Supporting Information

Construction of Diverse Polycyclic *N*-Heterocycles *via* Cascade Allylic Amination/Diels–Alder Reaction

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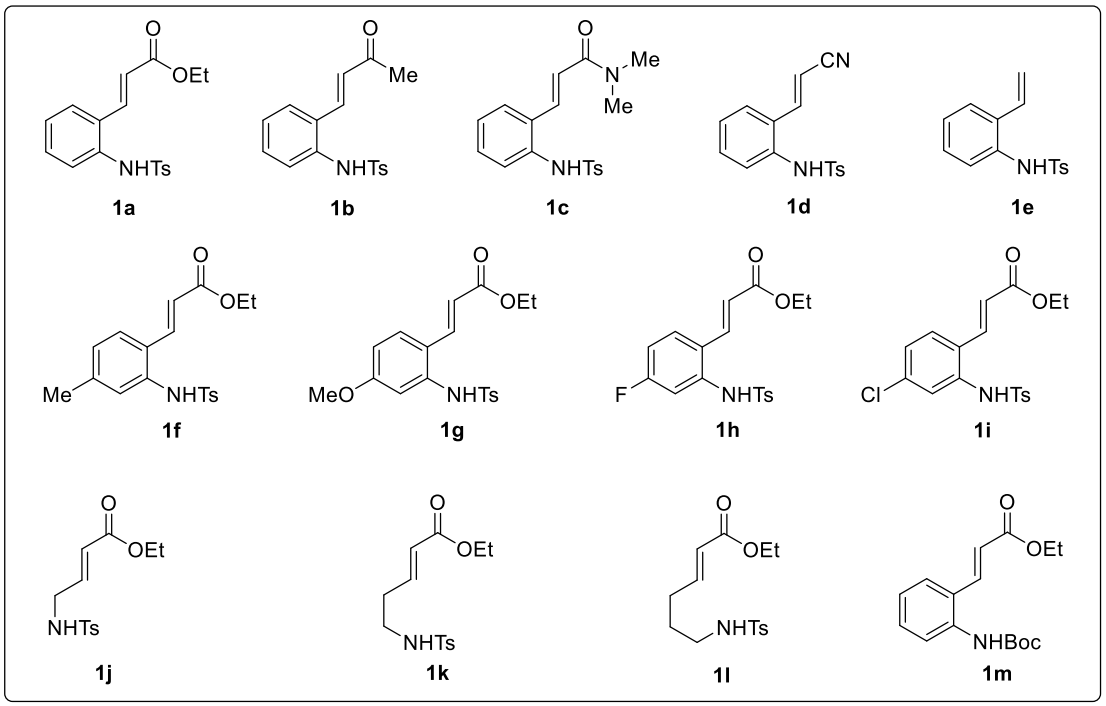
I. General Information

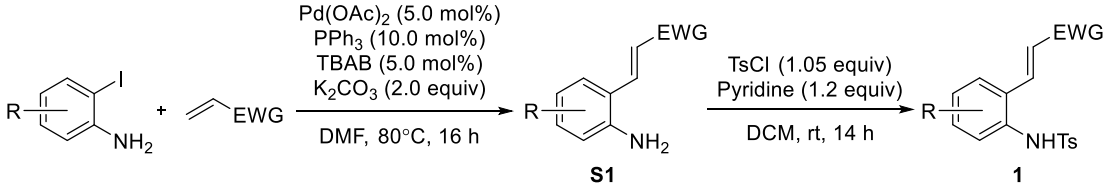
Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co. Lit., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous toluene, acetonitrile, dichloromethane, chloroform, methanol, and tetrahydrofuran were purified by the Innovative® solvent purification system. Other anhydrous solvents were purchased from J&K Scientific. ^{1}H, ^{13}C, and ^{19}F NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, acetone-d_6 at 2.05 ppm; ^{13}C NMR: $CDCl_3$ at 77.0 ppm, acetone-d_6 at 29.8 ppm). HRMS spectra were performed on a Waters mass spectrometer. The X-ray data was collected by SuperNova, Dual, Cu at zero, Atlas diffractometer.

II. Preparation of Substrates 1

Vinyl amines **1a-1m,** as shown below, were synthesized according to the following procedures.



General Procedure A: Preparation of *o*-tosylamidocinnamic acid derivatives (1a-1d, 1f-1i)[1].



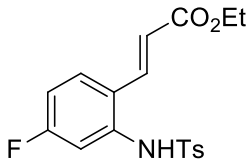
***o*-Vinyl anilines (S1)**: Under N_2 at room temperature, to an oven dried round bottom flask was charged with substituted *ortho*-iodoanilines (10.0 mmol, 1.0 equiv.), olefins (20.0 mmol, 2.0 equiv.), K_2CO_3 (2.8 g, 20.0 mmol, 2.0 equiv.), $Pd(OAc)_2$ (112.0 mg, 0.5 mmol, 5.0 mol%), PPh_3 (262.0 mg, 1.0 mmol, 10 mol%) and tetrabutylammonium bromide (TBAB) (161.0 mg, 0.5 mmol, 5.0 mol%) followed by the addition of DMF (40.0 mL). The mixture was allowed

[1] B. Harish, S. Yadav and S. Suresh, *Chem. Commun*., 2021, **57**, 231-234.

to stir at 80 °C for 12 h, and then diluted with EtOAc (50.0 mL), washed with water (20.0 × 3 mL), brine (40.0 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 3:1) to afford the *ortho*-aminocinnamic acid derivatives **S1**.

***o*-Tosylamidocinnamic acid derivatives (1):** Under air at room temperature, to a stirred solution of *ortho*-aminocinnamic acid derivatives **S1** (1.0 mmol, 1.0 equiv.) in dry DCM (8.0 mL) was added dry pyridine (0.1 mL, 1.2 mmol, 1.2 equiv.) followed by *p*-toluenesulfonyl chloride (200.0 mg, 1.1 mmol, 1.1 equiv.). The reaction mixture was stirred at room temperature for 14 h, and then dry MeOH (5.0 mL) was added. The mixture was concentrated under reduced pressure, and the residue was partitioned between EtOAc (20.0 mL) and 2 N HCl (20.0 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (20.0 × 3 mL). The combined organic layers were washed with saturated aqueous $NaHCO_3$ (20.0 mL), brine (20.0 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to afford the desired *o*-tosylamidocinnamic acid derivatives **1**.

Characterization data for new compounds.



1h

(*E*)-Ethyl-3-(4-fluoro-2-(4-methylphenylsulfonamido)phenyl)acrylate (1h) was prepared according to the General Procedure A as a white solid (chromatography eluent: Dichloromethane/EtOAc = 5:1) in 62% yield (670.0 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, J = 8.34 Hz, 2H), 7.50-7.36 (m, 2H), 7.28-7.19 (m, 3H), 7.14 (s, 1H), 6.90 (td, J_1 = 2.52 Hz, J_2 = 8.16 Hz, 1H), 6.09 (d, J

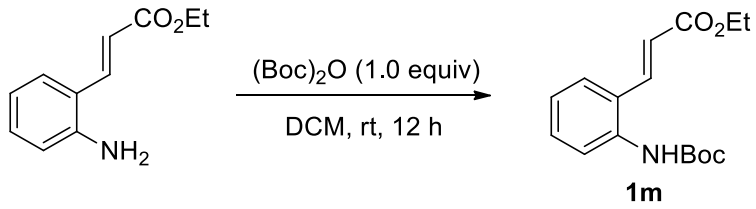
= 15.69 Hz, 1H), 4.24 (q, *J* = 7.14 Hz, 2H), 2.37 (s, 3H), 1.33 (t, *J* = 7.11 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.57, 164.47 (d, *J* = 249.75 Hz), 144.17, 137.96, 136.58 (d, *J* = 10.5 Hz), 135.66, 129.74, 128.66 (d, *J* = 9.0 Hz), 127.16, 125.45 (d, *J* = 3.0 Hz), 120.42 (d, *J* = 1.5 Hz), 114.03 (d, *J* = 21.75 Hz), 113.29 (d, *J* = 24.0 Hz), 60.91, 21.46, 14.19 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -107.58 ppm.

HRMS (CI^+) calculated for $C_{18}H_{19}FNO_4S$ $[M + H]^+$: 364.1019, found: 364.1018.

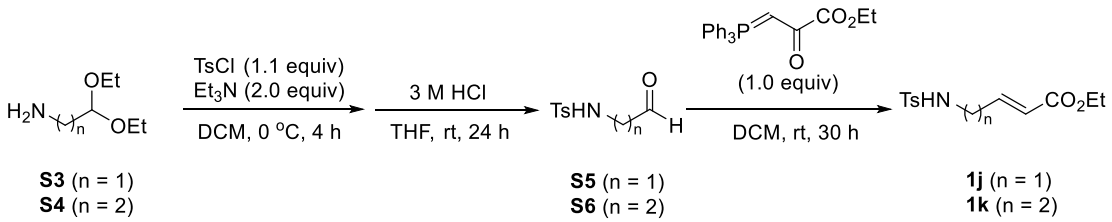
Preparation of ethyl (*E*)-3-(2-((*tert*-butoxycarbonyl)amino)phenyl)acrylate 1m.



1m

Ethyl (*E*)-3-(2-((*tert*-butoxycarbonyl)amino)phenyl)acrylate (1m): Under N_2 at room temperature, to an oven dried 100-mL Schlenk flask was charged with a solution of (*E*)-ethyl 3-(2-aminophenyl)acrylate (573.0 mg, 3.0 mmol, 1.0 equiv.) in DCM (20.0 mL) followed by the addition of $(Boc)_2O$ (655.0 mg, 3.0 mmol, 1.0 equiv.). The reaction mixture was stirred for 12 h at room temperature. The mixture was diluted with DCM (30.0 mL), washed with saturated aqueous $NaHCO_3$ (20.0 mL), water (20.0 × 3 mL), brine (40.0 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to afford **1m** in 86% yield (755.0 mg).

Preparation of 4-tosylamino-enoic ester derivatives (1j-1k)[2].



S3 (n = 1)
S4 (n = 2)

S5 (n = 1)
S6 (n = 2)

1j (n = 1)
1k (n = 2)

4-Methyl-*N*-(2-oxoethyl)benzenesulfonamide (S5): At 0 °C, to a stirred solution of 2,2-diethoxyethan-1-amine **S3** (0.7 mL, 5.0 mmol, 1.0 equiv.) and anhydrous Et_3N (1.4 mL, 10.0 mmol, 2.0 equiv.) in DCM (10.0 mL) was added dropwise a solution of *p*-toluenesulfonyl chloride (1.1 g, 5.5 mmol, 1.1 equiv.) in DCM (10.0 mL) over 0.5 h. Then the reaction mixture was stirred at 0 °C for another 12 h. The mixture was diluted with DCM (30.0 mL), washed with 1 M aq. HCl (50.0 mL), water (10.0 mL), and saturated aq. $NaHCO_3$ (100.0 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 4:1) to afforded the *N*-(2,2-diethoxyethyl)-4-methylbenzenesulfonamide as a white solid. The resulted solid was directly dissolved in THF (10.0 mL) followed by the addition of 3 M HCl (15.0 mL). Then the reaction mixture was stirred at room temperature for 24 h. The reaction mixture was diluted with EtOAc (50.0 mL), washed with brine (50.0 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to afford **S5** in >99% yield (1.1 g) which was used without further purification.

Ethyl (E)-4-((4-methylphenyl)sulfonamido)but-2-enoate (1j): At room temperature, to a solution of **S5** (639 mg, 3.0 mmol, 1.0 equiv.) in DCM (20.0 mL) was added Wittig reagent (1.13 g, 3.0 mmol, 1.0 equiv.). The solution was stirred at room temperature for 30 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 3:1) to afford **1j** as a brown solid in 31% yield (263.0 mg).

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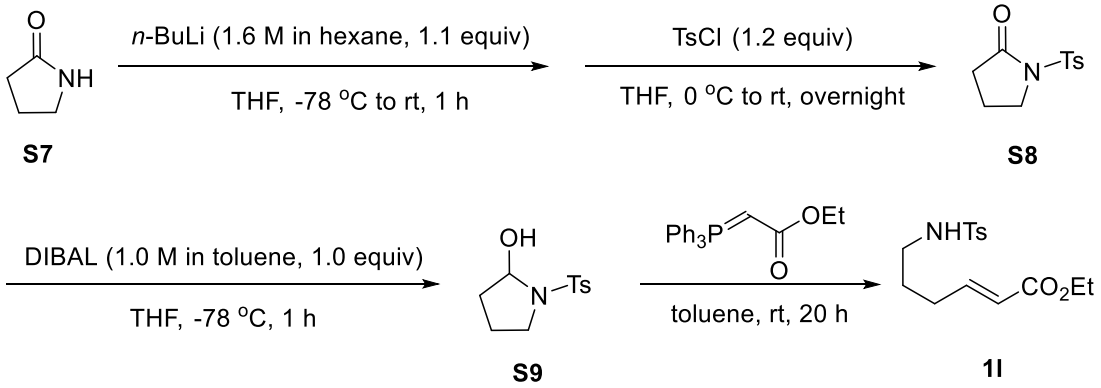
[2] B.-L. Zhao and D.-M. Du, *Asian J. Org. Chem.*, 2015, **4**, 1120-1126.

Compounds **1k** was prepared according to the above procedure.

Preparation of 4-tosylamino-2- enoic ester derivatives (1l)[3].



***N-p*-Tosylpyrrolidone (S8)**: Under N_2 at -78 °C, to an oven dried 200-mL flask was charged with 2-pyrrolidone (2.3 mL, 30.0 mmol, 1.0 equiv.) and anhydrous THF (120.0 mL) followed by dropwise addition of *n*-BuLi (1.6 M in hexanes, 13.8 mL, 33.0 mmol, 1.1 equiv.) over 10 min. The mixture was then stirred at -78 °C for 1 h then a solution of *p*-toluenesulfonyl chloride (6.8 g, 36.0 mmol, 1.2 equiv.) in THF (30.0 mL) was added dropwise over 20 min. The reaction was kept stirring at -78 °C for another 20 min and then warmed up to room temperature. After 12 h, the reaction was quenched by slowly adding saturated aqueous solution of NH_4Cl (30.0 mL) and extracted with EtOAc (100.0 × 3 mL). The combined organic layers were washed with brine (100 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by recrystallization from *n*-hexane to yield *N-p*-tosylpyrrolidone **S8** as a white solid in 70% yield (5.0 g).

Hemiaminal (**S9)**: Under N_2 at -78 °C, to a stirred solution of **S6** (2.4 g, 10.0 mmol, 1.0 equiv.) in THF (20.0 mL) was added DIBAL (1.0 M solution in toluene, 10.0 mL, 10.0 mmol, 1.0 equiv.). The resulting mixture was stirred at -78 °C for 1 h. The reaction mixture was quenched with MeOH and added a

[3] (a) W. L. Jia, N. Westerveld and K. M. Wong, *Org. Lett*., 2019, **21**, 9339-9342. (b) T. Azuma, A. Murata and Y. Kobayashi, *Org. Lett*., 2014, **16**, 4256-4259.

saturated solution of potassium sodium tartrate (30 mL). The organic layer was separated and the aqueous layer was extracted with DCM (30.0 × 3 mL). The combined organic layers were washed with brine (50 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to give the crude hemiaminal **S9** in 89% yield (2.2 g) which was used for the next step without further purification.

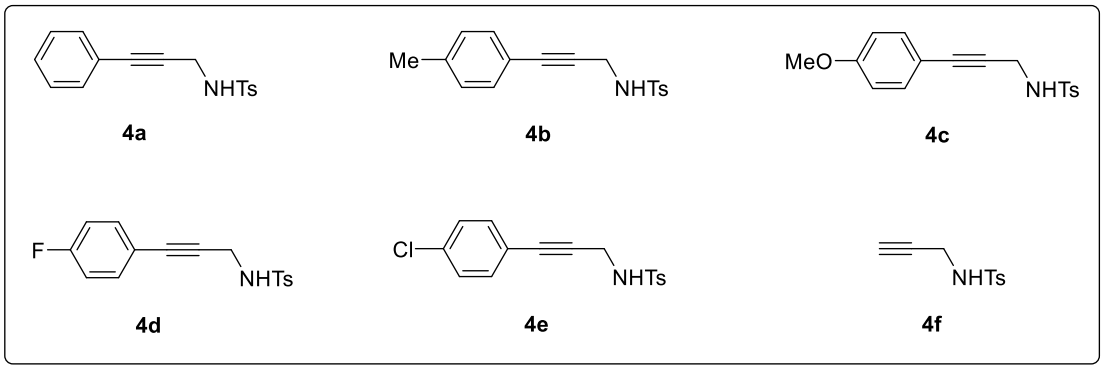
4-tosylamino-2- enoic ester derivatives (1l): At room temperature, to a stirred solution of crude hemiaminal **S9** (724.0 mg, 3.0 mmol, 1.0 equiv.) in toluene (25.0 mL) was added Wittig reagent (2.1 g, 6.0 mmol, 2.0 equiv.). The solution was stirred at room temperature for 30 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 7:1) to afford **1j** as a colorless oil in 97.0% yield (907.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.24 Hz, 2H), 7.29 (d, *J* = 8.16 Hz, 2H), 6.87-6.76 (m, 1H), 5.73 (d, *J* = 15.68 Hz, 1H), 4.97 (s, 1H), 4.15 (q, *J* = 7.18 Hz, 2H), 3.00-2.87 (m, 2H), 2.41 (s, 3H), 2.22-2.14 (m, 2H), 1.66-1.55 (m, 2H), 1.26 (t, *J* = 7.12 Hz, 3H) ppm.

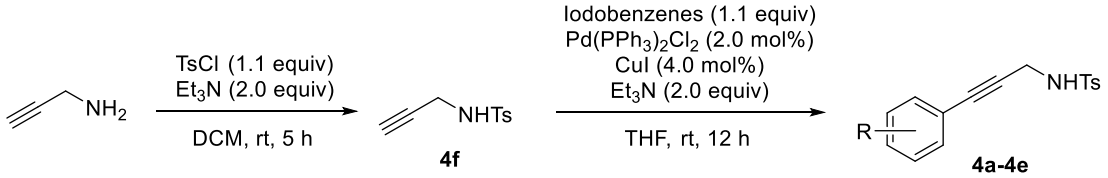
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.40, 147.29, 143.44, 136.79, 129.70, 127.00, 122.08, 60.23, 42.40, 28.93, 27.92, 21.45, 14.18 ppm.

HRMS (CI^+) calculated for $C_{15}H_{22}NO_4S$ $[M + H]^+$: 312.1270, found: 312.1282.

Alkynyl amines **4a-4f,** as shown below, were synthesized according to the following procedure.



General Procedure B: Preparation of the 3-substituted propargyl amines (4a-4f)[4].



4-Methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide (4f): Under N_2 at 0 °C, to a stirred solution of commercially available propargylamine (2.0 mL, 30.0 mmol, 1.0 equiv.) in DCM (60.0 mL) was added triethylamine (4.2 mL, 45.0 mmol, 1.5 equiv.), followed by tosyl chloride (6.2 g, 33.0 mmol, 1.1 equiv.) portionwise. The resulting mixture was stirred at room temperature for 5 h. The reaction mixture was quenched with water (30.0 mL) and extracted with DCM (30.0 × 3 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to afford the quantitatively pure **4f** (5.9 g, 95%) as a white solid which was further purified by recrystallization from ether.

4-Methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (4a): under N_2 at room temperature, to an oven dried 50-mL flask was charged with phenyl iodides (0.7 mL, 6.0 mmol, 1.2 equiv.), $PdCl_2(PPh_3)_2$ (70.2 mg, 0.1 mmol, 2.0 mol%), CuI (38.0 mg, 0.2 mmol, 4.0 mol%.), Et_3N (1.4 mL, 10.0 mmol, 2.0 equiv.) and dry THF (30.0 mL)followed by the addition of **4f** (1.05 g, 5.0 mmol, 1.0 equiv.). The resulting reaction mixture was stirred at room temperature for 12 h. The mixture was quenched with saturated aqueous solution of NH_4Cl (30.0 mL) and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (30.0 × 3 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum

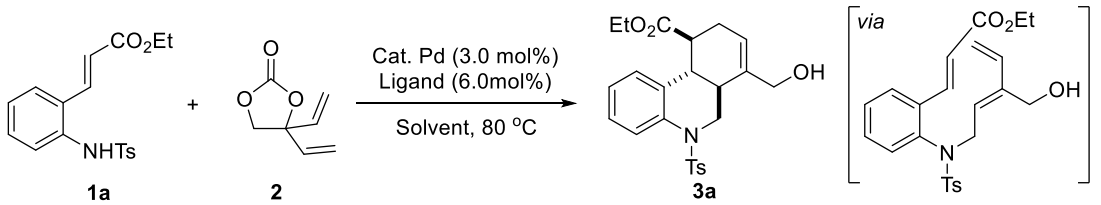
[4] (a) C. Chen, Y. Huang and Z. Zhang, *Chem. Commun.*, 2017, **53**, 4612-4615. (b) F. Bodinier, Y. Sanogo, J. Ardisson, *Chem. Commun.*, 2021, **57**, 3603-3606.

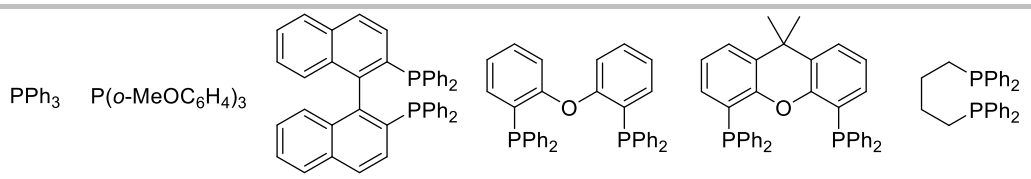
ether/EtOAc = 10:1) to give the desired product **4a** as white solid in 73% yield (1.1 g).

Compounds **4b-4e** was prepared according to the General Procedure B.

III. The Optimization of Reaction Conditions

Table S1. The optimization of reaction conditions[a]



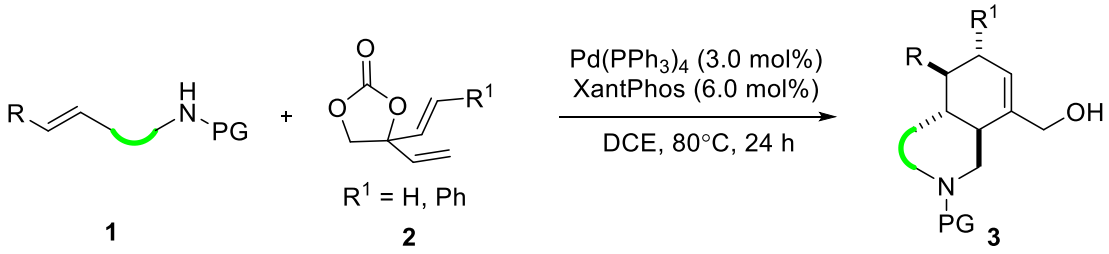


entry	solvent	Cat. Pd	ligand	Yield[b]
1	Toluene	$Pd(PPh_3)_4$	**L1**	61%
2	PhCl	$Pd(PPh_3)_4$	**L1**	81%
3	MeCN	$Pd(PPh_3)_4$	**L1**	50%
4	1,4-Dioxane	$Pd(PPh_3)_4$	**L1**	80%
5	THF	$Pd(PPh_3)_4$	**L1**	82%
6	EA	$Pd(PPh_3)_4$	**L1**	81%
7	DCE	$Pd(PPh_3)_4$	**L1**	84%
8	DCE	$Pd(PPh_3)_4$	**L2**	87%
9	DCE	$Pd(PPh_3)_4$	**L3**	69%
10	DCE	$Pd(PPh_3)_4$	**L4**	88%
11	DCE	$Pd(PPh_3)_4$	**L5**	91%
12	DCE	$Pd(PPh_3)_4$	**L6**	88%
13	DCE	$PdCl_2$	**L5**	trace
14	DCE	$Pd(OAc)_2$	**L5**	<10%
15	DCE	$Pd_2(dba)_3$	**L5**	62%
16	DCE	$Pd(TFA)_2$	**L5**	trace

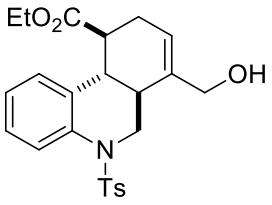
[a] Reaction conditions: **1a** (0.3 mmol), **2** (0.45 mmol), Cat. Pd (0.009 mmol, 3.0 mol%) and Ligand (0.018 mmol, 6.0 mol%) in Solvent (3.0 mL) at 80 °C for 24 h. [b] Determined by ^1H NMR using CH_2Br_2 as an internal standard.

IV. Synthesis of Hydrophenanthridine and Hydrogenated Isoquinoline Derivatives

General Procedure C:



Under N_2, to a solution of vinyl amines **1** (0.3 mmol, 1.0 equiv.) and divinyl-dioxolanones **2** (0.45 mmol, 1.5 equiv.) in DCE (3.0 mL) was added $Pd(PPh_3)_4$ (10.5 mg, 9.0×10^{-3} mmol, 3.0 mol%) and Xantphos (10.4 mg, 1.8×10^{-2} mmol, 6.0 mol%). The reaction mixture was stirred at 80 °C for 24 h. The reaction mixture was concentrated under reduced pressure, then the residue was directly purified by silica gel column chromatography (eluent: petroleum ether/EtOAc) to afford the desired product **3**.



3a

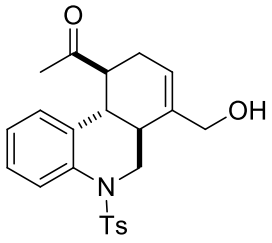
Ethyl 7- (hydroxymethyl)-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophen anthridine-10-carboxylate (3a) was prepared according to the General Procedure C as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 80% yield (106.0 mg, *dr* > 20:1).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (dd, J_1 = 8.07 Hz, J_2 = 1.08 Hz, 1H), 7.46 (d, J = 8.31 Hz, 2H), 7.28-7.25 (m, 1H), 7.21 (d, J = 8.13 Hz, 2H), 7.10 (td, J_1 = 7.62 Hz, J_2 = 1.14 Hz, 1H), 6.91 (d, J = 7.68 Hz, 1H), 5.75 (d, J = 5.79 Hz, 1H), 4.15-4.01 (m,

5H), 3.42 (t, J = 12.18 Hz, 1H), 2.62 (td, J_1 = 11.49 Hz, J_2 = 5.22 Hz, 1H), 2.49-2.34 (m, 4H), 2.28-2.13 (m, 1H), 2.07-1.86 (m, 2H), 1.18 (t, J = 7.11 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.03, 143.56, 137.11, 136.01, 135.79, 135.38, 129.57, 126.95, 126.80, 126.54, 125.54, 122.41, 122.08, 64.14, 60.53, 50.35, 40.72, 40.52, 38.85, 28.88, 21.46, 14.03 ppm.

HRMS (CI^+) calculated for $C_{24}H_{28}NO_5S$ $[M + H]^+$: 442.1688, found: 442.1689.



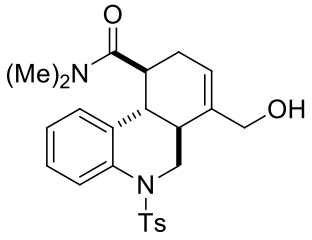
3b

1- (7- (Hydroxymethyl)-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthridin-10-yl) ethanone (3b) was prepared according to the General Procedure C as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 82% yield (100.9 mg, dr > 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 7.96 Hz, 1H), 7.41 (d, J = 8.16 Hz, 2H), 7.29-7.15 (m, 3H), 7.08 (t, J = 7.44 Hz, 1H), 6.65 (d, J = 7.6 Hz, 1H), 5.74 (d, J = 5.04 Hz, 1H), 4.12-3.97 (m, 3H), 3.45 (t, J = 11.84 Hz, 1H), 2.69 (td, J_1 = 11.64 Hz, J_2 = 5.28 Hz, 1H), 2.40-2.23 (m, 4H), 2.23-2.11 (m, 1H), 1.97-1.84 (m, 5H), 1.84-1.73 (m, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 210.99, 143.75, 137.11, 136.28, 135.77, 135.33, 129.61(2C), 127.22, 126.85, 125.92, 122.89, 121.85, 64.14, 50.51, 48.11, 41.03, 38.90, 28.04, 26.34, 21.40 ppm.

HRMS (CI^+) calculated for $C_{23}H_{26}NO_4S$ $[M + H]^+$: 412.1583, found: 412.1582.



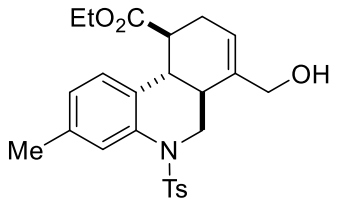
3c

7-(Hydroxymethyl)-*N*, *N*-dimethyl-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthridine-10-carboxamide (3c) was prepared according to the General Procedure C as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 74% yield (97.5 mg, *dr* > 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dd, J_1 = 8.08 Hz, J_2 = 0.92 Hz, 1H), 7.17 (d, *J* = 8.28 Hz, 2H), 6.99 (d, *J* = 8.04 Hz, 2H), 6.89-6.83 (m, 1H), 6.73 (td, J_1 = 1.00 Hz, J_2 = 7.60 Hz, 1H), 6.43 (d, *J* = 7.68 Hz, 1H), 5.80 (d, *J* = 5.38 Hz, 1H), 3.79-3.69 (m, 2H), 3.68-3.59 (m, 1H), 3.54 (t, *J* = 5.52 Hz, 1H), 3.06 (t, *J* = 12.04 Hz, 1H), 2.91 (s, 3H), 2.67-2.518 (m, 4H), 2.55 (s, 3H), 1.92-1.81 (m, 1H), 1.75-1.68 (m, 2H), 1.58-1.43 (m, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.32, 144.38, 138.70, 137.56, 137.06, 136.85, 130.44, 127.56, 126.78, 125.93, 125.63, 123.97, 122.30, 64.05, 51.20, 41.39, 40.33, 37.02, 35.36, 28.70, 21.27 ppm.

HRMS (CI^+) calculated for $C_{24}H_{29}N_2O_4S$ $[M + H]^+$: 441.1848, found: 441.1849.



3d

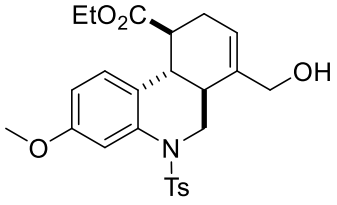
Ethyl-7-(hydroxymethyl)-3-methyl-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthri- dine-10-carboxylate（**3d**）was prepared according to the General Procedure C as a Colorless solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 86% yield (117.1 mg, *dr* > 20:1).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.45 (d, *J* = 8.28 Hz, 2H), 7.20 (d, *J* =

8.01 Hz, 2H), 6.90 (d, *J* = 7.86 Hz, 1H), 6.77 (d, *J* = 7.83 Hz, 1H), 5.72 (d, *J* = 5.67 Hz, 1H), 4.15-3.96 (m, 5H), 3.38 (t, *J* = 12.60 Hz, 1H), 2.45-2.34 (m, 4H), 2.33 (s, 3H), 2.24-2.08 (m, 1H), 2.04-1.79 (m, 2H), 1.74 (s, 1H), 1.17 (t, *J* = 7.11 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.09, 143.50, 136.77, 136.09, 135.64, 135.47, 134.14, 129.55, 127.26, 126.87, 126.28, 122.17, 122.09, 64.21, 60.51, 50.36, 40.86, 40.68, 38.61, 28.93, 21.48, 21.14, 14.06 ppm.

HRMS (CI^+) calculated for $C_{25}H_{30}NO_5S$ $[M + H]^+$: 456.1845, found: 456.1845.



3e

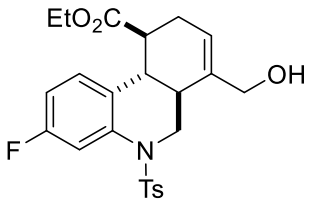
Ethyl-7-(hydroxymethyl)-3-methoxy-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthridine-10-carboxylate (3e) was prepared according to the General Procedure C as a colorless solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 87% yield (122.5 mg, *dr* = 10:1).

Major diastereomer

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.25 Hz, 2H), 7.31 (d, *J* = 2.58 Hz, 1H), 7.18 (d, *J* = 8.16 Hz, 2H), 6.77 (d, *J* = 8.52 Hz, 1H), 6.62 (dd, J_1 = 8.52 Hz, J_2 = 2.52 Hz, 1H), 5.70 (d, *J* = 3.24 Hz, 1H), 4.16-3.97 (m, 5H), 3.77 (s, 3H), 3.36 (t, *J* = 11.79 Hz, 1H), 2.54 (td, J_1 = 11.40 Hz, J_2 = 6.00 Hz, 1H), 2.43-2.29 (m, 4H), 2.21-2.06 (m, 2H), 2.03-1.77 (m, 2H), 1.15 (t, *J* = 7.11 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.17, 158.34, 143.61, 136.67, 135.95, 135.37, 129.57, 129.08, 126.87, 122.96, 122.18, 111.97, 111.27, 64.19, 60.54, 55.38, 50.44, 40.77, 40.72, 38.36, 28.92, 21.47, 14.04 ppm.

HRMS (CI^+) calculated for $C_{25}H_{30}NO_6S$ $[M + H]^+$: 472.1794, found: 472.1801.



3f

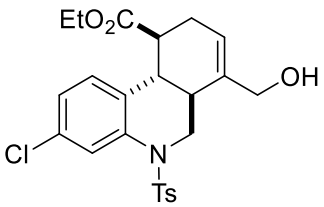
Ethyl-3-fluoro-7- (hydroxymethyl)-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthri- dine-10-carboxylate (3f) was prepared according to the General Procedure C as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 80% yield (109.7 mg, *dr* > 20:1).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55-7.45 (m, 3H), 7.22 (d, *J* = 5.07 Hz, 2H), 6.88-6.74 (m, 2H), 5.75 (d, *J* = 5.67 Hz, 1H), 4.18-3.98 (m, 5H), 3.39 (t, *J* = 12.15 Hz, 1H), 2.60 (td, J_1 = 11.46 Hz, J_2 = 5.28 Hz, 1H), 2.50-2.32 (m, 4H), 2.28-2.11 (m, 1H), 2.09-1.87 (m, 2H), 1.17 (t, *J* = 7.11 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.95, 161.29 (d, *J* = 242.75 Hz), 143.93, 137.15 (d, *J* = 10.81 Hz), 135.73, 135.24, 132.42 (d, *J* = 3.21 Hz), 129.71, 126.87, 123.35 (d, *J* = 9.18 Hz), 122.47, 113.56 (d, *J* = 25.11 Hz), 111.96 (d, *J* = 21.25 Hz), 64.27, 60.69, 50.42, 40.61, 40.48, 38.61, 28.85, 21.50, 14.04 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -114.39 ppm.

HRMS (CI^+) calculated for $C_{24}H_{27}FNO_5S$ $[M + H]^+$: 460.1594, found: 460.1594.



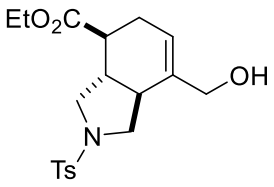
3g

Ethyl-3-chloro-7-(hydroxymethyl)-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthri- dine-10-carboxylate (3g) was prepared according to the General Procedure D as a yellow solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 86% yield (122.9 mg, *dr* = 19:1).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, *J* = 2.10 Hz, 1H), 7.48 (d, *J* = 8.31 Hz, 2H), 7.22 (d, *J* = 7.98 Hz, 2H), 7.06 (dd, J_1 = 8.28 Hz, J_2 =2.13 Hz, 1H), 6.81 (dd, J_1 = 8.28 Hz, J_2 = 0.72 Hz, 1H), 5.74 (d, *J* = 5.67 Hz, 1H), 4.17-3.97 (m, 5H), 3.39 (dd, J_1 = 12.18 Hz, J_2 = 11.28 Hz, 1H), 2.59 (td, J_1 = 11.43 Hz, J_2 = 5.25 Hz, 1H), 2.49-2.33 (m, 4H), 2.25-2.10 (m, 1H), 2.07-1.83 (m, 2H), 1.17 (t, *J* = 7.11 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.81, 143.95, 137.04, 135.74, 135.36, 135.20, 132.42, 129.73, 126.88, 126.27, 125.42, 123.47, 122.44, 64.25, 60.70, 50.38, 40.49, 40.45, 38.70, 28.81, 21.51, 14.05 ppm.

HRMS (CI^+) calculated for $C_{24}H_{27}ClNO_5S$ $[M + H]^+$: 476.1298, found: 476.1300.



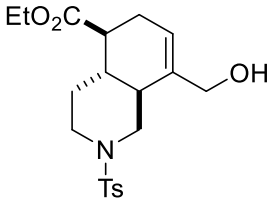
3h

Ethyl-7-(hydroxymethyl)-2-tosyl-2, 3, 3a, 4, 5, 7a-hexahydro-1*H*-isoindole-4–carboxylate (3h) was prepared according to the General Procedure C as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 59% yield (65.7 mg, *dr* > 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.12 Hz, 2H), 7.29 (d, *J* = 8.08 Hz, 2H), 5.57 (s, 1H), 4.16-4.09 (m, 2H), 4.01-3.93 (m, 2H), 3.80 (dd, J_1 = 8.96 Hz, J_2 = 6.96 Hz, 1H), 3.65 (dd, J_1 = 9.56 Hz, J_2 = 7.08 Hz, 1H), 3.09-2.90 (m, 2H), 2.48-2.37 (m, 5H), 2.33-2.21 (m, 2H), 1.93-1.75 (m, 2H), 1.24 (t, *J* = 7.12 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.68, 143.37, 135.94, 134.45, 129.72, 127.15, 123.07, 64.63, 60.78, 50.89, 50.03, 43.49, 42.99, 42.23, 29.16, 21.45, 14.15 ppm.

HRMS (CI^+) calculated for $C_{19}H_{26}NO_5S$ $[M + H]^+$: 380.1532, found: 380.1530.



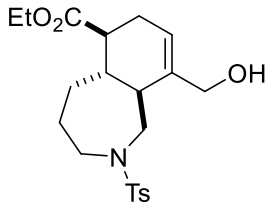
3i

Ethyl-8- (hydroxymethyl)-2-tosyl-1, 2, 3, 4, 4a, 5, 6, 8a-octahydroisoquinoline- 5-carboxylate (3i) was prepared according to the General Procedure C as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 85% yield (100.2 mg, *dr* > 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.20 Hz, 2H), 7.29 (d, *J* = 8.00 Hz, 2H), 5.70 (s, 1H), 4.21-4.03 (m, 4H), 4.00 (d, *J* = 12.64 Hz, 1H), 3.84 (d, *J* = 11.72 Hz, 1H), 2.40 (s, 3H), 2.37-2.18 (m, 5H), 2.08 (s, 1H), 2.01 (t, *J* = 11.28 Hz, 1H), 1.70-1.60 (m, 1H), 1.49-1.30 (m, 2H), 1.22 (t, *J* = 7.12 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.91, 143.49, 135.67, 133.01, 129.59, 127.53, 124.09, 64.09, 60.40, 48.87, 46.24, 44.55, 40.17, 40.10, 28.74, 28.69, 21.43, 14.18 ppm.

HRMS (CI^+) calculated for $C_{20}H_{28}NO_5S$ $[M + H]^+$: 394.1688, found: 394.1692.



3j

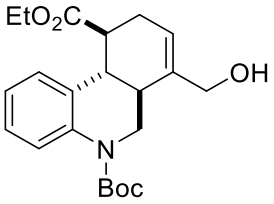
Ethyl 9-(hydroxymethyl)-2-tosyl-2,3,4,5,5a,6,7,9a-octahydro-1*H*-benzo[*c*] azepine-6-carboxylate (3j) was prepared according to the General Procedure C at 125 °C as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 16% yield (17.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.20 Hz, 2H), 7.29 (d, *J* = 8.08 Hz, 2H), 5.78 (d, *J* = 5.40 Hz, 1H), 4.22-4.10 (m, 3H), 4.01 (d, *J* = 12.80 Hz, 1H), 3.87 (dd, J_1 = 13.40 Hz, J_2 = 3.96 Hz, 1H), 3.40-3.21(m, 2H), 2.78 (dd, J_1 = 13.36 Hz, J_2 =

10.56 Hz, 1H), 2.41 (s, 3H), 2.33-2.27 (m, 1H), 2.27-2.17 (m, 2H), 1.99-1.76 (m, 3H), 1.76-1.63 (m, 3H) 1.26 (t, *J* = 7.12 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.71, 143.16, 137.34, 136.33, 129.70, 126.87, 124.42, 65.04, 60.39, 50.58, 46.80, 46.76, 44.39, 41.46, 32.18, 28.97, 27.63, 21.47, 14.25 ppm.

HRMS (CI^+) calculated for $C_{21}H_{30}NO_5S$ $[M + H]^+$: 408.1845, found: 408.1838.



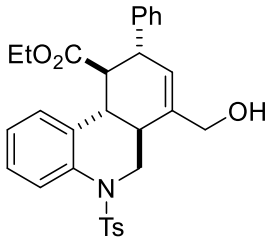
3k

5-*tert*-Butyl 10-ethyl 7- (hydroxymethyl)-6, 6a, 10, 10a-tetrahydrophenanthridine-5, 10 (9*H*)-dicarboxylate (3k) was prepared according to the General Procedure C as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 84% yield (98.0 mg, *dr* > 20:1).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.23-7.10 (m, 1H), 6.99 (d, *J* = 4.17 Hz, 2H), 5.82 (d, *J* = 5.61 Hz, 1H), 4.34-4.00 (m, 4H), 3.84 (dd, J_1 = 11.34 Hz, J_2 = 6.93 Hz, 1H), 3.48 (t, *J* = 12.24 Hz, 1H), 2.93-2.74 (m, 2H), 2.63-2.49 (m, 1H), 2.41-2.10 (m, 2H), 1.80 (s, 1H), 1.51 (s, 9H), 1.28 (t, *J* = 7.11 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.89, 154.02, 137.38, 136.70, 135.15, 126.16, 124.56, 123.56, 121.96, 121.73, 80.95, 64.33, 60.86, 49.18, 40.76, 39.80, 39.37, 29.17, 28.33, 14.12 ppm.

HRMS (CI^+) calculated for $C_{22}H_{30}NO_5$ $[M + H]^+$: 388.2124, found: 388.2124.



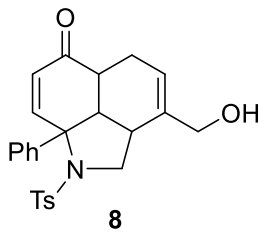
3l

Ethyl (6a, 9, 10, 10a)-7-(hydroxymethyl)-9-phenyl-5-tosyl-5,6,6a,9,10,10a-hexahydrophenanthridine-10-carboxylate (3l) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 88% yield (136.6 mg, *dr* > 20:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.52 Hz, 1H), 7.42 (d, *J* = 8.20 Hz, 2H), 7.25-7.05 (m, 7H), 6.80 (d, *J* = 7.16 Hz, 2H), 6.72 (d, *J* = 7.68 Hz, 1H), 5.79 (d, *J* = 4.40 Hz, 1H), 4.26-4.10 (m, 3H), 3.92-3.86 (m, 1H), 3.74-3.64 (m, 1H), 3.62-3.47 (m, 2H), 3.01 (dd, J_1 = 12.44 Hz, J_2 = 6.44 Hz, 2H), 2.31-2.19 (m, 4H), 2.06 (t, *J* = 11.80 Hz, 1H), 0.72 (t, *J* = 7.16 Hz, 3H) ppm.

^{13}C NMR(100 MHz, $CDCl_3$) δ 172.67, 143.23, 138.77, 137.71, 136.38, 135.66, 135.37, 129.58, 129.18, 128.00, 127.12, 126.90, 126.87, 126.74, 125.59, 124.96, 122.44, 64.33, 60.03, 50.53, 46.05, 43.15, 40.83, 34.22, 21.51, 13.50 ppm.

HRMS (CI^+) calculated for $C_{30}H_{32}NO_5S$ $[M + H]^+$: 518.2001, found: 518.2010 .



8

3-(Hydroxymethyl)-8a-phenyl-1-tosyl-2,2a,2a^1,5,5a,8a-hexahydrobenzo[*cd*]indol-6(1*H*)-one (8) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 2:1) in 52% yield (67.7 mg, *dr* = 6.3:1).

Major diastereomer

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61 (dd, J_1 = 10.44 Hz, J_2 = 2.32 Hz, 1H), 7.39 (d, *J* = 8.20 Hz, 2H), 7.32-7.22 (m, 5H), 7.18 (d, *J* = 8.12 Hz, 2H), 6.16 (d, *J* = 10.44 Hz, 1H), 5.55(d, *J* = 2.44 Hz, 1H), 4.19 (dd, J_1 = 8.60 Hz, J_2 = 6.88 Hz, 1H), 4.00 (s, 2H), 3.45 (dd, J_1 = 11.36 Hz, J_2 = 8.80 Hz, 1H), 3.00 (d, *J* = 19.28 Hz, 1H), 2.85-2.72 (m, 1H), 2.66-2.54 (m, 2H), 2.40 (s, 3H), 2.10-1.96 (m,1H), 1.83-1.62 (m,

1H) ppm.

^{13}C NMR (300 MHz, $CDCl_3$) δ 197.53, 147.94, 143.11, 140.40, 137.42, 135.53, 129.33, 128.43, 127.92, 127.63, 126.95, 126.30, 124.35, 69.87, 65.05, 56.05, 51.98, 39.26, 37.79, 23.47, 21.44 ppm.

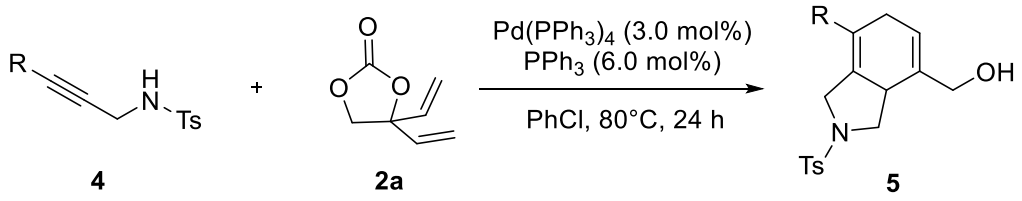
Minor diastereomer

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.20 Hz, 2H), 7.47-7.36 (m, 5H), 7.32-7.22 (m, 4H), 6.20 (d, *J* = 10.36 Hz, 1H), 5.67 (d, *J* = 5.04 Hz, 1H), 4.25 (t, *J* = 9.16 Hz, 1H), 3.92 (s, 2H), 3.28 (t, *J* = 9.80 Hz, 1H), 2.85-2.72 (m, 1H), 2.54-2.48 (m, 1H), 2.40 (s, 3H), 2.10-1.96 (m, 2H), 1.83-1.62 (m, 1H) ppm.

^{13}C NMR (300 MHz, $CDCl_3$) δ 199.23, 146.29, 143.67, 143.59, 136.39, 136.21, 129.51, 129.20, 128.64, 127.81, 126.99, 126.07, 123.20, 70.38, 66.13, 54.66, 54.49, 39.81, 34.87, 23.59, 21.49 ppm.

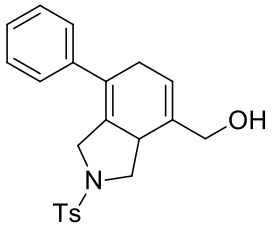
HRMS (CI^+) calculated for $C_{25}H_{26}NO_4S$ $[M + H]^+$: 436.1583, found: 436.1580.

General Procedure D:



4 **2a** **5**

Under N_2, to a solution of propynyl-*p*-toluenesulfonamide derivatives **4** (0.30 mmol, 1.0 equiv.) and divinyl-dioxolanone **2a** (0.45 mmol, 1.5 equiv.) in PhCl (3.0 mL) was added $Pd(PPh_3)_4$ (10.5 mg, 9.0×10^{-3} mmol, 3.0 mol%) and PPh_3 (4.6 mg, 1.8×10^{-2} mmol, 6.0 mol%). The reaction mixture was stirred at 80 °C for 24 h. The reaction mixture was concentrated under reduced pressure, then the residue was directly purified by silica gel column chromatography (eluent: petroleum ether/EtOAc) to afford the desired product **5**.



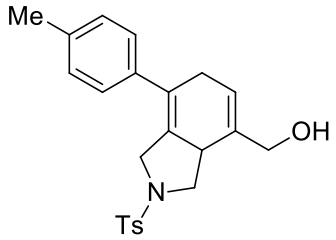
5a

(7-Phenyl-2-tosyl-2, 3, 3a, 6-tetrahydro-1*H*-isoindol-4-yl)methanol (5a) was prepared according to the General Procedure D as a colourless solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 83% yield (95.5 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.12 Hz, 2H), 7.38-7.21 (m, 5H), 7.10 (d, *J* = 7.08 Hz, 2H), 5.83 (s, 1H), 4.15 (d, *J* = 14.00 Hz, 1H), 4.09 (s, 2H), 3.99 (t, *J* = 8.32 Hz, 1H), 3.68 (d, *J* = 13.76 Hz, 1H), 3.37-3.23 (m, 1H), 3.19-3.05 (m, 1H), 3.00-2.86 (m, 1H), 2.77 (dd, J_1 = 11.08 Hz, J_2 = 9.08 Hz, 1H), 2.39 (s, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 143.38, 139.64, 134.07, 133.70, 130.24, 129.63, 129.34, 128.30, 127.45, 127.30, 127.22, 122.47, 65.04, 51.31, 49.64, 40.37, 32.12, 21.39 ppm.

HRMS (CI^+) calculated for $C_{22}H_{24}NO_3S$ $[M + H]^+$: 382.1477, found: 382.1469.



5b

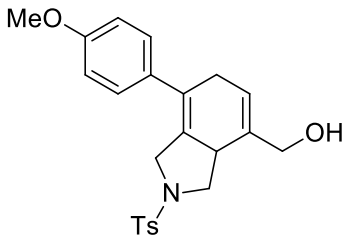
(7-(*p*-Tolyl)-2-tosyl-2, 3, 3a, 6-tetrahydro-1*H*-isoindol-4-yl)methanol (5b) was prepared according to the General Procedure D as a colourless solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 95% yield (112.2 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.25 Hz, 2H), 7.25 (d, *J* = 7.95 Hz, 2H), 7.13 (d, *J* = 7.89 Hz, 2H), 6.99 (d, *J* = 8.10 Hz, 2H), 5.81 (s, 1H), 4.16 (dt, J_1 = 3.80 Hz, J_2 = 1.41 Hz, 1H), 4.08 (s, 2H), 3.99 (dd, J_1 = 8.76 Hz, J_2 =7.71 Hz, 1H), 3.69

(d, J = 13.77 Hz, 1H), 3.38-3.20 (m, 1H), 3.19-3.03 (m, 1H), 2.97-2.81 (m, 1H), 2.76 (dd, J_1 = 11.25 Hz, J_2 = 8.91 Hz, 1H), 2.38 (s, 3H), 2.35 (s, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 143.32, 137.20, 136.65, 134.10, 133.78, 129.73, 129.61, 129.15, 128.96, 127.31, 127.10, 122.51, 65.06, 51.27, 49.71, 40.40, 32.10, 21.39, 21.05 ppm.

HRMS (CI^+) calculated for $C_{23}H_{26}NO_3S$ $[M + H]^+$: 396.1633, found: 396.1631.



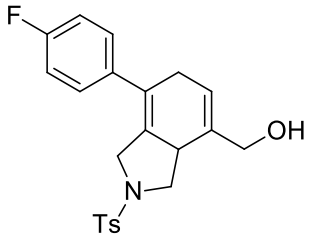
5c

(7-(4-Methoxyphenyl)-2-tosyl-2, 3, 3a, 6-tetrahydro-1*H*-isoindol-4-yl)methanol (5c) was prepared according to the General Procedure D as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 96% yield (117.9 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, J = 8.25 Hz, 2H), 7.29 (d, J = 8.04 Hz, 2H), 7.08 (d, J = 8.73 Hz, 2H), 6.91 (d, J = 8.76 Hz, 2H), 5.86 (s, 1H), 4.21 (dt, J_1 = 13.77 Hz, J_2 = 1.38 Hz, 1H), 4.13 (s, 2H), 4.03 (dd, J_1 = 8.67 Hz, J_2 = 7.77 Hz, 1H), 3.86 (s, 3H), 3.73 (d, J = 13.68 Hz, 1H), 3.43-3.25 (m, 1H), 3.23-3.07 (m, 1H), 3.02-2.85 (m, 1H), 2.79 (dd, J_1 = 11.22 Hz, J_2 = 8.88 Hz, 1H), 2.43 (s, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 158.84, 143.36, 134.16, 133.86, 131.94, 129.65, 129.36, 128.79, 128.43, 127.36, 122.62, 113.68, 65.20, 55.23, 51.29, 49.79, 40.47, 32.11, 21.44 ppm.

HRMS (CI^+) calculated for $C_{23}H_{26}NO_4S$ $[M + H]^+$: 412.1583, found: 412.1578.



5d

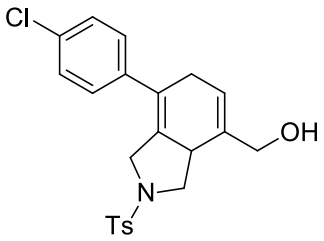
(7-(4-Fluorophenyl)-2-tosyl-2, 3, 3a, 6-tetrahydro-1*H*-isoindol-4-yl)methanol (5d) was prepared according to the General Procedure D as a white solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 86% yield (102.3 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.25 Hz, 2H), 7.26 (d, *J* = 7.98 Hz, 2H), 7.10-6.95 (m, 4H), 5.81 (s, 1H), 4.17-4.05 (m, 3H), 3.99 (t, *J* = 8.76 Hz, 1H), 3.62 (d, *J* = 13.74 Hz, 1H), 3.38-3.20 (m, 1H), 3.18-2.68 (m, 3H), 2.39 (s, 3H), 1.89 (s, 1H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.95 (d, *J* = 245.25 Hz), 143.49, 135.63 (d, *J* = 3.75 Hz), 134.13, 133.69, 130.58, 129.68, 128.93 (d, *J* = 8.25 Hz), 128.43, 127.35, 122.43, 115.28 (d, *J* = 21.0 Hz), 65.10, 51.29, 49.58, 40.43, 32.29, 21.44 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -114.17 ppm.

HRMS (CI^+) calculated for $C_{22}H_{23}FNO_3S$ $[M + H]^+$: 400.1383, found: 400.1376.



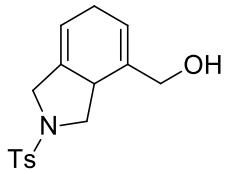
5e

(7-(4-Chlorophenyl)-2-tosyl-2, 3, 3a, 6-tetrahydro-1*H*-isoindol-4- yl)methanol (5e) was prepared according to the General Procedure D as a yellow solid, (chromatography eluent: petroleum ether/EtOAc = 3:1) in 90% yield (112.0 mg).

^{1}H NMR (300 MHz, acetone-d_6) δ 7.66 (d, *J* = 8.10 Hz, 2H), 7.38 (t, *J* = 8.16 Hz, 4H), 7.24 (d, *J* = 8.40 Hz, 2H), 5.78, (s, 1H), 4.21 (d, *J* = 13.95 Hz, 1H), 4.14-3.88 (m, 4H), 3.60 (d, *J* = 13.95 Hz, 1H), 3.39-3.05 (m, 2H), 2.98-2.85 (m, 2H), 2.39 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 144.14, 139.33, 135.74, 134.67, 133.29, 132.23, 130.31, 129.73, 129.03, 128.70, 128.07, 121.27, 64.69, 52.05, 50.12, 41.04, 32.20, 21.11 ppm.

HRMS (CI$^+$) calculated for $C_{22}H_{23}ClNO_3S$ [M + H]$^+$: 416.1087, found: 416.1082.



5f

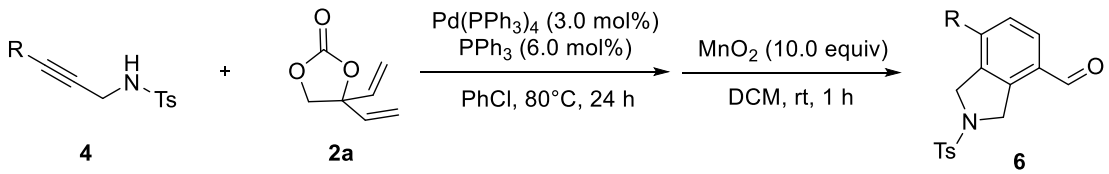
(2-Tosyl-2, 3, 3a, 6-tetrahydro-1*H*-isoindol-4-yl)methanol (5f) was prepared according to the General Procedure D as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 76% yield (69.6 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.82 (d, *J* = 8.20 Hz, 2H), 7.50 (d, *J* = 8.04 Hz, 2H), 5.75 (s, 1H), 5.67 (s, 1H), 4.17-4.00 (m, 4H), 3.95 (t, *J* = 5.52 Hz, 1H), 3.81 (d, *J* = 13.32 Hz, 1H), 3.18-3.07 (m, 1H), 2.80 (dd, J_1 = 11.16 Hz, J_2 = 9.20 Hz, 1H), 2.76-2.68 (m, 2H), 2.49 (s, 3H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 144.12, 136.04, 135.70, 134.62, 130.32, 128.17, 121.38, 117.45, 64.96, 52.80, 50.89, 39.25, 27.60, 21.15 ppm.

HRMS (CI$^+$) calculated for $C_{16}H_{20}NO_3S$ [M + H]$^+$: 306.1164, found: 306.1163.

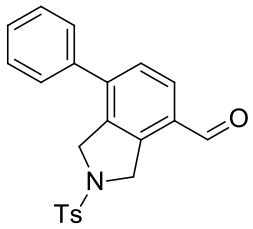
General Procedure E：



4 **2a** **6**

Under N_2, to a solution of propynyl-*p*-toluenesulfonamide derivatives **4** (0.30 mmol, 1.0 equiv.) and divinyl-dioxolanone **2a** (0.45 mmol, 1.5 equiv.) in

PhCl (3.0 mL) was added $Pd(PPh_3)_4$ (10.5 mg, 9.0×10^{-3} mmol, 3.0 mol%) and PPh_3 (4.6 mg, 1.8×10^{-2} mmol, 6.0 mol%). The reaction mixture was stirred at 80 °C for 24 h. The reaction mixture was evaporated under pressure, the residue was dissolved in DCM (5.0 mL) followed by the addition of MnO_2 (261 mg, 3.0 mmol, 10.0 equiv). The resulting reaction mixture was stirred at room temperature for another 1 h before it was filtered through a pad of Celite rinsing with DCM. The filtrate was concentrated under reduced pressure and purified by silica gel column chromatography (eluent: petroleum ether/EtOAc) to afford the desired product **6**.



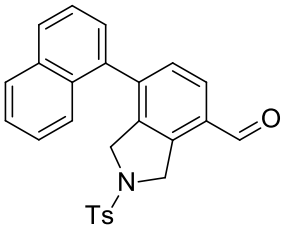
6a

7-Phenyl-2-tosylisoindoline-4-carbaldehyde (6a) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 76% yield (86.4 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.77 (d, *J* = 7.84 Hz, 2H), 7.53-7.40 (m, 4H), 7.39-7.27 (m, 4H) 4.97 (s, 2H), 4.65 (s, 2H), 2.39 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.57, 143.71, 142.79, 138.29, 137.87, 136.08, 133.50, 132.97, 129.86, 129.82, 128.91, 128.88, 128.61, 127.82, 127.55, 54.20, 52.58, 21.45 ppm.

HRMS (CI^+) calculated for $C_{22}H_{20}NO_3S$ $[M + H]^+$: 378.1164, found: 378.1162.



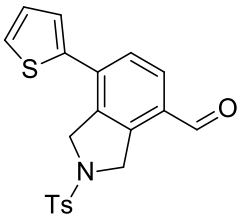
6b

7-(Naphthalen-1-yl)-2-tosylisoindoline-4-carbaldehyde (6b) was prepared according to the General Procedure E as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 37% yield (48.1 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.10 (s, 1H), 7.95 (d, *J* = 8.22 Hz, 2H), 7.84 (d, *J* = 7.68 Hz, 1H), 7.68 (d, *J* = 8.22 Hz, 2H), 7.58-7.50 (m, 2H), 7.49-7.23 (m, 6H), 5.12-4.95 (m, 2H), 4.41-4.22 (m, 2H), 2.40 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.65, 143.65, 141.78, 137.94, 137.42, 135.86, 133.62, 133.53, 132.63, 130.34, 130.25, 129.78 (2C), 129.01, 128.66, 127.54, 126.72, 126.30, 126.10, 125.28, 124.85, 54.55, 52.49, 21.47 ppm.

HRMS (CI^+) calculated for $C_{26}H_{22}NO_3S$ $[M + H]^+$: 428.1320, found: 428.1313.



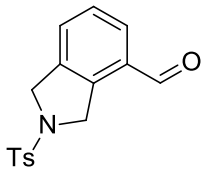
6c

7-(Thiophen-2-yl)-2-tosylisoindoline-4-carbaldehyde (6c) was prepared according to the General Procedure E as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 26% yield (30.0 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.81 (d, *J* = 8.19 Hz, 2H), 7.69 (q, *J* = 7.98 Hz, 2H), 7.48 (d, *J* = 5.04 Hz, 1H), 7.35-7.26 (m, 3H), 7.17 (dd, J_1 = 4.98 Hz, J_2 = 3.81 Hz, 1H), 4.97 (s, 2H), 4.83 (s, 2H), 2.39 (s, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 191.16, 143.79, 140.13, 138.65, 135.04, 134.62, 133.63, 132.91, 129.90, 129.52, 128.38, 127.71, 127.58, 127.36, 127.10, 54.11, 53.46, 21.49 ppm.

HRMS (CI^+) calculated for $C_{20}H_{18}NO_3S_2$ $[M + H]^+$: 384.0728, found: 384.0728.



6d

2-Tosylisoindoline-4-carbaldehyde (6d) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 3:1) in 53% yield (48.1 mg).

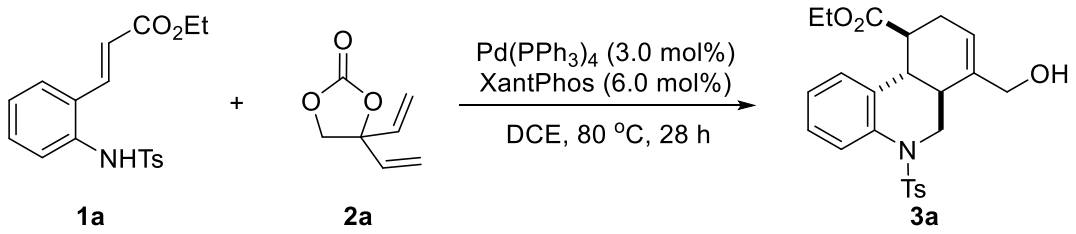
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.77 (d, *J* = 8.08 Hz, 2H), 7.69 (d, *J* = 7.20 Hz, 1H), 7.50-7.40 (m, 2H), 7.30 (d, *J* = 8.08 Hz, 2H), 4.90 (s, 2H), 4.62 (s, 2H), 2.38 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.89, 143.69, 138.07, 136.85, 133.48, 132.30, 131.18, 129.78, 128.49, 127.96, 127.49, 54.08, 52.60, 21.41 ppm.

HRMS (CI^+) calculated for $C_{16}H_{16}NO_3S$ $[M + H]^+$: 302.0851, found: 302.0850.

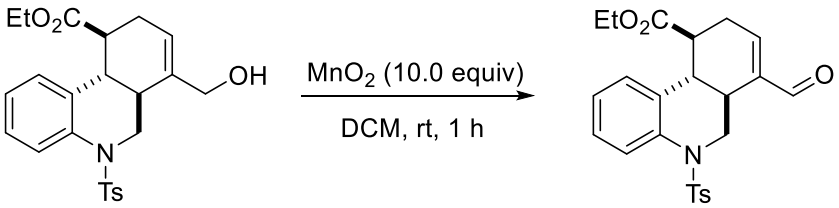
IV. Synthetic Transformation of Hydrophenanthridines

Scale-up reaction



1a **2a** **3a**

Under N_2, to a solution of ethyl (*E*)-3-(2-((4-methylphenyl)sulfonamido)-phenyl)-acrylate **1a** (933.3 mg, 2.7 mmol, 1.0 equiv.) and 4,4-divinyl-1,3-dioxolan-2-one **2a** (550.8 mg, 4.05 mmol, 1.5 equiv.) in DCE (27.0 mL) was added $Pd(PPh_3)_4$ (93.6 mg, 0.08 mmol, 3.0 mol%) and XantPhos (94.5 mg, 0.16 mmol, 6.0 mol%). The reaction mixture was stirred at 80 °C for 28 h. The reaction mixture was concentrated under reduced pressure, then the residue was directly purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 3:1) to afford the desired product **3a** in 89% yield (1.05 g).



3a **9**

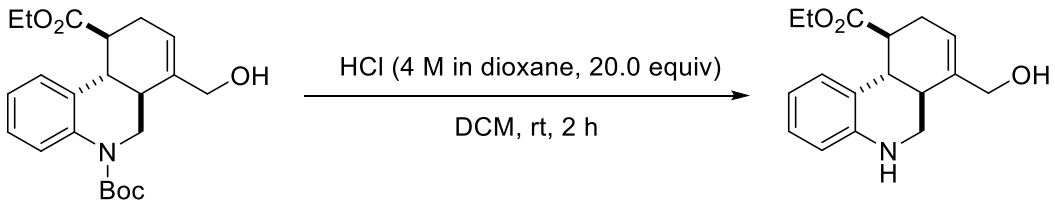
Ethyl-7-formyl-5-tosyl-5, 6, 6a, 9, 10, 10a- hexahydrophenanthridine-10-carboxylate (9)： Under air at room temperature, to a solution of hydrophenanthridine product **3a** (66.1 mg, 0.15 mmol) in DCM (2.0 mL) was added MnO_2 (130.4 mg, 1.5 mmol, 10.0 equiv). The reaction mixture was stirred at room temperature for 1 h before it was filtered through a pad of Celite rinsing with DCM. The filtrate was concentrated under reduced pressure, then the residue was purified by silica gel column chromatography

(eluent: petroleum ether/EtOAc = 3:1) to afford the desired product **9** as a colourless solid in 88% yield (57.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 7.70 (d, *J* = 8.04 Hz, 1H), 7.51 (d, *J* = 8.08 Hz, 2H), 7.31-7.21 (m, 3H), 7.13 (t, *J* = 7.60 Hz, 1H), 6.95 (d, *J* = 7.64 Hz, 1H), 6.87 (d, *J* = 5.76 Hz, 1H), 4.45 (dd, J_1 =11.64 Hz, J_2 = 7.12 Hz, 1H), 4.21-4.12 (m, 2H), 3.35 (t, *J* = 11.60 Hz, 1H), 2.82-2.63 (m, 2H), 2.41 (s, 3H), 2.38-2.26 (m, 2H), 2.03 (t, *J* = 11.08 Hz, 1H), 1.22 (td, J_1 = 7.04 Hz, J_2 = 0.56 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 192.30, 174.07, 148.50, 143.54, 141.19, 136.27, 136.19, 136.05, 129.65, 127.29, 126.85, 126.55, 125.65, 122.25, 60.95, 49.77, 39.89, 39.21, 38.54, 30.35, 21.49, 14.06 ppm.

HRMS (CI^+) calculated for $C_{24}H_{26}NO_5S$ $[M + H]^+$: 440.1532, found: 440.1534.



3m **10**

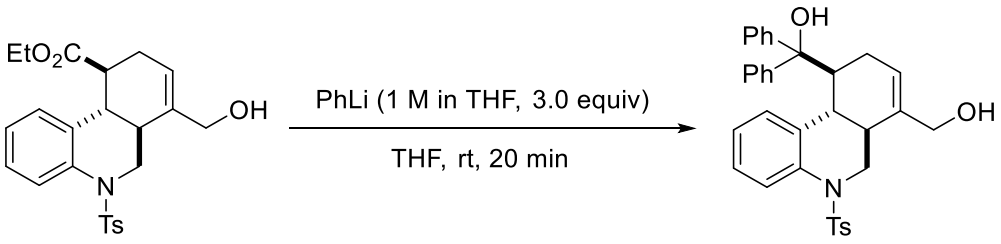
Ethyl-7- (hydroxymethyl)-5, 6, 6a, 9, 10, 10a- hexahydrophenanthridine-10-carboxylate (10) : Under air at room temperature, to a solution of hydrophenanthridine product **3m** (58.1 mg, 0.15 mmol) in DCM (2.0 mL) was added HCl (0.75 mL, 4.0 M in dioxane). The reaction mixture was stirred at room temperature for 2 hour. The reaction mixture was concentrated under reduced pressure, then the residue was directly purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 3:1) to afford the desired product **10** as a colourless solid in 73% yield (41.9 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 6.99 (t, *J* = 7.50 Hz, 1H), 6.86 (d, *J* = 7.65 Hz, 1H), 6.57 (t, *J* = 7.41 Hz, 1H), 6.47 (d, *J* = 7.86 Hz, 1H), 5.83 (d, *J* = 5.37 Hz, 1H), 4.34-3.98 (m, 4H), 3.76 (dd, J_1 = 10.35 Hz, J_2 = 5.10 Hz, 1H), 3.12 (t, *J* = 11.85 Hz,

1H), 3.01 (t, *J* = 11.19 Hz, 1H), 2.86-2.73 (m, 1H), 2.65-2.48 (m, 1H), 2.43-2.25 (m, 2H), 1.29 (t, *J* = 7.14 Hz, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 176.70, 144.35, 136.76, 127.15, 124.58, 123.67, 122.69, 116.31, 113.06, 64.76, 60.79, 46.38, 41.63, 39.67, 35.96, 29.67, 14.08 ppm.

HRMS (CI^+) calculated for $C_{17}H_{22}NO_3$ $[M + H]^+$: 288.1600, found: 288.1607.



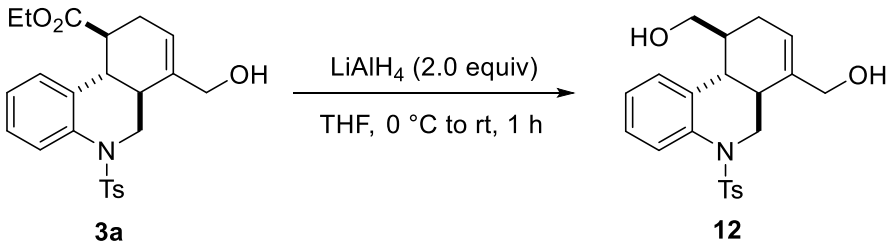
3a **11**

(7-(Hydroxymethyl)-5-tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthridin-10-yl)diphenylmethanol (11): Under N_2 at 0 °C, to a solution of hydrophenanthridine product **3a** (66.1 mg, 0.15 mmol) in THF (2.0 mL) was added PhLi (0.45 mL, 1 M in THF) dropwise. The reaction mixture was stirred at room temperature for 2 h. The reaction mixture was quenched by aq. NH_4Cl (5.0 mL) and extracted with ethyl acetate (5.0 × 3 mL). The combined organic layers were washed with water (10.0 mL), brine (10.0 mL), dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 3:1) to afford the desired product **11** as a white solid in 62% yield (51.7 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (dd, J_1 = 8.00 Hz, J_2 = 1.04 Hz, 1H), 7.45-7.36 (m, 3H), 7.28-7.11 (m, 12H), 7.00 (d, *J* = 8.08 Hz, 2H), 5.65 (t, *J* = 3.40 Hz, 1H), 4.11 (q, *J* = 5.84 Hz, 1H), 3.94 (q, *J* = 12.56 Hz, 2H), 3.83-3.72 (m, 2H), 2.36-2.25 (m, 5H), 2.20 (s, 1H), 2.13-2.02 (m, 1H), 1.98-1.87 (m, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 146.57, 146.20, 143.26, 139.27, 137.27, 136.27, 135.74, 129.43, 128.05, 127.86, 127.25, 127.10, 126.89, 126.84, 126.75, 126.70, 126.62, 126.00, 124.82, 123.80, 82.00, 63.52, 48.19, 41.21, 40.42, 39.39, 25.36, 21.56 ppm.

HRMS (CI$^+$) calculated for $C_{34}H_{34}NO_4S$ [M + H]$^+$: 552.2209, found:. 552.2207.



(5-Tosyl-5, 6, 6a, 9, 10, 10a-hexahydrophenanthridine -7, 10-diyl)dimethanol (12): Under N_2 at 0 °C, to a solution of hydrophenanthridine product **3a** (66.1 mg, 0.15 mmol) in THF (2.0 mL), was added $LiAlH_4$ (11.4 mg, 0.3mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for 1 h. The reaction mixture was quenched by aq. NH_4Cl (5.0mL) and extracted with ethyl acetate (5.0 × 3 mL). The combined organic layers were washed with water (10.0 mL), brine (10.0 mL), dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (chromatography eluent: petroleum ether/EtOAc = 1:1) to afford the desired product **12** as a white solid in 53% yield (31.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.88 Hz, 1H), 7.43 (d, *J* = 8.08 Hz, 2H), 7.31-7.24 (m, 1H), 7.23-7.12 (m, 4H), 5.75 (d, *J* = 4.12 Hz, 1H), 4.13-3.90 (m, 3H), 3.85 (d, *J* = 10.84 Hz, 1H), 3.45 (t, *J* = 11.76 Hz, 1H), 3.21 (dd, J_1 = 10.96 Hz, J_2 = 6.84 Hz, 1H), 2.48-2.30 (m, 4H), 2.18-1.94 (m, 2H), 1.87-1.20 (m, 4H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.63, 138.75, 136.46, 135.82, 135.21, 129.37, 27.93, 126.96 (2C), 126.05, 123.74, 122.76, 65.81, 64.85, 50.89, 42.43, 37.80, 33.80, 28.00, 21.47 ppm.

HRMS (CI$^+$) calculated for $C_{22}H_{26}NO_4S$ [M + H]$^+$: 400.1583, found: 400.1585.

V. Determination of Product Structure

The absolute stereochemistry of product **3a** was determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2191161). The data can be obtained free of charge via the internet at https://www.ccdc.cam.ac.uk/structures/. The measurements were taken in a Bruker D8 Venture CCD diffractometer. The data were integrated by Bruker D8 Venture with \f and \w scans absorption corrections. The structure solution and refinement were processed by ShelXL (Sheldrick, 2015). The stereochemistry of other products was assumed by analogy.

Method of crystallization: A solution of **3a** in EA and petroleum ether was evaporated the solvent slowly at room temperature.

Crystal data and structure for 3a

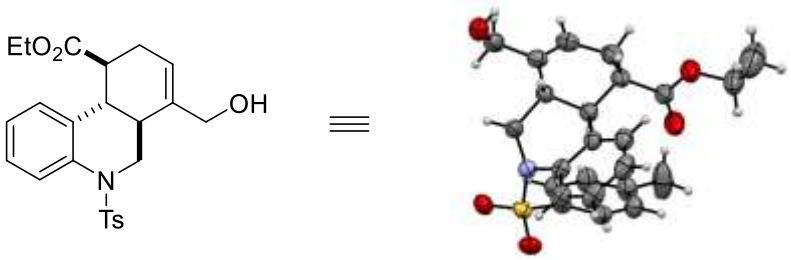


Table S1 Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{24}H_{27}NO_5S$
Formula weight	441.52
Temperature/K	193.00
Crystal system	monoclinic
Space group	Pc

a/Å	8.3476(14)
b/Å	12.016(2)
c/Å	11.2069(19)
α/°	90
β/°	96.481(6)
γ/°	90
Volume/Å^3	1116.9(3)
Z	2
ϱ_{calc}g/cm^3	1.313
μ/mm^{-1}	1.031
F(000)	468.0
Crystal size/mm^3	0.12 × 0.1 × 0.1
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	9.276 to 121.19
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 15, -14 ≤ l ≤ 14
Reflections collected	39835
Independent reflections	5028 [R_{int} = 0.0505, R_{sigma} = 0.0282]
Data/restraints/parameters	5028/3/294
Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ (I)]	R_1 = 0.0375, wR_2 = 0.0986
Final R indexes [all data]	R_1 = 0.0398, wR_2 = 0.1006
Largest diff. peak/hole / e Å^{-3}	0.17/-0.37
Flack parameter	0.062(7)

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for A. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	1811.8(6)	5815.0(5)	4630.1(5)	40.01(15)
O1	1543(2)	4741.7(15)	5138.7(16)	47.3(4)
O2	662(2)	6248.1(17)	3710.6(17)	48.9(4)
O3	8375(3)	3596.6(16)	5098(2)	59.7(5)
N1	3553(3)	5721.3(16)	4084.5(18)	38.6(4)
O5	8631(3)	9425.7(19)	5145(3)	69.4(7)
C5	2113(3)	6800(2)	5784(2)	39.9(5)
O4	6278(3)	9293.5(19)	5915(3)	80.0(9)
C13	5324(3)	7288(2)	3796(2)	42.1(5)
C4	2127(3)	7923(2)	5477(2)	42.4(5)
C8	4014(3)	6626(2)	3361(2)	39.8(5)
C14	6139(3)	6987(2)	5020(2)	43.5(5)
C12	5800(4)	8126(2)	3055(3)	51.9(6)
C11	4952(4)	8329(2)	1942(3)	57.9(7)
C10	3633(4)	7685(3)	1545(2)	55.5(7)
C6	2475(4)	6474(2)	6970(2)	47.3(6)
C15	6476(3)	5724.6(19)	4955(2)	39.4(5)
C9	3167(4)	6813(2)	2240(2)	47.4(6)
C20	8229(4)	7221(3)	6760(3)	57.2(7)
C19	8306(3)	5972(3)	6836(3)	52.6(6)
C17	7547(3)	5293(2)	6032(2)	45.1(5)
C21	7670(3)	7618(2)	5472(3)	48.8(6)
C16	4853(3)	5115(2)	4852(3)	45.7(5)
C3	2545(4)	8704(2)	6354(2)	47.5(6)
C22	7415(4)	8862(3)	5529(3)	57.2(7)
C18	7780(4)	4050(2)	6134(3)	52.8(6)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for A. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C2	2922(4)	8390(3)	7545(3)	54.6(7)
C7	2856(4)	7270(2)	7838(2)	55.0(7)
C1	3391(8)	9254(3)	8487(4)	92.5(17)
C23	8578(6)	10634(3)	5264(6)	90.5(15)
C24	9338(8)	10971(5)	6506(9)	93(3)
C24A	9750(30)	11014(14)	4510(20)	125(9)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for A. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	37.0(3)	45.4(3)	36.9(3)	1.7(2)	0.76(18)	-2.8(2)
O1	45.9(10)	46.8(10)	49.2(10)	3.8(8)	4.9(8)	-9.1(8)
O2	41.4(9)	61.6(11)	41.5(9)	1.1(8)	-5.8(7)	2.3(8)
O3	60.0(12)	44.4(10)	74.2(13)	-2.6(10)	5.2(10)	-2.4(9)
N1	40.8(11)	39.0(10)	35.6(9)	3.2(7)	1.9(8)	-0.5(7)
O5	54.2(12)	48.0(10)	109(2)	-6.1(12)	24.4(13)	-4.2(9)
C5	36.3(11)	45.3(12)	38.1(11)	2.2(9)	4.1(9)	-0.6(9)
O4	56.2(13)	51.4(12)	138(3)	-27.1(13)	35.6(15)	-3.9(10)
C13	44.6(12)	37.7(11)	45.7(12)	-0.1(9)	12.1(10)	0.3(9)
C4	42.3(12)	46.8(13)	38.0(11)	5.1(10)	4.5(9)	2.0(10)
C8	48.3(13)	37.4(11)	34.5(11)	-1.0(8)	8.7(9)	2.2(9)
C14	41.6(12)	42.4(12)	47.0(12)	-2.6(10)	7.1(10)	-2.2(10)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for A. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	56.3(16)	43.7(13)	58.5(15)	4.4(11)	18.6(13)	-2.0(11)
C11	78(2)	46.6(14)	53.5(15)	11.9(12)	25.6(14)	7.7(14)
C10	78(2)	52.9(15)	37.2(12)	6.3(11)	14.2(12)	11.4(13)
C6	57.0(15)	46.8(13)	38.0(12)	5.4(10)	4.3(10)	-3.7(11)
C15	36.3(11)	41.0(12)	41.5(11)	0.3(9)	6.6(9)	-2.5(9)
C9	59.9(16)	45.7(13)	36.7(11)	-0.3(10)	5.6(10)	5.7(11)
C20	45.2(14)	61.2(17)	64.1(17)	-15.7(14)	1.9(12)	-0.5(12)
C19	42.3(14)	66.0(17)	48.6(14)	-1.0(12)	1.3(11)	-0.2(12)
C17	37.4(11)	52.4(14)	45.4(12)	6.3(11)	4.4(9)	-0.9(10)
C21	38.8(12)	44.0(13)	65.3(16)	-9.1(12)	13.2(12)	-1.7(10)
C16	40.5(12)	39.9(12)	55.0(13)	9.6(10)	-1.9(10)	-1.1(10)
C3	55.6(15)	42.4(13)	45.3(13)	4.9(10)	8.5(11)	-2.3(11)
C22	45.4(14)	43.8(13)	83(2)	-13.4(14)	10.3(13)	-0.1(11)
C18	45.7(14)	53.3(15)	57.6(15)	13.3(12)	-2.2(12)	-4.4(11)
C2	71.5(19)	50.0(14)	41.5(13)	0.5(11)	2.2(12)	-8.8(13)
C7	74.3(18)	52.5(15)	36.9(12)	5.9(11)	0.7(12)	-4.5(13)
C1	162(5)	58(2)	52.6(18)	-5.4(15)	-12(2)	-27(2)
C23	73(2)	47.8(17)	156(5)	-1(2)	35(3)	-4.6(16)
C24	68(4)	52(3)	158(8)	-27(4)	7(4)	1(2)
C24A	145(17)	73(9)	170(20)	9(10)	66(15)	10(10)

Table S4 Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

Table S4 Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4378(18)	C14	C21	1.523(4)
S1	O2	1.4249(19)	C12	C11	1.385(5)
S1	N1	1.643(2)	C11	C10	1.377(5)
S1	C5	1.751(3)	C10	C9	1.387(4)
O3	C18	1.422(4)	C6	C7	1.375(4)
N1	C8	1.434(3)	C15	C17	1.510(4)
N1	C16	1.495(3)	C15	C16	1.533(3)
O5	C22	1.332(4)	C20	C19	1.504(4)
O5	C23	1.459(4)	C20	C21	1.542(5)
C5	C4	1.392(3)	C19	C17	1.322(4)
C5	C6	1.386(4)	C17	C18	1.509(4)
O4	C22	1.204(4)	C21	C22	1.512(4)
C13	C8	1.394(4)	C3	C2	1.388(4)
C13	C14	1.505(4)	C2	C7	1.388(4)
C13	C12	1.391(4)	C2	C1	1.500(4)
C4	C3	1.376(4)	C23	C24	1.518(10)
C8	C9	1.389(3)	C23	C24A	1.442(17)
C14	C15	1.546(3)			

Table S5 Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	N1	105.69(11)	C7	C6	C5	119.3(3)
O1	S1	C5	109.24(11)	C17	C15	C14	113.2(2)
O2	S1	O1	119.45(12)	C17	C15	C16	109.6(2)
O2	S1	N1	107.92(11)	C16	C15	C14	108.0(2)

Table S5 Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	S1	C5	108.42(12)	C10	C9	C8	118.9(3)
N1	S1	C5	105.19(11)	C19	C20	C21	111.6(2)
C8	N1	S1	117.60(16)	C17	C19	C20	124.3(3)
C8	N1	C16	118.1(2)	C19	C17	C15	121.8(2)
C16	N1	S1	115.73(17)	C19	C17	C18	120.7(3)
C22	O5	C23	116.4(3)	C18	C17	C15	117.4(2)
C4	C5	S1	118.46(19)	C14	C21	C20	108.1(2)
C6	C5	S1	120.9(2)	C22	C21	C14	112.9(2)
C6	C5	C4	120.3(2)	C22	C21	C20	107.2(2)
C8	C13	C14	115.9(2)	N1	C16	C15	112.8(2)
C12	C13	C8	118.0(2)	C4	C3	C2	120.9(3)
C12	C13	C14	126.0(3)	O5	C22	C21	111.9(2)
C3	C4	C5	119.5(2)	O4	C22	O5	123.9(3)
C13	C8	N1	119.0(2)	O4	C22	C21	124.2(3)
C9	C8	N1	119.5(2)	O3	C18	C17	111.8(2)
C9	C8	C13	121.5(2)	C3	C2	C7	118.6(3)
C13	C14	C15	105.0(2)	C3	C2	C1	120.1(3)
C13	C14	C21	117.4(2)	C7	C2	C1	121.3(3)
C21	C14	C15	110.8(2)	C6	C7	C2	121.3(3)
C11	C12	C13	120.9(3)	O5	C23	C24	109.6(4)
C10	C11	C12	120.0(3)	C24A	C23	O5	103.4(8)
C11	C10	C9	120.5(3)				

Table S6 Torsion Angles for 3a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°

Table S6 Torsion Angles for 3a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N1	C8	C13	112.6(2)	C14	C15	C17	C19	-10.0(4)
S1	N1	C8	C9	-68.4(3)	C14	C15	C17	C18	172.5(2)
S1	N1	C16	C15	-134.5(2)	C14	C15	C16	N1	37.6(3)
S1	C5	C4	C3	-172.5(2)	C14	C21	C22	O5	-138.7(3)
S1	C5	C6	C7	173.8(2)	C14	C21	C22	O4	43.8(5)
O1	S1	N1	C8	170.90(17)	C12	C13	C8	N1	176.8(2)
O1	S1	N1	C16	-41.8(2)	C12	C13	C8	C9	-2.1(4)
O1	S1	C5	C4	-169.43(19)	C12	C13	C14	C15	-126.4(3)
O1	S1	C5	C6	16.4(3)	C12	C13	C14	C21	-2.9(4)
O2	S1	N1	C8	42.0(2)	C12	C11	C10	C9	-1.6(4)
O2	S1	N1	C16	-170.65(18)	C11	C10	C9	C8	2.4(4)
O2	S1	C5	C4	-37.7(2)	C6	C5	C4	C3	1.7(4)
O2	S1	C5	C6	148.1(2)	C15	C14	C21	C20	-62.7(3)
N1	S1	C5	C4	77.5(2)	C15	C14	C21	C22	178.9(2)
N1	S1	C5	C6	-96.6(2)	C15	C17	C18	O3	55.9(3)
N1	C8	C9	C10	-179.4(2)	C20	C19	C17	C15	-1.6(4)
C5	S1	N1	C8	-73.57(19)	C20	C19	C17	C18	175.9(3)
C5	S1	N1	C16	73.8(2)	C20	C21	C22	O5	102.3(3)
C5	C4	C3	C2	-1.3(4)	C20	C21	C22	O4	-75.2(4)
C5	C6	C7	C2	-1.6(5)	C19	C20	C21	C14	50.3(3)
C13	C8	C9	C10	-0.5(4)	C19	C20	C21	C22	172.3(2)
C13	C14	C15	C17	170.2(2)	C19	C17	C18	O3	-121.6(3)
C13	C14	C15	C16	-68.4(3)	C17	C15	C16	N1	161.2(2)
C13	C14	C21	C20	176.7(2)	C21	C14	C15	C17	42.6(3)
C13	C14	C21	C22	58.3(3)	C21	C14	C15	C16	164.0(2)

Table S6 Torsion Angles for 3a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C13	C12	C11	C10	-1.1(4)	C21	C20	C19	C17	-19.3(4)
C4	C5	C6	C7	-0.3(4)	C16	N1	C8	C13	-33.9(3)
C4	C3	C2	C7	-0.5(5)	C16	N1	C8	C9	145.1(2)
C4	C3	C2	C1	179.4(4)	C16	C15	C17	C19	-130.6(3)
C8	N1	C16	C15	12.6(3)	C16	C15	C17	C18	51.9(3)
C8	C13	C14	C15	50.7(3)	C3	C2	C7	C6	2.0(5)
C8	C13	C14	C21	174.2(2)	C22	O5	C23	C24	86.3(5)
C8	C13	C12	C11	2.9(4)	C22	O5	C23	C24A	-165.2(12)
C14	C13	C8	N1	-0.6(3)	C1	C2	C7	C6	-177.9(4)
C14	C13	C8	C9	-179.5(2)	C23	O5	C22	O4	2.9(6)
C14	C13	C12	C11	-180.0(3)	C23	O5	C22	C21	-174.6(4)

Table S7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3a.

Atom	*x*	*y*	*z*	U(eq)
H3	9229.67	3925.31	4976.48	90
H4	1850.16	8147.32	4666.89	51
H14	5343.93	7102.17	5611.8	52
H12	6719.37	8564.69	3316.6	62
H11	5279.79	8912.04	1451.29	69
H10	3038.08	7839.53	789.78	67
H6	2461.66	5708.11	7180.78	57
H15	7007.8	5570.87	4215.8	47
H9	2281.75	6351.77	1954.25	57
H20A	9308.4	7533.79	7023.58	69

Table S7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3a.

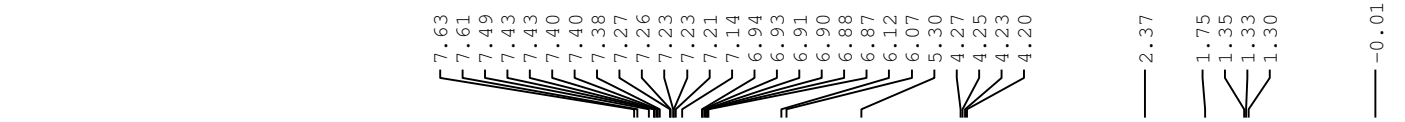
Atom	*x*	*y*	*z*	U(eq)
H20B	7472.42	7501.37	7310.12	69
H19	8940.03	5649.6	7504.42	63
H21	8527.46	7454.05	4941.71	59
H16A	4986.75	4365.9	4508.13	55
H16B	4518.5	5016.62	5664.99	55
H3A	2576.92	9468.12	6142.64	57
H18A	8547.78	3881.14	6849.99	63
H18B	6737.26	3693.75	6244.5	63
H7	3077.37	7048.13	8653.41	66
H1A	4507.3	9127.94	8833.85	139
H1B	2674.81	9202.81	9119.49	139
H1C	3298.33	9995.57	8121.32	139
H23A	7444.87	10892.47	5141.05	109
H23B	9169.24	10985.52	4645.65	109
H23C	7491.61	10925.98	4982.09	109
H23D	8873.82	10865.12	6107.98	109
H24A	8819.88	10562.21	7115.02	139
H24B	9193.52	11771.89	6616.8	139
H24C	10491.71	10795.03	6587.86	139
H24D	10832.42	10782.56	4854.44	188
H24E	9711.39	11826.97	4448.95	188
H24F	9515.82	10689.05	3704.7	188

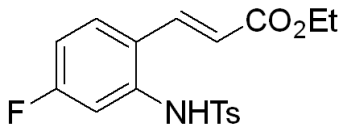
Table S8 Atomic Occupancy for 3a.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
H23A	0.668(16)	H23B	0.668(16)	H23C	0.332(16)
H23D	0.332(16)	C24	0.668(16)	H24A	0.668(16)
H24B	0.668(16)	H24C	0.668(16)	C24A	0.332(16)
H24D	0.332(16)	H24E	0.332(16)	H24F	0.332(16)

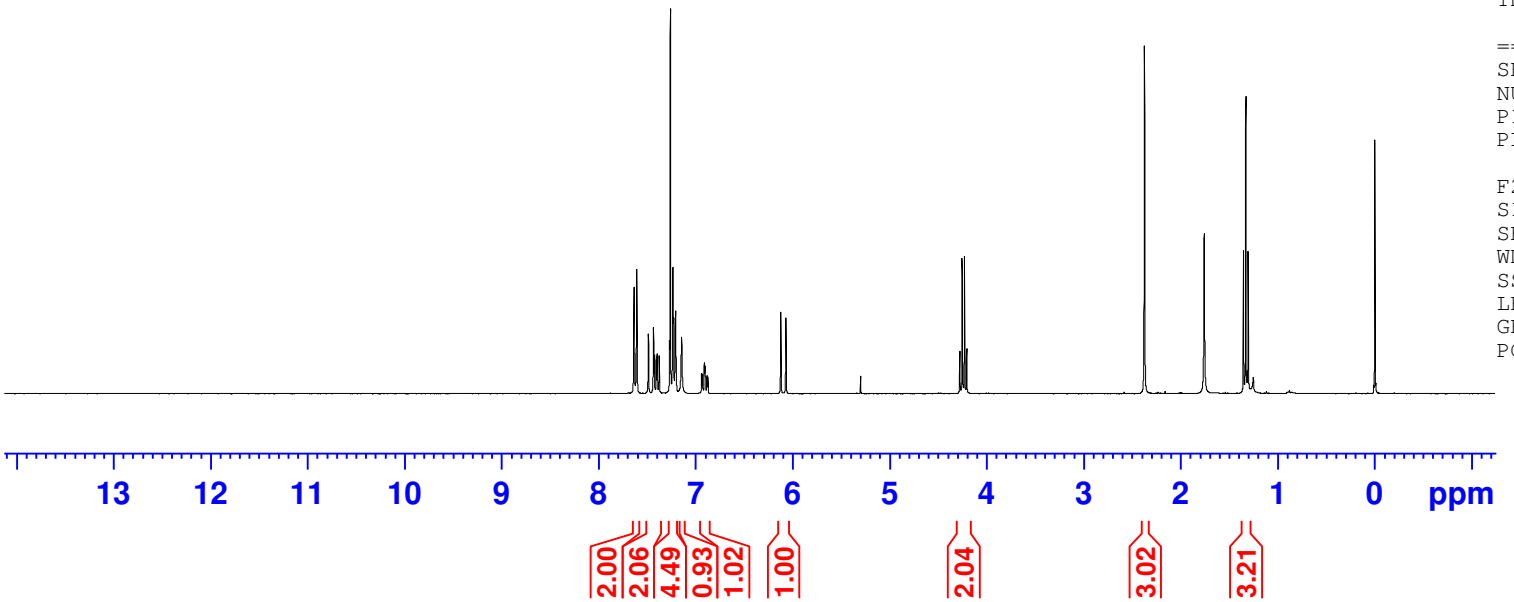
NMR Spectra

3sjwei 5113 yzk-2-61-fr 1h cdcl3



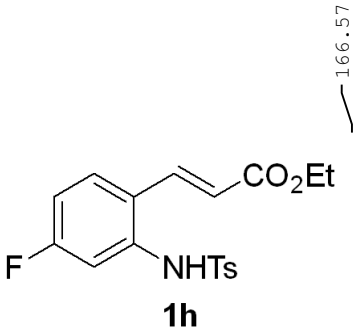


1h




```
Current Data Parameters
NAME            YZK-2-61
EXPNO               5113
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210828
Time               10.07
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   203
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300073 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

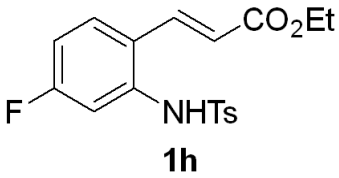
3sjwei 5139 yzk-2-61-ffr 13c cdcl3



1h


```
Current Data Parameters
NAME      1h-yzk-2-61-C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210830
Time              10.21
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4677536 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

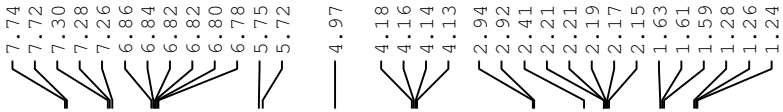
3sjwei 5114 yzk-2-61-fr 19f cdcl3

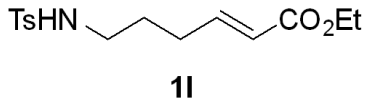


1h

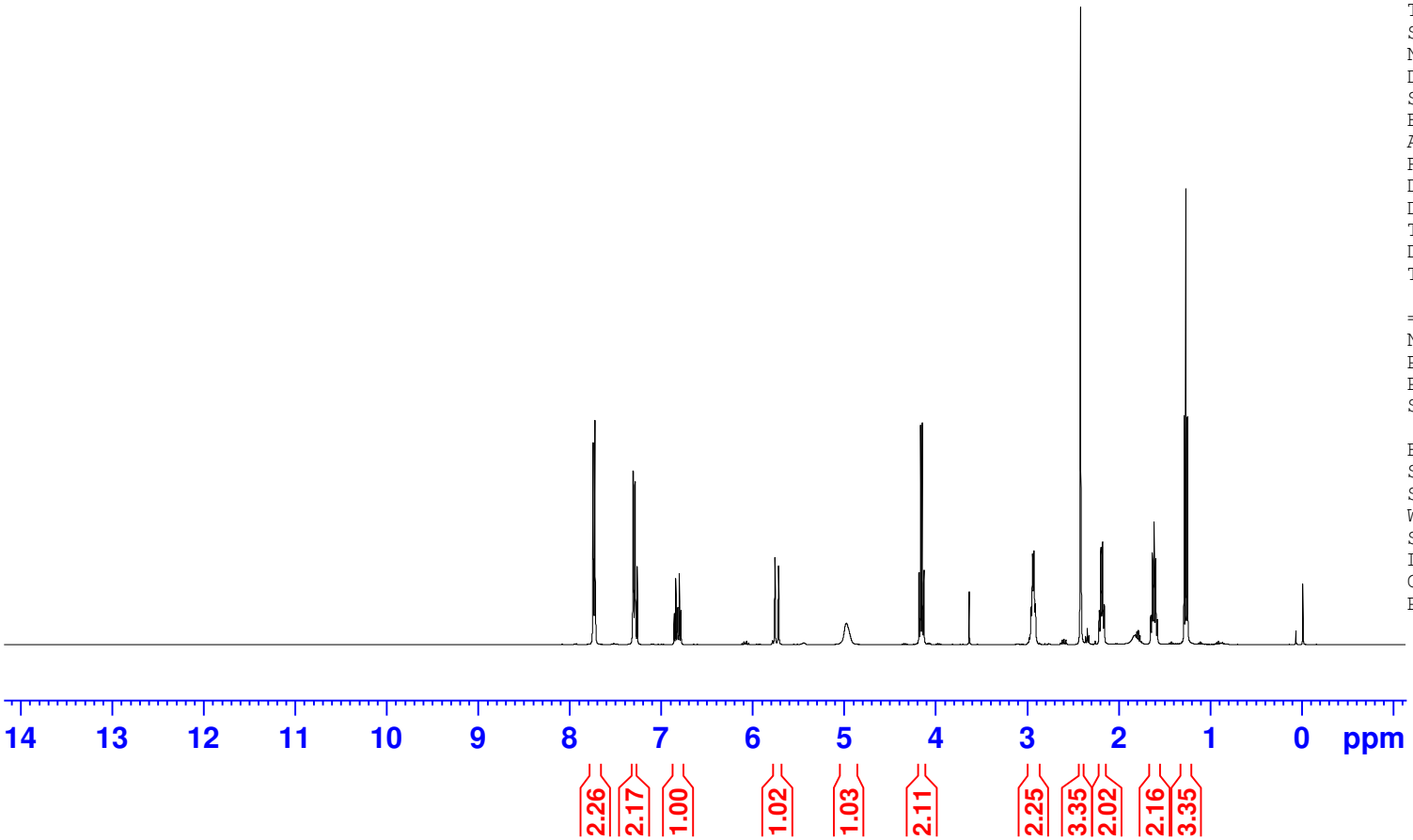

```
Current Data Parameters
NAME              workup
EXPNO               5114
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210828
Time               10.09
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD                131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            66964.289 Hz
FIDRES          0.510897 Hz
AQ             0.9786710 sec
RG                   203
DW                 7.467 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         282.3761148 MHz
NUC1                19F
P1                14.50 usec
PLW1         10.39999962 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         14.00000000 W
PLW12         0.17284000 W

F2 - Processing parameters
SI                 65536
SF           282.4043552 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

yzk-4-1b



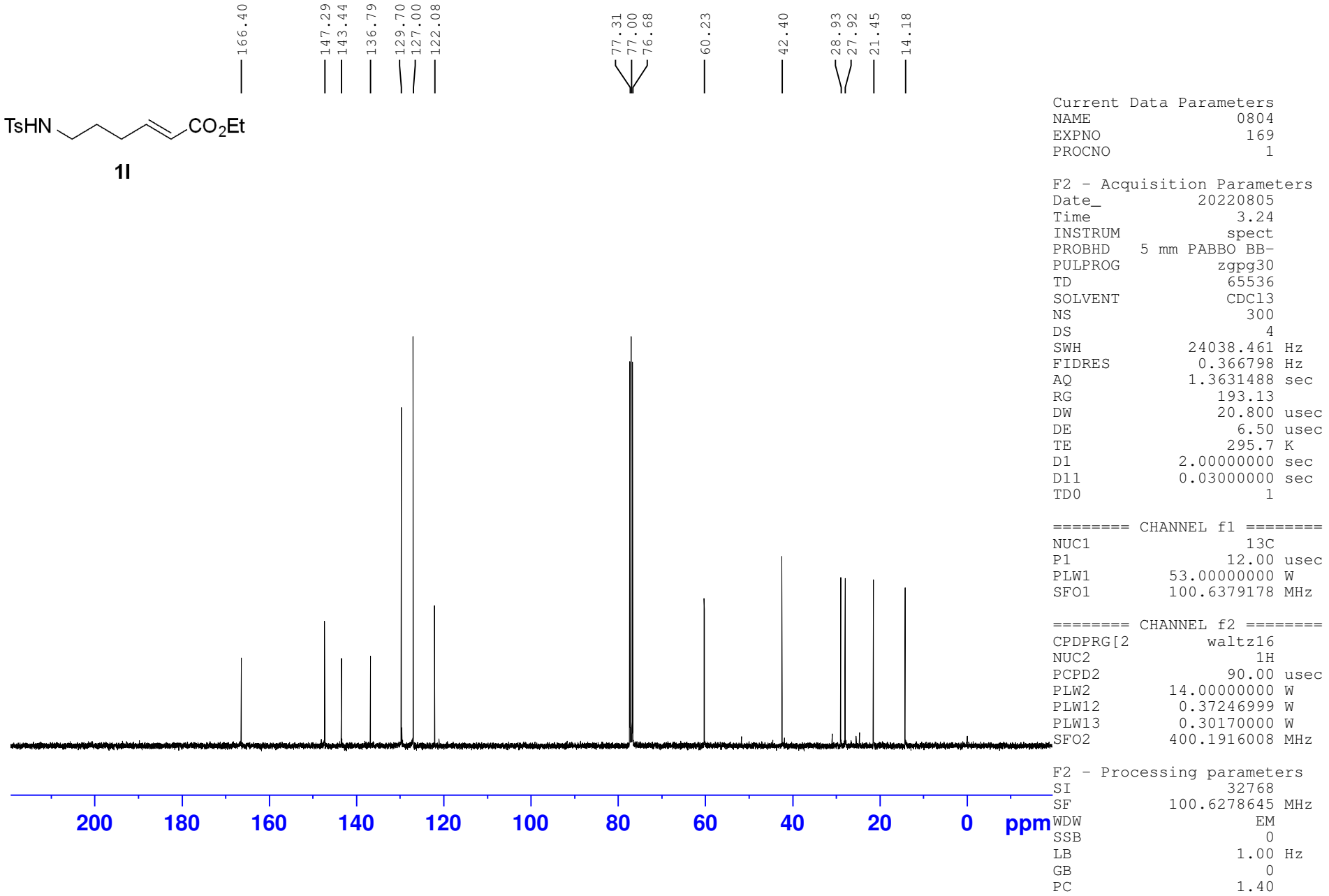


1l



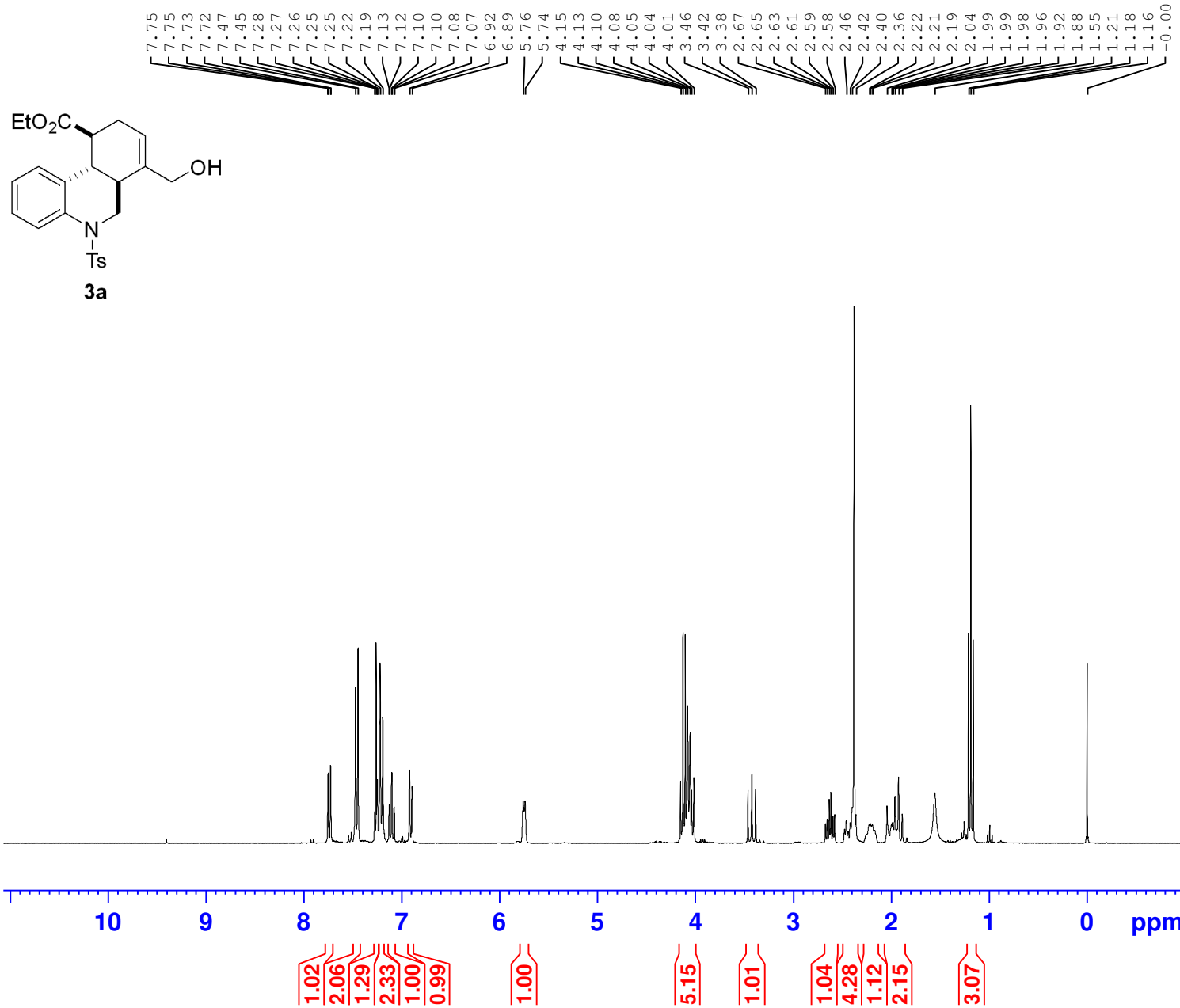

```
Current Data Parameters
NAME                  0804
EXPNO                  168
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220805
Time                  3.06
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                   90.23
DW                  60.800 usec
DE                   6.50 usec
TE                  294.9 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.68 usec
PLW1          14.00000000 W
SFO1          400.1924713 MHz

F2 - Processing parameters
SI                   65536
SF            400.1900163 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

yzk-4-1b



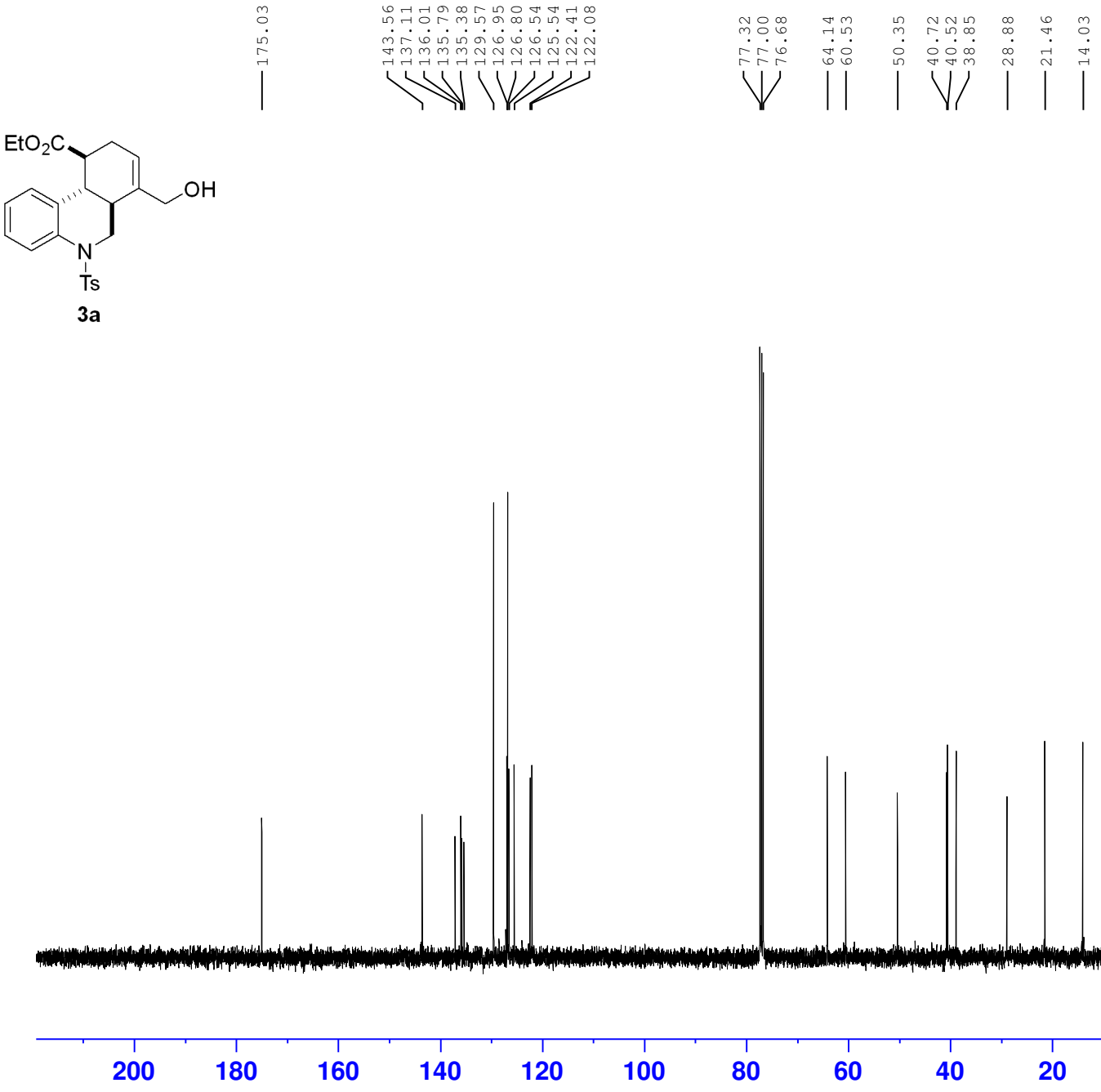

```
Current Data Parameters
NAME                  0804
EXPNO                  169
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220805
Time                   3.24
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      300
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   295.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                   12.00 usec
PLW1           53.00000000 W
SFO1          100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PLW2           14.00000000 W
PLW12           0.37246999 W
PLW13           0.30170000 W
SFO2          400.1916008 MHz

F2 - Processing parameters
SI                    32768
SF            100.6278645 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```

3sjwei 5491 yzk-2-97-fr 1h cdcl3



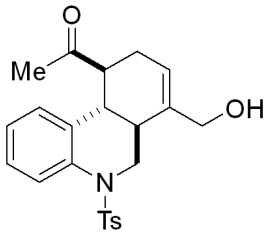

```
Current Data Parameters
NAME            YZK-2-97
EXPNO               5491
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210930
Time               10.08
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   161
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300072 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Yzk-2-52-fr

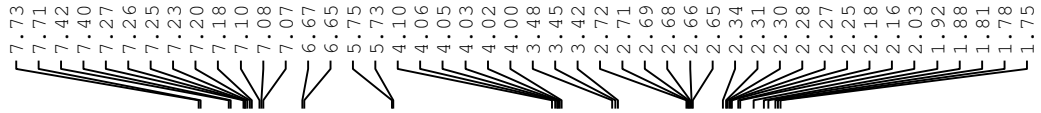


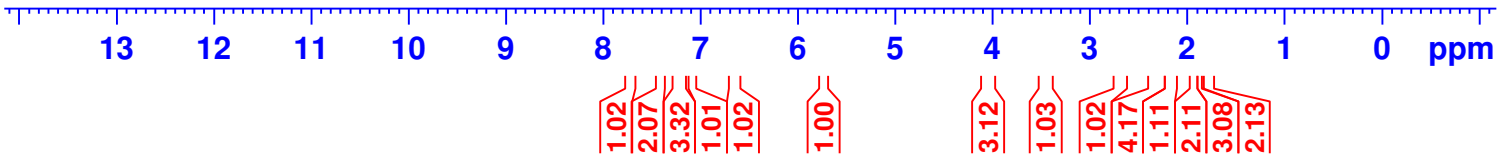

```
Current Data Parameters
NAME            YZK-2-52
EXPNO                 54
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211111
Time               19.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   57
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               293.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.90 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.35839999 W
PLW13        0.29030001 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278682 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

4sunjianwei8/207 YZK-2-74-fr



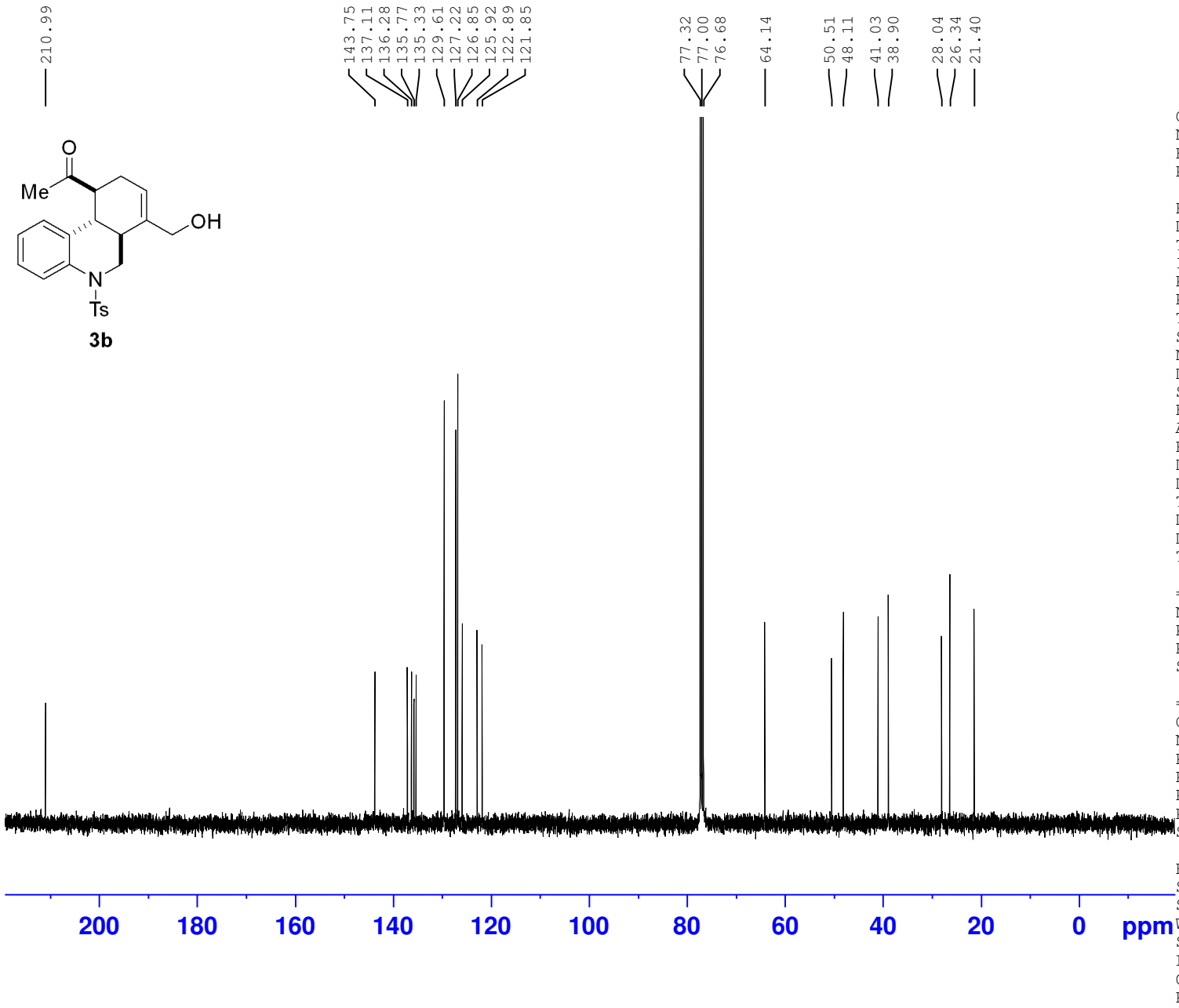
3b





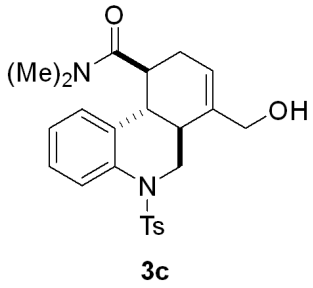

```
Current Data Parameters
NAME            YZK-2-74
EXPNO                207
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210908
Time               14.54
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 68.24
DW                60.800 usec
DE                 6.50 usec
TE                294.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.40 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900173 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

4sunjianwei8/208 YZK-2-74-fr




```
Current Data Parameters
NAME      3b-yzk-2-74-C
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20210908
Time              15.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  432
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               295.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.90 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2           90.00 usec
PLW2        14.00000000 W
PLW12        0.35839999 W
PLW13        0.29030001 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278661 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

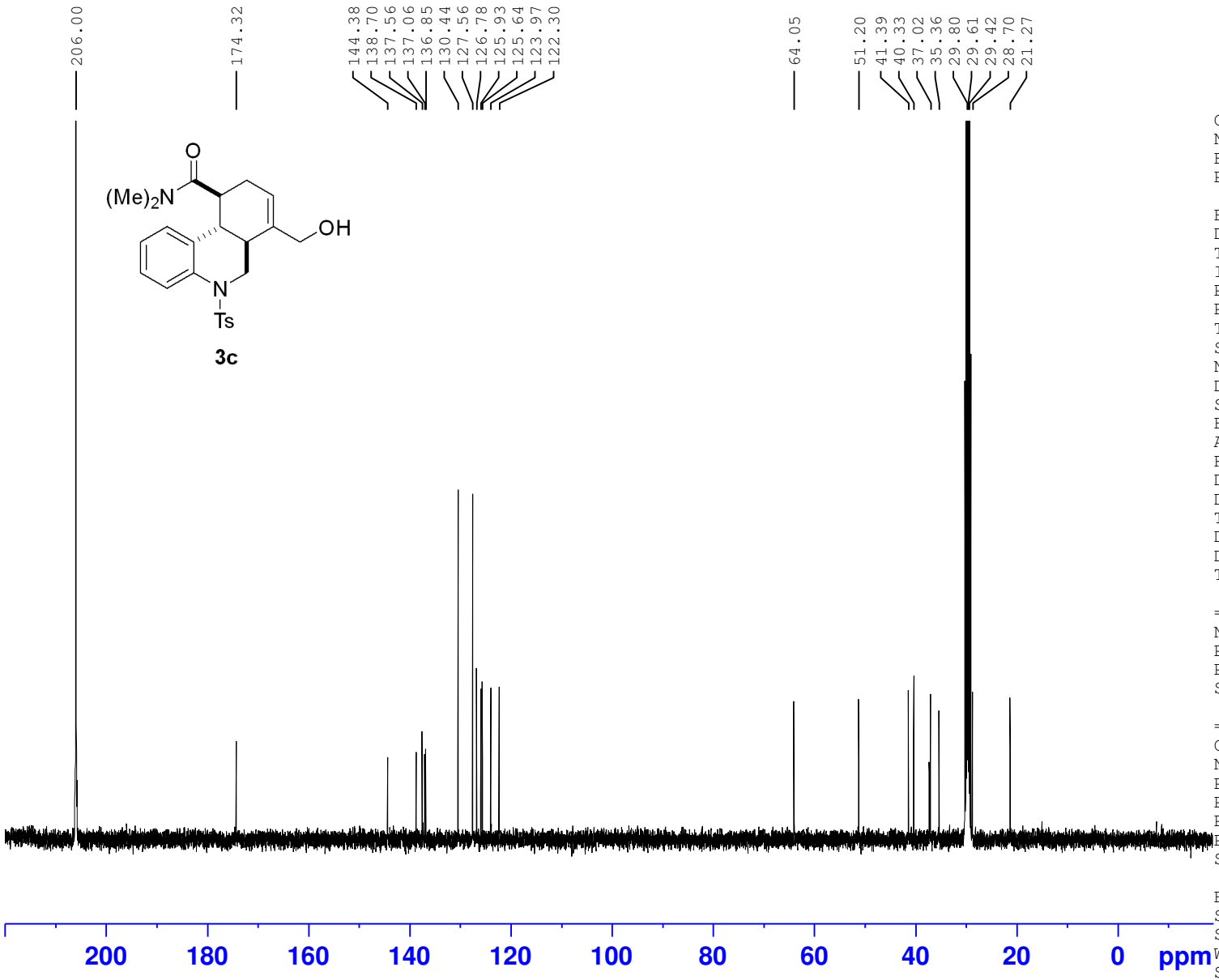
Yzk-3-21-fr



3c

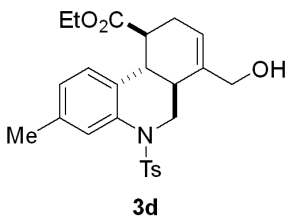

```
Current Data Parameters
NAME       3c-yzk-3-21-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211111
Time               20.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                113.67
DW                60.800 usec
DE                 6.50 usec
TE                293.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.40 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1901467 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Yzk-3-21-fr

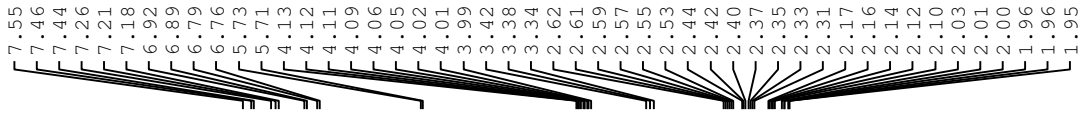



```
Current Data Parameters
NAME                  3-21
EXPNO                   58
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211111
Time                 20.19
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       280
DS                         4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                  193.13
DW                  20.800 usec
DE                   6.50 usec
TE                  294.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.90 usec
PLW1          53.00000000 W
SFO1         100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PLW2          14.00000000 W
PLW12          0.35839999 W
PLW13          0.29030001 W
SFO2         400.1916008 MHz

F2 - Processing parameters
SI                    32768
SF           100.6277928 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

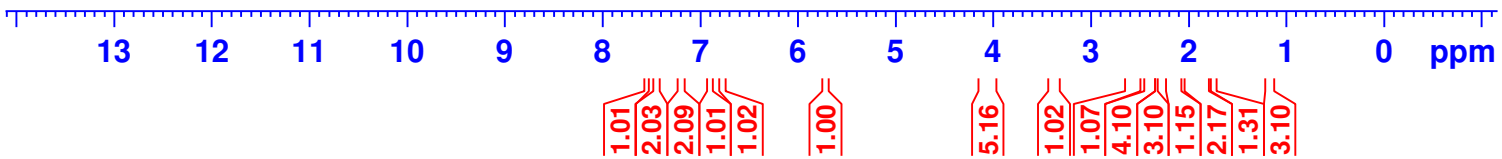
3sjwei 5215 yzk-2-58-fr 1h cdcl3



3d

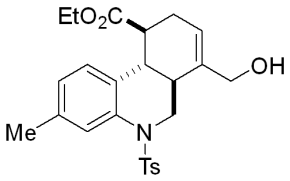



```
Current Data Parameters
NAME      3f-yzk-2-58-H
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20210904
Time              10.58
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                 90.5
DW               83.200 usec
DE                6.50 usec
TE               -59.1 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                1H
P1                10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                65536
SF          300.1300073 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



3sjwei 5216 yzk-2-58-fr 13ccdcl3

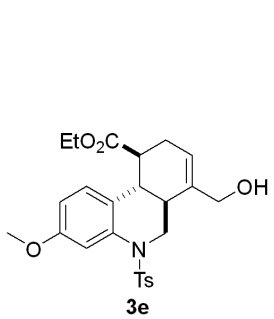
175.09
143.50
136.77
136.09
135.64
135.47
134.14
129.55
127.26
126.87
126.28
122.17
122.09
77.42
77.00
76.57
64.21
60.51
50.36
40.86
40.68
38.61
28.93
21.48
21.14
14.06



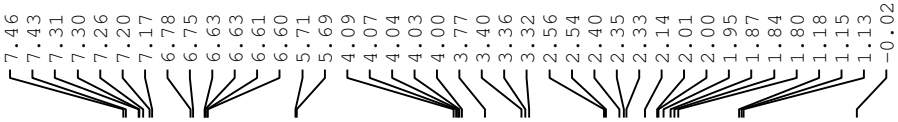
3d

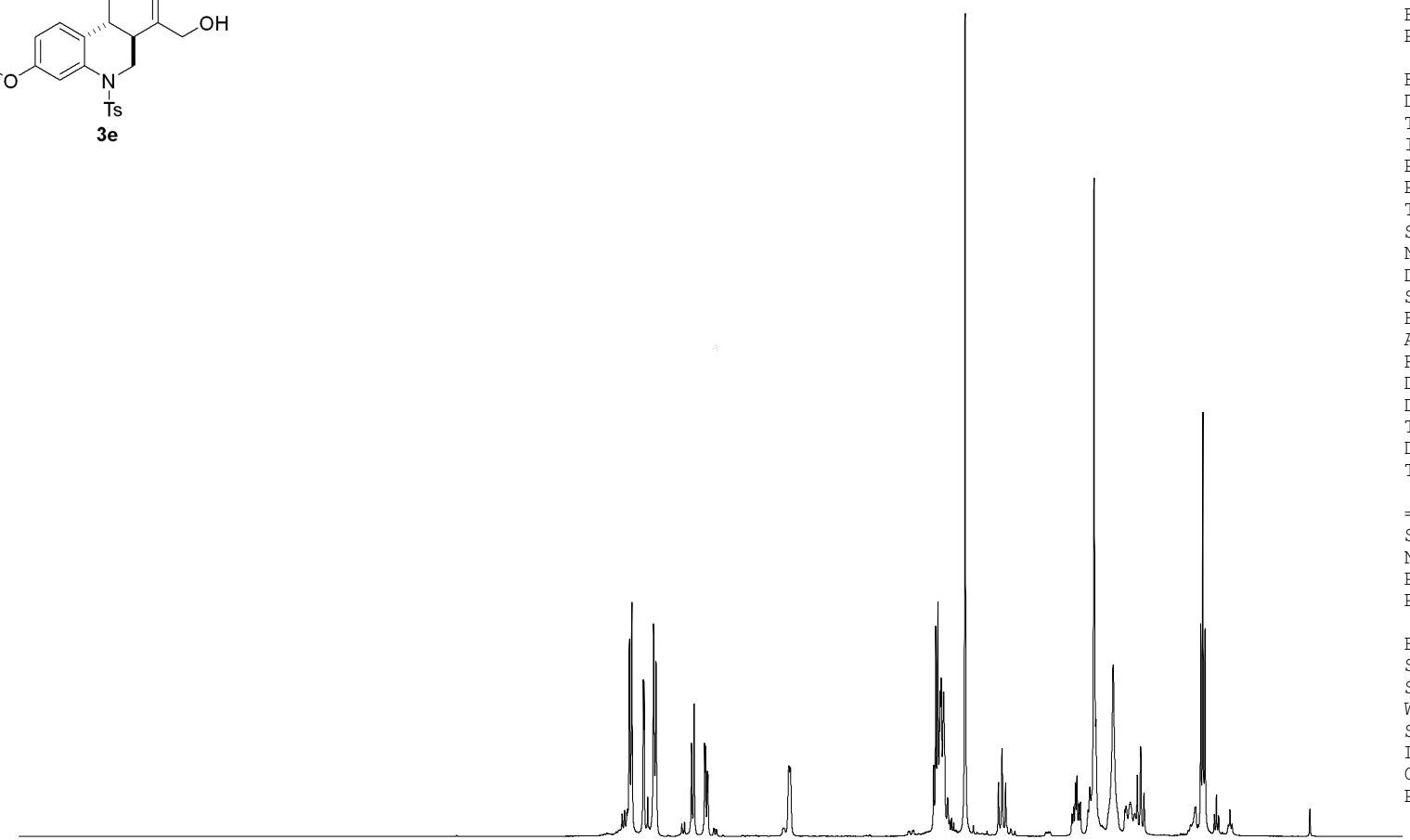

```
Current Data Parameters
NAME      3f-yzk-2-58-C
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20210904
Time              11.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  600
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                32768
SF           75.4677545 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

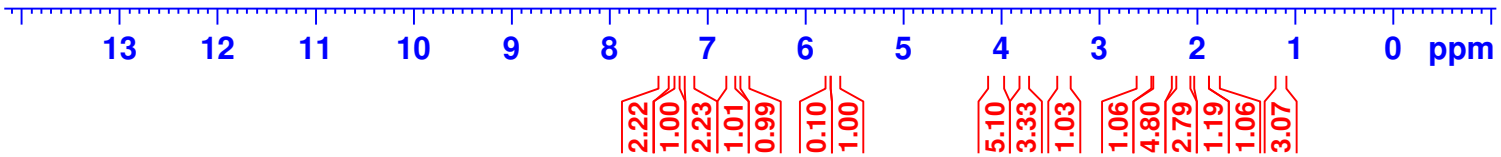
3sjwei 5321 yzk-2-81-fr 1h cdcl3



3e

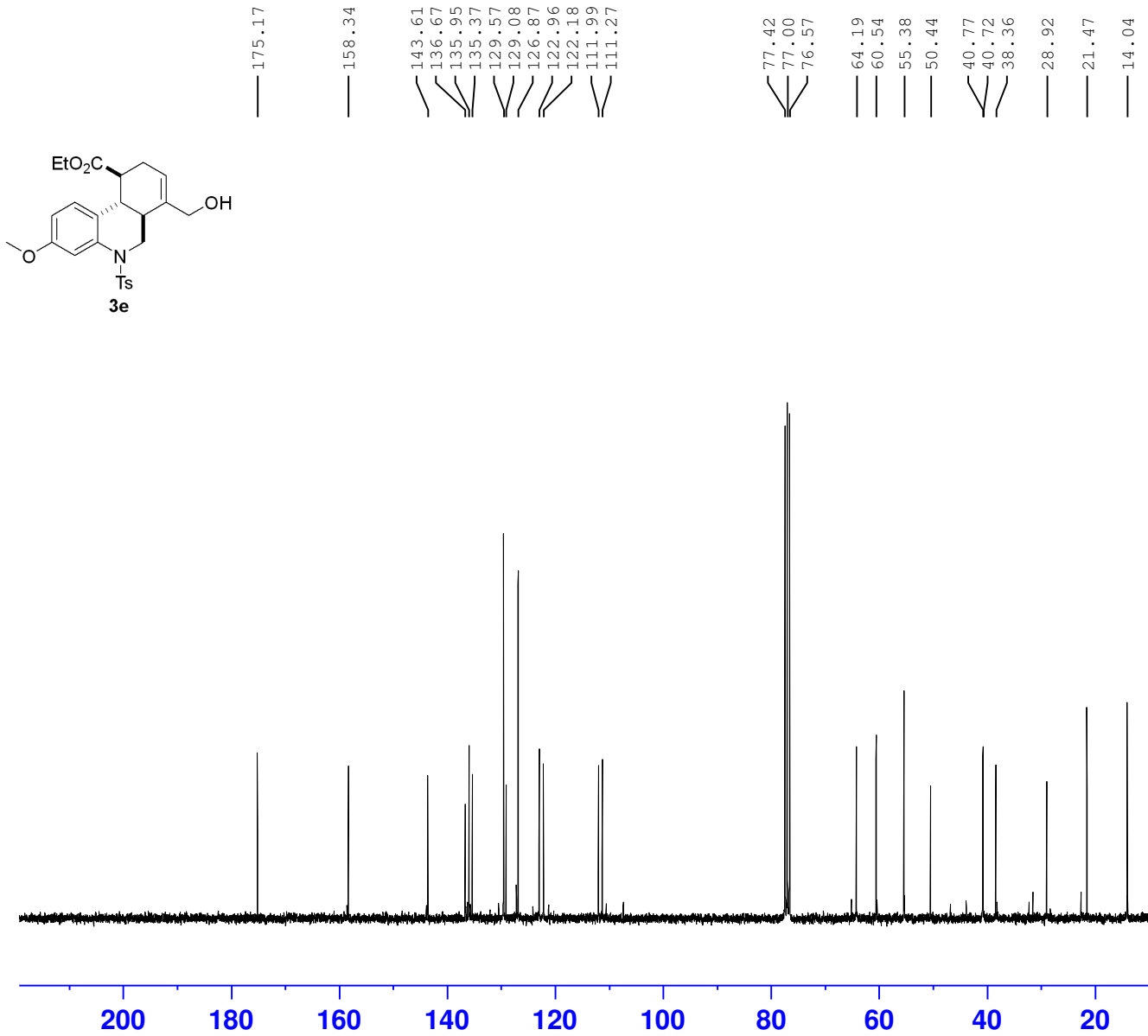







```
Current Data Parameters
NAME            YZK-2-81
EXPNO               5321
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210914
Time                9.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                    32
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300071 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3sjwei 5418yzk-2-81-fr 13c cdcl3



Current Data Parameters
NAME 3g-yzk-2-81-C
EXPNO 1
PROCNO 1

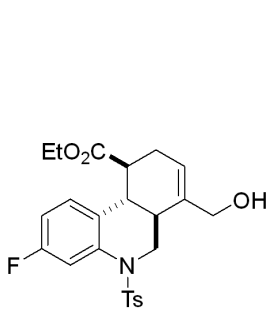
F2 - Acquisition Parameters
Date_ 20210925
Time 10.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

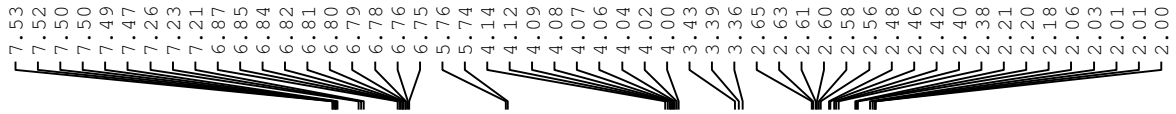
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

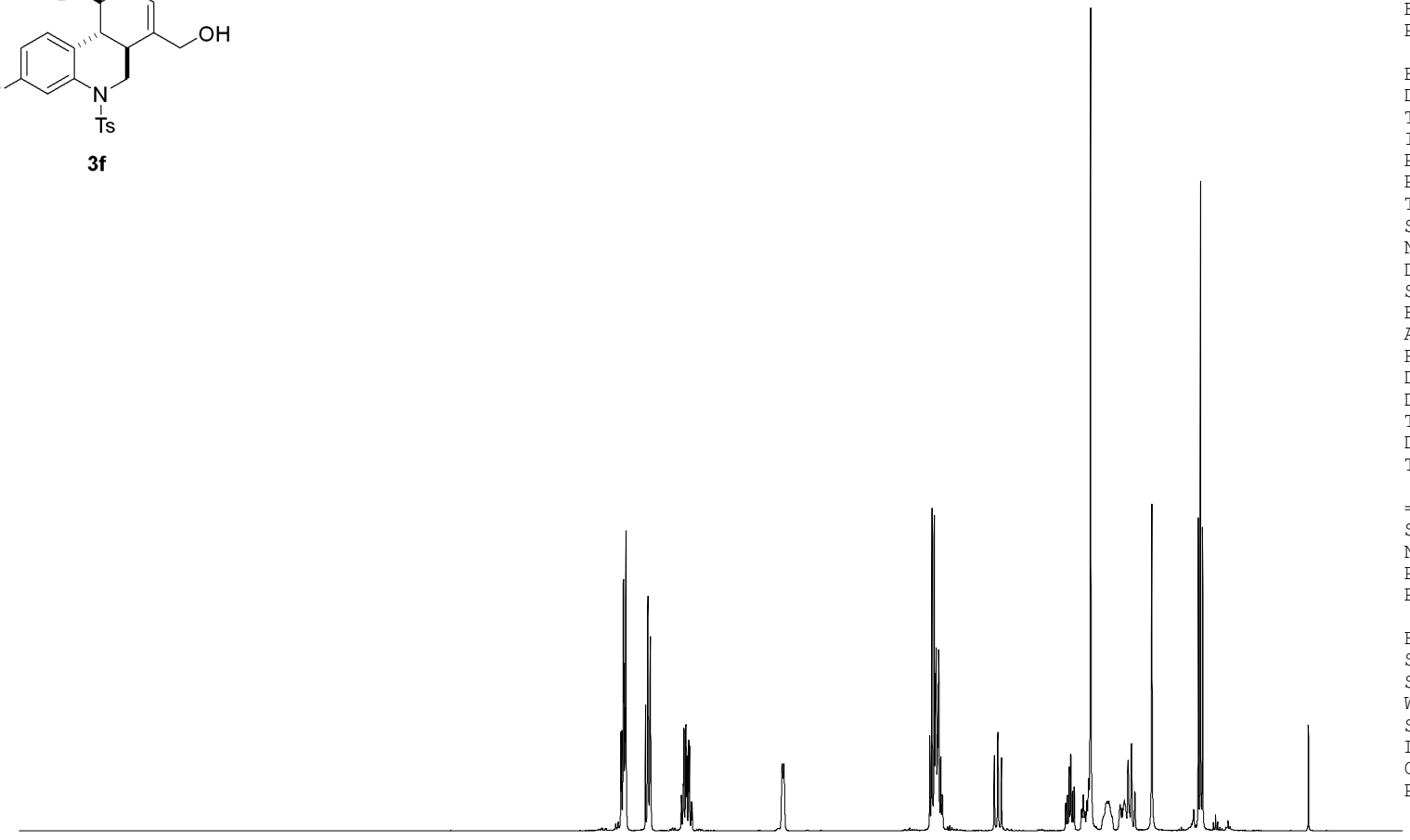
F2 - Processing parameters
SI 32768
SF 75.4677552 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

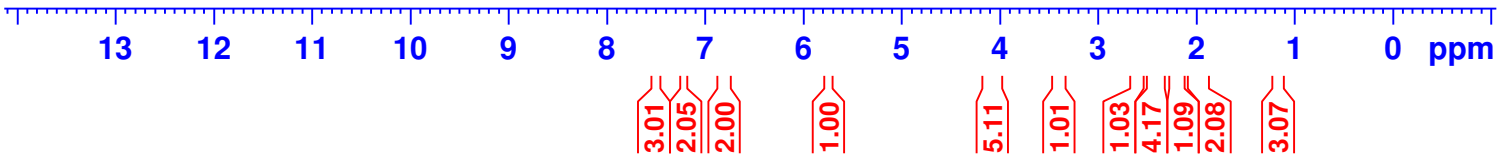
3sjwei 5304 yzk-2-80-fr 1h cdcl3



3f



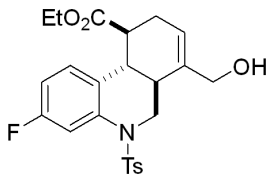





```
Current Data Parameters
NAME            YZK-2-80
EXPNO               5304
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210910
Time                9.20
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   114
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                 65536
SF          300.1300070 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3sjwei 5317 yzk-2-80-fr 13c cdcl3

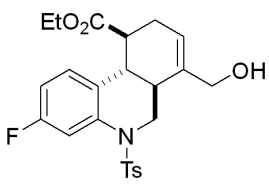
174.95
162.91
159.67
143.93
137.22
137.08
135.73
135.24
132.44
132.39
129.71
126.87
123.41
123.29
122.47
113.72
113.39
112.10
111.82
77.42
77.00
76.57
64.27
60.69
50.42
40.61
40.48
38.61
28.85
21.50
14.04



3f


```
Current Data Parameters
NAME       3h-yzk-2-80-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210911
Time               10.10
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4677538 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

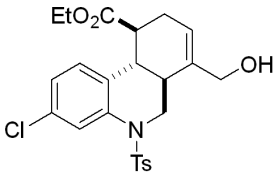
3sjwei 5305 yzk-2-80-fr 19f cdcl3



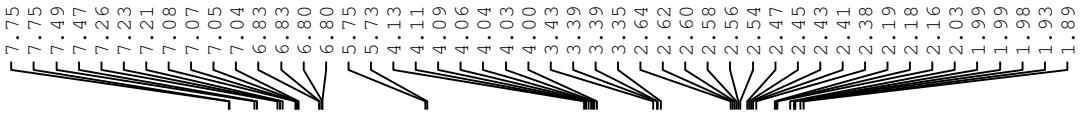
3f

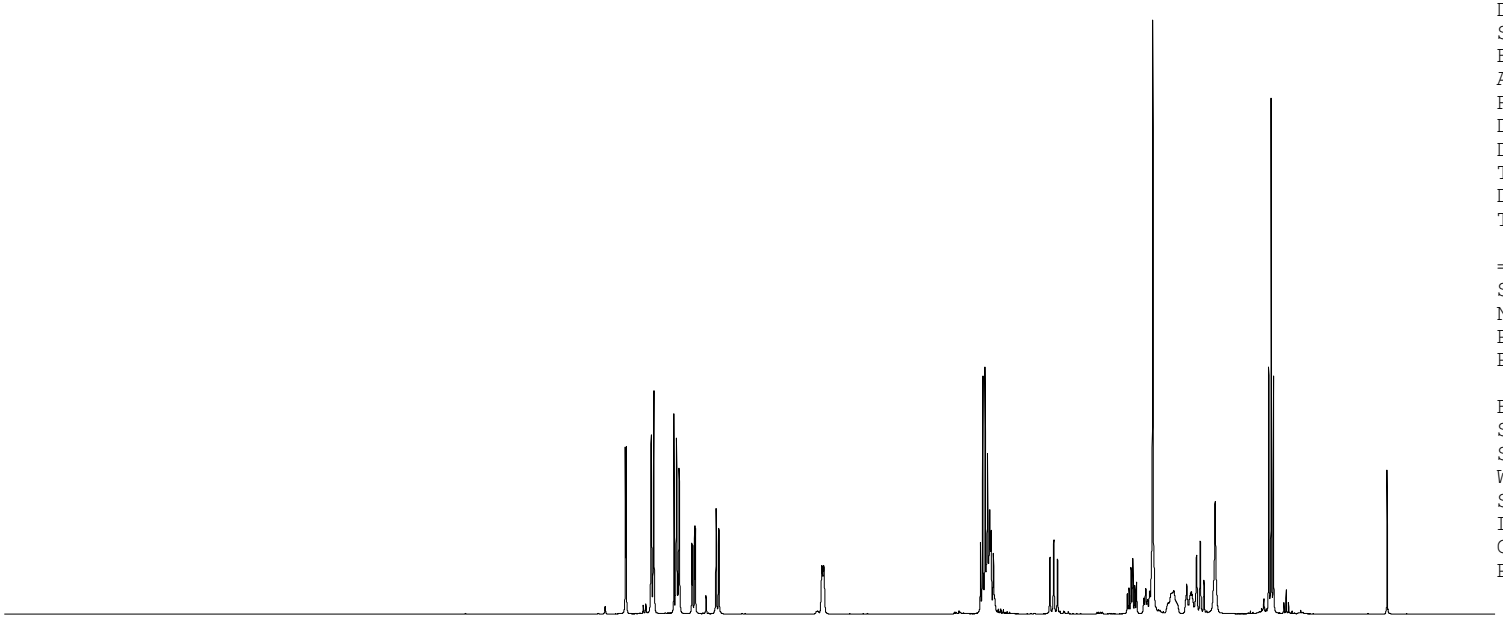

```
Current Data Parameters
NAME                  workup
EXPNO                   5305
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210910
Time                    9.23
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG          zgfhigqn.2
TD                     131072
SOLVENT                 CDCl3
NS                         16
DS                          4
SWH                66964.289 Hz
FIDRES              0.510897 Hz
AQ                  0.9786710 sec
RG                        203
DW                      7.467 usec
DE                      6.50 usec
TE                     -59.1 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             282.3761148 MHz
NUC1                    19F
P1                    14.50 usec
PLW1             10.39999962 W

======== CHANNEL f2 ========
SFO2             300.1312005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W

F2 - Processing parameters
SI                      65536
SF               282.4043552 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

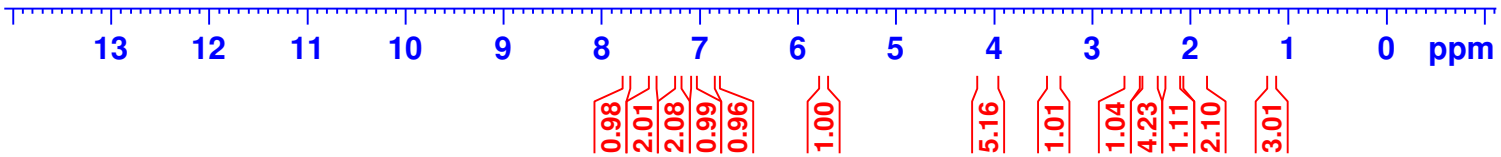
3sjwei 5164 yzk-2-68-fr 1h cdcl3



3g

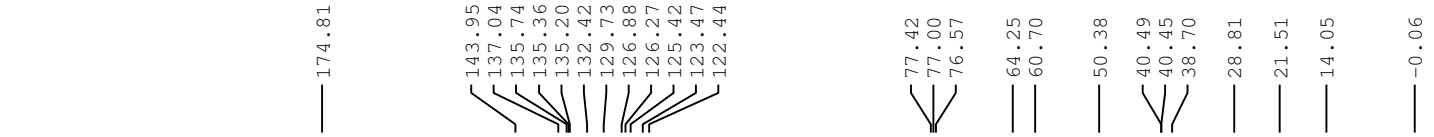


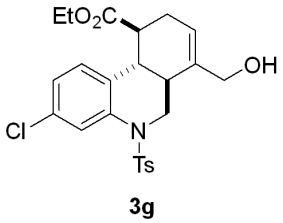




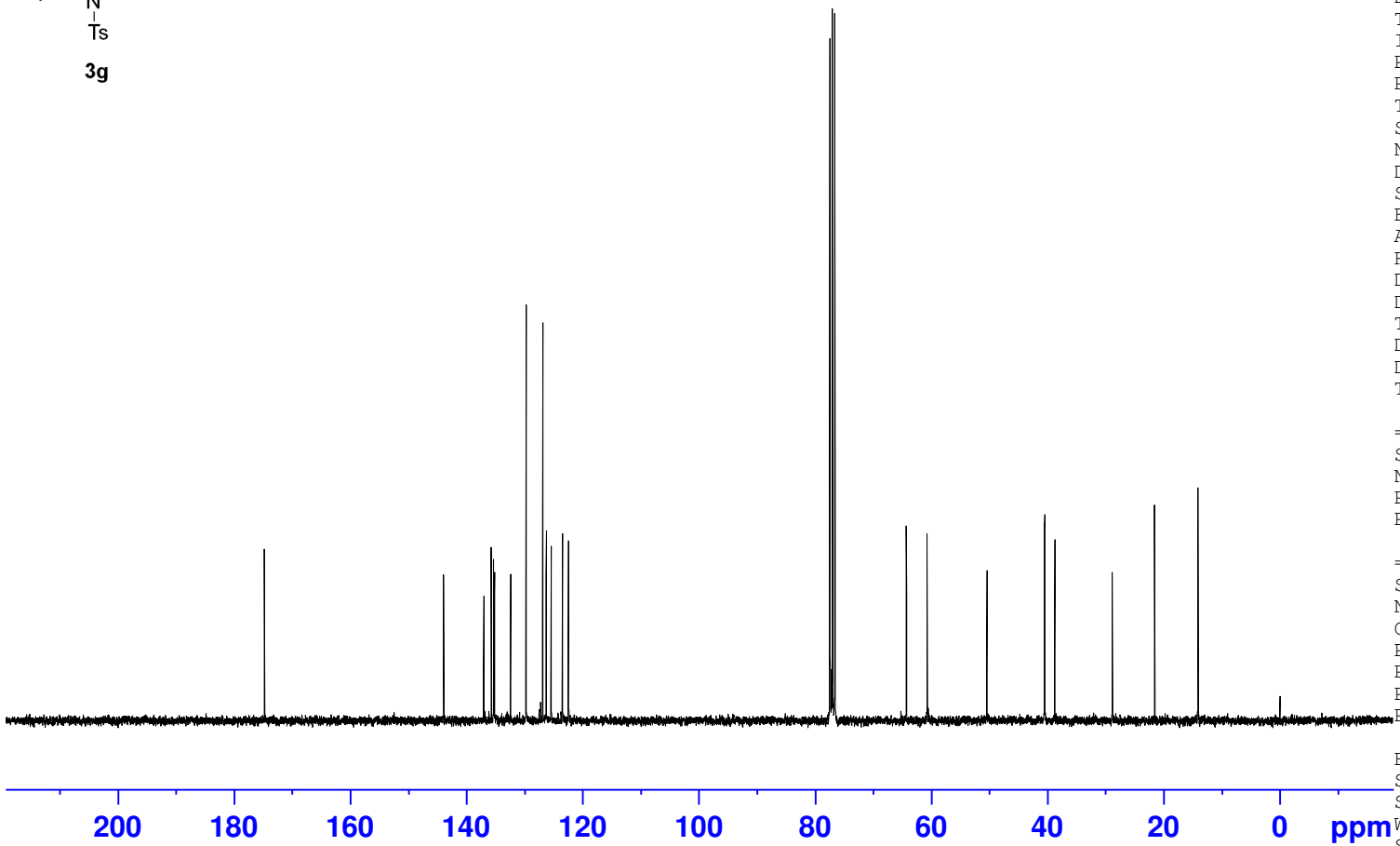

```
Current Data Parameters
NAME            YZK-2-68
EXPNO               5164
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210901
Time               10.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   101
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300072 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3sjwei 5165 yzk-2-68-fr 13c cdcl3



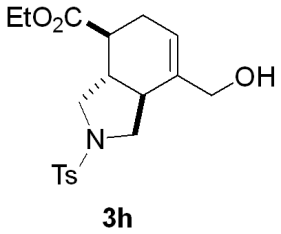


3g

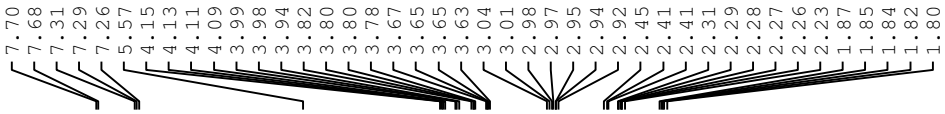


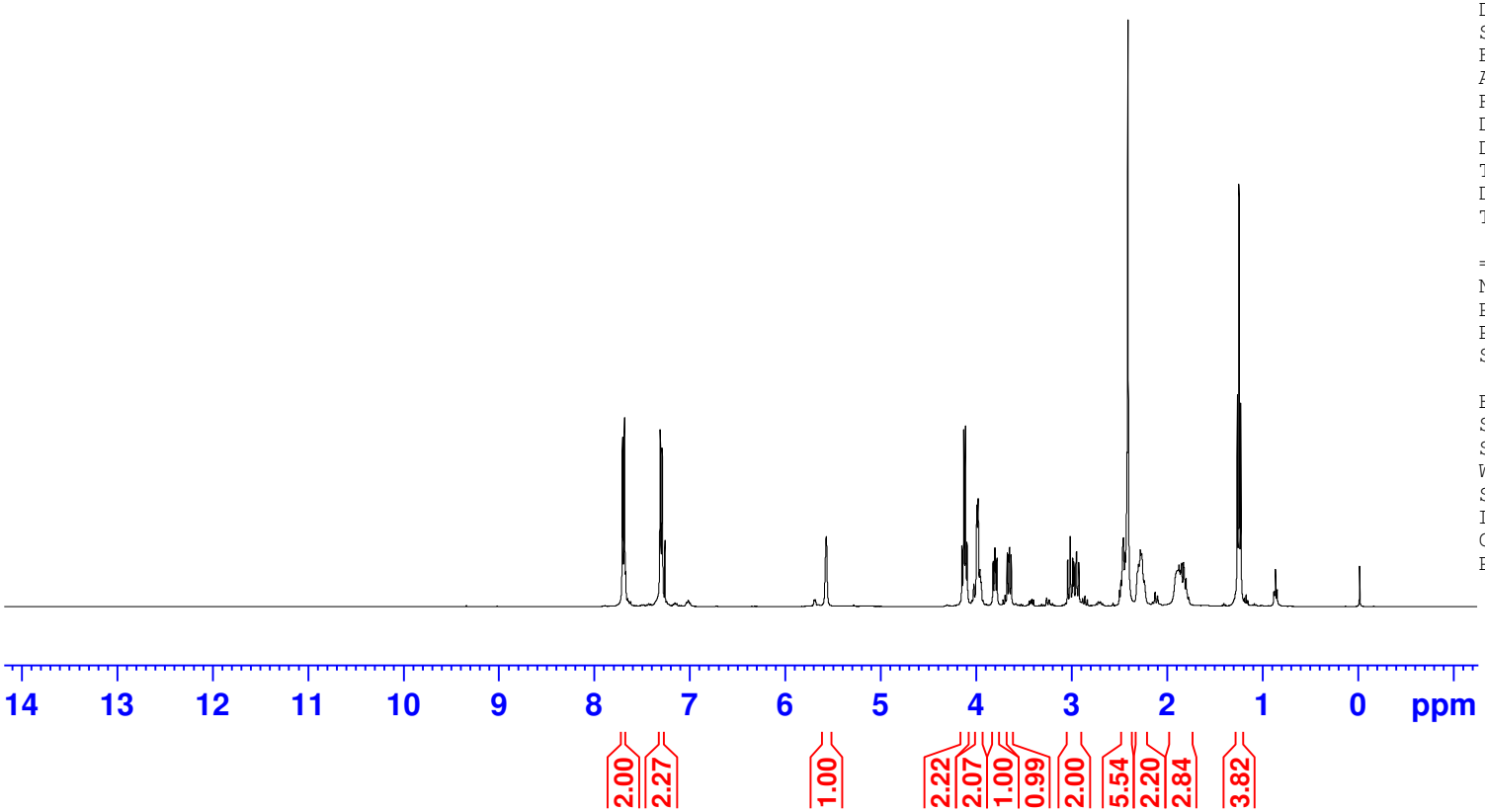

```
Current Data Parameters
NAME      3i-yzk-2-68-C
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20210901
Time               10.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  800
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                32768
SF          75.4677536 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

YZK-3-17-fr



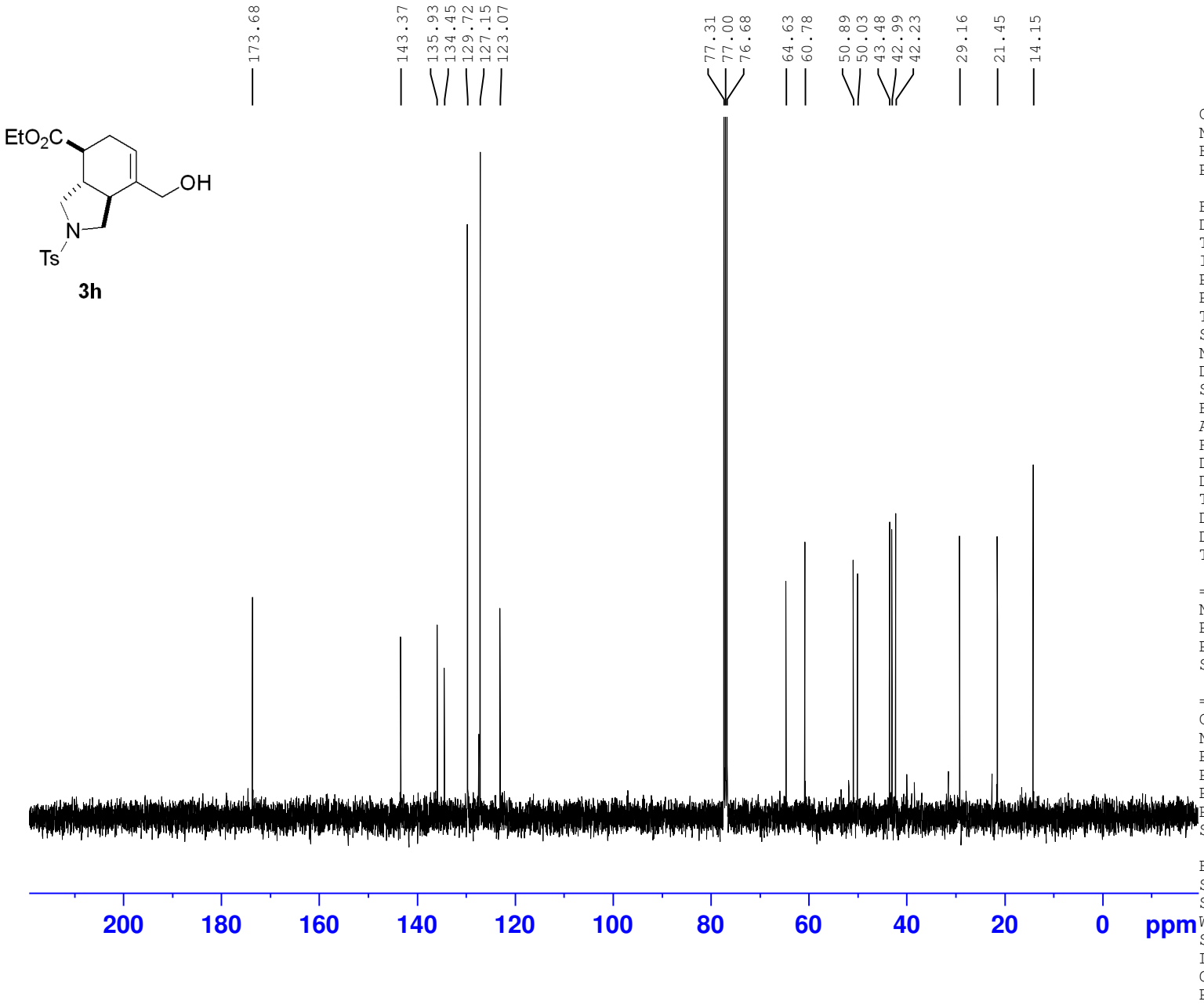
3h





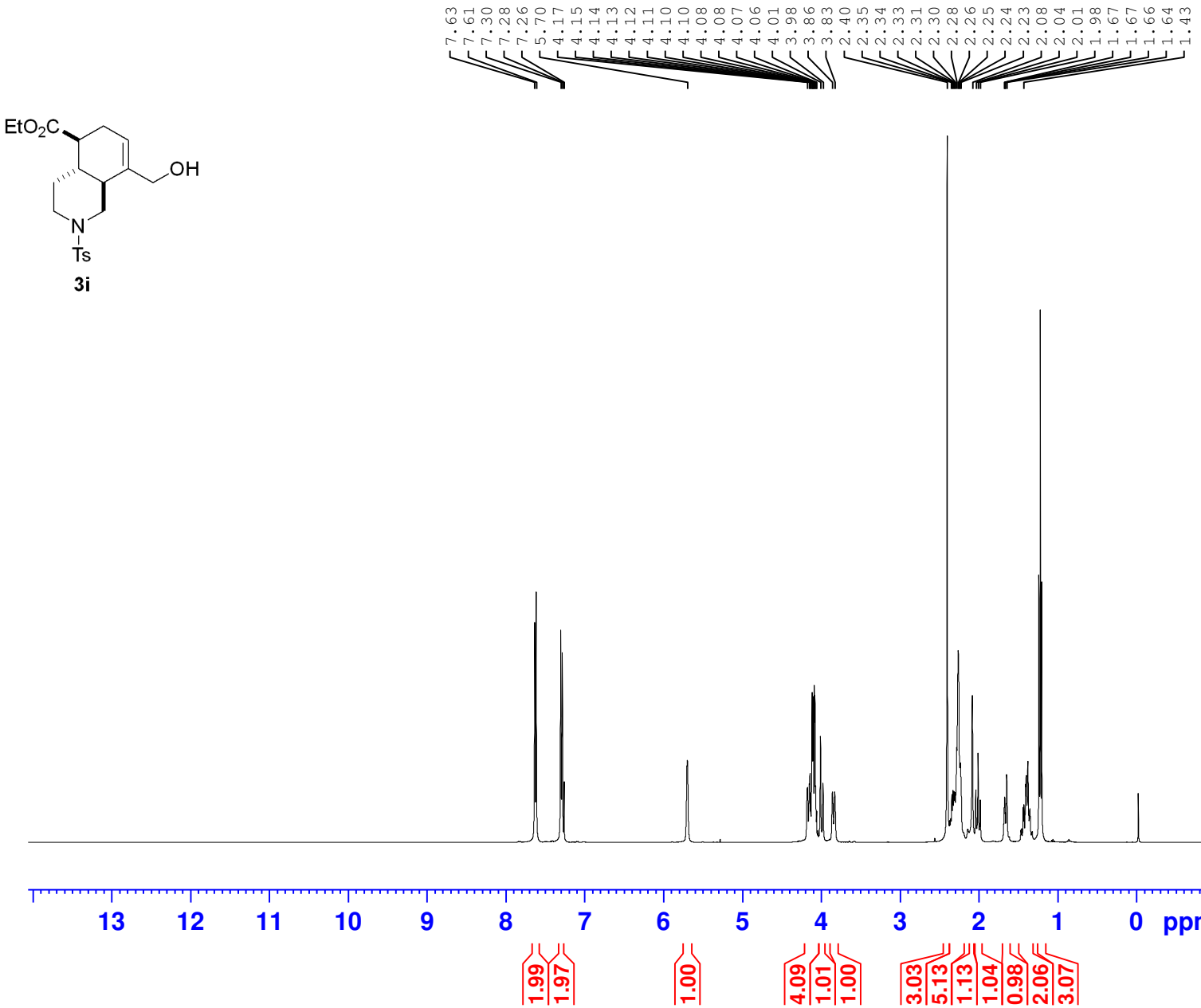

```
Current Data Parameters
NAME                  3-17
EXPNO                    7
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211020
Time                 10.16
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                   61.19
DW                  60.800 usec
DE                   6.50 usec
TE                  294.3 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.40 usec
PLW1           14.00000000 W
SFO1           400.1924713 MHz

F2 - Processing parameters
SI                   65536
SF             400.1900169 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

YZK-3-17-fr



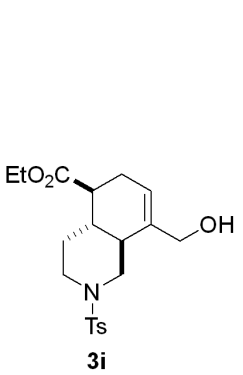

```
Current Data Parameters
NAME       3j-yzk-3-17-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211020
Time               10.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   66
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               295.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.90 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.35839999 W
PLW13        0.29030001 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278668 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

YZK-3-12-fr




```
Current Data Parameters
NAME                  3-12
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20211014
Time                 10.50
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       8
DS                       2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                    53.3
DW                  60.800 usec
DE                   6.50 usec
TE                  294.4 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.40 usec
PLW1          14.00000000 W
SFO1          400.1924713 MHz

F2 - Processing parameters
SI                   65536
SF            400.1900167 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

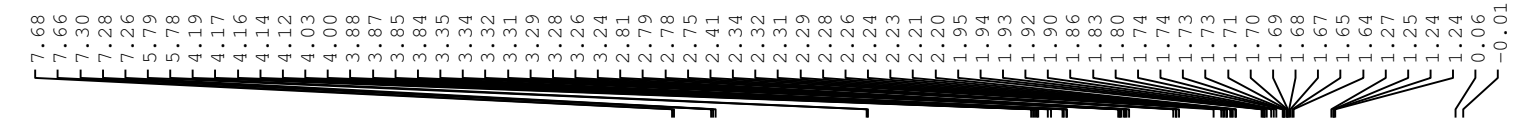
YZK-3-12-fr

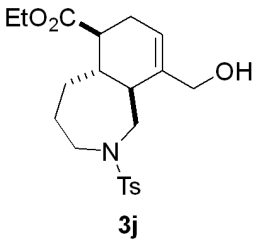


3i


```
Current Data Parameters
NAME                  3-12
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211014
Time                 10.54
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      63
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   295.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.90 usec
PLW1           53.00000000 W
SFO1          100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PLW2           14.00000000 W
PLW12           0.35839999 W
PLW13           0.29030001 W
SFO2          400.1916008 MHz

F2 - Processing parameters
SI                   32768
SF            100.6278675 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

yzk-5-31

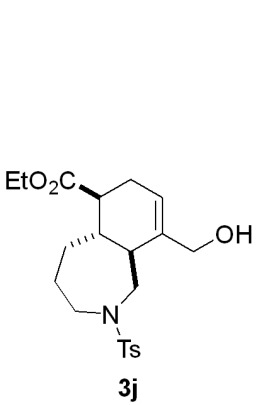




3j


```
Current Data Parameters
NAME        31-7YH-H NMR
EXPNO                44
PROCNO                1

F2 - Acquisition Parameters
Date_          20220812
Time              21.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               140.02
DW               60.800 usec
DE                6.50 usec
TE                294.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                65536
SF          400.1900168 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

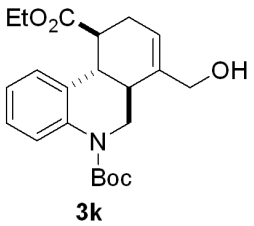
yzk-5-31



3j


```
Current Data Parameters
NAME                  0812
EXPNO                   73
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220813
Time                   0.56
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                  193.13
DW                  20.800 usec
DE                   6.50 usec
TE                  295.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  12.00 usec
PLW1          53.00000000 W
SFO1         100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2               90.00 usec
PLW2          14.00000000 W
PLW12          0.37246999 W
PLW13          0.30170000 W
SFO2         400.1916008 MHz

F2 - Processing parameters
SI                   32768
SF           100.6278616 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

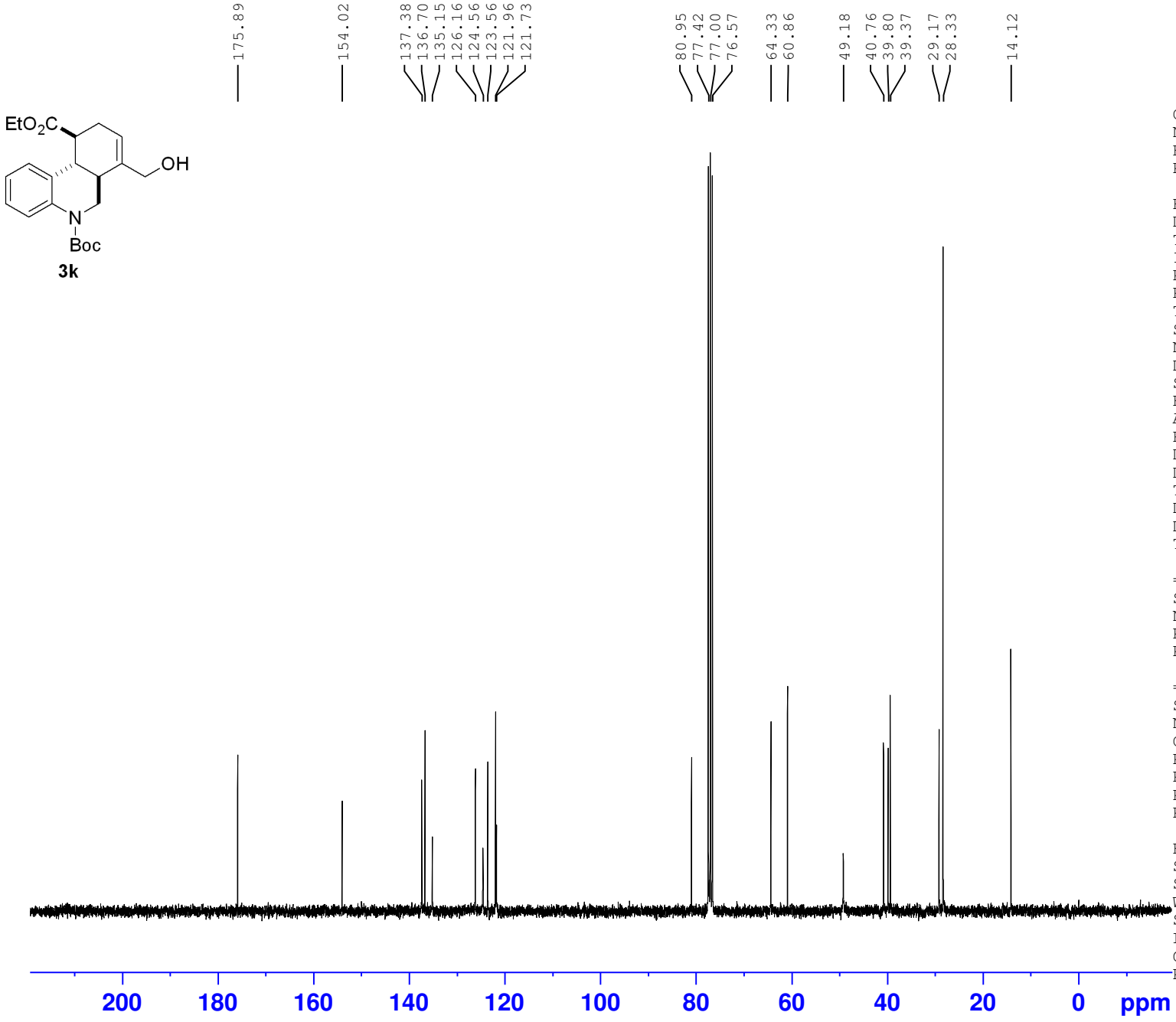
3sjwei 5615 yzk-3-34-fr 1h cdcl3



3k

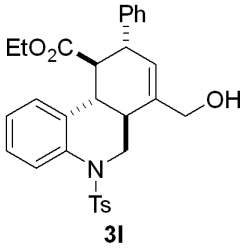

```
Current Data Parameters
NAME                  3-34
EXPNO                 5615
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211113
Time                  12.46
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4525952 sec
RG                     101
DW                  83.200 usec
DE                   6.50 usec
TE                  -59.1 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                    1H
P1                  10.00 usec
PLW1          14.00000000 W

F2 - Processing parameters
SI                   65536
SF            300.1300072 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

3sjwei 5616 yzk-3-34-fr 13c cdcl3




```
Current Data Parameters
NAME                  3-34
EXPNO                 5616
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211113
Time                  13.26
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      600
DS                        4
SWH              18028.846 Hz
FIDRES            0.275098 Hz
AQ               1.8175317 sec
RG                      203
DW                 27.733 usec
DE                   6.50 usec
TE                  -59.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4752949 MHz
NUC1                    13C
P1                    9.50 usec
PLW1           34.20000076 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           14.00000000 W
PLW12           0.17284000 W
PLW13           0.14000000 W

F2 - Processing parameters
SI                    32768
SF              75.4677541 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

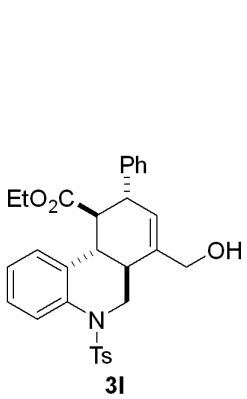
YZK-4-40



3l


```
Current Data Parameters
NAME       3n-yzk-4-40H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220615
Time              14.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    6
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               100.49
DW               60.800 usec
DE                6.50 usec
TE               295.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.40 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                65536
SF          400.1900167 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

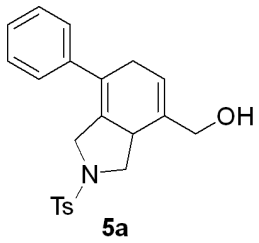
YZK-4-40



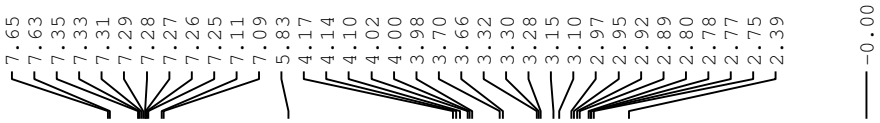
3l

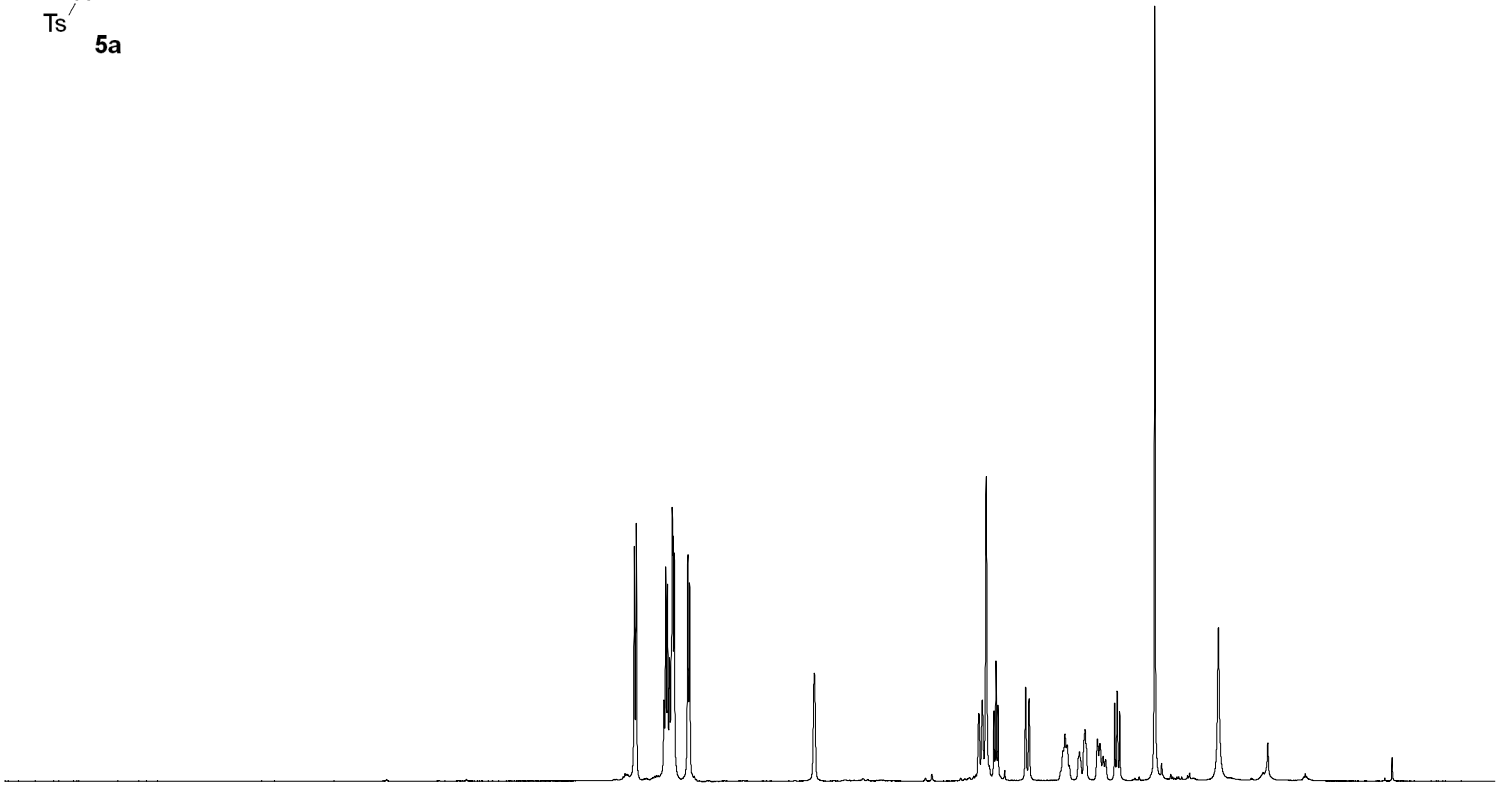

```
Current Data Parameters
NAME                  0616
EXPNO                    5
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220616
Time                 17.11 h
INSTRUM              Avance
PROBHD    Z116098_0833 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      400
DS                        4
SWH              23809.523 Hz
FIDRES            0.726609 Hz
AQ                1.3762560 sec
RG                  50.1934
DW                  21.000 usec
DE                   6.50 usec
TE                  295.5 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1
SFO1           100.6228298 MHz
NUC1                    13C
P0                   3.33 usec
P1                  10.00 usec
PLW1           87.89900208 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2          waltz65
PCPD2                90.00 usec
PLW2           20.73200035 W
PLW12           0.25595000 W
PLW13           0.12874000 W

F2 - Processing parameters
SI                    32768
SF             100.6127760 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                     1.40
```

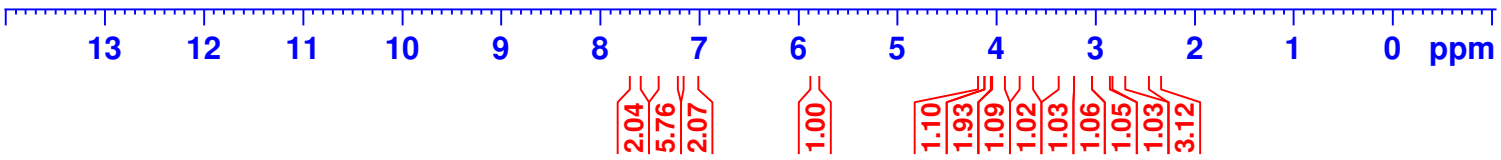
YZK-4-48



5a

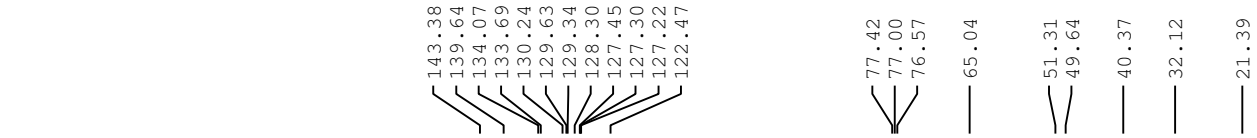


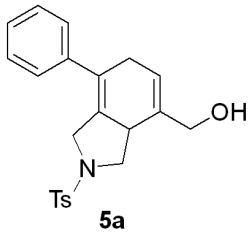




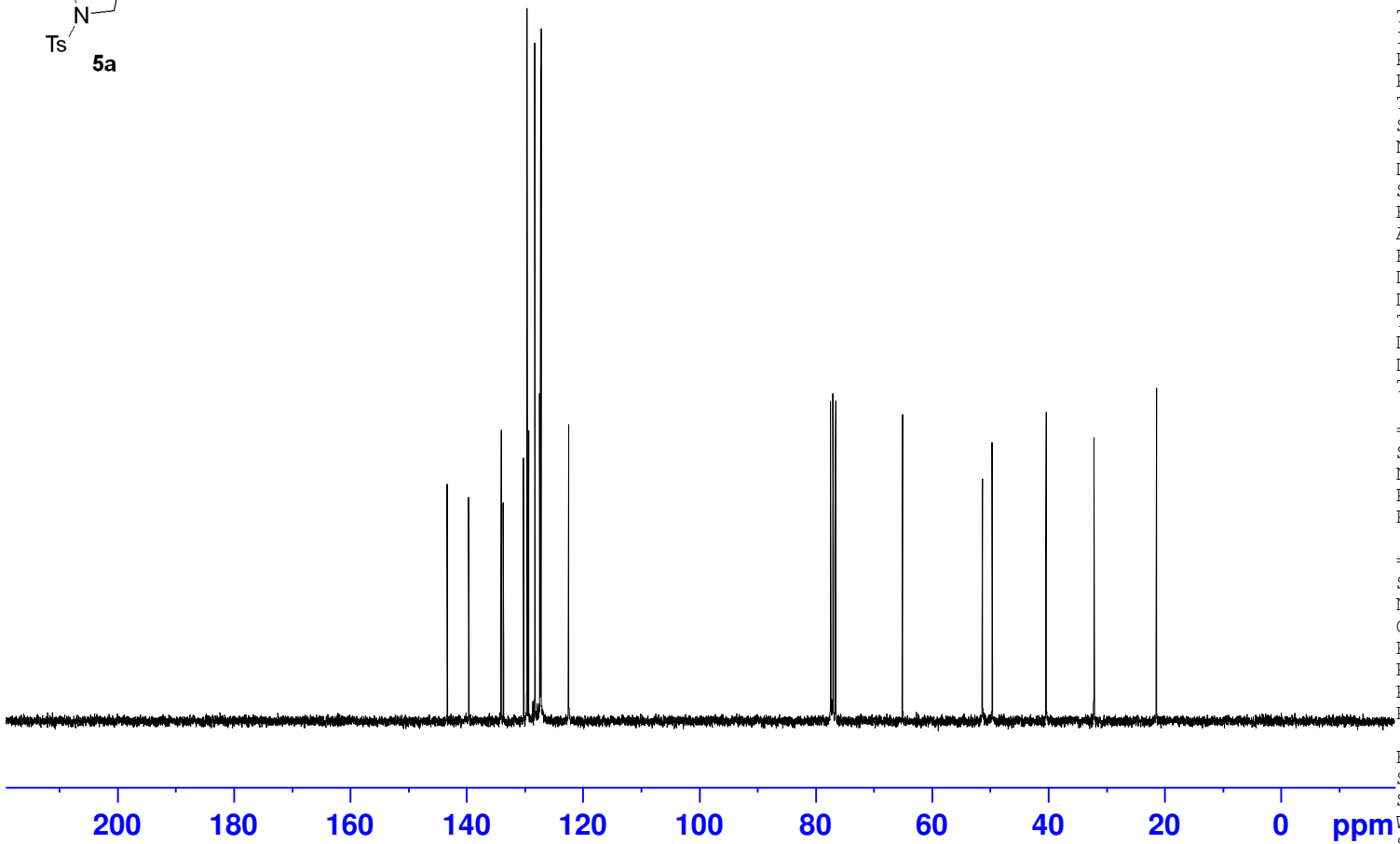

```
Current Data Parameters
NAME                  0617
EXPNO                   88
PROCNO                   1

F2 - Acquisition Parameters
Date_            20220617
Time                16.15
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                  90.23
DW                 60.800 usec
DE                  6.50 usec
TE                 294.9 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.40 usec
PLW1          14.00000000 W
SFO1          400.1924713 MHz

F2 - Processing parameters
SI                  65536
SF            400.1900180 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

3sjwei 5316 yzk-2-82-fr 13c cdcl3



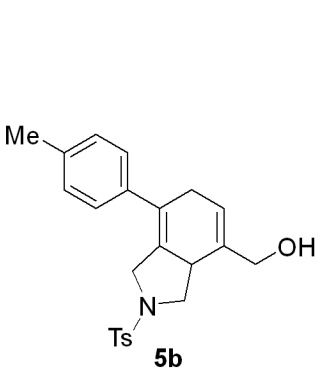


5a




```
Current Data Parameters
NAME      5a-yzk-2-82-C
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20210911
Time               9.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4677596 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

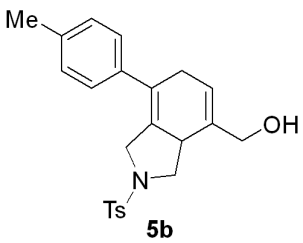
3sjwei 5390 yzk-2-90 1h cdcl3



5b

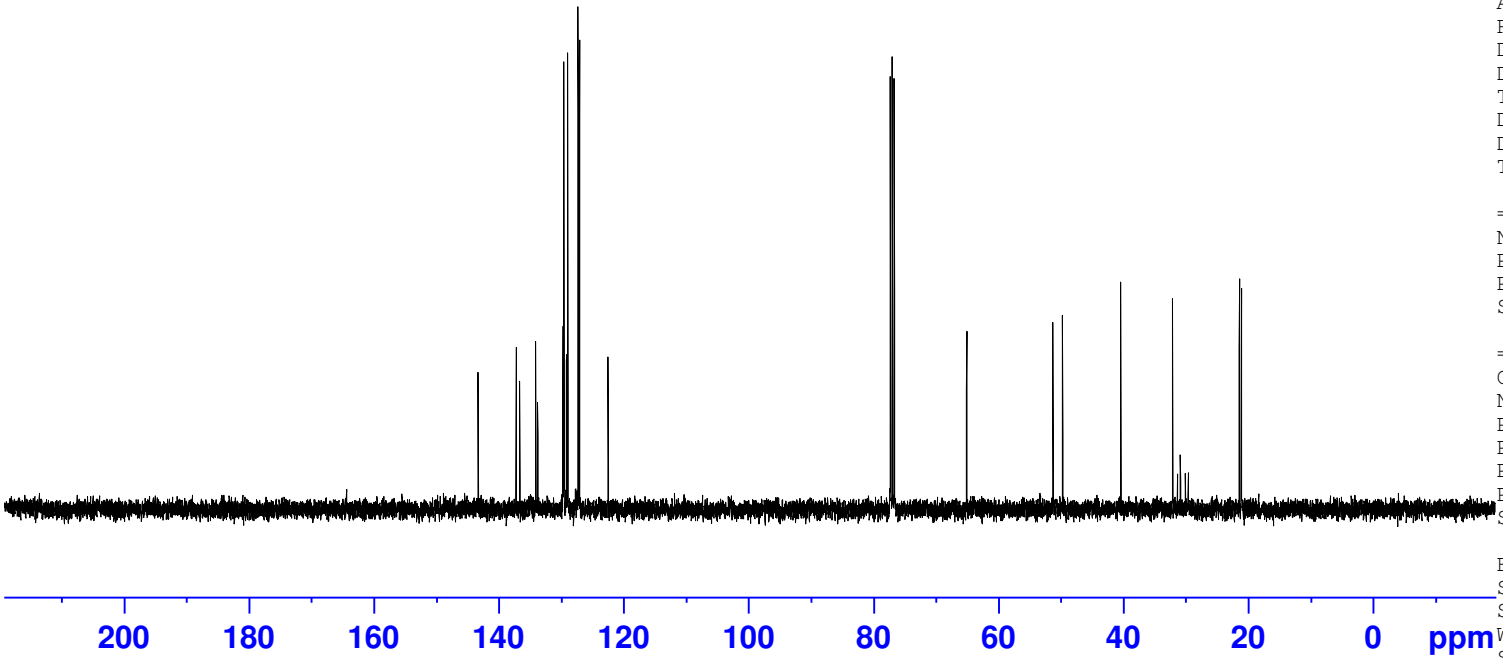

```
Current Data Parameters
NAME                  YZK-2-90
EXPNO                     5390
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210918
Time                      9.36
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 6009.615 Hz
FIDRES              0.091699 Hz
AQ                  5.4525952 sec
RG                         57
DW                    83.200 usec
DE                     6.50 usec
TE                     -59.1 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             300.1318534 MHz
NUC1                       1H
P1                      10.00 usec
PLW1             14.00000000 W

F2 - Processing parameters
SI                      65536
SF               300.1300080 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

yzk-3-27-fr



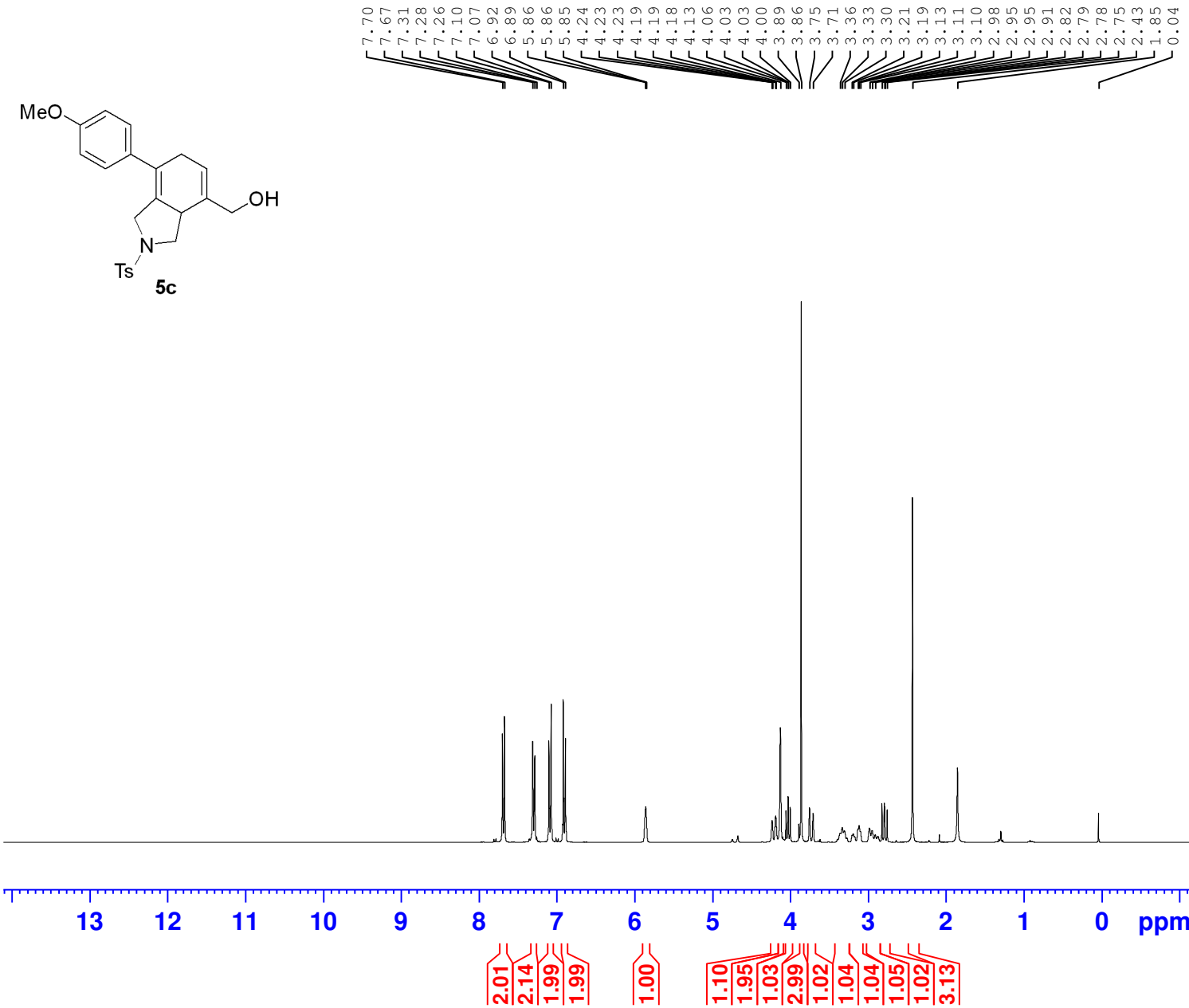
5b

143.32
137.20
136.65
134.10
133.78
129.73
129.61
129.15
128.96
127.31
127.10
122.51
77.31
76.99
76.68
65.06
51.27
49.71
40.40
32.10
21.39
21.05



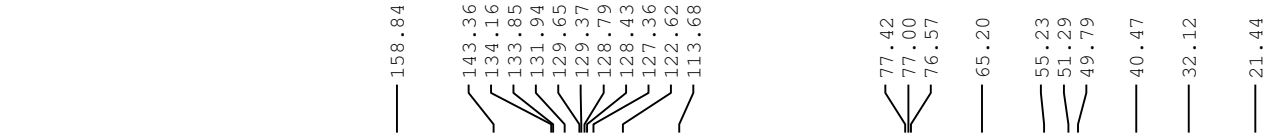

```
Current Data Parameters
NAME                   w
EXPNO                 33
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211028
Time               14.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               294.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.90 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.35839999 W
PLW13        0.29030001 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278720 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

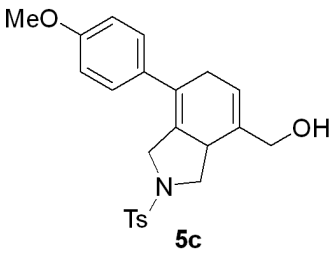
3sjwei 5360 yzk-2-91-fr 1h cdcl3



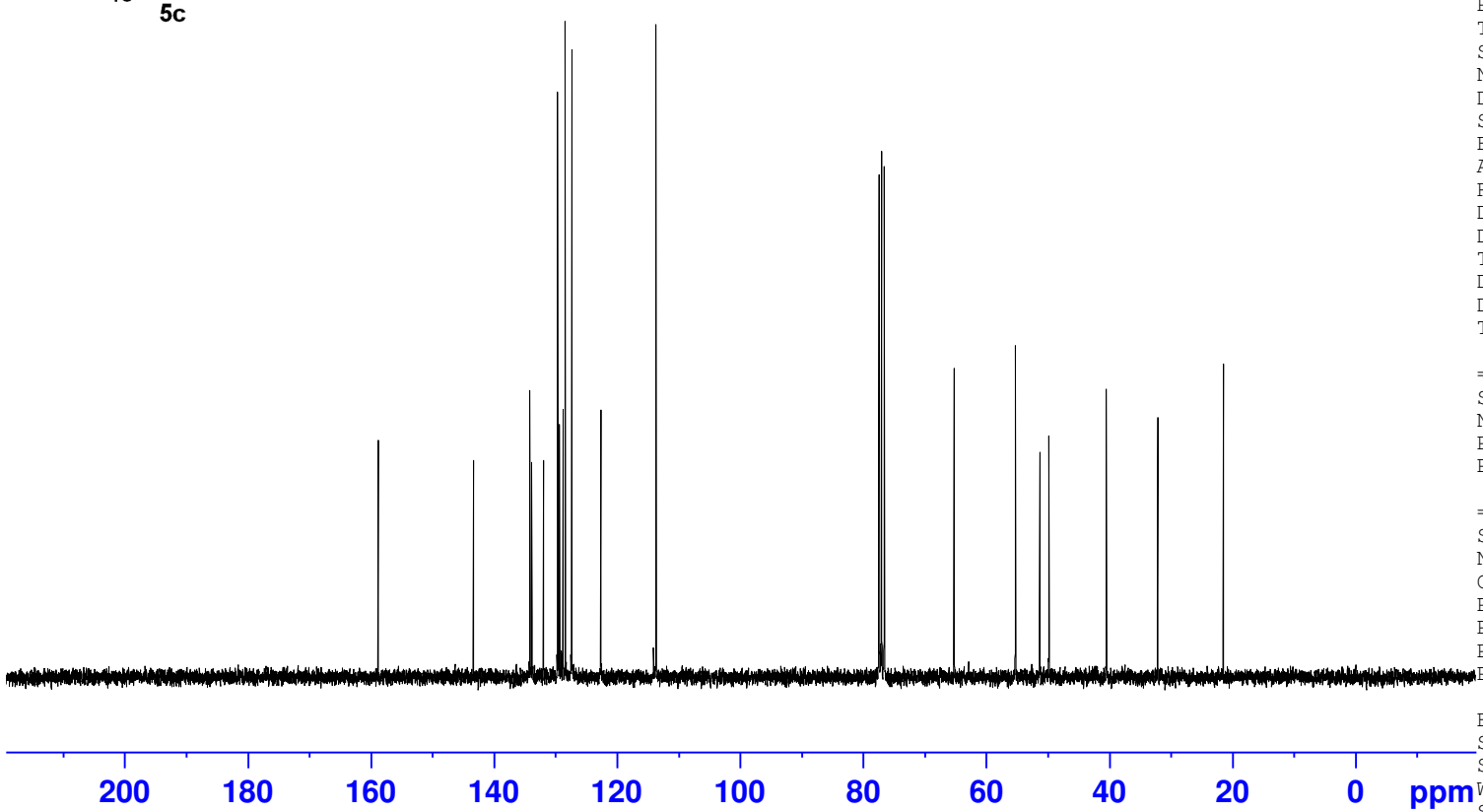

```
Current Data Parameters
NAME      5c-yzk-2-91-H
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20210917
Time                9.25
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ             5.4525952 sec
RG                  90.5
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                 65536
SF          300.1299940 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3sjwei 5399 yzk-2-91-fr 13c cdcl3



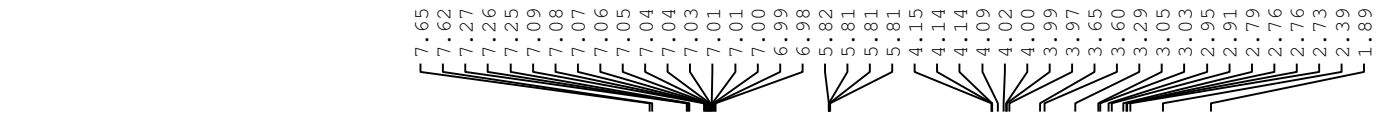


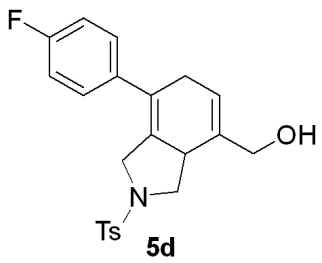
5c



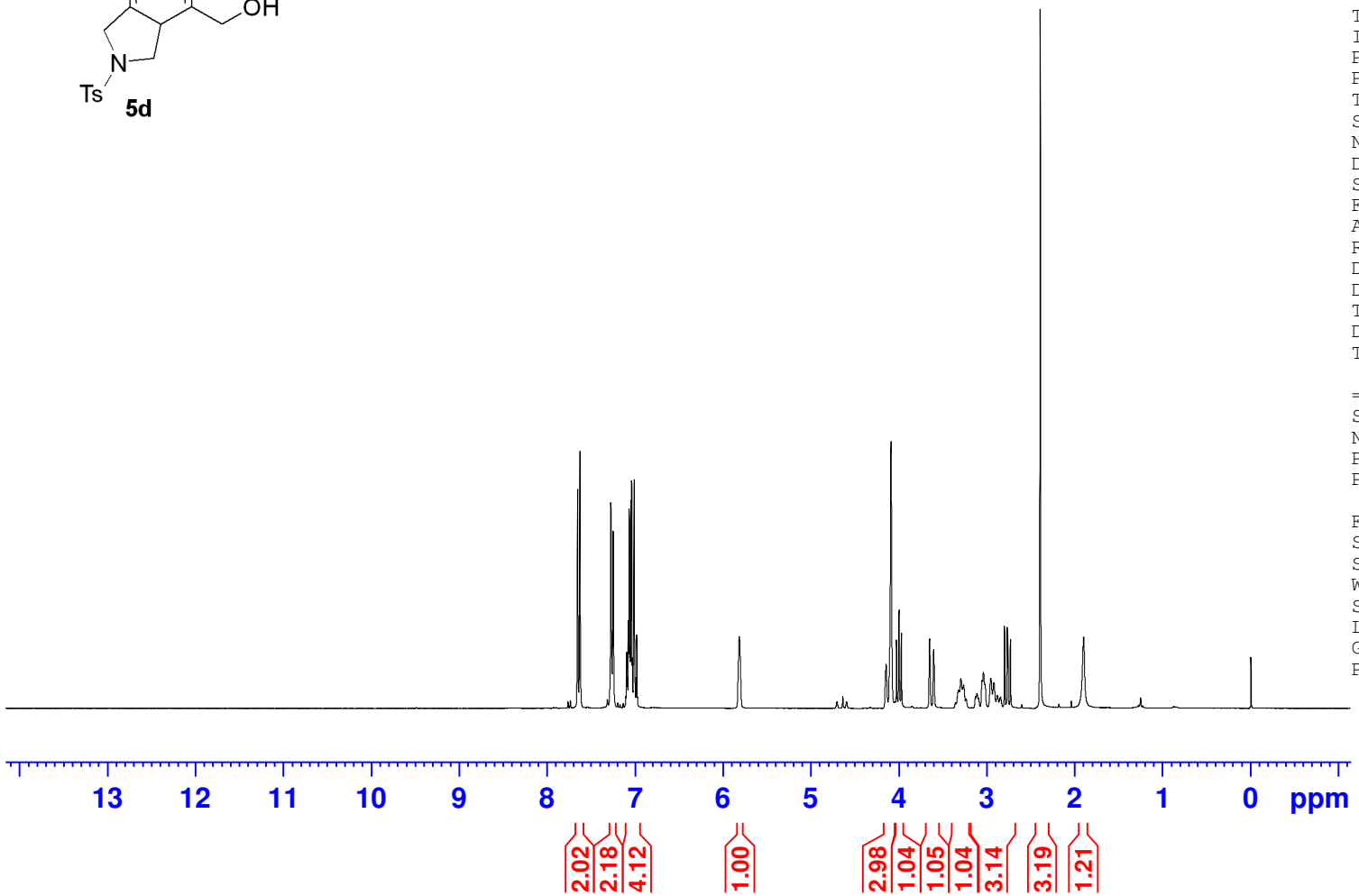

```
Current Data Parameters
NAME      5c-yzk-2-91-C
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20210918
Time               10.53
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4677553 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

3sjwei 5363 yzk-2-88-fr 1h cdcl3



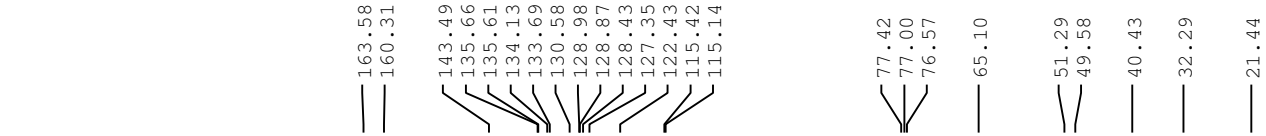


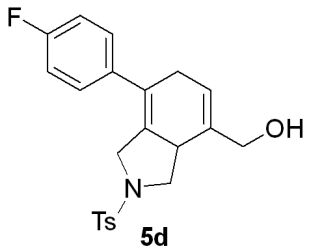
5d




```
Current Data Parameters
NAME            YZK-2-88
EXPNO               5363
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210916
Time               10.46
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                  80.6
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300074 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3sjwei 5376 yzk-2-88-fr 13c cdcl3

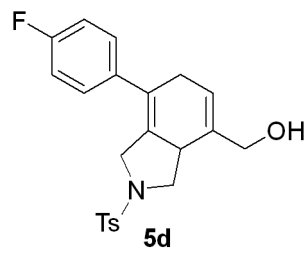




5d


```
Current Data Parameters
NAME      5d-yzk-2-88-C
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20210917
Time               11.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4677557 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

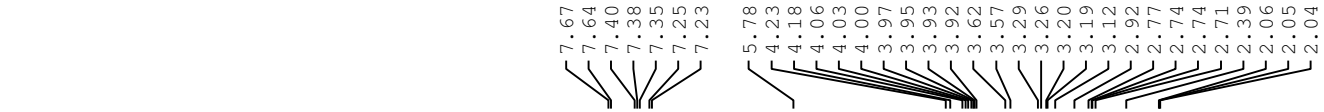
3sjwei 5364 yzk-2-88-fr 19f cdcl3

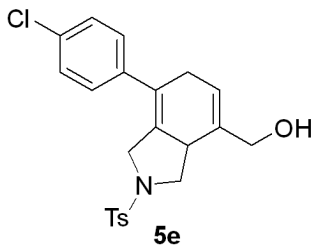


5d

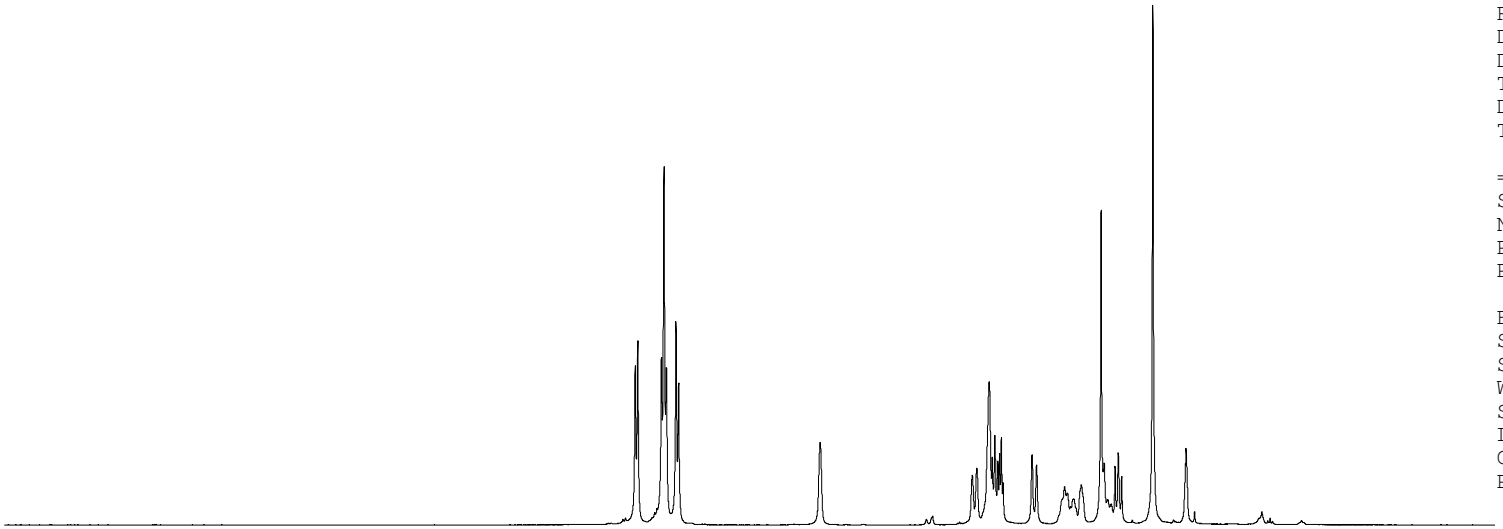

```
Current Data Parameters
NAME              workup
EXPNO               5364
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210916
Time               10.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD                131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            66964.289 Hz
FIDRES          0.510897 Hz
AQ             0.9786710 sec
RG                   203
DW                 7.467 usec
DE                 6.50 usec
TE                -59.1 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         282.3761148 MHz
NUC1                19F
P1                14.50 usec
PLW1         10.39999962 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         14.00000000 W
PLW12         0.17284000 W

F2 - Processing parameters
SI                 65536
SF           282.4043552 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

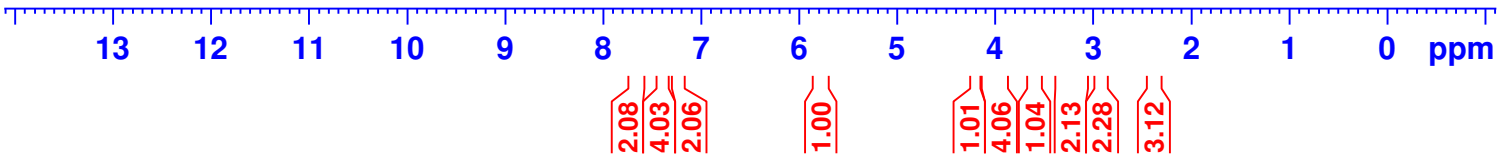
3sjwei 5603 yzk-3-39 1h acetone





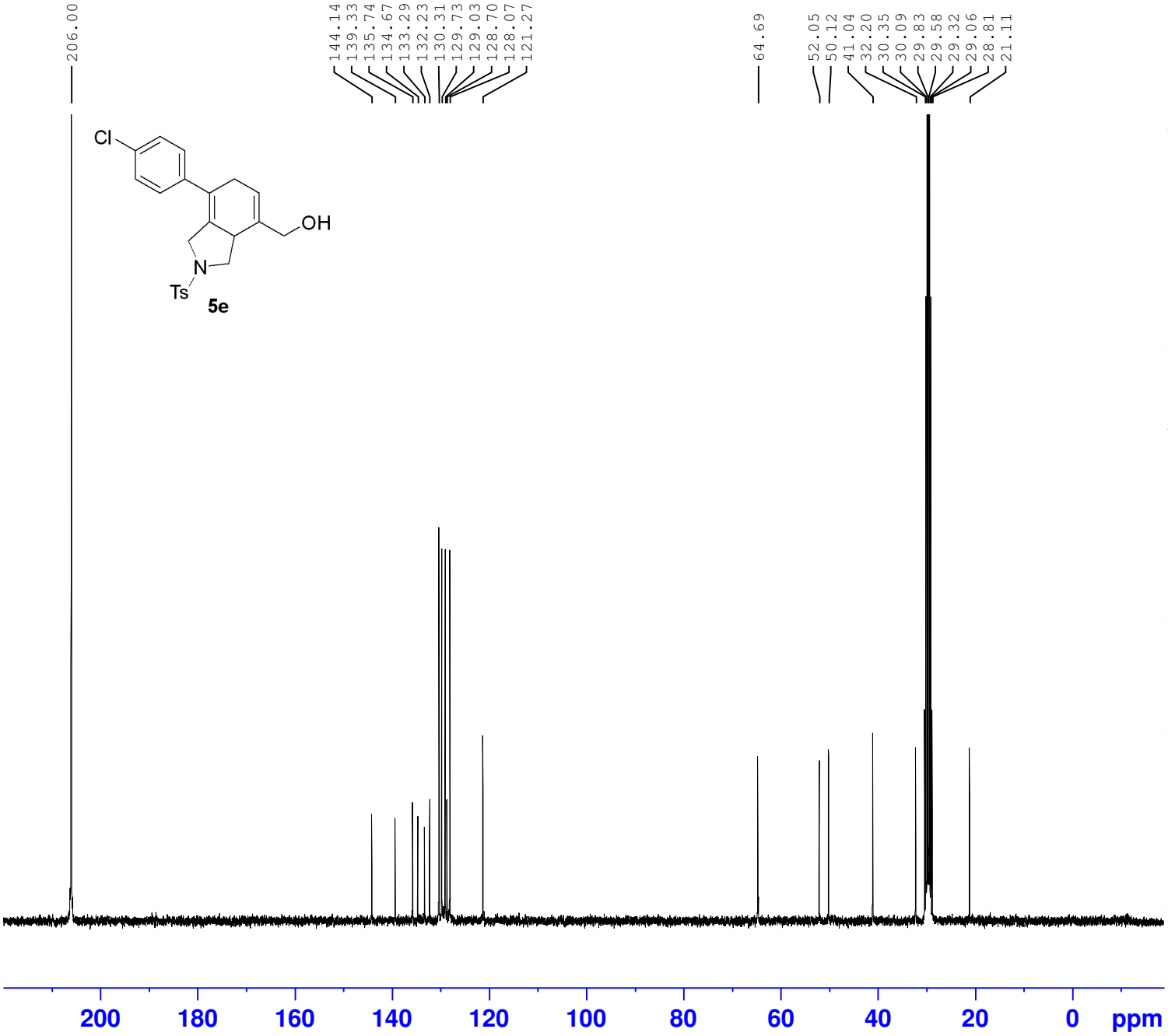
5e





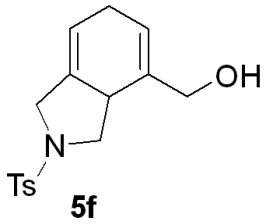

```
Current Data Parameters
NAME                  3-39
EXPNO                 5603
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211113
Time                 10.03
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                       16
DS                        2
SWH               6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      101
DW                   83.200 usec
DE                    6.50 usec
TE                   -59.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                    1H
P1                   10.00 usec
PLW1           14.00000000 W

F2 - Processing parameters
SI                    65536
SF             300.1300052 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

3sjwei 5604 yzk-3-39 13c acetone

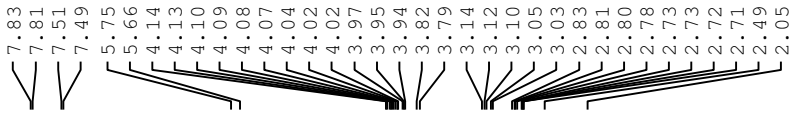


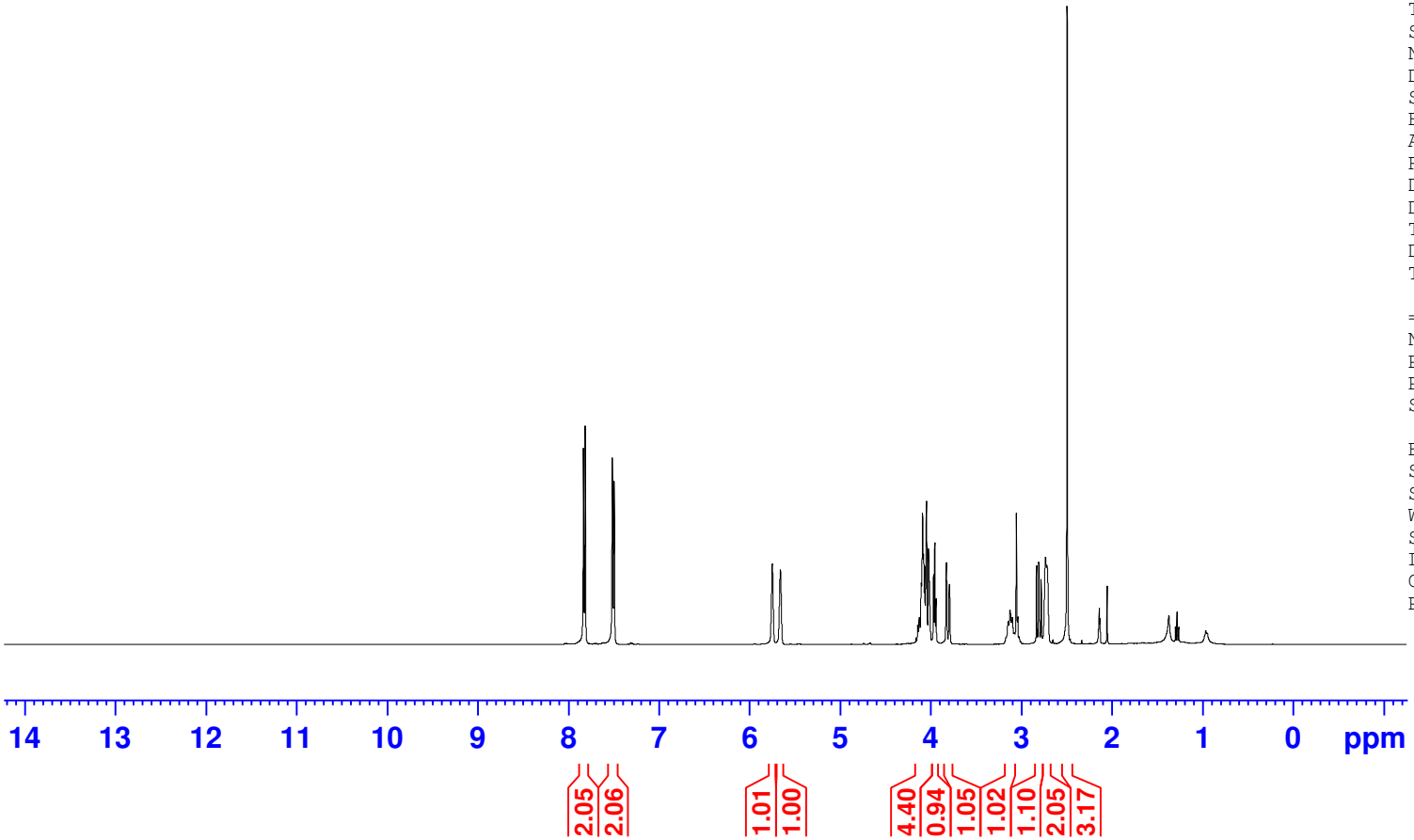

```
Current Data Parameters
NAME                  3-39
EXPNO                 5604
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211113
Time                 10.50
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                     700
DS                       4
SWH              18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175317 sec
RG                     203
DW                27.733 usec
DE                 6.50 usec
TE                -59.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4752949 MHz
NUC1                  13C
P1                  9.50 usec
PLW1          34.20000076 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          14.00000000 W
PLW12          0.17284000 W
PLW13          0.14000000 W

F2 - Processing parameters
SI                   32768
SF            75.4677050 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

YZK-3-32-fr



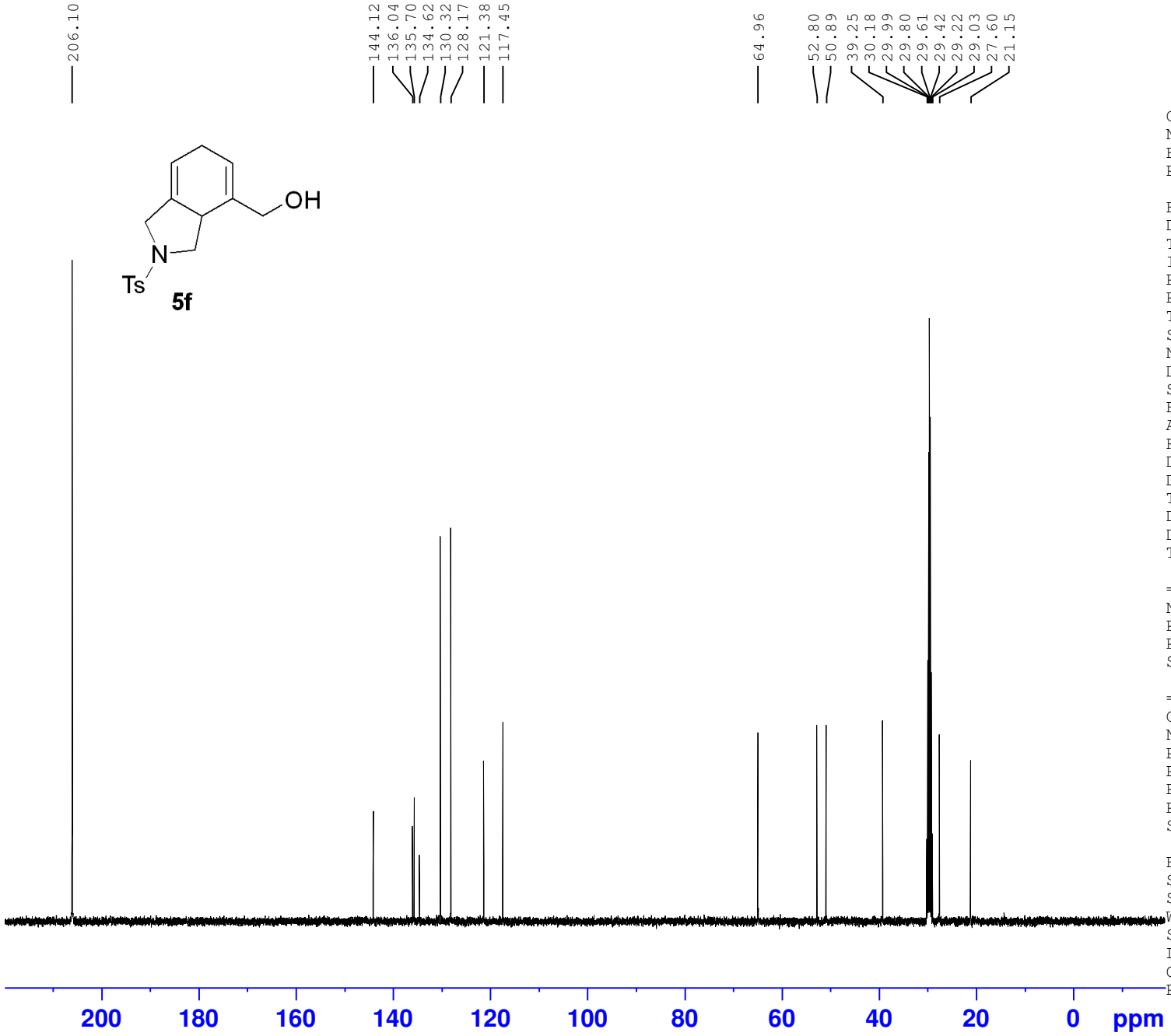
5f





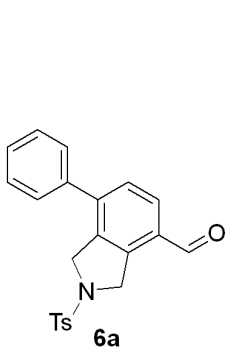

```
Current Data Parameters
NAME                  3-32
EXPNO                   36
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211029
Time                 14.50
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                        8
DS                        2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    29.75
DW                   60.800 usec
DE                    6.50 usec
TE                   294.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.40 usec
PLW1           14.00000000 W
SFO1           400.1924713 MHz

F2 - Processing parameters
SI                    65536
SF             400.1899775 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

YZK-3-32-fr




```
Current Data Parameters
NAME                  3-32
EXPNO                   37
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211029
Time                  14.53
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                      60
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                  193.13
DW                  20.800 usec
DE                   6.50 usec
TE                  294.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.90 usec
PLW1          53.00000000 W
SFO1         100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PLW2          14.00000000 W
PLW12          0.35839999 W
PLW13          0.29030001 W
SFO2         400.1916008 MHz

F2 - Processing parameters
SI                    32768
SF           100.6277995 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

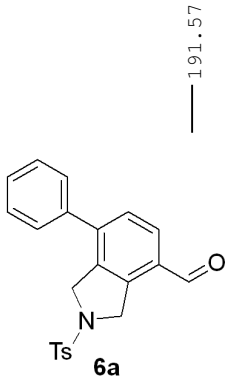
YZK-3-85



6a


```
Current Data Parameters
NAME                  3-85
EXPNO                  232
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211214
Time                  19.51
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    68.24
DW                   60.800 usec
DE                    6.50 usec
TE                   292.5 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.40 usec
PLW1           14.00000000 W
SFO1           400.1924713 MHz

F2 - Processing parameters
SI                    65536
SF             400.1900179 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

YZK-3-85



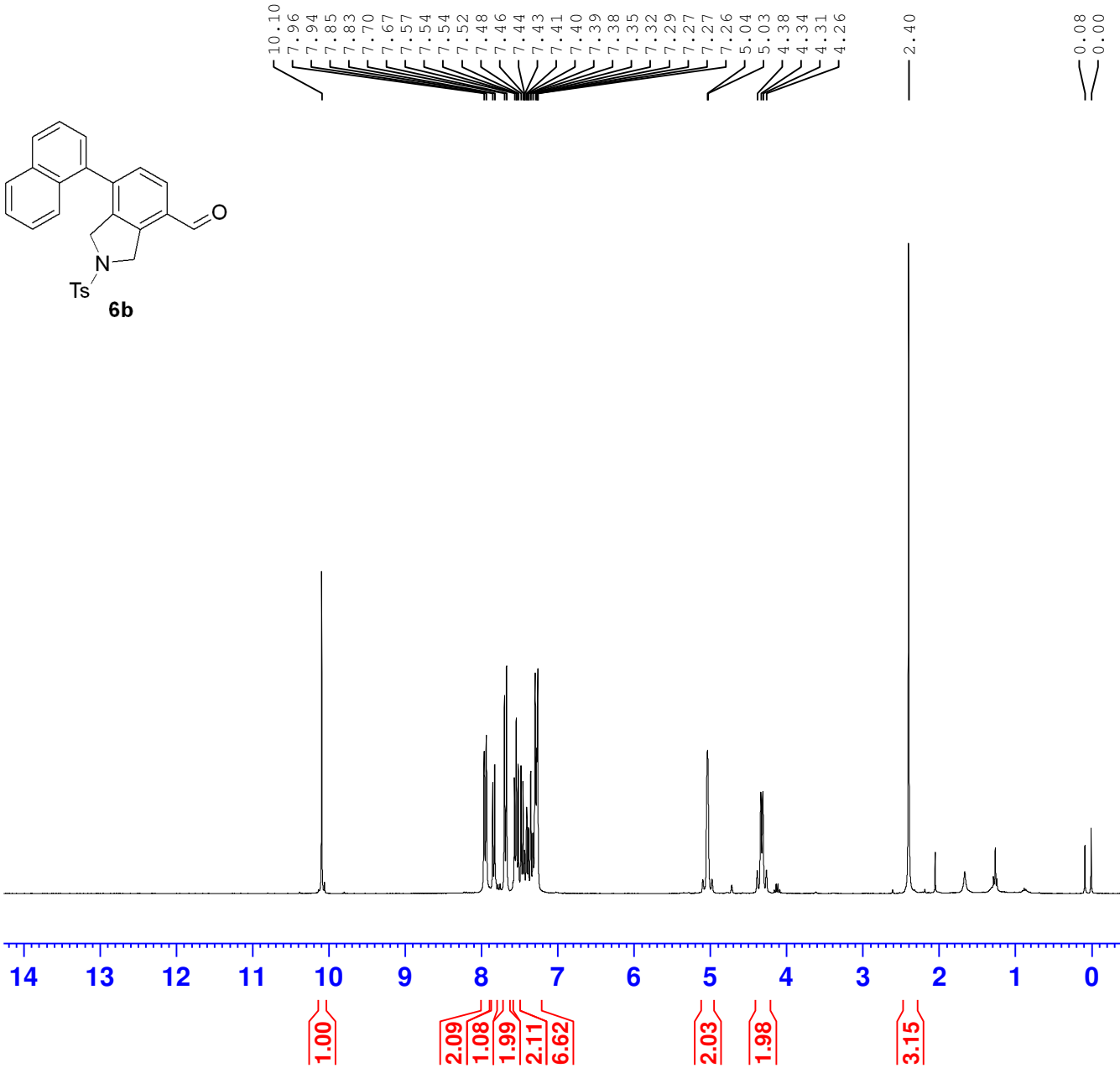
6a

191.57
143.71
142.79
138.29
137.87
136.08
133.50
132.97
129.86
129.82
128.91
128.88
128.61
127.82
127.55
77.31
77.00
76.68
54.20
52.58
21.45

200 180 160 140 120 100 80 60 40 20 0 ppm

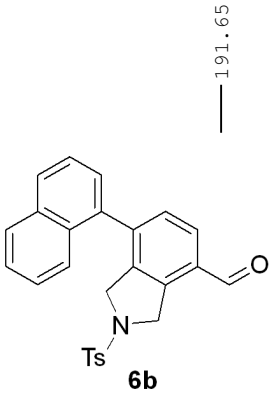
```
Current Data Parameters
NAME       6a-yzk-3-85-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211214
Time               19.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  110
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               293.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.90 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.35839999 W
PLW13        0.29030001 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF          100.6278682 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

3sjwei 5710 yzk-3-74-mno2 1h cdcl3




```
Current Data Parameters
NAME                  3-74
EXPNO                 5710
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211211
Time                  9.32
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4525952 sec
RG                     128
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                    1H
P1                  10.00 usec
PLW1          14.00000000 W

F2 - Processing parameters
SI                   65536
SF            300.1300074 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

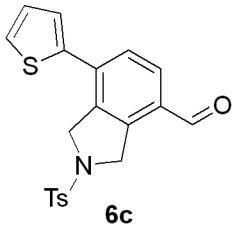
3sjwei 5711 yzk-3-74-mno2 13c cdcl3



6b


```
Current Data Parameters
NAME                  3-74
EXPNO                 5711
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211211
Time                  9.41
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     100
DS                       4
SWH             18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175317 sec
RG                     203
DW                27.733 usec
DE                 6.50 usec
TE                -59.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4752949 MHz
NUC1                  13C
P1                  9.50 usec
PLW1          34.20000076 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          14.00000000 W
PLW12          0.17284000 W
PLW13          0.14000000 W

F2 - Processing parameters
SI                   32768
SF            75.4677556 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

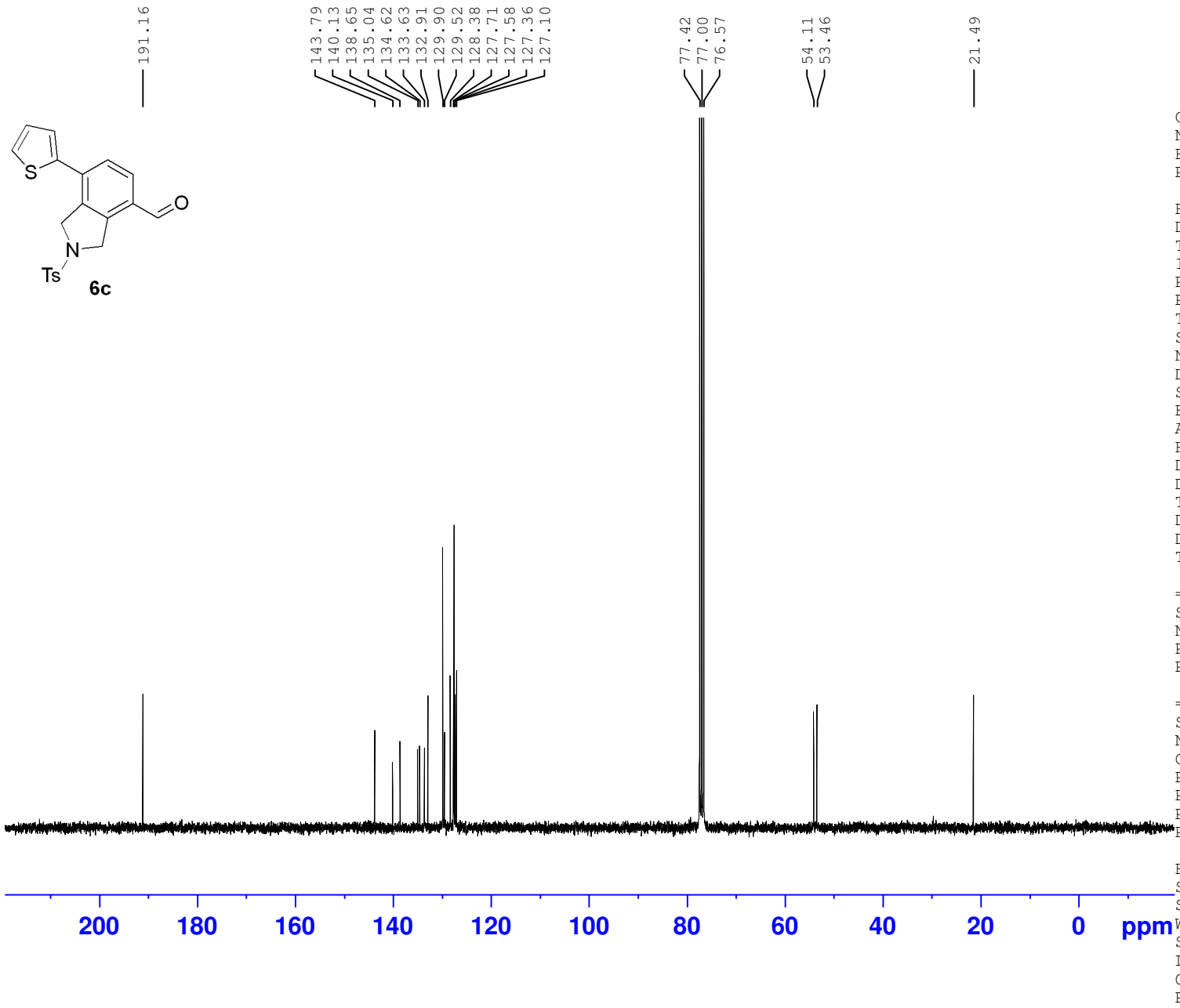
3sjwei 5741yzk-3-92-fr-mno2 1h cdcl3



6c

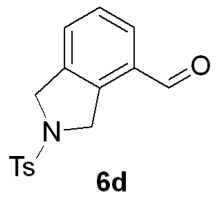

```
Current Data Parameters
NAME                  3-92
EXPNO                 5741
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211223
Time                 11.30
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4525952 sec
RG                    181
DW                 83.200 usec
DE                  6.50 usec
TE                 -59.1 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                   1H
P1                  10.00 usec
PLW1          14.00000000 W

F2 - Processing parameters
SI                  65536
SF            300.1300073 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

3sjwei 5742 yzk-3-92-fr-mno2 13c cdcl3




```
Current Data Parameters
NAME                  3-92
EXPNO                 5742
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211223
Time                  12.37
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175317 sec
RG                      203
DW                  27.733 usec
DE                   6.50 usec
TE                  -59.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4752949 MHz
NUC1                   13C
P1                    9.50 usec
PLW1           34.20000076 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           14.00000000 W
PLW12           0.17284000 W
PLW13           0.14000000 W

F2 - Processing parameters
SI                    32768
SF              75.4677530 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

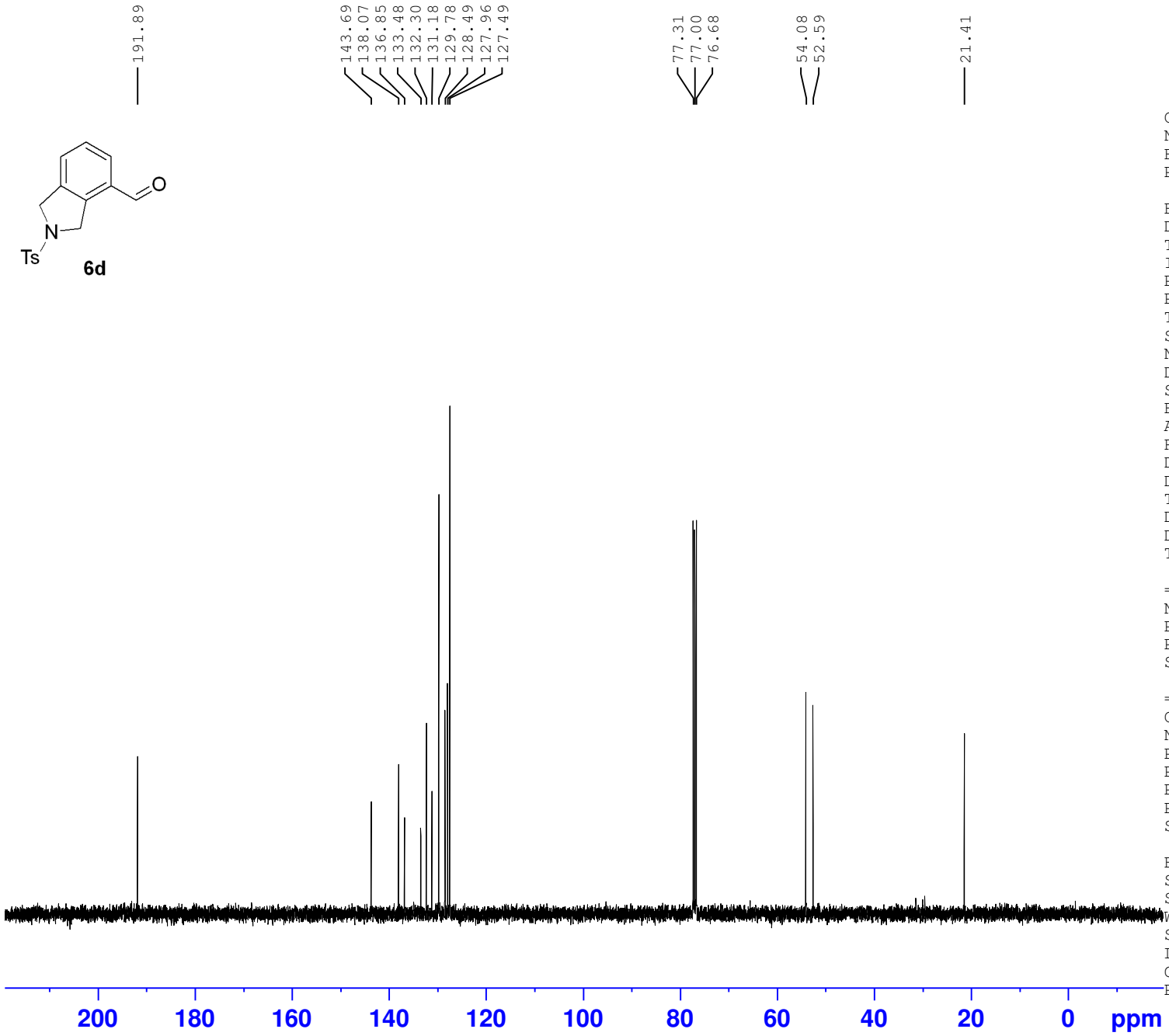
YZK-3-57-MnO2



6d

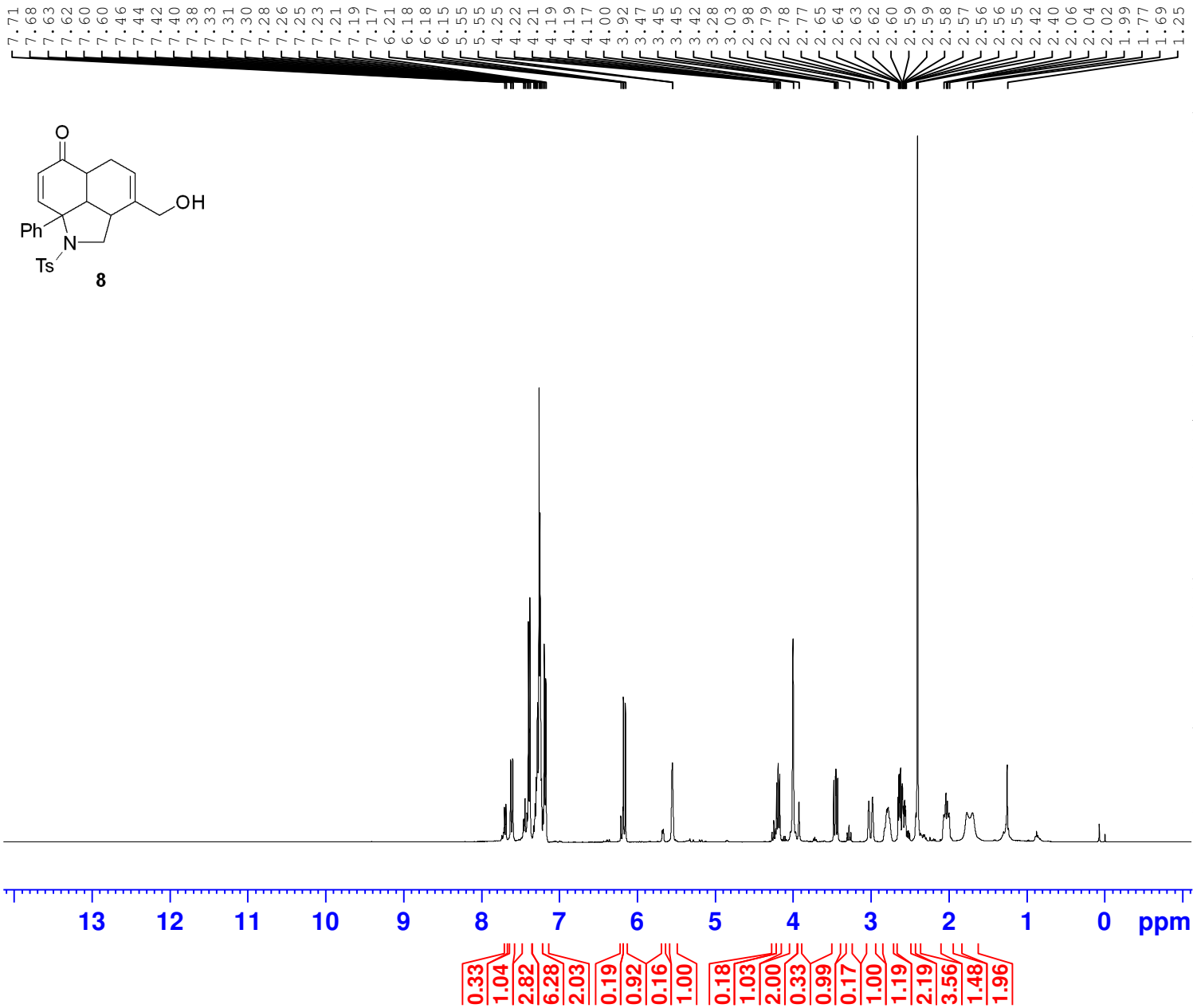

```
Current Data Parameters
NAME                  3-57
EXPNO                  155
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211129
Time                 20.00
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                   61.19
DW                  60.800 usec
DE                   6.50 usec
TE                  292.9 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.40 usec
PLW1          14.00000000 W
SFO1          400.1924713 MHz

F2 - Processing parameters
SI                   65536
SF            400.1900162 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

YZK-3-57-MnO2



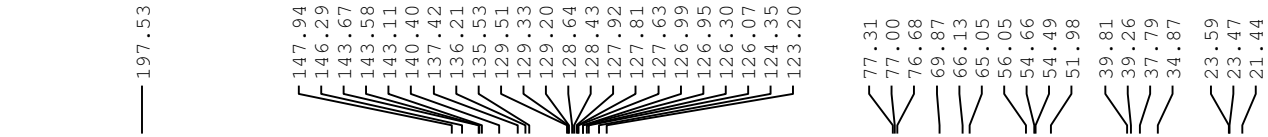

```
Current Data Parameters
NAME                  3-57
EXPNO                  156
PROCNO                   1

F2 - Acquisition Parameters
Date_            20211129
Time                20.03
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    38
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                193.13
DW                20.800 usec
DE                 6.50 usec
TE                293.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.90 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2         14.00000000 W
PLW12         0.35839999 W
PLW13         0.29030001 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF          100.6278702 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

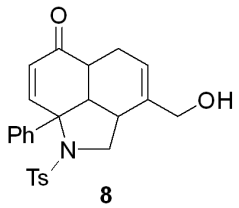
YZK-4-64



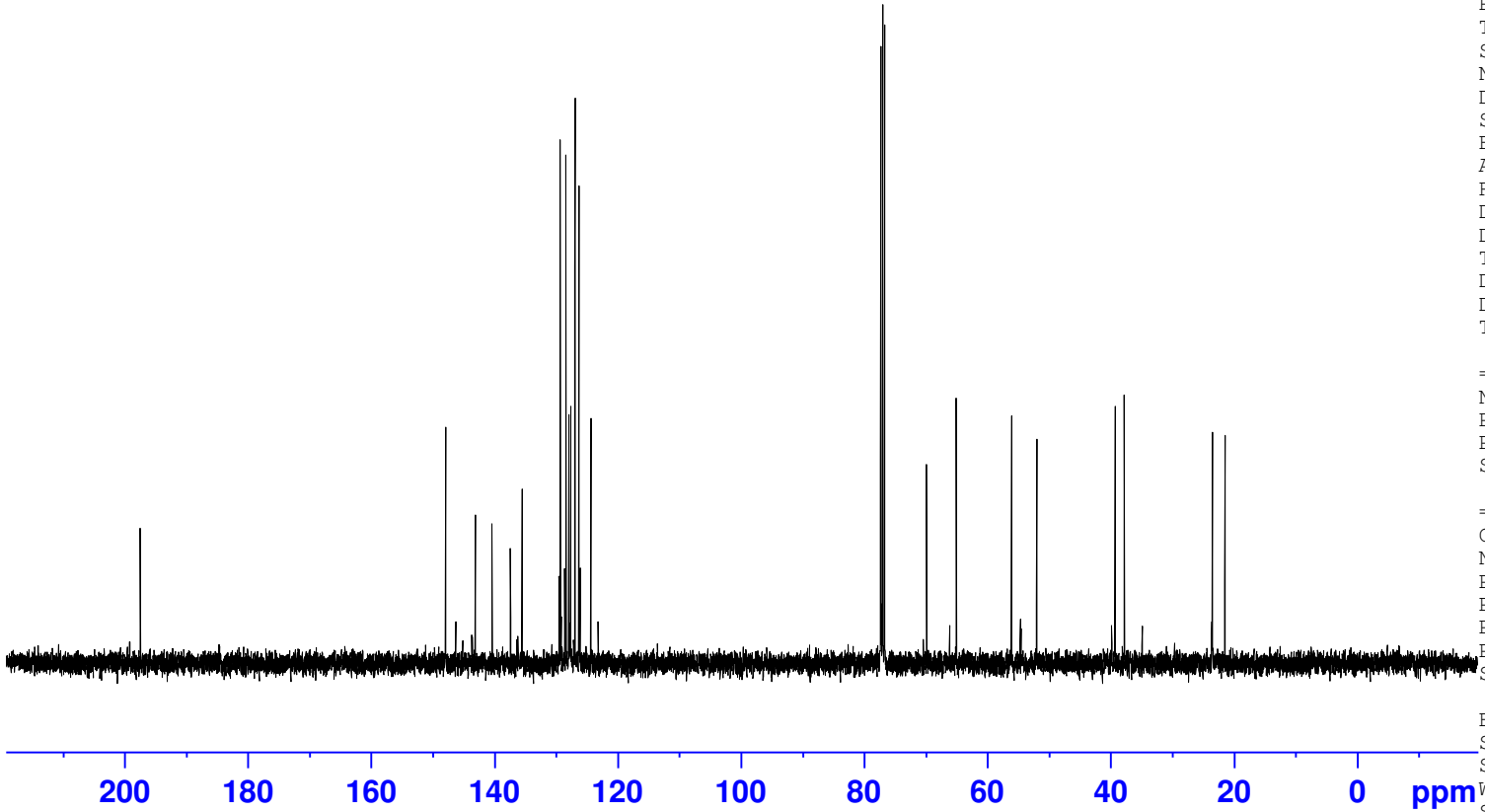

```
Current Data Parameters
NAME                  0701
EXPNO                  143
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220701
Time                 19.49
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9922944 sec
RG                  75.43
DW                60.800 usec
DE                 6.50 usec
TE                294.7 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                  65536
SF           400.1900247 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

YZK-4-64



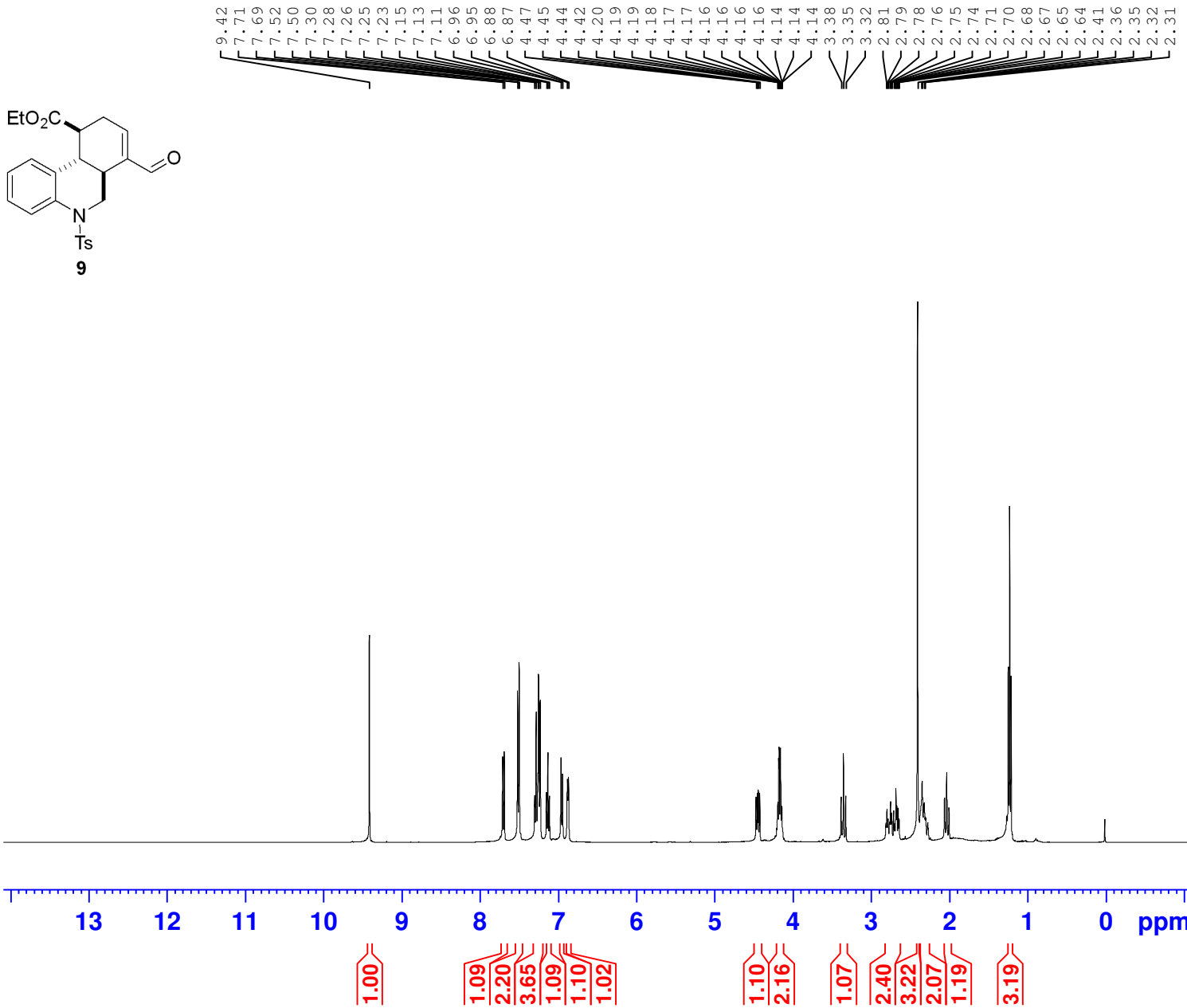


8



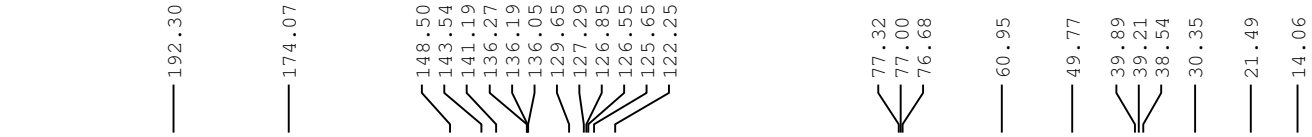

```
Current Data Parameters
NAME       8-yzk-4-64-C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220701
Time              19.53
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                193.13
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278667 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

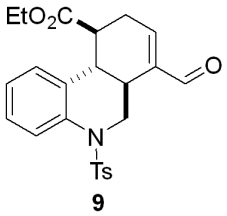
YZK-4-38




```
Current Data Parameters
NAME                  0605
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220606
Time                 21.15 h
INSTRUM              Avance
PROBHD   Z116098_0833 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8196.722 Hz
FIDRES             0.250144 Hz
AQ                3.9976959 sec
RG                  82.3452
DW                  61.000 usec
DE                   13.54 usec
TE                   292.8 K
D1              1.00000000 sec
TD0                      1
SFO1           400.1324708 MHz
NUC1                    1H
P0                   3.33 usec
P1                  10.00 usec
PLW1           20.73200035 W

F2 - Processing parameters
SI                    65536
SF             400.1300013 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

YZK-4-38





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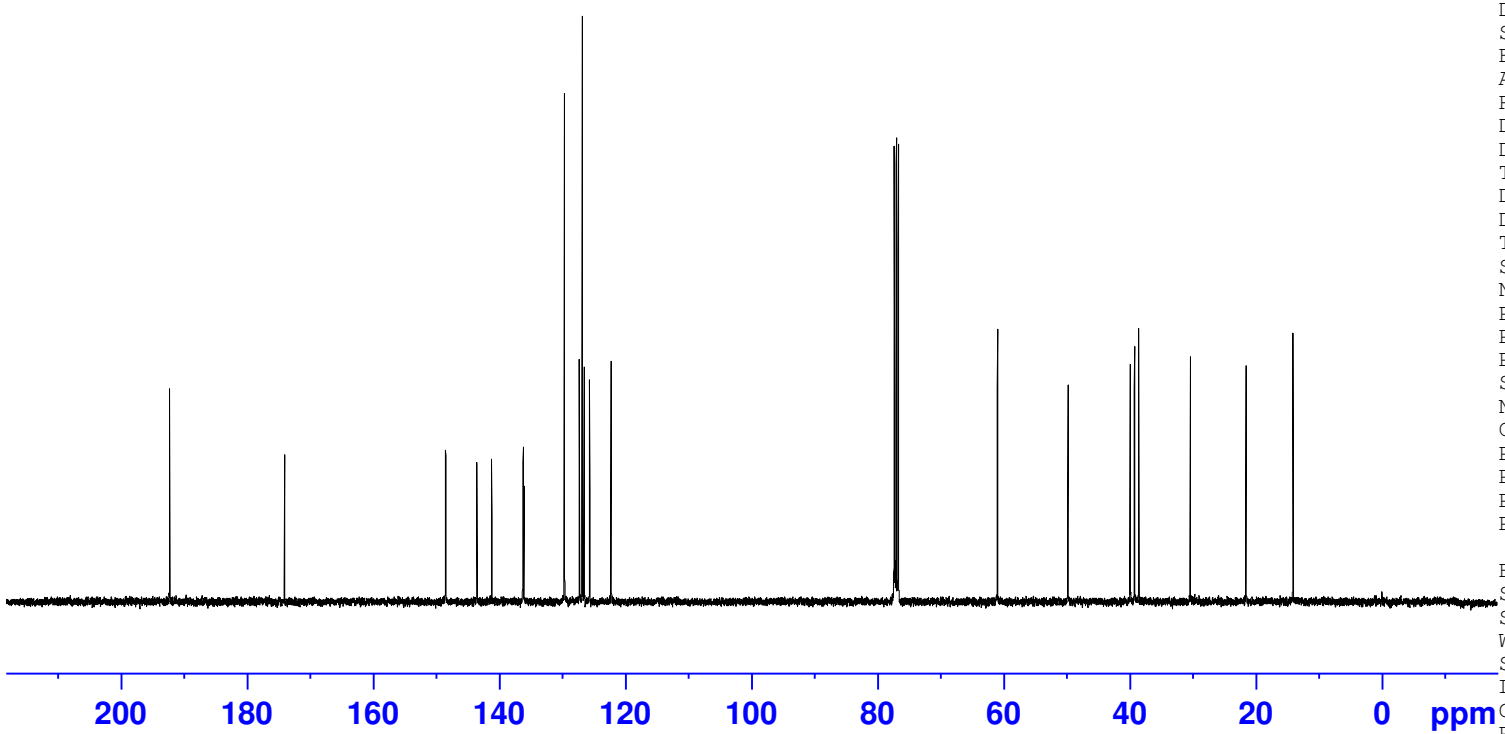
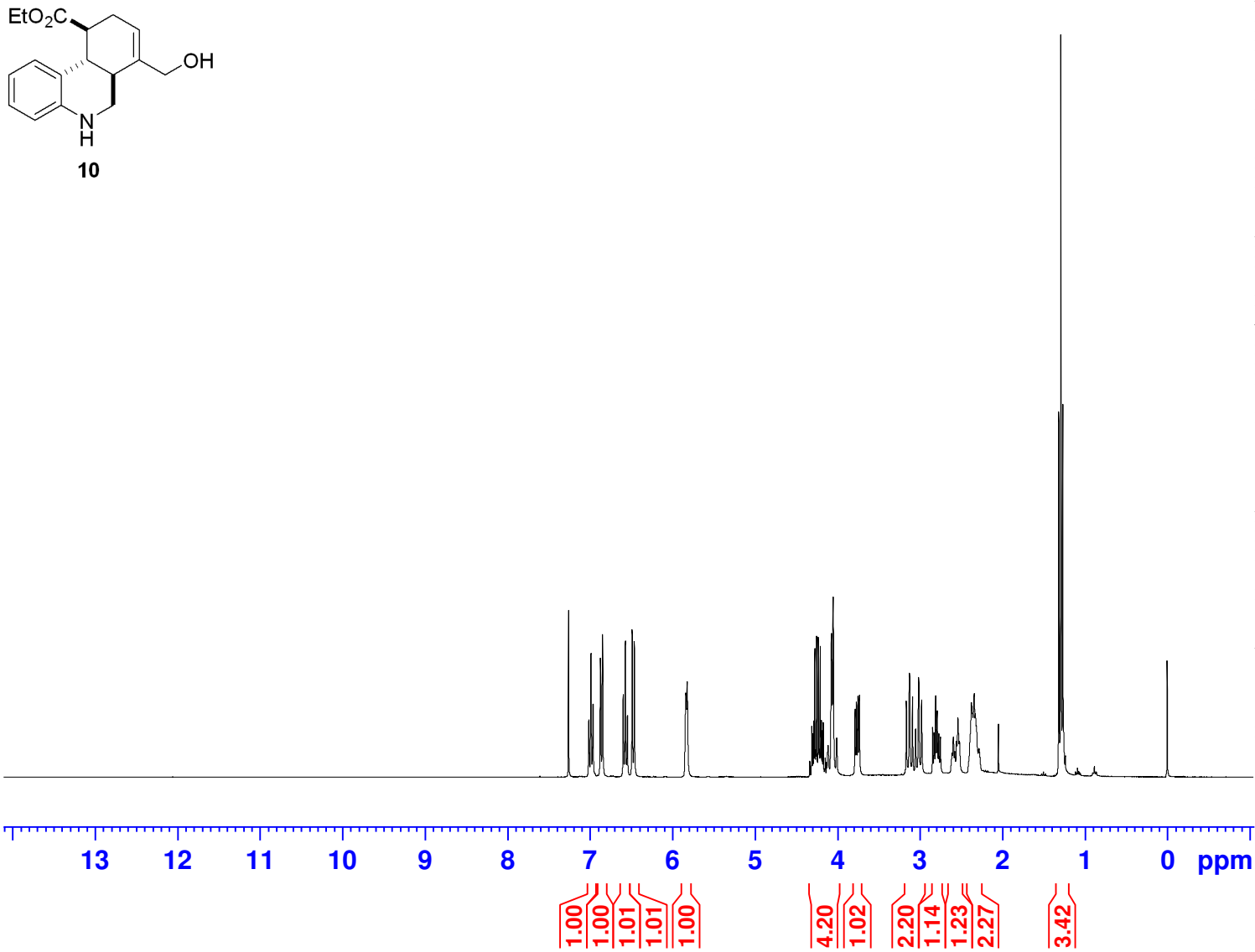


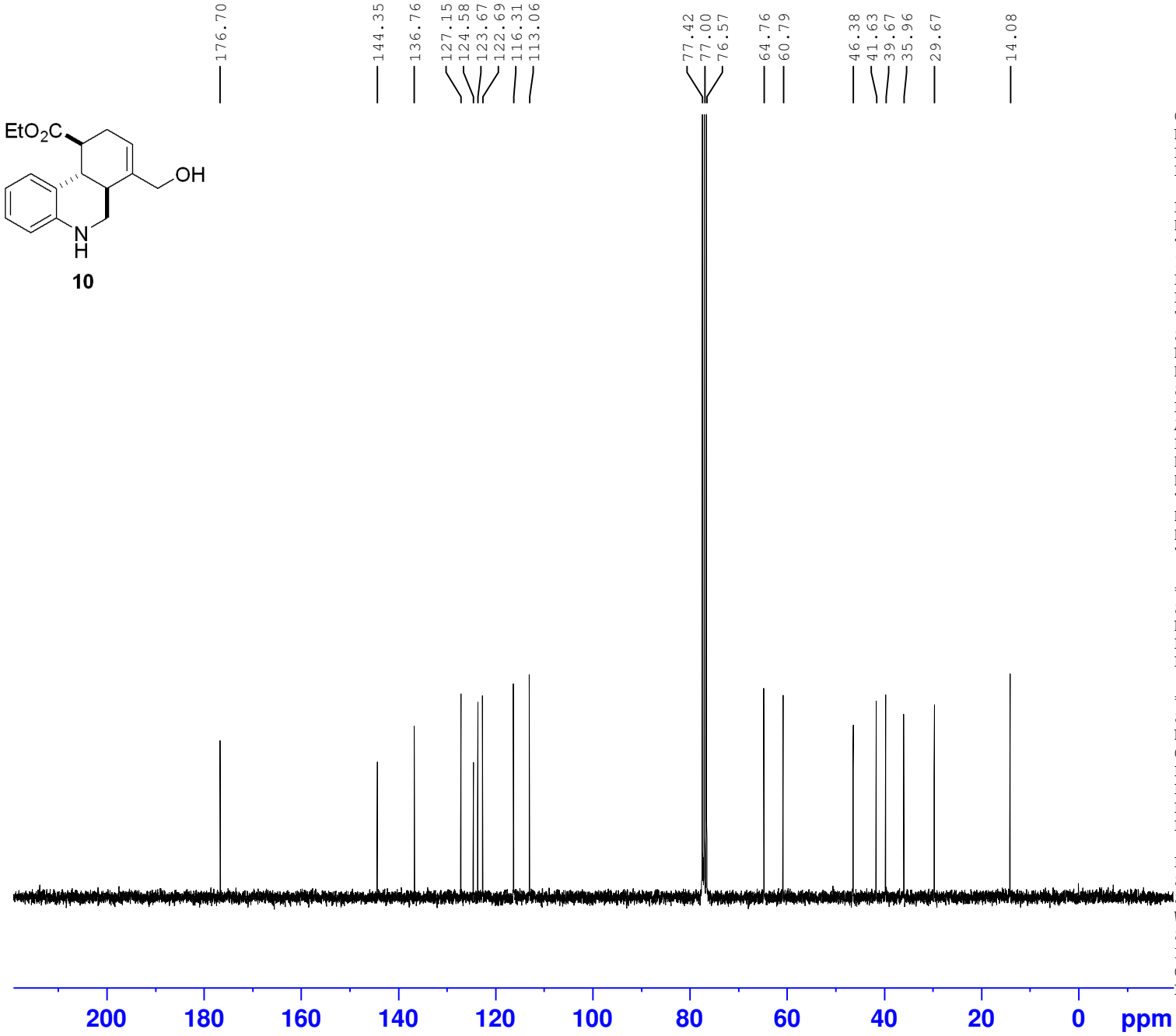

```
Current Data Parameters
NAME      11-yzk-4-38-C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220605
Time              19.43 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                51.55
DW               21.000 usec
DE                6.50 usec
TE               298.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         87.89900208 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2         20.73200035 W
PLW12         0.25595000 W
PLW13         0.12874000 W

F2 - Processing parameters
SI                32768
SF          100.6127735 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

3sjwei 5731 yzk-3-90 1h cdcl3



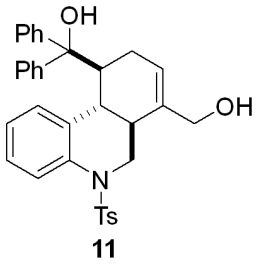

```
Current Data Parameters
NAME                  3-90
EXPNO                 5731
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211218
Time                  9.55
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4525952 sec
RG                     144
DW                  83.200 usec
DE                   6.50 usec
TE                  -59.1 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                    1H
P1                  10.00 usec
PLW1          14.00000000 W

F2 - Processing parameters
SI                   65536
SF            300.1300071 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

3sjwei 5732 yzk-3-90 13c cdcl3




```
Current Data Parameters
NAME                  3-90
EXPNO                 5732
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211218
Time                 10.35
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     600
DS                       4
SWH             18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175317 sec
RG                     203
DW                27.733 usec
DE                 6.50 usec
TE                -59.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4752949 MHz
NUC1                  13C
P1                  9.50 usec
PLW1          34.20000076 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2          14.00000000 W
PLW12          0.17284000 W
PLW13          0.14000000 W

F2 - Processing parameters
SI                    32768
SF             75.4677541 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

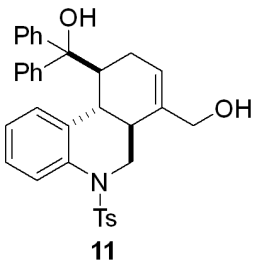
YZK-4-26



11


```
Current Data Parameters
NAME                  4-26
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220606
Time                 21.10 h
INSTRUM              Avance
PROBHD   Z116098_0833 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8196.722 Hz
FIDRES            0.250144 Hz
AQ               3.9976959 sec
RG                  97.6563
DW                  61.000 usec
DE                   13.54 usec
TE                   292.9 K
D1              1.00000000 sec
TD0                      1
SFO1           400.1324708 MHz
NUC1                    1H
P0                   3.33 usec
P1                  10.00 usec
PLW1           20.73200035 W

F2 - Processing parameters
SI                   65536
SF             400.1300100 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

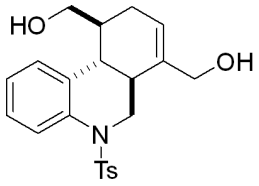
YZK-4-26



11


```
Current Data Parameters
NAME      13-yzk-4-26-C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220605
Time              17.34 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG               48.4406
DW               21.000 usec
DE                6.50 usec
TE                298.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1         87.89900208 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2         20.73200035 W
PLW12         0.25595000 W
PLW13         0.12874000 W

F2 - Processing parameters
SI                32768
SF          100.6127727 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

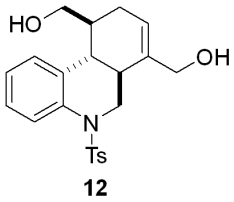
YZK-4-10



12


```
Current Data Parameters
NAME                  4-10
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220117
Time                 14.26 h
INSTRUM              Avance
PROBHD    Z116098_0833 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8196.722 Hz
FIDRES             0.250144 Hz
AQ                3.9976959 sec
RG                      101
DW                   61.000 usec
DE                   13.54 usec
TE                   293.0 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                     1H
P0                   3.33 usec
P1                   10.00 usec
PLW1           20.73200035 W

F2 - Processing parameters
SI                    65536
SF             400.1300099 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```

YZK-4-10



12

143.63
138.75
136.46
135.82
135.21
129.37
127.93
126.96
126.05
123.74
122.76
77.31
77.00
76.68
65.81
64.85
50.89
42.43
37.80
33.80
28.01
21.47
-0.03

200 180 160 140 120 100 80 60 40 20 0 ppm

```
Current Data Parameters
NAME                   wk
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220118
Time                0.40 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG              48.6724
DW               21.000 usec
DE                6.50 usec
TE                294.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6228298 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         87.89900208 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2         20.73200035 W
PLW12         0.25595000 W
PLW13         0.12874000 W

F2 - Processing parameters
SI                 32768
SF          100.6127727 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```