Supporting Information

for

Nickel-Catalyzed Acetamidation and Lactamization of Arylboronic Acids

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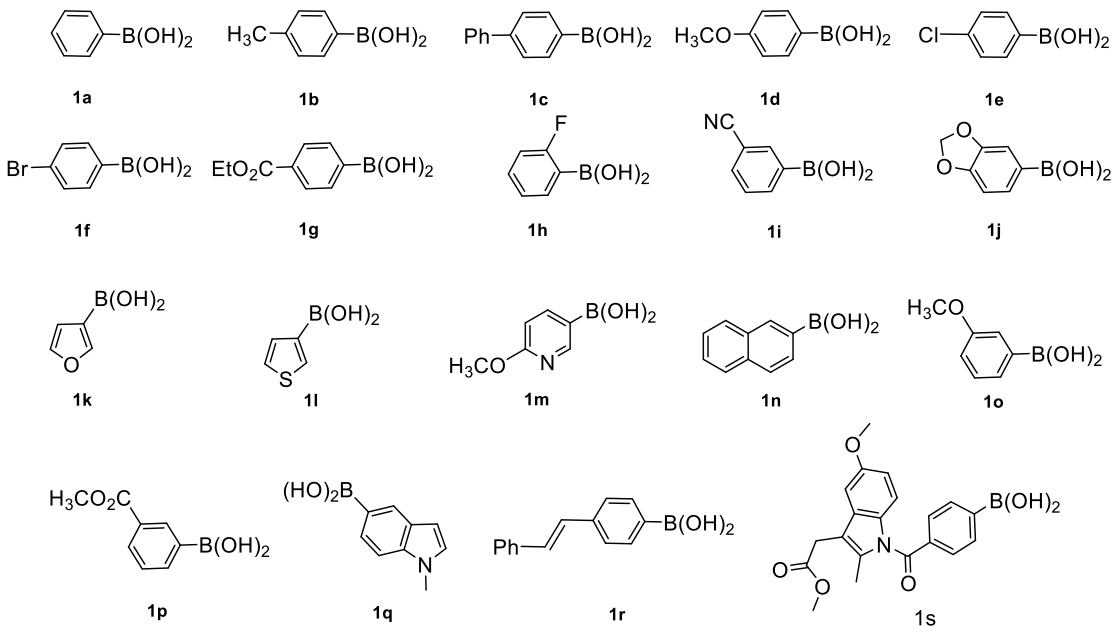
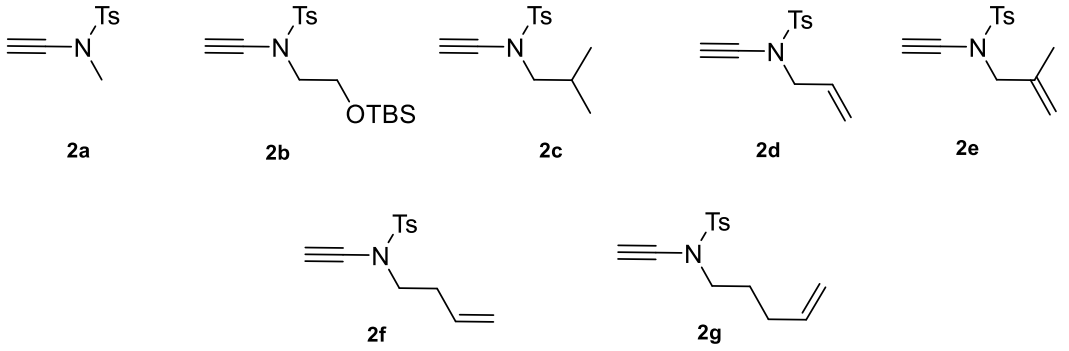
1. General Information:

Infrared spectra were obtained on a FTIR spectrometer. ^{1}H NMR and ^{13}C NMR spectra were recorded on BRUKER AVANCE III 400 spectrometer. $CDCl_3$ was used as solvent. Chemical shifts were referenced relative to residual solvent. The following abbreviations are used to describe peak patterns where appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (*J*) are reported in Hertz (Hz). HRMS were performed on Agilent Technologies 6224 TOF LC/MS (ESI). Melting points were measured with micro melting point apparatus.

Ethyl acetate (EA), Acetonitrile, Petroleum ether (PE), *N*-hydroxyphthalimide (NHPI), Triethylamine, 4,4'-di-*tert*-butyl-2,2'-bipyridine (di-*t*Bubipy), $NiCl_2$-$6H_2O$, DMF and Dioxane were commercial available. Boronic acids (**1a-1o, 1r**) were commercial available and (**1p, 1q, 1s**) were prepared according the literature.[1, 2, 3] The Ynamides (**2a-2g**) were prepared according the literature.[4]



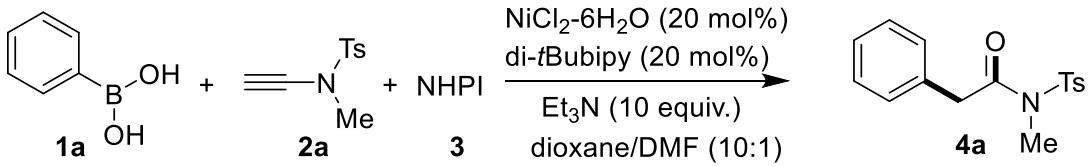


2. Typical Procedure for the synthesis of 4a and 5a.

a) Preparation of $NiCl_2$•$6H_2O$/di-*t*Bubipy Stock Solution (0.05 M in DMF)

A 25 mL two-neck flask was charged with $NiCl_2$•$6H_2O$ (118.5 mg, 0.5 mmol) and di-*t*Bubipy (134.2 mg, 0.5 mmol). The flask was then evacuated and purged with Argon three times. DMF (10.0 mL) was added and the resulting mixture was stirred at room temperature for several hours to give a homogeneous green solution, which could be used for several days without appreciable deterioration

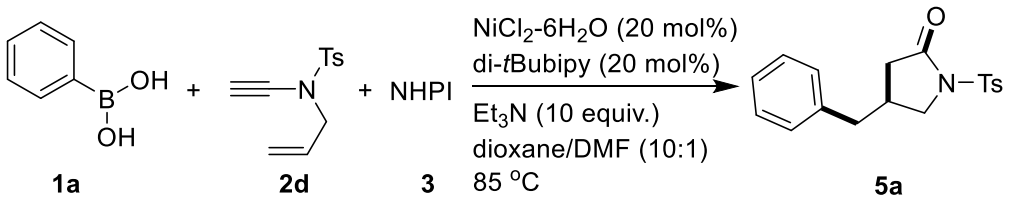
b) Nickel-Catalyzed Acetamidation reaction.



A schlenk tube was added *N*-ethynyl-*N*, 4-dimethylbenzenesulfonamide **2a** (20.9 mg, 0.1 mmol) and NHPI **3** (17.1 mg, 0.105 mmol), then evacuated and purged with Argon three times. Afterwards, CH_2Cl_2 (2 mL) were added as solvent. The solution was stirred under reflux for 6 hours, then concentrated and dissolved in dioxane (4 mL). Phenylboronic acid **1a** (36.3 mg, 0.3 mmol) was added quickly. Et_3N (139 μL, 1 mmol) and a solution of $NiCl_2$•$6H_2O$/di-*t*Bubipy (0.05M in DMF, 0.4 mL) was added successively and the schlenk was immediately placed in a preheated 85 °C oil bath under stirring. After the reaction was fully consumed about 3 hours, the reaction mixture was allowed to cool to room temperature, diluted with CH_2Cl_2, washed with water and brine, dried over Na_2SO_4 and concentrated under vacuum. The purification was performed by flash column chromatography on silica gel using ethyl

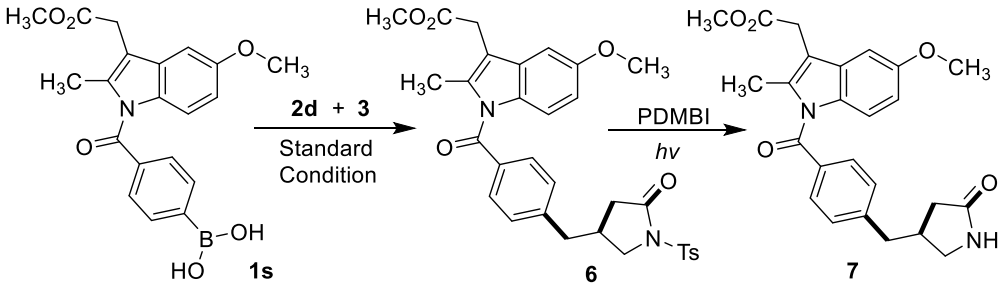
acetate/petroleum ether (v/v, 1:15) as eluent to give **4a** (28.9 mg, 95% yield).

c) **Nickel-Catalyzed Lactamization reaction.**



A schlenk tube was added *N*-ethynyl-*N*, 4-dimethylbenzenesulfonamide **2d** (23.5 mg, 0.1 mmol) and NHPI **3** (17.1 mg, 0.105 mmol), then evacuated and purged with Argon three times. Afterwards, CH_2Cl_2 (2 mL) were added as solvent. The solution was stirred under reflux for 6 hours, then concentrated and dissolved in dioxane (4 mL). Phenylboronic acid **1a** (36.3 mg, 0.3 mmol) was added quickly. Et_3N (139 μL, 1 mmol) and a solution of $NiCl_2$•$6H_2O$/di-*t*Bubipy (0.05M in DMF, 0.4 mL) was added successively and the schlenk was immediately placed in a preheated 85 °C oil bath under stirring. After the reaction was fully consumed about 3 hours, the reaction mixture was allowed to cool to room temperature, diluted with CH_2Cl_2, washed with water and brine, dried over Na_2SO_4 and concentrated under vacuum. The purification was performed by flash column chromatography on silica gel using ethyl acetate/petroleum ether (v/v, 1:10) as eluent to give **5a** (22.0 mg, 67% yield).

3. Synthetic Application

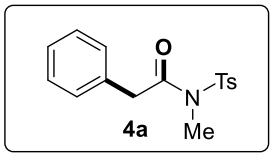


A two-neck flask was added *N*-ethynyl-*N*, 4-dimethylbenzenesulfonamide **2d** (117.5 mg, 0.5 mmol) and NHPI **3** (85.6 mg, 0.525 mmol), then evacuated and purged with Argon three times. Afterwards, CH_2Cl_2 (10 mL) were added as solvent. The solution was stirred under reflux for 6 hours, then concentrated and dissolved in dioxane (20 mL). **1s** (571.5 mg, 1.5 mmol) was added quickly. Et_3N (0.69 mL, 5

mmol) and a solution of $NiCl_2$•$6H_2O$/di-*t*Bubipy (0.05M in DMF, 2 mL) was added successively and the flask was immediately placed in a preheated 85 °C oil bath under stirring. After the reaction was fully consumed about 3 hours, the reaction mixture was allowed to cool to room temperature, diluted with CH_2Cl_2, washed with water and brine, dried over Na_2SO_4 and concentrated under vacuum. The purification was performed by flash column chromatography on silica gel using ethyl acetate/petroleum ether (v/v, 1:5) as eluent to give **6** (132.1 mg, 45% yield).

A mixture of **6** (117.6 mg, 0.2 mmol) and PDMBI (53.7 mg, 0.24 mmol) in 2.1 mL of acetonitrile containing 30 μL of water was irradiated with a Pyrex filtered (>300 nm) high-pressure mercury lamp under argon atmosphere at ambient temperature. After completion of the reaction as monitored by TLC, the solvent was removed under reduced pressure and **7** (59.6 mg, 69 % yield) was isolated from the residual by flash column chromatography using CH_2Cl_2/methanol (v/v, 50:1) as eluent.

4. Characterization of 4.



N-methyl-2-phenyl-*N*-tosylacetamide

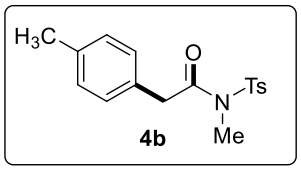
Oil (28.9 mg, 95% yield), R_f = 0.7 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.27 – 7.17 (m, 5H), 7.06 (d, *J* = 7.9 Hz, 2H), 3.97 (s, 2H), 3.20 (s, 3H), 2.37 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.40, 145.09, 136.10, 133.54, 129.99, 129.49, 128.70, 127.64, 127.28, 43.19, 33.41, 21.76.

IR (KBr) *v* 3067, 3037, 3009, 2961, 2920, 1699, 1595, 1514, 1458, 1413, 1341, 1245, 1162, 1073, 859, 807, 718, 669, 562 cm^{-1}.

HRMS (ESI) calcd for $C_{16}H_{18}NO_3S$ ($M+H^+$): 304.1007; Found: 304.1009.



N-methyl-2-(p-tolyl)-*N*-tosylacetamide

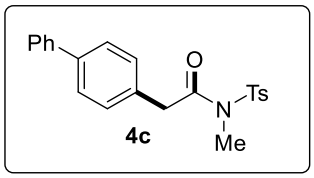
White solid, m. p. 96.0-96.7 ºC (27.6 mg, 87% yield), R_f = 0.7 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 4.00 (s, 2H), 3.29 (s, 3H), 2.46 (s, 3H), 2.33 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.62, 145.03, 136.93, 136.18, 130.40, 129.95, 129.40, 129.33, 127.67, 42.81, 33.41, 21.76, 21.19.

IR (KBr) *v* 3054, 3017, 2981, 2967, 1698, 1595, 1518, 1458, 1411, 1341, 1160, 1069, 857, 812, 724, 671 cm^{-1}.

HRMS (ESI) calcd for $C_{17}H_{20}NO_3S$ ($M+H^+$): 318.1164; Found: 318.1160.



2-([1,1'-biphenyl]-4-yl)-*N*-methyl-*N*-tosylacetamide

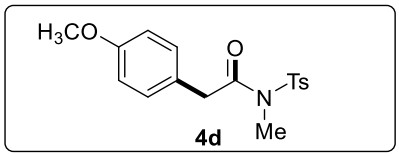
White solid, m. p. 88.7-89.4 ºC (34.2 mg, 90% yield), R_f = 0.7 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.50 – 7.40 (m, 3H), 7.39 – 7.31 (m, 3H), 7.28 – 7.19 (m, 3H), 7.12 (d, *J* = 8.2 Hz, 2H), 4.01 (s, 2H), 3.23 (s, 3H), 2.35 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.53, 145.16, 140.26, 136.08, 134.45, 132.54, 130.03, 129.94, 128.89, 127.64, 127.43, 127.16, 115.78, 42.84, 33.49, 21.76.

IR (KBr) *v* 3053, 2960, 2923, 1698, 1600, 1486, 1411, 1343, 1253, 1162, 1073, 860, 814, 764, 713, 692, 539 cm^{-1}.

HRMS (ESI) calcd for $C_{22}H_{22}NO_3S$ ($M+H^+$): 380.1320; Found: 380.1321.



2-(4-methoxyphenyl)-*N*-methyl-*N*-tosylacetamide

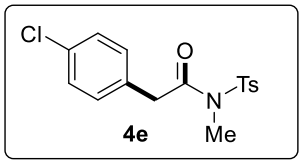
White solid, m. p. 108.8-109.5 ºC (22.3 mg, 67% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 3.98 (s, 2H), 3.79 (s, 3H), 3.29 (s, 3H), 2.45 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.78, 158.82, 145.03, 136.16, 134.39, 130.53, 129.96, 127.63, 114.11, 55.35, 42.29, 33.39, 21.73.

IR (KBr) *v* 3049. 2958, 2928, 1701, 1610, 1511, 1459, 1342, 1243, 1162, 1073, 1034, 861, 813, 718, 670, 566 cm^{-1}.

HRMS (ESI) calcd for $C_{17}H_{20}NO_4S$ ($M+H^+$): 334.1113; Found: 334.1109.



2-(4-chlorophenyl)-*N*-methyl-*N*-tosylacetamide

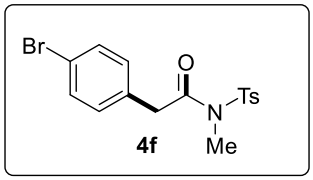
White solid, m. p. 112.2-113.0 ºC (24.6 mg, 73% yield), R_f = 0.7 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 4.00 (s, 2H), 3.25 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.08, 145.29, 136.06, 133.30, 132.10, 130.97, 130.12, 128.81, 127.54, 42.47, 33.45, 21.79.

IR (KBr) *v* 3068, 2961, 2920. 1697, 1595, 1491, 1413, 1340, 1162, 1073, 855, 807, 704, 677, 548 cm^{-1}.

HRMS (ESI) calcd for $C_{16}H_{17}ClNO_3S$ ($M+H^+$): 338.0618; Found: 338.0615.



2-(4-bromophenyl)-*N*-methyl-*N*-tosylacetamide

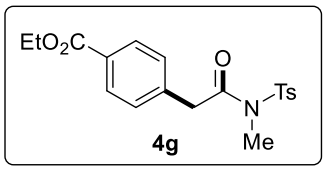
White solid, m. p. 127.1-128.2 ºC (23.4 mg, 61% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:10).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 4.03 (s, 2H), 3.28 (s, 3H), 2.46 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.98, 145.30, 136.01, 132.60, 131.76, 131.33, 130.12, 127.53, 121.39, 42.53, 33.45, 21.80.

IR (KBr) *v* 3065, 2960, 2923, 1697, 1592, 1486, 1410, 1340, 1244, 1161, 1071, 854, 805, 702, 672, 629, 540 cm^{-1}.

HRMS (ESI) calcd for $C_{16}H_{17}BrNO_3S$ ($M+H^+$): 382.0113; Found: 382.0111.



Ethyl 4-(2-((*N*,4-dimethylphenyl)sulfonamido)-2-oxoethyl)benzoate

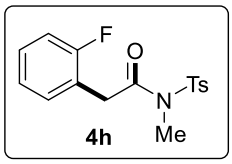
White solid, 113.1-113.9 ºC (25 mg, 66% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.72 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.3 Hz, 2H), 4.37 (d, *J* = 7.2 Hz, 2H), 4.13 (s, 2H), 3.29 (s, 3H), 2.46 (s, 3H), 1.39 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.78, 166.47, 145.33, 138.70, 135.98, 130.13, 129.90, 129.60, 129.54, 127.55, 61.11, 43.13, 33.46, 21.80, 14.47.

IR (KBr) *v* 3056, 2982, 2923, 1707, 1610, 1473, 1420, 1348, 1281, 1161, 1075, 1022, 850, 805, 767, 700, 673, 544 cm^{-1}.

HRMS (ESI) calcd for $C_{19}H_{22}NO_5S$ ($M+H^+$): 376.1219; Found: 376.1217.



2-(2-fluorophenyl)-*N*-methyl-*N*-tosylacetamide

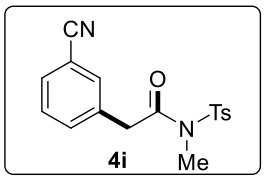
White solid, m. p. 88.9-89.7 ºC (14.3 mg, 44% yield), R_f = 0.6 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.19 (s, 1H), 7.07 – 6.90 (m, 3H), 4.02 (s, 2H), 3.24 (s, 3H), 2.39 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.46, 161.09 (d, *J* = 246.1 Hz), 145.23 , 136.09 , 131.64 (d, *J* = 3.8 Hz), 130.15 , 129.33 (d, *J* = 8.2 Hz), 127.54 , 124.27 (d, *J* = 3.6 Hz), 121.30 (d, *J* = 15.9 Hz), 115.41 (d, *J* = 21.5 Hz), 37.06 (d, *J* = 3.0 Hz), 33.40 , 21.81.

IR (KBr) *v* 3048, 2962, 2926, 1706, 1590, 1493, 1455, 1411, 1351, 1233, 1172, 1076, 873, 812, 762, 738, 705, 666, 618, 543 cm^{-1}.

HRMS (ESI) calcd for $C_{16}H_{17}FNO_3S$ ($M+H^+$): 322.0913; Found: 322.0913.



2-(3-cyanophenyl)-*N*-methyl-*N*-tosylacetamide

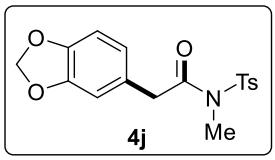
White solid, m. p. 97.2-98.3 ºC (18 mg, 55% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 2.8 Hz, 1H), 7.45 – 7.40 (m, 2H), 7.39 – 7.35 (m, 3H), 4.11 (s, 2H), 3.30 (s, 3H), 2.48 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.45, 145.62, 135.19, 134.41, 133.21, 131.05, 130.30, 129.85, 129.41, 127.42, 118.68, 112.67, 42.47, 33.47, 21.83.

IR (KBr) *v* 2920, 2223, 1714, 1595, 1356, 1162, 1073, 847, 811, 709, 672, 535 cm^{-1}.

HRMS (ESI) calcd for $C_{17}H_{17}N_2O_3S$ ($M+H^+$): 329.0960; Found: 329.0958.



2-(benzo[*d*][1,3]dioxol-5-yl)-*N*-methyl-*N*-tosylacetamide

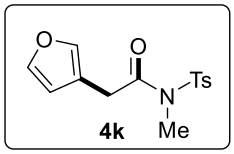
White solid, m. p. 89.1-90.0 ºC (17 mg, 49% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 7.9 Hz, 1H), 6.63 – 6.53 (m, 2H), 5.93 (s, 2H), 3.95 (s, 2H), 3.29 (s, 3H), 2.46 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.60, 147.87, 146.88, 136.17, 134.45, 130.03, 127.62, 127.04, 122.71, 110.02, 108.40, 101.17, 42.77, 33.45, 21.78.

IR (KBr) *v* 3065. 2998, 2976, 1723, 1642, 1428, 1342, 1208, 1073, 1032, 855, 843, 782, 671, 568 cm^{-1}.

HRMS (ESI) calcd for $C_{17}H_{18}NO_5S$ ($M+H^+$): 348.0906; Found: 348.0908.



2-(furan-3-yl)-*N*-methyl-*N*-tosylacetamide

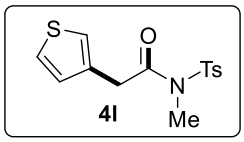
White solid, m. p. 95.6-97.1 ºC (13.4 mg, 46% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.37 – 7.23 (m, 4H), 6.28 – 6.22 (m, 1H), 3.85 (s, 2H), 3.24 (s, 3H), 2.40 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.97, 143.10, 140.84, 136.10, 134.46, 130.11, 127.57, 123.74, 111.62, 33.40, 25.17, 21.79.

IR (KBr) *v* 3126, 2963, 2924, 1699, 1597, 1497, 1465, 1347, 1268, 1172, 1078, 1021, 908, 867, 814, 689, 543 cm^{-1}.

HRMS (ESI) calcd for $C_{14}H_{16}NO_4S$ ($M+H^+$): 294.0800; Found: 294.0799.



N-methyl-2-(thiophen-3-yl)-*N*-tosylacetamide

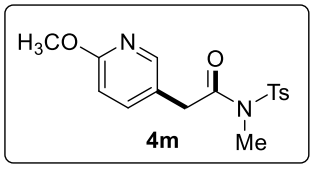
White solid, m. p. 114.5-115.7 ºC (17.8 mg, 58% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.24 – 7.20 (m, 1H), 7.02 – 6.97 (m, 1H), 6.92 – 6.86 (m, 1H), 4.05 (s, 2H), 3.23 (s, 3H), 2.40 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.97, 145.15, 136.05, 133.23, 130.05, 128.72, 127.59, 125.87, 123.35, 37.93, 33.38, 21.78.

IR (KBr) *v* 3094, 2960, 2920, 1698, 1595, 1468, 1405, 1347, 1255, 1235, 1172, 1073, 837, 802, 757, 685, 591, 536 cm^{-1}.

HRMS (ESI) calcd for $C_{14}H_{16}NO_3S_2$ ($M+H^+$): 310.0572; Found: 310.0570.



2-(6-methoxypyridin-3-yl)-*N*-methyl-*N*-tosylacetamide

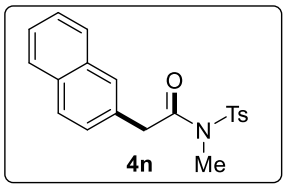
Solid (14.7 mg, 44% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.90 (d, *J* = 2.5 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.40 (dd, J_1 = 8.5, J_2 = 2.5 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 6.70 (d, *J* = 8.5 Hz, 1H), 3.98 (s, 2H), 3.91 (s, 3H), 3.31 (s, 3H), 2.47 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.25, 163.54, 147.26, 145.35, 140.12, 136.07, 130.19, 127.51, 122.09, 110.87, 53.60, 39.51, 33.46, 21.82.

IR (KBr) *v* 3058, 3014, 2978, 2956, 1696, 1673, 1480, 1358, 1076, 867, 765, 673 556 cm^{-1}.

HRMS (ESI) calcd for $C_{16}H_{19}N_2O_4S$ ($M+H^+$): 335.1066; Found: 335.1066.



N-methyl-2-(naphthalen-2-yl)-*N*-tosylacetamide

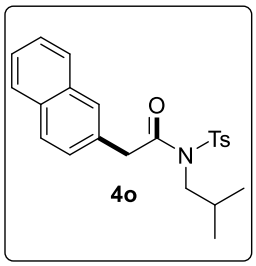
White solid, m. p. 114.6-115.7 ºC (34.2 mg, 92% yield), R_f = 0.8 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 – 7.66 (m, 2H), 7.64 – 7.59 (m, 3H), 7.43 (d, *J* = 1.7 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.22 – 7.13 (m, 3H), 4.12 (s, 2H), 3.23 (s, 3H), 2.32 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.40, 145.08, 136.08, 133.44, 132.55, 130.98, 129.95, 128.34, 128.09, 127.74, 127.72, 127.60, 127.49, 126.24, 126.00, 43.31, 33.49, 21.72.

IR (KBr) *v* 3054, 2960, 2920, 1747, 1695, 1596, 1458, 1343, 1161, 1072, 847, 810, 712, 673, 574, 555 cm^{-1}.

HRMS (ESI) calcd for $C_{20}H_{20}NO_3S$ ($M+H^+$): 354.1164; Found: 354.1161.



N-isobutyl-2-(naphthalen-2-yl)-*N*-tosylacetamide

White solid, m. p. 70.9-72.1 ºC (32 mg, 81% yield), R_f = 0.7 (EtOAc/Petroleum ether 1:5).

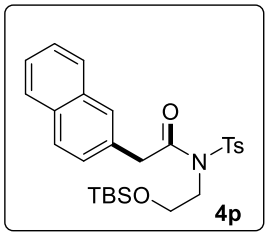
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 – 7.68 (m, 1H), 7.67 – 7.62 (m, 3H), 7.61 – 7.56 (m, 1H), 7.40 – 7.31 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.11 – 7.05 (m, 1H), 4.04 (s, 2H), 3.62 (d, *J* = 7.5 Hz, 2H), 2.33 (s, 3H), 2.16 – 1.96 (m, 1H), 0.88 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.60, 144.90, 137.06, 133.42, 132.53, 131.08,

129.95, 129.92, 128.27, 128.03, 127.72, 127.63, 127.44, 126.21, 125.96, 54.11, 43.29, 28.80, 21.72, 20.12.

IR (KBr) *v* 3056, 2961, 2873, 1693, 1595, 1465, 1435, 1347, 1312, 1162, 1086, 1017, 848, 815, 727, 672, 578, 541 cm^{-1}.

HRMS (ESI) calcd for $C_{23}H_{26}NO_3S$ ($M+H^+$): 396.1633; Found: 396.1632.



4p

N-(2-((tert-butyldimethylsilyl)oxy)ethyl)-2-(naphthalen-2-yl)-*N*-tosylacetamide

White solid, m. p. 106.8-108.1 ^oC (38 mg, 76% yield), R_f = 0.6 (EtOAc/Petroleum ether 1:5).

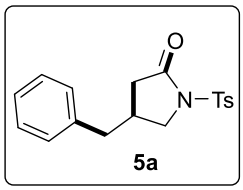
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82 – 7.72 (m, 3H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.45 – 7.34 (m, 3H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 1.6 Hz, 1H), 4.09 (s, 2H), 3.94 (t, *J* = 5.5 Hz, 2H), 3.85 (t, *J* = 5.6 Hz, 2H), 2.37 (s, 3H), 0.86 (s, 9H), 0.05 (s, 6H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.51, 144.82, 136.82, 133.47, 132.56, 130.90, 129.70, 128.41, 128.17, 127.85, 127.74, 127.71, 127.31, 126.26, 126.01, 62.19, 48.67, 43.16, 26.02, 21.75, 18.41, -5.31.

IR (KBr) *v* 3050, 2950, 2928, 1884, 1693, 1596, 1464, 1411, 1351, 1294, 1255, 1165, 1118, 1067, 938, 838, 779, 667, 572 cm^{-1}.

HRMS (ESI) calcd for $C_{27}H_{36}NO_4SSi$ ($M+H^+$): 498.2134; Found: 498.2135.

5. Characterization of 5.



5a

4-benzyl-1-tosylpyrrolidin-2-one

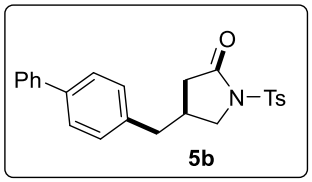
Oil (22 mg, 67% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.84 (d, *J* = 8.3 Hz, 2H), 7.31 – 7.20 (m, 4H), 7.19 – 7.13 (m, 1H), 7.06 – 7.00 (m, 2H), 3.85 (dd, J_1 = 10.0, J_2 = 6.6 Hz, 1H), 3.49 (dd, J_1 = 10.0, J_2 = 5.8 Hz, 1H), 2.77 – 2.54 (m, 3H), 2.46 (dd, J_1 = 17.3, J_2 = 7.4 Hz, 1H), 2.37 (s, 3H), 2.15 (dd, J_1 = 17.3, J_2 = 6.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.63, 145.34, 138.18, 135.29, 129.83, 128.94, 128.80, 128.20, 126.99, 52.04, 39.66, 38.64, 33.63, 21.83.

IR (KBr) *v* 3067, 2961, 2924, 1740, 1361, 1261, 1167, 1088, 1020, 876, 803, 703, 669 cm^{-1}.

HRMS (ESI) calcd for $C_{18}H_{20}NO_3S$ ($M+H^+$): 330.1164; Found: 330.1163.



5b

4-([1,1'-biphenyl]-4-ylmethyl)-1-tosylpyrrolidin-2-one

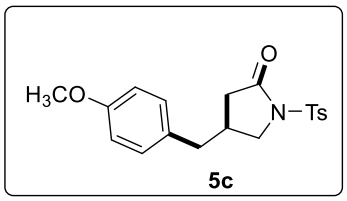
Solid (23 mg, 57% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.94 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.49 – 7.42 (m, 2H), 7.39 – 7.33 (m, 3H), 7.19 (d, *J* = 8.1 Hz, 2H), 3.97 (dd, J_1 = 10.0, J_2 = 6.5 Hz, 1H), 3.61 (dd, J_1 = 10.0, J_2 = 5.7 Hz, 1H), 2.84 – 2.66 (m, 3H), 2.58 (dd, J_1 = 17.3, J_2 = 7.4 Hz, 1H), 2.45 (s, 3H), 2.27 (dd, J_1 = 17.3, J_2 = 6.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.61, 145.35, 140.74, 139.97, 137.19, 135.28, 129.84, 129.24, 128.94, 128.20, 127.63, 127.46, 127.13, 52.04, 39.28, 38.65, 33.58, 21.82.

IR (KBr) *v* 3025, 2960, 1739, 1595, 1483, 1350, 1201, 1164, 1119, 1080, 952, 811, 761, 656, 592, 556 cm^{-1}.

HRMS (ESI) calcd for $C_{24}H_{24}NO_3S$ ($M+H^+$): 406.1477; Found: 406.1476.



5c

4-(4-methoxybenzyl)-1-tosylpyrrolidin-2-one

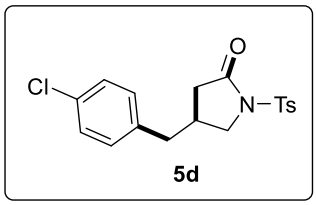
White solid m. p. 108.6-109.9 ºC (19.4 mg, 54% yield), R_f = 0.3 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 3.91 (dd, J_1 = 10.0, J_2 = 6.5 Hz, 1H), 3.80 (s, 3H), 3.55 (dd, J_1 = 10.0, J_2 = 5.5 Hz, 1H), 2.71 – 2.47 (m, 4H), 2.45 (s, 3H), 2.21 (dd, J_1 = 17.0, J_2 = 6.4 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.72, 158.59, 145.32, 135.30, 130.18, 129.82, 129.78, 128.19, 114.30, 55.42, 52.00, 38.78, 38.59, 33.77, 21.83.

IR (KBr) *v* 3067, 2998, 2923, 1735, 1596, 1513, 1353, 1248, 1166, 1123, 1033, 956, 811, 741, 663, 566, 547 cm^{-1}.

HRMS (ESI) calcd for $C_{19}H_{22}NO_4S$ ($M+H^+$): 360.1270; Found: 360.1268.



5d

4-(4-chlorobenzyl)-1-tosylpyrrolidin-2-one

oil (18 mg, 50% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:4).

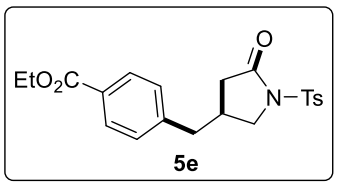
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 3.92 (dd, J_1 = 10.1, J_2 = 6.6 Hz, 1H), 3.55 (dd, J_1 = 10.1, J_2 = 5.7 Hz, 1H), 2.78 – 2.58 (m, 3H), 2.53 (dd, J_1 = 17.1, J_2 = 7.5 Hz, 1H), 2.46 (s, 3H), 2.21 (dd, J_1 = 17.1, J_2 = 6.6 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.38, 145.43, 136.60, 135.16, 132.86, 130.12, 129.86, 129.08, 128.18, 51.85, 38.95, 38.50, 33.46, 21.84.

IR (KBr) *v* 3056, 2952, 2921, 2858, 1738, 1596, 1490, 1359, 1168, 1090, 957, 808,

744, 664, 600, 555 cm^{-1}.

HRMS (ESI) calcd for $C_{18}H_{19}ClNO_3S$ ($M+H^+$): 364.0774; Found: 364.0773.



5e

Ethyl 4-((5-oxo-1-tosylpyrrolidin-3-yl)methyl)benzoate

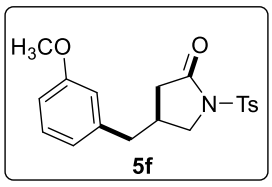
Oil (21 mg, 52% yield), R_f = 0.2 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.99 (d, *J* = 8.2 Hz, 2H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.2 Hz, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.92 (dd, J_1 = 10.1, J_2 = 7.0 Hz, 1H), 3.55 (dd, J_1 = 10.1, J_2 = 6.1 Hz, 1H), 2.86 – 2.63 (m, 3H), 2.54 (dd, J_1 = 17.3, J_2 = 7.7 Hz, 1H), 2.45 (s, 3H), 2.22 (dd, J_1 = 17.3, J_2 = 7.2 Hz, 1H), 1.40 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.31, 166.43, 145.44, 143.35, 135.18, 130.22, 129.86, 129.40, 128.79, 128.20, 61.15, 51.90, 39.58, 38.54, 33.35, 21.83, 14.46.

IR (KBr) *v* 3052, 2980, 2927, 1736, 1710, 1493, 1348, 1281, 1160, 1072, 805, 767, 700, 660, 556 cm^{-1}.

HRMS (ESI) calcd for $C_{21}H_{24}NO_5S$ ($M+H^+$): 402.1375; Found: 402.1377.



5f

4-(3-methoxybenzyl)-1-tosylpyrrolidin-2-one

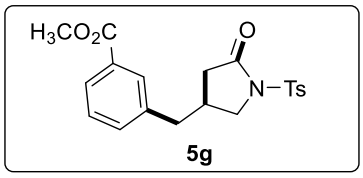
Oil (21 mg, 58% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.20 (m, 1H), 6.83 – 6.75 (m, 1H), 6.72 – 6.63 (m, 2H), 3.92 (dd, J_1 = 9.9, J_2 = 6.6 Hz, 1H), 3.80 (s, 3H), 3.56 (dd, J_1 = 9.9, J_2 = 5.7 Hz, 1H), 2.76 – 2.60 (m, 3H), 2.54 (dd, J_1 = 17.2, J_2 = 7.6 Hz, 1H), 2.45 (s, 3H), 2.23 (dd, J_1 = 17.2, J_2 = 6.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.65, 159.97, 145.35, 139.74, 135.22, 129.94, 129.83, 128.17, 121.09, 114.78, 111.94, 55.32, 52.02, 39.64, 38.64, 33.52, 21.83.

IR (KBr) *v* 3068, 2958, 2921, 1738, 1599, 1489, 1457, 1359, 1262, 1168, 1035, 957, 875, 812, 740, 700, 664, 599, 557 cm^{-1}.

HRMS (ESI) calcd for $C_{19}H_{22}NO_4S$ ($M+H^+$): 360.1270; Found: 360.1269.



5g

Methyl 3-((5-oxo-1-tosylpyrrolidin-3-yl)methyl)benzoate

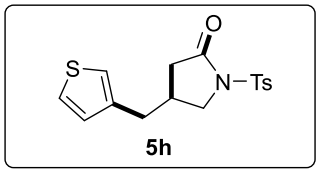
Oil (15 mg, 39% yield), R_f = 0.3 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.96 – 7.86 (m, 3H), 7.80 (d, *J* = 1.7 Hz, 1H), 7.46 – 7.23 (m, 4H), 4.04 – 3.80 (m, 4H), 3.55 (dd, J_1 = 10.1, J_2 = 5.9 Hz, 1H), 2.82 – 2.60 (m, 3H), 2.54 (dd, J_1 = 17.9, J_2 = 7.0 Hz, 1H), 2.45 (s, 3H), 2.22 (dd, J_1 = 17.9, J_2 = 6.1 Hz, 1H).

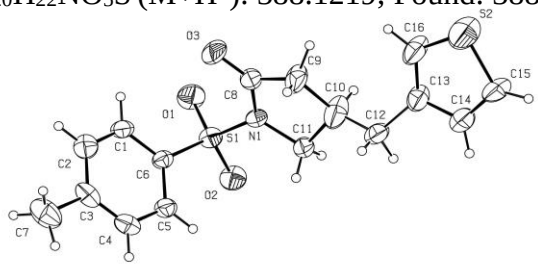
^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.36, 166.93, 145.40, 138.54, 135.14, 133.33, 130.78, 129.85, 129.76, 129.03, 128.25, 128.15, 52.35, 51.90, 39.33, 38.50, 33.45, 21.82.

IR (KBr) *v* 3067, 2958, 2919, 2880, 1734, 1594, 1438, 1362, 1294, 1275, 1161, 1124, 1040, 963, 808, 756, 702, 662, 602, 557 cm^{-1}.

HRMS (ESI) calcd for $C_{20}H_{22}NO_5S$ ($M+H^+$): 388.1219; Found: 388.1221.



5h



4-(thiophen-3-ylmethyl)-1-tosylpyrrolidin-2-one

Yellow solid (16 mg, 48% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:5).

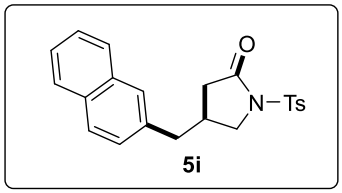
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.32 – 7.28 (m, 1H), 6.98 – 6.92 (m, 1H), 6.91 – 6.84 (m, 1H), 3.96 (dd, J_1 = 10.1, J_2

= 6.9 Hz, 1H), 3.57 (dd, J_1 = 10.1, J_2 = 5.8 Hz, 1H), 2.83 – 2.61 (m, 3H), 2.56 (dd, J_1= 17.2, J_2 = 7.8 Hz, 1H), 2.45 (s, 3H), 2.22 (dd, J_1 = 17.2, J_2 = 6.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.59, 145.37, 138.44, 135.21, 129.84, 128.17, 127.87, 126.55, 121.97, 52.08, 38.61, 34.13, 32.90, 21.83.

IR (KBr) *v* 3120, 2923, 2856, 1734, 1595, 1487, 1353, 1287, 1188, 1168, 1127, 1087, 958, 812, 776, 664, 599, 557 cm^{-1}.

HRMS (ESI) calcd for $C_{16}H_{18}NO_3S_2$ ($M+H^+$): 336.0728; Found: 336.0729.



5i

4-(naphthalen-2-ylmethyl)-1-tosylpyrrolidin-2-one

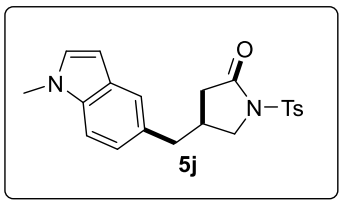
Oil (21 mg, 55% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, J = 8.3 Hz, 2H), 7.85 – 7.74 (m, 3H), 7.58 – 7.44 (m, 3H), 7.35 (d, J = 8.0 Hz, 2H), 7.24 (dd, J_1 = 8.4, J_2 = 1.6 Hz, 1H), 3.94 (dd, J_1 = 10.1, J_2 = 7.1 Hz, 1H), 3.63 (dd, J_1 = 10.1, J_2 = 6.2 Hz, 1H), 2.94 – 2.70 (m, 3H), 2.56 (dd, J_1 = 17.4, J_2 = 7.8 Hz, 1H), 2.45 (s, 3H), 2.29 (dd, J_1 = 17.4, J_2 = 7.3 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.64, 145.35, 135.62, 135.22, 133.56, 132.41, 129.83, 128.69, 128.17, 127.79, 127.60, 127.37, 126.90, 126.49, 125.91, 52.05, 39.81, 38.63, 33.48, 21.83.

IR (KBr) *v* 3051, 2919, 2858, 1736, 1596, 1484, 1358, 1168, 1092, 956, 814, 749, 663, 600, 557 cm^{-1}.

HRMS (ESI) calcd for $C_{22}H_{22}NO_3S$ ($M+H^+$): 380.1320; Found: 380.1318.



5j

4-((1-methyl-1H-indol-5-yl)methyl)-1-tosylpyrrolidin-2-one

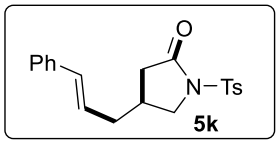
Solid (25 mg, 65% yield), R_f = 0.2 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.40 – 7.31 (m, 3H), 7.30 – 7.24 (m, 1H), 7.07 (d, *J* = 3.1 Hz, 1H), 6.96 (dd, J_1 = 8.4, J_2 = 1.6 Hz, 1H), 6.51 – 6.38 (m, 1H), 3.91 (dd, J_1 = 10.0, J_2 = 7.0 Hz, 1H), 3.80 (s, 3H), 3.61 (dd, J_1 = 10.0, J_2 = 6.1 Hz, 1H), 2.87 – 2.63 (m, 3H), 2.53 (dd, J_1 = 17.3, J_2 = 7.7 Hz, 1H), 2.45 (s, 3H), 2.27 (dd, J_1 = 17.3, J_2 = 7.3 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.98, 145.23, 135.80, 135.34, 129.80, 129.52, 128.92, 128.82, 128.16, 122.47, 120.72, 109.60, 100.68, 52.15, 39.77, 38.69, 34.23, 33.03, 21.83.

IR (KBr) *v* 3109, 3078, 2997, 2928, 1739, 1594, 1496, 1362, 1173, 1062, 953, 807, 749, 659, 609, 554 cm^{-1}.

HRMS (ESI) calcd for $C_{21}H_{23}N_2O_3S$ ($M+H^+$): 383.1429; Found: 383.1426.



4-cinnamyl-1-tosylpyrrolidin-2-one

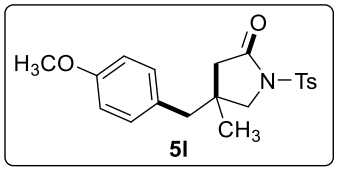
White solid, m. p. 90.1-90.6 ºC (23 mg, 65% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.84 (d, *J* = 8.3 Hz, 2H), 7.29 – 7.18 (m, 6H), 7.19 – 7.13 (m, 1H), 6.32 (d, *J* = 15.8 Hz, 1H), 6.07 – 5.90 (m, 1H), 3.96 (dd, J_1 = 10.0, J_2 = 7.4 Hz, 1H), 3.51 (dd, J_1 = 10.0, J_2 = 6.0 Hz, 1H), 2.63 – 2.39 (m, 2H), 2.36 (s, 3H), 2.31 – 2.18 (m, 2H), 2.15 (dd, J_1 = 16.8, J_2 = 6.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.67, 145.30, 136.84, 135.27, 133.29, 129.81, 128.72, 128.17, 127.70, 126.25, 125.59, 52.05, 38.35, 37.17, 31.63, 21.82.

IR (KBr) *v* 3030, 2963, 2920, 1733, 1593, 1486, 1447, 1353, 1191, 1165, 1126, 958, 818, 740, 699, 660, 610, 561 cm^{-1}.

HRMS (ESI) calcd for $C_{20}H_{22}NO_3S$ ($M+H^+$): 356.1320; Found: 356.1318.



4-(4-methoxybenzyl)-4-methyl-1-tosylpyrrolidin-2-one

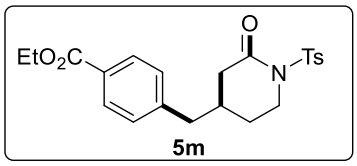
Oil (17 mg, 46% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.92 – 3.70 (m, 4H), 3.49 (d, *J* = 10.0 Hz, 1H), 2.69 – 2.53 (m, 2H), 2.51 – 2.36 (m, 4H), 2.13 (d, *J* = 16.9 Hz, 1H), 1.03 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.56, 158.72, 145.28, 135.34, 131.19, 129.81, 128.57, 128.12, 114.00, 57.55, 55.39, 45.43, 44.31, 37.50, 24.56, 21.83.

IR (KBr) *v* 3058, 2983, 2920, 1738, 1495, 1435, 1372, 1263, 1167, 1092, 1017, 877, 812, 740, 687, 561 cm^{-1}.

HRMS (ESI) calcd for $C_{20}H_{24}NO_4S$ ($M+H^+$): 374.1426; Found: 374.1424.



Ethyl 4-((2-oxo-1-tosylpiperidin-4-yl)methyl)benzoate

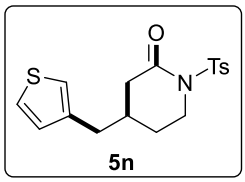
Oil (17 mg, 41% yield), R_f = 0.3 (EtOAc/Petroleum ether 1:5).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.97 (d, *J* = 7.9 Hz, 2H), 7.90 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 4.21 (td, J_1 = 12.2, J_2 = 4.5 Hz, 1H), 3.57 (td, J_1 = 11.8, J_2 = 4.2 Hz, 1H), 2.63 (t, *J* = 6.4 Hz, 2H), 2.53 – 2.37 (m, 4H), 2.24 – 1.90 (m, 3H), 1.58 – 1.50 (m, 1H), 1.39 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.54, 166.51, 145.03, 143.77, 135.94, 130.00, 129.46, 129.11, 129.07, 128.86, 61.10, 46.01, 41.72, 40.27, 34.30, 28.91, 21.81, 14.47.

IR (KBr) *v* 3068, 2915, 2856, 1717, 1608, 1479, 1388, 1357, 1279, 1163, 1114, 1023, 912, 867, 816, 764, 712, 692, 650, 553 cm^{-1}.

HRMS (ESI) calcd for $C_{22}H_{26}NO_5S$ ($M+H^+$): 416.1532; Found: 416.1530.



5n

4-(thiophen-3-ylmethyl)-1-tosylpiperidin-2-one

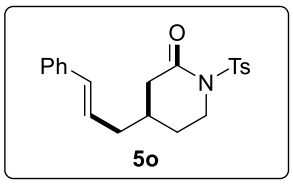
Oil (16 mg, 48% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.21 – 7.16 (m, 1H), 6.87 – 6.82 (m, 1H), 6.81 – 6.76 (m, 1H), 4.13 (td, J_1 = 12.3, J_2 = 5.2 Hz, 1H), 3.52 (td, J_1 = 11.7, J_2 = 4.1 Hz, 1H), 2.54 (d, *J* = 6.1 Hz, 2H), 2.42 (dd, J_1 = 12.4, J_2 = 2.2 Hz, 1H), 2.35 (s, 3H), 2.09 – 1.91 (m, 3H), 1.50 – 1.41 (m, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.88, 144.96, 138.72, 136.01, 129.44, 128.85, 128.25, 126.13, 121.90, 46.10, 40.28, 35.96, 33.87, 29.00, 21.80.

IR (KBr) *v* 2922, 2864, 1692, 1389, 1353, 1273, 1167, 1107, 814, 687, 548 cm^{-1}.

HRMS (ESI) calcd for $C_{17}H_{20}NO_3S_2$ ($M+H^+$): 350.0885; Found: 350.0882.



5o

4-cinnamyl-1-tosylpiperidin-2-one

Solid (19 mg, 51% yield), R_f = 0.3 (EtOAc/Petroleum ether 1:5).

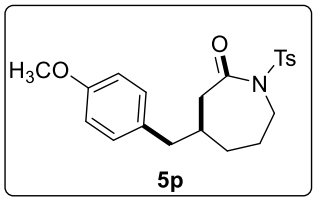
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.36 – 7.29 (m, 6H), 7.25 – 7.19 (m, 1H), 6.47 – 6.32 (m, 1H), 6.17 – 6.01 (m, 1H), 4.25 – 4.16 (m, 1H), 3.71 – 3.60 (m, 1H), 2.61 – 2.51 (m, 1H), 2.43 (s, 3H), 2.26 – 2.07 (m, 4H), 2.02 – 1.93 (m, 1H), 1.60 – 1.49 (m, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.96, 144.94, 137.06, 136.06, 132.98, 129.45,

128.83, 128.71, 127.54, 126.22, 126.17, 46.08, 40.25, 38.74, 32.74, 28.97, 21.80.

IR (KBr) *v* 2958, 2926, 1692, 1642, 1400, 1353, 1269, 1168, 1124, 1092, 968, 806, 689, 545 cm^{-1}.

HRMS (ESI) calcd for $C_{21}H_{23}NNaO_3S$ ($M+Na^+$): 392.1296; Found: 392.1295.



5p

4-(4-methoxybenzyl)-1-tosylazepan-2-one

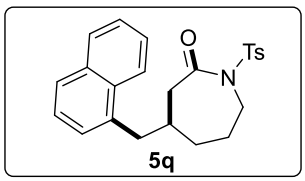
Oil (14 mg, 36% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:4).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 8.6 Hz, 2H), 6.81 (d, *J* = 8.7 Hz, 2H), 4.31 – 4.03 (m, 2H), 3.78 (s, 3H), 2.74 – 2.41 (m, 6H), 2.21 – 2.07 (m, 1H), 2.06 – 1.91 (m, 2H), 1.91 – 1.77 (m, 2H), 1.74 – 1.62 (m, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.58, 157.96, 144.83, 141.01, 136.35, 129.30, 129.18, 127.37, 114.05, 55.38, 46.32, 43.87, 37.28, 36.01, 32.56, 30.64, 21.82.

IR (KBr) *v* 3056, 2960, 2922, 1692, 1610, 1512, 1352, 1248, 1168, 1089, 1031, 807, 688, 550 cm^{-1}.

HRMS (ESI) calcd for $C_{21}H_{25}NNaO_4S$ ($M+Na^+$): 410.1402; Found: 410.1402.



5q

4-(naphthalen-1-ylmethyl)-1-tosylazepan-2-one

White solid, m. p. 50.1-50.9 ºC (16 mg, 40% yield), R_f = 0.5 (EtOAc/Petroleum ether 1:5).

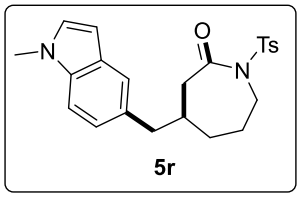
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.99 (d, *J* = 8.3 Hz, 2H), 7.83 – 7.70 (m, 3H), 7.53 – 7.40 (m, 3H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.19 (m, 1H), 4.37 – 4.08 (m, 2H), 2.84 – 2.58 (m, 3H), 2.48 (s, 3H), 2.27 – 2.04 (m, 3H), 2.03 – 1.85 (m, 2H), 1.84

– 1.73 (m, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.55, 145.95, 144.88, 136.38, 133.58, 132.19, 129.36, 129.24, 128.60, 127.71, 127.65, 126.29, 125.57, 125.32, 124.51, 46.41, 44.77, 36.91, 35.98, 32.40, 30.75, 21.86.

IR (KBr) *v* 3067, 2987, 2922, 2853, 1690, 1603, 1443, 1349, 1164, 1115, 1078, 814, 750, 678, 628, 541 cm^{-1}.

HRMS (ESI) calcd for $C_{24}H_{26}NO_3S$ ($M+H^+$): 408.1633; Found: 408.1634.



5r

4-((1-methyl-1H-indol-5-yl)methyl)-1-tosylazepan-2-one

Oil (23 mg, 56% yield), R_f = 0.4 (EtOAc/Petroleum ether 1:4).

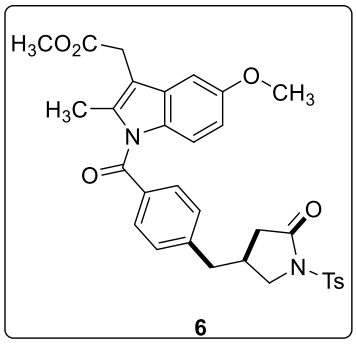
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.99 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.31 – 7.29 (m, 1H), 7.24 (d, *J* = 8.5 Hz, 1H), 7.04 (d, *J* = 3.1 Hz, 1H), 6.94 (dd, J_1 = 8.4, J_2 = 1.5 Hz, 1H), 6.42 – 6.37 (m, 1H), 4.35 – 4.09 (m, 2H), 3.77 (s, 3H), 2.74 – 2.55 (m, 3H), 2.47 (s, 3H), 2.21 – 2.01 (m, 3H), 1.99 – 1.83 (m, 2H), 1.79 – 1.69 (m, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.78, 144.77, 139.98, 136.41, 135.43, 129.36, 129.32, 129.23, 128.59, 120.51, 118.03, 109.49, 100.69, 46.37, 44.83, 37.72, 32.99, 31.56, 30.66, 29.83, 21.84.

IR (KBr) *v* 3067, 2992, 2934, 1694, 1465, 1423, 1337, 1245, 1134, 1078, 1017, 865, 809, 679, 556 cm^{-1}.

HRMS (ESI) calcd for $C_{23}H_{27}N_2O_3S$ ($M+H^+$): 411.1742; Found: 411.1739.

6. Characterization of 6 and 7



6

Methyl 2-(5-methoxy-2-methyl-1-(4-((5-oxo-1-tosylpyrrolidin-3-yl) methyl)benzoyl)-1H-indol-3-yl)acetate

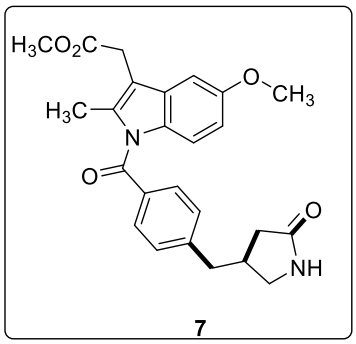
Yellow solid, m. p. 64.7-65.6 ^{o}C (132.1 mg, 45% yield), R_f = 0.2 (EtOAc/Petroleum ether 1:3).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 6.96 (d, *J* = 2.4 Hz, 1H), 6.85 (d, *J* = 9.0 Hz, 1H), 6.66 (dd, J_1 = 9.0, J_2 = 2.5 Hz, 1H), 3.95 (dd, J_1 = 10.0, J_2 = 7.1 Hz, 1H), 3.84 (s, 3H), 3.71 (s, 3H), 3.68 (s, 2H), 3.58 (dd, J_1 = 10.0, J_2 = 6.3 Hz, 1H), 2.86 – 2.67 (m, 3H), 2.56 (dd, J_1 = 17.3, J_2 = 7.8 Hz, 1H), 2.44 (s, 3H), 2.38 (s, 3H), 2.24 (dd, J_1 = 17.3, J_2 = 7.4 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100MHz) δ 172.22, 171.54, 169.09, 156.02, 145.47, 143.52, 136.10, 135.05, 134.31, 130.96, 130.66, 130.43, 129.86, 129.13, 128.14, 115.03, 112.35, 111.56, 101.30, 55.81, 52.28, 51.87, 39.54, 38.48, 33.26, 30.24, 21.81, 13.44.

IR (KBr) *v* 3434, 2958, 2926, 1738, 1679, 1603, 1477, 1358, 1321, 1217, 1168, 1072, 1030, 962, 812, 743, 663, 599, 556 cm^{-1}.

HRMS (ESI) calcd for $C_{32}H_{33}N_2O_7S$ ($M+H^+$): 589.2008; Found: 589.2008.



7

Methyl 2-(5-methoxy-2-methyl-1-(4-((5-oxopyrrolidin-3-yl)methyl) benzoyl)-1H-indol-3-yl)acetate

Yellow oil (59.6 mg, 69% yield), R_f = 0.2 (CH_2Cl_2/methanol 40:1).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.66 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 6.96 (d, *J* = 2.4 Hz, 1H), 6.88 (d, *J* = 9.0 Hz, 1H), 6.80 (br, 1H), 6.65 (dd, J_1 = 9.0, J_2 = 2.5 Hz, 1H), 3.83 (s, 3H), 3.70 (s, 3H), 3.67 (s, 2H), 3.55 – 3.39 (m, 1H), 3.19 – 3.07 (m, 1H), 2.91 – 2.75 (m, 3H), 2.53 – 2.40 (m, 1H), 2.36 (s, 3H), 2.20 – 2.06 (m, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.47, 169.21, 156.01, 144.73, 136.06, 134.00, 131.04, 130.62, 130.24, 129.13, 114.99, 112.25, 111.56, 101.32, 55.79, 52.18, 47.61, 40.42, 36.56, 36.03, 30.21, 13.33.

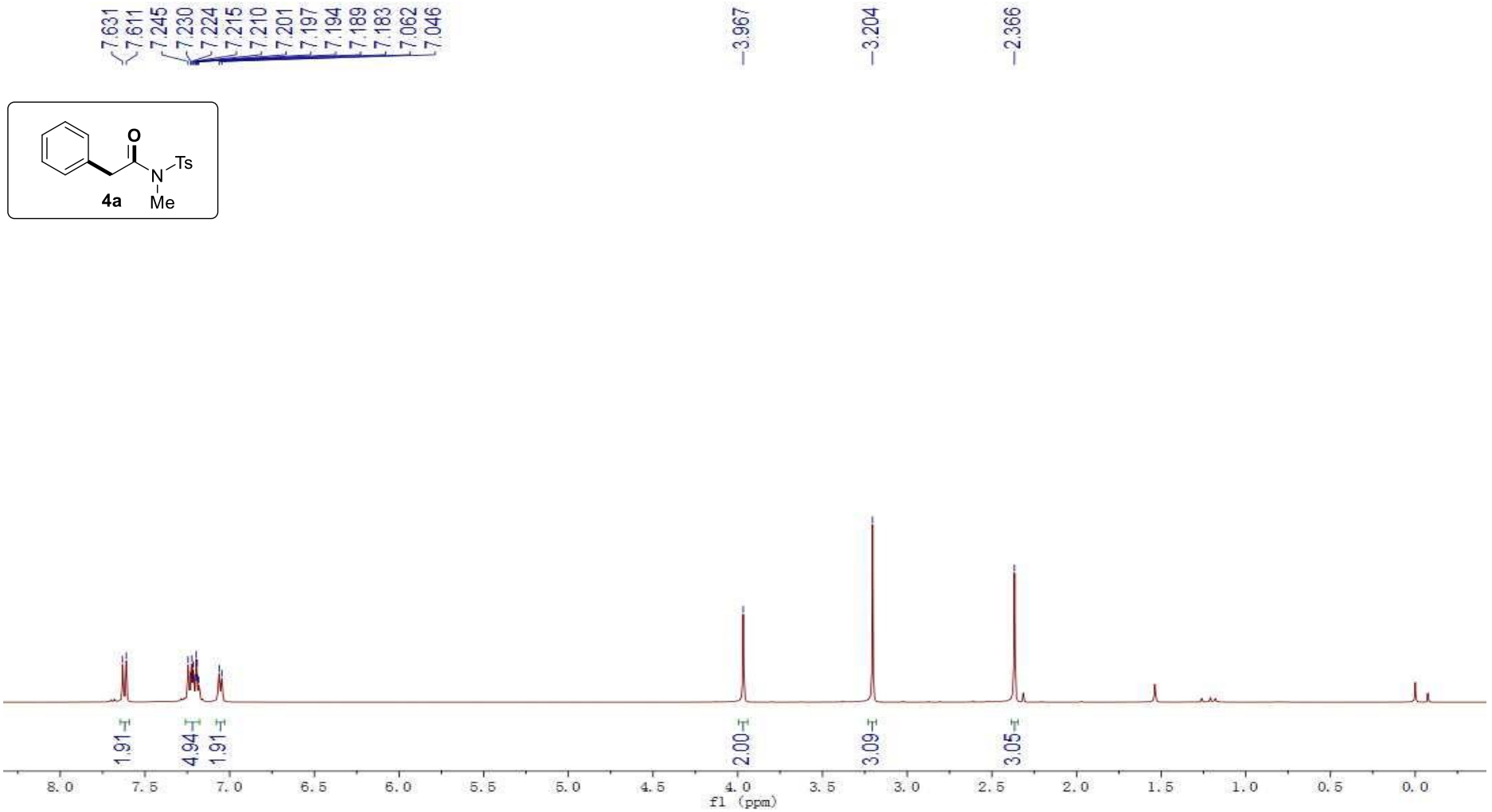
IR (KBr) *v* 3097, 2965, 2919, 1737, 1656, 1495, 1301, 1168, 1070, 812, 743, 660, 594, 556 cm^{-1}.

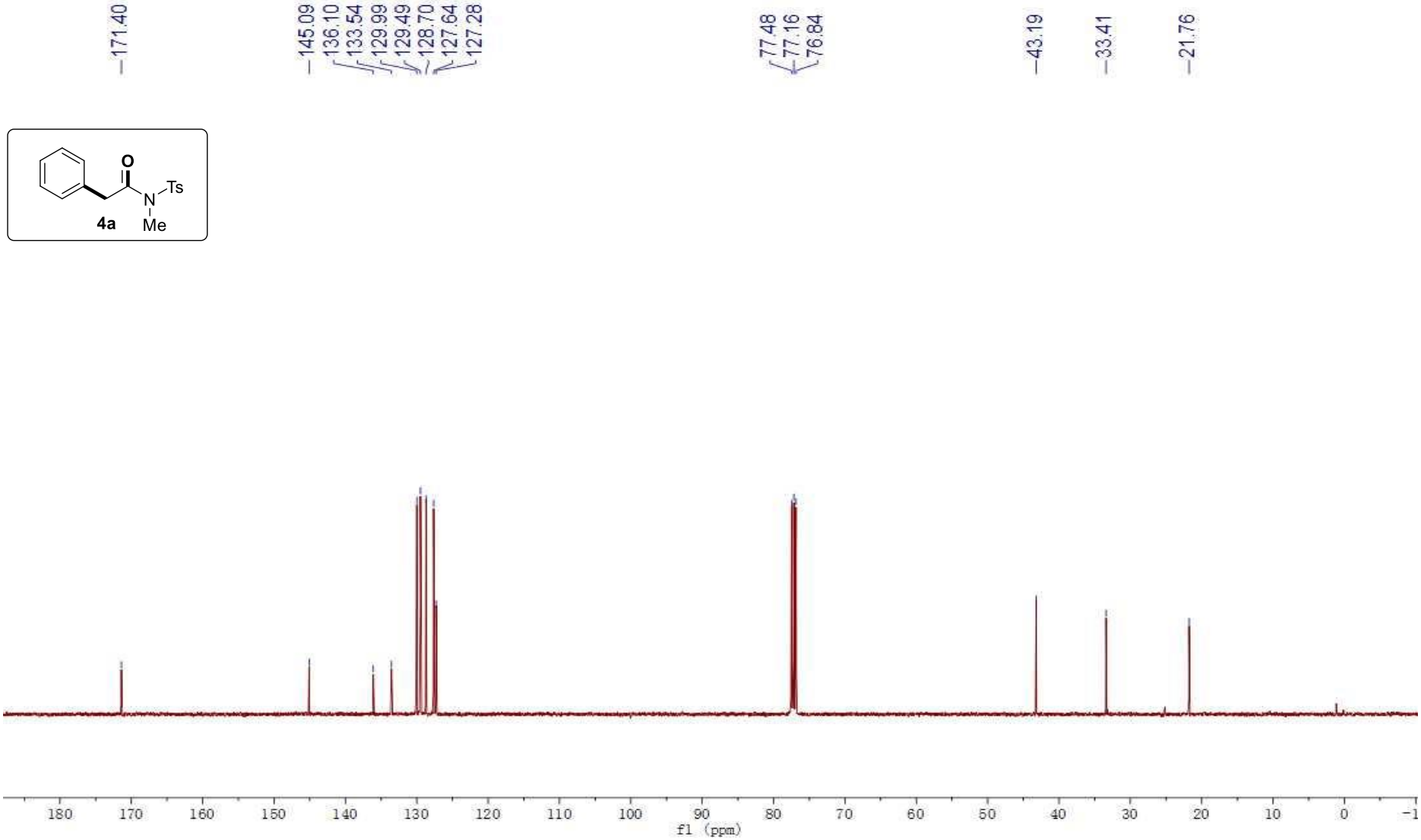
HRMS (ESI) calcd for $C_{25}H_{27}N_2O_5$ ($M+H^+$): 435.1920; Found: 435.1919.

7. References

1. Xie, F.; Zhao, H.; Li, D.; Chen, H.; Quan, H.; Shi, X.; Lou, L.; Hu, Y. *J. Med. Chem.* **2011**, *54*, 3200.
2. Dalal, A.; Loannis, S.et.*al*. *J. Am. Chem. Soc.* **2016**, *138*, 12767.
3. Molander, G. A.; Trice, S. L. J.; Dreher. S. D. *J. Am. Chem. Soc.* **2010**, *132*, 17701.
4. Steven, J.; Mansfield, C. D.; Campbell, M. W.; Edward, A. A. *Chem. Commun*. **2015**, *51*, 3316.

8. Copies of NMR Spectra

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33.41
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O
N
Ts
Me
4a
180
170
160
150
140
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110
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90
80
70
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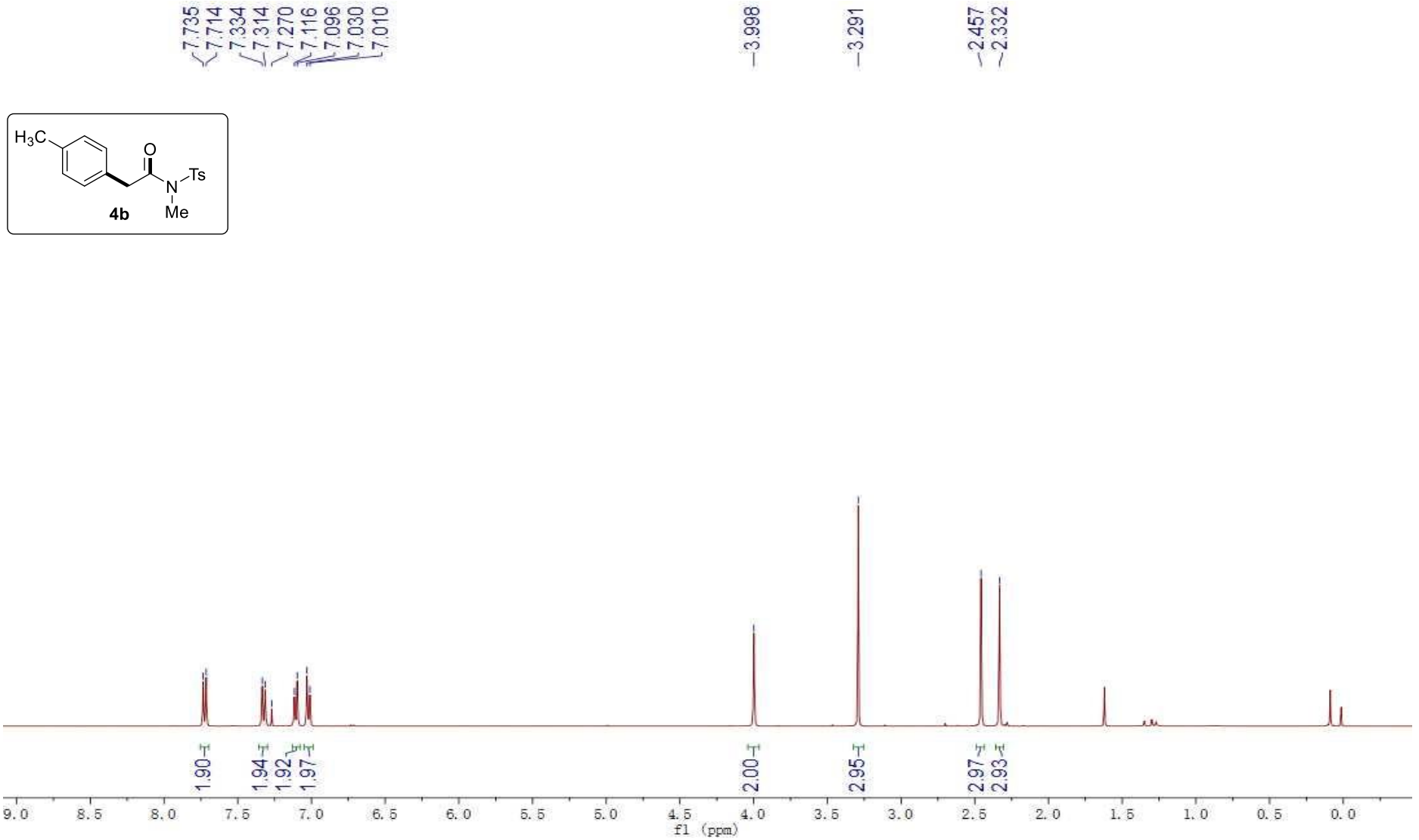
40
30
20
10
0
-1
f1 (ppm)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H3C
O
N
Ts
Me
4b
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1.94
1.92
1.97
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2.95
2.97
2.93
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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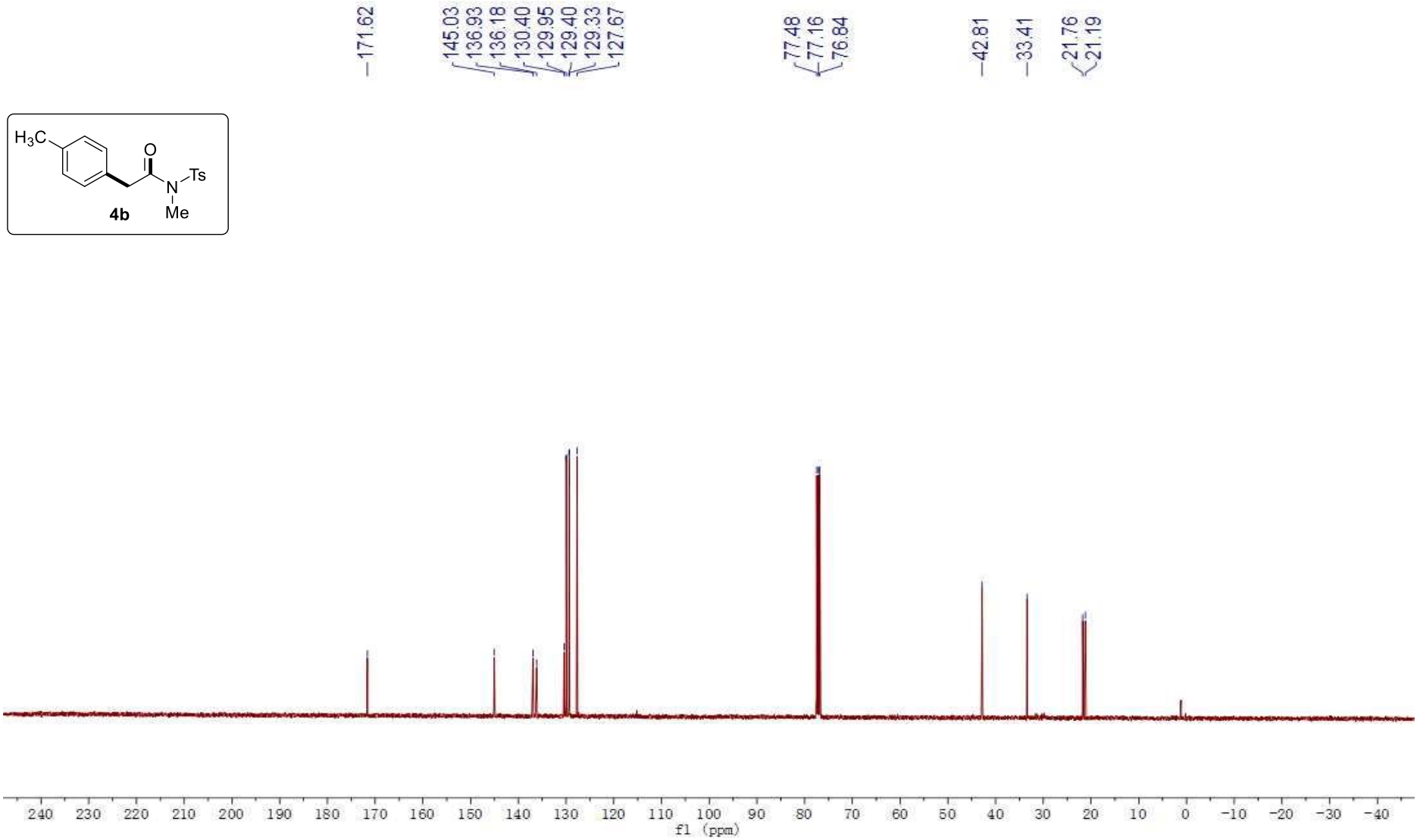
0.0
f1 (ppm)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33.41
21.76
21.19
H3C
O
N
Ts
Me
4b
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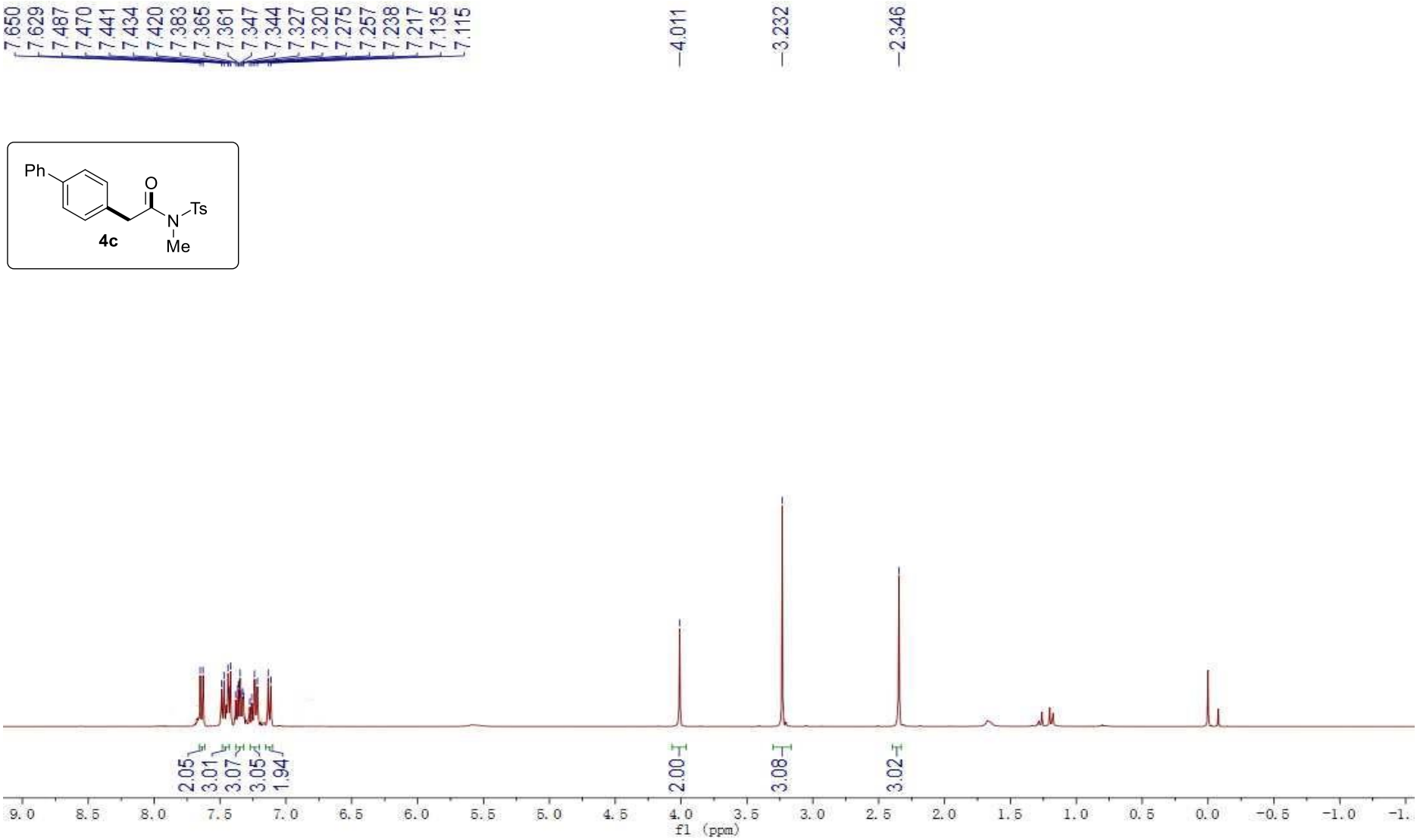
f1 (ppm)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7.383
7.365
7.361
7.347
7.344
7.327
7.320
7.275
7.257
7.238
7.217
7.135
7.115
4.011
3.232
2.346
Ph
O
N
Ts
Me
4c
2.05
3.01
3.07
3.05
1.94
2.00
3.08
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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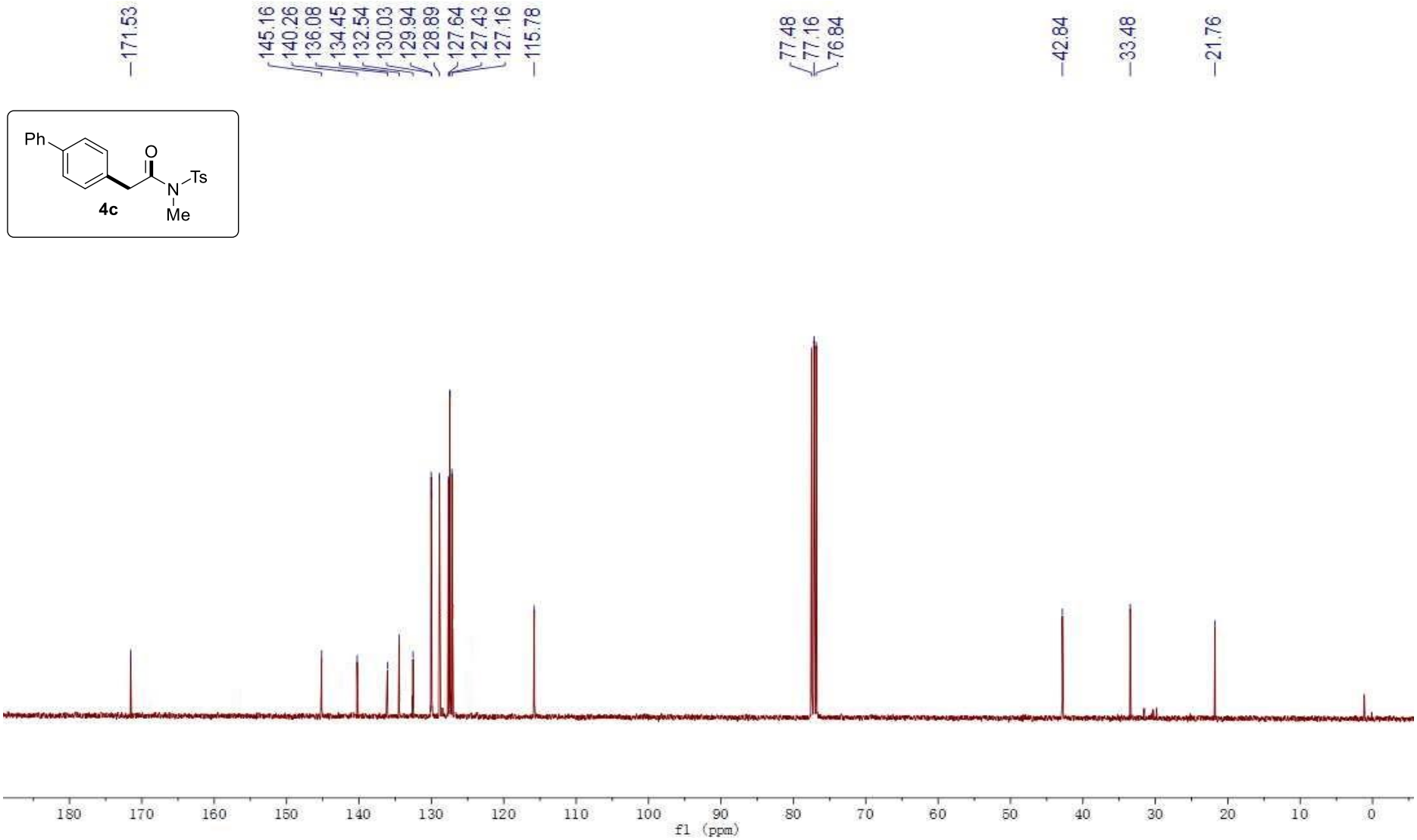
f1 (ppm)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132.54
130.03
129.94
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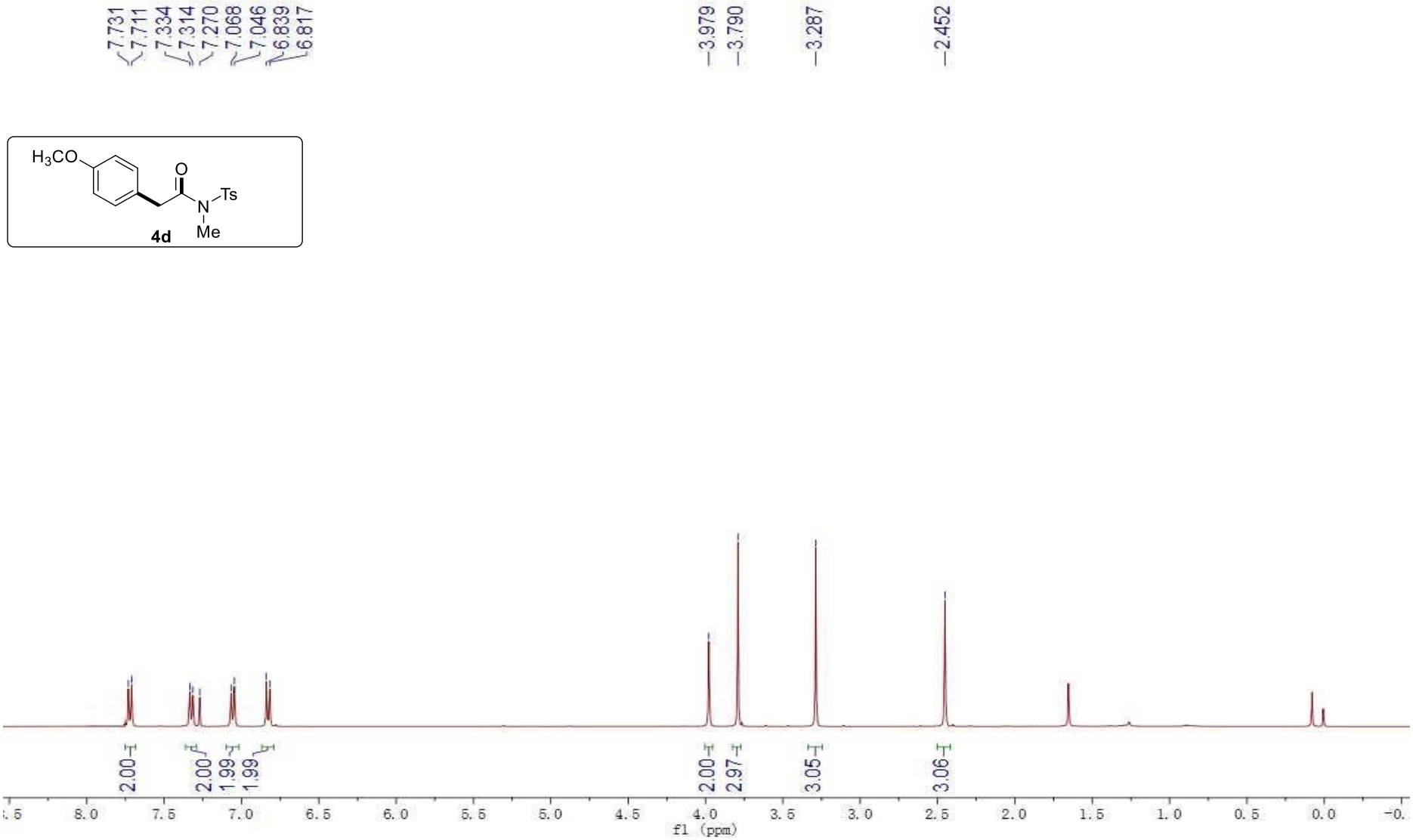
127.64
127.43
127.16
115.78
77.48
77.16
76.84
42.84
33.48
21.76
Ph
O
N
Ts
Me
4c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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3.287
2.452
H3CO
O
N
Ts
Me
4d
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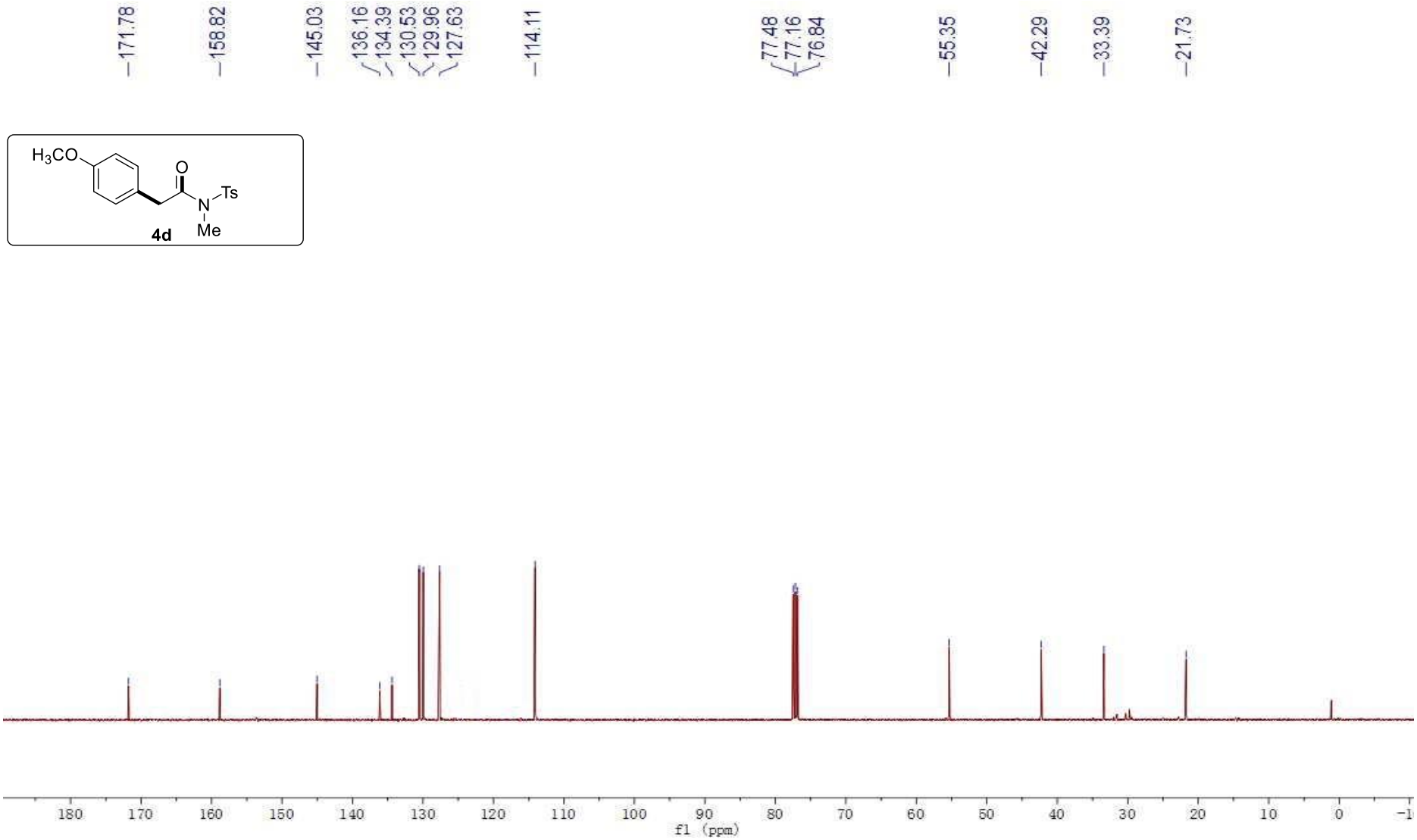
2.00
1.99
1.99
2.00
2.97
3.05
3.06
f1 (ppm)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127.63
114.11
77.48
77.16
76.84
55.35
42.29
33.39
21.73
H3CO
O
N
Ts
Me
4d
180
170
160
150
140
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120
110
100
90
80
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60
50
40
30
20
10
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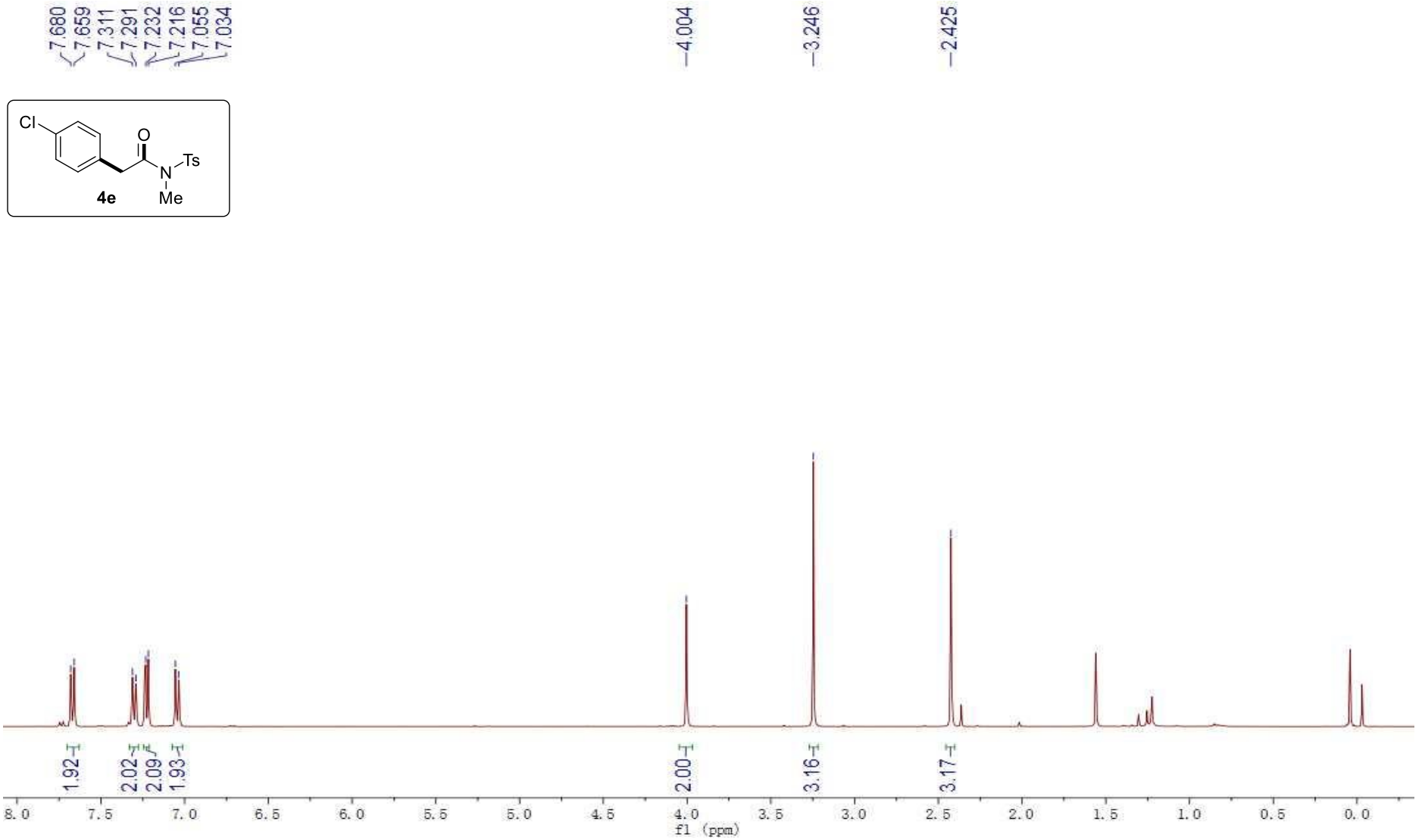
-1
f1 (ppm)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7.034
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3.246
2.425
Cl
O
N
Ts
Me
4e
1.92
2.02
2.09
1.93
2.00
3.16
3.17
8.0
7.5
7.0
6.5
6.0
5.5
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1.0
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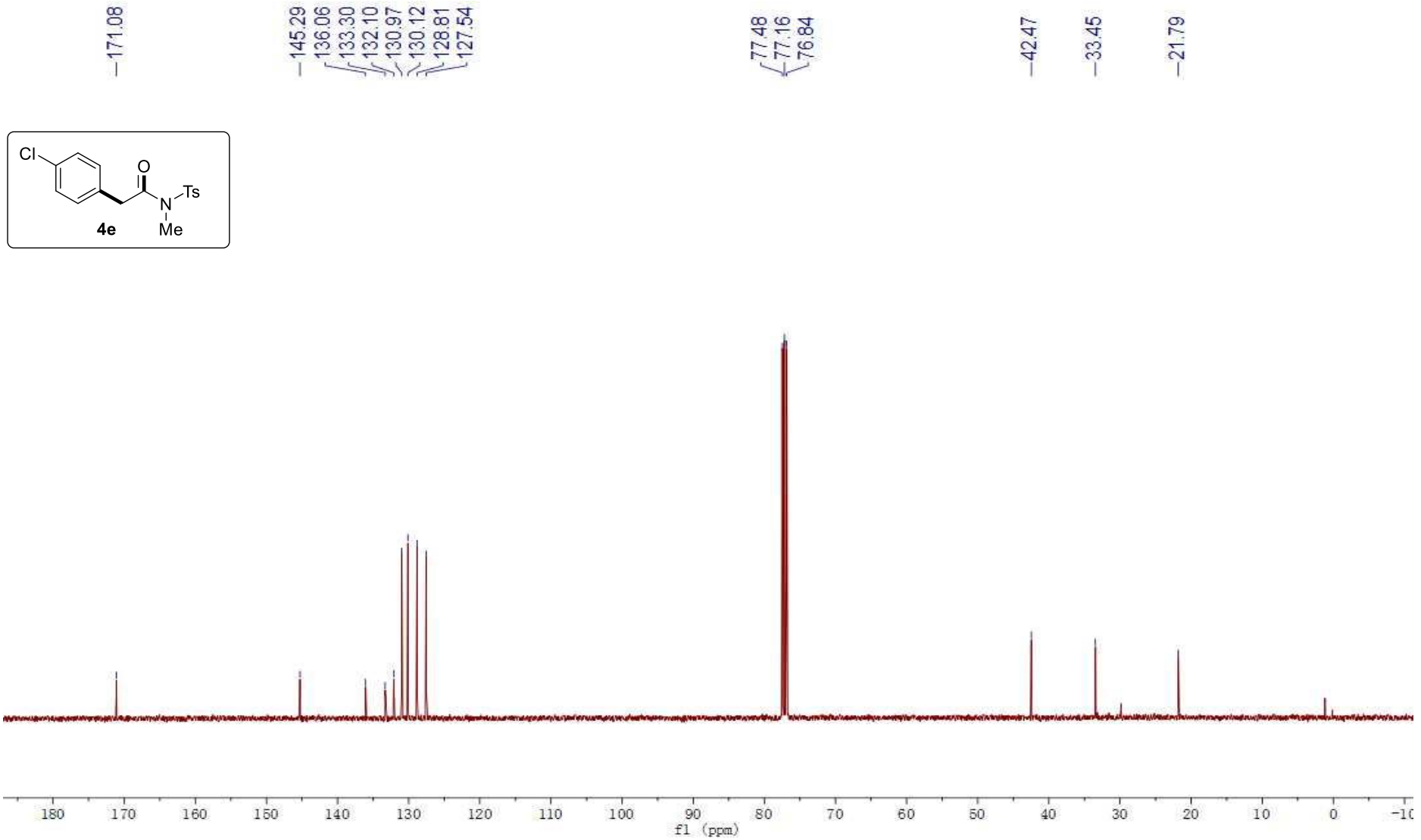
0.0
f1 (ppm)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133.30
132.10
130.97
130.12
128.81
127.54
77.48
77.16
76.84
42.47
33.45
21.79
Cl
O
N
Ts
Me
4e
180
170
160
150
140
130
120
110
100
90
80
70
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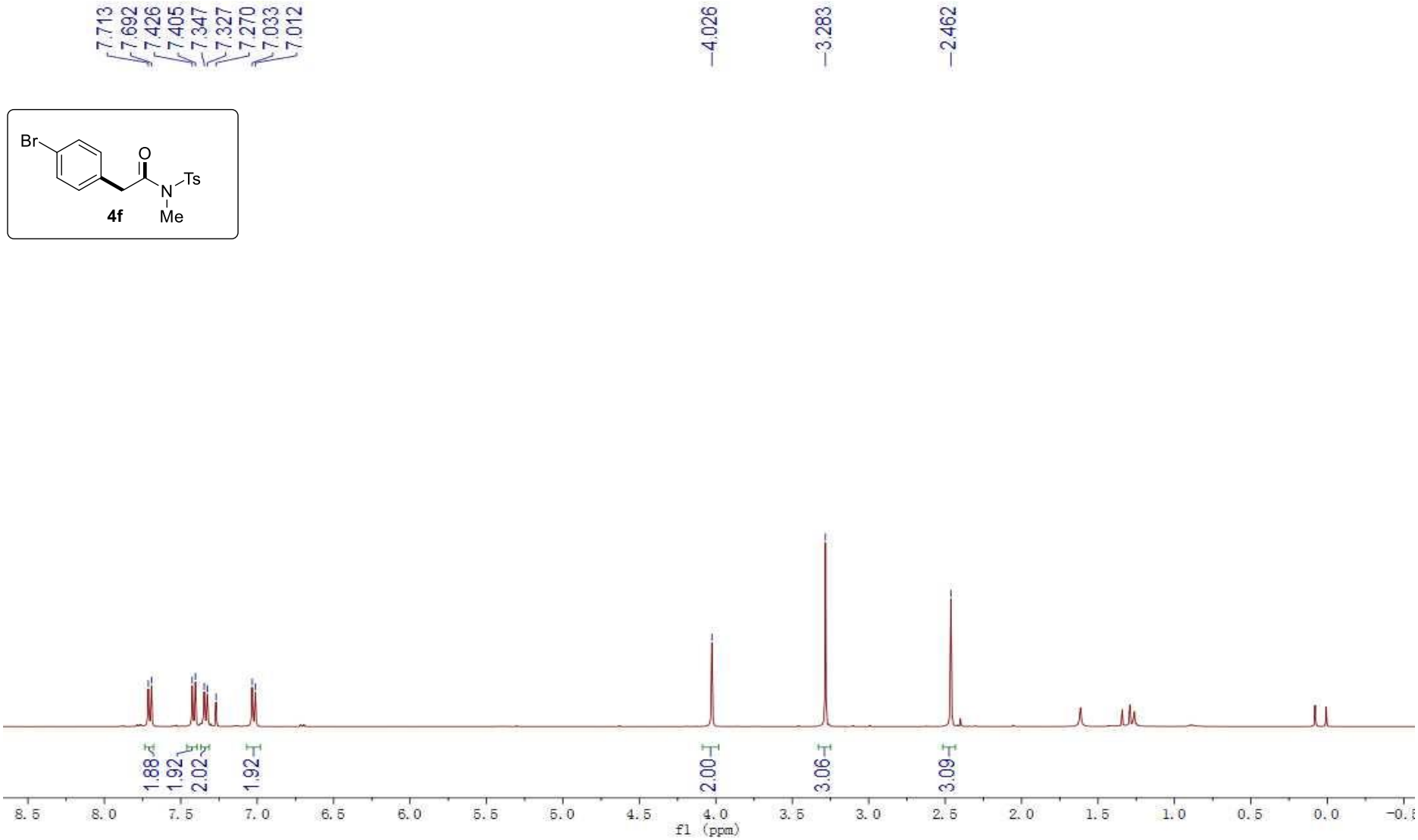
50
40
30
20
10
0
f1 (ppm)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7.426
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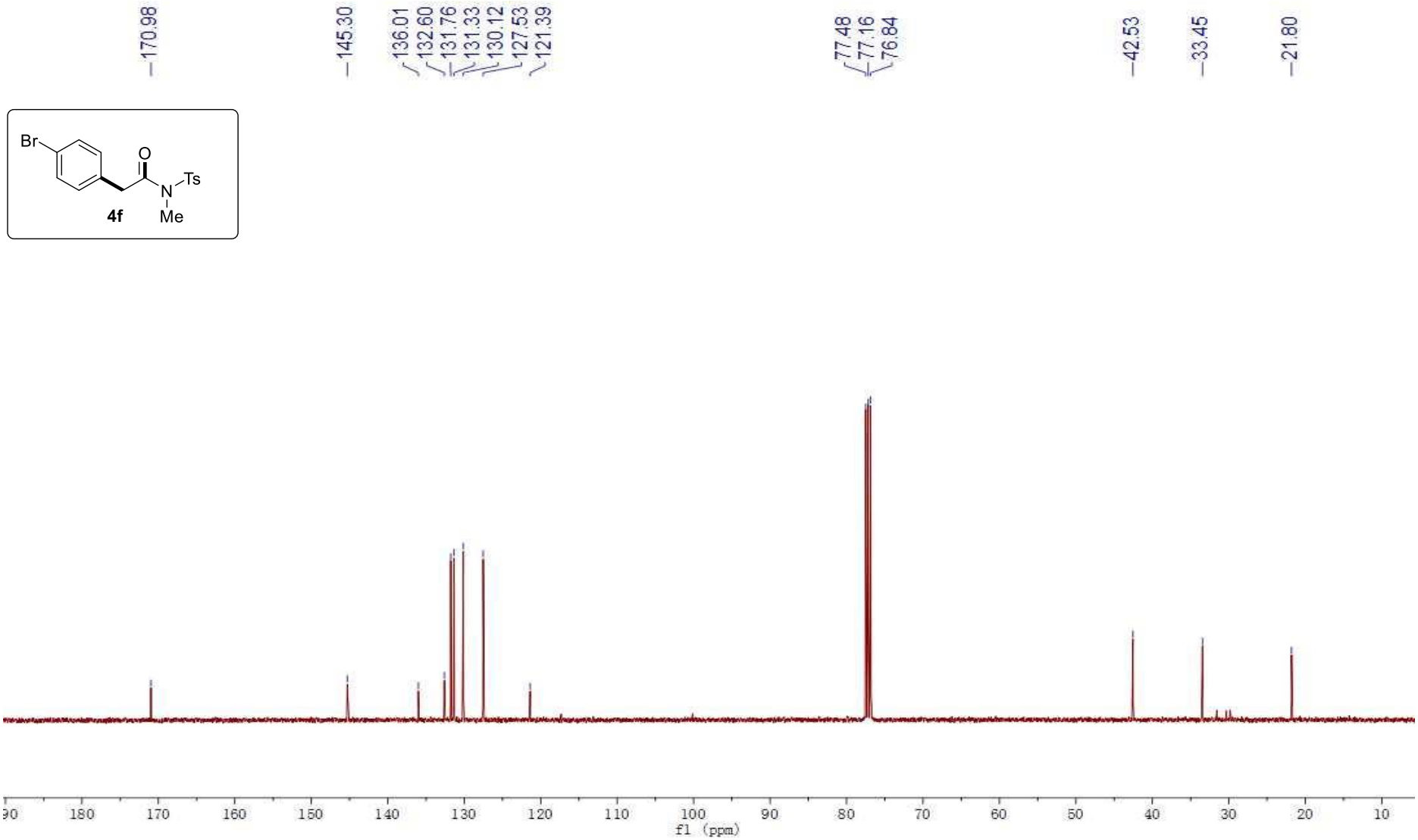
7.347
7.327
7.270
7.033
7.012
4.026
3.283
2.462
Br
O
N
Ts
Me
4f
1.88
1.92
2.02
1.92
2.00
3.06
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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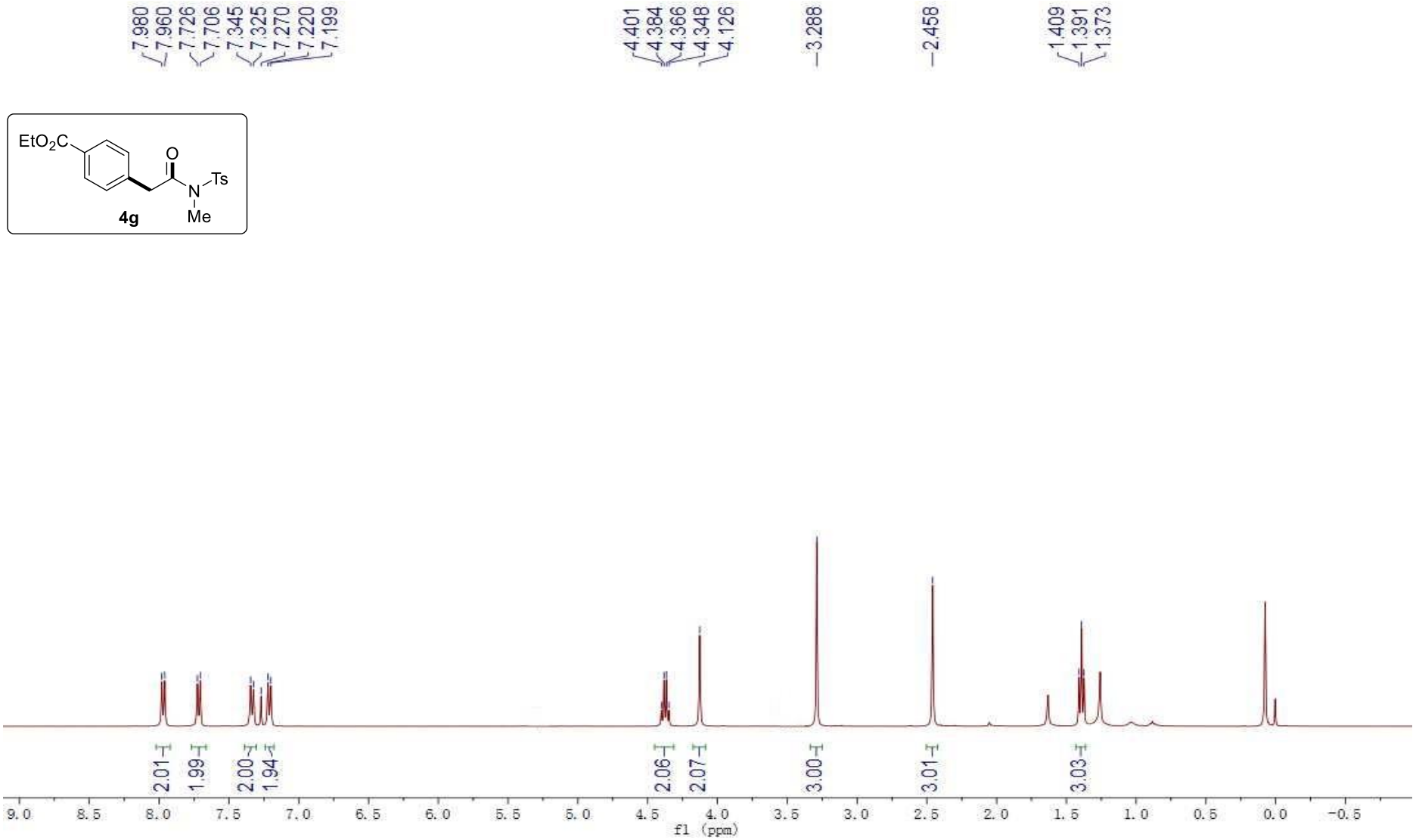
145.30
136.01
132.60
131.76
131.33
130.12
127.53
121.39
77.48
77.16
76.84
42.53
33.45
21.80
Br
O
N
Ts
Me
4f
f1 (ppm)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7.726
7.706
7.345
7.325
7.270
7.220
7.199
4.401
4.384
4.366
4.348
4.126
3.288
2.458
1.409
1.391
1.373
EtO2C
O
N
Ts
Me
4g
2.01
1.99
2.00
1.94
2.06
2.07
3.00
3.01
3.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
2.0
1.5
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0.0
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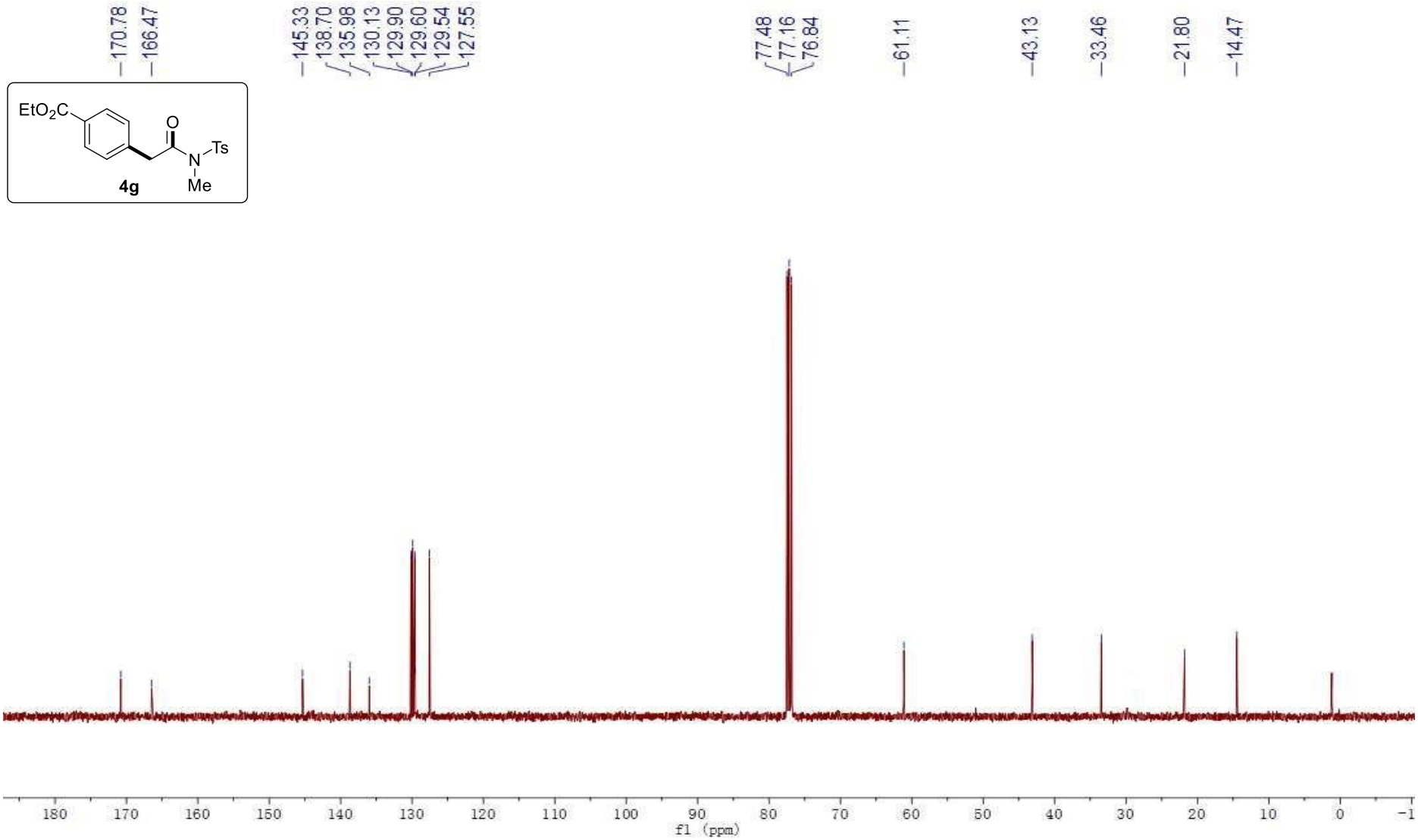
f1 (ppm)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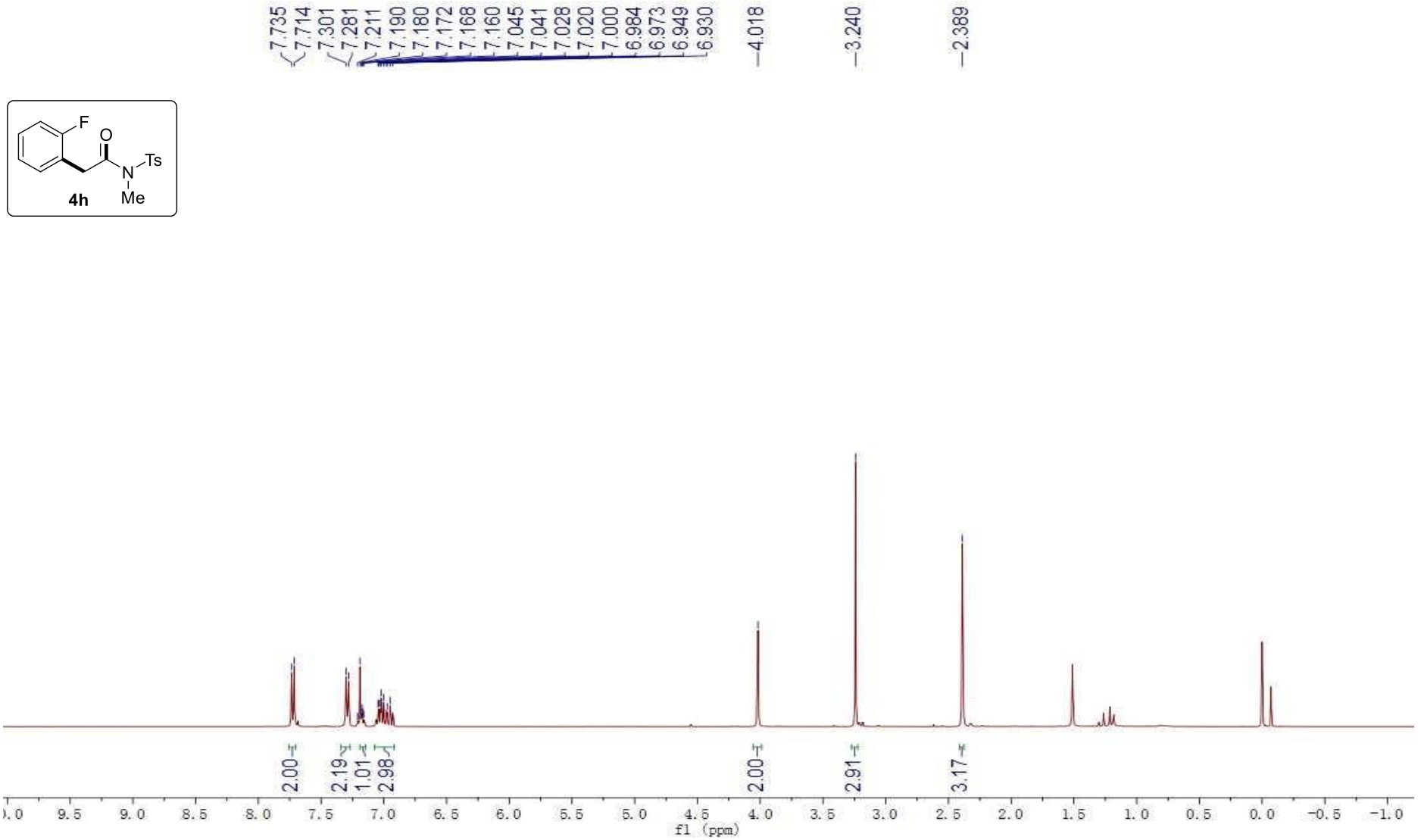
138.70
135.98
130.13
129.90
129.60
129.54
127.55
77.48
77.16
76.84
61.11
43.13
33.46
21.80
14.47
EtO2C
O
N
Ts
Me
4g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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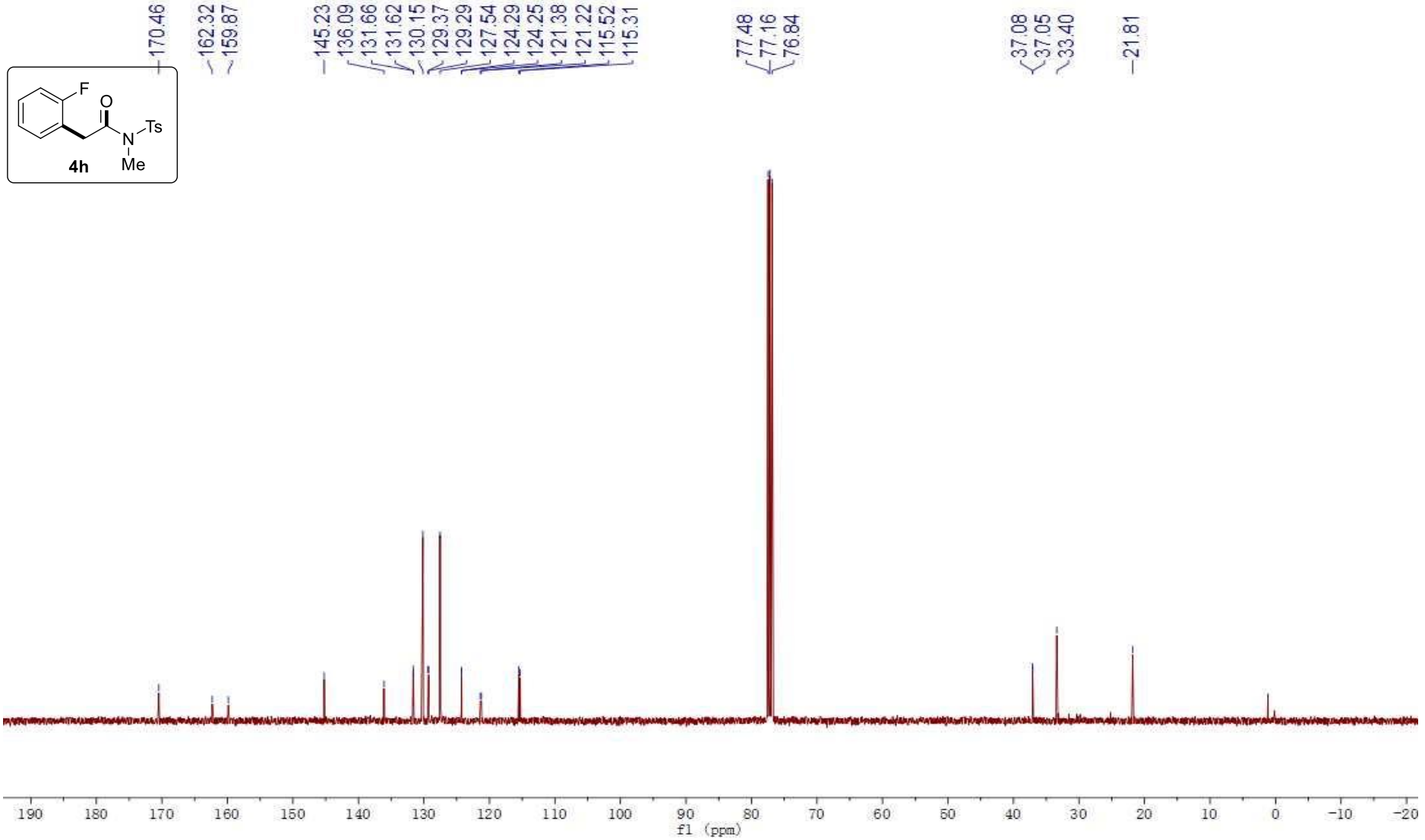
7.172
7.168
7.160
7.045
7.041
7.028
7.020
7.000
6.984
6.973
6.949
6.930
4.018
3.240
2.389
F
O
N
Ts
Me
4h
2.00
2.19
1.01
2.98
2.00
2.91
3.17
f1 (ppm)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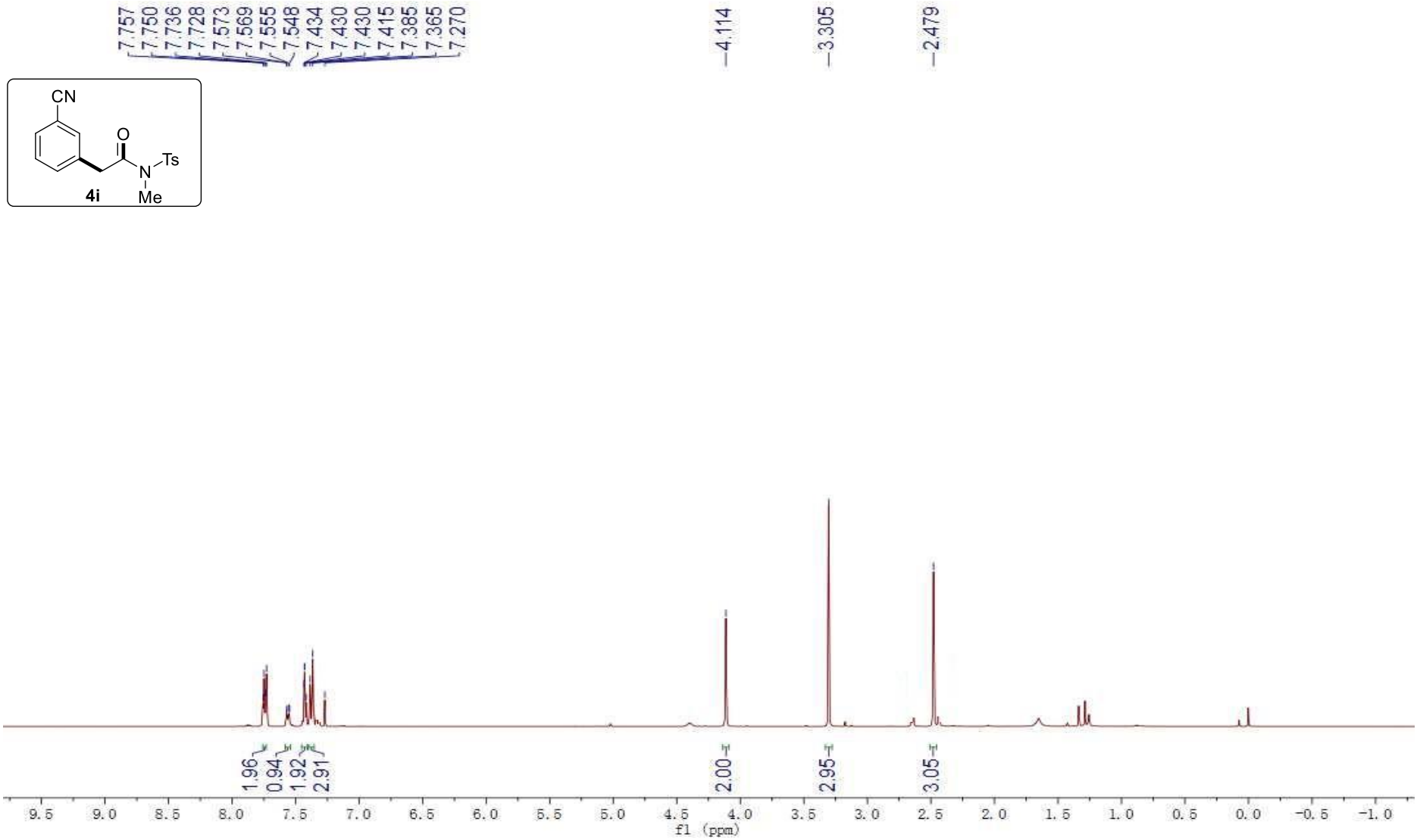
159.87
145.23
136.09
131.66
131.62
130.15
129.37
129.29
127.54
124.29
124.25
121.38
121.22
115.52
115.31
77.48
77.16
76.84
37.08
37.05
33.40
21.81
F
O
N
Ts
Me
4h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)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7.555
7.548
7.434
7.430
7.430
7.415
7.385
7.365
7.270
4.114
3.305
2.479
CN
O
N
Ts
Me
4i
1.96
0.94
1.92
2.91
2.00
2.95
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
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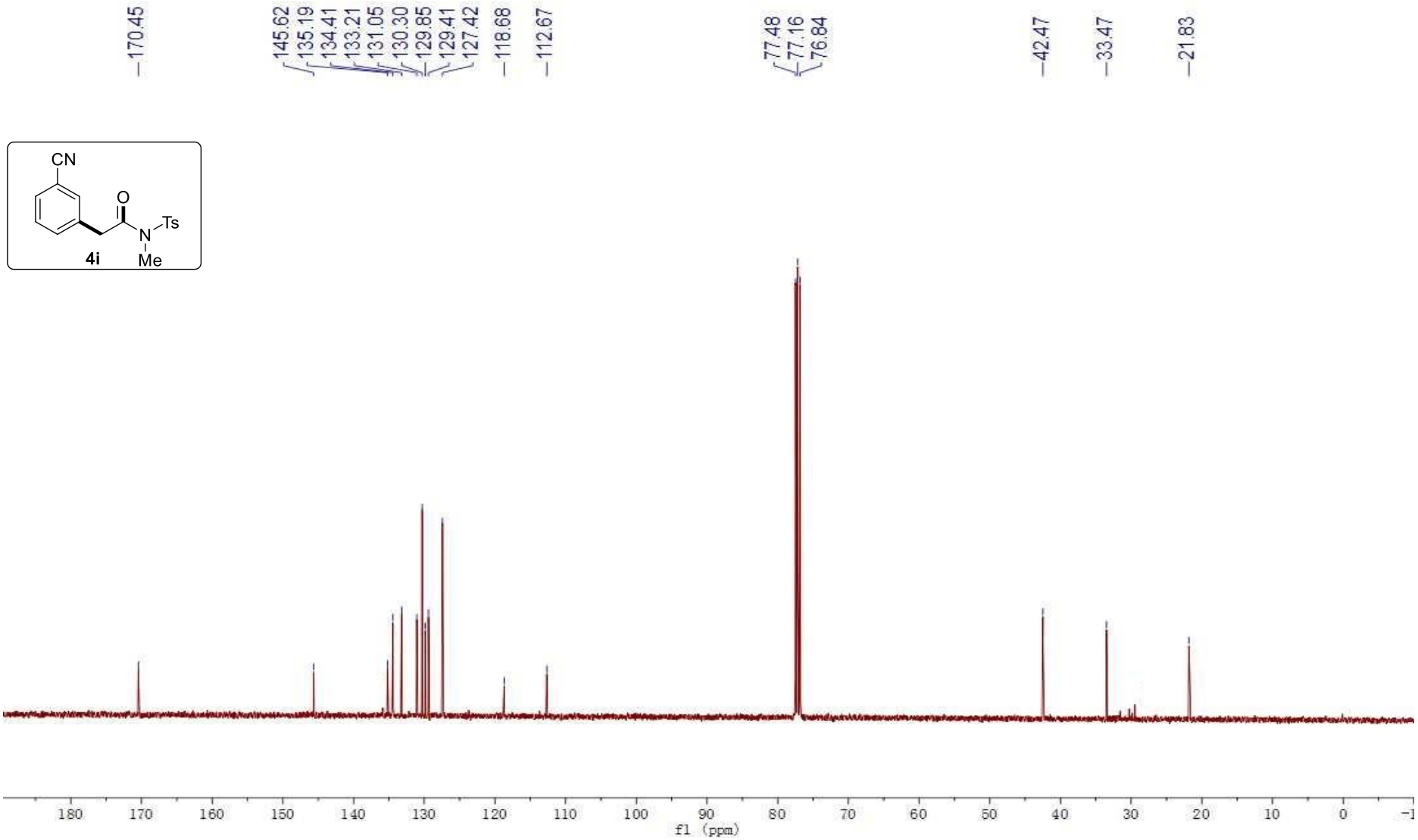
0.0
-0.5
-1.0
f1 (ppm)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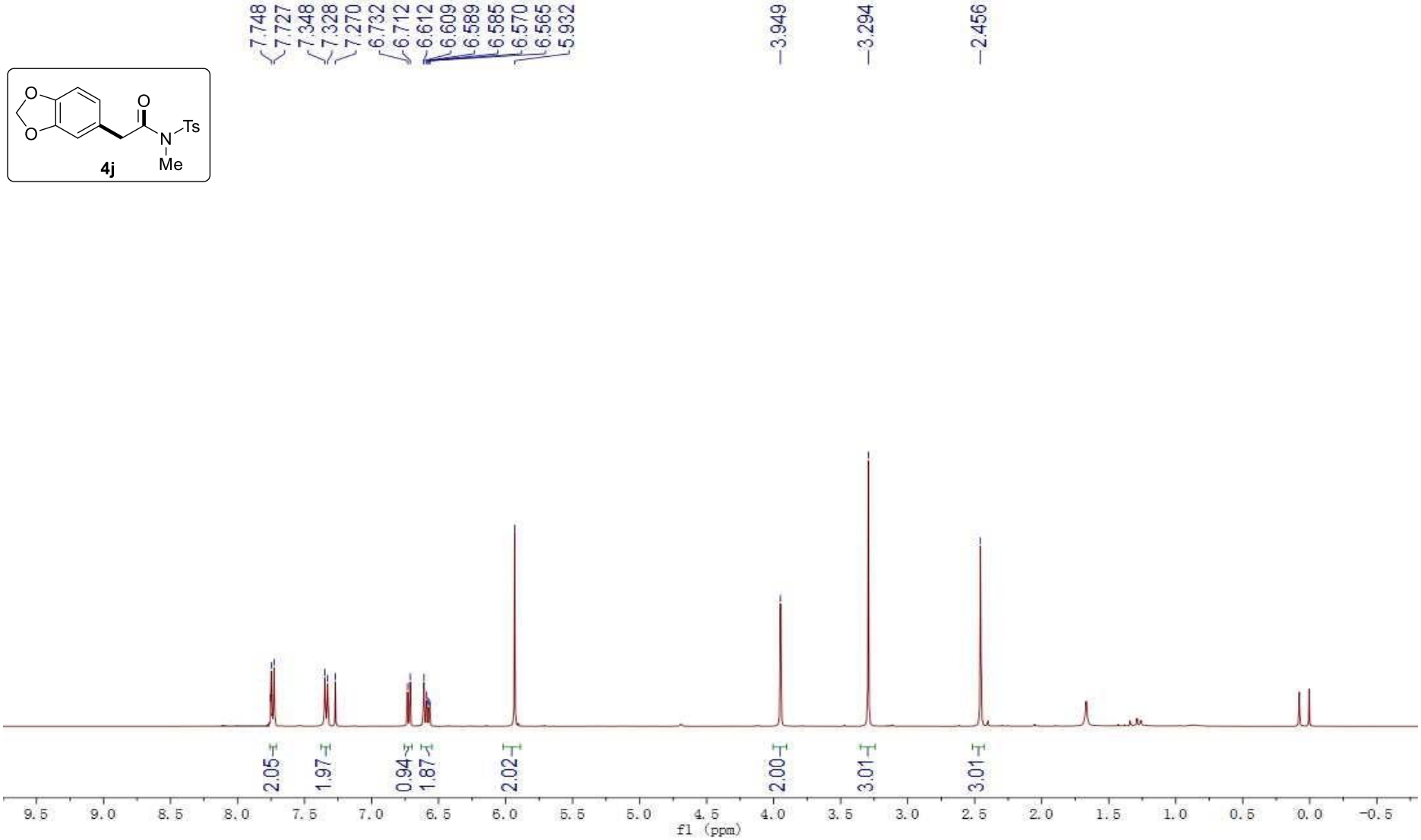
135.19
134.41
133.21
131.05
130.30
129.85
129.41
127.42
118.68
112.67
77.48
77.16
76.84
42.47
33.47
21.83
CN
O
N
Ts
Me
4i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.565
5.932
3.949
3.294
2.456
O
O
O
N
Ts
Me
4j
2.05
1.97
0.94
1.87
2.02
2.00
3.01
3.01
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
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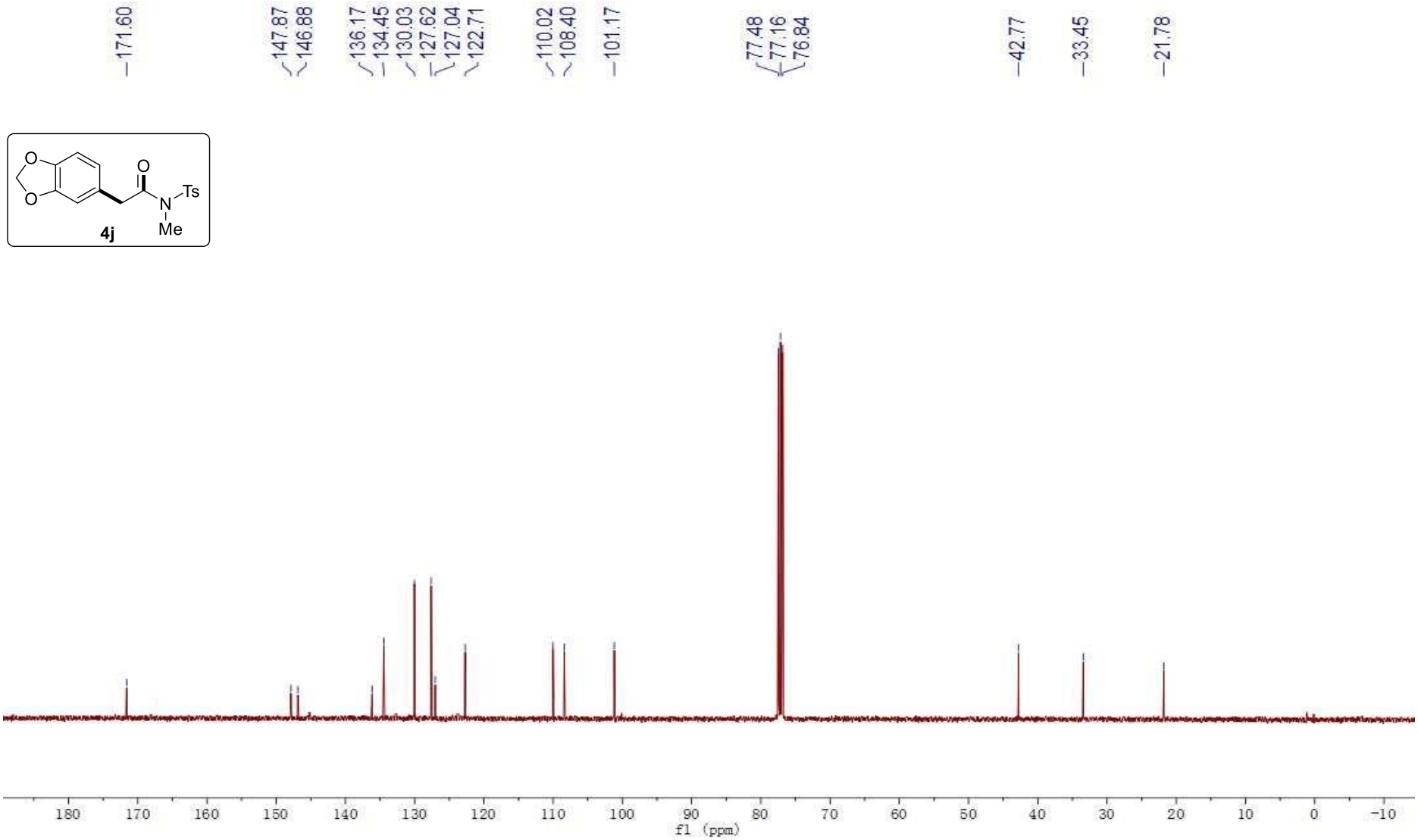
0.0
-0.5
f1 (ppm)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127.62
127.04
122.71
110.02
108.40
101.17
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77.16
76.84
42.77
33.45
21.78
O
O
O
N
Ts
Me
4j
180
170
160
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140
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120
110
100
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80
70
60
50
40
30
20
10
0
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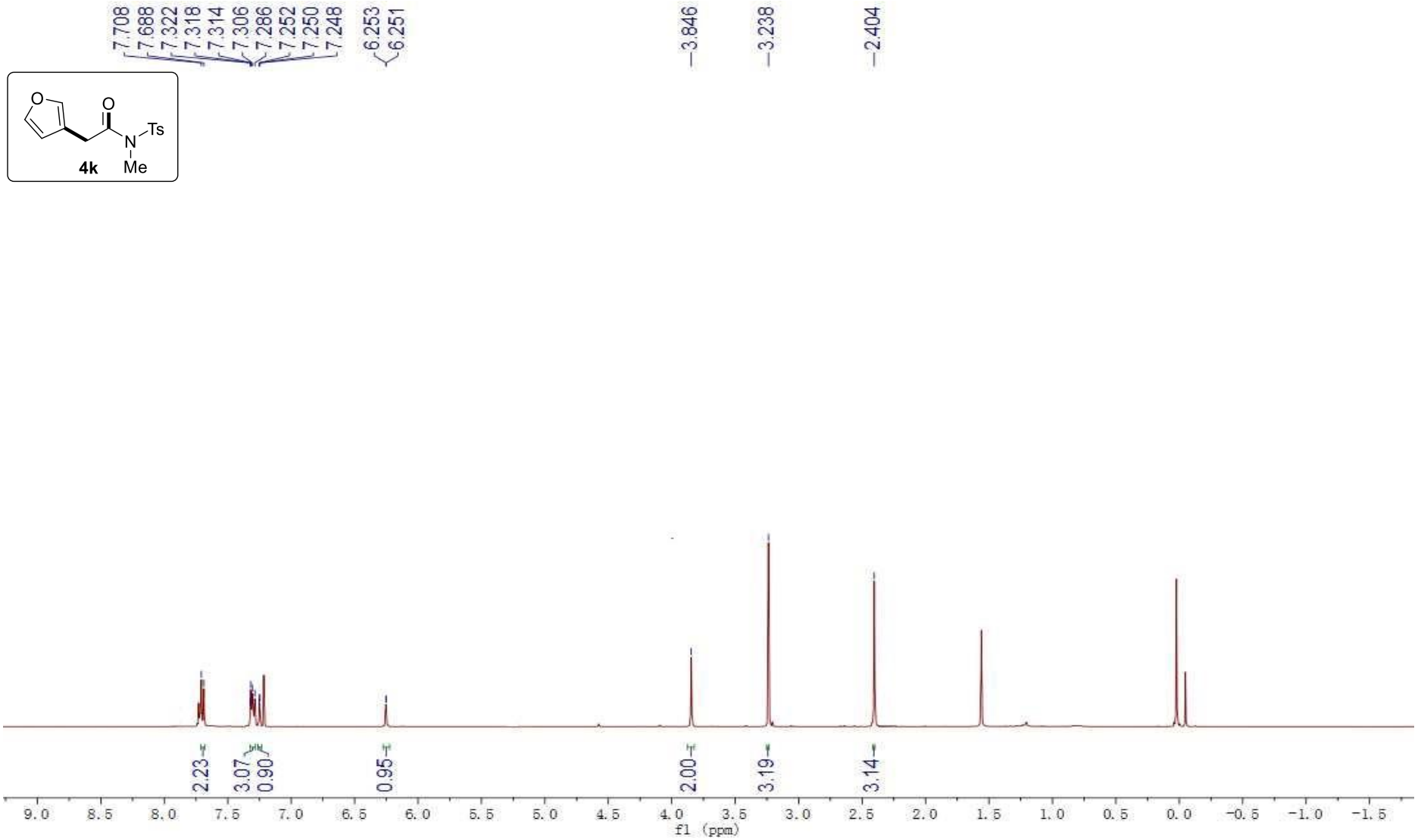
f1 (ppm)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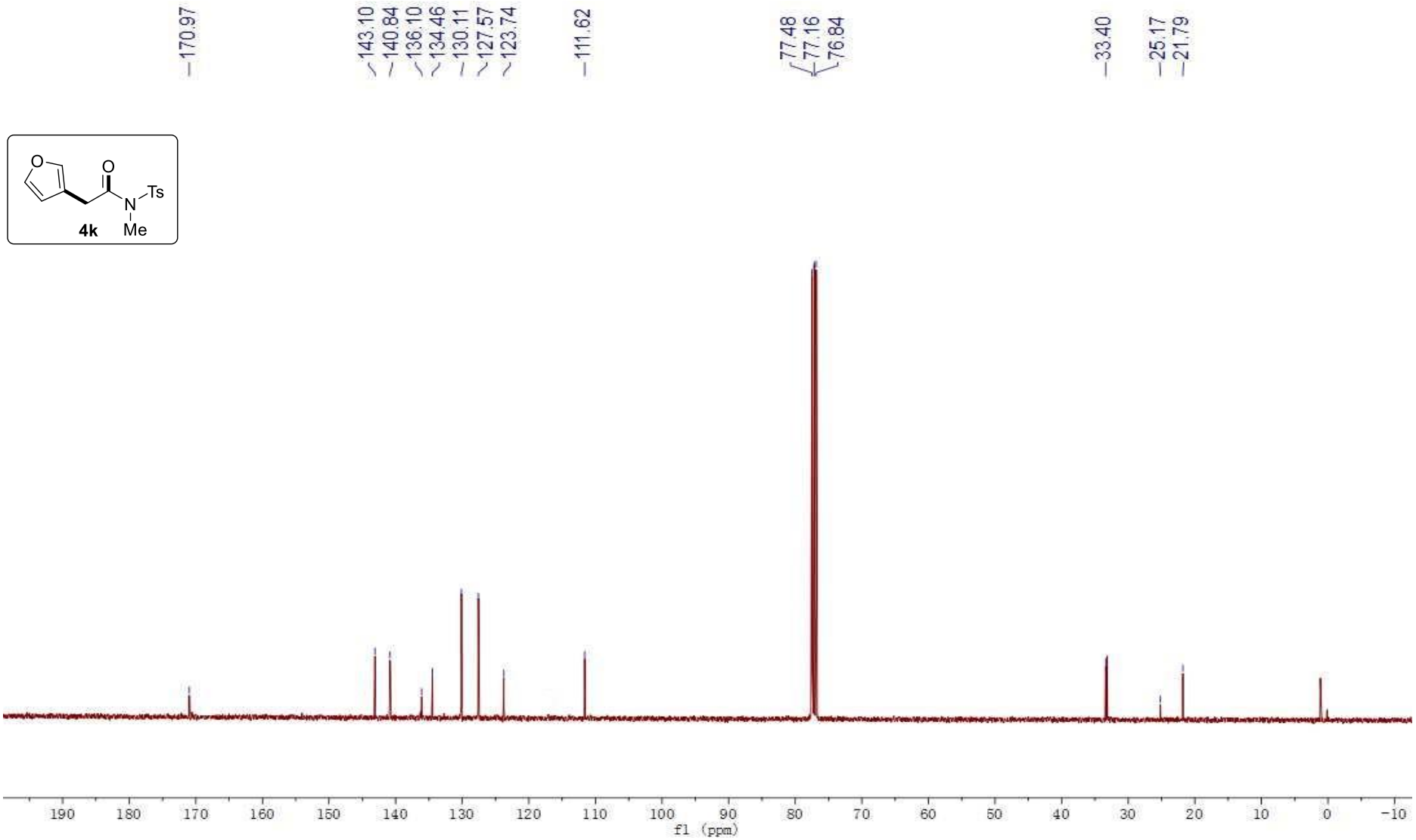
7.248
6.253
6.251
3.846
3.238
2.404
O
O
N
Ts
Me
4k
2.23
3.07
0.90
0.95
2.00
3.19
3.14
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)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136.10
134.46
130.11
127.57
123.74
111.62
77.48
77.16
76.84
33.40
25.17
21.79
O
O
N
Ts
Me
4k
190
180
170
160
150
140
130
120
110
100
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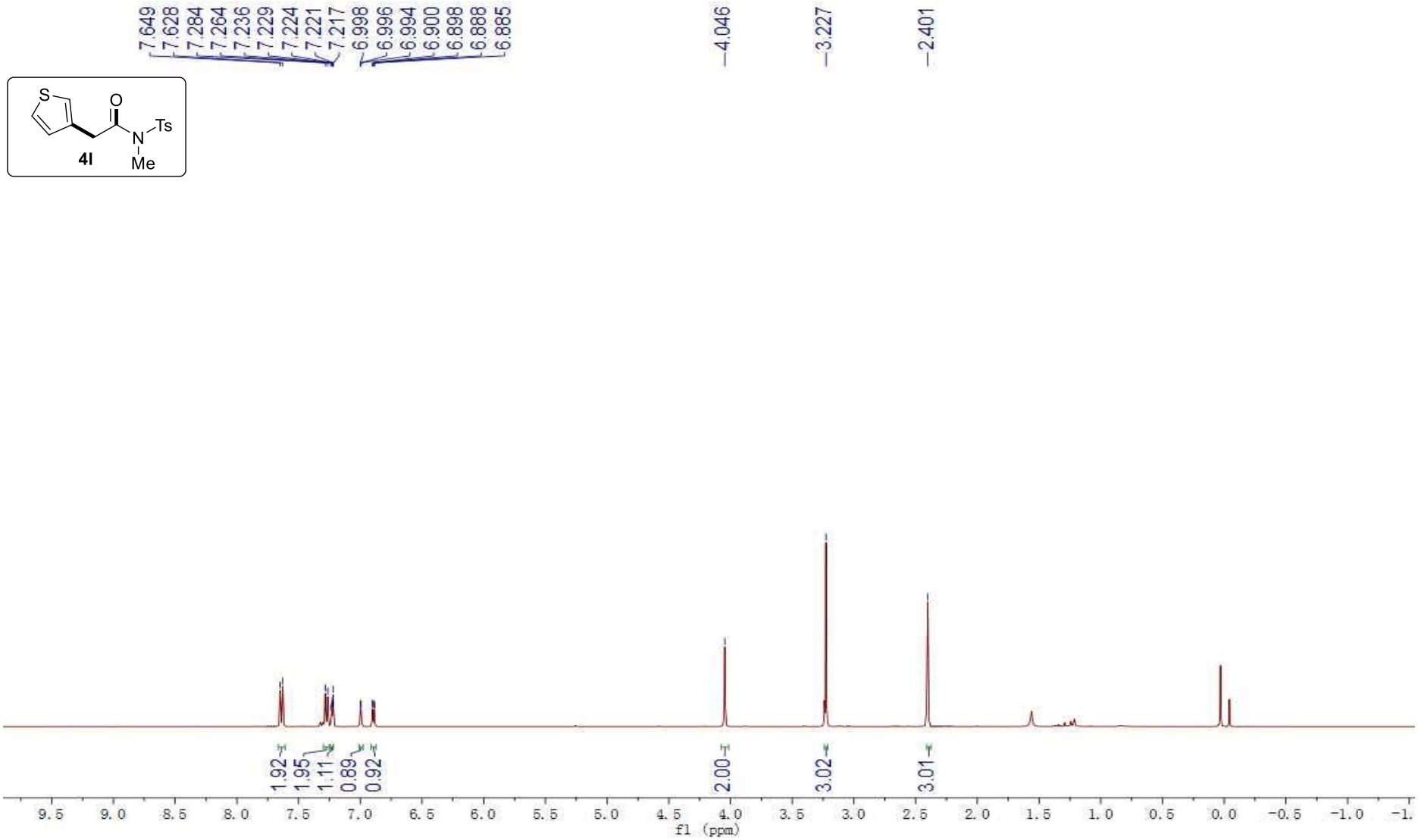
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.221
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6.998
6.996
6.994
6.900
6.898
6.888
6.885
4.046
3.227
2.401
S
O
N
Ts
Me
4l
1.92
1.95
1.11
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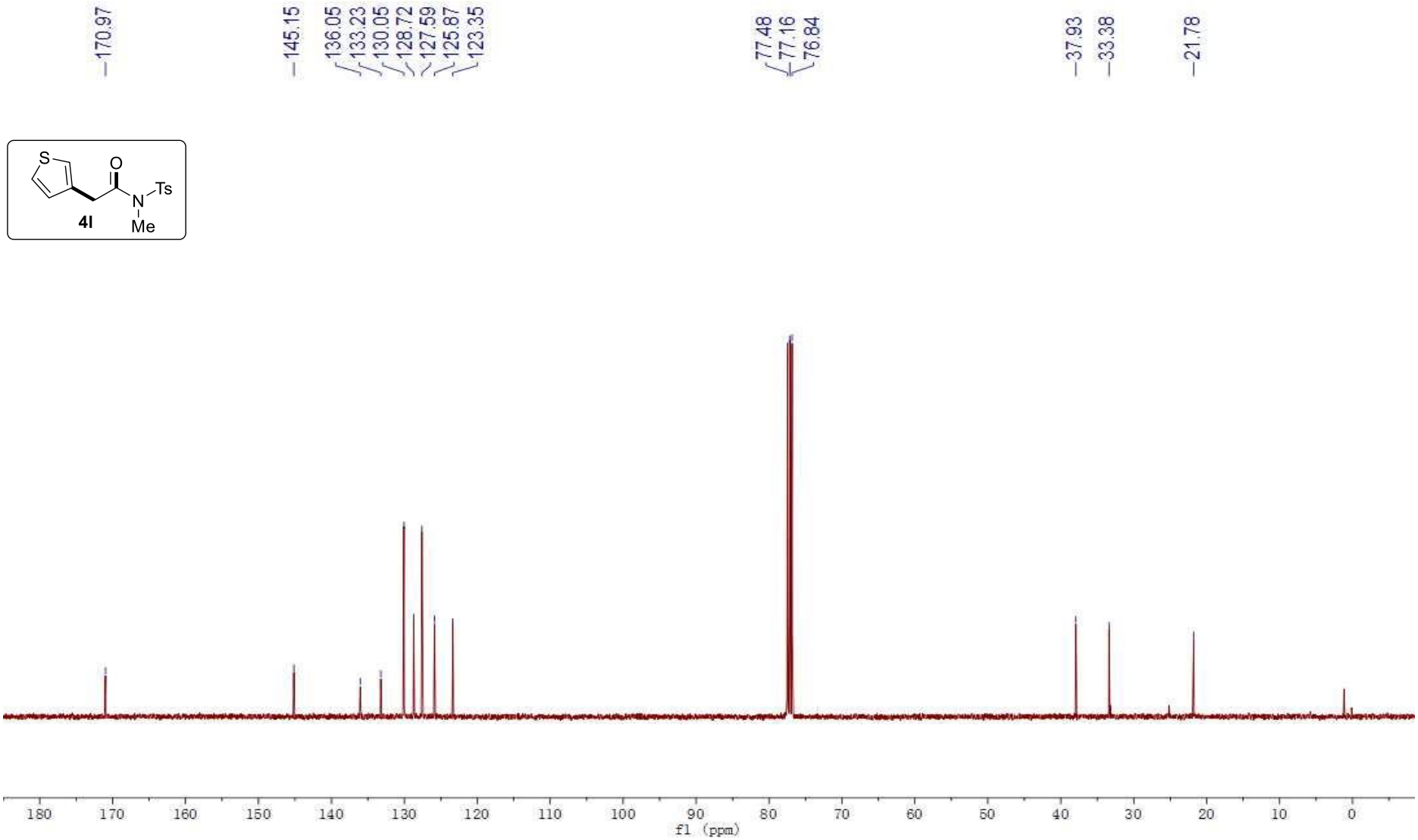
2.00
3.02
3.01
f1 (ppm)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130.05
128.72
127.59
125.87
123.35
77.48
77.16
76.84
37.93
33.38
21.78
S
O
N
Ts
Me
4l
180
170
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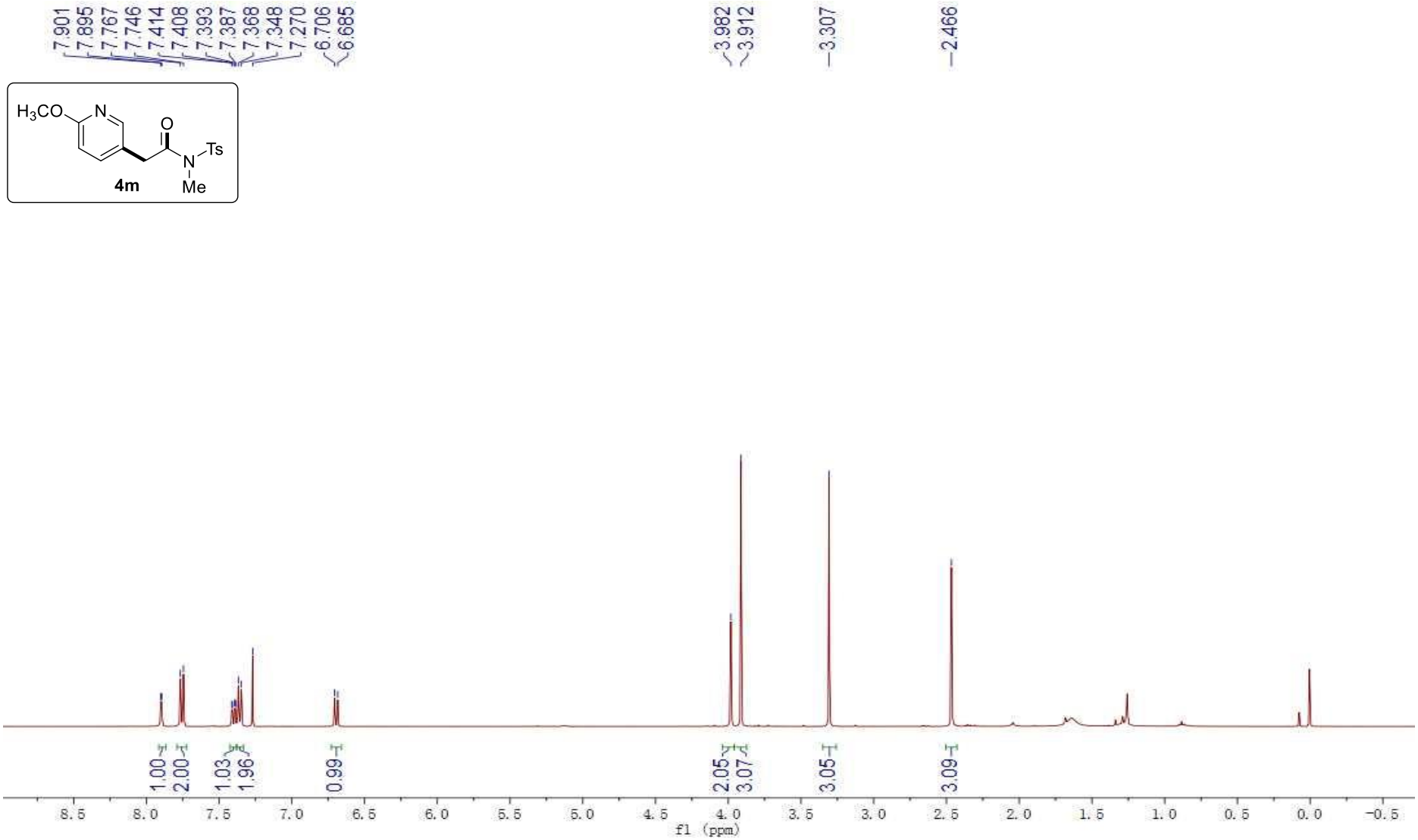
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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3.982
3.912
3.307
2.466
H3CO
N
O
Ts
N
Me
4m
1.00
2.00
1.03
1.96
0.99
2.05
3.07
3.05
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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0.5
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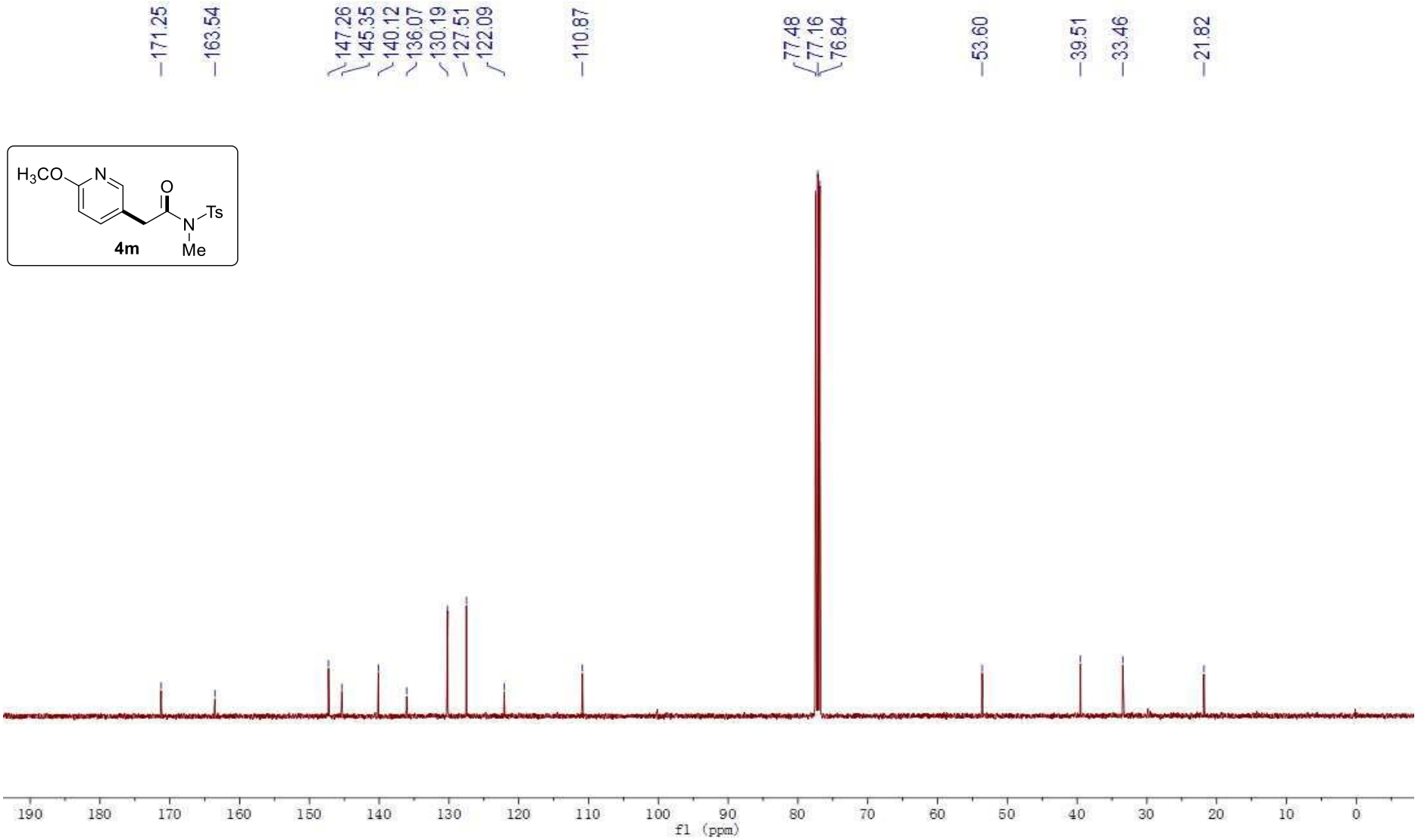
f1 (ppm)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127.51
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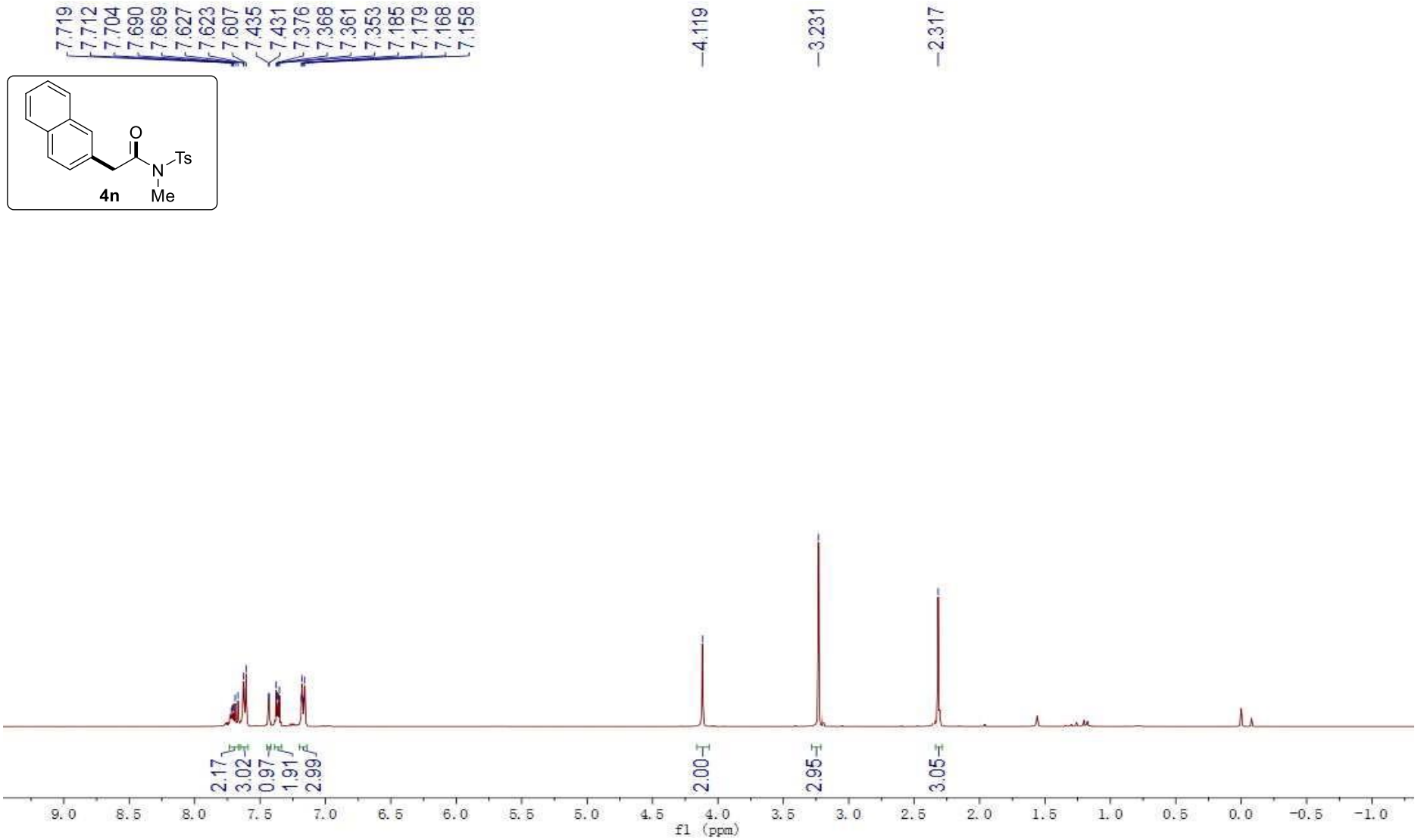
110.87
77.48
77.16
76.84
53.60
39.51
33.46
21.82
H3CO
N
O
N
Ts
Me
4m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.690
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7.607
7.435
7.431
7.376
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7.361
7.353
7.185
7.179
7.168
7.158
4.119
3.231
2.317
O
N
Ts
Me
4n
2.17
3.02
0.97
1.91
2.99
2.00
2.95
3.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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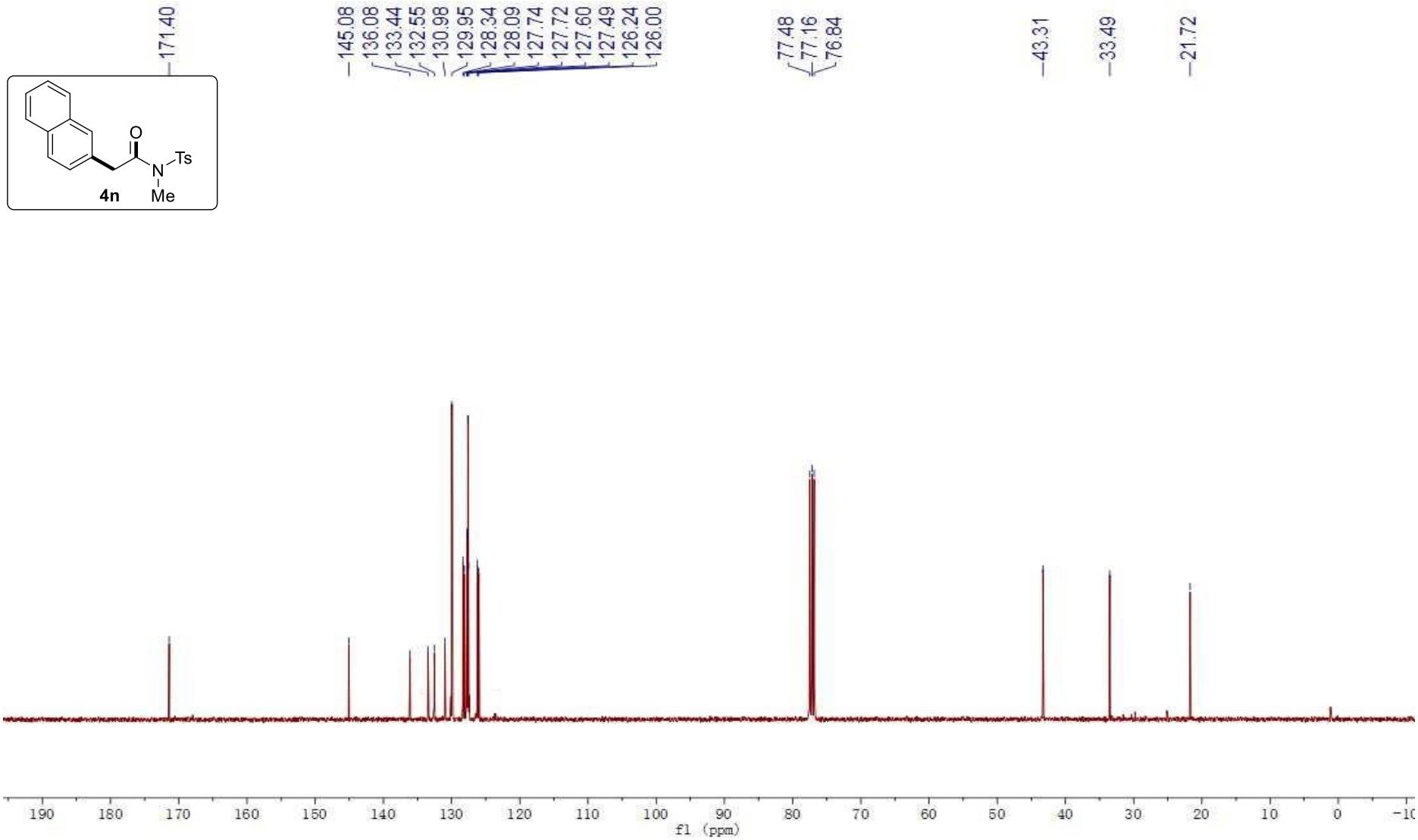
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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132.55
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129.95
128.34
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127.74
127.72
127.60
127.49
126.24
126.00
77.48
77.16
76.84
43.31
33.49
21.72
O
N
Ts
Me
4n
190
180
170
160
150
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130
120
110
100
90
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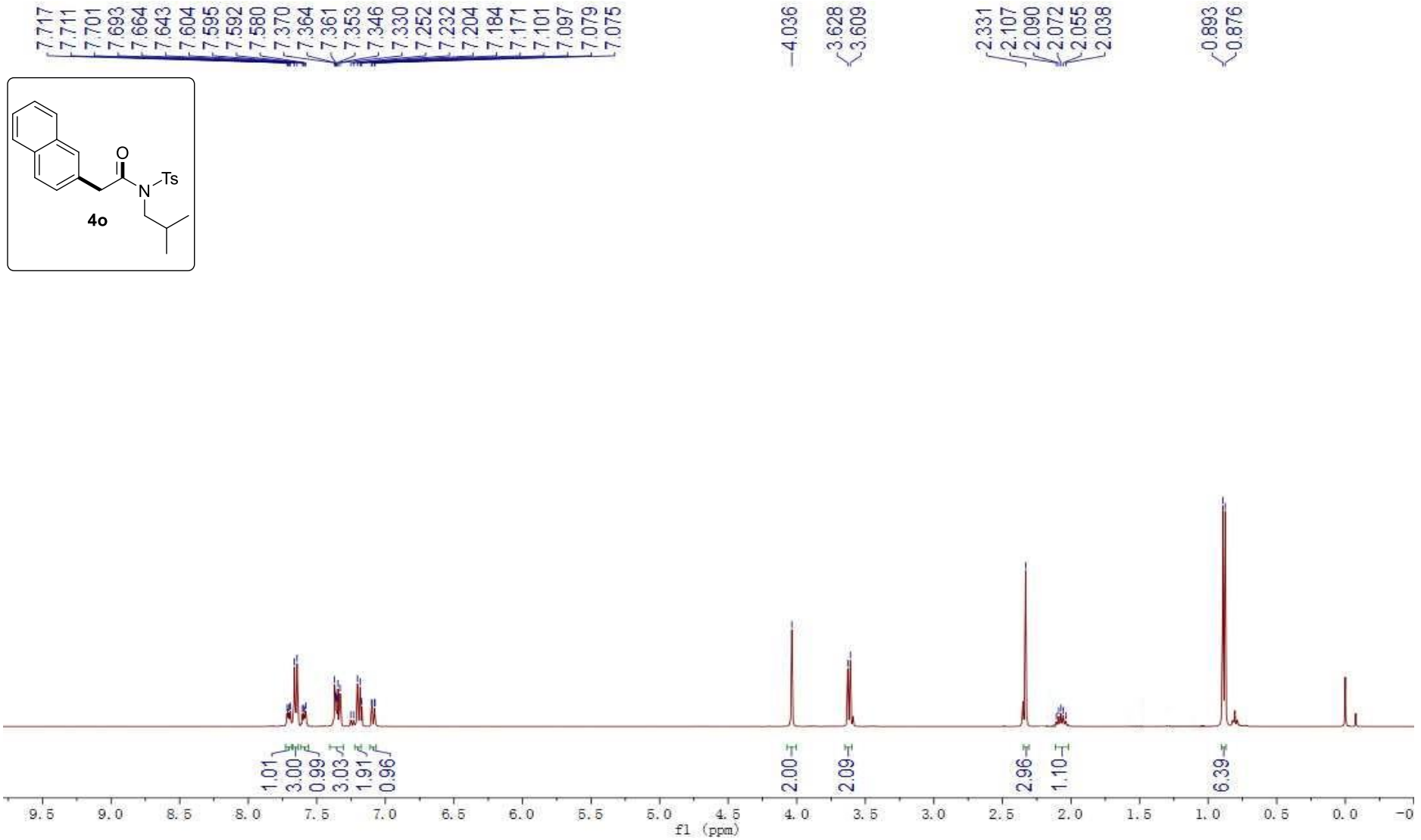
70
60
50
40
30
20
10
0
f1 (ppm)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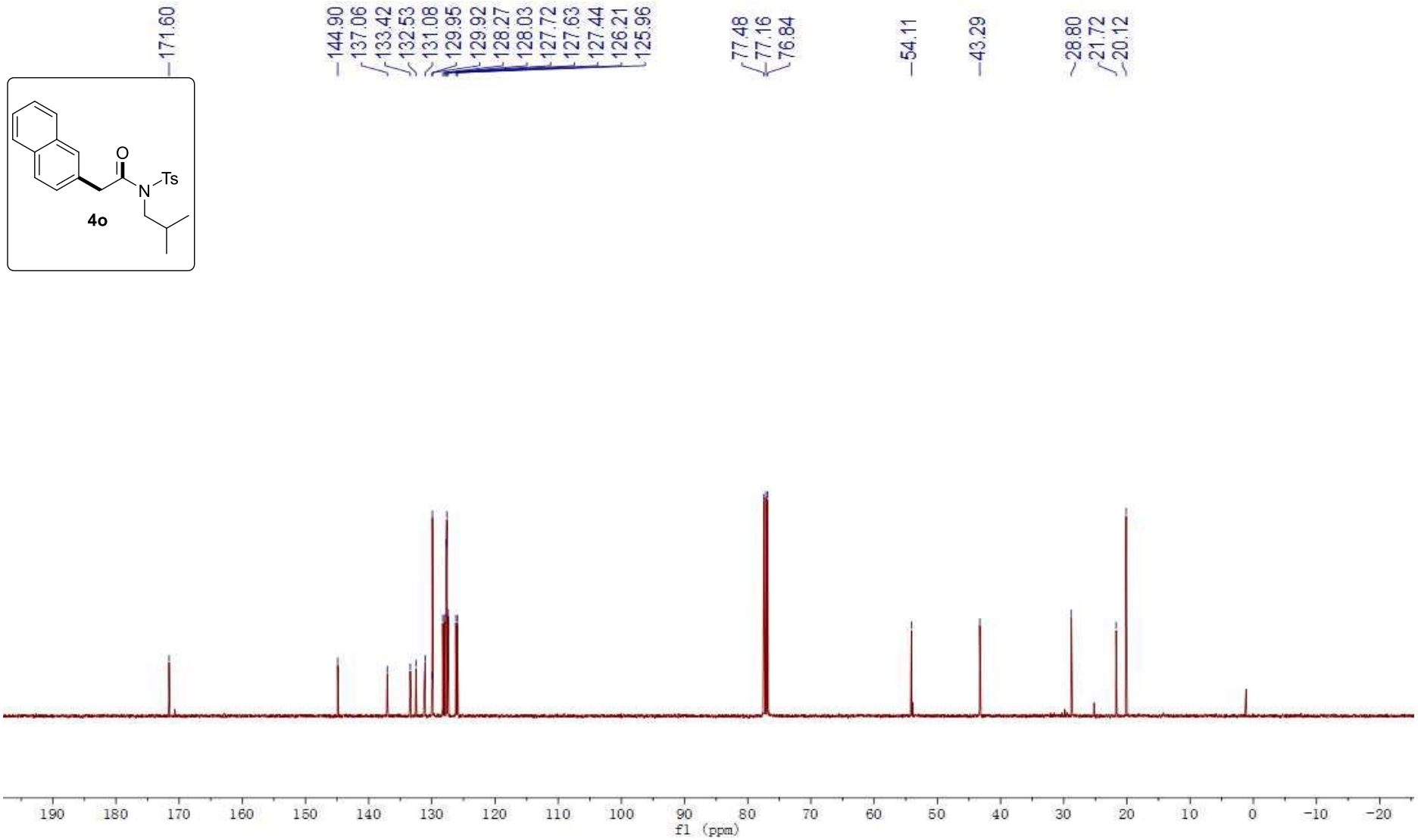
7.604
7.595
7.592
7.580
7.370
7.364
7.361
7.353
7.346
7.330
7.252
7.232
7.204
7.184
7.171
7.101
7.097
7.079
7.075
4.036
3.628
3.609
2.331
2.107
2.090
2.072
2.055
2.038
0.893
0.876
O
N
Ts
4o
1.01
3.00
0.99
3.03
1.91
0.96
2.00
2.09
2.96
1.10
6.39
f1 (ppm)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129.92
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128.03
127.72
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127.44
126.21
125.96
77.48
77.16
76.84
54.11
43.29
28.80
21.72
20.12
O
N
Ts
4o
190
180
170
160
150
140
130
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90
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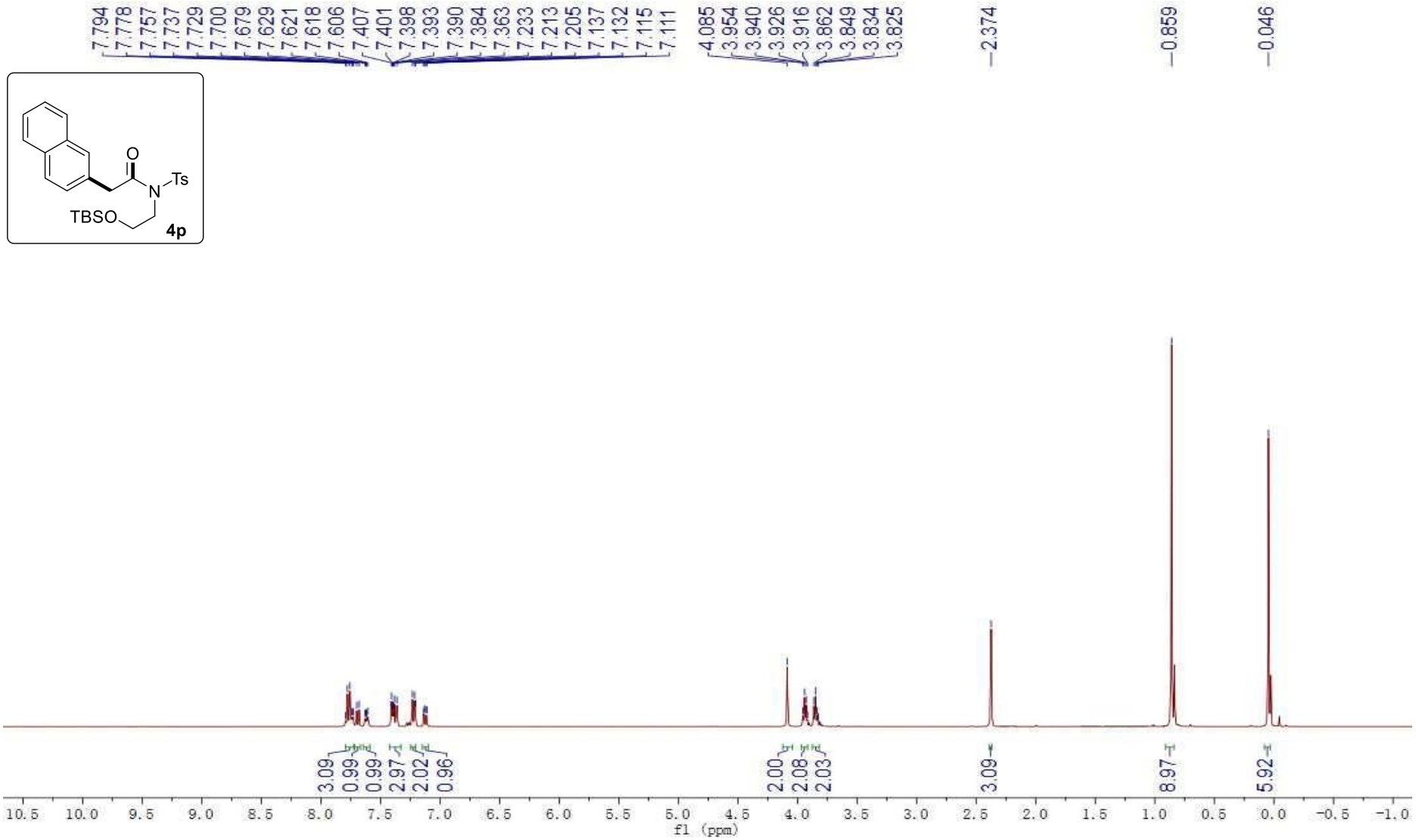
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)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7.618
7.606
7.407
7.401
7.398
7.393
7.390
7.384
7.363
7.233
7.213
7.205
7.137
7.132
7.115
7.111
4.085
3.954
3.940
3.926
3.916
3.862
3.849
3.834
3.825
2.374
0.859
0.046
O
N
Ts
TBSO
4p
3.09
0.99
0.99
2.97
2.02
0.96
2.00
2.08
2.03
3.09
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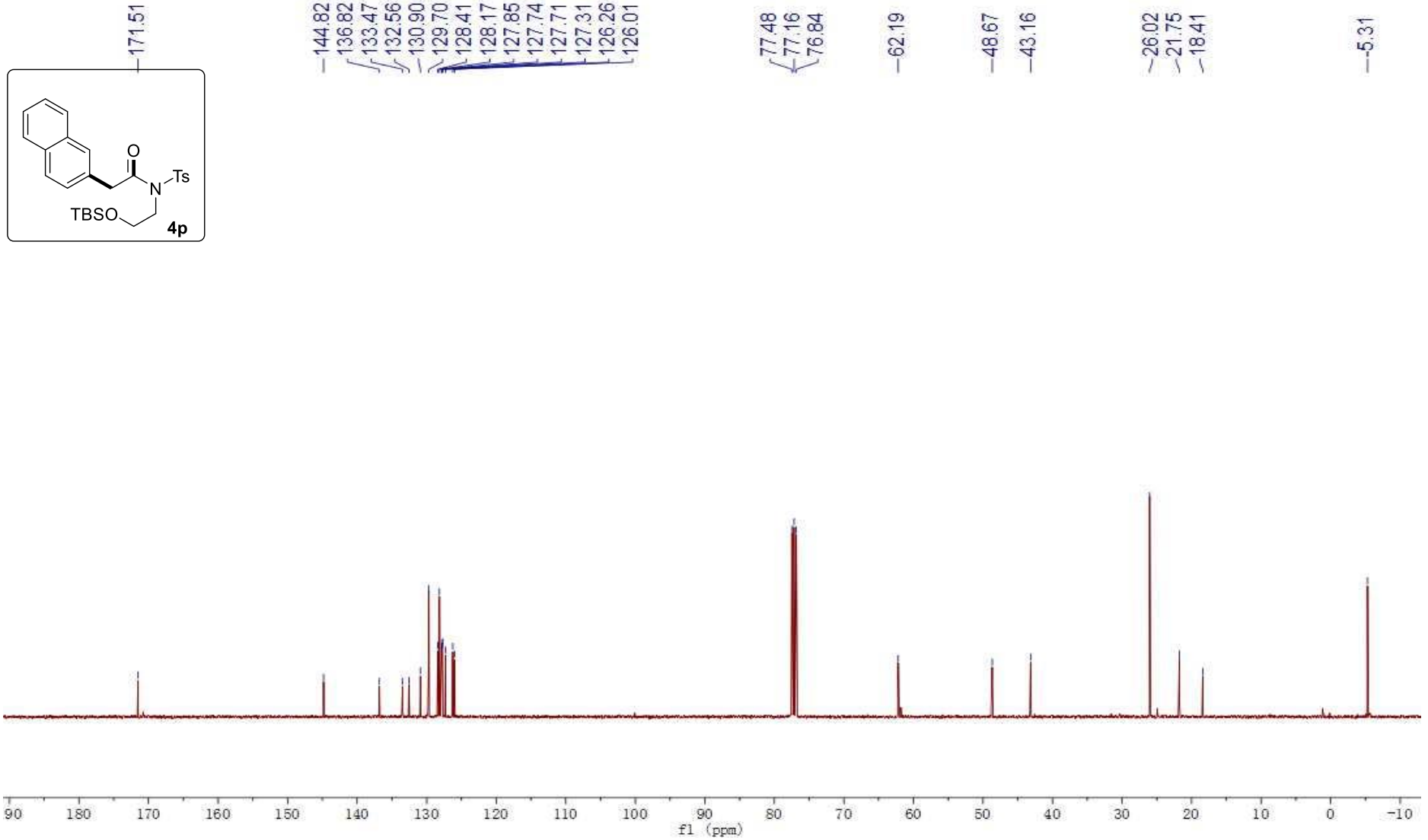
5.92
f1 (ppm)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129.70
128.41
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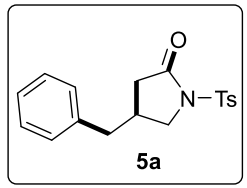
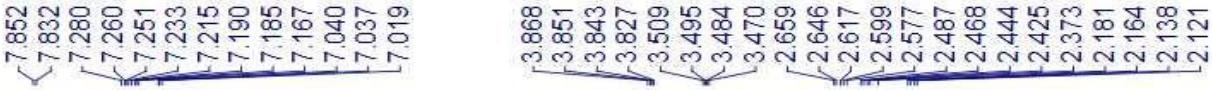
127.85
127.74
127.71
127.31
126.26
126.01
77.48
77.16
76.84
62.19
48.67
43.16
26.02
21.75
18.41
-5.31
O
N
Ts
TBSO
4p
f1 (ppm)


O
N–Ts

5a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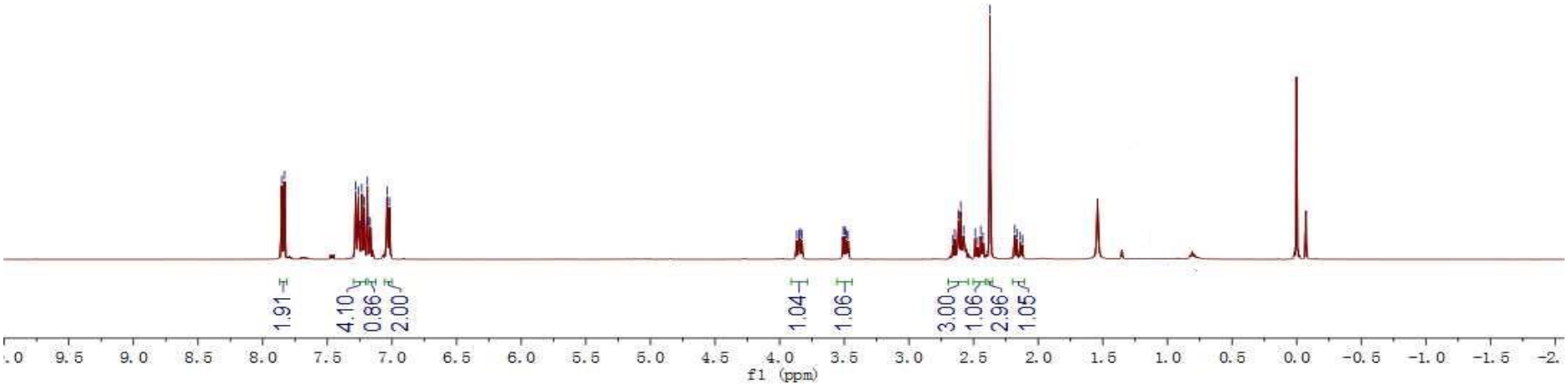
7.190
7.185
7.167
7.040
7.037
7.019
3.868
3.851
3.843
3.827
3.509
3.495
3.484
3.470
2.659
2.646
2.617
2.599
2.577
2.487
2.468
2.444
2.425
2.373
2.181
2.164
2.138
2.121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4.10
0.86
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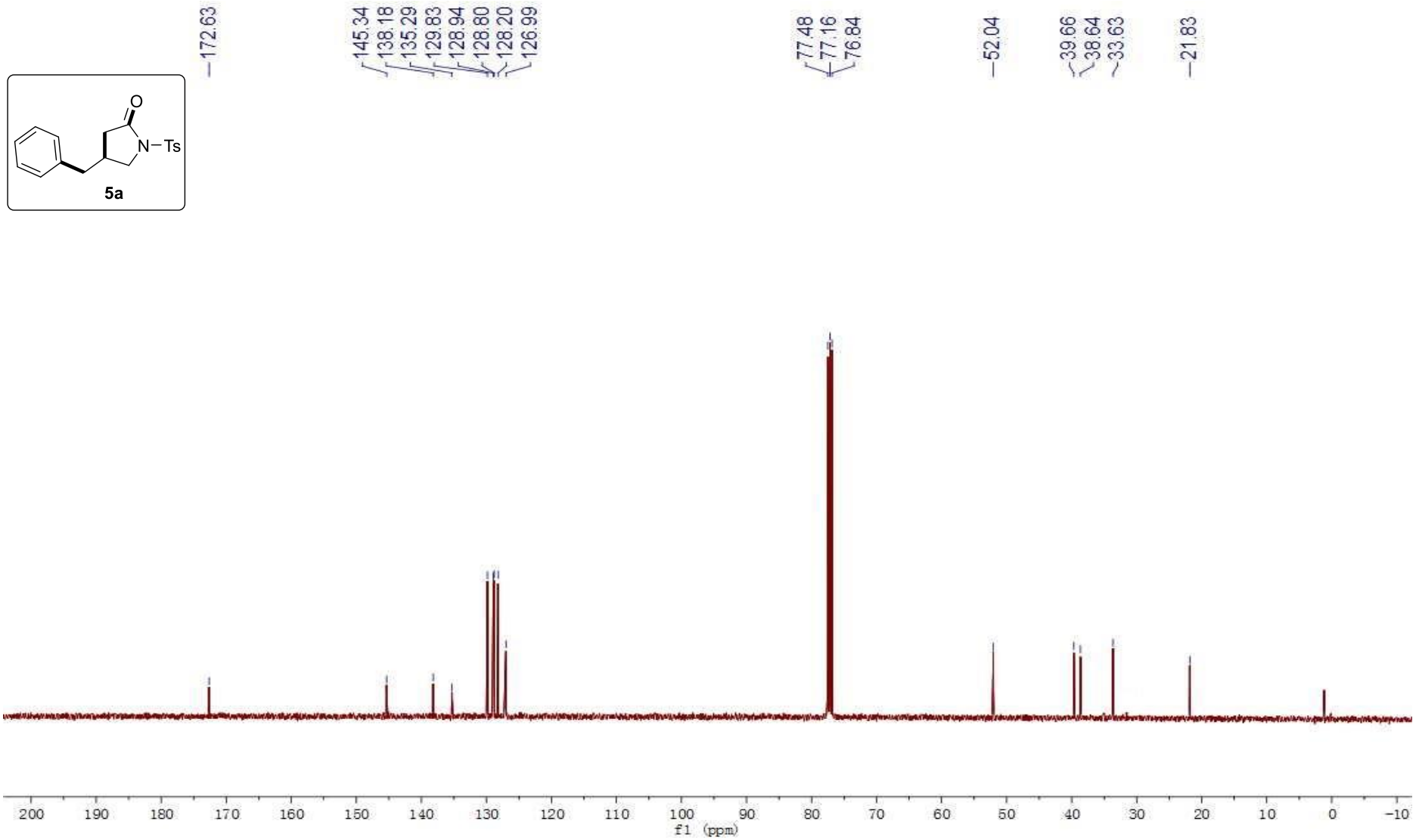
1.04
1.06
3.00
1.06
2.96
1.05
f1 (ppm)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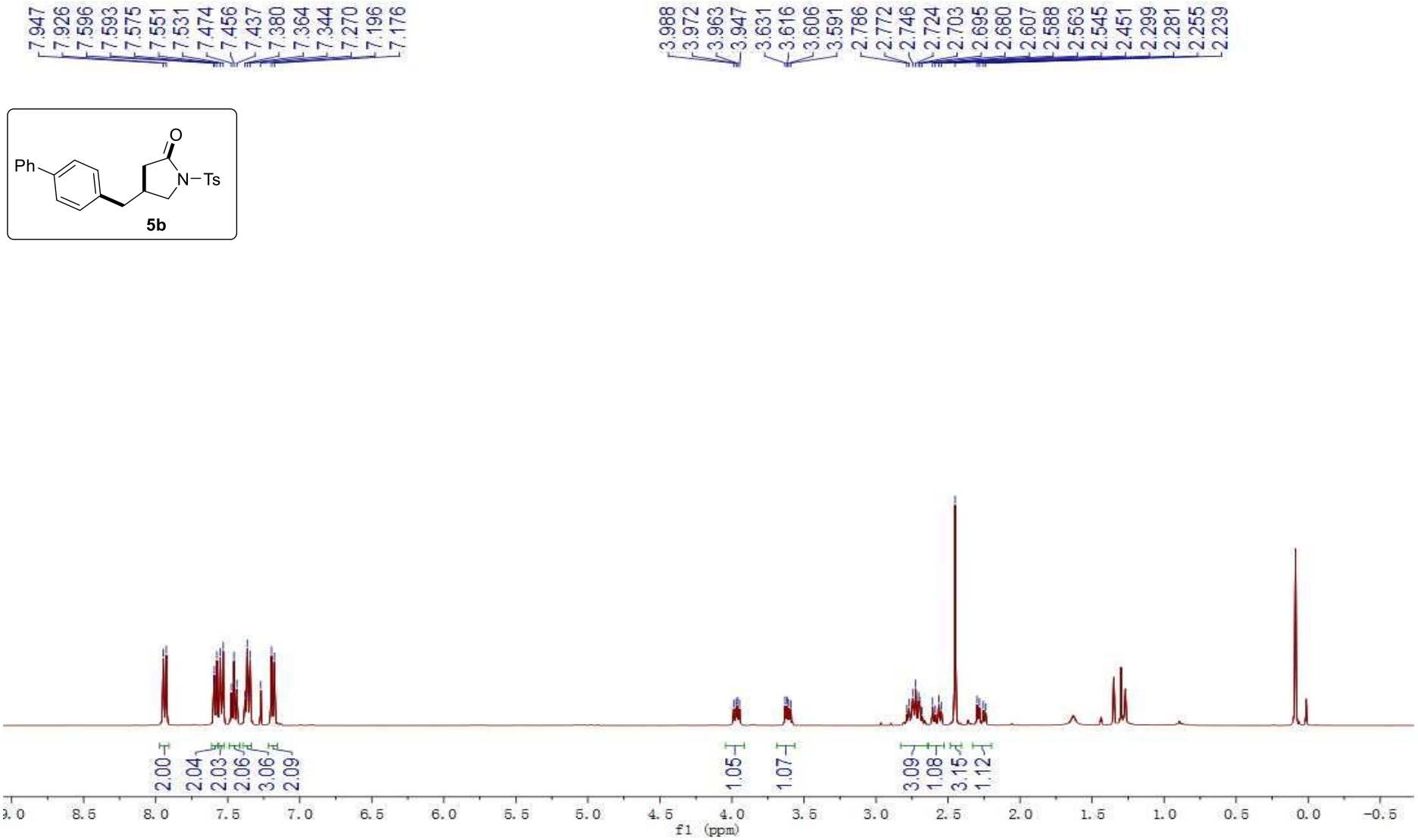
135.29
129.83
128.94
128.80
128.20
126.99
77.48
77.16
76.84
52.04
39.66
38.64
33.63
21.83
O
N−Ts
5a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.593
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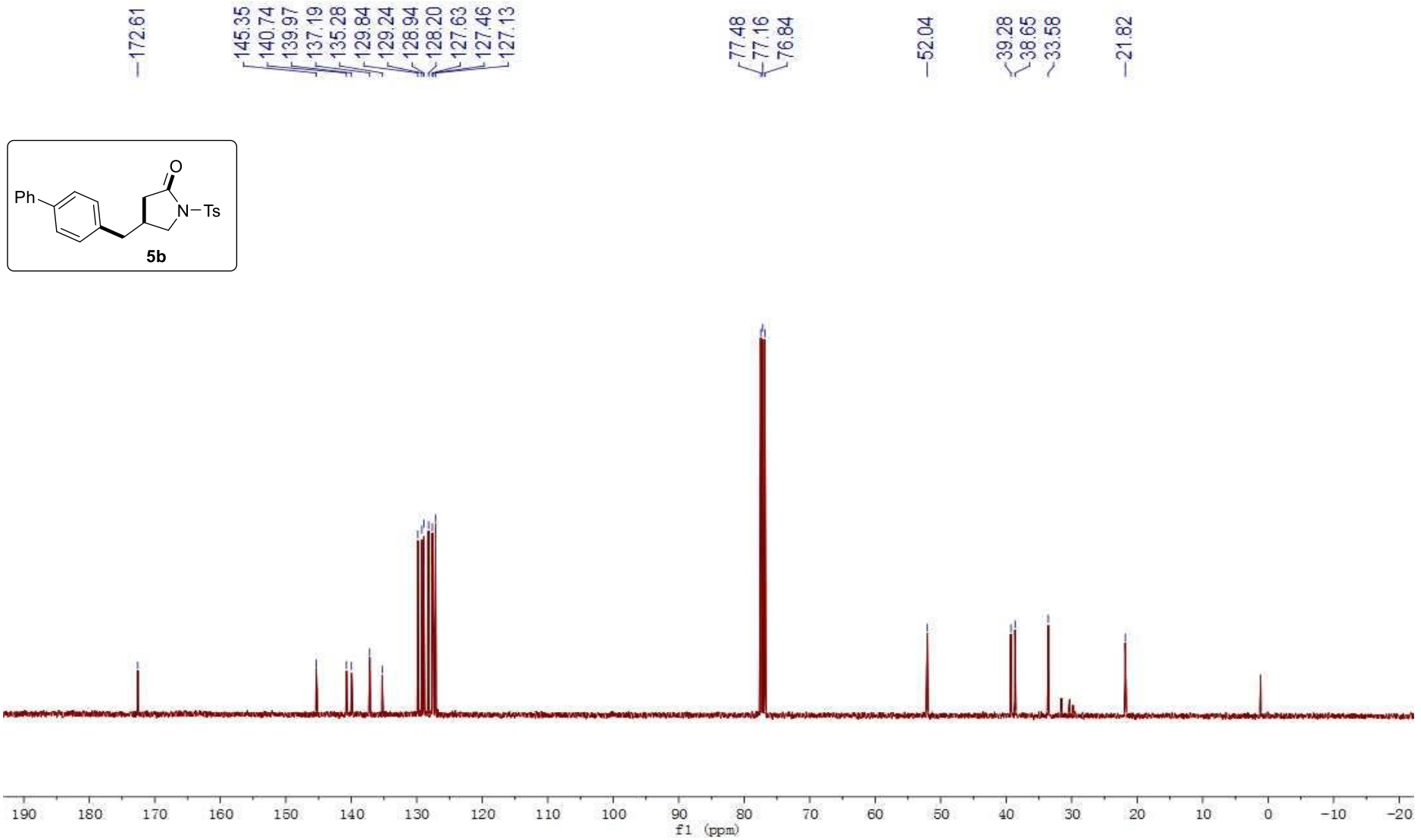
7.474
7.456
7.437
7.380
7.364
7.344
7.270
7.196
7.176
3.988
3.972
3.963
3.947
3.631
3.616
3.606
3.591
2.786
2.772
2.746
2.724
2.703
2.695
2.680
2.607
2.588
2.563
2.545
2.451
2.299
2.281
2.255
2.239
Ph
O
N−Ts
5b
2.00
2.04
2.03
2.06
3.06
2.09
1.05
1.07
3.09
1.08
3.15
1.12
f1 (ppm)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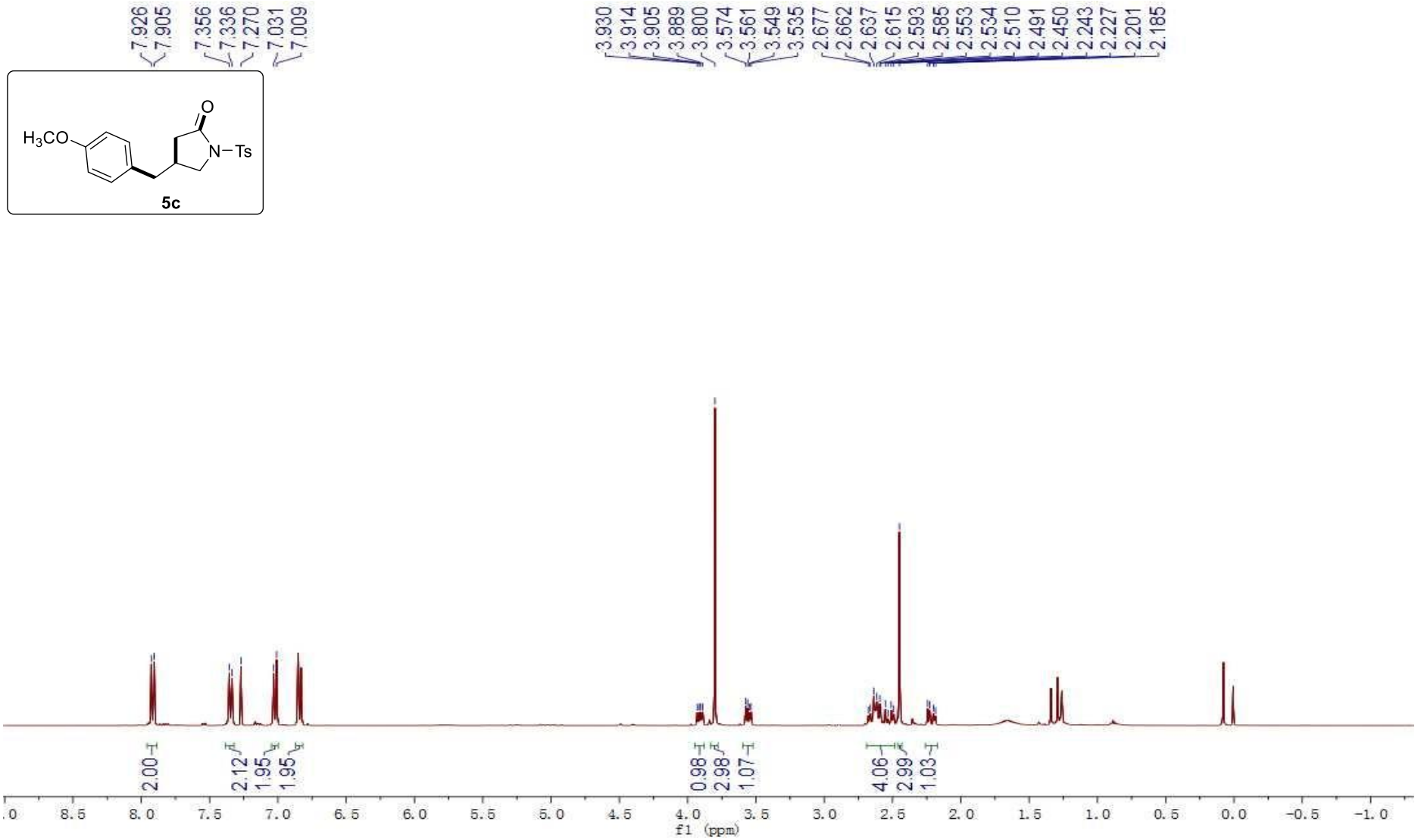
140.74
139.97
137.19
135.28
129.84
129.24
128.94
128.20
127.63
127.46
127.13
77.48
77.16
76.84
52.04
39.28
38.65
33.58
21.82
Ph
O
N−Ts
5b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)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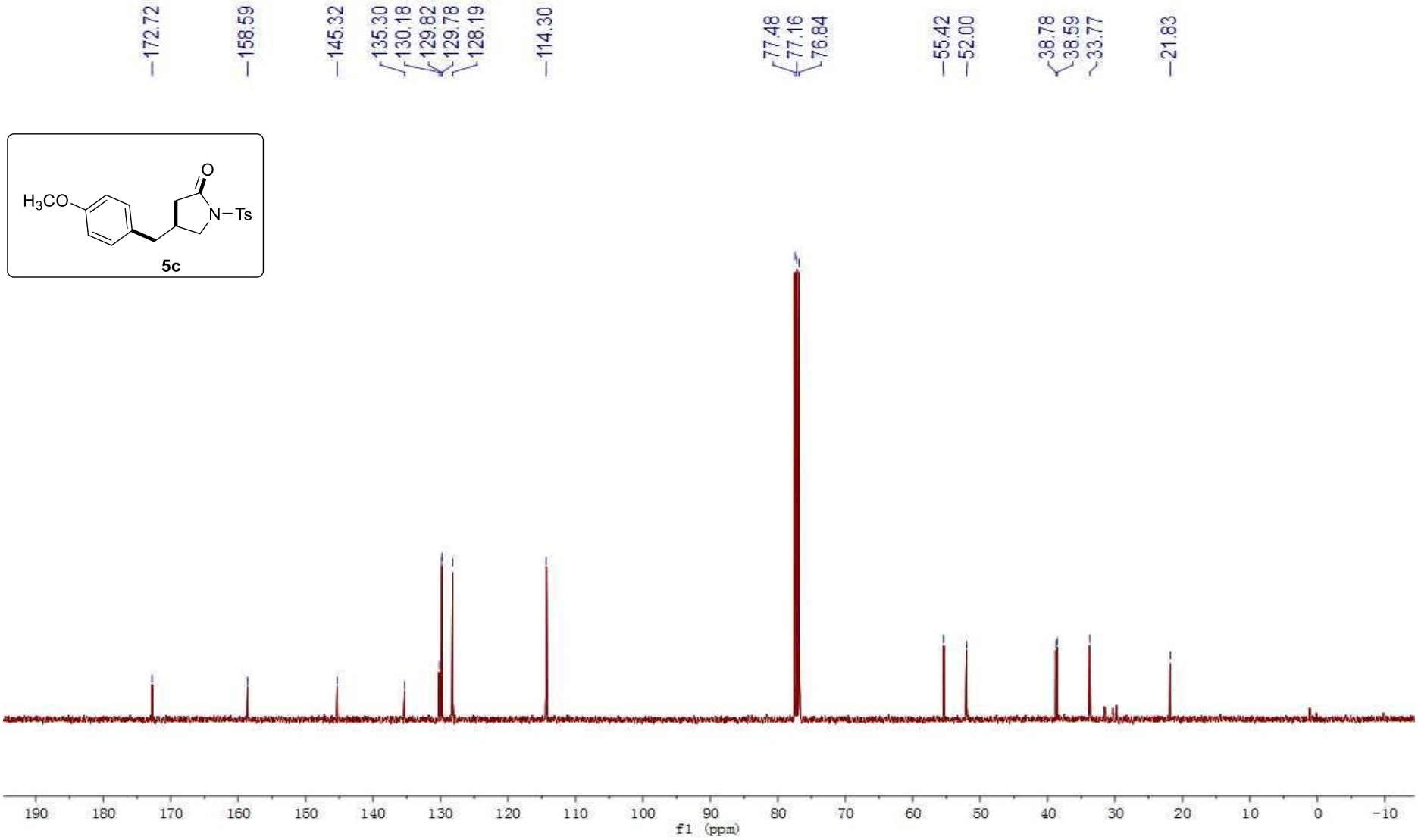
3.914
3.905
3.889
3.800
3.574
3.561
3.549
3.535
2.677
2.662
2.637
2.615
2.593
2.585
2.553
2.534
2.510
2.491
2.450
2.243
2.227
2.201
2.185
H3CO
O
N−Ts
5c
2.00
2.12
1.95
1.95
0.98
2.98
1.07
4.06
2.99
1.03
f1 (ppm)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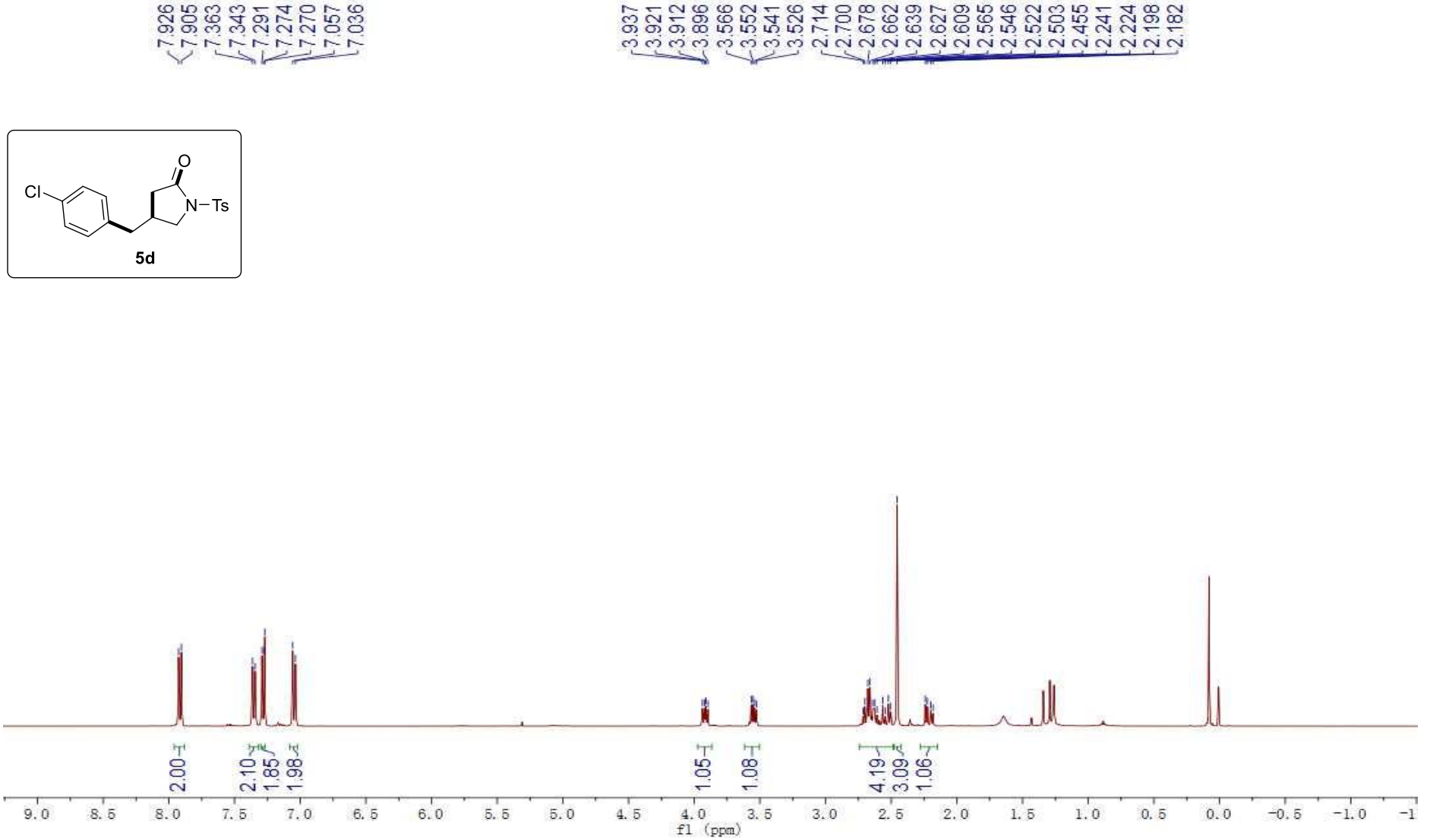
158.59
145.32
135.30
130.18
129.82
129.78
128.19
114.30
77.48
77.16
76.84
55.42
52.00
38.78
38.59
33.77
21.83
H3CO
O
N−Ts
5c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.343
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7.274
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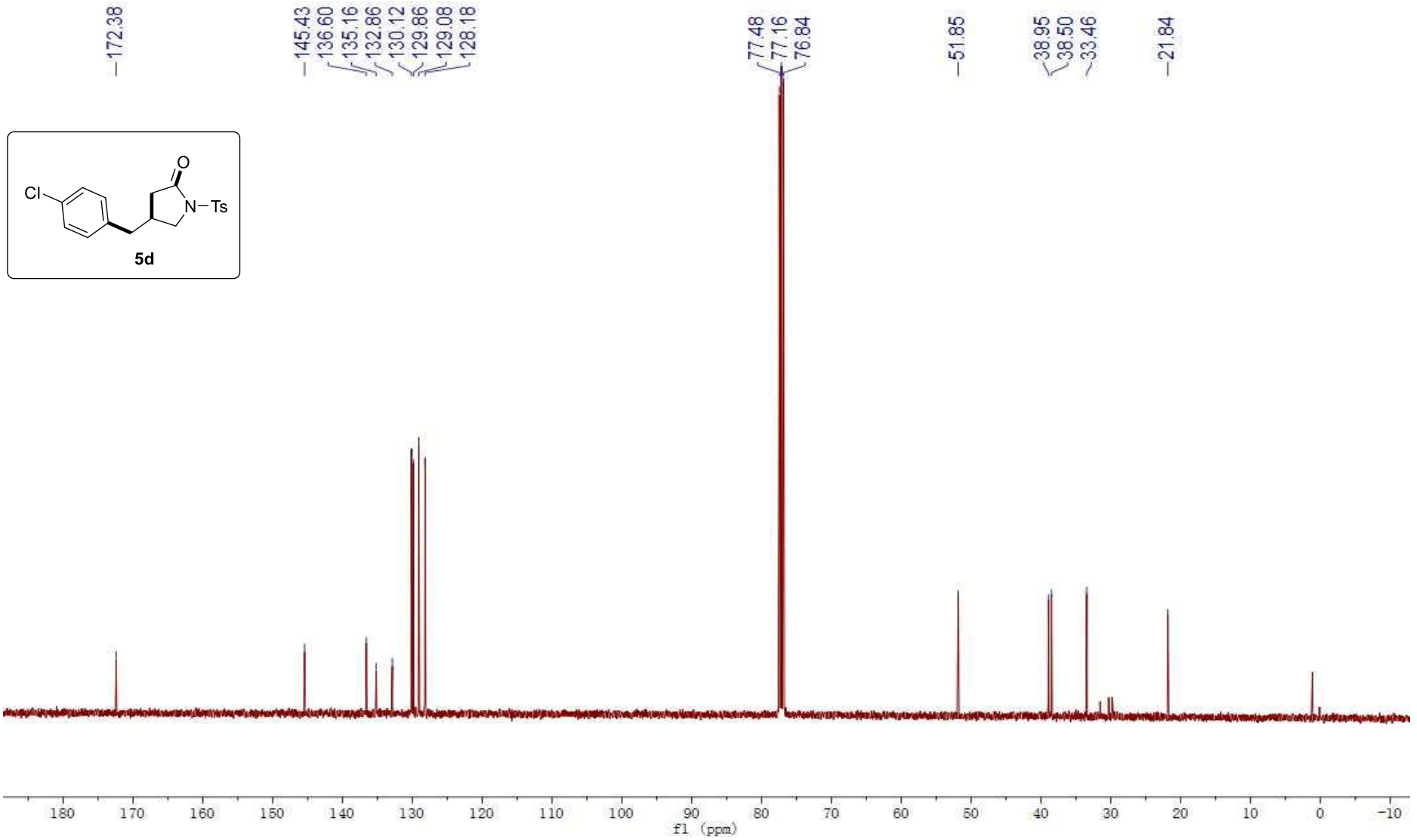
7.057
7.036
3.937
3.921
3.912
3.896
3.566
3.552
3.541
3.526
2.714
2.700
2.678
2.662
2.639
2.627
2.609
2.565
2.546
2.522
2.503
2.455
2.241
2.224
2.198
2.182
Cl
O
N–Ts
5d
2.00
2.10
1.85
1.98
1.05
1.08
4.19
3.09
1.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1
f1 (ppm)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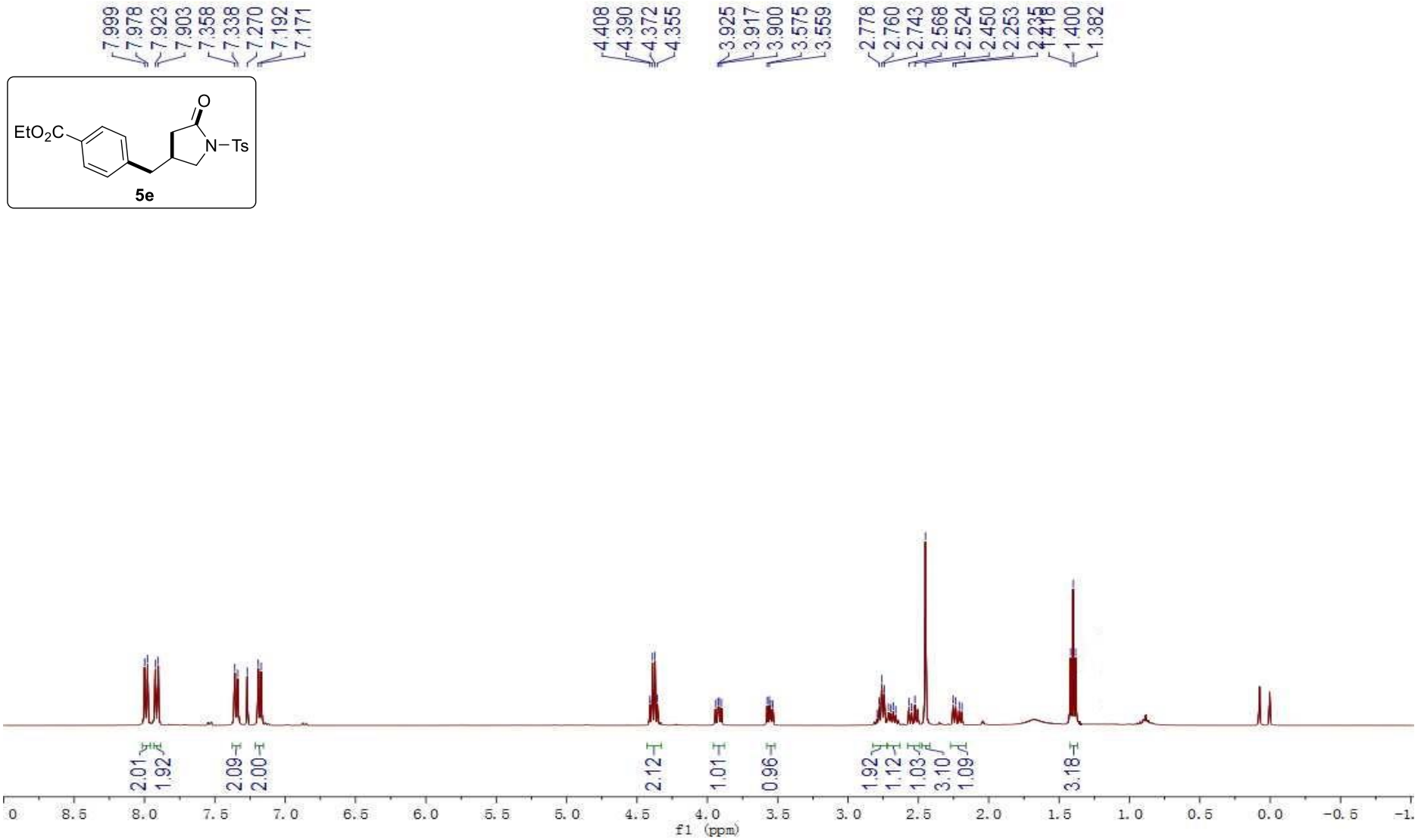
132.86
130.12
129.86
129.08
128.18
77.48
77.16
76.84
51.85
38.95
38.50
33.46
21.84
Cl
O
N–Ts
5d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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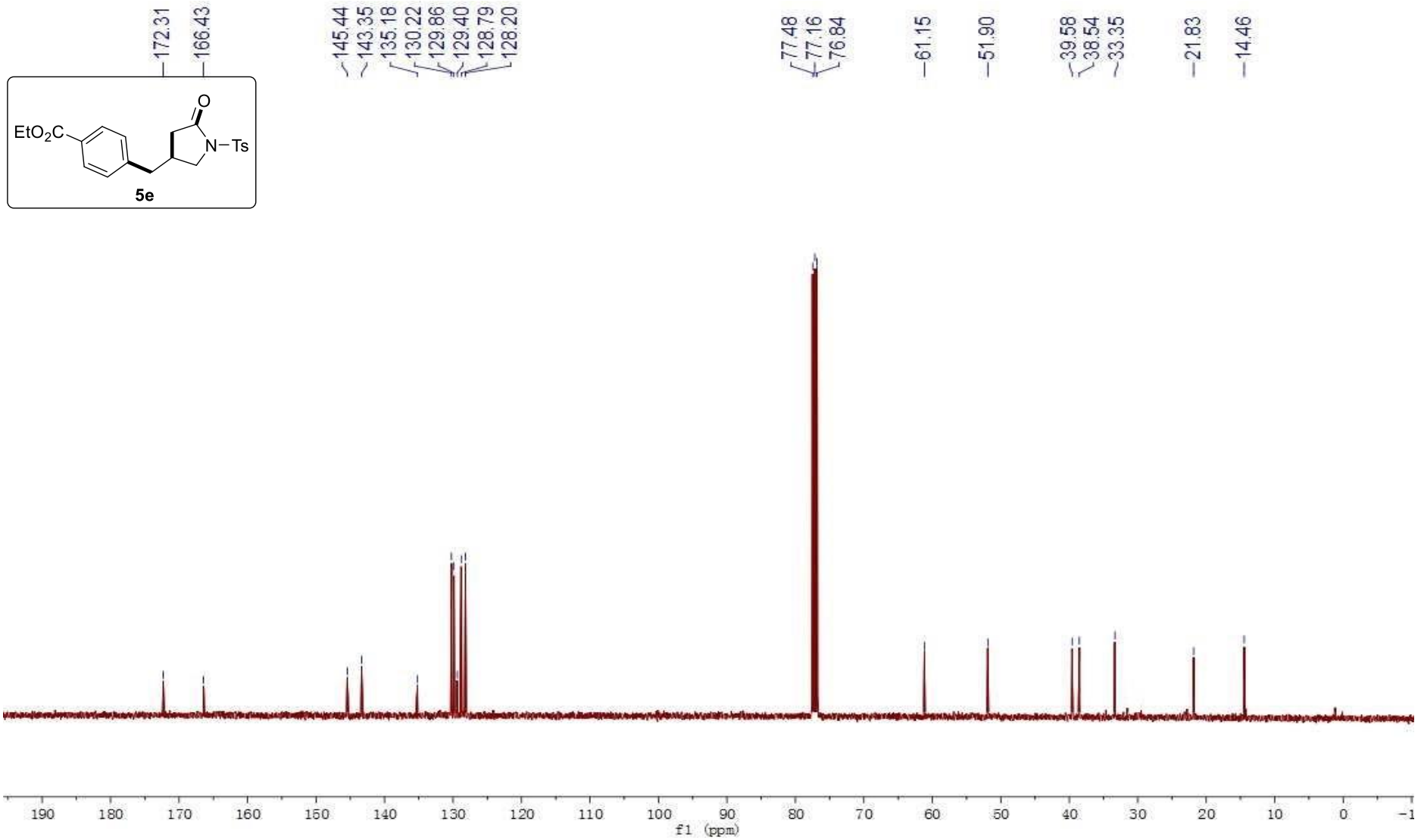
7.338
7.270
7.192
7.171
4.408
4.390
4.372
4.355
3.925
3.917
3.900
3.575
3.559
2.778
2.760
2.743
2.568
2.524
2.450
2.253
1.400
1.382
EtO2C
O
N−Ts
5e
2.01
1.92
2.09
2.00
2.12
1.01
0.96
1.92
1.12
1.03
3.10
1.09
3.18
f1 (ppm)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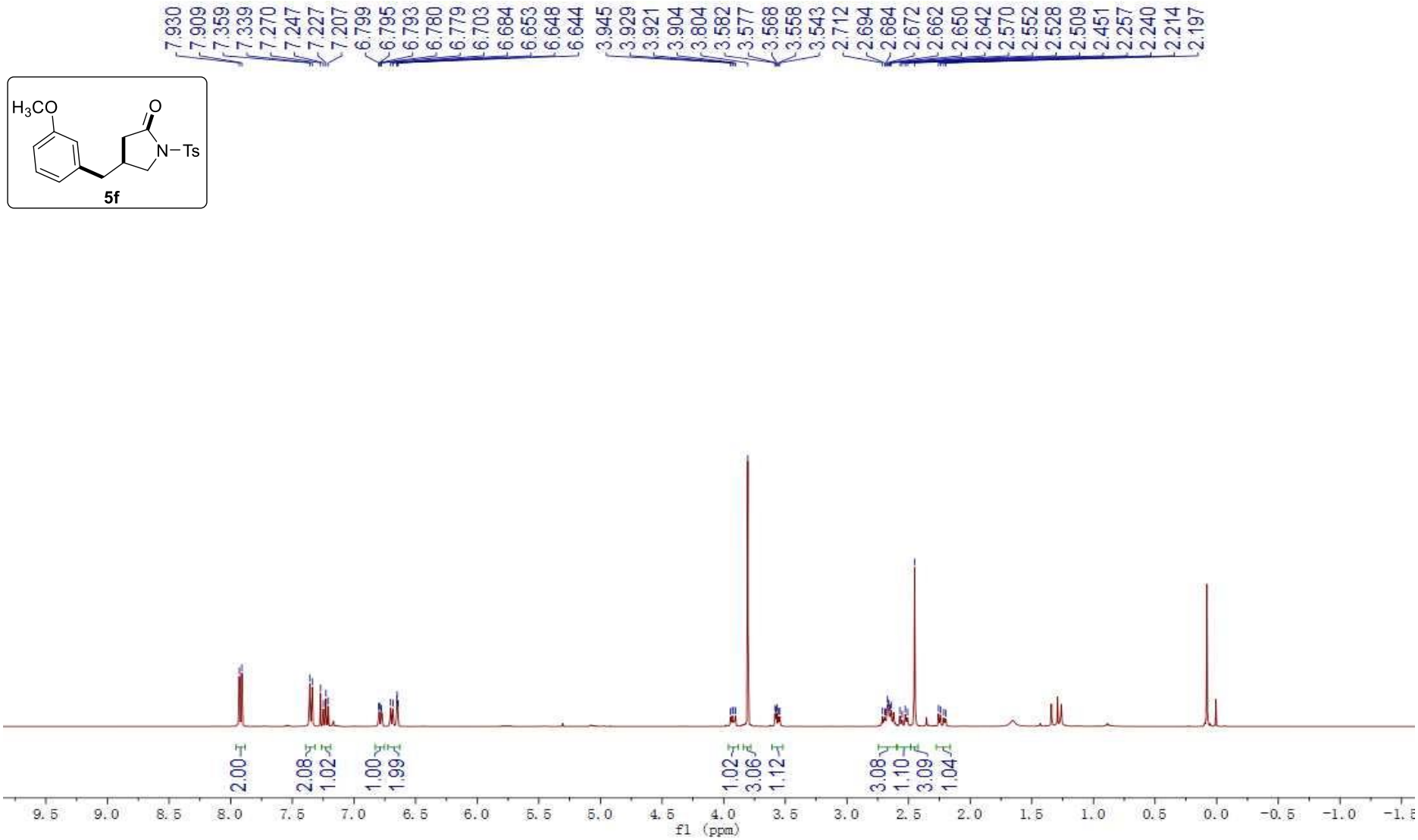
130.22
129.86
129.40
128.79
128.20
77.48
77.16
76.84
61.15
51.90
39.58
38.54
33.35
21.83
14.46
EtO2C
O
N–Ts
5e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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7.207
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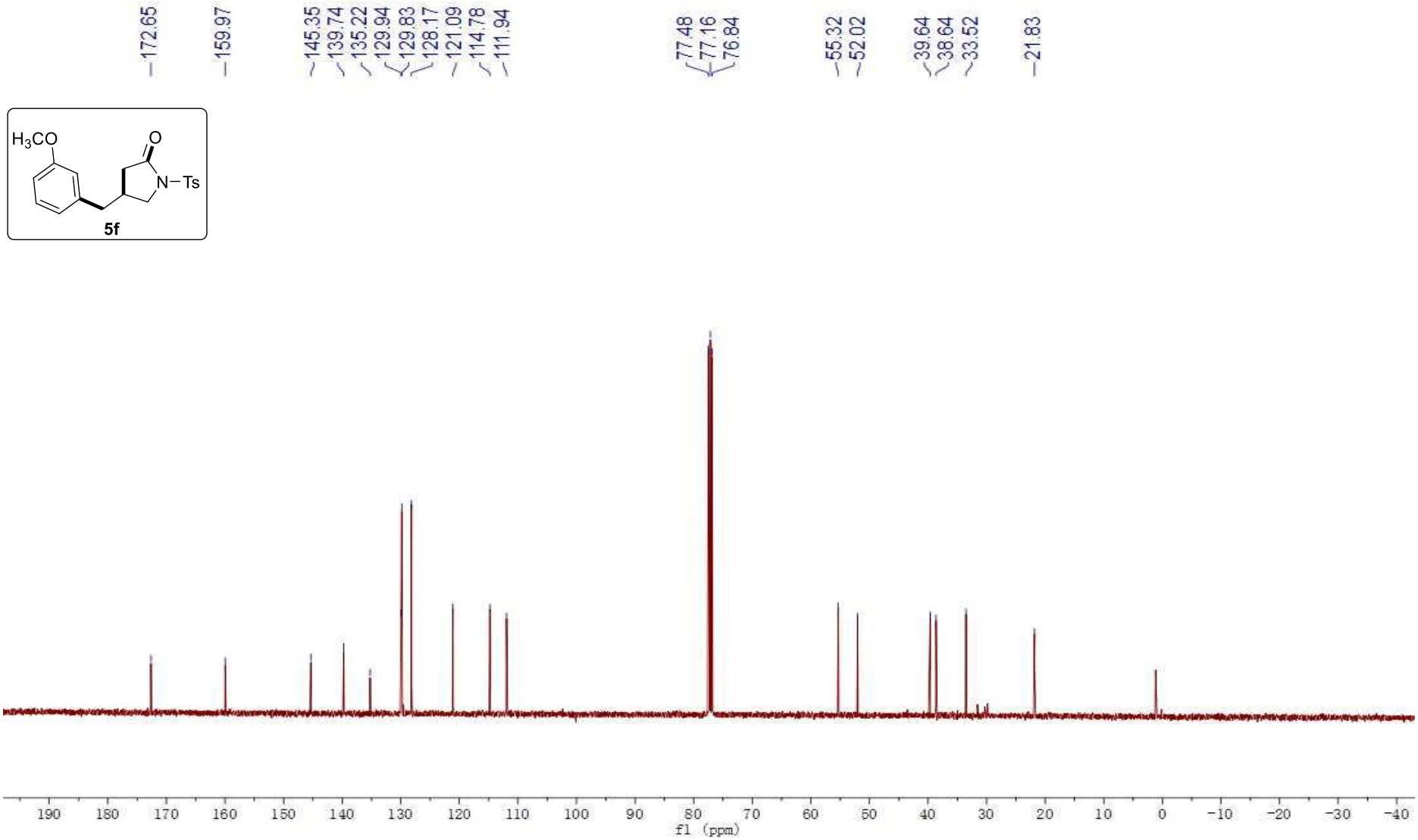
6.780
6.779
6.703
6.684
6.653
6.648
6.644
3.945
3.929
3.921
3.904
3.804
3.582
3.577
3.568
3.558
3.543
2.712
2.694
2.684
2.672
2.662
2.650
2.642
2.570
2.552
2.528
2.509
2.451
2.257
2.240
2.214
2.197
H3CO
O
N−Ts
5f
2.00
2.08
1.02
1.00
1.99
1.02
3.06
1.12
3.08
1.10
3.09
1.04
f1 (ppm)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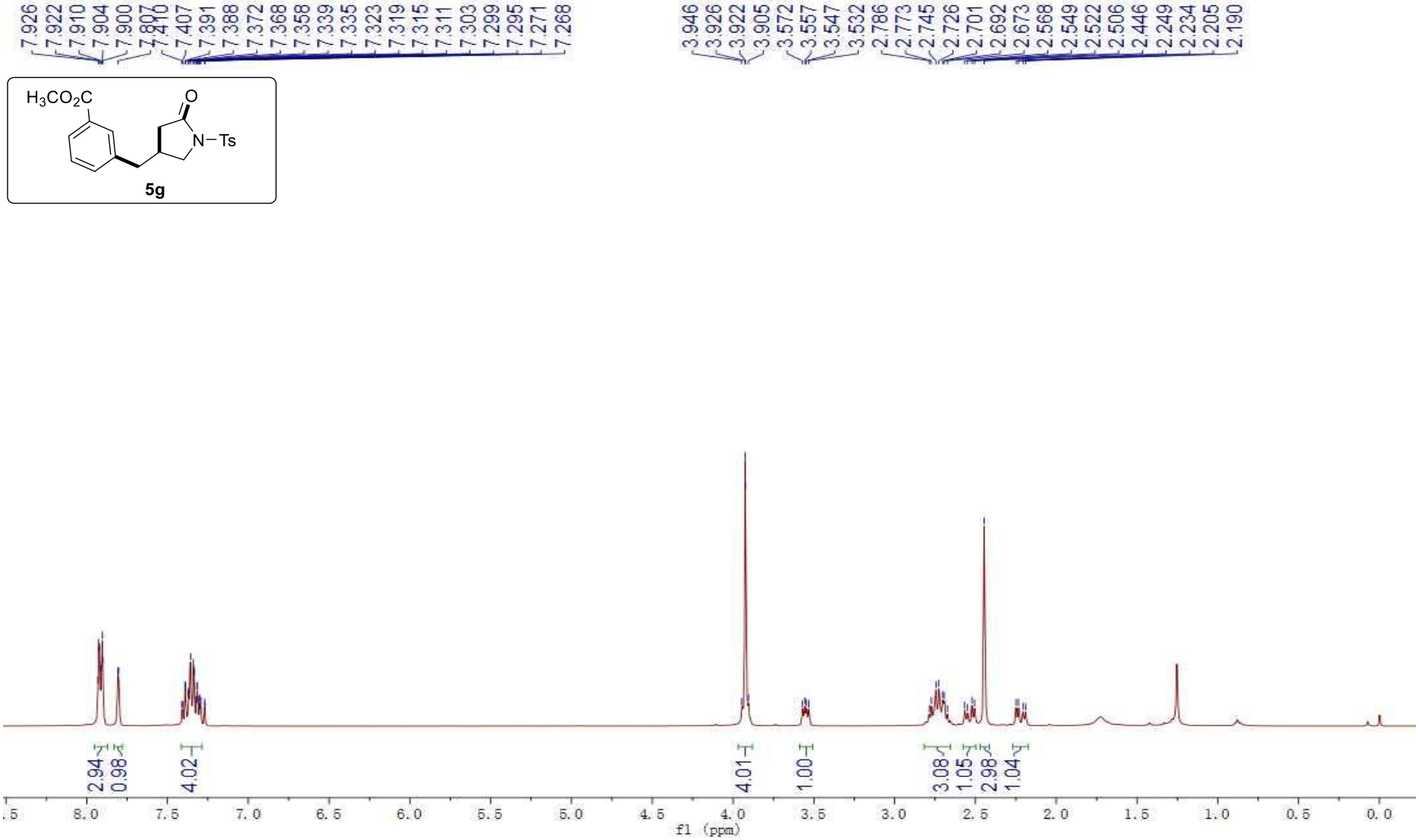
135.22
129.94
129.83
128.17
121.09
114.78
111.94
77.48
77.16
76.84
55.32
52.02
39.64
38.64
33.52
21.83
H3CO
O
N−Ts
5f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30 −40
f1 (ppm)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7.323
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7.303
7.299
7.295
7.271
7.268
3.946
3.926
3.922
3.905
3.572
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3.547
3.532
2.786
2.773
2.745
2.726
2.701
2.692
2.673
2.568
2.549
2.522
2.506
2.446
2.249
2.234
2.205
2.190
H3CO2C
O
N−Ts
5g
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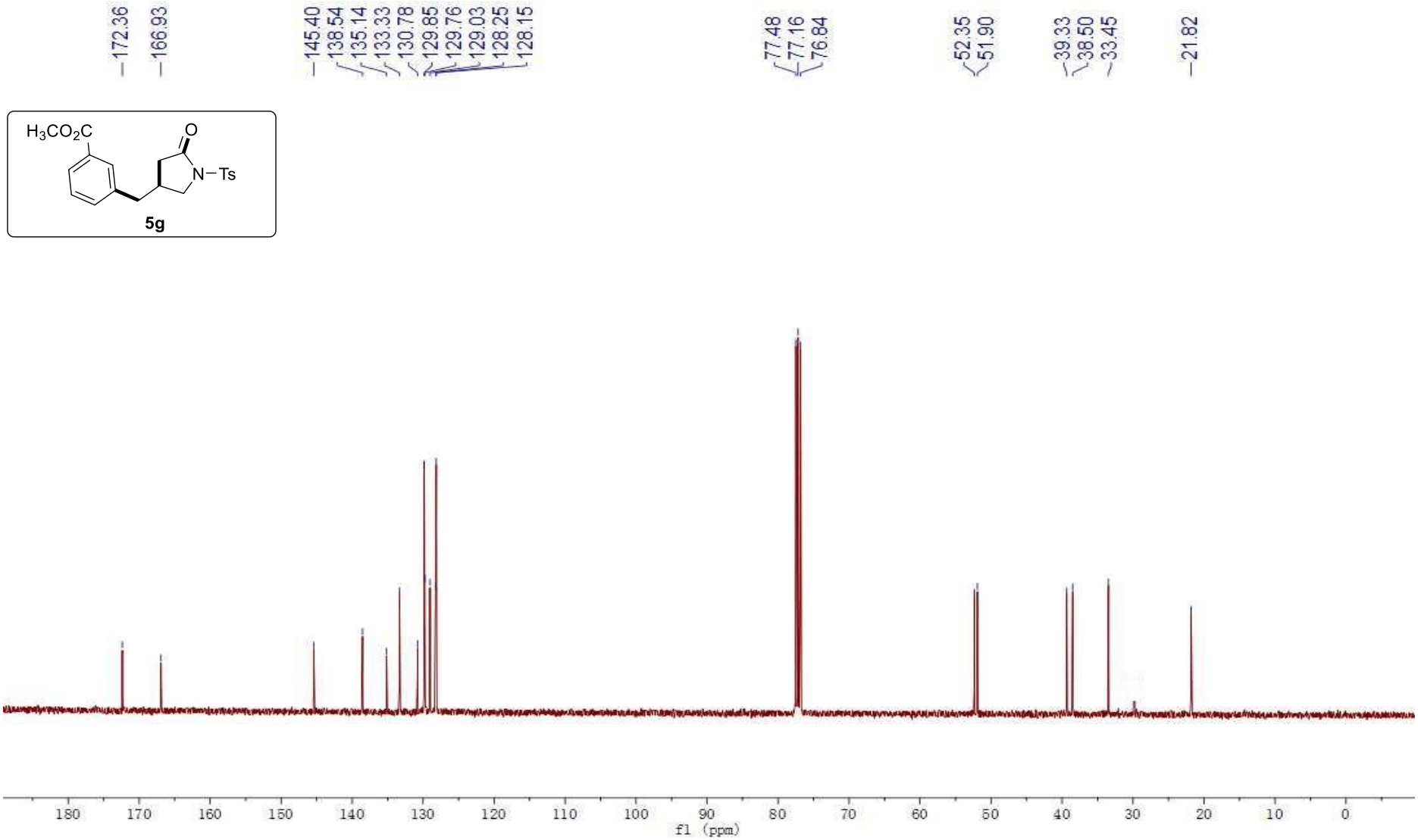
0.98
4.02
4.01
1.00
3.08
1.05
2.98
1.04
f1 (ppm)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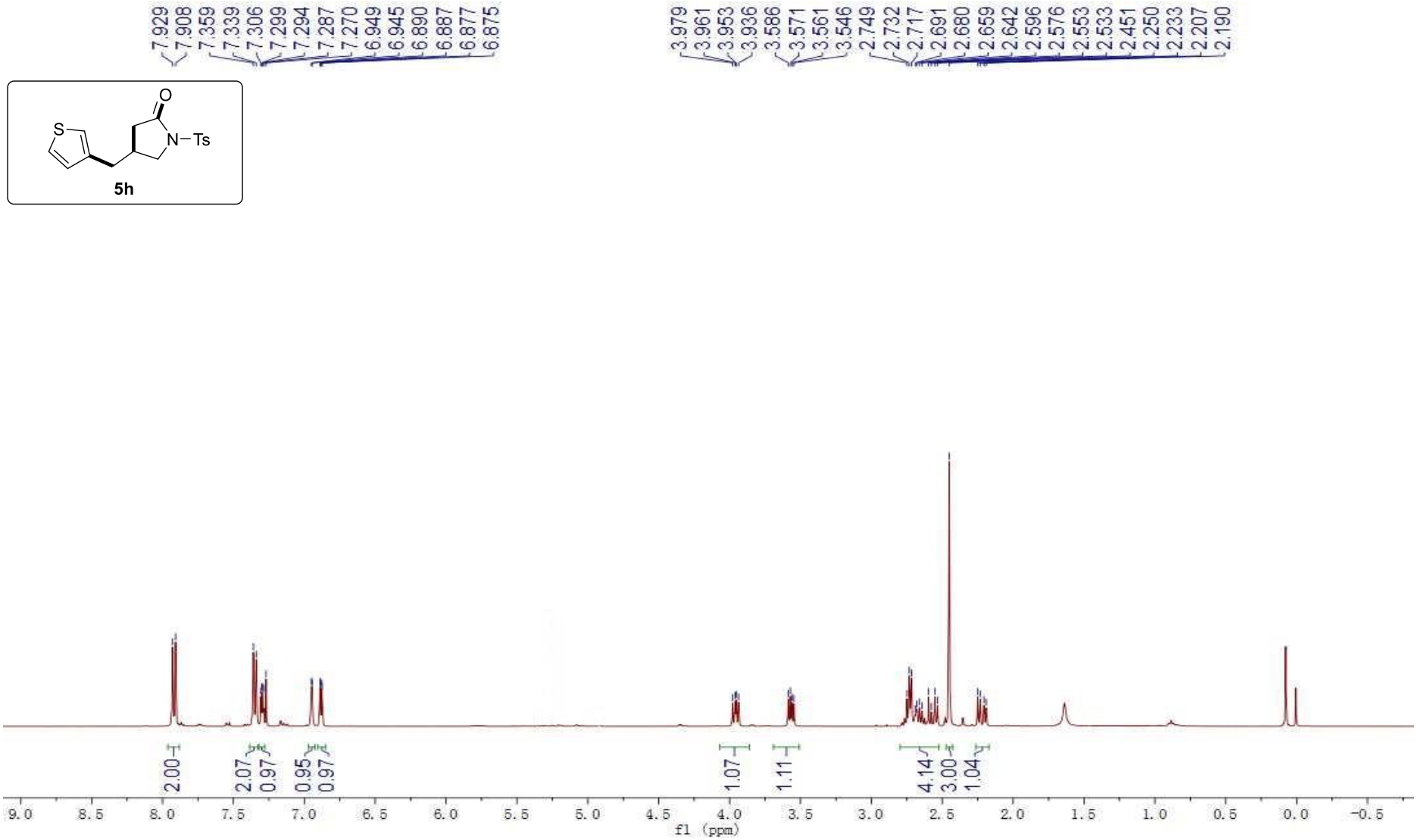
133.33
130.78
129.85
129.76
129.03
128.25
128.15
77.48
77.16
76.84
52.35
51.90
39.33
38.50
33.45
21.82
H3CO2C
O
N−Ts
5g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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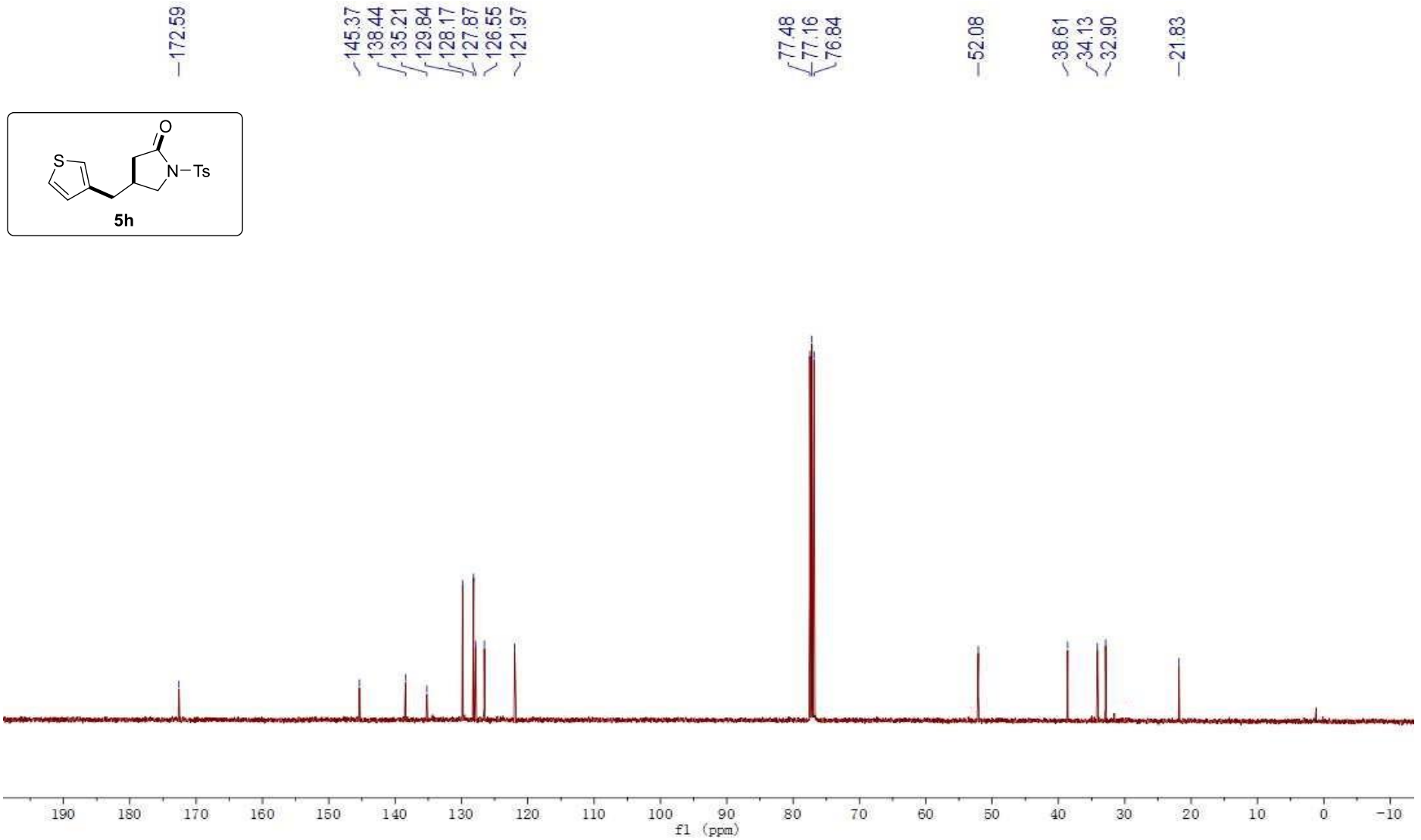
6.887
6.877
6.875
3.979
3.961
3.953
3.936
3.586
3.571
3.561
3.546
2.749
2.732
2.717
2.691
2.680
2.659
2.642
2.596
2.576
2.553
2.533
2.451
2.250
2.233
2.207
2.190
O
S
N−Ts
5h
2.00
2.07
0.97
0.95
0.97
1.07
1.11
4.14
3.00
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)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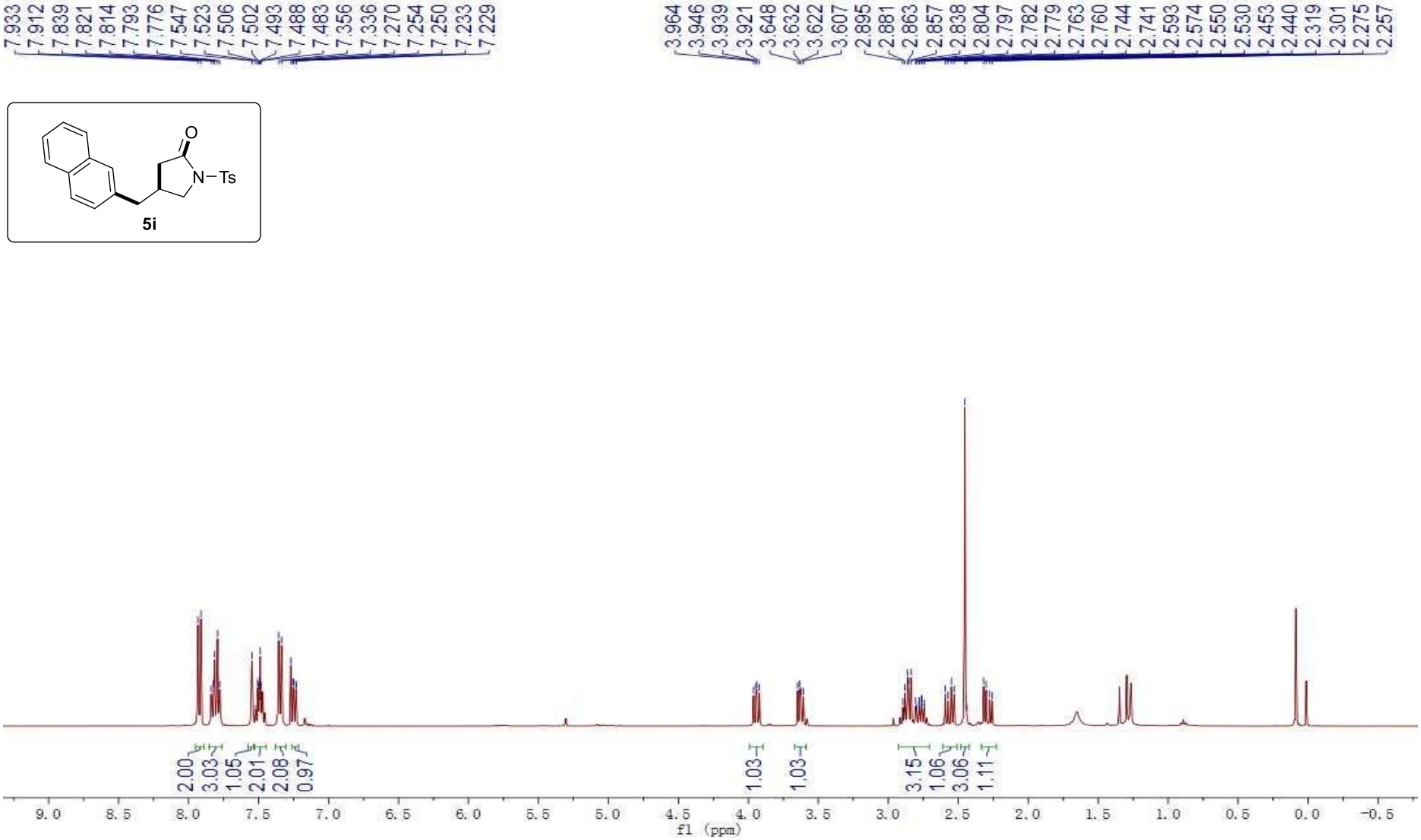
128.17
127.87
126.55
121.97
77.48
77.16
76.84
52.08
38.61
34.13
32.90
21.83
O
S
N−Ts
5h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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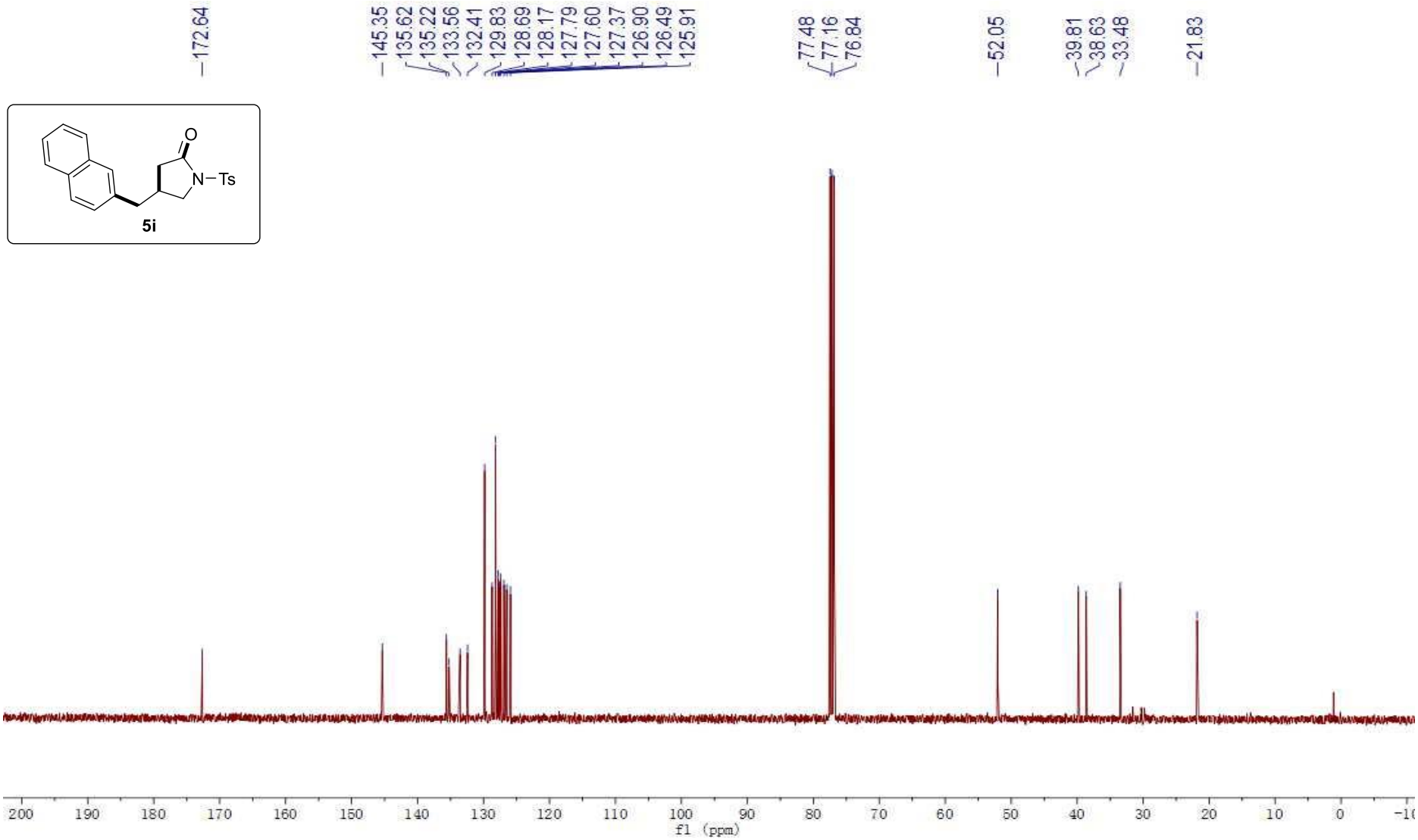
2.453
2.440
2.319
2.301
2.275
2.257
O
N−Ts
5i
2.00
3.03
1.05
2.01
2.08
0.97
1.03
1.03
3.15
1.06
3.06
1.11
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)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132.41
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128.69
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127.79
127.60
127.37
126.90
126.49
125.91
77.48
77.16
76.84
52.05
39.81
38.63
33.48
21.83
O
N–Ts
5i
200
190
180
170
160
150
140
130
120
110
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90
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50
40
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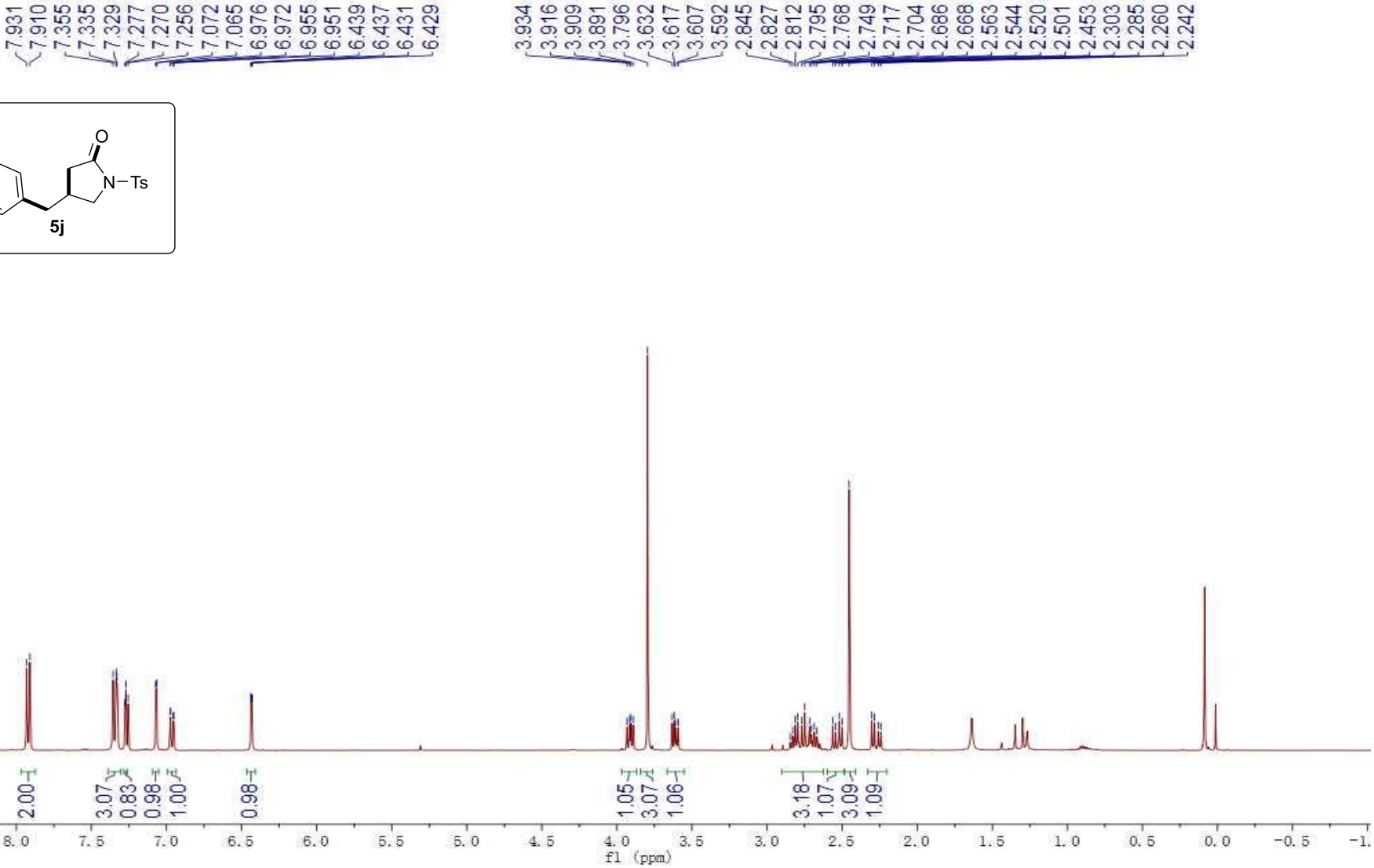
f1 (ppm)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6.972
6.955
6.951
6.439
6.437
6.431
6.429
3.934
3.916
3.909
3.891
3.796
3.632
3.617
3.607
3.592
2.845
2.827
2.812
2.795
2.768
2.749
2.717
2.704
2.686
2.668
2.563
2.544
2.520
2.501
2.453
2.303
2.285
2.260
2.242
N
O
N−Ts
5j
2.00
3.07
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3.07
1.06
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1.07
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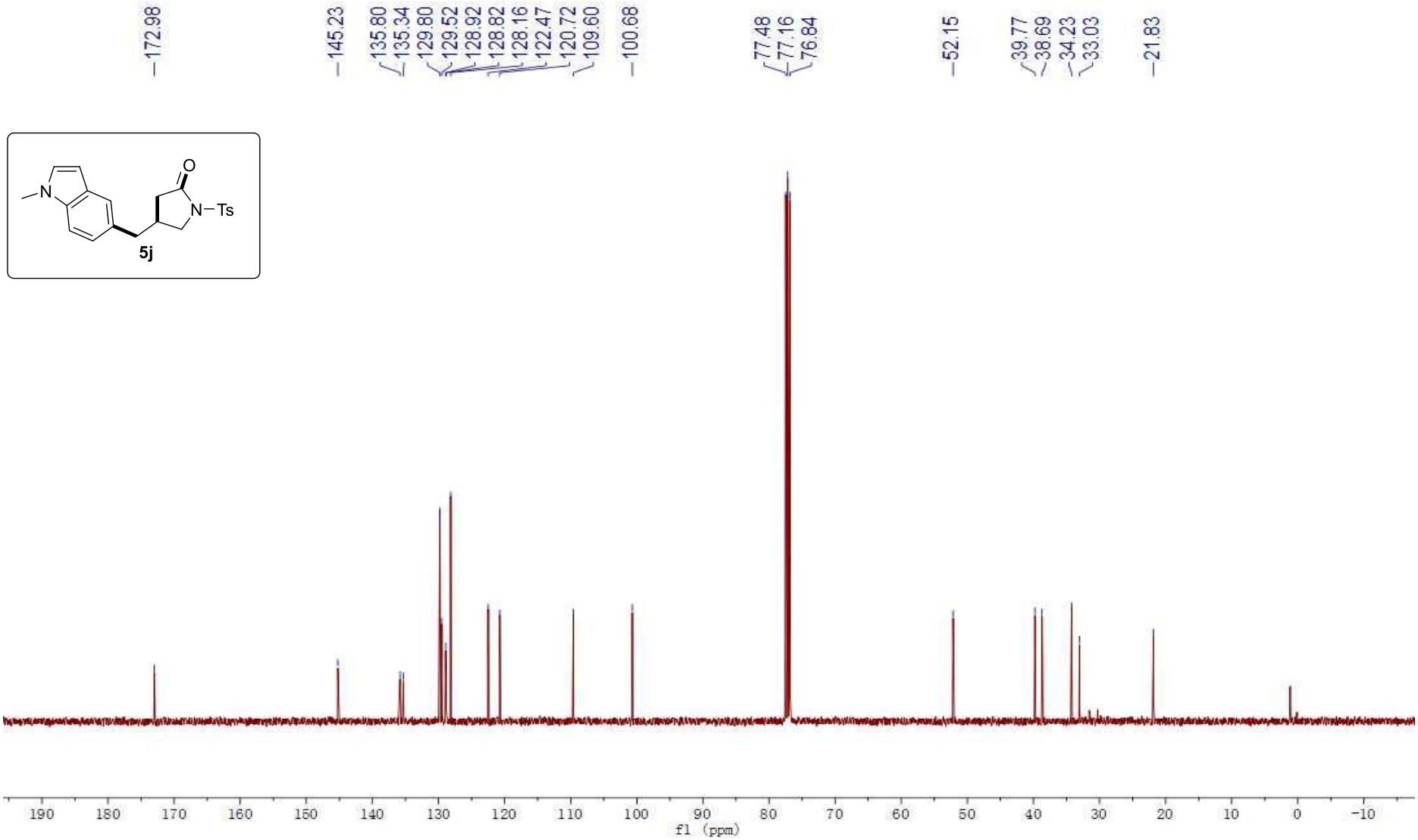
1.09
f1 (ppm)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135.34
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129.52
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122.47
120.72
109.60
100.68
77.48
77.16
76.84
52.15
39.77
38.69
34.23
33.03
21.83
N
O
N–Ts
5j
190
180
170
160
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120
110
100
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80
70
60
50
40
30
20
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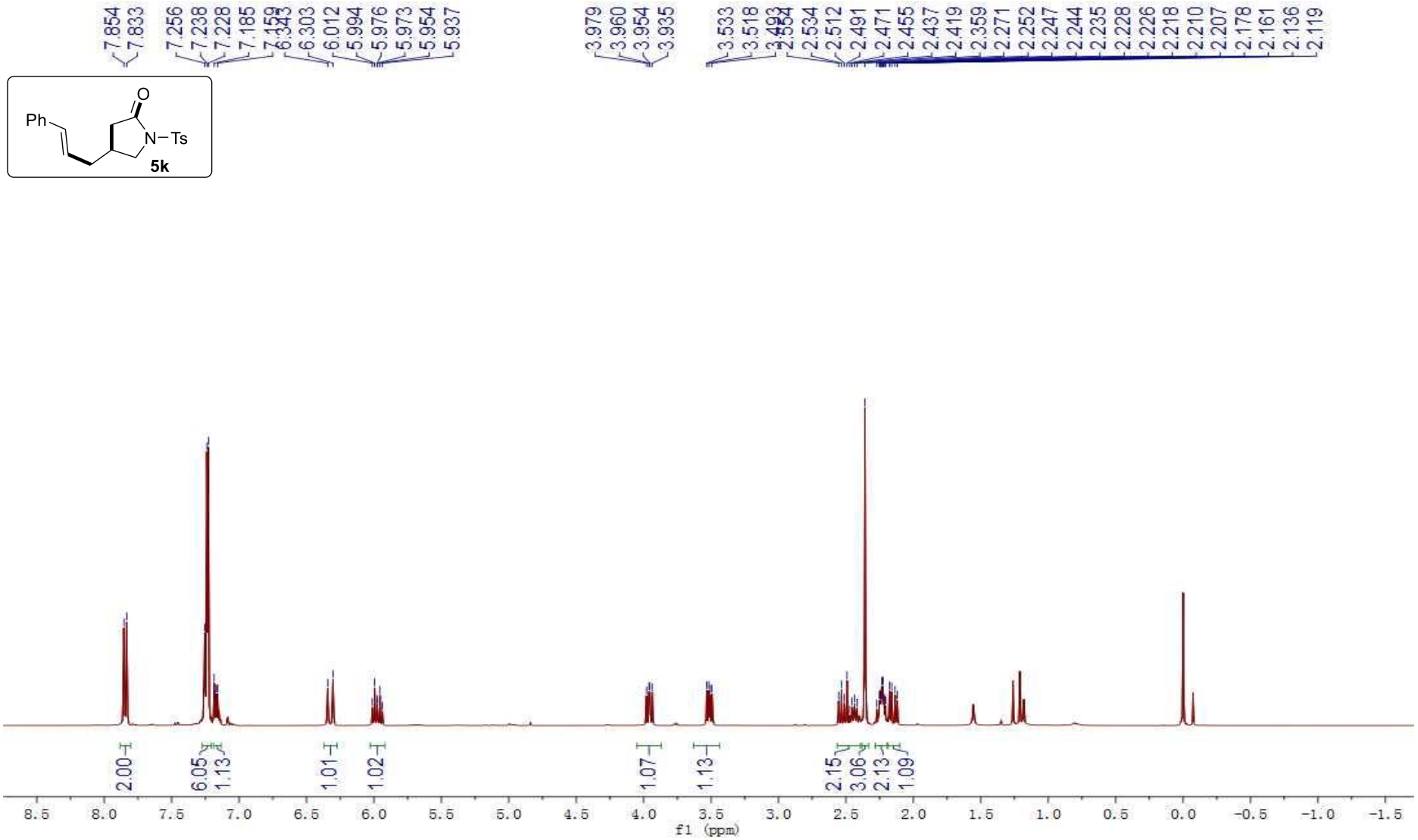
0
−10
f1 (ppm)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6.012
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5.937
3.979
3.960
3.954
3.935
3.533
3.518
2.534
2.512
2.491
2.471
2.455
2.437
2.419
2.359
2.271
2.252
2.247
2.244
2.235
2.228
2.226
2.218
2.210
2.207
2.178
2.161
2.136
2.119
Ph
O
N−Ts
5k
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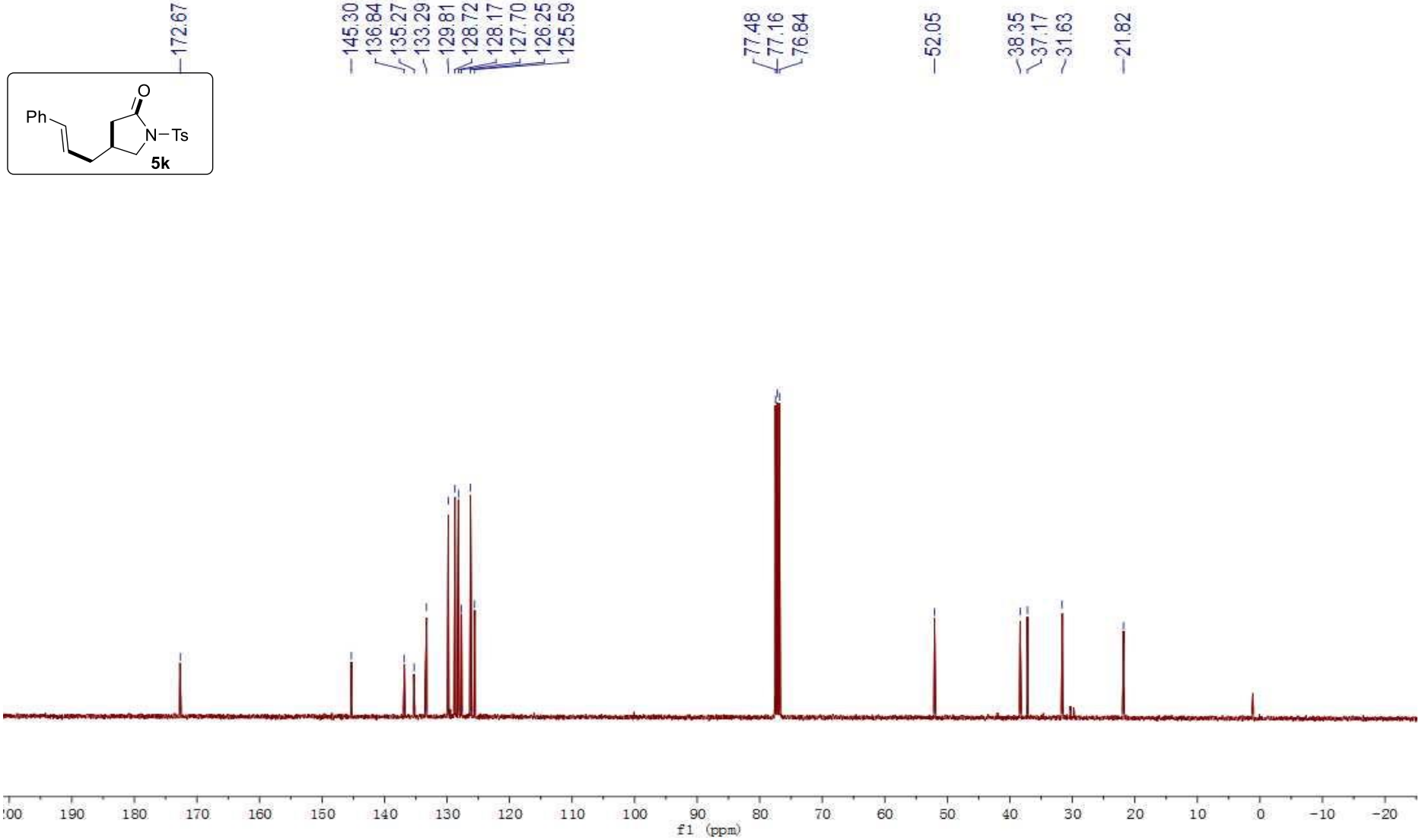
1.01
1.02
1.07
1.13
2.15
3.06
2.13
1.09
f1 (ppm)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126.25
125.59
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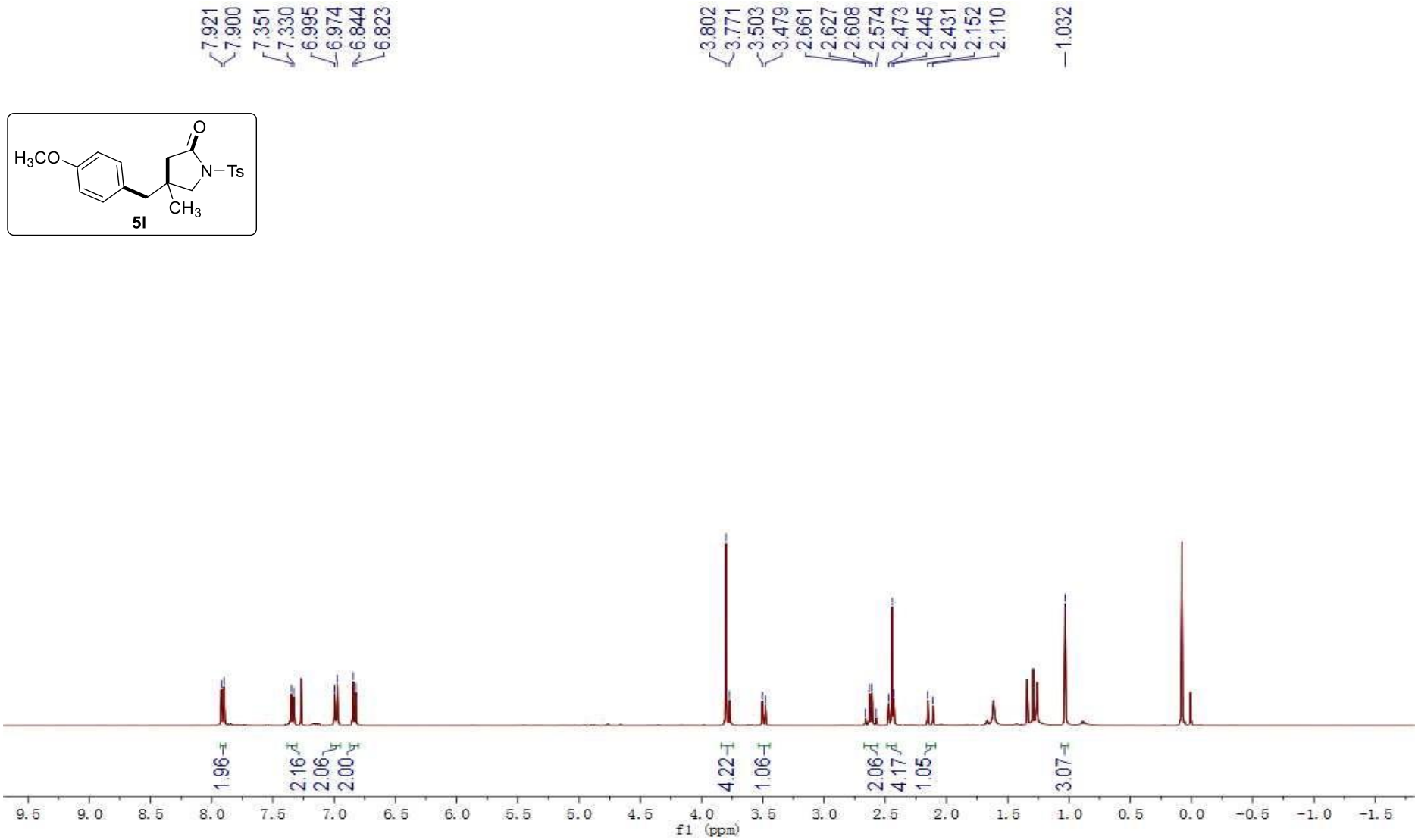
52.05
38.35
37.17
31.63
21.82
Ph
N−Ts
O
5k
f1 (ppm)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3.771
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3.479
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2.627
2.608
2.574
2.473
2.445
2.431
2.152
2.110
1.032
H3CO
O
N−Ts
CH3
5l
1.96
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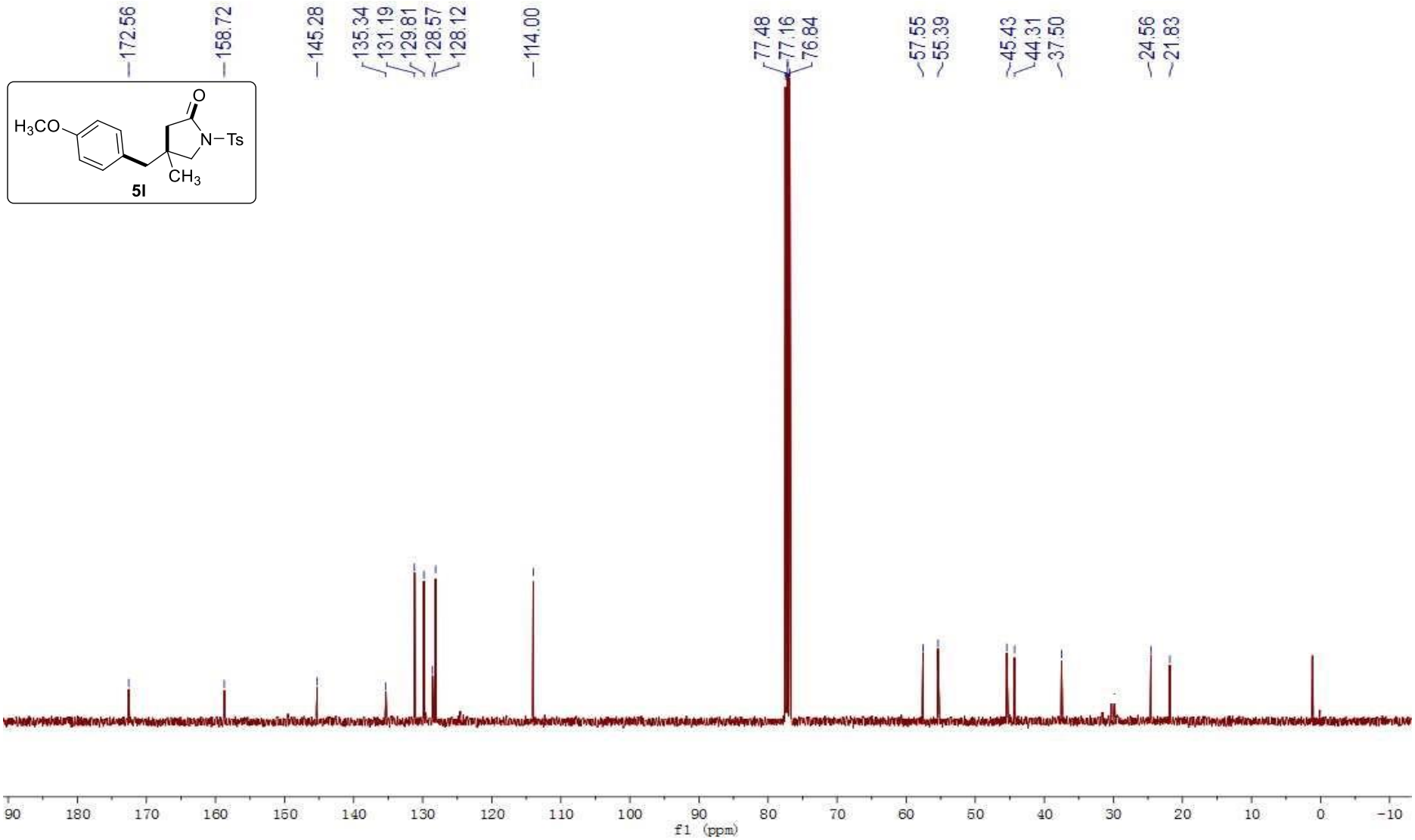
2.06
2.00
4.22
1.06
2.06
4.17
1.05
3.07
f1 (ppm)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77.16
76.84
57.55
55.39
45.43
44.31
37.50
24.56
21.83
H3CO
O
N−Ts
CH3
5l
90
180
170
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140
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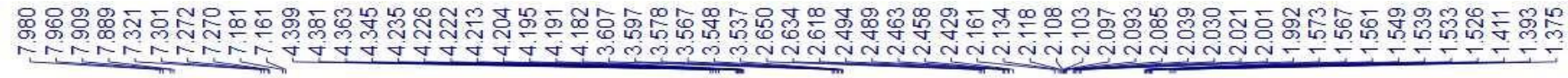
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.909
7.889
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7.270
7.181
7.161
4.399
4.381
4.363
4.345
4.235
4.226
4.222
4.213
4.204
4.195
4.191
4.182
3.607
3.597
3.578
3.567
3.548
3.537
2.650
2.634
2.618
2.494
2.489
2.463
2.458
2.429
2.161
2.134
2.118
2.108
2.103
2.097
2.093
2.085
2.039
2.030
2.021
2.001
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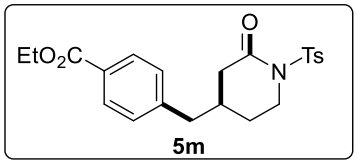
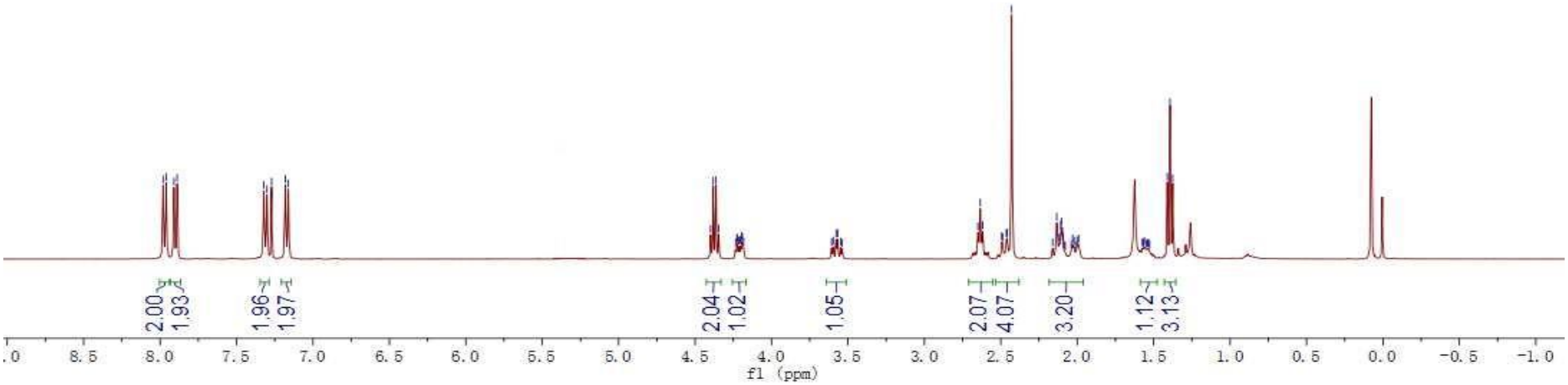
1.573
1.567
1.561
1.549
1.539
1.533
1.526
1.411
1.393
1.375


EtO2C
O
N
Ts

5m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1.93
1.96
1.97
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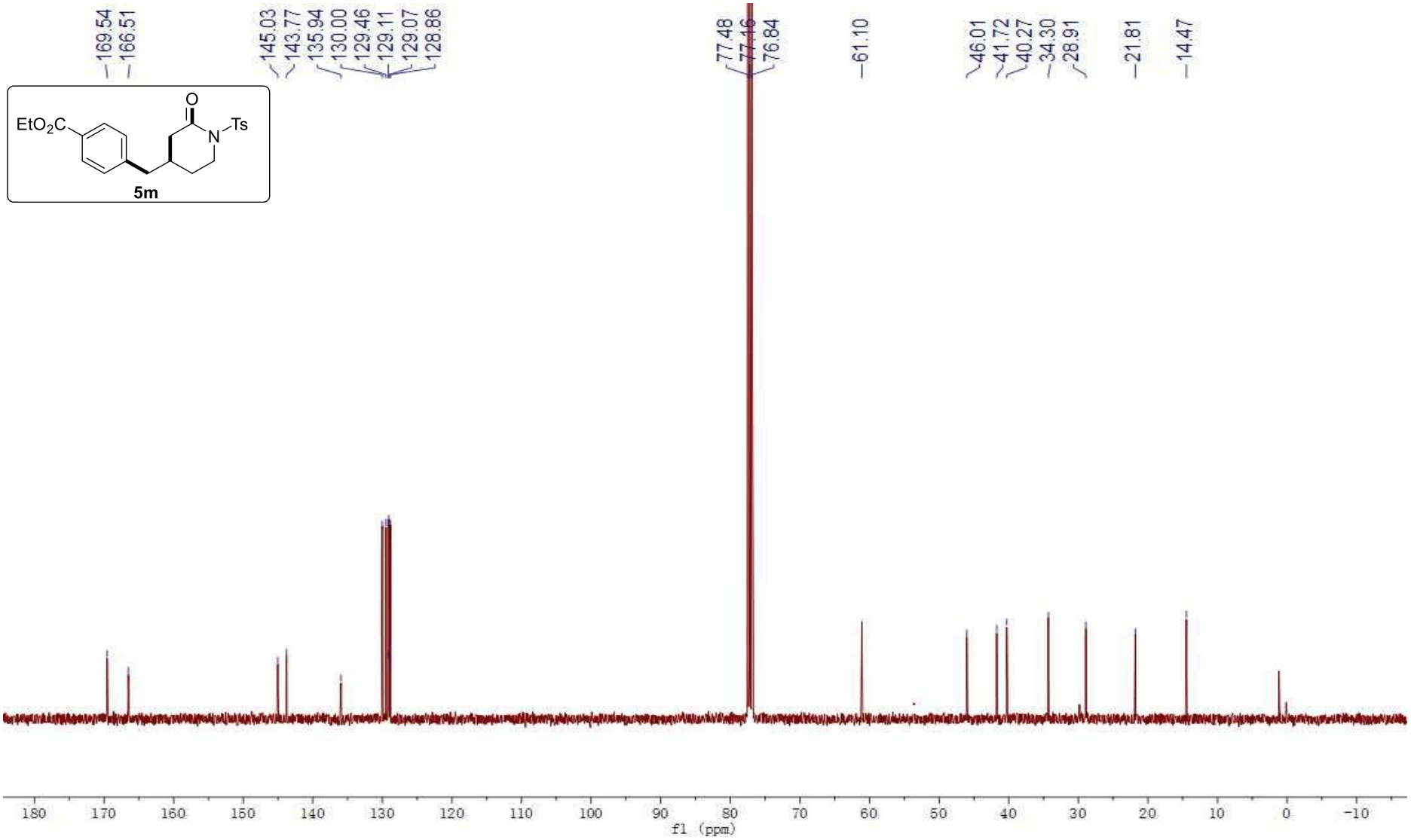
1.02
1.05
2.07
4.07
3.20
1.12
3.13
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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166.51
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143.77
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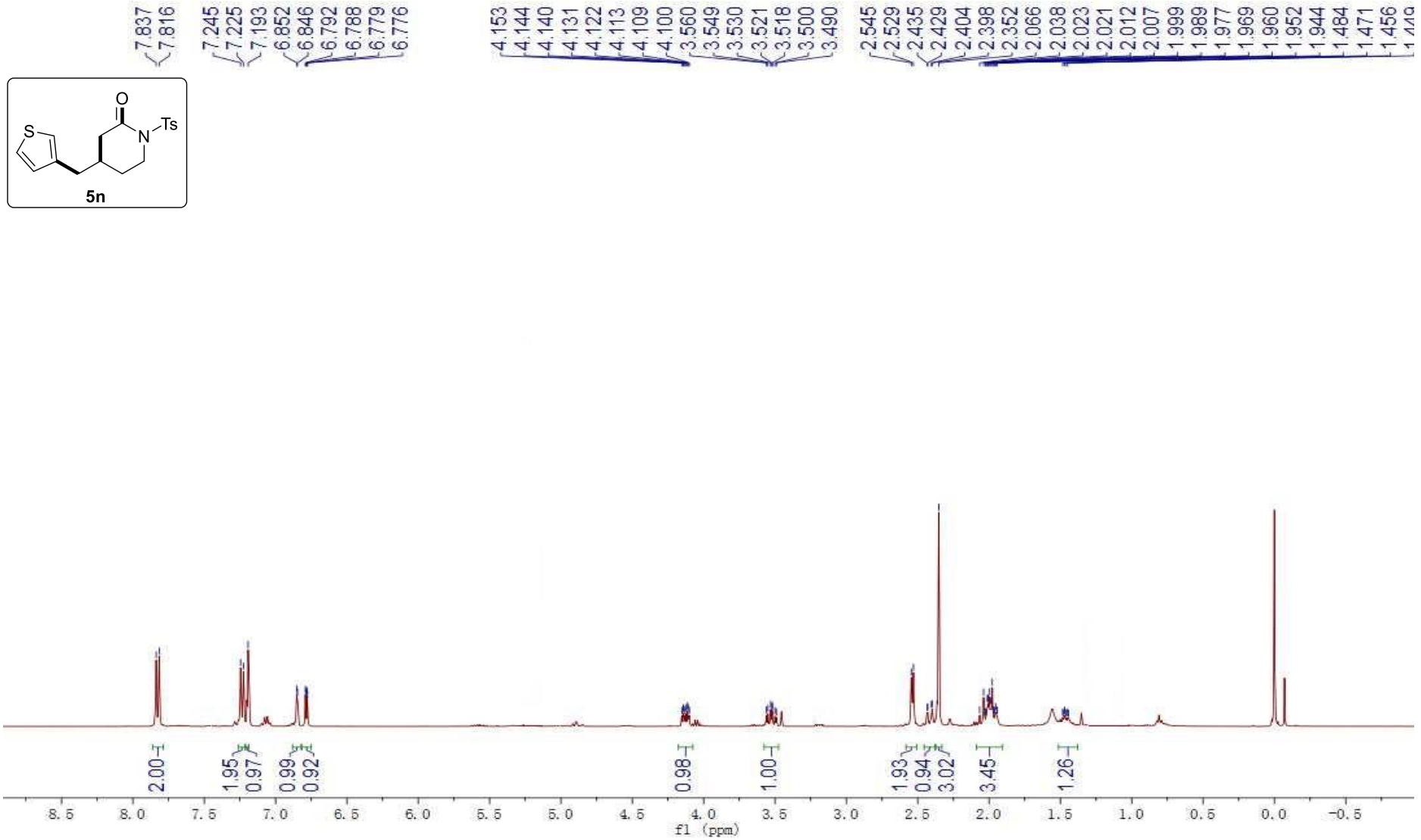
130.00
129.46
129.11
129.07
128.86
77.48
77.16
76.84
61.10
46.01
41.72
40.27
34.30
28.91
21.81
14.47
EtO2C
O
N
Ts
5m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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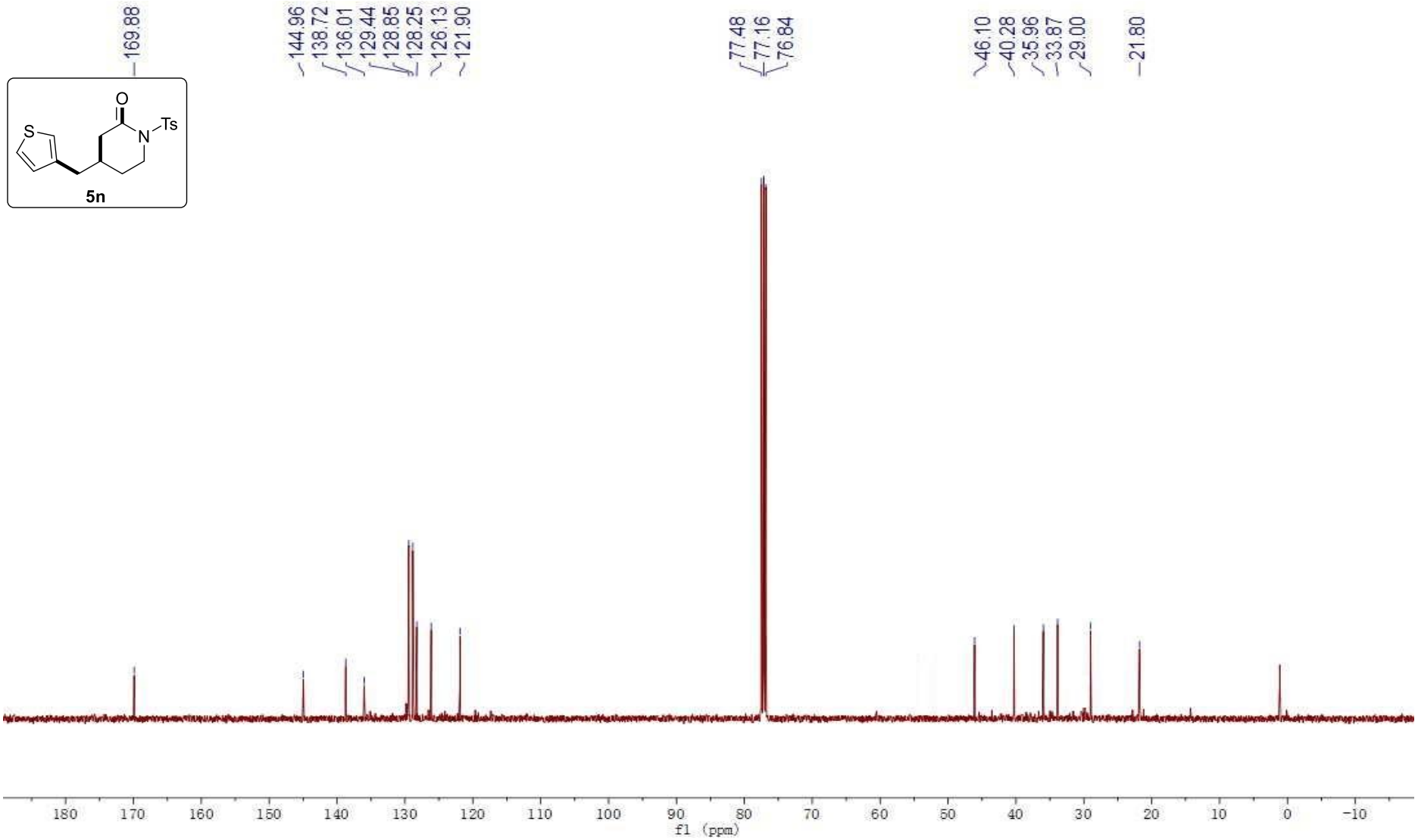
6.792
6.788
6.779
6.776
4.153
4.144
4.140
4.131
4.122
4.113
4.109
4.100
3.560
3.549
3.530
3.521
3.518
3.500
3.490
2.545
2.529
2.435
2.429
2.404
2.398
2.352
2.066
2.038
2.023
2.021
2.012
2.007
1.999
1.989
1.977
1.969
1.960
1.952
1.944
1.484
1.471
1.456
O
S
N
Ts
5n
2.00
1.95
0.97
0.99
0.92
0.98
1.00
1.93
0.94
3.02
3.45
1.26
f1 (ppm)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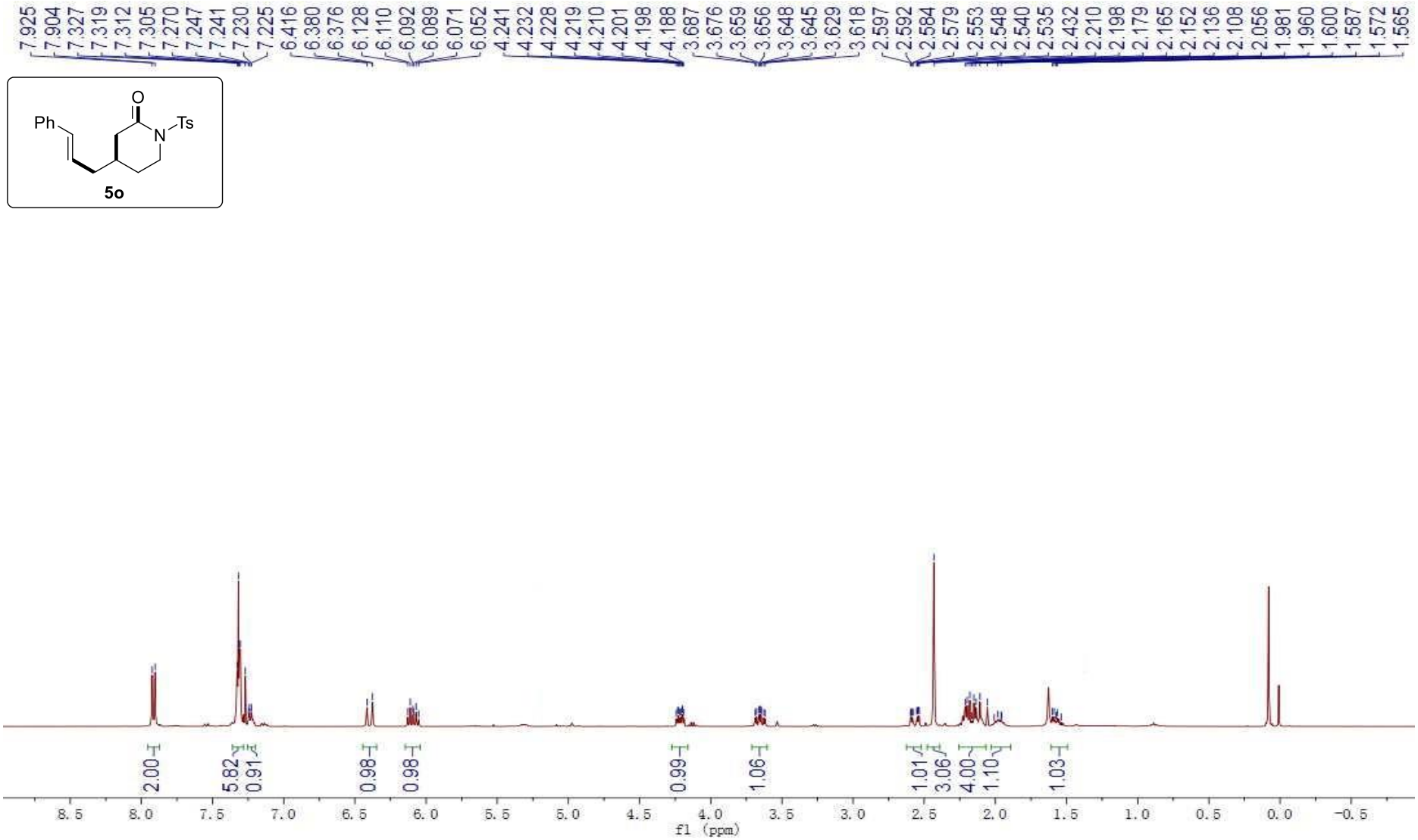
126.13
121.90
77.48
77.16
76.84
46.10
40.28
35.96
33.87
29.00
21.80
O
S
N
Ts
5n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.247
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7.230
7.225
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6.380
6.376
6.128
6.110
6.092
6.089
6.071
6.052
4.241
4.232
4.228
4.219
4.210
4.201
4.198
4.188
3.687
3.676
3.659
3.656
3.648
3.645
3.629
3.618
2.597
2.592
2.584
2.579
2.553
2.548
2.540
2.535
2.432
2.210
2.198
2.179
2.165
2.152
2.136
2.108
2.056
1.981
1.960
1.600
1.587
1.572
1.565
Ph
O
N
Ts
5o
2.00
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0.98
0.99
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1.01
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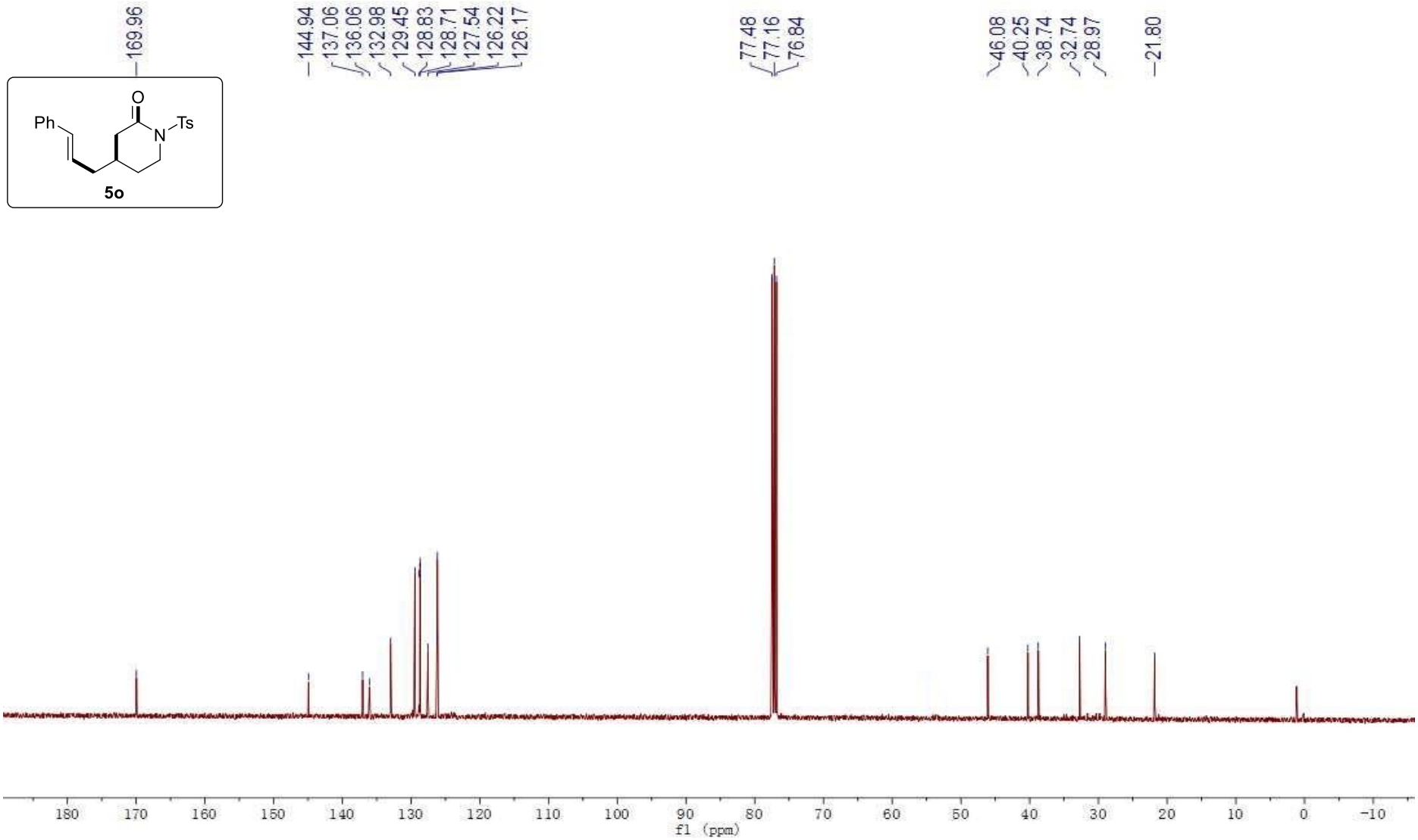
4.00
1.10
1.03
f1 (ppm)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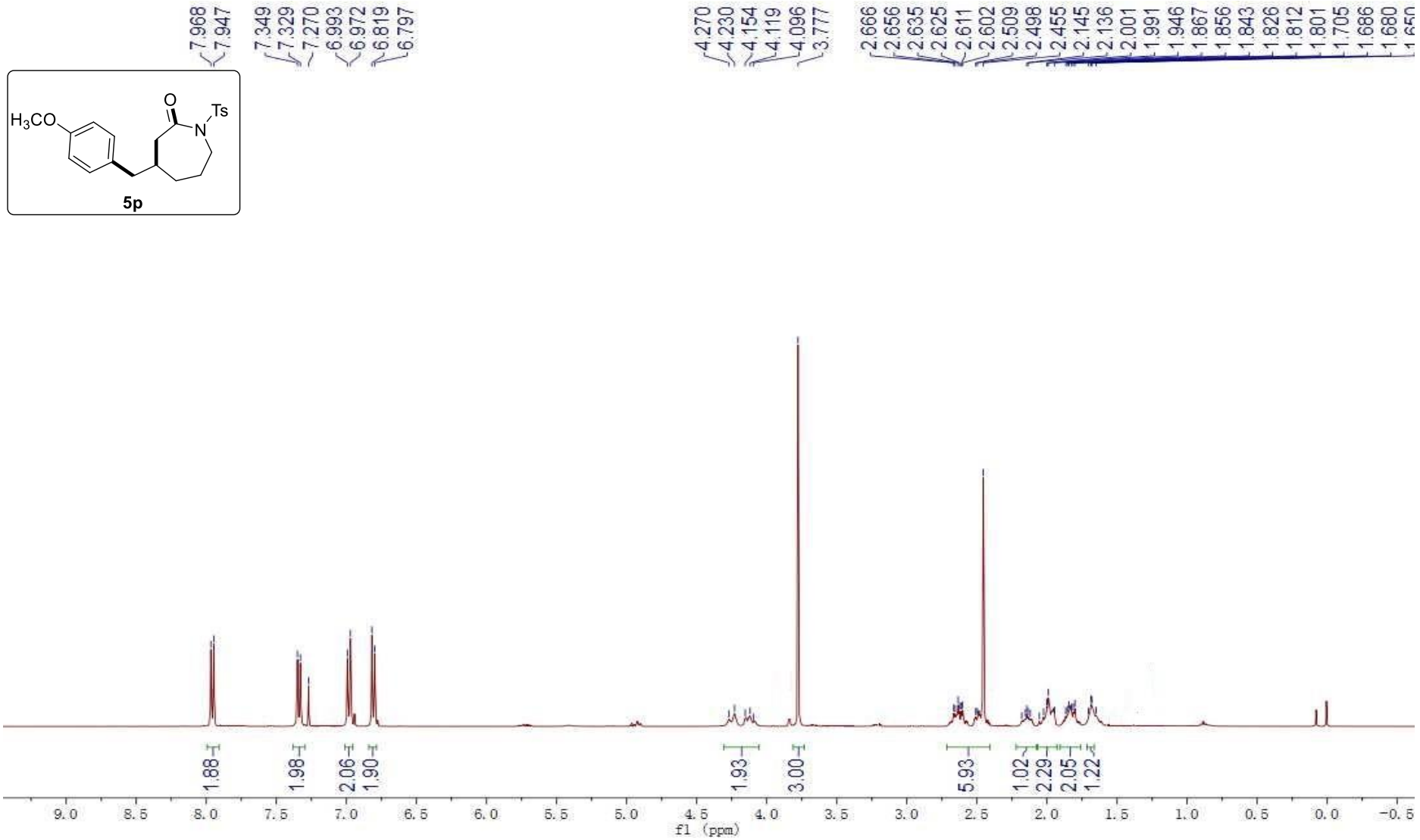
126.22
126.17
77.48
77.16
76.84
46.08
40.25
38.74
32.74
28.97
21.80
Ph
O
N
Ts
5o
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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4.119
4.096
3.777
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2.656
2.635
2.625
2.611
2.602
2.509
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2.455
2.145
2.136
2.001
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1.826
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1.801
1.705
1.686
1.680
H3CO
O
N
Ts
5p
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1.98
2.06
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3.00
5.93
1.02
2.29
2.05
1.22
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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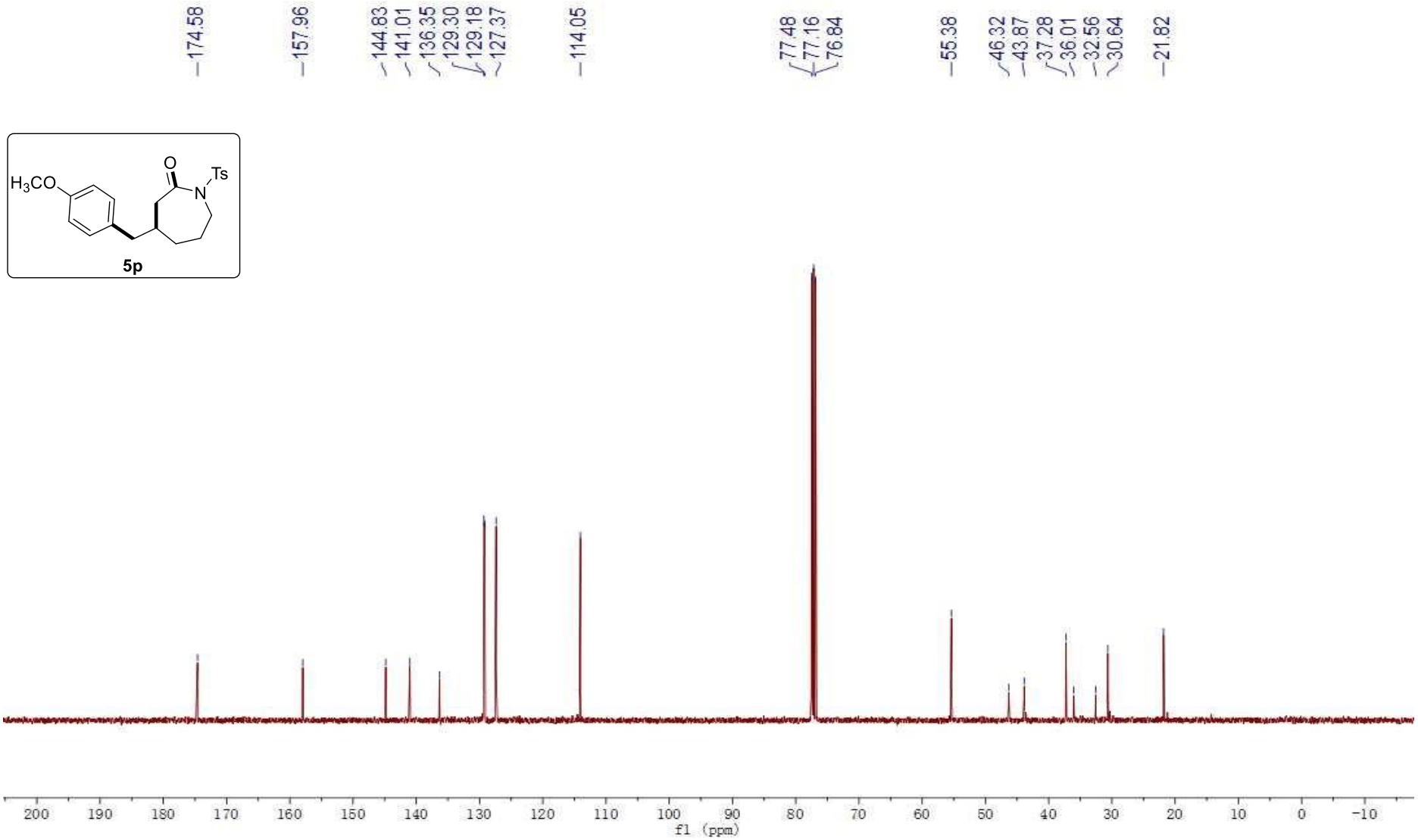
0.5
0.0
-0.5
f1 (ppm)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76.84
55.38
46.32
43.87
37.28
36.01
32.56
30.64
21.82
H3CO
O
N
Ts
5p
200
190
180
170
160
150
140
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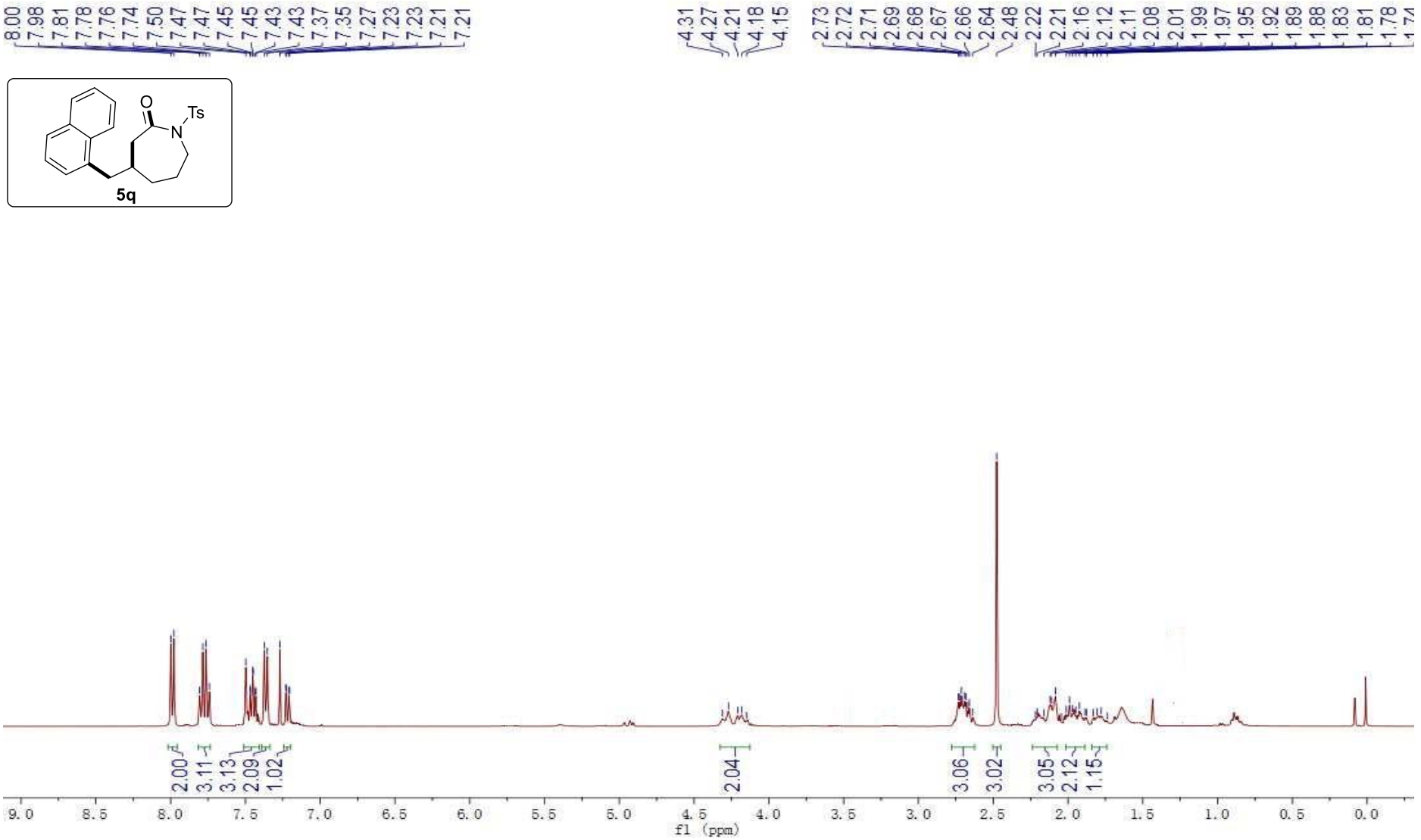
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.43
7.37
7.35
7.27
7.23
7.23
7.21
7.21
4.31
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4.21
4.18
4.15
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2.72
2.71
2.69
2.68
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2.21
2.16
2.12
2.11
2.08
2.01
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1.97
1.95
1.92
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1.88
1.83
1.81
1.78
O
N
Ts
5q
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1.02
2.04
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2.12
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6.0
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1.0
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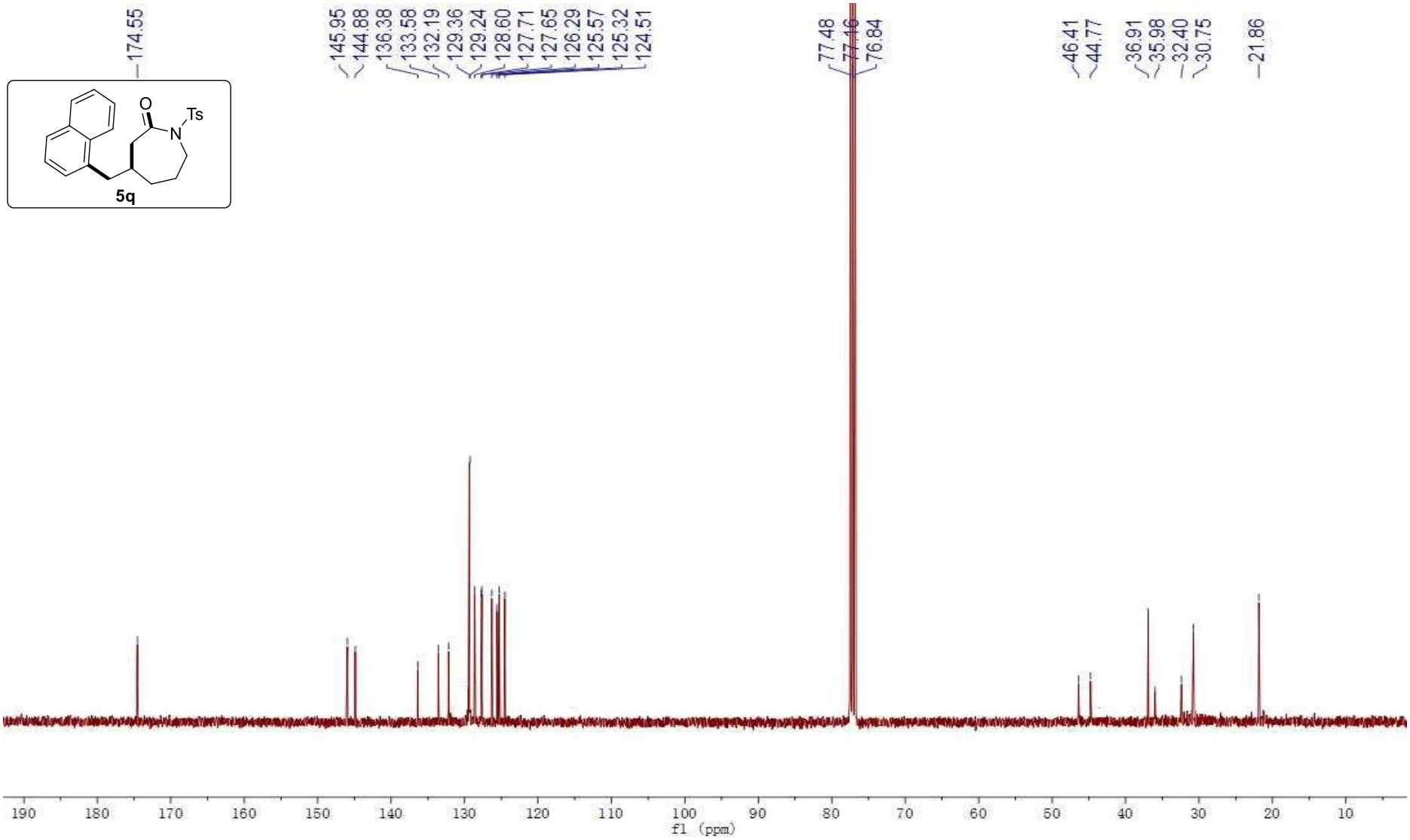
0.0
f1 (ppm)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127.71
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126.29
125.57
125.32
124.51
77.48
77.16
76.84
46.41
44.77
36.91
35.98
32.40
30.75
21.86
O
N
Ts
5q
190
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100
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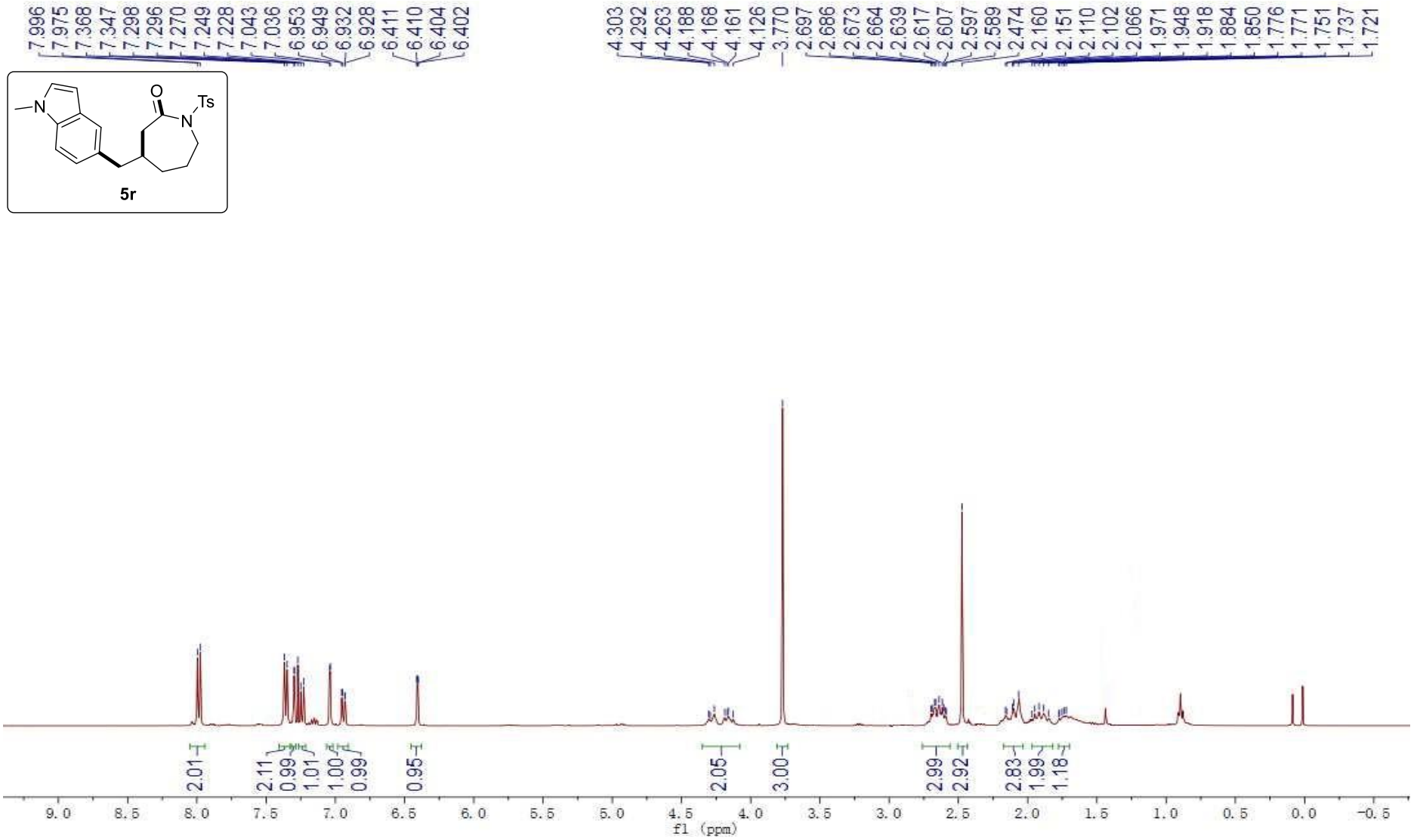
f1 (ppm)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6.949
6.932
6.928
6.411
6.410
6.404
6.402
4.303
4.292
4.263
4.188
4.168
4.161
4.126
3.770
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2.686
2.673
2.664
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2.617
2.607
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2.066
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1.884
1.850
1.776
1.771
1.751
1.737
1.721
N
O
N
Ts
5r
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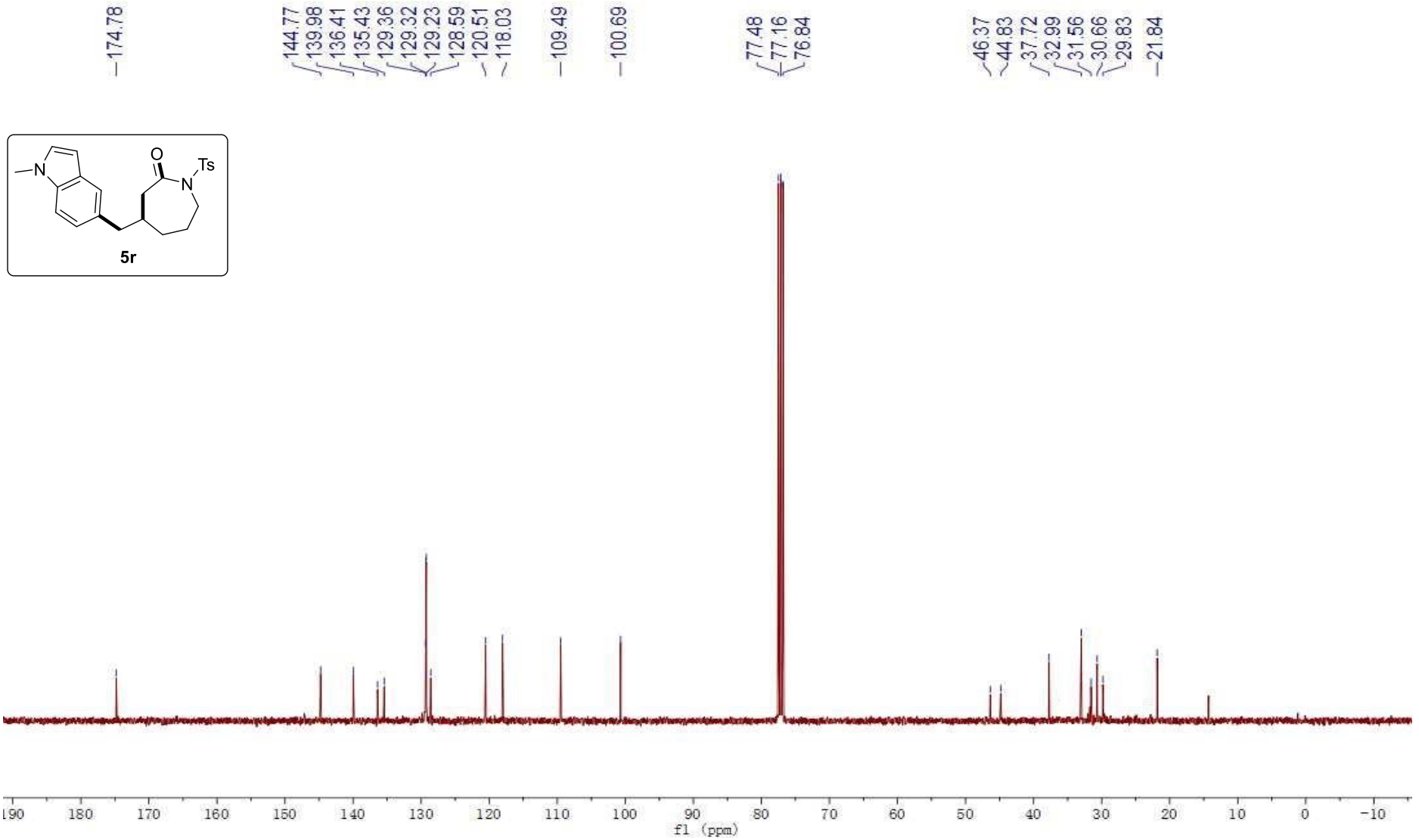
2.11
0.99
1.01
1.00
0.99
0.95
2.05
3.00
2.99
2.92
2.83
1.99
1.18
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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120.51
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109.49
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77.48
77.16
76.84
46.37
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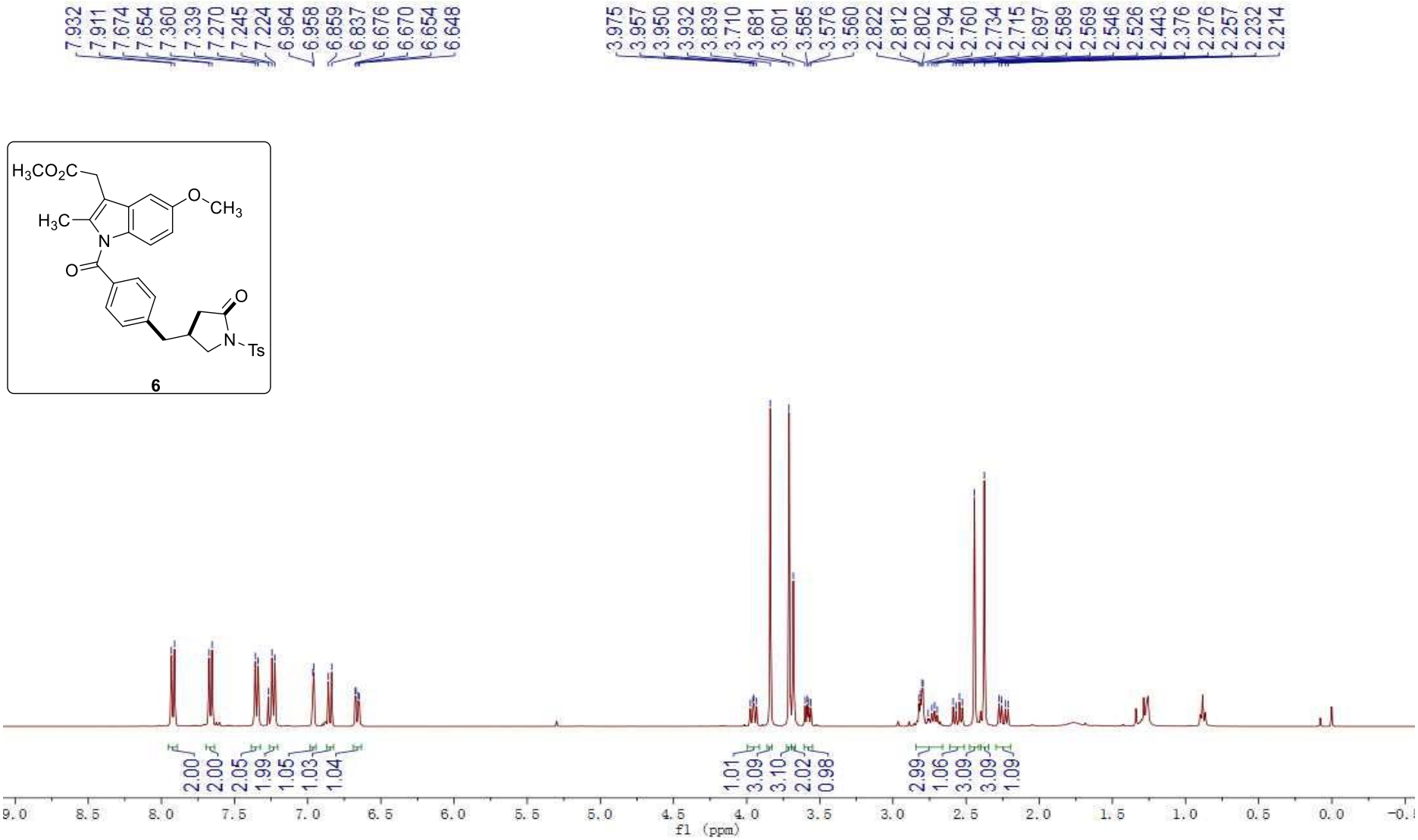
32.99
31.56
30.66
29.83
21.84
N
O
N
Ts
5r
f1 (ppm)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6.837
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6.670
6.654
6.648
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3.957
3.950
3.932
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3.710
3.681
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2.214
H3CO2C
H3C
N
O
CH3
O
O
N
Ts
6
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2.00
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1.99
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1.03
1.04
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5.0
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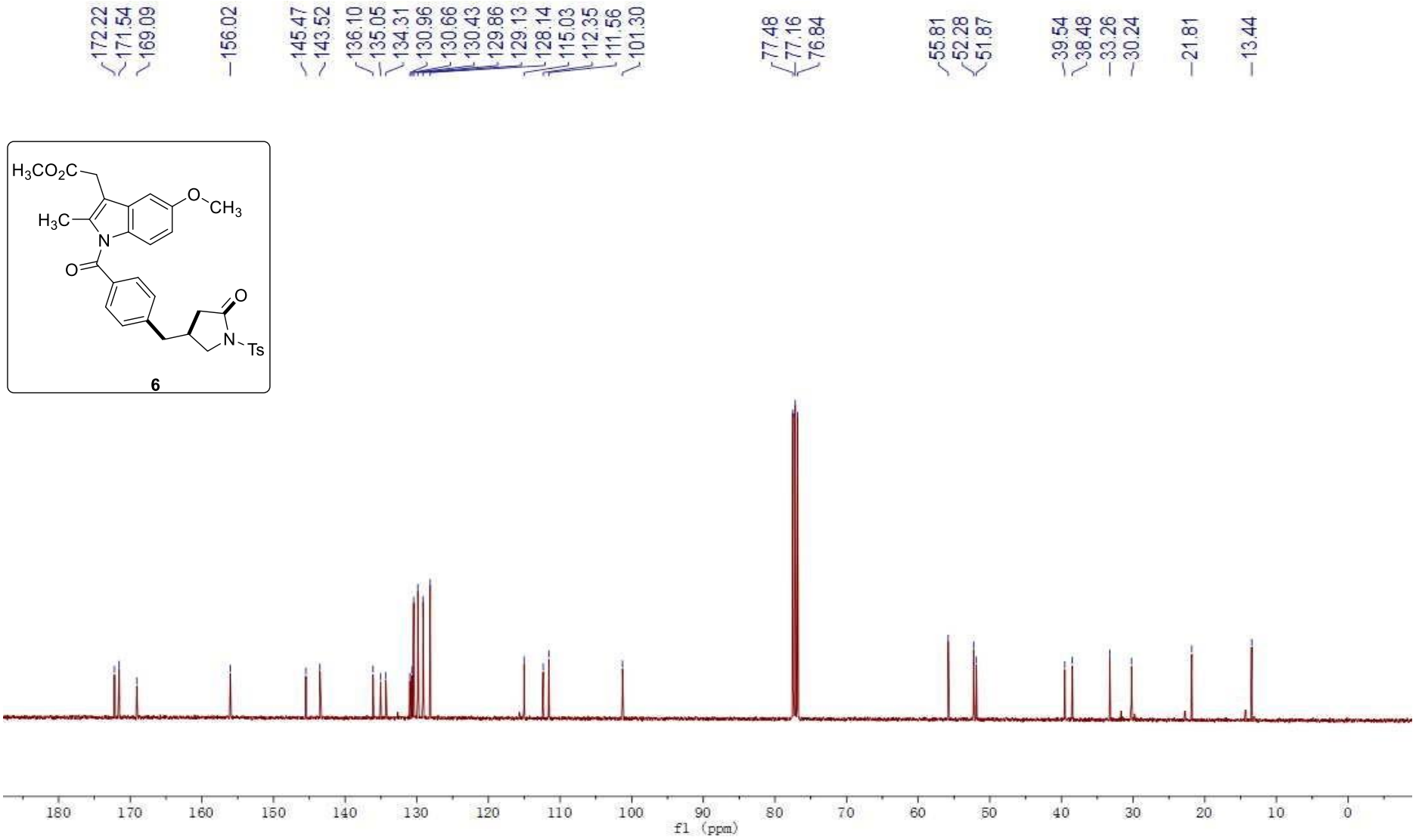
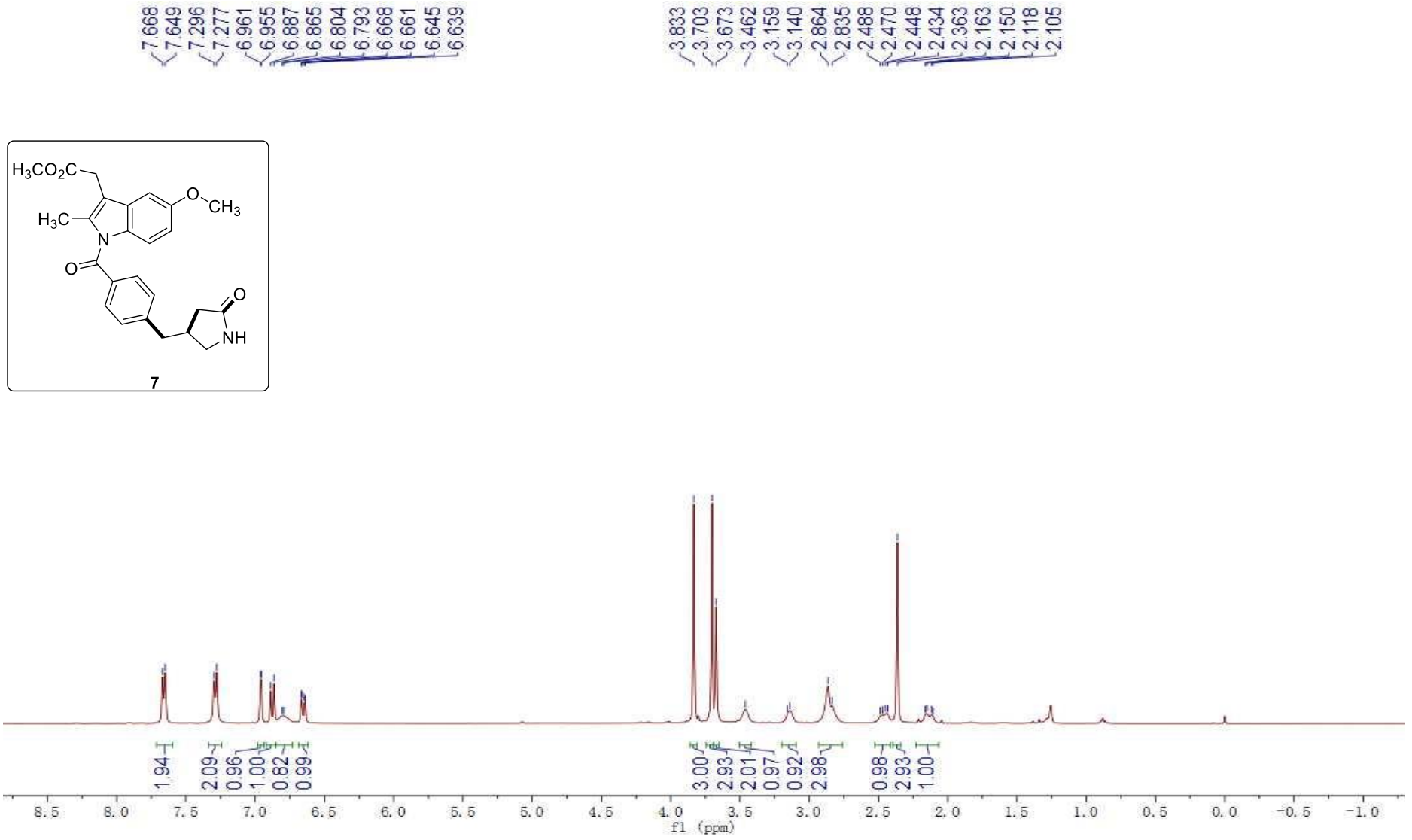
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


172.22
171.54
169.09
156.02
145.47
143.52
136.10
135.05
134.31
130.96
130.66
130.43
129.86
129.13
128.14
115.03
112.35
111.56
101.30
77.48
77.16
76.84
55.81
52.28
51.87
39.54
38.48
33.26
30.24
21.81
13.44
H3CO2C
H3C
O
CH3
N
O
O
N
Ts
6
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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7.296
7.277
6.961
6.955
6.887
6.865
6.804
6.793
6.668
6.661
6.645
6.639
3.833
3.703
3.673
3.462
3.159
3.140
2.864
2.835
2.488
2.470
2.448
2.434
2.363
2.163
2.150
2.118
2.105
H3CO2C
H3C
N
O
CH3
O
O
NH
7
1.94
2.09
0.96
1.00
0.82
0.99
3.00
2.93
2.01
0.97
0.92
2.98
0.98
2.93
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.5
2.0
1.5
1.0
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0.0
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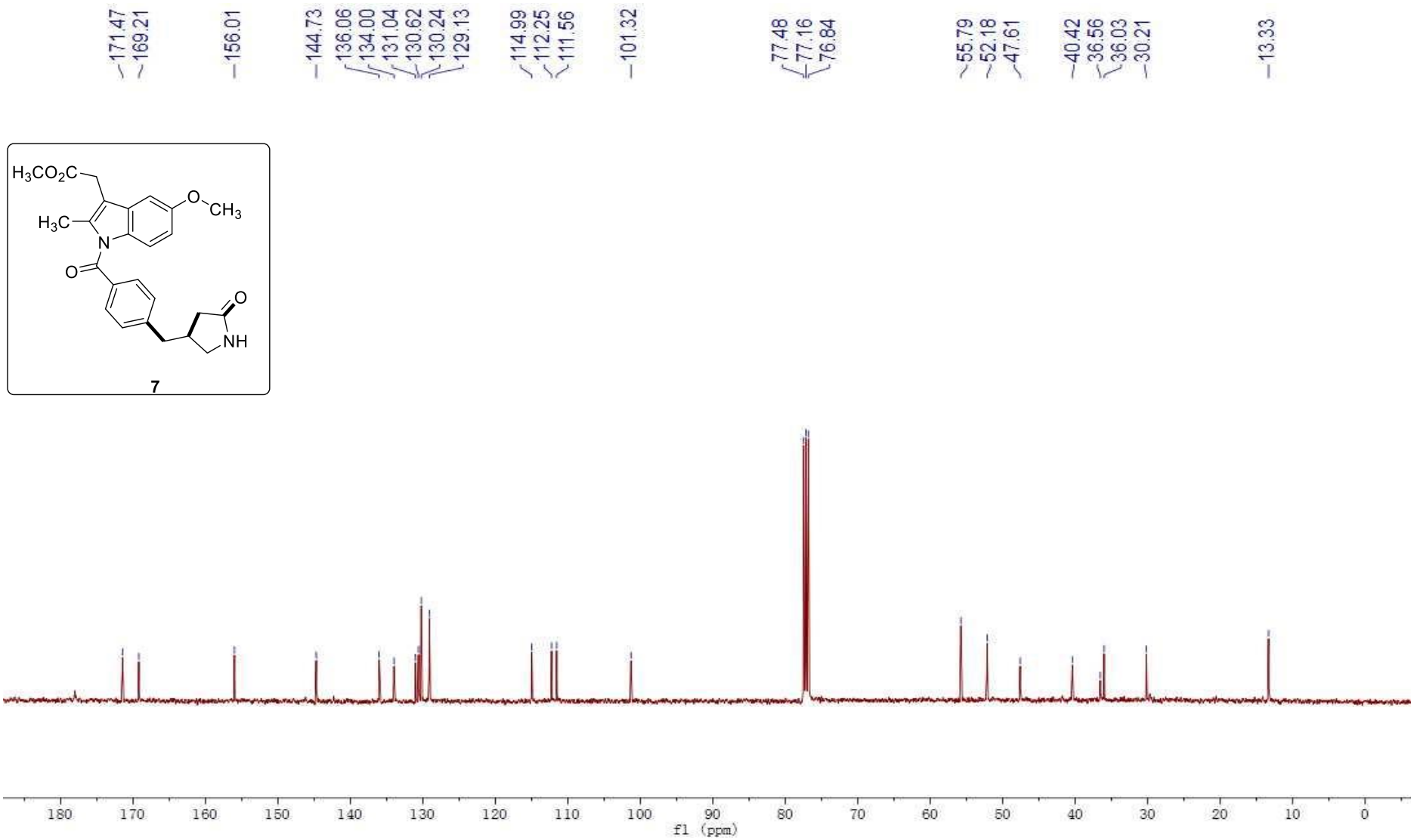
-1.0
f1 (ppm)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169.21
156.01
144.73
136.06
134.00
131.04
130.62
130.24
129.13
114.99
112.25
111.56
101.32
77.48
77.16
76.84
55.79
52.18
47.61
40.42
36.56
36.03
30.21
13.33
H3CO2C
H3C
N
O
CH3
O
O
NH
7
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)