Electronic supplementary information for

Innate Pharmacophore Assisted Selective C-H Functionalization to Therapeutically Important Nicotinamides

Zehua Song,[†] Guotong Wang,[†] Wei Li,[†] Shengkun Li *,[†]

[†] Department of Pesticide Science, College of Plant Protection, Nanjing Agricultural University, Weigang 1, Xuanwu District, Nanjing 210095, People's Republic of China.

*Corresponding Author (Email: SKL505@outlook.com)

Content

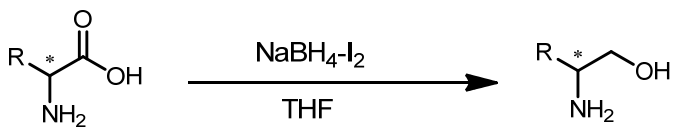
General Information

Unless otherwise mentioned, all solvents and reagents were purchased from commercial sources (Energy or Meryer Chemicals etc.), they were analytically pure and used without further purification. Anhydrous solvents were dried and distilled by standard techniques before use. Silica gel GF_{254} and column chromatography silica gel for isolation (200-300 mesh) were both purchased from Qingdao Broadchem Industrial Co., Ltd. Reaction progress was monitored by thin-layer chromatography (TLC) on silica gel GF254 with phosphomolybdic acid and ultraviolet (UV_{254nm}) detection. ^{1}HNMR and ^{13}CNMR spectra were recorded on a Bruker AV 400 or 600 spectrometers with $CDCl_3$ as solvent and tetramethylsilane as the internal standard. The chemical shifts (δ) were recorded in parts per million (ppm). Data for ^{1}H NMR are reported as follows: chemical shift (δ: ppm), multiplicity (s, singlet; d,doublet; t, triplet; q, quartet; and m, multiplet), coupling constant (Hz), integration and assignment (*H*). Data for ^{13}C NMR are reported in terms of chemical shift (δ: ppm), with (*C*) standing for quaternary carbon, (*CH*) standing for tertiary carbon, (CH_2) standing for secondary carbon, and (CH_3) standing for primary carbon. Elemental analyses were performed on Elementar Vairo EL instrument (Germany). Melting points (m.p.) were recorded on Shenguang WRS-1B melting point apparatus and are uncorrected. Electrospray ionization mass spectrometry (ESI-MS) data were obtained with Waters Xevo TQ-S Micro-Spectrometer. The single crystal diffraction was carried out on Bruker SMART APEX CCD diffractometer.

General Procedure for the Preparation of Nicotinamides

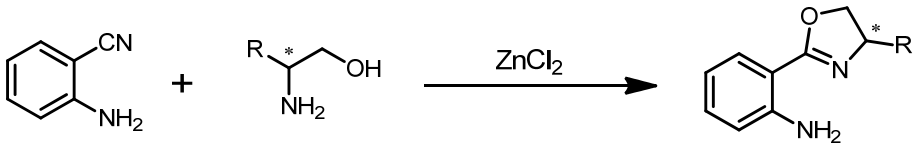
The synthesis of the nicotinamides in Tables 1~3 was carried out according to the previous methods reported by us and others[1-3].

Step 1, general synthesis of amino alcohol



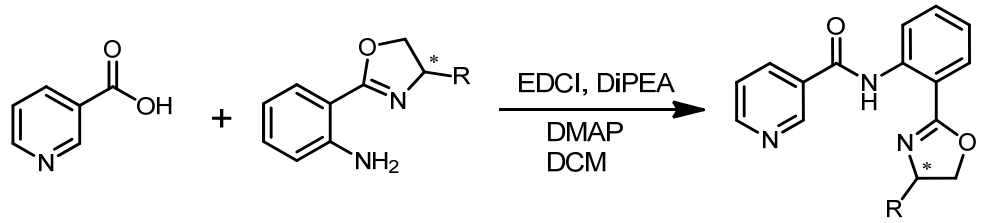
A three-neck round-bottom Schlenk flask fitted with a magnetic stir bar, a reflux condenser, and an addition funnel was charged with sodium borohydride (0.95 g, 25 mmol) and 50 mL of anhydrous tetrahydrofuran (THF) under a N_2 atmosphere, and then specific amino acid (10 mmol) was added in one portion and cooled to 0 °C with an ice bath. A solution of iodine (2.54 g, 10 mmol) in dry THF (25 mL) was added slowly and dropwise with an addition funnel under vigorous stirring. After completion of the iodine addition, the whole system was put into a preheated oil bath (80 °C) and stirred vigorously. The progress of the reaction was monitored by TLC until the reaction was complete (~12 h). The flask was then cooled to room temperature, and cold water was added cautiously to quench the reaction. The solvent was removed under vacuum; 20 mL of 20% aqueous KOH was added to the white paste; and the solution was stirred for 1 h and extracted by dichloromethane (DCM, 30 mL × 5), The organic extracts were combined and dried over sodium sulfate, concentrated in vacuum to afford amino alcohol intermediate, and used for the next step without further purification.

Step 2, general synthesis of 2-(2-Oxazolinyl)aniline



To an oven-dried tube under a nitrogen atomosphere was added 2-aminobenzonitrile (118 mg, 1 mmol), specific amino alcohols (1.2 mmol) and freshly flame-dried $ZnCl_2$ (13 mg, 10% mmol). The mixture was sealed with Teflon tape and stirred at 150 °C, and the reaction progress was monitored by TLC until the consumption of aminobenzonitrile (6−8 h). The reaction mixture was quenched and suspended with ethyl acetate (50 mL); NaOH (30%, 5 mL) was added; and the organic phase was washed with H_2O (10 mL × 2) and saturated aqueous NaCl (10 mL), then dried over anhydrous sodium sulfate, filtered, and concentrated by evaporation under vacuum to give the crude product, which was subject to flash chromatography purification on silica gel (hexane/EtOAc) to give the desired 2-(2-Oxazolinyl)anilines in moderate to good yields.

Step 3, general synthesis of nicotinamides



To a dried Schlenk flask charged with the 2-(4,5-dihydrooxazol-2-yl)anilines (1 mmol) and the pyridyl acid (1.05 mmol) were added anhydrous DCM (8 mL) and *N*,*N*-diisopropylethylamine (DIPEA, 1.5 mmol). The mixture was vigorously stirred and was added N-(3-(dimethylamino)propyl)-N-ethylcarbodiimide hydrochloride (EDCI−HCl, 0.211 g, 1.1 mmol) and 4-dimethylaminopyridine (DMAP, 0.012 g, 0.1 mmol). Then, the mixture was stirred overnight at room temperature until the full consumption of 2-(2-Oxazolinyl)aniline detected by TLC. The mixture was quenched by the addition of a saturated aqueous solution of NH_4Cl (20 mL) and separated. The water phase was extracted with DCM (15 mL × 3), and the combined organic phase was washed with water (10 mL × 2) and saturated aqueous NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (hexane/EtOAc) to give the desired nicotinamides for C-H functionalization.

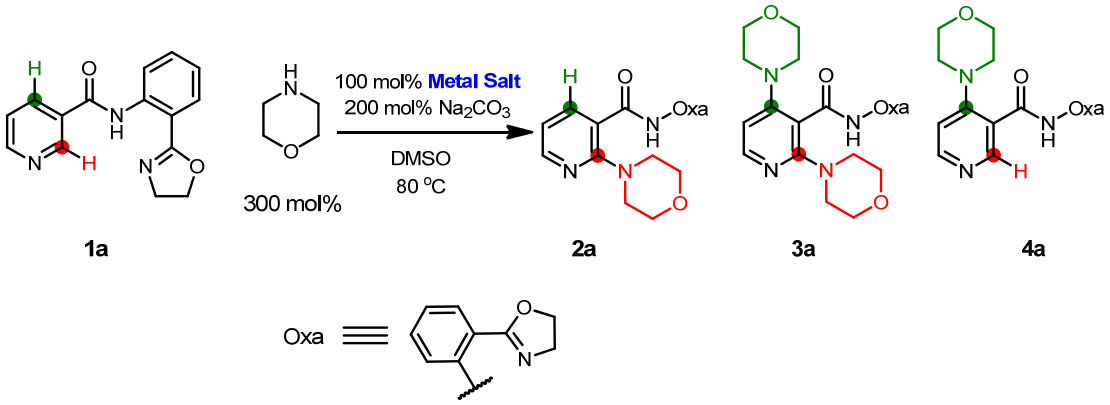
Optimization of the C-H functionalization of Nicotinamides

General procedure

To a 10 mL sealed tube was added N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide **1a** (100 mg, 0.376 mmol, 1 equiv), metal salts (100 mol%), morpholine (300 mol%), base (200 mol%), solvent (2 mL). The reaction mixture was put into a preheated oil bath (80 ℃) and stirred for 6 h under air. NH_3-H_2O (28%, 4 mL) were added to the mixture and stirred vigorously for 15 min, then the mixture was poured to EtOAc (30 mL) and the tube was rinsed by EtOAc (2 mL × 3), the combined organic phase was with water (10 mL × 2), and saturated NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (V_{hexane}/ V_{EtOAc} = 1 : 1 to EtOAc) to give the desired products.

NOTE: All the data was based on isolated products and starting materials

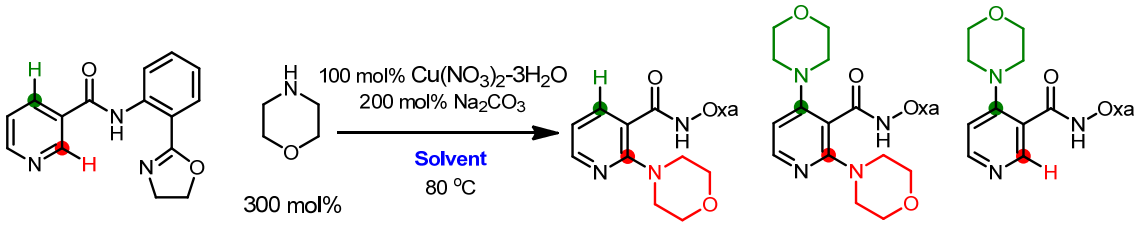
Table 1，Optimization of metal salts



1a **2a** **3a** **4a**

Entry	Metal Source	Conv. (%)	Yield (%)			Selectivity
			2a	**3a**	**4a**	**2a/4a**
1	$Cu(OAc)_2$	100	5	16	56	1:11.2
2	$CuCl_2$	45	13	11	46	1:3.5
3	CuCl	68	8	trace	50	1:6.3
4	$CuBr_2$	40	15	trace	57	1:3.8
5	CuBr	83	8	5	63	1:7.9
6	$CuSO_4·5H_2O$	100	30	trace	17	1.8:1
7	**$Cu(NO_3)_2·3H_2O$**	**93**	**63**	**5**	**trace**	**>20:1**
8	$Cu(OTf)_2$	80	47	trace	9	5.2:1
9	$Cu(ClO_4)_2·6H_2O$	100	45	2	12	3.8:1
10	$Cu_2(OH)_2CO_3$	<5	trace	trace	trace	
11	**$(C_8H_{15}O_2)_2Cu$**	**85**	**trace**	**trace**	**61**	**<1:20**
12	$Cu(BF_4)_2·6H_2O$	93	34	3	7	4.9:1
13	Cu	<5	trace	trace	trace	
14	CuO	<5	trace	trace	trace	
15	$Zn(OAc)_2$	8	trace	trace	trace	
16	$FeCl_2·4H_2O$	<5	trace	trace	trace	
17	$NiCl_2·6H_2O$	<5	trace	trace	trace	
18	$CoCl_2·6H_2O$	<5	trace	trace	trace	

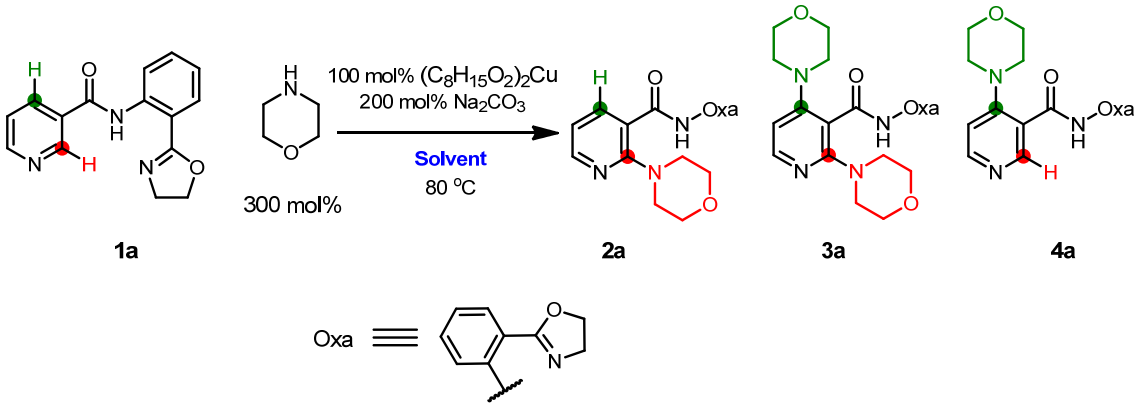
Table 2, Optimization of solvents with $Cu(NO_3)_2 \cdot 3H_2O$



1a **2a** **3a** **4a**

Entry	Solvent	Conv. (%)	Products Distribution			Selectivity
			2a	**3a**	**4a**	**2a/4a**
1	DMSO	93	63	5	trace	＞20:1
2	DMF	75	61	trace	trace	＞20:1
3	DMAc	77	61	trace	trace	＞20:1
4	NMP	82	44	trace	trace	＞20:1
5	1,4-dioxane	38	54	trace	14	3.9:1
6	MeCN	46	39	trace	trace	＞20:1
7	EtOH	53	24	trace	trace	＞20:1
8	H_2O	15	trace	trace	trace	
9	*n*-BuOH	48	24	trace	trace	＞20:1
10	*t*-Am-OH	56	46	trace	trace	＞20:1
11	DCE	13	trace	trace	trace	
12	Toluene	18	trace	trace	trace	

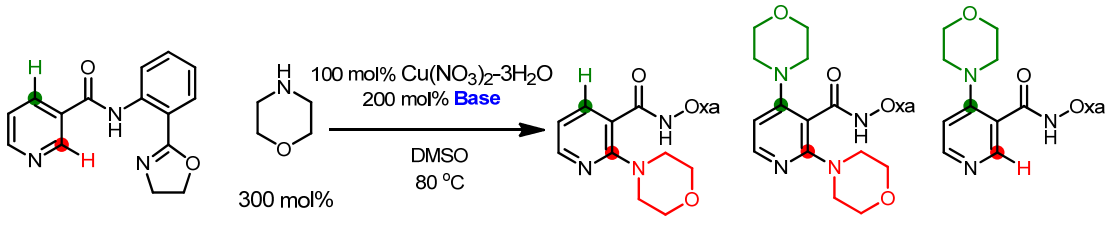
Table 3, Optimization of solvents with $(C_8H_{15}O_2)_2Cu$



1a **2a** **3a** **4a**

Entry	Solvent	Conv. (%)	Products Distribution			Selectivity
			2a	**3a**	**4a**	**2a/4a**
1	DMSO	85	Trace	Trace	61	＜1:20
2	DMAc	85	Trace	Trace	65	＜1:20
3	NMP	63	Trace	Trace	73	＜1:20
4	1,4-dioxane	38	Trace	Trace	22	＜1:20
5	MeCN	23	Trace	Trace	26	＜1:20
6	EtOH	51	10	Trace	Trace	＞20:1
7	H_2O	12	Trace	Trace	Trace	N.A.
8	*n*-BuOH	43	16	Trace	Trace	＞20:1
9	*t*-Am-OH	56	Trace	Trace	12	＜1:20
10	DCE	19	Trace	Trace	48	＜1:20
11	Toluene	15	Trace	Trace	Trace	N.A.

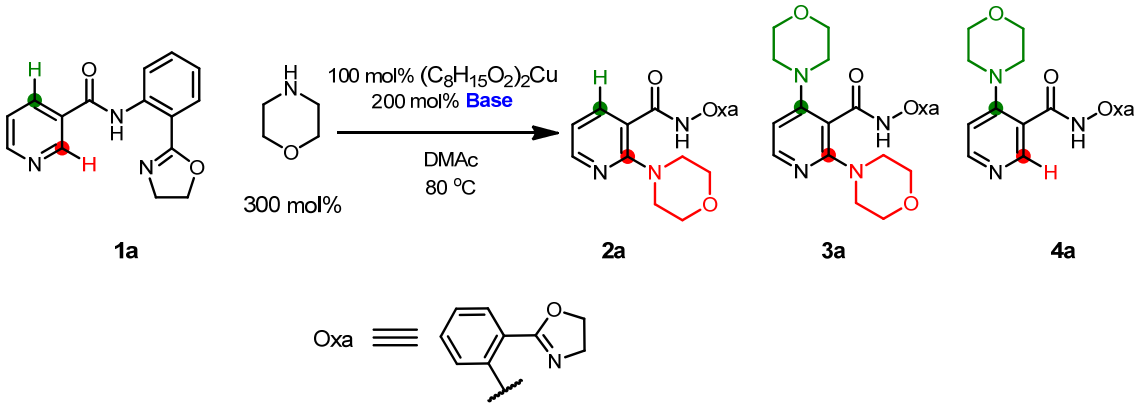
Table 4, Optimization of bases with $Cu(NO_3)_2 \cdot 3H_2O$



1a **2a** **3a** **4a**

Entry	Base	Conv. (%)	Products Distribution			Selectivity
			2a	**3a**	**4a**	**2a/4a**
1	Na_2CO_3	93	63	5	trace	＞20:1
2	CS_2CO_3	91	60	trace	14	4.3:1
3	$NaHCO_3$	93	45	trace	trace	＞20:1
4	K_3PO_4	50	54	trace	trace	＞20:1
5	DBU	20	34	trace	trace	＞20:1
6	Morpholine	35	39	trace	trace	＞20:1
7	N-Methylmorpholine	33	53	Trace	34	1.6:1
8	NEt_3	28	46	Trace	27	1.7:1
9	Pyridine	31	37	Trace	17	2.2:1
10	t-BuOK	30	33	trace	trace	＞20:1
11	NaOH	28	30	trace	trace	＞20:1
12	K_2CO_3	93	56	trace	trace	＞20:1

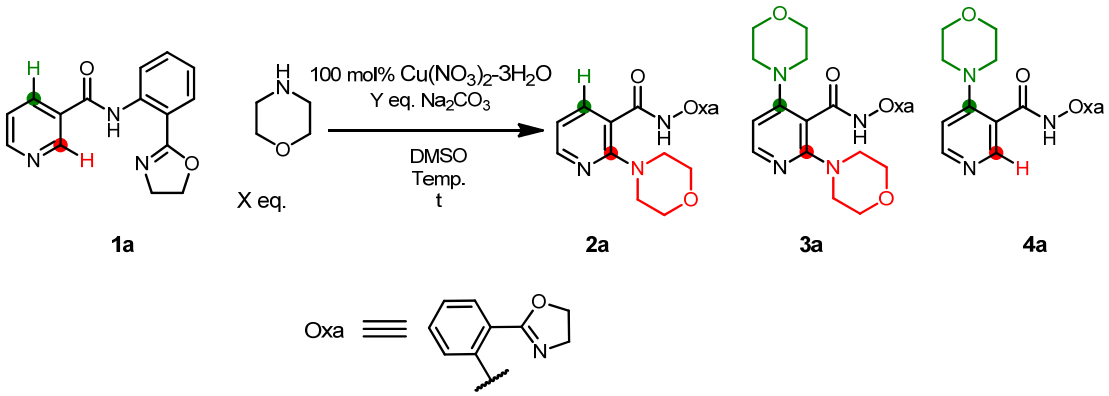
Table 5, Optimization of bases with $(C_8H_{15}O_2)_2Cu$



1a **2a** **3a** **4a**

Entry	Solvent	Conv. (%)	Products Distribution			Selectivity
			2a	**3a**	**4a**	**2a/4a**
1	Na_2CO_3	85	5	5	65	<1:20
2	CS_2CO_3	60	trace	trace	trace	
3	$NaHCO_3$	70	6	trace	52	1:8.7
4	K_3PO_4	71	29	trace	23	1.2:1
5	Morpholine	64	13	trace	67	1:5.2
6	N-Methylmorpholine	60	9	trace	65	1:7.2
7	NEt_3	76	13	6	70	1:5.4
8	Pyridine	73	17	trace	56	1:3.3
9	t-BuOK	55	trace	trace	25	<1:20
10	NaOH	95	trace	trace	6	<1:20
11	K_2CO_3	63	trace	trace	36	<1:20

Table 6, Optimization of other parameters

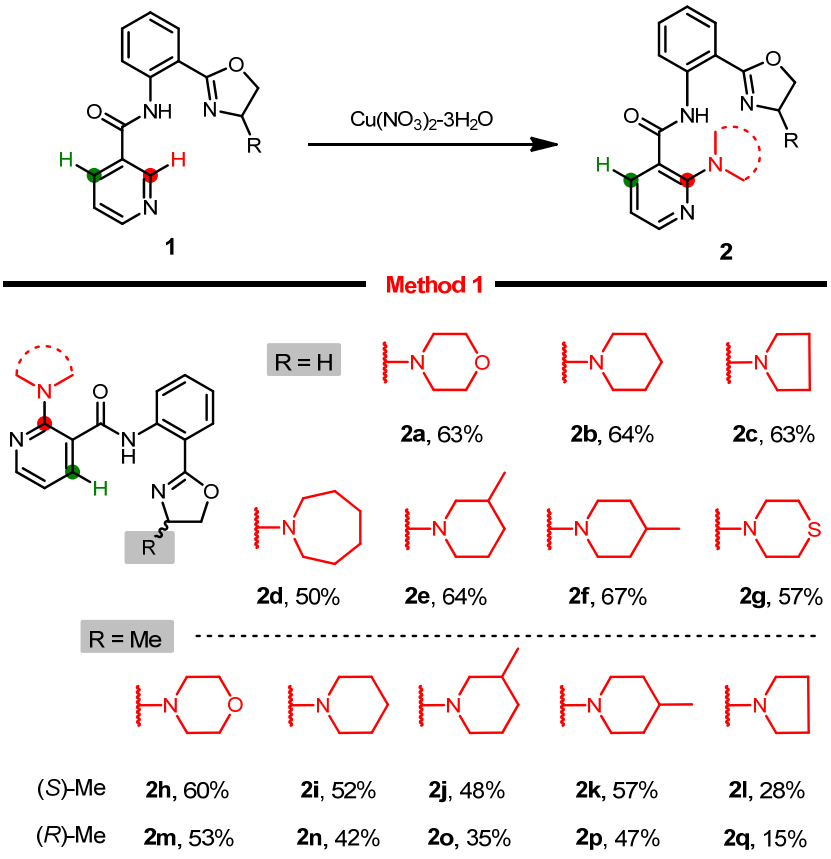


entry	Na_2CO_3	Temp	Morpholine	t	Yield (%)			Conv.(%)	**2a**/**4a**
					2a	**3a**	**4a**		
1	2eq	80	3eq	6h	63	trace	trace	93	＞20:1
2	2eq	80	1eq	6h	56	trace	trace	47	＞20:1
3	2eq	80	5eq	6h	60	trace	trace	95	＞20:1
4	2eq	40	3eq	6h	56	trace	trace	67	＞20:1
5[a]	2eq	80	3eq	6h	64	trace	trace	53	＞20:1
6	2eq	120	3eq	6h	53	trace	trace	93	＞20:1
7	2eq	100	3eq	6h	57	trace	trace	93	＞20:1
8	2eq	60	3eq	6h	55	trace	trace	89	＞20:1
9	2eq	80	3eq	3h	50	trace	trace	86	＞20:1
10	2eq	80	3eq	12h	57	trace	trace	93	＞20:1
11	3eq	80	3eq	6h	61	trace	trace	89	＞20:1
12	1eq	80	3eq	6h	53	trace	trace	85	＞20:1

General Procedure for N-*ortho*-amination of Nicotinamides

To a 10 mL sealed tube was added nicotinamide **1** (0.376 mmol, 1 equiv.), $Cu(NO_3)_2{\cdot}3H_2O$ (90 mg, 0.376 mmol), secondary amine (300 mol%), Na_2CO_3 (80 mg, 0.752 mmol) and DMSO (2 mL). The reaction mixture was put into a preheated oil bath (80 ℃) and stirred for 6 h under air. NH_3-H_2O (28%, 4 mL) were added to the mixture and stirred vigorously for 15 min, then the mixture was poured to EtOAc (30 mL) and the tube was rinsed by EtOAc (2 mL × 3), the combined organic phase was with water (10 mL × 2), and saturated NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (V_{hexane}/ V_{EtOAc} = 1 : 1 to EtOAc) to give the desired products.

NOTE: All the data were isolated yields

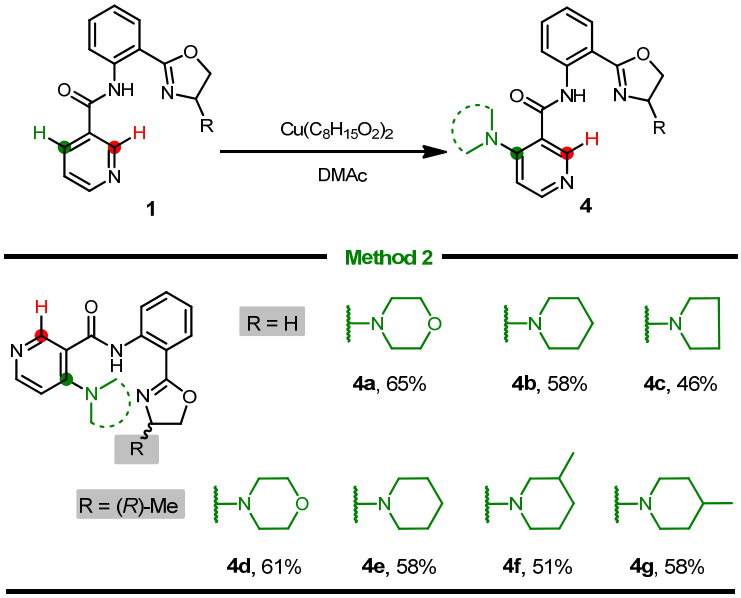


General Procedure for N-*para*-amination of Nicotinamides

To a 10 mL sealed tube was added nicotinamide **1** (0.376 mmol, 1 equiv), $Cu(C_8H_{15}O_2)_2$ (131 mg, 0.376 mmol), secondary amine (300 mol%), Na_2CO_3 (80 mg, 0.752 mmol) and DMAc (2

mL). The reaction mixture was put into a preheated oil bath (80 ℃) and stirred for 6 h under air. NH_3-H_2O (28%, 4 mL) were added to the mixture and stirred vigorously for 15 min, then the mixture was poured to EtOAc (30 mL) and the tube was rinsed by EtOAc (2 mL × 3), the combined organic phase was with water (10 mL × 2), and saturated NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (V_{hexane}/ V_{EtOAc} = 1 : 1 to EtOAc) to give the desired products.

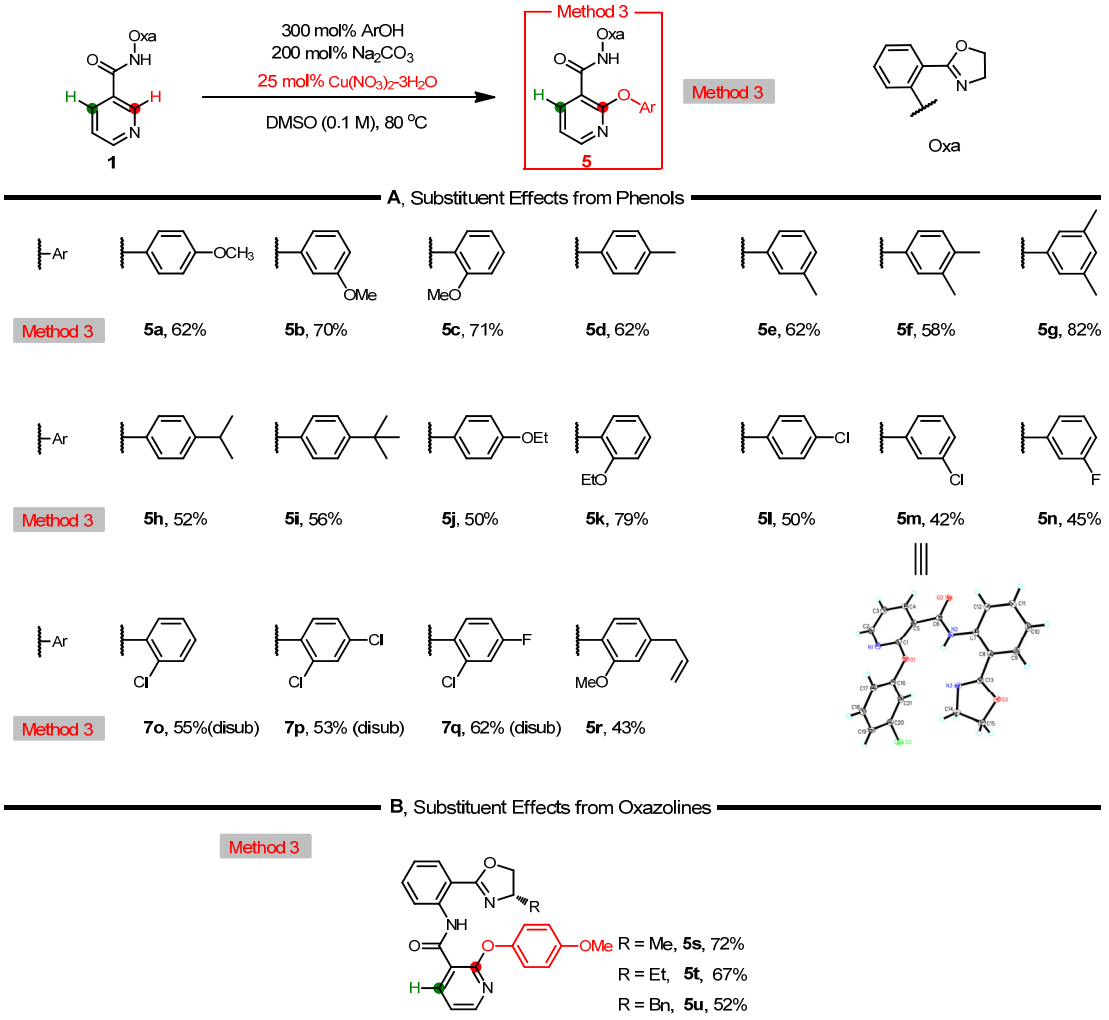
NOTE: All the data were isolated yields



General Procedure for N-*ortho*-etherification of Nicotinamides

To a 10 mL sealed tube was added nicotinamide **1** (0.187 mmol, 1 equiv), $Cu(NO_3)_2 \cdot 3H_2O$ (11.3 mg, 0.047 mmol), phenol (300 mol%), Na_2CO_3 (40 mg, 0.374 mmol) and DMSO (1.9 mL). The reaction mixture was put into a preheated oil bath (80 ℃) and stirred for 6 h under air. NH_3-H_2O (28%, 2 mL) were added to the mixture and stirred vigorously for 15 min, then the mixture was poured to EtOAc (15 mL) and the tube was rinsed by EtOAc (2 mL × 3), the combined organic phase was with water (10 mL × 2), and saturated NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (V_{hexane}/ V_{EtOAc} = 1 : 1 to EtOAc) to give the desired products.

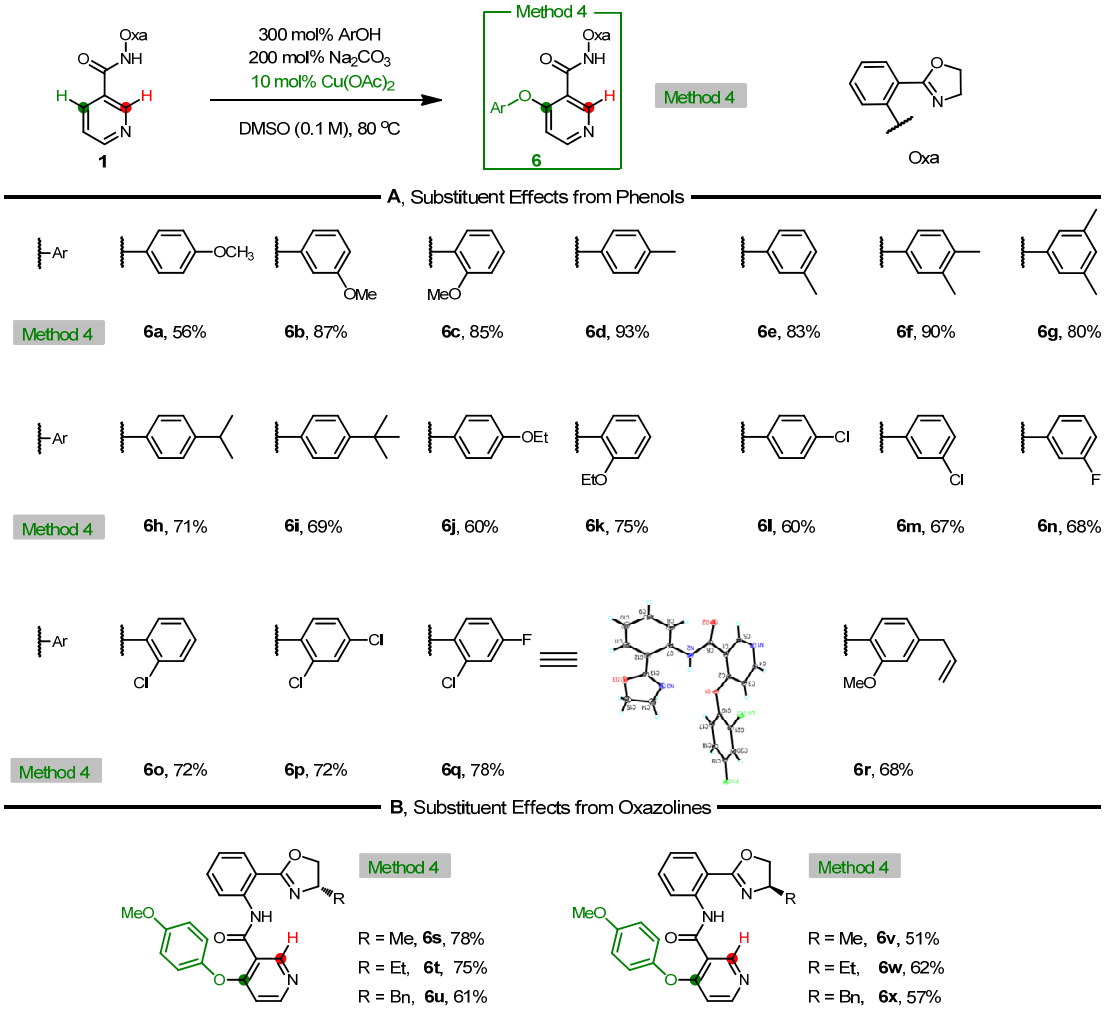
NOTE: All the data were isolated yields



General Procedure for N-*para*-etherification of Nicotinamides

To a 10 mL sealed tube was added nicotinamide **1** (0.187 mmol, 1 equiv), $Cu(OAc)_2$ (3.4 mg, 0.0187 mmol), phenol (300 mol%), Na_2CO_3 (40 mg, 0.374 mmol) and DMSO (1.9 mL). The reaction mixture was put into a preheated oil bath (80 ℃) and stirred for 6 h under air. NH_3-H_2O (28%, 2 mL) were added to the mixture and stirred vigorously for 15 min, then the mixture was poured to EtOAc (15 mL) and the tube was rinsed by EtOAc (2 mL × 3), the combined organic phase was with water (10 mL × 2), and saturated NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (V_{hexane}/ V_{EtOAc} = 1 : 1 to EtOAc) to give the desired products.

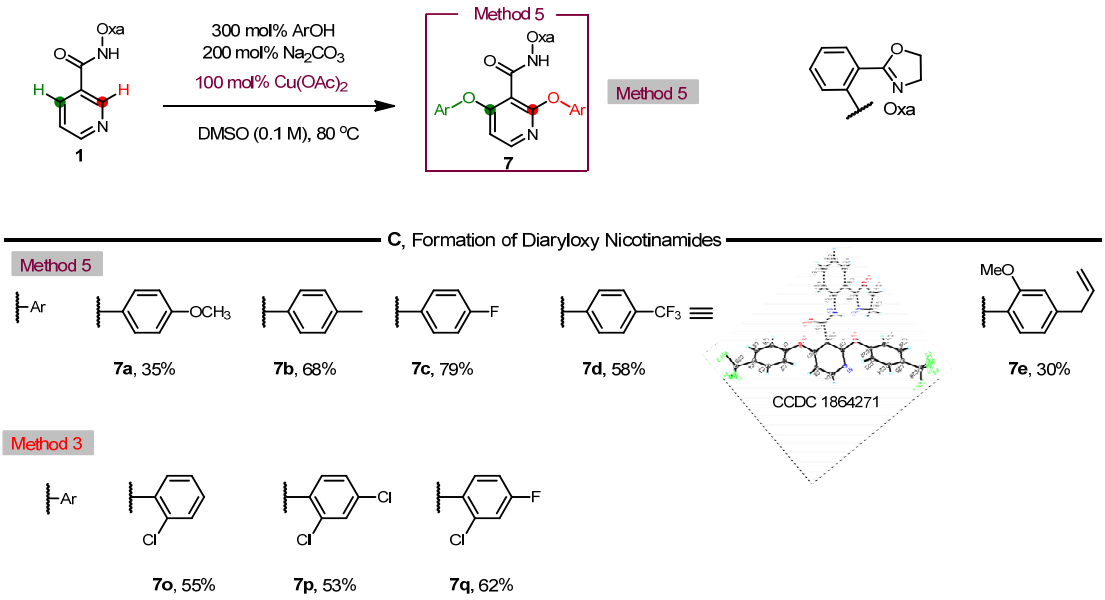
NOTE: All the data were isolated yields



General Procedure for di-etherification of Nicotinamides

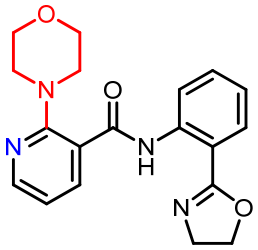
To a 10 mL sealed tube was added nicotinamide **1** (0.187 mmol, 1 equiv), $Cu(OAc)_2$ (34 mg, 0.187 mmol), phenol (300 mol%), Na_2CO_3 (40 mg, 0.374 mmol) and DMSO (1.9 mL). The reaction mixture was put into a preheated oil bath (80 ℃) and stirred for 6 h under air. NH_3-H_2O (28%, 2 mL) were added to the mixture and stirred vigorously for 15 min, then the mixture was poured to EtOAc (15 mL) and the tube was rinsed by EtOAc (2 mL × 3), the combined organic phase was with water (10 mL × 2), and saturated NaCl (10 mL) successively, dried over anhydrous sodium sulfate, concentrated under vacuum, and purified by chromatography on silica gel (V_{hexane}/ V_{EtOAc} = 1 : 1 to EtOAc) to give the desired products.

NOTE: All the data were isolated yields; Di-etherification of Nicotinamides was also observed in method 3, when some phenols with electron-withdrawing groups were used.



Typical Characteristic Data in Amination

Amination of Nicotinamide **1a** with Morpholine to produce **2a**, **3a** or **4a**



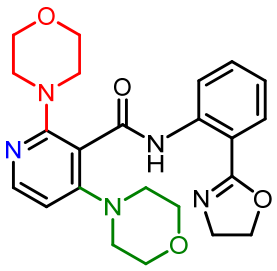
N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-morpholinonicotinamide (**2a**), white solid, yield 63%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.41 (t, J = 4.72 Hz, 4H, NCH_2 × 2), 3.71 (t, J = 4.72 Hz, 4H, OCH_2 × 2), 4.04 (t, J = 9.52 Hz, 2H, NCH_2-CH_2 O), 4.37 (t, J = 9.52 Hz, 2H, NCH_2-CH_2 O), 6.91 (dd, J_1 = 7.48 Hz, J_2 = 4.8 Hz, 1H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.91 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 7.95 (dd, J_1 = 7.48 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.32 (dd, J_1 = 4.8 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 8.89 (d, J = 8.4 Hz, 1H, *Aromatic H*), 12.85 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 49.9 (2 × CH_2), 54.8 (CH_2), 66.2 (CH_2), 66.6 (2 ×

CH$_2$), 113.6 (*C*), 116.0 (*CH*), 119.9 (*CH*), 121.4 (*C*), 122.8 (*CH*), 129.5 (*CH*), 132.7 (*CH*), 139.4 (*CH*), 139.6 (*C*), 149.5 (*CH*), 158.5 (*C*), 164.3 (*C*), 166.9 (*C*).

ESI-MS: calcd for $C_{19}H_{21}N_4O_3$ [M+ H]$^+$: 353.16, found: 353.18.

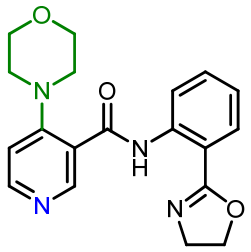
The structure of compound **2a** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1864263.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2,4-dimorpholinonicotinamide (**3a**), white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.17 (t, *J* = 4.64 Hz, 4H, N*CH*$_2$ × 2), 3.30 (t, *J* = 4.48 Hz, 4H, N*CH*$_2$ × 2), 3.64 (t, *J* = 4.64 Hz, 4H, O*CH*$_2$ × 2), 3.69 (t, *J* = 4.48 Hz, 4H, O*CH*$_2$ × 2), 3.97 (t, *J* = 9.44 Hz, 2H, N*CH*$_2$-CH_2O), 4.36 (t, *J* = 9.44 Hz, 2H, NCH_2-*CH*$_2$O), 6.55 (d, *J* = 5.72 Hz, 1H, *Aromatic H*), 7.14 (dd, J_1 = 8.24 Hz, J_2 = 8.24 Hz, 1H, *Aromatic H*), 7.53 (m, 1H, *Aromatic H*), 7.92 (dd, J_1 = 7.92 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.17 (d, *J* = 5.72 Hz, 1H, *Aromatic H*), 8.89 (d, *J* = 8.44 Hz, 1H, *Aromatic H*), 12.54 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 50.5 (2 × *CH*$_2$), 51.4 (2 × *CH*$_2$), 54.8(*CH*$_2$), 66.1 (*CH*$_2$), 66.8 (2 × *CH*$_2$), 67.0 (2 × *CH*$_2$), 107.8 (*CH*), 113.2 (*C*), 116.6 (*C*), 119.4 (*CH*), 122.7 (*CH*), 129.5 (*CH*), 132.8 (*CH*), 140.0 (*C*), 149.1 (*CH*), 158.1 (*C*), 160.5 (*C*), 164.4 (*C*), 167.3 (*C*).

ESI-MS: calcd for $C_{23}H_{28}N_5O_4$ [M+ H]$^+$: 438.21, found: 438.22.

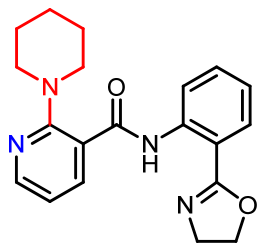


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-morpholinonicotinamide (**4a**), White solid, yield 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.26 (t, *J* = 4.76 Hz, 4H, N*CH*$_2$ × 2), 3.75 (t, *J* = 4.76 Hz, 4H, O*CH*$_2$ × 2), 4.05 (t, *J* = 9.44 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.38 (t, *J* = 9.44 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.82 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 7.15 (m, 1H, *Aromatic H*), 7.53 (m, 1H, *Aromatic H*), 7.92 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.44 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 8.68 (s, 1H, *Aromatic H*), 8.88 (d, *J* = 8.48 Hz, 1H, *Aromatic H*), 12.85 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 50.5 (2 × *CH*$_2$), 54.7 (*CH*$_2$), 66.2 (*CH*$_2$), 66.3 (2 × *CH*$_2$), 111.4 (*CH*), 113.5 (*C*), 119.8 (*CH*), 122.9 (*CH*), 123.1 (*C*), 129.4 (*CH*), 132.7 (*CH*), 139.6 (*C*), 151.0 (*CH*), 151.9 (*CH*), 155.1 (*C*), 164.5 (*C*), 166.3 (*C*).

ESI-MS: calcd for $C_{19}H_{21}N_4O_3$ $[M+H]^+$: 353.16, found: 353.17.

The structure of compound **4a** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1864265.

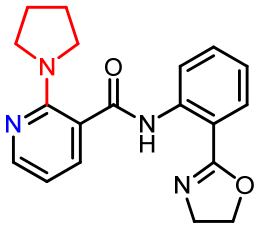


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(piperidin-1-yl)nicotinamide (**2b**), white solid, yield 64%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.54-1.61 (m, 6H, NCH$_2$-*CH*$_2$*CH*$_2$*CH*$_2$),

3.31-3.36 (m, 4H, N*CH*$_2$ × 2), 4.06 (t, *J* = 9.40 Hz, 2H, N*CH*$_2$-CH$_2$ O), 4.36 (t, *J* = 9.40 Hz, 2H, NCH$_2$-*CH*$_2$ O), 6.84 (dd, J_1 = 7.48 Hz, J_2 = 4.84 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 7.93 (dd, J_1 = 7.44 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 8.30 (dd, J_1 = 4.8 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.91 (d, *J* = 8.4 Hz, 1H, *Aromatic H*), 12.75 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, CDCl$_3$) δ 24.4 (*CH*$_2$), 25.6 (2 × *CH*$_2$), 51.0(2 × *CH*$_2$), 54.9 (*CH*$_2$), 66.2 (*CH*$_2$), 113.7 (*C*), 115.2 (*CH*), 120.1 (*CH*), 121.3 (*C*), 122.5 (*CH*), 129.3 (*CH*), 132.5 (*CH*), 139.3 (*CH*), 139.8 (*C*), 149.4 (*CH*), 159.5 (*C*), 164.1 (*C*), 167.3 (*C*).

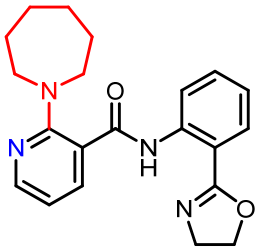
ESI-MS: calcd for $C_{20}H_{23}N_4O_2$ $[M+H]^+$: 351.18, found: 351.20.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(pyrrolidin-1-yl)nicotinamide (**2c**), white solid, yield 63%. ^{1}H NMR (400 MHz, CDCl$_3$) δ 1.89-1.92 (m, 4H, NCH$_2$-*CH*$_2$*CH*$_2$), 3.48-3.52 (m, 4H, N-*CH*$_2$ × 2), 4.07 (t, *J* = 9.48 Hz, 2H, N*CH*$_2$-CH$_2$ O), 4.38 (t, *J* = 9.48 Hz, 2H, NCH$_2$-*CH*$_2$ O), 6.63 (dd, J_1 = 7.52 Hz, J_2 = 4.96 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.78 (dd, J_1 = 7.44 Hz, J_2 = 1.88 Hz, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.96 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.25 (dd, J_1 = 4.8 Hz, J_2 = 1.84 Hz, 1H, *Aromatic H*), 8.91 (d, *J* = 8.44 Hz, 1H, *Aromatic H*), 12.61 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 25.7 (2 × *CH_2*), 49.2 (2 × *CH_2*), 54.7 (*CH_2*), 66.2 (*CH_2*), 111.1 (*CH*), 113.2 (*C*), 117.4 (*C*), 119.6 (*CH*), 122.4 (*CH*), 129.2 (*CH*), 132.7 (*CH*), 137.8 (*CH*), 140.1 (*C*), 149.4 (*CH*), 155.1 (*C*), 164.6 (*C*), 167.8 (*C*).

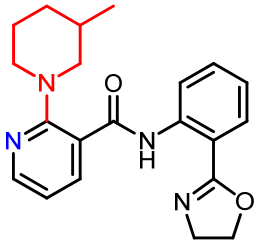
ESI-MS: calcd for $C_{19}H_{21}N_4O_2$ [M+ H]$^+$: 337.17, found: 337.18.



2-(azepan-1-yl)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**2d**), white solid, yield 50%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.49-1.54 (m, 4H, NCH_2CH_2-*CH_2* × 2), 1.76-1.84 (m, 4H, NCH_2-*CH_2* CH_2 × 2), 3.52-3.57 (m, 4H, N-*CH_2*CH_2CH_2 × 2), 4.07 (t, *J* = 9.40 Hz, 2H, N*CH_2*-CH_2 O), 4.37 (t, *J* = 9.40 Hz, 2H, NCH_2-*CH_2* O), 6.66 (dd, J_1 = 7.44 Hz, J_2 = 4.72 Hz, 1H, *Aromatic H*), 7.11 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.81 (dd, J_1 = 7.44 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.96 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.23 (dd, J_1 = 4.76 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 8.93 (d, *J* = 8.48 Hz, 1H, *Aromatic H*), 12.57 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 28.1 (2 × *CH_2*), 28.4 (2 × *CH_2*), 50.4 (2 × *CH_2*), 54.8 (*CH_2*), 66.2 (*CH_2*), 111.9 (*CH*), 113.3 (*C*), 117.6 (*C*), 119.6 (*CH*), 122.3 (*CH*), 129.3 (*CH*), 132.7 (*CH*), 138.7 (*CH*), 140.1, 148.8 (*CH*), 157.7 (*C*), 164.5 (*C*), 168.2 (*C*).

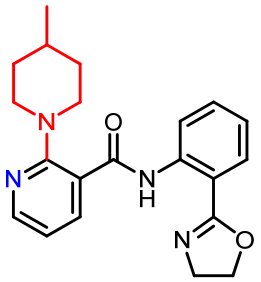
ESI-MS: calcd for $C_{21}H_{25}N_4O_2$ [M+ H]$^+$: 365.20, found: 365.24.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(3-methylpiperidin-1-yl)nicotinamide (**2e**), white solid, yield 64%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.82 (d, J = 6.72 Hz, 3H, *CH*$_3$-CH), 1.45-1.77 (m, 5H), 2.52 (dd, J_1 = 12.64 Hz, J_2 = 10.68 Hz, 1H), 2.83 (m, 1H), 3.69-3.78 (m, 2H), 4.01-4.08 (m, 2H), 4.35 (t, J = 9.40 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.84 (dd, J_1 = 7.44 Hz, J_2 = 4.76 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 7.93 (dd, J_1 = 7.44 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.30 (dd, J_1 = 4.8 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 8.89 (d, J = 8.0 Hz, 1H, *Aromatic H*), 12.73 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.3, 25.3, 30.9, 33.1, 50.6, 54.8, 57.6, 66.1, 113.7, 115.1, 120.0, 121.3, 122.5, 129.3, 132.5, 139.3, 139.8, 149.4, 159.3, 164.1, 167.3.

ESI-MS: calcd for $C_{21}H_{25}N_4O_2$ $[M+H]^+$: 365.20, found: 365.22.

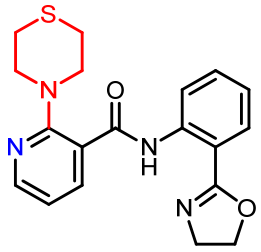


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(4-methylpiperidin-1-yl)nicotinamide (**2f**), white solid, yield 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.87 (d, J = 6.52 Hz, 3H, *CH*$_3$-CH), 1.13-1.26 (m, 2H), 1.50 (m, 1H), 1.56-1.66 (m, 2H), 2.85-2.97 (m, 2H), 3.77-3.86 (m, 2H), 4.06 (t, J = 9.52 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.36 (t, J = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O),

6.83 (dd, J_1 = 7.08 Hz, J_2 = 4.80 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 7.93 (dd, J_1 = 7.44 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.29 (dd, J_1 = 4.84 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.92 (d, J = 8.44 Hz, 1H, *Aromatic H*), 12.72 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 22.0, 30.8, 33.9 (2 × *CH_2*), 50.2 (2 × *CH_2*), 54.9, 66.2, 113.7, 115.0, 120.0, 121.1, 122.5, 129.3, 132.5, 139.3, 139.8, 149.3, 159.2, 164.1, 167.3.

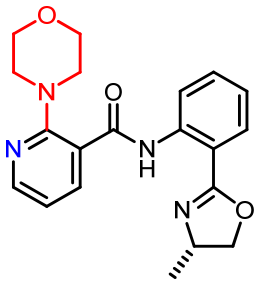
ESI-MS: calcd for $C_{21}H_{25}N_4O_2$ $[M+H]^+$: 365.20, found: 365.22.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-thiomorpholinonicotinamide (**2g**), yield 57%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62-2.70 (m, 4H, S*CH_2* × 2), 3.65-3.73 (m, 4H, N*CH_2* × 2), 4.06 (t, J = 9.44 Hz, 2H, N*CH_2*-CH_2 O), 4.38 (t, J = 9.44 Hz, 2H, NCH_2-*CH_2* O), 6.90 (dd, J_1 = 7.48 Hz, J_2 = 4.8 Hz, 1H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.91 (dd, J_1 = 7.96 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 7.94 (dd, J_1 = 7.52 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.31 (dd, J_1 = 4.84 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.89 (d, J = 8.44 Hz, 1H, *Aromatic H*), 12.77 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 27.0 (2 × *CH_2*), 52.3 (2 × *CH_2*), 54.8, 66.2, 113.6, 115.9, 120.0, 121.6, 122.8, 129.5, 132.6, 139.5, 139.6, 149.4, 158.9, 164.3, 166.9.

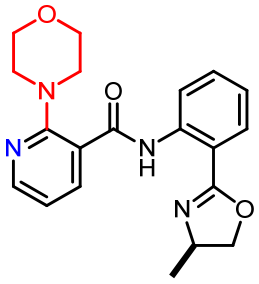
ESI-MS: calcd for $C_{19}H_{21}N_4O_2S$ $[M+H]^+$: 369.14, found: 369.17.



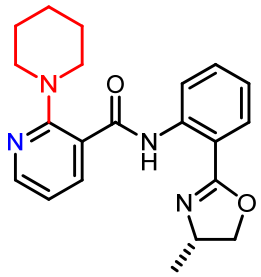
(S)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-morpholinonicotinamide (**2h**), yield 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.24 (d, J = 6.52 Hz, 3H, NCH-*CH*$_3$), 3.39-3.48 (m, 4H, N*CH*$_2$-CH_2O × 2), 3.68-3.78 (m, 4H, NCH_2*CH*$_2$-O × 2), 3.88 (dd, J_1 = 7.92 Hz, J_2 = 7.92 Hz, 1H), 4.37 (m, 1H), 4.47 (dd, J_1 = 8.16 Hz, J_2 = 7.92 Hz, 1H), 6.89 (dd, J_1 = 7.48 Hz, J_2 = 4.8 Hz, 1H, *Aromatic H*), 7.13 (dd, J_1 = 7.60 Hz, J_2 = 7.60 Hz, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.88 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 7.92 (dd, J_1 = 7.52 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.31 (dd, J_1 = 4.80 Hz, J_2 = 1.88 Hz, 1H, *Aromatic H*), 8.85 (d, J = 8.44 Hz, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 49.8 (2 × *CH*$_2$), 62.1, 66.6 (2 × *CH*$_2$), 72.7, 113.7, 115.6, 119.9, 121.2, 122.8, 129.4, 132.6, 139.1, 139.6, 149.4, 158.4, 163.1, 167.0.

ESI-MS: calcd for $C_{20}H_{23}N_4O_3$ $[M+H]^+$: 367.18, found: 367.21.



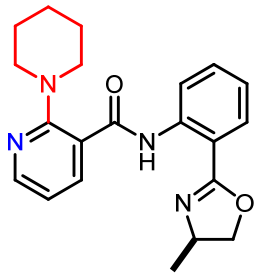
(R)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-morpholinonicotinamide (**2m**), yield 53%. Similar NMR Data to that of compound **2h**.



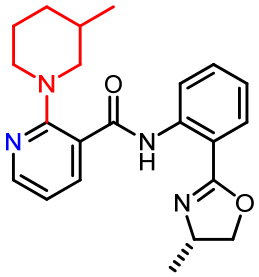
(S)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(piperidin-1-yl)nicotinamide (**2i**), yield 52%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.25 (d, J = 6.44 Hz, 3H, NCH-*CH*$_3$), 1.50-1.59 (m, 6H, NCH$_2$*CH*$_2$ *CH*$_2$ *CH*$_2$), 3.31-3.42 (m, 4H, N*CH*$_2$ × 2), 3.86 (dd, J_1 = 7.80 Hz, J_2 = 7.80 Hz, 1H), 4.38 (m, 1H), 4.45 (dd, J_1 = 9.44 Hz, J_2 = 7.80 Hz, 1H), 6.81 (dd, J_1 = 7.52 Hz, J_2 = 4.88 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 7.92 (dd, J_1 = 7.44 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.29 (dd, J_1 = 4.88 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.85 (d, J = 8.40 Hz, 1H, *Aromatic H*), 12.71 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 24.5, 25.7 (2 × *CH*$_2$), 50.9 (2 × *CH*$_2$), 62.1, 72.7, 113.8, 114.8, 120.1, 121.1, 122.5, 129.3, 132.4, 139.1, 139.8, 149.3, 159.3, 162.8, 167.4.

ESI-MS: calcd for $C_{21}H_{25}N_4O_2$ $[M+H]^+$: 365.20, found: 365.22.



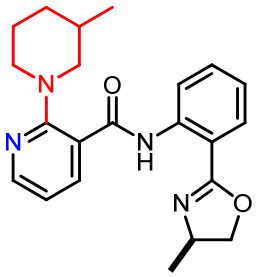
(R)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(piperidin-1-yl)nicotinamide (**2n**), yield 42%. Similar NMR Data to that of compound **2i**.



N-(2-((S)-4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(3-methylpiperidin-1-yl)nicotinamide (**2j**), 1:1 dr, white solid, yield 48%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.82 (d, J = 6.40 Hz, 1.5H, *CH*$_3$-CH), 0.83 (d, J = 6.48 Hz, 1.5H, *CH*$_3$-CH), 1.01 (m, 1H), 1.50-1.62 (m, 2H), 1.65-1.77 (m, 2H), 2.53 (m, 1H), 2.84 (m, 1H), 3.72-3.82 (m, 2H), 3.85 (dd, J_1 = 7.96 Hz, J_2 = 7.88 Hz, 1H), 4.35 (m, 1H), 4.44 (dd, J_1 = 9.44 Hz, J_2 = 7.96 Hz, 1H), 6.81 (dd, J_1 = 7.52 Hz, J_2 = 4.88 Hz, 1H, *Aromatic H*), 7.11 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.84 Hz, J_2 = 1.52 Hz, 1H, *Aromatic H*), 7.90 (m, 1H, *Aromatic H*), 8.28 (dd, J_1 = 4.88 Hz, J_2 = 1.84 Hz, 1H, *Aromatic H*), 8.83 (d, J = 8.48 Hz, 1H, *Aromatic H*), 12.65 and 12.68 (s, 1H, CO*NH*).

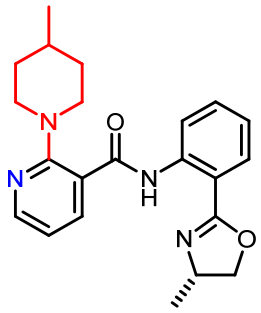
^{13}C NMR (100 MHz, $CDCl_3$) δ 19.2 (19.3), 21.3 (21.4), 25.3 (25.4), 30.8 (30.9), 33.1, 50.5, 57.5, 62.1, 72.7, 113.8, 114.7, 120.1, 121.0, 122.5, 129.3, 132.4, 139.1, 139.8, 149.3, 159.2, 162.8, 167.4.

ESI-MS: calcd for $C_{22}H_{27}N_4O_2$ [M+ H] $^{+}$: 379.21, found: 379.24.



N-(2-((R)-4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(3-methylpiperidin-1-

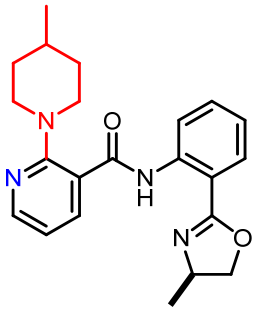
yl)nicotinamide (**2o**), 1:1 dr, white solid, yield 35%. Similar NMR Data to that of compound **2j**.



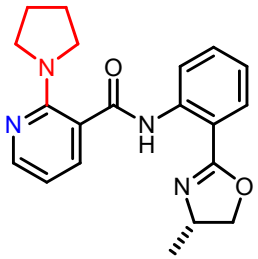
(S)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(4-methylpiperidin-1-yl)nicotinamide (**2k**), 1:1 dr, white solid, yield 57%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (d, J = 6.44 Hz, 3H, *CH*$_3$-CH), 1.16-1.26 (m, 2H), 1.25 (d, J = 6.44 Hz, 3H, *CH*$_3$-CH-N), 1.51 (m, 1H), 1.57-1.65 (m, 2H), 2.87-2.97 (m, 2H), 3.81-3.90 (m, 3H), 4.37 (m, 1H), 4.44 (m, 1H), 6.79 (dd, J_1 = 7.44 Hz, J_2 = 4.76 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.36 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.44 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 8.27 (dd, J_1 = 4.84 Hz, J_2 = 1.92 Hz, 1H, *Aromatic H*), 8.86 (d, J = 8.44 Hz, 1H, *Aromatic H*), 12.67 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 21.9, 30.9, 33.9 (34.0), 50.0 (50.2), 62.1, 72.7, 113.8, 114.5, 120.1, 120.9, 122.5, 129.3, 132.4, 139.0, 139.8, 149.3, 159.0, 162.9, 167.4.

ESI-MS: calcd for $C_{22}H_{27}N_4O_2$ $[M+H]^+$: 379.21, found: 379.25.



(R)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(4-methylpiperidin-1-yl)nicotinamide (**2p**), 1:1 dr, white solid, yield 47%. Similar NMR Data to that of compound **2k**.

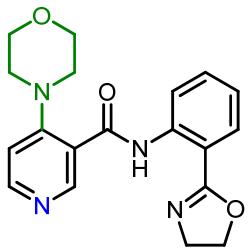


(S)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(pyrrolidin-1-yl)nicotinamide (**2l**), white solid, yield 28%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.30 (d, J = 6.44 Hz, 3H, *CH*$_3$-CH), 1.87-1.99 (m, 4H, NCH$_2$-*CH*$_2$ × 2), 3.44-3.59 (m, 4H, N*CH*$_2$ × 2), 3.91 (dd, J_1 = 7.64 Hz, J_2 = 7.56 Hz, 1H), 4.37 (m, 1H), 4.46 (dd, J_1 = 9.28 Hz, J_2 = 7.64 Hz, 1H), 6.63 (dd, J_1 = 7.40 Hz, J_2 = 4.80 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.81 (dd, J_1 = 7.44 Hz, J_2 = 1.84 Hz, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.96 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.26 (dd, J_1 = 4.88 Hz, J_2 = 1.88 Hz, 1H, *Aromatic H*), 8.89 (d, J = 8.40 Hz, 1H, *Aromatic H*), 12.70 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 25.7 (*CH*$_2$ × 2), 49.2 (*CH*$_2$ × 2), 61.9, 72.7, 110.9, 113.3, 117.4, 119.6, 122.4, 129.2, 132.6, 137.8, 140.1, 149.3, 155.0, 163.3, 167.7.

ESI-MS: calcd for $C_{20}H_{23}N_4O_2$ $[M+H]^+$: 351.18, found: 351.22.

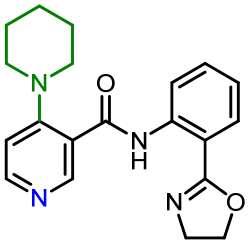


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-morpholinonicotinamide (**4a**), White solid, yield 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.26 (t, *J* = 4.76 Hz, 4H, N*CH*$_2$ × 2), 3.75 (t, *J* = 4.76 Hz, 4H, O*CH*$_2$ × 2), 4.05 (t, *J* = 9.44 Hz, 2H, N*CH*$_2$-CH_2O), 4.38 (t, *J* = 9.44 Hz, 2H, NCH_2-*CH*$_2$O), 6.82 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 7.15 (m, 1H, *Aromatic H*), 7.53 (m, 1H, *Aromatic H*), 7.92 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.44 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 8.68 (s, 1H, *Aromatic H*), 8.88 (d, *J* = 8.48 Hz, 1H, *Aromatic H*), 12.85 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 50.5 (2 × *CH*$_2$), 54.7 (*CH*$_2$), 66.2 (*CH*$_2$), 66.3 (2 × *CH*$_2$), 111.4 (*CH*), 113.5 (*C*), 119.8 (*CH*), 122.9 (*CH*), 123.1 (*C*), 129.4 (*CH*), 132.7 (*CH*), 139.6 (*C*), 151.0 (*CH*), 151.9 (*CH*), 155.1 (*C*), 164.5 (*C*), 166.3 (*C*).

ESI-MS: calcd for $C_{19}H_{21}N_4O_3$ $[M+ H]^+$: 353.16, found: 353.17.

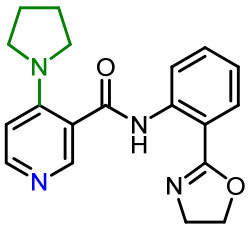
The structure of compound **4a** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1864265.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(piperidin-1-yl)nicotinamide (**4b**), white solid, yield 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.57-1.69 (m, 6H, $NCH_2CH_2CH_2CH_2$), 3.21-3.23 (m, 4H, N-CH_2 × 2), 4.05 (t, J = 9.36 Hz, 2H, NCH_2-CH_2O), 4.36 (t, J = 9.36 Hz, 2H, NCH_2-CH_2O), 6.82 (d, J = 5.88 Hz, 1H, *Aromatic H*), 7.13 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.90 (dd, J_1 = 7.96 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.37 (d, J = 5.84 Hz, 1H, *Aromatic H*), 8.64 (s, 1H, *Aromatic H*), 8.91 (dd, J_1 = 8.48 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.71 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 24.0, 25.4 (2 × CH_2), 51.7 (2 × CH_2), 54.8, 66.2, 111.6, 113.5, 120.0, 122.6, 122.8, 129.3, 132.6, 139.8, 151.1, 151.6, 155.7, 164.3, 166.7.

ESI-MS: calcd for $C_{20}H_{23}N_4O_2$ $[M+H]^+$: 351.18, found: 351.21.

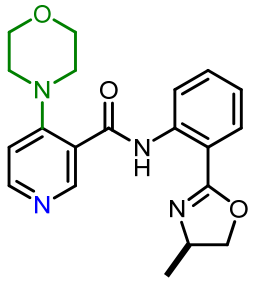


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(pyrrolidin-1-yl)nicotinamide (**4c**), white solid, yield 46%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94-1.97 (m, 4H, $NCH_2CH_2CH_2$), 3.36-3.40 (m, 4H, N-CH_2 × 2), 4.08 (t, J = 9.28 Hz, 2H, NCH_2-CH_2O), 4.38 (t, J = 9.28 Hz, 2H, NCH_2-CH_2O), 6.56 (d, J = 6.12 Hz, 1H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.91 (dd, J_1 = 7.84 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*),

8.23 (d, J = 6.08 Hz, 1H, *Aromatic H*), 8.52 (s, 1H, *Aromatic H*), 8.90 (dd, J_1 = 8.44 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 12.72 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 25.7 (2 × *CH*$_2$), 49.8 (2 × *CH*$_2$), 54.8, 66.3, 108.6, 113.4, 118.8, 119.6, 122.6, 129.3, 132.6, 140.0, 149.7, 150.0, 150.3, 164.6, 167.4.

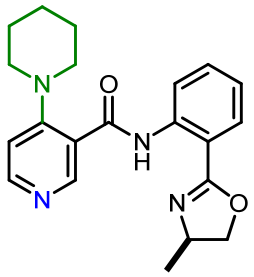
ESI-MS: calcd for $C_{19}H_{21}N_4O_2$ [M+ H]$^+$: 337.17, found: 337.15.



(R)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-morpholinonicotinamide (**4d**), white solid, yield 61%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.26 (d, J = 6.60 Hz, 3H, NCH*CH*$_3$), 3.24-3.27 (m, 4H, N*CH*$_2$ × 2), 3.74-3.77 (m, 4H, O*CH*$_2$ × 2), 3.90 (dd, J_1 = 8.04 Hz, J_2 = 7.98 Hz, 1H), 4.37 (m, 1H), 4.47 (dd, J_1 = 9.36 Hz, J_2 = 8.04 Hz, 1H), 6.80 (d, J = 5.88 Hz, 1H, *Aromatic H*), 7.15 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.92 Hz, J_2 = 1.08 Hz, 1H, *Aromatic H*), 8.44 (d, J = 5.88 Hz, 1H, *Aromatic H*), 8.68 (s, 1H, *Aromatic H*), 8.85 (d, J = 8.40 Hz, 1H, *Aromatic H*), 12.86 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 50.4 (2 × *CH*$_2$), 62.0, 66.3 (2 × *CH*$_2$), 72.7, 111.2, 113.6, 119.8, 120.8, 122.9, 129.4, 132.7, 139.7, 150.8, 151.9, 155.1, 163.2, 166.3.

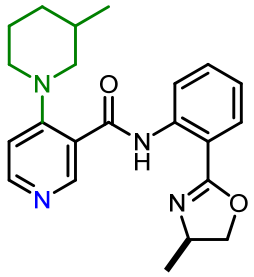
ESI-MS: calcd for $C_{20}H_{23}N_4O_3$ [M+ H]$^+$: 367.18, found: 367.16.



(R)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(piperidin-1-yl)nicotinamide (**4e**), white solid, yield 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.26 (d, J = 6.44 Hz, 3H, NCH*CH₃*), 1.52-1.65 (m, 6H, NCH₂*CH₂ CH₂ CH₂*), 3.19-3.29 (m, 4H, N*CH₂* × 2), 3.87(dd, J_1 = 7.76 Hz, J_2 = 7.76 Hz, 1H), 4.37 (m, 1H), 4.46 (dd, J_1 = 9.36 Hz, J_2 = 7.76 Hz, 1H), 6.79 (d, J = 5.92 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.88 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.36 (d, J = 5.88 Hz, 1H, *Aromatic H*), 8.62 (s, 1H, *Aromatic H*), 8.86 (d, J = 8.40 Hz, 1H, *Aromatic H*), 12.72 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 24.0, 25.4 (2 × *CH₂*), 51.5 (2 × *CH₂*), 62.0, 72.7, 113.3, 113.7, 119.9, 122.6, 129.2, 132.5, 139.8, 140.5, 150.8, 151.4, 155.7, 163.0, 166.7.

ESI-MS: calcd for $C_{21}H_{25}N_4O_2$ $[M+H]^+$: 365.20, found: 365.18.

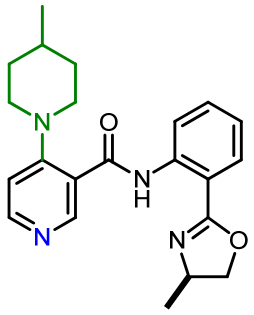


N-(2-((R)-4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(3-methylpiperidin-1-yl)nicotinamide (**4f**), 1:1 dr, white solid, yield 51%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.82 (d, J = 3.10 Hz, 1.5H, NCH₂CH*CH₃*), 0.84 (d, J = 3.10 Hz, 1.5H, NCH₂CH*CH₃*), 1.03

(m,1H), 1.26 (t, J = 6.52 Hz, 3H, NCH*CH*$_3$), 1.55-1.79 (m, 4H), 2.53 (m, 1H), 2.84 (m, 1H), 3.45-3.57 (m, 2H), 3.87 (m, 1H), 4.36 (m, 1H), 4.46 (dd, J_1 = 9.32 Hz, J_2 = 7.84 Hz, 1H), 6.79 (d, J = 5.84 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.36 (d, J = 5.76 Hz, 1H, *Aromatic H*), 8.62 (s, 1H, *Aromatic H*), 8.85 (d, J = 8.40 Hz, 1H, *Aromatic H*), 12.68 and 12.69 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.0 (19.1), 21.4 (21.5), 24.9 (25.0), 30.7, 32.57 (32.62), 50.9 (51.0), 58.2 (58.3), 62.0, 72.7, 111.4, 113.7, 119.9, 122.6, 129.3, 132.6, 139.8, 150.8, 151.4, 155.3, 155.4, 163.0, 166.8.

ESI-MS: calcd for $C_{22}H_{27}N_4O_2$ $[M+H]^+$: 379.21, found: 379.20.



(R)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methylpiperidin-1-yl)nicotinamide (**4g**), 1:1 dr, white solid, yield 58%.

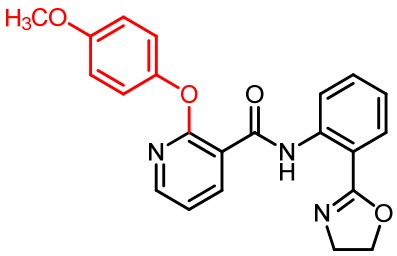
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (d, J = 6.48 Hz, 3H, *CH*$_3$-CH), 1.23-1.31 (m, 2H), 1.27 (d, J = 7.16 Hz, 3H, *CH*$_3$-CH-N), 1.53 (m, 1H), 1.61-1.67 (m, 2H), 2.87-2.96 (m, 2H), 3.54-3.64 (m, 2H), 3.89 (m, 1H), 4.37 (m, 1H), 4.44 (m, 1H), 6.79 (d, J = 5.96 Hz, 1H, *Aromatic H*), 7.13 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.88 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.35 (d, J = 5.72 Hz, 1H, *Aromatic H*),

8.62 (s, 1H, *Aromatic H*), 8.87 (d, *J* = 8.40 Hz, 1H, *Aromatic H*), 12.71 (s, 1H, CO*NH*).

ESI-MS: calcd for $C_{22}H_{27}N_4O_2$ $[M+H]^+$: 379.21, found: 379.20.

Typical Characteristic Data in Etherification

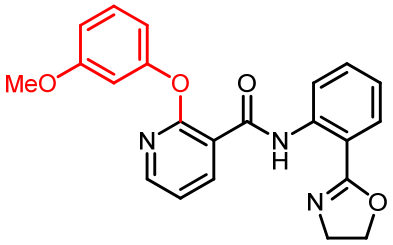
Etherification of Nicotinamide **1a** with 4-methoxyphenol to produce **5a**, **6a** or **7a**



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-morpholinonicotinamide (**5a**), white solid, yield 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.69 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 3.83 (s, 3H, O*CH*$_3$), 4.23 (t, *J* = 9.52 Hz, 2H, NCH_2-*CH*$_2$O), 6.94~7.00 (m, 2H, *Aromatic H*), 7.10~7.19 (m, 4H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.88 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.49 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.94 (d, *J* = 8.44 Hz, 1H, *Aromatic H*), 12.92 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.0, 55.6, 66.0, 114.6 (2 × *CH*), 114.7, 118.6, 119.0, 121.3, 123.0, 123.1 (2 × *CH*), 129.4, 132.2, 139.4, 142.1, 146.6, 150.0, 156.8, 160.4, 163.4, 163.7.

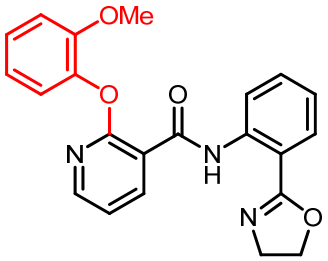
ESI-MS: calcd for $C_{22}H_{20}N_3O_4$ $[M+H]^+$: 390.15, found: 390.20.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(3-methoxyphenoxy)nicotinamide (**5b**), white solid, yield 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.69 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 3.81 (s, 3H, O*CH*$_3$), 4.23 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.78~6.84 (m, 3H, *Aromatic H*), 7.11~7.17 (m, 2H, *Aromatic H*), 7.34 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.84 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.26 (dd, J_1 = 4.84 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.49 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.93 (dd, J_1 = 8.52 Hz, J_2 = 1.08 Hz, 1H, *Aromatic H*), 12.92 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 55.4, 66.0, 108.2, 110.9, 114.4, 114.6, 118.9, 119.3, 121.3, 123.0, 129.4, 129.9, 132.2, 139.4, 142.1, 150.1, 154.4, 160.0, 160.7, 163.3, 163.7.

ESI-MS: calcd for $C_{22}H_{20}N_3O_4$ [M+ H] $^{+}$: 390.15, found: 390.20.

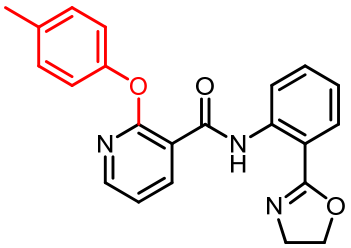


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(2-methoxyphenoxy)nicotinamide (**5c**), white solid, yield 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.61 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 3.72 (s, 3H, O*CH*$_3$), 4.20 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 7.02~7.06 (m, 2H, *Aromatic H*), 7.10~7.14 (m, 2H, *Aromatic H*), 7.23~7.26 (m, 2H, *Aromatic H*), 7.51 (m,

1H, *Aromatic H*), 7.87 (dd, J_1 = 7.88 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.20 (dd, J_1 = 4.80 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.54 (dd, J_1 = 7.60 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.96 (dd, J_1 = 8.56 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.91 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.8, 55.9, 66.0, 112.9, 114.9, 118.2, 118.6, 121.0, 121.6, 122.9, 123.5, 126.4, 129.3, 132.1, 139.5, 142.1, 142.3, 150.0, 151.9, 160.1, 163.4, 163.6.

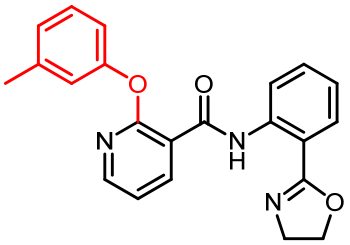
ESI-MS: calcd for $C_{22}H_{20}N_3O_4$ $[M+H]^+$: 390.15, found: 390.20.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(p-tolyloxy)nicotinamide (**5d**), white solid, yield 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H, *CH₃*), 3.67 (t, *J* = 9.48 Hz, 2H, N*CH₂*-CH_2O), 4.22 (t, *J* = 9.48 Hz, 2H, NCH_2-*CH₂*O), 7.09-7.15 (m, 4H, *Aromatic H*), 7.23-7.26 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.84 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.49 (dd, J_1 = 7.56 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.94 (dd, J_1 = 8.56 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.93 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.0, 54.9, 66.0, 114.7, 118.6, 119.1, 121.3, 121.9 (2 × *CH*), 122.9, 129.3, 130.1 (2 × *CH*), 132.2, 134.8, 139.5, 142.0, 150.0, 151.0, 160.3, 163.4, 163.7.

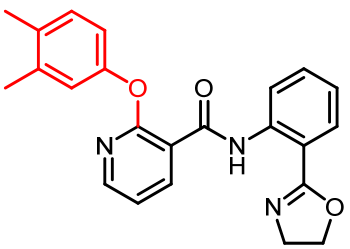
ESI-MS: calcd for $C_{22}H_{20}N_3O_3$ [M+ H] $^+$: 374.15, found: 374.13.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(m-tolyloxy)nicotinamide (**5e**), white solid, yield 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H, *CH*$_3$), 3.65 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 4.22 (t, *J* = 9.52 Hz, 2H, NCH_2-*CH*$_2$O), 7.01-7.08 (m, 3H, *Aromatic H*), 7.10-7.15 (m, 2H, *Aromatic H*), 7.32 (dd, $J_1 = J_2$ = 7.64 Hz, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.88 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.25 (dd, J_1 = 4.80 Hz, J_2 = 2.00Hz, 1H, *Aromatic H*), 8.49 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.93 (dd, J_1 = 8.60 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.91 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 54.9, 66.0, 114.7, 118.8, 119.16, 119.18, 121.3, 122.7, 123.0, 126.0, 129.3, 129.4, 132.2, 139.4, 139.7, 142.1, 150.1, 153.3, 160.2, 163.4, 163.7.

ESI-MS: calcd for $C_{22}H_{20}N_3O_3$ [M+ H] $^+$: 374.15, found: 374.13.

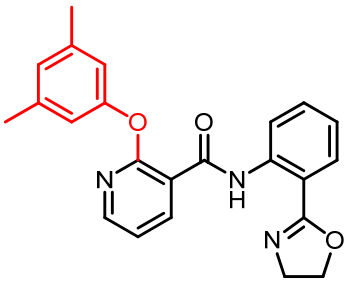


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(3,4-dimethylphenoxy)nicotinamide (**5f**),

white solid, yield 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H, *CH₃*), 2.28 (s, 3H, *CH₃*), 3.70 (t, *J* = 9.60 Hz, 2H, N*CH₂*-CH_2O), 4.22 (t, *J* = 9.60 Hz, 2H, NCH_2-*CH₂*O), 6.96 (dd, J_1 = 8.12 Hz, J_2 = 2.56 Hz, 1H, *Aromatic H*), 7.01 (d, *J* = 2.44 Hz, 1H, *Aromatic H*), 7.09-7.15 (m, 2H, *Aromatic H*), 7.19 (d, *J* = 8.08 Hz, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.88 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.25 (dd, J_1 = 4.84 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.48 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.93 (dd, J_1 = 8.56 Hz, J_2 = 1.08 Hz, 1H, *Aromatic H*), 12.91 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.3, 20.0, 54.9, 66.0, 114.7, 118.5, 119.0, 119.4, 121.3, 122.9, 123.2, 129.3, 130.5, 132.2, 133.4, 138.0, 139.5, 142.0, 150.1, 151.1, 160.5, 163.5, 163.7.

ESI-MS: calcd for $C_{23}H_{22}N_3O_3$ $[M+H]^+$: 388.17, found: 388.14.

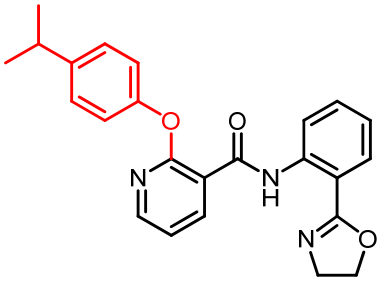


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(3,5-dimethylphenoxy)nicotinamide (**5g**), white solid, yield 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 6H, 2 × *CH₃*), 3.67 (t, *J* = 9.56 Hz, 2H, N*CH₂*-CH_2O), 4.23 (t, *J* = 9.56 Hz, 2H, NCH_2-*CH₂*O), 6.84 (s, 2H, 2 × *Aromatic H*), 6.88 6.84 (s, 1H, *Aromatic H*), 7.10-7.14 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.88 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.26 (dd, J_1 = 4.84 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.48 (dd, J_1 = 7.60 Hz, J_2 = 2.04 Hz, 1H,

Aromatic H), 8.93 (dd, J_1 = 8.52 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.89 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4 (2 × *CH*$_3$), 54.9, 66.0, 114.7, 118.6, 119.1, 119.8 (2 × *CH*), 121.3, 122.9, 127.0, 129.3, 132.2, 139.3 (2 × *C*), 139.4, 142.0, 150.2, 153.3, 160.3, 163.4, 163.7.

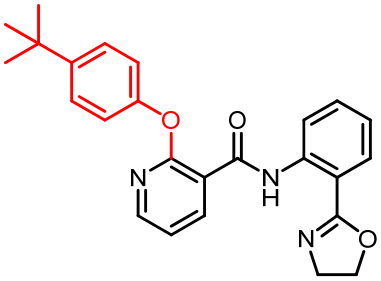
ESI-MS: calcd for $C_{23}H_{22}N_3O_3$ [M+ H]$^+$: 388.17, found: 388.14.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(4-isopropylphenoxy)nicotinamide (**5h**), white solid, yield 52%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.27 (d, *J* = 6.96 Hz, 6H, 2 × *CH*$_3$), 2.95 (q, *J* = 6.96 Hz, 1H, *CH*), 3.65 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.21 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 7.10-7.16 (m, 4H, *Aromatic H*), 7.26-7.30 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.25 (dd, J_1 = 4.92 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.48 (dd, J_1 = 7.52 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.92 (dd, J_1 = 8.56 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 12.91 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 24.1 (2 × *CH*$_3$), 33.6, 54.8, 66.0, 114.7, 118.7, 119.3, 121.3, 121.7 (2 × *CH*), 122.9, 127.5 (2 × *CH*), 129.3, 132.2, 139.4, 142.1, 145.6, 150.0, 151.2, 160.2, 163.4, 163.7.

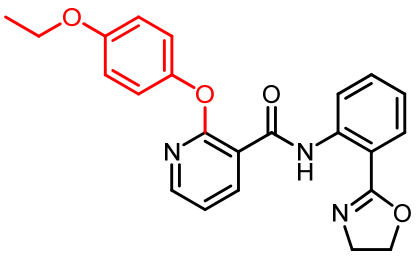
ESI-MS: calcd for $C_{24}H_{24}N_3O_3$ [M+ H]$^+$: 402.18, found: 402.20.



2-(4-(tert-butyl)phenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**5i**), white solid, yield 56%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.34 (s, 9H, 3 × *CH*$_3$), 3.65 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 4.21 (t, *J* = 9.52 Hz, 2H, NCH_2-*CH*$_2$O), 7.10-7.16 (m, 4H, *Aromatic H*), 7.43-7.46 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.80 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.26 (dd, J_1 = 4.84 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.48 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.92 (dd, J_1 = 8.56 Hz, J_2 = 1.20 Hz, 1H, *Aromatic H*), 12.90 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 31.5 (3 × *CH*$_3$), 34.5, 54.8, 66.0, 114.7, 118.7, 119.3, 121.25 (2 × *CH*), 121.29, 122.9, 126.4 (2 × *CH*), 129.3, 132.2, 139.4, 142.0, 147.8, 150.0, 151.0, 160.1, 163.4, 163.7.

ESI-MS: calcd for $C_{25}H_{26}N_3O_3$ $[M+H]^+$: 416.20, found: 416.18.

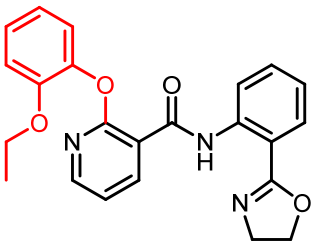


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(4-ethoxyphenoxy)nicotinamide (**5j**), white solid, yield 50%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.43 (t, *J* = 7.0 Hz, 3H, *CH*$_3$), 3.65 (t, *J* = 9.64 Hz, 2H, N*CH*$_2$-CH_2O), 4.04 (q, *J* = 7.0 Hz, 2H, *CH*$_2$-O), 4.22 (t, *J* =

9.64 Hz, 2H, NCH$_2$-*CH$_2$*O), 6.96 (dd, J_1 = 6.72 Hz, J_2 = 2.32 Hz, 2H, 2 × *Aromatic H*), 7.09-7.17 (m, 4H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.84 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.84 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.49 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.94 (dd, J_1 = 8.60 Hz, J_2 = 1.20 Hz, 1H, *Aromatic H*), 12.93 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 55.0, 63.8, 66.0, 114.7, 115.2 (2 × *CH*), 118.6, 118.9, 121.3, 122.95, 123.01 (2 × *CH*), 129.4, 132.2, 139.4, 142.1, 146.5, 150.0, 156.2, 160.5, 163.4, 163.7.

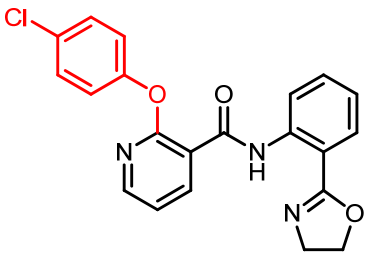
ESI-MS: calcd for $C_{23}H_{22}N_3O_4$ [M+ H] $^+$: 404.16, found: 404.17.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(2-ethoxyphenoxy)nicotinamide (**5k**), white solid, yield 79%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.03 (t, *J* = 6.96 Hz, 3H, *CH$_3$*), 3.59 (t, *J* = 9.52 Hz, 2H, N*CH$_2$*-CH$_2$O), 3.93 (q, *J* = 6.96 Hz, 2H, *CH$_2$*-O), 4.19 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH$_2$*O), 6.98-7.06 (m, 2H, *Aromatic H*), 7.09-7.14 (m, 2H, *Aromatic H*), 7.22 (m, 1H, *Aromatic H*), 7.29 (dd, J_1 = 7.84 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.88 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.20 (dd, J_1 = 4.84 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.55 (dd, J_1 = 7.60 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.96 (dd, J_1 = 8.56 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.91 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 14.6, 54.8, 64.3, 66.0, 114.0, 115.0, 118.2, 118.6, 120.9, 121.6, 122.9, 123.3, 126.2, 129.3, 132.1, 139.5, 142.0, 142.9, 149.9, 151.0, 160.3, 163.48, 163.49.

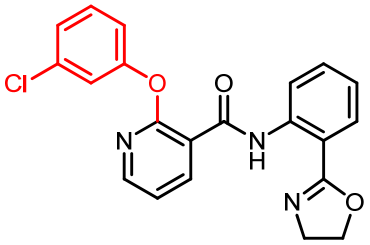
ESI-MS: calcd for $C_{23}H_{22}N_3O_4$ $[M+H]^+$: 404.16, found: 404.17.



2-(4-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**5l**), white solid, yield 50%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (t, J = 9.48 Hz, 2H, N*CH*$_2$-CH_2O), 4.25 (t, J = 9.48 Hz, 2H, NCH_2-*CH*$_2$O), 7.12-7.21 (m, 4H, *Aromatic H*), 7.39-7.43 (m, 2H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.80 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.48 (dd, J_1 = 7.52 Hz, J_2 = 2.04 Hz, 1H, *Aromatic H*), 8.93 (dd, J_1 = 8.48 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.91 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 66.0, 114.5, 119.2, 119.4, 121.2, 123.1, 123.5 (2 × *CH*), 129.4, 129.6 (2 × *CH*), 130.4, 132.3, 139.4, 142.2, 149.9, 151.8, 159.7, 163.2, 163.9.

ESI-MS: calcd for $C_{21}H_{17}ClN_3O_3$ $[M+H]^+$: 394.10, found: 394.11.

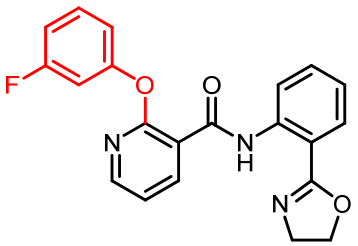


2-(3-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**5m**), white solid, yield 42%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.70 (t, J = 9.60 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.25 (t, J = 9.60 Hz, 2H, NCH$_2$-*CH*$_2$O), 7.11-7.19 (m, 3H, *Aromatic H*), 7.24 (m, 1H, *Aromatic H*), 7.28 (dd, $J_1 = J_2$ = 2.08 Hz, 1H, *Aromatic H*), 7.37 (dd, $J_1 = J_2$ = 8.04 Hz, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 8.36 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.26 (dd, J_1 = 4.84 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.47 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.92 (dd, J_1 = 8.56 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.89 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 66.0, 114.5, 119.3, 119.6, 120.5, 121.2, 122.8, 123.0, 125.3, 129.4, 130.3, 132.3, 134.7, 139.4, 142.1, 149.9, 154.0, 159.5, 163.1, 163.9.

ESI-MS: calcd for $C_{21}H_{17}ClN_3O_3$ $[M+H]^+$: 394.10, found: 394.11.

The structure of compound **5m** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1867348.

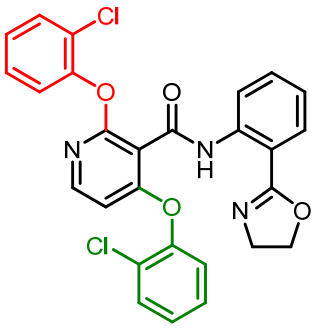


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-(3-fluorophenoxy)nicotinamide (**5n**), white solid, yield 45%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71 (t, J = 9.56 Hz, 2H, N*CH*$_2$-CH$_2$O),

4.25 (t, J = 9.56 Hz, 2H, NCH$_2$-*CH$_2$*O), 6.95-7.05 (m, 3H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.18 (dd, J_1 = 7.60 Hz, J_2 = 4.80 Hz, 1H, *Aromatic H*), 7.39 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.88 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.26 (dd, J_1 = 4.80 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.48 (dd, J_1 = 7.56 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.92 (dd, J_1 = 8.56 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 12.90 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, CDCl$_3$) δ 54.8, 66.0, 110.1 (d, J_{CF} = 23.84 Hz), 112.1 (d, J_{CF} = 20.78 Hz), 114.5, 117.8 (d, J_{CF} = 3.47 Hz), 119.4, 119.6, 121.2, 123.1, 129.4, 130.2 (d, J_{CF} = 9.42 Hz), 132.3, 139.4, 142.1, 149.9, 154.4 (d, J_{CF} = 10.79 Hz), 159.4, 162.9 (d, J_{CF} = 248.27 Hz), 163.2, 163.9.

ESI-MS: calcd for $C_{21}H_{17}FN_3O_3$ $[M+H]^+$: 378.13, found: 378.15.

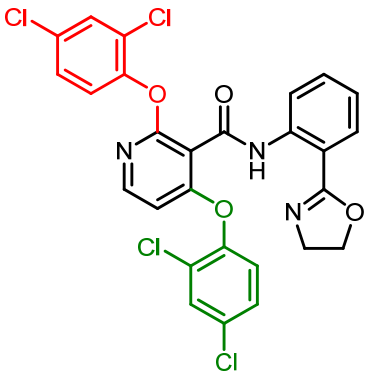


2,4-bis(2-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**7o**), white solid, yield 55%. ^{1}H NMR (400 MHz, CDCl$_3$) δ 4.04 (t, J = 9.40 Hz, 2H, N*CH$_2$*-CH$_2$O), 4.35 (t, J = 9.40 Hz, 2H, NCH$_2$-*CH$_2$*O), 6.27 (d, J = 5.88 Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.14-7.23 (m, 2H, *Aromatic H*), 7.26~7.34 (m, 4H, *Aromatic H*), 7.40~7.47 (m, 2H, *Aromatic H*), 7.50 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 7.95 (d, J = 5.92 Hz, 1H, *Aromatic H*), 9.02 (d, J = 8.40

Hz, 1H, *Aromatic H*), 12.86 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 66.1, 106.2, 111.2, 113.6, 120.3, 122.8, 123.5, 124.3, 126.4, 127.1, 127.3, 127.5, 127.8, 128.4, 129.2, 130.4, 131.0, 132.6, 139.8, 148.7, 149.6, 149.7, 160.9, 161.7, 163.3, 164.3.

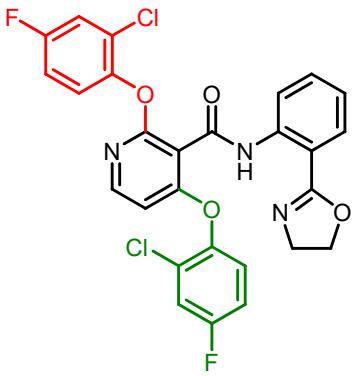
ESI-MS: calcd for $C_{27}H_{20}Cl_2N_3O_4$ $[M+H]^+$: 520.08, found: 520.11.



2,4-bis(2,4-dichlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**7p**), white solid, yield 53%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.02 (t, J = 9.44 Hz, 2H, N*CH*$_2$-CH_2O), 4.36 (t, J = 9.44 Hz, 2H, NCH_2-*CH*$_2$O), 6.29 (d, J = 5.80 Hz, 1H, *Aromatic H*), 7.13 (m, 1H, *Aromatic H*), 7.19-7.23 (m, 2H, *Aromatic H*), 7.27~7.32 (m, 2H, *Aromatic H*), 7.44 (d, J = 2.36 Hz, 1H, *Aromatic H*), 7.47 (d, J = 2.44 Hz, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.60 Hz, 1H, *Aromatic H*), 7.97 (d, J = 5.92 Hz, 1H, *Aromatic H*), 8.98 (d, J = 8.44 Hz, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

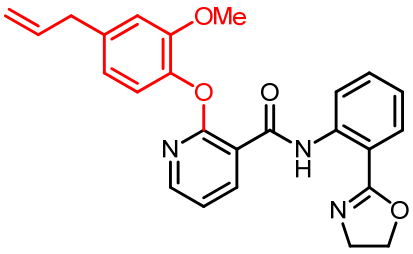
^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 66.1, 106.4, 111.3, 113.5, 120.2, 123.0, 124.2, 125.1, 128.0, 128.1, 128.4, 128.6, 129.2, 130.2, 130.8, 131.2, 132.0, 132.6, 139.6, 148.3, 148.5, 148.8, 160.7, 161.2, 163.1, 164.5.

ESI-MS: calcd for $C_{27}H_{18}Cl_4N_3O_4$ $[M+H]^+$: 590.00, found: 590.04.



2,4-bis(2-chloro-4-fluorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**7q**), white solid, yield 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.03 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.36 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.99-7.06 (m, 2H, *Aromatic H*), 7.13 (m, 1H, *Aromatic H*), 7.18 (dd, J_1 = 8.04 Hz, J_2 = 3.0 Hz, 1H, *Aromatic H*), 7.22 (dd, J_1 = 7.92 Hz, J_2 = 3.08 Hz, 1H, *Aromatic H*), 7.23-7.28 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.88 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 7.96 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 9.01 (d, *J* = 8.44 Hz, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

ESI-MS: calcd for $C_{27}H_{18}Cl_2F_2N_3O_4$ $[M+H]^+$: 556.06, found: 556.09.

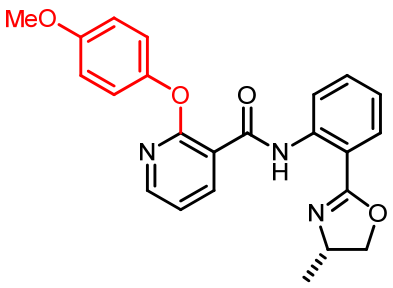


2-(4-allyl-2-methoxyphenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**5r**), white solid, yield 43%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.43 (d, *J* = 6.76 Hz, 2H, Ph*CH*$_2$), 3.66 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH$_2$O), 3.71 (s, 3H, O*CH*$_3$), 4.22 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 5.08-5.16 (m, 2H), 6.01 (m, 1H), 6.85-6.87 (m, 2H, *Aromatic*

H), 7.08-7.19 (m, 3H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.21 (dd, J_1 = 4.80 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.53 (dd, J_1 = 7.60 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.95 (dd, J_1 = 8.56 Hz, J_2 = 1.08 Hz, 1H, *Aromatic H*), 12.90 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 40.2, 54.9, 55.9, 66.0, 113.2, 114.9, 116.1, 118.2, 118.5, 120.9, 121.6, 122.9, 123.1, 129.3, 132.1, 137.2, 138.4, 139.5, 140.4, 142.1, 150.1, 151.6, 160.2, 163.5, 163.6.

ESI-MS: calcd for $C_{25}H_{24}N_3O_4$ $[M+H]^+$: 430.18, found: 430.16.

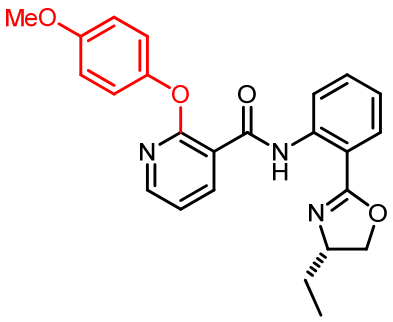


(S)-2-(4-methoxyphenoxy)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl) nicotinamide (**5s**), white solid, yield 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08 (d, J = 6.6 Hz, 3H, NCH-*CH*$_3$), 3.82 (m, 1H), 3.83 (s, 3H, O-*CH*$_3$), 4.06 (m, 1H), 4.31 (dd, J_1 = 9.24 Hz, J_2 = 8.00 Hz, 1H), 6.93-6.97 (m, 2H, *Aromatic H*), 7.09-7.17 (m, 4H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.84 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.88 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.43 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.87 (dd, J_1 = 8.48 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 12.75 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 55.6, 62.1, 72.6, 114.6 (2 × *CH*), 114.9, 118.5, 119.3, 121.4, 122.99 (2 × *CH*), 123.02, 129.3, 132.2, 139.3, 141.7, 146.6, 149.9, 156.8,

160.5, 162.6, 163.5.

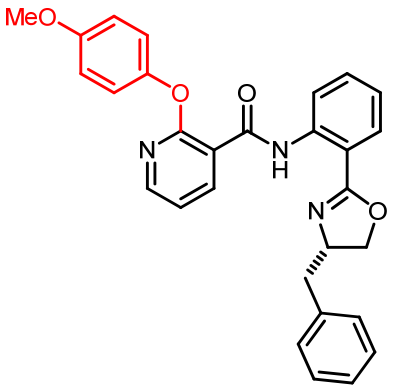
ESI-MS: calcd for $C_{23}H_{22}N_3O_4$ $[M+H]^+$: 404.16, found: 404.14.



(S)-N-(2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(4-methoxyphenoxy)nicotinamide (**5t**), white solid, yield 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.78 (t, J = 7.40 Hz, 3H, CH_2-*CH_3*), 1.36-1.51 (m, 2H, *CH_2*-CH_3), 3.82 (s, 3H, O-*CH_3*), 3.91-4.00 (m, 2H), 4.30 (m, 1H), 6.92-6.97 (m, 2H, *Aromatic H*), 7.08-7.17 (m, 4H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.80 Hz, J_2 = 1.96 Hz, 1H, *Aromatic H*), 8.37 (dd, J_1 = 7.56 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.87 (dd, J_1 = 8.44 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 10.0, 28.6, 55.6, 68.0, 70.8, 114.5 (2 × *CH*), 114.7, 118.4, 119.7, 121.2, 122.89 (2 × *CH*), 122.99, 129.3, 132.2, 139.4, 141.2, 146.7, 149.8, 156.8, 160.4, 162.7, 163.7.

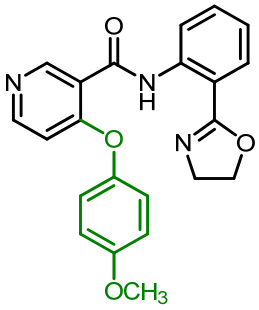
ESI-MS: calcd for $C_{24}H_{24}N_3O_4$ $[M+H]^+$: 418.18, found: 418.21.



(S)-N-(2-(4-benzyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(4-methoxyphenoxy) nicotinamide (**5u**), white solid, yield 52%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (dd, J_1 = 13.52 Hz, J_2 = 7.28 Hz, 1H, Ph-*CH*), 2.79 (dd, J_1 = 13.52 Hz, J_2 = 6.32 Hz, 1H, Ph-*CH*), 3.78 (s, 3H, O-CH_3), 4.01 (dd, J_1 = 8.08 Hz, J_2 = 6.04 Hz, 1H), 4.17 (dd, J_1 = 9.16 Hz, J_2 = 8.08 Hz, 1H), 4.24 (m, 1H), 6.88-6.94 (m, 4H, *Aromatic H*), 7.03-7.14 (m, 7H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.24 (dd, J_1 = 4.84 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.43 (dd, J_1 = 7.52 Hz, J_2 = 2.00 Hz, 1H, *Aromatic H*), 8.90 (dd, J_1 = 8.52 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 12.76 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 42.1, 55.5, 67.9, 70.5, 114.5 (2 × *CH*), 114.6, 118.6, 119.2, 121.3, 122.9 (2 × *CH*), 123.0, 126.6, 128.3 (2 × *CH*), 129.2 (2 × *CH*), 129.4, 132.4, 137.7, 139.5, 141.7, 146.5, 149.9, 156.7, 160.4, 163.1, 163.6.

ESI-MS: calcd for $C_{29}H_{26}N_3O_4$ $[M+H]^+$: 480.19, found: 480.20.

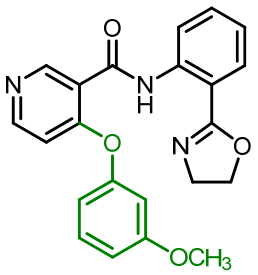


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methoxyphenoxy)nicotinamide (**6a**), white solid, yield 56%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (t, *J* = 9.72 Hz, 2H, N*CH*$_2$-CH$_2$O), 3.85 (s, 3H, O*CH*$_3$), 4.26 (t, *J* = 9.72 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.62 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 6.96~7.01 (m, 2H, *Aromatic H*), 7.10~7.16 (m, 3H, *Aromatic H*), 7.52 (dd, J_1 = 8.04 Hz, J_2 = 7.84 Hz, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.64 Hz, J_2 = 5.84 Hz, 1H, *Aromatic H*), 8.45 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 8.96 (d, *J* = 8.48 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.0, 55.7, 66.0, 109.7, 114.3, 115.2 (2 × *CH*), 120.9, 121.0, 122.5 (2 × *CH*), 122.9, 129.4, 132.4, 139.5, 146.6, 153.1, 153.4, 157.5, 162.9, 163.0, 164.0.

ESI-MS: calcd for $C_{22}H_{20}N_3O_4$ [M+ H] $^{+}$: 390.15, found: 390.20; calcd for $C_{22}H_{19}N_3NaO_4$ [M+ Na] $^{+}$: 412.13, found: 412.24.

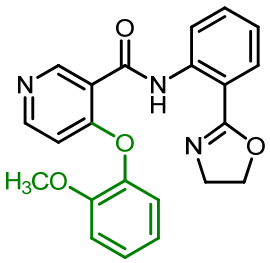
The structure of compound **6a** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1864262.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(3-methoxyphenoxy)nicotinamide (**6b**), white solid, yield 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (t, *J* = 8.96 Hz, 2H, N*CH*$_2$-CH_2O), 3.82 (s, 3H, O*CH*$_3$), 4.26 (t, *J* = 8.96 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.68-6.76 (m, 2H, *Aromatic H*), 6.77-6.88 (m, 2H, *Aromatic H*), 7.13 (m, 1H, *Aromatic H*), 7.37 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.88 Hz, J_2 = 1.76 Hz, 1H, *Aromatic H*), 8.45 (d, *J* = 9.40 Hz, 1H, *Aromatic H*), 8.95 (d, *J* = 8.52 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 55.6, 66.0, 107.5, 110.3, 111.6, 113.4, 114.2, 120.9, 121.3, 123.0, 129.3, 130.7, 132.4, 139.5, 153.1, 153.4, 154.5, 161.3, 162.2, 162.9, 164.0.

ESI-MS: calcd for $C_{22}H_{20}N_3O_4$ $[M+H]^+$: 390.15, found: 390.20.

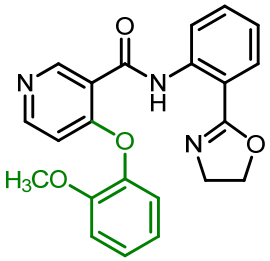


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(2-methoxyphenoxy)nicotinamide (**6c**), white solid, yield 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 3.76 (s, 3H, O*CH*$_3$), 4.24 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.52 (d, *J* = 5.80

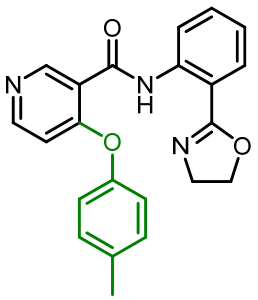
Hz, 1H, *Aromatic H*), 7.01-7.07 (m, 2H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.22 (dd, J_1 = 7.68 Hz, J_2 = 1.60 Hz, 1H, *Aromatic H*), 7.29 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.42 (d, J = 5.84 Hz, 1H, *Aromatic H*), 8.97 (dd, J_1 = 8.52 Hz, J_2 = 1.2 Hz, 1H, *Aromatic H*), 9.19 (s, 1H, *Aromatic H*), 12.82 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.8, 55.8, 66.0, 109.4, 113.0, 114.4, 120.2, 121.25, 121.33, 122.9, 123.2, 127.3, 129.3, 132.3, 139.6, 141.5, 151.6, 152.9, 153.4, 162.4, 163.1, 163.9.

ESI-MS: calcd for $C_{22}H_{20}N_3O_4$ $[M+H]^+$: 390.15, found: 390.20.



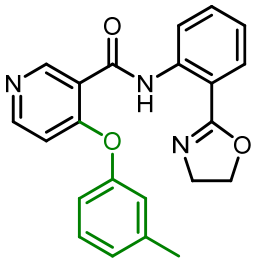
N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(2-methoxyphenoxy)nicotinamide (**6c**), white solid, yield 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (t, J = 9.52 Hz, 2H, N*CH*$_2$-CH$_2$O), 3.76 (s, 3H, O*CH*$_3$), 4.24 (t, J = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.52 (d, J = 5.80 Hz, 1H, *Aromatic H*), 7.01-7.07 (m, 2H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.22 (dd, J_1 = 7.68 Hz, J_2 = 1.60 Hz, 1H, *Aromatic H*), 7.29 (m, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.42 (d, J = 5.84 Hz, 1H, *Aromatic H*), 8.97 (dd, J_1 = 8.52 Hz, J_2 = 1.2 Hz, 1H, *Aromatic H*), 9.19 (s, 1H, *Aromatic H*), 12.82 (s, 1H, CO*NH*).



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(p-tolyloxy)nicotinamide (**6d**), white solid, yield 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (s, 3H, *CH_3*), 3.76 (t, *J* = 9.48 Hz, 2H, N*CH_2*-CH_2O), 4.25 (t, *J* = 9.48 Hz, 2H, NCH_2-*CH_2*O), 6.64 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 7.06-7.10 (m, 2H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.24-7.28 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.42 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 8.95 (dd, J_1 = 8.56 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 54.9, 66.0, 110.0, 114.3, 121.0, 121.1, 121.3 (2 × *CH*), 122.9, 129.3, 130.8 (2 × *CH*), 132.4, 135.8, 139.5, 151.1, 153.0, 153.4, 162.6, 163.0, 164.0.

ESI-MS: calcd for $C_{22}H_{20}N_3O_3$ $[M+H]^+$: 374.15, found: 374.13.

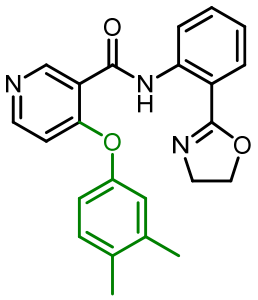


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(m-tolyloxy)nicotinamide (**6e**), white solid, yield 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (s, 3H, *CH_3*), 3.75 (t, *J* = 9.60 Hz, 2H, N*CH_2*-CH_2O), 4.25 (t, *J* = 9.60 Hz, 2H, NCH_2-*CH_2*O), 6.67 (d, *J* = 5.80 Hz, 1H,

Aromatic H), 6.98-7.01 (m, 2H, *Aromatic H*), 7.10-7.14 (m, 2H, *Aromatic H*), 7.35 (dd, $J_1 = J_2 = 7.68$ Hz, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, $J_1 = 7.92$ Hz, $J_2 = 1.64$ Hz, 1H, *Aromatic H*), 8.46 (d, $J = 5.92$ Hz, 1H, *Aromatic H*), 8.95 (dd, $J_1 = 8.52$ Hz, $J_2 = 1.12$ Hz, 1H, *Aromatic H*), 9.16 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 54.9, 66.0, 110.2, 114.3, 118.4, 121.0, 121.2, 122.0, 123.0, 126.8, 129.3, 130.0, 132.4, 139.5, 140.7, 153.0, 153.37, 153.40, 162.4, 163.0, 164.0.

ESI-MS: calcd for $C_{22}H_{20}N_3O_3$ $[M+H]^+$: 374.15, found: 374.13.

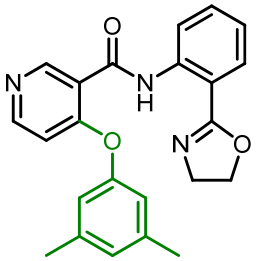


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(3,4-dimethylphenoxy)nicotinamide (**6f**), white solid, yield 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.29 (s, 3H, *CH*$_3$), 2.30 (s, 3H, *CH*$_3$), 3.77 (t, $J = 9.52$ Hz, 2H, N*CH*$_2$-CH$_2$O), 4.25 (t, $J = 9.52$ Hz, 2H, NCH$_2$-*CH*$_2$O), 6.65 (d, $J = 5.80$ Hz, 1H, *Aromatic H*), 6.92 (dd, $J_1 = 8.12$ Hz, $J_2 = 2.56$ Hz, 1H, *Aromatic H*), 6.97 (d, $J = 2.52$ Hz, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.20 (d, $J = 8.12$ Hz, 1H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, $J_1 = 7.84$ Hz, $J_2 = 1.68$ Hz, 1H, *Aromatic H*), 8.44 (d, $J = 5.88$ Hz, 1H, *Aromatic H*), 8.95 (dd, $J_1 = 8.52$ Hz, $J_2 = 1.2$ Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.3, 20.0, 54.9, 66.0, 110.1, 114.3, 118.6, 121.0, 121.1, 122.4, 122.9, 129.3, 131.1, 132.3, 134.4, 138.9, 139.5, 151.2, 153.0, 153.4, 162.7,

163.1, 164.0.

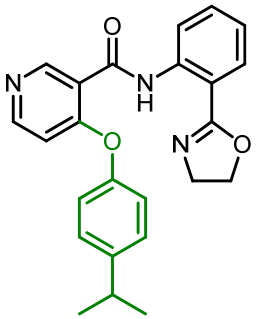
ESI-MS: calcd for $C_{23}H_{22}N_3O_3$ $[M+H]^+$: 388.17, found: 388.14.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(3,5-dimethylphenoxy)nicotinamide (**6g**), white solid, yield 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 6H, 2 × *CH*$_3$), 3.76 (t, *J* = 9.56 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.26 (t, *J* = 9.56 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.67 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 6.81 (s, 2H, *Aromatic H*), 6.93 (s, 1H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.46 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 8.95 (dd, J_1 = 8.52 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.81 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3(2 × *CH*$_3$), 54.9, 66.0, 110.3, 114.3, 119.0 (2 × *CH*), 121.1, 122.9, 127.6, 129.3, 132.4, 139.5, 140.2 (2 × *C*), 153.0, 153.3, 153.4, 162.5, 163.0, 164.0.

ESI-MS: calcd for $C_{23}H_{22}N_3O_3$ $[M+H]^+$: 388.17, found: 388.14.

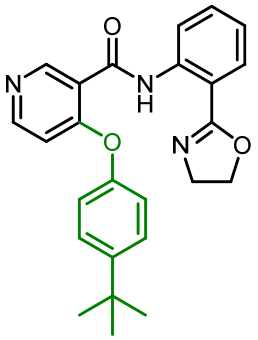


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(4-isopropylphenoxy)nicotinamide (**6h**),

white solid, yield 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (d, *J* = 6.92 Hz, 6H, 2 × *CH₃*), 2.95 (q, *J* = 6.92 Hz, 1H, *CH*), 3.75 (t, *J* = 9.48 Hz, 2H, N*CH₂*-CH_2O), 4.24 (t, *J* = 9.48 Hz, 2H, NCH_2-*CH₂*O), 6.67 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 7.08-7.15 (m, 3H, *Aromatic H*), 7.28-7.33 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.46 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 8.95 (dd, J_1 = 8.56 Hz, J_2 = 1.20 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.82 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 24.1 (2 × *CH₃*), 33.7, 54.9, 66.0, 110.1, 114.3, 121.0, 121.2 (2 × *CH*), 122.9, 128.1 (2 × *CH*), 129.3, 132.4, 139.5, 146.8, 151.2, 153.1, 153.4, 162.5, 163.1, 164.0.

ESI-MS: calcd for $C_{24}H_{24}N_3O_3$ $[M+H]^+$: 402.18, found: 402.20.

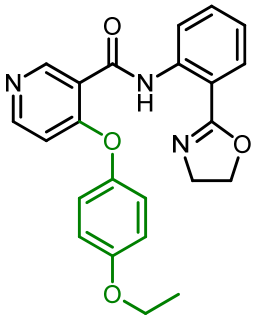


4-(4-(tert-butyl)phenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6i**), white solid, yield 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.35 (s, 9H, 3 × *CH₃*), 3.76 (t, *J* = 9.44 Hz, 2H, N*CH₂*-CH_2O), 4.25 (t, *J* = 9.44 Hz, 2H, NCH_2-*CH₂*O), 6.68 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 7.08-7.15 (m, 3H, *Aromatic H*), 7.44-7.49 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.46 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 8.95 (dd, J_1 = 8.52 Hz, J_2 = 1.20 Hz, 1H, *Aromatic*

H), 9.15 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 31.5 (3 × *CH_3*), 34.6, 54.8, 66.0, 110.2, 114.2, 120.8 (2 × *CH*), 121.0, 121.2, 122.9, 127.1 (2 × *CH*), 129.3, 132.4, 139.5, 149.1, 151.0, 153.1, 153.4, 162.5, 163.0, 164.0.

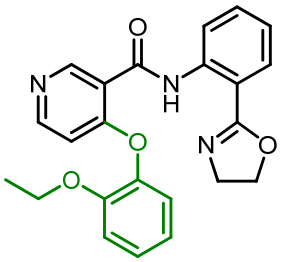
ESI-MS: calcd for $C_{25}H_{26}N_3O_3$ [M+ H] $^+$: 416.20, found: 416.18.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(4-ethoxyphenoxy)nicotinamide (**6j**), white solid, yield 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.45 (t, *J* = 6.96 Hz, 3H, *CH_3*), 3.77 (t, *J* = 9.48 Hz, 2H, N*CH_2*-CH_2O), 4.06 (q, *J* = 6.96 Hz, 2H, *CH_2*-O), 4.26 (t, *J* = 9.48 Hz, 2H, NCH_2-*CH_2*O), 6.63 (d, *J* = 5.84 Hz, 1H, *Aromatic H*), 6.96-6.99 (m, 2H, *Aromatic H*), 7.08-7.15 (m, 3H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.84 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.45 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 8.96 (dd, J_1 = 8.52 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 14.8, 55.0, 64.0, 66.0, 109.8, 114.3, 115.8 (2 × *CH*), 120.8, 121.0, 122.5 (2 × *CH*), 123.0, 129.4, 132.4, 139.5, 146.5, 153.1, 153.4, 156.9, 162.93, 163.03, 164.0.

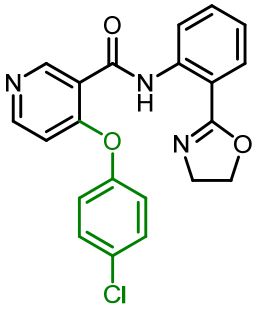
ESI-MS: calcd for $C_{23}H_{22}N_3O_4$ [M+ H] $^+$: 404.16, found: 404.17.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(2-ethoxyphenoxy)nicotinamide (**6k**), white solid, yield 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16 (t, *J* = 6.96 Hz, 3H, *CH₃*), 3.69 (t, *J* = 9.48 Hz, 2H, N*CH₂*-CH_2O), 3.99 (q, *J* = 6.96 Hz, 2H, *CH₂*-O), 4.23 (t, *J* = 9.48 Hz, 2H, NCH_2-*CH₂*O), 6.56 (d, *J* = 5.76 Hz, 1H, *Aromatic H*), 7.01-7.05 (m, 2H, *Aromatic H*), 7.12 (m, 1H, *Aromatic H*), 7.23-7.28 (m, 2H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.56 Hz, 1H, *Aromatic H*), 8.42 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 8.97 (dd, J_1 = 8.56 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 9.20 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 14.6, 54.8, 64.4, 66.0, 109.7, 114.1, 114.5, 120.2, 121.2, 121.3, 122.9, 123.2, 127.2, 129.3, 132.2, 139.6, 141.9, 150.8, 152.7, 153.3, 162.5, 163.1, 163.8.

ESI-MS: calcd for $C_{23}H_{22}N_3O_4$ $[M+H]^+$: 404.16, found: 404.17.

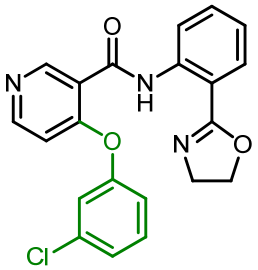


4-(4-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6l**), white solid, yield 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (t, *J* = 9.52 Hz, 2H, N*CH₂*-CH_2O),

4.28 (t, J = 9.52 Hz, 2H, NCH$_2$-*CH$_2$*O), 6.66 (d, J = 5.80 Hz, 1H, *Aromatic H*), 7.12-7.17 (m, 3H, *Aromatic H*), 7.41-7.47 (m, 2H, *Aromatic H*), 7.52 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.96 Hz, J_2 = 1.60 Hz, 1H, *Aromatic H*), 8.50 (d, J = 5.80 Hz, 1H, *Aromatic H*), 8.94 (d, J = 8.48 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, CDCl$_3$) δ 54.9, 66.0, 110.2, 114.1, 120.9, 121.6, 122.7 (2 × *CH*), 123.1, 129.4, 130.4 (2 × *CH*), 131.4, 132.5, 139.4, 152.1, 153.2, 153.4, 161.9, 162.8, 164.2.

ESI-MS: calcd for C$_{21}$H$_{17}$ClN$_3$O$_3$ [M+ H] $^+$: 394.10, found: 394.11.

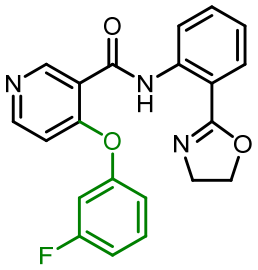


4-(3-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6m**), white solid, yield 67%. ^{1}H NMR (400 MHz, CDCl$_3$) δ 3.80 (t, J = 9.52 Hz, 2H, N*CH$_2$*-CH$_2$O), 4.29 (t, J = 9.52 Hz, 2H, NCH$_2$-*CH$_2$*O), 6.70 (d, J = 5.72 Hz, 1H, *Aromatic H*), 7.09-7.16 (m, 2H, *Aromatic H*), 7.24 (dd, J_1 = J_2 = 2.20 Hz, 1H, *Aromatic H*), 7.29 (m, 1H, *Aromatic H*), 7.41 (dd, J_1 = J_2 = 8.08 Hz, 1H, *Aromatic H*), 7. 52 (m, 1H, *Aromatic H*), 7.88 (dd, J_1 = 7.92 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.52 (d, J = 5.80 Hz, 1H, *Aromatic H*), 8.93 (d, J = 8.36 Hz, 1H, *Aromatic H*), 9.15 (s, 1H, *Aromatic H*), 12.82 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, CDCl$_3$) δ 54.9, 66.0, 110.4, 114.1, 119.6, 120.8, 121.7, 121.9,

123.1, 126.2, 129.4, 131.1, 132.5, 135.6, 139.4, 153.2, 153.4, 154.2, 161.6, 162.7, 164.2.

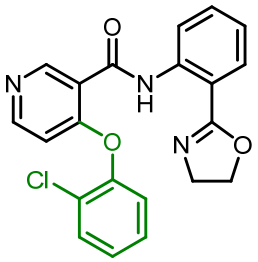
ESI-MS: calcd for $C_{21}H_{17}ClN_3O_3$ $[M+H]^+$: 394.10, found: 394.11.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(3-fluorophenoxy)nicotinamide (**6n**), white solid, yield 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 4.29 (t, *J* = 9.52 Hz, 2H, NCH_2-*CH*$_2$O), 6.72 (d, *J* = 5.76 Hz, 1H, *Aromatic H*), 6.95 (m, 1H, *Aromatic H*), 6.98-7.06 (m, 2H, *Aromatic H*), 7.14 (dd, J_1 = J_2 = 7.64 Hz, 1H, *Aromatic H*), 7.44 (m, 1H, *Aromatic H*), 7. 52 (m, 1H, *Aromatic H*), 7.89 (dd, J_1 = 7.84 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.52 (d, *J* = 5.96 Hz, 1H, *Aromatic H*), 8.93 (d, *J* = 8.20 Hz, 1H, *Aromatic H*), 9.14 (s, 1H, *Aromatic H*), 12.83 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.8, 66.0, 109.3 (d, J_{CF} = 23.95 Hz), 110.5, 113.0 (d, J_{CF} = 20.91 Hz), 114.1, 117.0, 120.8, 121.8, 123.1, 129.4, 131.2 (d, J_{CF} = 9.43 Hz), 132.5, 139.4, 153.2, 153.3, 154.6 (d, J_{CF} = 10.61 Hz), 161.5, 162.74, 163.5 (d, J_{CF} = 247.59 Hz), 164.2.

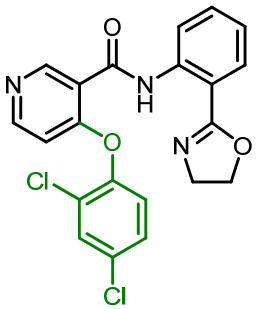
ESI-MS: calcd for $C_{21}H_{17}FN_3O_3$ $[M+H]^+$: 378.13, found: 378.15.



4-(2-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6o**), white solid, yield 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (t, *J* = 9.56 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.26 (t, *J* = 9.56 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.50 (d, *J* = 5.76 Hz, 1H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.28-7.32 (m, 2H, *Aromatic H*), 7.40 (m, 1H, *Aromatic H*), 7.49-7.57 (m, 2H, *Aromatic H*), 7.89 (dd, J_1 = 7.84 Hz, J_2 = 1.60 Hz, 1H, *Aromatic H*), 8.49 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 8.96 (dd, J_1 = 8.48 Hz, J_2 = 1.12 Hz, 1H, *Aromatic H*), 9.21 (s, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.8, 66.0, 109.5, 114.4, 120.7, 121.1, 123.0, 123.7, 127.4 (2), 128.6, 129.4, 131.3, 132.3, 139.5, 149.1, 153.2, 153.5, 161.3, 162.7, 164.0.

ESI-MS: calcd for $C_{21}H_{17}ClN_3O_3$ $[M+H]^+$: 394.10, found: 394.11.

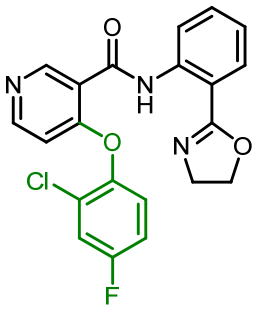


4-(2,4-dichlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6p**), white solid, yield 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (t, *J* = 9.48 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.30 (t, *J* = 9.48 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.51 (d, *J* = 5.76 Hz, 1H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.24 (d, *J* = 8.64 Hz, 1H, *Aromatic H*), 7.37 (dd, J_1 = 8.68

Hz, J_2 = 2.44 Hz, 1H, *Aromatic H*), 7.49-7.56 (m, 2H, *Aromatic H*), 7.89 (dd, J_1 = 7.88 Hz, J_2 = 1.52 Hz, 1H, *Aromatic H*), 8.51 (d, *J* = 5.92 Hz, 1H, *Aromatic H*), 8.95 (d, *J* = 8.48 Hz, 1H, *Aromatic H*), 9.18 (s, 1H, *Aromatic H*), 12.81 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.8, 66.0, 109.5, 114.2, 121.0, 121.1, 123.1, 124.4, 128.4, 128.8, 129.4, 131.0, 132.3, 132.4, 139.4, 148.0, 153.3, 153.4, 160.9, 162.6, 164.1.

ESI-MS: calcd for $C_{21}H_{16}Cl_2N_3O_3$ $[M+H]^+$: 428.06, found: 428.04.

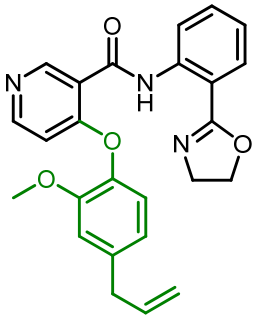


4-(2-chloro-4-fluorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6q**), white solid, yield 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (t, *J* = 9.48 Hz, 2H, N*CH*$_2$-CH_2O), 4.29 (t, *J* = 9.48 Hz, 2H, NCH_2-*CH*$_2$O), 6.49 (d, *J* = 5.76 Hz, 1H, *Aromatic H*), 7.09-7.17 (m, 2H, *Aromatic H*), 7.27-7.31 (m, 2H, *Aromatic H*), 7.53 (m, 1H, *Aromatic H*), 7.90 (dd, J_1 = 7.92 Hz, J_2 = 1.60 Hz, 1H, *Aromatic H*), 8.50 (d, *J* = 5.76 Hz, 1H, *Aromatic H*), 8.96 (d, *J* = 8.36 Hz, 1H, *Aromatic H*), 9.19 (s, 1H, *Aromatic H*), 12.81 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 66.0, 109.3, 114.3, 115.6 (d, J_{CF} = 22.87 Hz), 118.4 (d, J_{CF} = 26.0 Hz), 121.1, 123.1, 124.5 (d, J_{CF} = 8.97 Hz), 128.4 (d, J_{CF} = 10.78 Hz), 129.4, 132.4, 139.4, 145.5 (d, J_{CF} = 3.6 Hz), 153.3, 160.1(d, J_{CF} = 247.92 Hz), 161.2, 162.7, 164.1.

ESI-MS: calcd for $C_{21}H_{16}ClFN_3O_3$ $[M+H]^+$: 412.09, found: 412.06.

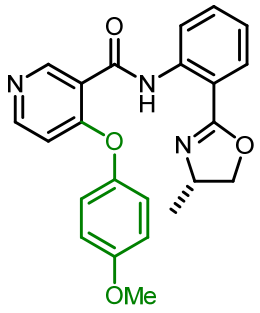
The structure of compound **6q** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1867347.



4-(4-allyl-2-methoxyphenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6r**), white solid, yield 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.43 (d, *J* = 6.68 Hz, 2H, Ph*CH*$_2$), 3.75 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH$_2$O), 3.75 (s, 3H, O*CH*$_3$), 4.25 (t, *J* = 9.52 Hz, 2H, NCH$_2$-*CH*$_2$O), 5.11-5.16 (m, 2H), 5.99 (m, 1H), 6.52 (d, *J* = 5.80 Hz, 1H, *Aromatic H*), 6.83-6.88 (m, 2H, *Aromatic H*), 7.09-7.15 (m, 2H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.42 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 8.97 (dd, J_1 = 8.52 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 9.18 (s, 1H, *Aromatic H*), 12.81 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 40.1, 54.9, 55.8, 66.0, 109.4, 113.2, 114.4, 116.4, 120.1, 121.2, 121.3, 122.85, 122.93, 129.3, 132.3, 136.9, 139.6 (2), 139.7, 151.4, 152.9, 153.3, 162.5, 163.1, 163.9.

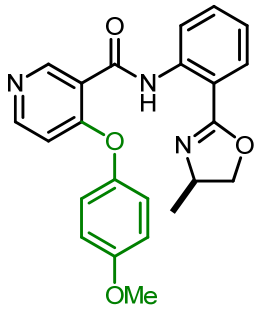
ESI-MS: calcd for $C_{25}H_{24}N_3O_4$ $[M+H]^+$: 430.18, found: 430.16.



(S)-4-(4-methoxyphenoxy)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl) nicotinamide (**6s**), white solid, yield 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16 (d, J = 6.6 Hz, 3H, NCH-*CH*$_3$), 3.83 (s, 3H, O-*CH*$_3$), 3.87 (dd, J_1 = 8.08 Hz, J_2 = 7.20 Hz, 1H), 4.18 (m, 1H), 4.36 (dd, J_1 = 9.32 Hz, J_2 = 8.08 Hz, 1H), 6.65 (d, J = 5.88 Hz, 1H, *Aromatic H*), 6.94-6.99 (m, 2H, *Aromatic H*), 7.08-7.16 (m, 3H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.88 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.45 (d, J = 5.80 Hz, 1H, *Aromatic H*), 8.90 (dd, J_1 = 8.44 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 9.08 (s, 1H, *Aromatic H*), 12.75 (s, 1H, CO*NH*).

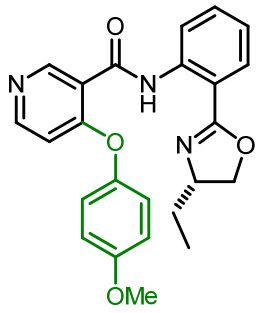
^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 55.7, 62.1, 72.6, 110.0, 114.4, 115.2 (2 × *CH*), 121.0, 121.5, 122.4 (2 × *CH*), 123.0, 129.3, 132.3, 139.4, 146.8, 152.7, 153.0, 157.5, 162.9, 163.0, 163.1.

ESI-MS: calcd for $C_{23}H_{22}N_3O_4$ $[M+H]^+$: 404.16, found: 404.14.



(R)-4-(4-methoxyphenoxy)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)

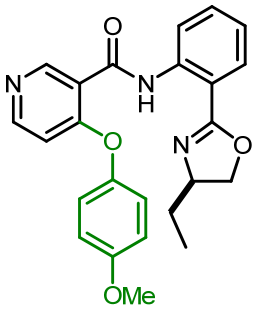
nicotinamide (**6v**), white solid, yield 51%. Similar NMR Data to that of compound **6s**.



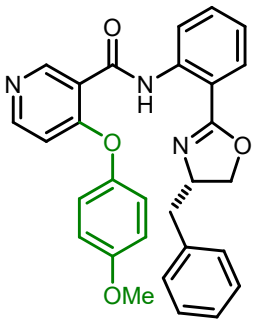
(S)-N-(2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methoxyphenoxy)nicotinamide (**6t**), white solid, yield 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.82 (t, J = 7.36 Hz, 3H, CH_2-*CH_3*), 1.43-1.51 (m, 2H, *CH_2*-CH_3), 3.83 (s, 3H, O-*CH_3*), 3.96 (dd, J_1 = 8.08 Hz, J_2 = 7.28 Hz, 1H), 4.07 (m, 1H), 4.35 (dd, J_1 = 9.36 Hz, J_2 = 8.08 Hz, 1H), 6.65 (d, J = 5.84 Hz, 1H, *Aromatic H*), 6.93-6.97 (m, 2H, *Aromatic H*), 7.07-7.16 (m, 3H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.45 (d, J = 5.84 Hz, 1H, *Aromatic H*), 8.89 (dd, J_1 = 8.48 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 9.03 (s, 1H, *Aromatic H*), 12.84 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 10.1, 28.8, 55.7, 68.0, 70.8, 110.1, 114.2, 115.2 (2 × *CH*), 120.8, 122.3 (2 × *CH*), 123.0, 129.2, 132.4, 139.5, 146.8, 152.2, 152.9, 157.4, 163.0, 163.1, 163.2.

ESI-MS: calcd for $C_{24}H_{24}N_3O_4$ $[M+H]^+$: 418.18, found: 418.21.



(R)-N-(2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methoxyphenoxy) nicotinamide (**6w**), white solid, yield 62%. Similar NMR Data to that of compound **6t**.

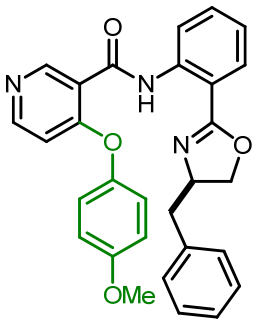


(S)-N-(2-(4-benzyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methoxyphenoxy)nicotinamide (**6u**), white solid, yield 61%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.65 (dd, J_1 = 13.24 Hz, J_2 = 6.36 Hz, 1H, Ph-*CH*), 2.81 (dd, J_1 = 13.24 Hz, J_2 = 7.20 Hz, 1H, Ph-*CH*), 3.80 (s, 3H, O-CH_3), 4.04 (dd, J_1 = 8.24 Hz, J_2 = 6.32 Hz, 1H), 4.25 (dd, J_1 = 9.28 Hz, J_2 = 8.24 Hz, 1H), 4.33 (m, 1H), 6.48 (d, J = 5.80 Hz, 1H, *Aromatic H*), 6.76-6.79 (m, 2H, *Aromatic H*), 6.86-6.89 (m, 2H, *Aromatic H*), 7.03-7.10 (m, 5H, *Aromatic H*), 7.13 (m, 1H, *Aromatic H*), 7.53 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.96 Hz, J_2 = 1.72 Hz, 1H, *Aromatic H*), 8.44 (d, J = 5.84 Hz, 1H, *Aromatic H*), 8.93 (dd, J_1 = 8.56 Hz, J_2 = 1.16 Hz, 1H, *Aromatic H*), 9.10 (s, 1H, *Aromatic H*), 12.71 (s, 1H, CO*NH*).

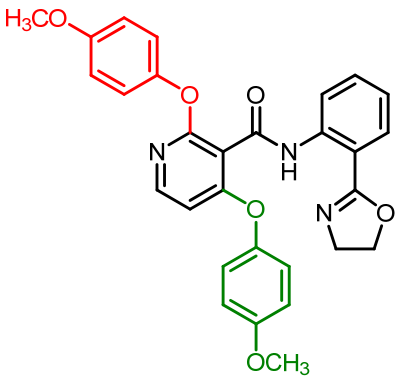
^{13}C NMR (100 MHz, $CDCl_3$) δ 42.4, 55.7, 68.0, 70.6, 110.0, 114.1, 115.1 (2 × *CH*),

120.9, 121.4, 122.3 (2 × *CH*), 123.0, 126.6, 128.3 (2 × *CH*), 129.1 (2 × *CH*), 129.4, 132.5, 137.7, 139.6, 146.5, 152.91, 152.93, 157.4, 162.7, 163.2, 163.4.

ESI-MS: calcd for $C_{29}H_{26}N_3O_4$ $[M+H]^+$: 480.19, found: 480.20.



(R)-N-(2-(4-benzyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methoxyphenoxy)nicotinamide (**6x**), white solid, yield 57%. Similar NMR Data to that of compound **6u**.

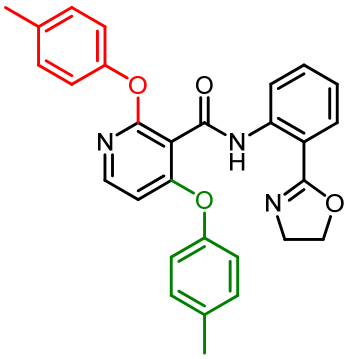


N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2,4-bis(4-methoxyphenoxy)nicotinamide (**7a**), white solid, yield 35%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (s, 3H, O*CH*$_3$), 3.80 (s, 3H, O*CH*$_3$), 4.07 (t, *J* = 9.40 Hz, 2H, N*CH*$_2$-CH_2O), 4.35 (t, *J* = 9.40 Hz, 2H, NCH_2-*CH*$_2$O), 6.35 (dd, J_1 = 5.88 Hz, J_2 = 1.04 Hz, 1H, *Aromatic H*), 6.85~6.93 (m, 4H, *Aromatic H*), 7.05~7.15 (m, 5H, *Aromatic H*), 7.50 (dd, J_1 = 8.08 Hz, J_2 = 7.88 Hz, 1H, *Aromatic H*), 7.88 (m, 1H, *Aromatic H*), 7.96 (dd, J_1 = 5.88 Hz, J_2 = 1.08 Hz, 1H,

Aromatic H), 9.01 (d, *J* = 8.52 Hz, 1H, *Aromatic H*), 12.75 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 55.6, 55.7, 66.1, 106.2, 111.3, 113.4, 114.5 (2 × *CH*), 115.0 (2 × *CH*), 120.1, 122.2 (2 × *CH*), 122.7 (2 × *CH*), 122.8, 129.2, 132.7, 139.8, 147.1, 147.5, 148.8, 156.6, 157.2, 162.1, 162.2, 164.6, 164.9.

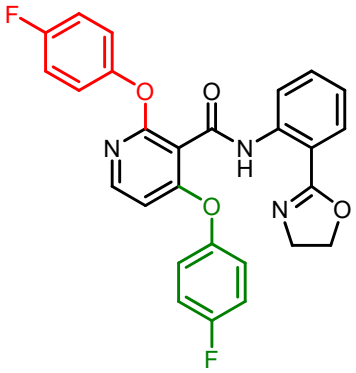
ESI-MS: calcd for $C_{29}H_{26}N_3O_6$ [M+ H]$^+$: 512.18, found: 512.20; calcd for $C_{29}H_{25}N_3NaO_6$ [M+ H]$^+$: 534.16, found: 534.24.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2,4-bis(p-tolyloxy)nicotinamide (**7b**), white solid, yield 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.33 (s, 3H, Ph*CH*$_3$), 2.35 (s, 3H, Ph*CH*$_3$), 4.06 (t, *J* = 9.56 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.34 (t, *J* = 9.56 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.38 (d, *J* = 5.92 Hz, 1H, *Aromatic H*), 6.99-7.08 (m, 4H, *Aromatic H*), 7.11 (m, 1H, *Aromatic H*), 7.15~7.21 (m, 4H, *Aromatic H*), 7.49 (m, 1H, *Aromatic H*), 7.87 (dd, J_1 = 7.88 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 7.96 (d, *J* = 5.92 Hz, 1H, *Aromatic H*), 9.00 (d, *J* = 8.48 Hz, 1H, *Aromatic H*), 12.74 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 20.9, 54.9, 66.1, 106.5, 111.7, 113.4, 120.2, 120.9 (2 × *CH*), 121.5 (2 × *CH*), 122.7, 129.2, 130.0 (2 × *CH*), 130.5 (2 × *CH*), 132.6, 134.4, 135.3, 139.9, 148.8, 151.5, 151.9, 162.06, 162.11, 164.5, 164.6.

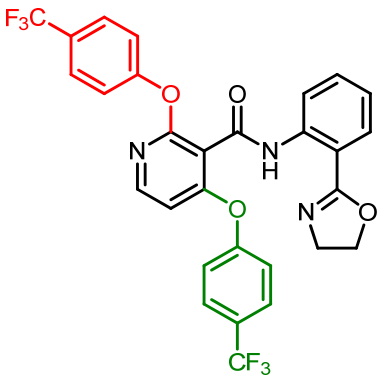
ESI-MS: calcd for $C_{29}H_{26}N_3O_4$ [M+ H]$^+$: 480.19, found: 480.17.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2,4-bis(4-fluorophenoxy)nicotinamide (**7c**), white solid, yield 79%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.05 (t, *J* = 9.40 Hz, 2H, N*CH*$_2$-CH$_2$O), 4.36 (t, *J* = 9.40 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.40 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 7.02-7.19 (m, 9H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.89 (d, *J* = 7.84 Hz, 1H, *Aromatic H*), 7.99 (dd, J_1 = 5.92 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 8.99 (d, *J* = 8.52 Hz, 1H, *Aromatic H*), 12.76 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 54.9, 66.1, 106.6, 111.8, 113.4, 116.0, 116.2, 116.7, 116.9, 120.1, 122.6 (d, J_{CF} = 8.43 Hz), 122.9, 123.2 (d, J_{CF} = 8.36 Hz), 129.3, 132.7, 139.7, 148.9, 149.4, 150.0, 159.8 (d, J_{CF} = 243.33 Hz), 160.1 (d, J_{CF} = 241.53 Hz), 161.7, 164.5.

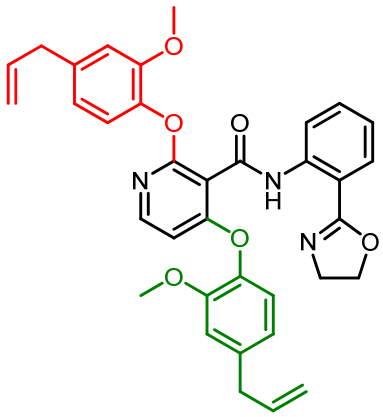
ESI-MS: calcd for $C_{27}H_{20}F_2N_3O_4$ $[M+H]^+$: 488.14, found: 488.26; calcd for $C_{27}H_{19}F_2N_3NaO_4$ $[M+Na]^+$: 510.12, found: 510.21.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2,4-bis(4-(trifluoromethyl)phenoxy) nicotinamide (**7d**), white solid, yield 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.01 (t, *J* = 9.60 Hz, 2H, N*CH*$_2$-CH_2O), 4.36 (t, *J* = 9.60 Hz, 2H, NCH$_2$-*CH*$_2$O), 6.54 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 7.14 (m, 1H, *Aromatic H*), 7.25-7.33 (m, 4H, *Aromatic H*), 7.51 (m, 1H, *Aromatic H*), 7.63-7.70 (m, 4H, *Aromatic H*), 7.89 (dd, J_1 = 7.92 Hz, J_2 = 1.68 Hz, 1H, *Aromatic H*), 8.07 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 8.93 (d, *J* = 8.28 Hz, 1H, *Aromatic H*), 12.82 (s, 1H, CO*NH*).

ESI-MS: calcd for $C_{29}H_{20}F_6N_3O_4$ $[M+H]^+$: 588.14, found: 588.25.

The structure of compound **7d** was unambiguously confirmed by X-ray diffraction and was deposited at the CCDC with the number 1864271.



2,4-bis(4-allyl-2-methoxyphenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl) nicotinamide (**7e**), white solid, yield 30%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.37 (d, *J* = 6.68 Hz, 2H, Ph*CH*$_2$), 3.37 (d, *J* = 6.68 Hz, 2H, Ph*CH*$_2$), 3.74 (s, 3H, O*CH*$_3$), 3.76 (s, 3H, O*CH*$_3$), 4.08 (d, *J* = 6.68 Hz, 2H, Ph*CH*$_2$), 4.35 (t, *J* = 9.52 Hz, 2H, N*CH*$_2$-CH_2O), 5.04-5.14 (m, 4H), 6.26 (d, *J* = 5.92 Hz, 1H, *Aromatic H*), 6.72-6.79 (m, 4H, *Aromatic H*), 7.04-7.11 (m, 3H, *Aromatic H*), 7.47 (m, 1H, *Aromatic H*), 7.86 (dd, J_1 = 7.92 Hz, J_2 = 1.64 Hz, 1H, *Aromatic H*), 7.89 (d, *J* = 5.88 Hz, 1H, *Aromatic H*), 9.03 (dd, *J* =

8.12 Hz, 1H, *Aromatic H*), 12.66 (s, 1H, CO*NH*).

^{13}C NMR (100 MHz, $CDCl_3$) δ 40.0, 40.1, 55.0, 56.0, 56.1, 66.0, 105.8, 113.5, 113.6, 116.0, 116.2, 120.4, 120.9, 121.1, 122.5, 122.6, 122.9, 123.1, 129.1, 132.5, 137.0, 137.3, 137.7, 137.9, 138.9, 140.0, 140.9, 141.0, 148.5, 151.5, 151.7, 161.8, 162.3, 164.37, 164.40,

ESI-MS: calcd for $C_{35}H_{34}N_3O_6$ $[M+H]^+$: 592.24, found: 592.31.

X-ray Crystallographic Data

Compound list with crystallographic data

2a (CCDC 1864263),

4a (CCDC 1864265),

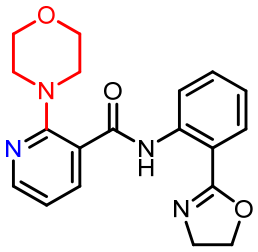
5m (CCDC 1867348),

6a (CCDC 1864262),

6q (CCDC 1867347),

7d (CCDC 1864271),

Diflufenican (CCDC 1864261)



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-morpholinonicotinamide (**2a**),

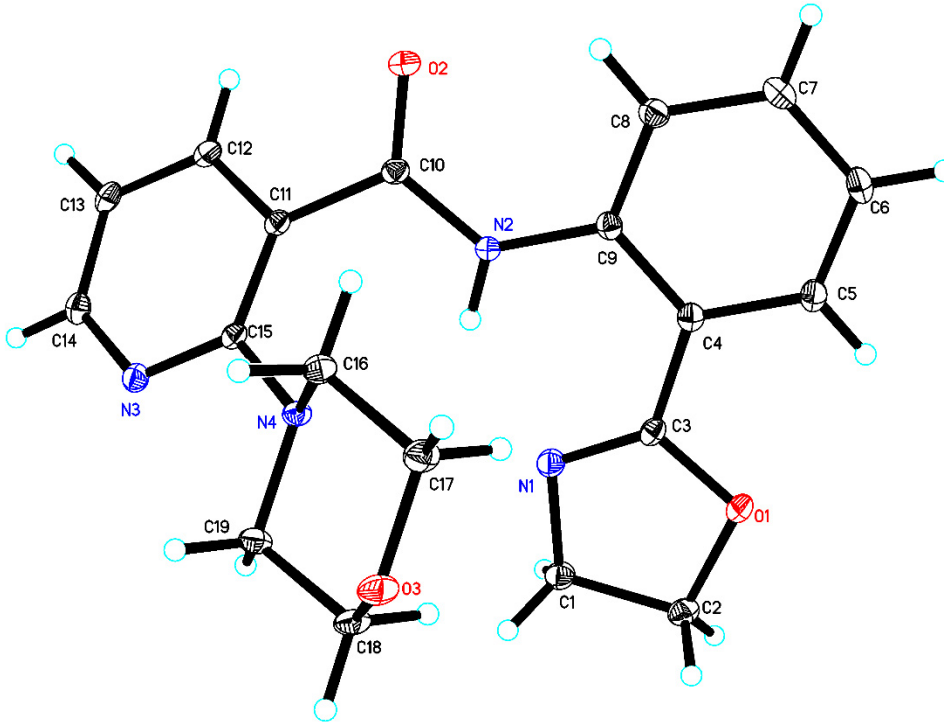


Table 1 Crystal data and structure refinement for 2a.

Identification code	**2a**
Empirical formula	$C_{19}H_{20}N_4O_3$
Formula weight	352.39
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.8860(4)
b/Å	9.5658(7)
c/Å	11.4661(7)
α/°	86.429(5)
β/°	79.097(5)
γ/°	77.958(6)

Volume/Å^3	830.42(9)
Z	2
ρ_{calc}g/cm^3	1.409
μ/mm^{-1}	0.801
F(000)	372.0
Crystal size/mm^3	0.25 × 0.2 × 0.16
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.854 to 147.156
Index ranges	-8 ≤ h ≤ 9, -8 ≤ k ≤ 11, -14 ≤ l ≤ 14
Reflections collected	5513
Independent reflections	3233 [R_{int} = 0.0148, R_{sigma} = 0.0167]
Data/restraints/parameters	3233/0/235
Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ (I)]	R_1 = 0.0396, wR_2 = 0.1037
Final R indexes [all data]	R_1 = 0.0410, wR_2 = 0.1047
Largest diff. peak/hole / e Å^{-3}	0.31/-0.24

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

Atom	*x*	*y*	*z*	U(eq)
O1	7111.4(13)	8433.4(11)	4731.8(8)	24.5(2)
O2	982.8(13)	4957.8(10)	6861.0(8)	23.4(2)
O3	1918.4(13)	10763.7(10)	8437.9(9)	23.4(2)
N4	2543.4(14)	7752.4(11)	8800.7(9)	15.6(2)
N3	2844.7(14)	6049.1(12)	10335.8(9)	18.0(2)
N2	3190.2(14)	6238.9(11)	6541.4(9)	16.2(2)
N1	6081.8(15)	7411.1(12)	6475.2(10)	20.1(2)
C9	3330.0(17)	6573.7(13)	5320.8(11)	15.6(3)
C15	2532.4(16)	6345.1(13)	9232.2(11)	14.9(3)
C11	2220.0(16)	5308.4(13)	8517.7(11)	14.9(3)
C3	5954.4(16)	7686.7(13)	5393.5(11)	16.3(3)
C10	2052.2(16)	5493.7(13)	7230.6(11)	15.9(3)
C12	2042.6(16)	3986.0(13)	9044.4(11)	17.4(3)
C13	2331.3(17)	3689.1(13)	10195.7(11)	19.1(3)
C5	4847.6(18)	7611.5(14)	3535.2(11)	20.0(3)
C14	2788.4(17)	4728.5(14)	10787.8(11)	19.6(3)

C4	4683.3(16)	7284.8(13)	4754.8(11)	16.3(3)
C8	2157.5(17)	6257.9(14)	4644.3(12)	19.1(3)
C6	3680.0(19)	7288.2(15)	2880.4(12)	22.5(3)
C16	915.6(17)	8538.9(13)	8429.1(12)	18.2(3)
C19	3197.0(18)	8660.0(14)	9520.7(12)	19.8(3)
C2	8121.3(18)	8823.3(15)	5547.7(12)	21.7(3)
C18	3482.5(19)	9994.8(14)	8795.5(13)	22.2(3)
C7	2328.8(18)	6627.5(15)	3443.1(12)	21.6(3)
C1	7612.3(17)	7954.5(15)	6679.9(12)	21.3(3)
C17	1277.9(19)	9878.9(14)	7734.7(13)	22.2(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for EN-1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	27.2(5)	31.1(5)	19.5(5)	5.1(4)	-3.8(4)	-17.6(4)
O2	26.0(5)	27.0(5)	22.4(5)	0.9(4)	-6.9(4)	-15.2(4)
O3	27.2(5)	13.3(4)	31.2(5)	-0.3(4)	-8.0(4)	-4.9(4)
N4	17.5(5)	12.9(5)	17.6(5)	-0.2(4)	-4.5(4)	-4.4(4)
N3	19.7(5)	17.8(5)	16.4(5)	1.1(4)	-2.3(4)	-4.6(4)
N2	17.7(5)	18.8(5)	13.9(5)	0.2(4)	-3.3(4)	-7.7(4)
N1	17.2(5)	25.8(6)	19.0(5)	2.3(4)	-4.8(4)	-7.8(4)
C9	16.9(6)	14.4(6)	14.7(6)	-1.4(5)	-2.0(5)	-1.5(4)
C15	12.7(6)	14.6(6)	16.6(6)	0.2(5)	-0.2(4)	-3.6(4)
C11	13.1(6)	14.3(6)	16.6(6)	-0.5(5)	-0.3(4)	-3.3(4)
C3	14.7(6)	14.7(6)	17.7(6)	0.6(5)	0.8(5)	-2.7(5)
C10	16.6(6)	13.0(6)	17.9(6)	-1.6(5)	-1.8(5)	-3.5(5)
C12	15.8(6)	14.3(6)	21.0(6)	-1.7(5)	1.4(5)	-4.2(5)
C13	19.0(6)	14.3(6)	21.3(6)	3.7(5)	1.6(5)	-3.4(5)
C5	23.4(7)	18.8(6)	16.4(6)	1.1(5)	-1.2(5)	-3.7(5)
C14	21.2(6)	19.2(6)	16.9(6)	3.5(5)	-1.6(5)	-3.1(5)
C4	17.2(6)	13.6(6)	16.7(6)	-0.5(5)	-2.3(5)	-0.9(5)
C8	18.4(6)	20.2(6)	18.9(6)	-2.7(5)	-3.3(5)	-4.1(5)
C6	28.2(7)	24.2(7)	14.1(6)	0.1(5)	-4.4(5)	-2.4(5)
C16	17.6(6)	15.4(6)	22.1(6)	-0.2(5)	-4.6(5)	-3.5(5)
C19	23.7(7)	16.1(6)	21.8(6)	-2.4(5)	-7.3(5)	-5.9(5)
C2	18.8(6)	22.4(7)	25.6(7)	0.6(5)	-4.2(5)	-8.2(5)
C18	26.4(7)	15.0(6)	28.4(7)	0.0(5)	-7.9(6)	-8.7(5)
C7	22.9(7)	23.6(7)	19.1(6)	-4.2(5)	-7.2(5)	-2.4(5)
C1	17.8(6)	25.8(7)	22.5(7)	1.3(5)	-5.6(5)	-8.0(5)

C17	26.7(7)	16.8(6)	24.9(7)	2.6(5)	-9.1(5)	-5.3(5)

Table 4 Bond Lengths for EN-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C3	1.3642(15)	C9	C8	1.4017(18)
O1	C2	1.4484(16)	C15	C11	1.4123(17)
O2	C10	1.2232(16)	C11	C10	1.5029(17)
O3	C18	1.4162(17)	C11	C12	1.3897(17)
O3	C17	1.4280(16)	C3	C4	1.4705(18)
N4	C15	1.4062(16)	C12	C13	1.3839(18)
N4	C16	1.4695(16)	C13	C14	1.3804(19)
N4	C19	1.4623(16)	C5	C4	1.4013(18)
N3	C15	1.3365(17)	C5	C6	1.3843(19)
N3	C14	1.3415(17)	C8	C7	1.3889(18)
N2	C9	1.4050(16)	C6	C7	1.386(2)
N2	C10	1.3662(16)	C16	C17	1.5159(17)
N1	C3	1.2701(17)	C19	C18	1.5130(18)
N1	C1	1.4718(16)	C2	C1	1.5312(18)
C9	C4	1.4173(18)			

Table 5 Bond Angles for EN-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	O1	C2	105.98(10)	O2	C10	N2	124.57(12)
C18	O3	C17	109.74(10)	O2	C10	C11	119.95(11)
C15	N4	C16	116.25(10)	N2	C10	C11	115.45(11)
C15	N4	C19	116.16(10)	C13	C12	C11	119.58(12)
C19	N4	C16	110.09(10)	C14	C13	C12	118.47(11)
C15	N3	C14	118.12(11)	C6	C5	C4	121.13(13)
C10	N2	C9	127.84(11)	N3	C14	C13	123.28(12)
C3	N1	C1	106.91(11)	C9	C4	C3	122.64(11)
N2	C9	C4	118.90(11)	C5	C4	C9	119.44(12)
C8	C9	N2	122.48(12)	C5	C4	C3	117.92(12)
C8	C9	C4	118.60(11)	C7	C8	C9	120.56(12)
N4	C15	C11	120.88(11)	C5	C6	C7	119.28(12)
N3	C15	N4	116.64(11)	N4	C16	C17	109.33(10)
N3	C15	C11	122.48(11)	N4	C19	C18	108.19(10)
C15	C11	C10	126.27(11)	O1	C2	C1	103.61(10)

C12	C11	C15	117.59(11)	O3	C18	C19	112.34(11)
C12	C11	C10	116.15(11)	C6	C7	C8	120.95(12)
O1	C3	C4	115.16(11)	N1	C1	C2	104.29(10)
N1	C3	O1	117.71(12)	O3	C17	C16	110.63(11)
N1	C3	C4	127.13(12)				

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for EN-1.

Atom	*x*	*y*	*z*	U(eq)
H2	3908	6539	6898	19
H12	1732	3305	8626	21
H13	2220	2810	10562	23
H5	5757	8053	3159	24
H14	3072	4502	11537	24
H8	1257	5797	5003	23
H6	3801	7512	2072	27
H16A	7	8795	9122	22
H16B	501	7940	7938	22
H19A	4297	8154	9739	24
H19B	2347	8913	10243	24
H2A	7804	9841	5694	26
H2B	9376	8568	5241	26
H18A	3916	10608	9263	27
H18B	4375	9729	8096	27
H7	1525	6429	3010	26
H1A	8574	7173	6796	26
H1B	7301	8554	7371	26
H17A	2144	9616	7022	27
H17B	202	10406	7496	27

Experimental

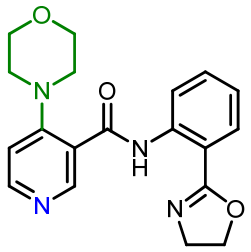
Single crystals of $C_{19}H_{20}N_4O_3$ **[2a]** were **[]**. A suitable crystal was selected and **[]** on a **SuperNova, Dual, Cu at zero, AtlasS2** diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [2a]

Crystal Data for $C_{19}H_{20}N_4O_3$ (M =352.39 g/mol): triclinic, space group P-1 (no. 2), a = 7.8860(4) Å, b = 9.5658(7) Å, c = 11.4661(7) Å, α = 86.429(5)°, β = 79.097(5)°, γ = 77.958(6)°, V = 830.42(9) Å^3, Z = 2, T = 100.00(10) K, μ(Cu Kα) = 0.801 mm^{-1}, *Dcalc* = 1.409 g/cm^3, 5513 reflections measured (7.854° ≤ 2Θ ≤ 147.156°), 3233 unique (R_{int} = 0.0148, R_{sigma} = 0.0167) which were used in all calculations. The final R_1 was 0.0396 (I > 2σ(I)) and wR_2 was 0.1047 (all data).



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-morpholinonicotinamide (**4a**)

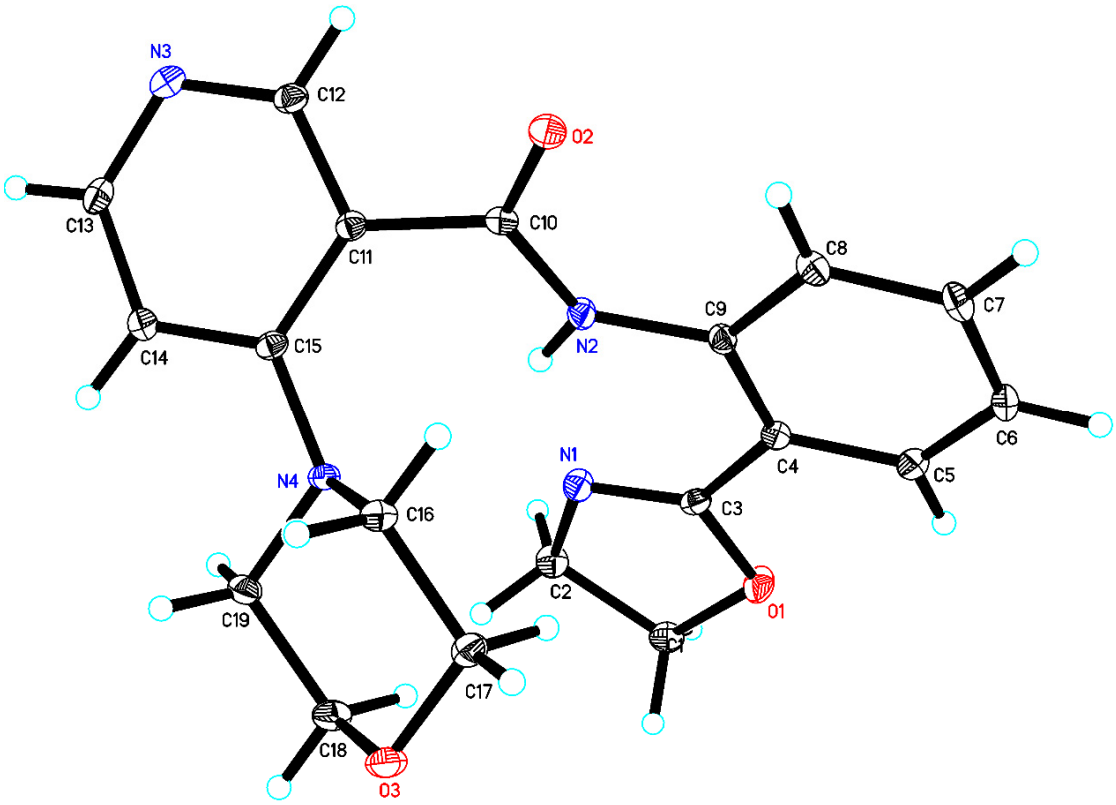


Table 1 Crystal data and structure refinement for 4a.

Identification code	**4a**
Empirical formula	$C_{19}H_{20}N_4O_3$
Formula weight	352.39
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.7358(5)
b/Å	9.6039(6)
c/Å	11.6310(7)
α/°	85.647(5)
β/°	76.146(5)
γ/°	78.816(5)

Volume/Å^3	822.64(9)
Z	2
ρ_{calc}g/cm^3	1.423
μ/mm^{-1}	0.099
F(000)	372.0
Crystal size/mm^3	0.31 × 0.21 × 0.13
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	7.22 to 58.986
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -11 ≤ l ≤ 15
Reflections collected	6220
Independent reflections	3834 [R_{int} = 0.0189, R_{sigma} = 0.0405]
Data/restraints/parameters	3834/0/235
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.1048
Final R indexes [all data]	R_1 = 0.0588, wR_2 = 0.1137
Largest diff. peak/hole / e Å^{-3}	0.32/-0.25

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

Atom	*x*	*y*	*z*	U(eq)
O2	1001.5(15)	4807.2(12)	6979.0(9)	22.0(3)
O3	1772.2(15)	10621.6(11)	8414.0(9)	22.6(3)
O1	7191.7(16)	8515.4(12)	4762.9(9)	25.6(3)
N2	3285.3(16)	6102.2(13)	6594.6(10)	16.2(3)
N1	6181.9(17)	7364.1(14)	6480.0(11)	19.2(3)
N3	2563.0(17)	3369.4(14)	10138.7(11)	19.9(3)
N4	2439.4(16)	7633.0(12)	8865.7(10)	15.2(3)
C8	2241(2)	6157.2(16)	4753.3(13)	18.7(3)
C11	2268.3(19)	5160.9(15)	8579.3(12)	14.6(3)
C3	6026.8(19)	7709.1(15)	5429.1(12)	15.5(3)
C9	3404.3(19)	6507.6(15)	5397.8(12)	14.9(3)
C4	4733.2(19)	7319.5(15)	4827.8(12)	15.8(3)
C10	2096.9(19)	5342.2(15)	7316.6(12)	15.2(3)
C5	4843(2)	7757.2(16)	3643.8(13)	20.3(3)
C12	2270.4(19)	3789.8(16)	9067.8(13)	17.6(3)
C15	2464.3(19)	6226.7(15)	9285.6(12)	14.8(3)

C6	3655(2)	7436.2(17)	3025.9(13)	21.5(3)
C14	2731(2)	5790.0(16)	10411.1(13)	18.6(3)
C1	8247(2)	8860.1(17)	5542.8(13)	21.0(3)
C13	2797(2)	4388.6(17)	10781.8(13)	20.1(3)
C16	839(2)	8354.5(16)	8439.6(13)	18.1(3)
C19	2974(2)	8599.2(16)	9578.1(13)	19.1(3)
C2	7735(2)	7929.0(17)	6651.7(13)	20.5(3)
C7	2368(2)	6630.3(17)	3579.5(13)	21.1(3)
C18	3310(2)	9931.7(16)	8846.5(14)	21.7(3)
C17	1270(2)	9672.1(16)	7719.8(13)	20.8(3)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	25.1(6)	24.1(6)	21.4(5)	0.6(4)	-7.5(4)	-13.3(5)
O3	28.0(6)	13.9(5)	27.3(6)	0.7(4)	-8.9(5)	-4.5(5)
O1	30.7(6)	31.9(7)	19.5(5)	6.1(5)	-6.5(5)	-20.4(5)
N2	17.2(6)	19.7(7)	13.8(6)	0.6(5)	-4.7(5)	-7.6(5)
N1	18.9(6)	23.2(7)	18.2(6)	1.7(5)	-6.9(5)	-8.2(5)
N3	20.2(7)	17.7(7)	21.7(6)	3.4(5)	-4.0(5)	-5.5(5)
N4	19.2(6)	11.5(6)	16.7(6)	0.5(5)	-6.7(5)	-4.1(5)
C8	18.1(7)	20.8(8)	17.6(7)	-4.9(6)	-3.1(6)	-4.0(6)
C11	12.9(7)	14.7(7)	15.7(7)	0.1(5)	-2.0(5)	-3.3(5)
C3	14.9(7)	12.5(7)	17.4(7)	0.3(5)	-0.5(5)	-2.6(6)
C9	16.1(7)	14.6(7)	13.0(6)	-1.9(5)	-2.7(5)	-0.9(6)
C4	17.3(7)	14.3(7)	15.5(7)	-1.1(5)	-3.4(5)	-2.3(6)
C10	15.5(7)	12.7(7)	17.5(7)	-1.4(5)	-3.6(5)	-2.6(5)
C5	25.6(8)	17.7(8)	17.5(7)	1.3(6)	-3.3(6)	-6.4(6)
C12	16.4(7)	15.6(7)	20.1(7)	-0.2(6)	-1.4(6)	-4.7(6)
C15	12.6(7)	14.2(7)	17.3(7)	1.2(5)	-1.7(5)	-4.2(5)
C6	28.9(9)	24.1(8)	12.6(7)	0.5(6)	-6.1(6)	-6.6(7)
C14	22.2(8)	19.0(8)	15.2(7)	-1.4(6)	-3.8(6)	-5.5(6)
C1	18.5(8)	20.6(8)	25.7(8)	-1.0(6)	-5.5(6)	-7.4(6)
C13	21.3(8)	23.2(8)	16.1(7)	5.6(6)	-4.9(6)	-6.6(6)
C16	18.7(7)	14.5(7)	21.7(7)	-0.4(6)	-5.8(6)	-3.0(6)
C19	23.9(8)	15.5(7)	19.9(7)	-2.4(6)	-7.5(6)	-5.0(6)
C2	16.9(7)	24.4(8)	21.8(7)	-0.9(6)	-5.7(6)	-6.1(6)
C7	22.8(8)	25.6(8)	17.2(7)	-4.9(6)	-8.3(6)	-3.8(6)
C18	23.7(8)	16.5(8)	27.2(8)	-1.0(6)	-7.8(6)	-6.3(6)

C17	25.8(8)	17.2(8)	20.6(7)	2.3(6)	-8.4(6)	-4.4(6)

Table 4 Bond Lengths for EN-3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C10	1.2228(18)	C8	C7	1.392(2)
O3	C18	1.4274(18)	C11	C10	1.500(2)
O3	C17	1.4263(19)	C11	C12	1.394(2)
O1	C3	1.3628(18)	C11	C15	1.412(2)
O1	C1	1.4507(19)	C3	C4	1.467(2)
N2	C9	1.4028(18)	C9	C4	1.418(2)
N2	C10	1.3714(19)	C4	C5	1.396(2)
N1	C3	1.2694(19)	C5	C6	1.384(2)
N1	C2	1.4705(19)	C15	C14	1.395(2)
N3	C12	1.3375(19)	C6	C7	1.386(2)
N3	C13	1.340(2)	C14	C13	1.377(2)
N4	C15	1.3990(18)	C1	C2	1.529(2)
N4	C16	1.4725(18)	C16	C17	1.511(2)
N4	C19	1.4655(19)	C19	C18	1.512(2)
C8	C9	1.401(2)			

Table 5 Bond Angles for EN-3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C17	O3	C18	109.99(11)	C5	C4	C9	119.33(14)
C3	O1	C1	106.09(11)	O2	C10	N2	124.13(13)
C10	N2	C9	128.34(13)	O2	C10	C11	121.07(13)
C3	N1	C2	107.03(12)	N2	C10	C11	114.76(13)
C12	N3	C13	115.45(13)	C6	C5	C4	121.14(15)
C15	N4	C16	117.31(12)	N3	C12	C11	125.07(14)
C15	N4	C19	117.41(11)	N4	C15	C11	121.74(12)
C19	N4	C16	109.85(11)	C14	C15	N4	122.02(14)
C7	C8	C9	120.20(14)	C14	C15	C11	116.22(13)
C12	C11	C10	115.32(13)	C5	C6	C7	119.52(14)
C12	C11	C15	118.41(13)	C13	C14	C15	120.37(14)
C15	C11	C10	126.25(13)	O1	C1	C2	103.56(12)
O1	C3	C4	115.16(12)	N3	C13	C14	124.33(14)
N1	C3	O1	117.64(14)	N4	C16	C17	109.35(12)
N1	C3	C4	127.20(14)	N4	C19	C18	109.16(12)

N2	C9	C4	118.64(13)	N1	C2	C1	104.48(12)
C8	C9	N2	122.37(13)	C6	C7	C8	120.80(14)
C8	C9	C4	118.98(13)	O3	C18	C19	112.43(13)
C9	C4	C3	122.54(12)	O3	C17	C16	110.88(12)
C5	C4	C3	118.13(14)				

Table 6 Torsion Angles for EN-3.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C3	C4	C9	-178.76(13)	C12	N3	C13	C14	0.7(2)
O1	C3	C4	C5	2.03(19)	C12	C11	C10	O2	44.18(19)
O1	C1	C2	N1	-10.75(15)	C12	C11	C10	N2	-133.94(14)
N2	C9	C4	C3	2.2(2)	C12	C11	C15	N4	-178.73(13)
N2	C9	C4	C5	-178.64(13)	C12	C11	C15	C14	2.9(2)
N1	C3	C4	C9	2.2(2)	C15	N4	C16	C17	-164.20(12)
N1	C3	C4	C5	-177.06(14)	C15	N4	C19	C18	165.99(12)
N4	C15	C14	C13	-178.23(13)	C15	C11	C10	O2	-137.35(15)
N4	C16	C17	O3	-59.42(16)	C15	C11	C10	N2	44.5(2)
N4	C19	C18	O3	56.95(16)	C15	C11	C12	N3	-4.6(2)
C8	C9	C4	C3	-178.79(13)	C15	C14	C13	N3	-2.1(2)
C8	C9	C4	C5	0.4(2)	C1	O1	C3	N1	-4.79(18)
C11	C15	C14	C13	0.1(2)	C1	O1	C3	C4	176.03(12)
C3	O1	C1	C2	9.43(15)	C13	N3	C12	C11	2.7(2)
C3	N1	C2	C1	8.40(16)	C16	N4	C15	C11	56.38(18)
C3	C4	C5	C6	-179.46(13)	C16	N4	C15	C14	-125.36(15)
C9	N2	C10	O2	5.3(2)	C16	N4	C19	C18	-56.56(15)
C9	N2	C10	C11	-176.65(13)	C19	N4	C15	C11	-169.33(13)
C9	C8	C7	C6	0.8(2)	C19	N4	C15	C14	8.9(2)
C9	C4	C5	C6	1.3(2)	C19	N4	C16	C17	58.30(15)
C4	C5	C6	C7	-2.0(2)	C2	N1	C3	O1	-2.60(18)
C10	N2	C9	C8	-0.1(2)	C2	N1	C3	C4	176.47(14)
C10	N2	C9	C4	178.94(13)	C7	C8	C9	N2	177.56(13)
C10	C11	C12	N3	173.99(13)	C7	C8	C9	C4	-1.5(2)
C10	C11	C15	N4	2.9(2)	C18	O3	C17	C16	58.67(16)
C10	C11	C15	C14	-175.51(14)	C17	O3	C18	C19	-57.90(16)
C5	C6	C7	C8	0.9(2)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for EN-3.

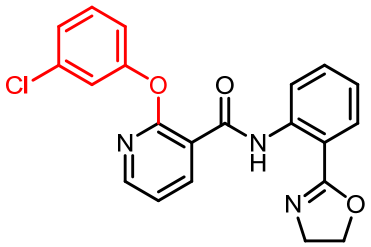
Atom	*x*	*y*	*z*	U(eq)
H2	4057	6364	6917	19
H8	1381	5607	5111	22
H5	5730	8273	3264	24
H12	2052	3115	8614	21
H6	3720	7759	2245	26
H14	2866	6449	10914	22
H1A	7928	9859	5726	25
H1B	9534	8632	5188	25
H13	3017	4133	11528	24
H16A	-172	8613	9108	22
H16B	501	7721	7955	22
H19A	4065	8141	9825	23
H19B	2022	8840	10283	23
H2A	8733	7165	6720	25
H2B	7401	8486	7359	25
H7	1580	6403	3162	25
H18A	3625	10584	9327	26
H18B	4330	9688	8180	26
H17A	2253	9405	7037	25
H17B	218	10146	7435	25

Experimental

Single crystals of $C_{19}H_{20}N_4O_3$ **[4a]** were **[]**. A suitable crystal was selected and **[]** on a **SuperNova, Dual, Cu at zero, AtlasS2** diffractometer. The crystal was kept at 100.00(10) K during data collection.

Crystal structure determination of [4a]

Crystal Data for $C_{19}H_{20}N_4O_3$ (*M* =352.39 g/mol): triclinic, space group P-1 (no. 2), *a* = 7.7358(5) Å, *b* = 9.6039(6) Å, *c* = 11.6310(7) Å, *α* = 85.647(5), *β* = 76.146(5) , *γ* = 78.816(5) , *V* = 822.64(9) Å^3, *Z* = 2, *T* = 100.00(10) K, μ(Mo Kα) = 0.099 mm^{-1}, *Dcalc* = 1.423 g/cm^3, 6220 reflections measured (7.22° ≤ 2Θ ≤ 58.986°), 3834 unique (R_{int} = 0.0189, R_{sigma} = 0.0405) which were used in all calculations. The final R_1 was 0.0458 (I > 2σ(I)) and wR_2 was 0.1137 (all data).



2-(3-chlorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**5m**)

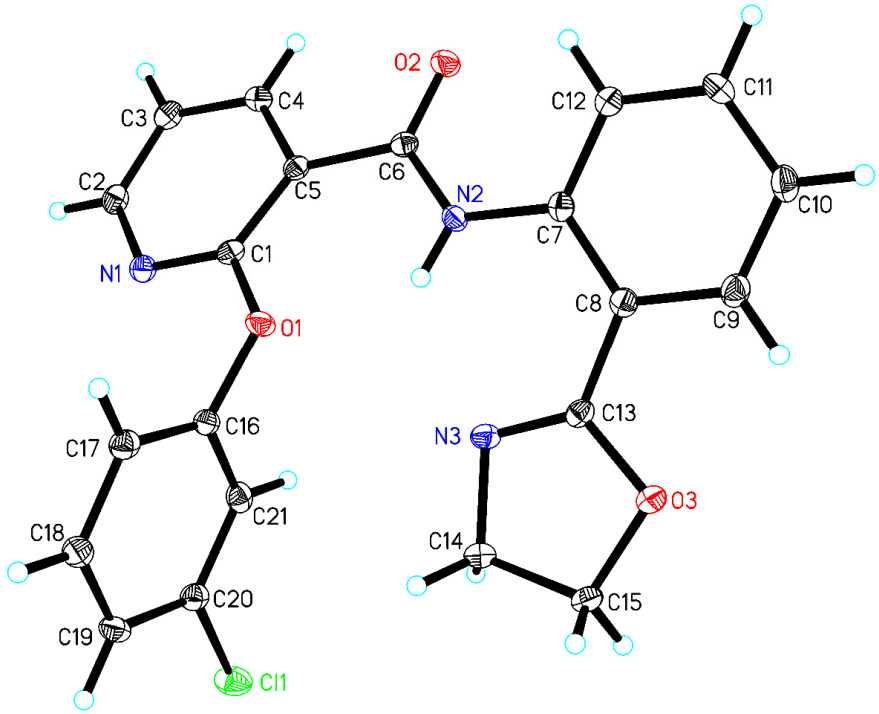


Table 1 Crystal data and structure refinement for 5m.

Identification code	**5m**
Empirical formula	$C_{21}H_{16}ClN_3O_3$
Formula weight	393.82
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.0444(10)
b/Å	10.7234(12)
c/Å	11.5467(13)
α/°	71.104(10)
β/°	70.410(11)
γ/°	73.474(10)
Volume/Å^3	870.4(2)
Z	2
ρ_{calc}g/cm^3	1.503

μ/mm^{-1}	0.249
F(000)	408.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.096 to 59.172
Index ranges	-11 ≤ h ≤ 11, -14 ≤ k ≤ 13, -15 ≤ l ≤ 13
Reflections collected	11524
Independent reflections	4192 [R_{int} = 0.0448, R_{sigma} = 0.0583]
Data/restraints/parameters	4192/0/253
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0561, wR_2 = 0.1276
Final R indexes [all data]	R_1 = 0.0759, wR_2 = 0.1414
Largest diff. peak/hole / e Å^{-3}	0.37/-0.33

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 54-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	7399.7(9)	4631.7(6)	10634.9(6)	34.06(19)
O1	6278.7(19)	8288.9(16)	6717.1(13)	22.7(3)
O2	5675(2)	8382.6(16)	3213.6(14)	25.3(4)
O3	12823(2)	5591.3(16)	4939.4(15)	27.2(4)
N2	7768(2)	7903.7(17)	4308.0(16)	19.1(4)
N1	3226(2)	8443.2(18)	7576.4(17)	21.4(4)
N3	9898(2)	6305.4(18)	5882.0(17)	21.3(4)
C7	9333(3)	7762(2)	3296(2)	18.9(4)
C6	6047(3)	8239(2)	4202(2)	18.7(4)
C16	6478(3)	7979(2)	7949(2)	21.0(5)
C1	4621(3)	8374(2)	6575(2)	19.0(4)
C13	11145(3)	6294(2)	4853(2)	19.5(4)
C3	1304(3)	8734(2)	6263(2)	23.2(5)
C5	4525(3)	8406(2)	5370.5(19)	17.9(4)
C8	10985(3)	6993(2)	3556(2)	20.4(4)
C12	9310(3)	8406(2)	2031(2)	20.6(4)
C17	6545(3)	8989(2)	8418(2)	22.9(5)
C4	2796(3)	8621(2)	5237(2)	20.0(4)
C14	10712(3)	5495(2)	6931(2)	22.5(5)

C19	7206(3)	7298(2)	10280(2)	23.4(5)
C2	1588(3)	8611(2)	7412(2)	22.9(5)
C21	6733(3)	6630(2)	8618(2)	23.0(5)
C18	6918(3)	8639(2)	9581(2)	24.3(5)
C11	10851(3)	8278(2)	1055(2)	23.3(5)
C20	7106(3)	6316(2)	9781(2)	22.3(5)
C15	12719(3)	5137(2)	6284(2)	24.1(5)
C9	12534(3)	6898(2)	2539(2)	24.8(5)
C10	12473(3)	7520(2)	1297(2)	26.7(5)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 54-1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	46.8(4)	25.2(3)	32.0(3)	0.4(2)	-19.1(3)	-8.3(3)
O1	16.7(7)	34.0(9)	17.0(8)	-5.2(6)	-5.8(6)	-4.2(6)
O2	21.3(8)	34.3(9)	20.6(8)	-6.6(7)	-8.0(6)	-3.4(7)
O3	19.1(8)	34.9(9)	23.8(8)	-6.5(7)	-7.6(7)	1.6(7)
N2	17.9(9)	25.0(10)	15.5(9)	-6.6(7)	-4.3(7)	-4.2(7)
N1	18.6(9)	23.4(9)	20.8(9)	-5.0(8)	-3.9(7)	-4.0(7)
N3	20.7(9)	23.5(10)	21.2(9)	-4.2(8)	-9.3(8)	-3.7(7)
C7	19.0(10)	18.6(10)	21.1(11)	-7.7(8)	-4.0(8)	-5.2(8)
C6	20.1(10)	16.0(10)	20.6(11)	-3.0(8)	-7.2(9)	-4.1(8)
C16	13.5(10)	29.4(12)	16.6(10)	-5.2(9)	-2.7(8)	-1.2(8)
C1	17.8(10)	16.2(10)	21.6(11)	-1.6(8)	-6.6(8)	-3.4(8)
C13	17.0(10)	19.0(10)	25.3(11)	-7.5(9)	-7.8(9)	-3.1(8)
C3	17.0(10)	23.2(11)	30.9(12)	-6.8(9)	-7.5(9)	-4.9(8)
C5	17.7(10)	14.8(10)	19.9(11)	-2.3(8)	-5.3(8)	-3.2(8)
C8	20.0(11)	21.2(11)	22.0(11)	-7.5(9)	-6.1(9)	-4.1(8)
C12	19.5(11)	20.2(11)	22.3(11)	-5.9(9)	-5.6(9)	-3.5(8)
C17	17.9(11)	25.6(12)	22.9(11)	-4.0(9)	-4.6(9)	-4.1(9)
C4	22.4(11)	18.6(10)	21.3(11)	-3.9(9)	-8.1(9)	-5.9(8)
C14	23.1(11)	22.4(11)	22.8(11)	-2.6(9)	-10.6(9)	-4.2(9)
C19	20.3(11)	32.6(12)	18.4(11)	-4.6(9)	-7.2(9)	-6.6(9)
C2	17.5(11)	23.3(11)	25.2(12)	-6.2(9)	-1.2(9)	-5.0(8)
C21	18.8(11)	28.9(12)	23.2(11)	-10.5(9)	-2.4(9)	-6.7(9)
C18	21.1(11)	28.1(12)	24.7(12)	-7.6(9)	-6.0(9)	-5.4(9)
C11	28.0(12)	27.7(12)	15.7(10)	-4.5(9)	-5.0(9)	-9.7(9)
C20	17.6(10)	25.8(11)	20.8(11)	-3.2(9)	-4.1(9)	-4.8(9)
C15	21.4(11)	24.0(11)	24.9(12)	-3.4(9)	-10.6(9)	0.5(9)

C9	17.8(11)	30.5(12)	27.2(12)	-10.6(10)	-4.9(9)	-4.1(9)
C10	20.7(11)	34.6(13)	23.7(12)	-11.5(10)	0.5(9)	-6.8(9)

Table 4 Bond Lengths for 54-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C20	1.747(2)	C16	C21	1.394(3)
O1	C16	1.405(2)	C1	C5	1.408(3)
O1	C1	1.371(2)	C13	C8	1.472(3)
O2	C6	1.227(2)	C3	C4	1.384(3)
O3	C13	1.365(2)	C3	C2	1.379(3)
O3	C15	1.450(3)	C5	C4	1.396(3)
N2	C7	1.412(3)	C8	C9	1.402(3)
N2	C6	1.364(3)	C12	C11	1.375(3)
N1	C1	1.319(3)	C17	C18	1.384(3)
N1	C2	1.348(3)	C14	C15	1.529(3)
N3	C13	1.273(3)	C19	C18	1.399(3)
N3	C14	1.476(3)	C19	C20	1.385(3)
C7	C8	1.421(3)	C21	C20	1.388(3)
C7	C12	1.403(3)	C11	C10	1.392(3)
C6	C5	1.508(3)	C9	C10	1.383(3)
C16	C17	1.379(3)			

Table 5 Bond Angles for 54-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C16	118.90(16)	C1	C5	C6	128.43(18)
C13	O3	C15	106.01(16)	C4	C5	C6	115.67(18)
C6	N2	C7	125.03(18)	C4	C5	C1	115.90(19)
C1	N1	C2	117.15(19)	C7	C8	C13	122.78(19)
C13	N3	C14	106.93(17)	C9	C8	C7	118.87(19)
N2	C7	C8	119.84(18)	C9	C8	C13	118.35(19)
C12	C7	N2	121.24(18)	C11	C12	C7	120.7(2)
C12	C7	C8	118.88(19)	C16	C17	C18	118.4(2)
O2	C6	N2	123.4(2)	C3	C4	C5	120.5(2)
O2	C6	C5	118.39(18)	N3	C14	C15	104.54(17)
N2	C6	C5	118.23(18)	C20	C19	C18	118.4(2)
C17	C16	O1	119.64(19)	N1	C2	C3	123.7(2)
C17	C16	C21	122.29(19)	C20	C21	C16	117.7(2)

C21	C16	O1	117.90(19)	C17	C18	C19	121.4(2)
O1	C1	C5	117.88(18)	C12	C11	C10	120.9(2)
N1	C1	O1	117.39(18)	C19	C20	Cl1	120.07(17)
N1	C1	C5	124.72(19)	C19	C20	C21	121.9(2)
O3	C13	C8	115.51(18)	C21	C20	Cl1	118.03(17)
N3	C13	O3	117.75(19)	O3	C15	C14	104.01(16)
N3	C13	C8	126.73(19)	C10	C9	C8	121.3(2)
C2	C3	C4	117.88(19)	C9	C10	C11	119.3(2)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 54-1.

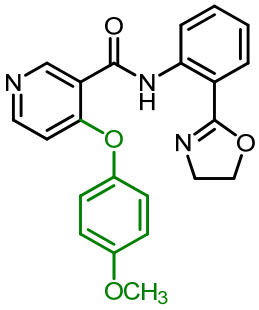
Atom	*x*	*y*	*z*	U(eq)
H2	7909.66	7768.57	5047.83	23
H3	146.28	8887.64	6180.92	28
H12	8241.43	8924.19	1851.07	25
H17	6344.49	9883.92	7962.9	28
H4	2645.56	8688.85	4453.23	24
H14A	10213.11	4689.56	7371.55	27
H14B	10508.72	6009.27	7536.02	27
H19	7457.2	7070.55	11060.59	28
H2A	592.55	8646.64	8112.25	28
H21	6655.05	5964.34	8295.84	28
H18	6978.94	9309.23	9904.68	29
H11	10807.23	8705.39	221.85	28
H15A	13407.64	5596.58	6500.76	29
H15B	13166.81	4175.17	6529.07	29
H9	13622.7	6406.6	2703.36	30
H10	13506.08	7432.02	630.65	32

Experimental

Single crystals of $C_{21}H_{16}ClN_3O_3$ **[5m]** were **[]**. A suitable crystal was selected and **[]** on a **SuperNova, Dual, Cu at zero, AtlasS2** diffractometer. The crystal was kept at 100.00(10) K during data collection.

Crystal structure determination of [5m]

Crystal Data for $C_{21}H_{16}ClN_3O_3$ (M =393.82 g/mol): triclinic, space group P-1 (no. 2), a = 8.0444(10) Å, b = 10.7234(12) Å, c = 11.5467(13) Å, α = 71.104(10)°, β = 70.410(11)°, γ = 73.474(10)°, V = 870.4(2) Å^3, Z = 2, T = 100.00(10) K, μ(MoKα) = 0.249 mm^{-1}, *Dcalc* = 1.503 g/cm^3, 11524 reflections measured (4.096° ≤ 2Θ ≤ 59.172°), 4192 unique (R_{int} = 0.0448, R_{sigma} = 0.0583) which were used in all calculations. The final R_1 was 0.0561 (I > 2σ(I)) and wR_2 was 0.1414 (all data).



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-4-(4-methoxyphenoxy)nicotinamide (**6a**),

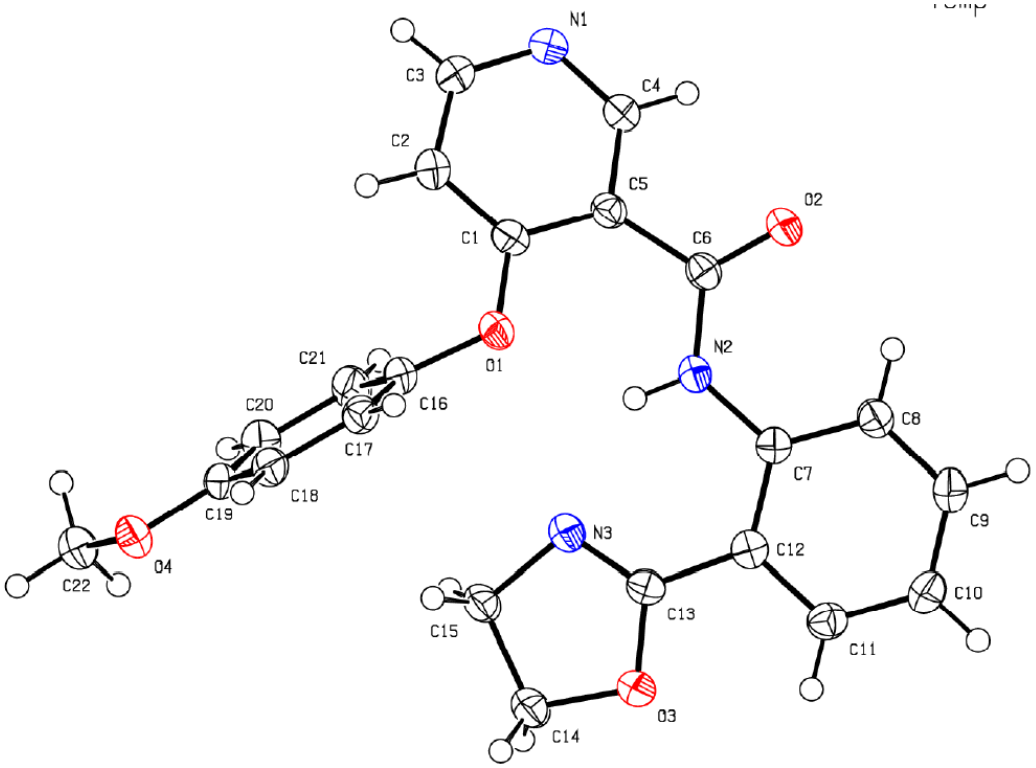


Table 1 Crystal data and structure refinement for E0-6-2-4.

Identification code	E0-6-2-4
Empirical formula	$C_{22}H_{19}N_3O_4$
Formula weight	389.40
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.75620(10)
b/Å	23.4732(3)
c/Å	8.8632(2)
α/°	90
β/°	92.210(2)
γ/°	90
Volume/Å^3	1820.35(5)
Z	4

ρ_{calc}g/cm^3	1.421
μ/mm^{-1}	0.819
F(000)	816.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.532 to 147.968
Index ranges	-10 ≤ h ≤ 10, -28 ≤ k ≤ 14, -10 ≤ l ≤ 10
Reflections collected	9852
Independent reflections	3593 [R_{int} = 0.0255, R_{sigma} = 0.0280]
Data/restraints/parameters	3593/0/263
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0382, wR_2 = 0.0967
Final R indexes [all data]	R_1 = 0.0435, wR_2 = 0.0990
Largest diff. peak/hole / e Å^{-3}	0.16/-0.27

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for E0-6-2-4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	6680.0(11)	6548.7(4)	6012.4(11)	30.6(2)
O4	9554.6(11)	6807.7(4)	11636.5(10)	29.1(2)
O3	9098.8(11)	4525.0(4)	6509.8(10)	30.8(2)
O2	4381.2(12)	5944.2(4)	2215(1)	33.3(2)
N2	5970.9(12)	5612.2(5)	4124.1(12)	23.7(2)
N3	7625.2(13)	5309.5(5)	6663.1(12)	27.7(3)
N1	2295.9(16)	7110.9(6)	4790.1(15)	40.1(3)
C12	7637.8(14)	4781.9(6)	4277.8(14)	23.9(3)
C6	4943.3(14)	5987.0(6)	3498.0(14)	23.4(3)
C7	6567.6(14)	5121.8(5)	3440.9(14)	22.9(3)
C19	8736.6(15)	6751.1(5)	10295.5(15)	24.1(3)
C17	8762.5(15)	6876.1(6)	7595.9(15)	26.1(3)
C18	9470.4(15)	6930.5(6)	9014.2(15)	26.0(3)
C13	8095.8(14)	4903.1(6)	5859.6(15)	23.9(3)
C5	4433.0(15)	6472.6(6)	4459.9(14)	24.4(3)
C16	7311.9(15)	6645.0(6)	7474.6(15)	26.0(3)
C4	2980.0(16)	6686.9(6)	4085.6(15)	28.9(3)
C1	5233.0(16)	6735.2(6)	5665.1(15)	28.1(3)
C8	6146.1(15)	4955.1(6)	1967.7(15)	26.8(3)
C11	8250.7(16)	4299.3(6)	3602.2(16)	28.3(3)

C9	6757.9(16)	4468.8(6)	1341.2(15)	28.7(3)
C21	6557.5(16)	6474.8(6)	8732.0(16)	30.6(3)
C15	8350.4(16)	5244.3(6)	8178.4(15)	28.7(3)
C20	7264.8(16)	6528.5(6)	10154.0(16)	29.5(3)
C14	9301.1(17)	4698.5(6)	8077.1(15)	30.9(3)
C22	8796.2(17)	6658.8(6)	12980.9(15)	31.8(3)
C10	7814.1(16)	4140.3(6)	2147.8(16)	30.4(3)
C2	4557.2(19)	7186.4(7)	6402.6(18)	40.5(4)
C3	3104(2)	7353.5(7)	5931.8(19)	46.6(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for E0-6-2-4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	26.5(5)	36.4(5)	28.2(5)	-7.9(4)	-7.6(4)	2.8(4)
O4	27.4(5)	35.8(5)	23.7(5)	-1.9(4)	-2.8(4)	-2.9(4)
O3	32.9(5)	33.1(5)	26.2(5)	-1.0(4)	-4.5(4)	8.1(4)
O2	37.0(6)	40.0(6)	22.3(5)	-4.7(4)	-6.9(4)	8.8(4)
N2	24.9(5)	26.3(6)	19.8(5)	-2.3(4)	-1.6(4)	1.1(4)
N3	30.7(6)	30.7(6)	21.6(5)	0.3(5)	-0.9(4)	2.4(5)
N1	42.9(8)	40.2(7)	36.1(7)	-9.4(6)	-13.2(6)	16.6(6)
C12	22.4(6)	25.6(6)	24.0(6)	0.8(5)	2.8(5)	-2.8(5)
C6	21.9(6)	26.8(7)	21.6(6)	0.9(5)	0.3(5)	-2.2(5)
C7	20.9(6)	24.8(6)	23.0(6)	-0.7(5)	3.1(5)	-2.5(5)
C19	24.6(6)	21.4(6)	26.1(6)	-3.3(5)	-3.5(5)	0.4(5)
C17	28.3(7)	23.1(6)	26.9(7)	-1.3(5)	0.4(5)	-1.3(5)
C18	22.2(6)	24.4(7)	31.3(7)	-3.8(5)	-1.8(5)	-3.6(5)
C13	20.9(6)	25.5(7)	25.1(6)	3.0(5)	0.9(5)	-0.5(5)
C5	27.1(7)	23.9(6)	21.9(6)	2.0(5)	-1.6(5)	-0.9(5)
C16	26.0(7)	24.6(6)	26.8(7)	-5.5(5)	-6.0(5)	1.4(5)
C4	32.4(7)	28.1(7)	25.7(7)	-1.5(5)	-5.7(5)	4.0(6)
C1	28.3(7)	28.5(7)	27.0(7)	0.3(5)	-5.3(5)	2.3(5)
C8	25.1(7)	31.0(7)	24.2(7)	-1.5(5)	-0.3(5)	-0.5(5)
C11	26.9(7)	28.8(7)	29.4(7)	0.8(6)	2.7(5)	2.1(5)
C9	29.2(7)	33.0(7)	24.1(6)	-5.6(5)	2.6(5)	-4.1(6)
C21	22.4(7)	34.8(8)	34.3(7)	-5.1(6)	-2.2(5)	-5.0(5)
C15	30.1(7)	34.0(7)	21.7(6)	0.7(5)	-1.7(5)	1.8(6)
C20	26.5(7)	33.2(7)	28.9(7)	-1.7(6)	3.0(5)	-3.4(5)
C14	32.8(7)	36.1(8)	23.4(7)	1.2(6)	-2.9(5)	2.6(6)
C22	35.0(8)	34.8(8)	25.6(7)	0.2(6)	0.0(6)	0.6(6)

C10	31.4(7)	29.0(7)	31.1(7)	-5.7(6)	5.3(6)	1.4(6)
C2	46.8(9)	36.9(8)	36.4(8)	-13.7(7)	-15.7(7)	10.9(7)
C3	51.7(10)	43.4(9)	43.2(9)	-16.9(8)	-17.0(8)	23.1(8)

Table 4 Bond Lengths for E0-6-2-4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C16	1.4077(15)	C6	C5	1.5018(18)
O1	C1	1.3645(16)	C7	C8	1.3990(18)
O4	C19	1.3703(15)	C19	C18	1.3915(19)
O4	C22	1.4297(16)	C19	C20	1.3918(19)
O3	C13	1.3609(16)	C17	C18	1.3859(18)
O3	C14	1.4518(16)	C17	C16	1.3815(19)
O2	C6	1.2256(15)	C5	C4	1.3961(19)
N2	C6	1.3613(17)	C5	C1	1.3978(18)
N2	C7	1.4104(17)	C16	C21	1.376(2)
N3	C13	1.2687(17)	C1	C2	1.389(2)
N3	C15	1.4713(16)	C8	C9	1.3861(19)
N1	C4	1.3299(19)	C11	C10	1.3817(19)
N1	C3	1.339(2)	C9	C10	1.382(2)
C12	C7	1.4182(18)	C21	C20	1.3884(19)
C12	C13	1.4710(18)	C15	C14	1.532(2)
C12	C11	1.3981(19)	C2	C3	1.381(2)

Table 5 Bond Angles for E0-6-2-4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C16	119.00(10)	N3	C13	C12	126.72(12)
C19	O4	C22	117.07(11)	C4	C5	C6	115.27(11)
C13	O3	C14	105.97(10)	C4	C5	C1	116.61(12)
C6	N2	C7	127.04(11)	C1	C5	C6	128.12(12)
C13	N3	C15	107.22(11)	C17	C16	O1	117.53(12)
C4	N1	C3	116.02(13)	C21	C16	O1	121.00(12)
C7	C12	C13	122.69(12)	C21	C16	C17	121.29(12)
C11	C12	C7	119.25(12)	N1	C4	C5	125.52(13)
C11	C12	C13	118.02(12)	O1	C1	C5	117.68(12)
O2	C6	N2	124.10(12)	O1	C1	C2	123.18(12)
O2	C6	C5	118.12(12)	C2	C1	C5	119.07(13)
N2	C6	C5	117.75(11)	C9	C8	C7	120.81(13)

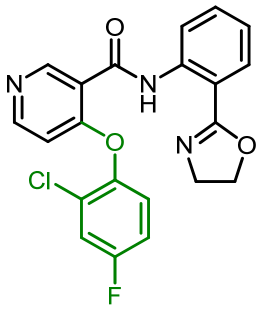
N2	C7	C12	118.87(11)	C10	C11	C12	121.43(13)
C8	C7	N2	122.71(12)	C10	C9	C8	120.90(13)
C8	C7	C12	118.42(12)	C16	C21	C20	119.83(13)
O4	C19	C18	115.86(11)	N3	C15	C14	104.47(11)
O4	C19	C20	124.46(12)	C21	C20	C19	119.67(13)
C18	C19	C20	119.68(12)	O3	C14	C15	104.13(10)
C16	C17	C18	118.98(13)	C11	C10	C9	119.17(13)
C17	C18	C19	120.52(12)	C3	C2	C1	118.62(14)
O3	C13	C12	115.17(11)	N1	C3	C2	124.14(14)
N3	C13	O3	118.09(12)				

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for E0-6-2-4.

Atom	*x*	*y*	*z*	U(eq)
H2	6290.84	5682.01	5034.95	28
H17	9256.29	6993.32	6739.03	31
H18	10443.65	7088.18	9110.35	31
H4	2445.38	6518.83	3275.06	35
H8	5446.87	5173.19	1401.72	32
H11	8967.8	4080.55	4143.44	34
H9	6453.51	4362.11	364.79	34
H21	5576.47	6324.34	8629.32	37
H15A	7586.03	5206.99	8935.77	34
H15B	8997.36	5568.7	8430.29	34
H20	6757.61	6416.29	11007.63	35
H14A	10369.18	4772.68	8335.51	37
H14B	8929.6	4407.46	8747.69	37
H22A	8540.51	6261.12	12955.31	48
H22B	7879.34	6880.32	13045.05	48
H22C	9459.34	6734.98	13845.14	48
H10	8225.78	3816.28	1717.03	36
H2A	5072.78	7372.02	7196.92	49
H3	2657.44	7653.56	6439.82	56

Crystal structure determination of [E0-6-2-4]

Crystal Data for $C_{22}H_{19}N_3O_4$ (M =389.40 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 8.75620(10) Å, b = 23.4732(3) Å, c = 8.8632(2) Å, β = 92.210(2)°, V = 1820.35(5) Å^3, Z = 4, T = 150.00(10) K, μ(CuKα) = 0.819 mm^{-1}, *Dcalc* = 1.421 g/cm^3, 9852 reflections measured (7.532° ≤ 2Θ ≤ 147.968°), 3593 unique (R_{int} = 0.0255, R_{sigma} = 0.0280) which were used in all calculations. The final R_1 was 0.0382 (I > 2σ(I)) and wR_2 was 0.0990 (all data).



4-(2-chloro-4-fluorophenoxy)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (**6q**)

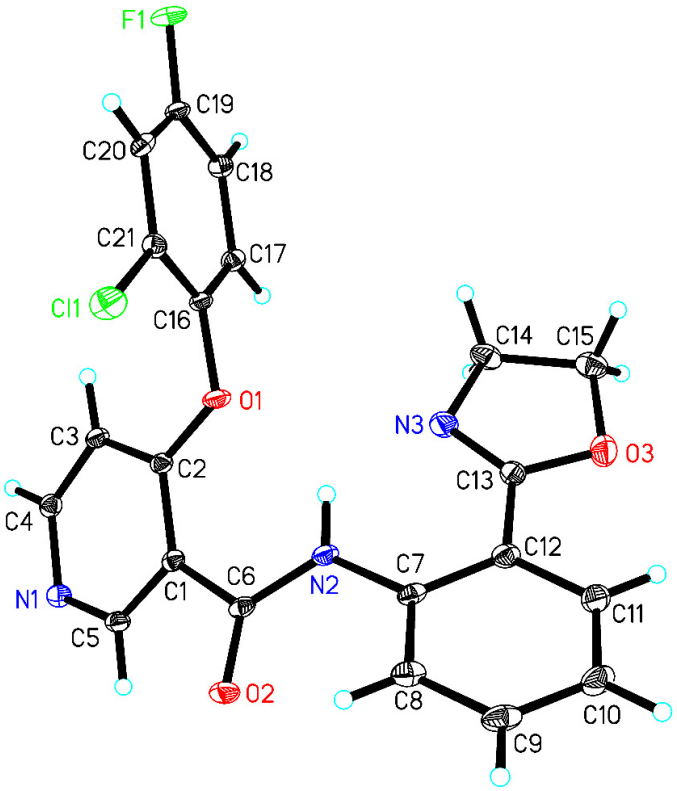


Table 1 Crystal data and structure refinement for 6q.

Identification code	**6q**
Empirical formula	$C_{21}H_{15}ClFN_3O_3$
Formula weight	411.81
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.3959(4)
b/Å	19.3566(12)
c/Å	12.7098(9)
α/°	90
β/°	91.147(6)
γ/°	90

Volume/Å^3	1819.2(2)
Z	4
ρ_{calc}g/cm^3	1.504
μ/mm^{-1}	0.250
F(000)	848.0
Crystal size/mm^3	0.14 × 0.13 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.208 to 59.036
Index ranges	-10 ≤ h ≤ 8, -26 ≤ k ≤ 26, -17 ≤ l ≤ 17
Reflections collected	14810
Independent reflections	4489 [R_{int} = 0.0370, R_{sigma} = 0.0415]
Data/restraints/parameters	4489/0/262
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0445, wR_2 = 0.1002
Final R indexes [all data]	R_1 = 0.0575, wR_2 = 0.1079
Largest diff. peak/hole / e Å^{-3}	0.29/-0.43

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 58-3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	10208.2(5)	3654.8(2)	7800.1(4)	33.96(14)
F1	5419.8(13)	1810.2(5)	8097.7(8)	29.4(2)
O1	7131.2(16)	4478.4(5)	7088.1(9)	22.1(3)
O2	9517.9(15)	6355.5(6)	6530.5(9)	24.3(3)
O3	3339.4(17)	6054.9(7)	9807.8(10)	34.2(3)
N2	7676.1(17)	5820.9(6)	7701.7(10)	19.1(3)
N1	7692.8(17)	5208.7(7)	4023.3(11)	20.9(3)
N3	4549.2(19)	5369.9(7)	8571.5(11)	26.2(3)
C2	7303.3(19)	4696.3(7)	6070.6(12)	16.7(3)
C6	8474(2)	5887.6(7)	6750.4(12)	17.7(3)
C5	8114(2)	5584.6(8)	4877.5(13)	19.4(3)
C16	6677(2)	3792.1(7)	7287.7(12)	17.4(3)
C18	4489(2)	2886.5(8)	7423.7(12)	19.9(3)
C1	7937.6(19)	5371.1(7)	5915.2(12)	16.7(3)
C4	7099(2)	4567.4(8)	4206.5(13)	20.0(3)
C19	5848(2)	2466.2(7)	7808.2(12)	18.9(3)
C3	6902(2)	4286.4(8)	5196.7(12)	19.2(3)
C21	8021(2)	3353.1(8)	7667.3(12)	19.2(3)
C7	7733(2)	6321.8(8)	8508.3(12)	19.7(3)

C20	7611(2)	2676.6(8)	7948.9(13)	20.2(3)
C17	4912(2)	3564.8(8)	7171.7(12)	19.5(3)
C12	6255(2)	6384.8(8)	9187.5(13)	22.4(3)
C13	4703(2)	5906.2(8)	9143.5(12)	21.4(3)
C8	9220(2)	6759.5(8)	8660.1(13)	25.2(4)
C11	6272(3)	6903.0(9)	9946.0(13)	29.2(4)
C14	2782(2)	5054.8(9)	8807.0(14)	28.8(4)
C9	9202(3)	7267.3(9)	9431.3(14)	31.7(4)
C10	7726(3)	7349.0(9)	10068.4(14)	34.1(4)
C15	2116(2)	5467.3(9)	9743.5(15)	30.5(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 58-3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	18.7(2)	29.3(2)	53.8(3)	0.3(2)	-1.6(2)	-5.31(16)
F1	35.3(6)	12.9(5)	39.8(6)	7.6(4)	-5.2(5)	-5.1(4)
O1	34.7(6)	11.5(5)	19.9(6)	0.8(4)	-0.4(5)	-4.6(5)
O2	26.2(6)	17.8(6)	28.8(7)	0.3(5)	1.9(5)	-8.0(5)
O3	33.1(7)	33.3(7)	36.5(8)	-6.9(6)	11.0(6)	-2.4(6)
N2	22.8(7)	12.6(6)	22.0(7)	-0.6(5)	-0.3(5)	-3.4(5)
N1	21.6(6)	19.7(7)	21.2(7)	1.4(5)	-0.3(6)	-0.1(5)
N3	28.4(7)	23.8(7)	26.3(8)	-2.5(6)	2.1(6)	-8.3(6)
C2	15.4(7)	14.2(7)	20.5(8)	2.3(6)	0.6(6)	1.9(6)
C6	16.5(7)	12.5(7)	24.0(8)	2.7(6)	-3.1(6)	2.5(6)
C5	17.6(7)	15.4(7)	25.4(8)	3.7(6)	0.7(6)	0.2(6)
C16	25.7(8)	10.5(7)	16.2(7)	0.0(5)	1.4(6)	-1.3(6)
C18	19.2(7)	18.5(8)	21.9(8)	-0.9(6)	-1.3(6)	-3.0(6)
C1	13.0(7)	14.5(7)	22.6(8)	0.5(6)	-0.3(6)	1.6(6)
C4	18.4(7)	19.1(8)	22.7(8)	-3.3(6)	0.4(6)	-0.6(6)
C19	27.0(8)	10.1(7)	19.6(8)	1.1(6)	0.5(6)	-1.3(6)
C3	19.5(7)	13.2(7)	24.9(8)	-0.6(6)	1.8(6)	-1.3(6)
C21	17.6(7)	19.3(8)	20.8(8)	-1.6(6)	1.7(6)	-2.6(6)
C7	27.3(8)	12.8(7)	18.7(8)	2.0(6)	-5.6(7)	-0.6(6)
C20	22.8(8)	14.1(7)	23.8(8)	-0.3(6)	-1.0(7)	5.2(6)
C17	21.9(8)	17.0(8)	19.5(8)	1.4(6)	-2.3(6)	2.7(6)
C12	30.5(9)	18.7(8)	17.8(8)	1.9(6)	-3.5(7)	-1.7(7)
C13	26.4(8)	20.5(8)	17.3(8)	2.3(6)	0.0(7)	0.8(7)
C8	30.4(9)	20.6(8)	24.3(9)	3.6(6)	-6.1(7)	-4.6(7)
C11	44.8(11)	23.1(8)	19.7(8)	-0.7(7)	0.7(8)	-2.1(8)
C14	27.5(9)	31.0(9)	27.9(9)	3.7(7)	-1.0(7)	-10.2(7)
C9	45.8(11)	22.7(9)	26.1(9)	2.2(7)	-11.9(8)	-12.6(8)

C10	57.6(12)	22.4(9)	22.2(9)	-5.5(7)	-4.9(9)	-8.1(8)
C15	24.3(8)	31.1(10)	36.1(10)	8.0(8)	2.2(8)	-1.6(7)

Table 4 Bond Lengths for 58-3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C21	1.7247(16)	C5	C1	1.391(2)
F1	C19	1.3612(17)	C16	C21	1.387(2)
O1	C2	1.3687(18)	C16	C17	1.382(2)
O1	C16	1.3947(17)	C18	C19	1.375(2)
O2	C6	1.2260(18)	C18	C17	1.389(2)
O3	C13	1.359(2)	C4	C3	1.381(2)
O3	C15	1.455(2)	C19	C20	1.375(2)
N2	C6	1.362(2)	C21	C20	1.392(2)
N2	C7	1.411(2)	C7	C12	1.412(2)
N1	C5	1.339(2)	C7	C8	1.398(2)
N1	C4	1.339(2)	C12	C13	1.475(2)
N3	C13	1.271(2)	C12	C11	1.391(2)
N3	C14	1.478(2)	C8	C9	1.388(2)
C2	C1	1.403(2)	C11	C10	1.385(3)
C2	C3	1.392(2)	C14	C15	1.523(3)
C6	C1	1.506(2)	C9	C10	1.381(3)

Table 5 Bond Angles for 58-3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O1	C16	119.52(12)	C20	C19	C18	123.76(14)
C13	O3	C15	105.55(13)	C4	C3	C2	118.55(14)
C6	N2	C7	124.92(13)	C16	C21	Cl1	119.40(12)
C4	N1	C5	115.78(14)	C16	C21	C20	120.48(14)
C13	N3	C14	106.90(14)	C20	C21	Cl1	120.12(12)
O1	C2	C1	117.23(13)	N2	C7	C12	119.42(14)
O1	C2	C3	123.77(13)	C8	C7	N2	121.92(15)
C3	C2	C1	119.00(14)	C8	C7	C12	118.67(15)
O2	C6	N2	123.94(14)	C19	C20	C21	117.13(14)
O2	C6	C1	119.21(14)	C16	C17	C18	119.53(14)
N2	C6	C1	116.75(13)	C7	C12	C13	122.28(14)
N1	C5	C1	125.66(14)	C11	C12	C7	119.31(15)
C21	C16	O1	118.23(14)	C11	C12	C13	118.39(16)
C17	C16	O1	120.95(13)	O3	C13	C12	115.46(14)
C17	C16	C21	120.71(14)	N3	C13	O3	117.98(15)

C19	C18	C17	118.37(14)	N3	C13	C12	126.54(15)
C2	C1	C6	127.08(14)	C9	C8	C7	120.50(17)
C5	C1	C2	116.62(14)	C10	C11	C12	121.57(17)
C5	C1	C6	116.29(13)	N3	C14	C15	104.06(14)
N1	C4	C3	124.36(15)	C10	C9	C8	120.93(17)
F1	C19	C18	118.41(14)	C9	C10	C11	118.92(16)
F1	C19	C20	117.80(13)	O3	C15	C14	104.07(13)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 58-3.

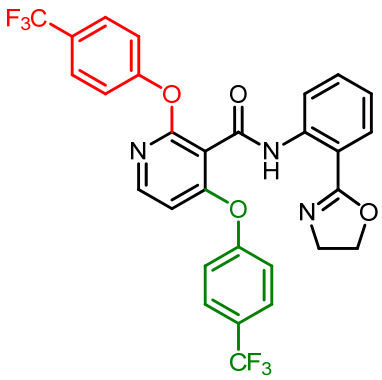
Atom	*x*	*y*	*z*	U(eq)
H2	7093.33	5445.21	7819.59	23
H5	8563.78	6026.89	4767.59	23
H18	3316.07	2720.58	7334.61	24
H4	6797.89	4292.77	3628.61	24
H3	6510.69	3833.24	5277.77	23
H20	8492.86	2379.87	8220.4	24
H17	4014.42	3863.98	6926.54	23
H8	10228.98	6709.99	8241.38	30
H11	5284.12	6951.14	10381.21	35
H14A	2920.07	4570.27	8986.19	35
H14B	1950.33	5095.96	8210.62	35
H9	10197.17	7556.57	9520.13	38
H10	7707.99	7697.73	10571.37	41
H15A	877.75	5618.3	9626.65	37
H15B	2183.41	5194.42	10383.19	37

Experimental

Single crystals of $C_{21}H_{15}ClFN_3O_3$ **[6q]** were **[]**. A suitable crystal was selected and **[]** on a **SuperNova, Dual, Cu at zero, AtlasS2** diffractometer. The crystal was kept at 99.99(10) K during data collection.

Crystal structure determination of [6q]

Crystal Data for $C_{21}H_{15}ClFN_3O_3$ (M =411.81 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 7.3959(4) Å, b = 19.3566(12) Å, c = 12.7098(9) Å, β = 91.147(6)°, V = 1819.2(2) Å^3, Z = 4, T = 99.99(10) K, μ(MoKα) = 0.250 mm^{-1}, *Dcalc* = 1.504 g/cm^3, 14810 reflections measured (4.208° ≤ 2Θ ≤ 59.036°), 4489 unique (R_{int} = 0.0370, R_{sigma} = 0.0415) which were used in all calculations. The final R_1 was 0.0445 (I > 2σ(I)) and wR_2 was 0.1079 (all data).



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2,4-bis(4-(trifluoromethyl)phenoxy) nicotinamide (**7d**)

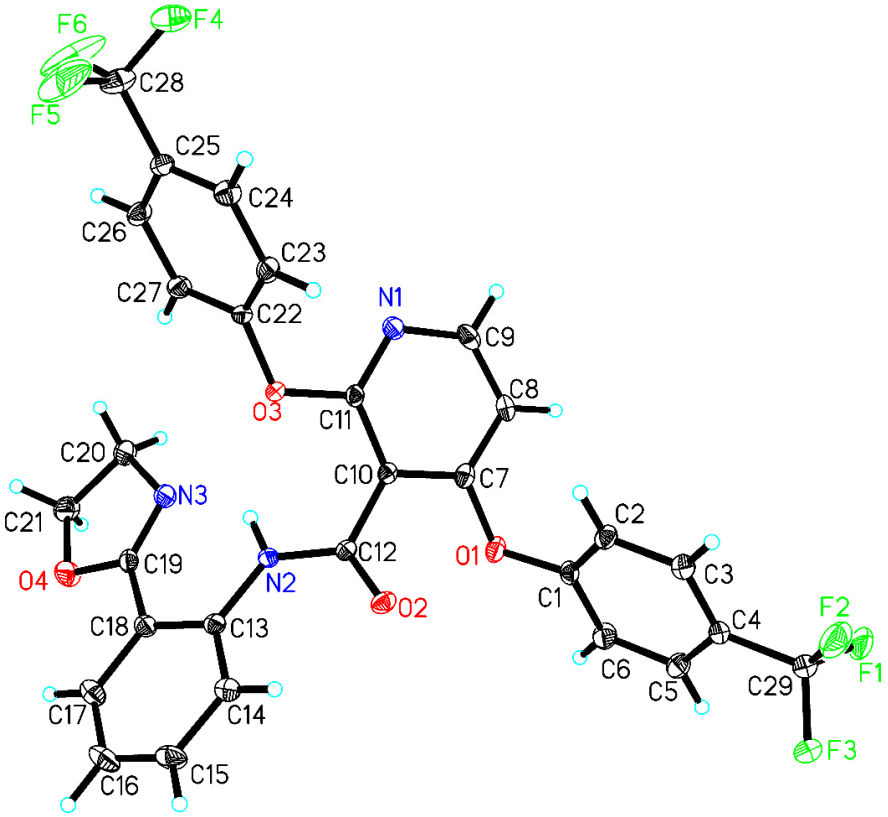


Table 1 Crystal data and structure refinement for 7d.

Identification code	**7d**
Empirical formula	$C_{29}H_{19}F_6N_3O_4$
Formula weight	587.47
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.9357(8)

b/Å	13.7866(8)
c/Å	11.8725(7)
α/°	90
β/°	93.908(5)
γ/°	90
Volume/Å^3	2602.3(3)
Z	4
ρ_{calc}g/cm^3	1.499
μ/mm^{-1}	0.130
F(000)	1200.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.534 to 59.172
Index ranges	-21 ≤ h ≤ 21, -12 ≤ k ≤ 19, -11 ≤ l ≤ 16
Reflections collected	13946
Independent reflections	6166 [R_{int} = 0.0347, R_{sigma} = 0.0566]
Data/restraints/parameters	6166/7/379
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0643, wR_2 = 0.1500
Final R indexes [all data]	R_1 = 0.0902, wR_2 = 0.1664
Largest diff. peak/hole / e Å^{-3}	0.66/-0.60

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for X_48. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	*x*	*y*	*z*	U(eq)
F3	503.6(9)	4083.2(12)	6449.3(15)	44.8(4)
O3	6823.0(9)	5589.1(11)	5949.8(14)	25.2(4)
O2	4906.3(9)	3850.9(12)	5553.6(14)	25.6(4)
O1	4369.3(10)	4561.7(12)	7607.6(14)	28.1(4)
O4	8561.5(11)	2192.3(13)	6999.2(17)	37.5(5)
F2	645.2(10)	5524.5(14)	5812(2)	70.0(7)
N2	6305.1(11)	3659.3(13)	6072.6(15)	19.8(4)
F1	490.5(10)	5293.0(15)	7568(2)	69.0(7)
N1	6141.0(12)	6683.1(15)	7063.4(17)	25.9(4)
N3	7854.2(12)	3600.4(15)	7110.4(18)	27.6(5)
F5	9214.3(16)	8303(2)	3433.4(18)	90.9(9)
C13	6478.9(14)	2764.6(16)	5574.1(18)	21.0(5)
C11	6168.5(13)	5811.1(16)	6588.5(18)	19.9(5)

C12	5558.3(13)	4138.2(16)	6043.7(17)	18.2(4)
C22	7353.6(14)	6333.3(16)	5626.2(19)	21.2(5)
C10	5570.3(13)	5070.7(16)	6698.3(18)	18.4(4)
C7	4923.8(14)	5292.6(17)	7380.3(19)	22.3(5)
C19	7878.4(14)	2747.6(17)	6701.6(19)	23.6(5)
C1	3514.9(14)	4710.7(17)	7366.3(19)	23.1(5)
C25	8463.4(14)	7687.5(17)	4902.5(19)	23.2(5)
C18	7248.5(15)	2299.2(17)	5899.1(19)	23.8(5)
C8	4871.8(15)	6189.0(18)	7898.0(19)	25.7(5)
F6	9778.3(14)	8445(2)	5057(2)	108.4(10)
C27	8188.6(14)	6281.7(17)	6016(2)	25.8(5)
C9	5483.2(15)	6855.1(18)	7700(2)	28.4(5)
C26	8748.4(14)	6962.8(18)	5649(2)	27.0(5)
C14	5925.2(15)	2324.1(18)	4764.0(19)	25.8(5)
C2	3202.2(14)	5421.5(18)	6631(2)	25.1(5)
C3	2341.1(15)	5499.6(18)	6400(2)	27.6(5)
C23	7063.1(14)	7041.9(18)	4878(2)	26.2(5)
C4	1802.0(15)	4859.1(18)	6897(2)	27.7(5)
C24	7619.7(15)	7720.0(18)	4513(2)	27.4(5)
C6	2985.3(15)	4064.9(19)	7863(2)	31.1(6)
F4	8756.6(17)	9304.7(15)	4490(3)	117.7(12)
C20	8643.4(15)	3744.1(19)	7818(2)	32.8(6)
C28	9062.5(18)	8424(2)	4498(2)	38.2(6)
C15	6121.8(18)	1426.7(19)	4318(2)	34.5(6)
C5	2128.1(16)	4145.4(19)	7627(2)	33.6(6)
C17	7418.1(17)	1386.5(18)	5451(2)	33.3(6)
C16	6855.6(19)	952(2)	4668(2)	39.9(7)
C29	868.7(16)	4940(2)	6678(3)	39.1(7)
C21	9064.5(16)	2748(2)	7834(3)	36.8(6)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for X_48. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F3	29.5(8)	34.1(9)	71.1(12)	-12.5(8)	5.7(8)	-9.1(7)
O3	18.9(8)	19.7(8)	37.8(9)	-4.4(7)	8.8(7)	-3.5(6)
O2	19.9(8)	26.2(9)	29.9(9)	1.2(7)	-4.7(7)	-4.2(7)
O1	19.5(8)	29.6(9)	35.9(9)	10.5(8)	7.3(7)	3.2(7)
O4	26.9(9)	28.2(10)	55.8(12)	-2.0(9)	-8.6(9)	9.6(8)
F2	29.0(9)	53.7(12)	123.9(19)	25.1(12)	-18.9(11)	-3.3(8)

N2	17.1(8)	19.6(10)	22.6(9)	-4.3(8)	-1.1(7)	-0.8(7)
F1	26.0(8)	69.3(14)	114.2(17)	-49.8(13)	22.0(10)	-5.4(8)
N1	21.0(9)	24.4(10)	31.7(11)	-6.0(9)	-2.5(8)	1.4(8)
N3	20.3(9)	27.1(11)	34.7(11)	-4.1(9)	-3.1(9)	1.8(8)
F5	109.7(19)	114(2)	53.4(12)	-2.0(13)	36.3(12)	-63.9(16)
C13	24.5(11)	19.7(11)	19.3(10)	1.5(9)	5.0(9)	-2.8(9)
C11	14.9(10)	22.3(12)	22.2(10)	-1.1(9)	-0.6(9)	2.4(9)
C12	18.3(10)	19.8(11)	16.5(10)	3.6(9)	1.8(8)	-1.8(9)
C22	20.4(10)	17.4(11)	26.4(11)	-4.6(9)	4.9(9)	-3.5(9)
C10	15.2(9)	20.3(11)	19.1(10)	3.4(9)	-2.6(8)	1.8(9)
C7	18.8(10)	27.1(12)	21.0(11)	6.4(10)	1.2(9)	2.9(9)
C19	20.6(11)	23.4(12)	27.3(11)	3.6(10)	5.7(9)	3.9(9)
C1	20.8(11)	24.4(12)	25.0(11)	0.3(10)	8.0(9)	3.1(9)
C25	24.0(11)	22.2(12)	23.5(11)	-0.2(10)	2.6(9)	-3.7(10)
C18	28.1(12)	20.7(12)	23.1(11)	1.6(9)	5.7(10)	-0.2(10)
C8	24.3(11)	30.4(13)	22.8(11)	-0.4(10)	3.8(9)	9.5(10)
F6	69.0(13)	131.3(19)	117.8(18)	85.5(16)	-45.9(13)	-69.8(14)
C27	24.0(11)	21.7(12)	31.3(12)	5.1(10)	-0.9(10)	0.5(10)
C9	31.5(13)	25.7(13)	27.1(12)	-8.5(10)	-3.6(10)	8.1(11)
C26	18.4(10)	29.2(13)	32.7(12)	2.0(11)	-3.2(10)	-3.2(10)
C14	31.5(12)	24.9(12)	21.2(11)	0.5(10)	2.7(10)	-2.5(10)
C2	22.0(11)	27.2(13)	26.8(11)	4.2(10)	6.6(9)	-2.0(10)
C3	25.3(12)	26.8(13)	30.6(12)	0.5(11)	1.2(10)	1.4(10)
C23	17.9(10)	29.7(13)	30.4(12)	-2.5(11)	-2.9(10)	0.6(10)
C4	22.0(11)	23.5(12)	38.4(14)	-5.8(11)	7.0(10)	-0.1(10)
C24	29.3(12)	26.2(13)	26.2(12)	4.9(10)	-1.7(10)	0.3(10)
C6	29.5(12)	28.7(13)	36.2(13)	10.7(11)	10.2(11)	1.6(11)
F4	100.2(19)	33.4(12)	230(4)	29.9(17)	88(2)	-5.3(12)
C20	18.8(11)	34.1(14)	44.5(15)	-2.9(12)	-5.1(11)	2.7(10)
C28	37.9(14)	35.0(14)	40.3(14)	13.8(12)	-6.4(12)	-11.7(12)
C15	47.0(16)	30.4(14)	25.9(12)	-8.7(11)	1.9(12)	-7.3(12)
C5	27.8(12)	31.0(14)	43.9(15)	3.7(12)	16.5(11)	-4.3(11)
C17	39.1(14)	24.7(13)	36.5(14)	-2.4(11)	4.6(12)	6.7(11)
C16	58.9(18)	26.2(14)	35.2(14)	-11.4(12)	7.2(13)	2.8(13)
C29	26.4(13)	26.5(14)	65.1(19)	-8.2(14)	7.8(13)	-3.1(11)
C21	24.8(12)	34.3(15)	50.2(16)	3.0(13)	-7.0(12)	1.4(11)

Table 4 Bond Lengths for X_48.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

F3	C29	1.337(3)	C10	C7	1.387(3)
O3	C11	1.365(3)	C7	C8	1.385(3)
O3	C22	1.400(3)	C19	C18	1.472(3)
O2	C12	1.222(2)	C1	C2	1.383(3)
O1	C7	1.379(3)	C1	C6	1.386(3)
O1	C1	1.387(3)	C25	C26	1.391(3)
O4	C19	1.358(3)	C25	C24	1.392(3)
O4	C21	1.451(3)	C25	C28	1.495(3)
F2	C29	1.335(4)	C18	C17	1.400(3)
N2	C13	1.404(3)	C8	C9	1.371(4)
N2	C12	1.359(3)	F6	C28	1.280(3)
F1	C29	1.343(3)	C27	C26	1.386(3)
N1	C11	1.330(3)	C14	C15	1.390(4)
N1	C9	1.354(3)	C2	C3	1.385(3)
N3	C19	1.274(3)	C3	C4	1.391(3)
N3	C20	1.478(3)	C23	C24	1.379(3)
F5	C28	1.314(4)	C4	C5	1.388(4)
C13	C18	1.414(3)	C4	C29	1.496(3)
C13	C14	1.399(3)	C6	C5	1.380(3)
C11	C10	1.409(3)	F4	C28	1.308(4)
C12	C10	1.502(3)	C20	C21	1.527(4)
C22	C27	1.381(3)	C15	C16	1.379(4)
C22	C23	1.379(3)	C17	C16	1.383(4)

Table 5 Bond Angles for X_48.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	O3	C22	119.12(17)	C17	C18	C13	119.4(2)
C7	O1	C1	118.97(17)	C17	C18	C19	118.9(2)
C19	O4	C21	106.00(19)	C9	C8	C7	117.2(2)
C12	N2	C13	127.85(18)	C22	C27	C26	119.1(2)
C11	N1	C9	116.4(2)	N1	C9	C8	124.4(2)
C19	N3	C20	107.08(19)	C27	C26	C25	119.9(2)
N2	C13	C18	118.42(19)	C15	C14	C13	120.0(2)
C14	C13	N2	122.6(2)	C1	C2	C3	119.3(2)
C14	C13	C18	119.0(2)	C2	C3	C4	119.9(2)
O3	C11	C10	115.87(19)	C22	C23	C24	119.2(2)
N1	C11	O3	119.1(2)	C3	C4	C29	120.9(2)
N1	C11	C10	125.0(2)	C5	C4	C3	119.9(2)
O2	C12	N2	124.7(2)	C5	C4	C29	119.1(2)

O2	C12	C10	120.30(19)	C23	C24	C25	120.1(2)
N2	C12	C10	114.99(18)	C5	C6	C1	119.0(2)
C27	C22	O3	117.2(2)	N3	C20	C21	104.1(2)
C23	C22	O3	120.90(19)	F5	C28	C25	112.7(2)
C23	C22	C27	121.7(2)	F6	C28	F5	106.6(3)
C11	C10	C12	123.87(19)	F6	C28	C25	114.5(2)
C7	C10	C11	115.4(2)	F6	C28	F4	107.5(3)
C7	C10	C12	120.5(2)	F4	C28	F5	101.8(3)
O1	C7	C10	117.7(2)	F4	C28	C25	112.8(2)
O1	C7	C8	120.4(2)	C16	C15	C14	121.1(2)
C8	C7	C10	121.7(2)	C6	C5	C4	120.5(2)
O4	C19	C18	115.5(2)	C16	C17	C18	120.8(2)
N3	C19	O4	117.8(2)	C15	C16	C17	119.6(2)
N3	C19	C18	126.7(2)	F3	C29	F1	105.5(2)
C2	C1	O1	122.8(2)	F3	C29	C4	112.5(2)
C2	C1	C6	121.3(2)	F2	C29	F3	106.7(2)
C6	C1	O1	115.8(2)	F2	C29	F1	106.1(2)
C26	C25	C24	120.0(2)	F2	C29	C4	112.9(2)
C26	C25	C28	120.3(2)	F1	C29	C4	112.6(2)
C24	C25	C28	119.7(2)	O4	C21	C20	104.16(19)
C13	C18	C19	121.8(2)				

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for X_48.

Atom	*x*	*y*	*z*	U(eq)
H2	6721.5	3938.24	6440.69	24
H8	4440.31	6332.81	8360.3	31
H27	8372.84	5796.96	6518.98	31
H9	5443.75	7465.83	8024.87	34
H26	9313.5	6935.18	5900.35	32
H14	5425.4	2631.83	4523.67	31
H2A	3566.28	5842.74	6294.56	30
H3	2123.56	5979.76	5913.45	33
H23	6498.48	7062.17	4622.97	31
H24	7431.46	8199.58	4006.15	33
H6	3204.31	3584.3	8347.43	37
H20A	8527.9	3946.06	8574.96	39
H20B	8995.45	4228.13	7491.02	39
H15	5752.46	1141.65	3775.07	41

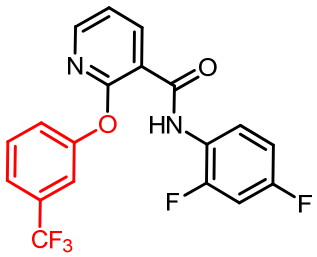
H5	1766.43	3718.61	7959.05	40
H17	7915	1068.5	5681.76	40
H16	6971.53	343.32	4378.8	48
H21A	9642.3	2798.24	7631.01	44
H21B	9057.65	2452.48	8574.67	44

Experimental

Single crystals of $C_{29}H_{19}F_6N_3O_4$ **[7d]** were **[]**. A suitable crystal was selected and **[]** on a **SuperNova, Dual, Cu at zero, AtlasS2** diffractometer. The crystal was kept at 100.00(10) K during data collection.

Crystal structure determination of [7d]

Crystal Data for $C_{29}H_{19}F_6N_3O_4$ (M =587.47 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 15.9357(8) Å, b = 13.7866(8) Å, c = 11.8725(7) Å, β = 93.908(5)°, V = 2602.3(3) Å^3, Z = 4, T = 100.00(10) K, μ(MoKα) = 0.130 mm^{-1}, *Dcalc* = 1.499 g/cm^3, 13946 reflections measured (4.534° ≤ 2Θ ≤ 59.172°), 6166 unique (R_{int} = 0.0347, R_{sigma} = 0.0566) which were used in all calculations. The final R_1 was 0.0643 (I > 2σ(I)) and wR_2 was 0.1664 (all data).



N-(2,4-difluorophenyl)-2-(3-(trifluoromethyl)phenoxy)nicotinamide (Diflufenican)

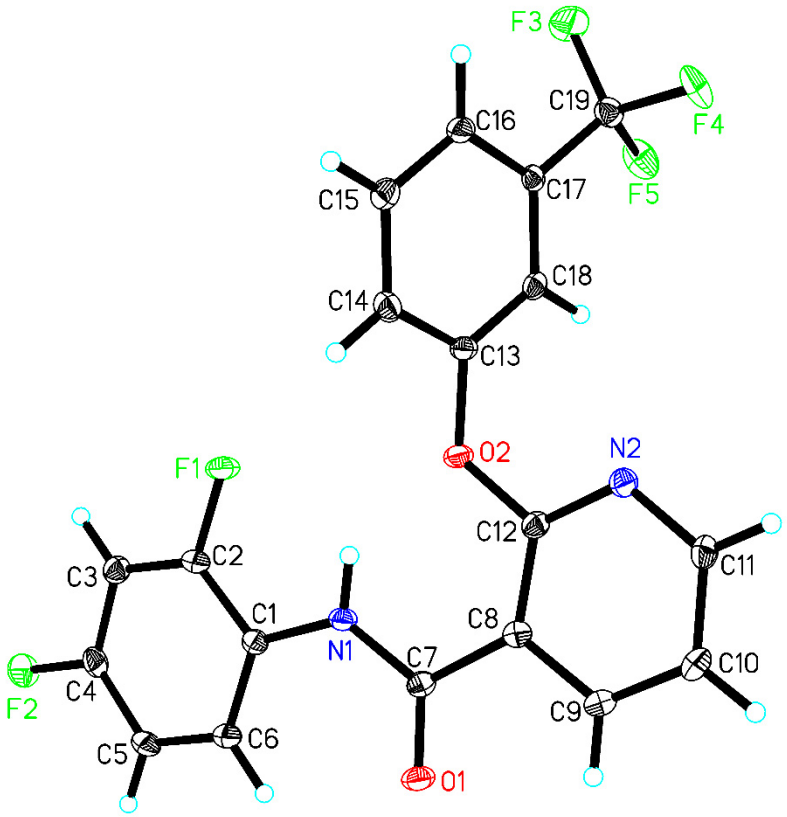


Table 1 Crystal data and structure refinement for Diflufenican.

Identification code	Diflufenican
Empirical formula	$C_{19}H_{11}F_5N_2O_2$
Formula weight	394.30
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.1293(6)
b/Å	8.5068(4)
c/Å	15.8667(9)
α/°	90

β/°	92.925(5)
γ/°	90
Volume/Å^3	1635.02(15)
Z	4
ρ_{calc}g/cm^3	1.602
μ/mm^{-1}	0.144
F(000)	800.0
Crystal size/mm^3	0.15 × 0.14 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.142 to 59.042
Index ranges	-16 ≤ h ≤ 14, -10 ≤ k ≤ 11, -22 ≤ l ≤ 13
Reflections collected	8760
Independent reflections	3905 [R_{int} = 0.0331, R_{sigma} = 0.0488]
Data/restraints/parameters	3905/0/253
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0499, wR_2 = 0.1058
Final R indexes [all data]	R_1 = 0.0718, wR_2 = 0.1188
Largest diff. peak/hole / e Å^{-3}	0.27/-0.29

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for exp_1053. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F(1)	4741.7(8)	8497.6(12)	5961.0(8)	29.9(3)
F(2)	8279.4(10)	9547.8(14)	5028.8(8)	39.1(3)
F(4)	-265.6(10)	6991.0(15)	8900.4(8)	39.0(3)
F(5)	1327.8(10)	7807.8(16)	9339.8(7)	39.1(3)
F(3)	130.8(12)	9429.8(15)	8816.5(8)	47.7(4)
O(2)	3220(1)	5701.7(14)	6862.7(9)	25.3(3)
O(1)	5880.4(10)	3031.9(15)	6071.9(9)	28.7(3)
N(2)	2356.8(12)	3450.4(18)	7287.1(10)	22.8(4)
N(1)	5106.3(12)	5459.5(17)	6083(1)	21.3(3)
C(8)	4136.4(14)	3257(2)	6678.4(11)	20.0(4)
C(17)	961.8(14)	7724(2)	7868.3(11)	18.2(4)
C(12)	3217.5(14)	4089(2)	6950.6(12)	20.7(4)
C(18)	1898.0(14)	6809(2)	7786.6(12)	19.8(4)
C(16)	396.2(14)	8369(2)	7167.2(12)	22.2(4)

C(1)	5944.4(14)	6391(2)	5764.8(11)	19.8(4)
C(9)	4110.0(15)	1647(2)	6802.2(12)	23.2(4)
C(13)	2244.5(14)	6547(2)	6983.2(12)	20.7(4)
C(7)	5120.7(14)	3899(2)	6251.3(12)	20.6(4)
C(2)	5750.3(14)	7997(2)	5726.7(12)	22.0(4)
C(6)	6965.6(15)	5862(2)	5515.8(12)	24.9(4)
C(19)	541.7(16)	7990(2)	8723.7(13)	25.4(4)
C(10)	3216.9(16)	940(2)	7155.0(13)	26.1(4)
C(11)	2361.6(16)	1880(2)	7383.0(12)	24.5(4)
C(3)	6498.9(15)	9082(2)	5480.6(12)	25.0(4)
C(14)	1713.1(15)	7193(2)	6281.1(12)	24.6(4)
C(15)	781.5(15)	8115(2)	6374.9(12)	25.5(4)
C(4)	7506.4(16)	8502(2)	5256.9(13)	26.3(4)
C(5)	7746.7(15)	6933(2)	5259.3(13)	27.4(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for exp_1053. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F(1)	23.3(6)	20.4(6)	47.0(8)	-2.0(5)	10.2(5)	4.2(4)
F(2)	34.6(7)	30.5(7)	53.8(9)	4.5(6)	17.7(6)	-9.2(5)
F(4)	34.3(7)	51.2(8)	33.0(7)	-4.9(6)	16.2(6)	-17.6(6)
F(5)	35.5(7)	60.5(9)	21.1(6)	-2.9(6)	-0.1(5)	-6.0(6)
F(3)	72.8(9)	32.1(7)	39.8(8)	-7.7(6)	18.6(7)	16.3(7)
O(2)	20.7(6)	14.8(6)	41.3(9)	0.7(6)	10.4(6)	2.1(5)
O(1)	23.6(7)	20.9(7)	42.3(9)	-0.6(6)	7.9(6)	5.6(5)
N(2)	20.3(8)	20.9(8)	27.3(9)	1.3(7)	2.2(7)	-1.1(6)
N(1)	17.0(7)	18.7(8)	28.6(9)	-1.2(7)	5.2(7)	2.1(6)
C(8)	19.5(9)	20.7(9)	19.6(9)	-1.6(7)	-1.5(7)	0.8(7)
C(17)	20.6(8)	14.0(8)	20.3(9)	-0.5(7)	4.5(7)	-3.5(7)
C(12)	20.7(9)	17.4(9)	24(1)	-0.1(8)	0.2(8)	-0.3(7)
C(18)	19.8(9)	15.7(8)	23.7(10)	2.9(7)	-0.6(7)	-2.4(7)
C(16)	17.8(9)	18.9(9)	30.0(11)	2.3(8)	3.3(8)	0.8(7)
C(1)	18.8(9)	21.1(9)	19.6(9)	-0.8(8)	1.1(7)	0.0(7)
C(9)	23.2(9)	19.6(9)	26.5(10)	-2.5(8)	-0.7(8)	3.5(7)
C(13)	16.8(8)	15.0(8)	30.7(11)	-0.4(8)	5.7(8)	-0.4(7)
C(7)	19.6(9)	19.5(9)	22.5(10)	-0.7(8)	-1.1(8)	1.5(7)
C(2)	18.8(9)	23.9(9)	23.4(10)	-2.6(8)	2.9(8)	3.1(7)
C(6)	23.6(9)	23.1(9)	28.3(11)	-0.5(8)	5.5(8)	4.0(8)
C(19)	25.1(10)	24(1)	27.5(11)	-1.9(8)	4.4(8)	-2.8(8)

C(10)	31.5(10)	17.3(9)	29.3(11)	2.2(8)	-1.7(9)	-0.6(8)
C(11)	24.6(9)	22.1(9)	26.9(10)	4.3(8)	1.3(8)	-4.5(8)
C(3)	28(1)	21.5(9)	25.6(10)	0.2(8)	1.6(8)	-0.4(8)
C(14)	28.6(10)	25.7(10)	20(1)	0.1(8)	6.0(8)	0.1(8)
C(15)	26.2(10)	26.5(10)	23.7(10)	4.7(8)	-0.5(8)	2.2(8)
C(4)	25.1(10)	27.5(10)	26.8(10)	2.1(9)	7.1(8)	-6.9(8)
C(5)	21.0(9)	29.8(10)	32.1(11)	0.1(9)	9.8(8)	3.2(8)

Table 4 Bond Lengths for exp_1053.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F(1)	C(2)	1.365(2)	C(17)	C(18)	1.388(2)
F(2)	C(4)	1.355(2)	C(17)	C(16)	1.389(3)
F(4)	C(19)	1.337(2)	C(17)	C(19)	1.491(3)
F(5)	C(19)	1.339(2)	C(18)	C(13)	1.381(3)
F(3)	C(19)	1.334(2)	C(16)	C(15)	1.380(3)
O(2)	C(12)	1.379(2)	C(1)	C(2)	1.387(2)
O(2)	C(13)	1.406(2)	C(1)	C(6)	1.394(2)
O(1)	C(7)	1.225(2)	C(9)	C(10)	1.382(3)
N(2)	C(12)	1.314(2)	C(13)	C(14)	1.373(3)
N(2)	C(11)	1.345(2)	C(2)	C(3)	1.366(3)
N(1)	C(1)	1.403(2)	C(6)	C(5)	1.390(3)
N(1)	C(7)	1.354(2)	C(10)	C(11)	1.373(3)
C(8)	C(12)	1.407(2)	C(3)	C(4)	1.381(3)
C(8)	C(9)	1.384(2)	C(14)	C(15)	1.390(3)
C(8)	C(7)	1.505(2)	C(4)	C(5)	1.366(3)

Table 5 Bond Angles for exp_1053.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(12)	O(2)	C(13)	119.27(13)	O(1)	C(7)	C(8)	120.63(16)
C(12)	N(2)	C(11)	117.24(16)	N(1)	C(7)	C(8)	116.23(15)
C(7)	N(1)	C(1)	128.49(15)	F(1)	C(2)	C(1)	116.62(15)
C(12)	C(8)	C(7)	127.95(16)	F(1)	C(2)	C(3)	119.02(16)
C(9)	C(8)	C(12)	115.45(16)	C(3)	C(2)	C(1)	124.36(17)
C(9)	C(8)	C(7)	116.58(16)	C(5)	C(6)	C(1)	120.00(18)
C(18)	C(17)	C(16)	121.29(17)	F(4)	C(19)	F(5)	105.98(16)
C(18)	C(17)	C(19)	119.27(17)	F(4)	C(19)	C(17)	112.50(16)
C(16)	C(17)	C(19)	119.42(16)	F(5)	C(19)	C(17)	112.54(16)

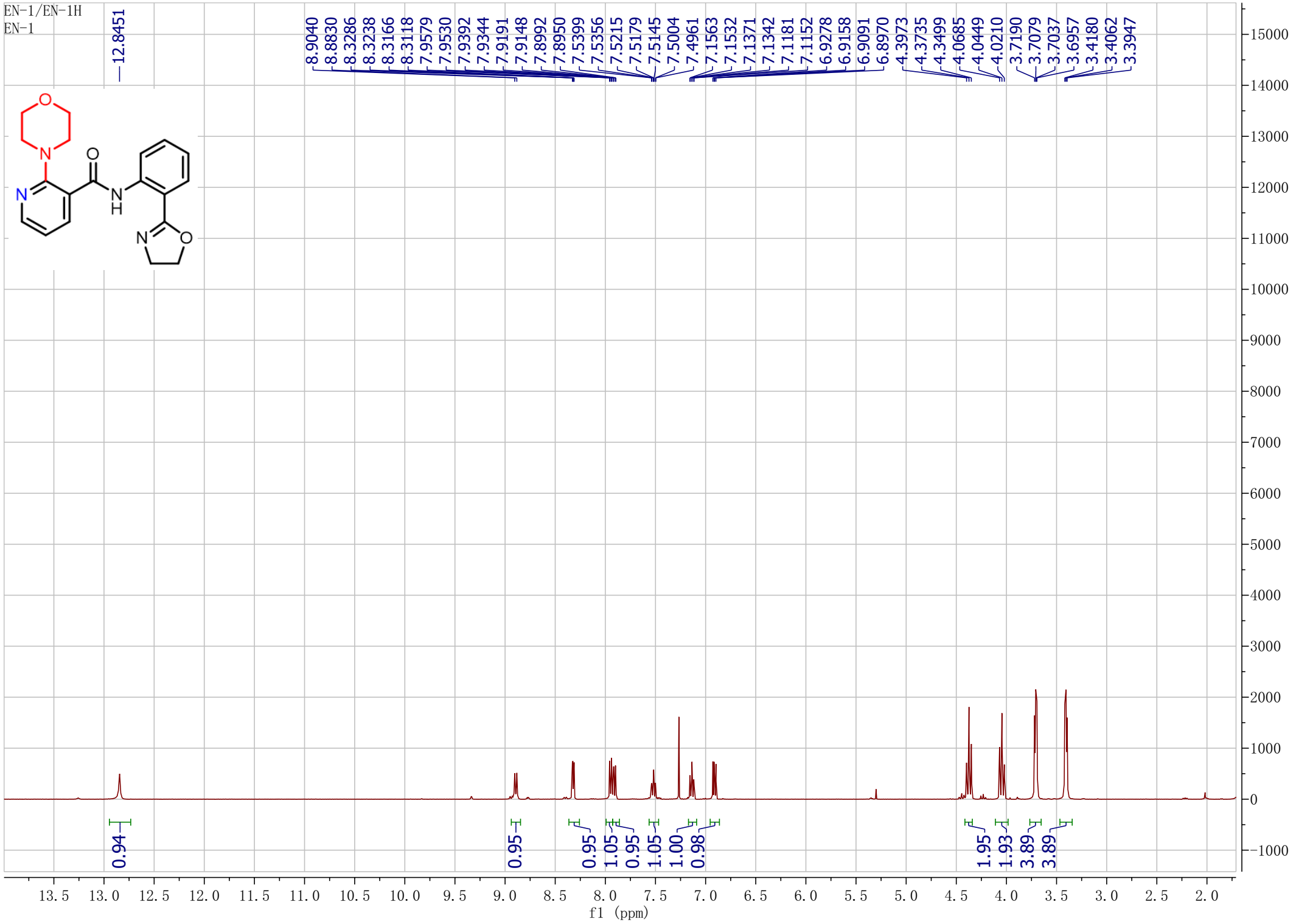
O(2)	C(12)	C(8)	117.62(15)	F(3)	C(19)	F(4)	106.18(16)
N(2)	C(12)	O(2)	117.27(15)	F(3)	C(19)	F(5)	106.36(16)
N(2)	C(12)	C(8)	125.11(17)	F(3)	C(19)	C(17)	112.74(16)
C(13)	C(18)	C(17)	117.74(17)	C(11)	C(10)	C(9)	118.17(18)
C(15)	C(16)	C(17)	119.42(17)	N(2)	C(11)	C(10)	123.20(17)
C(2)	C(1)	N(1)	116.58(15)	C(2)	C(3)	C(4)	116.23(18)
C(2)	C(1)	C(6)	117.19(16)	C(13)	C(14)	C(15)	119.32(17)
C(6)	C(1)	N(1)	126.18(17)	C(16)	C(15)	C(14)	120.04(18)
C(10)	C(9)	C(8)	120.81(17)	F(2)	C(4)	C(3)	117.88(17)
C(18)	C(13)	O(2)	120.40(17)	F(2)	C(4)	C(5)	119.45(17)
C(14)	C(13)	O(2)	117.25(16)	C(5)	C(4)	C(3)	122.67(17)
C(14)	C(13)	C(18)	122.15(17)	C(4)	C(5)	C(6)	119.52(17)
O(1)	C(7)	N(1)	123.15(16)				

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for exp_1053.

Atom	*x*	*y*	*z*	U(eq)
H(1)	4504.72	5943.04	6184.55	26
H(18)	2278.81	6386.09	8257.23	24
H(16)	-236.32	8965.6	7231.25	27
H(9)	4700.45	1033.71	6646.08	28
H(6)	7124.46	4792.3	5521.22	30
H(10)	3196.06	-141.74	7235.69	31
H(11)	1755.83	1406.92	7615.17	29
H(3)	6339.12	10151.16	5464.56	30
H(14)	1973.78	7015.15	5748.28	30
H(15)	417.41	8561.39	5903.5	31
H(5)	8427.87	6584.24	5090.65	33

Crystal structure determination of [Diflufenican**]**

Crystal Data for $C_{19}H_{11}F_5N_2O_2$ (M =394.30 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 12.1293(6) Å, b = 8.5068(4) Å, c = 15.8667(9) Å, β = 92.925(5)°, V = 1635.02(15) Å^3, Z = 4, T = 100.00(10) K, μ(MoKα) = 0.144 mm^{-1}, *Dcalc* = 1.602 g/cm^3, 8760 reflections measured (5.142° ≤ 2Θ ≤ 59.042°), 3905 unique (R_{int} = 0.0331, R_{sigma} = 0.0488) which were used in all calculations. The final R_1 was 0.0499 (I > 2σ(I)) and wR_2 was 0.1188 (all data).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8.3118
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7.9530
7.9392
7.9344
7.9191
7.9148
7.8992
7.8950
7.5399
7.5356
7.5215
7.5179
7.5145
7.5004
7.4961
7.1563
7.1532
7.1371
7.1342
7.1181
7.1152
6.9278
6.9158
6.9091
6.8970
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4.3499
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4.0210
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3.7079
3.7037
3.6957
3.4180
3.4062
3.3947
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0.95
0.95
1.05
0.95
1.05
1.00
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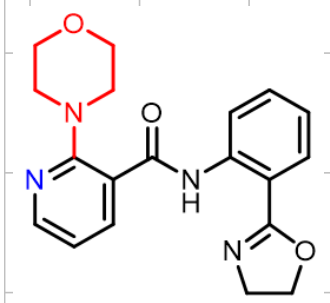
1.95
1.93
3.89
3.89
f1 (ppm)

EN-1/EN-1C
EN-1



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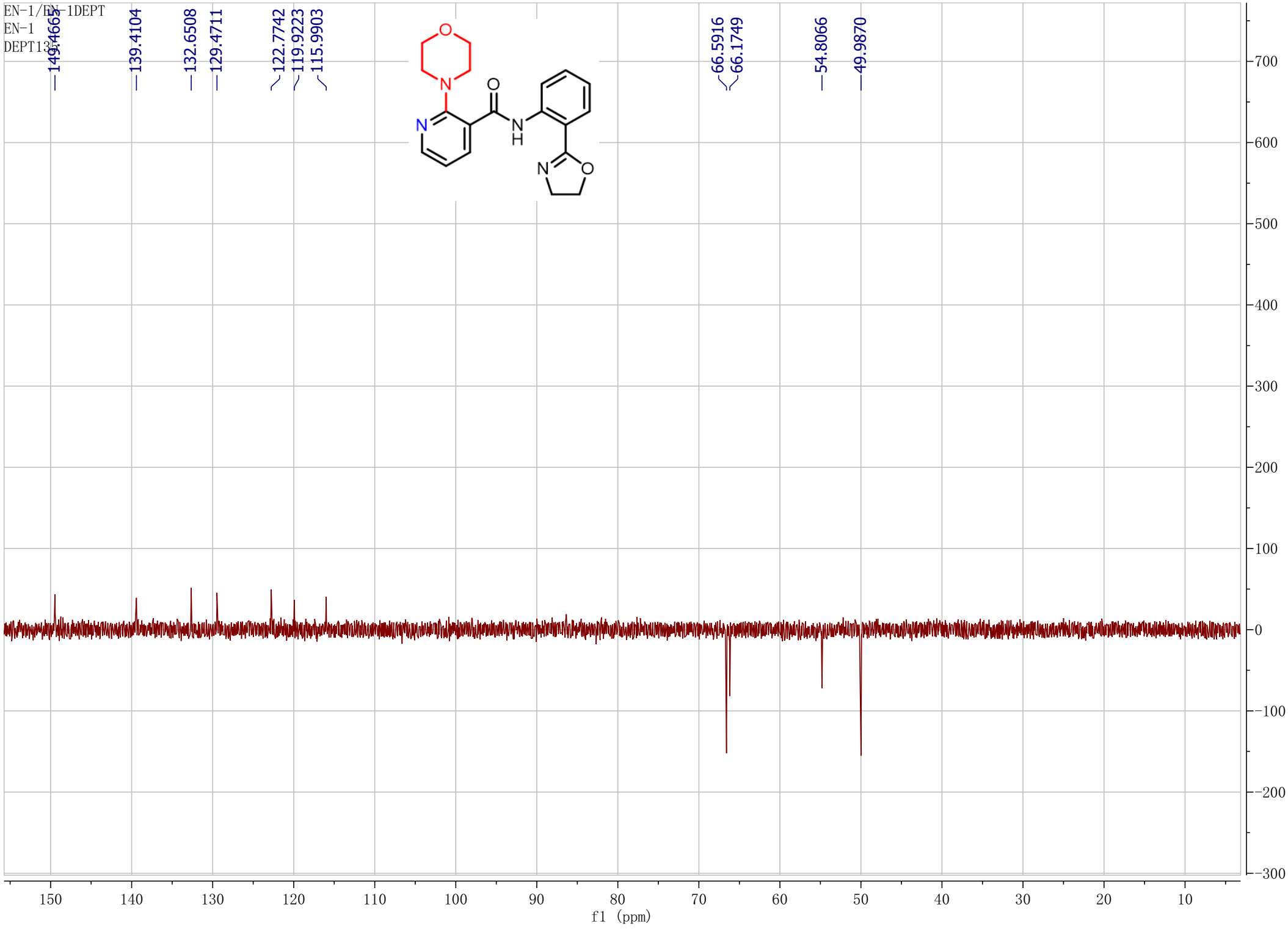
158.4614
149.4655
139.6111
139.4135
132.6521
129.4704
122.7804
121.4312
119.9182
115.9970
113.6056
66.5891
66.1743
54.8048
49.9860

5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)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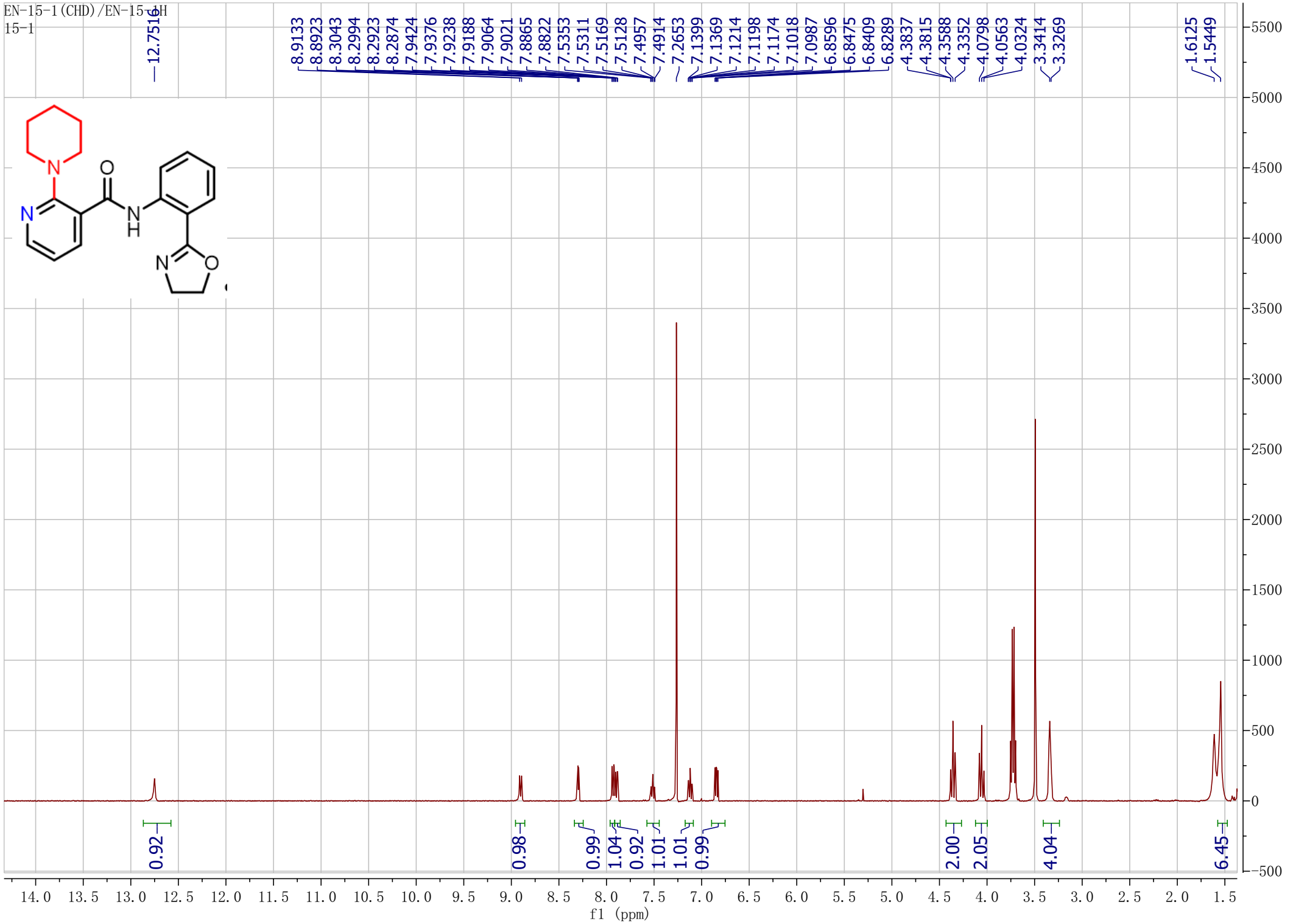
66.5916
66.1749
54.8066
49.9870
O
N
O
N
H
N
O
700
600
500
400
300
200
100
0
-100
-200
-300
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.9238
7.9188
7.9064
7.9021
7.8865
7.8822
7.5353
7.5311
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7.1214
7.1198
7.1174
7.1018
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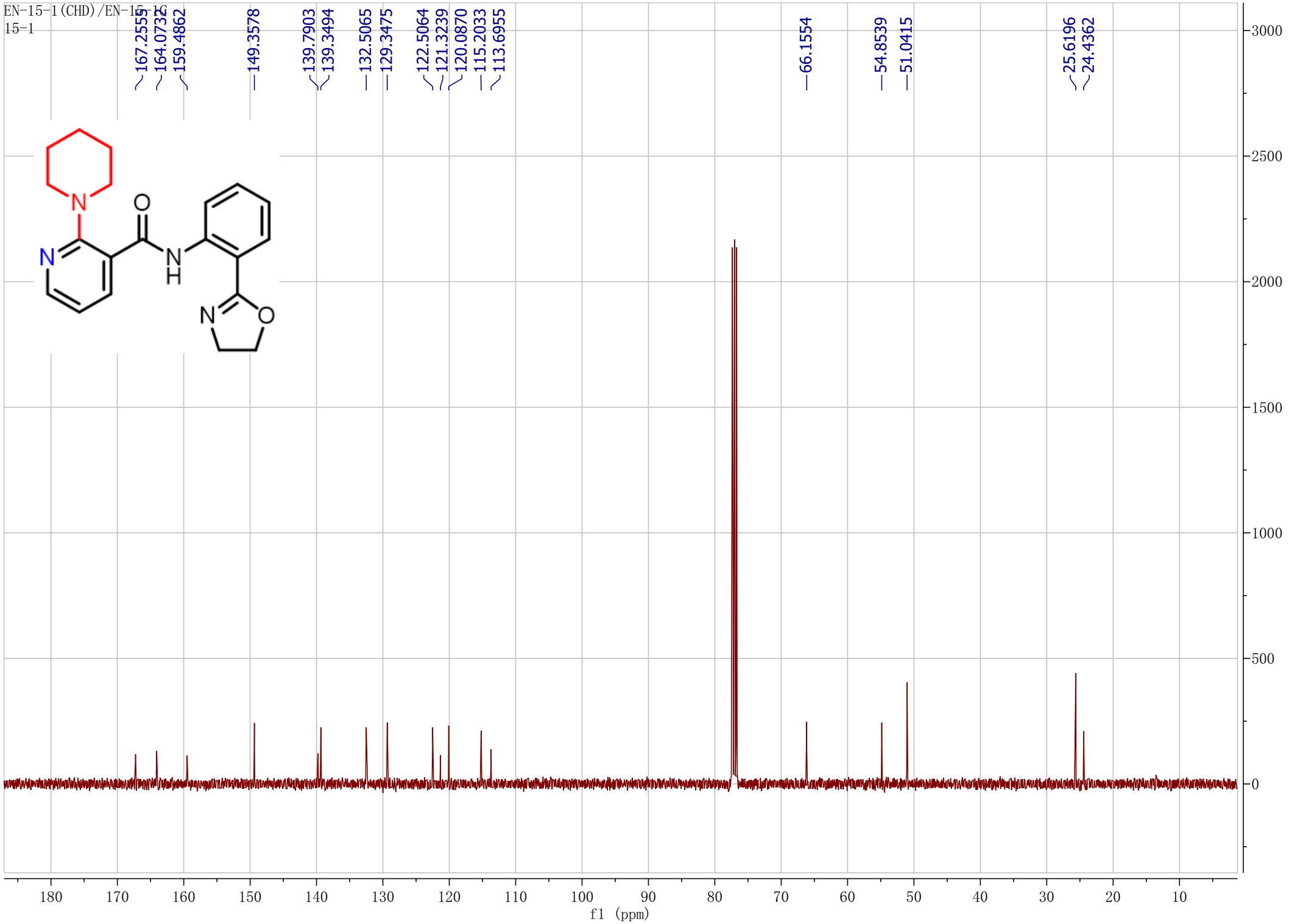
f1 (ppm)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122.5064
121.3239
120.0870
115.2033
113.6955
66.1554
54.8539
51.0415
25.6196
24.4362
N
O
N
H
N
O
3000
2500
2000
1500
1000
500
0
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120
110
100
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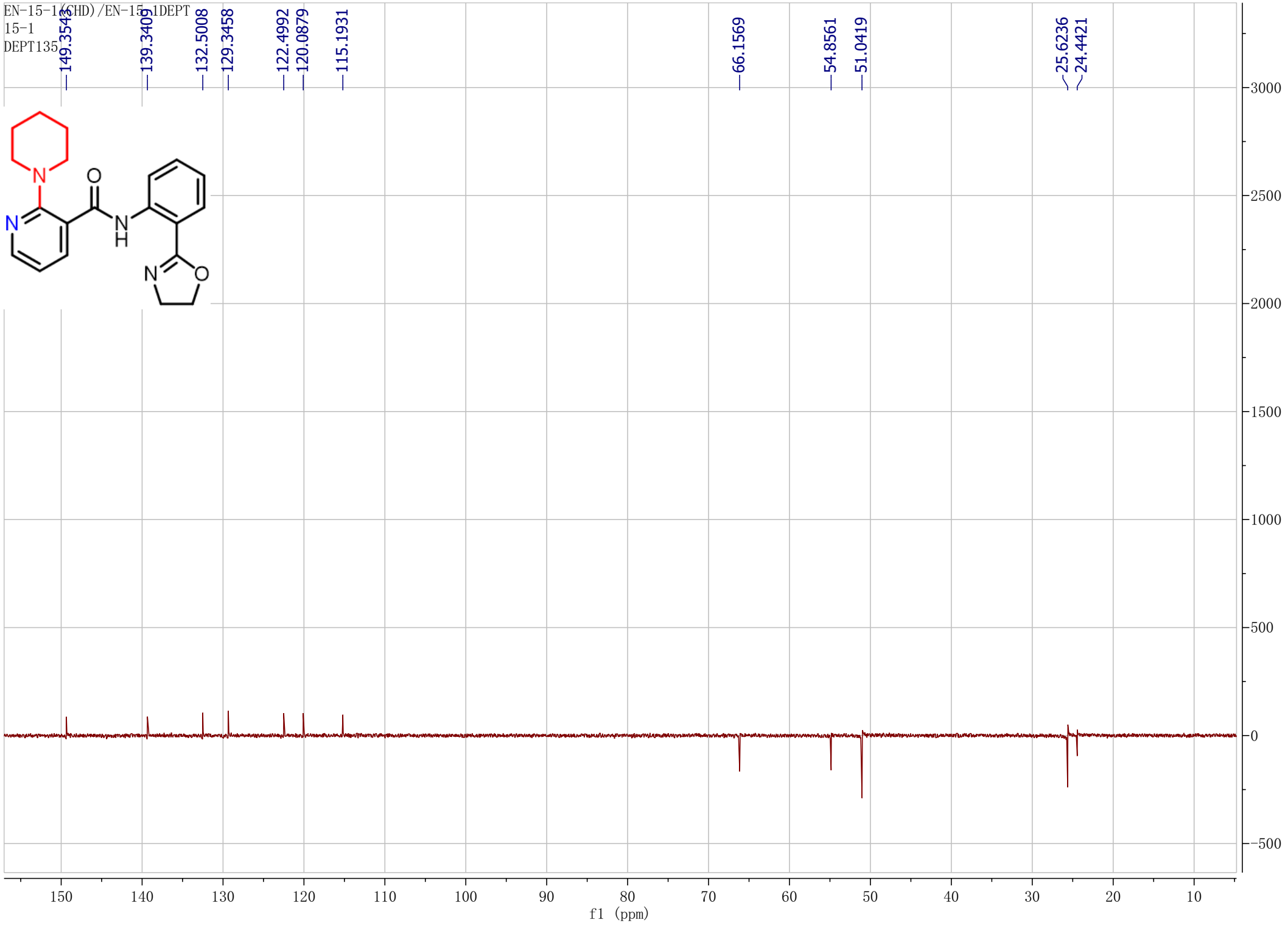
80
70
60
50
40
30
20
10
f1 (ppm)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54.8561
51.0419
25.6236
24.4421
O
N
N
H
N
O
3000
2500
2000
1500
1000
500
0
-500
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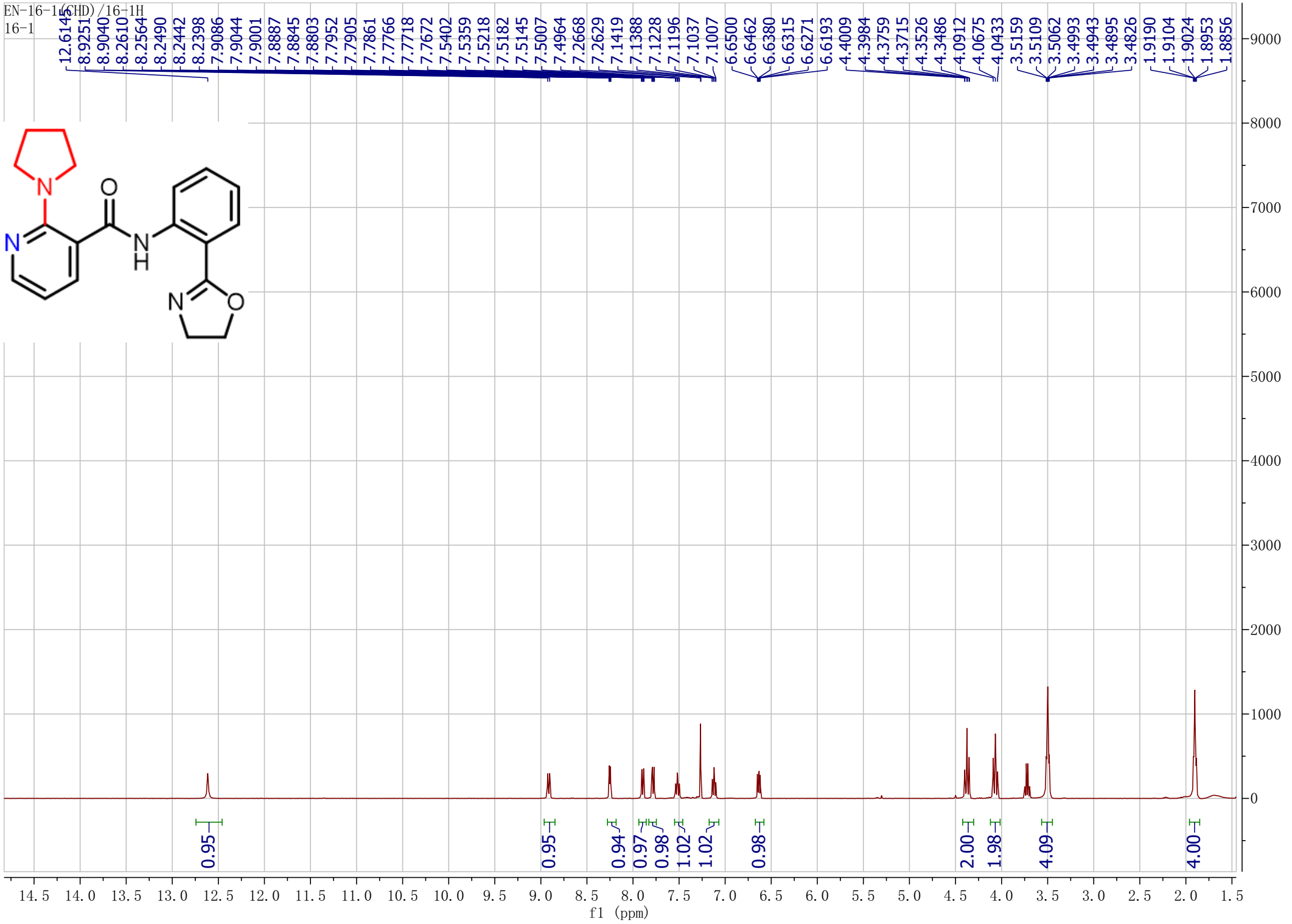
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.9001
7.8887
7.8845
7.8803
7.7952
7.7905
7.7861
7.7766
7.7718
7.7672
7.5402
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7.5182
7.5145
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7.4964
7.2668
7.2629
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4.3715
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3.4895
3.4826
1.9190
1.9104
1.9024
1.8953
1.8856
0.95
0.95
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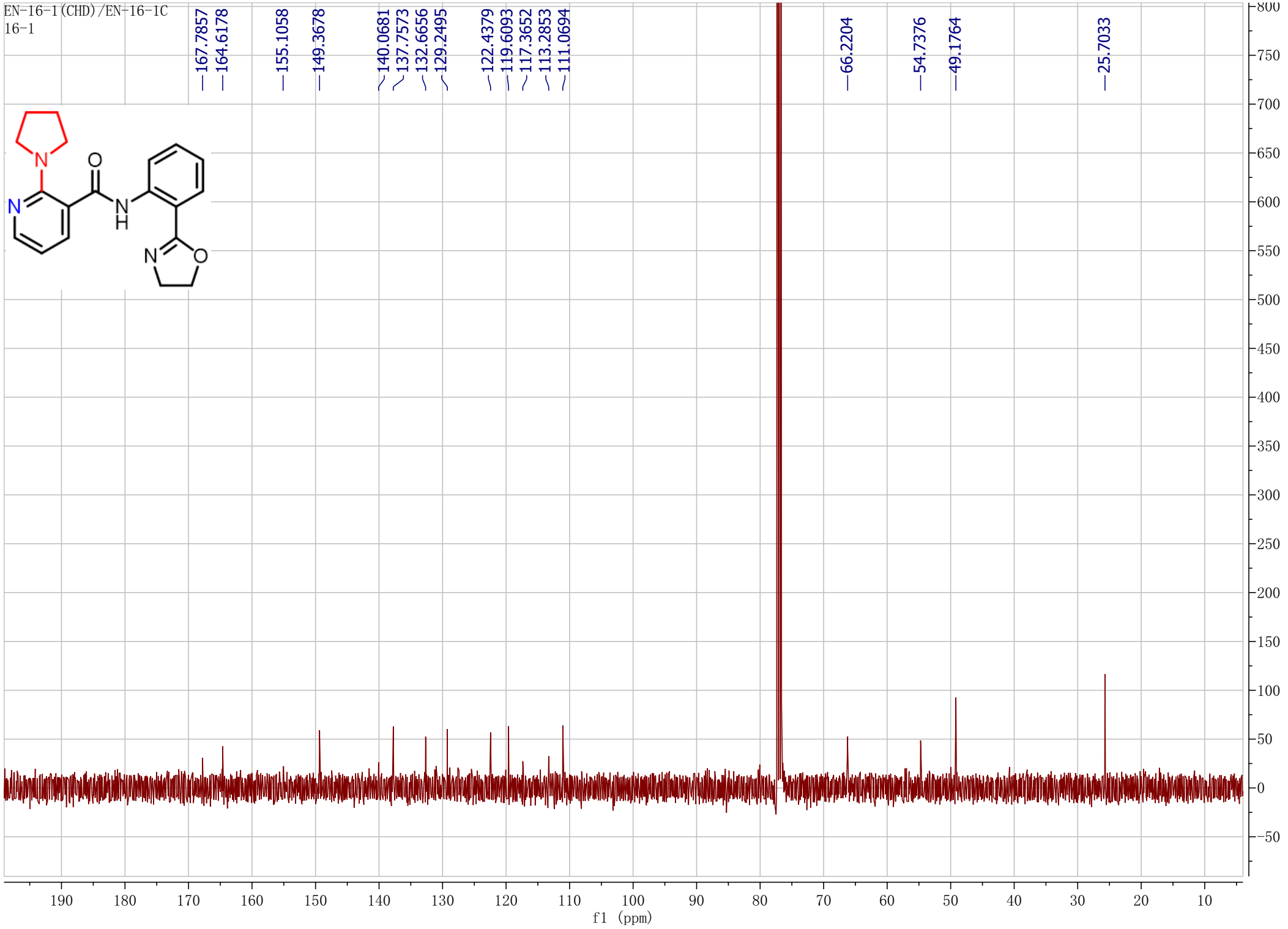
1.02
1.02
0.98
2.00
1.98
4.09
4.00
f1 (ppm)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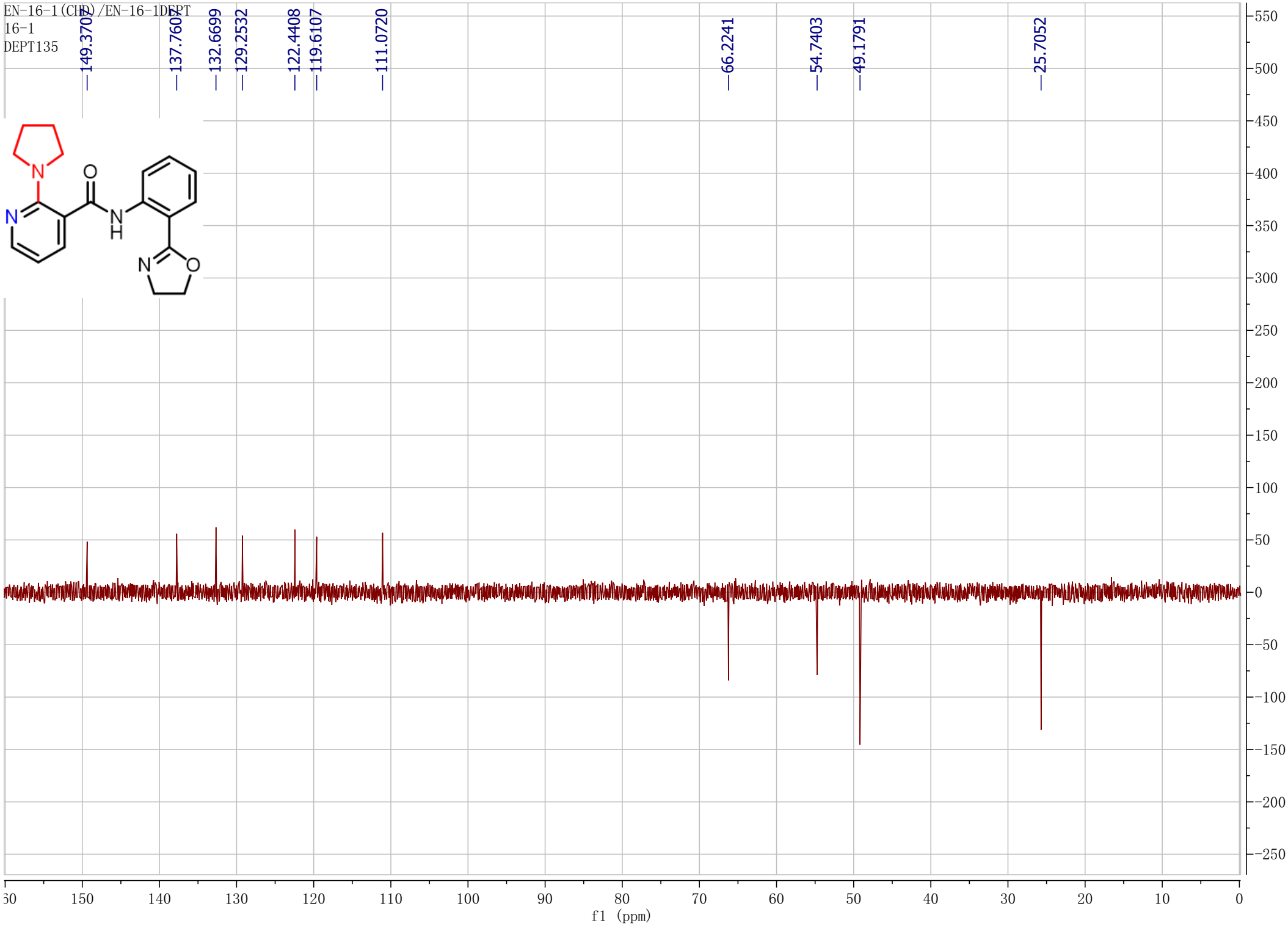
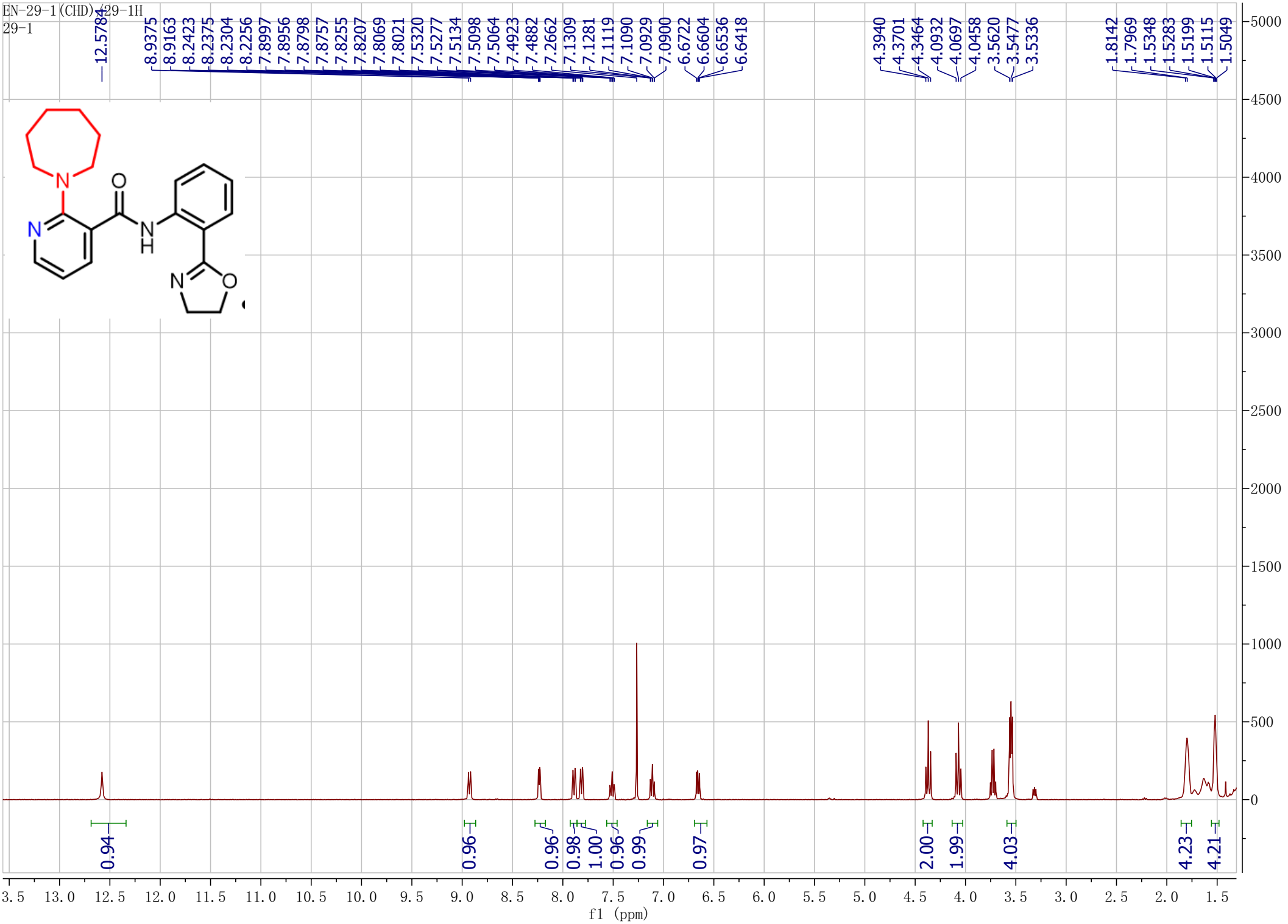
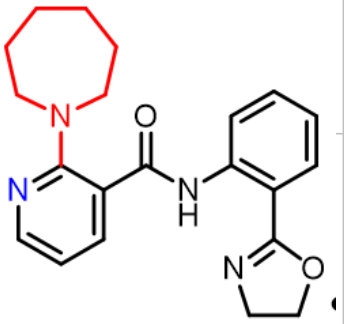
137.7573
132.6656
129.2495
122.4379
119.6093
117.3652
113.2853
111.0694
66.2204
54.7376
49.1764
25.7033
N
O
N
H
N
O
f1 (ppm)


EN-16-1(CHD)/EN-16-1DEPT
16-1
DEPT135
149.3703
137.7605
132.6699
129.2532
122.4408
119.6107
111.0720
66.2241
54.7403
49.1791
25.7052
N
O
N
H
N
O
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


EN-29-1(CHD)-29-1H
29-1
12.5784
8.9375
8.9163
8.2423
8.2375
8.2304
8.2256
7.8997
7.8956
7.8798
7.8757
7.8255
7.8207
7.8069
7.8021
7.5320
7.5277
7.5134
7.5098
7.5064
7.4923
7.4882
7.2662
7.1309
7.1281
7.1119
7.1090
7.0929
7.0900
6.6722
6.6604
6.6536
6.6418
4.3940
4.3701
4.3464
4.0932
4.0697
4.0458
3.5620
3.5477
3.5336
1.8142
1.7969
1.5348
1.5283
1.5199
1.5115
1.5049
0.94
0.96
0.96
0.98
1.00
0.96
0.99
0.97
2.00
1.99
4.03
4.23
4.21
f1 (ppm)

EN-29-1(CHD)/EN-29-1C
29-1

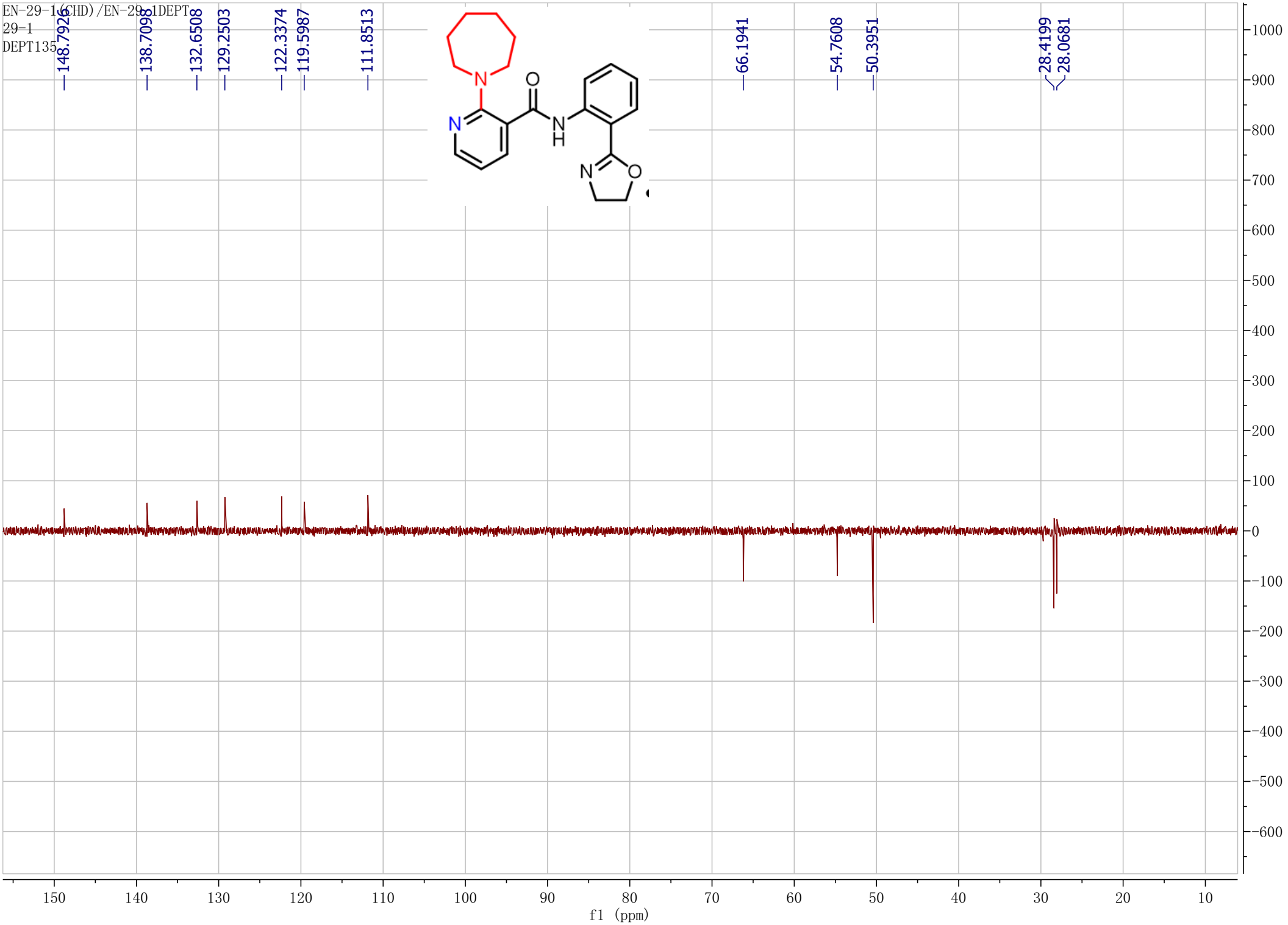


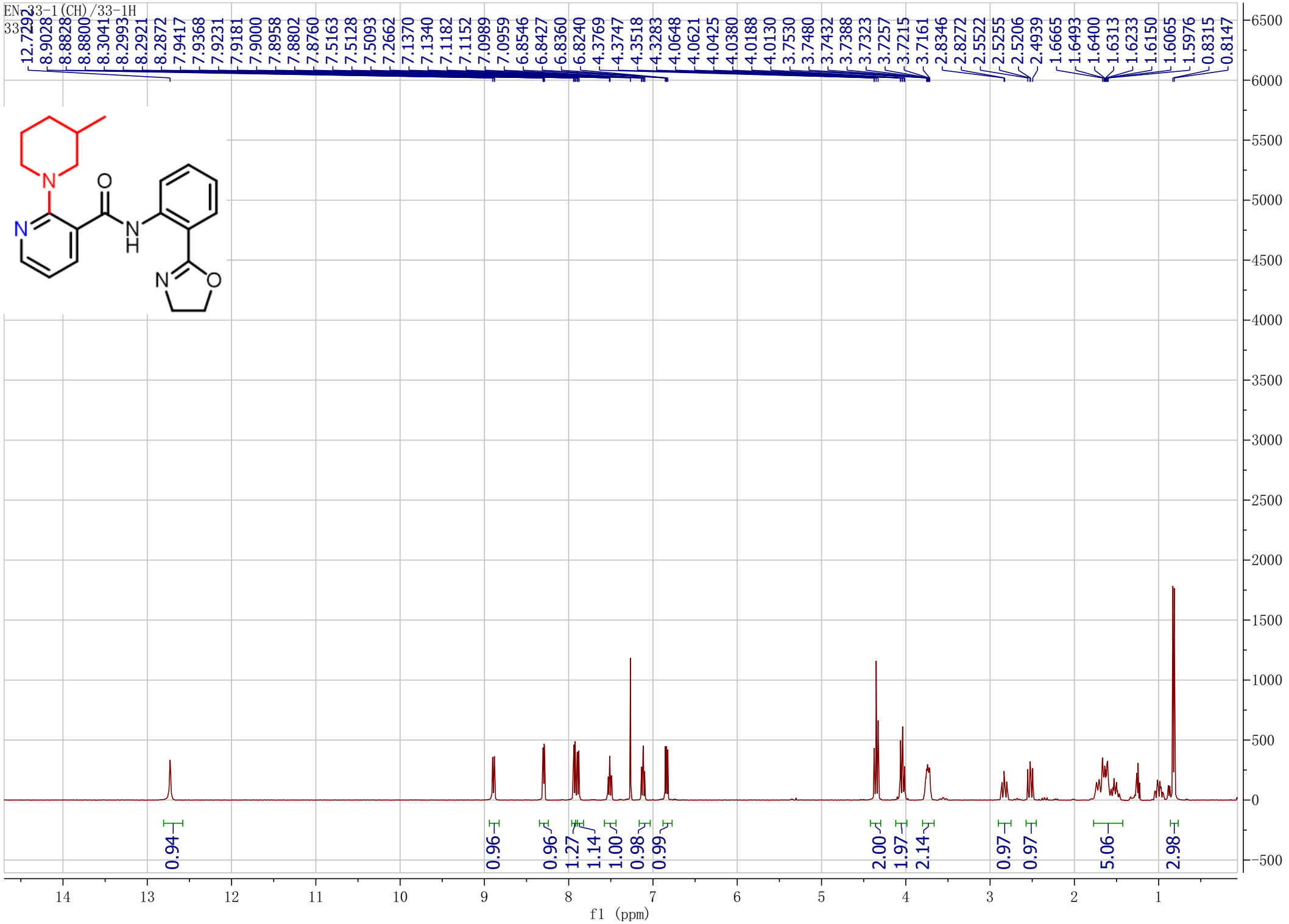
168.1526
164.5293
157.6924
148.7987
140.1151
138.7119
132.6519
129.2517
122.3361
119.6020
117.5736
113.2586
111.8522
66.1912
54.7573
50.3937
28.4159
28.0616

2500
2000
1500
1000
500
0

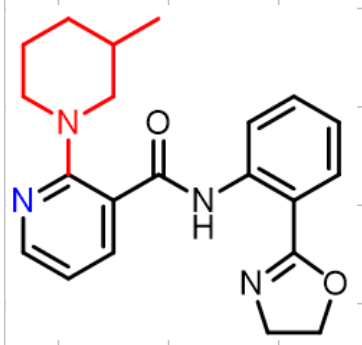
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)


EN-29-1(CHD)/EN-29-1DEPT
29-1
DEPT135
148.7926
138.7098
132.6508
129.2503
122.3374
119.5987
111.8513
66.1941
54.7608
50.3951
28.4199
28.0681
N
O
N
H
N
O
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
-300
-400
-500
-600
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


EN-33-1(CH)/33-1H
12.729
8.9028
8.8828
8.8800
8.3041
8.2993
8.2921
8.2872
7.9417
7.9368
7.9231
7.9181
7.9000
7.8958
7.8802
7.8760
7.5163
7.5128
7.5093
7.2662
7.1370
7.1340
7.1182
7.1152
7.0989
7.0959
6.8546
6.8427
6.8360
6.8240
4.3769
4.3747
4.3518
4.3283
4.0648
4.0621
4.0425
4.0380
4.0188
4.0130
3.7530
3.7480
3.7432
3.7388
3.7323
3.7257
3.7215
3.7161
2.8346
2.8272
2.5522
2.5255
2.5206
2.4939
1.6665
1.6493
1.6400
1.6313
1.6233
1.6150
1.6065
1.5976
0.8315
0.8147
N
O
N
H
N
O
0.94
0.96
0.96
1.27
1.14
1.00
0.98
0.99
2.00
1.97
2.14
0.97
0.97
5.06
2.98
f1 (ppm)

EN-33-1(CH)/EN-33-1C
33-1

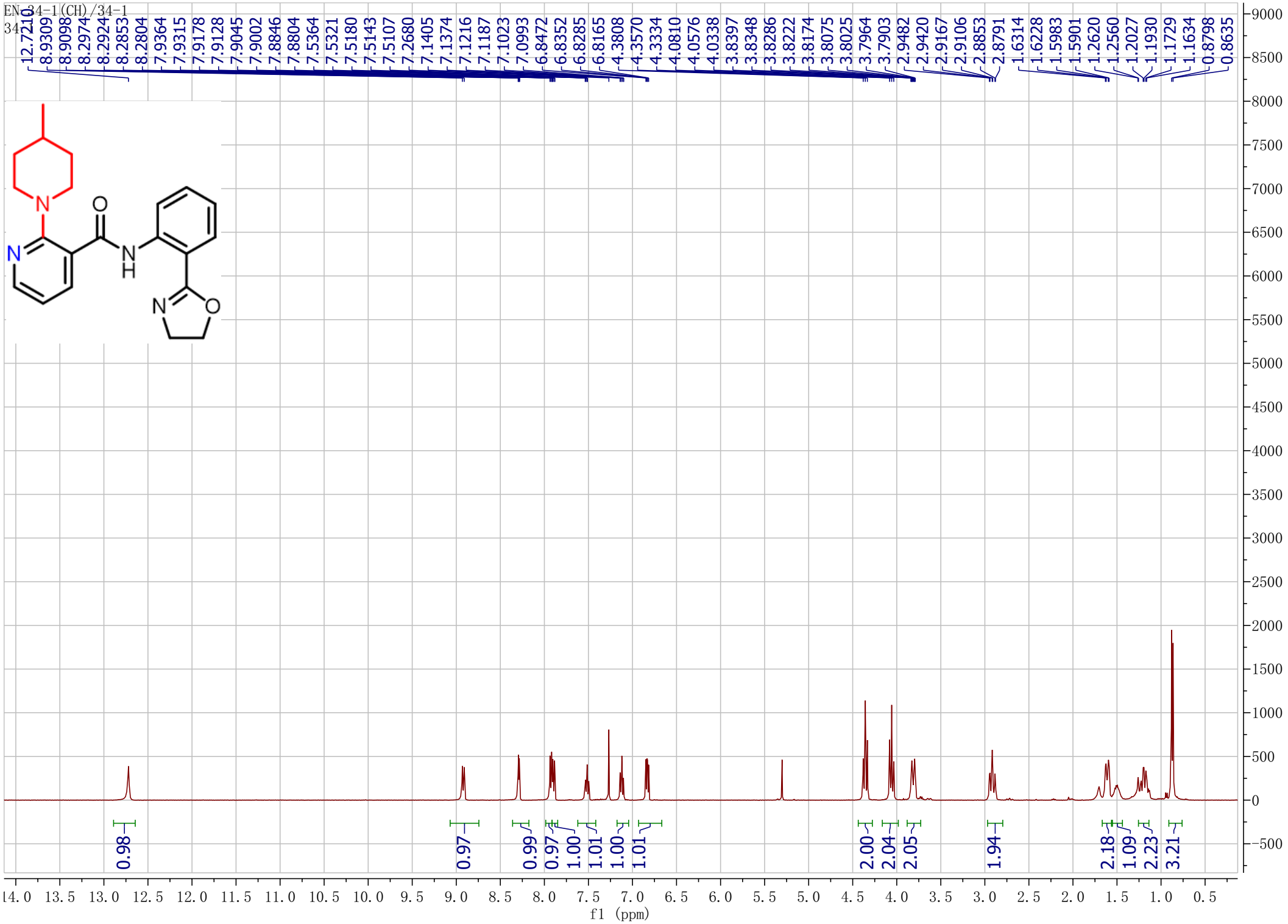


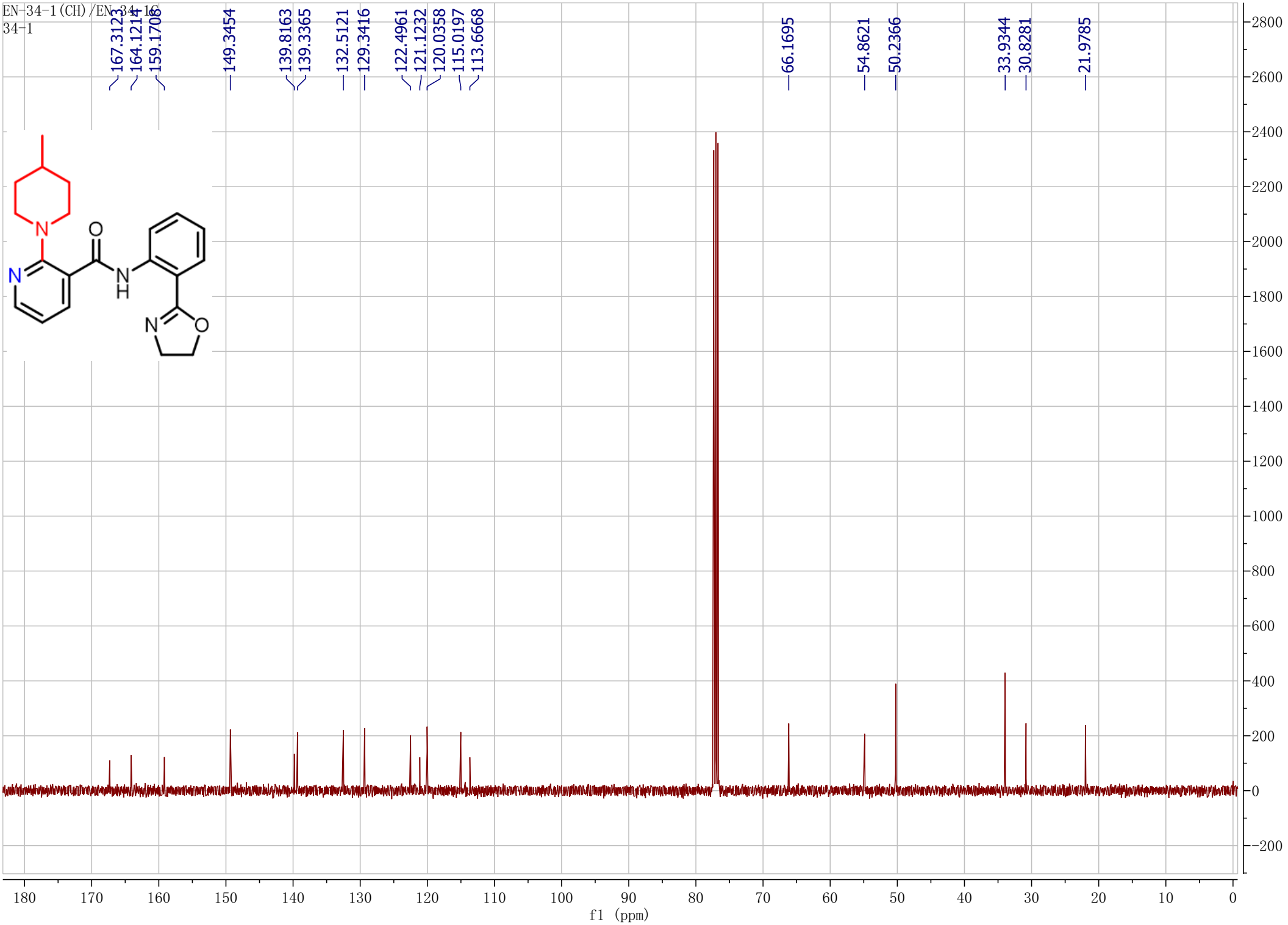
167.2526
164.0811
159.2898
149.3606
139.7757
139.3484
132.5145
129.3392
122.5038
121.2512
120.0481
115.1435
113.6853
66.1473
57.6277
54.8472
50.6387
33.0790
30.8517
25.2834
19.2972

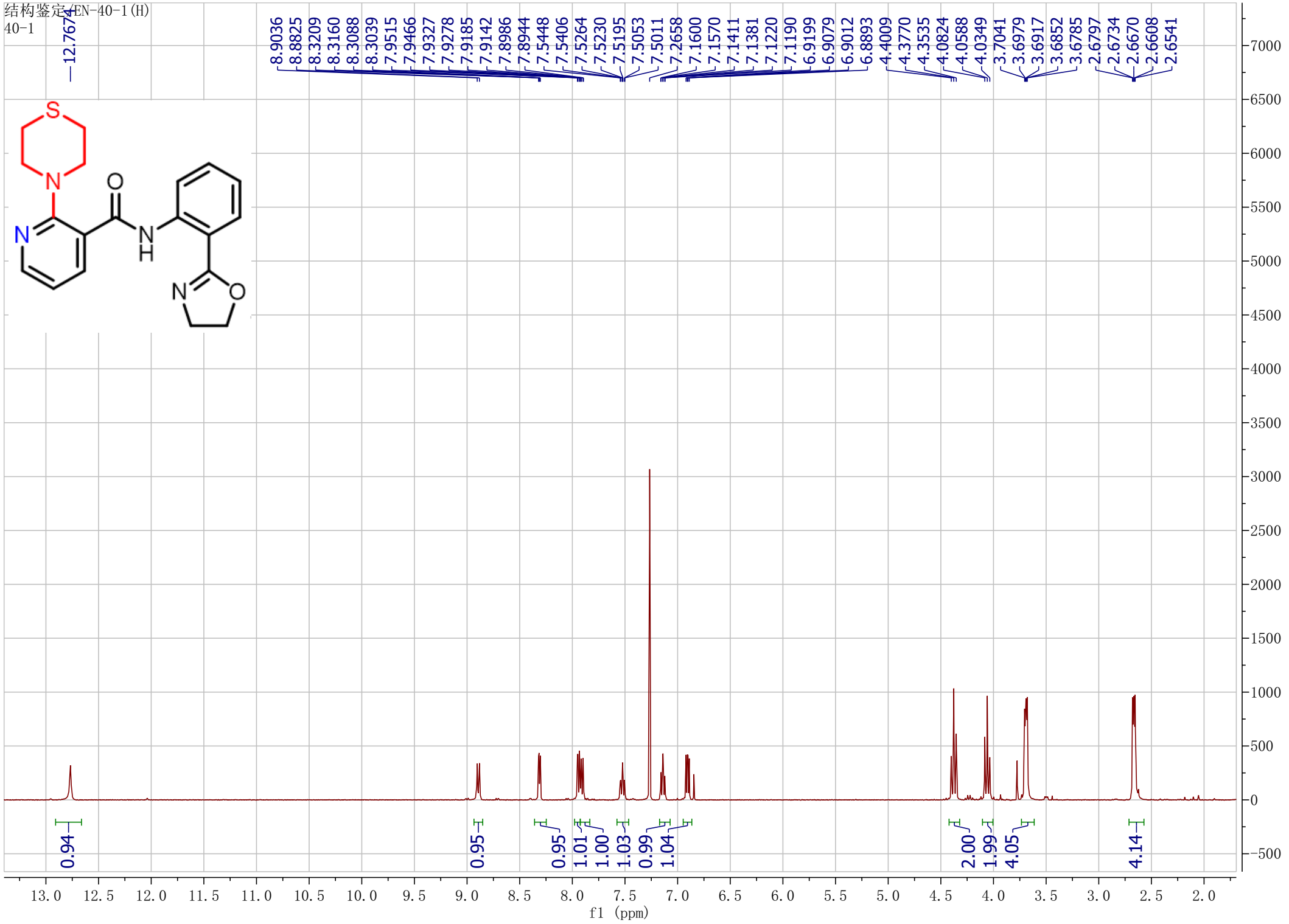
6500 6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0 −500

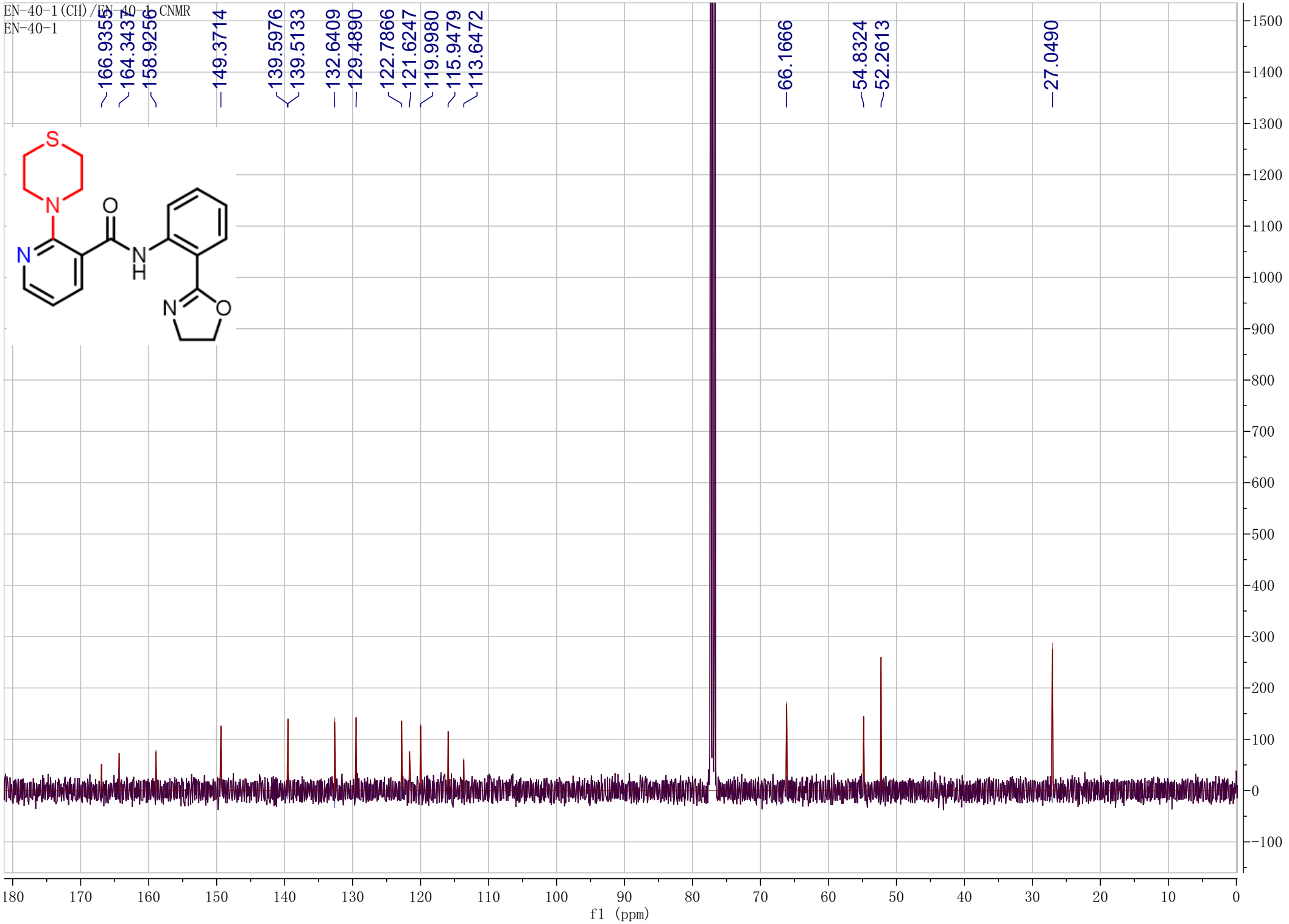
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)

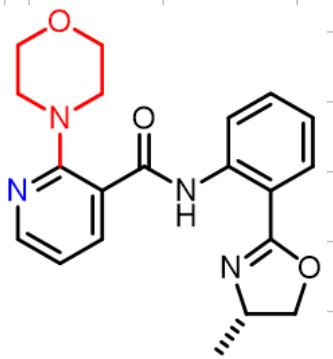

EN-34-1(CH)/34-1
34
12.7216
8.9309
8.9098
8.2974
8.2924
8.2853
8.2804
7.9364
7.9315
7.9178
7.9128
7.9045
7.9002
7.8846
7.8804
7.5364
7.5321
7.5180
7.5143
7.5107
7.2680
7.1405
7.1374
7.1216
7.1187
7.1023
7.0993
6.8472
6.8352
6.8285
6.8165
4.3808
4.3570
4.3334
4.0810
4.0576
4.0338
3.8397
3.8348
3.8286
3.8222
3.8174
3.8075
3.8025
3.7964
3.7903
2.9482
2.9420
2.9167
2.9106
2.8853
2.8791
1.6314
1.6228
1.5983
1.5901
1.2620
1.2560
1.2027
1.1930
1.1729
1.1634
0.8798
0.8635
O
N
N
H
N
O
0.98
0.97
0.99
0.97
1.00
1.01
1.00
1.01
2.00
2.04
2.05
1.94
2.18
1.09
2.23
3.21
f1 (ppm)


EN-34-1(CH)/EN-34-1C
34-1
167.3123
164.1214
159.1708
149.3454
139.8163
139.3365
132.5121
129.3416
122.4961
121.1232
120.0358
115.0197
113.6668
66.1695
54.8621
50.2366
33.9344
30.8281
21.9785
N
O
N
H
N
O
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


结构鉴定/EN-40-1(H)
40-1
12.7674
8.9036
8.8825
8.3209
8.3160
8.3088
8.3039
7.9515
7.9466
7.9327
7.9278
7.9185
7.9142
7.8986
7.8944
7.5448
7.5406
7.5264
7.5230
7.5195
7.5053
7.5011
7.2658
7.1600
7.1570
7.1411
7.1381
7.1220
7.1190
6.9199
6.9079
6.9012
6.8893
4.4009
4.3770
4.3535
4.0824
4.0588
4.0349
3.7041
3.6979
3.6917
3.6852
3.6785
2.6797
2.6734
2.6670
2.6608
2.6541
0.94
0.95
0.95
1.01
1.00
1.03
0.99
1.04
2.00
1.99
4.05
4.14
f1 (ppm)


EN-40-1(CH)/EN-40-1 CNMR
EN-40-1
166.9355
164.3437
158.9256
149.3714
139.5976
139.5133
132.6409
129.4890
122.7866
121.6247
119.9980
115.9479
113.6472
66.1666
54.8324
52.2613
27.0490
S
N
O
N
H
N
O
f1 (ppm)

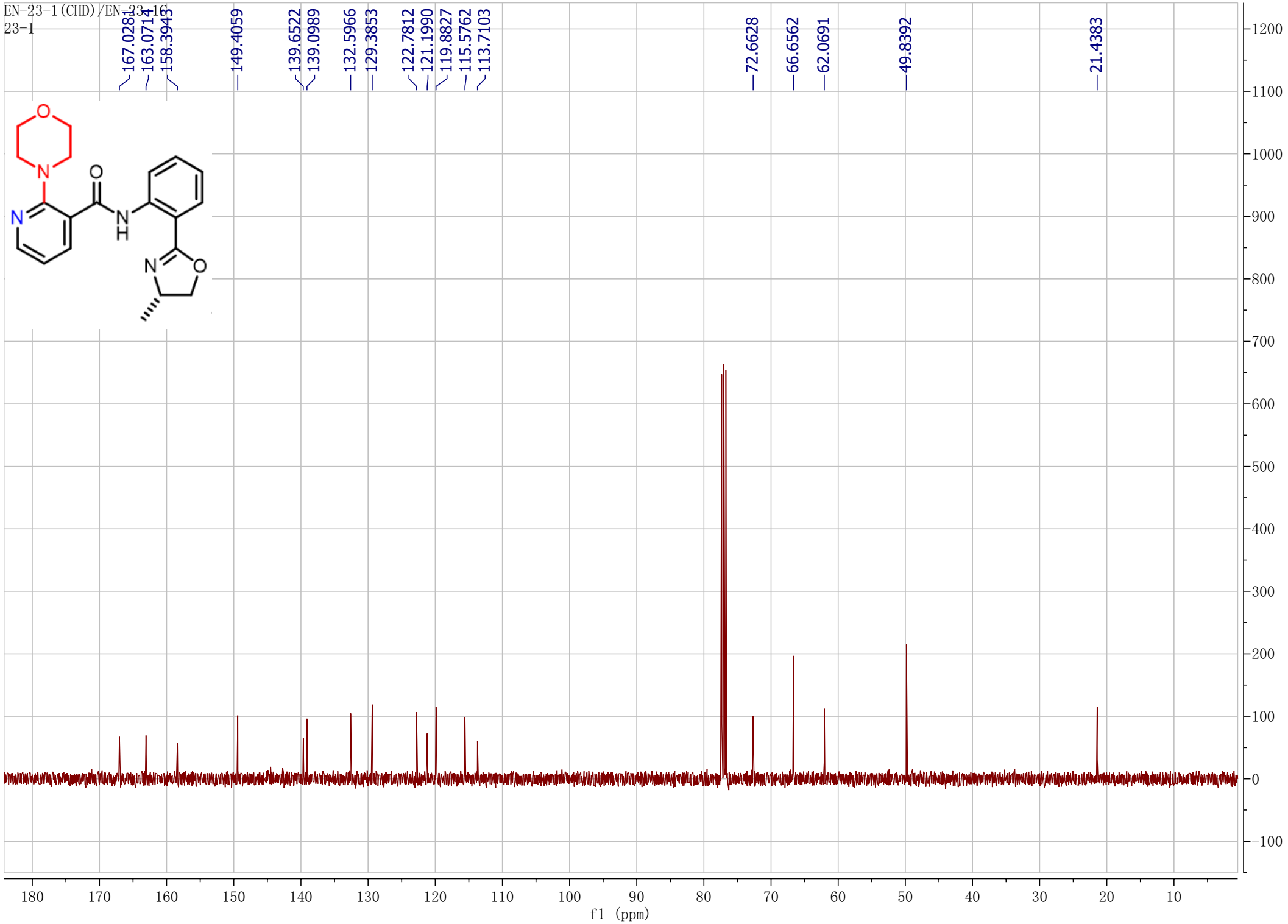
EN-23-1(CHD)/23-1H
23-1



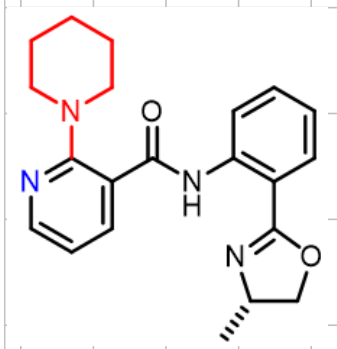
12.8453
8.8571
8.8360
8.3210
8.3163
8.3090
8.3043
7.9352
7.9302
7.9164
7.9115
7.8973
7.8932
7.8776
7.8735
7.5373
7.5335
7.5160
7.4979
7.4941
7.2757
7.1527
7.1337
7.1147
6.9039
6.8918
6.8852
6.8733
4.4889
4.4697
4.4661
4.4457
4.3933
4.3749
4.3574
4.3516
4.3408
4.3348
3.8949
3.8751
3.8553
3.7382
3.7343
3.7243
3.7129
3.4415
3.4321
3.4210
3.4109
1.2558
1.2395

0.98
0.94
1.00
1.98
1.00
0.98
0.99
1.00
0.97
1.19
4.03
4.00
3.10

f1 (ppm)


EN-23-1(CHD)/EN-23-1C
23-1
167.0281
163.0714
158.3943
149.4059
139.6522
139.0989
132.5966
129.3853
122.7812
121.1990
119.8827
115.5762
113.7103
72.6628
66.6562
62.0691
49.8392
21.4383
O
N
O
N
H
N
O
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

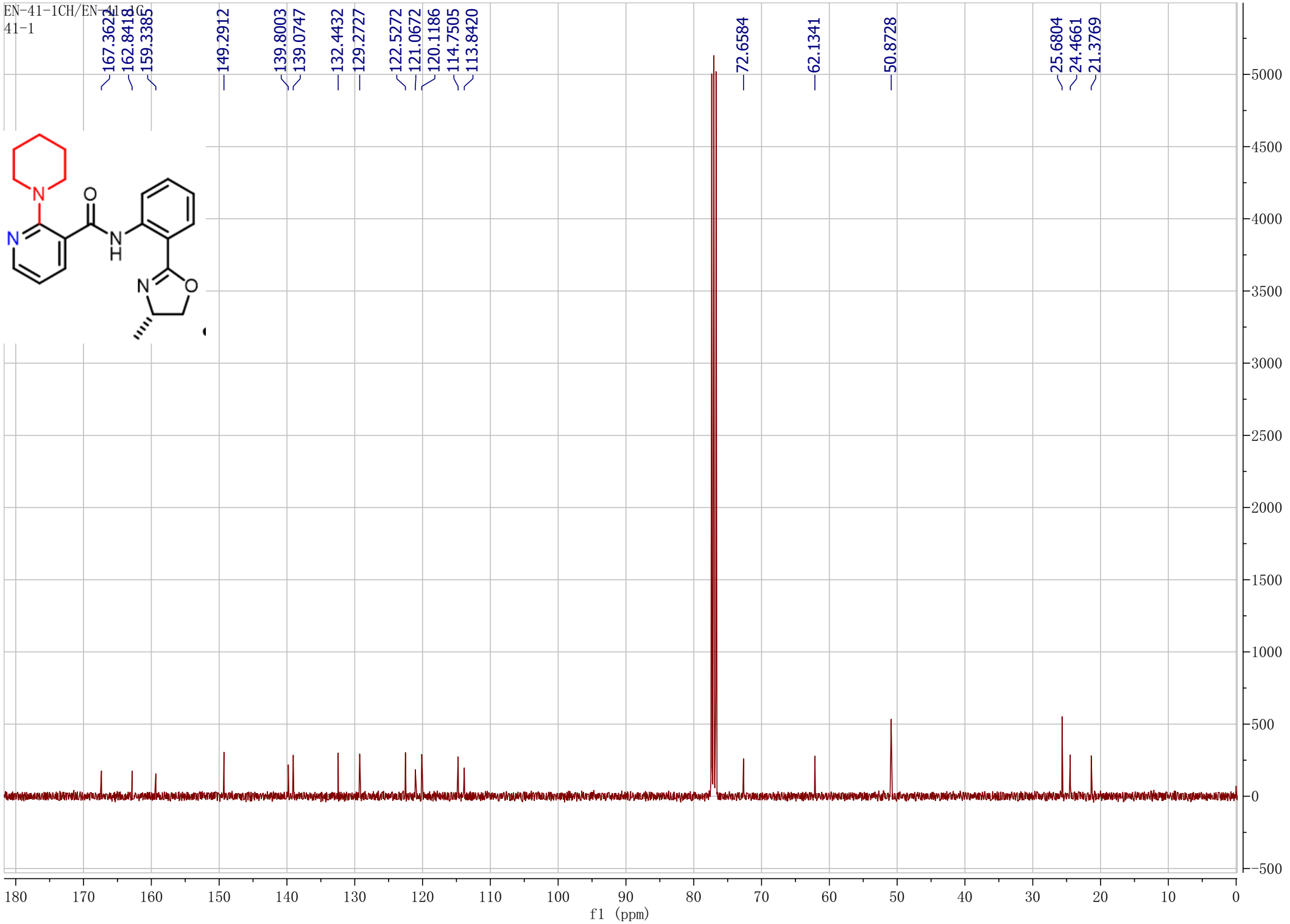
EN-41-1CH/41-1-H
41-1

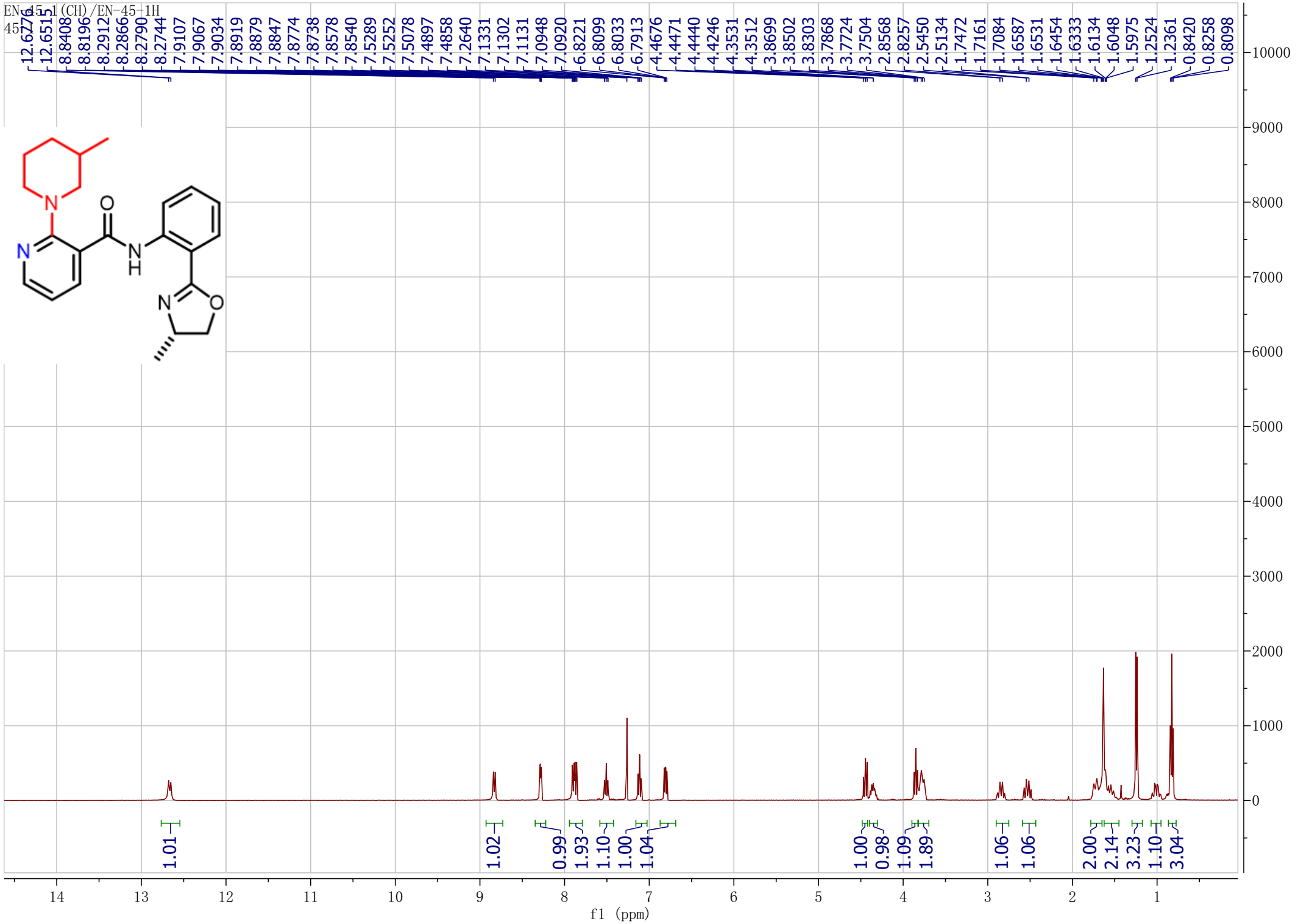


12.7108
8.8574
8.8364
8.2943
8.2893
8.2821
8.2773
7.9134
7.9085
7.8948
7.8899
7.8832
7.8789
7.8634
7.8592
7.5323
7.5281
7.5234
7.5139
7.5103
7.5070
7.4928
7.4887
7.2647
7.1381
7.1351
7.1192
7.1163
7.1002
7.0971
6.8298
6.8176
6.8110
6.7990
4.4759
4.4563
4.4523
4.4332
4.4002
4.3843
4.3810
4.3767
4.3681
4.3647
4.3605
4.3574
4.3416
3.8760
3.8565
3.8373
3.3784
3.3667
3.3524
1.5823
1.5673
1.5558
1.2552
1.2391

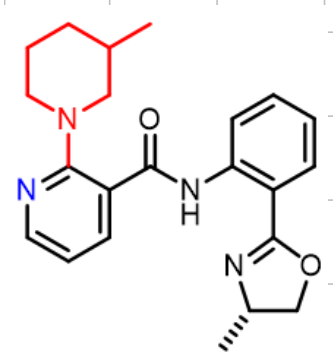
0.95
0.96
0.99
1.02
1.00
1.09
1.05
1.00
1.00
1.03
1.04
4.02
6.26
3.42

f1 (ppm)


EN-41-1CH/EN-41-1C
41-1
167.3625
162.8418
159.3385
149.2912
139.8003
139.0747
132.4432
129.2727
122.5272
121.0672
120.1186
114.7505
113.8420
72.6584
62.1341
50.8728
25.6804
24.4661
21.3769
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

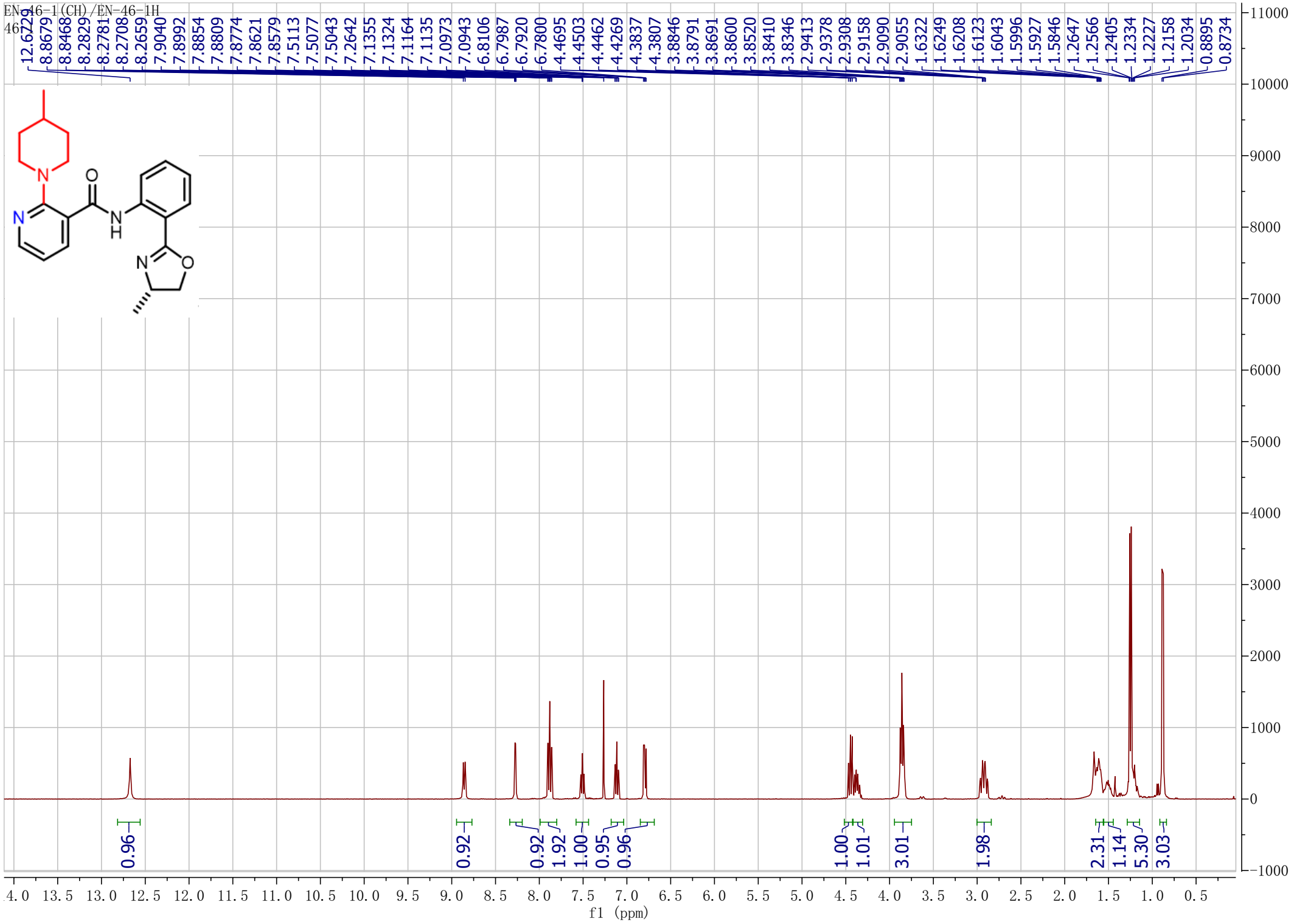

EN-45-1(CH)/EN-45-1H
12.6276
12.6515
8.8408
8.8196
8.2912
8.2866
8.2790
8.2744
7.9107
7.9067
7.9034
7.8919
7.8879
7.8847
7.8774
7.8738
7.8578
7.8540
7.5289
7.5252
7.5078
7.4897
7.4858
7.2640
7.1331
7.1302
7.1131
7.0948
7.0920
6.8221
6.8099
6.8033
6.7913
4.4676
4.4471
4.4440
4.4246
4.3531
4.3512
3.8699
3.8502
3.8303
3.7868
3.7724
3.7504
2.8568
2.8257
2.5450
2.5134
1.7472
1.7161
1.7084
1.6587
1.6531
1.6454
1.6333
1.6134
1.6048
1.5975
1.2524
1.2361
0.8420
0.8258
0.8098
N
O
N
H
N
O
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1.01
1.02
0.99
1.93
1.10
1.00
1.04
1.00
0.98
1.09
1.89
1.06
1.06
2.00
2.14
3.23
1.10
3.04
14
13
12
11
10
9
8
7
6
5
4
3
2
1
f1 (ppm)

EN-45-1(CH)/EN-45-1C
45-1

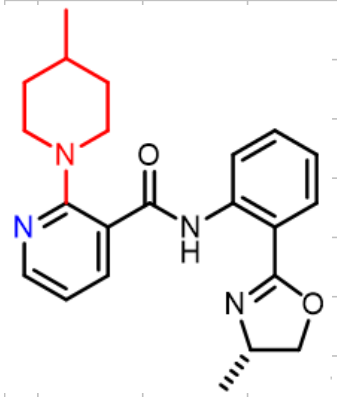


167.3523
162.8423
159.1786
149.3050
139.7837
139.0542
132.4461
129.2697
122.5213
121.0347
120.0842
114.7206
113.8418
72.6583
62.1367
57.4671
50.5094
33.1184
30.8921
30.8511
25.3827
25.2625
21.3960
21.3257
19.3178
19.2149

f1 (ppm)


EN-46-1(CH)/EN-46-1H
46
12.6220
8.8679
8.8468
8.2829
8.2781
8.2708
8.2659
7.9040
7.8992
7.8854
7.8809
7.8774
7.8621
7.8579
7.5113
7.5077
7.5043
7.2642
7.1355
7.1324
7.1164
7.1135
7.0973
7.0943
6.8106
6.7987
6.7920
6.7800
4.4695
4.4503
4.4462
4.4269
4.3837
4.3807
3.8846
3.8791
3.8691
3.8600
3.8520
3.8410
3.8346
2.9413
2.9378
2.9308
2.9158
2.9090
2.9055
1.6322
1.6249
1.6208
1.6123
1.6043
1.5996
1.5927
1.5846
1.2647
1.2566
1.2405
1.2334
1.2227
1.2158
1.2034
0.8895
0.8734
0.96
0.92
0.92
1.92
1.00
0.95
0.96
1.00
1.01
3.01
1.98
2.31
1.14
5.30
3.03
f1 (ppm)

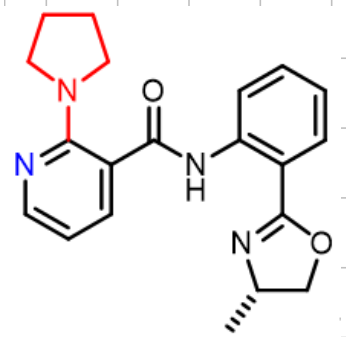
EN-46-1(CH)/EN-46-1C
46-1



167.4089
162.8833
159.0274
149.2810
139.8450
139.0456
132.4476
129.2585
122.5087
120.8532
120.0795
114.5460
113.8061
72.6656
62.1220
50.1619
49.9647
34.0263
33.9588
30.9055
21.9487
21.4128

f1 (ppm)

EN-48-1(CH)/EN-48-1H
48-1

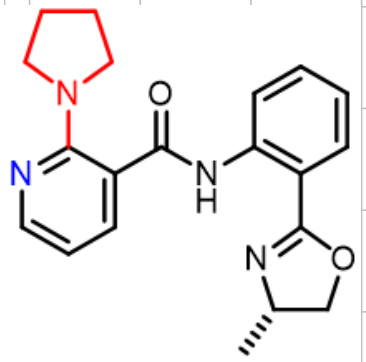


12.7034
8.9069
8.8859
8.2759
8.2712
8.2637
8.2589
7.8906
7.8864
7.8707
7.8666
7.8160
7.8114
7.7974
7.7927
7.5375
7.5333
7.5189
7.5146
7.4979
7.4938
7.1414
7.1384
7.1203
7.1032
7.1002
6.6461
6.6341
6.6276
6.6154
4.4873
4.4681
4.4641
4.4445
4.4131
4.3960
4.3893
4.3792
4.3733
3.9241
3.9050
3.8861
3.5575
3.5327
3.5158
3.5016
3.4893
3.4766
1.9363
1.9215
1.9050
1.8910
1.8840
1.3049
1.2888

0.96
0.93
1.00
0.97
1.02
0.98
0.99
0.99
1.03
1.05
1.00
4.24
4.28
3.28

f1 (ppm)

EN-48-1(CH)/EN-48-1C
48-1



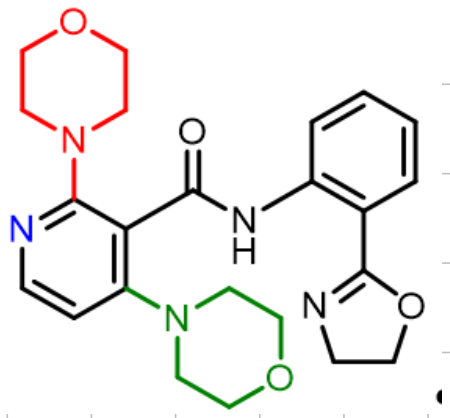
167.7474
163.3339
154.9890
149.2803
140.0936
137.7896
132.6427
129.1788
122.4468
119.5716
117.3978
113.3311
110.8921
72.6978
61.9072
49.2331
25.6958
21.4821

6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

EN-2/EN-2H
EN-2



12.5329

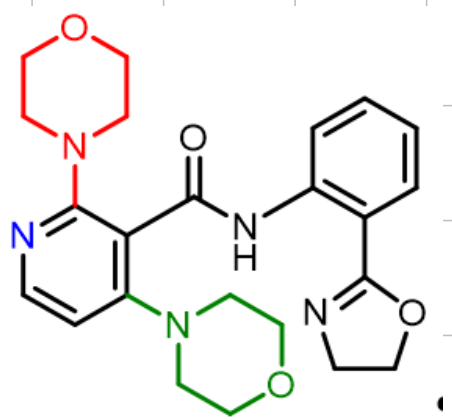
8.8985 8.8774 8.1788 8.1645 7.9305 7.9264 7.9107 7.9066 7.5504 7.5461 7.5287 7.5108 7.5067 7.2687 7.1651 7.1621 7.1445 7.1268 7.1239 6.5595 6.5452

4.3804 4.3565 4.3329 3.9898 3.9662 3.9423 3.6989 3.6870 3.6758 3.6711 3.6574 3.6453 3.6338 3.6257 3.3112 3.2997 3.2883 3.1797 3.1681 3.1566

0.91 0.95 0.98 0.96 1.06 0.98 0.97 2.00 2.03 4.13 4.05 4.30 3.99

f1 (ppm)

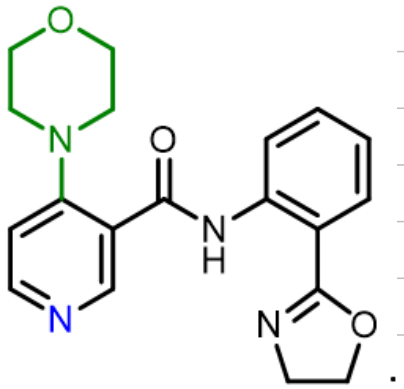
EN-2/EN-2C
EN-2



167.3337
164.3566
160.5099
158.1390
149.0737
140.0189
132.8443
129.5225
122.7055
119.3719
116.6226
113.2076
107.8198
67.0214
66.7848
66.1114
54.7812
51.4153
50.5345

f1 (ppm)

EN-3/EN-3H
EN3



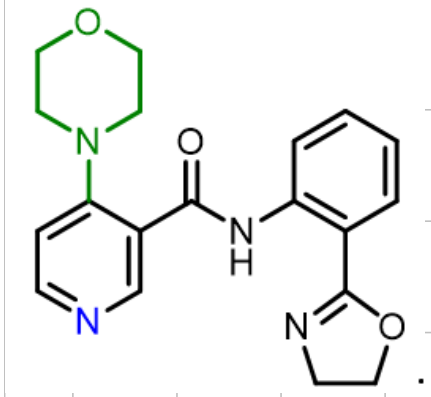
12.8498

8.8943
8.8731
8.6767
8.4483
8.4337
7.9280
7.9238
7.9082
7.9040
7.5493
7.5450
7.5307
7.5271
7.5238
7.5097
7.5055
7.2677
7.1729
7.1699
7.1539
7.1510
7.1349
7.1318
6.8245
6.8099
4.4076
4.3838
4.3603
4.0698
4.0462
4.0223
3.7608
3.7493
3.7374
3.2697
3.2578
3.2463

0.91
0.93
0.94
1.01
1.02
1.08
1.00
1.00
2.00
2.03
4.11
3.95

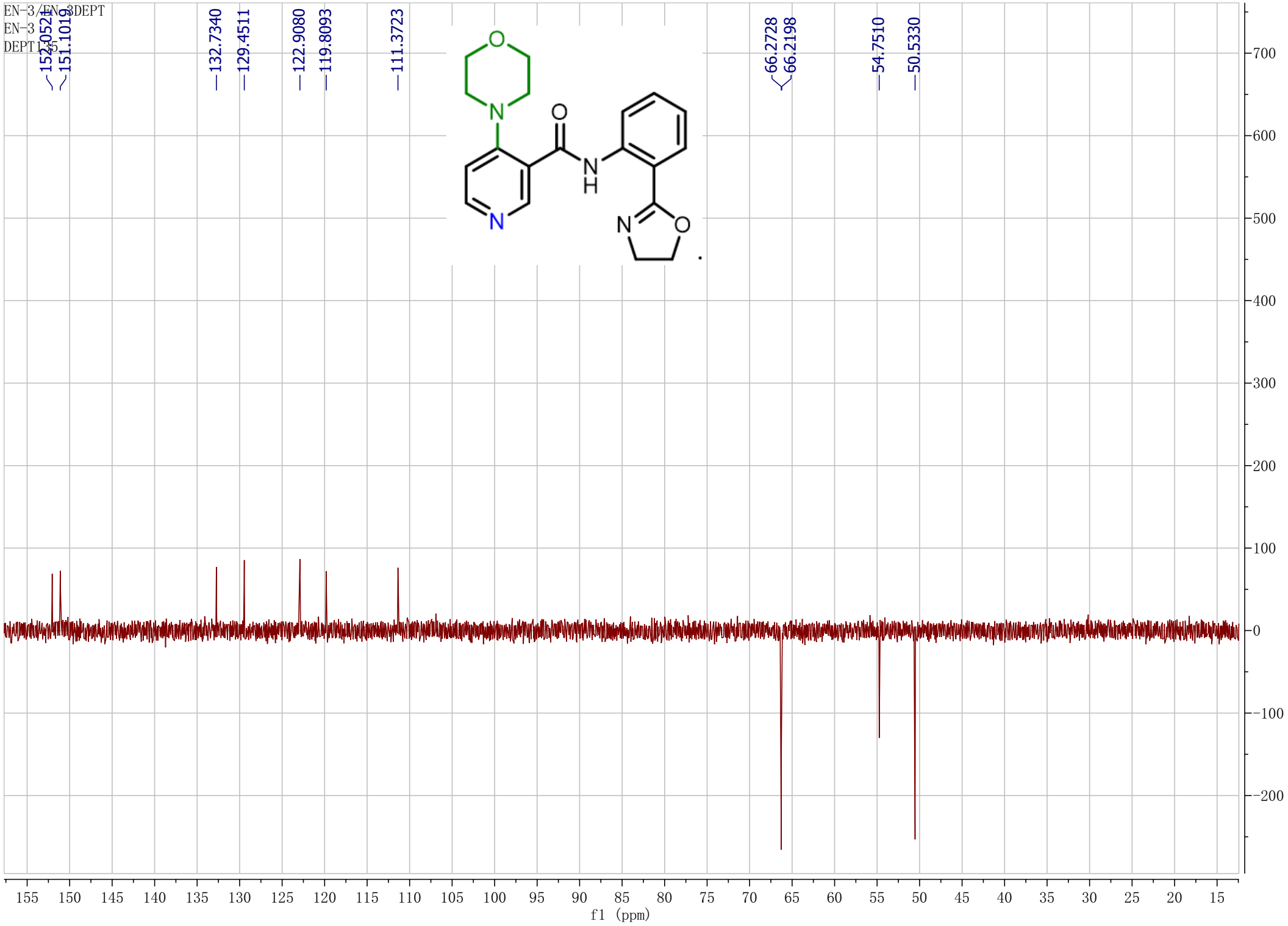
f1 (ppm)

EN-3/EN-3C
EN-3

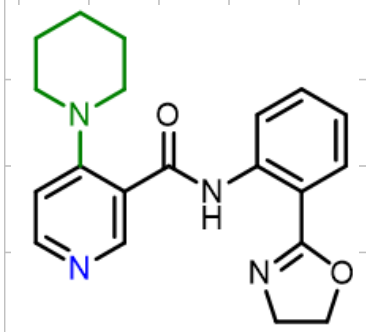


166.2591
164.4933
155.1346
151.8629
150.9534
139.6343
132.7333
129.4486
123.0652
122.9192
119.8085
113.5263
111.3515
66.2652
66.2240
54.7477
50.5313

f1 (ppm)


EN-3/EN-3DEPT
EN-3
DEPT135
152.0524
151.1019
132.7340
129.4511
122.9080
119.8093
111.3723
66.2728
66.2198
54.7510
50.5330
O
N
O
N
H
N
O
700
600
500
400
300
200
100
0
-100
-200
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

EN-15-2(CHD)/EN-15-2H
EN-15-2



12.7092

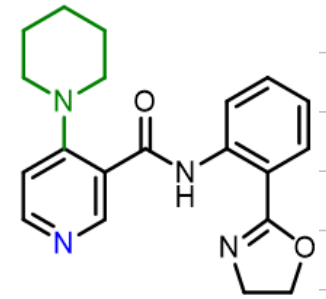
8.9252 8.9224 8.9040 8.9011 8.6374 8.3771 8.3625 7.9110 7.9068 7.8911 7.8870 7.5391 7.5348 7.5206 7.5171 7.5138 7.4994 7.4952 7.2683 7.1476 7.1446 7.1287 7.1257 7.1094 7.1065 6.8115 6.7968 4.3888 4.3867 4.3640 4.3403 4.0705 4.0471 4.0232 3.2311 3.2199 3.2064

1.6075 1.5953 1.5871 1.5746

0.97 0.97 0.96 0.98 1.00 1.02 1.01 1.00 2.00 2.01 4.00 6.22

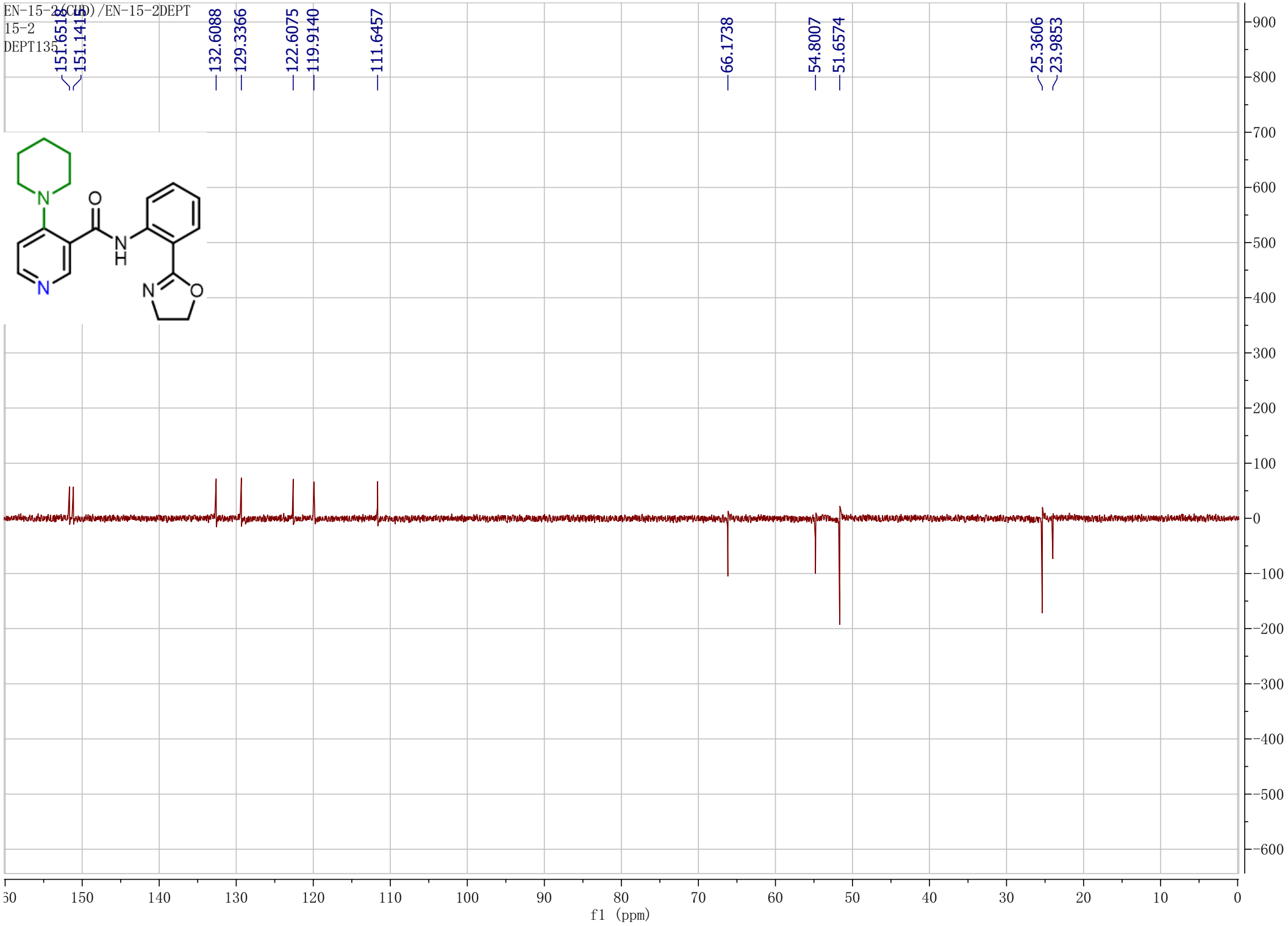
f1 (ppm)

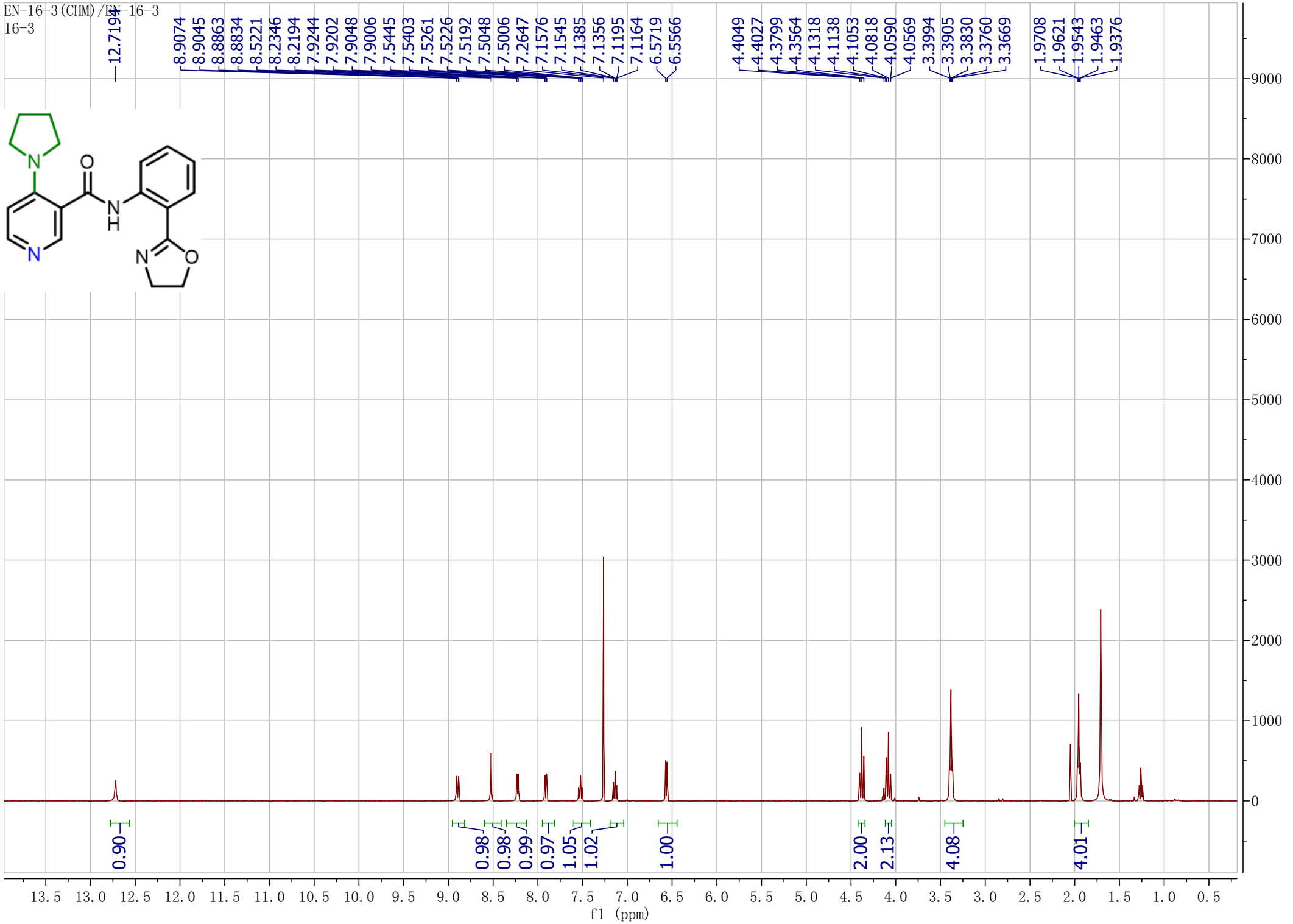
EN-15-2(CHD)/EN-15-2C
15-2

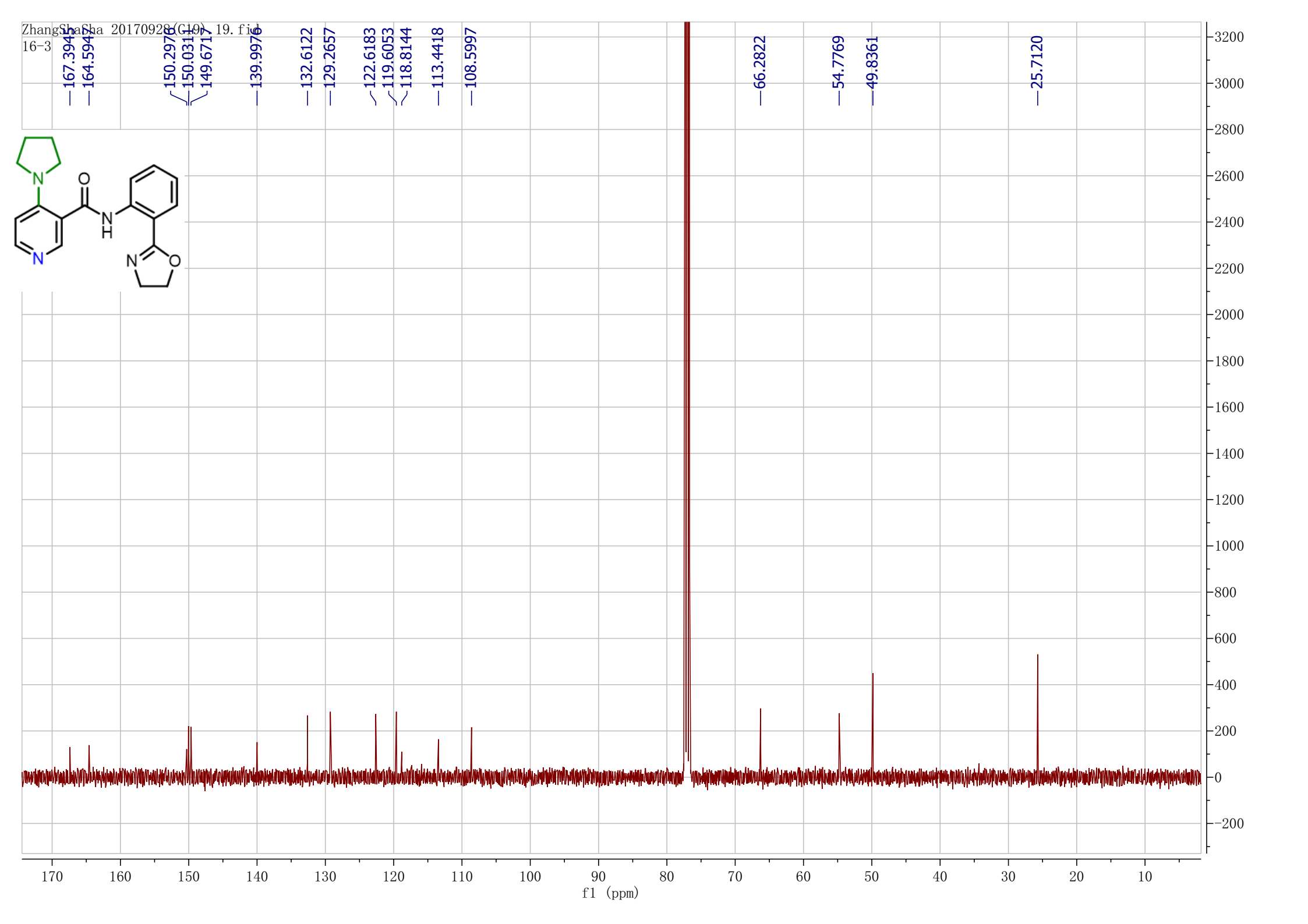


166.6725
164.2808
155.7253
151.6407
151.1344
139.8454
132.5984
129.3285
122.8205
122.5962
119.9091
113.5273
111.6347
66.1692
54.7968
51.6526
25.3581
23.9829

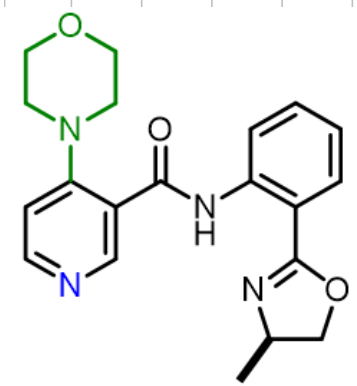
f1 (ppm)


EN-15-2(CHD)/EN-15-2DEPT
15-2
DEPT135
151.6518
151.1418
132.6088
129.3366
122.6075
119.9140
111.6457
66.1738
54.8007
51.6574
25.3606
23.9853
f1 (ppm)


EN-16-3(CHM)/EN-16-3
16-3
12.7194
8.9074
8.9045
8.8863
8.8834
8.5221
8.2346
8.2194
7.9244
7.9202
7.9048
7.9006
7.5445
7.5403
7.5261
7.5226
7.5192
7.5048
7.5006
7.2647
7.1576
7.1545
7.1385
7.1356
7.1195
7.1164
6.5719
6.5566
4.4049
4.4027
4.3799
4.3564
4.1318
4.1138
4.1053
4.0818
4.0590
4.0569
3.3994
3.3905
3.3830
3.3760
3.3669
1.9708
1.9621
1.9543
1.9463
1.9376
0.90
0.98
0.98
0.99
0.97
1.05
1.02
1.00
2.00
2.13
4.08
4.01
f1 (ppm)


ZhangShaSha 20170928(C19) 19.fid
16-3
167.3945
164.5941
150.2976
150.0311
149.6717
139.9976
132.6122
129.2657
122.6183
119.6053
118.8144
113.4418
108.5997
66.2822
54.7769
49.8361
25.7120
N
O
N
H
N
N
O
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

EN-23-3(CHDM)/23-3H

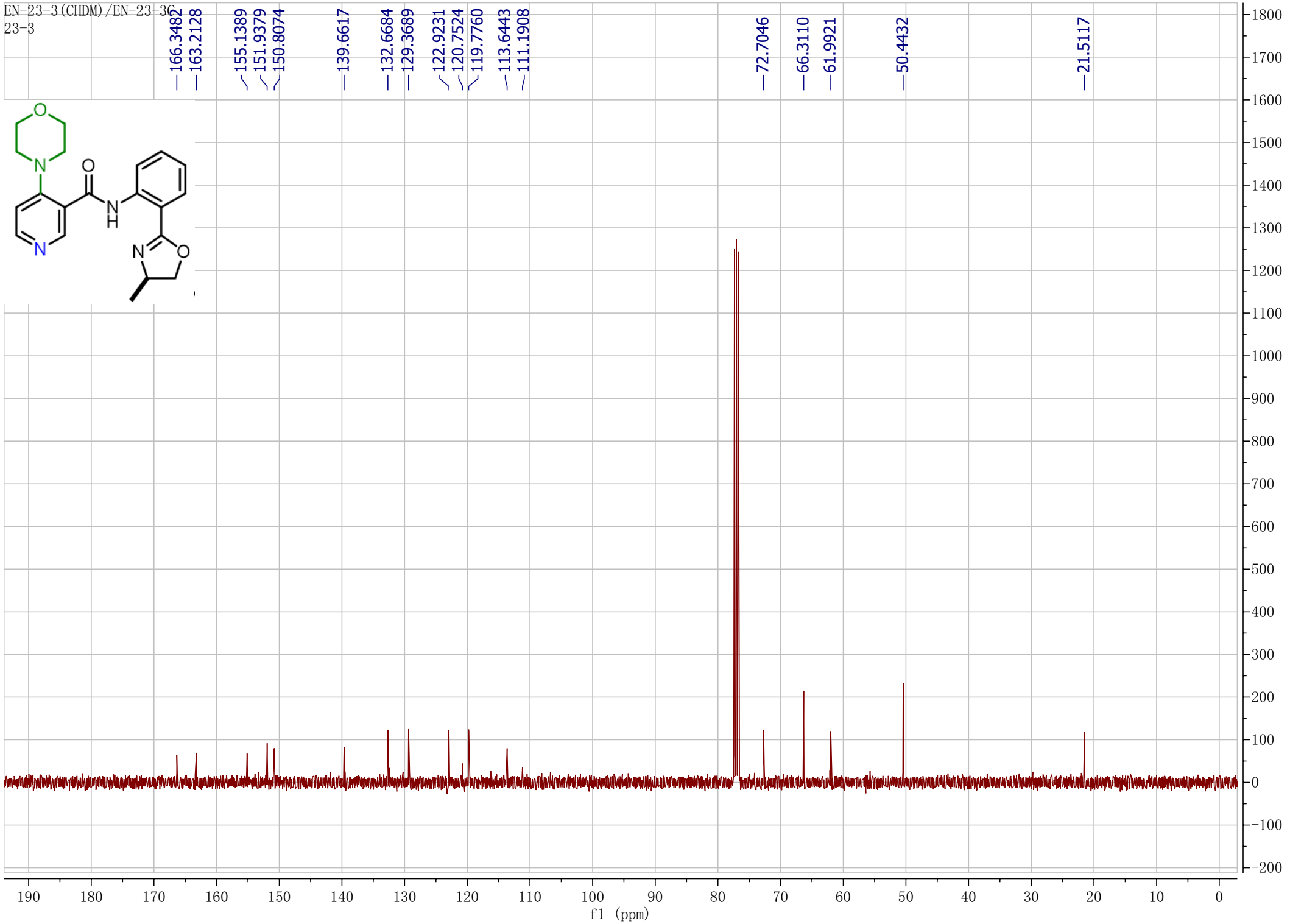


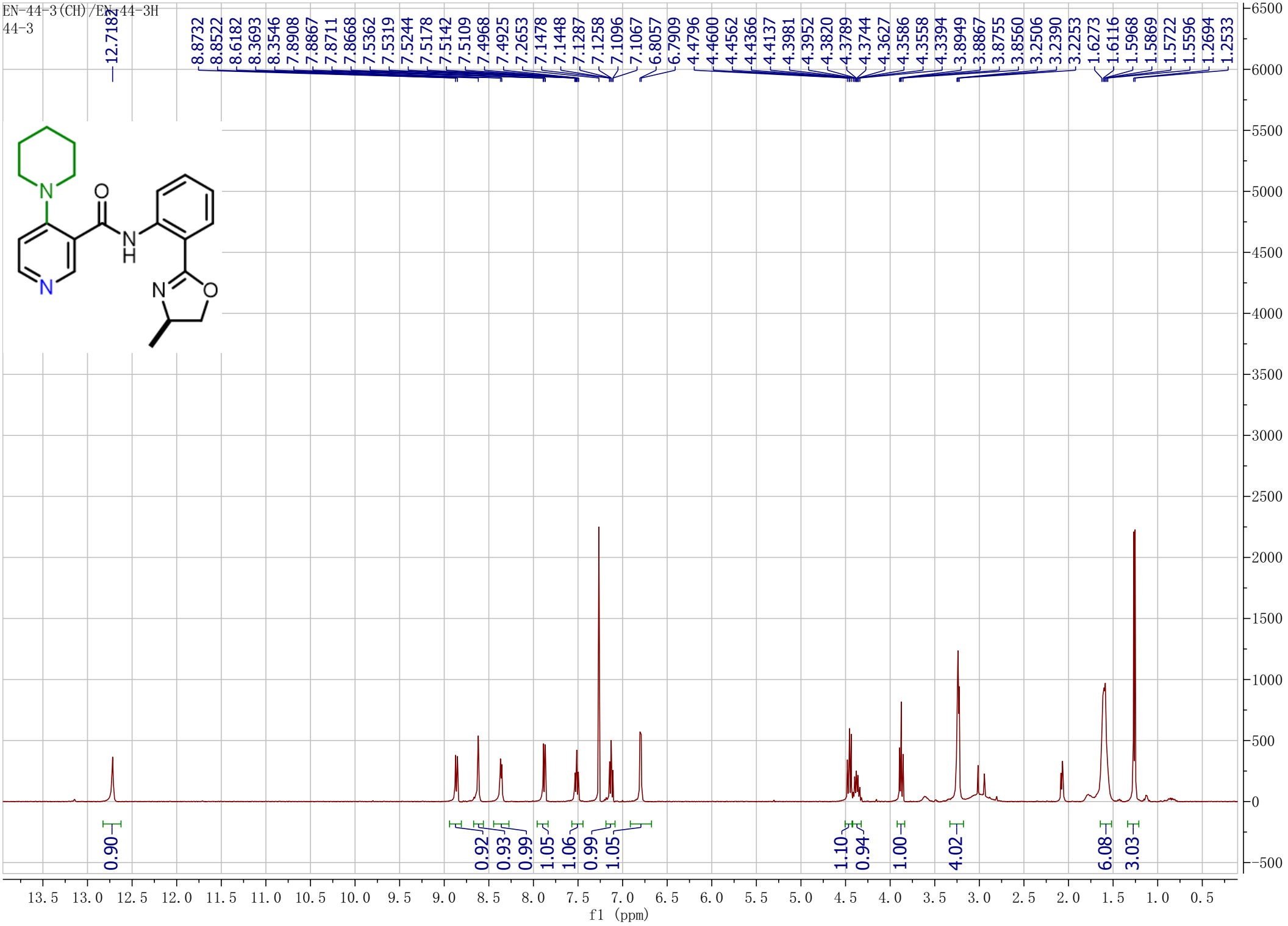
12.8648

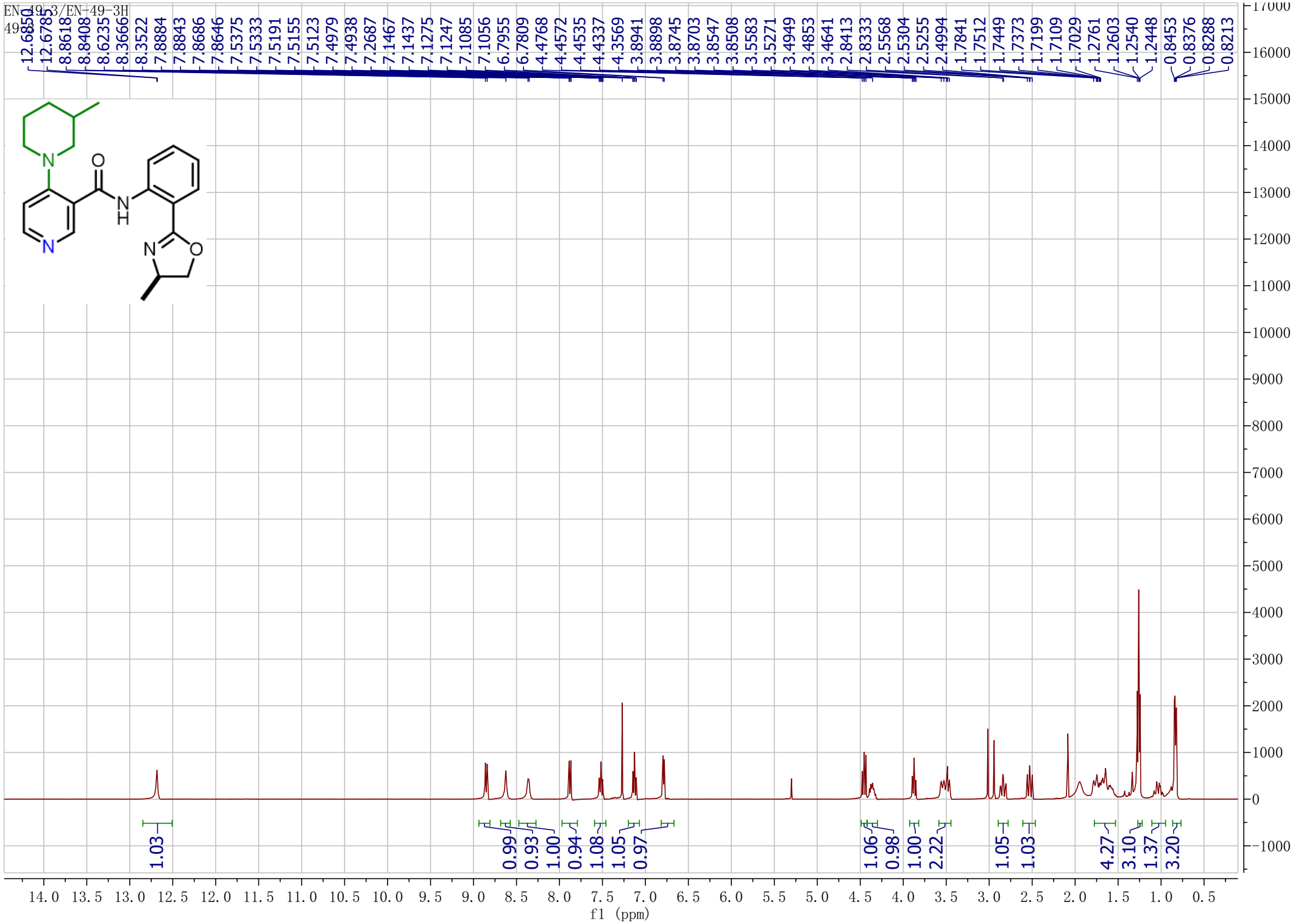
8.8542 8.8402 8.6767 8.4454 8.4359 8.4356 7.9026 7.8999 7.8894 7.8866 7.5385 7.5357 7.5262 7.5239 7.5217 7.5123 7.5094 7.2623 7.1629 7.1610 7.1507 7.1498 7.1488 7.1478 7.1375 7.1355 6.8083 6.7985 4.4858 4.4724 4.4702 4.4568 4.3887 4.3780 4.3758 4.3733 4.3649 4.3623 4.3602 4.3494 3.9092 3.8958 3.8825 3.7711 3.7633 3.7554 3.2657 3.2611 3.2578 3.2547 3.2500 1.2714 1.2604

0.89 0.97 0.94 0.90 1.00 1.06 1.07 0.98 1.06 1.00 1.03 3.98 3.93 3.09

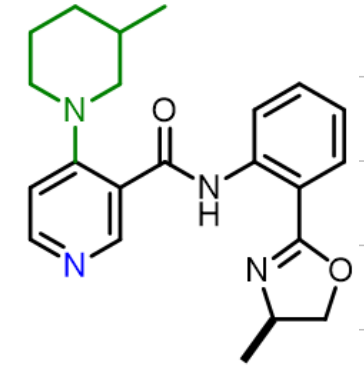
f1 (ppm)


EN-23-3(CHDM)/EN-23-3C
23-3
166.3482
163.2128
155.1389
151.9379
150.8074
139.6617
132.6684
129.3689
122.9231
120.7524
119.7760
113.6443
111.1908
72.7046
66.3110
61.9921
50.4432
21.5117
O
N
O
N
H
N
O
N
f1 (ppm)


EN-44-3(CH)/EN-44-3H
44-3
12.7182
8.8732
8.8522
8.6182
8.3693
8.3546
7.8908
7.8867
7.8711
7.8668
7.5362
7.5319
7.5244
7.5178
7.5142
7.5109
7.4968
7.4925
7.2653
7.1478
7.1448
7.1287
7.1258
7.1096
7.1067
6.8057
6.7909
4.4796
4.4600
4.4562
4.4366
4.4137
4.3981
4.3952
4.3820
4.3789
4.3744
4.3627
4.3586
4.3558
4.3394
3.8949
3.8867
3.8755
3.8560
3.2506
3.2390
3.2253
1.6273
1.6116
1.5968
1.5869
1.5722
1.5596
1.2694
1.2533
0.90
0.92
0.93
0.99
1.05
1.06
0.99
1.05
1.10
0.94
1.00
4.02
6.08
3.03
f1 (ppm)


EN-49-3/EN-49-3H
12.6785
8.8618
8.8408
8.6235
8.3666
8.3522
7.8884
7.8843
7.8686
7.8646
7.5375
7.5333
7.5191
7.5155
7.5123
7.4979
7.4938
7.2687
7.1467
7.1437
7.1275
7.1247
7.1085
7.1056
6.7955
6.7809
4.4768
4.4572
4.4535
4.4337
4.3569
3.8941
3.8898
3.8745
3.8703
3.8547
3.8508
3.5583
3.5271
3.4949
3.4853
3.4641
2.8413
2.8333
2.5568
2.5304
2.5255
2.4994
1.7841
1.7512
1.7449
1.7373
1.7199
1.7109
1.7029
1.2761
1.2603
1.2540
1.2448
0.8453
0.8376
0.8288
0.8213
1.03
0.99
0.93
1.00
0.94
1.08
1.05
0.97
1.06
0.98
1.00
2.22
1.05
1.03
4.27
3.10
1.37
3.20
f1 (ppm)

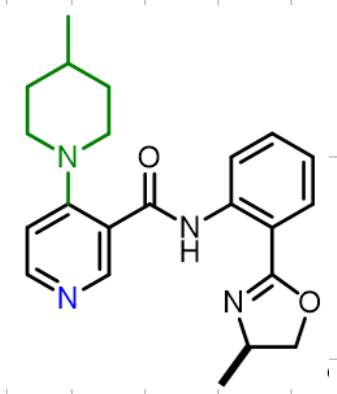
EN-49-3(CH)/EN-49-3 CNMR
EN-49-3



166.7507
163.0377
155.4411
155.3916
151.4045
150.7621
139.8208
132.5555
129.2602
122.6460
119.8815
113.6732
111.4292
72.6619
62.0433
58.3473
58.2080
51.0624
50.8803
32.6265
32.5787
30.7108
25.0888
24.9410
21.4916
21.4397
19.1366
19.0628

f1 (ppm)

EN-50-3/EN-50-3H
50-3



12.7115

8.8843 8.8633 8.6199 8.3608 8.3465 7.8933 7.8891 7.8736 7.8694 7.5401 7.5359 7.5225 7.5187 7.5006 7.4964 7.2635 7.1517 7.1487 7.1320 7.1136 7.1107 6.8008 6.7859 4.4791 4.4598 4.4559 4.4364 4.4039 4.3866 4.3677 3.9037 3.8845 3.8652 3.6079 3.5758 3.0164 2.9445 2.9162 2.8844 1.6618 1.6274 1.5540 1.5437 1.5279 1.3133 1.3065 1.2854 1.2772 1.2611 1.2547 1.2322 0.9213 0.9051

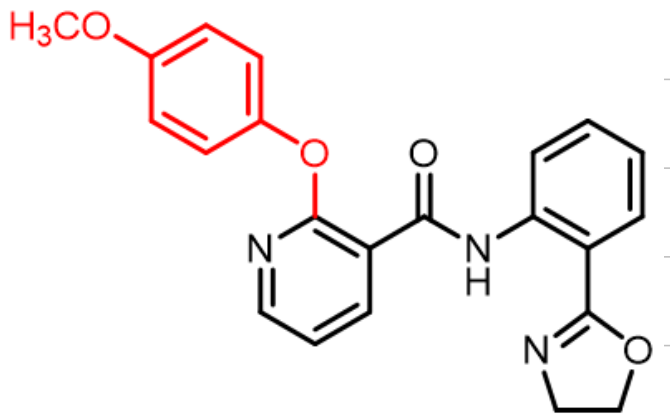
0.93 0.94 0.91 0.94 1.02 1.15 1.07 0.97 1.13 0.94 1.00 2.15 2.23 2.45 0.98 5.39 3.26

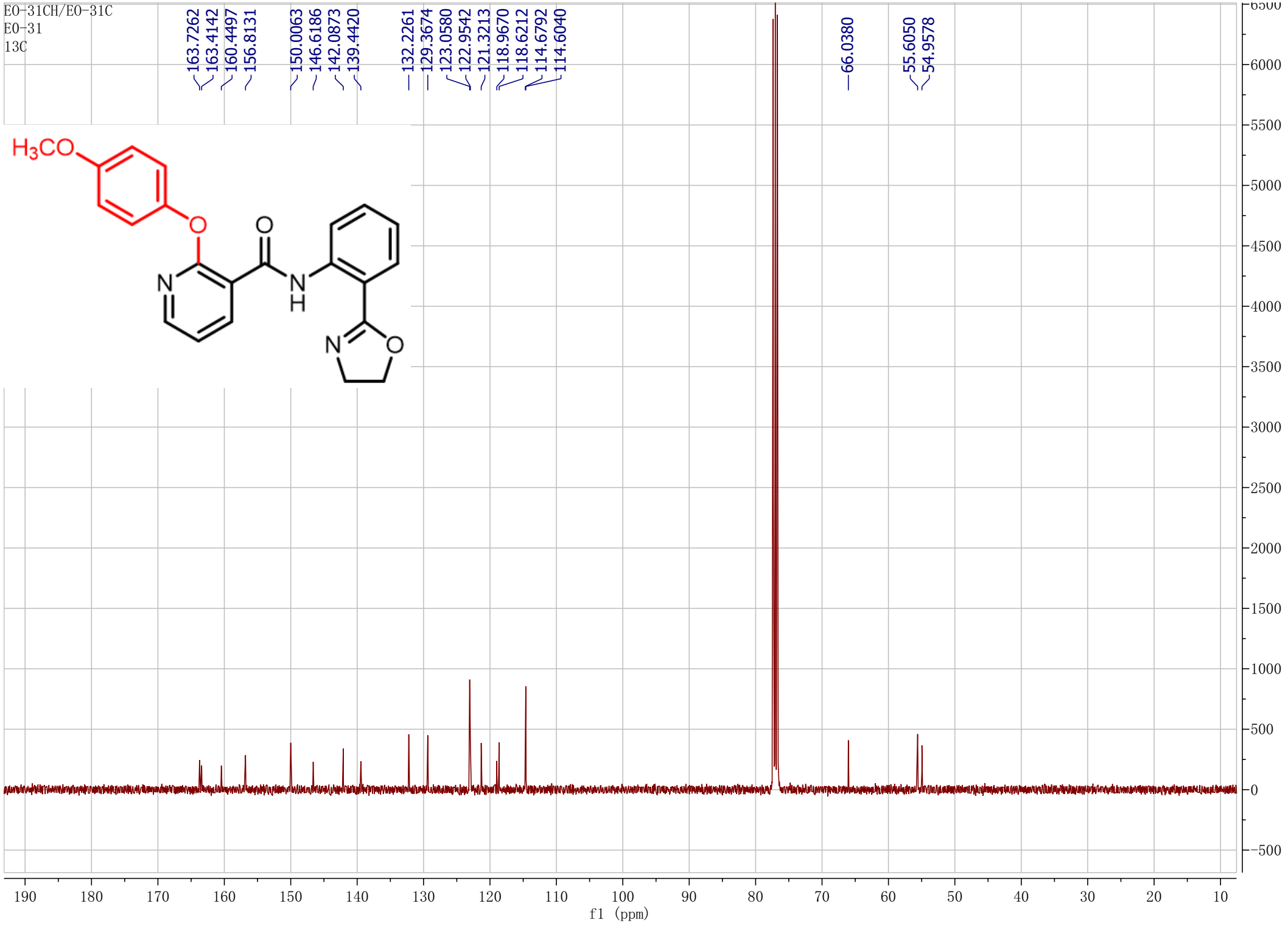
3000 2500 2000 1500 1000 500 0

13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

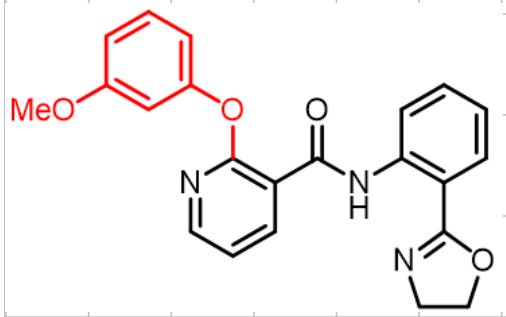
f1 (ppm)

EO-31CH/EO-31H
EO-31




EO-31CH/EO-31C
EO-31
13C
163.7262
163.4142
160.4497
156.8131
150.0063
146.6186
142.0873
139.4420
132.2261
129.3674
123.0580
122.9542
121.3213
118.9670
118.6212
114.6792
114.6040
66.0380
55.6050
54.9578
H3CO
O
O
N
N
H
N
O
f1 (ppm)

EO-13-1(CH)/EO-13-1H
EO-13-1



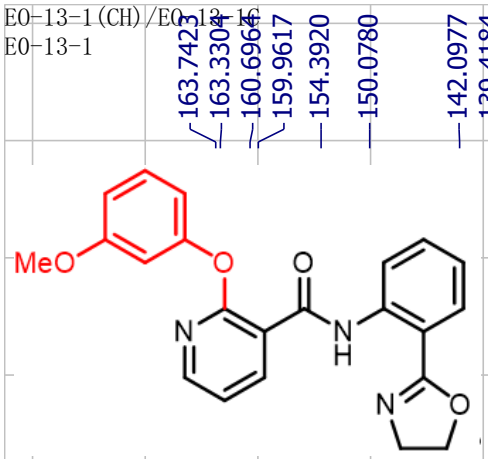
12.9234

8.9452 8.9424 8.9238 8.9211 8.5024 8.4974 8.4835 8.4784 8.2729 8.2678 8.2608 8.2558 7.8912 7.8870 7.8716 7.8673 7.5391 7.5348 7.5208 7.5169 7.5134 7.4994 7.4951 7.3637 7.3586 7.3455 7.3413 7.3241 7.3213 7.3182 7.1654 7.1530 7.1471 7.1337 7.1294 7.1128 7.1098 6.8452 6.8428 6.8397 6.8375 6.8253 6.8213 6.8165 6.8136 6.8031 6.7982 6.7945 6.7910 4.2534 4.2295 4.2057 3.8146 3.7110 3.6872 3.6633

0.93 0.97 0.99 1.00 0.99 1.05 1.04 2.08 2.94 2.00 3.06 2.01

f1 (ppm)

EO-13-1(CH)/EO-13-1C
EO-13-1

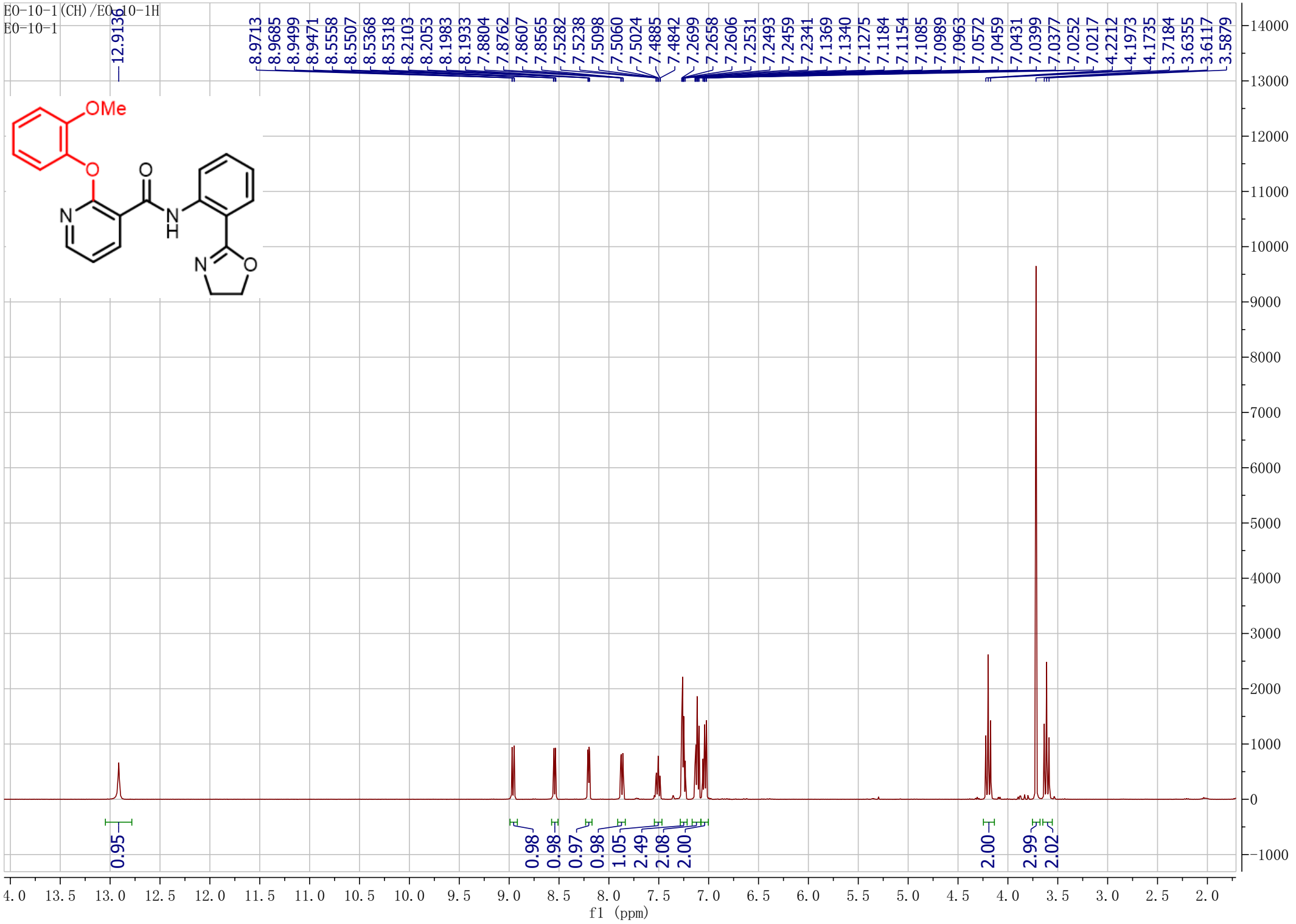


163.7423
163.3304
160.6966
159.9617
154.3920
150.0780
142.0977
139.4184
132.2411
129.8774
129.3575
122.9830
121.2688
119.2994
118.9248
114.6350
114.3772
110.8739
108.1971
66.0480
55.4487
54.8762

5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500

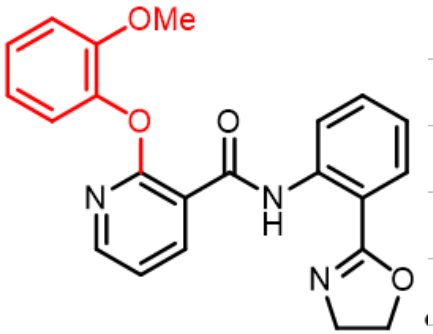
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)

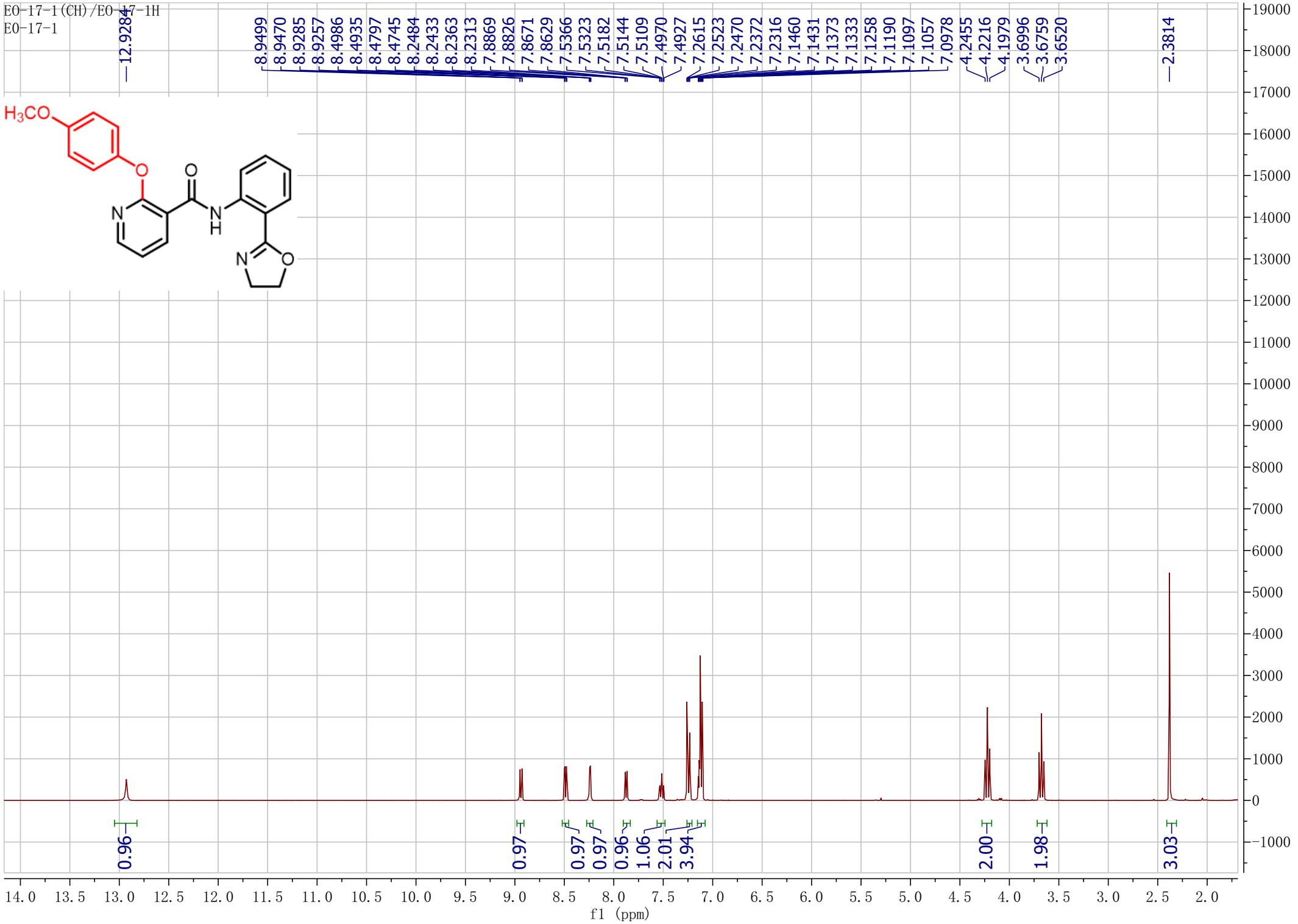

EO-10-1(CH)/EO-10-1H
EO-10-1
12.9136
8.9713
8.9685
8.9499
8.9471
8.5558
8.5507
8.5368
8.5318
8.2103
8.2053
8.1983
8.1933
7.8804
7.8762
7.8607
7.8565
7.5282
7.5238
7.5098
7.5060
7.5024
7.4885
7.4842
7.2699
7.2658
7.2606
7.2531
7.2493
7.2459
7.2341
7.1369
7.1340
7.1275
7.1184
7.1154
7.1085
7.0989
7.0963
7.0572
7.0459
7.0431
7.0399
7.0377
7.0252
7.0217
4.2212
4.1973
4.1735
3.7184
3.6355
3.6117
3.5879
OMe
O
N
O
N
H
N
O
0.95
0.98
0.98
0.97
0.98
1.05
2.49
2.08
2.00
2.00
2.99
2.02
f1 (ppm)

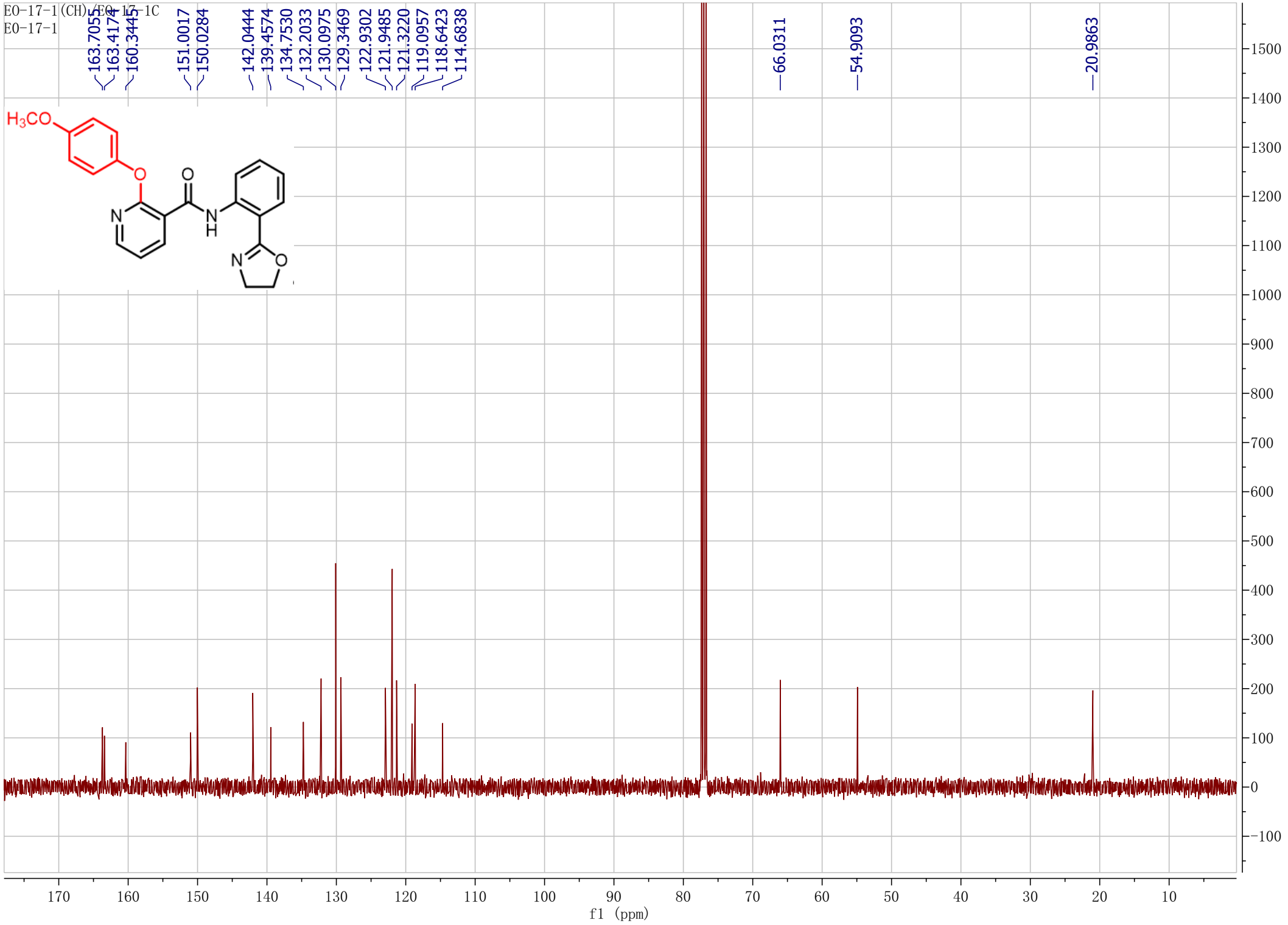
EO-10-1(CH)/EO-10-1C
EO-10-1

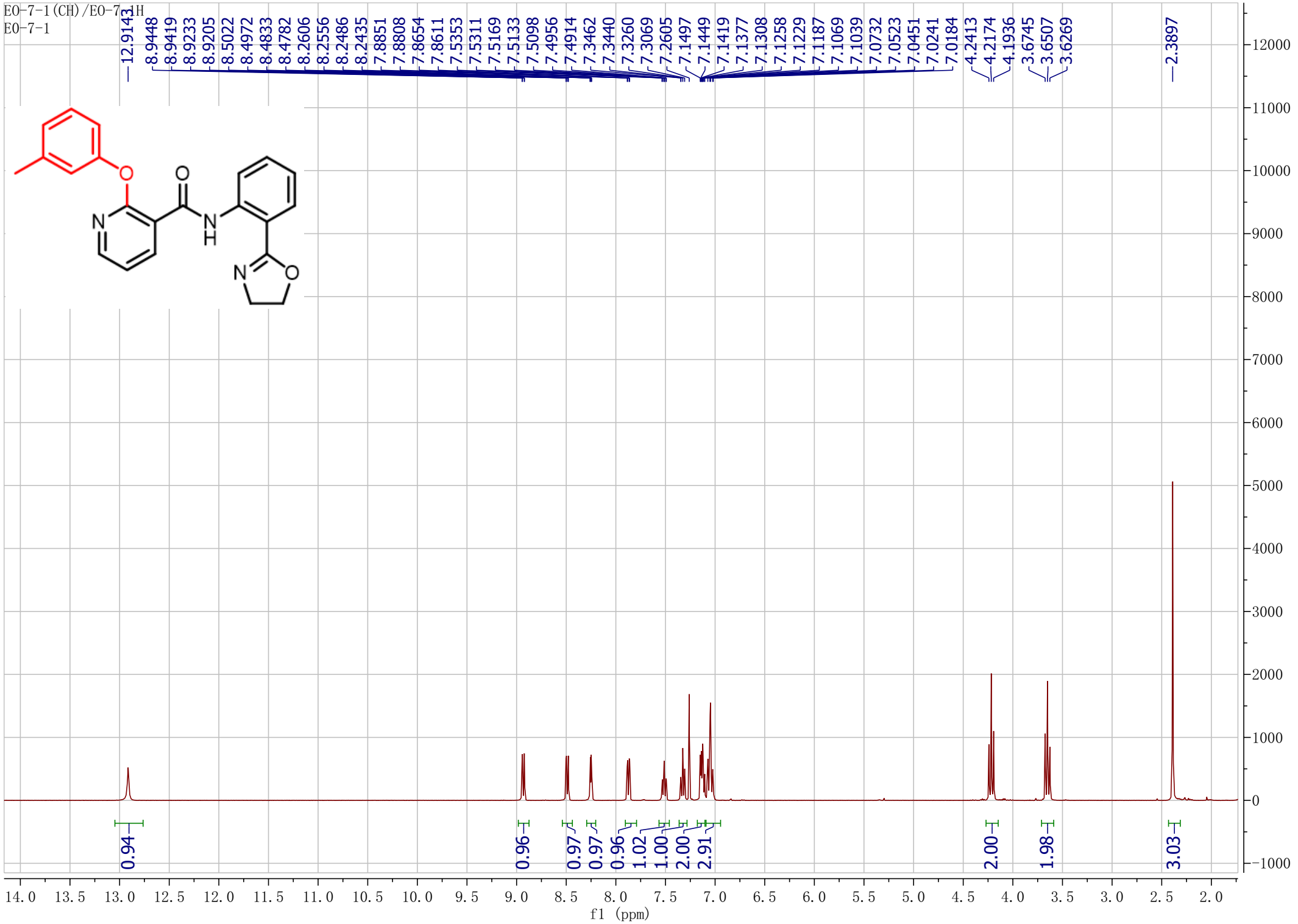
163.5923
163.4243
160.0988
151.8746
150.0409
142.2911
142.1044
139.5390
132.0860
129.3237
126.3643
123.4692
122.8647
121.5514
120.9880
118.5766
118.1557
114.9136
112.8980
65.9877
55.9290
54.8060

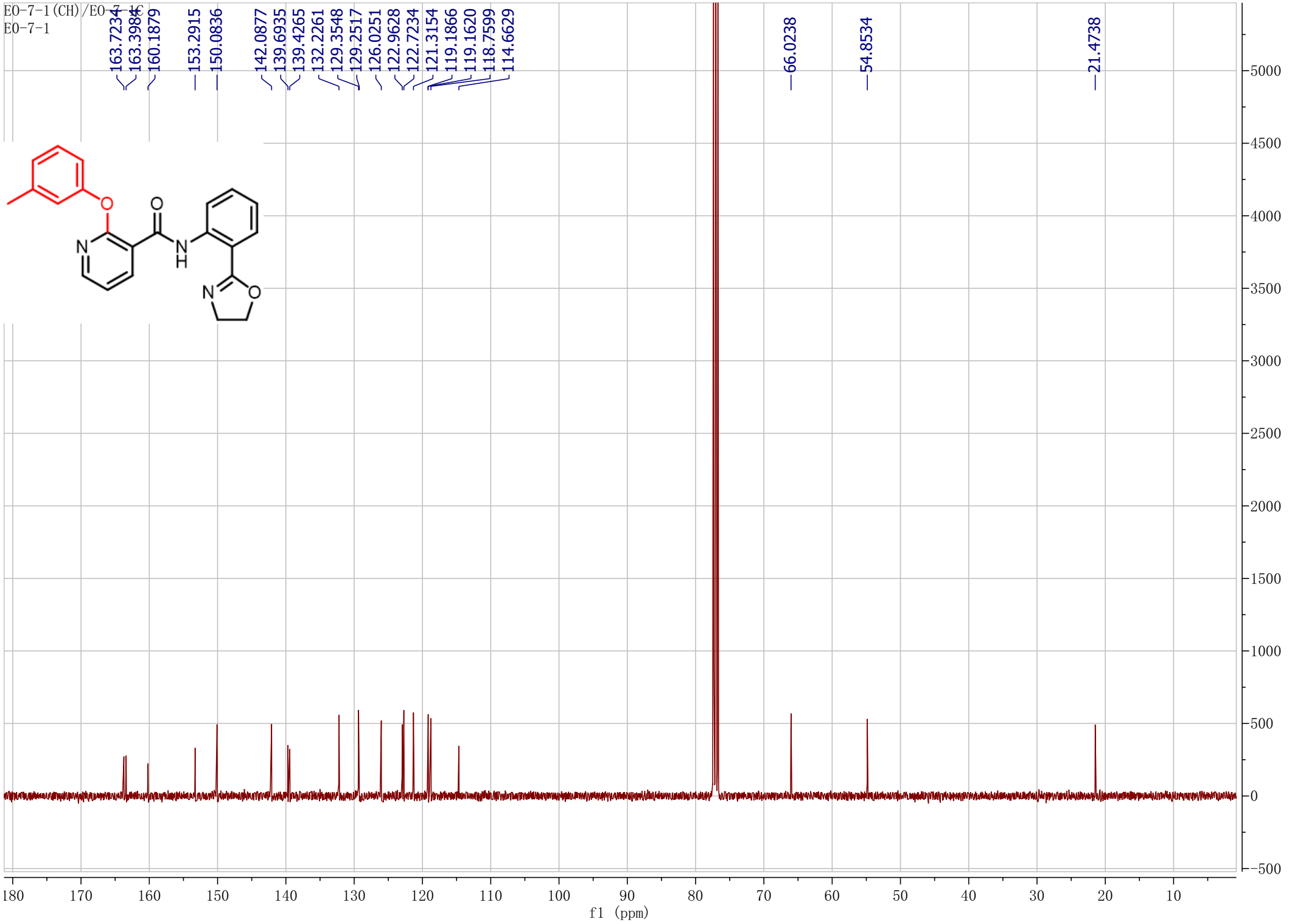


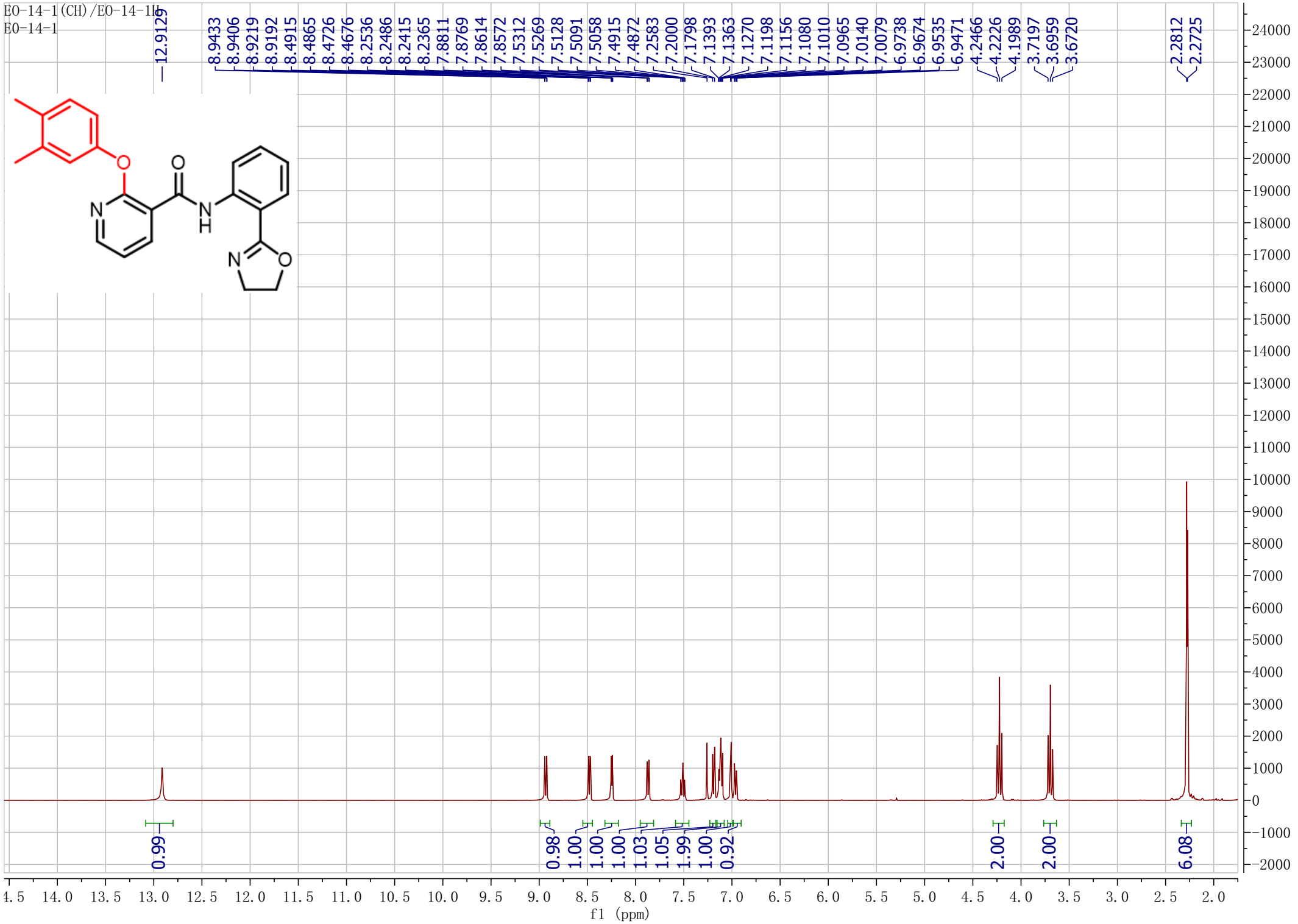
f1 (ppm)

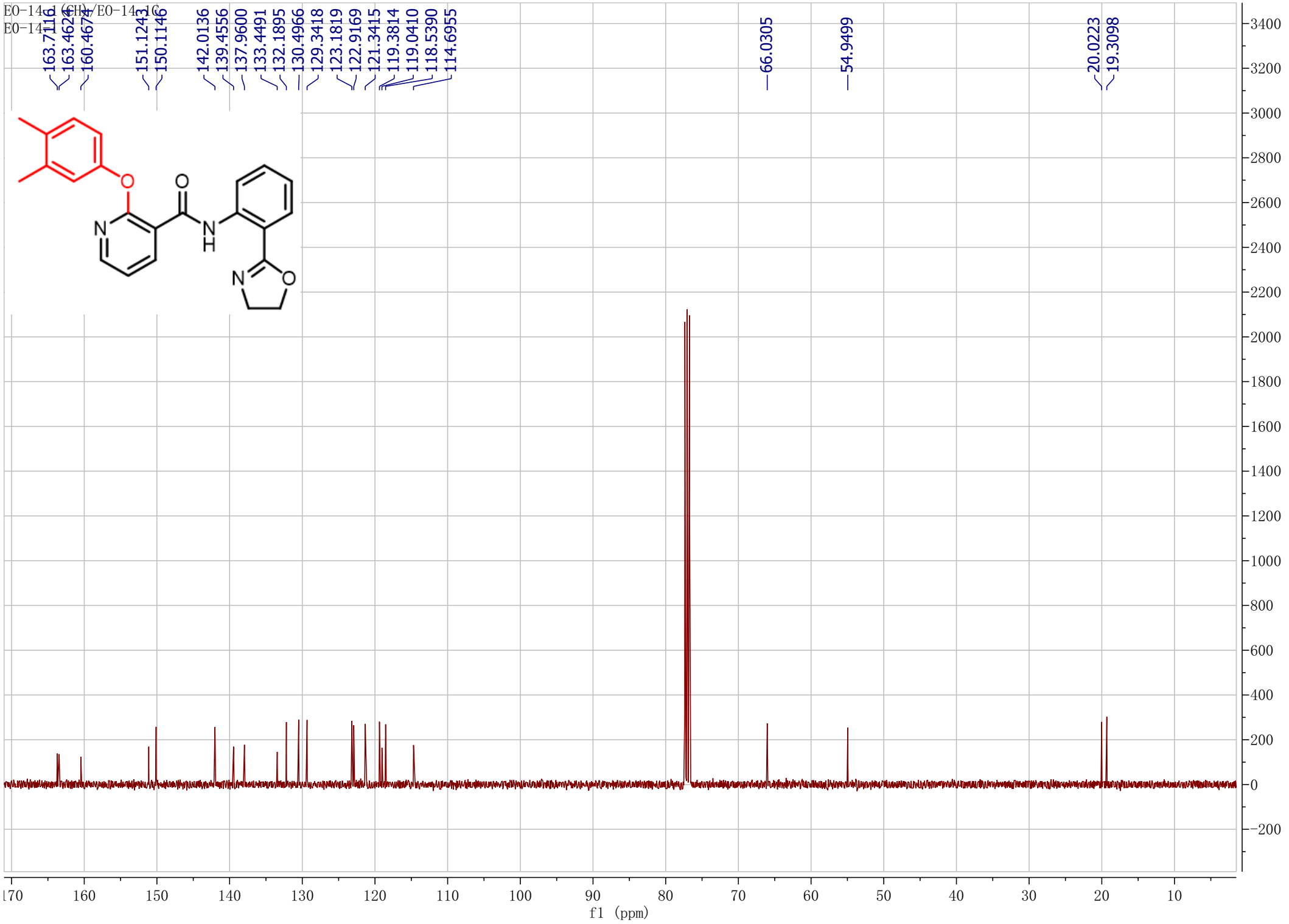

EO-17-1(CH)/EO-17-1H
EO-17-1
12.9284
8.9499
8.9470
8.9285
8.9257
8.4986
8.4935
8.4797
8.4745
8.2484
8.2433
8.2363
8.2313
7.8869
7.8826
7.8671
7.8629
7.5366
7.5323
7.5182
7.5144
7.5109
7.4970
7.4927
7.2615
7.2523
7.2470
7.2372
7.2316
7.1460
7.1431
7.1373
7.1333
7.1258
7.1190
7.1097
7.1057
7.0978
4.2455
4.2216
4.1979
3.6996
3.6759
3.6520
2.3814
H3CO
O
N
O
N
H
N
O
0.96
0.97
0.97
0.97
0.96
1.06
2.01
3.94
2.00
1.98
3.03
f1 (ppm)


EO-17-1(CH)/EO-17-1C
EO-17-1
163.7055
163.4174
160.3445
151.0017
150.0284
142.0444
139.4574
134.7530
132.2033
130.0975
129.3469
122.9302
121.9485
121.3220
119.0957
118.6423
114.6838
66.0311
54.9093
20.9863
H3CO
O
N
O
N
H
N
O
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

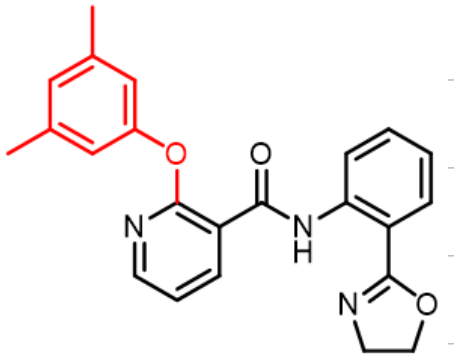

EO-7-1(CH)/EO-7-1H
EO-7-1
12.9143
8.9448
8.9419
8.9233
8.9205
8.5022
8.4972
8.4833
8.4782
8.2606
8.2556
8.2486
8.2435
7.8851
7.8808
7.8654
7.8611
7.5353
7.5311
7.5169
7.5133
7.5098
7.4956
7.4914
7.3462
7.3440
7.3260
7.3069
7.2605
7.1497
7.1449
7.1419
7.1377
7.1308
7.1258
7.1229
7.1187
7.1069
7.1039
7.0732
7.0523
7.0451
7.0241
7.0184
4.2413
4.2174
4.1936
3.6745
3.6507
3.6269
2.3897
0.94
0.96
0.97
0.97
0.96
1.02
1.00
2.00
2.91
2.00
1.98
3.03
f1 (ppm)


EO-7-1(CH)/EO-7-1C
EO-7-1
163.7234
163.3984
160.1879
153.2915
150.0836
142.0877
139.6935
139.4265
132.2261
129.3548
129.2517
126.0251
122.9628
122.7234
121.3154
119.1866
119.1620
118.7599
114.6629
66.0238
54.8534
21.4738
O
O
N
N
H
N
O
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


EO-14-1(CH)/EO-14-1H
EO-14-1
12.9129
8.9433
8.9406
8.9219
8.9192
8.4915
8.4865
8.4726
8.4676
8.2536
8.2486
8.2415
8.2365
7.8811
7.8769
7.8614
7.8572
7.5312
7.5269
7.5128
7.5091
7.5058
7.4915
7.4872
7.2583
7.2000
7.1798
7.1393
7.1363
7.1270
7.1198
7.1156
7.1080
7.1010
7.0965
7.0140
7.0079
6.9738
6.9674
6.9535
6.9471
4.2466
4.2226
4.1989
3.7197
3.6959
3.6720
2.2812
2.2725
0.99
0.98
1.00
1.00
1.00
1.03
1.05
1.99
1.00
0.92
2.00
2.00
6.08
f1 (ppm)


EO-14-1 (CH)/EO-14-1C
163.7116
163.4624
160.4674
151.1243
150.1146
142.0136
139.4556
137.9600
133.4491
132.1895
130.4966
129.3418
123.1819
122.9169
121.3415
119.3814
119.0410
118.5390
114.6955
66.0305
54.9499
20.0223
19.3098
O
O
N
N
H
N
O
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

EO-21-1(CH)/EO-21-1H
EO-21-1



12.8905

8.9390 8.9362 8.9177 8.9149 8.4967 8.4916 8.4777 8.4727 8.2704 8.2653 8.2583 8.2533 7.8842 7.8800 7.8645 7.8603 7.5330 7.5287 7.5146 7.5109 7.5075 7.4933 7.4891 7.2616 7.1431 7.1406 7.1288 7.1244 7.1217 7.1099 7.1049 7.1019 6.8843 6.8481

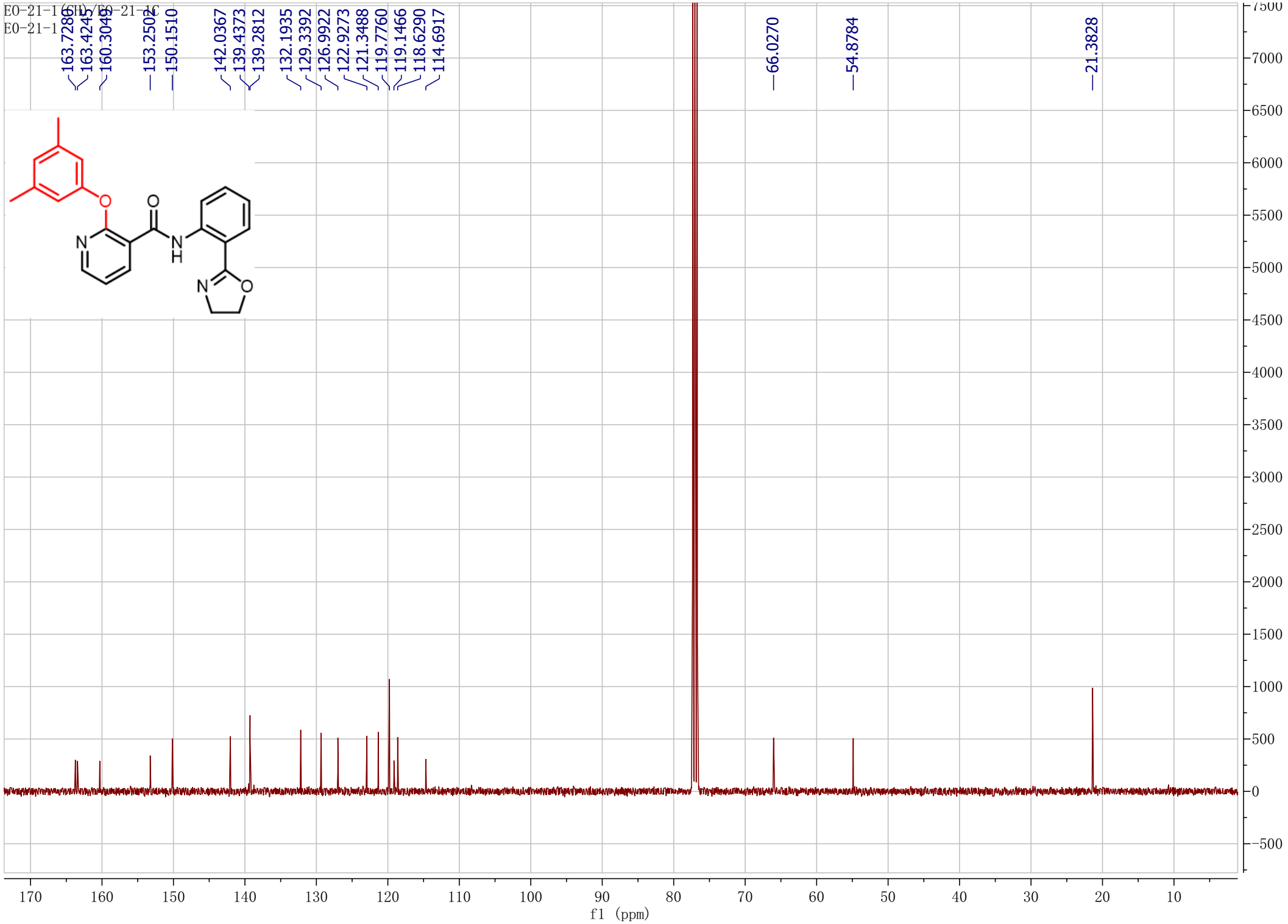
4.2519 4.2280 4.2043

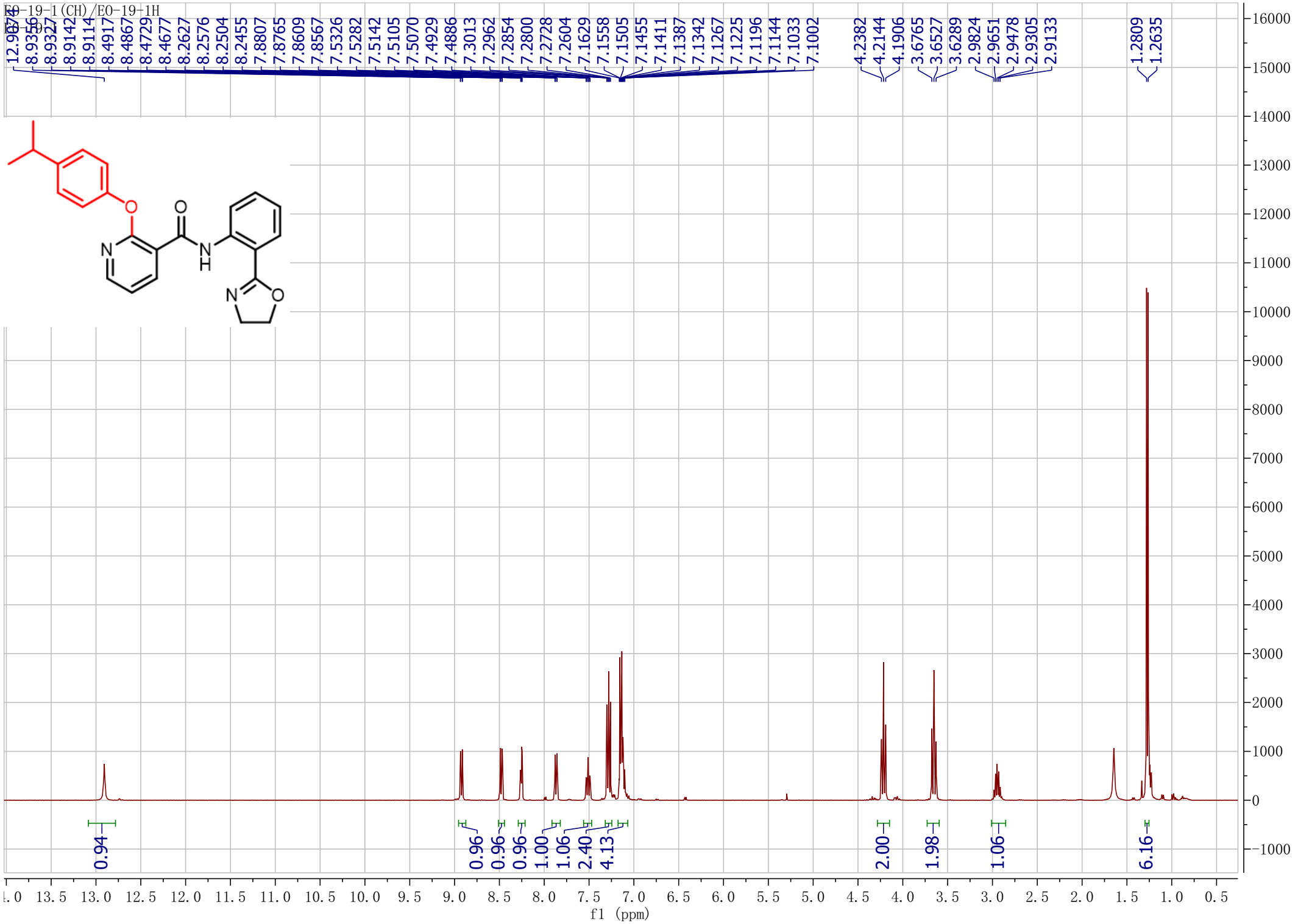
3.6989 3.6751 3.6513

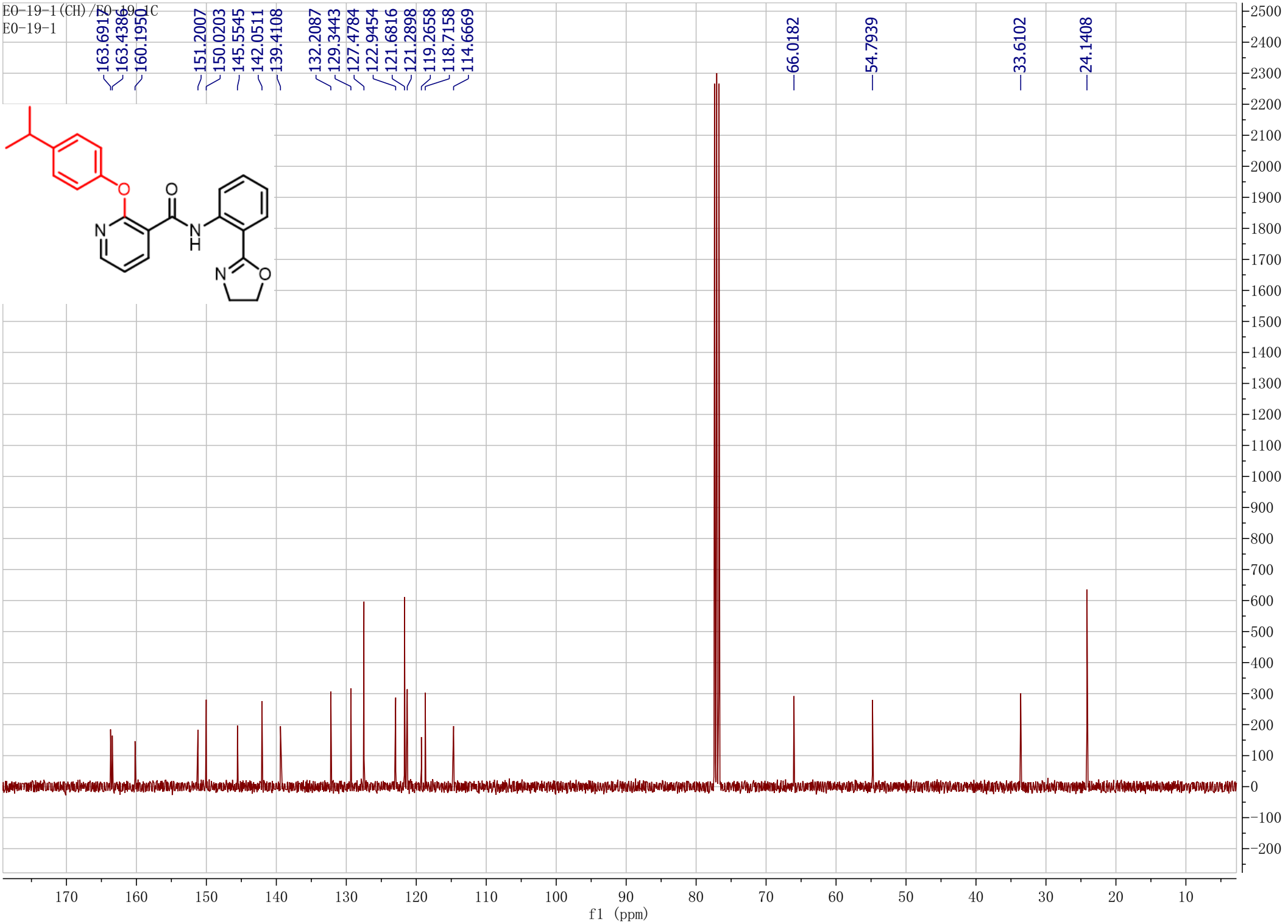
2.3455

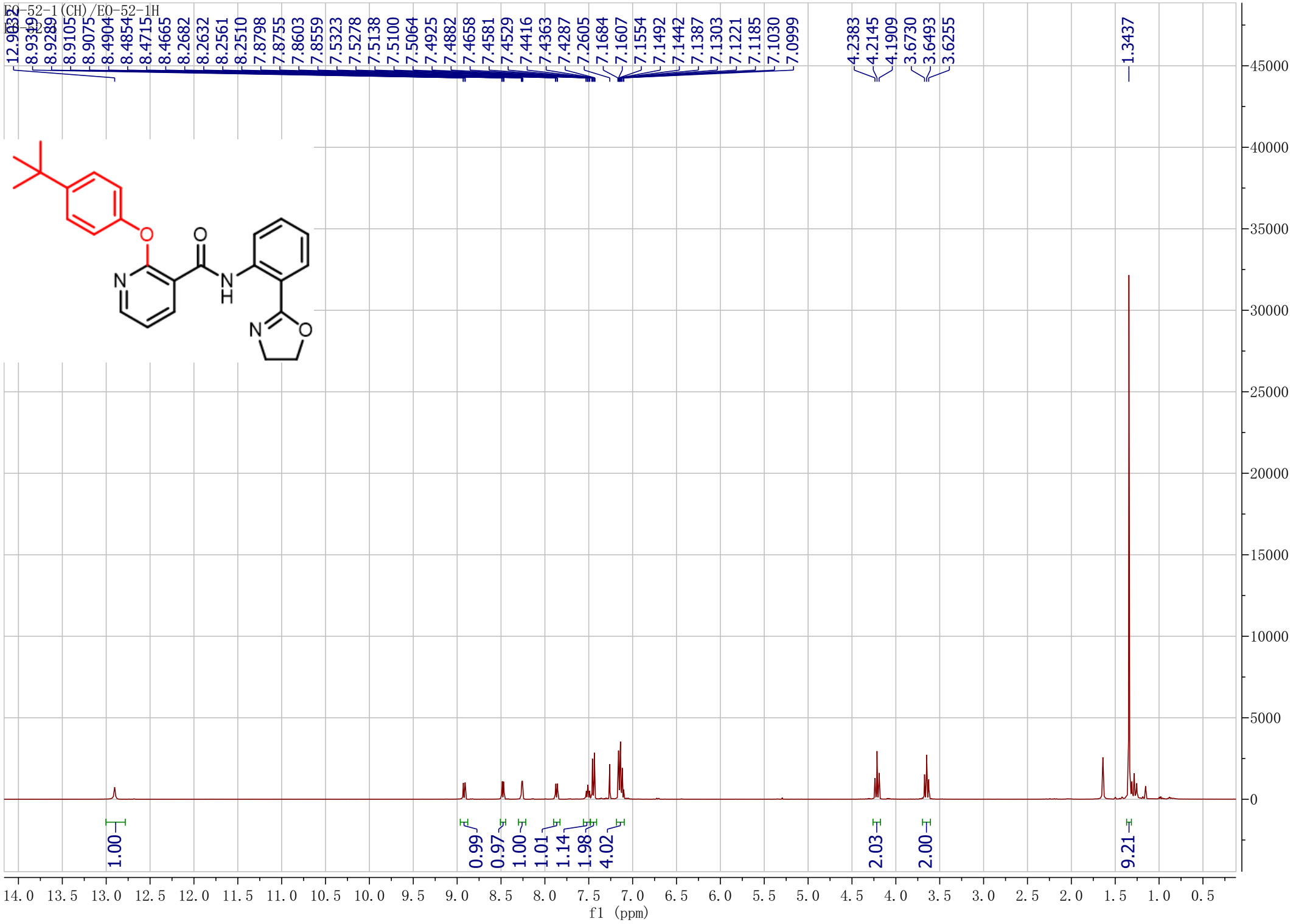
0.94 0.98 0.99 1.00 0.99 1.06 2.05 1.02 1.91 2.00 1.98 6.15

f1 (ppm)

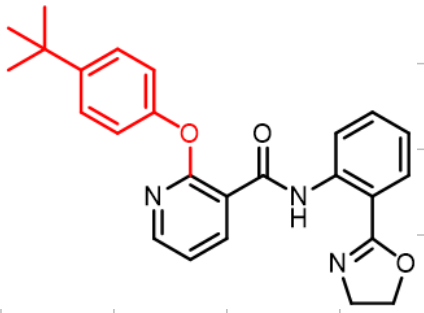

EO-21-1(CH)/EO-21-1C
EO-21-1
163.7286
163.4245
160.3046
153.2502
150.1510
142.0367
139.4373
139.2812
132.1935
129.3392
126.9922
122.9273
121.3488
119.7760
119.1466
118.6290
114.6917
66.0270
54.8784
21.3828
O
O
N
H
N
O
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


EO-19-1(CH)/EO-19-1H
12.9636
8.9356
8.9327
8.9142
8.9114
8.4917
8.4867
8.4729
8.4677
8.2627
8.2576
8.2504
8.2455
7.8807
7.8765
7.8609
7.8567
7.5326
7.5282
7.5142
7.5105
7.5070
7.4929
7.4886
7.3013
7.2962
7.2854
7.2800
7.2728
7.2604
7.1629
7.1558
7.1505
7.1455
7.1411
7.1387
7.1342
7.1267
7.1225
7.1196
7.1144
7.1033
7.1002
4.2382
4.2144
4.1906
3.6765
3.6527
3.6289
2.9824
2.9651
2.9478
2.9305
2.9133
1.2809
1.2635
O
O
N
N
H
N
O
0.94
0.96
0.96
0.96
1.00
1.06
2.40
4.13
2.00
1.98
1.06
6.16
f1 (ppm)


EO-19-1(CH)/EO-19-1C
EO-19-1
163.6915
163.4386
160.1950
151.2007
150.0203
145.5545
142.0511
139.4108
132.2087
129.3443
127.4784
122.9454
121.6816
121.2898
119.2658
118.7158
114.6669
66.0182
54.7939
33.6102
24.1408
O
O
N
N
H
N
O
2500
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


EO-52-1(CH)/EO-52-1H
12.9337
8.9339
8.9289
8.9105
8.9075
8.4904
8.4854
8.4715
8.4665
8.2682
8.2632
8.2561
8.2510
7.8798
7.8755
7.8603
7.8559
7.5323
7.5278
7.5138
7.5100
7.5064
7.4925
7.4882
7.4658
7.4581
7.4529
7.4416
7.4363
7.4287
7.2605
7.1684
7.1607
7.1554
7.1492
7.1442
7.1387
7.1303
7.1221
7.1185
7.1030
7.0999
4.2383
4.2145
4.1909
3.6730
3.6493
3.6255
1.3437
O
N
H
N
O
1.00
0.99
0.97
1.00
1.01
1.14
1.98
4.02
2.03
2.00
9.21
f1 (ppm)

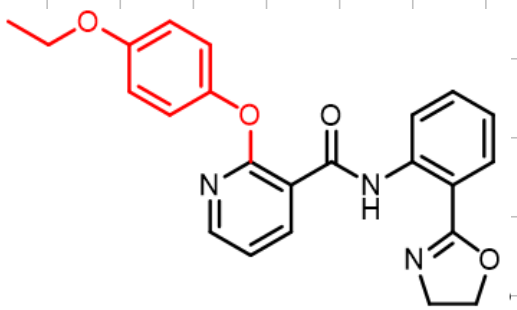
EO-52-1(CH)/EO-52-1C
EO-52-1



163.6990
163.4318
160.1368
150.9796
150.0034
147.8003
142.0329
139.4141
132.2004
129.3353
126.4338
122.9305
121.2867
121.2502
119.3556
118.7286
114.6694
66.0106
54.7626
34.4929
31.5154

f1 (ppm)

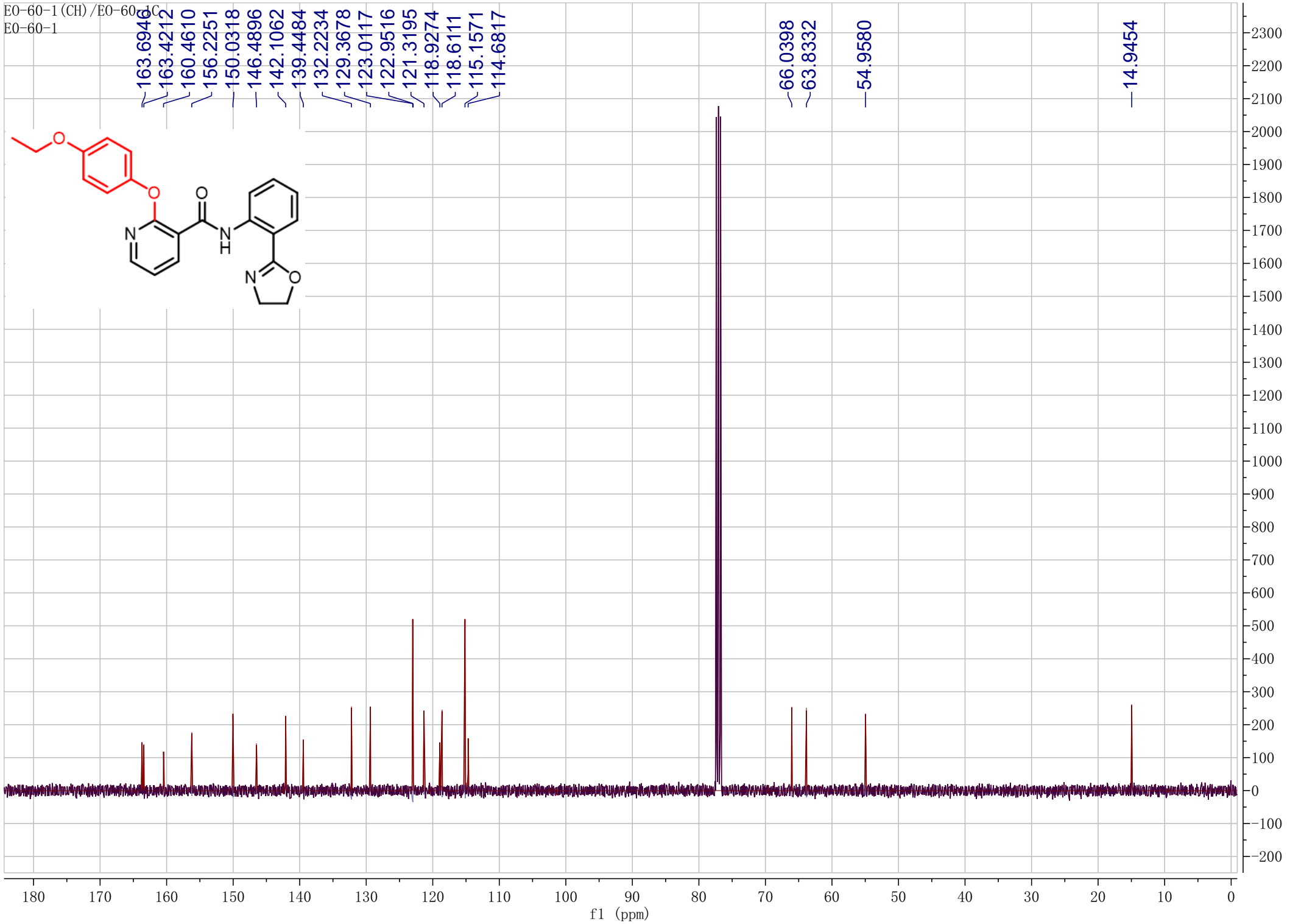
C-H 醚化结构鉴定/EO-60-1(H)
EO-60-1



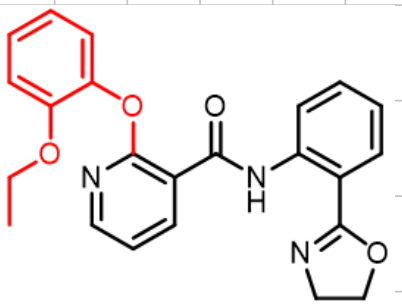
12.9256
8.9566
8.9536
8.9351
8.9322
8.5043
8.4993
8.4854
8.4804
8.2503
8.2453
8.2382
8.2332
7.8898
7.8855
7.8702
7.8660
7.5378
7.5335
7.5193
7.5156
7.5122
7.4980
7.4938
7.1555
7.1498
7.1483
7.1451
7.1387
7.1362
7.1329
7.1284
7.1244
7.1173
7.1100
7.1071
7.1052
6.9694
6.9636
6.9526
6.9469
4.2460
4.2219
4.1981
4.0752
4.0577
4.0403
4.0229
3.6950
3.6785
3.6547
1.4506
1.4331
1.4157

0.90
0.95
1.01
0.98
1.02
1.05
3.97
2.01
2.00
2.04
2.07
3.28

f1 (ppm)

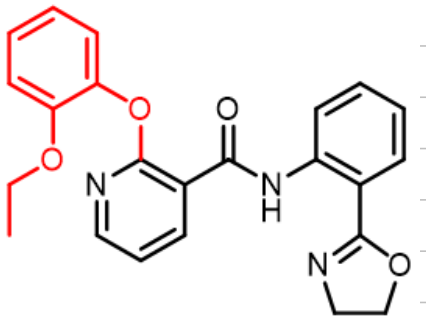

EO-60-1(CH)/EO-60-1C
EO-60-1
163.6946
163.4212
160.4610
156.2251
150.0318
146.4896
142.1062
139.4484
132.2234
129.3678
123.0117
122.9516
121.3195
118.9274
118.6111
115.1571
114.6817
66.0398
63.8332
54.9580
14.9454
O
O
O
N
N
H
N
O
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

EO-59-1(H)/EO-59-1H
EO-59-1



f1 (ppm)

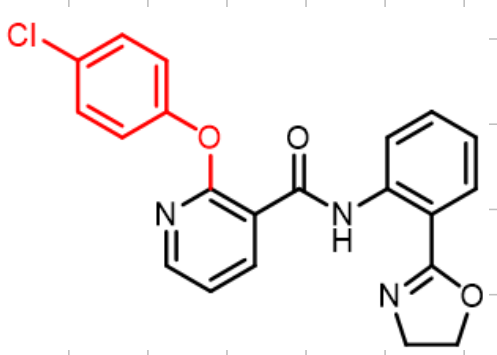
EO-59-1(CH)/EO-59-1C
EO-59-1



163.4907
163.4849
160.3293
150.9802
149.9485
142.8566
142.0446
139.5168
132.0733
129.3247
126.1898
123.2759
122.8692
121.5522
120.9520
118.5918
118.1944
114.9500
114.0015
65.9978
64.2925
54.7875
14.5780

f1 (ppm)

EO-53-1(CH)/EO-53-1H
EO-53-1

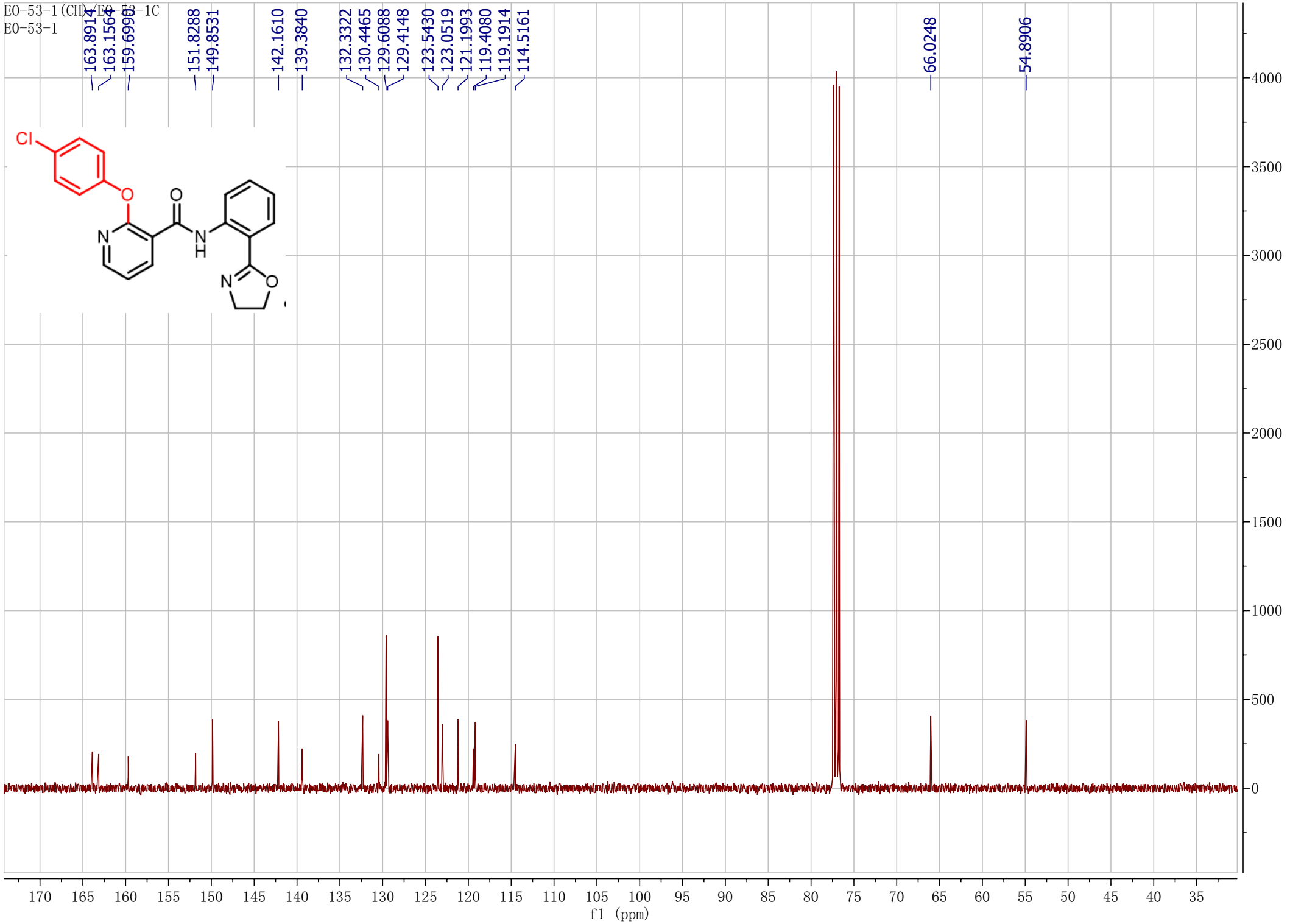


12.9074

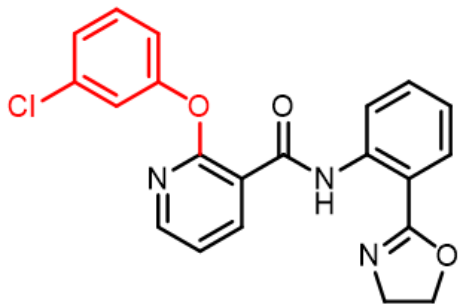
8.9422 8.9393 8.9209 8.9181 8.4950 8.4899 8.4762 8.4709 8.2486 8.2436 8.2366 8.2315 7.8989 7.8947 7.8791 7.8749 7.5450 7.5407 7.5266 7.5229 7.5194 7.5053 7.5010 7.4299 7.4216 7.4163 7.4051 7.3996 7.3914 7.2625 7.2080 7.1999 7.1944 7.1830 7.1778 7.1707 7.1639 7.1581 7.1551 7.1519 7.1390 7.1360 7.1199 7.1169 4.2699 4.2460 4.2224 3.6988 3.6751 3.6513

0.94 0.97 0.98 0.98 0.98 1.02 1.94 4.03 2.00 2.00

f1 (ppm)


EO-53-1(CH)-/EO-53-1C
EO-53-1
163.8914
163.1564
159.6996
151.8288
149.8531
142.1610
139.3840
132.3322
130.4465
129.6088
129.4148
123.5430
123.0519
121.1993
119.4080
119.1914
114.5161
66.0248
54.8906
Cl
O
O
N
N
H
N
O
4000
3500
3000
2500
2000
1500
1000
500
0
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

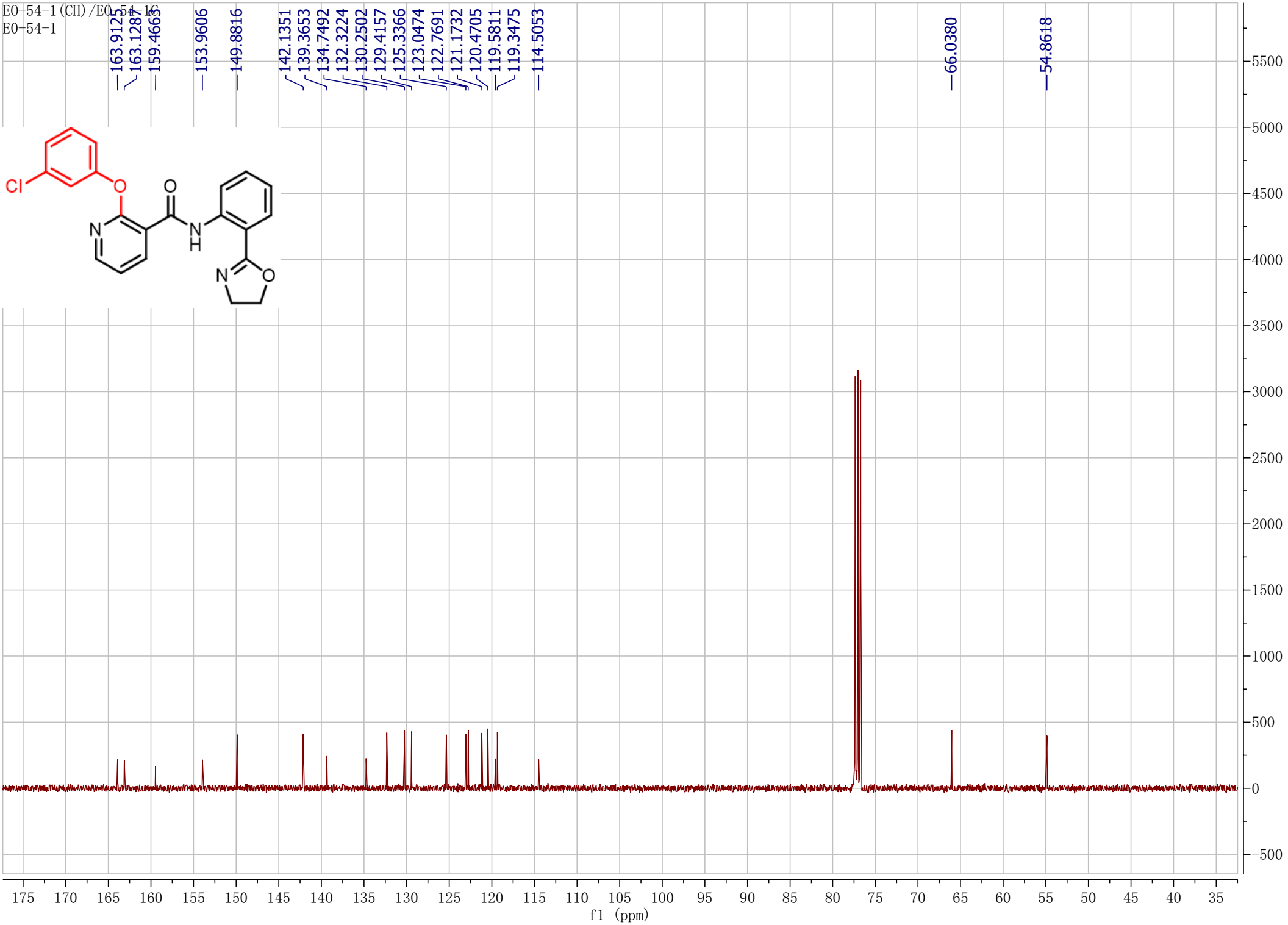
EO-54-1(CH)/EO-54-1H
EO-54-1



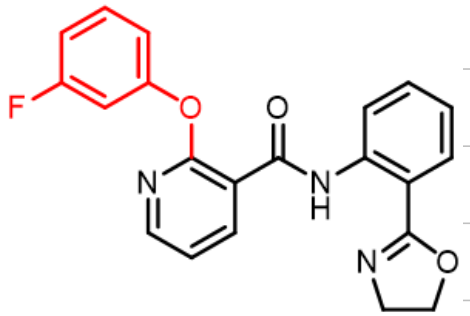
12.8886
8.9326
8.9298
8.9112
8.9084
8.4850
8.4800
8.4661
8.4611
8.2643
8.2594
8.2522
8.2472
7.8985
7.8942
7.8786
7.8744
7.5428
7.5383
7.5243
7.5205
7.5169
7.5028
7.4985
7.3927
7.3726
7.3522
7.2892
7.2840
7.2788
7.2613
7.2521
7.2495
7.2469
7.2445
7.2320
7.2293
7.2268
7.2244
7.1958
7.1837
7.1768
7.1648
7.1557
7.1521
7.1485
7.1430
7.1364
7.1336
7.1287
7.1174
7.1144
4.2752
4.2512
4.2276
3.7247
3.7010
3.6771

0.99
0.99
0.95
0.96
1.00
1.29
1.25
1.14
1.04
3.31
2.00
2.00

f1 (ppm)


EO-54-1(CH)/EO-54-1C
EO-54-1
163.9125
163.1287
159.4663
153.9606
149.8816
142.1351
139.3653
134.7492
132.3224
130.2502
129.4157
125.3366
123.0474
122.7691
121.1732
120.4705
119.5811
119.3475
114.5053
66.0380
54.8618
Cl
O
N
O
N
H
N
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

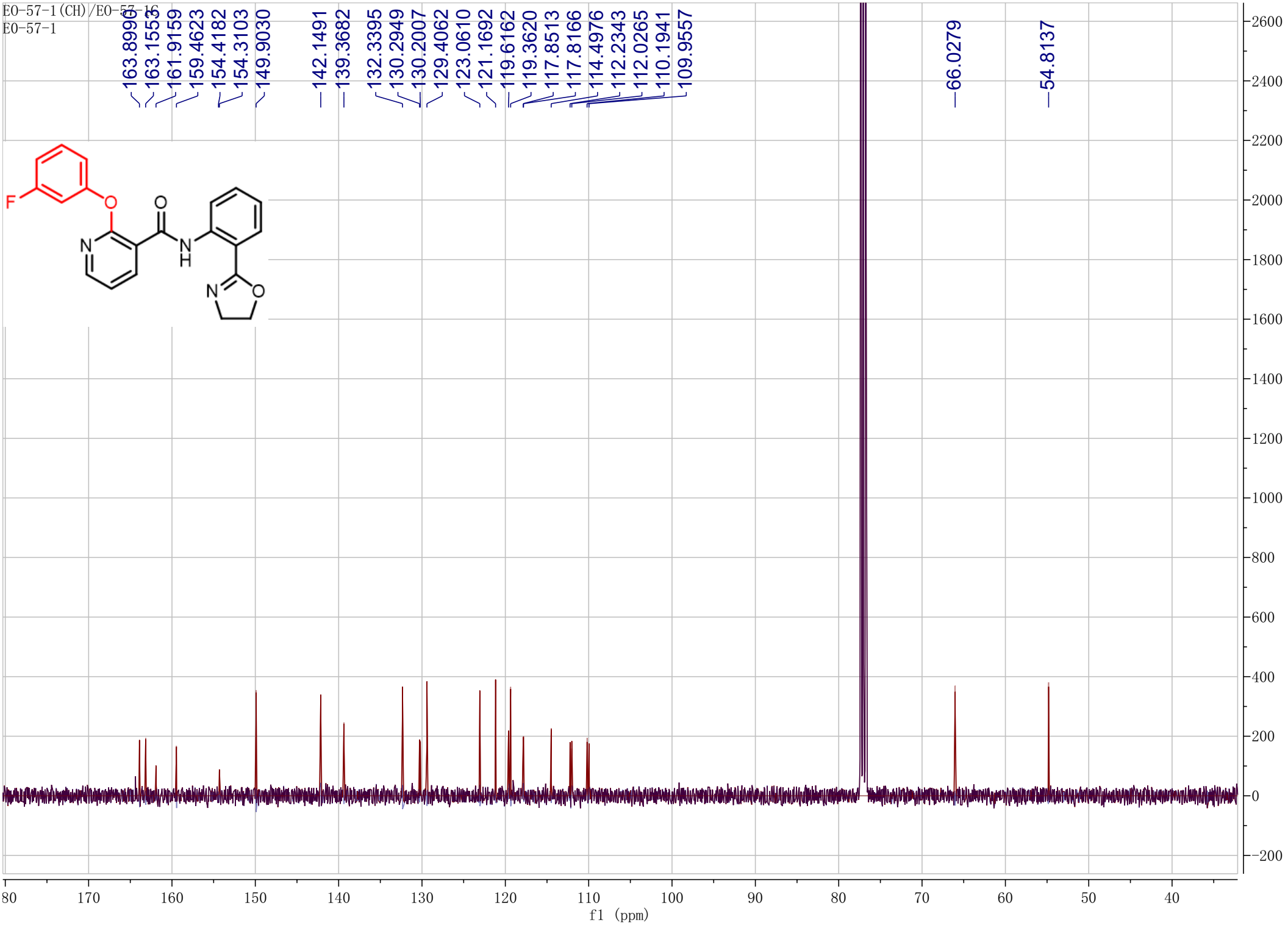
C-H 醚化结构鉴定/EO-57-1(H)
EO-57-1

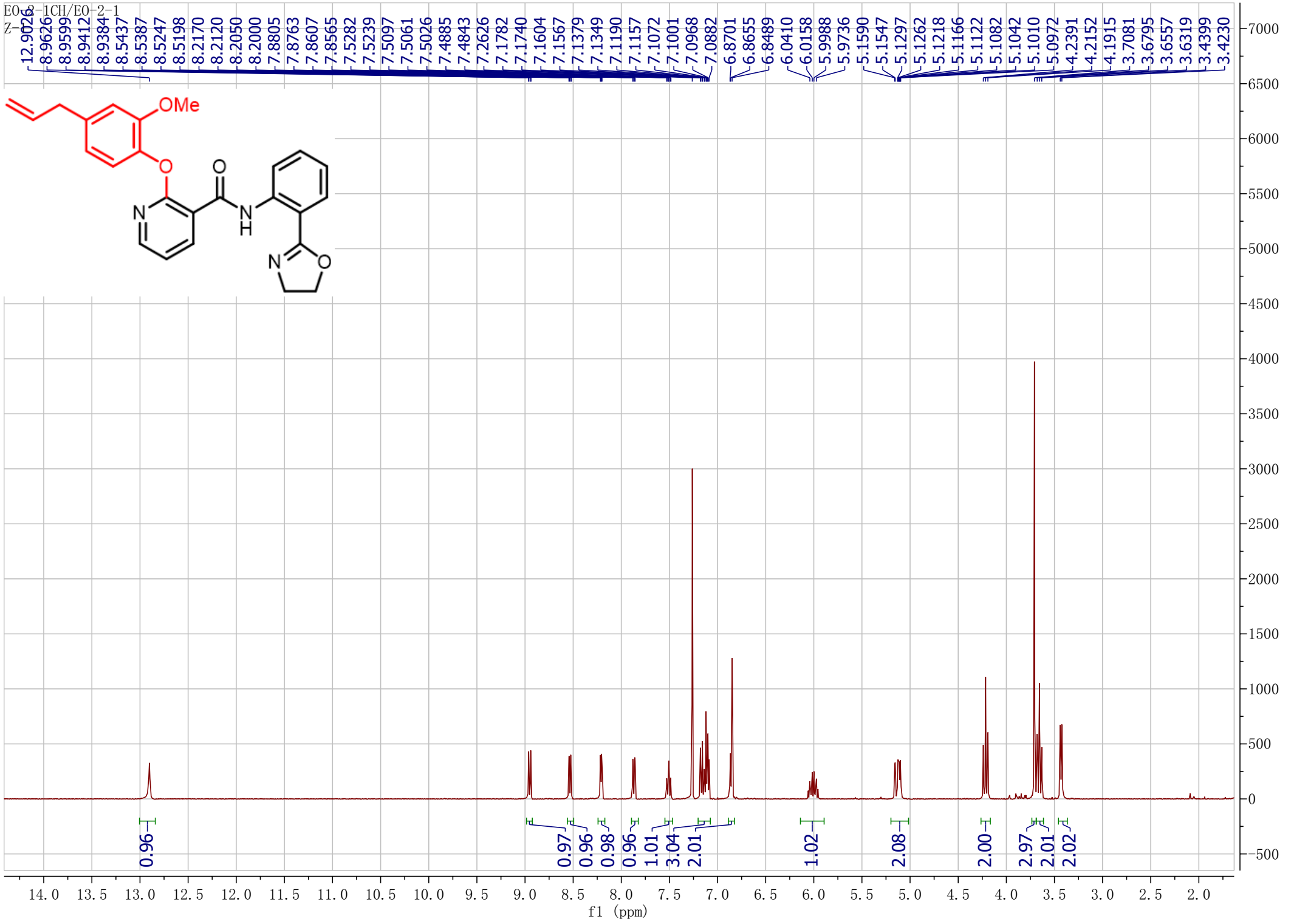


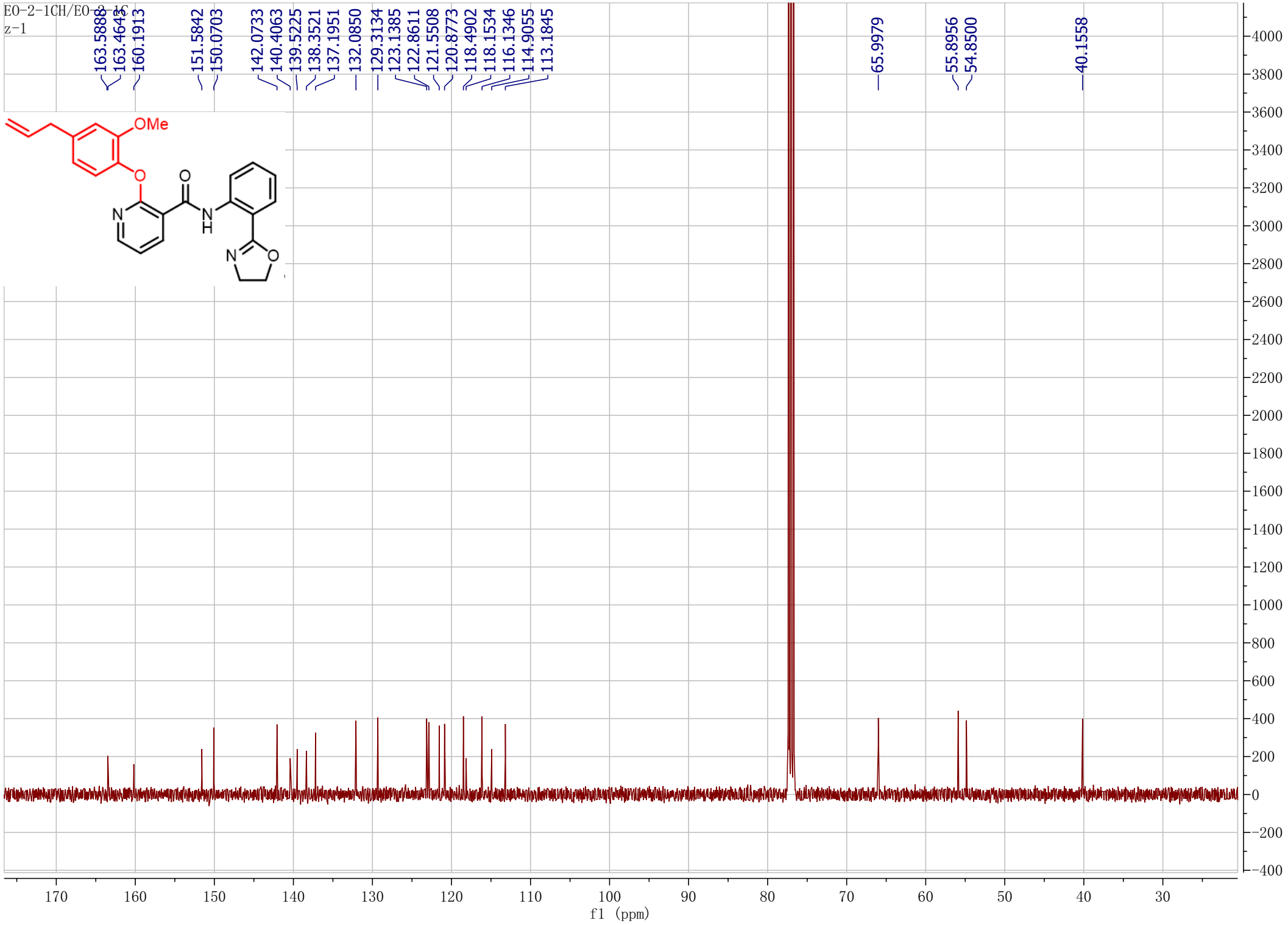
12.9018
8.9346
8.9317
8.9132
8.9103
8.4891
8.4842
8.4702
8.4652
8.2721
8.2672
8.2601
8.2551
7.8994
7.8952
7.8797
7.8754
7.5453
7.5412
7.5270
7.5231
7.5195
7.5057
7.5014
7.4101
7.4059
7.3895
7.3853
7.3689
7.2638
7.2001
7.1881
7.1811
7.1692
7.1585
7.1555
7.1395
7.1364
7.1204
7.1172
7.0527
7.0499
7.0455
7.0326
7.0302
7.0268
7.0243
7.0217
7.0161
7.0106
6.9982
6.9957
6.9925
6.9868
6.9749
6.9724
6.9687
6.9662
4.2723
4.2484
4.2247
3.7298
3.7124
3.6955

0.91
1.00
1.00
1.00
1.01
1.17
1.09
1.04
1.08
2.99
2.00
2.14

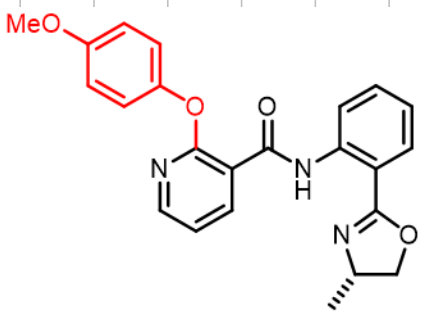
f1 (ppm)


EO-57-1(CH)/EO-57-1C
EO-57-1
163.8990
163.1553
161.9159
159.4623
154.4182
154.3103
149.9030
142.1491
139.3682
132.3395
130.2949
130.2007
129.4062
123.0610
121.1692
119.6162
119.3620
117.8513
117.8166
114.4976
112.2343
112.0265
110.1941
109.9557
66.0279
54.8137
F
O
O
N
N
H
N
O
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)


EO-2-1CH/EO-2-1
Z-
12.9026
8.9626
8.9599
8.9412
8.9384
8.5437
8.5387
8.5247
8.5198
8.2170
8.2120
8.2050
8.2000
7.8805
7.8763
7.8607
7.8565
7.5282
7.5239
7.5097
7.5061
7.5026
7.4885
7.4843
7.2626
7.1782
7.1740
7.1604
7.1567
7.1379
7.1349
7.1190
7.1157
7.1072
7.1001
7.0968
7.0882
6.8701
6.8655
6.8489
6.0410
6.0158
5.9988
5.9736
5.1590
5.1547
5.1297
5.1262
5.1218
5.1166
5.1122
5.1082
5.1042
5.1010
5.0972
4.2391
4.2152
4.1915
3.7081
3.6795
3.6557
3.6319
3.4399
3.4230
OMe
O
N
O
N
H
N
O
0.96
0.97
0.96
0.98
0.96
1.01
3.04
2.01
1.02
2.08
2.00
2.97
2.01
2.02
f1 (ppm)

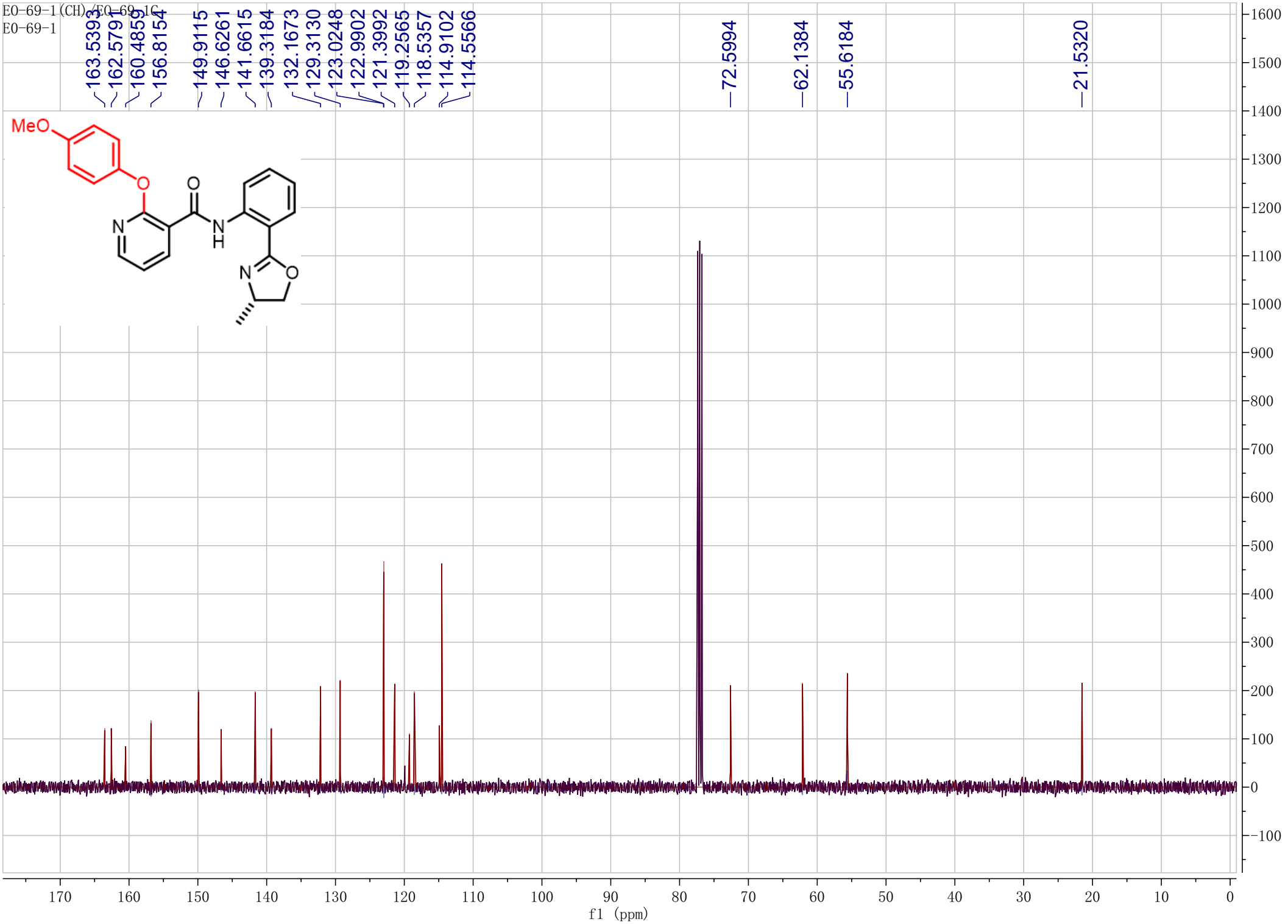

EO-2-1CH/EO-2-1C
z-1
163.5886
163.4643
160.1913
151.5842
150.0703
142.0733
140.4063
139.5225
138.3521
137.1951
132.0850
129.3134
123.1385
122.8611
121.5508
120.8773
118.4902
118.1534
116.1346
114.9055
113.1845
65.9979
55.8956
54.8500
40.1558
OMe
O
N
H
N
O
f1 (ppm)

C-H 醚化结构鉴定/EO-69-1(H)
EO-69

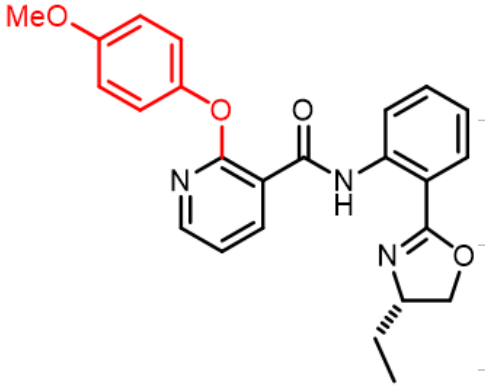


f1 (ppm)

EO-69-1(CH)/EO-69-1C
EO-69-1



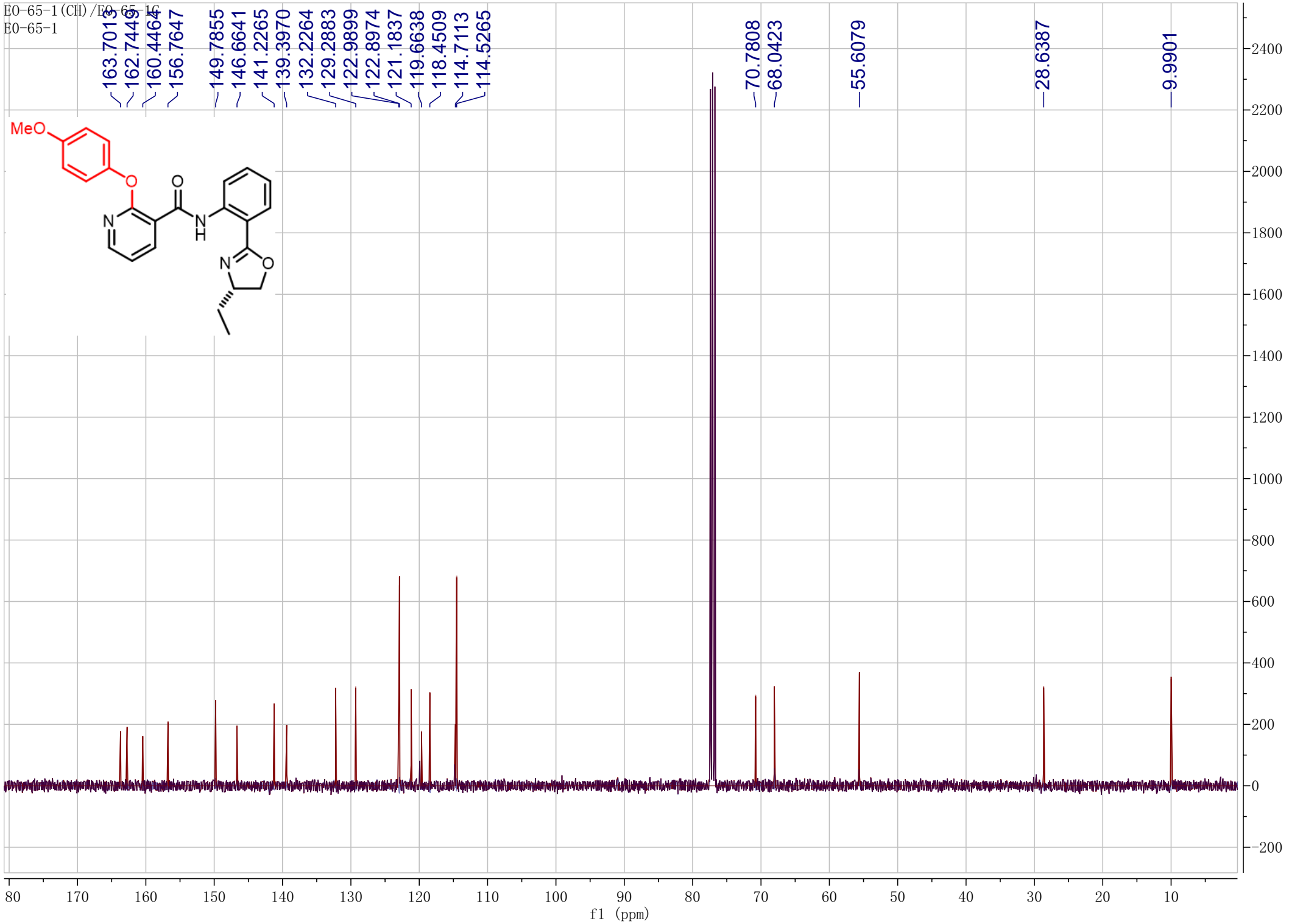
C-H 醚化结构鉴定/EO-65-1(H)
EO-65-1



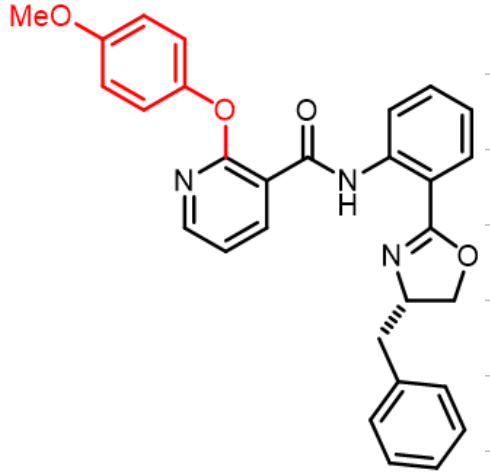
12.8265 8.8802 8.8774 8.8591 8.8563 8.3781 8.3731 8.3592 8.3543 8.2477 8.2428 8.2357 8.2307 7.8815 7.8773 7.8617 7.8575 7.5362 7.5320 7.5179 7.5142 7.5107 7.4965 7.4923 7.2637 7.1607 7.1548 7.1515 7.1486 7.1439 7.1381 7.1322 7.1294 7.1188 7.1066 7.1000 7.0878 6.9553 6.9494 6.9383 6.9327 4.2982 4.2952 3.9795 3.9655 3.9619 3.9586 3.9466 3.9410 3.9357 3.9318 3.9140 3.8211 1.4621 1.4481 1.4430 1.4290 1.4241 1.4196 1.4015 1.3838 0.7981 0.7796 0.7611

0.96 1.01 1.02 0.98 1.00 1.09 3.93 2.06 1.00 2.02 3.08 2.24 2.99

f1 (ppm)


EO-65-1(CH)/EO-65-1C
EO-65-1
163.7013
162.7449
160.4464
156.7647
149.7855
146.6641
141.2265
139.3970
132.2264
129.2883
122.9899
122.8974
121.1837
119.6638
118.4509
114.7113
114.5265
70.7808
68.0423
55.6079
28.6387
9.9901
MeO
O
N
O
N
H
N
O
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
−200
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

C-H 醚化结构鉴定/EO-68-1(H)
EO-68-1



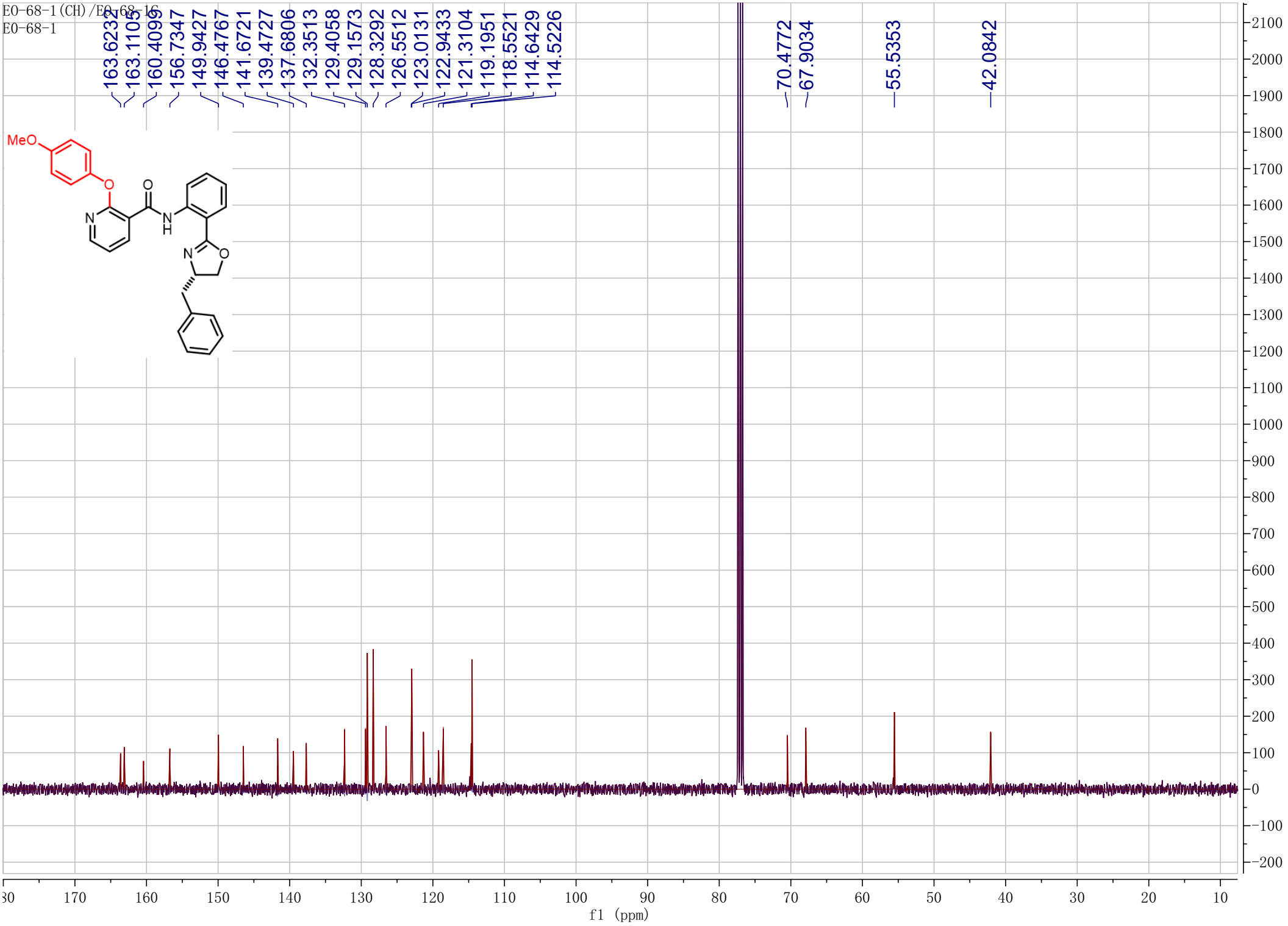
12.7617 8.9138 8.9109 8.8925 8.8896 8.4397 8.4347 8.4209 8.4158 8.2458 8.2408 8.2337 8.2287 7.8779 7.8737 7.8581 7.8538 7.5285 7.5249 7.5213 7.5073 7.1497 7.1467 7.1303 7.1274 7.1182 7.1115 7.1055 7.0991 7.0939 7.0848 7.0694 7.0637 7.0553 7.0504 7.0442 6.9420 6.9358 6.9260 6.9193 6.9127 6.9058 6.8991 6.8925 6.8827 6.8761 4.2378 4.2207 4.1916 4.1714 4.1685 4.1485 4.0242 4.0091 4.0040 3.9888 3.7806 2.7970 2.7788 2.7627 2.5807 2.5625 2.5469 2.5282

1.03 1.03 0.99 1.00 1.02 1.06 7.05 4.39 1.16 1.14 1.06 3.46 1.00 1.00

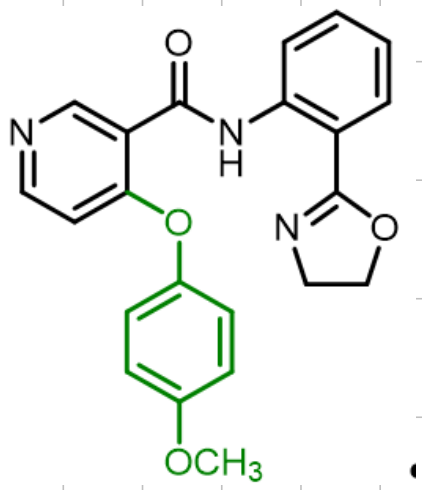
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0
f1 (ppm)

8500 8000 7500 7000 6500 6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0 -500

EO-68-1(CH)/EO-68-1C
EO-68-1



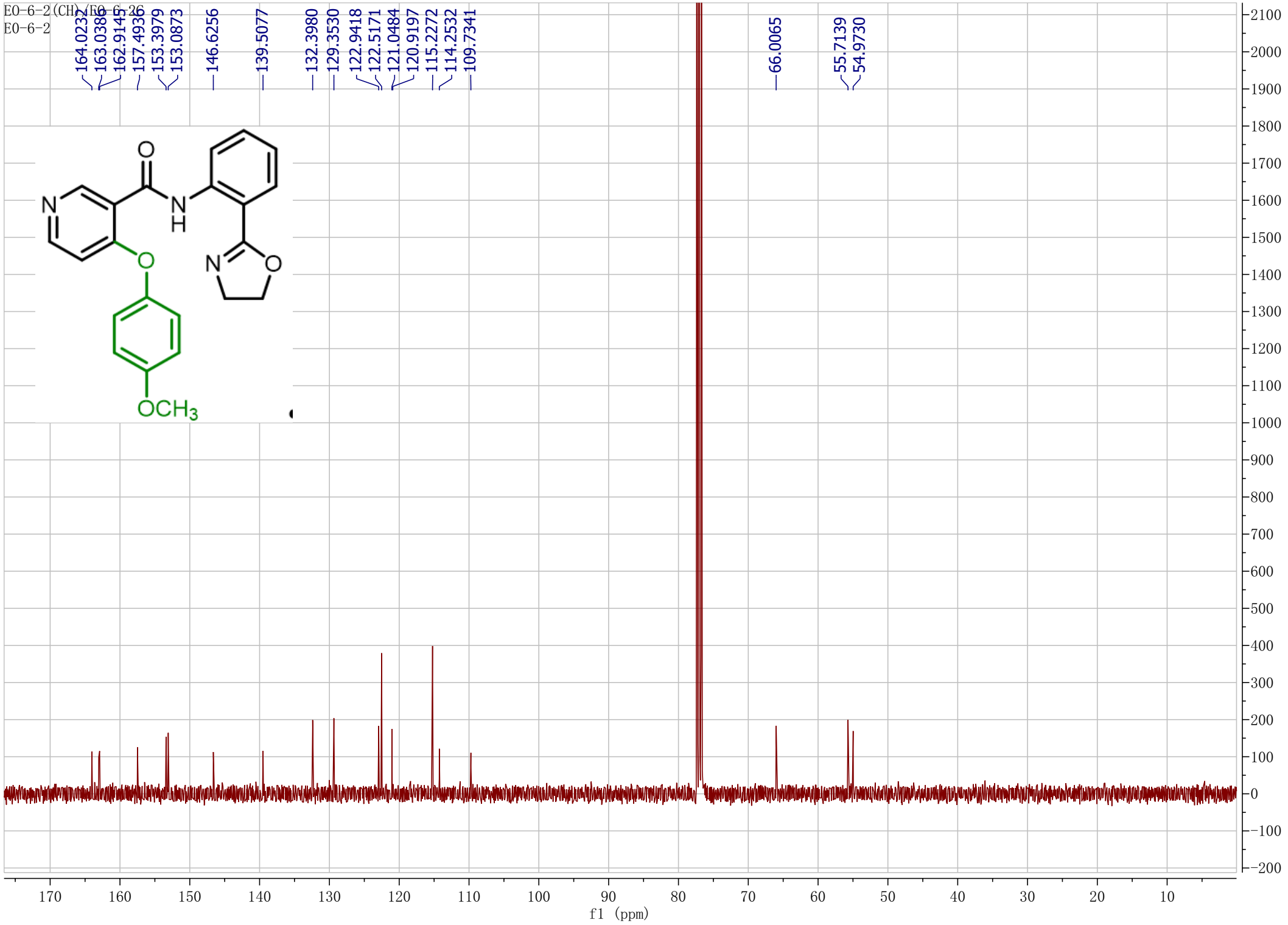
C-H 醚化结构鉴定/EO-6-2(H)
EO-6-2

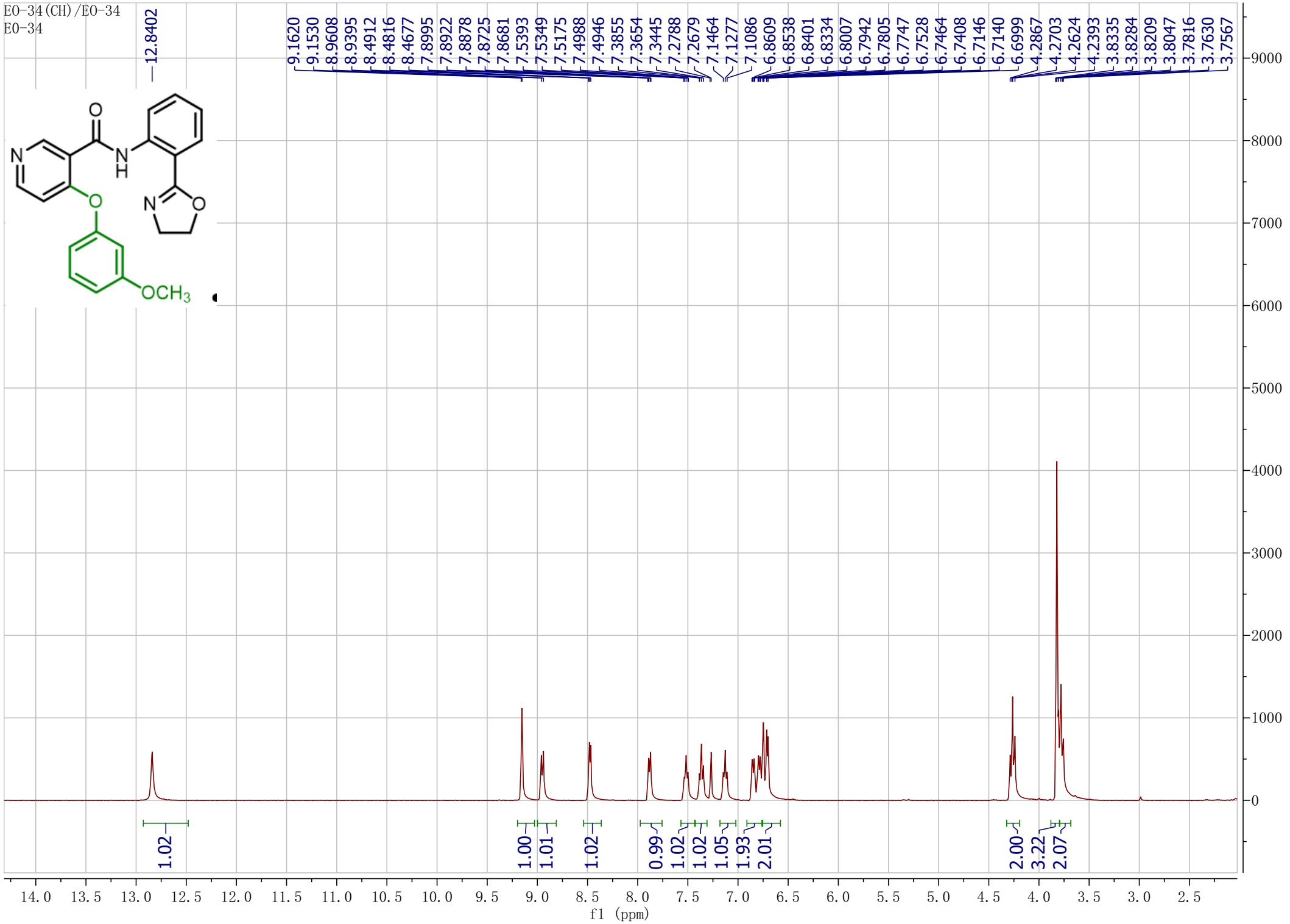


12.8342
9.1528
8.9740
8.9528
8.4613
8.4466
7.8927
7.8736
7.8590
7.5413
7.5217
7.5016
7.2651
7.1489
7.1367
7.1303
7.1140
6.9951
6.9789
6.9729
6.6329
6.6184
4.2870
4.2632
4.2395
3.8512
3.8075
3.8031
3.7999
3.7822
3.7579

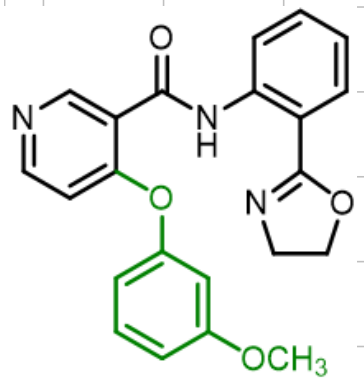
1.06
1.06
1.16
0.98
1.18
1.20
3.00
2.20
0.93
2.00
3.00
2.37

f1 (ppm)


EO-6-2(CH2)/EO-6-2C
EO-6-2
164.0231
163.0386
162.9145
157.4936
153.3979
153.0873
146.6256
139.5077
132.3980
129.3530
122.9418
122.5171
121.0484
120.9197
115.2272
114.2532
109.7341
66.0065
55.7139
54.9730
O
N
H
N
O
O
OCH3
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


EO-34(CH)/EO-34
EO-34
12.8402
9.1620
9.1530
8.9608
8.9395
8.4912
8.4816
8.4677
7.8995
7.8922
7.8878
7.8725
7.8681
7.5393
7.5349
7.5175
7.4988
7.4946
7.3855
7.3654
7.3445
7.2788
7.2679
7.1464
7.1277
7.1086
6.8609
6.8538
6.8401
6.8334
6.8007
6.7942
6.7805
6.7747
6.7528
6.7464
6.7408
6.7146
6.7140
6.6999
4.2867
4.2703
4.2624
4.2393
3.8335
3.8284
3.8209
3.8047
3.7816
3.7630
3.7567
O
N
H
N
O
N
O
OCH3
1.02
1.00
1.01
1.02
0.99
1.02
1.02
1.05
1.93
2.01
2.00
3.22
2.07
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
14.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)

EO-34(CH)/EO-34
Eo-34



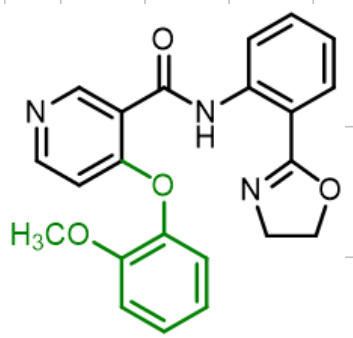
164.0436
162.9403
162.1710
161.2705
154.4575
153.3815
153.0850
139.4827
132.3940
130.6871
129.3402
122.9631
121.2863
120.9810
114.2274
113.4264
111.6109
110.3086
107.4879
66.0273
55.5735
54.8927

1500 1400 1300 1200 1100 1000 900 800 700 600 500 400 300 200 100 0 −100

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20

f1 (ppm)

EO-33(CH)/EO-33
EO-33



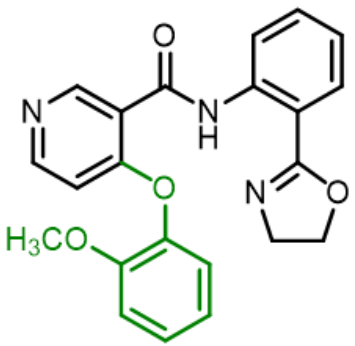
12.8232

9.1917 8.9904 8.9848 8.9818 8.9635 8.9606 8.4300 8.4154 7.8854 7.8811 7.8655 7.8612 7.5330 7.5288 7.5148 7.5111 7.5074 7.4935 7.4891 7.3170 7.3129 7.2986 7.2957 7.2926 7.2777 7.2736 7.2651 7.2362 7.2322 7.2170 7.2126 7.1404 7.1373 7.1212 7.1182 7.1022 7.0992 7.0615 7.0416 7.0376 7.0226 7.0190 6.5236 6.5091 4.2618 4.2379 4.2142 3.7649 3.7392 3.7154 3.6915

0.99 0.95 0.99 0.97 0.97 1.01 0.94 1.02 1.05 2.09 0.96 2.00 2.99 2.22

f1 (ppm)

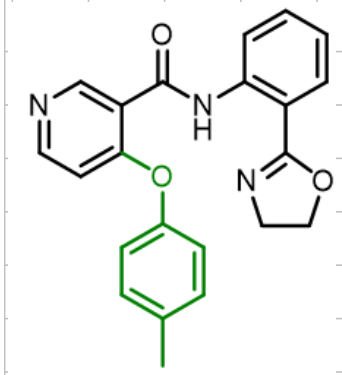
EO-33(CH)/EO-33C
EO-33



163.8985
163.1105
162.3567
153.3969
152.9299
151.6295
141.4965
139.5753
132.2812
129.3017
127.2866
123.2160
122.8751
121.3358
121.2581
120.1719
114.4430
113.0002
109.3951
65.9757
55.7902
54.8238

f1 (ppm)

EO-35(CH)/EO-35H
EO-35



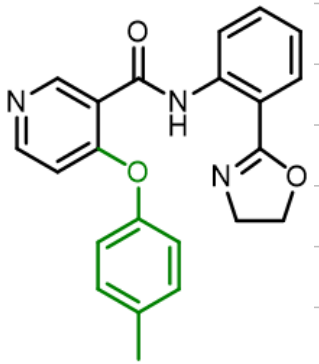
12.8439

9.1498
8.9654
8.9625
8.9440
8.9411
8.4676
8.4609
8.4462
7.8882
7.8839
7.8684
7.8641
7.5380
7.5335
7.5196
7.5159
7.5123
7.4983
7.4940
7.2837
7.2752
7.2662
7.2603
7.2548
7.1456
7.1426
7.1265
7.1236
7.1074
7.1044
7.0952
7.0882
7.0830
7.0721
7.0670
6.6542
6.6396
4.2774
4.2535
4.2298
3.7834
3.7597
3.7357
2.4009

0.93
0.97
0.97
0.99
0.97
1.04
2.43
1.10
1.97
0.96
2.00
1.98
3.05

f1 (ppm)

EO-35(CH)/EO-35C
EO-35
13C

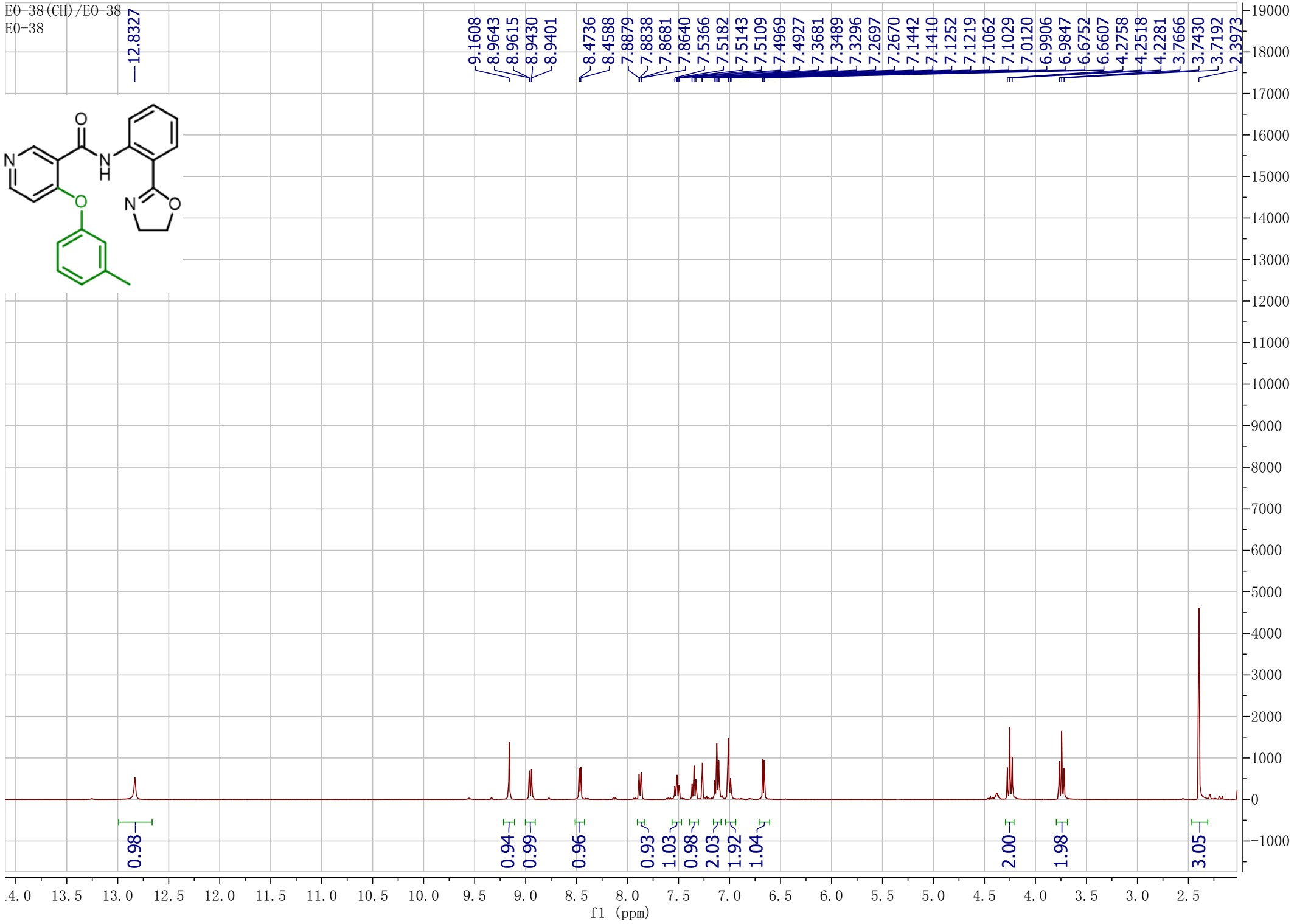


163.9898
163.0204
162.6329
153.3772
153.0123
151.0743
139.4947
135.8278
132.3687
130.7799
129.3349
122.9352
121.2609
121.0839
121.0397
114.2662
109.9853
66.0039
54.9131
20.9301

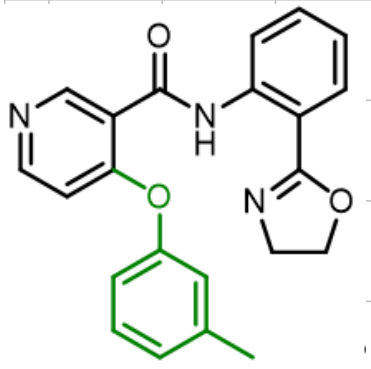
2100 2000 1900 1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800 700 600 500 400 300 200 100 0 −100 −200

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)


E0-38(CH)/E0-38
E0-38
12.8327
9.1608
8.9643
8.9615
8.9430
8.9401
8.4736
8.4588
7.8879
7.8838
7.8681
7.8640
7.5366
7.5182
7.5143
7.5109
7.4969
7.4927
7.3681
7.3489
7.3296
7.2697
7.2670
7.1442
7.1410
7.1252
7.1219
7.1062
7.1029
7.0120
6.9906
6.9847
6.6752
6.6607
4.2758
4.2518
4.2281
3.7666
3.7430
3.7192
2.3973
0.98
0.94
0.99
0.96
0.93
1.03
0.98
2.03
1.92
1.04
2.00
1.98
3.05
f1 (ppm)

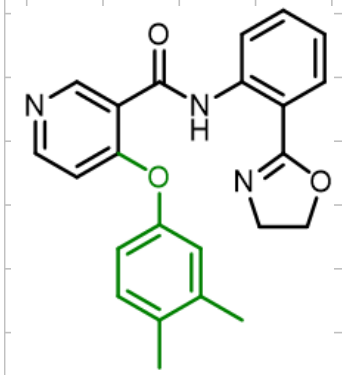
EO-38(CH)/EO-386
EO-38



164.0143
162.9945
162.4079
153.4014
153.3685
153.0358
140.6838
139.4771
132.3796
129.9738
129.3401
126.7682
122.9516
122.0144
121.1841
121.0319
118.3784
114.2543
110.2348
65.9986
54.8664
21.3883

f1 (ppm)

EO-37(CH)/EO-37
EO-37



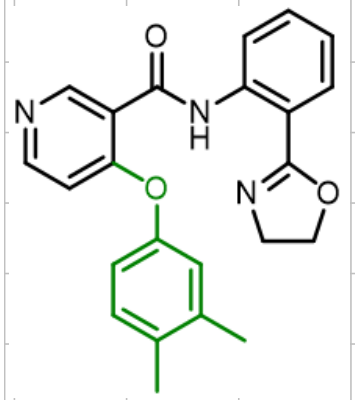
12.8250

9.1485
8.9642
8.9612
8.9429
8.9398
8.4490
8.4343
7.8828
7.8786
7.8632
7.8590
7.5274
7.5136
7.5097
7.5060
7.2676
7.2163
7.1960
7.1381
7.1349
7.1189
7.1159
7.0999
7.0969
6.9745
6.9682
6.9335
6.9271
6.9132
6.9067
6.6559
6.6414
4.2754
4.2515
4.2279
3.7922
3.7684
3.7445
2.2953
2.2904

0.96
0.91
1.00
0.97
0.97
1.13
0.98
1.06
0.95
0.98
0.95
2.00
1.95
6.04

f1 (ppm)

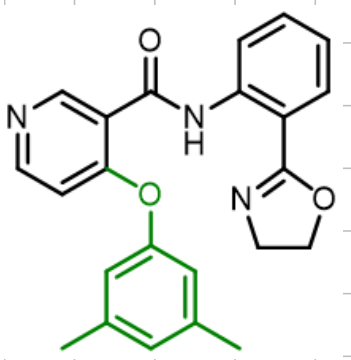
EO-37(CH)/EO-37
EO-37



163.9786
163.0746
162.7167
153.3591
153.0025
151.1657
139.4980
138.9228
134.4330
132.3432
131.0694
129.3294
122.9128
122.4315
121.0517
120.9940
118.5854
114.2815
110.0506
66.0012
54.9359
19.9703
19.2619

f1 (ppm)

EO-50(CH)/EO-50H
EO-50



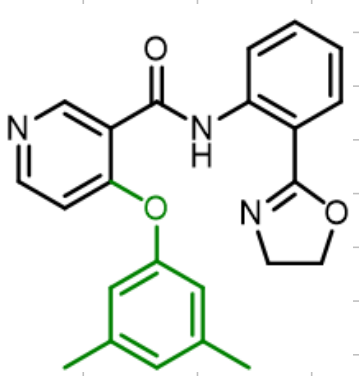
12.8090

9.1500
8.9631
8.9603
8.9418
8.9389
8.4653
8.4508
7.8870
7.8827
7.8672
7.8629
7.5402
7.5360
7.5319
7.5258
7.5178
7.5140
7.5104
7.4965
7.4922
7.2663
7.1426
7.1396
7.1238
7.1208
7.1047
7.1016
6.9314
6.8138
6.6803
6.6657
4.2820
4.2581
4.2345
3.7797
3.7560
3.7320
2.3515

0.94
0.95
0.95
0.96
0.94
1.24
1.00
0.98
1.92
0.97
2.02
2.00
6.00

f1 (ppm)

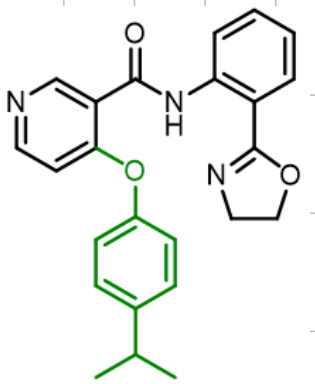
EO-50(CH)/EO-50C
EO-50



164.0075
163.0455
162.4807
153.4094
153.3085
153.0361
140.2420
139.4956
132.3670
129.3283
127.5894
122.9186
121.0570
119.0026
114.2616
110.2648
65.9969
54.8844
21.3178

f1 (ppm)

EO-51(CH)/EO-51H
EO-51

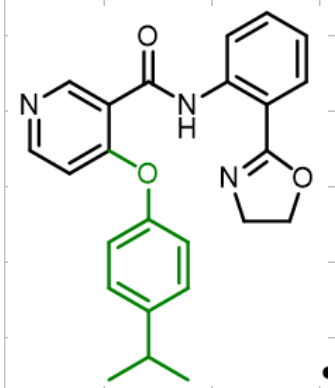


12.8229
9.1471
8.9585
8.9555
8.9371
8.9341
8.4647
8.4501
7.8859
7.8816
7.8660
7.8619
7.5360
7.5318
7.5177
7.5141
7.5104
7.4965
7.4922
7.3311
7.3233
7.3184
7.3075
7.3021
7.2950
7.2647
7.1427
7.1396
7.1238
7.1180
7.1125
7.1046
7.1016
7.0963
7.0890
6.6759
6.6614
4.2789
4.2552
4.2329
4.2313
3.7862
3.7625
3.7386
3.7300
2.9806
2.9634
2.9461
2.9288
1.2908
1.2735

0.98
0.94
0.96
0.97
0.97
1.04
1.97
2.93
0.98
2.00
2.01
0.97
6.37

f1 (ppm)

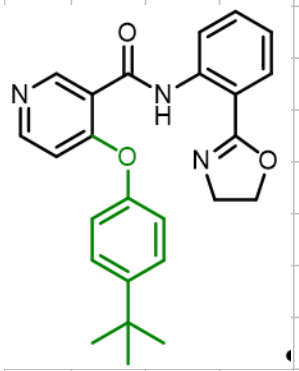
EO-51(CH)/EO-51C
EO-51



163.9983
163.0548
162.5493
153.4004
153.0604
151.2424
146.8274
139.4842
132.3727
129.3318
128.1396
122.9272
121.1940
121.0240
114.2540
110.1126
65.9937
54.8630
33.6656
24.1250

f1 (ppm)

EO-52(CH)/EO-52H
EO-52

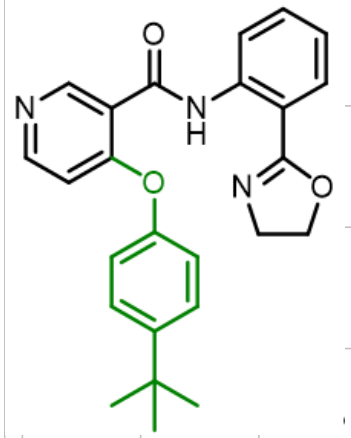


12.8254
9.1471
8.9555
8.9525
8.9342
8.9313
8.4664
8.4517
7.8837
7.8795
7.8639
7.8597
7.5329
7.5286
7.5146
7.5109
7.5073
7.4933
7.4889
7.4809
7.4756
7.4643
7.4591
7.4514
7.2674
7.1393
7.1364
7.1289
7.1208
7.1165
7.1042
7.0991
7.0915
6.6858
6.6713
4.2789
4.2550
4.2313
3.7880
3.7644
3.7404
1.3547

0.98
0.96
0.96
0.96
0.96
1.12
1.99
2.97
0.97
2.00
2.00
9.16

f1 (ppm)

EO-52(CH)/EO-52C
EO-52



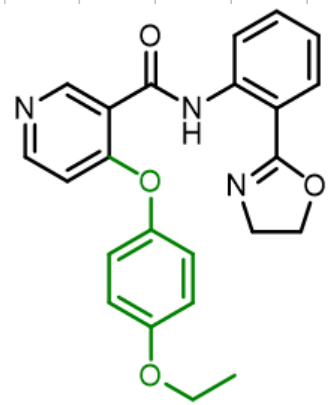
163.9936
163.0482
162.4996
153.3852
153.0503
150.9791
149.1346
139.4785
132.3574
129.3288
127.1121
122.9173
121.1880
121.0064
120.7976
114.2499
110.1600
65.9900
54.8467
34.6131
31.4648

5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20

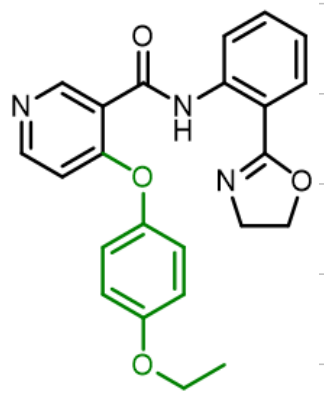
f1 (ppm)

EO-60-3(CH)/EO-60-3H
EO-60-3



f1 (ppm)

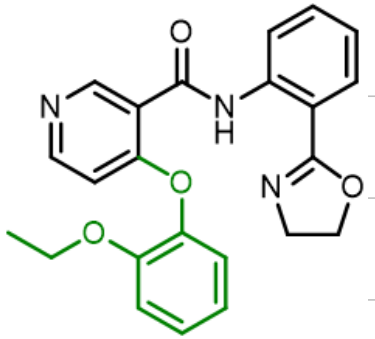
EO-60-3(CH)/EO-60-3C
EO-60-3



163.9755
163.0347
162.9372
156.8960
153.4035
153.0754
146.4587
139.4927
132.3541
129.3543
122.9332
122.4704
121.0436
120.8482
115.7626
114.2794
109.7517
66.0023
63.9770
54.9622
14.8454

f1 (ppm)

EO-59-3CH/EO-59-3H
EO-59-3

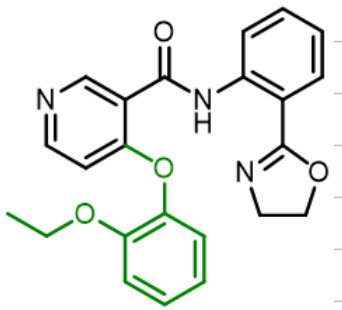


12.8284
9.1992
8.9897
8.9868
8.9683
8.9653
8.4312
8.4167
7.8868
7.8829
7.8670
7.8631
7.5356
7.5315
7.5173
7.5135
7.5102
7.4959
7.4920
7.2846
7.2809
7.2690
7.2606
7.2565
7.2526
7.2458
7.2419
7.2360
7.2321
7.1430
7.1400
7.1233
7.1049
7.1019
7.0465
7.0434
7.0370
7.0334
7.0264
7.0167
7.0131
7.0075
6.5670
6.5526
4.2566
4.2329
4.2091
4.0163
3.9988
3.9814
3.9640
3.7308
3.7174
3.7125
3.6944
3.6705
1.1738
1.1564
1.1391

0.97 0.97 0.98 0.99 0.98 1.07 2.42 1.09 2.05 1.09 2.00 1.99 2.23 2.98

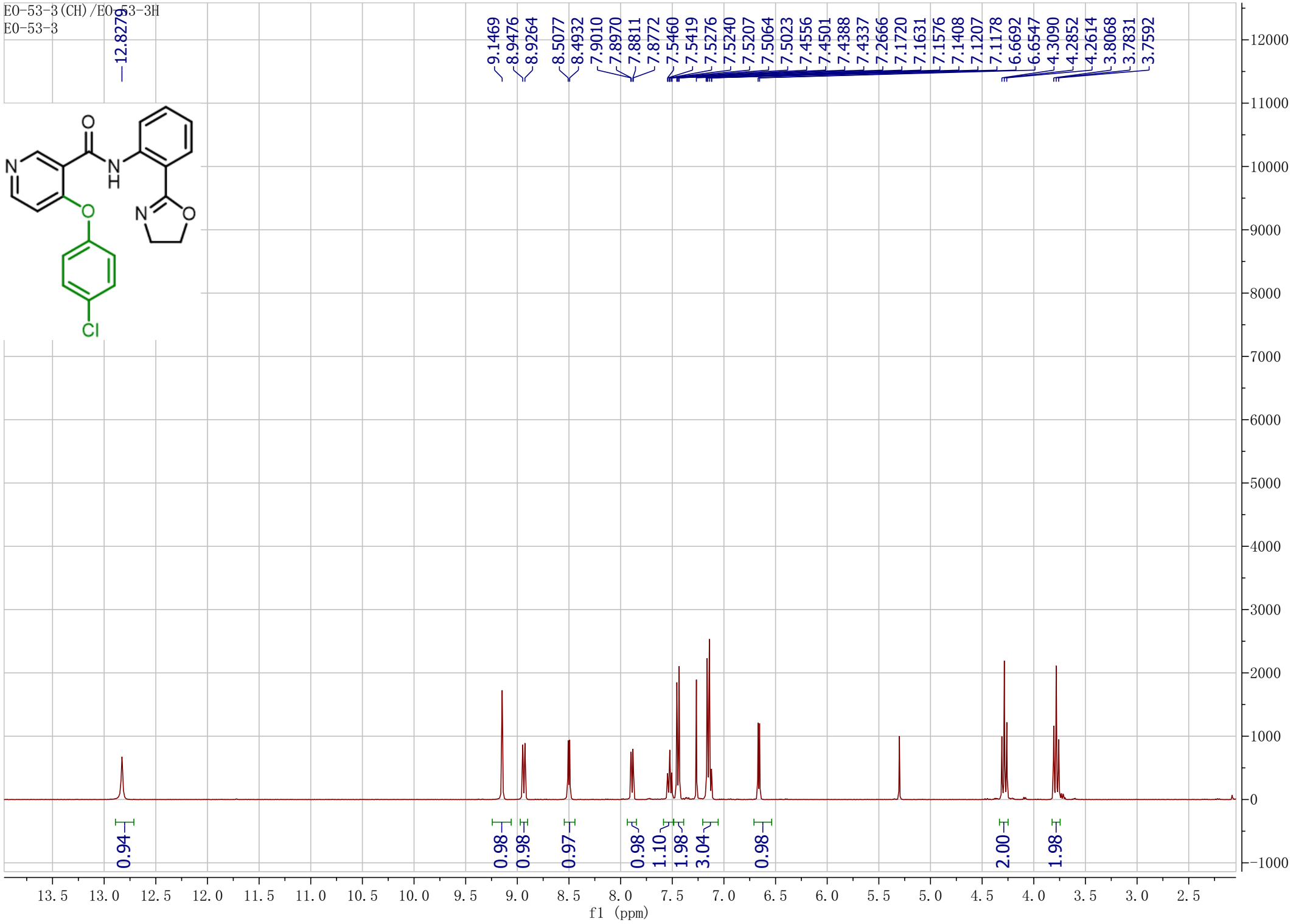
f1 (ppm)

EO-59-3CH/EO-59-3C
EO-59-3

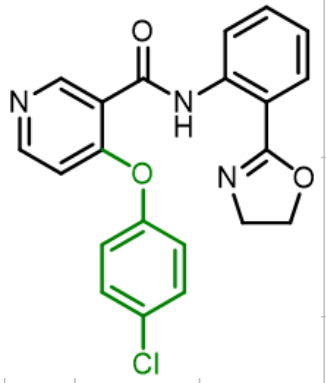


163.8115
163.1466
162.5369
153.3086
152.7321
150.8150
141.9287
139.5570
132.2414
129.3082
127.1507
123.1918
122.8689
121.2608
121.2058
120.1916
114.4834
114.1416
109.7309
65.9765
64.3503
54.8095
14.5539

f1 (ppm)


EO-53-3(CH)/EO-53-3H
EO-53-3
12.8279
9.1469
8.9476
8.9264
8.5077
8.4932
7.9010
7.8970
7.8811
7.8772
7.5460
7.5419
7.5276
7.5240
7.5207
7.5064
7.5023
7.4556
7.4501
7.4388
7.4337
7.2666
7.1720
7.1631
7.1576
7.1408
7.1207
7.1178
6.6692
6.6547
4.3090
4.2852
4.2614
3.8068
3.7831
3.7592
O
N
H
N
O
O
N
Cl
0.94
0.98
0.98
0.97
0.98
1.10
1.98
3.04
0.98
2.00
1.98
f1 (ppm)

EO-53-3(CH)/EO-53-3C
EO-53-3



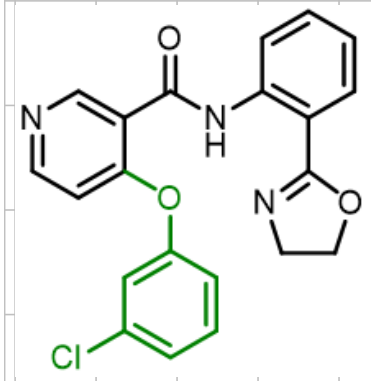
164.2008
162.7507
161.8973
153.3657
153.1914
152.0847
139.4290
132.4861
131.3631
130.4044
129.3915
123.0505
122.7408
121.6070
120.8823
114.1090
110.1710
66.0228
54.8889

4000
3500
3000
2500
2000
1500
1000
500
0

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30

f1 (ppm)

EO-54-3(CH)/EO-54-3H
EO-54-3



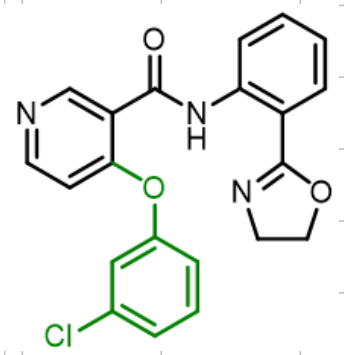
12.8153

9.1481 8.9415 8.9206 8.5321 8.5176 7.8991 7.8950 7.8793 7.8753 7.5428 7.5387 7.5244 7.5205 7.5173 7.5031 7.4991 7.4294 7.4092 7.3890 7.3072 7.3044 7.3019 7.2999 7.2868 7.2824 7.2797 7.2684 7.2467 7.2412 7.2358 7.1551 7.1522 7.1354 7.1211 7.1165 7.1140 7.1009 7.0956 7.0933 6.7069 6.6926 4.3116 4.2878 4.2640 3.8250 3.8013 3.7775

0.96 0.94 1.00 0.96 1.00 1.09 0.99 0.99 0.97 2.04 0.97 2.00 1.99

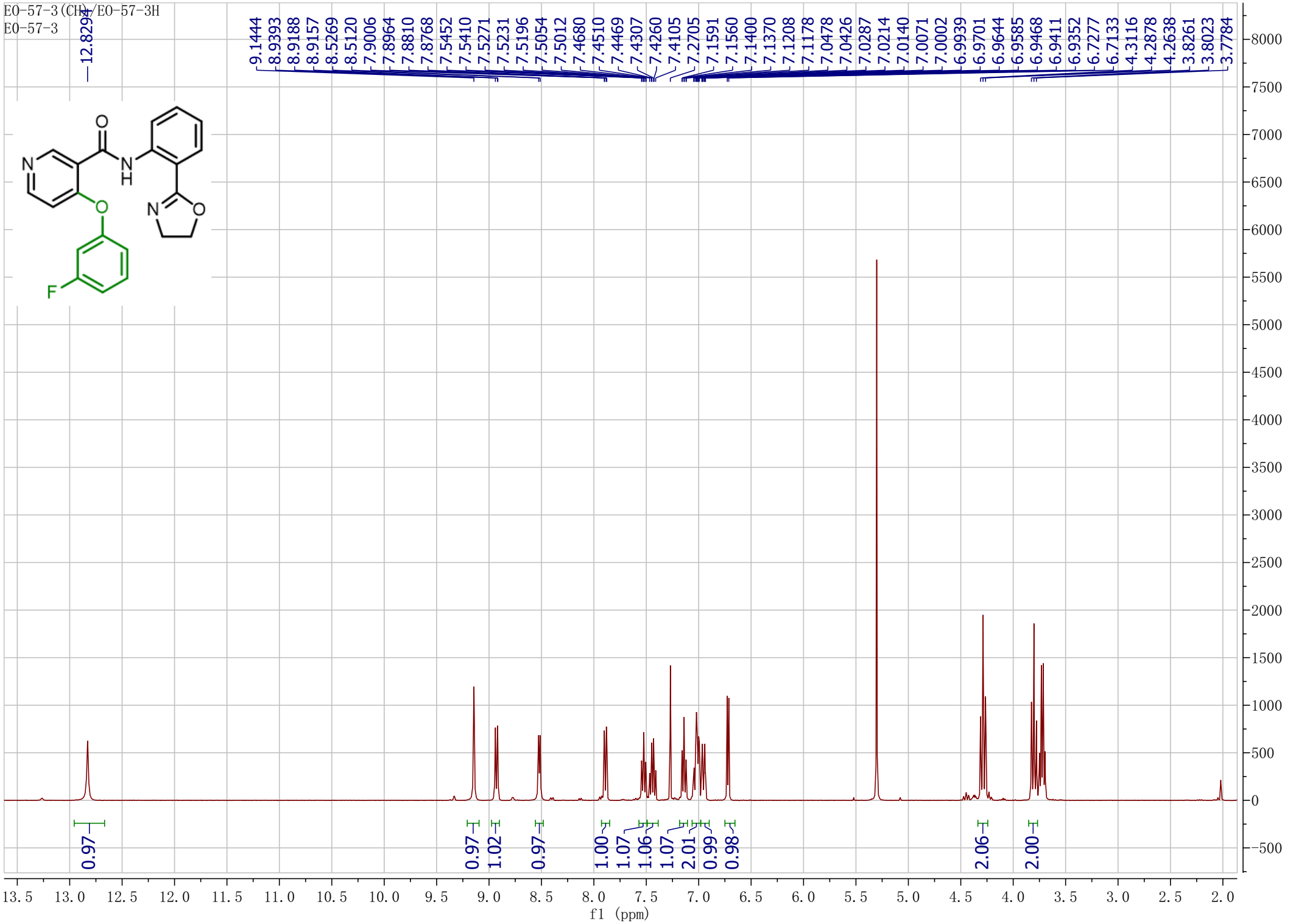
f1 (ppm)

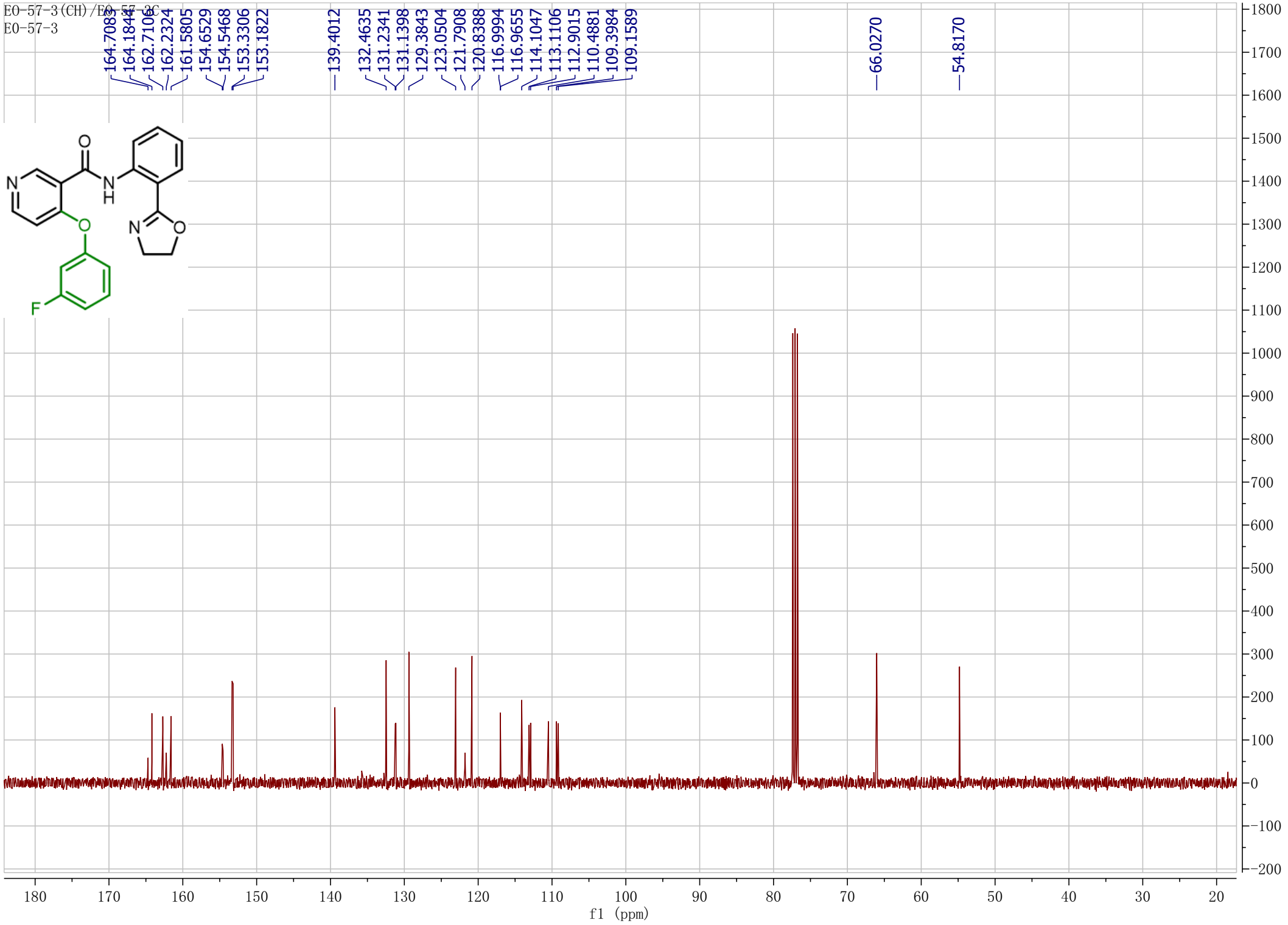
EO-54-3(CH)/EO-54-3C
EO-54-3



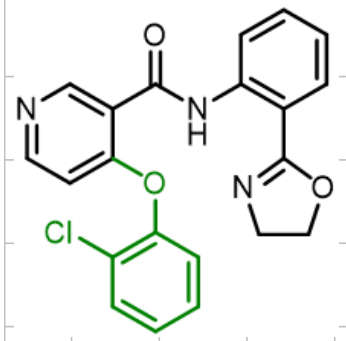
164.1951
162.6960
161.5732
154.1972
153.3743
153.2147
139.3972
135.5839
132.4763
131.1041
129.4003
126.2006
123.0543
121.9171
121.7213
120.8415
119.6043
114.0987
110.4141
66.0372
54.8595

f1 (ppm)


EO-57-3(CH3)/EO-57-3H
EO-57-3
12.8299
9.1444
8.9393
8.9188
8.9157
8.5269
8.5120
7.9006
7.8964
7.8810
7.8768
7.5452
7.5410
7.5271
7.5231
7.5196
7.5054
7.5012
7.4680
7.4510
7.4469
7.4307
7.4260
7.4105
7.2705
7.1591
7.1560
7.1400
7.1370
7.1208
7.1178
7.0478
7.0426
7.0287
7.0214
7.0140
7.0071
7.0002
6.9939
6.9701
6.9644
6.9585
6.9468
6.9411
6.9352
6.7277
6.7133
4.3116
4.2878
4.2638
3.8261
3.8023
3.7784
0.97
0.97
1.02
0.97
1.00
1.07
1.06
1.07
2.01
0.99
0.98
2.06
2.00
f1 (ppm)


EO-57-3(CH)/EO-57-3C
EO-57-3
164.7083
164.1844
162.7106
162.2324
161.5805
154.6529
154.5468
153.3306
153.1822
139.4012
132.4635
131.2341
131.1398
129.3843
123.0504
121.7908
120.8388
116.9994
116.9655
114.1047
113.1106
112.9015
110.4881
109.3984
109.1589
66.0270
54.8170
f1 (ppm)

EO-55-3(CH)/EO-55-3H
EO-55-3



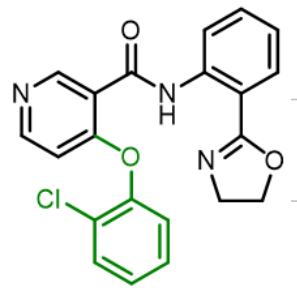
12.8365

9.2104 8.9769 8.9741 8.9557 8.9529 8.4913 8.4768 7.9028 7.8988 7.8832 7.8792 7.5568 7.5522 7.5459 7.5413 7.5355 7.5323 7.5270 7.5237 7.5201 7.5059 7.5018 7.4191 7.4152 7.4010 7.3979 7.3951 7.3806 7.3767 7.3165 7.2976 7.2931 7.2807 7.2766 7.2685 7.1581 7.1553 7.1385 7.1201 7.1172 6.5110 6.4966 4.2820 4.2581 4.2344 3.7616 3.7378 3.7307 3.7136

0.94 0.97 1.00 0.99 0.97 2.09 1.03 1.96 1.05 0.96 2.00 2.45

f1 (ppm)

EO-55-3(CH)/EO-55-3C
EO-55-3



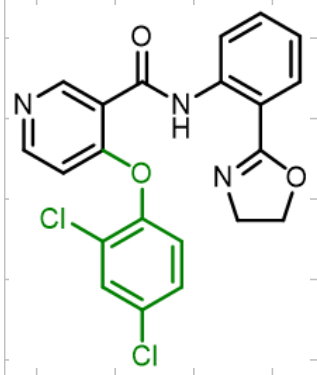
163.9575
162.7525
161.2667
153.5128
153.1775
149.1163
139.4661
132.3306
131.2557
129.3656
128.5881
127.4434
123.6946
123.0209
121.1473
120.7456
114.3670
109.5427
65.9818
54.7865

2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30

f1 (ppm)

EO-56-3(CH)/EO-56-3H
EO-56-3



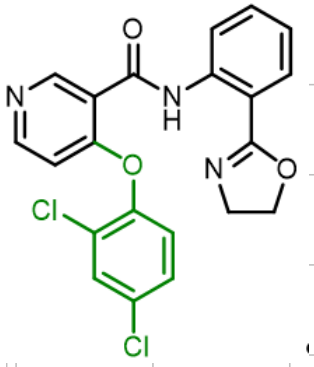
12.8133

9.1846
8.9555
8.9343
8.5150
8.5002
7.9097
7.9059
7.8900
7.8861
7.5579
7.5514
7.5442
7.5285
7.5250
7.5219
7.5076
7.5038
7.3853
7.3792
7.3636
7.3576
7.2684
7.2553
7.2337
7.1645
7.1618
7.1450
7.1265
7.1235
6.5184
6.5040
4.3151
4.2913
4.2676
3.8204
3.7967
3.7729

0.95 0.95 0.98 0.96 0.98 1.96 1.00 0.96 1.00 0.97 2.00 1.99

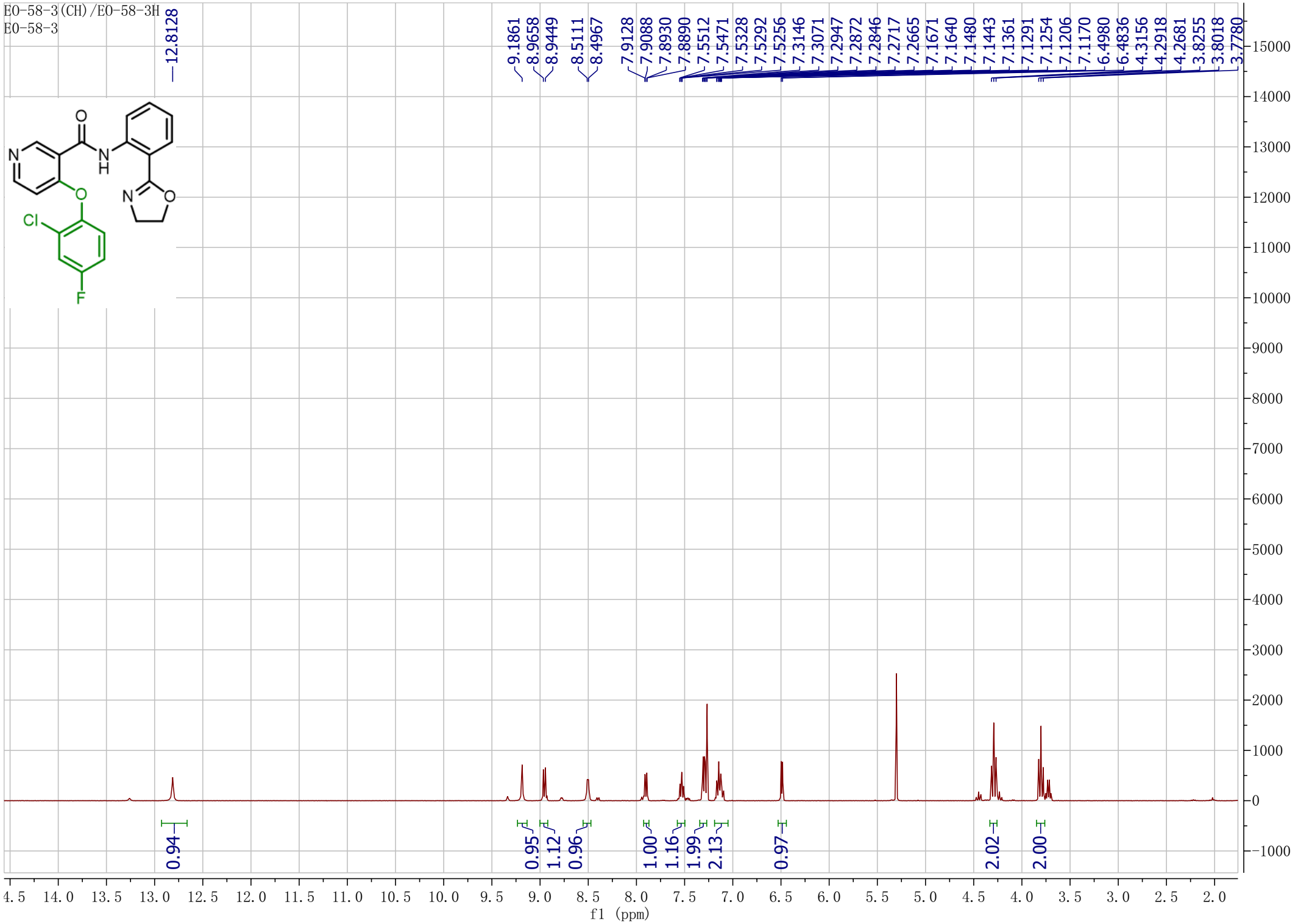
f1 (ppm)

EO-56-3(CH)/EO-56-3C
EO-56-3

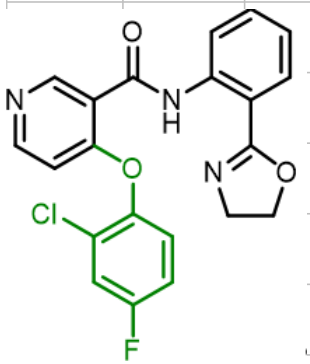


164.1224
162.5805
160.9345
153.3796
153.2599
147.9723
139.4163
132.4161
132.2749
130.9843
129.3976
128.7773
128.3517
124.4326
123.0908
121.0711
121.0092
114.2321
109.5184
66.0125
54.8415

f1 (ppm)

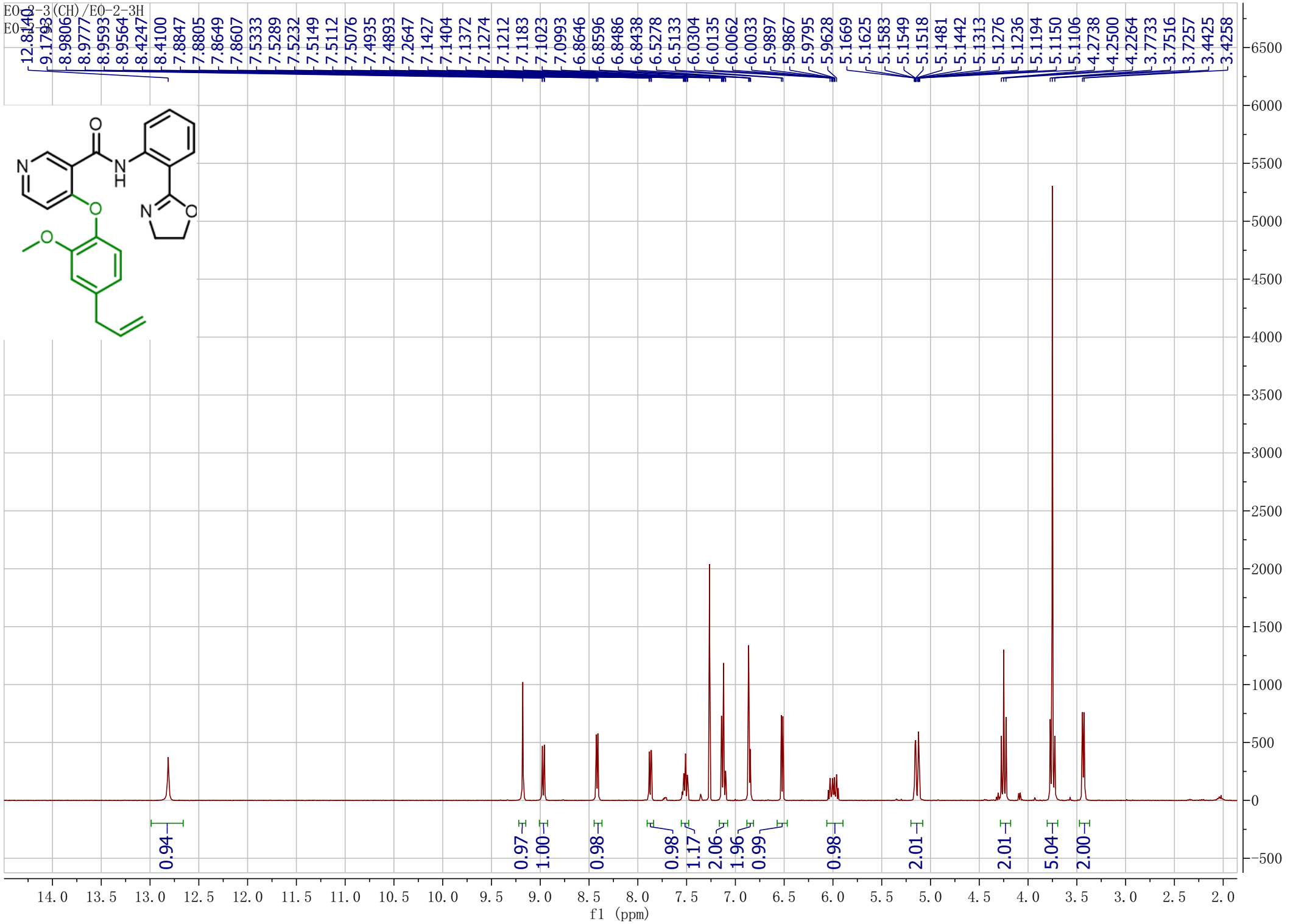

EO-58-3(CH)/EO-58-3H
EO-58-3
12.8128
9.1861
8.9658
8.9449
8.5111
8.4967
7.9128
7.9088
7.8930
7.8890
7.5512
7.5471
7.5328
7.5292
7.5256
7.3146
7.3071
7.2947
7.2872
7.2846
7.2717
7.2665
7.1671
7.1640
7.1480
7.1443
7.1361
7.1291
7.1254
7.1206
7.1170
6.4980
6.4836
4.3156
4.2918
4.2681
3.8255
3.8018
3.7780
0.94
0.95
1.12
0.96
1.00
1.16
1.99
2.13
0.97
2.02
2.00
f1 (ppm)

EO-58-3(CH)/EO-58-3C
EO-58-3

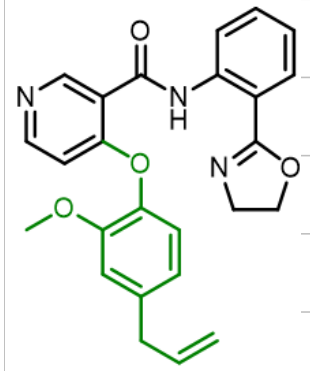


164.1302
162.6695
161.2854
161.2224
158.8062
153.3517
153.2349
145.4810
145.4450
139.4383
132.4270
129.3911
128.4688
128.3610
124.5868
124.4971
123.0829
121.0615
118.5204
118.2604
115.7254
115.4967
114.2590
109.3130
66.0039
54.8474

f1 (ppm)


EO-2-3(CH)/EO-2-3H
EO-2-3H
12.8140
9.1793
8.9806
8.9777
8.9593
8.9564
8.4247
8.4100
7.8847
7.8805
7.8649
7.8607
7.5333
7.5289
7.5232
7.5149
7.5112
7.5076
7.4935
7.4893
7.2647
7.1427
7.1404
7.1372
7.1274
7.1212
7.1183
7.1023
7.0993
6.8646
6.8596
6.8486
6.8438
6.5278
6.5133
6.0304
6.0135
6.0062
6.0033
5.9897
5.9867
5.9795
5.9628
5.1669
5.1625
5.1583
5.1549
5.1518
5.1481
5.1442
5.1313
5.1276
5.1236
5.1194
5.1150
5.1106
4.2738
4.2500
4.2264
3.7733
3.7516
3.7257
3.4425
3.4258
0.94
0.97
1.00
0.98
0.98
1.17
2.06
1.96
0.99
0.98
2.01
2.01
5.04
2.00
f1 (ppm)

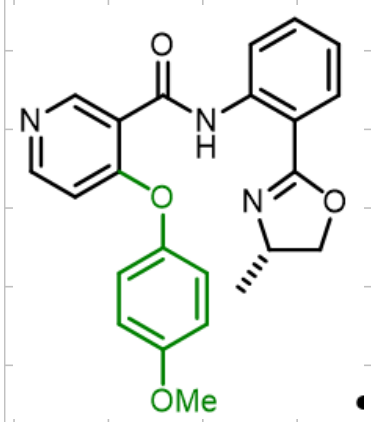
EO-2-3(CH)/EO-2-36
EO-23



163.8869
163.1476
162.4917
153.3471
152.9137
151.3846
139.6784
139.5663
136.8527
132.2636
129.2907
122.9396
122.8538
121.2530
121.2085
120.1495
116.4484
114.4425
113.2275
109.3864
65.9843
55.7549
54.8609
40.0799

f1 (ppm)

EO-69-3(CH)/EO-69-3H
EO-69-3



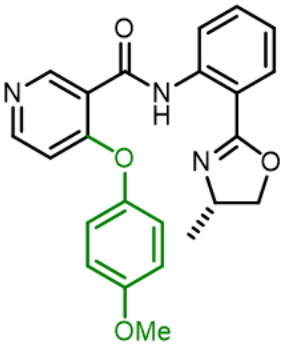
12.7470

9.0816 8.9099 8.9070 8.8888 8.8859 8.4611 8.4466 7.8869 7.8828 7.8672 7.8629 7.5353 7.5311 7.5171 7.5134 7.5098 7.4959 7.4916 7.2679 7.1520 7.1491 7.1330 7.1300 7.1207 7.1144 7.1108 7.1039 7.0980 7.0889 6.9844 6.9753 6.9694 6.9584 6.9527 6.6522 6.6375 4.3802 4.3600 4.3569 4.3368 4.2067 4.1897 4.1836 4.1728 4.1666 4.1496 3.8872 3.8692 3.8670 3.8491 3.8378 3.7995

0.98 0.98 0.98 0.99 0.99 1.11 3.12 2.10 1.00 1.00 0.98 2.03 3.26

f1 (ppm)

EO-69-3(CH)/EO-69-36
EO-69-3

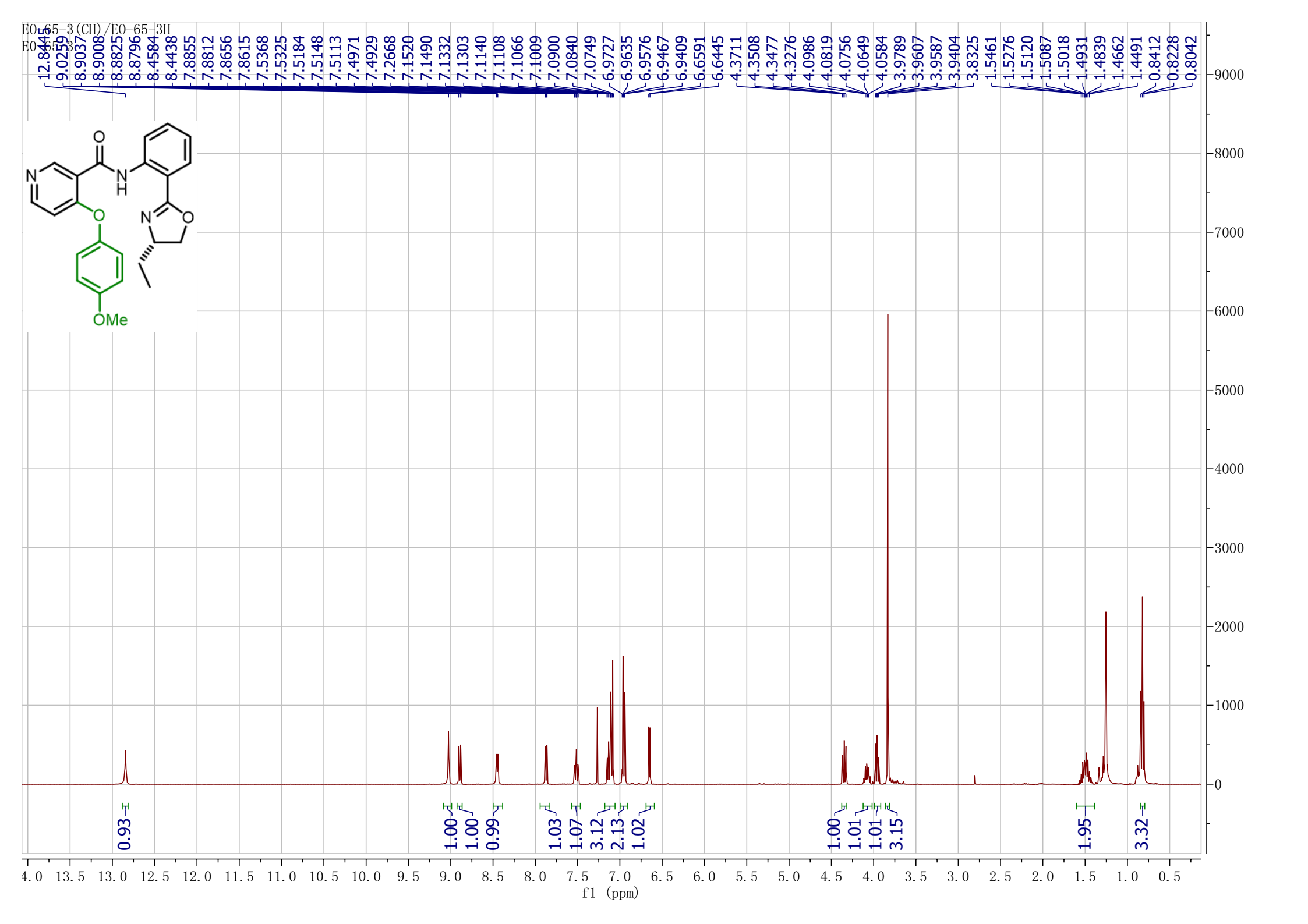


163.1358
163.0569
162.9139
157.4708
152.9930
152.6597
146.7533
139.4288
132.3449
129.2669
122.9897
122.3687
121.5265
120.9852
115.2112
114.4003
109.9638
72.5900
62.0862
55.7091
21.5915

5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

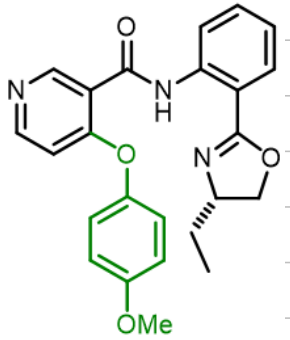
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)

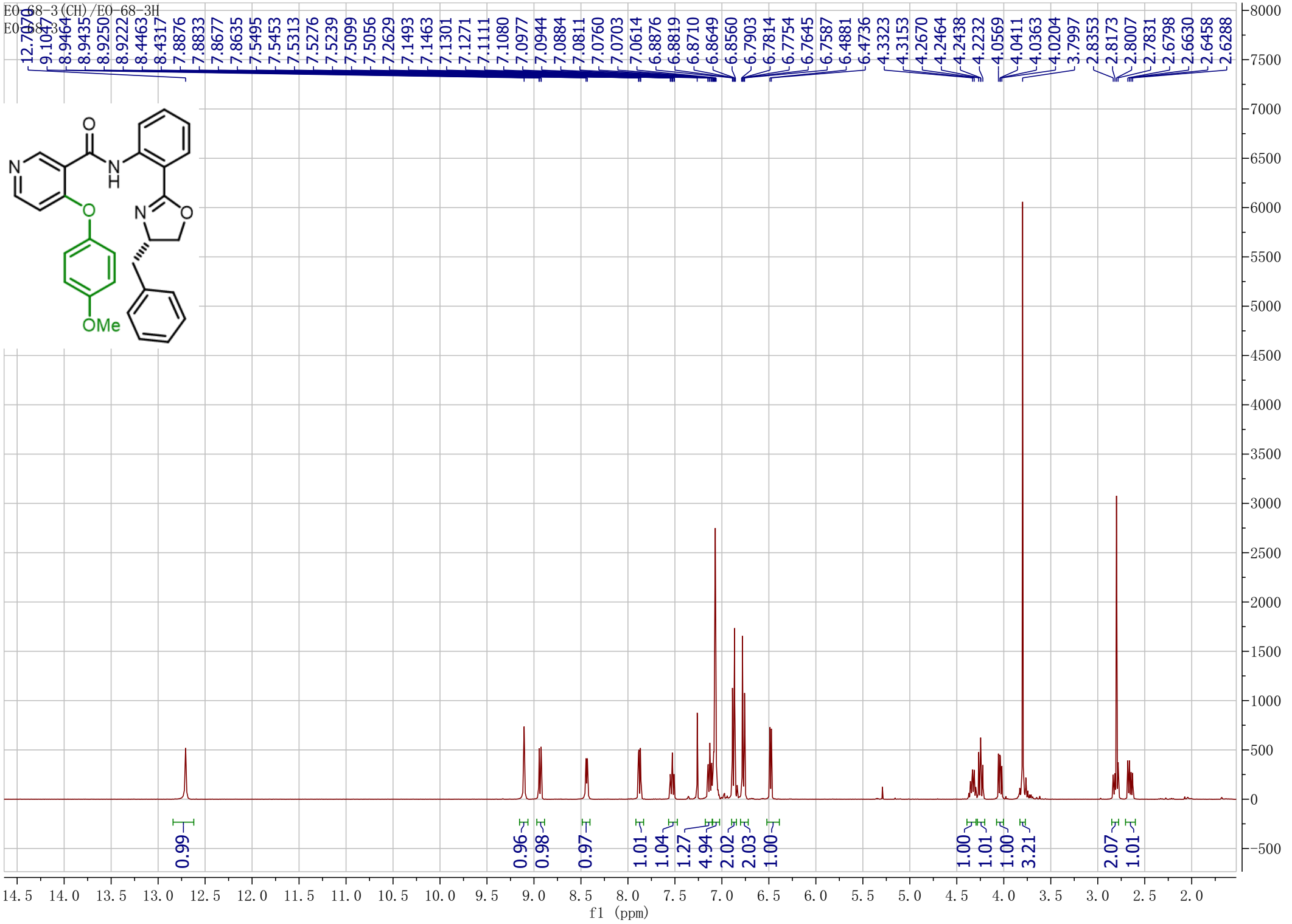

EO-65-3(CH)/EO-65-3H
EO-65-3
12.8446
9.0259
8.9037
8.9008
8.8825
8.8796
8.4584
8.4438
7.8855
7.8812
7.8656
7.8615
7.5368
7.5325
7.5184
7.5148
7.5113
7.4971
7.4929
7.2668
7.1520
7.1490
7.1332
7.1303
7.1140
7.1108
7.1066
7.1009
7.0900
7.0840
7.0749
6.9727
6.9635
6.9576
6.9467
6.9409
6.6591
6.6445
4.3711
4.3508
4.3477
4.3276
4.0986
4.0819
4.0756
4.0649
4.0584
3.9789
3.9607
3.9587
3.9404
3.8325
1.5461
1.5276
1.5120
1.5087
1.5018
1.4931
1.4839
1.4662
1.4491
0.8412
0.8228
0.8042
N
O
N
H
O
N
O
OMe
0.93
1.00
1.00
0.99
1.03
1.07
3.12
2.13
1.02
1.00
1.01
1.01
3.15
1.95
3.32
f1 (ppm)

EO-65-3(CH)/EO-65-3C
EO-65-3

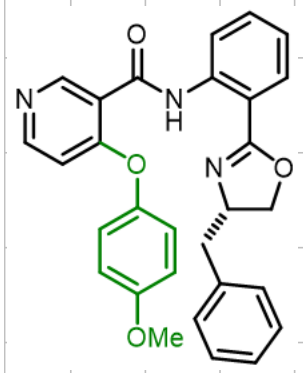
163.2253
163.0788
162.9613
157.4060
152.9023
152.1968
146.8476
139.5175
132.3910
129.2434
122.9518
122.2698
120.7724
115.1760
114.2270
110.0580
70.8293
68.0430
55.6957
28.7550
10.0505



f1 (ppm)


EO-68-3(CH)/EO-68-3H
EO-68-3
12.7676
9.1047
8.9464
8.9435
8.9250
8.9222
8.4463
8.4317
7.8876
7.8833
7.8677
7.8635
7.5495
7.5453
7.5313
7.5276
7.5239
7.5099
7.5056
7.2629
7.1493
7.1463
7.1301
7.1271
7.1111
7.1080
7.0977
7.0944
7.0884
7.0811
7.0760
7.0703
7.0614
6.8876
6.8819
6.8710
6.8649
6.8560
6.7903
6.7814
6.7754
6.7645
6.7587
6.4881
6.4736
4.3323
4.3153
4.2670
4.2464
4.2438
4.2232
4.0569
4.0411
4.0363
4.0204
3.7997
2.8353
2.8173
2.8007
2.7831
2.6798
2.6630
2.6458
2.6288
O
N
H
N
O
O
OMe
0.99
0.96
0.98
0.97
1.01
1.04
1.27
4.94
2.02
2.03
1.00
1.00
1.01
1.00
3.21
2.07
1.01
f1 (ppm)

EO-68-3(CH3)/EO-68-3C
EO-68-3

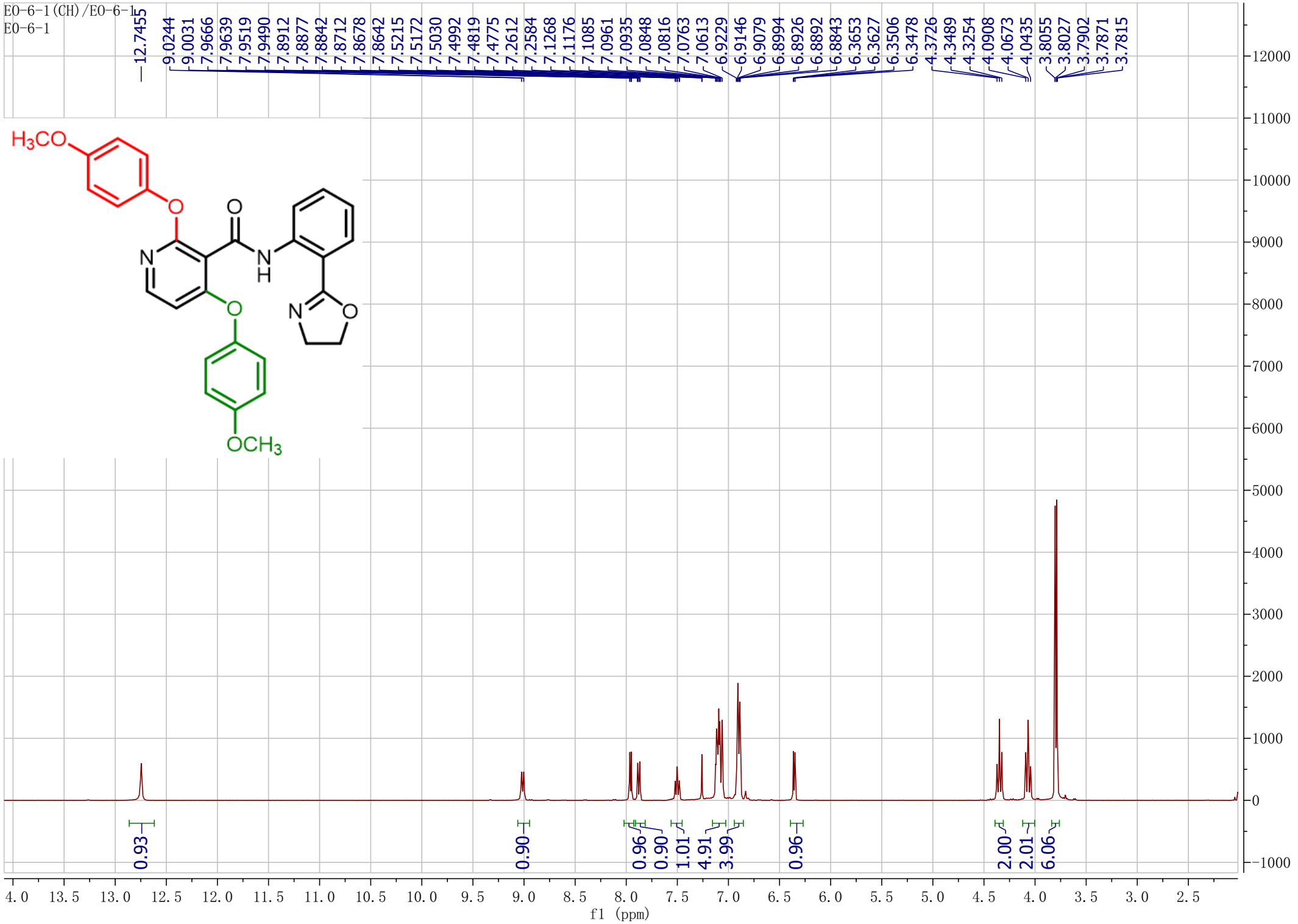


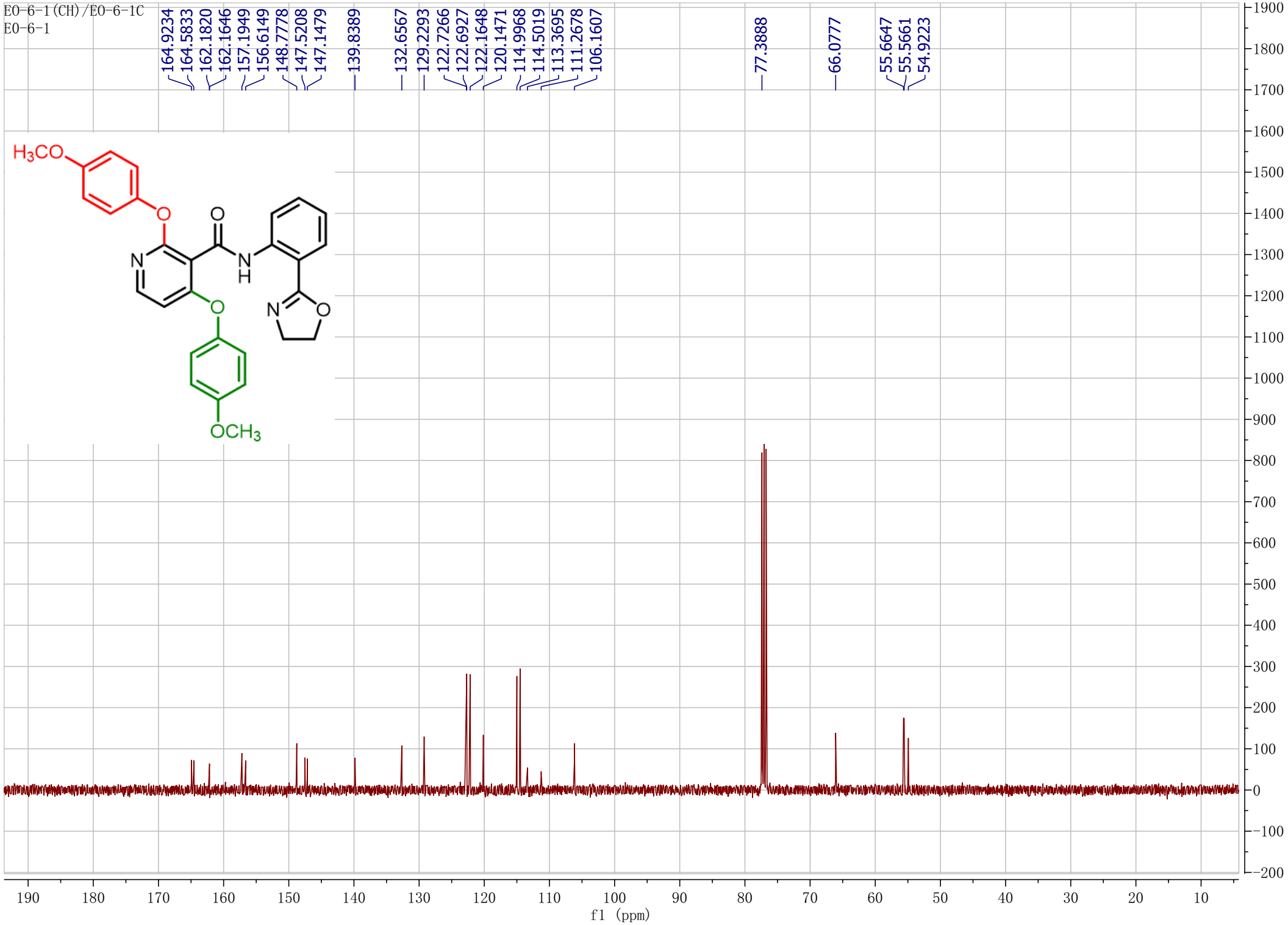
163.3628
163.2046
162.7494
157.3838
152.9341
152.9087
146.5199
139.6013
137.7312
132.5287
129.4122
129.0798
128.3370
126.6334
122.9668
122.3179
121.3624
120.9185
115.1297
114.1333
109.9651
70.6214
68.0436
55.6545
42.3757

13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000

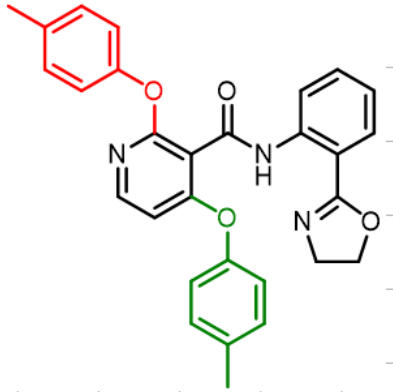
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40

f1 (ppm)


EO-6-1(CH)/EO-6-1
EO-6-1
12.7455
9.0244
9.0031
7.9666
7.9639
7.9519
7.9490
7.8912
7.8877
7.8842
7.8712
7.8678
7.8642
7.5215
7.5172
7.5030
7.4992
7.4819
7.4775
7.2612
7.2584
7.1268
7.1176
7.1085
7.0961
7.0935
7.0848
7.0816
7.0763
7.0613
6.9229
6.9146
6.9079
6.8994
6.8926
6.8892
6.8843
6.3653
6.3627
6.3506
6.3478
4.3726
4.3489
4.3254
4.0908
4.0673
4.0435
3.8055
3.8027
3.7902
3.7871
3.7815
H3CO
O
O
N
O
N
H
N
O
O
OCH3
0.93
0.90
0.96
0.90
1.01
4.91
3.99
0.96
2.00
2.01
6.06
f1 (ppm)


EO-6-1(CH)/EO-6-1C
EO-6-1
164.9234
164.5833
162.1820
162.1646
157.1949
156.6149
148.7778
147.5208
147.1479
139.8389
132.6567
129.2293
122.7266
122.6927
122.1648
120.1471
114.9968
114.5019
113.3695
111.2678
106.1607
77.3888
66.0777
55.6647
55.5661
54.9223
H3CO
O
O
N
N
H
O
N
O
OCH3
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

EO-17CH/EO-17H
EO-17



12.7402

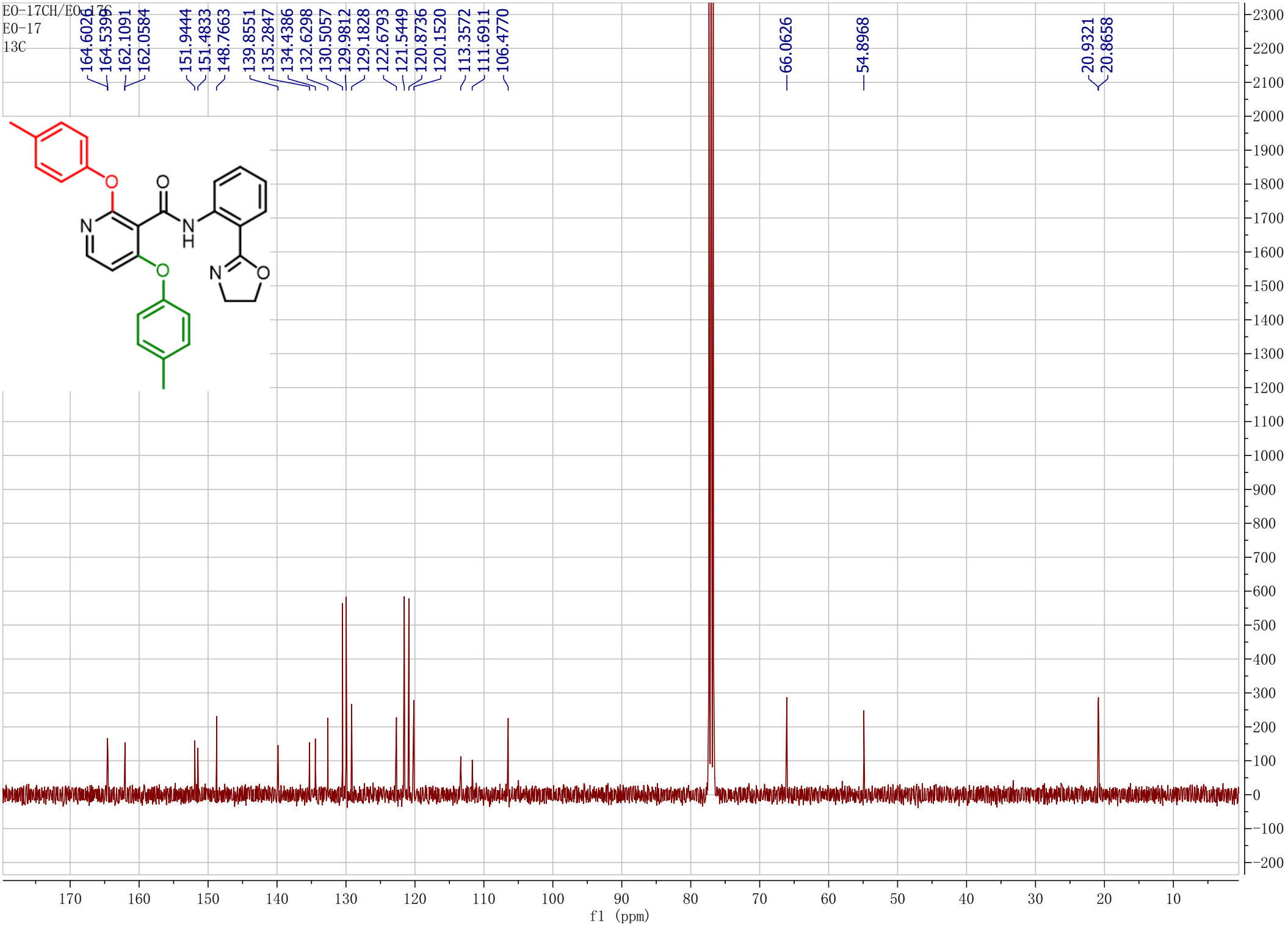
9.0125 8.9913 7.9653 7.9505 7.8827 7.8786 7.8630 7.8590 7.5173 7.5131 7.4987 7.4953 7.4921 7.4775 7.4734 7.2596 7.1944 7.1817 7.1737 7.1612 7.1222 7.1194 7.1029 7.1001 7.0830 7.0759 7.0703 7.0599 7.0548 7.0479 7.0410 7.0357 7.0248 7.0199 7.0122 6.3878 6.3730

4.3674 4.3435 4.3200 4.0861 4.0627 4.0387

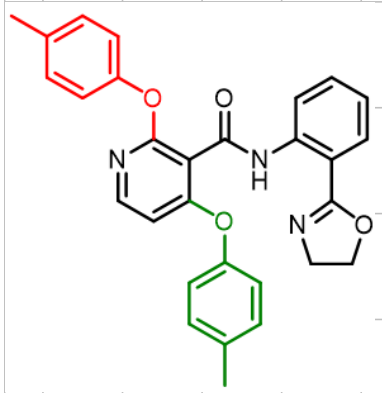
2.3486 2.3316

0.94 0.92 0.94 0.94 0.97 3.86 1.24 3.88 0.97 2.00 1.98 6.06

f1 (ppm)


EO-17CH/EO-17C
EO-17
13C
164.6026
164.5396
162.1091
162.0584
151.9444
151.4833
148.7663
139.8551
135.2847
134.4386
132.6298
130.5057
129.9812
129.1828
122.6793
121.5449
120.8736
120.1520
113.3572
111.6911
106.4770
66.0626
54.8968
20.9321
20.8658
f1 (ppm)

EO-16(CH)/EO-16
EO-16



12.7594

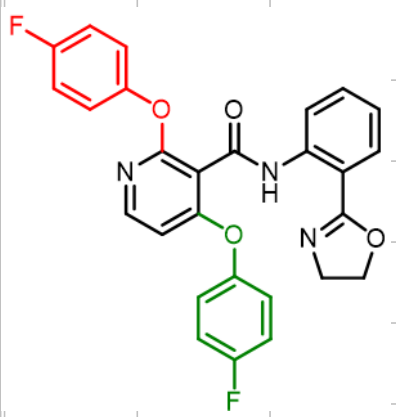
9.0007
8.9794
8.0034
7.9993
7.9886
7.9845
7.9010
7.8814
7.5315
7.5116
7.4914
7.1717
7.1677
7.1608
7.1551
7.1461
7.1364
7.1273
7.1230
7.1154
7.1106
7.0898
7.0659
7.0470
7.0425
6.4029
6.3882

4.3850
4.3640
4.3596
4.3376
4.0730
4.0495
4.0257

0.92
0.93
0.96
0.95
1.03
8.90
0.95
2.00
1.96

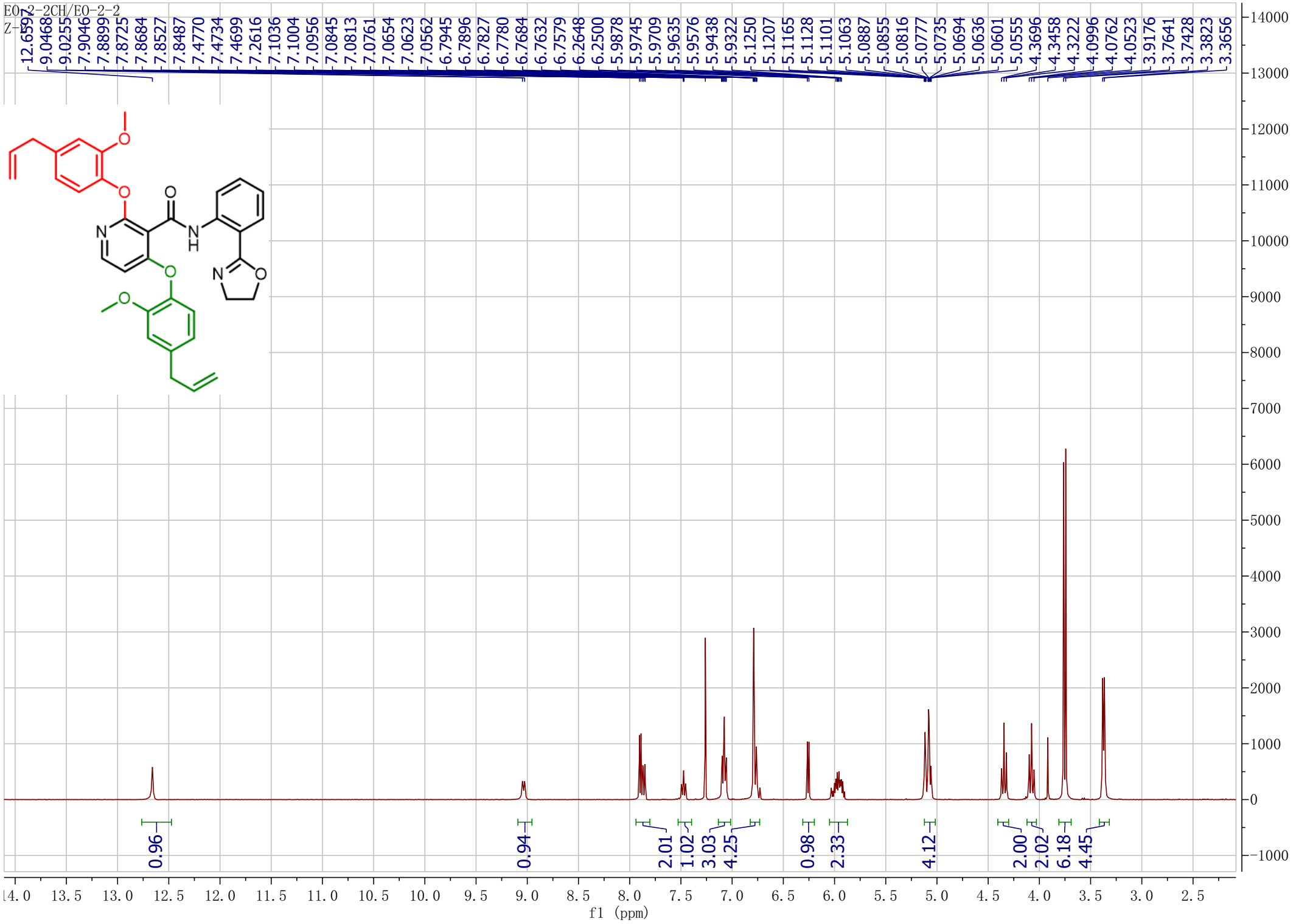
f1 (ppm)

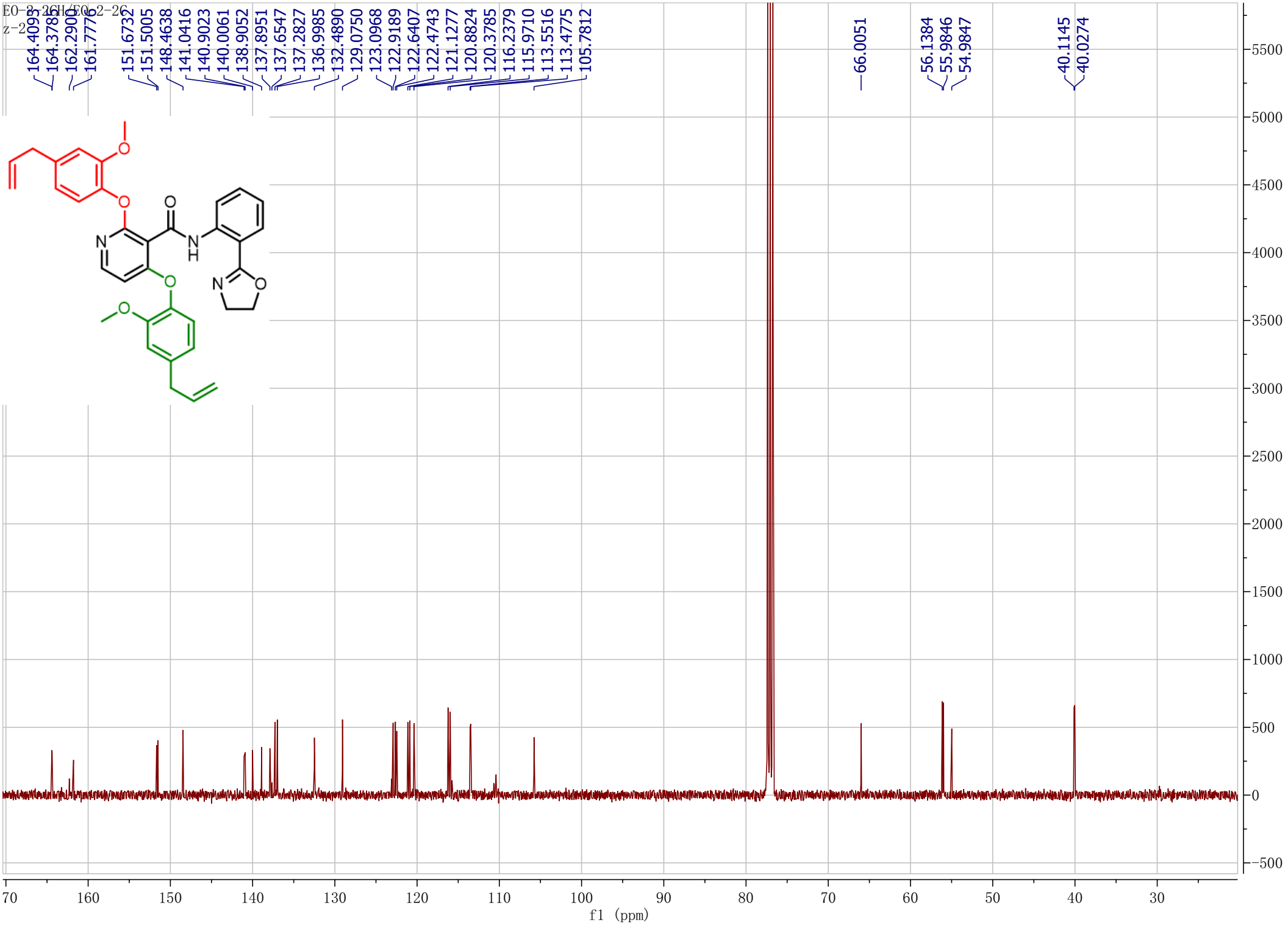
EO-16(CH)/EO-16C
EO-16

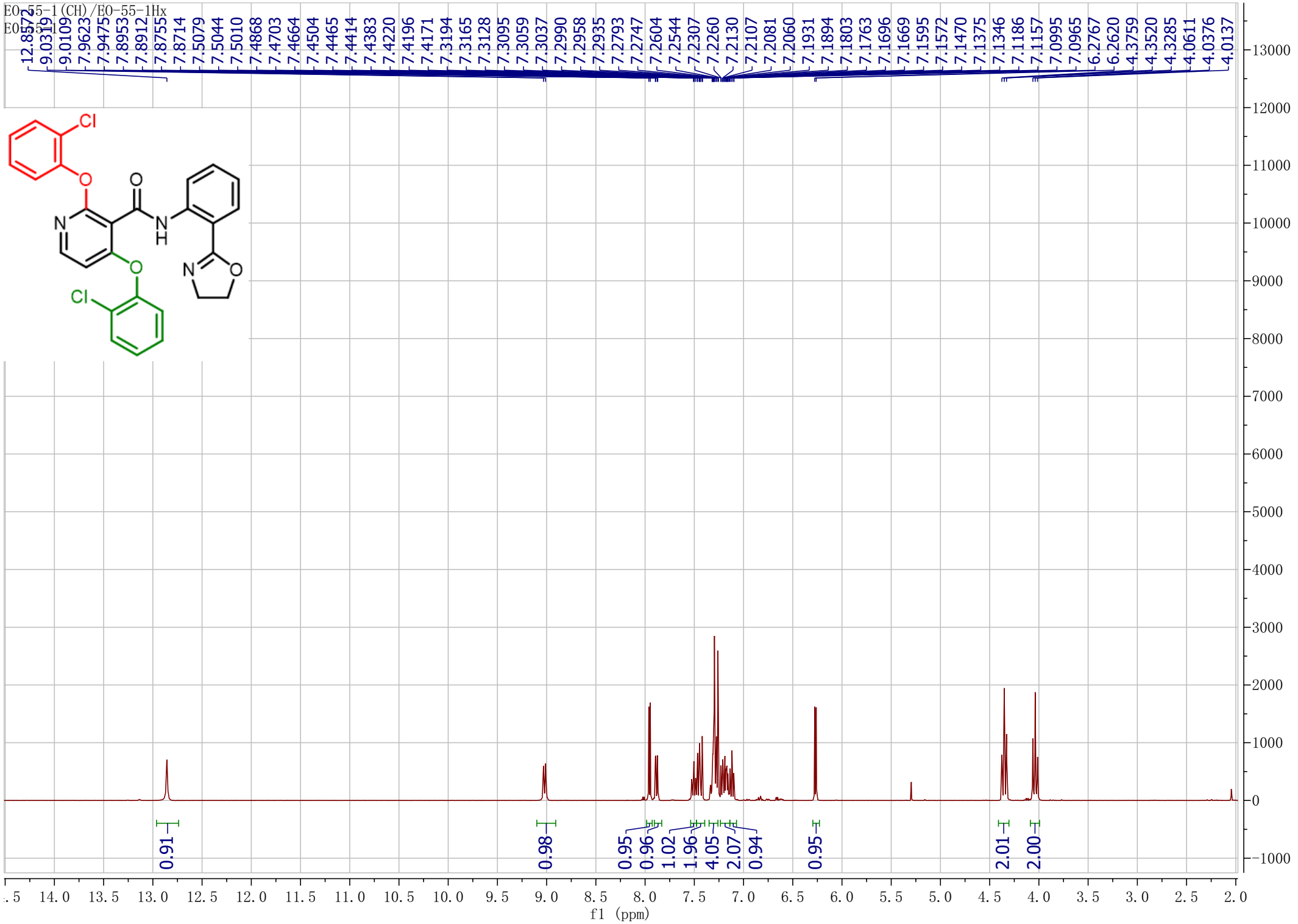


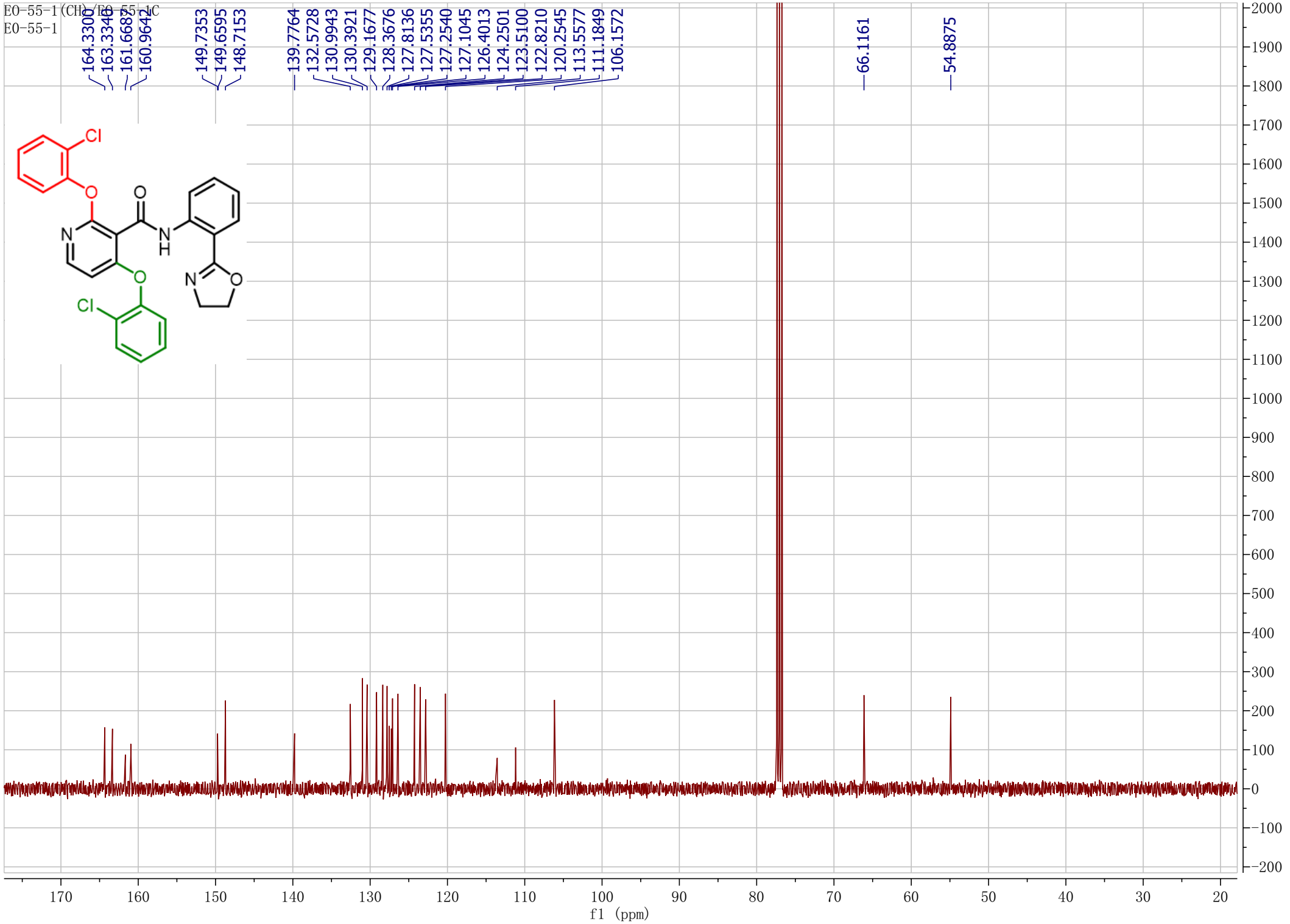
164.6908
164.4190
161.7649
161.6862
161.3085
160.9508
158.8752
158.5355
149.9963
149.4476
148.8757
139.6994
132.7405
129.3000
123.1975
123.1139
122.9048
122.5954
122.5111
120.0944
116.9121
116.6782
116.2007
115.9678
113.3555
111.7965
106.6303
66.1004
54.8809

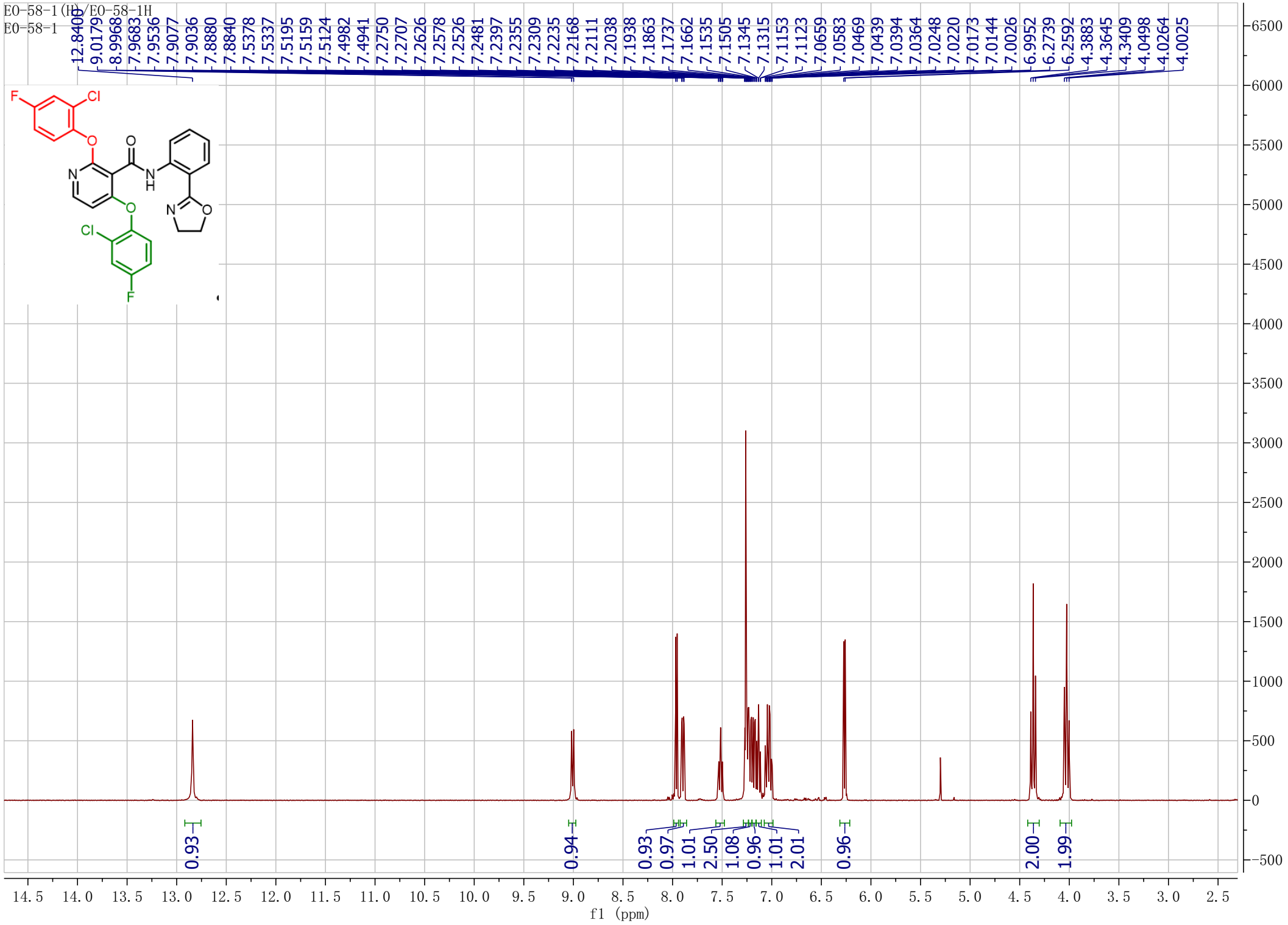
f1 (ppm)

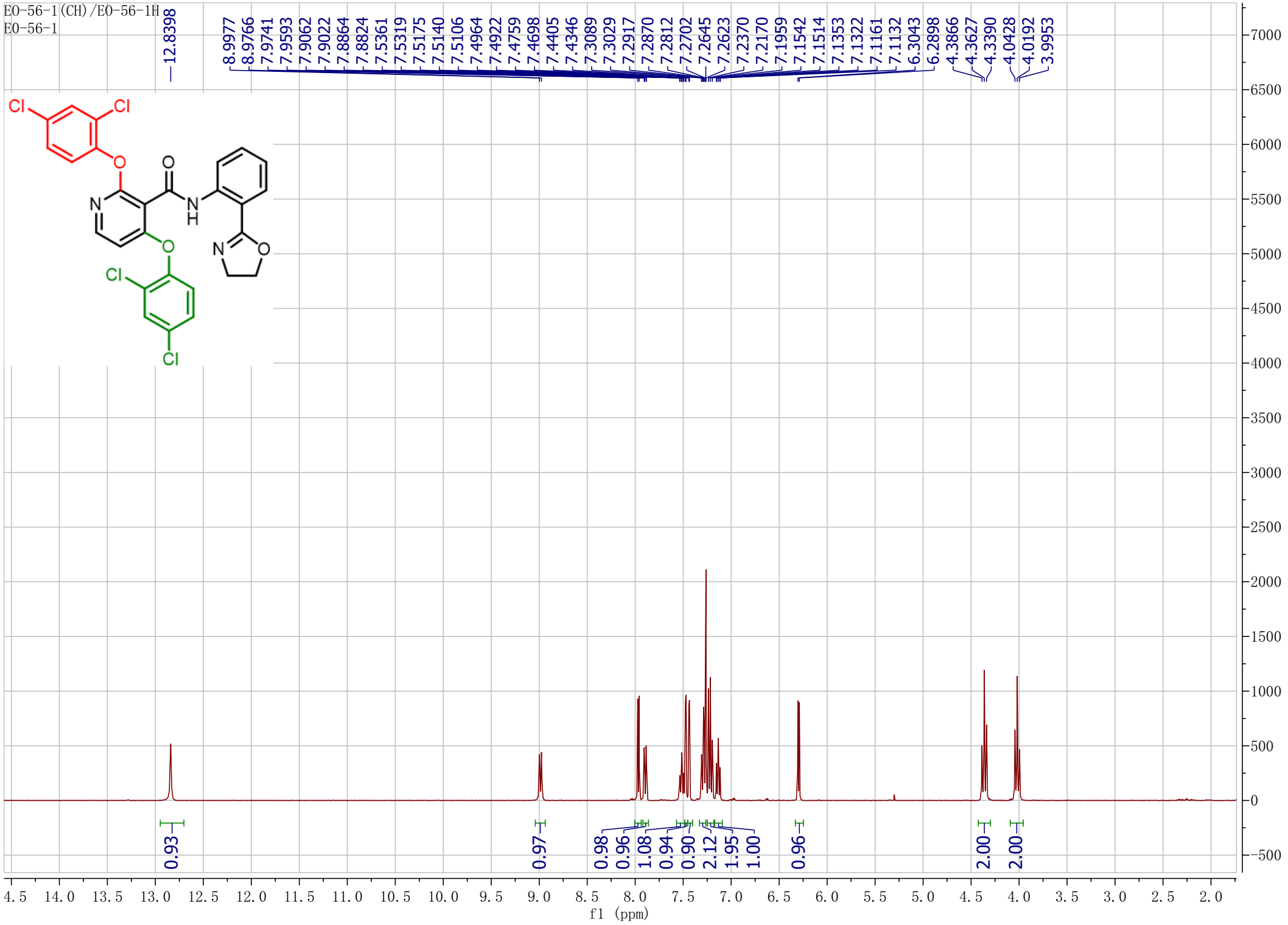

EO-2-2CH/EO-2-2
Z-
12.659
9.0468
9.0255
7.9046
7.8899
7.8725
7.8684
7.8527
7.8487
7.4770
7.4734
7.4699
7.2616
7.1036
7.1004
7.0956
7.0845
7.0813
7.0761
7.0654
7.0623
7.0562
6.7945
6.7896
6.7827
6.7780
6.7684
6.7632
6.7579
6.2648
6.2500
5.9878
5.9745
5.9709
5.9635
5.9576
5.9438
5.9322
5.1250
5.1207
5.1165
5.1128
5.1101
5.1063
5.0887
5.0855
5.0816
5.0777
5.0735
5.0694
5.0636
5.0601
5.0555
4.3696
4.3458
4.3222
4.0996
4.0762
4.0523
3.9176
3.7641
3.7428
3.3823
3.3656
0.96
0.94
2.01
1.02
3.03
4.25
0.98
2.33
4.12
2.00
2.02
6.18
4.45
f1 (ppm)


EO-2-26H/EO-2-26
z-2
164.4093
164.3780
162.2900
161.7776
151.6732
151.5005
148.4638
141.0416
140.9023
140.0061
138.9052
137.8951
137.6547
137.2827
136.9985
132.4890
129.0750
123.0968
122.9189
122.6407
122.4743
121.1277
120.8824
120.3785
116.2379
115.9710
113.5516
113.4775
105.7812
66.0051
56.1384
55.9846
54.9847
40.1145
40.0274
O
O
O
N
H
N
O
N
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)


EO-55-1(CH)/EO-55-1Hx
EO-55-1
12.8572
9.0319
9.0109
7.9623
7.9475
7.8953
7.8912
7.8755
7.8714
7.5079
7.5044
7.5010
7.4868
7.4703
7.4664
7.4504
7.4465
7.4414
7.4383
7.4220
7.4196
7.4171
7.3194
7.3165
7.3128
7.3095
7.3059
7.3037
7.2990
7.2958
7.2935
7.2793
7.2747
7.2604
7.2544
7.2307
7.2260
7.2130
7.2107
7.2081
7.2060
7.1931
7.1894
7.1803
7.1763
7.1696
7.1669
7.1595
7.1572
7.1470
7.1375
7.1346
7.1186
7.1157
7.0995
7.0965
6.2767
6.2620
4.3759
4.3520
4.3285
4.0611
4.0376
4.0137
Cl
O
O
N
N
H
O
N
O
Cl
0.91
0.98
0.95
0.96
1.02
1.96
4.05
2.07
0.94
0.95
2.01
2.00
f1 (ppm)


EO-55-1(CH)/EO-55-1C
EO-55-1
164.3300
163.3346
161.6685
160.9642
149.7353
149.6595
148.7153
139.7764
132.5728
130.9943
130.3921
129.1677
128.3676
127.8136
127.5355
127.2540
127.1045
126.4013
124.2501
123.5100
122.8210
120.2545
113.5577
111.1849
106.1572
66.1161
54.8875
Cl
O
O
N
O
N
H
N
O
Cl
f1 (ppm)


EO-58-1(H)/EO-58-1H
EO-58-1
12.8400
9.0179
8.9968
7.9683
7.9536
7.9077
7.9036
7.8880
7.8840
7.5378
7.5337
7.5195
7.5159
7.5124
7.4982
7.4941
7.2750
7.2707
7.2626
7.2578
7.2526
7.2481
7.2397
7.2355
7.2309
7.2235
7.2168
7.2111
7.2038
7.1938
7.1863
7.1737
7.1662
7.1535
7.1505
7.1345
7.1315
7.1153
7.1123
7.0659
7.0583
7.0469
7.0439
7.0394
7.0364
7.0248
7.0220
7.0173
7.0144
7.0026
6.9952
6.2739
6.2592
4.3883
4.3645
4.3409
4.0498
4.0264
4.0025
F
Cl
O
N
H
O
N
O
O
Cl
F
0.93
0.94
0.93
0.97
1.01
2.50
1.08
0.96
1.01
2.01
0.96
2.00
1.99
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)


EO-56-1(CH)/EO-56-1H
EO-56-1
12.8398
8.9977
8.9766
7.9741
7.9593
7.9062
7.9022
7.8864
7.8824
7.5361
7.5319
7.5175
7.5140
7.5106
7.4964
7.4922
7.4759
7.4698
7.4405
7.4346
7.3089
7.3029
7.2917
7.2870
7.2812
7.2702
7.2645
7.2623
7.2370
7.2170
7.1959
7.1542
7.1514
7.1353
7.1322
7.1161
7.1132
6.3043
6.2898
4.3866
4.3627
4.3390
4.0428
4.0192
3.9953
Cl
Cl
O
N
O
N
H
O
N
O
Cl
Cl
0.93
0.97
0.98
0.96
1.08
0.94
0.90
2.12
1.95
1.00
0.96
2.00
2.00
f1 (ppm)