DMSO/$SOCl_2$-mediated C(sp^2)−H amination: switchable synthesis of 3-unsubstituted indole and 3-methylthioindole derivatives

Jingran Zhang,[a] Xiaoxian Li,[a] Xuemin Li,[a] Haofeng Shi,[a] Fengxia Sun[b] and Yunfei Du*[a]

[a]*School of Pharmaceutical Science and Technology, Tianjin University, Tianjin 300072, China.*

[b]*College of Chemical and Pharmaceutical Engineering, Hebei University of Science and Technology; Hebei Research Center of Pharmaceutical and Chemical Engineering, Shijiazhuang 050018, China.*

Tel: +86-22-27406121; duyunfeier@tju.edu.cn

Supporting Information

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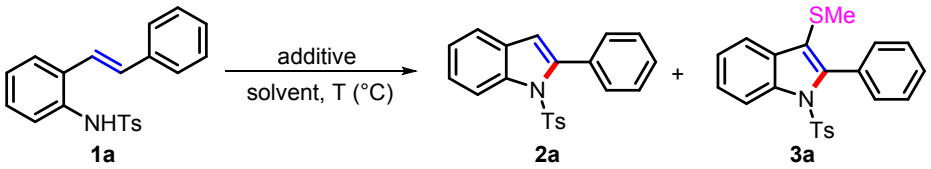
I. General Information

^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz or 600 MHz spectrometer at 25 ^{o}C. Chemical shifts values are given in ppm and referred as the internal standard to TMS: 0.00 ppm. Chemical shifts were expressed in parts per million (δ) downfield from the internal standard tetramethylsilane, and were reported as s (singlet), d (doublet), t (triplet), q (quadruple), dd (doublet of doublet), m (multiplet), etc. The coupling constants *J*, are reported in Hertz (Hz). High resolution mass spectrometry (HRMS) was obtained on a Q-TOF micro spectrometer. Melting points were determined with a Micromelting point apparatus. TLC plates were visualized by exposure to ultraviolet light.

Reagents and solvents were purchased as reagent grade and were used without further purification. All reactions were performed in standard glassware, heated at 70 ^{o}C for 3 h before used. The starting materials **1** were prepared according to literature methods.[1] Flash column chromatography was performed over silica gel (200-300 m) using a mixture of ethyl acetate (EtOAc) and petroleum ether (PE).

II. Details for Optimization of Reaction Conditions

Table S1. Optimization of reaction conditions for synthesis of 3a[2]



entry	solvent	additive (equiv)	T (°C)	time (min)	yield (%)[b]	
					2a	**3a**
S1	DMSO	$SOCl_2$ (3.0)	rt	30	92	0
S2	DMSO	$SOCl_2$ (3.5)	rt	30	86	0
S3	DMSO	$SOCl_2$ (4.0)	rt	30	85	0
S4	DMSO	$SOCl_2$ (3.0)	70	30	80	10
S5	DMSO	$SOCl_2$ (3.5)	70	50	43	35
S6	DMSO	$SOCl_2$ (3.8)	70	50	25	48
S7	**DMSO**	**$SOCl_2$ (4.0)**	**70**	**40**	**0**	**55**
S8	DMSO	$SOCl_2$ (4.2)	70	30	0	26
S9	DMSO	$SOCl_2$ (4.5)	70	30	0	trace
S10	DMSO	$SOCl_2$ (4.0)	80	40	0	39
S11	DMSO	$SOCl_2$ (4.0)	90	40	0	26
S12[c]	DMSO	$SOCl_2$ (4.0)	70	40	0	50

[a] Reaction conditions: **1a** (0.5 mmol), DMSO (1 mL), unless otherwise stated. [b] Isolated yields.

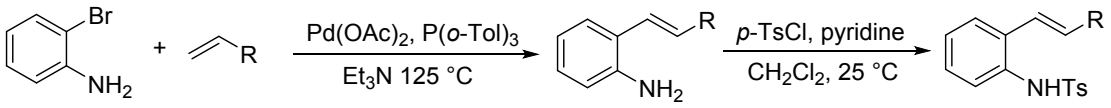
[c] Reaction conditions: **1a** (0.5 mmol), DMSO (1 mL), reacted at rt for 30 min and then reacted at 70 °C.

The conditions were further optimized to improve the yield of 3-methylthioindole **3a**, and the results were shown below. When the reaction was carried out at room temperature, the increasing of the dosage of $SOCl_2$ could not enable the conversion of indole **2a** to 3-methylthioindole **3a** (Table S1, entries S1-S3). To our delight, when the reaction was run at 70 °C by reacting substrate **1a** with 3.0 equiv of $SOCl_2$, product **3a** was obtained in 10% yield, together with 80% yield of 3-unsubstituted indole **2a**. With the increasing dosage of $SOCl_2$, the formation of more

product **3a** and the depletion of product **2a** were observed. When 4.0 equiv of $SOCl_2$ was applied, product **3a** was obtained in 55% yield, with no isolation of product **2a** (Table S1, entries S4-S7). However, further increasing the equiv of $SOCl_2$ led to a lower-yielding of product 3a, due to the formation of some more unidentified byproducts (Table S1, entries S8-S9). Attempts to further improve the outcome by raising and lowering the temperature proved to be futile. Combining all the testing results, the optimized conditions of DMSO/$SOCl_2$-mediated synthesis of 3-methylthioindole **3a** were concluded to be: 0.5 mmol of **1a** with 4.0 equiv of $SOCl_2$ in DMSO (1 mL) at 70 ^{o}C.

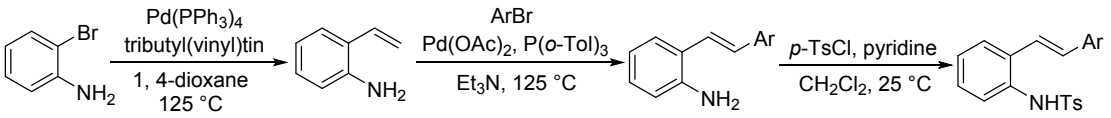
III. Experimental Procedures and Spectroscopic Data

1. Typical procedure for the synthesis of 2-styrylaniline derivatives 1 (1a-z, 1aa-af):



Method A: To a solution of 2-bromoaniline (2.7 g, 15.5 mmol) in Et_3N (15.0 mL, 1.0 M) were added $Pd(OAc)_2$ (34.8 mg, 0.155 mmol, 1 mol%), P(*o*-Tol)$_3$ (398.0 mg, 1.241 mmol, 8 mol%), and olefin (18.62 mmol). After being stirred at 125 ^oC overnight, the reaction mixture was poured into water and then the product was extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (EtOAc/petroleum ether = 1/5) to afford the corresponding 2-styrylaniline products.

To a solution of 2-styrylaniline (1.95 g, 10.0 mmol) in pyridine (20 mL) was added *p*-toluenesulfonyl chloride (2.10 g, 11.0 mmol) at 0 ^oC. After being stirred at 25 ^oC for 2 hours, the reaction mixture was poured into water and then the product was extracted with CH_2Cl_2 (3 x 30 mL), dried over Na_2SO_4, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (EtOAc/petroleum ether = 1/5) to give the corresponding product **1**.



Method B: To a solution of 2-bromoaniline (1.801 mmol, 309.8 mg) in 1,4-dioxane (0.13 M, 14.0 mL) were added $Pd(PPh_3)_4$ (2 mol%, 0.0360 mmol, 41.6 mg), tributyl(vinyl)tin (2.161 mmol, 0.7 mL). The resulting mixture was heated to 125 °C with stir for 4 hours. When the reaction was completed, the reaction mixture was cooled to room temperature and 10% KF aqueous solution (22 mL) was added. Then the mixture was allowed to stand for 2 h and then filtered with celite. The reaction mixture was extracted with EtOAc (3 x 30 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was

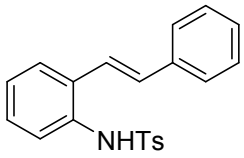
purified by column chromatography on silica gel (CH_2Cl_2 : *n*-hexane = 1:1) to give 2-vinylaniline (188.0 mg, 83%) as a brown oil.

To a solution of 2-vinylaniline (1.19 g, 10.0 mmol) in Et_3N (10 mL) were added $Pd(OAc)_2$ (1 mol%), P(*o*-Tol)$_3$ (8 mol%), and ArBr (1.88 g, 12.0 mmol). After being stirred at 125 ^oC overnight, the reaction mixture was poured into water and then the product was extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (EtOAc/petroleum ether = 1/5) to afford the corresponding 2-styrylaniline product.

To a solution of 2-styrylaniline (1.95 g, 10.0 mmol) in pyridine (20mL) was added *p*-toluenesulfonyl chloride (2.10 g, 11.0 mmol) at 0 °C. After being stirred at 25 ^oC for 2 hours, the reaction mixture was poured into water and then the product was extracted with CH_2Cl_2 (3 x 30 mL), dried over Na_2SO_4, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (EtOAc/petroleum ether = 1/5) to give the corresponding product **1**.

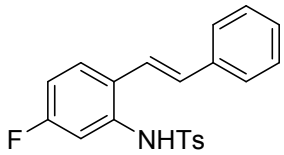
2. Spectroscopic Data of 2-Styrylaniline Derivatives 1 (1a-z, 1aa-af):

(*E*)-4-Methyl-*N*-(2-styrylphenyl) benzenesulfonamide (1a)



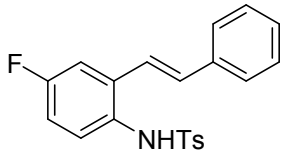
Following the general procedure **Method A**, **1a** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 79%); m.p. 144-146 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^1H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.49 (dd, *J* = 7.1, 2.1 Hz, 1H), 7.38 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.35 – 7.31 (m, 4H), 7.30 – 7.26 (m, 1H), 7.26 – 7.20 (m, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.81 (dd, *J* = 43.4, 16.1 Hz, 2H), 6.68 (s, 1H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.9, 136.7, 136.6, 133.3, 133.3, 132.2, 129.7, 128.6, 128.4, 128.1, 127.2, 127.1, 126.8, 126.7, 126.6, 122.7, 21.5. HRMS (ESI) calcd for $C_{21}H_{19}NNaO_2S^+$ [M + Na^+] 372.1029, found 372.1028.

(*E*)-*N*-(5-Fluoro-2-styrylphenyl)-4-methylbenzenesulfonamide (1b)



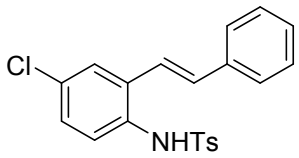
Following the general procedure **Method A**, **1b** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 71%); m.p. 114-116 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.2 Hz, 2H), 7.40 (dd, *J* = 8.6, 6.2 Hz, 1H), 7.37 – 7.26 (m, 5H), 7.19 (dd, *J* = 9.7, 2.5 Hz, 3H), 6.90 (td, *J* = 8.3, 2.6 Hz, 1H), 6.79 – 6.65 (m, 3H), 2.32 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.2 (d, $^1J_{C\text{-}F}$ = 247.1 Hz), 144.3, 136.5,136.4, 134.7 (d, $^3J_{C\text{-}F}$ = 10.2 Hz), 132.7 (d, $^4J_{C\text{-}F}$ = 3.8 Hz), 129.8, 128.7, 128.3, 128.2, 128.1 (d, $^4J_{C\text{-}F}$ = 2.5 Hz), 127.2, 126.6, 121.6, 113.7 (d, $^2J_{C\text{-}F}$ = 21.4 Hz), 112.2 (d, $^2J_{C\text{-}F}$ = 24.6 Hz), 21.5. HRMS (ESI) calcd for $C_{21}H_{18}FNNaO_2S^+$ [M + Na^+] 390.0934, found 390.0936.

(*E*)-*N*-(4-Fluoro-2-styrylphenyl)-4-methylbenzenesulfonamide (1c)



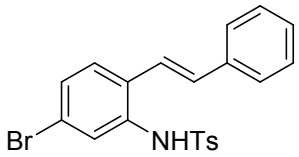
Following the general procedure **Method A**, **1c** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 69%); m.p. 151-153 °C. R_f = 0.57 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.26 (m, 6H), 7.20 (dd, *J* = 9.6, 2.9 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.95 – 6.89 (m, 1H), 6.78 (dd, *J* = 48.5, 16.1 Hz, 3H), 2.25 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.7 (d, $^1J_{C\text{-}F}$ = 245.4 Hz), 144.03, 136.5 (d, $^3J_{C\text{-}F}$ = 8.2 Hz), 136.35, 136.33, 132.71, 130.1 (d, $^3J_{C\text{-}F}$ = 8.8 Hz), 129.71, 129.0 (d, $^4J_{C\text{-}F}$ = 2.4 Hz), 128.64, 128.37, 127.21, 126.86, 121.96, 115.2 (d, $^2J_{C\text{-}F}$ = 22.8 Hz), 112.5 (d, $^2J_{C\text{-}F}$ = 23.2 Hz), 21.42. HRMS (ESI) calcd for $C_{21}H_{18}FNNaO_2S^+$ [M + Na^+] 390.0934, found 390.0936.

(*E*)-*N*-(4-Chloro-2-styrylphenyl)-4-methylbenzenesulfonamide (1d)



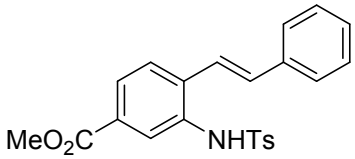
Following the general procedure **Method A**, **1d** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 79%); m.p. 143-145 °C. R_f = 0.39 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.40 (d, *J* = 2.4 Hz, 1H), 7.30 – 7.20 (m, 6H), 7.13 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.85 (s, 1H), 6.72 (q, *J* = 16.1 Hz, 2H), 2.21 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.1, 136.3, 136.3, 135.1, 133.2, 132.9, 131.8, 129.8, 128.7, 128.43, 128.41, 128.2, 127.2, 126.9, 126.3, 121.5, 21.5. HRMS (ESI) calcd for $C_{21}H_{18}ClNNaO_2S^+$ [M + Na^+] 406.0639, found 406.0638.

(*E*)-*N*-(5-Bromo-2-styrylphenyl)-4-methylbenzenesulfonamide (1e)



Following the general procedure **Method A**, **1e** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A pale yellow solid (yield: 78%); m.p. 148-150 °C. R_f = 0.59 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.56 (s, 1H), 7.37 – 7.27 (m, 7H), 7.18 (d, *J* = 7.9 Hz, 2H), 6.79 – 6.72 (m, 3H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.3, 136.4, 136.3, 134.4, 132.9, 131.9, 130.0, 129.8, 129.1, 128.7, 128.4, 127.8, 127.2, 126.7, 121.6, 121.5, 21.5. HRMS (ESI) calcd for $C_{21}H_{18}BrNNaO_2S^+$ [M + Na^+] 450.0134, found 450.0136.

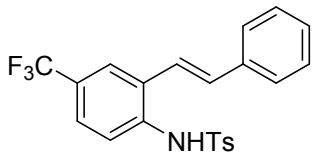
Methyl (*E*)-3-((4-methylphenyl)sulfonamido)-4-styrylbenzoate (1f)



Following the general procedure **Method A**, **1f** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 69%); m.p. 182-

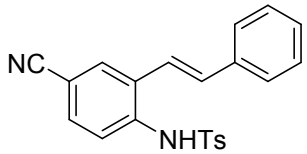
184 °C. R_f = 0.35 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 1.5 Hz, 1H), 7.88 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.2 Hz, 1H), 7.38 – 7.27 (m, 5H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.96 – 6.85 (m, 3H), 3.91 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.2, 144.1, 137.9, 136.4, 136.3, 134.0, 133.4, 129.9, 129.8, 128.7, 128.6, 128.2, 128.1, 127.2, 127.0, 126.4, 121.9, 52.3, 21.4. HRMS (ESI) calcd for $C_{23}H_{21}NNaO_4S^+$ [M + Na^+] 430.1083, found 430.1086.

(*E*)-4-Methyl-*N*-(2-styryl-4-(trifluoromethyl)phenyl)benzenesulfonamide (1g)



Following the general procedure **Method A**, **1g** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 78%); m.p. 116-118 °C. R_f = 0.38 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 3H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.47 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.34 (ddd, *J* = 25.2, 16.7, 7.1 Hz, 5H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.11 (s, 1H), 6.86 (q, *J* = 16.1 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.4, 136.6, 136.3, 136.10, 134.4, 132.3, 129.9, 128.8, 128.7, 128.3(q, $^2J_{C\text{-}F}$ = 32.7 Hz), 127.2, 126.9, 125.0(q, $^4J_{C\text{-}F}$ = 3.6 Hz), 124.7, 124.0(q, $^4J_{C\text{-}F}$ = 3.7 Hz), 123.0, 121.2, 21.5. HRMS (ESI) calcd for $C_{22}H_{18}F_3NNaO_2S^+$ [M + Na^+] 440.0903, found 440.0905.

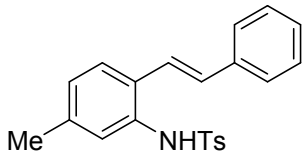
(*E*)-*N*-(4-Cyano-2-styrylphenyl)-4-methylbenzenesulfonamide (1h)



Following the general procedure **Method A**, **1h** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 69%); m.p. 164-166 °C. R_f = 0.45 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 5.0, 3.2 Hz, 3H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.49 (s, 1H), 7.45 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.39 (d, *J* = 7.1 Hz, 2H), 7.31 (dt, *J* = 20.8, 7.0 Hz, 3H), 7.20 (d, *J* = 8.2 Hz,

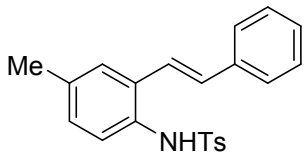
2H), 6.85 (dd, J = 54.4, 16.0 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.7, 137.7, 136.0, 135.9, 135.2, 132.0, 131.6, 131.0, 130.0, 128.9, 128.8, 127.2, 127.0, 123.6, 120.3, 118.4, 109.3, 21.6. HRMS (ESI) calcd for $C_{22}H_{18}N_2NaO_2S^+$ [M + Na^+] 397.0981, found 397.0981.

(*E*)-4-Methyl-*N*-(5-methyl-2-styrylphenyl)benzenesulfonamide (1i)



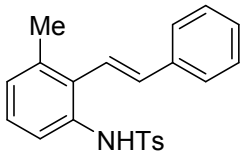
Following the general procedure **Method A**, **1i** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 75%); m.p. 154-156 °C. R_f = 0.45 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 7.9 Hz, 1H), 7.33 – 7.22 (m, 5H), 7.21 (s, 1H), 7.13 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 7.9 Hz, 1H), 6.73 (q, J = 16.1 Hz, 2H), 6.63 (s, 1H), 2.32 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.8, 138.6, 136.9, 136.7, 133.1, 131.2, 130.4, 129.6, 128.6, 128.0, 127.9, 127.5, 127.2, 126.6, 126.3, 122.6, 21.4, 21.2. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1185, found 386.1186.

(*E*)-4-Methyl-*N*-(4-methyl-2-styrylphenyl)benzenesulfonamide (1j)



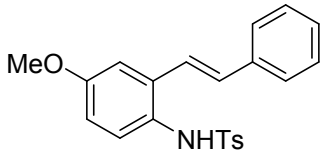
Following the general procedure **Method A**, **1j** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 69%); m.p. 117-119 °C. R_f = 0.30 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, J = 8.3 Hz, 2H), 7.36 – 7.26 (m, 6H), 7.23 (d, J = 8.1 Hz, 1H), 7.15 (d, J = 8.4 Hz, 2H), 7.05 (dd, J = 8.1, 1.5 Hz, 1H), 6.77 (s, 2H), 6.43 (s, 1H), 2.34 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.8, 137.1, 136.8, 136.7, 133.5, 131.7, 130.7, 129.6, 129.2, 128.6, 127.9, 127.4, 127.2, 126.9, 126.6, 122.9, 21.4, 21.1. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1185, found 386.1186.

(*E*)-4-Methyl-*N*-(3-methyl-2-styrylphenyl)benzenesulfonamide (1k)



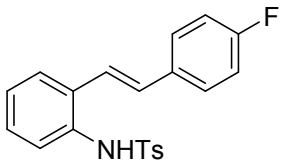
Following the general procedure **Method A**, **1k** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A brown solid (yield: 75%); m.p. 128-130 °C. R_f = 0.65 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.36 (ddt, *J* = 21.4, 14.3, 7.2 Hz, 5H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.16 (t, *J* = 7.9 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.85 (s, 1H), 6.58 (d, *J* = 16.8 Hz, 1H), 6.28 (d, *J* = 16.8 Hz, 1H), 2.41 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.8, 137.5, 136.8, 136.3, 136.1, 134.1, 129.9, 129.7, 128.8, 128.5, 127.8, 127.2, 126.8, 126.5, 122.8, 119.7, 21.6, 20.7. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1185, found 386.1186.

(*E*)-*N*-(4-Methoxy-2-styrylphenyl)-4-methylbenzenesulfonamide (1l)



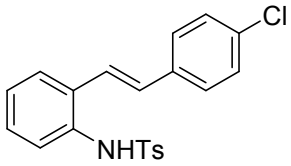
Following the general procedure **Method A**, **1l** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 77%); m.p. 142-144 °C. R_f = 0.40 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.26 (m, 5H), 7.22 (d, *J* = 8.8 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 2.9 Hz, 1H), 6.81 (d, *J* = 16.1 Hz, 1H), 6.78 (dd, *J* = 8.8, 2.9 Hz, 1H), 6.74 (d, *J* = 16.1 Hz, 1H), 6.51 (s, 1H), 3.83 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9, 143.7, 136.7, 136.6, 136.0, 131.6, 130.1, 129.6, 128.6, 128.1, 127.3, 126.7, 126.0, 123.0, 114.0, 110.9, 55.5, 21.4. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_3S^+$ [M + Na^+] 402.1134, found 402.1136.

(*E*)-*N*-(2-(4-Fluorostyryl)phenyl)-4-methylbenzenesulfonamide (1m)



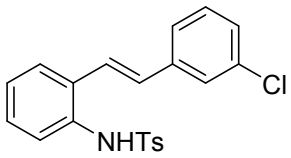
Following the general procedure **Method B**, **1m** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 85%); m.p. 167-169 °C. R_f = 0.43 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.48 (dd, *J* = 6.6, 2.7 Hz, 1H), 7.35 – 7.29 (m, 3H), 7.25 – 7.20 (m, 2H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.00 (t, *J* = 8.6 Hz, 2H), 6.89 (s, 1H), 6.86 (d, *J* = 16.1 Hz, 1H), 6.74 (d, *J* = 16.1 Hz, 1H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.6 (d, $^1J_{C\text{-}F}$ = 248.0 Hz), 143.9, 136.6, 133.3, 133.1 (d, $^4J_{C\text{-}F}$ = 3.2 Hz), 130.7, 129.6, 128.3 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 128.3, 127.2, 127.1, 126.8, 126.4, 122.7, 115.5 (d, $^2J_{C\text{-}F}$ = 21.8 Hz), 100.0, 21.4. HRMS (ESI) calcd for $C_{21}H_{18}FNNaO_2S^+$ [M + Na^+] 390.0934, found 390.0936.

(*E*)-*N*-(2-(4-Chlorostyryl)phenyl)-4-methylbenzenesulfonamide (1n)



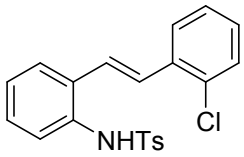
Following the general procedure **Method B**, **1n** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 67%); m.p. 195-197 °C. R_f = 0.39 (30% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, DMSO) δ 9.79 (s, 1H), 7.70 – 7.63 (m, 1H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.6 Hz, 2H), 7.27 – 7.22 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.13 (m, 1H), 7.10 (d, *J* = 16.3 Hz, 1H), 6.92 (d, *J* = 16.3 Hz, 1H), 2.16 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 142.9, 137.1, 136.0, 133.9, 133.2, 131.9, 129.5, 128.5, 128.2, 128.1, 128.0, 126.9, 126.5, 125.5, 124.4, 20.8. HRMS (ESI) calcd for $C_{21}H_{18}ClNNaO_2S^+$ [M + Na^+] 406.0639, found 406.0638.

(*E*)-*N*-(2-(3-Chlorostyryl)phenyl)-4-methylbenzenesulfonamide (1o)



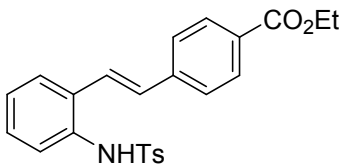
Following the general procedure **Method B**, **1o** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 83%); m.p. 131-133 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.37 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.29 – 7.20 (m, 5H), 7.20 – 7.16 (m, 3H), 6.74 (dd, *J* = 52.3, 16.1 Hz, 2H), 6.67 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.0, 138.7, 136.7, 134.6, 133.4, 133.1, 130.5, 129.8, 129.8, 128.8, 127.9, 127.6, 127.3, 127.2, 126.5, 126.3, 125.0, 124.3, 21.4. HRMS (ESI) calcd for $C_{21}H_{18}ClNNaO_2S^+$ [M + Na^+] 406.0639, found 406.0638.

(*E*)-*N*-(2-(2-Chlorostyryl)phenyl)-4-methylbenzenesulfonamide (1p)



Following the general procedure **Method B**, **1p** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A brown solid (yield: 81%); m.p. 162-164 °C. R_f = 0.45 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.58 – 7.54 (m, 1H), 7.44 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.32 (dd, *J* = 5.6, 3.7 Hz, 1H), 7.26 – 7.18 (m, 5H), 7.14 (d, *J* = 8.1 Hz, 2H), 6.91 (d, *J* = 16.1 Hz, 1H), 6.74 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.0, 136.5, 134.9, 133.5, 133.4, 133.3, 129.8, 129.7, 129.0, 128.8, 127.9, 127.3, 127.2, 127.0, 126.9, 126.8, 126.8, 125.4, 21.5. HRMS (ESI) calcd for $C_{21}H_{18}ClNNaO_2S^+$ [M + Na^+] 406.0639, found 406.0638.

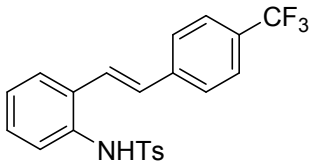
Ethyl (*E*)-4-(2-((4-methylphenyl)sulfonamido)styryl)benzoate (1q)



Following the general procedure **Method B**, **1q** was purified by silica gel

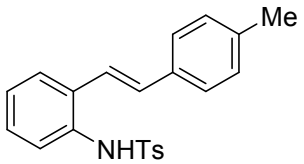
chromatography (10% EtOAc/petroleum ether). A white solid (yield: 82%); m.p. 152-153 °C. R_f = 0.40 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.52 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.40 – 7.32 (m, 3H), 7.26 – 7.22 (m, 2H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.01 (d, *J* = 16.1 Hz, 1H), 6.89 (s, 1H), 6.80 (d, *J* = 16.1 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.27 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.4, 144.0, 141.1, 136.5, 133.5, 133.1, 130.7, 129.9, 129.7, 129.6, 128.9, 127.4, 127.3, 127.2, 126.5, 126.5, 125.4, 61.0, 21.5, 14.4. HRMS (ESI) calcd for $C_{24}H_{23}NNaO_4S^+$ [M + Na^+] 444.1240, found 444.1242.

(*E*)-4-Methyl-*N*-(2-(4-(trifluoromethyl)styryl)phenyl)benzenesulfonamide (1r)



Following the general procedure **Method B**, **1r** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 79%); m.p. 162-164 °C. R_f = 0.45 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.58 – 7.51 (m, 3H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.32 – 7.28 (m, 1H), 7.25 (dd, *J* = 5.8, 4.0 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 16.2 Hz, 1H), 6.82 (d, *J* = 16.1 Hz, 1H), 6.77 (s, 1H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.0, 140.3, 136.5, 133.5, 133.0, 130.2, 129.7, 129.6 (q, $^2J_{C\text{-}F}$ = 31.8 Hz), 129.0, 127.3, 127.3, 127.2, 126.8, 126.6, 125.6, 125.5 (q, $^3J_{C\text{-}F}$ = 3.8 Hz), 124.2(q, $^1J_{C\text{-}F}$ = 270.1 Hz), 21.4. HRMS (ESI) calcd for $C_{22}H_{18}F_3NNaO_2S^+$ [M + Na^+] 440.0903, found 440.0905.

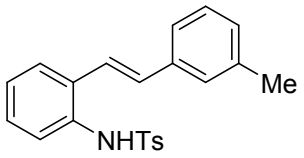
(*E*)-4-Methyl-*N*-(2-(4-methylstyryl)phenyl)benzenesulfonamide (1s)



Following the general procedure **Method B**, **1s** was purified by silica gel

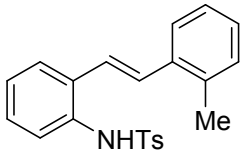
chromatography (10% EtOAc/petroleum ether). A white solid (yield: 77%); m.p. 159-161 °C. R_f = 0.33 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.46 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.38 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.22 (ddd, *J* = 16.1, 10.7, 5.0 Hz, 4H), 7.16 (dd, *J* = 15.2, 8.0 Hz, 4H), 6.80 – 6.67 (m, 2H), 6.50 (s, 1H), 2.37 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.2, 136.7, 133.9, 133.2, 133.2, 132.4, 129.7, 129.4, 128.2, 127.2, 127.0, 126.6, 126.6, 126.5, 121.6, 21.5, 21.3. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1185, found 386.1186.

(*E*)-4-Methyl-*N*-(2-(3-methylstyryl)phenyl)benzenesulfonamide (1t)



Following the general procedure **Method B**, **1t** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 70%); m.p. 117-119 °C. R_f = 0.60 (30% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 7.2, 2.1 Hz, 1H), 7.39 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.26 – 7.20 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 7.2 Hz, 3H), 6.74 (d, *J* = 2.5 Hz, 2H), 6.47 (s, 1H), 2.38 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 138.2, 136.6, 136.6, 133.2, 133.1, 132.6, 129.7, 129.0, 128.6, 128.4, 127.2, 127.2, 127.0, 126.6, 126.6, 123.9, 122.3, 21.5, 21.4. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1191, found 386.1190.

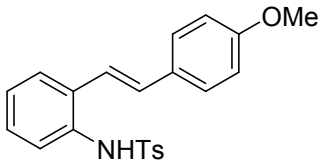
(*E*)-4-Methyl-*N*-(2-(2-methylstyryl)phenyl)benzenesulfonamide (1u)



Following the general procedure **Method B**, **1u** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 67%); m.p. 148-149 °C. R_f = 0.40 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.50 (dd, *J* = 6.5, 2.8 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.28 (dd, *J* =

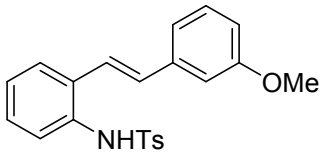
7.2, 4.6 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.21 – 7.14 (m, 5H), 7.05 (d, *J* = 16.0 Hz, 1H), 6.71 (d, *J* = 16.0 Hz, 1H), 6.68 (s, 1H), 2.34 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 136.7, 135.8, 135.7, 133.4, 133.3, 130.4, 130.1, 129.7, 128.4, 128.1, 127.2, 127.0, 126.8, 126.6, 126.2, 125.5, 123.9, 21.5, 19.9. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1191, found 386.1192.

(*E*)-*N*-(2-(4-Methoxystyryl)phenyl)-4-methylbenzenesulfonamide (1v)



Following the general procedure **Method B**, **1v** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 90%); m.p. 122-124 °C. R_f = 0.40 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.48 – 7.42 (m, 1H), 7.40 – 7.32 (m, 1H), 7.29 – 7.22 (m, 2H), 7.23 – 7.16 (m, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.88 – 6.81 (m, 2H), 6.77 (s, 1H), 6.70 (s, 2H), 3.82 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.7, 143.8, 136.7, 133.5, 133.1, 131.7, 129.6, 128.0, 127.2, 126.9, 126.6, 126.4, 120.5, 114.1, 55.4, 21.5. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_3S^+$ [M + Na^+] 402.1134, found 402.1136.

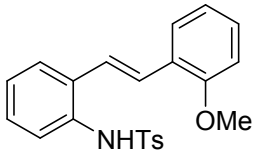
(*E*)-*N*-(2-(3-Methoxystyryl)phenyl)-4-methylbenzenesulfonamide (1w)



Following the general procedure **Method B**, **1w** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 90%); m.p. 104-105 °C. R_f = 0.70 (30% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.49 (dd, *J* = 7.0, 2.3 Hz, 1H), 7.40 (dd, *J* = 7.3, 2.0 Hz, 1H), 7.26 – 7.19 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.08 (s, 1H), 6.97 – 6.79 (m, 4H), 6.72 (d, *J* = 16.1 Hz, 1H), 3.83 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.8, 143.9, 138.2, 136.5, 133.4, 133.3, 131.9, 129.7, 129.6, 128.4, 127.2, 126.5, 123.0,

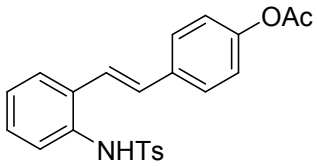
119.5, 113.8, 111.9, 55.3, 21.5 (2 carbons are missing due to overlapping). HRMS (ESI) calcd for $C_{22}H_{21}NNaO_3S^+$ [M + Na^+] 402.1140, found 402.1142.

(*E*)-*N*-(2-(2-Methoxystyryl)phenyl)-4-methylbenzenesulfonamide (1x)



Following the general procedure **Method B**, **1x** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 67%); m.p. 163-165 °C. R_f = 0.43 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.50 (dd, *J* = 7.0, 2.3 Hz, 1H), 7.39 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.28 (dd, *J* = 6.6, 2.0 Hz, 1H), 7.25 (s, 1H), 7.24 – 7.18 (m, 2H), 7.16 (dd, *J* = 12.1, 8.7 Hz, 3H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 8.5 Hz, 1H), 6.78 (d, *J* = 16.3 Hz, 1H), 6.51 (s, 1H), 3.87 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 143.9, 136.6, 133.4, 133.2, 129.7, 129.3, 128.2, 127.6, 127.2, 126.9, 126.8, 126.1, 125.7, 123.0, 120.7, 110.9, 55.5, 21.5. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_3S^+$ [M + Na^+] 402.1134, found 402.1136.

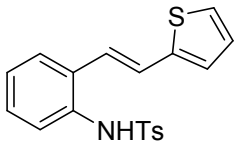
(*E*)-4-(2-((4-Methylphenyl)sulfonamido)styryl)phenyl acetate (1y)



Following the general procedure **Method B**, **1y** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 87%); m.p. 140-141 °C. R_f = 0.30 (20% EtOAc/petroleum ether);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.48 (dd, *J* = 6.8, 2.5 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.25 – 7.18 (m, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.96 (s, 1H), 6.85 (d, *J* = 16.1 Hz, 1H), 6.73 (d, *J* = 16.1 Hz, 1H), 2.31 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 150.3, 143.9, 136.5, 134.6, 133.3, 133.3, 130.7, 129.7, 128.5, 127.7, 127.2, 127.1, 127.1, 126.4, 123.0, 121.8, 21.5, 21.2.

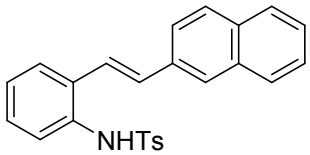
HRMS (ESI) calcd for $C_{23}H_{21}NNaO_4S^+$ [M + Na^+] 430.1089, found 430.1088.

(*E*)-4-Methyl-*N*-(2-(2-(thiophen-2-yl)vinyl)phenyl)benzenesulfonamide (1z)



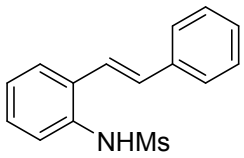
Following the general procedure **Method B**, **1z** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A yellow solid (yield: 76%); m.p. 117-119 °C. R_f = 0.55 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.41 (td, *J* = 7.5, 1.5 Hz, 2H), 7.25 – 7.18 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.98 (dd, *J* = 5.5, 2.5 Hz, 2H), 6.87 (d, *J* = 15.9 Hz, 1H), 6.72 (s, 1H), 6.59 (d, *J* = 15.9 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.9, 142.3, 136.4, 133.1, 133.0, 129.7, 128.4, 127.6, 127.2, 126.7, 126.3, 125.1, 125.0, 122.1, 21.5. HRMS (ESI) calcd for $C_{19}H_{17}NNaO_2S_2^+$ [M + Na^+] 378.0593, found 378.0596.

(*E*)-4-Methyl-*N*-(2-(2-(naphthalen-2-yl)vinyl)phenyl)benzenesulfonamide (1aa)



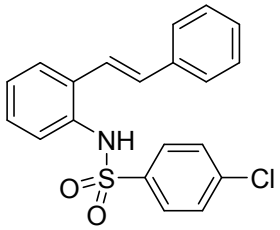
Following the general procedure **Method B**, **1aa** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 86%); m.p. 138-140 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81 – 7.77 (m, 2H), 7.75 (d, *J* = 8.6 Hz, 1H), 7.68 (s, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.49 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.48 – 7.43 (m, 2H), 7.41 – 7.36 (m, 1H), 7.27 – 7.20 (m, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 6.95 (dd, *J* = 44.2, 16.1 Hz, 2H), 6.85 (s, 1H), 2.19 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.9, 136.6, 134.3, 133.6, 133.4, 133.3, 133.2, 132.1, 129.7, 128.4, 128.3, 128.1, 127.7, 127.2, 127.2, 127.0, 127.0, 126.5, 126.4, 126.2, 123.6, 123.0, 21.4. HRMS (ESI) calcd for $C_{25}H_{21}NNaO_2S^+$ [M + Na^+] 422.1185, found 422.1186.

(*E*)-*N*-(2-Styrylphenyl)methanesulfonamide (1ab)



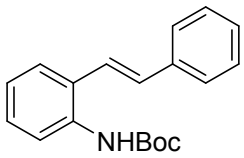
Following the general procedure **Method A** using methanesulfonyl chloride as the sulfonylation reagent, **1ab** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 81%); m.p. 110-112 °C. R_f = 0.31 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.50 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.36 – 7.26 (m, 4H), 7.06 (d, *J* = 16.1 Hz, 1H), 6.51 (s, 1H), 3.02 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.8, 133.5, 132.9, 132.5, 128.8, 128.7, 128.3, 127.0, 126.9, 126.9, 125.1, 122.8, 40.0. HRMS (ESI) calcd for $C_{15}H_{15}NNaO_2S^+$ [M + Na^+] 296.0716, found 296.0718.

(*E*)-4-Chloro-*N*-(2-styrylphenyl)benzenesulfonamide (1ac)



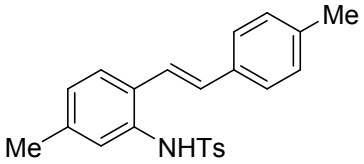
Following the general procedure **Method A** using 4-chlorobenzenesulfonyl chloride as the sulfonylation reagent, **1ac** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 80%); m.p. 129-131 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 – 7.61 (m, 2H), 7.51 – 7.47 (m, 1H), 7.37 – 7.30 (m, 5H), 7.30 – 7.26 (m, 3H), 7.26 – 7.22 (m, 2H), 6.88 (d, *J* = 16.1 Hz, 1H), 6.82 (s, 1H), 6.75 (d, *J* = 16.1 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.6, 137.9, 136.6, 133.6, 132.8, 132.5, 129.3, 128.7, 128.6, 128.5, 128.3, 127.6, 127.0, 126.8, 126.7, 122.6. HRMS (ESI) calcd for $C_{20}H_{16}ClNNaO_2S^+$ [M + Na^+] 392.0482, found 392.0483.

***tert*-butyl (*E*)-(2-styrylphenyl)carbamate (1ad)**



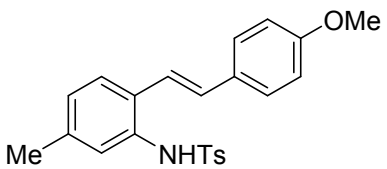
Following the general procedure **Method A** using $(Boc)_2O$ in $ClCH_2CH_2Cl$ in place of *p*-TsCl in pyridine, **1ad** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 73%); mp 130-132 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.52 (t, *J* = 8.5 Hz, 3H), 7.39 (t, *J* = 6.9 Hz, 2H), 7.36 – 7.26 (m, 2H), 7.14 (dd, *J* = 20.9, 13.2 Hz, 2H), 7.00 (d, *J* = 16.0 Hz, 1H), 6.45 (s, 1H), 1.54 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.2, 137.2, 135.4, 132.4, 128.8, 128.4, 128.1, 126.9, 126.7, 124.3, 123.6, 122.1, 80.7, 28.4. HRMS (ESI) calcd for $C_{19}H_{21}NNaO_2^+$ [M + Na^+] 318.1465, found 318.1468.

(*E*)-4-Methyl-*N*-(5-methyl-2-(4-methylstyryl)phenyl)benzenesulfonamide(1ae)



Following the general procedure **Method B**, **1ae** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 88%); m.p. 158-160 °C. R_f = 0.70 (20% EtOAc/petroleum ether); ^1H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.23 (s, 1H), 7.15 (q, *J* = 8.1 Hz, 6H), 7.03 (d, *J* = 8.2 Hz, 1H), 6.66 (q, *J* = 16.1 Hz, 2H), 6.50 (s, 1H), 2.36 (s, 3H), 2.33 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 138.5, 137.9, 136.7, 134.1, 132.9, 131.3, 130.4, 129.6, 129.3, 128.0, 127.3, 127.2, 126.5, 126.3, 121.5, 21.5, 21.3, 21.2. HRMS (ESI) calcd for $C_{23}H_{23}NNaO_2S^+$ [M + Na^+] 400.1347, found 400.1348.

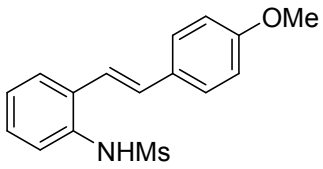
(*E*)-*N*-(2-(4-Methoxystyryl)-5-methylphenyl)-4-methylbenzenesulfonamide(1af)



Following the general procedure **Method B**, **1af** was purified by silica gel

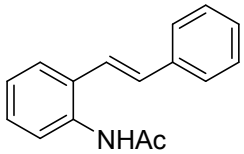
chromatography (10% EtOAc/petroleum ether). A white solid (yield: 83%); m.p. 132-134 °C. R_f = 0.40 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.19 (t, *J* = 9.1 Hz, 5H), 7.02 (d, *J* = 7.8 Hz, 1H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.67 (d, *J* = 16.1 Hz, 1H), 6.51 (d, *J* = 16.1 Hz, 1H), 6.35 (s, 1H), 3.84 (s, 3H), 2.33 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 143.9, 138.3, 136.7, 132.8, 131.0, 130.4, 129.6, 129.6, 127.9, 127.8, 127.2, 127.2, 126.2, 120.3, 114.1, 55.4, 21.5, 21.2. HRMS (ESI) calcd for $C_{23}H_{23}NNaO_3S^+$ [M + Na^+] 416.1291, found 416.1293.

(*E*)-*N*-(2-(4-Methoxystyryl)phenyl)methanesulfonamide (1ag)



Following the general procedure **Method B** using methanesulfonyl chloride as the sulfonylation reagent, **1ag** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 81%); m.p. 115-117 °C. R_f = 0.35 (30% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 7.0, 2.3 Hz, 1H), 7.53 – 7.46 (m, 3H), 7.28 (dd, *J* = 4.0, 2.5 Hz, 1H), 7.21 (d, *J* = 16.1 Hz, 1H), 7.00 (d, *J* = 16.0 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.81 (s, 1H), 3.83 (s, 3H), 3.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 133.2, 132.7, 132.5, 129.5, 128.4, 128.2, 126.9, 126.8, 125.0, 120.4, 114.3, 55.4, 40.0. HRMS (ESI) calcd for $C_{16}H_{17}NNaO_3S^+$ [M + Na^+] 326.0827, found 326.0828.

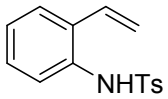
(*E*)-*N*-(2-styrylphenyl)acetamide (1ah)



Following the general procedure **Method A** using AcCl in place of *p*-TsCl, **1ah** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 84%); mp 140-141 °C. R_f = 0.58 (10% EtOAc/petroleum ether); ^{1}H NMR (600

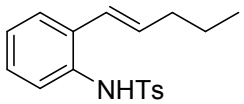
MHz, DMSO) δ 9.63 (s, 1H), 7.76 (d, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.39 (dd, *J* = 19.9, 12.0 Hz, 3H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.23 – 7.15 (m, 2H), 2.12 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 168.6, 137.3, 135.6, 130.8, 129.5, 128.7, 127.7, 127.6, 126.6, 126.1, 125.4, 125.2, 124.1, 23.4. HRMS (ESI) calcd for $C_{16}H_{15}NNaO^+$ [M + Na^+] 260.1046, found 260.1048.

4-methyl-*N*-(2-vinylphenyl)benzenesulfonamide (1ai)



Following the general procedure **Method B**, **1ai** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 76%); mp 114-116 °C. R_f = 0.20 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.36 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.20 (dd, *J* = 13.2, 4.9 Hz, 3H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.71 (s, 1H), 6.58 (dd, *J* = 17.4, 11.0 Hz, 1H), 5.50 (d, *J* = 17.4 Hz, 1H), 5.25 (d, *J* = 11.0 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.9, 136.5, 133.2, 132.8, 131.6, 129.6, 128.6, 127.3, 126.9, 126.5, 125.0, 118.1, 21.6. HRMS (ESI) calcd for $C_{15}H_{15}NNaO_2S^+$ [M + Na^+] 296.0716, found 296.0718.

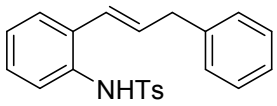
(*E*)-4-methyl-*N*-(2-(pent-1-en-1-yl)phenyl)benzenesulfonamide (1aj)



Following the general procedure **Method A**, **1aj** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 68%); mp 76-78 °C. R_f = 0.43 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 7.9 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.11 (t, *J* = 7.3 Hz, 1H), 6.62 (s, 1H), 6.11 (d, *J* = 15.7 Hz, 1H), 5.92 (dt, *J* = 15.6, 6.9 Hz, 1H), 2.37 (s, 3H), 2.13 – 1.93 (m, 2H), 1.51 – 1.31 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.7, 136.6, 135.7,

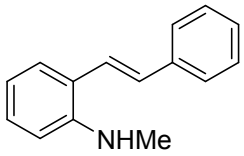
132.9, 132.7, 129.6, 127.7, 127.2, 127.1, 126.3, 124.7, 124.0, 35.2, 22.2, 21.5, 13.7. HRMS (ESI) calcd for $C_{18}H_{21}NNaO_2S^+$ [M + Na^+] 338.1185, found 338.1187.

(*E*)-4-methyl-*N*-(2-(3-phenylprop-1-en-1-yl)phenyl)benzenesulfonamide(1ak)



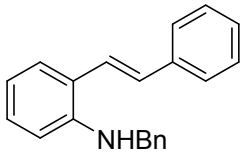
Following the general procedure **Method A**, **1ak** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (yield: 75%); mp 125-127 °C. R_f = 0.28 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.27 (m, 4H), 7.25 – 7.20 (m, 2H), 7.18 – 7.12 (m, 4H), 6.57 (s, 1H), 6.28 (d, *J* = 15.9 Hz, 1H), 6.09 (dt, *J* = 15.9, 6.4 Hz, 1H), 3.25 (dd, *J* = 6.3, 1.2 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.8, 136.8, 136.7, 134.9, 132.5, 132.0, 130.5, 129.6, 128.6, 127.7, 127.6, 127.2, 127.1, 126.28, 126.26, 124.3, 35.1, 21.5. HRMS (ESI) calcd for $C_{22}H_{21}NNaO_2S^+$ [M + Na^+] 386.1185, found 386.1188.

(*E*)-N-methyl-2-styrylaniline (1al)



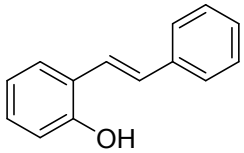
Following the general procedure **Method A** using MeI in place of *p*-TsCl, **1al** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A yellow oil (yield: 45%). R_f = 0.65 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.8 Hz, 2H), 7.39 (dd, *J* = 13.5, 7.4 Hz, 3H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.24 (s, 1H), 7.17 (d, *J* = 16.0 Hz, 1H), 6.98 (d, *J* = 16.0 Hz, 1H), 6.80 (t, *J* = 7.4 Hz, 1H), 6.71 (d, *J* = 8.1 Hz, 1H), 4.16 (s, 1H), 2.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 137.7, 130.9, 129.1, 128.7, 127.6, 127.3, 126.5, 124.4, 124.1, 117.6, 110.5, 31.0. HRMS (ESI) calcd for $C_{15}H_{15}NNa^+$ [M + Na^+] 232.1097, found 232.1096.

(*E*)-*N*-benzyl-2-styrylaniline (1am)



Following the general procedure **Method A** using BnCl in place of *p*-TsCl, **1am** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A yellow oil (yield: 48%). R_f = 0.65 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.4 Hz, 2H), 7.35 – 7.29 (m, 3H), 7.26 (t, *J* = 7.0 Hz, 4H), 7.21 – 7.12 (m, 3H), 7.08 (dd, *J* = 14.5, 6.5 Hz, 2H), 6.90 (d, *J* = 16.0 Hz, 1H), 6.70 (t, *J* = 7.2 Hz, 1H), 6.60 (d, *J* = 7.8 Hz, 1H), 4.31 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.4, 139.1, 137.7, 131.1, 129.0, 128.7, 127.62, 127.56, 127.5, 127.3, 126.5, 124.4, 117.9, 111.5, 48.6. HRMS (ESI) calcd for $C_{21}H_{19}NNa^+$ [M + Na^+] 308.1410, found 308.1416.

(*E*)-2-styrylphenol (1an)



Following the general procedure **Method A** step 1, **1an** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A yellow solid (yield: 82%); mp 140-142 °C. R_f = 0.55 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 3H), 7.39 (d, *J* = 4.7 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.27 (d, *J* = 13.9 Hz, 1H), 7.18 – 7.08 (m, 2H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 4.96 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 137.6, 130.2, 128.7, 127.7, 127.3, 126.6, 124.7, 123.0, 121.2, 116.0. HRMS (ESI) calcd for $C_{14}H_{12}NaO^+$ [M + Na^+] 219.0780, found 219.0785.

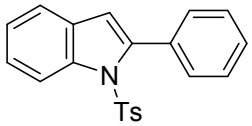
3. General Procedure for the Synthesis of 3-Unsubstituted Indoles Derivatives 2 (2a-2ac):

To a solution of substrate **1** (0.5 mmol) in DMSO (1 mL) was slowly added $SOCl_2$ (1.5 mmol, 179 mg) at 25 °C. The mixture was kept stirring at 25 °C until TLC indicated that total consumption of substrate **1**. Then the reaction mixture was

quenched with saturated aq. $NaHCO_3$ solution (5 mL) and water (20 mL), extracted with EtOAc (3 × 20 mL), combined the organic phase then evaporated the solvent, purified by flash column chromatography (5% EtOAc/petroleum ether) to afford the desired compound **2**.

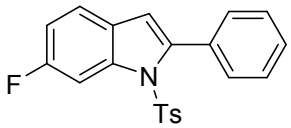
4. Spectroscopic Data of 3-Unsubstituted Indoles Derivatives 2 (2a-ac):

2-Phenyl-1-tosyl-1*H*-indole (2a)



Following the general procedure, **2a** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (159 mg, 92%); m.p. 145-147 °C. R_f = 0.59 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.4 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.45 – 7.39 (m, 4H), 7.37 – 7.32 (m, 1H), 7.26 – 7.23 (m, 2H), 7.02 (d, *J* = 8.3 Hz, 2H), 6.53 (s, 1H), 2.27 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.5, 142.2, 138.3, 134.8, 132.5, 130.6, 130.4, 129.2, 128.7, 127.5, 126.8, 124.8, 124.3, 120.7, 116.7, 113.6, 21.5. HRMS (ESI) calcd for $C_{21}H_{17}NNaO_2S^+$ [M + Na^+] 370.0878, found 370.0882.

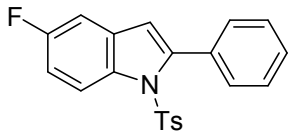
6-Fluoro-2-phenyl-1-tosyl-1*H*-indole (2b)



Following the general procedure, **2b** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (168 mg, 92%); m.p. 103-105 °C. R_f = 0.61 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 10.4, 2.1 Hz, 1H), 7.49 – 7.39 (m, 5H), 7.36 (dd, *J* = 8.5, 5.4 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 8.1 Hz, 2H), 7.02 (td, *J* = 8.8, 2.3 Hz, 1H), 6.49 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.7, 160.1, 144.8, 142.4(d, $^4J_{C\text{-}F}$ = 4.3 Hz), 138.6(d, $^3J_{C\text{-}F}$ = 12.5 Hz), 134.7, 132.1, 130.4, 129.3, 128.7, 127.5, 126.9, 126.7, 121.3(d, $^3J_{C\text{-}F}$ = 9.7 Hz), 112.8, 112.6(d, $^2J_{C\text{-}F}$ = 24.1 Hz), 104.0(d, $^2J_{C\text{-}F}$ = 28.6 Hz), 21.5. HRMS (ESI)

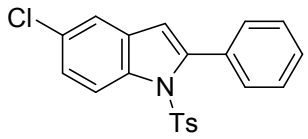
calcd for $C_{21}H_{16}FNNaO_2S^+$ [M + Na^+] 388.0783, found 388.0782.

5-Fluoro-2-phenyl-1-tosyl-1*H*-indole (2c)



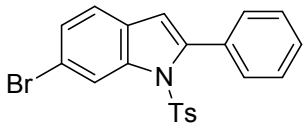
Following the general procedure, **2c** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A pale yellow solid (165 mg, 91%); m.p. 113-115 °C. R_f = 0.57 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 8.9, 4.5 Hz, 1H), 7.51 – 7.39 (m, 5H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.12 – 7.02 (m, 4H), 6.50 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.2(d, $^1J_{C\text{-}F}$ = 239.7 Hz), 144.7, 144.0, 134.6, 134.5, 132.1, 131.6(d, $^3J_{C\text{-}F}$ = 10.0 Hz), 130. 3, 129.3, 128.9, 127.6, 126.8, 117.9(d, $^3J_{C\text{-}F}$ = 9.2 Hz), 113.2(d, $^4J_{C\text{-}F}$ = 3.8 Hz), 112.5(d, $^2J_{C\text{-}F}$ = 25.0 Hz), 106.3(d, $^2J_{C\text{-}F}$ = 23.8 Hz), 21.5. HRMS (ESI) calcd for $C_{21}H_{16}FNNaO_2S^+$ [M + Na^+] 388.0783, found 388.0781.

5-Chloro-2-phenyl-1-tosyl-1*H*-indole (2d)



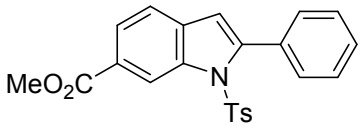
Following the general procedure, **2d** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (165 mg, 83%); m.p. 142-143 °C. R_f = 0.61 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.9 Hz, 1H), 7.52 – 7.39 (m, 6H), 7.31 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 8.1 Hz, 2H), 6.48 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 143.6, 136.6, 134.4, 131.9, 131.8, 130.4, 130.0, 129.4, 129.0, 127.6, 126.8, 124.9, 120.3, 117.7, 112.7, 21.6. HRMS (ESI) calcd for $C_{21}H_{16}ClNNaO_2S^+$ [M + Na^+] 404.0488, found 404.0485.

6-Bromo-2-phenyl-1-tosyl-1*H*-indole (2e)



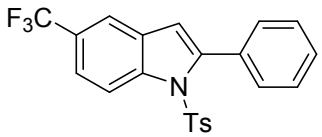
Following the general procedure, **2e** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (186 mg, 87%); m.p. 156-157 °C. R_f = 0.46 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.48 – 7.36 (m, 6H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.06 (d, *J* = 8.2 Hz, 2H), 6.48 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.9, 142.6, 138.9, 134.7, 131.9, 130.4, 129.4, 129.3, 128.9, 127.6, 127.5, 126.9, 121.7, 119.6, 118.3, 112.8, 21.6. HRMS (ESI) calcd for $C_{21}H_{16}BrNNaO_2S^+$ [M + Na^+] 449.9983, found 449.9981.

Methyl 2-phenyl-1-tosyl-1*H*-indole-6-carboxylate (2f)



Following the general procedure, **2f** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (181 mg, 86%); m.p. 165-166 °C. R_f = 0.21 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.01 (s, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.45 (ddd, *J* = 20.2, 15.4, 7.5 Hz, 6H), 7.30 – 7.21 (m, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 6.56 (s, 1H), 3.98 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.4, 145.2, 144.9, 137.7, 134.6, 134.2, 131.8, 130.4, 129.4, 129.1, 127.6, 126.9, 126.5, 125.6, 120.4, 118.3, 113.1, 52.3, 21.6. HRMS (ESI) calcd for $C_{23}H_{19}NNaO_4S^+$ [M + Na^+] 428.0932, found 428.0933.

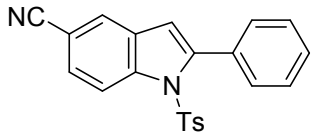
2-Phenyl-1-tosyl-5-(trifluoromethyl)-1*H*-indole (2g)



Following the general procedure, **2g** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (151 mg, 73%); m.p. 123-125 °C. R_f = 0.67

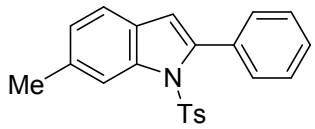
(20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 (d, J = 8.8 Hz, 1H), 7.75 (s, 1H), 7.52 – 7.39 (m, 5H), 7.28 (m, 2H), 7.08 (d, J = 8.1 Hz, 2H), 6.59 (s, 1H), 2.31 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.1, 143.7, 139.7, 134.8, 131.6, 130.6, 130.0, 129.5, 129.1, 127.6, 126.8, 126.5(q, $^2J_{C\text{-}F}$ = 21.4 Hz), 125.4, 121.4(q, $^4J_{C\text{-}F}$ = 2.4 Hz), 118.1(q, $^4J_{C\text{-}F}$ = 2.7 Hz), 116.7, 112.7, 21.5. HRMS (ESI) calcd for $C_{22}H_{16}F_3NNaO_2S^+$ [M + Na^+] 438.0752, found 438.0750.

2-Phenyl-1-tosyl-1*H*-indole-5-carbonitrile (2h)



Following the general procedure, **2h** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (121 mg, 65%); m.p. 118-119 °C. R_f = 0.25 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, J = 8.7 Hz, 1H), 7.80 (d, J = 1.1 Hz, 1H), 7.61 (dd, J = 8.7, 1.6 Hz, 1H), 7.51 – 7.40 (m, 5H), 7.24 (d, 2H), 7.08 (d, J = 8.1 Hz, 2H), 6.57 (s, 1H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 144.1, 139.9, 134.6, 131.2, 130.5, 130.2, 129.5, 129.3, 127.6, 126.8, 125.4, 119.3, 117.1, 112.0, 107.7, 21.6. HRMS (ESI) calcd for $C_{22}H_{16}N_2NaO_2S^+$ [M + Na^+] 395.0830, found 395.0833.

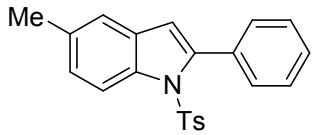
6-Methyl-2-phenyl-1-tosyl-1*H*-indole (2i)



Following the general procedure, **2i** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (176 mg, 98%); m.p. 178-180 °C. R_f = 0.69 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.47 (d, J = 4.6 Hz, 2H), 7.40 (s, 3H), 7.30 (d, J = 7.8 Hz, 1H), 7.24 (t, J = 8.4 Hz, 2H), 7.08 (d, J = 7.7 Hz, 1H), 7.02 (d, J = 7.9 Hz, 2H), 6.47 (s, 1H), 2.51 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.4, 141.5, 138.8, 134.9, 134.8, 132.6, 130.3, 129.2, 128.5, 128.3, 127.5, 126.8, 125.8, 120.3, 116.9, 113.6, 22.1, 21.5. HRMS (ESI) calcd

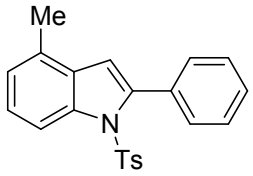
for $C_{22}H_{19}NNaO_2S^+$ [M + Na^+] 384.1034, found 384.1038.

5-Methyl-2-phenyl-1-tosyl-1*H*-indole (2j)



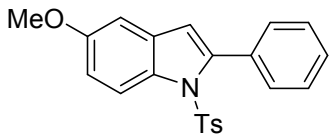
Following the general procedure, **2j** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A pale yellow solid (174 mg, 96%); m.p. 111-113 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 1H), 7.50 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.46 – 7.39 (m, 3H), 7.27 (s, 1H), 7.24 (d, *J* = 12.1 Hz, 2H), 7.17 (dd, *J* = 8.6, 1.3 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.47 (s, 1H), 2.41 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 142.3, 136.5, 134.6, 134.0, 132.5, 130.8, 130.3, 129.2, 128.6, 127.5, 126.8, 126.2, 120.6, 116.4, 113.6, 21.5, 21.3. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_2S^+$ [M + Na^+] 384.1029, found 384.1028.

4-Methyl-2-phenyl-1-tosyl-1*H*-indole (2k)



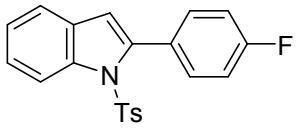
Following the general procedure, **2k** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (165 mg, 91%); m.p. 163-164 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.4 Hz, 1H), 7.52 (dd, *J* = 6.9, 2.8 Hz, 2H), 7.43 (dd, *J* = 5.1, 1.9 Hz, 3H), 7.33 – 7.29 (m, 2H), 7.26 (d, *J* = 15.8 Hz, 1H), 7.06 (t, *J* = 7.7 Hz, 3H), 6.59 (d, *J* = 0.7 Hz, 1H), 2.43 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 141.4, 138.0, 134.8, 132.7, 130.4, 130.2, 130.1, 129.2, 128.6, 127.5, 126.8, 124.8, 124.7, 114.1, 112.1, 21.6, 18.4. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_2S^+$ [M + Na^+] 384.1029, found 384.1028.

5-Methoxy-2-phenyl-1-tosyl-1*H*-indole (2l)



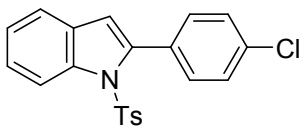
Following the general procedure, **2l** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (143 mg, 76%); m.p. 123-125 °C. R_f = 0.48 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 9.1 Hz, 1H), 7.51 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.46 – 7.39 (m, 3H), 7.24 (d, *J* = 8.3 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.96 (dd, *J* = 9.1, 2.6 Hz, 1H), 6.88 (d, *J* = 2.5 Hz, 1H), 6.48 (s, 1H), 3.83 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 144.4, 143.1, 134.4, 132.9, 132.4, 131.8, 130.2, 129.2, 128.7, 127.5, 126.8, 117.8, 113.9, 113.4, 103.2, 55.6, 21.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_3S^+$ [M + Na^+] 400.0978, found 400.0978.

2-(4-Fluorophenyl)-1-tosyl-1*H*-indole (2m)



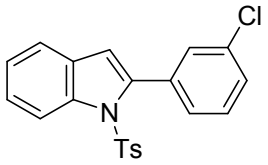
Following the general procedure, **2m** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (152 mg, 83%); m.p. 135-137 °C. R_f = 0.62 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.4 Hz, 1H), 7.45 (ddd, *J* = 8.8, 5.8, 2.8 Hz, 3H), 7.36 (ddd, *J* = 8.5, 7.3, 1.3 Hz, 1H), 7.30 – 7.22 (m, 3H), 7.10 (t, *J* = 8.7 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.51 (s, 1H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1(d, $^1J_{C\text{-}F}$ = 249.5 Hz), 144.7, 140.9, 138.2, 134.6, 132.1(d, $^3J_{C\text{-}F}$ = 8.3 Hz), 130.4, 129.3, 128.4(d, $^4J_{C\text{-}F}$ = 3.4 Hz), 126.7, 125.0, 124.4, 120.7, 116.7, 114.6 (d, $^2J_{C\text{-}F}$ = 21.6 Hz), 113.7, 21.6. HRMS (ESI) calcd for $C_{21}H_{16}FNNaO_2S^+$ [M + Na^+] 388.0783, found 388.0782.

2-(4-Chlorophenyl)-1-tosyl-1*H*-indole (2n)



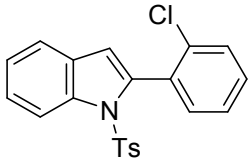
Following the general procedure, **2n** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (178 mg, 94%); m.p. 138-140 °C. R_f = 0.61 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 1H), 7.43 (dd, *J* = 8.5, 2.4 Hz, 3H), 7.40 – 7.34 (m, 3H), 7.26 (t, *J* = 8.0 Hz, 3H), 7.03 (d, *J* = 8.2 Hz, 2H), 6.53 (s, 1H), 2.27 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.7, 140.8, 138.4, 134.8, 134.6, 131.5, 130.9, 130.5, 129.3, 127.9, 126.8, 125.1, 124.5, 120.8, 116.7, 114.0, 21.5. HRMS (ESI) calcd for $C_{21}H_{16}ClNNaO_2S^+$ [M + Na^+] 404.0488, found 404.0489.

2-(3-chlorophenyl)-1-tosyl-1*H*-indole (2o)



Following the general procedure, **2o** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (152 mg, 79%); m.p. 49-50 °C. R_f = 0.52 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.32 (t, *J* = 7.6 Hz, 1H), 7.50 – 7.34 (m, 6H), 7.28 (ddd, *J* = 6.8, 5.2, 3.0 Hz, 3H), 7.07 (d, *J* = 8.1 Hz, 2H), 6.57 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.8, 140.4, 138.4, 134.6, 134.2, 133.4, 130.3, 130.0, 129.3, 128.8, 128.7, 126.8, 125.2, 124.5, 120.9, 116.6, 114.2, 21.5. HRMS (ESI) calcd for $C_{21}H_{16}ClNNaO_2S^+$ [M + Na^+] 404.0488, found 404.0488.

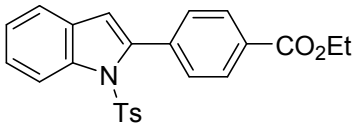
2-(2-Chlorophenyl)-1-tosyl-1*H*-indole (2p)



Following the general procedure, **2p** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A colorless oil (130 mg, 68%);. R_f = 0.48 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.4 Hz, 1H), 7.50 (dd, *J* = 13.8, 7.8 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.31 (m, 4H), 7.28 (d, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.63 (s, 1H), 2.31 (s, 3H). ^{13}C NMR (151 MHz,

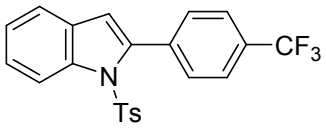
$CDCl_3$) δ 144.7, 137.4, 137.2, 135.3, 135.1, 133.0, 131.6, 130.1, 129.8, 129.43, 129.40, 127.0, 125.8, 125.0, 123.9, 121.0, 115.7, 113.8, 21.5. HRMS (ESI) calcd for $C_{21}H_{16}ClNNaO_2S^+$ [M + Na^+] 404.0488, found 404.0485.

Ethyl 4-(1-tosyl-1*H*-indol-2-yl)benzoate (2q)



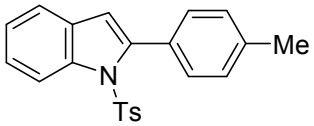
Following the general procedure, **2q** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (155 mg, 74%); m.p. 118-119 °C. R_f = 0.25 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.24 (s, 1H), 7.04 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.61 (s, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 2.28 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 144.8, 141.1, 138.6, 136.8, 134.3, 130.5, 130.4, 130.1, 129.3, 128.8, 126.8, 125.3, 124.6, 121.0, 116.8, 114.9, 61.1, 21.6, 14.4. HRMS (ESI) calcd for $C_{24}H_{21}NNaO_4S^+$ [M + Na^+] 442.1089, found 442.1088.

1-Tosyl-2-(4-(trifluoromethyl)phenyl)-1*H*-indole (2r)



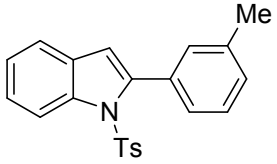
Following the general procedure, **2r** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (141 mg, 68%); m.p. 164-165 °C. R_f = 0.53 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.66 (q, *J* = 8.3 Hz, 4H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.39 (ddd, *J* = 8.5, 7.3, 1.3 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.61 (s, 1H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 140.5, 138.5, 136.1, 134.3, 130.4, 129.4, 126.7, 125.4, 124.6, 124.5(q, $^4J_{C\text{-}F}$ = 3.7 Hz), 121.0, 116.7, 115.0, 21.6. HRMS (ESI) calcd for $C_{22}H_{16}F_3NNaO_2S^+$ [M + Na^+] 438.0752, found 438.0756.

2-(*p*-Tolyl)-1-tosyl-1*H*-indole (2s)



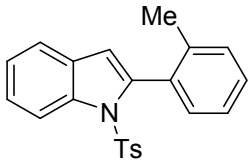
Following the general procedure, **2s** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (167 mg, 92%); m.p. 101-103 °C. R_f = 0.46 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 3H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 3H), 7.22 (s, 1H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.50 (s, 1H), 2.43 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 142.3, 138.7, 138.2, 134.6, 130.7, 130.2, 129.6, 129.2, 128.3, 126.8, 124.6, 124.3, 120.6, 116.7, 113.3, 21.6, 21.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_2S^+$ [M + Na^+] 384.1034, found 384.1038.

2-(*m*-Tolyl)-1-tosyl-1*H*-indole (2t)



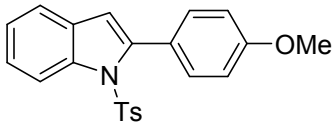
Following the general procedure, **2t** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (141 mg, 78%); m.p. 132-133 °C. R_f = 0.43 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 9.1 Hz, 1H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.38 (ddd, *J* = 9.7, 5.7, 1.5 Hz, 4H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.11 (dd, *J* = 8.0, 3.6 Hz, 3H), 6.47 (s, 1H), 2.32 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 140.3, 139.3, 137.3, 135.6, 132.1, 130.9, 130.1, 129.6, 129.4, 129.1, 126.9, 124.7, 124.6, 123.8, 120.7, 115.7, 112.3, 21.6, 20.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_2S^+$ [M + Na^+] 384.1034, found 384.1036.

2-(*o*-Tolyl)-1-tosyl-1*H*-indole (2u)



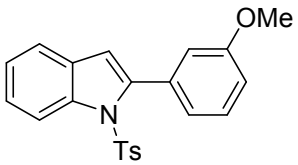
Following the general procedure, **2u** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (168 mg, 93%); m.p. 98-100 °C. R_f = 0.54 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 9.1 Hz, 1H), 7.50 (d, *J* = 7.3 Hz, 1H), 7.42 – 7.34 (m, 4H), 7.28 (t, *J* = 7.1 Hz, 2H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 3H), 6.47 (s, 1H), 2.32 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 140.3, 139.4, 137.3, 135.6, 132.1, 130.9, 130.1, 129.6, 129.4, 129.1, 126.9, 124.7, 124.6, 123.8, 120.7, 115.7, 112.3, 21.6, 20.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_2S^+$ [M + Na^+] 384.1034, found 384.1036.

2-(4-Methoxyphenyl)-1-tosyl-1*H*-indole (2v)



Following the general procedure, **2v** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (170 mg, 90%); m.p. 135-137 °C. R_f = 0.42 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.9 Hz, 1H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.25 – 7.27 (m, 3H), 7.04 (d, *J* = 8.1 Hz, 1H), 6.95 (d, *J* = 8.8 Hz, 1H), 6.48 (s, 1H), 3.89 (s, 1H), 2.28 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 144.5, 142.0, 138.2, 134.7, 131.7, 130.6, 129.2, 126.8, 124.7, 124.5, 124.3, 120.5, 116.7, 113.0, 112.9, 55.3, 21.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_3S^+$ [M + Na^+] 400.0983, found 400.0986.

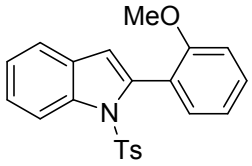
2-(3-Methoxyphenyl)-1-tosyl-1*H*-indole (2w)



Following the general procedure, **2w** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (162 mg, 86%); m.p. 108-110 °C. R_f = 0.46

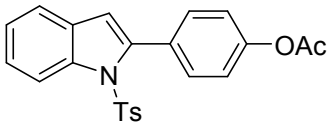
(10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.33 (m, 5H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 3H), 6.99 (dd, *J* = 8.3, 2.5 Hz, 1H), 6.56 (s, 1H), 3.86 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 144.6, 142.0, 138.3, 134.6, 133.7, 130.5, 129.2, 128.5, 126.9, 124.8, 124.3, 122.8, 120.7, 116.7, 115.9, 114.5, 113.7, 55.4, 21.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_3S^+$ [M + Na^+] 400.0983, found 400.0982.

2-(2-Methoxyphenyl)-1-tosyl-1*H*-indole (2x)



Following the general procedure, **2x** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (172 mg, 91%); m.p. 78-80 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.29 (m, 1H), 7.26 – 7.20 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 6.55 (s, 1H), 3.78 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 144.3, 138.0, 137.4, 135.8, 131.8, 130.6, 130.2, 129.3, 126.8, 124.4, 123.6, 121.9, 120.7, 119.6, 115.6, 112.4, 110.5, 55.5, 21.5. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_3S^+$ [M + Na^+] 400.0983, found 400.0981.

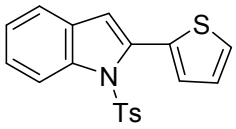
4-(1-Tosyl-1*H*-indol-2-yl)phenyl acetate (2y)



Following the general procedure, **2y** was purified by silica gel chromatography (10% EtOAc/petroleum ether). A white solid (180 mg, 89%); m.p. 97-99 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 9.0 Hz, 1H), 7.50 (d, *J* = 8.7 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.36 (ddd, *J* = 8.5, 7.3, 1.3 Hz, 1H), 7.25-7.29 (m, *3*H), 7.16 (d, *J* = 8.7 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.54 (s, 1H),

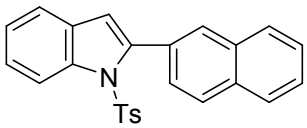
2.35 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.4, 151.0, 144.7, 141.1, 138.3, 134.6, 131.5, 130.4, 130.0, 129.3, 126.8, 124.9, 124.4, 120.8, 120.7, 116.7, 113.8, 21.6, 21.3. HRMS (ESI) calcd for $C_{23}H_{19}NnaO_4S^+$ [M + Na^+] 428.0932, found 428.0932.

2-(Thiophen-2-yl)-1-tosyl-1*H*-indole (2z)



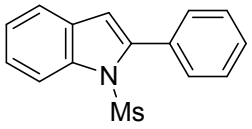
Following the general procedure, **2z** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A pale yellow solid (119 mg, 67%); m.p. 90-91 °C. R_f = 0.59 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.40 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.38 – 7.30 (m, 4H), 7.29 – 7.23 (m, 1H), 7.11 (dd, *J* = 5.1, 3.6 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.63 (s, 1H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 138.3, 134.9, 134.0, 132.4, 130.6, 129.9, 129.4, 127.1, 127.0, 126.8, 125.2, 124.3, 120.8, 116.5, 114.5, 21.6. HRMS (ESI) calcd for $C_{19}H_{15}NNaO_2S_2^+$ [M + Na^+] 376.0442, found 376.0446.

2-(Naphthalen-2-yl)-1-tosyl-1*H*-indole (2aa)



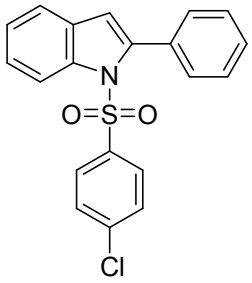
Following the general procedure, **2aa** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (191 mg, 96%); m.p. 152-153 °C. R_f = 0.52 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.3 Hz, 1H), 7.88 (t, *J* = 10.5 Hz, 4H), 7.69 (d, *J* = 8.3 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.26 (t, *J* = 14.4 Hz, 3H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.62 (s, 1H), 2.25 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.2, 138.5, 134.7, 134.7, 133.3, 132.7, 130.7, 130.2, 129.2, 128.8, 128.6, 128.2, 127.9, 126.9, 126.8, 126.6, 126.4, 124.9, 124.4, 120.8, 116.7, 114.2, 21.5. HRMS (ESI) calcd for $C_{25}H_{19}NNaO_2S^+$ [M + Na^+] 420.1034, found 420.1036.

1-(Methylsulfonyl)-2-phenyl-1*H*-indole (2ab)



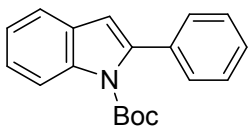
Following the general procedure, **2ab** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (126 mg, 92%); m.p. 120-122 °C. R_f = 0.38 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.1 Hz, 1H), 7.59 (d, *J* = 7.3 Hz, 1H), 7.57 – 7.54 (m, 2H), 7.45 – 7.40 (m, 3H), 7.40 – 7.32 (m, 2H), 6.70 (s, 1H), 2.72 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.0, 138.0, 132.0, 130.3, 130.2, 128.9, 127.8, 125.2, 124.6, 121.1, 115.9, 113.1, 39.5. HRMS (ESI) calcd for $C_{21}H_{17}NNaO_2S^+$ [M + Na^+] 370.0878, found 370.0882.

1-((4-Chlorophenyl)sulfonyl)-2-phenyl-1*H*-indole (2ac)



Following the general procedure, **2ac** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (177 mg, 96%); m.p. 186-188 °C. R_f = 0.59 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.4 Hz, 1H), 7.53 – 7.39 (m, 6H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 8.7 Hz, 3H), 7.18 (d, *J* = 8.6 Hz, 2H), 6.55 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.1, 140.2, 138.3, 135.9, 132.1, 130.7, 130.3, 128.9, 128.9, 128.2, 127.7, 125.1, 124.7, 121.0, 116.7, 114.2. HRMS (ESI) calcd for $C_{20}H_{14}ClNNaO_2S^+$ [M + Na^+] 390.0331, found 390.0336.

***tert*-butyl 2-phenyl-1*H*-indole-1-carboxylate (2ad)**



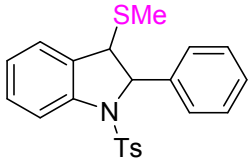
Following the general procedure, **2ad** was purified by silica gel chromatography (2% EtOAc/petroleum ether). A colorless oil (104 mg, 71%). R_f = 0.69 (5% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.9 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.36 – 7.23 (m, 6H), 7.17 (dd, *J* = 7.5, 0.9 Hz, 1H), 6.49 (s, 1H), 1.23 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2, 140.5, 137.5, 135.0, 129.2, 128.7, 127.8, 127.6, 124.3, 122.9, 120.5, 115.2, 109.9, 83.4, 27.6. HRMS (ESI) calcd for $C_{19}H_{19}NNaO_2^+$ [M + Na^+] 316.1308, found 316.1306.

5. The Procedure for the Synthesis of Indoline 2a':

To a solution of substrate **1** (0.5 mmol) in DMSO (1 mL) was slowly added $SOCl_2$ (1.0 mmol, 119 mg) at 25 °C. The reaction mixture was kept stirring at 25 °C until TLC indicated the total consumption of substrate **1**. Then the reaction mixture was quenched with saturated aq. $NaHCO_3$ solution (5 mL) and water (20 mL), extracted with EtOAc (3×20 mL), combined the organic phase then evaporated the solvent, purified by flash column chromatography (5% EtOAc/petroleum ether) to afford the desired compound **2a** (125 mg, 72%) and compound **2a'** (40 mg, 20%).

6. Spectroscopic data of Indoline 2a':

3-(Methylthio)-2-phenyl-1-tosylindoline (2a')



Following the procedure, **2a'** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid; mp: 146-147 °C. R_f = 0.42 (10% EtOAc/petroleum ether);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.25 (m, 6H), 7.18 (d, *J* = 8.1 Hz, 3H), 7.06 (td, *J* = 7.5, 0.8 Hz, 1H), 5.20 (d, *J* = 3.1 Hz, 1H), 4.06 (d, *J* = 3.0 Hz, 1H), 2.34 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2, 142.1, 141.7, 135.1, 129.6, 129.5, 129.4, 128.9, 128.0, 127.5, 126.0, 125.7, 124.4, 115.0, 72.8, 54.6, 21.6, 12.6. HRMS (ESI)

calcd for $C_{22}H_{21}NNaO_2S_2^+$ [M + Na^+] 418.0911, found 418.0916.

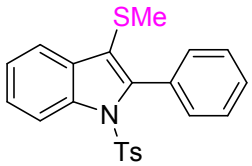
7. General Procedure for the Synthesis of 3-Methylthioindole Derivatives 3 (3a-l):

Method A: To a solution of substrate **1** (0.5 mmol) in DMSO (1 mL) was slowly added $SOCl_2$ (2.0 mmol, 239 mg) at 25 °C. The mixture was kept stirring at 70 °C until TLC indicated the total consumption of substrate **1**. Then the reaction mixture was quenched with saturated aq. $NaHCO_3$ solution (5 mL) and water (20 mL), extracted with EtOAc (3 x 20 mL), combined the organic phase then evaporated the solvent, purified by flash column chromatography (3% EtOAc/petroleum ether) to afford the desired 3-methylthioindole derivatives **3**.

Method B: To a solution of substrate **1** (0.5 mmol) in DMSO (1 mL) was slowly added $SOCl_2$ (1.75 mmol, 209 mg) at 25 °C. The mixture was kept stirring at 70 °C until TLC indicated the total consumption of substrate **1**. Then the reaction mixture was quenched with saturated aq. $NaHCO_3$ solution (5 mL) and water (20 mL), extracted with EtOAc (3×20 mL), combined the organic phase then evaporated the solvent, purified by flash column chromatography (3% EtOAc/petroleum ether) to afford the desired 3-methylthioindole derivatives **3**.

8. Spectroscopic Data of 3-Methylthioindoles Derivatives 3 (3a-l):

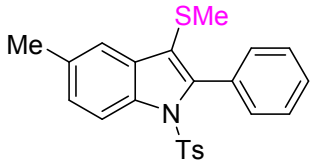
3-(Methylthio)-2-phenyl-1-tosyl-1*H*-indole (3a)



Following the general procedure **Method A**, **3a** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (109 mg, 55%); mp: 104-105 °C. R_f = 0.45 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.3 Hz, 1H), 7.70 (dd, *J* = 7.7, 0.7 Hz, 1H), 7.51 – 7.41 (m, 4H), 7.41 – 7.35 (m, 3H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 2.31 (s, 3H), 2.07 (s,

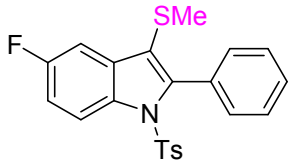
3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 142.7, 137.0, 135.2, 131.8, 131.2, 130.7, 129.4, 129.1, 127.2, 126.9, 125.5, 124.3, 119.9, 117.4, 116.2, 21.6, 18.3. HRMS (ESI) calcd for $C_{22}H_{19}NNaO_2S_2^+$ [M + Na^+] 416.0749, found 416.0748.

5-Methyl-3-(methylthio)-2-phenyl-1-tosyl-1*H*-indole (3b)



Following the general procedure **Method B**, **3b** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (153 mg, 75%); mp: 119-121°C. R_f = 0.62 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.5 Hz, 1H), 7.48 (dd, *J* = 11.7, 4.1 Hz, 4H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.31 (dd, *J* = 14.4, 7.6 Hz, 3H), 7.07 (d, *J* = 8.2 Hz, 2H), 2.50 (s, 3H), 2.31 (s, 3H), 2.08 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 142.9, 135.3, 135.1, 134.2, 131.8, 131.5, 130.8, 129.4, 129.0, 127.2, 126.9, 126.9, 119.8, 117.3, 116.0, 21.6, 21.4, 18.4. HRMS (ESI) calcd for $C_{23}H_{21}NNaO_2S_2^+$ [M + Na^+] 430.0906, found 430.0906.

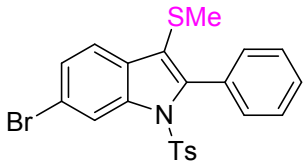
5-Fluoro-3-(methylthio)-2-phenyl-1-tosyl-1*H*-indole (3c)



Following the general procedure **Method A**, **3c** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (105 mg, 51%); mp: 120-121 °C. R_f = 0.45 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 9.1, 4.4 Hz, 1H), 7.47 (ddd, *J* = 15.8, 7.7, 2.1 Hz, 3H), 7.39 – 7.35 (m, 2H), 7.33 (dd, *J* = 8.4, 2.5 Hz, 1H), 7.28 (s, 1H), 7.26 (s, 1H), 7.14 (td, *J* = 9.0, 2.6 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 2.33 (s, 3H), 2.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3(d, $^1J_{C\text{-}F}$ = 240.7 Hz), 145.1, 144.6, 134.9, 133.2, 132.7(d, $^3J_{C\text{-}F}$ = 10.0 Hz), 131.7, 130.3, 129.5, 129.3, 127.3, 126.9, 117.6(d, $^3J_{C\text{-}F}$ = 9.0 Hz), 117.2(d, $^4J_{C\text{-}F}$ = 3.8 Hz), 113.4(d, $^2J_{C\text{-}F}$ = 25.0 Hz), 105.5(d, $^2J_{C\text{-}F}$ = 24.3 Hz), 21.6, 18.2. HRMS (ESI)

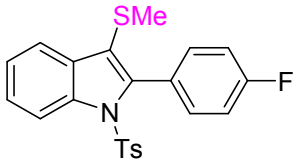
calcd for $C_{22}H_{18}FNNaO_2S_2^+$ [M + Na^+] 434.0655, found 434.0656.

6-Bromo-3-(methylthio)-2-phenyl-1-tosyl-1*H*-indole (3d)



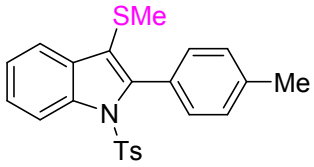
Following the general procedure **Method A**, **3d** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (125 mg, 53%); mp: 138-139 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 1.4 Hz, 1H), 7.57 – 7.40 (m, 5H), 7.32 (d, *J* = 6.9 Hz, 2H), 7.28 (s, 1H), 7.25 (s, 1H), 7.10 (d, *J* = 8.2 Hz, 2H), 2.33 (s, 3H), 2.03 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 143.2, 137.6, 135.0, 131.8, 130.1, 130.0, 129.6, 129.3, 127.6, 127.3, 127.0, 121.0, 119.1, 117.0, 21.6, 18.4. HRMS (ESI) calcd for $C_{22}H_{18}BrNNaO_2S_2^+$ [M + Na^+] 493.9855, found 493.9856.

2-(4-Fluorophenyl)-3-(methylthio)-1-tosyl-1*H*-indole (3e)



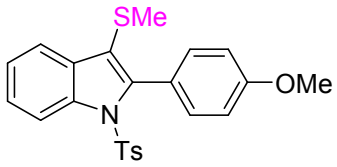
Following the general procedure **Method A**, **3e** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (64 mg, 31%); mp: 123-125 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.3 Hz, 1H), 7.69 (dd, *J* = 7.7, 0.7 Hz, 1H), 7.44 (ddd, *J* = 8.4, 7.3, 1.4 Hz, 1H), 7.40 – 7.32 (m, 3H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.19 – 7.11 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 2.32 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2(d, $^1J_{C\text{-}F}$ = 247.8 Hz), 145.0, 141.6, 137.0, 135.1, 133.6(d, $^3J_{C\text{-}F}$ = 8.4 Hz), 131.0, 129.5, 126.8, 126.5(d, $^4J_{C\text{-}F}$ = 3.4 Hz), 125.7, 124.4, 119.9, 117.7, 116.2, 114.5(d, $^2J_{C\text{-}F}$ = 21.6 Hz), 21.6, 18.3. HRMS (ESI) calcd for $C_{22}H_{18}FNNaO_2S_2^+$ [M + Na^+] 434.0655, found 434.0656.

3-(Methylthio)-2-(*p*-tolyl)-1-tosyl-1*H*-indole (3f)



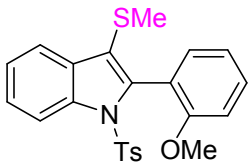
Following the general procedure **Method A**, **3f** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (143 mg, 70%); mp: 131-133 °C. R_f = 0.45 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.2 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.45 – 7.34 (m, 2H), 7.32 – 7.26 (m, 6H), 7.07 (d, *J* = 8.1 Hz, 2H), 2.47 (s, 3H), 2.31 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 143.0, 139.1, 137.0, 135.1, 131.6, 131.2, 129.4, 128.0, 127.7, 126.9, 125.4, 124.3, 119.8, 117.2, 116.2, 21.6, 21.6, 18.3. HRMS (ESI) calcd for $C_{23}H_{21}NNaO_2S_2^+$ [M + Na^+] 430.0911, found 430.0913.

2-(4-Methoxyphenyl)-3-(methylthio)-1-tosyl-1*H*-indole (3g)



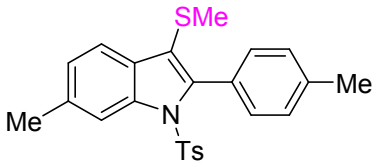
Following the general procedure **Method B**, **3g** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (173 mg, 82%); mp: 147-148 °C. R_f = 0.45 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.2 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.45 – 7.34 (m, 2H), 7.32 – 7.26 (m, 4H), 7.06 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 4H), 2.31 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 144.8, 142.7, 137.0, 135.2, 133.1, 131.1, 129.3, 126.9, 125.3, 124.3, 122.7, 119.7, 117.0, 116.3, 112.7, 55.3, 21.6, 18.3. HRMS (ESI) calcd for $C_{23}H_{21}NNaO_3S_2^+$ [M + Na^+] 446.0861, found 446.0861.

2-(2-Methoxyphenyl)-3-(methylthio)-1-tosyl-1*H*-indole (3h)



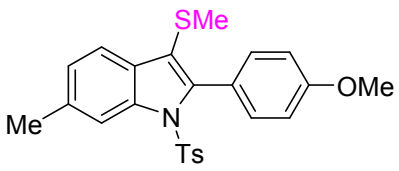
Following the general procedure **Method B**, **3h** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (163 mg, 77%); mp: 154-156 °C. R_f = 0.42 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.70 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.48 (ddd, *J* = 8.3, 7.5, 1.8 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.34 (td, *J* = 7.5, 1.1 Hz, 1H), 7.14 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.04 (td, *J* = 7.4, 1.0 Hz, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 3.69 (s, 3H), 2.32 (s, 3H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 144.5, 139.4, 136.7, 135.9, 133.0, 131.0, 130.9, 129.3, 127.0, 125.1, 123.7, 120.1, 119.7, 119.5, 116.6, 115.4, 110.5, 55.3, 21.6, 18.3. HRMS (ESI) calcd for $C_{23}H_{21}NNaO_3S_2^+$ [M + Na^+] 446.0861, found 446.0862.

6-Methyl-3-(methylthio)-2-(*p*-tolyl)-1-tosyl-1*H*-indole (3i)



Following the general procedure **Method A**, **3i** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (131 mg, 62%); mp: 163-164 °C. R_f = 0.55 (10% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 5.5 Hz, 4H), 7.19 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 8.1 Hz, 2H), 2.57 (s, 3H), 2.47 (s, 3H), 2.33 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 142.2, 138.9, 137.4, 135.6, 135.3, 131.6, 129.3, 129.0, 128.0, 127.8, 126.9, 125.7, 119.4, 117.1, 116.4, 22.1, 21.6, 21.6, 18.3. HRMS (ESI) calcd for $C_{24}H_{23}NNaO_2S_2^+$ [M + Na^+] 444.1062, found 444.1063.

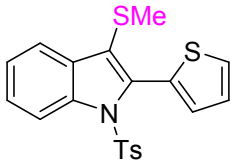
2-(4-Methoxyphenyl)-6-methyl-3-(methylthio)-1-tosyl-1*H*-indole (3j)



Following the general procedure **Method B**, **3j** was purified by silica gel

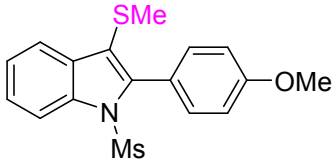
chromatography (3% EtOAc/petroleum ether). A white solid (138 mg, 63%); mp: 131-133 °C. R_f = 0.50 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.24 (m, 5H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 3H), 2.55 (s, 3H), 2.31 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 144.7, 142.0, 137.4, 135.5, 135.3, 133.1, 129.3, 129.1, 126.8, 125.7, 122.9, 119.3, 117.0, 116.4, 112.7, 55.3, 22.1, 21.6, 18.3. HRMS (ESI) calcd for $C_{24}H_{23}NNaO_3S_2^+$ [M + Na^+] 460.1012, found 460.1013.

3-(Methylthio)-2-(thiophen-2-yl)-1-tosyl-1*H*-indole (3k)



Following the general procedure **Method A**, **3k** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (130 mg, 65%); mp: 80-81 °C. R_f = 0.40 (20% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.54 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.43 (ddd, *J* = 8.5, 7.3, 1.3 Hz, 1H), 7.39 – 7.32 (m, 3H), 7.16 (ddd, *J* = 8.6, 4.8, 3.5 Hz, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 2.32 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.8, 137.3, 135.3, 135.0, 132.2, 130.8, 130.2, 129.4, 128.6, 126.9, 126.4, 125.9, 124.3, 119.9, 119.7, 116.1, 21.6, 18.6. HRMS (ESI) calcd for $C_{20}H_{17}NNaO_2S_3^+$ [M + Na^+] 422.0314, found 422.0316.

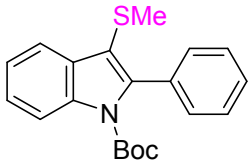
2-(4-Methoxyphenyl)-1-(methylsulfonyl)-3-(methylthio)-1*H*-indole (3l)



Following the general procedure **Method B**, **3l** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (127 mg, 73%); mp: 123-125 °C. R_f = 0.45 (20% EtOAc/petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ

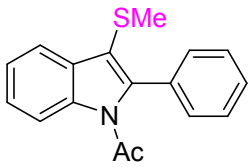
8.20 – 8.09 (m, 1H), 7.81 – 7.75 (m, 1H), 7.47 – 7.39 (m, 4H), 7.06 – 6.96 (m, 2H), 3.88 (s, 3H), 2.80 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 142.5, 136.7, 132.8, 131.1, 125.6, 124.5, 122.4, 120.0, 116.9, 115.6, 113.1, 55.3, 40.6, 18.4. HRMS (ESI) calcd for $C_{17}H_{17}NNaO_3S_2^+$ [M + Na^+] 370.0542, found 370.0543.

tert-butyl 3-(methylthio)-2-phenyl-1*H*-indole-1-carboxylate (3m)



Following the general procedure **Method A**, **3m** was purified by silica gel chromatography (2% EtOAc/petroleum ether). A colorless oil (102 mg, 60%). R_f = 0.59 (5% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (d, J = 8.2 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.46 – 7.39 (m, 6H), 7.35 (dd, J = 8.6, 5.4 Hz, 1H), 2.18 (s, 3H), 1.24 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 142.1, 136.6, 133.7, 130.3, 130.0, 128.0, 127.7, 125.0, 123.2, 119.5, 115.3, 114.2, 83.6, 27.5, 18.8. HRMS (ESI) calcd for $C_{20}H_{21}NNaO_2S^+$ [M + Na^+] 362.1185, found 362.1188.

1-(3-(methylthio)-2-phenyl-1*H*-indol-1-yl)ethan-1-one (3n)



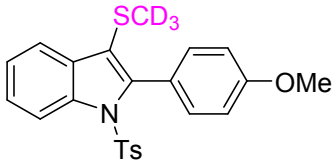
Following the general procedure **Method A**, **3n** was purified by silica gel chromatography (5% EtOAc/petroleum ether). A white solid (101 mg, 72%); m.p. 135-137 °C. R_f = 0.52 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, J = 7.9 Hz, 1H), 7.78 (d, J = 7.3 Hz, 1H), 7.54 – 7.50 (m, 3H), 7.47 (dd, J = 7.7, 1.7 Hz, 2H), 7.40 (dtd, J = 20.3, 7.3, 1.1 Hz, 2H), 2.19 (s, 3H), 1.97 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.1, 141.2, 136.8, 132.7, 130.5, 130.0, 129.2, 128.6, 125.9, 124.0, 119.5, 116.3, 115.9, 27.7, 18.7. HRMS (ESI) calcd for $C_{17}H_{15}NNaOS^+$ [M + Na^+] 304.0767, found 304.0765.

9. General Procedure for the Synthesis of 3-(d_3-Methylthio) Indole Derivative 3':

To a solution of substrate **1** (0.5 mmol) in DMSO (1 mL) was slowly added $SOCl_2$ (1.75 mmol, 209 mg) at 25 °C. The mixture was kept stirring at 70 °C until TLC indicated the total consumption of substrate **1v**. Then the reaction mixture was quenched with saturated aq. $NaHCO_3$ solution (5 mL) and water (20 mL), extracted with EtOAc (3 x 20 mL), combined the organic phase then evaporated the solvent, purified by flash column chromatography (3% EtOAc/petroleum ether) to afford the desired compound **3'** (165 mg, 78%).

10. Spectroscopic Data of 3-(d_3-Methylthio) Indole Derivative 3':

2-(4-Methoxyphenyl)-3-(d_3-methylthio)-1-tosyl-1*H*-indole (3')



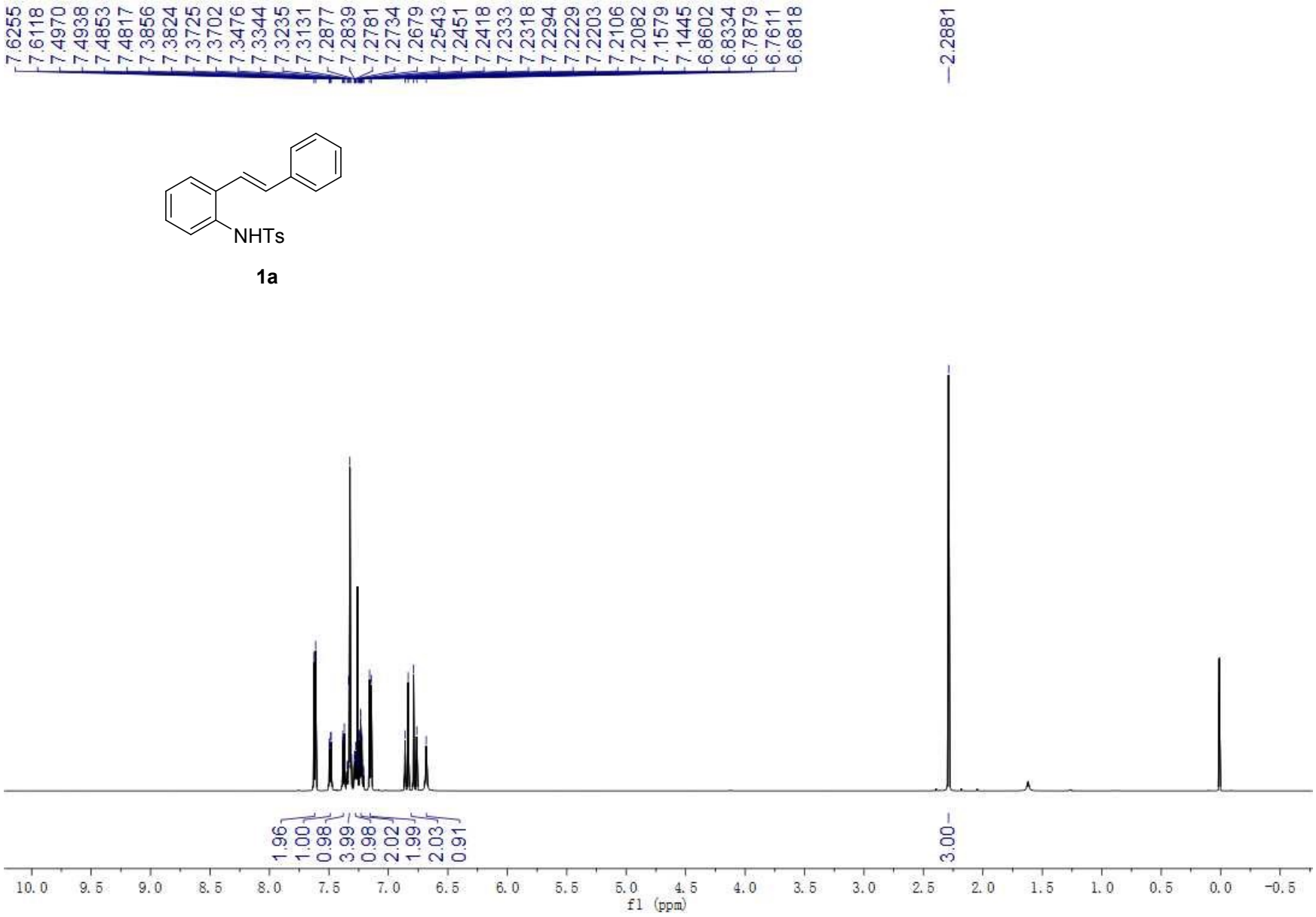
Following the procedure, **3'** was purified by silica gel chromatography (3% EtOAc/petroleum ether). A white solid (165 mg, 78%); mp: 146-147 °C. R_f = 0.50 (10% EtOAc/petroleum ether); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.3 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.35 (td, *J* = 7.7, 0.8 Hz, 1H), 7.28 (dd, *J* = 11.6, 8.6 Hz, 4H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.97 (d, *J* = 8.7 Hz, 2H), 3.89 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.2, 144.7, 142.7, 137.0, 135.3, 133.1, 131.3, 129.3, 126.9, 125.3, 124.2, 122.7, 119.7, 116.9, 116.3, 112.7, 55.3, 21.5. HRMS (ESI) calcd for $C_{23}H_{18}D_3NNaO_3S_2^+$ [M + Na^+] 446.0855, found 446.0856.

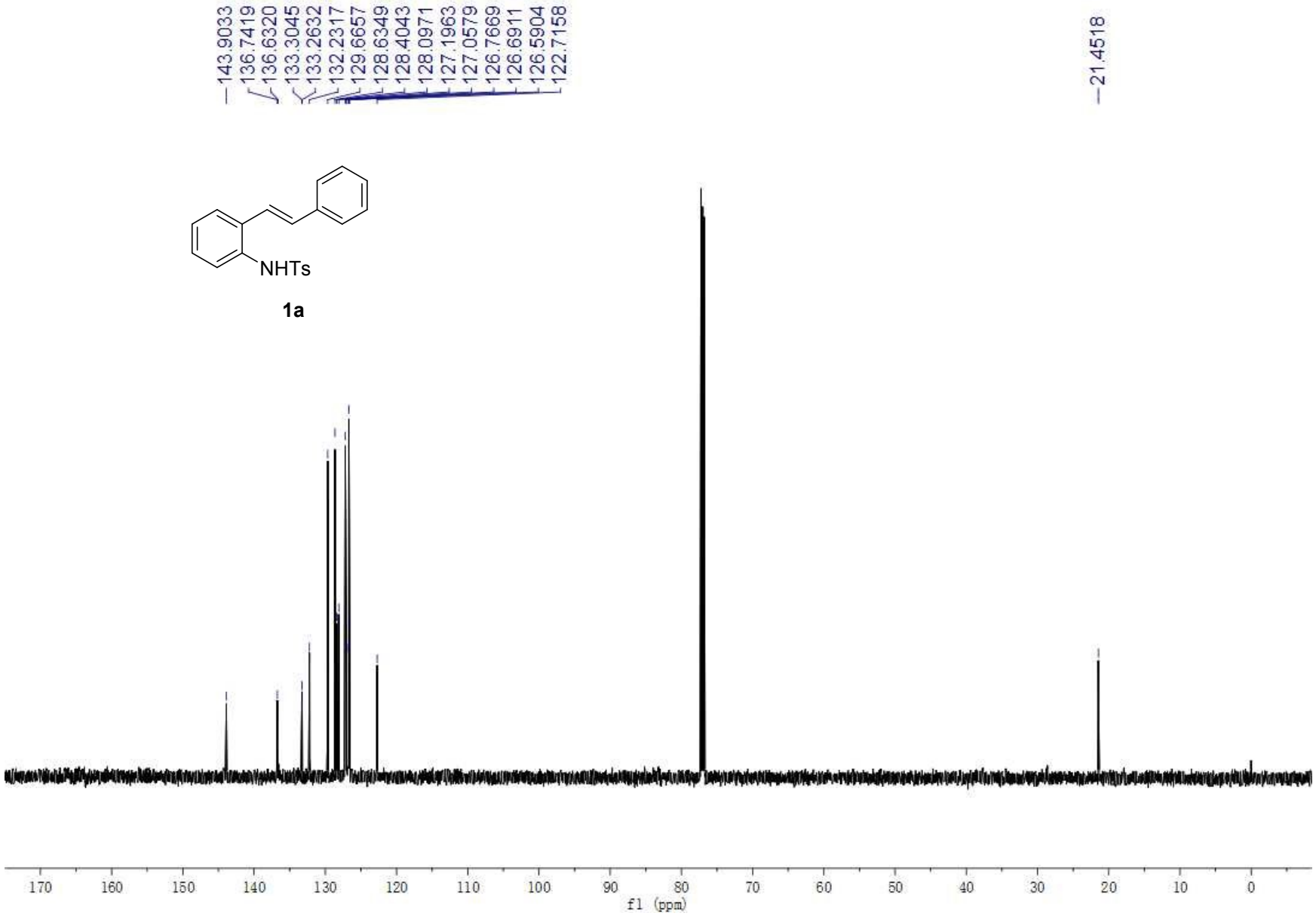
IV. References:

(1) (a) Y. H. Jang and S. W. Youn, *Org. Lett.*, 2014, **16**, 3720-3723; (b) Y. L. Li, J. Li, A. L. Ma, Y. N. Huang and J. Deng, *J. Org. Chem.*, 2015, **80**, 3841-3851; (c) S. Ortgies and A. Breder, *Org. Lett.*, 2015, **17**, 2748-2751.

(2) J. F. Zou, W. S. Huang, L. Li, Z. Xu, Z. J. Zheng, K. F. Yang and L. W. Xu, *RSC Adv.*, 2015, **5**, 30389-30393.

V. ^{1}H and ^{13}C NMR Spectra of Compounds 1a-af, 2a-ac, 2a', 3a-l and 3':

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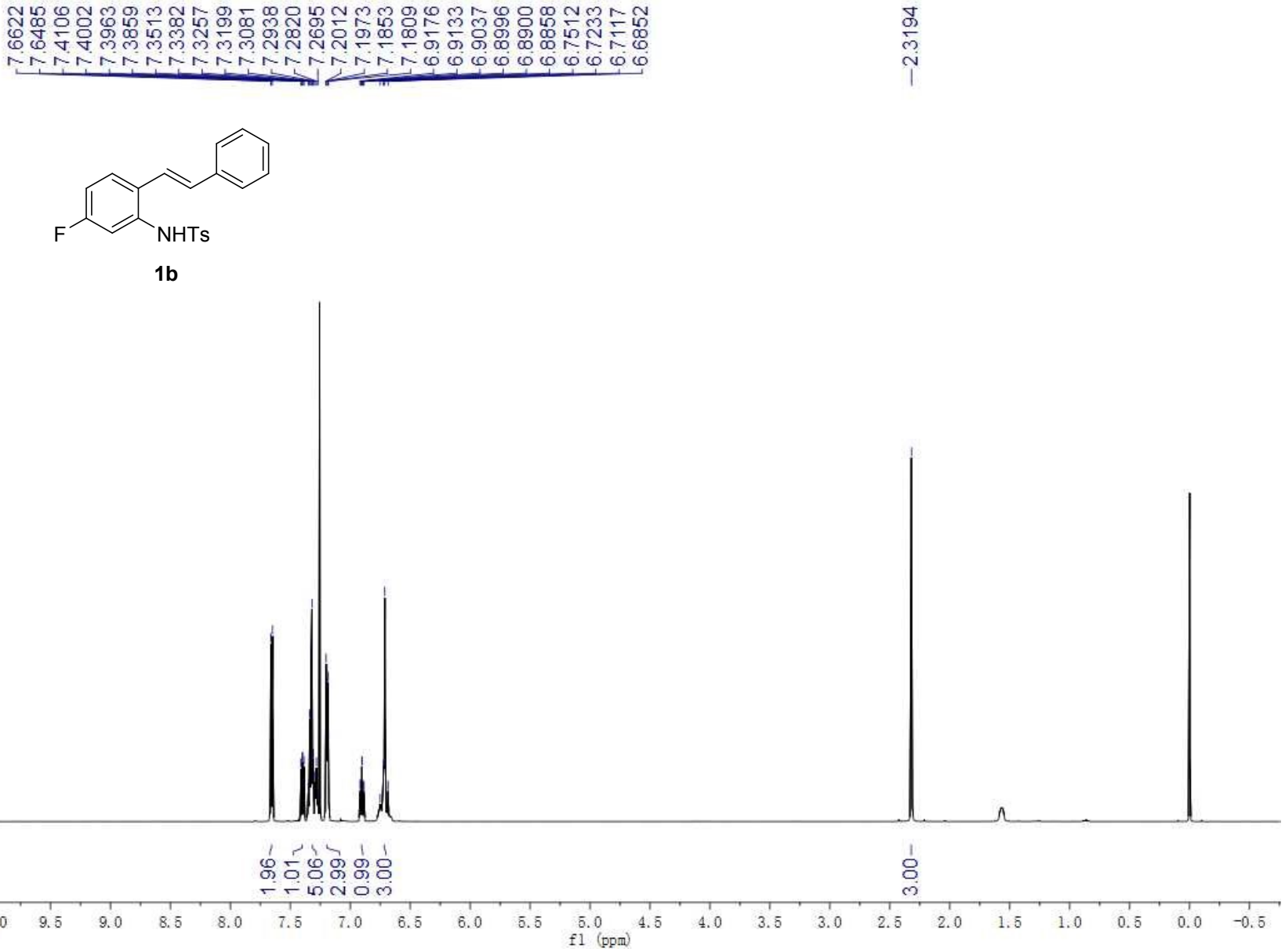
133.3045
133.2632
132.2317
129.6657
128.6349
128.4043
128.0971
127.1963
127.0579
126.7669
126.6911
126.5904
122.7158
21.4518
NHTs
1a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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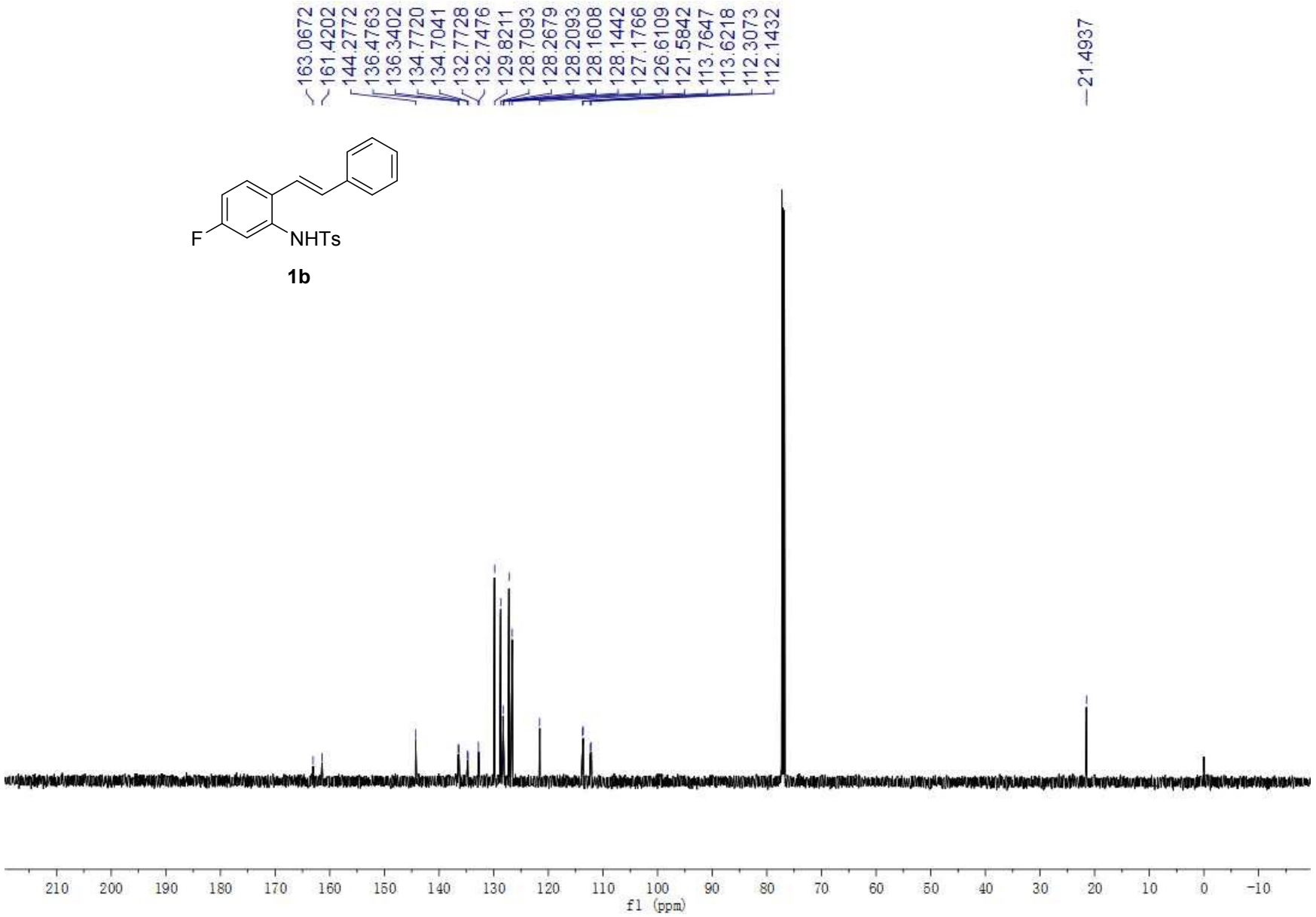
7.3081
7.2938
7.2820
7.2695
7.2012
7.1973
7.1853
7.1809
6.9176
6.9133
6.9037
6.8996
6.8900
6.8858
6.7512
6.7233
6.7117
6.6852
2.3194
F
NHTs
1b
1.96
1.01
5.06
2.99
0.99
3.00
3.00
f1 (ppm)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128.7093
128.2679
128.2093
128.1608
128.1442
127.1766
126.6109
121.5842
113.7647
113.6218
112.3073
112.1432
21.4937
F
NHTs
1b
210
200
190
180
170
160
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140
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120
110
100
90
80
70
60
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40
30
20
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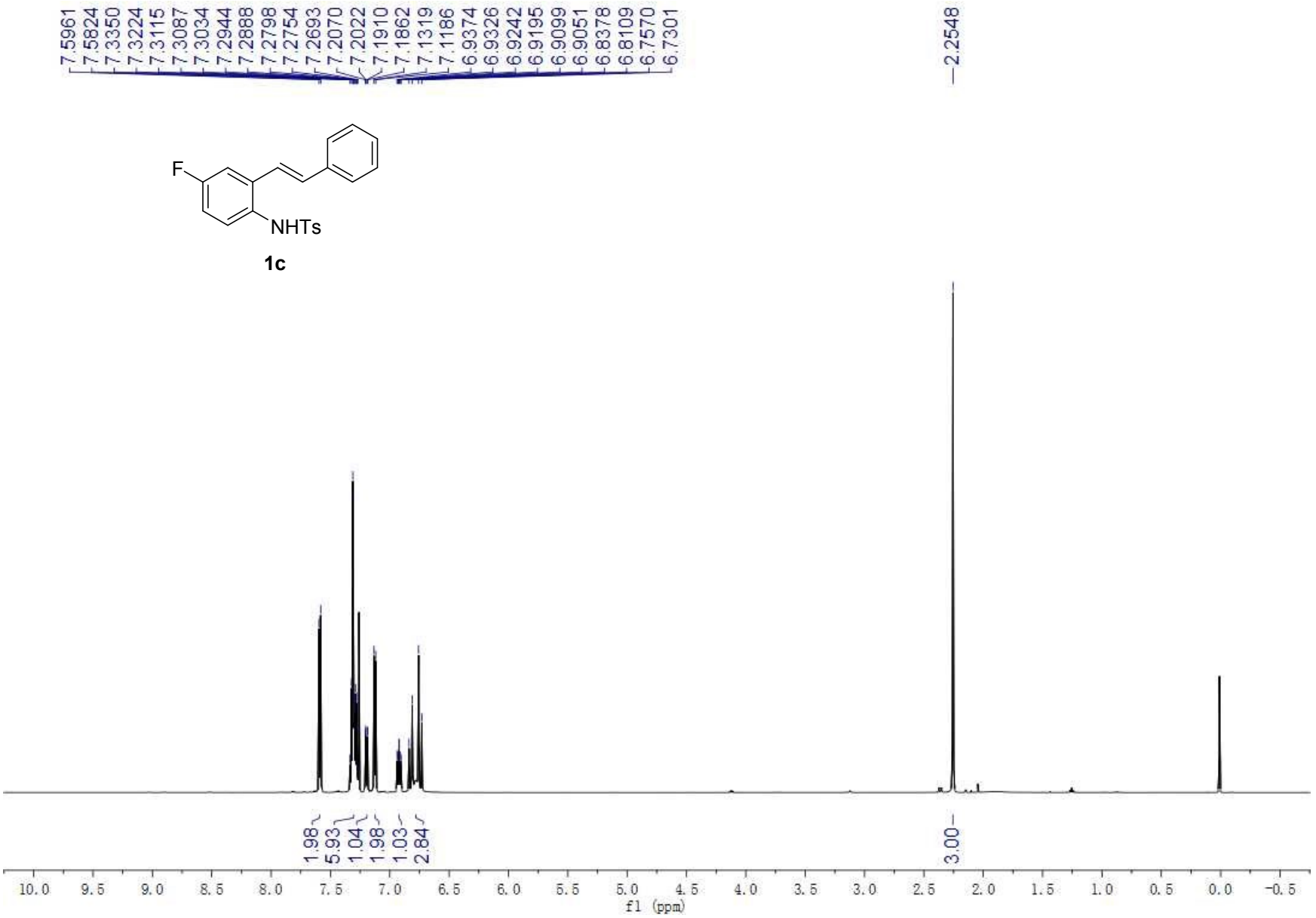
0
-10
f1 (ppm)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7.3115
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7.2754
7.2693
7.2070
7.2022
7.1910
7.1862
7.1319
7.1186
6.9374
6.9326
6.9242
6.9195
6.9099
6.9051
6.8378
6.8109
6.7570
6.7301
2.2548
F
NHTs
1c
1.98
5.93
1.04
1.98
1.03
2.84
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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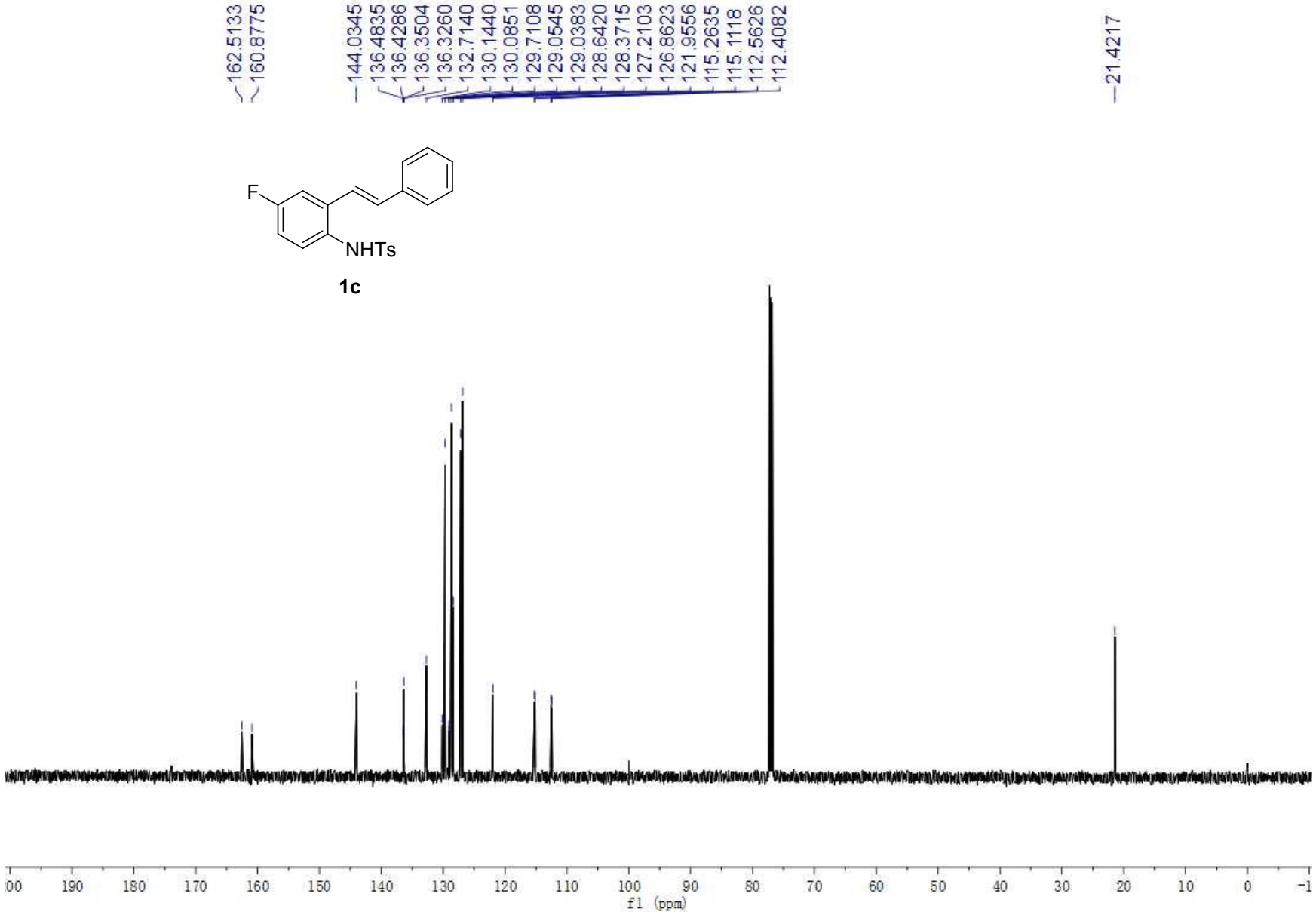
f1 (ppm)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144.0345
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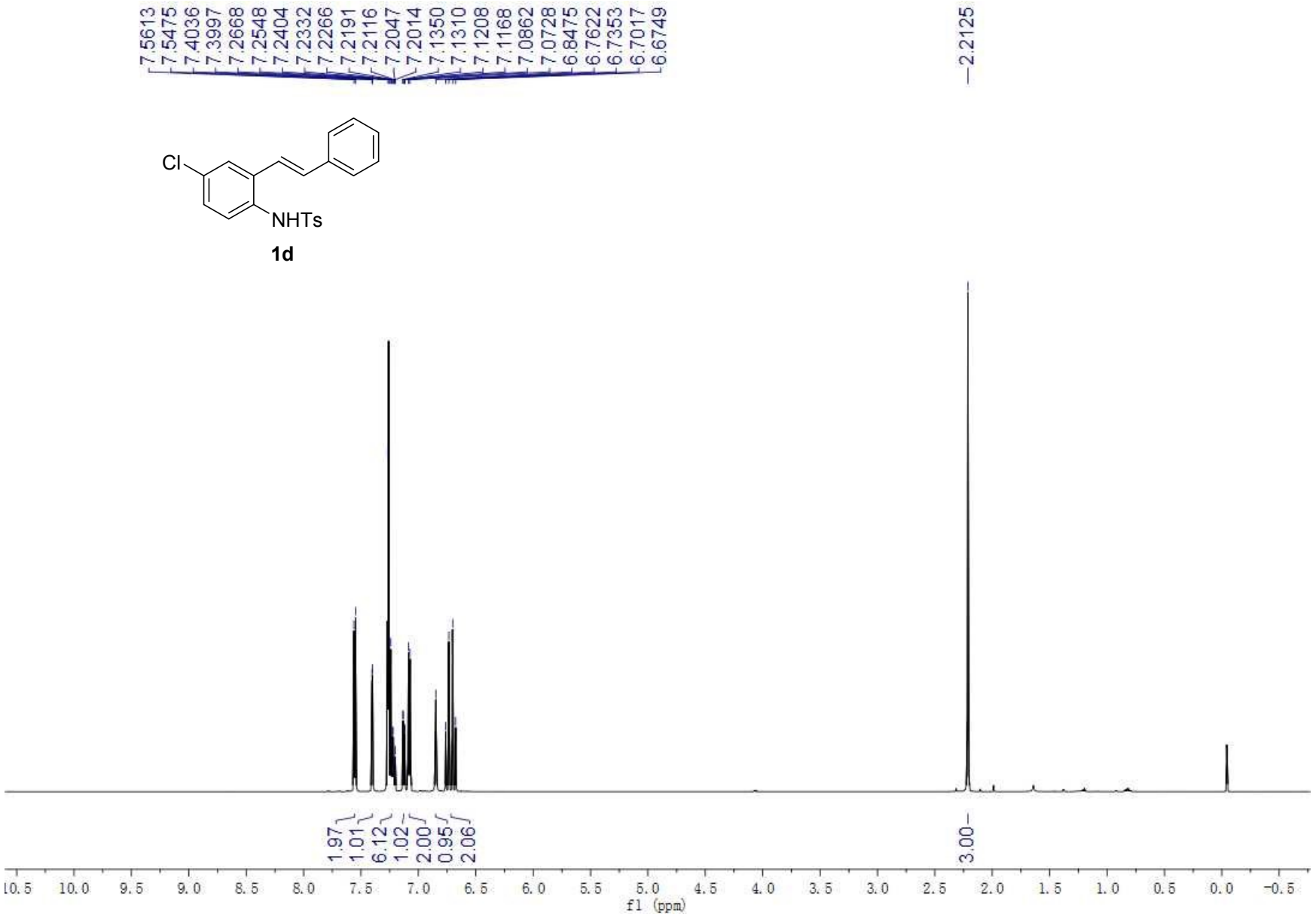
129.7108
129.0545
129.0383
128.6420
128.3715
127.2103
126.8623
121.9556
115.2635
115.1118
112.5626
112.4082
21.4217
F
NHTs
1c
f1 (ppm)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7.2116
7.2047
7.2014
7.1350
7.1310
7.1208
7.1168
7.0862
7.0728
6.8475
6.7622
6.7353
6.7017
6.6749
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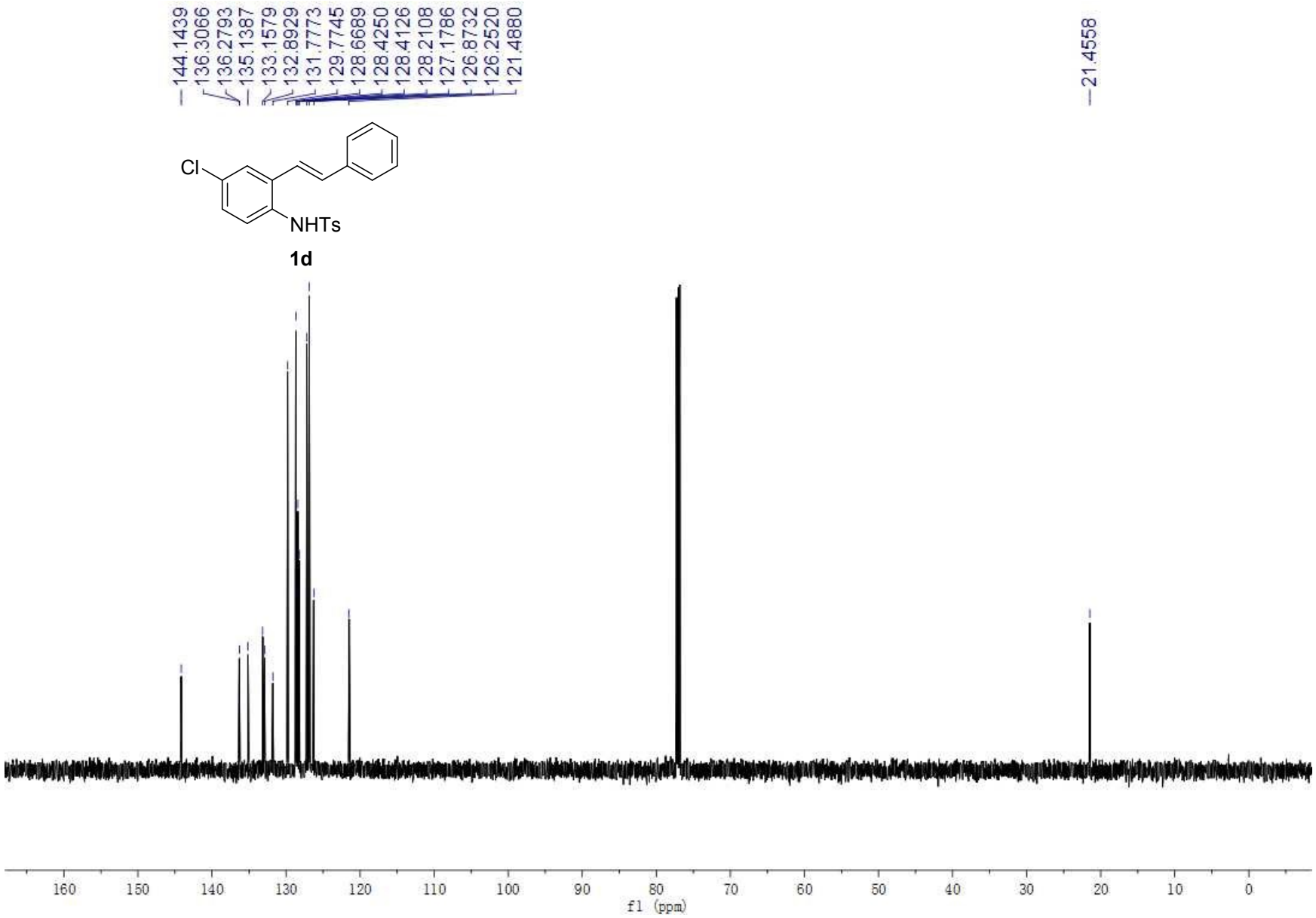
f1 (ppm)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128.2108
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126.8732
126.2520
121.4880
21.4558
Cl
NHTs
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130
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110
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90
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70
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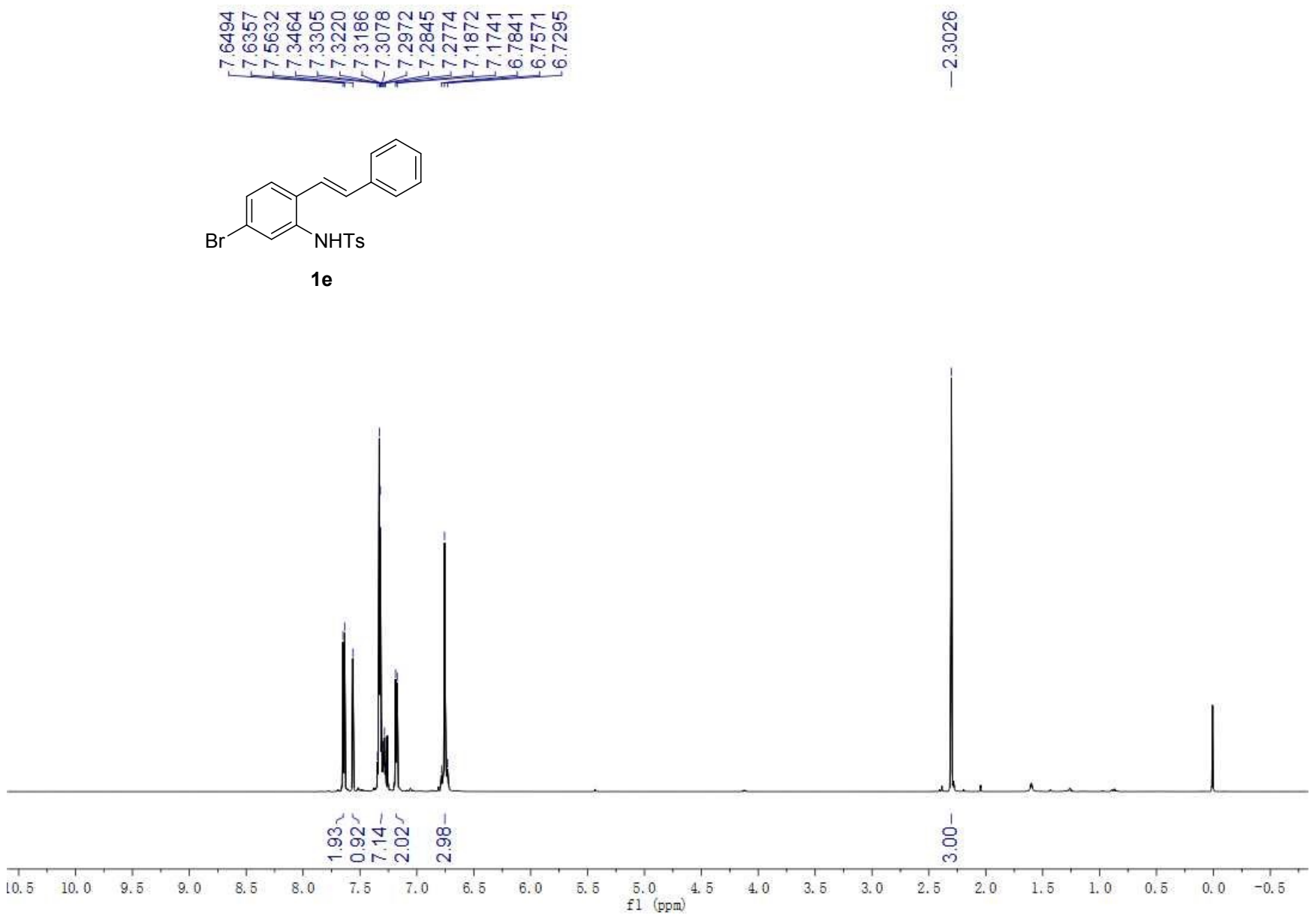
50
40
30
20
10
0
f1 (ppm)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7.1872
7.1741
6.7841
6.7571
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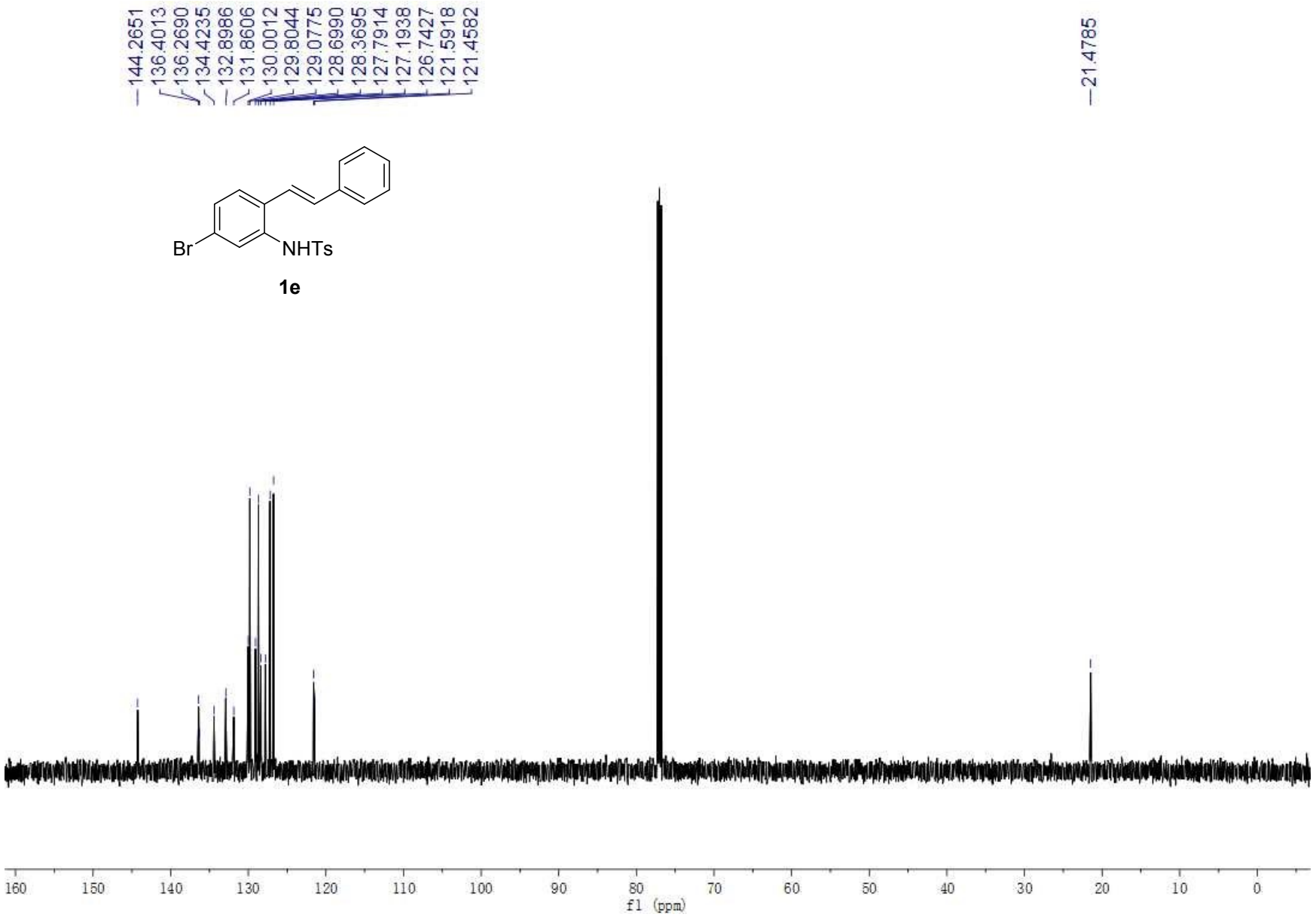
2.98
3.00
f1 (ppm)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127.1938
126.7427
121.5918
121.4582
21.4785
Br
NHTs
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90
80
70
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50
40
30
20
10
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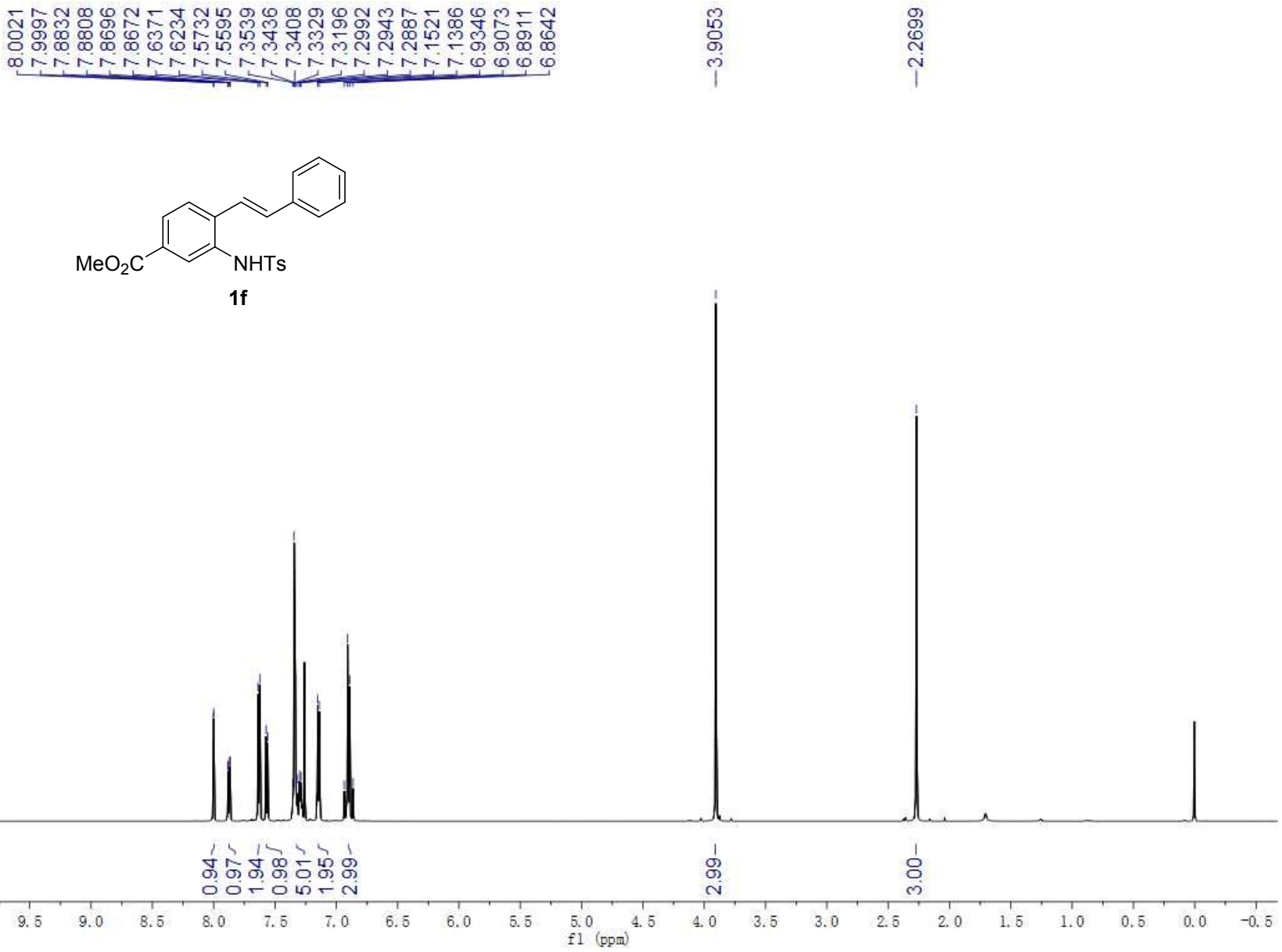
f1 (ppm)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7.2887
7.1521
7.1386
6.9346
6.9073
6.8911
6.8642
3.9053
2.2699
MeO2C
NHTs
1f
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0.97
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0.98
5.01
1.95
2.99
2.99
3.00
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9.0
8.5
8.0
7.5
7.0
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6.0
5.5
5.0
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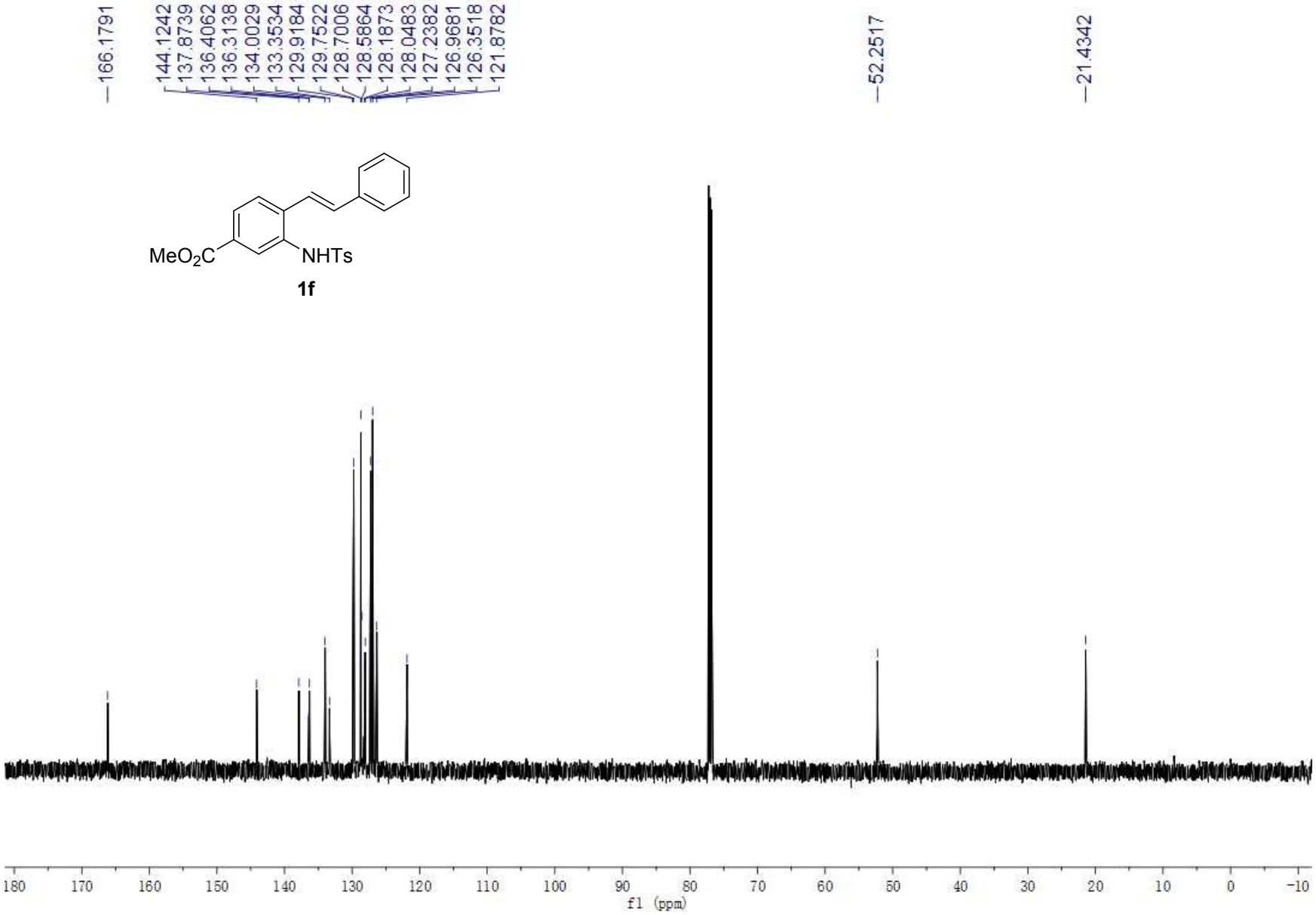
f1 (ppm)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126.3518
121.8782
52.2517
21.4342
MeO2C
NHTs
1f
180
170
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120
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100
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80
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60
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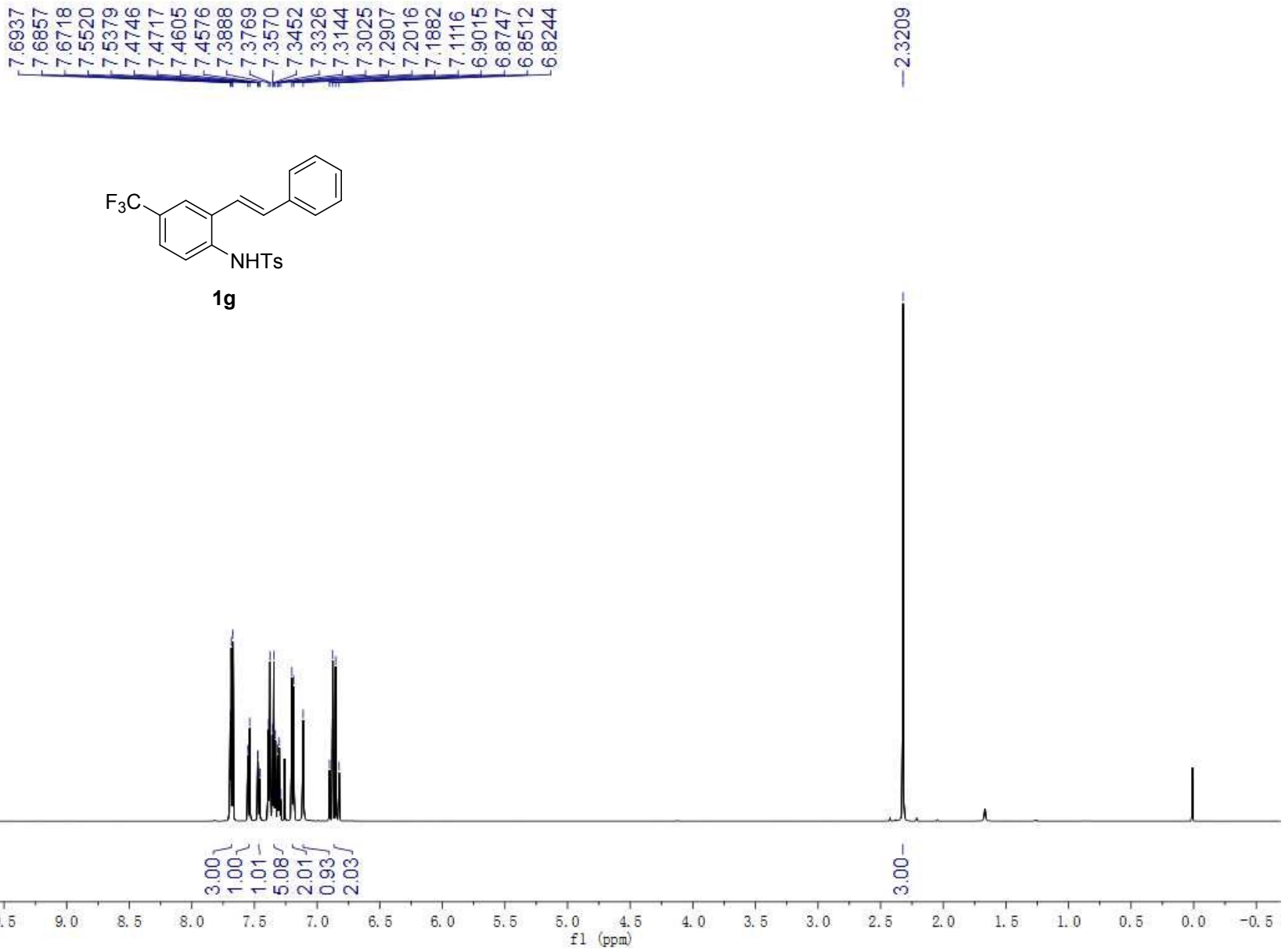
40
30
20
10
0
-10
f1 (ppm)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7.1116
6.9015
6.8747
6.8512
6.8244
2.3209
F3C
NHTs
1g
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1.00
1.01
5.08
2.01
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2.03
3.00
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
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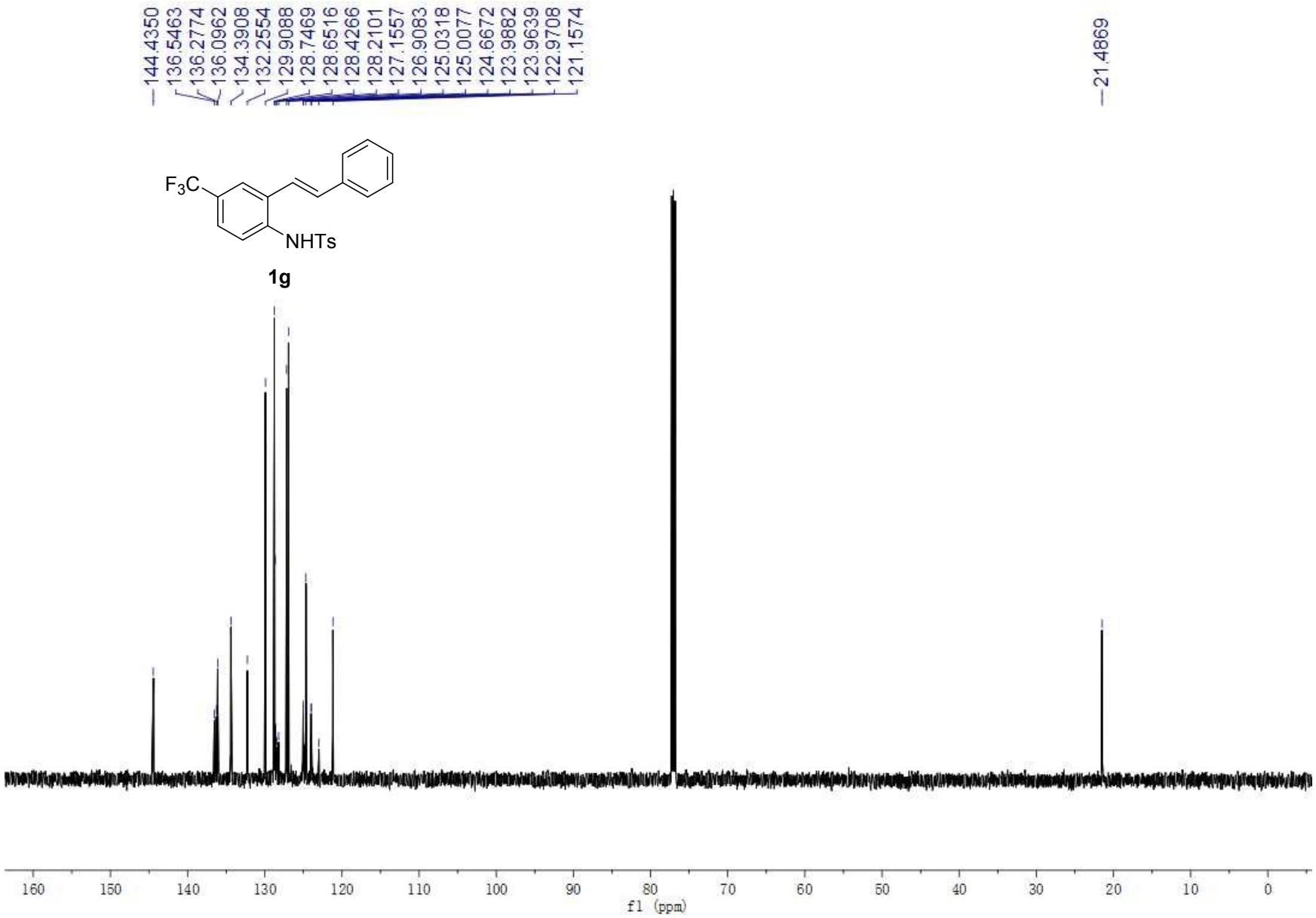
f1 (ppm)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127.1557
126.9083
125.0318
125.0077
124.6672
123.9882
123.9639
122.9708
121.1574
21.4869
F3C
NHTs
1g
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130
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90
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50
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30
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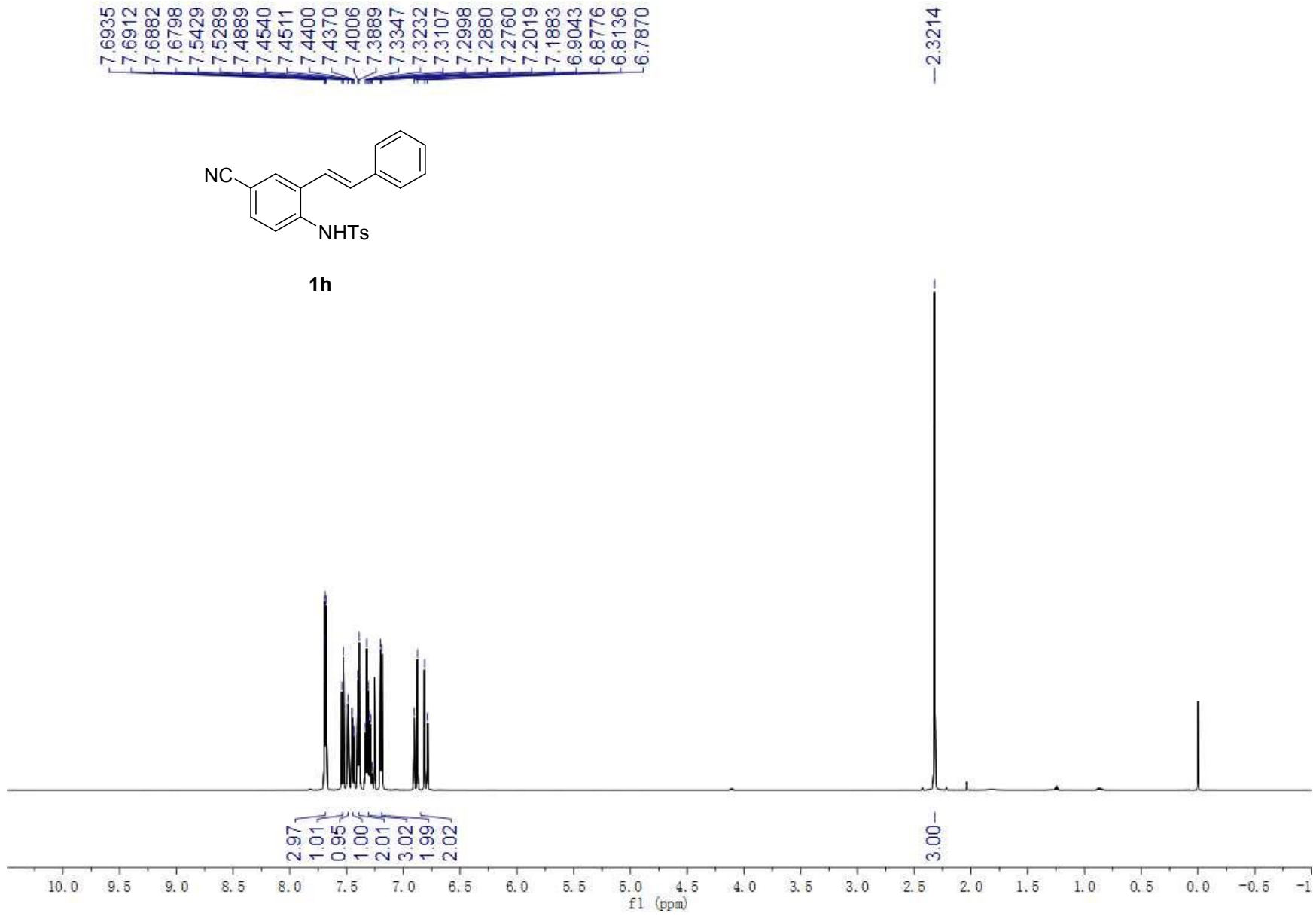
10
0
f1 (ppm)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7.1883
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6.8776
6.8136
6.7870
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NC
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3.02
1.99
2.02
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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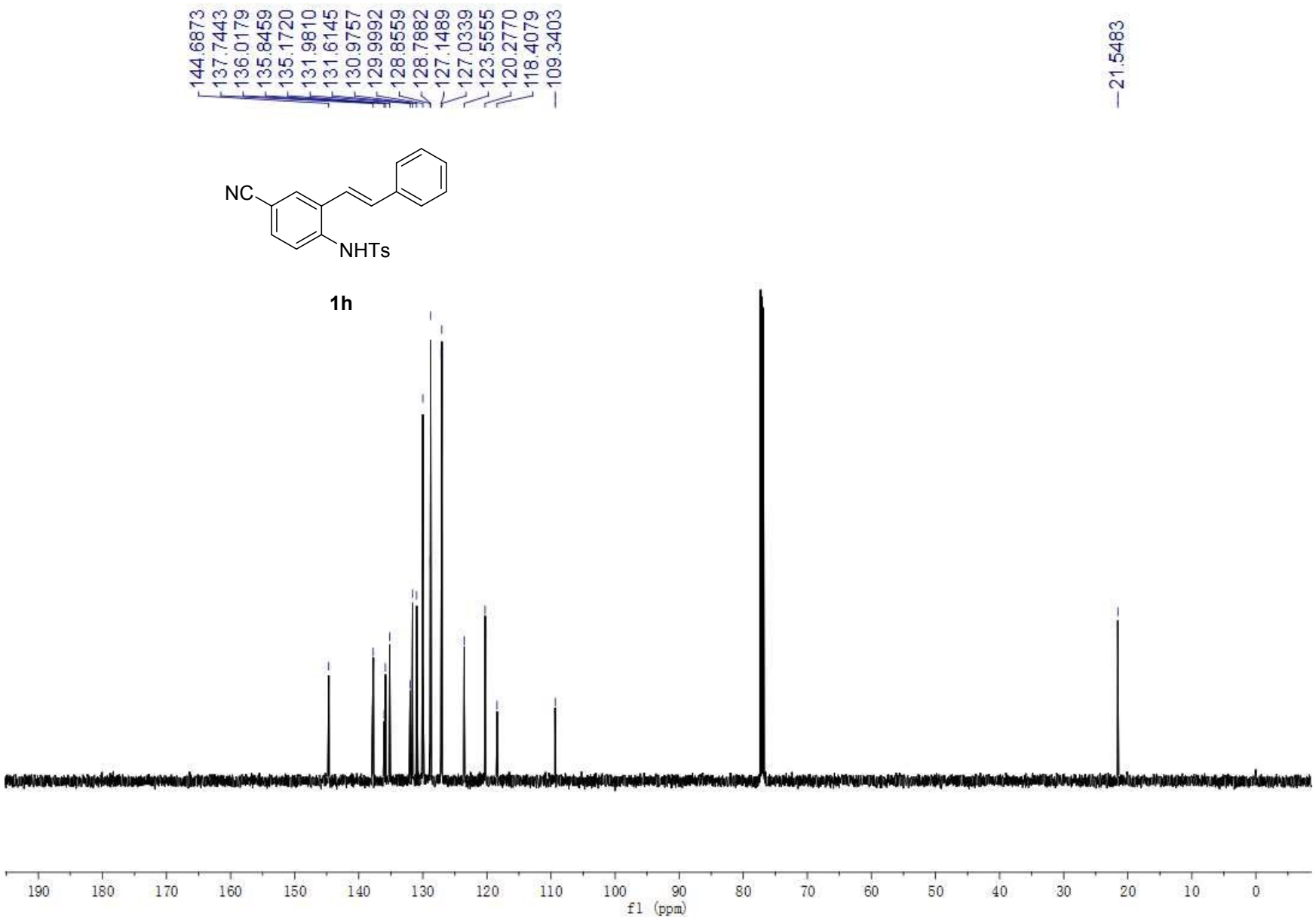
-1
f1 (ppm)

1h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NC
NHTs
1h
190
180
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50
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10
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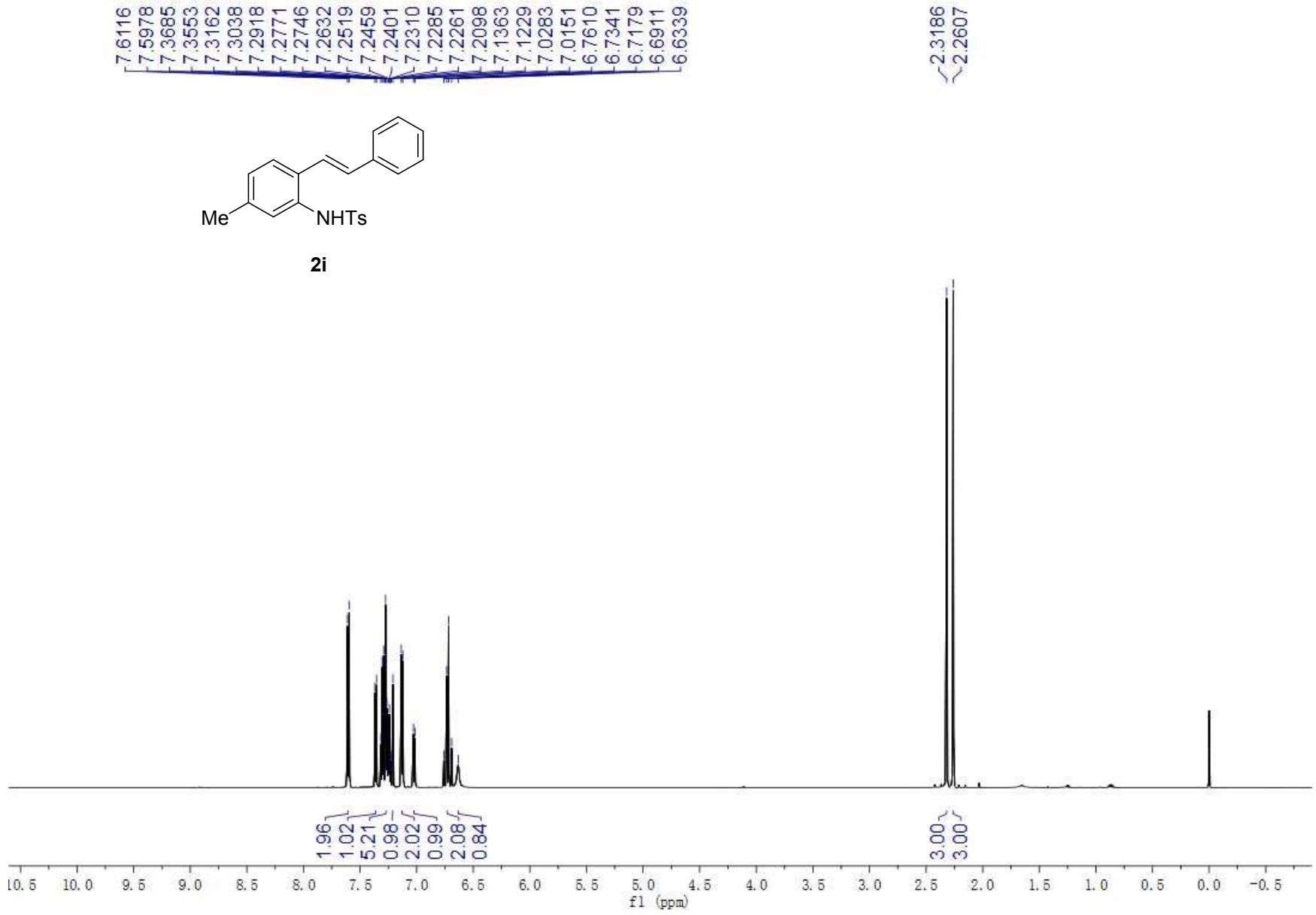
f1 (ppm)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7.2519
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7.2401
7.2310
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6.7341
6.7179
6.6911
6.6339
2.3186
2.2607
Me
NHTs
1.96
1.02
5.21
0.98
2.02
0.99
2.08
0.84
3.00
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
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2.5
2.0
1.5
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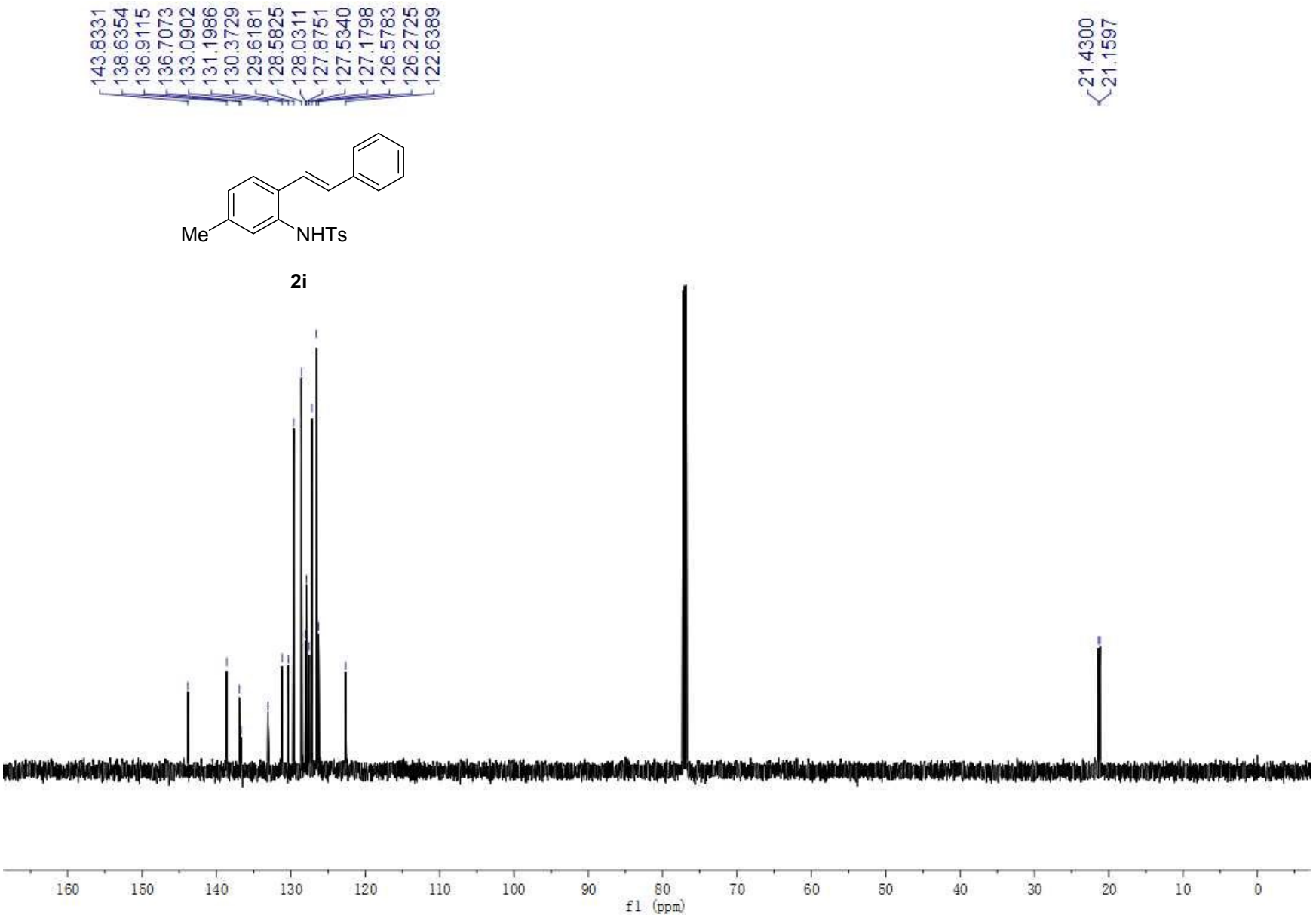
0.5
0.0
-0.5
f1 (ppm)

2i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127.1798
126.5783
126.2725
122.6389
21.4300
21.1597
Me
NHTs
2i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.6086
7.5948
7.3402
7.3276
7.3153
7.3055
7.2981
7.2954
7.2839
7.2773
7.2652
7.2331
7.2195
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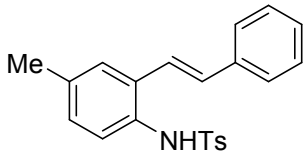
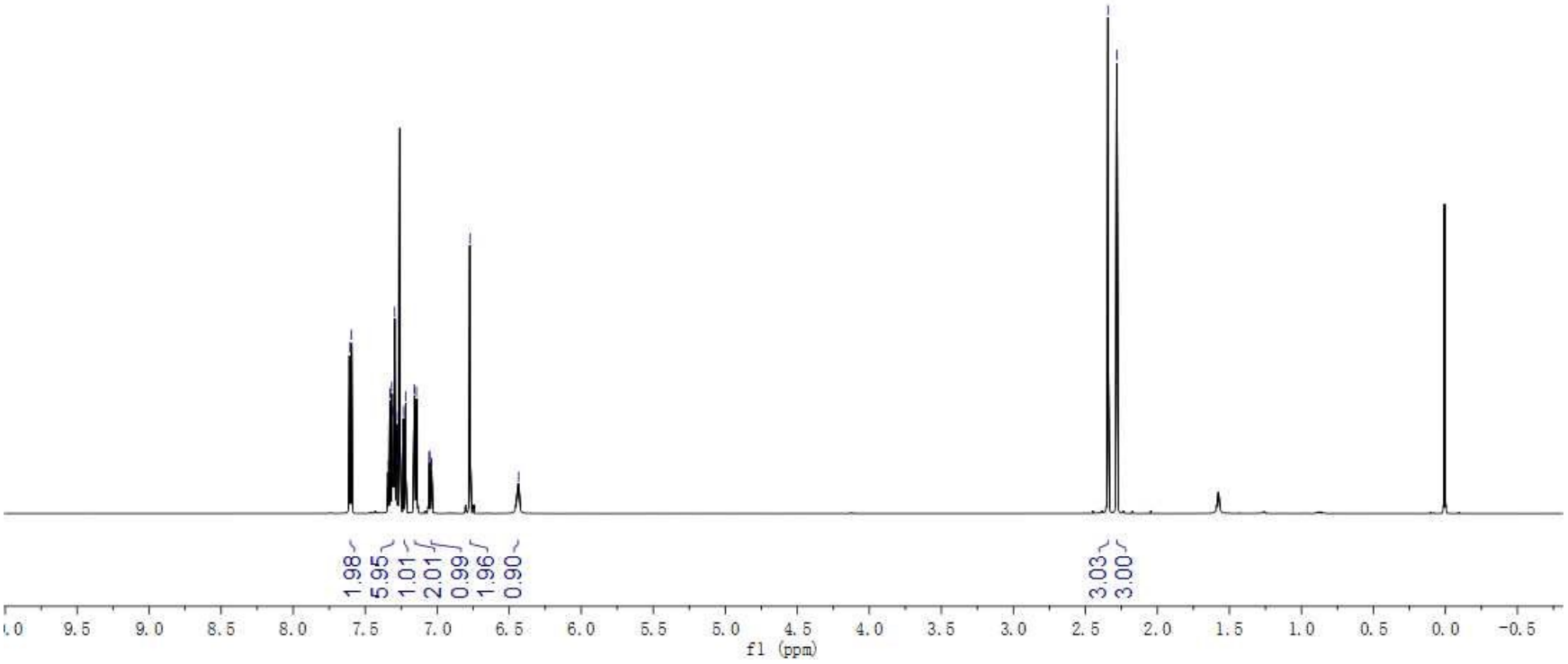
2.3427
2.2814


Me
NHTs

1j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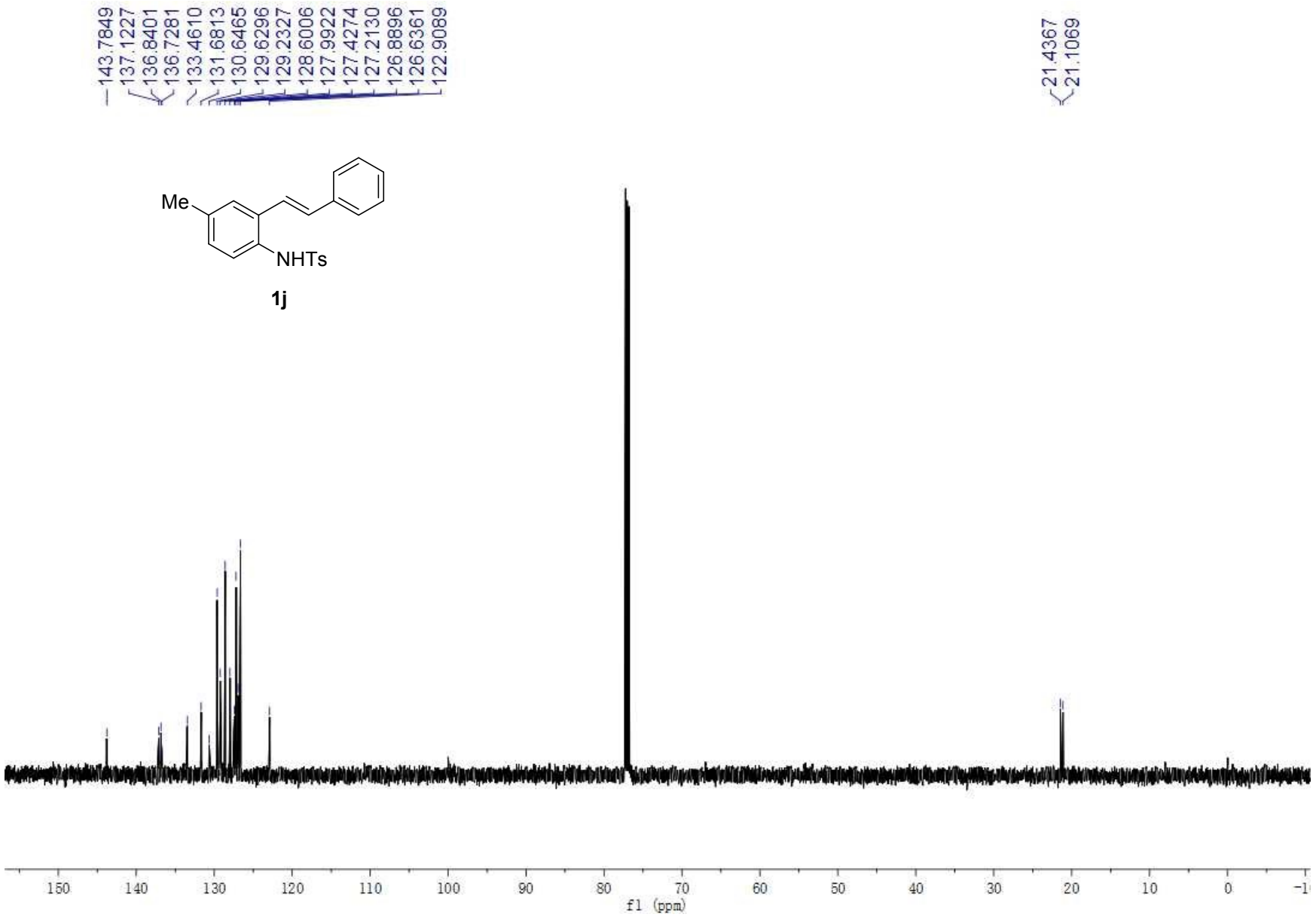
2.01
0.99
1.96
0.90
3.03
3.00
f1 (ppm)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129.2327
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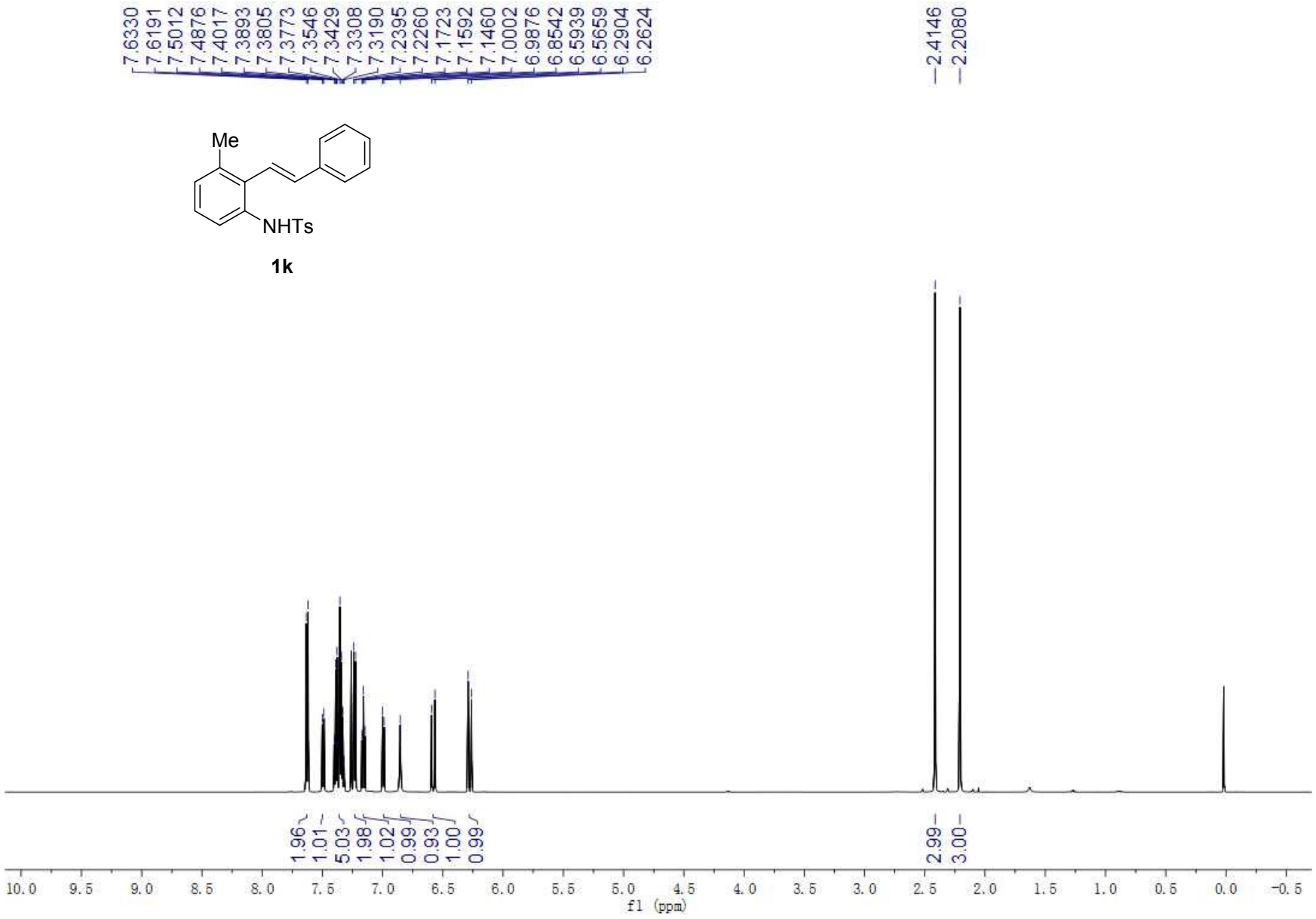
127.9922
127.4274
127.2130
126.8896
126.6361
122.9089
21.4367
21.1069
Me
NHTs
1j
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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7.3429
7.3308
7.3190
7.2395
7.2260
7.1723
7.1592
7.1460
7.0002
6.9876
6.8542
6.5939
6.5659
6.2904
6.2624
2.4146
2.2080
Me
NHTs
1k
1.96
1.01
5.03
1.98
1.02
0.99
0.93
1.00
0.99
2.99
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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0.5
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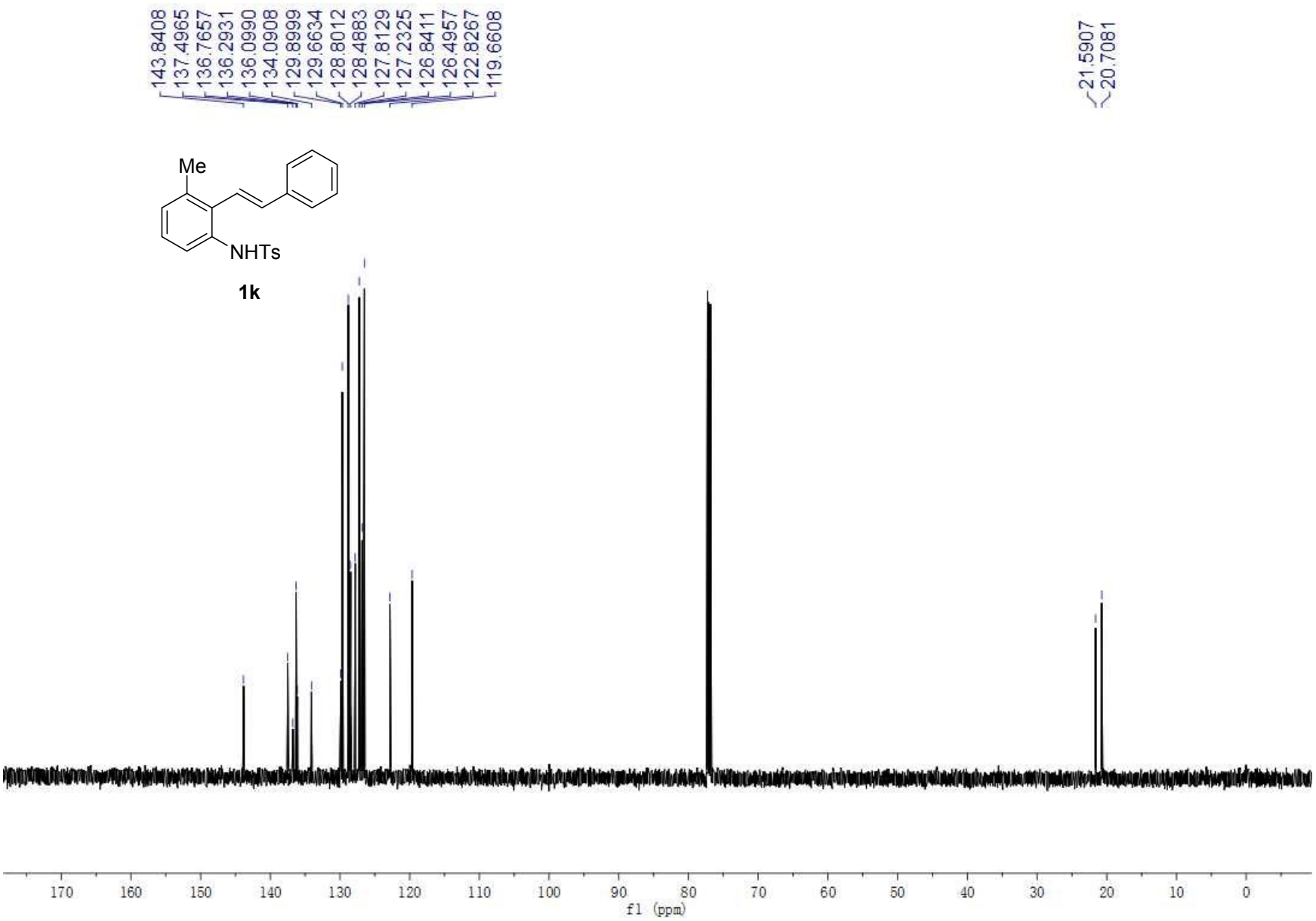
-0.5
f1 (ppm)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127.2325
126.8411
126.4957
122.8267
119.6608
21.5907
20.7081
Me
NHTs
1k
170
160
150
140
130
120
110
100
90
80
70
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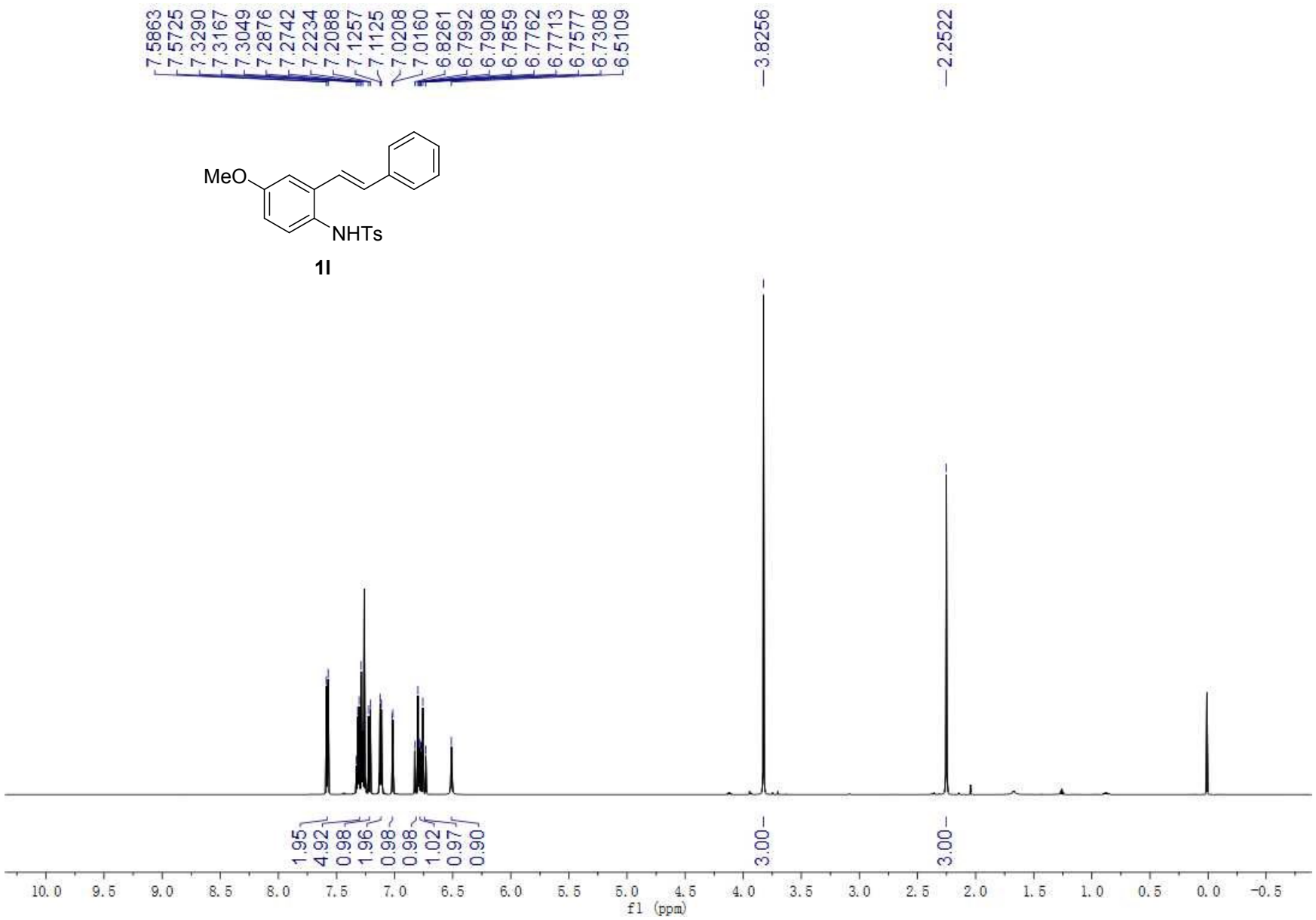
50
40
30
20
10
0
f1 (ppm)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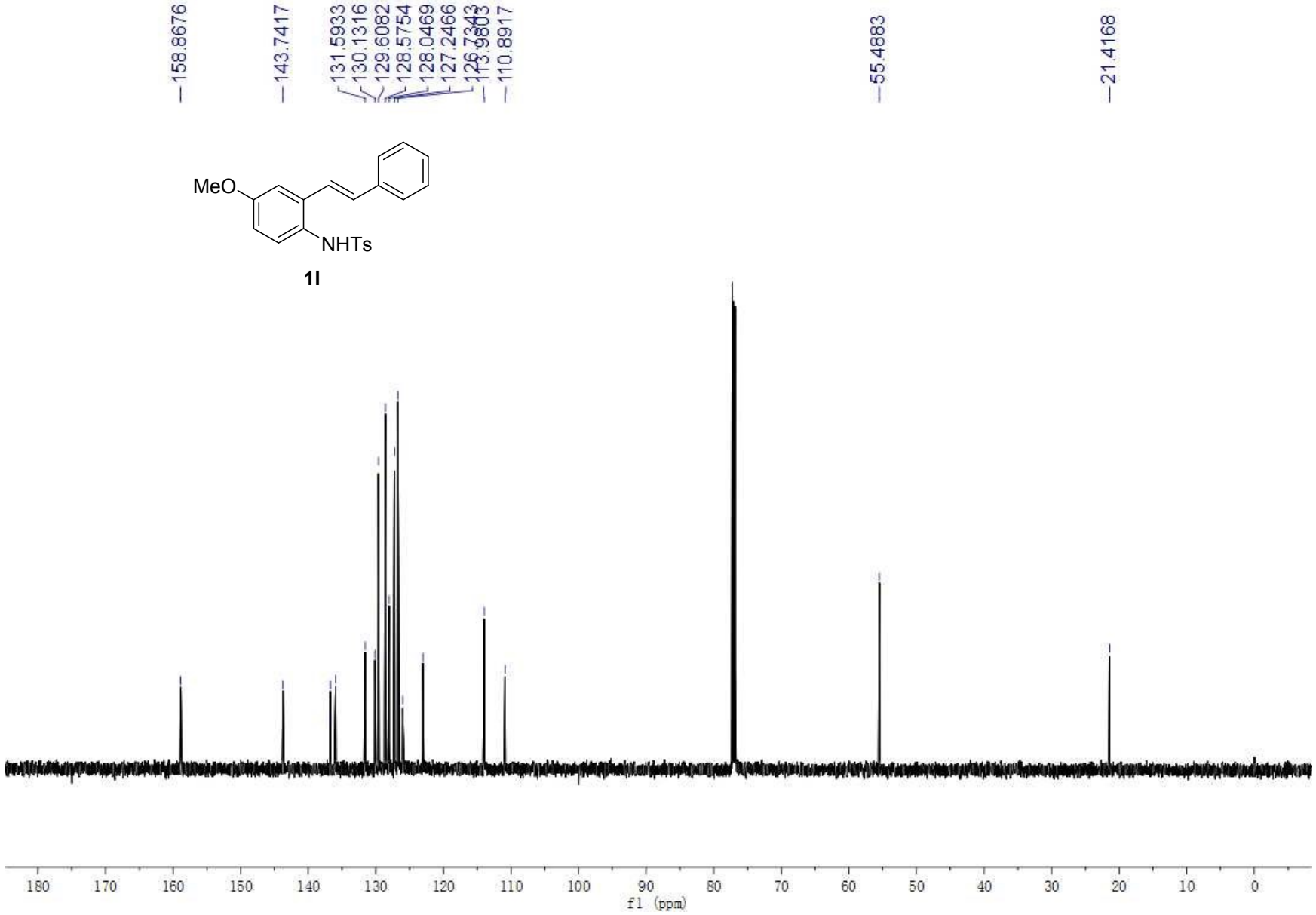
7.2742
7.2234
7.2088
7.1257
7.1125
7.0208
7.0160
6.8261
6.7992
6.7908
6.7859
6.7762
6.7713
6.7577
6.7308
6.5109
3.8256
2.2522
MeO
NHTs
1l
1.95
4.92
0.98
1.96
0.98
0.98
1.02
0.97
0.90
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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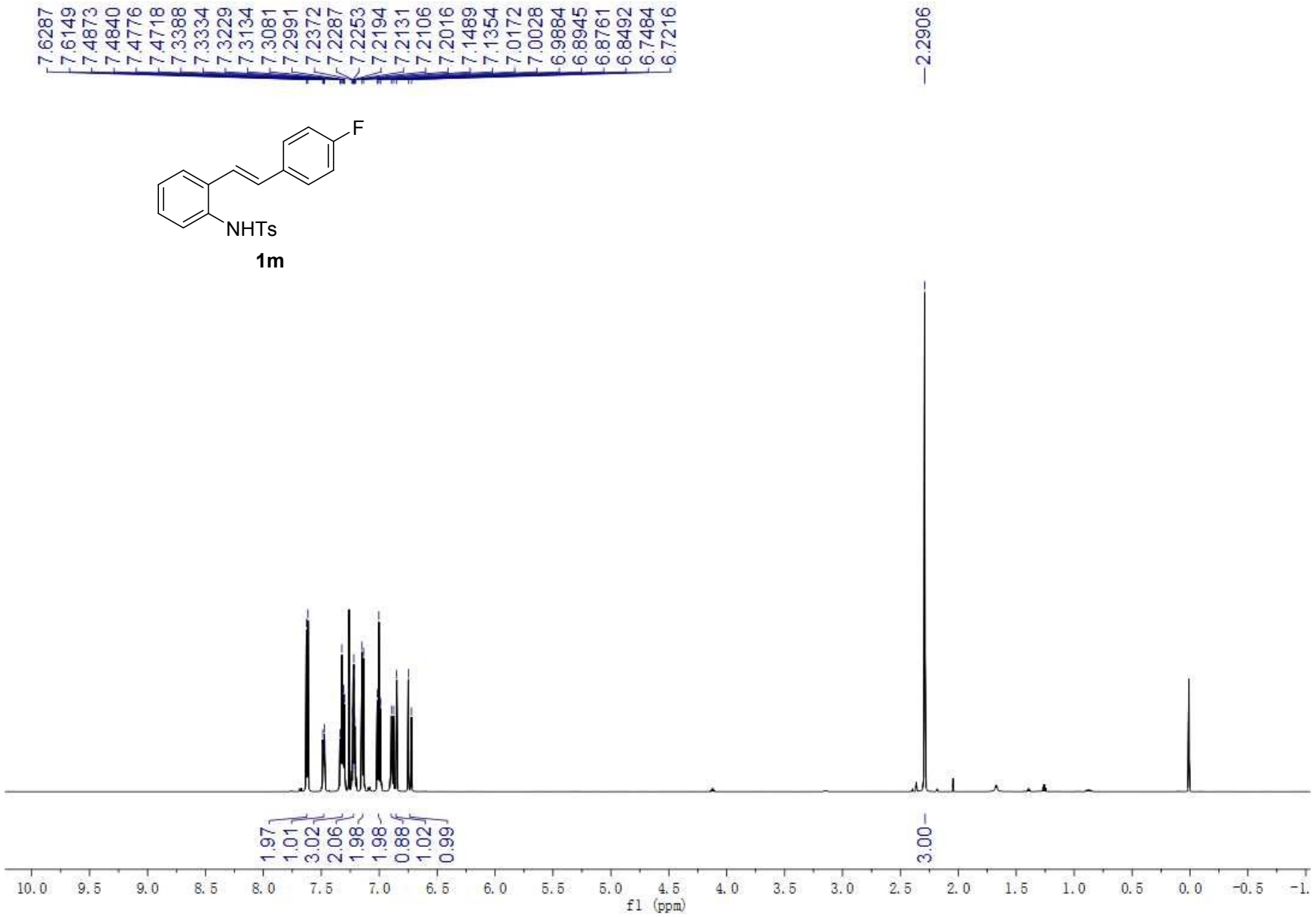
55.4883
21.4168
MeO
NHTs
1l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2991
7.2372
7.2287
7.2253
7.2194
7.2131
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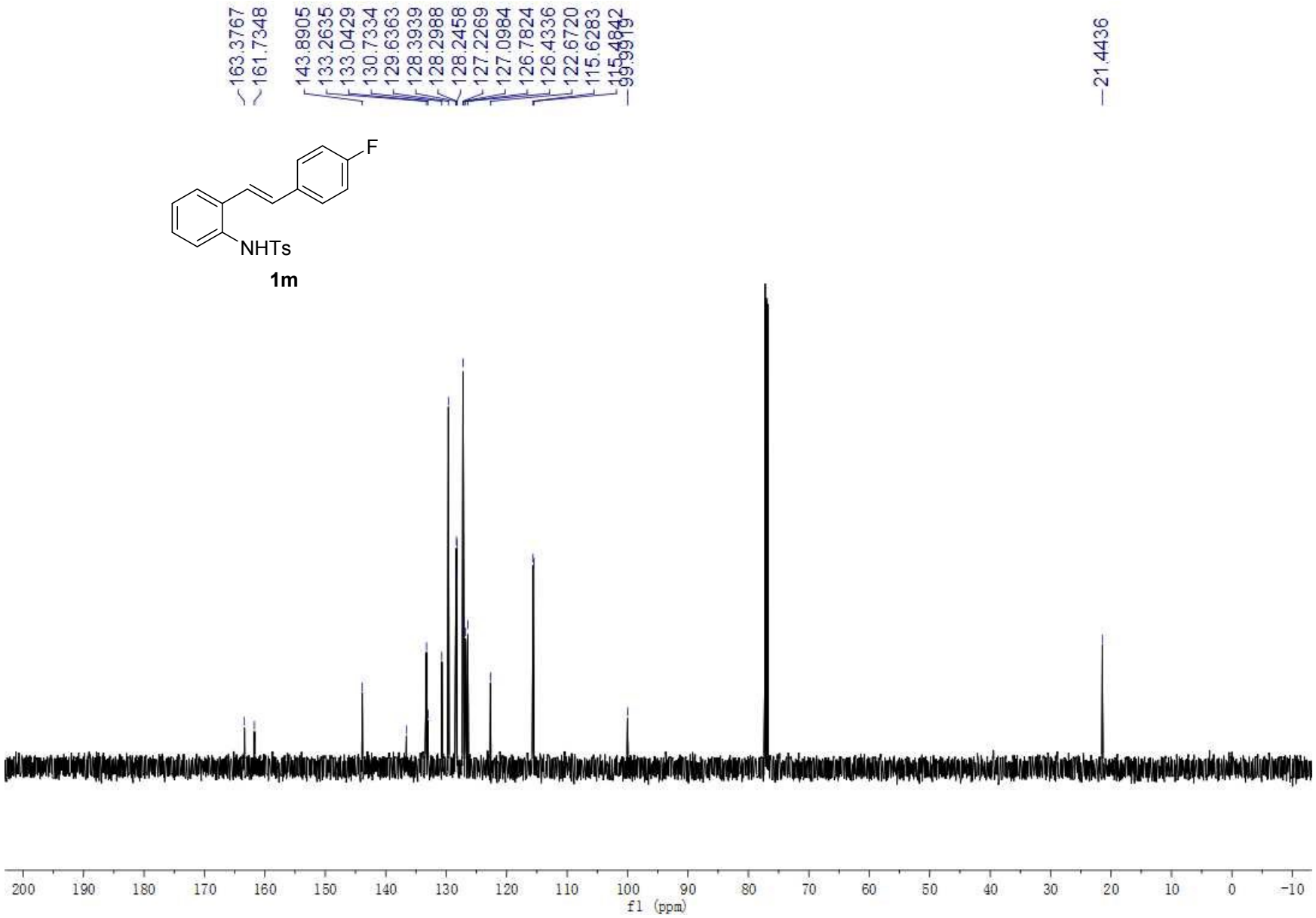
7.2016
7.1489
7.1354
7.0172
7.0028
6.9884
6.8945
6.8761
6.8492
6.7484
6.7216
2.2906
F
NHTs
1m
1.97
1.01
3.02
2.06
1.98
1.98
0.88
1.02
0.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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143.8905
133.2635
133.0429
130.7334
129.6363
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128.2988
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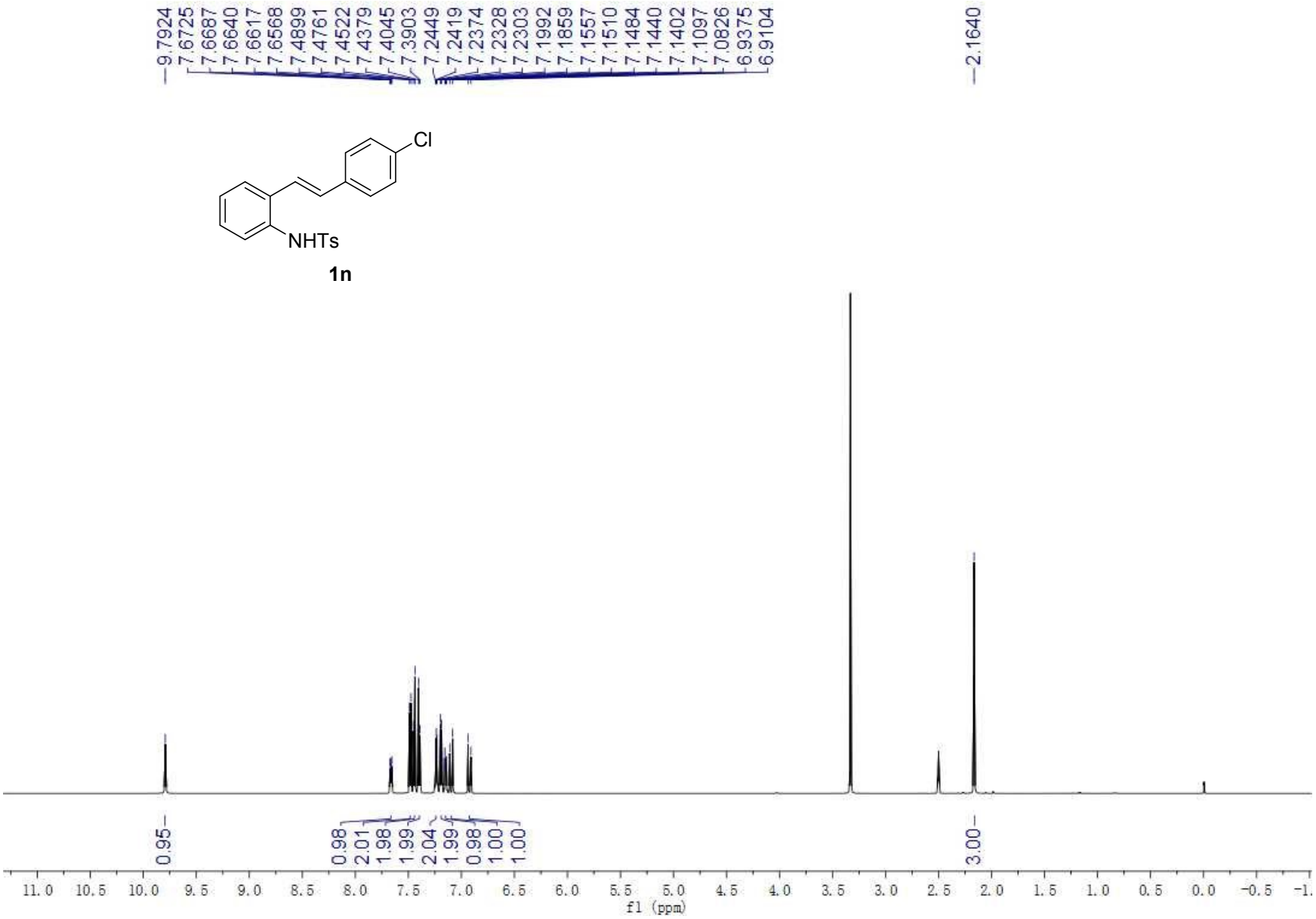
127.2269
127.0984
126.7824
126.4336
122.6720
115.6283
115.4842
99.9919
21.4436
F
NHTs
1m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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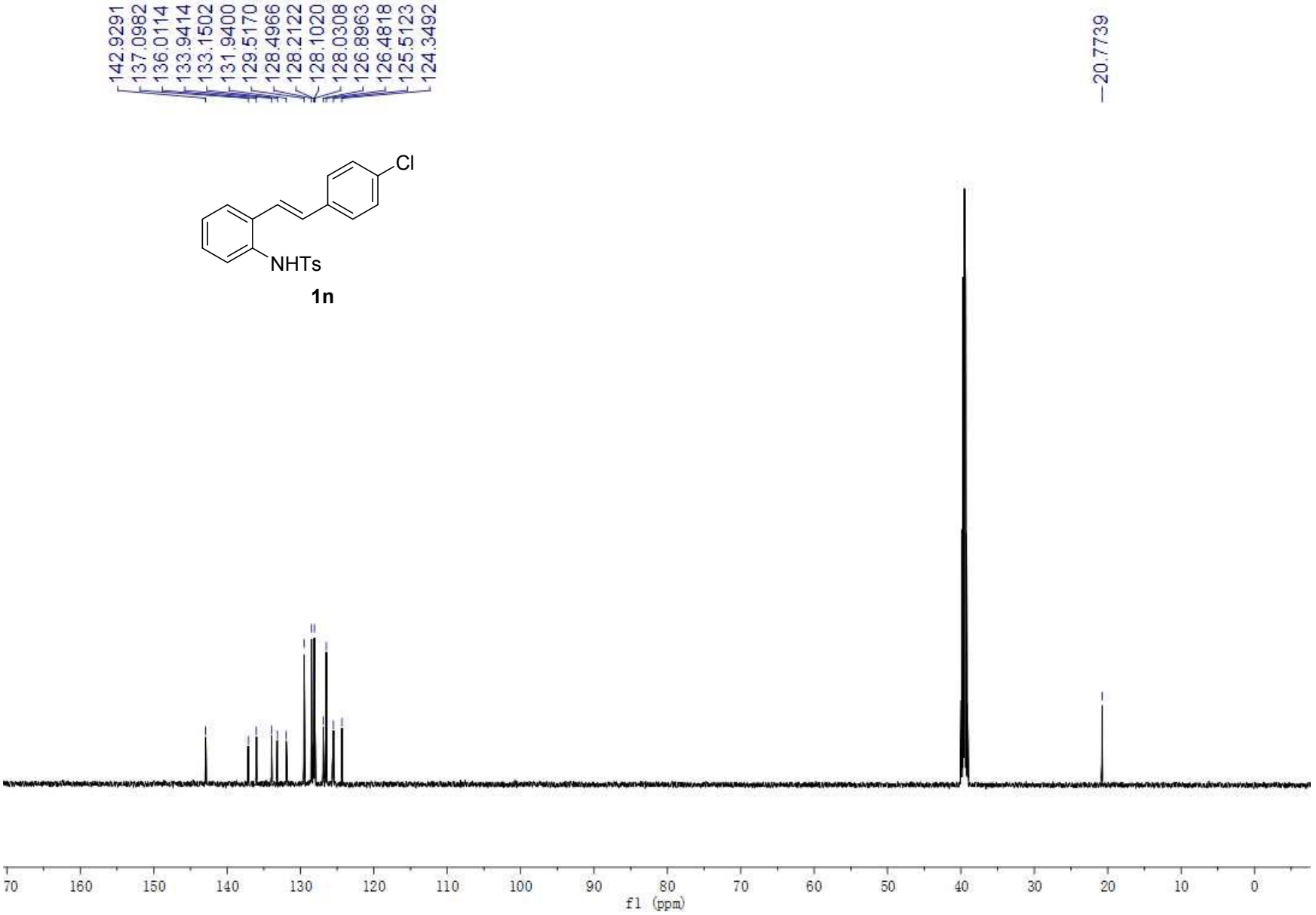
7.6568
7.4899
7.4761
7.4522
7.4379
7.4045
7.3903
7.2449
7.2419
7.2374
7.2328
7.2303
7.1992
7.1859
7.1557
7.1510
7.1484
7.1440
7.1402
7.1097
7.0826
6.9375
6.9104
2.1640
Cl
NHTs
1n
0.95
0.98
2.01
1.98
1.99
2.04
1.99
0.98
1.00
1.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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131.9400
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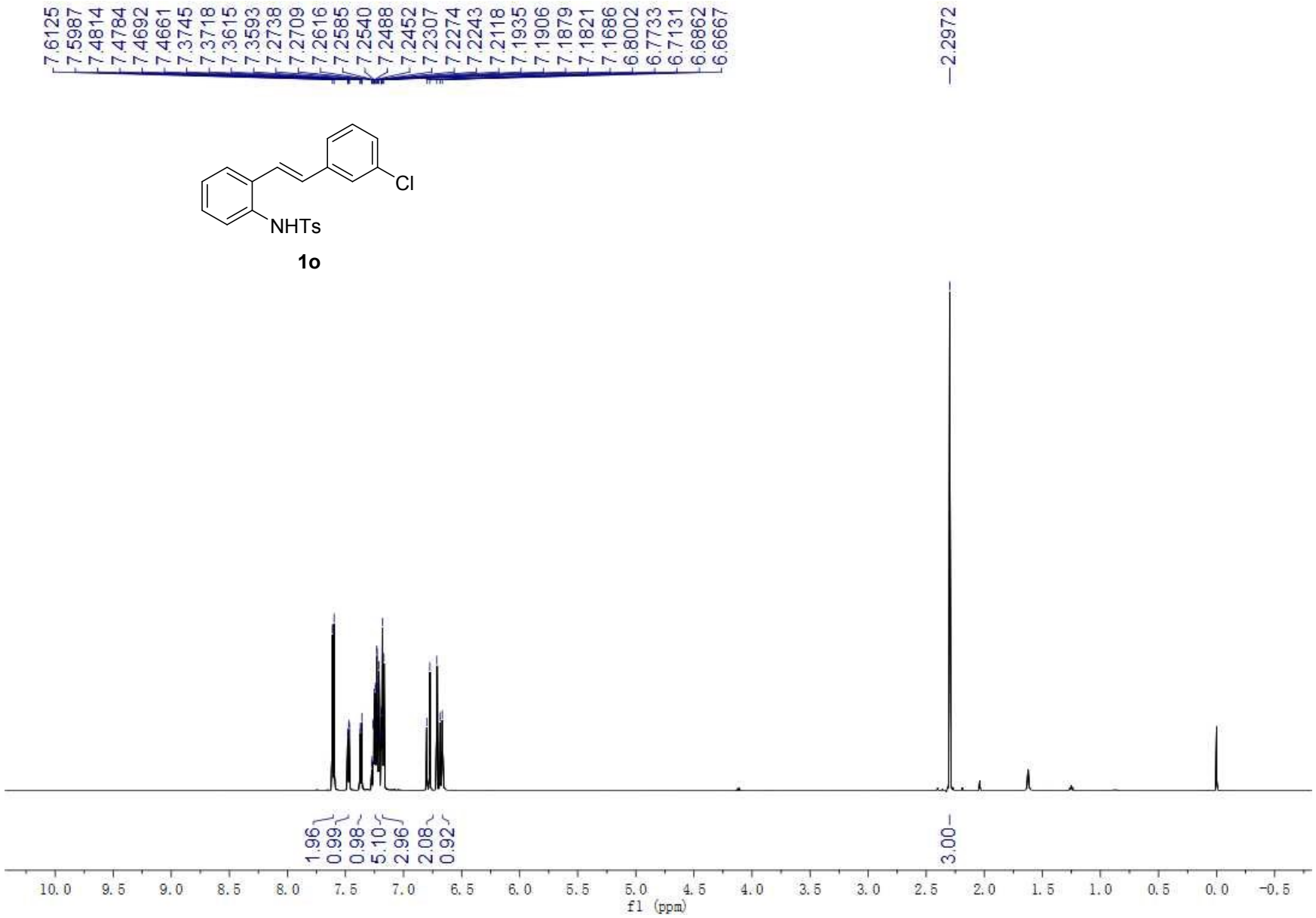
128.2122
128.1020
128.0308
126.8963
126.4818
125.5123
124.3492
20.7739
Cl
NHTs
1n
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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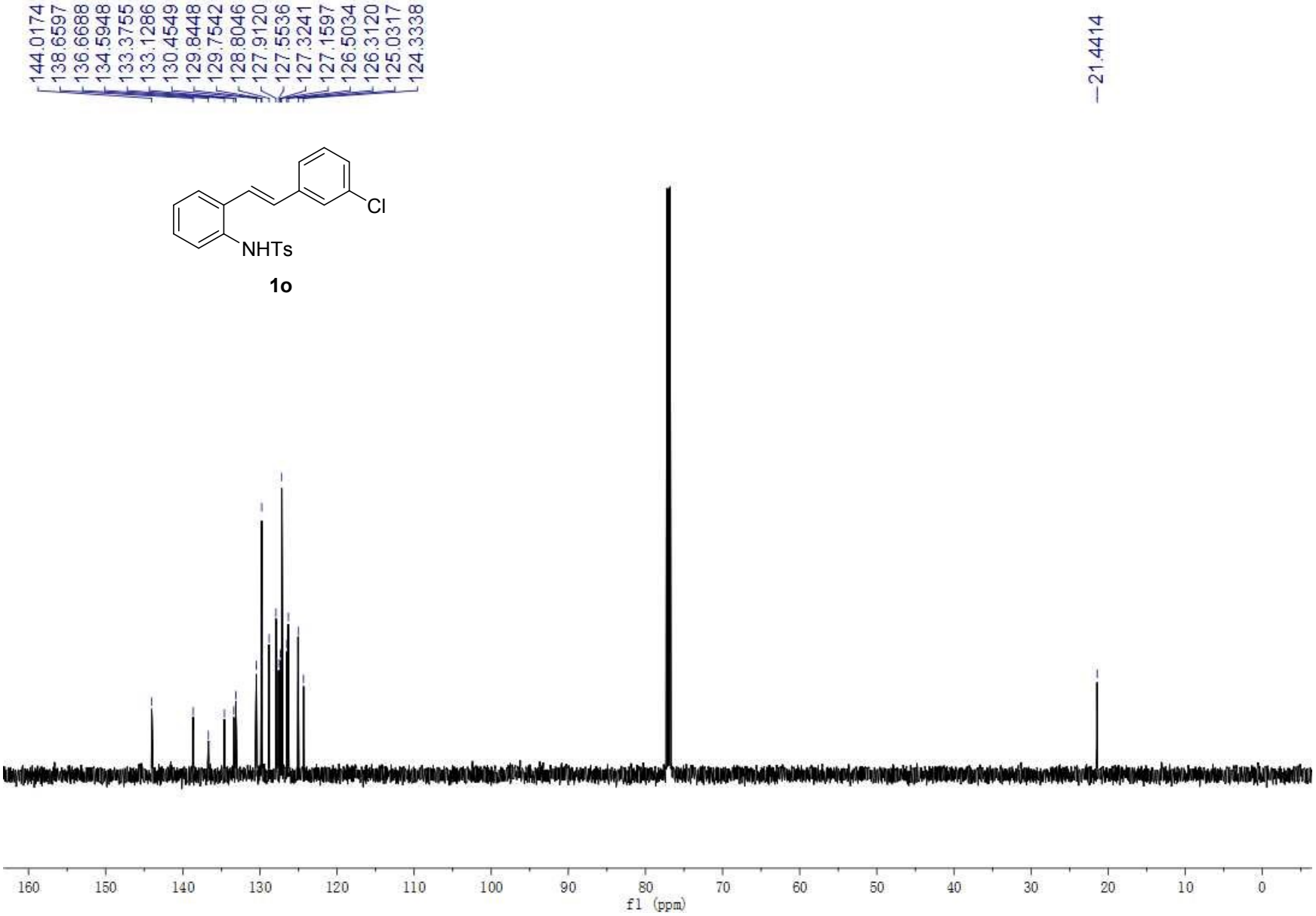
7.2738
7.2709
7.2616
7.2585
7.2540
7.2488
7.2452
7.2307
7.2274
7.2243
7.2118
7.1935
7.1906
7.1879
7.1821
7.1686
6.8002
6.7733
6.7131
6.6862
6.6667
2.2972
Cl
NHTs
1o
1.96
0.99
0.98
5.10
2.96
2.08
0.92
3.00
f1 (ppm)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130.4549
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127.9120
127.5536
127.3241
127.1597
126.5034
126.3120
125.0317
124.3338
21.4414
Cl
NHTs
1o
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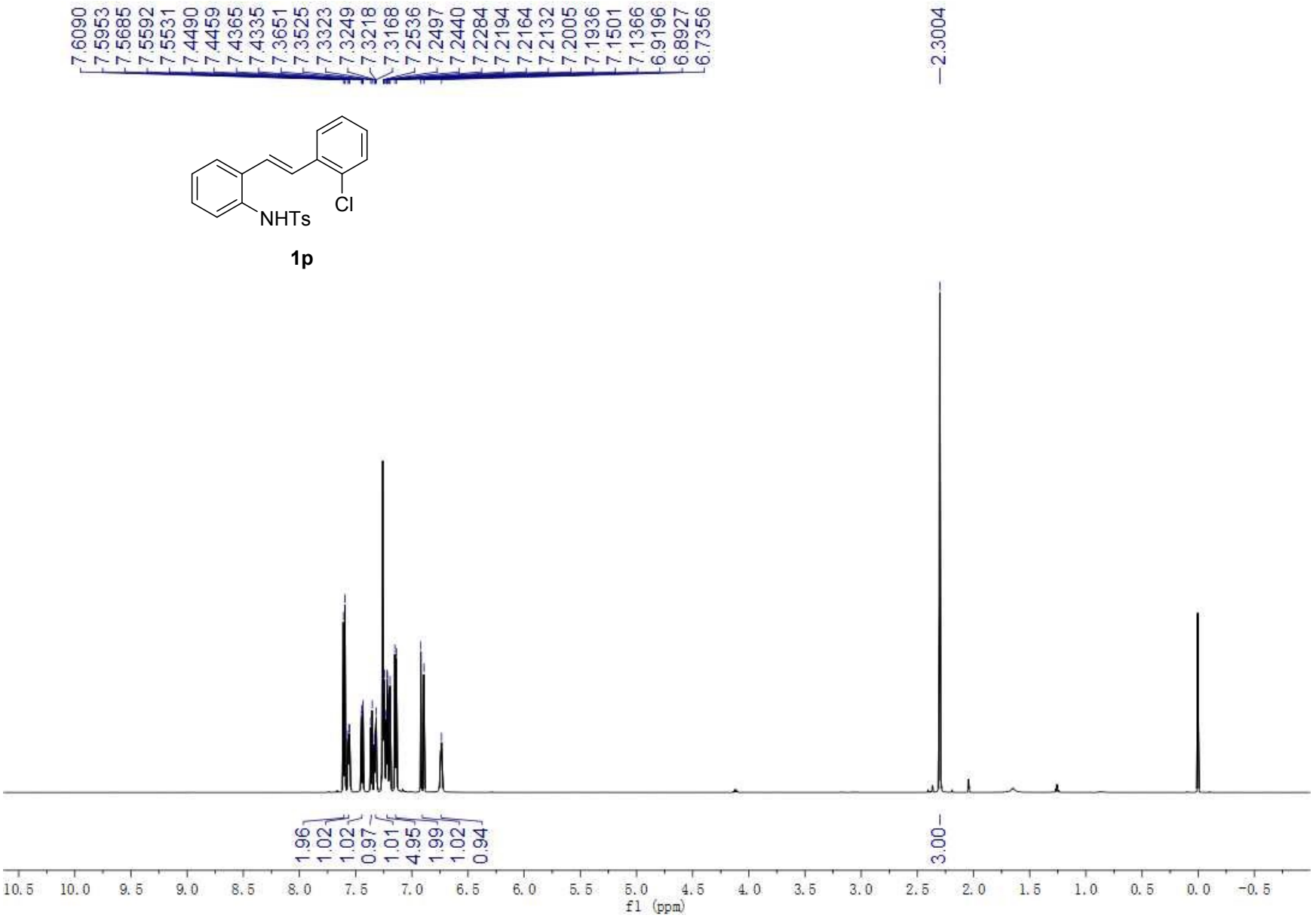
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3651
7.3525
7.3323
7.3249
7.3218
7.3168
7.2536
7.2497
7.2440
7.2284
7.2194
7.2164
7.2132
7.2005
7.1936
7.1501
7.1366
6.9196
6.8927
6.7356
2.3004
NHTs
Cl
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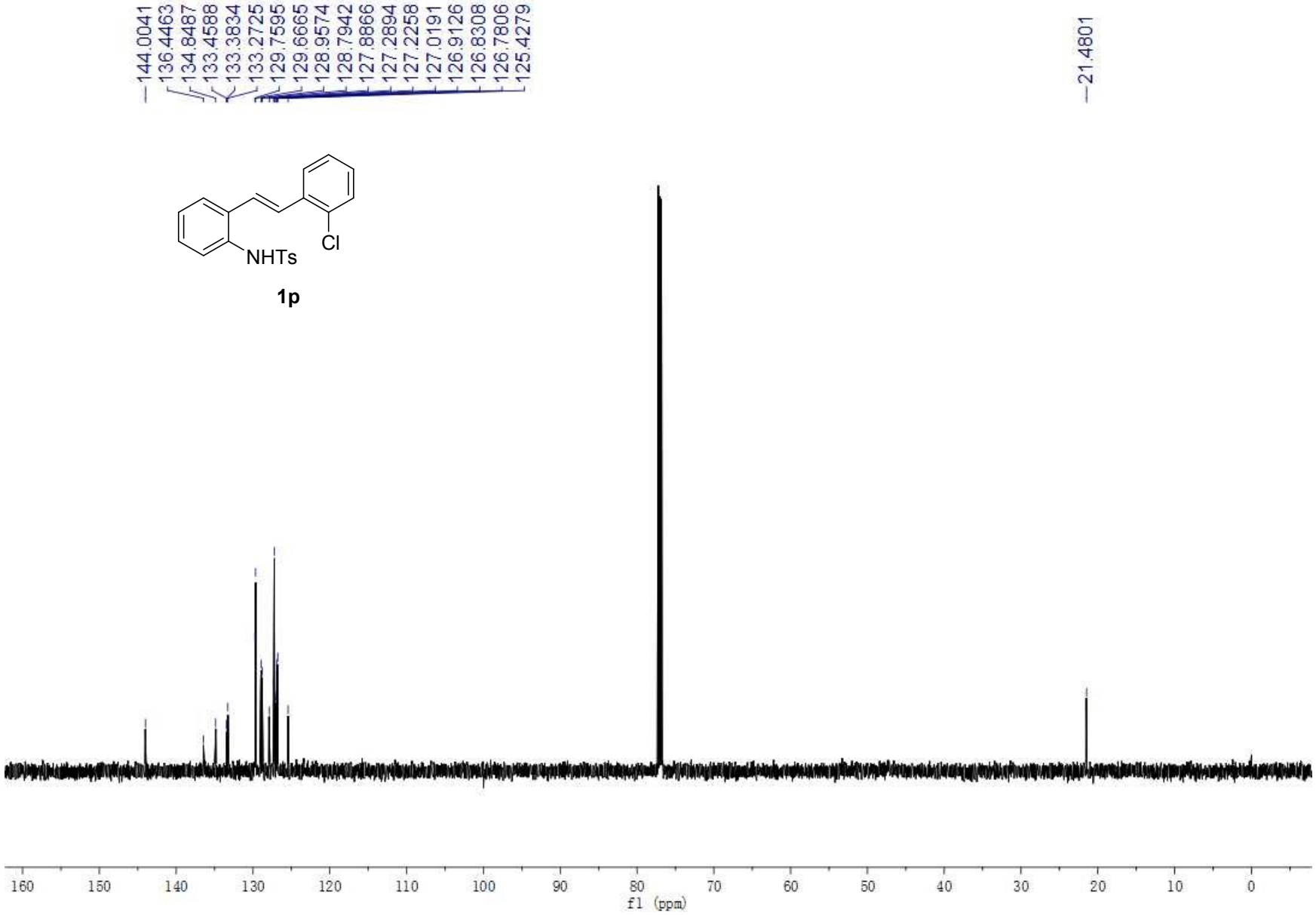
1.02
1.02
0.97
1.01
4.95
1.99
1.02
0.94
3.00
f1 (ppm)

1p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127.2894
127.2258
127.0191
126.9126
126.8308
126.7806
125.4279
21.4801
NHTs
Cl
1p
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150
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130
120
110
100
90
80
70
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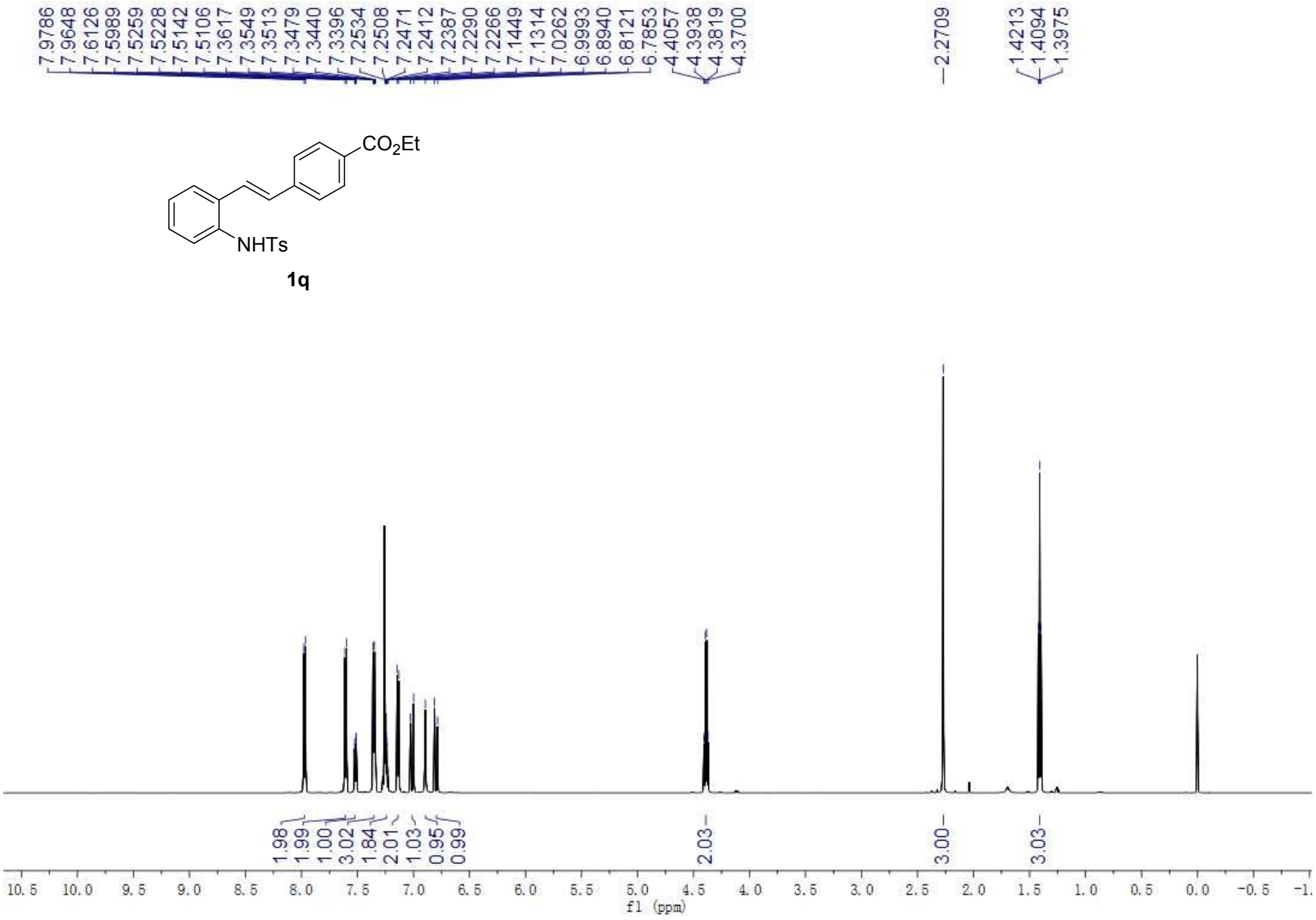
50
40
30
20
10
0
f1 (ppm)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7.3440
7.3396
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7.2508
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7.2412
7.2387
7.2290
7.2266
7.1449
7.1314
7.0262
6.9993
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6.8121
6.7853
4.4057
4.3938
4.3819
4.3700
2.2709
1.4213
1.4094
1.3975
CO2Et
NHTs
1q
1.98
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1.00
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1.03
0.95
0.99
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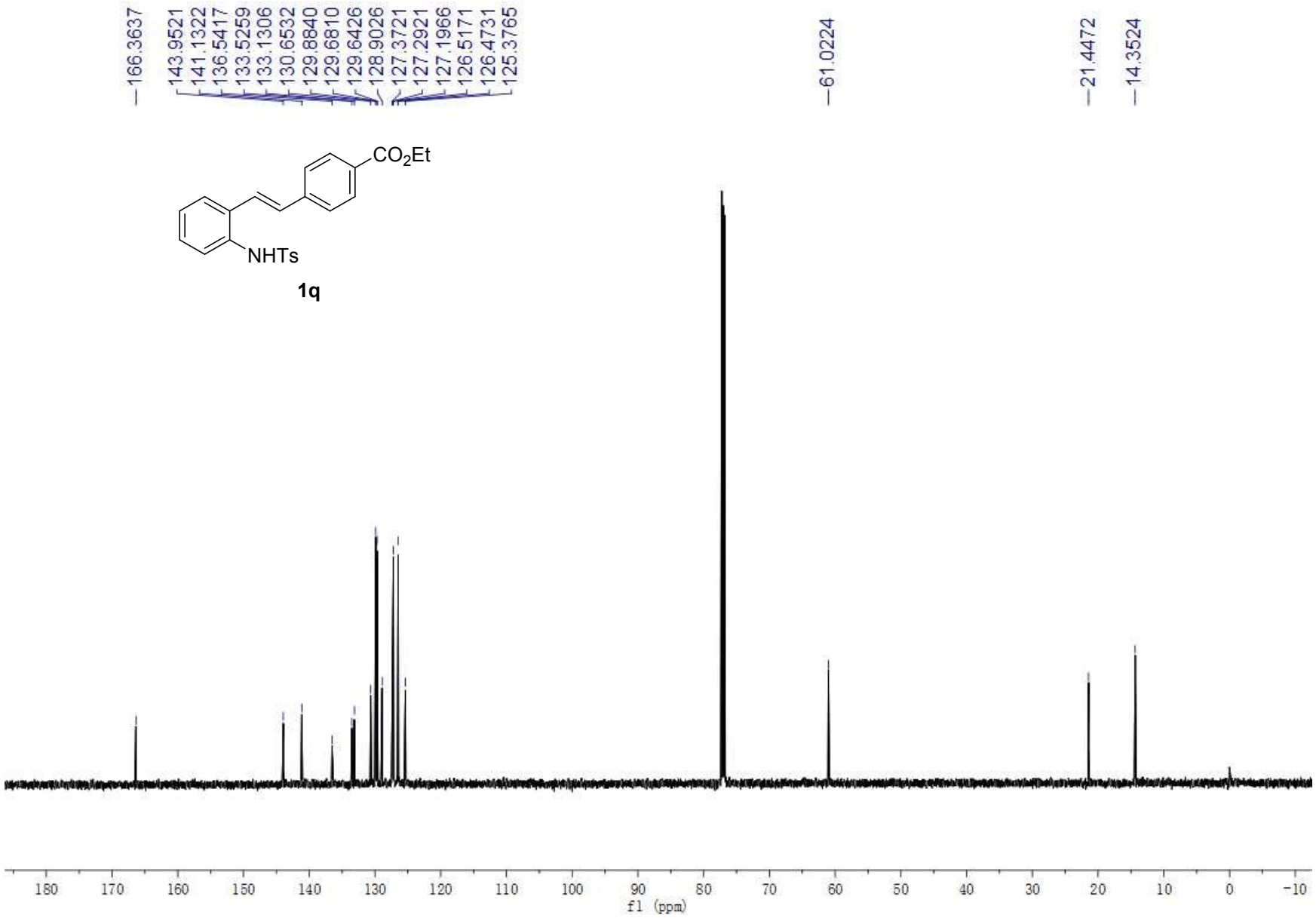
3.00
3.03
f1 (ppm)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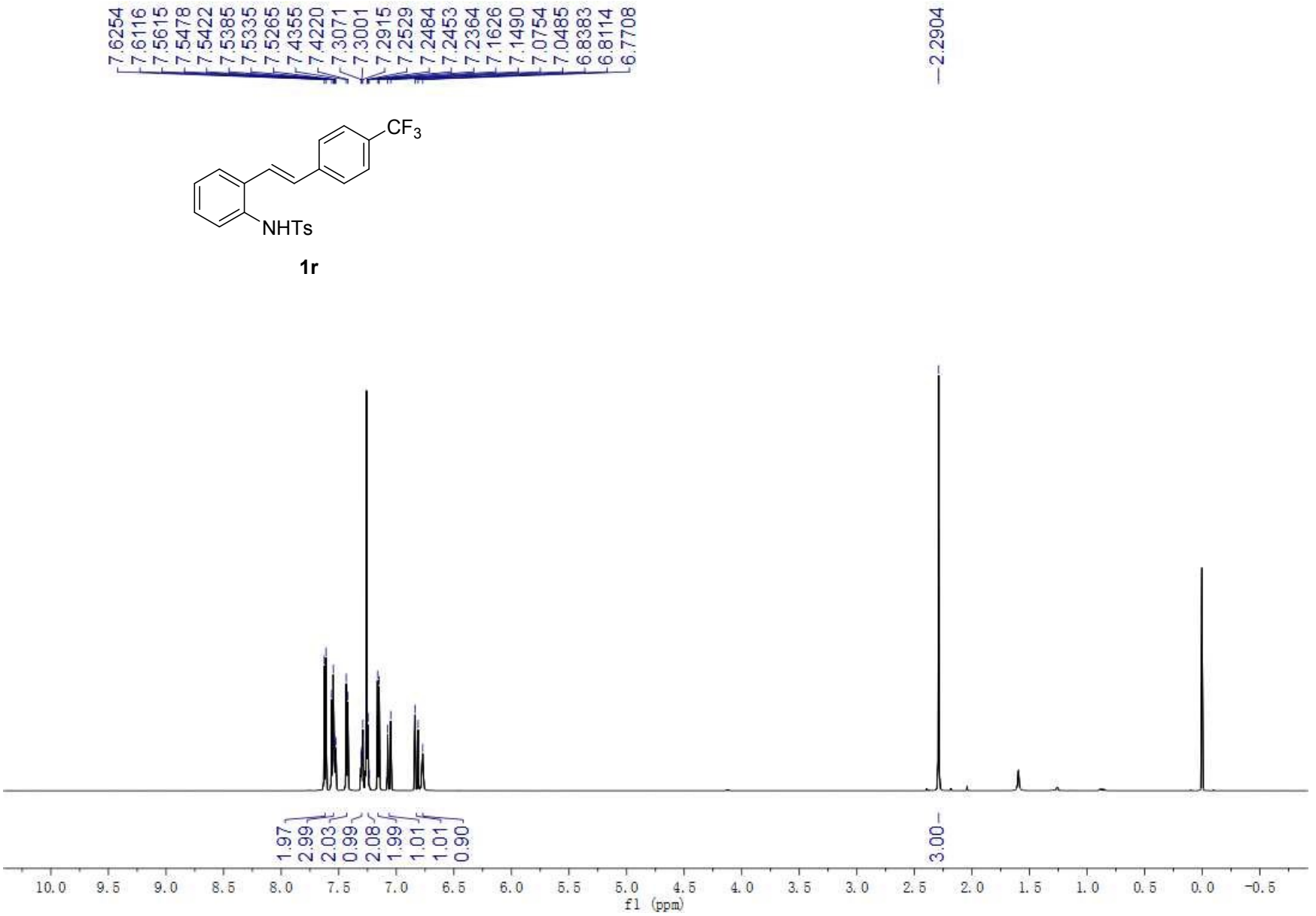
128.9026
127.3721
127.2921
127.1966
126.5171
126.4731
125.3765
61.0224
21.4472
14.3524
CO2Et
NHTs
1q
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.3001
7.2915
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7.2484
7.2453
7.2364
7.1626
7.1490
7.0754
7.0485
6.8383
6.8114
6.7708
2.2904
CF3
NHTs
1r
1.97
2.99
2.03
0.99
2.08
1.99
1.01
1.01
0.90
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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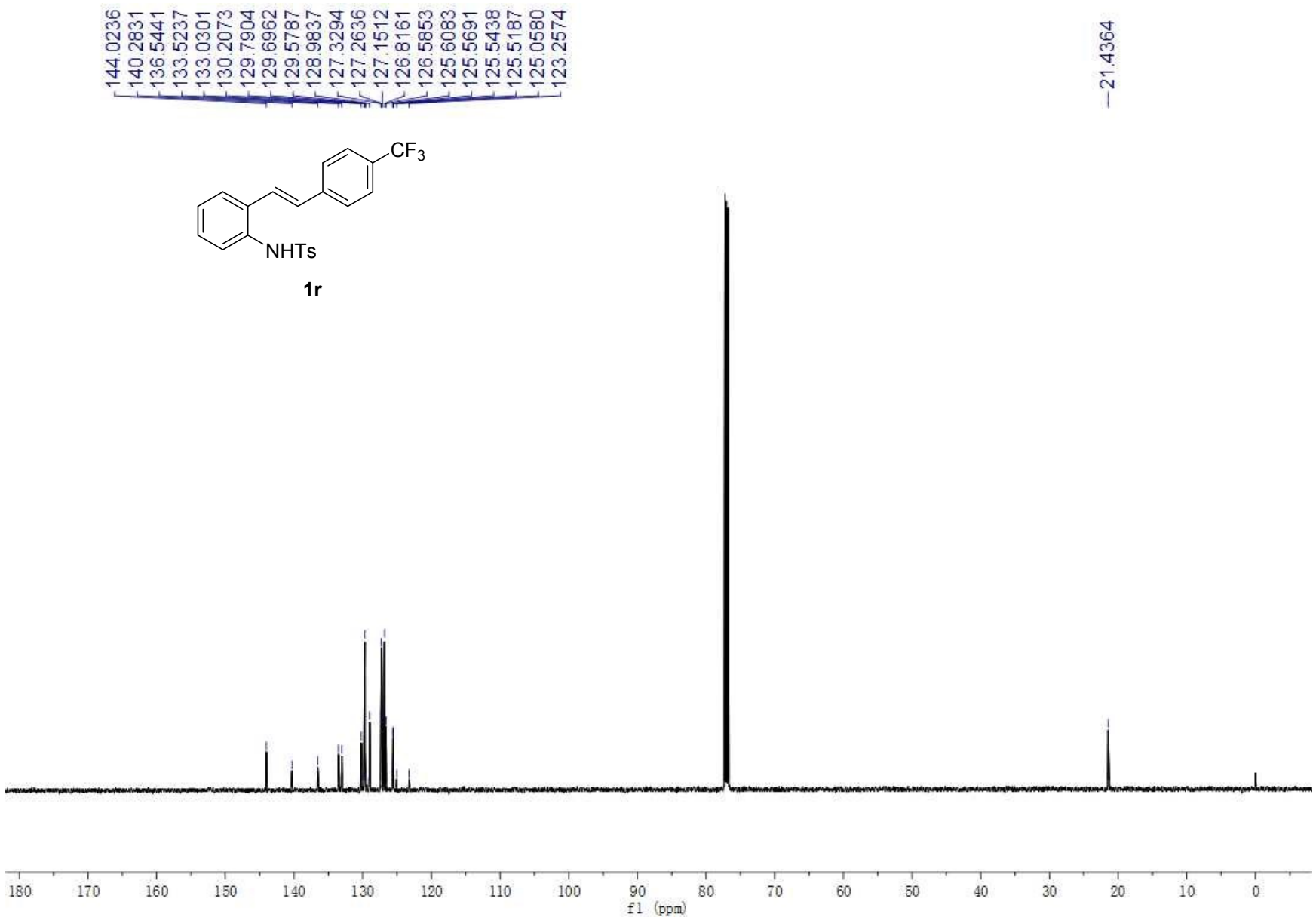
0.5
0.0
-0.5
f1 (ppm)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127.2636
127.1512
126.8161
126.5853
125.6083
125.5691
125.5438
125.5187
125.0580
123.2574
21.4364
CF3
NHTs
1r
180
170
160
150
140
130
120
110
100
90
80
70
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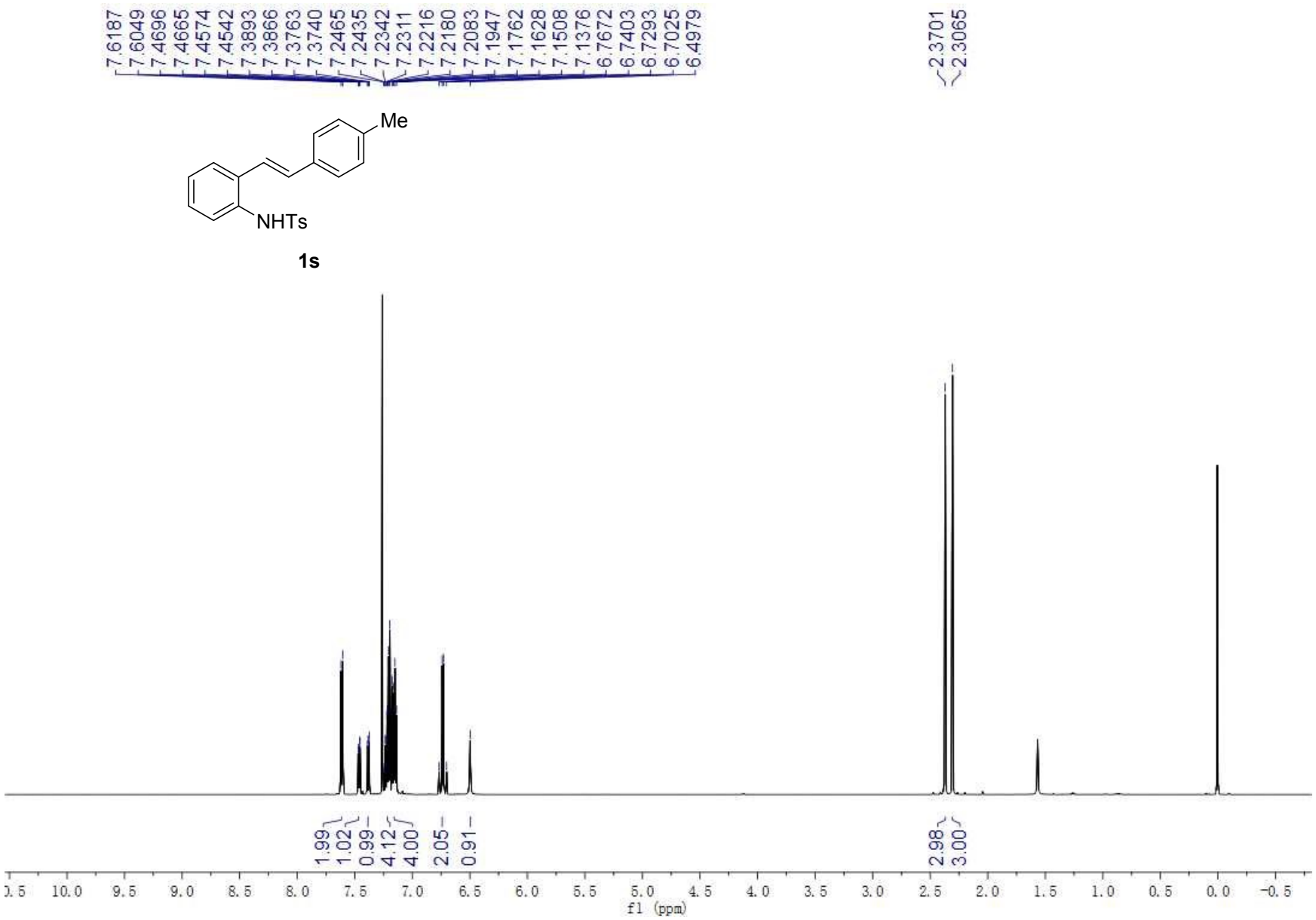
50
40
30
20
10
0
f1 (ppm)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7.2435
7.2342
7.2311
7.2216
7.2180
7.2083
7.1947
7.1762
7.1628
7.1508
7.1376
6.7672
6.7403
6.7293
6.7025
6.4979
2.3701
2.3065
Me
NHTs
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1.02
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4.00
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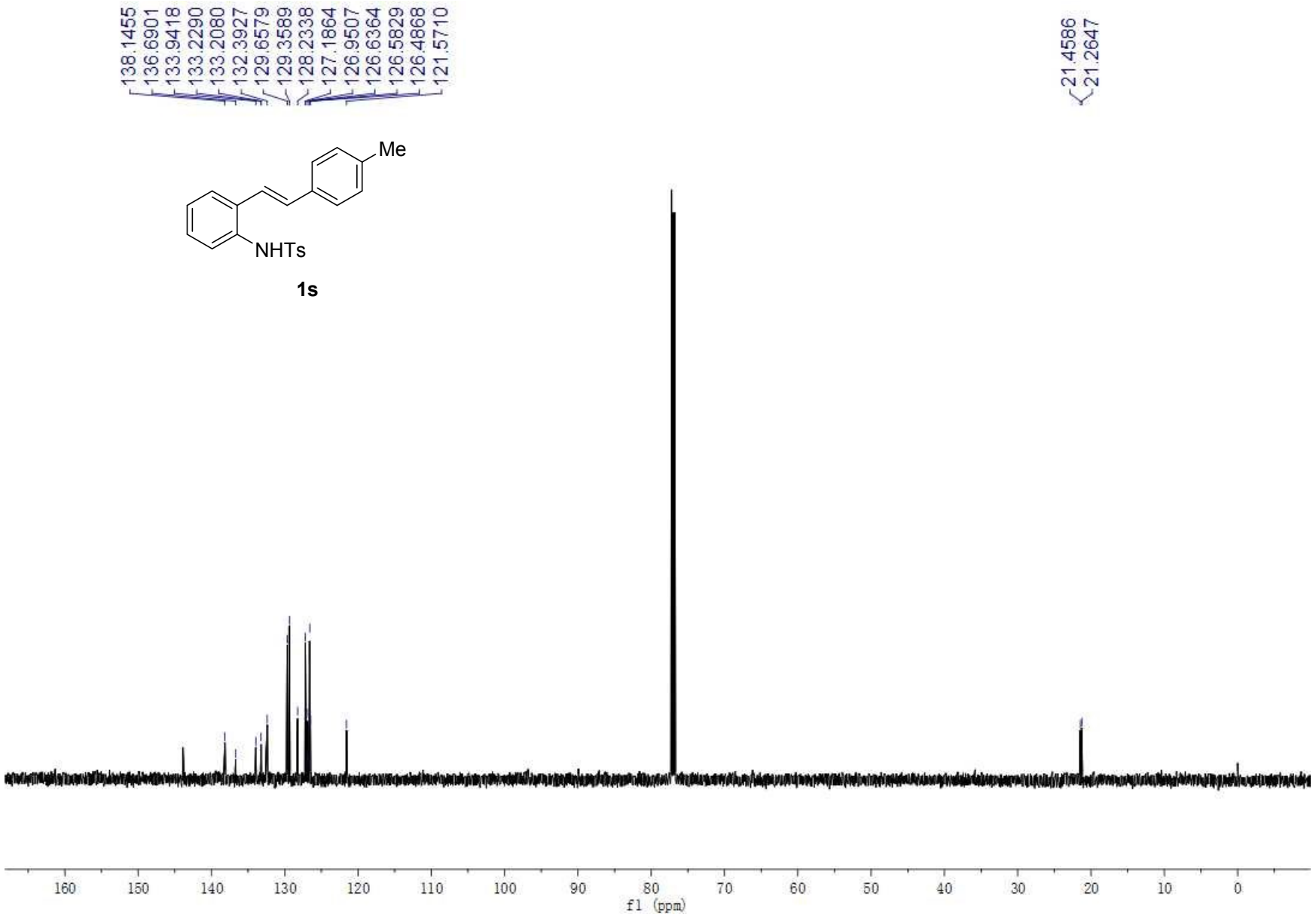
0.91
2.98
3.00
f1 (ppm)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126.5829
126.4868
121.5710
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21.2647
Me
NHTs
1s
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130
120
110
100
90
80
70
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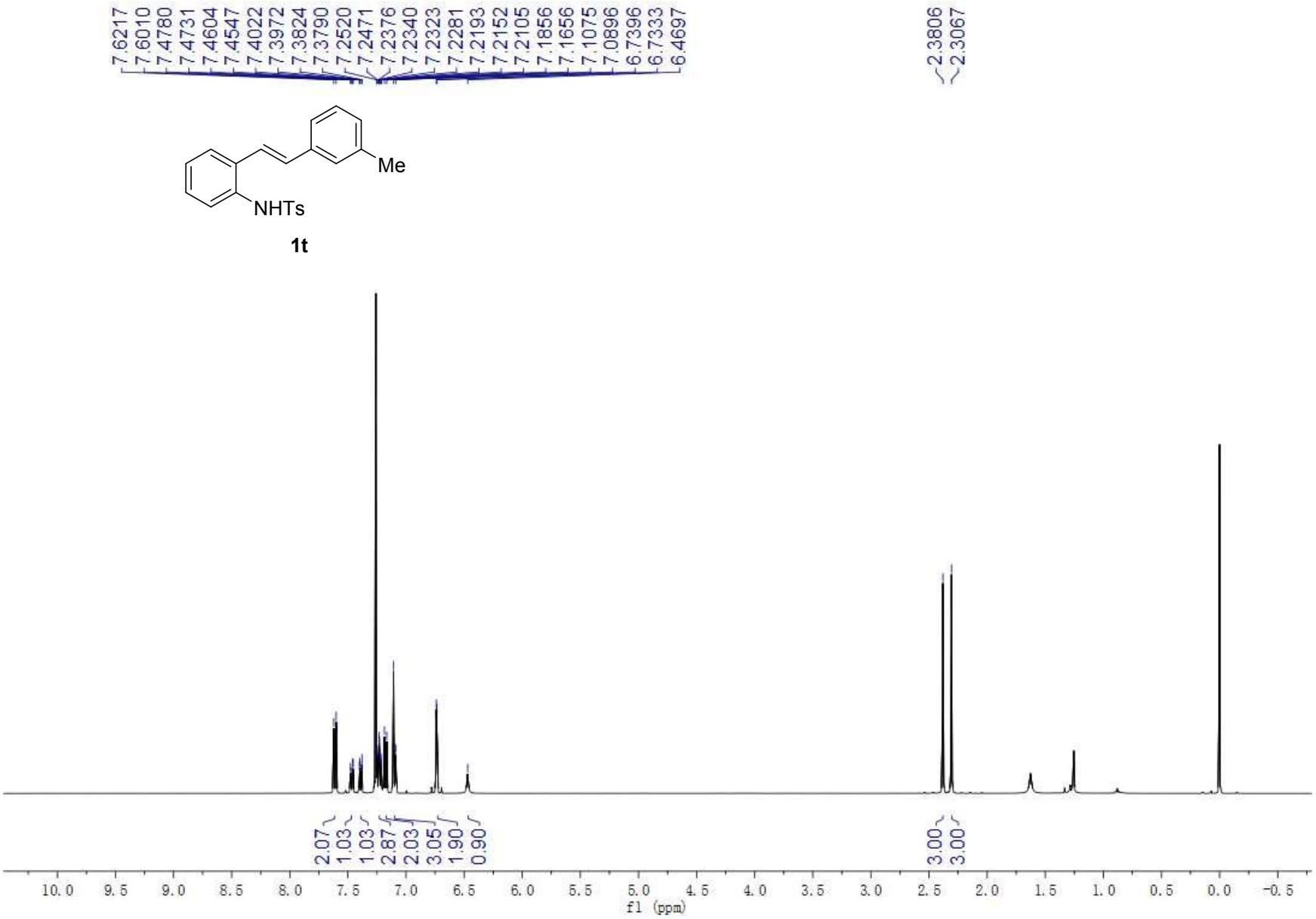
50
40
30
20
10
0
f1 (ppm)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7.2471
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7.2340
7.2323
7.2281
7.2193
7.2152
7.2105
7.1856
7.1656
7.1075
7.0896
6.7396
6.7333
6.4697
2.3806
2.3067
Me
NHTs
1t
2.07
1.03
1.03
2.87
2.03
3.05
1.90
0.90
3.00
3.00
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
1.5
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0.5
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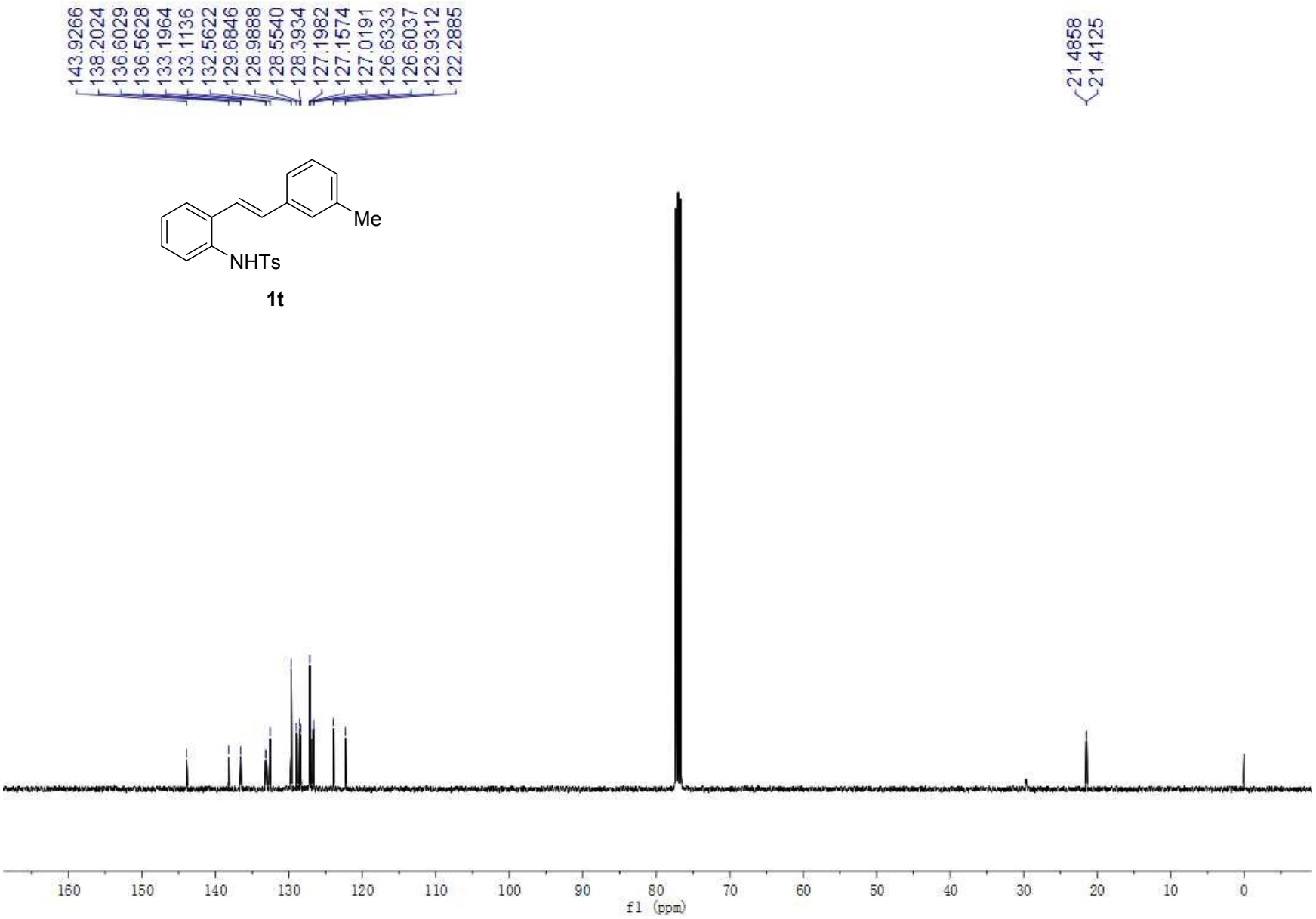
-0.5
f1 (ppm)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127.1574
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126.6333
126.6037
123.9312
122.2885
21.4858
21.4125
Me
NHTs
1t
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150
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130
120
110
100
90
80
70
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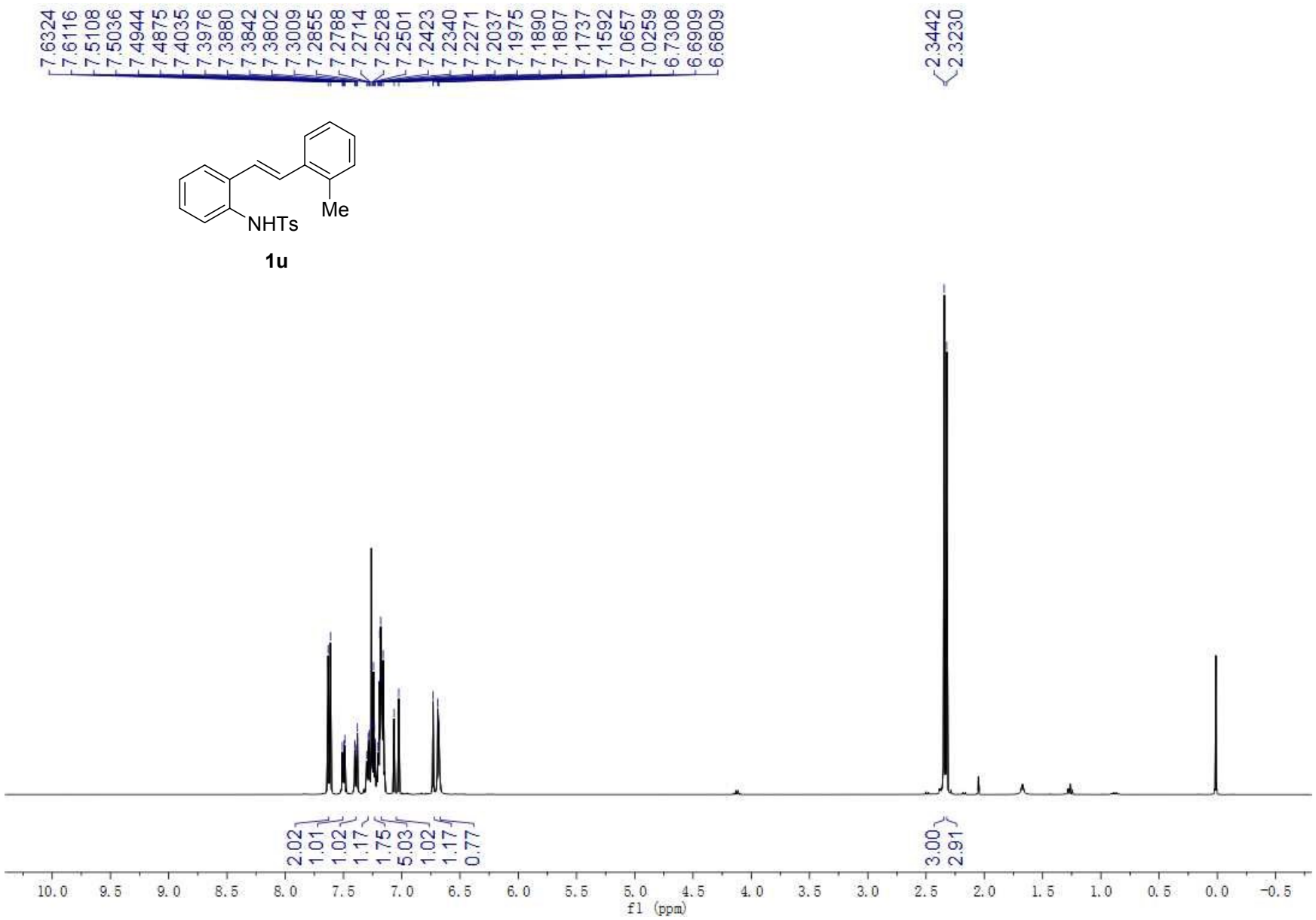
50
40
30
20
10
0
f1 (ppm)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7.2528
7.2501
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7.2271
7.2037
7.1975
7.1890
7.1807
7.1737
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6.6809
2.3442
2.3230
NHTs
Me
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1.01
1.02
1.17
1.75
5.03
1.02
1.17
0.77
3.00
2.91
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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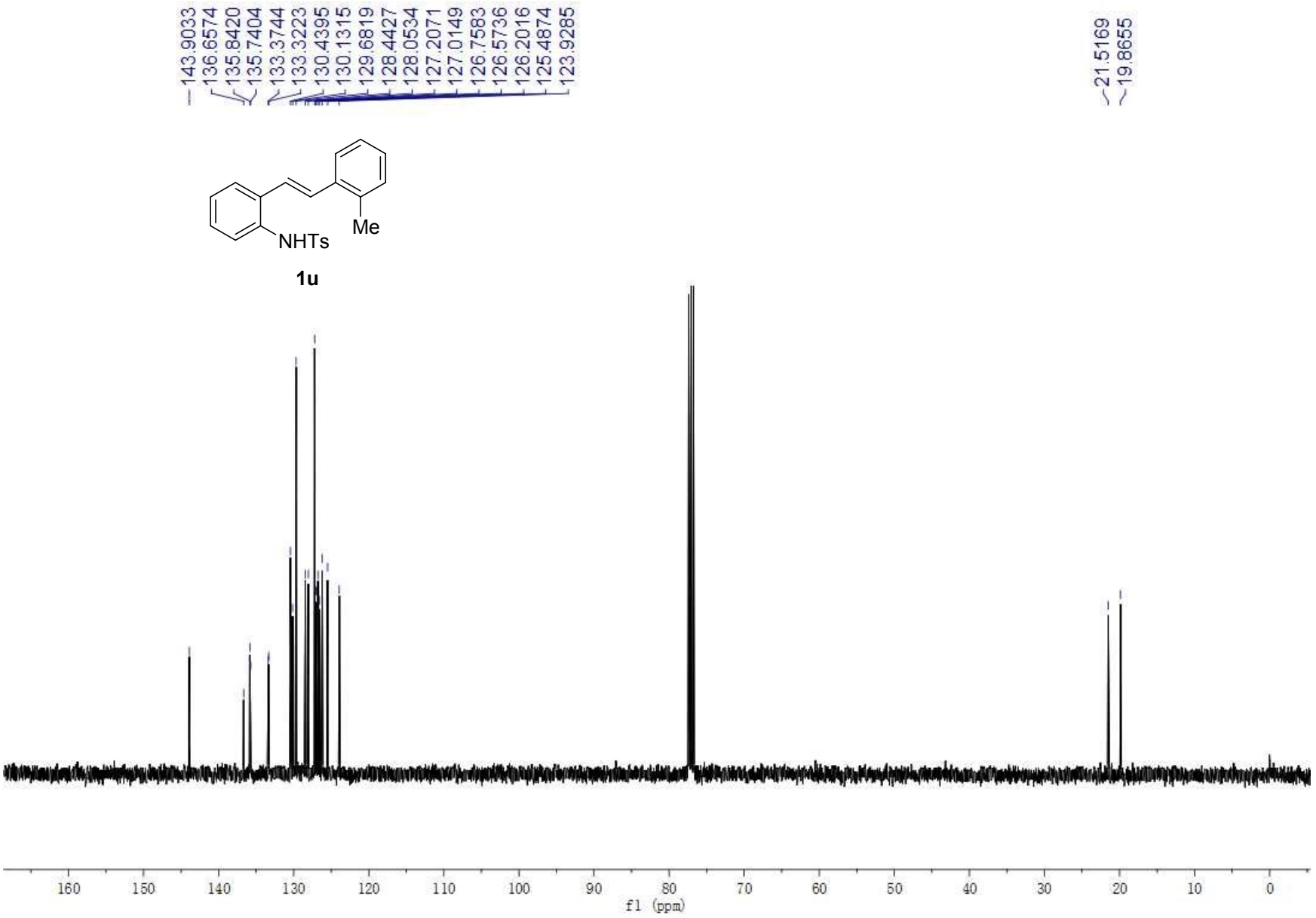
f1 (ppm)

1u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125.4874
123.9285
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NHTs
Me
1u
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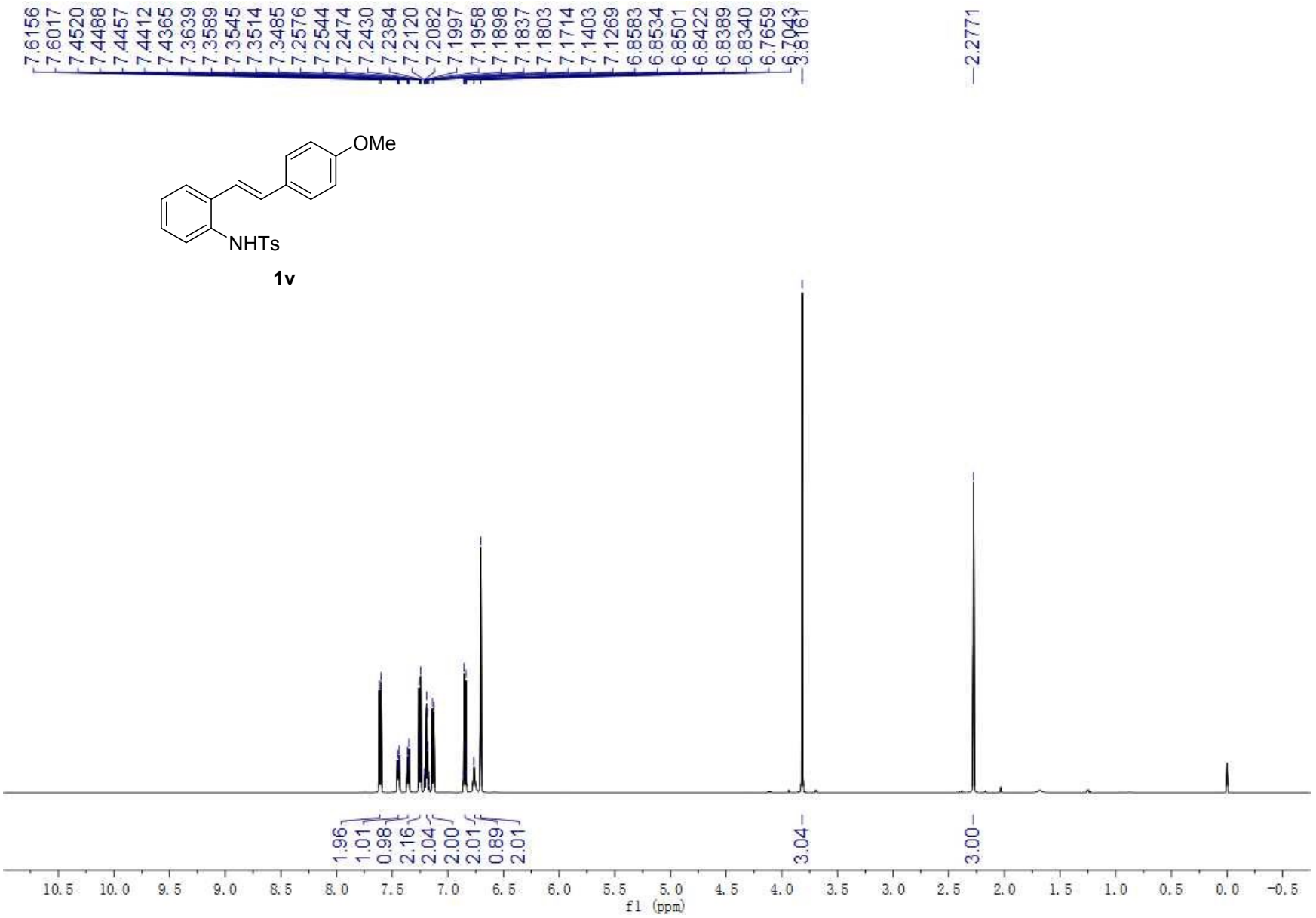
f1 (ppm)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7.2544
7.2474
7.2430
7.2384
7.2120
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7.1997
7.1958
7.1898
7.1837
7.1803
7.1714
7.1403
7.1269
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6.8534
6.8501
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6.7659
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3.8161
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OMe
NHTs
1v
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2.01
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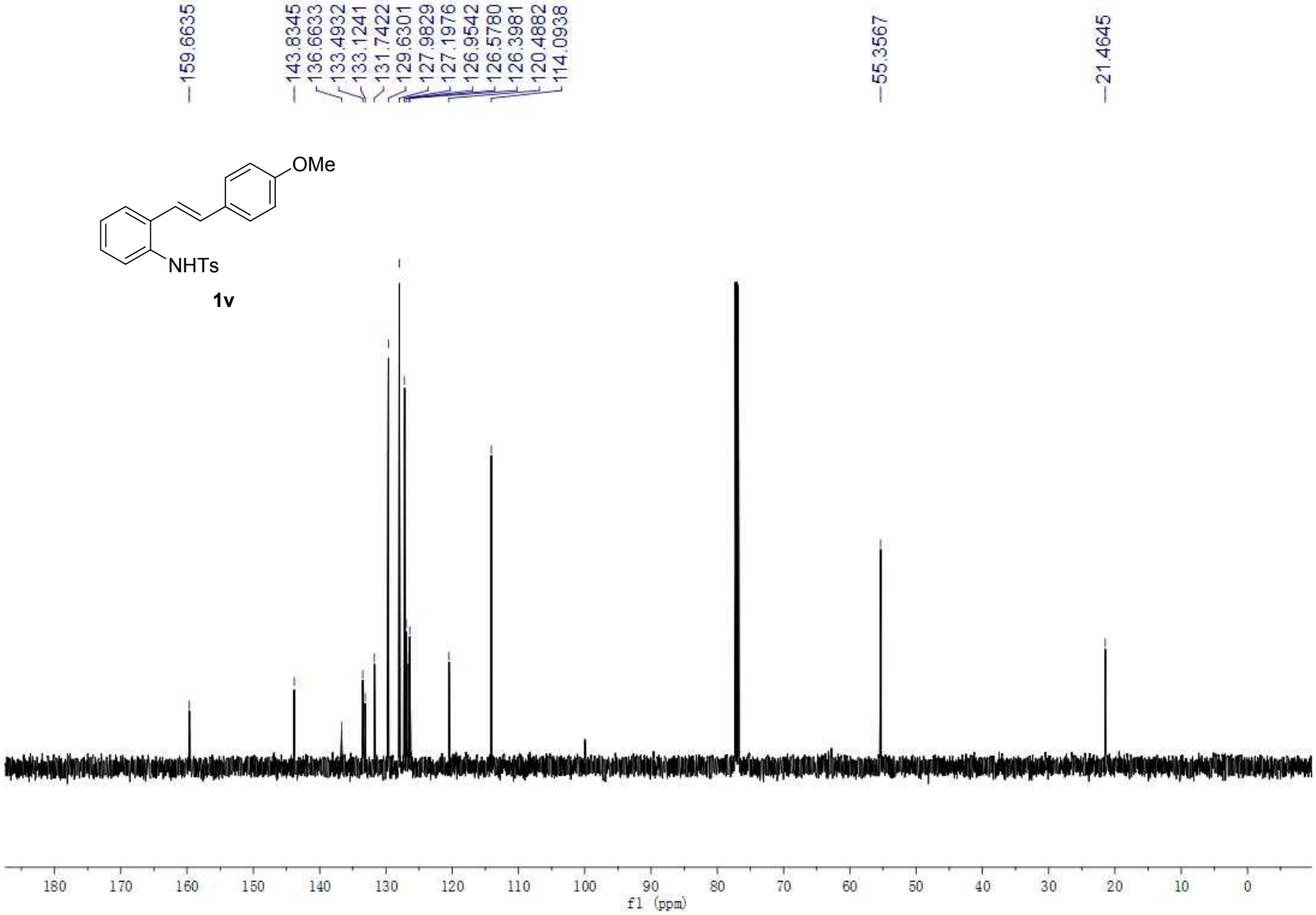
3.00
f1 (ppm)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55.3567
21.4645
OMe
NHTs
1v
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130
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110
100
90
80
70
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50
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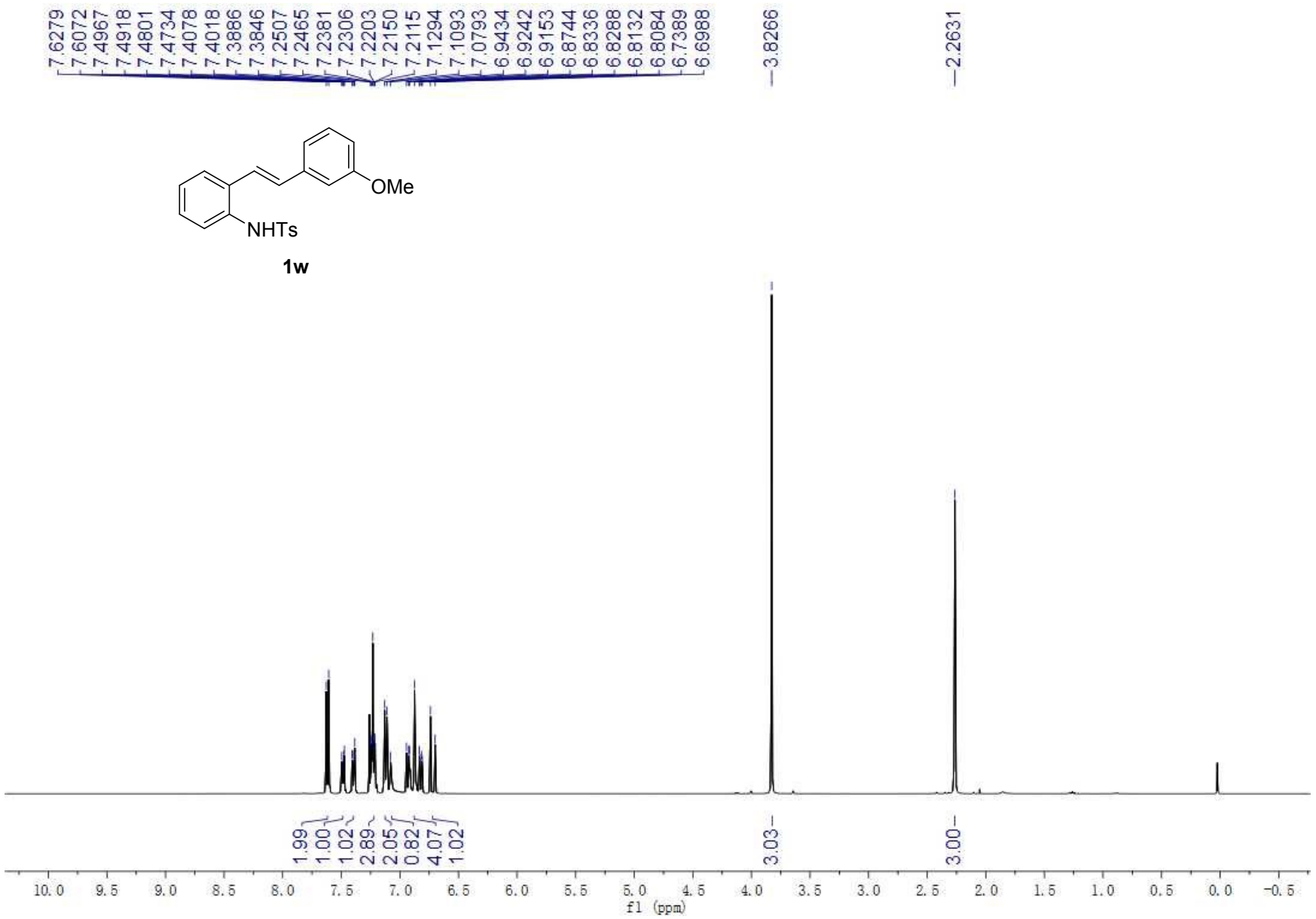
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7.2465
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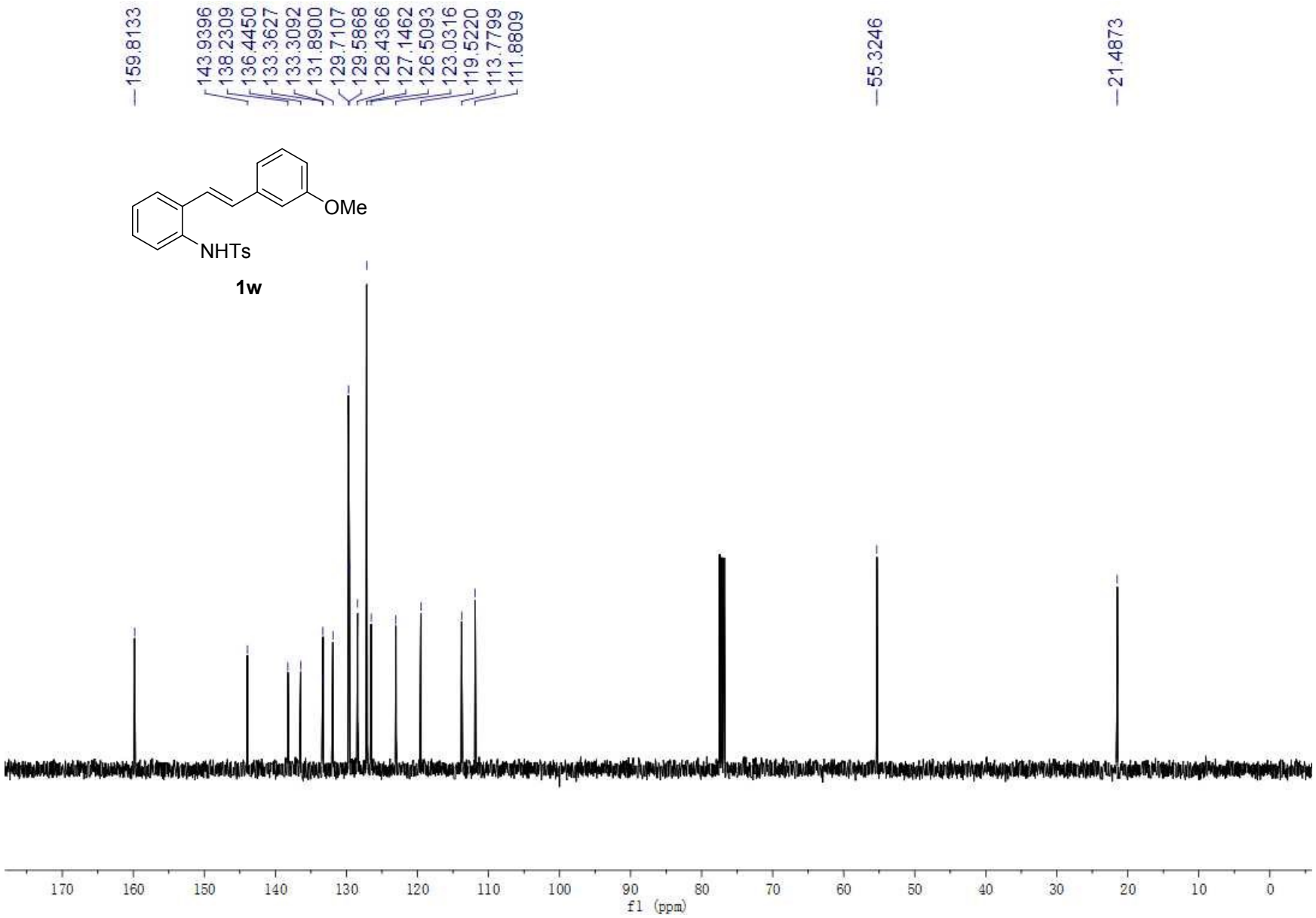
7.2306
7.2203
7.2150
7.2115
7.1294
7.1093
7.0793
6.9434
6.9242
6.9153
6.8744
6.8336
6.8288
6.8132
6.8084
6.7389
6.6988
3.8266
2.2631
OMe
NHTs
1w
1.99
1.00
1.02
2.89
2.05
0.82
4.07
1.02
3.03
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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123.0316
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113.7799
111.8809
55.3246
21.4873
OMe
NHTs
1w
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130
120
110
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90
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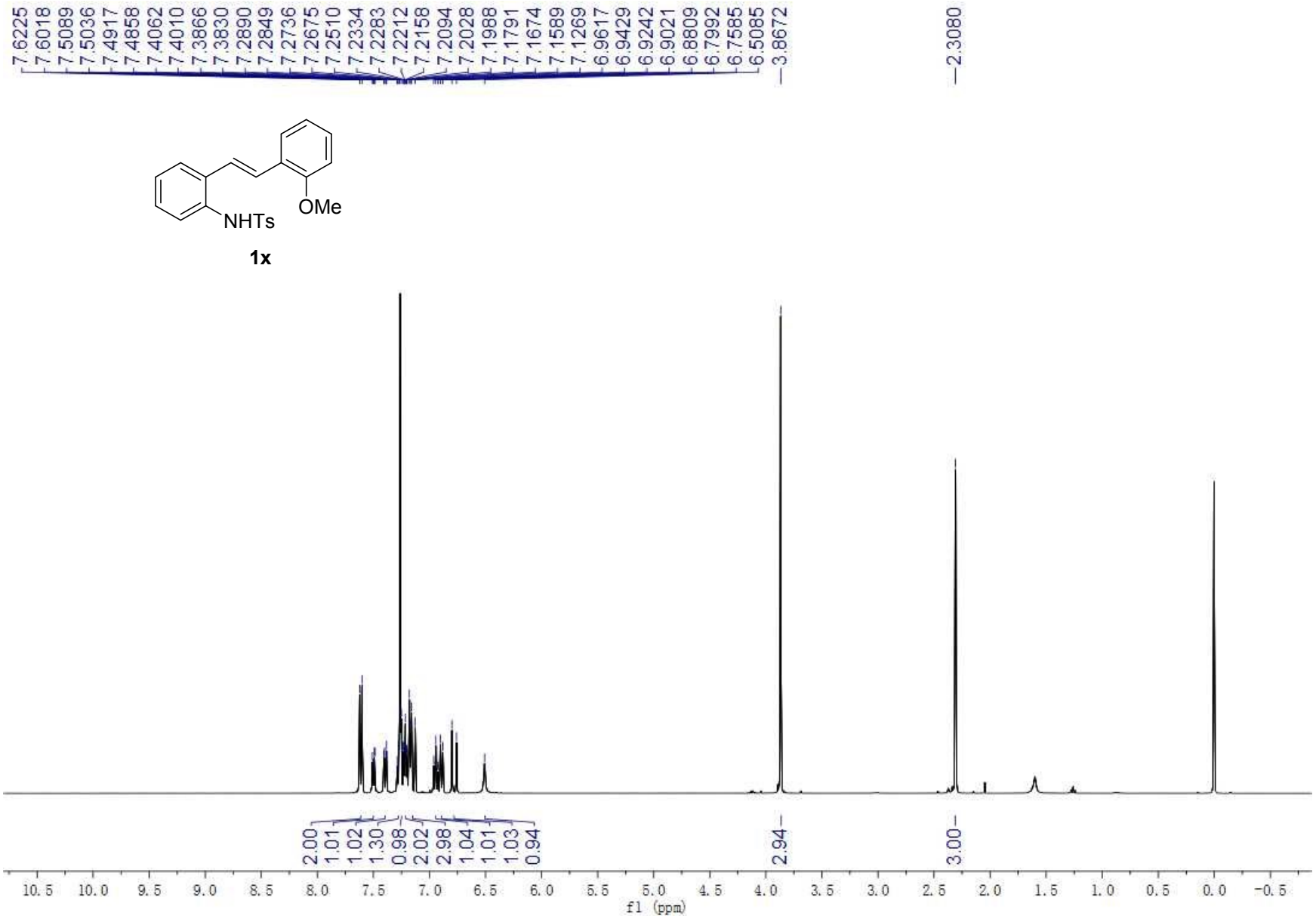
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7.2510
7.2334
7.2283
7.2212
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7.2094
7.2028
7.1988
7.1791
7.1674
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7.1269
6.9617
6.9429
6.9242
6.9021
6.8809
6.7992
6.7585
6.5085
3.8672
2.3080
NHTs
OMe
1x
2.00
1.01
1.02
1.30
0.98
2.02
2.98
1.04
1.01
1.03
0.94
2.94
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
1.5
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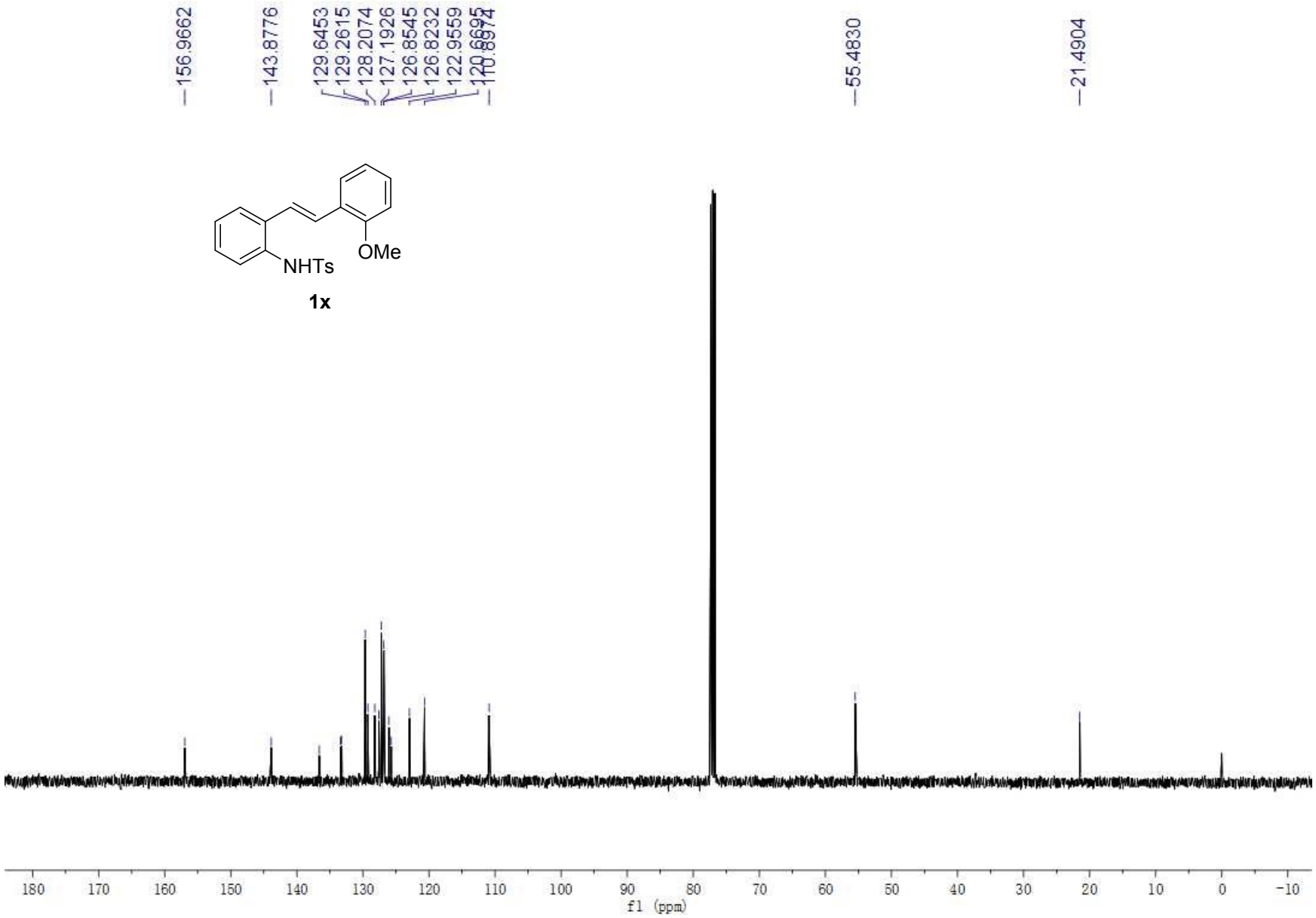
-0.5
f1 (ppm)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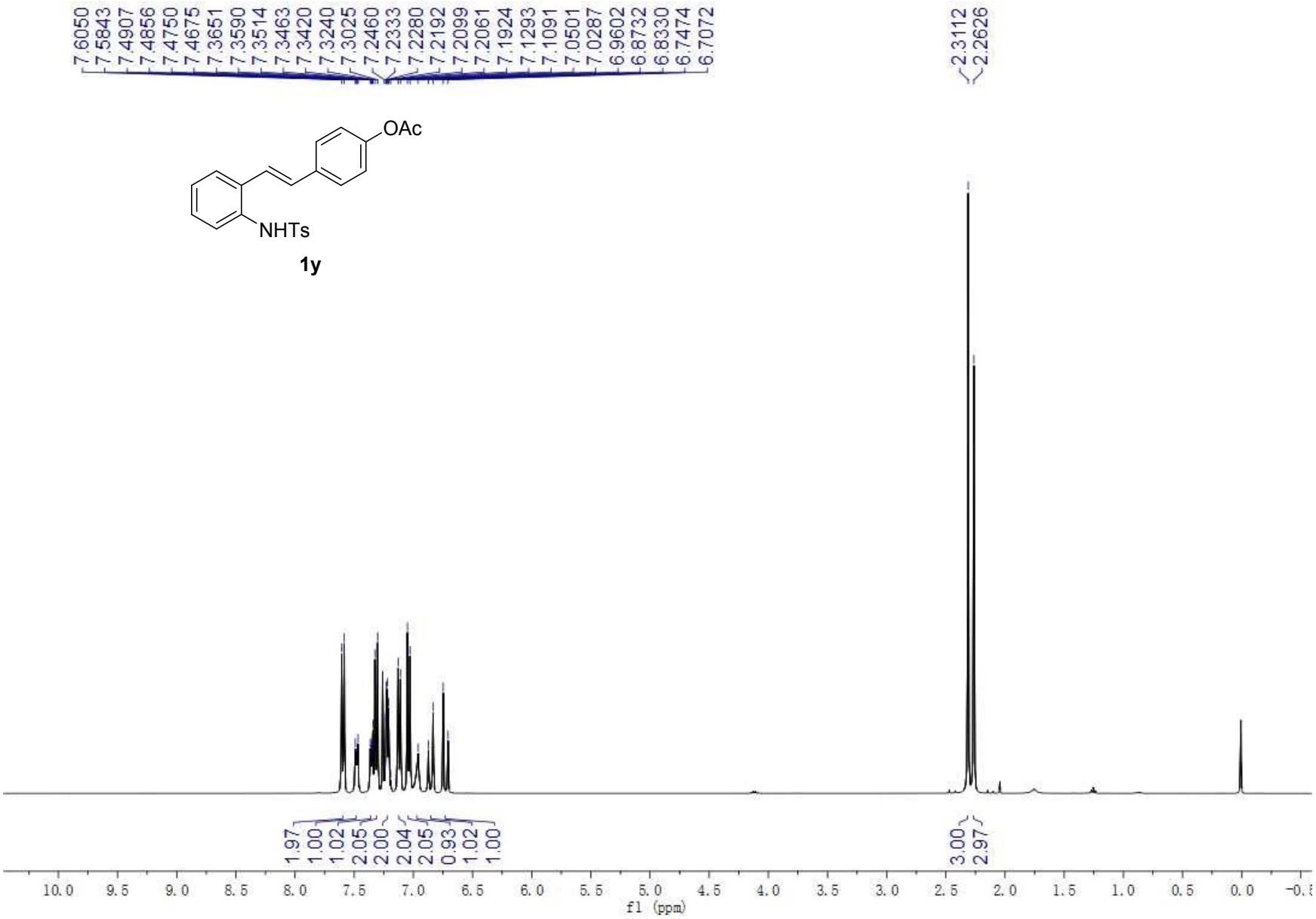
NHTs
OMe
1x
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.3420
7.3240
7.3025
7.2460
7.2333
7.2280
7.2192
7.2099
7.2061
7.1924
7.1293
7.1091
7.0501
7.0287
6.9602
6.8732
6.8330
6.7474
6.7072
2.3112
2.2626
OAc
NHTs
1y
1.97
1.00
1.02
2.05
2.00
2.04
2.05
0.93
1.02
1.00
3.00
2.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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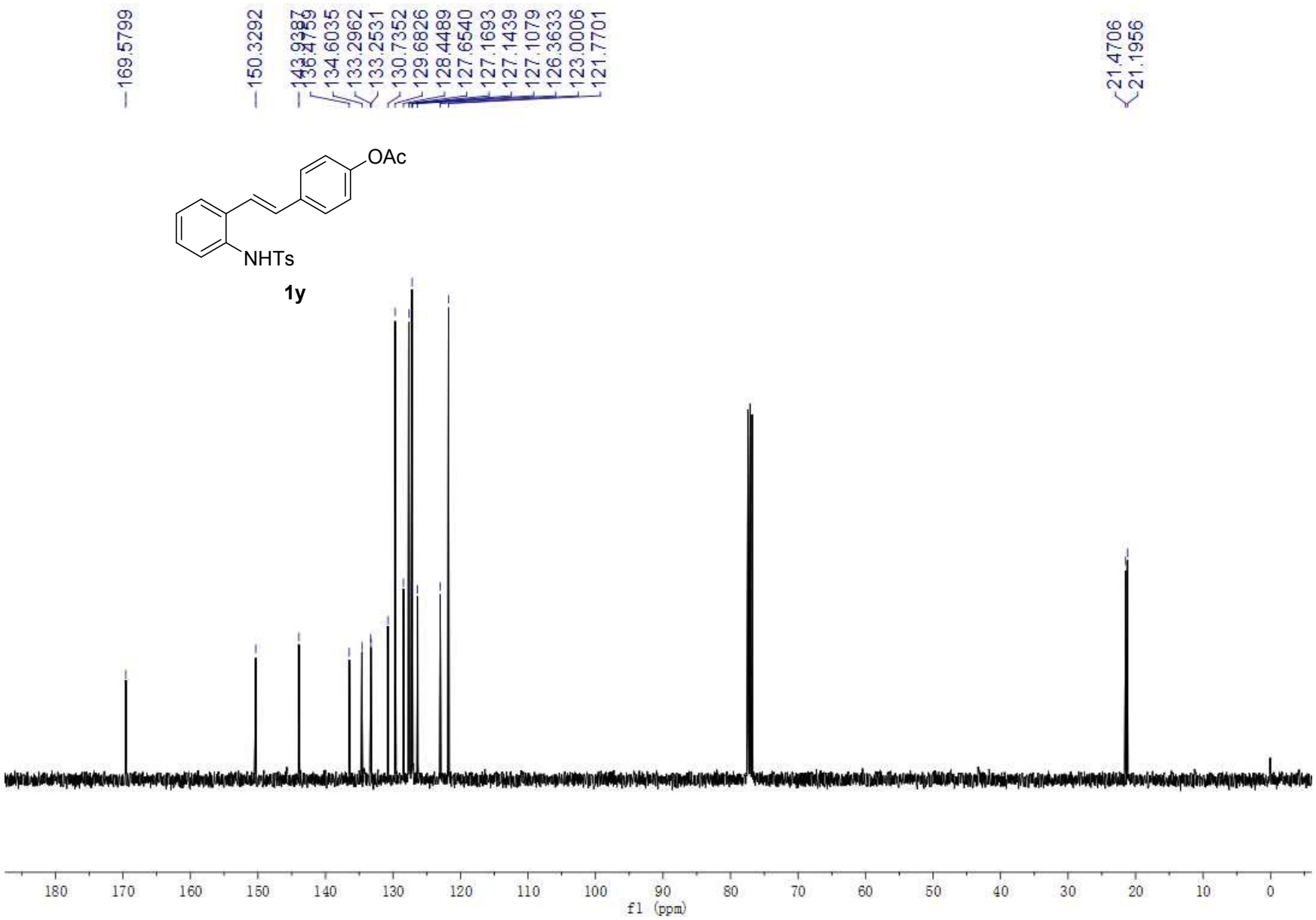
0.0
f1 (ppm)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126.3633
123.0006
121.7701
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21.1956
OAc
NHTs
1y
180
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160
150
140
130
120
110
100
90
80
70
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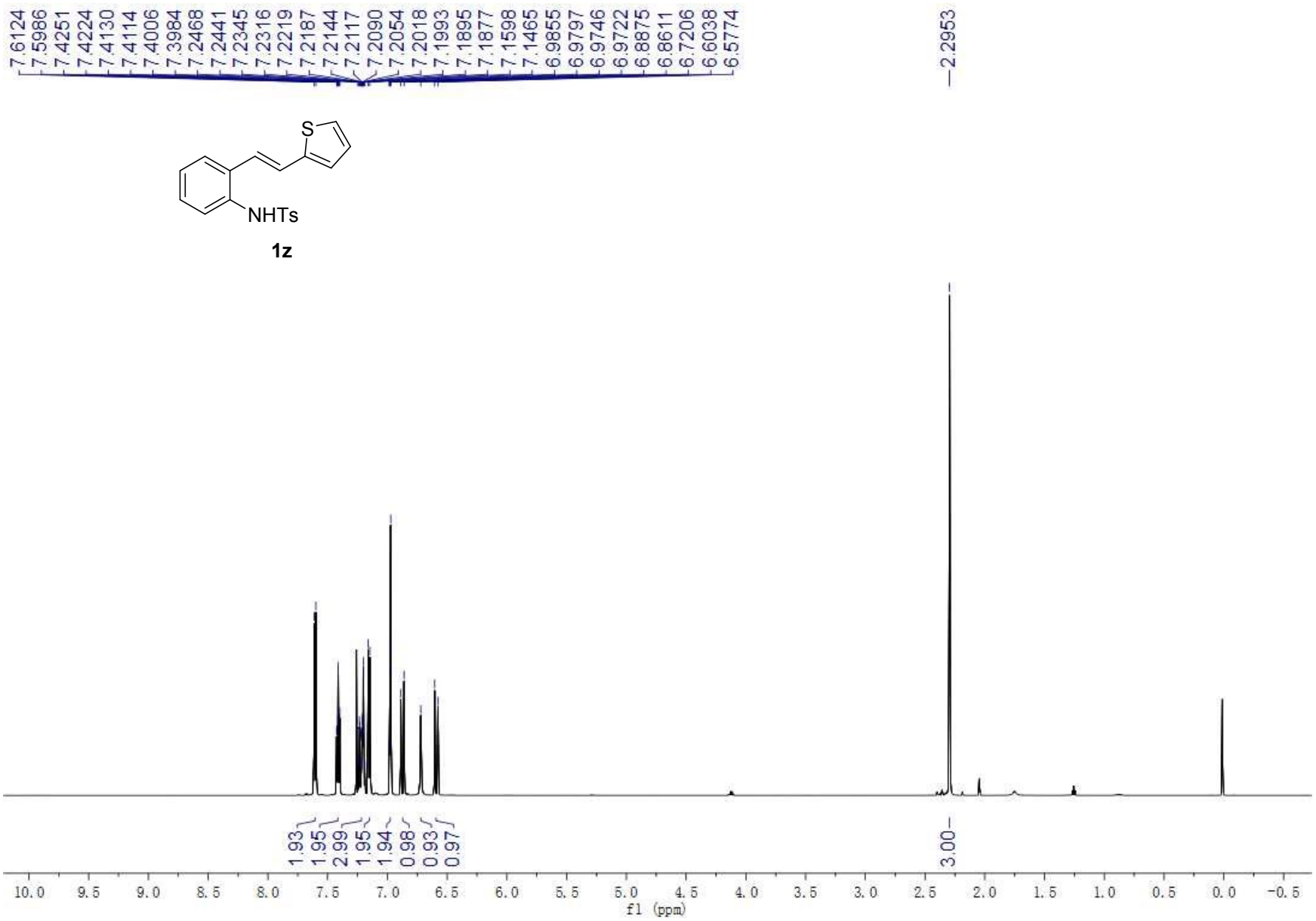
50
40
30
20
10
0
f1 (ppm)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7.2345
7.2316
7.2219
7.2187
7.2144
7.2117
7.2090
7.2054
7.2018
7.1993
7.1895
7.1877
7.1598
7.1465
6.9855
6.9797
6.9746
6.9722
6.8875
6.8611
6.7206
6.6038
6.5774
2.2953
S
NHTs
1z
1.93
1.95
2.99
1.95
1.94
0.98
0.93
0.97
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
5.5
5.0
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2.0
1.5
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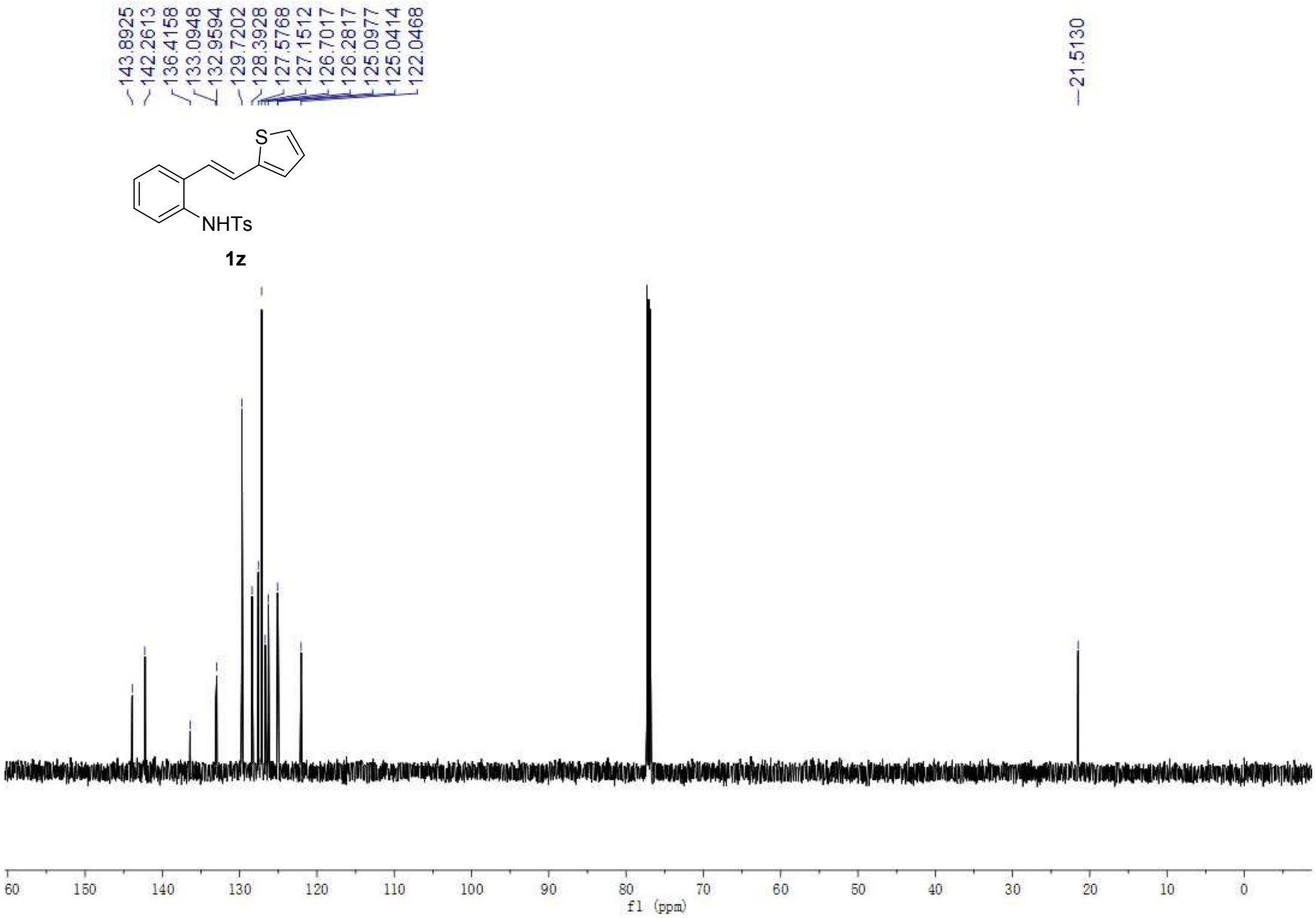
-0.5
f1 (ppm)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125.0977
125.0414
122.0468
21.5130
S
NHTs
1z
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130
120
110
100
90
80
70
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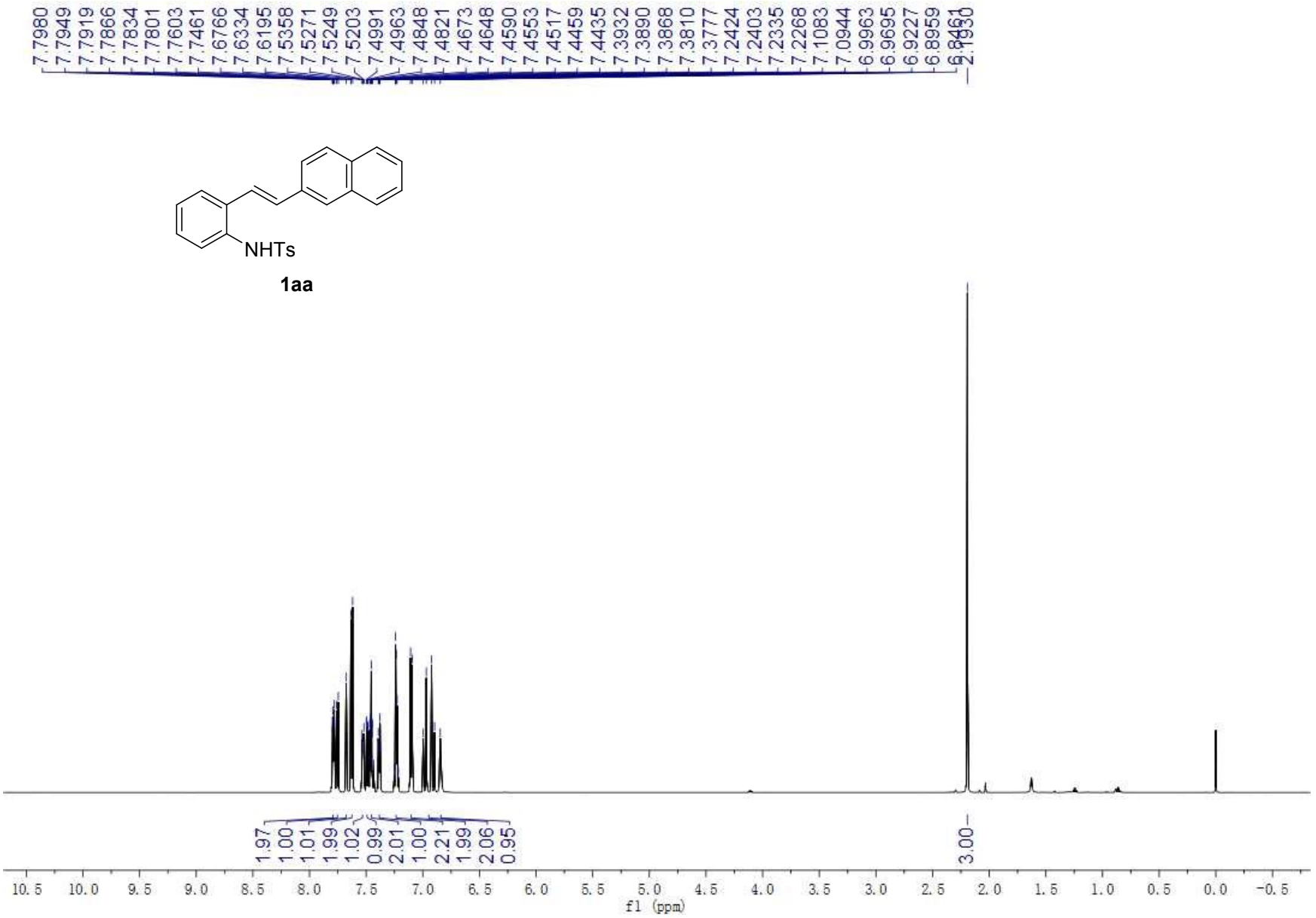
50
40
30
20
10
0
f1 (ppm)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7.4821
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7.4648
7.4590
7.4553
7.4517
7.4459
7.4435
7.3932
7.3890
7.3868
7.3810
7.3777
7.2424
7.2403
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2.1930
NHTs
1aa
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1.01
1.99
1.02
0.99
2.01
1.00
2.21
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2.06
0.95
3.00
10.5
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9.0
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6.0
5.5
5.0
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3.0
2.5
2.0
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0.5
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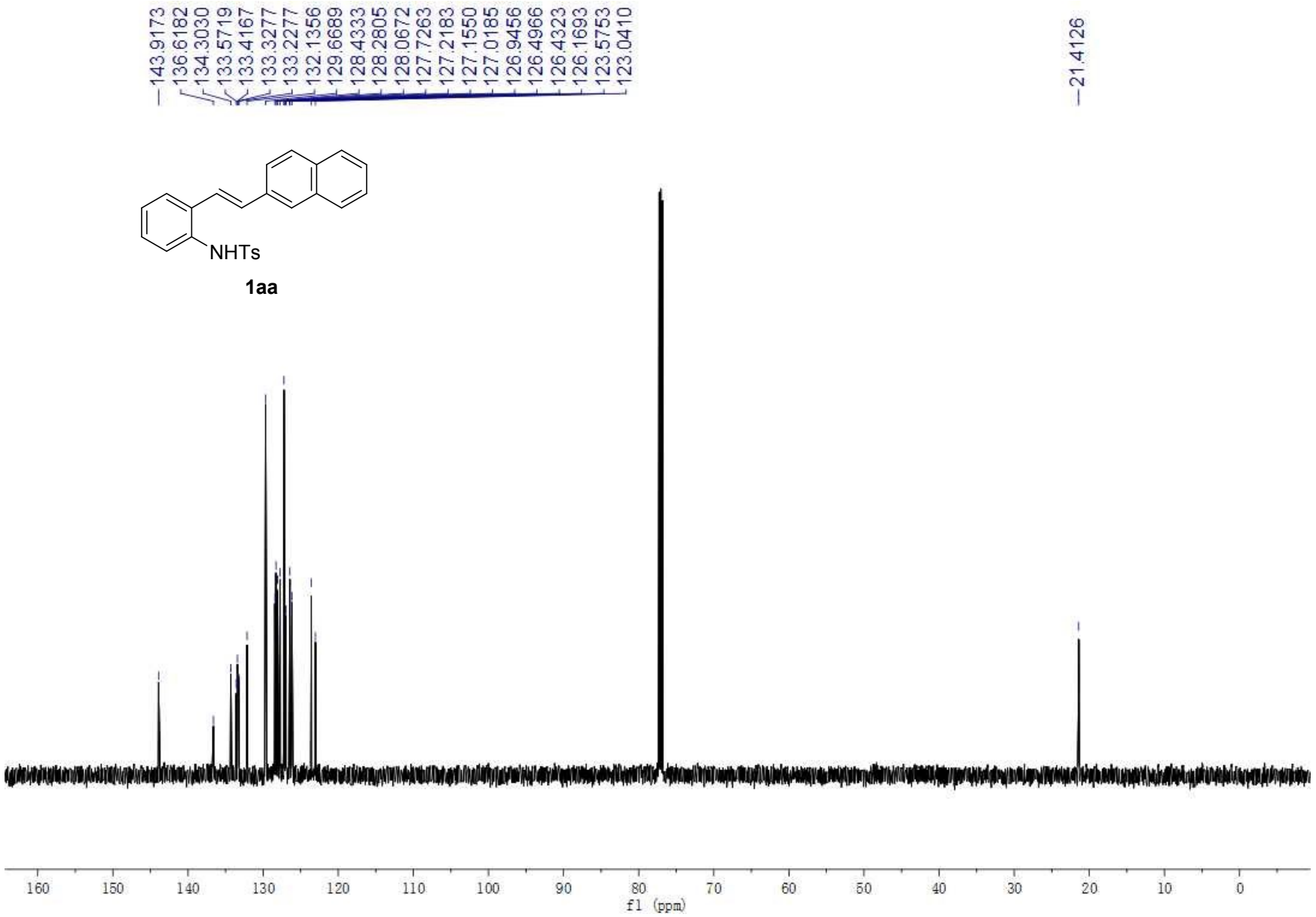
-0.5
f1 (ppm)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126.1693
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123.0410
21.4126
NHTs
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120
110
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90
80
70
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50
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30
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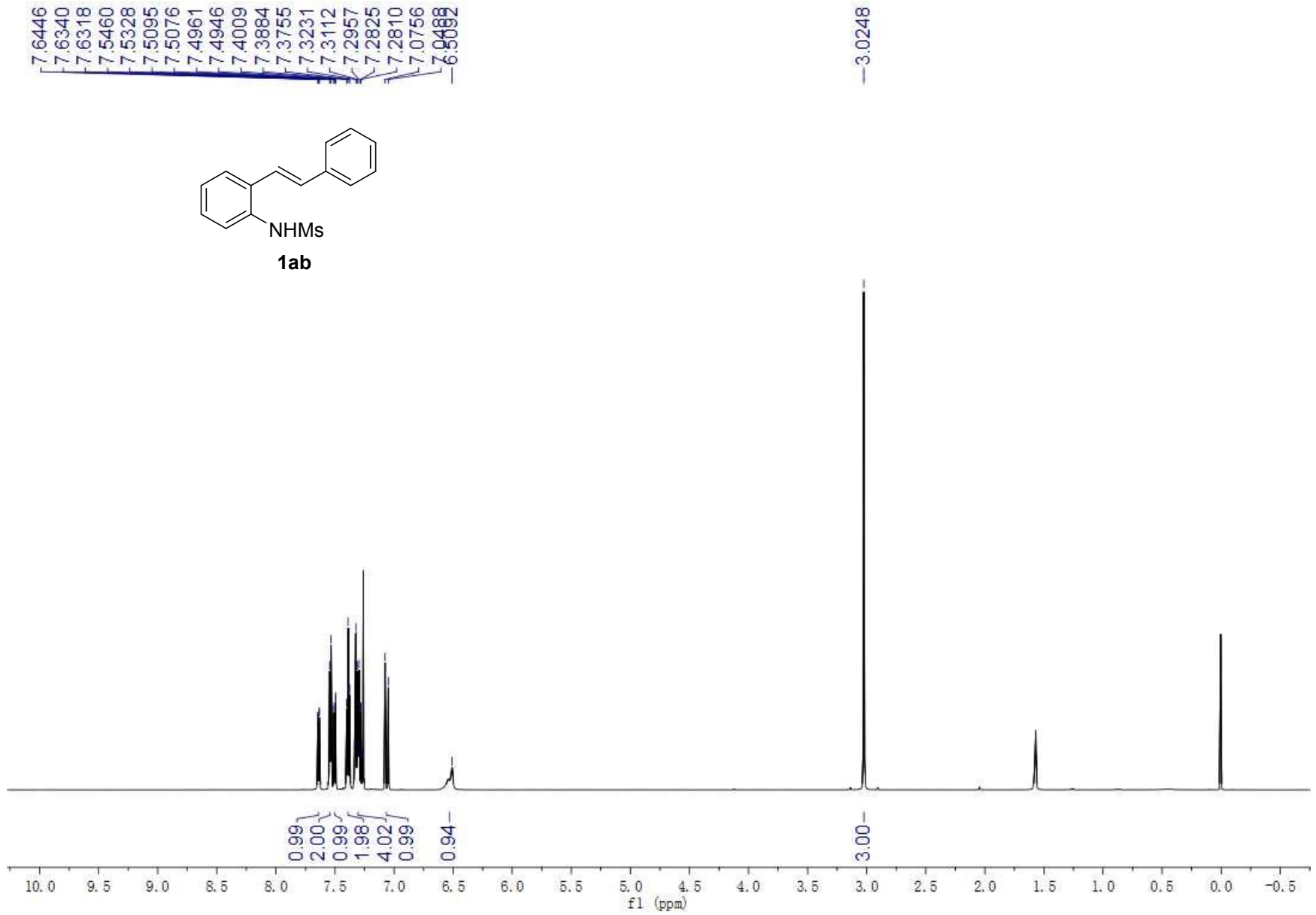
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7.2957
7.2825
7.2810
7.0756
7.0488
7.0392
6.5092
3.0248
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0.99
1.98
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0.99
0.94
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7.5
7.0
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6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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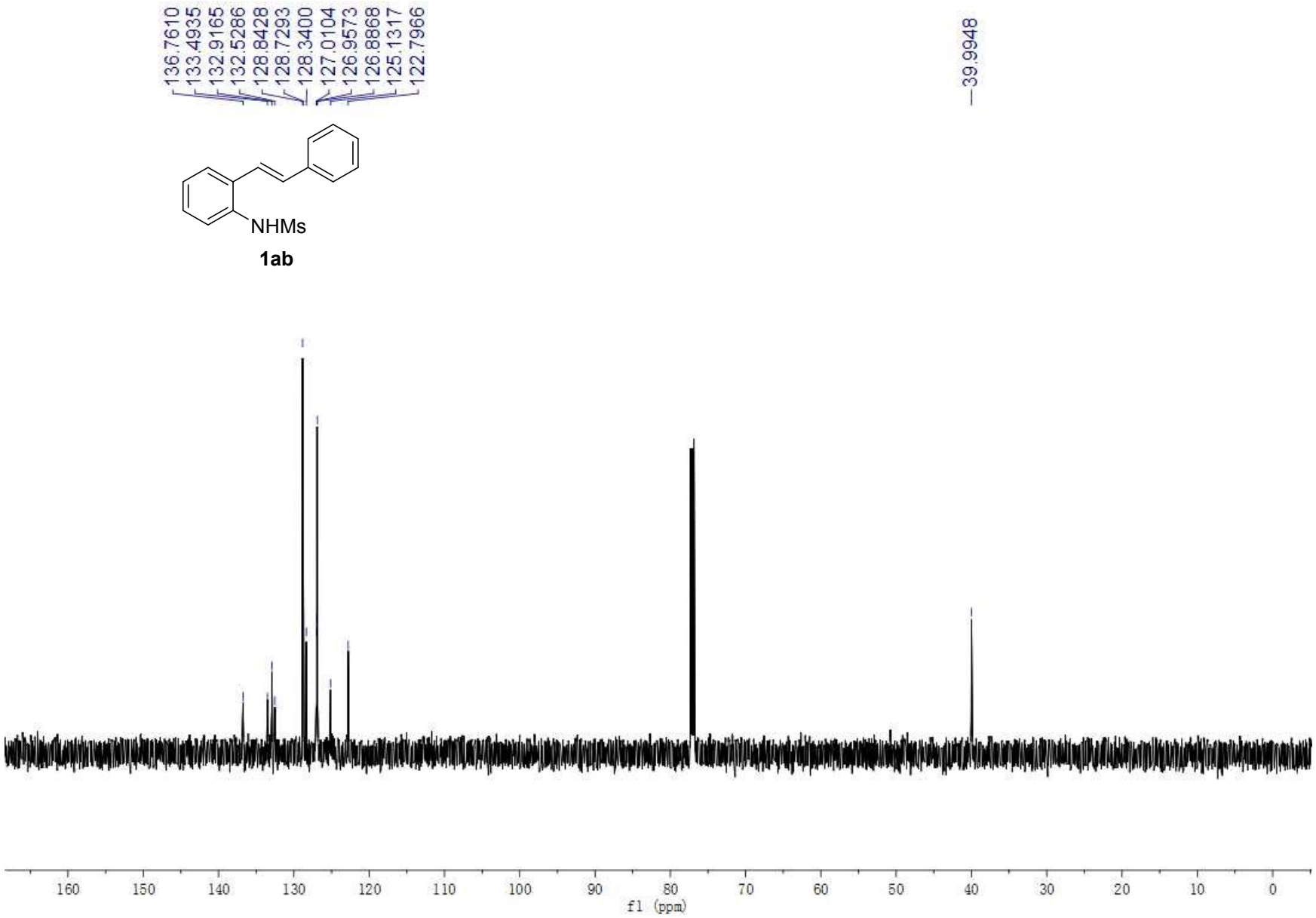
0.5
0.0
-0.5
f1 (ppm)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122.7966
39.9948
NHMs
1ab
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150
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130
120
110
100
90
80
70
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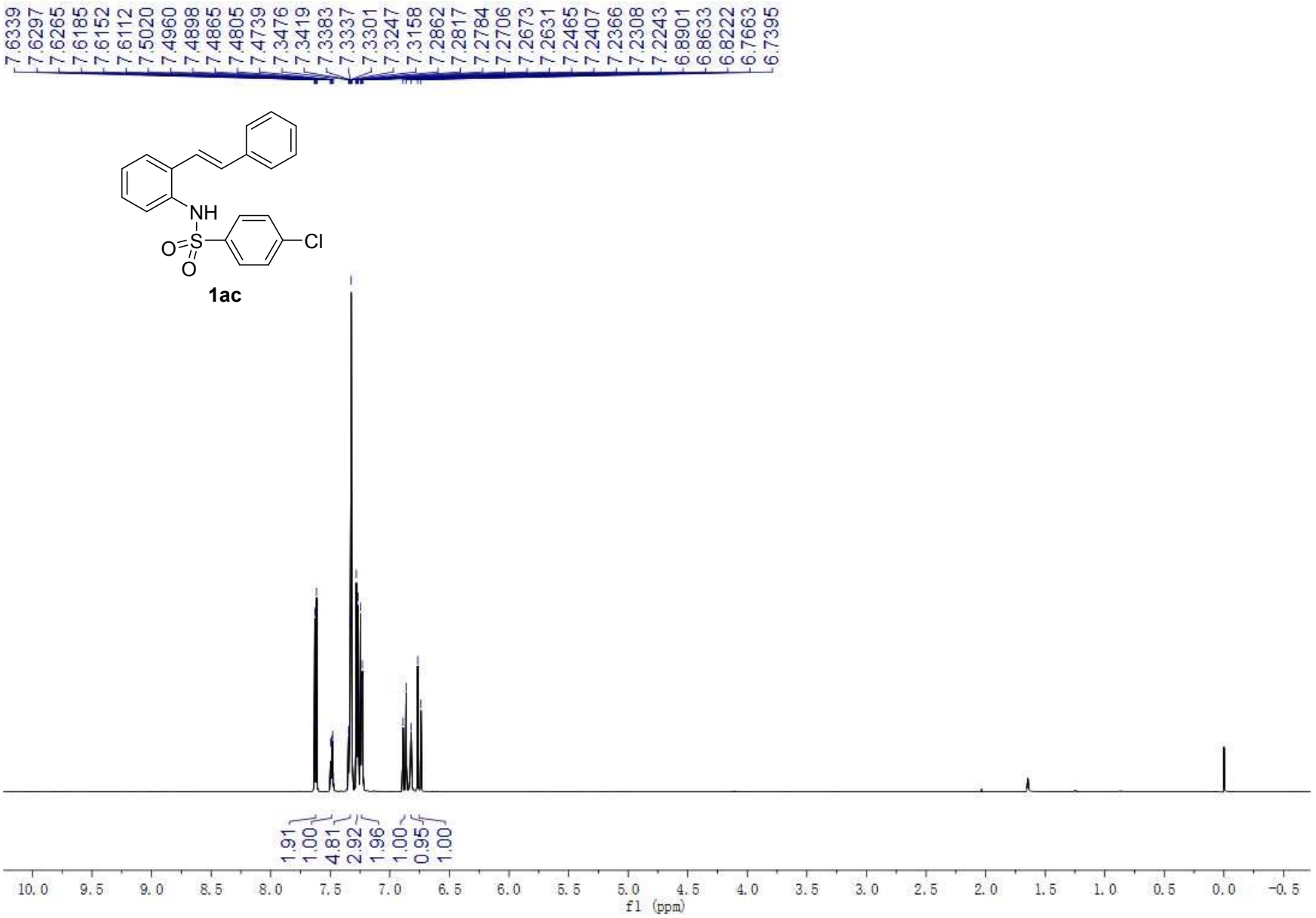
50
40
30
20
10
0
f1 (ppm)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NH
S
O
O
Cl
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2.92
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1.00
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9.0
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7.0
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6.0
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5.0
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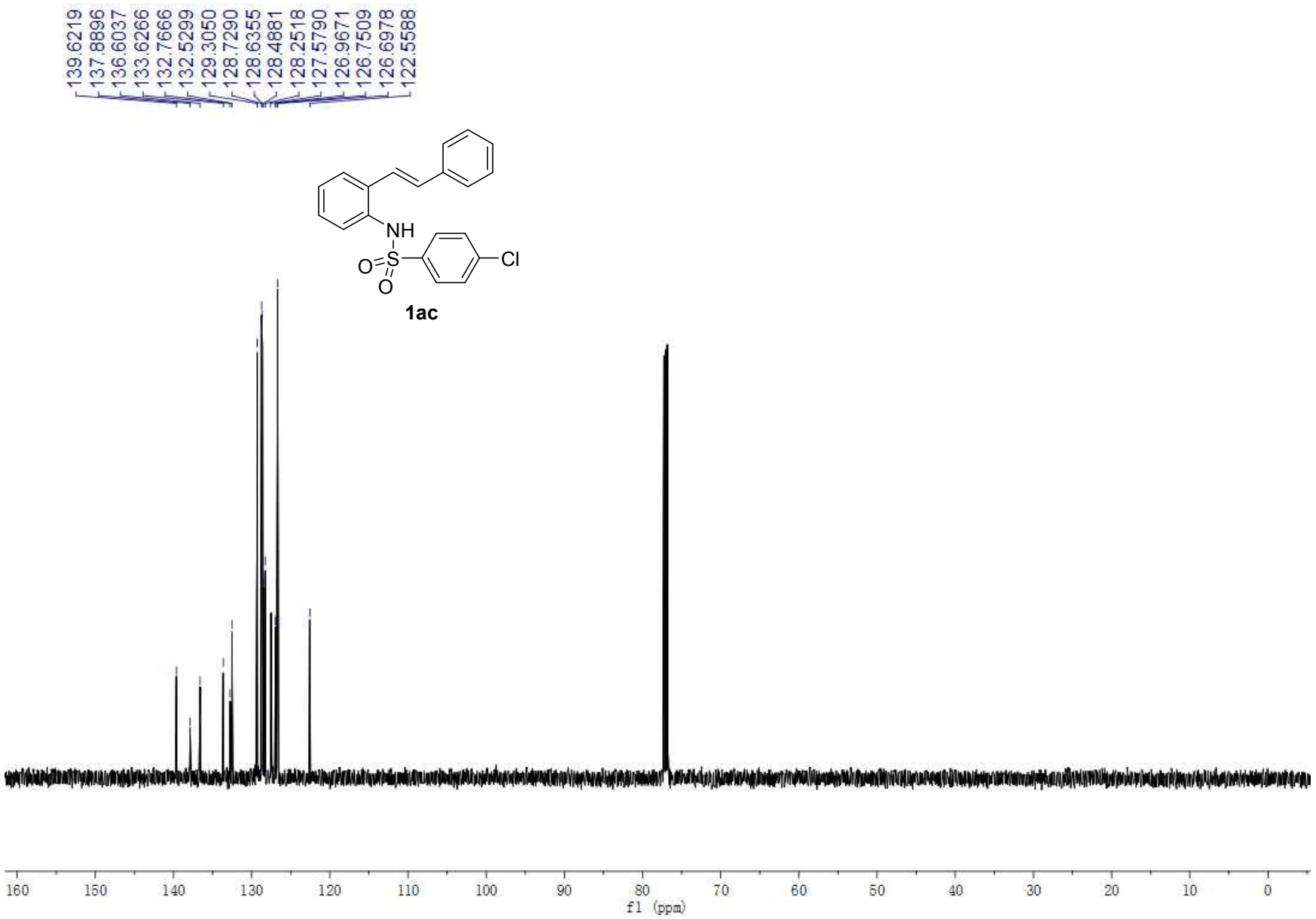
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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O
S
O
Cl
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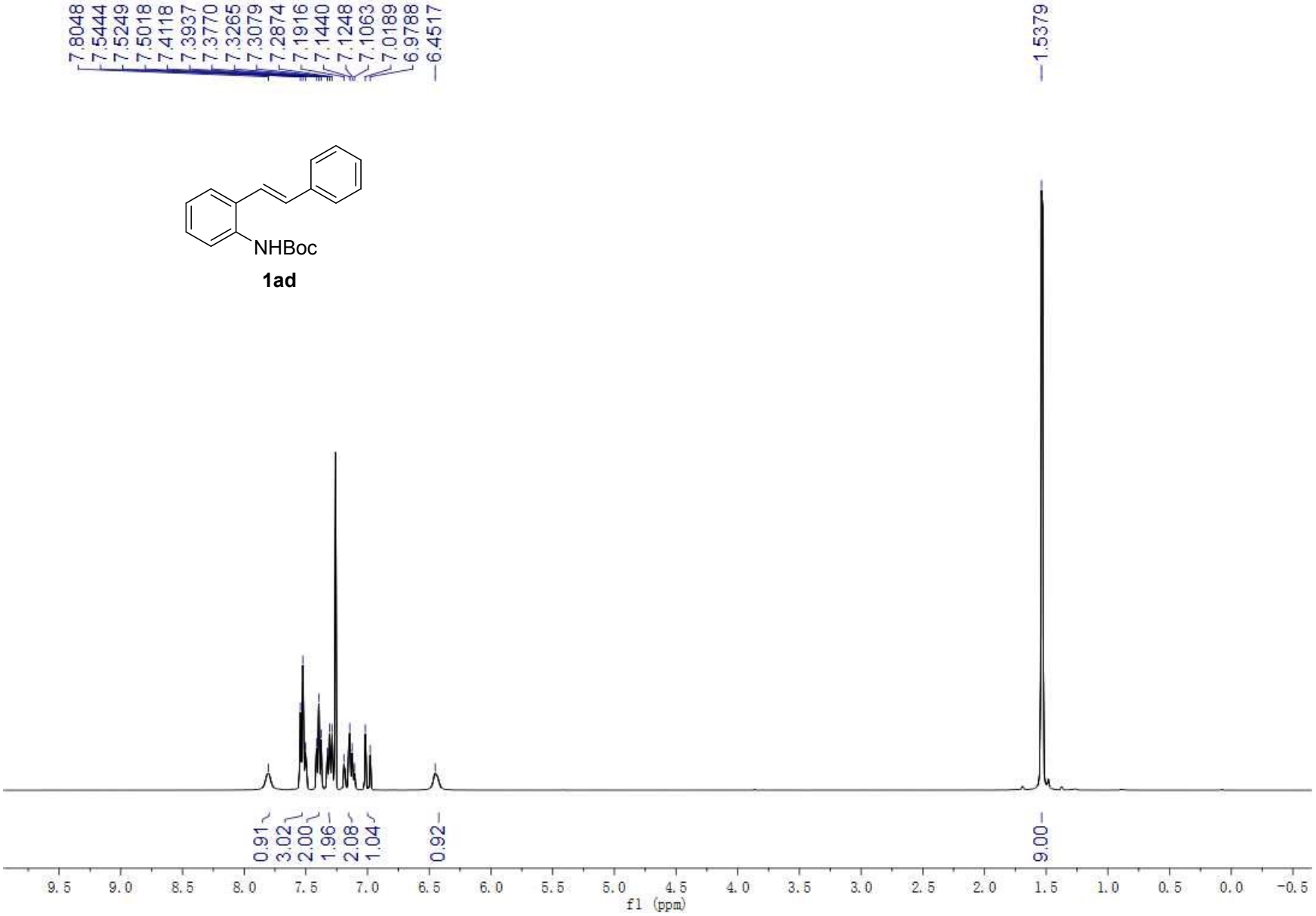
f1 (ppm)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NHBoc
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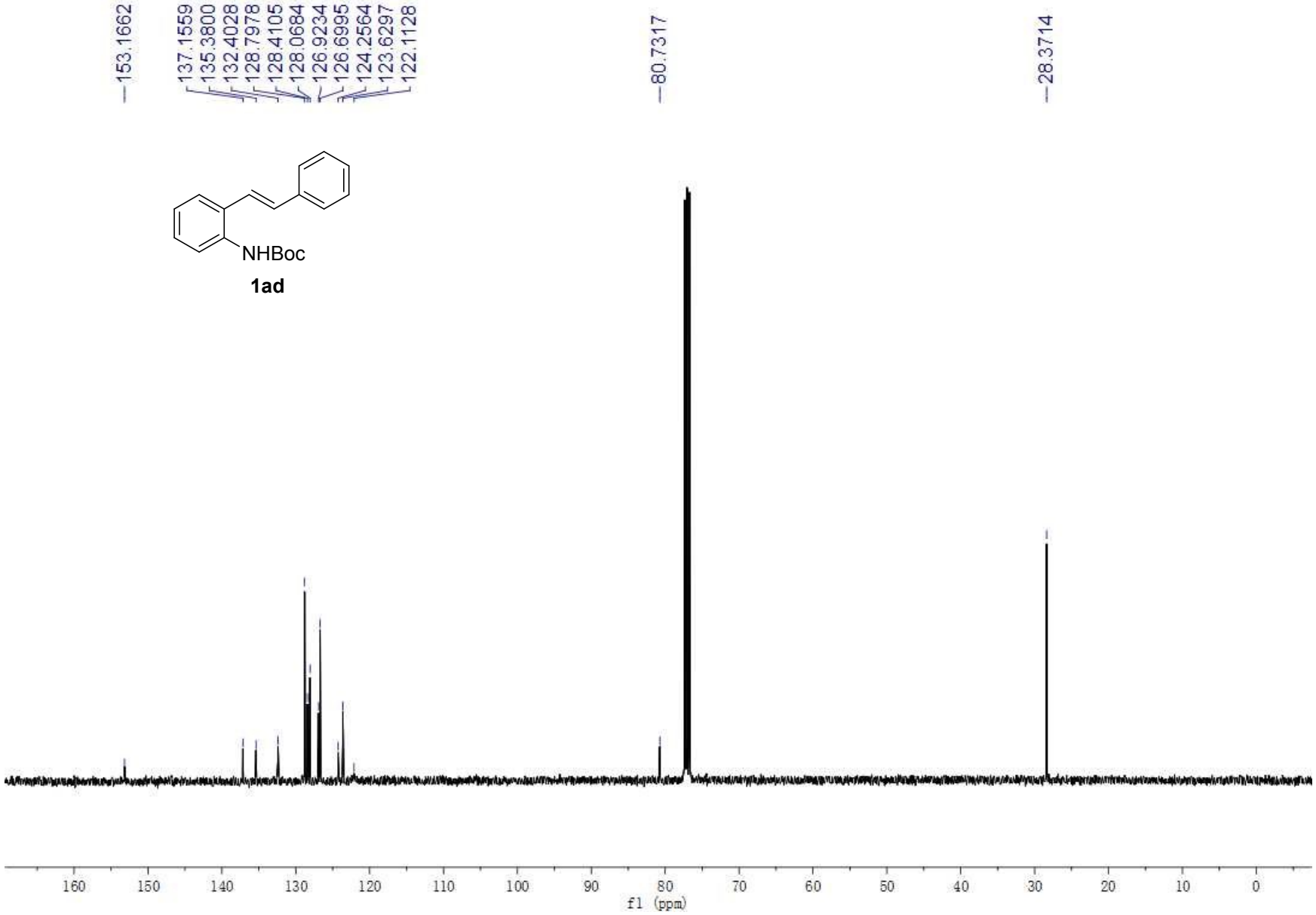
f1 (ppm)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NHBoc
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110
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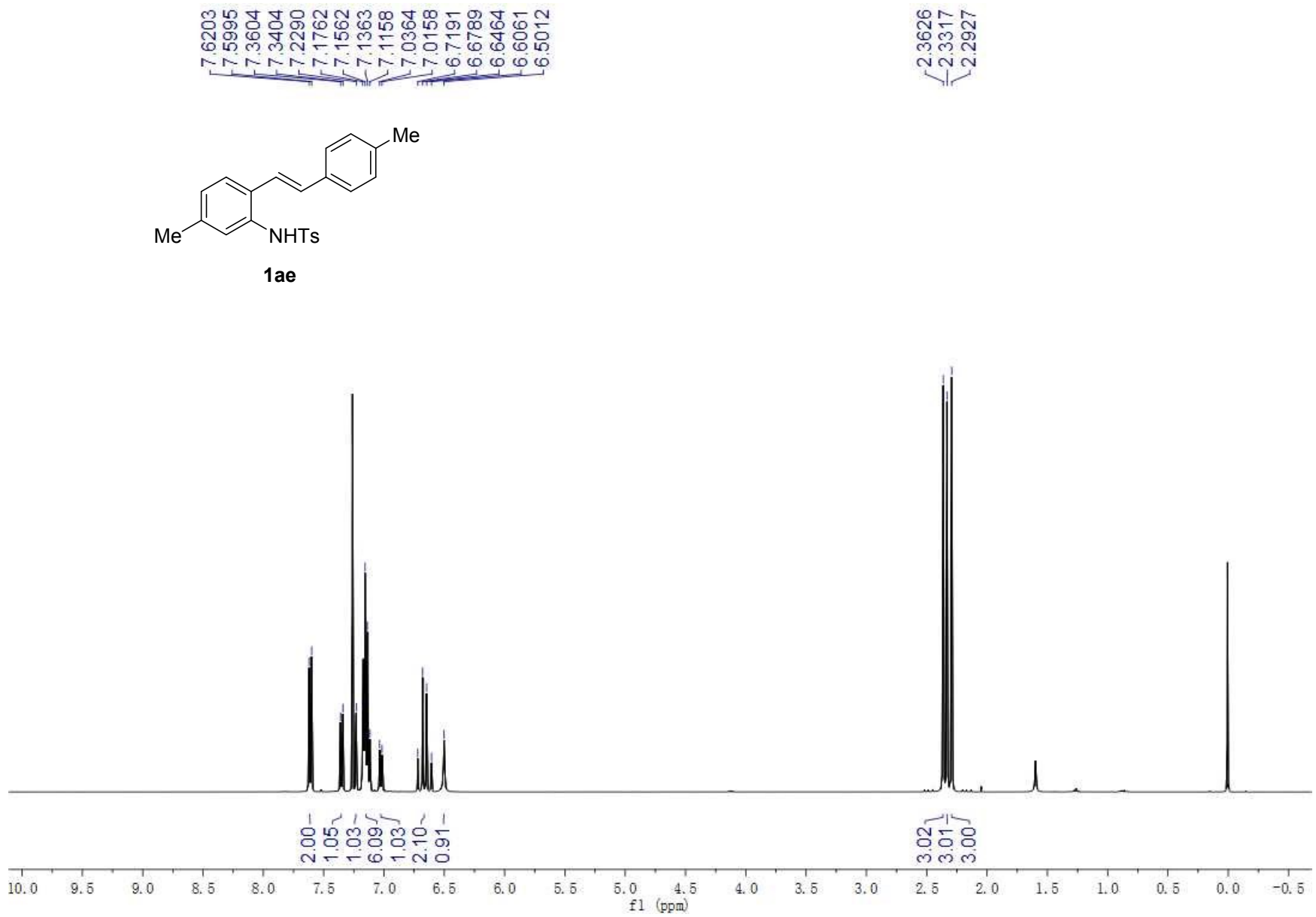
f1 (ppm)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2.2927
Me
Me
NHTs
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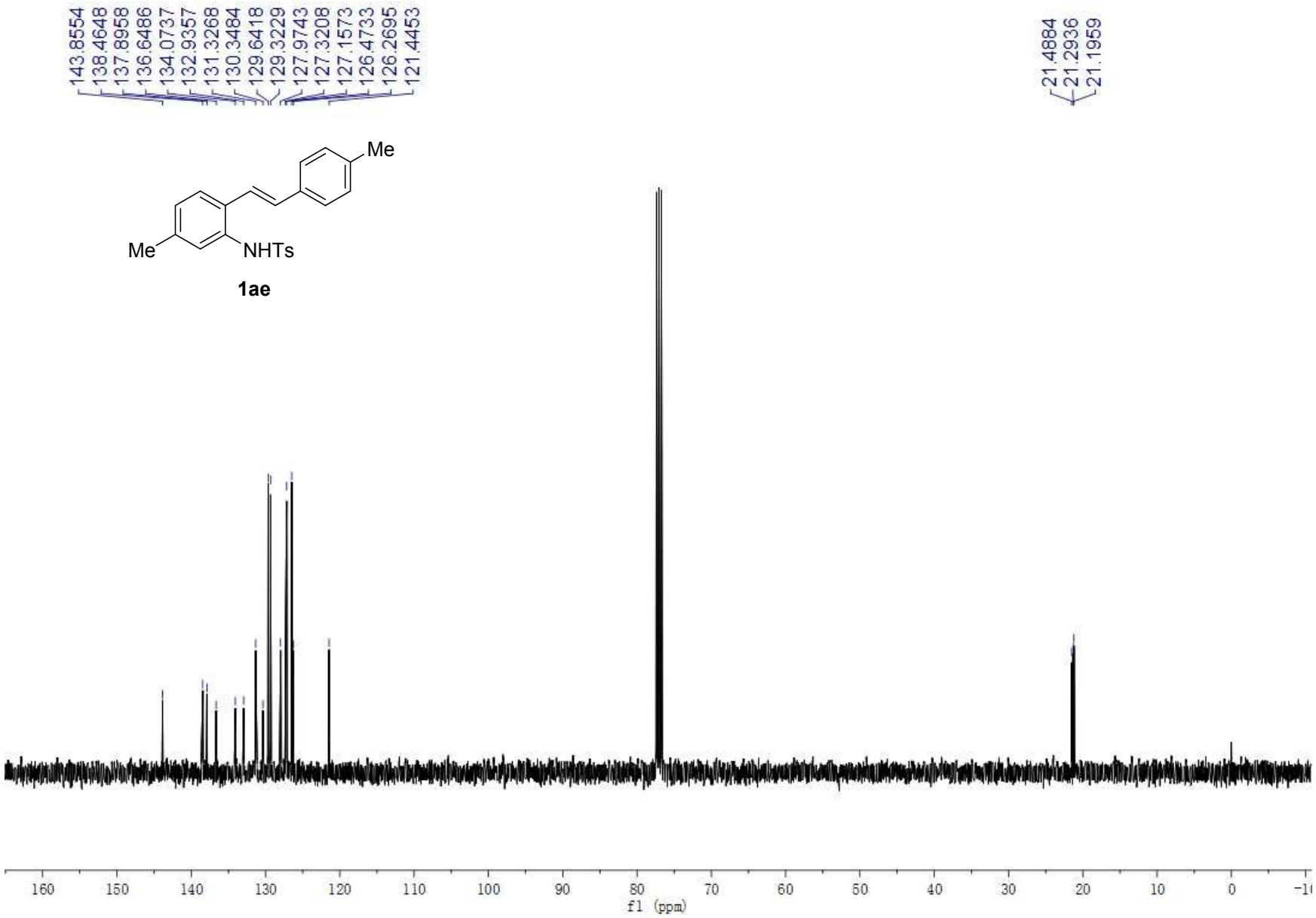
1.05
1.03
6.09
1.03
2.10
0.91
3.02
3.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

1ae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Me
Me
NHTs
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110
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90
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50
40
30
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10
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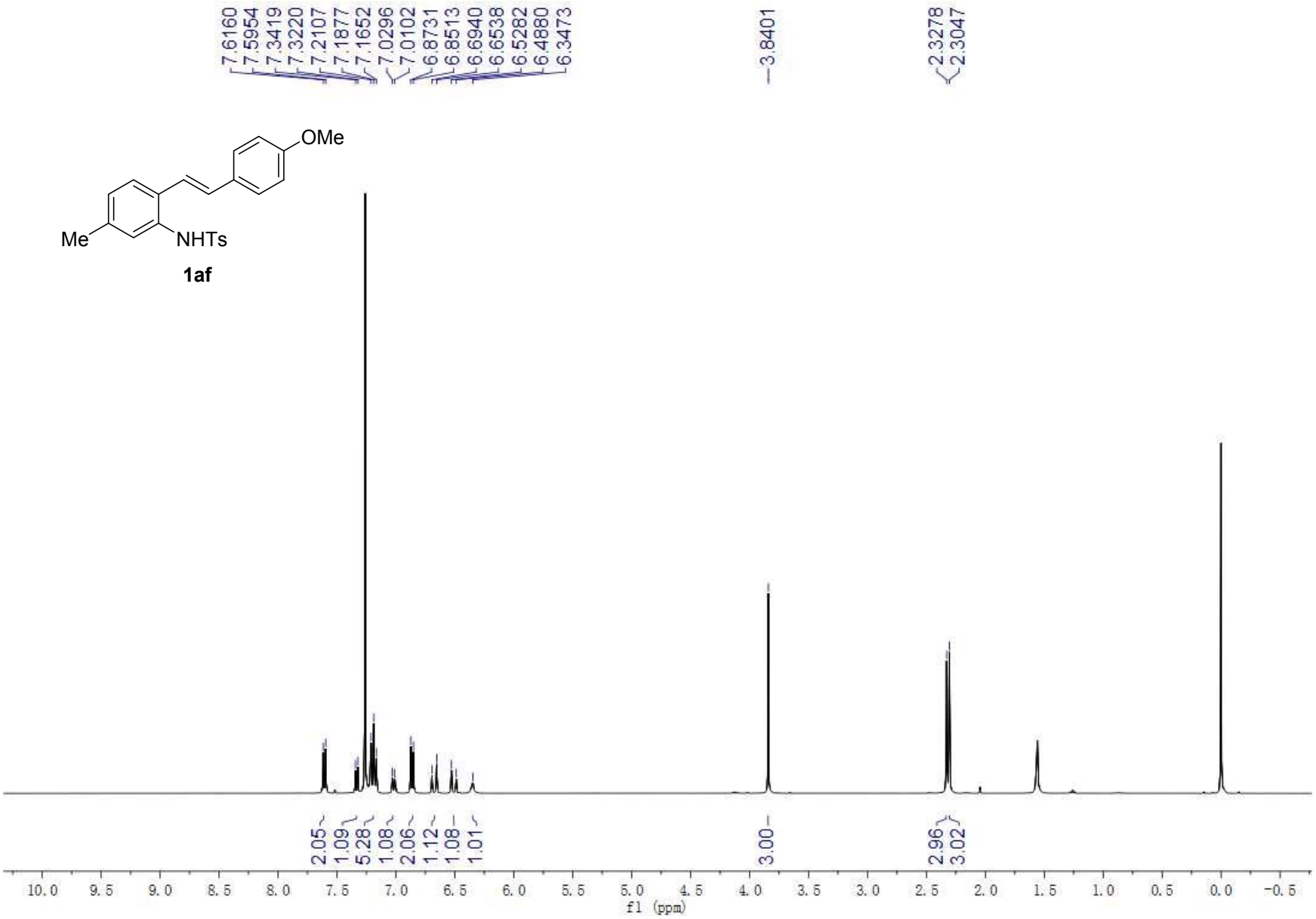
f1 (ppm)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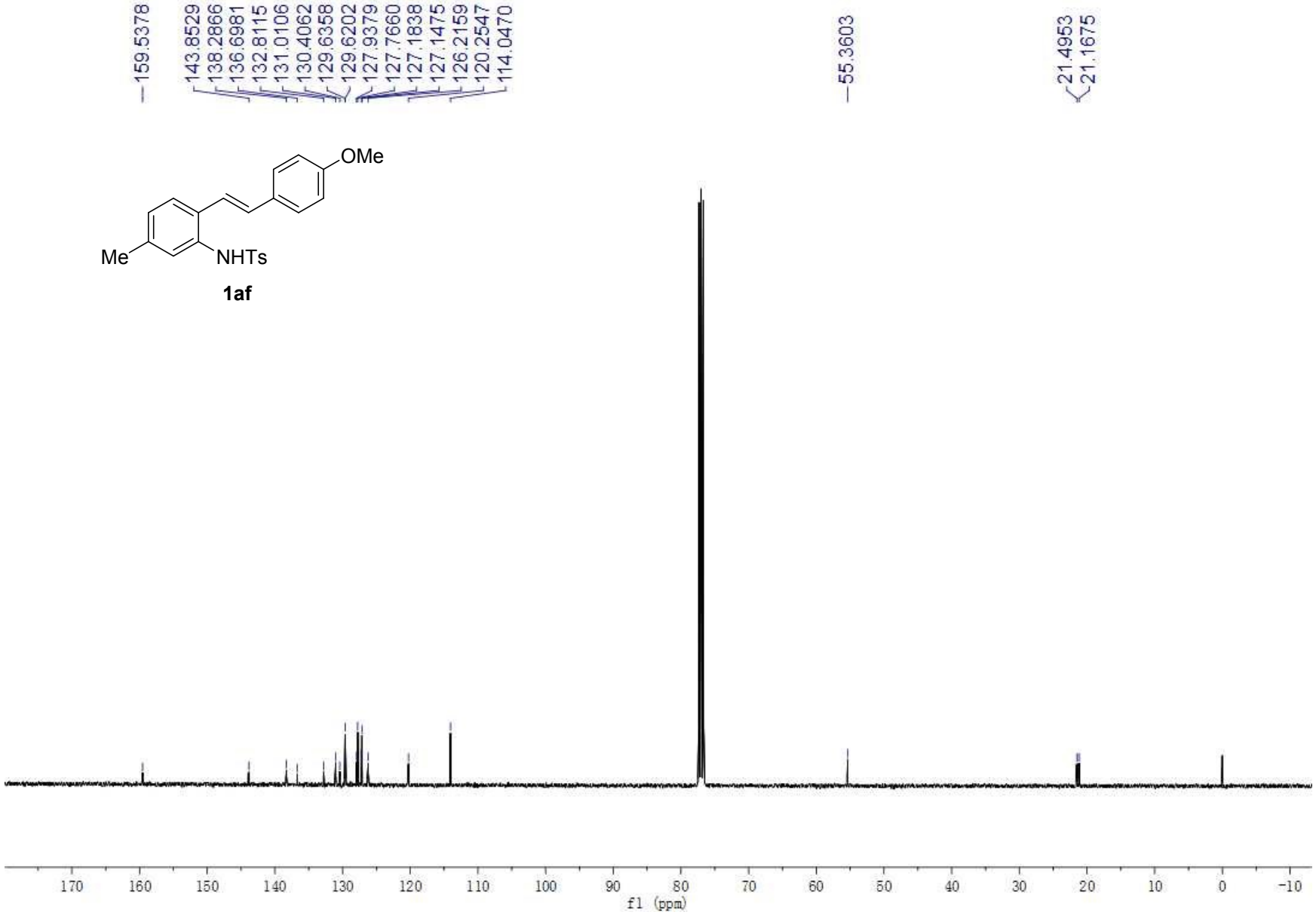
7.1877
7.1652
7.0296
7.0102
6.8731
6.8513
6.6940
6.6538
6.5282
6.4880
6.3473
3.8401
2.3278
2.3047
OMe
Me
NHTs
1af
2.05
1.09
5.28
1.08
2.06
1.12
1.08
1.01
3.00
2.96
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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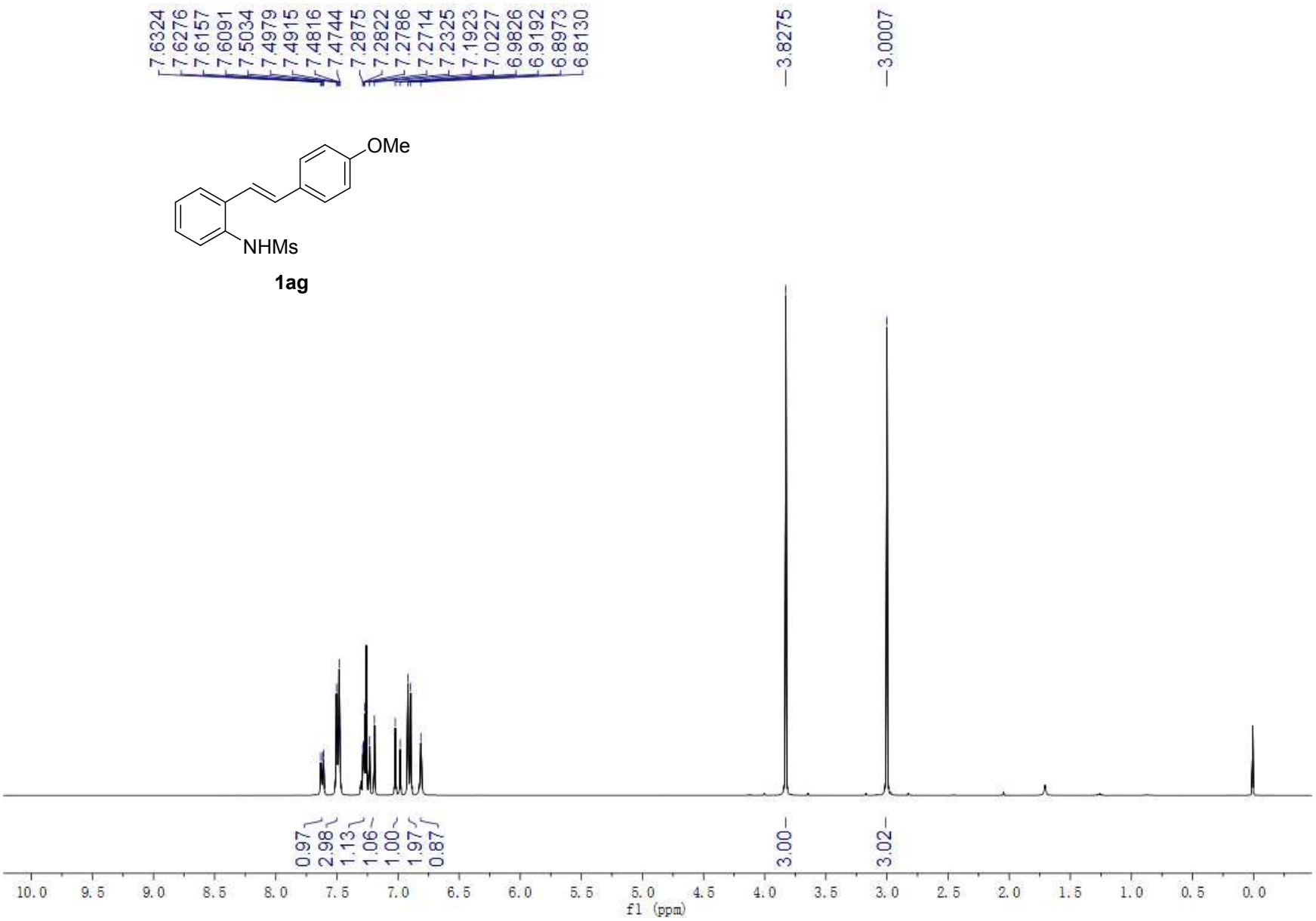
127.1838
127.1475
126.2159
120.2547
114.0470
55.3603
21.4953
21.1675
OMe
Me
NHTs
1af
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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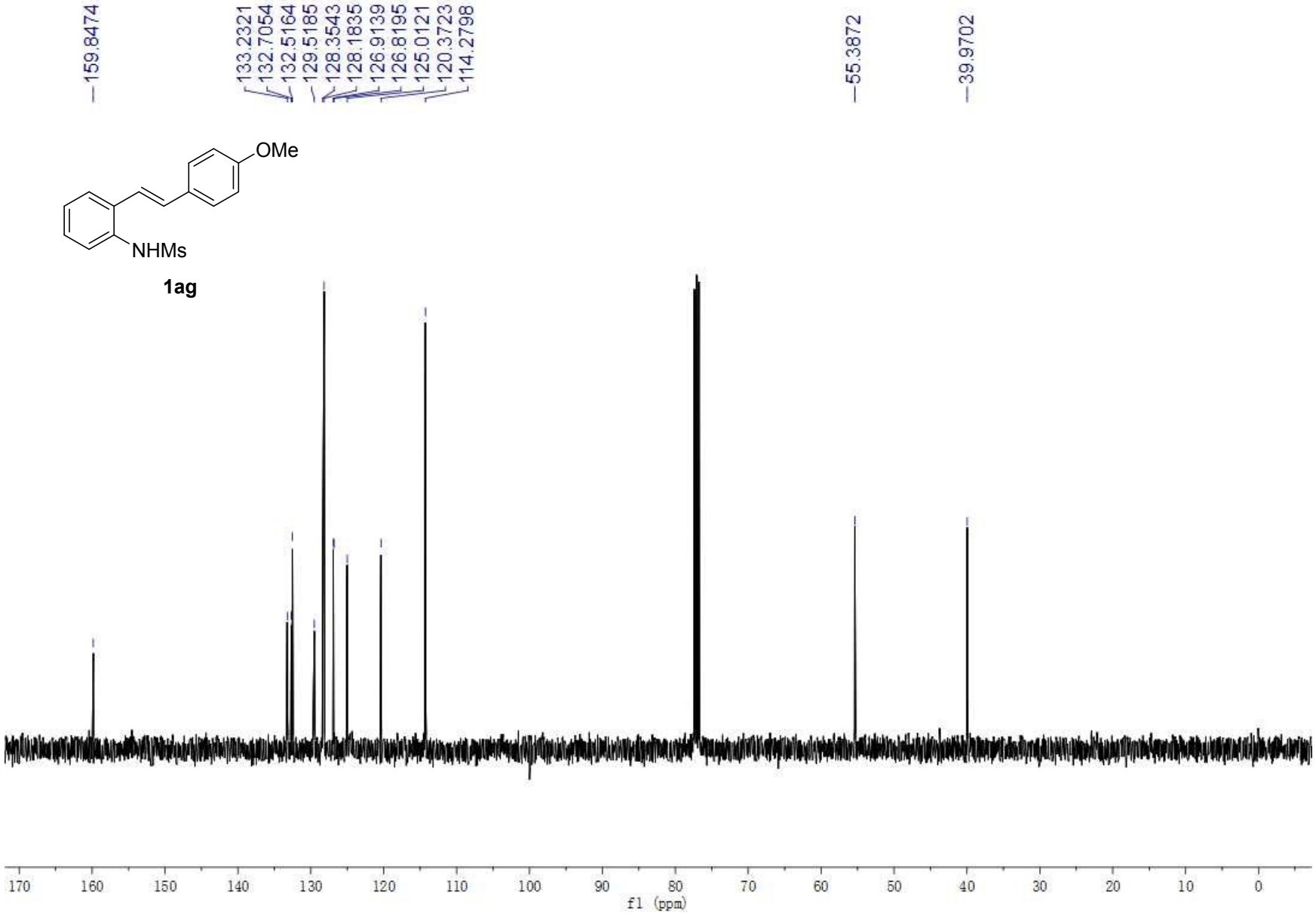
7.4979
7.4915
7.4816
7.4744
7.2875
7.2822
7.2786
7.2714
7.2325
7.1923
7.0227
6.9826
6.9192
6.8973
6.8130
3.8275
3.0007
OMe
NHMs
1ag
0.97
2.98
1.13
1.06
1.00
1.97
0.87
3.00
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.5185
128.3543
128.1835
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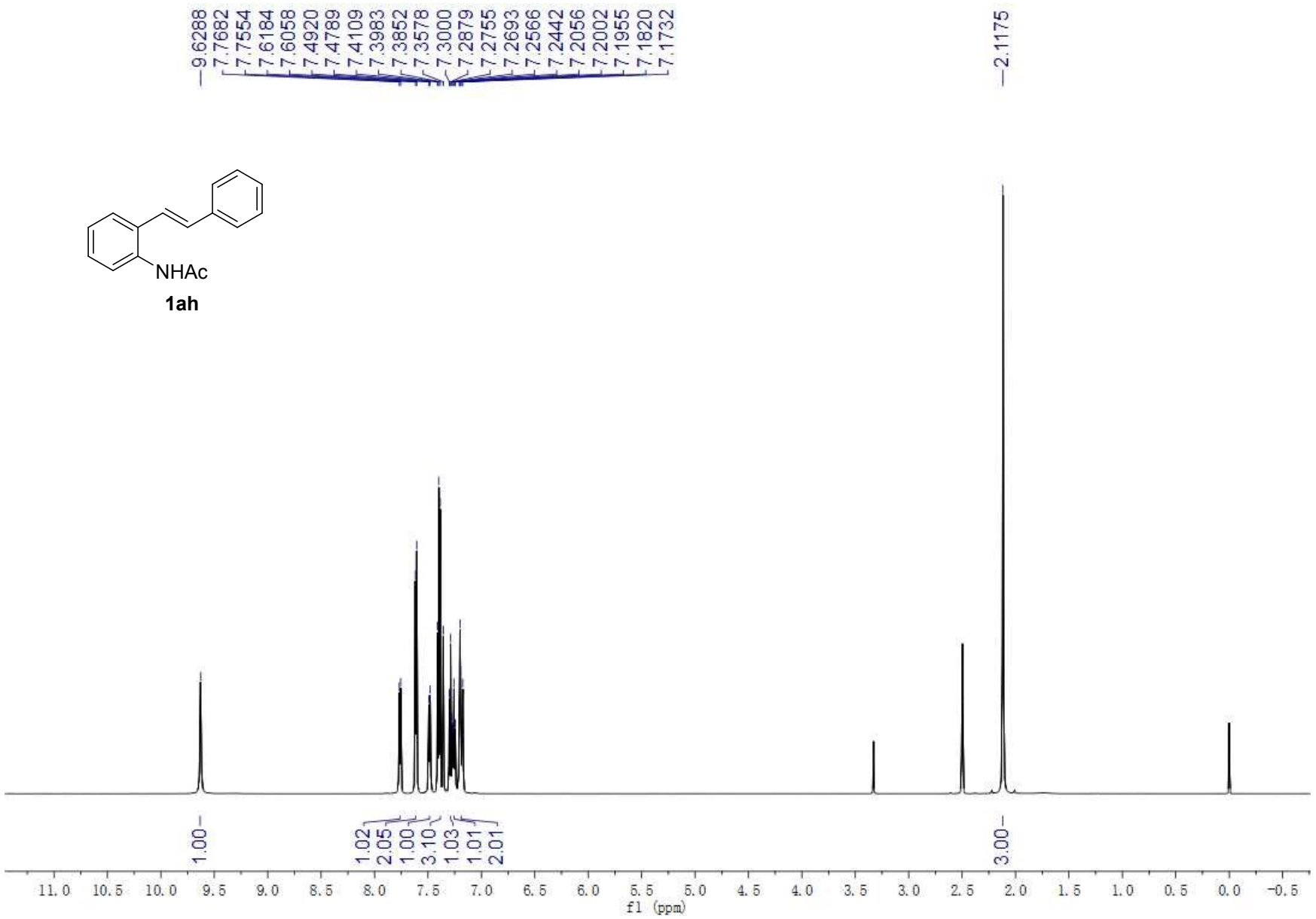
120.3723
114.2798
55.3872
39.9702
OMe
NHMs
1ag
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4789
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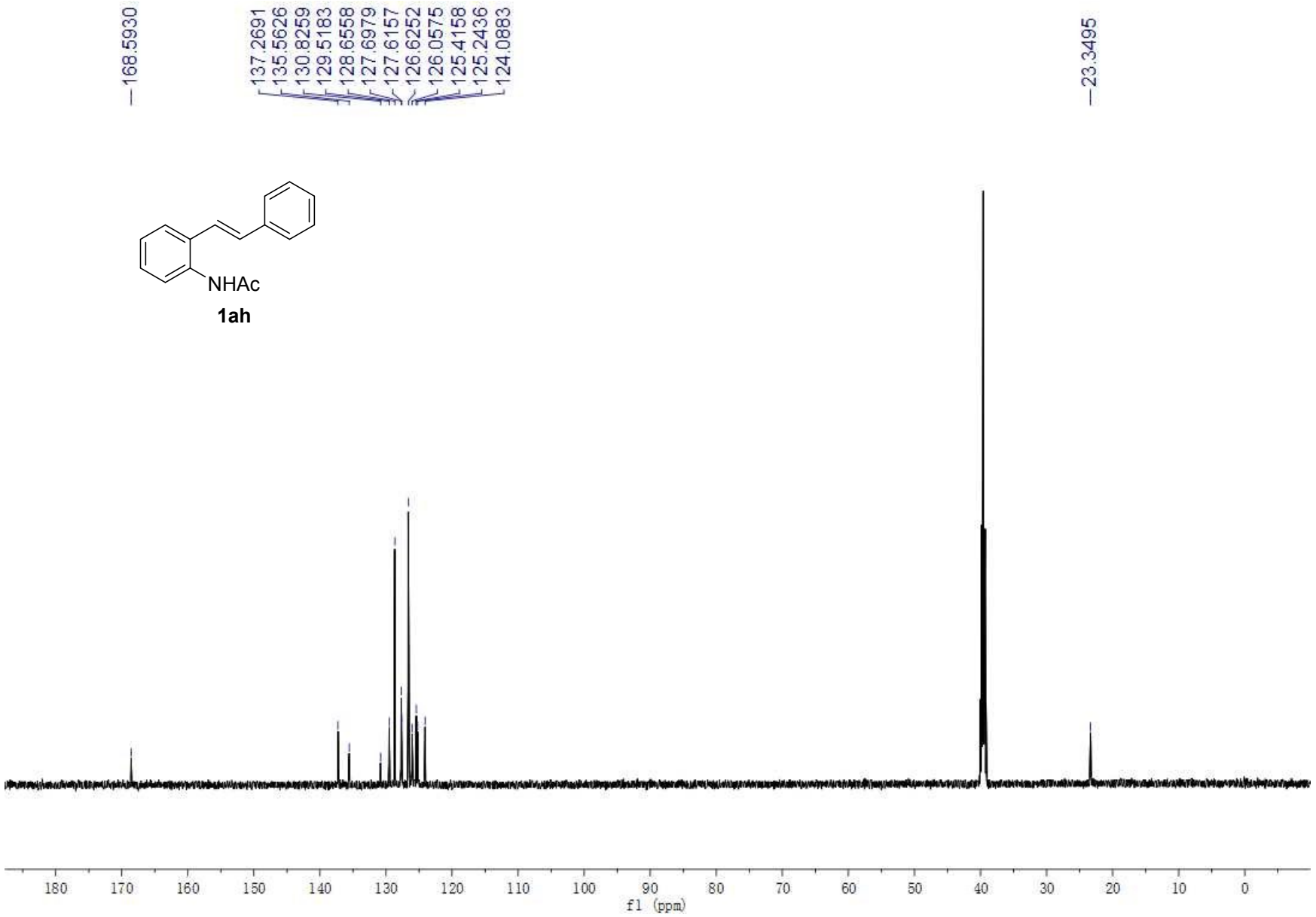
7.3983
7.3852
7.3578
7.3000
7.2879
7.2755
7.2693
7.2566
7.2442
7.2056
7.2002
7.1955
7.1820
7.1732
2.1175
NHAc
1ah
1.00
1.02
2.05
1.00
3.10
1.03
1.01
2.01
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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130.8259
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128.6558
127.6979
127.6157
126.6252
126.0575
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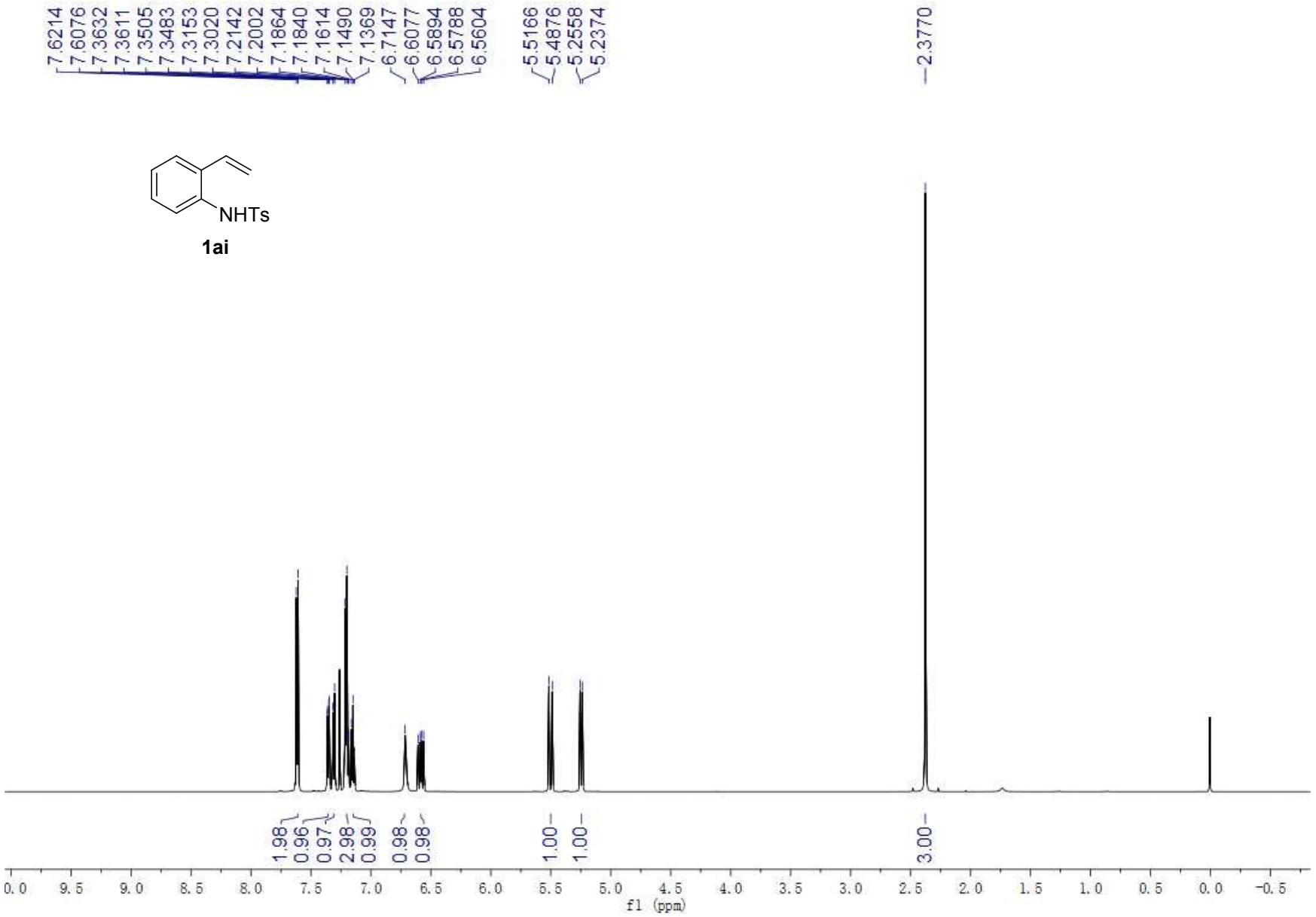
125.2436
124.0883
23.3495
NHAc
1ah
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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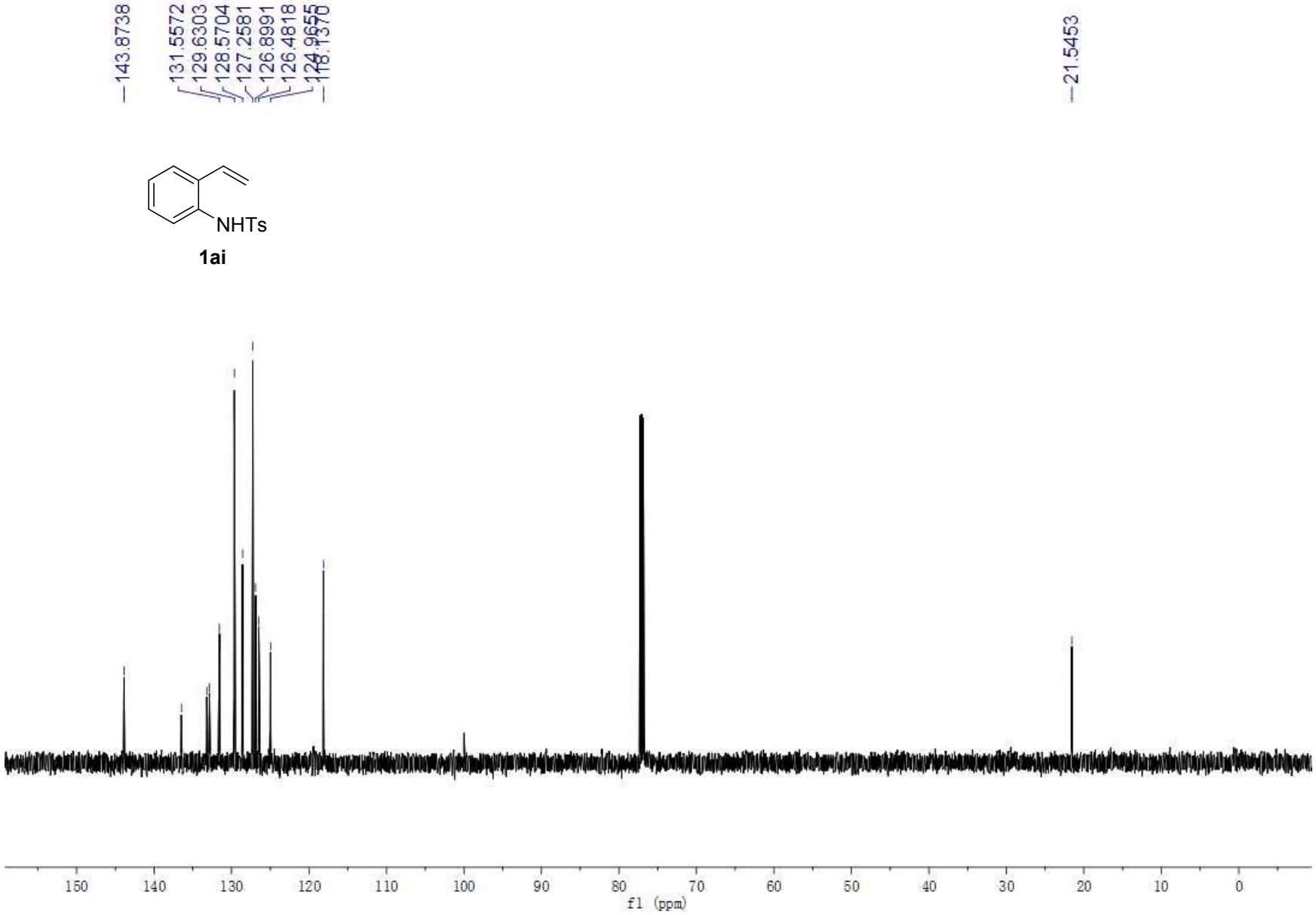
7.6076
7.3632
7.3611
7.3505
7.3483
7.3153
7.3020
7.2142
7.2002
7.1864
7.1840
7.1614
7.1490
7.1369
6.7147
6.6077
6.5894
6.5788
6.5604
5.5166
5.4876
5.2558
5.2374
2.3770
NHTs
1ai
1.98
0.96
0.97
2.98
0.99
0.98
0.98
1.00
1.00
3.00
f1 (ppm)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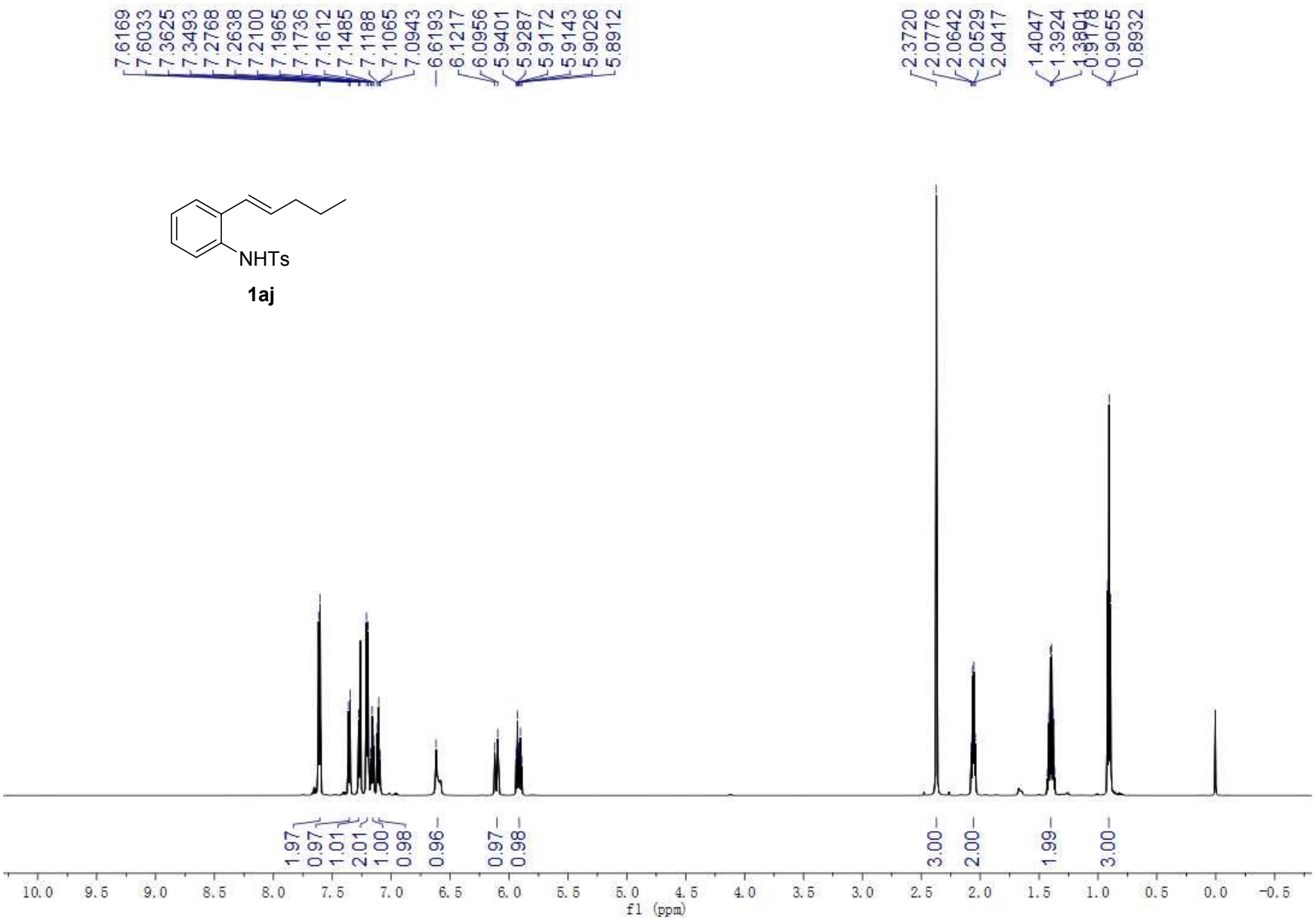
131.5572
129.6303
128.5704
127.2581
126.8991
126.4818
124.9655
118.1370
21.5453
NHTs
1ai
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3625
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7.2768
7.2638
7.2100
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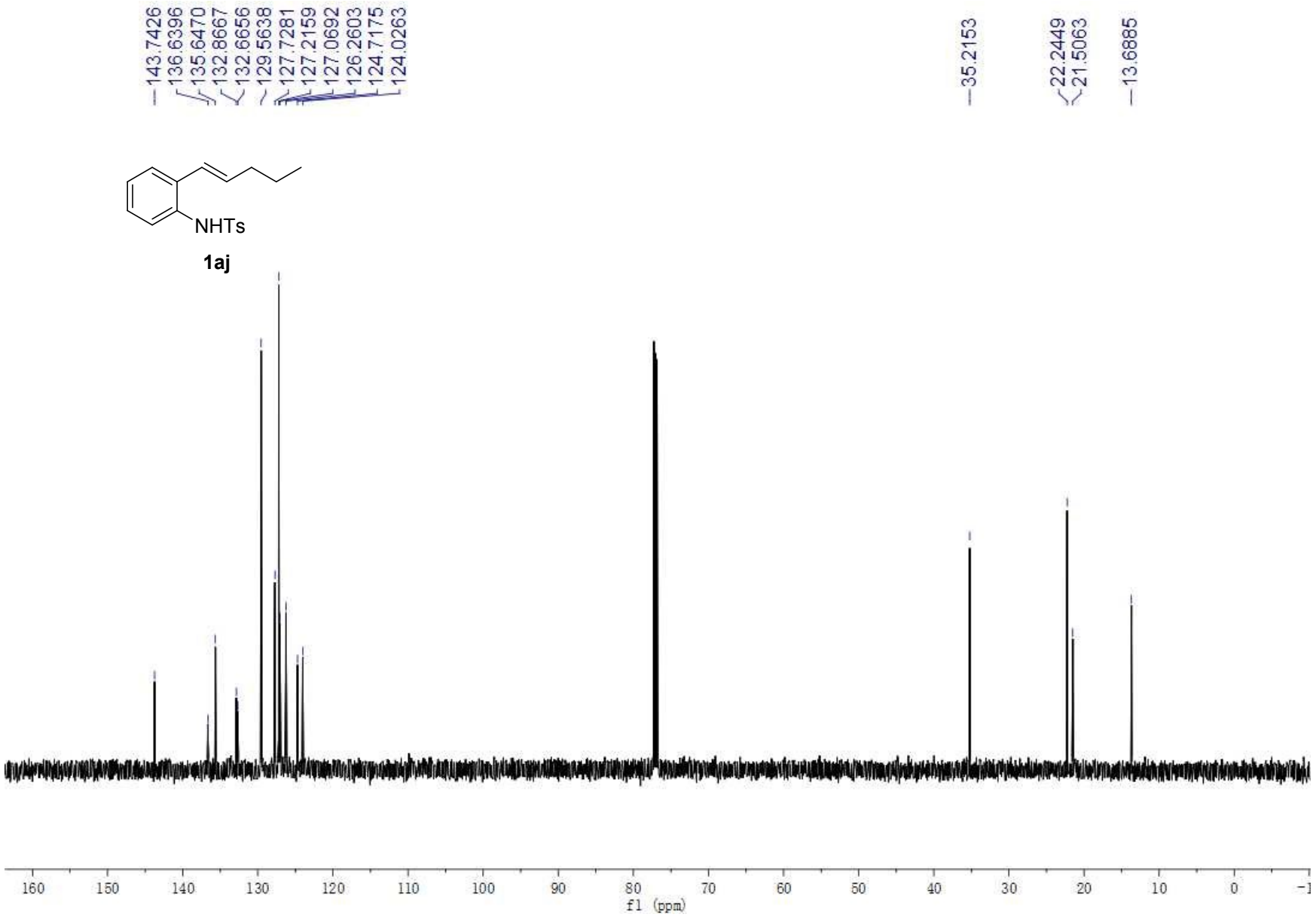
7.1736
7.1612
7.1485
7.1188
7.1065
7.0943
6.6193
6.1217
6.0956
5.9401
5.9287
5.9172
5.9143
5.9026
5.8912
2.3720
2.0776
2.0642
2.0529
2.0417
1.4047
1.3924
1.3891
0.9178
0.9055
0.8932
NHTs
1aj
1.97
0.97
1.01
2.01
1.00
0.98
0.96
0.97
0.98
3.00
2.00
1.99
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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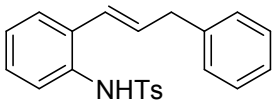
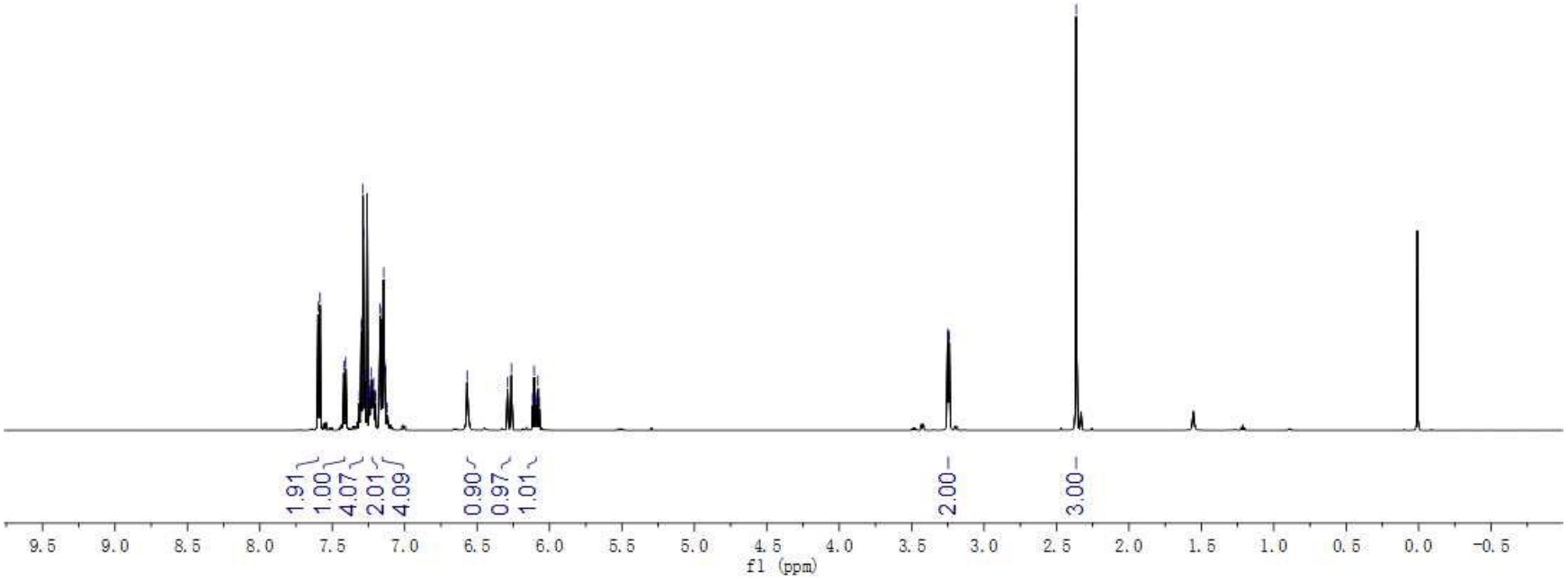
135.6470
132.8667
132.6656
129.5638
127.7281
127.2159
127.0692
126.2603
124.7175
124.0263
35.2153
22.2449
21.5063
13.6885
NHTs
1aj
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.5978
7.5841
7.4201
7.4068
7.2997
7.2881
7.2844
7.2736
7.2321
7.1697
7.1562
7.1449
7.1405
7.1349
6.2896
6.2631
6.1170
6.1064
6.0958
6.0905
6.0799
6.0693
3.2522
3.2503
3.2417
3.2397
2.3637


NHTs

1ak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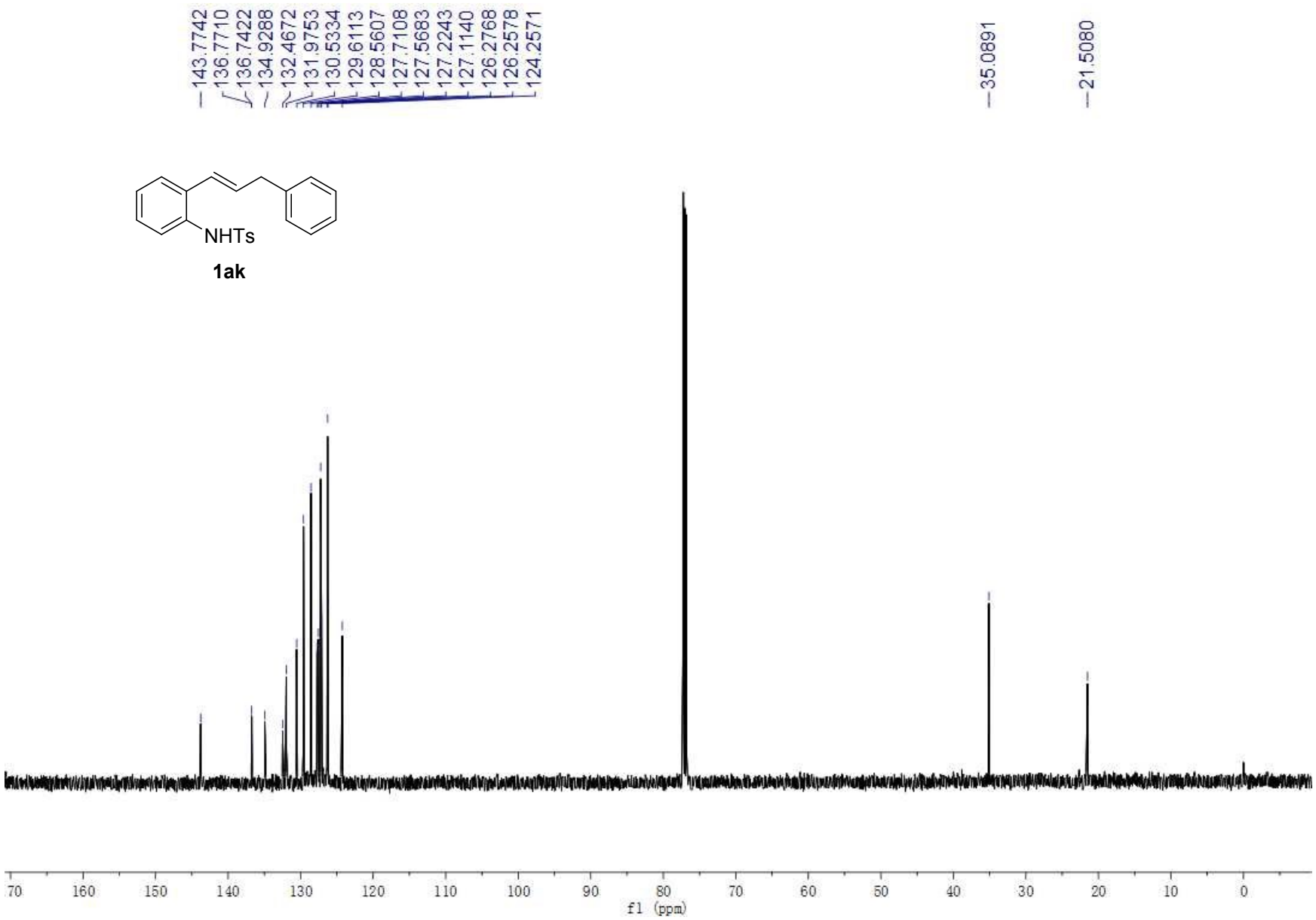
4.07
2.01
4.09
0.90
0.97
1.01
2.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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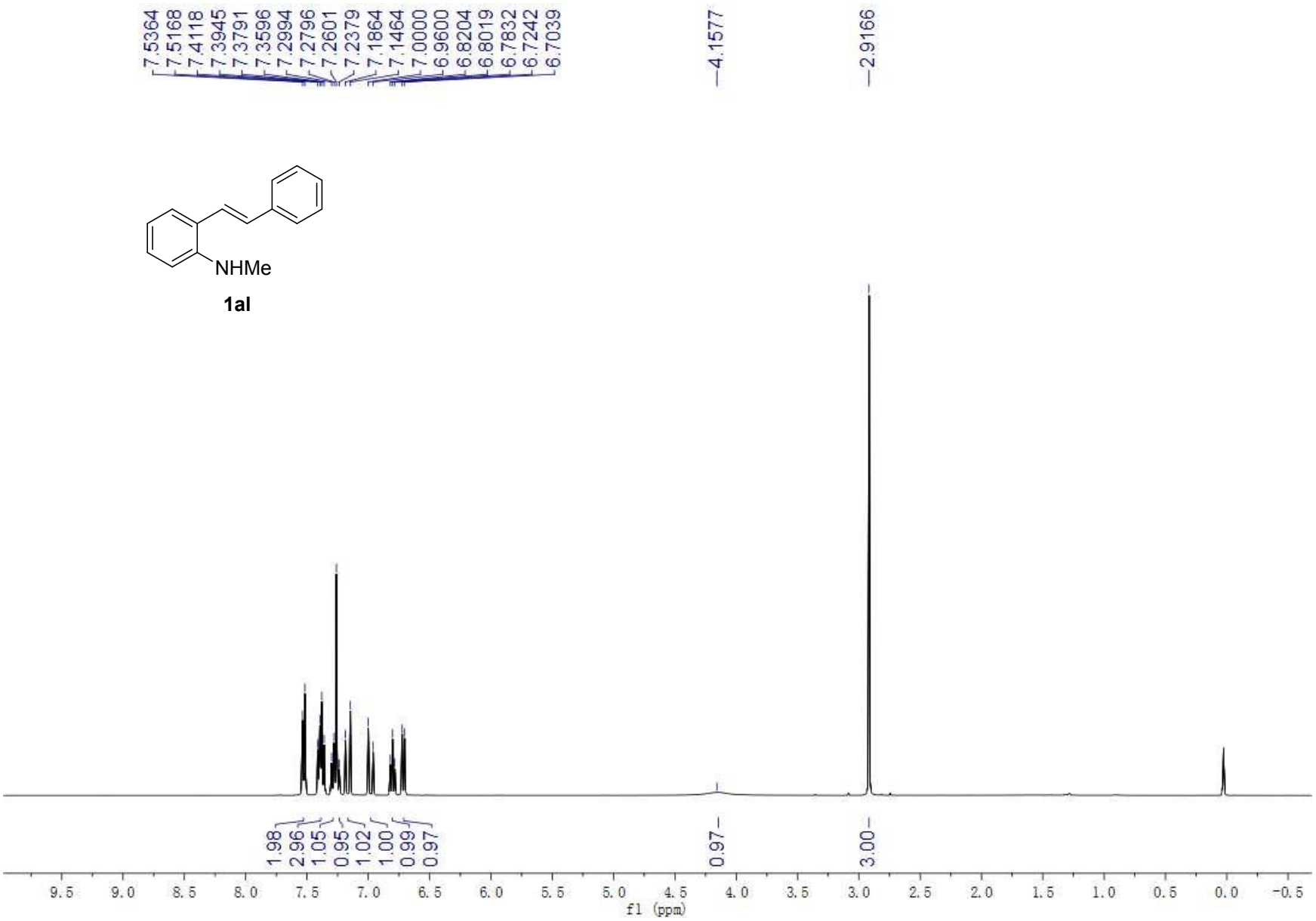
136.7422
134.9288
132.4672
131.9753
130.5334
129.6113
128.5607
127.7108
127.5683
127.2243
127.1140
126.2768
126.2578
124.2571
35.0891
21.5080
NHTs
1ak
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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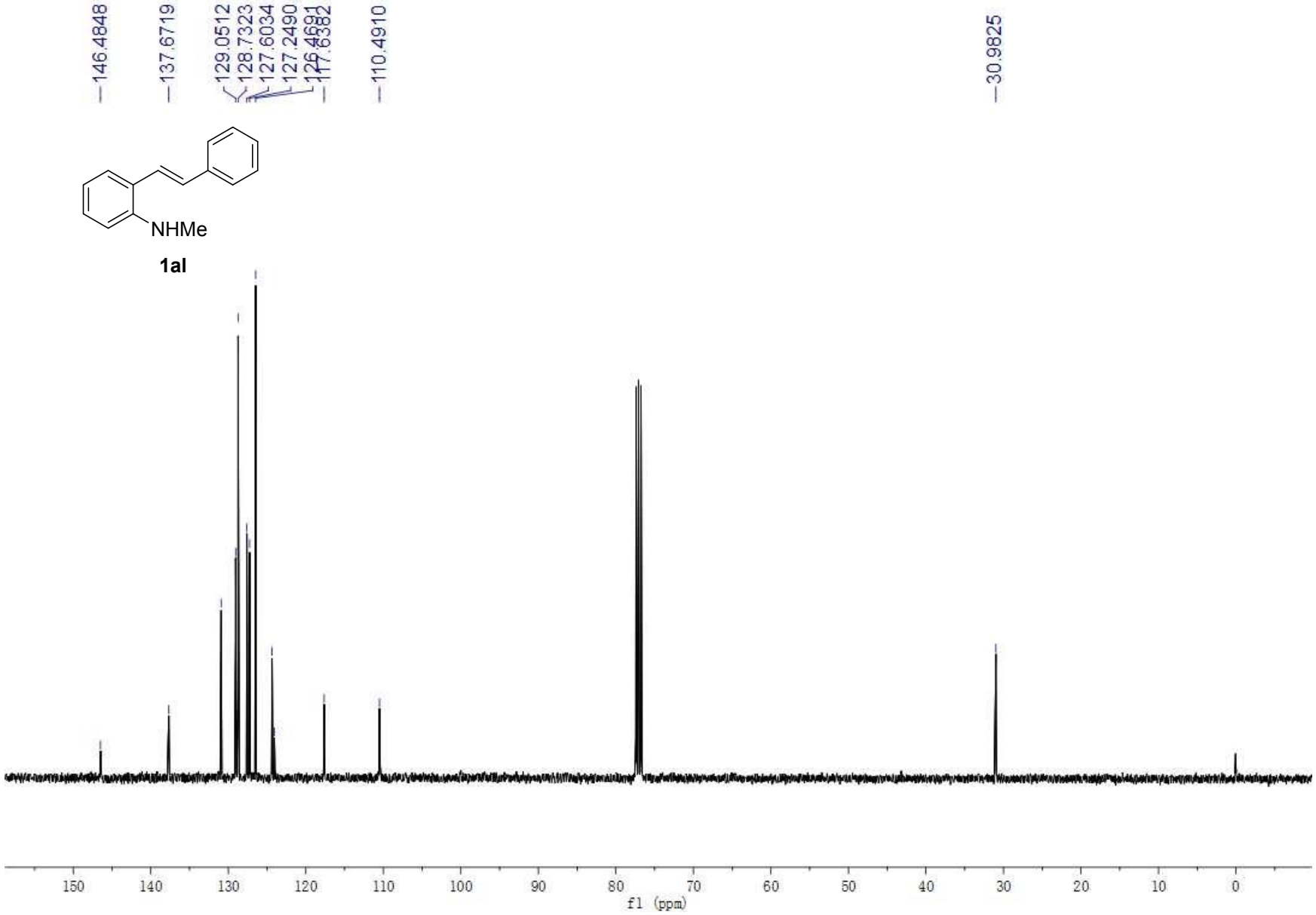
7.5168
7.4118
7.3945
7.3791
7.3596
7.2994
7.2796
7.2601
7.2379
7.1864
7.1464
7.0000
6.9600
6.8204
6.8019
6.7832
6.7242
6.7039
4.1577
2.9166
NHMe
1al
1.98
2.96
1.05
0.95
1.02
1.00
0.99
0.97
0.97
3.00
f1 (ppm)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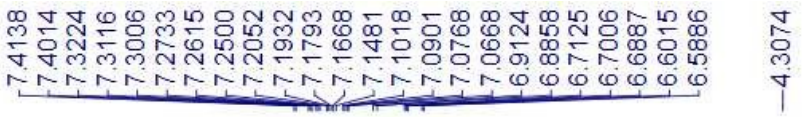
127.6034
127.2490
126.4691
117.6382
110.4910
30.9825
NHMe
1al
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2733
7.2615
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7.2052
7.1932
7.1793
7.1668
7.1481
7.1018
7.0901
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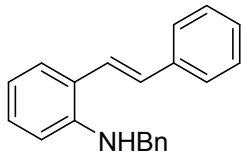
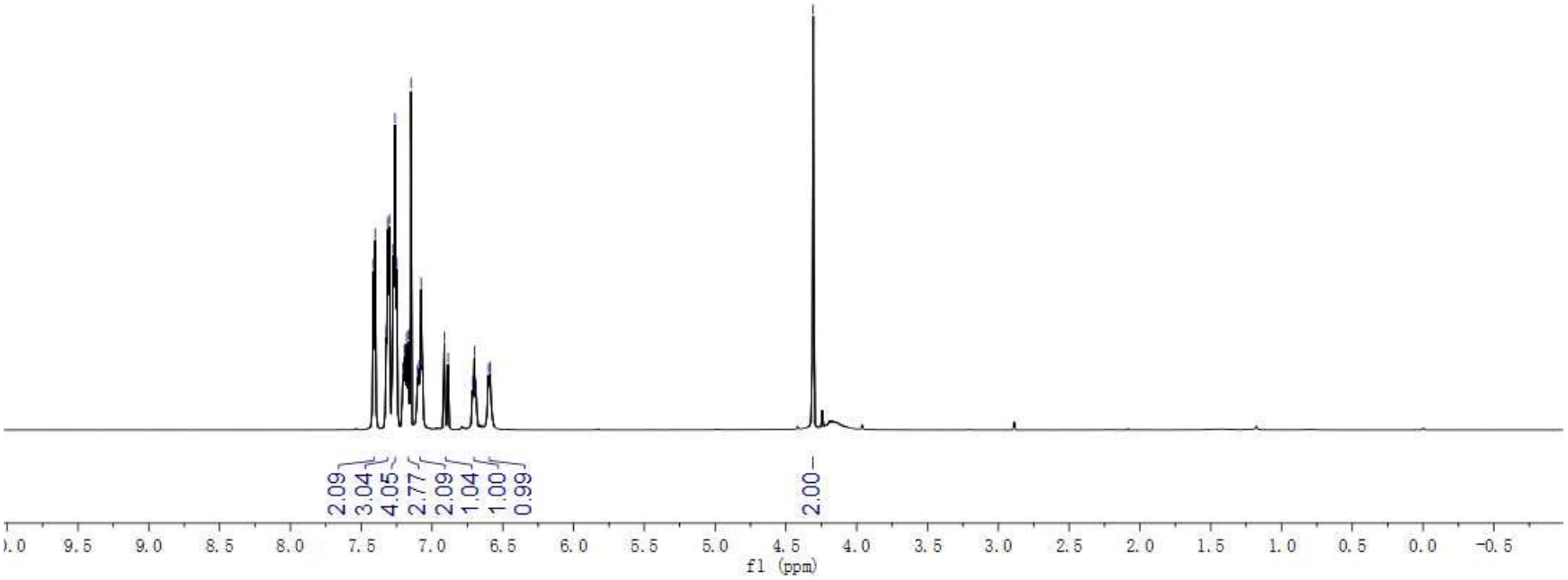
6.9124
6.8858
6.7125
6.7006
6.6887
6.6015
6.5886
4.3074


NHBn

1am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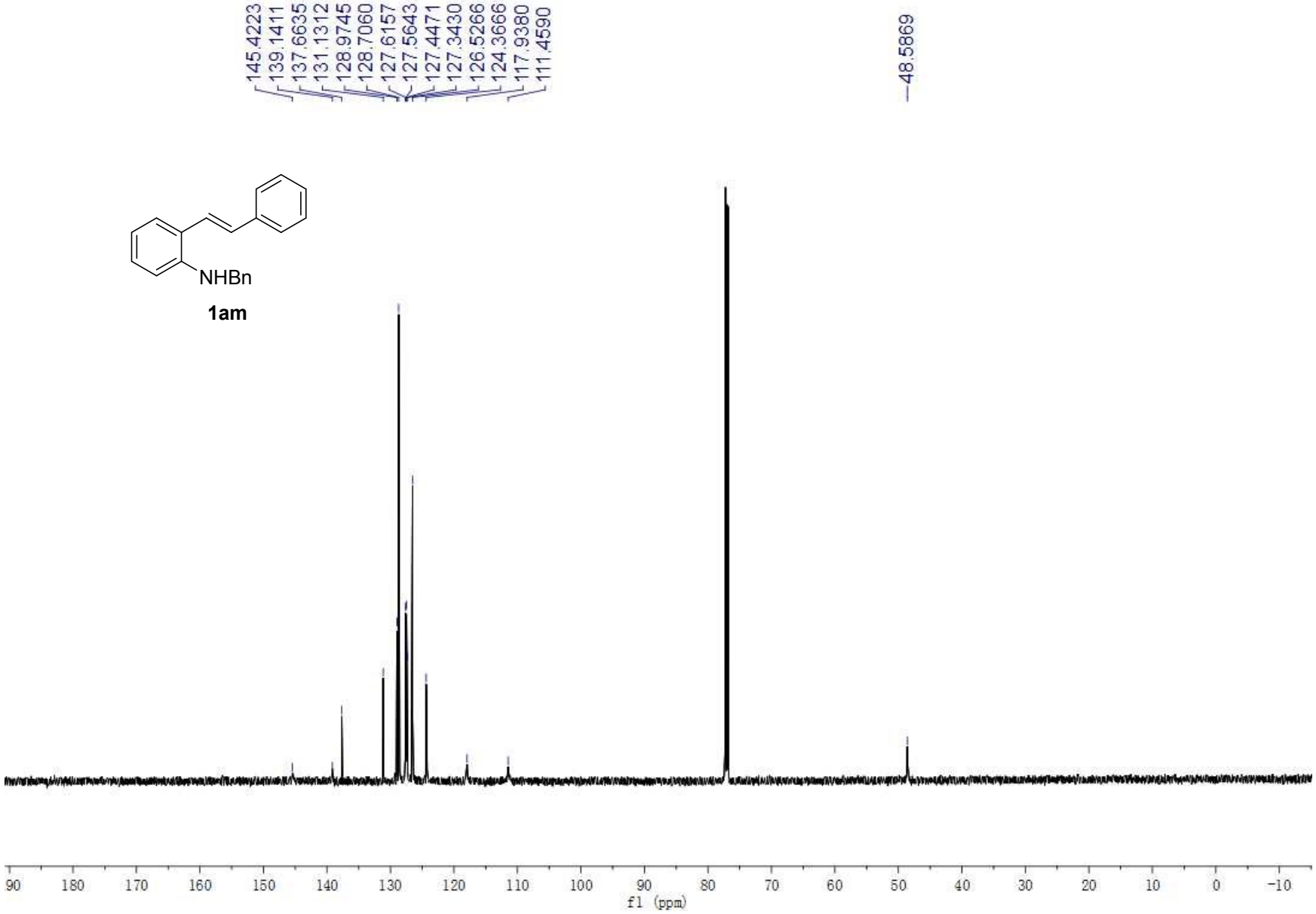
4.05
2.77
2.09
1.04
1.00
0.99
2.00
f1 (ppm)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128.9745
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127.6157
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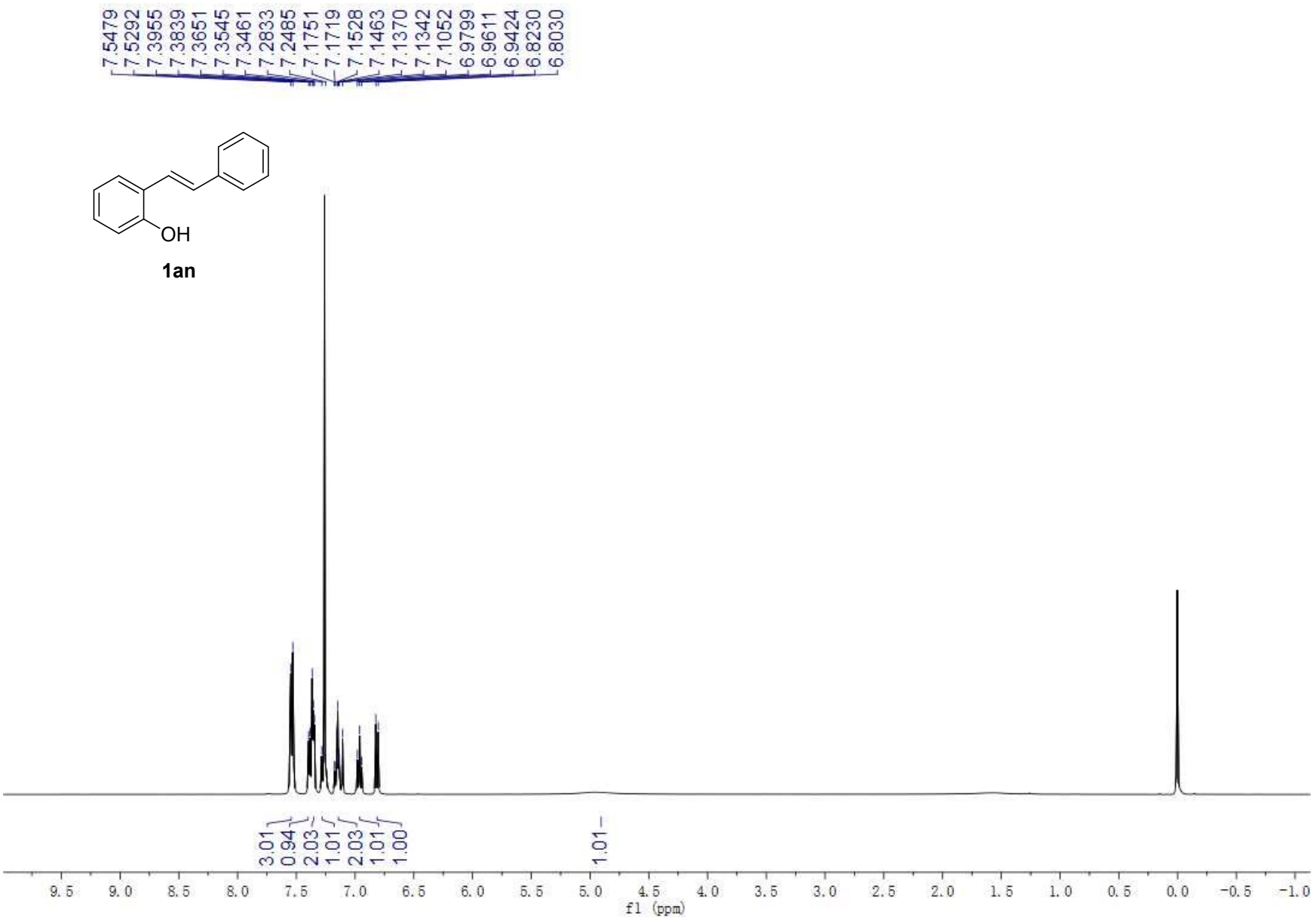
127.4471
127.3430
126.5266
124.3666
117.9380
111.4590
48.5869
NHBn
1am
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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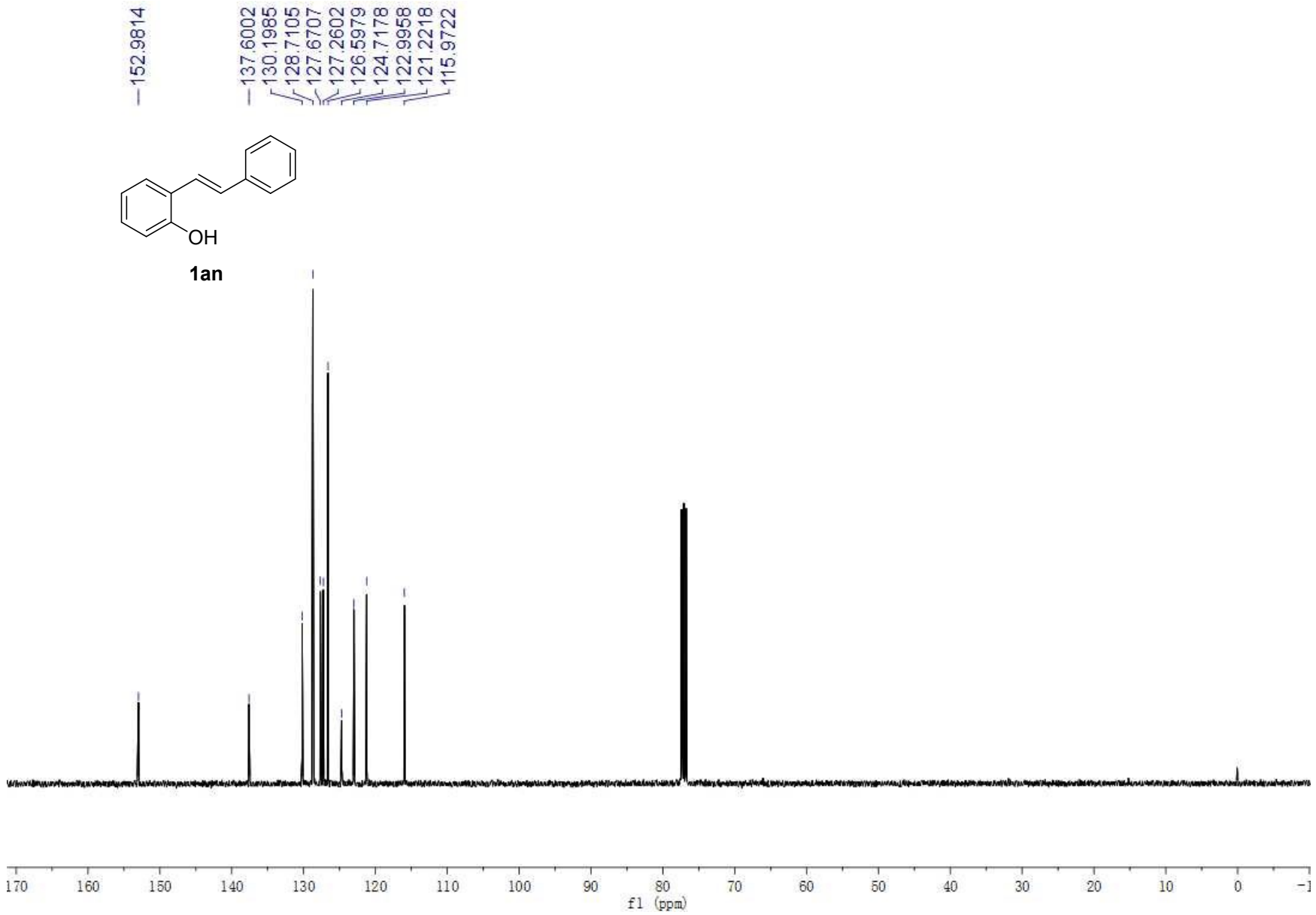
7.3651
7.3545
7.3461
7.2833
7.2485
7.1751
7.1719
7.1528
7.1463
7.1370
7.1342
7.1052
6.9799
6.9611
6.9424
6.8230
6.8030
OH
1an
3.01
0.94
2.03
1.01
2.03
1.01
1.00
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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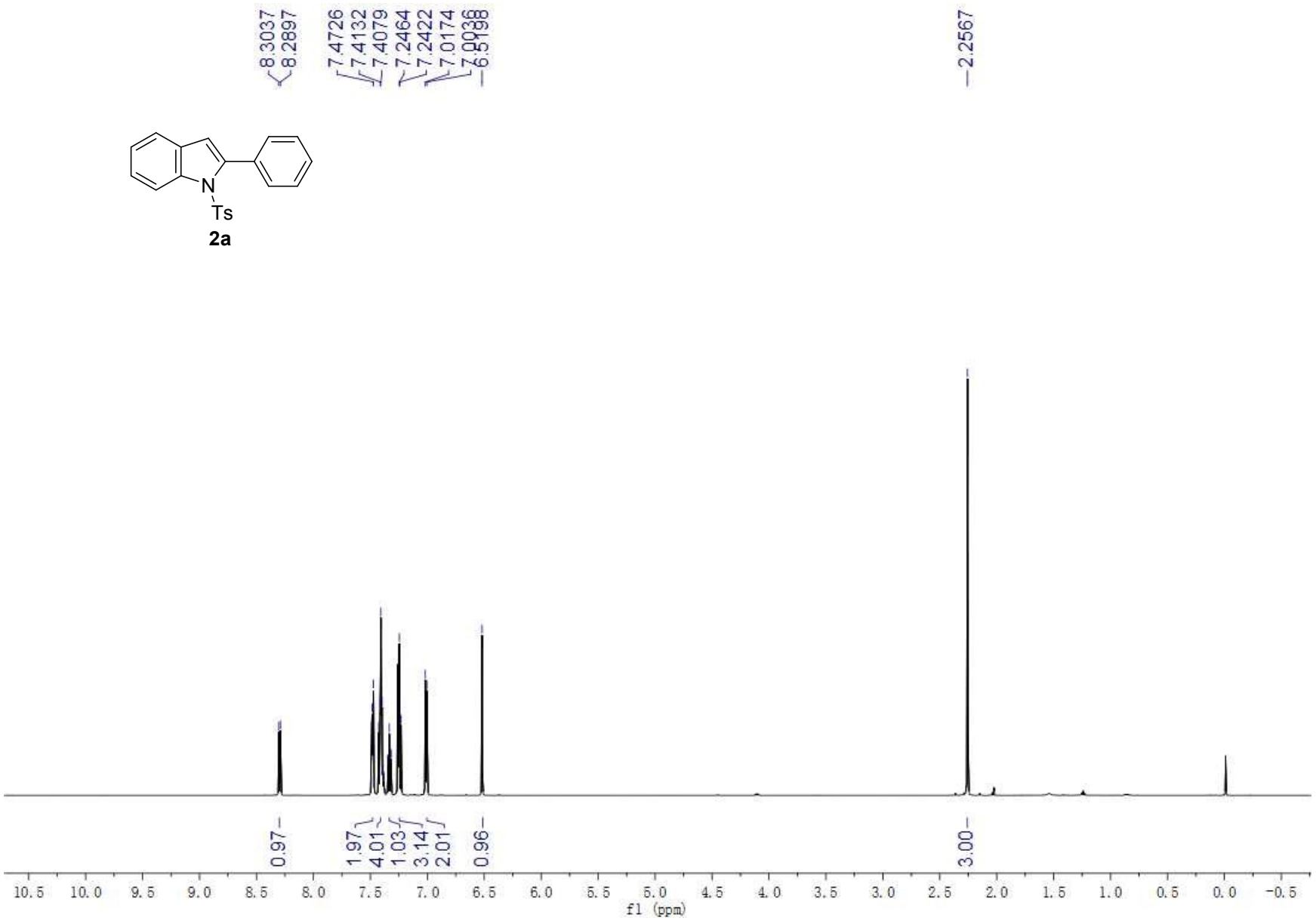
126.5979
124.7178
122.9958
121.2218
115.9722
OH
1an
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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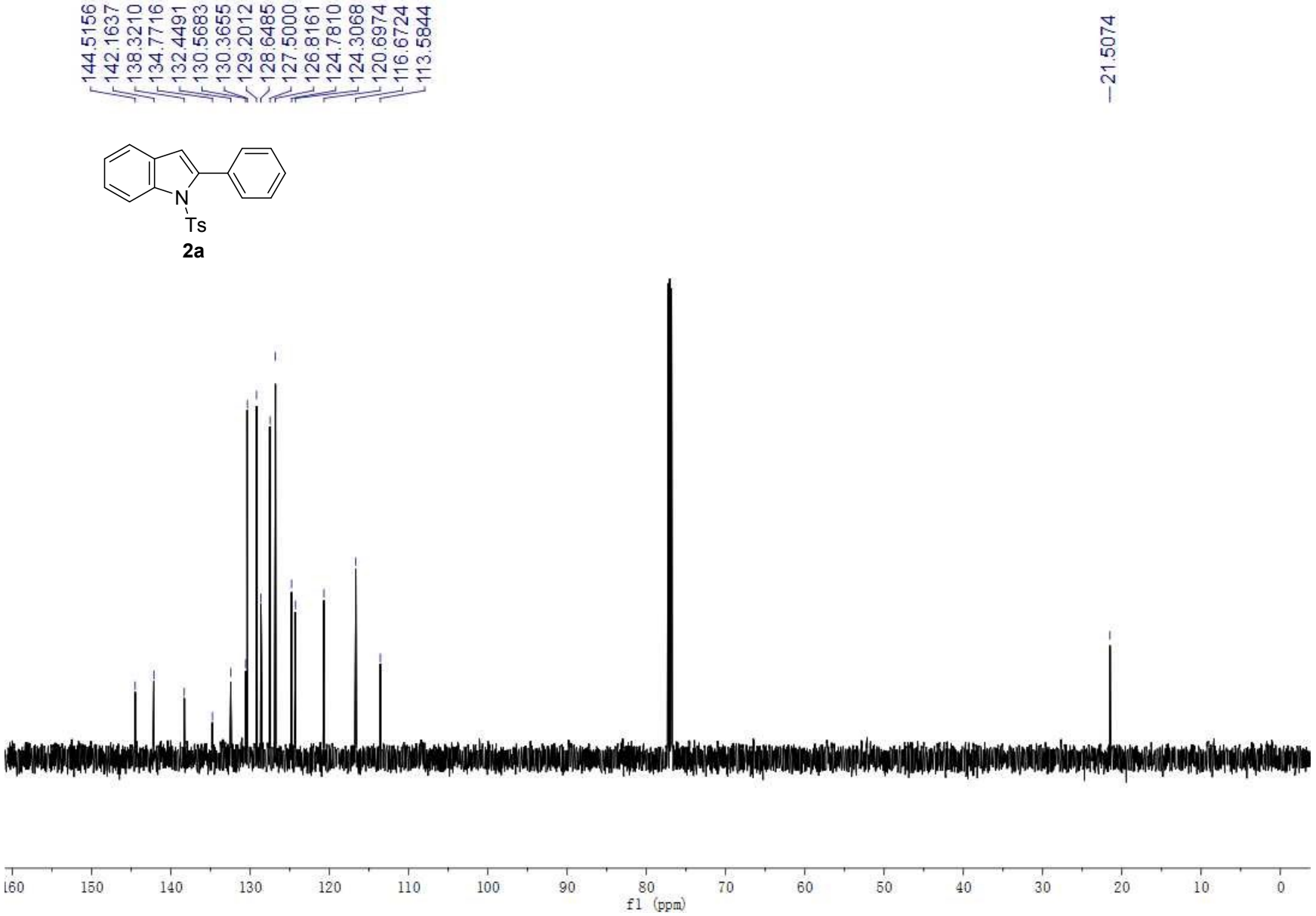
7.2422
7.0174
7.0038
6.5198
2.2567
N
Ts
2a
0.97
1.97
4.01
1.03
3.14
2.01
0.96
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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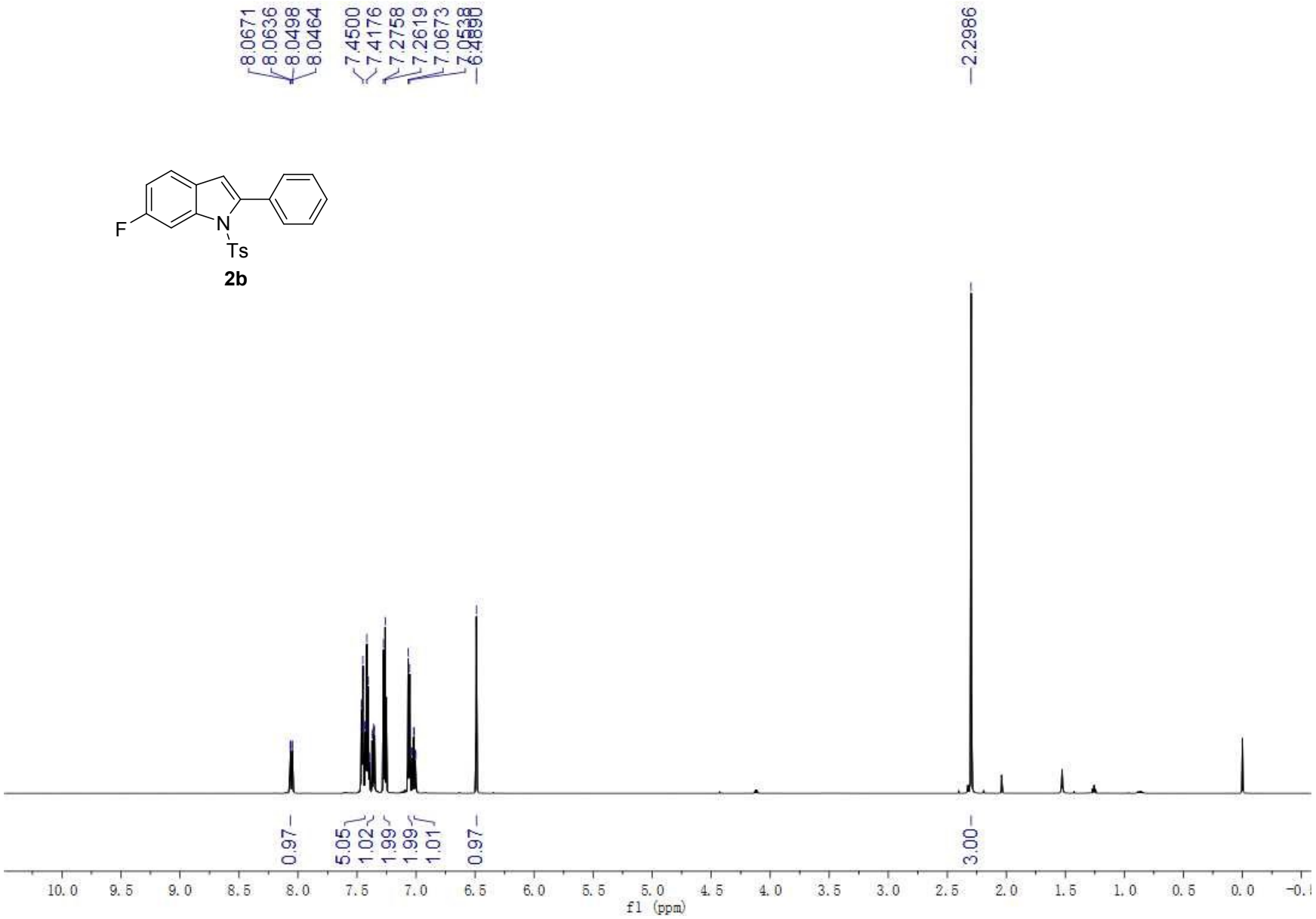
127.5000
126.8161
124.7810
124.3068
120.6974
116.6724
113.5844
21.5074
N
Ts
2a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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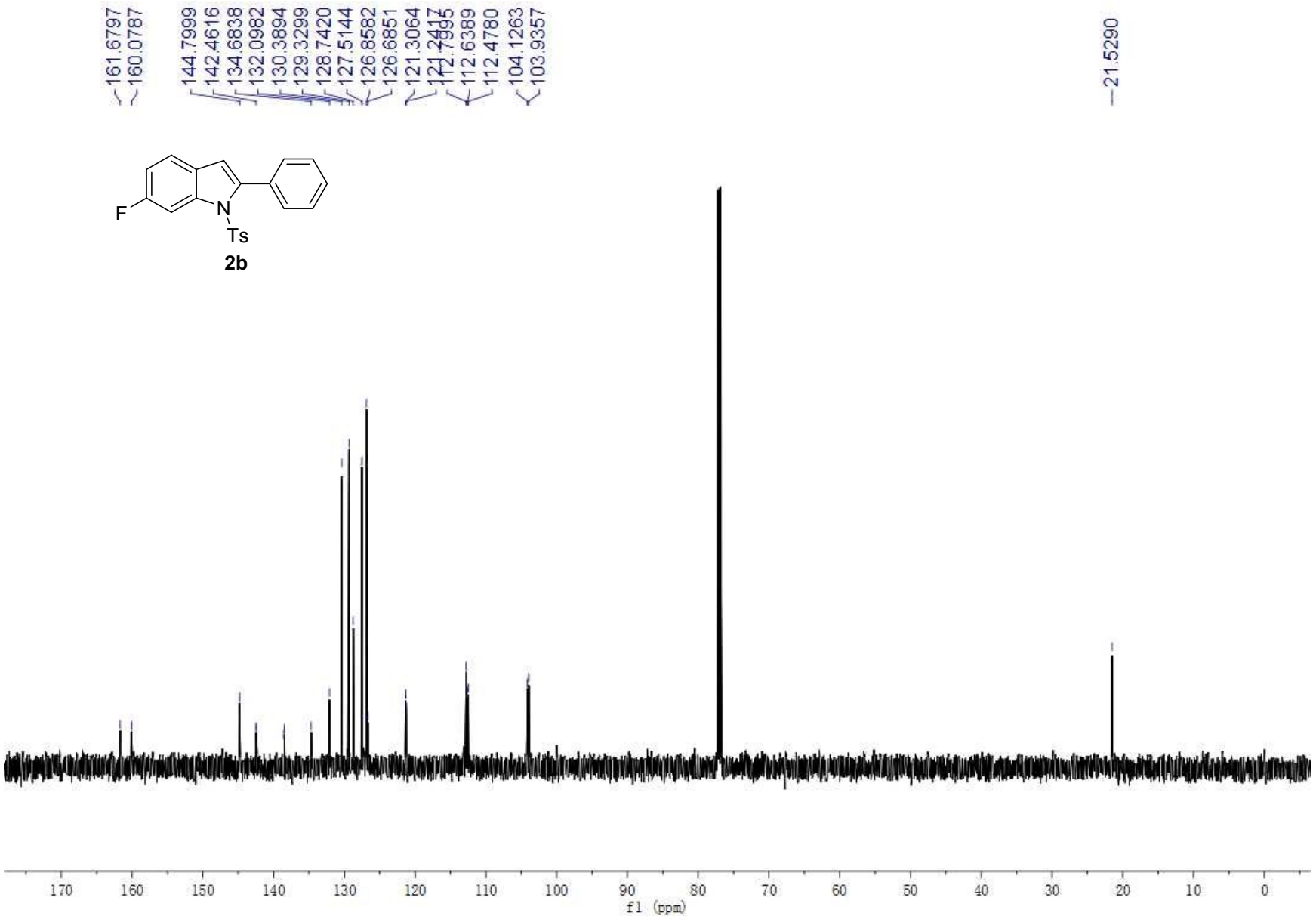
7.4176
7.2758
7.2619
7.0673
2.2986
F
N
Ts
2b
0.97
5.05
1.02
1.99
1.99
1.01
0.97
3.00
f1 (ppm)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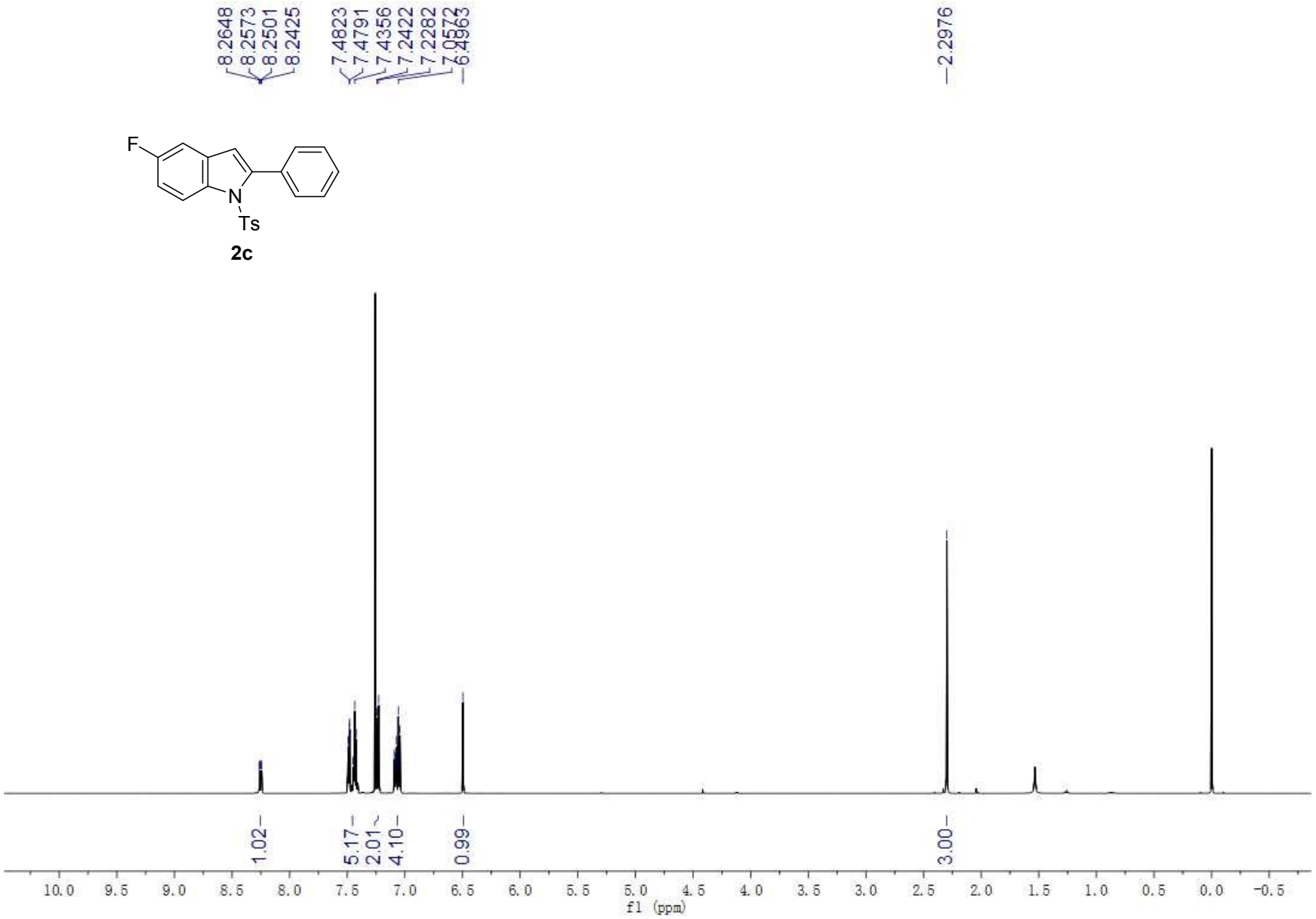
126.8582
126.6851
121.3064
121.2417
112.7995
112.6389
112.4780
104.1263
103.9357
21.5290
F
N
Ts
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4791
7.4356
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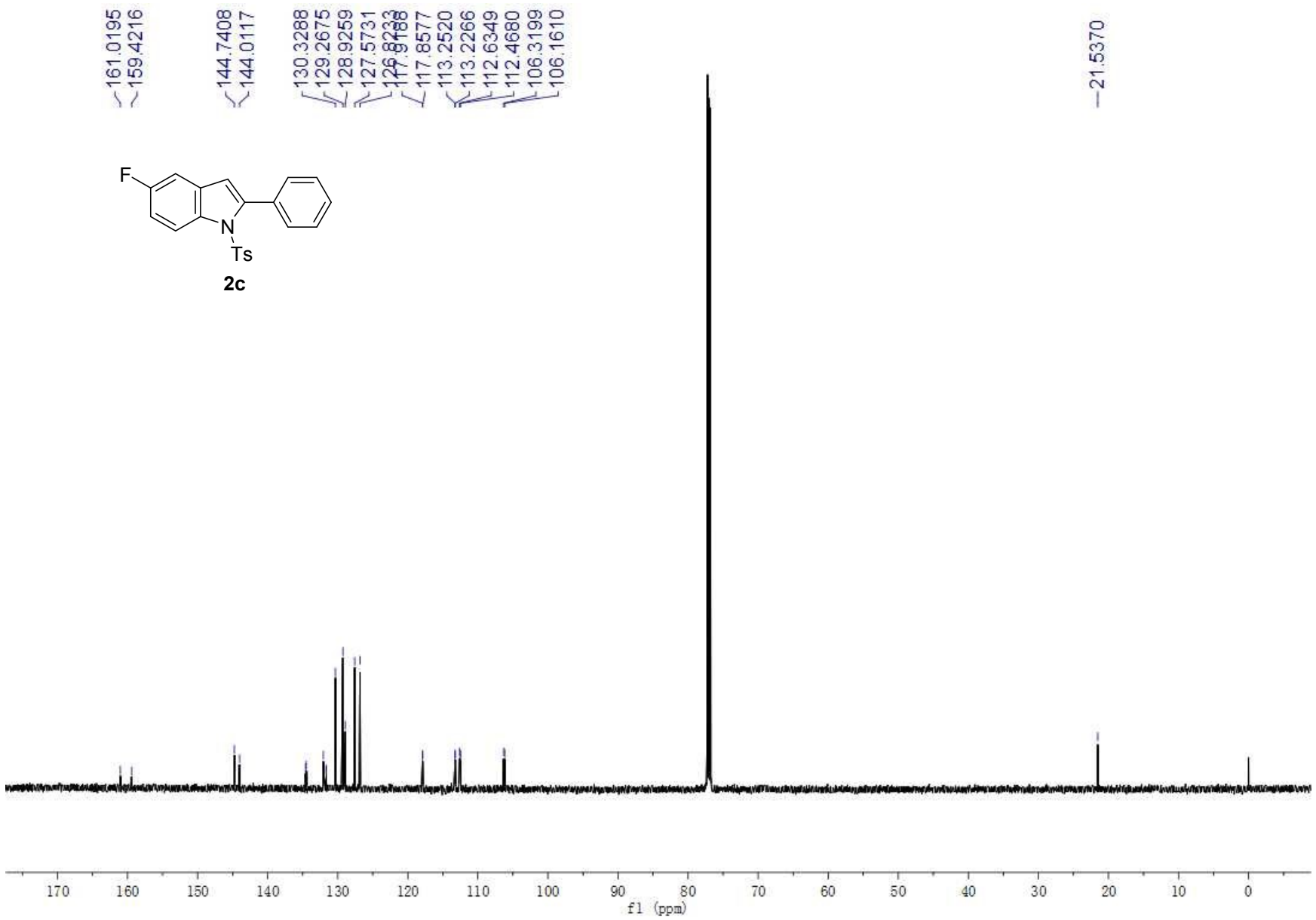
7.2282
7.0572
6.9963
2.2976
F
N
Ts
1.02
5.17
2.01
4.10
0.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

2c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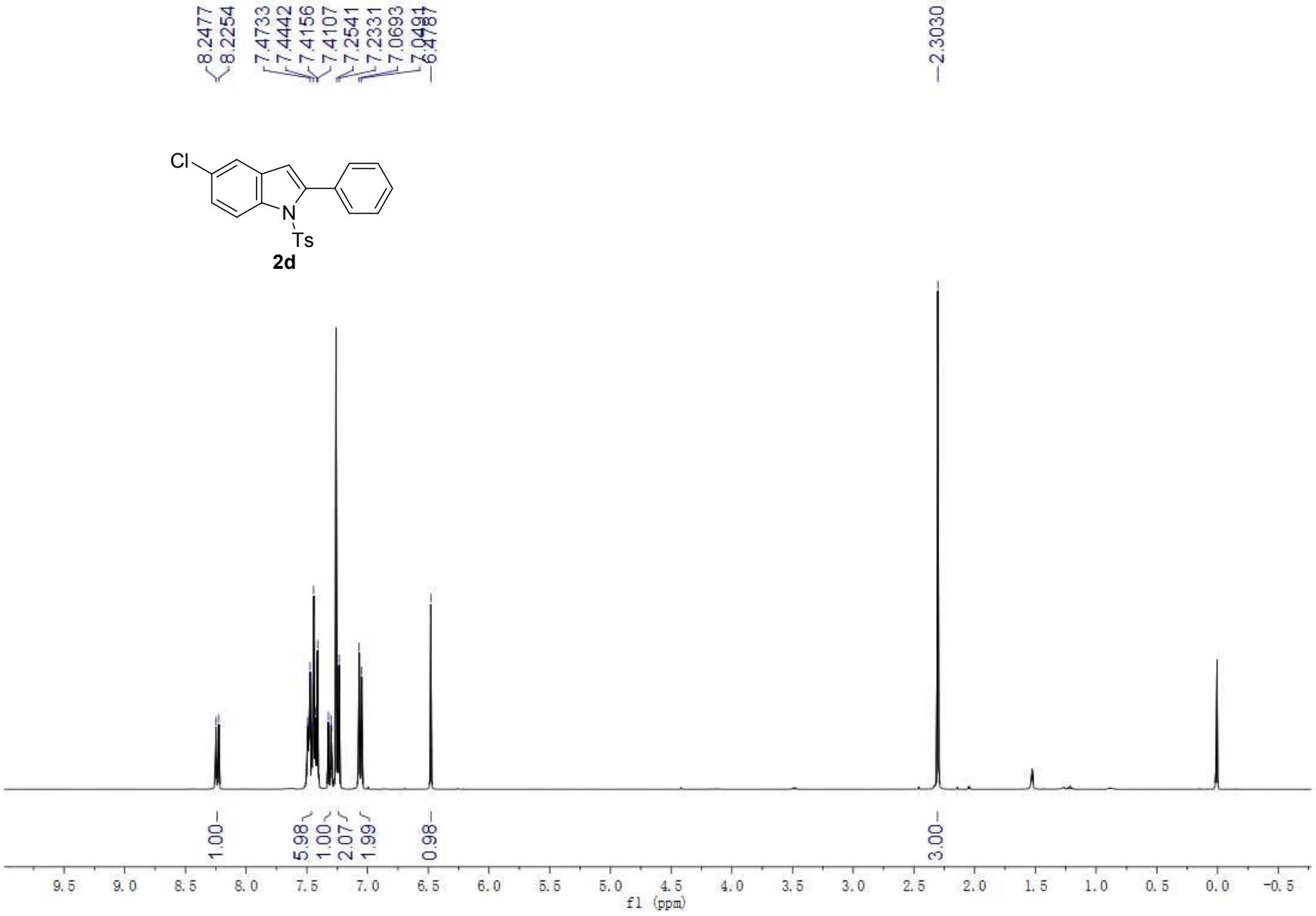
113.2520
113.2266
112.6349
112.4680
106.3199
106.1610
21.5370
F
N
Ts
2c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2541
7.2331
7.0693
7.0481
6.4787
2.3030
Cl
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Ts
2d
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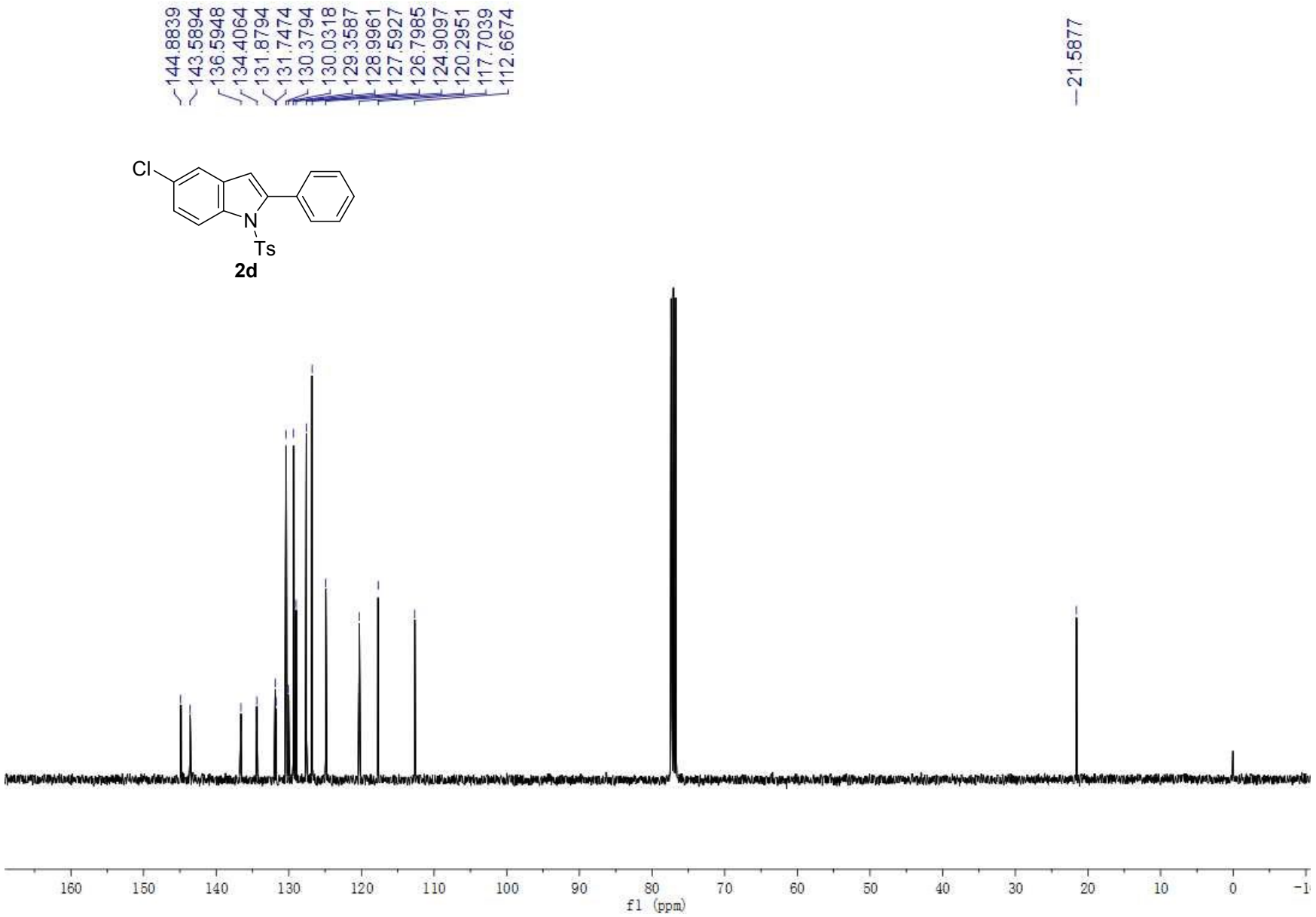
1.00
2.07
1.99
0.98
3.00
f1 (ppm)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131.7474
130.3794
130.0318
129.3587
128.9961
127.5927
126.7985
124.9097
120.2951
117.7039
112.6674
21.5877
Cl
N
Ts
2d
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140
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120
110
100
90
80
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40
30
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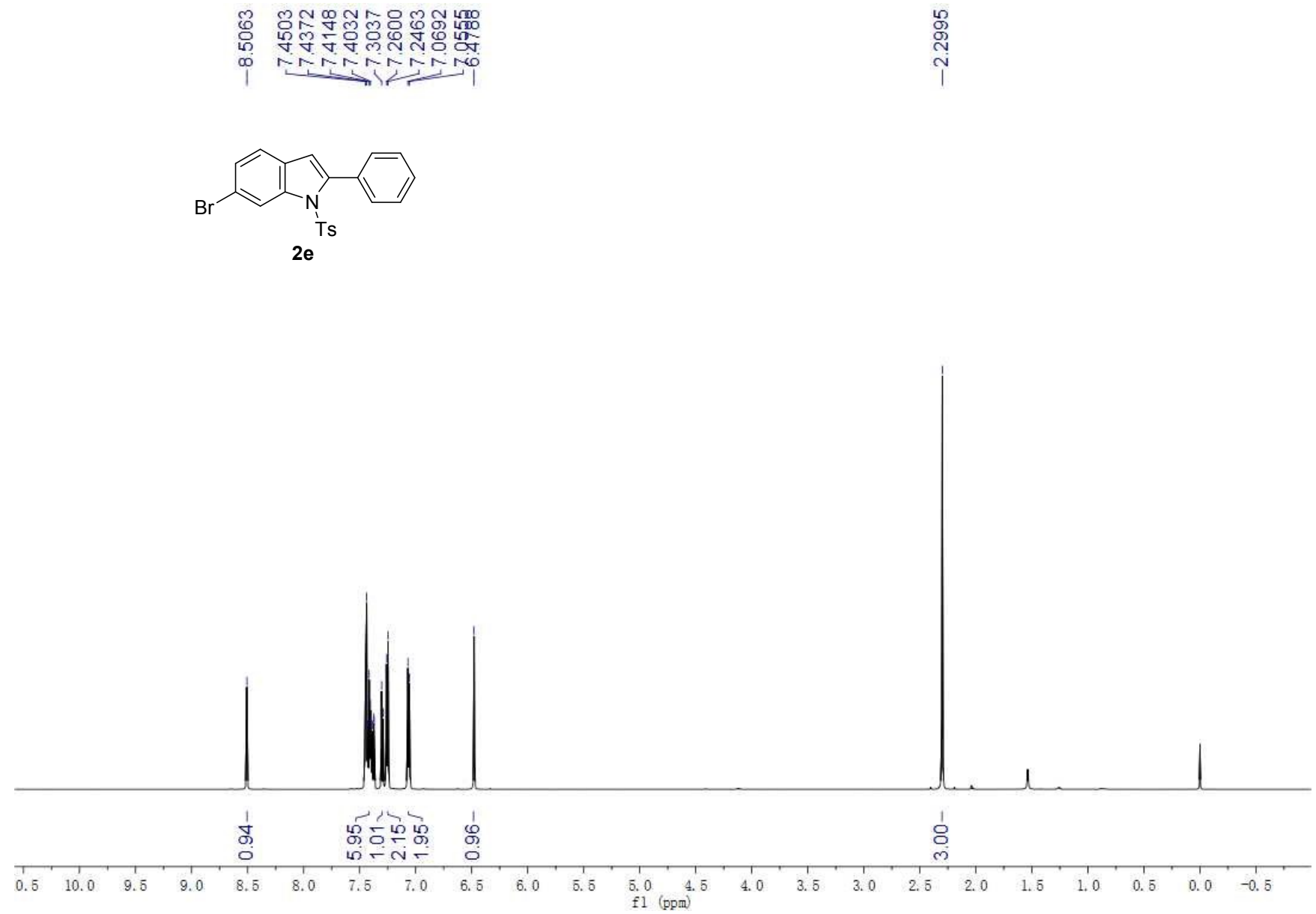
f1 (ppm)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Br
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Ts
2e
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2.15
1.95
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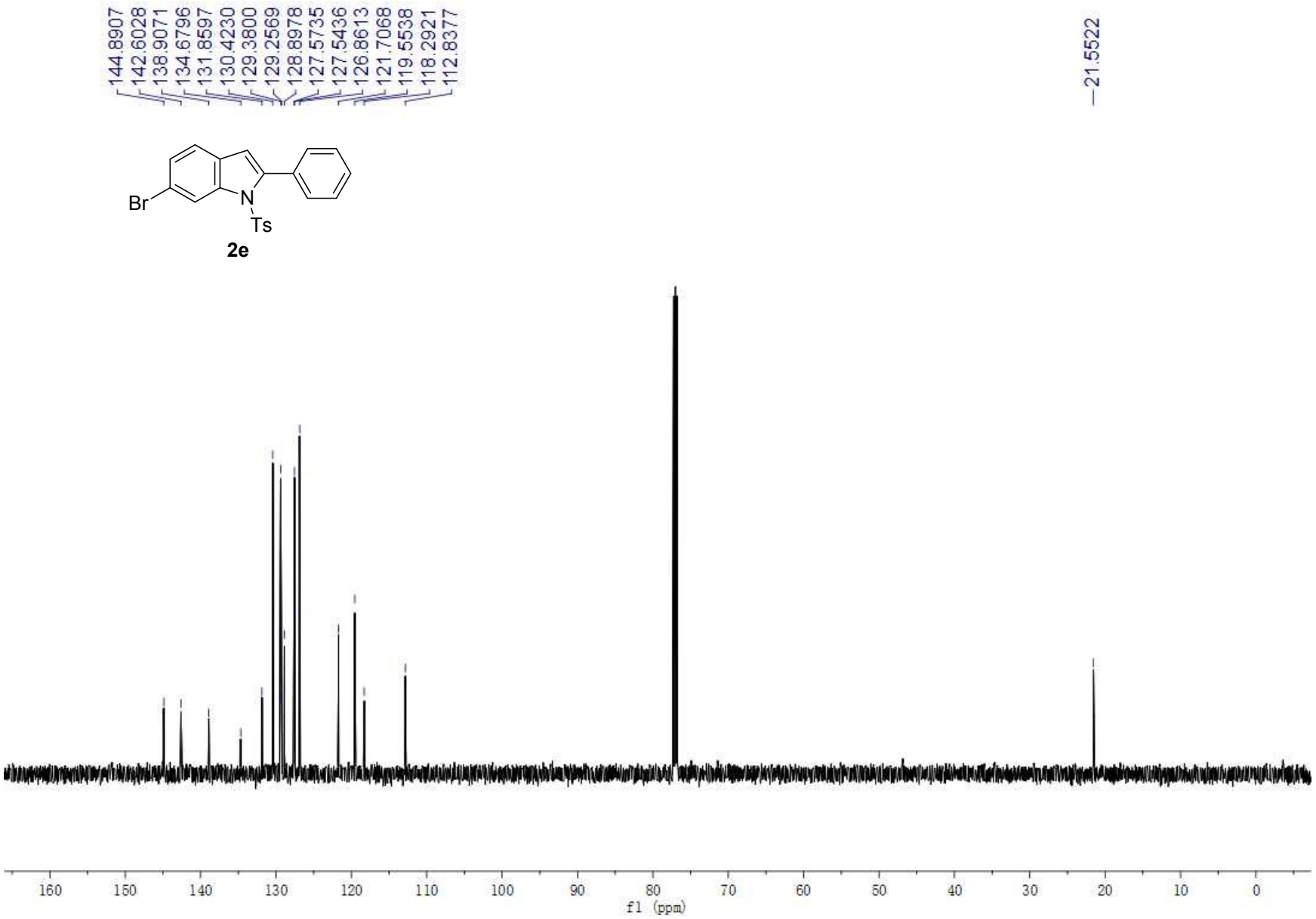
3.00
f1 (ppm)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119.5538
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21.5522
Br
N
Ts
2e
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110
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90
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70
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50
40
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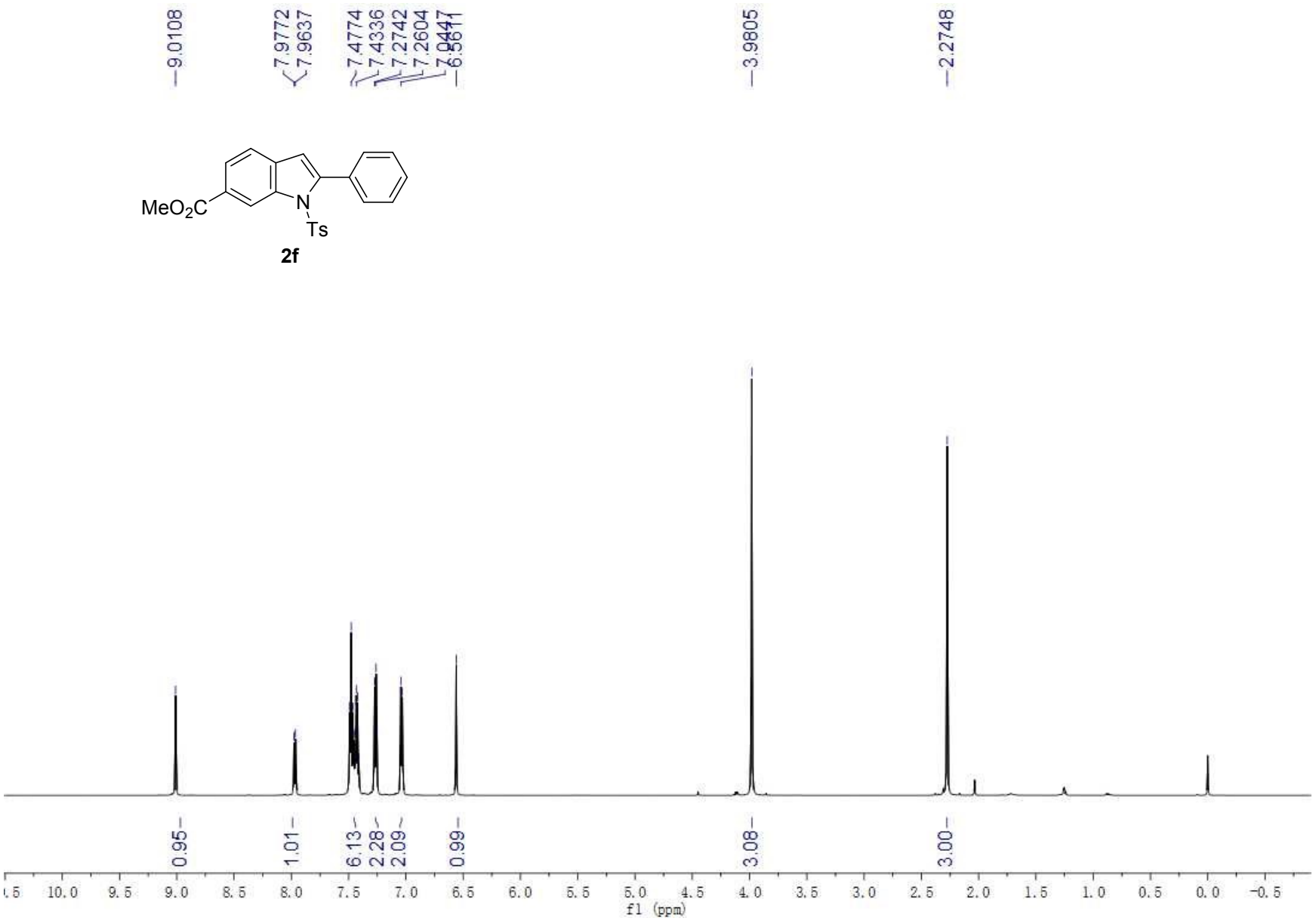
10
0
f1 (ppm)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6.9611
3.9805
2.2748
MeO2C
N
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2f
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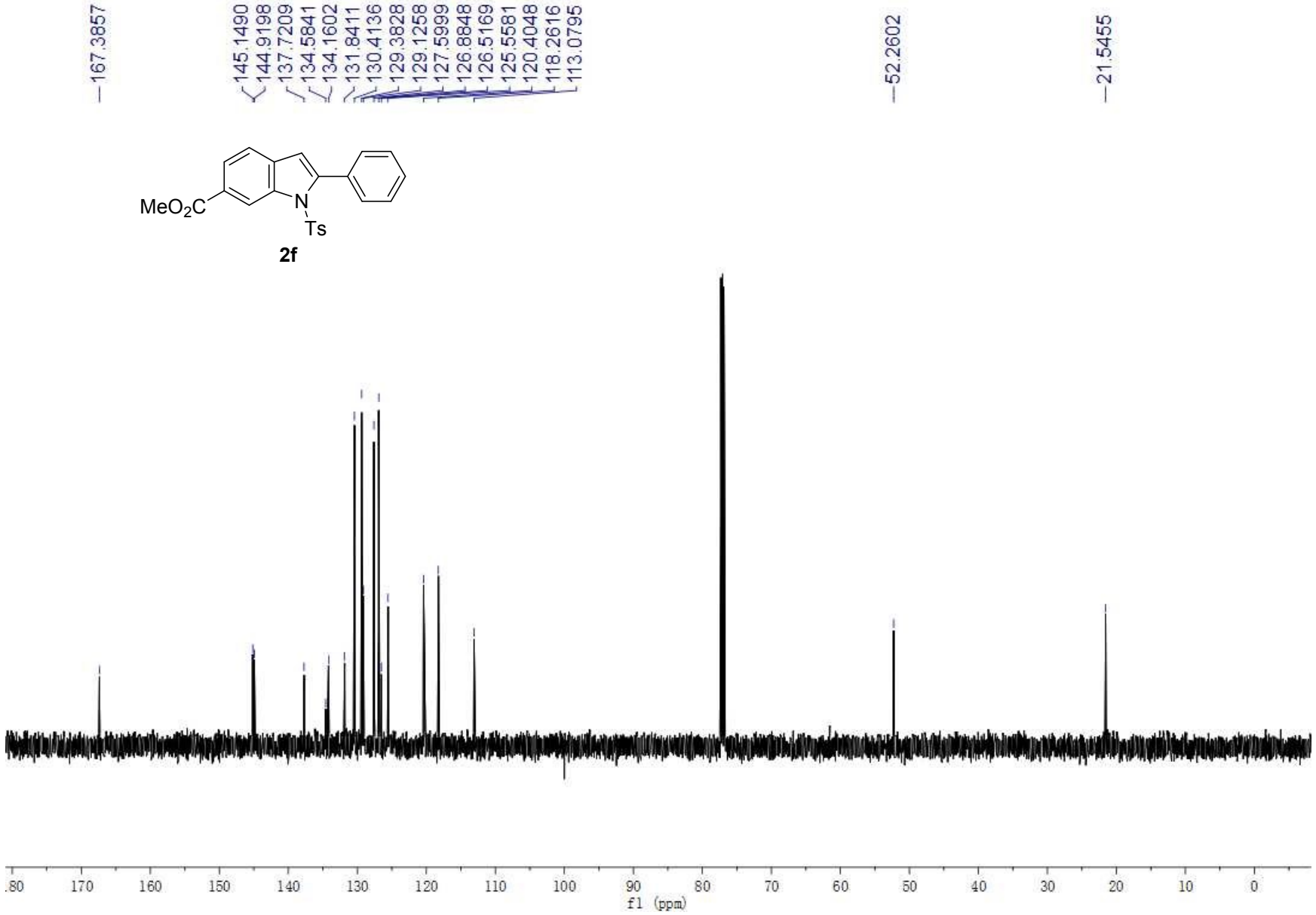
6.13
2.28
2.09
0.99
3.08
3.00
f1 (ppm)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126.8848
126.5169
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MeO2C
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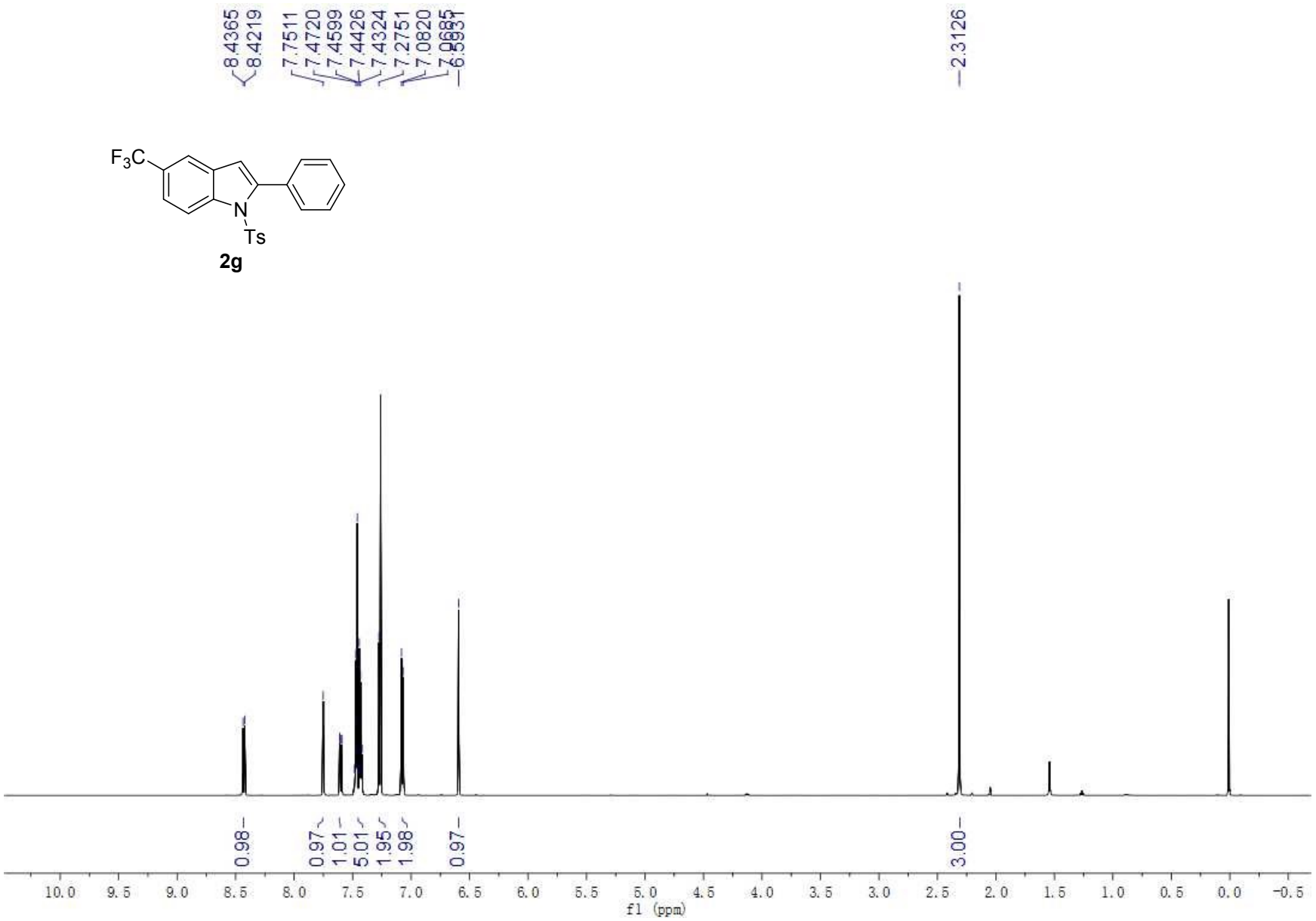
Ts
2f
f1 (ppm)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7.4599
7.4426
7.4324
7.2751
7.0820
2.3126
F3C
N
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2g
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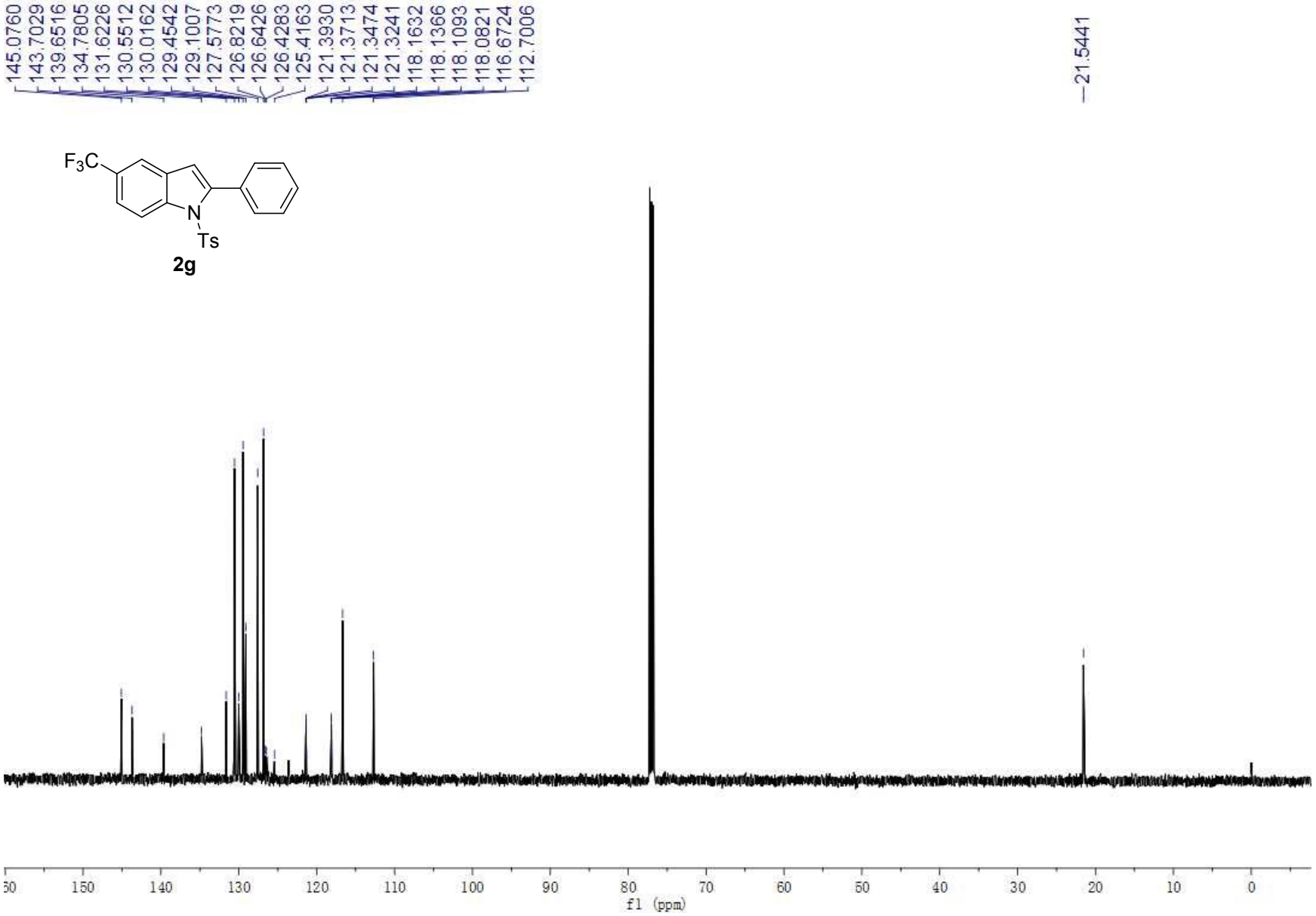
0.97
1.01
5.01
1.95
1.98
0.97
3.00
f1 (ppm)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126.8219
126.6426
126.4283
125.4163
121.3930
121.3713
121.3474
121.3241
118.1632
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118.0821
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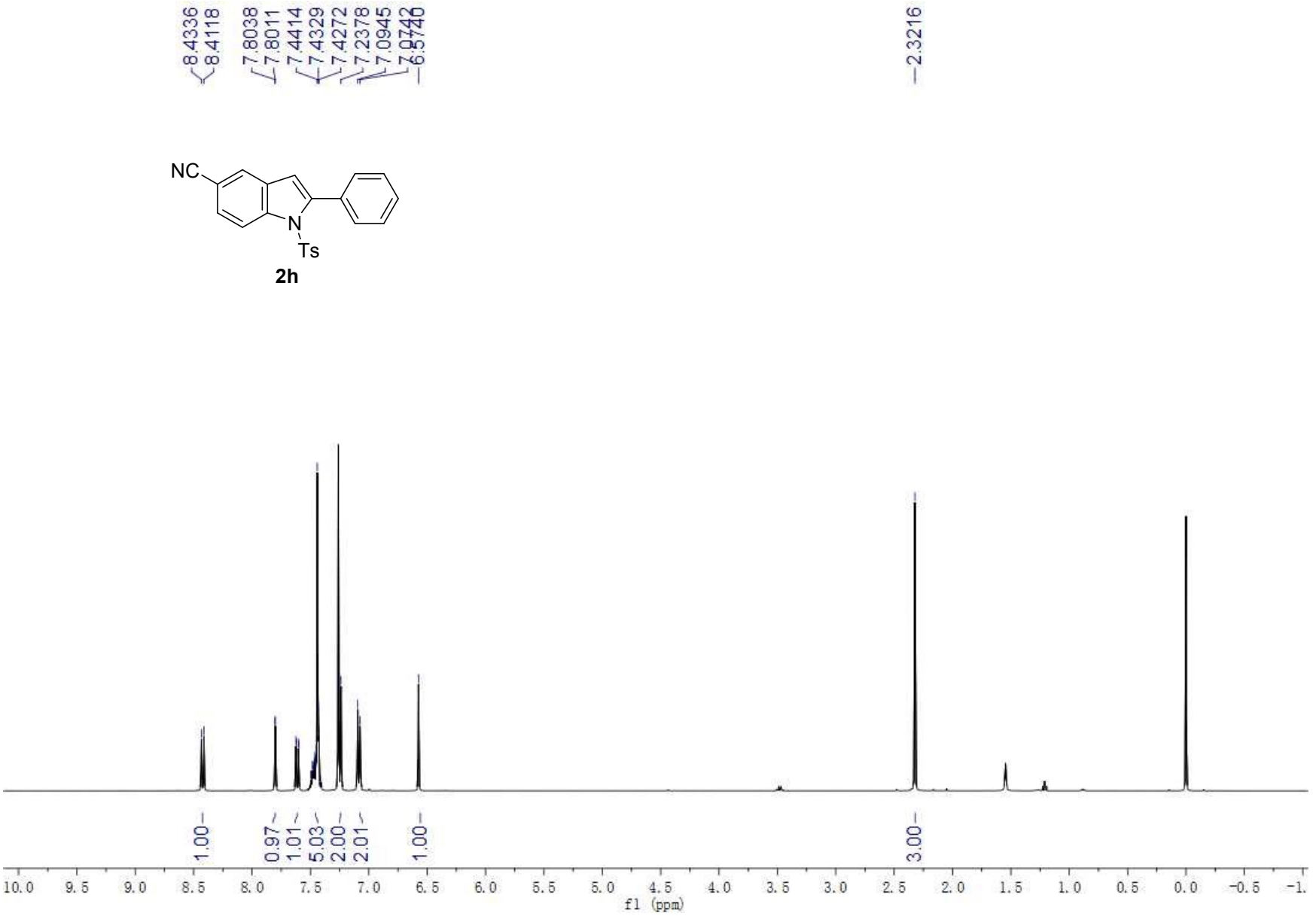
112.7006
21.5441
F3C
N
Ts
2g
f1 (ppm)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7.4329
7.4272
7.2378
7.0945
2.3216
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N
Ts
2h
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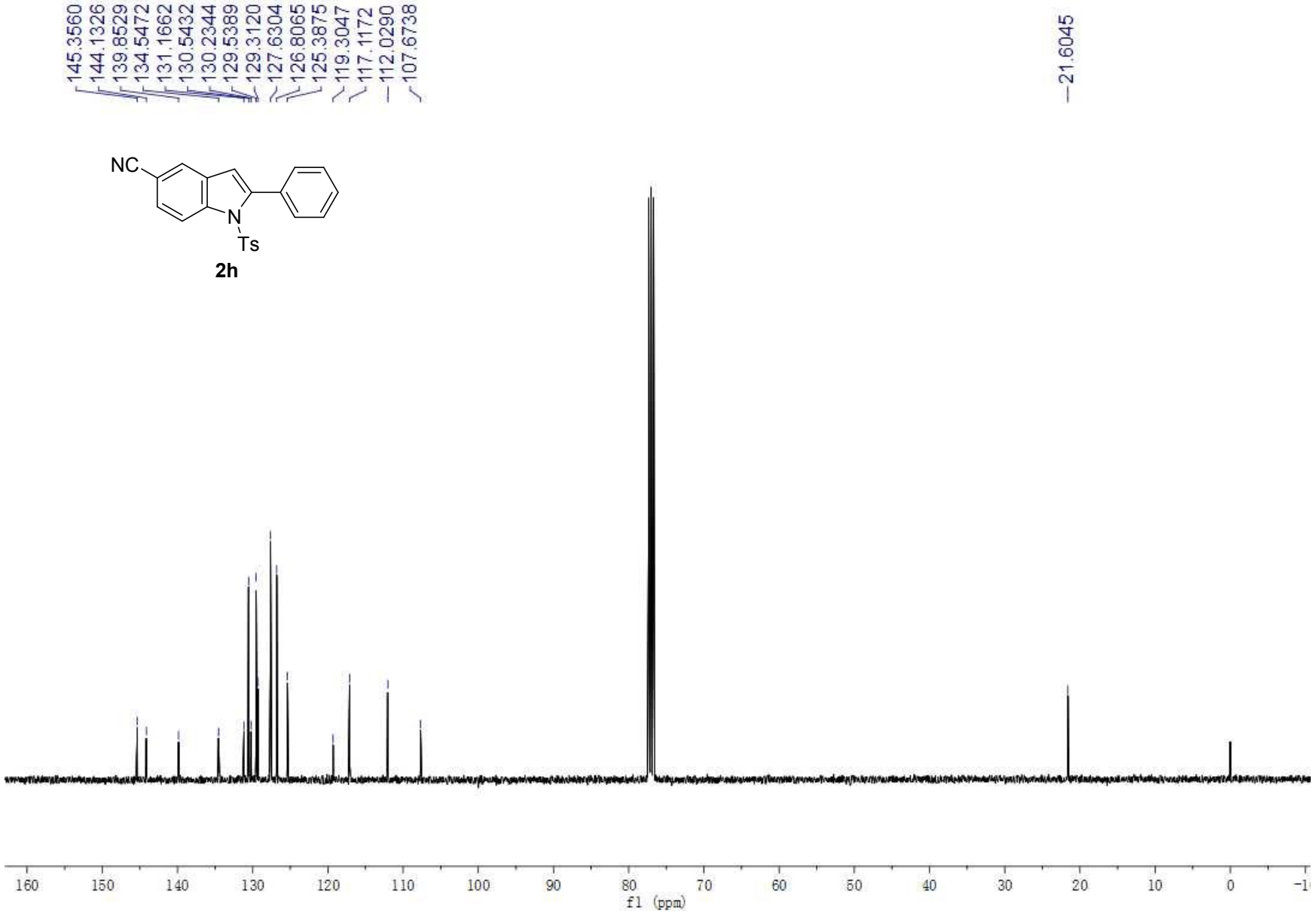
0.97
1.01
5.03
2.00
2.01
1.00
3.00
f1 (ppm)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130.2344
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129.3120
127.6304
126.8065
125.3875
119.3047
117.1172
112.0290
107.6738
21.6045
NC
N
Ts
2h
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120
110
100
90
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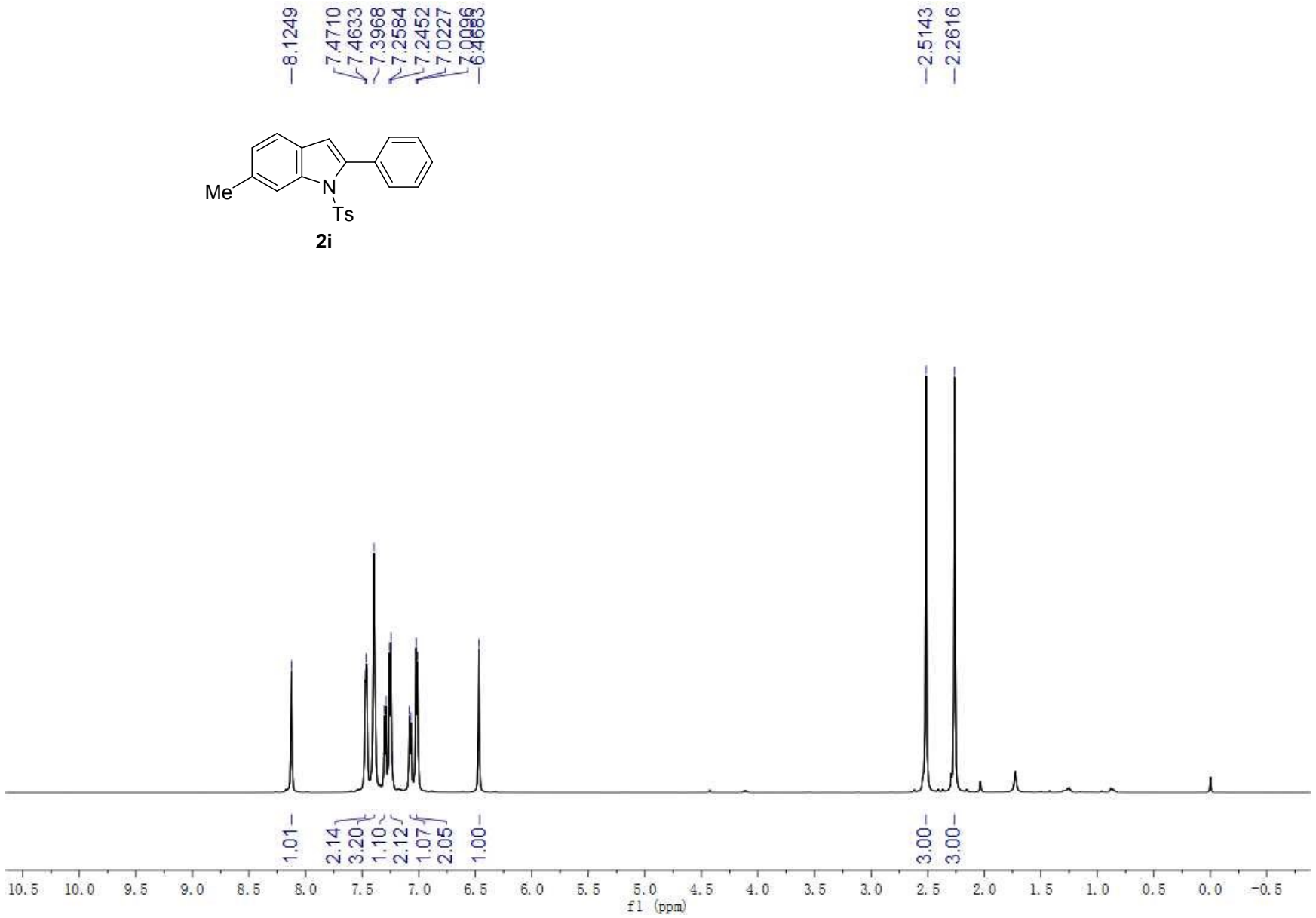
50
40
30
20
10
0
f1 (ppm)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7.2584
7.2452
7.0227
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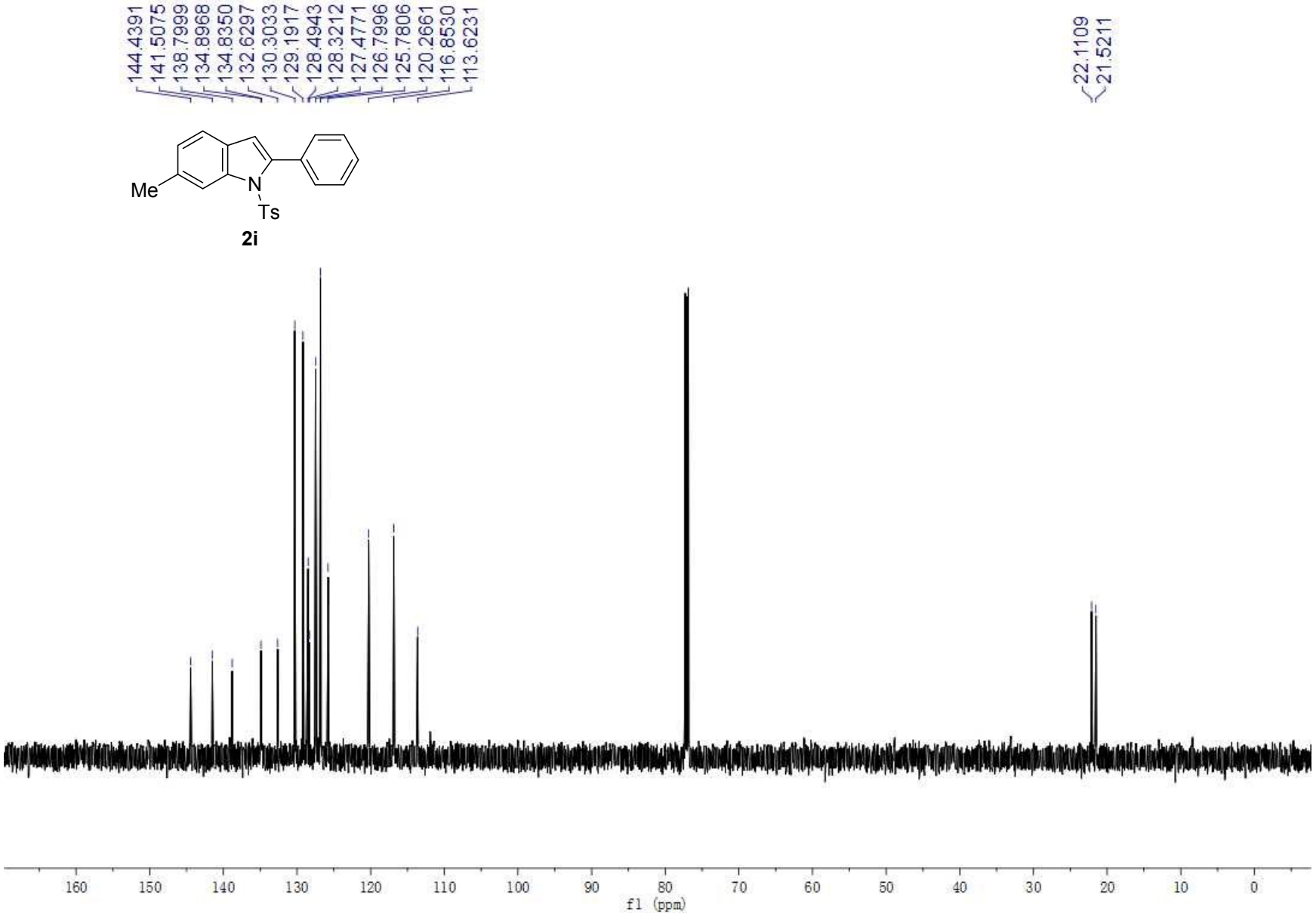
2.2616
Me
N
Ts
2i
1.01
2.14
3.20
1.10
2.12
1.07
2.05
1.00
3.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.4771
126.7996
125.7806
120.2661
116.8530
113.6231
22.1109
21.5211
Me
N
Ts
2i
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150
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130
120
110
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90
80
70
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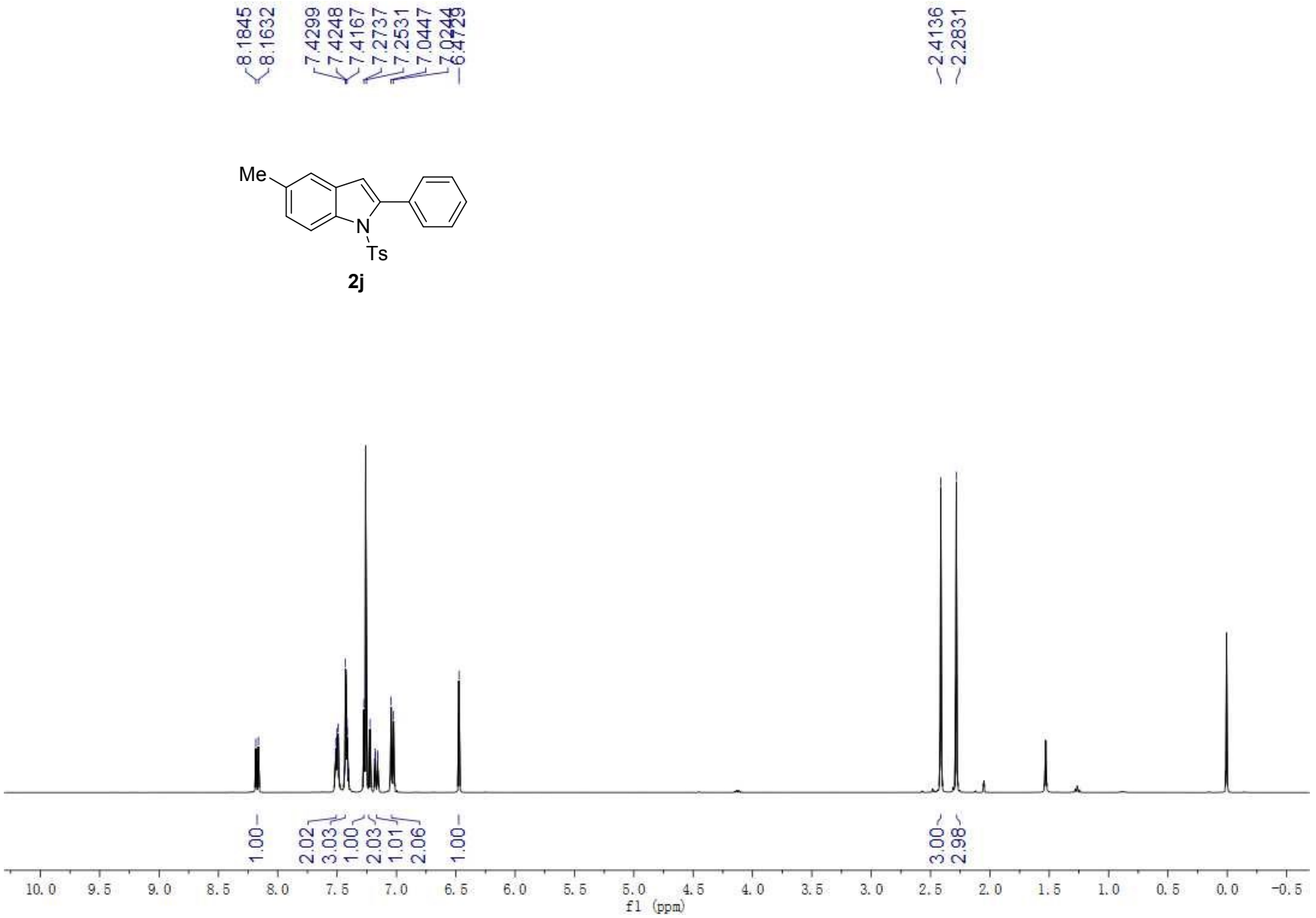
50
40
30
20
10
0
f1 (ppm)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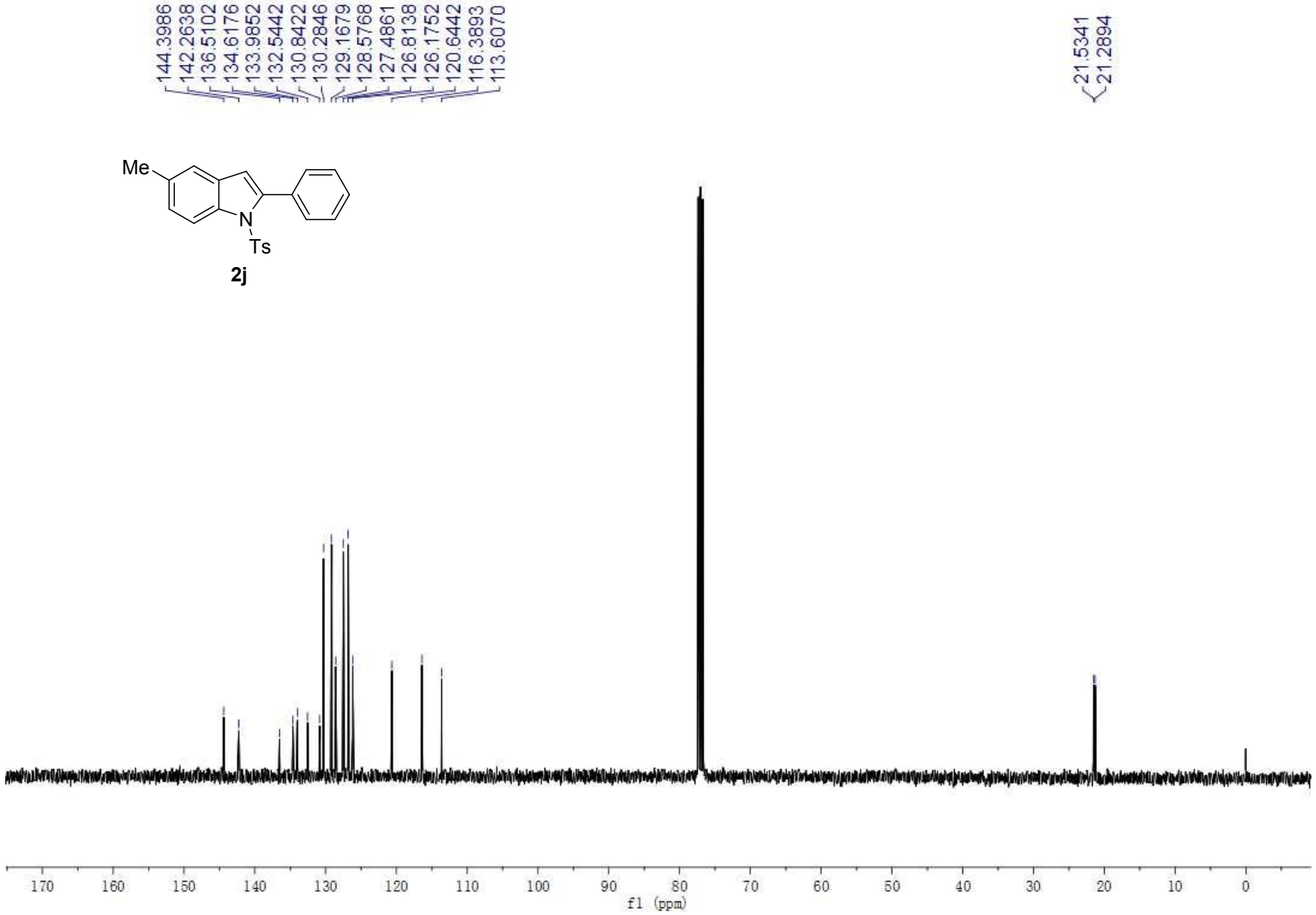
8.1632
7.4299
7.4248
7.4167
7.2737
7.2531
7.0447
2.4136
2.2831
Me
N
Ts
1.00
2.02
3.03
1.00
2.03
1.01
2.06
1.00
3.00
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

2j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126.8138
126.1752
120.6442
116.3893
113.6070
21.5341
21.2894
Me
N
Ts
2j
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130
120
110
100
90
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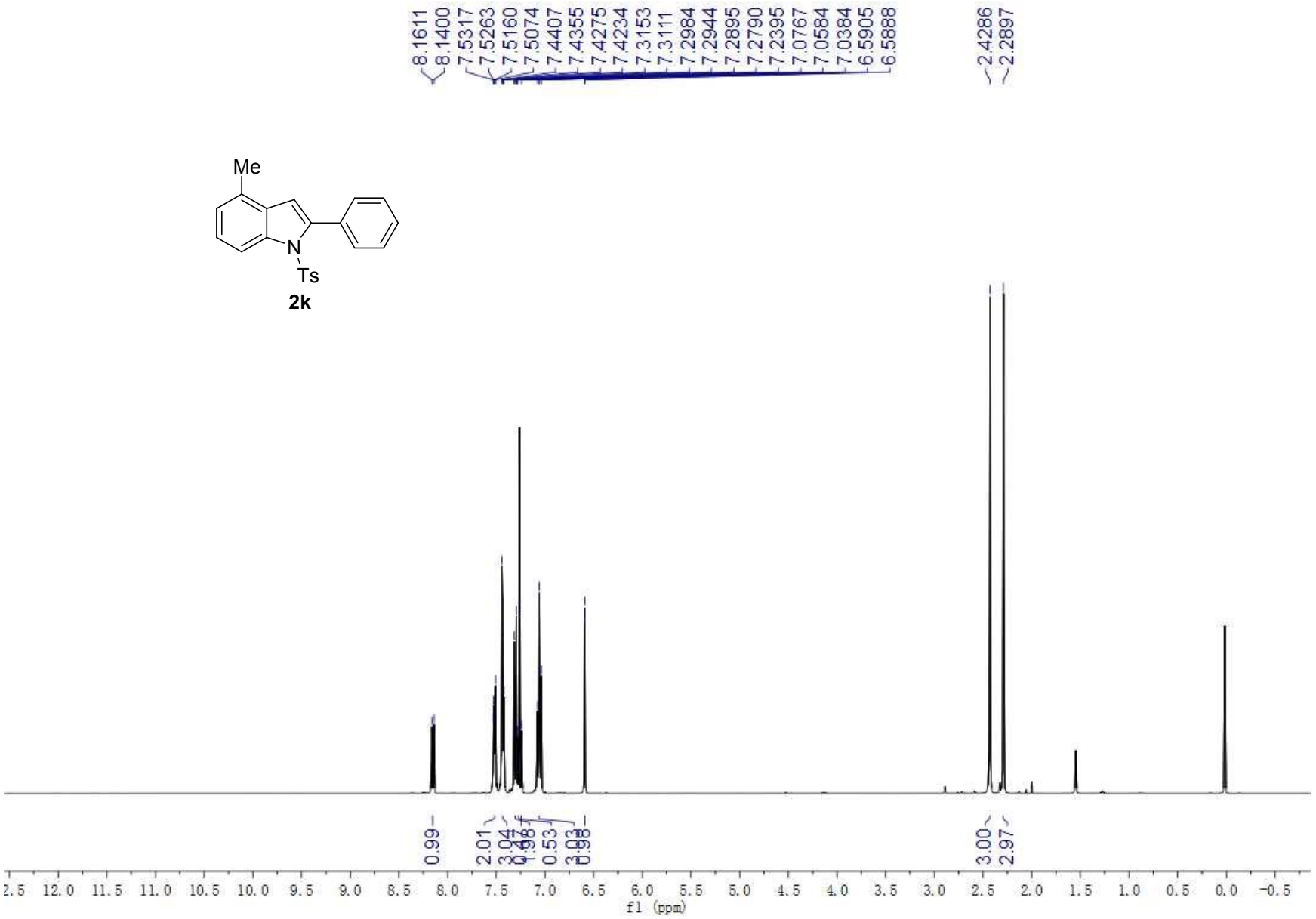
50
40
30
20
10
0
f1 (ppm)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7.3153
7.3111
7.2984
7.2944
7.2895
7.2790
7.2395
7.0767
7.0584
7.0384
6.5905
6.5888
2.4286
2.2897
Me
N
Ts
2k
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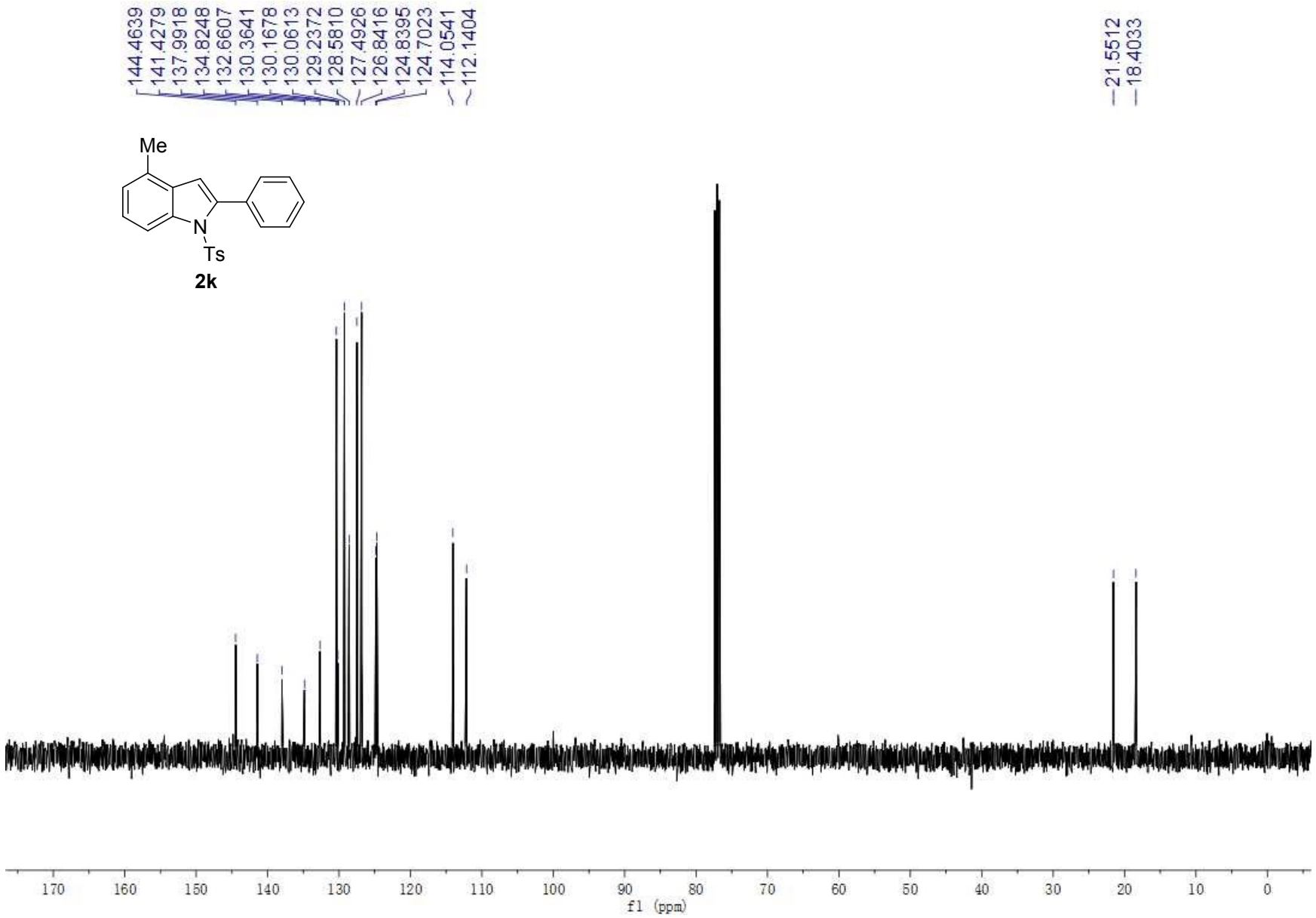
2.01
3.04
4.98
0.53
3.03
0.98
3.00
2.97
f1 (ppm)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127.4926
126.8416
124.8395
124.7023
114.0541
112.1404
21.5512
18.4033
Me
N
Ts
2k
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130
120
110
100
90
80
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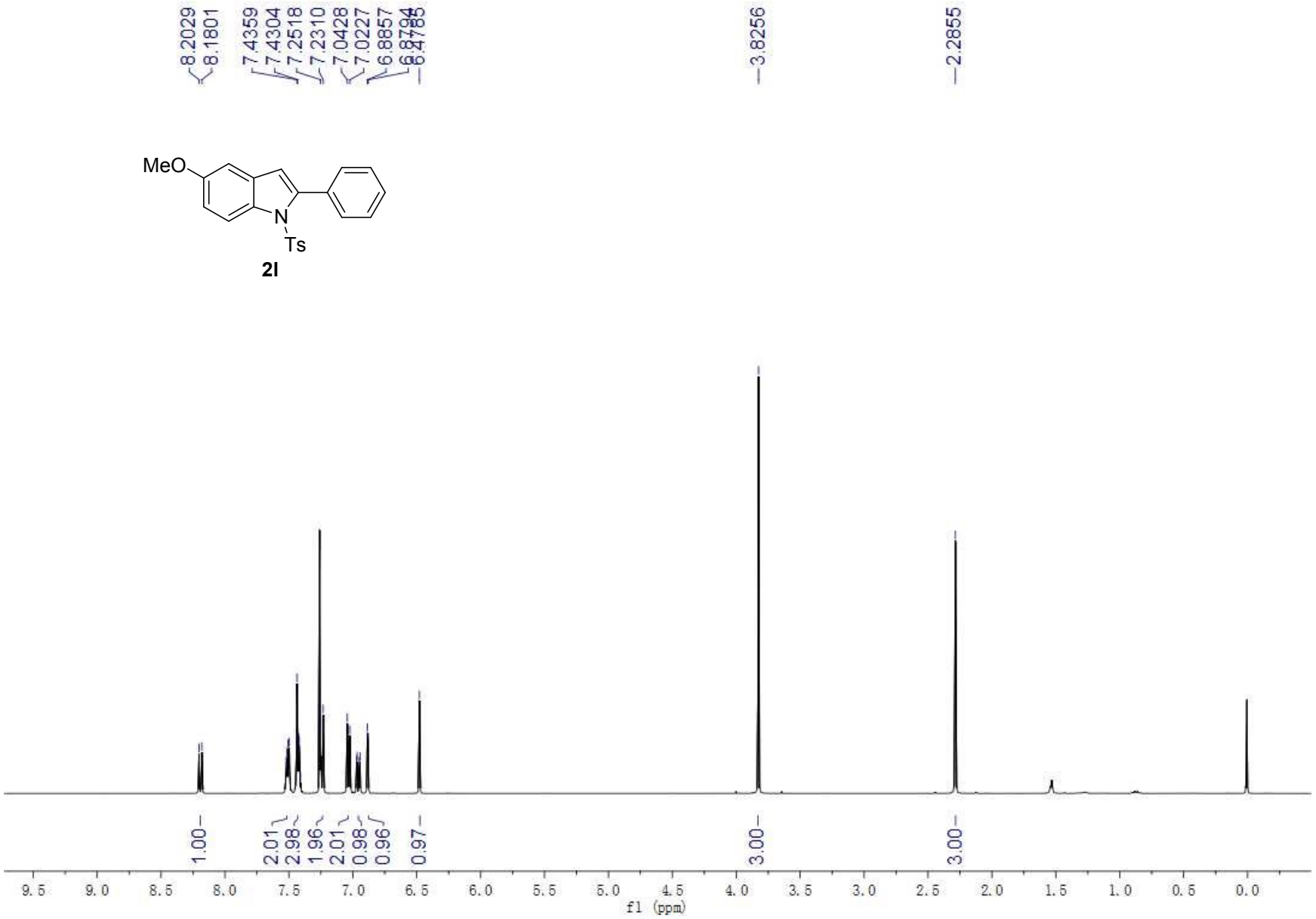
50
40
30
20
10
0
f1 (ppm)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6.8857
6.8794
6.8785
3.8256
2.2855
MeO
N
Ts
2l
1.00
2.01
2.98
1.96
2.01
0.98
0.96
0.97
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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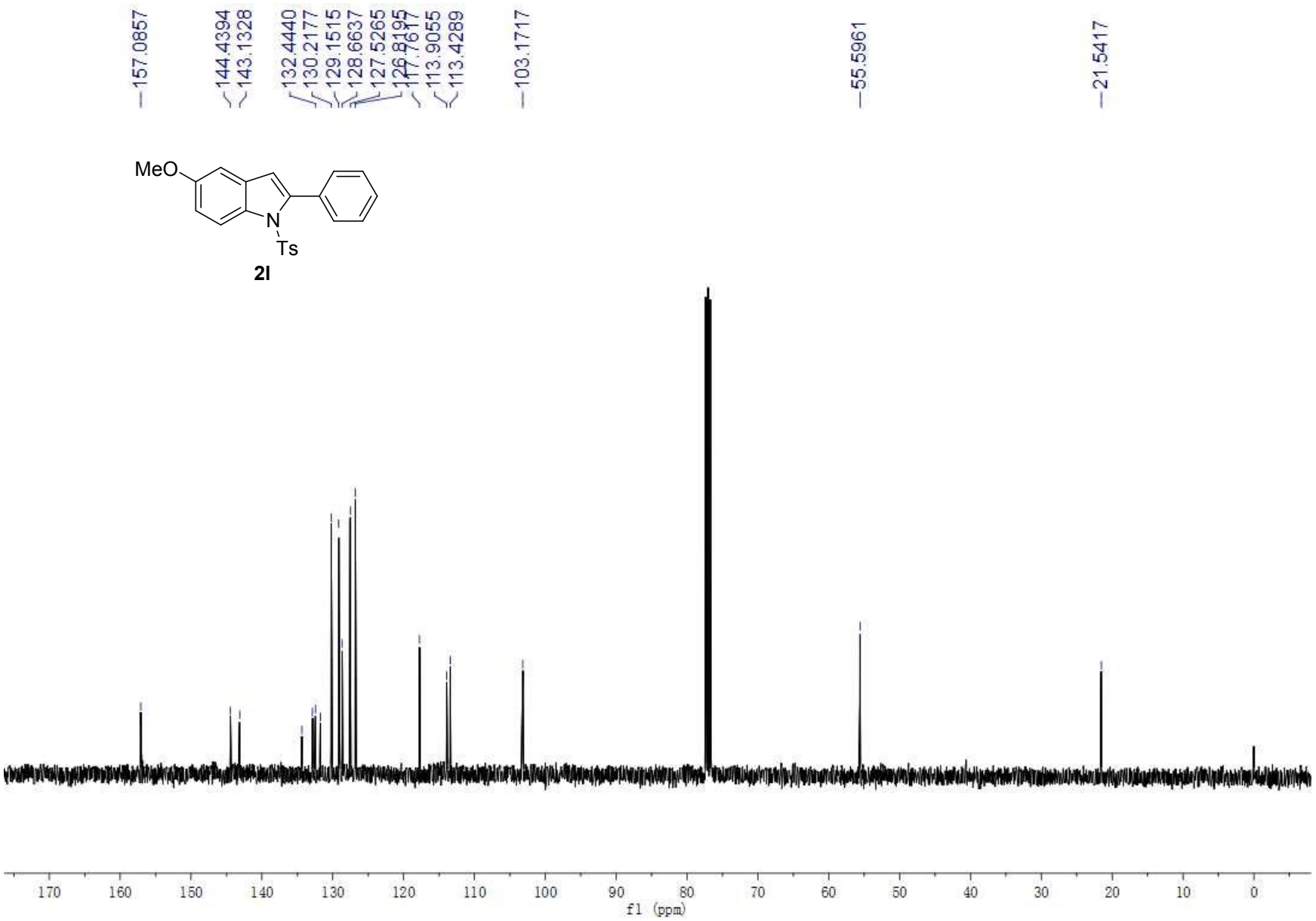
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113.9055
113.4289
103.1717
55.5961
21.5417
MeO
N
Ts
2l
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110
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90
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70
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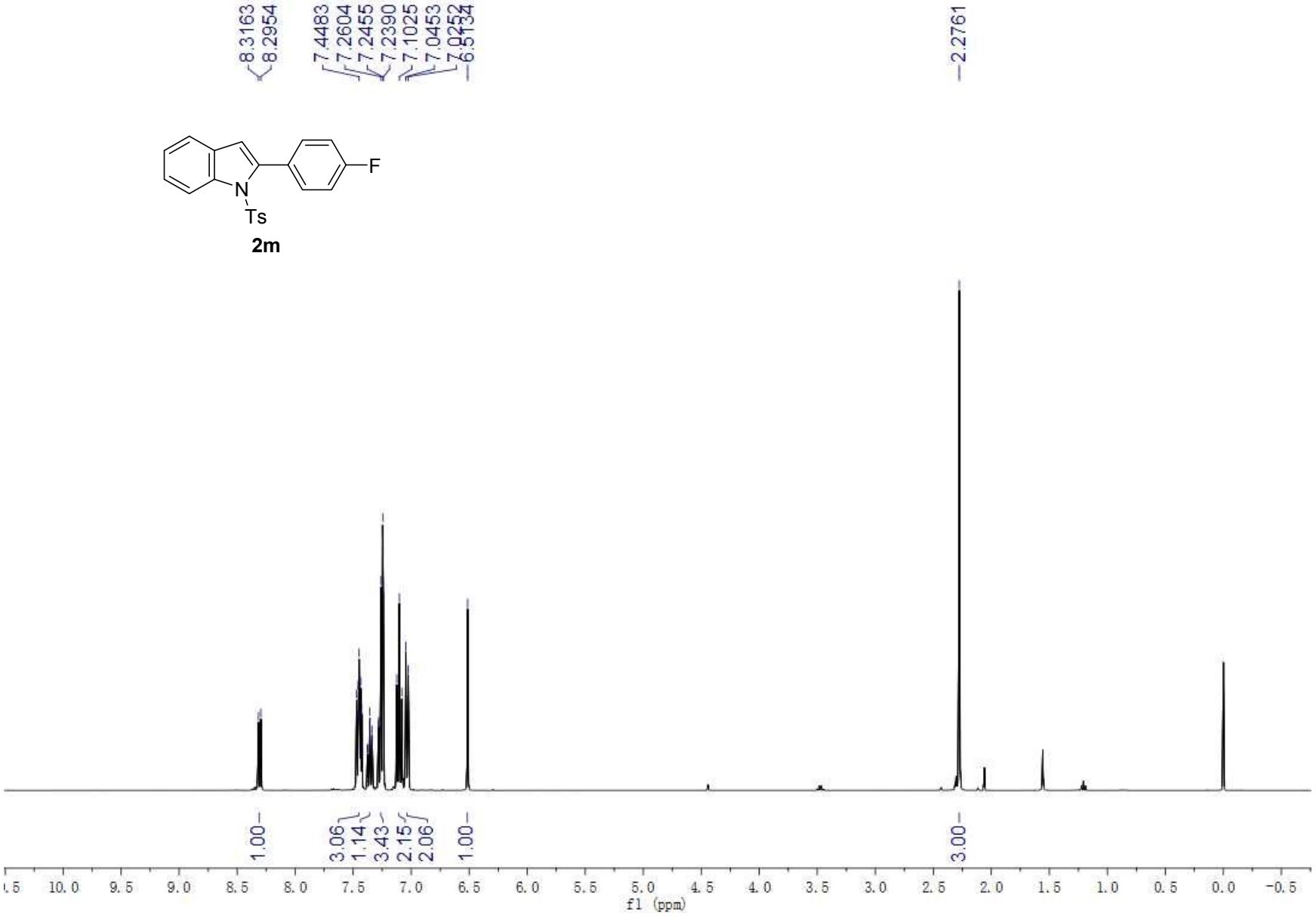
50
40
30
20
10
0
f1 (ppm)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7.1025
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2.2761
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N
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2.06
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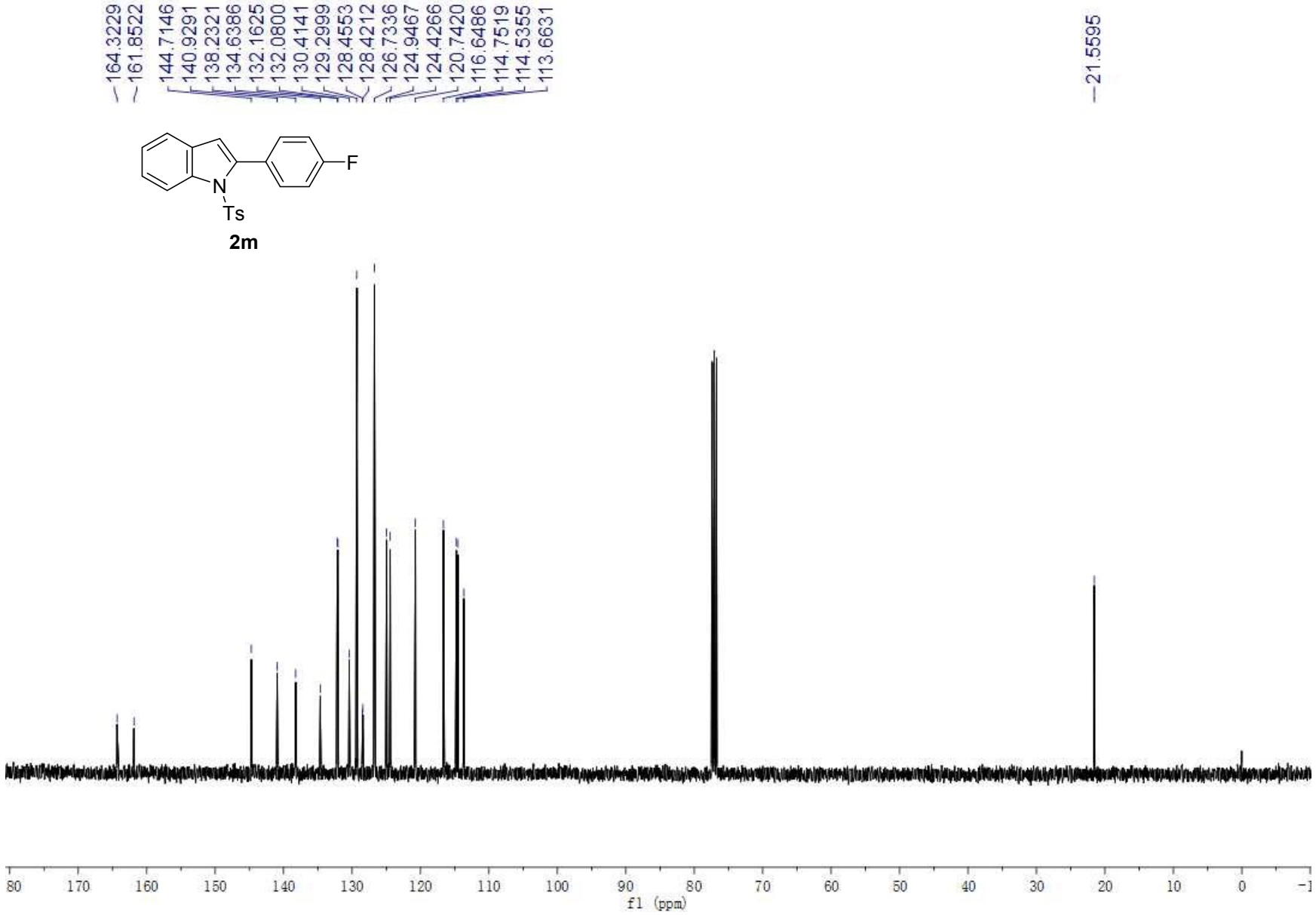
3.00
f1 (ppm)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128.4553
128.4212
126.7336
124.9467
124.4266
120.7420
116.6486
114.7519
114.5355
113.6631
21.5595
F
N
Ts
2m
80
170
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140
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120
110
100
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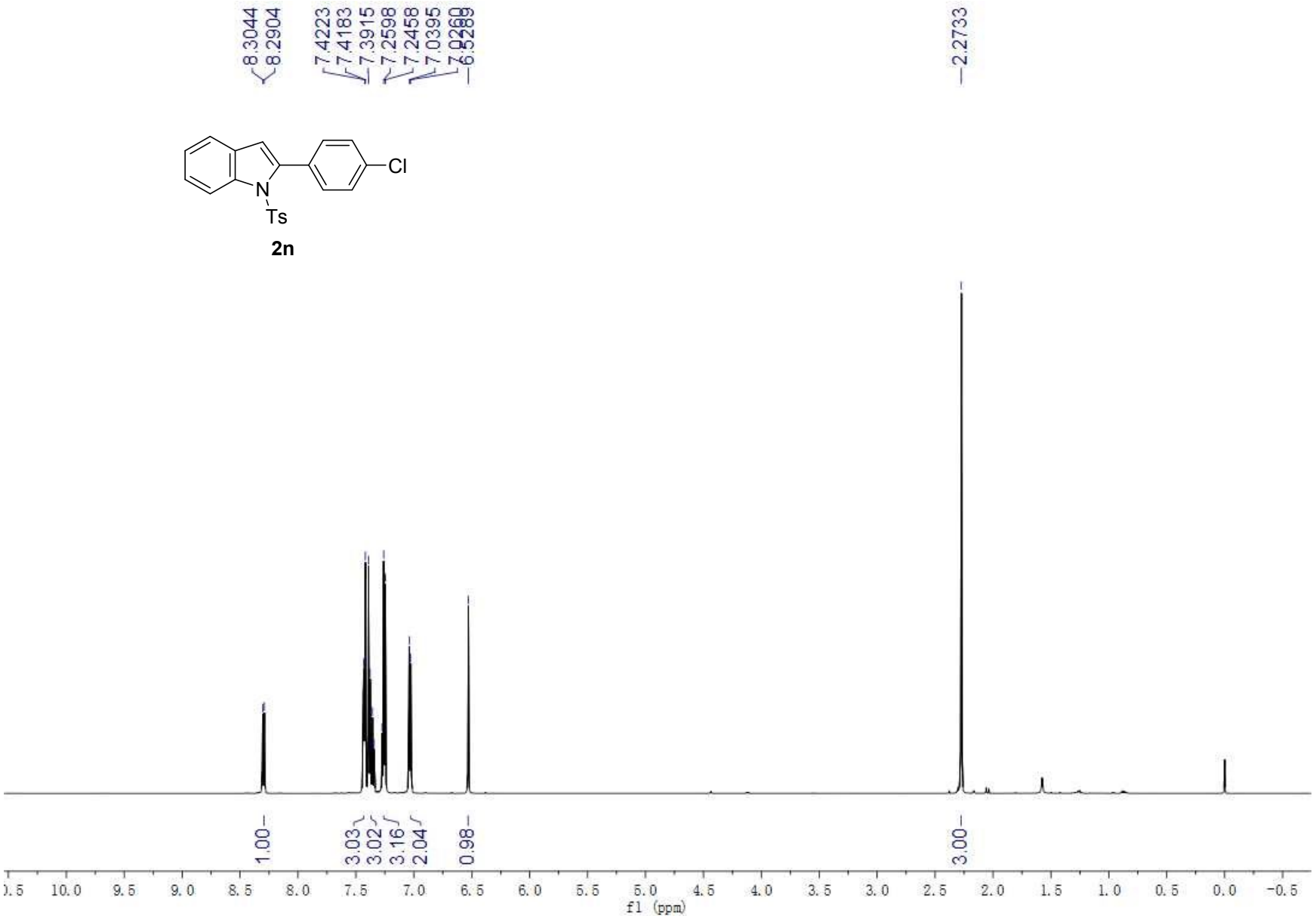
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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3.16
2.04
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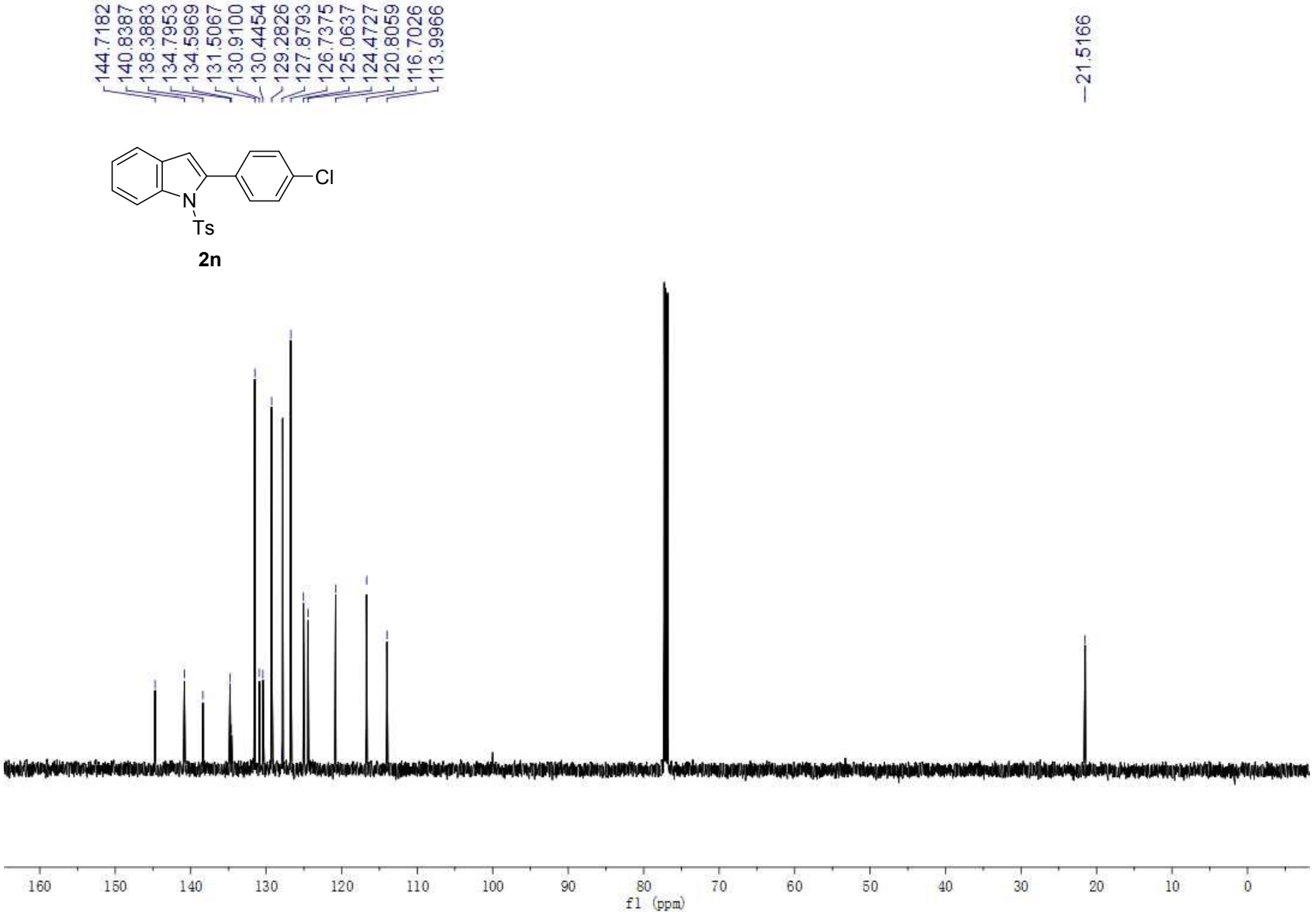
3.00
f1 (ppm)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125.0637
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120.8059
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113.9966
21.5166
Cl
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Ts
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50
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10
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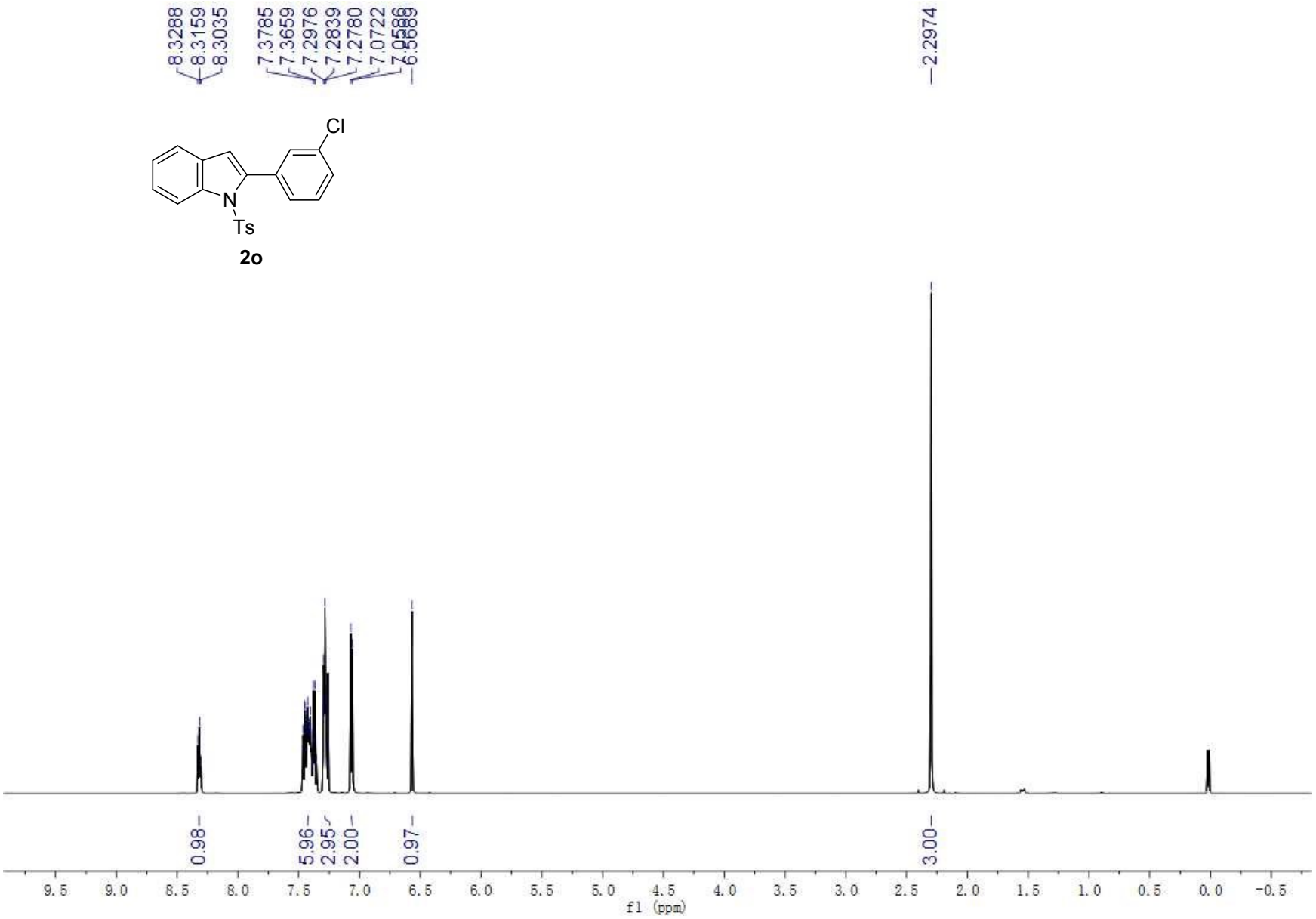
f1 (ppm)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Ts
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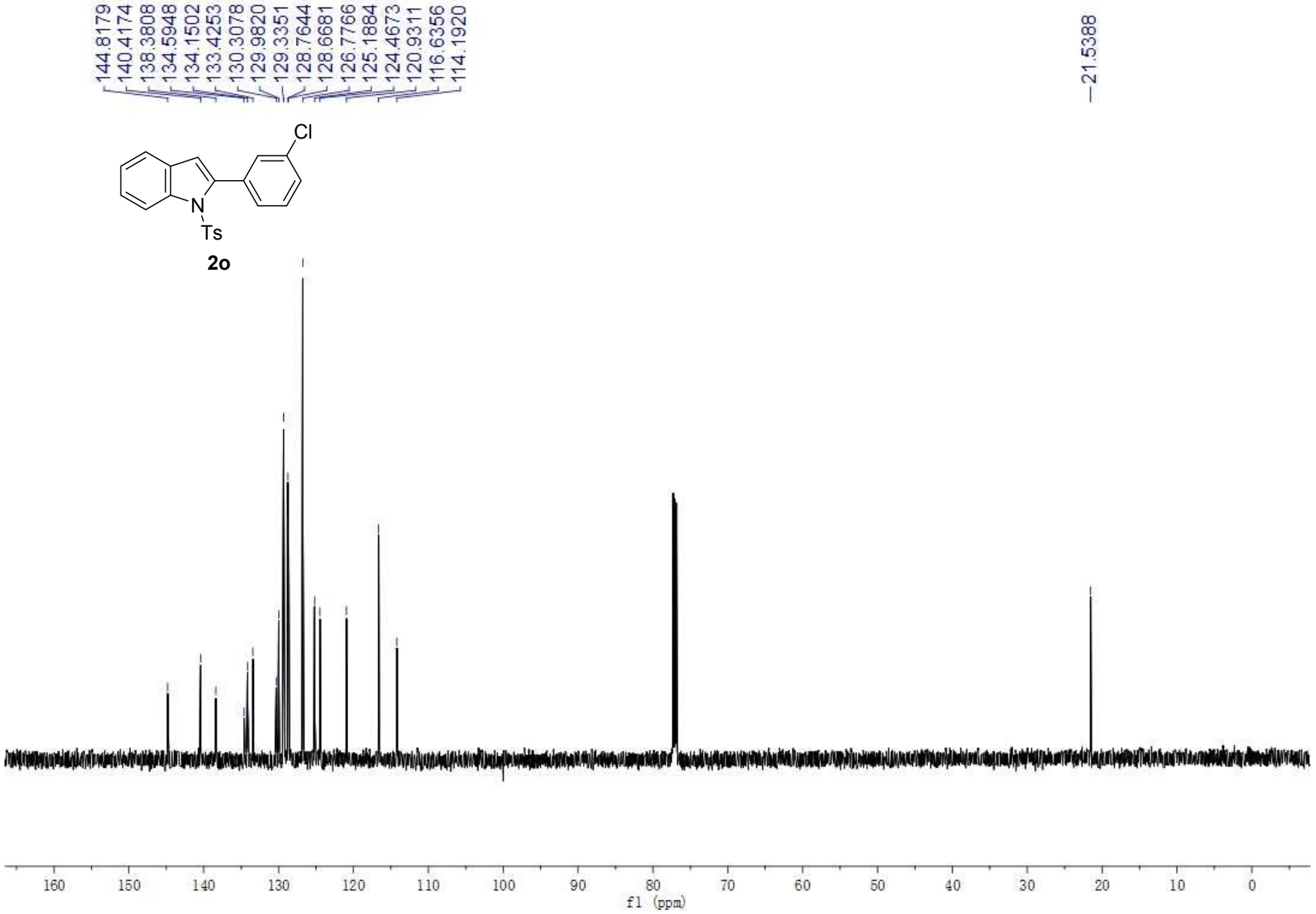
3.00
f1 (ppm)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126.7766
125.1884
124.4673
120.9311
116.6356
114.1920
21.5388
Cl
N
Ts
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150
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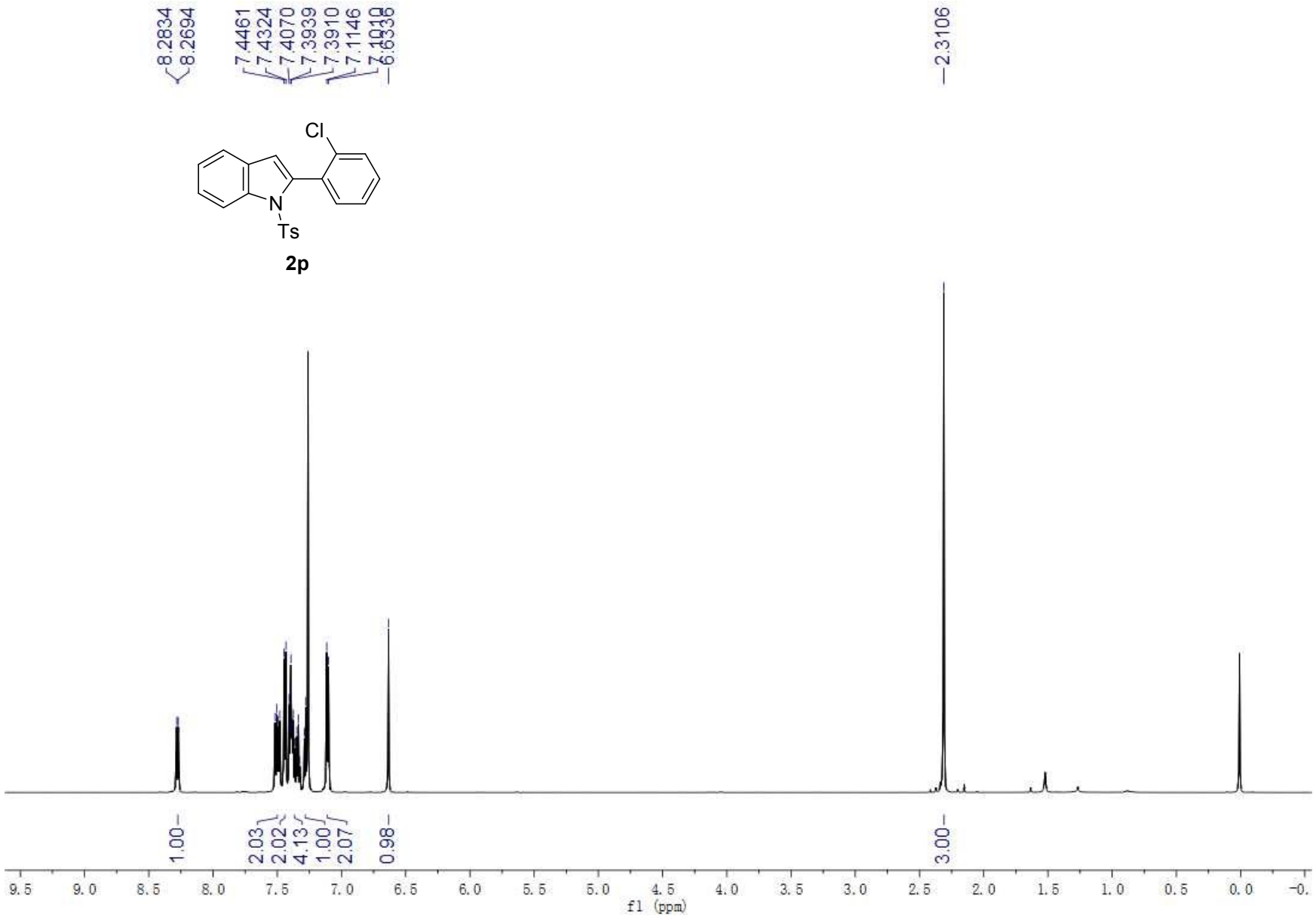
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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2.02
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1.00
2.07
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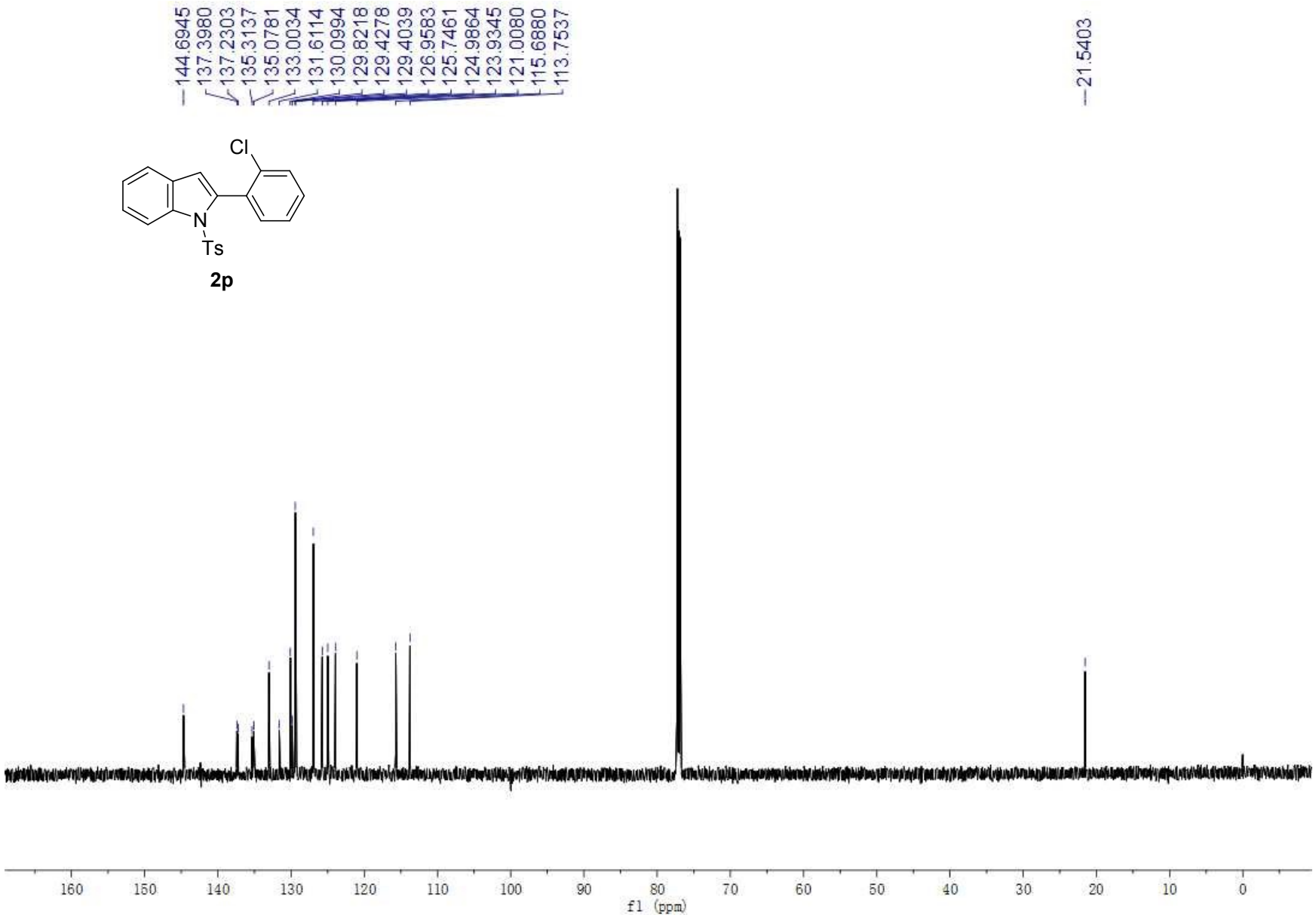
3.00
f1 (ppm)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Cl
N
Ts
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90
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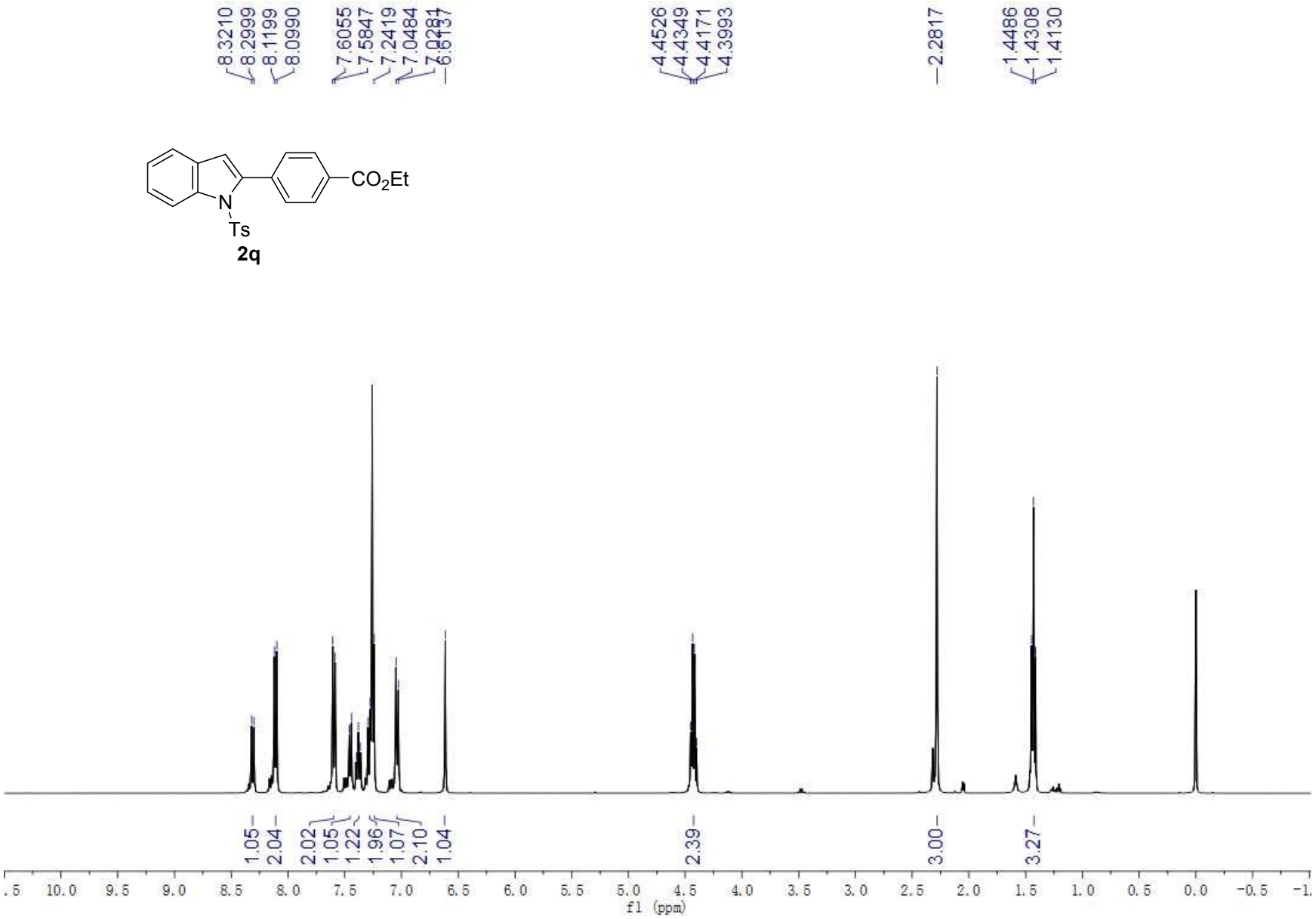
50
40
30
20
10
0
f1 (ppm)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4.4349
4.4171
4.3993
2.2817
1.4486
1.4308
1.4130
CO2Et
N
Ts
2q
1.05
2.04
2.02
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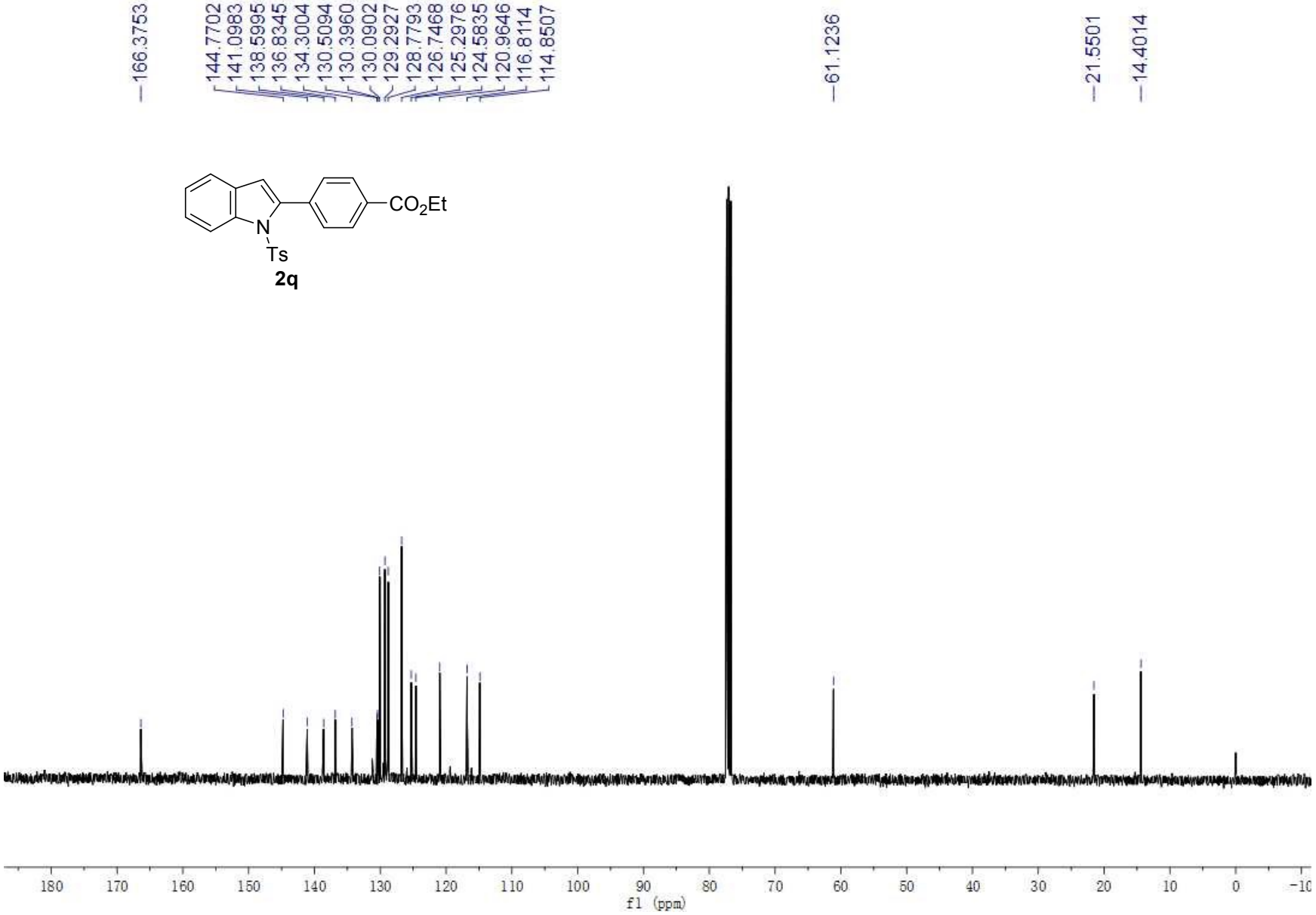
1.22
1.96
1.07
2.10
1.04
2.39
3.00
3.27
f1 (ppm)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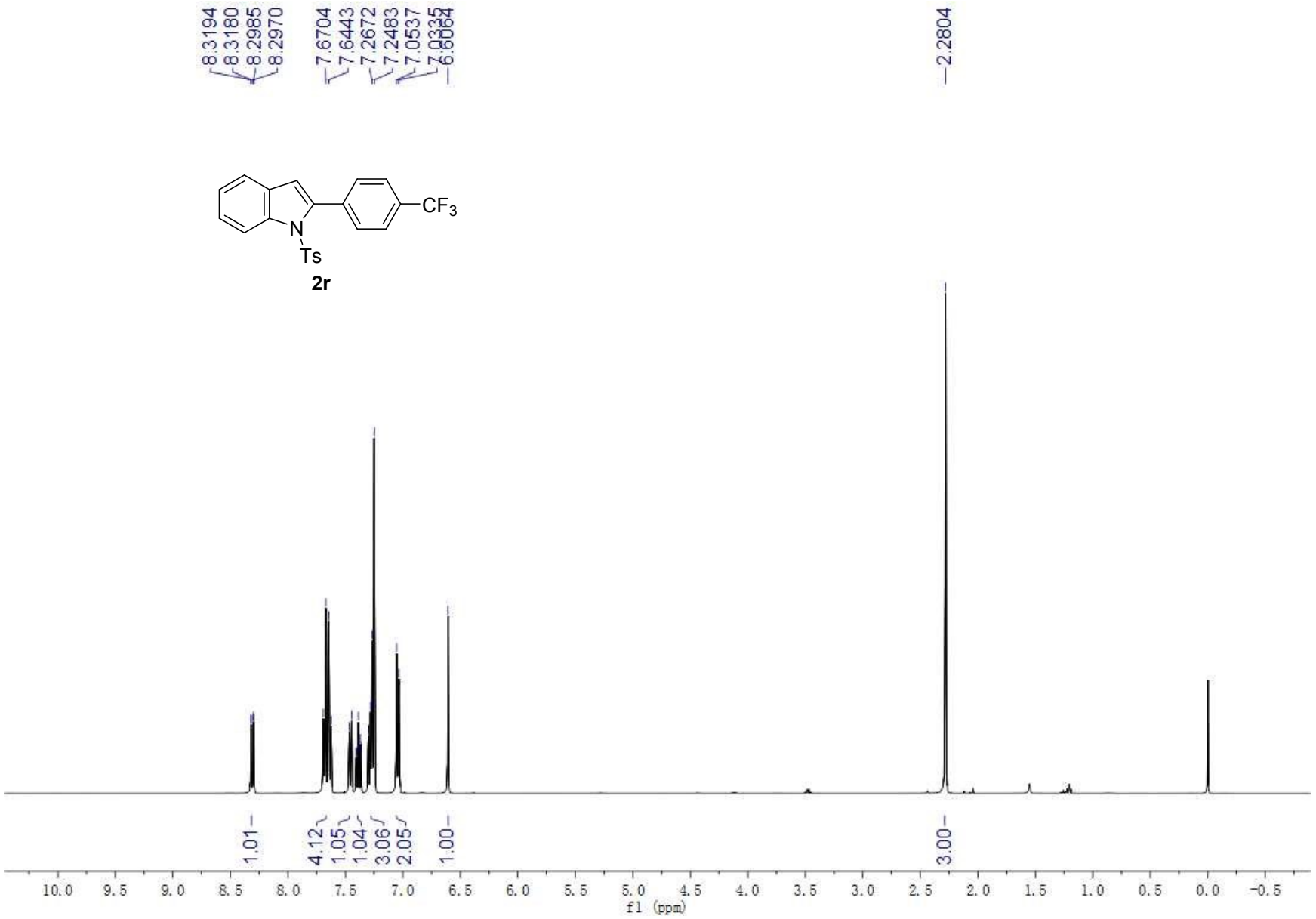
126.7468
125.2976
124.5835
120.9646
116.8114
114.8507
61.1236
21.5501
14.4014
CO2Et
N
Ts
2q
f1 (ppm)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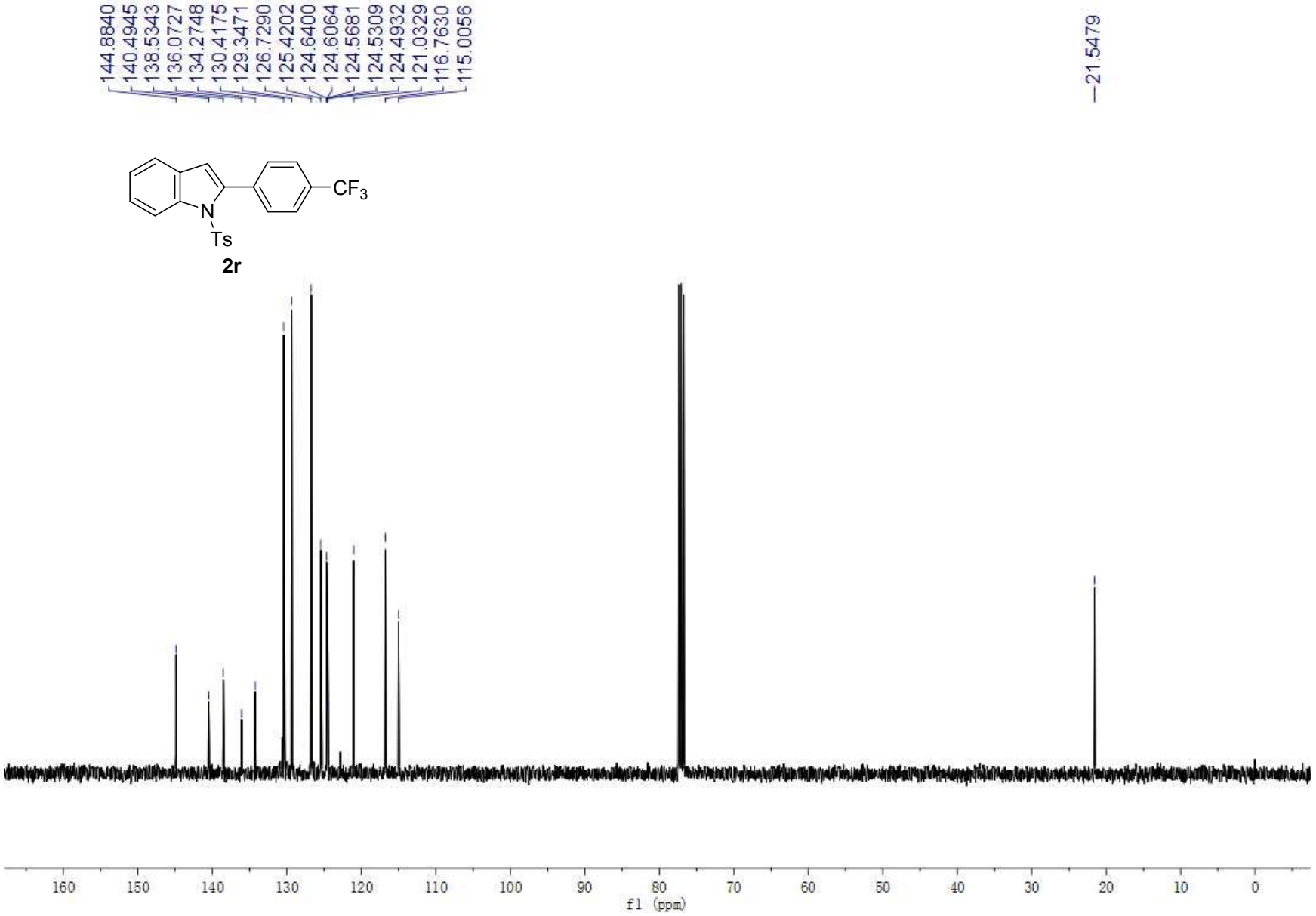
8.3180
8.2985
8.2970
7.6704
7.6443
7.2672
7.2483
7.0537
2.2804
CF3
N
Ts
2r
1.01
4.12
1.05
1.04
3.06
2.05
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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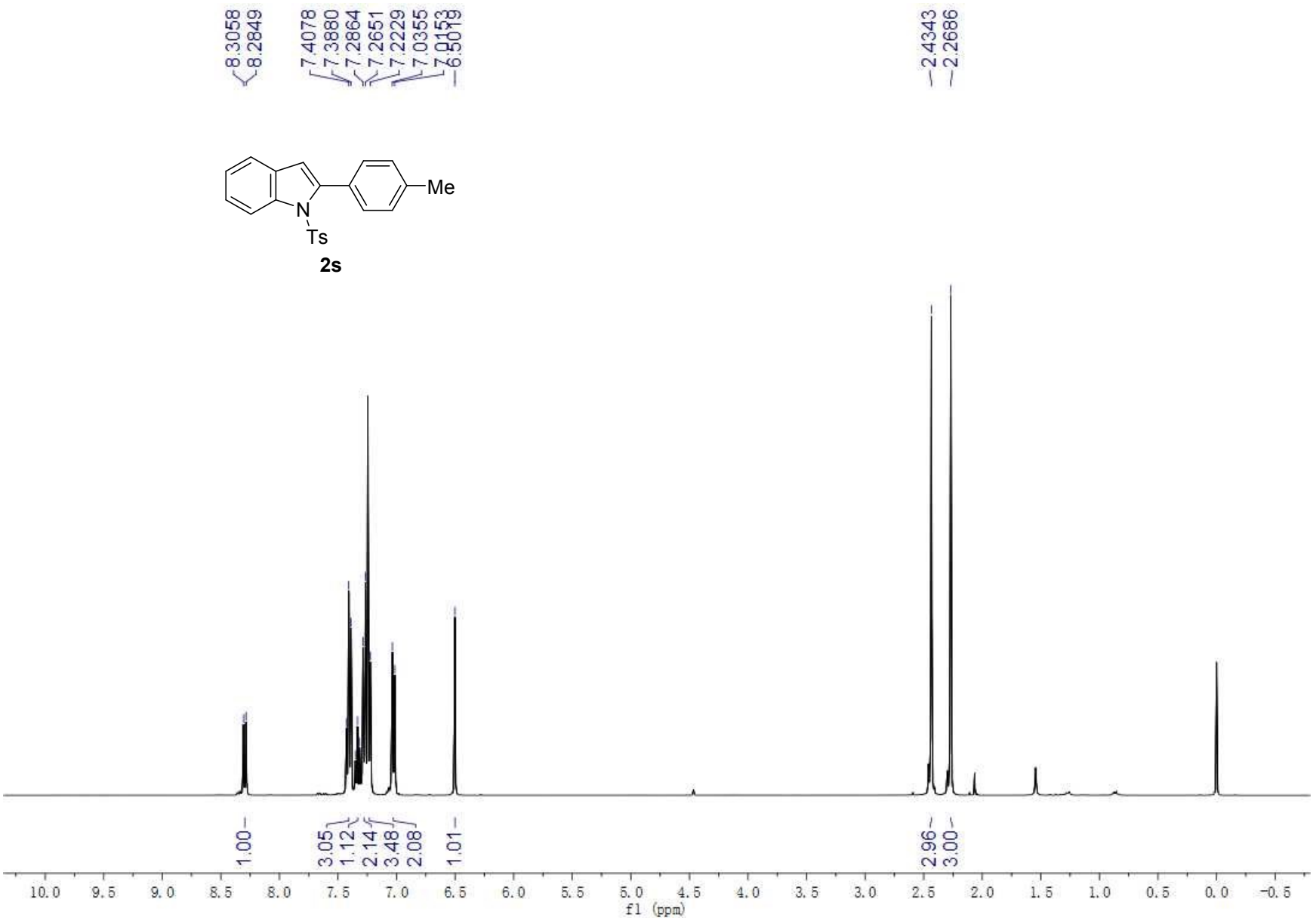
136.0727
134.2748
130.4175
129.3471
126.7290
125.4202
124.6400
124.6064
124.5681
124.5309
124.4932
121.0329
116.7630
115.0056
21.5479
CF3
N
Ts
2r
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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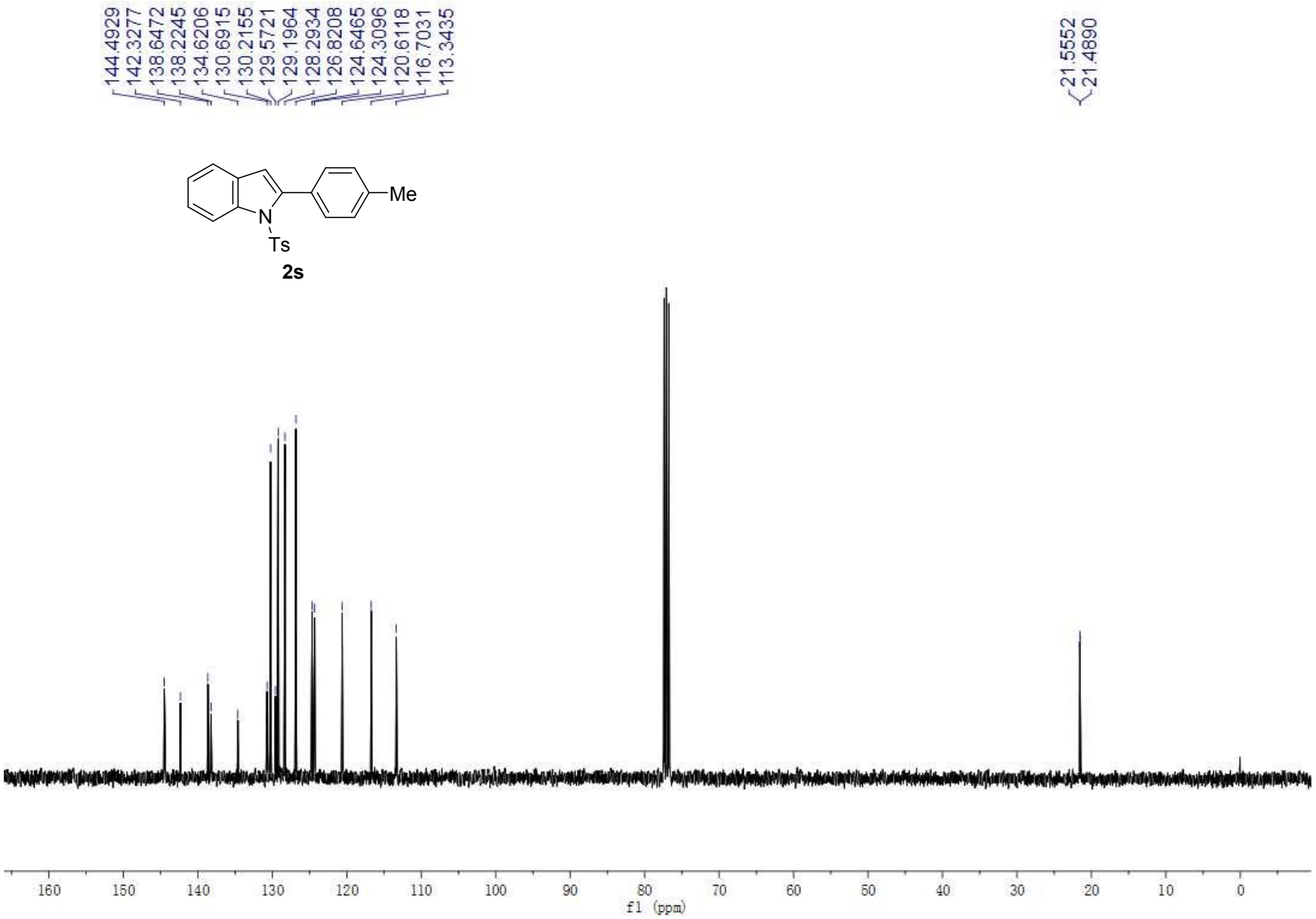
8.2849
7.4078
7.3880
7.2864
7.2651
7.2229
7.0355
7.0153
6.5019
2.4343
2.2686
Me
N
Ts
2s
1.00
3.05
1.12
2.14
3.48
2.08
1.01
2.96
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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142.3277
138.6472
138.2245
134.6206
130.6915
130.2155
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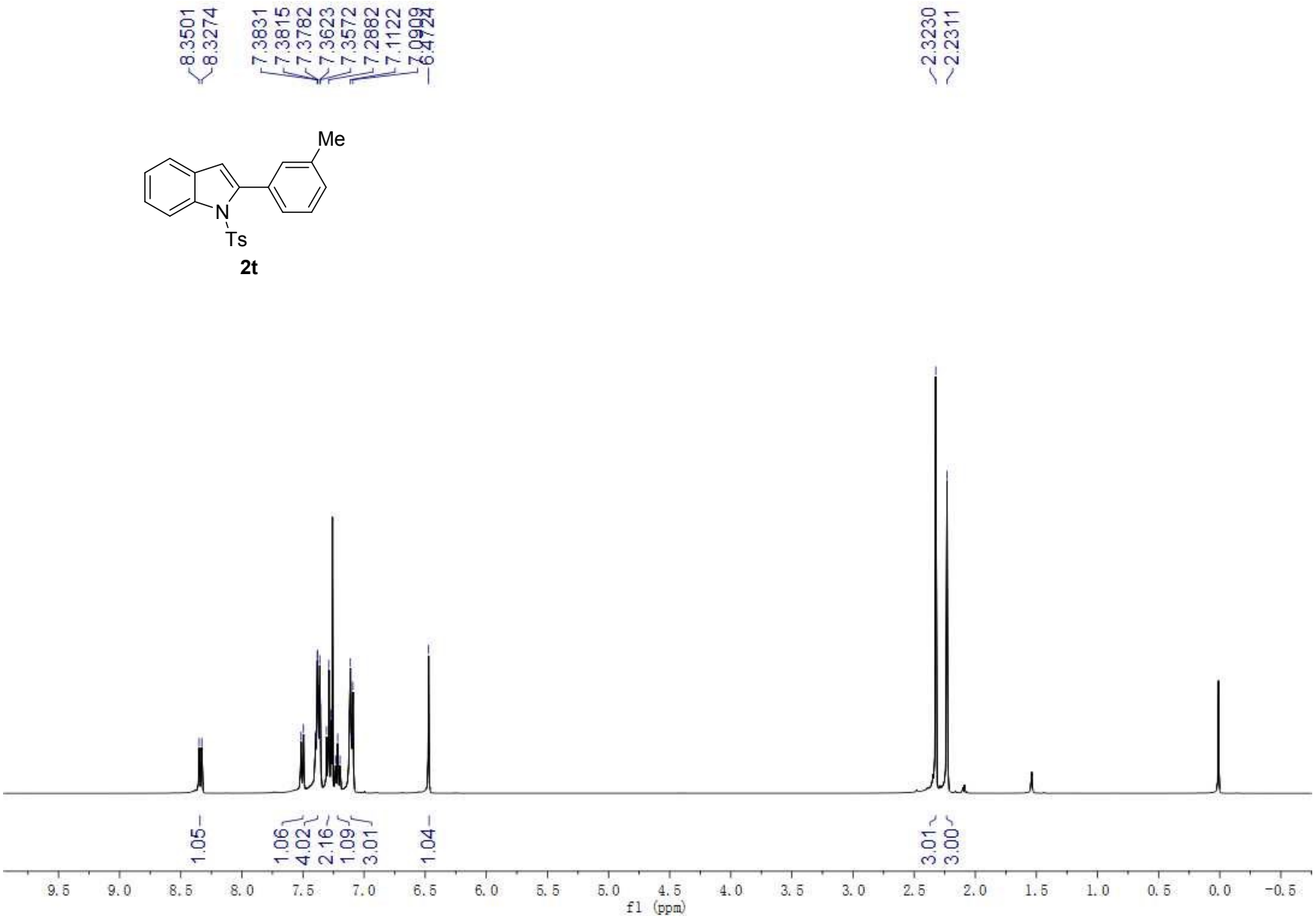
129.1964
128.2934
126.8208
124.6465
124.3096
120.6118
116.7031
113.3435
21.5552
21.4890
Me
N
Ts
2s
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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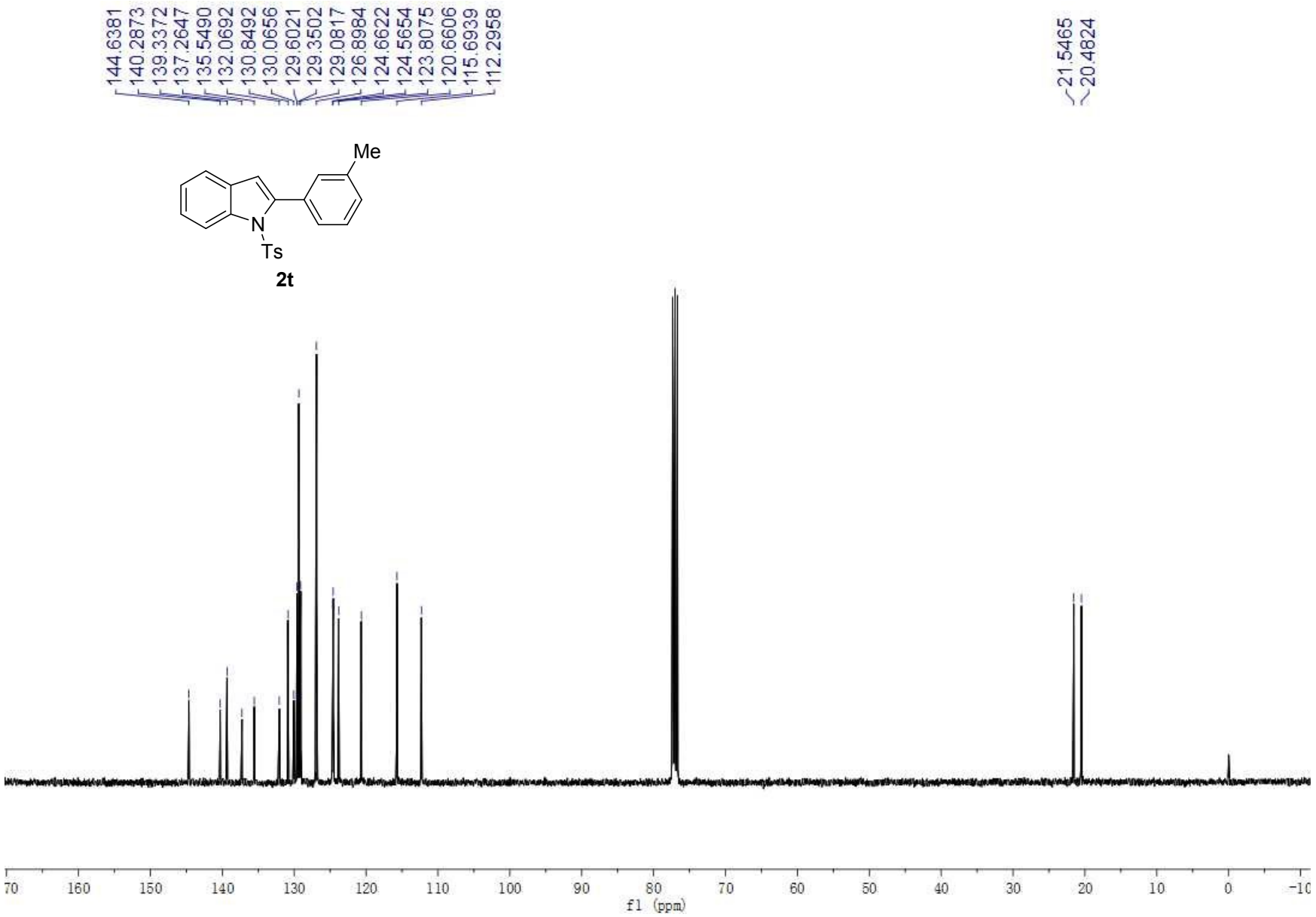
8.3274
7.3831
7.3815
7.3782
7.3623
7.3572
7.2882
7.1122
7.0999
6.4724
2.3230
2.2311
Me
N
Ts
1.05
1.06
4.02
2.16
1.09
3.01
1.04
3.01
3.00
f1 (ppm)

2t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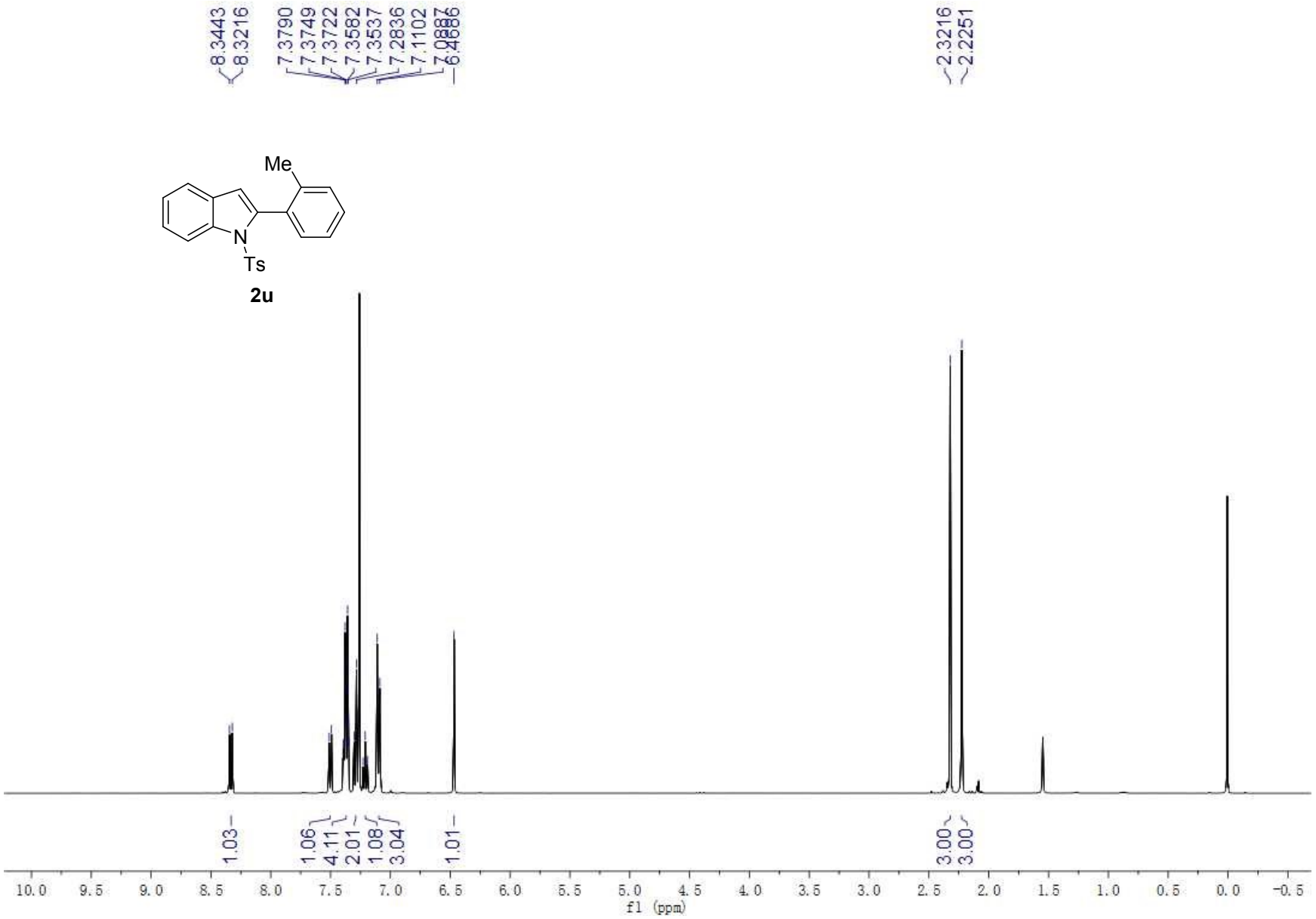
139.3372
137.2647
135.5490
132.0692
130.8492
130.0656
129.6021
129.3502
129.0817
126.8984
124.6622
124.5654
123.8075
120.6606
115.6939
112.2958
21.5465
20.4824
Me
N
Ts
2t
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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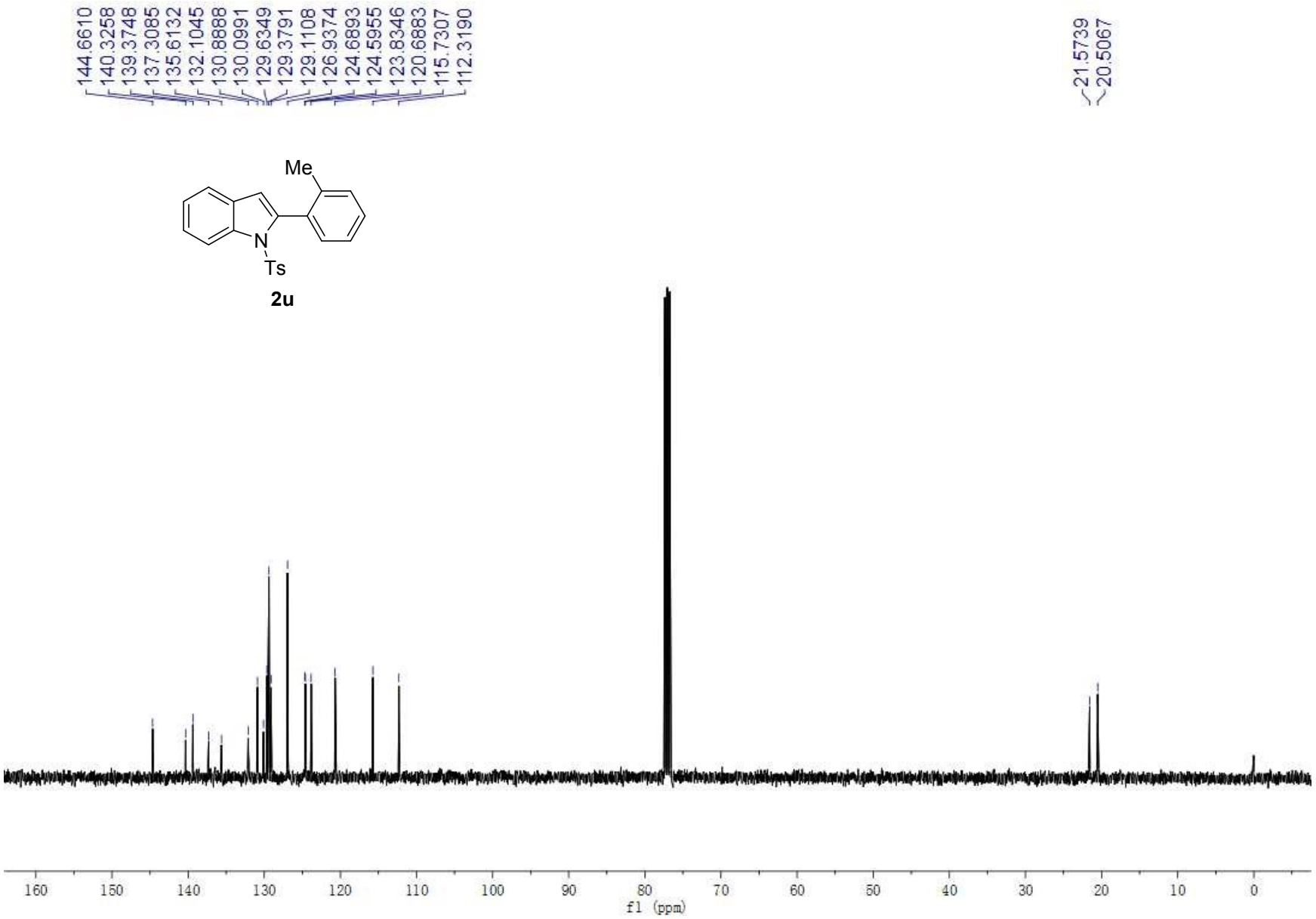
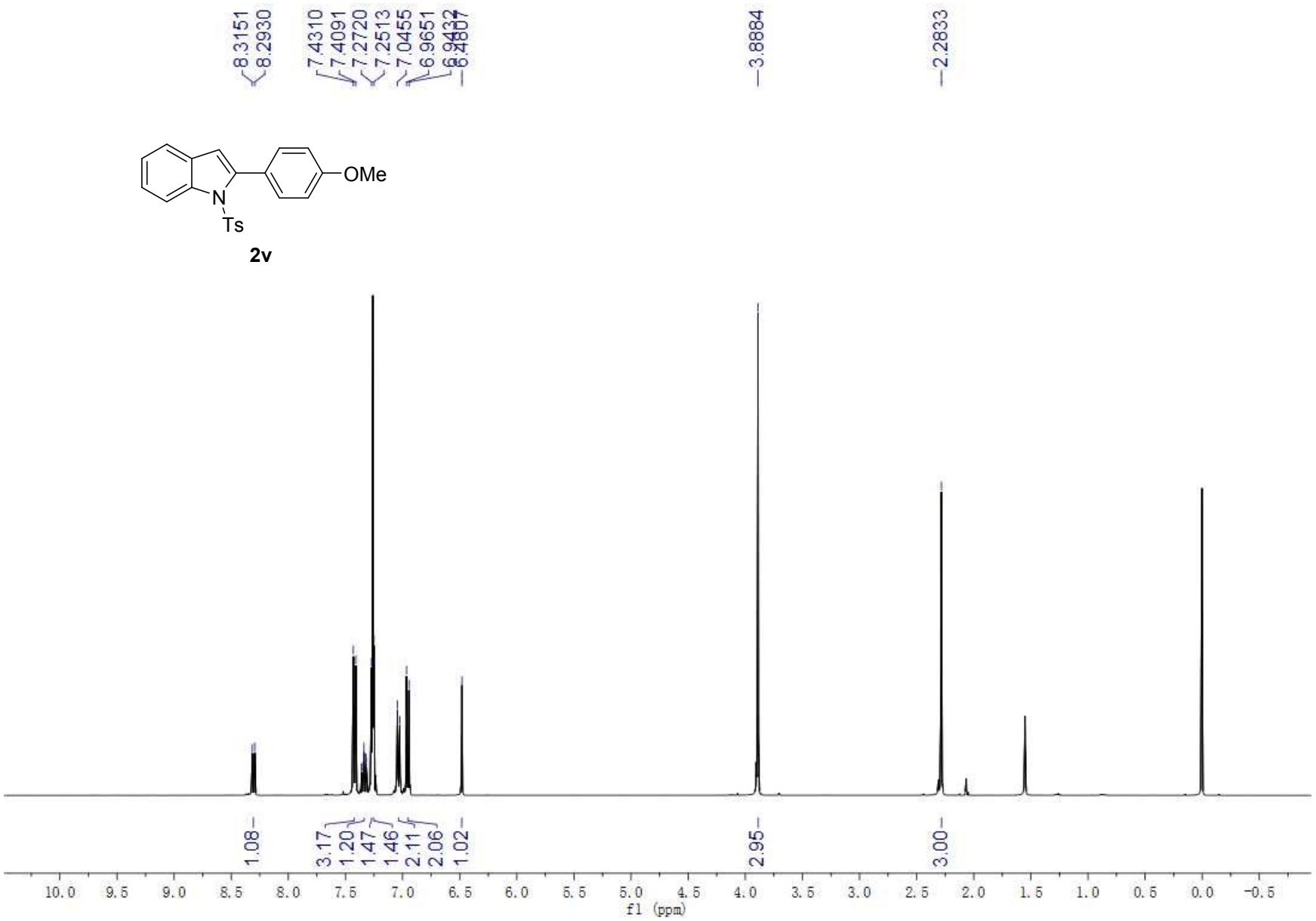
8.3216
7.3790
7.3749
7.3722
7.3582
7.3537
7.2836
7.1102
2.3216
2.2251
Me
N
Ts
2u
1.03
1.06
4.11
2.01
1.08
3.04
1.01
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


144.6610
140.3258
139.3748
137.3085
135.6132
132.1045
130.8888
130.0991
129.6349
129.3791
129.1108
126.9374
124.6893
124.5955
123.8346
120.6883
115.7307
112.3190
21.5739
20.5067
Me
N
Ts
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2u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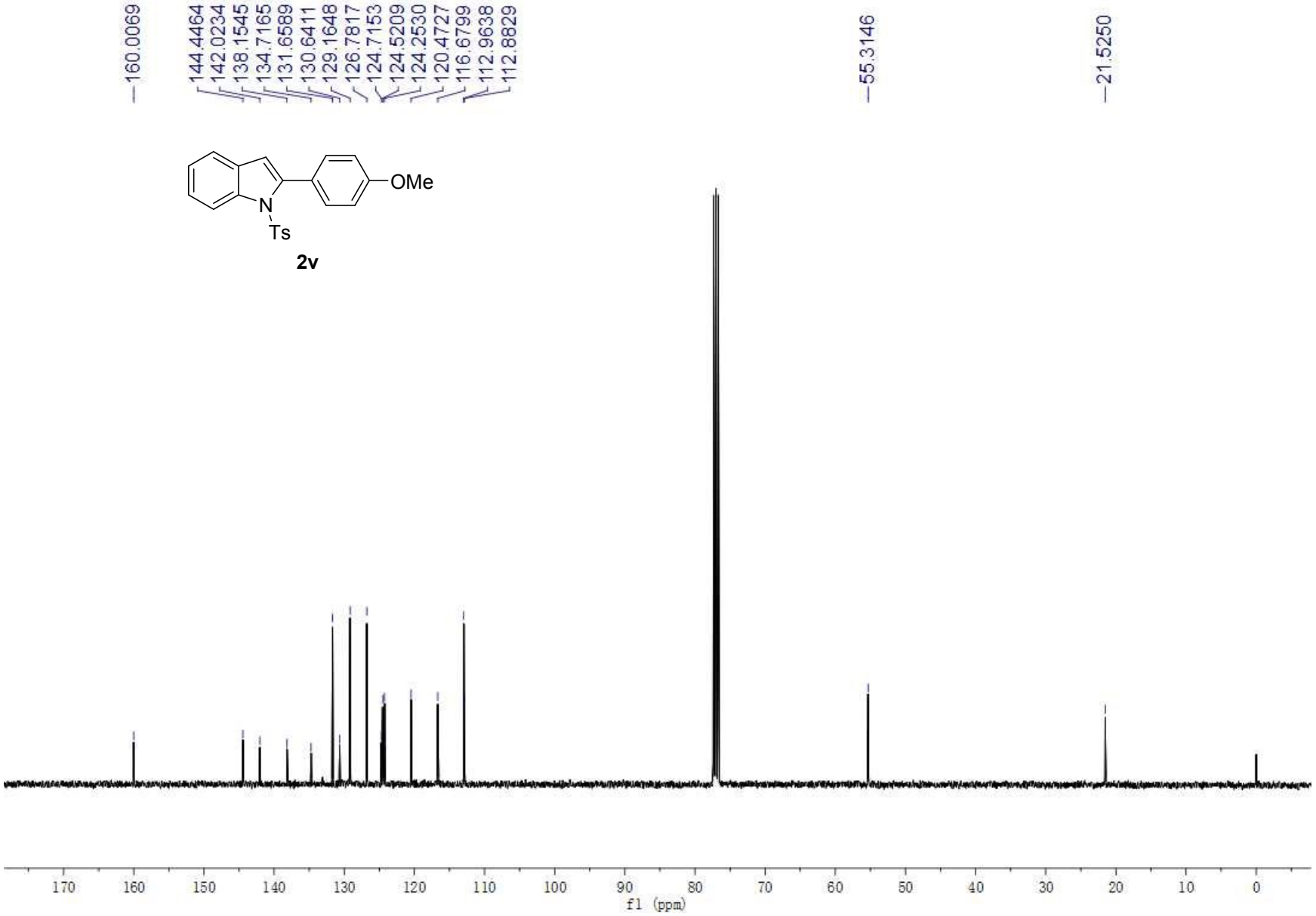
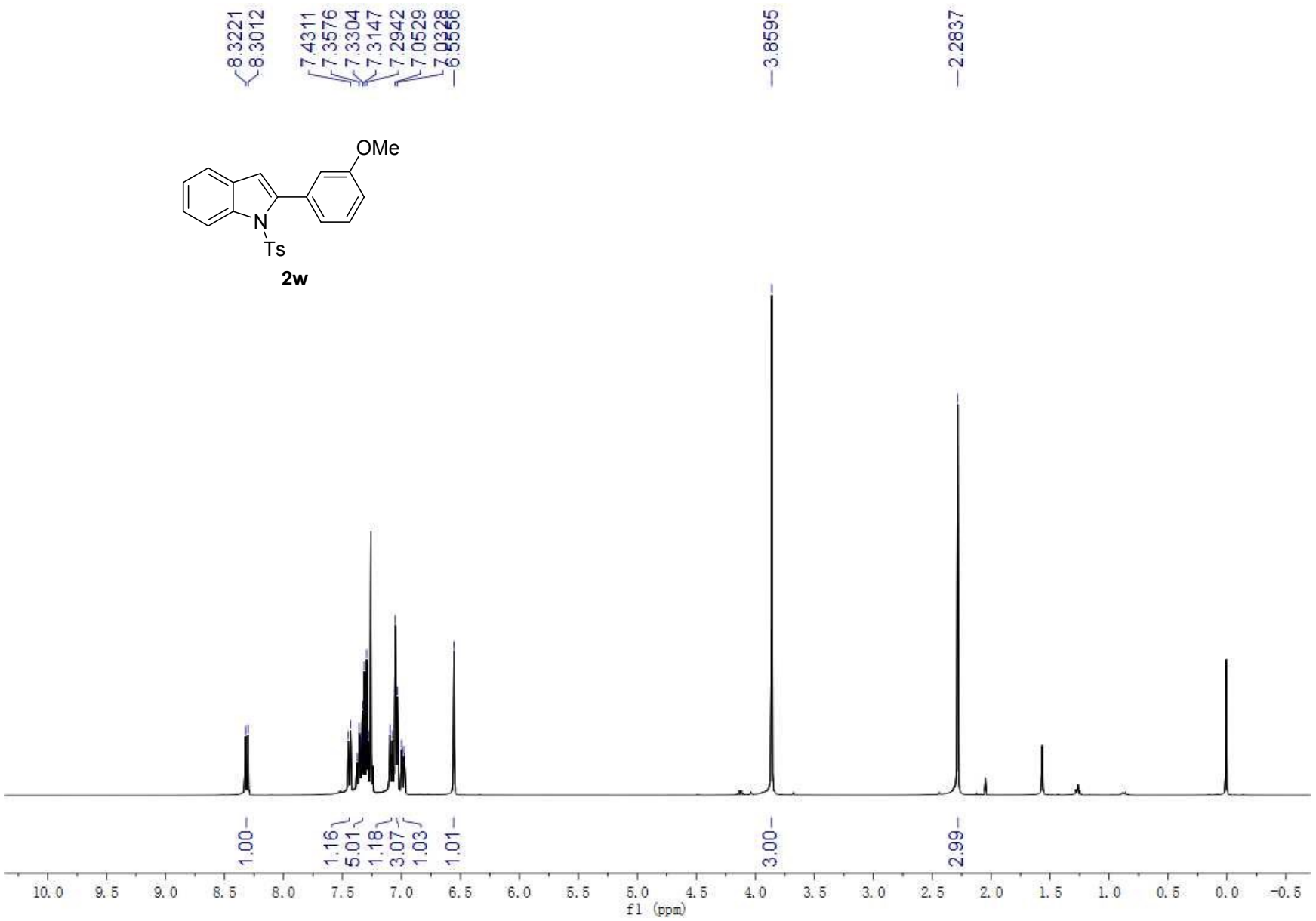
8.2930
7.4310
7.4091
7.2720
7.2513
7.0455
6.9651
3.8884
2.2833
OMe
N
Ts
2v
1.08
3.17
1.20
1.47
1.46
2.11
2.06
1.02
2.95
3.00
f1 (ppm)


160.0069
144.4464
142.0234
138.1545
134.7165
131.6589
130.6411
129.1648
126.7817
124.7153
124.5209
124.2530
120.4727
116.6799
112.9638
112.8829
55.3146
21.5250
OMe
N
Ts
2v
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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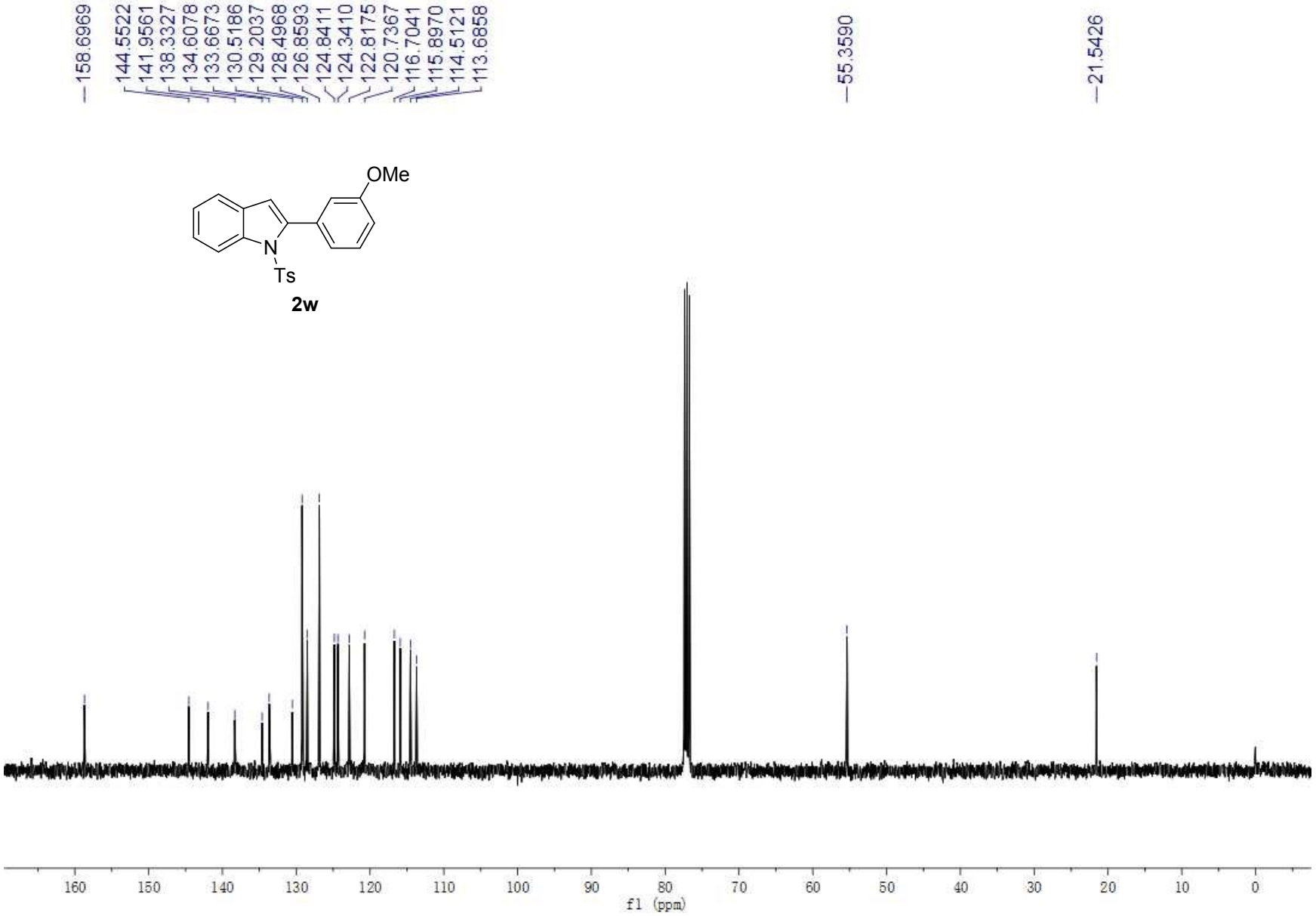
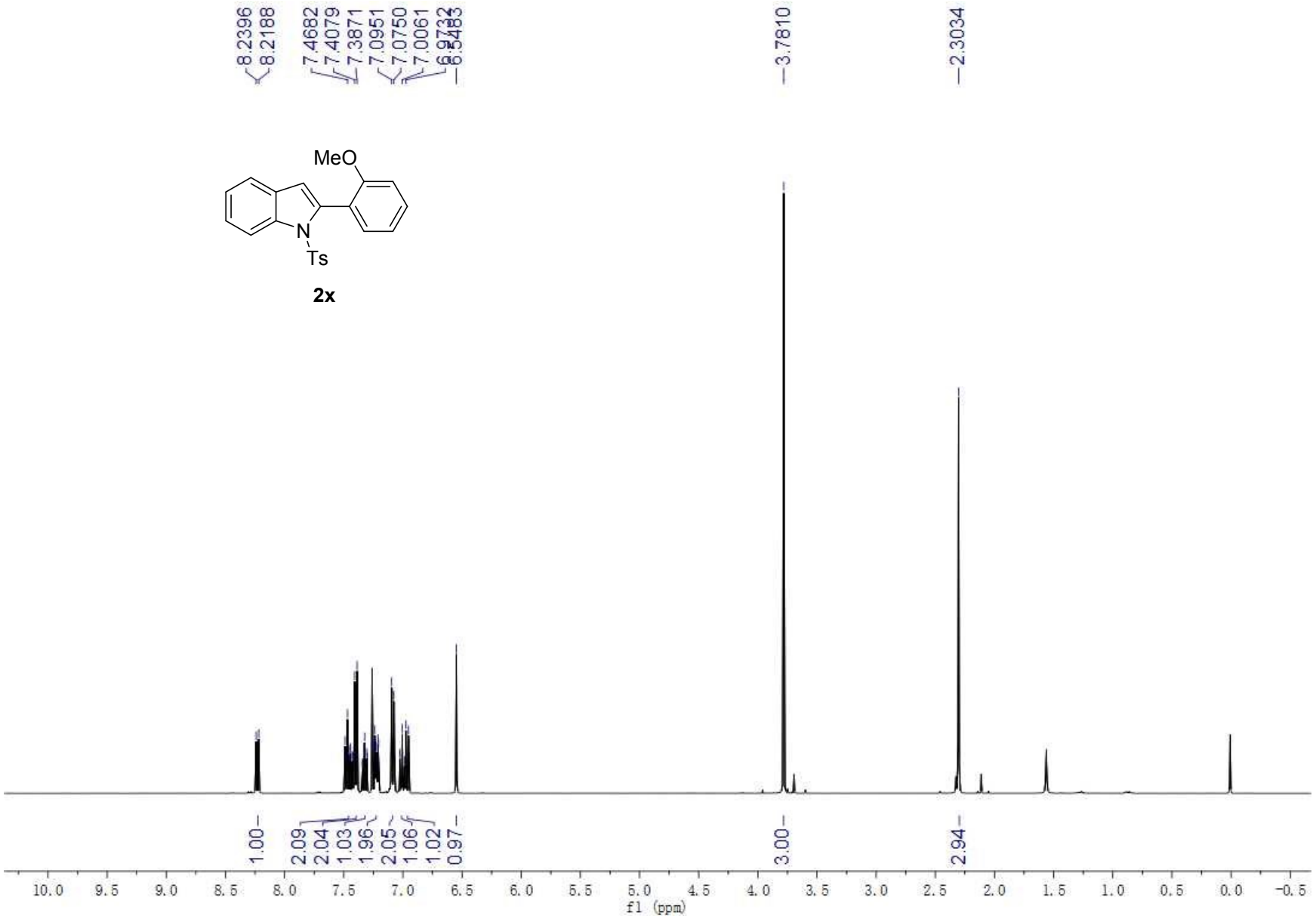
8.3012
7.4311
7.3576
7.3304
7.3147
7.2942
7.0529
3.8595
2.2837
OMe
N
Ts
2w
1.00
1.16
5.01
1.18
3.07
1.03
1.01
3.00
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


158.6969
144.5522
141.9561
138.3327
134.6078
133.6673
130.5186
129.2037
128.4968
126.8593
124.8411
124.3410
122.8175
120.7367
116.7041
115.8970
114.5121
113.6858
55.3590
21.5426
OMe
N
Ts
2w
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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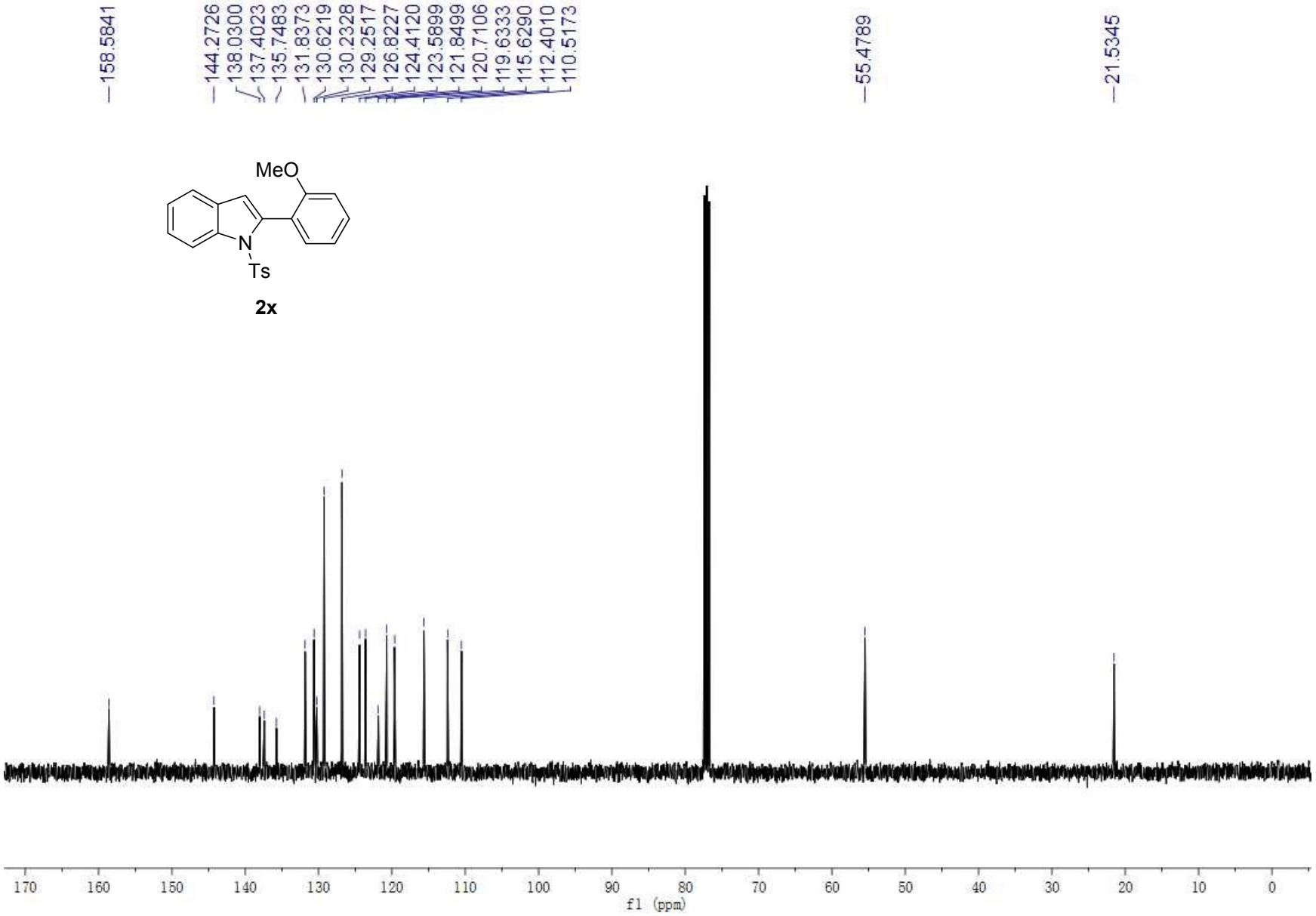
8.2188
7.4682
7.4079
7.3871
7.0951
7.0750
7.0061
3.7810
2.3034
MeO
N
Ts
2x
1.00
2.09
2.04
1.03
1.96
2.05
1.06
1.02
0.97
3.00
2.94
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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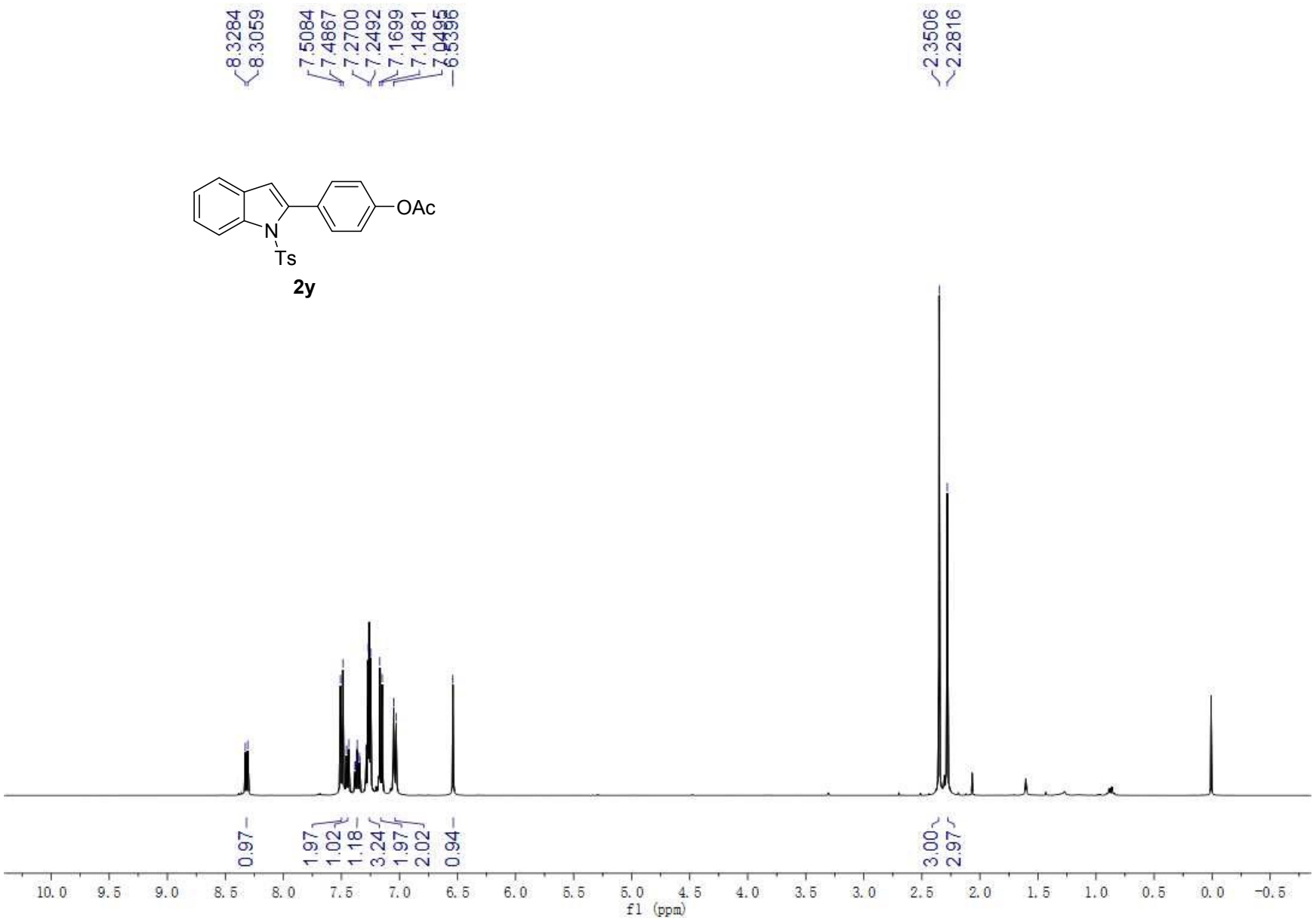
135.7483
131.8373
130.6219
130.2328
129.2517
126.8227
124.4120
123.5899
121.8499
120.7106
119.6333
115.6290
112.4010
110.5173
55.4789
21.5345
MeO
N
Ts
2x
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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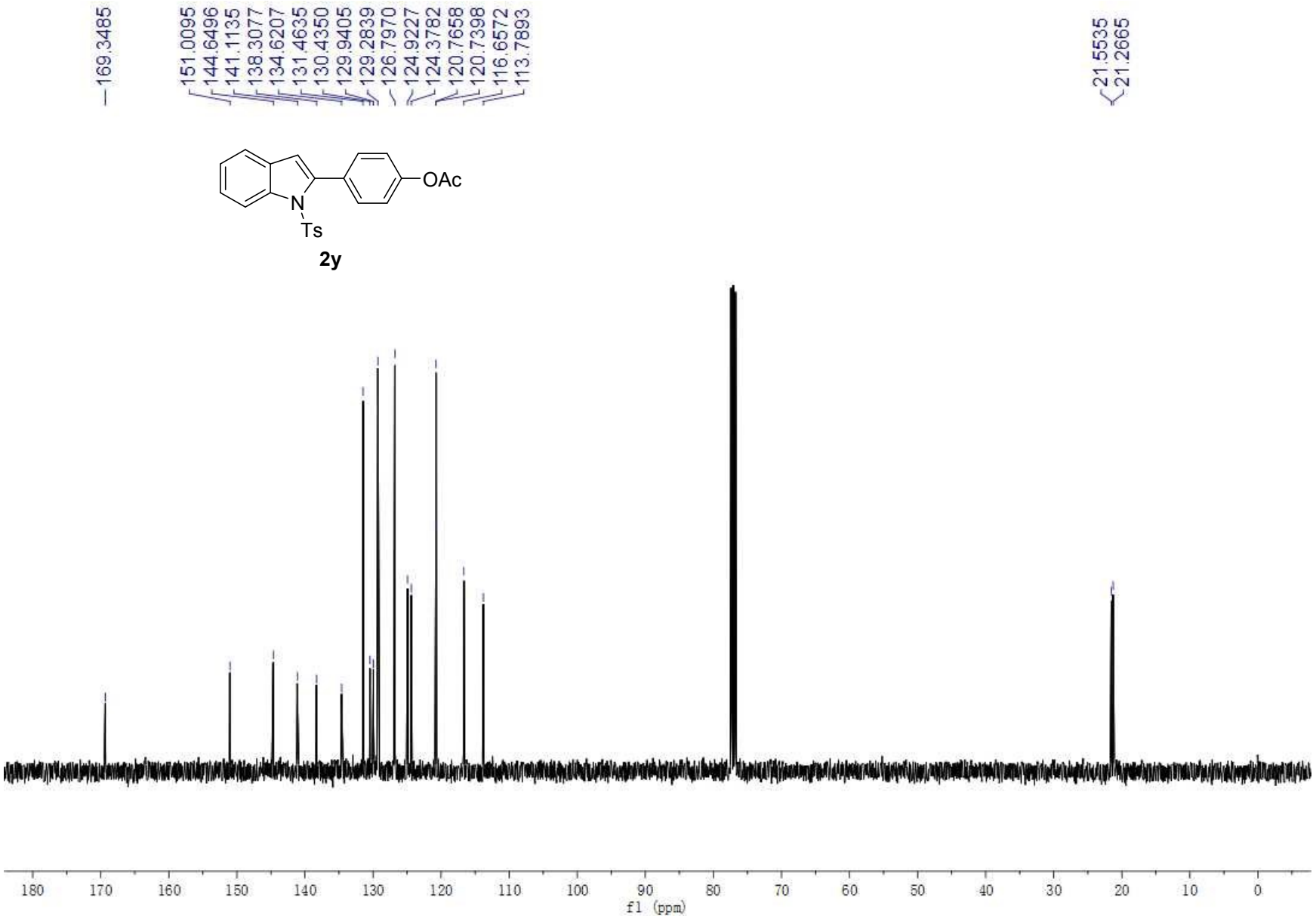
8.3059
7.5084
7.4867
7.2700
7.2492
7.1699
7.1481
2.3506
2.2816
OAc
N
Ts
2y
0.97
1.97
1.02
1.18
3.24
1.97
2.02
0.94
3.00
2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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141.1135
138.3077
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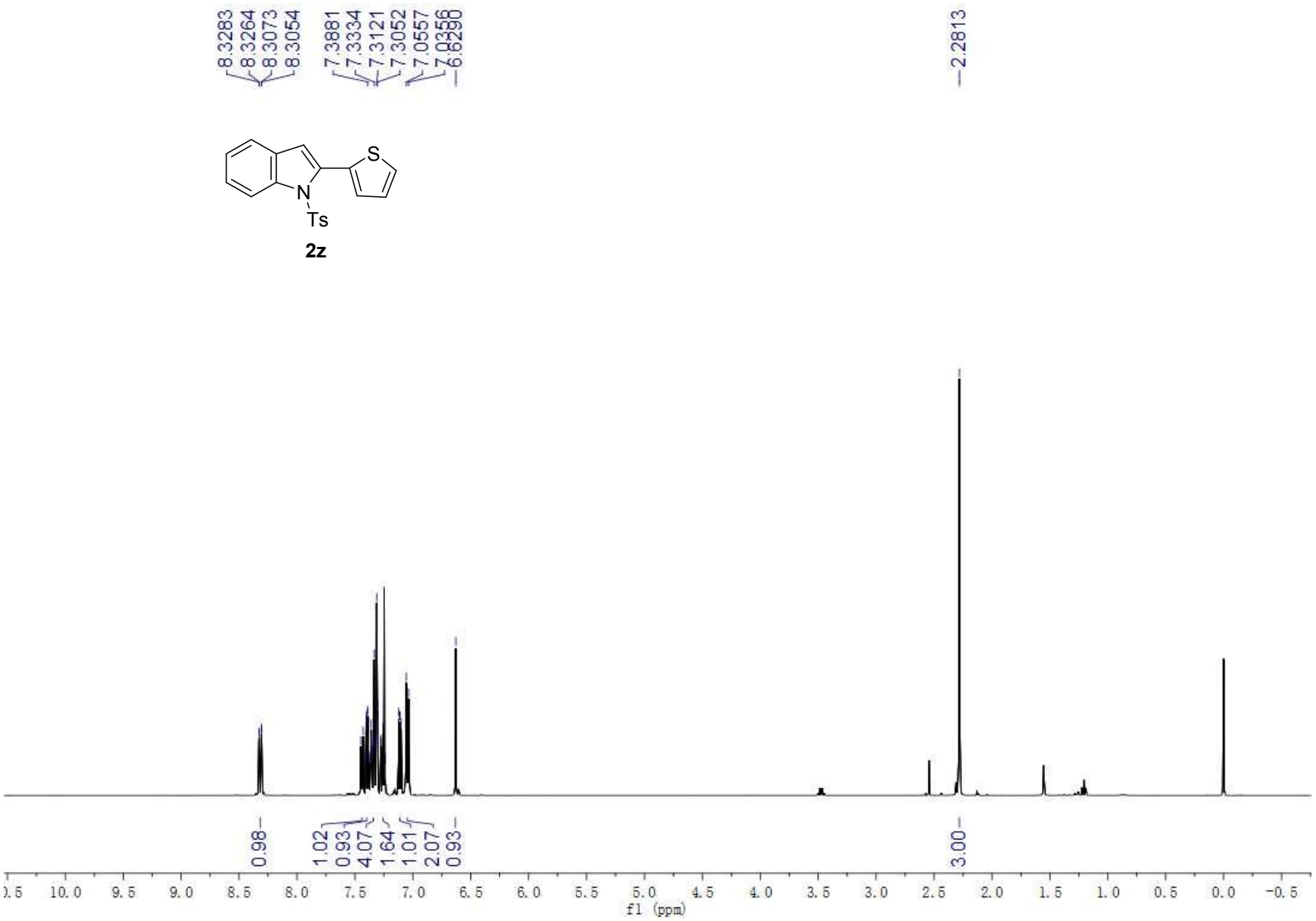
131.4635
130.4350
129.9405
129.2839
126.7970
124.9227
124.3782
120.7658
120.7398
116.6572
113.7893
21.5535
21.2665
OAc
N
Ts
2y
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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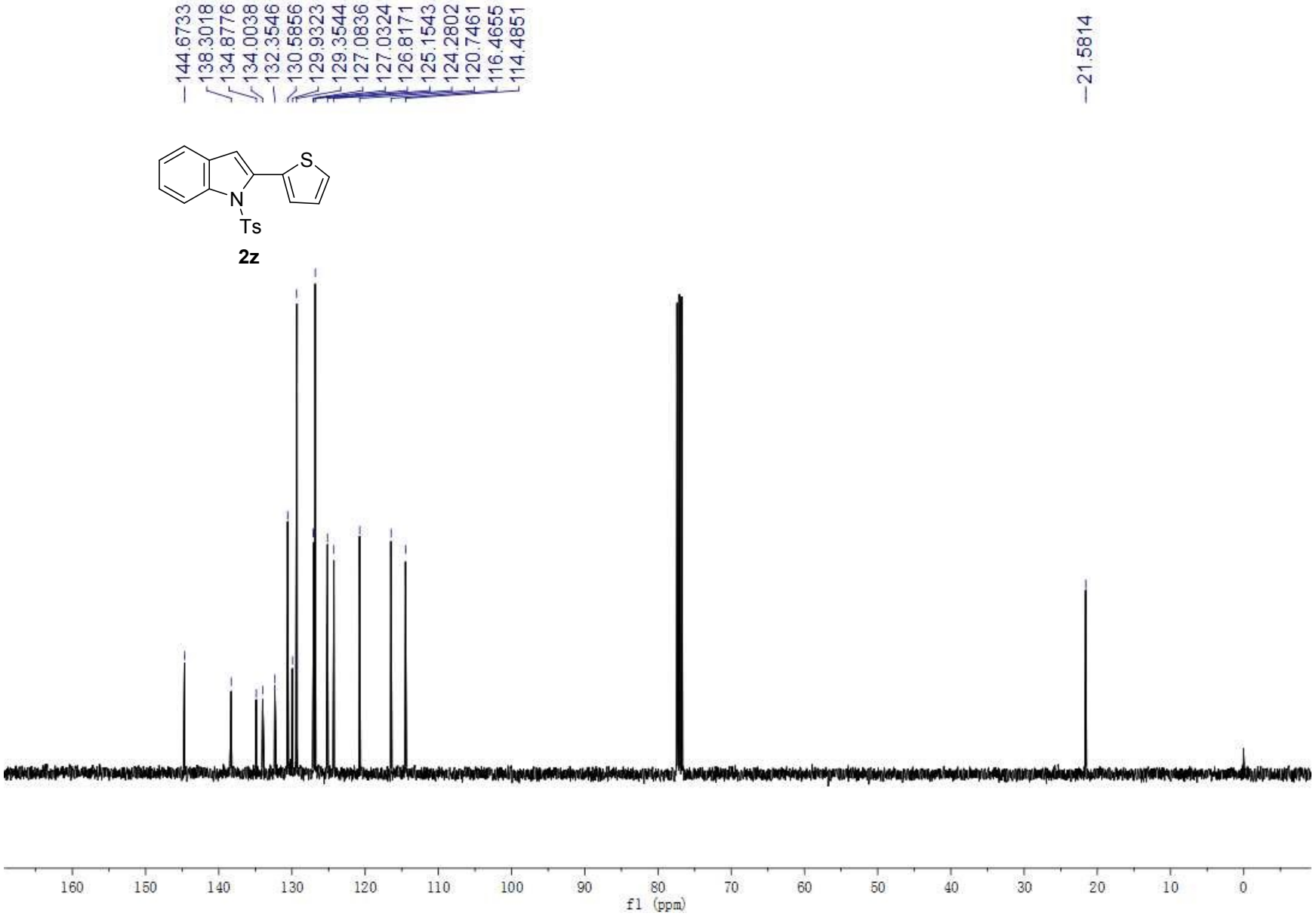
8.3073
8.3054
7.3881
7.3334
7.3121
7.3052
7.0557
2.2813
S
N
Ts
2z
0.98
1.02
0.93
4.07
1.64
1.01
2.07
0.93
3.00
f1 (ppm)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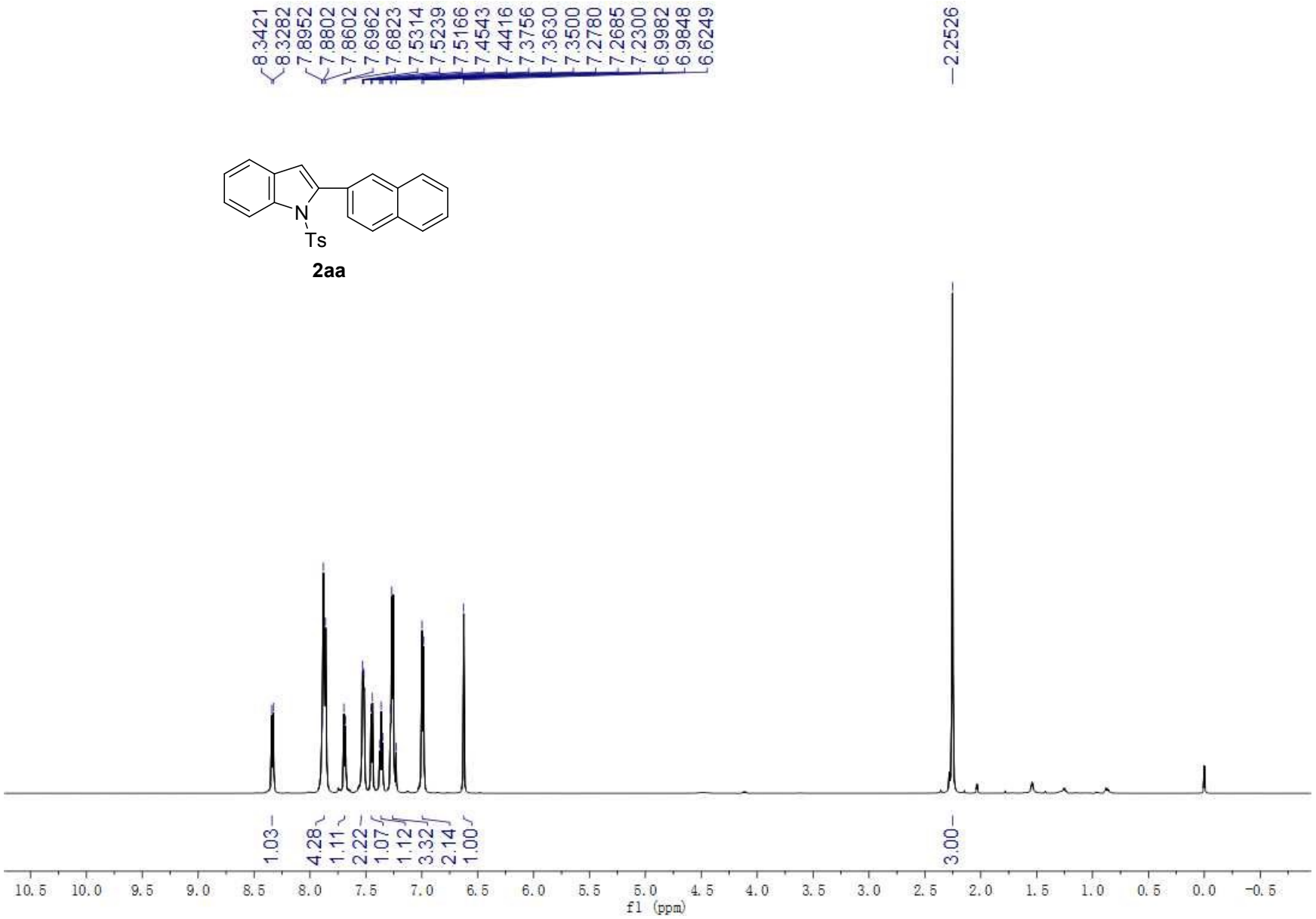
130.5856
129.9323
129.3544
127.0836
127.0324
126.8171
125.1543
124.2802
120.7461
116.4655
114.4851
21.5814
S
N
Ts
2z
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.8602
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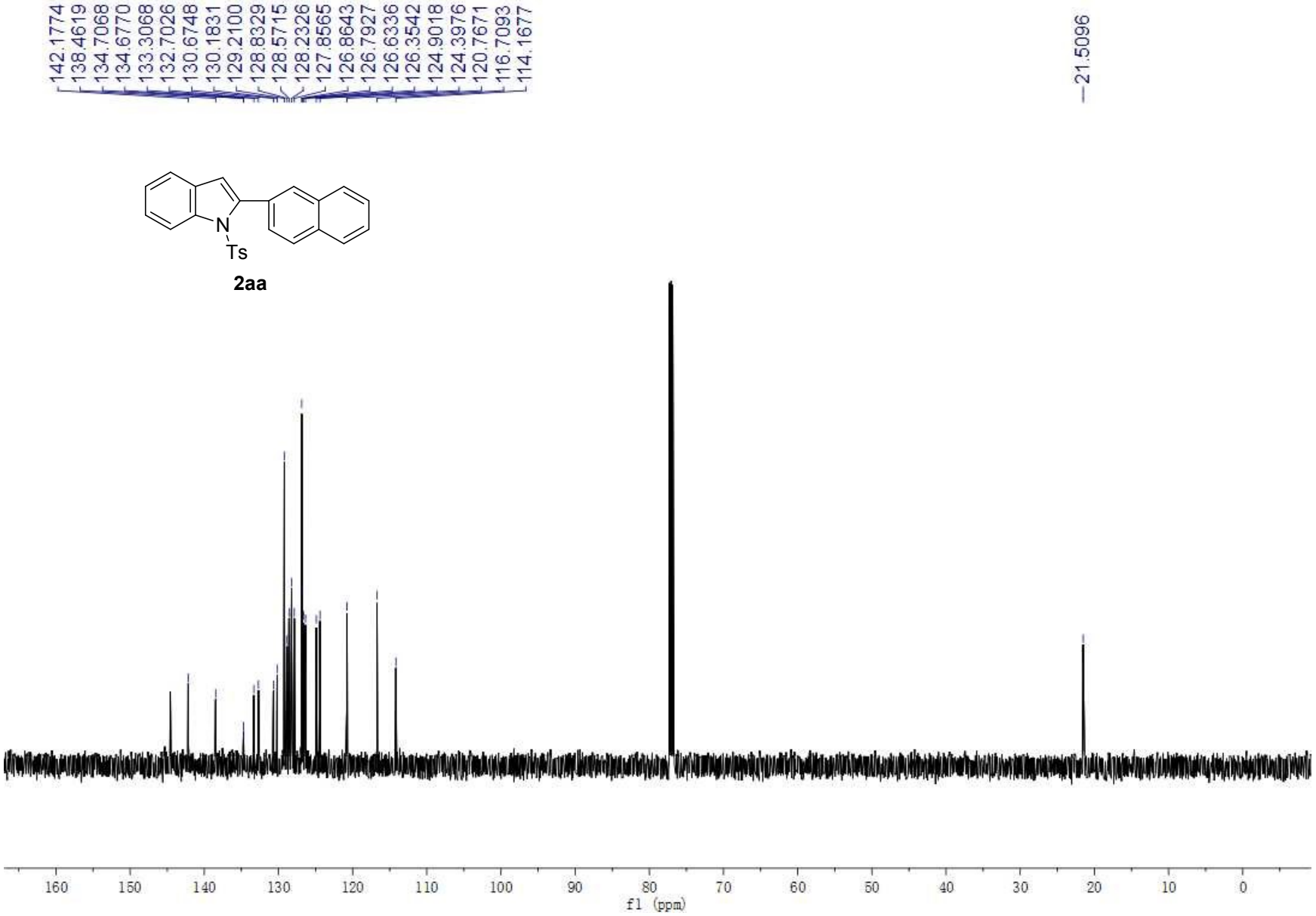
7.6823
7.5314
7.5239
7.5166
7.4543
7.4416
7.3756
7.3630
7.3500
7.2780
7.2685
7.2300
6.9982
6.9848
6.6249
2.2526
N
Ts
1.03
4.28
1.11
2.22
1.07
1.12
3.32
2.14
1.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

2aa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134.7068
134.6770
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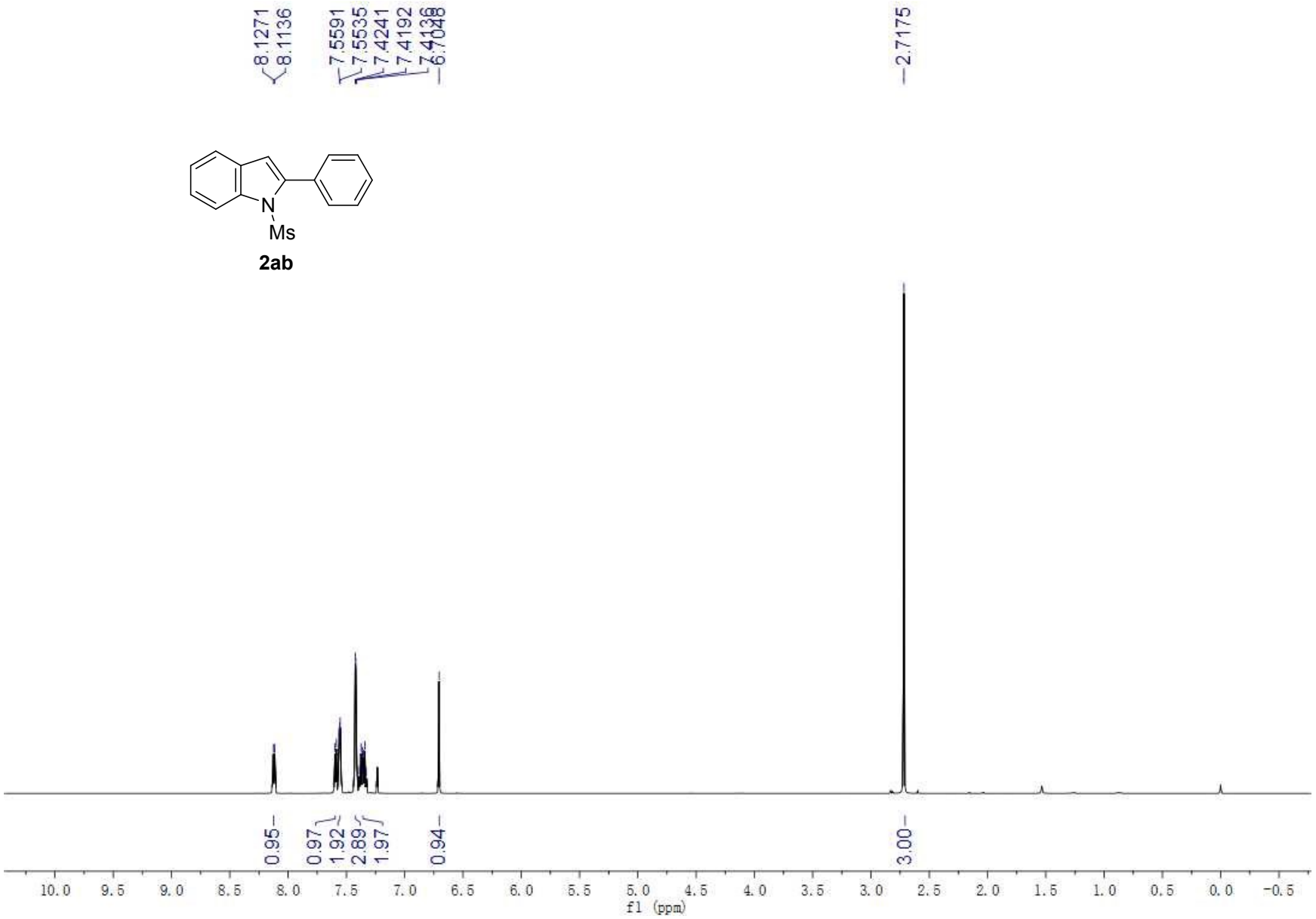
132.7026
130.6748
130.1831
129.2100
128.8329
128.5715
128.2326
127.8565
126.8643
126.7927
126.6336
126.3542
124.9018
124.3976
120.7671
116.7093
114.1677
21.5096
N
Ts
2aa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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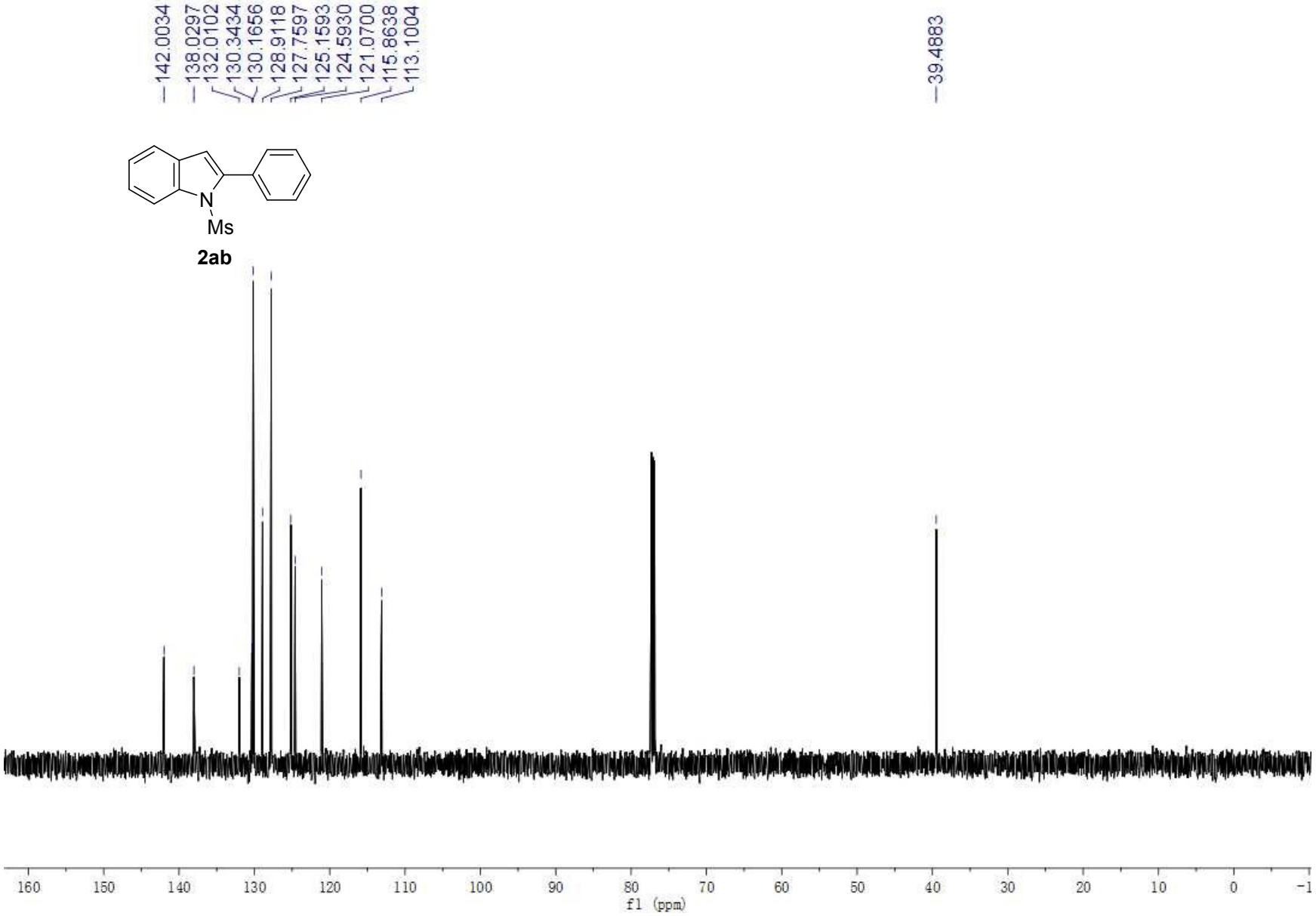
7.5591
7.5535
7.4241
7.4192
7.4138
7.4048
2.7175
N
Ms
2ab
0.95
0.97
1.92
2.89
1.97
0.94
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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138.0297
132.0102
130.3434
130.1656
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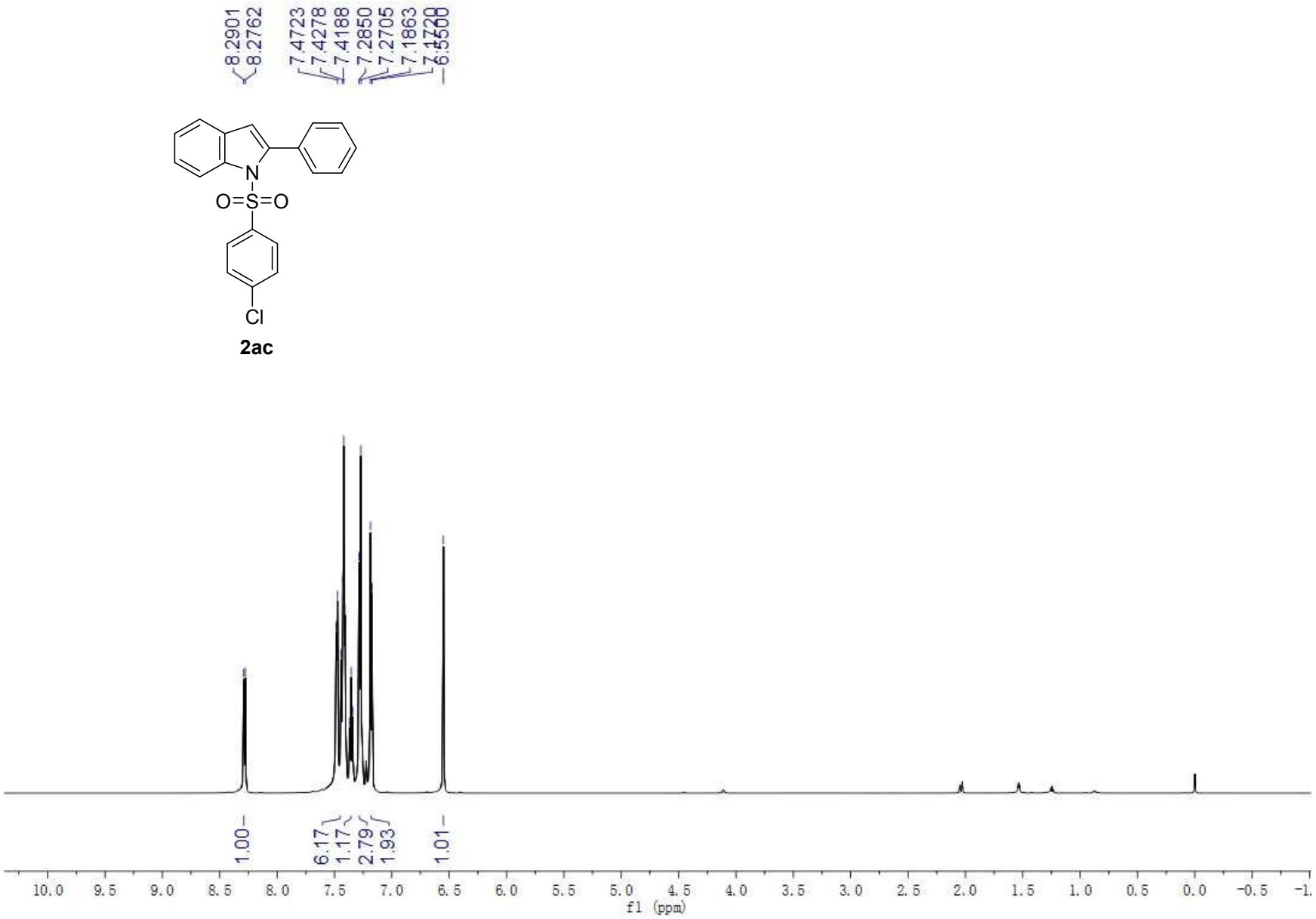
127.7597
125.1593
124.5930
121.0700
115.8638
113.1004
39.4883
N
Ms
2ab
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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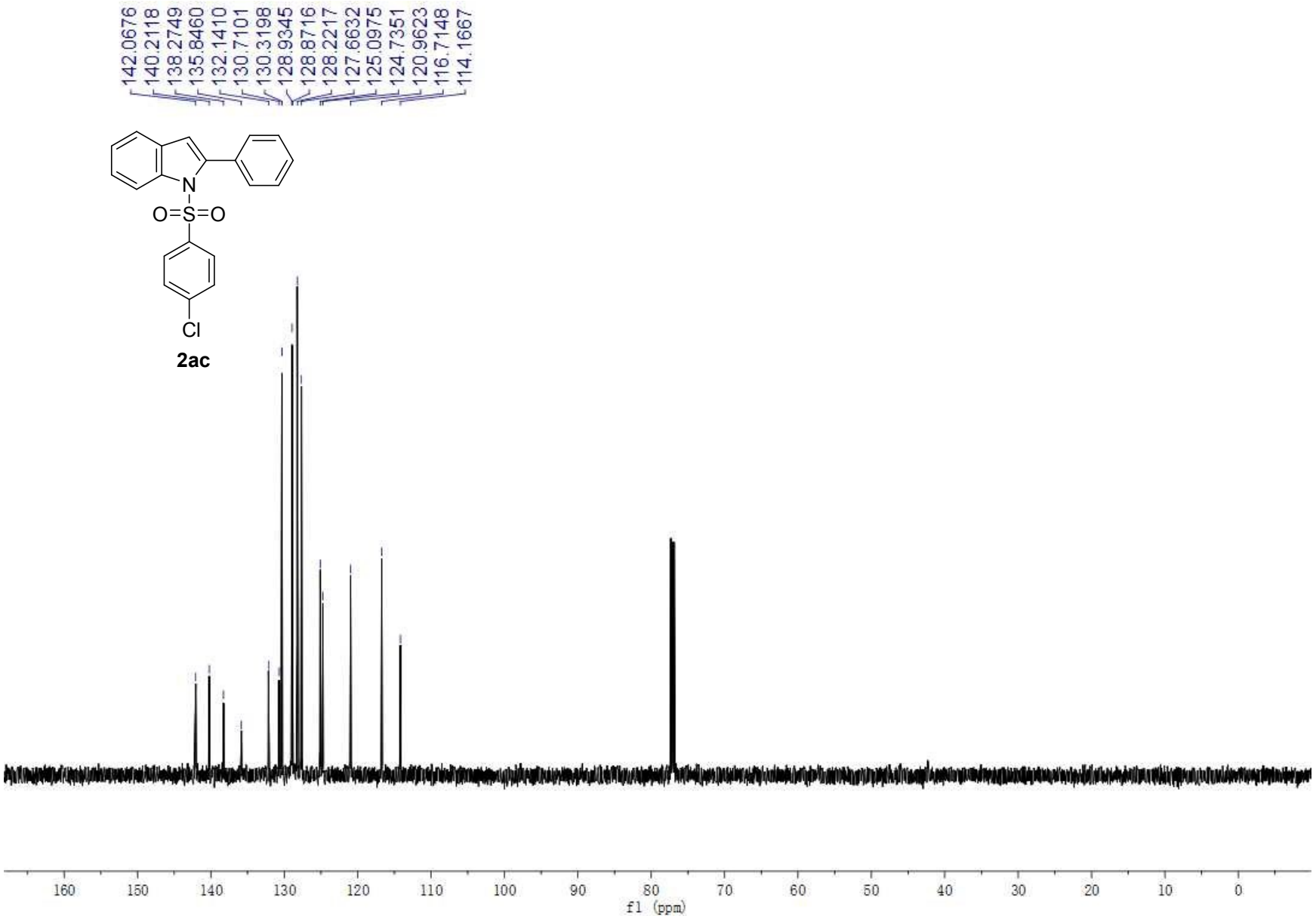
7.4723
7.4278
7.4188
7.2850
7.2705
7.1863
N
O=S=O
Cl
1.00
6.17
1.17
2.79
1.93
1.01
f1 (ppm)

2ac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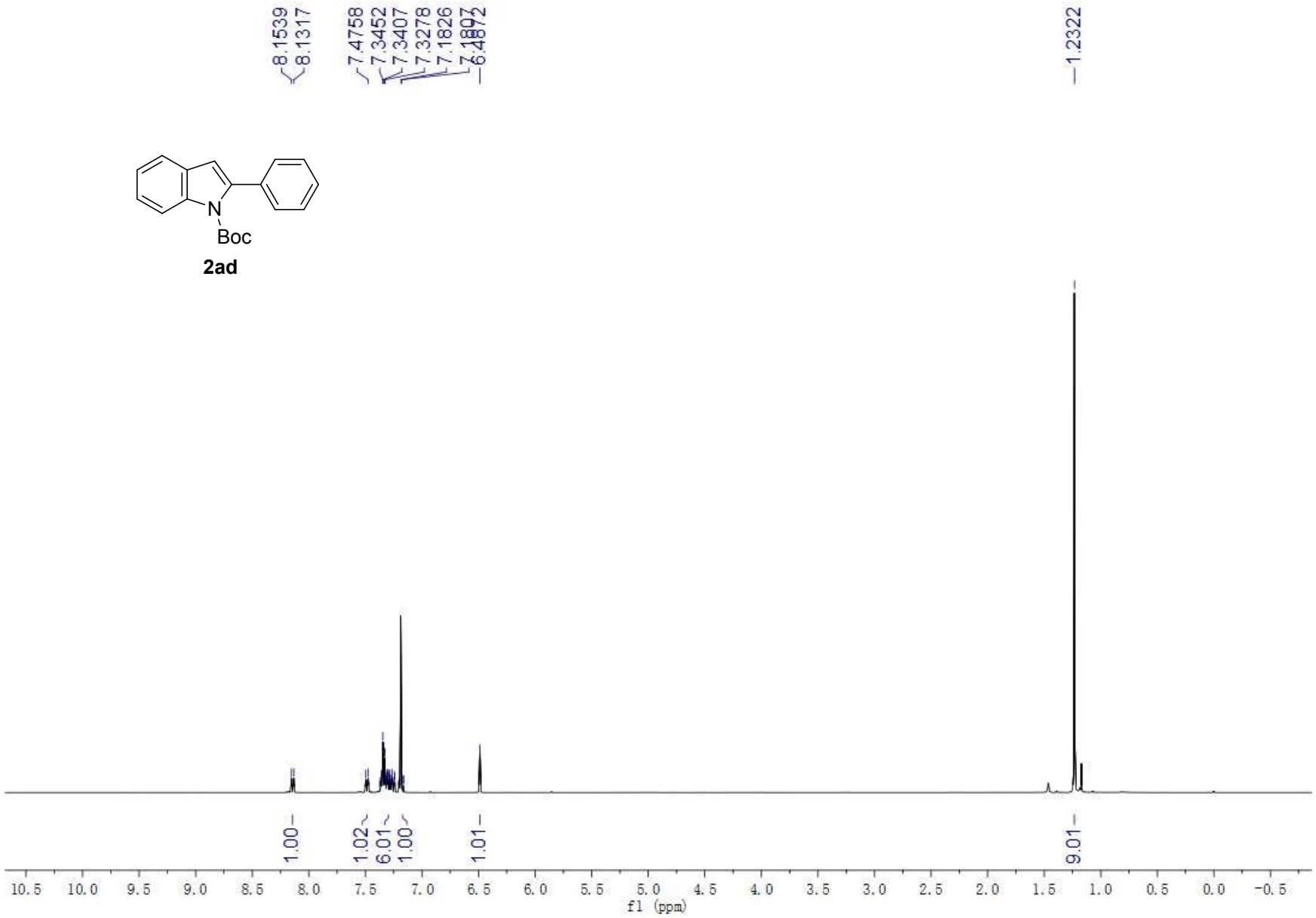
140.2118
138.2749
135.8460
132.1410
130.7101
130.3198
128.9345
128.8716
128.2217
127.6632
125.0975
124.7351
120.9623
116.7148
114.1667
N
O=S=O
Cl
2ac
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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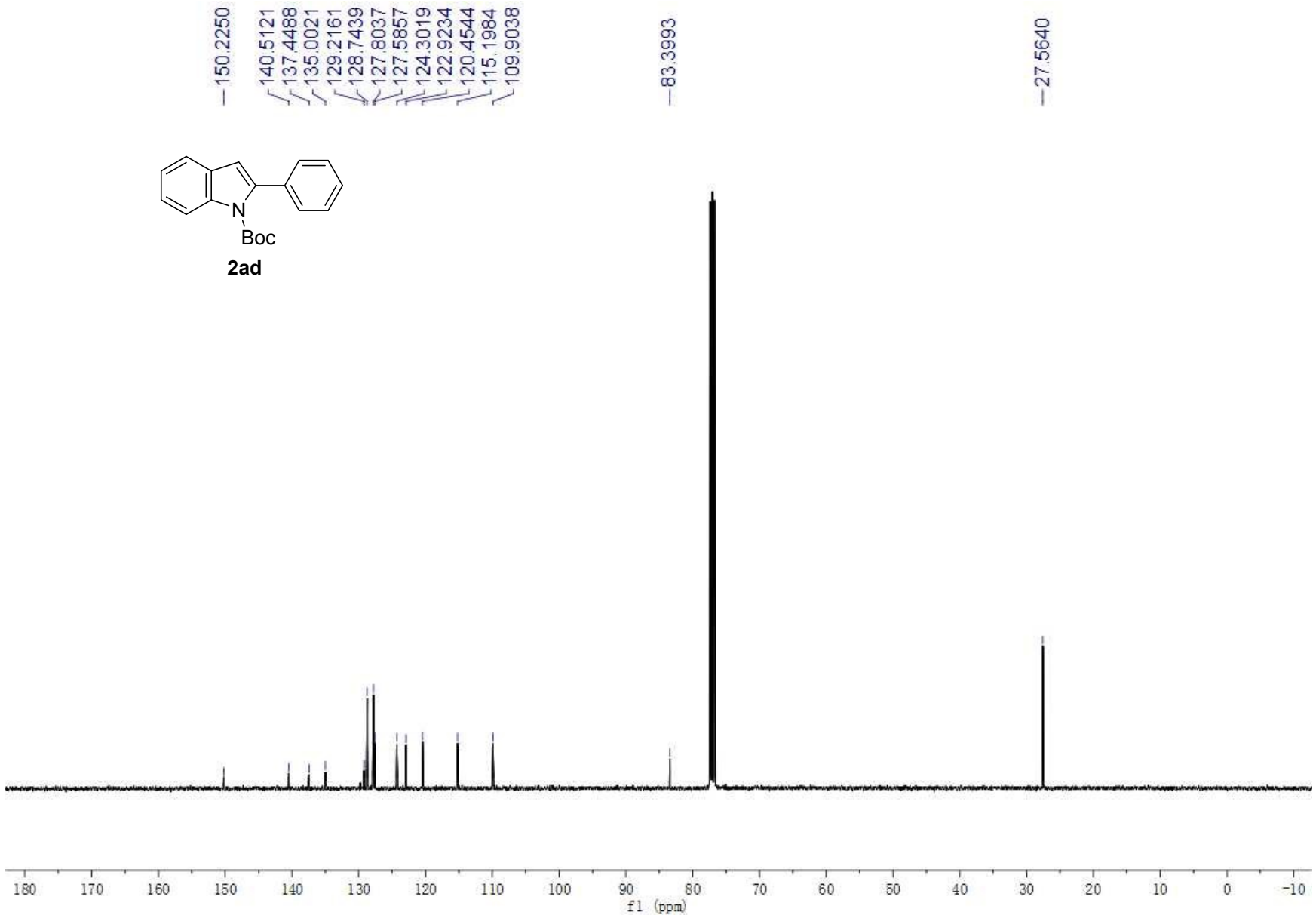
8.1317
7.4758
7.3452
7.3407
7.3278
7.1826
1.2322
N
Boc
1.00
1.02
6.01
1.00
1.01
9.01
f1 (ppm)

2ad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135.0021
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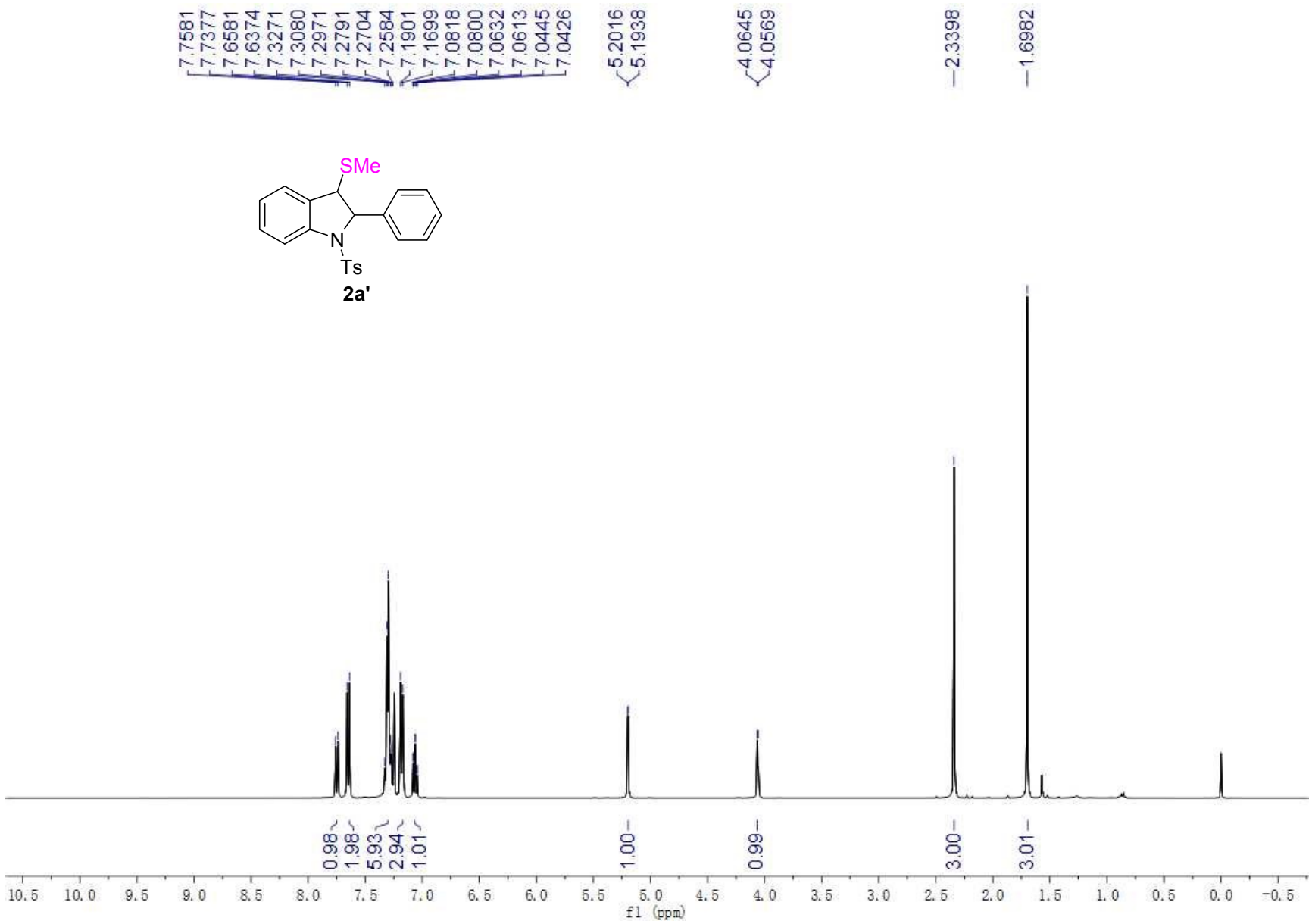
127.8037
127.5857
124.3019
122.9234
120.4544
115.1984
109.9038
83.3993
27.5640
N
Boc
2ad
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.7377
7.6581
7.6374
7.3271
7.3080
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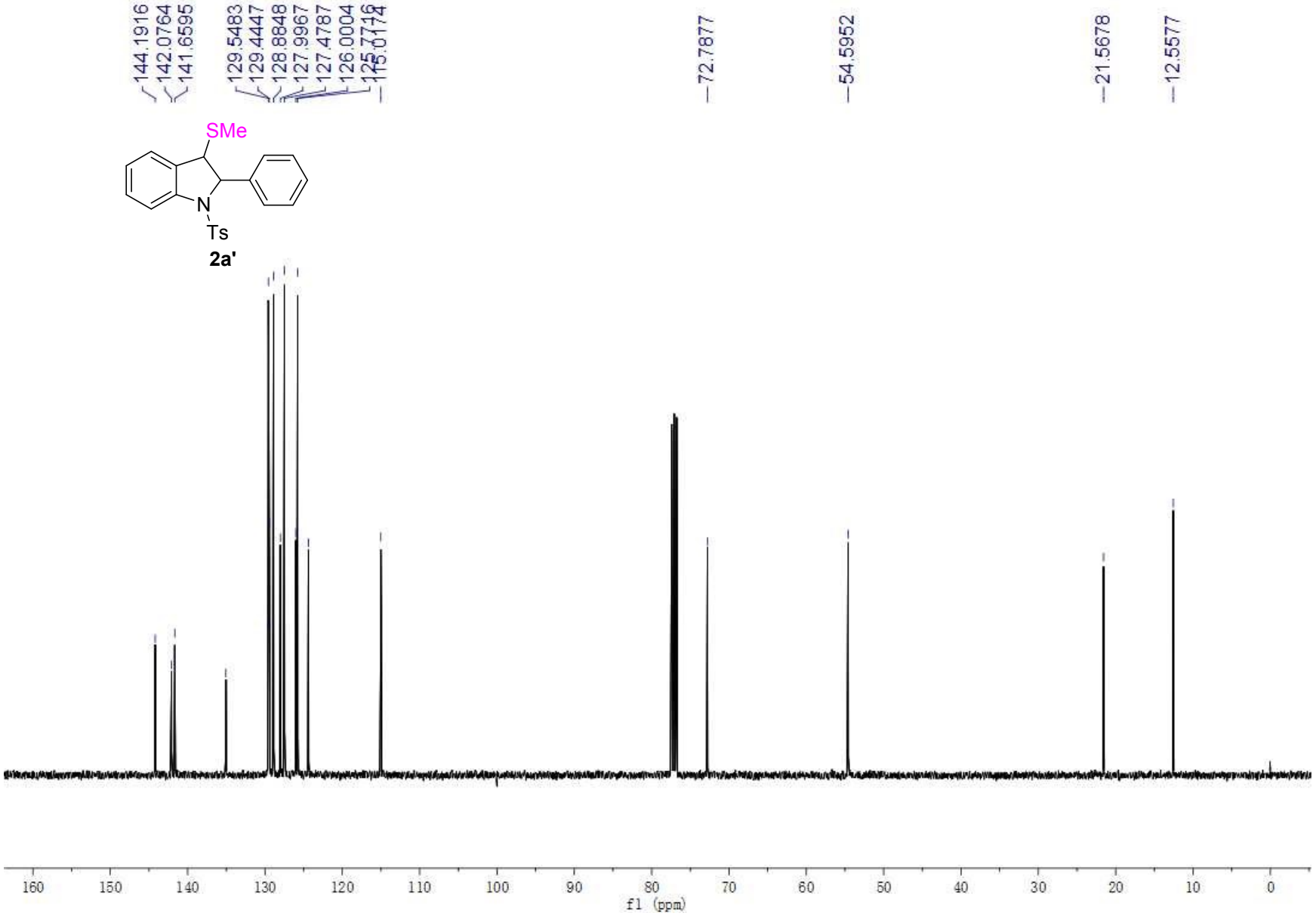
7.2704
7.2584
7.1901
7.1699
7.0818
7.0800
7.0632
7.0613
7.0445
7.0426
5.2016
5.1938
4.0645
4.0569
2.3398
1.6982
SMe
N
Ts
2a'
0.98
1.98
5.93
2.94
1.01
1.00
0.99
3.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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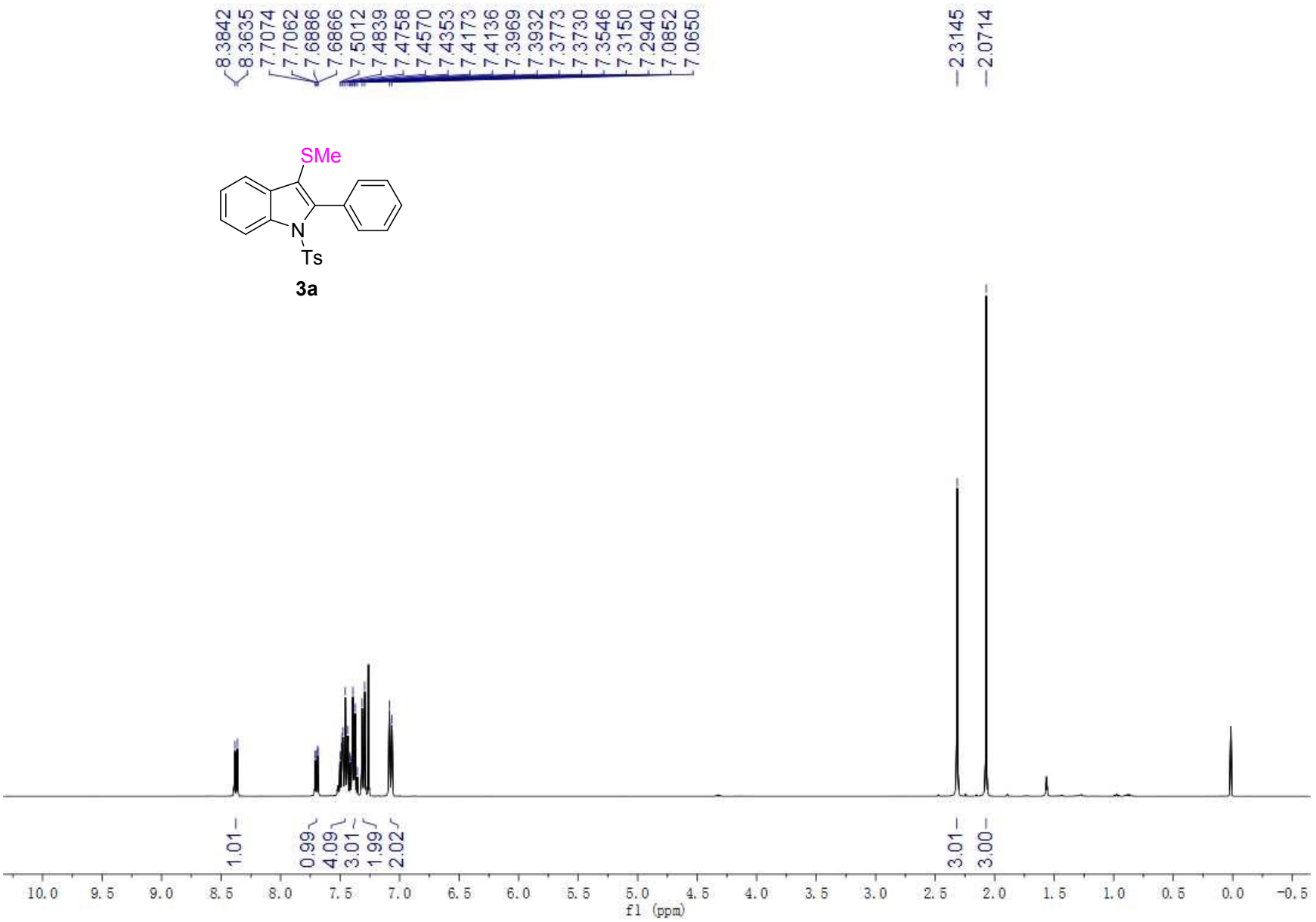
141.6595
129.5483
129.4447
128.8848
127.9967
127.4787
126.0004
125.7716
125.0174
72.7877
54.5952
21.5678
12.5577
SMe
N
Ts
2a'
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.3635
7.7074
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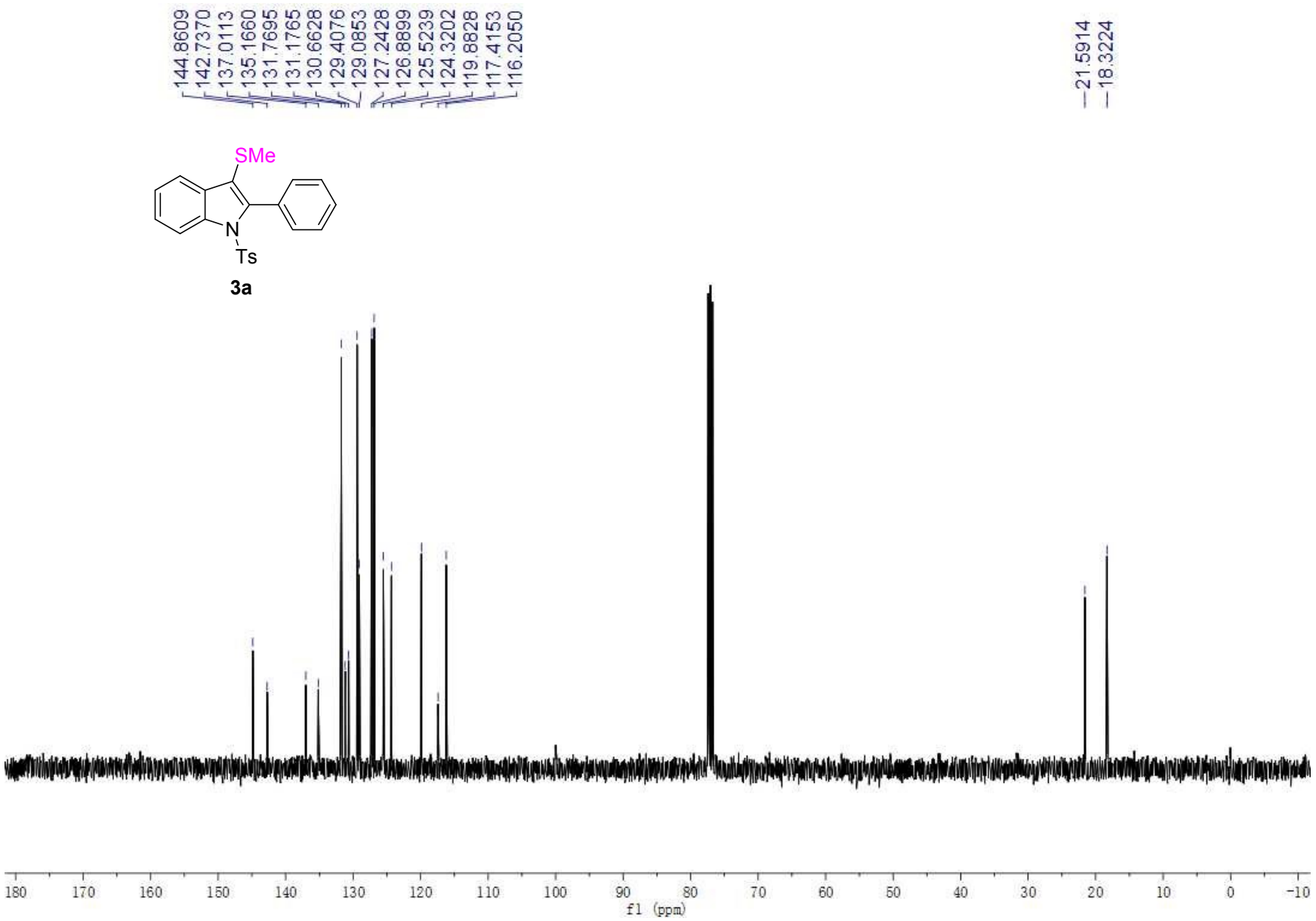
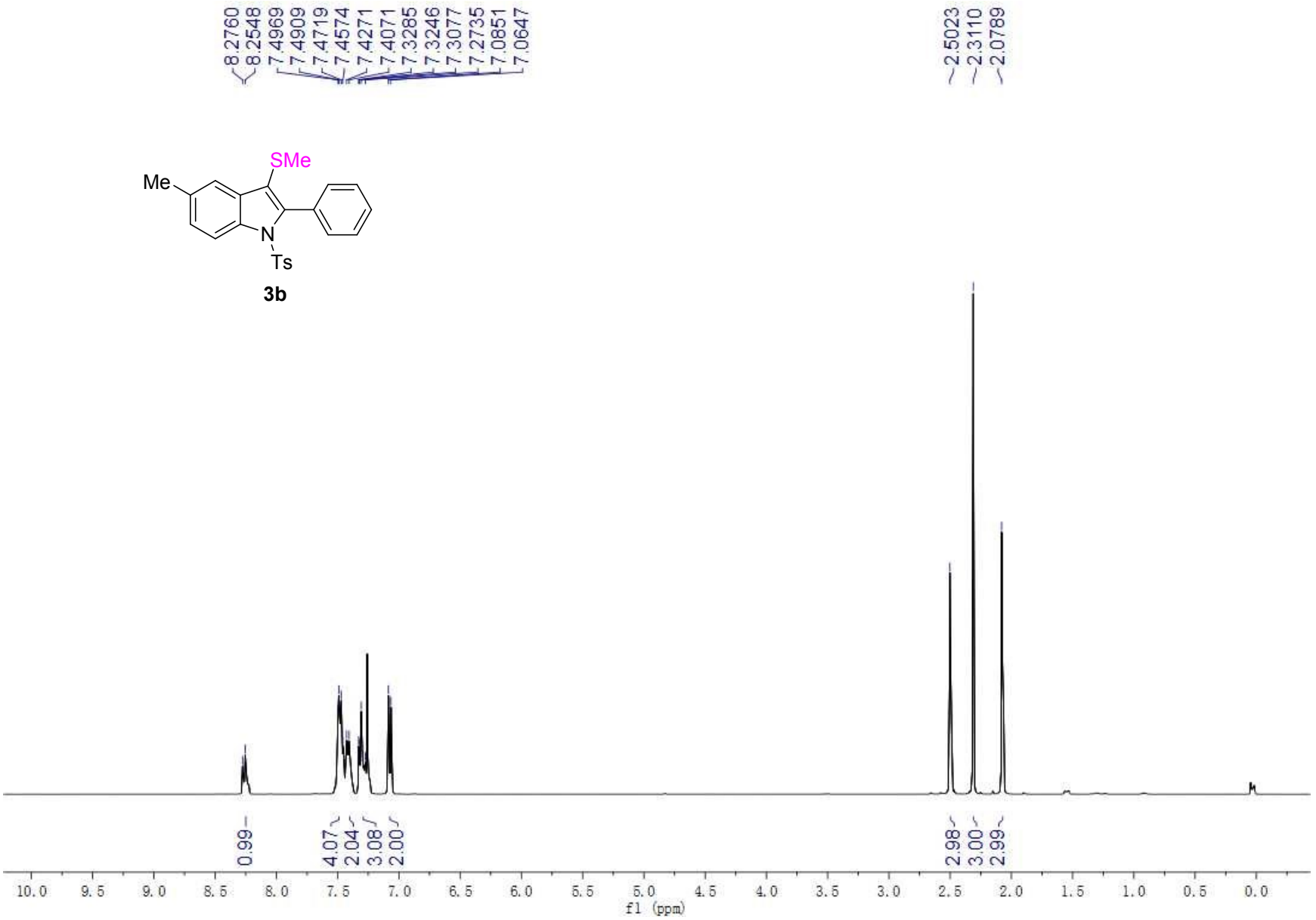
7.6886
7.6866
7.5012
7.4839
7.4758
7.4570
7.4353
7.4173
7.4136
7.3969
7.3932
7.3773
7.3730
7.3546
7.3150
7.2940
7.0852
7.0650
2.3145
2.0714
SMe
N
Ts
1.01
0.99
4.09
3.01
1.99
2.02
3.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3a


144.8609
142.7370
137.0113
135.1660
131.7695
131.1765
130.6628
129.4076
129.0853
127.2428
126.8899
125.5239
124.3202
119.8828
117.4153
116.2050
21.5914
18.3224
SMe
N
Ts
3a
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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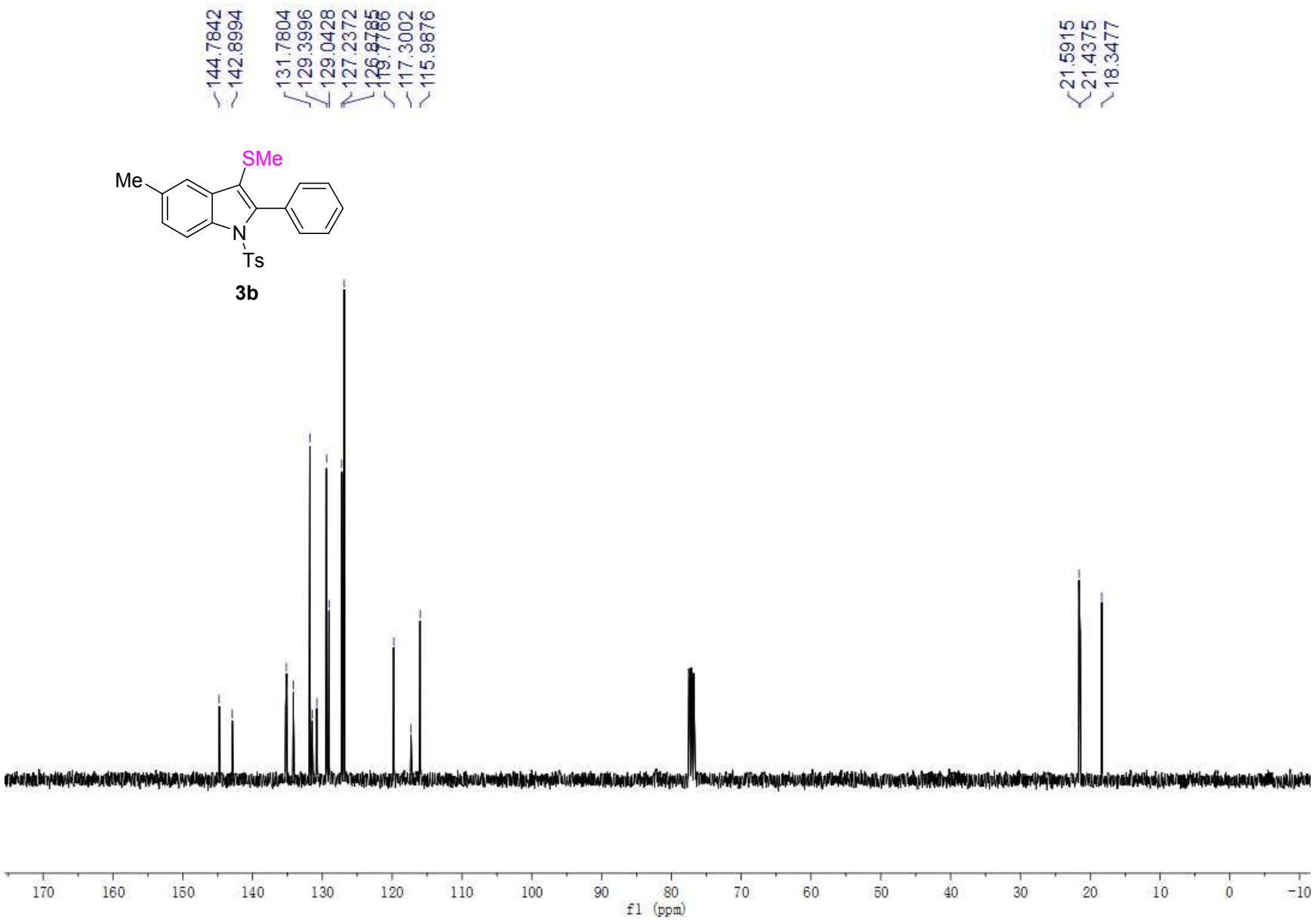
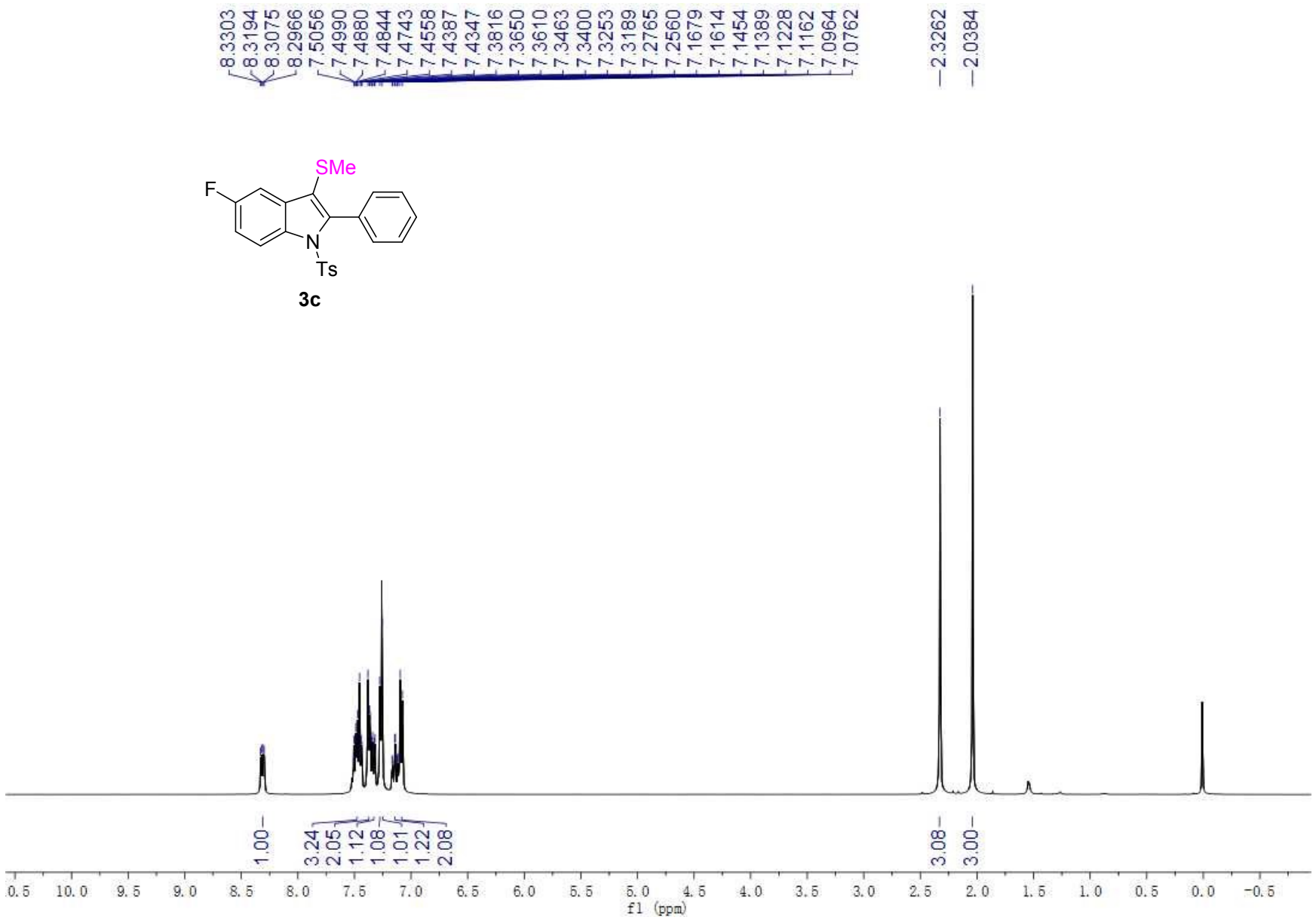
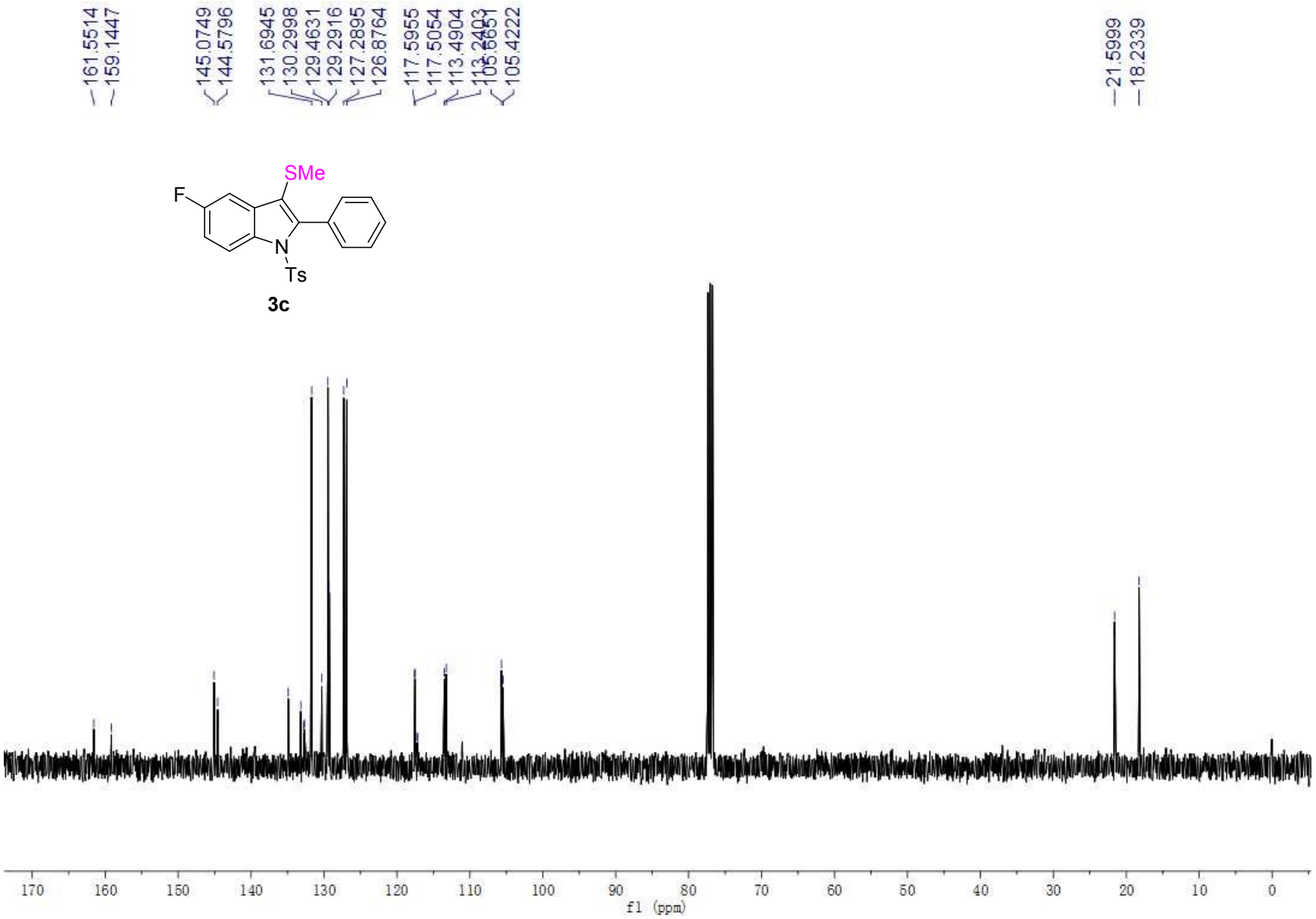
7.4969
7.4909
7.4719
7.4574
7.4271
7.4071
7.3285
7.3246
7.3077
7.2735
7.0851
7.0647
2.5023
2.3110
2.0789
SMe
Me
N
Ts
0.99
4.07
2.04
3.08
2.00
2.98
3.00
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

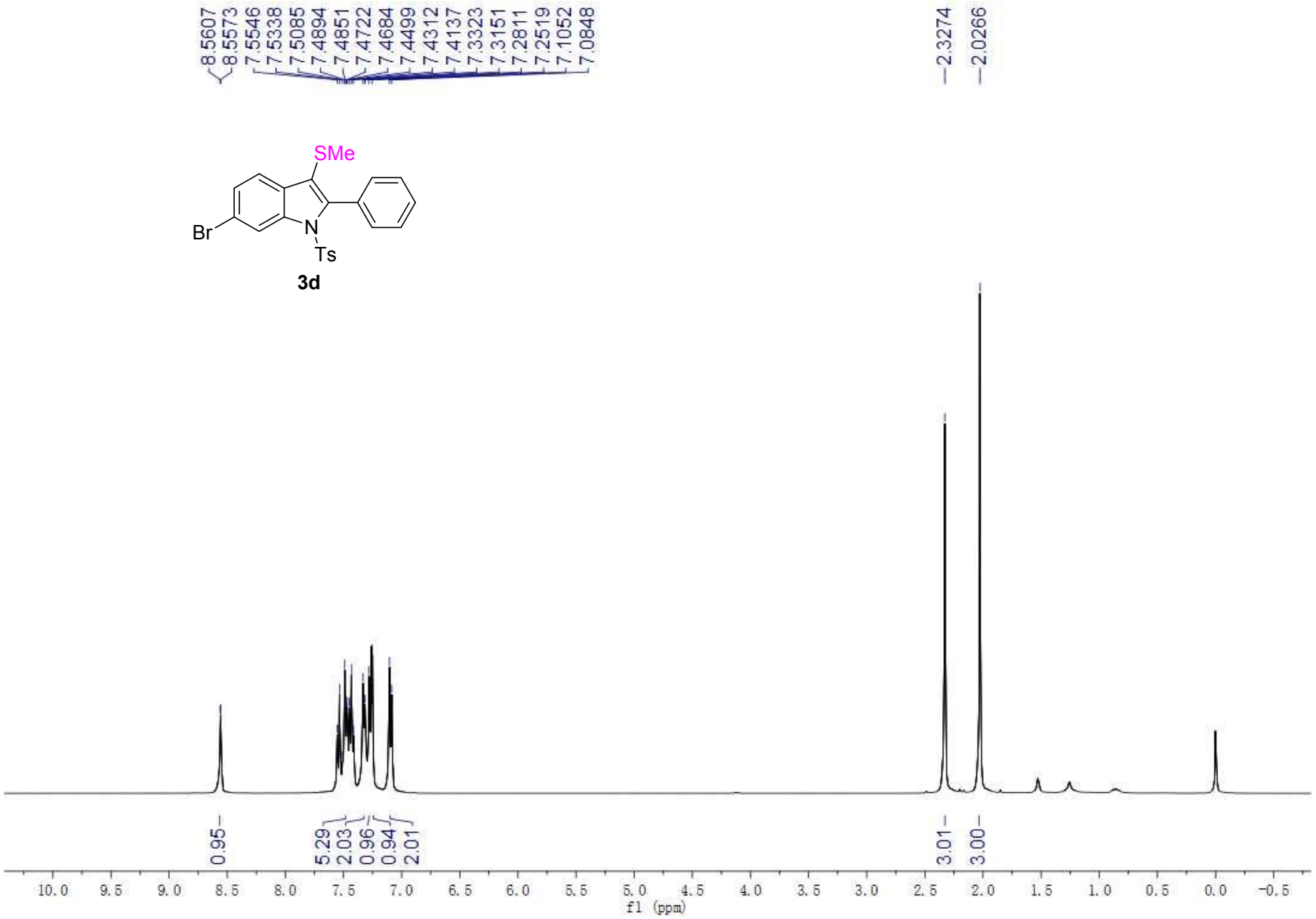
3b


144.7842
142.8994
131.7804
129.3996
129.0428
127.2372
126.8785
119.7788
117.3002
115.9876
21.5915
21.4375
18.3477
SMe
Me
N
Ts
3b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

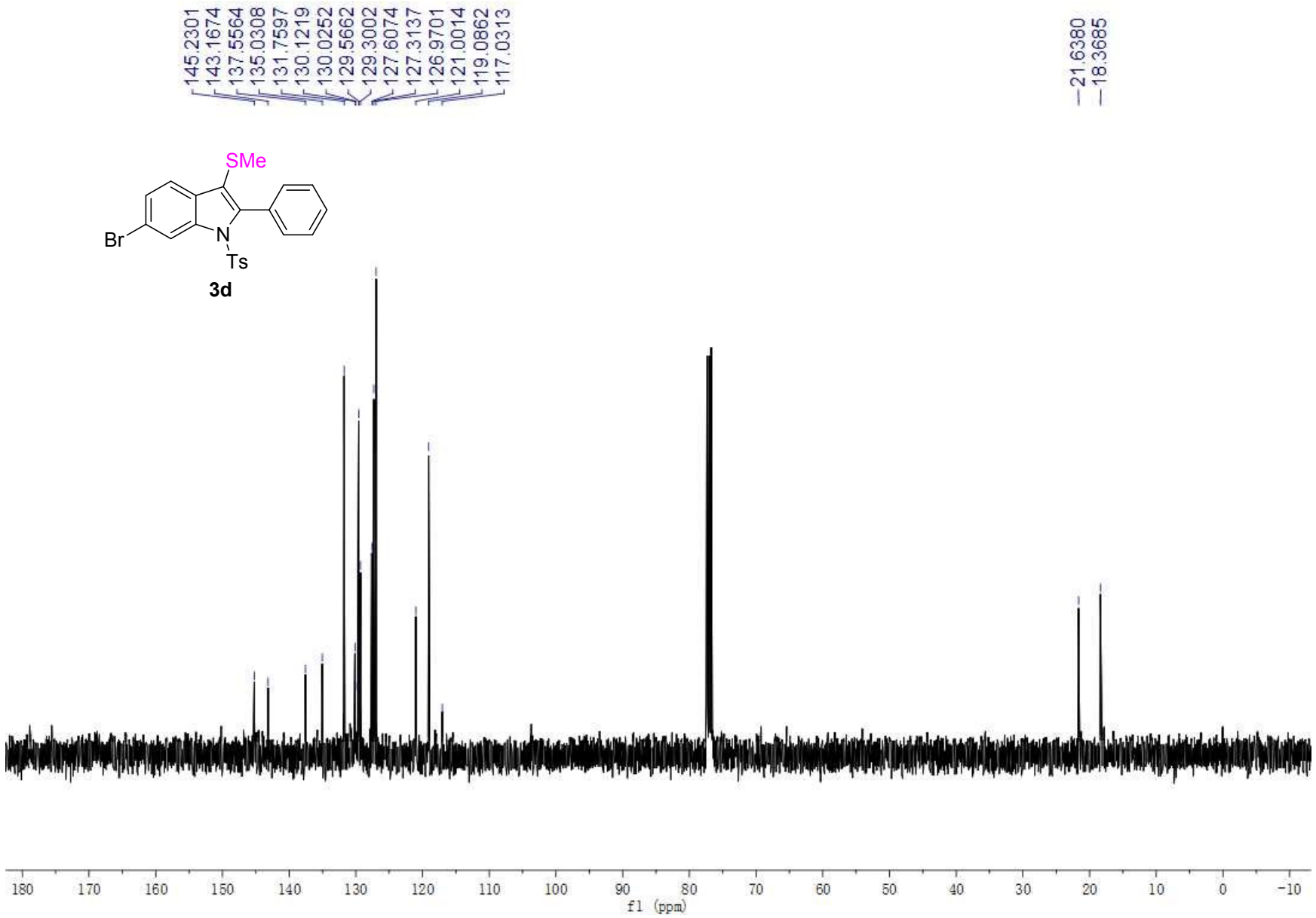

8.3303
8.3194
8.3075
8.2966
7.5056
7.4990
7.4880
7.4844
7.4743
7.4558
7.4387
7.4347
7.3816
7.3650
7.3610
7.3463
7.3400
7.3253
7.3189
7.2765
7.2560
7.1679
7.1614
7.1454
7.1389
7.1228
7.1162
7.0964
7.0762
2.3262
2.0384
SMe
F
N
Ts
1.00
3.24
2.05
1.12
1.08
1.01
1.22
2.08
3.08
3.00
f1 (ppm)

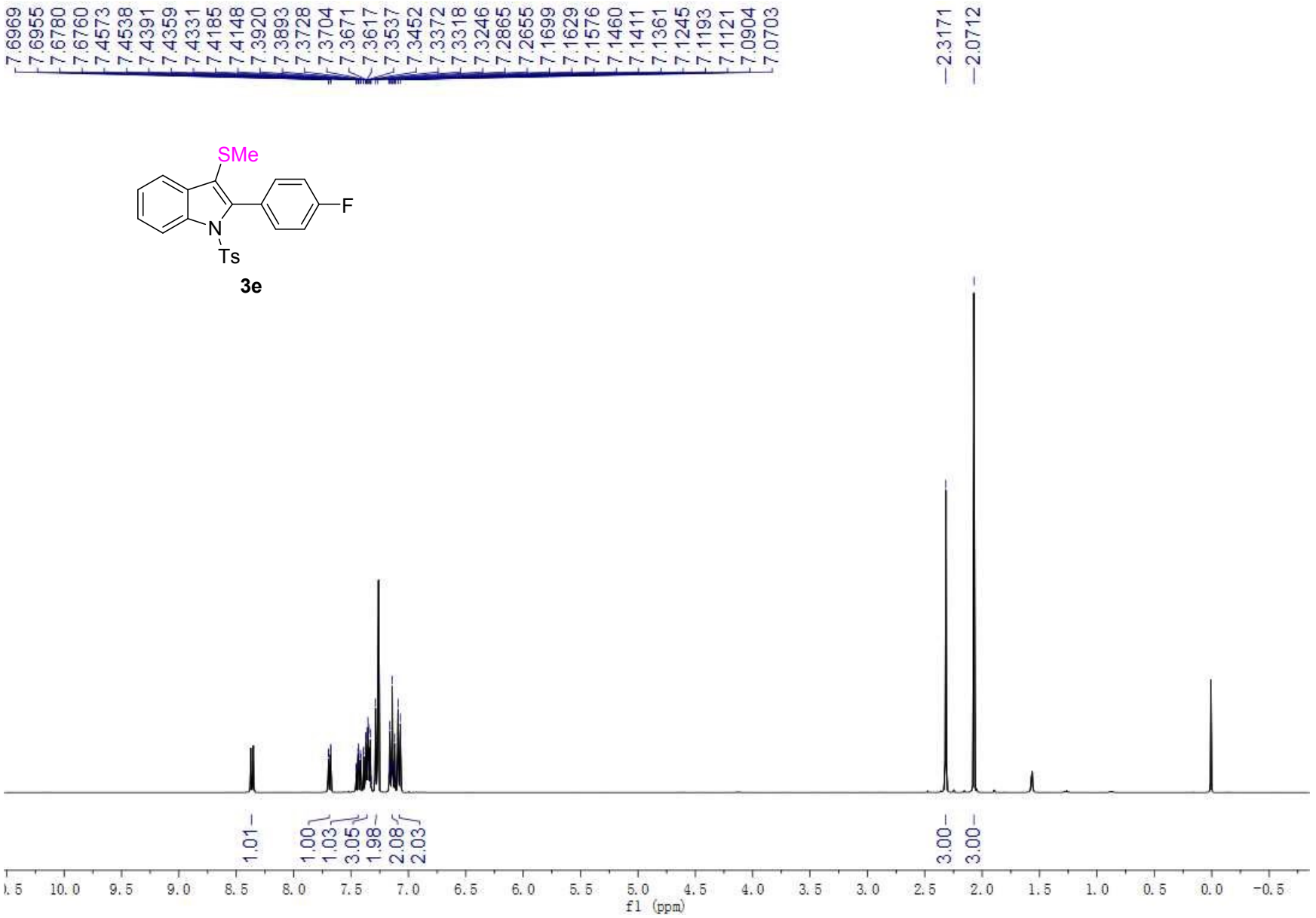
3c

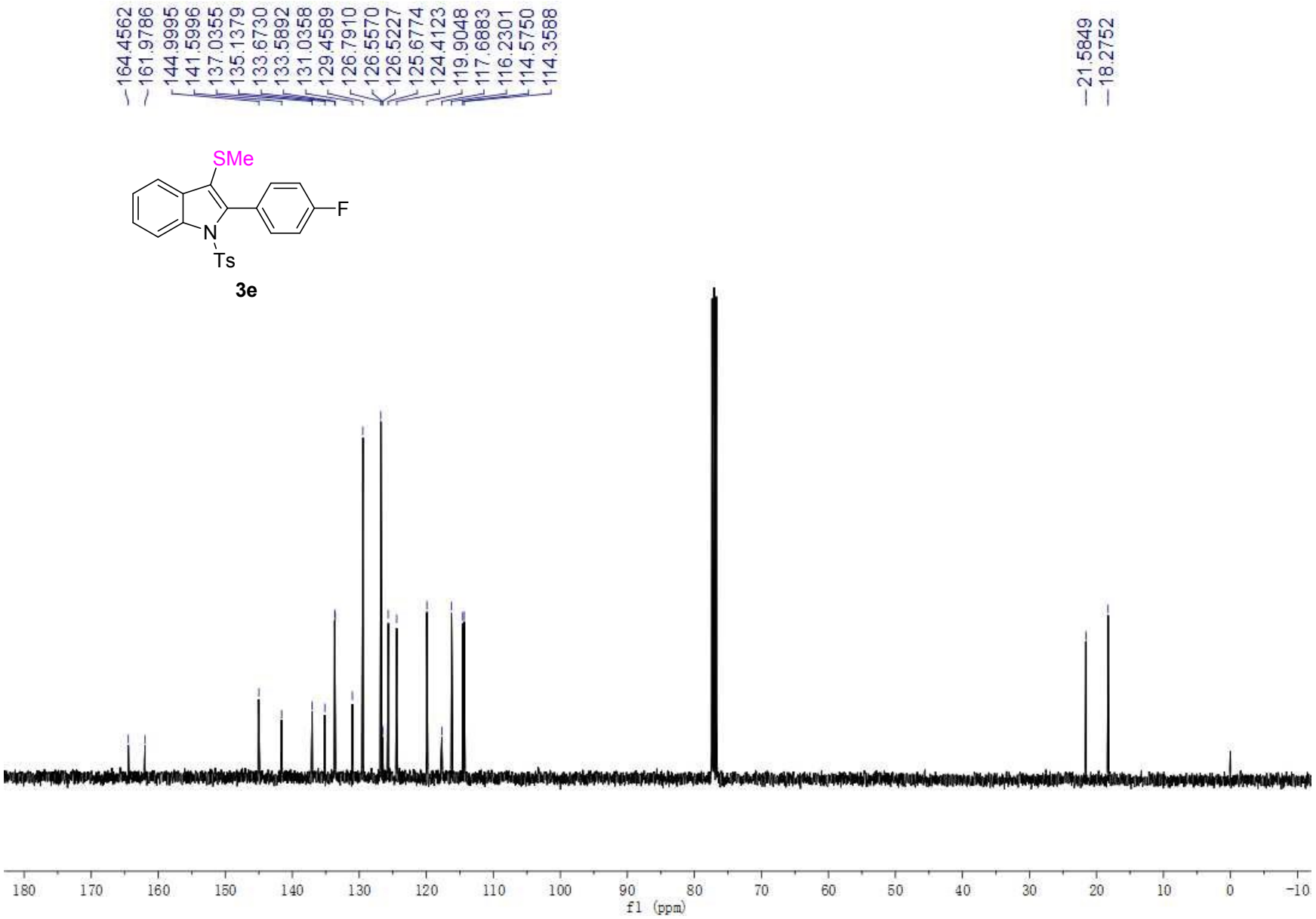

161.5514
159.1447
145.0749
144.5796
131.6945
130.2998
129.4631
129.2916
127.2895
126.8764
117.5955
117.5054
113.4904
113.2403
105.6651
105.4222
21.5999
18.2339
SMe
F
N
Ts
3c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.5607
8.5573
7.5546
7.5338
7.5085
7.4894
7.4851
7.4722
7.4684
7.4499
7.4312
7.4137
7.3323
7.3151
7.2811
7.2519
7.1052
7.0848
2.3274
2.0266
SMe
Br
N
Ts
0.95
5.29
2.03
0.96
0.94
2.01
3.01
3.00
10.0
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
-0.5
f1 (ppm)

3d


145.2301
143.1674
137.5564
135.0308
131.7597
130.1219
130.0252
129.5662
129.3002
127.6074
127.3137
126.9701
121.0014
119.0862
117.0313
21.6380
18.3685
SMe
Br
N
Ts
3d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.6969
7.6955
7.6780
7.6760
7.4573
7.4538
7.4391
7.4359
7.4331
7.4185
7.4148
7.3920
7.3893
7.3728
7.3704
7.3671
7.3617
7.3537
7.3452
7.3372
7.3318
7.3246
7.2865
7.2655
7.1699
7.1629
7.1576
7.1460
7.1411
7.1361
7.1245
7.1193
7.1121
7.0904
7.0703
2.3171
2.0712
SMe
F
N
Ts
3e
1.01
1.00
1.03
3.05
1.98
2.08
2.03
3.00
3.00
f1 (ppm)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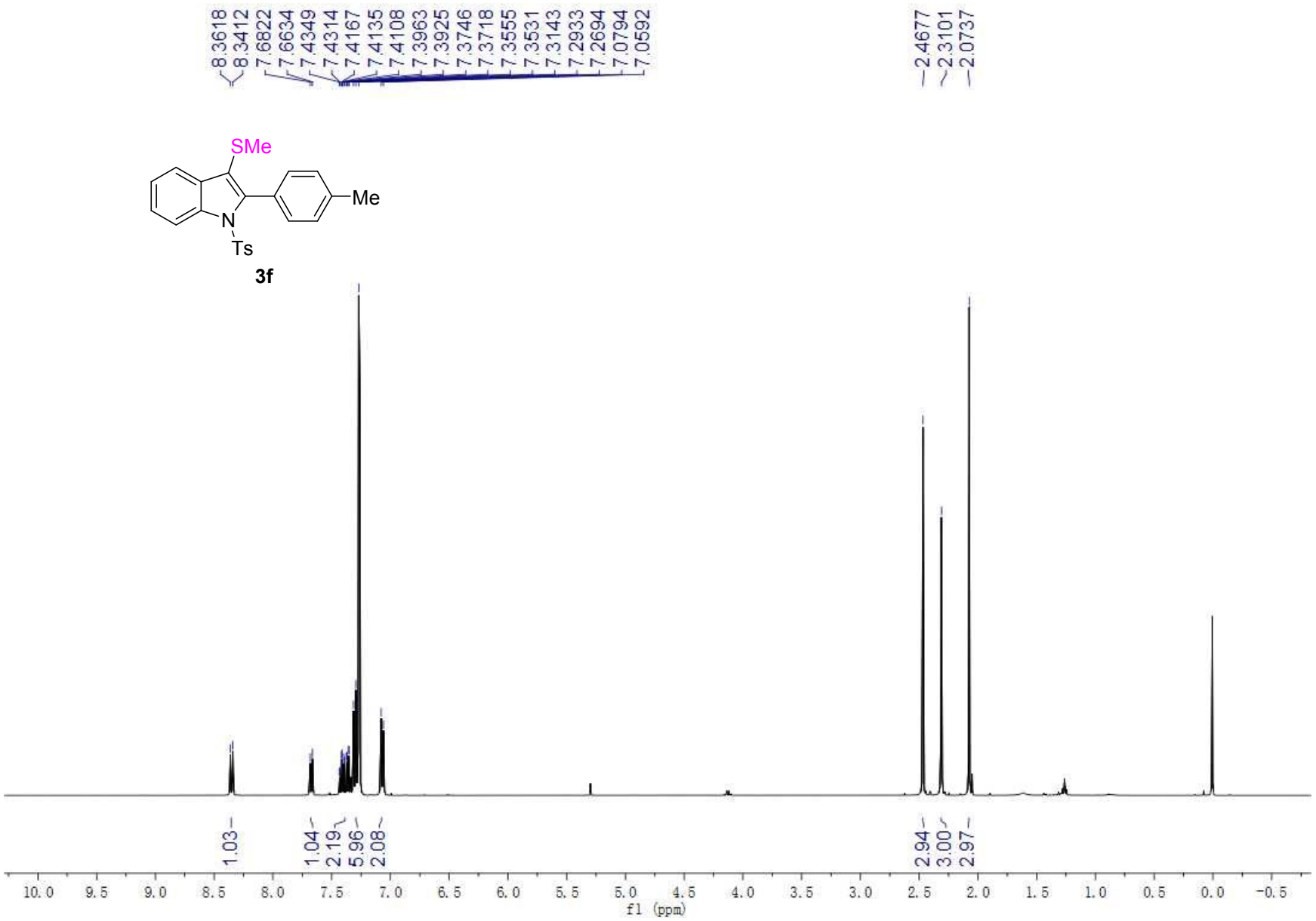
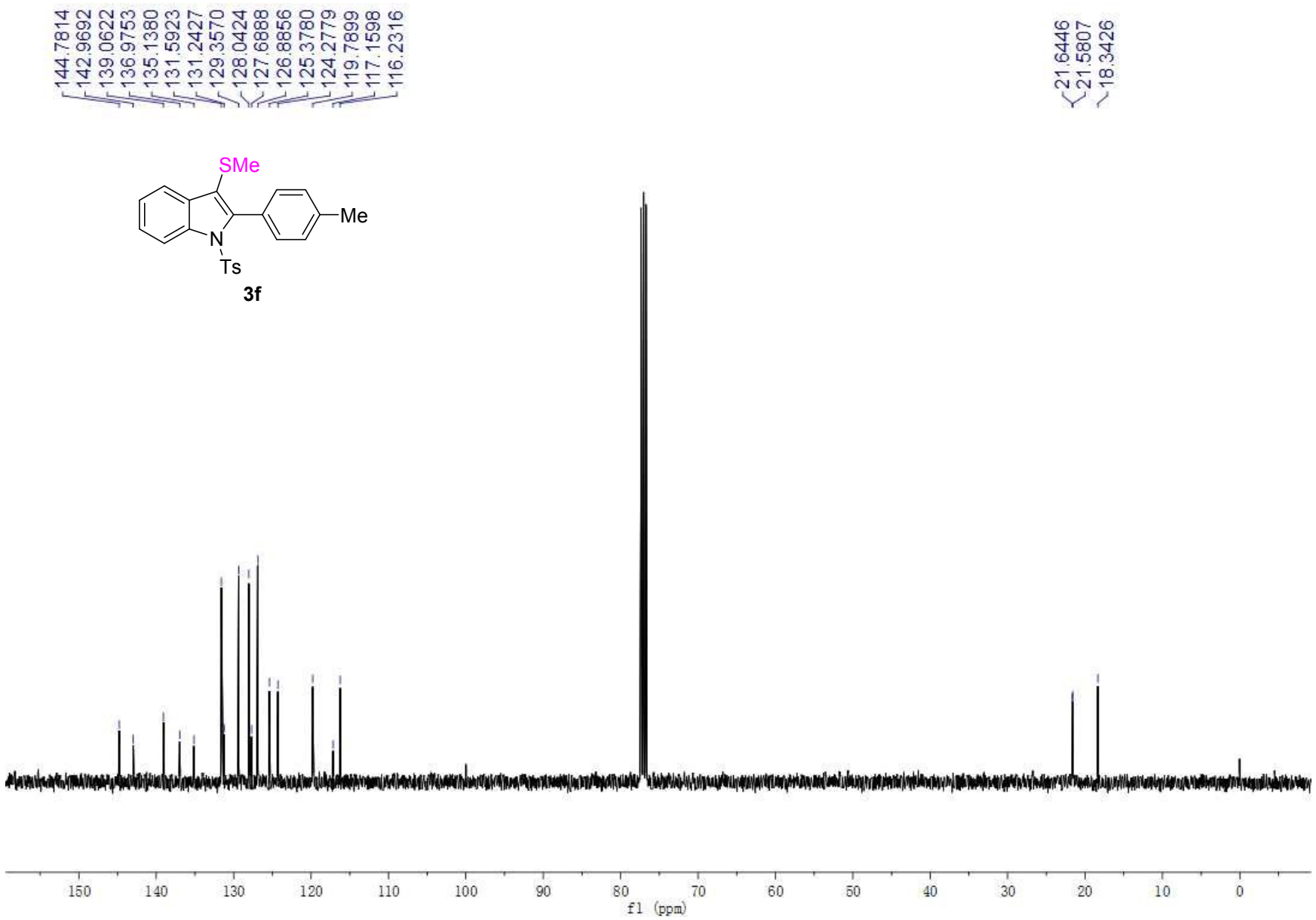
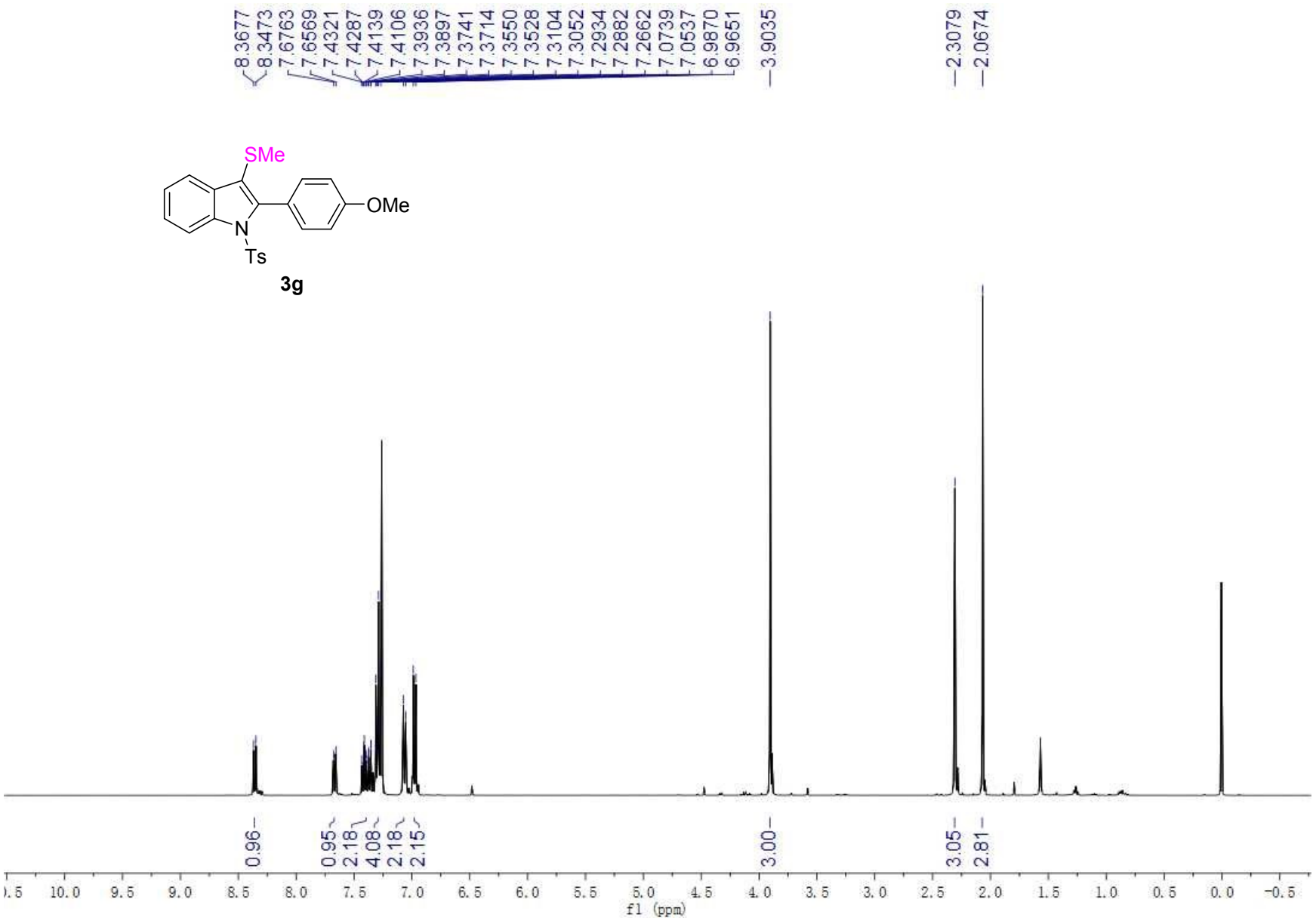
161.9786
144.9995
141.5996
137.0355
135.1379
133.6730
133.5892
131.0358
129.4589
126.7910
126.5570
126.5227
125.6774
124.4123
119.9048
117.6883
116.2301
114.5750
114.3588
21.5849
18.2752
SMe
F
N
Ts
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3e


8.3618
8.3412
7.6822
7.6634
7.4349
7.4314
7.4167
7.4135
7.4108
7.3963
7.3925
7.3746
7.3718
7.3555
7.3531
7.3143
7.2933
7.2694
7.0794
7.0592
2.4677
2.3101
2.0737
SMe
Me
N
Ts
3f
1.03
1.04
2.19
5.96
2.08
2.94
3.00
2.97
10.0
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
-0.5
f1 (ppm)


144.7814
142.9692
139.0622
136.9753
135.1380
131.5923
131.2427
129.3570
128.0424
127.6888
126.8856
125.3780
124.2779
119.7899
117.1598
116.2316
21.6446
21.5807
18.3426
SMe
Me
N
Ts
3f
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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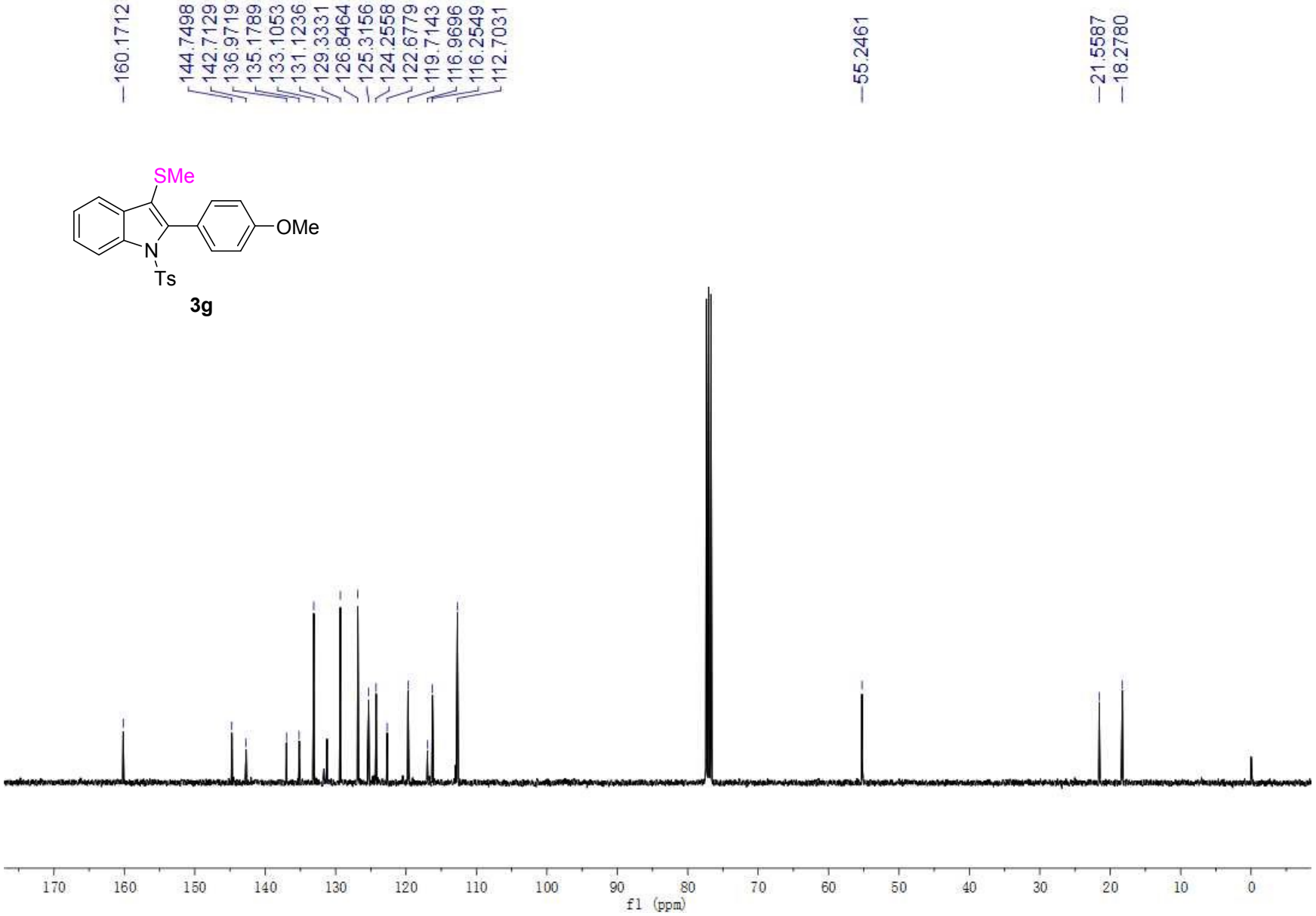
7.6763
7.6569
7.4321
7.4287
7.4139
7.4106
7.3936
7.3897
7.3741
7.3714
7.3550
7.3528
7.3104
7.3052
7.2934
7.2882
7.2662
7.0739
7.0537
6.9870
6.9651
3.9035
2.3079
2.0674
SMe
OMe
N
Ts
3g
0.96
0.95
2.18
4.08
2.18
2.15
3.00
3.05
2.81
f1 (ppm)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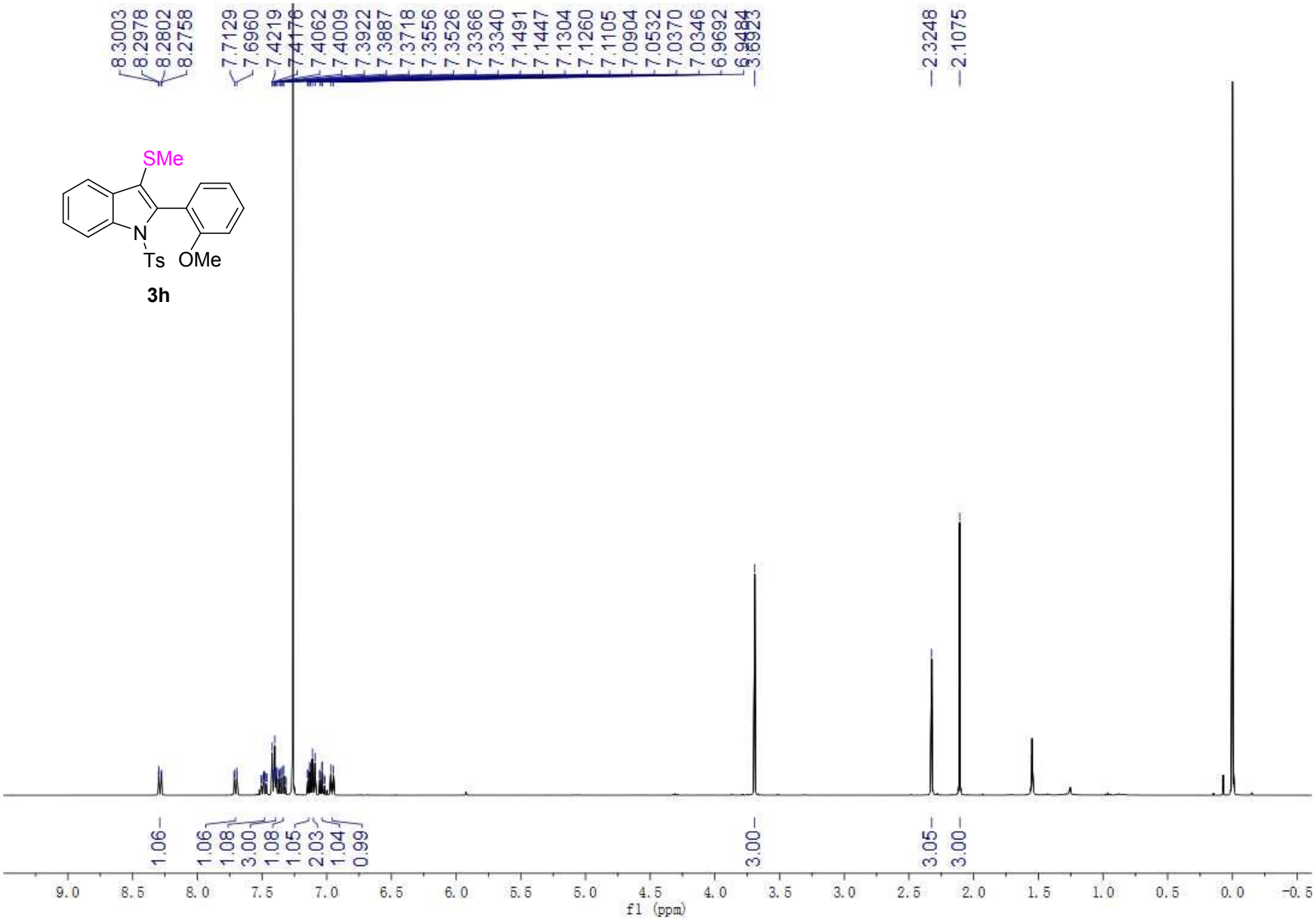
144.7498
142.7129
136.9719
135.1789
133.1053
131.1236
129.3331
126.8464
125.3156
124.2558
122.6779
119.7143
116.9696
116.2549
112.7031
55.2461
21.5587
18.2780
SMe
OMe
N
Ts
3g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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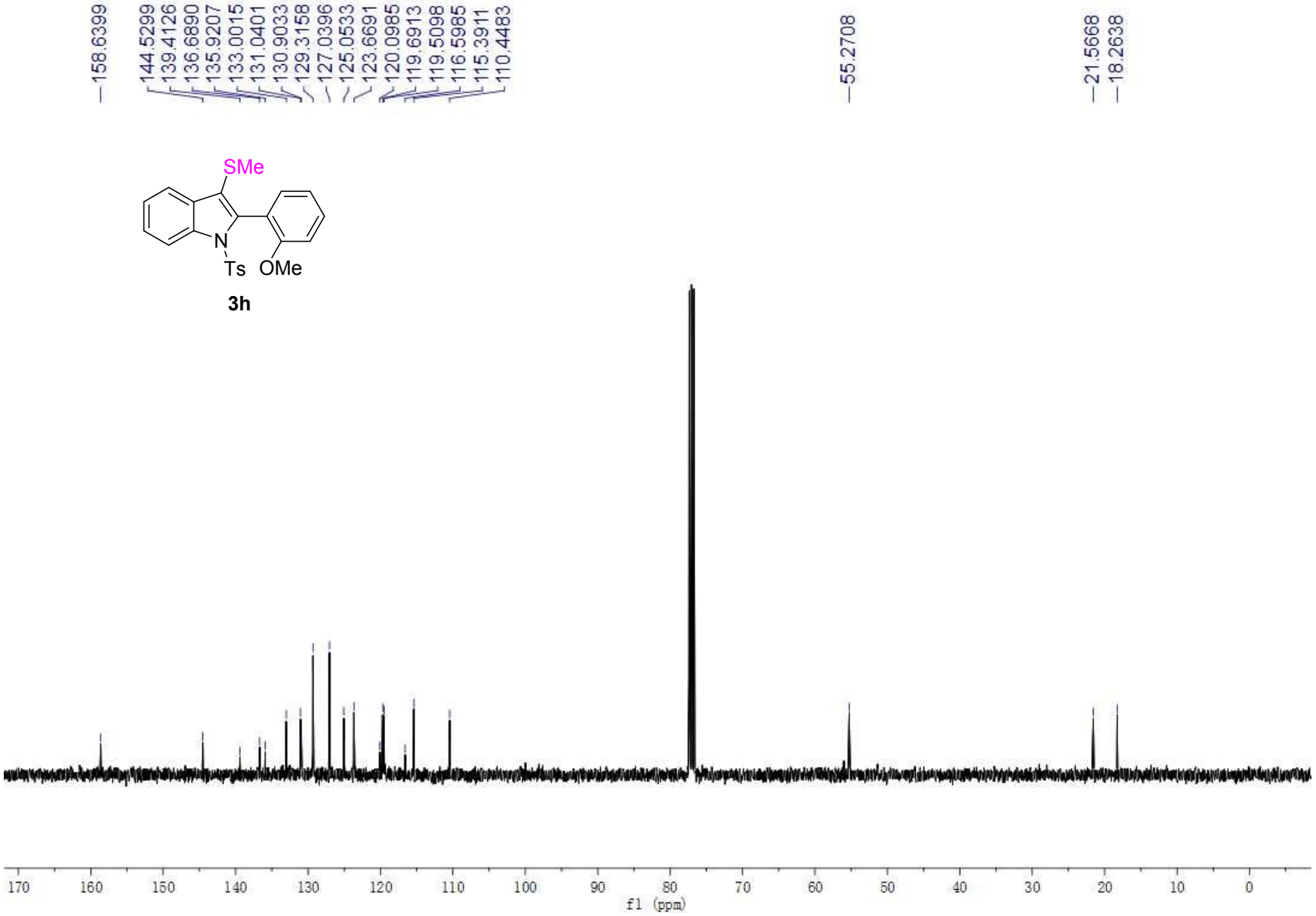
8.2978
8.2802
8.2758
7.7129
7.6960
7.4219
7.4178
7.4062
7.4009
7.3922
7.3887
7.3718
7.3556
7.3526
7.3366
7.3340
7.1491
7.1447
7.1304
7.1260
7.1105
7.0904
7.0532
7.0370
7.0346
6.9692
2.3248
2.1075
SMe
N
Ts
OMe
3h
1.06
1.06
1.08
3.00
1.08
1.05
2.03
1.04
0.99
3.00
3.05
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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136.6890
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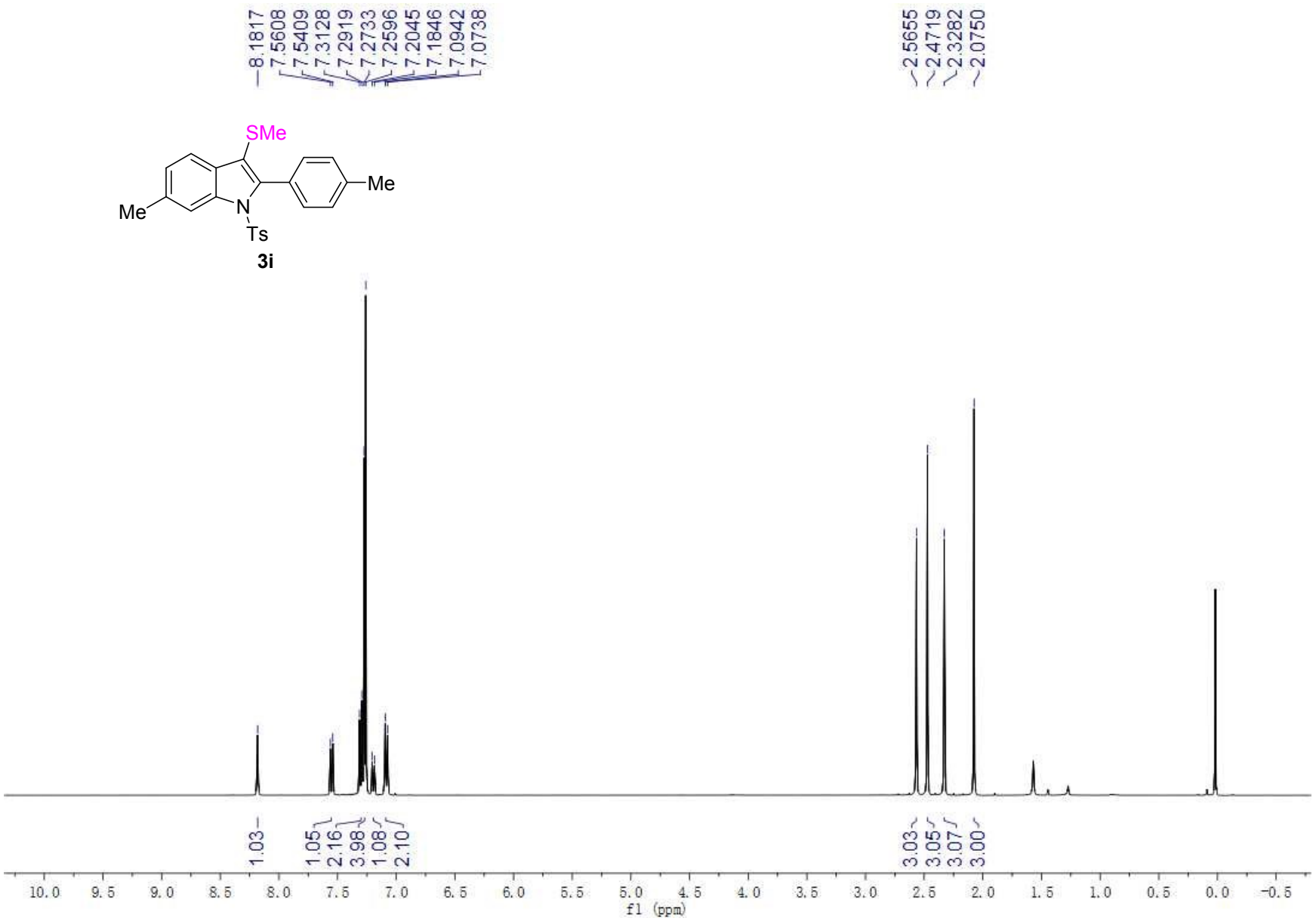
133.0015
131.0401
130.9033
129.3158
127.0396
125.0533
123.6691
120.0985
119.6913
119.5098
116.5985
115.3911
110.4483
55.2708
21.5668
18.2638
SMe
N
Ts
OMe
3h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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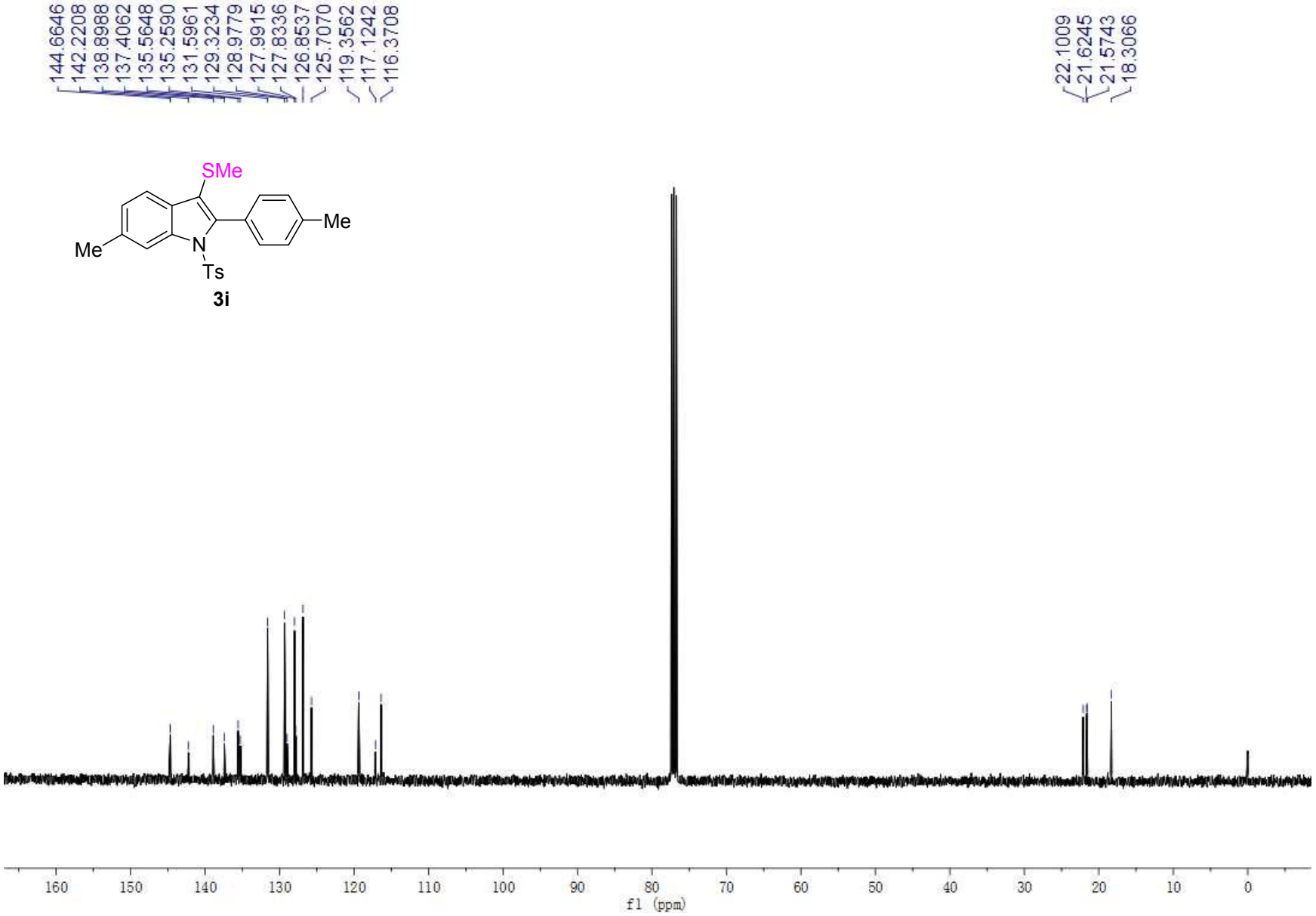
7.2919
7.2733
7.2596
7.2045
7.1846
7.0942
7.0738
2.5655
2.4719
2.3282
2.0750
SMe
Me
Me
N
Ts
3i
1.03
1.05
2.16
3.98
1.08
2.10
3.03
3.05
3.07
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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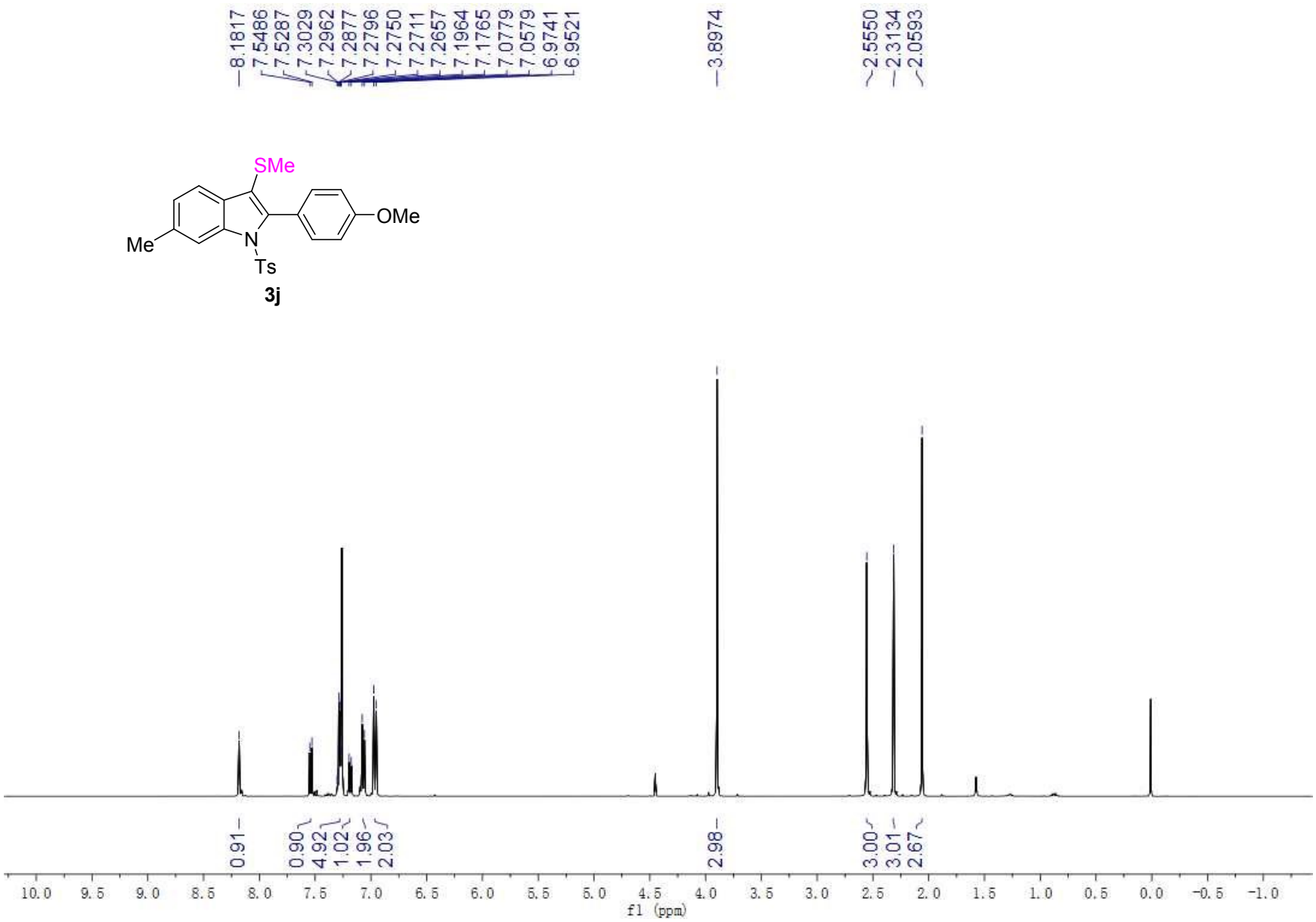
129.3234
128.9779
127.9915
127.8336
126.8537
125.7070
119.3562
117.1242
116.3708
22.1009
21.6245
21.5743
18.3066
SMe
Me
Me
N
Ts
3i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.1817
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7.5287
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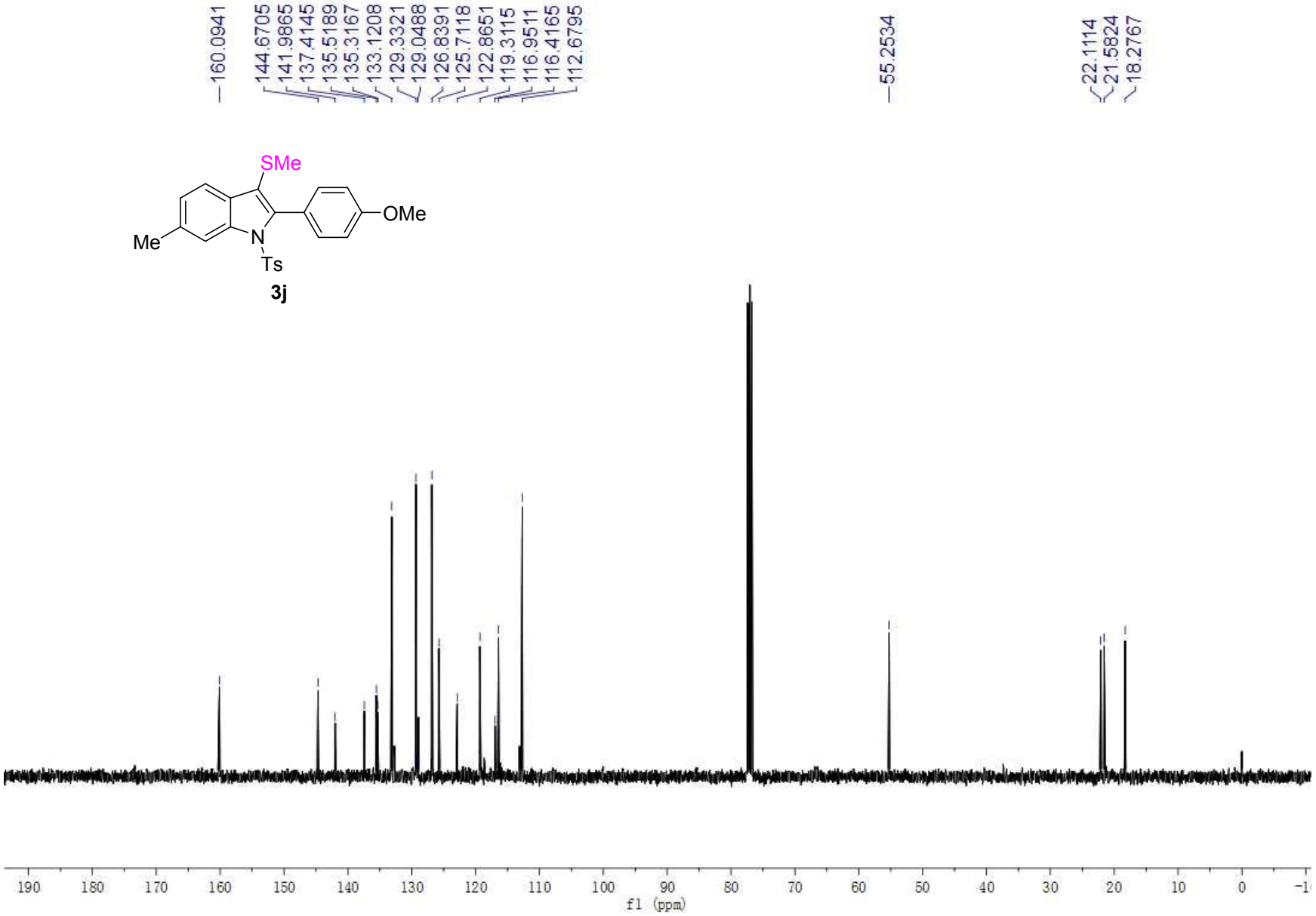
7.2962
7.2877
7.2796
7.2750
7.2711
7.2657
7.1964
7.1765
7.0779
7.0579
6.9741
6.9521
3.8974
2.5550
2.3134
2.0593
SMe
OMe
Me
N
Ts
0.91
0.90
4.92
1.02
1.96
2.03
2.98
3.00
3.01
2.67
f1 (ppm)

3j


160.0941
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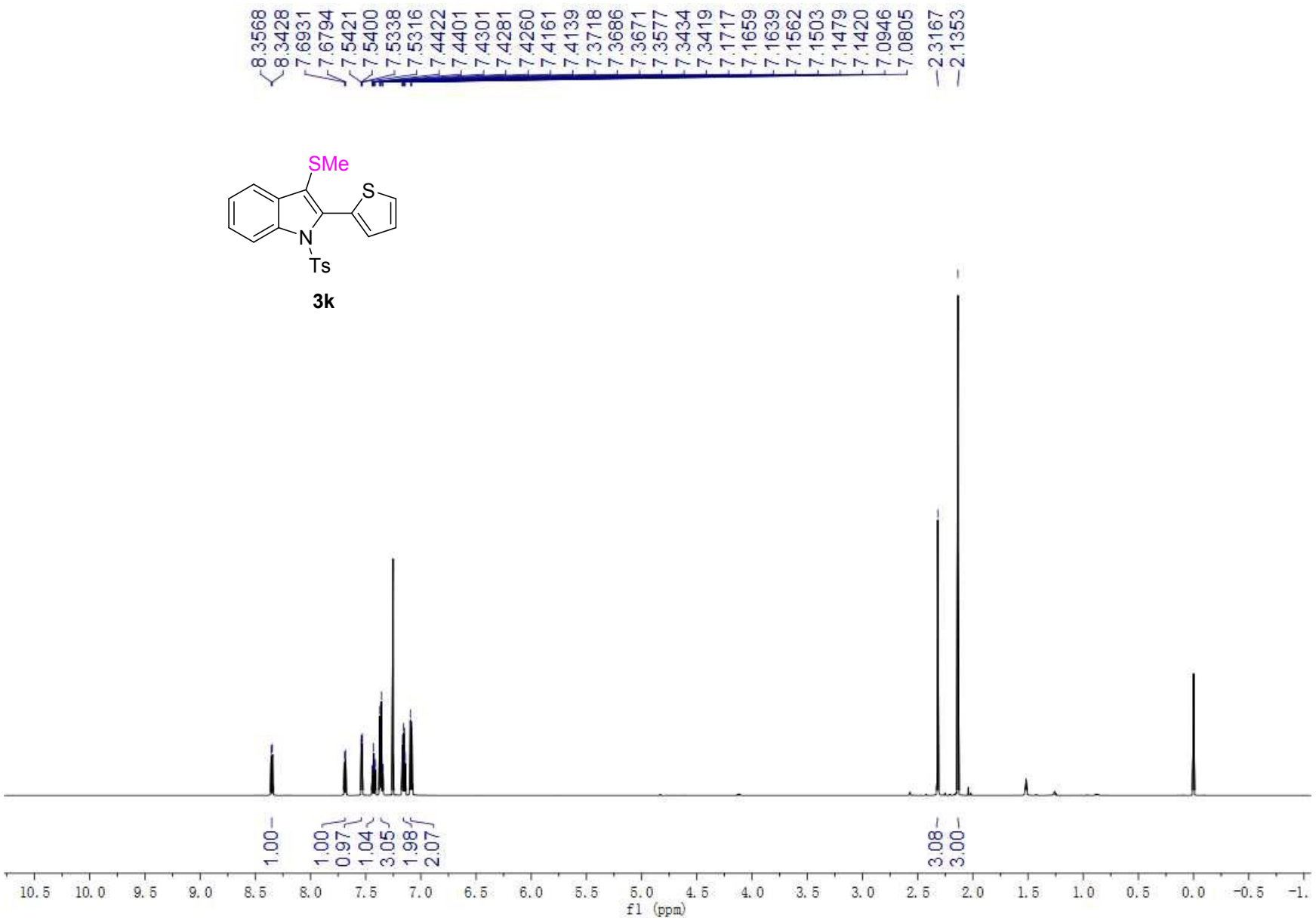
141.9865
137.4145
135.5189
135.3167
133.1208
129.3321
129.0488
126.8391
125.7118
122.8651
119.3115
116.9511
116.4165
112.6795
55.2534
22.1114
21.5824
18.2767
SMe
OMe
Me
N
Ts
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6794
7.5421
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7.5338
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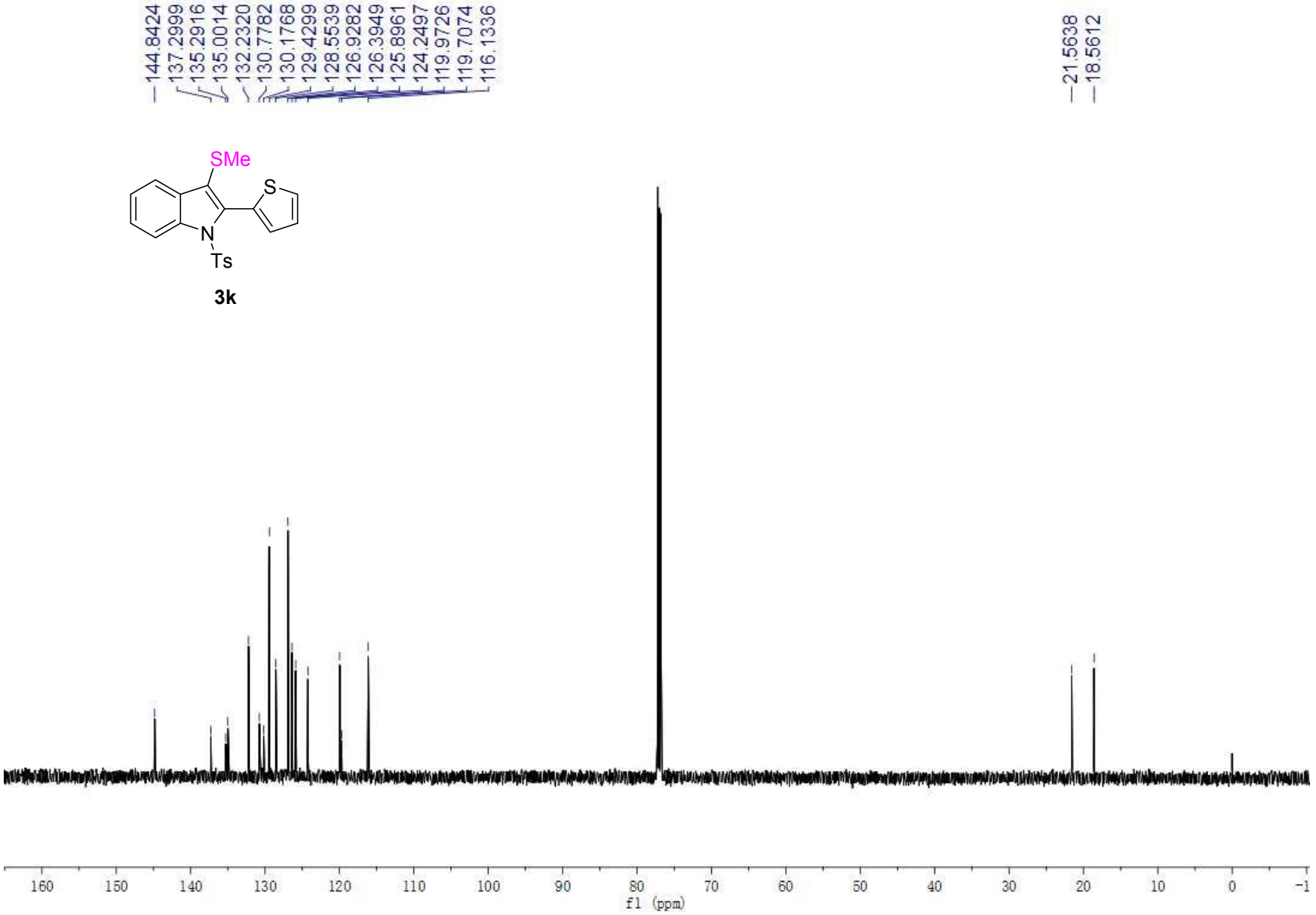
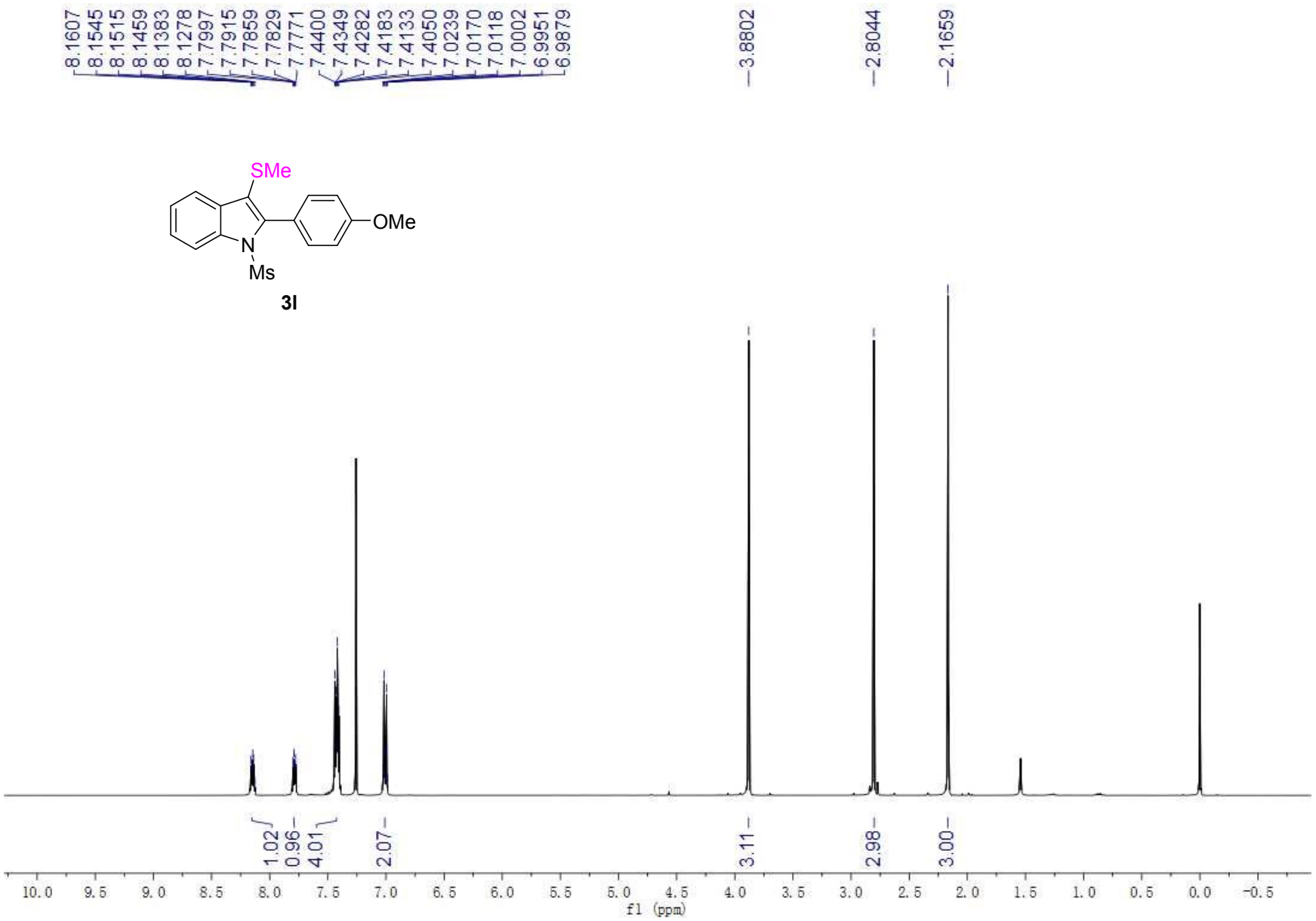
7.4422
7.4401
7.4301
7.4281
7.4260
7.4161
7.4139
7.3718
7.3686
7.3671
7.3577
7.3434
7.3419
7.1717
7.1659
7.1639
7.1562
7.1503
7.1479
7.1420
7.0946
7.0805
2.3167
2.1353
SMe
S
N
Ts
1.00
1.00
0.97
1.04
3.05
1.98
2.07
3.08
3.00
f1 (ppm)

3k


144.8424
137.2999
135.2916
135.0014
132.2320
130.7782
130.1768
129.4299
128.5539
126.9282
126.3949
125.8961
124.2497
119.9726
119.7074
116.1336
21.5638
18.5612
SMe
S
N
Ts
3k
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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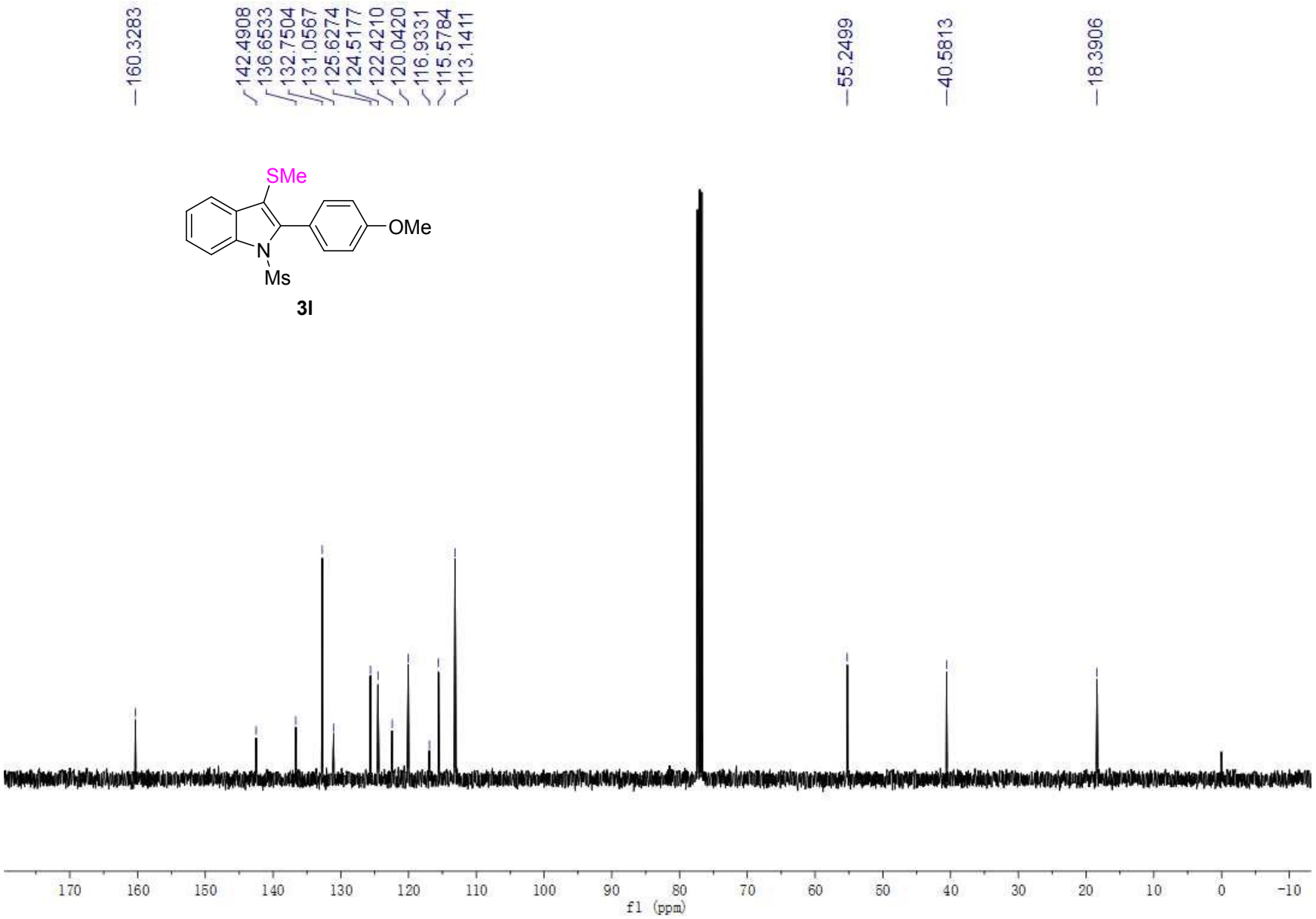
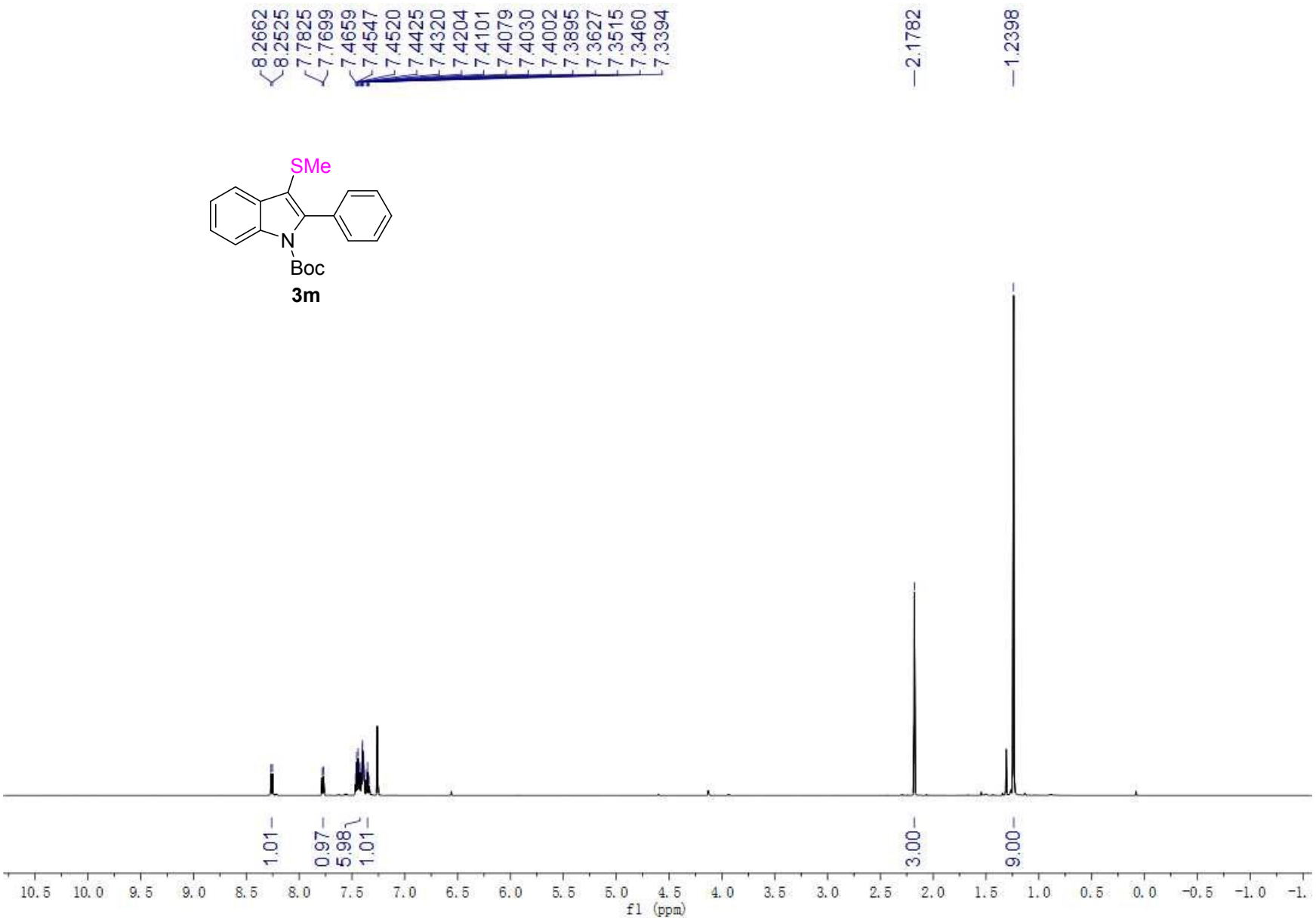
8.1545
8.1515
8.1459
8.1383
8.1278
7.7997
7.7915
7.7859
7.7829
7.7771
7.4400
7.4349
7.4282
7.4183
7.4133
7.4050
7.0239
7.0170
7.0118
7.0002
6.9951
6.9879
3.8802
2.8044
2.1659
SMe
OMe
N
Ms
1.02
0.96
4.01
2.07
3.11
2.98
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3l


160.3283
142.4908
136.6533
132.7504
131.0567
125.6274
124.5177
122.4210
120.0420
116.9331
115.5784
113.1411
55.2499
40.5813
18.3906
SMe
OMe
N
Ms
3l
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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8.2525
7.7825
7.7699
7.4659
7.4547
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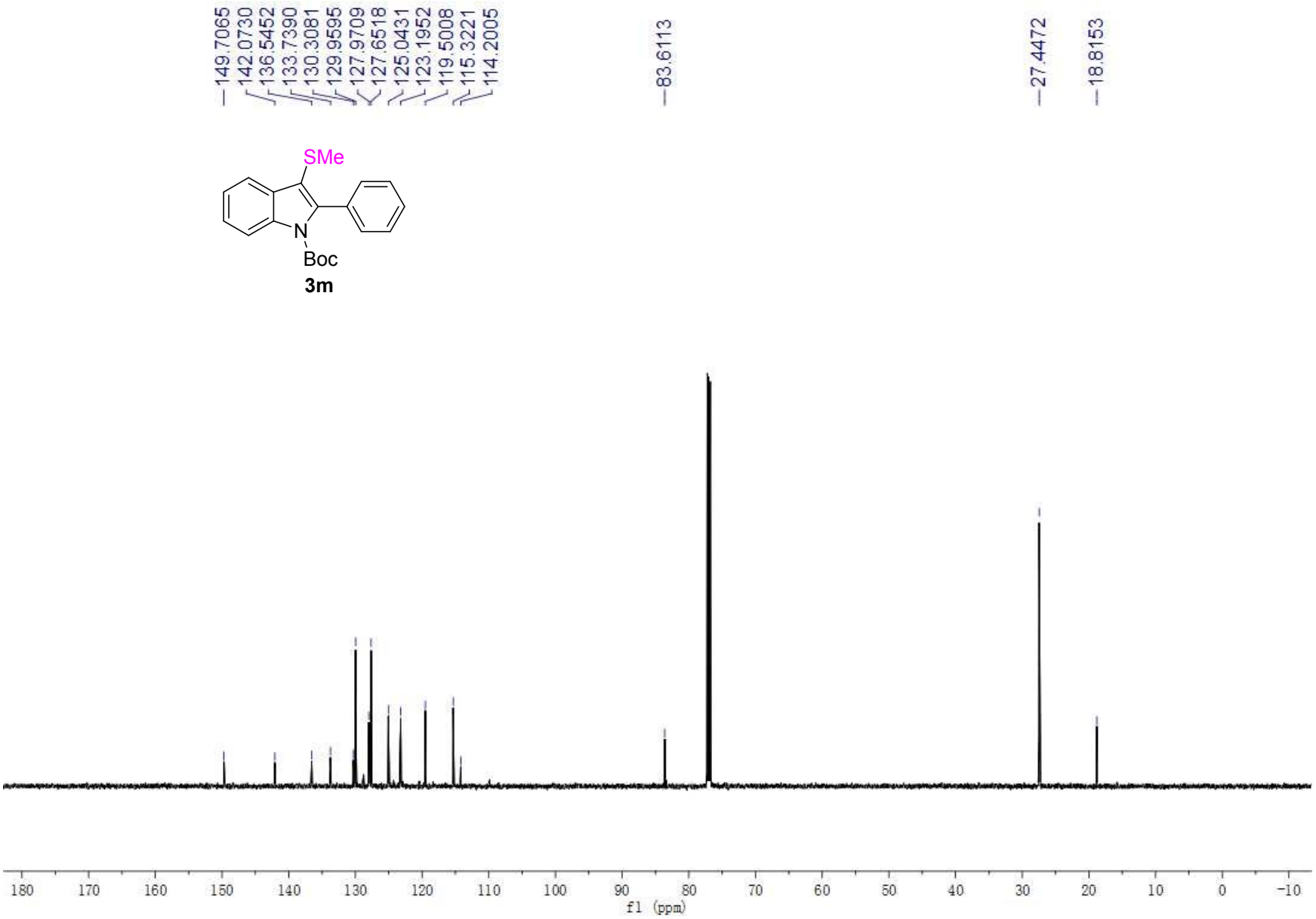
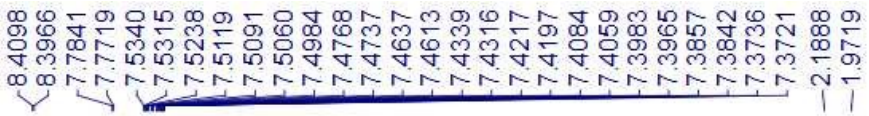
7.4320
7.4204
7.4101
7.4079
7.4030
7.4002
7.3895
7.3627
7.3515
7.3460
7.3394
2.1782
1.2398
SMe
N
Boc
3m
1.01
0.97
5.98
1.01
3.00
9.00
f1 (ppm)


149.7065
142.0730
136.5452
133.7390
130.3081
129.9595
127.9709
127.6518
125.0431
123.1952
119.5008
115.3221
114.2005
83.6113
27.4472
18.8153
SMe
N
Boc
3m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.4098
8.3966
7.7841
7.7719
7.5340
7.5315
7.5238
7.5119
7.5091
7.5060
7.4984
7.4768
7.4737
7.4637
7.4613
7.4339
7.4316
7.4217
7.4197
7.4084
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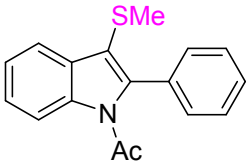
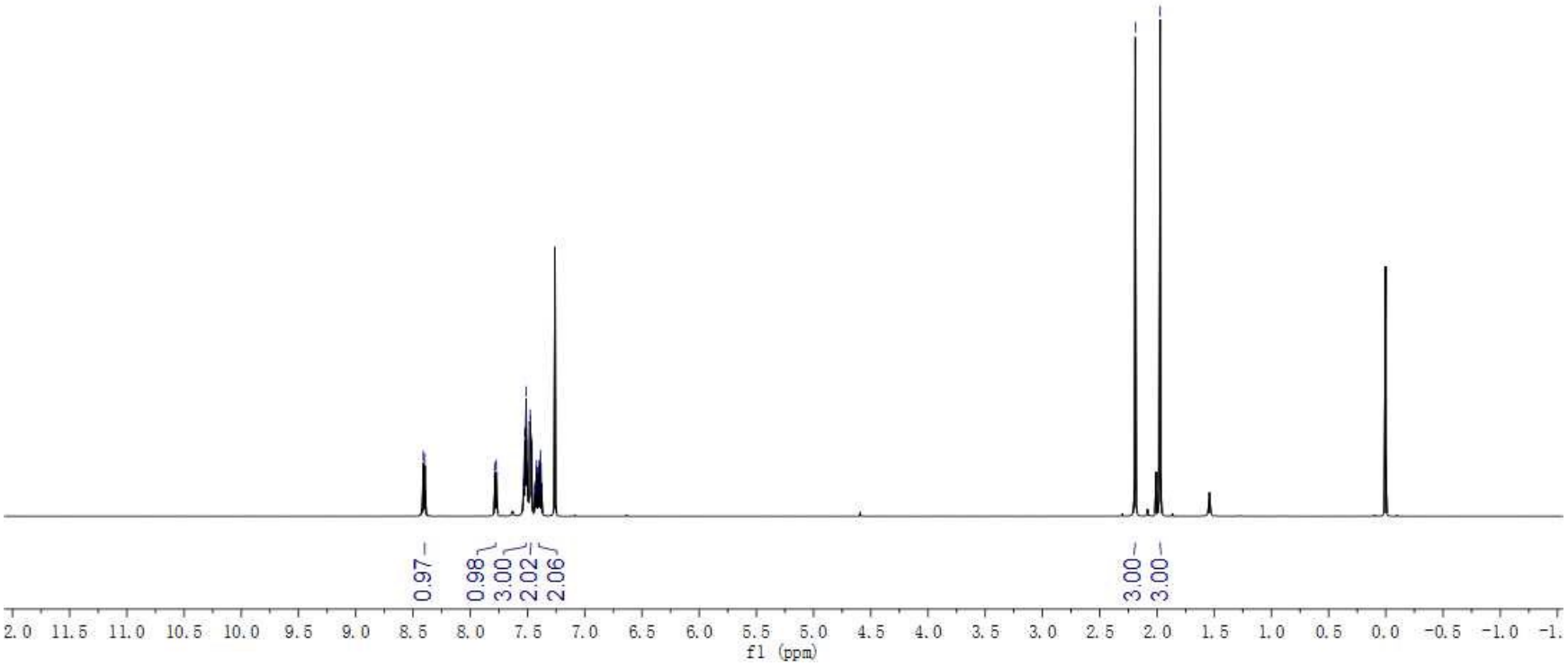
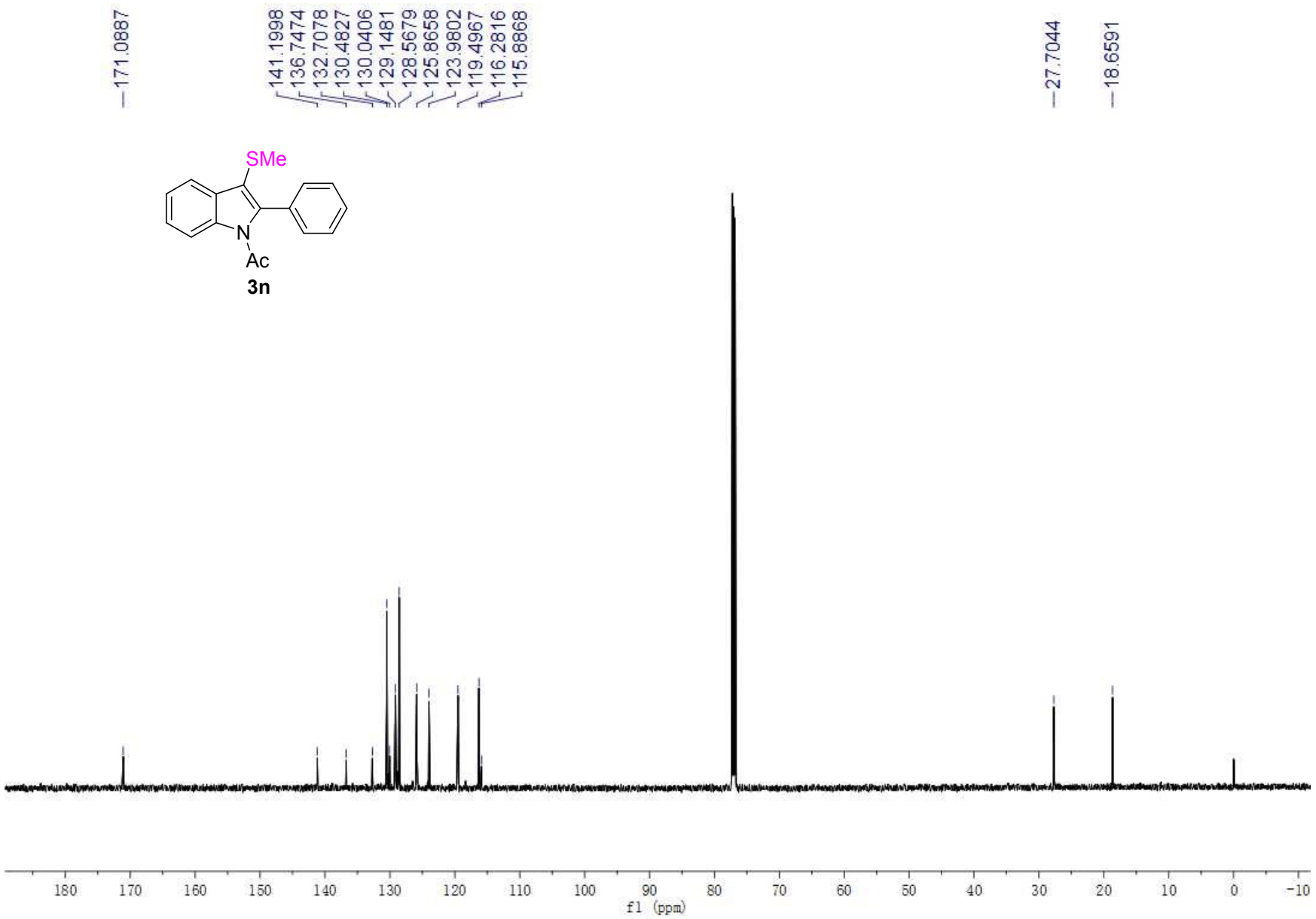
7.3983
7.3965
7.3857
7.3842
7.3736
7.3721
2.1888
1.9719


SMe
N
Ac

3n


0.97
0.98
3.00
2.02
2.06
3.00
3.00
2.0 11.5 11.0 10.5 10.0 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 -0.5 -1.0 -1.
f1 (ppm)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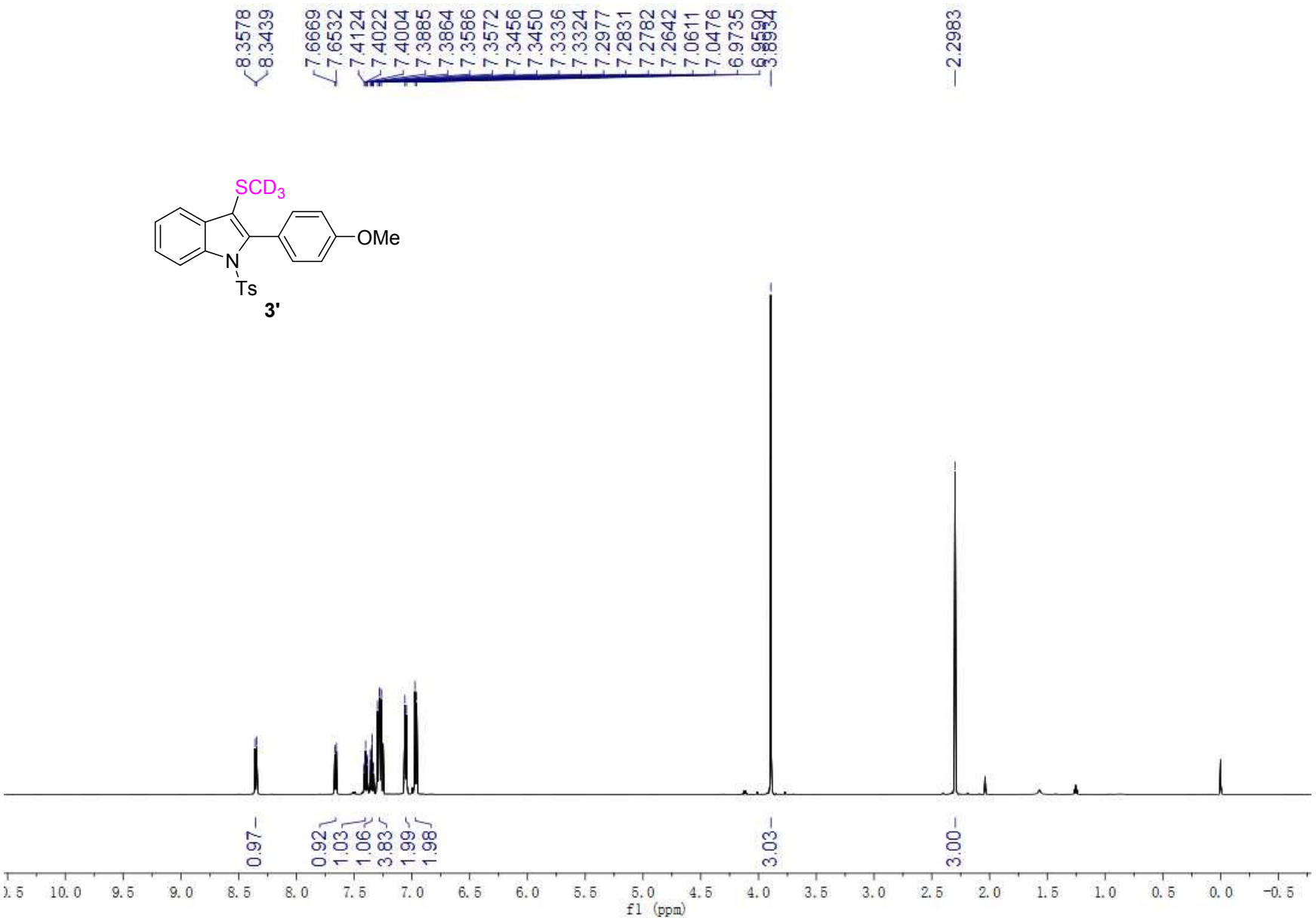
141.1998
136.7474
132.7078
130.4827
130.0406
129.1481
128.5679
125.8658
123.9802
119.4967
116.2816
115.8868
27.7044
18.6591
SMe
N
Ac
3n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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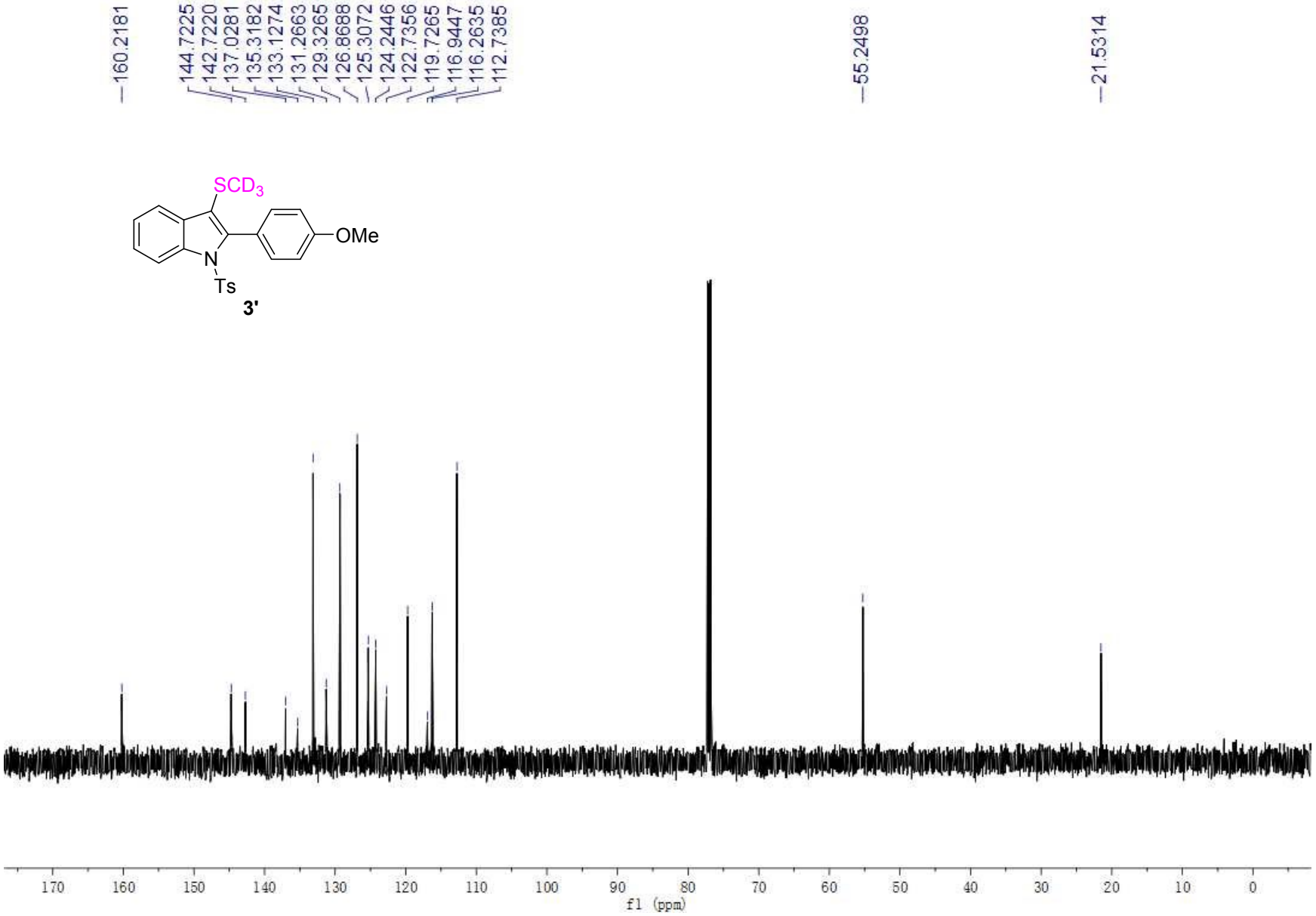
8.3439
7.6669
7.6532
7.4124
7.4022
7.4004
7.3885
7.3864
7.3586
7.3572
7.3456
7.3450
7.3336
7.3324
7.2977
7.2831
7.2782
7.2642
7.0611
7.0476
6.9735
2.2983
SCD3
OMe
N
Ts
3'
0.97
0.92
1.03
1.06
3.83
1.99
1.98
3.03
3.00
f1 (ppm)


160.2181
144.7225
142.7220
137.0281
135.3182
133.1274
131.2663
129.3265
126.8688
125.3072
124.2446
122.7356
119.7265
116.9447
116.2635
112.7385
55.2498
21.5314
SCD3
OMe
N
Ts
3'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)