Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

[3+2] cycloaddition for the assembly of indolizine-based heterocyclic sulfonyl fluorides

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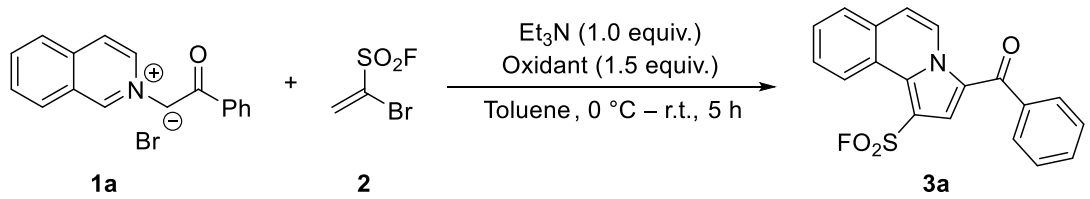
1. General Information

All reactions were carried out under an air atmosphere unless otherwise specified. Oil bath was used for the heating reactions. NMR spectra were recorded in $CDCl_3$, CD_2Cl_2, D_2O or DMSO-d_6 on a 500 MHz (for ^1H), 471 MHz (for ^{19}F), and 126 MHz (for ^{13}C) Bruker Avance spectrometer, and were internally referenced to solvent residual signals (note: $CDCl_3$: δ H = 7.264 ppm, δ C = 77.160 ppm; CD_2Cl_2: δ H = 5.320 ppm, δ C = 53.840 ppm; D_2O: δ H = 4.790 ppm; DMSO-d_6: δ H = 2.500 ppm, δ C = 39.520 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, m = multiplet. The coupling constants were reported in Hertz (Hz). The HPLC experiments were carried out on a Waters e2695 instrument (column: J&K, RP-C18, 5 μm, 4.6 × 150 mm), and the HPLC yields of the products were determined by using the corresponding pure compounds as the external standards. Melting points were measured and uncorrected. HRMS experiments were performed on a TOF-Q ESI instrument. Reagents used in the reactions were all purchased from commercial sources and used without further purification. The product spots on the thin layer chromatography (TLC) were visualized under ultraviolet light (254 nm or 365 nm) followed by staining with potassium permanganate or phosphomolybdic acid.

2. Optimization of the Reaction Conditions

Table S1 Screening of the oxidant[a]

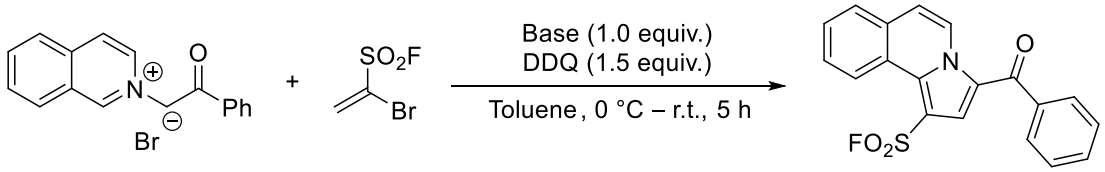


1a **2** **3a**

Entry	Oxidant (1.5 equiv.)	Yield (3a, %)[b]
1	**DDQ**	**46**
2	TEMPO	20
3	BQ	10
4	NFSI	26
5	AgO	40
6	$AgNO_3$	19
7	CuO	14
8	$CuBr_2$	8
9	$Cu(OAc)_2$	33
10	MnO_2	14
11	/	N.D.

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (112 mg, 0.6 mmol, 3.0 equiv.), Et_3N (20 mg, 0.2 mmol, 1.0 equiv.), oxidant (0.3 mmol, 1.5 equiv.) and toluene (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL). After the addition was over, the resulting mixture was stirred at room temperature for 5 h. [b]HPLC yield (t_R = 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)). N.D. = Not detectable.

Table S2 Screening of the base[a]

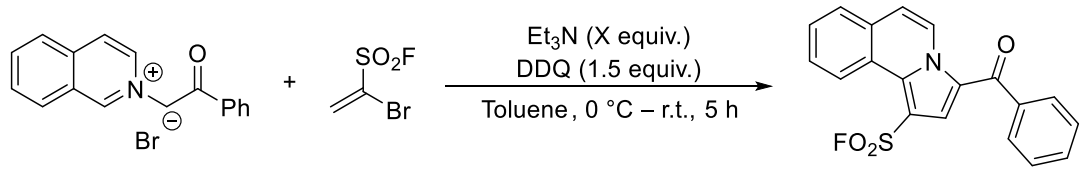


1a **2** **3a**

Entry	Base (1.0 equiv.)	Yield (3a, %)[b]
1	**Et_3N**	**45**
2	DABCO	28
3	DIPEA	42
4	TMEDA	40
5	DBU	14
6	Tripropylamine	24
7	Na_2CO_3	N.D.
8	$NaHCO_3$	N.D.
9	K_2CO_3	N.D.
10	$KHCO_3$	N.D.
11	$CsCO_3$	6
12	KH_2PO_4	N.D.
13	/	N.D.

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (112 mg, 0.6 mmol, 3.0 equiv.), base (0.2 mmol, 1.0 equiv.), DDQ (68 mg, 0.3 mmol, 1.5 equiv.) and toluene (0.1M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 °C. After the addition was over, the resulting mixture was stirred at room temperature for 5 h. [b]HPLC yield (t_R = 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)). N.D. = Not detectable.

Table S3 Screening of the Et_3N loading[a]

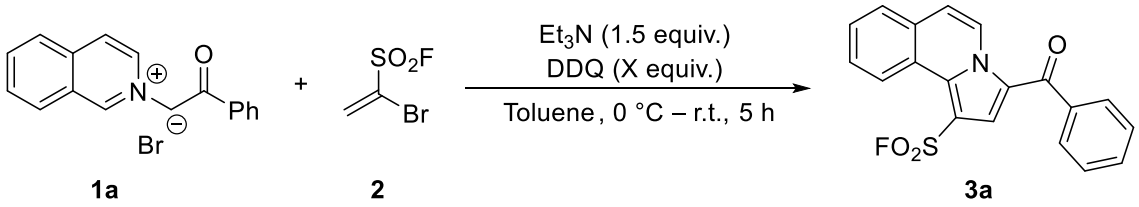


1a **2** **3a**

Entry	Et_3N (X equiv.)	Yield (3a, %)[b]
1	1.0	45
2	**1.5**	**50**
3	2.0	51
4	2.5	49
5	3.0	32

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (112 mg, 0.6 mmol, 3.0 equiv.), Et_3N (X equiv.), DDQ (68 mg, 0.3 mmol, 1.5 equiv.) and toluene (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 ℃. After the addition was over, the resulting mixture was stirred at room temperature for 5 h. [b]HPLC yield (t_R= 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)).

Table S4 Screening of the DDQ loading[a]

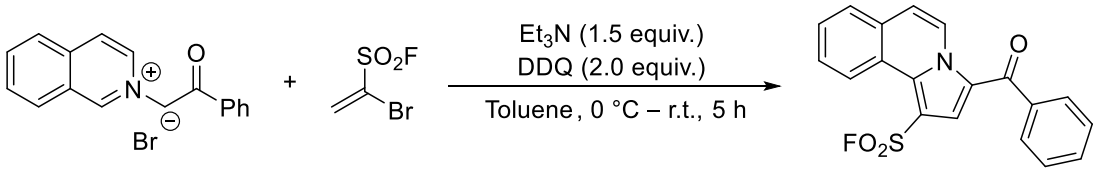


1a **2** **3a**

Entry	DDQ (X equiv.)	Yield (3a, %)[b]
1	0.5	29
2	1.0	43
3	1.5	49
4	**2.0**	**56**
5	3.0	50

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (112 mg, 0.6 mmol, 3.0 equiv.), Et_3N (30 mg, 0.3 mmol, 1.5 equiv.), DDQ (X equiv.) and toluene (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 ℃. After the addition was over, the resulting mixture was stirred at room temperature for 5 h. [b]HPLC yield (t_R= 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)).

Table S5 Screening of the BESF (**2**) loading[a]

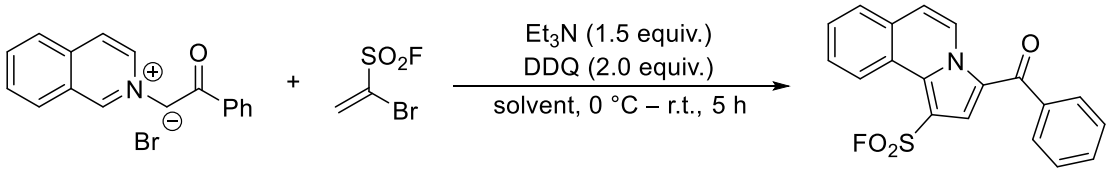


1a **2, (**X equiv.**)** **3a**

Entry	BESF (2, X equiv.)	Yield (3a, %)[b]
1	1.0	43
2	1.5	47
3	2.0	50
4	**2.5**	**55**
5	3.0	53
6	4.0	57
7	5.0	55
8	6.0	56
9	8.0	54
10	10.0	49

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (X equiv.), Et_3N (30 mg, 0.3 mmol, 1.5 equiv.), DDQ (91 mg, 0.4 mmol, 2.0 equiv.) and toluene (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 ℃. After the addition was over, the resulting mixture was stirred at room temperature for 5 h. [b]HPLC yield (t_R= 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)).

Table S6 Screening of the solvent[a]

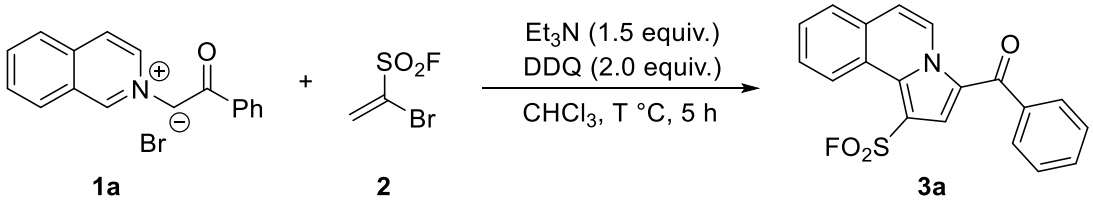


1a **2** **3a**

Entry	Solvent	Yield (3a, %)[b]
1	DCM	46
2	**$CHCl_3$**	**61**
3	DCE	48
4	Toluene	55
5	O-dichlorobenzene	54
6	Bromobenzene	53
7	Toluene/ $CHCl_3$ (v/v = 1:1)	58
8	Toluene/ $CHCl_3$ (v/v = 1:3)	47
9	Toluene/ $CHCl_3$ (v/v = 3:1)	57

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (95 mg, 0.5 mmol, 2.5 equiv.), Et_3N (30 mg, 0.3 mmol, 1.5 equiv.), DDQ (91 mg, 0.4 mmol, 2.0 equiv.) and solvent (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 ℃. After the addition was over, the resulting mixture was stirred at room temperature for 5 h. [b]HPLC yield (t_R= 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)).

Table S7 Screening of the temperature[a]

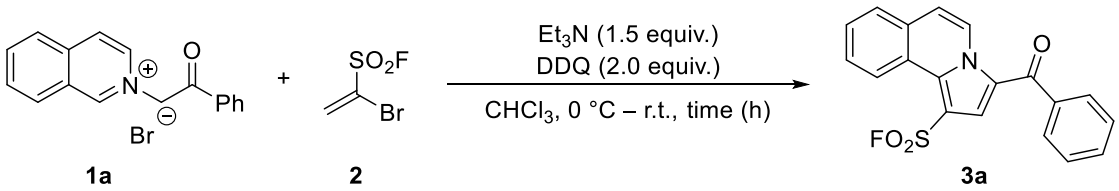


1a **2** **3a**

Entry	Temperature (°C)	Yield (3a, %)[b]
1	0	60
2	**25**	**62**
3	35	63
4	45	59
5	55	61
6	65	63

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (95 mg, 0.5 mmol, 2.5 equiv.), Et_3N (30 mg, 0.3 mmol, 1.5 equiv.), DDQ (91 mg, 0.4 mmol, 2.0 equiv.) and $CHCl_3$ (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 °C. After the addition was over, the resulting mixture was stirred at the corresponding temperature for 5 h. [b]HPLC yield (t_R= 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)).

Table S8 Screening of the time[a]



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

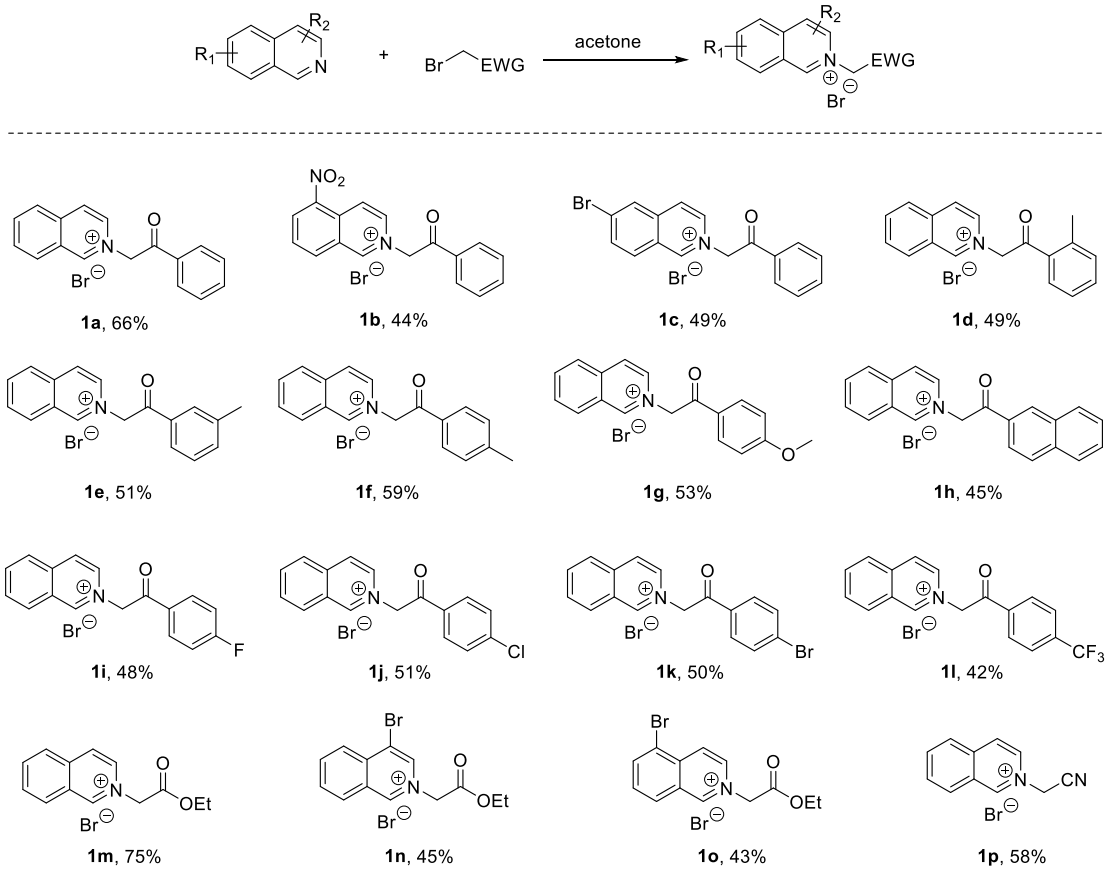
Entry	Time (h)	Yield (3a, %)[b]
1	0.5	55
2	**1.0**	**60**
3	2.0	56
4	4.0	63
5	7.0	64
6	18.0	61

[a]Reaction conditions: **1a** (65 mg, 0.2 mmol, 1.0 equiv.), **2** (95 mg, 0.5 mmol, 2.5 equiv.), Et_3N (30 mg, 0.3 mmol, 1.5 equiv.), DDQ (91 mg, 0.4 mmol, 2.0 equiv.) and $CHCl_3$ (0.1 M, 2.0 mL) were added to an oven-dried reaction tube (10 mL) at 0 ℃. After the addition was over, the resulting mixture was stirred at room temperature for the corresponding time. [b]HPLC yield (t_R= 5.912 min, λ_{max} = 261.8 nm; MeCN / H_2O = 80 : 20 (v / v)).

3. General Procedures

3.1 General procedures for synthesis of the salts 1 (with 1a as an example)

Isoquinoline (5 mmol) was added to a solution of the 2-bromoacetophenone (1.1 equiv.) in acetone (0.4 M) in a 50 mL round-bottom flask equipped with a magnetic stirring bar. The mixture was stirred for 24 h at room temperature. Filter the resulting precipitate and wash the residue with diethyl ether. Finally, the residue was dried in vacuum to obtain the product **1a**.

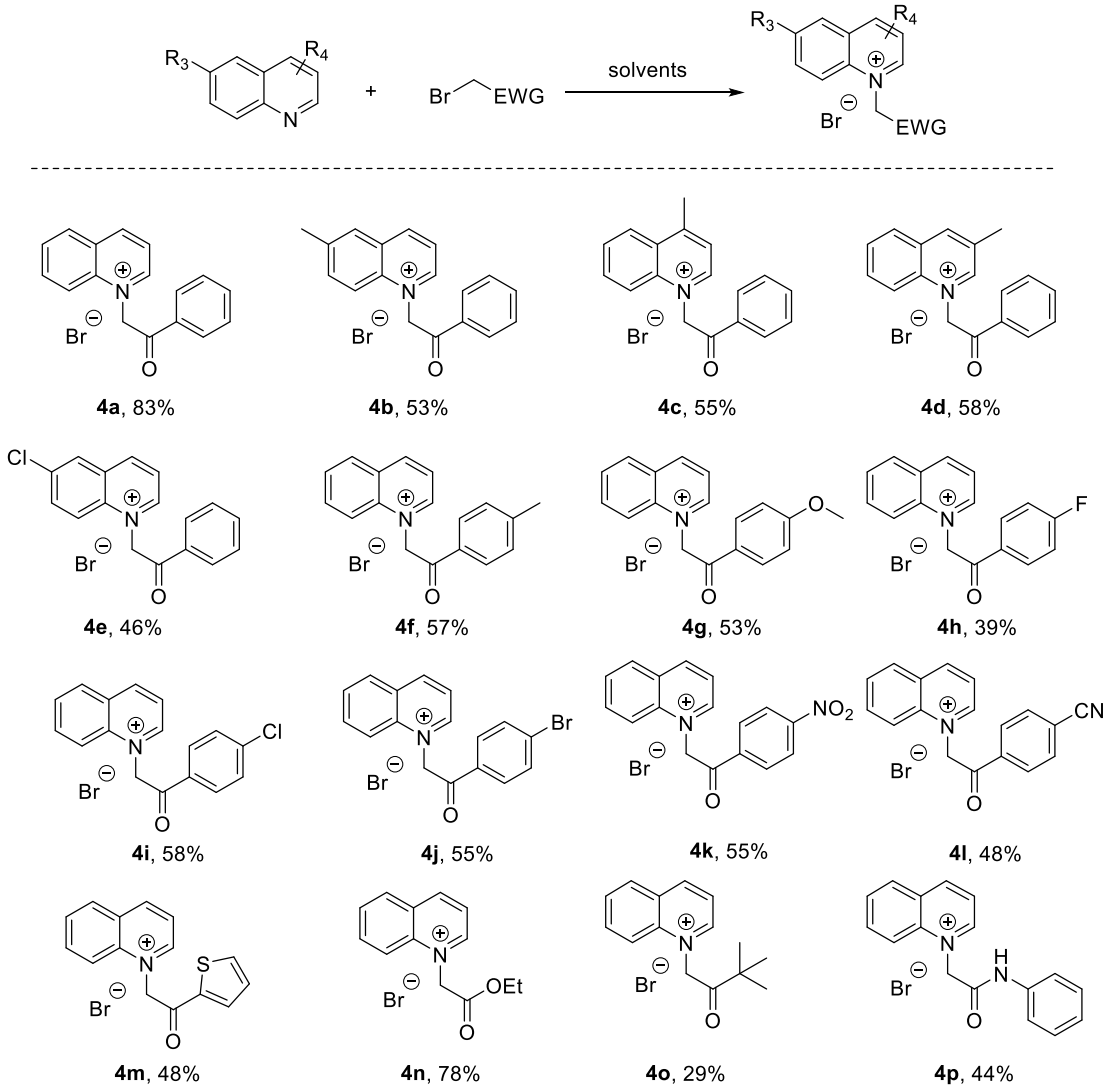


Scheme S1. Preparation of the salts 1

3.2 General procedures for synthesis of the salts 4 (with 4a as an example)

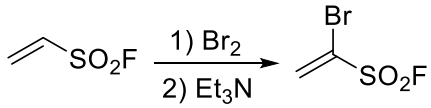
Quinoline (5 mmol) was added to a solution of the 2-bromoacetophenone (1.1 equiv.) in EtOAc (0.4 M) in a 50 mL round-bottom flask equipped with a magnetic stirring bar. The mixture was refluxed for 12 h, then cooled to room temperature upon completion. Filter the resulting precipitate and wash the residue with diethyl ether. Finally，the residue was dried in vacuum to obtain the product **4a**.

Note: Switched EtOAc to acetone for preparing **4m** and **4p**, toluene for synthesis of **4o** and reacted at room temperature.



Scheme S2. Preparation of the salts 4

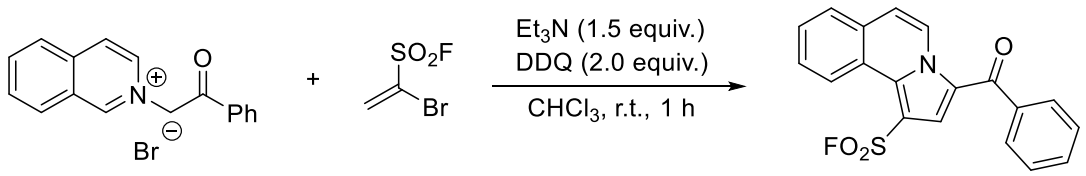
3.3 General procedures for synthesis of 1-bromoethene-1-sulfonyl fluoride 2[1]



2

Ethenesulfonyl fluoride, 33 g (300 mmol) was dissolved in 300 mL CH_2Cl_2 and placed in a 500 mL round-bottom flask equipped with a stirred bar under the irradiation of 50 W white light. To the flask was added 96 g (600 mmol, 31 mL) bromine in three portions in 30 minutes, the reaction was stirred for about 12-16 hours. After the ethenesulfonyl fluoride was completely consumed, the solution was washed with sodium thiosulfate solution until the color turned light yellow. Then dried over anhydrous Na_2SO_4, and concentrated to dryness. The residue was dissolved in 250 mL dry ether, and the mixture was cooled to -50 ℃. A solution of 31 g (300 mmol) of triethylamine in 60 mL dry ether was added in 30 minutes below -40 ℃. The mixture reacted vigorously to precipitate triethylamine hydrobromide. After warming slowly to room temperature with stirring, dilute sulfuric acid was added and the layers were separated. The layers were washed with acid, water and saturated sodium chloride solution, dried with anhydrous Na_2SO_4, concentrated to dryness. The residue was purified by reduced pressure distillation with a water pump at 85 ℃. The product weighed 42.8 g, 76 %.

3.4 General procedure for synthesis of compounds 3 (with 3a as an example)

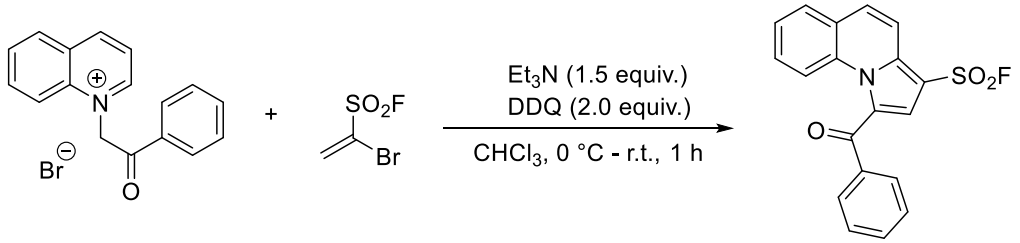


1a **2** **3a**

2-(2-oxo-2-phenylethyl)isoquinolin-2-ium bromide (**1a**, 328 mg, 1.0 mmol), BESF (**2**, 473 mg, 2.5 mmol) and $CHCl_3$ (0.2 M, 5.0 mL) were added to an oven-dried reaction tube (30 mL) equipped with a magnetic stirring bar. Et_3N (152 mg, 1.5 mmol) was dropped into the suspension at 0 ℃. Then DDQ (545 mg, 2.0 mmol) was added and the mixture was stirred at room temperature for 1 h. After the reaction was completed, the mixture was filtered, and the filter cake was washed with dichloromethane. The filtrate was extracted with dichloromethane (3×20 mL) and the combined organic layers were further washed with brine, and dried over anhydrous sodium sulfate. The solvent was

concentrated under reduced pressure and the residue was further purified by column chromatography on silica gel *via* gradient elution with petroleum ether/ dichloromethane (3:1 to 1:1, v/v) as eluent to afford pure heterocyclic sulfonyl fluoride **3a** as yellow solid (212 mg, 60% yield).

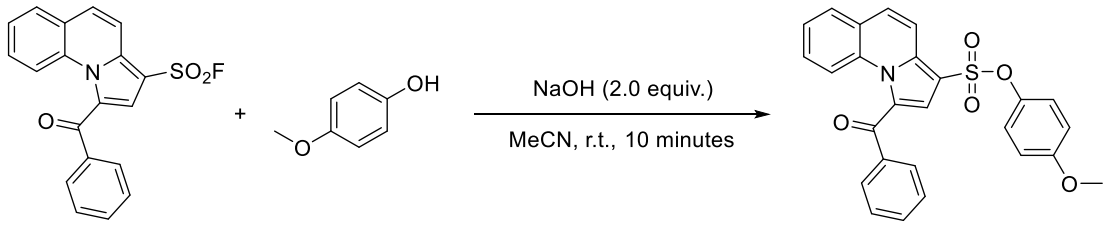
3.5 General procedure for synthesis of compounds 5 (with 5a as an example)



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

1-(2-oxo-2-phenylethyl)quinolin-1-ium bromide (**4a**, 328 mg, 1.0 mmol), BESF (**2**, 473 mg, 2.5 mmol) and $CHCl_3$ (0.2 M, 5.0 mL) were added to an oven-dried reaction tube (30 mL) equipped with a magnetic stirring bar. Et_3N (152 mg, 1.5 mmol) was dropped into the suspension at 0 ℃. Then DDQ (545 mg, 2.0 mmol) was added and the mixture was stirred at room temperature for 1 h. After the reaction was completed, the mixture was filtered, and the filter cake was washed with dichloromethane. The filtrate was extracted with dichloromethane (3×20 mL) and the combined organic layers were further washed with brine, and dried over anhydrous sodium sulfate. The solvent was concentrated under reduced pressure and the residue was further purified by column chromatography on silica gel *via* gradient elution with petroleum ether/ dichloromethane (3:1 to 1:1, v/v) as eluent to afford pure heterocyclic sulfonyl fluoride **5a** as light white solid (296 mg, 84% yield).

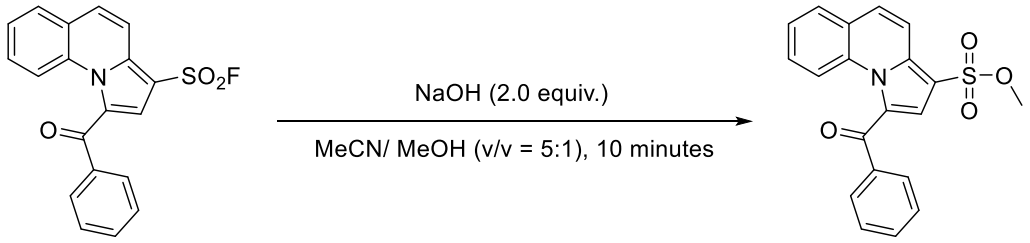
3.6 General procedure for synthesis of compound 6



5a 4-methoxyphenol **6**

1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5a**, 177 mg, 0.5 mmol), 4-methoxyphenol (74.4 mg, 0.6 mmol), NaOH (40 mg, 1.0 mmol) were added in a solution of acetonitrile (3 mL) and reacted at room temperature for 10 minutes. The reaction mixture was extracted with ethyl acetate (3×20 mL) and the combined organic layers were dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude product was further purified by column chromatography on silica gel by gradient elution with petroleum ether/dichloromethane (3:1 to 0:1, v/v) as eluent to obtain pure compound **6** as yellow solid (226 mg, 99% yield).

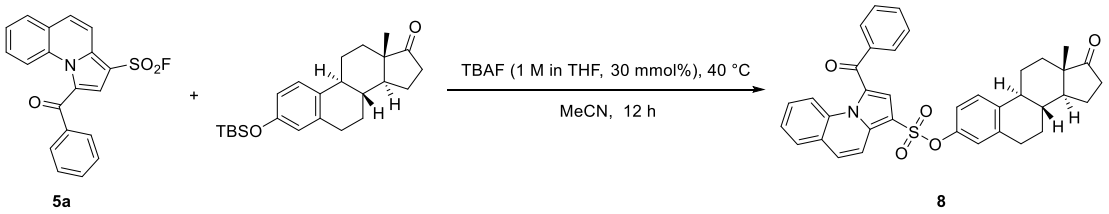
3.7 General procedure for synthesis of compound 7



5a **7**

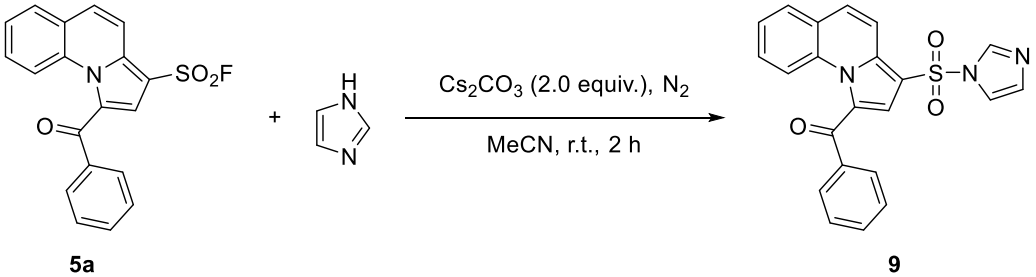
1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5a**, 177 mg, 0.5 mmol), and NaOH (40 mg, 1.0 mmol) were added in mixed solution (3 mL) of acetonitrile and methanol (5:1), and reacted at room temperature for 10 minutes. The reaction mixture was extracted with ethyl acetate (3×20 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude product was further purified by column chromatography on silica gel by gradient elution with petroleum ether/ dichloromethane (3:1 to 0:1, v/v) as eluent to obtain pure compound **7** as yellow solid (170 mg, 93% yield).

3.8 General procedure for synthesis of compound 8



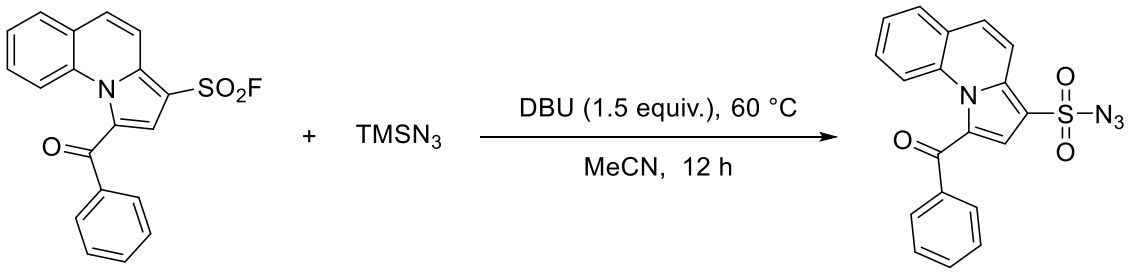
To a solution of compound **5a** (70 mg, 0.2 mmol) and TBS-protected estrone (77 mg, 0.2 mmol) dissolved in acetonitrile (2 mL) was added catalytic amount (30 mol%, 60 μL) of TBAF solution (tetrabutylammonium fluoride, 1 M in anhydrous THF), and the resulting mixture was stirred at 40 ℃ for 12 h. The reaction mixture was diluted with water and the aqueous phrase was extracted with dichloromethane (3×20 mL). The combined organic layers were washed with brine and dried over anhydrous Na_2SO_4 before being concentrated to dryness under vacuum. The residue was purified through silica gel chromatography with petroleum ether/ dichloromethane (1:1, v/v) as eluent to obtain pure compound **8** as yellow solid (68 mg, 55% yield).

3.9 General procedure for synthesis compound of 9



1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5a**, 177 mg, 0.5 mmol), imidazole (68 mg, 1.0 mmol) and Cs_2CO_3 (326 mg, 1.0 mmol) were added in mixed solution (3 mL) of acetonitrile, and reacted at room temperature under N_2 for 2 h. The reaction mixture was extracted with dichloromethane (3×20 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude product was further purified by column chromatography on silica gel by gradient elution with petroleum ether/ dichloromethane (1:1 to 0:1, v/v) as eluent to obtain pure compound **9** as white solid (184 mg, 92% yield).

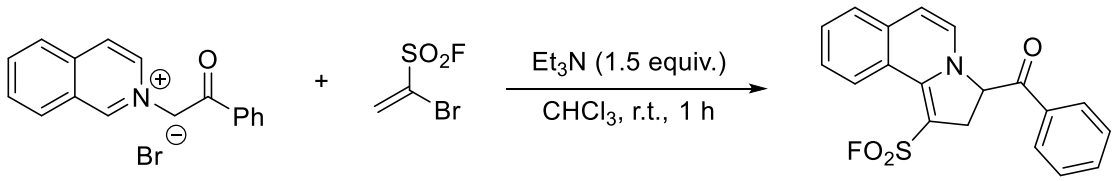
3.10 General procedure for synthesis of compound 10



5a **10**

To a stirred solution of compound **5a** (177 mg, 0.5 mmol) in MeCN (3 mL) was added DBU (228 mg,1.5 mmol) followed by $TMSN_3$ (144 mg, 1.25 mmol). The resultant solution was stirred at 60 ℃ for 2 h, then a further portion of $TMSN_3$ (86 mg, 0.75 mmol) was added and reacted for further 10 h. The reaction mixture was extracted with dichloromethane (3×20 mL) and the combined organic layers was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude product was further purified by column chromatography on silica gel by gradient elution with petroleum ether/ dichloromethane (1:1, v/v) as eluent to obtain pure compound **10** as yellow solid (152 mg, 81% yield).

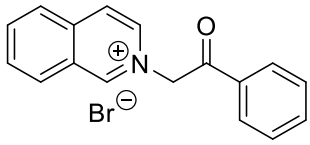
3.11 General procedure for synthesis of compound 11



1a **2** **11**

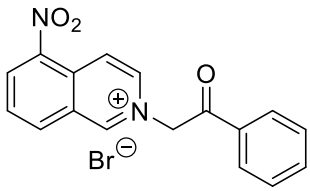
2-(2-oxo-2-phenylethyl)isoquinolin-2-ium bromide (**1a**, 656 mg, 1.0 mmol), BESF (**2**, 946 mg, 2.5 mmol) and $CHCl_3$ (0.2 M, 10.0 mL) were added to an oven-dried reaction tube (30 mL) equipped with a magnetic stirring bar. Et_3N (304 mg, 1.5 mmol) was dropped into the suspension at 0 ℃. The mixture was stirred at room temperature for 1 h. The mixture was extracted with dichloromethane (3×20 mL) and the combined organic layers were further washed with brine, and dried over anhydrous sodium sulfate. The solvent was concentrated under reduced pressure and the residue was further purified by column chromatography on silica gel *via* gradient elution with petroleum ether/ dichloromethane (1:1, v/v) as eluent to afford compound **11** as yellow solid (121 mg, 17% yield).

4. Characterization



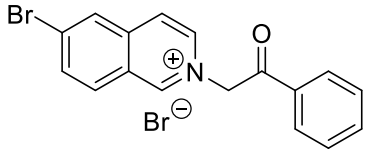
1a

2-(2-oxo-2-phenylethyl)isoquinolin-2-ium bromide (**1a**). White solid, 1079 mg, 66% yield. M.p. 208−210 ºC. General procedures for synthesis of the salts **1** was followed. The NMR data is identical to that reported in literature[2]. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.14 (s, 1H), 8.81 (dd, J_1 = 1.5 Hz, J_2 = 7.0 Hz, 1H), 8.71 (d, J = 6.5 Hz, 1H), 8.54 (d, J = 8.0 Hz, 1H), 8.43 (d, J = 8.0 Hz, 1H), 8.34 – 8.30 (m, 1H), 8.13 – 8.09 (m, 3H), 7.82 – 7.79 (m, 1H), 7.69 – 7.66 (m, 2H), 6.75 (s, 2H).



1b

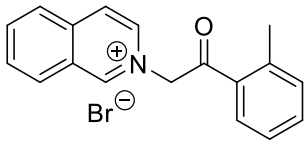
5-nitro-2-(2-oxo-2-phenylethyl)isoquinolin-2-ium bromide (**1b**). Yellow solid, 820 mg, 44% yield. M.p. 192−194 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.44 (s, 1H), 9.12 – 8.97 (m, 4H), 8.31 (s, 1H), 8.13 (s, 2H), 7.81 – 7.69 (m, 3H), 6.83 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 190.5, 152.7, 144.1, 139.0, 137.7, 134.8, 134.7, 133.4, 130.8, 129.5, 129.1, 128.3, 127.6, 121.3, 66.3. **HRMS-ESI** (m/z) calcd. for $[C_{17}H_{13}N_2O_3]^+$ ([M-Br]$^+$): 293.0921, found: 293.0925.



1c

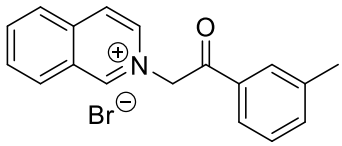
6-bromo-2-(2-oxo-2-phenylethyl)isoquinolin-2-ium bromide (**1c**). White solid, 997 mg, 49% yield. M.p. 235−237 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.14 (s, 1H), 8.84 (dd, J_1 = 1.5 Hz, J_2 =

7.0 Hz, 1H), 8.78 (d, J = 1.5 Hz, 1H), 8.64 (d, J = 7.0 Hz, 1H), 8.50 (d, J = 9.0 Hz, 1H), 8.25 (dd, J_1 = 2.0 Hz, J_2 = 9.0 Hz, 1H), 8.13 – 8.11 (m, 2H), 7.82 – 7.79 (m, 1H), 7.69 – 7.66 (m, 2H), 6.72 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 190.7, 151.8, 138.0, 137.4, 134.7, 134.6, 133.5, 132.3, 132.2, 129.7, 129.1, 128.3, 125.5, 124.4, 66.2. **HRMS-ESI** (m/z) calcd. for $[C_{17}H_{13}BrNO]^+$ ($[M\text{-}Br]^+$): 326.0175, found:326.0168.



1d

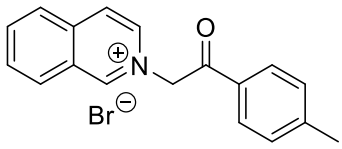
2-(2-oxo-2-(o-tolyl)ethyl)isoquinolin-2-ium bromide (**1d**). White solid, 838 mg, 49% yield. M.p. 229−230 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.17 (s, 1H), 8.83 (dd, J_1 = 1.5 Hz, J_2 = 7.0 Hz, 1H), 8.71 (d, J = 7.0 Hz, 1H), 8.55 (d, J = 8.5 Hz, 1H), 8.43 (d, J = 8.5 Hz, 1H), 8.32 (t, J = 8.0 Hz, 1H), 8.17 (d, J = 7.5 Hz, 1H), 8.11 (t, J = 8.0 Hz, 1H), 7.62 (t, J = 7.0 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 6.6 (s, 2H), 2.5 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 193.0, 151.6, 139.1, 137.3, 137.1, 136.3, 133.2, 133.1, 132.2, 131.3, 130.5, 129.7, 127.3, 126.8, 126.2, 125.3, 67.2, 21.1. **HRMS-ESI** (m/z) calcd. for $[C_{18}H_{16}NO]^+$ ($[M\text{-}Br]^+$): 262.1226, found: 262.1235.



1e

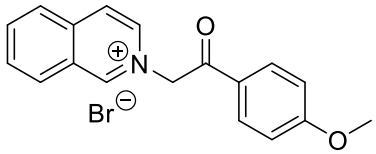
2-(2-oxo-2-(m-tolyl)ethyl)isoquinolin-2-ium bromide (**1e**). White solid, 872 mg, 51% yield. M.p. 262−263 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.06 (s, 1H), 8.76 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 1H), 8.70 (d, J = 6.5 Hz, 1H), 8.55 (d, J = 8.5 Hz, 1H), 8.43 (d, J = 8.5 Hz, 1H), 8.33 (t, J = 7.5 Hz, 1H), 8.12 (t, J = 7.5 Hz, 1H), 7.94 – 7.91 (m, 2H), 7.63 (d, J = 7.5 Hz, 1H), 7.57 (t, J = 7.5 Hz, 1H), 6.65 (s, 2H), 2.45 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 190.9, 151.6, 138.6, 137.4, 137.2, 136.3, 135.3, 133.6, 131.4, 130.6, 129.0, 128.5,

127.4, 126.8, 125.5, 125.4, 66.1, 20.8. **HRMS-ESI** (m/z) calcd. for $[C_{18}H_{16}NO]^+$ ([M-Br]$^+$): 262.1226, found: 262.1220.



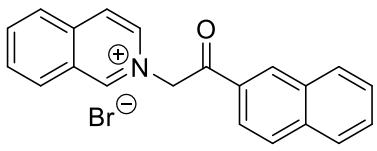
1f

2-(2-oxo-2-(p-tolyl)ethyl)isoquinolin-2-ium bromide (**1f**). White solid, 1009 mg, 59% yield. M.p. 217−219 ºC. General procedures for synthesis of the salts **1** was followed. The compound was reported in literature.[3] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.12 (d, J = 4.5 Hz, 1H), 8.80 – 8.78 (m, 1H), 8.70 (d, J = 7.0 Hz, 1H), 8.54 (d, J = 8.5 Hz, 1H), 8.42 (d, J = 8.0 Hz, 1H), 8.34 – 8.31 (m, 1H), 8.12 – 8.10 (m, 1H), 8.03 – 8.01 (m, 2H), 7.48 (d, J = 7.5 Hz, 2H), 6.69 (d, J = 5.0 Hz, 2H), 2.44 (s, 3H).



1g

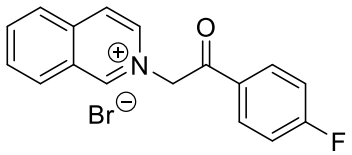
2-(2-(4-methoxyphenyl)-2-oxoethyl)isoquinolin-2-ium bromide (**1g**). White solid, 949 mg, 53% yield. M.p. 213−215 ºC. General procedures for synthesis of the salts **1** was followed. The compound was reported in literature.[3] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.12 (s, 1H), 8.79 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 1H), 8.69 (d, J = 7.0 Hz, 1H), 8.54 (d, J = 8.0 Hz, 1H), 8.42 (d, J = 8.5 Hz, 1H), 8.33 – 8.30 (m, 1H), 8.12 – 8.08 (m, 3H), 7.21 – 7.18 (m, 2H), 6.67 (s, 2H), 3.90 (s, 3H).



1h

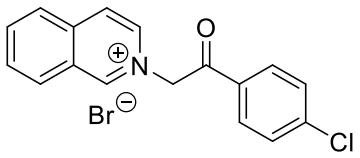
2-(2-(naphthalen-2-yl)-2-oxoethyl)isoquinolin-2-ium bromide (**1h**). White solid, 850 mg, 45% yield. M.p. 259−261 ºC. General procedures for synthesis of the salts **1** was

followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.14 (s, 1H), 8.93 (s, 1H), 8.83 (dd, J_1 = 1.5 Hz, J_2 = 6.5 Hz, 1H), 8.72 (d, J = 6.5 Hz, 1H), 8.57 (d, J = 8.0 Hz, 1H), 8.44 (d, J = 8.0 Hz, 1H), 8.36 – 8.32 (m, 1H), 8.25 (d, J = 8.0 Hz, 1H), 8.18 – 8.07 (m, 4H), 7.78 – 7.70 (m, 2H), 6.83 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 190.8, 151.7, 137.4, 137.2, 136.3, 135.6, 132.0, 131.3, 130.9, 130.7, 130.6, 129.7, 129.4, 128.8, 127.8, 127.4, 127.4, 126.8, 125.4, 123.2, 66.1. **HRMS-ESI** (m/z) calcd. for $[C_{21}H_{16}NO]^+$ ($[M\text{-}Br]^+$): 298.1226, found: 298.1222.



1i

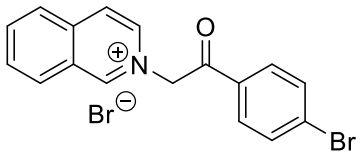
2-(2-(4-fluorophenyl)-2-oxoethyl)isoquinolin-2-ium bromide (**1i**). White solid, 836 mg, 48% yield. M.p. 203−204 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.10 (s, 1H), 8.79 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 1H), 8.71 (d, J = 6.5 Hz, 1H), 8.55 (d, J = 8.5 Hz, 1H), 8.43 (d, J = 8.5 Hz, 1H), 8.34 – 8.31 (m, 1H), 8.24 – 8.20 (m, 2H), 8.13 – 8.10 (m, 1H), 7.55 – 7.51 (m, 2H), 6.71 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 190.2, 167.3, 165.3, 152.2, 138.0, 137.8, 136.8, 132.1, 132.0 (d, J = 9.7 Hz), 131.5 (d, J = 100.9 Hz), 130.9 (d, J = 2.8 Hz), 127.9, 127.4, 126.0, 116.9 (d, J = 22.2 Hz), 66.5. **HRMS-ESI** (m/z) calcd. for $[C_{17}H_{13}FNO]^+$ ($[M\text{-}Br]^+$): 266.0976, found: 266.0985.



1j

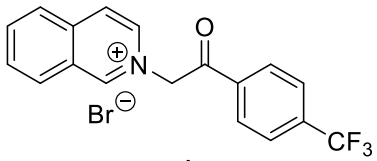
2-(2-(4-chlorophenyl)-2-oxoethyl)isoquinolin-2-ium bromide (**1j**). White solid, 923 mg, 51% yield. M.p. 215−217 ºC. General procedures for synthesis of the salts **1** was followed. The compound was reported in literature.[4] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.07 (s, 1H), 8.76 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 1H), 8.70 (d, J = 6.5 Hz, 1H), 8.55 (d, J = 8.5 Hz, 1H), 8.43 (d, J = 8.5 Hz, 1H), 8.35 – 8.32 (m, 1H), 8.14 – 8.10 (m, 3H),

7.78 – 7.76 (m, 2H), 6.68 (s, 2H).



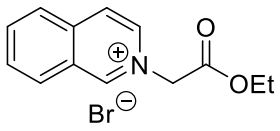
1k

2-(2-(4-bromophenyl)-2-oxoethyl)isoquinolin-2-ium bromide (**1k**). White solid, 1018 mg, 50% yield. M.p. 248−249 °C. General procedures for synthesis of the salts **1** was followed. The NMR data is identical to that reported in literature.[5] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.08 (s, 1H), 8.77 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 1H), 8.70 (d, J = 7.0 Hz, 1H), 8.55 (d, J = 8.5 Hz, 1H), 8.43 (d, J = 8.5 Hz, 1H), 8.35 – 8.31 (m, 1H), 8.13 – 8.10 (m, 1H), 8.07 – 8.04 (m, 2H), 7.92 – 7.90 (m, 2H), 6.68 (s, 2H).



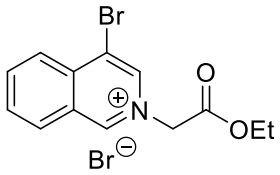
1l

2-(2-oxo-2-(4-(trifluoromethyl)phenyl)ethyl)isoquinolin-2-ium bromide (**1l**). White solid, 832 mg, 42% yield. M.p. 210−211 °C. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.15 (s, 1H), 8.83 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 1H), 8.73 (d, J = 7.0 Hz, 1H), 8.56 (d, J = 8.0 Hz, 1H), 8.43 (d, J = 8.5 Hz, 1H), 8.34 – 8.31 (m, 3H), 8.13 – 8.10 (m, 1H), 8.06 (d, J = 8.0 Hz, 2H), 6.82 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 190.6, 151.6, 137.5, 137.3, 136.9, 136.3, 133.6 (q, J = 32.2 Hz), 131.4, 130.6, 129.2, 127.4, 126.8, 126.1 (q, J = 3.7 Hz), 125.4, 123.6 (q, J = 273.4 Hz), 66.2. **HRMS-ESI** (m/z) calcd. for $[C_{18}H_{13}F_3NO]^+$ ($[M\text{-}Br]^+$): 316.0944, found: 316.0939.



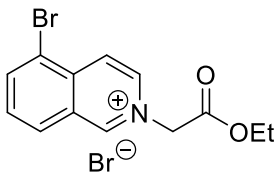
1m

2-(2-ethoxy-2-oxoethyl)isoquinolin-2-ium bromide (**1m**). White solid, 1110 mg, 75% yield. M.p. 194−196 ºC. General procedures for synthesis of the salts **1** was followed. The NMR data is identical to that reported in literature.[5] **^{1}H NMR** (500 MHz, D_2O) δ 9.72 (s, 1H), 8.50 (d, J = 6.5 Hz, 1H), 8.46 – 8.43 (m, 2H), 8.26 – 8.25 (m, 2H), 8.08 – 8.04 (m, 1H), 5.72 (s, 2H), 4.38 (q, J = 7.5 Hz, 2H), 1.33 (t, J = 7.5 Hz, 3H).



1n

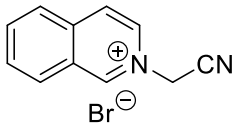
4-bromo-2-(2-ethoxy-2-oxoethyl)isoquinolin-2-ium bromide (**1n**). Light yellow solid, 844 mg, 45% yield. M.p. 135−137 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.34 (s, 1H), 9.39 (d, J = 1.0 Hz, 1H), 8.63 (d, J = 8.0 Hz, 1H), 8.48 – 8.44 (m, 1H), 8.38 (d, J = 8.5 Hz, 1H), 8.21– 8.18 (m, 1H), 5.89 (s, 2H), 4.26 (q, J = 7.0 Hz, 2H), 1.26 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.1, 151.8, 139.5, 137.2, 136.0, 132.3, 131.9, 126.7, 126.0, 120.8, 62.4, 60.0, 13.9. **HRMS-ESI** (m/z) calcd. for $[C_{13}H_{13}BrNO_2]^+$ ($[M\text{-}Br]^+$): 294.0124, found: 294.0131.



1o

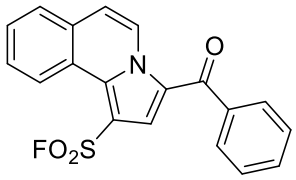
5-bromo-2-(2-ethoxy-2-oxoethyl)isoquinolin-2-ium bromide (**1o**). White solid, 806 mg, 43% yield. M.p. 202−204 ºC. General procedures for synthesis of the salts **1** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.30 (s, 1H), 8.94 (d, J = 7.0 Hz, 1H),

8.70 (d, J = 7.0 Hz, 1H), 8.66 (d, J = 7.5 Hz, 1H), 8.58 (d, J = 8.0 Hz, 1H), 8.01 (t, J = 7.5 Hz, 1H), 5.92 (s, 2H), 4.26 (q, J = 7.0 Hz, 2H), 1.27 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.2, 152.5, 141.0, 137.8, 136.0, 132.3, 130.9, 128.0, 124.3, 120.9, 62.4, 60.2, 13.9. **HRMS-ESI** (m/z) calcd. for $[C_{13}H_{13}BrNO_2]^+$ ($[M\text{-}Br]^+$): 294.0124, found: 294.0131.



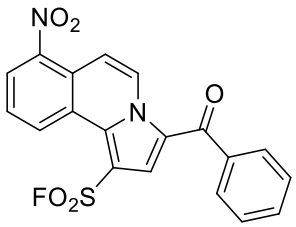
1p

2-(cyanomethyl)isoquinolin-2-ium bromide (**1p**). White solid, 722 mg, 58% yield. M.p. 203−205 ºC. General procedures for synthesis of the salts **1** was followed. The NMR data is identical to that reported in literature.[6] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.32 (s, 1H), 8.91 (dd, J_1 = 1.5 Hz, J_2 = 6.5 Hz, 1H), 8.71 (d, J = 7.0 Hz, 1H), 8.60 (d, J = 8.0 Hz, 1H), 8.41 (d, J = 8.5 Hz, 1H), 8.35 – 8.31 (m, 1H), 8.14 – 8.10 (m, 1H), 6.23 (s, 2H).



3a

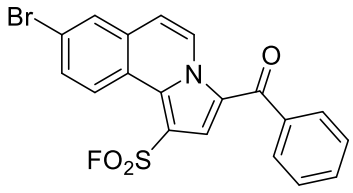
3-benzoylpyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3a**). Yellow solid, 212 mg, 60% yield. M.p. 198−199 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.66 (d, J = 7.5 Hz, 1H), 8.97 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 7.0 Hz, 4H), 7.79 – 7.74 (m, 2H), 7.65 (t, J = 7.5 Hz, 1H), 7.55 (t, J = 7.8 Hz, 2H), 7.43 (d, J = 7.5 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.67 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.9, 138.8, 134.7, 132.7, 130.9, 130.6, 129.3, 129.3, 129.1, 128.8, 127.6, 126.6(d, J = 2.5 Hz), 125.1, 123.7, 122.5, 117.1, 107.8 (d, J = 32.3 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{13}FNO_3S]^+$ ($[M+H]^+$): 354.0595, found: 354.0590.



3b

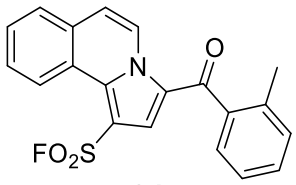
3-benzoyl-7-nitropyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3b**). Yellow solid, 295 mg, 74% yield. M.p. 211−213 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.81 (t, J = 6.8 Hz, 1H), 9.28 (t, J = 6.8 Hz, 1H), 8.42 (t, J = 6.5 Hz, 1H), 8.17 (t, J = 6.8 Hz, 1H), 7.93 – 7.87 (m, 4H), 7.69 (q, J = 6.8 Hz, 1H), 7.58 (q, J = 7.0 Hz, 2H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.68 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.8, 146.4, 138.2, 133.2, 132.7, 132.1, 132.1, 129.4, 129.0, 128.4, 128.0, 126.9, 124.1, 123.8, 110.9, 109.3 (d, J = 32.5 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}FN_2O_5S]^+$ ($[M+H]^+$): 399.0445, found: 399.0440.

Note: In the ^{13}C NMR spectrum of **3b**, theoretically, there should be seventeen peaks. Due to the compact overlaying, it is difficult to specify the overlaying peaks.



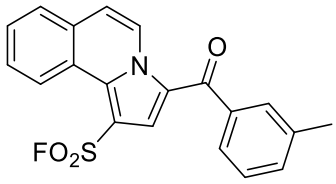
3c

3-benzoyl-8-bromopyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3c**). Yellow solid, 240 mg, 56% yield. M.p. 245−247 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.69 (d, J = 7.5 Hz, 1H), 8.84 (d, J = 8.5 Hz, 1H), 8.03 (s, 1H), 7.87 – 7.85 (m, 4H), 7.66 (t, J = 7.0 Hz, 1H), 7.56 (t, J = 7.5 Hz, 1H), 7.36 (d, J = 7.0 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.82 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.9, 138.7, 134.2, 132.9, 132.6, 132.2, 130.0, 129.3, 129.1, 128.9, 128.3 (d, J = 2.5 Hz), 126.2, 125.4, 124.0, 121.2, 116.0, 108.2 (d, J = 32.6 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}BrFNO_3S]^+$ ($[M+H]^+$): 431.9700, found: 431.9695.



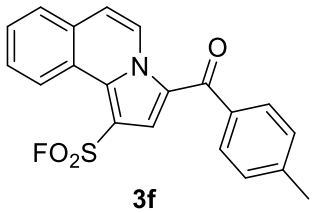
3d

3-(2-methylbenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3d**). Light yellow solid, 147 mg, 40% yield. M.p. 224−225 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.87 (d, J = 7.0 Hz, 1H), 8.90 (d, J = 9.0 Hz, 1H), 7.92 – 7.89 (m, 1H), 7.82 – 7.77 (m, 2H), 7.63 (s, 1H), 7.50 (d, J = 7.4 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.36 – 7.31 (m, 2H), 2.42 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.50 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 188.1, 138.7, 136.6, 134.8, 131.4, 131.0, 130.8, 130.7, 130.0, 129.4, 128.3, 127.7, 126.7 (d, J = 2.4 Hz), 125.6, 125.2, 124.4, 122.5, 117.4, 107.9 (d, J = 32.5 Hz), 19.8. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$):368.0751, found: 368.0748.



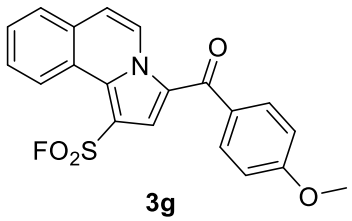
3e

3-(3-methylbenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3e**). White solid, 187 mg, 51% yield. M.p. 189−190 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.65 (d, J = 7.5 Hz, 1H), 8.97 (d, J = 8.0 Hz, 1H), 7.85 (s, 2H), 7.79 – 7.75 (m, 2H), 7.66 – 7.63 (m, 2H), 7.45 – 7.42 (m, 3H), 2.47 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.63 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.1, 138.8, 138.8, 134.7, 133.5, 130.8, 130.5, 129.7, 129.3, 129.1, 128.6, 127.6, 126.6 (d, J = 2.5 Hz), 126.5, 125.1, 123.8, 122.5, 117.1, 107.6 (d, J = 32.4 Hz), 21.6. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$):368.0751, found: 368.0748.



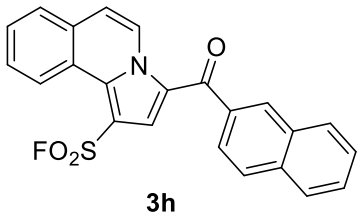
3f

3-(4-methylbenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3f**). Light yellow solid, 220 mg, 60% yield. M.p. 185−186 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.63 (d, J = 7.5 Hz, 1H), 8.97 (d, J = 8.0 Hz, 1H), 7.87 – 7.85 (m, 2H), 7.79 – 7.74 (m, 4H), 7.42 (d, J = 7.5 Hz, 1H), 7.36 (d, J = 8.0 Hz, 2H), 2.48 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.68 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.7, 143.6, 136.0, 134.6, 130.8, 130.5, 129.5, 129.5, 129.3, 128.8, 127.6, 126.6, (d, J = 2.3 Hz), 125.1, 123.8, 122.5, 117.0, 107.5 (d, J = 32.3 Hz), 21.8. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$):368.0751, found: 368.0758.



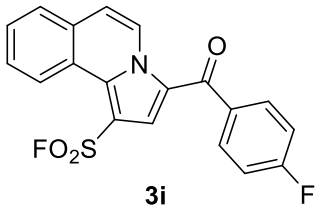
3g

3-(4-methoxybenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3g**). Light yellow solid, 195 mg, 51% yield. M.p. 204−206 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.54 (d, J = 7.5 Hz, 1H), 8.95 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 7.0 Hz, 2H), 7.83 (s, 2H), 7.74 (s, 2H), 7.38 (d, J = 7.5 Hz, 1H), 7.03 (d, J = 8.0 Hz, 2H), 3.92 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.74 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.5, 163.5, 134.5, 131.7, 131.2, 130.7, 130.4, 129.2, 128.1, 127.6, 126.5 (d, J = 2.3 Hz), 125.0, 123.9, 122.5, 116.8, 114.1, 107.3 (d, J = 32.1 Hz), 55.7. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_4S]^+$ ($[M+H]^+$): 384.0700, found: 384.0693.



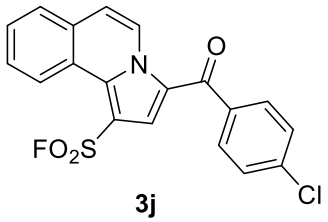
3h

3-(2-naphthoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3h**). Yellow solid, 173 mg, 43% yield. M.p. 205−207 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.65 (s, 1H), 8.98 (s, 1H), 8.37 (s, 1H), 7.99 – 7.76 (m, 8H), 7.62 (s, 2H), 7.41 (s, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.69 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.7, 135.9, 135.3, 134.7, 132.4, 130.8, 130.6, 130.5, 129.5, 129.3, 129.0, 128.8, 128.5, 127.9, 127.6, 127.2, 126.6 (d, J = 2.3 Hz), 125.2, 125.0, 123.8, 122.4, 117.0, 107.7 (d, J = 32.4 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{23}H_{15}FNO_3S]^+$ ($[M+H]^+$): 404.0751, found: 404.0759.



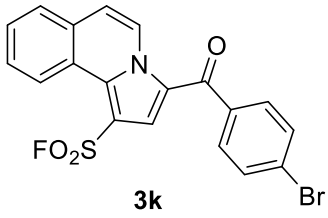
3i

3-(4-fluorobenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3i**). Yellow solid, 207 mg, 56% yield. M.p. 228−229 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 9.58 (d, J = 7.5 Hz, 1H), 8.95 – 8.93 (m, 1H), 7.92 – 7.89 (m, 3H), 7.81 – 7.77 (m, 3H), 7.48 (d, J = 7.5 Hz, 1H), 7.24 (t, J = 8.5 Hz, 2H). **^{19}F NMR** (471 MHz, CD_2Cl_2) δ 65.20 (s, 1F), −106.75 — −106.80 (m, 1F). **^{13}C NMR** (126 MHz, CD_2Cl_2) δ 184.6, 165.8 (d, J = 253.8 Hz), 135.5 (d, J = 3.2 Hz), 135.2, 132.2 (d, J = 9.2 Hz), 131.3, 130.9, 129.6, 129.0, 128.1, 126.7 (d, J = 2.5 Hz), 125.3, 124.0, 122.7, 117.5, 116.2 (d, J = 22.1 Hz), 107.8 (d, J = 32.4 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}F_2NO_3S]^+$ ($[M+H]^+$):372.0500, found: 372.0491.



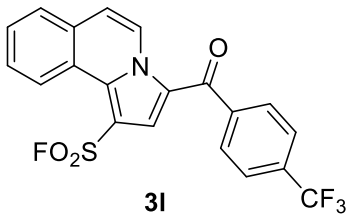
3j

3-(4-chlorobenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3j**). Light yellow solid, 237 mg, 61% yield. M.p. 215−216 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.63 (d, J = 7.5 Hz, 1H), 8.97 (d, J = 9.5 Hz, 1H), 7.89 – 7.87 (m, 1H), 7.82 (d, J = 2.5 Hz, 2H), 7.81 – 7.77 (m, 3H), 7.53 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 7.5 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.60 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.5, 139.2, 137.1, 134.9, 130.9, 130.7, 130.7 129.4, 129.2, 129.0, 127.7, 126.7 (d, J = 2.5 Hz), 125.0, 123.4, 122.4, 117.3, 108.0 (d, J = 32.4 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}ClFNO_3S]^+$ ($[M+H]^+$): 388.0205, found: 388.0210.



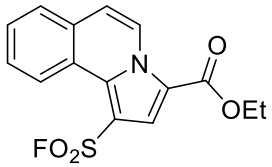
3k

3-(4-bromobenzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3k**). Light yellow solid, 242 mg, 56% yield. M.p. 217−218 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.63 (d, J = 7.5 Hz, 1H), 8.97 (d, J = 8.5 Hz, 1H), 7.89 – 7.86 (m, 1H), 7.82 (s, 1H), 7.81 – 7.76 (m, 2H), 7.72 (q, J = 8.8 Hz, 4H), 7.45 (d, J = 7.5 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.61 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.7, 137.5, 134.9, 132.2, 130.9, 130.8, 130.7, 129.4, 129.1, 127.7, 127.7, 126.7 (d, J = 2.4 Hz), 125.0, 123.3, 122.4, 117.3, 108.0 (d, J = 32.4 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}BrFNO_3S]^+$ ($[M+H]^+$): 431.9700, found: 431.9707.



3l

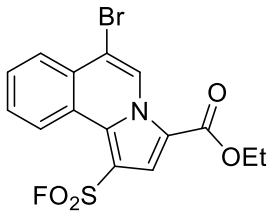
3-(4-(trifluoromethyl)benzoyl)pyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3l**). White solid, 248 mg, 59% yield. M.p. 214−215 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 9.68 (d, J = 7.5 Hz, 1H), 8.97 – 8.95 (m, 1H), 7.97 (d, J = 8.0 Hz, 2H), 7.95 – 7.93 (m, 1H), 7.85 (s, 1H), 7.83 – 7.80 (m, 4H), 7.53 (d, J = 7.5 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.11 (s, 1F), δ -63.32 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.6, 142.0, 135.2, 134.1 (q, J = 32.9 Hz), 131.1, 130.9, 129.6, 129.6, 129.5, 127.7, 126.8 (d, J = 2.5 Hz), 125.9 (q, J = 3.8 Hz), 125.0, 123.7 (q, J = 273.2 Hz), 123.2, 122.5, 117.6, 108.4 (d, J = 32.8 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{12}F_4NO_3S]^+$ ($[M+H]^+$): 422.0469, found: 422.0461.



3m

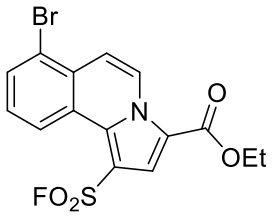
ethyl 1-(fluorosulfonyl)pyrrolo[2,1-a]isoquinoline-3-carboxylate (**3m**). White solid, 177 mg, 55% yield. M.p. 181−182 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, CD_2Cl_2) δ 9.39 (d, J = 7.5 Hz, 1H), 8.89 (d, J = 8.5 Hz, 1H), 8.04 (s, 1H), 7.76 (dd, J_1 = 1.0, J_2 = 7.5 Hz, 1H), 7.72 – 7.66 (m, 2H), 7.29 (d, J = 7.5 Hz, 1H), 4.43 (q, J = 7.0 Hz, 2H), 1.44 (t, J = 7.0 Hz, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.57 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.3, 133.8, 130.0, 129.9, 129.1, 127.5, 126.3 (d, J = 2.6 Hz), 124.9, 124.2, 122.6, 116.6, 116.5, 107.2 (d, J = 32.3 Hz), 61.3, 14.5.

HRMS-ESI (m/z) calcd. for $[C_{15}H_{13}FNO_4S]^+$ ($[M+H]^+$): 322.0544, found: 322.0550.



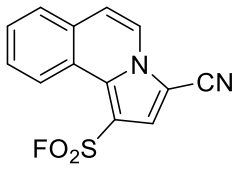
3n

ethyl 6-bromo-1-(fluorosulfonyl)pyrrolo[2,1-a]isoquinoline-3-carboxylate (**3n**). White solid, 316 mg, 79% yield. M.p. 196−197 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.91 – 8.90 (m, 1H), 8.20 – 8.17 (m, 1H), 8.03 (s, 1H), 7.81 – 7.77 (m, 2H), 4.45 (q, J = 7.0 Hz, 2H), 1.45 (t, J = 7.0 Hz, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.45 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.1, 132.9, 130.9, 130.1, 128.7, 127.3, 126.6 (d, J = 2.5 Hz), 125.4, 125.0, 122.6, 116.4, 113.1, 107.9 (d, J = 32.5 Hz), 61.6, 14.5. **HRMS-ESI** (m/z) calcd. for $[C_{15}H_{12}BrFNO_4S]^+$ ($[M+H]^+$): 399.9649, found: 399.9641.



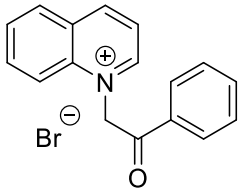
3o

ethyl 7-bromo-1-(fluorosulfonyl)pyrrolo[2,1-a]isoquinoline-3-carboxylate (**3o**). White solid, 216 mg, 54% yield. M.p. 225−227 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.52 (d, J = 7.5 Hz, 1H), 8.90 (d, J = 8.0 Hz, 1H), 8.10 (s, 1H), 7.97(dd, J_1 = 1.0 Hz, J_2 = 7.5 Hz, 1H), 7.81 (d, J = 7.5 Hz, 1H), 7.58 (t, J = 8.0 Hz, 1H), 4.45 (q, J = 7.0 Hz, 2H), 1.45 (t, J = 7.5 Hz, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.46 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.2, 134.0, 132.9, 129.6, 129.1, 125.9 (d, J = 2.5 Hz), 125.5, 125.5, 124.2, 122.5, 116.8, 115.3, 108.1 (d, J = 32.4 Hz), 61.5, 14.5. **HRMS-ESI** (m/z) calcd. for $[C_{15}H_{12}BrFNO_4S]^+$ ($[M+H]^+$): 399.9649, found: 399.9645.



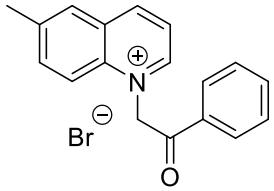
3p

3-cyanopyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**3l**). White solid, 197 mg, 72% yield. M.p. 189−190 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.92 (d, J = 8.0 Hz, 1H), 8.22 (d, J = 7.0 Hz, 1H), 7.88 (d, J = 7.5 Hz, 2H), 7.83 – 7.77 (m, 2H), 7.47 (d, J = 7.5 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 65.73 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 133.3, 130.9, 130.1, 130.1, 128.1, 126.4 (d, J = 2.4 Hz), 125.9, 122.7, 122.2, 117.9, 111.0, 108.3 (d, J = 33.6 Hz), 99.5. **HRMS-ESI** (m/z) calcd. for $[C_{13}H_8FN_2O_2S]^+$ ($[M+H]^+$): 275.0285, found: 275.0280.



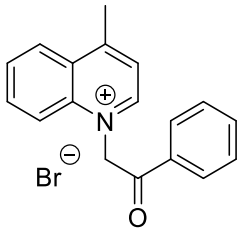
4a

1-(2-oxo-2-phenylethyl)quinolin-1-ium bromide (**4a**). White solid, 1361 mg, 83% yield. M.p. 203−205 ºC. General procedures for synthesis of the salts **4** was followed. The NMR data is identical to that reported in literature.[2] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.61 (dd, J_1 = 1.5 Hz, J_2 = 6.0 Hz, 1H), 9.48 (d, J = 8.0 Hz, 1H), 8.57 (dd, J_1 = 1.5 Hz, J_2 = 8.5 Hz, 1H), 8.47 (d, J = 9.0 Hz, 1H), 8.34 (dd, J_1 = 5.5 Hz, J_2 = 8.0 Hz, 1H), 8.24 – 8.20 (m, 1H), 8.18 – 8.16 (m, 2H), 8.06 (t, J = 7.5 Hz, 1H), 7.84 – 7.81 (m, 1H), 7.71 – 7.68 (m, 2H), 7.10(s, 2H).



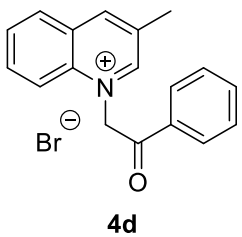
4b

6-methyl-1-(2-oxo-2-phenylethyl)quinolin-1-ium bromide (**4b**). White solid, 906 mg, 53% yield. M.p. 219−221 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[7] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.56 – 9.55 (m, 1H), 9.34 (d, J = 8.5 Hz, 1H), 8.37 (d, J = 9.0 Hz, 1H), 8.31 (s, 1H), 8.28 (dd, J_1 = 5.5 Hz, J_2 = 8.5 Hz, 1H), 8.18 – 8.16 (m, 2H), 8.06 (dd, J_1 = 2.0 Hz, J_2 = 9.5 Hz, 1H), 7.83 – 7.80 (m, 1H), 7.69 (t, J = 7.7 Hz, 2H), 7.10 (s, 2H), 2.60 (s, 3H).



4c

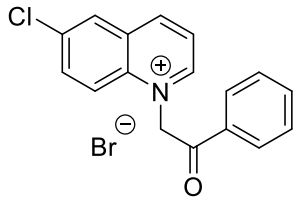
4-methyl-1-(2-oxo-2-phenylethyl)quinolin-1-ium bromide (**4c**). White solid, 940 mg, 55% yield. M.p. 225−226 ºC. General procedures for synthesis of the salts **4** was followed. The NMR data is identical to that reported in literature.[8] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.53 (d, J = 6.0 Hz, 1H), 8.60 – 8.57 (m, 1H), 8.42 (d, J = 9.0 Hz, 1H), 8.23 (d, J = 6.5 Hz, 1H), 8.20 – 8.16 (m, 3H), 8.05 – 8.02 (m, 1H), 7.83 – 7.79 (m, 1H), 7.68 (t, J = 7.5 Hz, 2H), 7.11 (s, 2H), 3.07 (s, 3H).



4d

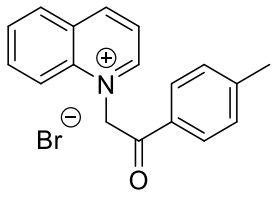
3-methyl-1-(2-oxo-2-phenylethyl)quinolin-1-ium bromide (**4d**). White solid, 991 mg, 58% yield. M.p. 226−227 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[7] **^{1}H NMR** (500 MHz, DMSO-d_6)

δ 9.64 (d, J = 2.0 Hz, 1H), 9.29 (s, 1H), 8.44 – 8.40 (m, 2H), 8.18 – 8.16 (m, 2H), 8.15 – 8.11 (m, 1H), 8.02 – 7.99 (m, 1H), 7.84 – 7.81 (m, 1H), 7.71 – 7.68 (m, 2H), 7.07 (s, 2H), 2.67 (s, 3H).



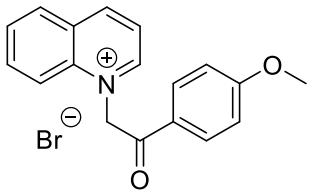
4e

6-chloro-1-(2-oxo-2-phenylethyl)quinolin-1-ium bromide (**4e**). Yellow solid, 832 mg, 46% yield. M.p. 203−205 °C. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[7] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.62 (dd, J_1 = 1.0 Hz, J_2 = 6.0 Hz, 1H), 9.40 (d, J = 8.0 Hz, 1H), 8.75 (d, J = 2.5 Hz, 1H), 8.55 (d, J = 9.5 Hz, 1H), 8.39 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 8.26 (dd, J_1 = 2.5 Hz, J_2 = 9.5 Hz, 1H), 8.16 – 8.14 (m, 2H), 7.84 – 7.81 (m, 1H), 7.71 – 7.68(m, 2H), 7.09 (s, 2H).



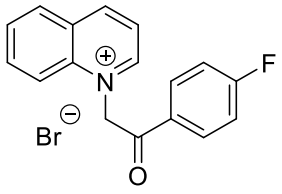
4f

1-(2-oxo-2-(p-tolyl)ethyl)quinolin-1-ium bromide (**4f**). White solid, 975 mg, 57% yield. M.p. 215−216 °C. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[3] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.58 (d, J = 5.5 Hz, 1H), 9.46 (d, J = 8.5 Hz, 1H), 8.56 (dd, J_1 = 1.5 Hz, J_2 = 8.5 Hz, 1H), 8.42 (d, J = 9.0 Hz, 1H), 8.33 (dd, J_1 = 5.5 Hz, J_2 = 8.0 Hz, 1H), 8.23 – 8.20 (m, 1H), 8.08 – 8.05 (m, 3H), 7.50 (d, J = 8.0 Hz, 2H), 7.04 (s, 2H), 2.46 (s, 3H).



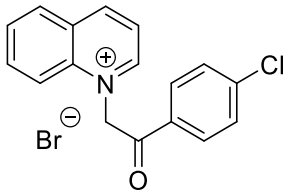
4g

1-(2-(4-methoxyphenyl)-2-oxoethyl)quinolin-1-ium bromide (**4g**). White solid, 949 mg, 53% yield. M.p. 218−220 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[3] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.55 – 9.53 (m, 1H), 9.45 (d, J = 8.5 Hz, 1H), 8.55 (dd, J_1 = 1.5 Hz, J_2 = 8.0 Hz, 1H), 8.40 (d, J = 9.0 Hz, 1H), 8.32 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 8.24 – 8.20 (m, 1H), 8.15 – 8.12 (m, 2H), 8.06 (t, J = 7.5Hz, 1H), 7.23 – 7.20 (m, 2H), 6.98 (s, 2H), 3.92 (s, 3H).



4h

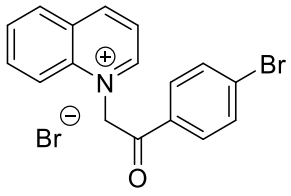
1-(2-(4-fluorophenyl)-2-oxoethyl)quinolin-1-ium bromide (**4h**). Yellow solid, 675 mg, 39% yield. M.p. 231−233 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[9] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.60 (dd, J_1 = 1.5 Hz, J_2 = 6.0 Hz, 1H), 9.48 (d, J = 8.5 Hz, 1H), 8.57 (dd, J_1 = 1.0 Hz, J_2 = 8.0 Hz, 1H),, 8.48 (d, J = 9.0 Hz, 1H), 8.34 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 8.28 – 8.20 (m, 3H), 8.06 (t, J = 7.5 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.10 (s, 2H).



4i

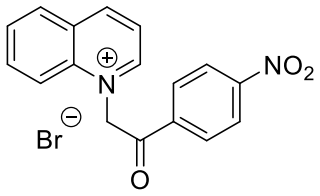
1-(2-(4-chlorophenyl)-2-oxoethyl)quinolin-1-ium bromide (**4i**). White solid, 1050 mg, 58% yield. M.p. 218−219 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[10] **^{1}H NMR** (500 MHz, DMSO-d_6)

δ 9.55 (dd, J_1 = 1.5 Hz, J_2 = 6.0 Hz, 1H), 9.46 (d, J = 8.0 Hz, 1H), 8.56 (dd, J_1 = 1.5 Hz, J_2 = 8.0 Hz, 1H), 8.48 (d, J = 9.0 Hz, 1H), 8.33 (dd, J_1 =6.0 Hz, J_2 = 8.5 Hz, 1H), 8.24 – 8.21 (m, 1H), 8.18 – 8.15 (m, 2H), 8.07 (t, J = 7.0 Hz, 1H), 7.80 – 7.77 (m, 2H), 7.04 (s, 2H).



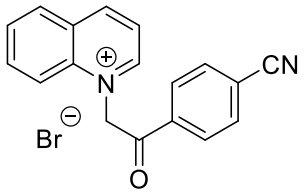
4j

1-(2-(4-bromophenyl)-2-oxoethyl)quinolin-1-ium bromide (**4j**). White solid, 1119 mg, 55% yield. M.p. 227−229 ºC. General procedures for synthesis of the salts **4** was followed. The NMR data is identical to that reported in literature.[6] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.65 (dd, J_1 = 1.5 Hz, J_2 = 6.0 Hz, 1H), 9.49 (d, J = 8.5 Hz, 1H), 8.58 – 8.56 (m, 1H), 8.49 (d, J = 9.0 Hz, 1H), 8.34 (dd, J_1 = 6.0 Hz, J_2 = 8.5 Hz, 1H), 8.23 – 8.19 (m, 1H), 8.11 – 8.08 (m, 2H), 8.05 (t, J = 7.5Hz, 1H), 7.93 – 7.90 (m, 2H), 7.13 (s, 2H).



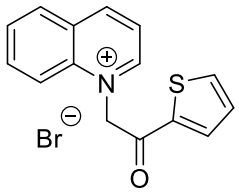
4k

1-(2-(4-nitrophenyl)-2-oxoethyl)quinolin-1-ium bromide (**4k**). Yellow solid, 1026 mg, 55% yield. M.p. 212−213 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[3] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.61 (dd, J_1 = 1.5 Hz, J_2 = 6.0 Hz, 1H), 9.49 (d, J = 8.5 Hz, 1H), 8.58 – 8.56 (m, 2H), 8.52 – 8.49 (m, 2H), 8.41 – 8.38 (m, 2H), 8.36 (dd, J_1 = 5.5 Hz, J_2 = 8.0 Hz, 1H), 8.25 – 8.21 (m, 1H), 8.08 (t, J = 7.5 Hz, 1H), 7.15 (s, 2H).



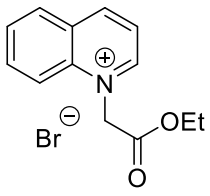
4l

1-(2-(4-cyanophenyl)-2-oxoethyl)quinolin-1-ium bromide (**4l**). White solid, 847 mg, 48% yield. M.p. 226−228 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[11] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.61 (dd, J_1 = 1.0 Hz, J_2 = 6.0 Hz, 1H), 9.49 (d, J = 8.5 Hz, 1H), 8.58 – 8.56 (m, 1H), 8.54 (d, J = 9.0 Hz, 1H), 8.36 – 8.30 (m, 3H), 8.24 – 8.18 (m, 3H), 8.08 – 8.05 (m, 1H), 7.14 (s, 2H).



4m

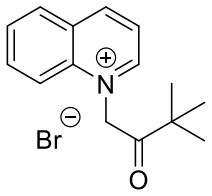
1-(2-oxo-2-(thiophen-2-yl)ethyl)quinolin-1-ium bromide (**4m**). Yellow solid, 802 mg, 48% yield. M.p. 199−201 ºC. General procedures for synthesis of the salts **4** was followed. The compound was reported in literature.[12] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.62 (dd, J_1 = 1.5 Hz, J_2 = 6.0 Hz, 1H), 9.47 (d, J = 8.5 Hz, 1H), 8.56 (dd, J_1 = 1.0 Hz, J_2 = 8.5 Hz, 1H), 8.46 – 8.42 (m, 2H), 8.33 (dd, J_1 = 5.5 Hz, J_2 = 8.0 Hz, 1H), 8.28 – 8.22 (m, 2H), 8.06 (t, J = 7.5 Hz, 1H), 7.47 (dd, J_1 = 3.5 Hz, J_2 = 5.0 Hz, 1H), 7.02 (s, 2H).



4n

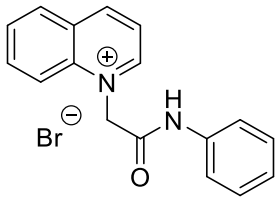
1-(2-ethoxy-2-oxoethyl)quinolin-1-ium bromide (**4n**). Brown solid, 1154 mg, 78% yield. M.p. 164−166 ºC. General procedures for synthesis of the salts **4** was followed. The NMR data is identical to that reported in literature.[5] **^{1}H NMR** (500 MHz,

DMSO-d_6) δ 9.64 – 9.62 (m, 1H), 9.46 (d, J = 8.5 Hz, 1H), 8.55 (dd, J_1 = 1.0 Hz, J_2 = 8.5 Hz, 1H), 8.46 (d, J = 9.0 Hz, 1H), 8.33 – 8.27 (m, 2H), 8.09 – 8.06 (m, 1H), 6.22 (s, 2H), 4.24 (q, J = 7.0 Hz, 2H), 1.24 (t, J = 7.0 Hz, 3H).



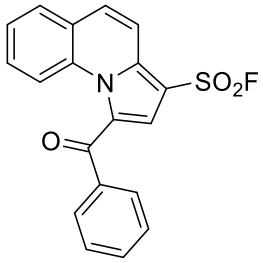
4o

1-(3,3-dimethyl-2-oxobutyl)quinolin-1-ium bromide (**4o**). Gray solid, 447 mg, 29% yield. M.p. 190−192 °C. General procedures for synthesis of the salts **4** was followed. The NMR data is identical to that reported in literature.[13] **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.56 (d, J = 5.5 Hz, 1H), 9.42 (d, J = 8.0 Hz, 1H), 8.53 (d, J = 8.0 Hz, 1H), 8.30 (dd, J_1 = 6.0 Hz, J_2 = 8.0 Hz, 1H), 8.27 – 8.21 (m, 2H), 8.05 (t, J = 7.5 Hz, 1H), 6.64 (s, 2H), 1.34 (s, 9H).



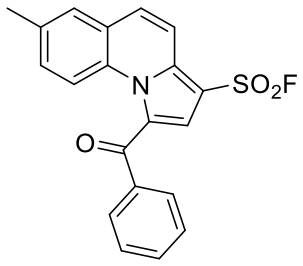
4p

1-(2-oxo-2-(phenylamino)ethyl)quinolin-1-ium bromide (**4p**). White solid, 755 mg, 44% yield. M.p. 229−231 °C. General procedures for synthesis of the salts **4** was followed. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.97 (s, 1H), 9.61 (dd, J_1 = 1.0 Hz, J_2 = 6.0 Hz, 1H), 9.42 (d, J = 8.0 Hz, 1H), 8.54 (dd, J_1 = 1.5 Hz, J_2 = 8.5 Hz, 1H), 8.47 (d, J = 9.0 Hz, 1H), 8.32 – 8.27 (m, 2H), 8.08 – 8.05 (m, 1H), 7.62 – 7.60 (m, 2H), 7.35 (t, J = 7.5 Hz, 2H), 7.11 (t, J = 7.5 Hz, 1H), 6.13 (s, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.7, 151.3, 148.5, 138.4, 138.0, 136.0, 130.7, 129.9, 129.3, 128.9, 124.1, 121.9, 119.3, 118.6, 59.2. **HRMS-ESI** (m/z) calcd. for $[C_{17}H_{15}N_2O]^+$ ($[M\text{-}Br]^+$): 263.1179, found: 263.1177.



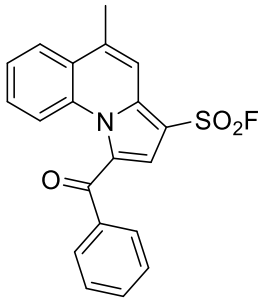
5a

1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5a**). White solid, 296 mg, 84% yield. M.p. 175−177 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, J = 8.0 Hz, 2H), 8.04 (dd, J_1 = 5.0, J_2 = 9.0 Hz, 2H), 7.90 – 7.85 (m, 2H), 7.72 (t, J = 7.5 Hz, 1H), 7.66 – 7.57 (m, 5H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.28 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.9, 138.6, 137.3, 133.9, 132.9, 131.2, 130.3, 129.9, 129.5, 129.0, 128.9, 127.1, 126.7, 125.1, 120.3, 115.2, 105.9 (d, J = 30.5 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{13}FNO_3S]^+$ ($[M+H]^+$): 354.0595, found: 354.0603.



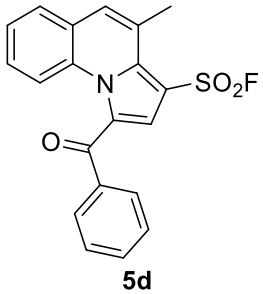
5b

1-benzoyl-7-methylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5b**). Yellow solid, 290 mg, 79% yield. M.p. 202−203 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, J = 7.5 Hz, 2H), 7.99 (d, J = 9.5 Hz, 1H), 7.93 (d, J = 9.0 Hz, 1H), 7.79 (d, J = 9.0 Hz, 1H), 7.71 (t, J = 7.5 Hz, 1H), 7.66 (s, 1H), 7.60 – 7.58 (m, 3H), 7.45 (d, J = 9.0 Hz, 1H), 2.52 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.25 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.9, 138.3, 137.4, 136.7, 133.8, 131.3, 131.1, 131.0, 130.3, 128.9, 128.9, 128.6, 127.2, 125.1, 120.1, 115.0, 105.5 (d, J = 30.2 Hz), 21.1. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$): 368.0751, found: 368.0750.



5c

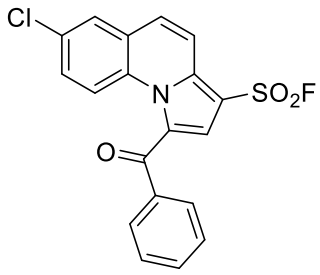
1-benzoyl-5-methylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5c**). Yellow solid, 135 mg, 37% yield. M.p. 207−208 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, CDCl3) δ 8.10 – 8.06 (m, 3H), 8.03 (d, J = 7.5 Hz, 1H), 7.87 (s, 1H), 7.71 (t, J = 7.5 Hz, 1H), 7.66 – 7.57 (m, 5H), 2.76 (s, 3H). **^{19}F NMR** (471 MHz, CDCl3) δ 72.08 (s, 1F). **^{13}C NMR** (126 MHz, CDCl3) δ 184.7, 139.3, 138.7, 137.4, 133.8, 132.7, 130.2, 129.5, 128.9, 128.6, 127.7, 126.6, 125.7, 125.3, 120.7, 114.8, 104.5 (d, J = 30.0 Hz), 19.8. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$): 368.0751, found: 368.0757.



5d

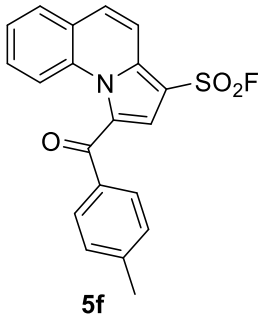
1-benzoyl-4-methylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5d**). Yellow solid, 338 mg, 92% yield. M.p. 205−207 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, J = 5.0 Hz, 2H), 7.88 (d, J = 6.5 Hz, 1H), 7.79 (d, J = 4.5 Hz, 1H), 7.72 (s, 2H), 7.63 – 7.54 (m, 5H), 2.86 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 73.81 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.8, 137.7, 137.2, 133.9, 131.6, 131.3, 130.3, 129.8, 129.0, 128.9, 128.3, 127.6, 126.6, 125.8, 125.1, 120.3, 107.7 (d, J = 32.5 Hz), 20.3 (d, J = 3.4 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$): 368.0751,

found: 368.0756.



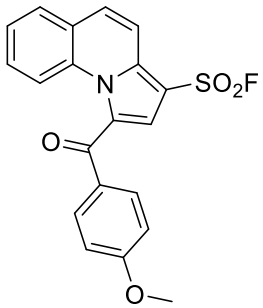
5e

1-benzoyl-7-chloropyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5e**). White solid, 340 mg, 88% yield. M.p. 188−190 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 8.02 (m, 4H), 7.84 (s, 1H), 7.73 (s, 2H), 7.62 – 7.56 (m, 4H). **^{19}F NMR** (471 MHz, CDCl3) δ 72.42 (s, 1F). **^{13}C NMR** (126 MHz, CDCl3) δ 184.9, 138.2, 137.2, 134.1, 132.4, 131.3, 130.3, 130.0, 129.9, 129.0, 129.0, 128.3, 127.3, 126.2, 121.9, 116.5, 106.6 (d, J = 30.9 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}ClFNO_3S]^+$ ($[M+H]^+$): 388.0205, found: 388.0210.



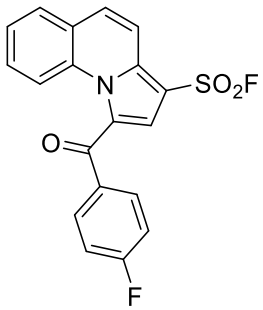
5f

1-(4-methylbenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5f**). Yellow solid, 297 mg, 81% yield. M.p. 187−189 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 (s, 4H), 7.87 – 7.83 (m, 2H), 7.60 – 7.56 (m, 3H), 7.39 (s, 2H), 2.51 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.35 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.8, 145.1, 138.3, 134.6, 132.8, 130.9, 130.5, 129.8, 129.7, 129.4, 128.9, 126.6, 126.5, 125.0, 120.2, 115.2, 105.6 (d, J = 30.1 Hz), 21.9. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_3S]^+$ ($[M+H]^+$): 368.0751, found: 368.0754.



5g

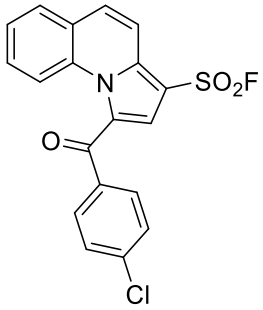
1-(4-methoxybenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5g**). White solid, 295 mg, 77% yield. M.p. 204−205 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, J = 8.5 Hz, 2H), 8.04 – 7.98 (m, 2H), 7.88 (d, J = 7.5 Hz, 1H), 7.82 (d, J = 9.0 Hz, 1H), 7.62 (t, J = 7.8 Hz, 1H), 7.58 – 7.55(m, 2H), 7.07 (d, J = 8.5 Hz, 2H), 3.95 (s, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.39 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.1, 164.5, 138.1, 132.9, 132.8, 130.7, 129.9, 129.8, 129.5, 128.8, 126.6, 125.7, 125.0, 120.1, 115.3, 114.3, 105.5 (d, J = 30.2 Hz), 55.8. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{15}FNO_4S]^+$ ($[M+H]^+$): 384.0700, found: 384.0709.



5h

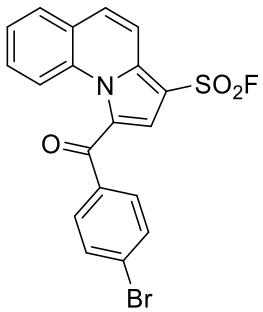
1-(4-fluorobenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5h**). Yellow solid, 330 mg, 89% yield. M.p. 201−203 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 – 8.13 (m, 2H), 8.04 (d, J = 9.5 Hz, 2H), 8.00 (d, J = 8.5 Hz, 2H), 7.90 (d, J = 7.5 Hz, 2H), 7.87 (d, J = 9.5 Hz, 2H), 7.67 – 7.64 (m, 1H), 7.61 – 7.58 (m, 2H), 7.28 (t, J = 8.5 Hz, 2H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.27 (s, 1F), −103.46 —

−103.52 (m, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 183.5, 166.4 (d, J = 257.0 Hz), 138.6, 133.6 (d, J = 3.0 Hz), 133.0 (d, J = 9.5 Hz), 132.8, 131.3, 130.0, 129.6, 128.5, 126.9, 126.8, 125.1, 120.2, 116.3 (d, J = 22.2 Hz), 115.2, 106.0 (d, J = 30.5 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}F_2NO_3S]^+$ ($[M+H]^+$): 372.0500, found: 372.0509.



5i

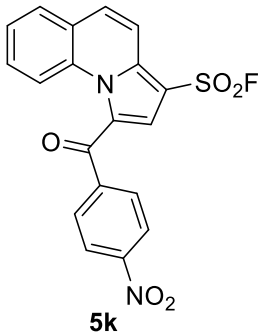
1-(4-chlorobenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5i**). Light yellow solid, 325 mg, 84% yield. M.p. 186−187 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.00 (m, 4H), 7.91 – 7.87 (m, 2H), 7.66 (t, J = 7.3 Hz, 1H), 7.61 – 7.57 (m, 4H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.24 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 183.6, 140.6, 138.7, 135.7, 132.9, 131.6, 131.4, 130.0, 129.6, 129.4, 128.4, 127.2, 126.8, 125.1, 120.2, 115.2, 106.1 (d, J = 30.6 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}ClFNO_3S]^+$ ($[M+H]^+$): 388.0205, found: 388.0209.



5j

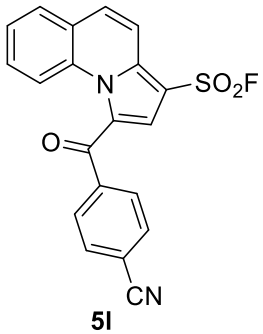
1-(4-bromobenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5j**). Yellow solid, 397 mg, 92% yield. M.p. 203−204 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz,

$CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.97 (d, J = 8.5 Hz, 2H), 7.91 – 7.87 (m, 2H), 7.74 (d, J = 8.5 Hz, 2H), 7.66 (t, J = 7.3 Hz, 1H), 7.61 – 7.58 (m, 2H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.24 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 183.7, 138.7, 136.1, 132.8, 132.3, 131.7, 131.4, 130.0, 129.6, 129.2, 128.4, 127.2, 126.8, 125.1, 120.2, 115.2, 106.1 (d, J = 30.6 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}BrFNO_3S]^+$ ($[M+H]^+$): 431.9700, found: 431.9707.



5k

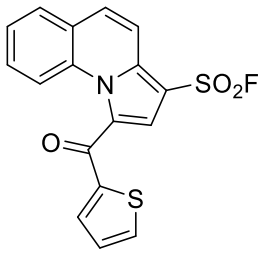
1-(4-nitrobenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5k**). Yellow solid, 358 mg, 90% yield. M.p. 224−225 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.43 (s, 2H), 8.29 (s, 3H), 8.15 (s, 1H), 8.04 – 8.00 (m, 2H), 7.86 (s, 1H), 7.76 – 7.71 (m, 2H). **^{19}F NMR** (471 MHz, DMSO-d_6) δ 72.82 (s, 1F). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 182.5, 150.2, 142.0, 138.3, 132.6, 132.0, 131.4, 130.0, 129.6, 128.5, 127.6, 126.9, 124.6, 123.8, 120.6, 114.2, 104.3 (d, J = 28.6 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{12}FN_2O_5S]^+$ ($[M+H]^+$): 399.0445, found: 399.0449.



5l

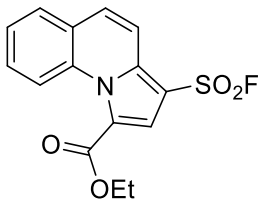
1-(4-cyanobenzoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5l**). Yellow solid, 336

mg, 89% yield. M.p. 220−222 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.18 (d, J = 8.0 Hz, 2H), 8.04 (d, J = 6.5 Hz, 2H), 7.93 – 7.89 (m, 4H), 7.69 (t, J = 7.3 Hz, 1H), 7.64 – 7.61 (m, 2H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.13 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 182.7, 140.9, 139.2, 132.9, 132.8, 132.0, 130.5, 130.1, 129.7, 128.3, 128.1, 127.0, 125.2, 120.3, 117.9, 117.0, 115.1, 106.6 (d, J = 30.9 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{12}FN_2O_3S]^+$ ($[M+H]^+$): 379.0547, found: 379.0537.



5m

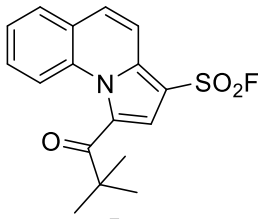
1-(thiophene-2-carbonyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5m**). White solid, 302 mg, 84% yield. M.p. 180−181 ºC. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 – 7.79 (m, 8H), 7.62 (s, 1H), 7.55 (s, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.42 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 177.2, 143.6, 138.3, 135.8, 135.3, 132.7, 130.9, 130.0, 129.5, 128.6, 128.0, 126.6, 125.8, 125.0, 120.0, 115.2, 105.7 (d, J = 30.2 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{17}H_{11}FNO_3S_2]^+$ ($[M+H]^+$): 360.0159, found: 360.0149.



5n

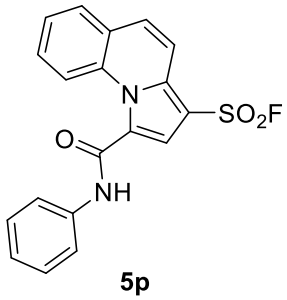
Ethyl 3-(fluorosulfonyl)pyrrolo[1,2-a]quinoline-1-carboxylate (**5n**). White solid, 167 mg, 52% yield. M.p. 123−125 ºC. Purification by column chromatography on silica gel

using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H** NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 8.5 Hz, 1H), 7.98 (d, J = 10.0 Hz, 2H), 7.84 (d, J = 7.5 Hz, 1H), 7.75 (d, J = 9.0 Hz, 1H), 7.69 (t, J = 7.3 Hz, 1H), 7.58 (t, J = 7.5 Hz, 1H), 4.48 (q, J = 7.2 Hz, 2H), 1.47 (t, J = 7.3 Hz, 3H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.19 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.0, 137.9, 133.2, 130.2, 129.5, 129.2, 126.7, 125.3, 125.2, 121.8, 120.4, 115.3, 105.8 (d, J = 30.4 Hz), 62.0, 14.5. **HRMS-ESI** (m/z) calcd. for $[C_{15}H_{13}FNO_4S]^+$ ($[M+H]^+$): 322.0544, found: 322.0536.



5o

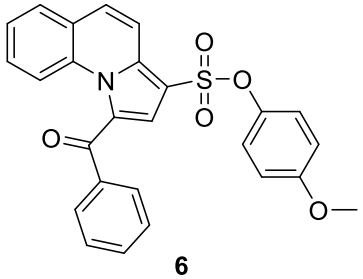
1-pivaloylpyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5o**). Light yellow solid, 150 mg, 45% yield. M.p. 135−137 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (d, J = 9.5 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 9.5 Hz, 1H), 7.67 (s, 1H), 7.65 – 7.59 (m, 2H), 7.55 (t, J = 7.3 Hz, 1H), 1.53 (s, 9H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 72.51 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 201.3, 137.1, 132.9, 130.0, 129.7, 129.7, 127.9, 126.3, 125.0, 120.3, 119.1, 115.3, 105.0 (d, J = 29.9 Hz), 45.2, 28.4. **HRMS-ESI** (m/z) calcd. for $[C_{17}H_{17}FNO_3S]^+$ ($[M+H]^+$): 334.0908, found: 334.0903.



5p

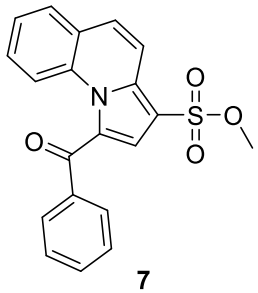
1-(phenylcarbamoyl)pyrrolo[1,2-a]quinoline-3-sulfonyl fluoride (**5o**). White solid, 151 mg, 41% yield. M.p. 260−262 °C. Purification by column chromatography on silica gel using petroleum ether / dichloromethane (3:1 to 1:1, v/v) as eluent. **^{1}H NMR** (500 MHz,

DMSO-d_6) δ 11.06 (s, 1H), 8.16 (d, J = 8.5 Hz, 1H), 8.09 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 9.5 Hz, 1H), 7.94 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 8.0 Hz, 2H), 7.77 (t, J = 7.5 Hz, 1H), 7.65 (t, J = 7.5 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.18 (t, J = 7.5 Hz, 1H). **^{19}F NMR** (471 MHz, DMSO-d_6) δ 73.61 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.5, 138.6, 135.3, 132.0, 130.0, 129.8, 129.6, 128.9, 126.5, 126.0, 124.3, 124.3, 120.2, 118.8, 118.5, 114.4, 102.5 (d, J = 28.7 Hz). **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{14}FN_2O_3S]^+$ ($[M+H]^+$): 369.0704, found: 369.0693.



6

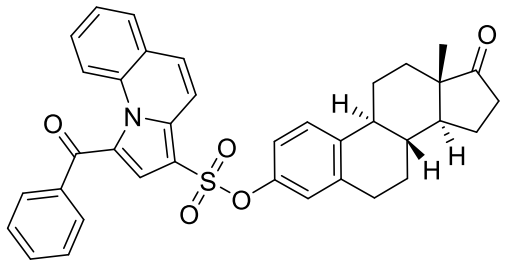
4-methoxyphenyl 1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonate (**6**). Yellow solid, 226 mg, 99% yield. M.p. 63−65 ºC. Purification by column chromatography on silica gel using dichloromethane as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.00 (m, 3H), 7.83 (s, 2H), 7.69 – 7.65 (m, 2H), 7.60 – 7.54 (m, 4H), 7.38 (s, 1H), 6.93 (d, J = 7.0 Hz, 2H), 6.74 (d, J = 7.5 Hz, 2H), 3.74 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.9, 158.4, 143.1, 138.0, 137.6, 133.6, 132.9, 130.2, 130.0, 129.4, 129.3, 128.7, 128.1, 127.9, 126.3, 125.0, 123.5, 120.2, 115.6, 114.6, 108.8, 55.6. **HRMS-ESI** (m/z) calcd. for $[C_{26}H_{20}NO_5S]^+$ ($[M+H]^+$): 458.1057, found: 458.1050.



7

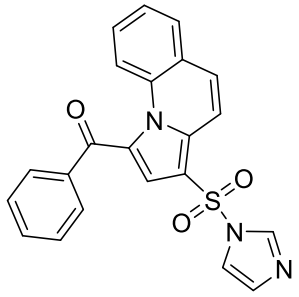
Methyl 1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonate (**7**). Yellow solid, 170 mg, 93% yield. M.p. 153–154 ºC. Purification by column chromatography on silica gel using

dichloromethane as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 – 8.00 (m, 4H), 7.85 (d, J = 4.5 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.69 (t, J = 7.5 Hz, 1H), 7.62 – 7.52 (m, 5H), 3.77 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.9, 137.8, 137.7, 133.6, 132.9, 130.3, 130.0, 129.4, 129.3, 128.8, 128.2, 127.7, 126.3, 125.0, 120.3, 115.7, 108.9, 56.3. **HRMS-ESI** (m/z) calcd. for $[C_{20}H_{16}NO_4S]^+$ ($[M+H]^+$):366.0795, found: 366.0798.



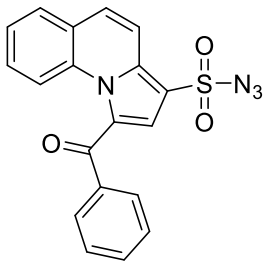
8

(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonate (**8**). Yellow solid, 66 mg, 55% yield. M.p. 202–203 °C. Purification by column chromatography on silica gel using ether/ dichloromethane (1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.66 (d, J = 7.5 Hz, 1H), 9.34 (d, J = 8.5 Hz, 1H), 7.88 – 7.86 (m, 1H), 7.81 – 7.74 (m, 4H), 7.66 (s, 1H), 7.61 – 7.57 (m, 1H), 7.49 (t, J = 7.5 Hz, 2H), 7.41 (d, J = 7.5 Hz, 1H), 7.08 (d, J = 8.5 Hz, 1H), 6.82 (d, J = 2.5 Hz, 1H), 6.67 (dd, J_1 = 2.5 Hz, J_2 = 8.5 Hz, 1H), 2.78 – 2.74 (m, 2H), 2.48 (dd, J_1 = 4.0 Hz, J_2 = 19.0 Hz,, 1H), 2.31 – 2.26 (m, 1H), 2.20 – 2.08 (m, 2H), 2.04 – 1.99 (m, 1H), 1.97 – 1.90 (m, 2H), 1.63 – 1.41 (m, 5H), 1.40 – 1.32 (m, 1H), 0.86 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 220.5, 185.9, 147.8, 139.1, 138.9, 138.6, 134.1, 132.4, 130.7, 130.2, 130.0, 129.4, 129.1, 128.7, 127.5, 127.4, 126.7, 125.1, 123.1, 123.0, 122.1, 118.9, 116.6, 111.2, 50.5, 48.0, 44.2, 37.9, 35.9, 31.6, 29.4, 26.2, 25.7, 21.7, 13.9. **HRMS-ESI** (m/z) calcd. for $[C_{37}H_{34}NO_5S]^+$ ($[M+H]^+$): 604.2152, found: 604.2160.



9

(3-((1H-imidazol-1-yl)sulfonyl)pyrrolo[1,2-a]quinolin-1-yl)(phenyl)methanone (**9**). White solid, 184 mg, 92% yield. M.p. 207–208 ºC. Purification by column chromatography on silica gel using petroleum ether/ dichloromethane (1:1 to 0:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 (s, 4H), 7.98 (d, J = 8.5 Hz, 1H), 7.87 – 7.82(m, 2H), 7.72 (s, 1H), 7.61 – 7.54 (m, 5H), 7.32 (s, 1H), 7.06 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.9, 137.6, 137.3, 136.2, 133.9, 132.8, 131.3, 131.1, 130.3, 129.9, 129.4, 129.0, 128.9, 126.6, 126.1, 125.0, 120.3, 117.1, 114.7, 111.0. **HRMS-ESI** (m/z) calcd. for $[C_{22}H_{16}N_3O_3S]^+$ ($[M+H]^+$): 402.0907, found: 402.0917.

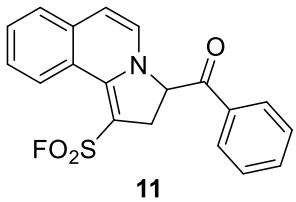


10

1-benzoylpyrrolo[1,2-a]quinoline-3-sulfonyl azide (**10**). Yellow solid, 152 mg, 92% yield. M.p. 165–166 ºC. Purification by column chromatography on silica gel using petroleum ether/ dichloromethane (1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 – 8.10 (m, 2H), 8.07 – 8.04 (m, 2H), 7.89 (dd, J_1 = 1.5 Hz, J_2 = 8.0 Hz, 1H), 7.83 (d, J = 9.0 Hz, 1H), 7.73 – 7.70 (t, J = 7.5 Hz, 1H), 7.66 – 7.63 (m, 1H), 7.61 – 7.57 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.1, 137.9, 137.5, 133.9, 132.9, 130.8, 130.4, 129.8, 129.5, 129.0, 128.5, 126.6, 125.2, 120.4, 115.4, 112.3. **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{13}N_4O_3S]^+$ ($[M+H]^+$): 377.0703, found: 377.0710.

Note: In the ^{13}C NMR spectrum of **10**, theoretically, there should be seventeen peaks.

Due to the compact overlaying, it is difficult to specify the overlaying peaks.



11

3-benzoyl-2,3-dihydropyrrolo[2,1-a]isoquinoline-1-sulfonyl fluoride (**11**). Yellow solid, 121 mg, 17% yield. M.p. 58–60 ºC. Purification by column chromatography on silica gel using petroleum ether/ dichloromethane (1:1, v/v) as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.65 (d, J = 7.5 Hz, 1H), 8.18 (d, J = 8.0 Hz, 1H), 7.87 – 7.85 (m, 2H), 7.81 (dd, J_1 = 1.0 Hz, J_2 = 8.0 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.65 – 7.60 (m, 2H), 7.56 – 7.52 (m, 2H), 7.17 (d, J = 7.0 Hz, 1H), 5.33 (dd, J_1 = 3.5 Hz, J_2 = 10.0 Hz, 1H), 4.44 (dd, J_1 = 3.5 Hz, J_2 = 16.0 Hz, 1H), 3.82 (dd, J_1 = 10.5 Hz, J_2 = 16.0 Hz, 1H). **^{19}F NMR** (471 MHz, $CDCl_3$) δ 44.28 (s, 1F). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.6, 140.3, 132.4, 131.7, 130.0, 129.3, 128.5, 128.3, 128.1 (d, J = 35.7 Hz), 125.9 (d, J = 2.6 Hz), 125.0, 123.3, 122.8, 114.1, 110.3, 58.0, 33.6. **HRMS-ESI** (m/z) calcd. for $[C_{19}H_{15}FNO_3S]^+$ ($[M+H]^+$): 356.0751, found: 356.0758.

5. References

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against Anopheles arabiensis, *Struct. Chem.*, 2020, **31**, 1533-1543.

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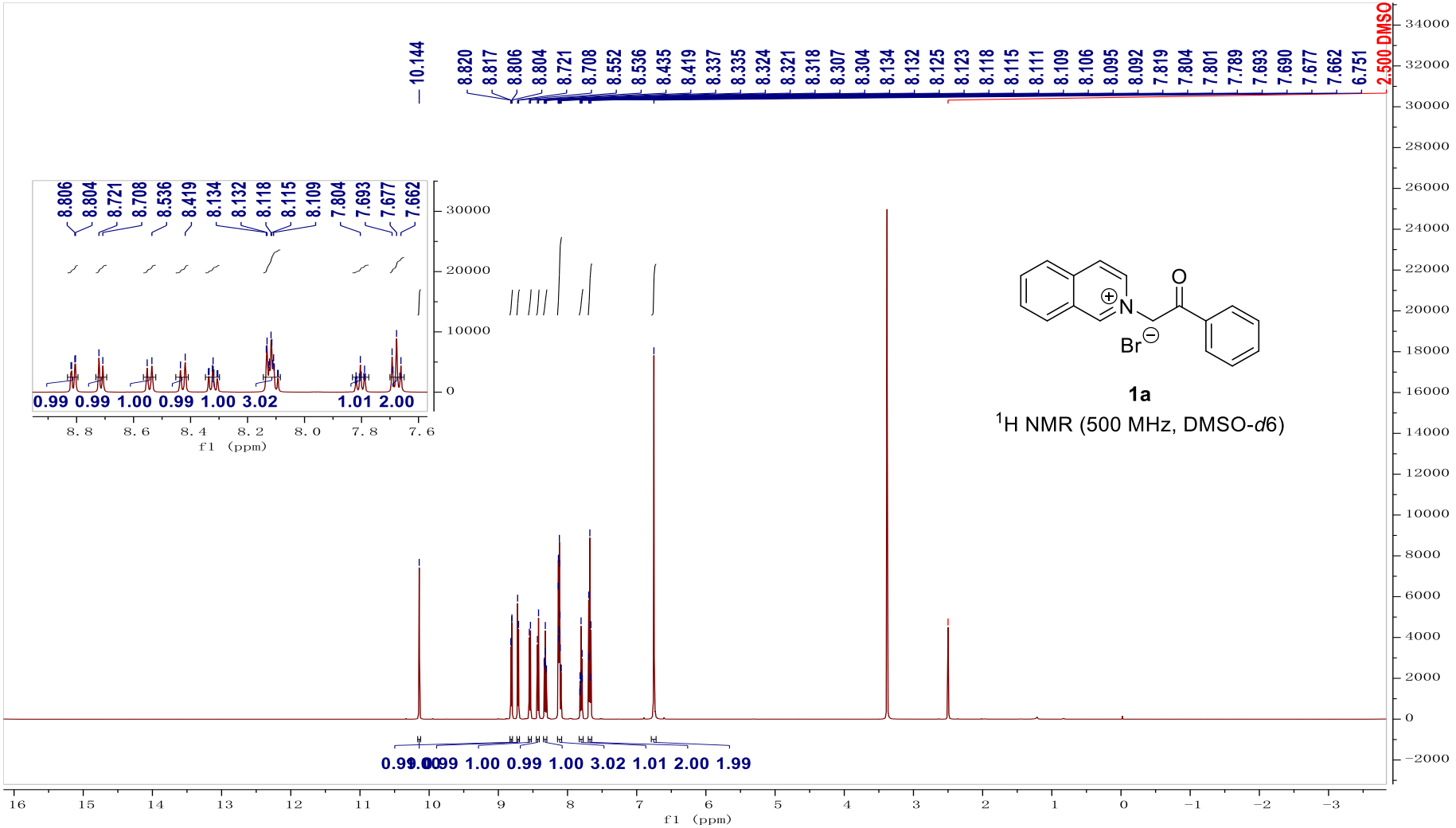
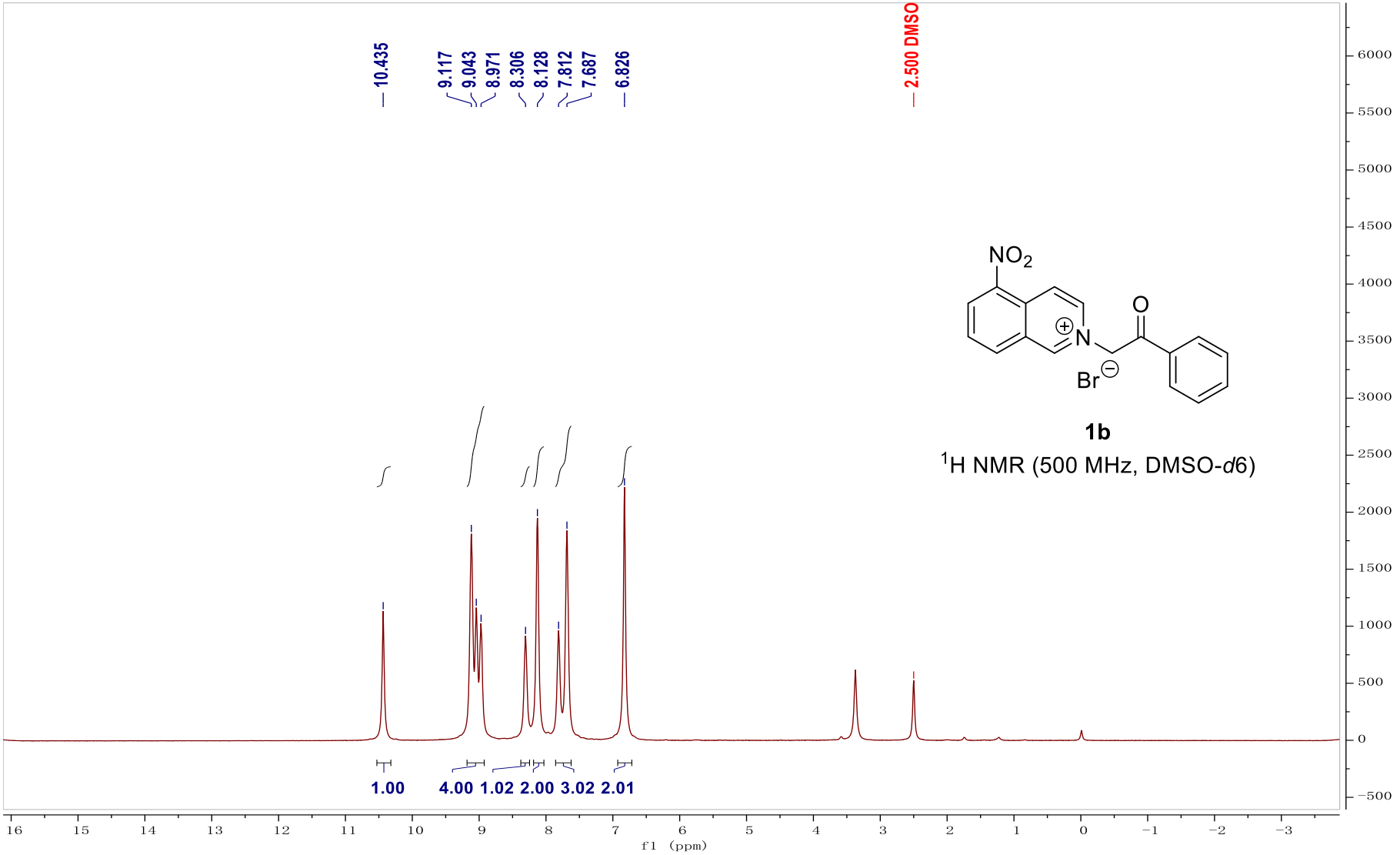
6. NMR spectra

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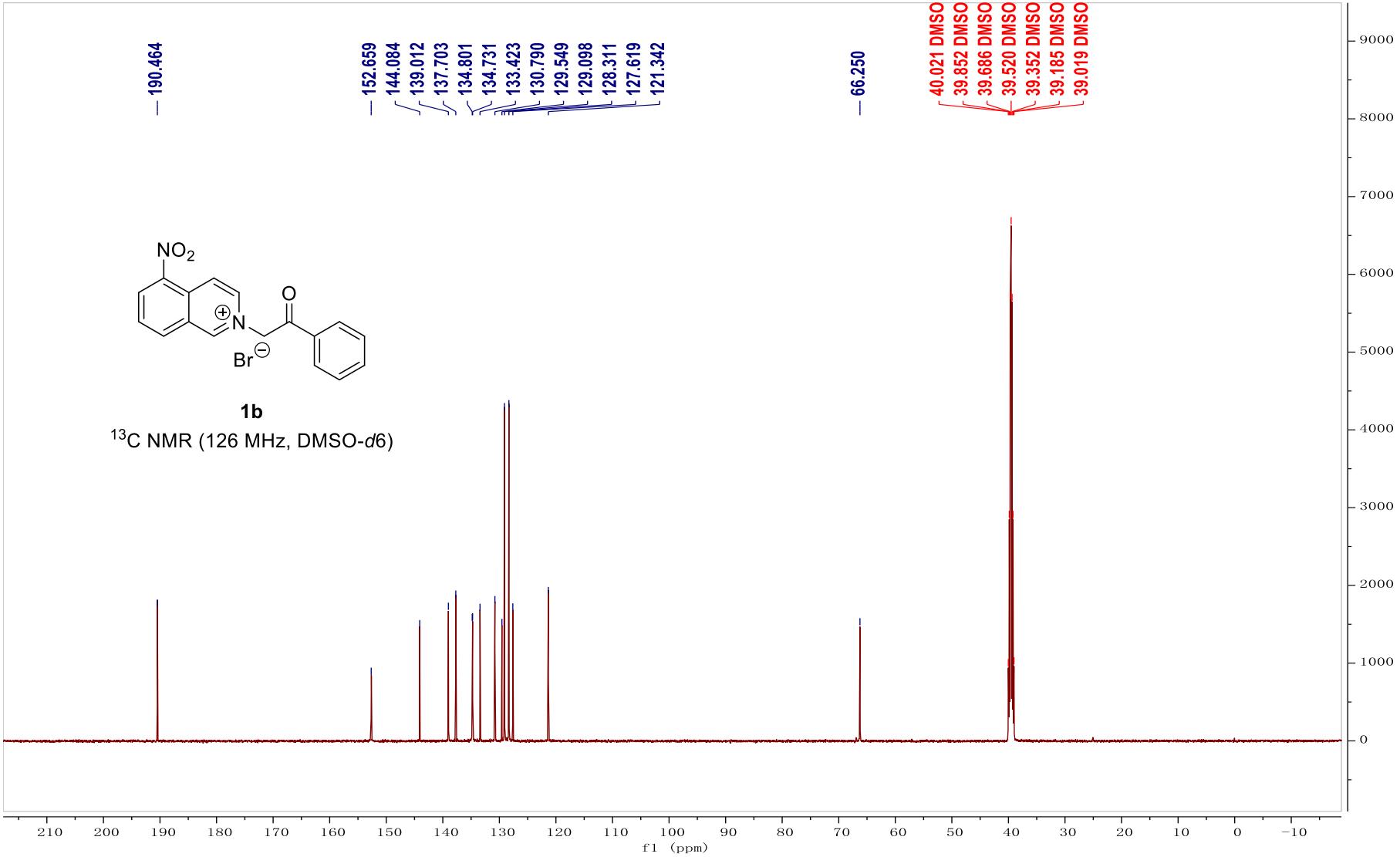
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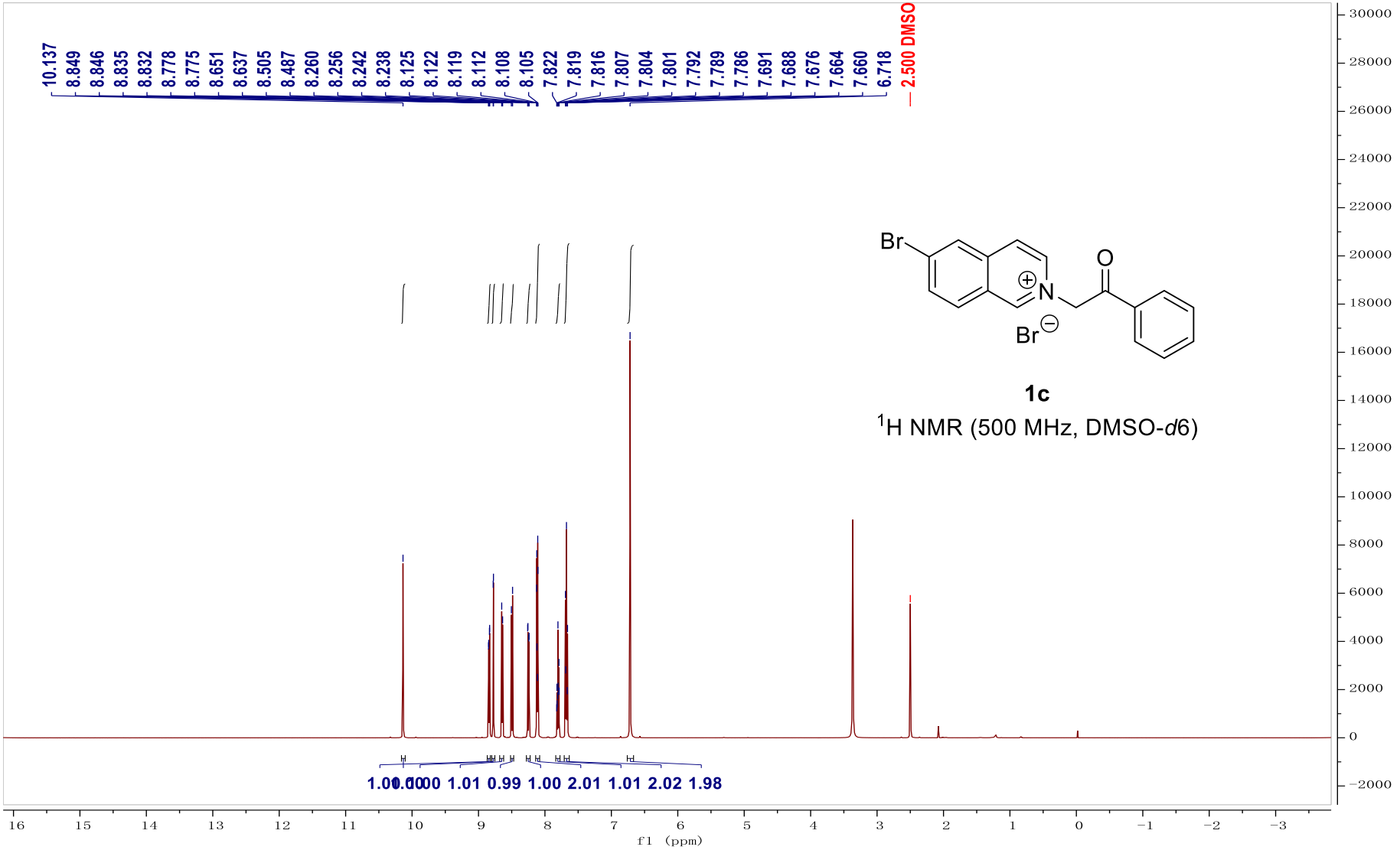
f1 (ppm)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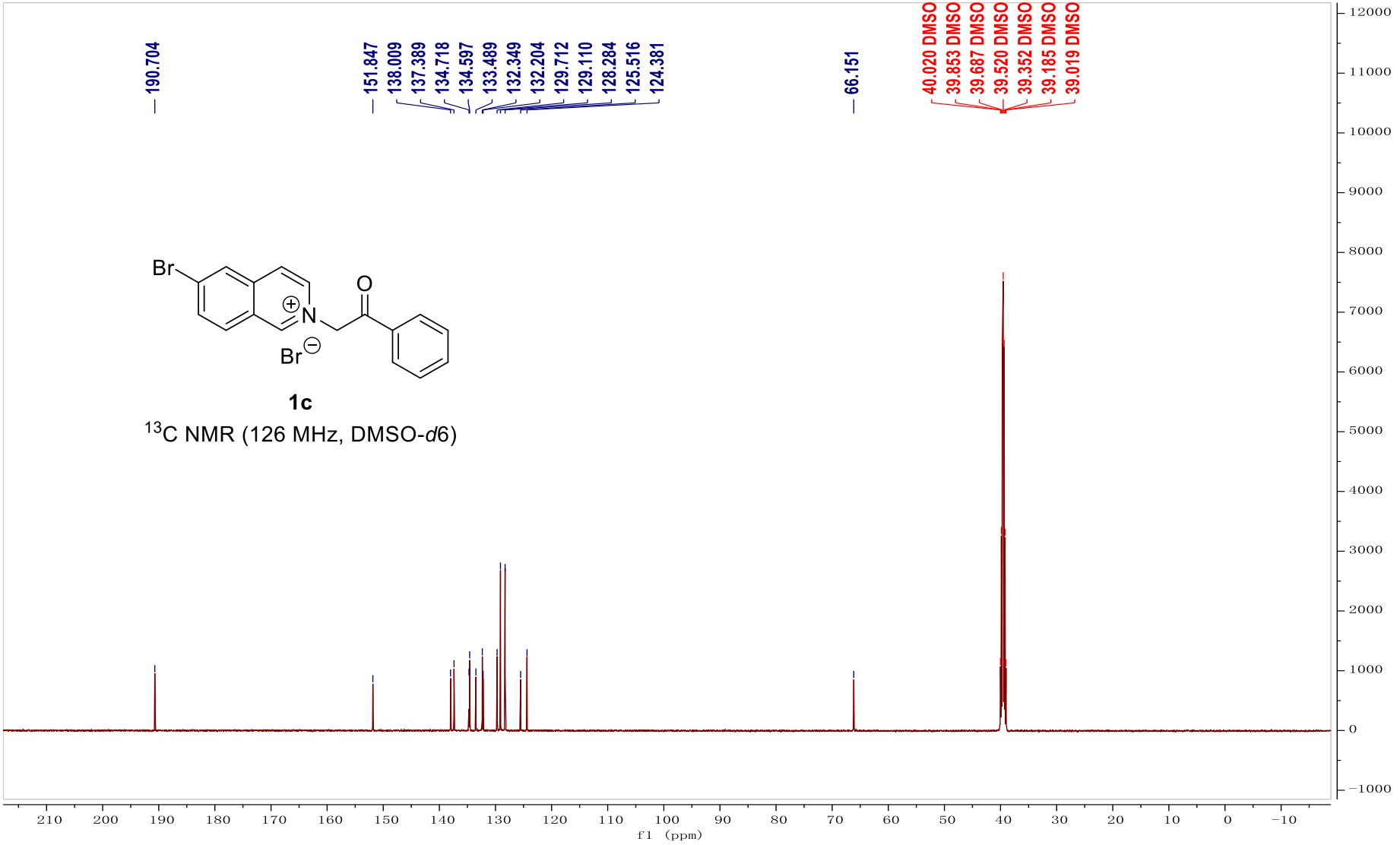
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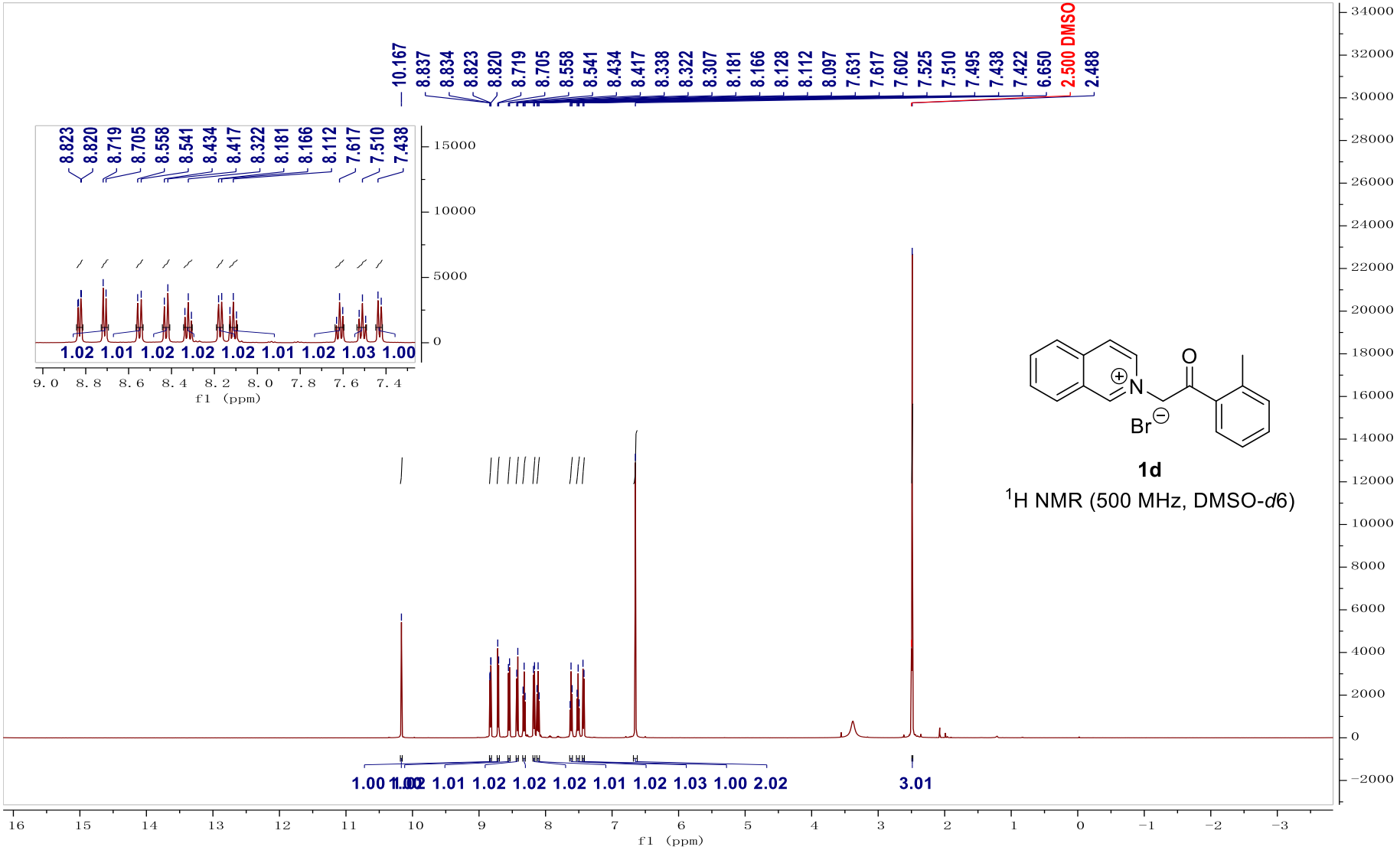
f1 (ppm)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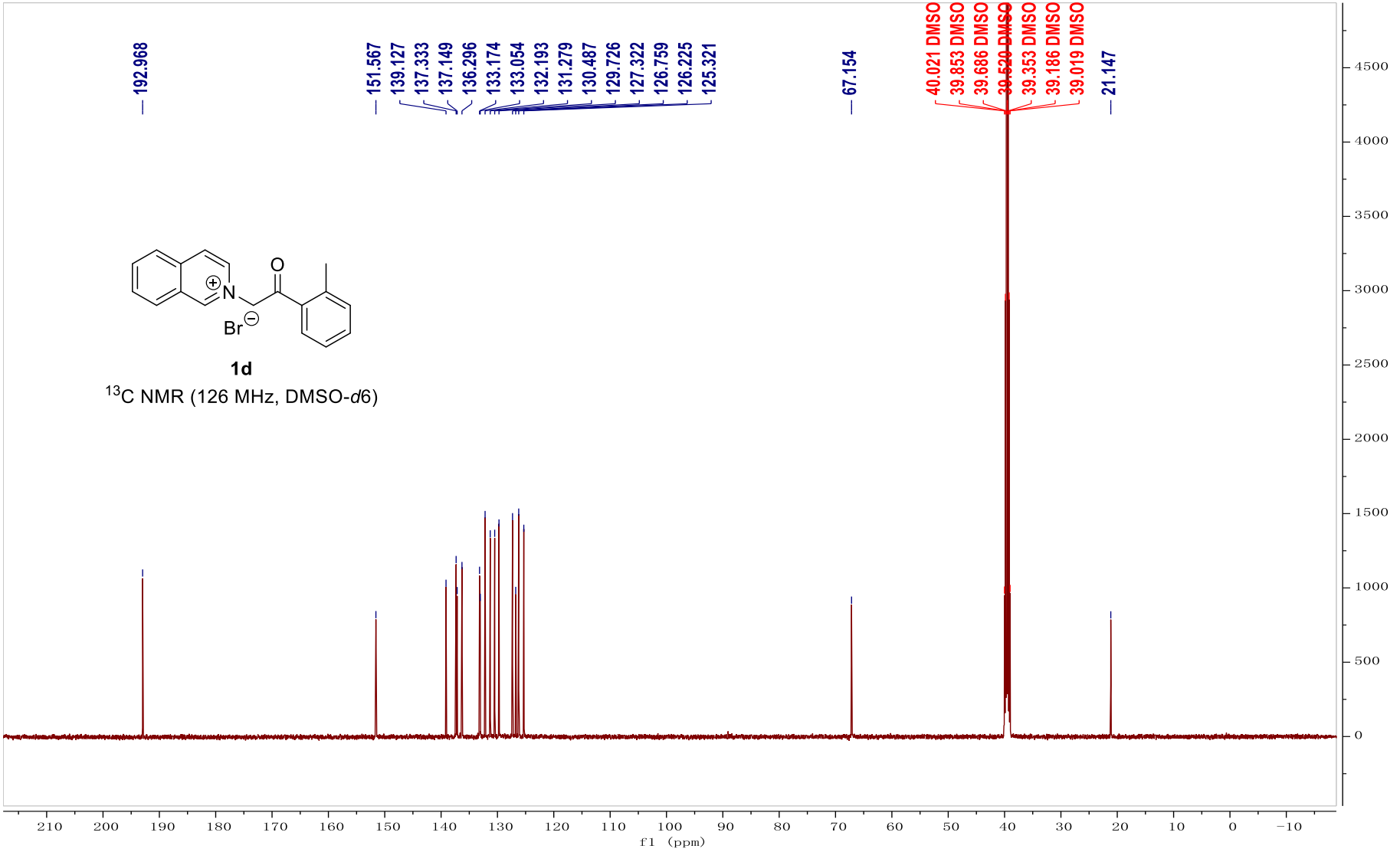
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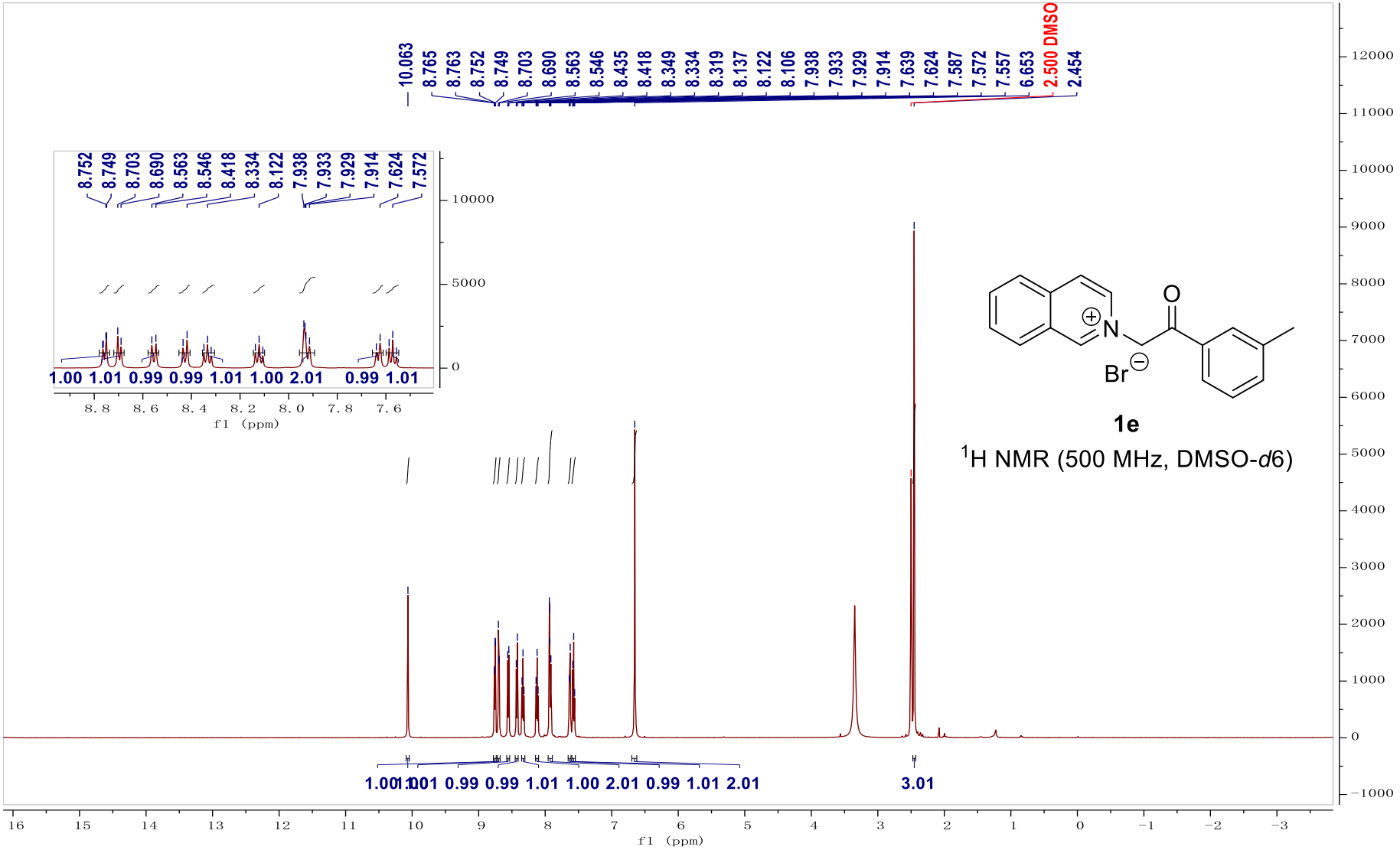
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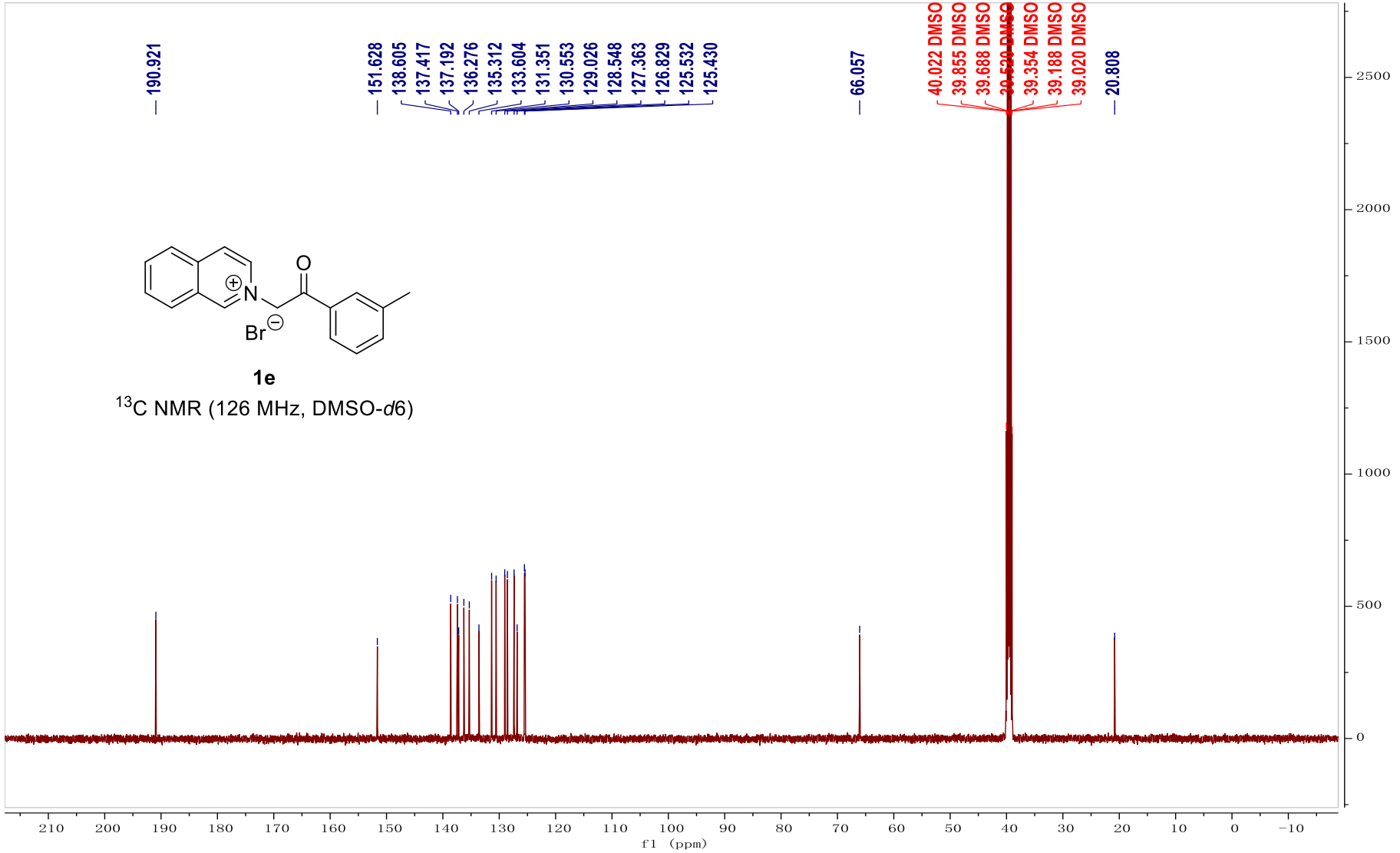
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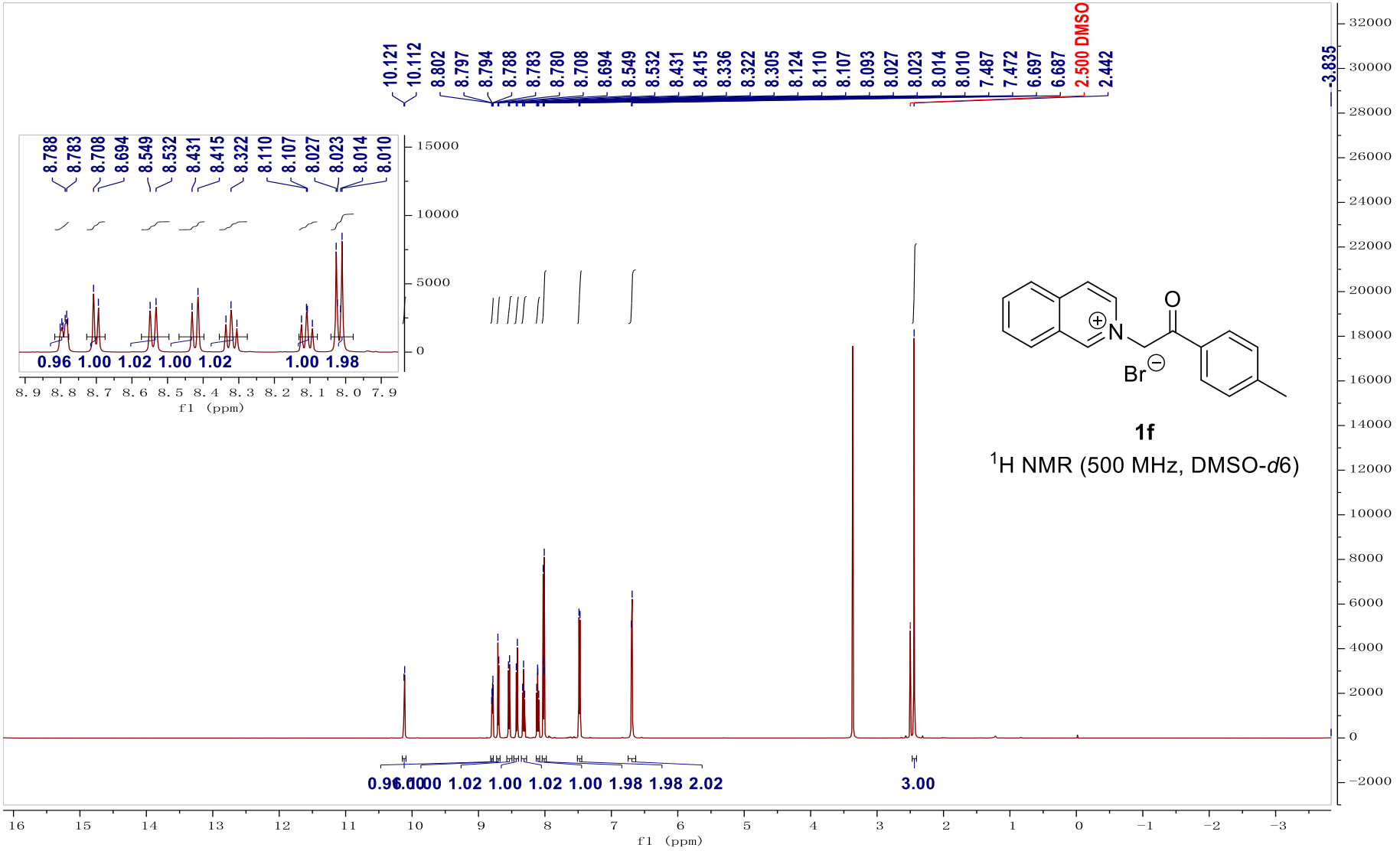
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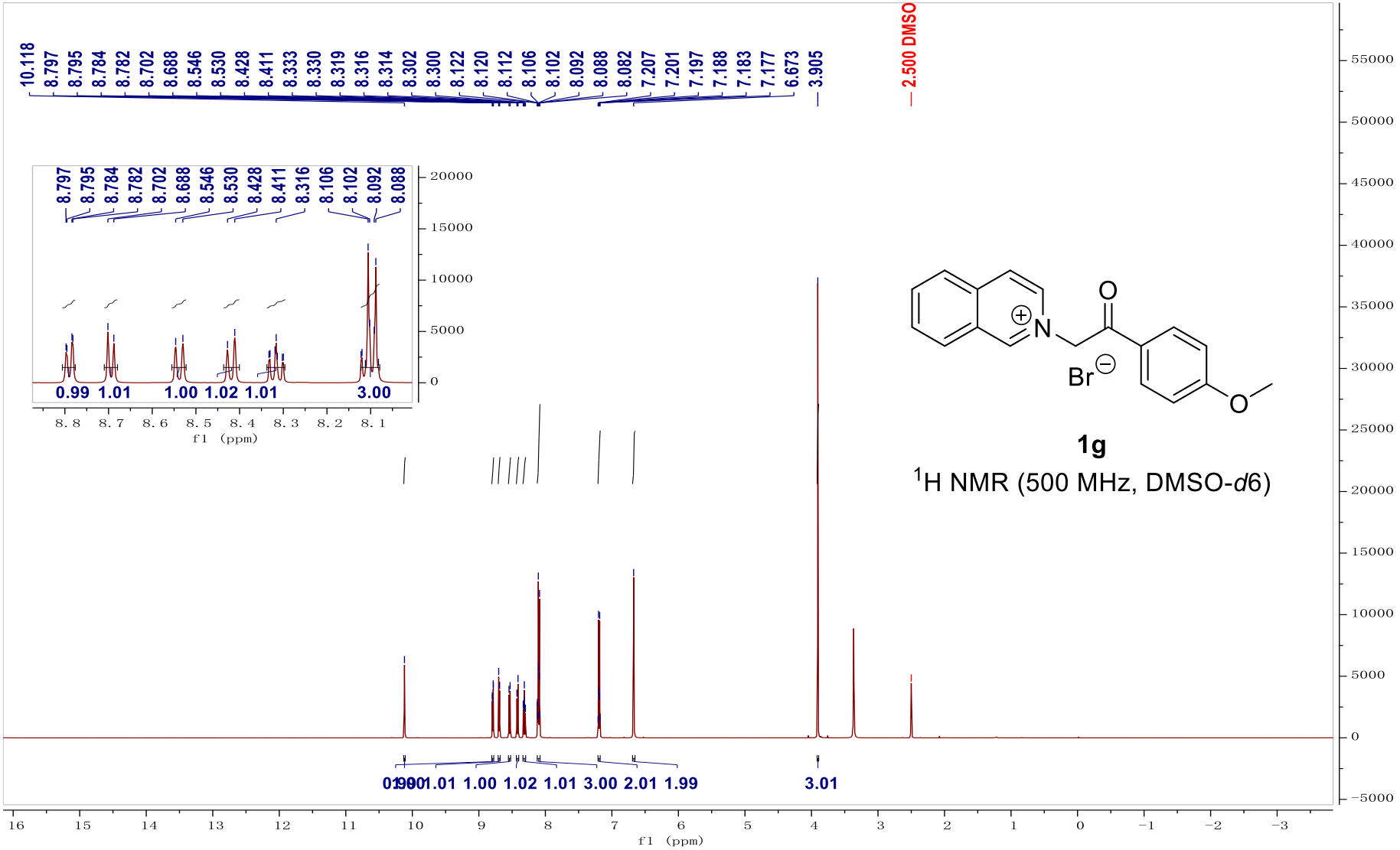
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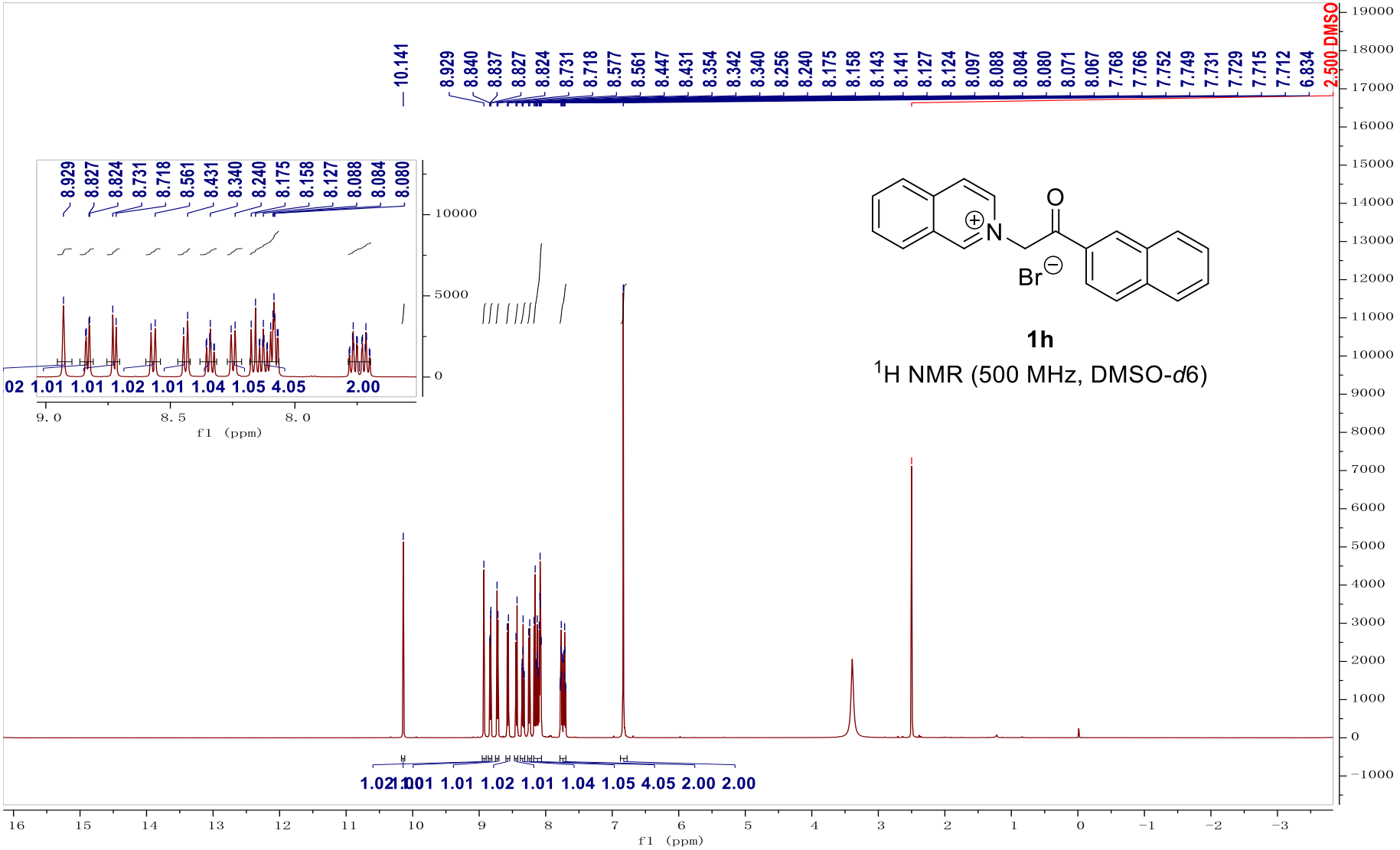
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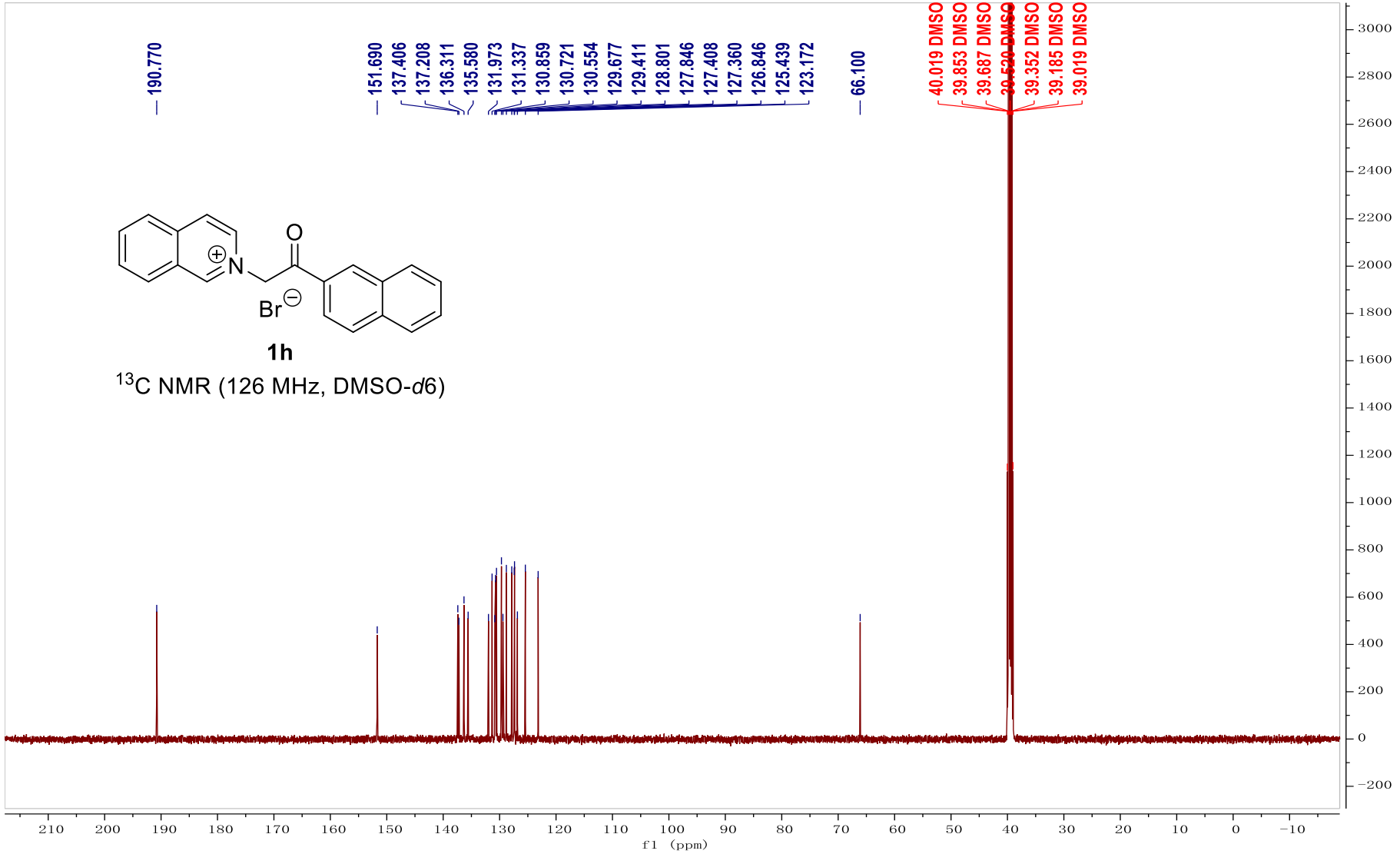
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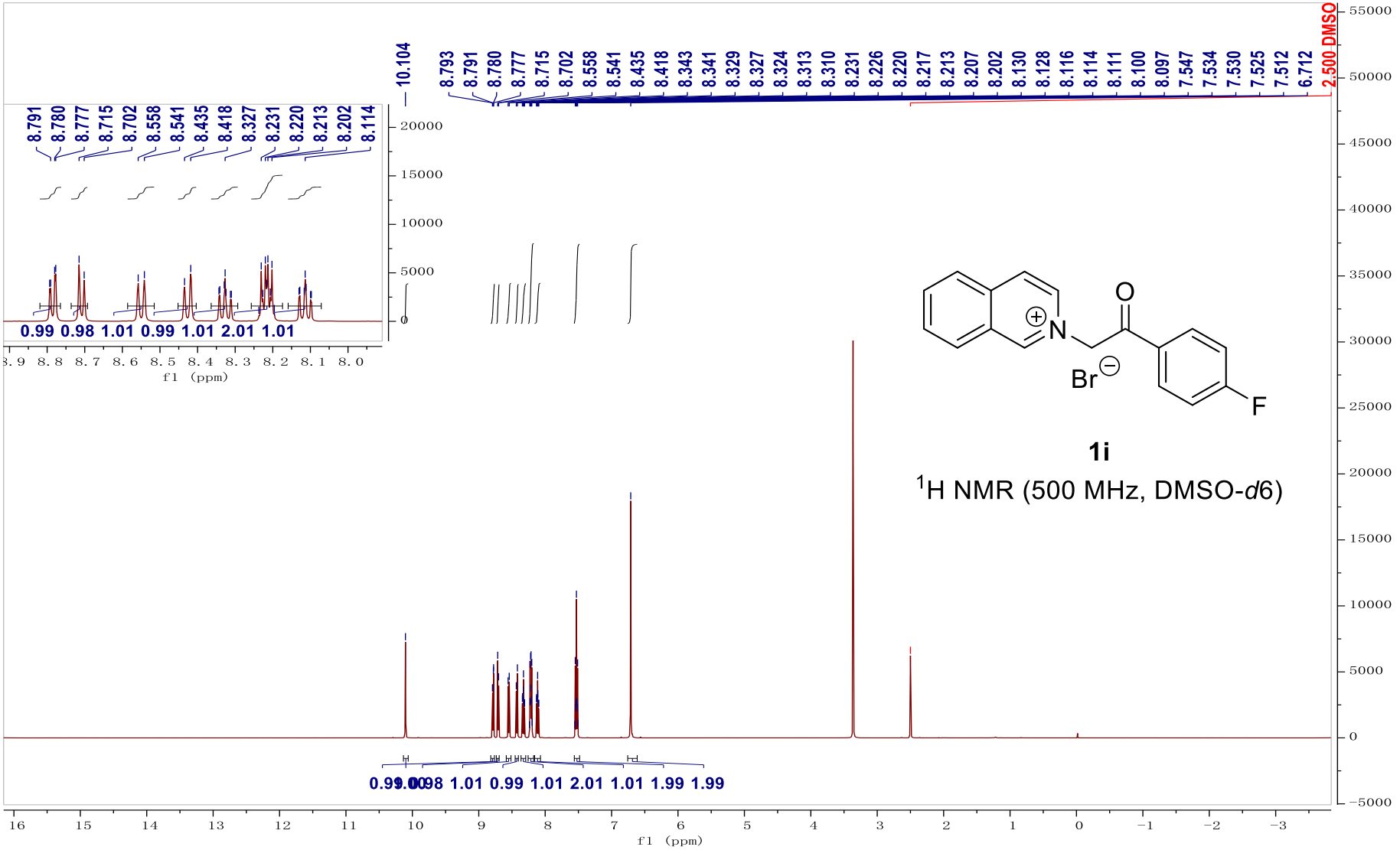
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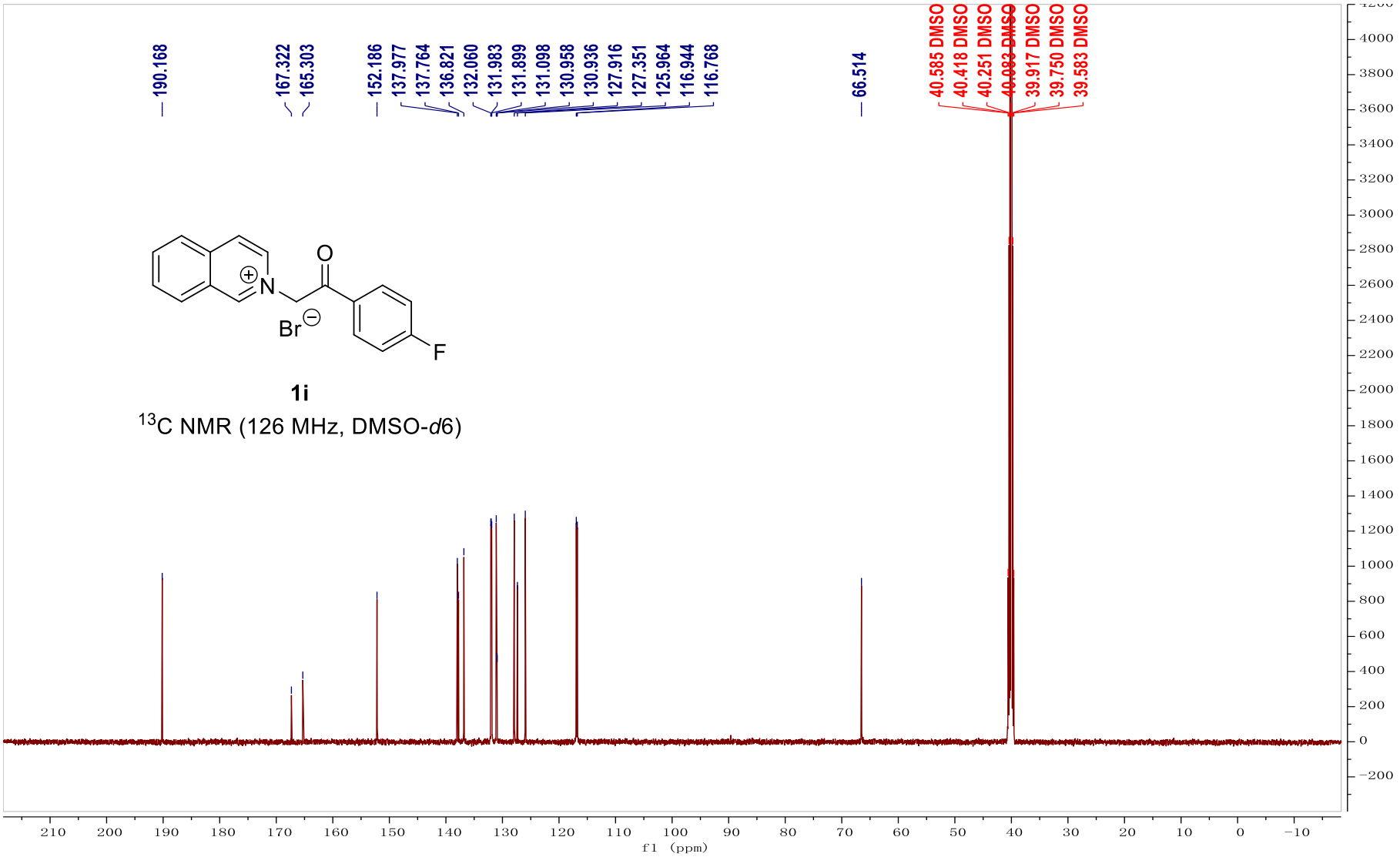
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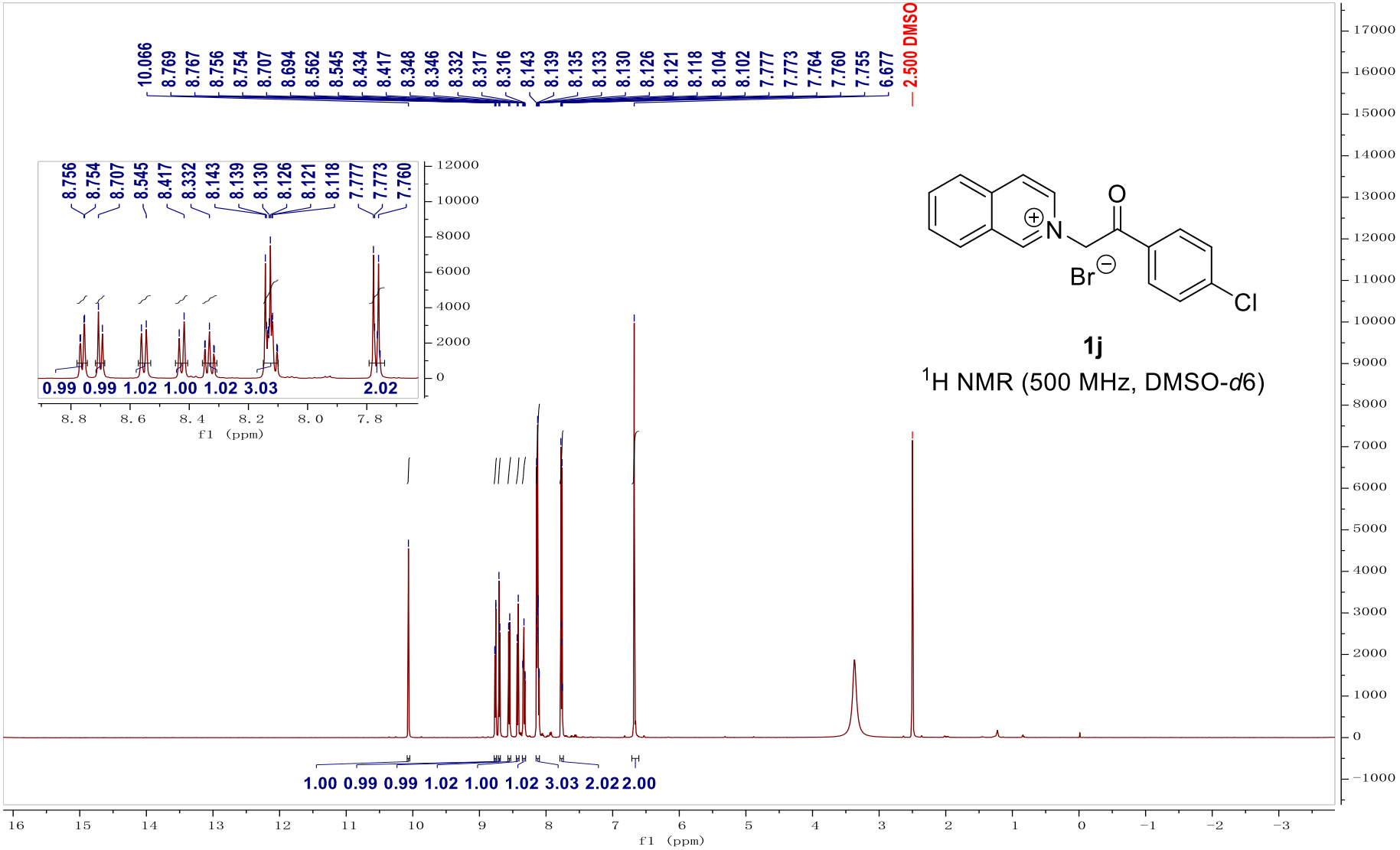
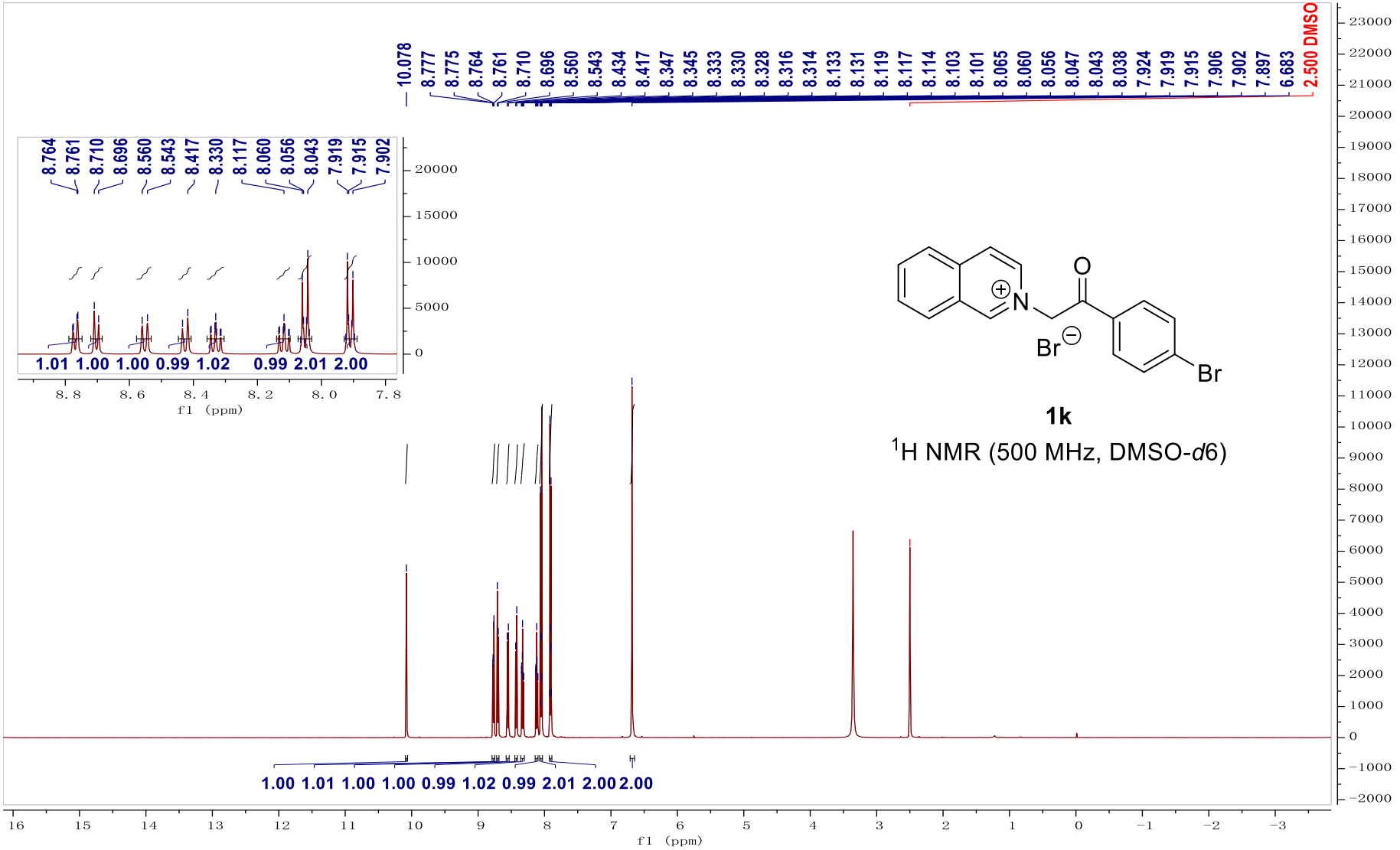
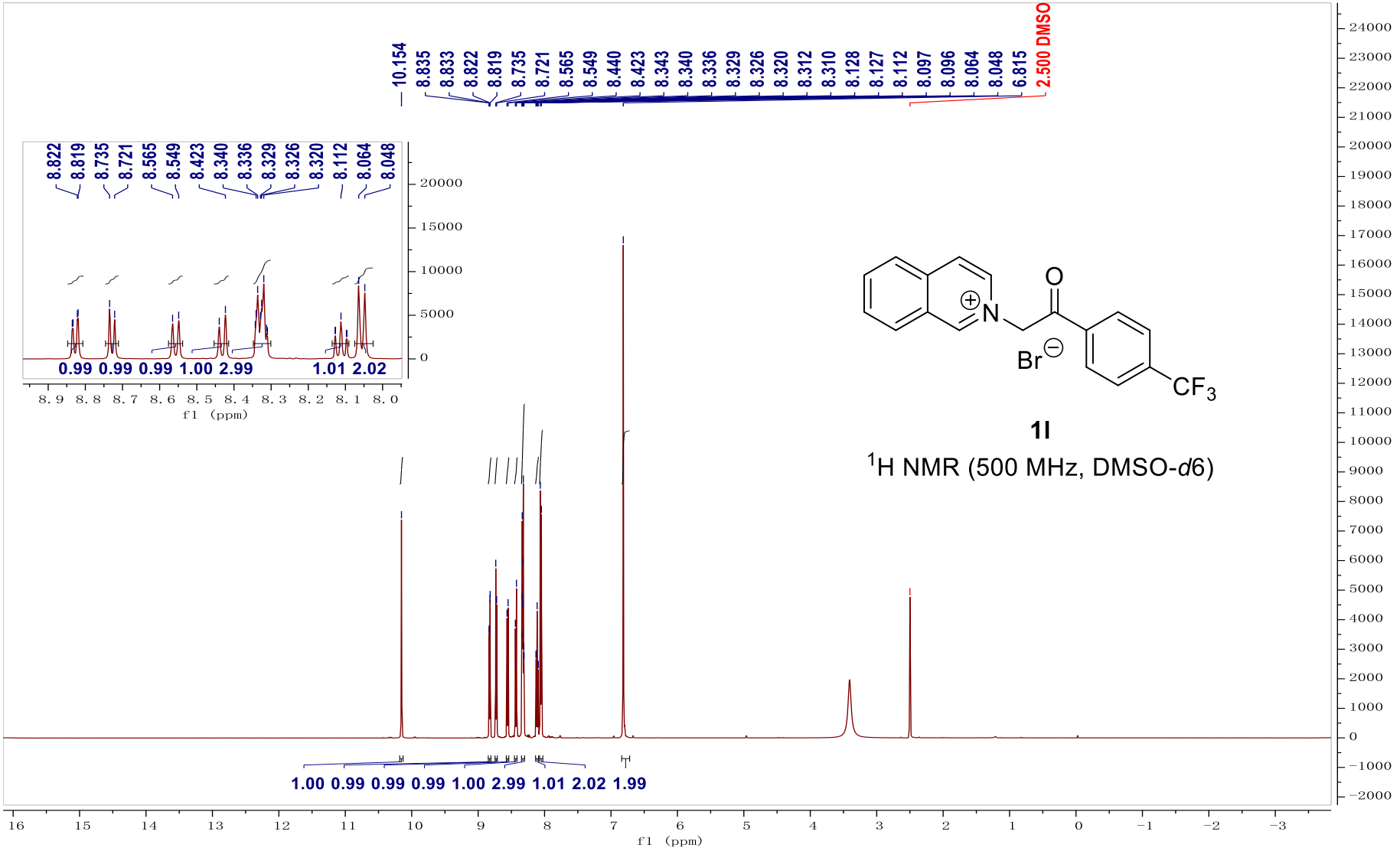
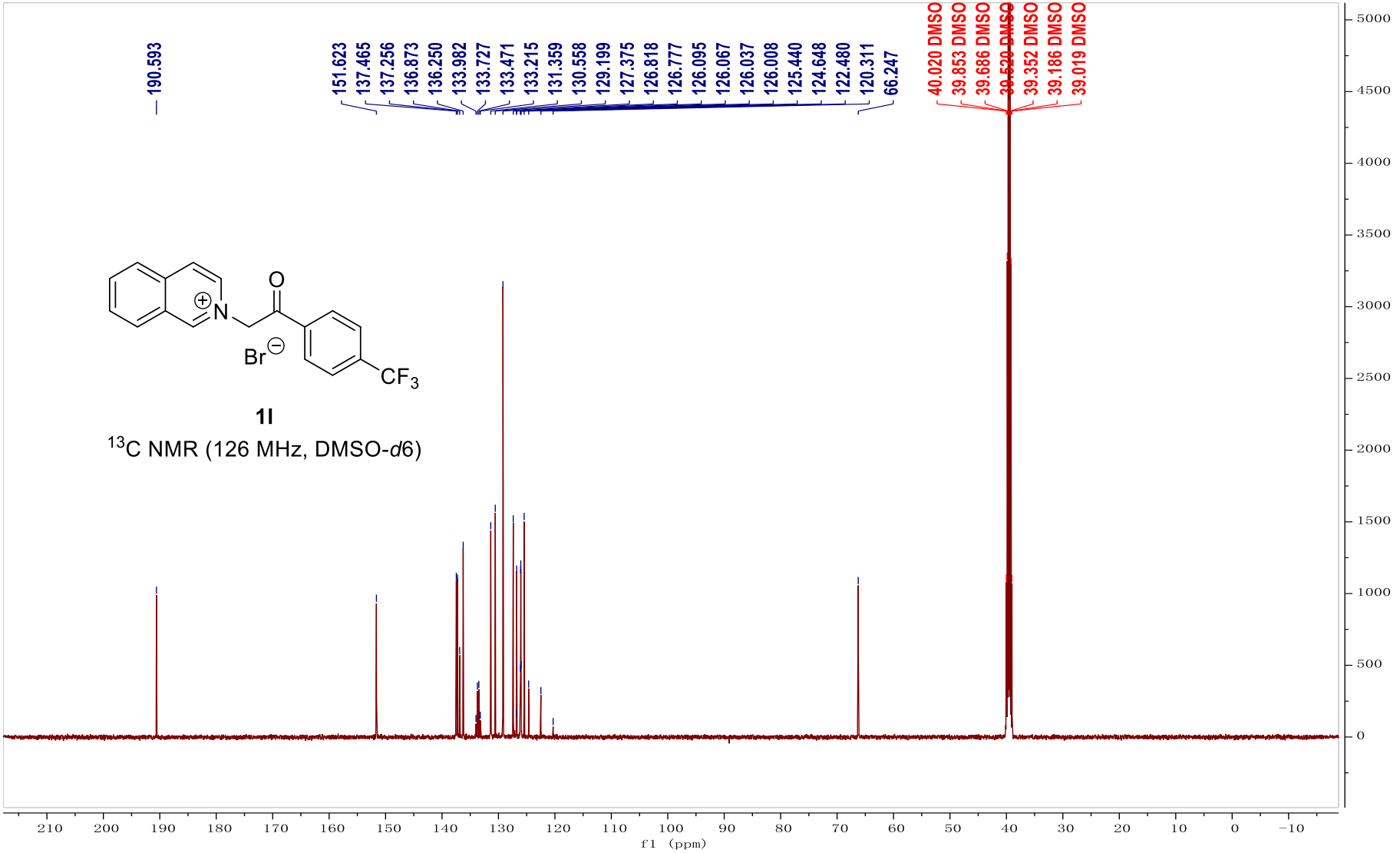
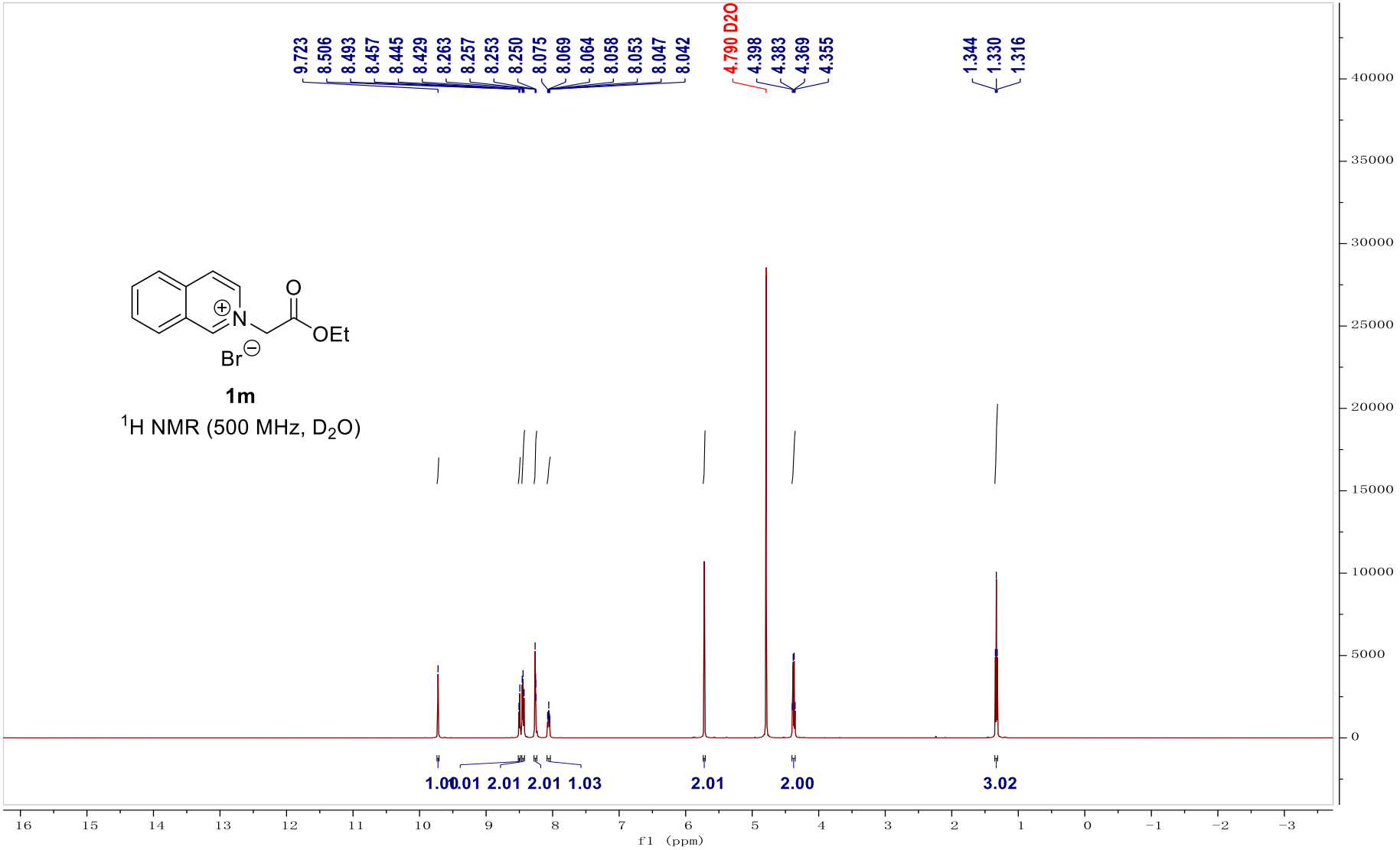
131.983
131.899
131.098
130.958
130.936
127.916
127.351
125.964
116.944
116.768
66.514
40.585 DMSO
40.418 DMSO
40.251 DMSO
40.083 DMSO
39.917 DMSO
39.750 DMSO
39.583 DMSO
O
N
Br
F
1i
13C NMR (126 MHz, DMSO-d6)
f1 (ppm)

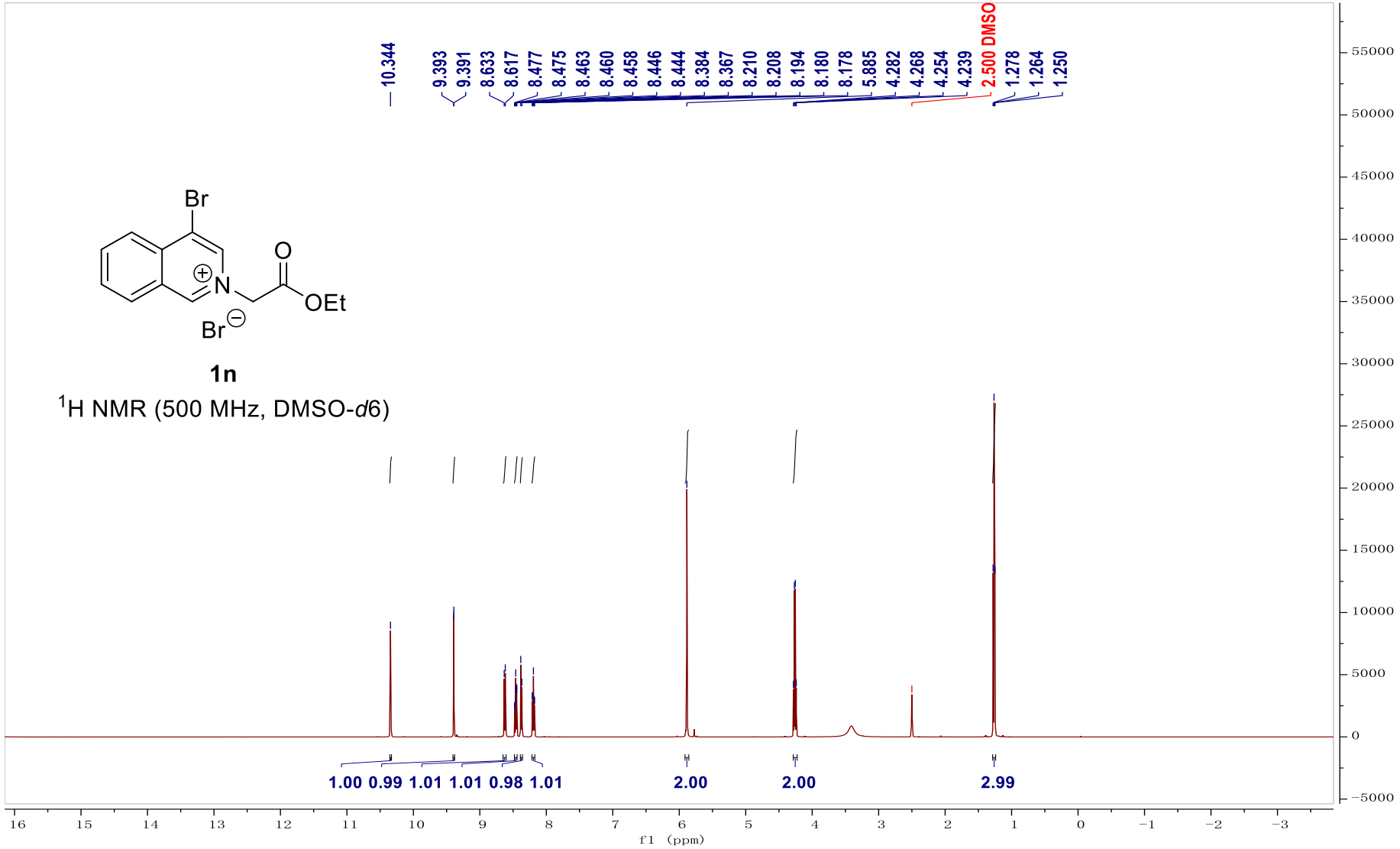

10.066
8.769
8.767
8.756
8.754
8.707
8.694
8.562
8.545
8.434
8.417
8.348
8.346
8.332
8.317
8.316
8.143
8.139
8.135
8.133
8.130
8.126
8.121
8.118
8.104
8.102
7.777
7.773
7.764
7.760
7.755
6.677
2.500 DMSO
0.99 0.99 1.02 1.00 1.02 3.03 2.02
1.00 0.99 0.99 1.02 1.00 1.02 3.03 2.02 2.00
f1 (ppm)
O
N
Br
Cl
1j
1H NMR (500 MHz, DMSO-d6)

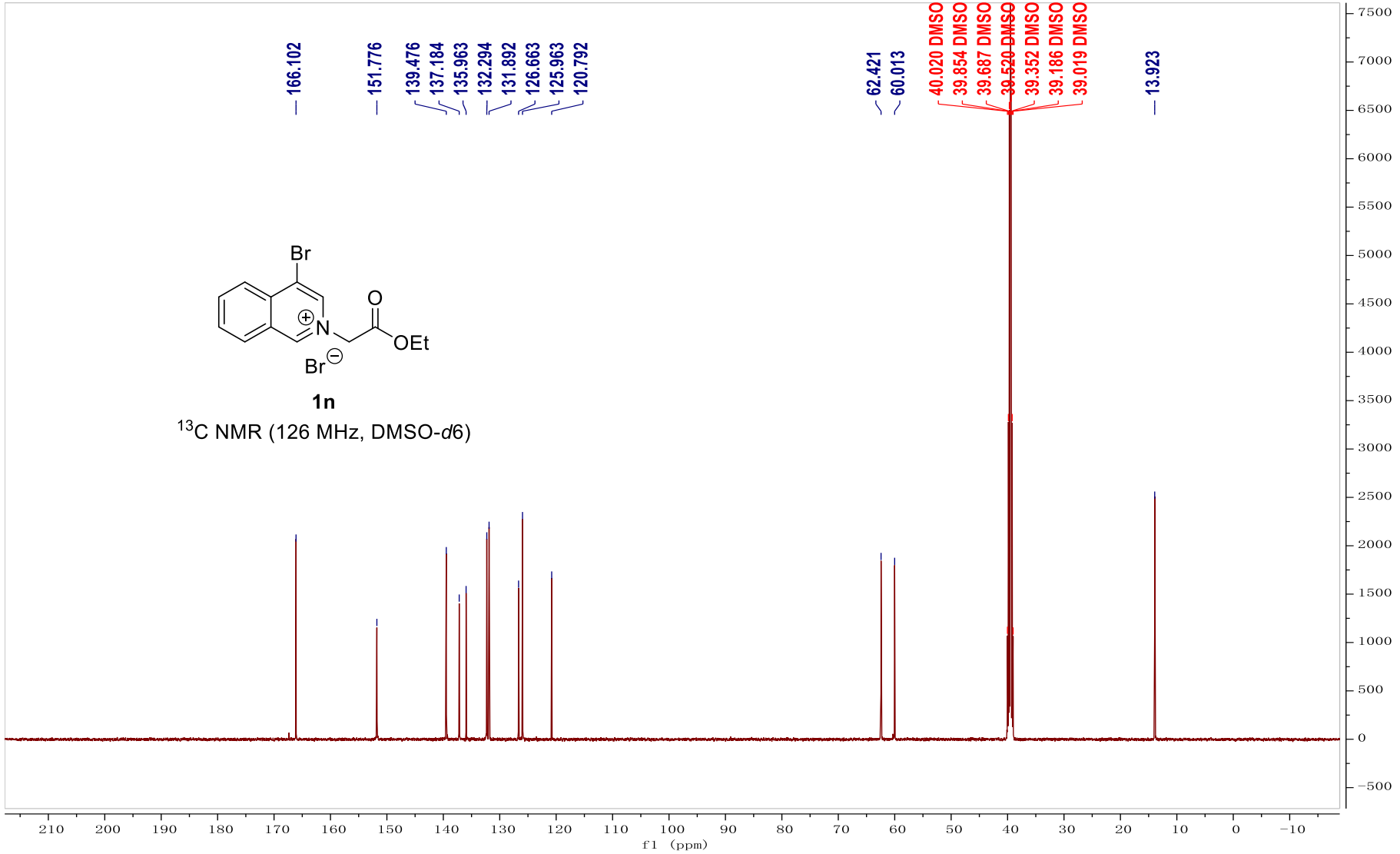

10.078
8.777
8.775
8.764
8.761
8.710
8.696
8.560
8.543
8.434
8.417
8.347
8.345
8.333
8.330
8.328
8.316
8.314
8.133
8.131
8.119
8.117
8.114
8.103
8.101
8.065
8.060
8.056
8.047
8.043
8.038
7.924
7.919
7.915
7.906
7.902
7.897
6.683
2.500 DMSO
1.00 1.01 1.00 1.00 0.99 1.02 0.99 2.01 2.00 2.00
f1 (ppm)
1.01 1.00 1.00 0.99 1.02 0.99 2.01 2.00
f1 (ppm)
O
N
Br
Br
1k
1H NMR (500 MHz, DMSO-d6)

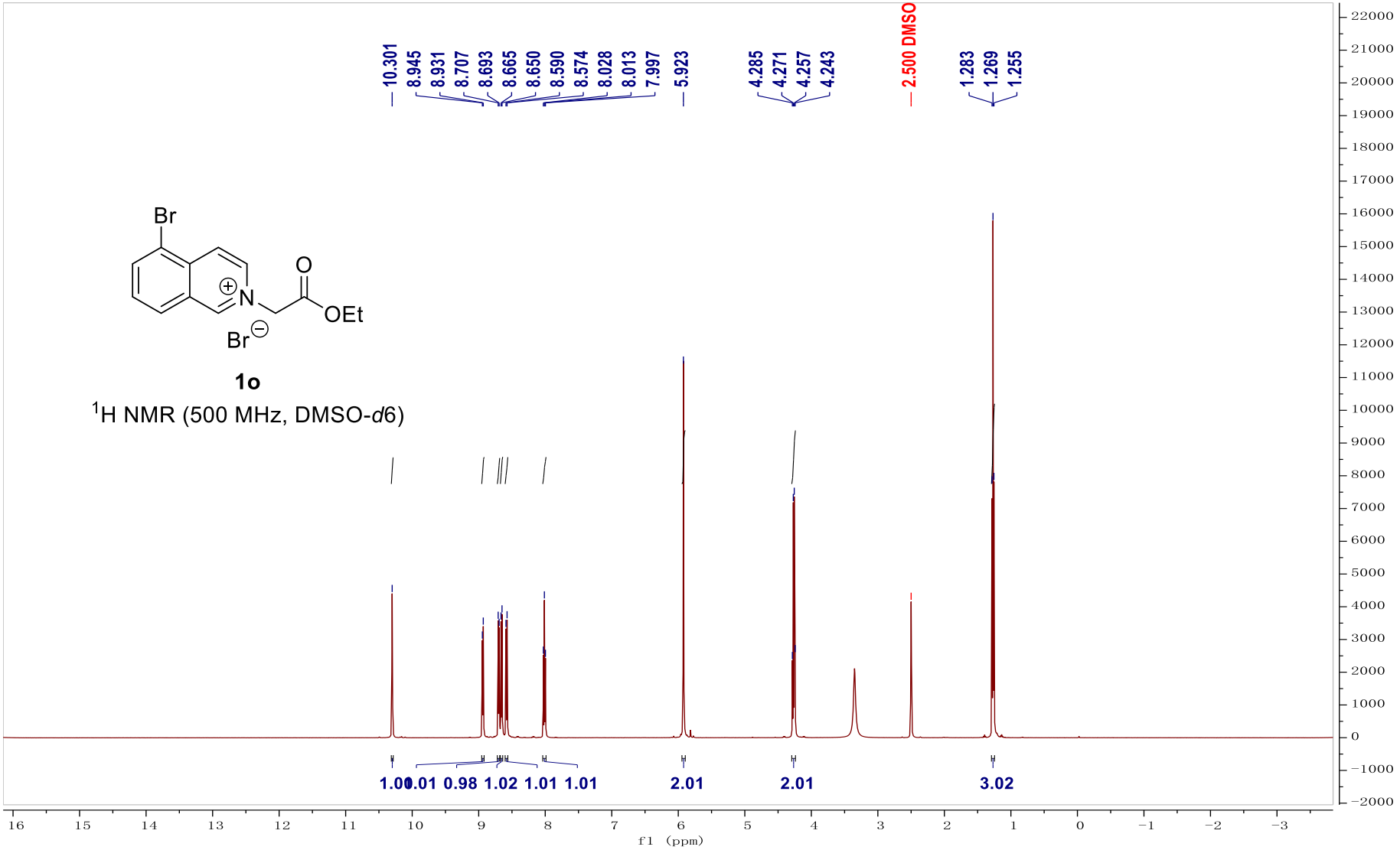

10.154
8.835
8.833
8.822
8.819
8.735
8.721
8.565
8.549
8.440
8.423
8.343
8.340
8.336
8.329
8.326
8.320
8.312
8.310
8.128
8.127
8.112
8.097
8.096
8.064
8.048
6.815
2.500 DMSO
0.99 0.99 0.99 1.00 2.99 1.01 2.02
1.00 0.99 0.99 0.99 1.00 2.99 1.01 2.02 1.99
f1 (ppm)
Br
CF3
1I
1H NMR (500 MHz, DMSO-d6)

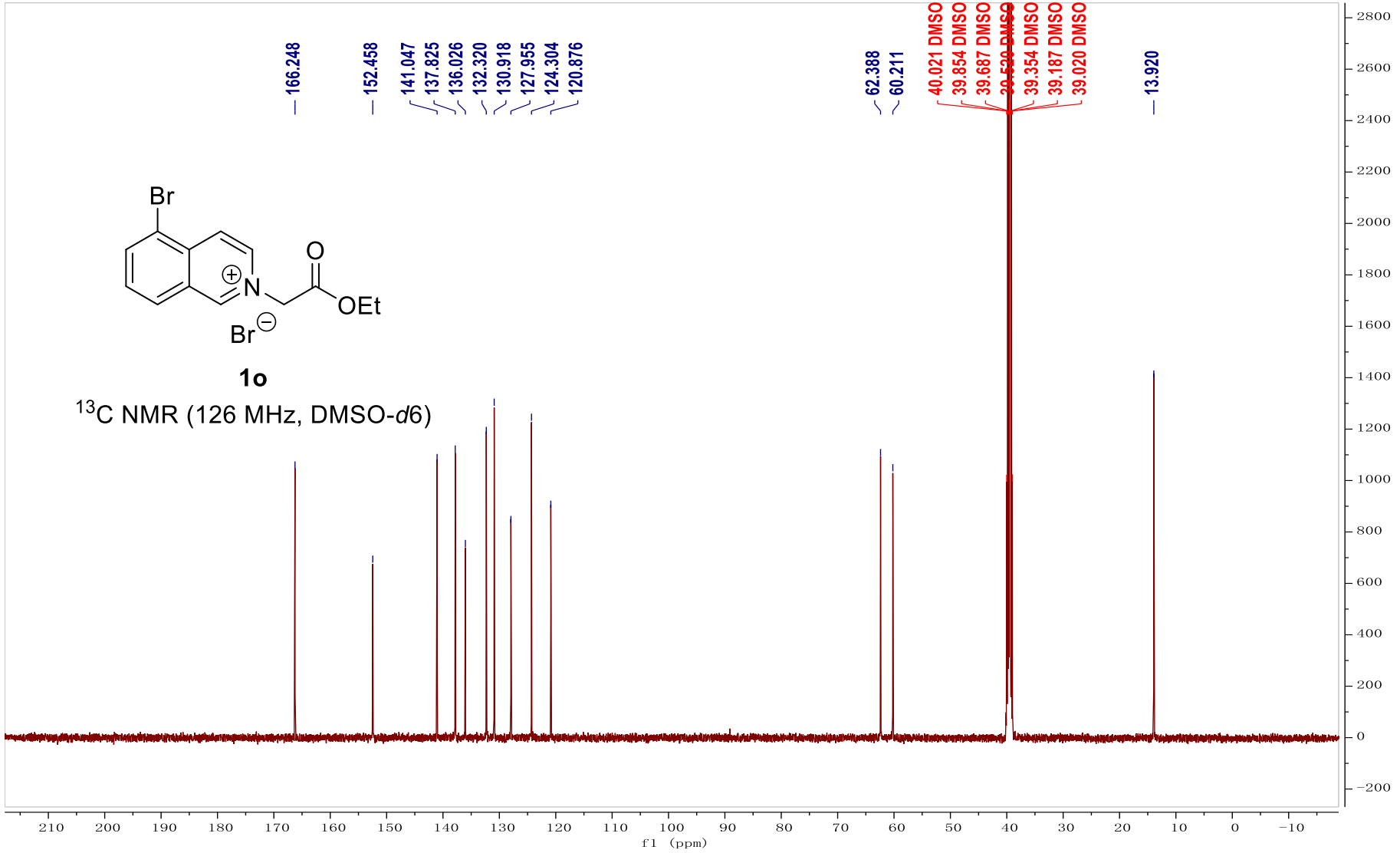

190.593
151.623
137.465
137.256
136.873
136.250
133.982
133.727
133.471
133.215
131.359
130.558
129.199
127.375
126.818
126.777
126.095
126.067
126.037
126.008
125.440
124.648
122.480
120.311
66.247
40.020 DMSO
39.853 DMSO
39.686 DMSO
39.520 DMSO
39.352 DMSO
39.186 DMSO
39.019 DMSO
O
N
Br
CF3
1l
13C NMR (126 MHz, DMSO-d6)
f1 (ppm)

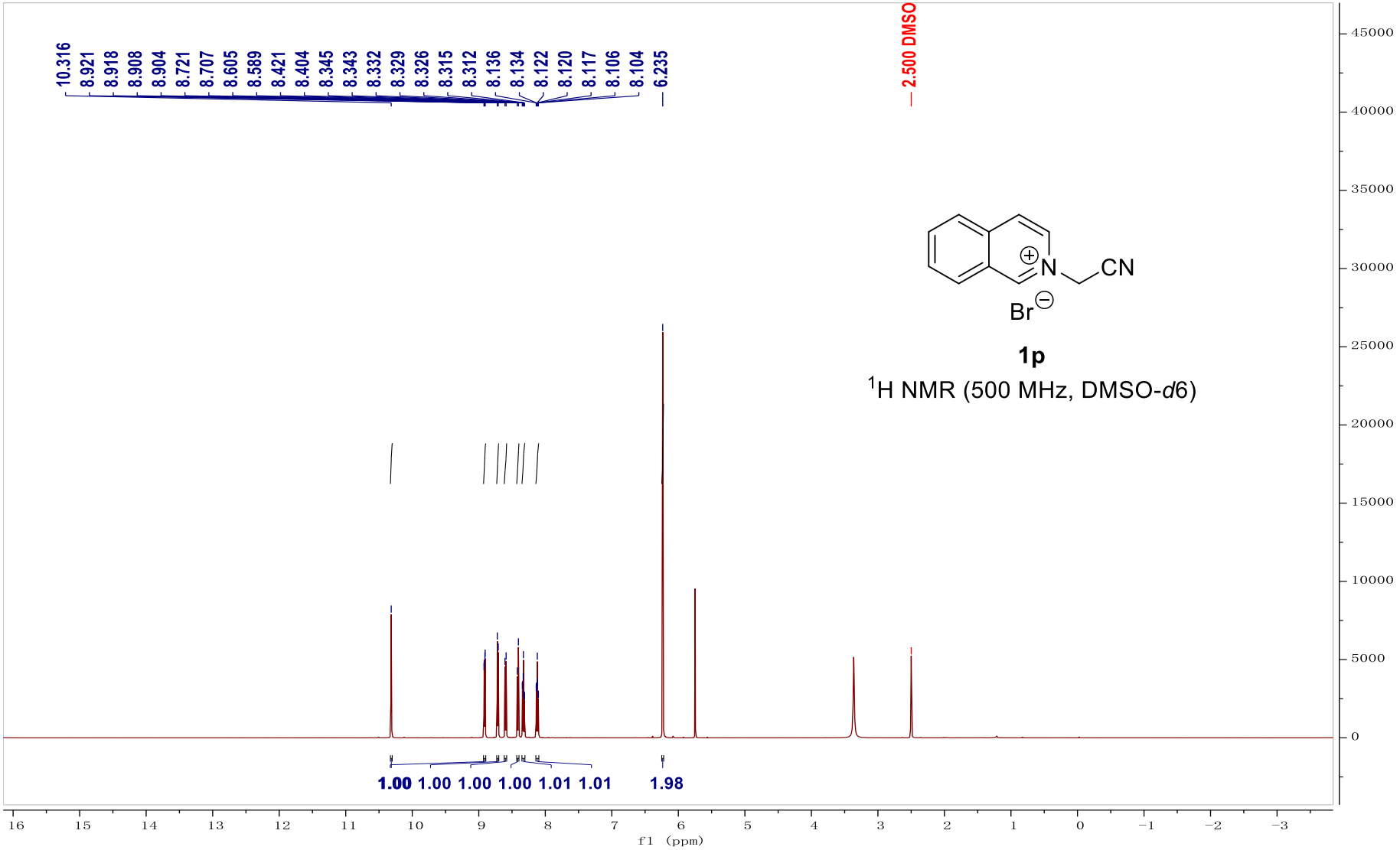

9.723
8.506
8.493
8.457
8.445
8.429
8.263
8.257
8.253
8.250
8.075
8.069
8.064
8.058
8.053
8.047
8.042
4.790 D2O
4.398
4.383
4.369
4.355
1.344
1.330
1.316
O
N
OEt
Br
1m
1H NMR (500 MHz, D2O)
1.00
1.01
2.01
2.01
1.03
2.01
2.00
3.02
f1 (ppm)

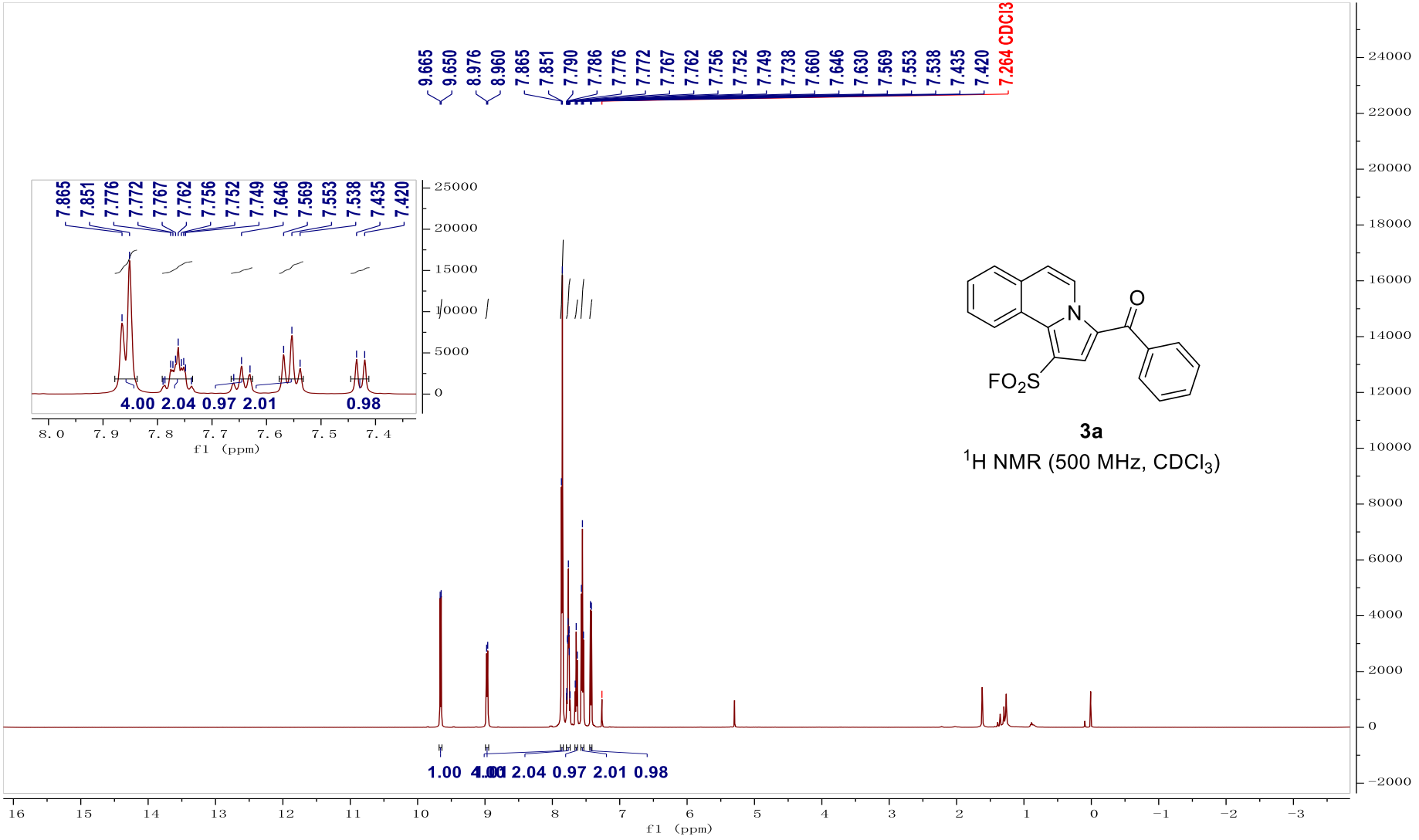

10.344
9.393
9.391
8.633
8.617
8.477
8.475
8.463
8.460
8.458
8.446
8.444
8.384
8.367
8.210
8.208
8.194
8.180
8.178
5.885
4.282
4.268
4.254
4.239
2.500 DMSO
1.278
1.264
1.250
Br
O
N
OEt
Br
1n
1H NMR (500 MHz, DMSO-d6)
1.00 0.99 1.01 1.01 0.98 1.01
2.00
2.00
2.99
f1 (ppm)

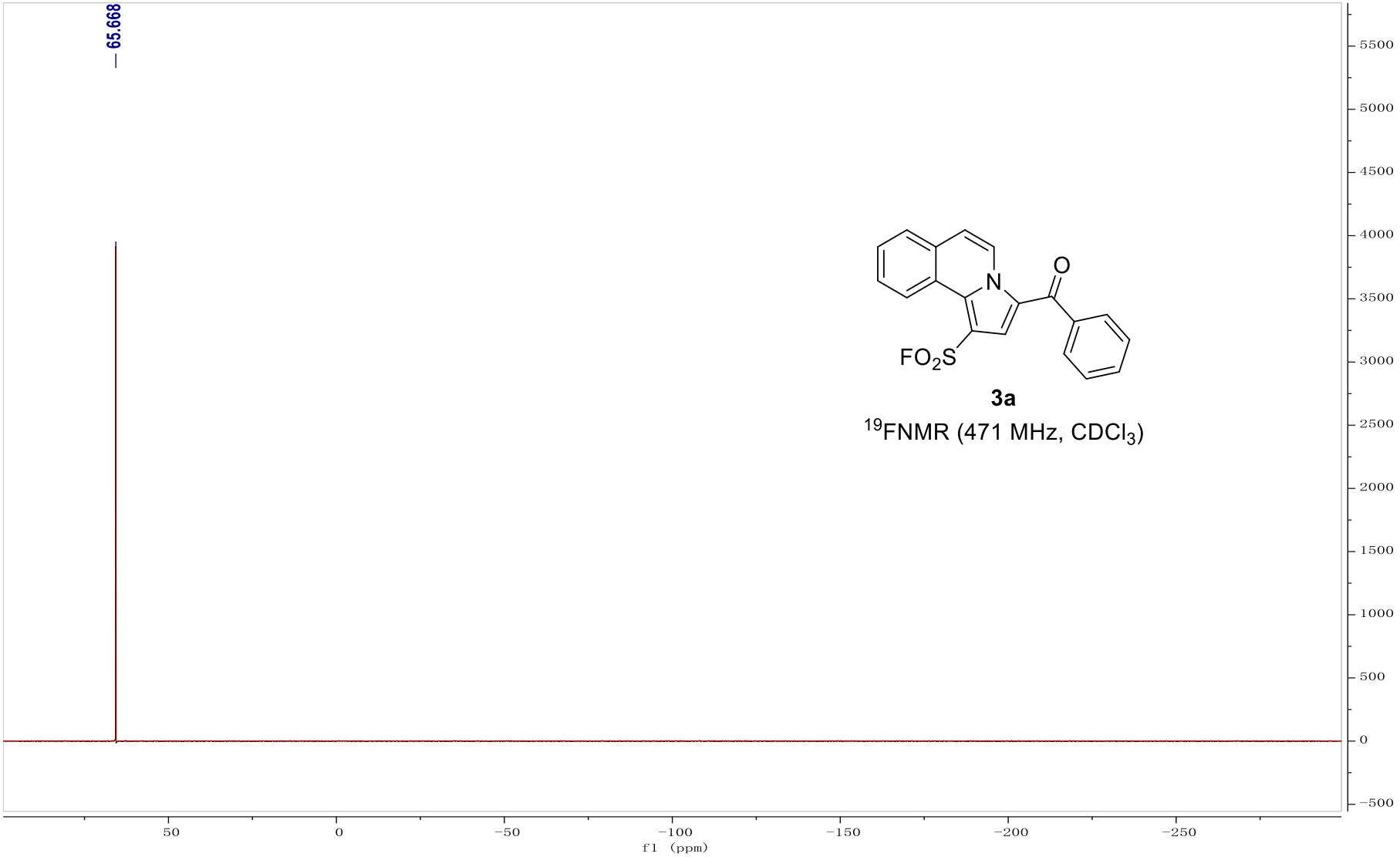

166.102
151.776
139.476
137.184
135.963
132.294
131.892
126.663
125.963
120.792
62.421
60.013
40.020 DMSO
39.854 DMSO
39.687 DMSO
39.520 DMSO
39.352 DMSO
39.186 DMSO
39.019 DMSO
13.923
Br
O
N
OEt
Br
1n
13C NMR (126 MHz, DMSO-d6)
f1 (ppm)


10.301
8.945
8.931
8.707
8.693
8.665
8.650
8.590
8.574
8.028
8.013
7.997
5.923
4.285
4.271
4.257
4.243
2.500 DMSO
1.283
1.269
1.255
Br
O
N
OEt
Br
1o
1H NMR (500 MHz, DMSO-d6)
1.00 0.01 0.98 1.02 1.01 1.01
2.01
2.01
3.02
f1 (ppm)


166.248
152.458
141.047
137.825
136.026
132.320
130.918
127.955
124.304
120.876
62.388
60.211
40.021 DMSO
39.854 DMSO
39.687 DMSO
39.520 DMSO
39.354 DMSO
39.187 DMSO
39.020 DMSO
13.920
Br
O
N
OEt
Br
1o
13C NMR (126 MHz, DMSO-d6)
f1 (ppm)

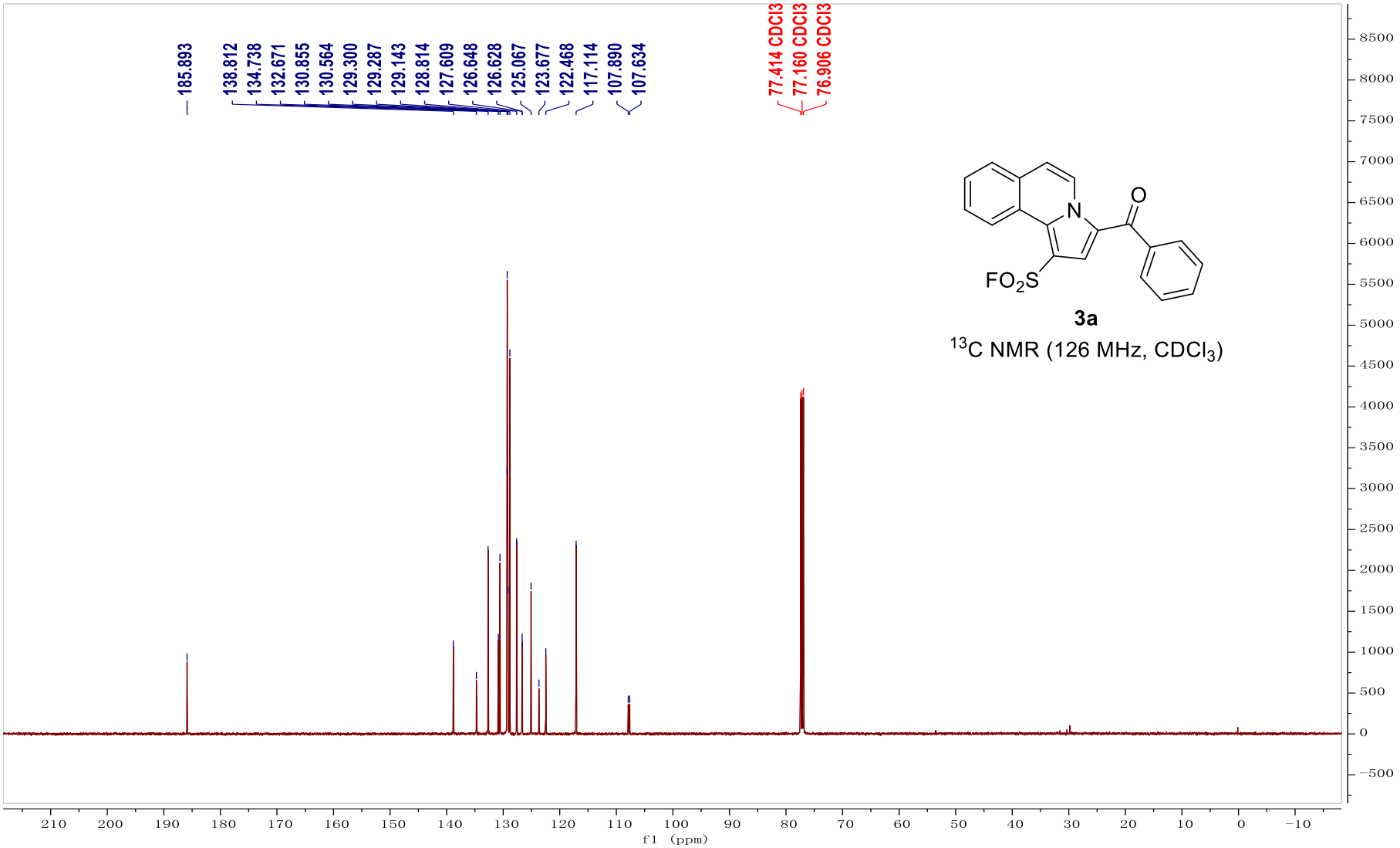

10.316
8.921
8.918
8.908
8.904
8.721
8.707
8.605
8.589
8.421
8.404
8.345
8.343
8.332
8.329
8.326
8.315
8.312
8.136
8.134
8.122
8.120
8.117
8.106
8.104
6.235
2.500 DMSO
N
CN
Br
1p
1H NMR (500 MHz, DMSO-d6)
1.00 1.00 1.00 1.00 1.01 1.01
1.98
f1 (ppm)

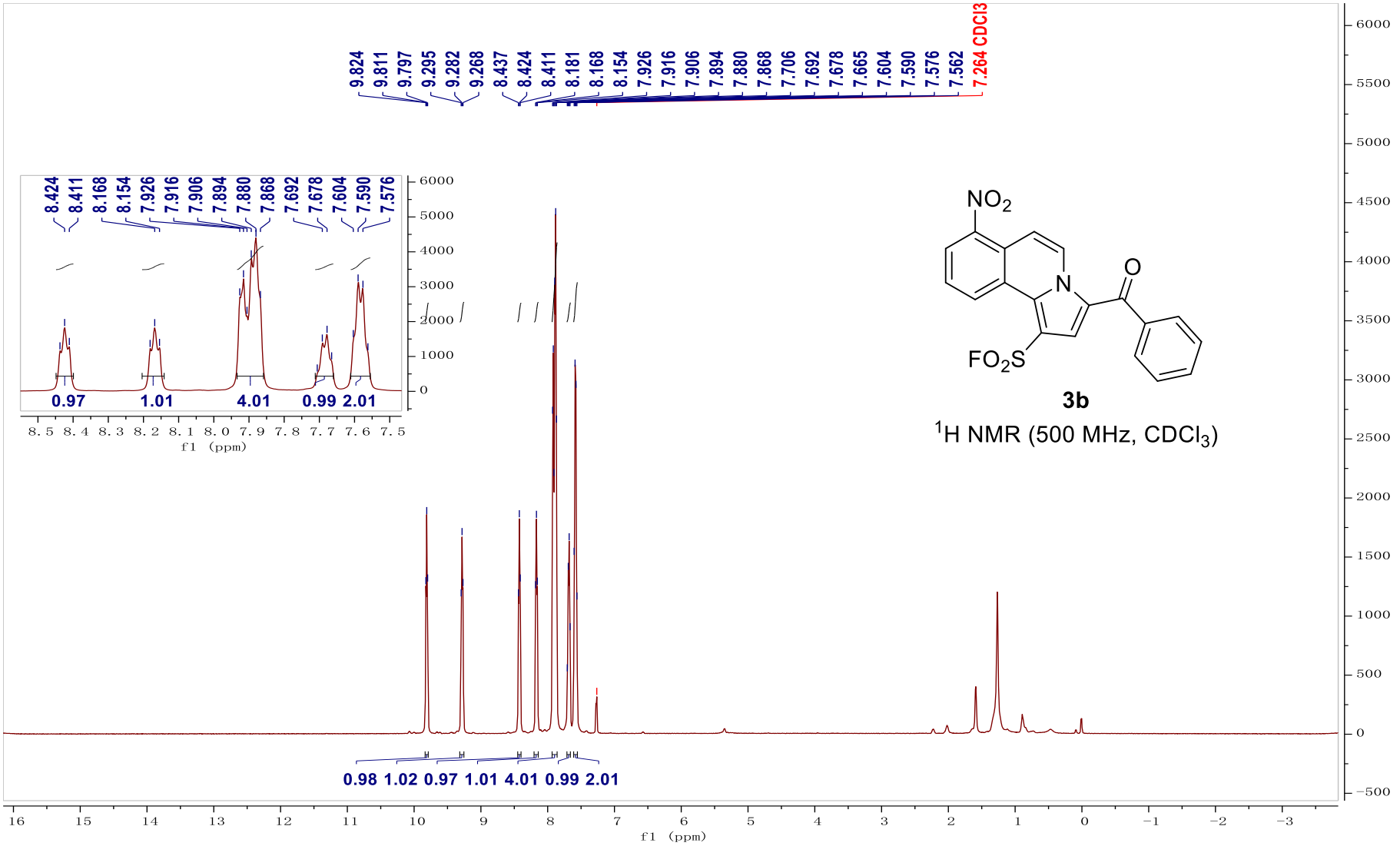

9.665
9.650
8.976
8.960
7.865
7.851
7.790
7.786
7.776
7.772
7.767
7.762
7.756
7.752
7.749
7.738
7.660
7.646
7.630
7.569
7.553
7.538
7.435
7.420
7.264 CDCl3
4.00 2.04 0.97 2.01 0.98
1.00 4.00 2.04 0.97 2.01 0.98
f1 (ppm)
O
N
FO2S
3a
1H NMR (500 MHz, CDCl3)

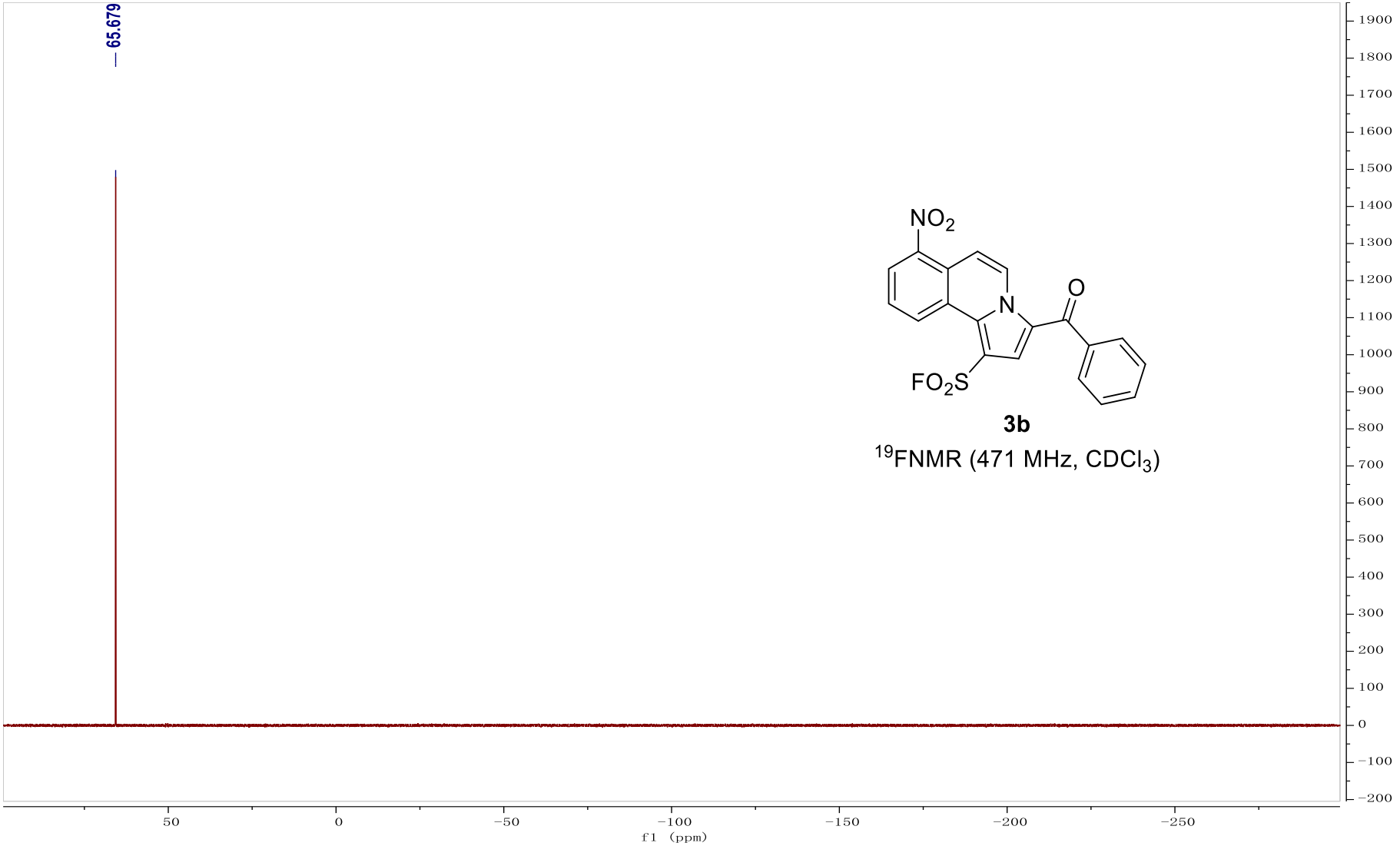


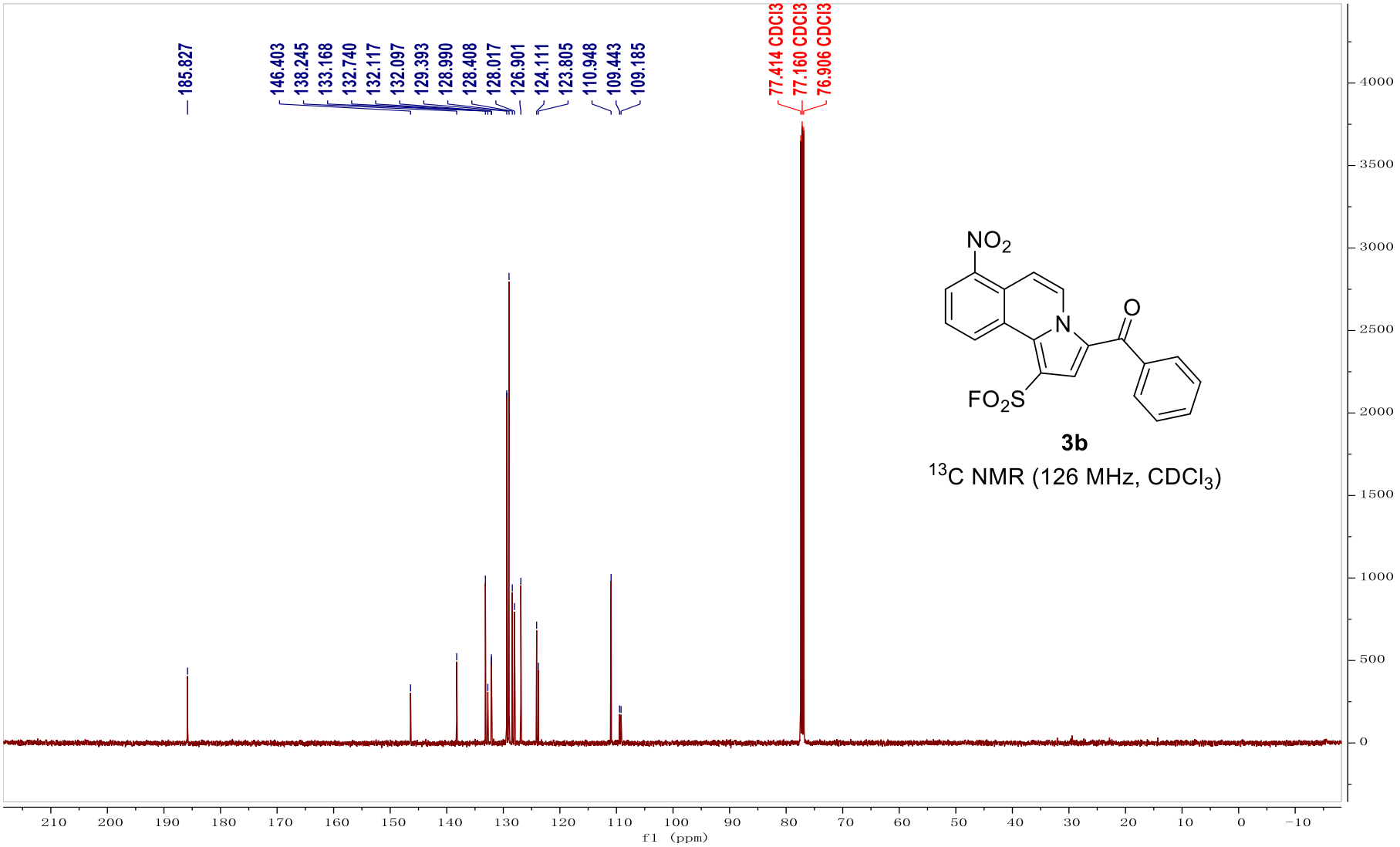
3a

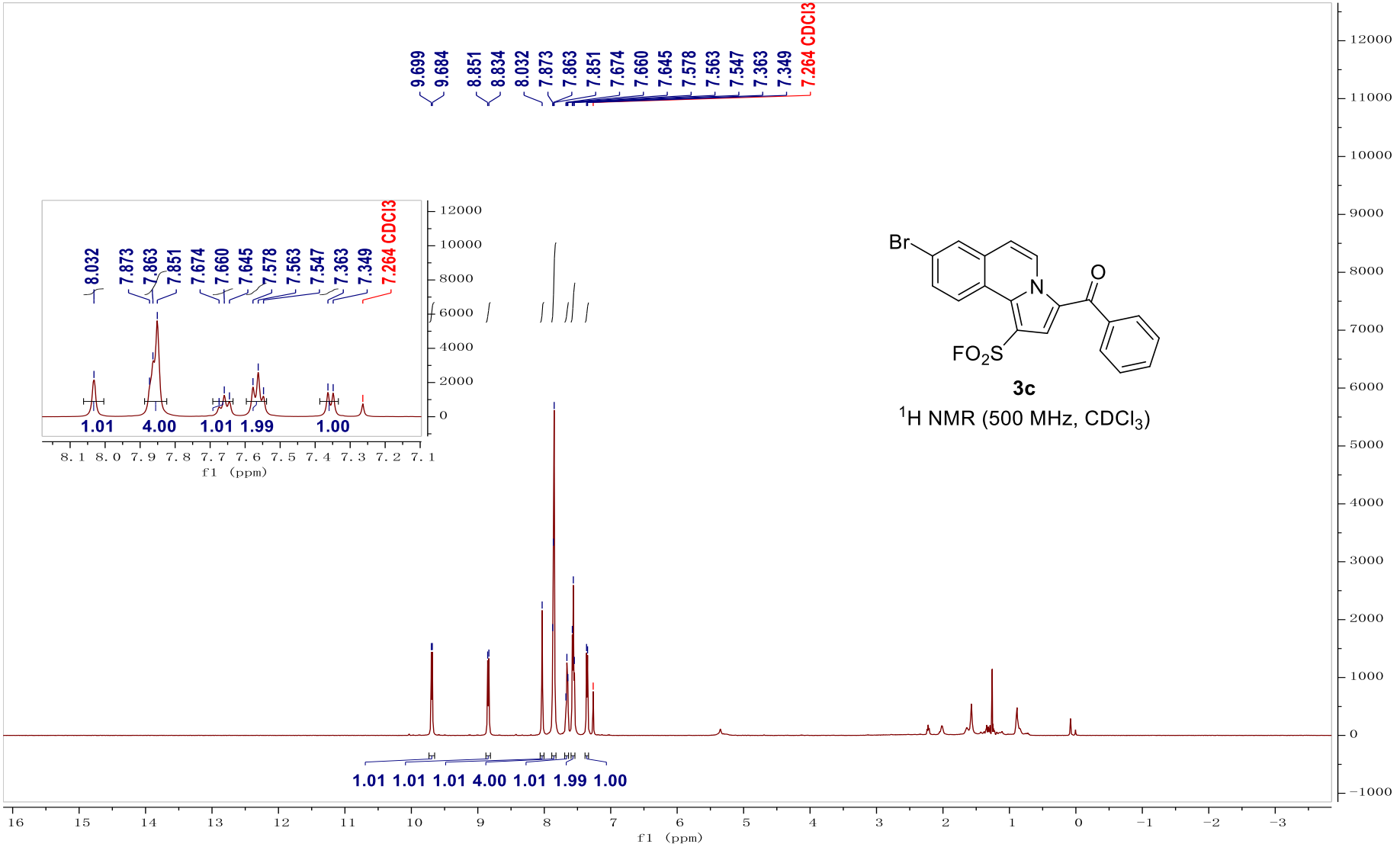
^{19}FNMR (471 MHz, $CDCl_3$)

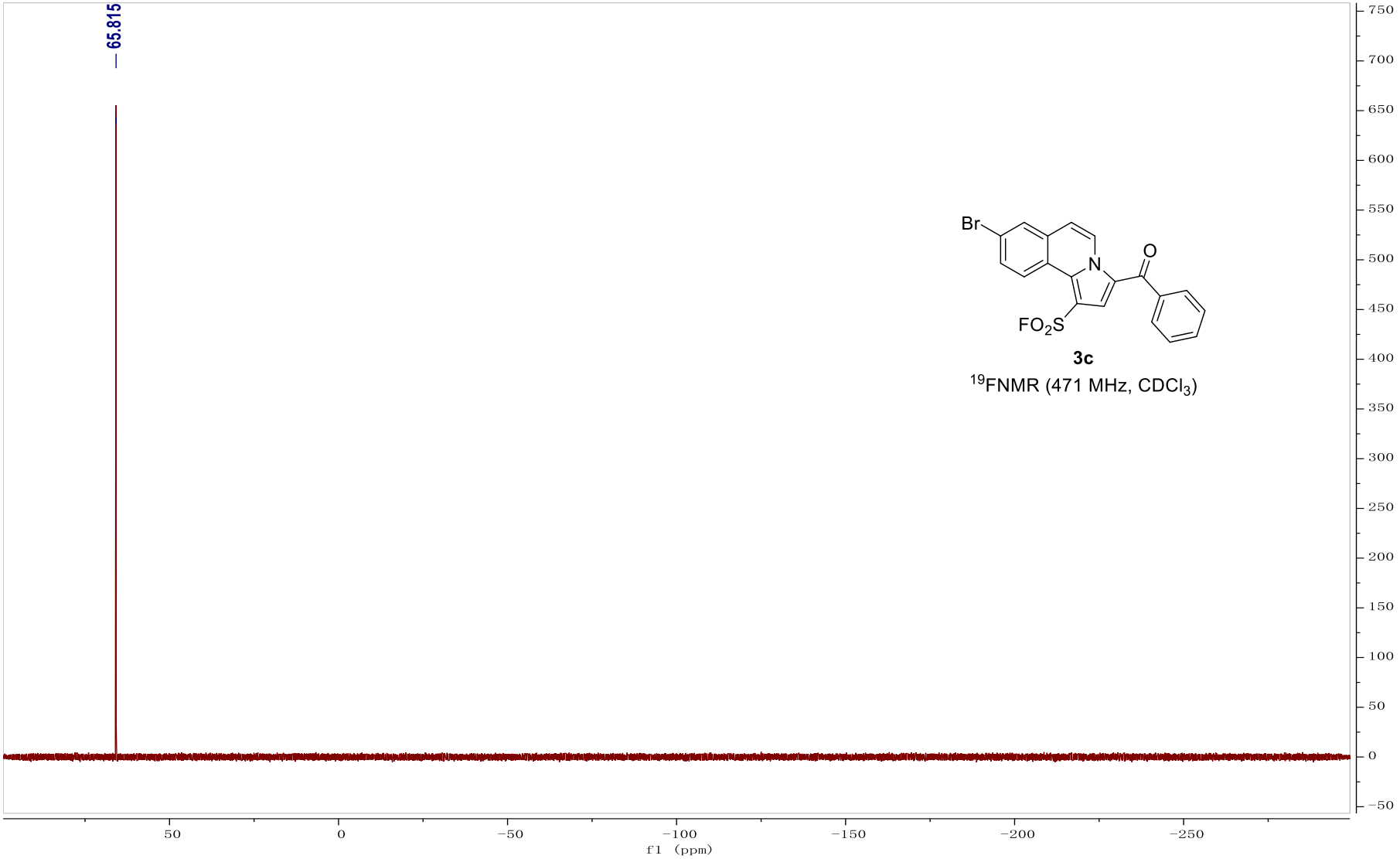

185.893
138.812
134.738
132.671
130.855
130.564
129.300
129.287
129.143
128.814
127.609
126.648
126.628
125.067
123.677
122.468
117.114
107.890
107.634
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
O
N
FO2S
3a
13C NMR (126 MHz, CDCl3)
f1 (ppm)

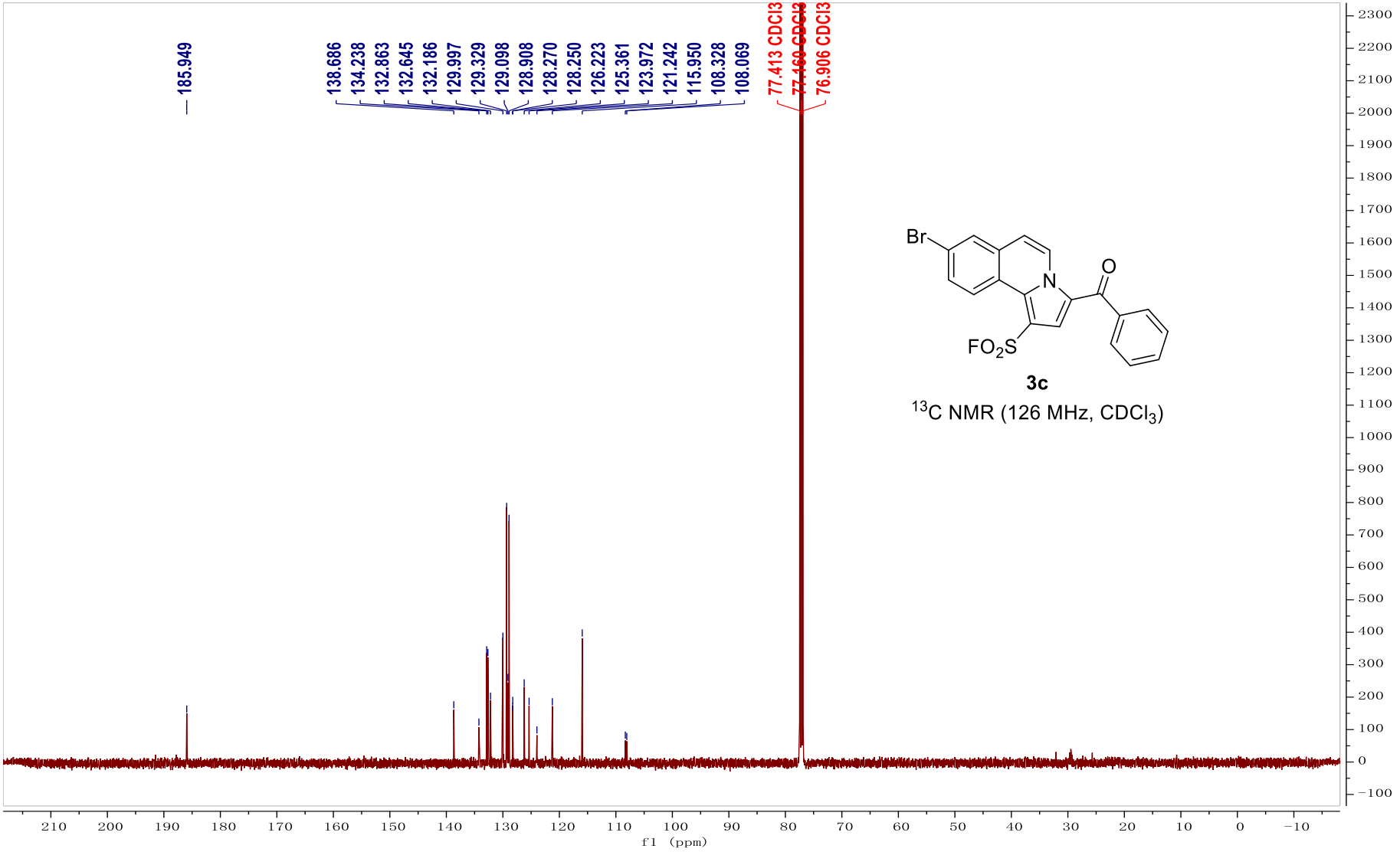

9.824
9.811
9.797
9.295
9.282
9.268
8.437
8.424
8.411
8.181
8.168
8.154
7.926
7.916
7.906
7.894
7.880
7.868
7.706
7.692
7.678
7.665
7.604
7.590
7.576
7.562
7.264 CDCl3
0.98 1.02 0.97 1.01 4.01 0.99 2.01
f1 (ppm)
0.97 1.01 4.01 0.99 2.01
NO2
N
O
FO2S
3b
1H NMR (500 MHz, CDCl3)

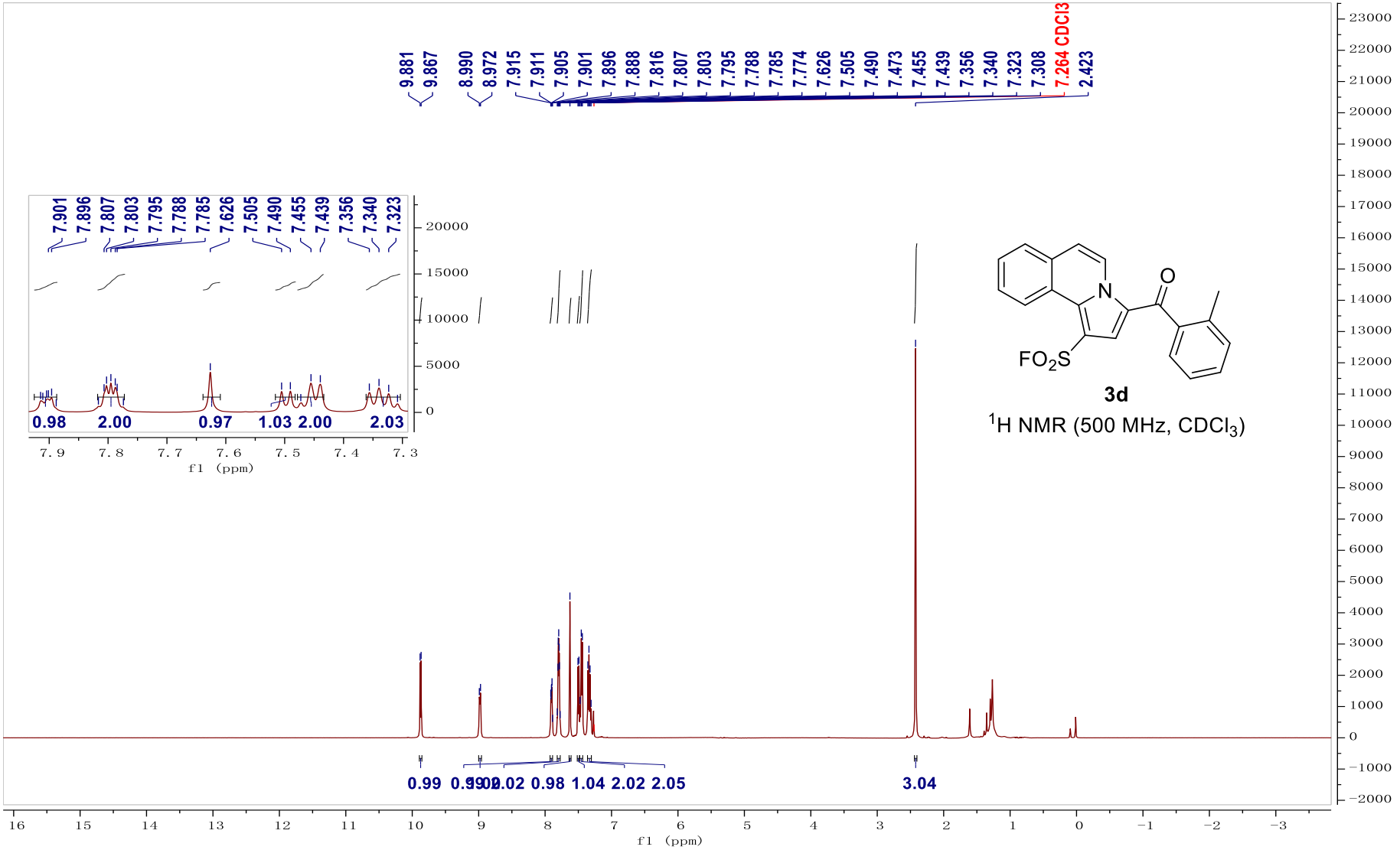

65.679
NO2
O
N
FO2S
3b
19FNMR (471 MHz, CDCl3)
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

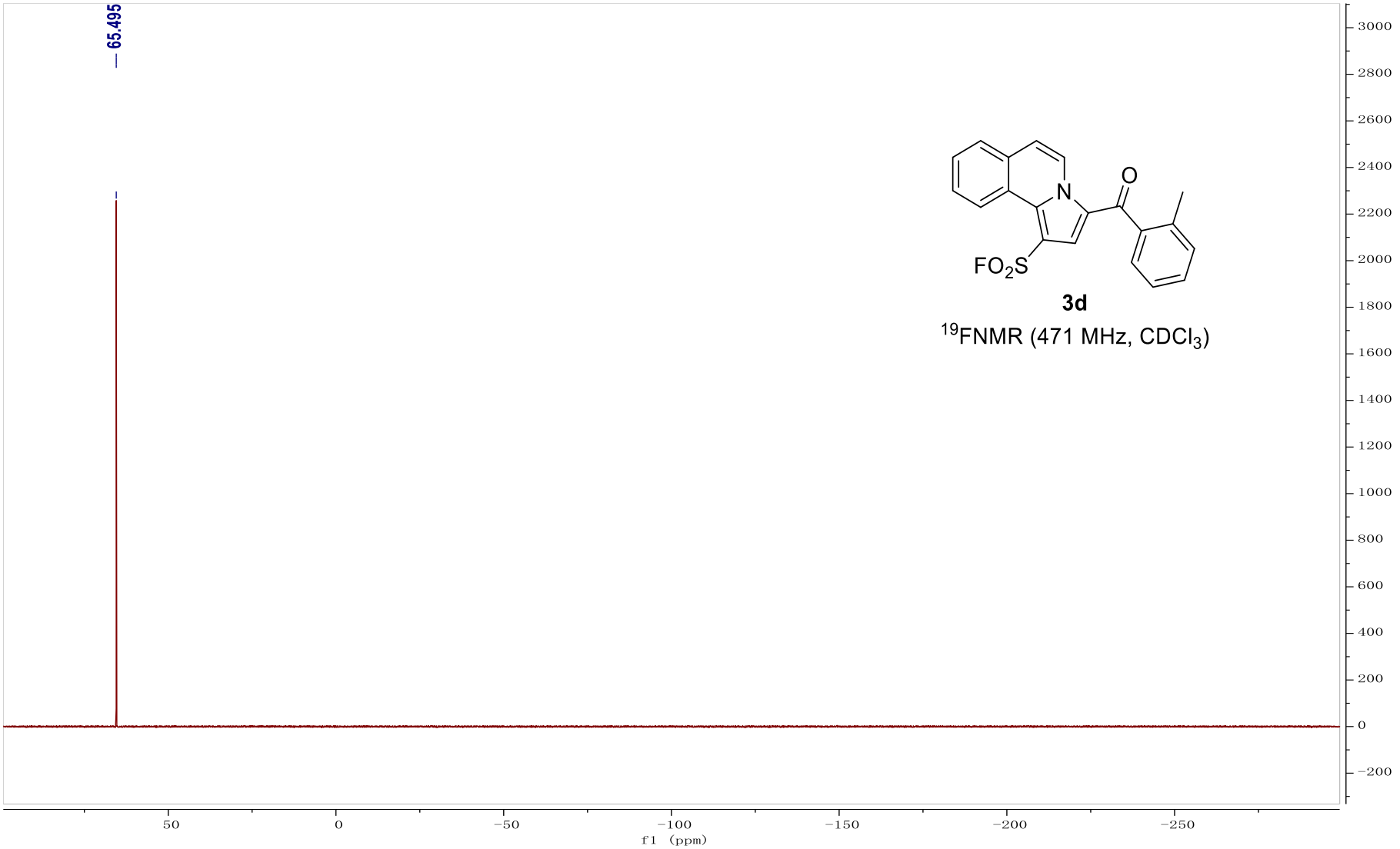

185.827
146.403
138.245
133.168
132.740
132.117
132.097
129.393
128.990
128.408
128.017
126.901
124.111
123.805
110.948
109.443
109.185
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
NO2
N
O
FO2S
3b
13C NMR (126 MHz, CDCl3)
f1 (ppm)

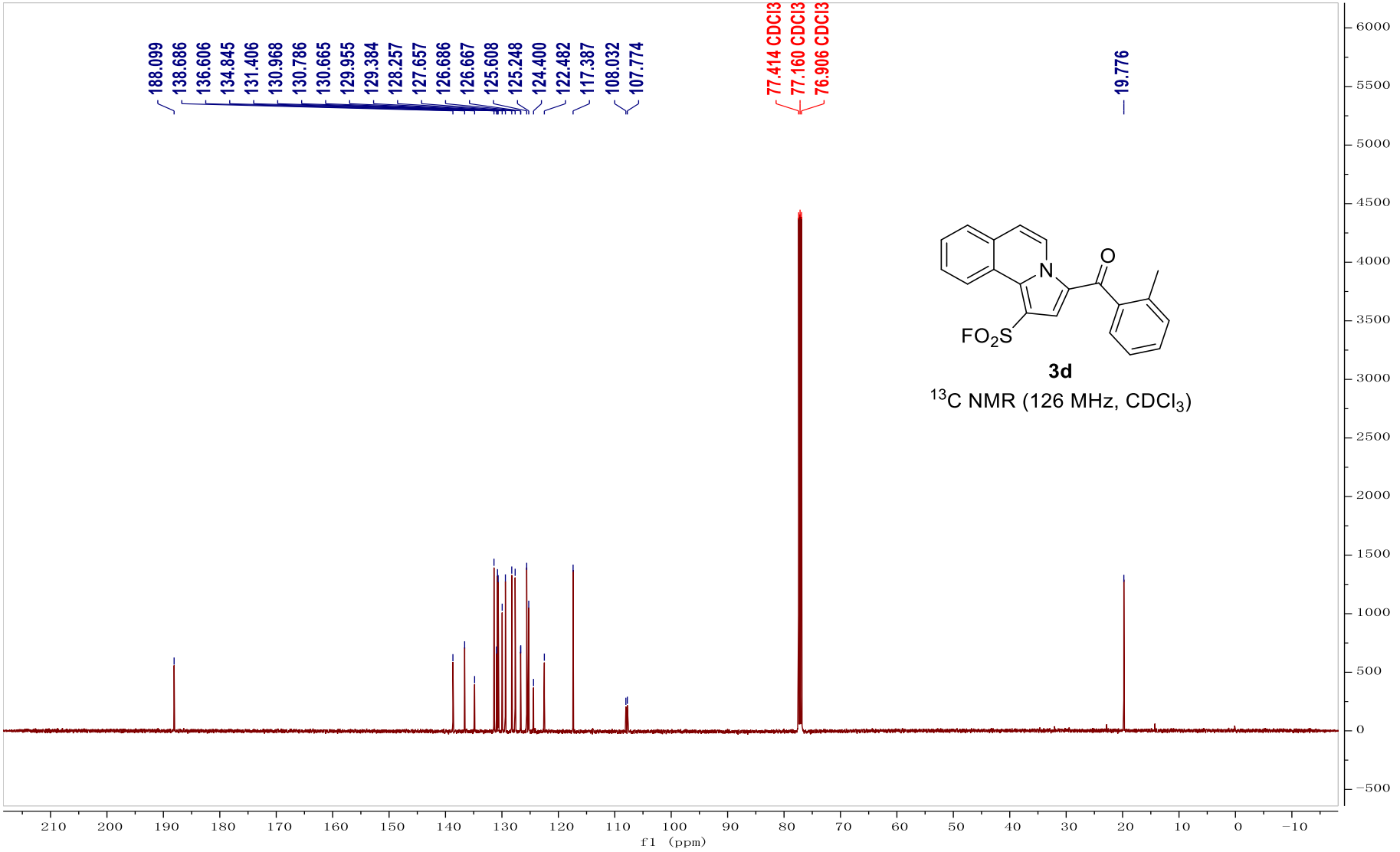

9.699
9.684
8.851
8.834
8.032
7.873
7.863
7.851
7.674
7.660
7.645
7.578
7.563
7.547
7.363
7.349
7.264 CDCl3
1.01 1.01 1.01 4.00 1.01 1.99 1.00
f1 (ppm)
Br
O
N
FO2S
3c
1H NMR (500 MHz, CDCl3)
1.01 4.00 1.01 1.99 1.00

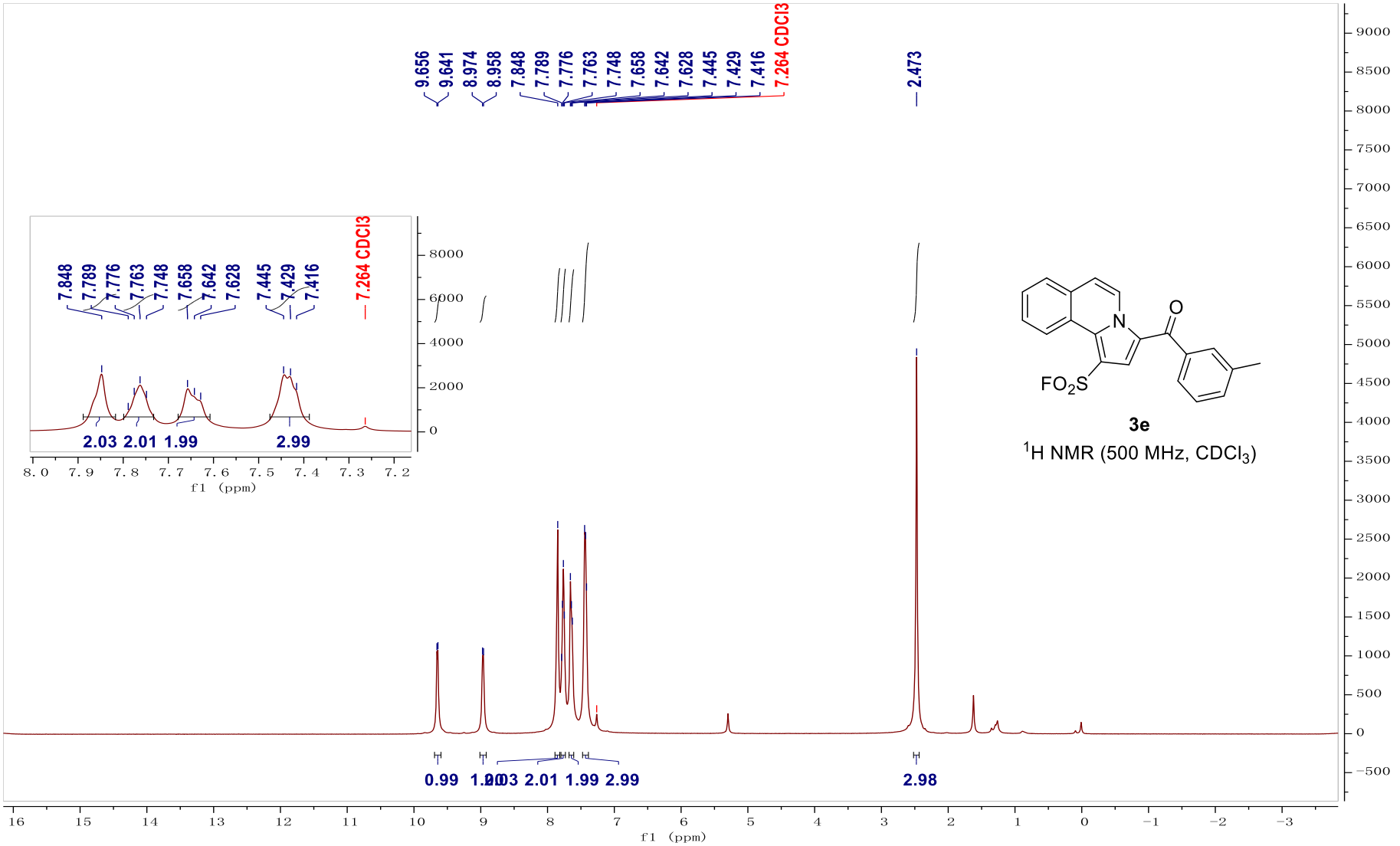

65.815
Br
N
O
FO2S
3c
19FNMR (471 MHz, CDCl3)
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
50
0
−50
−100
−150
−200
−250
f1 (ppm)

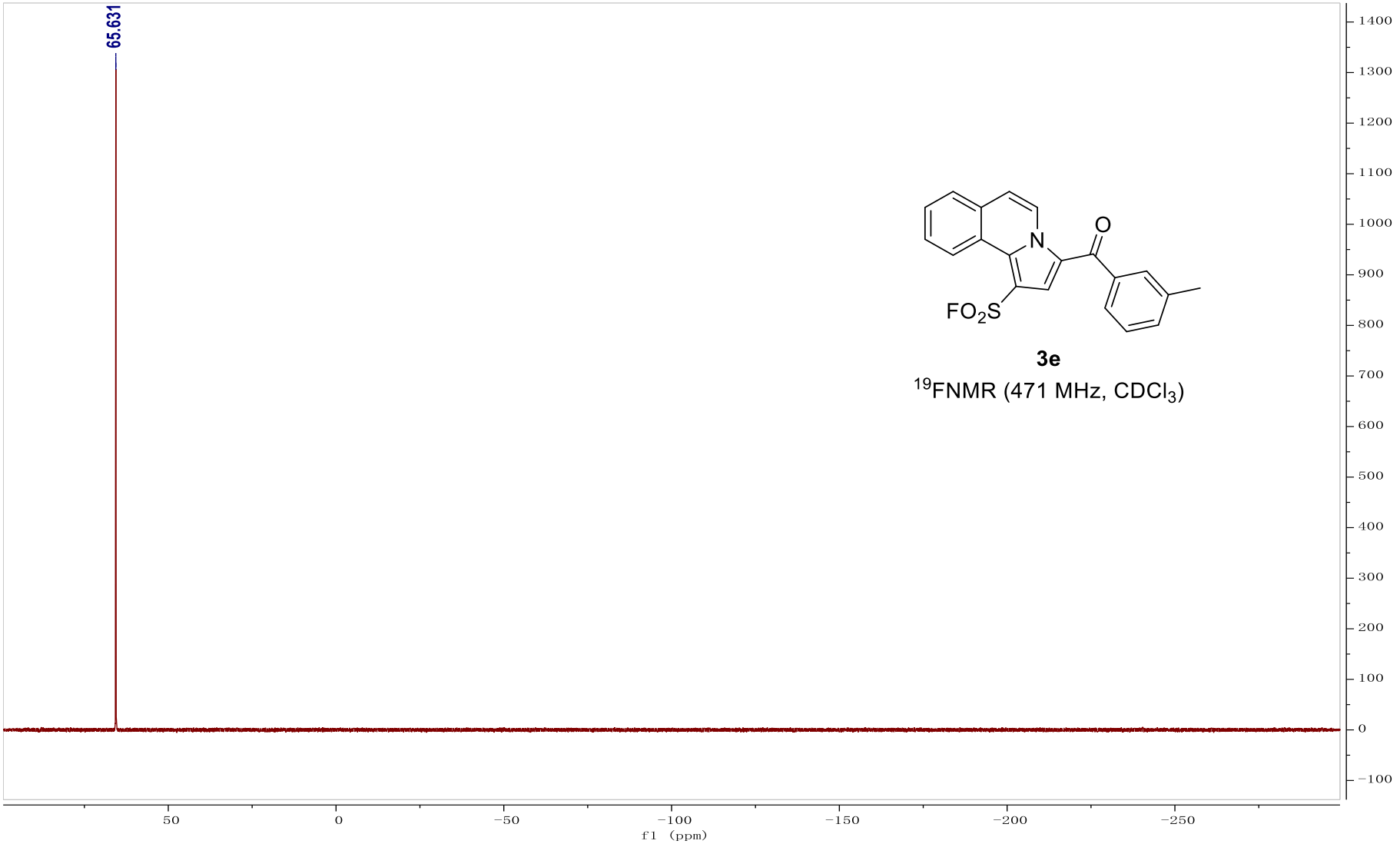

185.949
138.686
134.238
132.863
132.645
132.186
129.997
129.329
129.098
128.908
128.270
128.250
126.223
125.361
123.972
121.242
115.950
108.328
108.069
77.413 CDCl3
77.160 CDCl3
76.906 CDCl3
Br
O
N
FO2S
3c
13C NMR (126 MHz, CDCl3)
f1 (ppm)


9.881
9.867
8.990
8.972
7.915
7.911
7.905
7.901
7.896
7.888
7.816
7.807
7.803
7.795
7.788
7.785
7.774
7.626
7.505
7.490
7.473
7.455
7.439
7.356
7.340
7.323
7.308
7.264 CDCl3
2.423
0.99
1.02
0.98
1.04
2.02
2.05
3.04
f1 (ppm)
0.98
2.00
0.97
1.03
2.00
2.03
3d
1H NMR (500 MHz, CDCl3)


65.495
O
N
FO2S
3d
19FNMR (471 MHz, CDCl3)
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

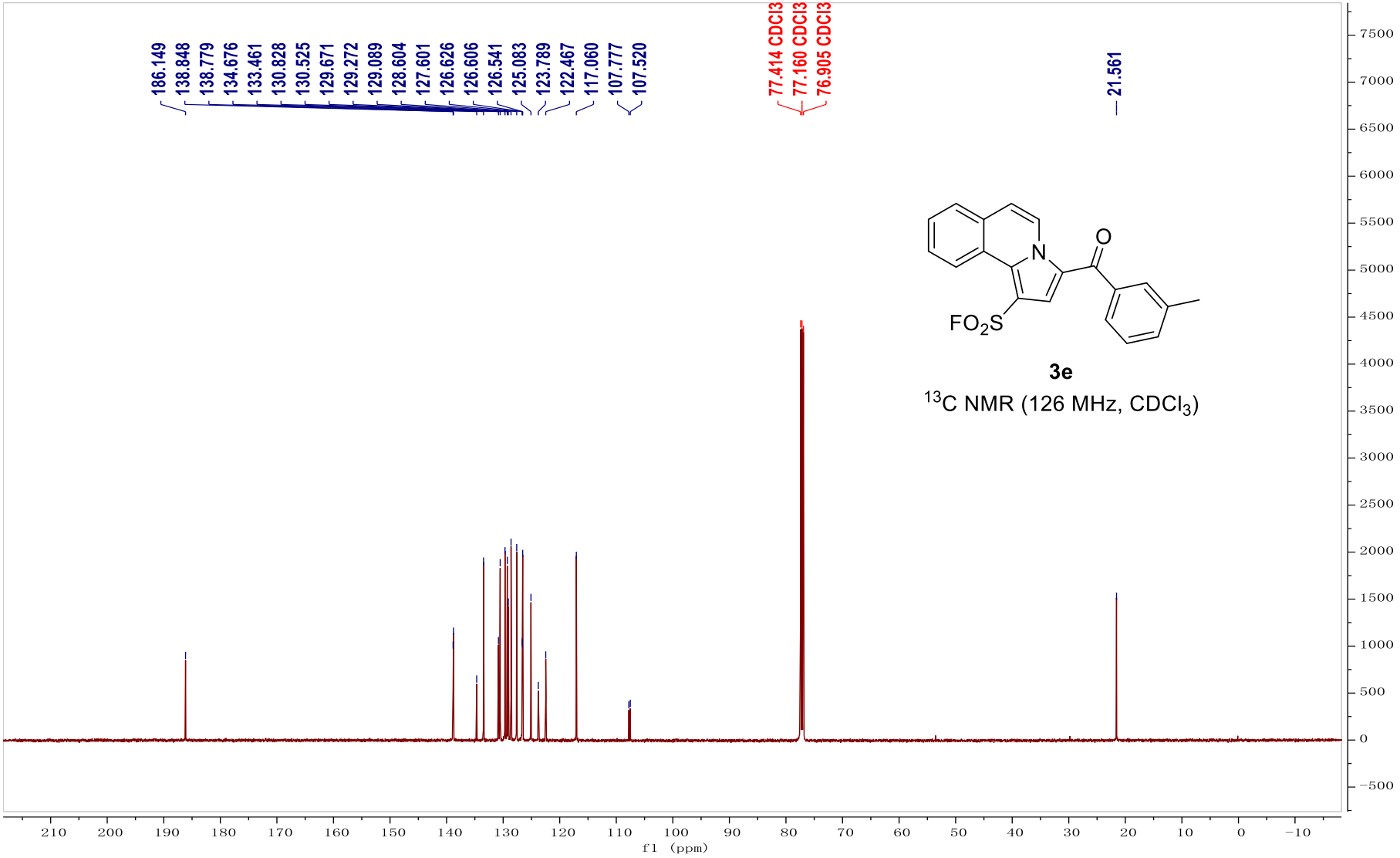

188.099
138.686
136.606
134.845
131.406
130.968
130.786
130.665
129.955
129.384
128.257
127.657
126.686
126.667
125.608
125.248
124.400
122.482
117.387
108.032
107.774
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
19.776
O
N
FO2S
3d
13C NMR (126 MHz, CDCl3)
f1 (ppm)

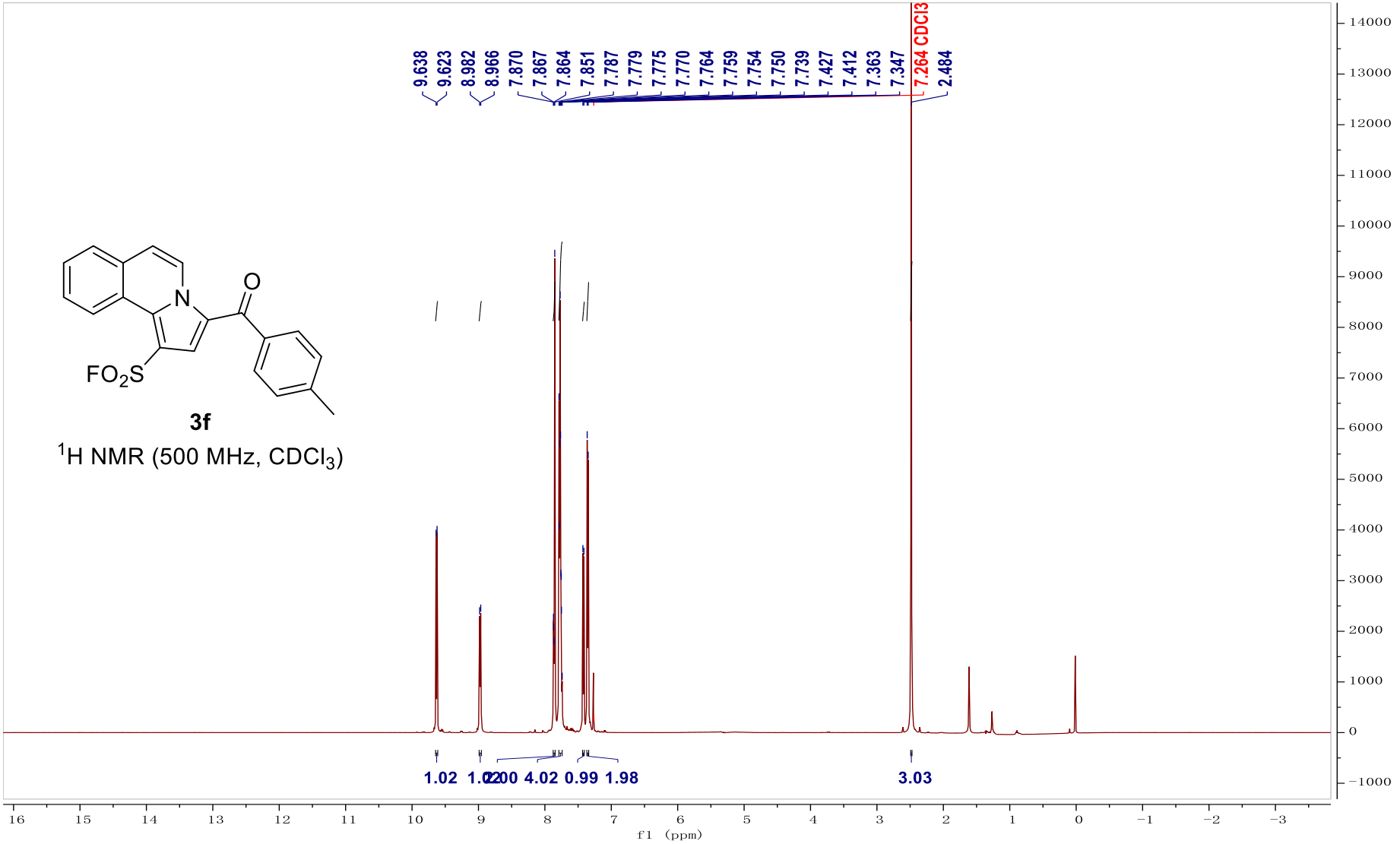

9.656
9.641
8.974
8.958
7.848
7.789
7.776
7.763
7.748
7.658
7.642
7.628
7.445
7.429
7.416
7.264 CDCl3
2.473
2.03 2.01 1.99
2.99
f1 (ppm)
0.99
2.03 2.01 1.99 2.99
2.98
f1 (ppm)
O
N
FO2S
3e
1H NMR (500 MHz, CDCl3)

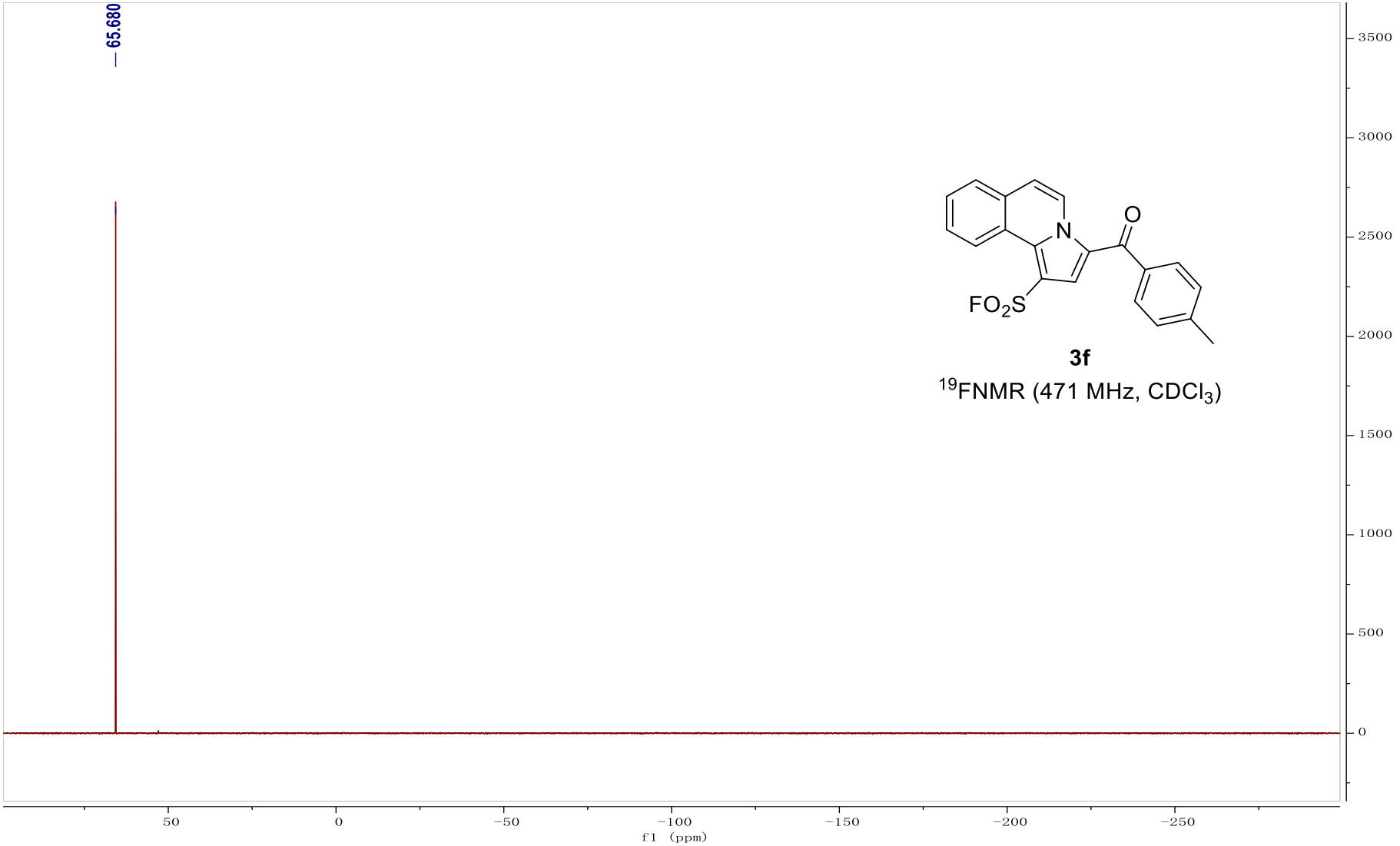


3e

^{19}FNMR (471 MHz, $CDCl_3$)

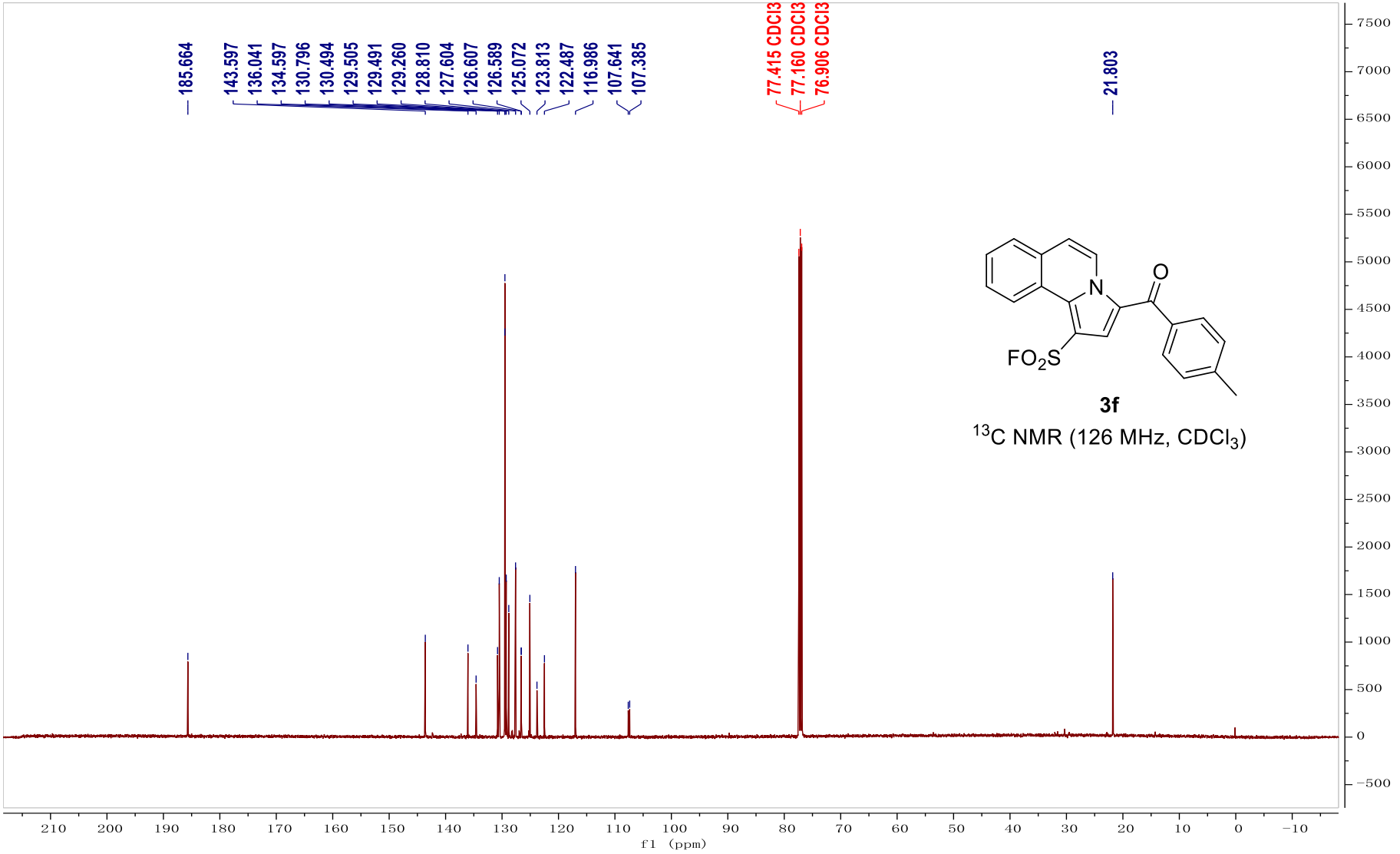

186.149
138.848
138.779
134.676
133.461
130.828
130.525
129.671
129.272
129.089
128.604
127.601
126.626
126.606
126.541
125.083
123.789
122.467
117.060
107.777
107.520
77.414 CDCl3
77.160 CDCl3
76.905 CDCl3
21.561
O
N
FO2S
3e
13C NMR (126 MHz, CDCl3)
f1 (ppm)

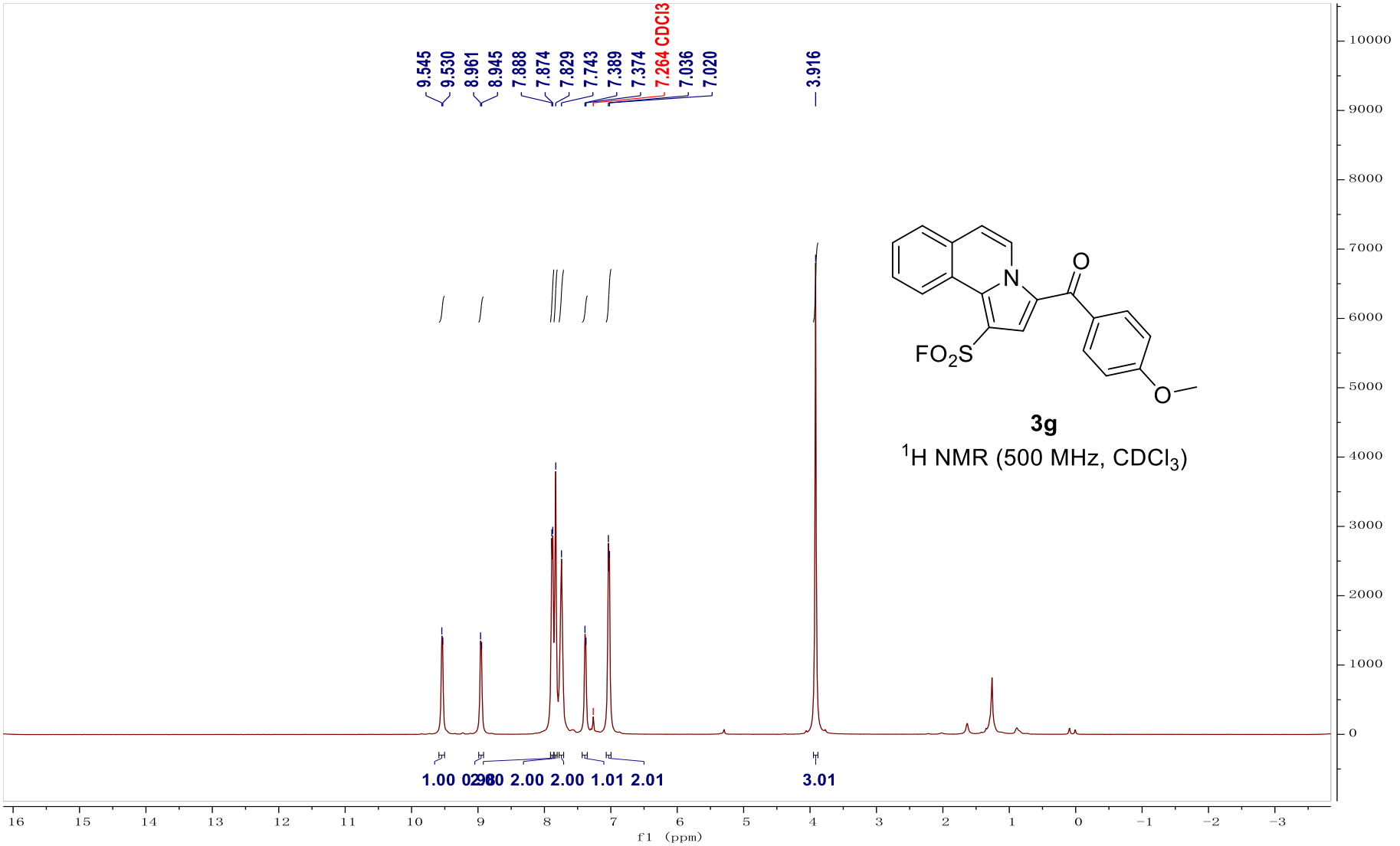

9.638
9.623
8.982
8.966
7.870
7.867
7.864
7.851
7.787
7.779
7.775
7.770
7.764
7.759
7.754
7.750
7.739
7.427
7.412
7.363
7.347
7.264 CDCl3
2.484
O
N
FO2S
3f
1H NMR (500 MHz, CDCl3)
1.02
1.02
2.00
4.02
0.99
1.98
3.03
f1 (ppm)

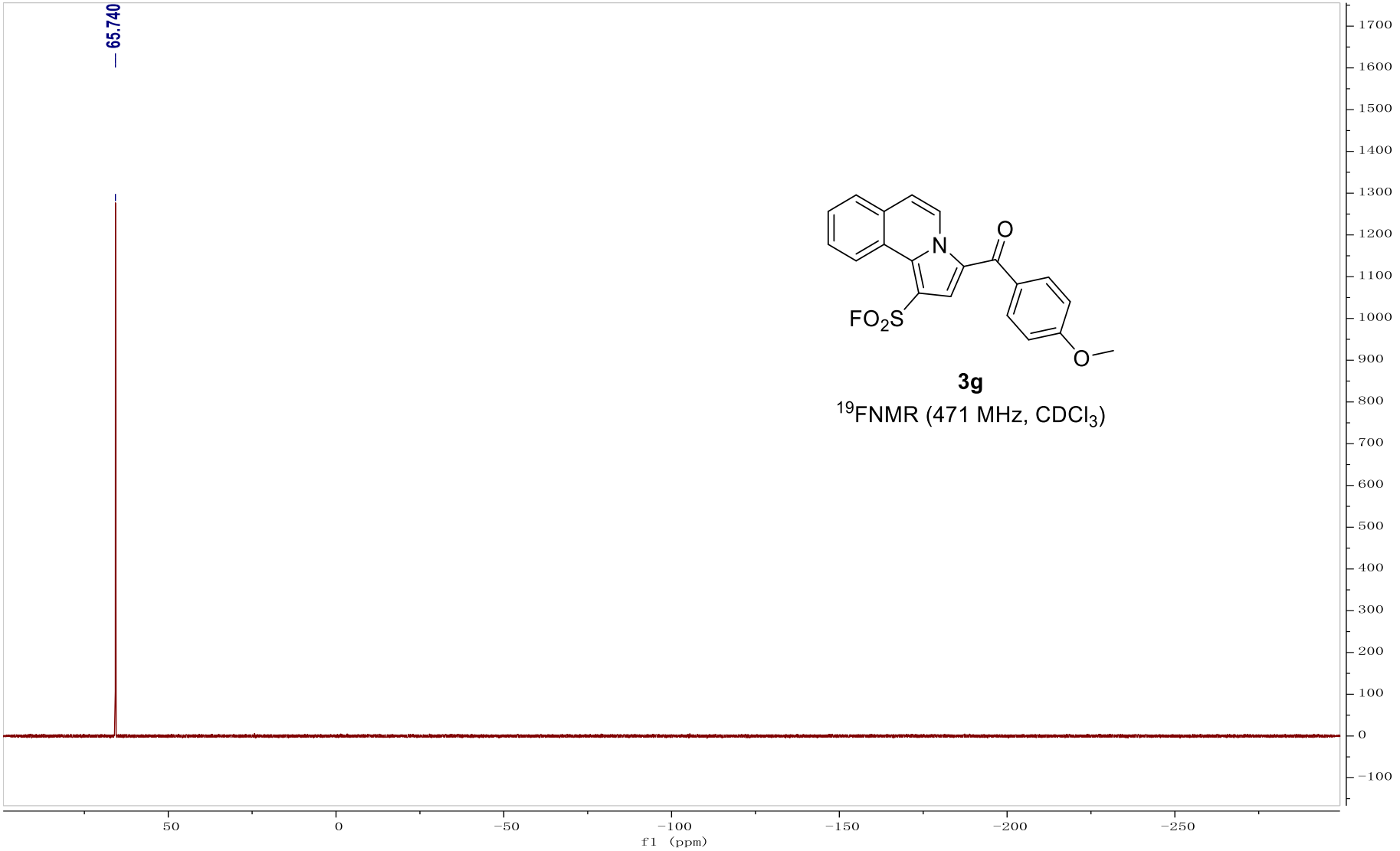


3f

^{19}FNMR (471 MHz, $CDCl_3$)

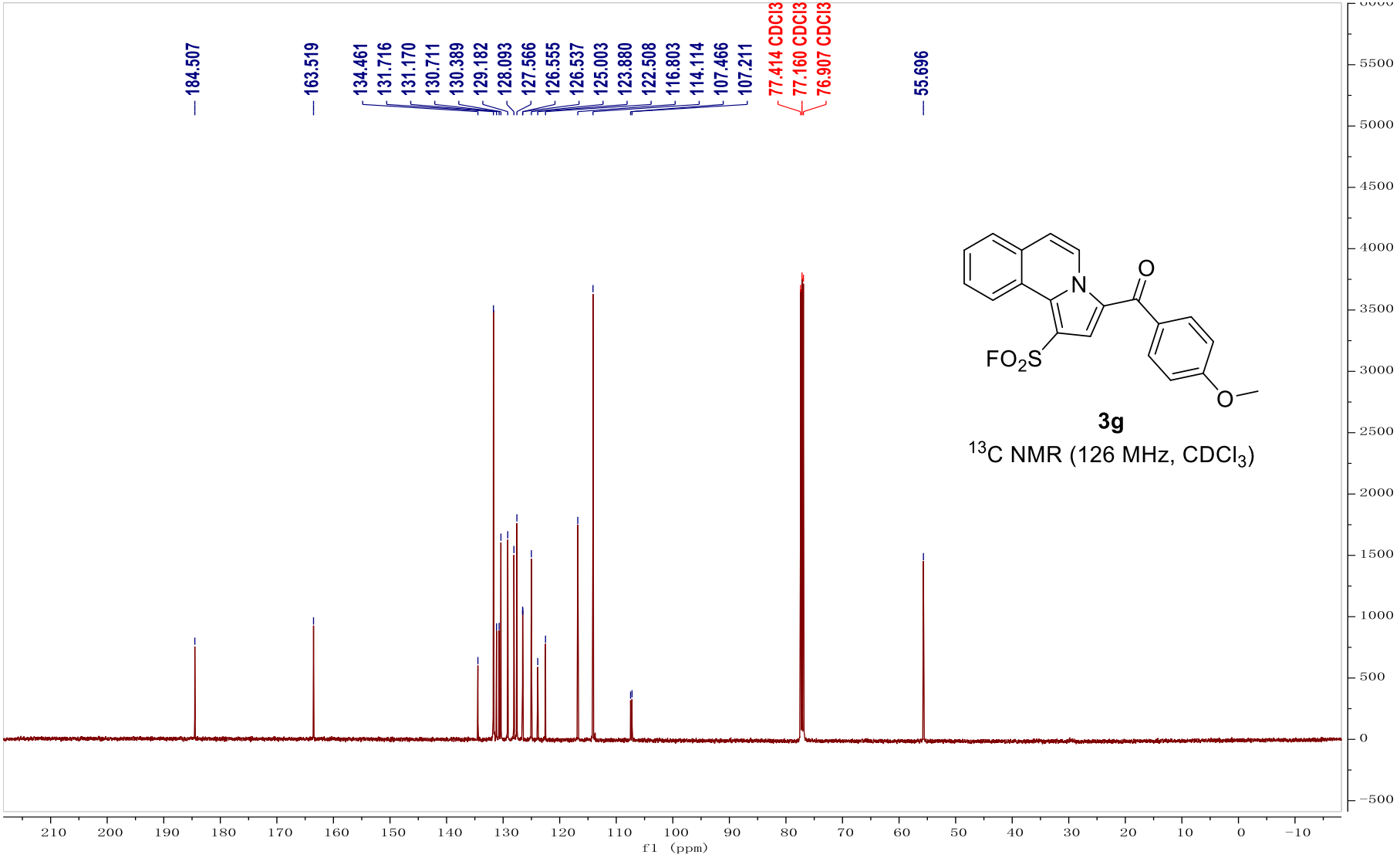

185.664
143.597
136.041
134.597
130.796
130.494
129.505
129.491
129.260
128.810
127.604
126.607
126.589
125.072
123.813
122.487
116.986
107.641
107.385
77.415 CDCl3
77.160 CDCl3
76.906 CDCl3
21.803
O
N
FO2S
3f
13C NMR (126 MHz, CDCl3)
f1 (ppm)

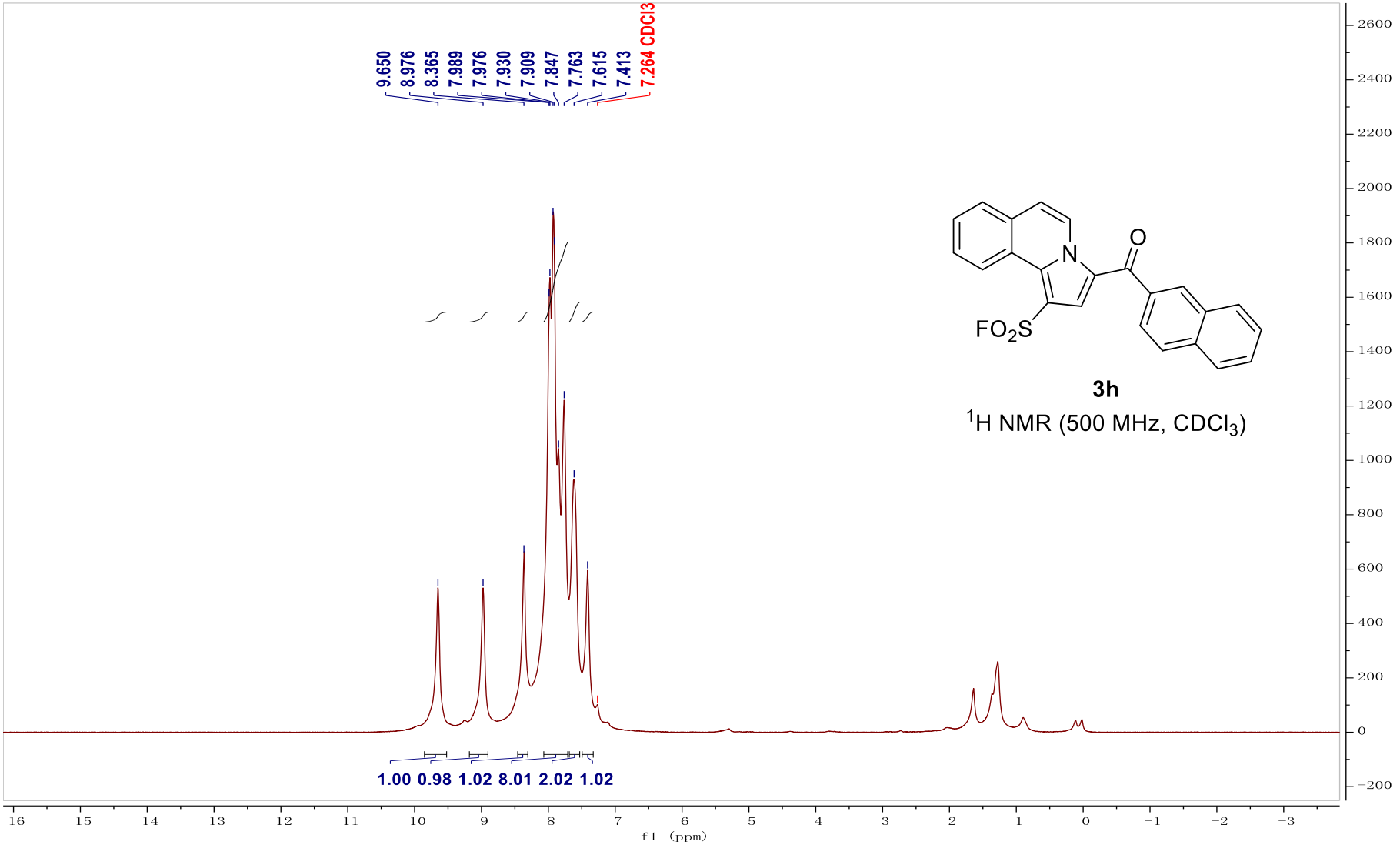

9.545
9.530
8.961
8.945
7.888
7.874
7.829
7.743
7.389
7.374
7.264 CDCl3
7.036
7.020
3.916
1.00
2.00
2.00
1.01
2.01
3.01
f1 (ppm)
3g
1H NMR (500 MHz, CDCl3)

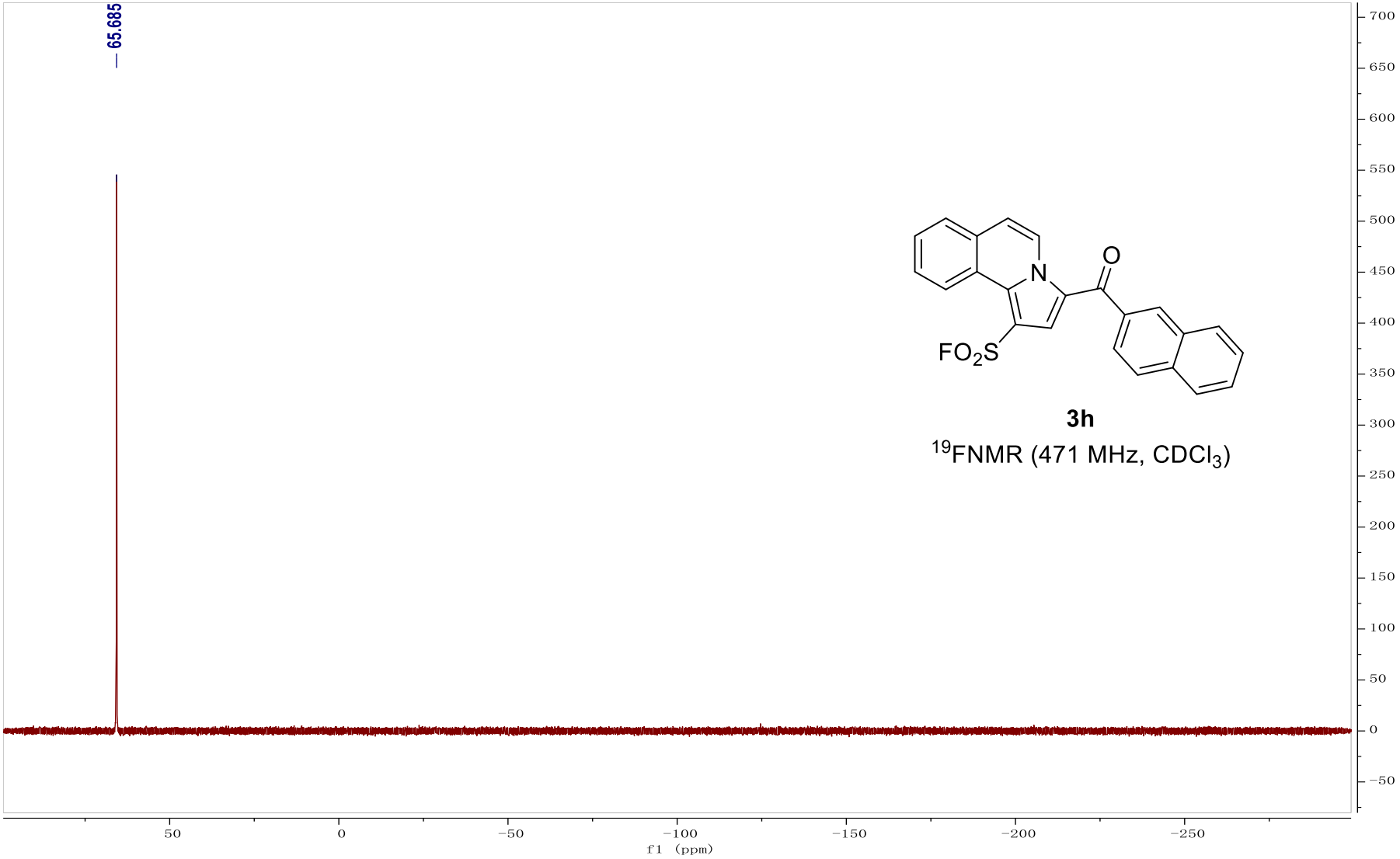


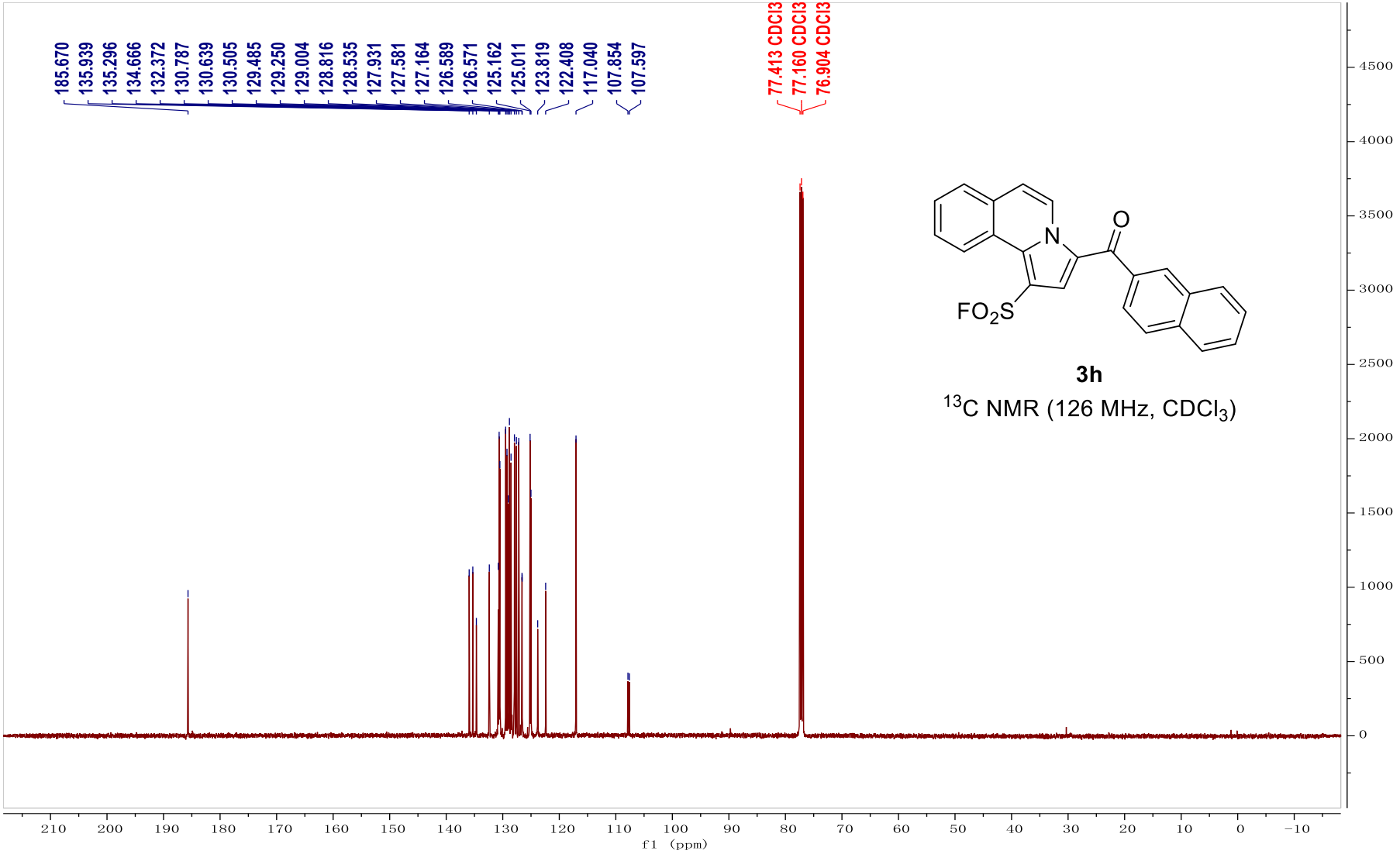
3g

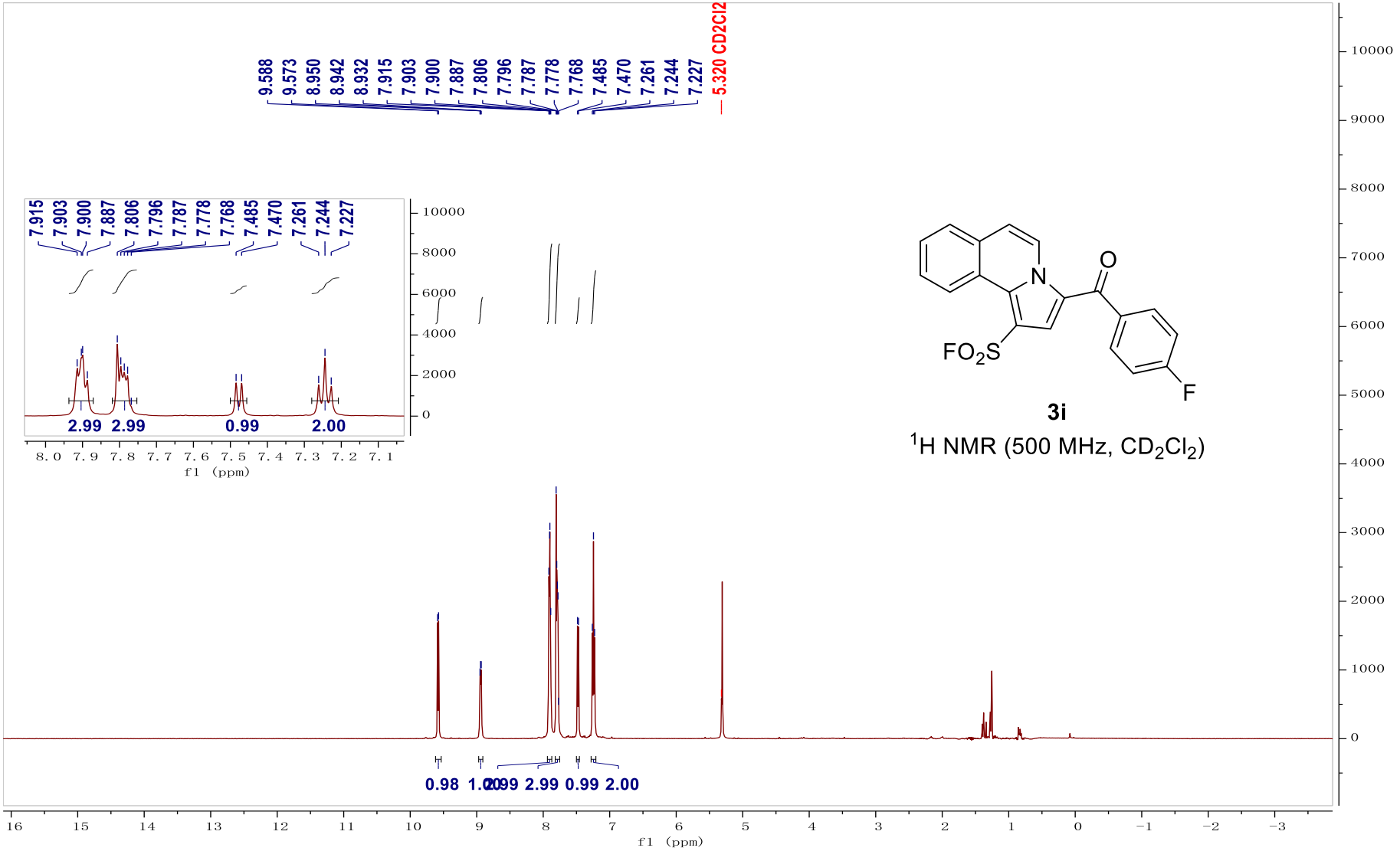
^{19}FNMR (471 MHz, $CDCl_3$)

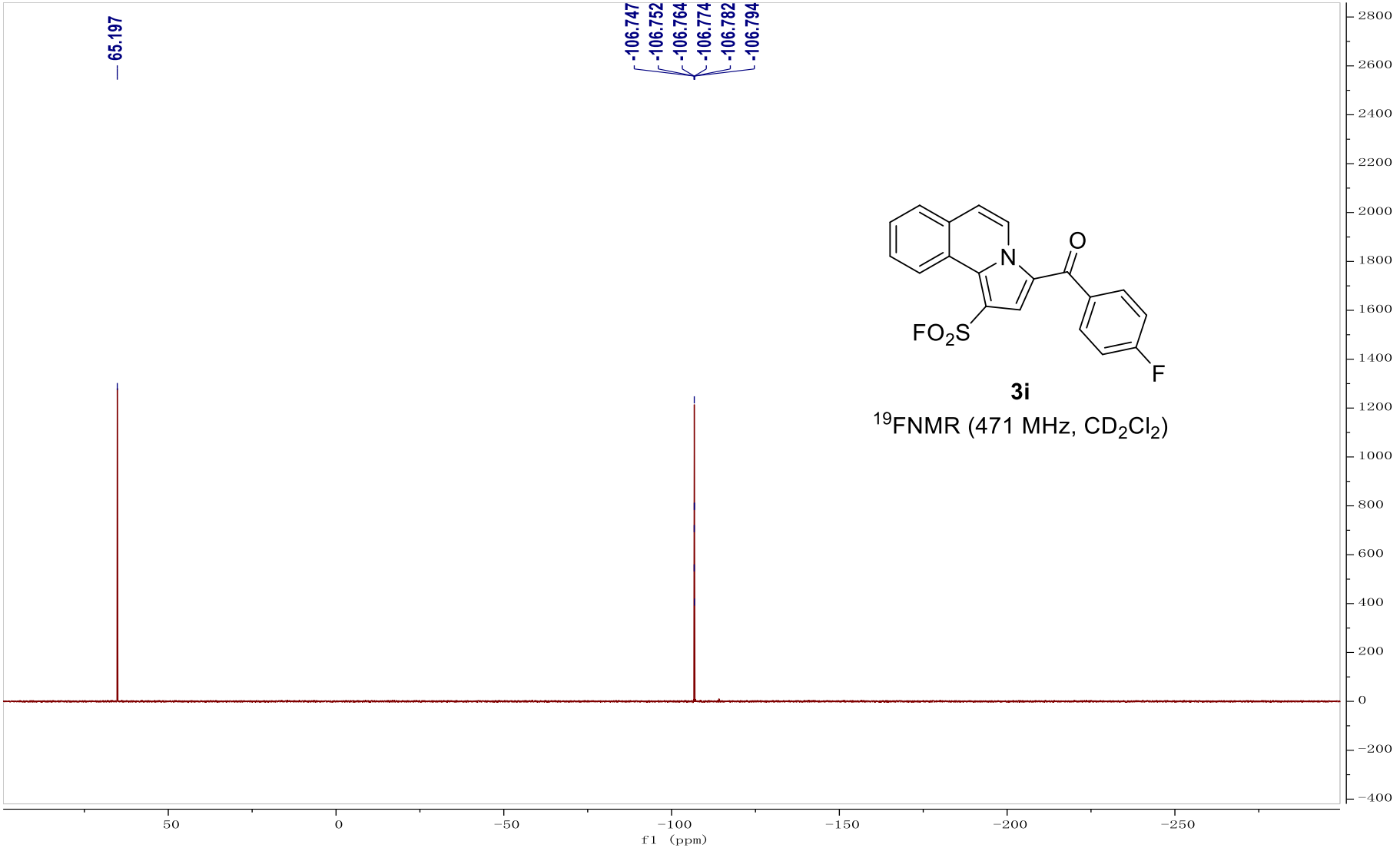

184.507
163.519
134.461
131.716
131.170
130.711
130.389
129.182
128.093
127.566
126.555
126.537
125.003
123.880
122.508
116.803
114.114
107.466
107.211
77.414 CDCl3
77.160 CDCl3
76.907 CDCl3
55.696
O
N
FO2S
O
3g
13C NMR (126 MHz, CDCl3)
f1 (ppm)

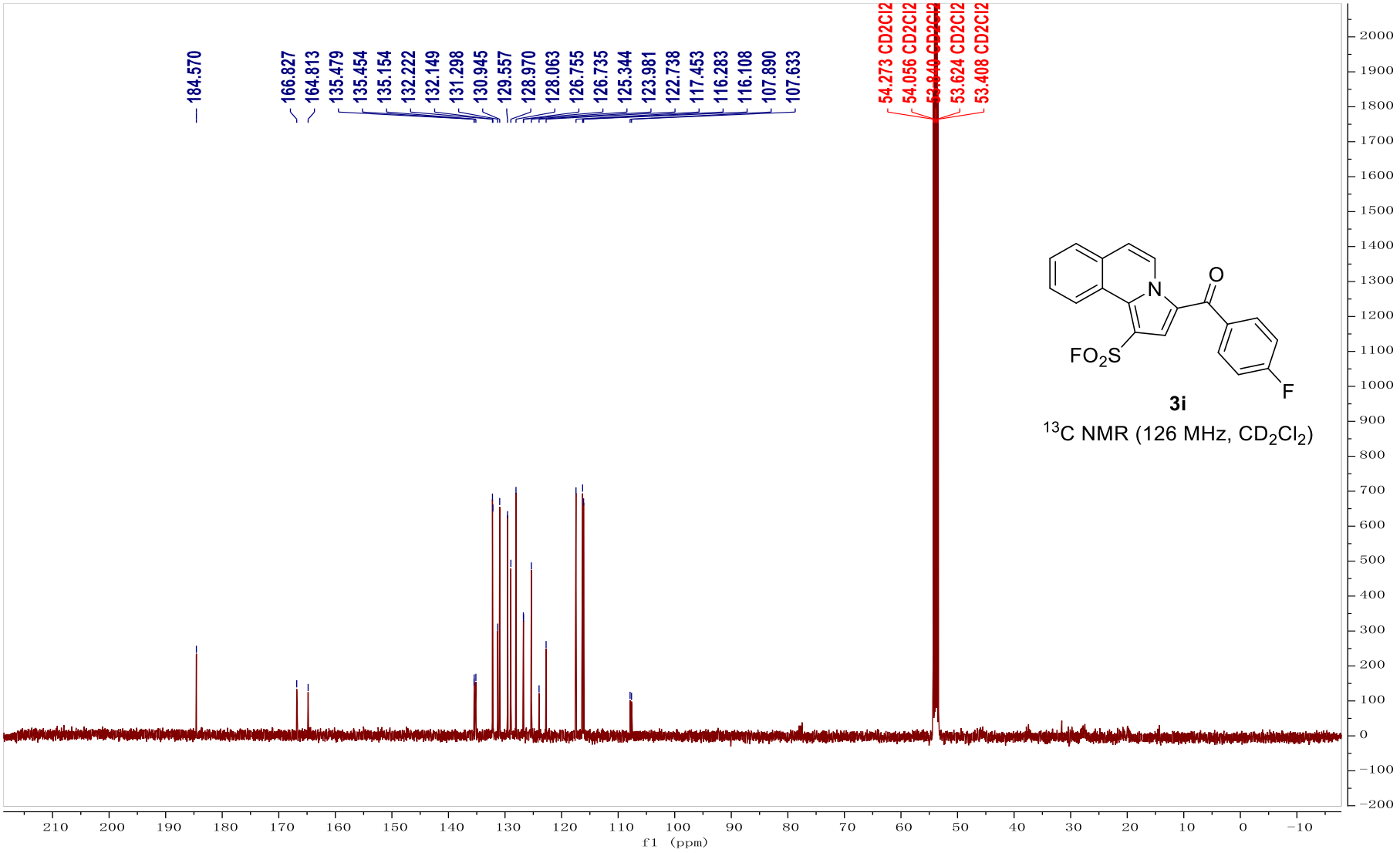

9.650
8.976
8.365
7.989
7.976
7.930
7.909
7.847
7.763
7.615
7.413
7.264 CDCl3
1.00 0.98 1.02 8.01 2.02 1.02
f1 (ppm)
O
N
FO2S
3h
1H NMR (500 MHz, CDCl3)

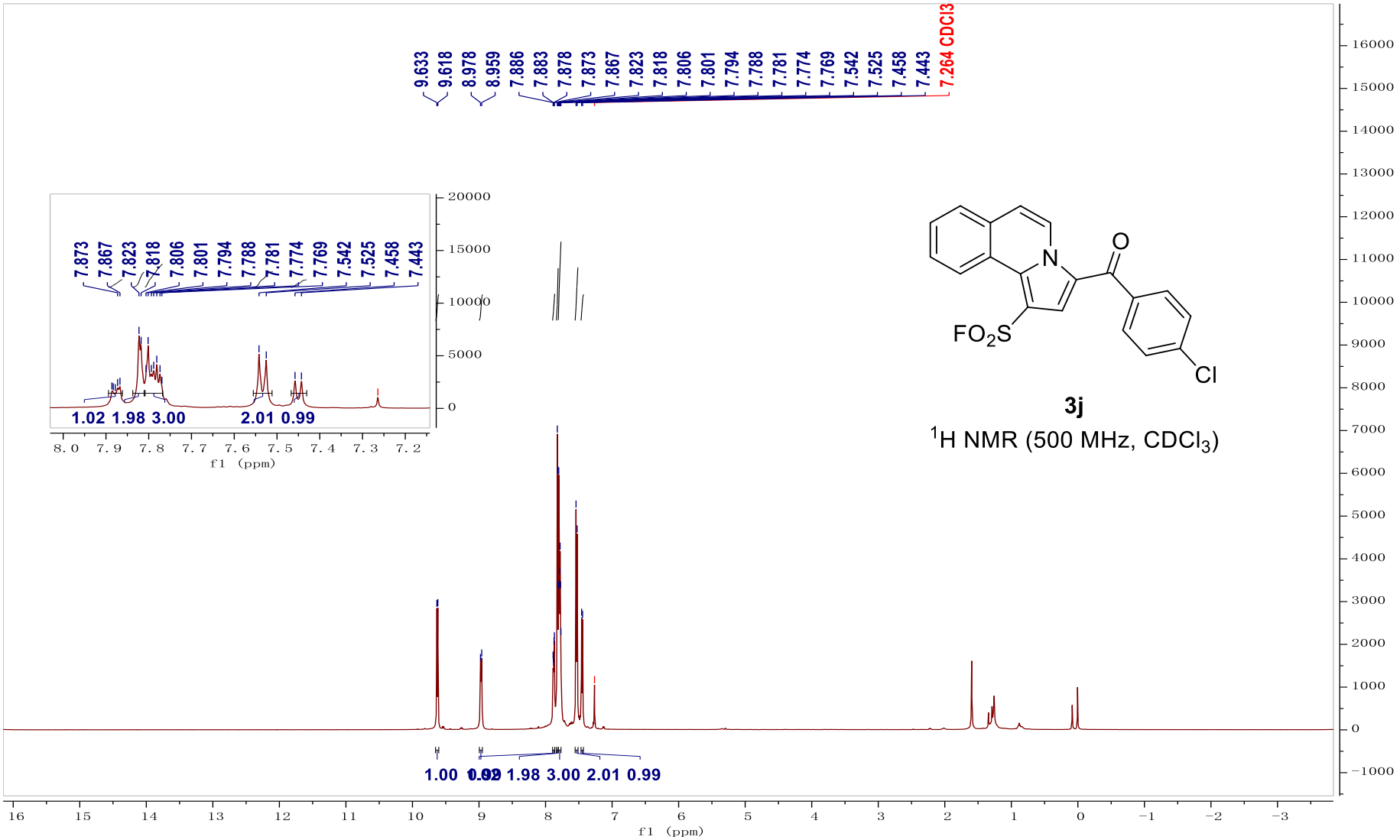

65.685
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
50
0
−50
−100
−150
−200
−250
f1 (ppm)
O
N
FO2S
3h
19FNMR (471 MHz, CDCl3)

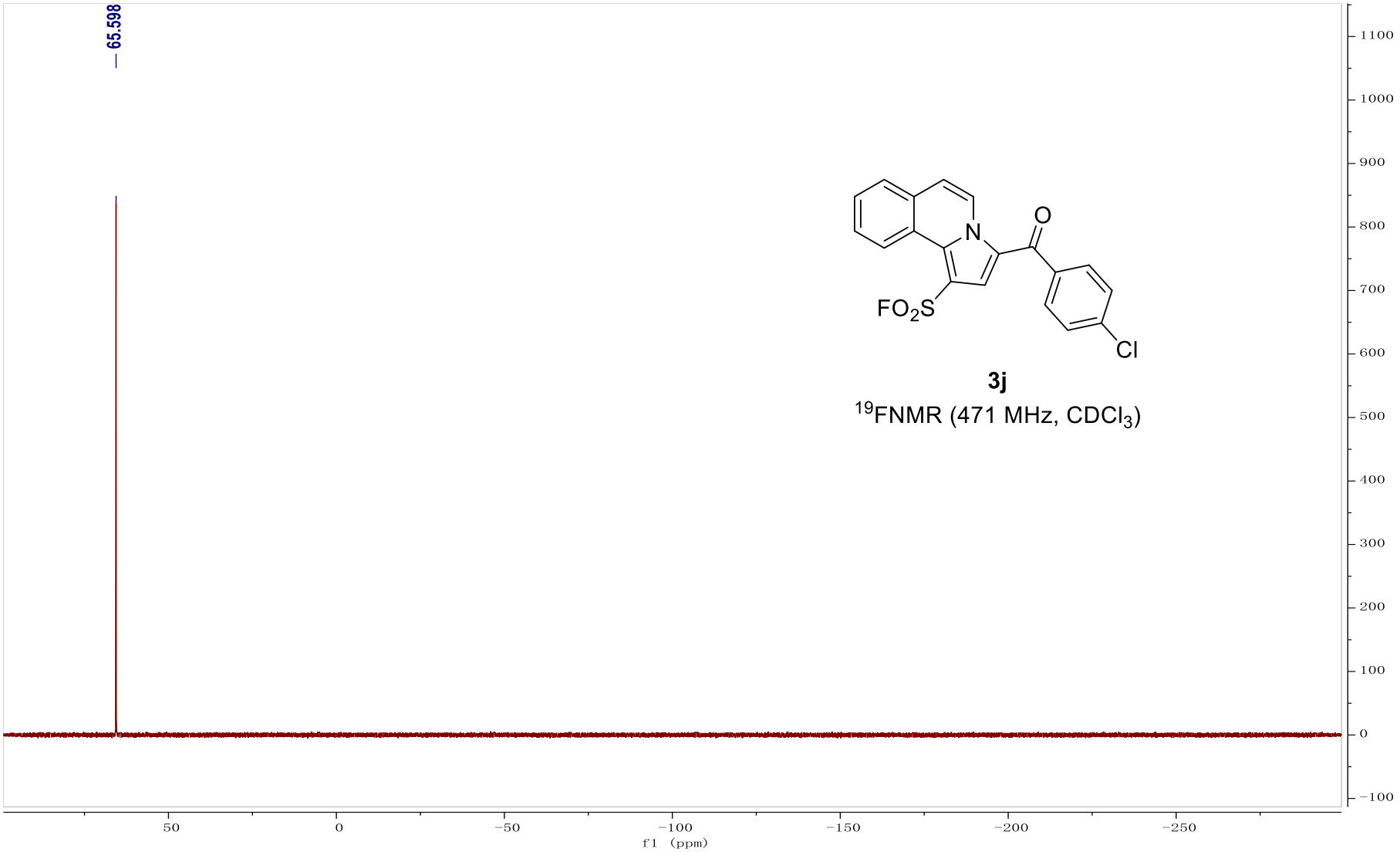

185.670
135.939
135.296
134.666
132.372
130.787
130.639
130.505
129.485
129.250
129.004
128.816
128.535
127.931
127.581
127.164
126.589
126.571
125.162
125.011
123.819
122.408
117.040
107.854
107.597
77.413 CDCl3
77.160 CDCl3
76.904 CDCl3
O
N
FO2S
3h
13C NMR (126 MHz, CDCl3)
f1 (ppm)


9.588
9.573
8.950
8.942
8.932
7.915
7.903
7.900
7.887
7.806
7.796
7.787
7.778
7.768
7.485
7.470
7.261
7.244
7.227
5.320 CD2Cl2
2.99 2.99 0.99 2.00
f1 (ppm)
0.98 1.00 2.99 2.99 0.99 2.00
f1 (ppm)
3i
1H NMR (500 MHz, CD2Cl2)


-65.197
-106.747
-106.752
-106.764
-106.774
-106.782
-106.794
O
N
FO2S
F
3i
19FNMR (471 MHz, CD2Cl2)
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
−400
50
0
−50
−100
−150
−200
−250
f1 (ppm)

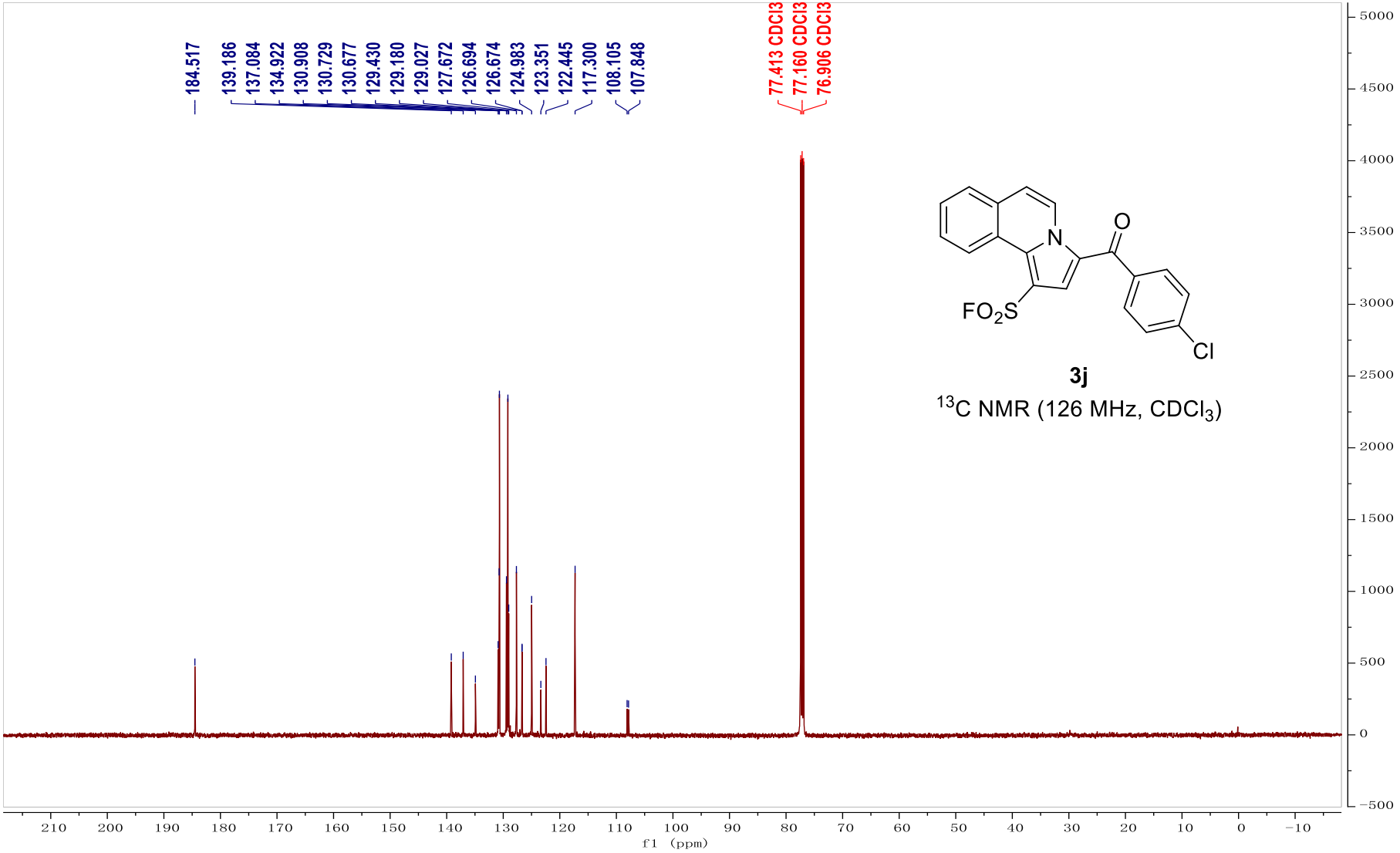

184.570
166.827
164.813
135.479
135.454
135.154
132.222
132.149
131.298
130.945
129.557
128.970
128.063
126.755
126.735
125.344
123.981
122.738
117.453
116.283
116.108
107.890
107.633
54.273 CD2Cl2
54.056 CD2Cl2
53.624 CD2Cl2
53.408 CD2Cl2
O
N
FO2S
F
3i
13C NMR (126 MHz, CD2Cl2)
f1 (ppm)

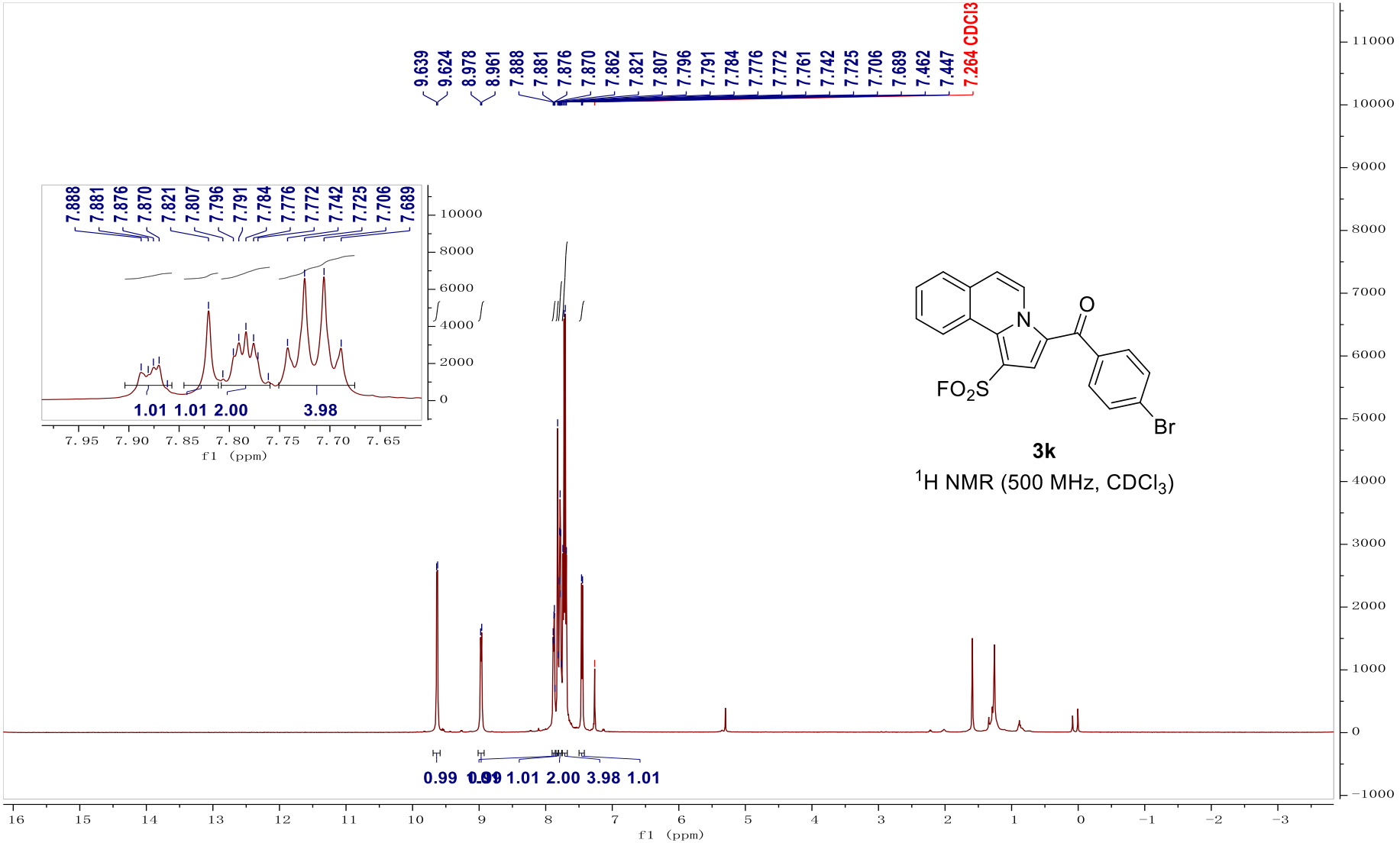

9.633
9.618
8.978
8.959
7.886
7.883
7.878
7.873
7.867
7.823
7.818
7.806
7.801
7.794
7.788
7.781
7.774
7.769
7.542
7.525
7.458
7.443
7.264 CDCl3
1.00 0.92 1.98 3.00 2.01 0.99
f1 (ppm)
1.02 1.98 3.00 2.01 0.99
FO2S
N
O
Cl
3j
1H NMR (500 MHz, CDCl3)

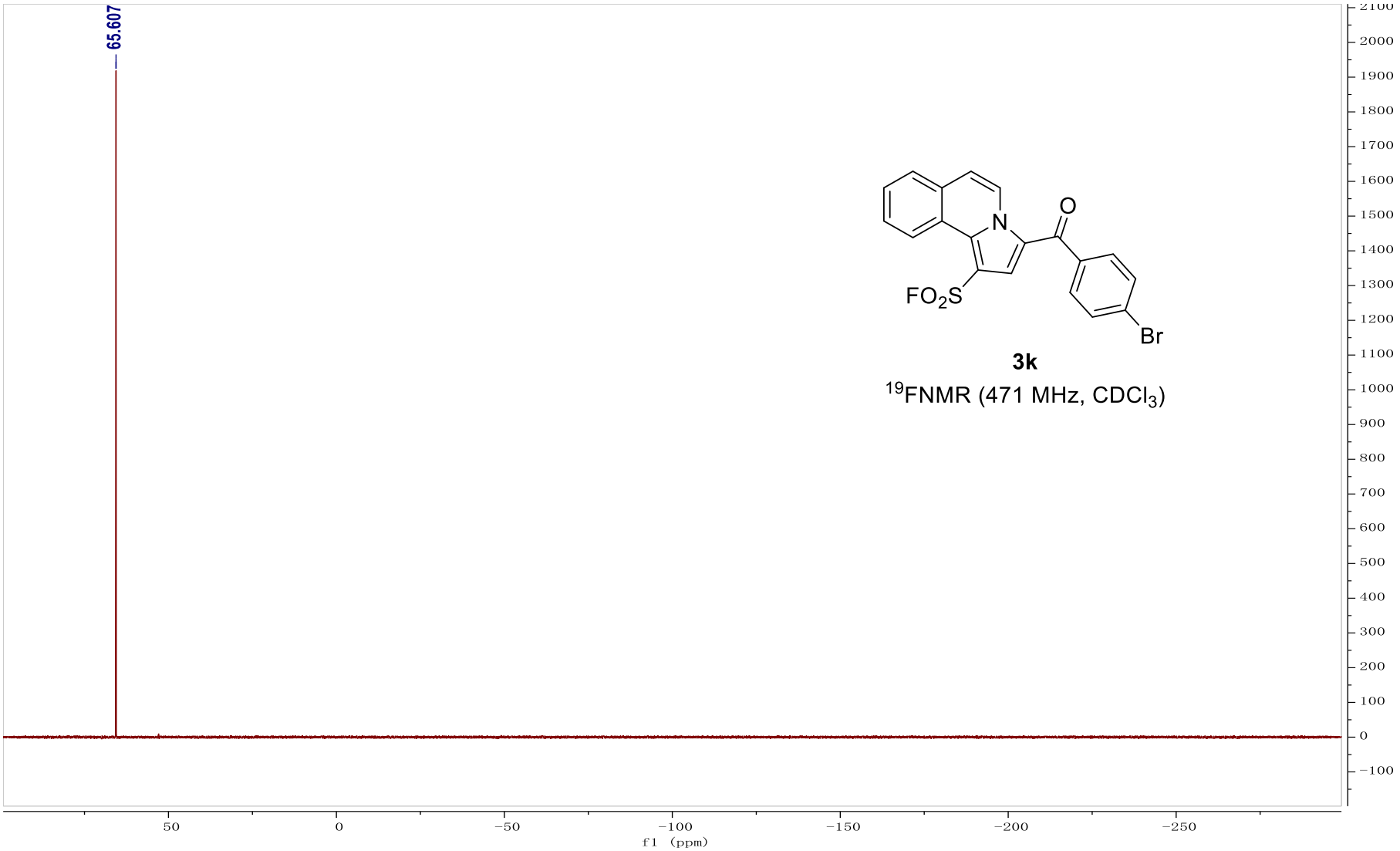


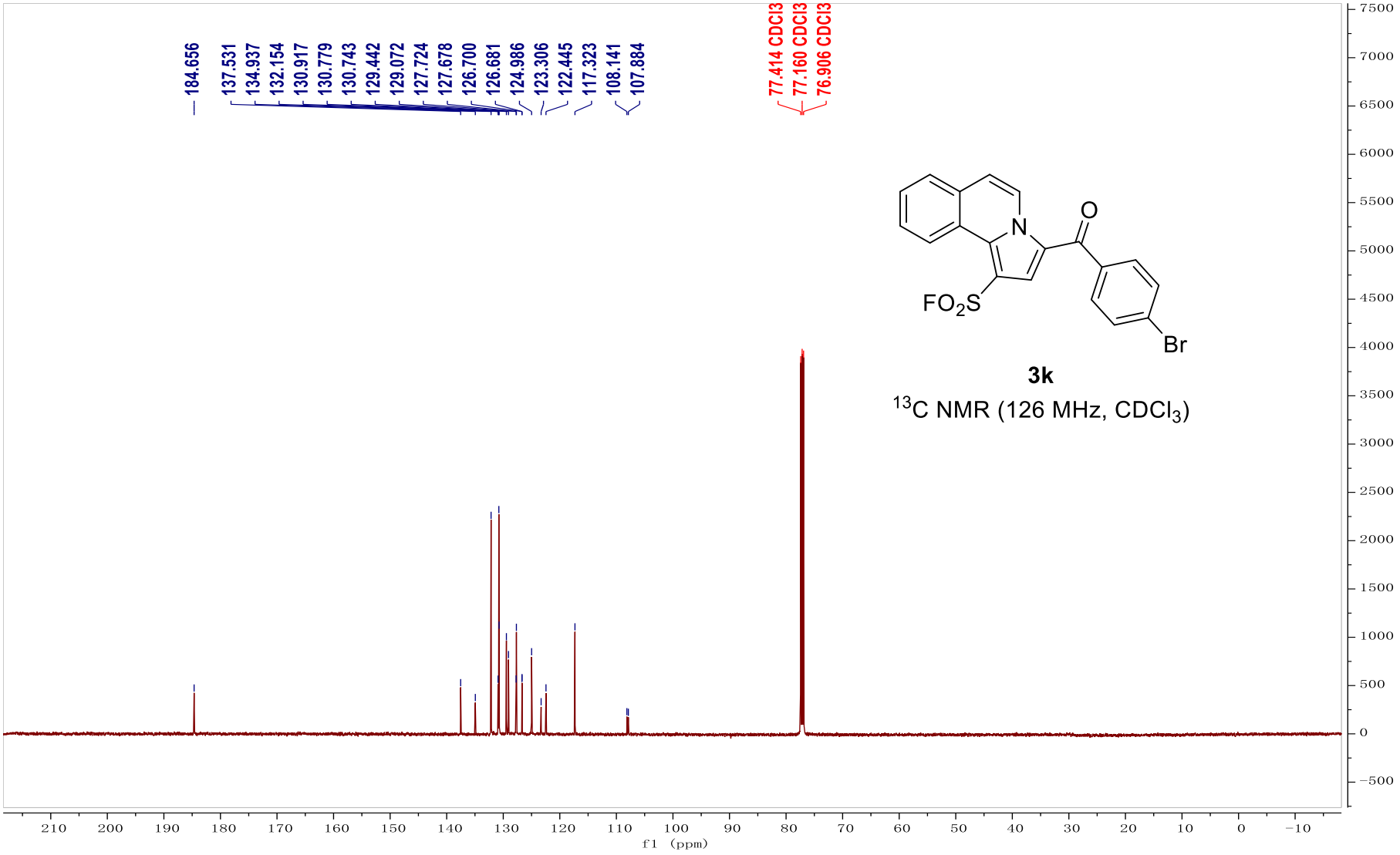
3j

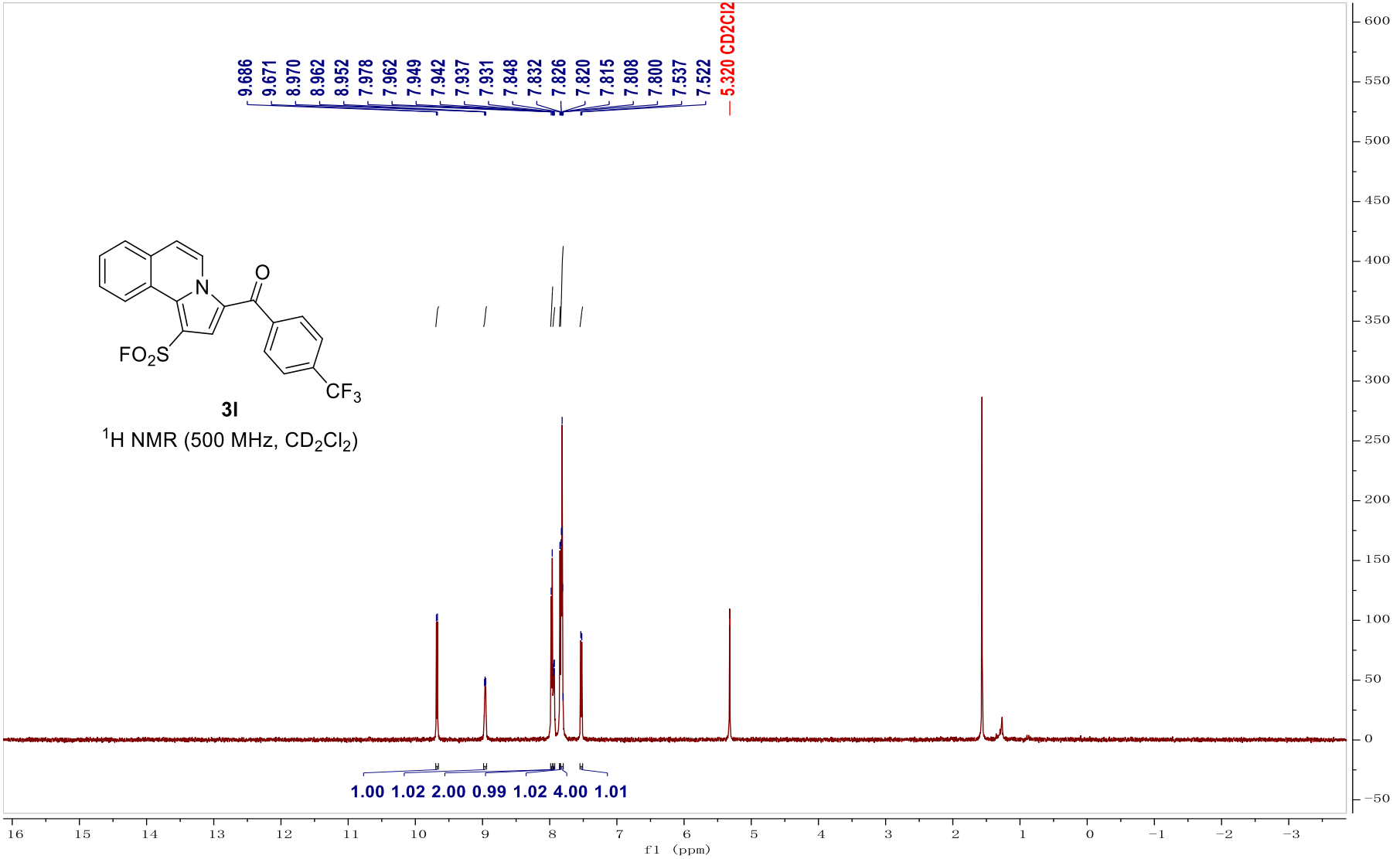
^{19}FNMR (471 MHz, $CDCl_3$)

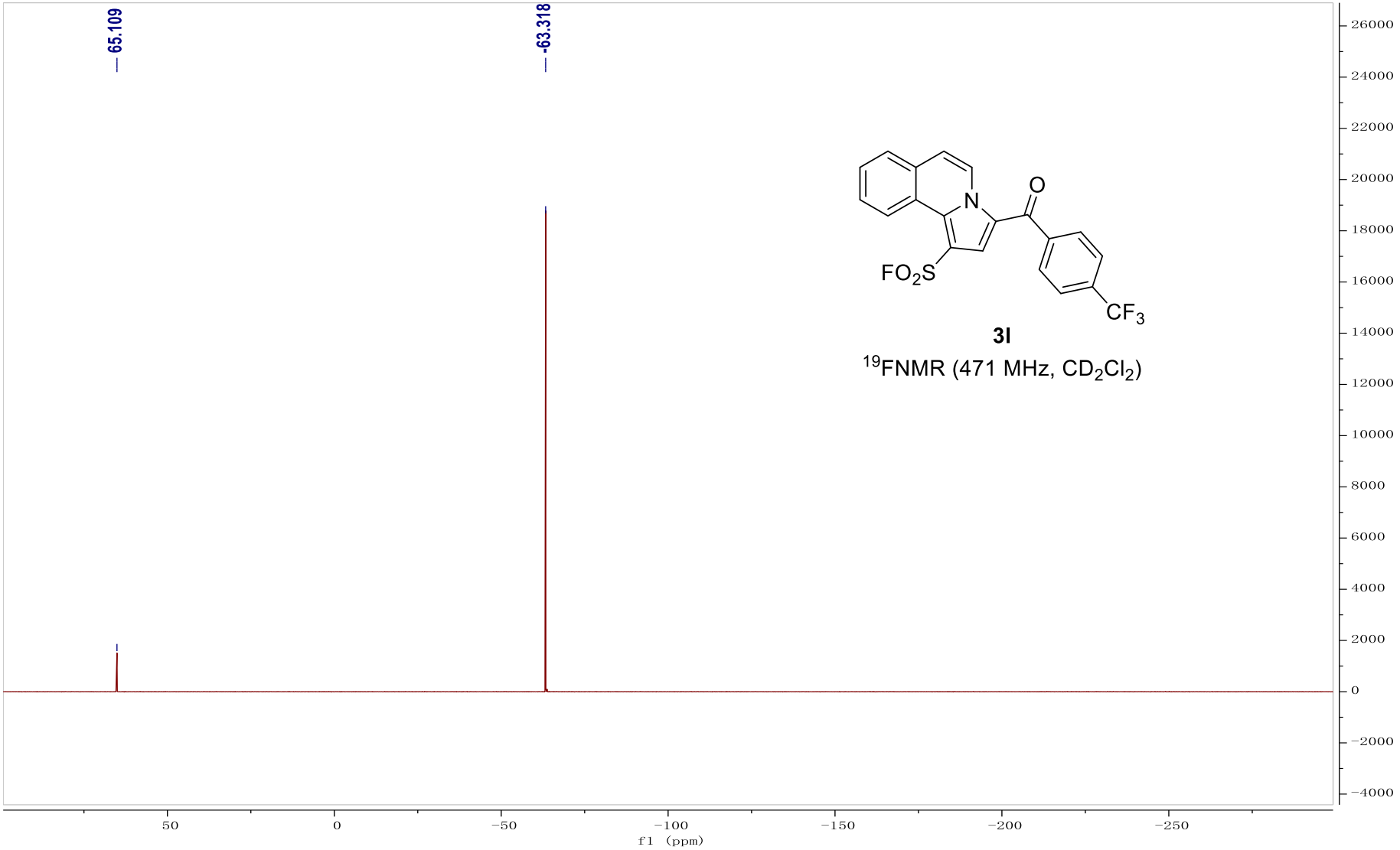

184.517
139.186
137.084
134.922
130.908
130.729
130.677
129.430
129.180
129.027
127.672
126.694
126.674
124.983
123.351
122.445
117.300
108.105
107.848
77.413 CDCl3
77.160 CDCl3
76.906 CDCl3
O
N
FO2S
Cl
3j
13C NMR (126 MHz, CDCl3)
f1 (ppm)

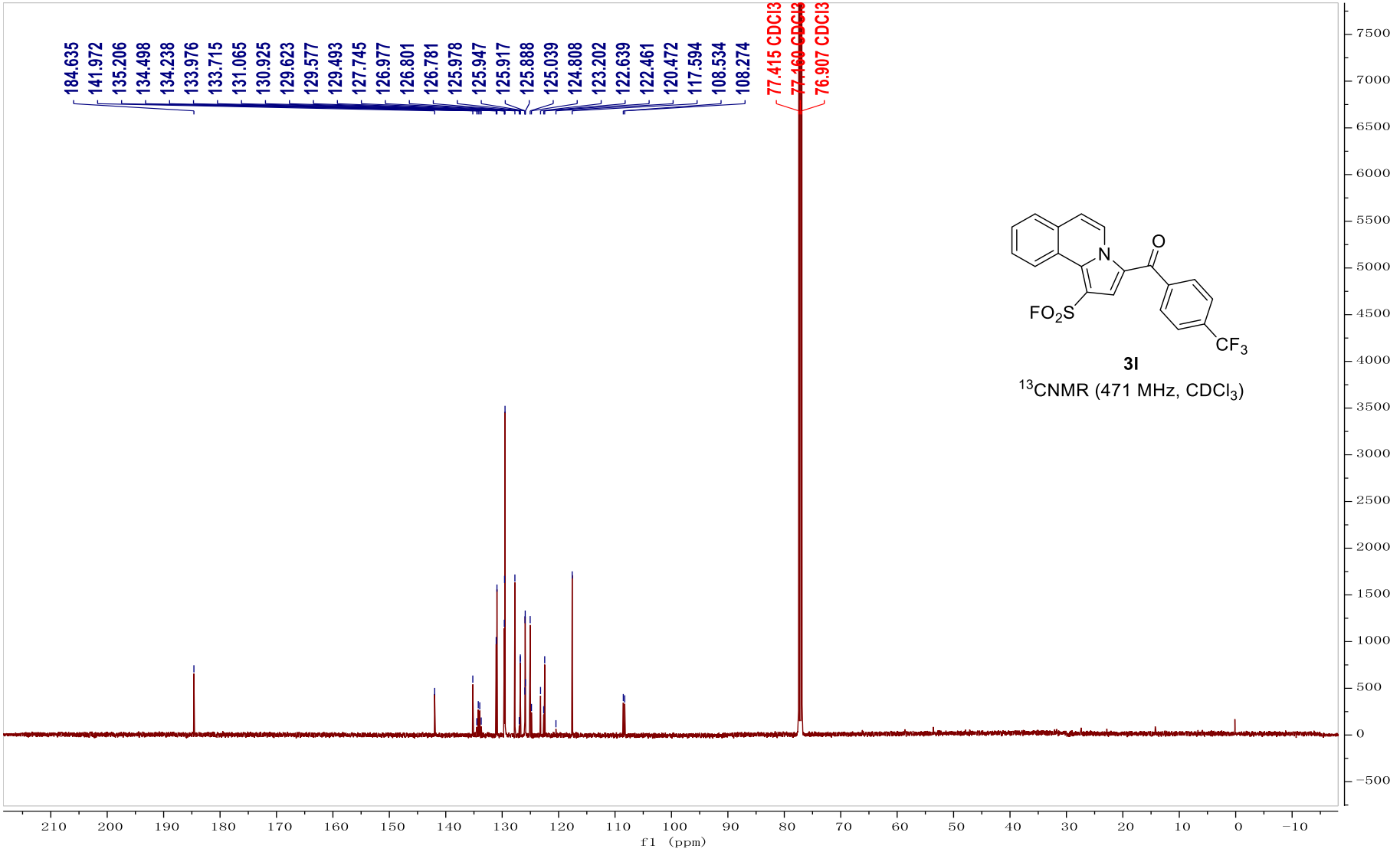

9.639
9.624
8.978
8.961
7.888
7.881
7.876
7.870
7.862
7.821
7.807
7.796
7.791
7.784
7.776
7.772
7.761
7.742
7.725
7.706
7.689
7.462
7.447
7.264 CDCl3
1.01 1.01 2.00 3.98
f1 (ppm)
0.99 0.99 1.01 2.00 3.98 1.01
f1 (ppm)
O
N
FO_2S
Br
3k
^{1}H NMR (500 MHz, $CDCl_3$)

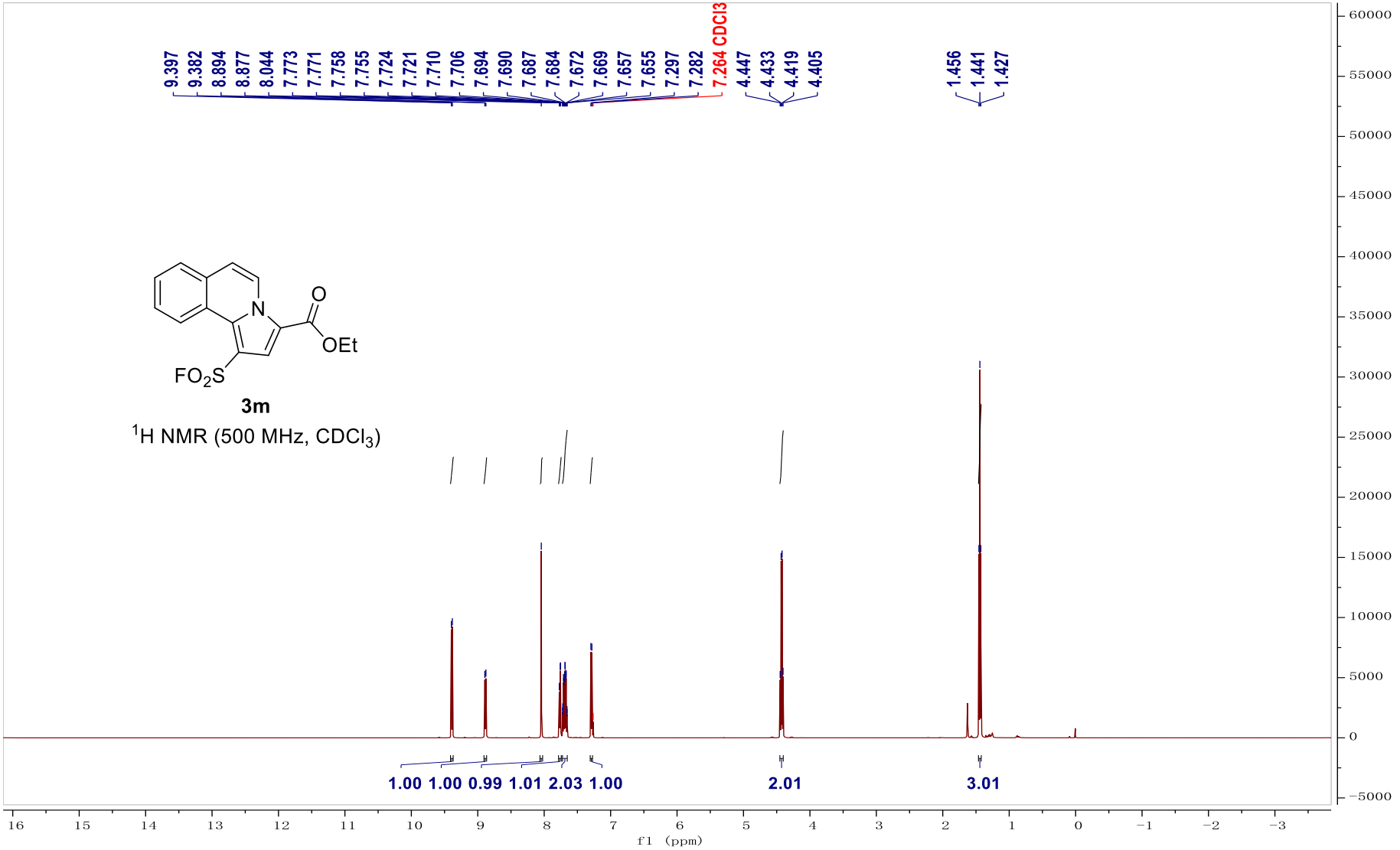

65.607
O
N
FO_2S
Br
3k
^{19}FNMR (471 MHz, $CDCl_3$)
f1 (ppm)

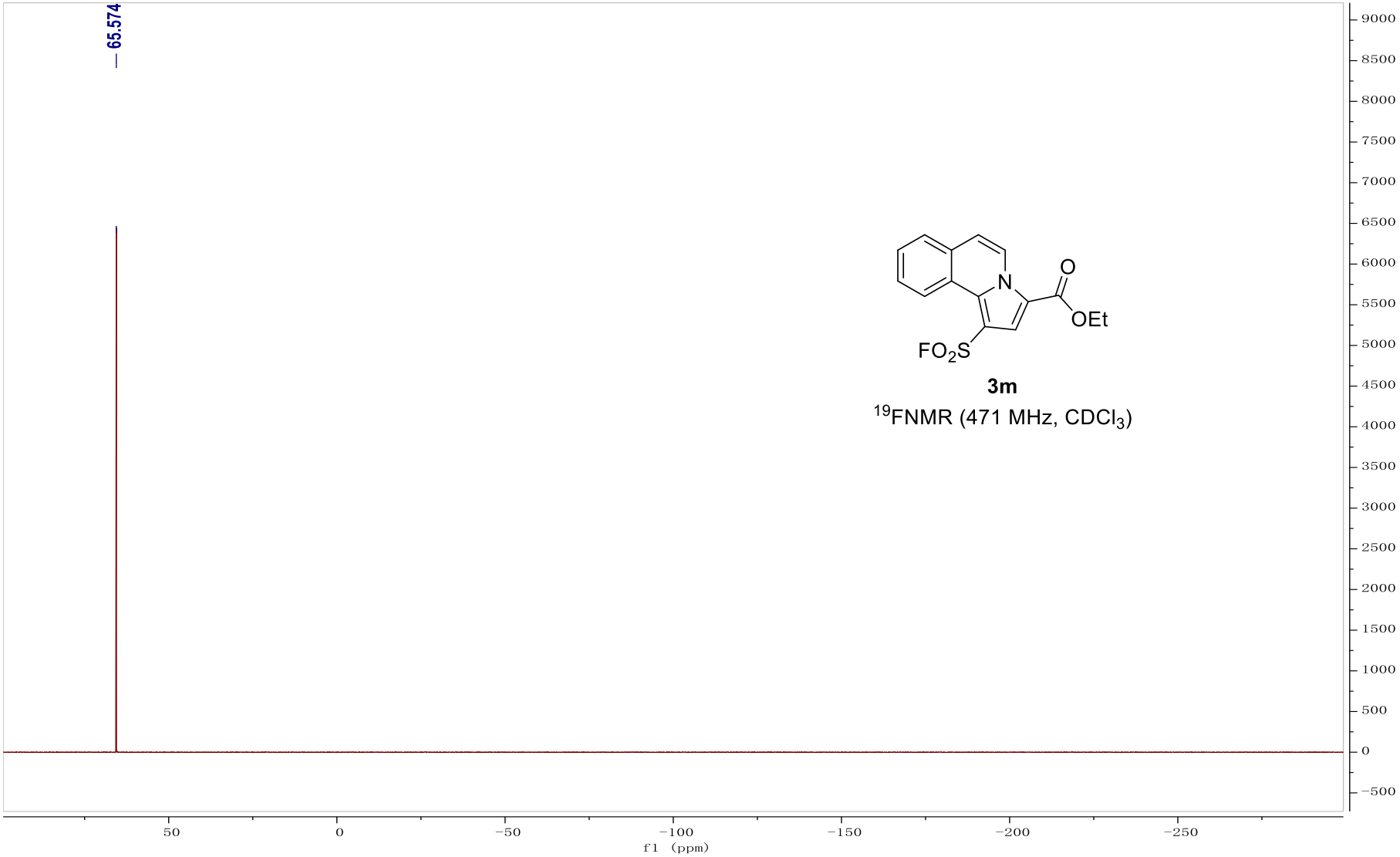

184.656
137.531
134.937
132.154
130.917
130.779
130.743
129.442
129.072
127.724
127.678
126.700
126.681
124.986
123.306
122.445
117.323
108.141
107.884
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
N
O
FO2S
Br
3k
13C NMR (126 MHz, CDCl3)
f1 (ppm)


9.686
9.671
8.970
8.962
8.952
7.978
7.962
7.949
7.942
7.937
7.931
7.848
7.832
7.826
7.820
7.815
7.808
7.800
7.537
7.522
5.320 CD2Cl2
O
N
FO2S
CF3
3l
1H NMR (500 MHz, CD2Cl2)
1.00 1.02 2.00 0.99 1.02 4.00 1.01
f1 (ppm)


65.109
-63.318
O
N
FO2S
CF3
3l
19FNMR (471 MHz, CD2Cl2)
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
−2000
−4000
50
0
−50
−100
−150
−200
−250
f1 (ppm)

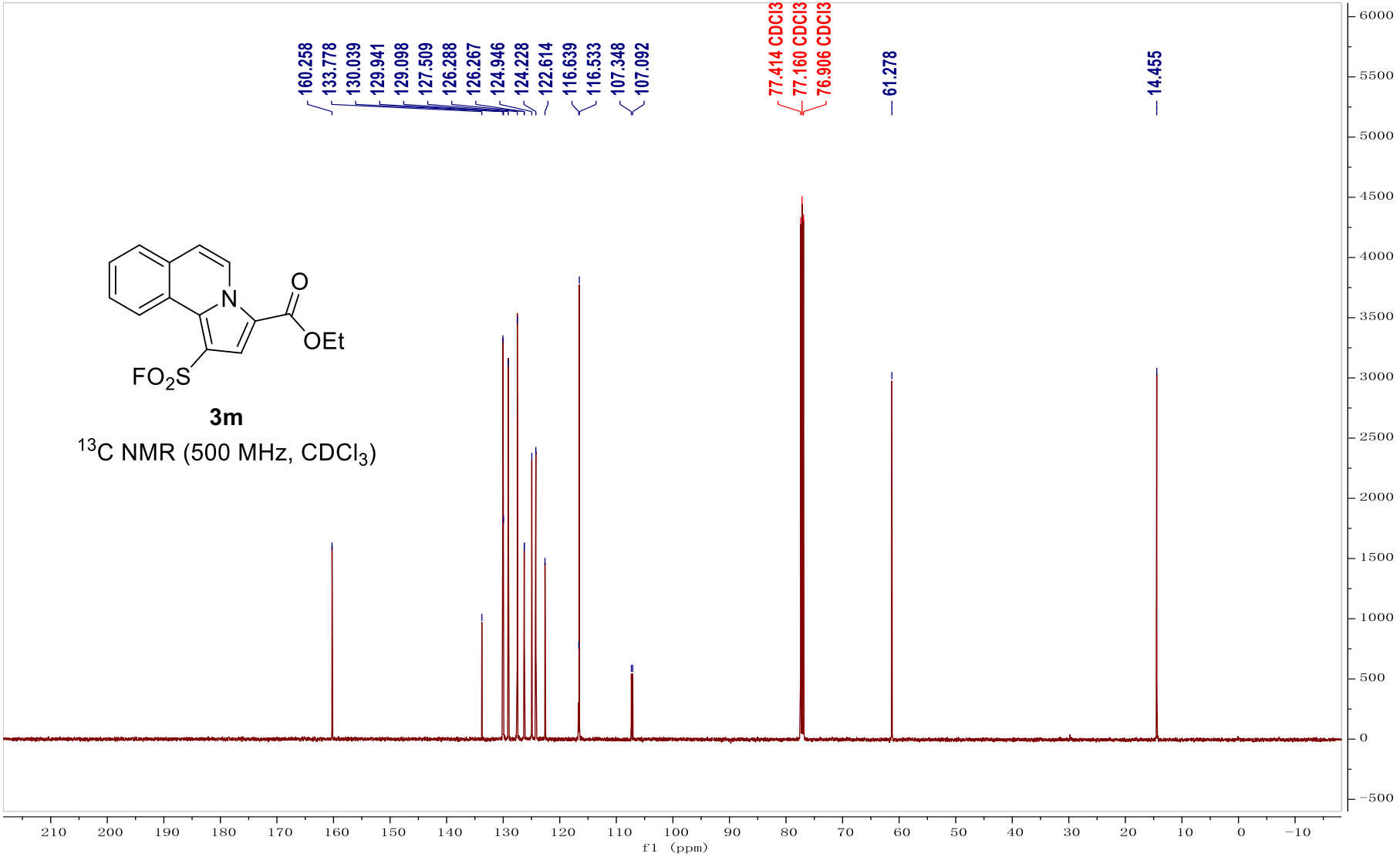

184.635
141.972
135.206
134.498
134.238
133.976
133.715
131.065
130.925
129.623
129.577
129.493
127.745
126.977
126.801
126.781
125.978
125.947
125.917
125.888
125.039
124.808
123.202
122.639
122.461
120.472
117.594
108.534
108.274
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
O
N
FO2S
CF3
3l
13CNMR (471 MHz, CDCl3)
f1 (ppm)

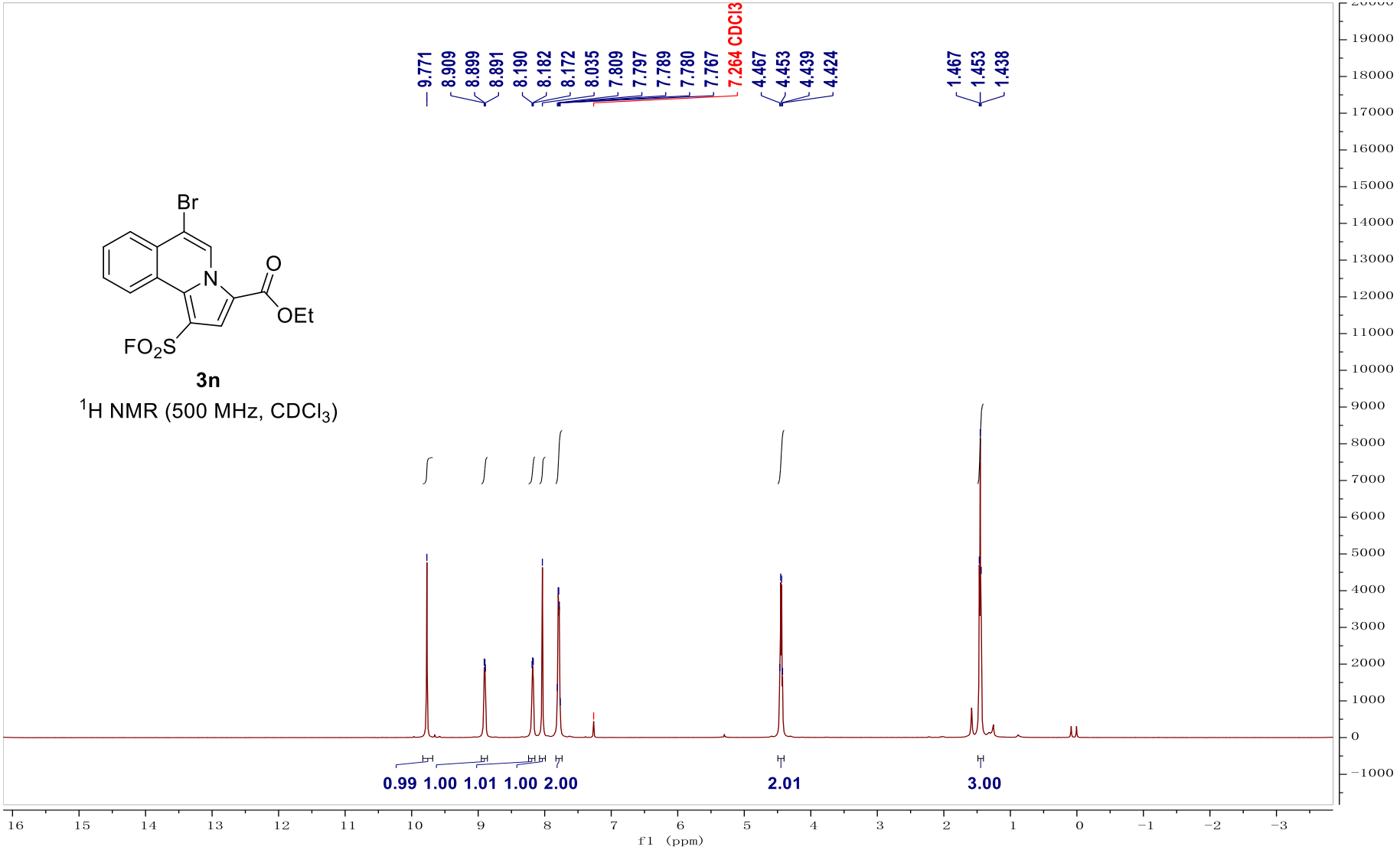

9.397
9.382
8.894
8.877
8.044
7.773
7.771
7.758
7.755
7.724
7.721
7.710
7.706
7.694
7.690
7.687
7.684
7.672
7.669
7.657
7.655
7.297
7.282
7.264 CDCl3
4.447
4.433
4.419
4.405
1.456
1.441
1.427
O
N
OEt
FO2S
3m
1H NMR (500 MHz, CDCl3)
1.00 1.00 0.99 1.01 2.03 1.00
2.01
3.01
f1 (ppm)

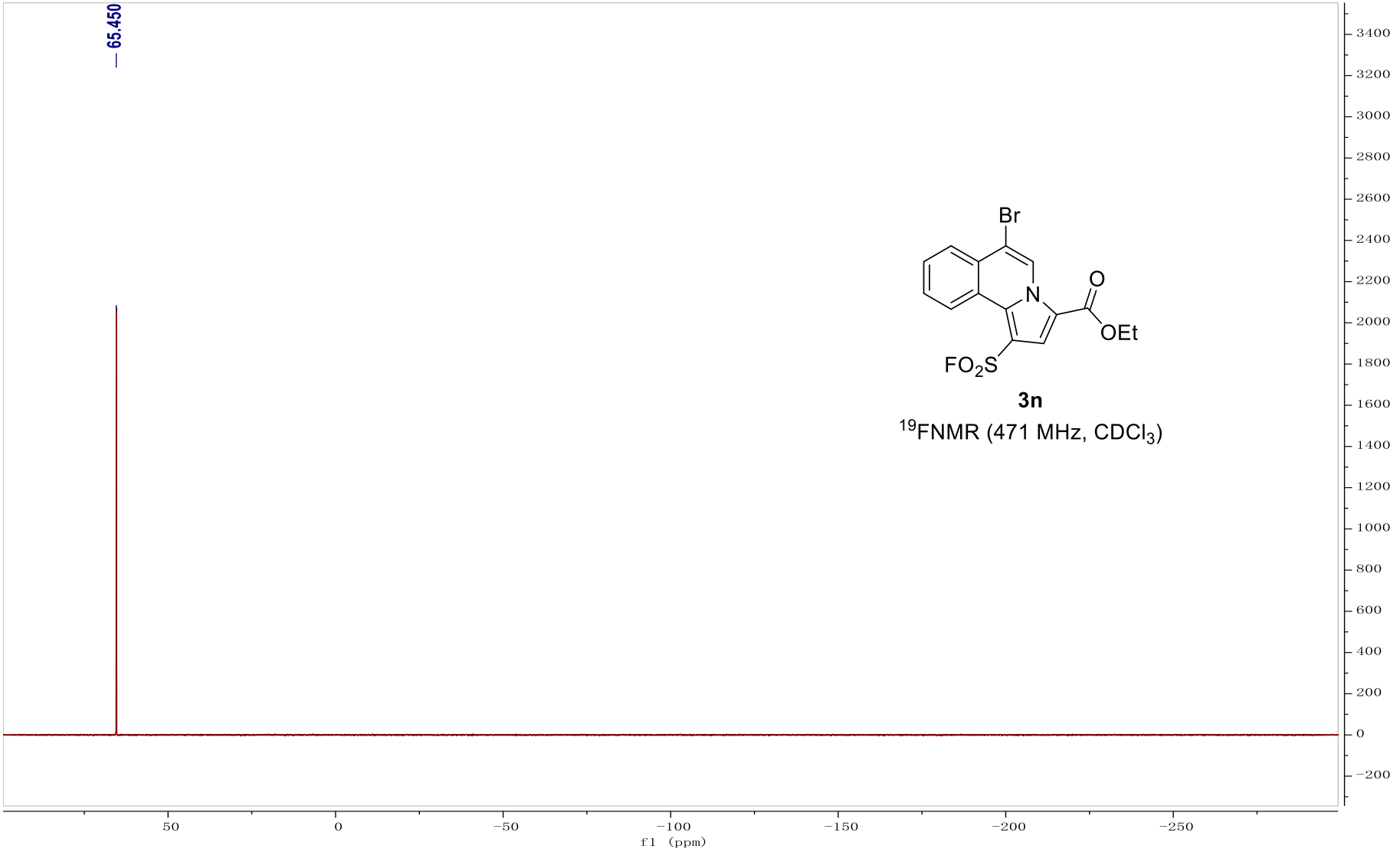


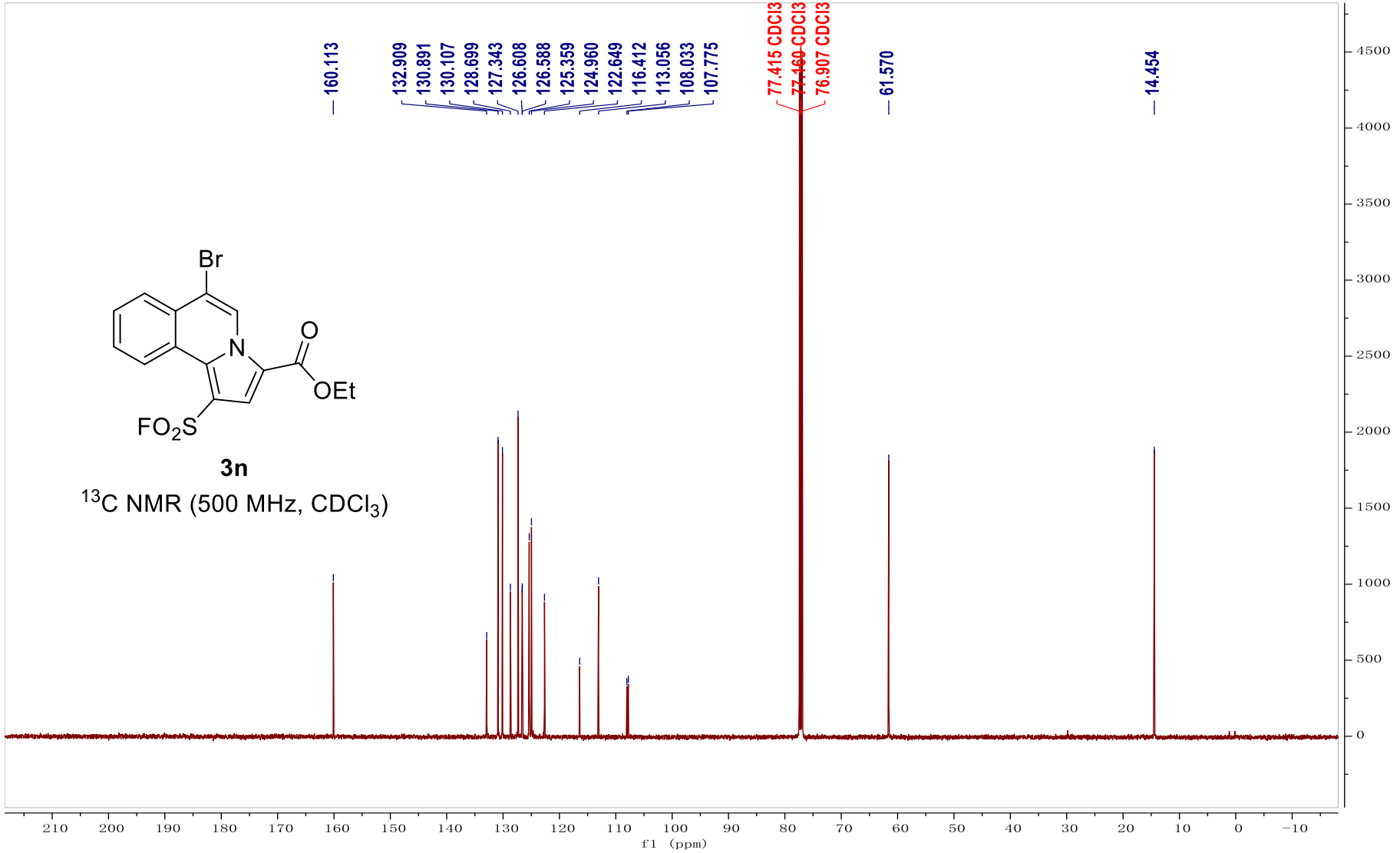
3m

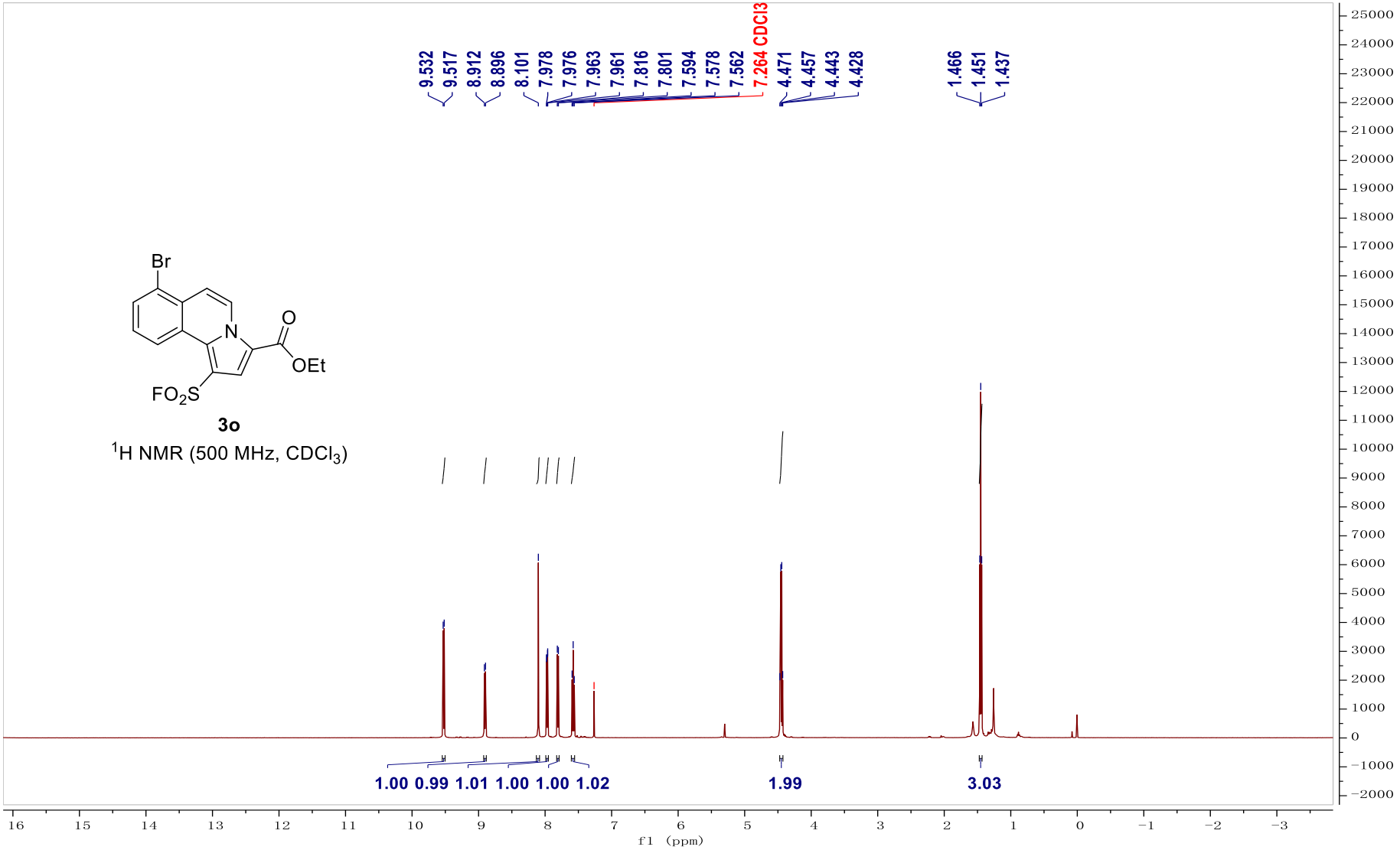
^{19}FNMR (471 MHz, $CDCl_3$)

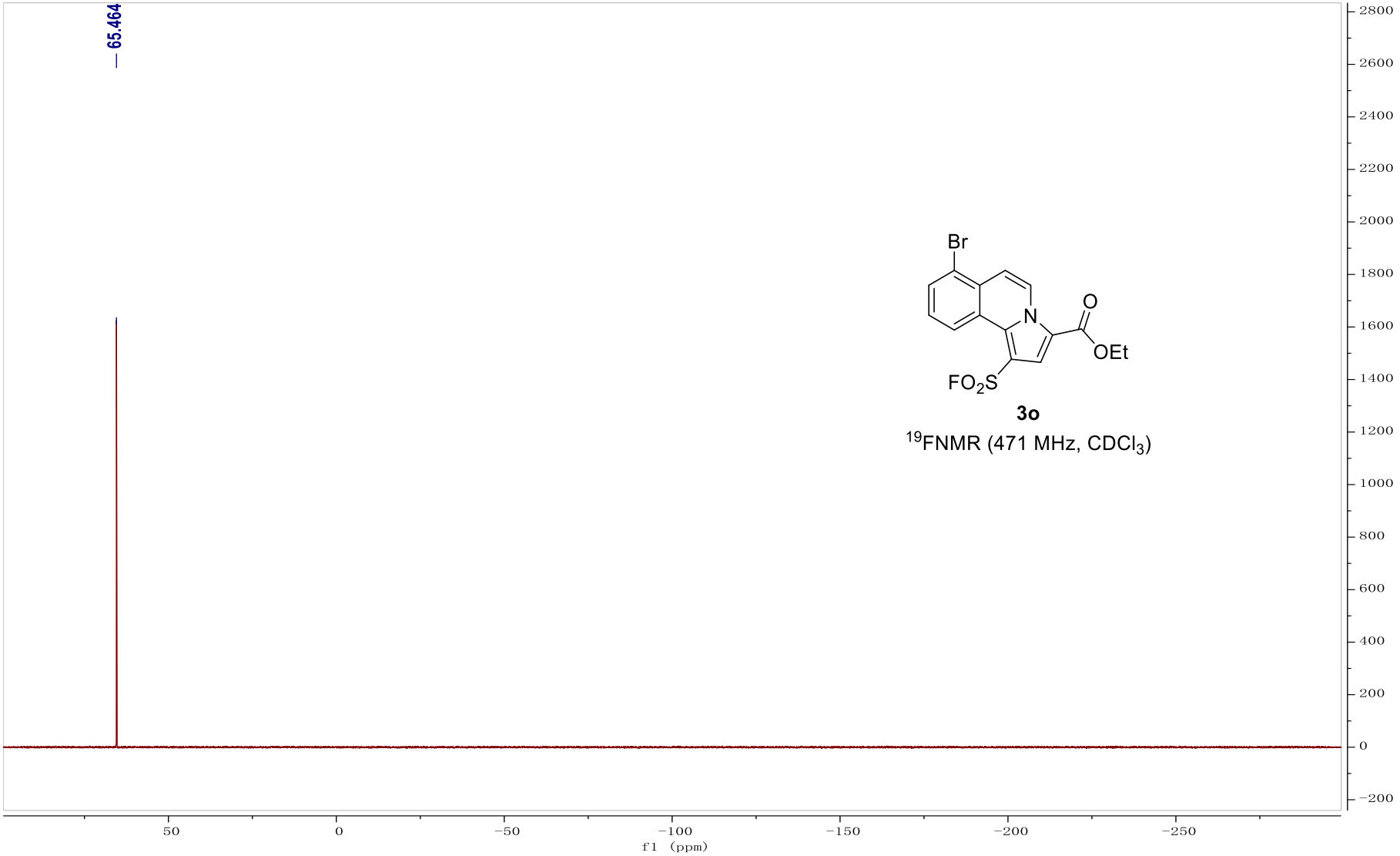

160.258
133.778
130.039
129.941
129.098
127.509
126.288
126.267
124.946
124.228
122.614
116.639
116.533
107.348
107.092
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
61.278
14.455
O
N
OEt
FO2S
3m
13C NMR (500 MHz, CDCl3)
f1 (ppm)

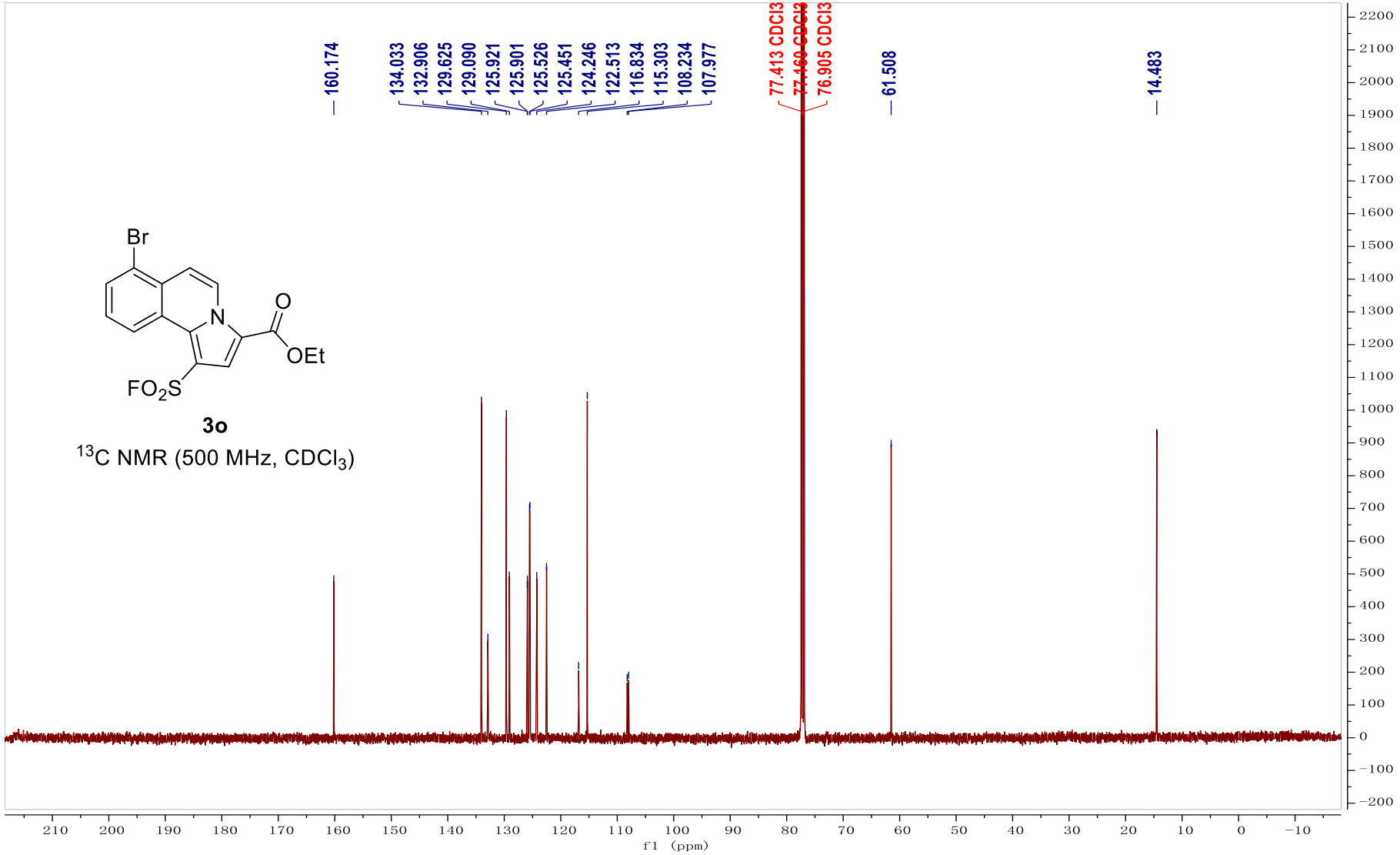

9.771
8.909
8.899
8.891
8.190
8.182
8.172
8.035
7.809
7.797
7.789
7.780
7.767
7.264 CDCl3
4.467
4.453
4.439
4.424
1.467
1.453
1.438
Br
O
N
OEt
FO2S
3n
1H NMR (500 MHz, CDCl3)
0.99 1.00 1.01 1.00 2.00
2.01
3.00
f1 (ppm)

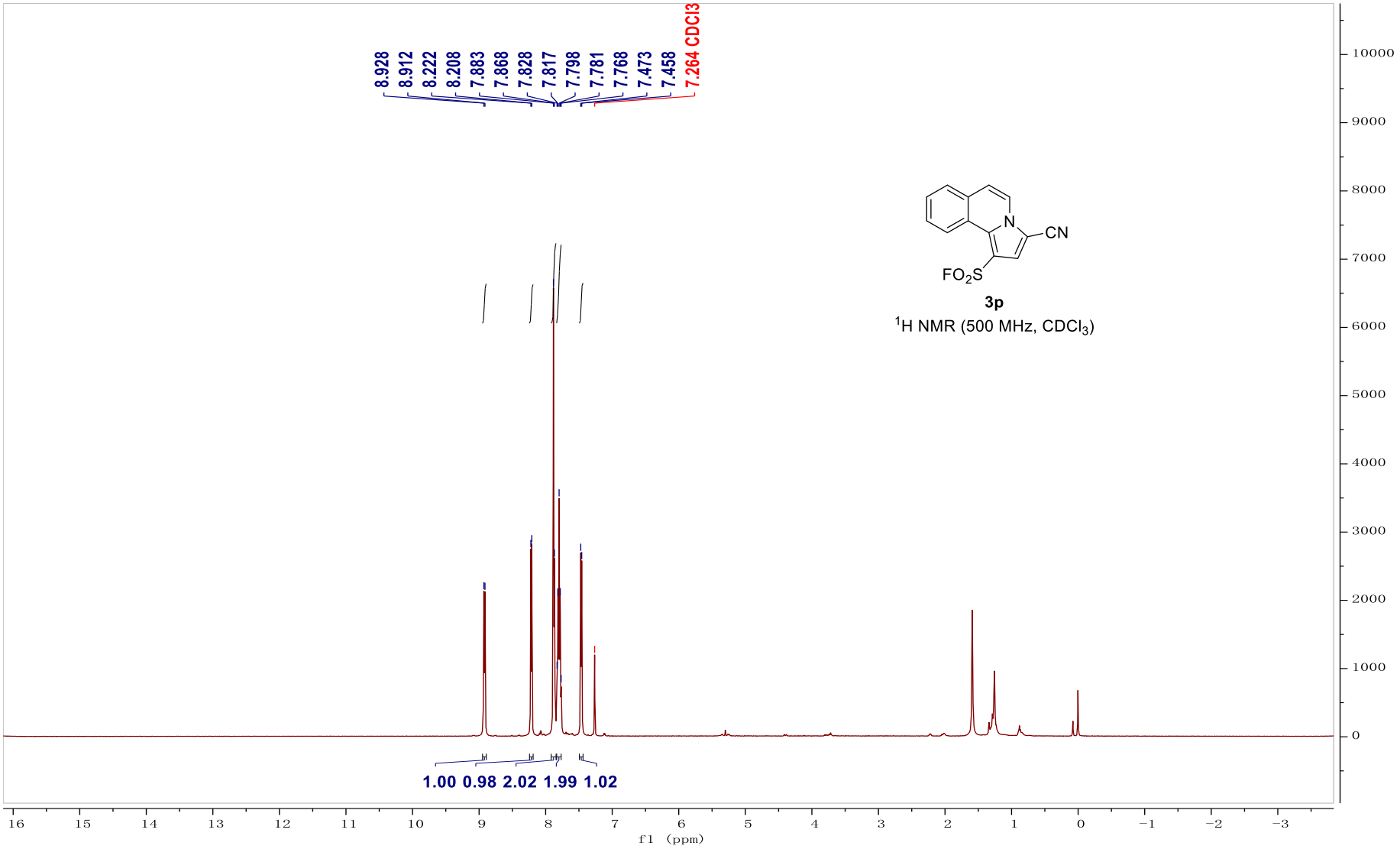

65.450
Br
N
O
OEt
FO2S
3n
19FNMR (471 MHz, CDCl3)
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

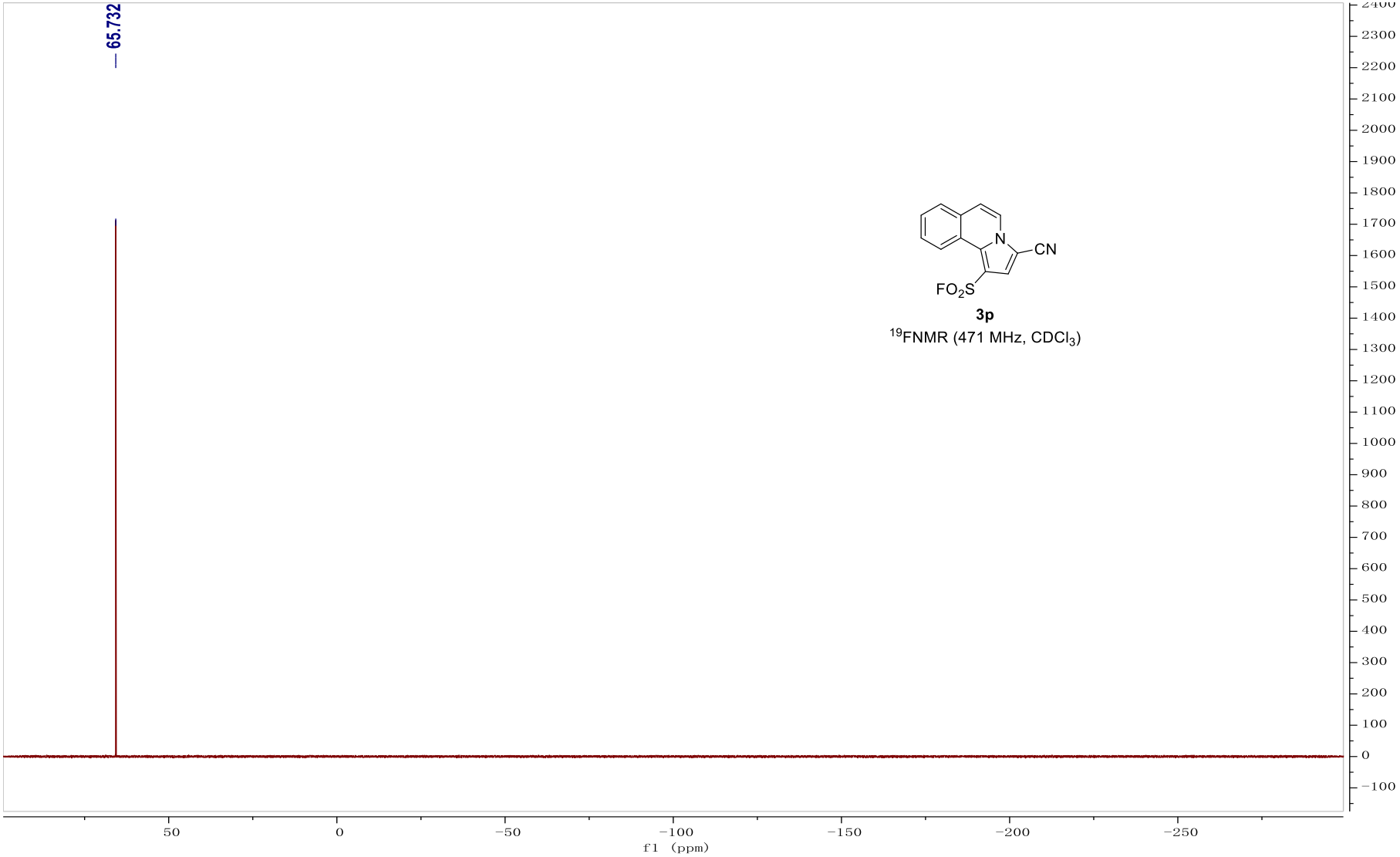

160.113
132.909
130.891
130.107
128.699
127.343
126.608
126.588
125.359
124.960
122.649
116.412
113.056
108.033
107.775
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
61.570
14.454
Br
O
N
OEt
FO2S
3n
13C NMR (500 MHz, CDCl3)
f1 (ppm)

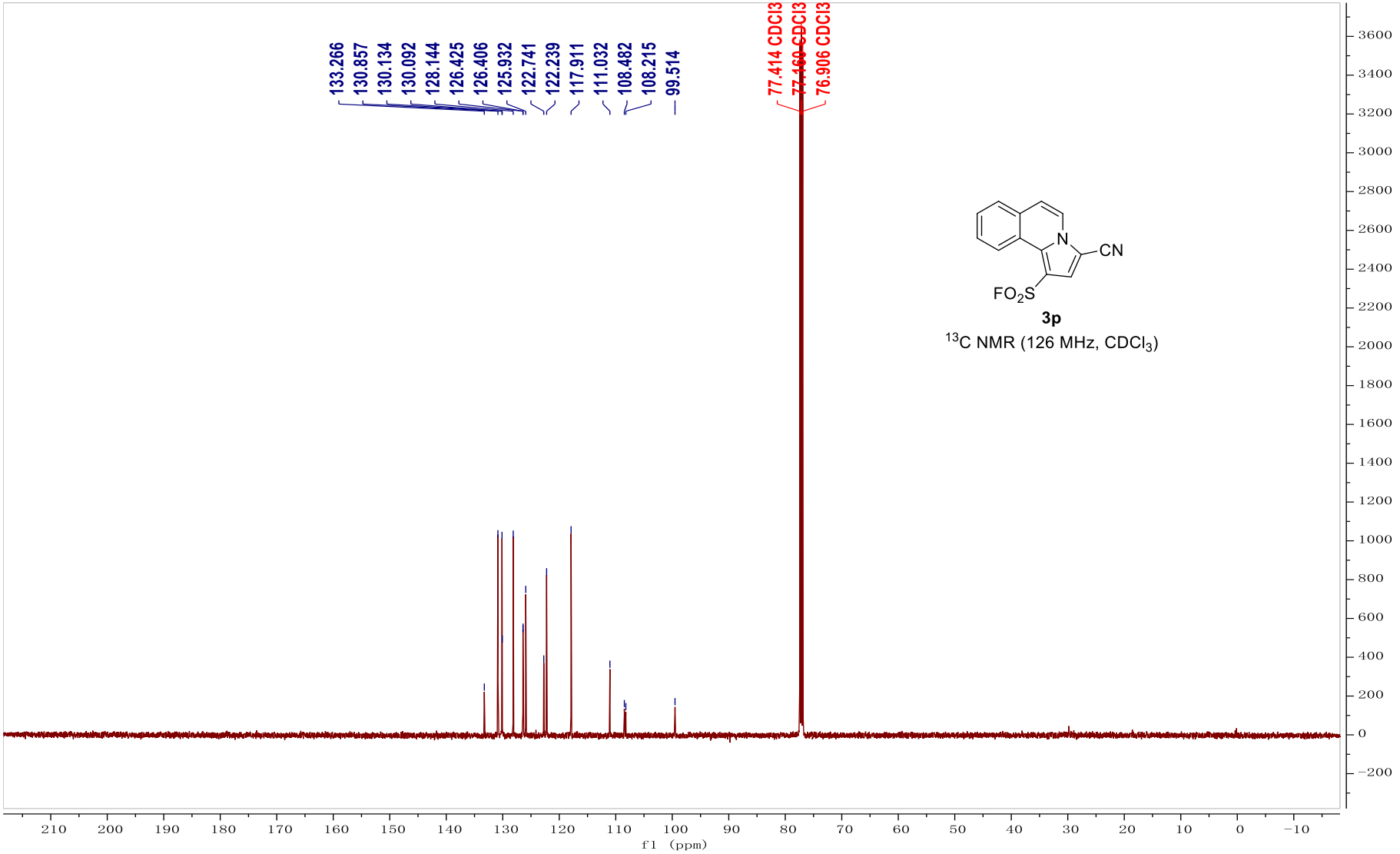

9.532
9.517
8.912
8.896
8.101
7.978
7.976
7.963
7.961
7.816
7.801
7.594
7.578
7.562
7.264 CDCl3
4.471
4.457
4.443
4.428
1.466
1.451
1.437
Br
O
N
OEt
FO2S
3o
1H NMR (500 MHz, CDCl3)
1.00 0.99 1.01 1.00 1.00 1.02
1.99
3.03
f1 (ppm)

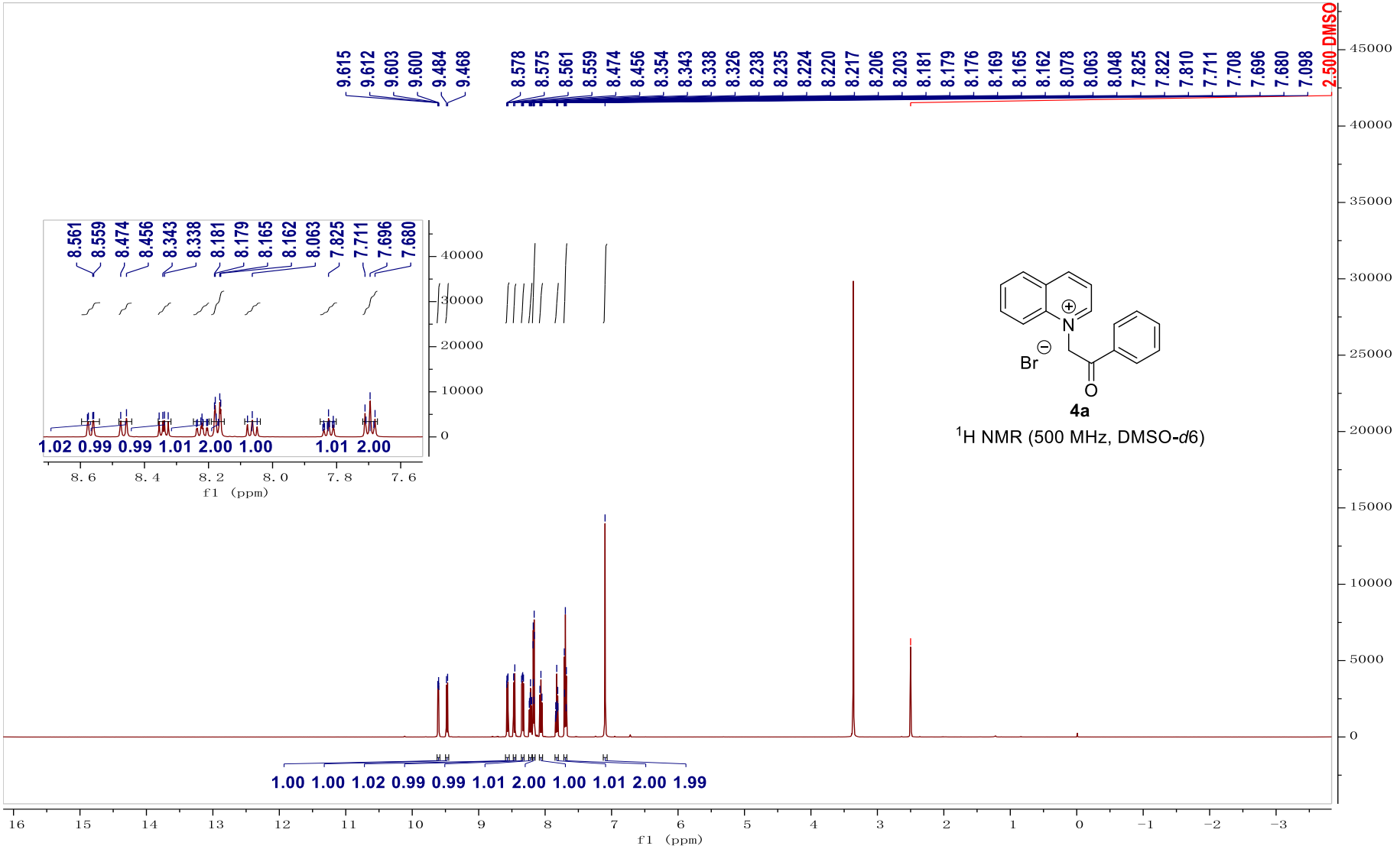

65.464
Br
O
N
OEt
FO2S
3o
19FNMR (471 MHz, CDCl3)
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

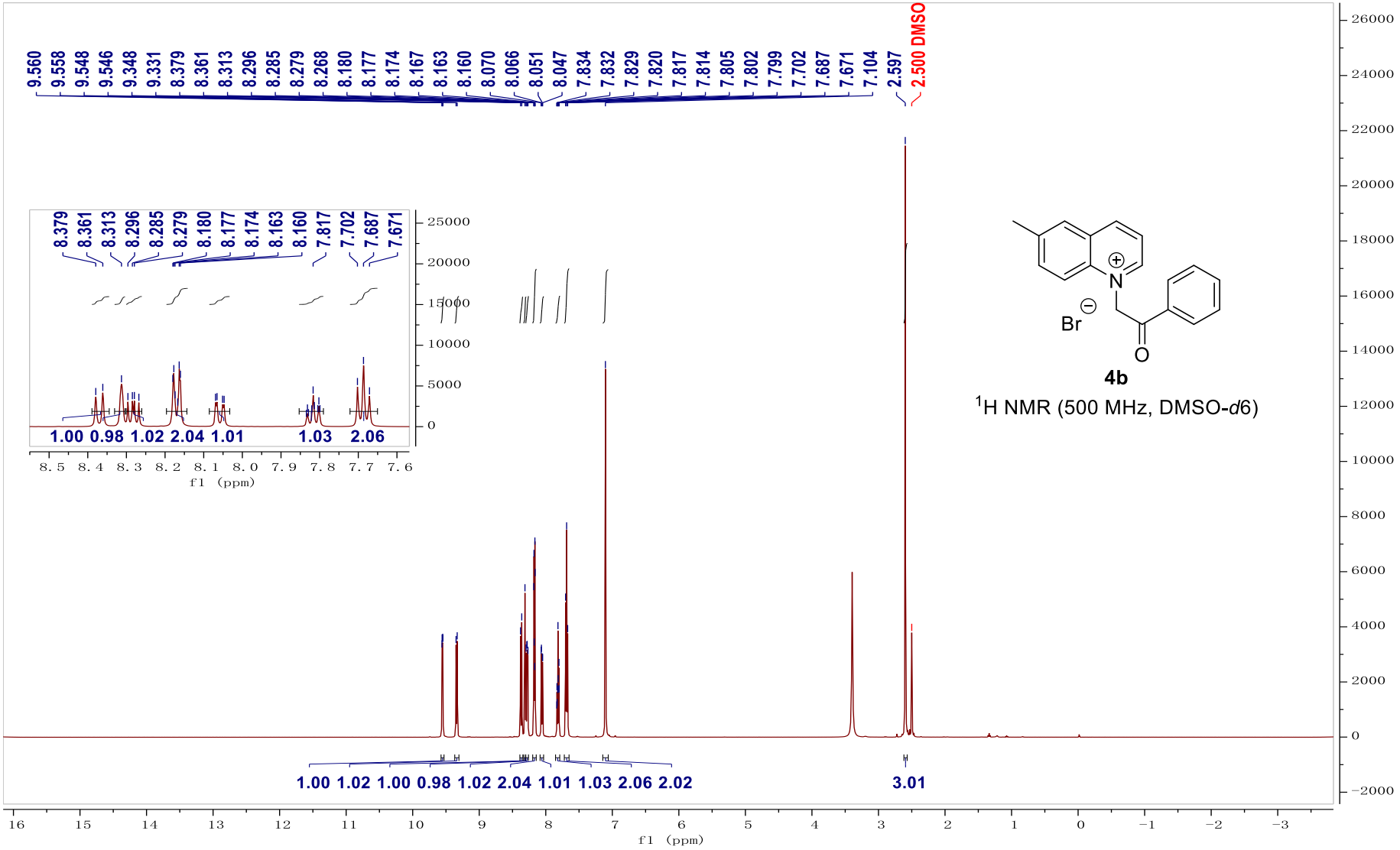

160.174
134.033
132.906
129.625
129.090
125.921
125.901
125.526
125.451
124.246
122.513
116.834
115.303
108.234
107.977
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
61.508
14.483
Br
O
N
OEt
FO2S
3o
13C NMR (500 MHz, CDCl3)
f1 (ppm)

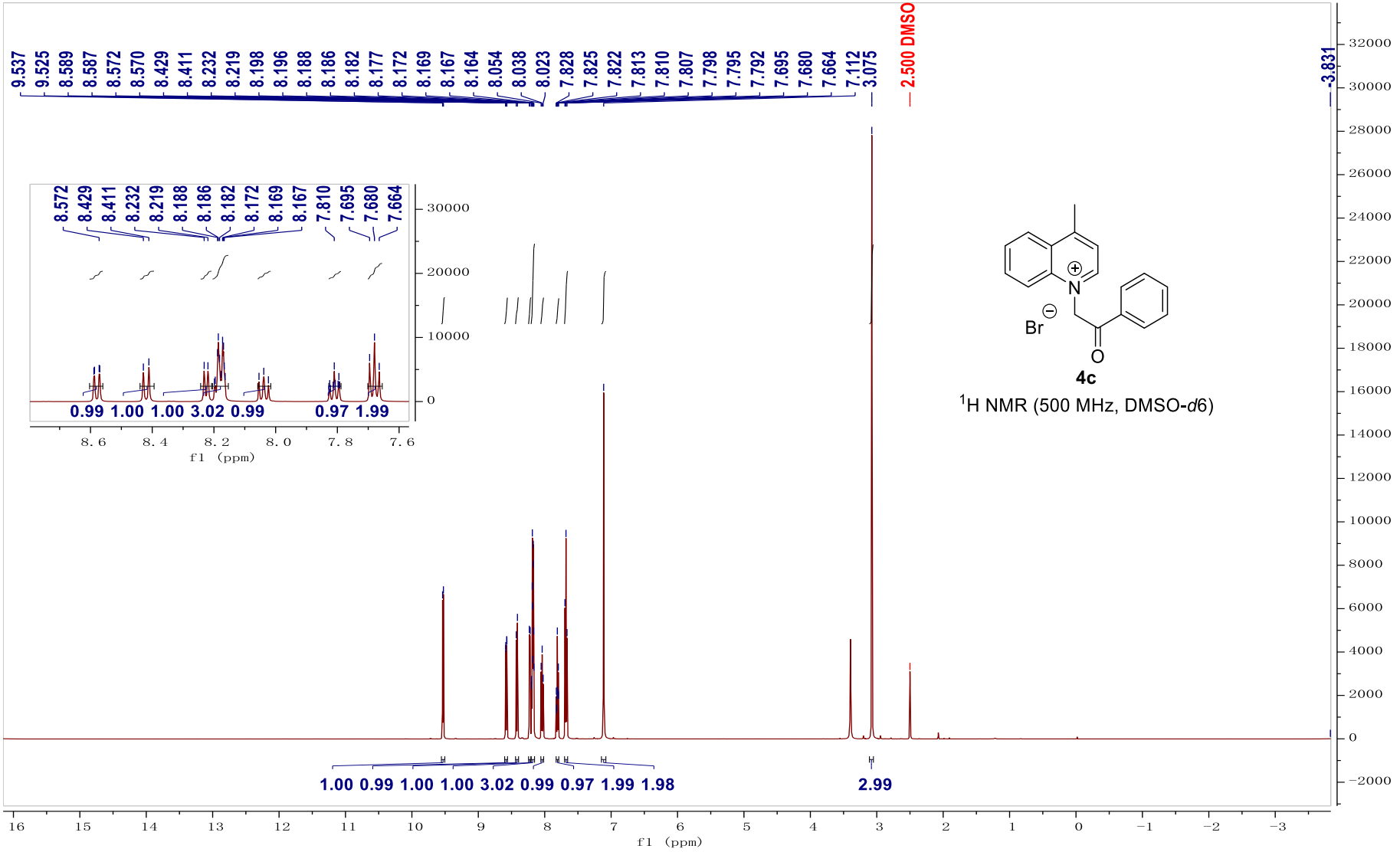

8.928
8.912
8.222
8.208
7.883
7.868
7.828
7.817
7.798
7.781
7.768
7.473
7.458
7.264 CDCl3
N
CN
FO2S
3p
1H NMR (500 MHz, CDCl3)
1.00 0.98 2.02 1.99 1.02
f1 (ppm)

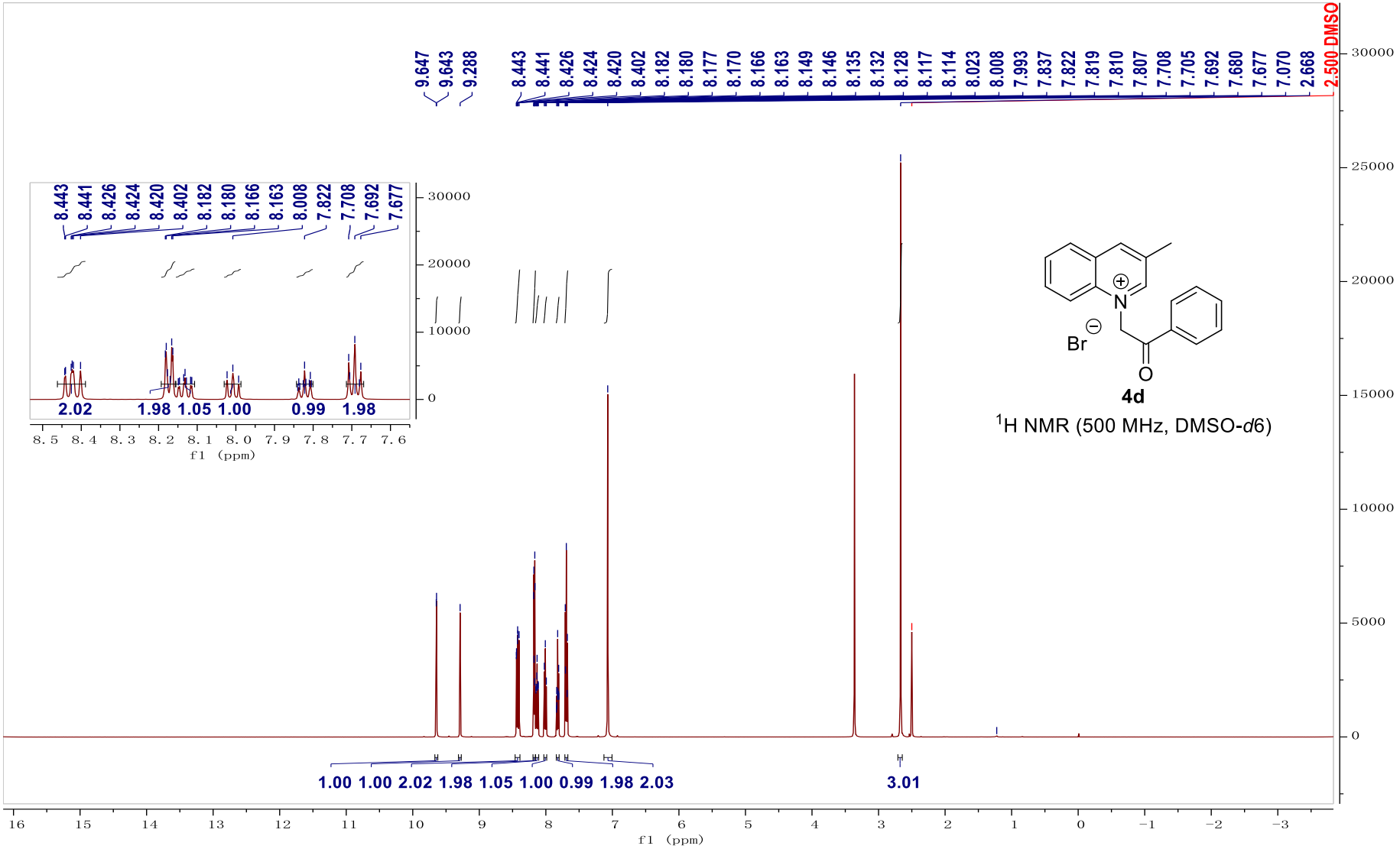

65.732
N
CN
FO2S
3p
19FNMR (471 MHz, CDCl3)
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
50
0
−50
−100
−150
−200
−250
f1 (ppm)

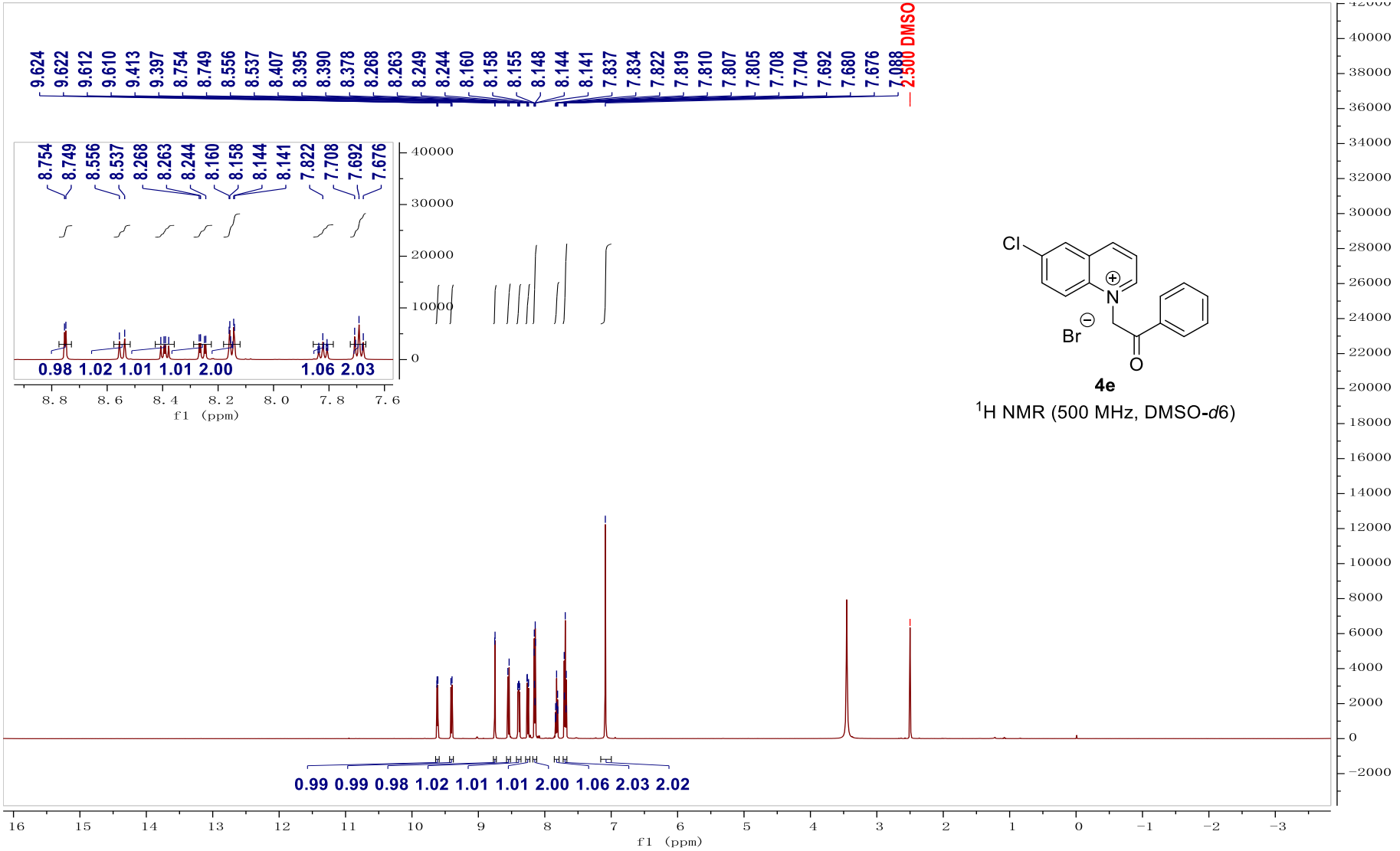

133.266
130.857
130.134
130.092
128.144
126.425
126.406
125.932
122.741
122.239
117.911
111.032
108.482
108.215
99.514
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
N
CN
FO2S
3p
13C NMR (126 MHz, CDCl3)
f1 (ppm)

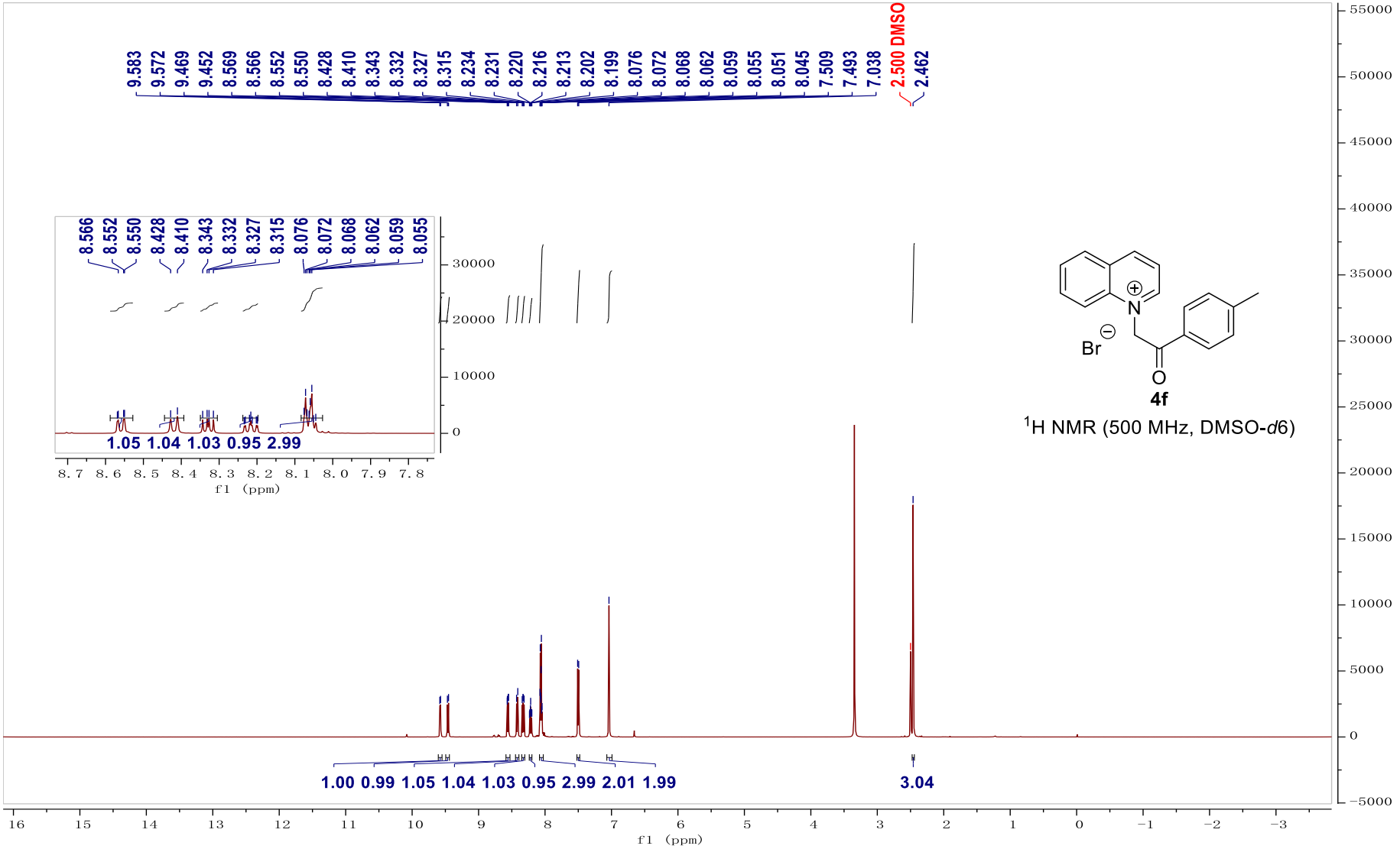

9.615 9.612 9.603 9.600 9.484 9.468
8.578 8.575 8.561 8.559 8.474 8.456 8.354 8.343 8.338 8.326 8.238 8.235 8.224 8.220 8.217 8.206 8.203 8.181 8.179 8.176 8.169 8.165 8.162 8.078 8.063 8.048 7.825 7.822 7.810 7.711 7.708 7.696 7.680 7.098
2.500 DMSO
8.561 8.559 8.474 8.456 8.343 8.338 8.181 8.179 8.165 8.162 8.063 7.825 7.711 7.696 7.680
1.02 0.99 0.99 1.01 2.00 1.00 1.01 2.00
f1 (ppm)
Br
4a
1H NMR (500 MHz, DMSO-d6)
1.00 1.00 1.02 0.99 0.99 1.01 2.00 1.00 1.01 2.00 1.99
f1 (ppm)

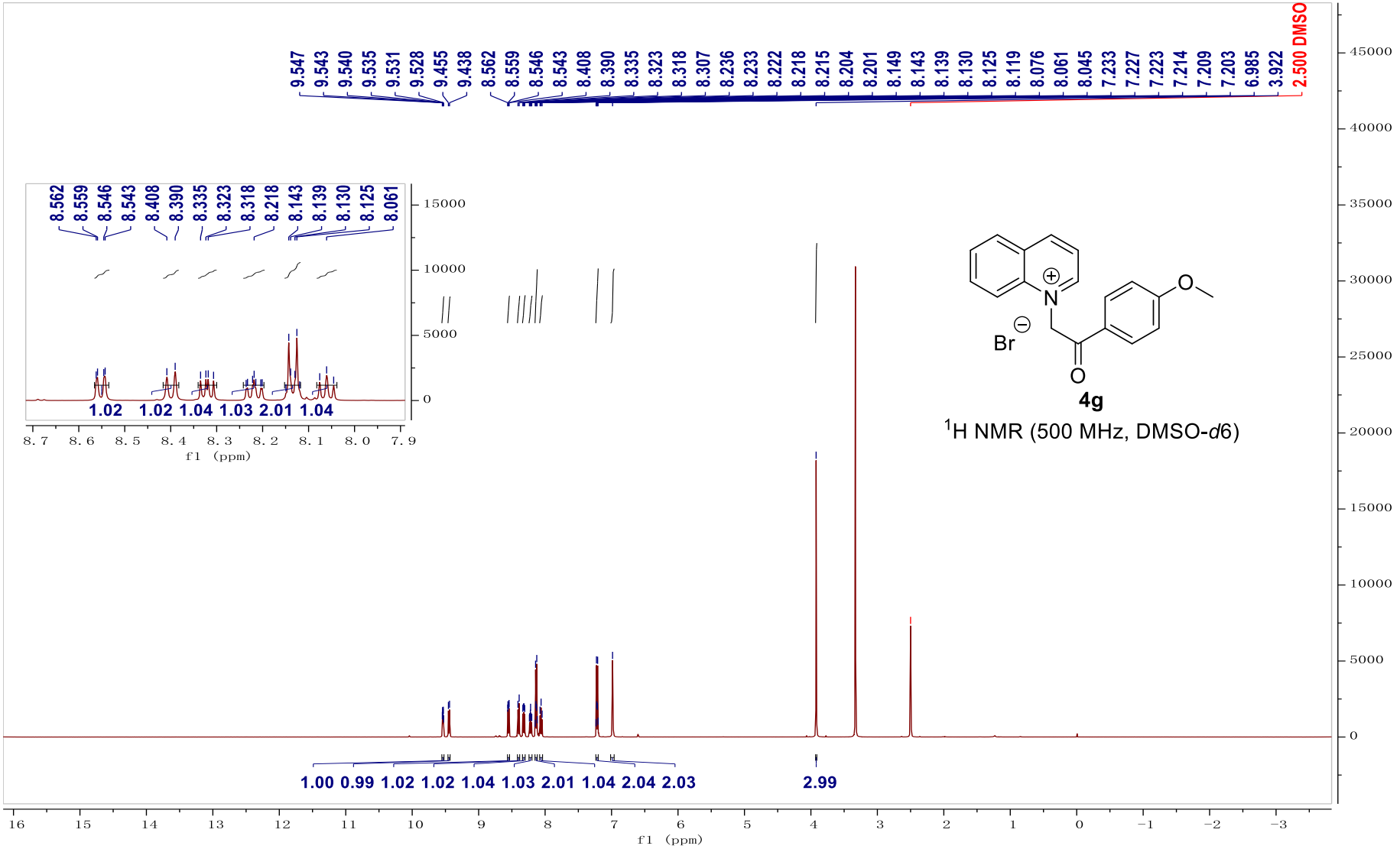

9.560 9.558 9.548 9.546 9.348 9.331 8.379 8.361 8.313 8.296 8.285 8.279 8.268 8.180 8.177 8.174 8.167 8.163 8.160 8.070 8.066 8.051 8.047 7.834 7.832 7.829 7.820 7.817 7.814 7.805 7.802 7.799 7.702 7.687 7.671 7.104 2.597 2.500 DMSO
1.00 1.02 1.00 0.98 1.02 2.04 1.01 1.03 2.06 2.02
3.01
f1 (ppm)
1.00 0.98 1.02 2.04 1.01 1.03 2.06
Br
4b
1H NMR (500 MHz, DMSO-d6)

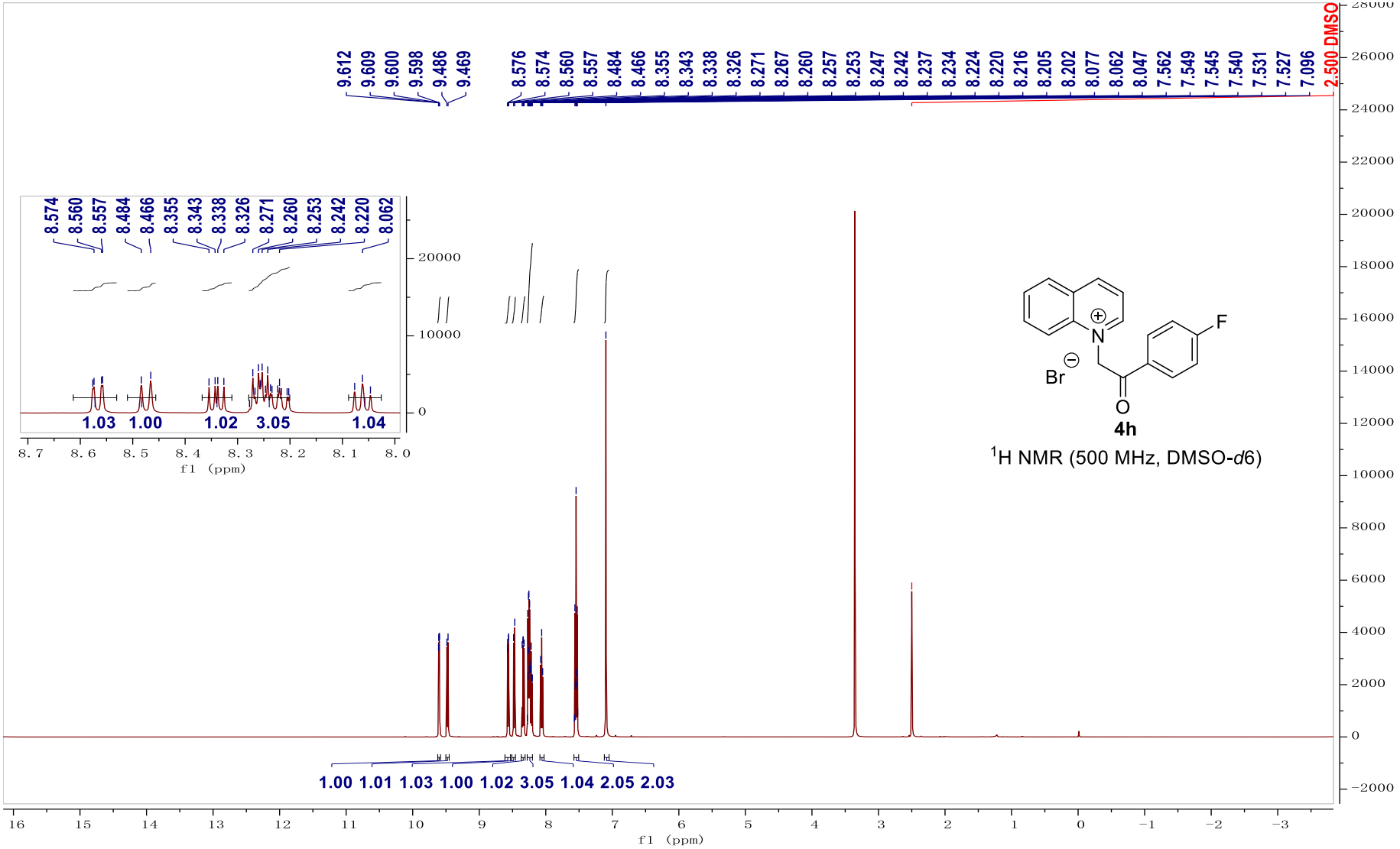

9.537 9.525 8.589 8.587 8.572 8.570 8.429 8.411 8.232 8.219 8.198 8.196 8.188 8.186 8.182 8.177 8.172 8.169 8.167 8.164 8.054 8.038 8.023 7.828 7.825 7.822 7.813 7.810 7.807 7.798 7.795 7.792 7.695 7.680 7.664 7.112 3.075
2.500 DMSO
3.831
8.572 8.429 8.411 8.232 8.219 8.188 8.186 8.182 8.172 8.169 8.167 7.810 7.695 7.680 7.664
0.99 1.00 1.00 3.02 0.99 0.97 1.99
f1 (ppm)
1.00 0.99 1.00 1.00 3.02 0.99 0.97 1.99 1.98
2.99
f1 (ppm)
Br
O
4c
1H NMR (500 MHz, DMSO-d6)

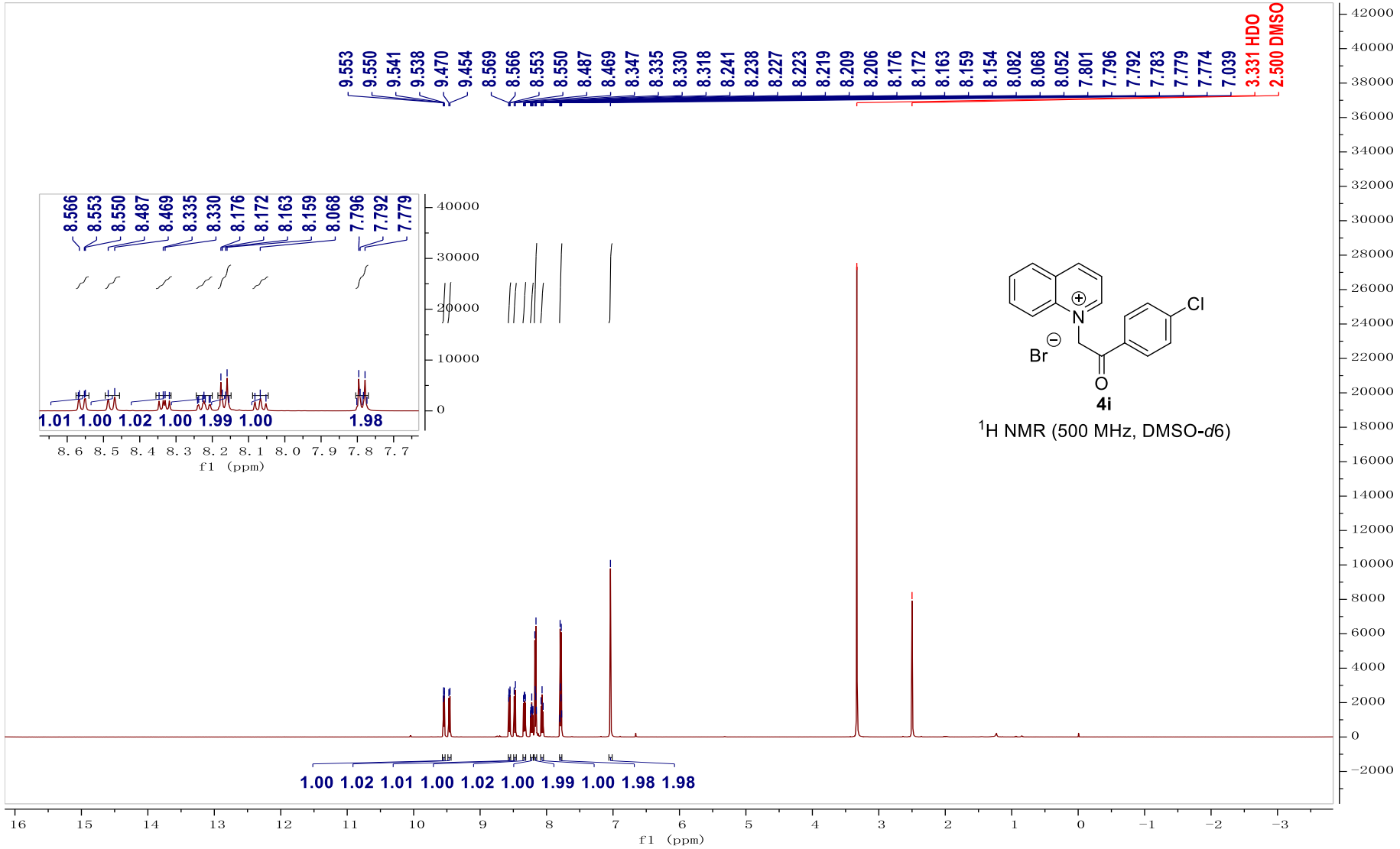

9.647
9.643
9.288
8.443
8.441
8.426
8.424
8.420
8.402
8.182
8.180
8.177
8.170
8.166
8.163
8.149
8.146
8.135
8.132
8.128
8.117
8.114
8.023
8.008
7.993
7.837
7.822
7.819
7.810
7.807
7.708
7.705
7.692
7.680
7.677
7.070
2.668
2.500 DMSO
1.00 1.00 2.02 1.98 1.05 1.00 0.99 1.98 2.03
3.01
f1 (ppm)
2.02
1.98 1.05 1.00
0.99
1.98
Br
N
O
4d
1H NMR (500 MHz, DMSO-d6)

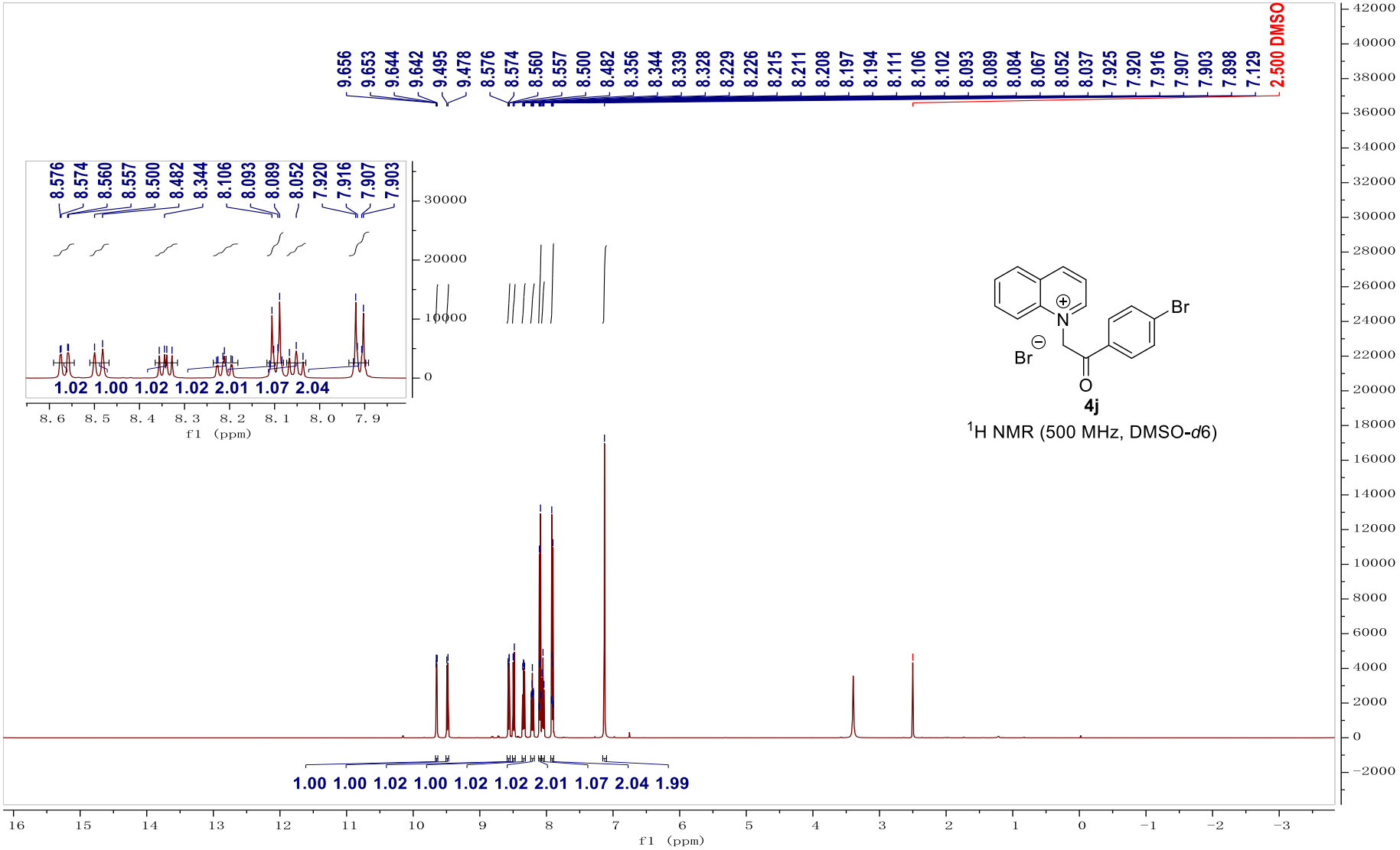

9.624 9.622 9.612 9.610 9.413 9.397 8.754 8.749 8.556 8.537 8.407 8.395 8.390 8.378 8.268 8.263 8.249 8.244 8.160 8.158 8.155 8.148 8.144 8.141 7.837 7.834 7.822 7.819 7.810 7.807 7.805 7.708 7.704 7.692 7.680 7.676 7.088
2.500 DMSO
0.99 0.99 0.98 1.02 1.01 1.01 2.00 1.06 2.03 2.02
f1 (ppm)
0.98 1.02 1.01 1.01 2.00 1.06 2.03
f1 (ppm)
Cl
N
Br
O
4e
1H NMR (500 MHz, DMSO-d6)

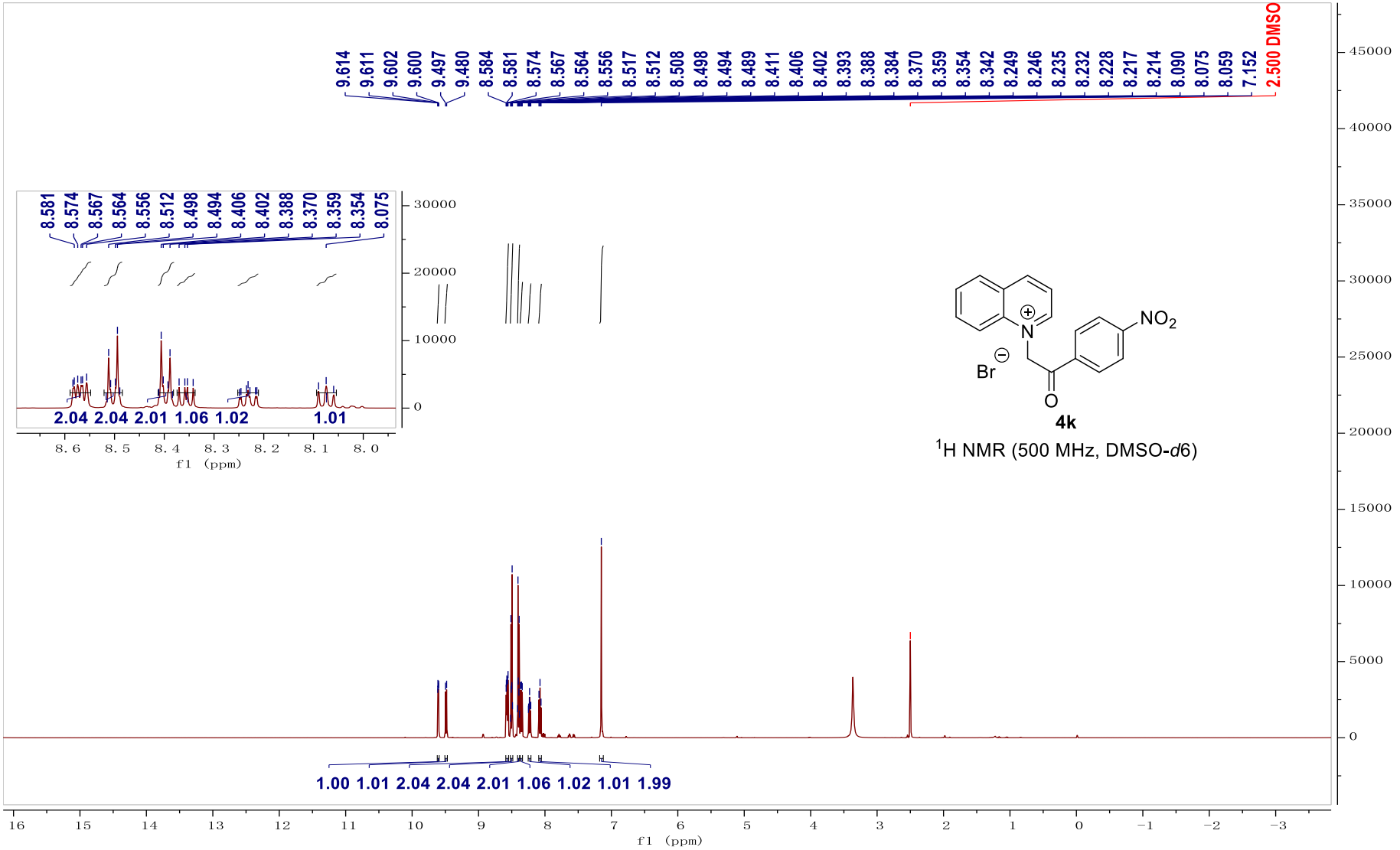

9.583
9.572
9.469
9.452
8.569
8.566
8.552
8.550
8.428
8.410
8.343
8.332
8.327
8.315
8.234
8.231
8.220
8.216
8.213
8.202
8.199
8.076
8.072
8.068
8.062
8.059
8.055
8.051
8.045
7.509
7.493
7.038
2.500 DMSO
2.462
1.00 0.99 1.05 1.04 1.03 0.95 2.99 2.01 1.99
3.04
f1 (ppm)
1.05 1.04 1.03 0.95 2.99
Br
O
4f
1H NMR (500 MHz, DMSO-d6)

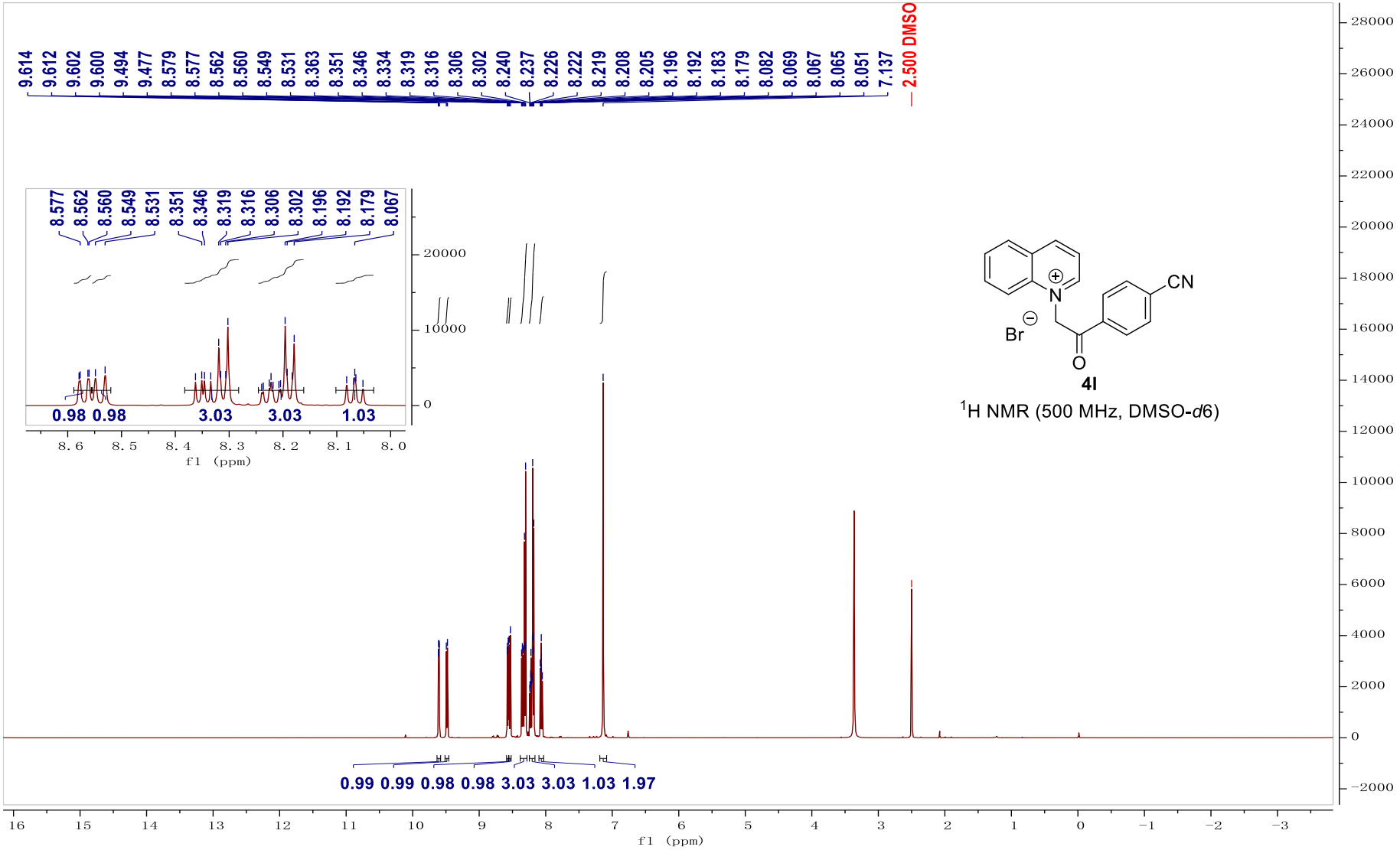

9.547 9.543 9.540 9.535 9.531 9.528 9.455 9.438 8.562 8.559 8.546 8.543 8.408 8.390 8.335 8.323 8.318 8.307 8.236 8.233 8.222 8.218 8.215 8.204 8.201 8.149 8.143 8.139 8.130 8.125 8.119 8.076 8.061 8.045 7.233 7.227 7.223 7.214 7.209 7.203 6.985 3.922 2.500 DMSO
1.00 0.99 1.02 1.02 1.04 1.03 2.01 1.04 2.04 2.03
2.99
f1 (ppm)
1.02 1.02 1.04 1.03 2.01 1.04
Br
O
4g
1H NMR (500 MHz, DMSO-d6)

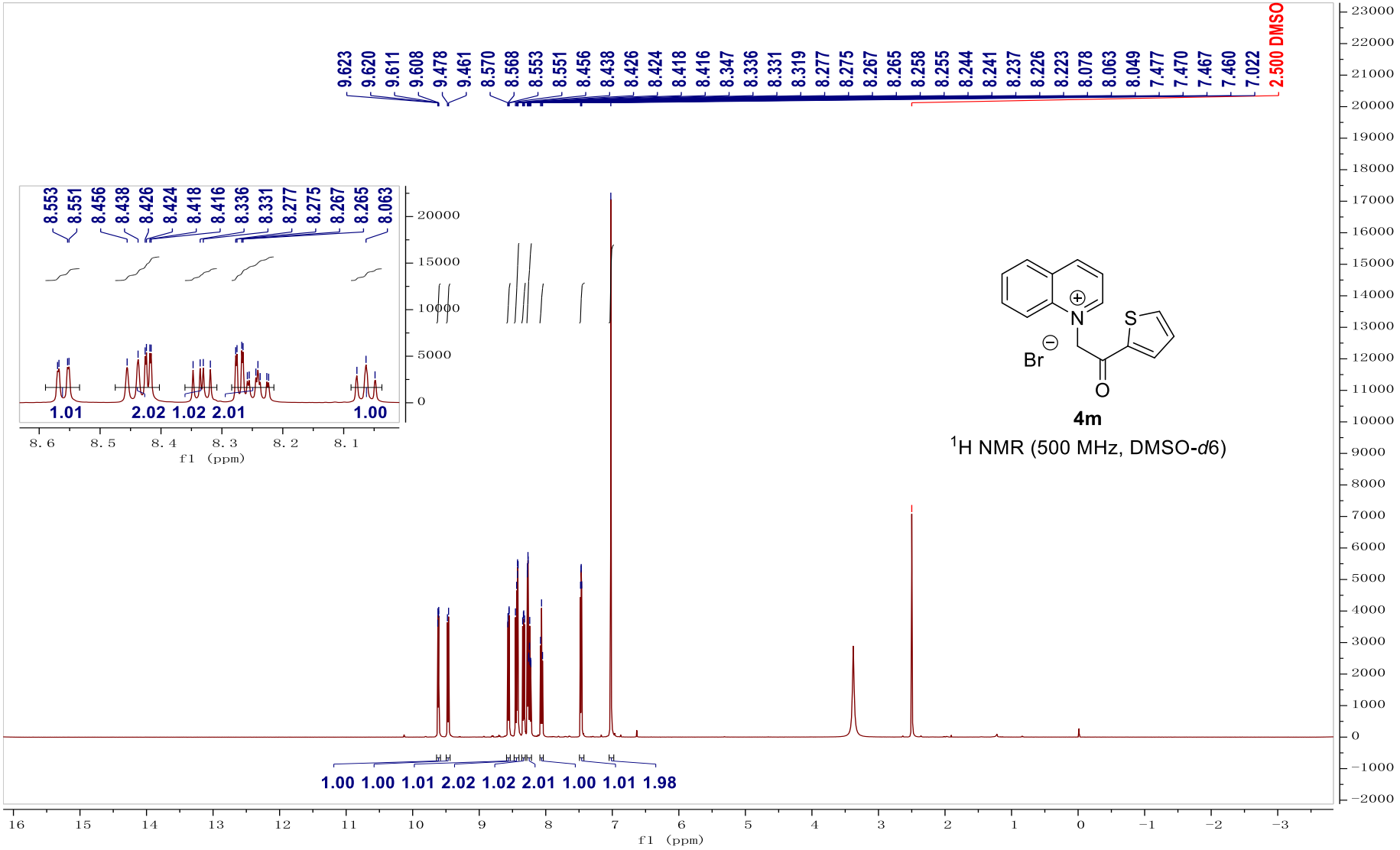

9.612 9.609 9.600 9.598 9.486 9.469
8.576 8.574 8.560 8.557 8.484 8.466 8.355 8.343 8.338 8.326 8.271 8.267 8.260 8.257 8.253 8.247 8.242 8.237 8.234 8.224 8.220 8.216 8.205 8.202 8.077 8.062 8.047 7.562 7.549 7.545 7.540 7.531 7.527 7.096
2.500 DMSO
1.00 1.01 1.03 1.00 1.02 3.05 1.04 2.05 2.03
f1 (ppm)
8.574 8.560 8.557 8.484 8.466 8.355 8.343 8.338 8.326 8.271 8.260 8.253 8.242 8.220 8.062
1.03 1.00 1.02 3.05 1.04
f1 (ppm)
Br
N
O
F
4h
1H NMR (500 MHz, DMSO-d6)

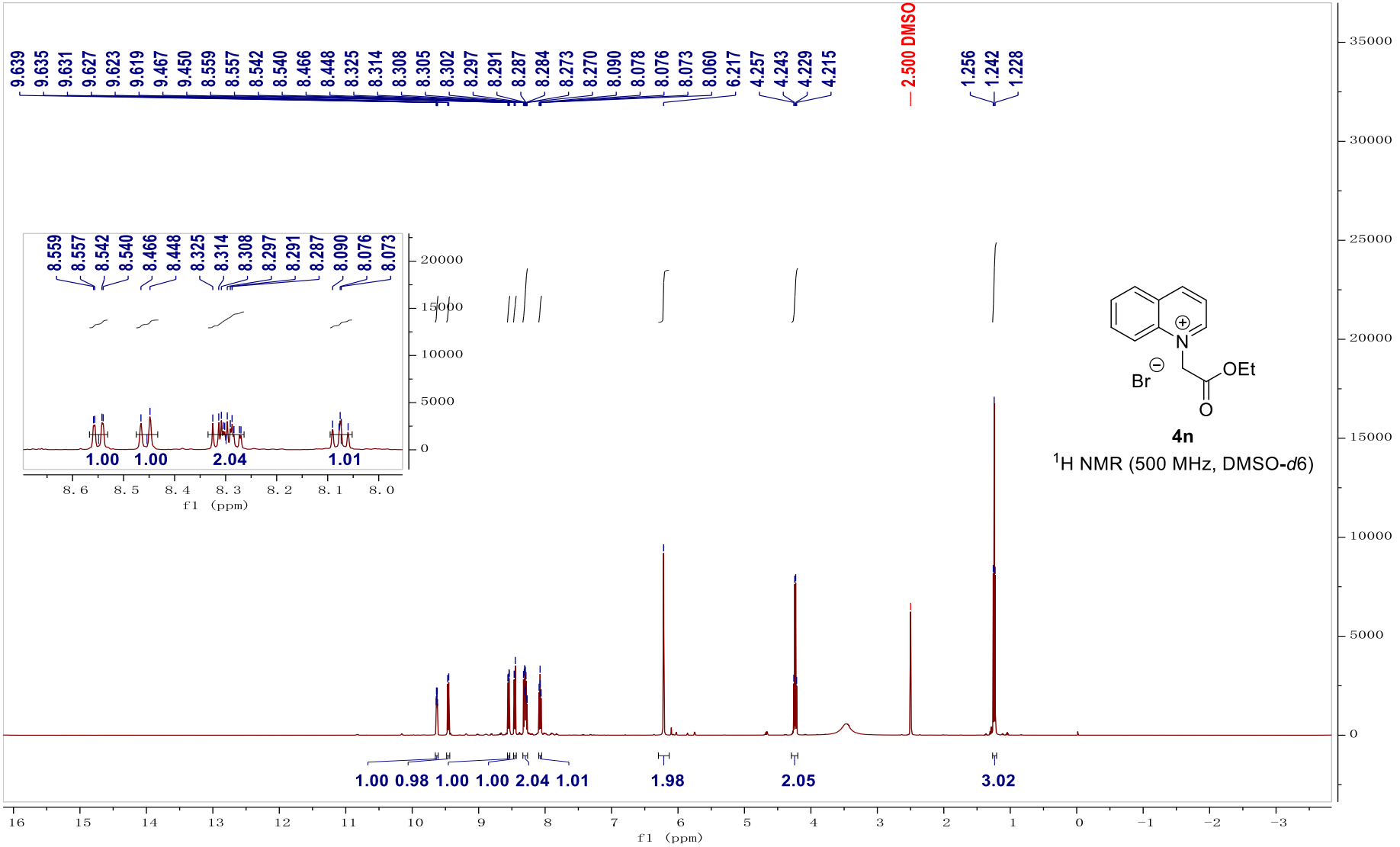

9.553
9.550
9.541
9.538
9.470
9.454
8.569
8.566
8.553
8.550
8.487
8.469
8.347
8.335
8.330
8.318
8.241
8.238
8.227
8.223
8.219
8.209
8.206
8.176
8.172
8.163
8.159
8.154
8.082
8.068
8.052
7.801
7.796
7.792
7.783
7.779
7.774
7.039
3.331 HDO
2.500 DMSO
1.00 1.02 1.01 1.00 1.02 1.00 1.99 1.00 1.98 1.98
f1 (ppm)
1.01 1.00 1.02 1.00 1.99 1.00
1.98
Br
N
O
Cl
4i
1H NMR (500 MHz, DMSO-d6)

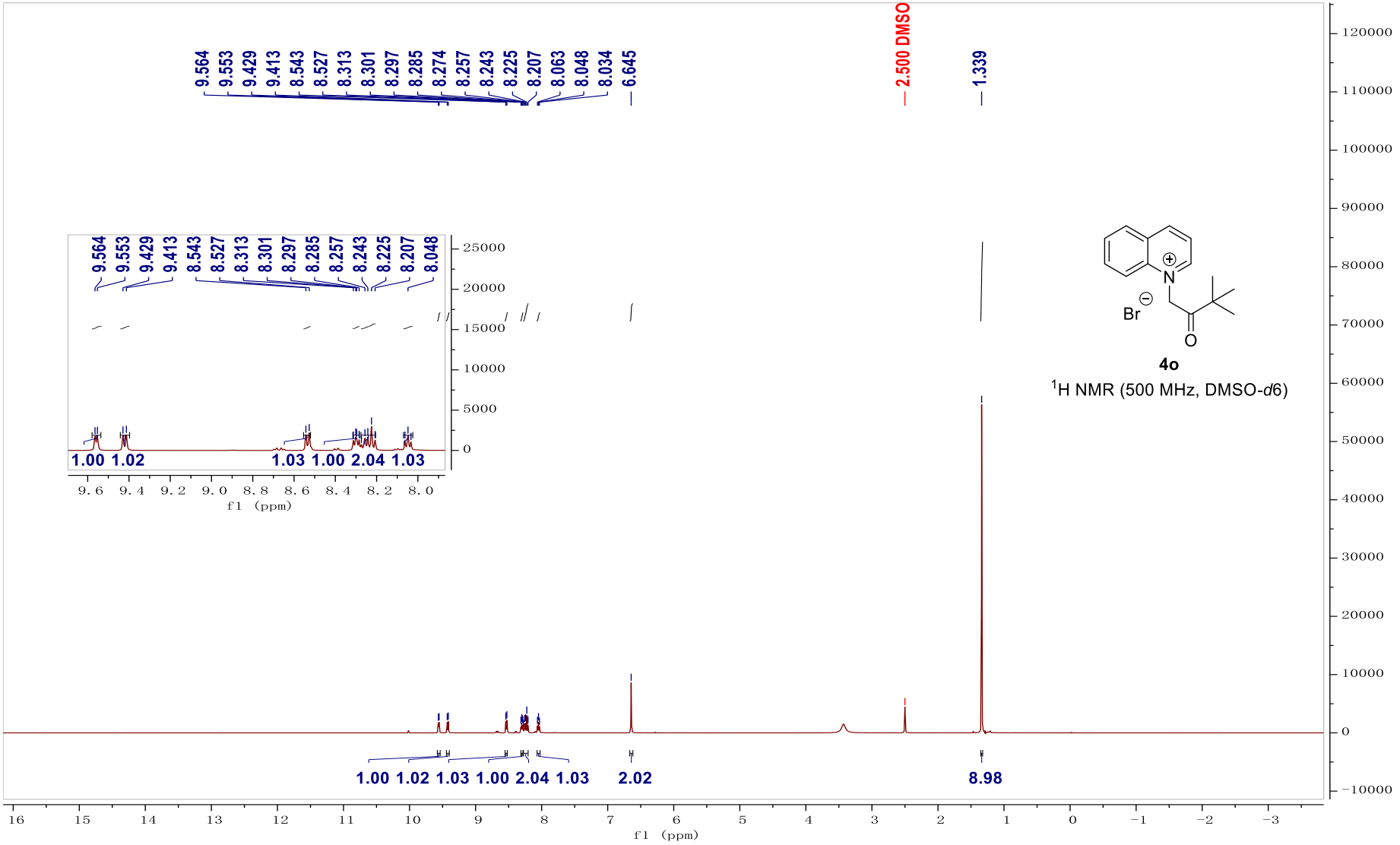

9.656 9.653 9.644 9.642 9.495 9.478 8.576 8.574 8.560 8.557 8.500 8.482 8.356 8.344 8.339 8.328 8.229 8.226 8.215 8.211 8.208 8.197 8.194 8.111 8.106 8.102 8.093 8.089 8.084 8.067 8.052 8.037 7.925 7.920 7.916 7.907 7.903 7.898 7.129 2.500 DMSO
1.00 1.00 1.02 1.00 1.02 1.02 2.01 1.07 2.04 1.99
f1 (ppm)
1.02 1.00 1.02 1.02 2.01 1.07 2.04
f1 (ppm)
Br
Br
O
4j
1H NMR (500 MHz, DMSO-d6)

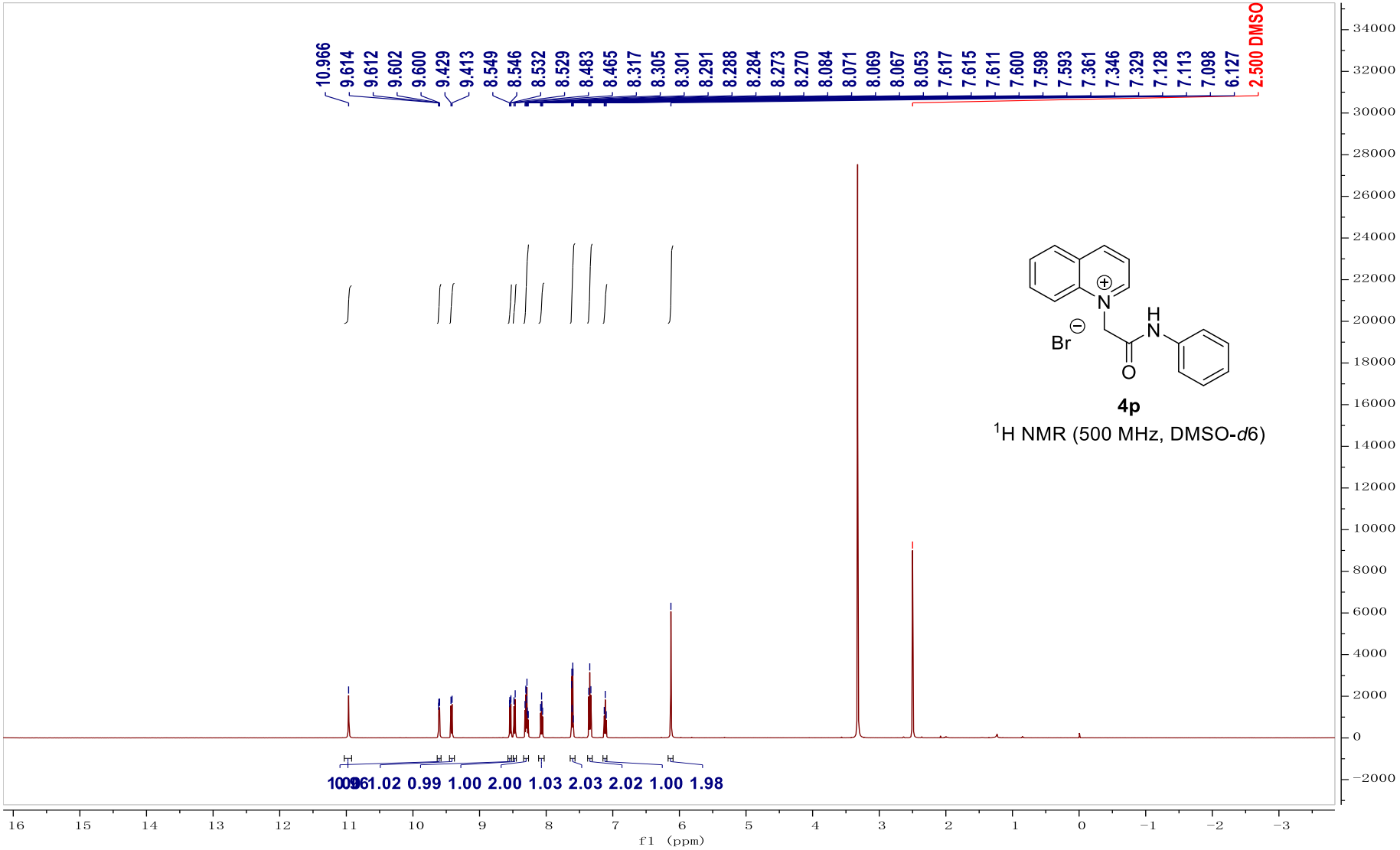

9.614 9.611 9.602 9.600 9.497 9.480 8.584 8.581 8.574 8.567 8.564 8.556 8.517 8.512 8.508 8.498 8.494 8.489 8.411 8.406 8.402 8.393 8.388 8.384 8.370 8.359 8.354 8.342 8.249 8.246 8.235 8.232 8.228 8.217 8.214 8.090 8.075 8.059 7.152 2.500 DMSO
8.581 8.574 8.567 8.564 8.556 8.512 8.498 8.494 8.406 8.402 8.388 8.370 8.359 8.354 8.075
2.04 2.04 2.01 1.06 1.02 1.01
f1 (ppm)
NO2
N
Br
O
4k
1H NMR (500 MHz, DMSO-d6)
1.00 1.01 2.04 2.04 2.01 1.06 1.02 1.01 1.99
f1 (ppm)

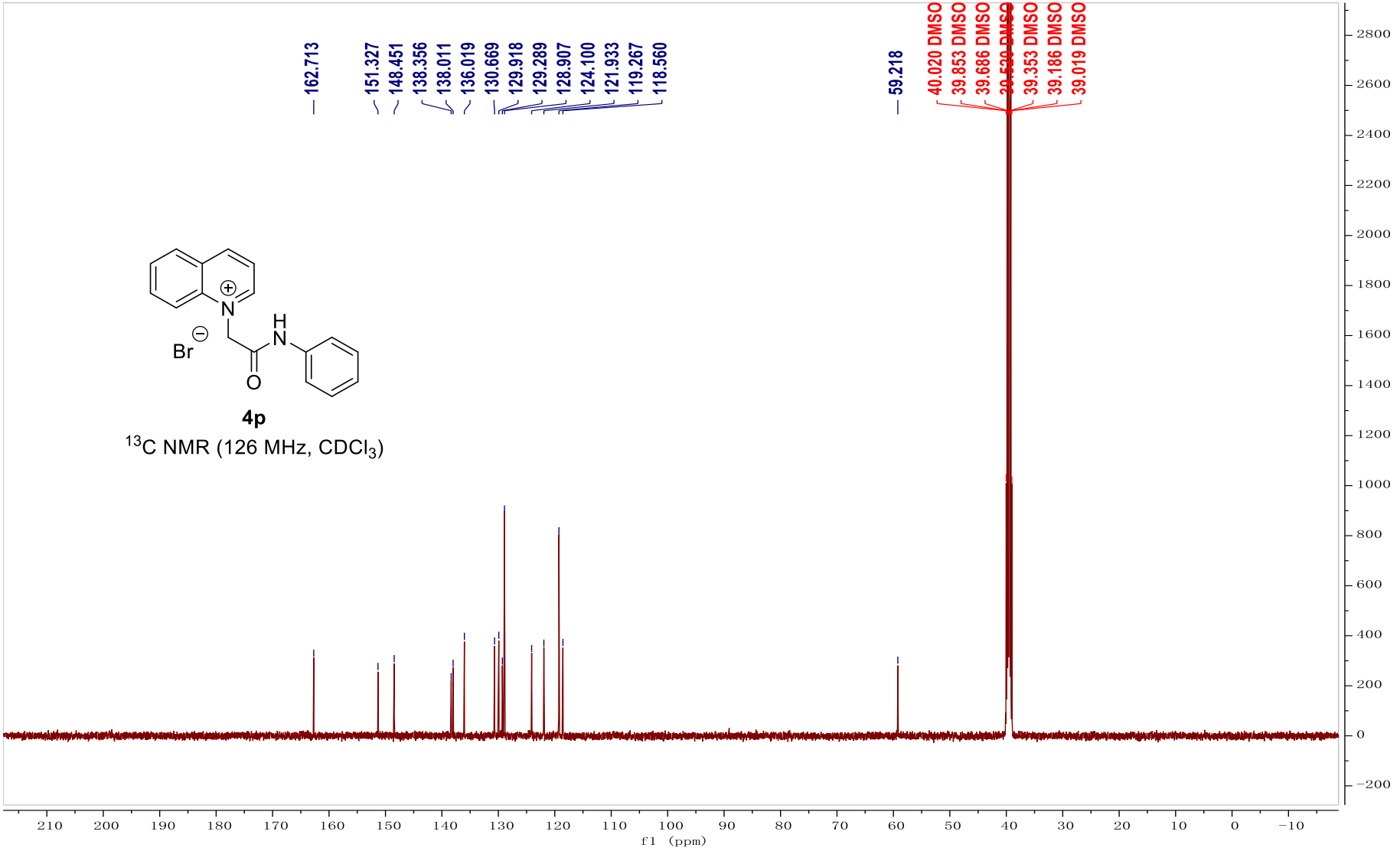

9.614 9.612 9.602 9.600 9.494 9.477 8.579 8.577 8.562 8.560 8.549 8.531 8.363 8.351 8.346 8.334 8.319 8.316 8.306 8.302 8.240 8.237 8.226 8.222 8.219 8.208 8.205 8.196 8.192 8.183 8.179 8.082 8.069 8.067 8.065 8.051 7.137
2.500 DMSO
8.577 8.562 8.560 8.549 8.531 8.351 8.346 8.319 8.316 8.306 8.302 8.196 8.192 8.179 8.067
0.98 0.98 3.03 3.03 1.03
f1 (ppm)
0.99 0.99 0.98 0.98 3.03 3.03 1.03 1.97
f1 (ppm)
CN
N
Br
O
4l
1H NMR (500 MHz, DMSO-d6)

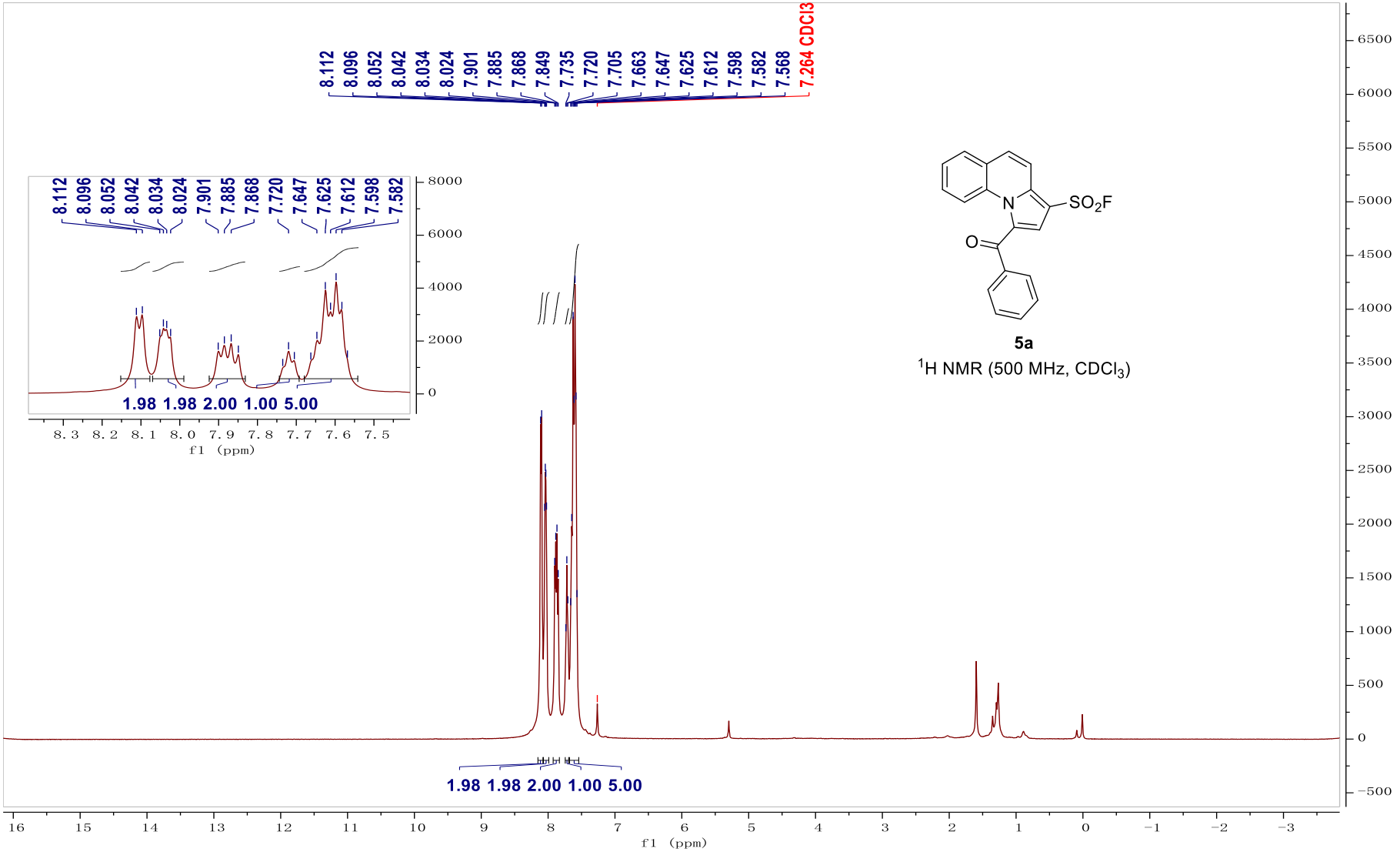

9.623 9.620 9.611 9.608 9.478 9.461 8.570 8.568 8.553 8.551 8.456 8.438 8.426 8.424 8.418 8.416 8.347 8.336 8.331 8.319 8.277 8.275 8.267 8.265 8.258 8.255 8.244 8.241 8.237 8.226 8.223 8.078 8.063 8.049 7.477 7.470 7.467 7.460 7.022 2.500 DMSO
8.553 8.551 8.456 8.438 8.426 8.424 8.418 8.416 8.336 8.331 8.277 8.275 8.267 8.265 8.063
1.01 2.02 1.02 2.01 1.00
f1 (ppm)
1.00 1.00 1.01 2.02 1.02 2.01 1.00 1.01 1.98
f1 (ppm)
Br
N
S
O
4m
1H NMR (500 MHz, DMSO-d6)

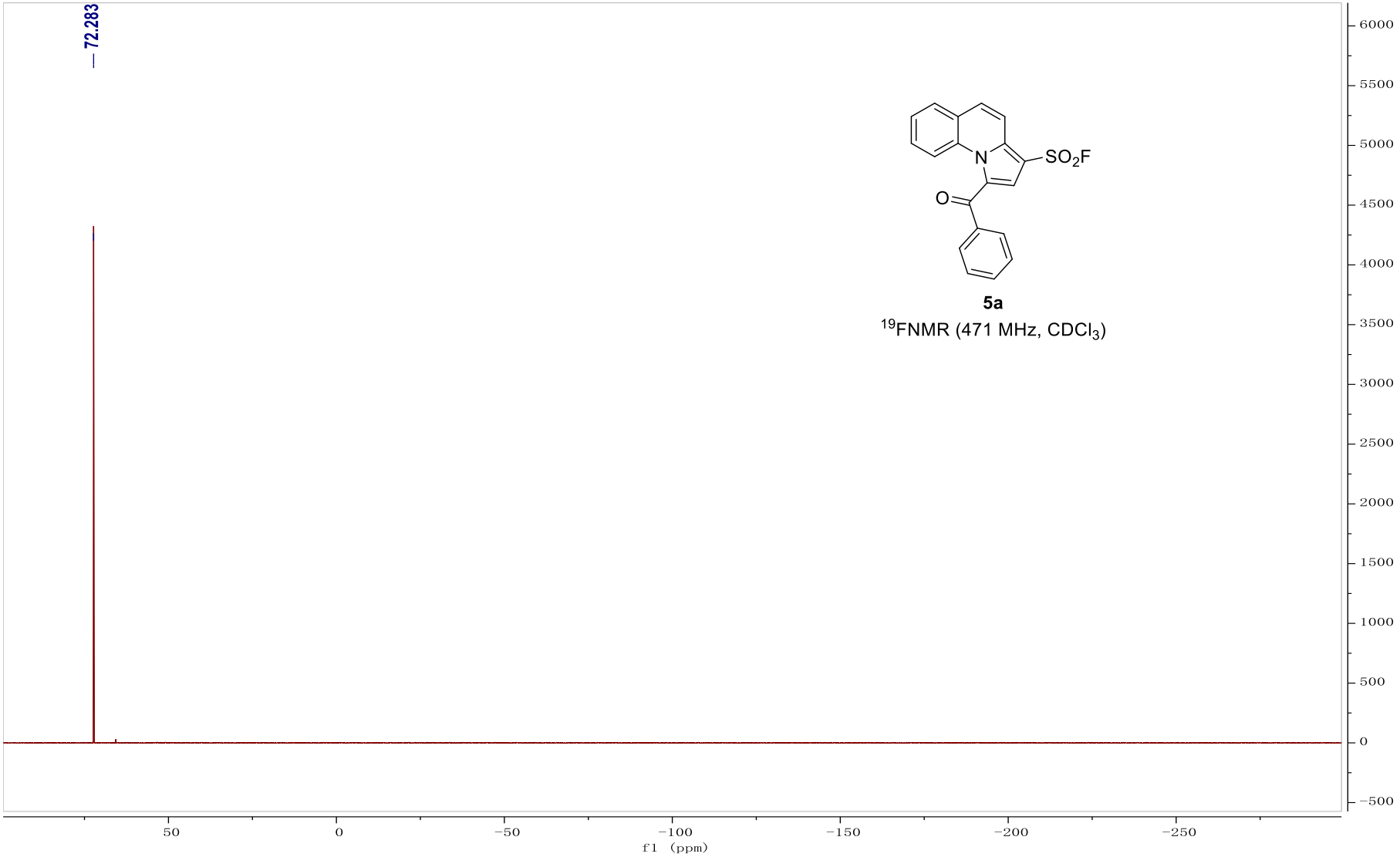

9.639 9.635 9.631 9.627 9.623 9.619 9.467 9.450 9.559 9.557 9.542 9.540 9.466 9.448 8.325 8.314 8.308 8.305 8.302 8.297 8.291 8.287 8.284 8.273 8.270 8.090 8.078 8.076 8.073 8.060 6.217 4.257 4.243 4.229 4.215
2.500 DMSO
1.256 1.242 1.228
1.00 0.98 1.00 1.00 2.04 1.01
1.98
2.05
3.02
f1 (ppm)
1.00 1.00 2.04 1.01
4n
1H NMR (500 MHz, DMSO-d6)

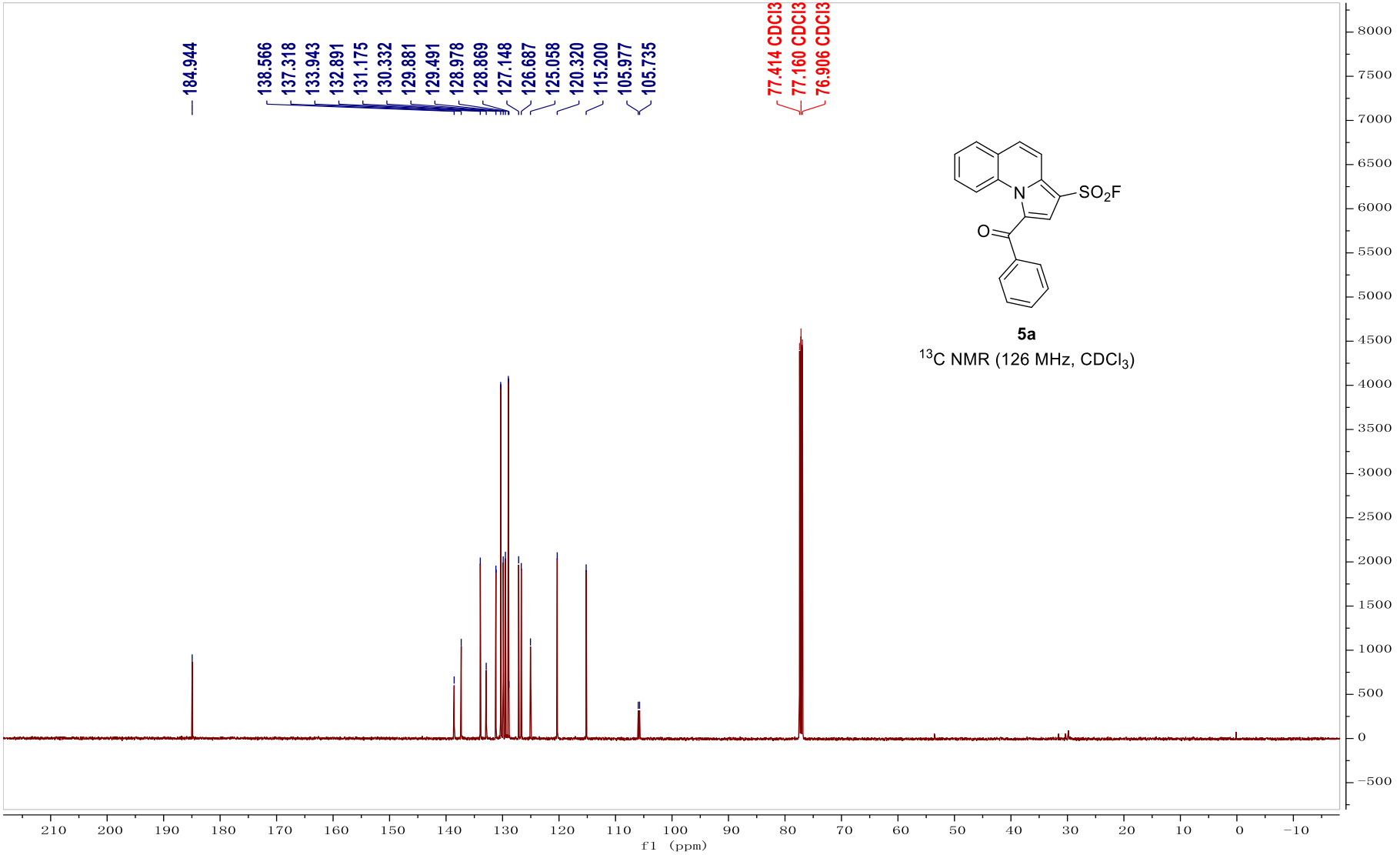

9.564
9.553
9.429
9.413
8.543
8.527
8.313
8.301
8.297
8.285
8.274
8.257
8.243
8.225
8.207
8.063
8.048
8.034
6.645
2.500 DMSO
1.339
1.00 1.02 1.03 1.00 2.04 1.03
2.02
8.98
f1 (ppm)
Br
O
4o
1H NMR (500 MHz, DMSO-d6)

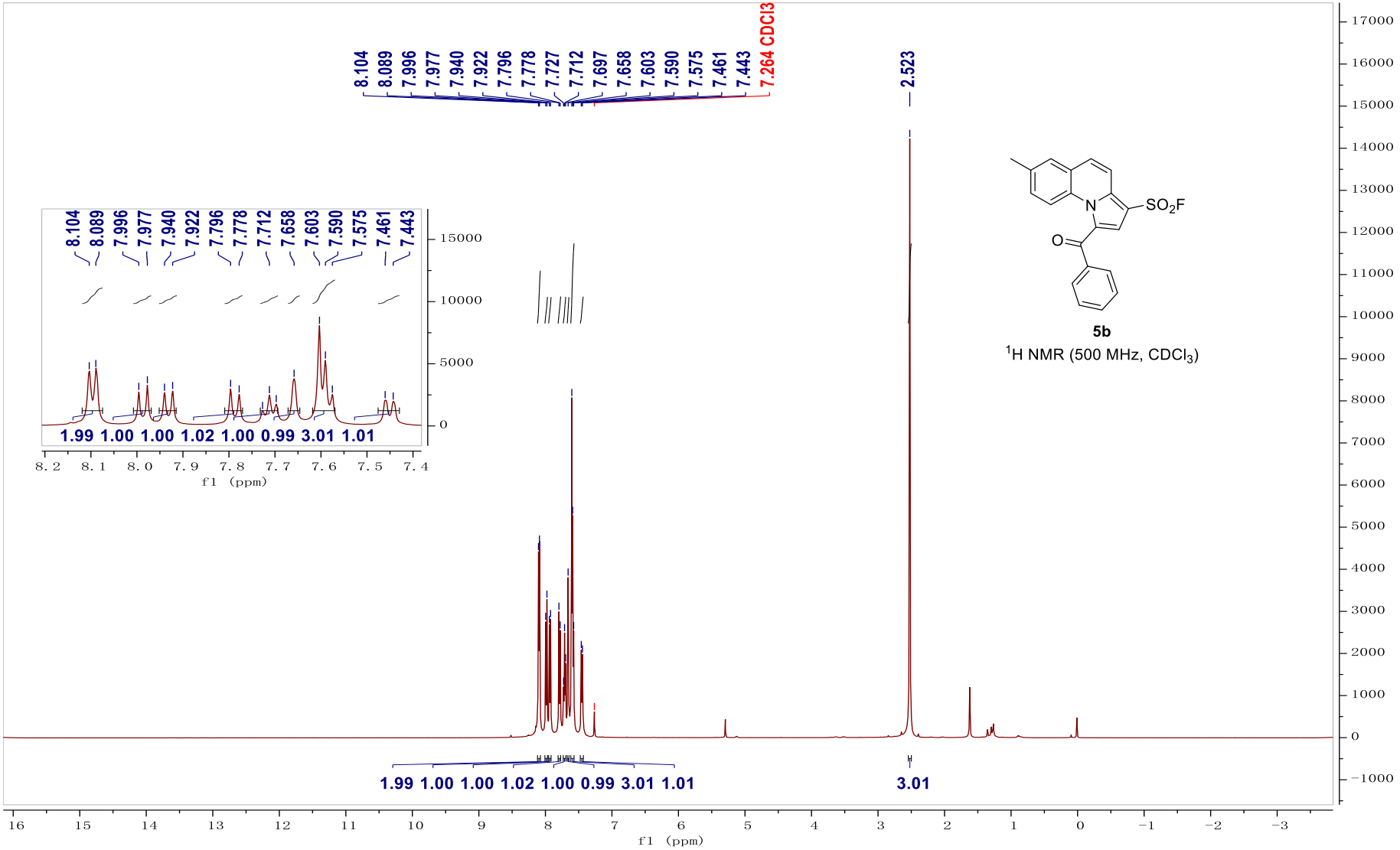

10.966
9.614
9.612
9.602
9.600
9.429
9.413
8.549
8.546
8.532
8.529
8.483
8.465
8.317
8.305
8.301
8.291
8.288
8.284
8.273
8.270
8.084
8.071
8.069
8.067
8.053
7.617
7.615
7.611
7.600
7.598
7.593
7.361
7.346
7.329
7.128
7.113
7.098
6.127
2.500 DMSO
1.00 0.96 1.02 0.99 1.00 2.00 1.03 2.03 2.02 1.00 1.98
Br
N
H
N
O
4p
1H NMR (500 MHz, DMSO-d6)
f1 (ppm)

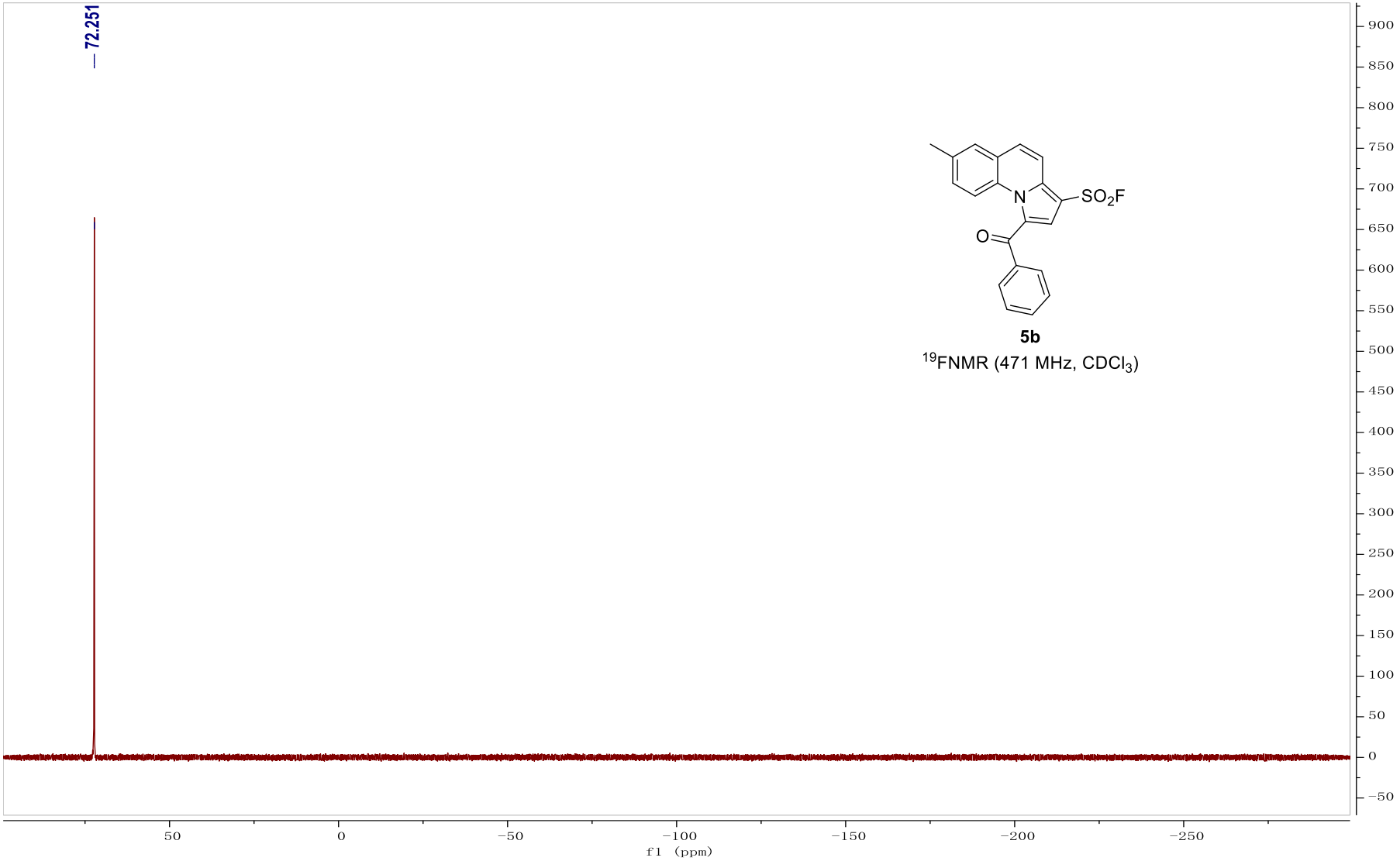

162.713
151.327
148.451
138.356
138.011
136.019
130.669
129.918
129.289
128.907
124.100
121.933
119.267
118.560
59.218
40.020 DMSO
39.853 DMSO
39.686 DMSO
39.520 DMSO
39.353 DMSO
39.186 DMSO
39.019 DMSO
Br
N
H
N
O
4p
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.112
8.096
8.052
8.042
8.034
8.024
7.901
7.885
7.868
7.849
7.735
7.720
7.705
7.663
7.647
7.625
7.612
7.598
7.582
7.568
7.264 CDCl3
1.98 1.98 2.00 1.00 5.00
f1 (ppm)
N
SO2F
O
5a
1H NMR (500 MHz, CDCl3)


72.283
N
SO2F
O
5a
19FNMR (471 MHz, CDCl3)
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
50
0
−50
−100
−150
−200
−250
f1 (ppm)

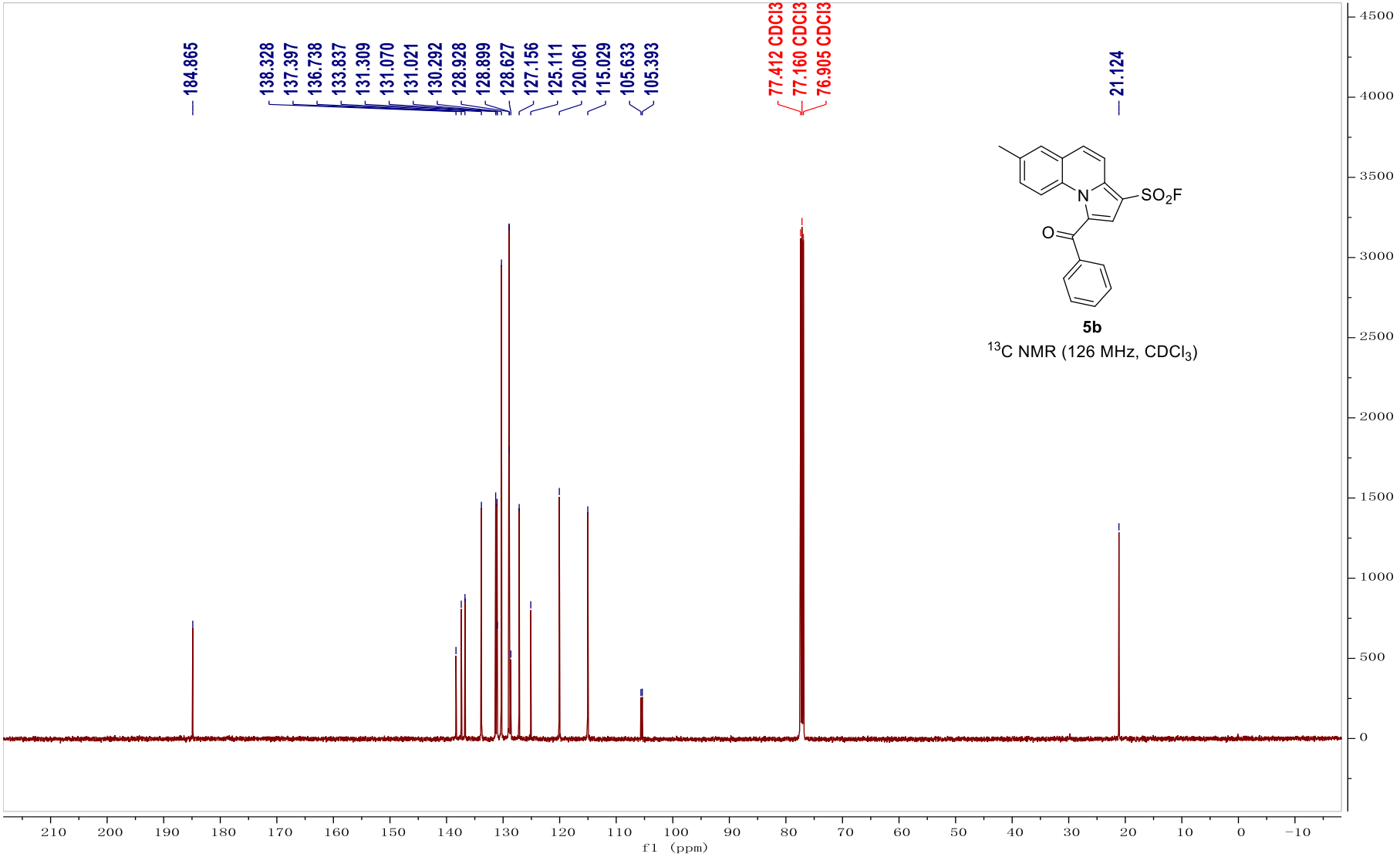

184.944
138.566
137.318
133.943
132.891
131.175
130.332
129.881
129.491
128.978
128.869
127.148
126.687
125.058
120.320
115.200
105.977
105.735
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
N
SO2F
O
5a
13C NMR (126 MHz, CDCl3)
f1 (ppm)

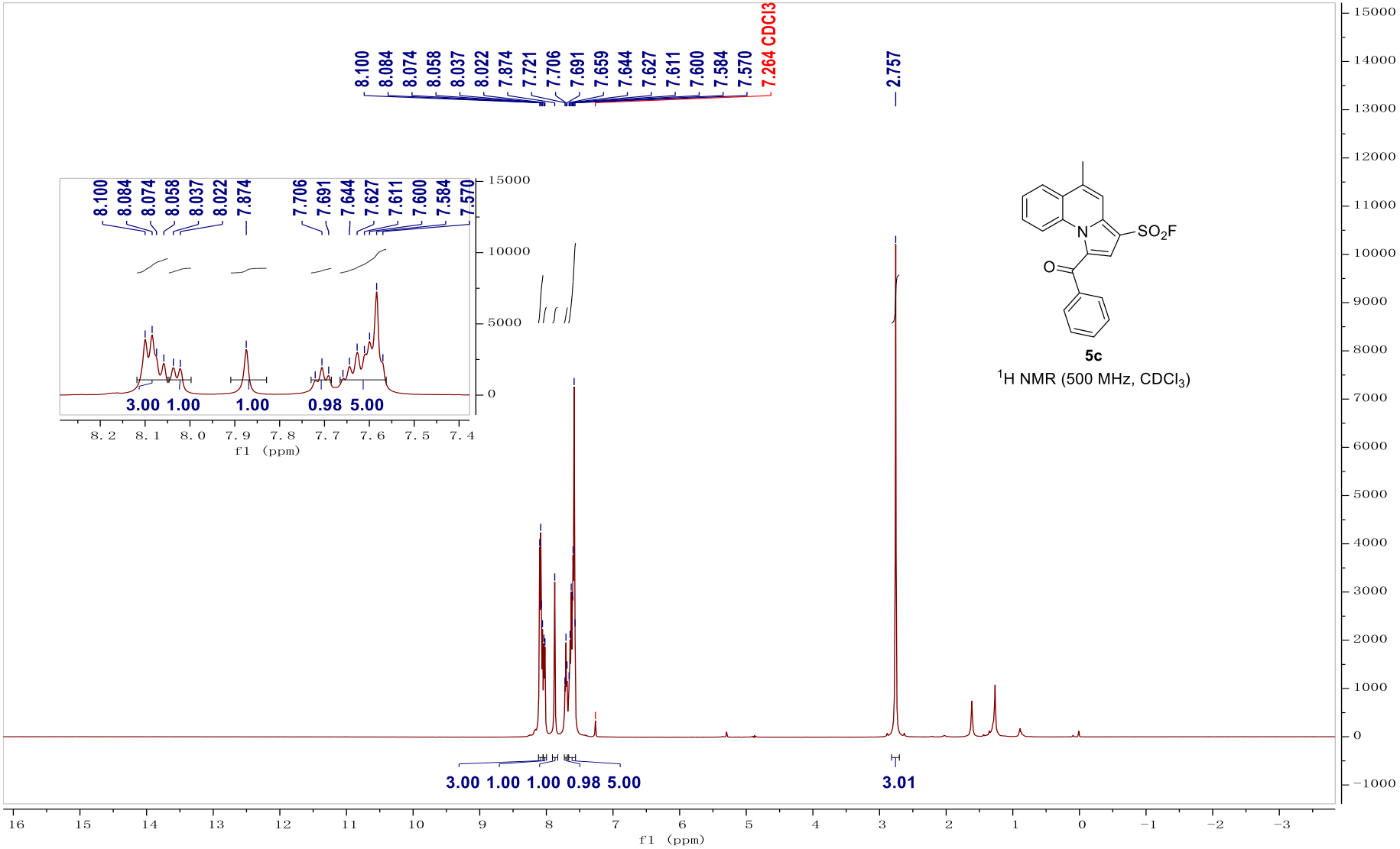

8.104
8.089
7.996
7.977
7.940
7.922
7.796
7.778
7.727
7.712
7.697
7.658
7.603
7.590
7.575
7.461
7.443
7.264 CDCl3
2.523
1.99 1.00 1.00 1.02 1.00 0.99 3.01 1.01
3.01
f1 (ppm)
N
SO2F
O
5b
1H NMR (500 MHz, CDCl3)

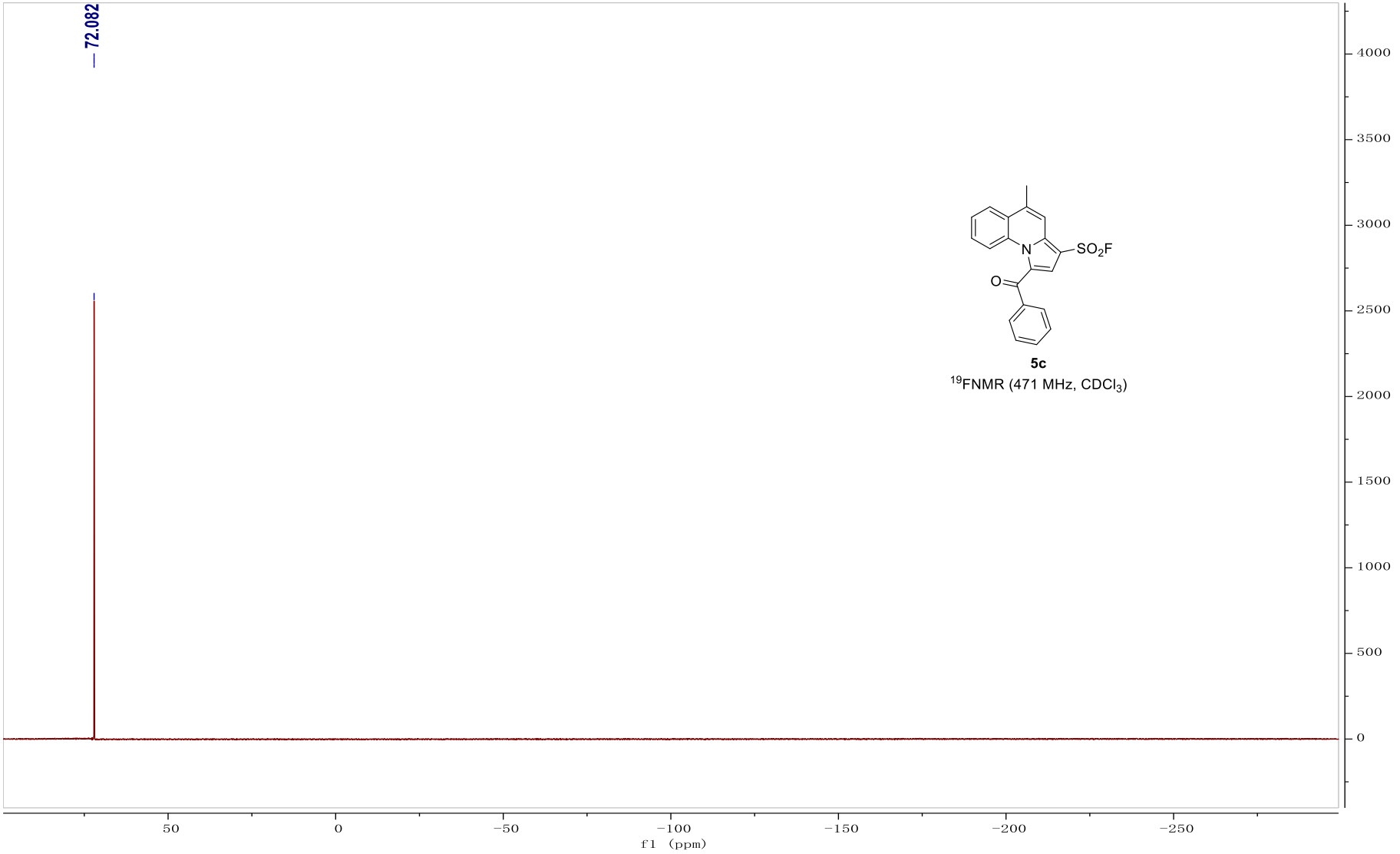


5b

^{19}FNMR (471 MHz, $CDCl_3$)

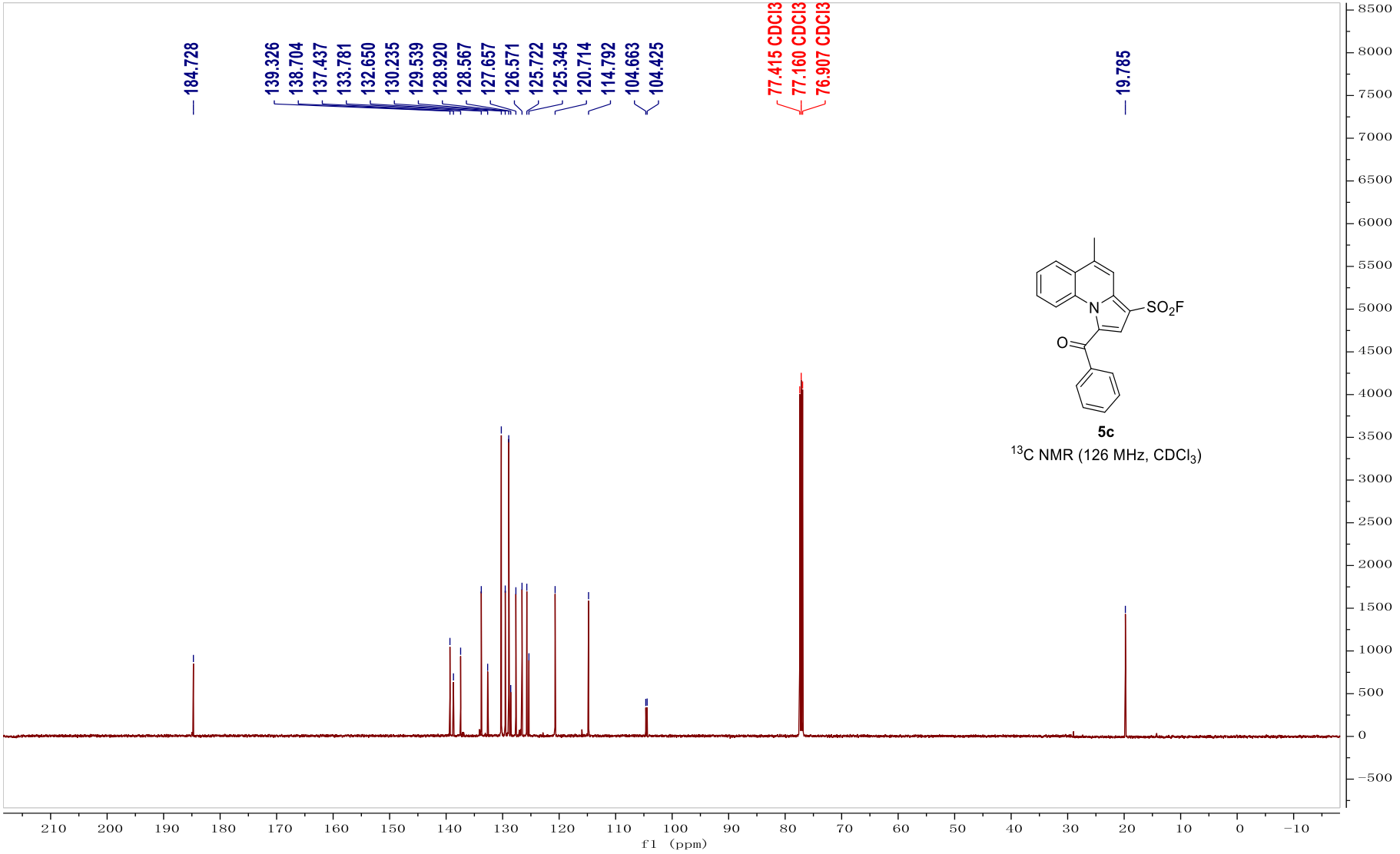

184.865
138.328
137.397
136.738
133.837
131.309
131.070
131.021
130.292
128.928
128.899
128.627
127.156
125.111
120.061
115.029
105.633
105.393
77.412 CDCl3
77.160 CDCl3
76.905 CDCl3
21.124
N
SO2F
O
5b
13C NMR (126 MHz, CDCl3)
f1 (ppm)

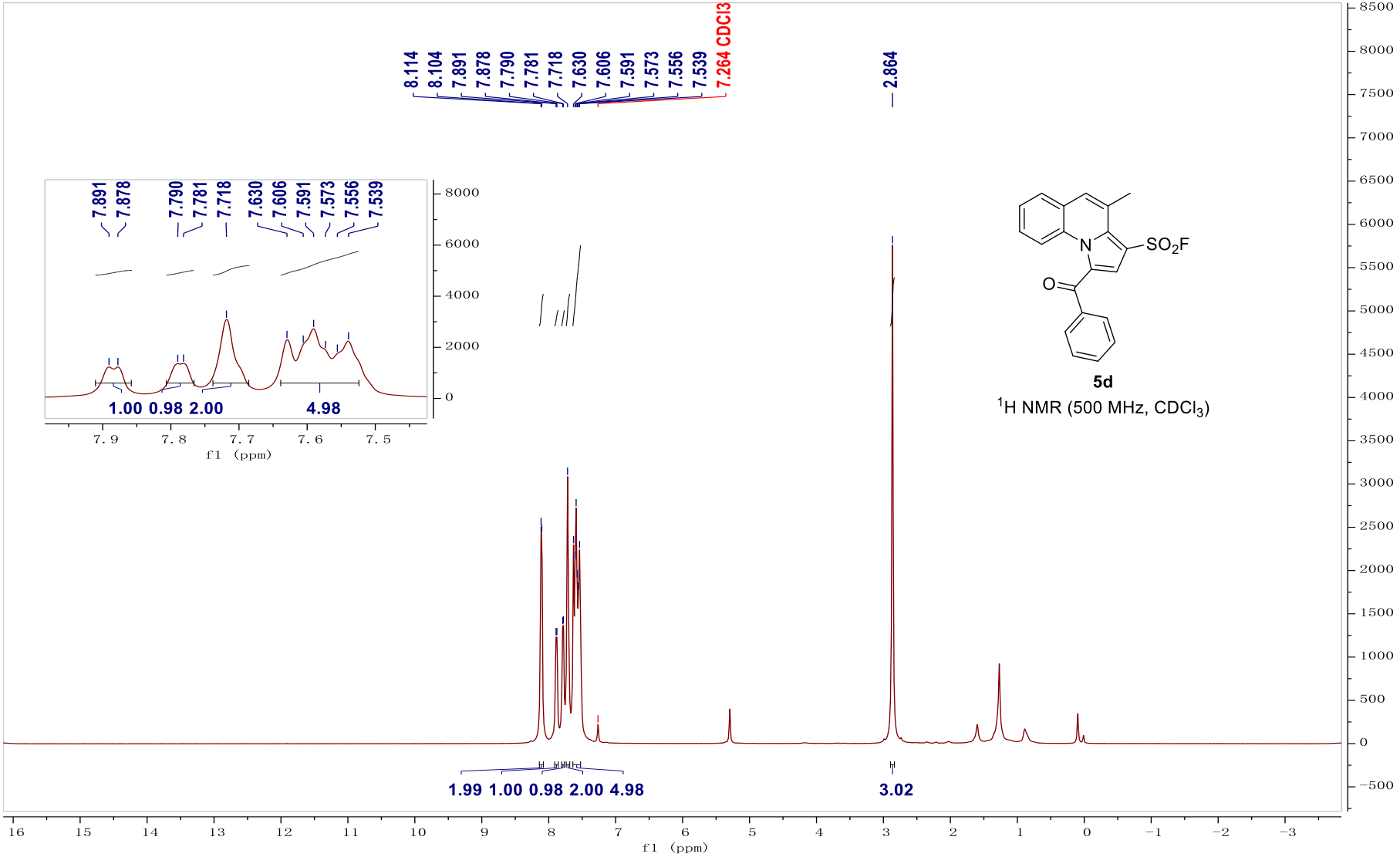

8.100
8.084
8.074
8.058
8.037
8.022
7.874
7.721
7.706
7.691
7.659
7.644
7.627
7.611
7.600
7.584
7.570
7.264 CDCl3
2.757
3.00 1.00 1.00 0.98 5.00
3.01
f1 (ppm)
3.00 1.00 1.00 0.98 5.00
f1 (ppm)
SO2F
N
O
5c
1H NMR (500 MHz, CDCl3)

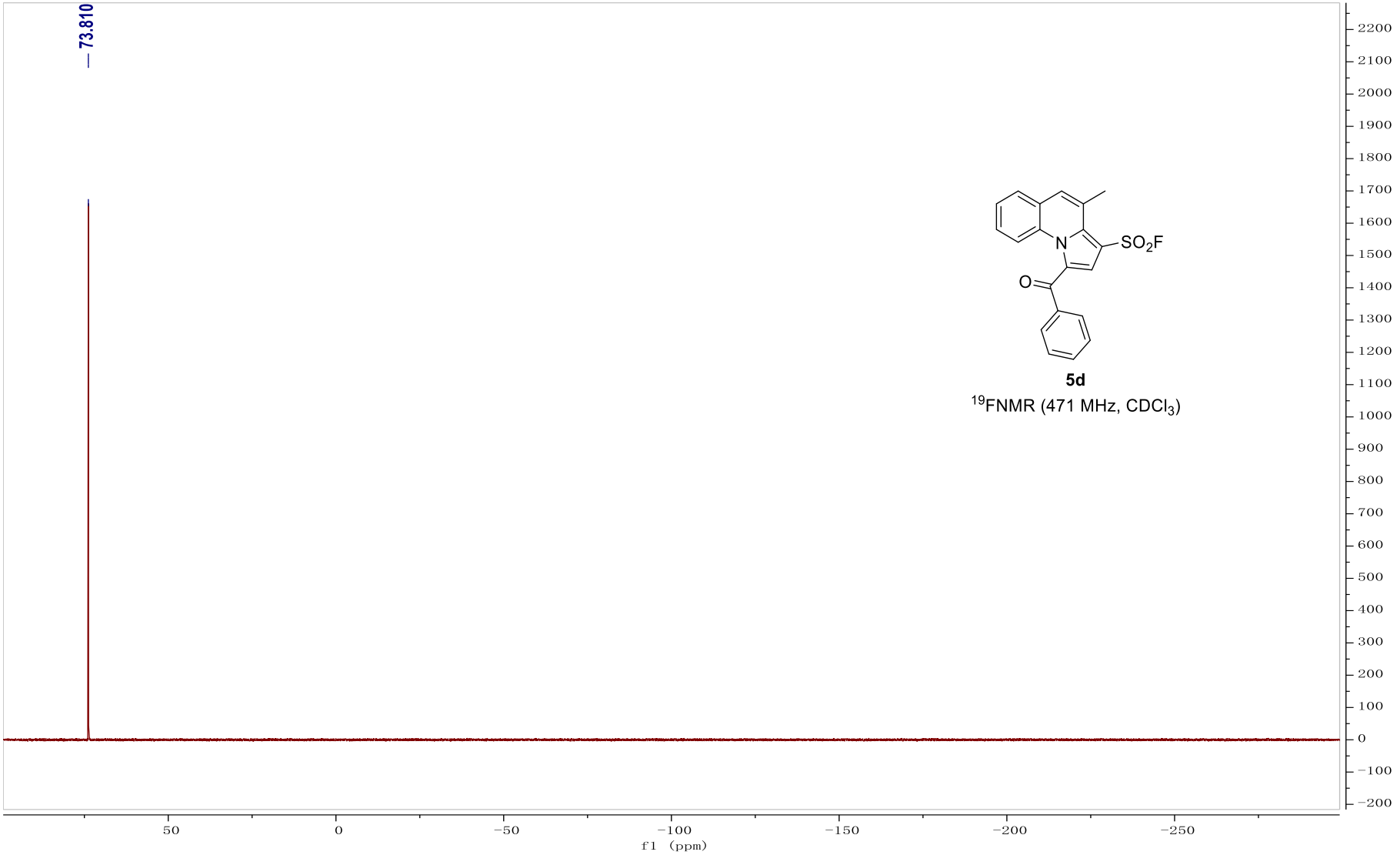


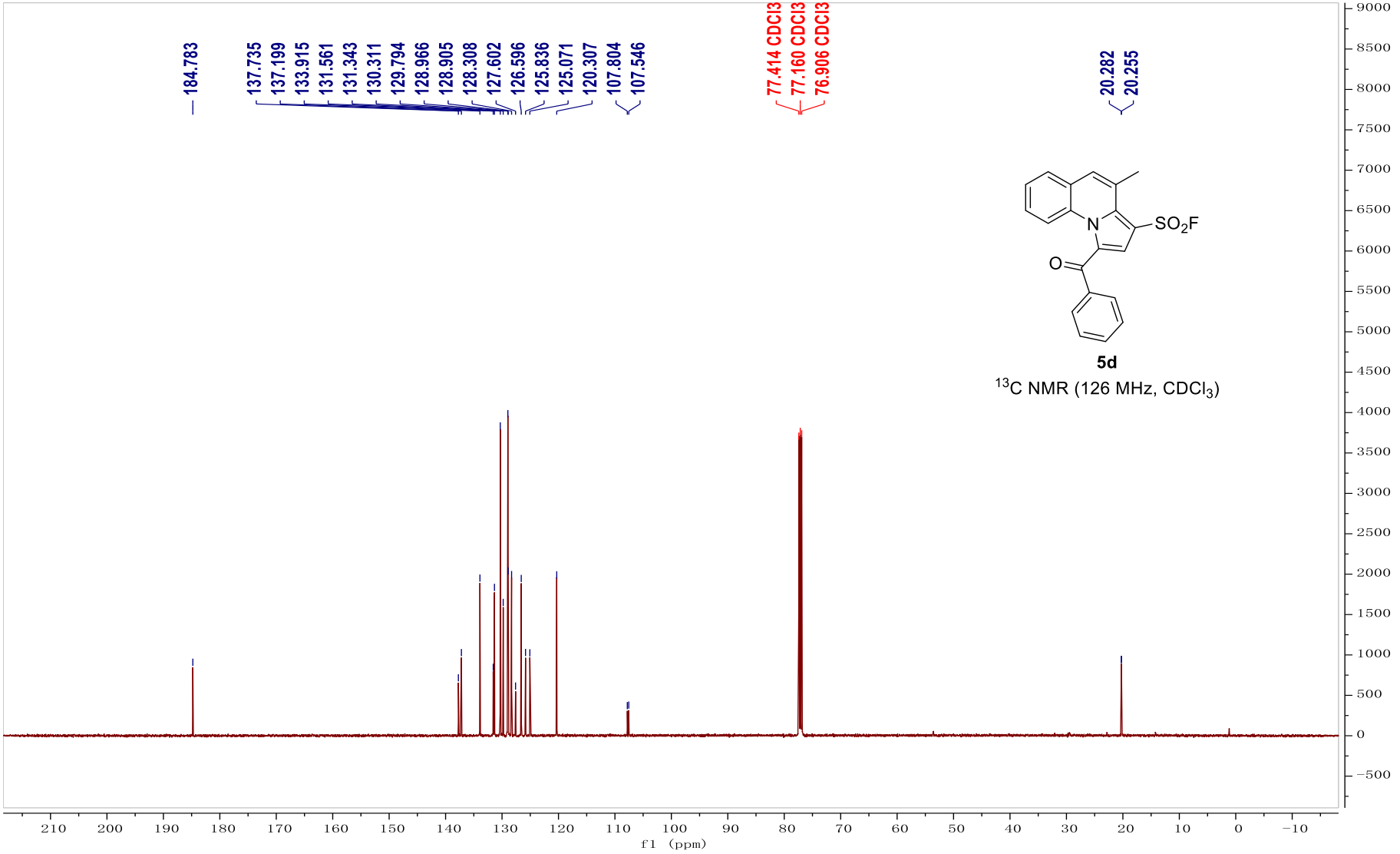
5c

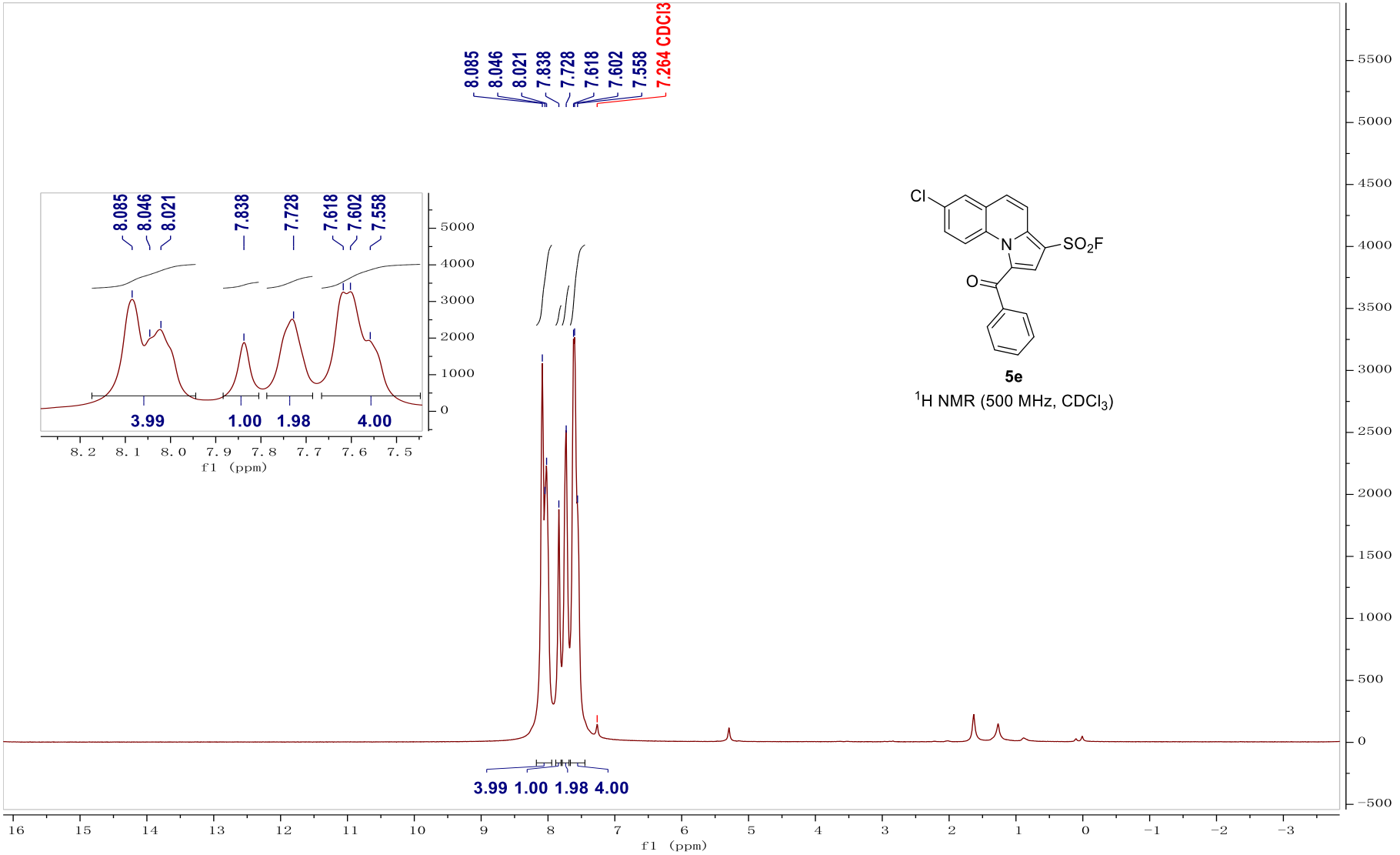
^{19}FNMR (471 MHz, $CDCl_3$)

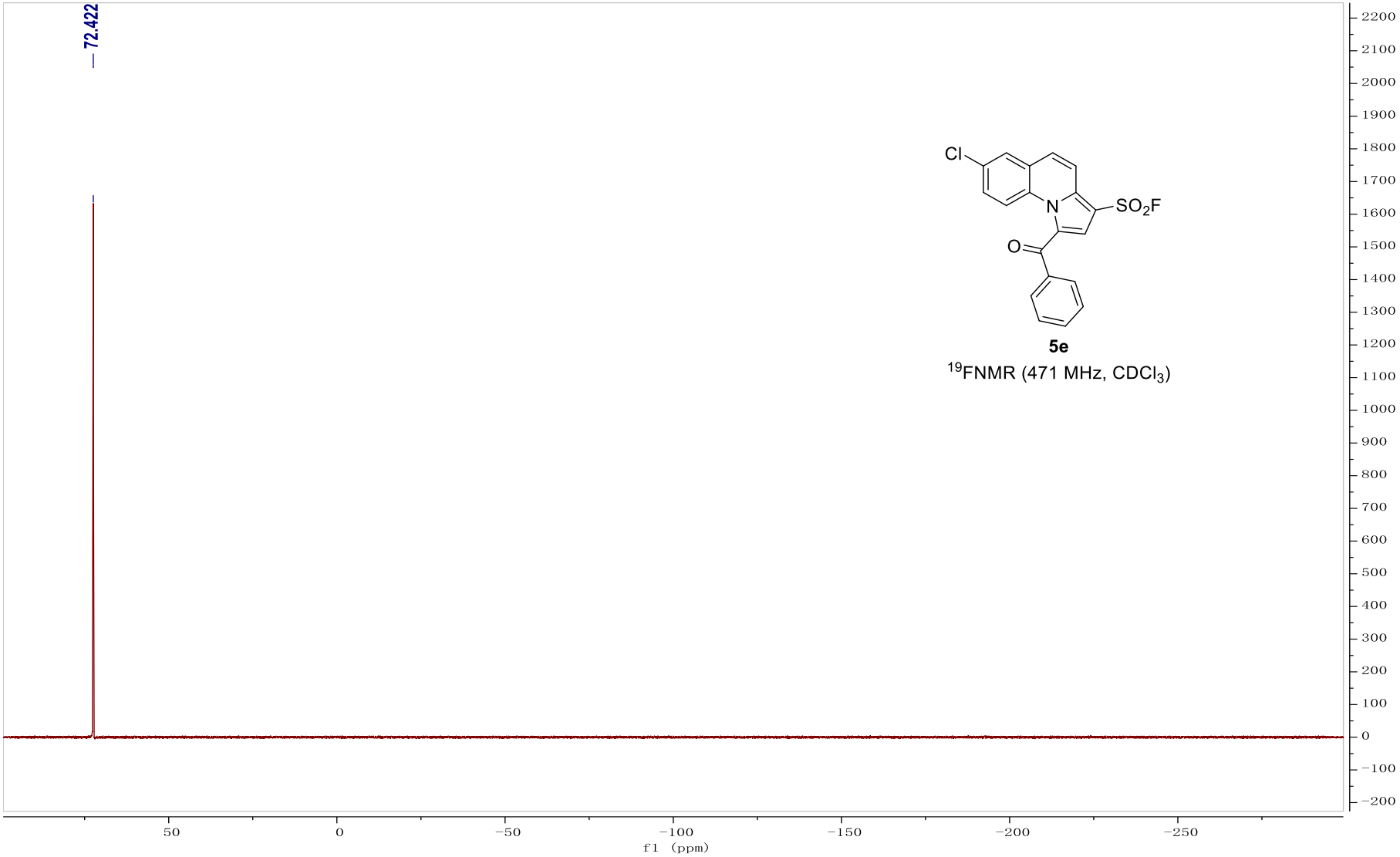

184.728
139.326
138.704
137.437
133.781
132.650
130.235
129.539
128.920
128.567
127.657
126.571
125.722
125.345
120.714
114.792
104.663
104.425
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
19.785
N
SO2F
O
5c
13C NMR (126 MHz, CDCl3)
f1 (ppm)

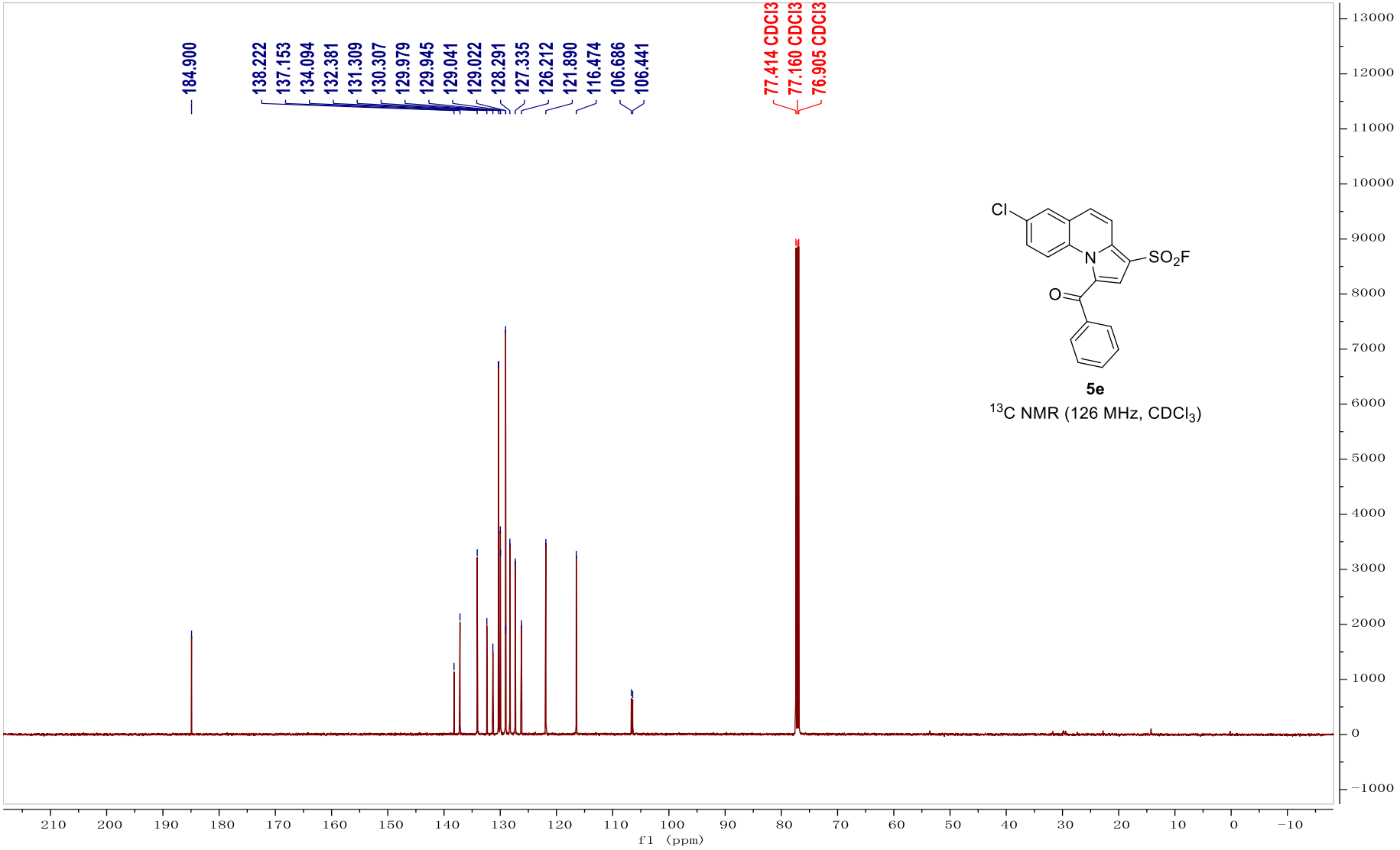

8.114
8.104
7.891
7.878
7.790
7.781
7.718
7.630
7.606
7.591
7.573
7.556
7.539
7.264 CDCl3
2.864
1.99 1.00 0.98 2.00 4.98
3.02
f1 (ppm)
1.00 0.98 2.00 4.98
f1 (ppm)
SO2F
O
N
5d
1H NMR (500 MHz, CDCl3)

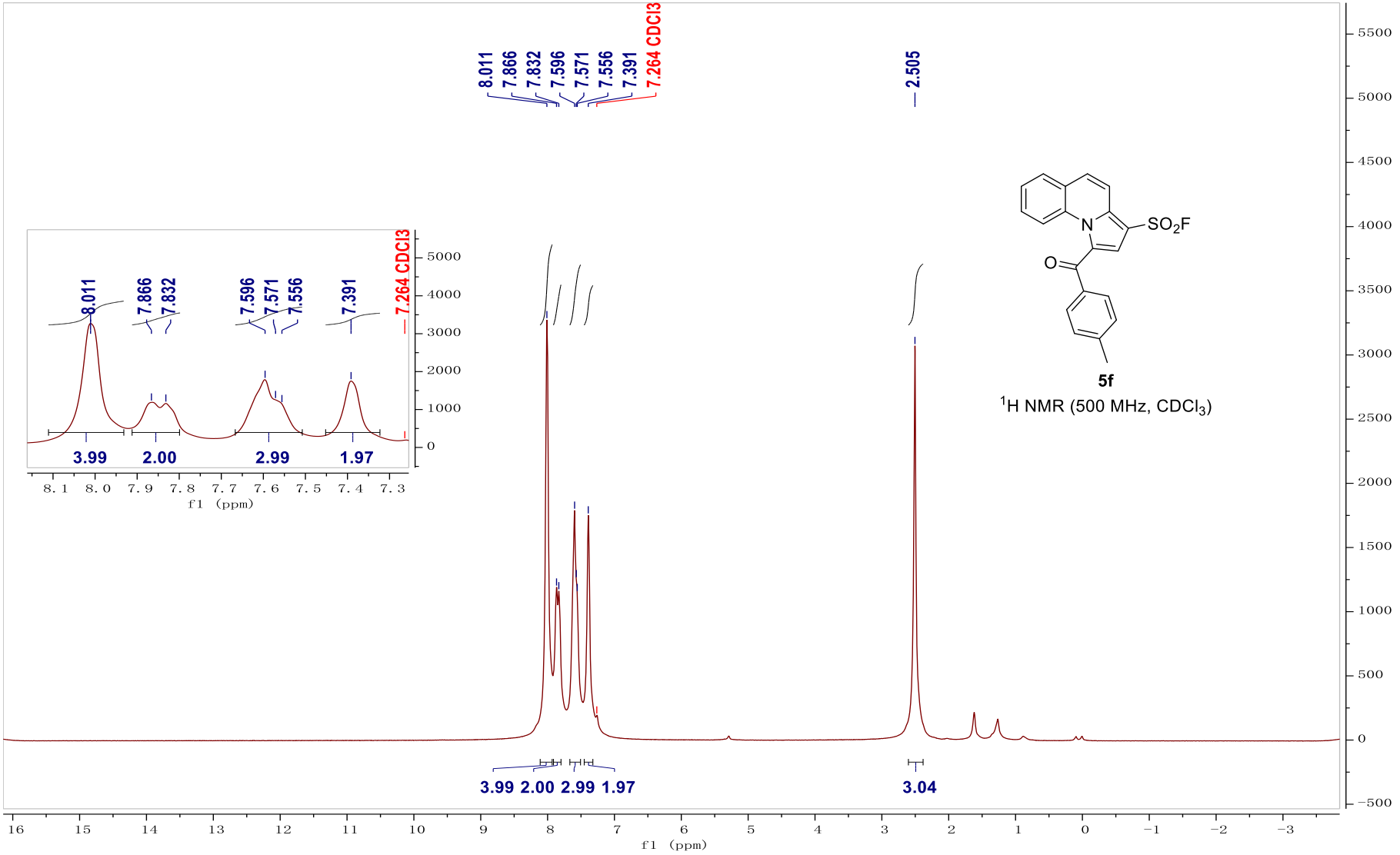

73.810
SO2F
N
O
5d
19FNMR (471 MHz, CDCl3)
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

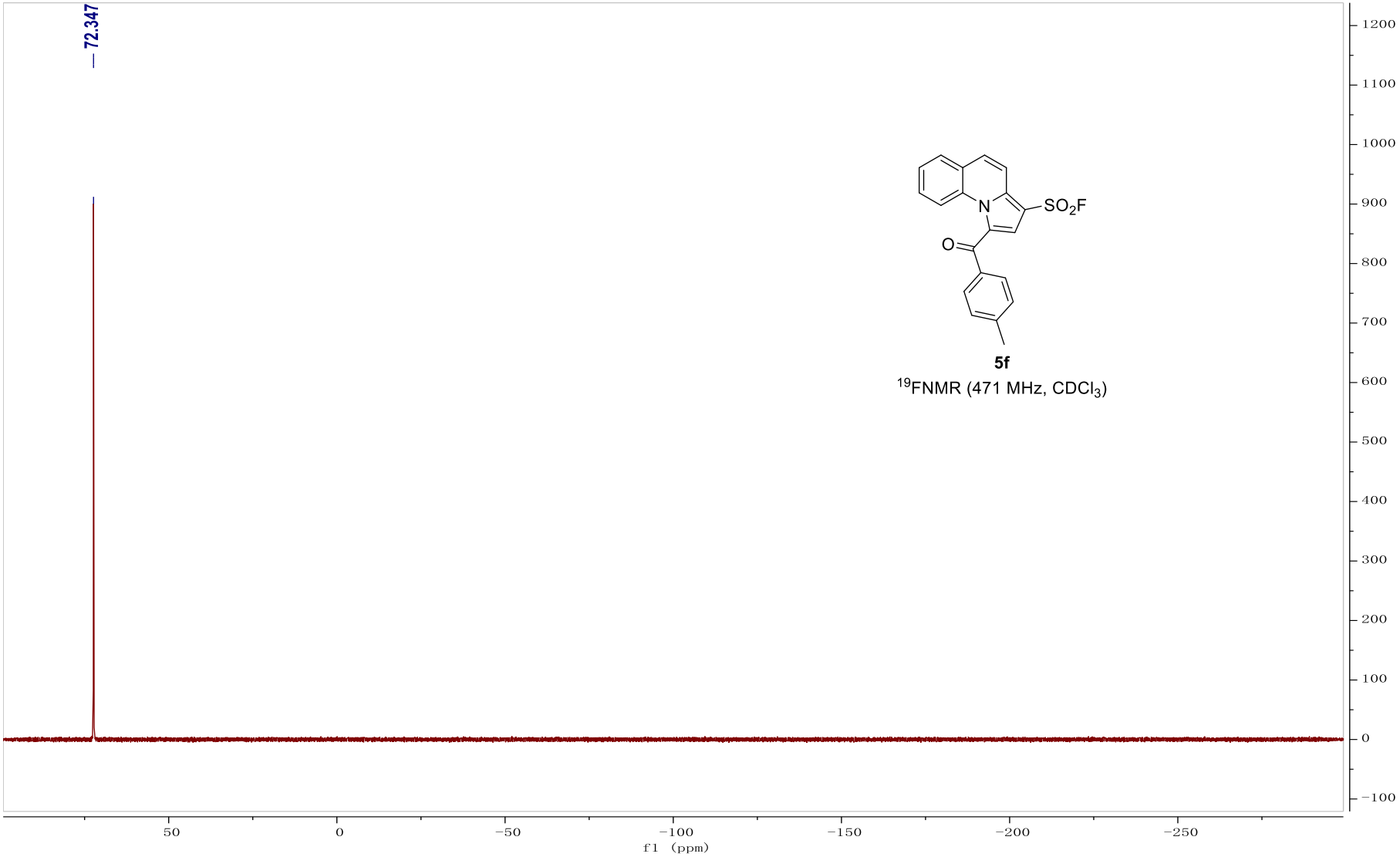

184.783
137.735
137.199
133.915
131.561
131.343
130.311
129.794
128.966
128.905
128.308
127.602
126.596
125.836
125.071
120.307
107.804
107.546
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
20.282
20.255
N
SO2F
O
5d
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.085
8.046
8.021
7.838
7.728
7.618
7.602
7.558
7.264 CDCl3
3.99 1.00 1.98 4.00
f1 (ppm)
Cl
N
SO2F
O
5e
1H NMR (500 MHz, CDCl3)


72.422
Cl
N
SO2F
O
5e
19FNMR (471 MHz, CDCl3)
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

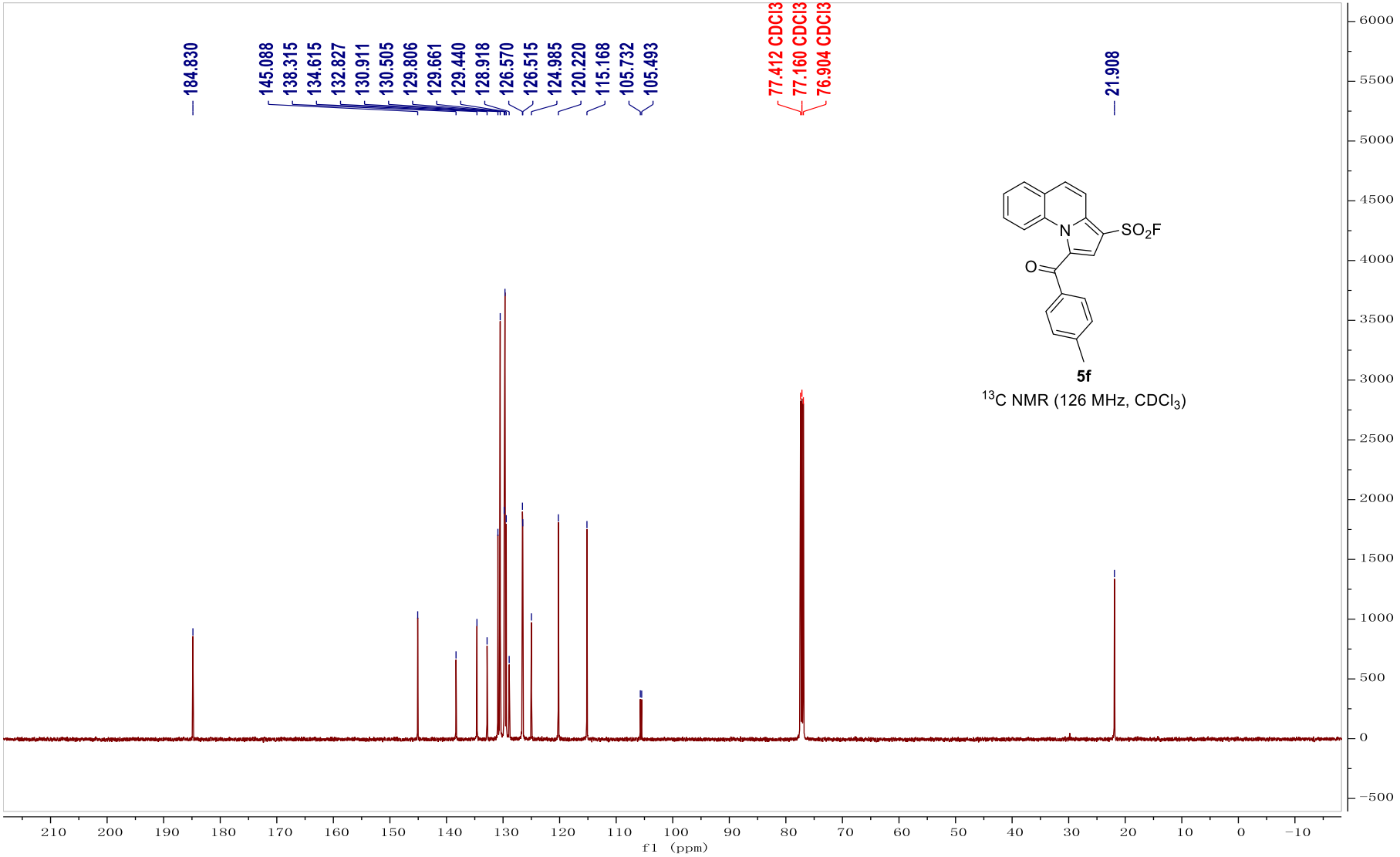

184.900
138.222
137.153
134.094
132.381
131.309
130.307
129.979
129.945
129.041
129.022
128.291
127.335
126.212
121.890
116.474
106.686
106.441
77.414 CDCl3
77.160 CDCl3
76.905 CDCl3
Cl
N
SO2F
O
5e
13C NMR (126 MHz, CDCl3)
f1 (ppm)

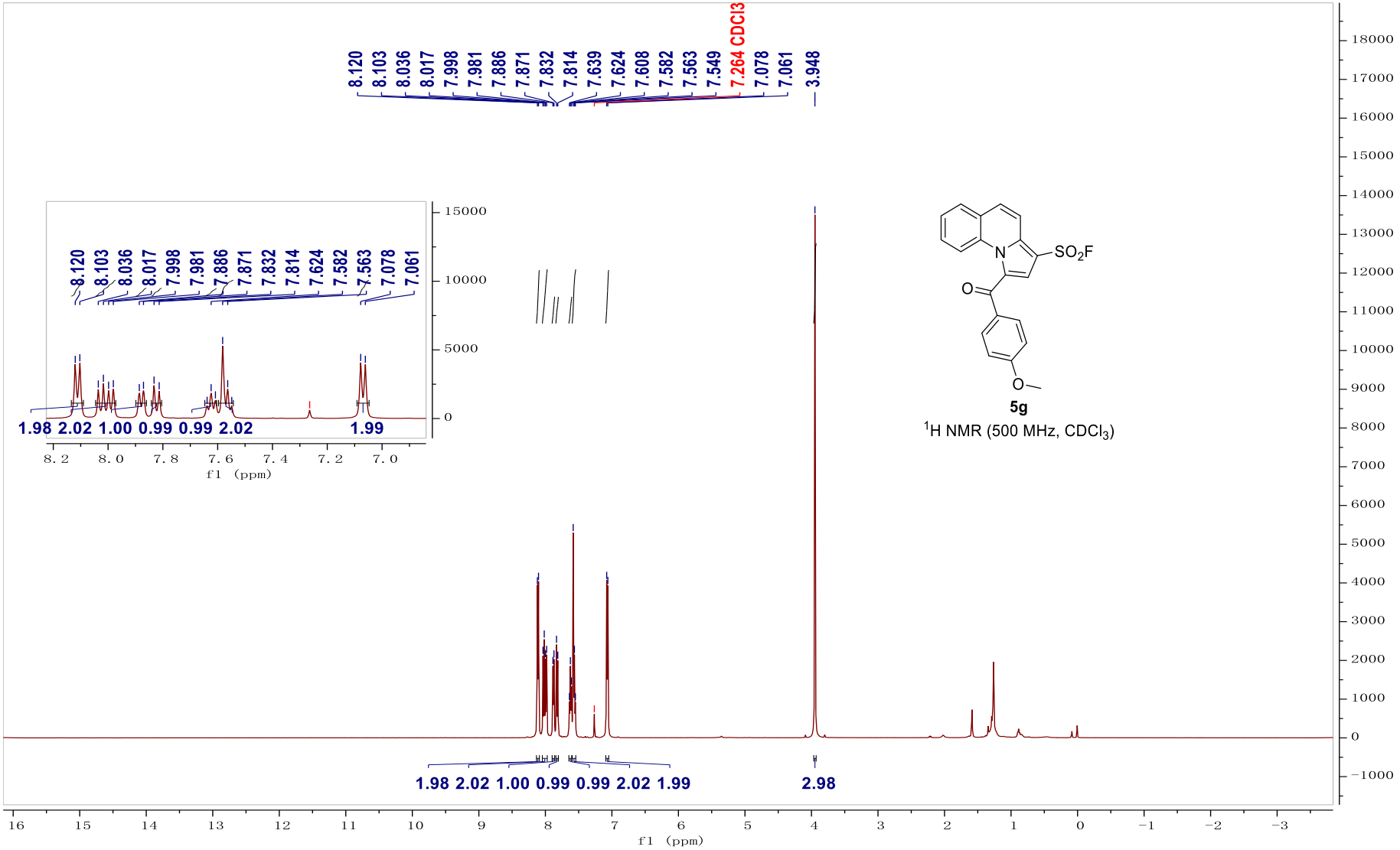

8.011
7.866
7.832
7.596
7.571
7.556
7.391
7.264 CDCl3
2.505
3.99 2.00 2.99 1.97
3.04
f1 (ppm)
5f
1H NMR (500 MHz, CDCl3)
SO2F
N
O

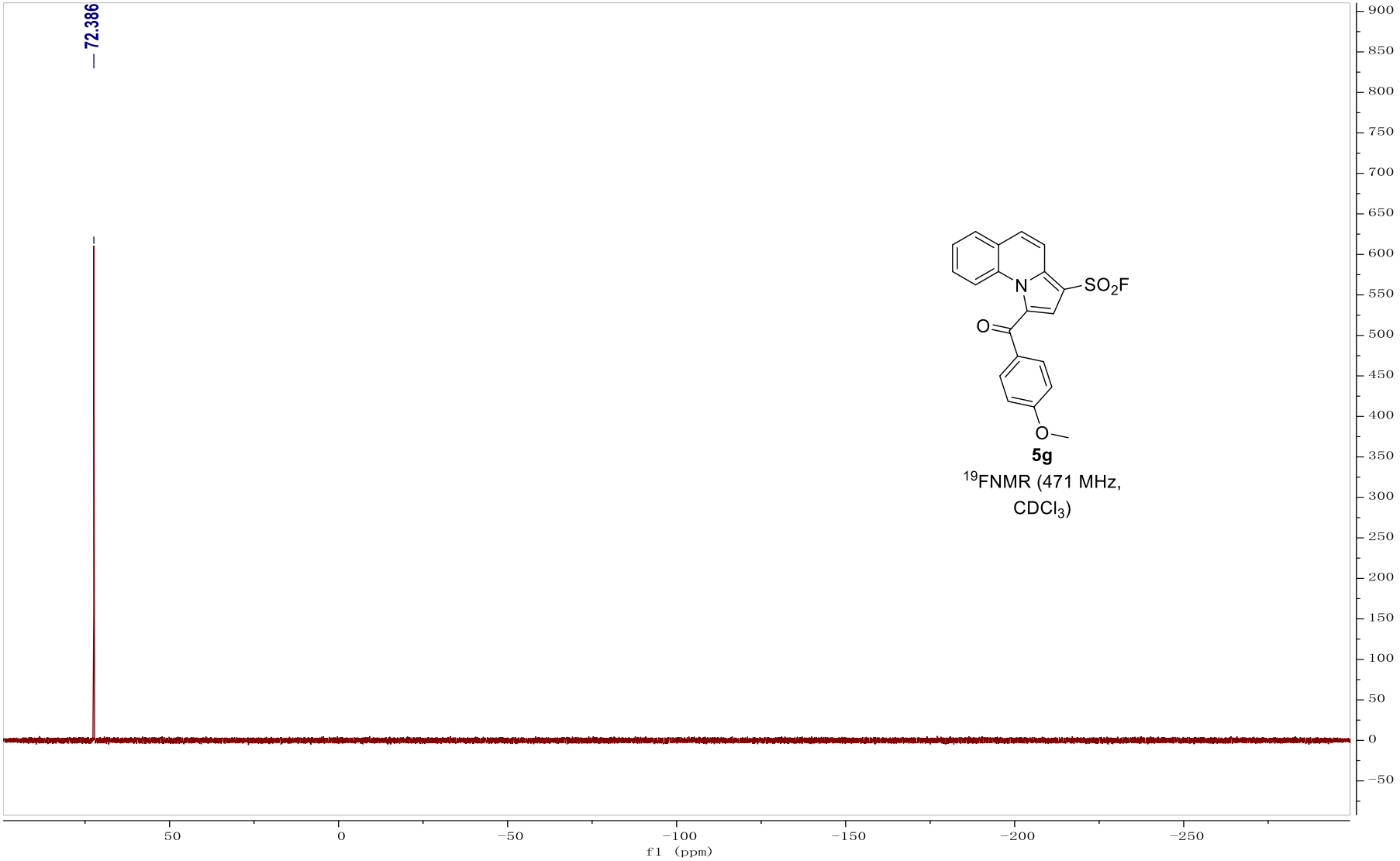


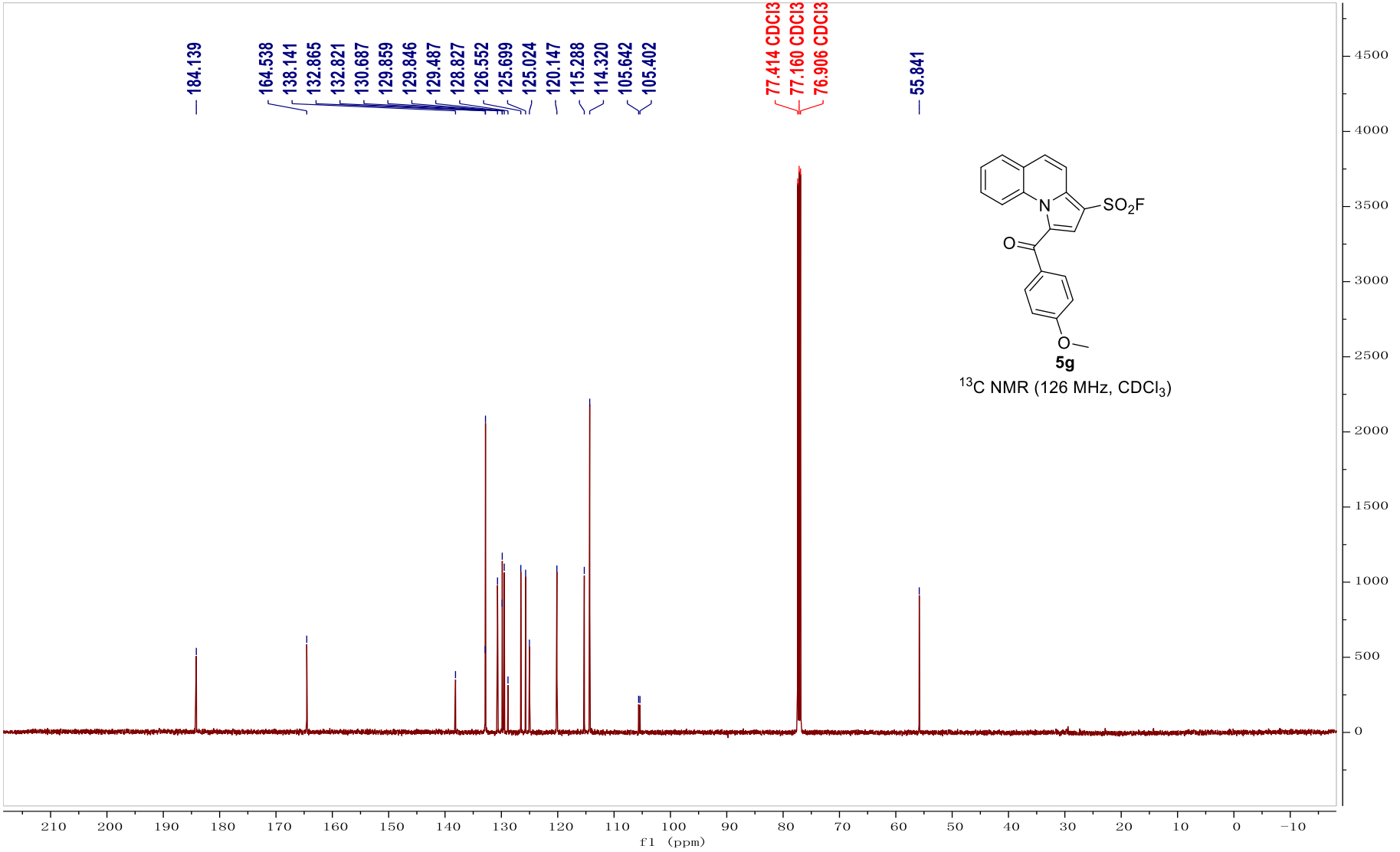
5f

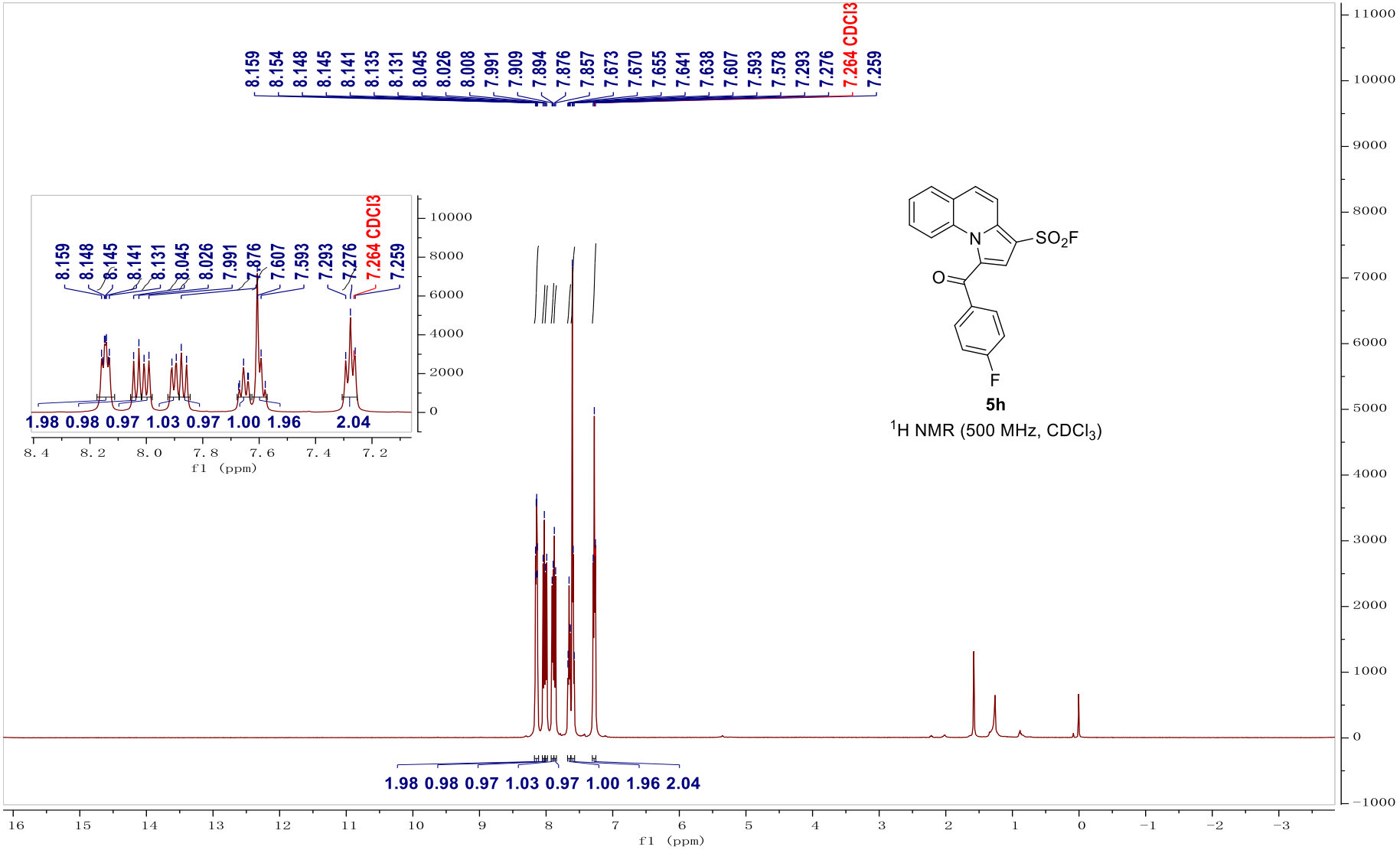
^{19}FNMR (471 MHz, $CDCl_3$)

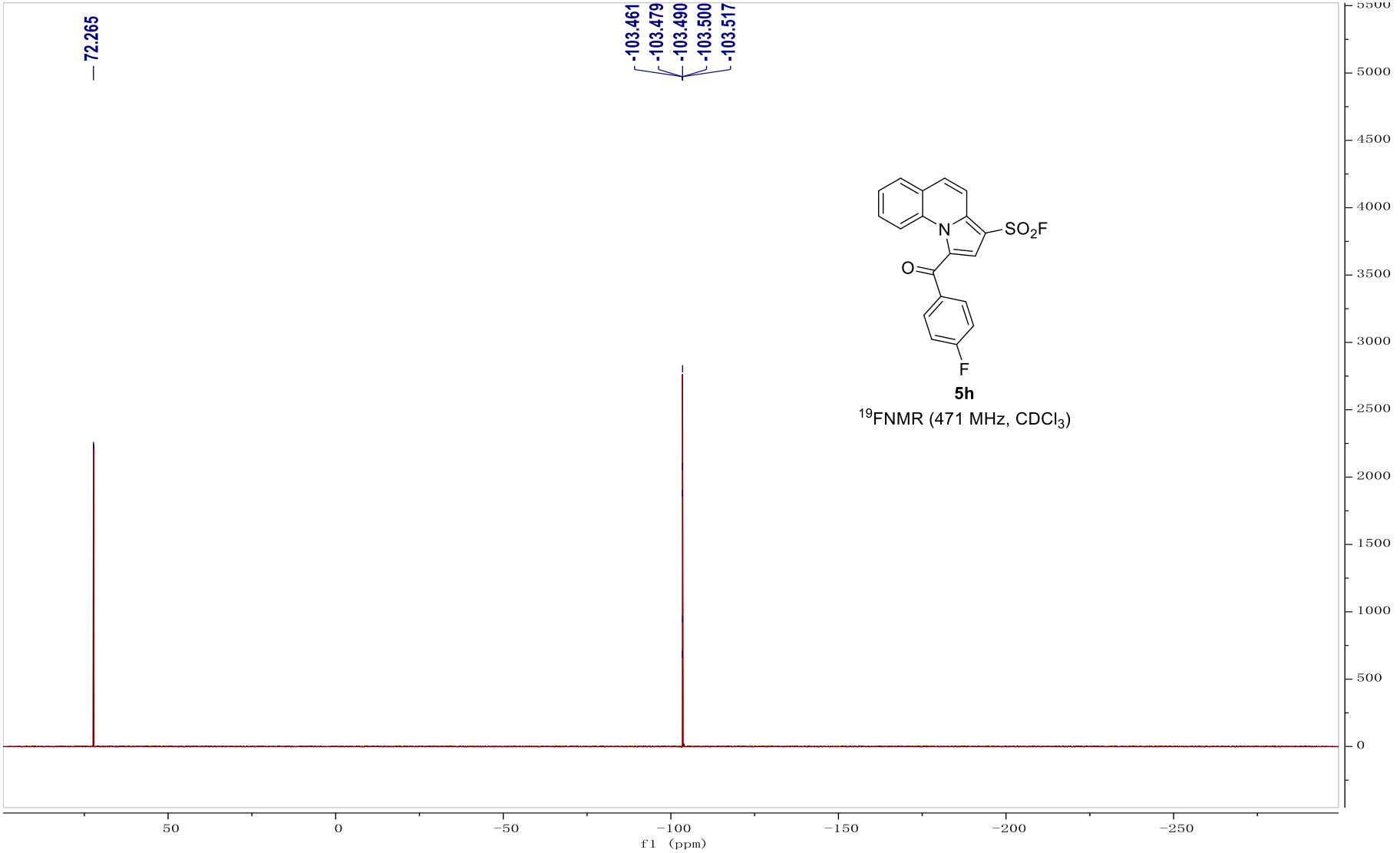

184.830
145.088
138.315
134.615
132.827
130.911
130.505
129.806
129.661
129.440
128.918
126.570
126.515
124.985
120.220
115.168
105.732
105.493
77.412 CDCl3
77.160 CDCl3
76.904 CDCl3
21.908
N
SO2F
O
5f
13C NMR (126 MHz, CDCl3)
f1 (ppm)

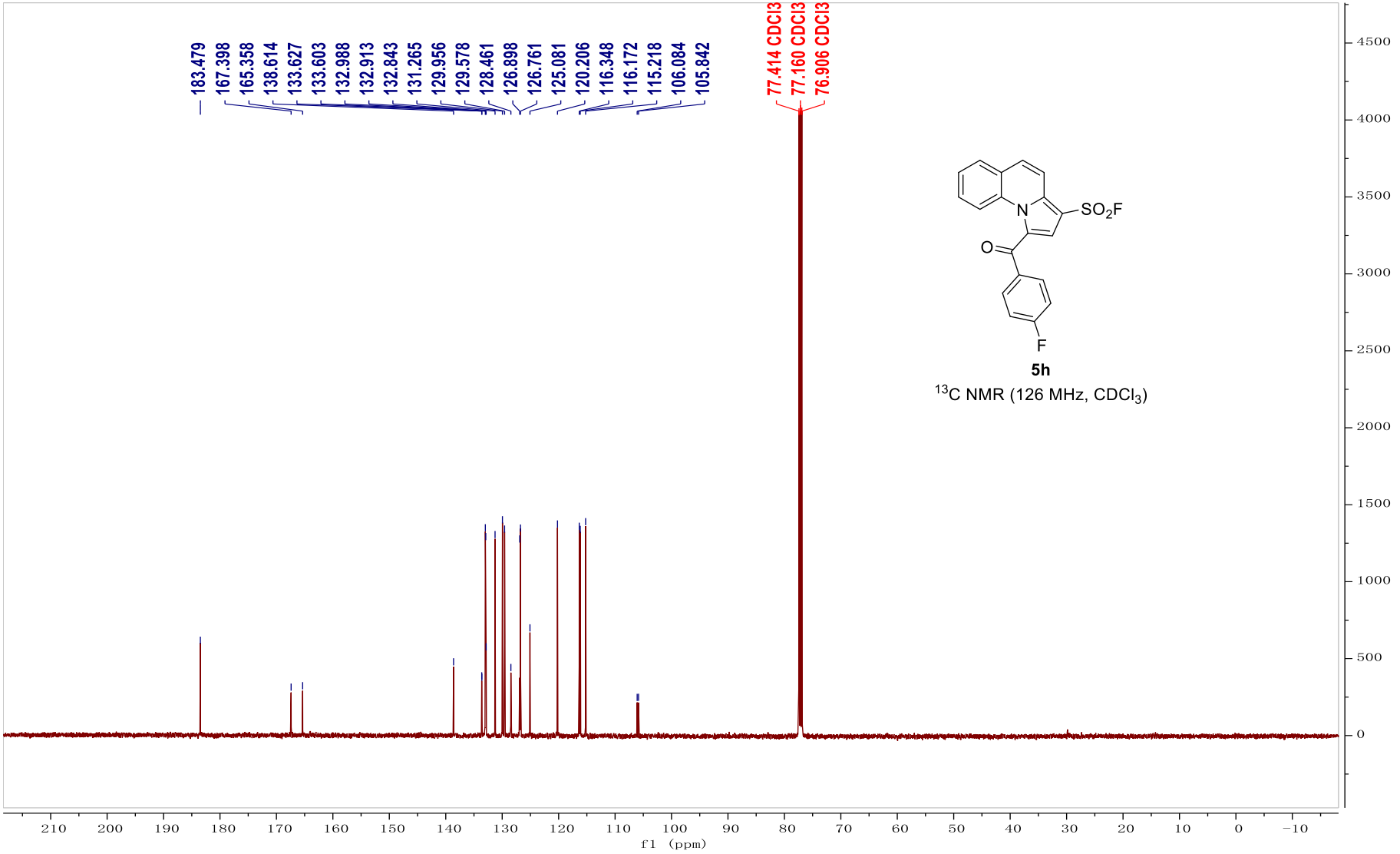

8.120
8.103
8.036
8.017
7.998
7.981
7.886
7.871
7.832
7.814
7.639
7.624
7.608
7.582
7.563
7.549
7.264 CDCl3
7.078
7.061
3.948
1.98 2.02 1.00 0.99 0.99 2.02 1.99
2.98
f1 (ppm)
SO2F
N
O
O
5g
1H NMR (500 MHz, CDCl3)

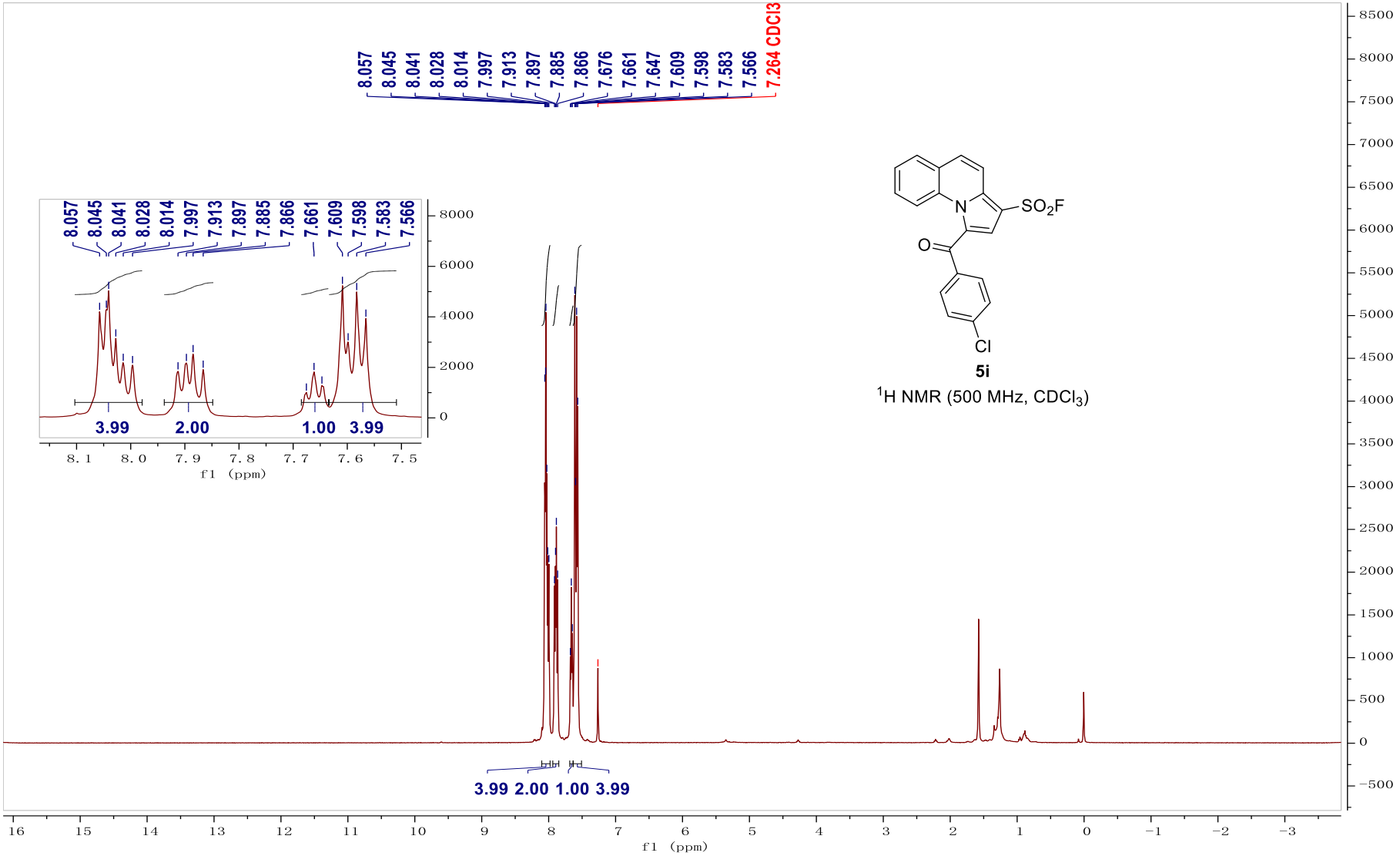

72.386
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
50
0
−50
−100
−150
−200
−250
f1 (ppm)
N
SO2F
O
O
5g
19FNMR (471 MHz,
CDCl3)

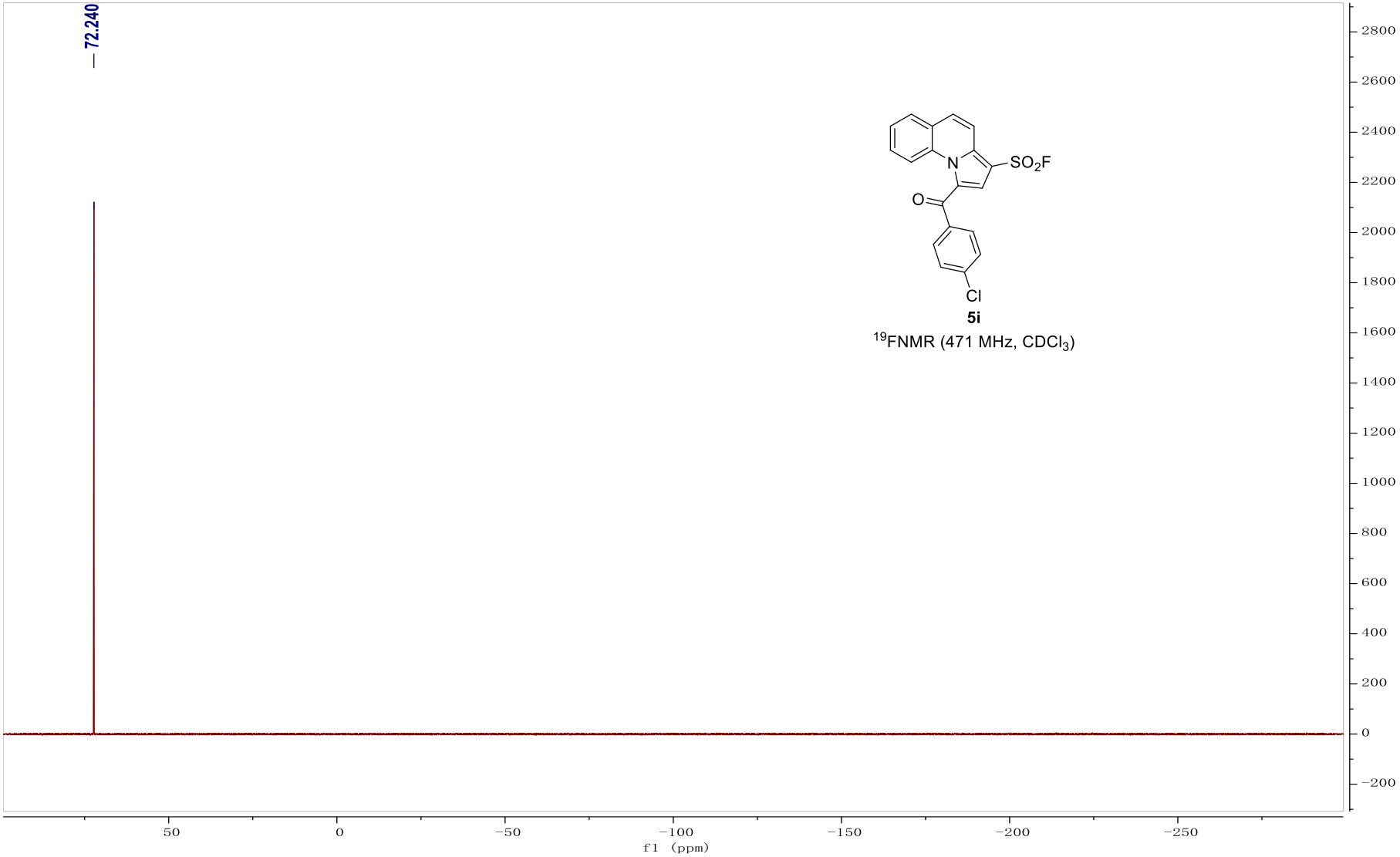

184.139
164.538
138.141
132.865
132.821
130.687
129.859
129.846
129.487
128.827
126.552
125.699
125.024
120.147
115.288
114.320
105.642
105.402
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
55.841
SO2F
N
O
O
5g
13C NMR (126 MHz, CDCl3)
f1 (ppm)

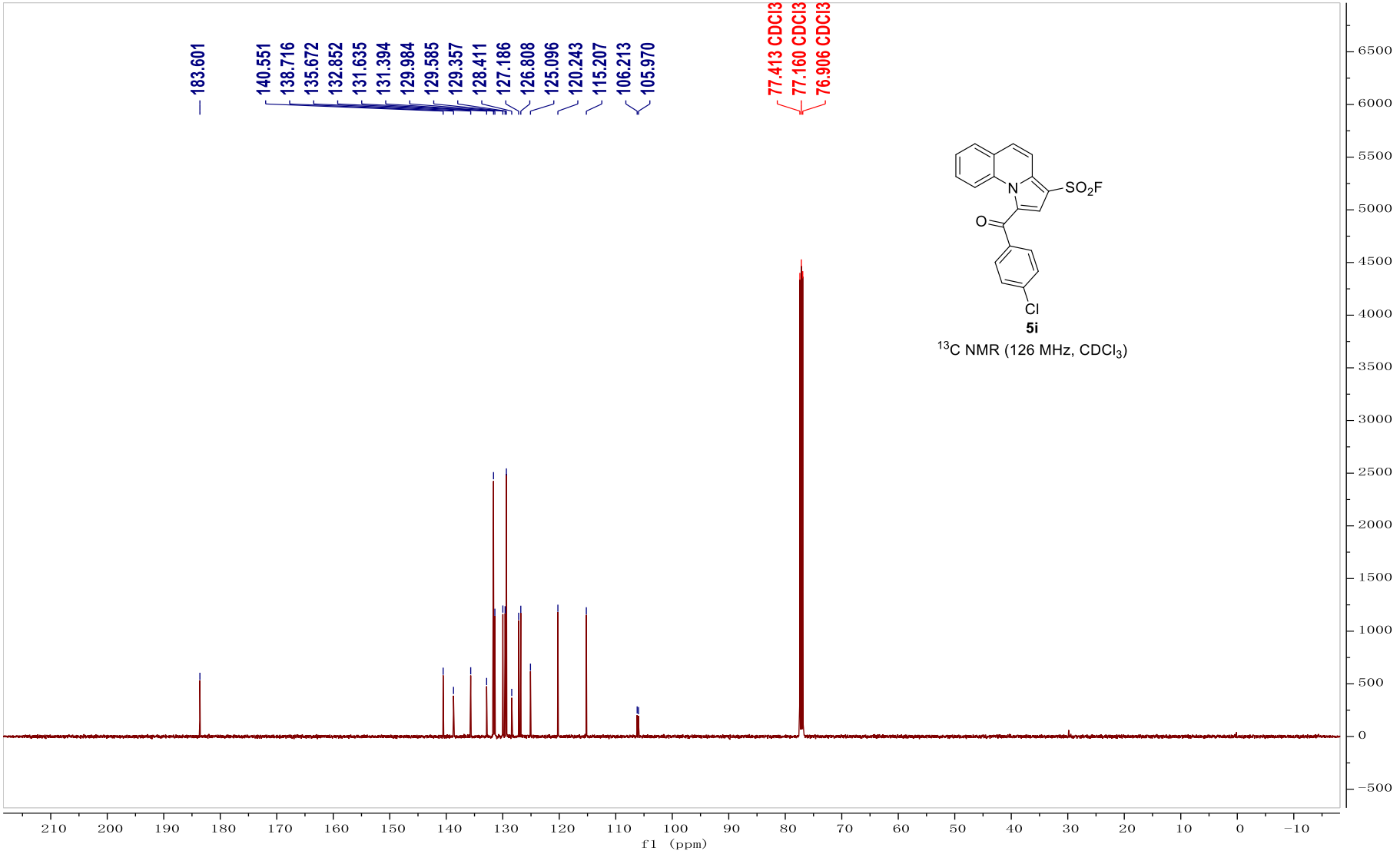

8.159 8.154 8.148 8.145 8.141 8.135 8.131 8.045 8.026 8.008 7.991 7.909 7.894 7.876 7.857 7.673 7.670 7.655 7.641 7.638 7.607 7.593 7.578 7.293 7.276 7.264 CDCl3 7.259
1.98 0.98 0.97 1.03 0.97 1.00 1.96 2.04
f1 (ppm)
SO2F
N
O
F
5h
1H NMR (500 MHz, CDCl3)

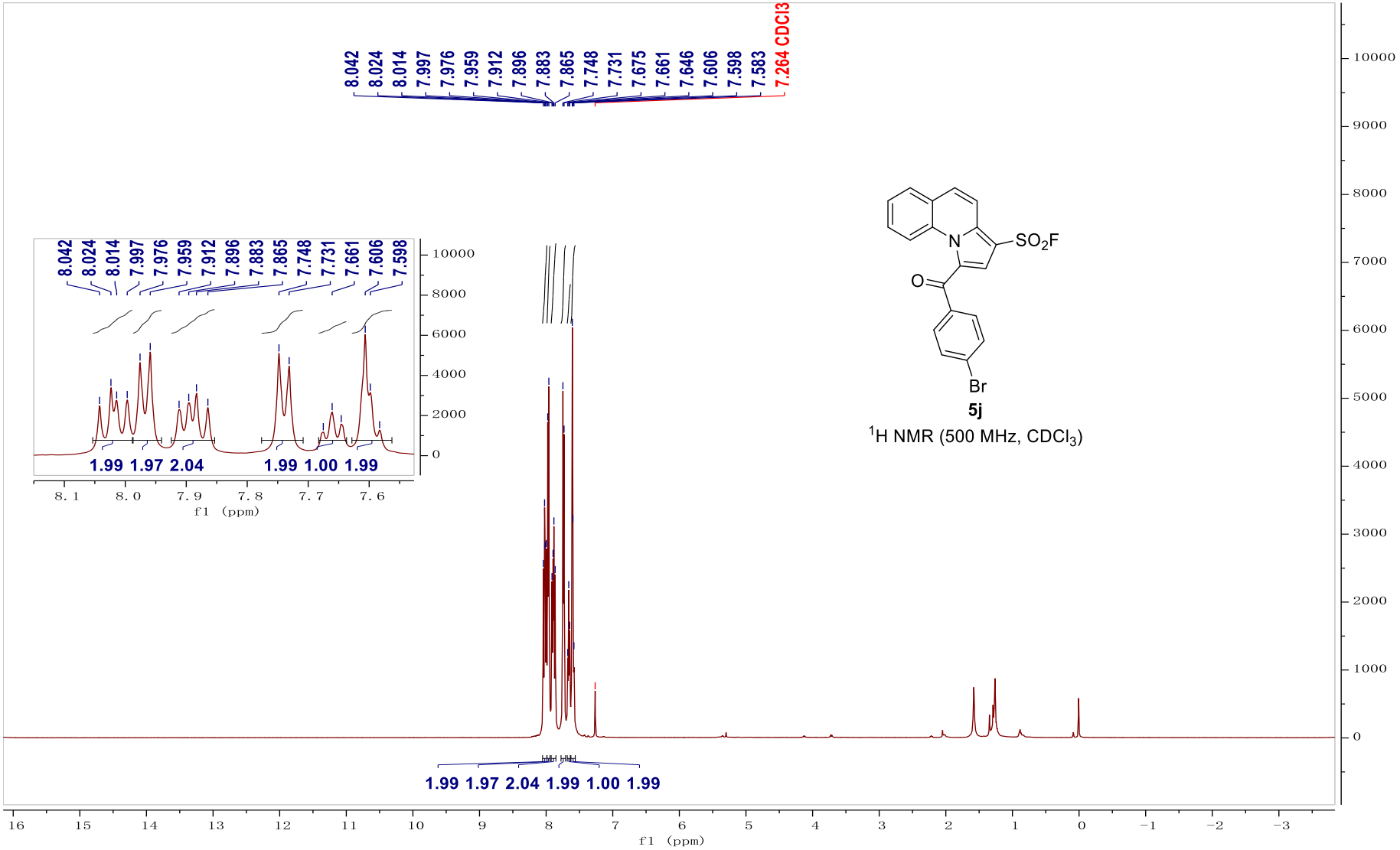

-72.265
-103.461
-103.479
-103.490
-103.500
-103.517
N
SO2F
O
F
5h
19FNMR (471 MHz, CDCl3)
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
50
0
−50
−100
−150
−200
−250
f1 (ppm)

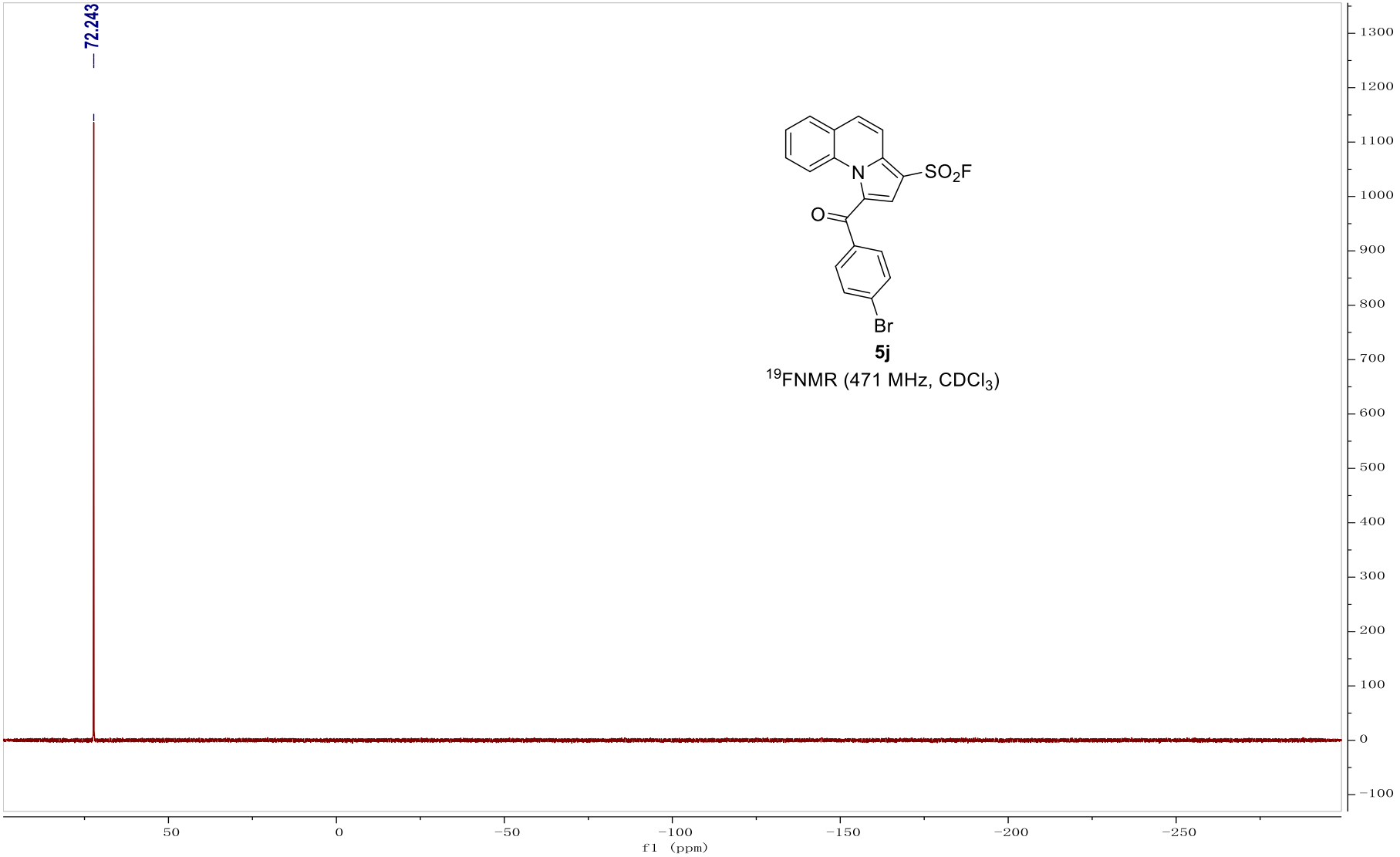

183.479
167.398
165.358
138.614
133.627
133.603
132.988
132.913
132.843
131.265
129.956
129.578
128.461
126.898
126.761
125.081
120.206
116.348
116.172
115.218
106.084
105.842
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
N
SO2F
O
F
5h
13C NMR (126 MHz, CDCl3)
f1 (ppm)

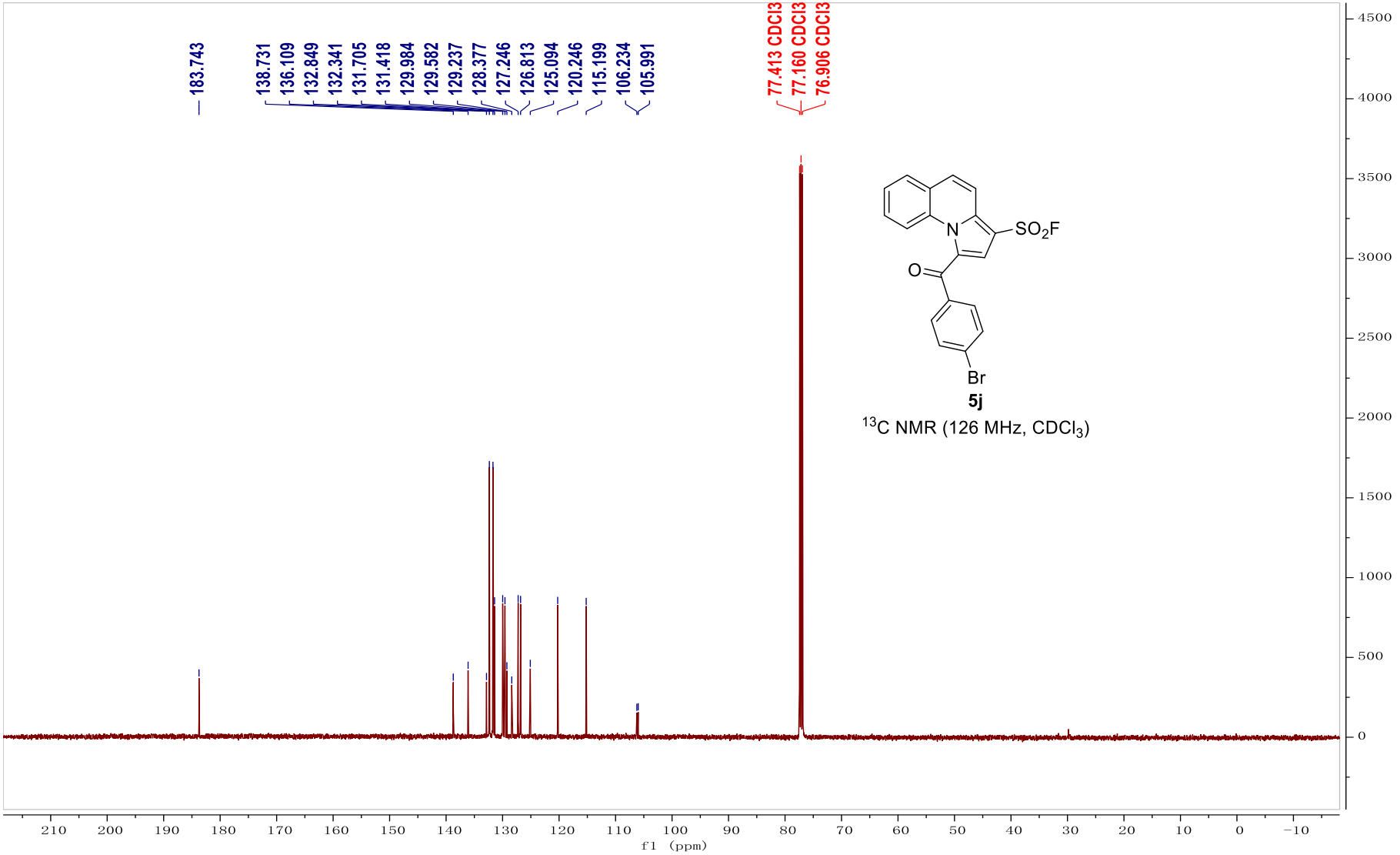

8.057
8.045
8.041
8.028
8.014
7.997
7.913
7.897
7.885
7.866
7.676
7.661
7.647
7.609
7.598
7.583
7.566
7.264 CDCl3
3.99 2.00 1.00 3.99
f1 (ppm)
SO2F
N
O
Cl
5i
1H NMR (500 MHz, CDCl3)

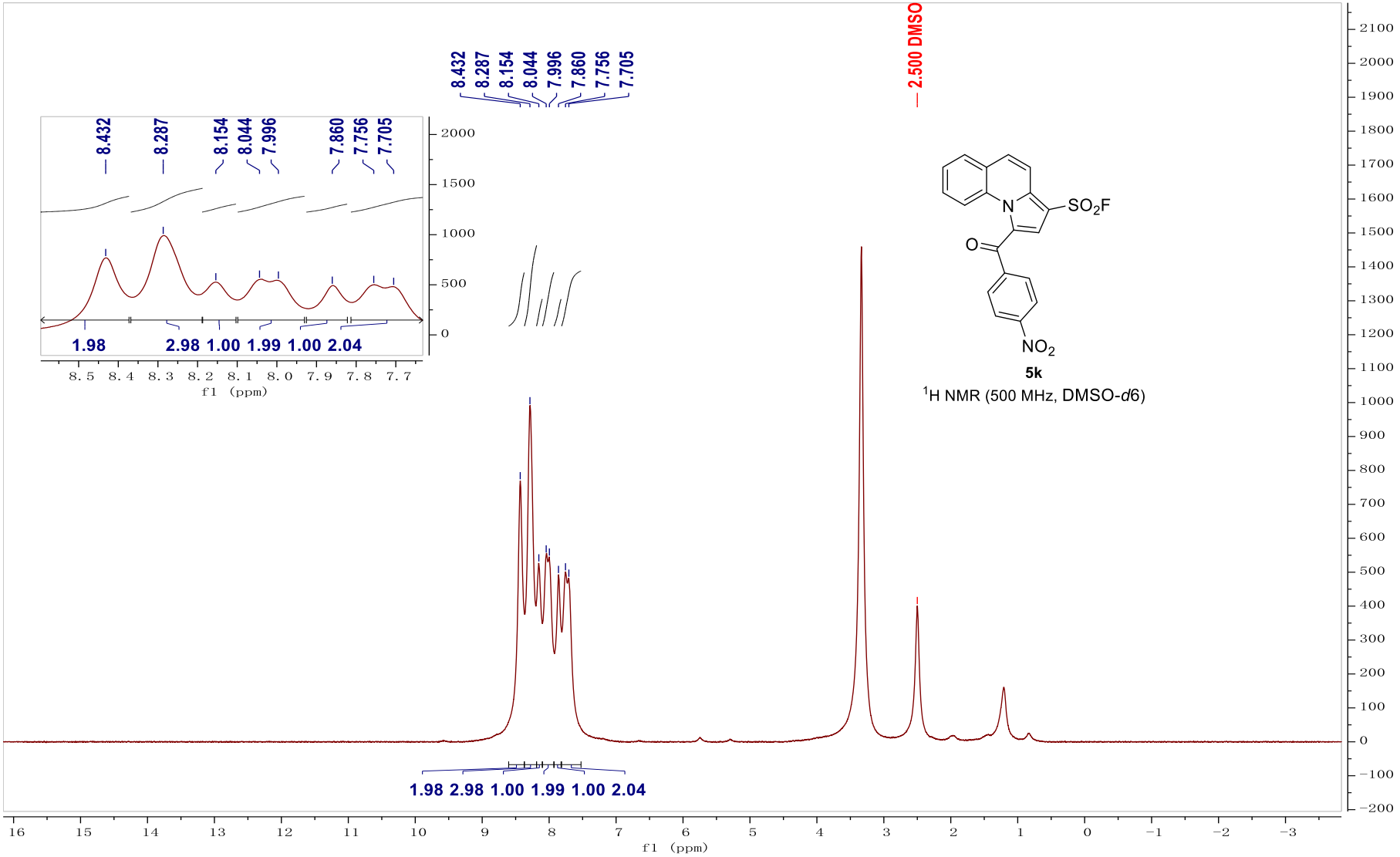

72.240
SO2F
N
O
Cl
5i
19FNMR (471 MHz, CDCl3)
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
50
0
−50
−100
−150
−200
−250
f1 (ppm)

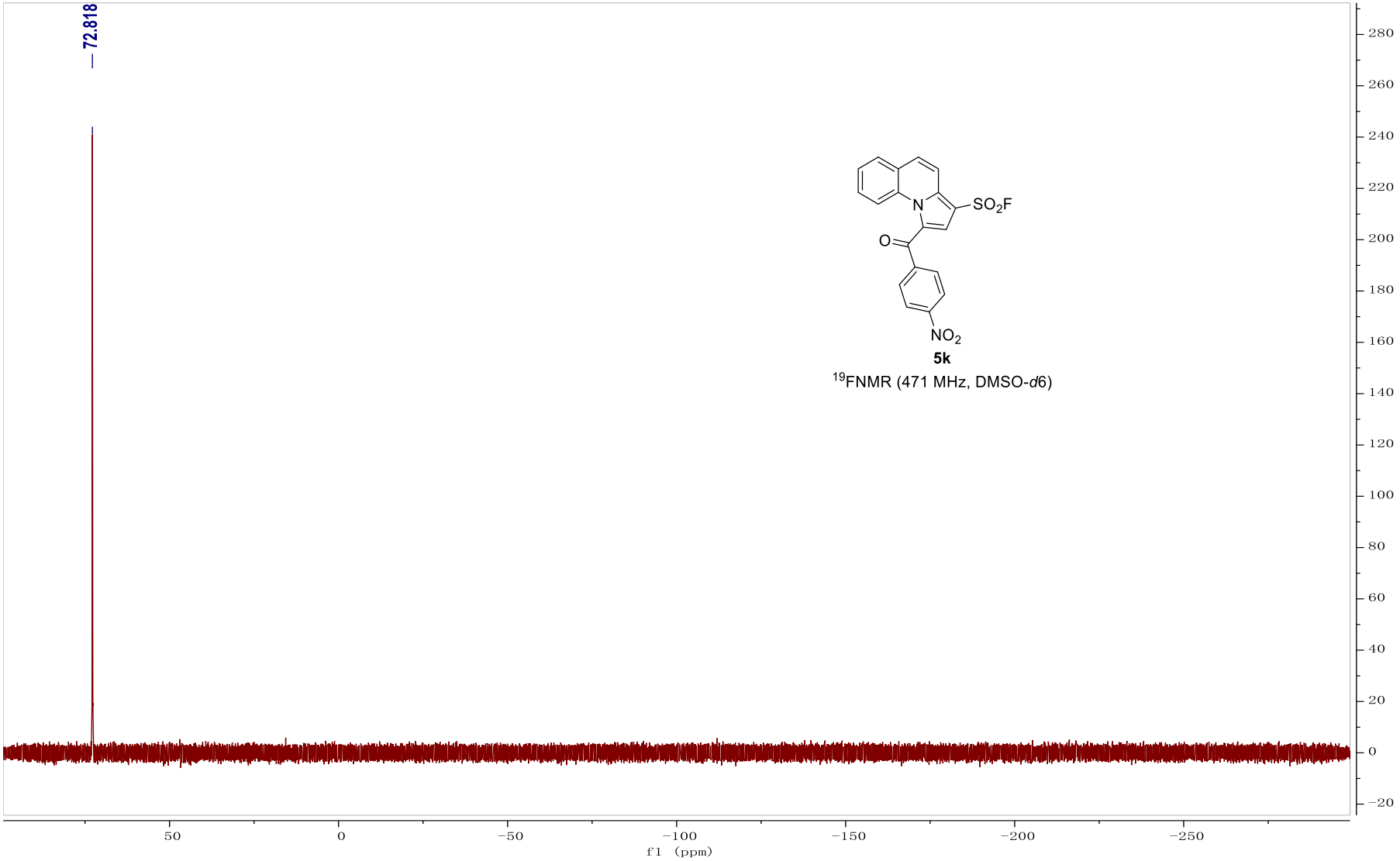

183.601
140.551
138.716
135.672
132.852
131.635
131.394
129.984
129.585
129.357
128.411
127.186
126.808
125.096
120.243
115.207
106.213
105.970
77.413 CDCl3
77.160 CDCl3
76.906 CDCl3
SO2F
N
O
Cl
5i
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.042
8.024
8.014
7.997
7.976
7.959
7.912
7.896
7.883
7.865
7.748
7.731
7.675
7.661
7.646
7.606
7.598
7.583
7.264 CDCl3
1.99 1.97 2.04 1.99 1.00 1.99
f1 (ppm)
SO2F
N
O
Br
5j
1H NMR (500 MHz, CDCl3)


72.243
N
SO2F
O
Br
5j
19FNMR (471 MHz, CDCl3)
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
50
0
−50
−100
−150
−200
−250
f1 (ppm)

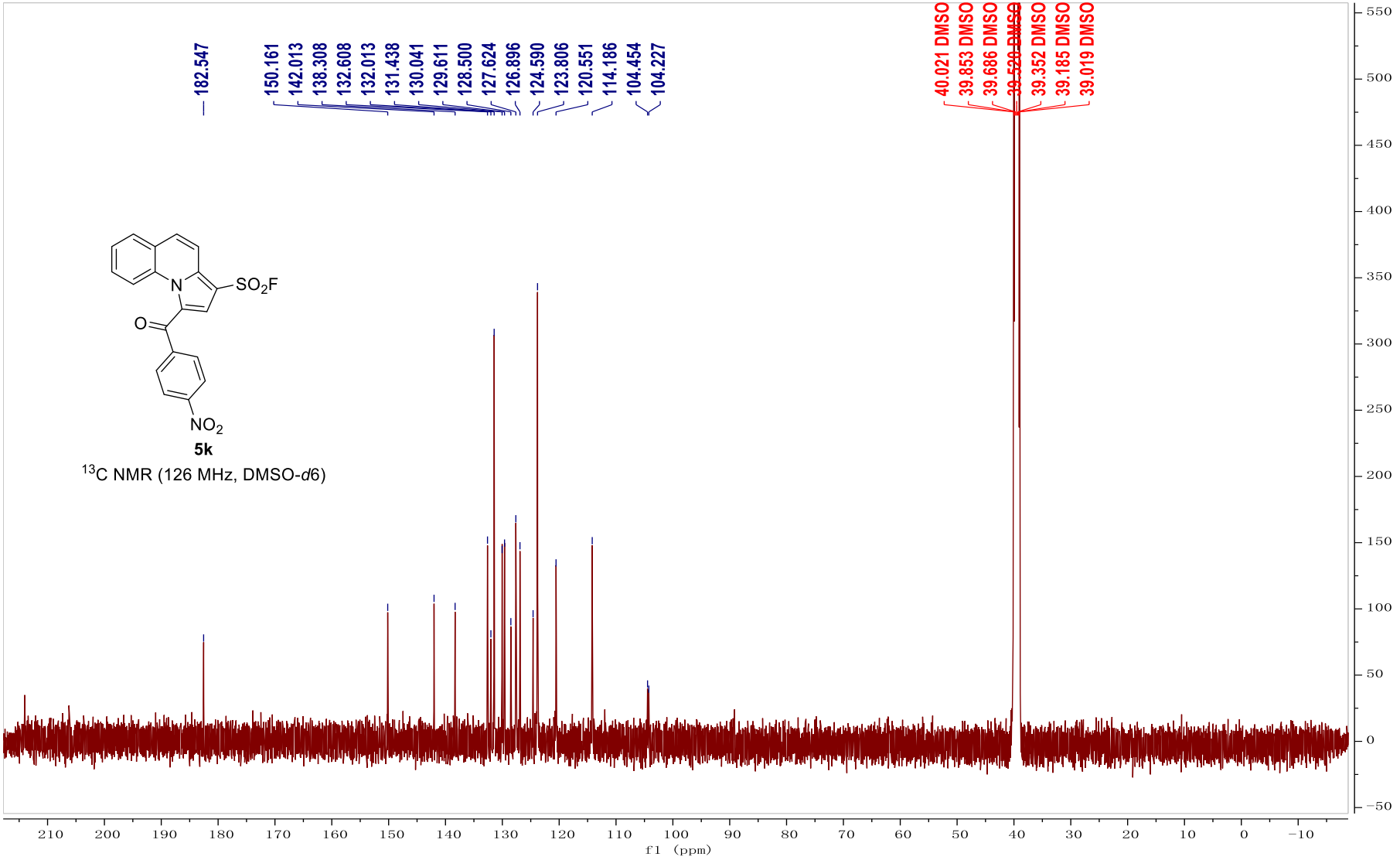

183.743
138.731
136.109
132.849
132.341
131.705
131.418
129.984
129.582
129.237
128.377
127.246
126.813
125.094
120.246
115.199
106.234
105.991
77.413 CDCl3
77.160 CDCl3
76.906 CDCl3
N
SO2F
O
Br
5j
13C NMR (126 MHz, CDCl3)
f1 (ppm)

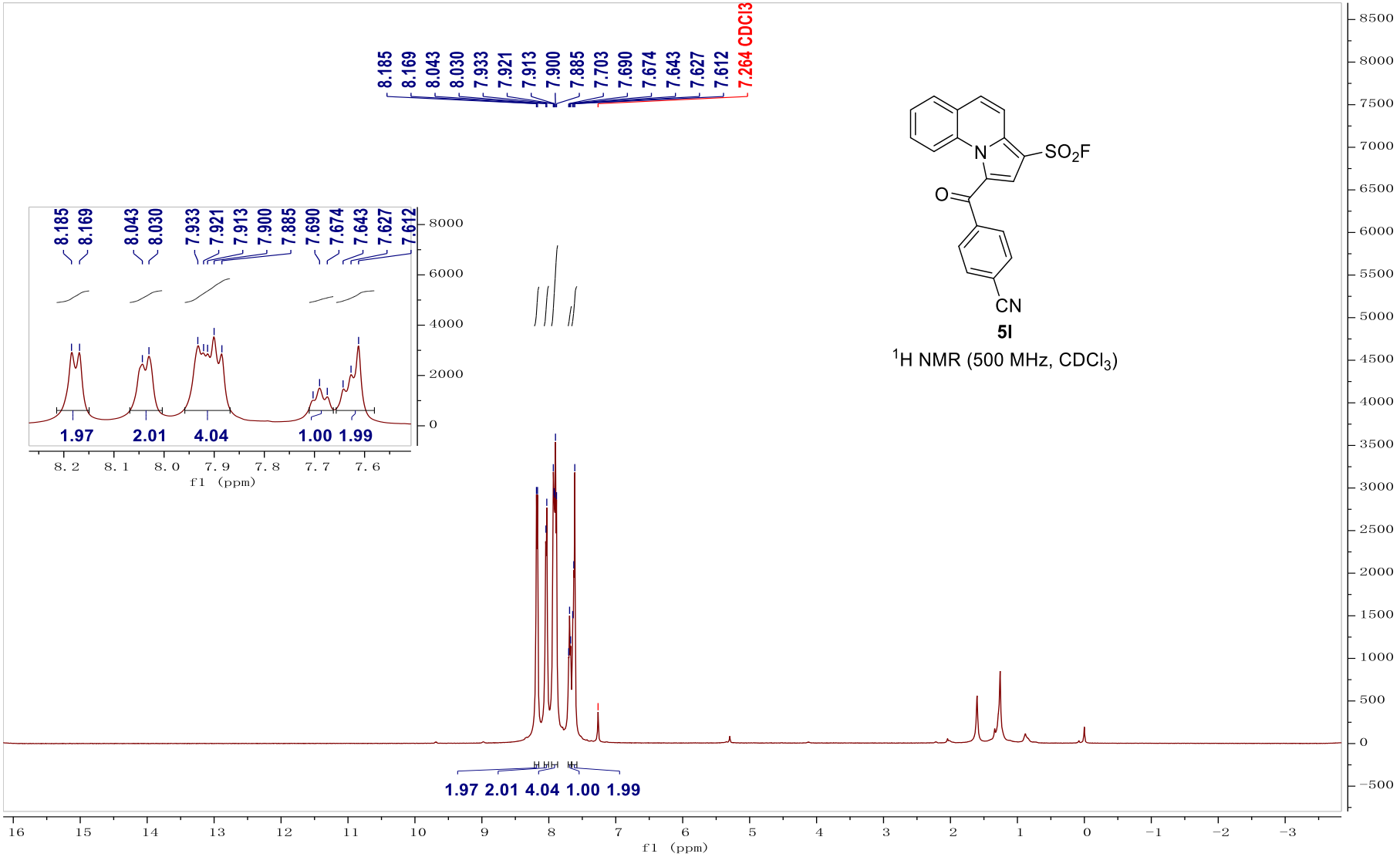

8.432
8.287
8.154
8.044
7.996
7.860
7.756
7.705
2.500 DMSO
1.98 2.98 1.00 1.99 1.00 2.04
f1 (ppm)
SO2F
N
O
NO2
5k
1H NMR (500 MHz, DMSO-d6)

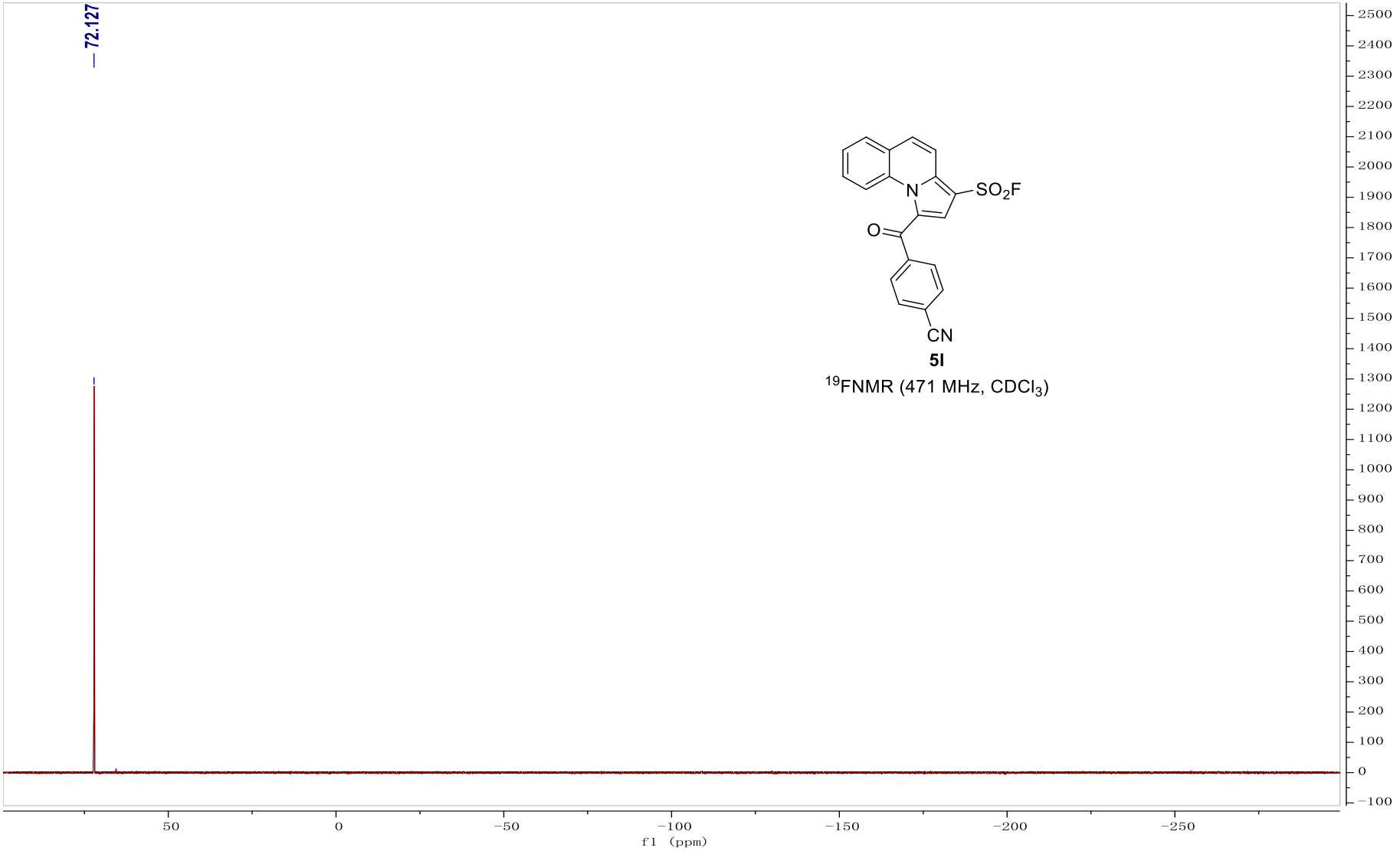


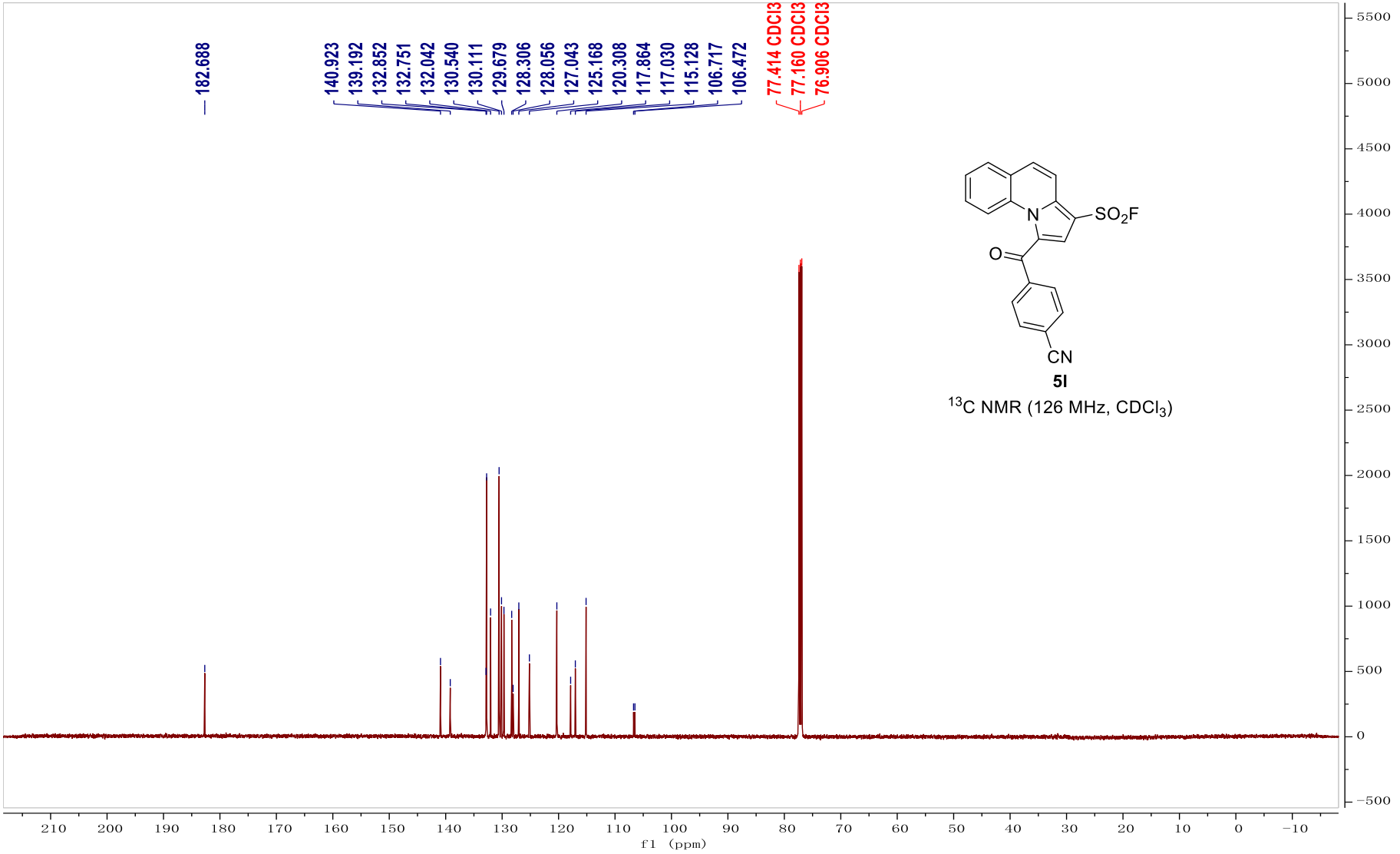
5k

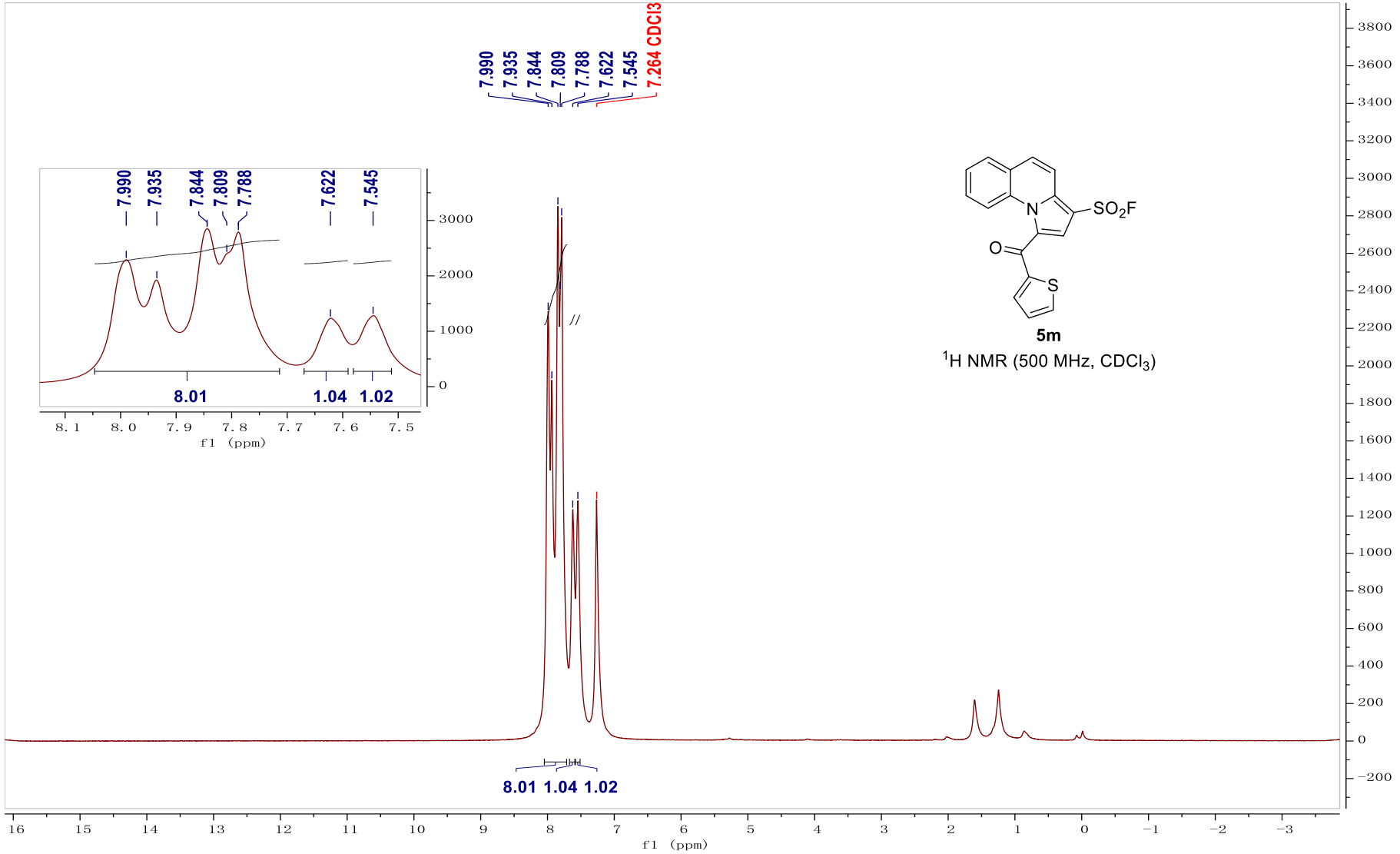
^{19}FNMR (471 MHz, DMSO-*d*6)

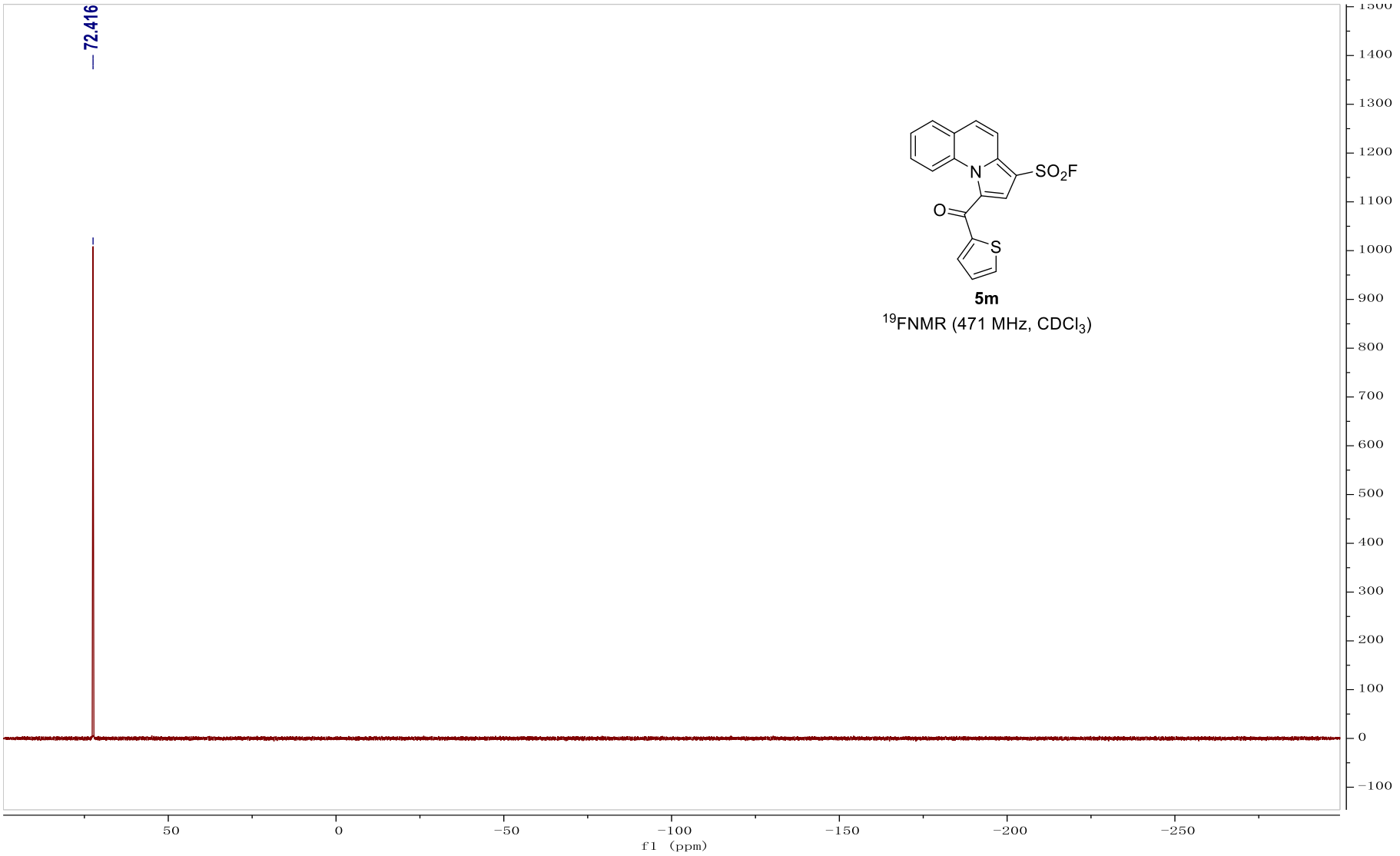

182.547
150.161
142.013
138.308
132.608
132.013
131.438
130.041
129.611
128.500
127.624
126.896
124.590
123.806
120.551
114.186
104.454
104.227
40.021 DMSO
39.853 DMSO
39.686 DMSO
39.520 DMSO
39.352 DMSO
39.185 DMSO
39.019 DMSO
SO2F
O
N
NO2
5k
13C NMR (126 MHz, DMSO-d6)
f1 (ppm)

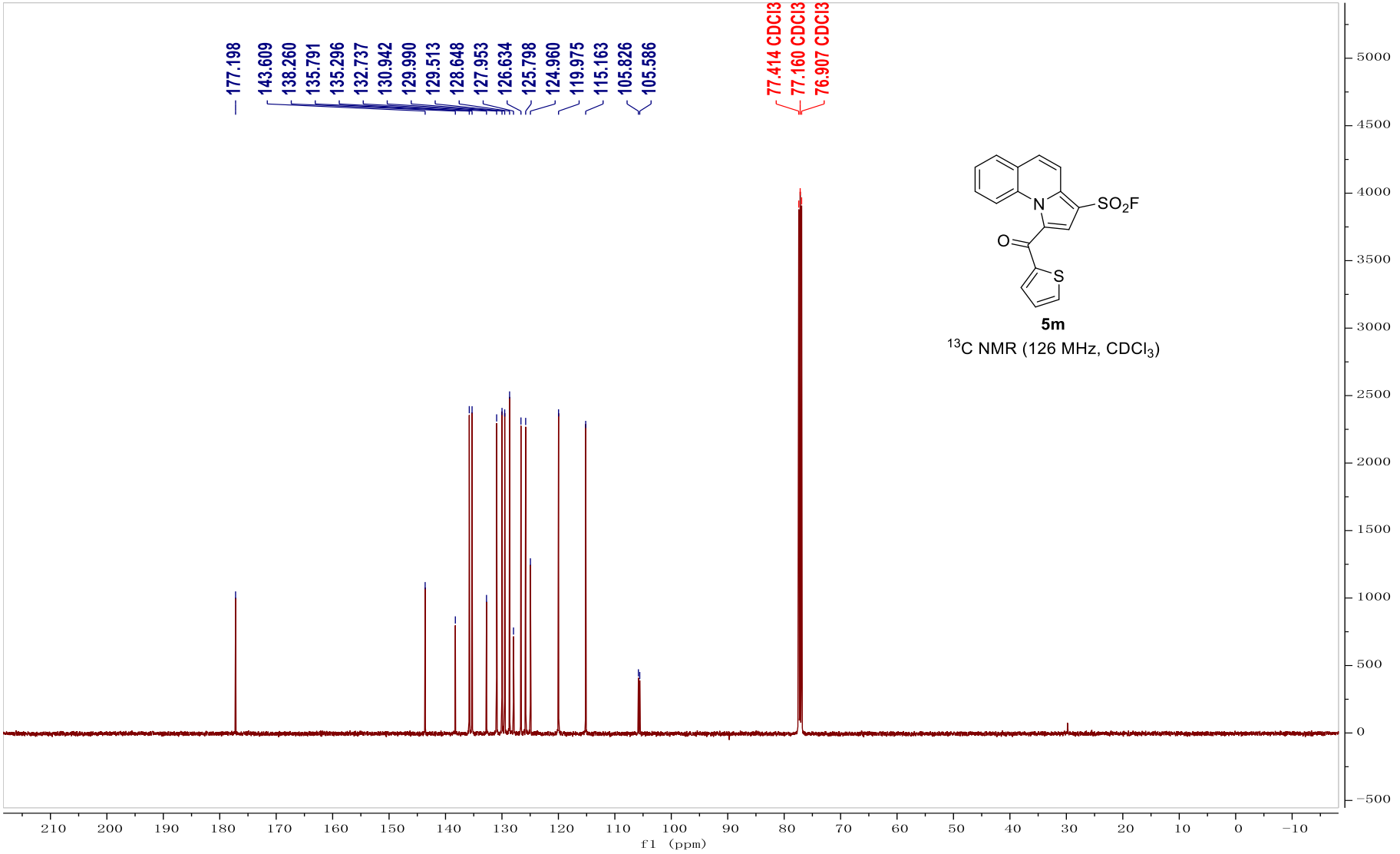

8.185
8.169
8.043
8.030
7.933
7.921
7.913
7.900
7.885
7.703
7.690
7.674
7.643
7.627
7.612
7.264 CDCl3
1.97 2.01 4.04 1.00 1.99
f1 (ppm)
N
SO2F
O
CN
5l
1H NMR (500 MHz, CDCl3)

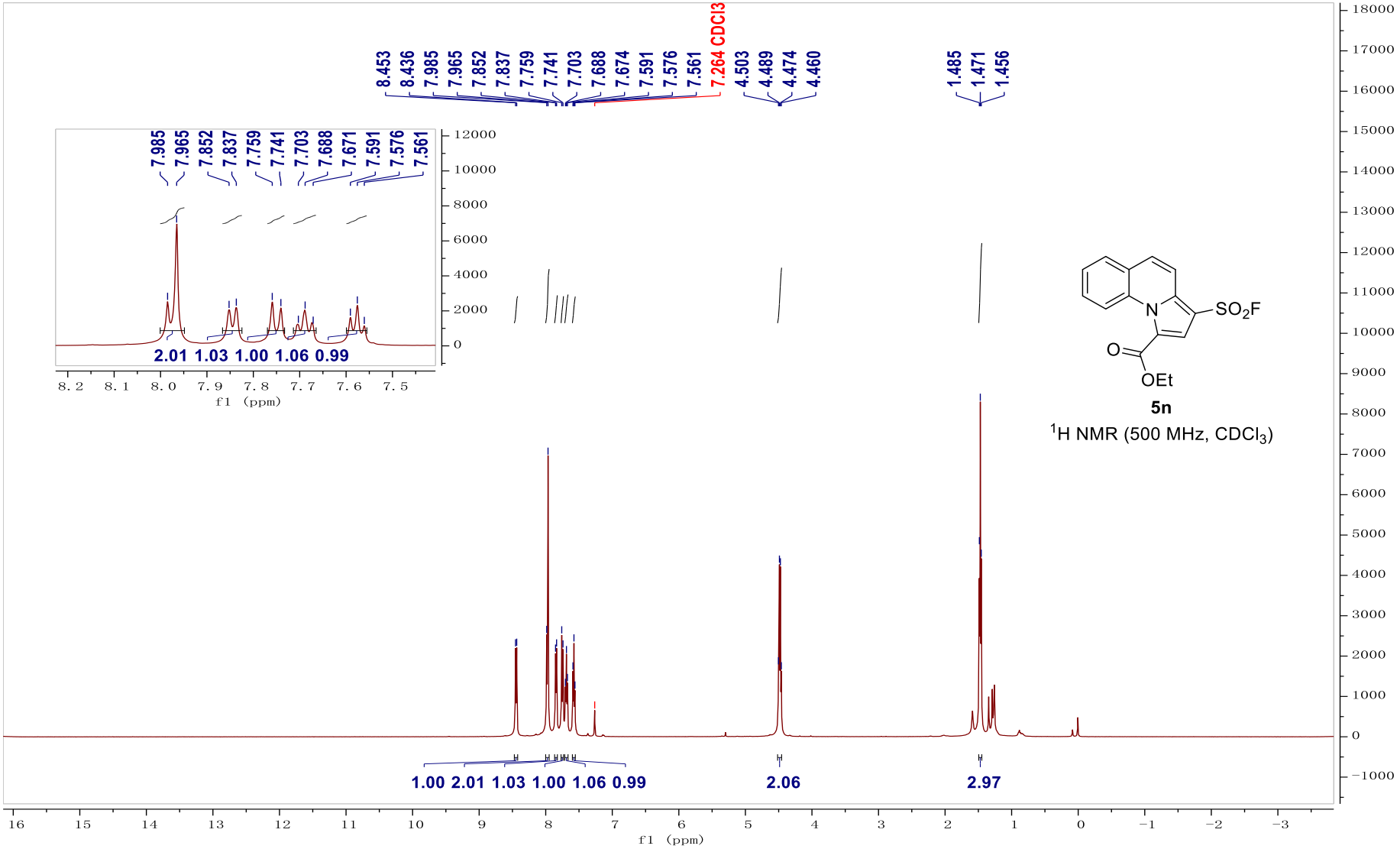

72.127
N
SO2F
O
CN
5l
19FNMR (471 MHz, CDCl3)
2500
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
50
0
−50
−100
−150
−200
−250
f1 (ppm)

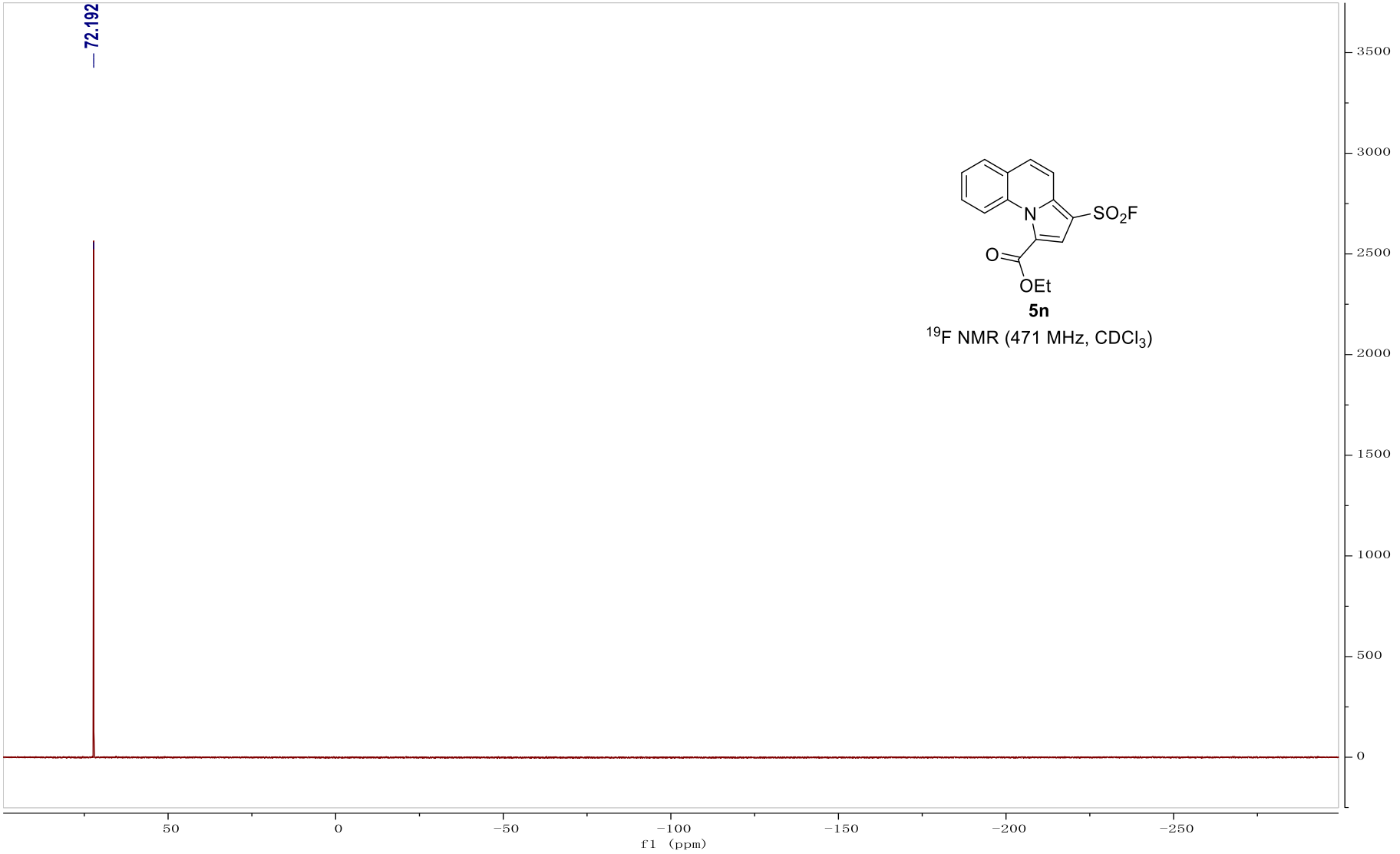

182.688
140.923
139.192
132.852
132.751
132.042
130.540
130.111
129.679
128.306
128.056
127.043
125.168
120.308
117.864
117.030
115.128
106.717
106.472
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
N
SO2F
O
CN
5l
13C NMR (126 MHz, CDCl3)
f1 (ppm)

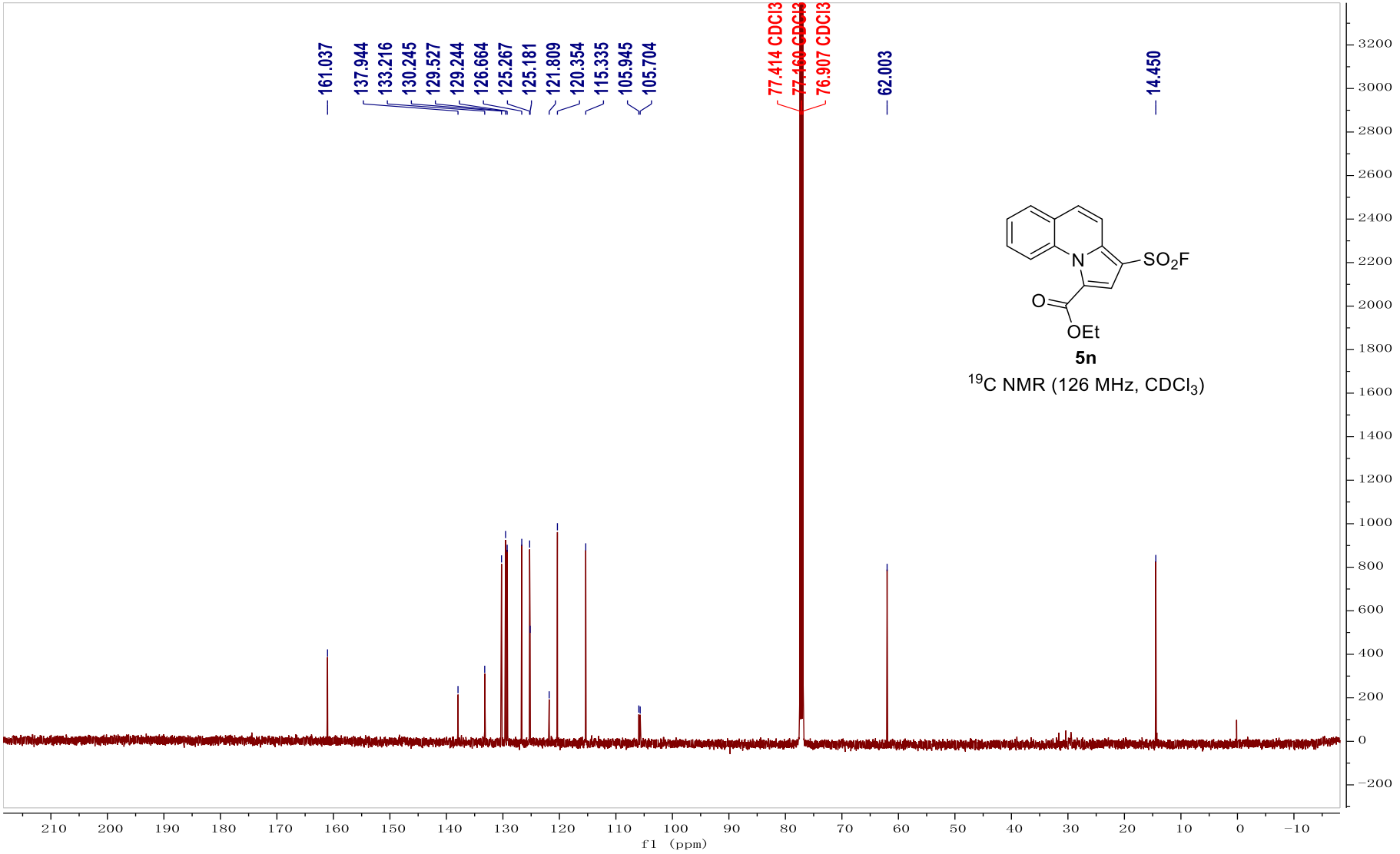

7.990
7.935
7.844
7.809
7.788
7.622
7.545
7.264 CDCl3
8.01
1.04
1.02
f1 (ppm)
5m
1H NMR (500 MHz, CDCl3)
SO2F
N
O
S
f1 (ppm)

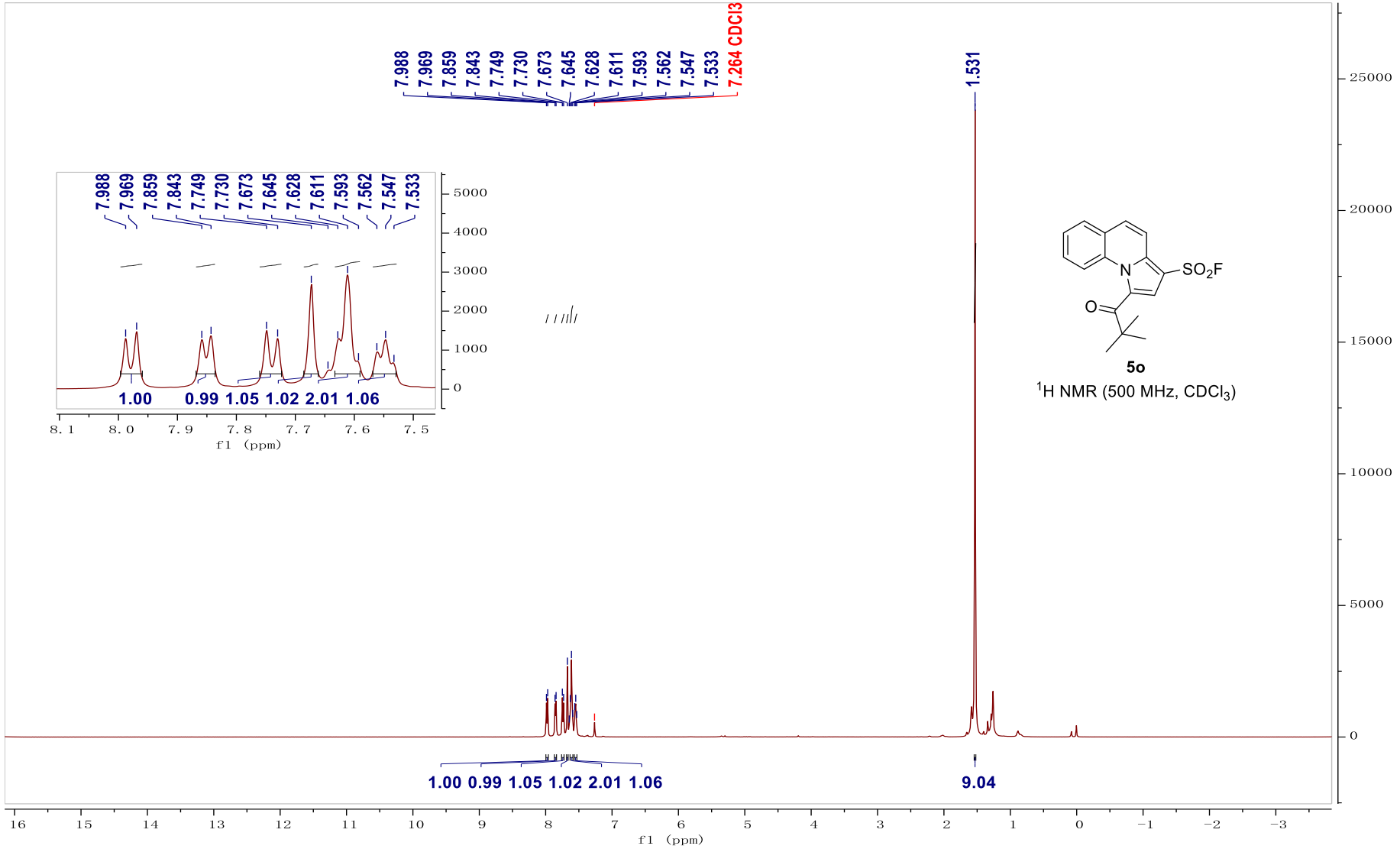

72.416
N
SO2F
O
S
5m
19FNMR (471 MHz, CDCl3)
50
0
−50
−100
−150
−200
−250
f1 (ppm)

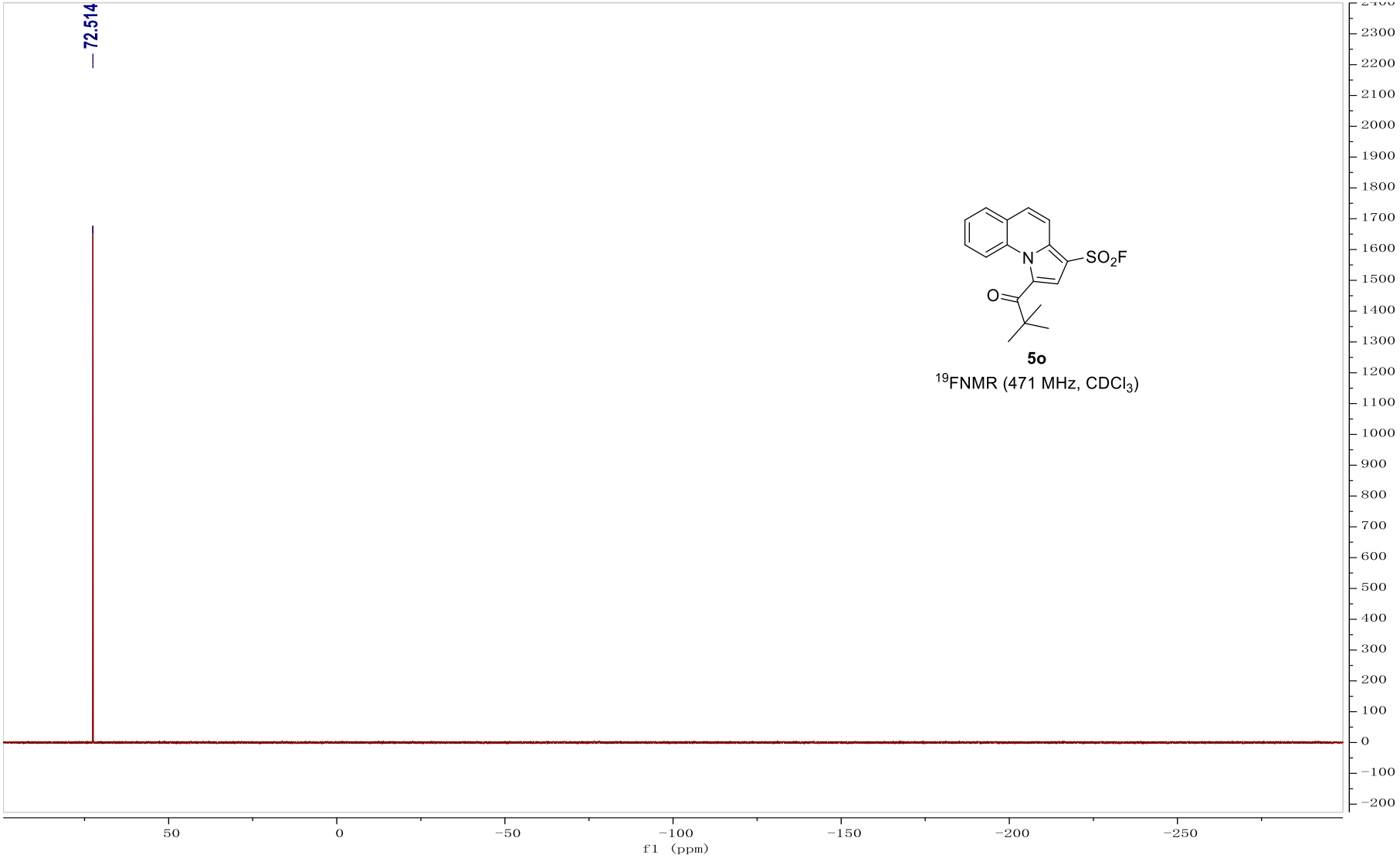

177.198
143.609
138.260
135.791
135.296
132.737
130.942
129.990
129.513
128.648
127.953
126.634
125.798
124.960
119.975
115.163
105.826
105.586
77.414 CDCl3
77.160 CDCl3
76.907 CDCl3
SO2F
N
O
S
5m
13C NMR (126 MHz, CDCl3)
f1 (ppm)

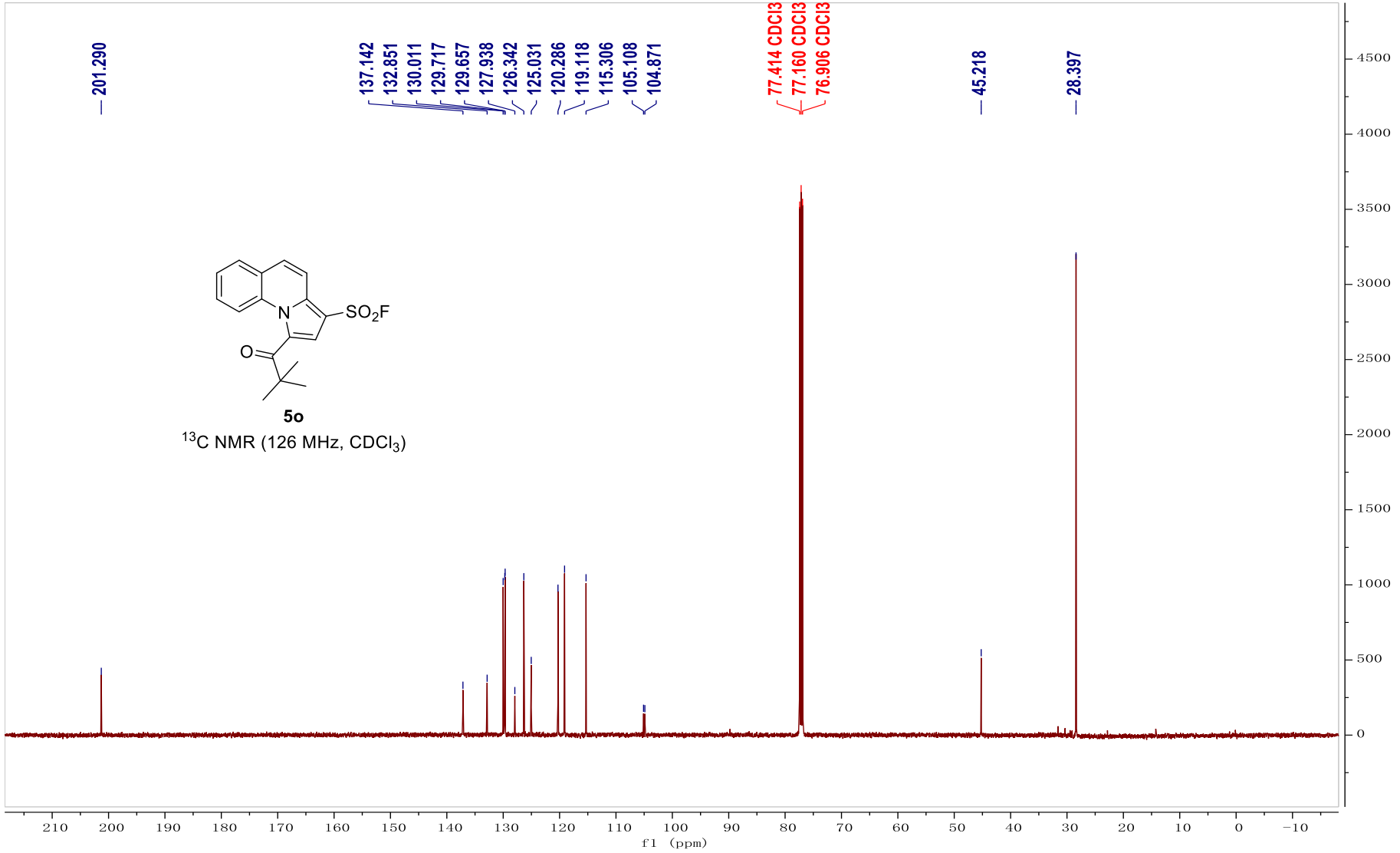

8.453
8.436
7.985
7.965
7.852
7.837
7.759
7.741
7.703
7.688
7.674
7.591
7.576
7.561
7.264 CDCl3
4.503
4.489
4.474
4.460
1.485
1.471
1.456
2.01 1.03 1.00 1.06 0.99
f1 (ppm)
1.00 2.01 1.03 1.00 1.06 0.99
2.06
2.97
f1 (ppm)
SO2F
N
O
OEt
5n
1H NMR (500 MHz, CDCl3)


72.192
3500
3000
2500
2000
1500
1000
500
0
50
0
−50
−100
−150
−200
−250
f1 (ppm)
N
SO2F
O
OEt
5n
19F NMR (471 MHz, CDCl3)


161.037
137.944
133.216
130.245
129.527
129.244
126.664
125.267
125.181
121.809
120.354
115.335
105.945
105.704
77.414 CDCl3
77.160 CDCl3
76.907 CDCl3
62.003
14.450
N
SO2F
O
OEt
5n
19C NMR (126 MHz, CDCl3)
f1 (ppm)

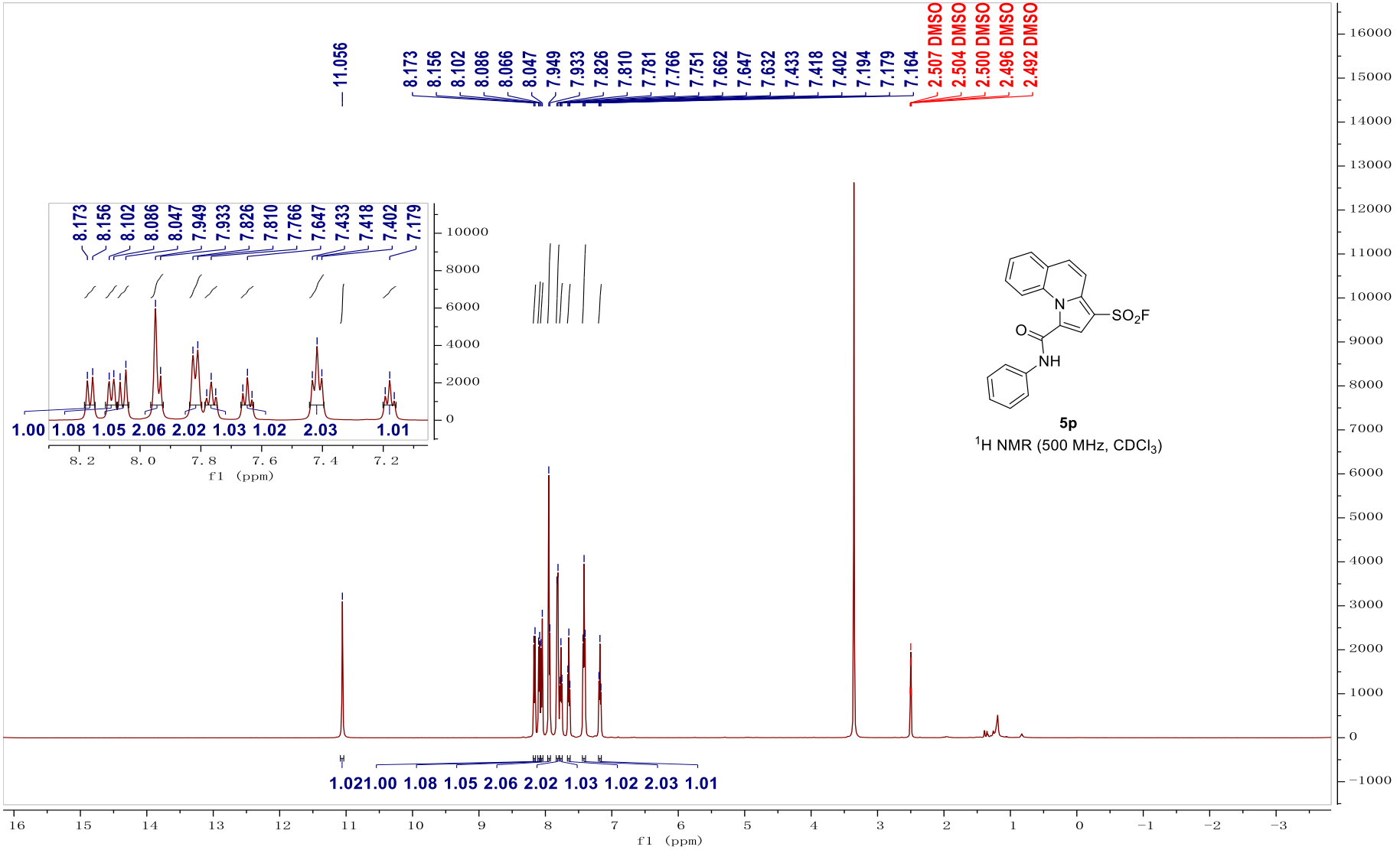

7.988
7.969
7.859
7.843
7.749
7.730
7.673
7.645
7.628
7.611
7.593
7.562
7.547
7.533
7.264 CDCl3
1.531
1.00 0.99 1.05 1.02 2.01 1.06
9.04
f1 (ppm)
SO2F
N
O
5o
1H NMR (500 MHz, CDCl3)

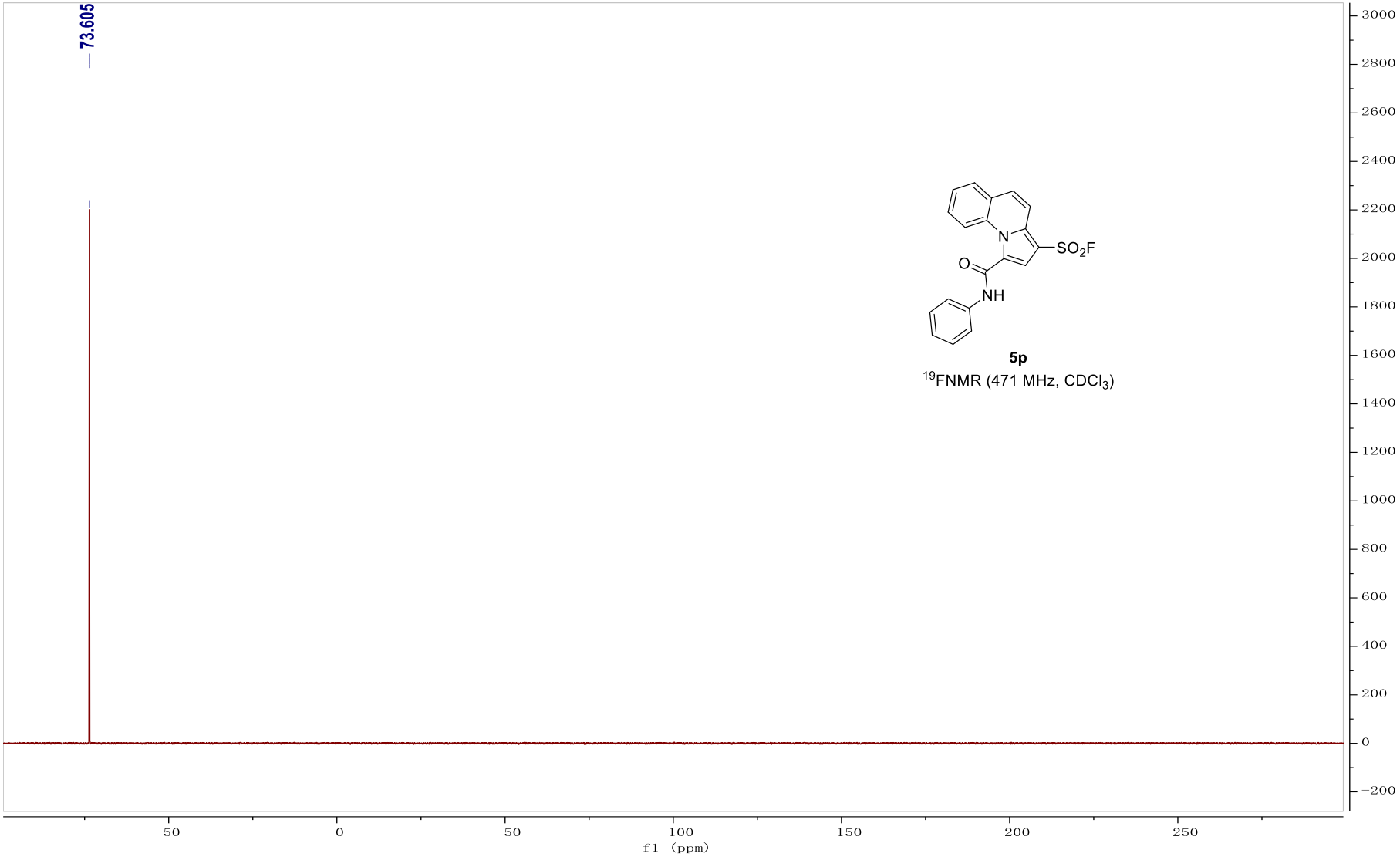

72.514
N
SO2F
O
5o
19FNMR (471 MHz, CDCl3)
50
0
−50
−100
−150
−200
−250
f1 (ppm)



5o

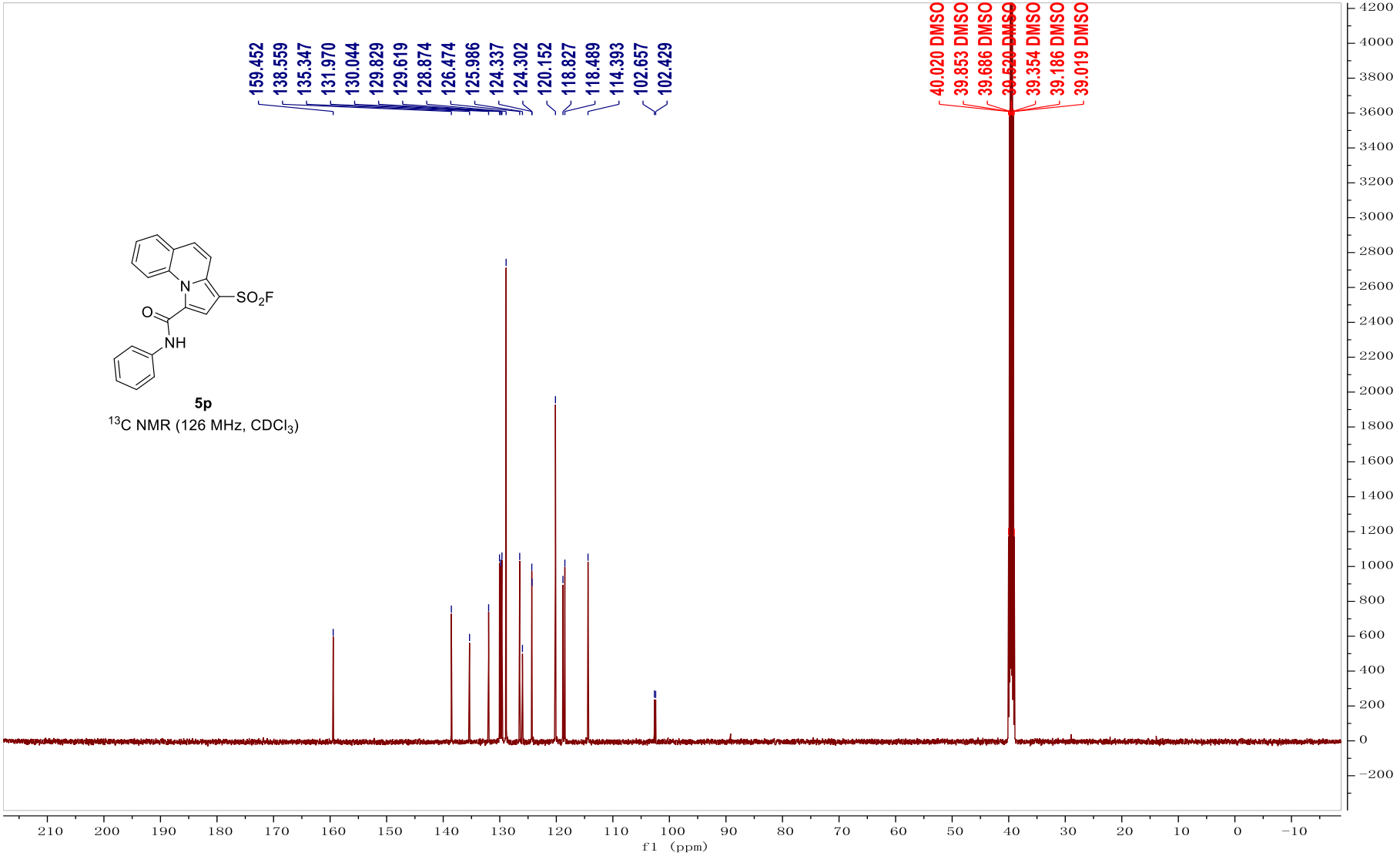
^{13}C NMR (126 MHz, $CDCl_3$)

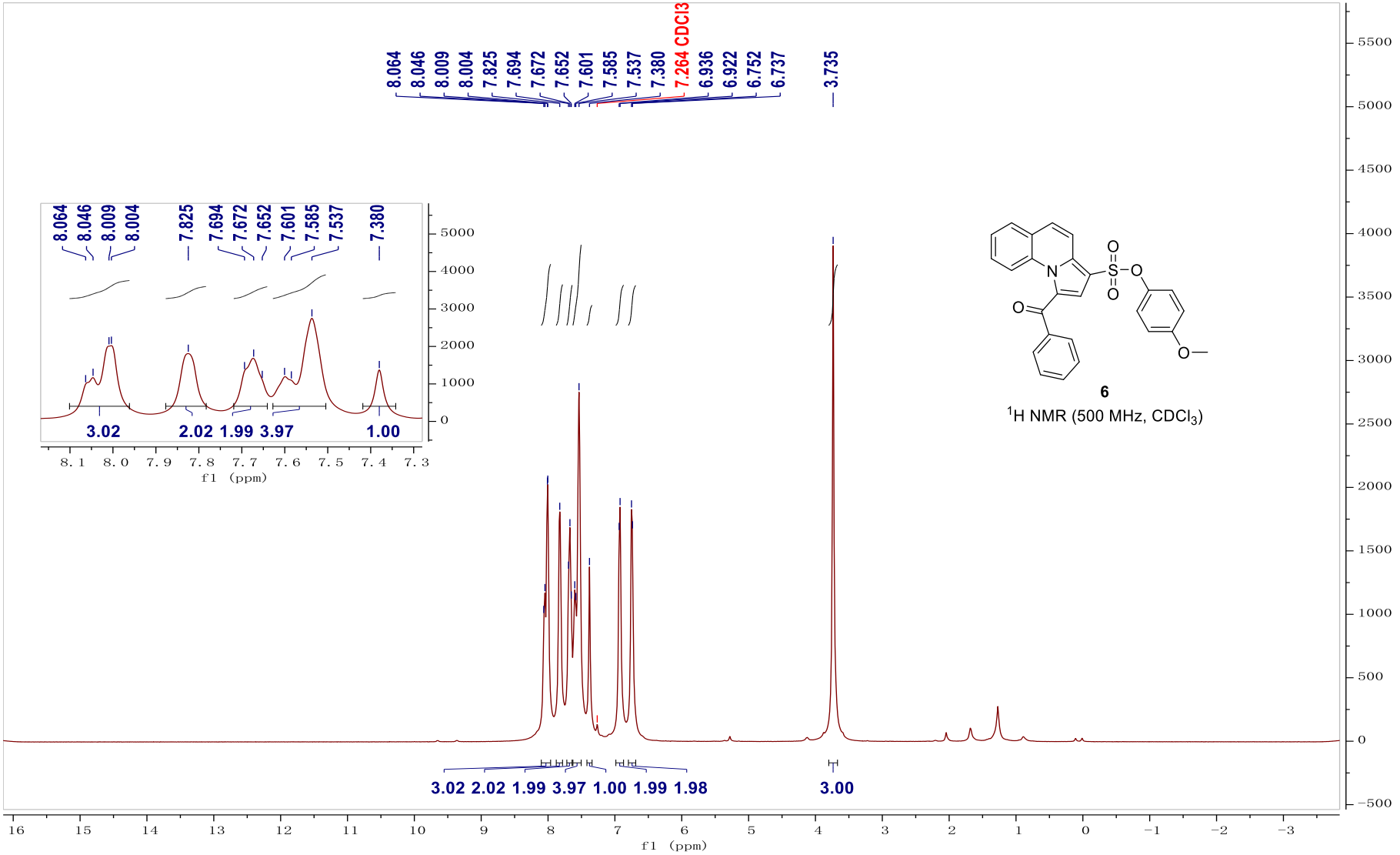

11.056
8.173
8.156
8.102
8.086
8.066
8.047
7.949
7.933
7.826
7.810
7.781
7.766
7.751
7.662
7.647
7.632
7.433
7.418
7.402
7.194
7.179
7.164
2.507 DMSO
2.504 DMSO
2.500 DMSO
2.496 DMSO
2.492 DMSO
1.00 1.08 1.05 2.06 2.02 1.03 1.02 2.03 1.01
f1 (ppm)
1.02 1.00 1.08 1.05 2.06 2.02 1.03 1.02 2.03 1.01
f1 (ppm)
N
O
NH
SO2F
5p
1H NMR (500 MHz, CDCl3)

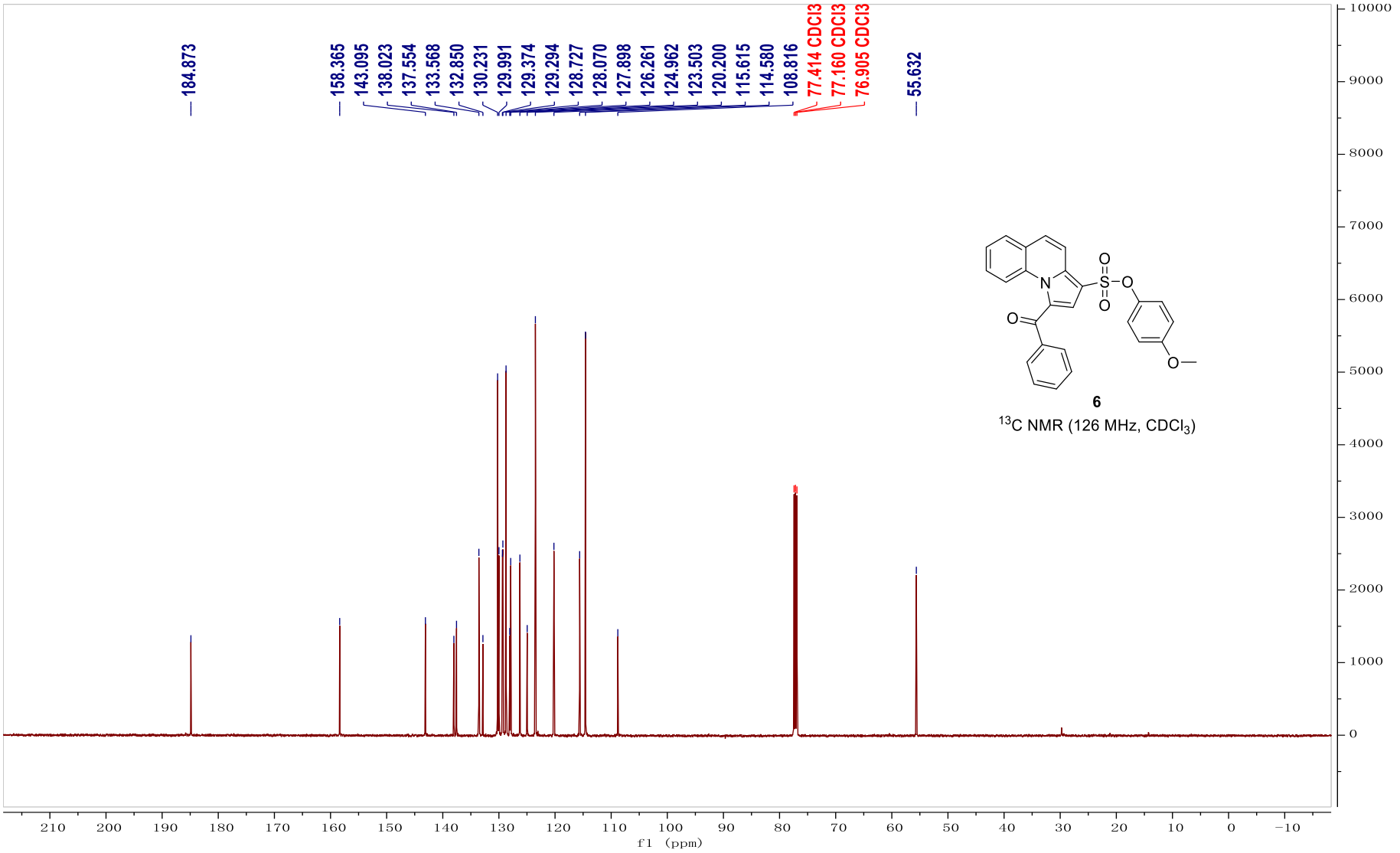


5p

^{19}FNMR (471 MHz, $CDCl_3$)

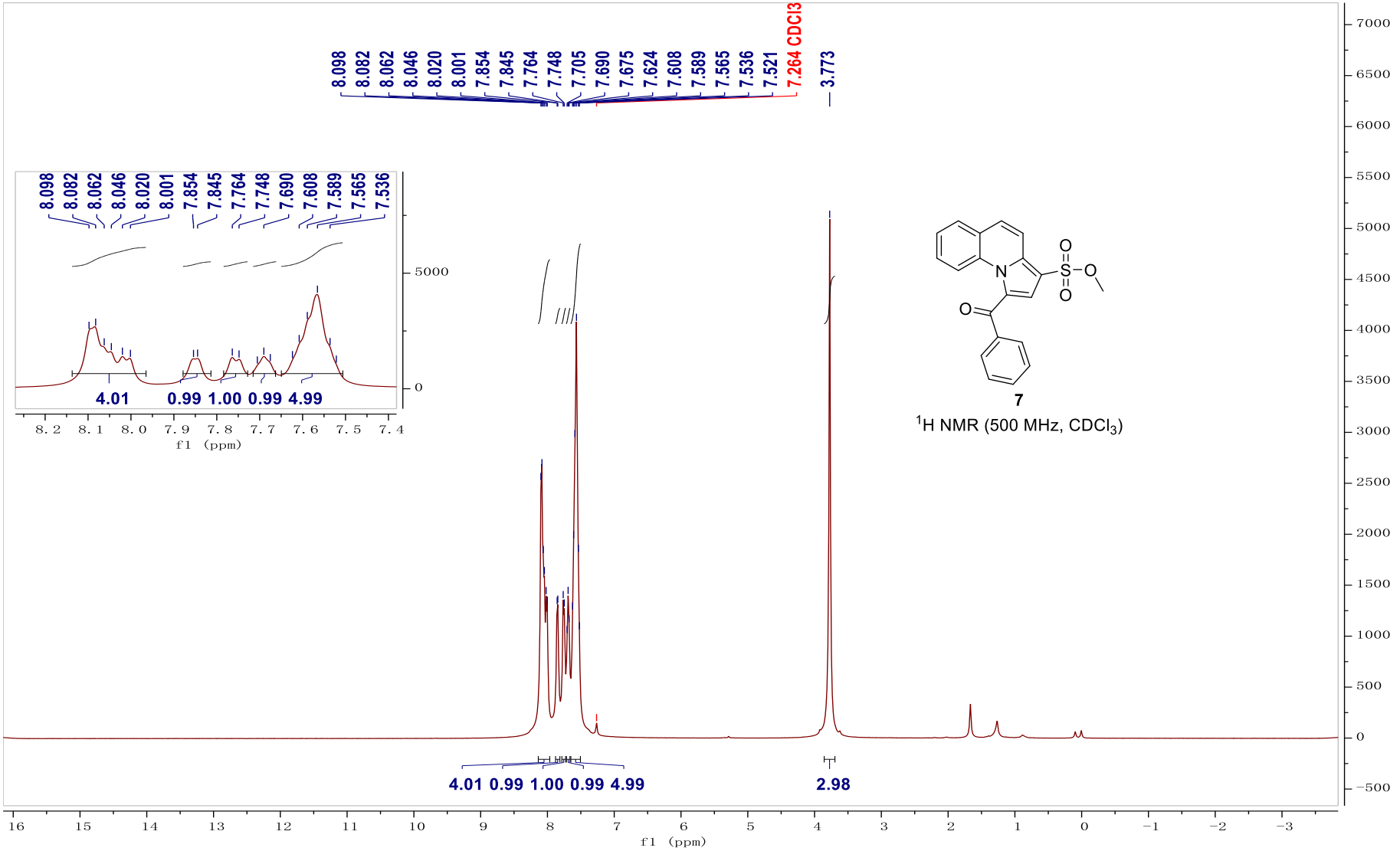

159.452
138.559
135.347
131.970
130.044
129.829
129.619
128.874
126.474
125.986
124.337
124.302
120.152
118.827
118.489
114.393
102.657
102.429
40.020 DMSO
39.853 DMSO
39.686 DMSO
39.520 DMSO
39.354 DMSO
39.186 DMSO
39.019 DMSO
SO2F
O
NH
5p
13C NMR (126 MHz, CDCl3)
f1 (ppm)

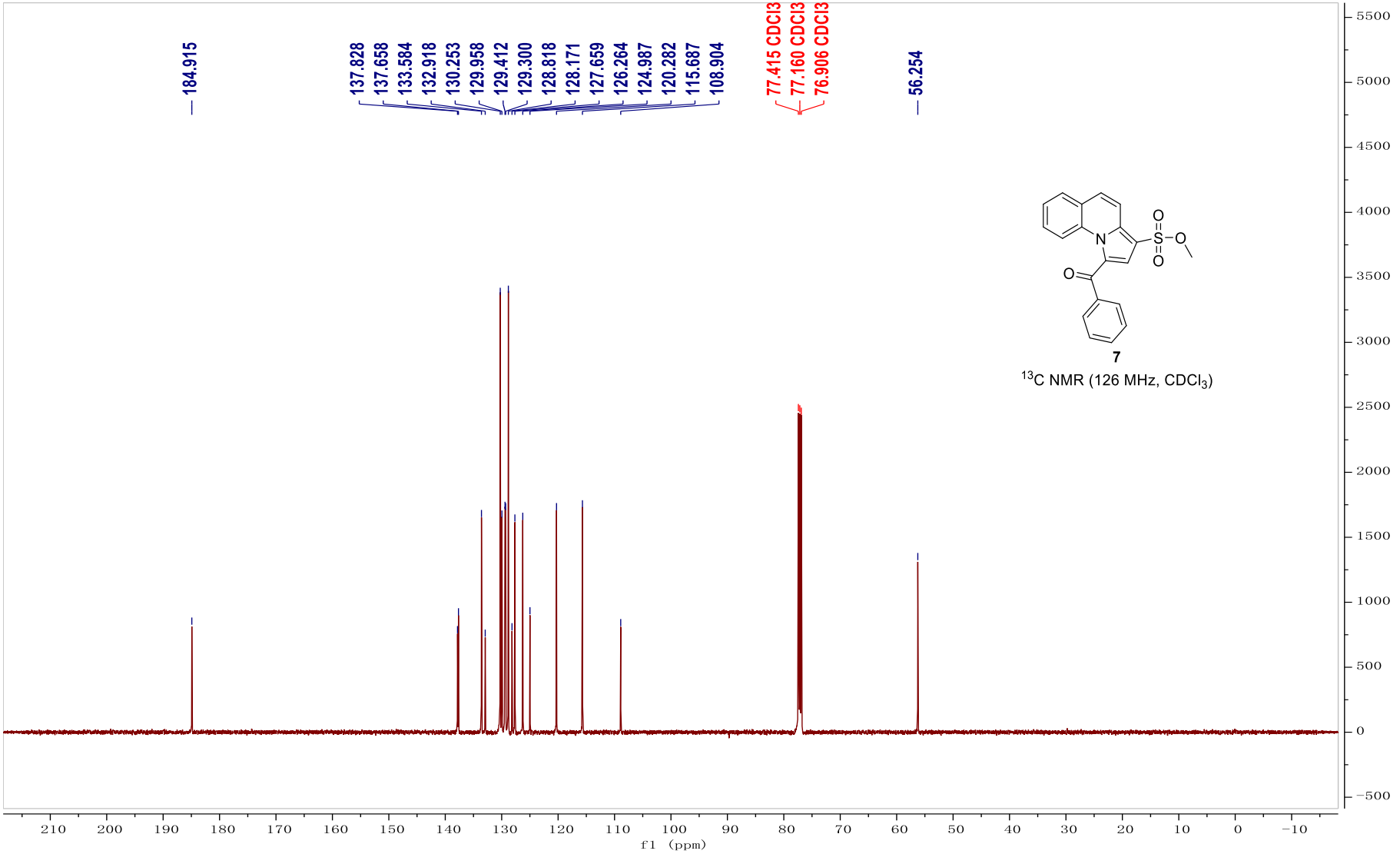

8.064
8.046
8.009
8.004
7.825
7.694
7.672
7.652
7.601
7.585
7.537
7.380
7.264 CDCl3
6.936
6.922
6.752
6.737
3.735
3.02 2.02 1.99 3.97 1.00 1.99 1.98
3.00
f1 (ppm)
3.02
2.02 1.99 3.97
1.00
6
1H NMR (500 MHz, CDCl3)

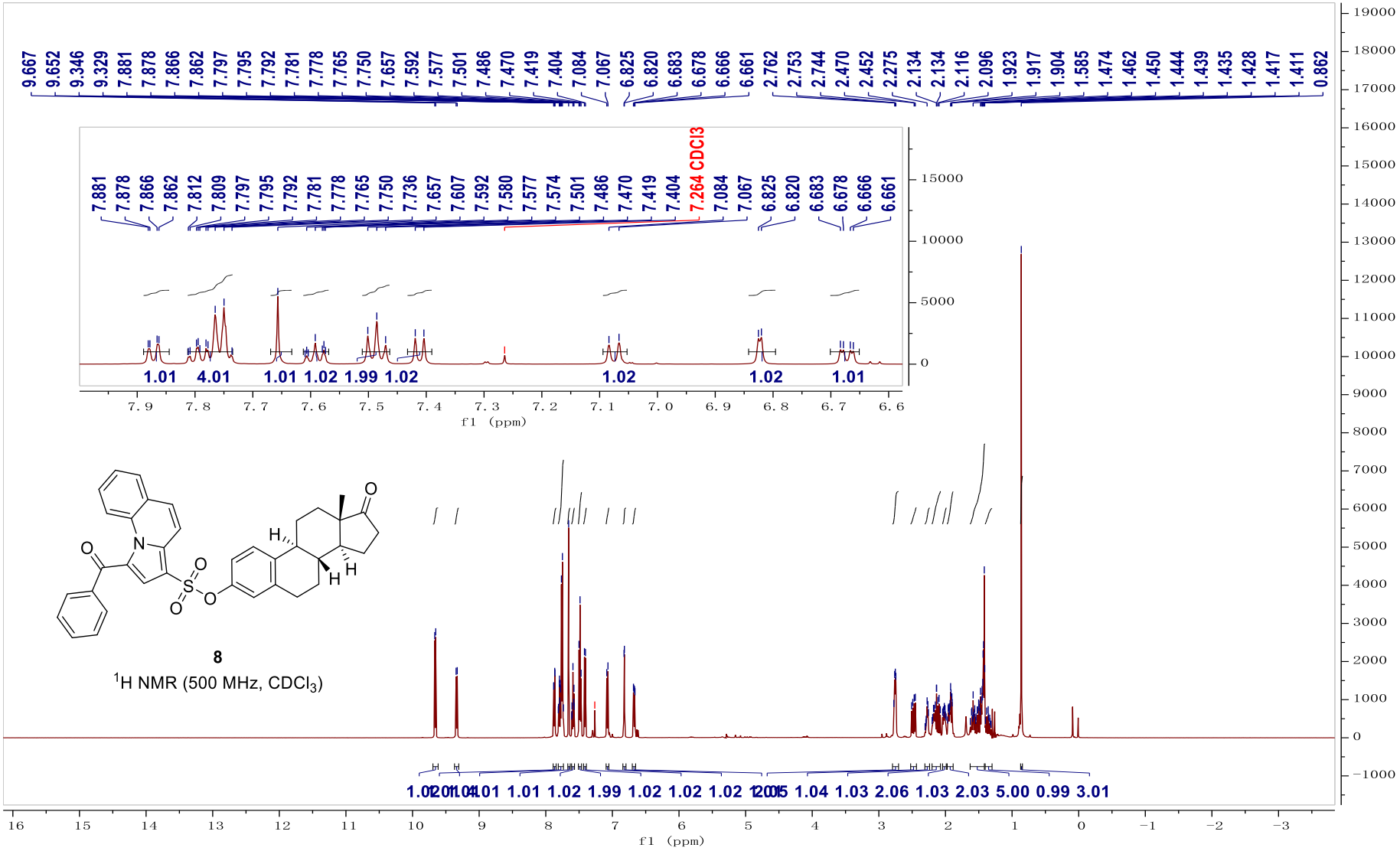


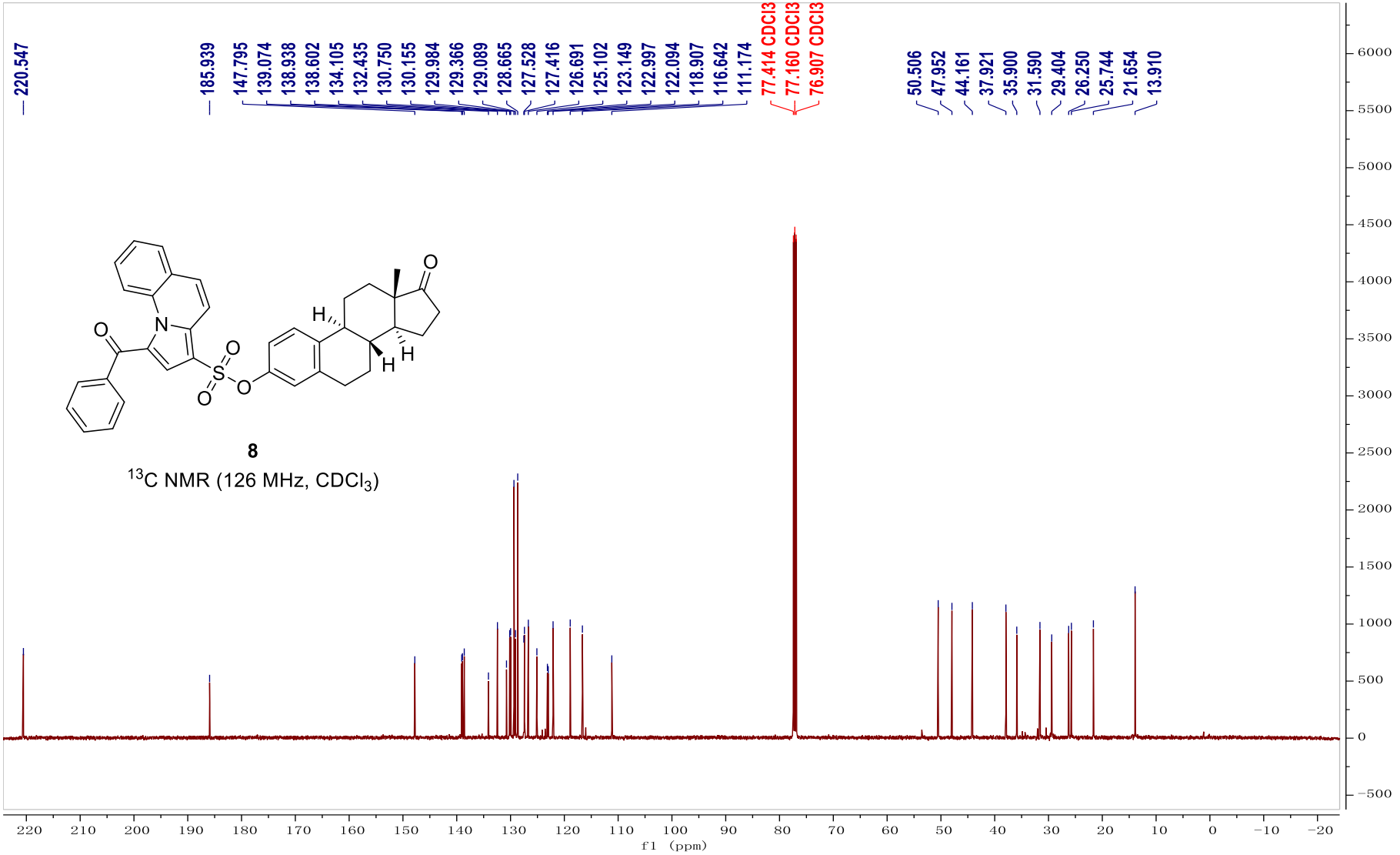
6

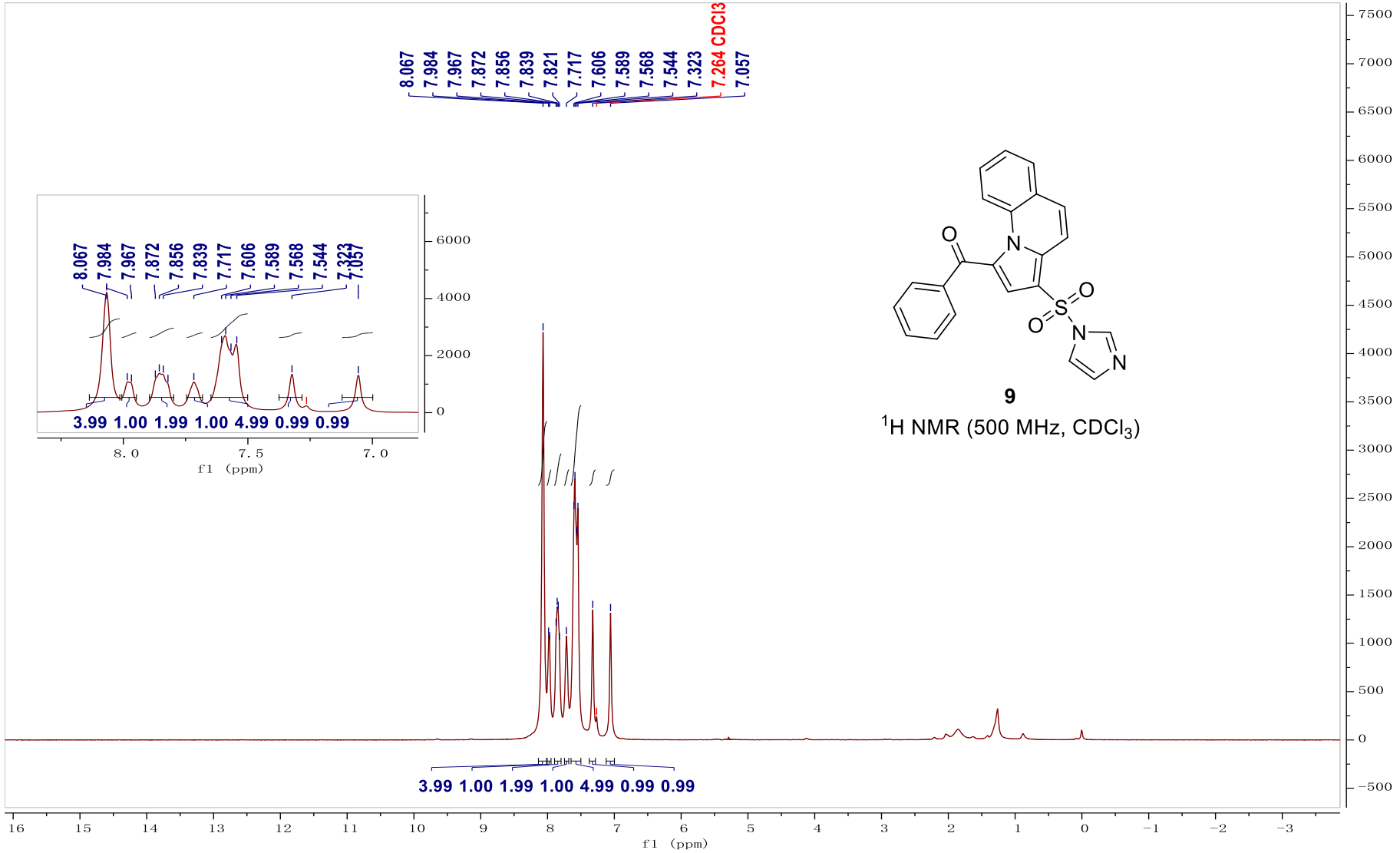
^{13}C NMR (126 MHz, $CDCl_3$)

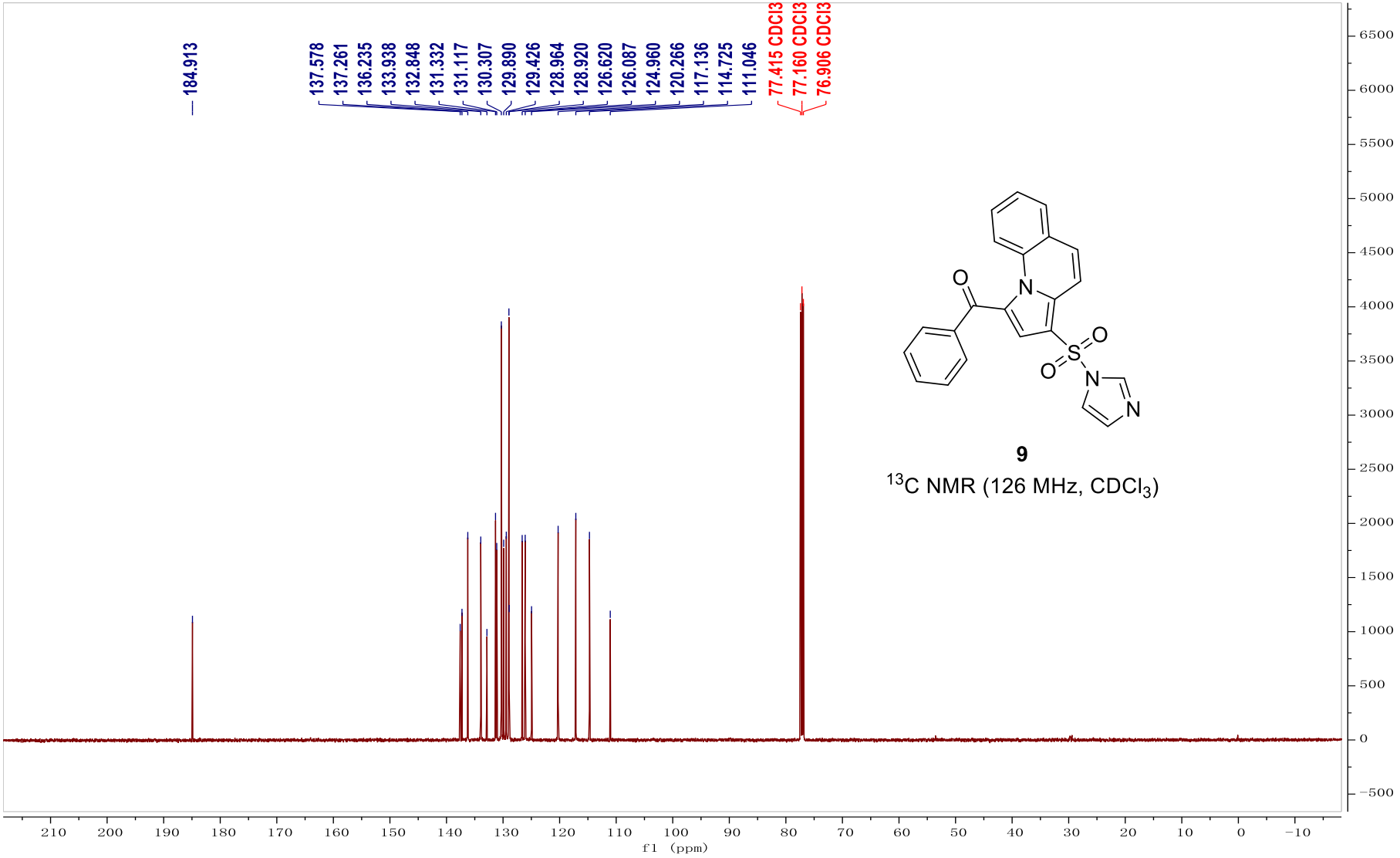

8.098
8.082
8.062
8.046
8.020
8.001
7.854
7.845
7.764
7.748
7.705
7.690
7.675
7.624
7.608
7.589
7.565
7.536
7.521
7.264 CDCl3
3.773
4.01 0.99 1.00 0.99 4.99
2.98
f1 (ppm)
7
1H NMR (500 MHz, CDCl3)

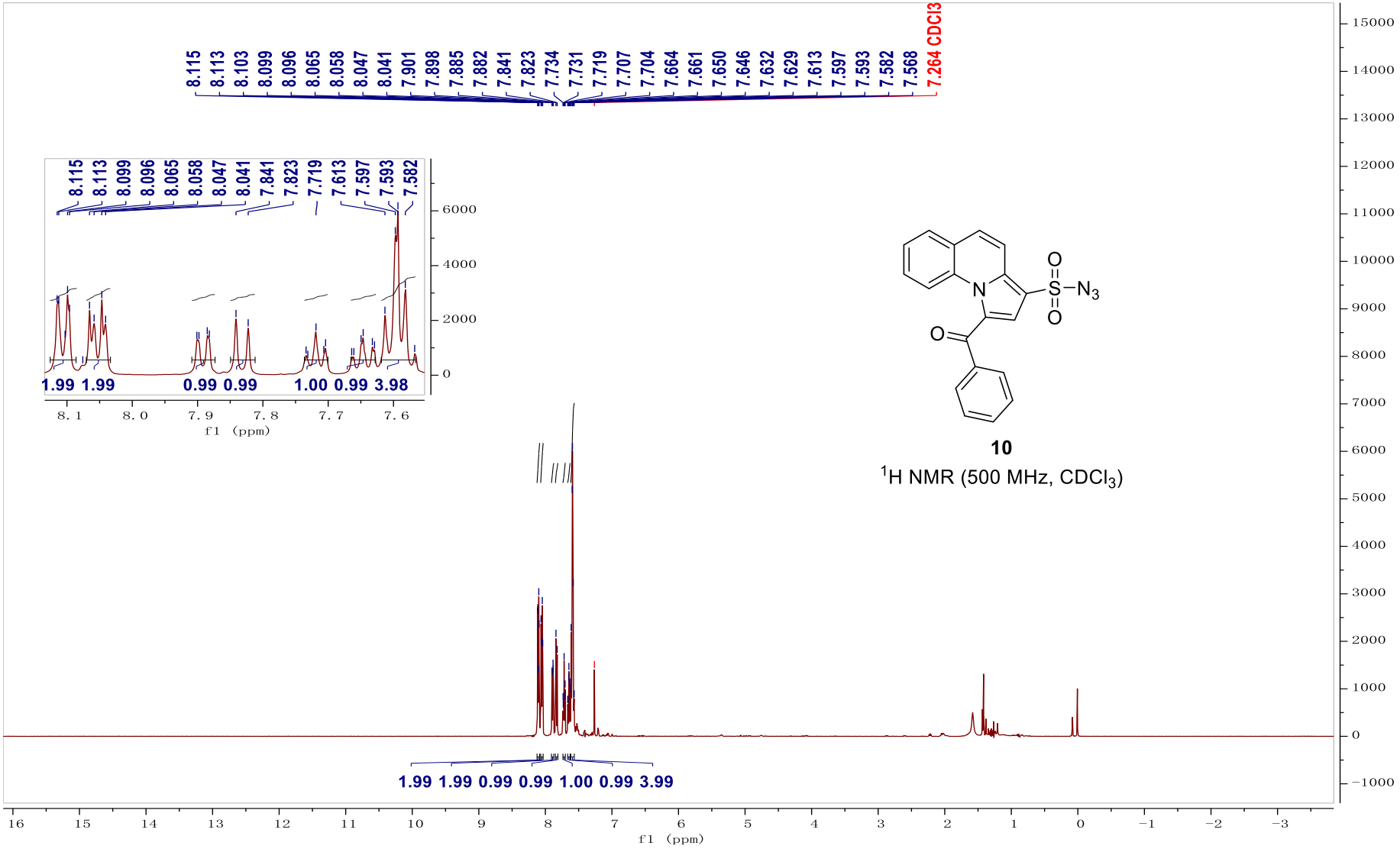

184.915
137.828
137.658
133.584
132.918
130.253
129.958
129.412
129.300
128.818
128.171
127.659
126.264
124.987
120.282
115.687
108.904
77.415 CDCl3
77.160 CDCl3
76.906 CDCl3
56.254
7
13C NMR (126 MHz, CDCl3)
f1 (ppm)

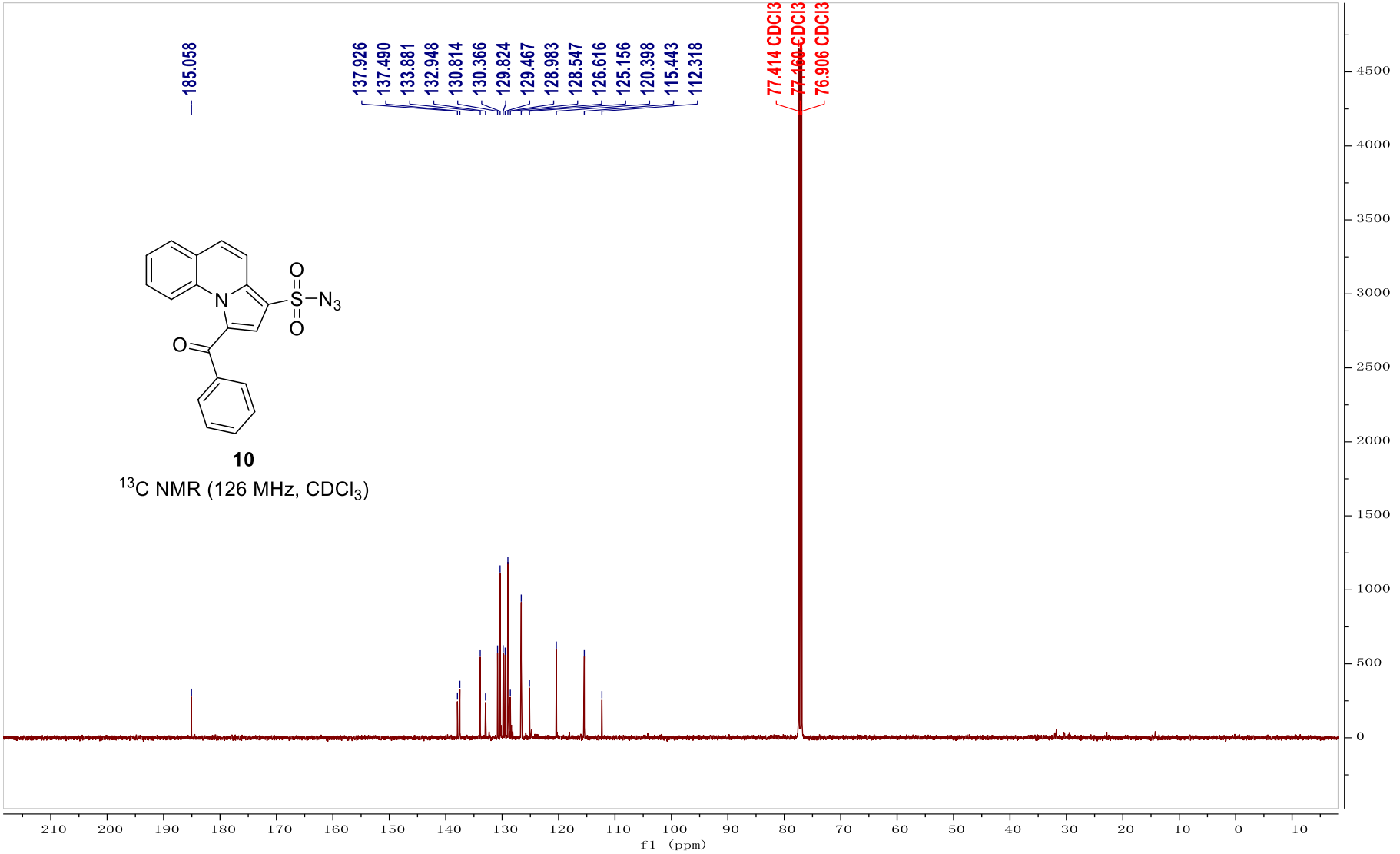

9.667 9.652 9.346 9.329 7.881 7.878 7.866 7.862 7.797 7.795 7.792 7.781 7.778 7.765 7.750 7.657 7.592 7.577 7.501 7.486 7.470 7.419 7.404 7.084 7.067 6.825 6.820 6.683 6.678 6.666 6.661 2.762 2.753 2.744 2.470 2.452 2.275 2.134 2.134 2.116 2.096 1.923 1.917 1.904 1.585 1.474 1.462 1.450 1.444 1.439 1.435 1.428 1.417 1.411 0.862
7.881 7.878 7.866 7.862 7.812 7.809 7.797 7.795 7.792 7.781 7.778 7.765 7.750 7.736 7.657 7.607 7.592 7.580 7.577 7.574 7.501 7.486 7.470 7.419 7.404 7.264 CDCl3 7.084 7.067 6.825 6.820 6.683 6.678 6.666 6.661
1.01 4.01 1.01 1.02 1.99 1.02 1.02 1.02 1.01
f1 (ppm)
1.01 2.01 1.04 1.01 1.01 1.02 1.99 1.02 1.02 1.02 2.05 1.04 1.03 2.06 1.03 2.03 5.00 0.99 3.01
f1 (ppm)
8
1H NMR (500 MHz, CDCl3)


220.547
185.939
147.795
139.074
138.938
138.602
134.105
132.435
130.750
130.155
129.984
129.366
129.089
128.665
127.528
127.416
126.691
125.102
123.149
122.997
122.094
118.907
116.642
111.174
77.414 CDCl3
77.160 CDCl3
76.907 CDCl3
50.506
47.952
44.161
37.921
35.900
31.590
29.404
26.250
25.744
21.654
13.910
O
N
O
S
O
O
H
H
H
8
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.067
7.984
7.967
7.872
7.856
7.839
7.821
7.717
7.606
7.589
7.568
7.544
7.323
7.264 CDCl3
7.057
3.99 1.00 1.99 1.00 4.99 0.99 0.99
f1 (ppm)
O
N
O
S
O
N
N
9
1H NMR (500 MHz, CDCl3)

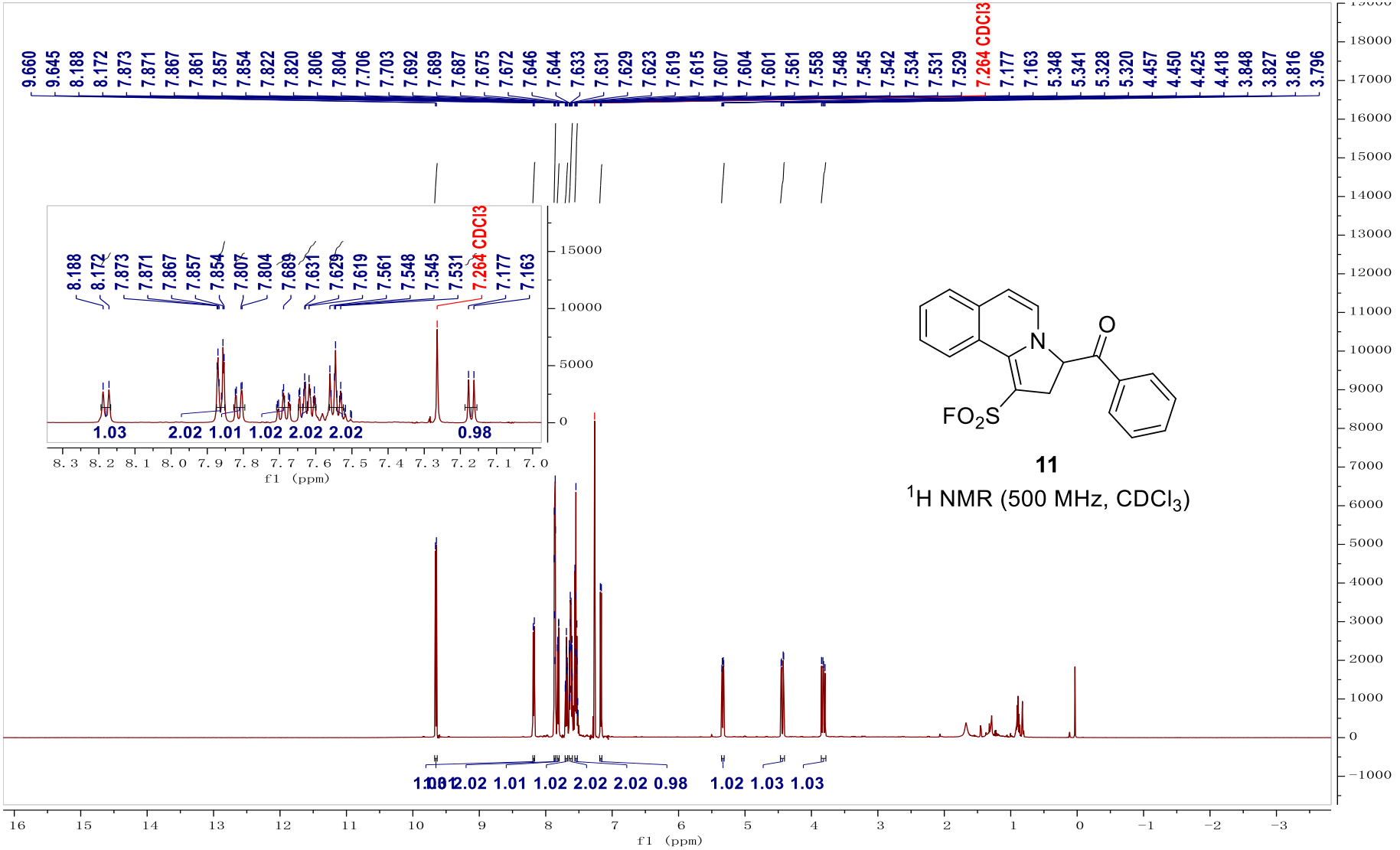

184.913
137.578
137.261
136.235
133.938
132.848
131.332
131.117
130.307
129.890
129.426
128.964
128.920
126.620
126.087
124.960
120.266
117.136
114.725
111.046
77.415 CDCl3
77.160 CDCl3
76.906 CDCl3
O
N
O
S
O
O
N
N
9
13C NMR (126 MHz, CDCl3)
f1 (ppm)

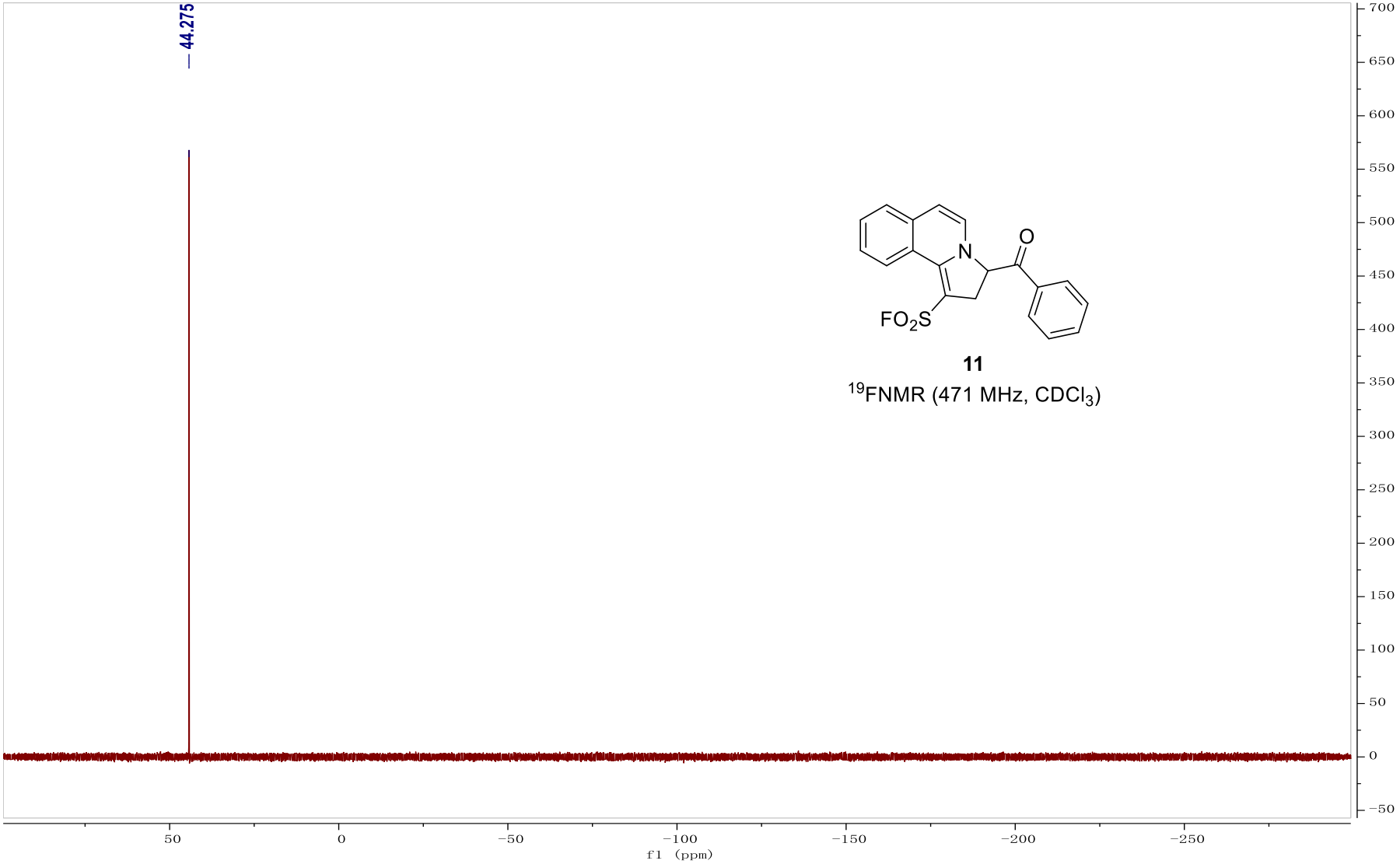

8.115
8.113
8.103
8.099
8.096
8.065
8.058
8.047
8.041
7.901
7.898
7.885
7.882
7.841
7.823
7.734
7.731
7.719
7.707
7.704
7.664
7.661
7.650
7.646
7.632
7.629
7.613
7.597
7.593
7.582
7.568
7.264 CDCl3
1.99 1.99 0.99 0.99 1.00 0.99 3.98
f1 (ppm)
10
1H NMR (500 MHz, CDCl3)
1.99 1.99 0.99 0.99 1.00 0.99 3.99
f1 (ppm)

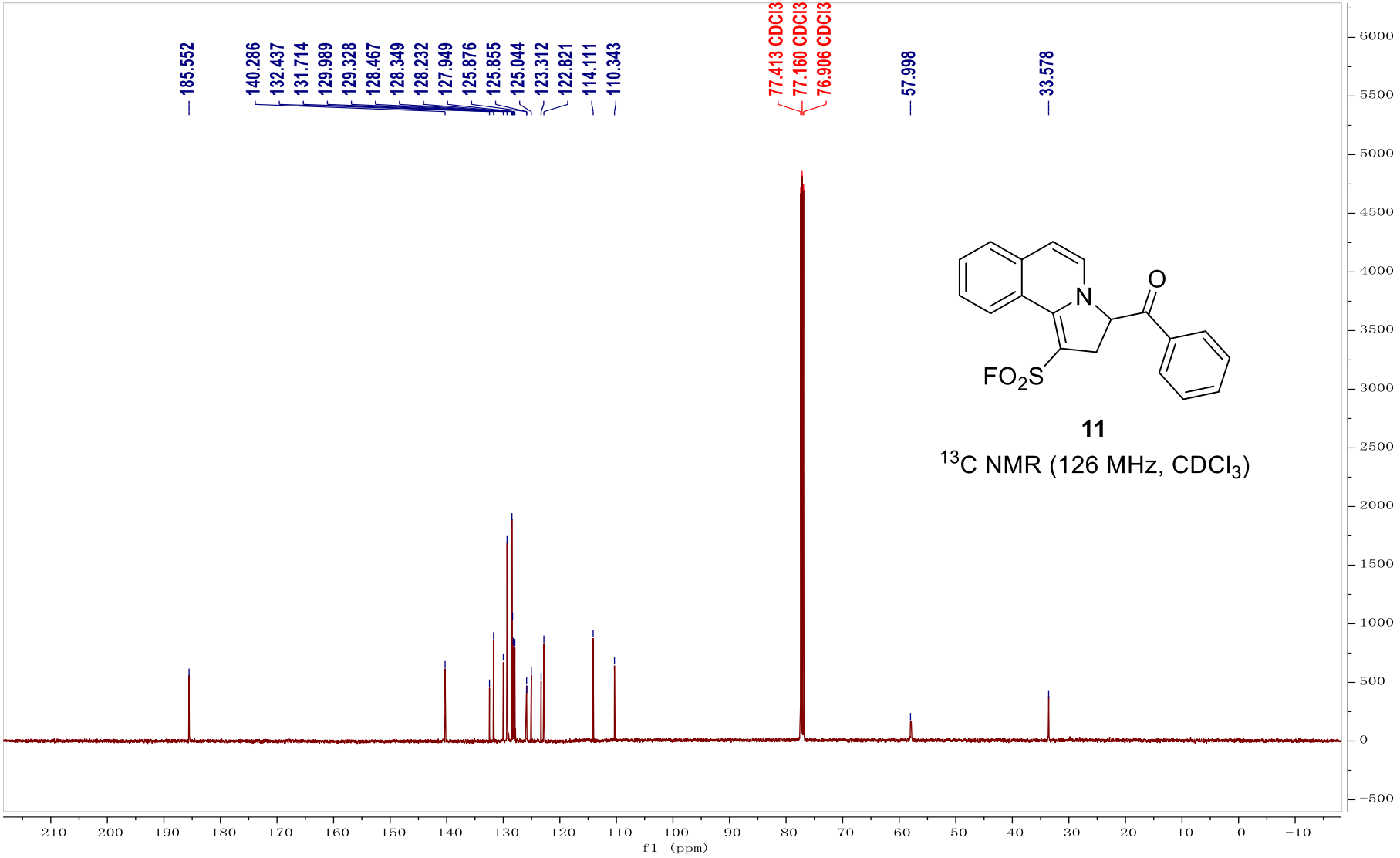


10

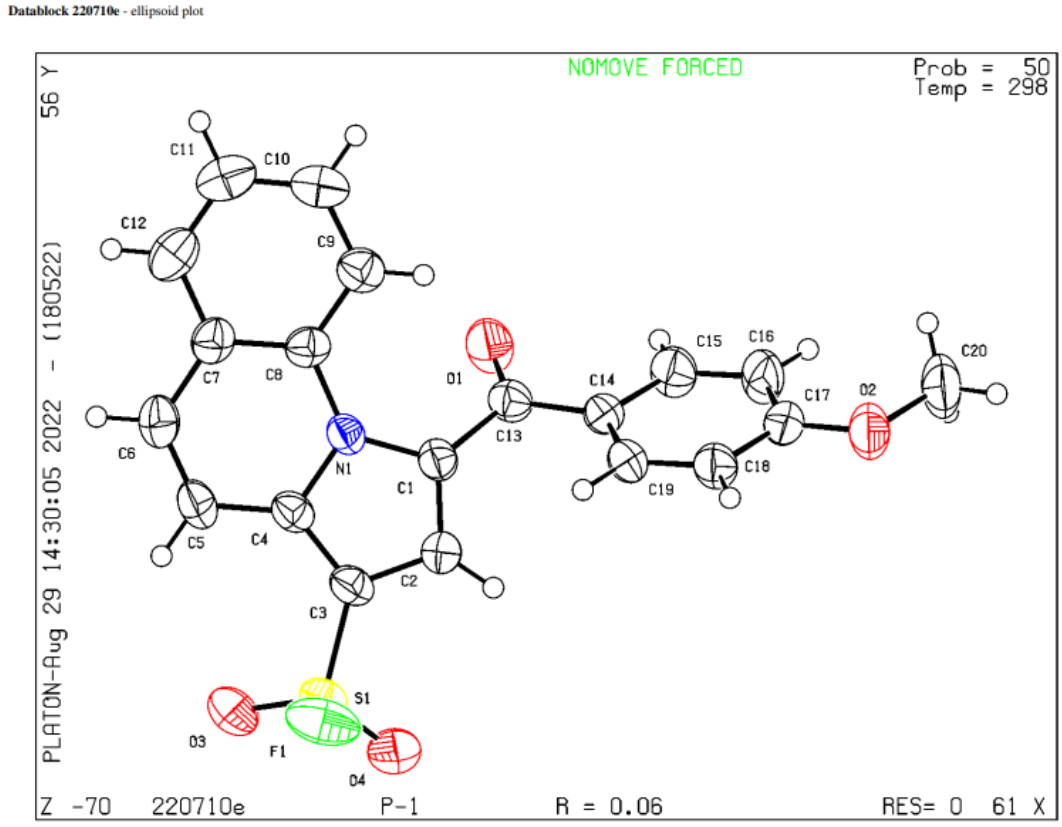
^{13}C NMR (126 MHz, $CDCl_3$)


9.660 9.645 8.188 8.172 7.873 7.871 7.867 7.861 7.857 7.854 7.822 7.820 7.806 7.804 7.706 7.703 7.692 7.689 7.687 7.675 7.672 7.646 7.644 7.633 7.631 7.629 7.623 7.619 7.615 7.607 7.604 7.601 7.561 7.558 7.548 7.545 7.542 7.534 7.531 7.529 7.264 CDCl3 7.177 7.163 5.348 5.341 5.328 5.320 4.457 4.450 4.425 4.418 3.848 3.827 3.816 3.796
1.03 2.02 1.01 1.02 2.02 2.02 0.98
f1 (ppm)
1.03 2.02 1.01 1.02 2.02 2.02 0.98 1.02 1.03 1.03
f1 (ppm)
O
N
FO2S
11
1H NMR (500 MHz, CDCl3)


44.275
O
N
FO2S
11
19FNMR (471 MHz, CDCl3)
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
50
0
−50
−100
−150
−200
−250
f1 (ppm)


185.552
140.286
132.437
131.714
129.989
129.328
128.467
128.349
128.232
127.949
125.876
125.855
125.044
123.312
122.821
114.111
110.343
77.413 CDCl3
77.160 CDCl3
76.906 CDCl3
57.998
33.578
O
N
FO2S
11
13C NMR (126 MHz, CDCl3)
f1 (ppm)

7. Data of Crystal Structure of 5g.



Approximately 150 mg of the purified compound **5g** was dissolved in $CHCl_3$ and placed under dark conditions to evaporate slowly. After several days, colorless crystals were obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart-1000 CDCC diffractometer (graphite-monochromated Mo Kα radiation, λ=0.71073 nm) at 293(2) K. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2204064).

Table S9 Crystal data and structure refinement for 220710e

Identification code	220710e
Empirical formula	$C_{20}H_{14}FNO_4S$
Formula weight	383.38
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1

Unit cell dimensions	a = 4.5757(4) A alpha = 76.640(2) deg. b = 10.3900(11) A beta = 83.509(3) deg. c = 18.9149(18) A gamma = 83.568(3) deg.
Volume	865.86(14) A^3
Z, Calculated density	2, 1.470 Mg/m^3
Absorption coefficient	0.224 mm^-1
F(000)	396
Crystal size	0.45 x 0.23 x 0.11 mm
Theta range for data collection	2.08 to 25.02 deg.
Limiting indices	-5<=h<=5, -12<=k<=12, -17<=l<=22
Reflections collected / unique	4275 / 2988 [R(int) = 0.0361]
Completeness to theta = 25.02	97.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9757 and 0.9057
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2988 / 0 / 245
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0633, wR2 = 0.1493
R indices (all data)	R1 = 0.0922, wR2 = 0.1613
Largest diff. peak and hole	0.253 and -0.377 e.A^{-3}

Table S10 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 220710e.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	-3136(2)	3863(1)	3357(1)	47(1)
F(1)	-623(5)	2754(2)	3600(2)	78(1)
N(1)	789(6)	7139(3)	3028(1)	37(1)
O(1)	469(7)	9120(2)	1626(1)	61(1)
O(2)	8072(8)	6697(3)	-867(2)	72(1)
O(3)	-4970(6)	3898(3)	4004(2)	71(1)
O(4)	-4197(7)	3511(3)	2759(2)	66(1)
C(1)	1097(8)	6912(3)	2311(2)	41(1)
C(2)	-129(8)	5750(3)	2342(2)	42(1)
C(3)	-1285(8)	5268(3)	3070(2)	43(1)
C(4)	-714(7)	6135(3)	3493(2)	40(1)
C(5)	-1428(8)	6171(4)	4238(2)	48(1)
C(6)	-538(9)	7158(4)	4494(2)	51(1)
C(7)	1246(8)	8139(3)	4038(2)	44(1)
C(8)	2035(7)	8097(3)	3303(2)	40(1)
C(9)	4033(8)	8948(3)	2878(2)	48(1)
C(10)	5106(9)	9887(4)	3170(3)	59(1)
C(11)	4209(10)	9996(4)	3884(3)	64(1)
C(12)	2387(9)	9106(4)	4318(2)	57(1)
C(13)	1528(8)	7977(3)	1626(2)	44(1)
C(14)	3141(8)	7585(3)	979(2)	40(1)
C(15)	3076(9)	8505(4)	307(2)	54(1)

C(16)	4646(10)	8248(4)	-321(2)	61(1)
C(17)	6381(10)	7052(4)	-285(2)	51(1)
C(18)	6470(9)	6116(3)	377(2)	48(1)
C(19)	4874(8)	6386(3)	993(2)	45(1)
C(20)	8117(15)	7642(5)	-1553(2)	97(2)

Table S11 Bond lengths [A] and angles [deg] for 220710e

S(1)-O(3)	1.409(3)
S(1)-O(4)	1.415(3)
S(1)-F(1)	1.562(2)
S(1)-C(3)	1.717(3)
N(1)-C(4)	1.391(4)
N(1)-C(1)	1.418(4)
N(1)-C(8)	1.422(4)
O(1)-C(13)	1.231(4)
O(2)-C(17)	1.370(5)
O(2)-C(20)	1.435(5)
C(1)-C(2)	1.374(5)
C(1)-C(13)	1.506(5)
C(2)-C(3)	1.415(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.397(5)
C(4)-C(5)	1.419(5)
C(5)-C(6)	1.350(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.439(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.405(5)
C(7)-C(12)	1.409(5)
C(8)-C(9)	1.398(5)
C(9)-C(10)	1.384(5)
C(9)-H(9)	0.9300
C(10)-C(11)	1.394(6)
C(10)-H(10)	0.9300

C(11)-C(12)	1.375(6)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.473(5)
C(14)-C(19)	1.396(5)
C(14)-C(15)	1.403(5)
C(15)-C(16)	1.383(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.390(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.399(5)
C(18)-C(19)	1.372(5)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
O(3)-S(1)-O(4)	121.11(18)
O(3)-S(1)-F(1)	104.13(18)
O(4)-S(1)-F(1)	104.44(17)
O(3)-S(1)-C(3)	111.28(18)
O(4)-S(1)-C(3)	110.74(17)
F(1)-S(1)-C(3)	103.04(16)
C(4)-N(1)-C(1)	109.1(3)
C(4)-N(1)-C(8)	121.1(3)
C(1)-N(1)-C(8)	129.4(3)
C(17)-O(2)-C(20)	117.6(3)
C(2)-C(1)-N(1)	107.4(3)
C(2)-C(1)-C(13)	124.1(3)

N(1)-C(1)-C(13)	124.4(3)
C(1)-C(2)-C(3)	108.1(3)
C(1)-C(2)-H(2)	125.9
C(3)-C(2)-H(2)	125.9
C(4)-C(3)-C(2)	108.6(3)
C(4)-C(3)-S(1)	127.1(3)
C(2)-C(3)-S(1)	124.3(3)
N(1)-C(4)-C(3)	106.8(3)
N(1)-C(4)-C(5)	120.0(3)
C(3)-C(4)-C(5)	133.2(3)
C(6)-C(5)-C(4)	119.4(3)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
C(5)-C(6)-C(7)	121.5(3)
C(5)-C(6)-H(6)	119.3
C(7)-C(6)-H(6)	119.3
C(8)-C(7)-C(12)	118.4(4)
C(8)-C(7)-C(6)	119.8(3)
C(12)-C(7)-C(6)	121.7(4)
C(9)-C(8)-C(7)	120.2(3)
C(9)-C(8)-N(1)	122.4(3)
C(7)-C(8)-N(1)	117.4(3)
C(10)-C(9)-C(8)	119.7(4)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	120.7(4)
C(9)-C(10)-H(10)	119.6
C(11)-C(10)-H(10)	119.6
C(12)-C(11)-C(10)	119.5(4)

C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2
C(11)-C(12)-C(7)	121.1(4)
C(11)-C(12)-H(12)	119.4
C(7)-C(12)-H(12)	119.4
O(1)-C(13)-C(14)	123.1(3)
O(1)-C(13)-C(1)	119.1(3)
C(14)-C(13)-C(1)	117.8(3)
C(19)-C(14)-C(15)	117.4(3)
C(19)-C(14)-C(13)	124.4(3)
C(15)-C(14)-C(13)	118.1(3)
C(16)-C(15)-C(14)	122.0(4)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(15)-C(16)-C(17)	119.0(4)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
O(2)-C(17)-C(16)	124.4(3)
O(2)-C(17)-C(18)	115.6(4)
C(16)-C(17)-C(18)	120.0(4)
C(19)-C(18)-C(17)	120.0(4)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(14)	121.6(3)
C(18)-C(19)-H(19)	119.2
C(14)-C(19)-H(19)	119.2
O(2)-C(20)-H(20A)	109.5
O(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5

O(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S12 Anisotropic displacement parameters (A^2 x 10^3) for 220710e

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	42(1)	46(1)	52(1)	-6(1)	3(1)	-14(1)
F(1)	64(2)	44(1)	117(2)	8(1)	-18(2)	-9(1)
N(1)	37(2)	34(2)	36(2)	-5(1)	4(1)	-2(1)
O(1)	81(2)	40(2)	53(2)	-5(1)	7(2)	10(1)
O(2)	114(3)	55(2)	43(2)	-13(1)	16(2)	-7(2)
O(3)	62(2)	82(2)	69(2)	-20(2)	23(2)	-35(2)
O(4)	69(2)	72(2)	65(2)	-19(2)	-4(2)	-30(2)
C(1)	44(2)	39(2)	37(2)	-8(2)	3(2)	-5(2)
C(2)	44(2)	42(2)	39(2)	-11(2)	0(2)	-6(2)
C(3)	38(2)	41(2)	46(2)	-6(2)	4(2)	-10(2)
C(4)	35(2)	36(2)	44(2)	-5(2)	4(2)	-3(2)
C(5)	48(2)	51(2)	39(2)	-4(2)	9(2)	-4(2)
C(6)	50(2)	58(2)	42(2)	-14(2)	5(2)	2(2)
C(7)	44(2)	39(2)	47(2)	-15(2)	-2(2)	7(2)
C(8)	37(2)	33(2)	49(2)	-12(2)	-3(2)	2(2)
C(9)	46(2)	42(2)	53(2)	-9(2)	-3(2)	-2(2)
C(10)	55(3)	44(2)	75(3)	-5(2)	-10(2)	-12(2)
C(11)	69(3)	48(2)	81(3)	-22(2)	-19(3)	-5(2)
C(12)	58(3)	54(2)	64(3)	-28(2)	-8(2)	11(2)
C(13)	50(2)	36(2)	43(2)	-5(2)	-3(2)	-3(2)
C(14)	49(2)	37(2)	35(2)	-5(2)	-5(2)	-7(2)
C(15)	72(3)	40(2)	45(2)	-2(2)	-6(2)	5(2)
C(16)	96(3)	47(2)	34(2)	1(2)	-6(2)	0(2)

C(17)	74(3)	46(2)	37(2)	-12(2)	0(2)	-14(2)
C(18)	60(3)	37(2)	44(2)	-6(2)	1(2)	0(2)
C(19)	57(2)	41(2)	33(2)	-1(2)	-3(2)	-9(2)
C(20)	174(6)	68(3)	40(3)	-11(2)	26(3)	-16(3)

Table S13 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 220710e.

	x	y	z	U(eq)
H(2)	-189	5350	1953	50
H(5)	-2499	5521	4547	57
H(6)	-1089	7205	4977	61
H(9)	4641	8884	2400	57
H(10)	6440	10452	2886	70
H(11)	4839	10666	4066	76
H(12)	1900	9142	4804	69
H(15)	1942	9312	284	65
H(16)	4543	8867	-762	73
H(18)	7611	5311	400	58
H(19)	4948	5756	1430	53
H(20A)	6174	7796	-1719	145
H(20B)	9472	7299	-1905	145
H(20C)	8734	8461	-1495	145

Table S14 Torsion angles [deg] for 220710e

C(4)-N(1)-C(1)-C(2)	-1.9(4)
C(8)-N(1)-C(1)-C(2)	170.5(3)
C(4)-N(1)-C(1)-C(13)	156.1(3)
C(8)-N(1)-C(1)-C(13)	-31.5(5)
N(1)-C(1)-C(2)-C(3)	1.8(4)
C(13)-C(1)-C(2)-C(3)	-156.3(3)
C(1)-C(2)-C(3)-C(4)	-1.0(4)
C(1)-C(2)-C(3)-S(1)	177.7(3)
O(3)-S(1)-C(3)-C(4)	21.4(4)
O(4)-S(1)-C(3)-C(4)	159.1(3)
F(1)-S(1)-C(3)-C(4)	-89.7(4)
O(3)-S(1)-C(3)-C(2)	-157.1(3)
O(4)-S(1)-C(3)-C(2)	-19.3(4)
F(1)-S(1)-C(3)-C(2)	91.9(3)
C(1)-N(1)-C(4)-C(3)	1.3(4)
C(8)-N(1)-C(4)-C(3)	-171.9(3)
C(1)-N(1)-C(4)-C(5)	-177.0(3)
C(8)-N(1)-C(4)-C(5)	9.8(5)
C(2)-C(3)-C(4)-N(1)	-0.2(4)
S(1)-C(3)-C(4)-N(1)	-178.9(3)
C(2)-C(3)-C(4)-C(5)	177.8(4)
S(1)-C(3)-C(4)-C(5)	-0.9(6)
N(1)-C(4)-C(5)-C(6)	-2.5(5)
C(3)-C(4)-C(5)-C(6)	179.8(4)
C(4)-C(5)-C(6)-C(7)	-3.1(6)
C(5)-C(6)-C(7)-C(8)	1.5(6)
C(5)-C(6)-C(7)-C(12)	-174.6(4)

C(12)-C(7)-C(8)-C(9)	3.5(5)
C(6)-C(7)-C(8)-C(9)	-172.8(3)
C(12)-C(7)-C(8)-N(1)	-178.2(3)
C(6)-C(7)-C(8)-N(1)	5.5(5)
C(4)-N(1)-C(8)-C(9)	167.1(3)
C(1)-N(1)-C(8)-C(9)	-4.6(5)
C(4)-N(1)-C(8)-C(7)	-11.2(5)
C(1)-N(1)-C(8)-C(7)	177.2(3)
C(7)-C(8)-C(9)-C(10)	-3.7(5)
N(1)-C(8)-C(9)-C(10)	178.1(3)
C(8)-C(9)-C(10)-C(11)	-0.2(6)
C(9)-C(10)-C(11)-C(12)	4.2(6)
C(10)-C(11)-C(12)-C(7)	-4.4(6)
C(8)-C(7)-C(12)-C(11)	0.5(6)
C(6)-C(7)-C(12)-C(11)	176.7(4)
C(2)-C(1)-C(13)-O(1)	124.7(4)
N(1)-C(1)-C(13)-O(1)	-29.7(5)
C(2)-C(1)-C(13)-C(14)	-53.6(5)
N(1)-C(1)-C(13)-C(14)	152.0(3)
O(1)-C(13)-C(14)-C(19)	166.3(4)
C(1)-C(13)-C(14)-C(19)	-15.5(5)
O(1)-C(13)-C(14)-C(15)	-10.0(6)
C(1)-C(13)-C(14)-C(15)	168.3(3)
C(19)-C(14)-C(15)-C(16)	0.2(6)
C(13)-C(14)-C(15)-C(16)	176.7(4)
C(14)-C(15)-C(16)-C(17)	-1.1(7)
C(20)-O(2)-C(17)-C(16)	1.9(6)
C(20)-O(2)-C(17)-C(18)	-178.3(4)
C(15)-C(16)-C(17)-O(2)	-178.8(4)

C(15)-C(16)-C(17)-C(18)	1.4(6)
O(2)-C(17)-C(18)-C(19)	179.3(3)
C(16)-C(17)-C(18)-C(19)	-0.8(6)
C(17)-C(18)-C(19)-C(14)	-0.1(6)
C(15)-C(14)-C(19)-C(18)	0.4(6)
C(13)-C(14)-C(19)-C(18)	-175.9(3)

Symmetry transformations used to generate equivalent atoms:

Table S15 Hydrogen bonds for 220710e [A and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)