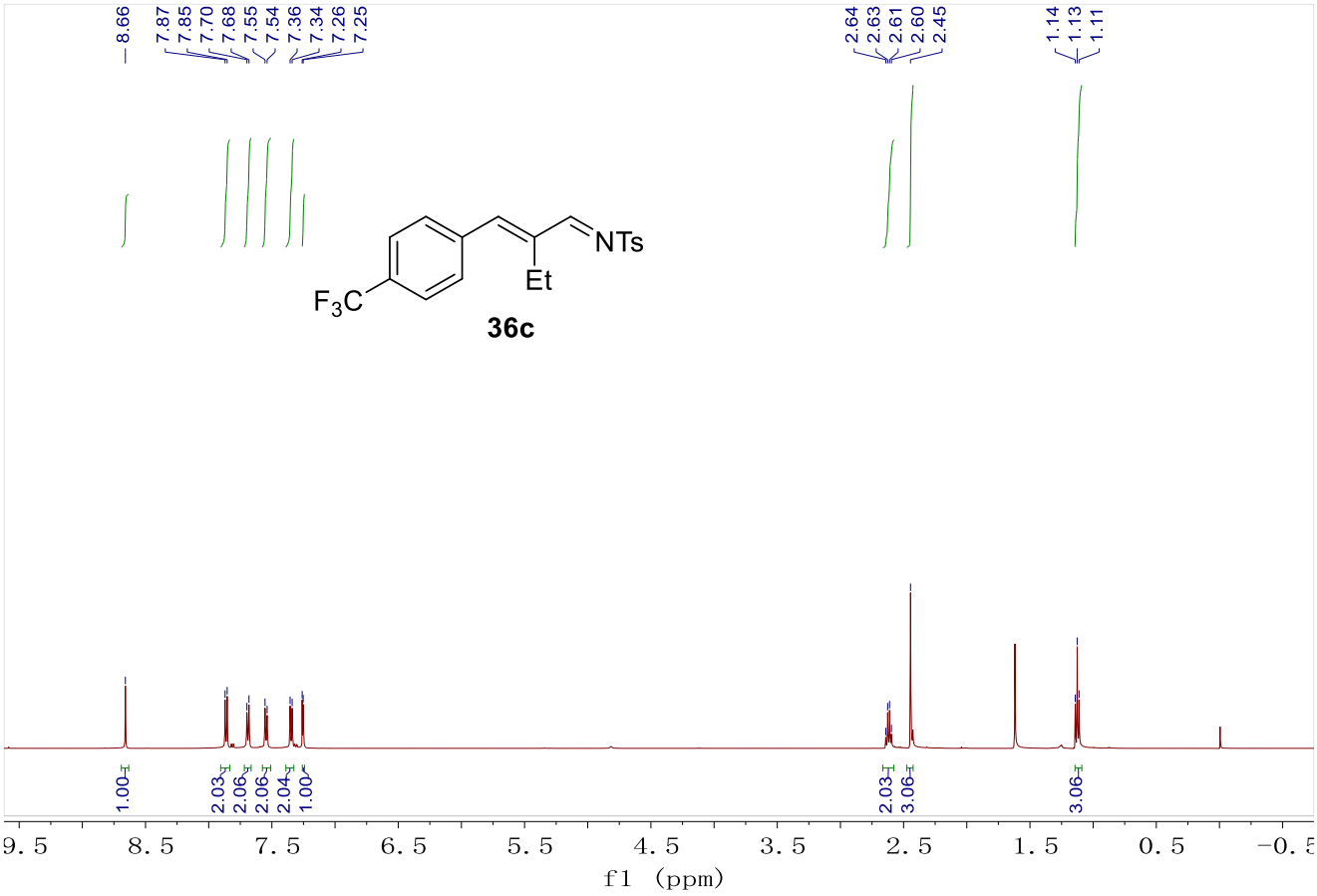
127.82
121.33
120.96
119.28
77.25
77.00
76.75
21.61
19.42
12.76
NTs
Et
F3CO
35c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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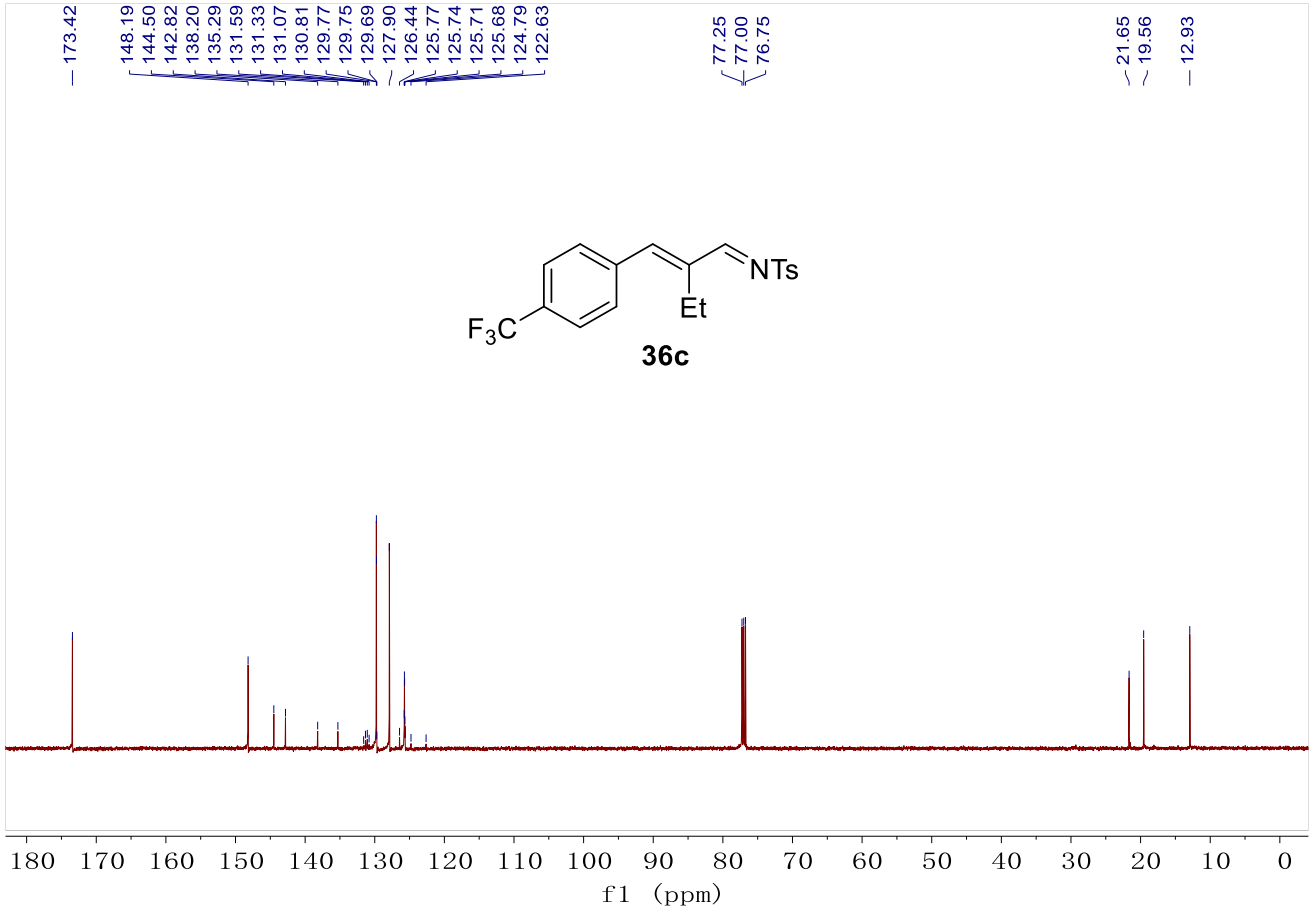
7.36
7.34
7.26
7.25
2.64
2.63
2.61
2.60
2.45
1.14
1.13
1.11
NTs
Et
F3C
36c
1.00
2.03
2.06
2.06
2.04
1.00
2.03
3.06
3.06
f1 (ppm)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142.82
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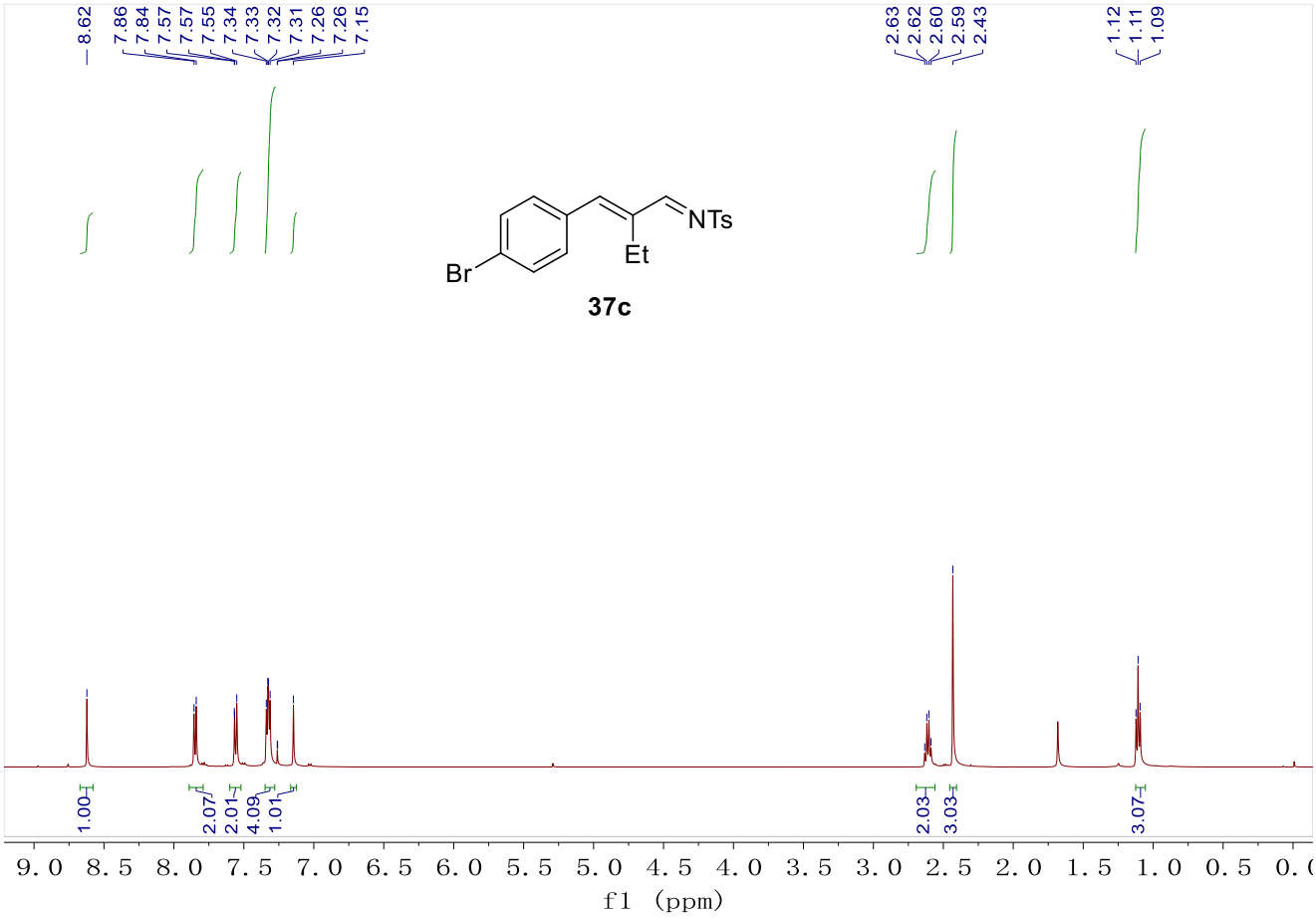
135.29
131.59
131.33
131.07
130.81
129.77
129.75
129.69
127.90
126.44
125.77
125.74
125.71
125.68
124.79
122.63
77.25
77.00
76.75
21.65
19.56
12.93
NTs
Et
F3C
36c
f1 (ppm)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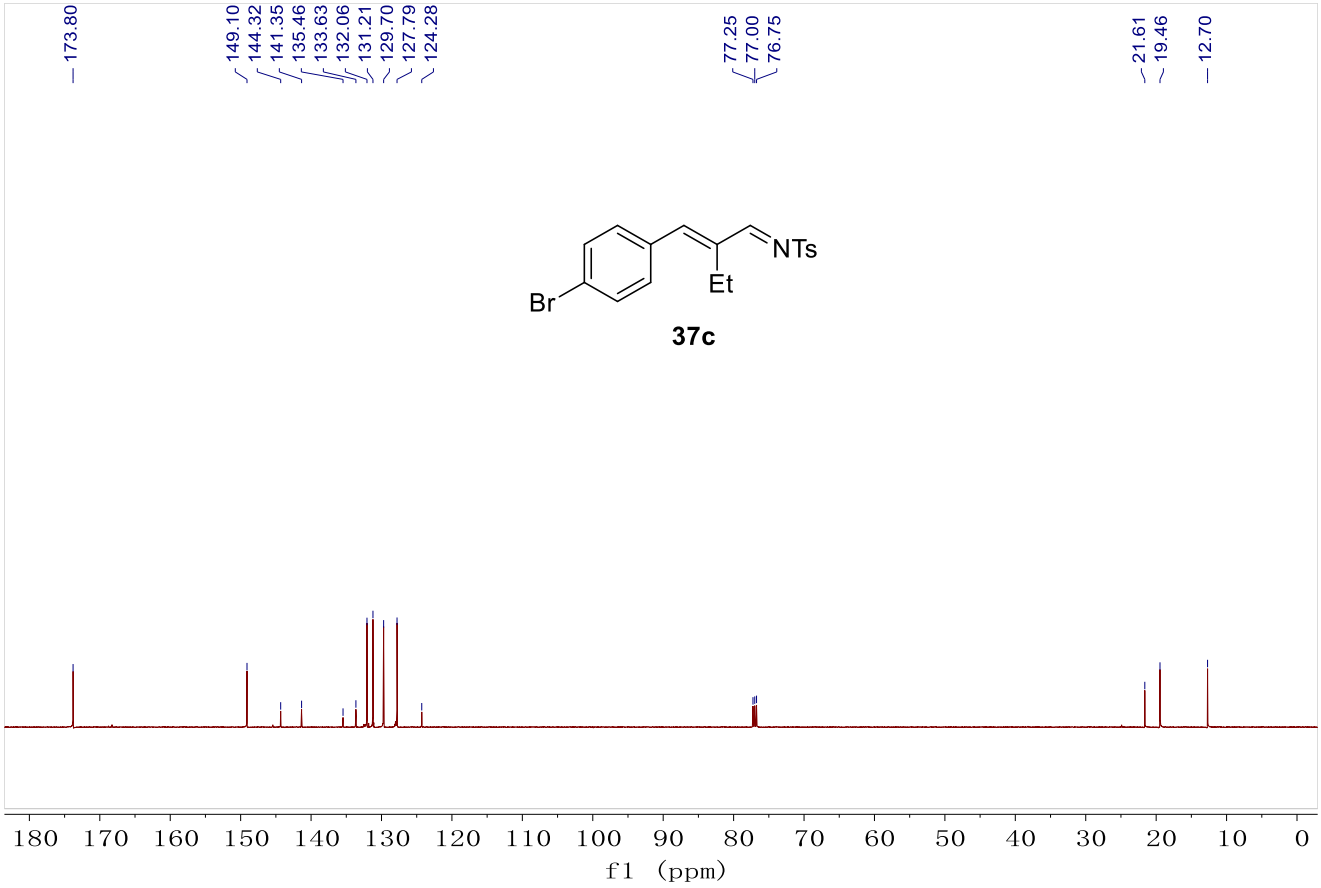
7.55
7.34
7.33
7.32
7.31
7.26
7.26
7.15
2.63
2.62
2.60
2.59
2.43
1.12
1.11
1.09
NTs
Et
Br
37c
1.00
2.07
2.01
4.09
1.01
2.03
3.03
3.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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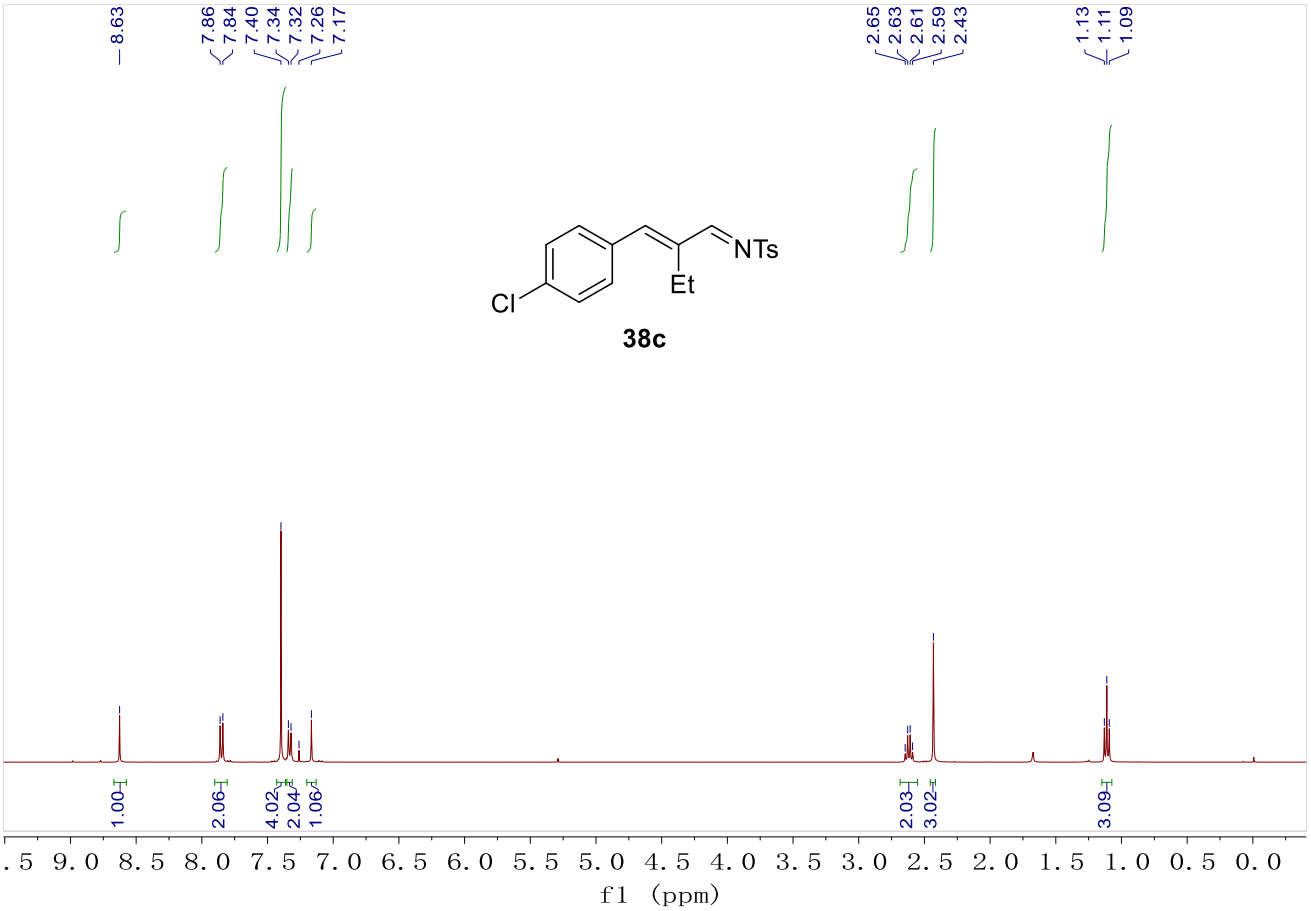
127.79
124.28
77.25
77.00
76.75
21.61
19.46
12.70
NTs
Et
Br
37c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.34
7.32
7.26
7.17
2.65
2.63
2.61
2.59
2.43
1.13
1.11
1.09
NTs
Et
Cl
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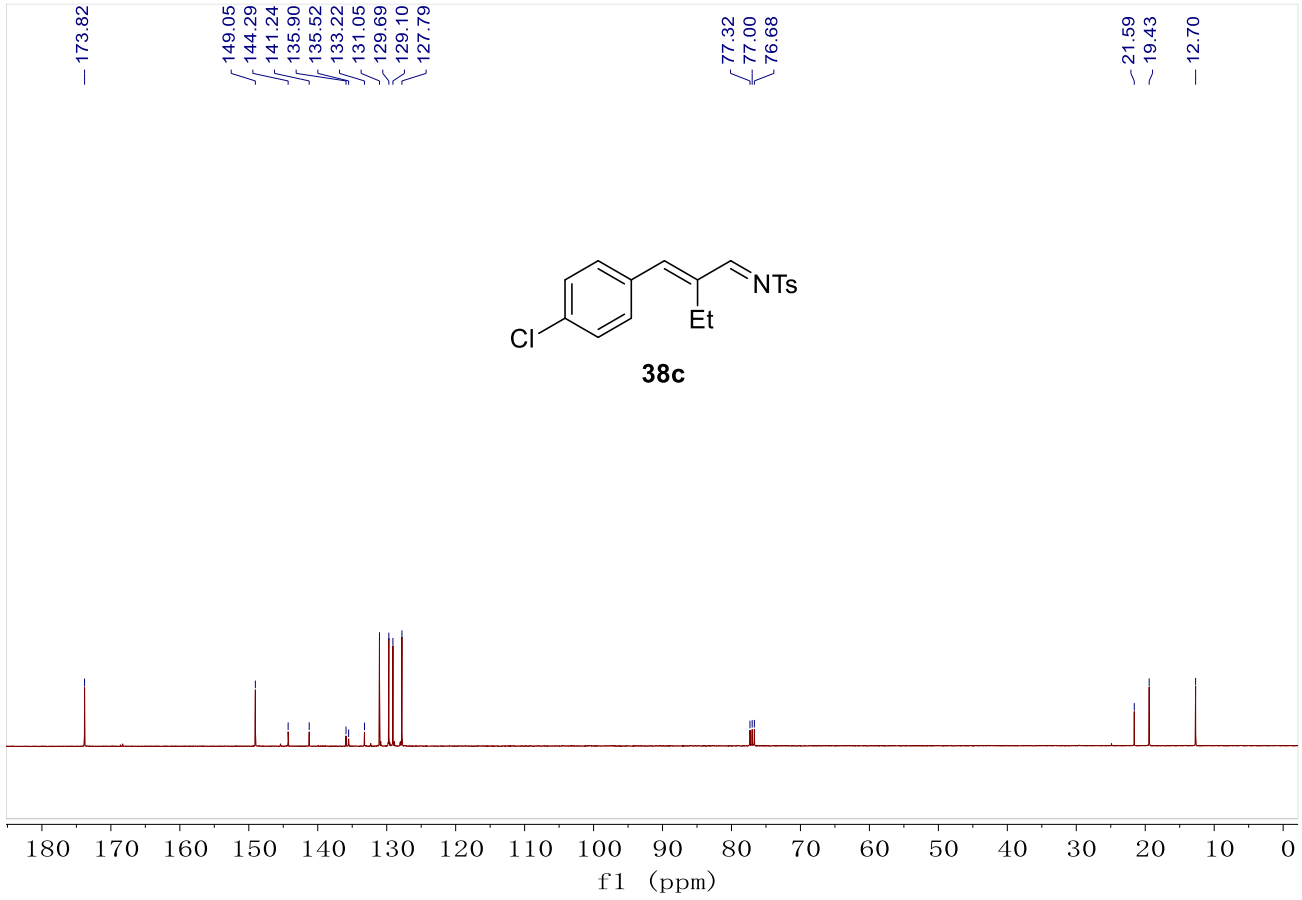
1.00
2.06
4.02
2.04
1.06
2.03
3.02
3.09
f1 (ppm)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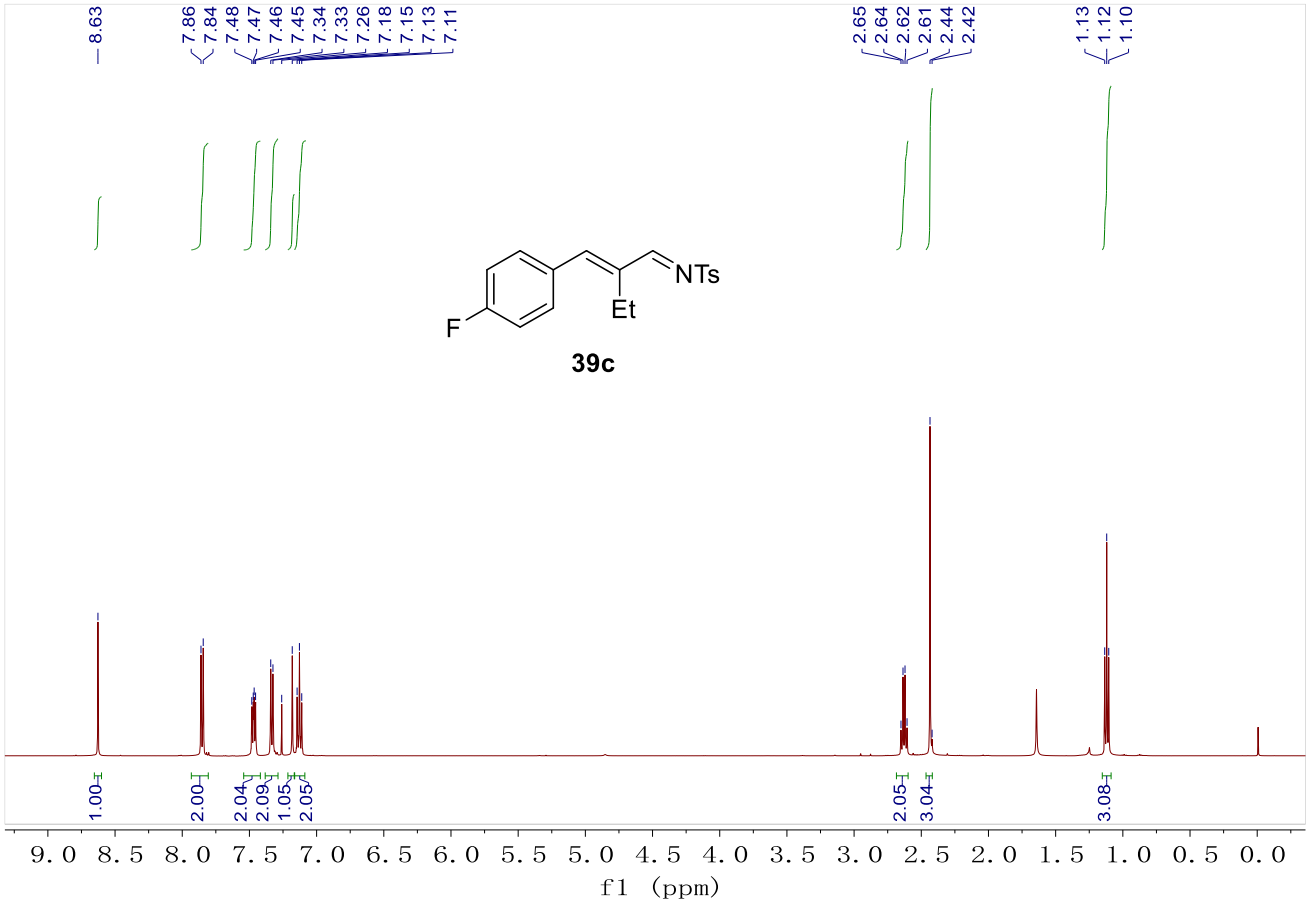
141.24
135.90
135.52
133.22
131.05
129.69
129.10
127.79
77.32
77.00
76.68
21.59
19.43
12.70
NTs
Et
Cl
38c
f1 (ppm)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7.86
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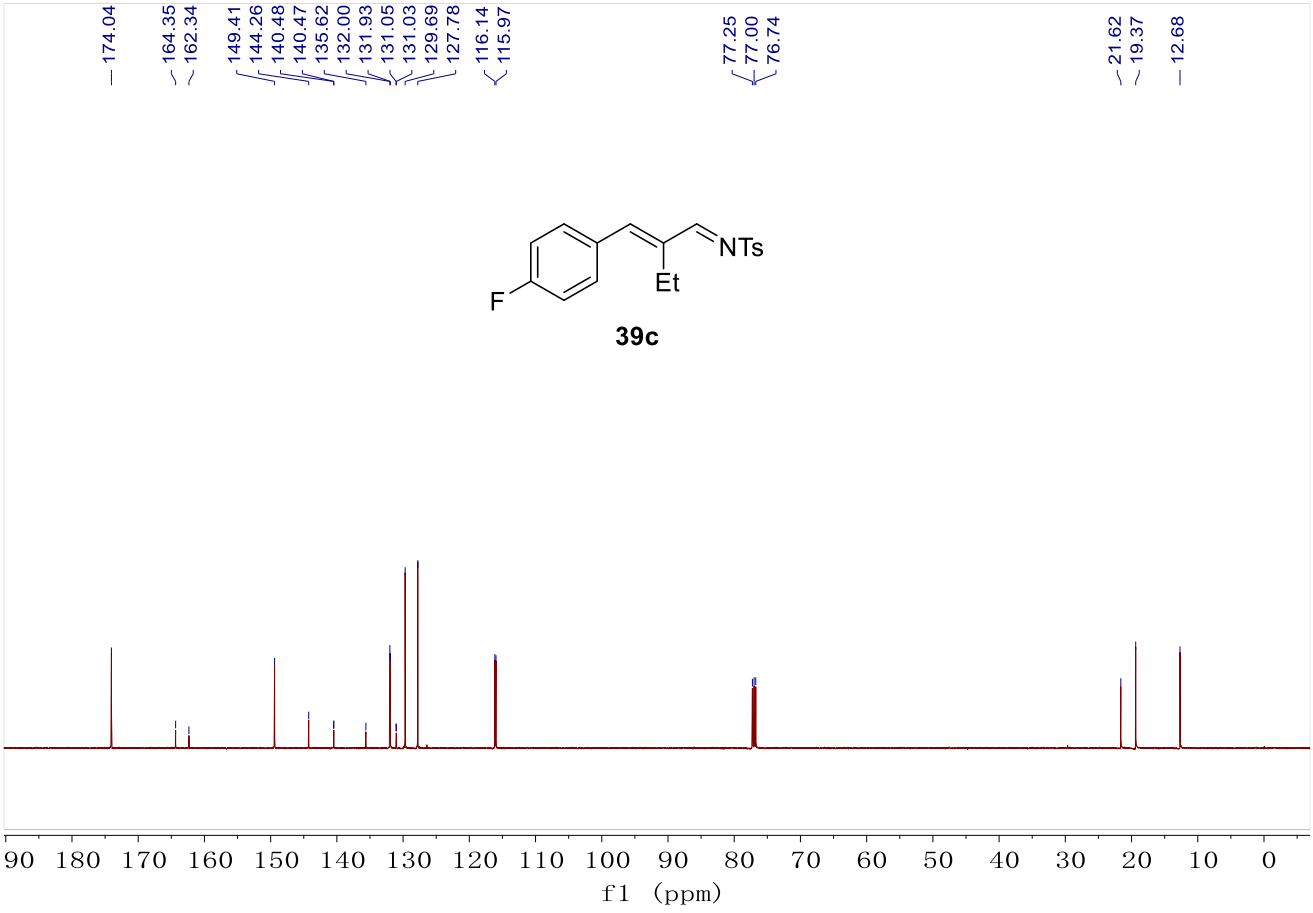
7.26
7.18
7.15
7.13
7.11
2.65
2.64
2.62
2.61
2.44
2.42
1.13
1.12
1.10
NTs
Et
F
39c
1.00
2.00
2.04
2.09
1.05
2.05
2.05
3.04
3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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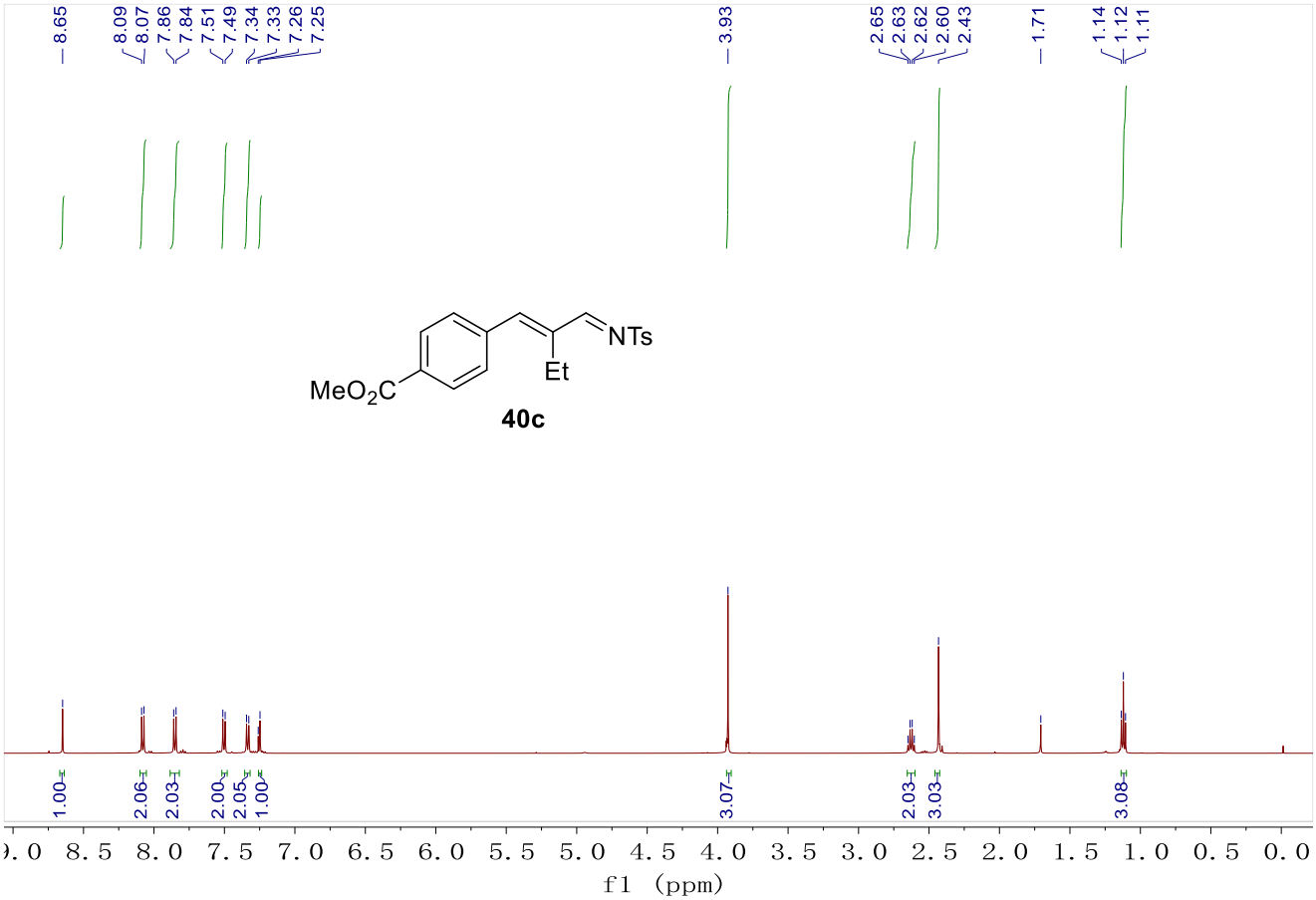
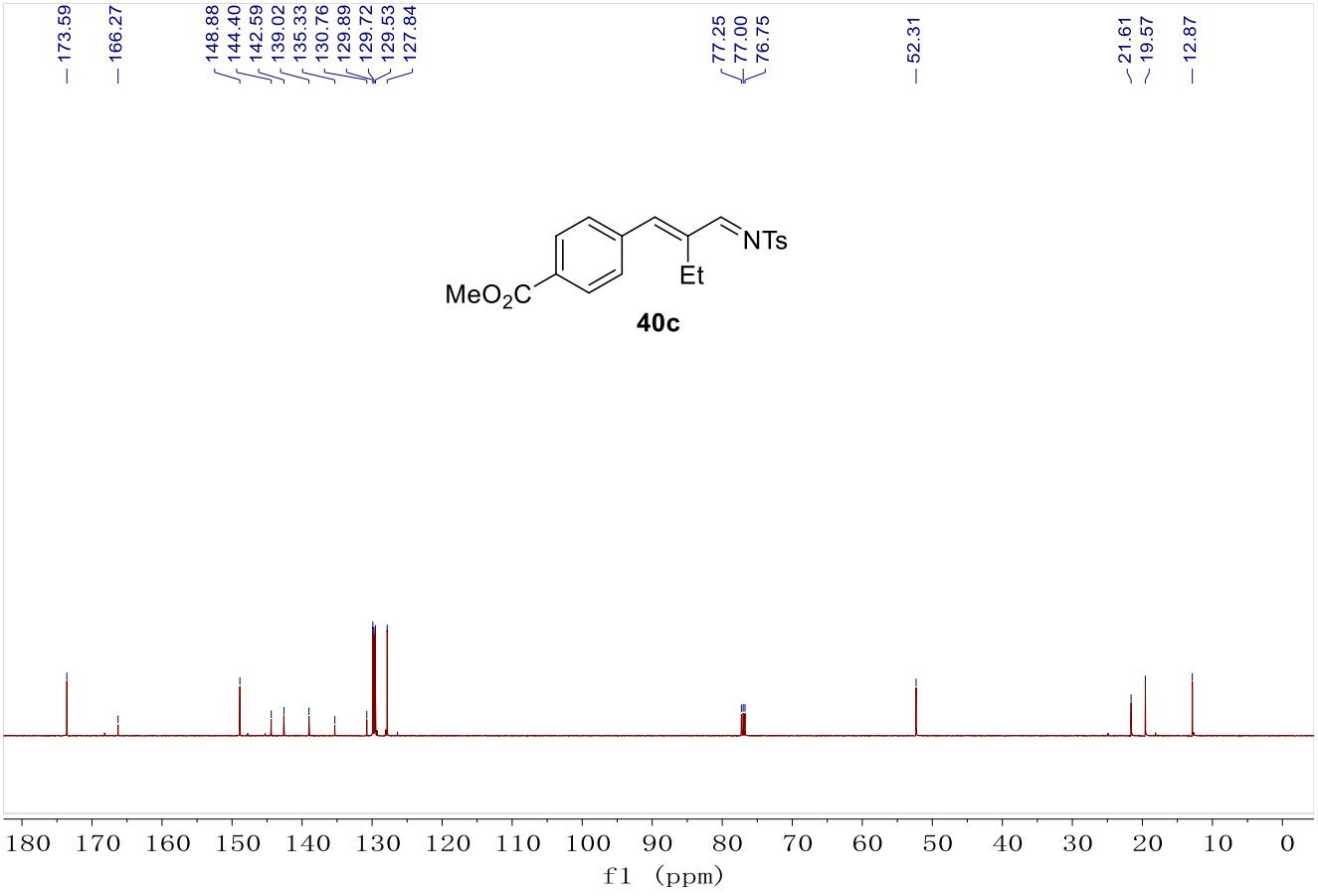
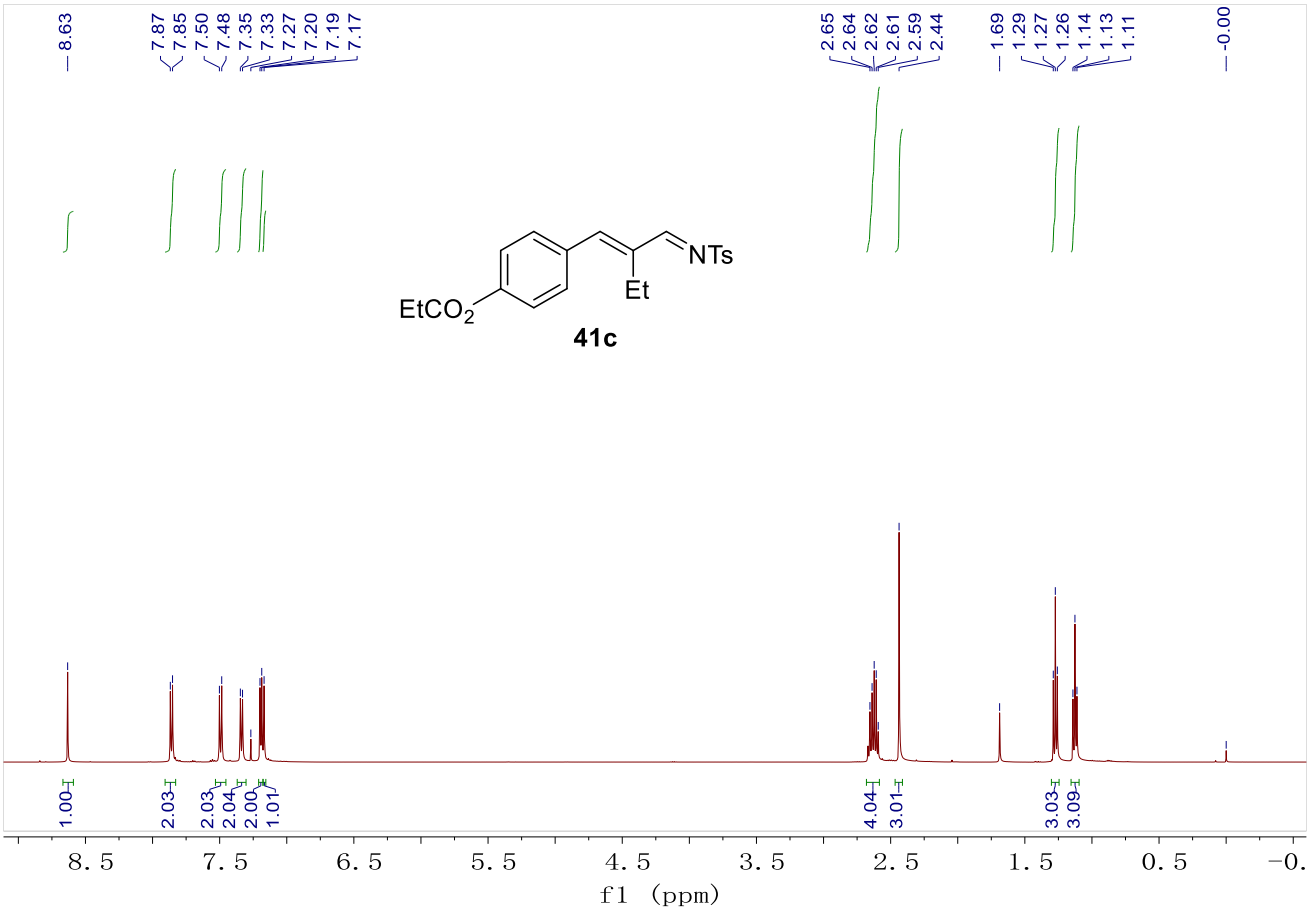
164.35
162.34
149.41
144.26
140.48
140.47
135.62
132.00
131.93
131.05
131.03
129.69
127.78
116.14
115.97
77.25
77.00
76.74
21.62
19.37
12.68
NTs
Et
F
39c
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.65
8.09
8.07
7.86
7.84
7.51
7.49
7.34
7.33
7.26
7.25
3.93
2.65
2.63
2.62
2.60
2.43
1.71
1.14
1.12
1.11
NTs
Et
MeO2C
40c
1.00
2.06
2.03
2.00
2.05
1.00
3.07
2.03
3.03
3.08
f1 (ppm)


173.59
166.27
148.88
144.40
142.59
139.02
135.33
130.76
129.89
129.72
129.53
127.84
77.25
77.00
76.75
52.31
21.61
19.57
12.87
NTs
Et
MeO2C
40c
f1 (ppm)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7.87
7.85
7.50
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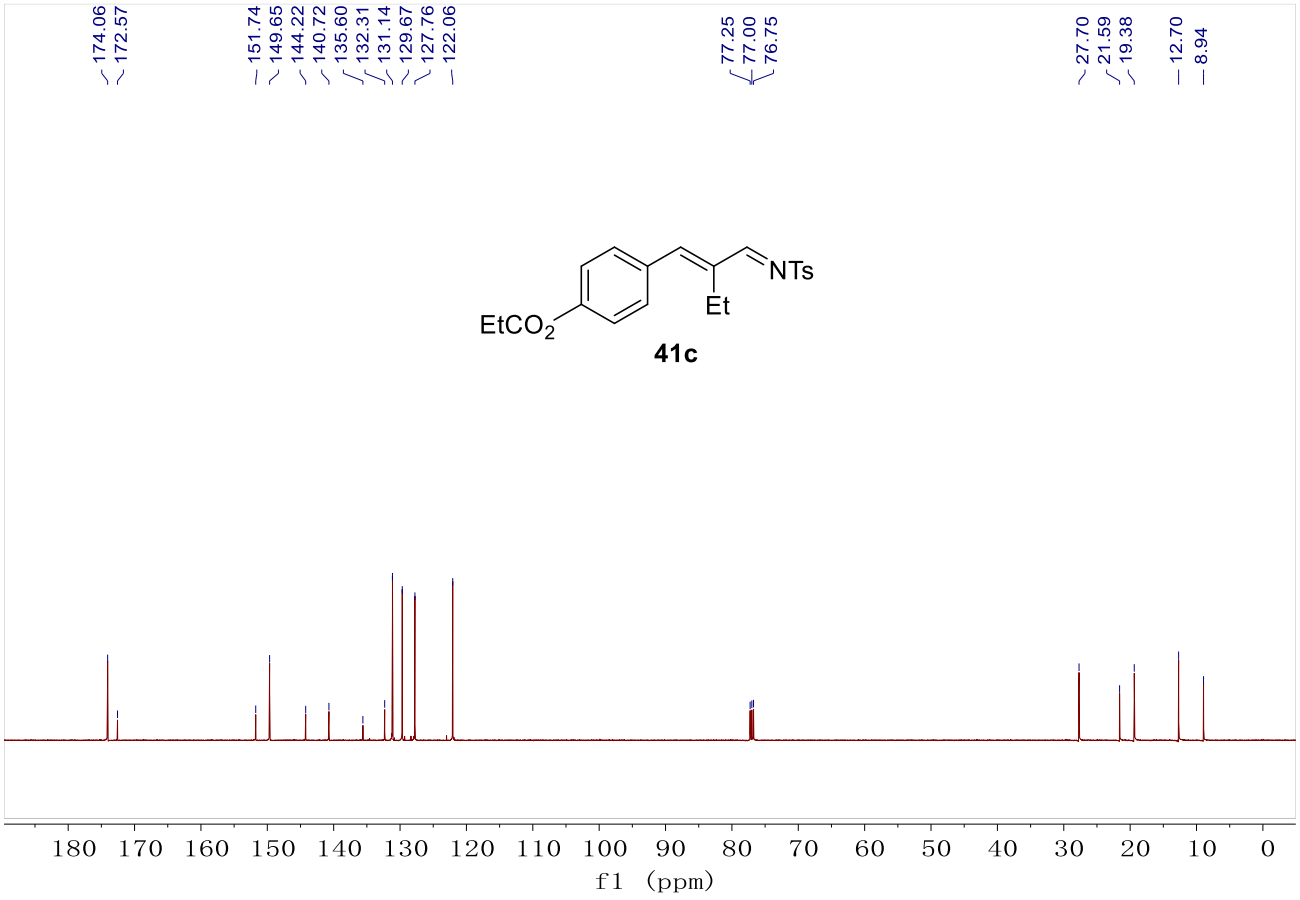
7.35
7.33
7.27
7.20
7.19
7.17
2.65
2.64
2.62
2.61
2.59
2.44
1.69
1.29
1.27
1.26
1.14
1.13
1.11
-0.00
NTs
Et
EtCO2
41c
1.00
2.03
2.03
2.04
2.00
1.01
4.04
3.01
3.03
3.09
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
f1 (ppm)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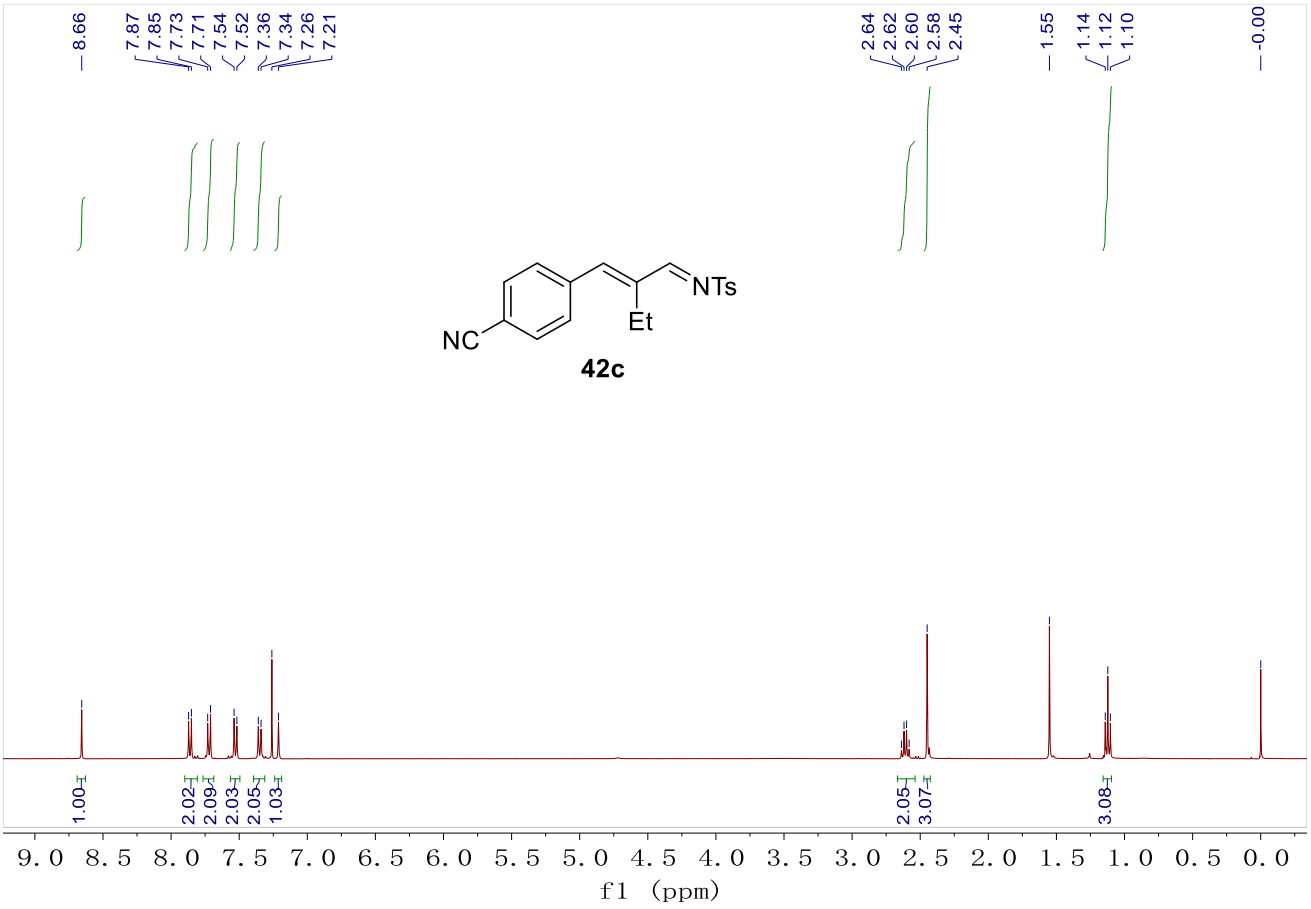
172.57
151.74
149.65
144.22
140.72
135.60
132.31
131.14
129.67
127.76
122.06
77.25
77.00
76.75
27.70
21.59
19.38
12.70
8.94
NTs
Et
EtCO2
41c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.85
7.73
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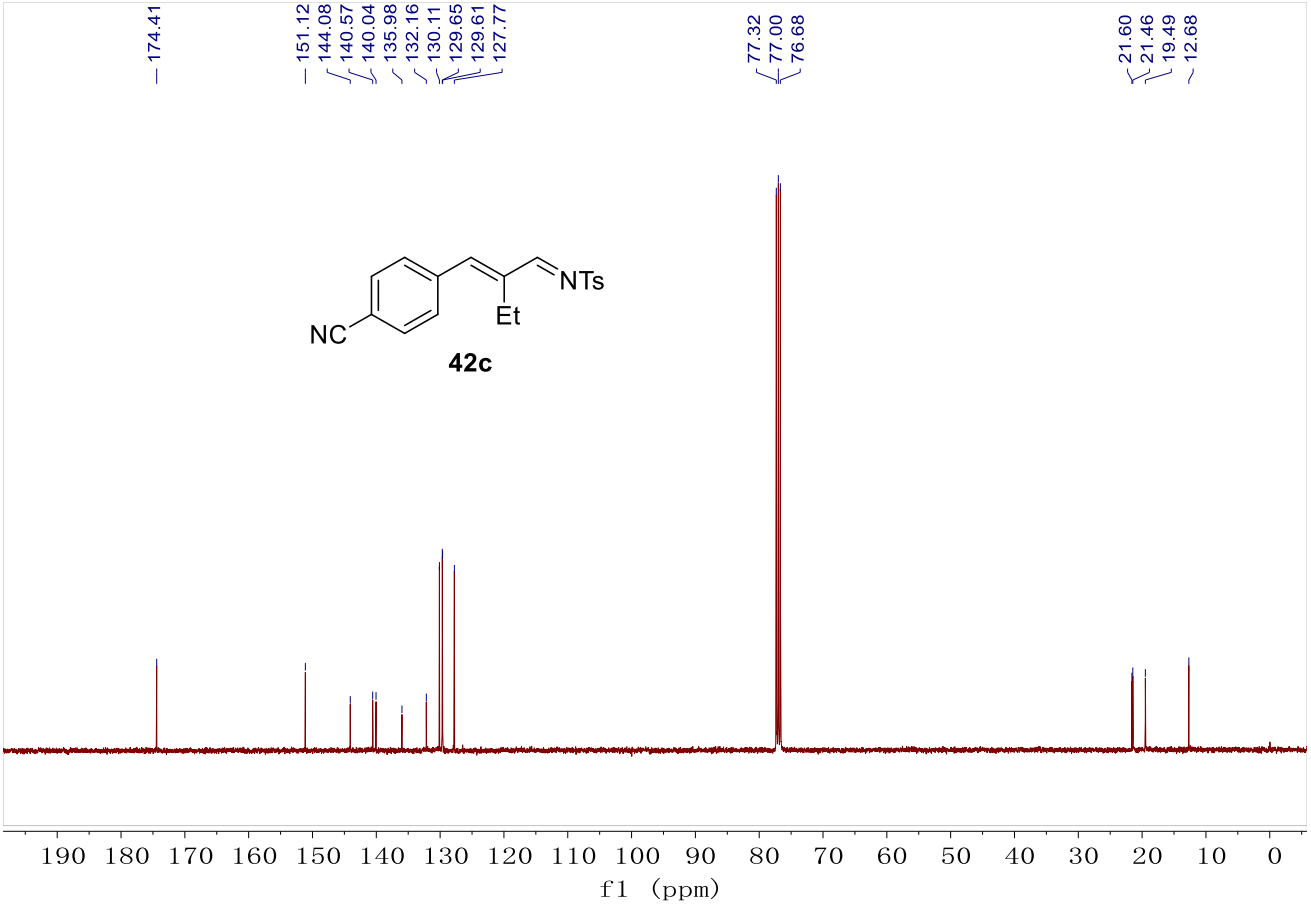
7.54
7.52
7.36
7.34
7.26
7.21
2.64
2.62
2.60
2.58
2.45
1.55
1.14
1.12
1.10
-0.00
NTs
Et
NC
42c
1.00
2.02
2.09
2.03
2.05
1.03
2.05
3.07
3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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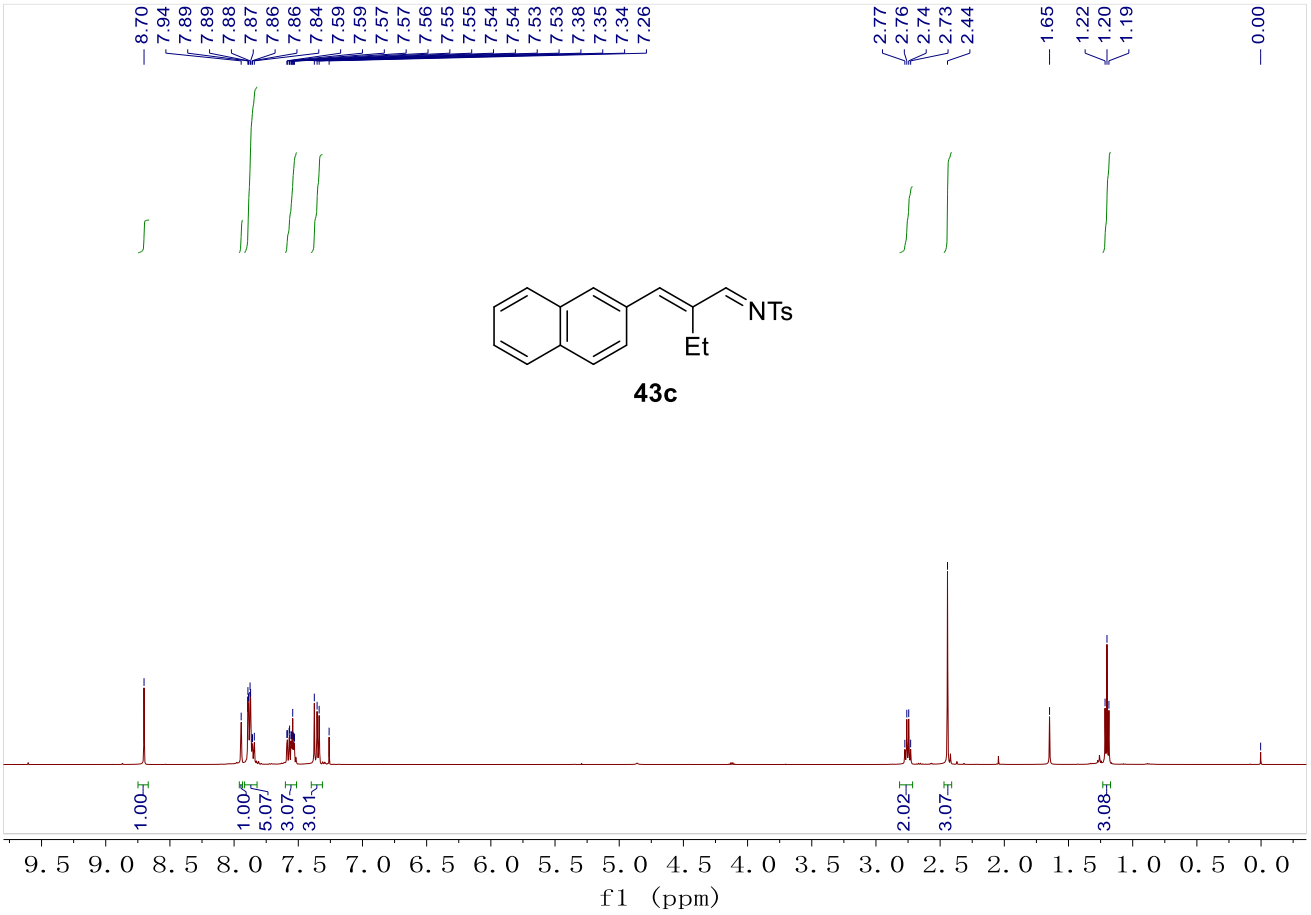
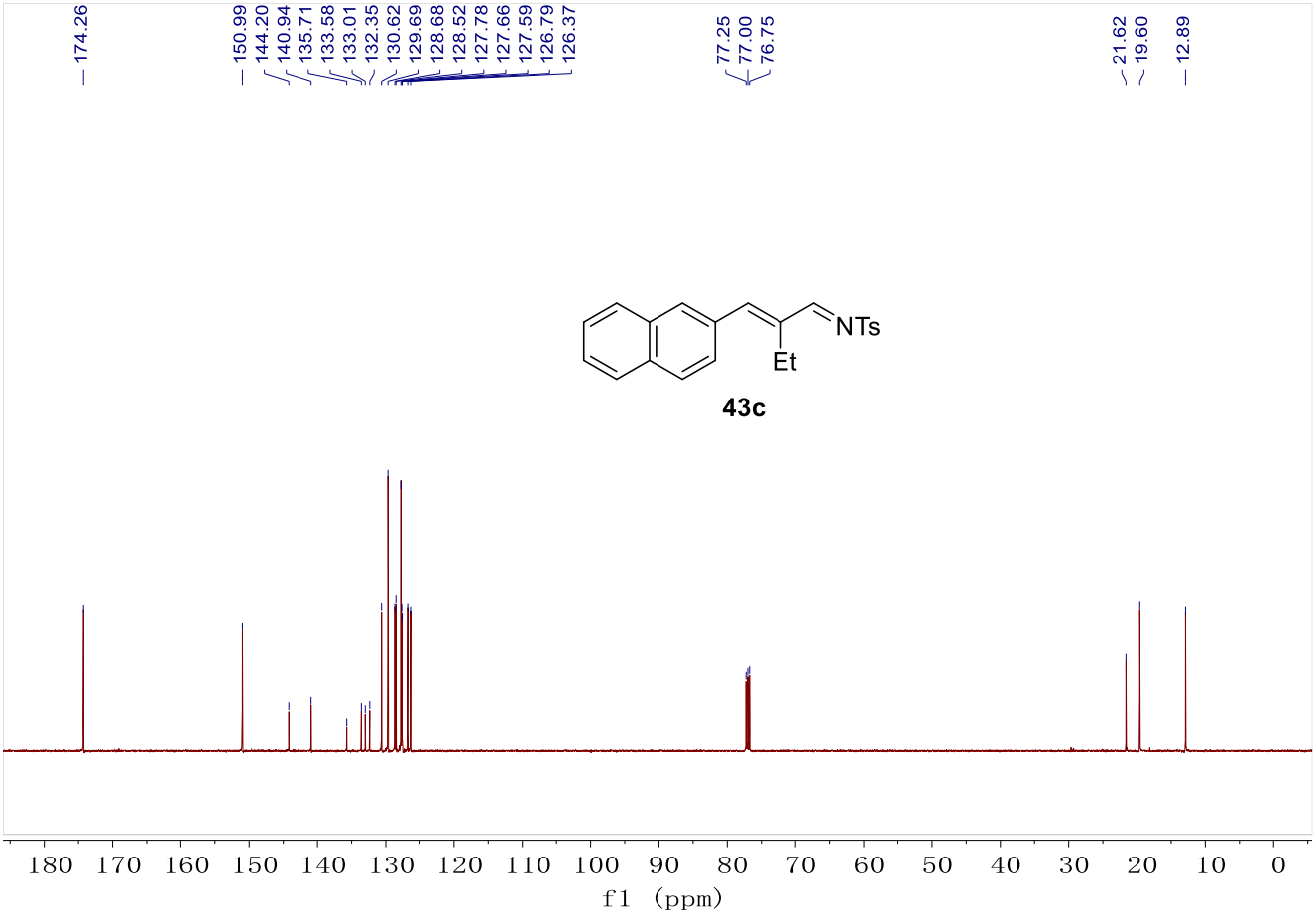
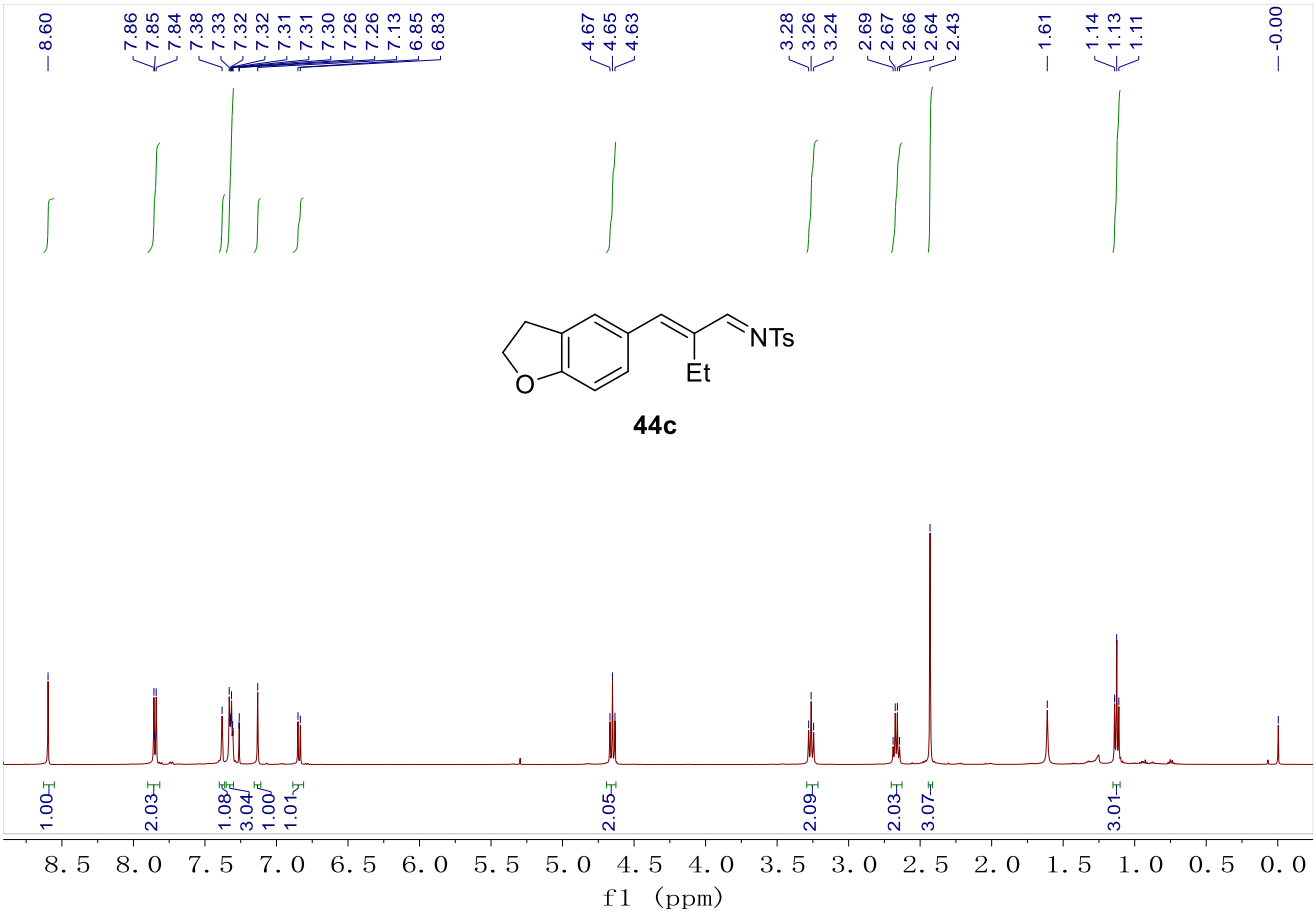
151.12
144.08
140.57
140.04
135.98
132.16
130.11
129.65
129.61
127.77
77.32
77.00
76.68
21.60
21.46
19.49
12.68
NTs
Et
NC
42c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.70
7.94
7.89
7.89
7.88
7.87
7.86
7.86
7.84
7.59
7.59
7.57
7.57
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.38
7.35
7.34
7.26
2.77
2.76
2.74
2.73
2.44
1.65
1.22
1.20
1.19
0.00
NTs
Et
1.00
1.00
5.07
3.07
3.01
2.02
3.07
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

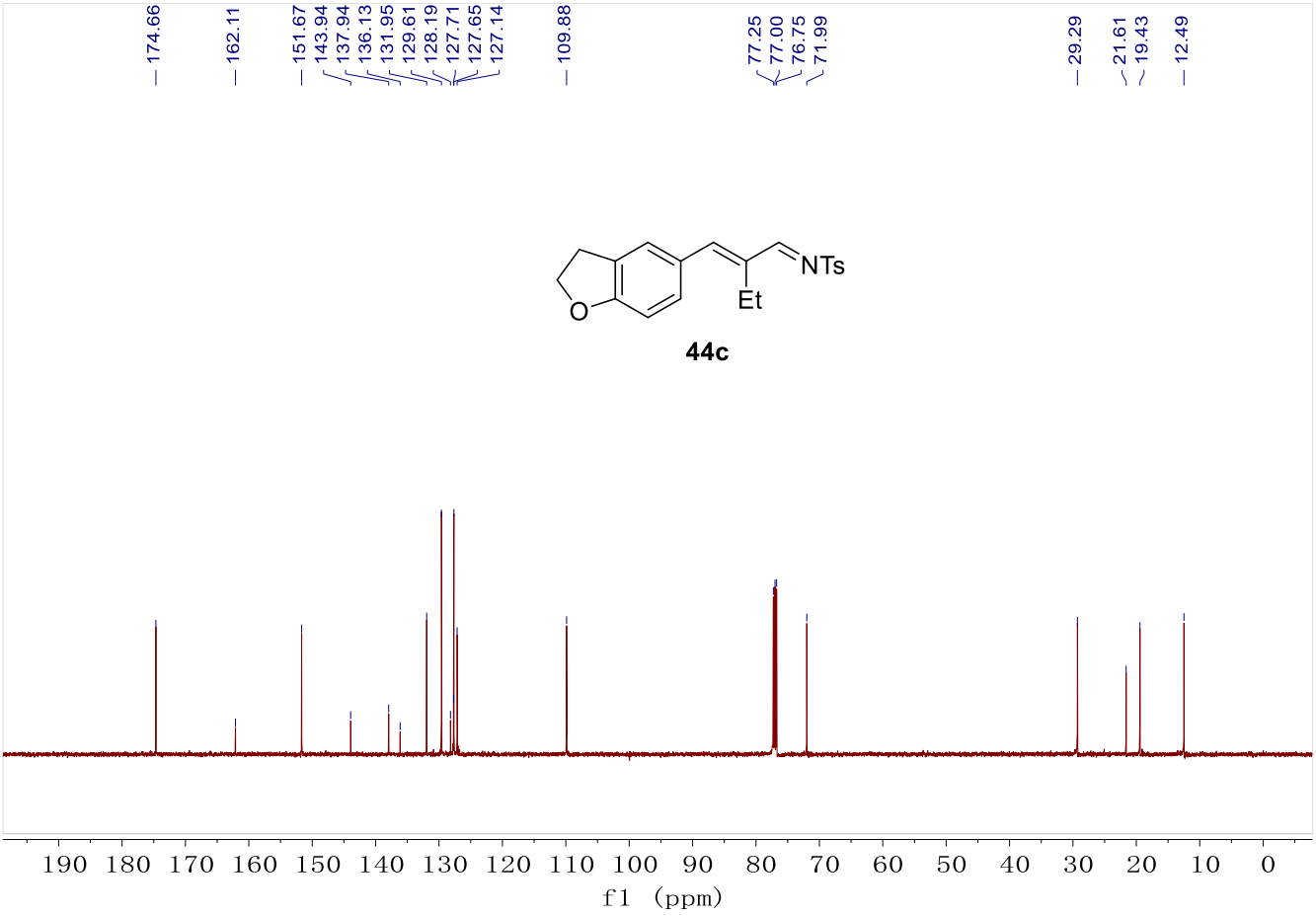
43c


174.26
150.99
144.20
140.94
135.71
133.58
133.01
132.35
130.62
129.69
128.68
128.52
127.78
127.66
127.59
126.79
126.37
77.25
77.00
76.75
21.62
19.60
12.89
NTs
Et
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

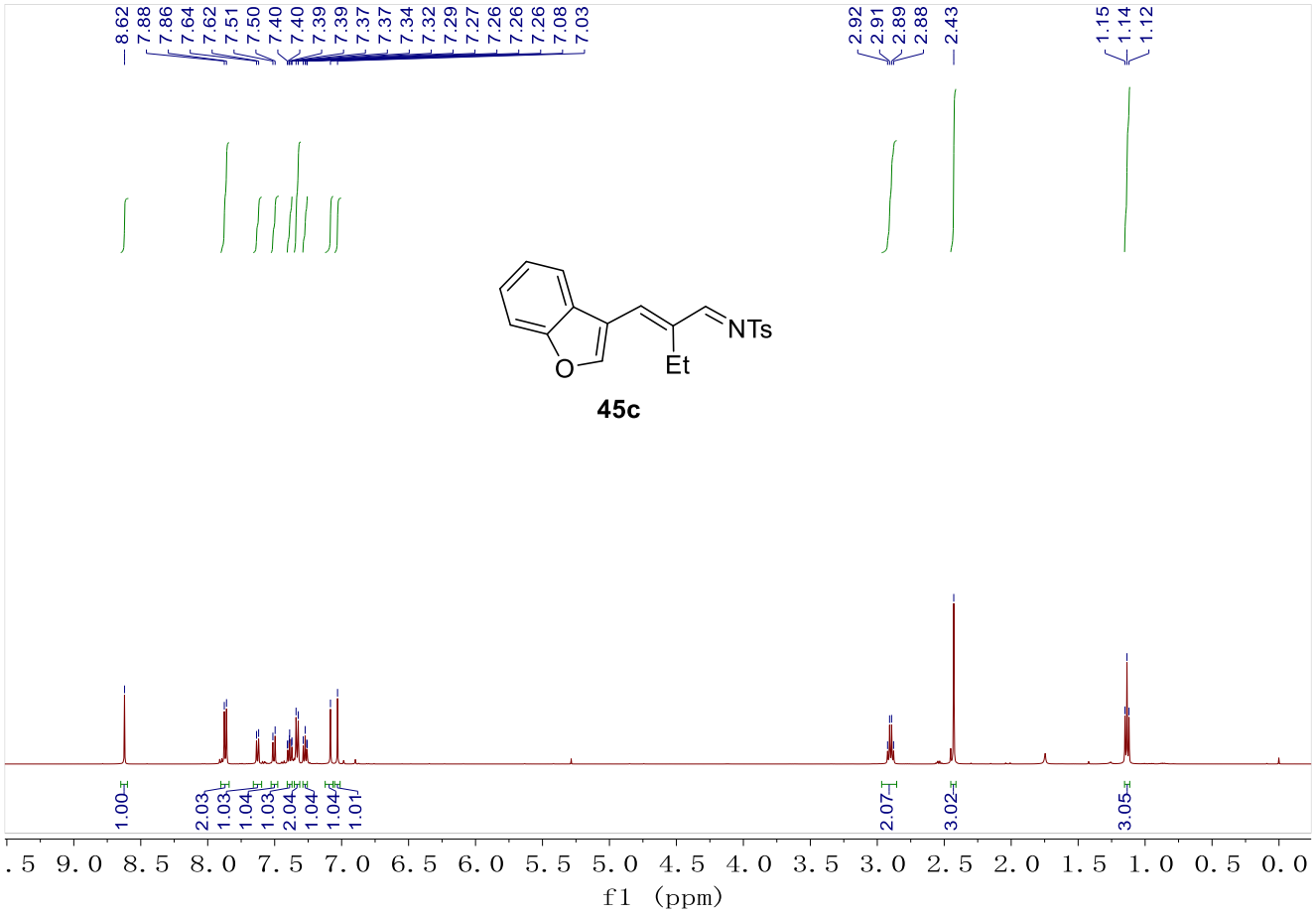
43c


8.60
7.86
7.85
7.84
7.38
7.33
7.32
7.32
7.31
7.31
7.30
7.26
7.26
7.13
6.85
6.83
4.67
4.65
4.63
3.28
3.26
3.24
2.69
2.67
2.66
2.64
2.43
1.61
1.14
1.13
1.11
-0.00
NTs
Et
O
1.00
2.03
1.08
3.04
1.00
1.01
2.05
2.09
2.03
3.07
3.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

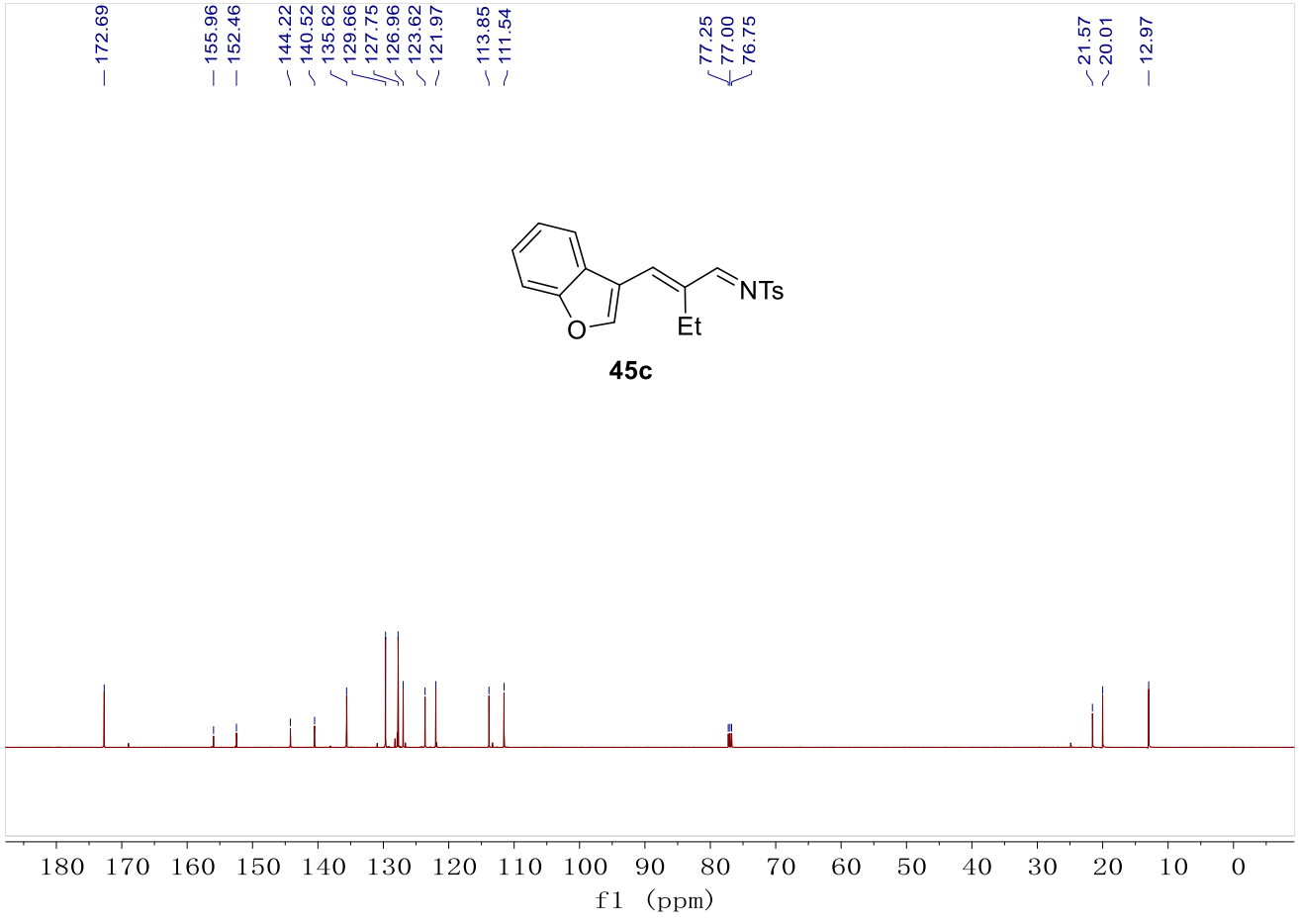
44c


174.66
162.11
151.67
143.94
137.94
136.13
131.95
129.61
128.19
127.71
127.65
127.14
109.88
77.25
77.00
76.75
71.99
29.29
21.61
19.43
12.49
NTs
Et
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

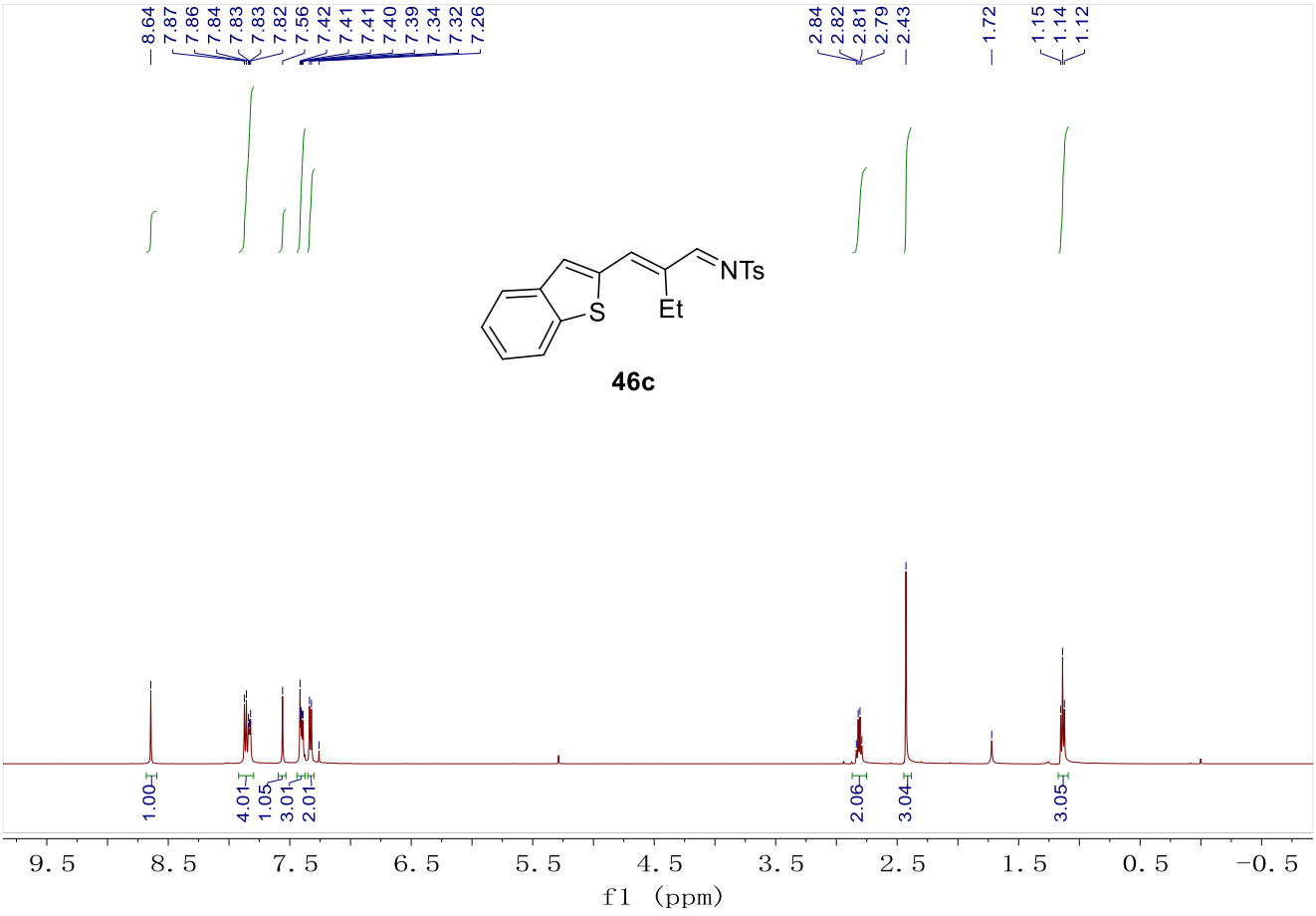
44c

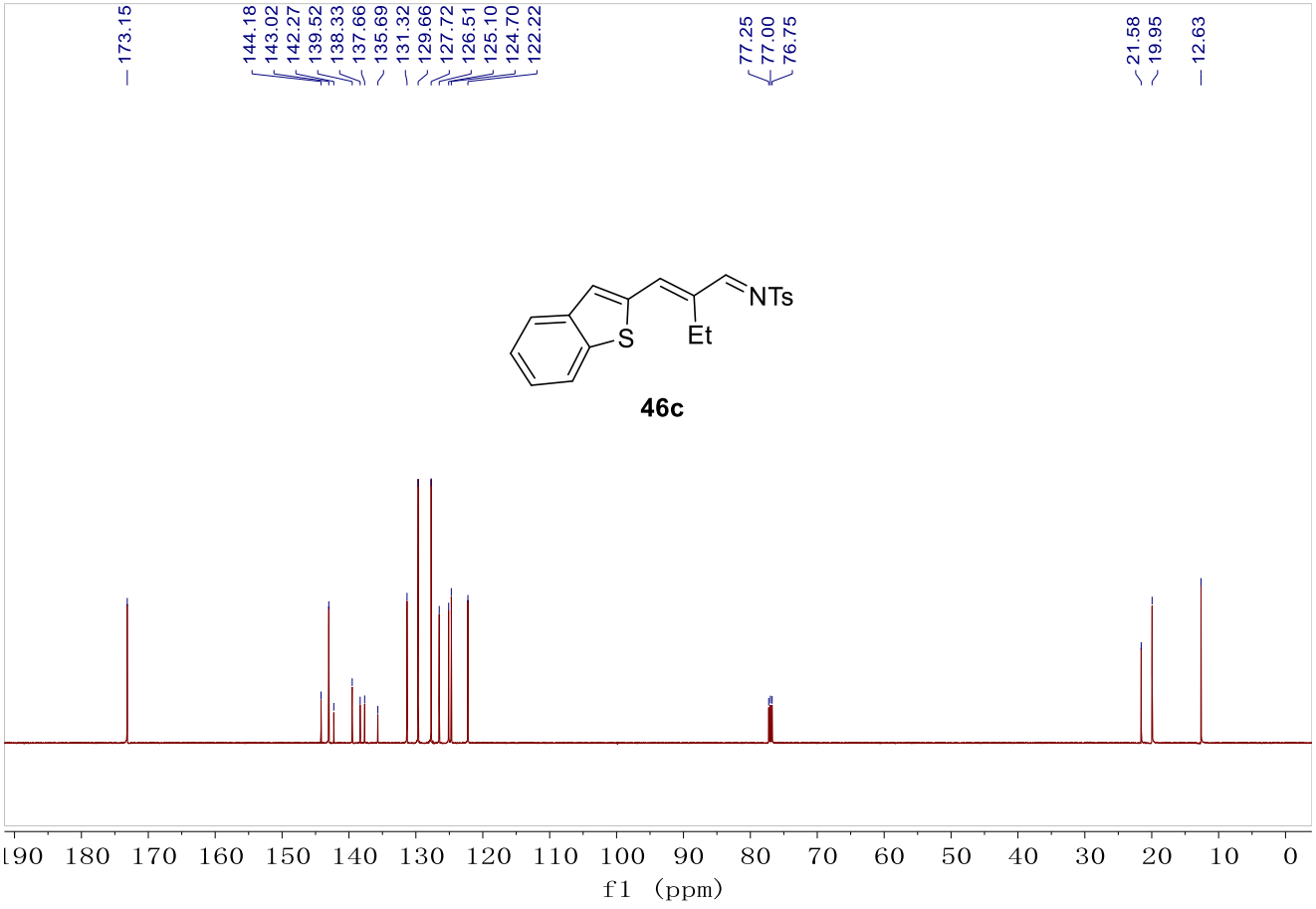

8.62
7.88
7.86
7.64
7.62
7.51
7.50
7.40
7.40
7.39
7.39
7.37
7.37
7.34
7.32
7.29
7.27
7.26
7.26
7.26
7.08
7.03
2.92
2.91
2.89
2.88
2.43
1.15
1.14
1.12
NTs
Et
O
1.00
2.03
1.03
1.04
1.03
2.04
1.04
1.04
1.01
2.07
3.02
3.05
f1 (ppm)

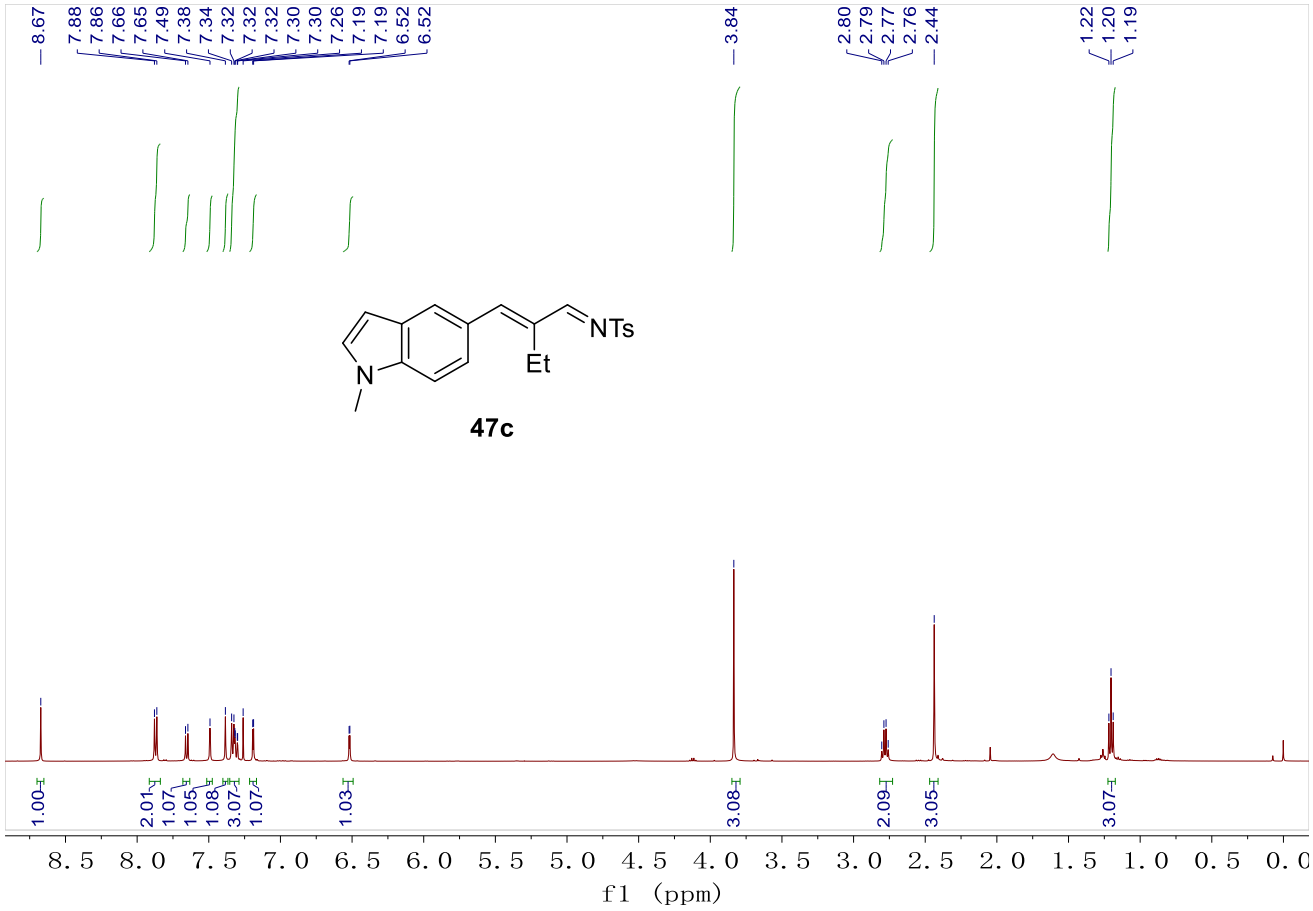
45c


172.69
155.96
152.46
144.22
140.52
135.62
129.66
127.75
126.96
123.62
121.97
113.85
111.54
77.25
77.00
76.75
21.57
20.01
12.97
NTs
Et
O
f1 (ppm)

45c


8.64
7.87
7.86
7.84
7.83
7.83
7.82
7.56
7.42
7.41
7.41
7.40
7.39
7.34
7.32
7.26
2.84
2.82
2.81
2.79
2.43
1.72
1.15
1.14
1.12
NTs
S
Et
46c
1.00
4.01
1.05
3.01
2.01
2.06
3.04
3.05
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)


173.15
144.18
143.02
142.27
139.52
138.33
137.66
135.69
131.32
129.66
127.72
126.51
125.10
124.70
122.22
77.25
77.00
76.75
21.58
19.95
12.63
NTs
S
Et
46c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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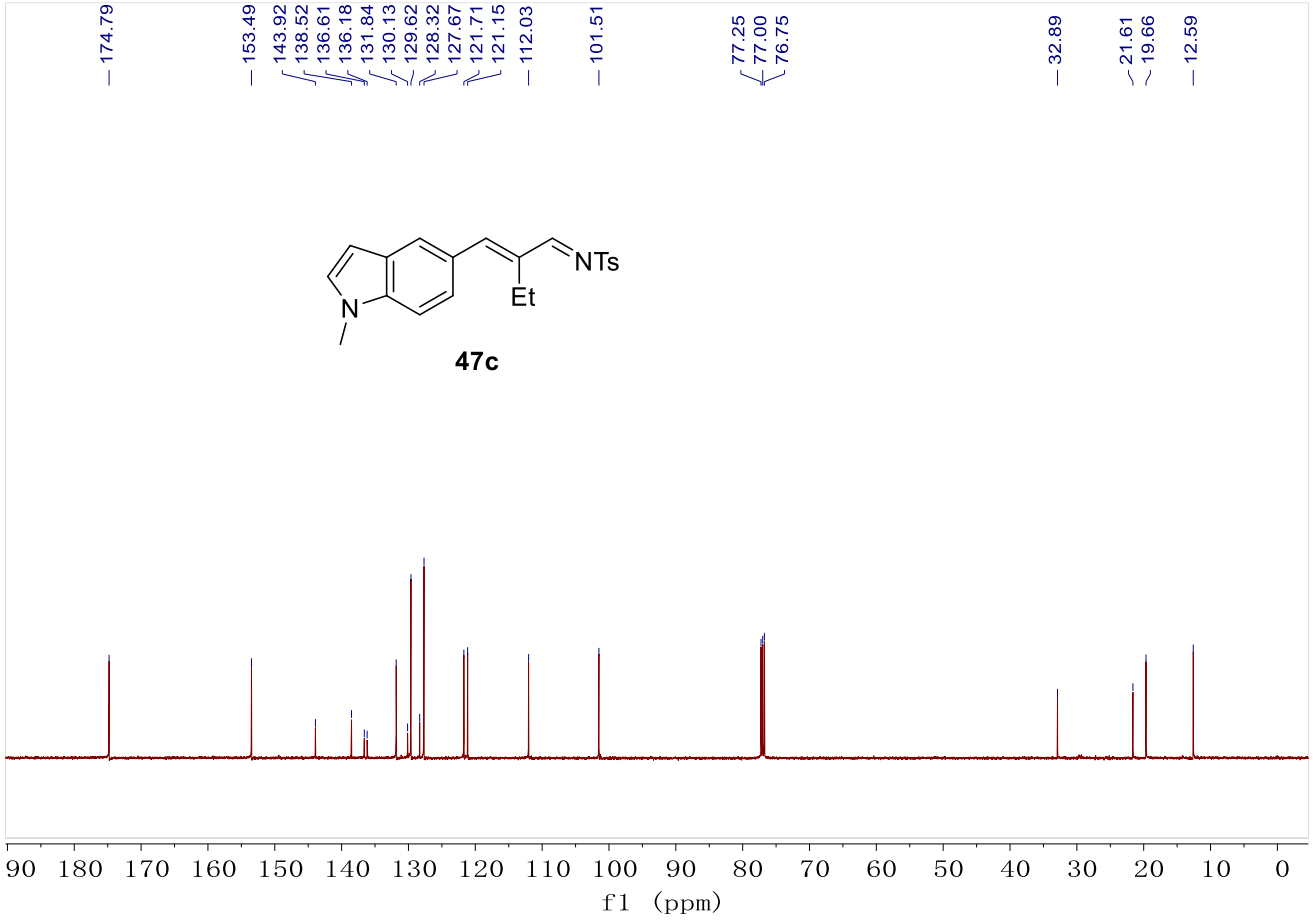
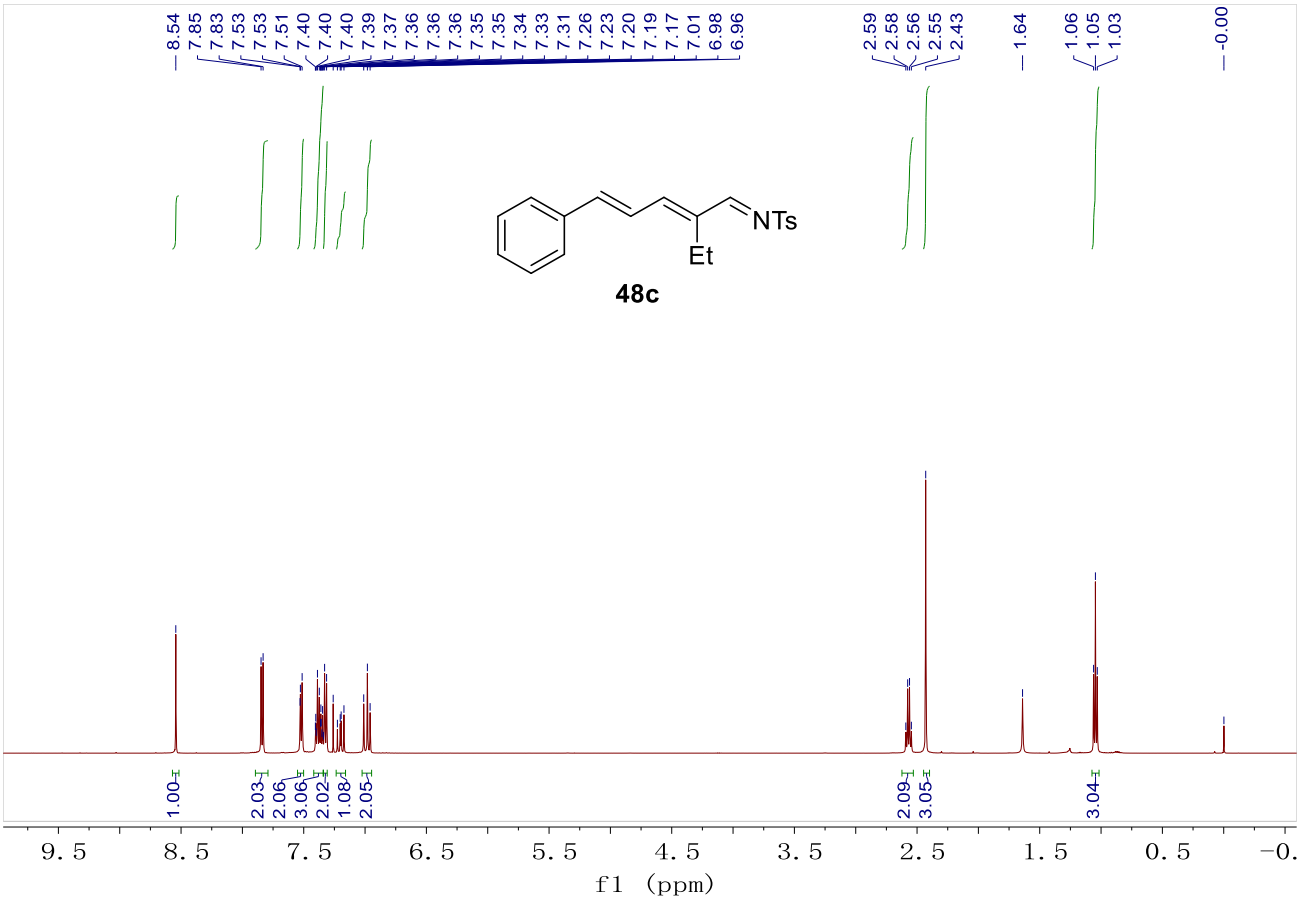
7.88
7.86
7.66
7.65
7.49
7.38
7.34
7.32
7.32
7.32
7.30
7.30
7.26
7.19
7.19
6.52
6.52
3.84
2.80
2.79
2.77
2.76
2.44
1.22
1.20
1.19
NTs
Et
N
1.00
2.01
1.07
1.05
1.08
3.07
1.07
1.03
3.08
2.09
3.05
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

47c


174.79
153.49
143.92
138.52
136.61
136.18
131.84
130.13
129.62
128.32
127.67
121.71
121.15
112.03
101.51
77.25
77.00
76.75
32.89
21.61
19.66
12.59
NTs
Et
N
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

47c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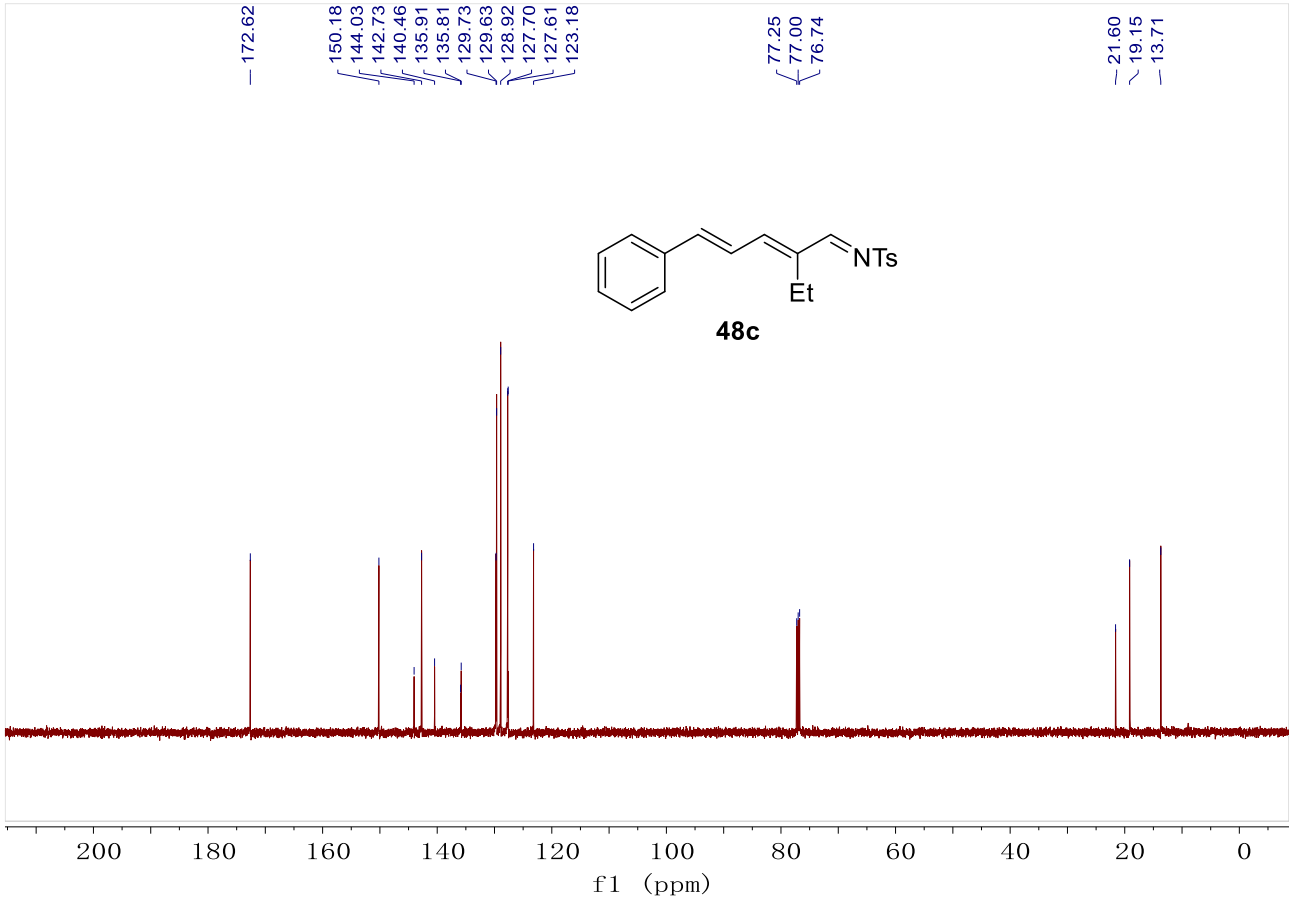
7.83
7.53
7.53
7.51
7.40
7.40
7.40
7.39
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.33
7.31
7.26
7.23
7.20
7.19
7.17
7.01
6.98
6.96
2.59
2.58
2.56
2.55
2.43
1.64
1.06
1.05
1.03
-0.00
NTs
Et
48c
1.00
2.03
2.06
3.06
2.02
1.08
2.05
2.09
3.05
3.04
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
f1 (ppm)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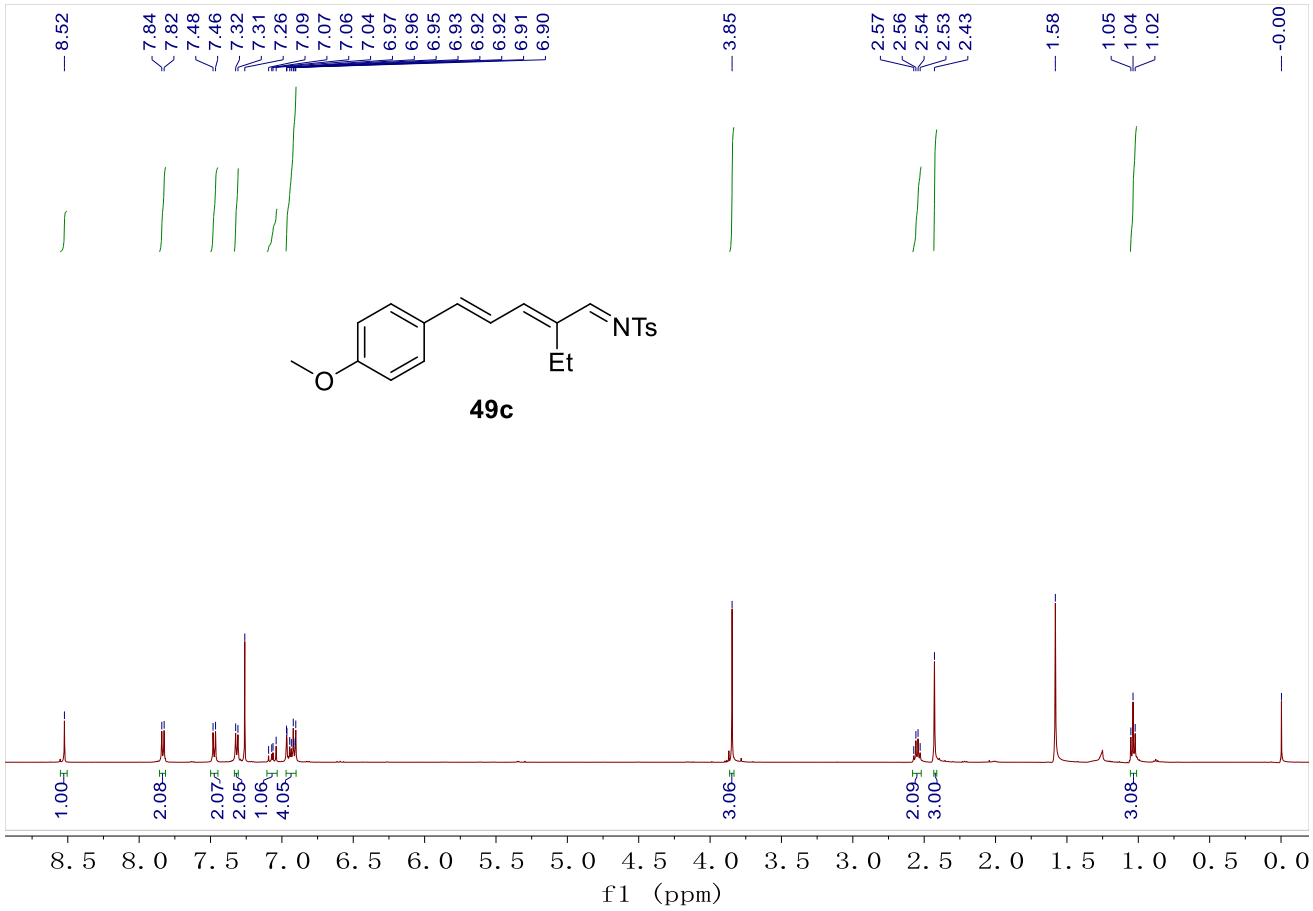
150.18
144.03
142.73
140.46
135.91
135.81
129.73
129.63
128.92
127.70
127.61
123.18
77.25
77.00
76.74
21.60
19.15
13.71
NTs
Et
48c
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)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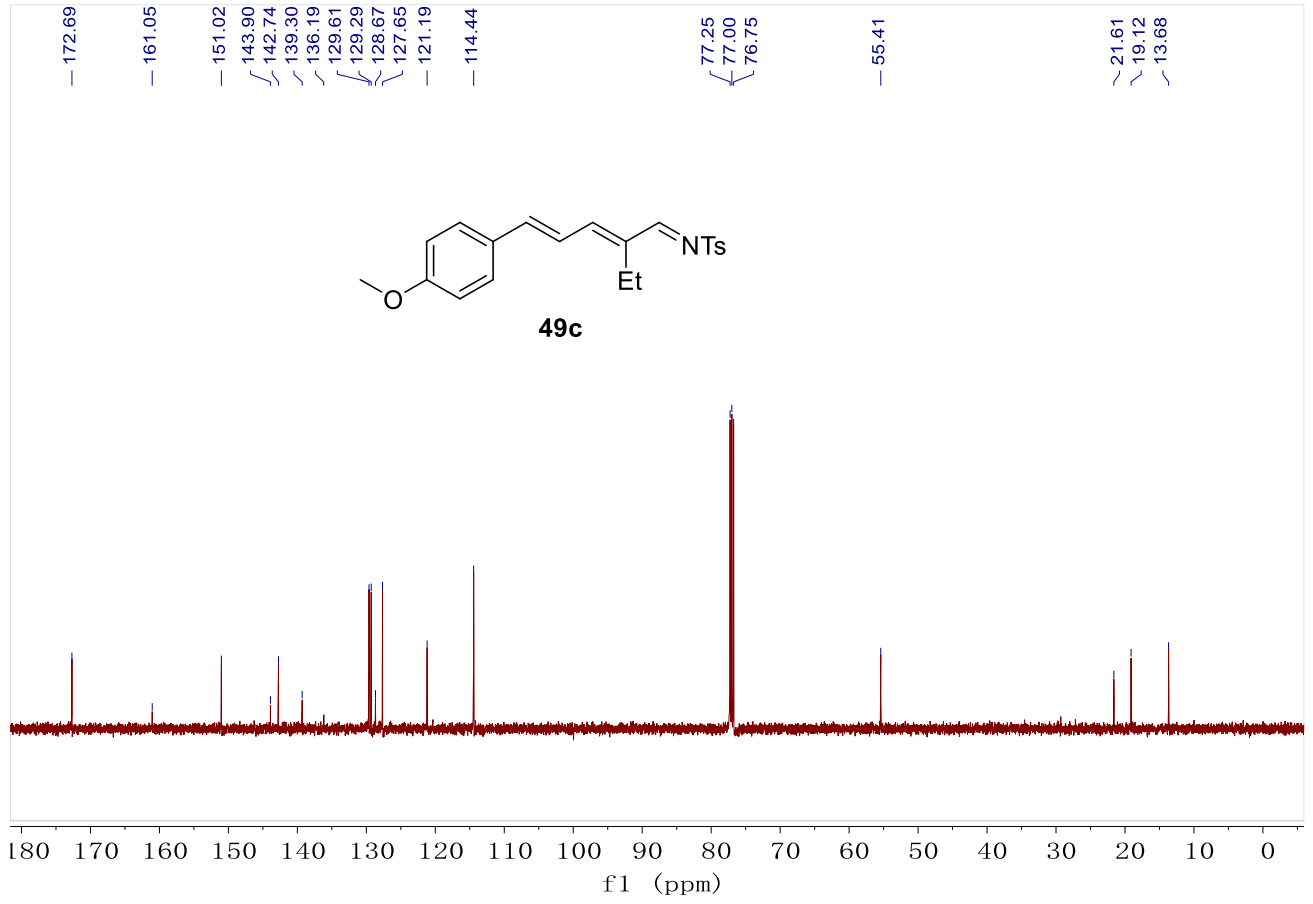
7.84
7.82
7.48
7.46
7.32
7.31
7.26
7.09
7.07
7.06
7.04
6.97
6.96
6.95
6.93
6.92
6.92
6.91
6.90
3.85
2.57
2.56
2.54
2.53
2.43
1.58
1.05
1.04
1.02
-0.00
NTs
Et
O
49c
1.00
2.08
2.07
2.05
1.06
4.05
3.06
2.09
3.00
3.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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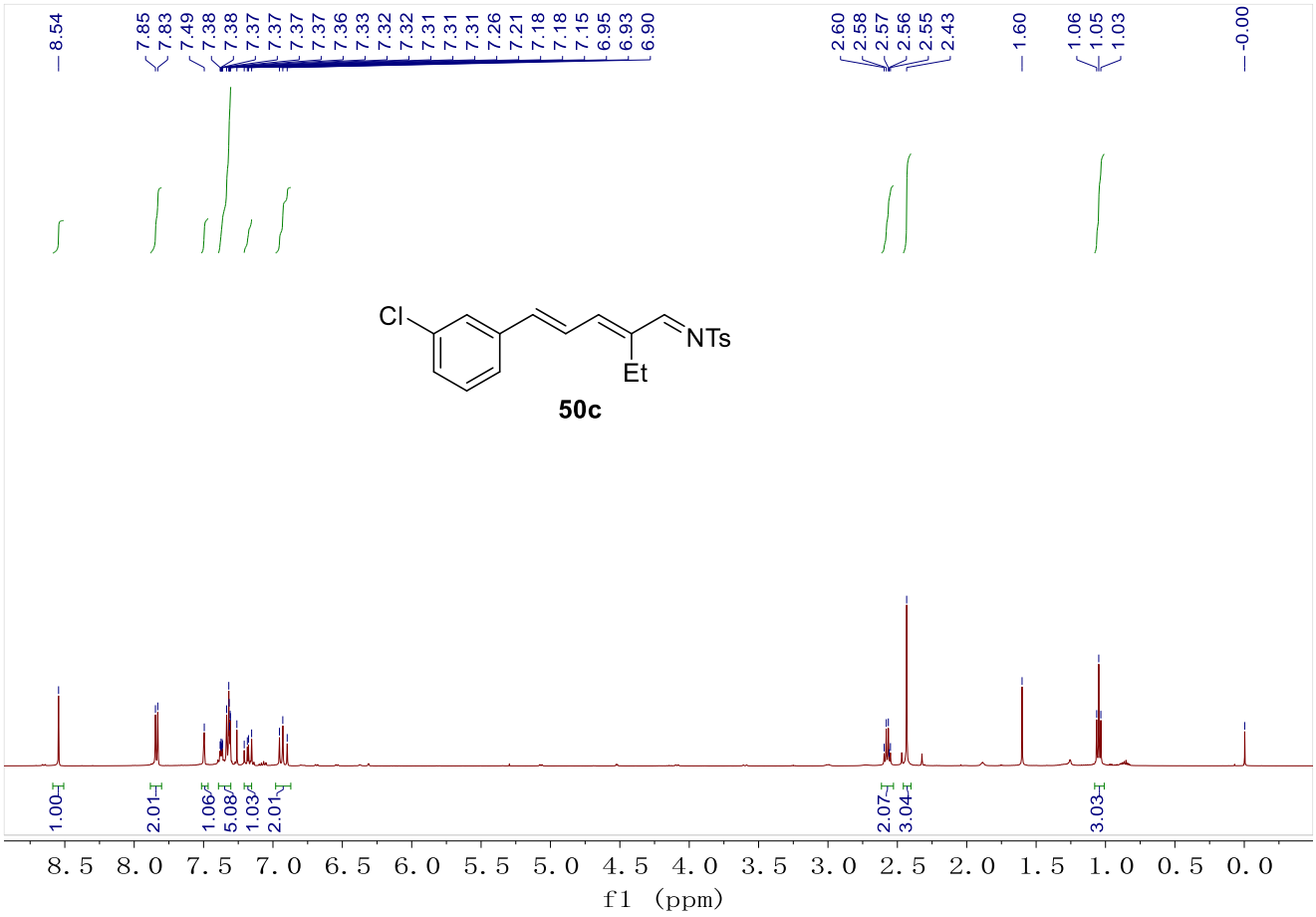
161.05
151.02
143.90
142.74
139.30
136.19
129.61
129.29
128.67
127.65
121.19
114.44
77.25
77.00
76.75
55.41
21.61
19.12
13.68
NTs
Et
O
49c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.83
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7.38
7.38
7.37
7.37
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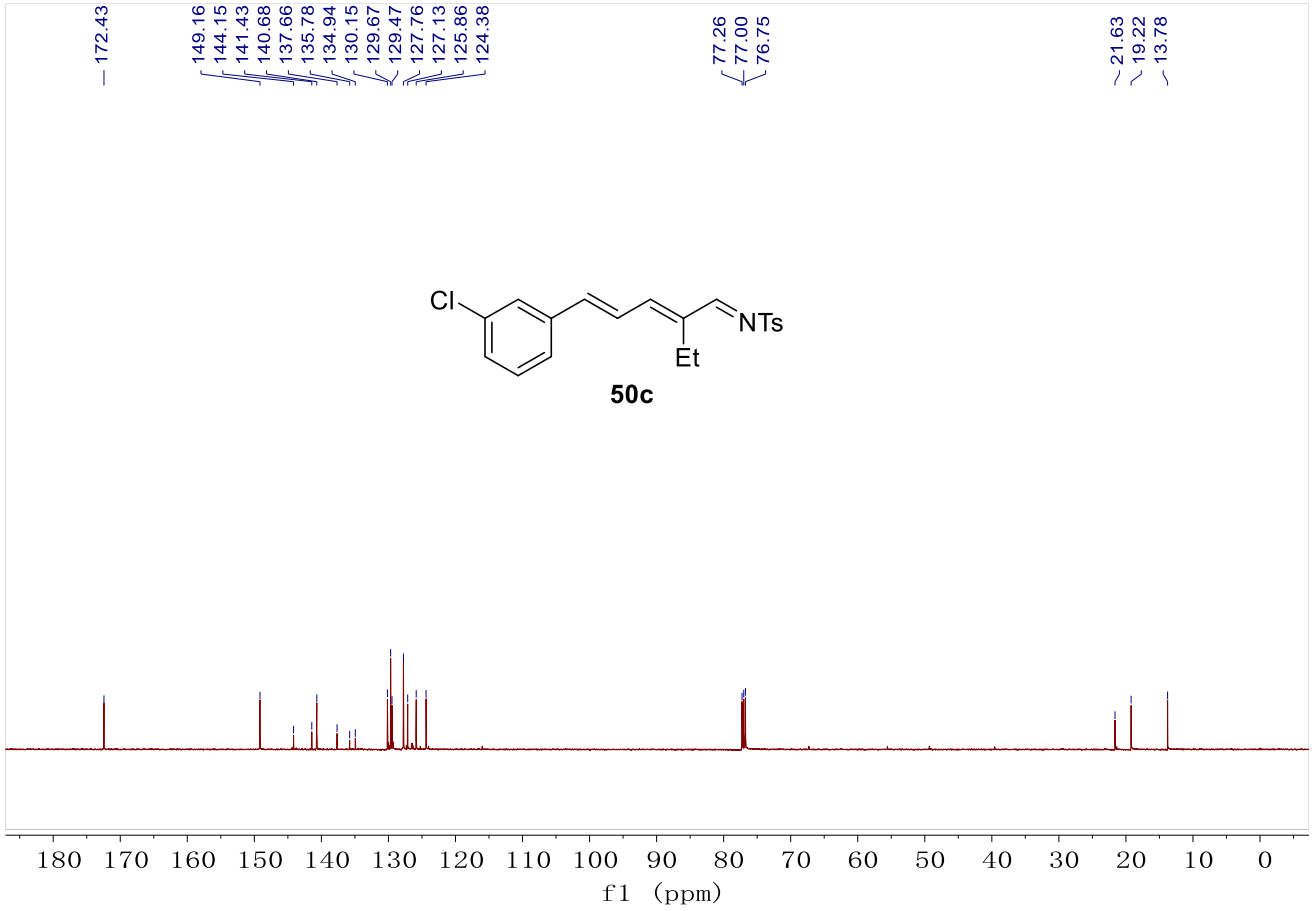
7.37
7.36
7.33
7.32
7.32
7.31
7.31
7.31
7.26
7.21
7.18
7.18
7.15
6.95
6.93
6.90
2.60
2.58
2.57
2.56
2.55
2.43
1.60
1.06
1.05
1.03
-0.00
Cl
NTs
Et
50c
1.00
2.01
1.06
5.08
1.03
2.01
2.07
3.04
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.43
149.16
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141.43
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137.66
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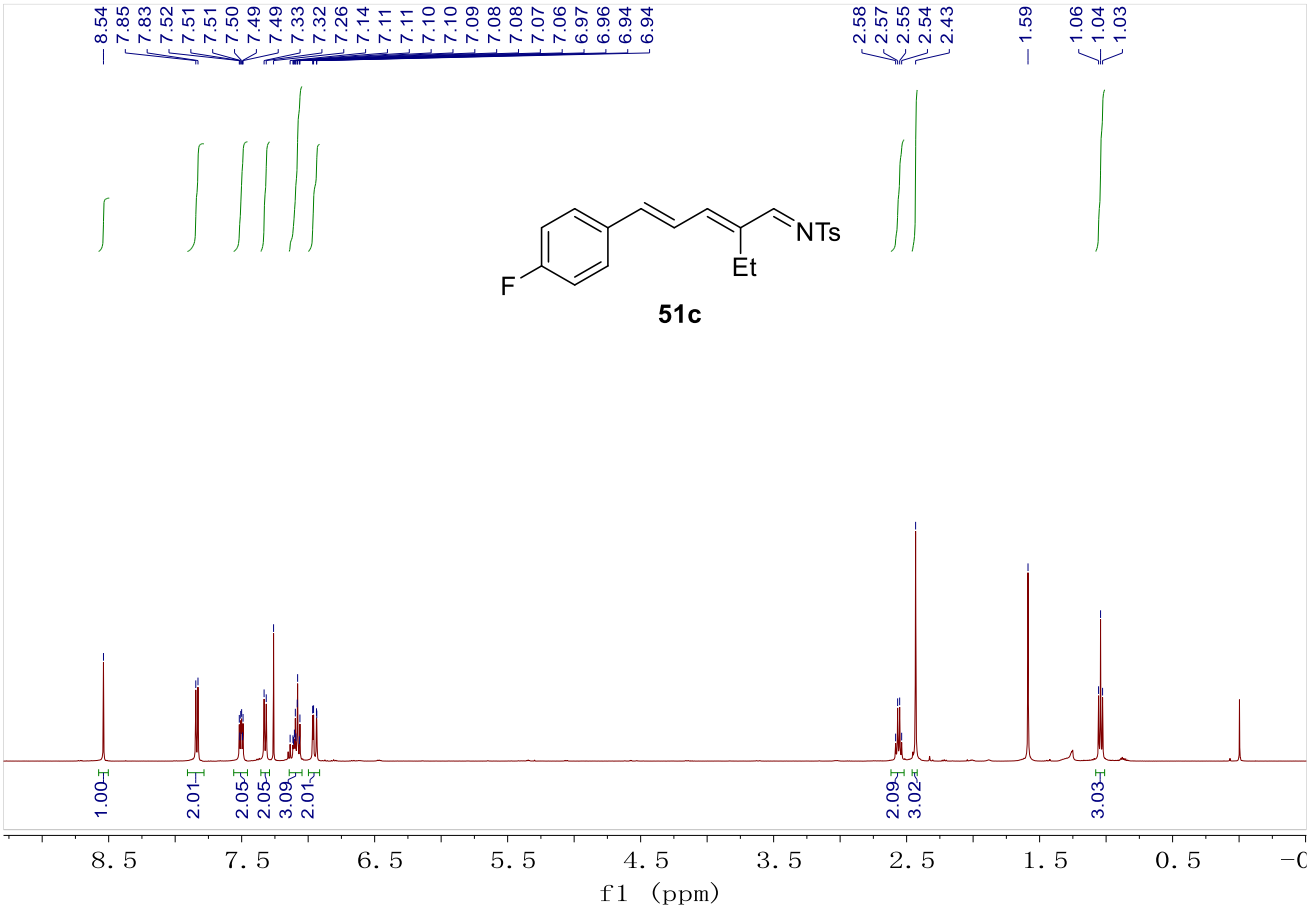
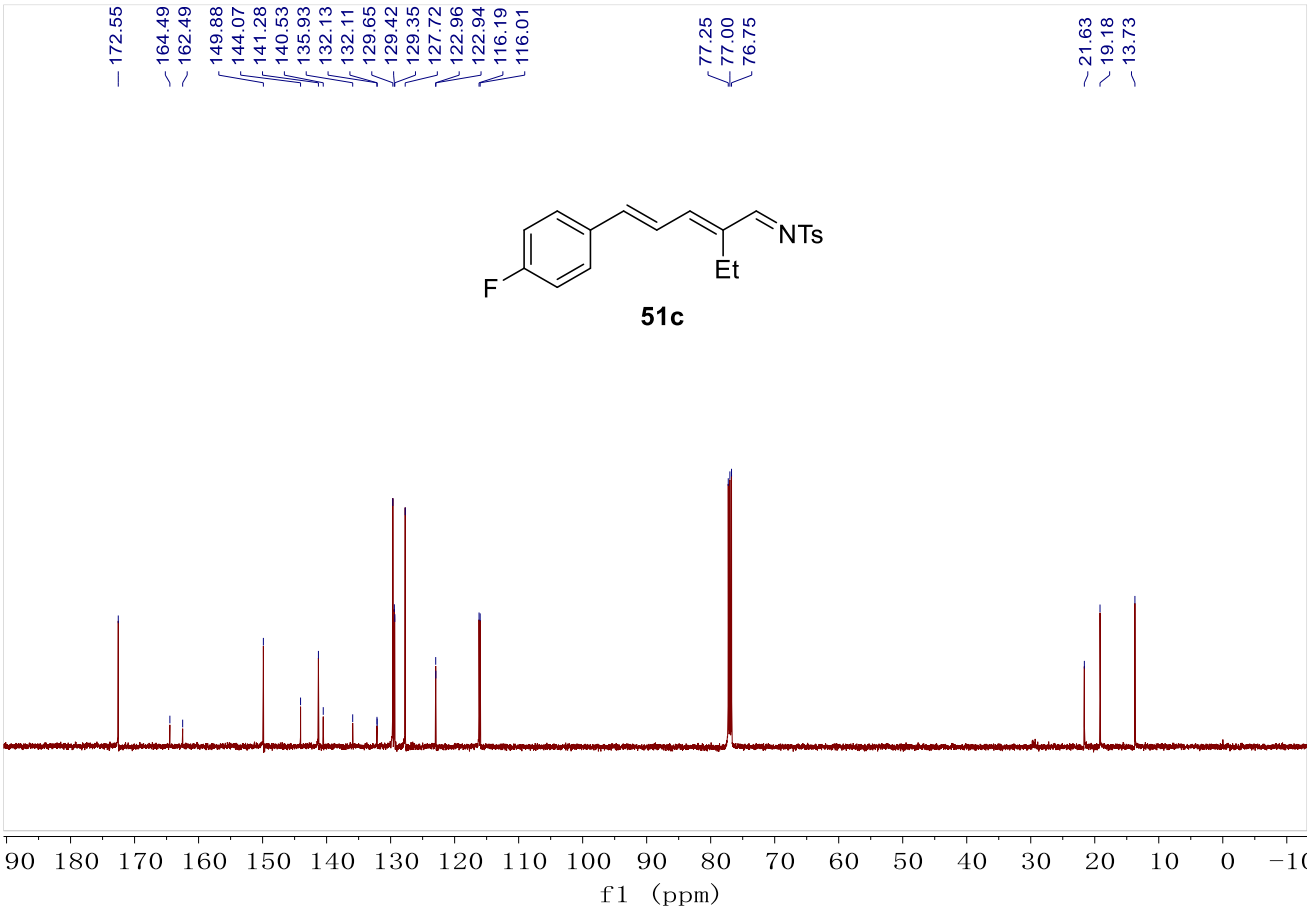
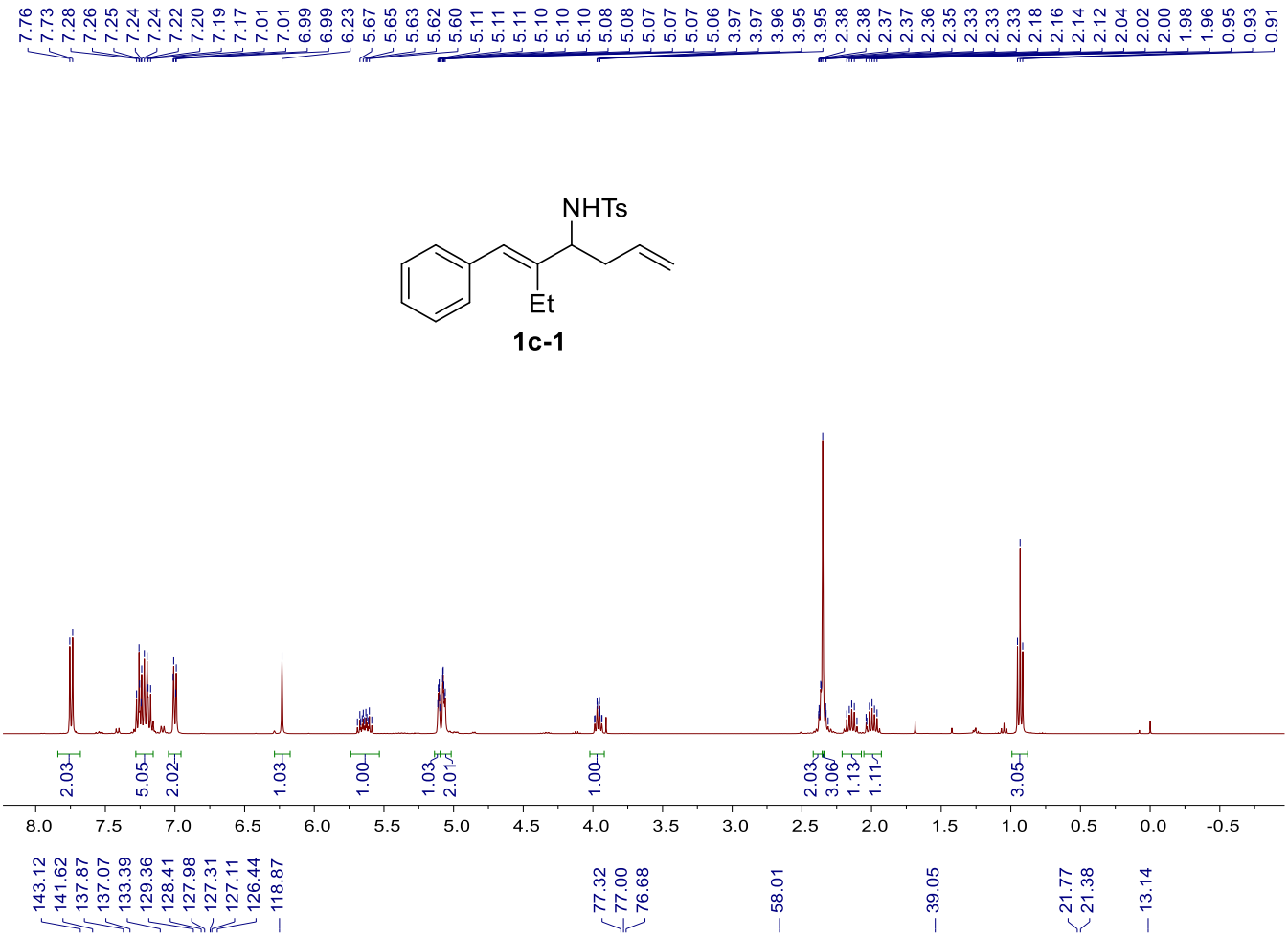
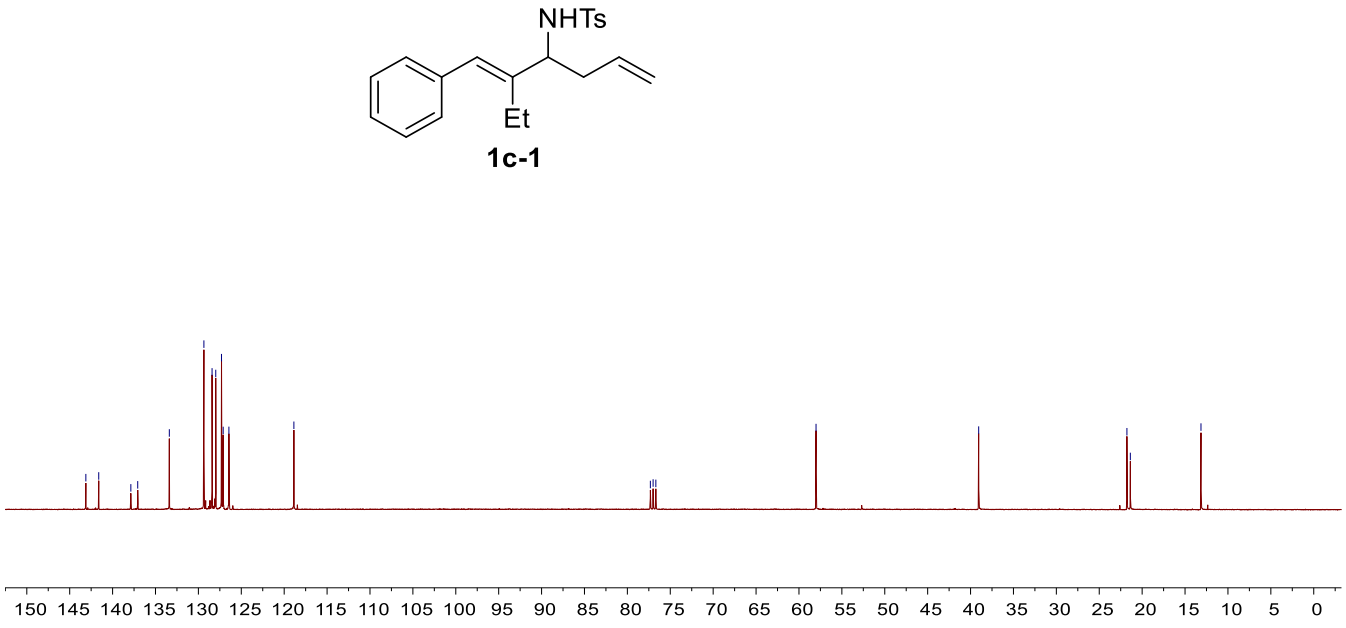
134.94
130.15
129.67
129.47
127.76
127.13
125.86
124.38
77.26
77.00
76.75
21.63
19.22
13.78
Cl
NTs
Et
50c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

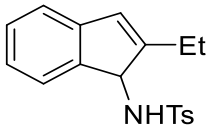

8.54
7.85
7.83
7.52
7.51
7.51
7.50
7.49
7.49
7.33
7.32
7.26
7.14
7.11
7.11
7.10
7.10
7.09
7.08
7.08
7.07
7.06
6.97
6.96
6.94
6.94
2.58
2.57
2.55
2.54
2.43
1.59
1.06
1.04
1.03
NTs
Et
F
51c
1.00
2.01
2.05
2.05
3.09
2.01
2.09
3.02
3.03
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


172.55
164.49
162.49
149.88
144.07
141.28
140.53
135.93
132.13
132.11
129.65
129.42
129.35
127.72
122.96
122.94
116.19
116.01
77.25
77.00
76.75
21.63
19.18
13.73
NTs
Et
F
51c
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

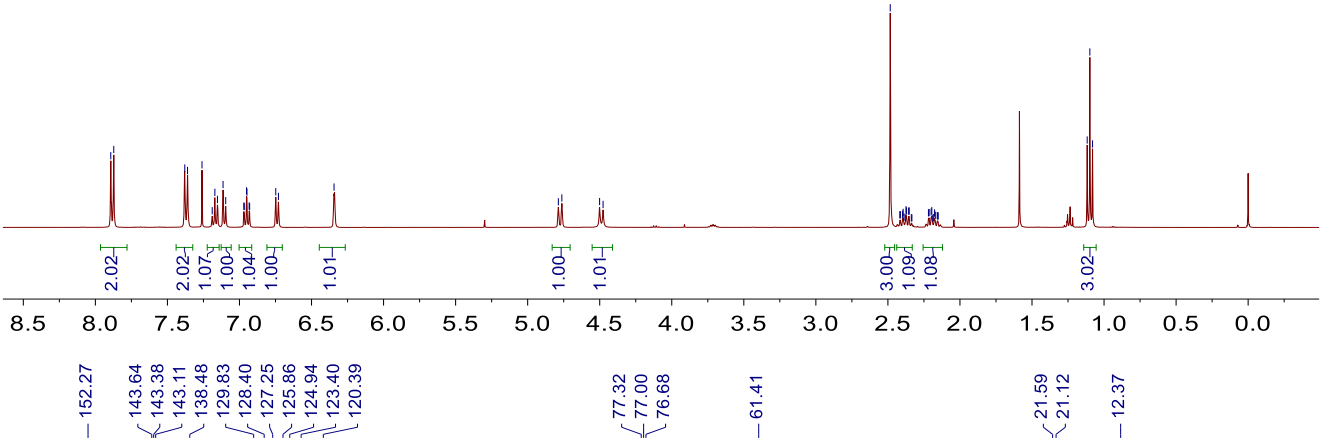

7.76 7.73 7.28 7.26 7.25 7.24 7.24 7.22 7.20 7.19 7.17 7.01 7.01 6.99 6.99 6.23
5.67 5.65 5.63 5.62 5.60 5.11 5.11 5.11 5.10 5.10 5.10 5.08 5.08 5.07 5.07 5.07 5.06 3.97 3.97 3.96 3.95 3.95 2.38 2.37 2.37 2.36 2.35 2.33 2.33 2.33 2.18 2.16 2.14 2.12 2.04 2.02 2.00 1.98 1.96 0.95 0.93 0.91
NHTs
Et
1c-1
2.03 5.05 2.02 1.03 1.00 1.03 2.01 1.00 2.03 3.06 1.13 1.11 3.05
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
143.12 141.62 137.87 137.07 133.39 129.36 128.41 127.98 127.31 127.11 126.44 118.87
77.32 77.00 76.68
58.01
39.05
21.77 21.38
13.14


NHTs
Et
1c-1
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

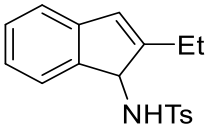

7.89
7.87
7.38
7.36
7.26
7.19
7.17
7.15
7.11
7.10
6.97
6.97
6.95
6.95
6.93
6.93
6.75
6.73
6.34
4.79
4.76
4.50
4.48
2.48
2.42
2.41
2.40
2.39
2.39
2.38
2.37
2.37
2.36
2.35
2.34
2.33
2.22
2.21
2.20
2.20
2.19
2.18
2.18
2.17
2.16
2.15
2.15
1.12
1.10
1.08


Et
NHTs

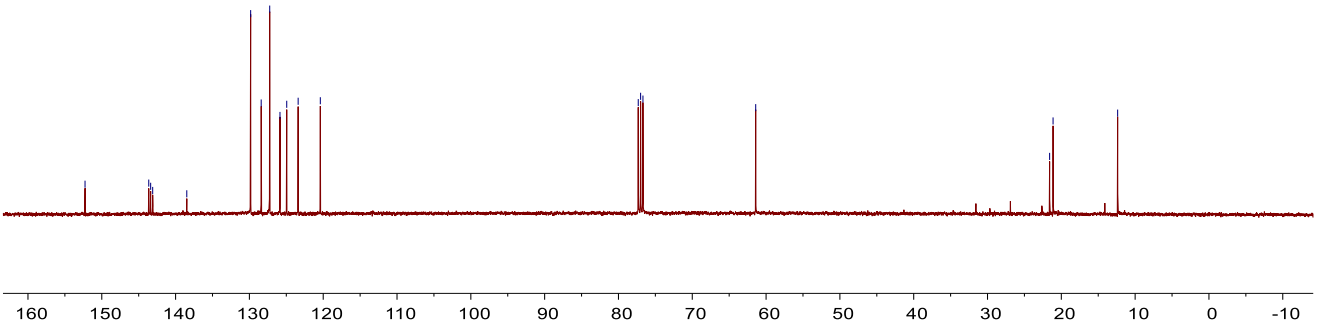
1c-2


2.02
2.02
1.07
1.00
1.04
1.00
1.01
1.00
1.01
3.00
1.09
1.08
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

152.27
143.64
143.38
143.11
138.48
129.83
128.40
127.25
125.86
124.94
123.40
120.39
77.32
77.00
76.68
61.41
21.59
21.12
12.37


Et
NHTs

1c-2


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


7.80
7.78
7.29
7.28
7.28
7.26
7.26
7.21
7.21
7.20
7.20
7.19
7.18
7.17
7.17
7.17
7.10
7.08
5.02
5.01
4.99
3.67
3.66
3.65
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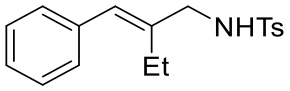
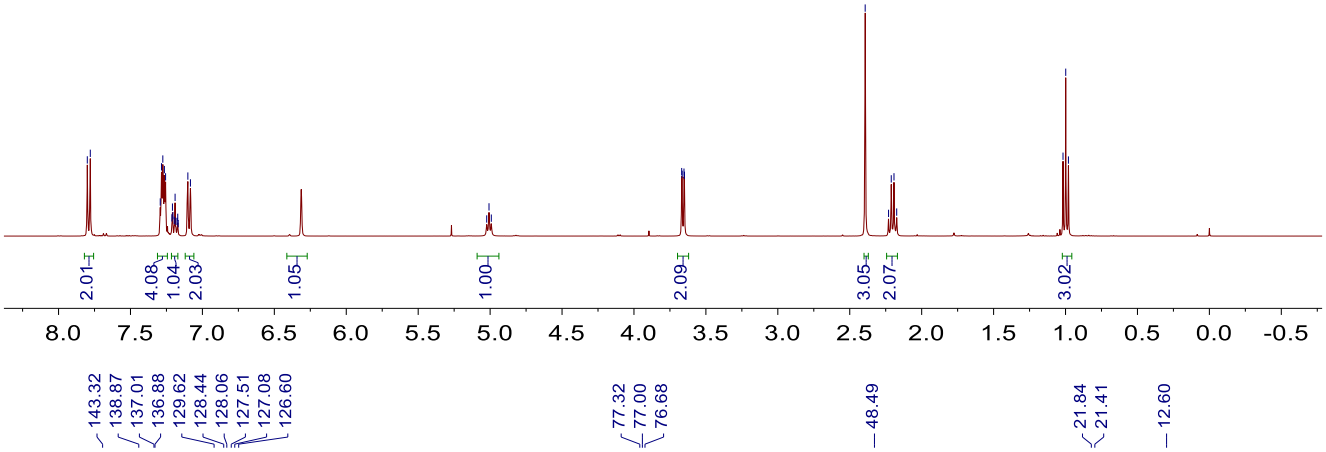
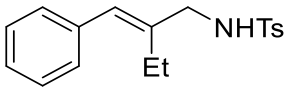
2.21
2.19
2.17
1.02
1.00
0.98


NHTs
Et

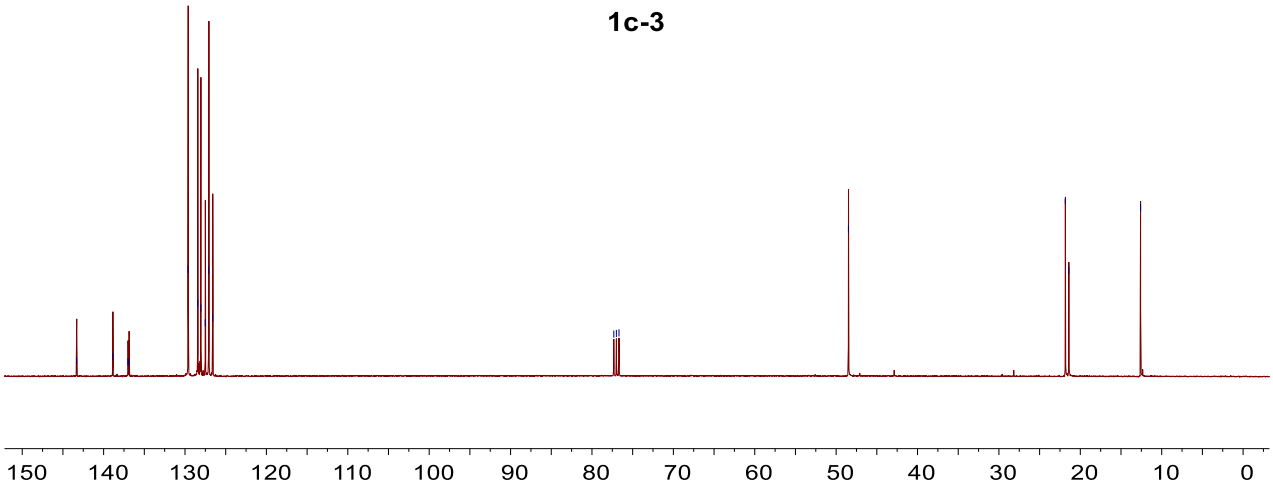
1c-3


2.01
4.08
1.04
2.03
1.05
1.00
2.09
3.05
2.07
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

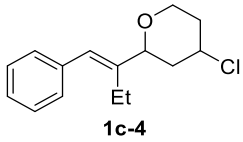
143.32
138.87
137.01
136.88
129.62
128.44
128.06
127.51
127.08
126.60
77.32
77.00
76.68
48.49
21.84
21.41
12.60


NHTs
Et

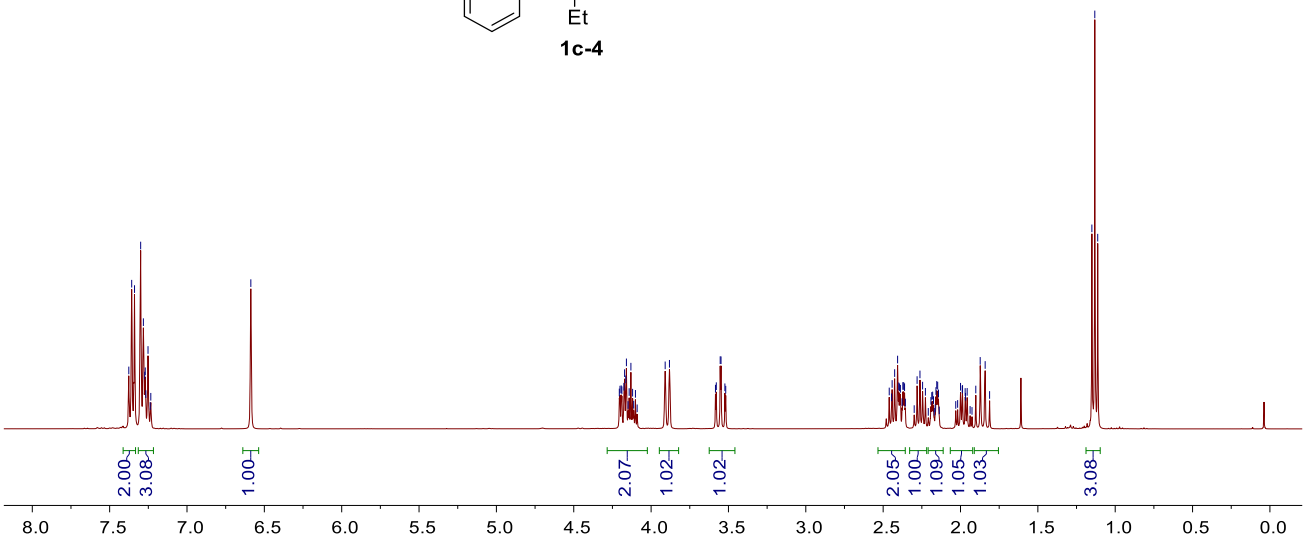
1c-3


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

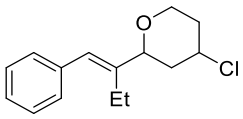

7.38 7.36 7.34 7.30 7.28 7.27 7.27 7.27 7.25 6.59 4.21 4.20 4.19 4.19 4.18 4.17 4.16 4.16 4.14 4.13 4.12 4.10 3.91 3.88 3.58 3.58 3.55 3.55 3.52 3.52 2.46 2.44 2.43 2.41 2.40 2.39 2.39 2.37 2.37 2.36 2.28 2.26 2.24 2.23 2.16 2.15 2.15 2.14 2.00 1.99 1.99 1.97 1.96 1.90 1.87 1.84 1.15 1.13 1.11


O
Cl
Et

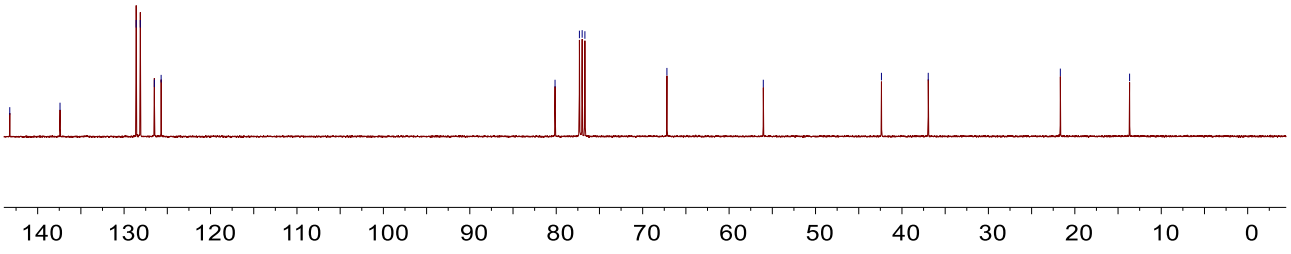
1c-4

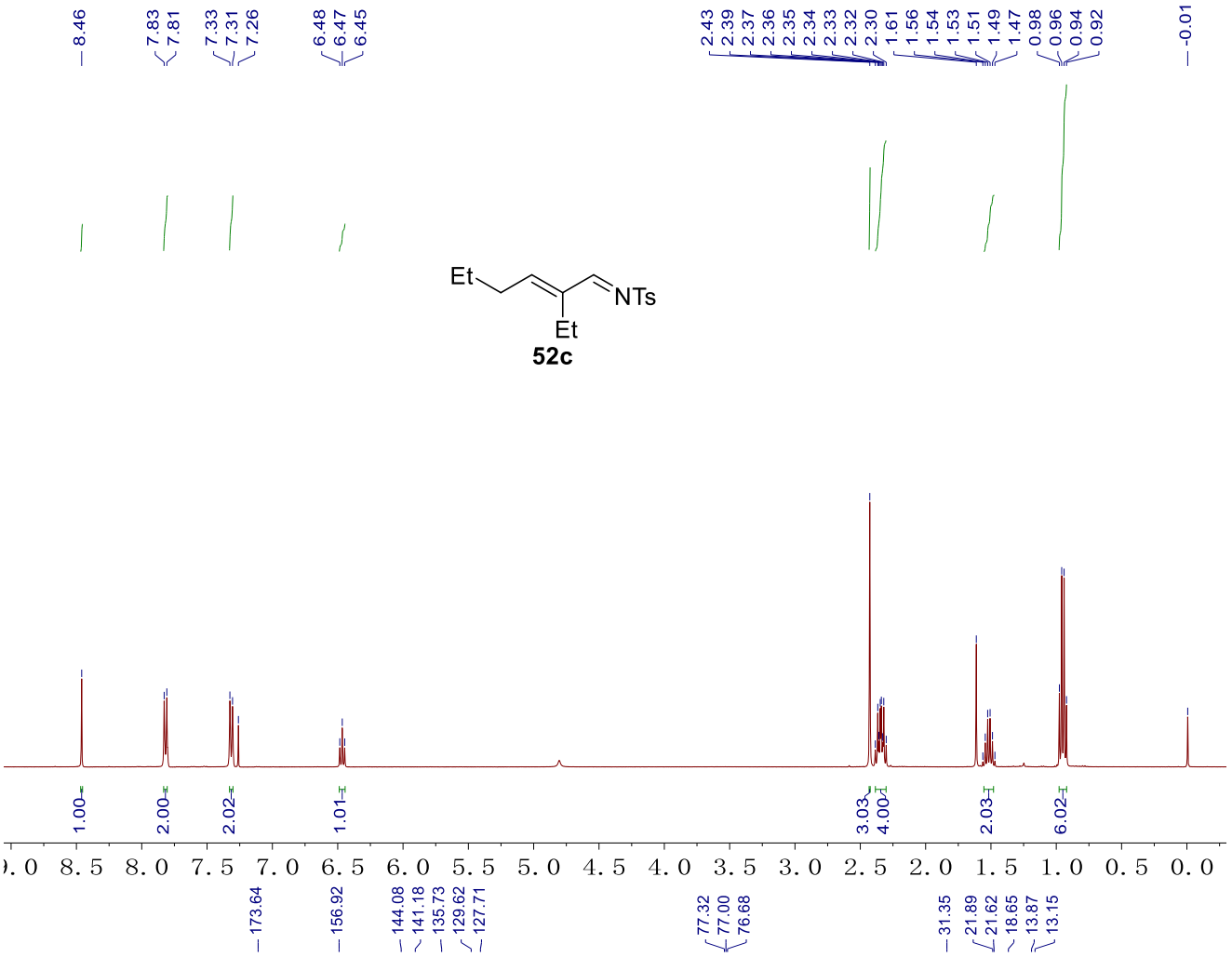

2.00 3.08 1.00 2.07 1.02 1.02 2.05 1.00 1.09 1.05 1.03 3.08
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

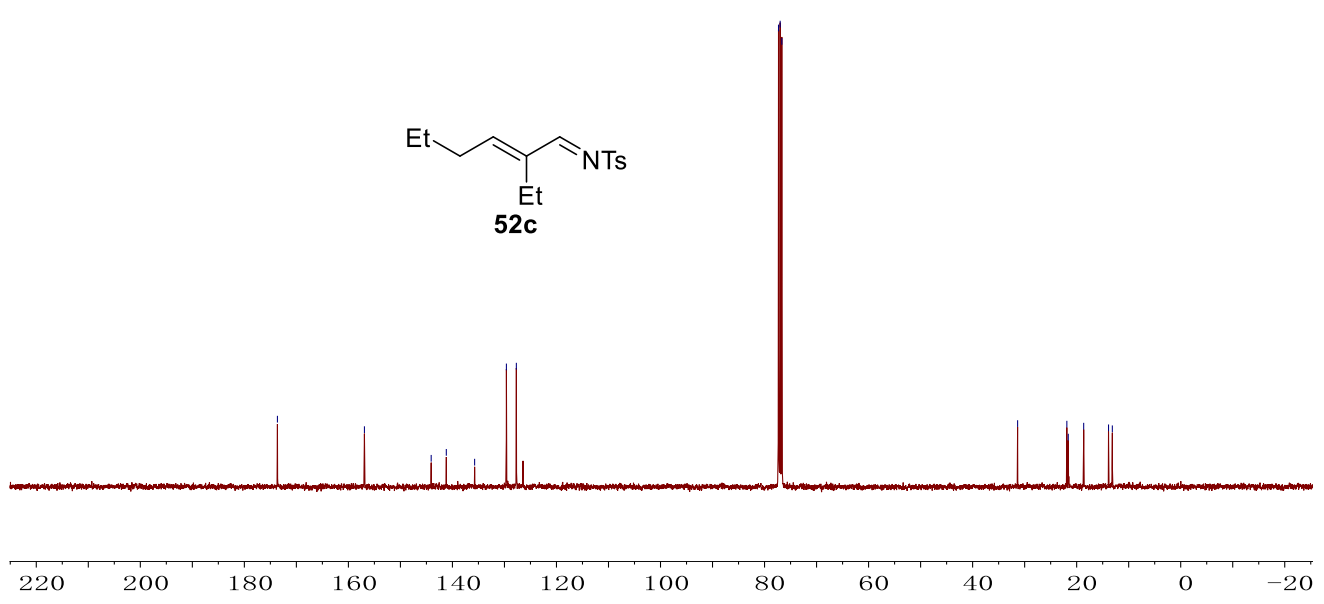

143.23
137.41
128.60
128.13
126.50
125.71
80.14
77.32
77.00
76.68
67.19
56.04
42.37
36.96
21.68
13.66

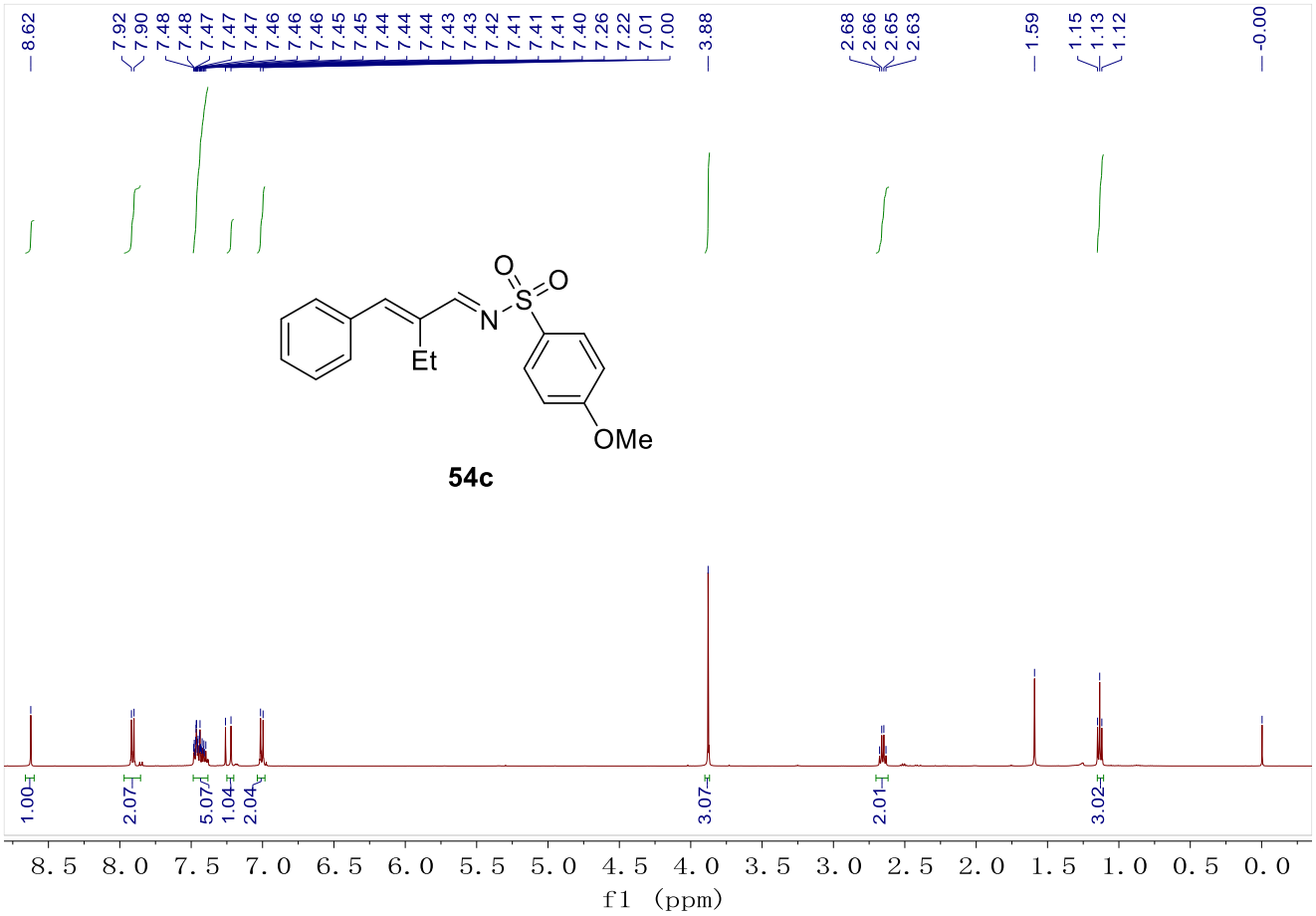

O
Cl
Et

1c-4

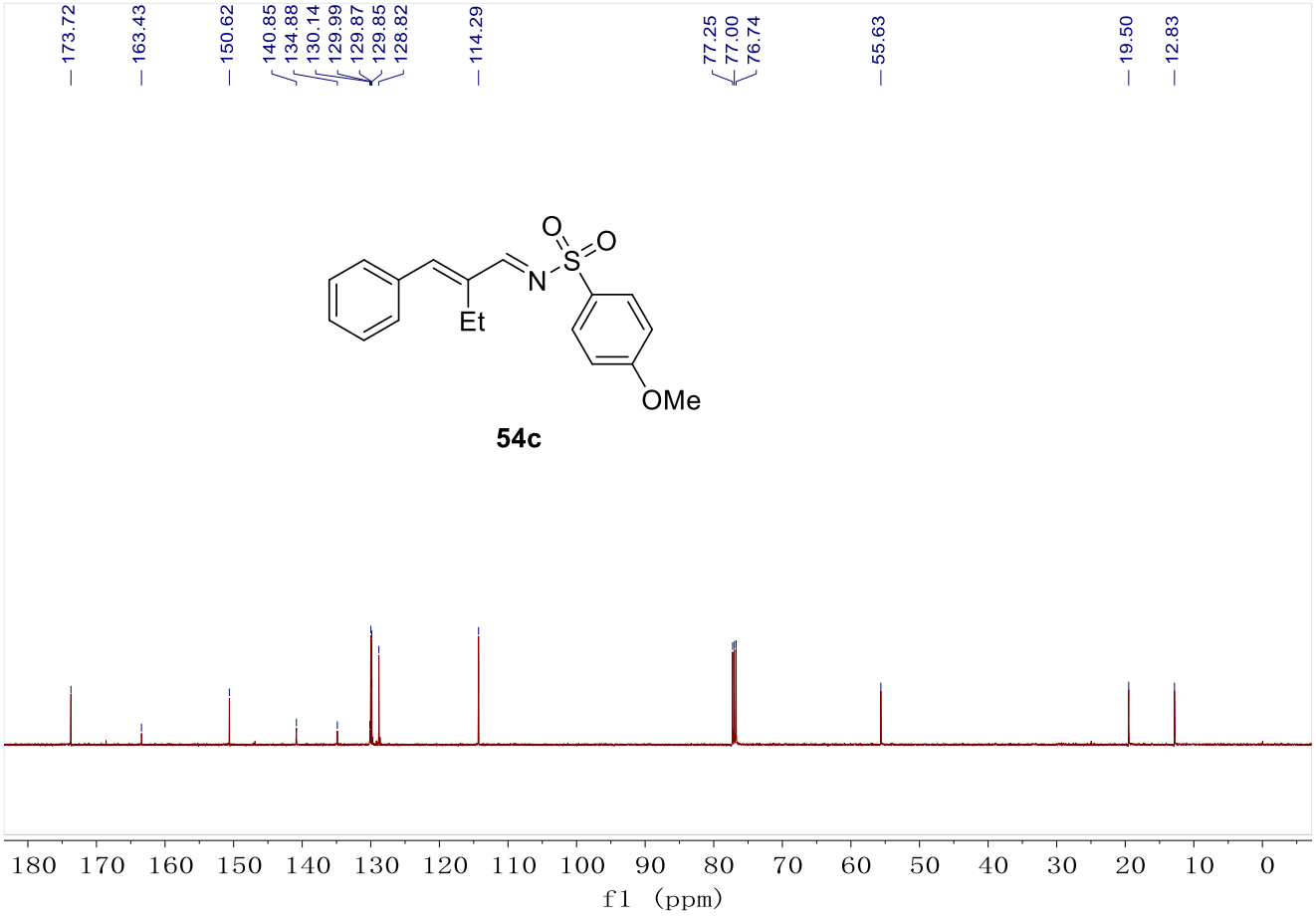

140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


8.46
7.83
7.81
7.33
7.31
7.26
6.48
6.47
6.45
2.43
2.39
2.37
2.36
2.35
2.34
2.33
2.32
2.30
1.61
1.56
1.54
1.53
1.51
1.49
1.47
0.98
0.96
0.94
0.92
-0.01
Et
NTs
Et
52c
1.00
2.00
2.02
1.01
3.03
4.00
2.03
6.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


173.64
156.92
144.08
141.18
135.73
129.62
127.71
77.32
77.00
76.68
31.35
21.89
21.62
18.65
13.87
13.15
Et
NTs
Et
52c
220 200 180 160 140 120 100 80 60 40 20 0 -20


8.62
7.92
7.90
7.48
7.47
7.47
7.47
7.46
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.42
7.41
7.41
7.41
7.40
7.26
7.22
7.01
7.00
3.88
2.68
2.66
2.65
2.63
1.59
1.15
1.13
1.12
0.00
O
O
S
N
Et
OMe
1.00
2.07
5.07
1.04
2.04
3.07
2.01
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

54c


173.72
163.43
150.62
140.85
134.88
130.14
129.99
129.87
129.85
128.82
114.29
77.25
77.00
76.74
55.63
19.50
12.83
O
O
S
N
Et
OMe
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

54c