Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Copper-Catalyzed Nitrene Transfer/Cyclization Cascade to Synthesize 3a-Nitrogenous Furoindolines and Pyrroloindolines

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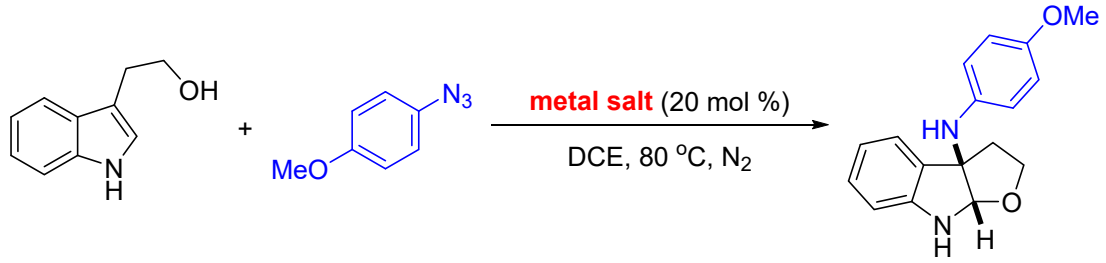
I. General Information

All manipulations were maintained under an atmosphere of argon unless otherwise stated. Commercially available reagents were used without further purification. Solvents were pre-dried over activated 4 Å molecular sieves and were refluxed over sodium-benzophenone (toluene, tetrahydrofurane), phosphorus pentoxide (chlorobenzene) or calcium hydride (dichloromethane, dichloroethane, acetonitrile) under an argon atmosphere and collected by distillation. Column chromatography was performed on silica gel (200-300 mesh). ^{1}H, ^{13}C, ^{11}B, and ^{19}F were recorded at 400 MHz, 101 MHz, 128 MHz, and 376 MHz, respectively. Melting points are uncorrected. Infrared spectra were prepared as KBr pellets and were recorded on a Varian Excalibur 3100 series FT-IR spectrometer. Mass spectra were recorded by the mass spectrometry service of Shanghai Institute of Organic Chemistry. **1a-1d**[1], **1e**[2], **1f**[3], **1g**[4], **1h,**[1] **1i**[5], **1j**[4], **1k-1l**[1], **1m**[6], **1n**[7], **1o**[8], **1p**[9],**1q**[10], **1r**[11], **5**[17], **6**[18] were synthesized according to the literature procedures. **L1 and L2** were purchased from Sigma Aldrich and used without further purification. **L3-L4**[12], **L5**[13], **L6-L8**[12], **L9**[14], **L10**[15], **L11**[16] were synthesized according to the literature procedures.

CAUTION: Organic azides are known to be potentially explosive compounds. Although under the conditions and scale described here we did not encounter any problems, appropriate precautions should be taken when handling these compounds in general. All azidation reactions and subsequent workups were performed behind a blast shield.

II. Optimization of reaction conditions.

Table S1. Optimization of the Reaction Conditions (Metal Salts)for the Synthesis of Product 3[a]

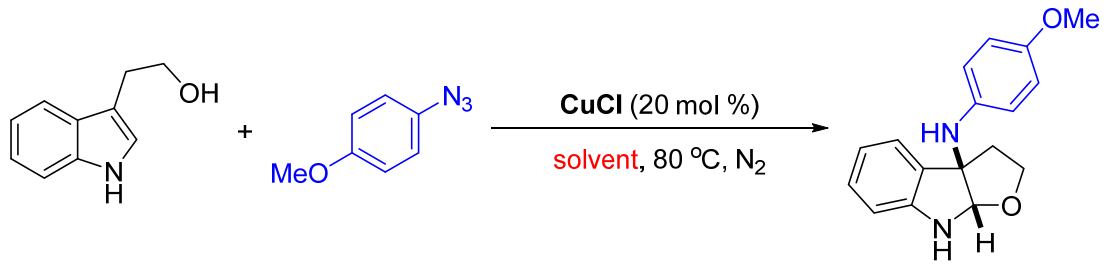


entry	catalyst	time (d)	Yield [b] (%)
1	CuCl	2	27

2	$FeCl_2$	2	NR[c]
3	$NiCl_2$	2	NR[c]
4	$(Cp^*RhCl_2)_2$	2	15
5	$CoCl_2$	2	NR[c]
6	$Pd(OAc)_2$	2	21
7	$(Cp^*IrCl_2)_2$	2	trace
8	$Zn(OTf)_2$	2	trace
9	$MnCl_2$	2	trace
10	$(Cp^*RuCl_2)_2$	2	trace
11	CuOAc	2	11.2
12	CuSCN	2	trace
13	$Cu(OAc)_2 \cdot H_2O$	2	23
14	CuCN	2	13
15	$CuSO_4 \cdot 5H_2O$	2	19
16	$Cu(ClO_4)_2 \cdot 6H_2O$	2	NR[c]
17	CuF_2	2	NR[c]
18	$CuBH_4(PPh_3)_2$	2	trace
19	$Cu(MeCN)_4PF_6$	2	trace

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (3 equiv), metal salt (20 mol %), DCE (2.0 mL), 80 °C, argon. [b] The yields of isolated products. [c] No Reaction. DCE = 1,2-dichloroethane.

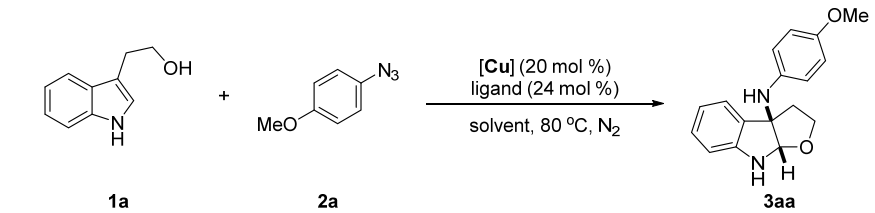
Table S2. Optimization of the Reaction Conditions (Solvents) for the Synthesis of Product 3[a]

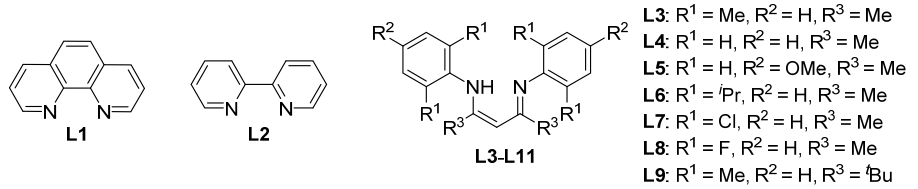


entry	solvent	time (d)	Yield [b] (%)
1	DCE	2	27
2	MeCN	2	trace
3	EtOH	2	NR[c]
4	THF	2	trace
5	PhMe	2	16
6	PhCl	2	27
7	NMP	2	NR[c]
8	DMF	2	NR[c]
9	dioxane	2	trace

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (3 equiv), CuCl (20 mol %), solvent (2.0 mL), 80 °C, argon. [b] The yields of isolated products. [c] No Reaction. DCE = 1,2-dichloroethane.

Table S3. Optimization of the Reaction Conditions (Ligands) for the Synthesis of Product 3[a]





L3: R^1 = Me, R^2 = H, R^3 = Me
L4: R^1 = H, R^2 = H, R^3 = Me
L5: R^1 = H, R^2 = OMe, R^3 = Me
L6: R^1 = ^{i}Pr, R^2 = H, R^3 = Me
L7: R^1 = Cl, R^2 = H, R^3 = Me
L8: R^1 = F, R^2 = H, R^3 = Me
L9: R^1 = Me, R^2 = H, R^3 = ^{t}Bu
L10: R^1 = H, R^2 = Br, R^3 = Me
L11: R^1 = Me, R^2 = Me, R^3 = Me

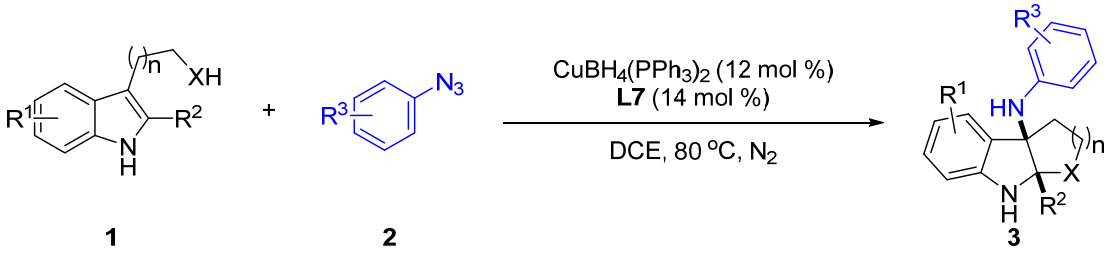
entry	[Cu]	ligand	solvent	time (h)	Yield [b] (%)
1	CuCl	--	PhCl	48	27
2	CuCl	**L1**	PhCl	12	13
3	CuCl	**L2**	PhCl	12	17
4	CuCl	**L3**	PhCl	12	45
5	CuOAc	**L3**	PhCl	12	45
6	CuSCN	**L3**	PhCl	12	70
7	$CuBH_4(PPh_3)_2$	**L3**	PhCl	12	88
8	$CuBH_4(PPh_3)_2$	**L4**	PhCl	24	trace
9	$CuBH_4(PPh_3)_2$	**L5**	PhCl	24	trace
10	$CuBH_4(PPh_3)_2$	**L6**	PhCl	12	64
11	$CuBH_4(PPh_3)_2$	**L7**	PhCl	0.5	92
12	$CuBH_4(PPh_3)_2$	**L8**	PhCl	24	trace
13	$CuBH_4(PPh_3)_2$	**L9**	PhCl	24	trace
14	$CuBH_4(PPh_3)_2$	**L10**	PhCl	24	trace
15	$CuBH_4(PPh_3)_2$	**L11**	PhCl	24	25
16	$CuBH_4(PPh_3)_2$	**L7**	DCE	0.5	95
17	$CuBH_4(PPh_3)_2$	**L7**	MeCN	12	77
18	$CuBH_4(PPh_3)_2$	**L7**	toluene	12	56
19[c]	$CuBH_4(PPh_3)_2$	**L7**	DCE	0.5	93
20[c, d]	$CuBH_4(PPh_3)_2$	**L7**	DCE	2	86
21[c, e]	$CuBH_4(PPh_3)_2$	**L7**	DCE	0.5	92
22[c, f]	$CuBH_4(PPh_3)_2$	**L7**	DCE	0.5	93
23[g]	$CuBH_4(PPh_3)_2$	**L7**	DCE	0.5	Trace

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (3 equiv), metal salt (20 mol %), ligand (24 mol %), solvent (2.0 mL), 80 °C, argon. [b] The yields of isolated products. [c] **2a** (1.5 equiv).

[d] metal salt (10 mol %), ligand (12 mol %). [e] metal salt (12 mol %), ligand (14 mol %). [f] metal salt (15 mol %), ligand (18 mol %). [g] 60 °C.

III. General Catalytic Reaction Procedure of Products

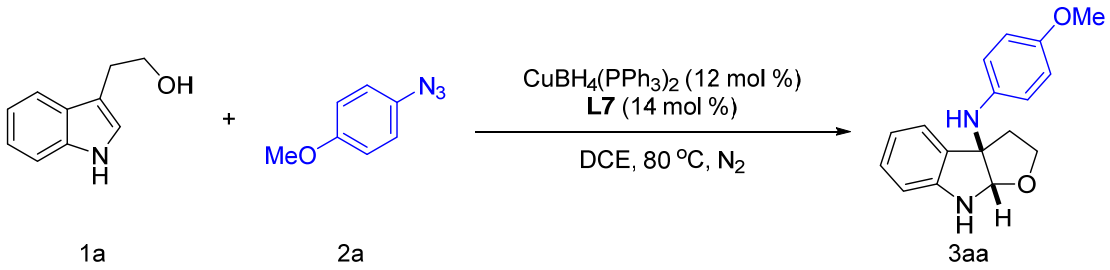
General Procedure:



1 2 3

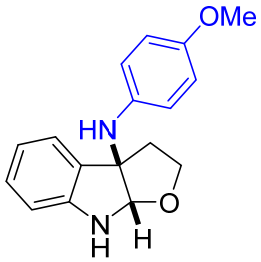
After stirring a mixture of $CuBH_4(PPh_3)_2$ (0.024 mmol, 12 mol %) and **L7** (0.028 mmol, 14 mol %) in dry DCE (2 mL) at 80 °C for 1 h, substrates **1** (0.20 mmol) and **2** (0.30 mmol) was added. The reaction mixture was stirred at 80 °C under argon atmosphere. After the disappearance of substrate **1** (monitored by TLC) and then the crude product was purified by silica gel flash chromatography to afford the desired product **3**.

General Procedure for gram Scale:



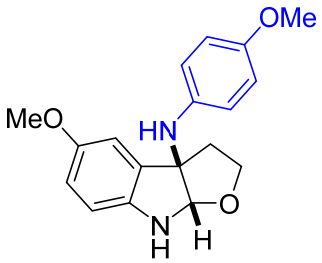
1a 2a 3aa

After stirring a mixture of $CuBH_4(PPh_3)_2$ (0.75 mmol, 12 mol %) and **L7** (0.89 mmol, 14 mol %) in dry DCE (30mL) at 80 °C for 1 h, substrates **1a** (6.20 mmol) and **2a** (9.30 mmol) was added. The reaction mixture was stirred at 80 °C under argon atmosphere. After the disappearance of substrate **1a** (monitored by TLC) and then the crude product was purified by silica gel flash chromatography to afford the desired product **3aa** (1.56 g, 5.52 mmol, 89 %).



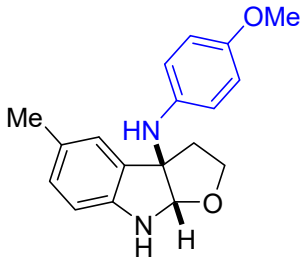
3aa

***N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3aa);** reaction temperature: 80 °C; reaction time: 30 min; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 132.9 – 135.9 °C); 92 % yield (51.4 mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.19 (d, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.76 (t, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.62 (d, *J* = 8.0 Hz, 1H), 6.47 (d, *J* = 8.8 Hz, 2H), 5.77 (s, 1H), 4.66 (s, 1H), 4.09 (t, *J* = 8.0 Hz, 1H), 3.72 – 3.63 (m, 4H), 2.51 (td, *J* = 11.7, 7.5 Hz, 1H), 2.29 (dd, *J* = 12.0, 4.8 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 152.9, 149.8, 139.7, 130.4, 129.6, 124.1, 119.5, 116.8, 114.9, 108.8, 95.7, 74.7, 66.0, 55.8, 42.4; **IR *v* (neat, cm^{-1}):** 3445, 2066, 1634, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{17}H_{19}N_2O_2^+$ $[M+H]^+$: 283.1441, found: 283.1431.



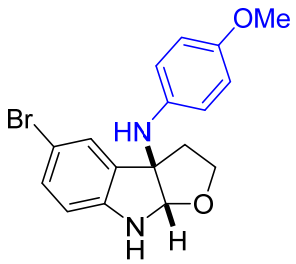
3ba

5-Methoxy-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ba); reaction temperature: 80 °C; reaction time: 2 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); yellow oil; 72 % yield (39.0 mg, 0.14 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 6.80 (d, *J* = 2.8 Hz, 1H), 6.72 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.56 (d, *J* = 8.8 Hz, 1H), 6.47 (d, *J* = 8.8 Hz, 2H), 5.75 (s, 1H), 4.46 (brs, 1H), 4.07 (t, *J* = 8.0 Hz, 1H), 3.75 – 3.63 (m, 7H), 2.46 (td, *J* = 11.6, 7.5 Hz, 1H), 2.29 (dd, *J* = 11.8, 4.6 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 154.0, 152.9, 143.6, 139.7, 131.8, 116.8, 115.1, 114.8, 110.0, 109.8, 96.5, 75.0, 65.8, 56.0, 55.7, 42.5; **IR *v* (neat, cm^{-1}):** 3446, 6005, 2325, 1552, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_3^+$ $[M+H]^+$: 313.1547, found: 313.1555.



3ca

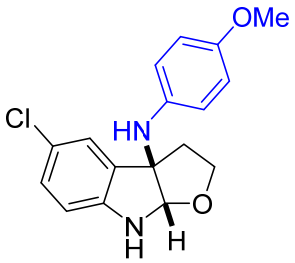
***N*-(4-methoxyphenyl)-5-methyl-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ca)**; reaction temperature: 80 °C; reaction time: 1 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 154.6 – 159.7 °C); 97 % yield (57.6 mg, 0.19 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.02 (s, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 8.8 Hz, 2H), 6.54 (d, *J* = 8.0 Hz, 1H), 6.48 (d, *J* = 7.2 Hz, 2H), 5.76 (s, 1H), 4.53 (brs, 1H), 4.12-4.04 (m, 1H), 3.91 (brs, 1H), 3.74 – 3.61 (m, 4H), 2.50 (td, *J* = 11.7, 7.5 Hz, 1H), 2.32 – 2.19 (m, 4H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 152.8, 147.5, 139.8, 130.7, 130.0, 128.8, 124.5, 116.6, 114.9, 108.8, 95.9, 74.6, 65.9, 55.7, 42.3, 21.0; **IR *v* (neat, cm^{-1}):** 3449, 3006, 2989, 1646, 1509, 1275, 1261, 779; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_2^+$ $[M+H]^+$: 297.1598, found: 297.1604.



3da

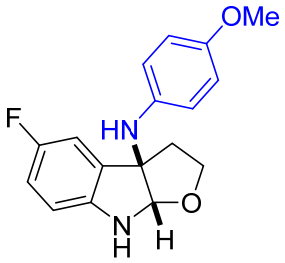
5-Bromo-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3da); reaction temperature: 80 °C; reaction time: 2 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 147.1 – 151.6 °C); 94 % yield (68.0 mg, 0.19 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.28 (d, *J* = 2.0 Hz, 1H), 7.21 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.68 (d, *J* = 8.8 Hz, 2H), 6.50 (d, *J* = 8.4 Hz, 1H), 6.45 (d, *J* = 8.8 Hz, 2H), 5.76 (s, 1H), 4.66 (s, 1H), 4.09 (t, *J* = 8.4 Hz, 1H), 3.70 (s, 3H), 3.69 - 3.62 (m, 1H), 2.46 (td, *J* = 11.7, 7.5 Hz, 1H), 2.29 (dd, *J* = 11.8, 5.0 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 153.0, 148.7, 139.2, 132.5, 132.2, 127.1, 116.7, 114.9, 110.9, 110.0, 95.8, 74.5, 65.8, 55.7, 42.9; **IR *v* (neat, cm^{-1}):** 3446, 2065,

1645, 1543, 1275, 1281, 750; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}BrN_2O_2^+$ $[M+H]^+$: 361.0546, found: 361.0542.



3ea

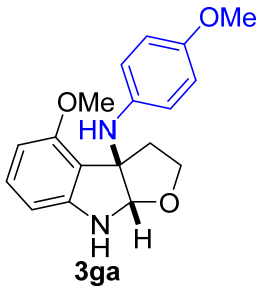
5-Chloro-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ea); reaction temperature: 80 °C; reaction time: 45 min; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 148.2 – 151.2 °C); 99 % yield (62.8 mg, 0.20 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.14 (d, *J* = 2.4 Hz, 1H), 7.07 (dd, *J* = 7.8, 2.2 Hz, 1H), 6.72 – 6.62 (m, 2H), 6.53 (d, *J* = 8.4 Hz, 1H), 6.49 – 6.41 (m, 2H), 5.77 (s, 1H), 4.66 (brs, 1H), 4.12-4.05 (m, 1H), 3.79 – 3.60 (m, 4H), 2.45 (td, *J* = 11.7, 7.5 Hz, 1H), 2.29 (dd, *J* = 12.0, 4.0 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 153.01, 148.3, 139.4, 132.2, 129.4, 124.3, 123.9, 116.7, 114.9, 109.5, 96.1, 74.5, 65.8, 55.7, 42.9; **IR *v* (neat, cm^{-1}):** 3445, 3006, 2989, 1646, 1275, 1261, 759; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}ClN_2O_2^+$ $[M+H]^+$: 317.1051, found: 317.1056.



3fa

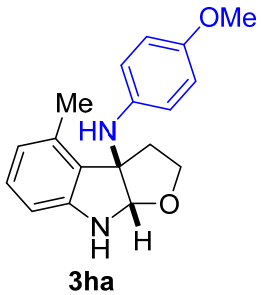
5-Fluoro-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3fa); reaction temperature: 80 °C; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 139.8 – 140.9 °C); 95 % yield (57.2 mg, 0.19 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 6.90 (dd, *J* = 8.0, 2.8 Hz, 1H), 6.87 – 6.80 (m, 1H), 6.70 – 6.63 (m, 2H), 6.54 (dd, *J* = 8.6, 4.1 Hz, 1H), 6.49 – 6.41 (m, 2H), 5.77 (s, 1H), 4.54 (brs, 1H), 4.13 – 4. 05(m, 1H), 3.74 – 3.62 (m, 4H), 2.45 (td, *J* = 11.6, 7.5 Hz, 1H), 2.34 -2.25 (m, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 158.6, 156.2, 153.1, 145.7, 139.5, 131.8 (d, *J* = 7.0 Hz), 115.9 (d, *J* =

23.5 Hz), 115.8 (d, J = 194.8 Hz), 111.2 (d, J = 23.7 Hz), 109.25 (d, J = 7.9 Hz), 96.7, 74.8, 65.8, 55.7, 43.0; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -125.07 (s, 1F); **IR *v* (neat, cm^{-1}):** 3440, 3006, 1645, 1410, 1275, 1261, 779; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}FN_2O_2^+$ $[M+H]^+$: 301.1347, found: 301.1350.



3ga

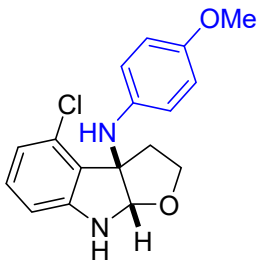
4-Methoxy-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ga); reaction temperature: 80 °C; reaction time: 4 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); brown solid (mp: 133.8 – 135.1 °C); 84 % yield (52.5 mg, 0.17 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.05 (t, J = 8.0 Hz, 1H), 6.66 (d, J = 8.9 Hz, 2H), 6.57 (d, J = 8.9 Hz, 2H), 6.24 (d, J = 8.0 Hz, 2H), 5.78 (s, 1H), 4.65 (brs, 1H), 4.14 – 4.04 (m, 1H), 3.77 (s, 3H), 3.72 – 3.62 (m, 4H), 2.52 - 2.41 (m, 2H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 152.7, 148.2, 139.6, 130.3, 129.9, 121.4, 119.6, 118.2, 116.6, 114.8, 95.4, 74.9, 66.0, 55.7, 41.8, 16.7; **IR *v* (neat, cm^{-1}):** 3446, 3006, 2065, 1640, 1275, 1260, 750; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_3^+$ $[M+H]^+$: 313.1547, found: 313.1551.



3ha

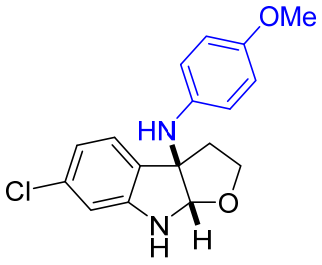
***N*-(4-methoxyphenyl)-4-methyl-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ha);** reaction temperature: 80 °C; reaction time: 5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 142.1 – 146.0 °C); 89 % yield (53.0 mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.02 (t, J = 7.7 Hz, 1H), 6.63 (d, J = 8.9 Hz, 2H), 6.47 (dd, J = 15.7, 7.7 Hz, 2H), 6.40 (d, J = 8.6 Hz, 2H), 5.75 (s, 1H), 4.61 (brs, 1H), 4.08 (dd, J = 12.0, 4.5 Hz, 1H), 3.76 – 3.64 (m, 4H), 2.46 (dd, J = 11.3, 4.6 Hz, 1H), 2.38 – 2.25 (m, 4H); **^{13}C{^{1}H} NMR (101 MHz,**

$CDCl_3$) δ 152.6, 150.0, 140.0, 135.2, 129.5, 126.6, 121.4, 116.0, 114.8, 106.4, 96.5, 74.7, 65.6, 55.7, 41.7, 17.6; **IR *v* (neat, cm^{-1}):**3446, 3006, 2064, 1646, 1275, 1261, 1750; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_2^+$ $[M+H]^+$: 297.1598, found: 297.1589.



3ia

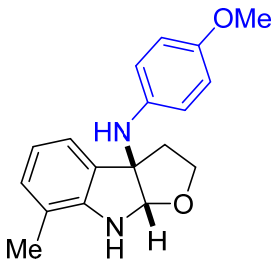
4-Chloro-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ia); reaction temperature: 80 ºC; reaction time: 3 h; petroleum ether/ethylacetate = 7:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 122.5 – 126.6 ºC); 92 % yield (58.1 mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.01 (t, *J* = 8.0 Hz, 1H), 6.64 (d, *J* =9.2 Hz, 2H), 6.60 (d, *J* = 8.0 Hz, 1H), 6.45-6.53 (m, 3H), 5.79 (s, 1H), 4.77 (brs, 1H), 4.28 (brs, 1H), 4.09 (t, *J* = 8.2 Hz, 1H), 3.71 – 3.59 (m, 4H), 2.65 (dd, *J* = 12.0, 4.8 Hz, 1H), 2.40 (td, *J* = 11.7, 7.4 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 153.0, 151.8, 139.6, 130.8, 130.6, 125.1, 119.7, 116.6, 114.7, 106.8, 96.8, 75.1, 65.9, 55.6, 40.5; **IR *v* (neat, cm^{-1}):** 3359, 2920, 2849, 1604, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}ClN_2O_2^+$ $[M+H]^+$: 317.1051, found: 317.1059.



3ja

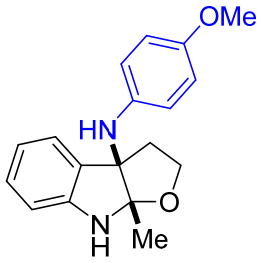
6-Chloro-*N*-(4-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ja); reaction temperature: 80 ºC; reaction time: 4 h; petroleum ether/ethylacetate = 10:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); gray solid (mp: 145.9 – 150.9 ºC); 84 % yield (53.3 mg, 0.17 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.06 (d, *J* = 8.0 Hz, 1H), 6.71 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.59 (d, *J* = 1.6 Hz, 1H), 6.44 (d, *J* = 9.2 Hz, 2H), 5.76 (s, 1H), 4.72 (s, 1H), 4.08 (t, *J* = 8.2 Hz, 1H), 3.70 (s, 3H), 3.68 – 3.62 (m, 1H), 2.45 (td, *J* = 11.7, 7.5 Hz, 1H), 2.26 (dd, *J* = 11.8, 5.0

Hz, 1H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 153.1, 150.7, 139.4, 135.1, 128.8, 124.9, 119.3, 116.9, 114.9, 108.7, 96.0, 74.2, 65.9, 55.7, 42.9; **IR *v* (neat, cm^{-1}):** 3445, 3006, 1066, 1645, 1470, 1275, 1261, 769; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}ClN_2O_2^+$ $[M+H]^+$: 317.1051, found: 317.1048.



3ka

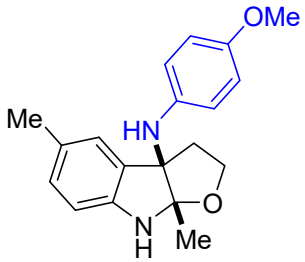
***N*-(4-methoxyphenyl)-7-methyl-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ka);** reaction temperature: 80 °C; reaction time: 5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 139.4 – 141.5 °C); 89 % yield (53.0 mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.06 (d, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 7.3 Hz, 1H), 6.72 (t, *J* = 7.5 Hz, 1H), 6.68 (d, *J* = 8.9 Hz, 2H), 6.48 (d, *J* = 8.8 Hz, 2H), 5.81 (s, 1H), 4.49 (brs, 1H), 4.09 (t, *J* = 8.3 Hz, 1H), 3.78 – 3.61 (m, 4H), 2.55 (td, *J* = 11.7, 7.6 Hz, 1H), 2.26 (dd, *J* = 12.0, 5.0 Hz, 1H), 2.18 (s, 3H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 152.7, 148.2, 139.6, 130.3, 129.9, 121.4, 119.6, 118.2, 116.6, 114.8, 95.4, 74.9, 66.0, 55.7, 41.8, 16.7; **IR *v* (neat, cm^{-1}):**3446, 3006, 3065, 1644, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_2^+$ $[M+H]^+$: 297.1598, found: 297.1588.



3la

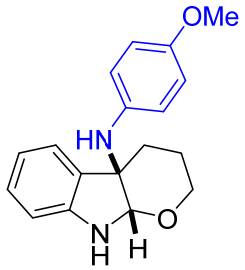
***N*-(4-methoxyphenyl)-8a-methyl-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3la);** reaction temperature: 80 °C; reaction time: 3.5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); yellow solid (mp: 124.8 – 128.3 °C); 87 % yield (51.5 mg, 0.17 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.11 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.70 (t, *J* = 7.4 Hz, 1H), 6.64-6.56 (m, 3H), 6.35 (d, *J* = 8.8 Hz, 2H), 4.57 (brs, 1H), 4.04 (brs, 1H), 3.94 (t, *J* = 7.6 Hz, 1H), 3.67 (s,

3H), 3.59-3.51 (m, 1H), 2.46-2.33 (m, 2H), 1.54 (s, 3H); **$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)** δ 152.3, 149.3, 139.5, 129.4, 129.2, 124.5, 119.3, 116.5, 114.5, 108.6, 101.8, 74.2, 64.8, 55.6, 43.9, 22.7; **IR *v* (neat, cm^{-1}):** 3440, 2065, 1644, 1510, 1275, 750, 518; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_2^+$ $[M+H]^+$: 297.1598, found: 297.1593.



3ma

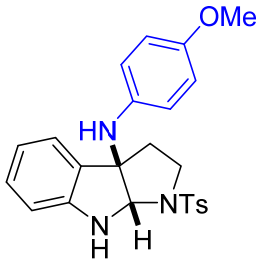
***N*-(4-methoxyphenyl)-5,8a-dimethyl-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ma);** reaction temperature: 80 °C; reaction time: 9 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); yellow solid (mp: 123.5 – 127.4°C); 94 % yield (53.3 mg, 0.17 mmol); **^1H NMR (400 MHz, $CDCl_3$)** δ 6.92 (d, *J* = 8.0 Hz, 1H), 6.86 (s, 1H), 6.61 (dd, *J* = 6.8, 2.0 Hz, 2H), 6.52 (d, *J* = 7.6 Hz, 1H), 6.37 (dd, *J* = 6.8, 2.4 Hz, 2H), 4.45 (brs, 1H), 4.03 (brs, 1H), 3.94 (t, *J* = 7.4 Hz, 1H), 3.67 (s, 3H), 3.59 - 3.50 (m, 1H), 2.46 – 2.31 (m, 2H), 2.20 (s, 3H), 1.52 (s, 3H); **$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$)** δ 152.2, 147.0, 139.6, 129.9, 129.5, 128.6, 124.9, 116.4, 114.5, 108.6, 102.1, 74.1, 64.8, 55.6, 43.8, 22.7, 20.9; **IR *v* (neat, cm^{-1}):** 3447, 2065, 1633, 1507, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{19}H_{23}N_2O_2^+$ $[M+H]^+$: 311.1754, found: 311.1763.



3na

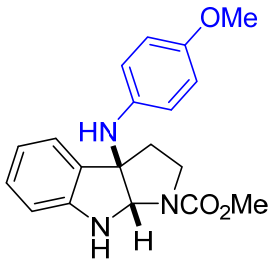
***N*-(4-methoxyphenyl)-3,4,9,9a-tetrahydropyrano[2,3-b]indol-4a(2*H*)-amine (3na);** reaction temperature: 80 °C; reaction time: 5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); yellow oil; 86 % yield (51.0 mg, 0.17 mmol); **^1H NMR (400 MHz, $CDCl_3$)** δ 7.17 -7.10 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.79 - 6.75 (m, 1H), 6.72 – 6.65 (m, 3H), 6.56 – 6.50 (m, 2H), 5.34 (s, 1H), 4.42 (s, 1H), 3.88 – 3.79 (m, 1H), 3.63 - 3.54 (m, 3H), 3.58 (m, 1H), 2.17 (m, 2H), 1.73 – 1.63 (m, 1H), 1.53 – 1.36

(m, 1H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 154.0, 148.8, 138.4, 131.2, 129.0, 123.5, 121.2, 119.2, 114.3, 110.1, 91.9, 63.5, 60.7, 55.6, 30.3, 20.6; **IR *v* (neat, cm^{-1}):** 3566, 3005, 1610, 1508, 1275, 1260, 750; **HRMS (ESI, m/z):** calcd for $C_{18}H_{21}N_2O_2^+$ $[M+H]^+$: 297.1598, found: 297.1589.



3oa

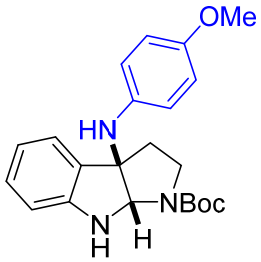
***N*-(4-methoxyphenyl)-1-tosyl-2,3,8,8a-tetrahydropyrrolo[2,3-b]indol-3a(1*H*)-amine (3oa);** reaction temperature: 80 °C; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 137.2 – 138.6 °C); 91 % yield (79.1mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.08 (m, 2H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.64 (d, *J* = 7.9 Hz, 1H), 6.61 – 6.55 (m, 2H), 6.31 – 6.25 (m, 2H), 5.54 (s, 1H), 4.86 (brs, 1H), 3.71 (s, 3H), 3.52 – 3.45 (m, 1H), 3.31 - 3.22 (m, 1H), 2.45 (s, 3H), 2.37 – 2.22 (m, 2H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 153.3, 149.0, 143.7, 138.4, 135.8, 129.9, 129.7, 127.3, 123.5, 119.5, 118.1, 114.6, 110.0, 79.6, 74.5, 55.6, 46.3, 38.3, 21.6; **IR *v* (neat, cm^{-1}):** 3446, 3006, 2066, 1635, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{24}H_{26}N_3O_3S^+$ $[M+H]^+$: 436.1689, found: 436.1687.



3pa

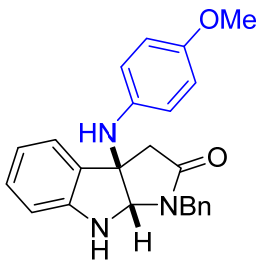
Methyl 3a-((4-methoxyphenyl)amino)-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indole-1(2H)-carboxylate (3pa); reaction temperature: 80 °C; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; TLC: R_f = 0.4 (PE / EA = 2:1, UV); yellow solid (mp: 142.3 – 144.4 °C); 91 % yield (61.8mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.07 (t, *J* = 7.2 Hz, 2H), 6.69 (q, *J* = 7.0 Hz, 1H), 6.65 – 6.59 (m, 2H), 6.55 (d, *J* = 7.7 Hz, 1H), 6.45 (dd, *J* = 16.5, 8.7 Hz, 2H), 5.50 (d, *J* = 12.1 Hz, 1H), 5.03 (s, 1H), 4.68 (s, 1H),

3.80 – 3.58 (m, 7H), 3.22 - 3.05 (m, 1H), 2.56 - 2.41 (m, 1H), 2.33 - 2.22 (m, 1H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 155.9, 155.2, 153.7, 153.4, 149.3, 149.0, 138.8, 138.7, 130.0, 129.8, 123.7, 119.5, 119.3, 119.0, 118.1, 114.7, 114.7, 109.9, 109.7, 78.0,, 77.4, , 74.2, 73.2, 55.7, 52.8, 52.6, 44.9, 44.7, 37.7, 37.5; **IR *v* (neat, cm^{-1}):** 3446, ; 3006, 2065, 1633, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{19}H_{22}N_3O_3^+$ $[M+H]^+$: 340.1656, found: 340.1663.



3qa

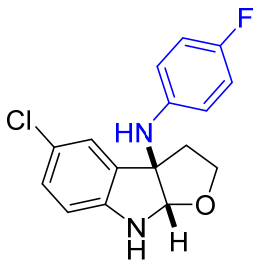
Tert-butyl 3a-((4-methoxyphenyl)amino)-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indole-1(2H)-carboxylate (3qa); reaction temperature: 80 ºC; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 161.1 – 165.1 ºC); 91 % yield (69.6mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.18 - 7.10 (m, 2H), 6.79 – 6.72 (m, 1H), 6.72 – 6.66 (m, 2H), 6.63 (d, *J* = 7.7 Hz, 1H), 6.52 (t, *J* = 9.6 Hz, 2H), 5.52 (d, *J* = 32.1 Hz, 1H), 5.11 (s, 1H), 4.68 (s, 1H), 3.71 (s, 3H), 3.65 (t, *J* = 7.8 Hz, 1H), 3.17 (dd, *J* = 18.3, 8.3 Hz, 1H), 2.58 – 2.47 (m, 1H), 2.36 - 2.28 (m, 1H), 1.54 – 1.44 (m, 9H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 154.9, 154.1, 153.7, 153.4, 149.5, 149.2, 138.9, 138.7, 130.1, 129.9, 129.8, 129.7, 123.8, 123.7, 119.4, 119.1, 118.1, 114.8, 114.7, 109.8, 109.6, 80.6, 80.2, 78.0, 77.8, 77.5, 74.2, 73.3, 55.7, 45.0, 44.4, 37.8, 37.7, 28.8, 28.6; **IR *v* (neat, cm^{-1}):** 3446, 3006, 1646, 1507, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{22}H_{28}N_2O_3^+$ $[M+H]^+$: 382.2125, found: 382.2129.



3ra

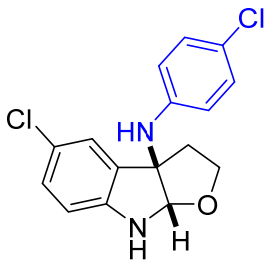
1-Benzyl-3a-((4-methoxyphenyl)amino)-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (3ra); reaction temperature: 80 ºC; reaction time: 3 h; petroleum

ether/ethylacetate = 8:1; TLC: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 168.7 – 175.2 ºC); 57 % yield (44.1mg, 0.11 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.37 – 7.27 (m, 5H), 7.22 – 7.16 (m, 1H), 6.92 – 6.86 (m, 1H), 6.67 (d, *J* = 7.9 Hz, 1H), 6.65 – 6.61 (m, 2H), 6.35 – 6.30 (m, 2H), 5.26 (s, 1H), 4.99 (d, *J* = 14.8 Hz, 1H), 4.41 (s, 1H), 4.21 (d, *J* = 14.8 Hz, 1H), 3.70 (s, 3H), 3.28 (d, *J* = 17.7 Hz, 1H), 2.96 (d, *J* = 17.7 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 171.9, 153.4, 147.9, 137.9, 136.3, 133.4, 130.4, 129.0, 128.4, 128.0, 124.1, 121.2, 117.1, 115.0, 112.0, 78.2, 67.0, 55.8, 44.2, 41.9. **IR *v* (neat, cm^{-1}):** 3445, 3006, 1645, 1511, 1275, 1261, 762; **HRMS (ESI, m/z):** calcd for $C_{24}H_{24}N_3O_2^+$ $[M+H]^+$: 386.1863, found: 386.1871.



3eb

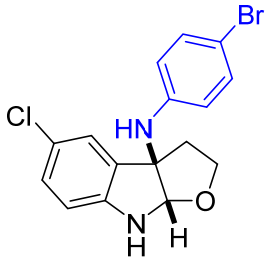
5-Chloro-*N*-(4-fluorophenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3eb); reaction temperature: 80 ºC; reaction time: 4 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 149.0 – 152.7 ºC); 90 % yield (54.8 mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.06 (d, *J* = 1.8 Hz, 1H), 7.01 (dd, *J* = 8.5, 1.9 Hz, 1H), 6.72 (t, *J* = 8.7 Hz, 2H), 6.47 (d, *J* = 8.3 Hz, 1H), 6.39 – 6.29 (m, 2H), 5.70 (s, 1H), 4.58 (brs, 1H), 4.02 (t, *J* = 8.3 Hz, 1H), 3.64-3.54 (m, 1H), 2.38 (td, *J* = 11.7, 7.5 Hz, 1H), 2.23 (dd, *J* = 11.9, 5.0 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 156.4 (d, *J* = 235.4 Hz), 148.2, 141.7 (d, *J* = 2.0 Hz), 131.5, 129.6, 124.2, 124.0, 115.8 (d, *J* = 28.7 Hz), 115.75, 109.5, 95.9, 74.2, 65.7, 43.1; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -126.50 (s, 1F). **IR *v* (neat, cm^{-1}):**3447, 3006, 1646, 1473, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{16}H_{15}ClFN_2O^+$ $[M+H]^+$: 305.0851, found: 305.0836.



3ec

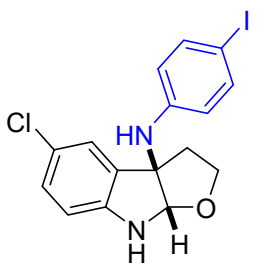
5-Chloro-*N*-(4-chlorophenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine

(3ec); reaction temperature: 80 °C; reaction time: 5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 174.7 – 175.6 °C); 81 % yield (52.3 mg, 0.16 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.12 (d, *J* = 2.0 Hz, 1H), 7.09 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 1H), 6.39 (d, *J* = 8.8 Hz, 2H), 5.78 (s, 1H), 4.67 (brs, 1H), 4.33 (brs, 1H), 4.10 (t, *J* = 8.2 Hz, 1H), 3.71 - 3.63 (m, 1H), 2.45 (td, *J* = 11.7, 7.5 Hz, 1H), 2.30 (dd, *J* = 12, 4.8 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 148.2, 144.0, 131.3, 129.7, 129.3, 124.1, 123.3, 115.7, 109.5, 95.9, 73.9, 65.7, 43.0; **IR *v* (neat, cm^{-1}):** 3420, 3006, 2990, 1633, 1476, 1275, 1261, 773; **HRMS (ESI, m/z):** calcd for $C_{16}H_{15}Cl_2N_2O^+$ $[M+H]^+$: 321.0556, found: 321.0563.



3ed

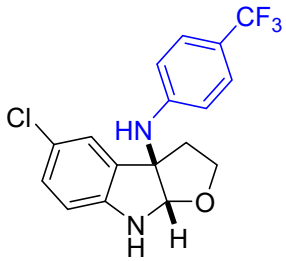
***N*-(4-bromophenyl)-5-chloro-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ed);** reaction temperature: 80 °C; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 183.8 – 184.8 °C); 75 % yield (54.5 mg, 0.15 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.15 (d, *J* = 8.8 Hz, 2H), 7.13-7.06 (m, 2H), 6.55 (d, *J* = 8.3 Hz, 1H), 6.34 (d, *J* = 8.8 Hz, 2H), 5.78 (s, 1H), 4.63 (brs, 1H), 4.34 (brs, 1H), 4.10 (t, *J* = 8.3 Hz, 1H), 3.71-3.62 (m, 1H), 2.45 (td, *J* = 11.7, 7.5 Hz, 1H), 2.30 (dd, *J* = 11.8, 4.7 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 148.2, 144.5, 132.1, 131.2, 129.7, 124.1, 116.1, 110.4, 109.5, 95.9, 73.9, 65.6, 43.0; **IR *v* (neat, cm^{-1}):** 3446, 3006, 2065, 1640, 1275, 1261, 779; **HRMS (ESI, m/z):** calcd for $C_{16}H_{15}BrClN_2O^+$ $[M+H]^+$: 365.0051, found: 365.0067.



3ee

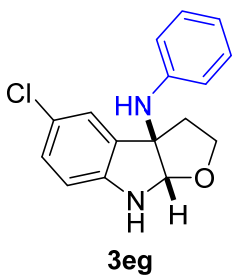
5-Chloro-*N*-(4-iodophenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine

(3ee); reaction temperature: 80 °C; reaction time: 4 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 192.6 – 196.3 °C); 88 % yield (72.6 mg, 0.18 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.33 (d, *J* = 8.7 Hz, 2H), 7.13 – 7.06 (m, 2H), 6.55 (d, *J* = 8.3 Hz, 1H), 6.24 (d, *J* = 8.7 Hz, 2H), 5.78 (s, 1H), 4.57 (brs, 2H), 4.10 (t, *J* = 8.3 Hz, 1H), 3.71 – 3.62 (m, 1H), 2.44 (td, *J* = 11.7, 7.5 Hz, 1H), 2.30 (dd, *J* = 11.9, 5.0 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 148.2, 145.1, 138.0, 131.2, 129.7, 124.1, 124.11, 116.7, 109.5, 95.9, 79.6, 73.8, 65.7, 43.1; **IR *v* (neat, cm^{-1}):**3446, 3006, 1646, 1507, 1275, 1261. 750; **HRMS (ESI, m/z):** calcd for $C_{16}H_{15}ClIN_2O^+$ $[M+H]^+$: 412.9912, found: 412.9902.



3ef

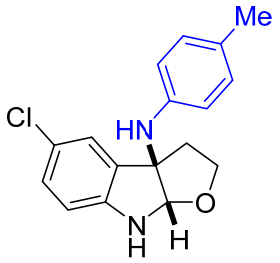
5-Chloro-*N*-(4-(trifluoromethyl)phenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ef); reaction temperature: 80 °C; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; TLC: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 177.1 – 179.8 °C); 77 % yield (54.5 mg, 0.15 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.32 (d, *J* = 8.6 Hz, 2H), 7.13 (d, *J* = 2.0 Hz, 1H), 7.12 – 7.08 (m, 1H), 6.57 (d, *J* = 8.3 Hz, 1H), 6.48 (d, *J* = 8.6 Hz, 2H), 5.81 (s, 1H), 4.70 (brs, 1H), 4.59 (brs, 1H), 4.13 (t, *J* = 7.8 Hz, 1H), 3.73 - 3.64 (m, 1H), 2.48 (td, *J* = 11.7, 7.4 Hz, 1H), 2.33 (dd, *J* = 11.8, 4.8 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 148.2, 148.1, 130.7, 129.8, 127.9 (q, *J* = 269.0 Hz), 126.7 (q, *J* = 3.8 Hz), 124.1, 124.0, 119.9 (q, *J* = 32.5 Hz), 113.5, 109.6, 95.8, 73.6, 65.6, 43.1; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -61.32 (s, 3F); **IR *v* (neat, cm^{-1}):** 3446, 3006, 1646, 1543, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{17}H_{15}ClF_3N_2O^+$ $[M+H]^+$: 355.0820, found: 355.0829.



3eg

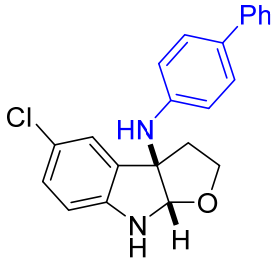
5-Chloro-*N*-phenyl-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3eg);

reaction temperature: 80 °C; reaction time: 5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 181.4 – 185.6 °C); 78 % yield (40.0 mg, 0.16 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.15 (d, *J* = 2.1 Hz, 1H), 7.12 – 7.05 (m, 3H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.55 (d, *J* = 8.4 Hz, 1H), 6.47 (d, *J* = 8.2 Hz, 2H), 5.83 (s, 1H), 4.70 (brs, 1H), 4.22 (brs, 1H), 4.11 (t, *J* = 8.0 Hz, 1H), 3.72 - 3.64 (m, 1H), 2.49 (td, *J* = 11.7, 7.5 Hz, 1H), 2.30 (dd, *J* = 12.0, 4.9 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 148.2, 145.5, 132.0, 129.5, 129.4, 124.2, 124.0, 118.5, 114.6, 109.5, 95.9, 73.9, 65.7, 42.9; **IR *v* (neat, cm^{-1}):**3420, 3006, 1633, 1508, 1479, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{16}H_{16}ClN_2O^+$ $[M+H]^+$: 287.0946, found: 287.0939.



3eh

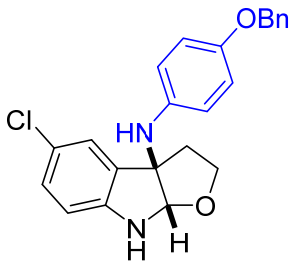
5-Chloro-*N*-(p-tolyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3eh); reaction temperature: 80 °C; reaction time: 5 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 183.3 – 184.8 °C); 86 % yield (51.9 mg, 0.17 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.15 (d, *J* = 2.4 Hz, 1H), 7.08 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.54 (d, *J* = 8.4 Hz, 1H), 6.40 (d, *J* = 8.4 Hz, 2H), 5.81 (s, 1H), 4.68 (brs, 1H), 4.09 (t, *J* = 7.8 Hz, 1H), 3.71 - 3.63 (m, 1H), 2.47 (td, *J* = 11.7, 7.5 Hz, 1H), 2.29 (dd, *J* = 12.0, 4.8 Hz, 1H), 2.19 (s, 3H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 148.2, 143.1, 132.1, 129.9, 129.4, 127.8, 124.2, 124.0, 114.9, 109.5, 96.0, 74.1, 65.7, 42.9, 20.4; **IR *v* (neat, cm^{-1}):** 3453, 2065, 1633, 1473, 1275, 1261, 773; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}ClN_2O^+$ $[M+H]^+$: 301.1102, found: 301.1112.



3ei

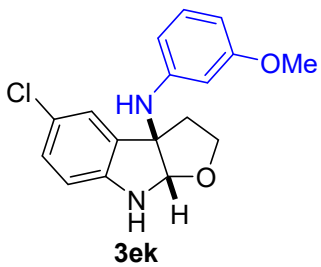
***N*-([1,1'-biphenyl]-4-yl)-5-chloro-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ei);** reaction temperature: 80 °C; reaction time: 4 h; petroleum

ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 227.1 – 239.0 °C); 93 % yield (67.5 mg, 0.19 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.48 (d, *J* = 8.1 Hz, 2H), 7.40 – 7.32 (m, 4H), 7.25 - 7.24 (m, 1H), 7.18 (d, *J* = 1.8 Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 1H), 6.61 - 6.50 (m, 3H), 5.87 (s, 1H), 4.69 (brs, 1H), 4.13 (t, *J* = 8.3 Hz, 1H), 3.75 – 3.64 (m, 1H), 2.52 (td, *J* = 11.8, 7.6 Hz, 1H), 2.33 (dd, *J* = 11.9, 4.9 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 157.7, 155.3, 148.3, 141.7, 141.72, 131.6, 129.6, 124.2, 124.0, 116.0, 115.8, 115.76, 109.5, 95.9, 74.3, 65.7, 43.0; **IR *v* (neat, cm^{-1}):**3446, 3006, 1646, 1473, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{22}H_{20}ClN_2O^+$ $[M+H]^+$: 363.1259, found: 363.1267.



3ej

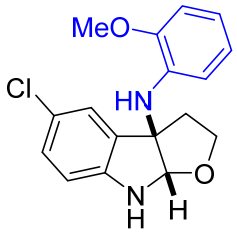
***N*-(4-(benzyloxy)phenyl)-5-chloro-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ej);** reaction temperature: 80 °C; reaction time: 4 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 163.2 – 188.5 °C); 95 % yield (74.1 mg, 0.19 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.41 - 7.28 (m, 5H), 7.15 (d, *J* = 2.0 Hz, 1H), 7.08 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.74 (d, *J* = 8.9 Hz, 2H), 6.53 (d, *J* = 8.3 Hz, 1H), 6.45 (d, *J* = 8.8 Hz, 2H), 5.77 (s, 1H), 4.94 (s, 2H), 4.66 (brs, 1H), 4.09 (t, *J* = 8.2 Hz, 1H), 3.69 – 3.58 (m, 1H), 2.55 – 2.43 (m, 1H), 2.29 (dd, *J* = 12.1, 4.8 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 152.2, 148.2, 139.6, 137.5, 132.0, 129.4, 128.6, 127.9, 127.6, 124.3, 123.9, 116.4, 116.0, 109.5, 96.0, 74.4, 70.7, 65.8, 42.9; **IR *v* (neat, cm^{-1}):** 3446, 3006, 1644, 1507, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{23}H_{22}ClN_2O_2^+$ $[M+H]^+$: 393.1364, found: 393.1359.



3ek

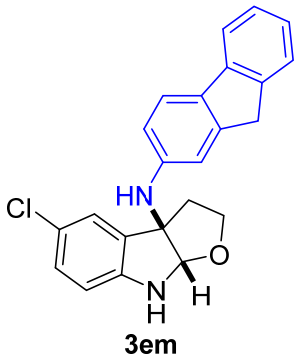
5-Chloro-*N*-(3-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3ek); reaction temperature: 80 °C; reaction time: 3 h; petroleum

ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); yellow solid (mp: 120.0 – 120.7 °C); 88 % yield (55.8 mg, 0.17 mmol); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.15 (d, *J* = 2.1 Hz, 1H), 7.08 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.99 (t, *J* = 8.1 Hz, 1H), 6.54 (d, *J* = 8.3 Hz, 1H), 6.27 (dd, *J* = 8.1, 2.2 Hz, 1H), 6.11 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.01 (t, *J* = 2.2 Hz, 1H), 5.83 (s, 1H), 4.76 (brs, 1H), 4.28 (brs, 1H), 4.14 – 4.05 (m, 1H), 3.71 – 3.62 (m, 4H), 2.46 (td, *J* = 11.7, 7.5 Hz, 1H), 2.30 (dd, *J* = 11.6, 4.6 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)** δ 160.7, 148.2, 146.8, 131.7, 130.1, 129.5, 124.1, 123.9, 109.4, 107.5, 103.7, 100.2, 96.0, 73.8, 65.6, 55.0, 43.1; **IR *v* (neat, cm^{-1}):** 3420, 3006, 2066, 1633, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}ClN_2O_2^+$ $[M+H]^+$: 317.1051, found: 317.1059.



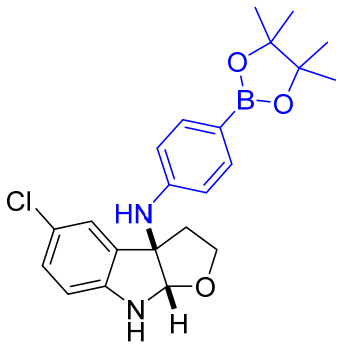
3el

5-Chloro-*N*-(2-methoxyphenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3el); reaction temperature: 80 °C; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); grew solid (mp: 166.3 – 167.4 °C); 94 % yield (60.0 mg, 0.19 mmol); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.16 (d, *J* = 2.1 Hz, 1H), 7.08 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.80 – 6.74 (m, 1H), 6.69 – 6.63 (m, 2H), 6.55 (d, *J* = 8.3 Hz, 1H), 6.29 (dd, *J* = 5.9, 3.5 Hz, 1H), 5.83 (s, 1H), 4.85 (brs, 1H), 4.73 (brs, 1H), 4.15 – 4.07 (m, 1H), 3.86 (s, 3H), 3.69 (ddd, *J* = 11.4, 9.2, 5.1 Hz, 1H), 2.55 (td, *J* = 11.7, 7.5 Hz, 1H), 2.35 – 2.27 (m, 1H); **^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)** δ 148.1, 147.1, 135.2, 132.0, 129.3, 124.1, 123.8, 121.1, 117.5, 111.7, 109.6, 109.4, 95.9, 73.4, 65.6, 55.5, 43.0; **IR *v* (neat, cm^{-1}):** 3446, 3006, 2065, 1640, 1275, 750, 668; **HRMS (ESI, m/z):** calcd for $C_{17}H_{18}ClN_2O_2^+$ $[M+H]^+$: 317.1051, found: 317.1050.



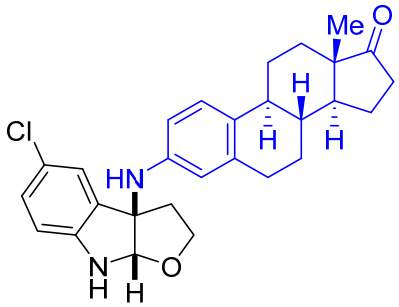
3em

5-Chloro-*N*-(9H-fluoren-2-yl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3em); reaction temperature: 80 ºC; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 222.8 – 228.3 ºC); 97 % yield (72.8 mg, 0.19 mmol); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.58 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.29 (t, *J* = 5.1 Hz, 1H), 7.19 – 7.14 (m, 2H), 7.10 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.70 (s, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 6.50 (dd, *J* = 8.2, 1.8 Hz, 1H), 5.88 (s, 1H), 4.70 (brs, 1H), 4.31 (brs, 1H), 4.14 (t, *J* = 7.8 Hz, 1H), 3.74 (d, *J* = 4.9 Hz, 2H), 3.73 – 3.66 (m, 1H), 2.56 (td, *J* = 11.7, 7.5 Hz, 1H), 2.32 (dd, *J* = 12.0, 4.6 Hz, 1H); **^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)** δ 148.3, 145.1, 142.4, 129.6, 126.8, 125.3, 124.8, 124.2, 124.1, 120.8, 118.8, 113.7, 111.6, 109.6, 100.1, 95.9, 65.9, 42.7, 37.1; **IR *v* (neat, cm^{-1}):**3446, 3006, 1646, 1507, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{23}H_{20}ClN_2O^+$ $[M+H]^+$: 375.1259, found: 375.1263.



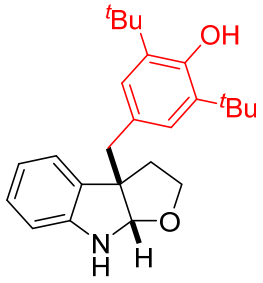
3en

5-Chloro-*N*-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-amine (3en); reaction temperature: 80 ºC; reaction time: 3 h; petroleum ether/ethylacetate = 8:1; **TLC**: R_f = 0.4 (PE / EA = 2:1, UV); white solid (mp: 183.1 – 188.7 ºC); 72 % yield (59.8 mg, 0.15 mmol); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.54 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 2.1 Hz, 1H), 7.07 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.54 (d, *J* = 8.3 Hz, 1H), 6.44 (d, *J* = 8.5 Hz, 2H), 5.83 (s, 1H), 4.62 (brs, 2H), 4.11 (t, *J* = 7.9 Hz, 1H), 3.70 – 3.72 (m, 1H), 2.48 (td, *J* = 11.7, 7.5 Hz, 1H), 2.30 (dd, *J* = 11.9, 4.5 Hz, 1H), 1.29 (s, 12H); **^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$)** δ 148.2, 148.0, 136.4, 131.5, 129.6, 124.1, 124.0, 113.5, 109.4, 96.1, 83.4, 73.7, 65.6, 43.0, 25.0, 24.9; **^{11}B NMR (128 MHz, CDCl$_3$)** δ 30.52; **IR *v* (neat, cm^{-1}):** 3446, 3006, 2065, 1640, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{22}H_{27}BClN_2O_3^+$ $[M+H]^+$: 413.1798, found: 413.1802.



3eo

(8*R*,9*S*,13*S*,14*S*)-3-((5-chloro-2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a-yl)amino)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H* cyclopenta[a]phenanthren-17-one (3eo); reaction temperature: 80 ºC; reaction time: 3 h; petroleum ether/ethylacetate = 50:1; TLC: R_f = 0.4 (PE / EA = 10:1, UV); white solid (mp: 169.8 – 172.2 ºC); 95 % yield (87.6 mg, 0.19 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.16 – 7.13 (m, 1H), 7.08 (dt, *J* = 8.3, 2.3 Hz, 1H), 7.00 (d, *J* = 8.5 Hz, 1H), 6.55 (dd, *J* = 8.3, 1.4 Hz, 1H), 6.28 (d, *J* = 9.0 Hz, 2H), 5.82 (d, *J* = 1.7 Hz, 1H), 4.09 (t, *J* = 8.2 Hz, 1H), 3.71 – 3.63 (m, 1H), 2.83 – 2.62 (m, 2H), 2.48 (dd, *J* = 19.0, 8.5 Hz, 2H), 2.28 (dd, *J* = 10.9, 5.5 Hz, 2H), 2.22 – 1.88 (m, 5H), 1.64 – 1.33 (m, 8H), 0.88 (s, 3H); **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ 221.1, 148.2, 143.4, 137.5, 132.1, 130.1, 129.5, 126.3, 124.3, 124.0, 115.1, 112.3, 109.4, 96.0, 73.9, 65.7, 50.6, 48.2, 44.1, 43.0, 38.6, 36.0, 31.7, 29.7, 26.7, 25.9, 21.7, 14.0; **IR *v* (neat, cm^{-1}):** 3445, 3006, 2989, 1633, 1475, 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{28}H_{32}ClN_2O_2^+$ $[M+H]^+$: 463.2147, found: 463.2141.



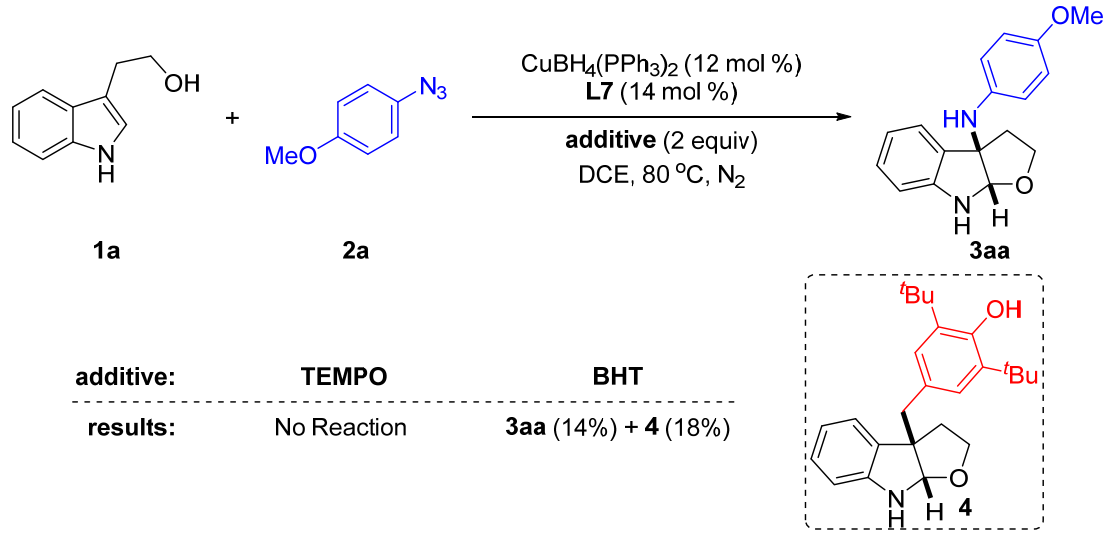
4

2,6-di-*tert*-butyl-4-((2,3,8,8a-tetrahydro-3a*H*-furo[2,3-b]indol-3a yl)methyl)phenol (4); reaction temperature: 80 ºC; reaction time: 3 h; petroleum ether/ethylacetate = 50:1; TLC: R_f = 0.4 (PE / EA = 10:1, UV); yellow oil; 18 % yield (13.6 mg, 0.04 mmol); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.05 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 7.3 Hz, 1H), 6.78 (s, 2H), 6.74 (t, *J* = 7.4 Hz, 1H), 6.53 (d, *J* = 7.8 Hz, 1H), 5.37 (s, 1H), 5.07 (s, 1H), 4.42 (s, 1H), 3.96 (t, *J* = 7.8 Hz, 1H), 3.58 – 3.48 (m, 1H), 3.12 (d, *J* = 13.5 Hz, 1H), 2.87 (d, *J* = 13.5 Hz, 1H), 2.29 (td, *J* = 11.5, 7.3 Hz, 1H), 2.14 (dd, *J* =

11.8, 4.7 Hz, 1H), 1.37 (s, 18H); **$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)** δ 152.4, 149.9, 135.3, 132.1, 128.4, 128.2, 126.7, 124.4, 118.7, 108.6, 97.3, 67.6, 59.2, 43.9, 39.8, 34.3, 30.4; **IR *v* (neat, cm^{-1}):** 3444, 3008, 2066, 1636. 1275, 1261, 750; **HRMS (ESI, m/z):** calcd for $C_{25}H_{34}NO_2^+$ $[M+H]^+$: 380.2584, found: 380.2588.

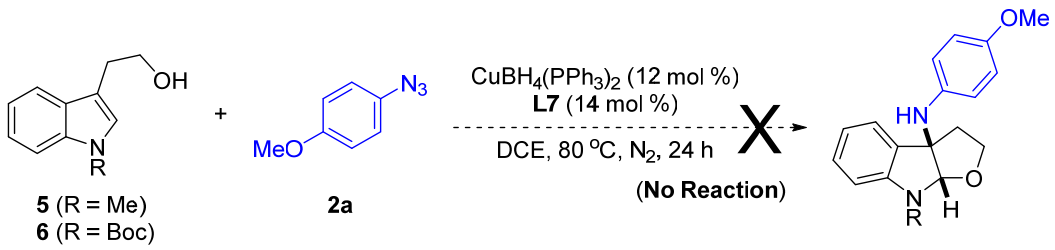
IV. Mechanistic Experiments:

(a) Radical inhibitation reactions



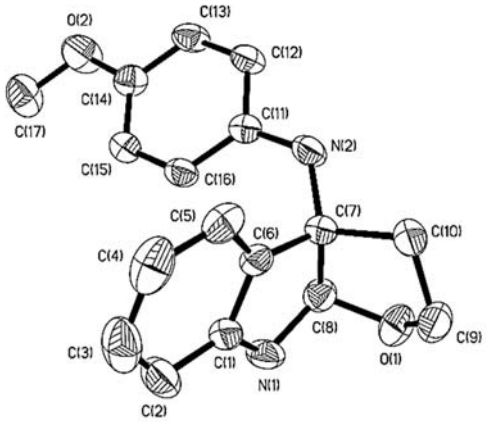
After stirring a mixture of $CuBH_4(PPh_3)_2$ (0.024 mmol, 12 mol %) and **L7** (0.028 mmol, 14 mol %) in dry DCE (2 mL) at 80 °C for 1 h, substrates **1a** (0.20 mmol) and **2a** (0.30 mmol) and **TEMPO** or **BHT** (0.40 mmol) was added. The reaction mixture was stirred at 80 °C under argon atmosphere. After the disappearance of substrate **1a** (monitored by TLC) and then the crude product was purified by silica gel flash chromatography to afford the desired product **3aa.**

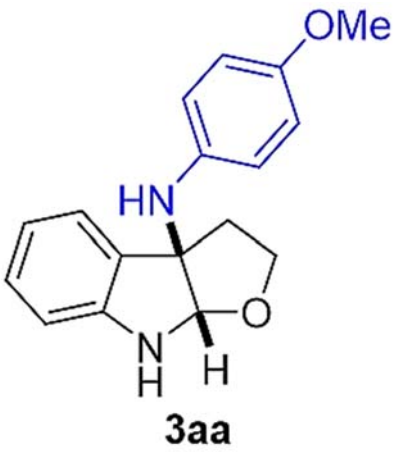
(b) Control experiments



After stirring a mixture of $CuBH_4(PPh_3)_2$ (0.024 mmol, 12 mol %) and **L7** (0.028 mmol, 14 mol %) in dry DCE (2 mL) at 80°C for 1 h, substrates **5** or **6** (0.20 mmol) and **2a** (0.30mmol) was added. The reaction mixture was stirred at 80 °C under argon atmosphere. And then the reaction was monitored by TLC.

V. Crystallographic Data





3aa

Table S4. Crystal data and structure refinement for **3aa** (CCDC: 1951998).

Identification code	d8v19607
Empirical formula	C17 H18 N2 O2
Formula weight	282.33
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 16.9108(15) Å a= 90°.
	b = 7.6555(6) Å b= 105.615(3)°.
	c = 11.6950(11) Å g = 90°.
Volume	1458.2(2) $Å^3$
Z	4
Density (calculated)	1.286 Mg/m^3
Absorption coefficient	0.085 mm^{-1}
F(000)	600
Crystal size	0.170 x 0.150 x 0.120 mm^3
Theta range for data collection	2.940 to 25.999°.
Index ranges	-20<=h<=20, -9<=k<=9, -14<=l<=14
Reflections collected	14661
Independent reflections	2857 [R(int) = 0.0495]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6041
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2857 / 0 / 196
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1112
R indices (all data)	R1 = 0.0591, wR2 = 0.1204
Extinction coefficient	0.027(5)

Largest diff. peak and hole	0.355 and -0.403 e.Å^{-3}

VI. Reference

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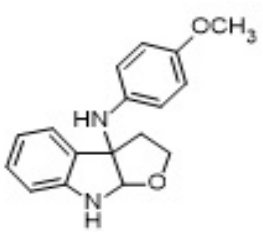
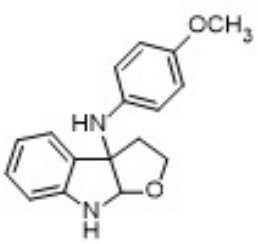


3aa

VII．NMR Spectra of New Compounds (^{1}H NMR, ^{13}C NMR, ^{19}F NMR, ^{11}B NMR)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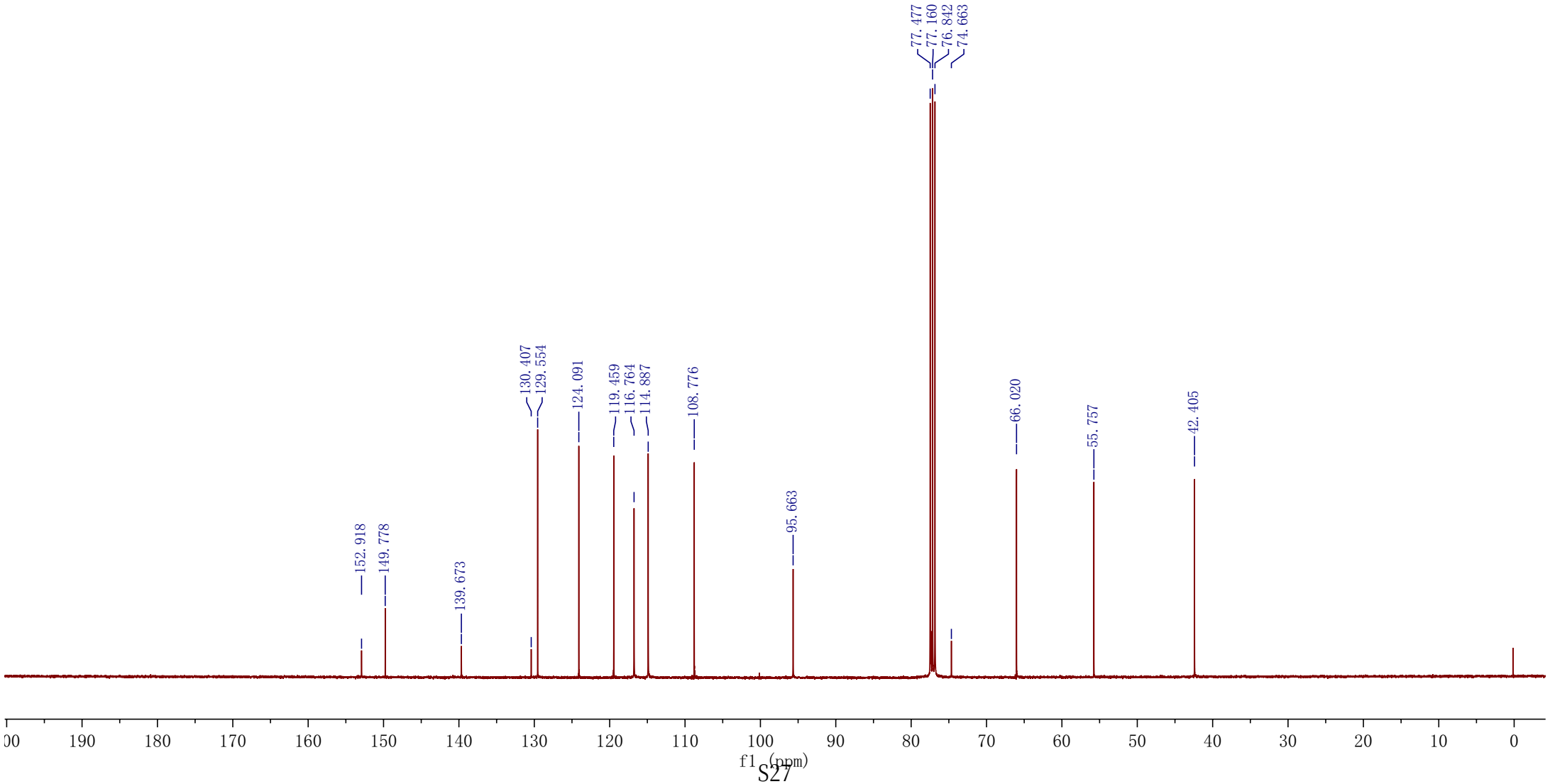
HN
O
N
H

3aa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77.160
76.842
74.663
152.918
149.778
139.673
130.407
129.554
124.091
119.459
116.764
114.887
108.776
95.663
66.020
55.757
42.405
190
180
170
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130
120
110
100
90
80
70
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50
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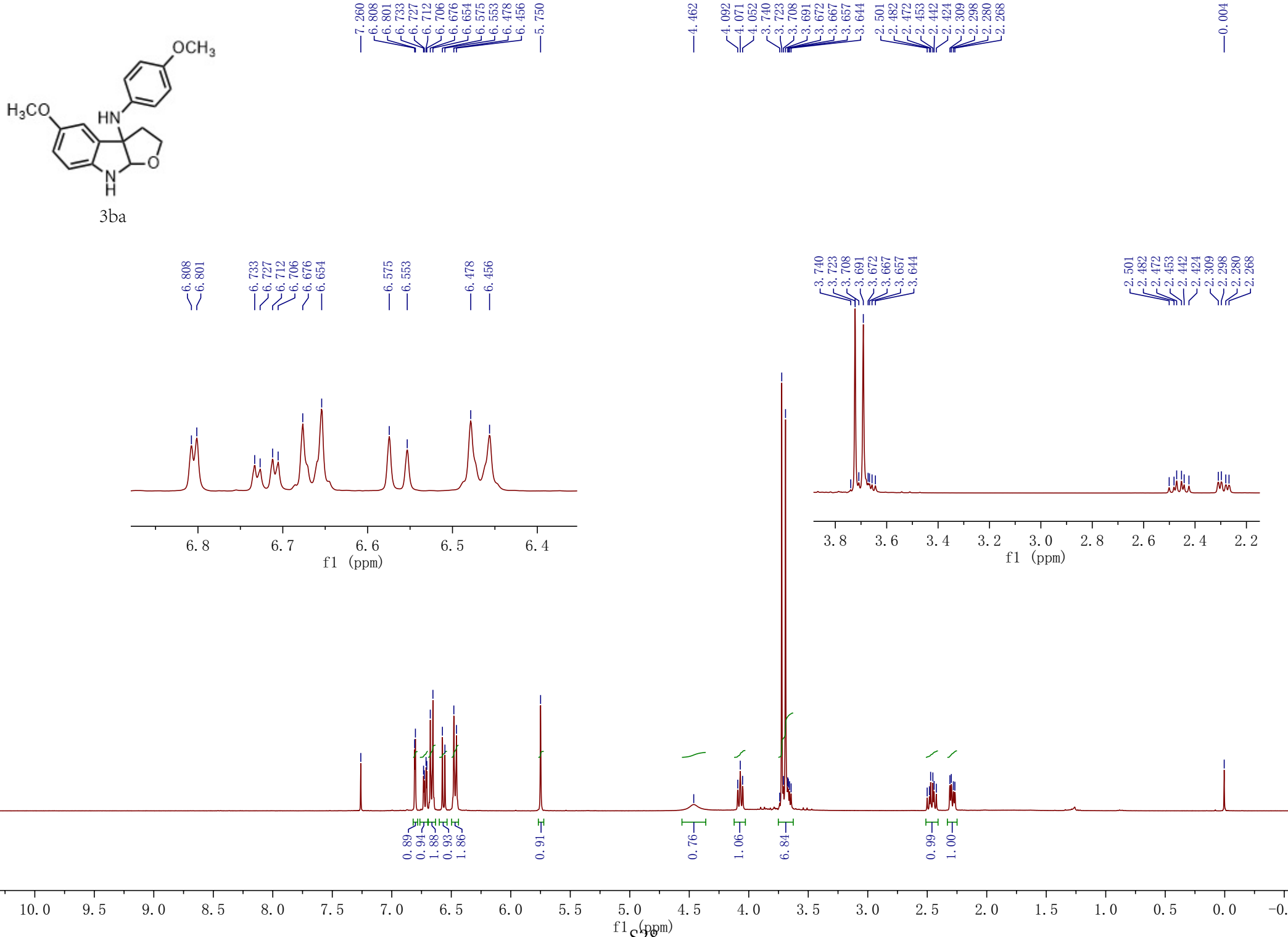
30
20
10
0
f1 (ppm)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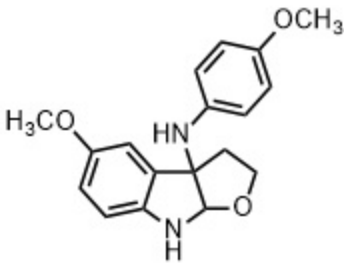
H3CO
HN
O
N
H
3ba
f1 (ppm)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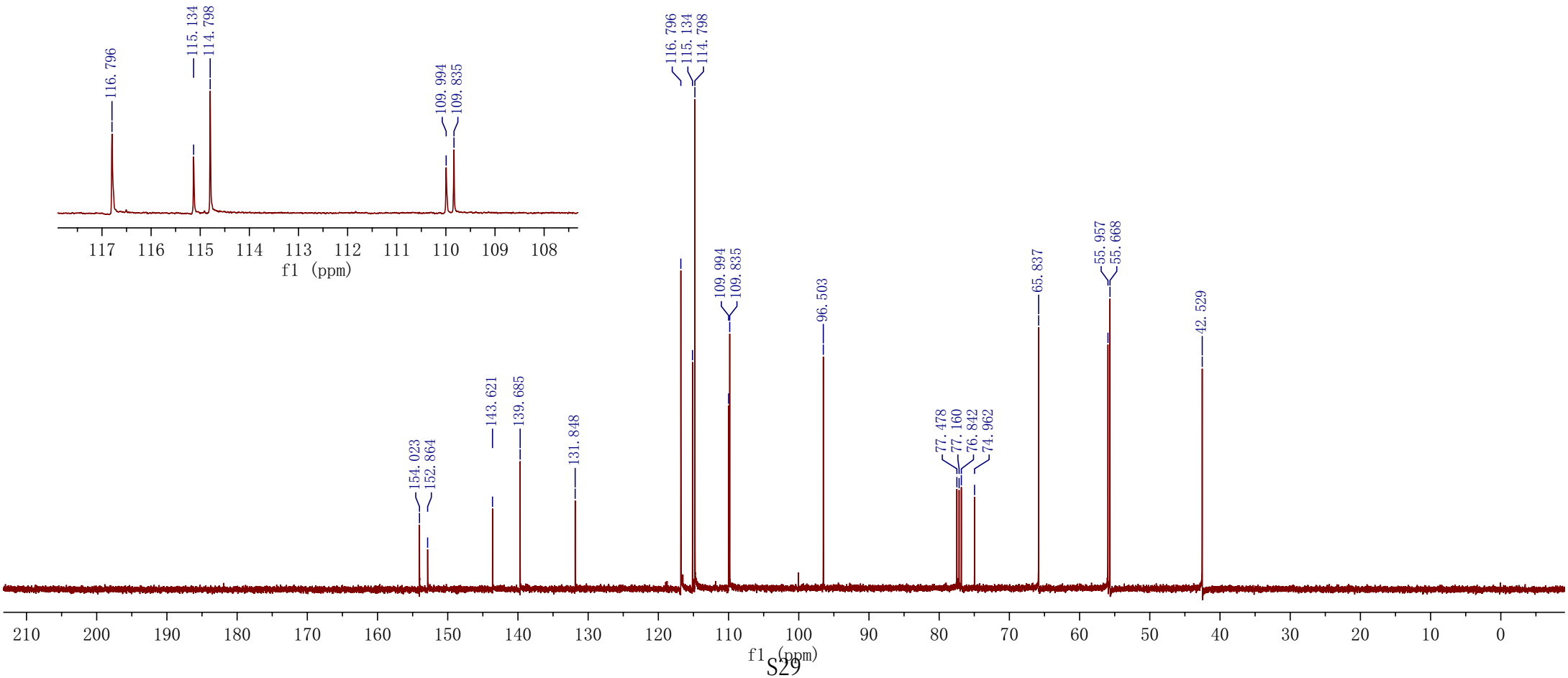
H3CO
HN
O
N
H

3ba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77.478
77.160
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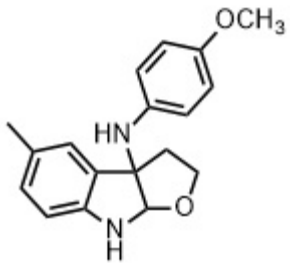
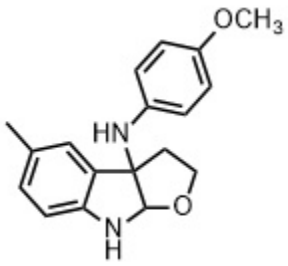
42.529
f1 (ppm)



3ca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O
N
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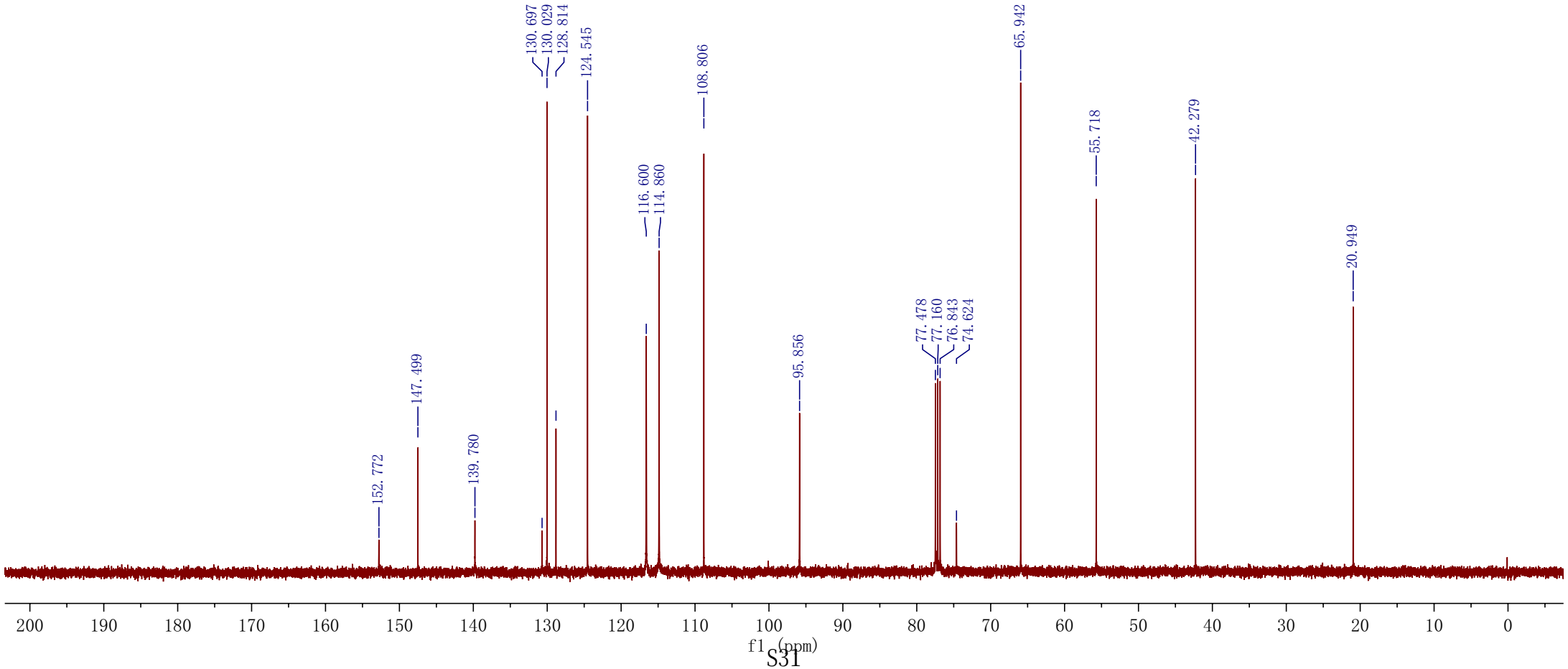
3ca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180
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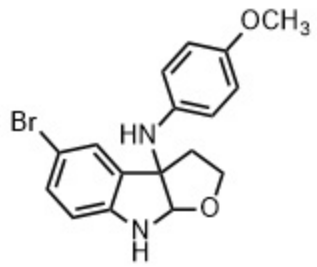
f1 (ppm)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Br
HN
O
N
H

3da

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6.486
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6.442
5.760
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4.107
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4.065
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3.692
3.678
3.668
3.663
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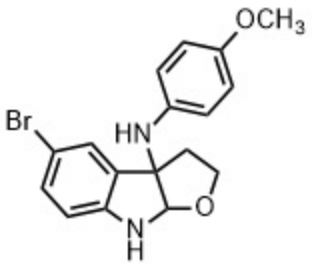
1.08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Br
HN
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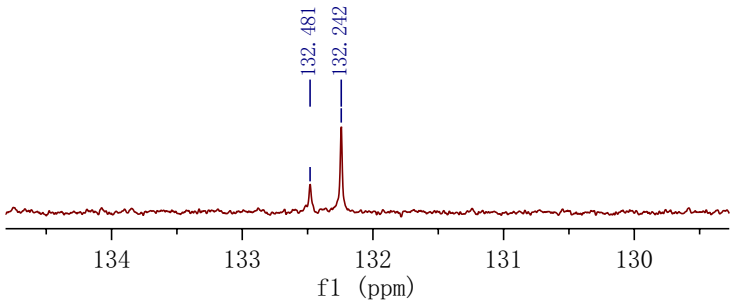
3da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131
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42. 884
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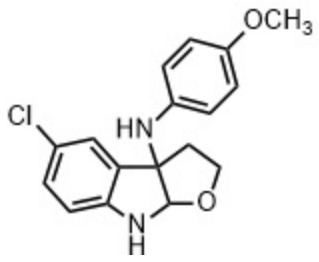
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3ea

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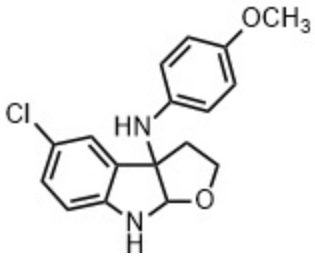
1.04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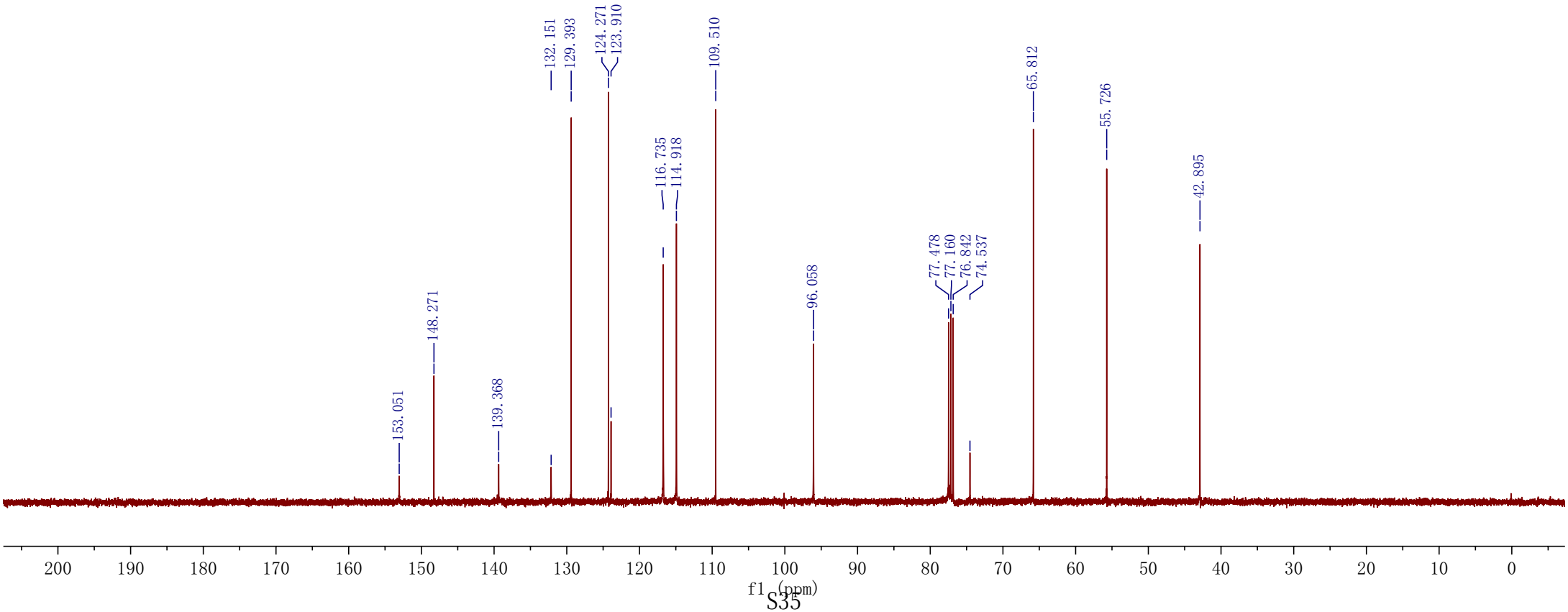
Cl
HN
N
H
O

3ea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76.842
74.537
65.812
55.726
42.895
200
190
180
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50
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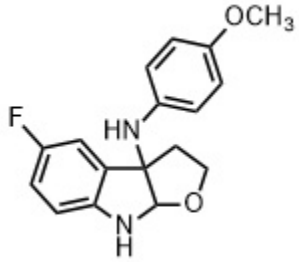
f1 (ppm)



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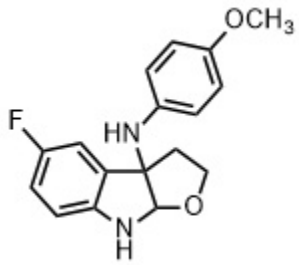
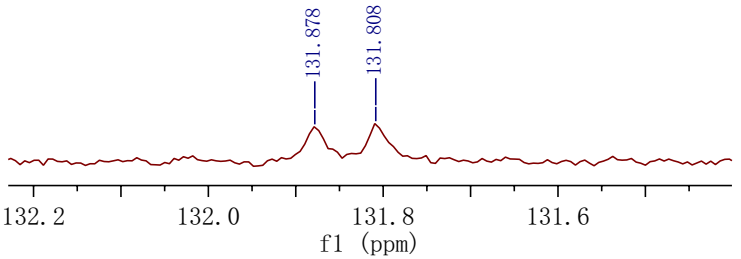

OCH3
F
HN
O
N
H

3fa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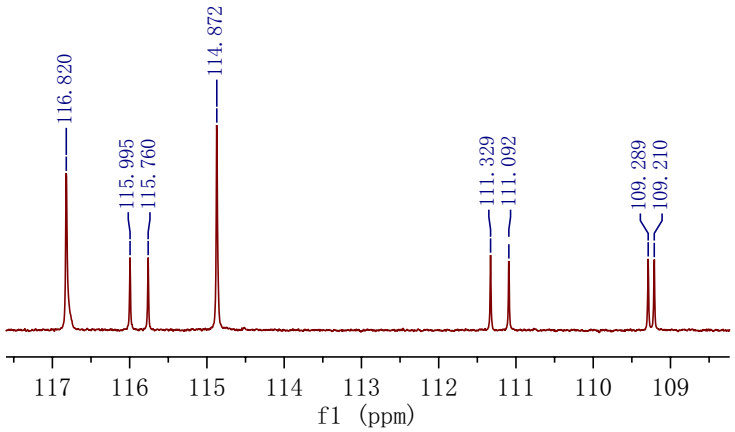
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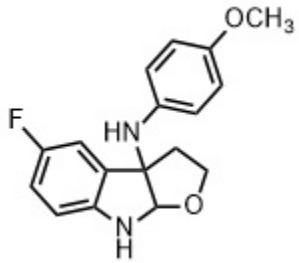
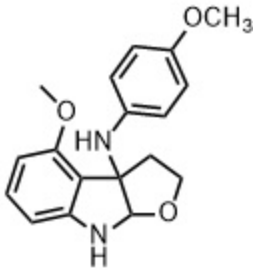
116
115
114
113
112
111
110
109
f1 (ppm)

116.820
115.995
115.760
114.872
111.329
111.092
109.289
109.210
65.775
55.695
43.003
96.653
77.478
77.160
76.843
74.755
158.562
156.211
153.050
145.720
139.459
131.878
131.808
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


OCH3
F
HN
O
N
H

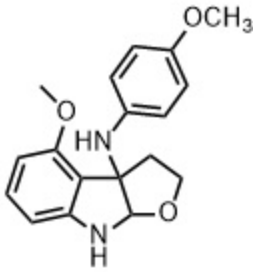
3fa

-125.067
1.00
90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

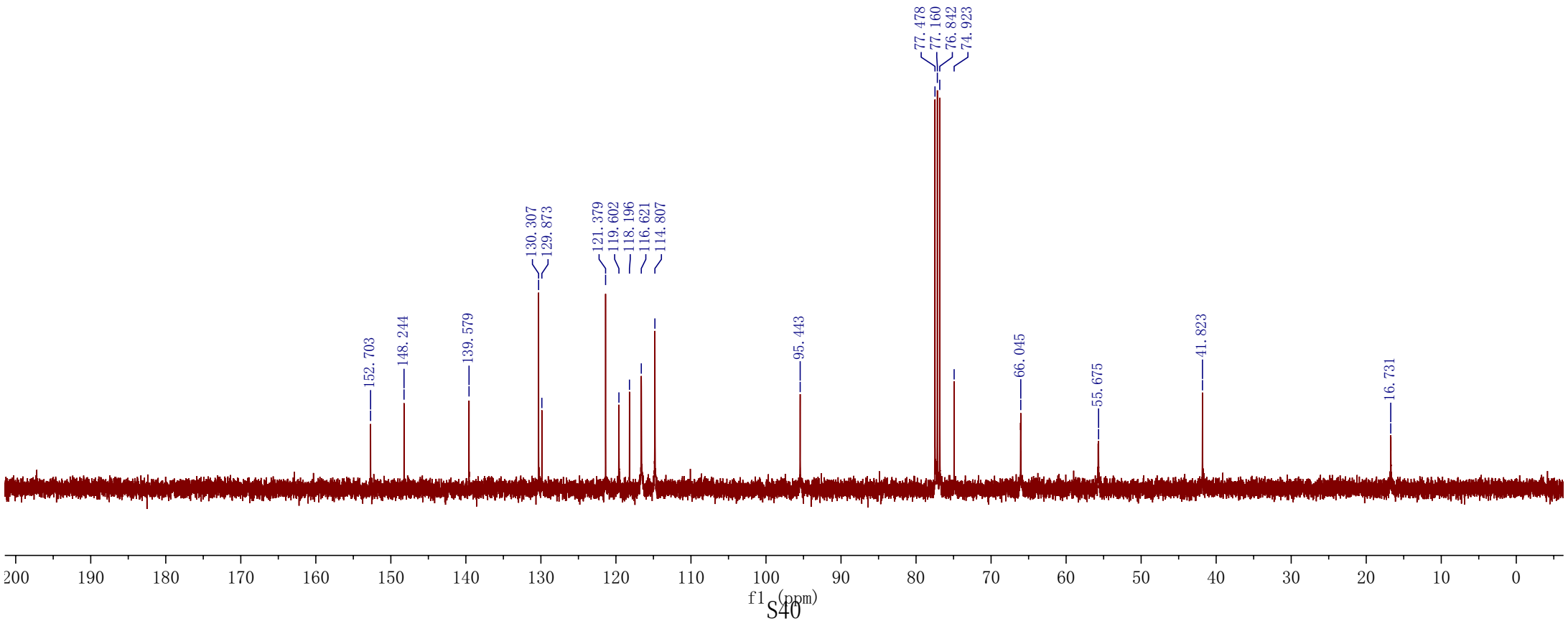

OCH3
O
HN
O
N
H

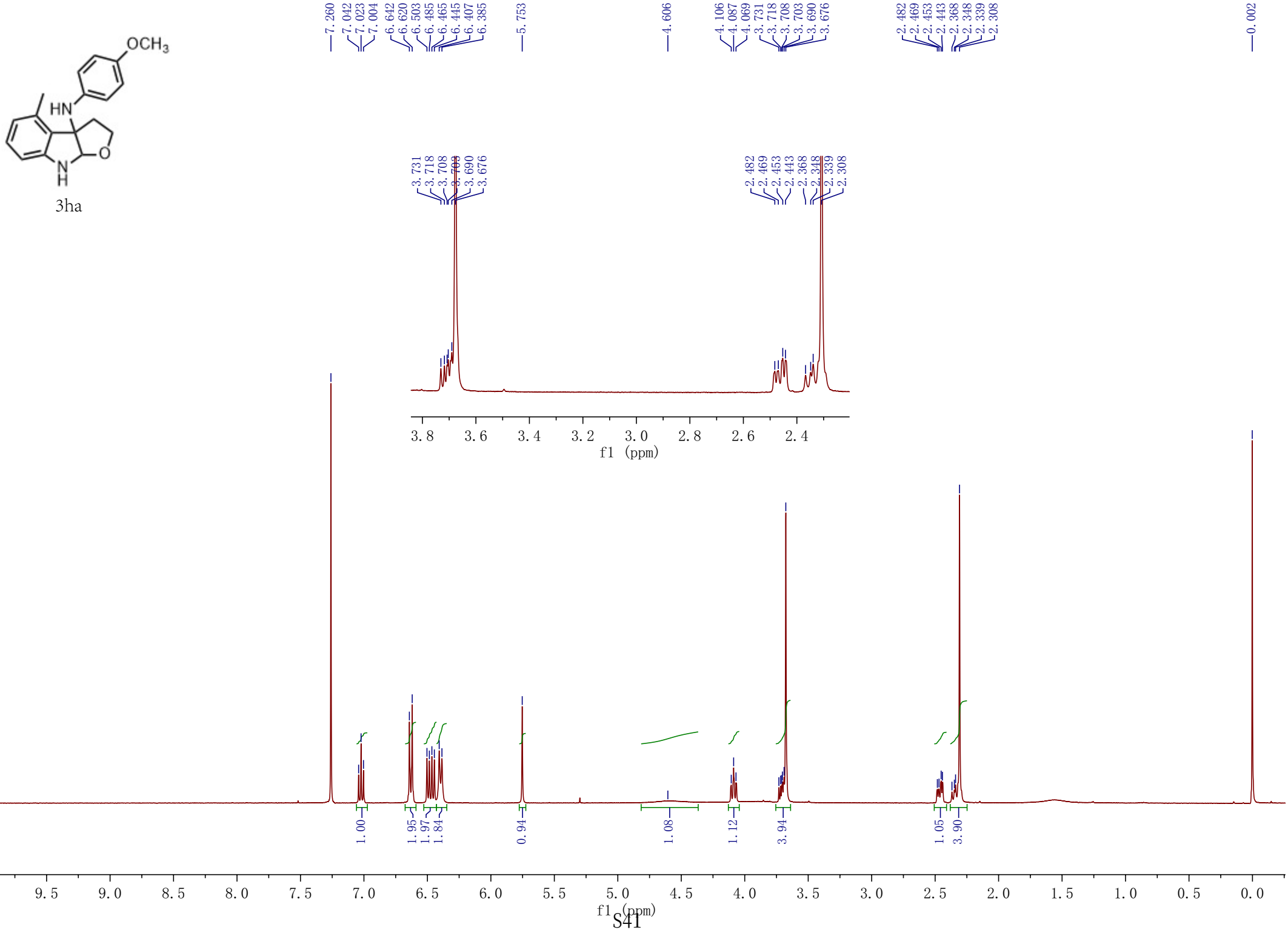
3ga

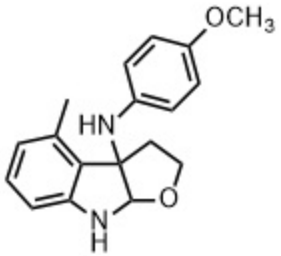
7.260
7.071
7.051
7.031
6.676
6.653
6.580
6.558
6.249
6.229
5.778
4.650
4.113
4.104
4.100
4.091
4.081
4.069
3.768
3.693
3.675
3.656
3.634
2.489
2.477
2.467
2.458
0.003
1.00
1.99
1.93
1.89
0.98
0.98
1.10
3.02
3.88
1.98
f1 (ppm)


OCH3
O
HN
O
N
H

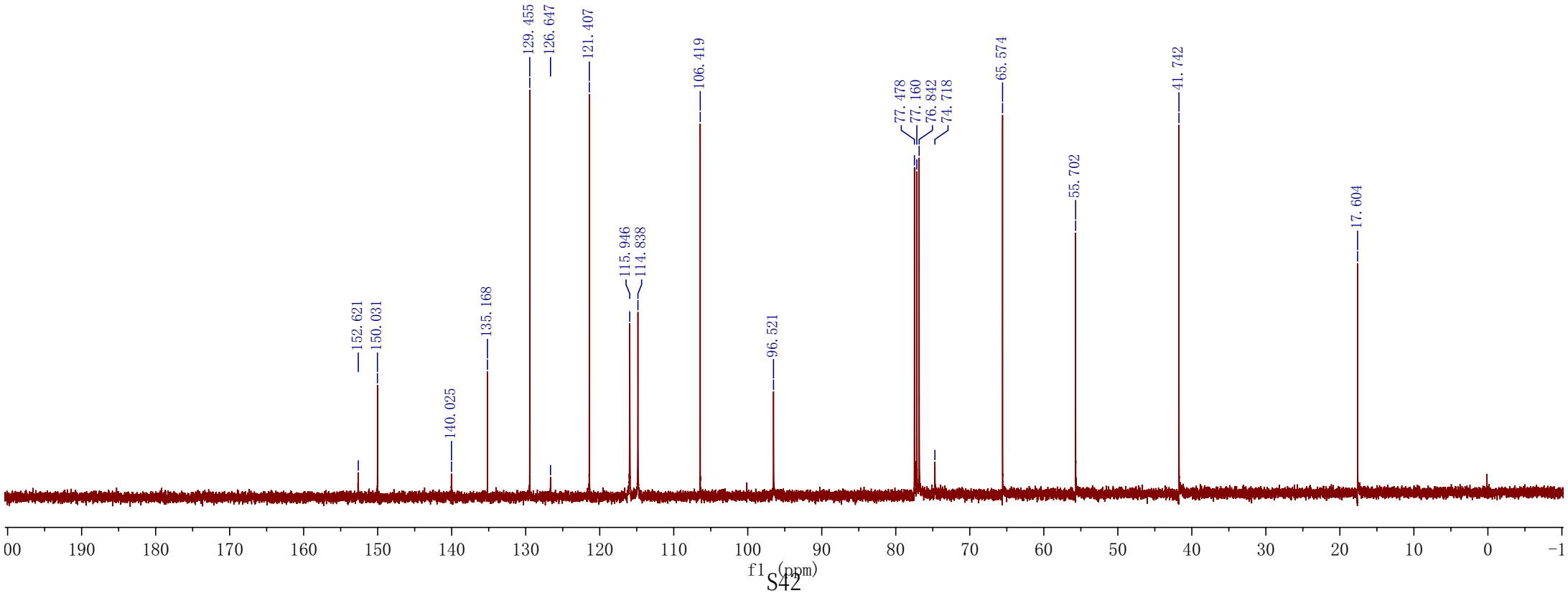
3ga

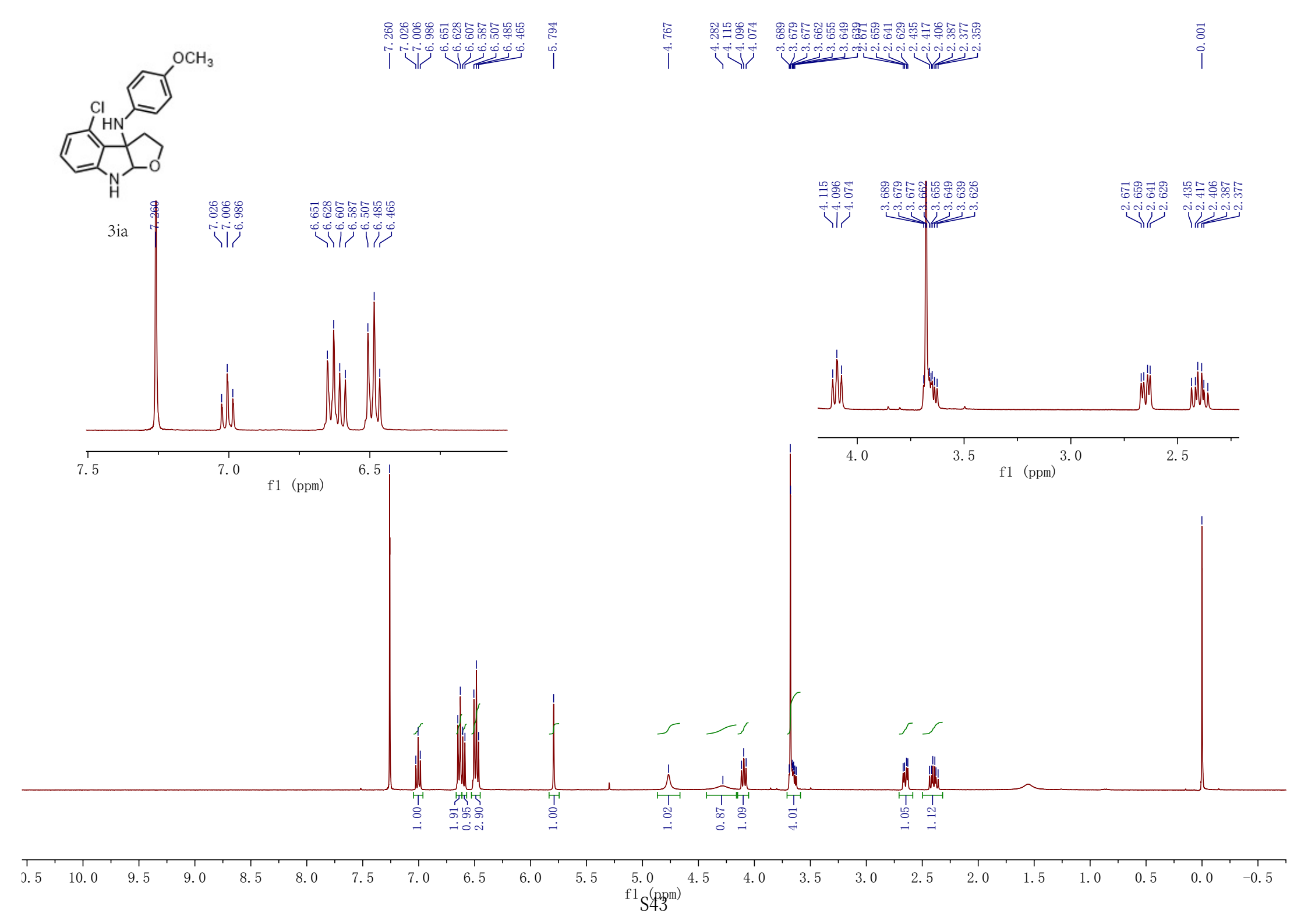

152.703
148.244
139.579
130.307
129.873
121.379
119.602
118.196
116.621
114.807
95.443
77.478
77.160
76.842
74.923
66.045
55.675
41.823
16.731
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

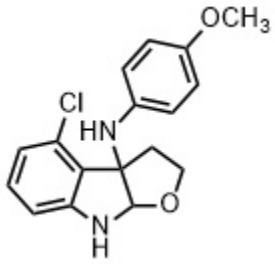

OCH3
HN
O
N
H
3ha
7.260
7.042
7.023
7.004
6.642
6.620
6.503
6.485
6.465
6.445
6.407
6.385
5.753
4.606
4.106
4.087
4.069
3.731
3.718
3.708
3.703
3.690
3.676
2.482
2.469
2.453
2.443
2.368
2.348
2.339
2.308
0.002
f1 (ppm)
1.00
1.95
1.97
1.84
0.94
1.08
1.12
3.94
1.05
3.90


OCH3
HN
N
H
O

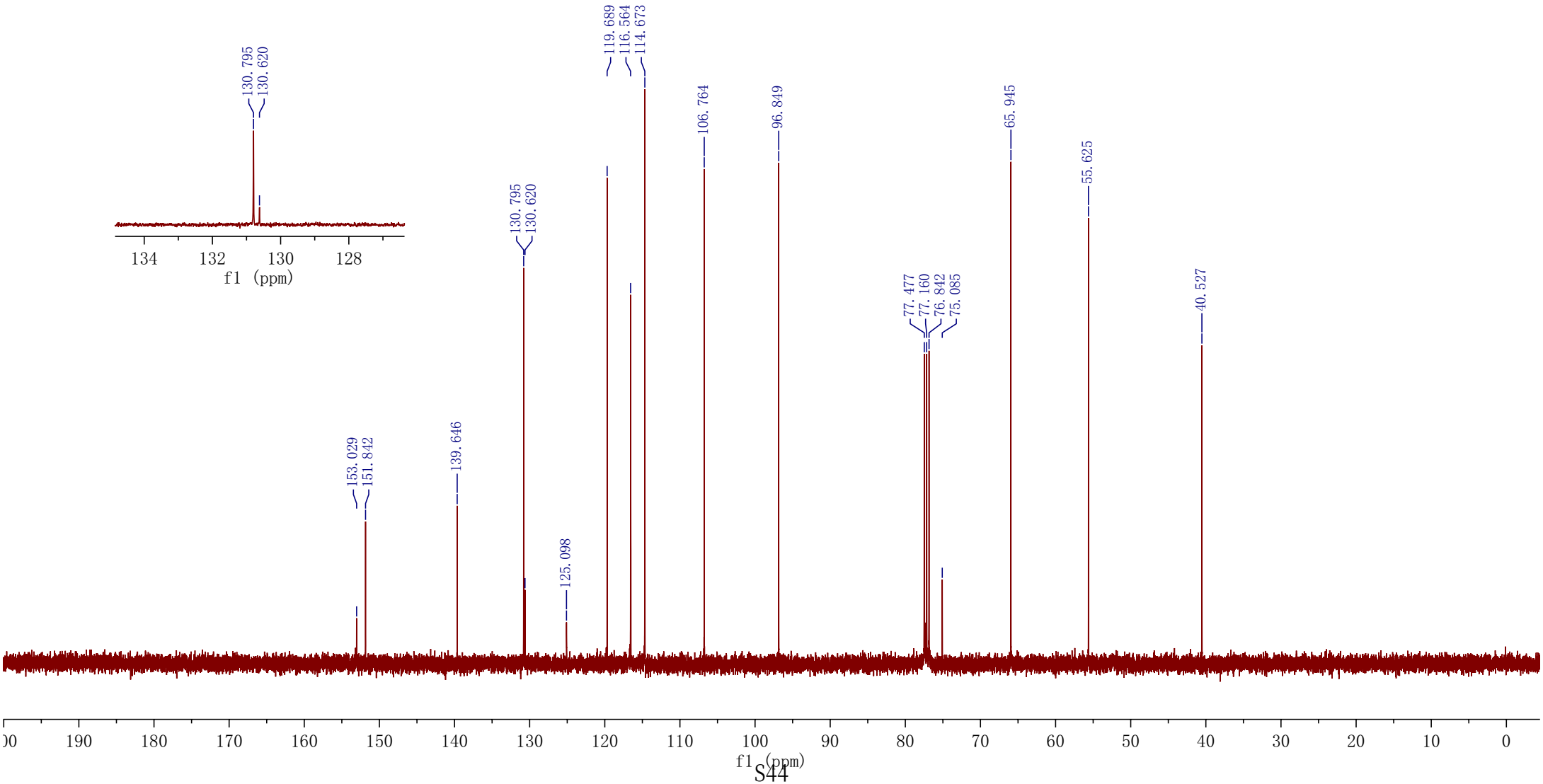
3ha

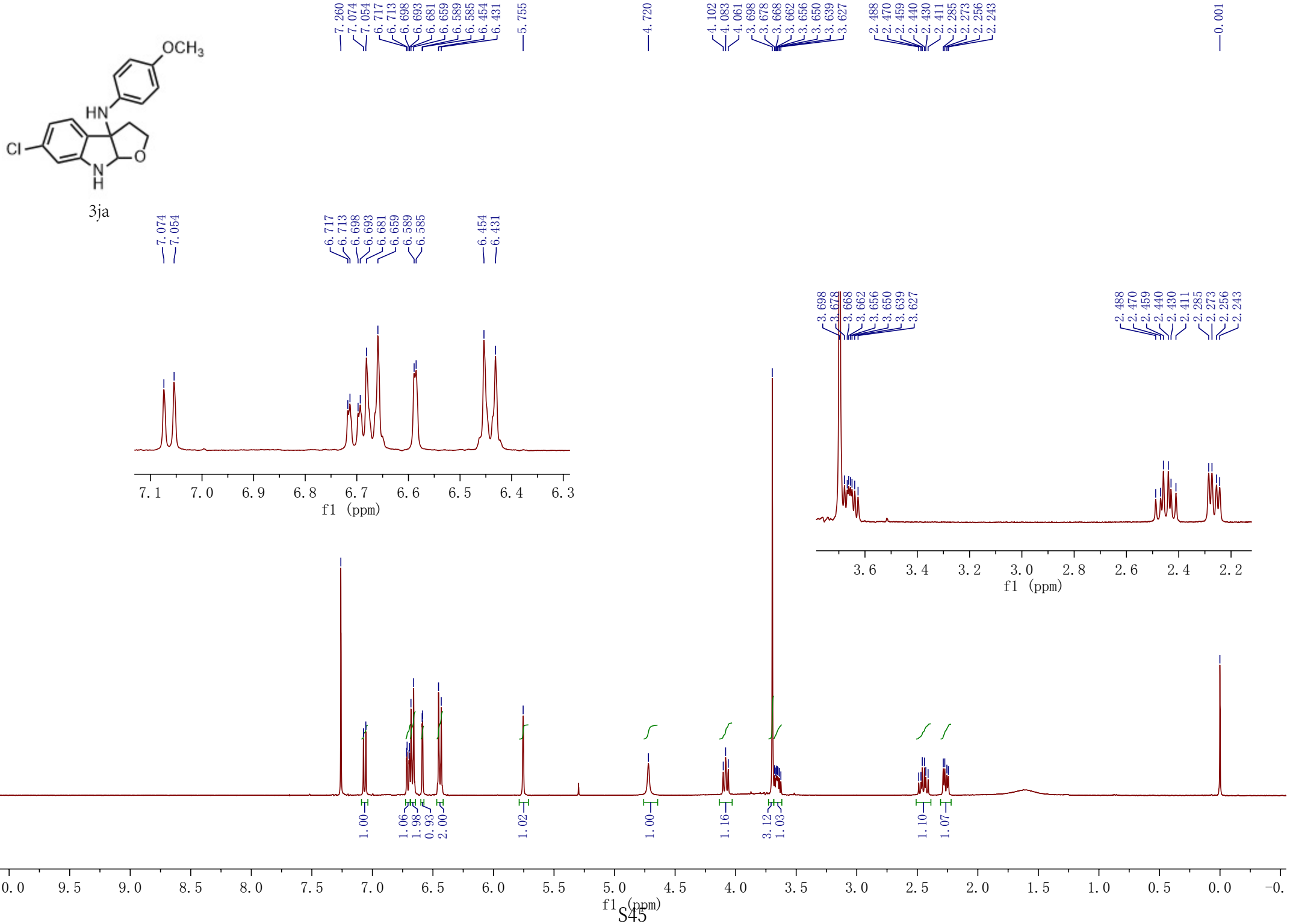

152.621
150.031
140.025
135.168
129.455
126.647
121.407
115.946
114.838
106.419
96.521
77.478
77.160
76.842
74.718
65.574
55.702
41.742
17.604
f1 (ppm)

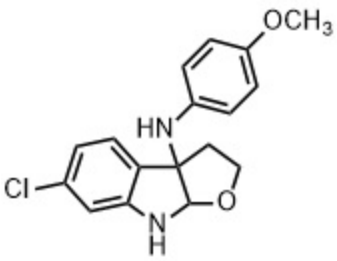

OCH3
Cl
HN
N
H
O
3ia
7.260
7.026
7.006
6.986
6.651
6.628
6.607
6.587
6.507
6.485
6.465
5.794
4.767
4.282
4.115
4.096
4.074
3.689
3.679
3.677
3.662
3.655
3.649
3.639
3.626
2.671
2.659
2.641
2.629
2.435
2.417
2.406
2.387
2.377
2.359
0.001
f1 (ppm)
1.00
1.91
0.95
2.90
1.00
1.02
0.87
1.09
4.01
1.05
1.12


OCH3
Cl
HN
N
H
O

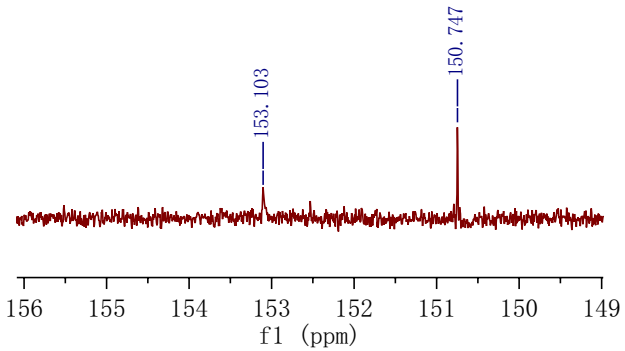
3ia

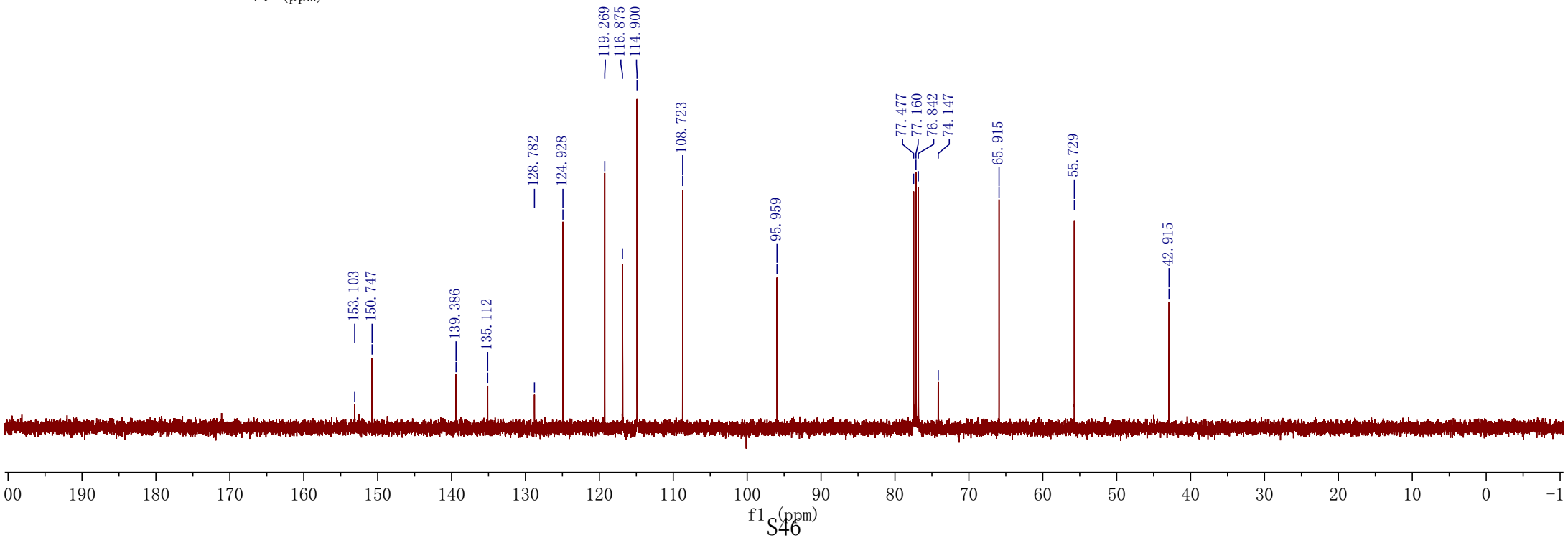

130.795
130.620
119.689
116.564
114.673
106.764
96.849
65.945
55.625
40.527
77.477
77.160
76.842
75.085
153.029
151.842
139.646
125.098
134
132
130
128
f1 (ppm)
f1 (ppm)

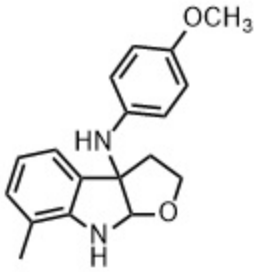

OCH3
HN
Cl
N
H
O
3ja
7.260
7.074
7.054
6.717
6.713
6.698
6.693
6.681
6.659
6.589
6.585
6.454
6.431
5.755
4.720
4.102
4.083
4.061
3.698
3.678
3.668
3.662
3.656
3.650
3.639
3.627
2.488
2.470
2.459
2.440
2.430
2.411
2.285
2.273
2.256
2.243
0.001
f1 (ppm)
1.00
1.06
1.98
0.93
2.00
1.02
1.00
1.16
3.12
1.03
1.10
1.07


OCH3
HN
Cl
O
N
H

3ja

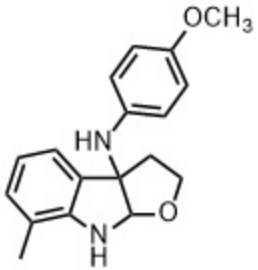

153.103
150.747
156
155
154
153
152
151
150
149
f1 (ppm)


153.103
150.747
139.386
135.112
128.782
124.928
119.269
116.875
114.900
108.723
95.959
77.477
77.160
76.842
74.147
65.915
55.729
42.915
f1 (ppm)

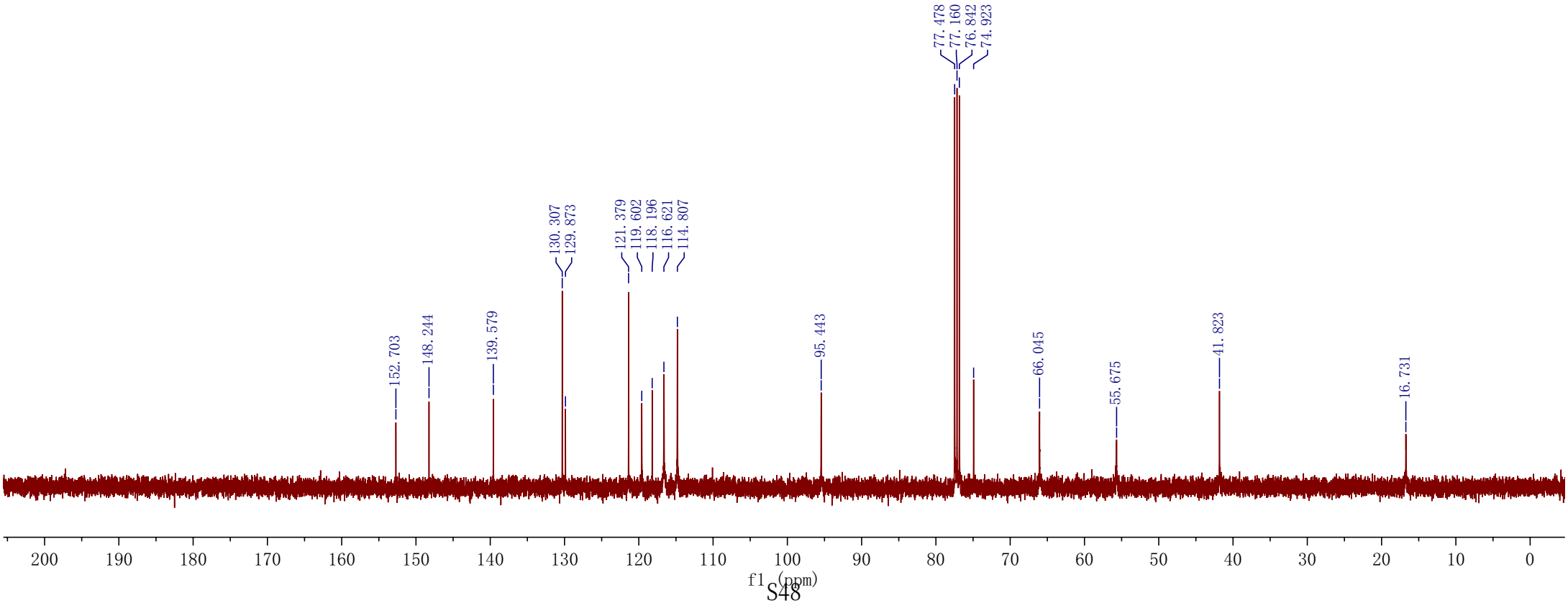

OCH3
HN
O
N
H

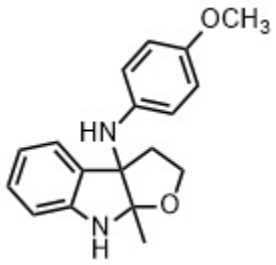
3ka

7.260
6.988
6.970
6.743
6.724
6.705
6.687
6.665
6.495
6.473
5.807
4.489
4.116
4.094
4.074
3.699
3.685
3.679
3.673
3.667
3.657
3.644
2.592
2.573
2.563
2.544
2.533
2.514
2.286
2.273
2.256
2.243
2.180
0.001
f1 (ppm)
1.04
1.05
1.12
2.00
2.03
1.00
1.00
1.36
4.34
1.19
1.12
3.09
f1 (ppm)


OCH3
HN
O
N
H

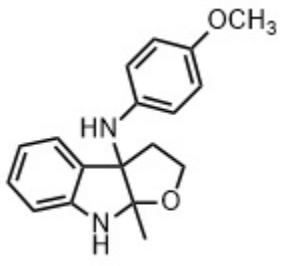
3ka


77.478
77.160
76.842
74.923
152.703
148.244
139.579
130.307
129.873
121.379
119.602
118.196
116.621
114.807
95.443
66.045
55.675
41.823
16.731
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

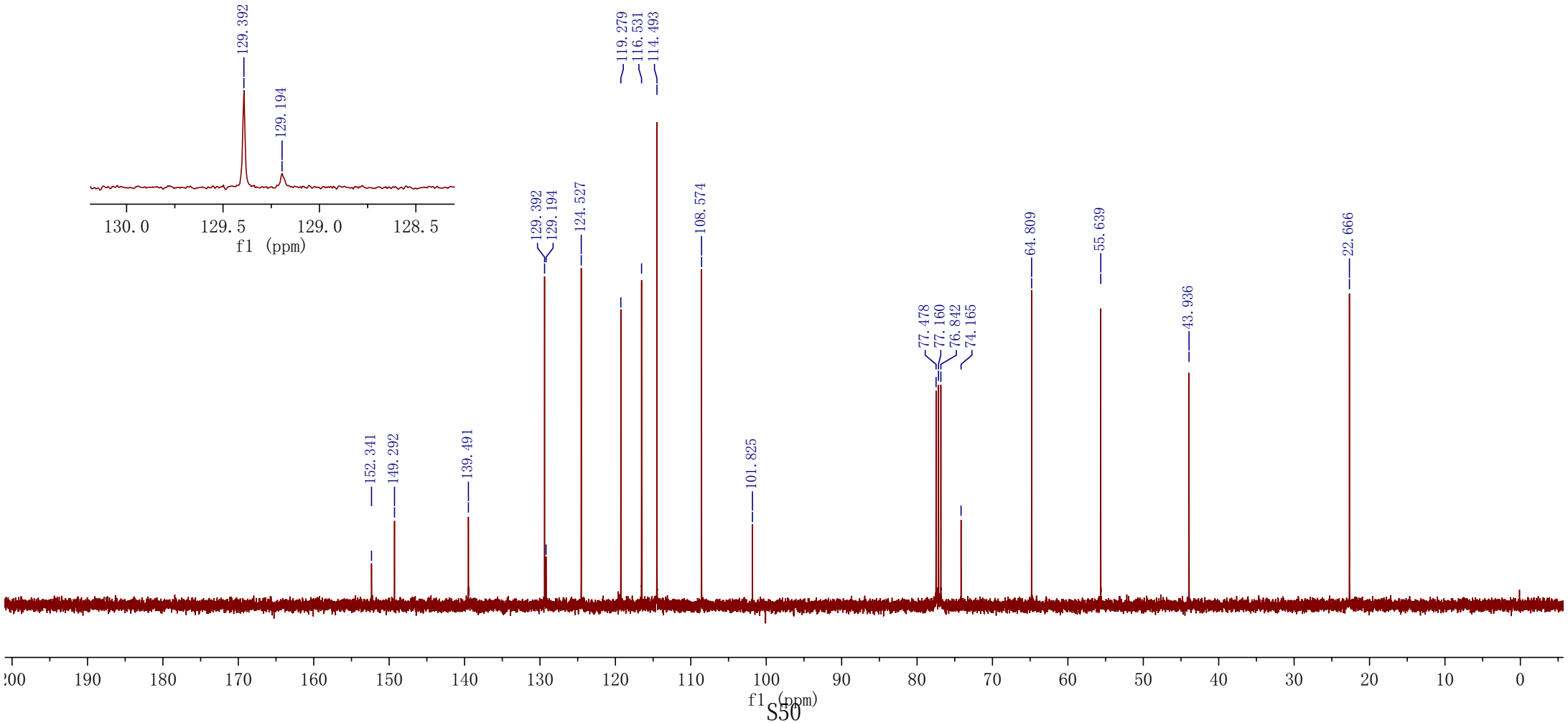

OCH3
HN
N
H
O

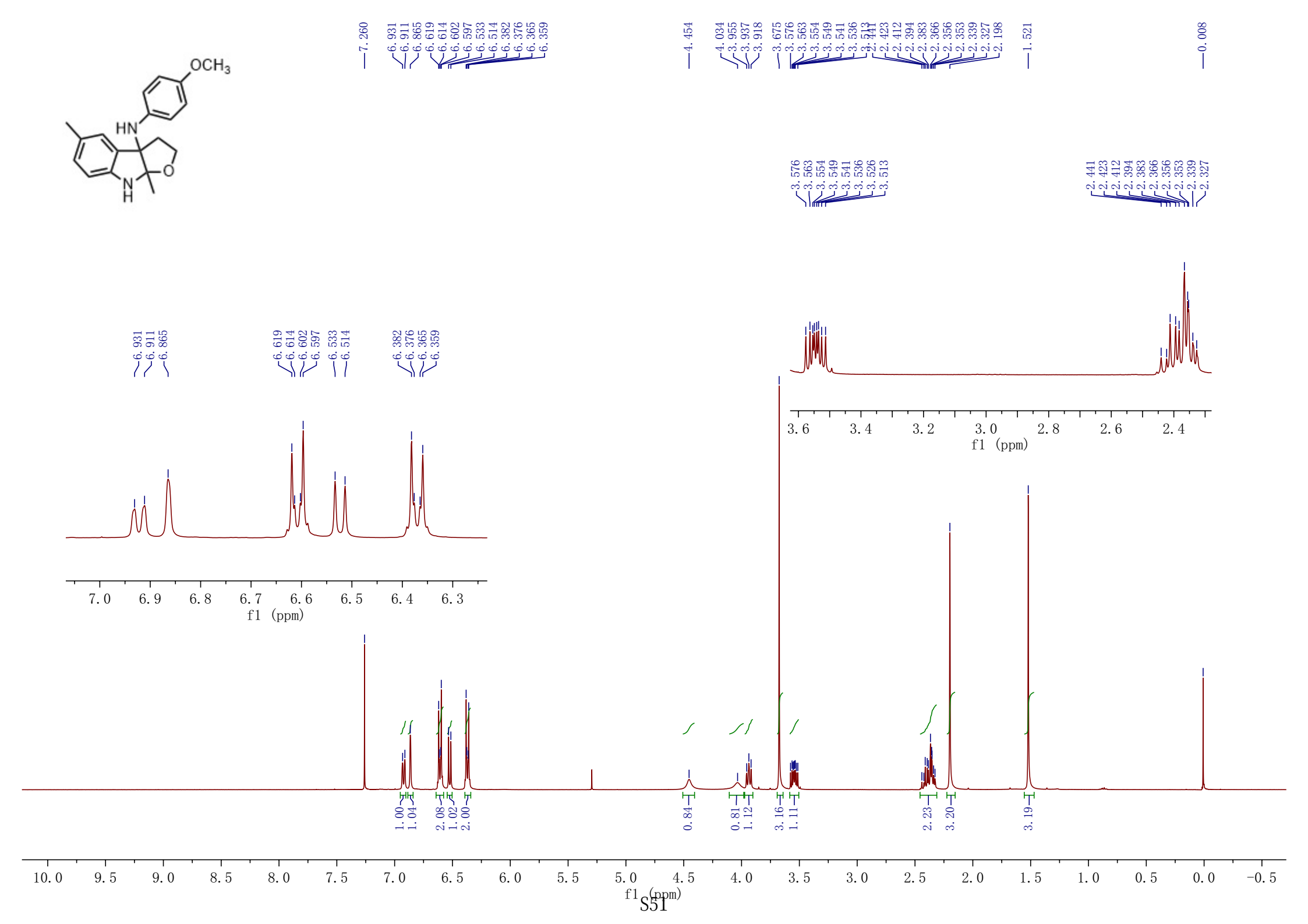
3la

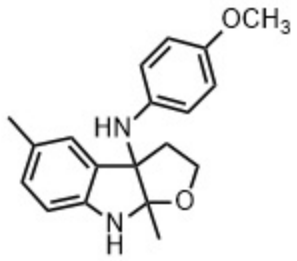
7.260
7.126
7.108
7.089
7.026
7.008
6.721
6.703
6.684
6.614
6.604
6.595
6.587
6.582
6.573
6.366
6.344
4.572
4.036
3.963
3.944
3.925
3.665
3.580
3.566
3.557
3.552
3.545
3.539
3.529
3.516
2.426
2.409
2.398
2.384
2.374
2.371
2.357
2.345
1.541
0.003
f1 (ppm)
1.00
1.00
0.97
2.87
1.98
0.90
0.70
1.14
2.99
1.07
2.02
3.23


OCH3
HN
N
H
O

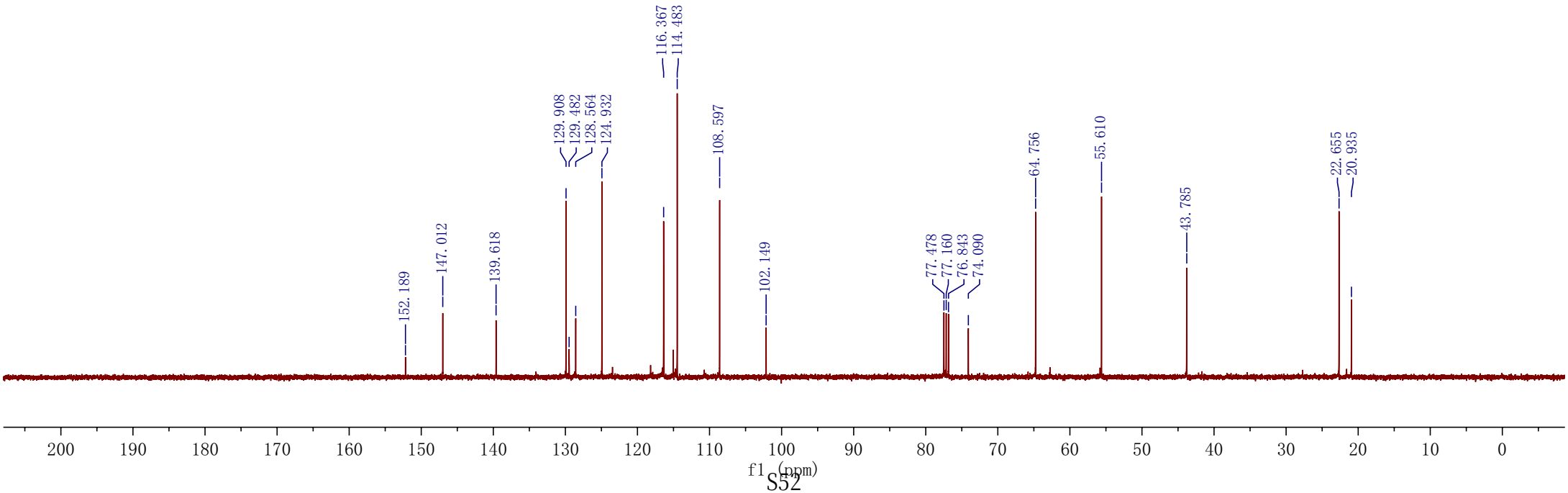
3la

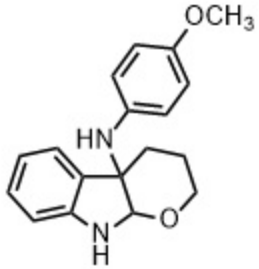

129.392
129.194
130.0
129.5
129.0
128.5
f1 (ppm)
119.279
116.531
114.493
129.392
129.194
124.527
108.574
64.809
55.639
43.936
22.666
77.478
77.160
76.842
74.165
152.341
149.292
139.491
101.825
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OCH3
HN
O
N
H
7.260
6.931
6.911
6.865
6.619
6.614
6.602
6.597
6.533
6.514
6.382
6.376
6.365
6.359
4.454
4.034
3.955
3.937
3.918
3.675
3.576
3.563
3.554
3.549
3.541
3.536
3.513
2.441
2.423
2.412
2.394
2.383
2.366
2.356
2.353
2.339
2.327
2.198
1.521
0.008
f1 (ppm)
1.00
1.04
2.08
1.02
2.00
0.84
0.81
1.12
3.16
1.11
2.23
3.20
3.19

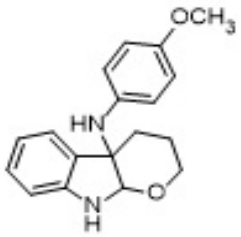

OCH3
HN
O
N
H

3ma

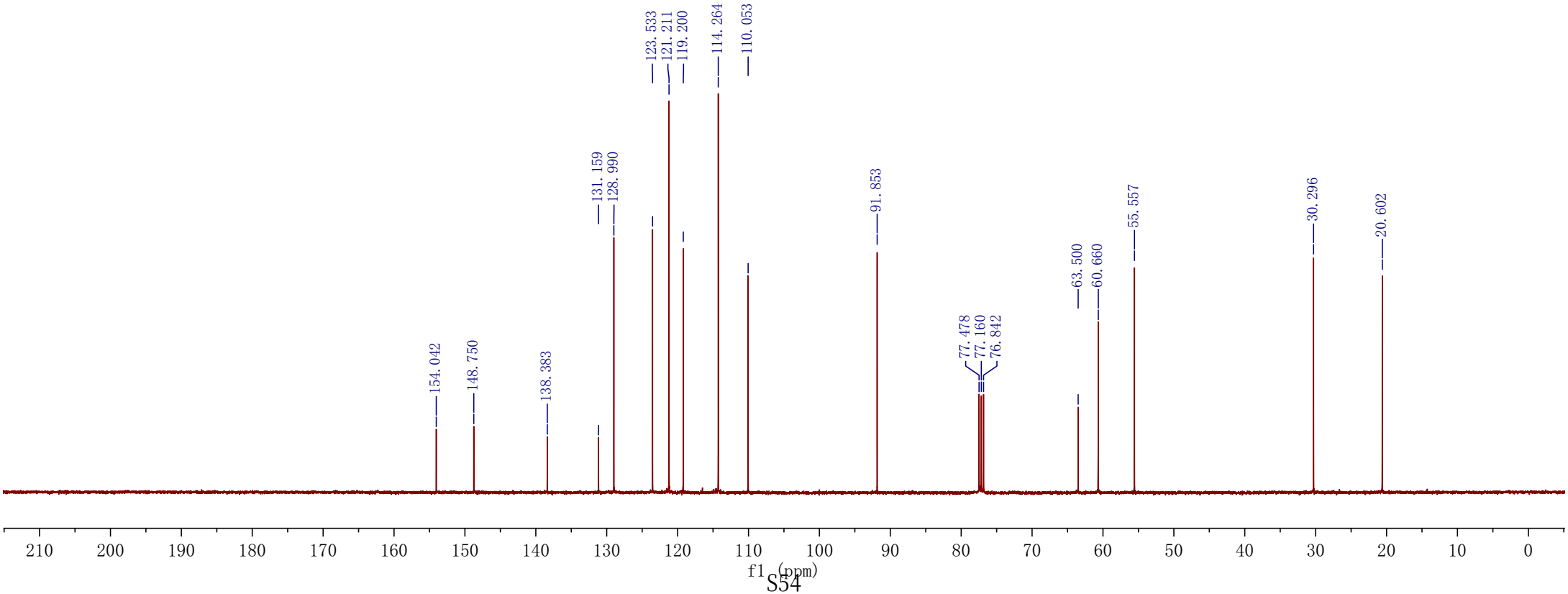

152.189
147.012
139.618
129.908
129.482
128.564
124.932
116.367
114.483
108.597
102.149
77.478
77.160
76.843
74.090
64.756
55.610
43.785
22.655
20.935
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

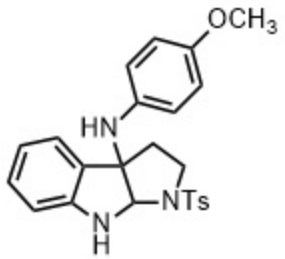


3na

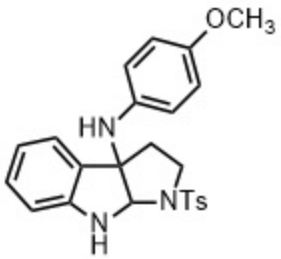

OCH3
HN
N
H
O

3na

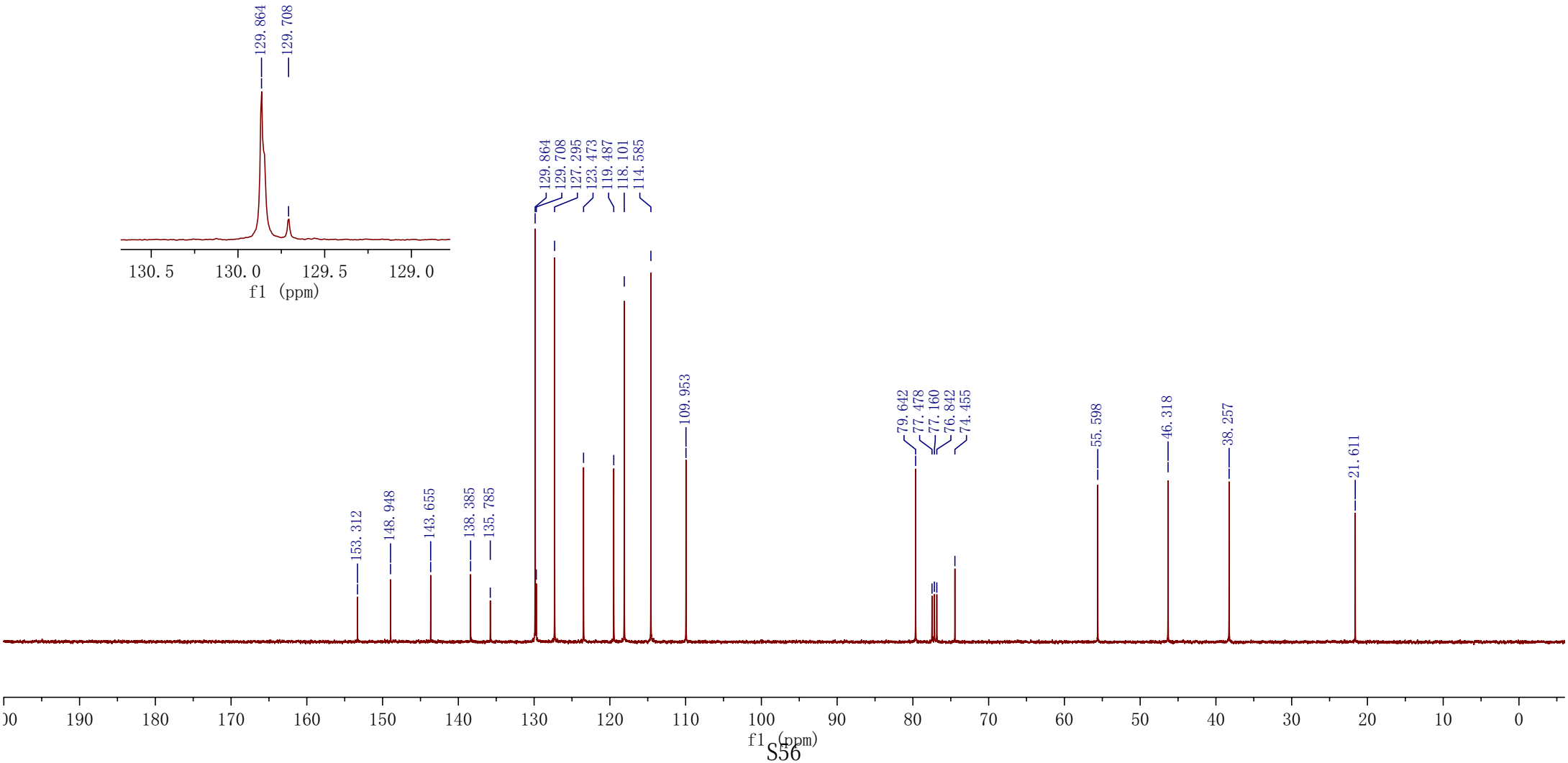

154.042
148.750
138.383
131.159
128.990
123.533
121.211
119.200
114.264
110.053
91.853
77.478
77.160
76.842
63.500
60.660
55.557
30.296
20.602
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

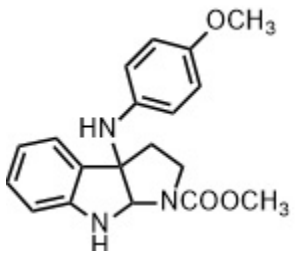


3oa


OCH3
HN
NTs
N
H

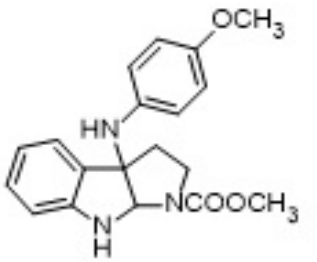
3oa


129.864
129.708
130.5
130.0
129.5
129.0
f1 (ppm)
129.864
129.708
127.295
123.473
119.487
118.101
114.585
153.312
148.948
143.655
138.385
135.785
109.953
79.642
77.478
77.160
76.842
74.455
55.598
46.318
38.257
21.611
f1 (ppm)

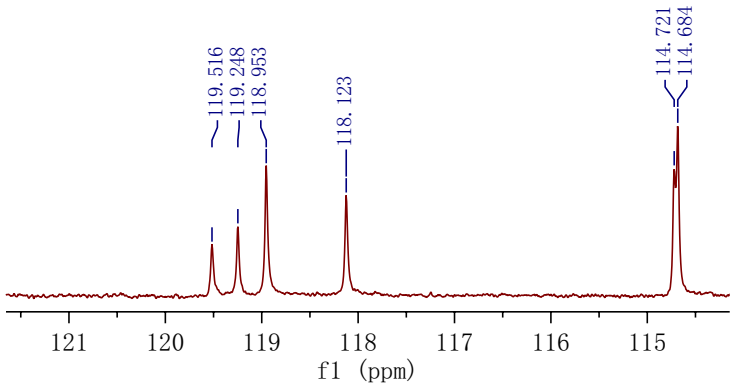

OCH3
HN
NCOOCH3
N
H

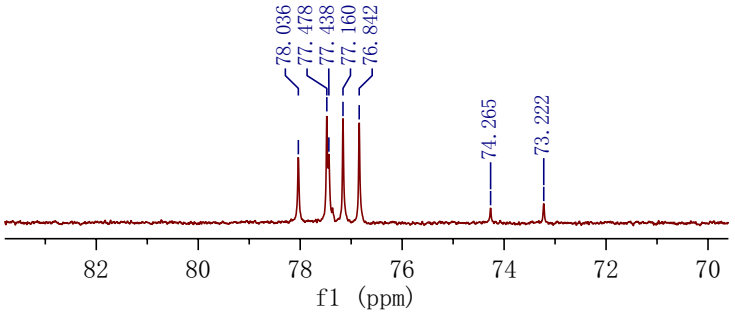
3pa

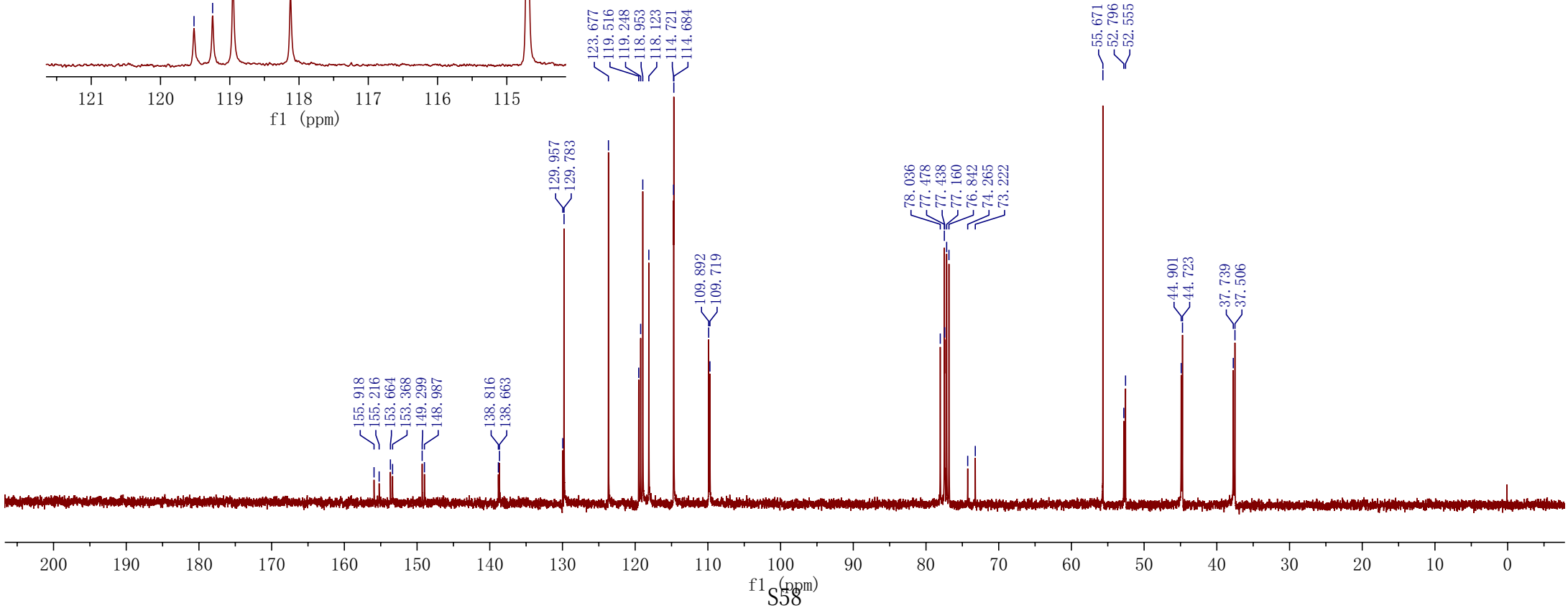
7.190
7.089
7.070
7.052
6.703
6.685
6.631
6.626
6.614
6.609
6.564
6.544
6.486
6.464
6.445
5.515
5.484
5.032
4.685
3.818
3.772
3.752
3.733
3.724
3.683
3.641
3.614
3.175
3.154
3.129
3.111
3.085
2.550
2.527
2.497
2.475
2.445
2.423
2.291
2.283
0.069
f1 (ppm)
1.93
0.99
1.85
0.98
2.03
1.00
0.54
0.55
7.02
1.15
1.12
1.05

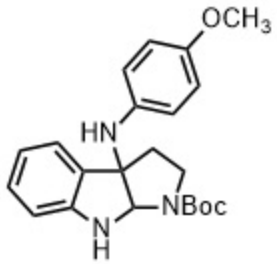

OCH3
HN
NCOOCH3
N
H

3pa


119.516
119.248
118.953
118.123
114.721
114.684
121
120
119
118
117
116
115
f1 (ppm)

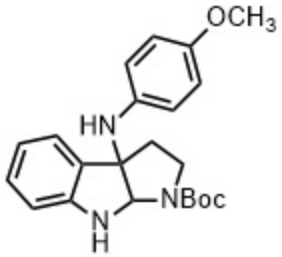

78.036
77.478
77.438
77.160
76.842
74.265
73.222
82
80
78
76
74
72
70
f1 (ppm)


123.677
119.516
119.248
118.953
118.123
114.721
114.684
129.957
129.783
109.892
109.719
78.036
77.478
77.438
77.160
76.842
74.265
73.222
55.671
52.796
52.555
44.901
44.723
37.739
37.506
155.918
155.216
153.664
153.368
149.299
148.987
138.816
138.663
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

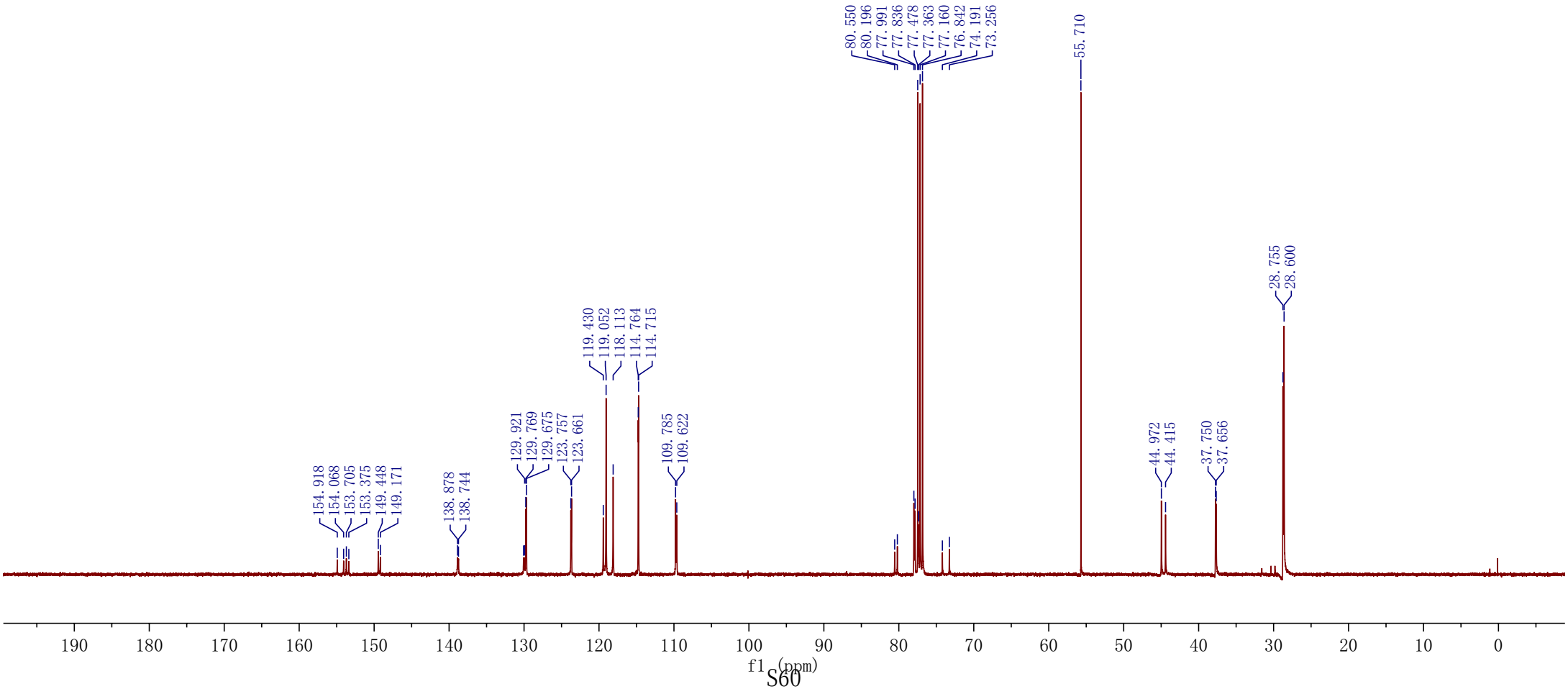

OCH3
HN
NBoc
N
H

3qa

7.260
6.775
6.756
6.737
6.718
6.705
6.694
6.684
6.672
6.642
6.623
6.548
6.523
6.500
5.559
5.479
5.109
4.684
3.772
3.753
3.711
3.666
3.647
3.627
3.205
3.182
3.157
3.139
2.539
2.527
2.516
2.330
2.321
1.509
1.478
1.458
0.002
6.9
6.8
6.7
6.6
6.5
6.4
f1 (ppm)
2.00
0.99
2.11
0.98
2.01
1.07
0.52
0.45
0.68
3.08
0.63
1.08
1.13
1.12
9.45
f1 (ppm)


OCH3
HN
NBoc
N
H

3qa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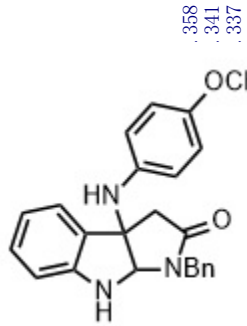
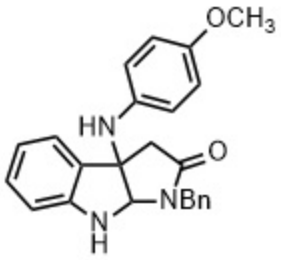
80.196
77.991
77.836
77.478
77.363
77.160
76.842
74.191
73.256
55.710
154.918
154.068
153.705
153.375
149.448
149.171
138.878
138.744
129.921
129.769
129.675
123.757
123.661
119.430
119.052
118.113
114.764
114.715
109.785
109.622
44.972
44.415
37.750
37.656
28.755
28.600
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

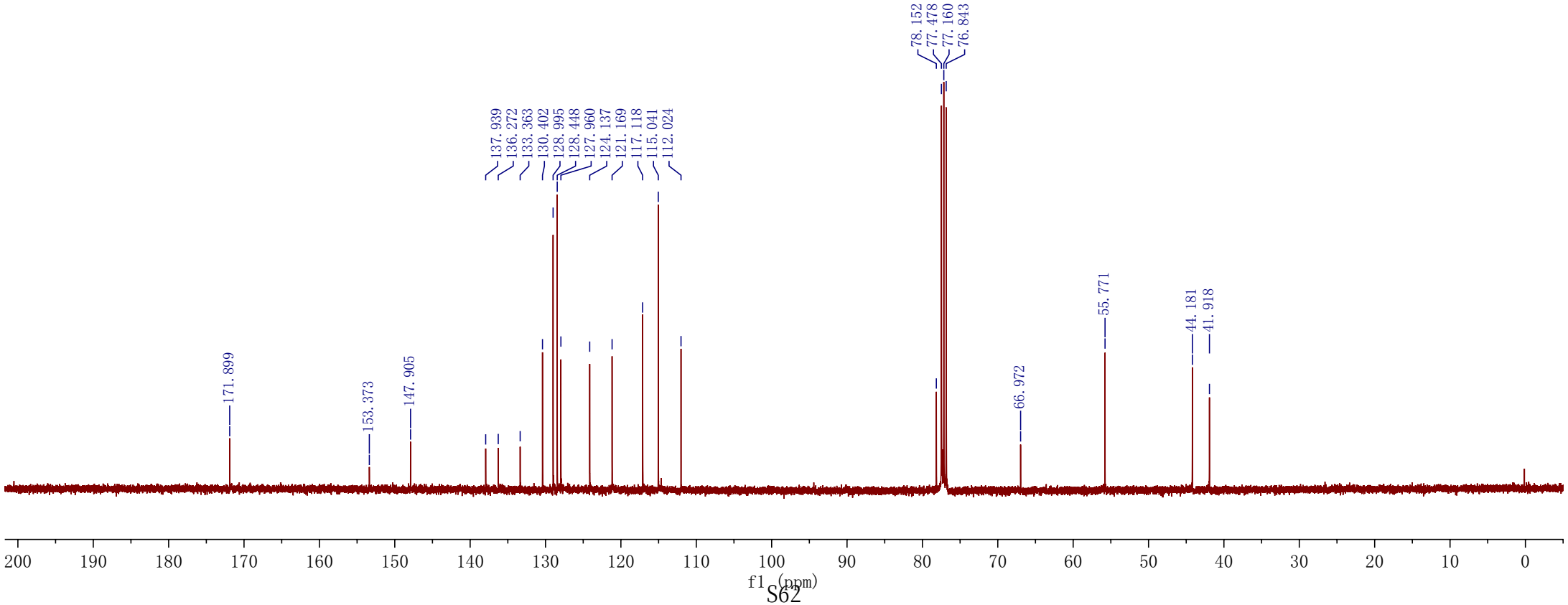

OCH3
HN
O
NBn
N
H

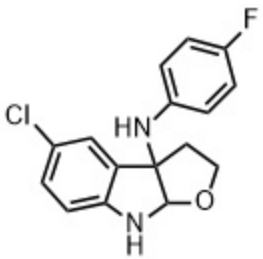
3ra

7.358
7.341
7.337
7.330
7.323
7.314
7.304
7.302
7.297
7.284
7.277
7.267
7.260
7.214
7.212
7.195
7.176
7.173
6.894
6.682
6.643
6.330
6.325
6.313
6.308
5.265
5.012
4.975
4.414
4.227
4.190
3.700
3.303
3.258
2.978
2.934
0.010
7.3
7.1
6.9
6.7
6.5
6.3
f1 (ppm)
5.43
1.10
1.02
1.03
1.98
2.00
1.00
1.03
0.94
1.04
3.10
1.04
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

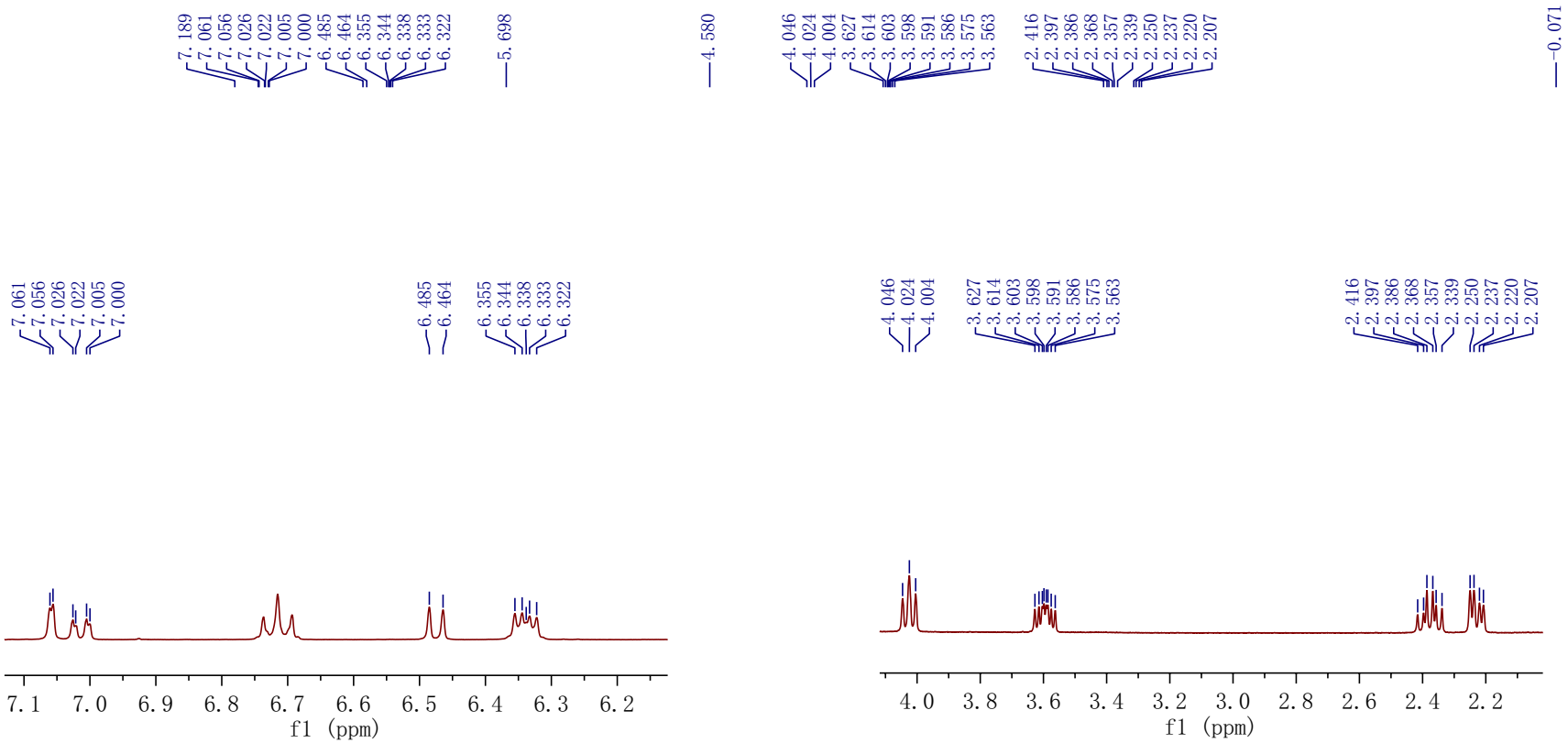

OCH3
HN
O
NBn
N
H

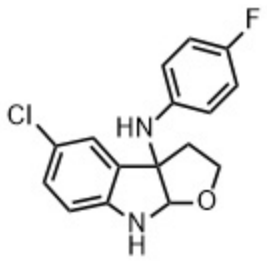
3ra


78.152
77.478
77.160
76.843
137.939
136.272
133.363
130.402
128.995
128.448
127.960
124.137
121.169
117.118
115.041
112.024
171.899
153.373
147.905
66.972
55.771
44.181
41.918
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

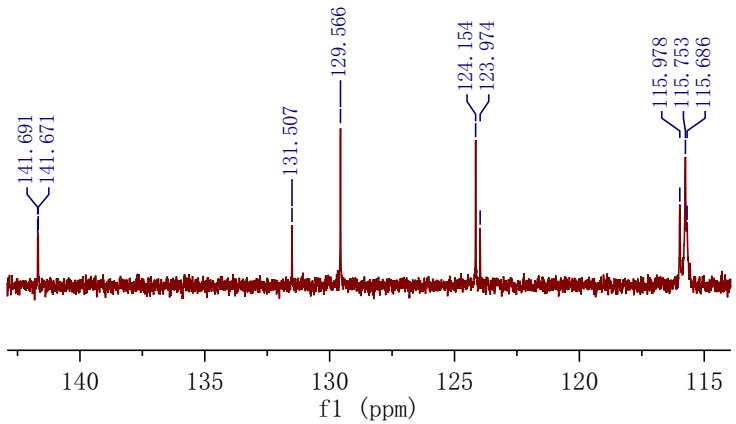

F
Cl
HN
O
N
H

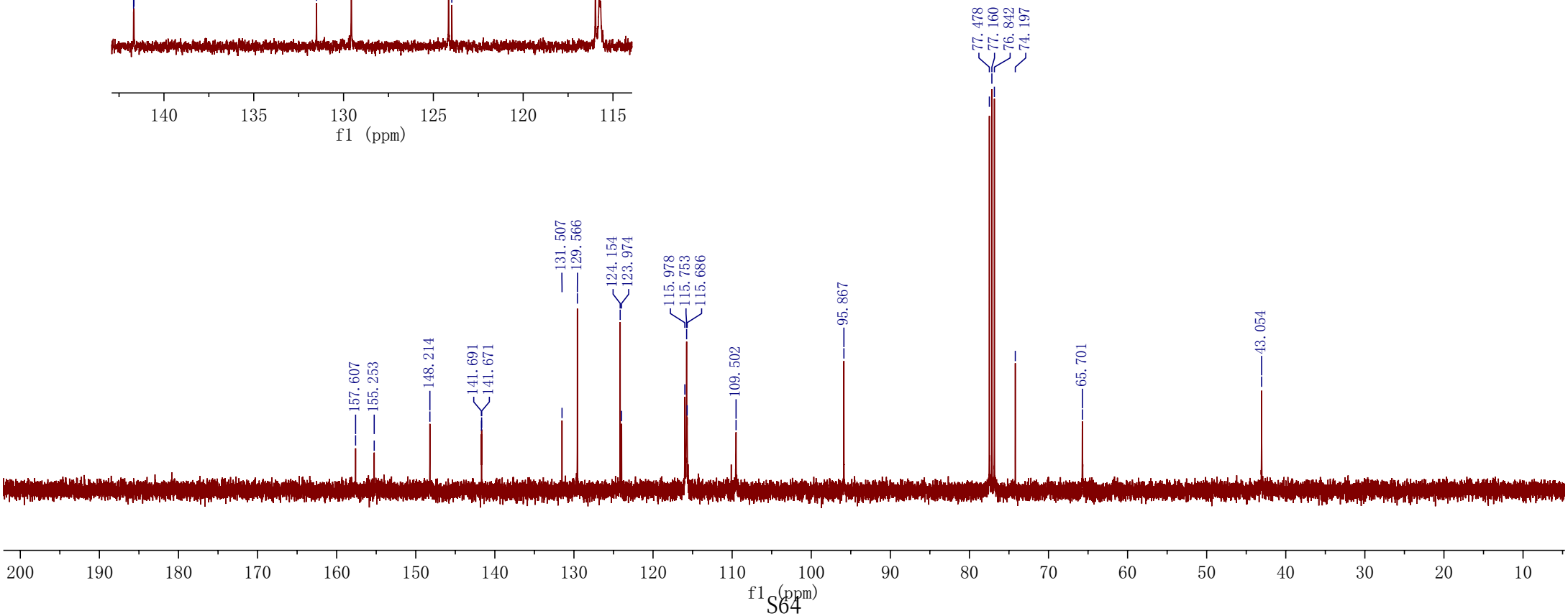
3eb

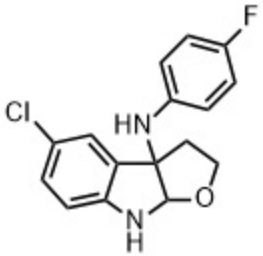

7.189
7.061
7.056
7.026
7.022
7.005
7.000
6.485
6.464
6.355
6.344
6.338
6.333
6.322
5.698
4.580
4.046
4.024
4.004
3.627
3.614
3.603
3.598
3.591
3.586
3.575
3.563
2.416
2.397
2.386
2.368
2.357
2.339
2.250
2.237
2.220
2.207
0.071
f1 (ppm)
f1 (ppm)
0.84
0.89
1.77
0.90
1.79
0.87
1.05
1.00
1.03
1.04
0.98
f1 (ppm)


F
Cl
HN
O
N
H

3eb

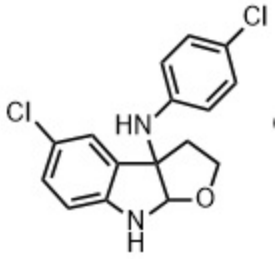

141.691
141.671
131.507
129.566
124.154
123.974
115.978
115.753
115.686
140
135
130
125
120
115
f1 (ppm)


157.607
155.253
148.214
141.691
141.671
131.507
129.566
124.154
123.974
115.978
115.753
115.686
109.502
95.867
77.478
77.160
76.842
74.197
65.701
43.054
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


F
Cl
HN
O
N
H

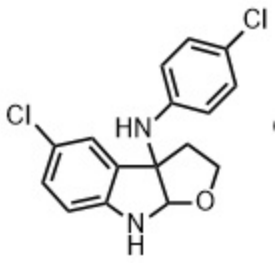
3eb

-126.497
1.00
90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

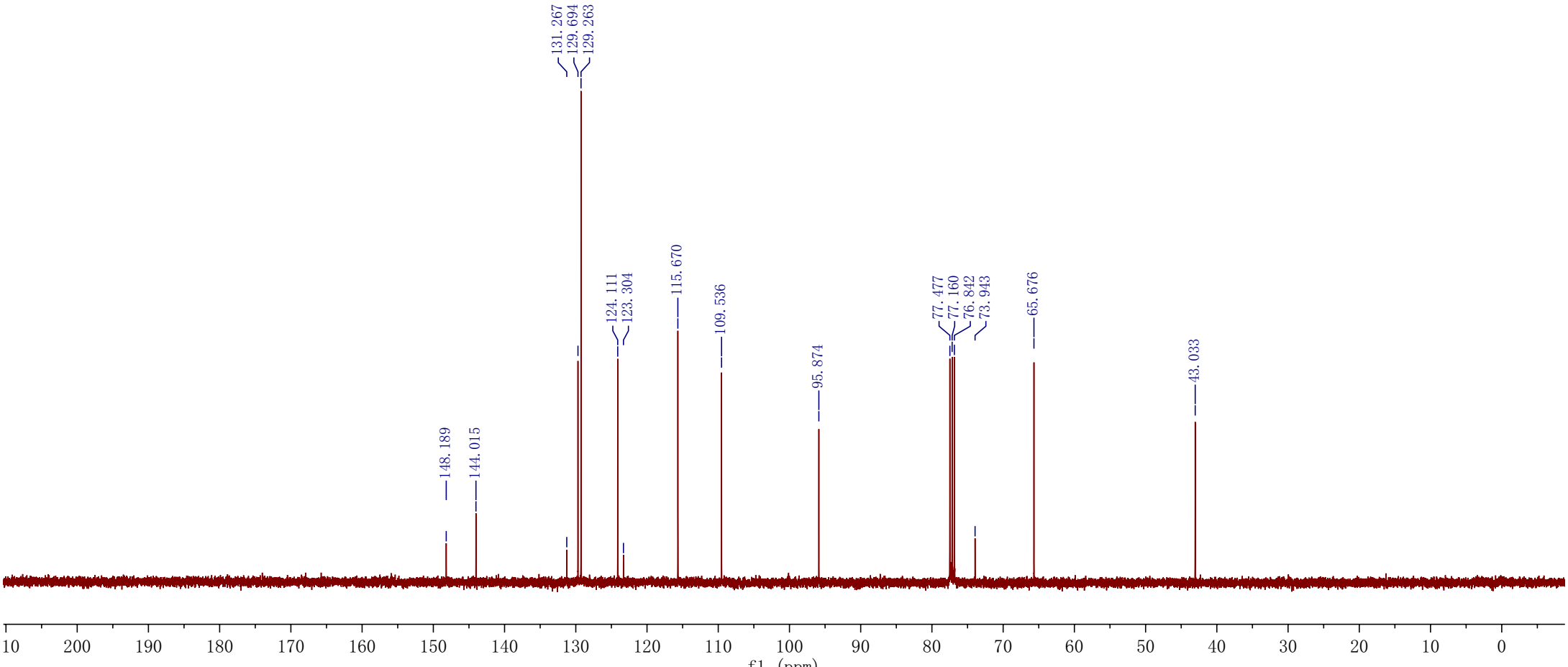

Cl
HN
Cl
N
H
O

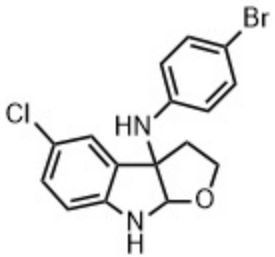
3ec

7.260
7.124
7.119
7.100
7.095
7.079
7.074
7.033
7.011
6.560
6.539
6.402
6.380
5.778
4.667
4.330
4.122
4.100
4.081
3.699
3.686
3.675
3.670
3.663
3.657
3.647
3.634
2.489
2.470
2.460
2.441
2.430
2.412
2.323
2.311
2.293
2.281
0.001
f1 (ppm)
0.98
1.00
1.93
1.02
2.05
0.95
1.14
0.90
1.05
1.03
1.05
1.03

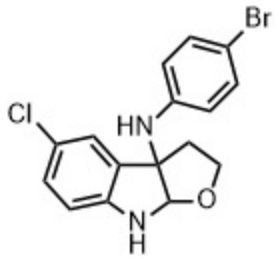

Cl
HN
Cl
O
N
H

3ec

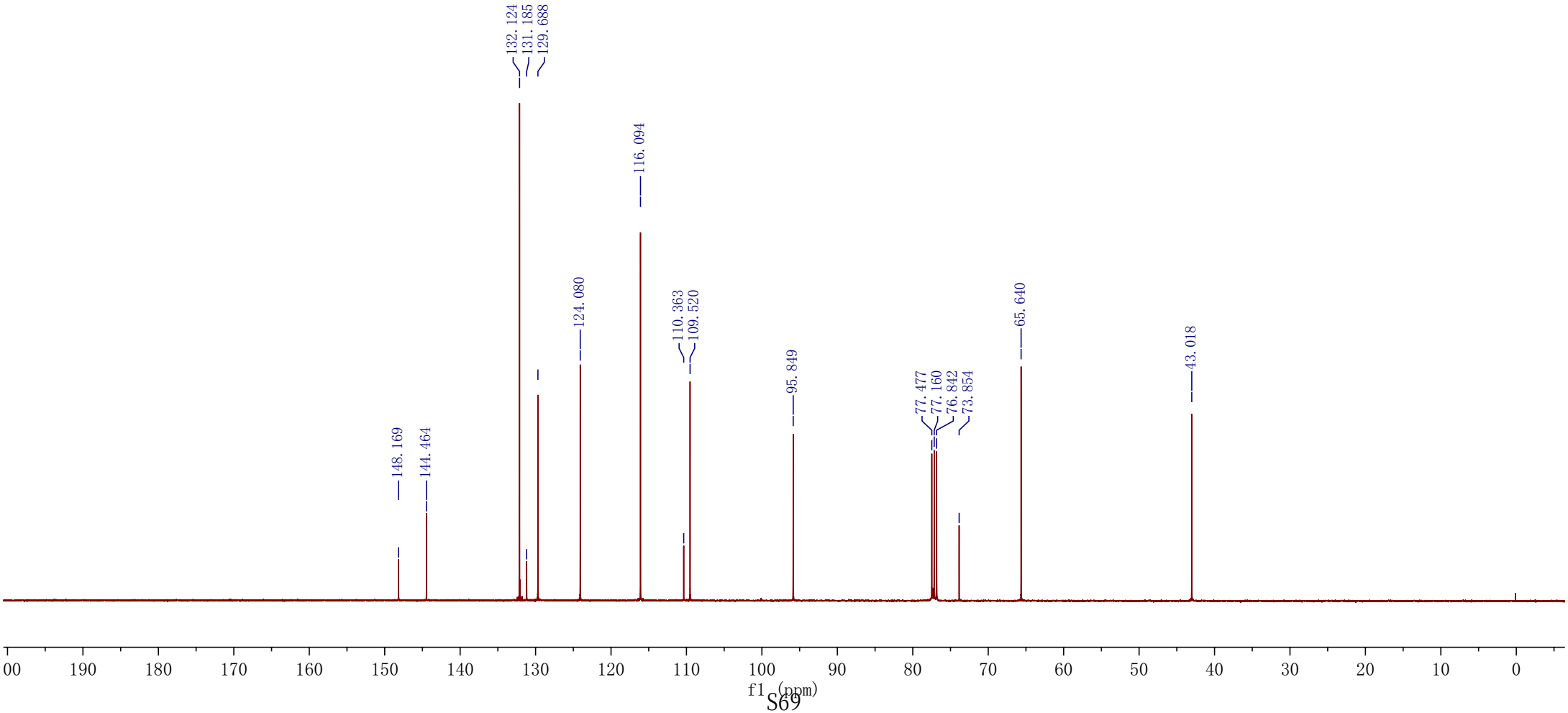

131.267
129.694
129.263
124.111
123.304
115.670
109.536
95.874
77.477
77.160
76.842
73.943
65.676
43.033
148.189
144.015
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

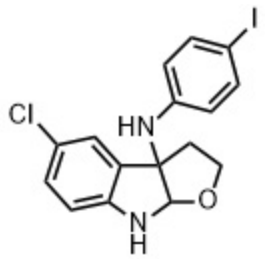


3ed


Br
Cl
HN
O
N
H

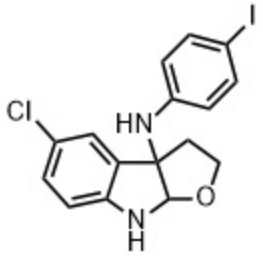
3ed


132. 124
131. 185
129. 688
116. 094
124. 080
110. 363
109. 520
95. 849
77. 477
77. 160
76. 842
73. 854
65. 640
43. 018
148. 169
144. 464
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

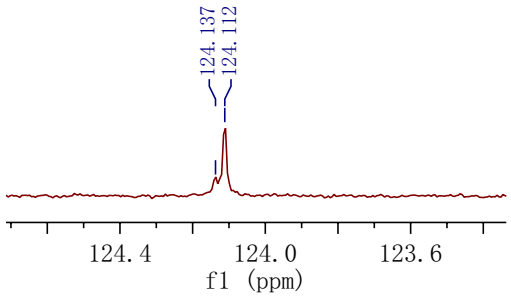

Cl
HN
I
O
N
H

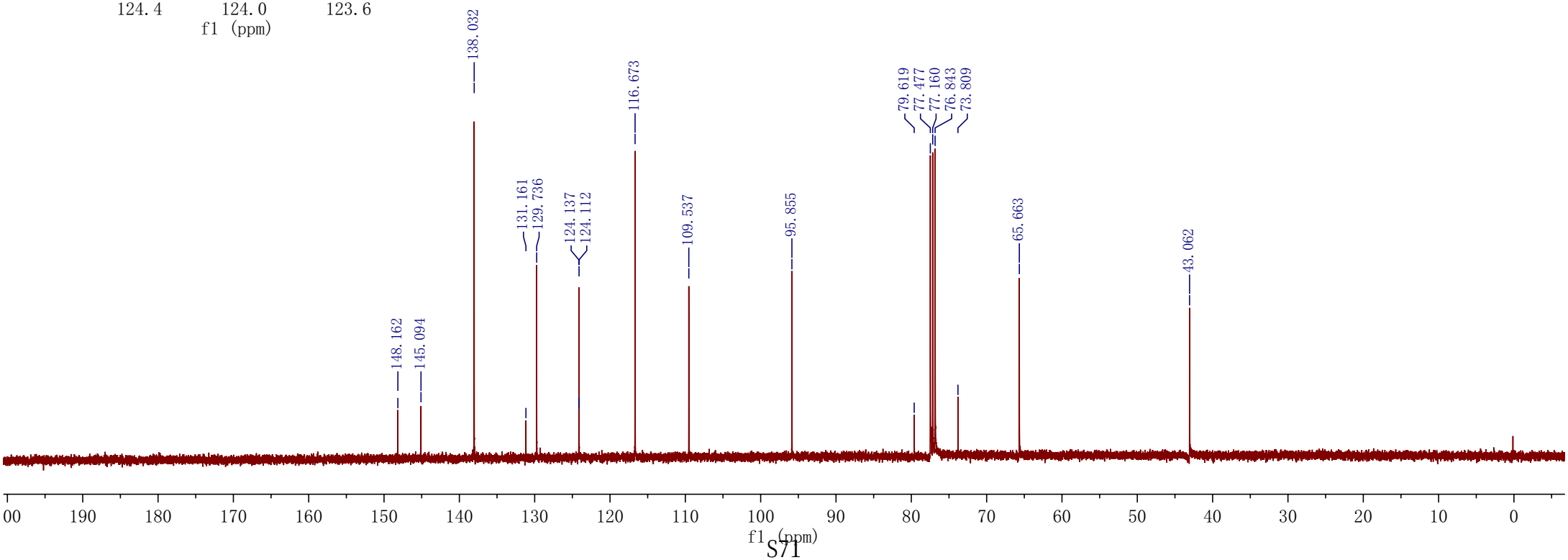
3ee

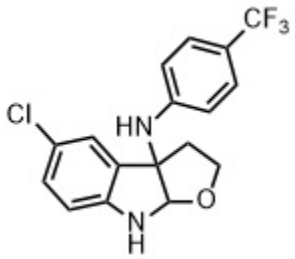
7.338
7.316
7.260
7.116
7.111
7.098
7.093
7.077
7.072
6.557
6.536
6.255
6.233
5.775
4.569
4.117
4.097
4.075
3.695
3.682
3.667
3.654
3.643
3.631
2.478
2.459
2.449
2.430
2.420
2.401
2.318
2.306
2.288
2.276
0.000
f1 (ppm)
2.00
2.01
1.03
2.02
1.00
1.98
1.20
1.16
1.21
1.15


I
Cl
HN
O
N
H

3ee

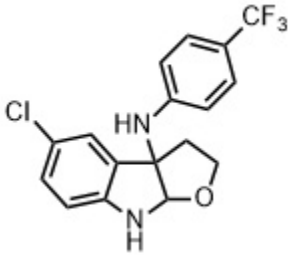

124.137
124.112
124.4
124.0
123.6
f1 (ppm)


138.032
116.673
131.161
129.736
124.137
124.112
109.537
95.855
79.619
77.477
77.160
76.843
73.809
65.663
43.062
148.162
145.094
f1 (ppm)


CF3
Cl
HN
O
N
H

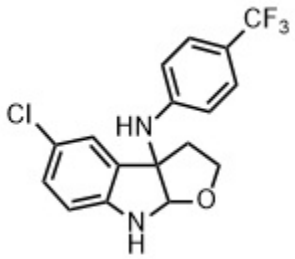
3ef

-61.321
3.00
8.0
-58.5
-59.0
-59.5
-60.0
-60.5
-61.0
-61.5
-62.0
-62.5
-63.0
f1 (ppm)

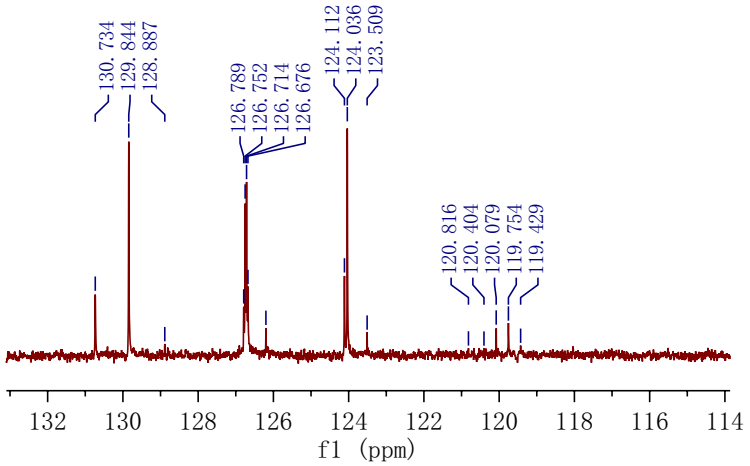

CF3
HN
Cl
O
N
H

3ef

7.327
7.305
7.260
7.132
7.127
7.118
7.097
7.092
6.581
6.560
6.495
6.474
5.806
4.704
4.592
4.142
4.123
4.103
3.716
3.703
3.693
3.687
3.680
3.675
3.664
3.652
2.514
2.496
2.485
2.466
2.456
2.437
2.355
2.343
2.326
2.314
0.003
f1 (ppm)
2.06
1.01
1.02
1.02
2.10
1.00
0.91
1.10
1.09
1.10
1.11
1.11


CF3
Cl
HN
O
N
H

3ef


130.734
129.844
128.887
126.789
126.752
126.714
126.676
124.112
124.036
123.509
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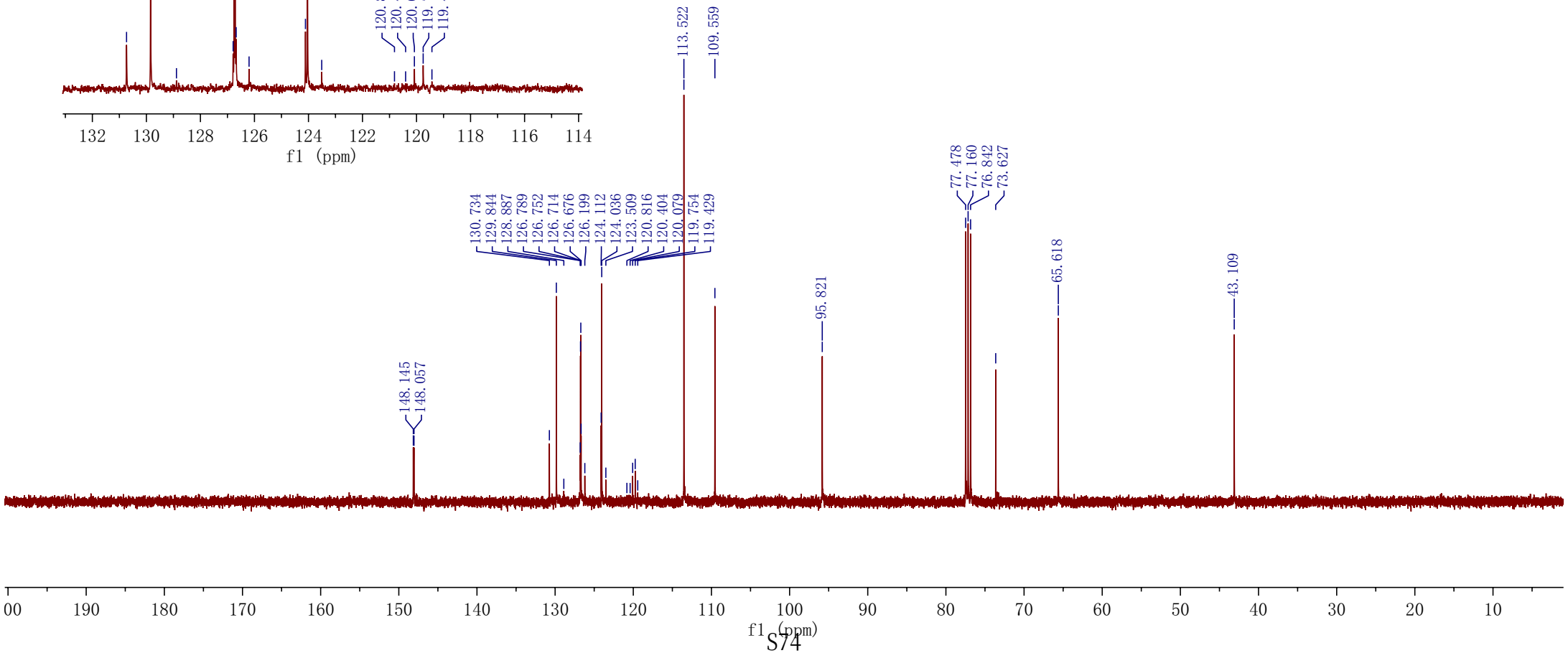
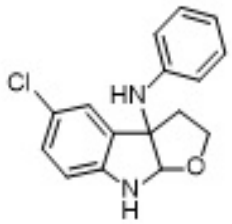
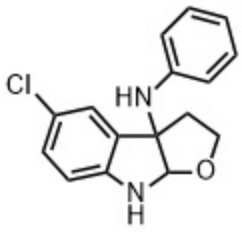
120.404
120.079
119.754
119.429
132
130
128
126
124
122
120
118
116
114
f1 (ppm)


130.734
129.844
128.887
126.789
126.752
126.714
126.676
126.199
124.112
124.036
123.509
120.816
120.404
120.079
119.754
119.429
113.522
109.559
77.478
77.160
76.842
73.627
65.618
43.109
95.821
148.145
148.057
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

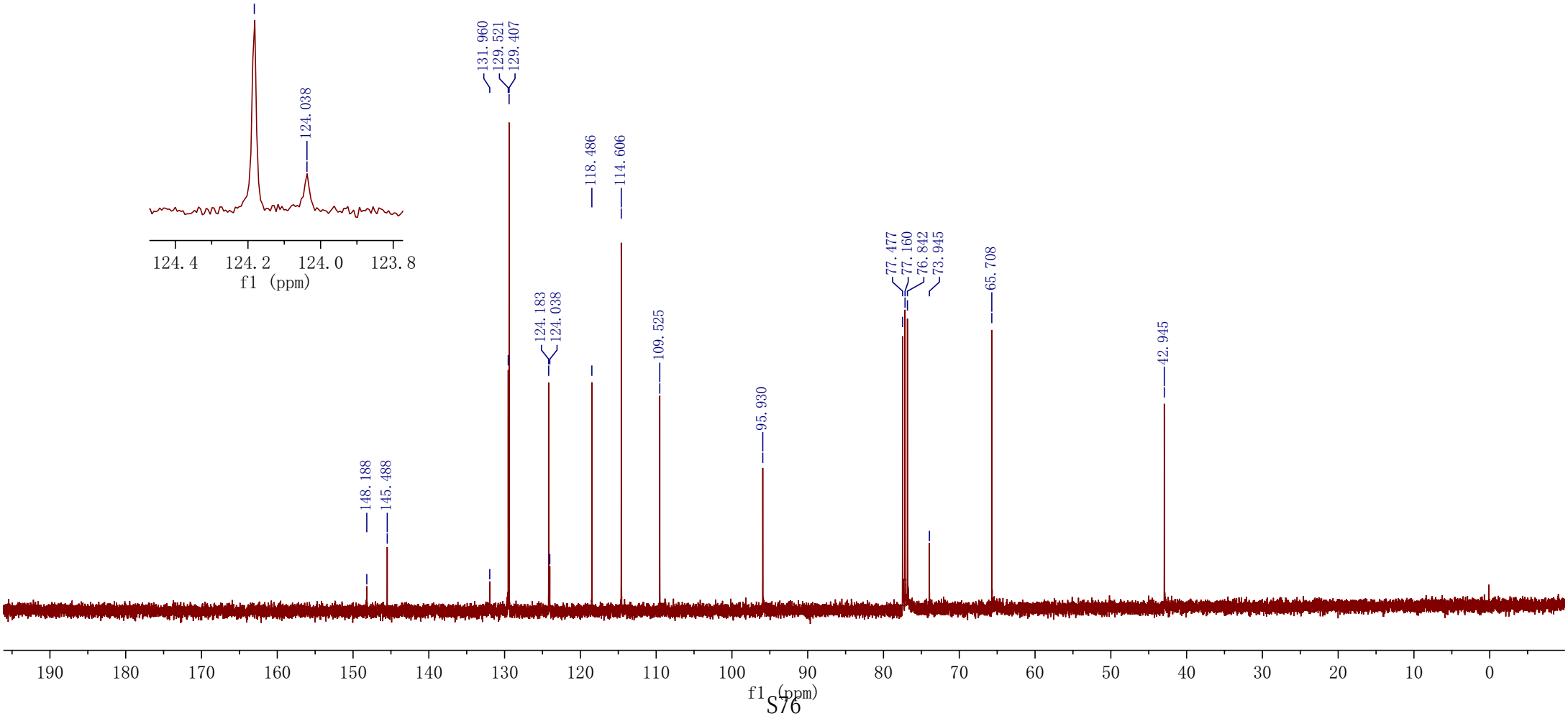

Cl
HN
O
N
H

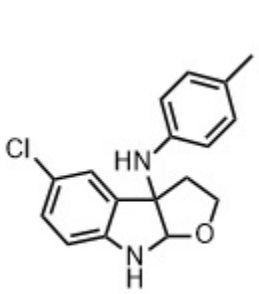
3eg

7.260
7.152
7.147
7.101
7.096
7.090
7.081
7.075
7.069
7.062
6.719
6.701
6.683
6.563
6.542
6.478
6.457
5.834
4.698
4.220
4.126
4.106
4.086
3.711
3.698
3.688
3.682
3.675
3.670
3.659
3.646
2.530
2.511
2.501
2.482
2.471
2.453
2.318
2.306
2.289
2.276
0.000
7.18
7.16
7.14
7.12
7.10
7.08
7.06
7.04
f1 (ppm)
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
f1 (ppm)
0.91
2.87
1.05
1.02
2.02
1.01
1.07
0.77
1.12
1.08
1.09
1.05
f1 (ppm)


Cl
HN
N
H
O

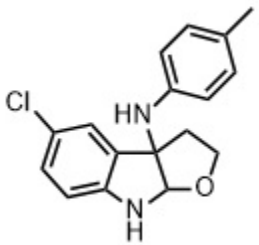
3eg


124.038
124.4
124.2
124.0
123.8
f1 (ppm)
131.960
129.521
129.407
118.486
114.606
124.183
124.038
109.525
95.930
77.477
77.160
76.842
73.945
65.708
42.945
148.188
145.488
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

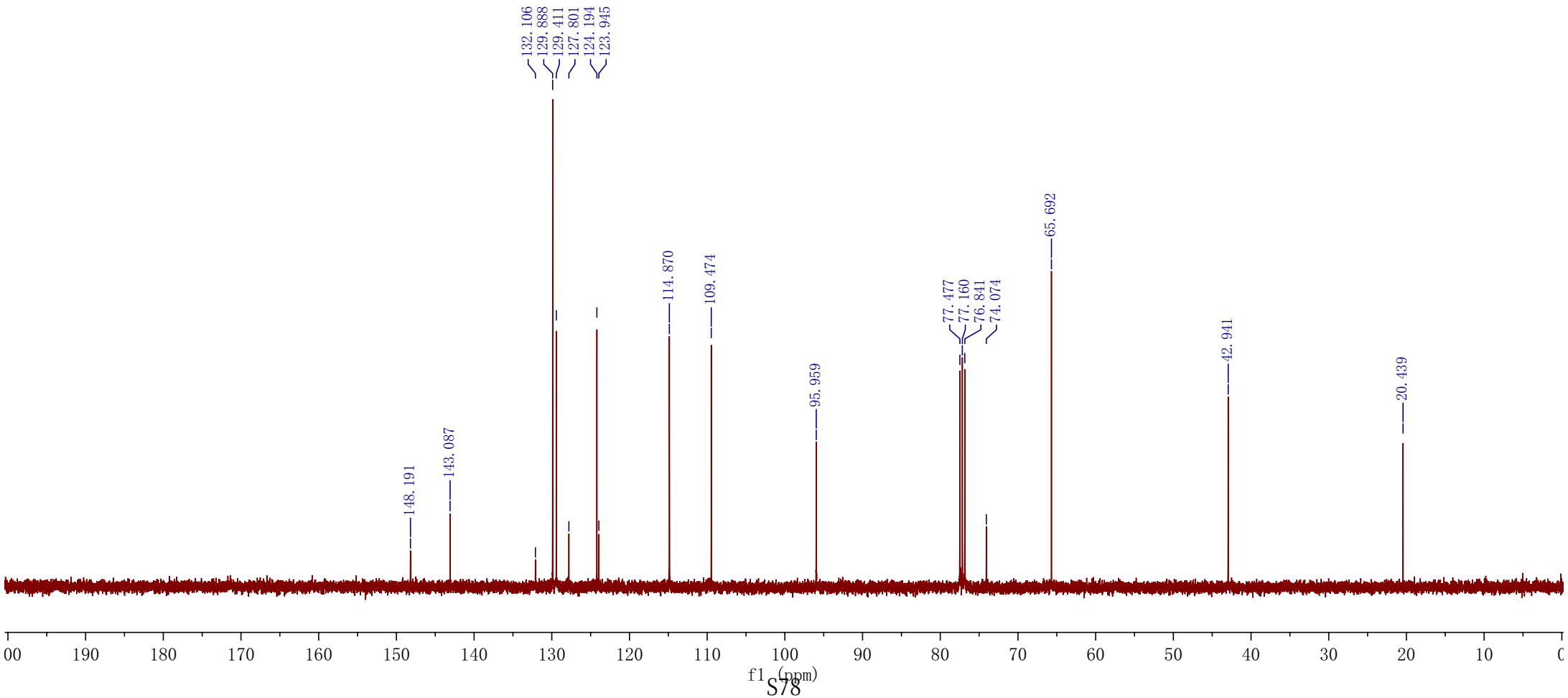

Cl
HN
O
N
H

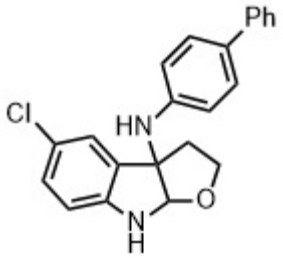
3eh

7.260
7.151
7.145
7.089
7.083
7.068
7.063
6.904
6.883
6.552
6.531
6.406
6.385
5.812
4.681
4.113
4.094
4.074
3.702
3.689
3.679
3.673
3.666
3.660
3.650
3.637
2.511
2.493
2.482
2.463
2.453
2.434
2.309
2.297
2.279
2.267
2.191
0.003
f1 (ppm)
1.00
1.01
2.04
1.03
2.03
1.01
0.88
1.27
1.11
1.09
1.07
3.10


Cl
HN
O
N
H

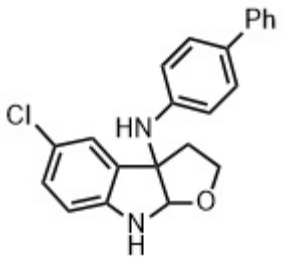
3eh


132.106
129.888
129.411
127.801
124.194
123.945
114.870
109.474
95.959
77.477
77.160
76.841
74.074
65.692
42.941
20.439
148.191
143.087
f1 (ppm)

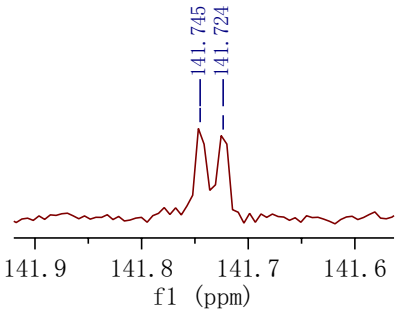

Ph
Cl
HN
O
N
H

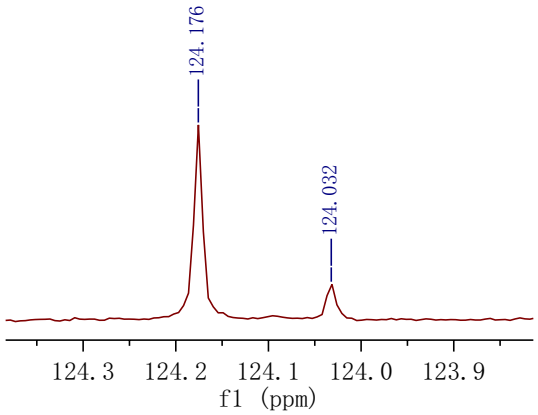
3ei

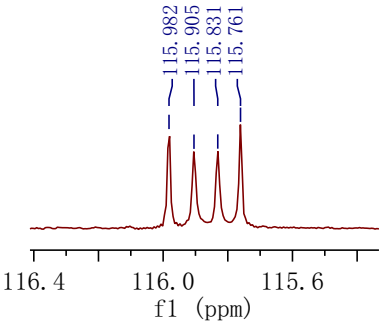
7.490
7.470
7.260
7.259
7.113
7.092
6.583
6.562
6.555
6.534
5.874
4.687
4.149
4.127
4.107
3.730
3.716
3.707
3.693
3.678
3.664
2.559
2.540
2.530
2.511
2.500
2.481
2.349
2.336
2.319
2.307
0.000
f1 (ppm)
2.05
4.00
1.03
1.01
1.04
3.02
1.00
1.23
1.20
1.35
1.22
1.25

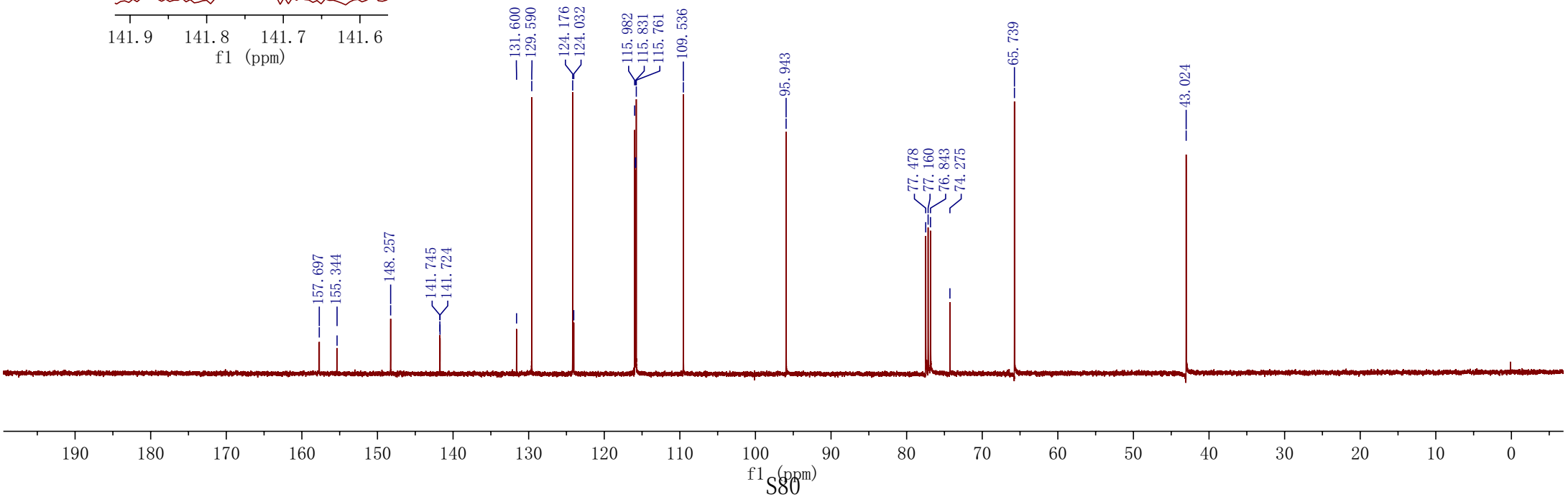

Ph
Cl
HN
O
N
H

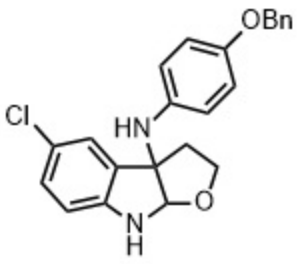
3ei


141.745
141.724
141.9
141.8
141.7
141.6
f1 (ppm)


124.176
124.032
124.3
124.2
124.1
124.0
123.9
f1 (ppm)

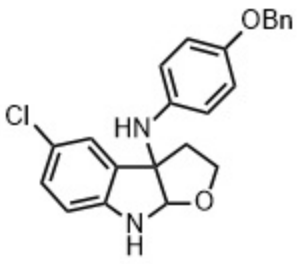

115.982
115.905
115.831
115.761
116.4
116.0
115.6
f1 (ppm)


157.697
155.344
148.257
141.745
141.724
131.600
129.590
124.176
124.032
115.982
115.831
115.761
109.536
95.943
77.478
77.160
76.843
74.275
65.739
43.024
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

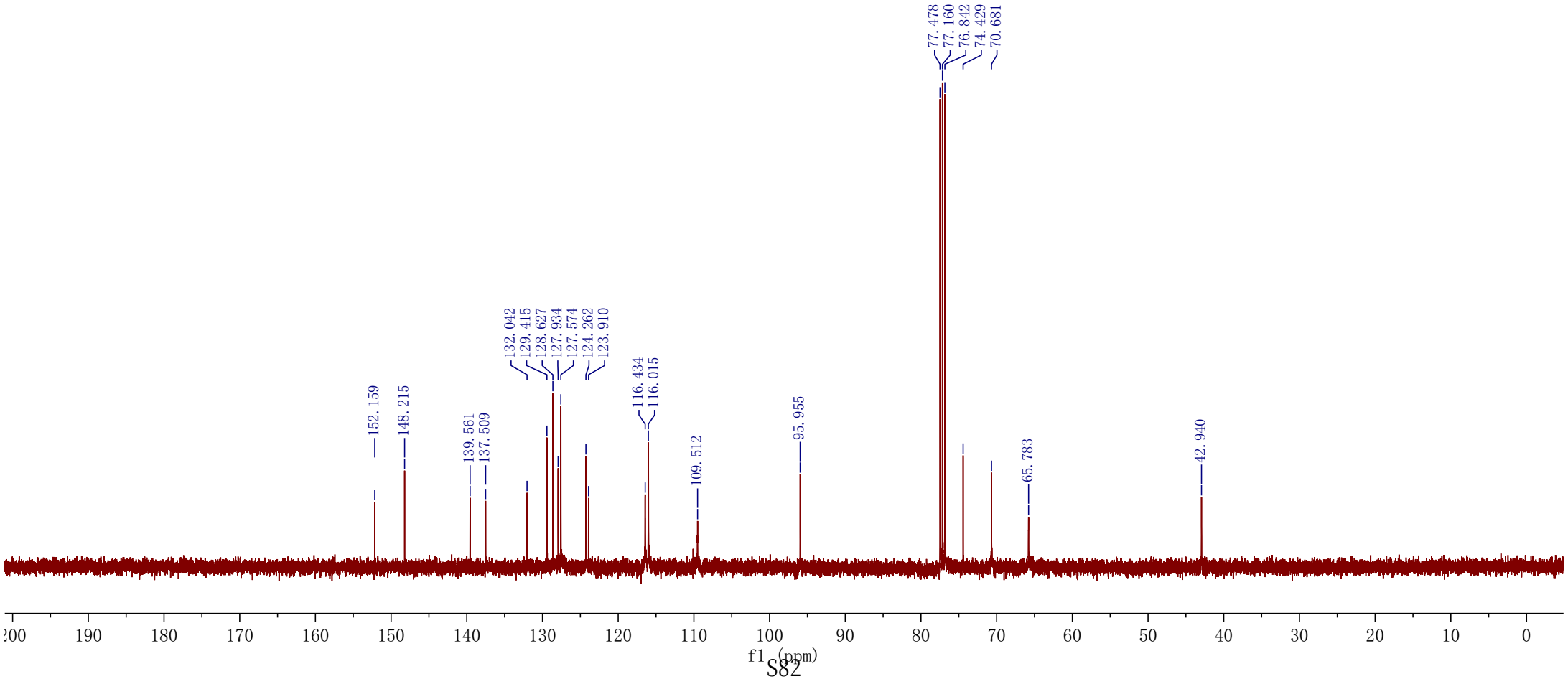

OBn
Cl
HN
O
N
H

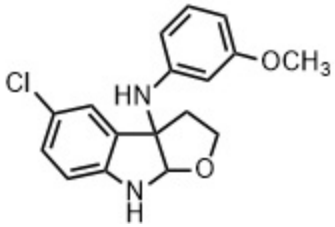
3ej

7.397
7.376
7.358
7.339
7.315
7.298
7.260
7.150
7.145
7.089
7.084
7.068
7.063
6.753
6.730
6.544
6.523
6.458
6.435
5.772
4.943
4.106
4.085
4.065
3.680
3.670
3.665
3.657
3.652
3.642
3.629
2.481
2.470
2.451
2.441
2.423
2.310
2.298
2.279
2.268
0.002
7.45
7.40
7.35
7.30
7.25
f1 (ppm)
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
f1 (ppm)
4.92
0.97
0.98
2.03
0.99
1.98
1.00
2.21
1.32
1.30
1.12
0.99
1.19
f1 (ppm)


OBn
Cl
HN
O
N
H

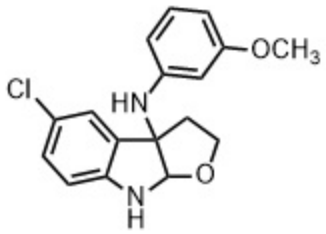
3ej


77.478
77.160
76.842
74.429
70.681
132.042
129.415
128.627
127.934
127.574
124.262
123.910
116.434
116.015
152.159
148.215
139.561
137.509
109.512
95.955
65.783
42.940
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

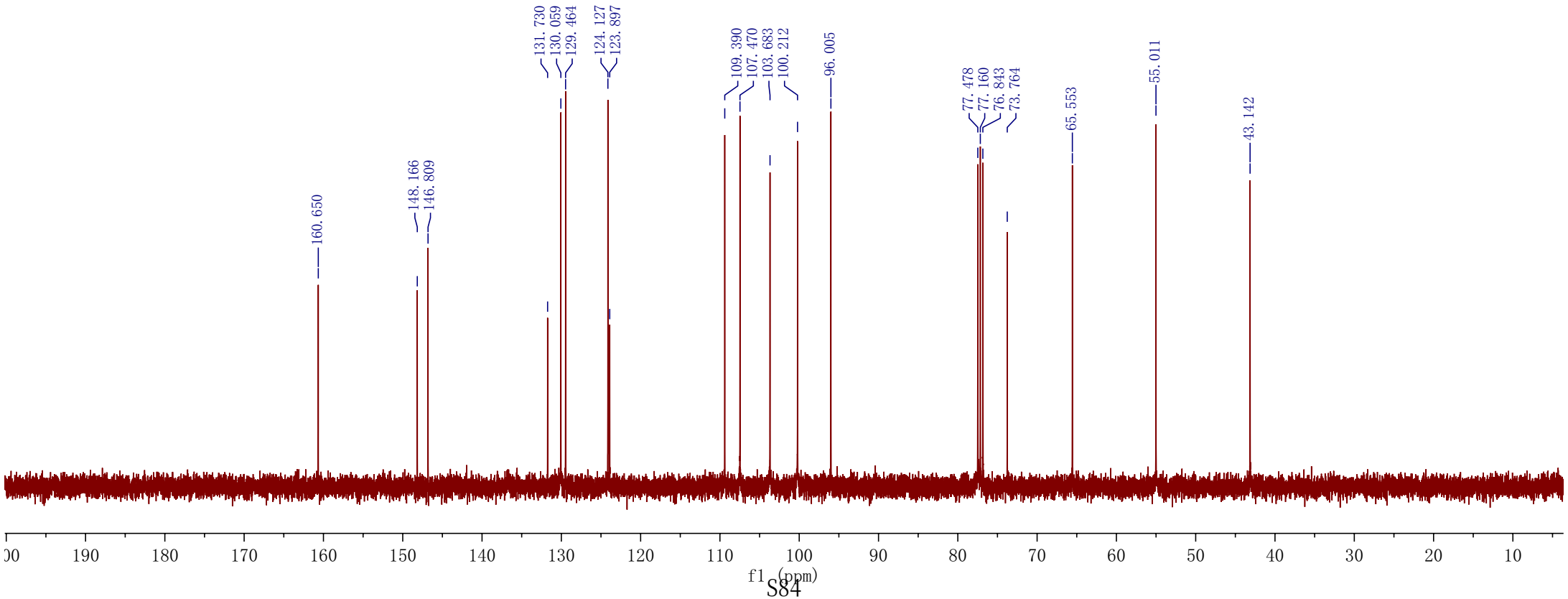

Cl
HN
OCH3
O
N
H

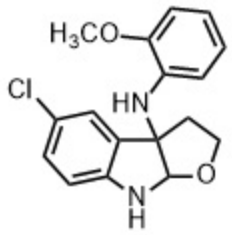
3ek

7.260
7.155
7.150
7.092
7.087
7.071
7.066
7.011
6.991
6.971
6.551
6.530
6.281
6.276
6.261
6.255
6.120
6.115
6.100
6.095
6.017
6.011
6.006
5.826
4.764
4.116
4.113
4.098
4.094
4.091
4.075
4.072
3.699
3.686
3.676
3.671
3.663
3.657
3.648
2.496
2.477
2.467
2.448
2.438
2.419
2.318
2.308
2.290
2.278
0.012
f1 (ppm)


OCH3
Cl
HN
N
H
O

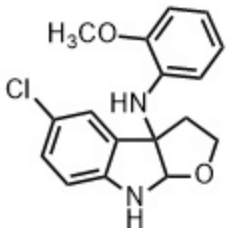
3ek


160.650
148.166
146.809
131.730
130.059
129.464
124.127
123.897
109.390
107.470
103.683
100.212
96.005
77.478
77.160
76.843
73.764
65.553
55.011
43.142
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

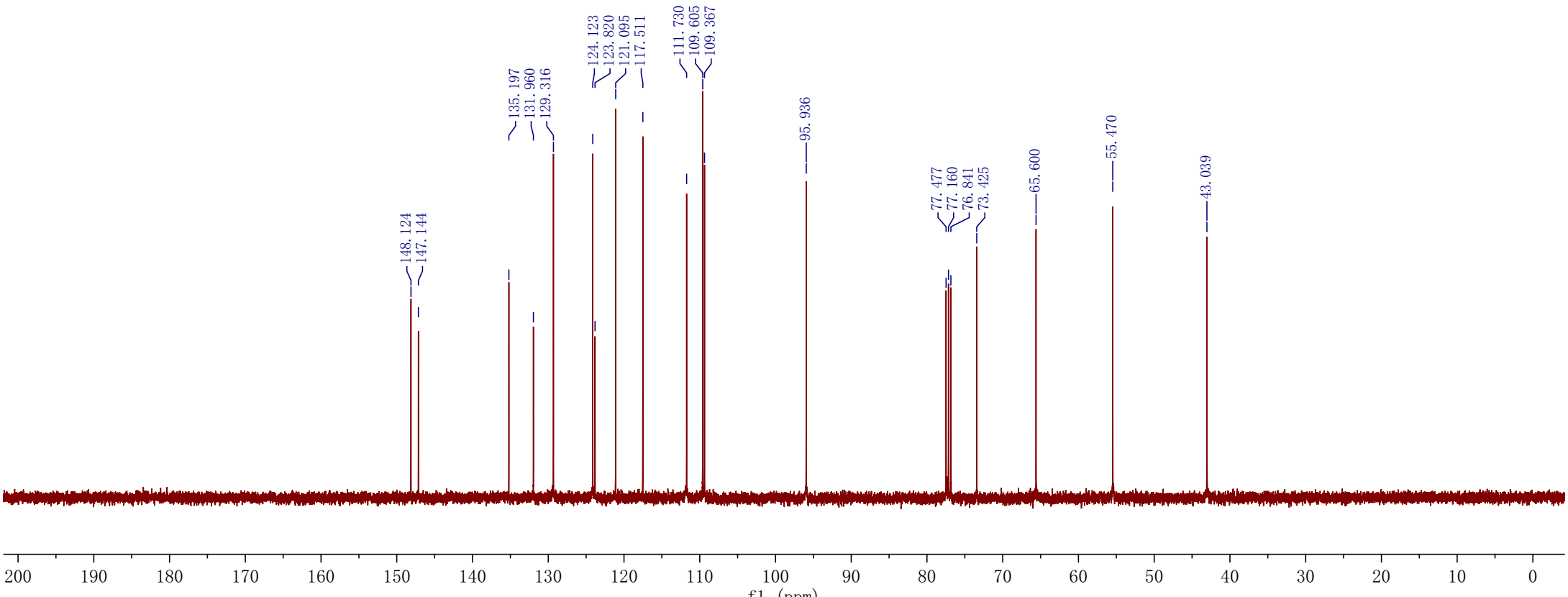

H3CO
Cl
HN
N
H
O

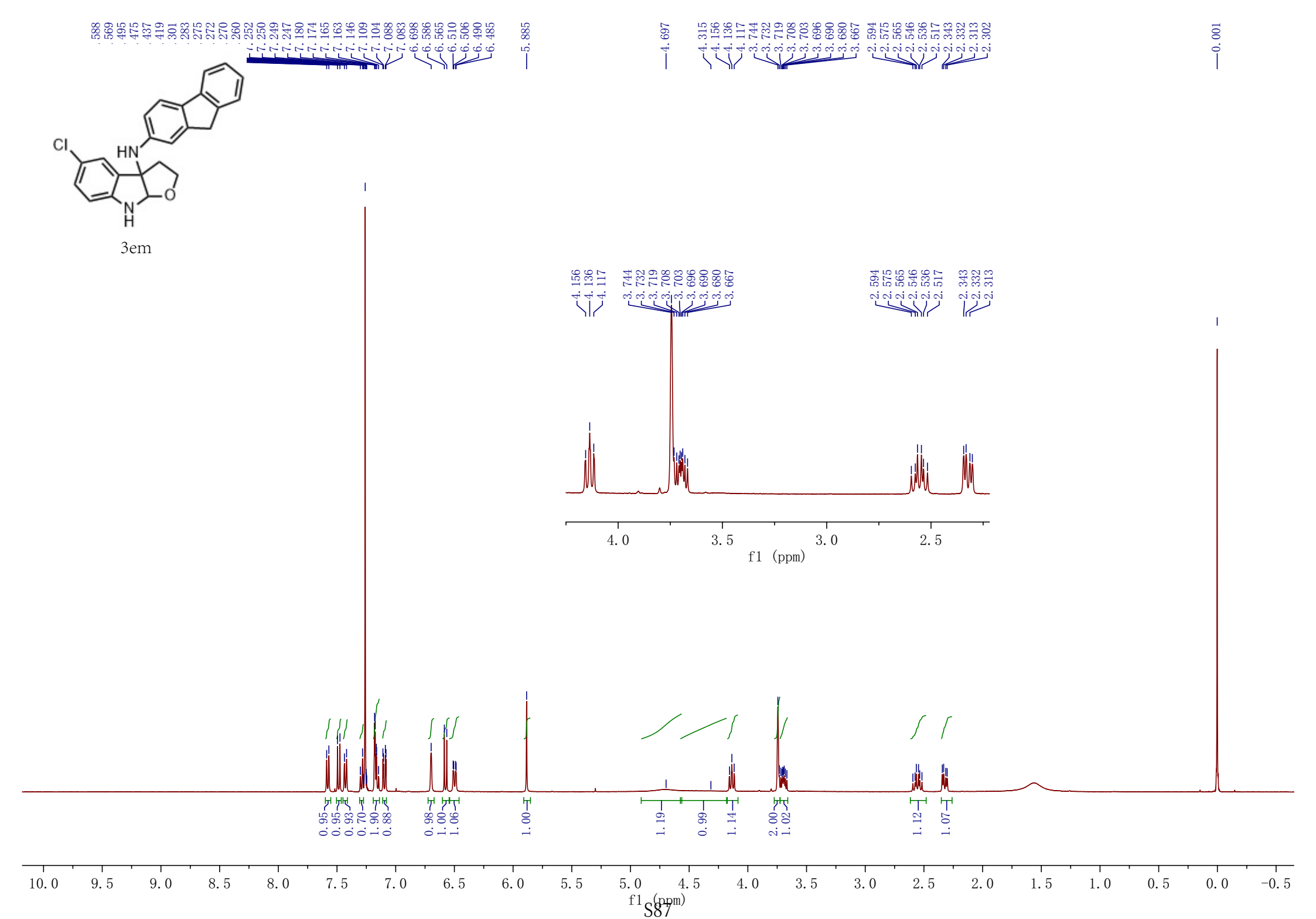
3el

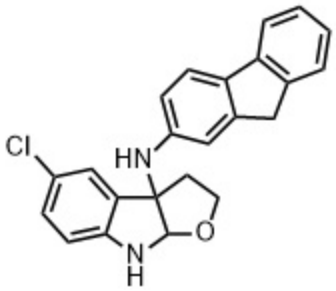
7.260
7.167
7.162
7.091
7.086
7.070
7.065
6.673
6.650
6.557
6.536
6.302
6.293
6.287
6.278
5.826
4.851
4.733
4.128
4.113
4.109
4.106
4.090
4.087
3.862
3.724
3.711
3.701
3.695
3.688
3.682
3.672
2.588
2.569
2.559
2.540
2.530
2.511
2.341
2.331
2.313
2.311
2.301
0.009
f1 (ppm)
1.00
1.02
1.09
2.12
1.05
1.06
1.04
0.95
0.89
1.10
3.28
1.11
1.11
1.09


H3CO
Cl
HN
O
N
H

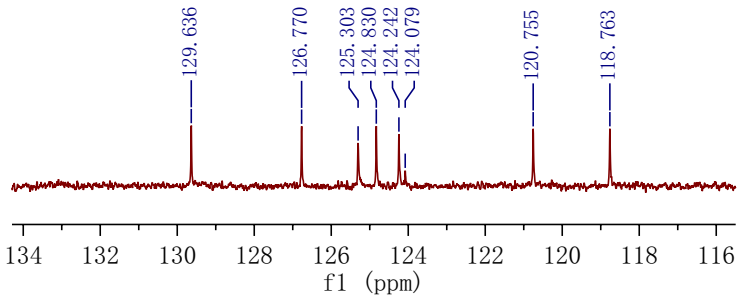
3el


148.124
147.144
135.197
131.960
129.316
124.123
123.820
121.095
117.511
111.730
109.605
109.367
95.936
77.477
77.160
76.841
73.425
65.600
55.470
43.039
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

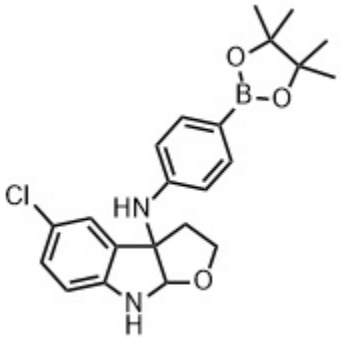

Cl
HN
O
N
H
3em
f1 (ppm)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
4.0 3.5 3.0 2.5
0.95 0.95 0.93 0.70 1.90 0.88 0.98 1.00 1.06 1.00 1.19 0.99 1.14 2.00 1.02 1.12 1.07


Cl
HN
O
N
H

3em

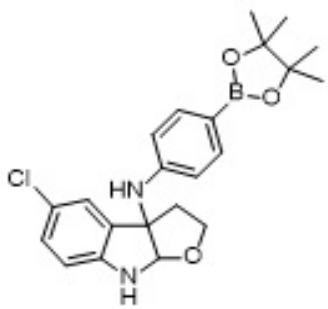

129.636
126.770
125.303
124.830
124.242
124.079
120.755
118.763
134
132
130
128
126
124
122
120
118
116
f1 (ppm)

77.478
77.160
76.843
148.249
145.145
142.385
129.636
126.770
125.303
124.830
124.242
124.079
120.755
118.763
113.729
111.553
109.567
100.135
95.923
65.858
42.721
37.127
f1 (ppm)

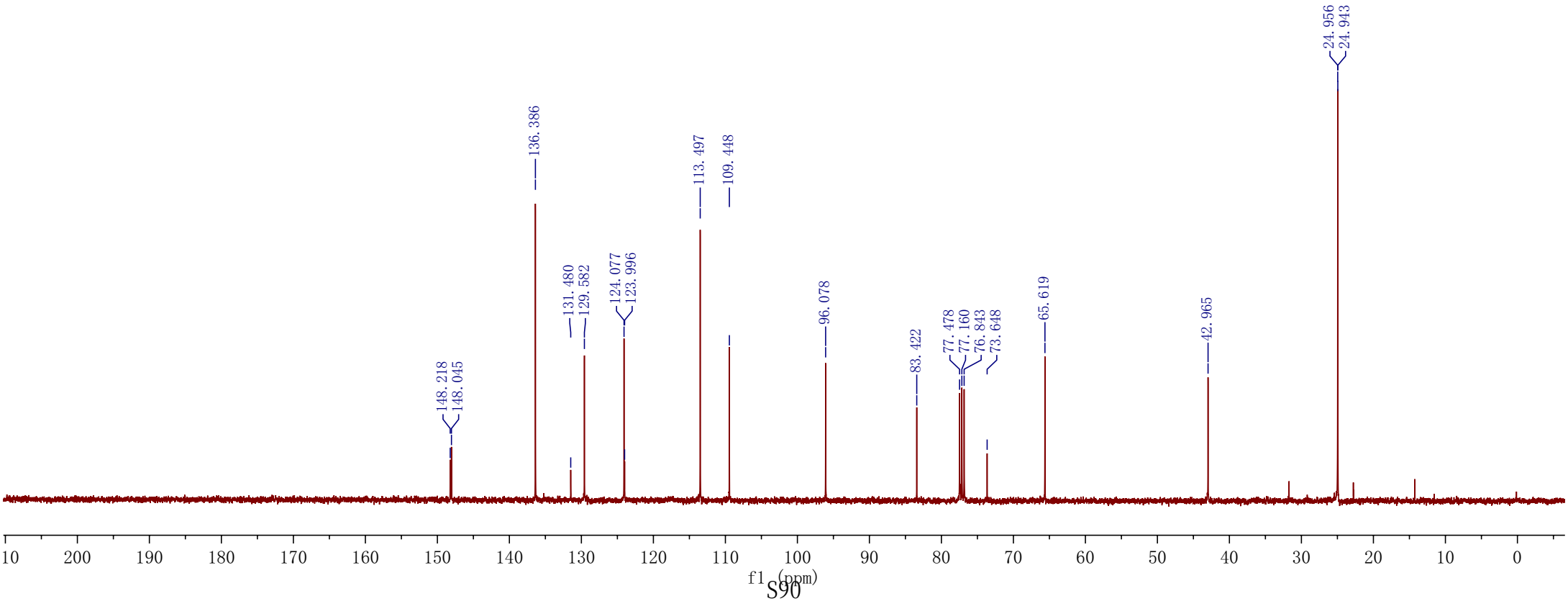

O
B
O
Cl
HN
O
N
H

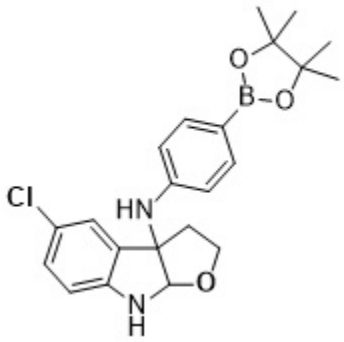
3en

7.549
7.528
7.260
7.119
7.114
7.081
7.060
6.529
6.455
6.433
5.832
4.620
4.125
4.105
4.085
3.707
3.694
3.684
3.678
3.671
3.666
3.655
3.643
2.521
2.502
2.492
2.473
2.463
2.444
2.325
2.314
2.295
2.284
1.286
0.002
f1 (ppm)
1.97
1.00
1.00
1.05
2.03
1.00
1.82
1.14
1.11
1.09
1.09
12.00
f1 (ppm)


Cl
HN
O
B
O
N
H
O

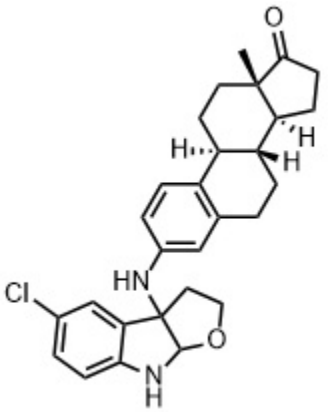
3en


148.218
148.045
136.386
131.480
129.582
124.077
123.996
113.497
109.448
96.078
83.422
77.478
77.160
76.843
73.648
65.619
42.965
24.956
24.943
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

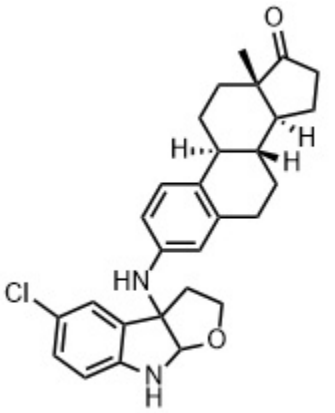

O
B
O
Cl
HN
O
N
H

3en

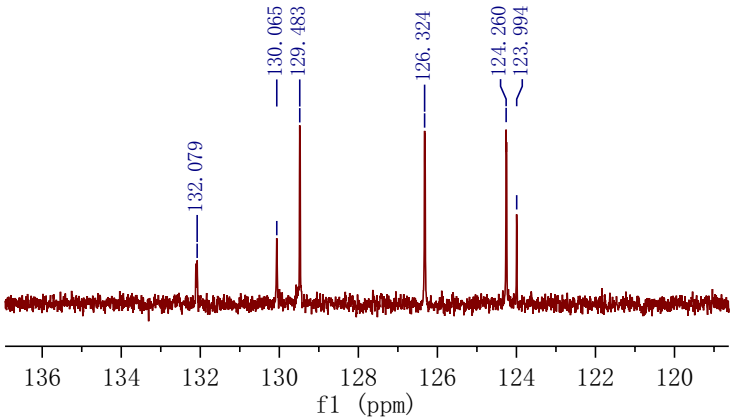
30.520
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
f1 (ppm)



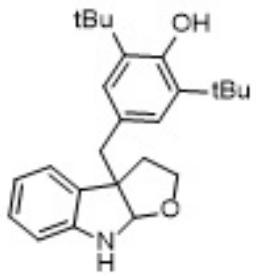
3eo


O
H
H
H
HN
Cl
O
N
H

3eo


132.079
130.065
129.483
126.324
124.260
123.994
136
134
132
130
128
126
124
122
120
f1 (ppm)

77.478
77.160
76.843
73.947
221.110
148.203
143.389
137.504
130.065
129.483
126.324
124.260
123.994
115.095
112.268
109.413
95.981
65.728
50.569
48.174
44.052
42.952
38.596
36.003
31.731
29.743
26.713
25.939
21.705
14.008
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


tBu
OH
tBu
O
N
H

4

7.260
7.067
7.048
7.029
6.861
6.842
6.778
6.754
6.736
6.717
6.544
6.525
5.368
5.071
4.424
3.981
3.961
3.942
3.552
3.543
3.536
3.525
3.515
3.133
3.099
2.890
2.856
2.324
2.306
2.296
2.277
2.267
2.249
2.160
2.149
2.131
2.119
1.368
0.023
1.10
0.99
1.86
1.05
1.00
0.94
0.97
1.08
1.21
1.12
1.10
1.17
1.27
1.14
17.59
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

7.067
7.048
7.029
6.861
6.842
6.778
6.754
6.736
6.717
6.544
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7.1
7.0
6.9
6.8
6.7
6.6
6.5
f1 (ppm)

3.981
3.961
3.942
3.565
3.552
3.543
3.536
3.525
3.515
3.503
3.133
3.099
2.890
2.856
2.324
2.306
2.296
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2.267
2.249
2.160
2.149
2.131
2.119
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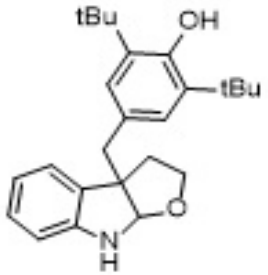
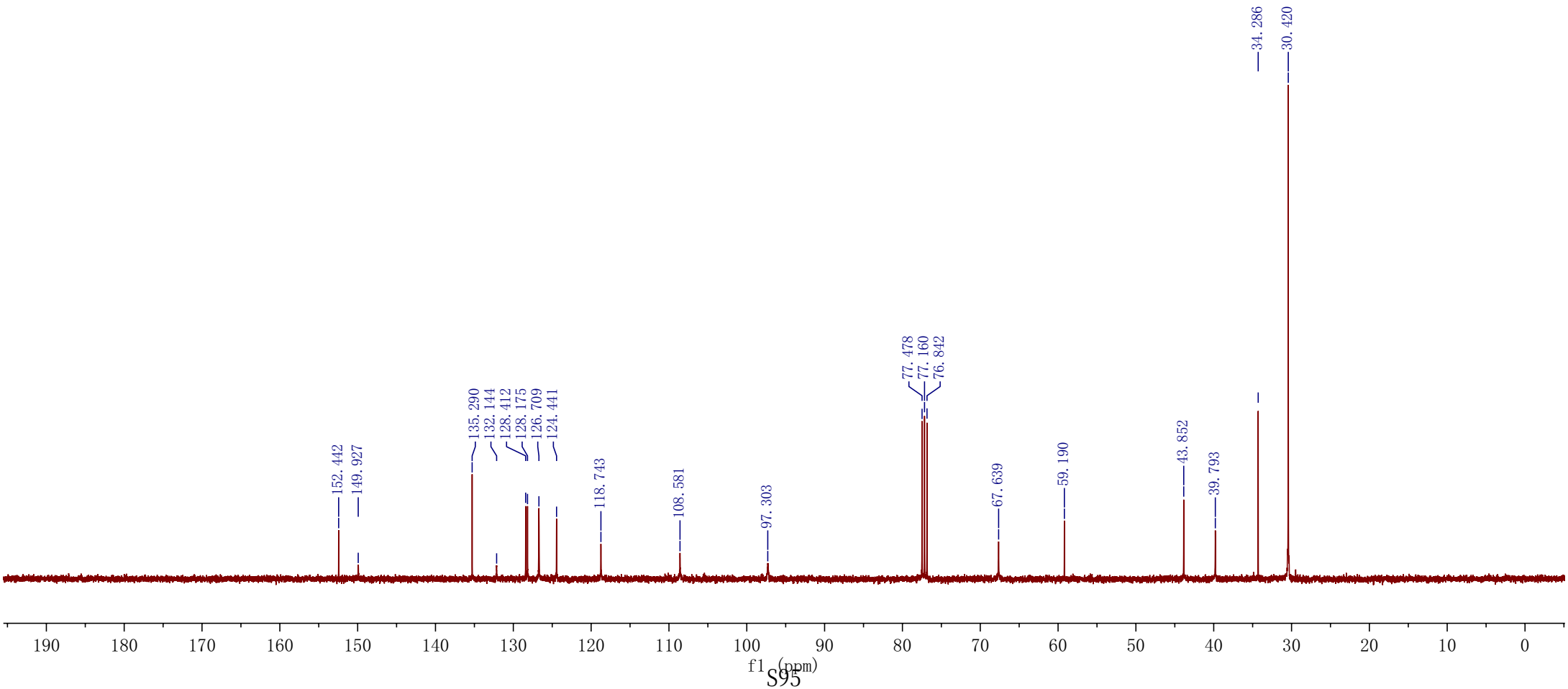
f1 (ppm)


tBu
OH
tBu
O
N
H

4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97.303
77.478
77.160
76.842
67.639
59.190
43.852
39.793
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)