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Supporting Information

For

Copper Catalyzed C-H Amination with Oximes: En Route to Primary Anilines

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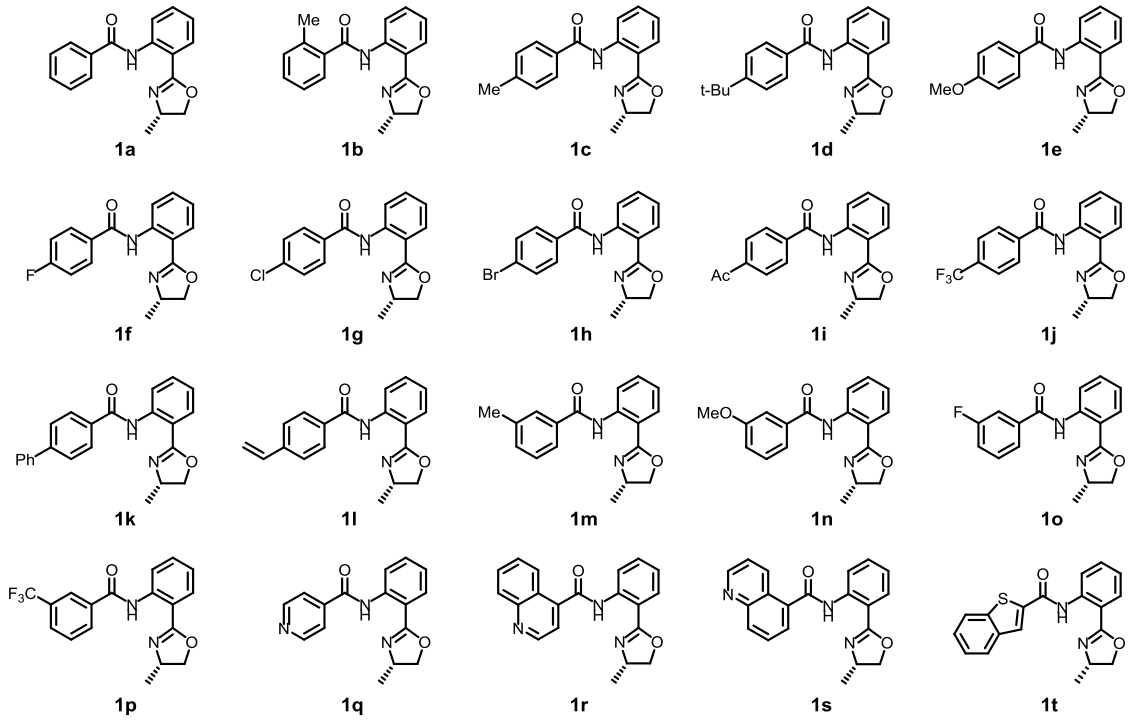
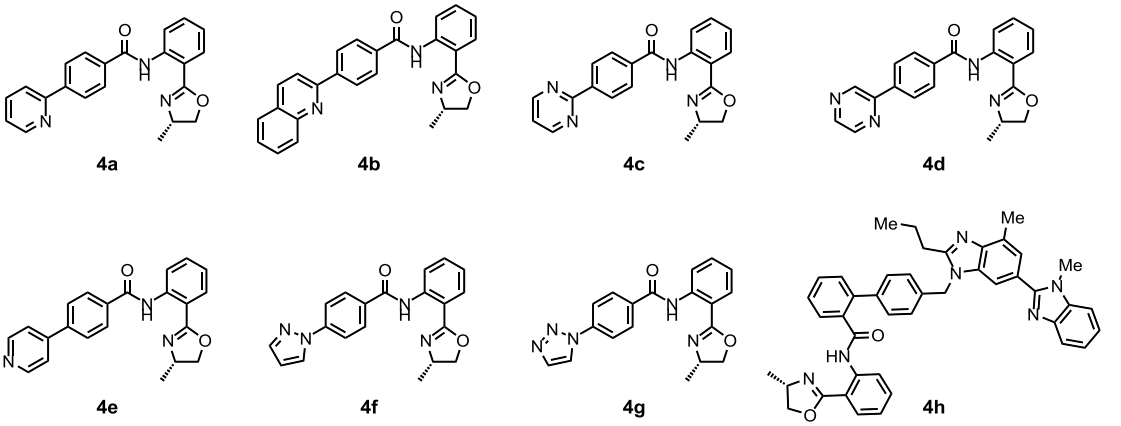
1. General Information

All commercial reagents were purchased from TCI, Sigma-Aldrich, Adamas-beta, 9-Ding chemistry and Energy Chemical of the highest purity grade. They were used without further purification unless specified. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AVANCE III 400，Bruker AVANCE III 500 and Bruker AVANCE III 600 (400 MHz，125 MHz and 150 MHz, respectively) instruments. ^{19}F NMR spectra were recorded on Bruker AVANCE III 500 instrument and are reported relative to the $CFCl_3$ as the internal standard. The peaks were internally referenced to TMS (0.00 ppm) or residual undeuterated solvent signal. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad. High resolution mass spectra were recorded at the Center for Mass Spectrometry, Shanghai Institute of Organic Chemistry and Shanghai Institute of Material Medica.

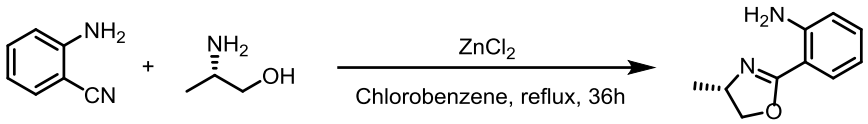
2. Experimental Section

2.1.1 Preparation of Substrates 1a-1t, 4a-4h.



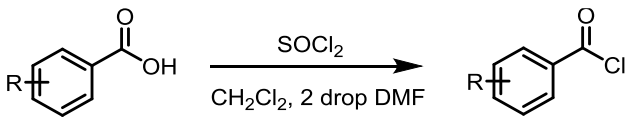


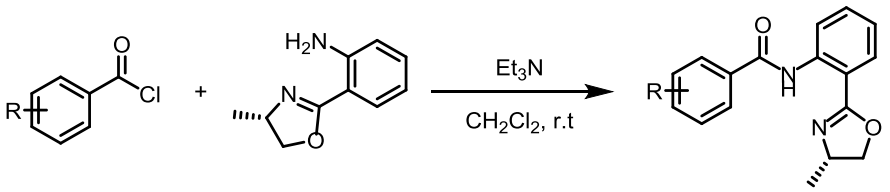
2.1.2 Synthesis of (*S*)-2-(4-methyl-4,5-dihydrooxazol-2-yl)aniline.[1,2]



2-aminobenzonitrile (19.8 g, 168 mmol) and $ZnCl_2$ (2.32 g, 17 mmol) was added to a 500 mL three-necked flask, and then suspended in chlorobenzene (240 mL) under nitrogen. L-Alaninol (39.2 ml, 504 mmol) was added to the suspension via a syringe. The mixture was slowly heated to reflux until no gas was produced. After refluxing for 36 hours, the reaction mixture was cooled down to room temperature and the solvent was removed in a rotary evaporator. CH_2Cl_2 (250 mL) was added to the residue and washed with saturated $NaHCO_3$ (150 mL) and H_2O (150 mL). The aqueous fraction was extracted with CH_2Cl_2 (250 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and the solvent was removed in a rotary evaporator. The crude product was purified by flash column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate to give yellow oil of the compound (*S*)-2-(4-methyl-4,5-dihydrooxazol -2-yl)aniline 23.4 g (79%).

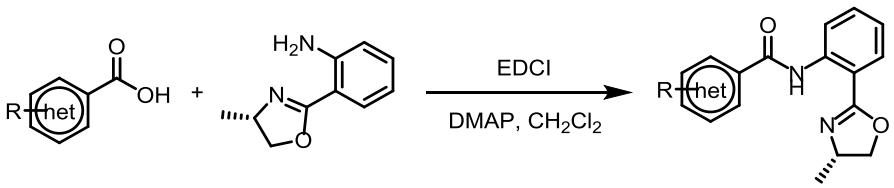
2.1.3 Preparation of Substrates 1a-1p.





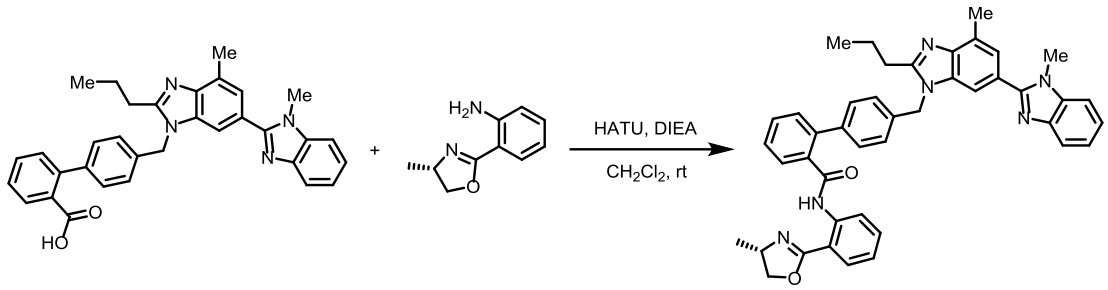
An acid chloride (5 mmol), prepared from the corresponding carboxylic acid and thionyl chloride and (*S*)-2-(4-methyl-4,5-dihydrooxazol-2-yl)aniline (5 mmol) were added to a 50 mL flask and then dissolved with CH_2Cl_2 (15 mL). Et_3N (7.5 mmol) was taken to the vigorously stirred solution via a syringe. The reaction mixture was stirred at room temperature for 6 h and quenched with saturated $NaHCO_3$. H_2O (100 mL) was added to the mixture and extracted with CH_2Cl_2 (50 mL x 3). Combined organic phase was washed with saturated NaCl (aq) and dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator. The crude product was purified by flash column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate to give colorless crystals of the product with the yield from 70% to 95%.

2.1.4 Preparation of Substrates 1q-1t, 4a-4g.[3]



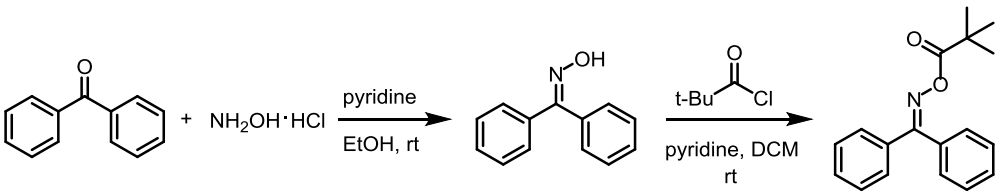
A heterocycle carboxylic acid (4 mmol) and (*S*)-2-(4-methyl-4,5-dihydrooxazol-2-yl)aniline (3 mmol) were taken to a 50 mL flask and dissolved with CH_2Cl_2 (20 mL). DMAP (0.5 mmol) and EDCI (6 mmol) were added to the mixture under ice bath and then stirred for 24 h at room temperature. Saturated $NaHCO_3$ was added to the mixture to quench reaction and then extracted with CH_2Cl_2 (50 mL x 3). Combined organic phase was washed with saturated NaCl (aq) and dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator. The crude product was purified by flash column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate with with the yield from 55% to 90%.

2.1.5 Preparation of Substrate 4h.[4]



Telmisartan (3 mmol) and DIEA (4.5 mmol) were dispersed with CH_2Cl_2 (15 mL) in a 50 mL flask. After the suspension turned transparent, HATU (4.5 mmol) was added.The solvent was stirred for 2 hours before (*S*)-2-(4-methyl-4,5dihydrooxazol -2-yl)aniline (4.5 mmol) was added, then stirred for another 8 hours at room temperature. Saturated $NaHCO_3$ was added to the mixture to quench reaction and then extracted with CH_2Cl_2 (30 mL x 3). Combined organic phase was washed with saturated NaCl (aq) and dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator. The crude product was purified by flash column chromatography on aluminum oxide with a gradient eluent of petroleum ether and ethyl acetate with the yield 75%.

2.1.6 Preparation of Aminated Agent 2a.[5]



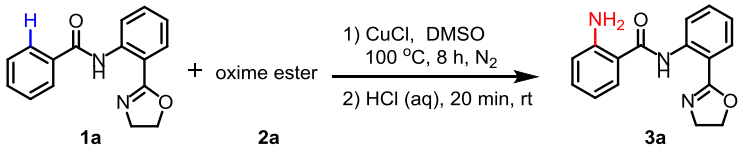
Hydroxylamine hydrochloride (2.86 g, 1.5 equiv) and pyridine (4.4 mL, 2.0 equiv) were added to the diphenylmethanone (5 g, 27.44 mmol) in 30 mL EtOH and the mixture was stirred at room temperature for 8 hours. The solvent was removed in vacuo and the resulting residue was dissolved in 20 mL DCM and washed with Dilute hydrochloric acid. Aqueous phase was extracted with CH_2Cl_2 three times, combined organic phase was washed with Saturated $NaHCO_3$ and brine, dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator. The crude product was dissolved in 30 mL DCM and cooled to 0 ℃. After the addition of pyridine (2.4 mL, 1.1 equiv), pivaloyl chloride (3.7 mL, 1.1 equiv) was added dropwise at 0 ℃. The mixture was stirred at room temperature overnight and quenched with water. The

aqueous layer was extracted with DCM three times and the combined organic layers were washed with saturated $NaHCO_3$ and brine, dried over Na_2SO_4, filtered and concentrated in vacuo. The crude product was recrystallized from DCM/Hexane to give colorless crystals of the product with 93% yield (7.2 g).

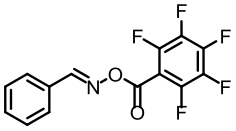
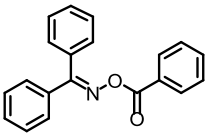
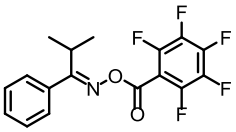
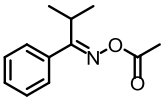
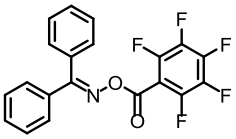
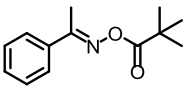
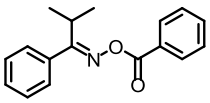
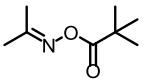
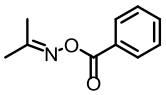
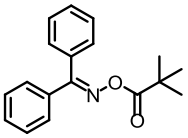
2.2 Optimization Studies

The reaction tube was directly placed into a pre-heated 90 ^oC oil bath.

Table S1. Screening of Oxime Esters.[a]

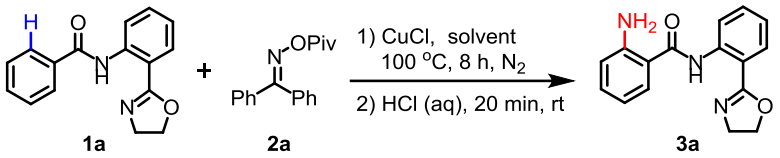


1a **2a** **3a**

entry	**2a**	Yield (%)	entry	**2a**	Yield (%)
1		trace	6		17
2		trace	7		trace
3		trace	8		N.R.
4		trace	9		N.R.
5		N.R.	10		25

[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuCl (20 mol %), DMSO (1 mL), 100 ^oC, 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). The yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as internal standard.

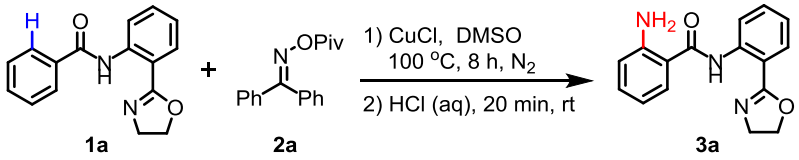
Table S2. Screening of the Solvents.[a]



entry	solvent	Yield (%)	entry	solvent	Yield (%)
1	DMSO	25	7	Chlorobenzene	N.R.
2	DMF	19	8	DMA	8
3	1,4-Dioxane	5	9	DMP	N.R.
4	CH_3CN	trace	10	THF	N.R.
5	HFIP	N.R.	11	Toluene	N.R.
6	DCE	N.R.	12	50%DMSO+50%DMF	24

[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuCl (20 mol %), solvent (1 mL), 100 °C, 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as internal standard.

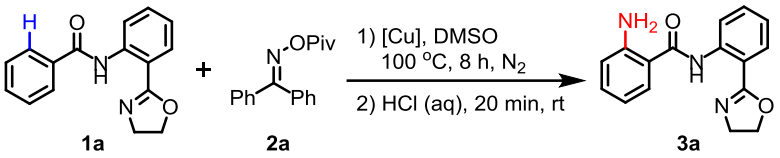
Table S3. The Effect of Concentration.[a]



entry	DMSO(mL)	Yield (%)
1	0.5	23
2	1	25
3	2	21
4	3	16
5	5	5

[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuCl (20 mol %), DMSO (x mL), 100 °C, 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as internal standard.

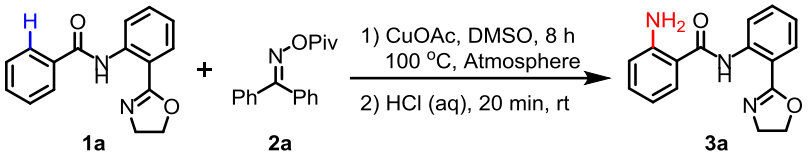
Table S4. Screening of the Copper Salts.[a]



entry	[Cu]	Yield (%)
1	Cu_2O	10
2	$CuBr{\cdot}SMe_2$	17
3	CuOAc	28
4	$Cu(OAc)_2$	21
5	CuI	21
6	CuBr	24
7	CuCl	25

[a] **1a** (0.1 mmol), **2a** (0.15 mmol), [Cu] (20 mol %), DMSO (1 mL), 100 °C, 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as internal standard.

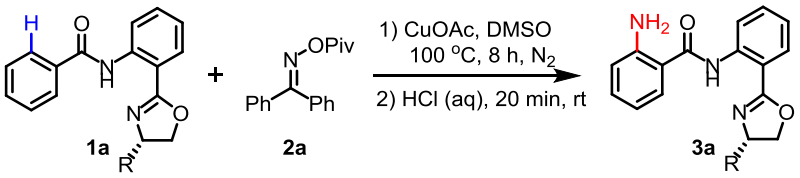
Table S5. The Effect of Atmosphere.[a]



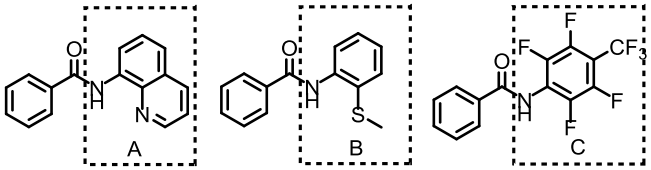
entry	Atmosphere	yield(%)
1	N_2	28
2	Air	25

[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuOAc (20 mol %), DMSO (1 mL), 100 °C, 8 h, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as internal standard.

Table S6. Screening of Directing Group.[a]



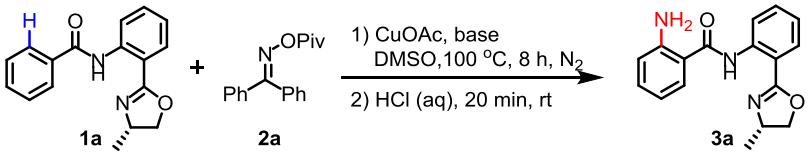
R=H	28%
R=Me	35%
R=^{i}Pr	20%
R=^{t}Bu	20%
R=Ph	26%
R=Bn	21%



N.R. N.R. N.R.

[a] **1a** (0.1 mmol), **2a** (0.15 mmol), CuOAc (20 mol %), DMSO (1 mL), 100 °C, 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as internal standard.

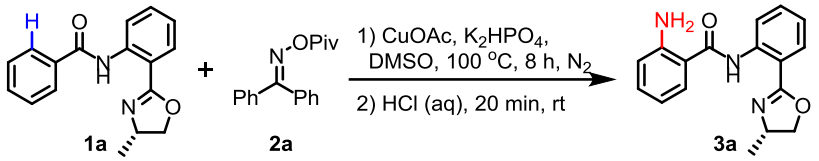
Table S7. Screening of Bases.[a]



entry	base	yield(%)	entry	base	yield(%)
1	Na_2CO_3	39	8	KH_2PO_4	42
2	K_2CO_3	16	9	NaOAc	41
3	Cs_2CO_3	0	10	NaF	40
4	$NaHCO_3$	36	11	KF	32
5	$KHCO_3$	37	12	CsF	35
6	K_3PO_4	35	13	Py	9
7	K_2HPO_4	46	14	---	40

[a] **1a** (0.1 mmol), **2a** (0.15 mmol), CuOAc (30 mol %), base (0.1 mmol), DMSO (1 mL), 100 °C, 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). The yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as internal standard.

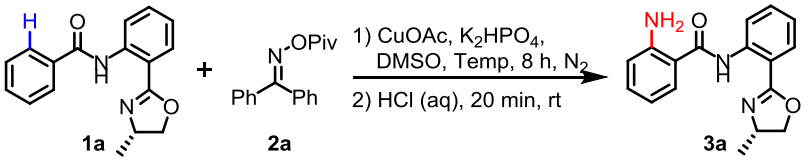
Table S8. Screening of Amount of CuOAc.[a]



entry	Cu	Yield (%)
1	0.2 eq	38
2	0.3 eq	46
3	0.6 eq	50
4	1.0 eq	52
5	1.5 eq	58

[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuOAc (x mmol), K_2HPO_4 (0.1 mmol), DMSO (1 mL), 100 °C , 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as internal standard.

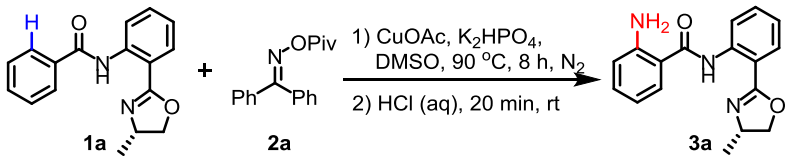
Table S9. Screening of Temperature.[a]



entry	Temp (°C)	Yield (%)
1	70	59
2	80	67
3	90	78
4	100	58

[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuOAc (0.15 mmol), DMSO (1 mL), K_2HPO_4 (0.1mmol), 8 h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as internal standard.

Table S10. Screening of Amount of 2a.[a]



entry	2a	Yield (%)
1	1.0 eq	68
2	1.5 eq	78
3	2.0 eq	64
4	3.0 eq	59

[a]**1a** (0.1 mmol), **2a** (x mmol), CuOAc (0.15 mol), K_2HPO_4 (0.1 mol), DMSO (1 mL), 90 °C, 8h, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as internal standard.

Table S11. Screening of Time.[a]

entry	t (h)	Yield (%)
1	8	38
2	10	45
3	12	49
4	14	48

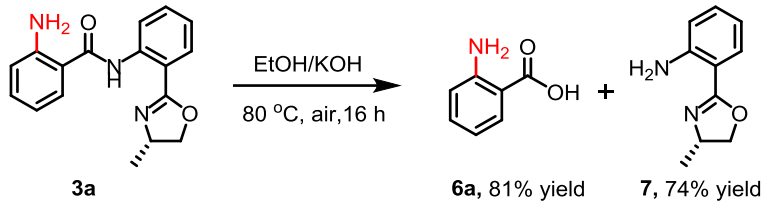
[a]**1a** (0.1 mmol), **2a** (0.15 mmol), CuOAc (30 mol %), K_2HPO_4 (0.1 mol), DMSO (1 mL), 90 °C, N_2, HCl (aq, 2 mol/L, 2 mL). the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as internal standard.

2.3 Typical Procedures for Copper Catalyzed Primary Amination of Aryl C–H Bond

To a 25 mL sealed tube was added substrates **1** (0.1 mmol, 1 equiv), CuOAc (0.15 mmol), K_2HPO_4 (0.1 mmol), DMSO (1 mL) and **2a** (0.15 mmol). The reaction tube was placed into a pre-heated oil bath and stirred at 90 °C for 8 h under N_2. Upon completion, 2 mL 2N HCl was added after cooling to room temperature. The resulting mixture was stirred at room temperature for 20 mins under air atmosphere before it was quenched with

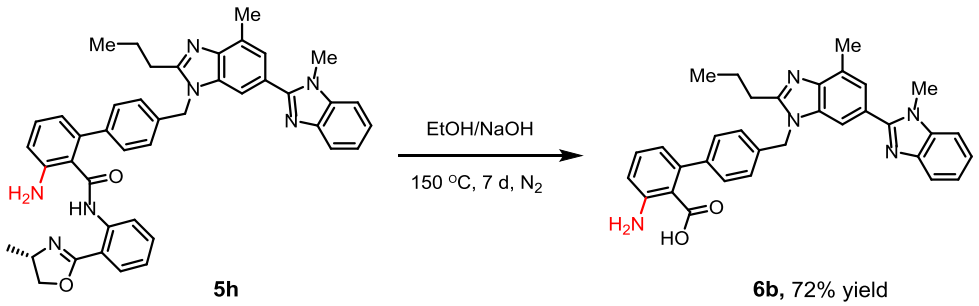
the addition of 2N NaOH (2 mL). Then EtOAc was added to dilute the mixture and washed with $NH_3 \cdot H_2O$ and saturated NaCl(aq). The organic fraction was dried over anhydrous Na_2SO_4, evaporated and the residue purified by a silica gel packed flash chromatography column, using ethyl acetate/hexane as the eluent.

2.4 Typical Procedure for Directing Group Removal.[6]



3a **6a**, 81% yield **7**, 74% yield

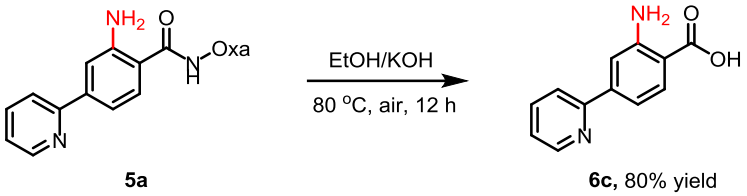
To a 50 mL round-bottomed flask was added **3a** (188 mg, 0.64 mmol), KOH (1428 mg, 25.5 mmol), EtOH (13 mL). The reaction mixture was stirred at 80 °C for 16 h under air. After completion, evaporated to remove solvent, and added EtOAc (40 mL x 3) to extract. The organic phase was dried over Na_2SO_4 evaporated and purified by flash column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate to recovery Directing Group **7** with a yield of 74% (83 mg). The water fraction was acidated with 1N HCl to PH 4~5, and then extracted with EtOAc. The organic fraction was dried over Na_2SO_4 evaporated and purified by flash column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate to get hydrolysis product **6a** with a yield of 81% (71 mg).



5h **6b**, 72% yield

To a 25 mL sealed tube was added **5h** (27.5 mg, 0.04 mmol), NaOH (160 mg, 4.0 mmol), EtOH (2 mL). The reaction mixture was stirred at 150 °C for 7 days under N_2. After completion, evaporated to remove solvent, diluted HCl solution was added to the

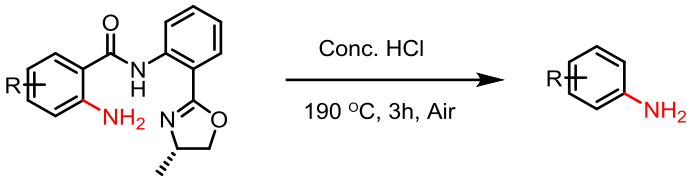
reaction mixture until pH is around 7, then the product was retracted from aqueous phase with dichloromethane and ethyl acetate. Organic fraction was dried over Na_2SO_4, evaporated and a crude product was obtained. The product was purified with flash column chromatography on silica gel (DCM:MeOH:HOAc = 10:1:0.2) to get hydrolysis product **6b** with a yield of 72% (15.2 mg).



5a **6c**, 80% yield

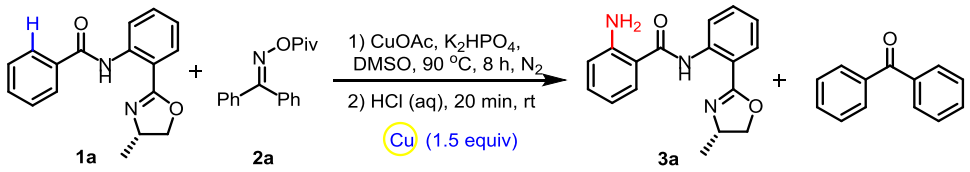
To a 15 mL sealed tube was added substrate **5a** (11.2 mg, 0.03 mmol), KOH (67.2 mg, 1.2 mmol), EtOH (0.5 ml). The reaction mixture was stirred at 80 °C for 12 h under air. Upon completion, 1N hydrochloric acid was added to acidify the mixture to around pH 7.0 and then extracted with dichloromethane. The organic fraction was dried over Na_2SO_4, evaporated and purified by flash column chromatography on silica gel (DCM:EtOAc:HCOOH = 3:1:0.03) to get hydrolysis product **6c** with a yield of 80% (5.1 mg).

2.5 Typical Procedure for Preparation of Aniline derivatives

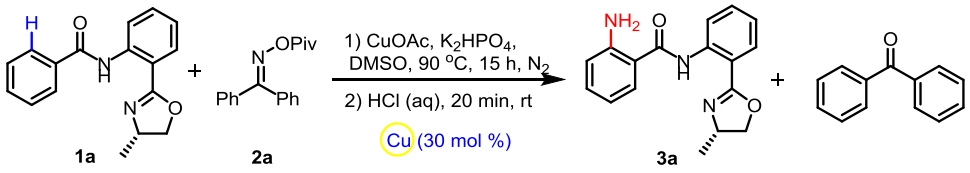


To a 15 mL sealed tube was added substrates **3 or 5** (0.03 mmol), conc.HCl (0.5 ml). The reaction mixture was stirred at 190 °C for 3 h under air. Upon completion, diluted NaOH solution was added to the reaction mixture until pH is around 9, then the product was retracted from aqueous phase with dichloromethane. Organic fraction was dried over Na_2SO_4, evaporated and a crude product was obtained. The product was purified by a silica gel packed flash chromatography column.

2.6 Typical Procedure for Gram-Scale Reaction.



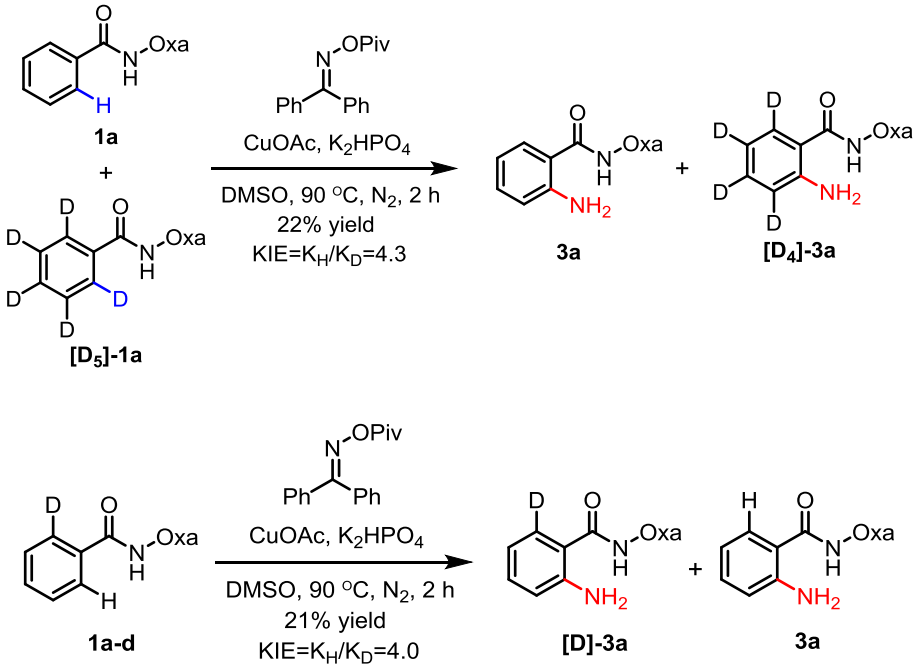
To a 250 mL sealed tube was added substrates **1a** (1.0 g, 3.57 mmol), CuOAc (656 mg, 5.36 mmol), K_2HPO_4 (621 mg, 3.57 mmol), **2a** (1.05 g, 3.57 mmol). and DMSO (18 mL) The reaction tube was placed into a pre-heated oil bath and stirred at 90 ^oC for 8 h under N_2. Upon completion, 36 mL 2N HCl was added after cooling to room temperature. The resulting mixture was stirred at room temperature for 40 min under air atmosphere before it was quenched with the addition of 2N NaOH (36 mL). Then EtOAc was added to dilute the mixture and washed with NH_3 H_2O and saturated NaCl (aq), Aqueous phase was extracted with EtOAc three times. Combined organic phase was washed with brine, dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator and purified by a silica gel packed flash chromatography column, using ethyl acetate/hexane as the eluent to afford the product **3a** with 62% yield (652 mg) and diphenylmethanone 91% yield (886 mg).



To a 250 mL sealed tube was added substrates **1a** (1.0 g, 3.57 mmol), CuOAc (131.3 mg, 1.67 mmol), K_2HPO_4 (621 mg, 3.57 mmol), **2a** (1.05 g, 3.57 mmol). and DMSO (18 mL) The reaction tube was placed into a pre-heated oil bath and stirred at 90 ^oC for 15 h under N_2. Upon completion, 36 mL 2N HCl was added after cooling to room temperature. The resulting mixture was stirred at room temperature for 40 min under air atmosphere before it was quenched with the addition of 2N NaOH (36 mL). Then EtOAc was added to dilute the mixture and washed with NH_3 H_2O and saturated NaCl (aq), Aqueous phase was extracted with EtOAc three times. Combined organic phase was washed with brine, dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator and purified by a silica gel packed flash chromatography column, using ethyl acetate/hexane as the eluent to afford the product **3a** with 45% yield (472 mg) and

diphenylmethanone 71% yield (688 mg).

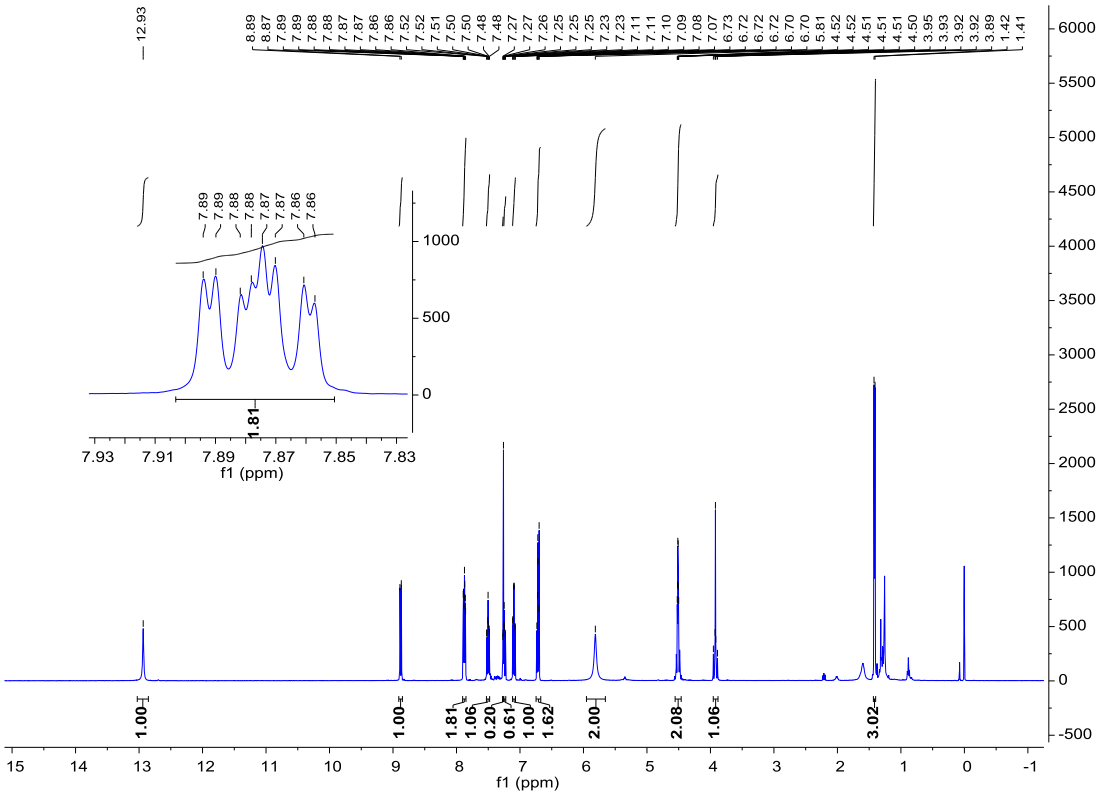
2.7 Procedure for Kinetic Isotope Effect Experiments



A. Intermolecular competition experiment between 1a and[D_5]-1a:

To a 25 mL sealed tube was added substrates (*S*)-N-(2-(4-methyl-4,5-dihydrooxazol -2-yl)phenyl)benzamide **1a** (0.05 mmol, 1 equiv), (*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide-2,3,4,5-d_4 **[D_5]-1a** (0.05 mmol, 1 equiv), CuOAc (0.15 mmol), K_2HPO_4 (0.1 mmol), DMSO (1 mL). Then the tube was placed into a pre-heated oil bath (90 ^oC) and stired for 2 h. Upon completion, 2 mL 2 N HCl was added after cooling to room temperature. The resulting mixture was stirred at room temperature for 20 min under air atmosphere before it was quenched with the addition of 2 N NaOH (2 mL). EtOAc was added to dilute the mixture and then washed with $NH_3 \cdot H_2O$ and saturated NaCl (aq). The organic fraction was dried over Na_2SO_4, evaporated and a mixture of product **3a** and **[D_4]-3a** was purified by flash column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. The distribution of **3a** and **[D_4]-3a** was calculated from the integrals of their respective ^1H NMR signals at 7.88 ppm (**3a** and **[D_4]-3a**) and 7.87 ppm (**3a**) (see Figure S1).

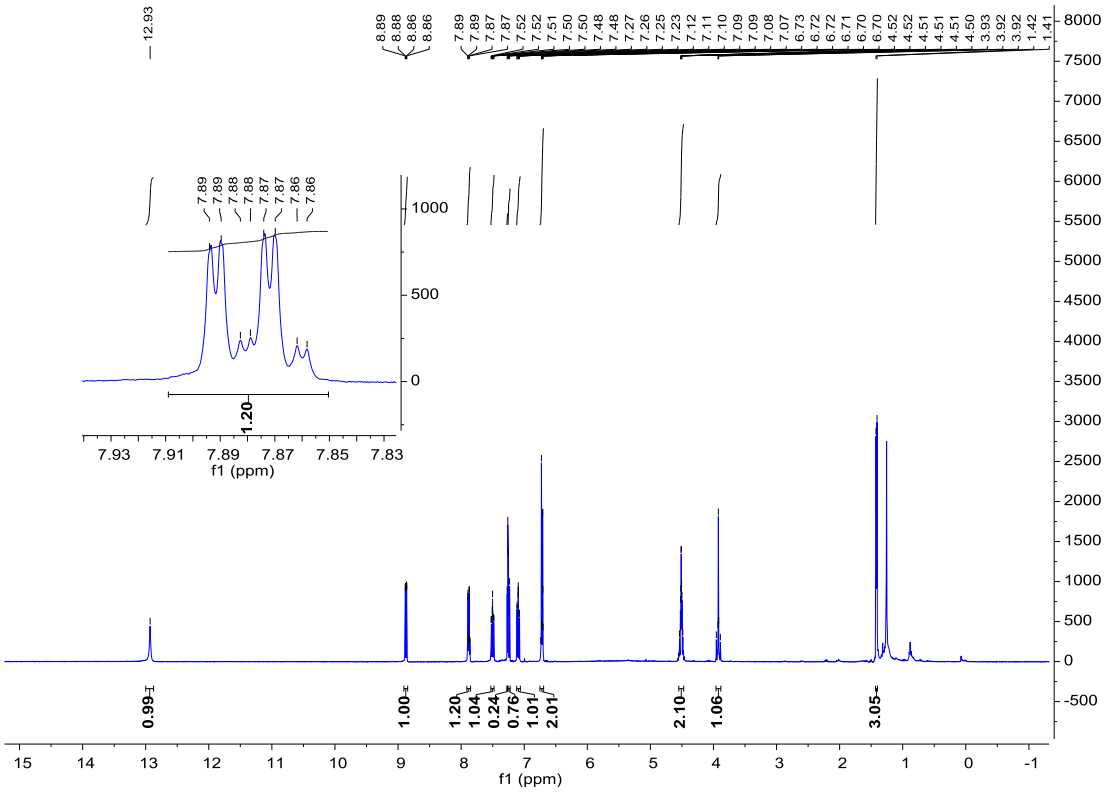
Figure S1. Detail of the ^{1}H NMR spectrum of the product mixture obtained in the intermolecular KIE experiment



B. **Intramolecular competition experiment between 1a and 1a-d:**

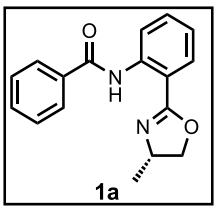
To a 25 mL sealed tube was added substrates (*S*)-N-(2-(4-methyl-4,5-dihydrooxazol -2-yl)phenyl)benzamide-2-d **1a-*d*** (0.1 mmol, 1 equiv), CuOAc (0.15 mmol), K_2HPO_4 (0.1 mmol), DMSO (1 mL). Then the tube was placed into a pre-heated oil bath (90 ^{o}C) and stired for 2 h. Upon completion, 2 mL 2N HCl was added after cooling to room temperature. The resulting mixture was stirred at room temperature for 20 min under air atmosphere before it was quenched with the addition of 2N NaOH (2 mL). EtOAc was added to dilute the mixture and then washed with $NH_3 \cdot H_2O$ and saturated NaCl (aq). The organic fraction was dried over Na_2SO_4, evaporated and a mixture of product **3a** and **[D]-3a** was purified by flash column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. The distribution of **3a** and **[D]-3a** was calculated from the integrals of their respective ^{1}H NMR signals at 7.88 ppm (**3a** and **[D]-3a**) and 7.87 ppm (**3a**) (see Figure S2).

Figure S2. Detail of the ^{1}H NMR spectrum of the product mixture obtained in the intramolecular KIE experiment



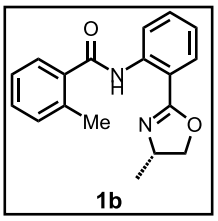
3. Analytical Data.

3.1 Characterization of Substrates.

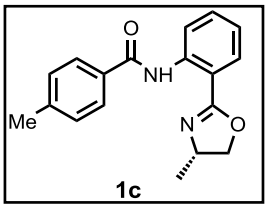


(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1a): white solid. Mp =101.2-102.6 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.14 (s, 1H), 8.98 (d, *J* = 8.4, 1H), 8.15 – 8.09 (m, 2H), 7.89 (dd, J = 7.9, 1.5 Hz, 1H), 7.58 – 7.46 (m, 4H), 7.14 – 7.07 (m, 1H), 4.59 – 4.45 (m, 2H), 3.97 – 3.87 (m, 1H), 1.43 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.98, 163.61, 140.20, 135.29, 132.61, 131.60, 129.15, 128.43, 127.71, 122.32, 119.71, 113.48, 72.68, 61.91, 21.45. **HRMS** (ESI-TOF) m/z Calcd for

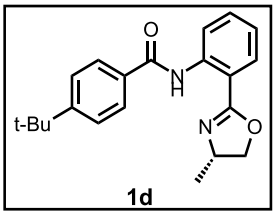
$C_{17}H_{16}N_2O_2$ $[M+H]^+$ 281.1285, found 281.1285.



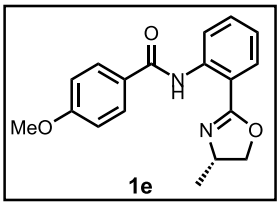
(*S*)-2-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1b): white solid. Mp =97.8-99.4 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.73 (s, 1H), 8.95 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 7.9, 1.6 Hz, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.57 – 7.47 (m, 1H), 7.39 – 7.32 (m, 1H), 7.31 – 7.23 (m, 2H), 7.17 – 7.07 (m, 1H), 4.51 – 4.23 (m, 2H), 3.88 (t, J = 7.6 Hz, 1H), 2.59 (s, 3H), 1.29 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.54, 163.30, 140.17, 137.32, 136.57, 132.49, 131.32, 130.10, 129.10, 127.54, 125.54, 122.33, 119.59, 113.41, 72.62, 61.82, 21.34, 20.35. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{18}N_2O_2$ $[M+H]^+$ 295.1441, found 295.1441.



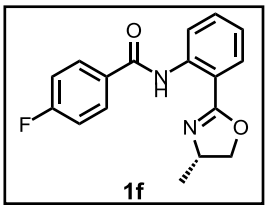
(*S*)-4-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1c): white solid. Mp =139.4-142.6 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.07 (s, 1H), 8.98 (dd, *J* = 8.5, 0.6 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 2H), 7.88 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.56 – 7.47 (m, 1H), 7.33 – 7.27 (m, 2H), 7.13 – 7.07 (m, 1H), 4.66 – 4.42 (m, 2H), 4.07 – 3.83 (m, 1H), 2.43 (s, 3H), 1.43 (d, J = 6.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$)δ 166.02, 163.66, 142.05, 140.38, 132.61, 132.58, 129.15, 127.77, 122.17, 119.74, 113.44, 72.70, 61.96, 21.46, 21.44. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{18}N_2O_2$ $[M+H]^+$ 295.1441, found 295.1441.



(*S*)-4-(tert-butyl)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1d): white solid. Mp =113.6-115.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.08 (s, 1H), 8.99 (dd, J = 8.5, 1.1 Hz, 1H), 8.10 – 8.04 (m, 2H), 7.89 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.53 – 7.49 (m, 3H), 7.10 (td, *J* = 7.9, 1.2 Hz, 1H), 4.63 – 4.46 (m, 2H), 4.00 – 3.89 (m, 1H), 1.46 (d, J = 6.3 Hz, 3H), 1.37 (s, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.95, 163.63, 155.11, 140.37, 132.62, 132.42, 129.16, 127.61, 125.41, 122.18, 119.75, 113.42, 72.68, 61.97, 34.94, 31.17, 21.60. **HRMS** (ESI-TOF) m/z Calcd for $C_{21}H_{24}N_2O_2$ $[M+H]^+$ 337.1910, found 337.1991.

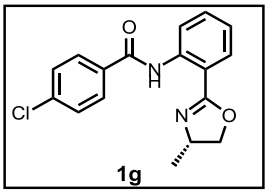


(*S*)-4-methoxy-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1e): white solid. Mp =132.8-134.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.01 (s, 1H), 8.95 (dd, J = 8.5, 1.2 Hz, 1H), 8.12 – 8.06 (m, 2H), 7.88 (dd, J = 7.9, 1.6 Hz, 1H), 7.51 (ddd, J = 8.7, 7.3, 1.7 Hz, 1H), 7.13 – 7.07 (m, 1H), 7.01 – 6.96 (m, 2H), 4.58 – 4.49 (m, 2H), 3.98 – 3.91 (m, 1H), 3.89 (s, 3H), 1.44 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.67, 163.76, 162.37, 140.49, 132.67, 129.65, 129.18, 127.77, 122.10, 119.73, 113.69, 113.37, 72.71, 61.99, 55.43, 21.56. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{18}N_2O_3$ $[M+H]^+$ 311.1390, found 311.1390.



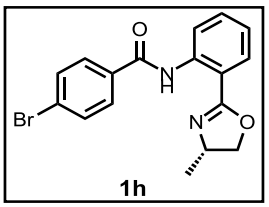
(*S*)-4-fluoro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1f): white solid. Mp =136.4-137.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.11 (s, 1H), 8.93 (d, *J* = 8.5 Hz, 1H), 8.18 – 8.09 (m, 2H), 7.93 – 7.86 (m, 1H), 7.52 (t, *J* = 7.9 Hz, 1H), 7.17 (t, *J* = 8.6 Hz, 2H), 7.12 (t, *J* = 7.6 Hz, 1H), 4.60 – 4.45 (m, 2H), 3.98 – 3.89 (m, 1H), 1.43 (d, *J* = 5.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.93, 164.92(d, J_{C-F} = 252.6 Hz), 163.84, 140.18, 132.74, 131.60(d, J_{C-F} = 2.9 Hz), 130.11(d, J_{C-F} = 9.0Hz) 129.25, 122.48,

119.76, 115.51 (d, J_{C-F} = 21.8 Hz), 113.52, 72.78, 61.96, 21.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{15}FN_2O_2$ $[M+H]^+$ 299.1191, found 299.1190.



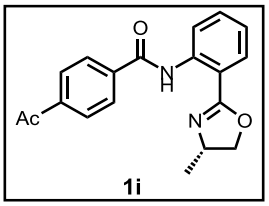
1g

(*S*)-4-chloro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1g): white solid. Mp =151.2-152.7 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.15 (s, 1H), 8.93 (dd, *J* = 8.5, 0.9 Hz, 1H), 8.10 – 8.04 (m, 2H), 7.89 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.49 – 7.44 (m, 2H), 7.16 – 7.09 (m, 1H), 4.59 – 4.51 (m, 2H), 4.00 – 3.89 (m, 1H), 1.43 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.90, 163.82, 140.08, 137.92, 133.82, 132.75, 129.25, 129.19, 128.75, 122.57, 119.77, 113.54, 72.78, 61.94, 21.51. **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{15}ClN_2O_2$ $[M+H]^+$ 315.0894, found 315.0895.



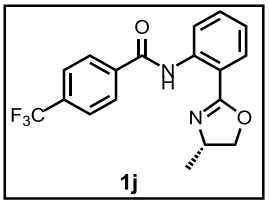
1h

(*S*)-4-bromo-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1h): white solid. Mp =150.9-152.4 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.16 (s, 1H), 8.93 (dd, *J* = 8.5, 0.9 Hz, 1H), 8.03 – 7.96 (m, 2H), 7.89 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.56 – 7.48 (m, 1H), 7.13 (td, *J* = 7.9, 1.2 Hz, 1H), 4.58 – 4.48 (m, 2H), 4.04 – 3.87 (m, 1H), 1.43 (d, *J* = 6.5, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.01, 163.81, 140.04, 134.27, 132.75, 131.73, 129.37, 129.25, 126.45, 122.60, 119.77, 113.55, 72.78, 61.93, 21.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{15}BrN_2O_2$ $[M+H]^+$ 359.0389, found 359.0390.



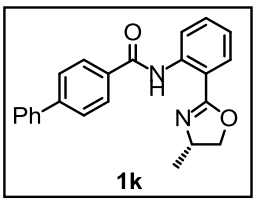
1i

(*S*)-4-acetyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1i): white solid. Mp =161.5-162.8 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.27 (s, 1H), 8.94 (d, *J* = 8.5 Hz, 1H), 8.20 (d, *J* = 8.3 Hz, 2H), 8.06 (d, *J* = 8.3 Hz, 2H), 7.89 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.57 – 7.48 (m, 1H), 7.18 – 7.10 (m, 1H), 4.59 – 4.48 (m, 2H), 4.03 – 3.86 (m, 1H), 2.66 (s, 3H), 1.44 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.55, 164.84, 163.74, 139.90, 139.22, 139.17, 132.71, 129.24, 128.39, 127.99, 122.74, 119.77, 113.63, 72.79, 61.91, 26.80, 21.50. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{18}N_2O_3$ $[M+H]^+$ 323.1389, found 323.1390.



1j

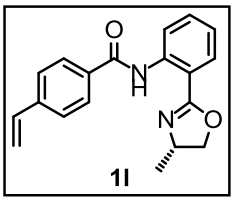
(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(trifluoromethyl)benzamide (1j): white solid. **^{1}** Mp =144.2-145.7 ºC. **H NMR** (400 MHz, $CDCl_3$) δ 13.28 (s, 1H), 8.94 (dd, *J* = 8.5, 1.0 Hz, 1H), 8.23 (d, *J* = 8.1 Hz, 2H), 7.90 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.59 – 7.50 (m, 1H), 7.19 – 7.11 (m, 1H), 4.61 – 4.48 (m, 2H), 4.04 – 3.88 (m, 1H), 1.44 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.54, 163.85, 139.88, 138.64, 133.26 (q, J_{C-F} = 33 Hz), 132.80, 129.30, 128.18, 125.51 (q, J_{C-F} = 3.8 Hz), 123.86 (q, J_{C-F} = 272.4 Hz), 122.85, 119.83, 113.67, 72.82, 61.93, 21.54. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{15}F_3N_2O_2$ $[M+H]^+$ 349.1158, found 349.1158.



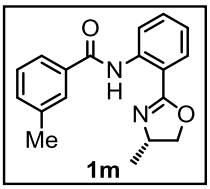
1k

(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-[1,1'-biphenyl]-4-carboxamide (1k): white solid. Mp =130.9-132.2 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.19 (s, 1H), 9.01 (d, *J* = 8.5 Hz, 1H), 8.26 – 8.16 (m, 2H), 7.91 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.77 – 7.71 (m, 2H), 7.69 – 7.64 (m, 2H), 7.54 (ddd, J = 8.7, 7.3, 1.6 Hz, 1H)., 7.51 – 7.45 (m, 2H), 7.43 – 7.38 (m, 1H), 7.13 (td, *J* = 7.9, 1.2 Hz, 1H), 4.73 – 4.42 (m, 2H), 4.31 – 3.72 (m, 1H), 1.46 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (151MHz, $CDCl_3$) δ 165.74, 163.70, 144.35,

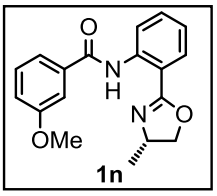
140.26, 140.05, 134.03, 132.67, 129.19, 128.86, 128.28, 127.94, 127.20, 127.13, 122.34, 119.75, 113.48, 72.72, 61.96, 21.54. **HRMS** (ESI-TOF) m/z Calcd for $C_{23}H_{20}N_2O_2$ $[M+H]^+$ 357.1596, found 357.1598.



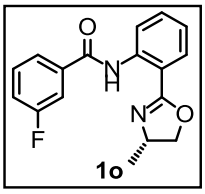
(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-vinylbenzamide (1l): white solid. Mp =123.1-124.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.13 (s, 1H), 8.97 (dd, *J* = 8.5, 1.0 Hz, 1H), 8.14 – 8.05 (m, 2H), 7.89 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.57 – 7.47 (m, 3H), 7.11 (ddd, *J* = 8.5, 7.7, 1.2 Hz, 1H), 6.78 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.88 (dd, *J* = 17.6, 0.7 Hz, 1H), 5.38 (dd, *J* = 10.9, 0.6 Hz, 1H), 4.63 – 4.46 (m, 2H), 3.99 – 3.89 (m, 1H), 1.44 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.63, 163.70, 140.72, 140.28, 136.04, 134.49, 132.65, 129.19, 128.07, 126.24, 122.32, 119.77, 115.92, 113.49, 72.73, 61.96, 21.51. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{18}N_2O_2$ $[M+H]^+$ 307.1440, found 307.1441.



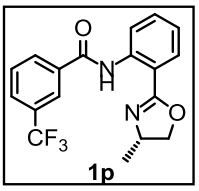
(*S*)-3-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1m): white solid. Mp =78.8-80.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.09 (s, 1H), 8.99 (d, *J* = 8.5 Hz, 1H), 7.99 – 7.85 (m, 3H), 7.57 – 7.47 (m, 1H), 7.43 – 7.32 (m, 2H), 7.16 – 7.05 (m, 1H), 4.60 – 4.44 (m, 2H), 3.99 – 3.89 (m, 1H), 2.45 (s, 3H), 1.45 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.18, 163.66, 140.32, 138.15, 135.31, 132.63, 132.33, 129.17, 128.38, 128.35, 124.91, 122.25, 119.74, 113.46, 72.69, 61.98, 21.45, 21.43. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{18}N_2O_2$ $[M+H]^+$ 295.1441, found 295.1441.



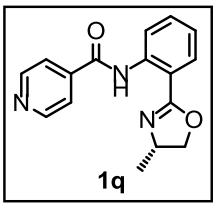
(*S*)-3-methoxy-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1n): white solid. Mp =77.4-78.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.11 (s, 1H), 8.97 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.89 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.76 – 7.65 (m, 2H), 7.58 – 7.48 (m, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.16 – 7.04 (m, 2H), 4.58 – 4.47 (m, 2H), 3.98 – 3.92 (m, 1H), 3.89 (s, 3H), 1.44 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.86, 163.65, 159.84, 140.20, 136.81, 132.67, 129.41, 129.20, 122.39, 119.78, 117.90, 113.54, 112.98, 72.74, 62.00, 55.43, 21.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{18}N_2O_3$ $[M+H]^+$ 311.1391, found 311.1391.



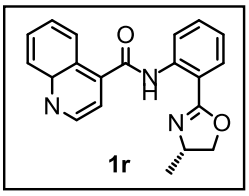
(*S*)-3-fluoro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (1o): white solid. Mp =180.1-181.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.13 (s, 1H), 8.86 – 8.74 (m, 1H), 7.81 – 7.77 (m, 1H), 7.77 – 7.72 (m, 1H), 7.56 (dd, *J* = 12.4, 4.6 Hz, 2H), 7.49 (td, *J* = 8.0, 5.6 Hz, 1H), 7.29 – 7.21 (m, 1H), 7.14 (td, *J* = 7.8, 1.1 Hz, 1H), 4.65 – 4.54 (m, 1H), 3.84 (dd, J = 11.2, 4.1 Hz, 1H), 3.68 (dd, J = 11.2, 3.4 Hz, 1H), 1.40 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.57, 164.19 (d, J_{C-F} = 2.1 Hz), 162.93 (d, J_{C-F} = 247.6 Hz), 139.91, 137.20 (d, J_{C-F} = 6.8 Hz), 133.12, 130.39 (d, J_{C-F} = 7.9 Hz), 126.58, 123.15,122.69 (d, J_{C-F} = 3.0 Hz), 121.64, 119.90, 118.85 (d, J_{C-F} = 21.5 Hz), 114.85 (d, J_{C-F} = 23.1 Hz), 49.21, 45.77, 17.93. **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{15}FN_2O_2$ $[M+H]^+$ 299.1192, found 299.1190.



(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-3-(trifluoromethyl)benzamide (1p): white solid. Mp =72.0-73.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.32 (s, 1H), 8.95 (dd, *J* = 8.5, 0.8 Hz, 1H), 8.41 (s, 1H), 8.33 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 7.9 Hz, 1H), 7.18 – 7.10 (m, 1H), 4.59 – 4.46 (m, 2H), 4.02 – 3.85 (m, 1H), 1.42 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$). δ 164.28, 163.80, 139.89, 136.10, 132.74, 131.50, 130.92 (q, J = 32.6 Hz), 129.29, 129.19, 128.15 (q, J = 3.7 Hz), 124.32 (q, J = 3.8 Hz), 123.89 (d, J = 272.3 Hz), 122.77, 119.74, 113.62, 72.84, 61.95, 21.25. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{15}F_3N_2O_2$ $[M+H]^+$ 349.1158, found 349.1158.

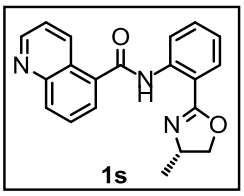


(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (1q): white solid. Mp =141.0-142.7 °C. **^{1}H NMR** (400 MHz,$CDCl_3$) δ 13.36 (s, 1H), 8.92 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.84 – 8.78 (m, 2H), 7.97 – 7.93 (m, 2H), 7.91 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.55 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.17 (m, *J* = 7.6, 1.2 Hz, 1H), 4.6 – 4.52 (m, 2H), 4.03 – 3.86 (m, 1H), 1.45 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.87, 163.80, 150.55, 142.39, 139.55, 132.80, 129.30, 123.09, 121.42, 119.86, 113.72, 72.83, 61.89, 21.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{16}H_{15}N_3O_2$ $[M+H]^+$ 282.1237, found 282.1237.

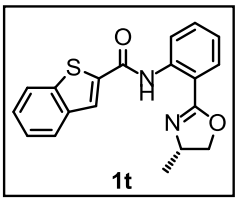


(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)quinoline-3-carboxamide (1r): white solid. Mp =130.0-131.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.20 (s, 1H), 9.02 (dd, *J* = 12.1, 6.4 Hz, 2H), 8.54 (d, *J* = 8.5 Hz, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 7.91 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.83 – 7.74 (m, 1H), 7.71 (d, *J* = 4.4 Hz, 1H), 7.61 (m, *J* = 19.5, 7.5 Hz, 2H), 7.19 (t, *J* = 7.6 Hz, 1H), 4.45 (t, *J* = 8.7 Hz, 1H), 4.31 (q, *J* = 8.2, 7.7 Hz, 1H), 3.88

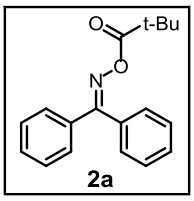
(t, *J* = 8.0 Hz, 1H), 1.20 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.86, 163.42, 149.78, 149.02, 142.08, 139.65, 132.73, 129.88, 129.78, 129.24, 127.57, 125.80, 124.77, 123.17, 119.86, 119.00, 113.70, 72.77, 61.73, 21.34. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{17}N_3O_2$ $[M+H]^+$ 332.1388, found 332.1394.



(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)quinoline-6-carboxamide (1s): white solid. Mp =143.0-144.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.11 (s, 1H), 9.06 (m, *J* = 8.6, 1.7, 0.9 Hz, 1H), 9.01 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.97 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.26 (m, *J* = 8.6, 1.1 Hz, 1H), 8.03 (dd, *J* = 7.2, 1.3 Hz, 1H), 7.91 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.77 (dd, *J* = 8.5, 7.2 Hz, 1H), 7.57 (m, *J* = 8.8, 7.4, 1.7 Hz, 1H), 7.49 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.17 (m, *J* = 7.7, 1.2 Hz, 1H), 4.47 (dd, *J* = 9.4, 8.0 Hz, 1H), 4.42 – 4.30 (m, 1H), 3.90 (t, *J* = 7.9 Hz, 1H), 1.27 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 166.84, 163.43, 150.73, 148.33, 139.98, 134.54, 134.52, 132.65, 129.20, 128.08, 126.45, 126.25, 122.79, 121.91, 119.64, 113.56, 72.69, 61.76, 21.38. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{17}N_3O_2$ $[M+H]^+$ 332.1388, found 332.1394.

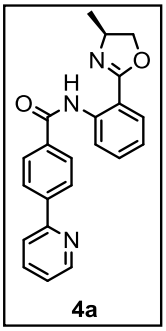


(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzo[b]thiophene-2-carboxamide (1t): white solid. Mp =150.8-151.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.34 (s, 1H), 8.88 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.08 (d, *J* = 0.8 Hz, 1H), 7.93 – 7.84 (m, 3H), 7.53 (m, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.43 (m, *J* = 7.2, 5.6 Hz, 2H), 7.13 (m, *J* = 7.6, 1.2 Hz, 1H), 4.67 – 4.51 (m, 2H), 3.97 (t, *J* = 7.5 Hz, 1H), 1.52 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 163.76, 161.09, 141.42, 140.86, 139.83, 139.23, 132.72, 129.20, 126.26, 125.56, 125.06, 124.75, 122.76, 122.55, 119.66, 113.30, 72.79, 61.96, 21.55. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{16}N_2O_2S$ $[M+H]^+$ 337.1005, found 337.1005.



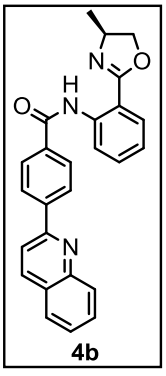
2a

diphenylmethanone O-pivaloyl oxime (2a)： white solid.[7] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (dd, J = 8.4, 1.4 Hz, 2H), 7.48 – 7.41 (m, 4H), 7.39 – 7.33 (m, 2H), 7.32 – 7.27 (m, 2H), 1.09 (s, 9H).



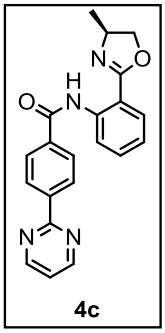
4a

(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyridin-2-yl)benzamide (4a): white solid. Mp =133.0-134.0 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.23 (s, 1H), 8.99 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.76 – 8.72 (m, 1H), 8.27 – 8.22 (m, 2H), 8.16 – 8.12 (m, 2H), 7.90 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.81 (m, *J* = 8.0, 6.3, 1.4 Hz, 2H), 7.54 (m, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.29 (m, *J* = 6.7, 4.8, 2.0 Hz, 1H), 7.13 (m, *J* = 7.6, 1.2 Hz, 1H), 4.59 – 4.50 (m, 2H), 4.00 – 3.92 (m, 1H), 1.47 (d, *J* = 6.2 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.56, 163.64, 156.21, 149.77, 142.20, 140.18, 136.85, 135.48, 132.63, 129.17, 128.22, 126.88, 122.69, 122.38, 120.85, 119.73, 113.50, 72.71, 61.92, 21.53. **HRMS** (ESI-TOF) m/z Calcd for $C_{22}H_{19}N_3O_2$ $[M+H]^+$ 358.1549, found 358.1550.



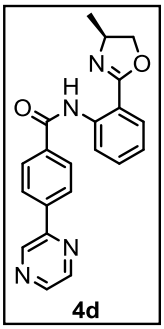
4b

(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(quinolin-2-yl)benzamide (4b): white solid. Mp =170.1-171.0 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.26 (s, 1H), 9.01 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 2H), 8.26 (dd, *J* = 8.5, 4.8 Hz, 3H), 8.20 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.95 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.91 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.86 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.76 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.59-7.52 (m, 2H), 7.14 (td, *J* = 7.7, 1.1 Hz, 1H), 4.63 – 4.47 (m, 2H), 3.99 – 3.94 (m, 1H), 1.47 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.63, 163.71, 156.18, 148.27, 142.52, 140.23, 136.98, 135.82, 132.70, 129.87, 129.76, 129.22, 128.33, 127.61, 127.51, 127.37, 126.67, 122.46, 119.82, 118.98, 113.57, 72.77, 61.99, 21.64. **HRMS** (ESI-TOF) m/z Calcd for $C_{26}H_{21}N_3O_2$ $[M+H]^+$ 673.3286, found 673.3279.

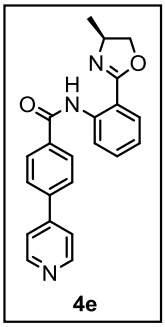


4c

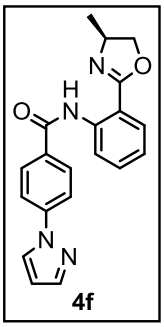
(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyrimidin-2-yl)benzamide (4c): white solid. Mp =157.2-158.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.27 (s, 1H), 9.00 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.87 (d, *J* = 4.9 Hz, 2H), 8.61 – 8.56 (m, 2H), 8.29 – 8.24 (m, 2H), 7.91 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.55 (d, *J* = 1.4 Hz, 1H), 7.26 (t, *J* = 4.9 Hz 1H), 7.14 (ddd, *J* = 7.9, 7.4, 1.2 Hz, 1H), 4.58 – 4.51 (m, 2H), 4.02 – 3.91 (m, 1H), 1.48 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.57, 163.91, 163.71, 157.34, 140.39, 140.19, 137.17, 132.72, 129.21, 128.24, 128.09, 122.49, 119.82, 119.57, 113.57, 72.79, 61.99, 21.58. **HRMS** (ESI-TOF) m/z Calcd for $C_{21}H_{18}N_4O_2$ $[M+H]^+$ 359.1497, found 359.1503.



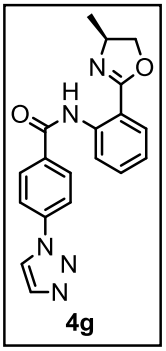
(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyrazin-2-yl)benzamide (4d): white solid. Mp =184.3-185.9 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.26 (s, 1H), 9.12 (d, *J* = 1.5 Hz, 1H), 8.99 (dd, *J* = 8.7, 1.2 Hz, 1H), 8.69 (dd, *J* = 2.5, 1.6 Hz, 1H), 8.57 (d, *J* = 2.5 Hz, 1H), 8.31 – 8.25 (m, 2H), 8.20 – 8.14 (m, 2H), 7.94 – 7.88 (m, 1H), 7.54 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.14 (ddd, *J* = 7.9, 7.3, 1.2 Hz, 1H), 4.58 – 4.52 (m, 2H), 3.99 – 3.94 (m, 1H), 1.47 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.29, 163.77, 151.76, 144.31, 143.55, 142.43, 140.11, 139.19, 136.50, 132.75, 129.24, 128.52, 126.99, 122.58, 119.81, 113.58, 72.78, 61.97, 21.61. **HRMS** (ESI-TOF) m/z Calcd for $C_{21}H_{18}N_4O_2$ $[M+H]^+$ 359.1496, found 359.1503.



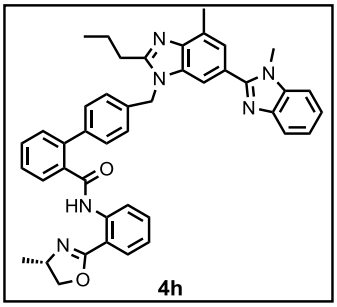
(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyridin-4-yl)benzamide (4e): white solid. Mp =182.0-183.2 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.23 (s, 1H), 8.98 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.71 (s, 2H), 8.24 – 8.20 (m, 2H), 7.90 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.79 – 7.73 (m, 2H), 7.61 – 7.50 (m, 3H)., 7.13 (td, *J* = 7.7, 1.2 Hz, 1H), 4.56 – 4.49 (m, 2H), 4.00 – 3.91 (m, 1H), 1.46 (d, *J* = 6.2 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.27, 163.80, 150.40, 147.27, 141.21, 140.11, 135.81, 132.77, 129.26, 128.58, 127.15, 122.59, 121.68, 119.80, 113.55, 72.77, 61.96, 21.60. **HRMS** (ESI-TOF) m/z Calcd for $C_{22}H_{19}N_3O_2$ $[M+H]^+$ 358.1548, found 358.1550.



(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(1H-pyrazol-1-yl)benzamide (4f): white solid. Mp =179.3-180.8 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.19 (s, 1H), 8.96 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.26 – 8.19 (m, 2H), 8.02 (dd, *J* = 2.6, 0.6 Hz, 1H), 7.89 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.86 – 7.82 (m, 2H), 7.77 (dd, *J* = 1.8, 0.6 Hz, 1H), 7.53 (ddd, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.12 (ddd, *J* = 7.9, 7.3, 1.2 Hz, 1H), 6.51 (dd, *J* = 2.5, 1.8 Hz, 1H), 4.58 – 4.48 (m, 2H), 3.99 – 3.90 (m, 1H), 1.45 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.01, 163.78, 142.33, 141.76, 140.16, 133.02, 132.73, 129.27, 129.23, 126.82, 122.47, 119.74, 118.48, 113.50, 108.31, 72.77, 61.95, 21.56. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{18}N_4O_2$ $[M+H]^+$ 347.1497, found 347.1503.

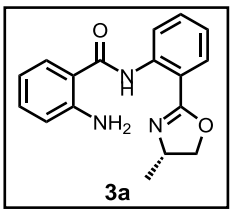


(*S*)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(1H-1,2,3-triazol-1-yl)benzamide (4g): white solid. Mp =177.3-179.2 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.24 (s, 1H), 8.98 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.29 – 8.20 (m, 4H), 7.92 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.88 (s, 2H), 7.54 (ddd, J = 8.7, 7.5, 1.6 Hz, 1H), 7.14 (ddd, J = 7.9, 7.4, 1.2 Hz, 1H), 4.60 – 4.50 (m, 2H), 4.01 – 3.91 (s, 1H), 1.47 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 164.93, 163.80, 141.85, 140.12, 136.12, 134.22, 132.75, 129.24, 129.11, 122.53, 119.76, 118.66, 113.53, 72.79, 61.96, 21.55. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{17}N_5O_2$ $[M+H]^+$ 348.1449, found 348.1455.



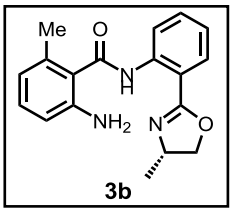
(*S*)-4'-((1,7'-dimethyl-2'-propyl-1H,3'H-[2,5'-bibenzo[d]imidazol]-3'-yl)methyl)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-[1,1'-biphenyl]-2-carboxamide (4h): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.47 (s, 1H), 8.69 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.73 – 7.69 (m, 2H), 7.49 (td, *J* = 7.5, 1.5 Hz, 1H), 7.46 – 7.34 (m, 8H), 7.31 – 7.28 (m, 2H), 7.05 – 6.97 (m, 3H), 5.37 (s, 2H), 4.32 – 4.16 (m, 2H), 3.80 – 3.71 (m, 4H), 2.89 – 2.79 (m, 2H), 2.75 (s, 3H), 1.86 – 1.73 (m, 2H), 1.18 (d, J = 6.4 Hz, 3H), 0.99 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$)δ 168.36, 162.94, 156.45, 154.66, 143.08, 142.91, 140.37, 139.78, 139.73, 136.85, 136.67, 134.98, 134.75, 132.38, 130.51, 130.19, 129.43, 129.30, 128.97, 128.30, 127.41, 125.98, 123.87, 122.43, 122.41, 122.25, 119.55, 113.31, 109.48, 108.75, 72.48, 61.72, 45.94, 31.82, 29.77, 21.79, 21.38, 16.86, 14.02. **HRMS** (ESI-TOF) m/z Calcd for $C_{43}H_{40}N_6O_2$ $[M+H]^+$ 673.3286, found 673.3279.

3.2 Characterization of Products 3a-3t,5a-5h,6a-6k,7,8,9

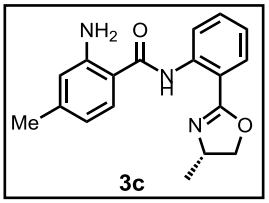


(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3a): white solid. Mp =109.1-110.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.93 (s, 1H), 8.88 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.86 (ddd, *J* = 8.2, 2.9, 1.5 Hz, 2H), 7.49 (ddd, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.26 – 7.19 (m, 1H), 7.07 (td, *J* = 7.6, 1.2 Hz, 1H), 6.70 (t, *J* = 7.5 Hz, 2H), 5.82 (s, br, 2H), 4.53 – 4.41 (m, 2H), 3.94 – 3.83 (m, 1H), 1.39 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.59, 163.53, 149.87, 140.36, 132.49, 132.45, 129.17, 128.44, 122.02, 119.62, 117.35, 116.26, 116.16, 113.52, 72.71, 61.94, 21.42. **HRMS** (ESI-TOF) m/z

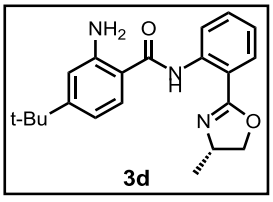
Calcd for $C_{17}H_{17}N_3O_2$ $[M+H]^+$ 296.1395, found 296.1394.



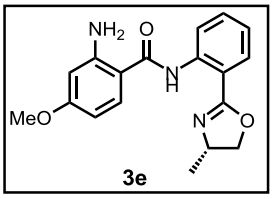
(*S*)-2-amino-6-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3b): white solid**.** Mp =95.6-96.9 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.60 (s, 1H), 8.97 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 7.9, 1.7 Hz, 1H), 7.52 (ddd, J = 8.8, 7.4, 1.7 Hz, 1H), 7.12 (td, J = 7.7, 1.2 Hz, 1H), 7.07 (t, J = 7.8 Hz, 1H), 6.65 – 6.54 (m, 2H), 4.37 – 4.30 (m, 2H), 3.87 (t, J = 7.7 Hz, 1H), 2.43 (s, 3H), 1.24 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (126 MHz, CDCl3) δ 168.40, 163.01, 145.34, 139.75, 135.36, 132.49, 130.08, 129.16, 123.40, 122.58, 120.32, 119.78, 113.90, 113.53, 72.62, 61.82, 21.25, 20.67. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_2$ $[M+H]^+$ 310.1546, found 310.1550.



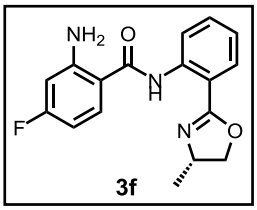
(*S*)-2-amino-4-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3c): white solid. Mp =135.6-136.9 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.88 (s, 1H), 8.87 (dd, J = 8.5, 1.1 Hz, 1H), 7.87 (dd, J = 7.9, 1.7 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.49 (ddd, J = 8.7, 7.3, 1.7 Hz, 1H), 7.08 (ddd, J = 7.9, 7.3, 1.2 Hz, 1H), 6.56 – 6.50 (m, 2H), 5.81 (s, br, 2H), 4.57 – 4.44 (m, 2H), 3.97 – 3.87 (m, 1H), 2.29 (s, 3H), 1.42 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.61, 163.57, 150.05, 143.09, 140.52, 132.44, 129.17, 128.45, 121.86, 119.62, 117.65, 117.60, 113.60, 113.46, 72.71, 61.98, 21.45, 21.41. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_2$ $[M+H]^+$ 310.1550, found 310.1550.



(*S*)-2-amino-4-(tert-butyl)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3d): white solid. Mp =124.5-125.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.88 (s, 1H), 8.89 (dd, J = 8.5, 1.1 Hz, 1H), 7.88 (dd, J = 7.9, 1.6 Hz, 1H), 7.83 (d, J = 8.5 Hz, 1H), 7.49 (ddd, J = 8.8, 7.3, 1.7 Hz, 1H), 7.08 (ddd, J = 7.9, 7.3, 1.2 Hz, 1H), 6.75 (dd, J = 8.5, 1.9 Hz, 1H), 6.71 (d, J = 1.9 Hz, 1H), 5.85 (s, br, 2H), 4.56 – 4.48 (m, 2H), 3.97 – 3.88 (m, 1H), 1.44 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.50, 163.54, 156.12, 149.94, 140.53, 132.44, 129.17, 128.20, 121.85, 119.64, 114.25, 114.10, 113.45, 113.41, 72.70, 61.99, 34.69, 30.93, 21.55. **HRMS** (ESI-TOF) m/z Calcd for $C_{21}H_{25}N_3O_2$ $[M+H]^+$ 352.2019, found 352.2020.

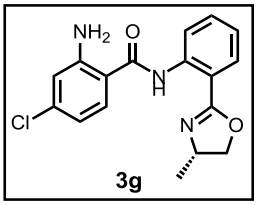


(*S*)-2-amino-4-methoxy-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3e): white solid. Mp =103.4-104.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.81 (s, 1H), 8.84 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.87 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.49 (d, *J* = 1.5 Hz, 1H), 7.07 (d, *J* = 1.2 Hz, 1H), 6.29 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.16 (d, *J* = 2.5 Hz, 1H), 5.98 (s, br, 2H), 4.55 – 4.46 (m, 2H), 3.95 – 3.87 (m, 1H). 3.80 (s, 3H), 1.41 (d, *J* = 5.8 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.33, 163.60, 163.03, 152.12, 140.60, 132.42, 130.22, 129.15, 121.70, 119.54, 113.34, 109.38, 104.11, 100.29, 72.68, 61.95, 55.13, 21.46. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_3$ $[M+H]^+$ 326.1499, found 326.1499.



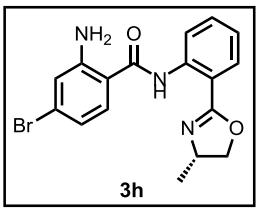
(*S*)-2-amino-4-fluoro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3f): white solid. Mp =126.2-127.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.90 (s, 1H), 8.83 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.87 (ddd, *J* = 9.8, 6.7, 4.0 Hz, 2H), 7.50 (ddd, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.09 (td, *J* = 7.5, 1.2 Hz, 1H), 6.43 – 6.34 (m, 2H), 6.01 (s, br, 2H), 4.56 – 4.42 (m,

2H), 3.97 – 3.88 (m, 1H), 1.40 (d, *J* = 6.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.83 , 165.48 (d, J = 249.9 Hz), 163.65 , 152.15 (d, J = 12.0 Hz), 140.27 , 132.48 , 130.77 (d, J = 11.2 Hz), 129.20 , 122.09 , 119.57 , 113.48 , 112.61 (d, J = 1.6 Hz), 103.82 (d, J = 22.5 Hz), 102.85 (d, J = 24.0 Hz). 72.73, 61.90, 21.40. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -107.97 (s). **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{16}FN_3O_2$ $[M+H]^+$ 314.1300, found 314.1299.



(*S*)-2-amino-4-chloro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide

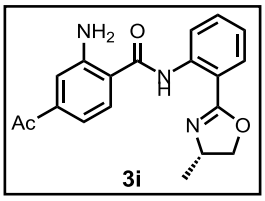
(3g): white solid. Mp =114.0-115.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.95 (s, 1H), 8.83 (dd, J = 8.5, 1.1 Hz, 1H), 7.88 (dd, J = 7.9, 1.7 Hz, 1H), 7.79 (d, J = 8.5 Hz, 1H), 7.50 (ddd, J = 8.7, 7.4, 1.7 Hz, 1H), 7.10 (td, J = 7.7, 1.2 Hz, 1H), 6.70 (d, J = 2.1 Hz, 1H), 6.67 (dd, J = 8.4, 2.1 Hz, 1H), 5.92 (s, br, 2H), 4.55 – 4.48 (m, 2H), 3.98 – 3.89 (m, 1H), 1.41 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.85, 163.69, 150.85, 140.19, 138.34, 132.56, 129.78, 129.25, 122.26, 119.63, 116.59, 116.49, 114.63, 113.55, 72.78, 61.94, 21.48. **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{16}ClN_3O_2$ $[M+H]^+$ 330.1003, found 330.1004.



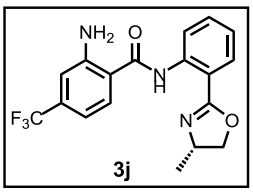
(*S*)-2-amino-4-bromo-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide

(3h): white solid. Mp =117.8-119.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.96 (s, 1H), 8.83 (dd, J = 8.6, 1.1 Hz, 1H), 7.88 (dd, J = 7.9, 1.7 Hz, 1H), 7.71 (d, J = 8.6 Hz, 1H), 7.50 (t, J = 1.5 Hz, 1H), 7.10 (td, J = 7.6, 1.2 Hz, 1H), 6.87 (d, J = 1.9 Hz, 1H), 6.82 (dd, J = 8.5, 1.9 Hz, 1H)., 5.90 (s, br, 2H), 4.55 – 4.47 (m, 2H), 3.96 – 3.88 (m, 1H), 1.41 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.92, 163.67, 150.91, 140.16, 132.54, 129.80, 129.24, 126.86, 122.26, 119.62, 119.30, 114.99, 113.55, 72.78, 61.93, 21.46.

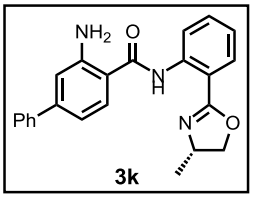
HRMS (ESI-TOF) m/z Calcd for $C_{17}H_{16}BrN_3O_2$ $[M+H]^+$ 374.0495, found 374.0499.



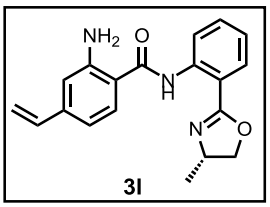
(*S*)-4-acetyl-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3i): white solid. Mp =138.5-139.8 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 13.05 (s, 1H), 8.87 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.89 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.51 (ddd, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.12 (td, *J* = 7.7, 1.2 Hz, 1H), 5.91 (s, br, 2H), 4.54 – 4.47 (m, 2H), 3.97 – 3.90 (m, 1H), 2.59 (s, 3H), 1.42 (d, *J* = 5.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.98, 167.72, 163.64, 149.74, 140.04, 139.90, 132.55, 129.25, 128.77, 122.46, 119.67, 119.61, 117.12, 115.58, 113.66, 72.79, 61.92, 26.78, 21.50. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{19}N_3O_3$ $[M+H]^+$ 372.1705, found 372.1707.



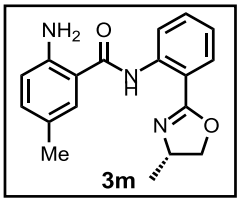
(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(trifluoromethyl)benzamide (3j): white solid. Mp =146.5-147.9 ºC. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 13.08 (s, 1H), 8.86 (dd, J = 8.5, 1.2 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.90 (dd, J = 7.9, 1.7 Hz, 1H), 7.52 (ddd, J = 8.7, 7.3, 1.7 Hz, 1H), 7.13 (td, J = 7.6, 1.2 Hz, 1H), 6.96 – 6.89 (m, 2H), 5.98 (s, br, 2H), 4.57 – 4.48 (m, 2H), 4.00 – 3.90 (m, 1H), 1.42 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.54 , 163.72 , 149.74 , 140.02 , 134.01 (q, J = 32.9 Hz), 132.60 , 129.30 , 129.14 , 123.69 (q, J = 272.5 Hz), 122.54 , 119.70 , 118.67 , 113.97 (q, J = 3.8 Hz), 113.69 , 112.35 (q, J = 3.8 Hz), 72.83 , 61.94 , 21.51. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.61 (s). **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{16}F_3N_3O_2$ $[M+H]^+$ 364.1261, found 364.1267.



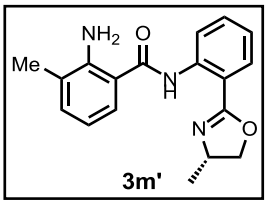
(*S*)-3-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-[1,1'-biphenyl]-4-carboxamide (3k): white solid. Mp =134.5-135.6 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.00 (s, 1H), 8.91 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.52 (s, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.10 (s, 1H), 7.00 – 6.90 (m, 2H), 5.95 (s, br, 2H), 4.57 – 4.47 (m, 2H), 3.97 – 3.88 (m, 1H), 1.44 (d, J = 5.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.41, 163.58, 150.23, 145.23, 140.40, 140.28, 132.47, 129.19, 128.99, 128.69, 127.86, 127.04, 122.02, 119.62, 115.64, 115.46, 115.02, 113.50 , 72.72, 61.95, 21.47. **HRMS** (ESI-TOF) m/z Calcd for $C_{23}H_{21}N_3O_2$ $[M+H]^+$ 372.1705, found 372.1707.



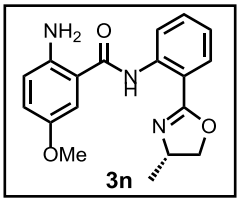
(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-vinylbenzamide (3l): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.94 (s, 1H), 8.87 (dd, J = 8.5, 1.1 Hz, 1H), 7.88 (dd, J = 7.9, 1.7 Hz, 1H), 7.84 (d, J = 8.3 Hz, 1H), 7.50 (ddd, J = 8.8, 7.3, 1.7 Hz, 1H), 7.09 (td, J = 7.6, 1.2 Hz, 1H), 6.81 (dd, J = 8.3, 1.7 Hz, 1H), 6.71 (d, J = 1.6 Hz, 1H), 6.64 (dd, J = 17.6, 10.8 Hz, 1H), 5.86 (s, br, 2H), 5.81 (dd, J = 17.6, 0.9 Hz, 1H), 5.33 (dd, J = 10.8, 0.8 Hz, 1H), 4.58 – 4.46 (m, 2H), 3.97 – 3.88 (m, 1H), 1.43 (d, J = 6.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.31, 163.56, 150.13, 141.44, 140.38, 136.23, 132.46, 129.18, 128.74, 122.00, 119.62, 115.67, 115.41, 115.22, 114.14, 113.49. 72.72, 61.95, 21.48. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{19}N_3O_2$ $[M+H]^+$ 338.1498, found 338.1499.



(*S*)-2-amino-5-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3m): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.88 (s, 1H), 8.91 (dd, J = 8.5, 1.2 Hz, 1H), 7.89 (dd, J = 7.8, 1.7 Hz, 1H), 7.72 – 7.64 (m, 1H), 7.50 (ddd, J = 8.7, 7.2, 1.7 Hz, 1H), 7.12 – 7.06 (m, 2H), 6.64 (d, J = 8.3 Hz, 1H), 5.66 (s, br, 2H), 4.58 – 4.45 (m, 2H), 3.99 – 3.85 (m, 1H), 2.31 (s, 3H), 1.44 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.64, 163.59, 147.65, 140.45, 133.45, 132.49, 129.21, 128.40, 125.32, 121.97, 119.59, 117.52, 116.14, 113.43, 72.68, 62.02, 21.47, 20.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_2$ $[M+H]^+$ 310.1550, found 310.1550.

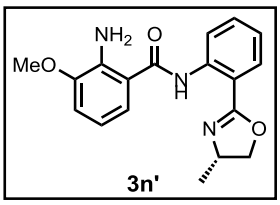


(*S*)-2-amino-3-methyl-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3m') white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.92 (s, 1H), 8.88 (dd, J = 8.5, 1.2 Hz, 1H), 7.88 (dd, J = 7.9, 1.7 Hz, 1H), 7.77 (dd, J = 8.3, 1.4 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.18 (d, J = 7.2 Hz, 1H), 7.12 – 7.05 (m, 1H), 6.67 (t, J = 7.6 Hz, 1H), 5.87 (s, br, 2H), 4.56 – 4.44 (m, 2H), 3.96 – 3.87 (m, 1H), 2.20 (s, 3H), 1.41 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.64, 163.59, 147.65, 140.45, 133.45, 132.49, 129.21, 128.40, 125.32, 121.97, 119.59, 117.52, 116.14, 113.43, 72.68, 62.02, 21.47, 20.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_2$ $[M+H]^+$ 310.1550, found 310.1550.

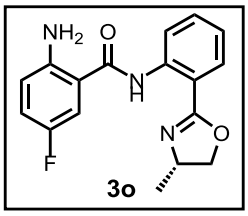


(*S*)-2-amino-5-methoxy-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3n): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.85 (s, 1H), 8.87 (dd, J = 8.5,

1.2 Hz, 1H), 7.89 (dd, J = 7.9, 1.7 Hz, 1H), 7.50 (ddd, J = 8.8, 7.4, 1.7 Hz, 1H), 7.42 (d, J = 2.8 Hz, 1H), 7.10 (td, J = 7.6, 1.2 Hz, 1H), 6.93 (dd, J = 8.8, 2.8 Hz, 1H), 6.68 (d, J = 8.9 Hz, 1H), 5.46 (s, br, 2H), 4.56 – 4.42 (m, 2H), 3.99 – 3.85 (m, 1H), 3.81 (s, 3H), 1.39 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.21, 163.56, 150.93, 144.07, 140.26, 132.44, 129.20, 122.10, 120.22, 119.66, 118.63, 116.70, 113.52, 112.81, 72.67, 62.01, 56.08, 21.48. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_3$ $[M+H]^+$ 326.1498, found 326.1499.

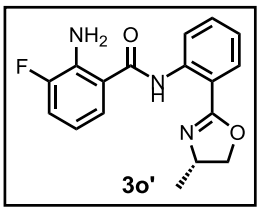


(*S*)-2-amino-3-methoxy-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3n'): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.90 (s, 1H), 8.89 (dd, *J* = 8.5, 1.2 Hz, 1H), 7.87 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.09 (td, *J* = 7.6, 1.2 Hz, 1H), 6.85 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.66 (t, *J* = 8.0 Hz, 1H), 6.12 (s, br, 2H), 4.57 – 4.44 (m, 2H), 3.96 – 3.88 (m, 1H), 3.89 (s, 3H), 1.41 (d, *J* = 5.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.68, 163.52, 147.61, 141.00, 140.43, 132.46, 129.17, 121.97, 120.05, 119.68, 115.40, 114.67, 113.53, 111.77, 72.73, 61.99, 55.72, 21.46. **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{19}N_3O_3$ $[M+H]^+$ 326.1498, found 326.1499.

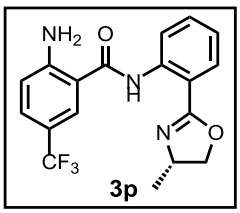


(*S*)-2-amino-5-fluoro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3o): white solid. Mp =149.7-150.8 ^{o}C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.99 (s, 1H), 8.86 (dd, J = 8.5, 1.1 Hz, 1H), 7.88 (dd, J = 7.9, 1.7 Hz, 1H), 7.66 (dd, J = 8.2, 1.3 Hz, 1H), 7.51 (ddd, J = 8.9, 7.3, 1.8 Hz, 1H), 7.13 – 7.06 (m, 2H), 6.63 (td, J = 8.0, 5.2 Hz, 1H), 5.90 (s, br, 2H), 4.58 – 4.46 (m, 2H), 3.97 – 3.88 (m, 1H), 1.41 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.77 (d, J = 2.7 Hz), 163.62, 152.00 (d, J = 239.8 Hz), 140.14, 139.09 (d, J = 13.8 Hz), 132.54, 129.23, 123.51 (d, J = 3.6 Hz), 122.30, 119.68, 118.02

(d, J = 4.5 Hz), 117.13 (d, J = 19.0 Hz), 114.73 (d, J = 7.4 Hz), 113.61, 72.76, 61.94, 21.44. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -128.31 (s). **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{16}FN_3O_2$ $[M+H]^+$ 314.1295, found 314.1299.

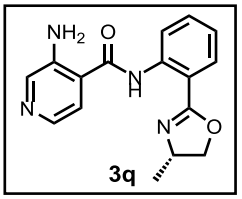


(*S*)-2-amino-3-fluoro-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (3o'): white solid. Mp =154.6-155.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.00 (s, 1H), 8.86 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.89 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.66 (dd, *J* = 10.2, 2.9 Hz, 1H), 7.50 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.11 (ddd, *J* = 7.9, 7.3, 1.2 Hz, 1H), 7.01 (ddd, *J* = 8.9, 7.7, 2.9 Hz, 1H), 6.66 (dd, *J* = 9.0, 4.7 Hz, 1H), 5.68 (s, br, 2H), 4.56 – 4.50 (m, 2H), 3.97 – 3.91 (m, 1H), 1.47 (d, *J* = 1.8 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.53, 163.68, 154.33 (d, J = 234.5 Hz), 146.32, 140.16, 132.58, 129.24, 122.32, 120.03 (d, J = 23.0 Hz), 119.53, 118.43 (d, J = 7.3 Hz), 116.11 (d, J = 5.5 Hz), 114.07 (d, J = 23.8 Hz), 113.57, 72.86, 62.01, 21.27. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -135.58 (s). **HRMS** (ESI-TOF) m/z Calcd for $C_{17}H_{16}FN_3O_2$ $[M+H]^+$ 314.1295, found 314.1299.

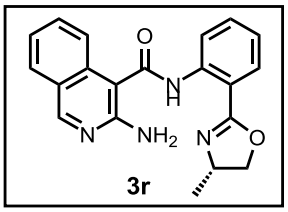


(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-5-(trifluoromethyl)benzamide (3p): white solid. Mp =166.3-167.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.15 (s, 1H), 8.86 (dd, J = 8.5, 1.1 Hz, 1H), 8.22 – 8.17 (m, 1H), 7.91 (dd, J = 7.9, 1.7 Hz, 1H), 7.51 (t, J = 1.4 Hz, 1H), 7.45 (dd, J = 8.6, 2.0 Hz, 1H), 7.13 (dd, J = 7.5, 1.2 Hz, 1H), 6.73 (d, J = 8.6 Hz, 1H), 6.24 (s, br, 2H), 4.59 – 4.45 (m, 2H), 3.99 – 3.91 (m, 1H), 1.39 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.49, 163.63, 152.34, 140.05, 132.52, 129.31, 128.97 (q, *J* = 3.4 Hz), 126.23 (q, *J* = 4.0 Hz), 124.63 (q, *J* = 270.7 Hz), 122.43, 119.57, 117.96 (q, *J* = 33.1 Hz), 117.12, 114.96, 113.67, 72.86, 61.98, 21.17. **^{19}F**

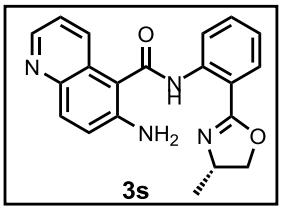
NMR (471 MHz, $CDCl_3$) δ -61.10 (s). **HRMS** (ESI-TOF) m/z Calcd for $C_{18}H_{16}F_3N_3O_2$ $[M+H]^+$ 364.1266, found 364.1267.



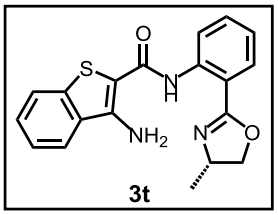
(*S*)-3-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)nicotinamide (3q): white solid. Mp =151.2-152.9 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.19 (s, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.21 (s, 1H), 7.99 (d, J = 5.3 Hz, 1H), 7.90 (d, J = 7.9 Hz, 1H), 7.65 (d, J = 5.3 Hz, 1H), 7.52 (t, J = 8.0 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 5.79 (s, br, 2H), 4.58 – 4.49 (m, 2H), 3.99 – 3.90 (m, 1H), 1.43 (d, J = 5.6 Hz, 3H). **^{13}C NMR**(126 MHz, $CDCl_3$) δ 166.82, 163.69, 144.46, 141.14, 139.70, 137.24, 132.61, 129.30, 122.77, 120.79, 120.49, 119.71, 113.74, 72.85, 61.91, 21.45. **HRMS** (ESI-TOF) m/z Calcd for $C_{16}H_{17}N_4O_2$ $[M+H]^+$ 297.1341, found 297.1346.



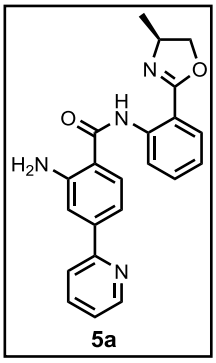
(*S*)-4-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)quinoline-3-carboxamide (3r): white solid. Mp =181.6-182.9 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.20 (s, 1H), 9.02 (d, J = 8.0 Hz, 1H), 8.56 (s, 1H), 8.07 – 8.03 (m, 1H), 8.01 – 7.97 (m, 1H), 7.88 (dd, J = 7.9, 1.6 Hz, 1H), 7.57 (ddd, J = 8.7, 7.4, 1.7 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.17 (td, J = 7.6, 1.2 Hz, 1H), 4.99 (s, br, 2H), 4.36 (dd, J = 9.3, 8.1 Hz, 1H), 4.11 – 3.97 (m, 1H), 3.78 (t, J = 8.1 Hz, 1H), 0.84 (d, J = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.90, 162.88, 144.31, 142.50, 139.54, 138.71, 132.59, 129.57, 129.21, 127.50, 125.18, 124.90, 124.03, 123.07, 119.93, 118.21, 113.76, 72.73, 61.61, 20.85. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{18}N_4O_2$ $[M+H]^+$ 347.1498, found 347.1503.



(*S*)-5-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)quinoline-6-carboxamide (3s): white solid. Mp =181.9-182.9 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.01 (s, 1H), 9.03 (dd, J = 8.4, 1.3 Hz, 1H), 8.63 (dd, J = 4.2, 1.6 Hz, 1H), 8.43 (ddd, J = 8.7, 1.6, 0.9 Hz, 1H), 7.95 (dd, J = 9.0, 0.8 Hz, 1H), 7.87 (dd, J = 7.9, 1.7 Hz, 1H), 7.56 (ddd, J = 8.8, 7.4, 1.7 Hz, 1H), 7.28 (q, J = 2.2 Hz, 1H), 7.18 – 7.14 (m, 2H), 5.21 (s, br, 2H), 4.35 (dd, J = 9.4, 8.2 Hz, 1H), 4.09 – 3.98 (m, 1H), 3.77 (t, J = 8.1 Hz, 1H), 0.85 (d, J = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.06, 162.96, 146.19, 145.27, 143.19, 139.86, 133.08, 132.58, 132.38, 129.21, 126.89, 122.74, 122.42, 121.48, 119.81, 113.59, 111.79, 72.67, 61.61, 20.92. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{18}N_4O_2$ $[M+H]^+$ 352.1113, found 352.1114.

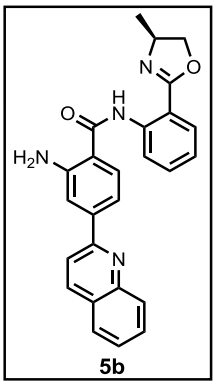


(*S*)-3-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)benzo[b]thiophene-2-carboxamide (**3t**): white solid. Mp =179.6-181.0 ºC. **^{1}H NMR**(400 MHz, $CDCl_3$) δ 12.65 (s, 1H), 8.86 (d, J = 8.5 Hz, 1H), 7.87 (dd, J = 7.9, 1.6 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.37 (t, J = 7.6 Hz, 1H), 7.08 (t, J = 7.6 Hz, 1H), 6.26 (s, br, 2H), 4.67 – 4.55 (m, 1H), 4.54 – 4.47 (m, 1H), 3.94 (t, J = 7.8 Hz, 1H), 1.51 (d, J = 6.7 Hz, 3H). **^{13}C NMR** (126 MHz, CDCl3) δ 164.84, 163.34, 148.00, 140.44, 138.42, 132.25, 132.22, 129.03, 127.79, 123.93, 123.13, 121.83, 121.02, 119.73, 113.25, 102.60, 72.78, 62.01, 21.61. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{17}N_3O_2S$ $[M+H]^+$ 352.1113, found 352.1114.



5a

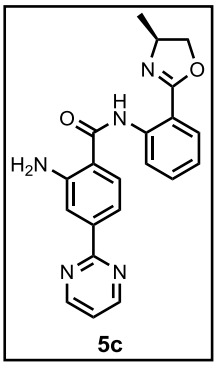
(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyridin-2-yl)benzamide (**5a**): white solid. Mp =160.0-161.8 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.04 (s, 1H), 8.91 (dd, J = 8.5, 1.1 Hz, 1H), 8.72 (dt, J = 4.9, 1.4 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.90 (dd, J = 7.9, 1.7 Hz, 1H), 7.79 – 7.75 (m, 2H), 7.53 (ddd, J = 8.8, 7.3, 1.7 Hz, 1H), 7.39 (d, J = 1.8 Hz, 1H), 7.36 – 7.33 (m, 1H), 7.28 (td, J = 5.4, 2.7 Hz, 1H), 7.12 (td, J = 7.6, 1.2 Hz, 1H), 5.99 (s, br, 2H), 4.58 – 4.49 (m, 2H), 3.98 – 3.91 (m, 1H), 1.45 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.31, 163.57, 156.45, 150.26, 149.60, 142.94, 140.34, 136.74, 132.47, 129.19, 129.00, 122.64, 122.09, 120.85, 119.66, 116.37, 115.60, 114.84, 113.55, 72.74, 61.95, 21.53. **HRMS** (ESI-TOF) m/z Calcd for $C_{22}H_{20}N_4O_2$ $[M+H]^+$ 373.1653, found 373.1659.



5b

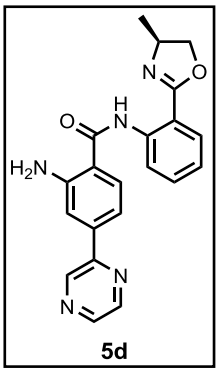
(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(quinolin-2-yl)benzamide (**5b**): white solid. Mp =167.4-169.0 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.05 (s, 1H), 8.91 (dd, J = 8.5, 1.1 Hz, 1H), 8.24 (d, J = 8.3 Hz, 1H), 8.19 (dd, J = 8.4, 1.0 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.92 – 7.87 (m, 2H), 7.84 (dd, J = 8.1, 1.4 Hz, 1H), 7.75 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.58 – 7.51 (m, 3H), 7.51 – 7.47 (m, 1H), 7.11 (td, J = 7.6, 1.2 Hz, 1H), 6.02 (s, br, 2H), 4.57 – 4.47 (m, 2H), 3.99 – 3.90 (m, 1H), 1.46 (d, J =

6.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.36, 163.62, 156.46, 150.31, 148.20, 143.26, 140.37, 136.77, 132.51, 129.76, 129.23, 129.09, 127.46, 127.43, 126.54, 122.14, 119.73, 119.06, 116.71, 116.30, 115.51, 113.61, 72.78, 62.00, 21.59. **HRMS** (ESI-TOF) m/z Calcd for $C_{26}H_{22}N_4O_2$ $[M+H]^+$ 423.1811, found 423.1816.



5c

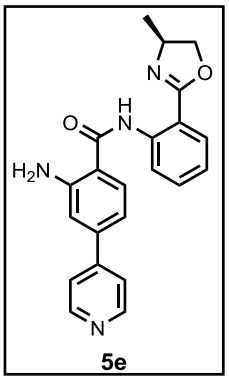
(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyrimidin-2-yl)benz amide (**5c**): white solid. Mp =195.6-196.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.07 (s, 1H), 8.90 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.84 (d, *J* = 4.8 Hz, 2H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.89 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.84 (d, *J* = 1.7 Hz, 1H), 7.78 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.52 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.24 (t, *J* = 4.8 Hz, 1H), 7.11 (ddd, *J* = 8.3, 7.5, 1.2 Hz, 1H), 5.96 (s, br, 2H), 4.62 – 4.44 (m, 2H), 3.99 – 3.89 (m, 1H), 1.44 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.28, 164.01, 163.59, 157.20, 150.11, 140.94, 140.32, 132.51, 129.21, 128.89, 122.18, 119.71, 119.49, 117.87, 117.03, 115.89, 113.61, 72.79, 61.99, 21.58. **HRMS**(ESI-TOF) m/z Calcd for $C_{21}H_{19}N_5O_2$ $[M+H]^+$ 374.1607, found 374.1612.



5d

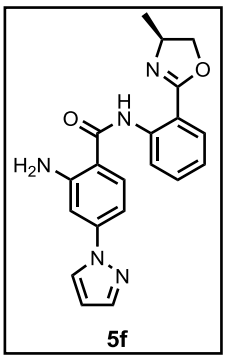
(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyrazin-2-yl)benza mide (**5d**): white solid. Mp =166.3-167.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.05 (s,

1H), 8.91 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.26 – 8.22 (m, 1H), 8.19 (dq, *J* = 8.4, 0.9 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.87 (m, 1H), 7.84 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.75 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.59 – 7.51 (m, 1H), 7.51 – 7.47 (m, 1H), 7.11 (td, *J* = 7.6, 1.2 Hz, 1H), 6.02 (s, br, 2H), 4.58 – 4.45 (m, 2H), 3.99 – 3.91 (m, 1H), 1.46 (d, J = 6.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.06, 163.63, 151.89, 150.33, 144.12, 143.41, 142.40, 140.23, 139.82, 132.52, 129.29, 129.23, 122.24, 119.67, 117.14, 115.53, 114.52, 113.59, 72.77, 61.95, 21.55. **HRMS** (ESI-TOF) m/z Calcd for $C_{21}H_{19}N_5O_2$ $[M+H]^+$ 374.1606, found 374.1612.



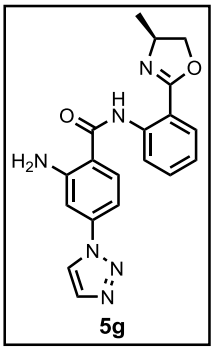
5e

(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(pyridin-4-yl)benzamide (**5e**): white solid. Mp =187.2-188.6 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.03 (s, 1H), 8.88 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.66 (s, 2H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.89 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.55 – 7.46 (m, 3H), 7.11 (td, *J* = 7.6, 1.2 Hz, 1H), 6.96 (d, *J* = 7.9 Hz, 2H), 5.99 (s, br, 2H), 4.58 – 4.45 (m, 2H), 3.98 – 3.89 (m, 1H), 1.43 (d, J = 6.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$)δ 168.06, 163.67, 150.30, 150.14, 147.64, 142.01, 140.22, 132.54, 129.33, 129.25, 122.26, 121.61, 119.65, 116.47, 115.55, 114.90, 113.57, 72.76, 61.95, 21.51. **HRMS** (ESI-TOF) m/z Calcd for $C_{22}H_{20}N_4O_2$ $[M+H]^+$ 373.1652, found 373.1659.



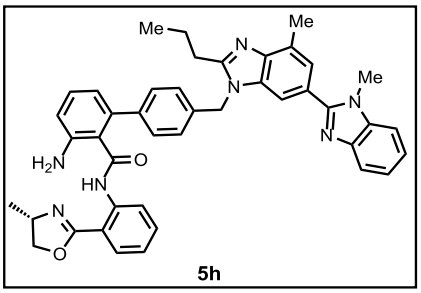
5f

(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(1H-pyrazol-1-yl)benzamide (**5f**): white solid. Mp =169.1-170.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.98 (s, 1H), 8.86 (dd, J = 8.5, 1.1 Hz, 1H), 7.99 – 7.95 (m, 2H), 7.89 (dd, J = 7.9, 1.7 Hz, 1H), 7.74 (dd, J = 1.8, 0.6 Hz, 1H), 7.51 (ddd, J = 8.7, 7.3, 1.7 Hz, 1H), 7.13 – 7.06 (m, 2H), 7.04 (dd, J = 8.6, 2.2 Hz, 1H), 6.48 (dd, J = 2.5, 1.8 Hz, 1H), 6.06 (s, br, 2H), 4.57 – 4.48 (m, 2H), 3.97 – 3.88 (m, 1H), 1.43 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.89, 163.65, 151.15, 142.93, 141.39, 140.29, 132.50, 130.08, 129.21, 126.77, 122.11, 119.60, 114.00, 113.50, 107.90, 106.68, 106.39, 72.74, 61.93, 21.52. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{19}N_5O_2$ $[M+H]^+$ 362.1605, found 362.1612.



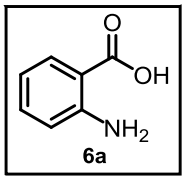
5g

(*S*)-2-amino-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-4-(1H-1,2,3-triazol-1-yl)benzamide (**5g**): white solid. Mp =172.6-173.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.03 (s, 1H), 8.86 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.00 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.88 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.83 (s, 2H), 7.51 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.10 (td, *J* = 7.6, 1.2 Hz, 1H), 6.09 (s, br, 2H), 4.57 – 4.45 (m, 2H), 3.98 – 3.89 (m, 1H), 1.43 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.84, 163.66, 150.93, 142.40, 140.24, 135.80, 132.52, 129.98, 129.22, 122.19, 119.61, 115.03, 113.54, 106.73, 106.54, 72.77, 61.94, 21.51. **HRMS** (ESI-TOF) m/z Calcd for $C_{19}H_{18}N_6O_2$ $[M+H]^+$ 363.1558, found 363.1564.



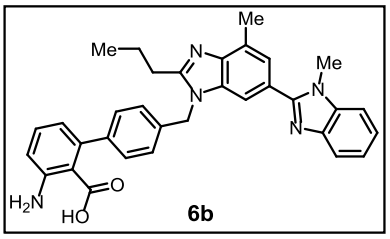
5h

(*S*)-3-amino-4'-((1,7'-dimethyl-2'-propyl-1H,3'H-[2,5'-bibenzo[d]imidazol]-3'-yl)methyl)-N-(2-(4-methyl-4,5-dihydrooxazol-2-yl)phenyl)-[1,1'-biphenyl]-2-carboxamide (**5h**): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 11.95 (s, 1H), 8.73 (d, J = 8.4 Hz, 1H), 7.87 – 7.81 (m, 1H), 7.50 (dd, J = 7.8, 1.6 Hz, 1H), 7.47 – 7.44 (m, 2H), 7.42 – 7.36 (m, 4H), 7.36 – 7.32 (m, 2H), 7.22 (t, J = 7.8 Hz, 1H), 6.92 (d, J = 8.0 Hz, 2H), 6.87 (td, J = 7.6, 1.2 Hz, 1H), 6.73 (dt, J = 7.5, 1.6 Hz, 2H), 5.31 (d, J = 3.3 Hz, 2H), 4.61 (s, br, 2H), 4.13 – 4.02 (m, 2H), 3.82 (s, 3H), 3.64 – 3.55 (m, 1H), 2.78 (s, 3H), 2.74 – 2.68 (m, 2H), 1.72 (h, J = 7.4 Hz, 2H), 1.07 (d, J = 6.2 Hz, 3H), 0.93 (t, J = 7.3 Hz, 3H).; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.43, 162.18, 156.53, 154.36, 146.15, 143.07, 142.12, 140.77, 139.85, 139.46, 136.45, 135.09, 134.58, 132.09, 130.46, 129.44, 129.31, 128.79, 125.63 , 123.76, 123.37, 122.73, 122.59, 122.29, 121.41, 119.60, 119.35, 119.32, 115.54, 113.28 , 109.55, 108.75, 72.27, 61.64, 46.82, 31.88, 29.63, 21.62, 21.22, 16.89, 13.93.; **HRMS** (ESI-TOF) m/z Calcd for $C_{43}H_{41}N_7O_2$ $[M+H]^+$ 688.3395, found 688.3401.



6a

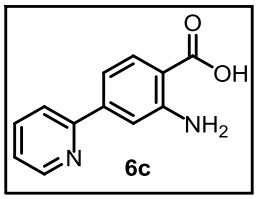
2-aminobenzoic acid (6a): light yellow solid**.**[15] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (dd, J = 8.3, 1.7 Hz, 1H), 7.32 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 6.74 – 6.62 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.71, 151.08, 135.12, 132.11, 116.77, 116.44, 109.48. **HRMS** (ESI-TOF) m/z Calcd for $C_7H_7NO_2$ $[M-H]^-$ 136.0404, found 136.0401



6b

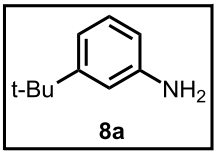
3-amino-4'-((1,7'-dimethyl-2'-propyl-1H,3'H-[2,5'-bibenzo[d]imidazol]-3'-yl)methyl)-[1,1'-biphenyl]-2-carboxylic acid (6b)： white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 – 8.21 (m, 1H), 7.35 – 7.28 (m, 5H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.14 – 7.08 (m, 2H), 7.04 (s, 1H), 6.93 (s, 1H), 6.70 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 7.3 Hz, 1H), 5.37 (s, 2H), 3.71 (s, 3H), 3.10 (t, *J* = 7.8 Hz, 2H), 2.69 (s, 3H), 2.03 – 1.90 (m, 2H),

1.14 (t, *J* = 7.3, 1.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.67, 156.62, 153.96, 149.01, 144.20, 143.84, 143.27, 141.07, 135.65, 134.52, 133.15, 130.88, 129.09, 128.85, 126.91, 123.64 , 123.14, 123.09, 121.92, 119.65, 118.18, 115.78, 115.73, 111.53, 109.48, 48.84, 31.86, 29.98, 22.43, 17.04, 14.16. **HRMS** (ESI-TOF) m/z Calcd for $C_{33}H_{31}N_5O_2$ $[M+H]^+$ 530.2551, found 530.2556.



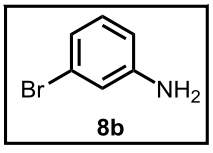
6c

2-amino-4-(pyridin-2-yl)benzoic acid (6c): white sticky foam. **^{1}H NMR** (400 MHz, $(CD_3)_2CO$) δ 8.71 (dt, J = 4.8, 1.6 Hz, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.96 – 7.88 (m, 2H), 7.65 (d, J = 1.8 Hz, 1H), 7.39 (ddd, J = 6.7, 4.7, 1.7 Hz, 1H), 7.34 (dd, J = 8.4, 1.7 Hz, 1H), 6.64 (s, 2H). **^{13}C NMR** (126 MHz, $(CD_3)_2CO$) δ 170.70, 157.69, 153.71, 151.25, 145.94, 138.50, 133.53, 124.55, 122.15, 116.25, 115.10, 111.60. **HRMS** (ESI-TOF) m/z Calcd for $C_{12}H_{10}N_2O_2$ $[M+H]^+$ 215.0815, found 215.0818.



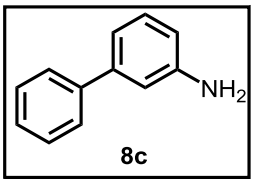
8a

3-(tert-butyl)aniline (8a)[8]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (t, *J* = 7.8 Hz, 1H), 6.81 (ddd, *J* = 7.8, 1.9, 1.0 Hz, 1H), 6.73 (t, *J* = 2.1 Hz, 1H), 6.53 (ddd, *J* = 7.8, 2.3, 1.0 Hz, 1H), 3.64 (s, br, 2H), 1.29 (s, 9H).



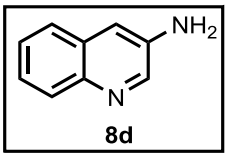
8b

3-bromoaniline (8b)[9]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (t, *J* = 7.9 Hz, 1H), 6.86 (ddd, *J* = 7.9, 1.8, 1.0 Hz, 1H), 6.84 (t, *J* = 2.1 Hz, 1H), 6.59 (ddd, *J* = 7.9, 2.3, 1.0 Hz, 1H), 3.71 (s, br, 2H).



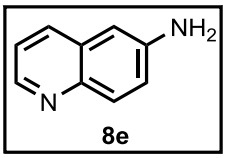
8c

[1,1'-biphenyl]-3-amine (8c)[10]: **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 – 7.55 (m, 2H), 7.45 – 7.40 (m, 2H), 7.37 – 7.31 (m, 1H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.05 – 7.00 (m, 1H), 6.94 (t, *J* = 2.0 Hz, 1H), 6.71 (ddd, *J* = 7.8, 2.3, 1.0 Hz, 1H), 3.76 (s, br, 2H).



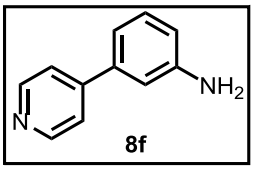
8d

quinolin-3-amine (8d)[11]**: ^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 2.8 Hz, 1H), 8.00 – 7.93 (m, 1H), 7.63 – 7.55 (m, 1H), 7.51 – 7.38 (m, 2H), 7.24 (d, *J* = 2.8, 1H), 3.91 (s, br, 2H).



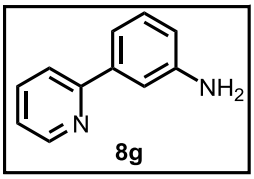
8e

quinolin-6-amine (8e)[11]**: ^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.66 (dd, *J* = 4.2, 1.6 Hz, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.90 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.27 (dd, *J* = 8.0, 4.2 Hz, 1H), 7.16 (dd, *J* = 8.9, 2.6 Hz, 1H), 6.90 (d, *J* = 2.6 Hz, 1H), 3.96 (s, br, 2H),



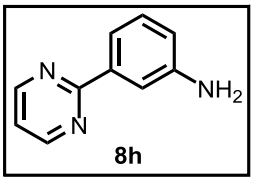
8f

3-(pyridin-4-yl)aniline (8f)[12]**: ^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.66 – 8.60 (m, 2H), 7.50 – 7.44 (m, 2H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.02 (ddd, *J* = 7.7, 1.7, 1.0 Hz, 1H), 6.93 (t, *J* = 2.0 Hz, 1H), 6.76 (ddd, *J* = 8.0, 2.4, 0.9 Hz, 1H), 3.81 (s, br, 2H).



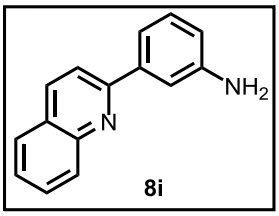
8g

3-(pyridin-2-yl)aniline (8g)[13]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (dt, *J* = 4.7, 1.3 Hz, 1H), 7.74 (td, *J* = 7.5, 7.1, 1.8 Hz, 1H), 7.70 (dt, *J* = 8.0, 1.3 Hz, 1H), 7.39 (t, *J* = 2.0 Hz, 1H), 7.32 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.27 (t, *J* = 7.7 Hz, 1H), 7.22(ddd, *J* = 6.6, 4.7, 1.5 Hz, 1H), 6.75 (ddd, *J* = 7.7, 2.4, 1.1 Hz, 1H), 3.75 (s, br, 2H).



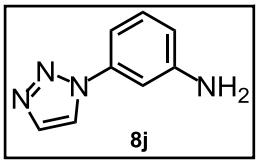
8h

3-(pyrimidin-2-yl)aniline (8h)[14]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.8 Hz, 2H), 7.84 (ddd, *J* = 7.8, 1.6, 1.0 Hz, 1H), 7.79 – 7.76 (m, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.18 (t, *J* = 4.8 Hz, 1H), 6.82 (ddd, *J* = 7.8, 2.5, 1.0 Hz, 1H), 3.79 (s, br, 2H).



8i

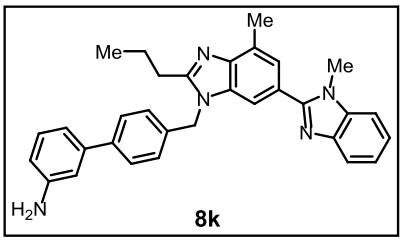
2-(3-aminophenyl)quinoline (8i)[15]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.6 Hz, 1H), 8.16 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.85 (d, *J* = 8.6 Hz, 1H), 7.83 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.72 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.57 (t, *J* = 2.1 Hz, 1H), 7.52 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.48 (ddd, *J* = 7.8, 1.7, 1.0 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 6.80 (ddd, *J* = 7.8, 2.4, 1.0 Hz, 1H), 3.83 (s, br, 2H).



8j

3-(1H-1,2,3-triazol-1-yl)aniline (8j)[16]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 2H),

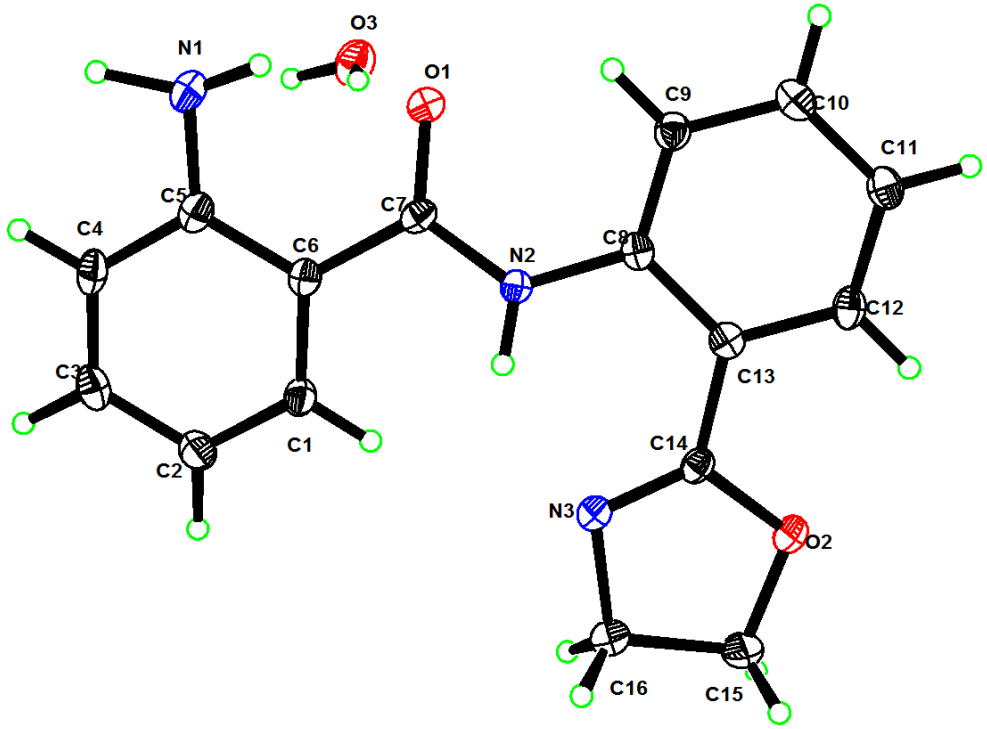
7.46 (ddd, *J* = 8.0, 2.1, 0.9 Hz, 1H), 7.42 (t, *J* = 2.2 Hz, 1H), 7.25 (t, *J* = 8.0 Hz, 1H), 6.66 (ddd, *J* = 8.0, 2.3, 0.9 Hz, 1H), 3.83 (s, br, 2H).



8k

4'-((1,7'-dimethyl-2'-propyl-1H,3'H-[2,5'-bibenzo[d]imidazol]-3'-yl)methyl)-[1,1'-biphenyl]-3-amine (8k): white sticky foam. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 – 7.78 (m, 1H), 7.51 (s, 1H), 7.47 (d, J = 8.1 Hz, 2H), 7.43 (s, 1H), 7.37 – 7.33 (m, 1H), 7.32 – 7.27 (m, 2H), 7.19 (t, J = 7.8 Hz, 1H), 7.10 (d, J = 7.9 Hz, 2H), 6.90 (d, J = 7.7 Hz, 1H), 6.82 (s, 1H), 6.65 (dd, J = 7.9, 2.2 Hz, 1H), 5.43 (s, 2H), 3.77 (s, 3H), 2.96 – 2.89 (m, 2H), 2.77 (s, 3H), 1.87 (h, J = 7.5 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H).; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.67, 154.28, 146.77, 143.20, 141.67, 141.46, 141.13, 136.26, 135.02, 134.62, 129.99, 129.73, 129.51, 127.62, 126.53, 123.77, 122.85, 122.75, 119.18, 117.40, 114.29, 113.62, 109.63, 109.34 , 47.10, 31.85, 29.81, 21.83, 16.90, 14.07.; **HRMS** (ESI-TOF) m/z Calcd for $C_{32}H_{31}N_5$ $[M-H]^-$ 484.2507, found 484.2520.

3.3.1 X-ray Crystallographic Data of 3a-A.



Crystal data

$2(C_{16}H_{15}N_3O_2)\ 0.5(H_4O_2)$	D_x = 1.428 Mg m^{-3}
M_r = 580.63	Mo $K\alpha$ radiation, λ = 0.71073 Å
Orthorhombic, *Fdd*2	Cell parameters from 1035 reflections
a = 29.697 (4) Å	θ = 2.7–27.5 °
b = 33.356 (5) Å	μ = 0.10 mm^{-1}
c = 5.4539 (8) Å	*T* = 170 K
V = 5402.4 (14) Å^3	Block, colourless
Z = 8	0.25 × 0.18 × 0.1 mm
F(000) = 2448	

Data collection

Bruker APEX-II CCD diffractometer	1855 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{int} = 0.058$
Absorption correction: multi-scan *SADABS2008*/1 (Bruker,2008) was used for absorption correction. wR2(int) was 0.0590 before and 0.0429 after correction. The Ratio of minimum to maximum transmission is 0.8637. The $\lambda/2$ correction factor is 0.0015.	$\theta_{max} = 25.0$ °, $\theta_{min} = 1.8$ °
$T_{min} = 0.644$, $T_{max} = 0.746$	$h = -34 \rightarrow 29$
9526 measured reflections	$k = -38 \rightarrow 39$
2262 independent reflections	$l = -6 \rightarrow 6$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rangle_{max} = 0.15$ e Å^{-3}
2262 reflections	$\Delta\rangle_{min} = -0.17$ e Å^{-3}
203 parameters	Absolute structure: Flack x determined using 633 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
6 restraints	Flack parameter: 0.3 (10)
Primary atom site location: dual	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are

estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O2	0.44217 (7)	0.63272 (7)	-0.1272 (4)	0.0332 (6)	
O1	0.34560 (8)	0.74402 (7)	0.6582 (5)	0.0371 (6)	
O3	0.2500	0.7500	0.5445 (8)	0.0447 (10)	
H3A	0.2756	0.7451	0.6074	0.067*	0.5
H3B	0.2296	0.7388	0.6296	0.067*	0.5
N2	0.38244 (8)	0.69290 (8)	0.4684 (5)	0.0247 (6)	
H2	0.3866	0.6668	0.4701	0.030*	
N3	0.40825 (9)	0.62472 (8)	0.2391 (6)	0.0291 (7)	
N1	0.30274 (10)	0.72957 (9)	1.0752 (6)	0.0373 (8)	
H1A	0.3198	0.7439	0.9798	0.045*	
C14	0.42527 (10)	0.64867 (10)	0.0823 (6)	0.0244 (8)	
C13	0.42870 (10)	0.69244 (9)	0.1028 (7)	0.0242 (7)	
C7	0.35261 (9)	0.70742 (10)	0.6358 (6)	0.0254 (8)	
C8	0.40755 (9)	0.71427 (10)	0.2929 (6)	0.0227 (7)	
C5	0.30395 (10)	0.69035 (10)	0.9975 (7)	0.0279 (8)	
C1	0.32594 (10)	0.63667 (9)	0.7226 (7)	0.0295 (8)	
H1	0.3418	0.6277	0.5817	0.035*	
C6	0.32797 (10)	0.67764 (9)	0.7859 (6)	0.0251 (8)	
C12	0.45387 (9)	0.71305 (10)	-0.0731 (6)	0.0283 (8)	
H12	0.4683	0.6984	-0.2004	0.034*	
C9	0.41241 (10)	0.75578 (10)	0.3008 (6)	0.0282 (8)	
H9	0.3987	0.7707	0.4293	0.034*	

C3	0.27861 (11)	0.62212 (11)	1.0644 (7)	0.0343 (9)	
H3	0.2617	0.6035	1.1585	0.041*	
C10	0.43718 (10)	0.77549 (11)	0.1217 (8)	0.0317 (8)	
H10	0.4397	0.8039	0.1276	0.038*	
C4	0.28005 (10)	0.66151 (10)	1.1324 (7)	0.0328 (9)	
H4	0.2644	0.6697	1.2757	0.039*	
C11	0.45824 (10)	0.75458 (10)	-0.0654 (6)	0.0297 (8)	
H11	0.4754	0.7683	-0.1862	0.036*	
C16	0.41328 (12)	0.58381 (10)	0.1411 (7)	0.0362 (9)	
H16A	0.3835	0.5709	0.1187	0.043*	
H16B	0.4318	0.5671	0.2522	0.043*	
C2	0.30184 (11)	0.60933 (11)	0.8576 (7)	0.0342 (9)	
H2A	0.3011	0.5819	0.8101	0.041*	
C15	0.43683 (13)	0.58975 (10)	-0.1047 (8)	0.0407 (10)	
H15A	0.4665	0.5762	-0.1062	0.049*	
H15B	0.4183	0.5790	-0.2405	0.049*	
H1B	0.2849 (14)	0.7286 (8)	1.239 (6)	0.103 (19)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0413 (13)	0.0325 (14)	0.0258 (14)	0.0014 (10)	0.0084 (11)	-0.0044 (11)
O1	0.0478 (15)	0.0269 (13)	0.0366 (17)	0.0032 (11)	0.0129 (12)	-0.0011 (12)
O3	0.042 (2)	0.057 (3)	0.035 (3)	0.009 (2)	0.000	0.000
N2	0.0293 (14)	0.0236 (14)	0.0212 (17)	0.0009 (11)	0.0026 (12)	0.0004 (12)
N3	0.0329 (15)	0.0267 (15)	0.0278 (18)	0.0008 (12)	0.0056 (13)	-0.0019 (13)
N1	0.0410 (18)	0.0392 (18)	0.032 (2)	0.0050 (13)	0.0115 (14)	-0.0034 (15)
C14	0.0234 (15)	0.0295 (19)	0.020 (2)	0.0037 (14)	-0.0006 (15)	-0.0019 (15)
C13	0.0197 (15)	0.0276 (18)	0.025 (2)	-0.0005 (13)	-0.0046 (14)	0.0012 (16)

C7	0.0264 (16)	0.0271 (19)	0.023 (2)	0.0036 (13)	-0.0015 (14)	-0.0047 (16)
C8	0.0195 (15)	0.0288 (18)	0.0199 (19)	-0.0011 (14)	-0.0039 (14)	0.0035 (14)
C5	0.0246 (17)	0.038 (2)	0.022 (2)	0.0060 (14)	-0.0031 (15)	0.0002 (15)
C1	0.0326 (18)	0.033 (2)	0.023 (2)	0.0014 (15)	0.0034 (15)	0.0007 (17)
C6	0.0221 (16)	0.031 (2)	0.022 (2)	0.0003 (14)	-0.0011 (13)	0.0009 (15)
C12	0.0234 (16)	0.039 (2)	0.022 (2)	-0.0018 (15)	-0.0001 (15)	0.0016 (16)
C9	0.0294 (18)	0.0305 (19)	0.025 (2)	-0.0013 (14)	-0.0001 (15)	-0.0010 (16)
C3	0.0308 (18)	0.043 (2)	0.029 (2)	-0.0024 (16)	-0.0015 (17)	0.0120 (18)
C10	0.0327 (18)	0.0303 (19)	0.032 (2)	-0.0053 (15)	-0.0041 (16)	0.0047 (17)
C4	0.0293 (17)	0.049 (2)	0.020 (2)	0.0058 (16)	0.0030 (14)	0.0055 (17)
C11	0.0280 (17)	0.035 (2)	0.026 (2)	-0.0041 (15)	-0.0025 (15)	0.0047 (17)
C16	0.043 (2)	0.029 (2)	0.037 (3)	0.0022 (15)	0.0064 (18)	-0.0031 (17)
C2	0.0376 (19)	0.032 (2)	0.033 (2)	-0.0031 (15)	0.0003 (18)	0.0035 (17)
C15	0.056 (2)	0.027 (2)	0.039 (3)	0.0011 (16)	0.0091 (18)	-0.0053 (18)

Geometric parameters (Å, º)

O2—C14	1.357 (4)	C1—H1	0.9500
O2—C15	1.447 (4)	C1—C6	1.411 (4)
O1—C7	1.244 (3)	C1—C2	1.374 (5)
O3—H3A	0.8500	C12—H12	0.9500
O3—H3B	0.8492	C12—C11	1.392 (4)
N2—H2	0.8800	C9—H9	0.9500
N2—C7	1.361 (4)	C9—C10	1.388 (5)
N2—C8	1.407 (4)	C3—H3	0.9500
N3—C14	1.275 (4)	C3—C4	1.366 (5)
N3—C16	1.473 (4)	C3—C2	1.389 (5)
N1—H1A	0.8708	C10—H10	0.9500
N1—C5	1.375 (4)	C10—C11	1.385 (5)

N1—H1B	1.04 (2)	C4—H4	0.9500
C14—C13	1.468 (4)	C11—H11	0.9500
C13—C8	1.414 (5)	C16—H16A	0.9900
C13—C12	1.397 (5)	C16—H16B	0.9900
C7—C6	1.481 (5)	C16—C15	1.525 (5)
C8—C9	1.393 (4)	C2—H2A	0.9500
C5—C6	1.422 (5)	C15—H15A	0.9900
C5—C4	1.404 (5)	C15—H15B	0.9900
C14—O2—C15	106.0 (3)	C11—C12—H12	119.4
H3A—O3—H3B	109.4	C8—C9—H9	119.9
C7—N2—H2	115.8	C10—C9—C8	120.2 (3)
C7—N2—C8	128.4 (3)	C10—C9—H9	119.9
C8—N2—H2	115.8	C4—C3—H3	120.0
C14—N3—C16	107.3 (3)	C4—C3—C2	120.0 (3)
H1A—N1—H1B	145.9	C2—C3—H3	120.0
C5—N1—H1A	108.9	C9—C10—H10	119.4
C5—N1—H1B	104.3 (15)	C11—C10—C9	121.3 (3)
O2—C14—C13	115.4 (3)	C11—C10—H10	119.4
N3—C14—O2	117.8 (3)	C5—C4—H4	118.9
N3—C14—C13	126.9 (3)	C3—C4—C5	122.2 (4)
C8—C13—C14	122.5 (3)	C3—C4—H4	118.9
C12—C13—C14	118.3 (3)	C12—C11—H11	120.6
C12—C13—C8	119.2 (3)	C10—C11—C12	118.8 (3)
O1—C7—N2	121.6 (3)	C10—C11—H11	120.6
O1—C7—C6	121.4 (3)	N3—C16—H16A	110.9
N2—C7—C6	117.0 (3)	N3—C16—H16B	110.9
N2—C8—C13	118.2 (3)	N3—C16—C15	104.2 (3)

C9—C8—N2	122.5 (3)	H16A—C16—H16B	108.9
C9—C8—C13	119.2 (3)	C15—C16—H16A	110.9
N1—C5—C6	123.2 (3)	C15—C16—H16B	110.9
N1—C5—C4	118.5 (3)	C1—C2—C3	119.3 (3)
C4—C5—C6	118.3 (3)	C1—C2—H2A	120.3
C6—C1—H1	118.9	C3—C2—H2A	120.3
C2—C1—H1	118.9	O2—C15—C16	104.7 (3)
C2—C1—C6	122.3 (3)	O2—C15—H15A	110.8
C5—C6—C7	119.8 (3)	O2—C15—H15B	110.8
C1—C6—C7	122.4 (3)	C16—C15—H15A	110.8
C1—C6—C5	117.8 (3)	C16—C15—H15B	110.8
C13—C12—H12	119.4	H15A—C15—H15B	108.9
C11—C12—C13	121.3 (3)		
O2—C14—C13—C8	171.4 (3)	C7—N2—C8—C9	14.3 (5)
O2—C14—C13—C12	-8.5 (4)	C8—N2—C7—O1	-3.4 (5)
O1—C7—C6—C5	-15.1 (5)	C8—N2—C7—C6	175.1 (3)
O1—C7—C6—C1	162.7 (3)	C8—C13—C12—C11	-0.4 (4)
N2—C7—C6—C5	166.4 (3)	C8—C9—C10—C11	-1.2 (5)
N2—C7—C6—C1	-15.8 (4)	C6—C5—C4—C3	-1.1 (5)
N2—C8—C9—C10	-179.3 (3)	C6—C1—C2—C3	-0.2 (5)
N3—C14—C13—C8	-8.5 (5)	C12—C13—C8—N2	-179.9 (3)
N3—C14—C13—C12	171.5 (3)	C12—C13—C8—C9	-0.2 (4)
N3—C16—C15—O2	-1.2 (4)	C9—C10—C11—C12	0.6 (5)
N1—C5—C6—C7	-1.0 (5)	C4—C5—C6—C7	178.5 (3)
N1—C5—C6—C1	-178.9 (3)	C4—C5—C6—C1	0.6 (5)
N1—C5—C4—C3	178.4 (3)	C4—C3—C2—C1	-0.3 (5)
C14—O2—C15—C16	1.8 (3)	C16—N3—C14—O2	1.3 (4)

C14—N3—C16—C15	0.0 (4)	C16—N3—C14—C13	-178.8 (3)
C14—C13—C8—N2	0.2 (4)	C2—C1—C6—C7	-177.8 (3)
C14—C13—C8—C9	179.8 (3)	C2—C1—C6—C5	0.0 (5)
C14—C13—C12—C11	179.6 (3)	C2—C3—C4—C5	1.0 (5)
C13—C8—C9—C10	1.0 (4)	C15—O2—C14—N3	-2.1 (4)
C13—C12—C11—C10	0.2 (5)	C15—O2—C14—C13	178.0 (3)
C7—N2—C8—C13	-166.1 (3)		

3.3.2 X-ray Crystallographic Data of 5a.

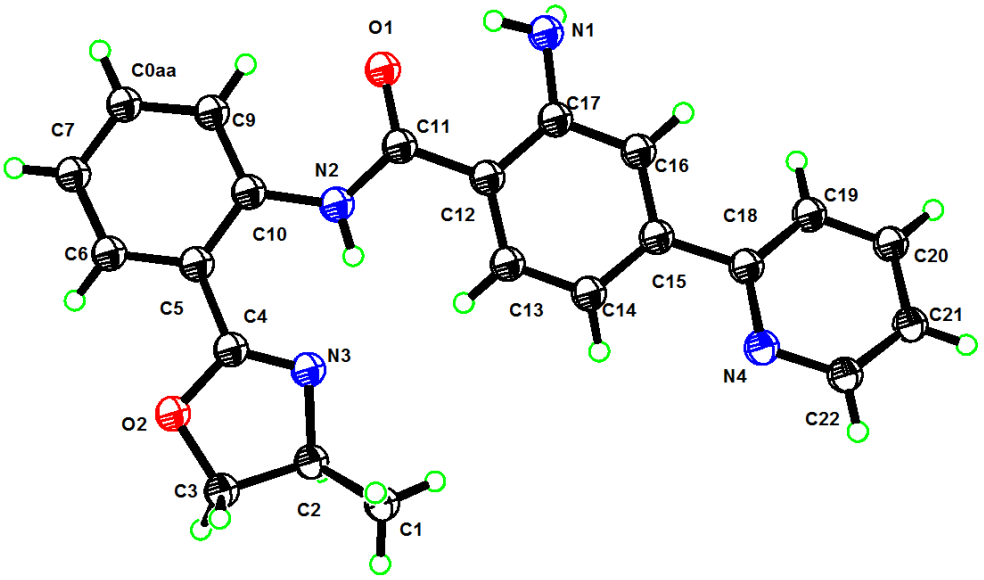


Table S12 Crystal data and structure refinement for mo_2017795_0m.

Identification code	mo_2017795_0m
Empirical formula	$C_{22}H_{20}N_4O_2$
Formula weight	372.42
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1$
a/Å	12.646(2)
b/Å	8.4619(16)
c/Å	17.452(3)
α/°	90
β/°	90.459(5)
γ/°	90
Volume/Å^3	1867.5(6)

Z	4
ρ_{calc}g/cm^3	1.325
μ/mm^{-1}	0.088
F(000)	784.0
Crystal size/mm^3	0.18 × 0.11 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/ °	2.334 to 54.942
Index ranges	-16 ≤ h ≤ 16, -10 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected	17022
Independent reflections	8399 [R_{int} = 0.0601, R_{sigma} = 0.1120]
Data/restraints/parameters	8399/446/510
Goodness-of-fit on F^2	0.966
Final R indexes [I>=2σ (I)]	R_1 = 0.0607, wR_2 = 0.1164
Final R indexes [all data]	R_1 = 0.1385, wR_2 = 0.1516
Largest diff. peak/hole / e Å^{-3}	0.20/-0.20
Flack parameter	-2(2)

Table S13 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for mo_2017795_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	3592(3)	4514(4)	127.0(18)	50.8(10)
O2	652(3)	1030(4)	2553.5(19)	52(1)
O3	5503(3)	1330(5)	2540(2)	57.5(10)
O4	8614(3)	4832(5)	4888.9(19)	55(1)
N2	2839(3)	3427(5)	1170(2)	41.6(10)
N6	7756(3)	3822(5)	3855(2)	43.1(11)
N5	6982(3)	2809(5)	2517(2)	46.5(11)
N3	2244(3)	2236(5)	2525(2)	45.7(11)
C11	3585(4)	4344(6)	832(3)	35.7(11)
N1	5271(4)	6343(6)	245(2)	58.9(13)
C12	4383(4)	5090(5)	1336(3)	33.5(11)
C35	10174(4)	6305(6)	3940(3)	41.9(12)
C14	5107(4)	5650(6)	2607(3)	38.7(12)
C32	6890(4)	3068(6)	4214(3)	44.2(13)

C17	5180(4)	6050(6)	1013(3)	38.5(12)
C10	1977(4)	2634(6)	832(3)	40.0(12)
C27	6158(4)	2242(6)	3750(3)	43.9(13)
N7	10234(4)	6739(7)	4704(2)	68.2(15)
C37	10939(4)	6509(6)	2672(3)	38.6(11)
C5	1284(4)	1805(6)	1318(3)	40.2(12)
C18	6683(4)	7437(6)	2785(3)	39.0(12)
N4	6400(4)	7697(6)	3524(3)	64.1(14)
C33	8558(4)	4630(6)	4185(3)	40.0(12)
C36	10919(4)	6897(6)	3438(3)	45.4(13)
C4	1444(4)	1734(6)	2148(3)	40.7(12)
C13	4384(4)	4924(6)	2135(3)	37.7(12)
C16	5912(4)	6782(6)	1508(3)	39.8(12)
C8	12593(4)	7950(6)	2472(3)	42.1(13)
C38	10185(4)	5418(6)	2395(3)	42.7(13)
C26	6274(4)	2170(6)	2916(3)	44.5(13)
C39	9440(4)	4825(6)	2880(3)	40.7(12)
C34	9387(4)	5244(6)	3665(3)	39.3(12)
C15	5894(4)	6604(6)	2295(3)	37.5(11)
C24	6751(4)	2462(6)	1698(3)	47.6(13)
C2	2091(4)	1781(6)	3337(3)	47.7(13)
C40	11734(4)	7236(6)	2153(3)	43.6(13)
C9	1784(4)	2638(7)	50(3)	52.7(14)
C19	7633(4)	7935(7)	2498(3)	45.0(13)
N41	11535(4)	7206(6)	1378(3)	74.1(16)
C25	5808(4)	1338(7)	1745(3)	53.5(14)
C3	926(4)	1267(7)	3351(3)	52.7(14)
C31	6752(4)	3100(8)	5003(3)	60.2(16)
C20	8314(5)	8737(7)	2969(4)	64.8(17)
C44	13290(4)	8668(7)	1997(4)	70.6(18)
C7	255(4)	984(8)	219(3)	63.6(17)
C6	435(4)	983(7)	996(3)	53.3(15)
C22	7105(6)	8494(8)	3973(4)	75.0(19)
C23	7694(4)	1789(7)	1296(3)	64.6(17)
C21	8046(6)	9042(8)	3715(4)	75.0(19)

C0AA	928(4)	1801(8)	-249(3)	65.8(18)
C1	2363(5)	3118(7)	3880(3)	65.3(17)
C42	12272(7)	7952(9)	921(4)	83(2)
C30	5902(5)	2317(8)	5326(4)	76(2)
C28	5315(4)	1493(8)	4098(3)	61.7(16)
C43	13134(6)	8706(8)	1228(5)	86(2)
C29	5179(5)	1529(9)	4880(4)	78(2)

Table S14 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for mo_2017795 _0m. 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	62(2)	59(2)	32.0(19)	-2.1(18)	1.5(17)	-8(2)
O2	51(2)	57(2)	49(2)	10.8(19)	4.1(16)	-6.4(19)
O3	54(2)	55(2)	63(2)	-4(2)	-9.2(18)	-10(2)
O4	66(2)	64(3)	35(2)	1.7(19)	-2.6(17)	-8(2)
N2	42(2)	49(3)	34(2)	4(2)	-1.0(18)	-1(2)
N6	43(2)	52(3)	34(2)	-4(2)	-0.7(19)	0(2)
N5	43(2)	53(3)	44(2)	-9(2)	-3.5(19)	1(2)
N3	47(2)	51(3)	39(2)	3(2)	3.1(19)	0(2)
C11	38(3)	35(3)	34(3)	4(2)	1(2)	9(2)
N1	63(3)	79(4)	35(2)	1(2)	9(2)	-13(3)
C12	38(2)	32(3)	31(2)	4(2)	5.5(19)	7(2)
C35	46(3)	44(3)	35(3)	-7(2)	-11(2)	5(2)
C14	48(3)	37(3)	32(3)	7(2)	1(2)	2(2)
C32	42(3)	46(3)	44(3)	-3(2)	4(2)	6(2)
C17	48(3)	36(3)	31(3)	0(2)	5(2)	3(2)
C10	33(2)	48(3)	39(3)	-1(2)	0(2)	3(2)
C27	41(3)	42(3)	48(3)	-5(2)	2(2)	5(2)
N7	79(4)	87(4)	39(2)	-11(3)	0(2)	-29(3)
C37	41(3)	35(3)	40(3)	0(2)	-6(2)	10(2)
C5	34(2)	45(3)	42(3)	4(2)	-2(2)	8(2)
C18	46(3)	34(3)	37(3)	2(2)	-5(2)	8(2)

N4	79(3)	65(3)	48(3)	2(3)	-7(2)	8(3)
C33	47(3)	40(3)	33(3)	-3(2)	-6(2)	8(2)
C36	47(3)	46(3)	42(3)	-5(2)	-4(2)	-1(3)
C4	40(3)	37(3)	45(3)	5(2)	3(2)	4(2)
C13	39(3)	36(3)	38(3)	6(2)	6(2)	0(2)
C16	44(3)	41(3)	35(3)	4(2)	8(2)	0(2)
C8	34(2)	39(3)	53(3)	-1(3)	0(2)	1(2)
C38	47(3)	42(3)	39(3)	-6(2)	1(2)	0(3)
C26	35(3)	41(3)	57(3)	-9(3)	-5(2)	7(2)
C39	45(3)	42(3)	35(3)	-3(2)	-10(2)	-2(2)
C34	44(3)	39(3)	35(3)	-4(2)	-9(2)	4(2)
C15	40(3)	38(3)	35(2)	6(2)	1(2)	2(2)
C24	58(3)	39(3)	46(3)	-1(2)	-15(2)	4(3)
C2	60(3)	47(3)	36(3)	7(2)	-1(2)	7(3)
C40	48(3)	34(3)	48(3)	-1(2)	2(2)	7(2)
C9	53(3)	61(4)	44(3)	-4(3)	-2(2)	2(3)
C19	39(3)	44(3)	52(3)	3(3)	-3(2)	1(3)
N41	102(4)	67(4)	53(3)	4(3)	5(3)	16(3)
C25	59(3)	46(3)	55(3)	-6(3)	-11(3)	2(3)
C3	60(3)	54(3)	44(3)	7(3)	5(2)	3(3)
C31	58(3)	72(4)	51(3)	-6(3)	11(3)	1(3)
C20	46(3)	54(4)	95(4)	14(4)	-15(3)	-5(3)
C44	43(3)	53(4)	117(5)	6(4)	14(3)	2(3)
C7	49(3)	80(5)	62(4)	5(3)	-14(3)	-10(3)
C6	42(3)	65(4)	53(3)	7(3)	-5(2)	-6(3)
C22	97(5)	76(5)	51(4)	-4(3)	-18(3)	10(4)
C23	71(4)	76(4)	46(3)	-7(3)	3(3)	3(3)
C21	79(4)	57(4)	88(5)	-8(4)	-43(4)	12(4)
C0AA	57(3)	93(5)	47(3)	-4(3)	-9(3)	-11(3)
C1	89(4)	64(4)	43(3)	-1(3)	-5(3)	-3(4)
C42	129(6)	65(5)	55(4)	12(3)	25(4)	21(4)
C30	77(4)	95(5)	58(4)	-3(4)	24(3)	-13(4)
C28	47(3)	67(4)	72(4)	-13(3)	7(3)	-6(3)
C43	102(5)	51(4)	106(5)	9(4)	61(4)	26(4)
C29	68(4)	87(5)	77(4)	-7(4)	27(3)	-18(4)

Table S15 Bond Lengths for mo_2017795_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C11	1.239(5)	C37	C38	1.410(7)
O2	C4	1.368(5)	C37	C40	1.491(7)
O2	C3	1.445(6)	C5	C4	1.463(7)
O3	C26	1.369(6)	C5	C6	1.394(7)
O3	C25	1.443(6)	C18	N4	1.360(6)
O4	C33	1.242(5)	C18	C15	1.486(7)
N2	C11	1.360(6)	C18	C19	1.371(7)
N2	C10	1.406(6)	N4	C22	1.361(8)
N6	C32	1.418(6)	C33	C34	1.486(7)
N6	C33	1.349(6)	C16	C15	1.382(6)
N5	C26	1.260(6)	C8	C40	1.358(7)
N5	C24	1.486(6)	C8	C44	1.358(7)
N3	C4	1.275(6)	C38	C39	1.367(7)
N3	C2	1.482(6)	C39	C34	1.416(6)
C11	C12	1.475(7)	C24	C25	1.528(7)
N1	C17	1.369(5)	C24	C23	1.501(7)
C12	C17	1.415(6)	C2	C3	1.537(7)
C12	C13	1.402(6)	C2	C1	1.514(7)
C35	N7	1.383(6)	C40	N41	1.374(7)
C35	C36	1.386(7)	C9	C0AA	1.392(7)
C35	C34	1.422(7)	C19	C20	1.366(8)
C14	C13	1.371(6)	N41	C42	1.384(8)
C14	C15	1.396(6)	C31	C30	1.386(8)
C32	C27	1.410(7)	C20	C21	1.372(9)
C32	C31	1.390(7)	C44	C43	1.355(9)
C17	C16	1.405(7)	C7	C6	1.373(7)
C10	C5	1.412(7)	C7	C0AA	1.371(8)
C10	C9	1.383(6)	C22	C21	1.358(9)
C27	C26	1.466(7)	C42	C43	1.369(10)
C27	C28	1.386(7)	C30	C29	1.370(9)
C37	C36	1.377(6)	C28	C29	1.377(8)

Table S16 Bond Angles for mo_2017795_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	O2	C3	105.5(4)	N3	C4	O2	117.4(4)
C26	O3	C25	105.3(4)	N3	C4	C5	126.9(4)
C11	N2	C10	129.0(4)	C14	C13	C12	123.2(4)
C33	N6	C32	128.3(4)	C15	C16	C17	123.1(5)
C26	N5	C24	108.1(4)	C40	C8	C44	118.0(6)
C4	N3	C2	107.3(4)	C39	C38	C37	119.7(5)
O1	C11	N2	120.5(5)	O3	C26	C27	114.9(5)
O1	C11	C12	122.2(4)	N5	C26	O3	117.7(5)
N2	C11	C12	117.3(4)	N5	C26	C27	127.4(5)
C17	C12	C11	119.6(4)	C38	C39	C34	123.1(5)
C13	C12	C11	123.1(4)	C35	C34	C33	120.6(4)
C13	C12	C17	117.3(4)	C39	C34	C35	116.5(5)
N7	C35	C36	118.8(5)	C39	C34	C33	122.8(5)
N7	C35	C34	121.8(5)	C14	C15	C18	121.8(4)
C36	C35	C34	119.5(4)	C16	C15	C14	117.9(5)
C13	C14	C15	119.9(4)	C16	C15	C18	120.3(4)
C27	C32	N6	118.4(4)	N5	C24	C25	102.7(4)
C31	C32	N6	122.2(5)	N5	C24	C23	112.0(4)
C31	C32	C27	119.4(5)	C23	C24	C25	114.3(5)
N1	C17	C12	124.1(5)	N3	C2	C3	102.8(4)
N1	C17	C16	117.4(4)	N3	C2	C1	111.9(4)
C16	C17	C12	118.5(4)	C1	C2	C3	114.5(5)
N2	C10	C5	117.9(4)	C8	C40	C37	118.4(5)
C9	C10	N2	122.9(5)	C8	C40	N41	123.4(5)
C9	C10	C5	119.2(5)	N41	C40	C37	118.1(5)
C32	C27	C26	121.4(5)	C10	C9	C0AA	120.0(5)
C28	C27	C32	118.6(5)	C20	C19	C18	118.9(5)
C28	C27	C26	120.0(5)	C40	N41	C42	116.1(6)
C36	C37	C38	118.1(5)	O3	C25	C24	105.6(4)
C36	C37	C40	120.6(5)	O2	C3	C2	104.2(4)
C38	C37	C40	121.3(4)	C30	C31	C32	119.9(6)

C10	C5	C4	122.3(4)	C19	C20	C21	120.3(6)
C6	C5	C10	119.0(5)	C43	C44	C8	121.7(7)
C6	C5	C4	118.6(5)	C0AA	C7	C6	119.3(5)
N4	C18	C15	116.3(4)	C7	C6	C5	121.3(5)
N4	C18	C19	122.3(5)	C21	C22	N4	123.4(6)
C19	C18	C15	121.4(5)	C22	C21	C20	118.3(7)
C18	N4	C22	116.8(5)	C7	C0AA	C9	121.2(5)
O4	C33	N6	121.9(5)	C43	C42	N41	121.6(7)
O4	C33	C34	121.4(5)	C29	C30	C31	121.2(6)
N6	C33	C34	116.6(4)	C29	C28	C27	121.8(6)
C37	C36	C35	123.1(5)	C44	C43	C42	119.1(7)
O2	C4	C5	115.7(4)	C30	C29	C28	119.1(6)

Table S17 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for mo_2017795_0m.

Atom	***x***	***y***	***z***	**U(eq)**
H2	2904	3317	1658	50
H6A	7772	3755	3363	52
H1A	5789	5788	70	71
H1B	4693	6065	15	71
H14	5074	5507	3135	46
H7A	10397	7724	4733	82
H7B	9626	6588	4909	82
H36	11429	7590	3627	54
H13	3869	4290	2356	45
H16	6434	7416	1295	48
H8	12701	7946	3000	51
H38	10194	5104	1885	51
H39	8946	4113	2686	49
H24	6530	3438	1440	57
H2A	2540	868	3456	57
H9	2225	3200	-275	63
H19	7810	7730	1992	54

H25A	5230	1709	1423	64
H25B	6007	285	1580	64
H3A	842	296	3640	63
H3B	487	2080	3577	63
H31	7228	3645	5314	72
H20	8962	9079	2783	78
H44	13889	9146	2205	85
H7	-318	436	12	76
H6	-18	424	1313	64
H22	6933	8673	4483	90
H23A	8257	2551	1300	97
H23B	7505	1540	776	97
H23C	7923	847	1554	97
H21	8498	9609	4035	90
H0AA	810	1796	-776	79
H1C	3098	3382	3831	98
H1D	2225	2795	4397	98
H1E	1939	4026	3757	98
H42	12179	7941	391	100
H30	5822	2327	5856	92
H28	4827	952	3796	74
H43	13606	9236	913	103
H29	4604	1025	5102	93

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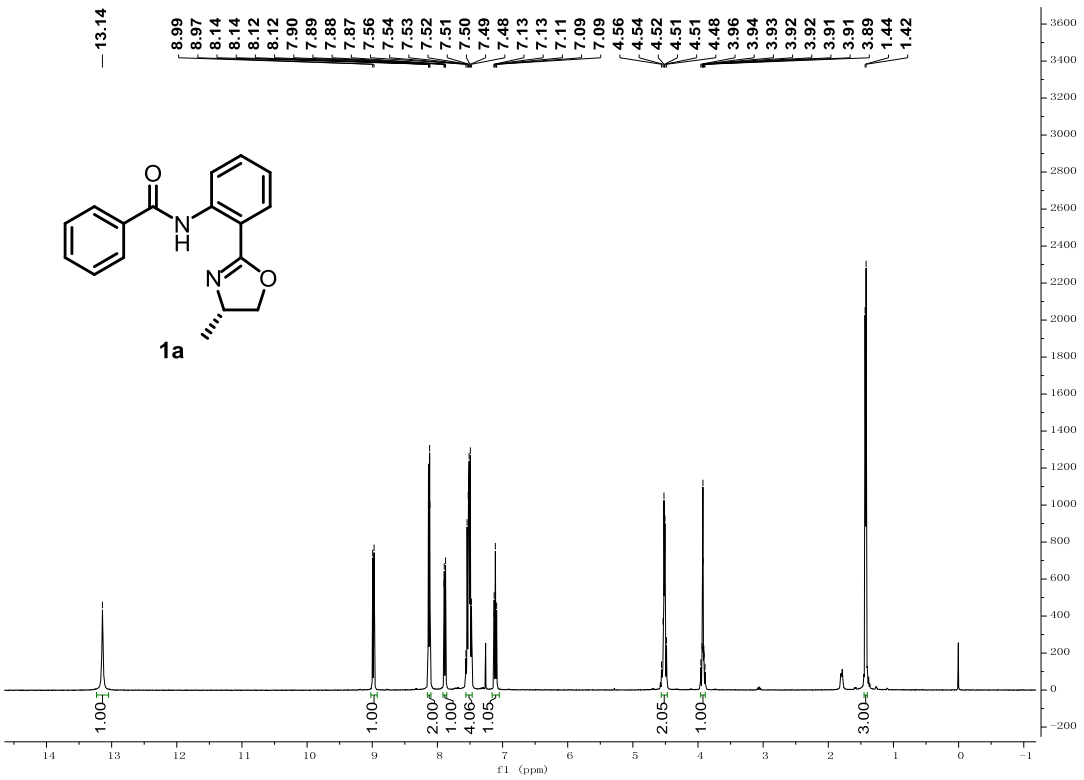
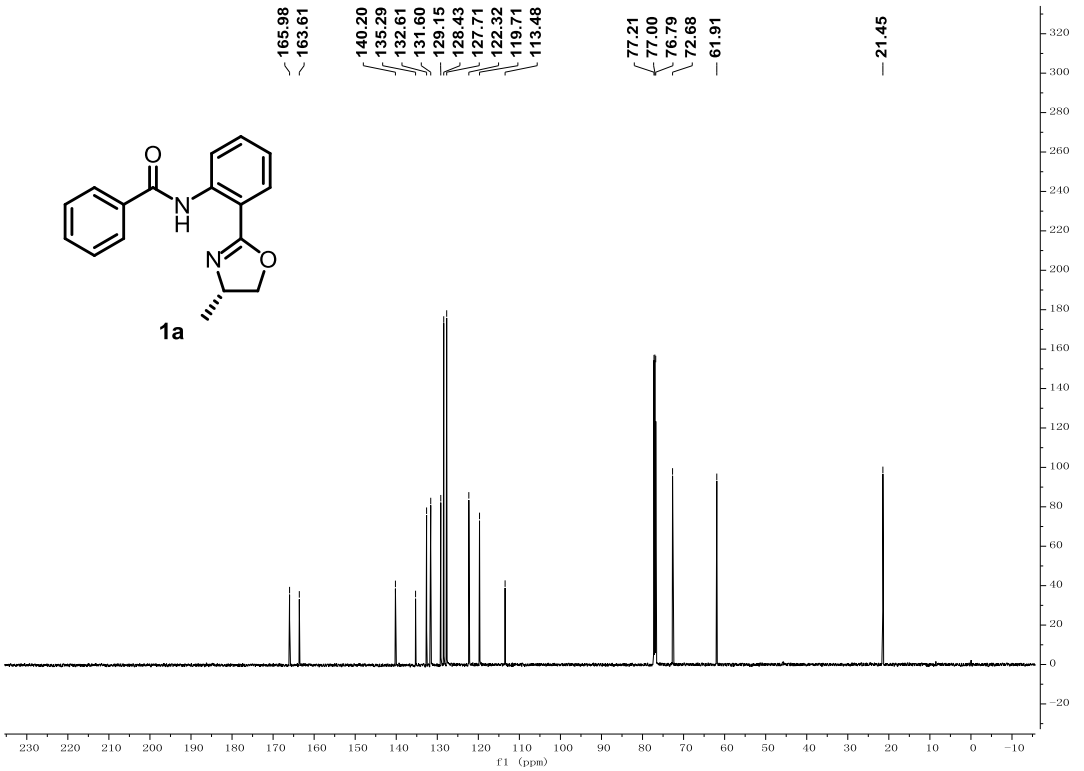
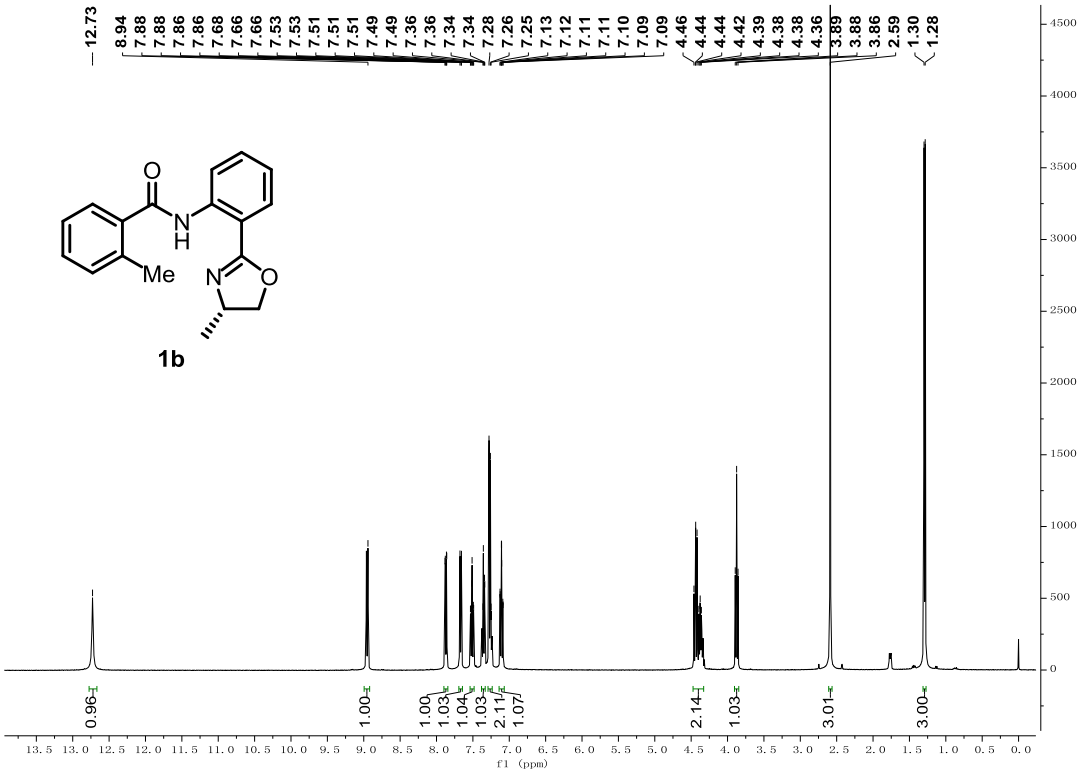
5. NMR Spectra for New Compounds.



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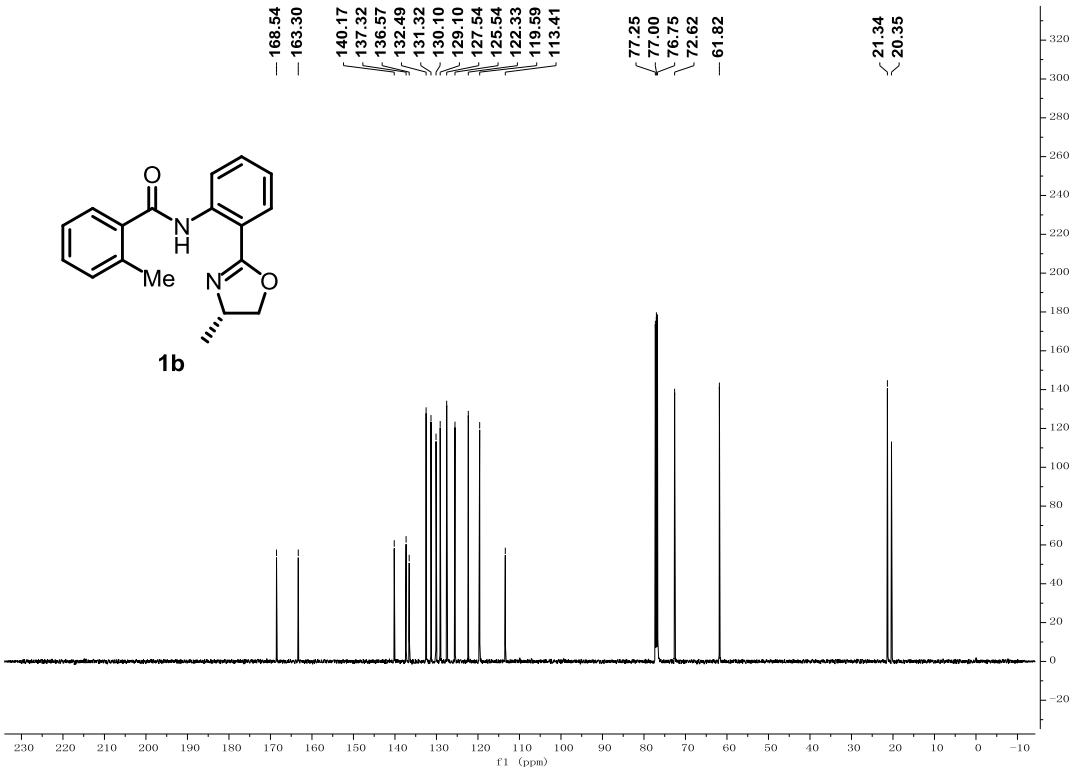
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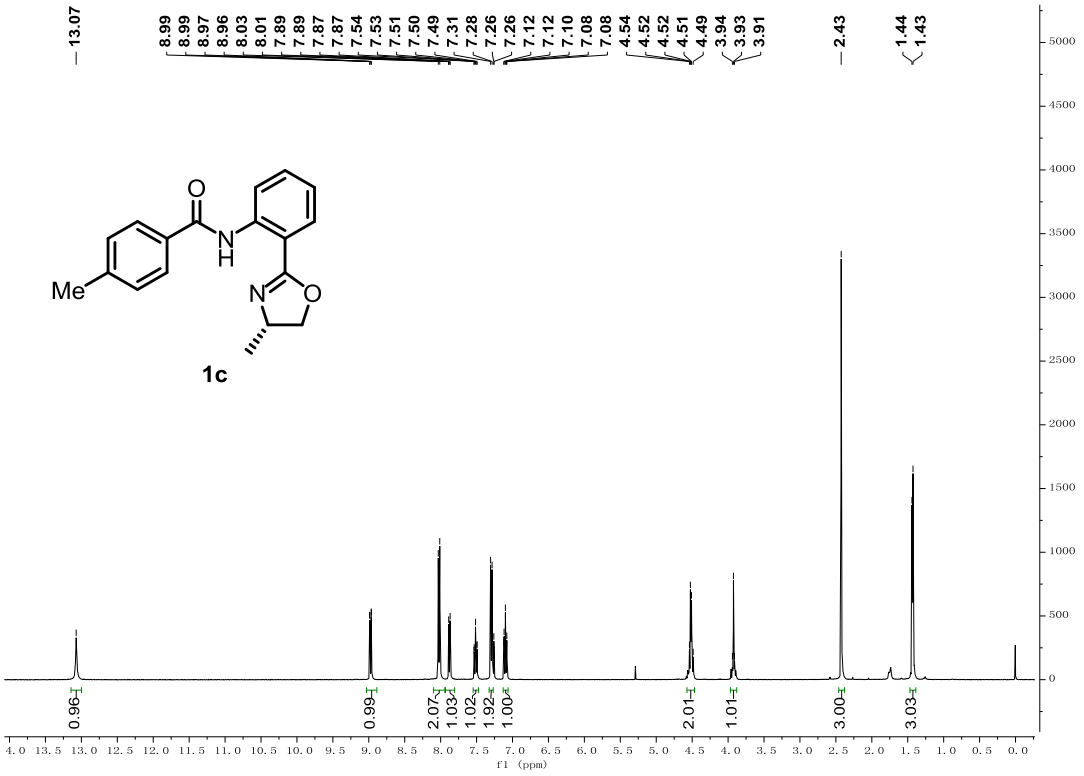
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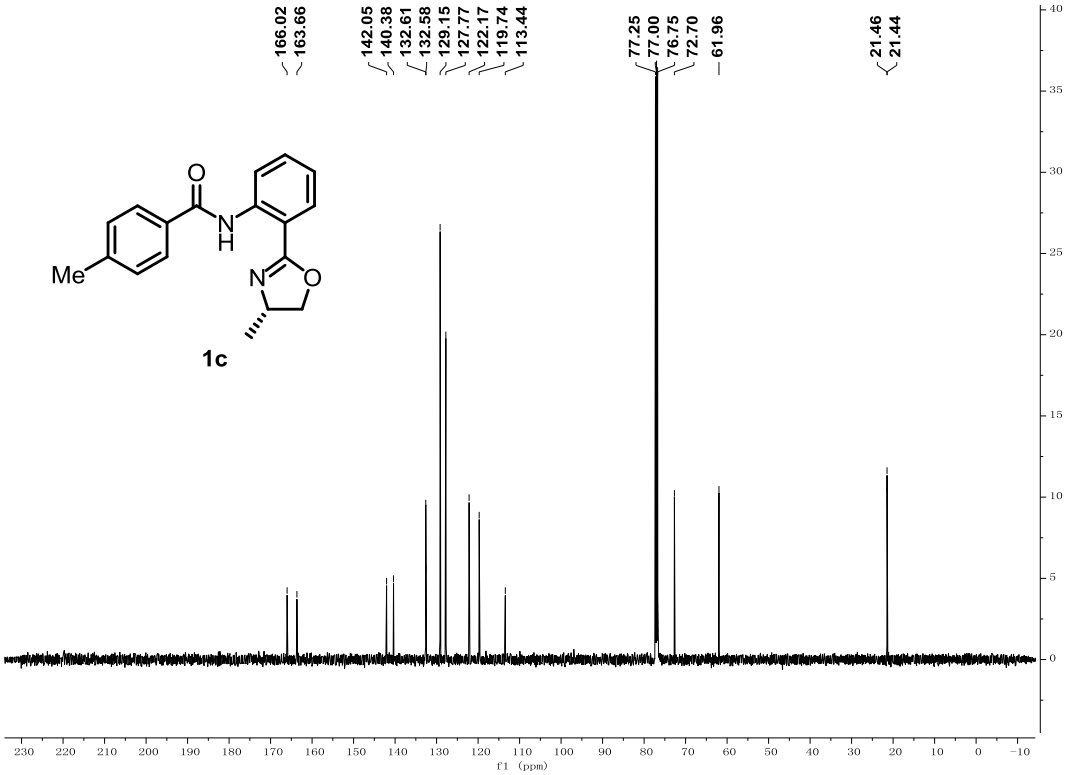
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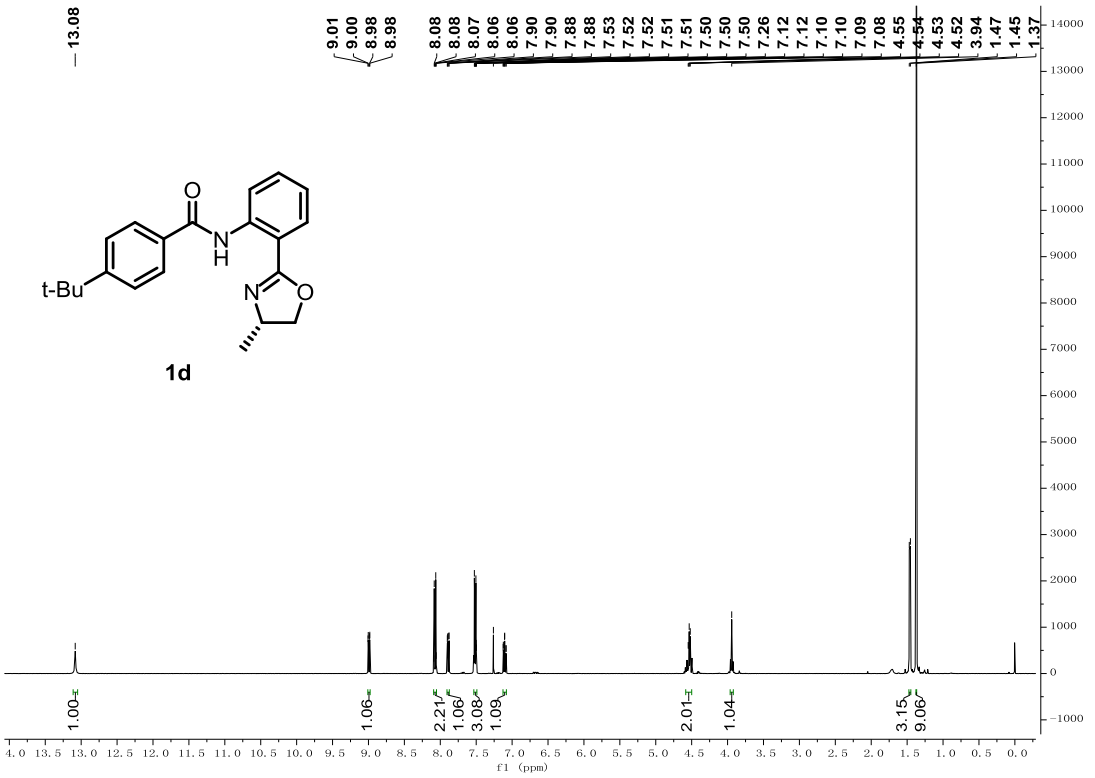
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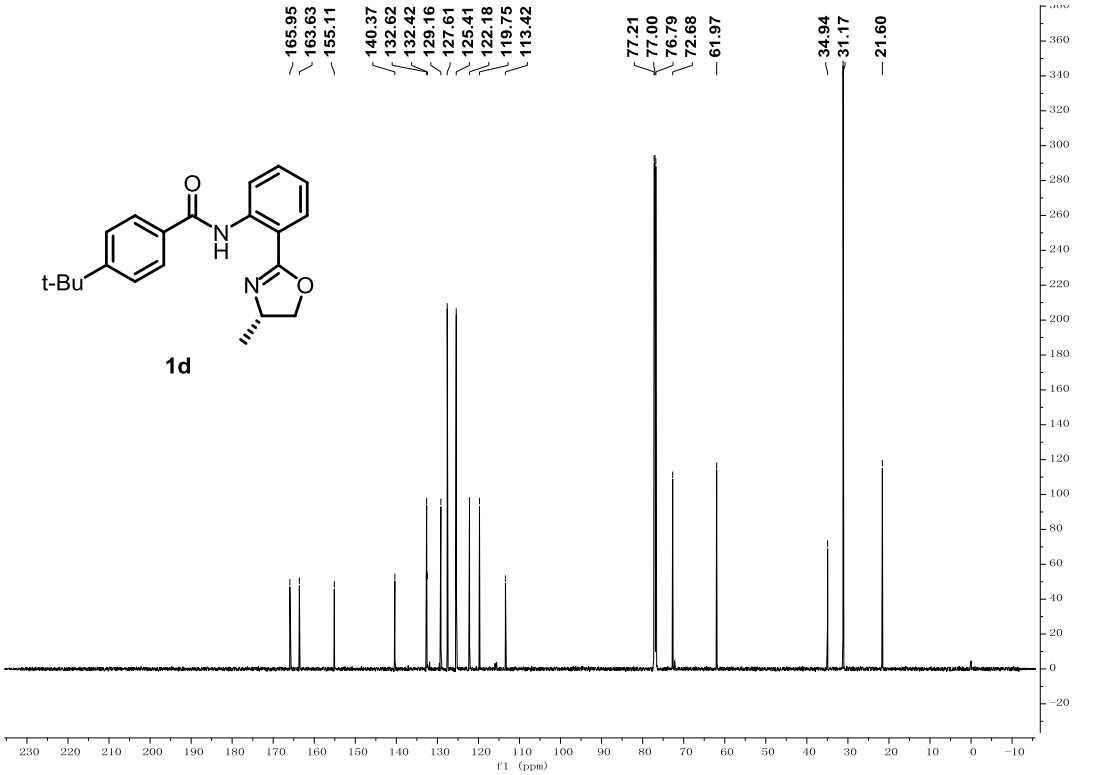
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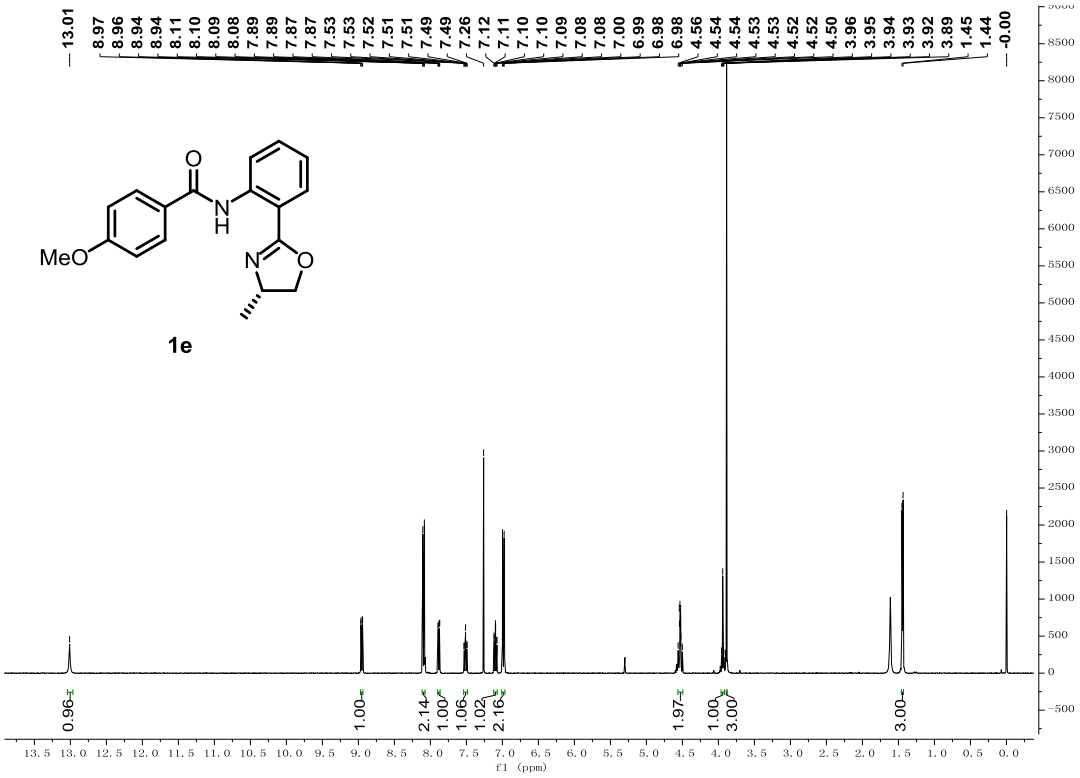
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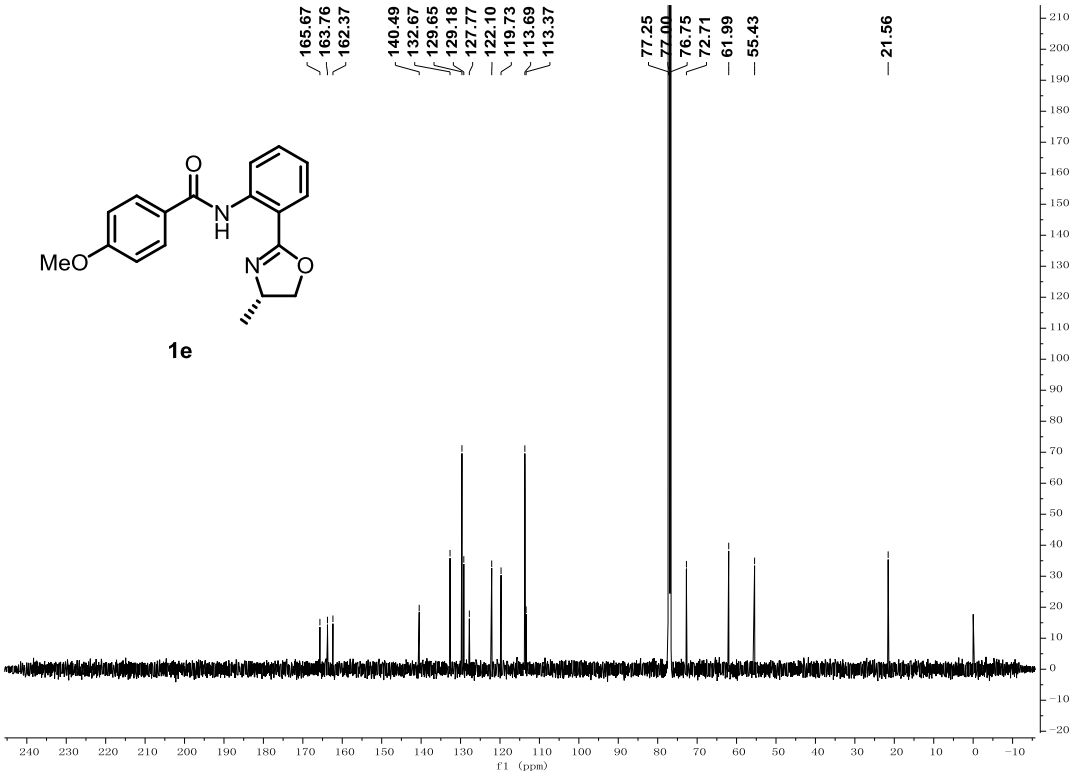
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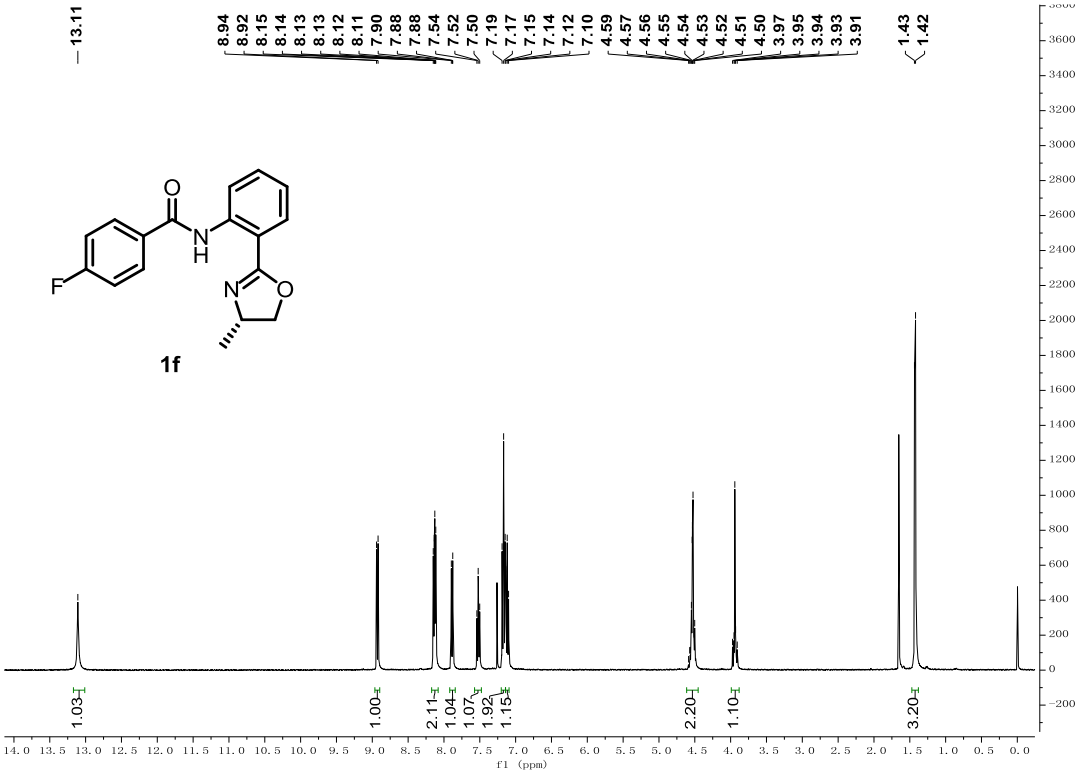
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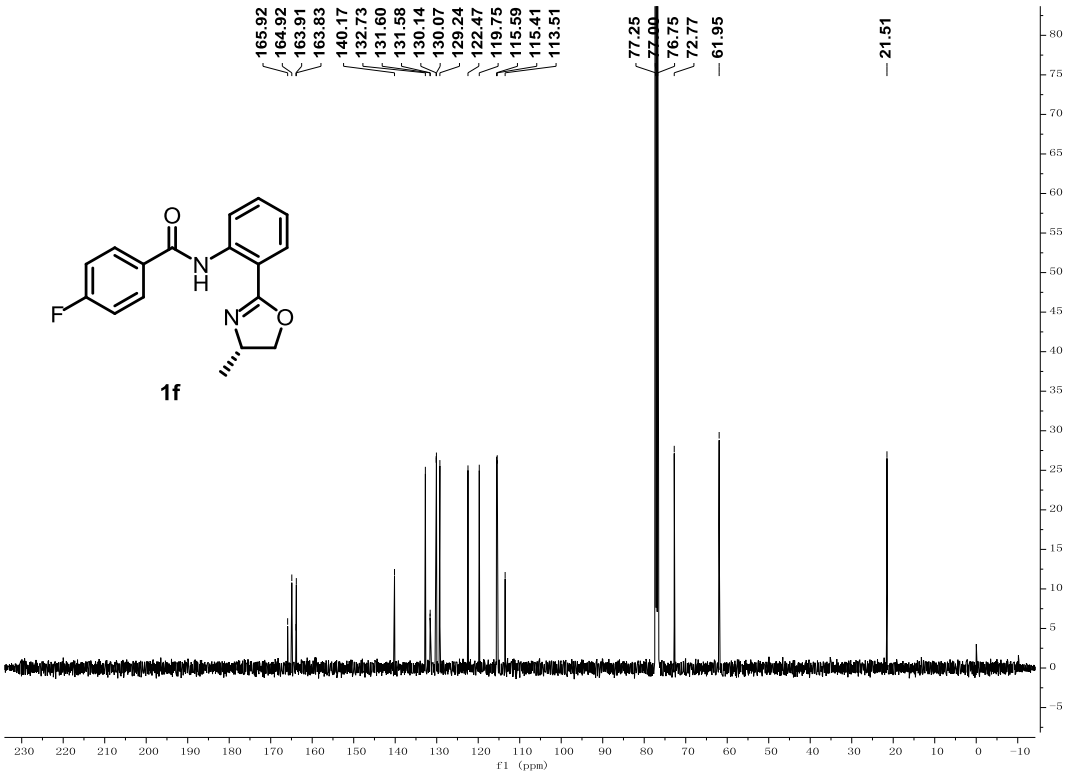
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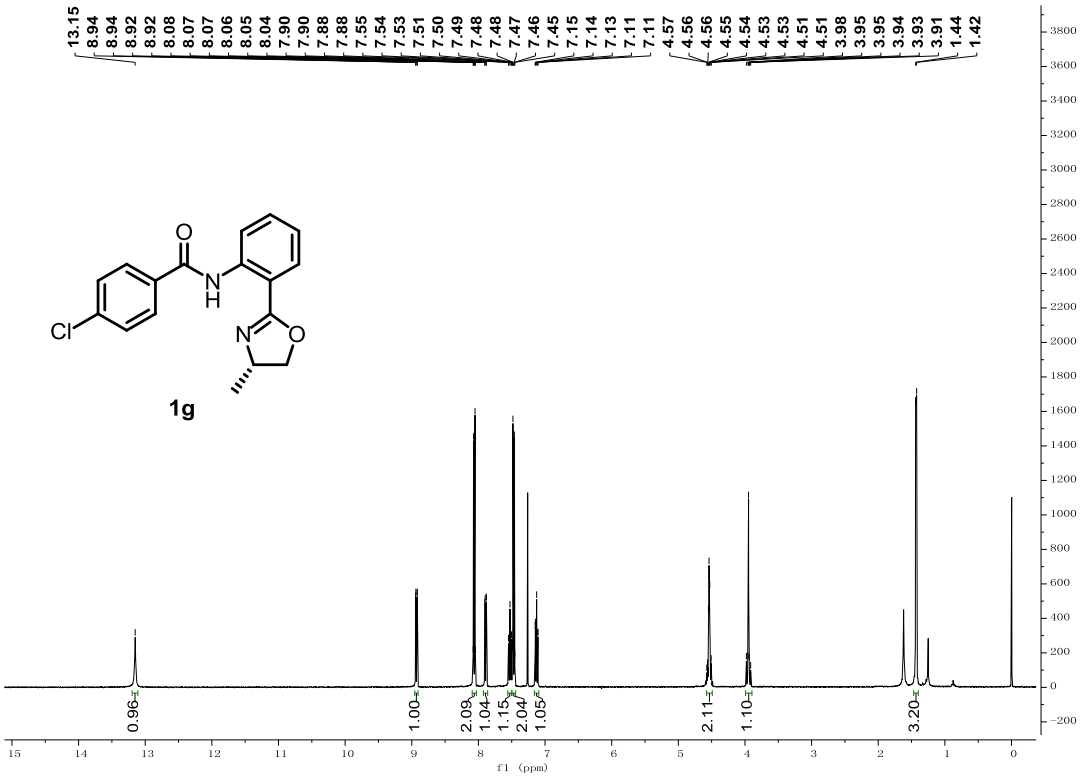
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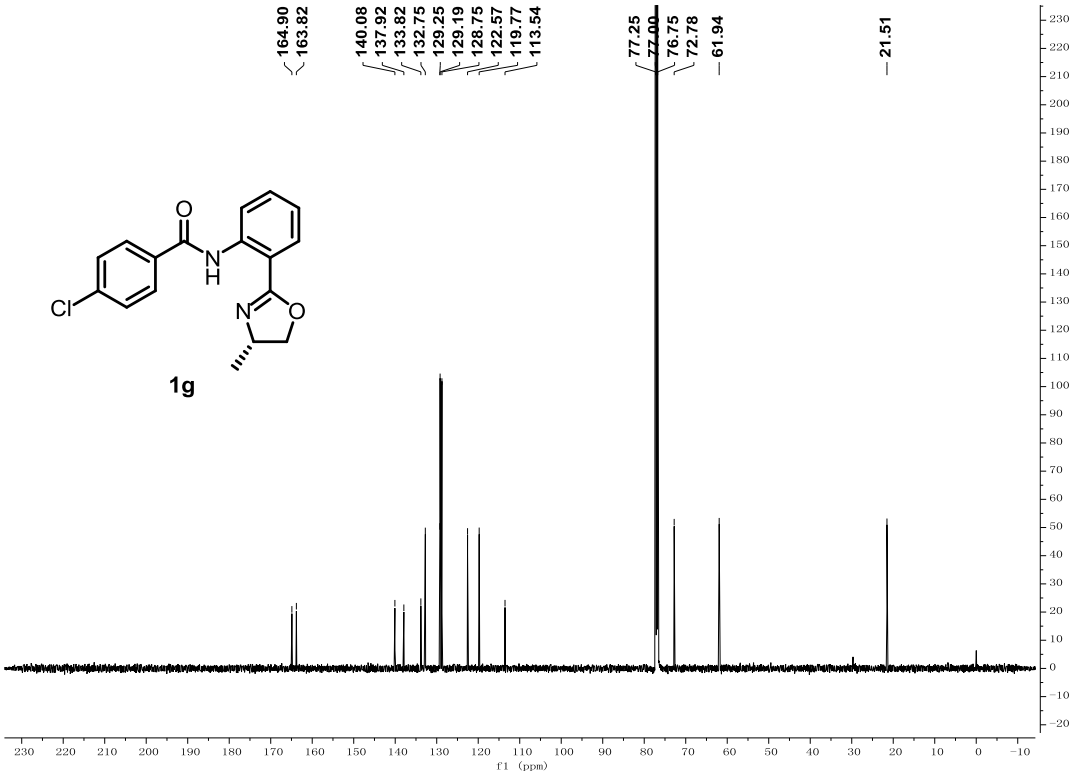
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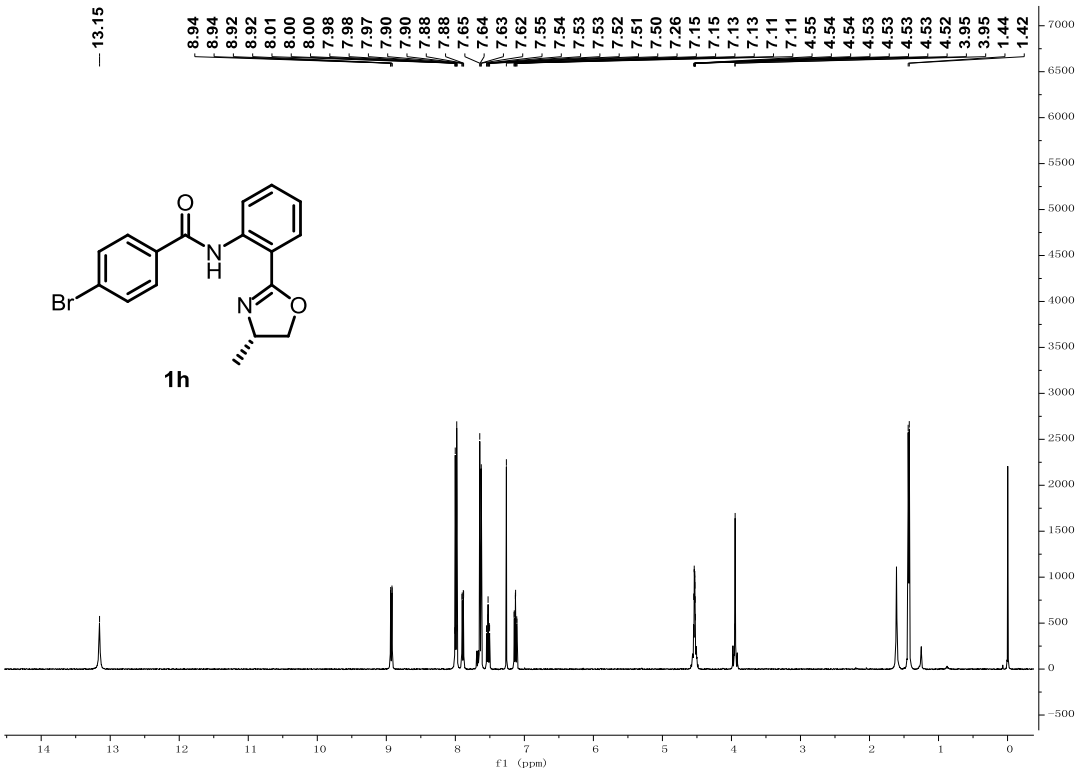
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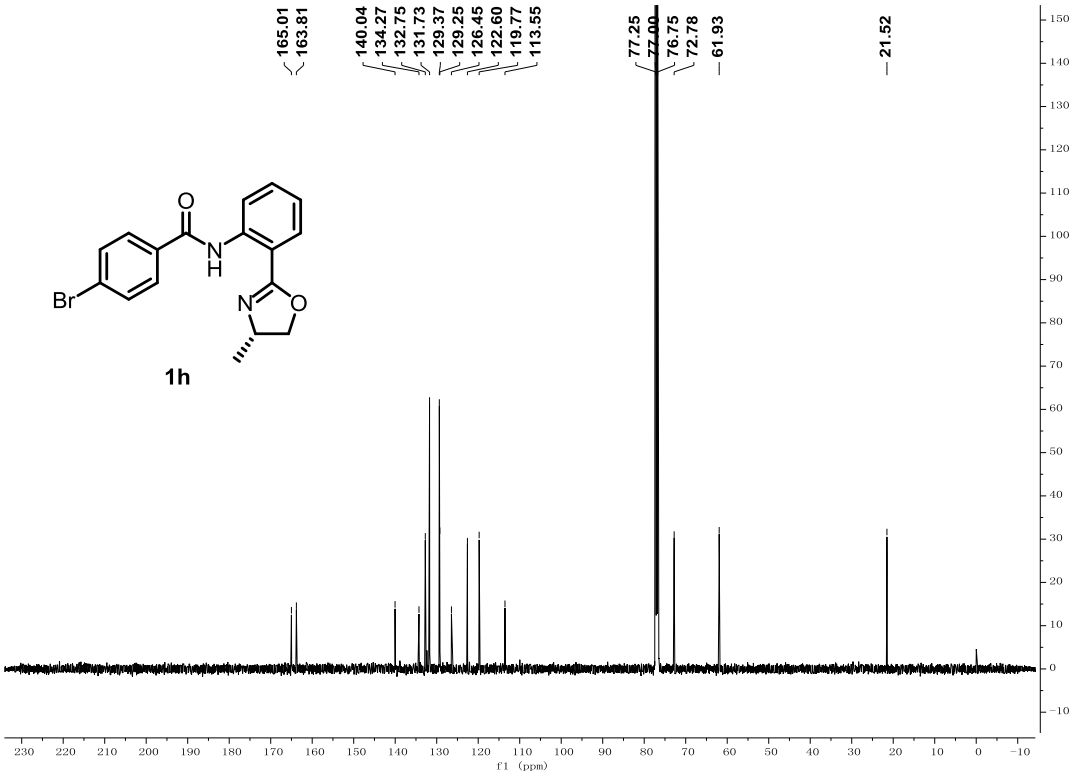
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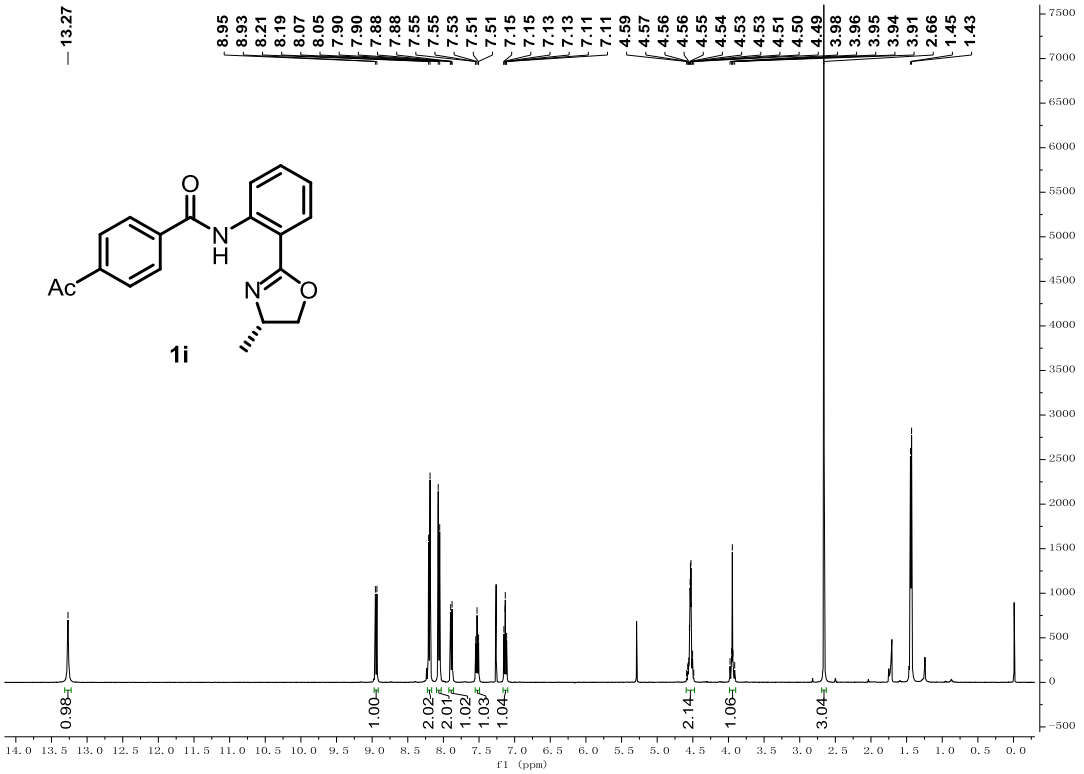
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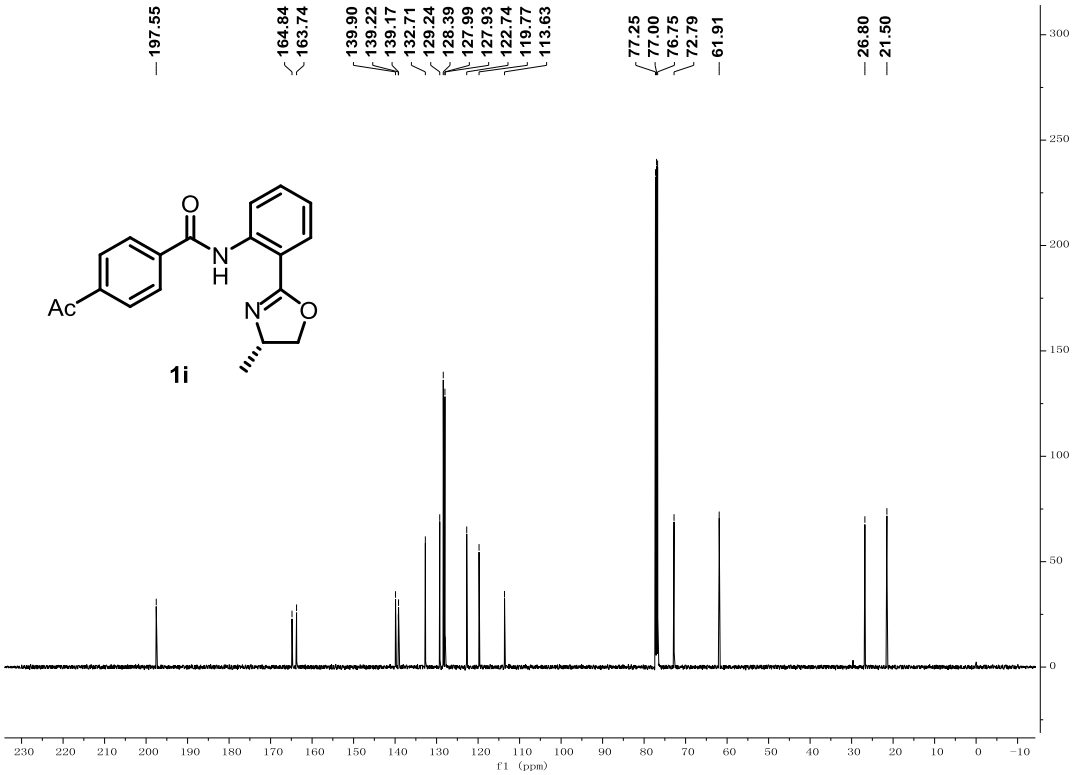
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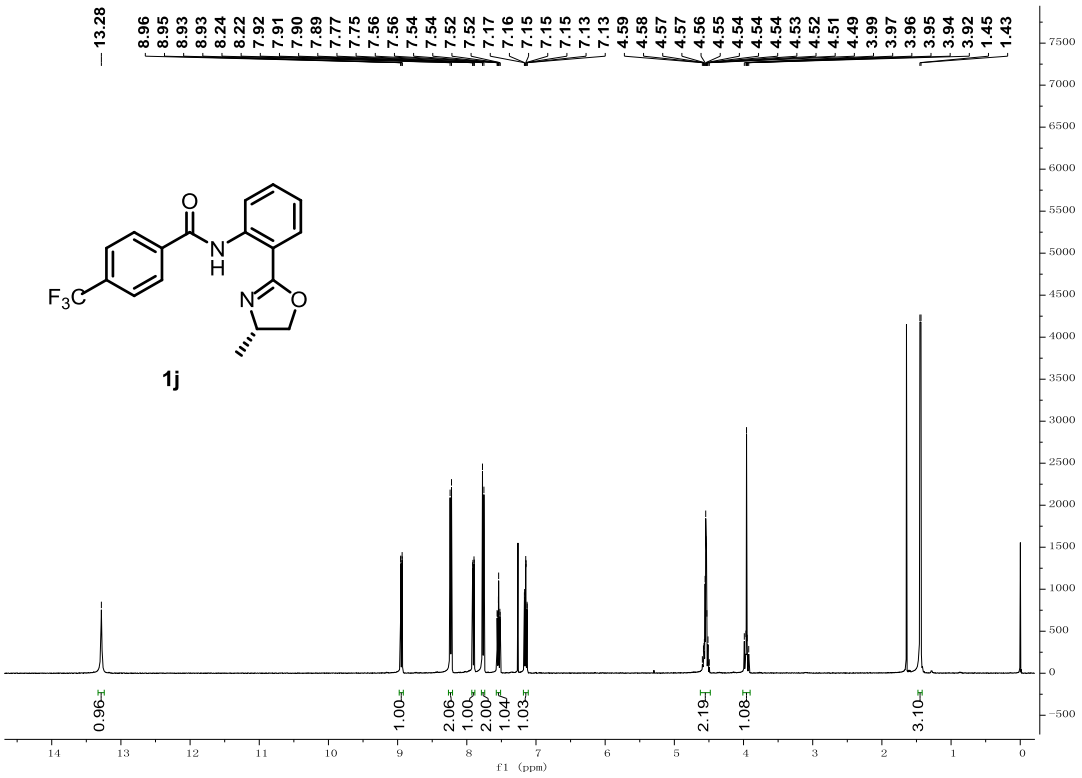
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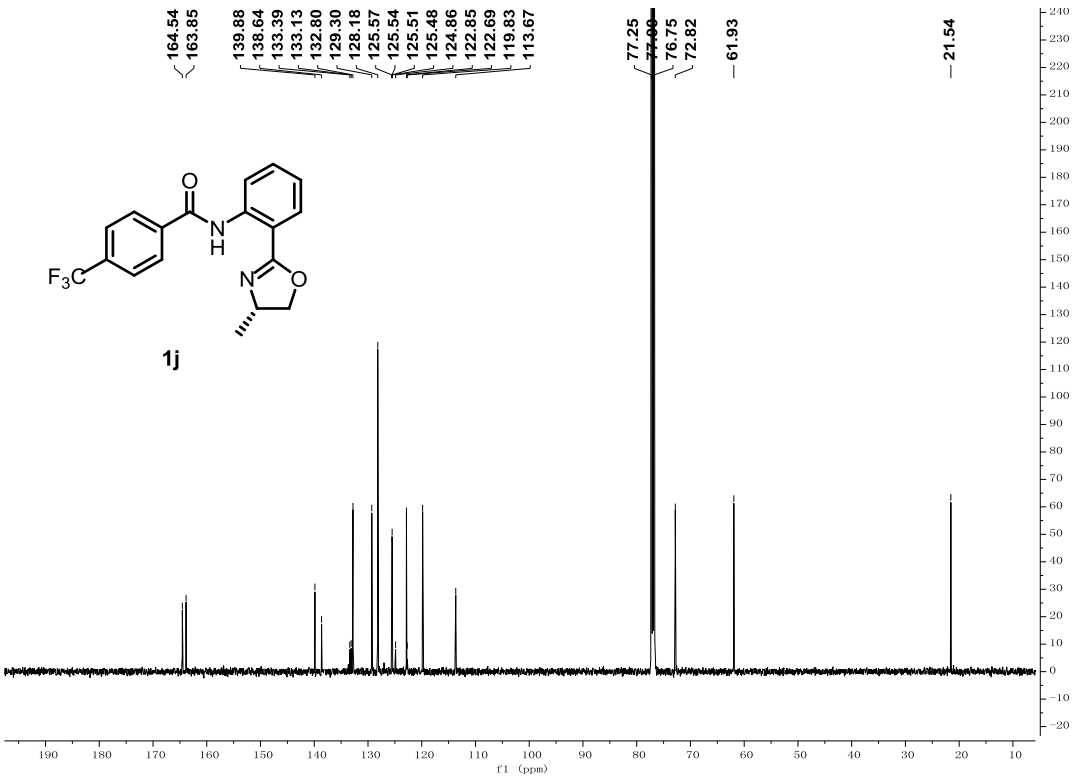
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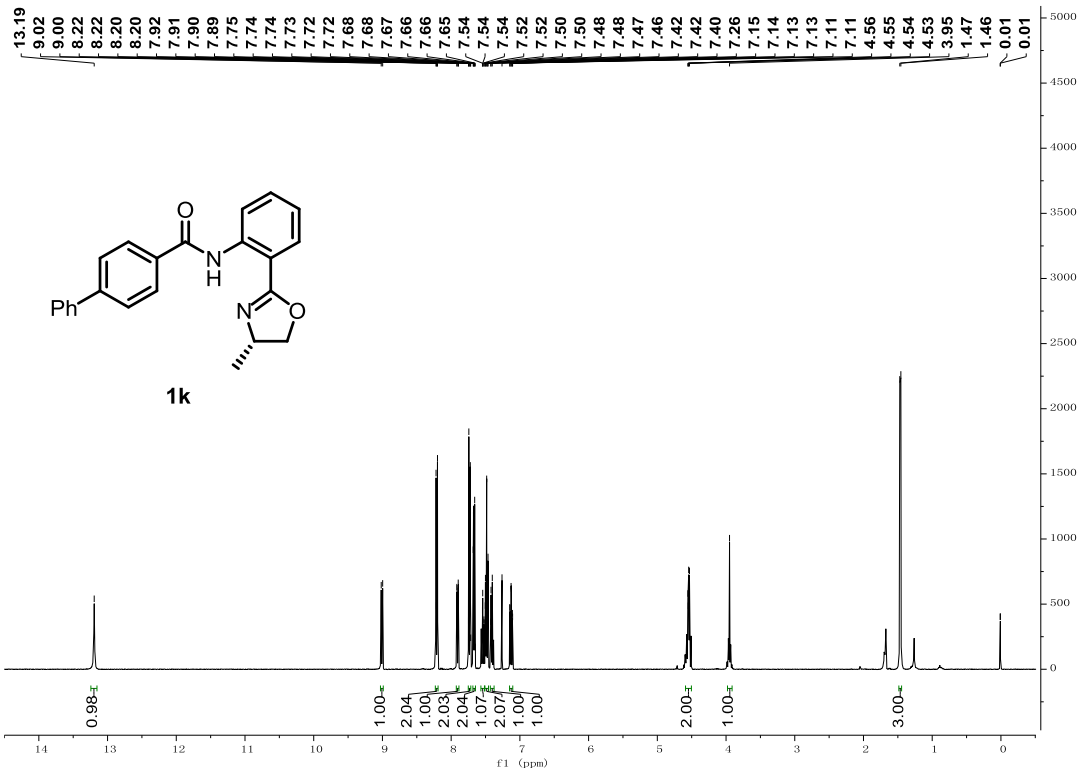
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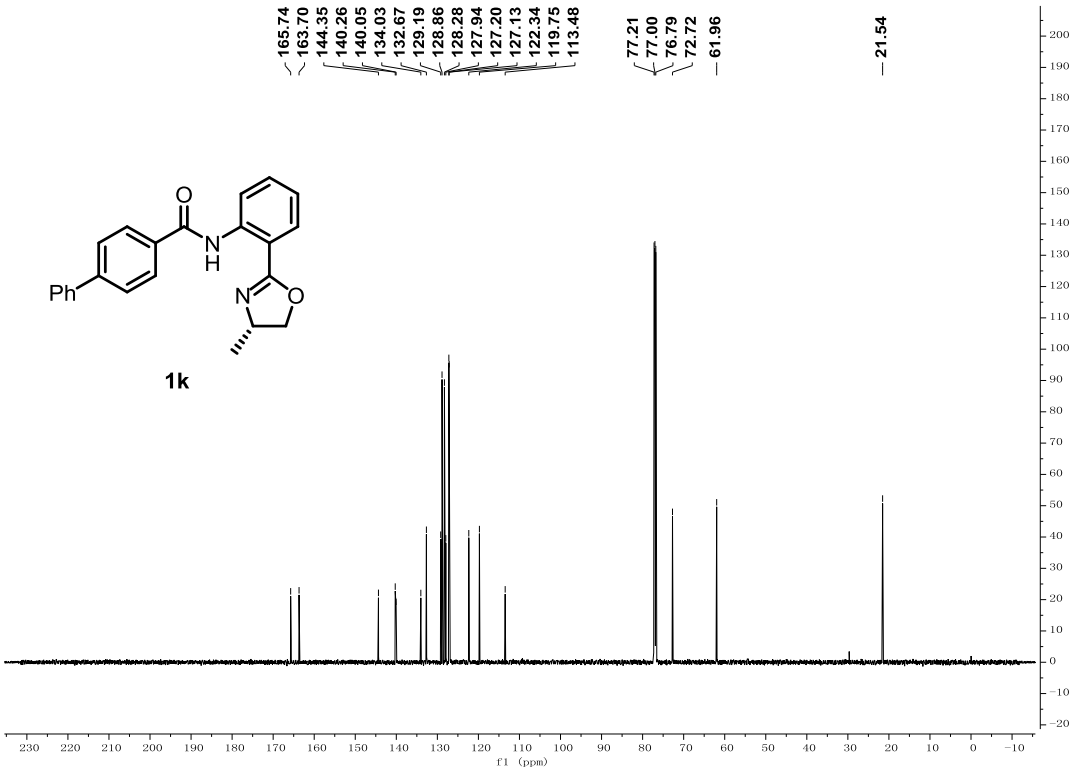
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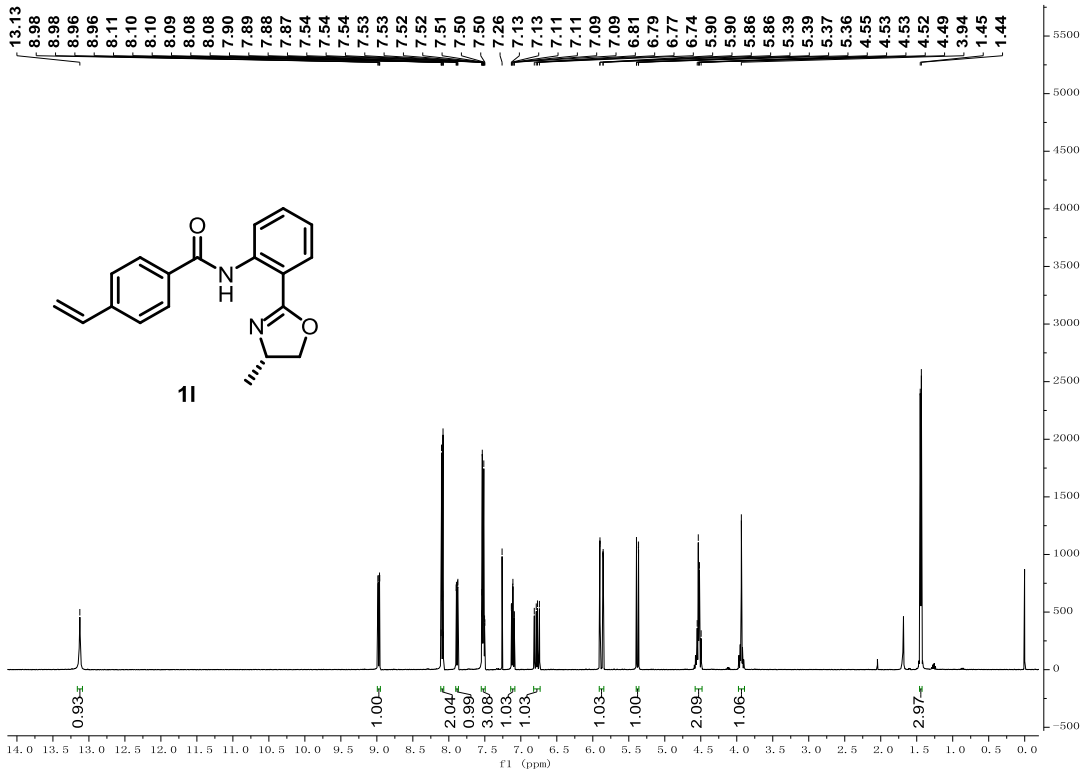
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0.93
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1.00
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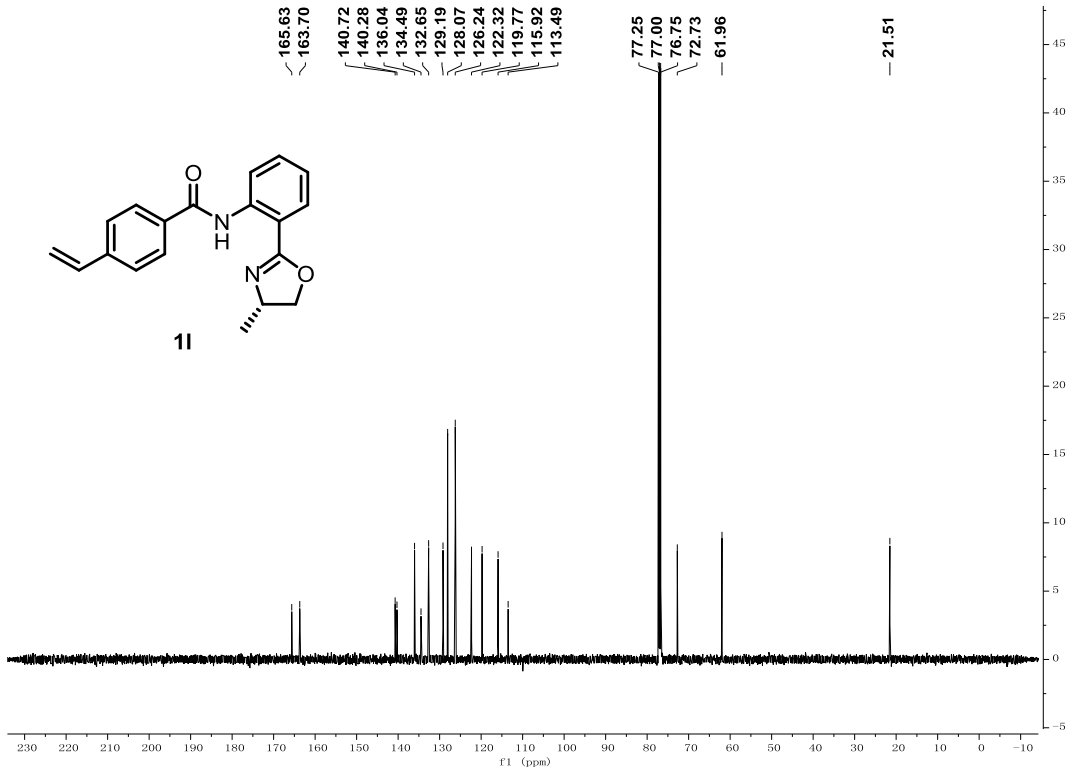
1.06
2.97
f1 (ppm)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126.24
122.32
119.77
115.92
113.49
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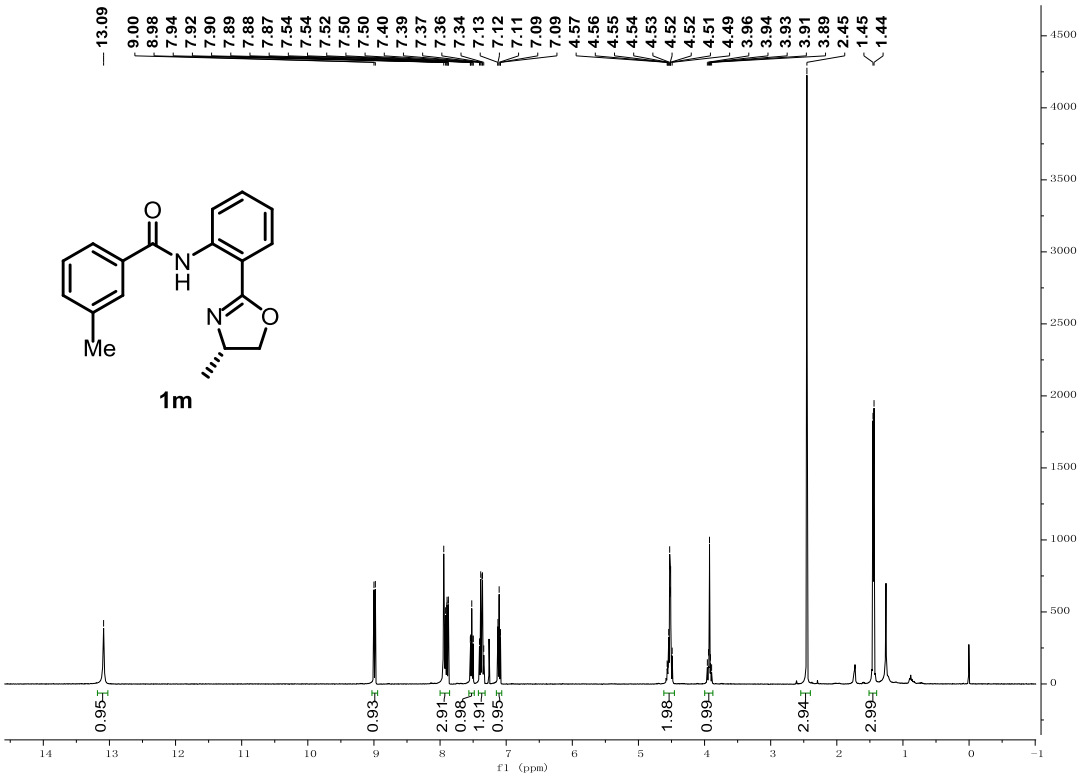
77.00
76.75
72.73
61.96
21.51
O
N
H
N
O
1l
f1 (ppm)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7.50
7.50
7.40
7.39
7.37
7.36
7.34
7.13
7.12
7.11
7.09
7.09
4.57
4.56
4.55
4.54
4.53
4.52
4.52
4.51
4.49
3.96
3.94
3.93
3.91
3.89
2.45
1.45
1.44
0.95
0.93
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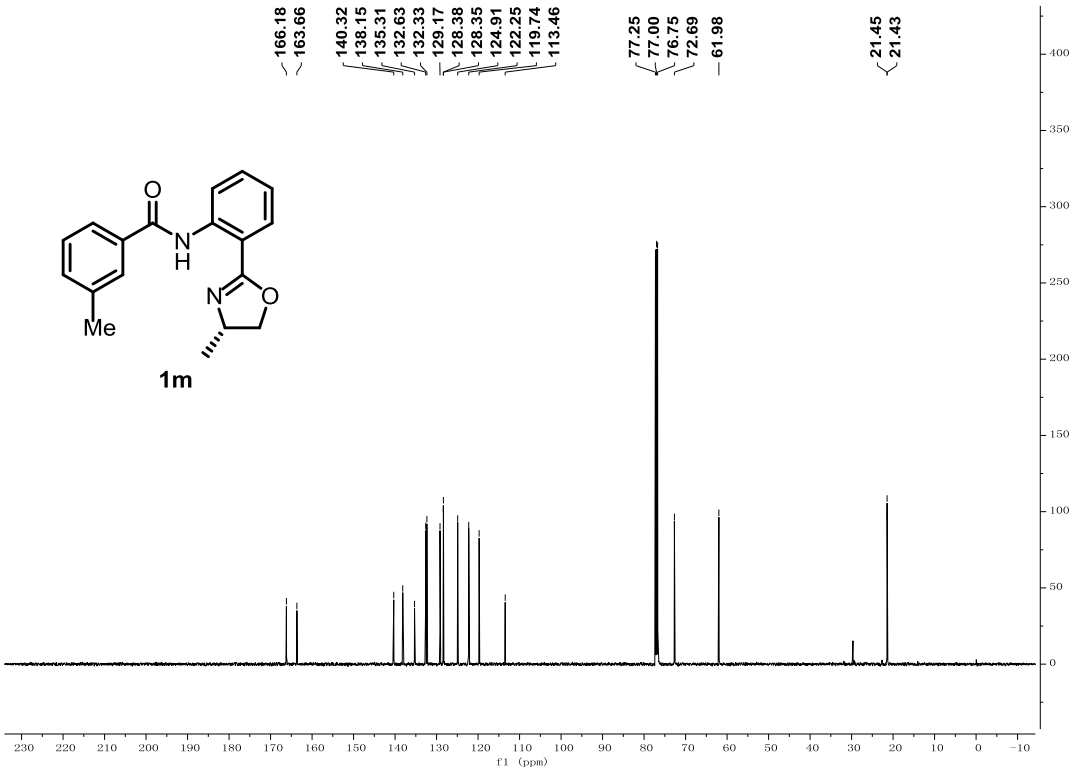
0.98
1.91
0.95
1.98
0.99
2.94
2.99
f1 (ppm)
1m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129.17
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128.35
124.91
122.25
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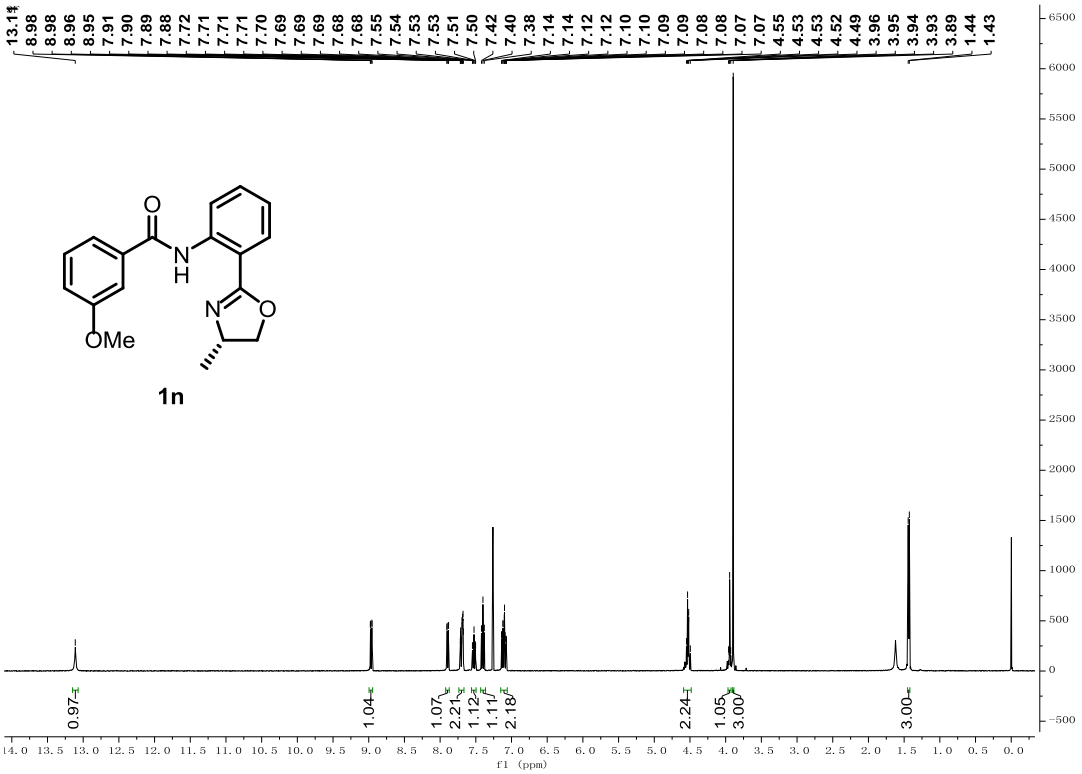
77.25
77.00
76.75
72.69
61.98
21.45
21.43
f1 (ppm)
1m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7.70
7.69
7.69
7.69
7.68
7.68
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7.54
7.53
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7.10
7.10
7.09
7.09
7.08
7.08
7.07
7.07
4.55
4.53
4.53
4.52
4.49
3.96
3.95
3.94
3.93
3.89
1.44
1.43
O
N
H
N
O
OMe
1n
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1.12
1.11
2.18
2.24
1.05
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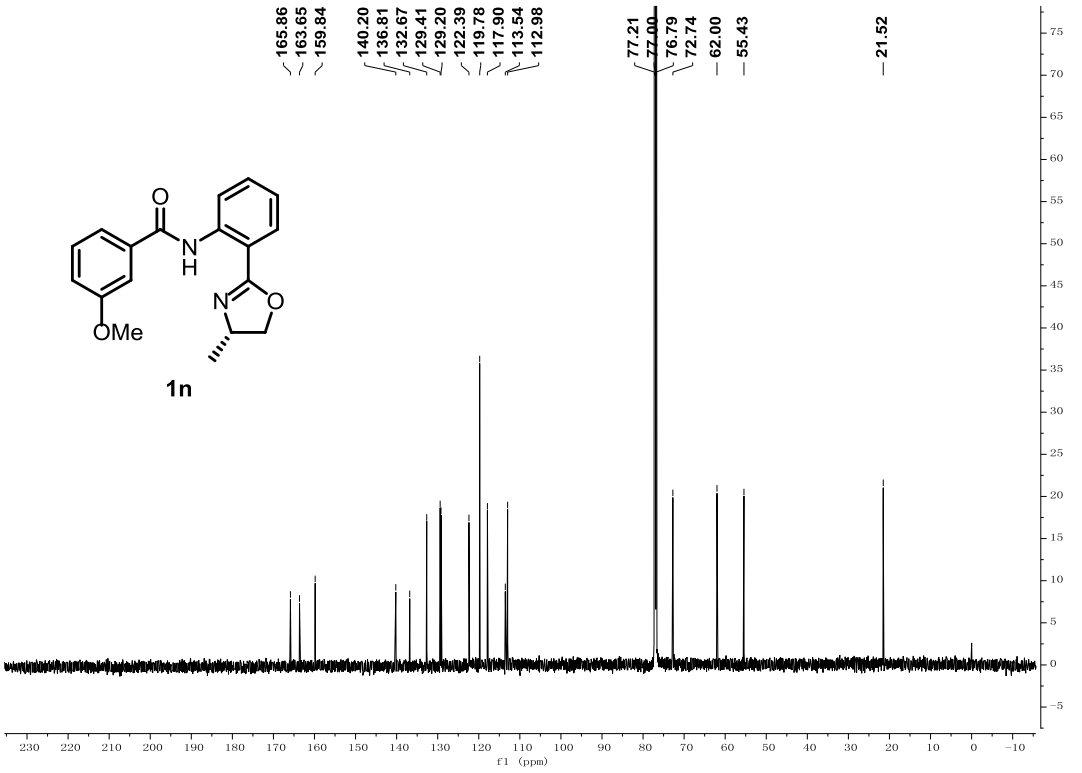
3.00
f1 (ppm)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117.90
113.54
112.98
77.21
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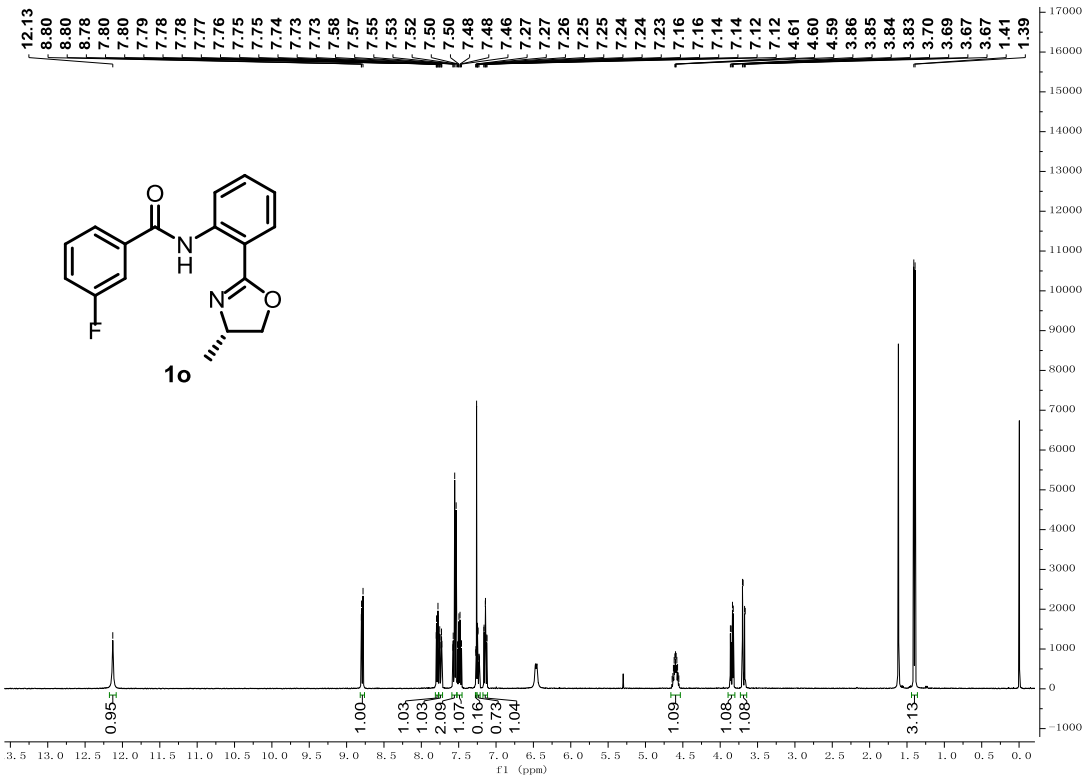
72.74
62.00
55.43
21.52
O
N
H
N
O
OMe
1n
f1 (ppm)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7.77
7.76
7.75
7.75
7.74
7.73
7.73
7.58
7.57
7.55
7.53
7.52
7.50
7.50
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7.48
7.46
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.23
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7.16
7.14
7.14
7.12
7.12
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4.60
4.59
3.86
3.85
3.84
3.83
3.70
3.69
3.67
3.67
1.41
1.39
O
N
H
N
O
F
1o
0.95
1.00
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1.03
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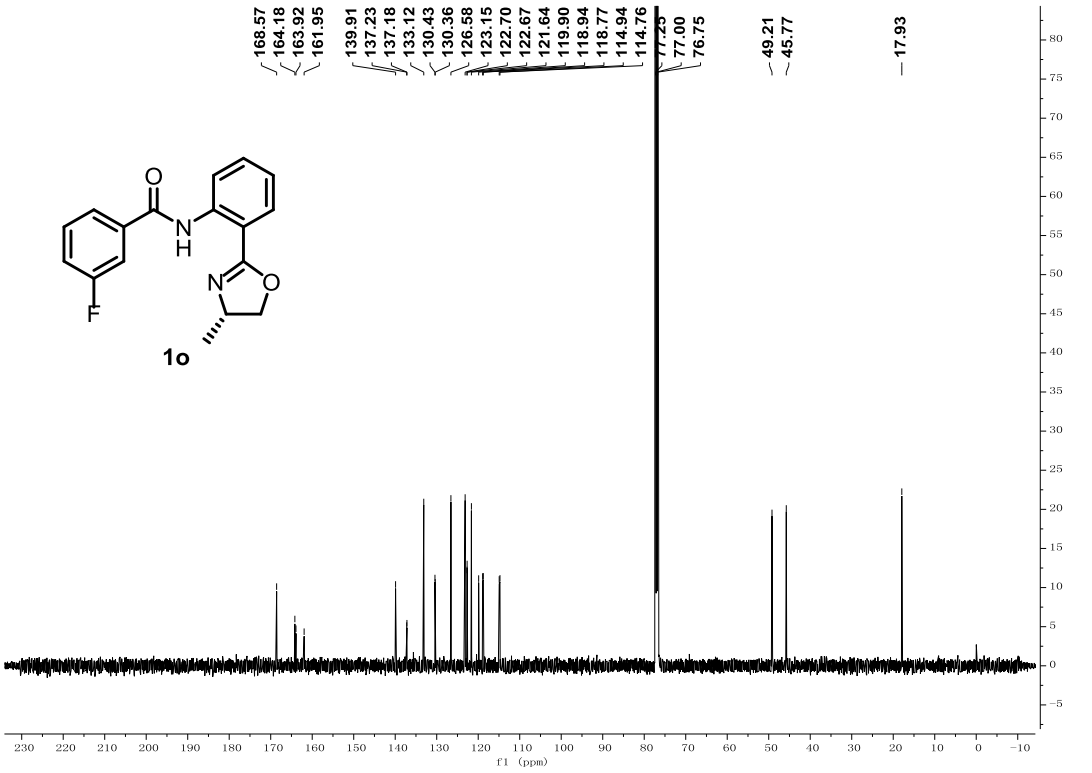
1.07
0.16
0.73
1.04
1.09
1.08
1.08
3.13
f1 (ppm)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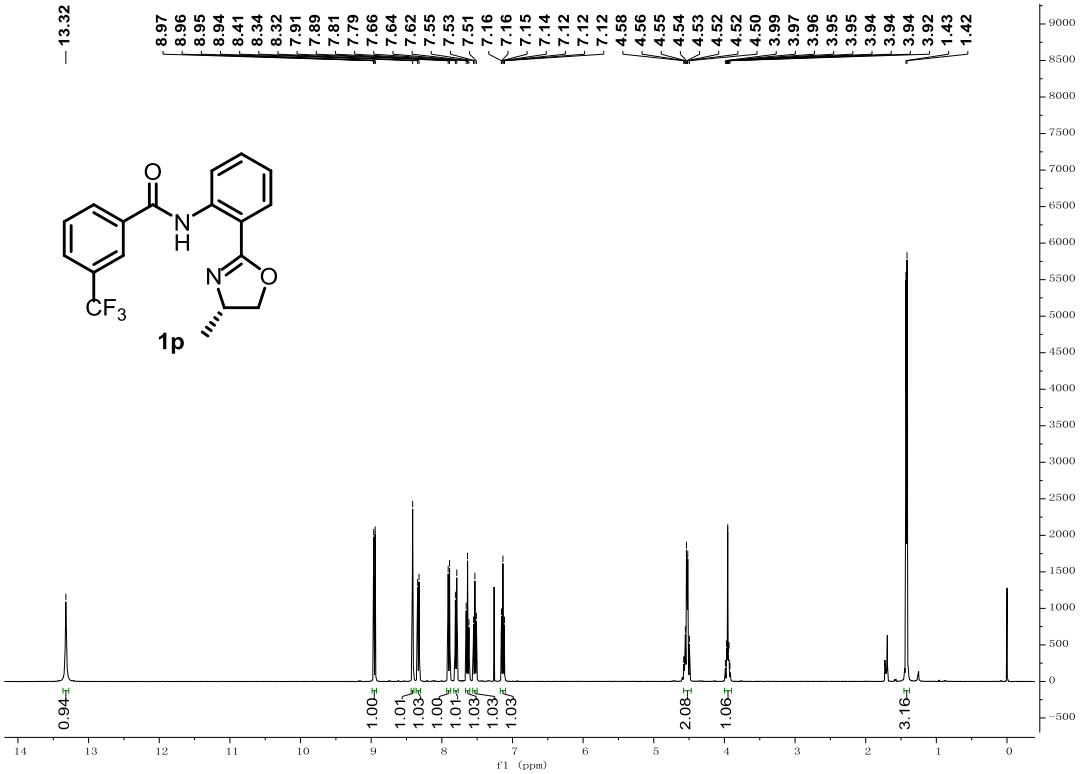
137.23
137.18
133.12
130.43
130.36
126.58
123.15
122.70
122.67
121.64
119.90
118.94
118.77
114.94
114.76
77.25
77.00
76.75
49.21
45.77
17.93
O
N
H
N
O
F
1o
f1 (ppm)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8.94
8.41
8.34
8.32
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7.89
7.81
7.79
7.66
7.64
7.62
7.55
7.53
7.51
7.16
7.16
7.15
7.14
7.12
7.12
7.12
4.58
4.56
4.55
4.54
4.53
4.52
4.52
4.50
3.99
3.97
3.96
3.95
3.95
3.94
3.94
3.94
3.92
1.43
1.42
O
N
H
N
O
CF3
1p
0.94
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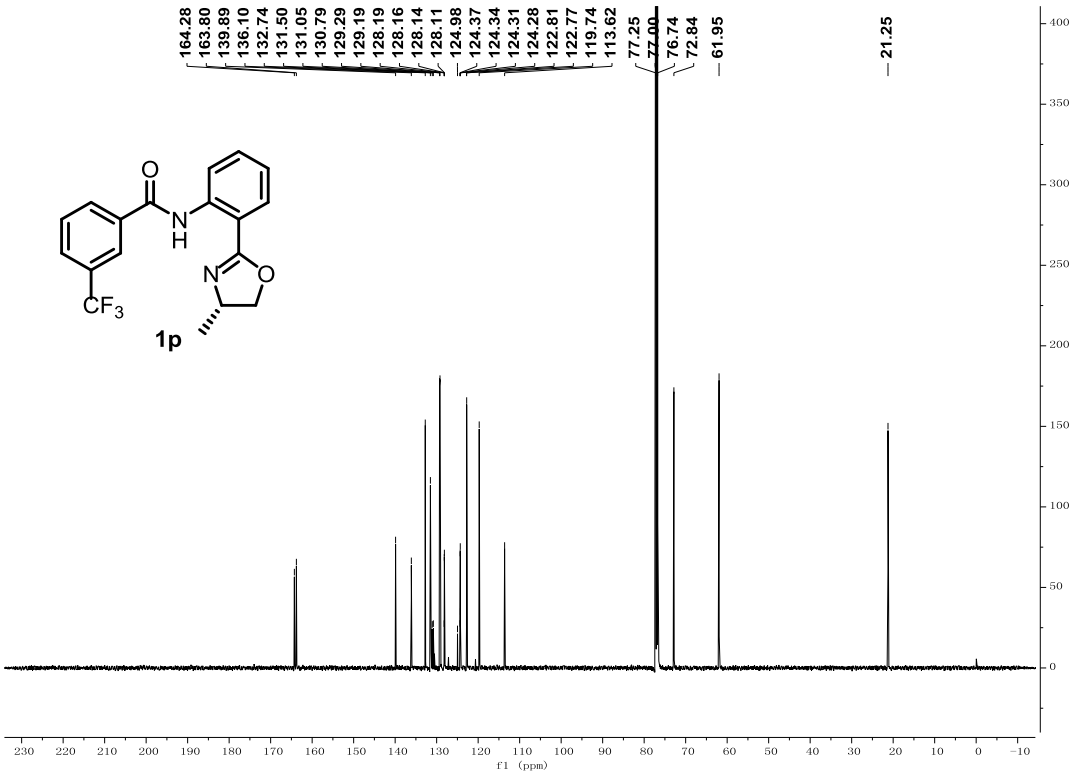
1.00
1.01
1.03
1.03
1.03
2.08
1.06
3.16
f1 (ppm)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129.19
128.19
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128.14
128.11
124.98
124.37
124.34
124.31
124.28
122.81
122.77
119.74
113.62
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77.00
76.74
72.84
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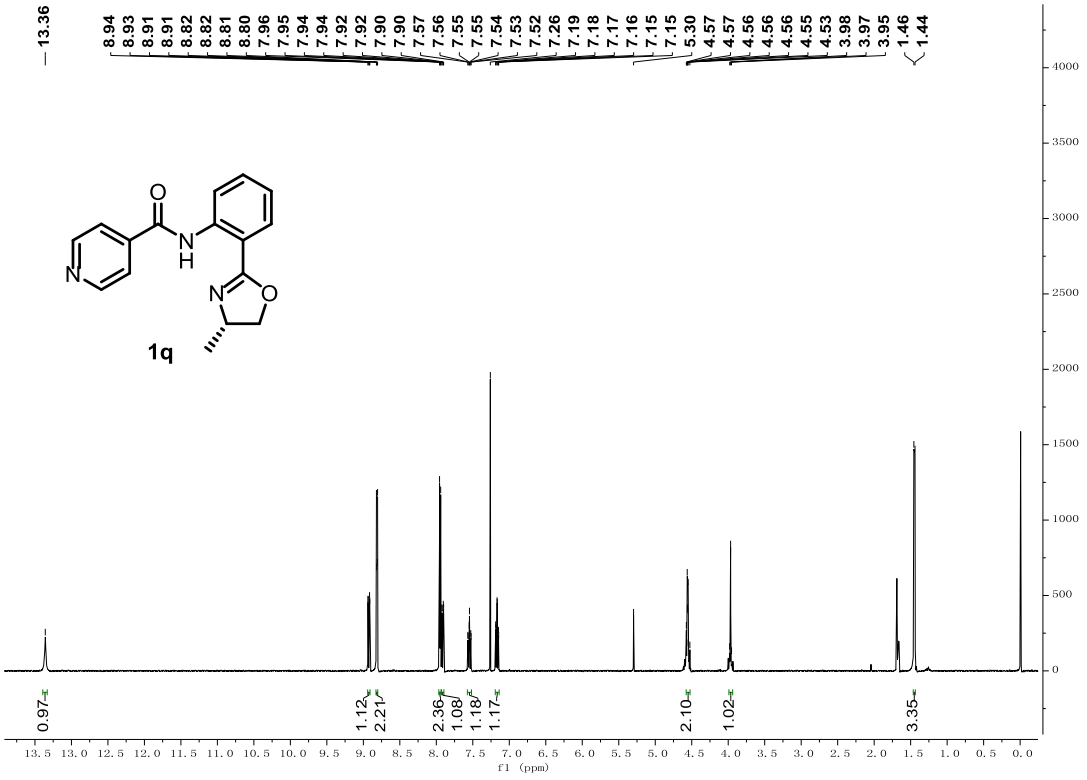
21.25
O
N
H
N
O
CF3
1p
f1 (ppm)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7.95
7.94
7.94
7.92
7.92
7.90
7.90
7.57
7.56
7.55
7.55
7.54
7.53
7.52
7.26
7.19
7.18
7.17
7.16
7.15
7.15
5.30
4.57
4.57
4.56
4.56
4.56
4.55
4.53
3.98
3.97
3.95
1.46
1.44
1q
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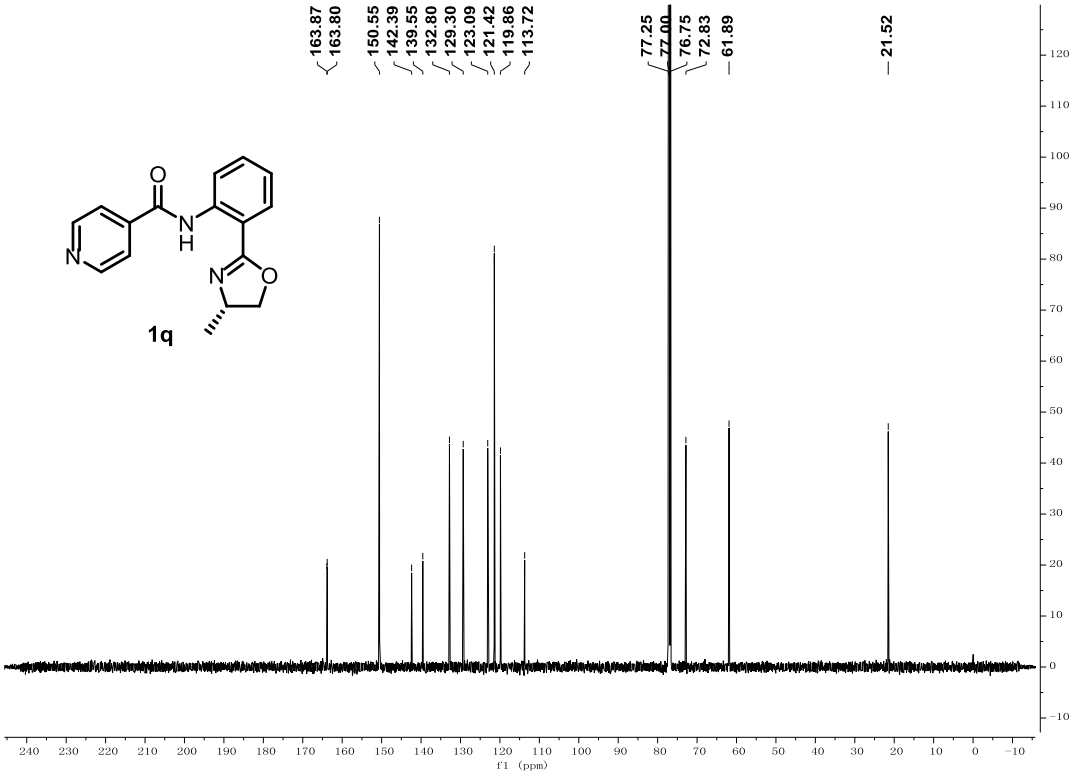
2.21
2.36
1.08
1.18
1.17
2.10
1.02
3.35
f1 (ppm)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139.55
132.80
129.30
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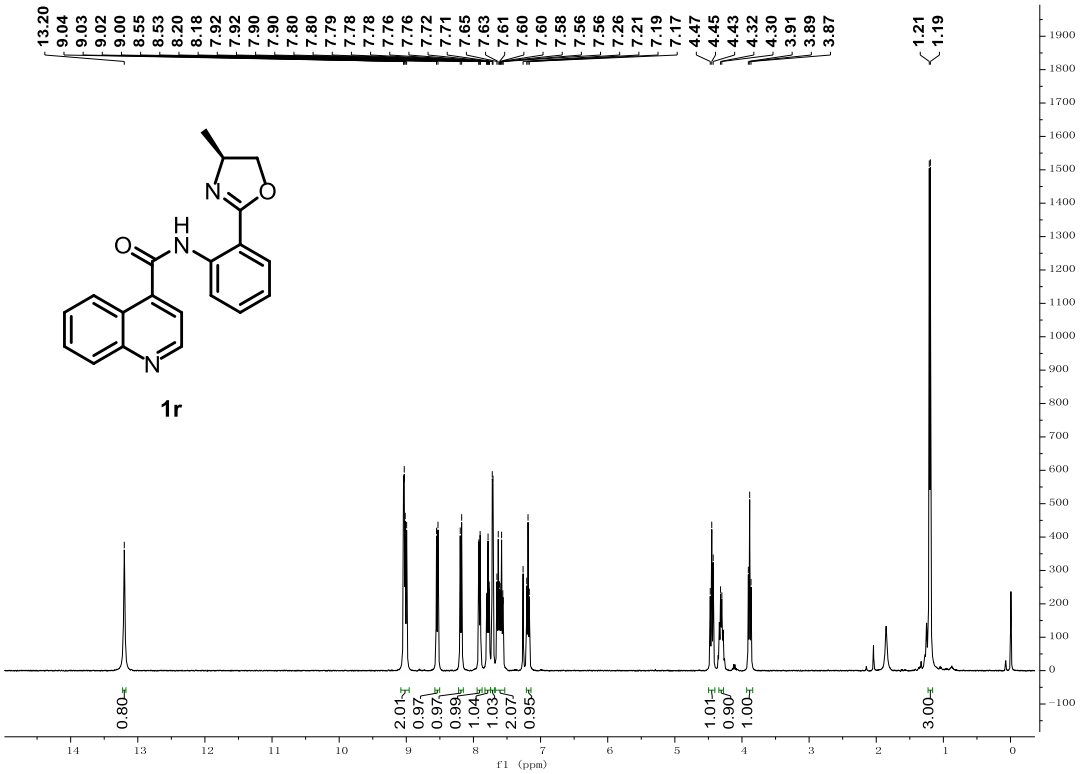
119.86
113.72
77.25
77.00
76.75
72.83
61.89
21.52
1q
f1 (ppm)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7.92
7.90
7.90
7.80
7.80
7.79
7.78
7.78
7.76
7.76
7.72
7.71
7.65
7.63
7.61
7.60
7.60
7.58
7.56
7.56
7.26
7.21
7.19
7.17
4.47
4.45
4.43
4.32
4.30
3.91
3.89
3.87
1.21
1.19
1r
0.80
2.01
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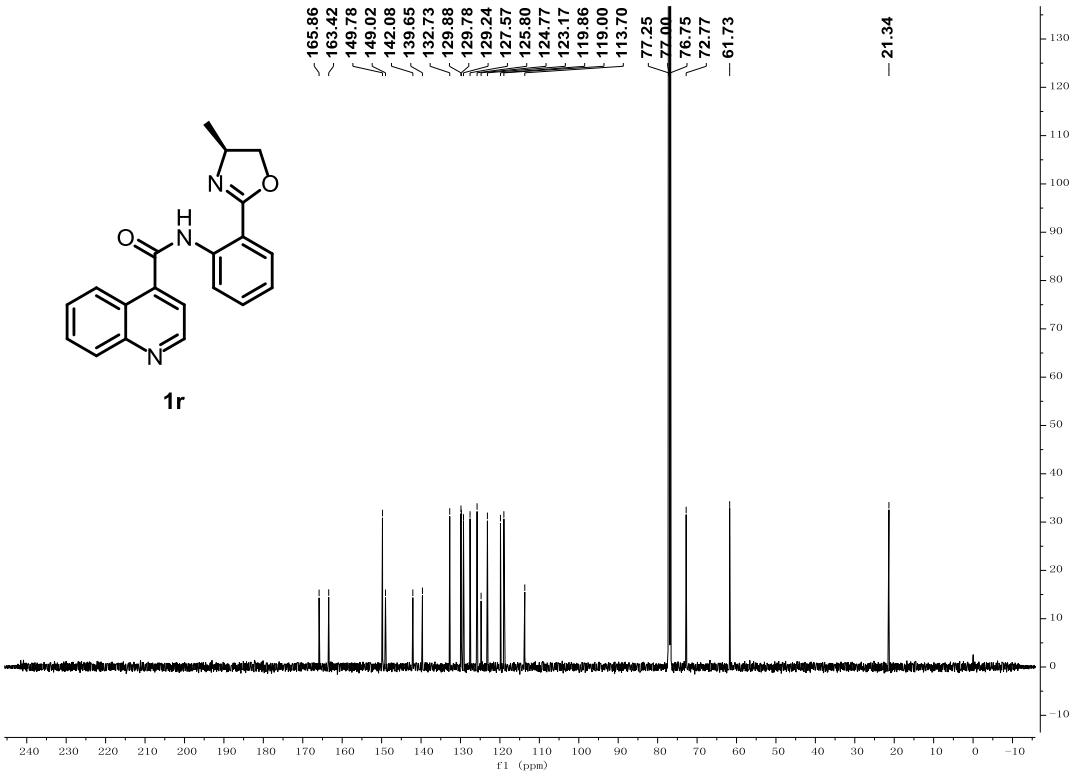
0.97
0.99
1.04
1.03
2.07
0.95
1.01
0.90
1.00
3.00
f1 (ppm)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129.78
129.24
127.57
125.80
124.77
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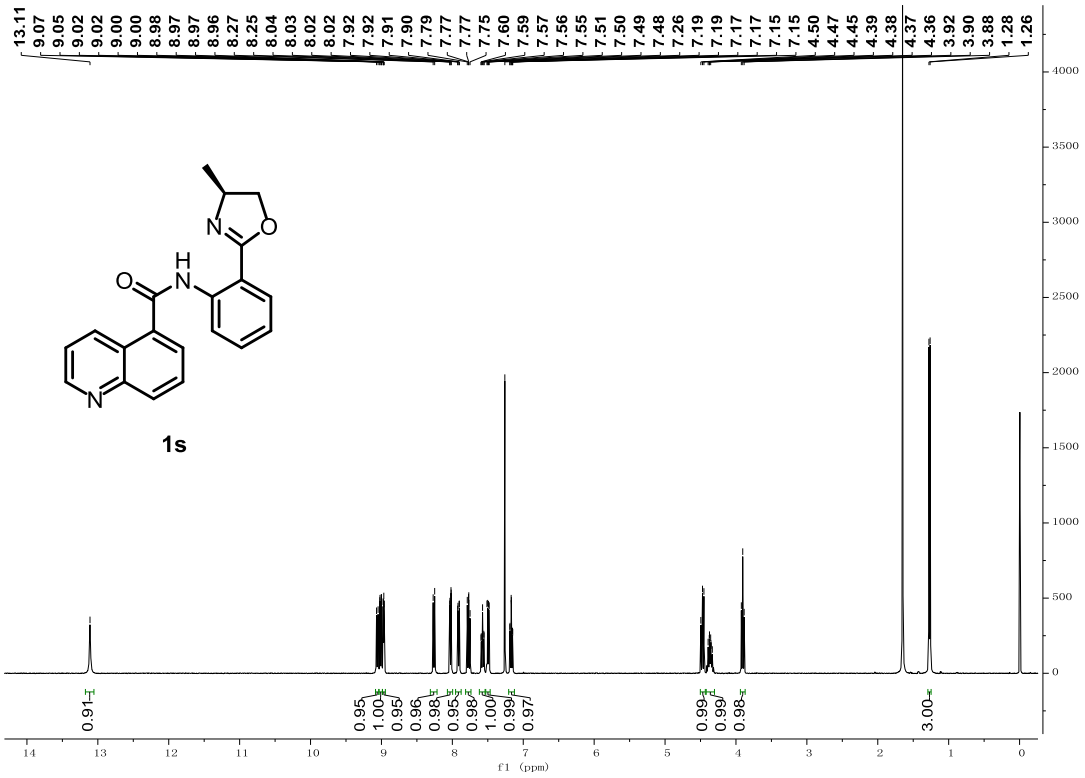
77.25
77.00
76.75
72.77
61.73
21.34
1r
f1 (ppm)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9.02
9.02
9.00
9.00
8.98
8.97
8.97
8.96
8.27
8.25
8.04
8.03
8.02
8.02
7.92
7.92
7.91
7.90
7.79
7.77
7.77
7.75
7.60
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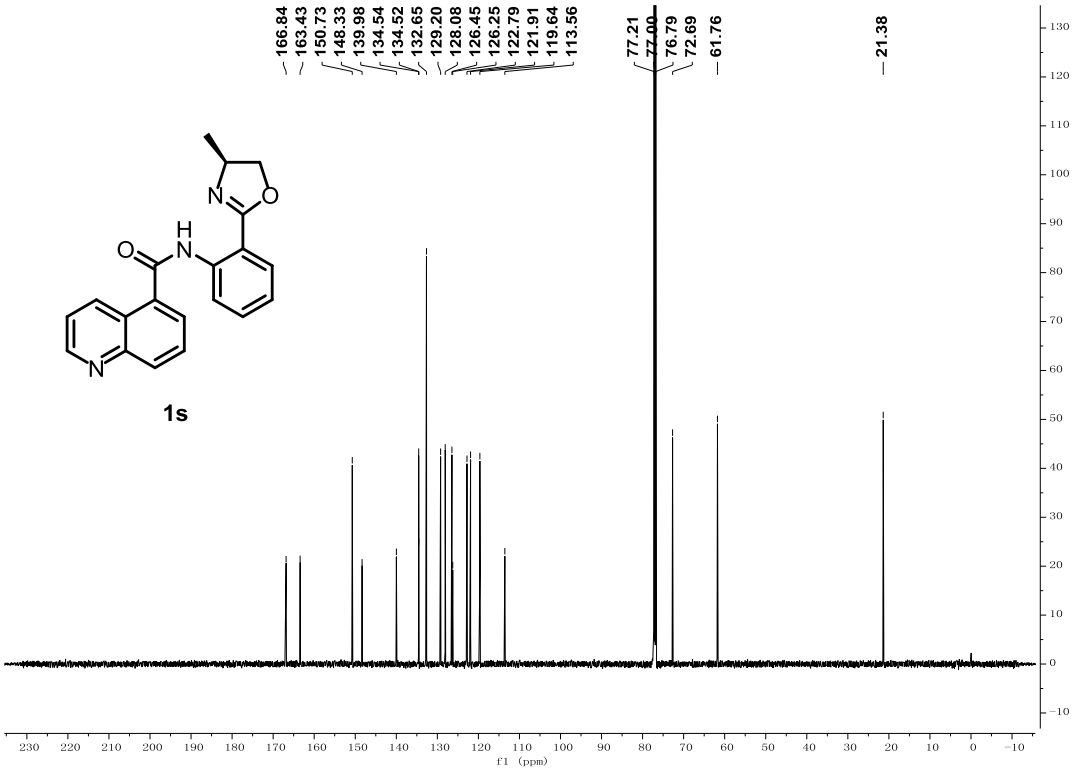
7.56
7.55
7.51
7.50
7.49
7.48
7.26
7.19
7.19
7.17
7.17
7.15
7.15
4.50
4.47
4.45
4.39
4.38
4.37
4.36
3.92
3.90
3.88
1.28
1.26
1s
0.91
0.95
1.00
0.95
0.96
0.98
0.95
0.98
1.00
0.99
0.97
0.99
0.99
0.98
3.00
f1 (ppm)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126.25
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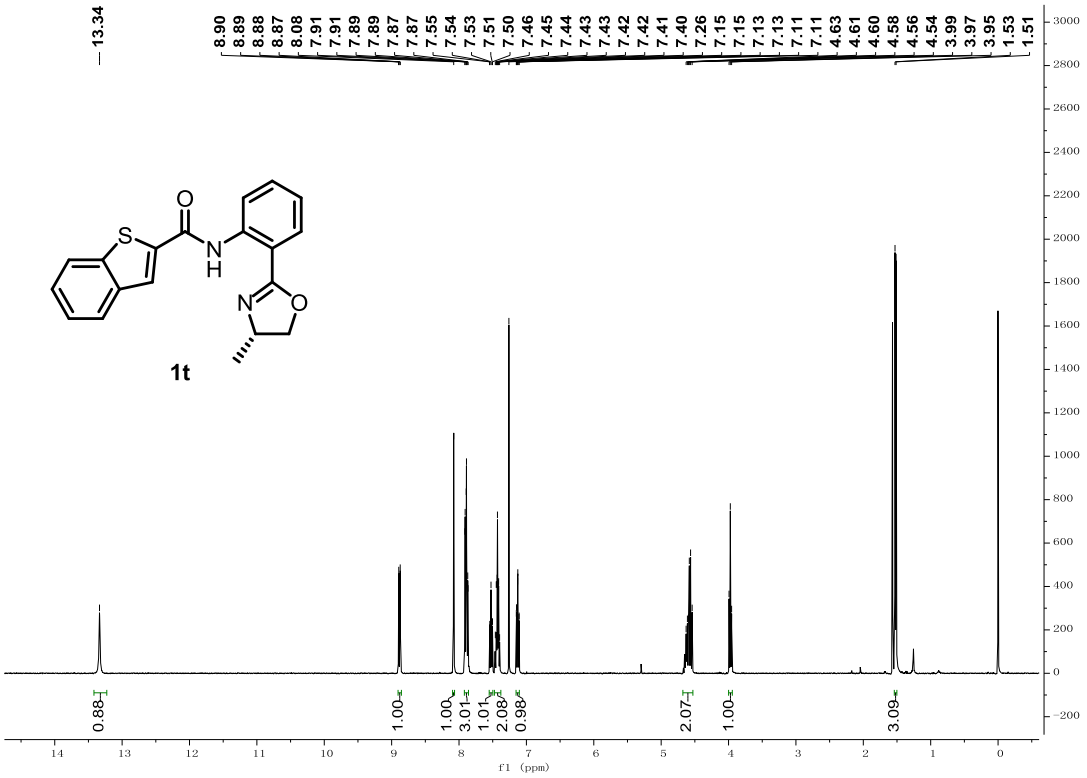
77.00
76.79
72.69
61.76
21.38
1s
f1 (ppm)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8.08
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7.89
7.87
7.87
7.55
7.54
7.53
7.51
7.50
7.46
7.45
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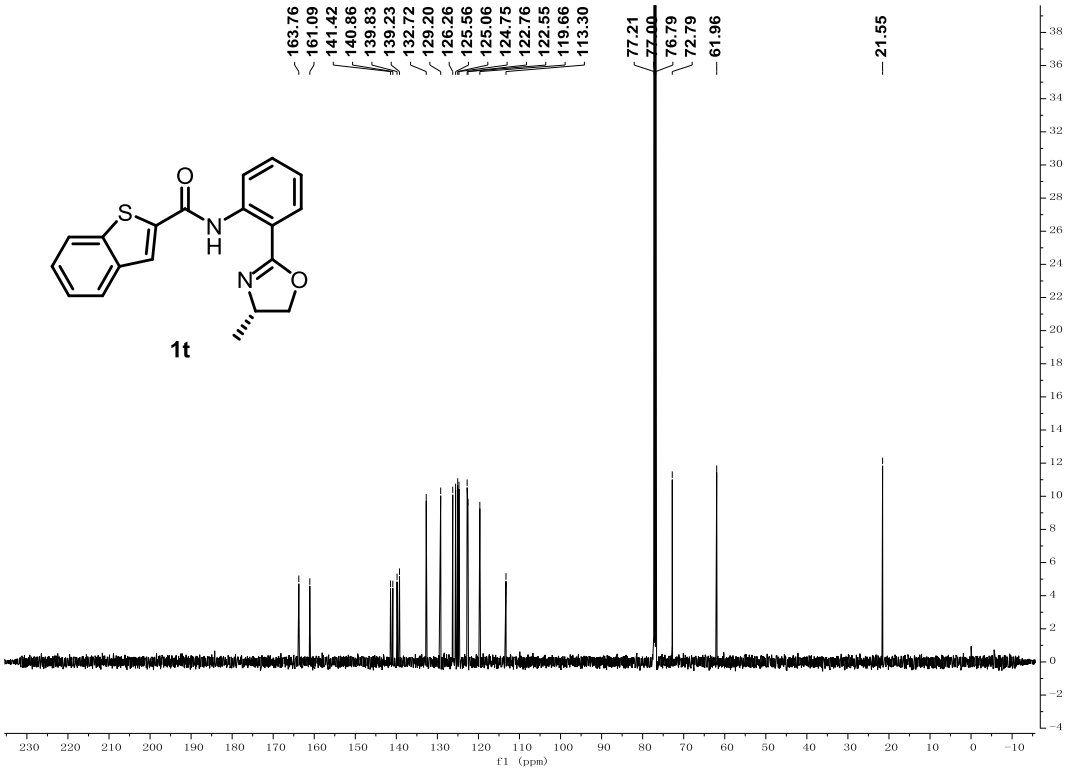
7.43
7.43
7.42
7.42
7.41
7.40
7.26
7.15
7.15
7.13
7.13
7.11
7.11
4.63
4.61
4.60
4.58
4.56
4.54
3.99
3.97
3.95
1.53
1.51
1t
0.88
1.00
1.00
3.01
1.01
2.08
0.98
2.07
1.00
3.09
f1 (ppm)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129.20
126.26
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125.06
124.75
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122.55
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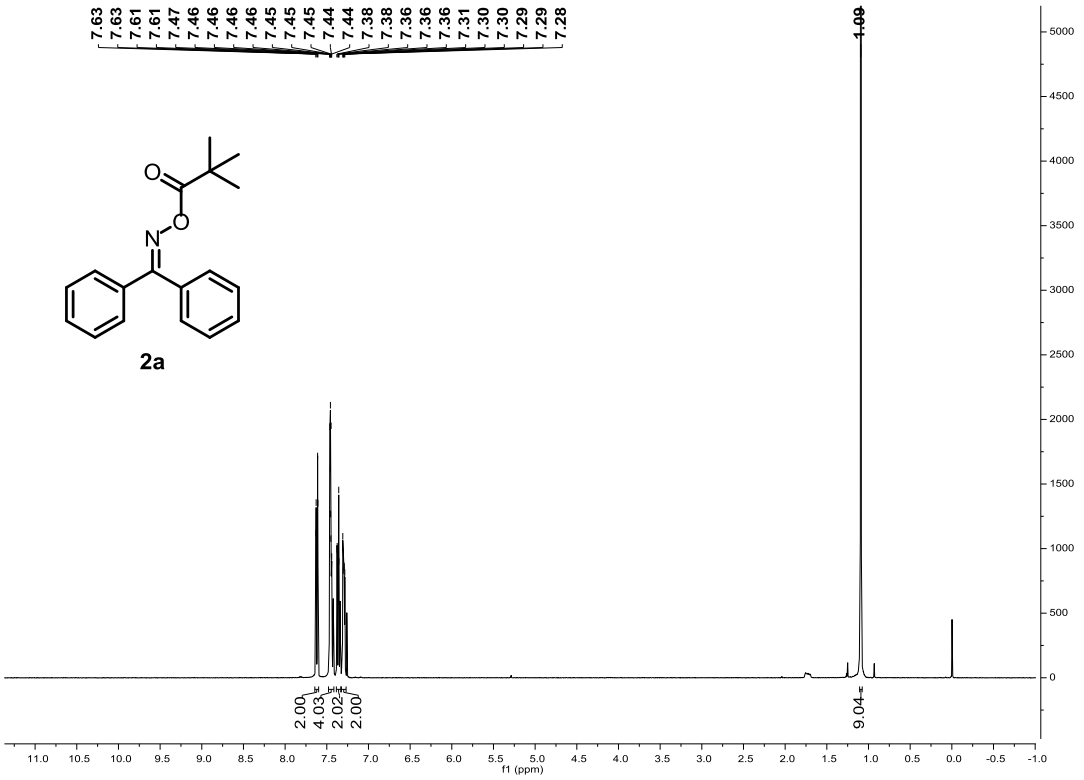
113.30
77.21
77.00
76.79
72.79
61.96
21.55
1t
f1 (ppm)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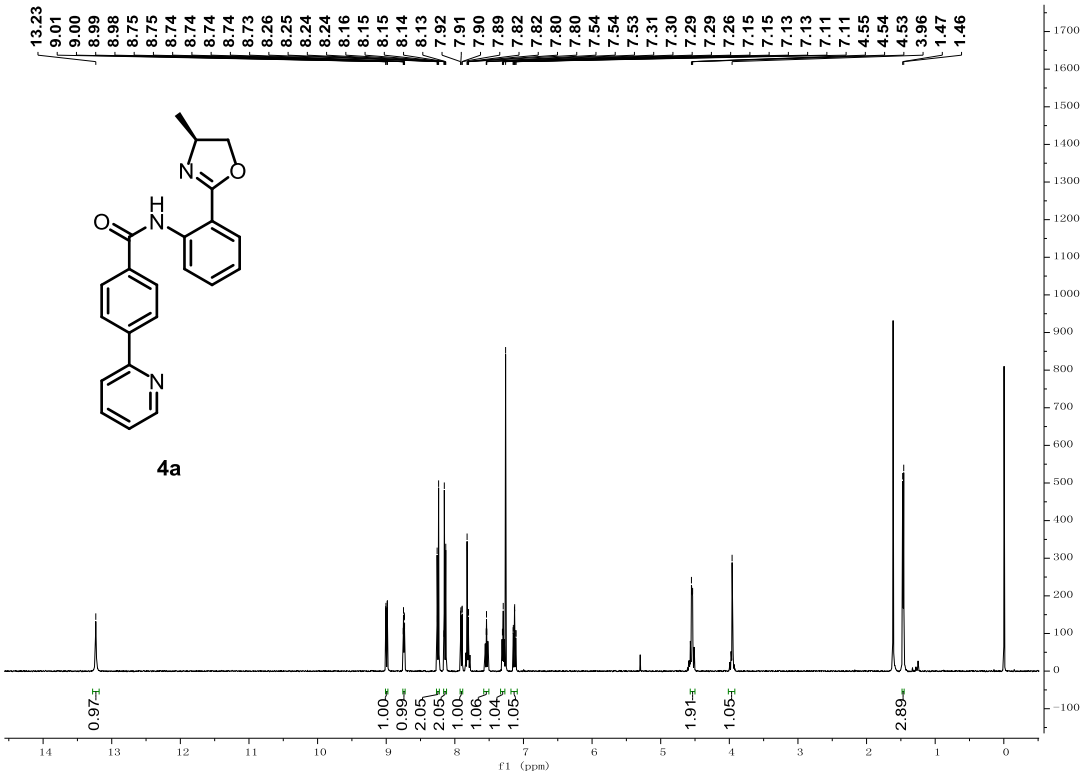
7.46
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.38
7.36
7.36
7.31
7.30
7.30
7.29
7.29
7.28
1.00
2.00
4.03
2.02
2.00
9.04
f1 (ppm)

2a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8.74
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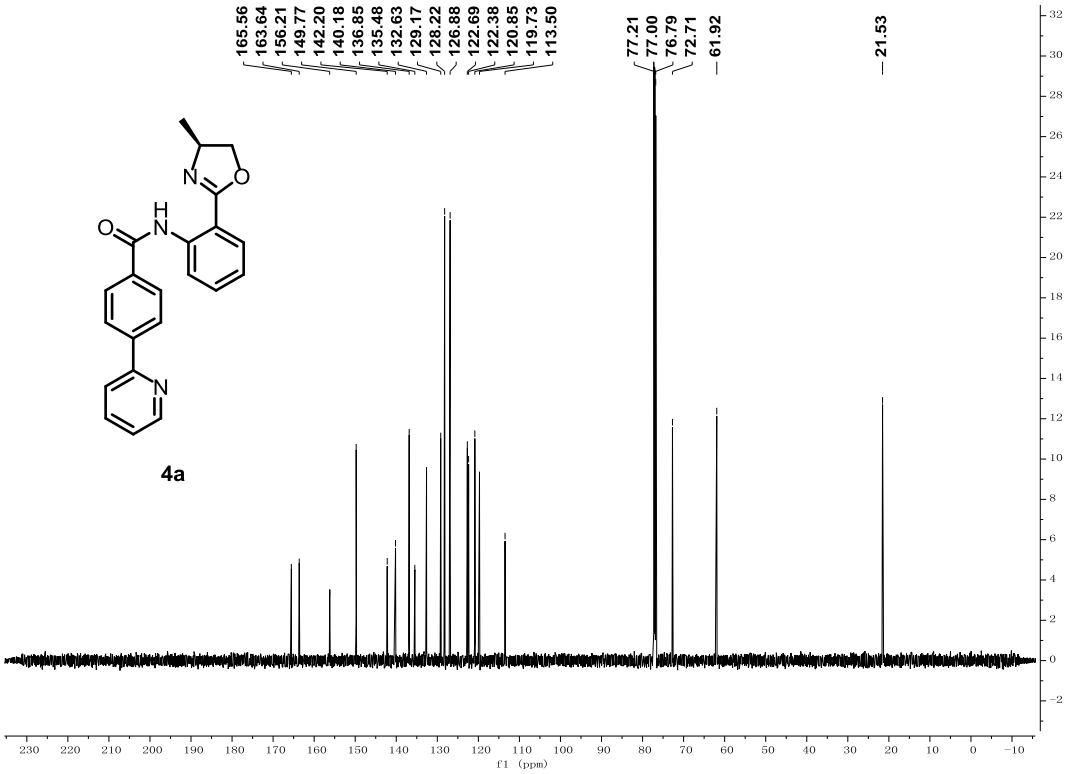
8.74
8.73
8.26
8.25
8.24
8.24
8.16
8.15
8.15
8.14
8.13
7.92
7.91
7.90
7.89
7.82
7.82
7.80
7.80
7.54
7.54
7.53
7.31
7.30
7.29
7.29
7.26
7.15
7.15
7.13
7.13
7.11
7.11
4.55
4.54
4.53
3.96
1.47
1.46
0.97
1.00
0.99
2.05
2.05
1.00
1.06
1.04
1.05
1.91
1.05
2.89
f1 (ppm)

4a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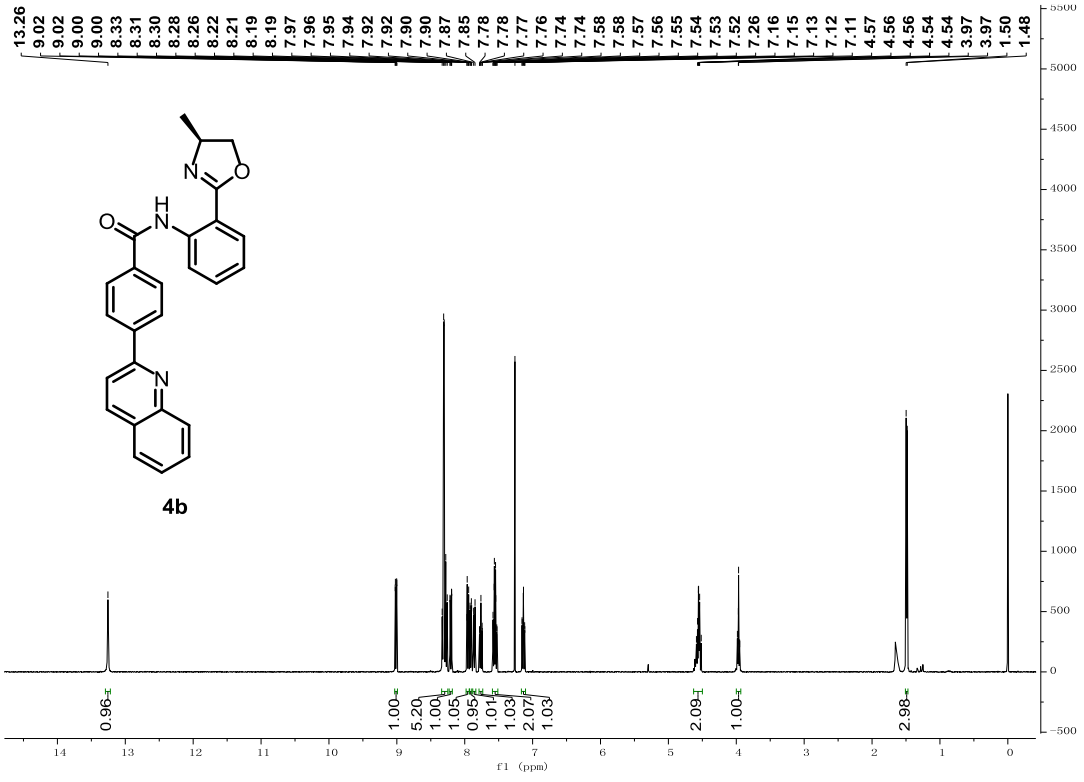
135.48
132.63
129.17
128.22
126.88
122.69
122.38
120.85
119.73
113.50
77.21
77.00
76.79
72.71
61.92
21.53
4a
f1 (ppm)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9.00
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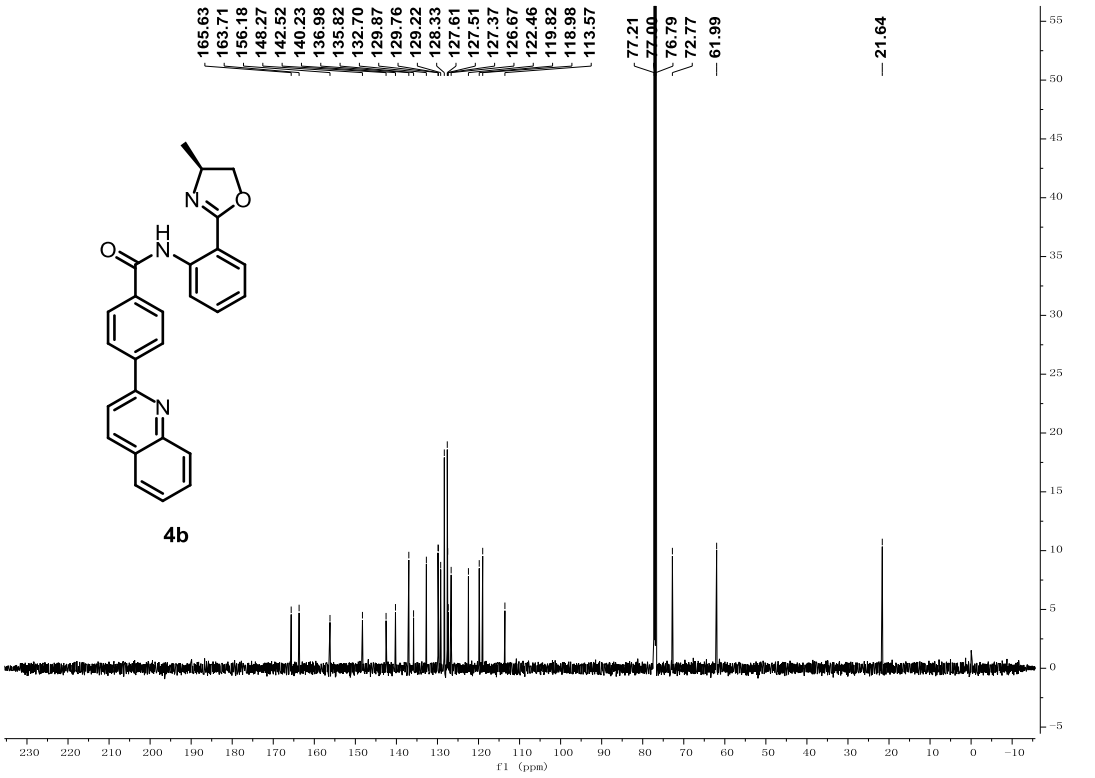
8.30
8.28
8.26
8.22
8.21
8.19
8.19
7.97
7.96
7.95
7.94
7.92
7.92
7.90
7.90
7.87
7.85
7.78
7.78
7.77
7.76
7.74
7.74
7.58
7.58
7.57
7.56
7.55
7.54
7.53
7.52
7.26
7.16
7.15
7.13
7.12
7.11
4.57
4.56
4.56
4.54
4.54
3.97
3.97
1.50
1.48
0.96
1.00
5.20
1.00
1.05
0.95
1.01
1.03
2.07
1.03
2.09
1.00
2.98
4b
f1 (ppm)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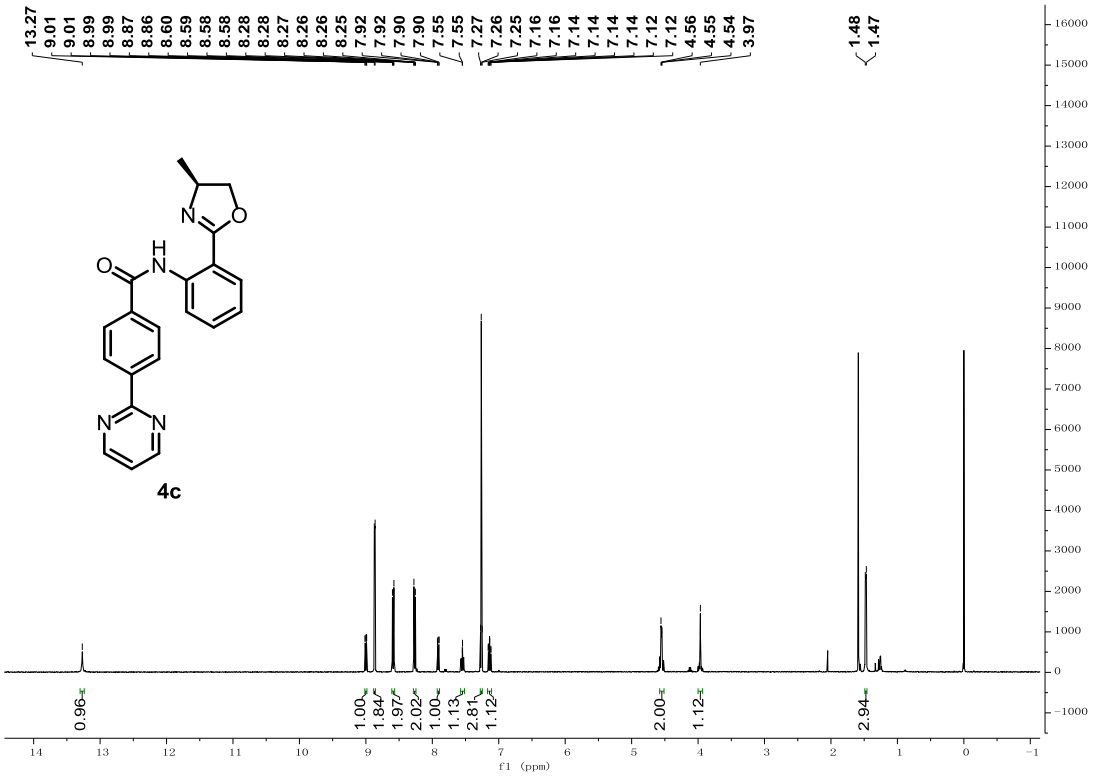
142.52
140.23
136.98
135.82
132.70
129.87
129.76
129.22
128.33
127.61
127.51
127.37
126.67
122.46
119.82
118.98
113.57
77.21
77.00
76.79
72.77
61.99
21.64
4b
f1 (ppm)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8.87
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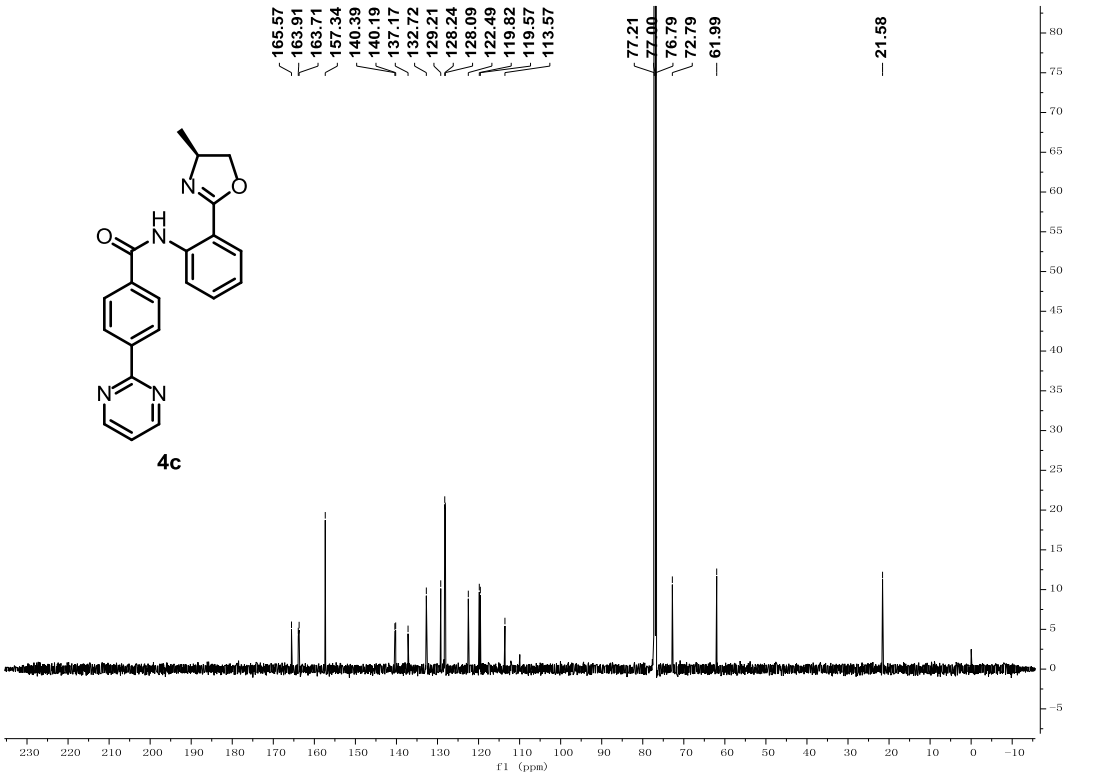
8.58
8.28
8.28
8.27
8.26
8.26
8.25
7.92
7.92
7.90
7.90
7.55
7.55
7.27
7.26
7.25
7.16
7.16
7.14
7.14
7.14
7.14
7.12
7.12
4.56
4.55
4.54
3.97
1.48
1.47
4c
0.96
1.00
1.84
1.97
2.02
1.00
1.13
2.81
1.12
2.00
1.12
2.94
f1 (ppm)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128.24
128.09
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113.57
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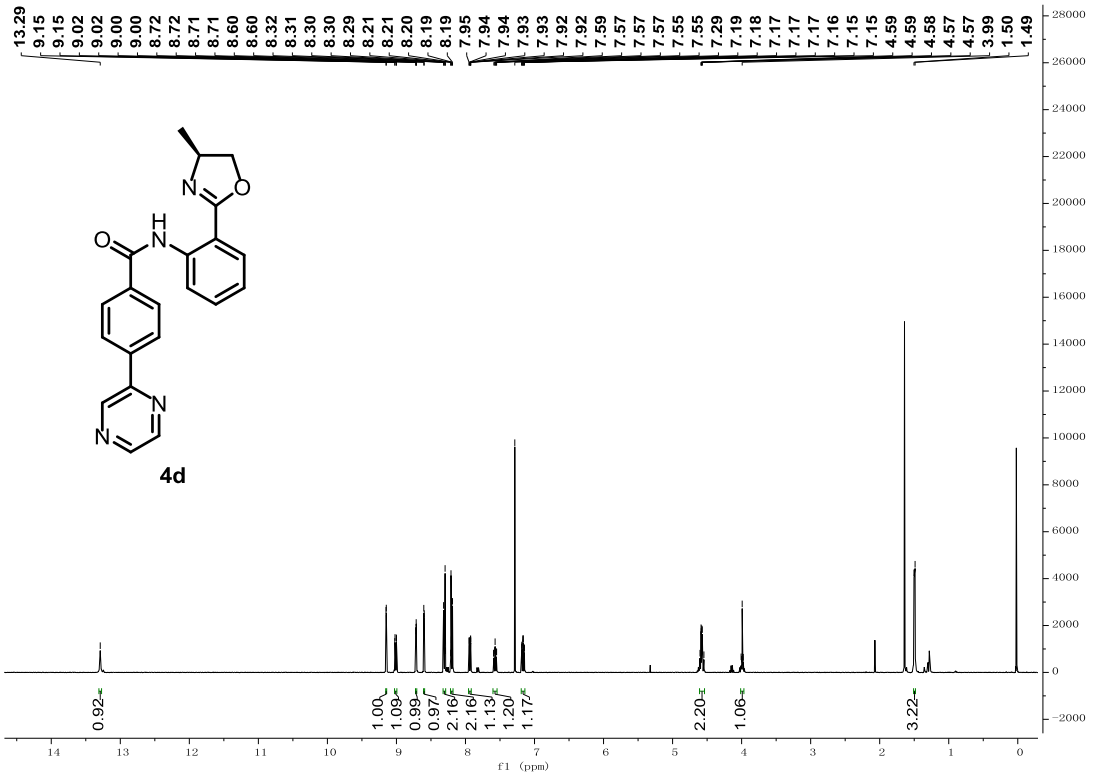
77.00
76.79
72.79
61.99
21.58
f1 (ppm)

4c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8.60
8.32
8.31
8.30
8.30
8.29
8.21
8.21
8.20
8.19
8.19
7.95
7.94
7.94
7.93
7.93
7.92
7.92
7.59
7.57
7.57
7.57
7.55
7.55
7.29
7.19
7.18
7.17
7.17
7.17
7.16
7.15
7.15
4.59
4.59
4.58
4.57
4.57
3.99
1.50
1.49
0.92
1.00
1.09
0.99
0.97
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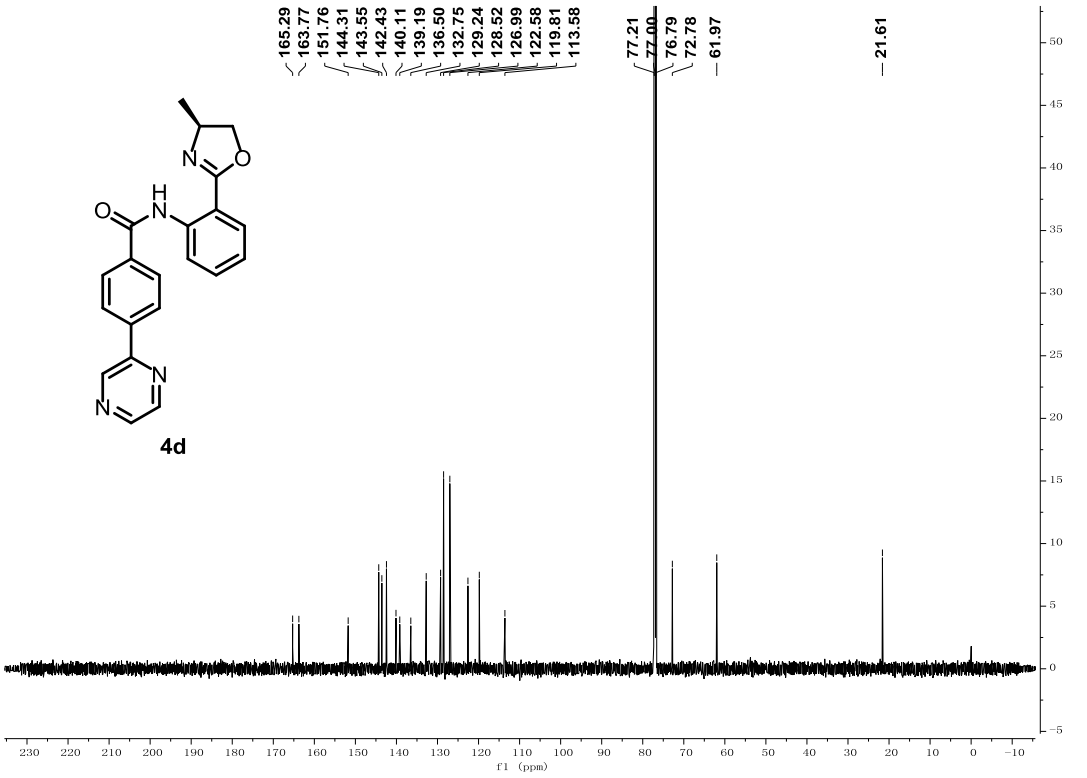
2.16
1.13
1.20
1.17
2.20
1.06
3.22
f1 (ppm)

4d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128.52
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113.58
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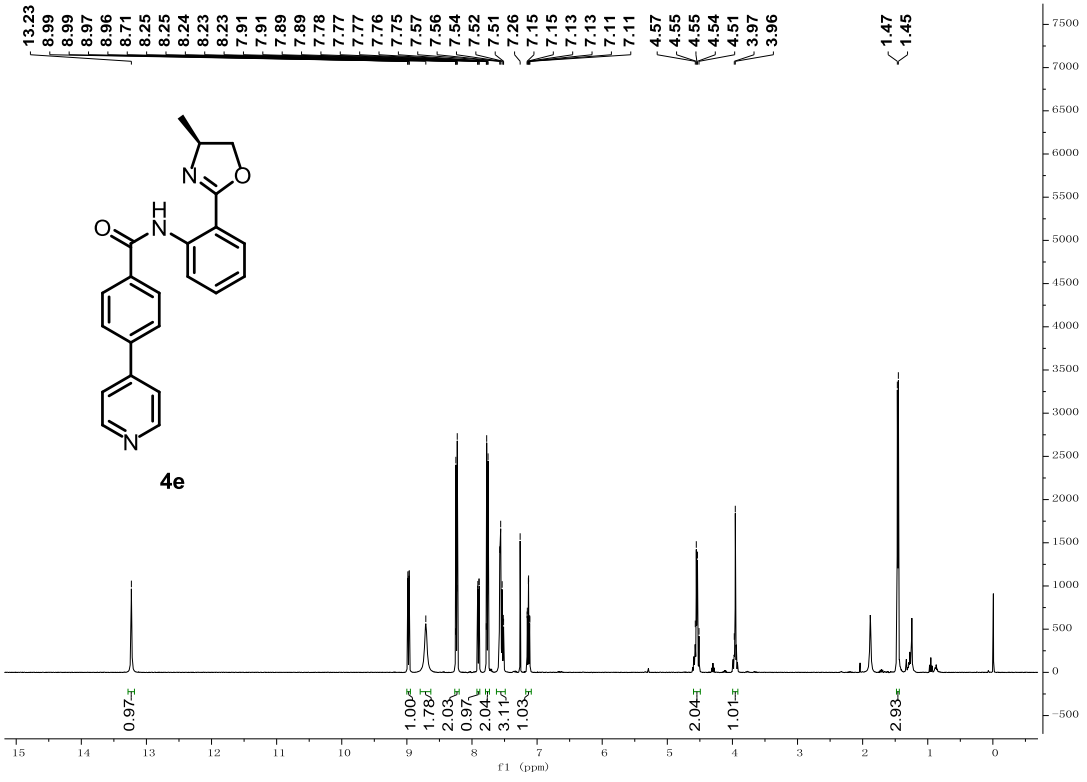
77.00
76.79
72.78
61.97
21.61
4d
f1 (ppm)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7.89
7.78
7.77
7.77
7.76
7.75
7.57
7.56
7.54
7.52
7.51
7.26
7.15
7.15
7.13
7.13
7.11
7.11
4.57
4.55
4.55
4.54
4.51
3.97
3.96
1.47
1.45
4e
0.97
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0.97
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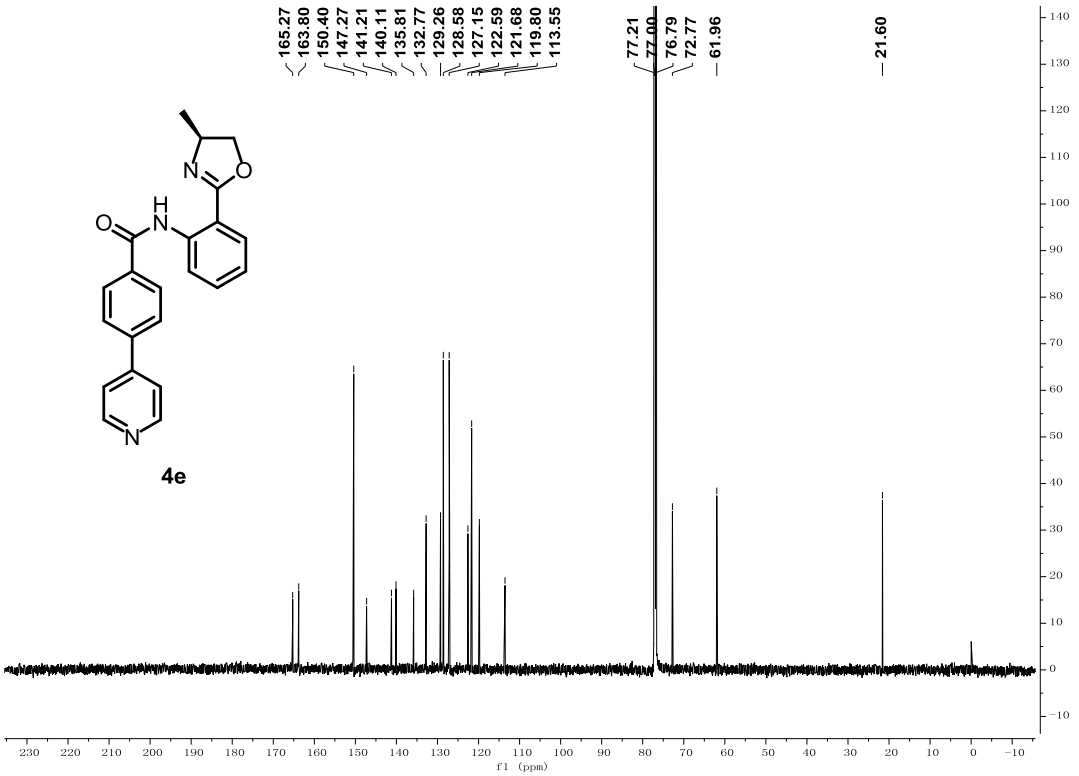
3.11
1.03
2.04
1.01
2.93
f1 (ppm)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127.15
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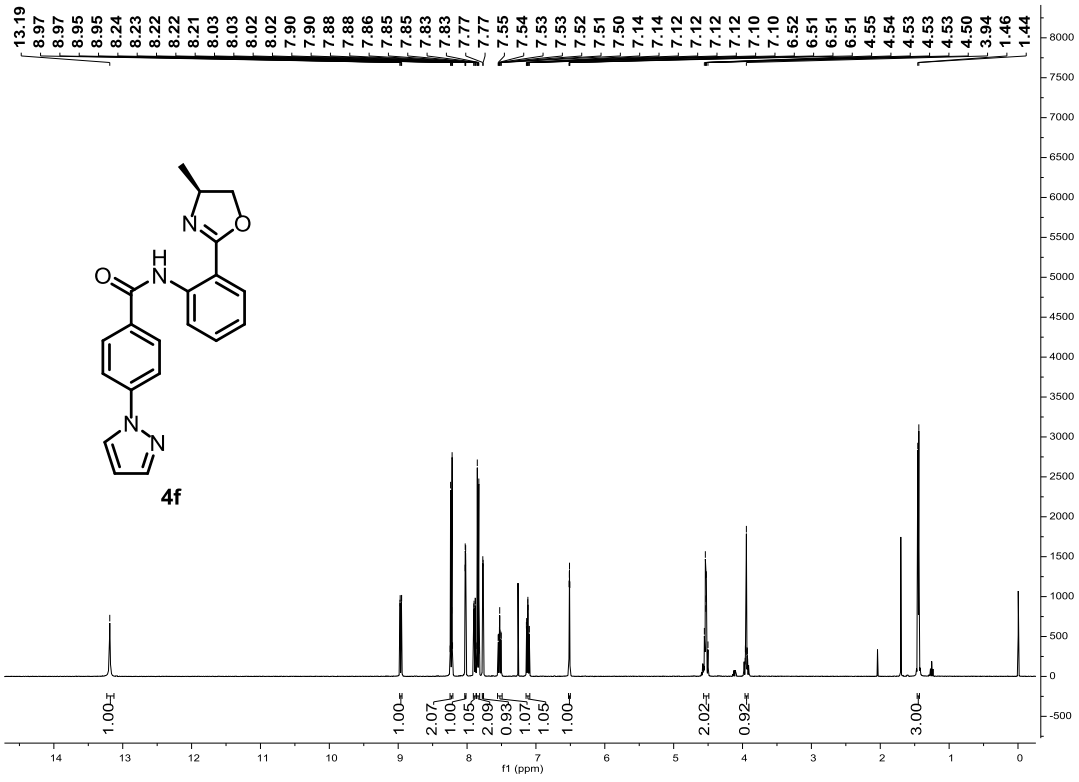
76.79
72.77
61.96
21.60
4e
f1 (ppm)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8.22
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8.03
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7.88
7.86
7.85
7.85
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7.83
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7.77
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7.53
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7.51
7.50
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7.12
7.12
7.10
7.10
6.52
6.51
6.51
6.51
4.55
4.54
4.53
4.53
4.53
4.50
3.94
1.46
1.44
4f
1.00
1.00
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1.00
1.05
2.09
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1.07
1.05
1.00
2.02
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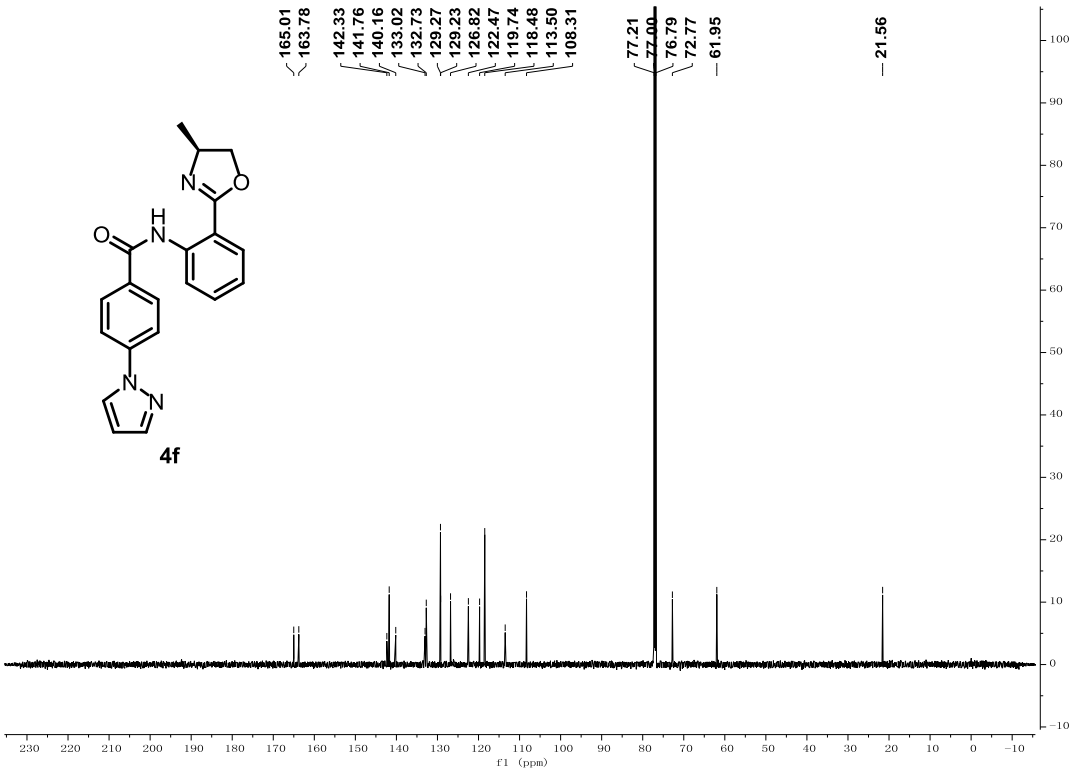
3.00
f1 (ppm)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140.16
133.02
132.73
129.27
129.23
126.82
122.47
119.74
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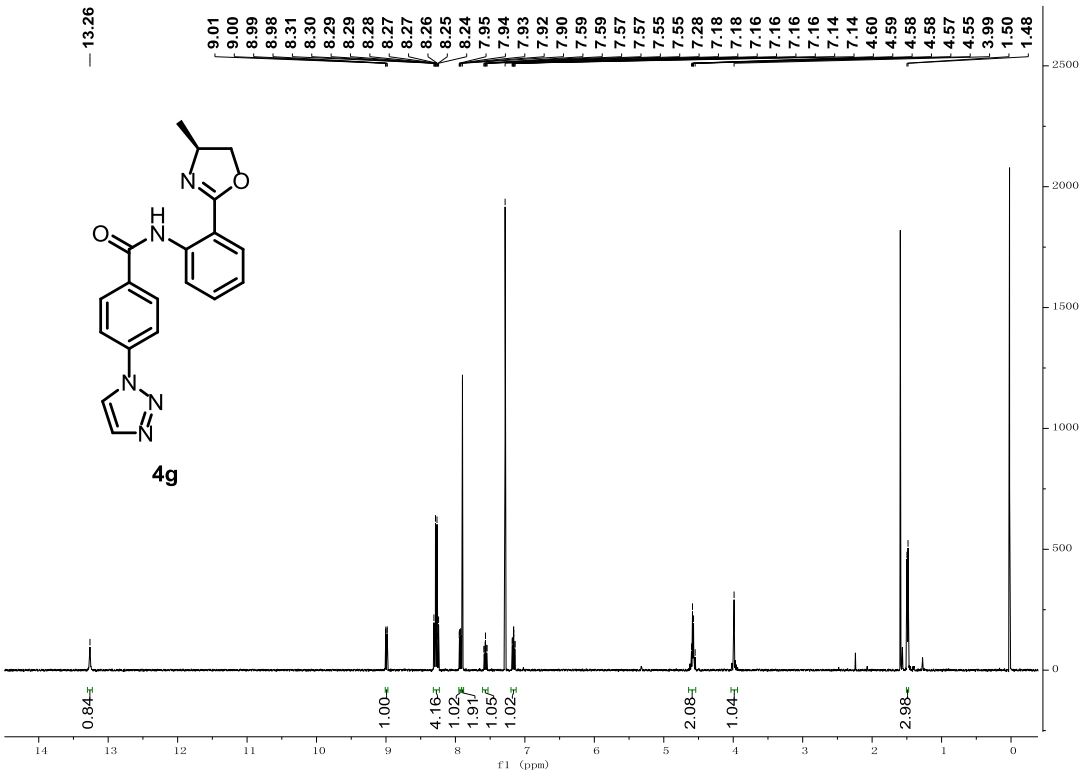
113.50
108.31
77.21
77.00
76.79
72.77
61.95
21.56
f1 (ppm)

4f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8.29
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8.28
8.27
8.27
8.26
8.25
8.24
7.95
7.94
7.93
7.92
7.90
7.59
7.59
7.57
7.57
7.55
7.55
7.28
7.18
7.18
7.16
7.16
7.16
7.14
7.14
4.60
4.59
4.58
4.58
4.57
4.55
3.99
1.50
1.48
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1.00
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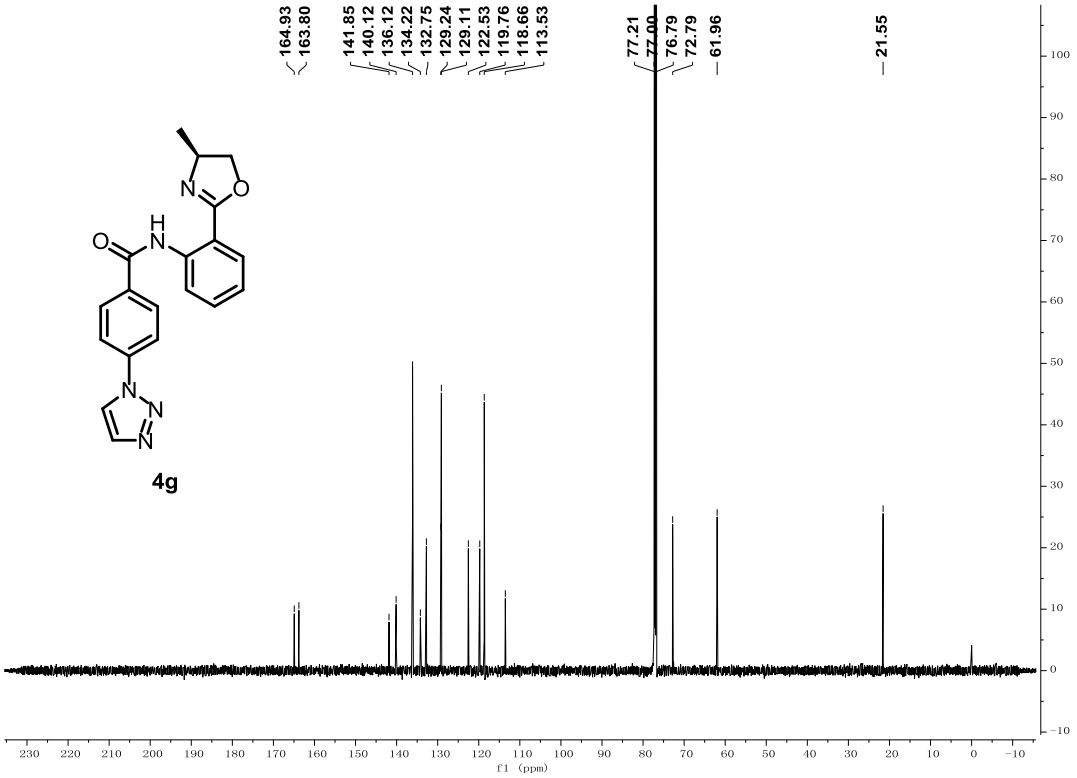
1.02
1.91
1.05
1.02
2.08
1.04
2.98
f1 (ppm)

4g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136.12
134.22
132.75
129.24
129.11
122.53
119.76
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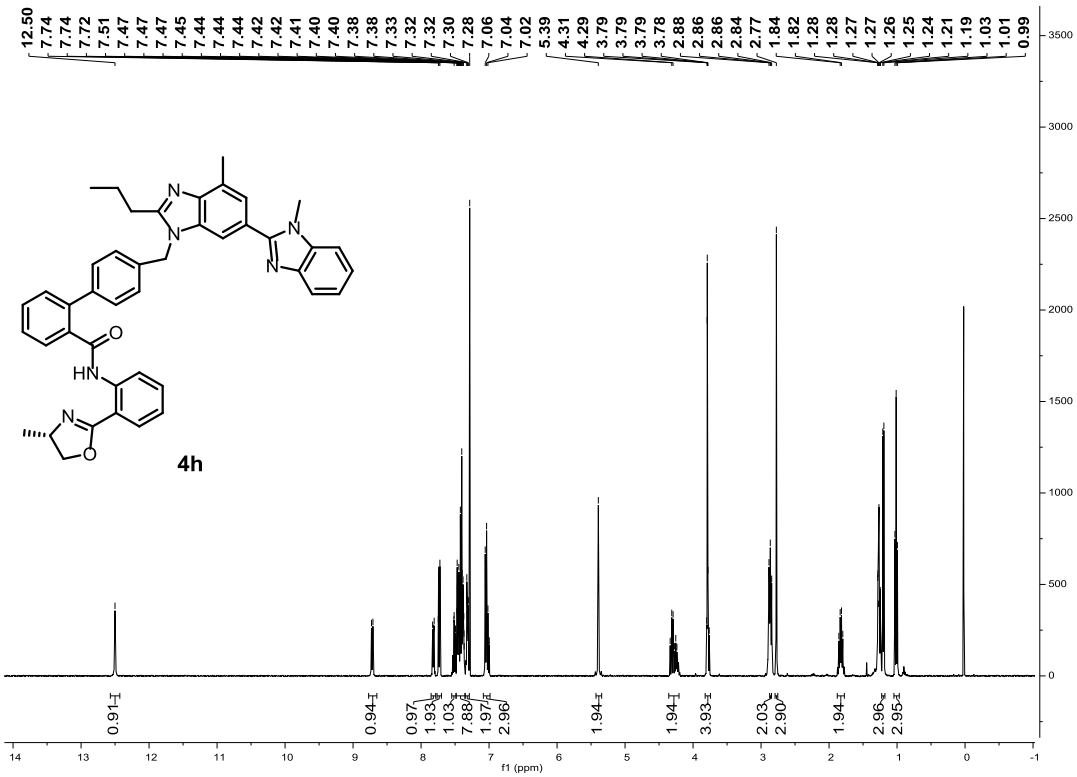
113.53
77.21
77.00
76.79
72.79
61.96
21.55
f1 (ppm)

4g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7.33
7.32
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7.06
7.04
7.02
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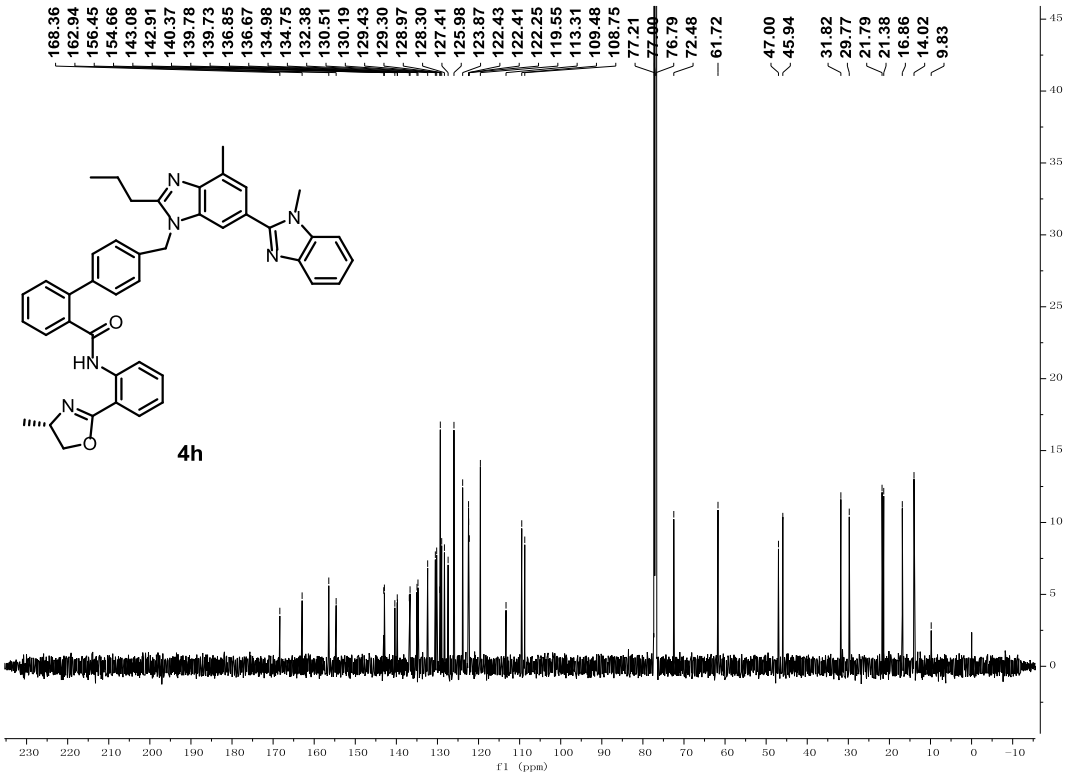
4.31
4.29
3.79
3.79
3.79
3.78
2.88
2.86
2.86
2.84
2.77
1.84
1.82
1.28
1.28
1.27
1.27
1.26
1.25
1.24
1.21
1.19
1.03
1.01
0.99
0.91
0.94
0.97
1.93
1.03
7.88
1.97
2.96
1.94
1.94
3.93
2.03
2.90
1.94
2.96
2.95
f1 (ppm)

4h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142.91
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139.78
139.73
136.85
136.67
134.98
134.75
132.38
130.51
130.19
129.43
129.30
128.97
128.30
127.41
125.98
123.87
122.43
122.41
122.25
119.55
113.31
109.48
108.75
77.21
77.00
76.79
72.48
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31.82
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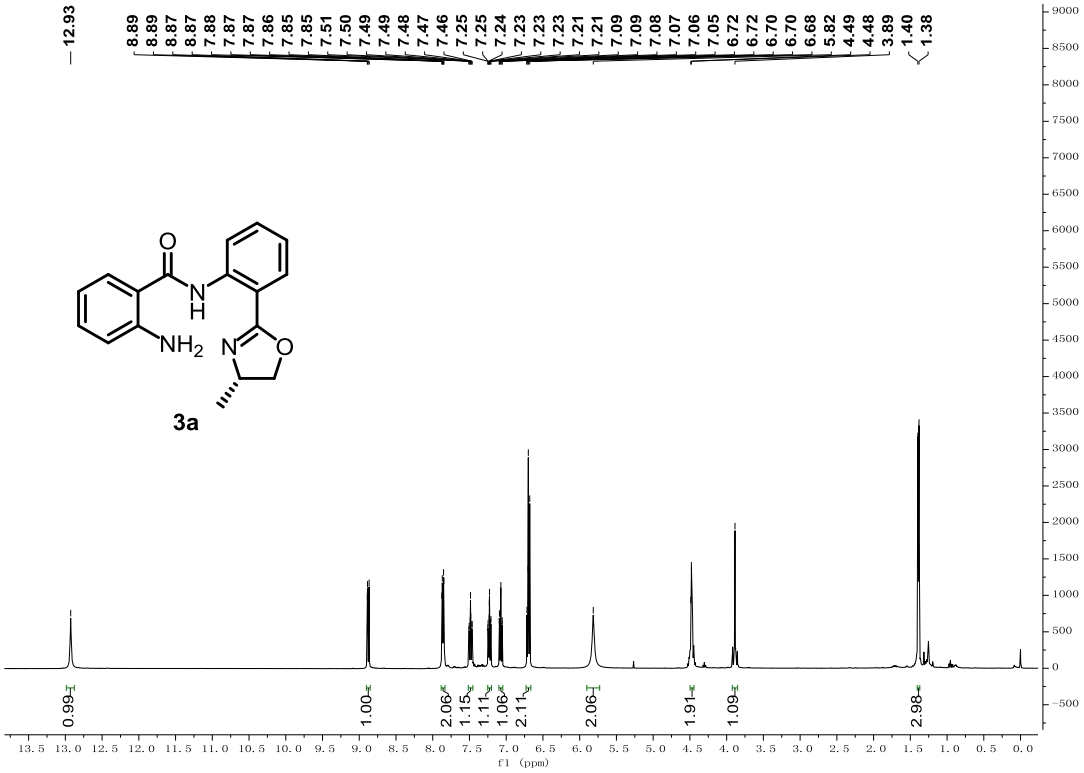
21.79
21.38
16.86
14.02
9.83
4h
f1 (ppm)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7.85
7.85
7.51
7.50
7.49
7.49
7.48
7.47
7.46
7.25
7.25
7.24
7.23
7.23
7.23
7.21
7.21
7.09
7.09
7.08
7.07
7.06
7.05
6.72
6.72
6.70
6.70
6.68
5.82
4.49
4.48
3.89
1.40
1.38
3a
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1.00
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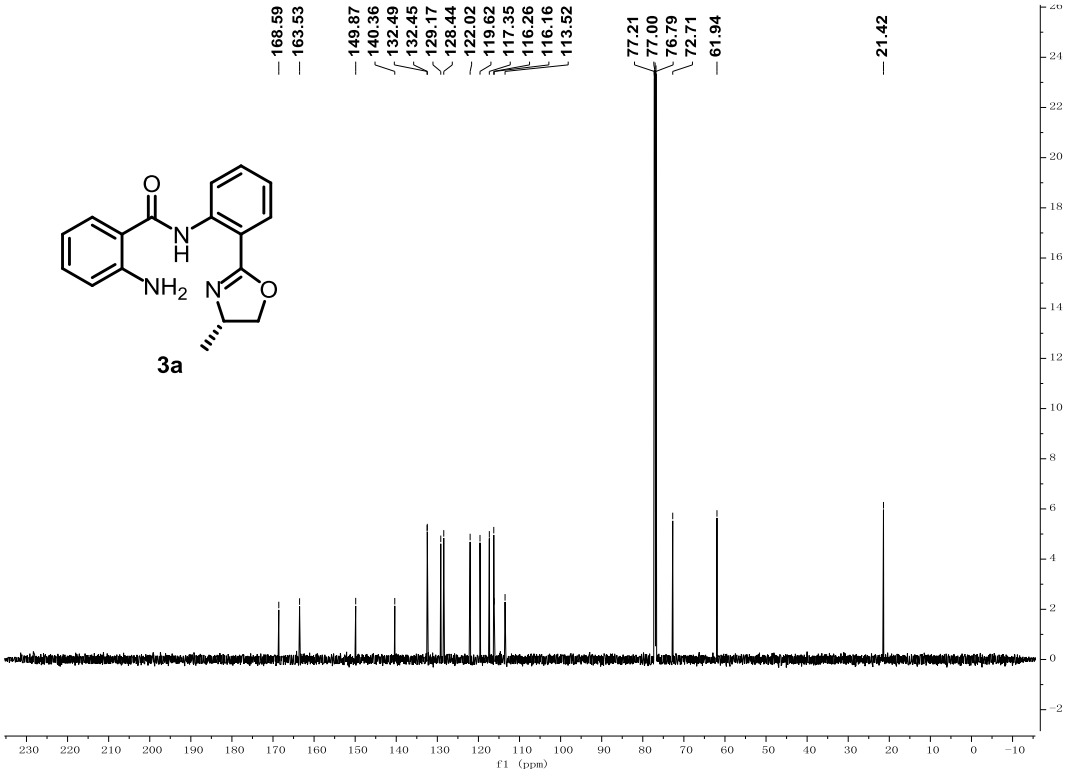
1.15
1.11
1.06
2.11
2.06
1.91
1.09
2.98
f1 (ppm)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122.02
119.62
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116.26
116.16
113.52
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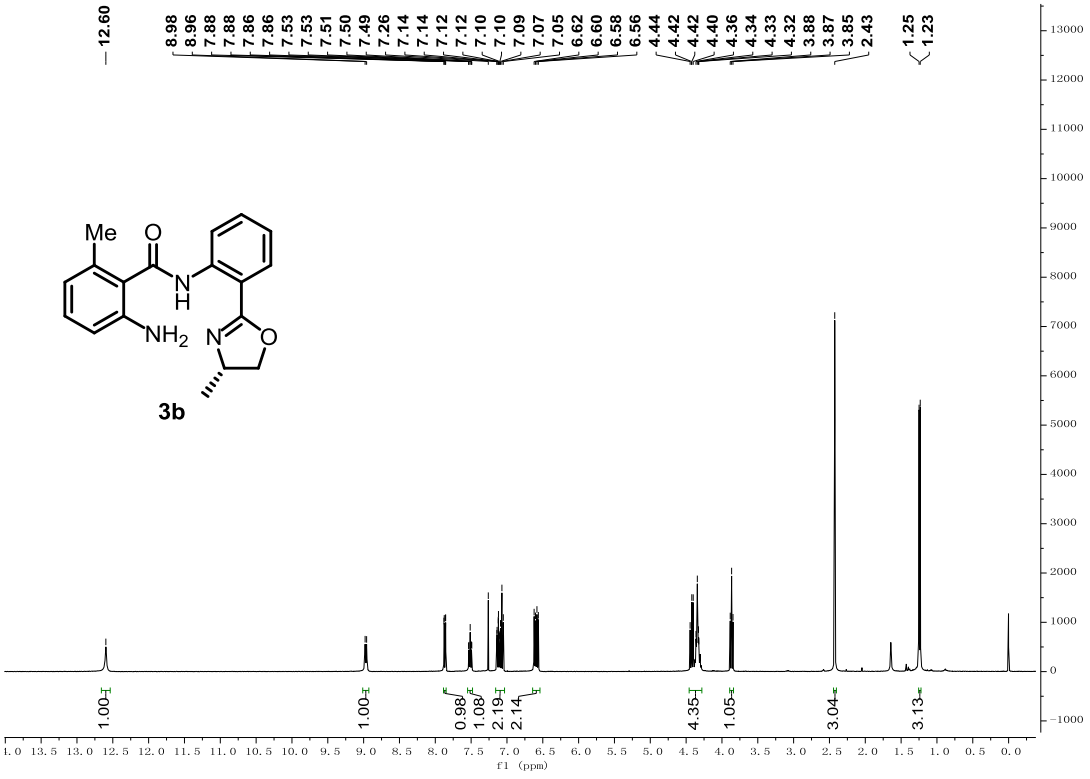
76.79
72.71
61.94
21.42
O
N
H
NH2
N
O
3a
f1 (ppm)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7.86
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7.51
7.50
7.49
7.26
7.14
7.14
7.12
7.12
7.10
7.10
7.09
7.07
7.05
6.62
6.60
6.58
6.56
4.44
4.42
4.42
4.40
4.36
4.34
4.33
4.32
3.88
3.87
3.85
2.43
1.25
1.23
Me
O
N
H
NH2
N
O
3b
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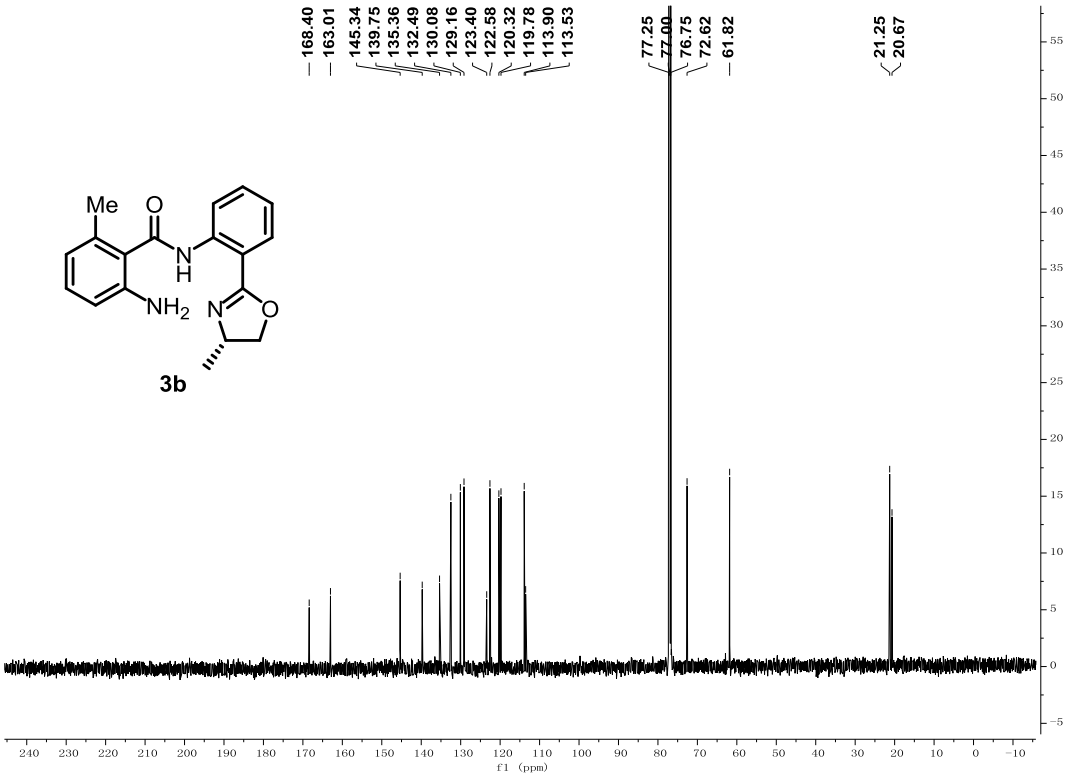
1.00
0.98
1.08
2.19
2.14
4.35
1.05
3.04
3.13
f1 (ppm)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122.58
120.32
119.78
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113.53
77.25
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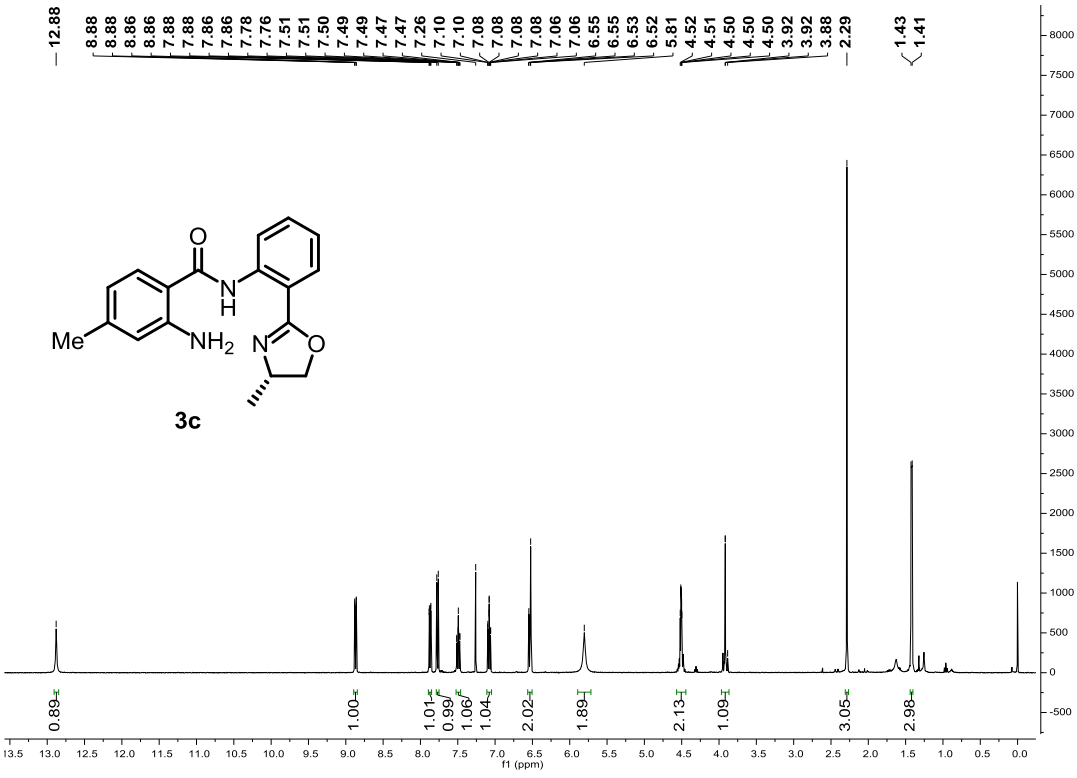
O
N
H
NH2
N
O
3b
f1 (ppm)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7.50
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7.47
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7.26
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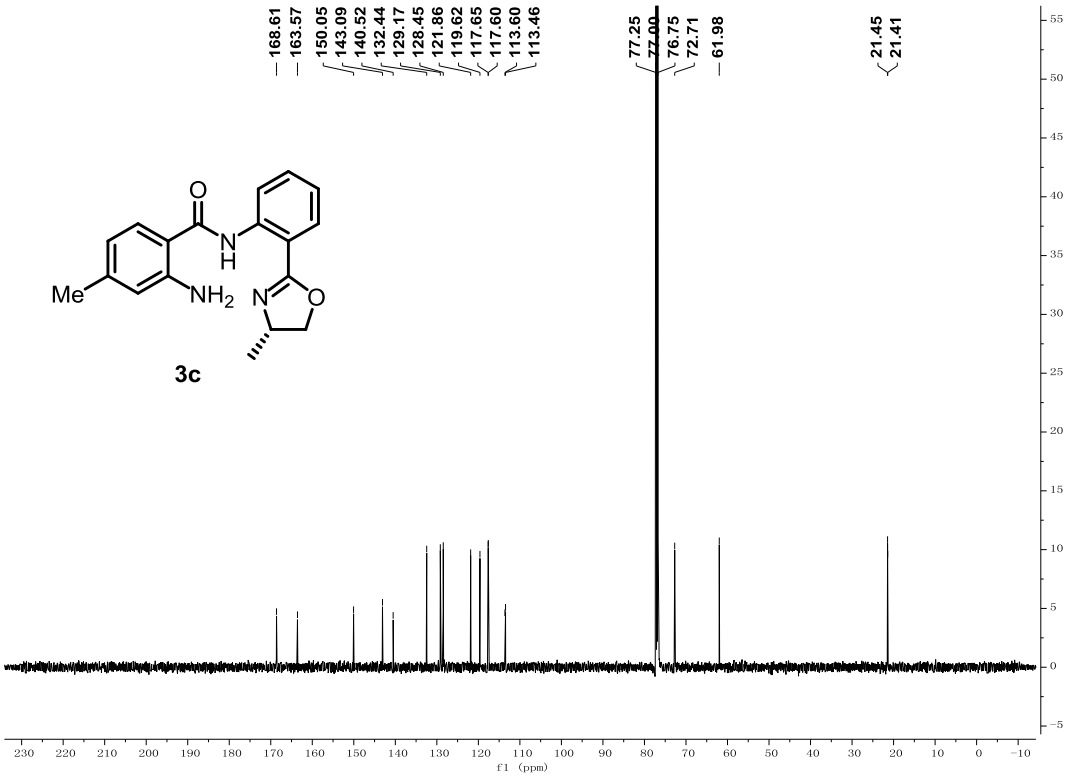
7.10
7.08
7.08
7.08
7.08
7.06
7.06
6.55
6.55
6.53
6.52
5.81
4.52
4.51
4.50
4.50
4.50
3.92
3.92
3.88
2.29
1.43
1.41
O
N
H
Me
NH2
N
O
3c
0.89
1.00
1.01
0.99
1.06
1.04
2.02
1.89
2.13
1.09
3.05
2.98
f1 (ppm)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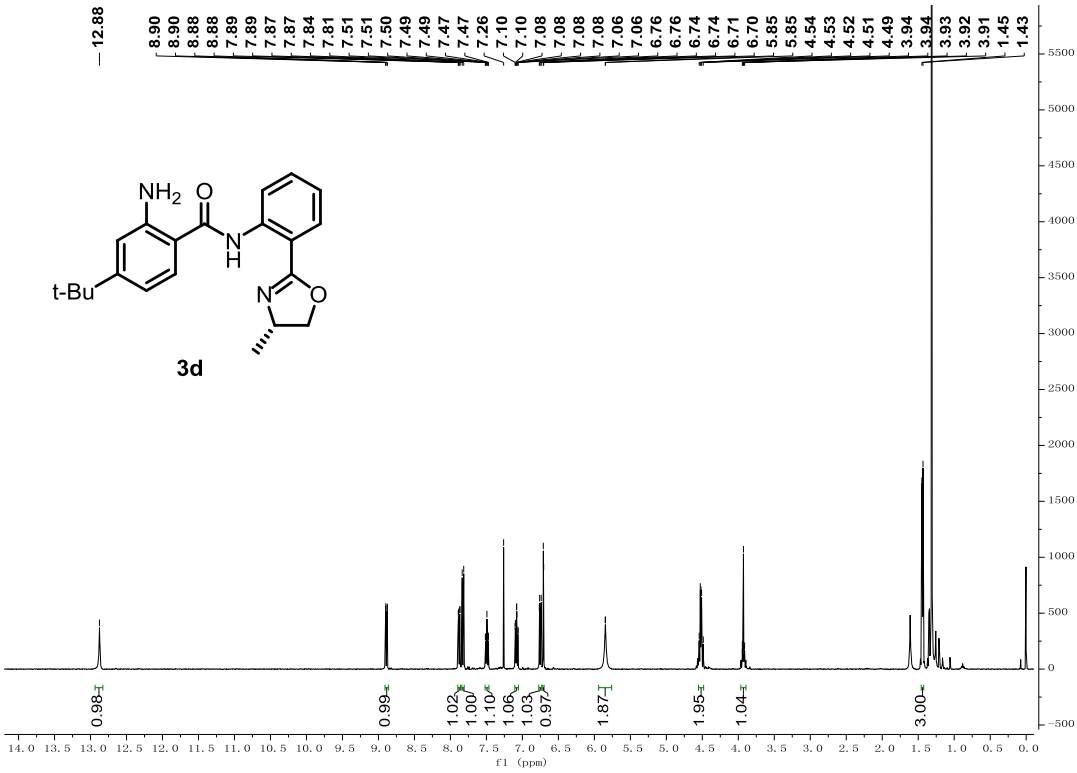
132.44
129.17
128.45
121.86
119.62
117.65
117.60
113.60
113.46
77.25
77.00
76.75
72.71
61.98
21.45
21.41
Me
NH2
O
N
H
N
O
3c
f1 (ppm)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7.50
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7.08
7.06
7.06
6.76
6.76
6.74
6.74
6.71
6.70
5.85
5.85
4.54
4.53
4.52
4.51
4.49
3.94
3.94
3.93
3.92
3.91
1.45
1.43
NH2
O
N
H
t-Bu
N
O
3d
0.98
0.99
1.02
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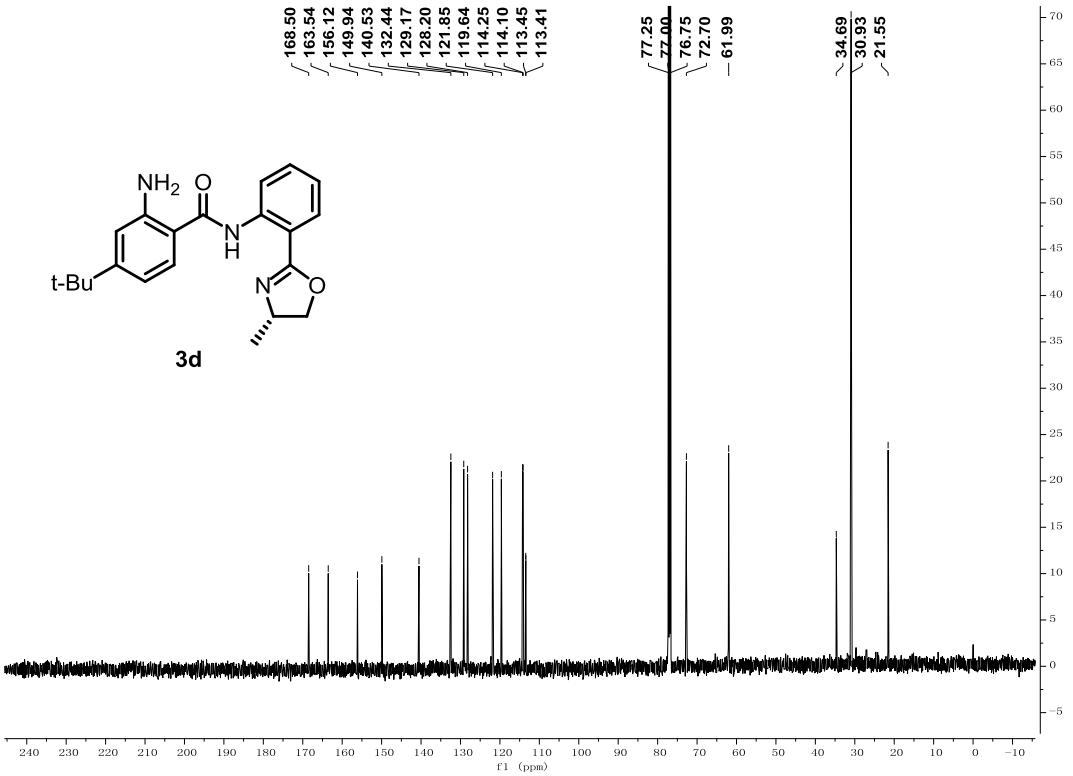
1.10
1.06
1.03
0.97
1.87
1.95
1.04
3.00
f1 (ppm)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132.44
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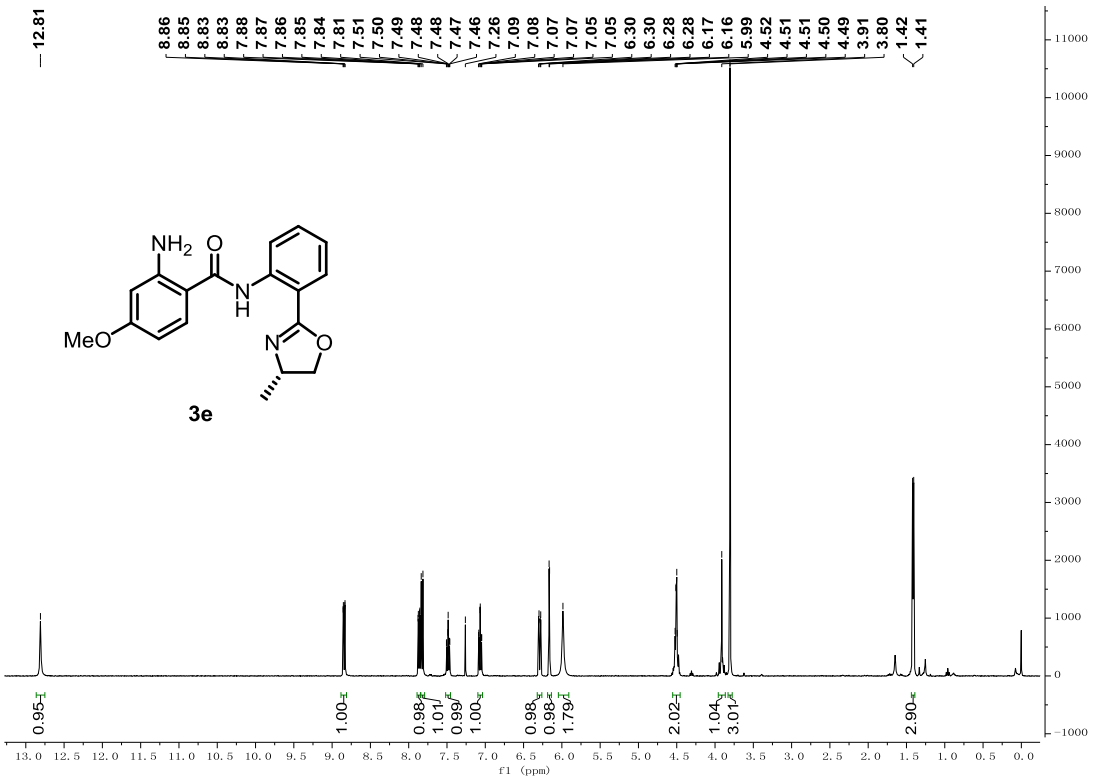
128.20
121.85
119.64
114.25
114.10
113.45
113.41
77.25
77.00
76.75
72.70
61.99
34.69
30.93
21.55
NH2
O
N
H
t-Bu
N
O
f1 (ppm)

3d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7.85
7.84
7.81
7.51
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7.49
7.48
7.48
7.47
7.46
7.26
7.09
7.08
7.07
7.07
7.05
7.05
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6.17
6.16
5.99
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4.51
4.51
4.50
4.49
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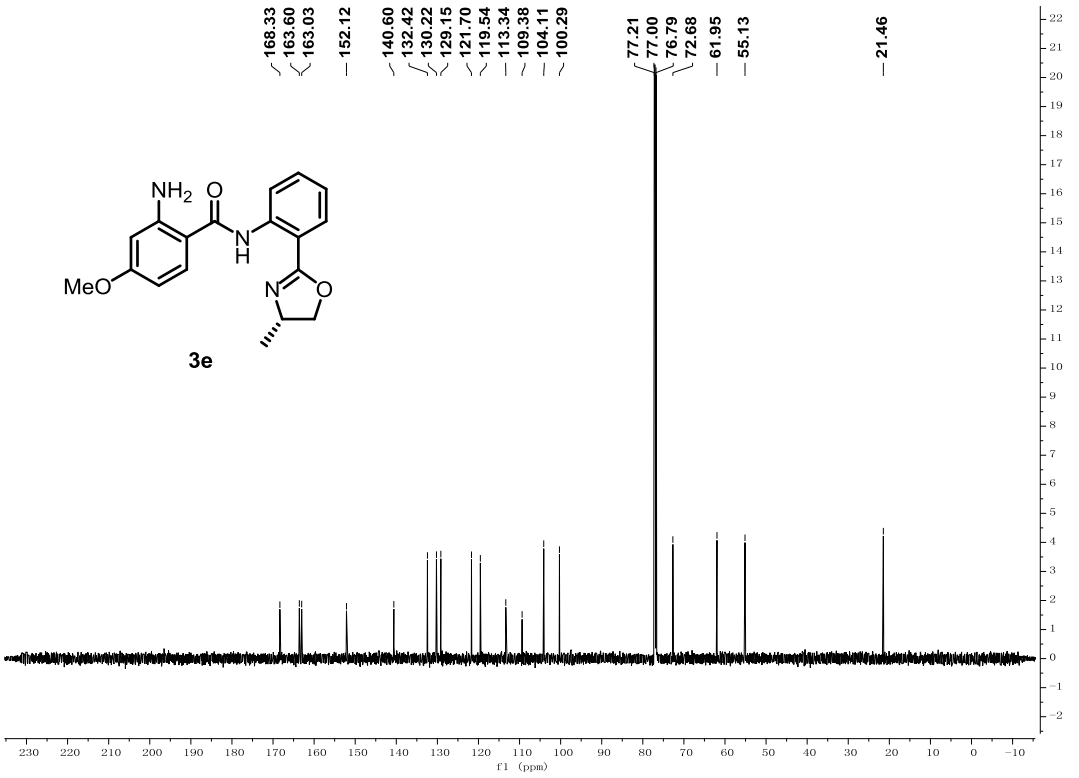
3.80
1.42
1.41
NH2
O
N
H
MeO
N
O
0.95
1.00
0.98
1.01
0.99
1.00
0.98
0.98
1.79
2.02
1.04
3.01
2.90
f1 (ppm)

3e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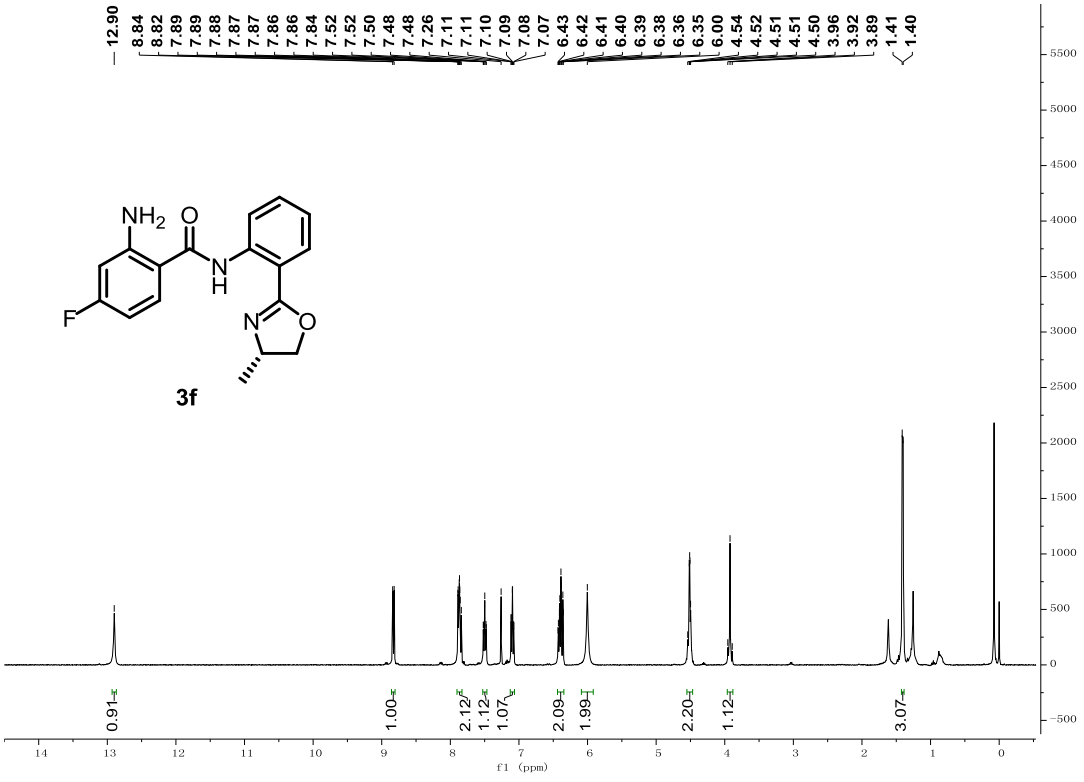
119.54
113.34
109.38
104.11
100.29
77.21
77.00
76.79
72.68
61.95
55.13
21.46
NH2
O
N
H
MeO
N
O
f1 (ppm)

3e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7.87
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7.86
7.84
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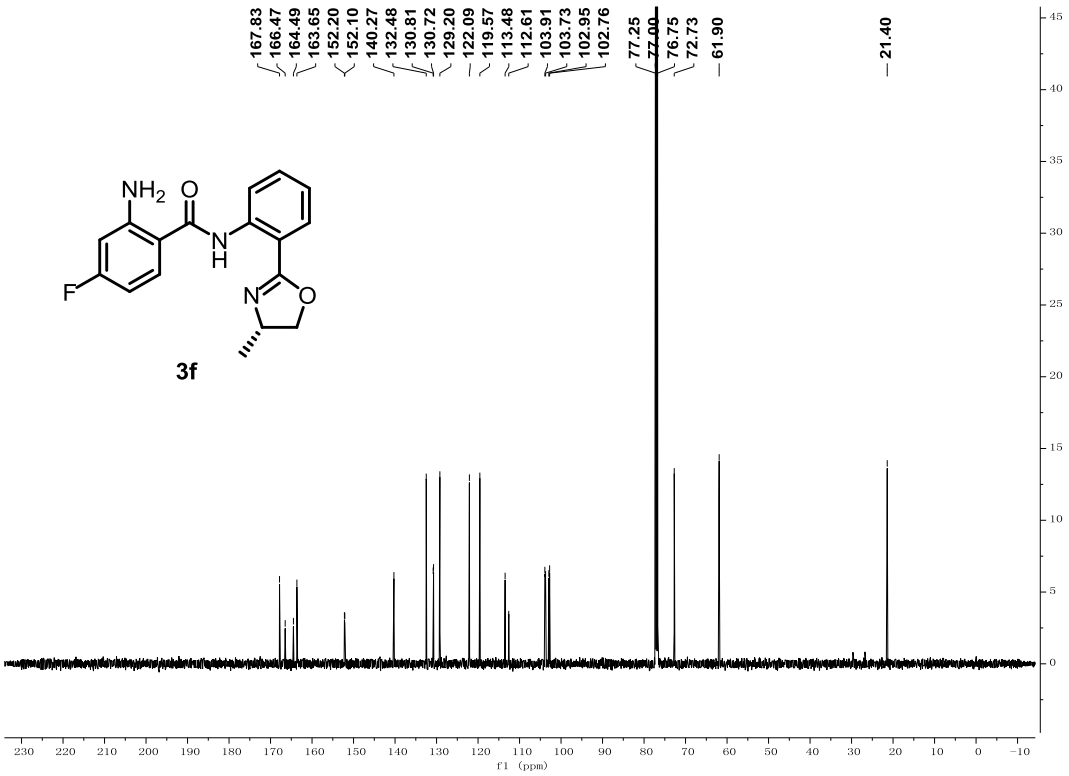
7.52
7.50
7.48
7.48
7.26
7.11
7.11
7.10
7.09
7.08
7.07
6.43
6.42
6.41
6.40
6.39
6.38
6.36
6.35
6.00
4.54
4.52
4.51
4.51
4.50
3.96
3.92
3.89
1.41
1.40
NH2
O
N
H
F
N
O
0.91
1.00
2.12
1.12
1.07
2.09
1.99
2.20
1.12
3.07
f1 (ppm)

3f


167.83
166.47
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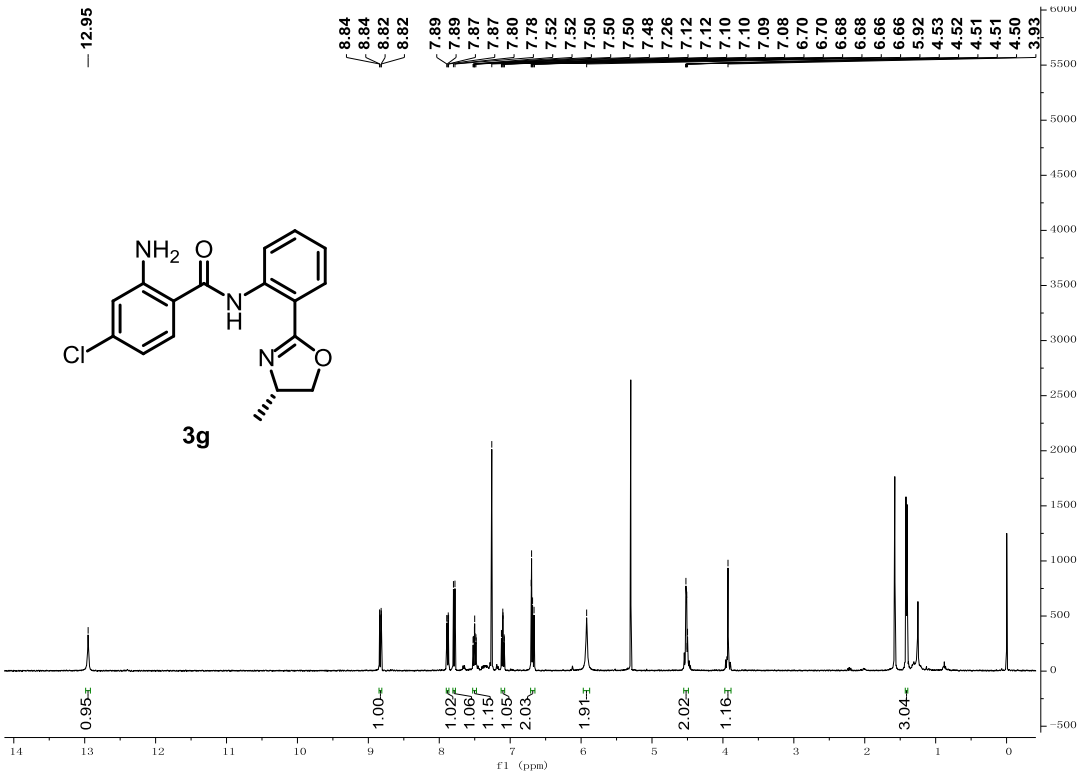
163.65
152.20
152.10
140.27
132.48
130.81
130.72
129.20
122.09
119.57
113.48
112.61
103.91
103.73
102.95
102.76
77.25
77.00
76.75
72.73
61.90
21.40
NH2
O
N
H
F
N
O
3f
f1 (ppm)


-107.97
NH2
O
N
H
F
N
O
3f
f1 (ppm)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7.52
7.50
7.50
7.50
7.48
7.26
7.12
7.12
7.10
7.10
7.09
7.08
6.70
6.70
6.68
6.68
6.66
6.66
5.92
4.53
4.52
4.51
4.51
4.50
3.93
NH2
O
N
H
Cl
N
O
3g
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1.15
1.05
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2.02
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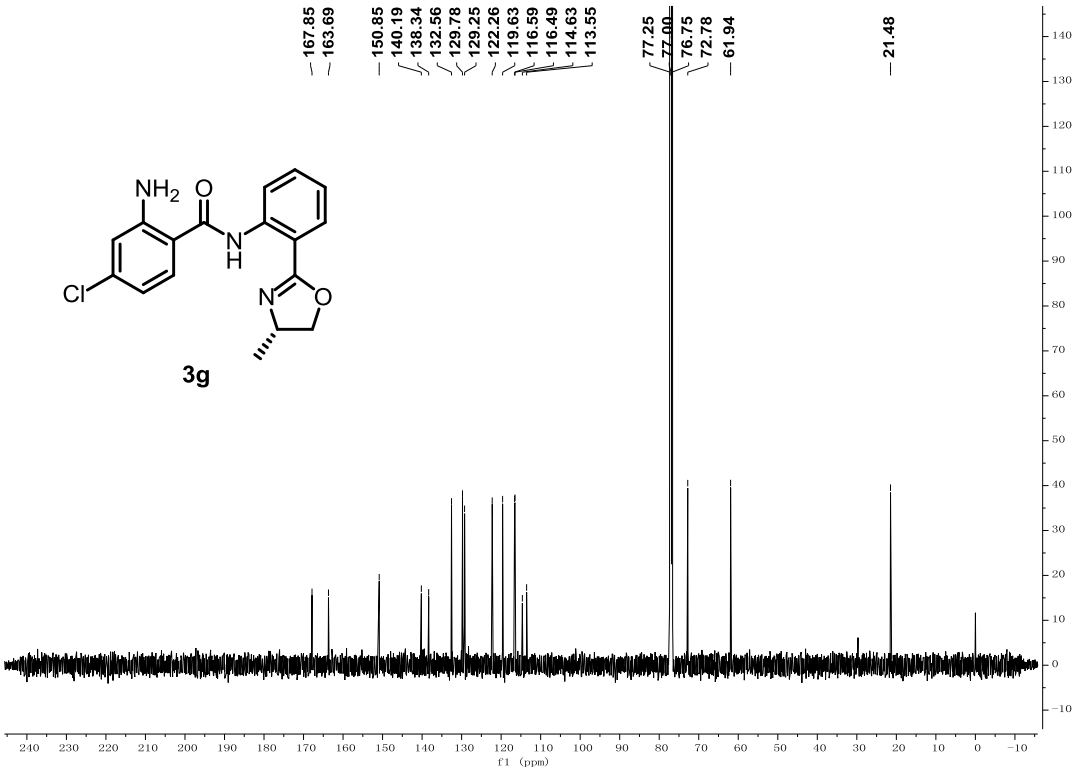
f1 (ppm)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114.63
113.55
77.25
77.00
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72.78
61.94
21.48
NH2
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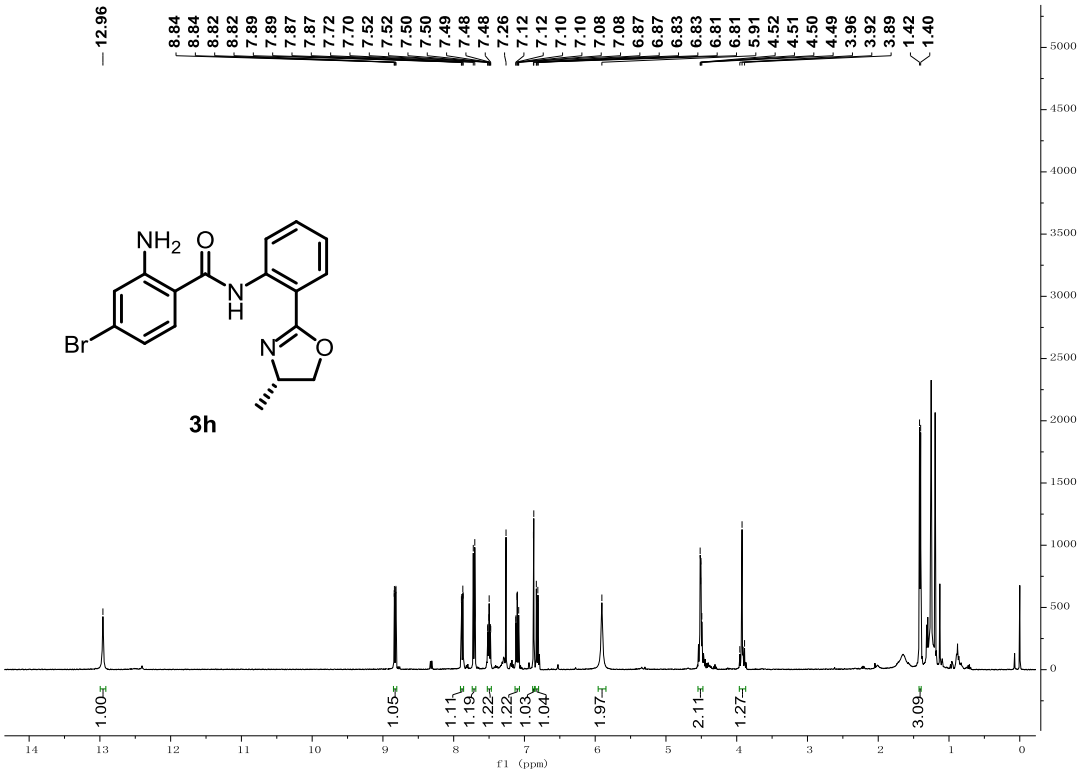
N
H
Cl
N
O
3g
f1 (ppm)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7.49
7.48
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5.91
4.52
4.51
4.50
4.49
3.96
3.92
3.89
1.42
1.40
NH2
O
N
H
Br
N
O
3h
1.00
1.05
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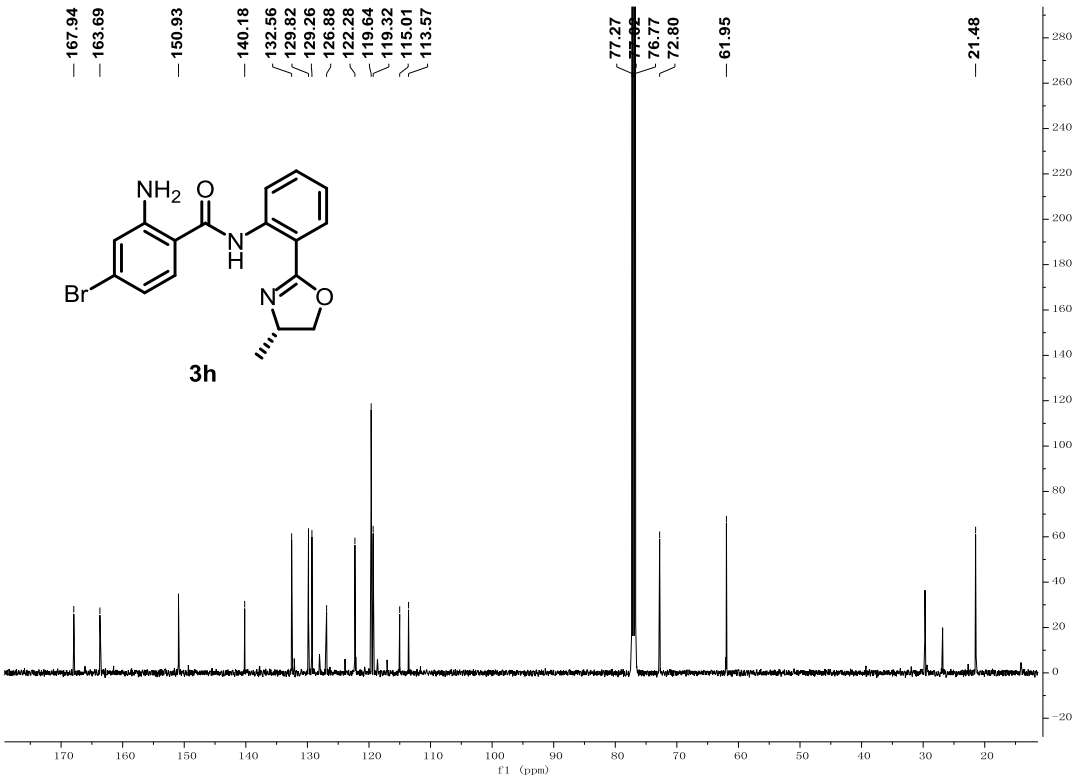
1.22
1.22
1.03
1.04
1.97
2.11
1.27
3.09
f1 (ppm)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21.48
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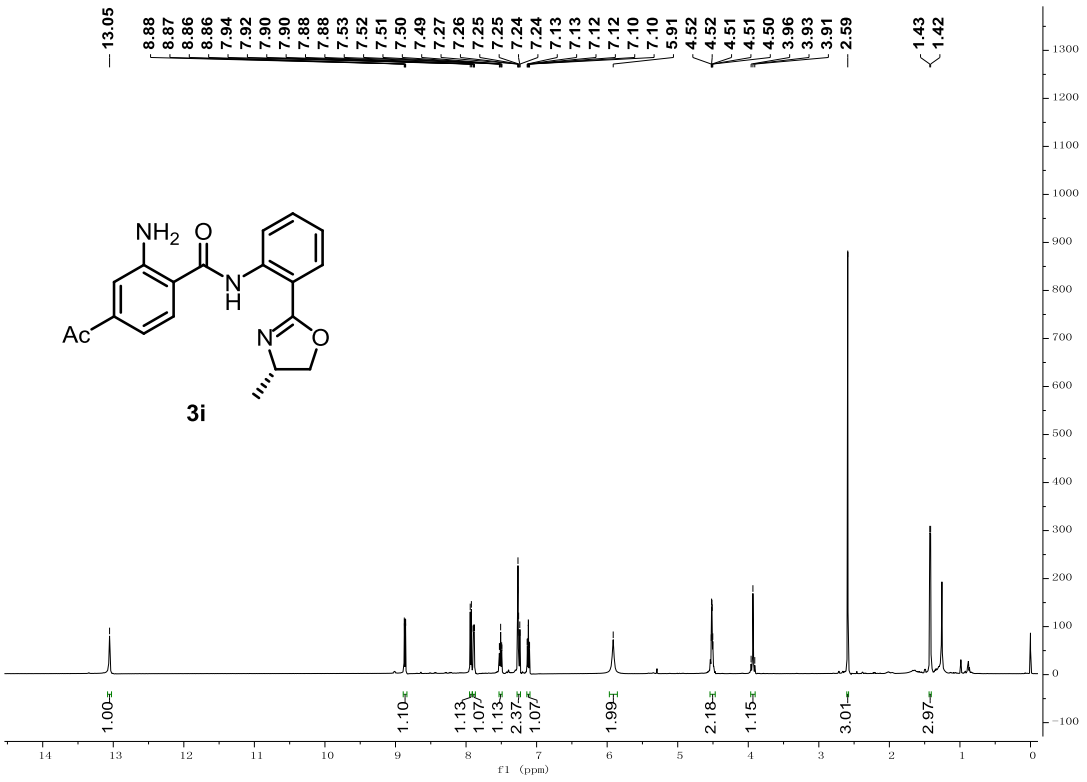
H
Br
N
O
3h
f1 (ppm)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7.26
7.25
7.25
7.24
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7.13
7.13
7.12
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7.10
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4.52
4.51
4.51
4.50
3.96
3.93
3.91
2.59
1.43
1.42
NH2
O
N
H
Ac
N
O
3i
1.00
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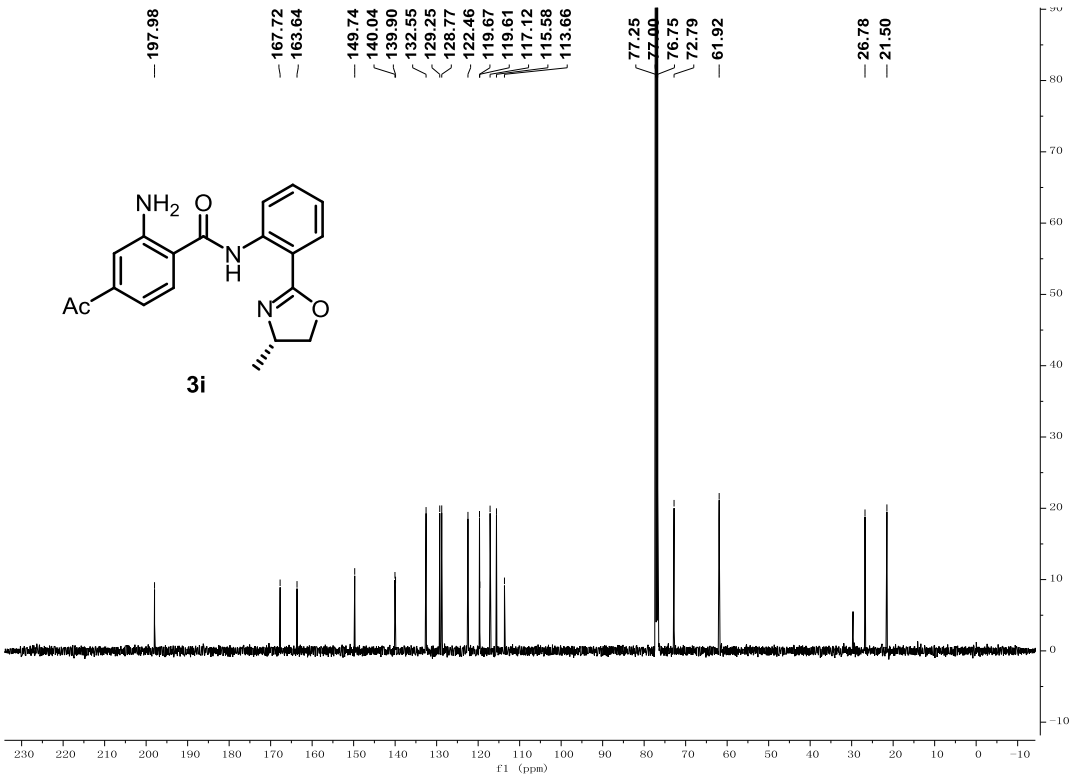
1.13
2.37
1.07
1.99
2.18
1.15
3.01
2.97
f1 (ppm)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113.66
77.25
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61.92
26.78
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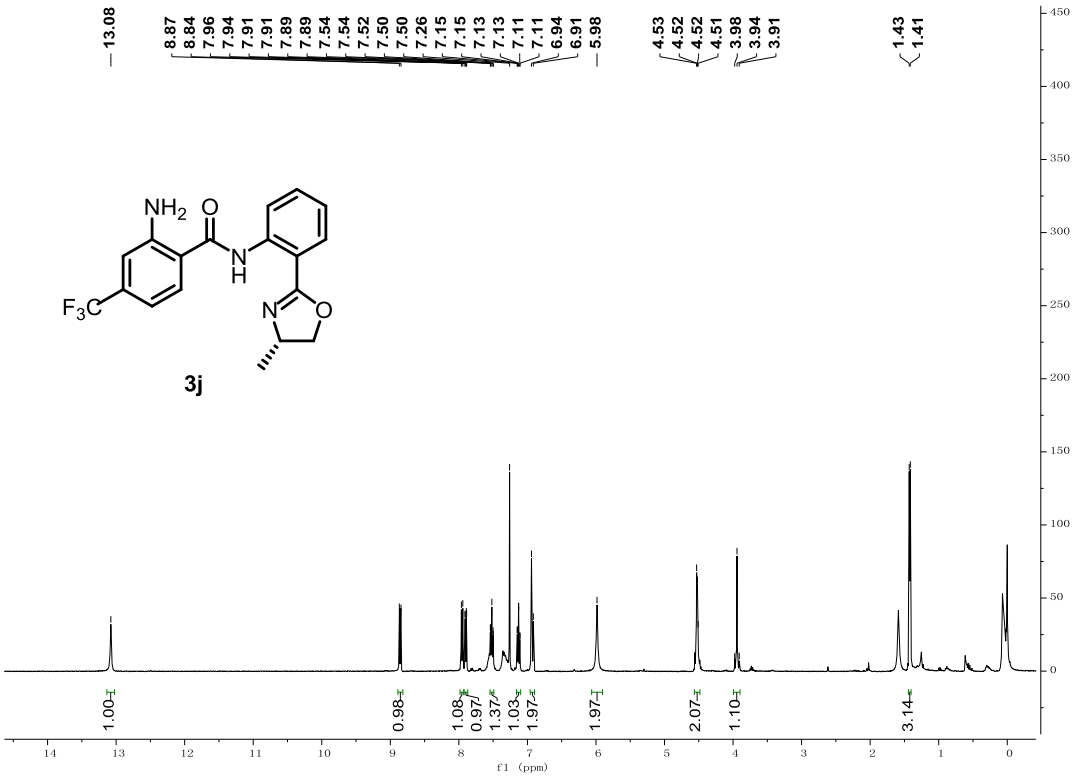
N
H
Ac
N
O
3i
f1 (ppm)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7.89
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7.54
7.52
7.50
7.50
7.26
7.15
7.15
7.13
7.11
7.11
6.94
6.91
5.98
4.53
4.52
4.52
4.51
3.98
3.94
3.91
1.43
1.41
NH2
O
N
H
F3C
N
O
3j
1.00
0.98
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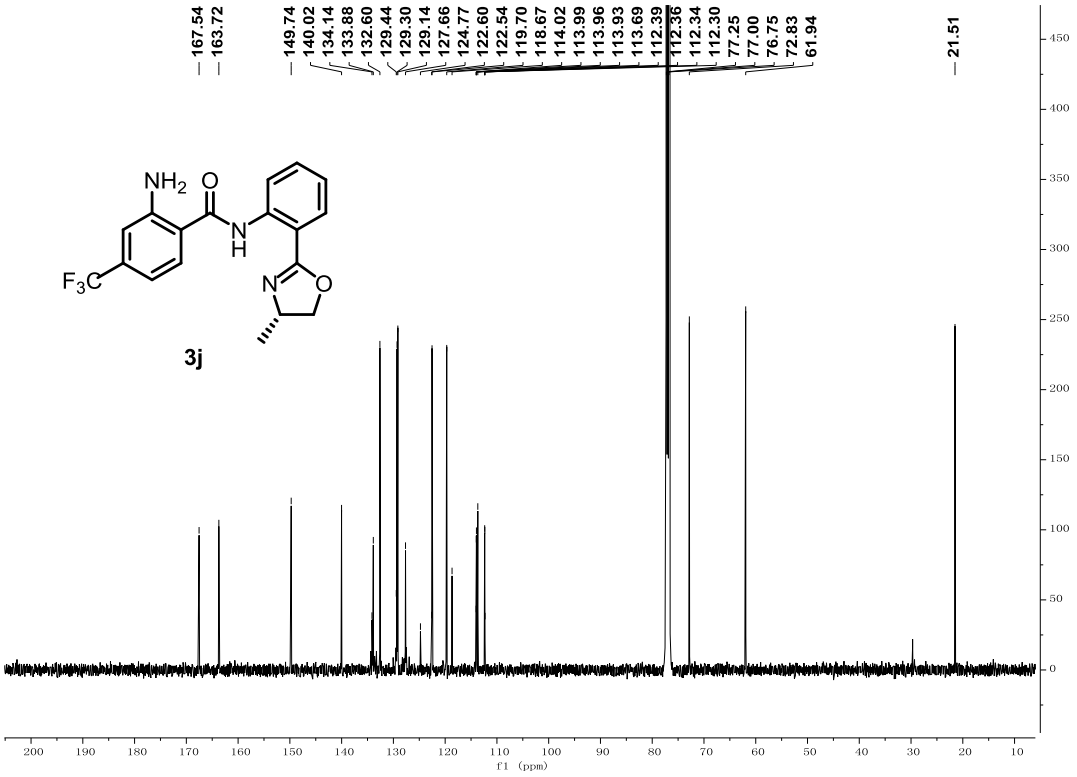
0.97
1.37
1.03
1.97
1.97
2.07
1.10
3.14
f1 (ppm)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124.77
122.60
122.54
119.70
118.67
114.02
113.99
113.96
113.93
113.69
112.39
112.36
112.34
112.30
77.25
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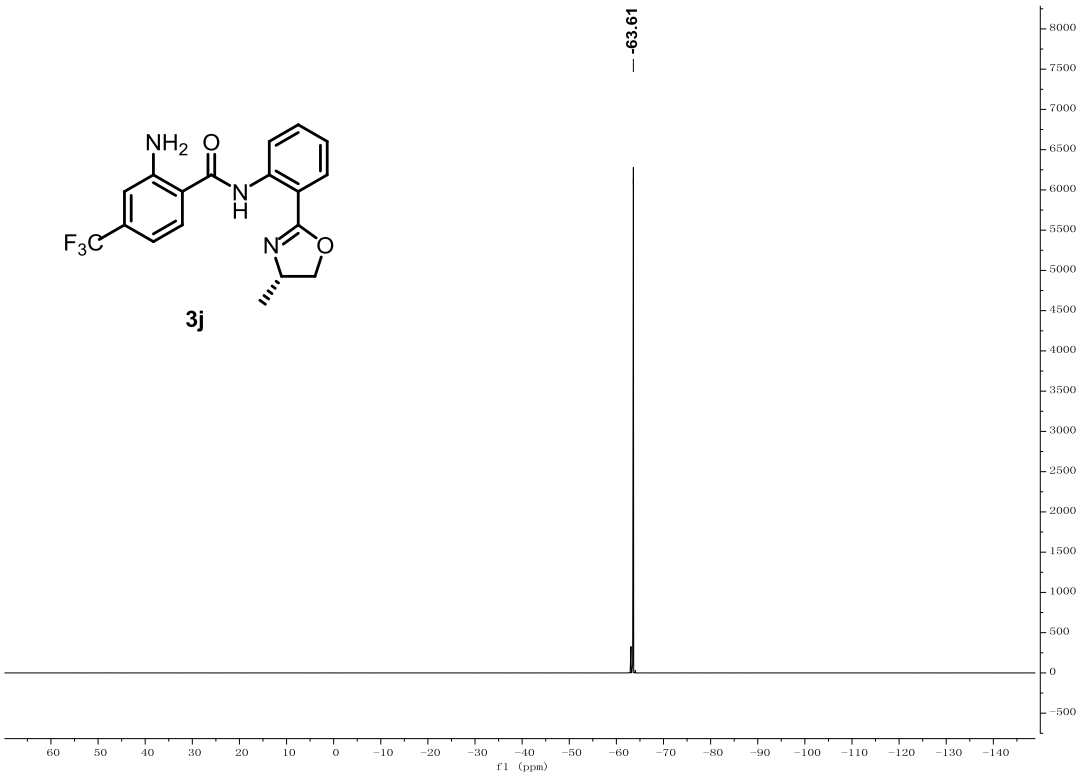
72.83
61.94
21.51
NH2
O
N
H
F3C
N
O
3j
f1 (ppm)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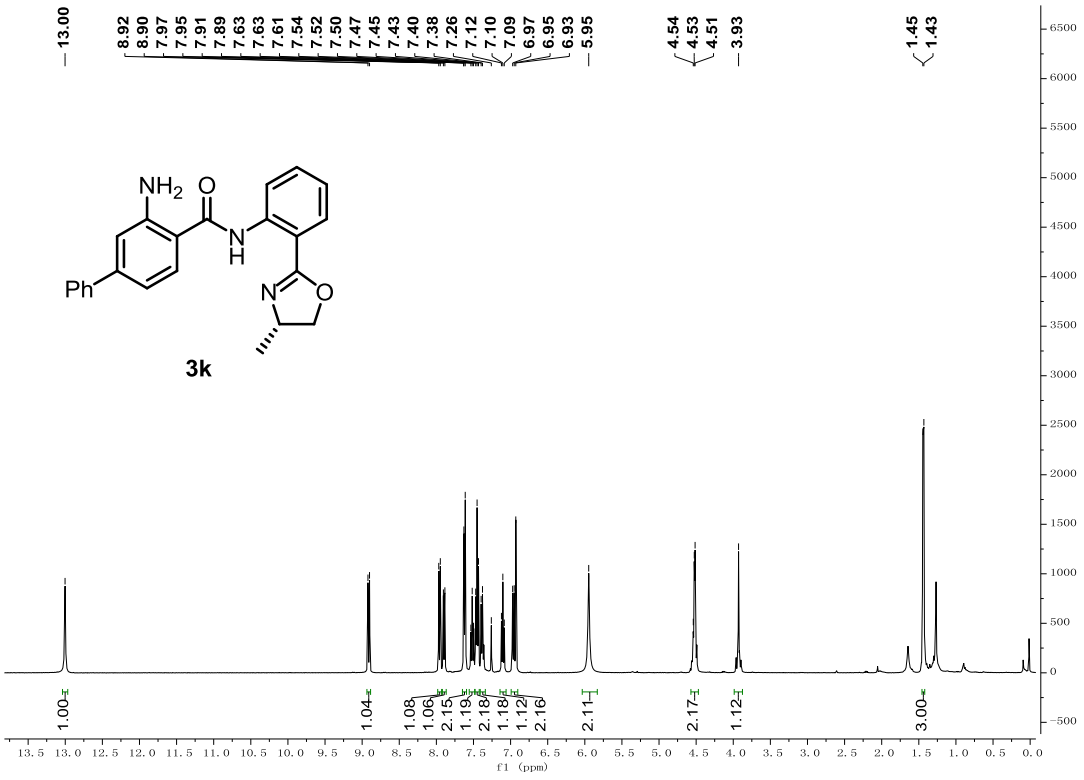
f1 (ppm)

3j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7.43
7.40
7.38
7.26
7.12
7.10
7.09
6.97
6.95
6.93
5.95
4.54
4.53
4.51
3.93
1.45
1.43
1.00
1.04
1.08
1.06
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1.19
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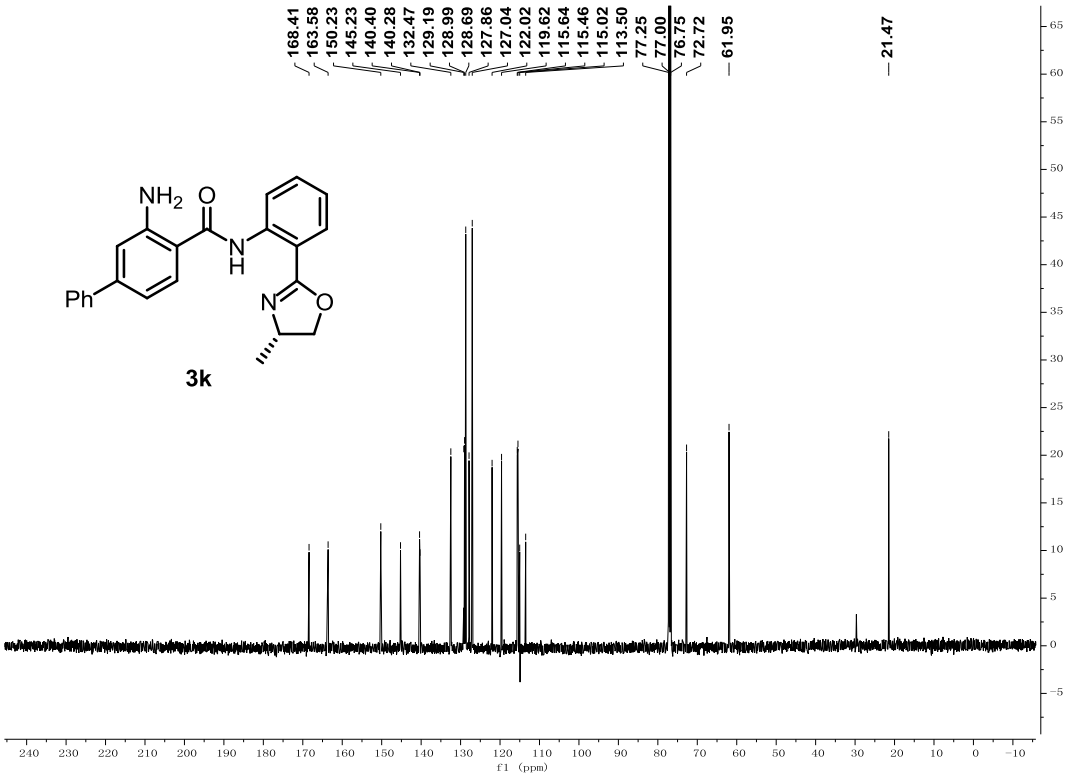
1.18
1.12
2.16
2.11
2.17
1.12
3.00
f1 (ppm)

3k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122.02
119.62
115.64
115.46
115.02
113.50
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72.72
61.95
21.47
NH2
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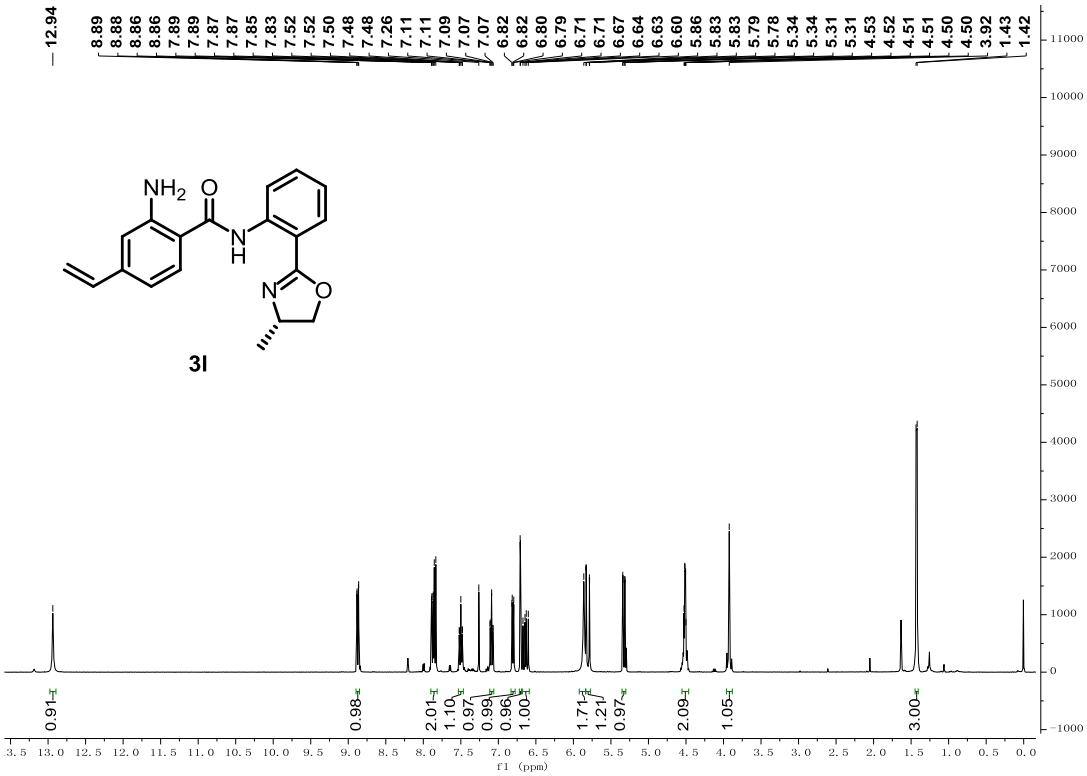
N
H
Ph
N
O
3k
f1 (ppm)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7.48
7.26
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5.83
5.79
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5.34
5.34
5.31
5.31
4.53
4.52
4.51
4.51
4.50
4.50
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1.43
1.42
NH2
O
N
H
N
O
3l
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0.98
2.01
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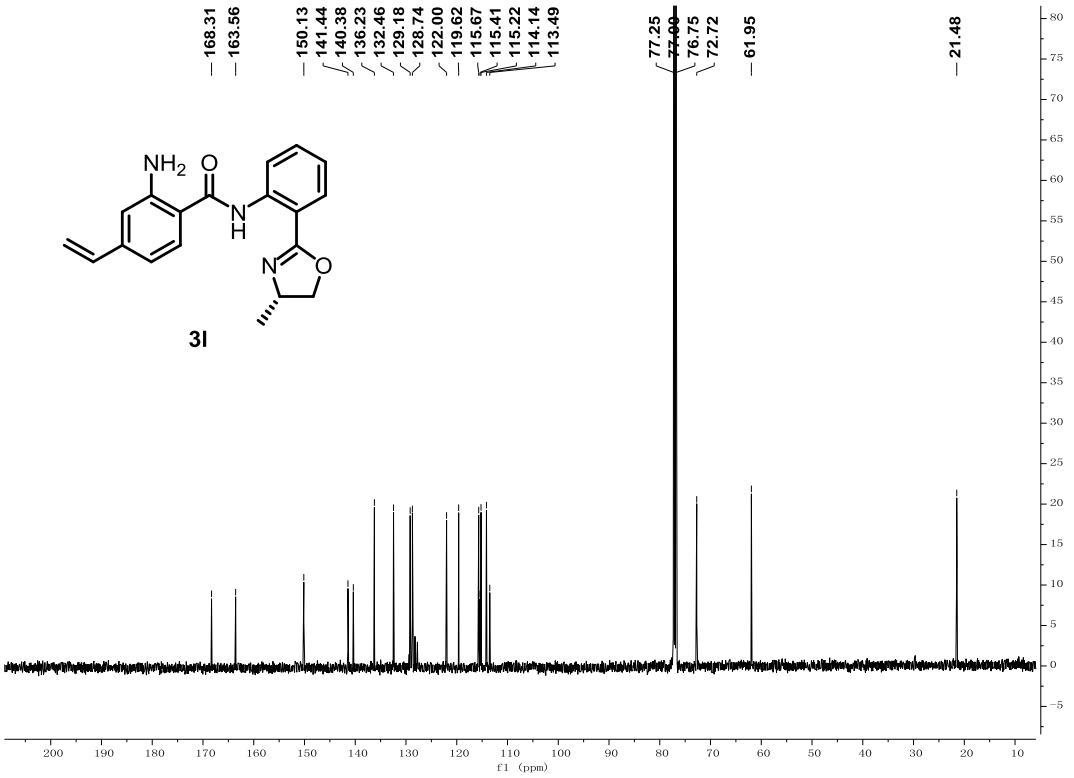
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113.49
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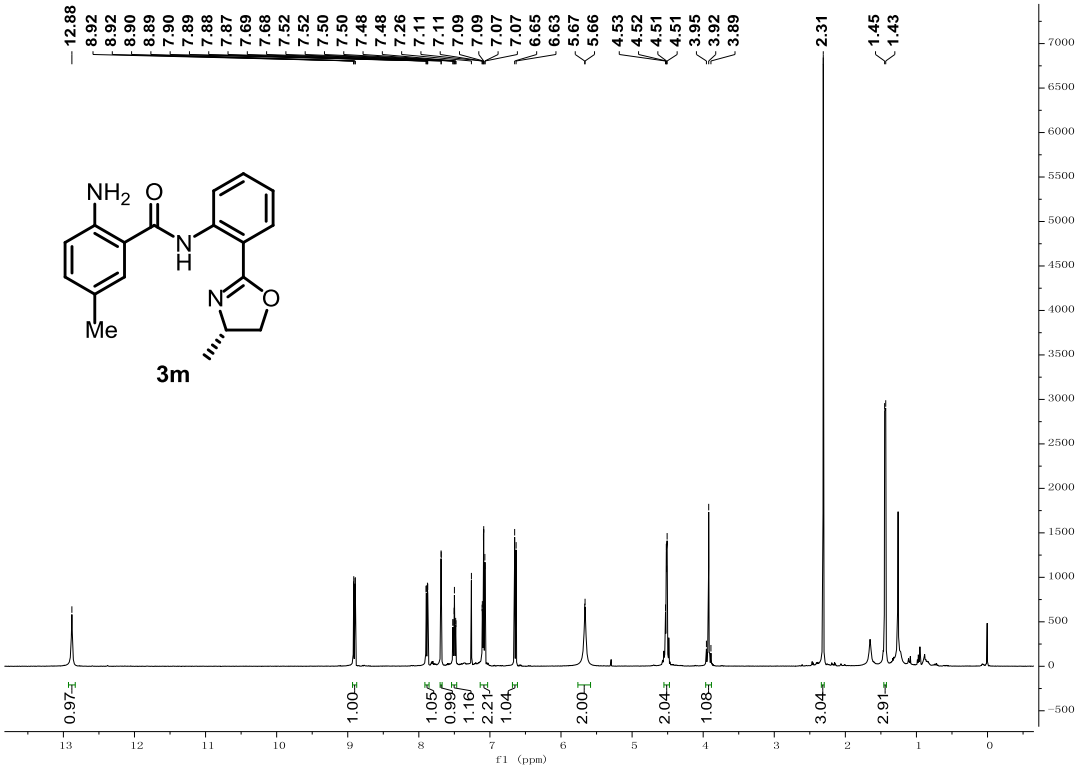
72.72
61.95
21.48
NH2
O
N
H
N
O
3l
f1 (ppm)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7.52
7.50
7.50
7.48
7.48
7.26
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7.11
7.09
7.09
7.07
7.07
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6.63
5.67
5.66
4.53
4.52
4.51
4.51
3.95
3.92
3.89
2.31
1.45
1.43
NH2
O
N
H
N
O
Me
3m
0.97
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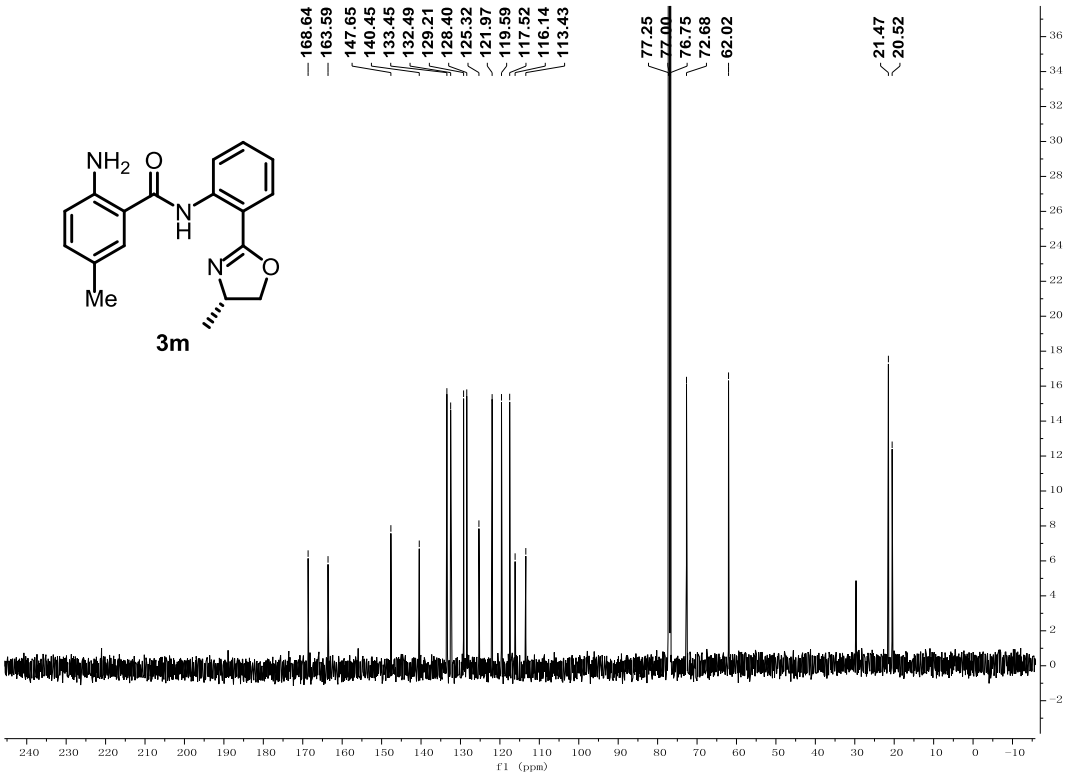
2.91
f1 (ppm)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116.14
113.43
77.25
77.00
76.75
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62.02
21.47
20.52
NH2
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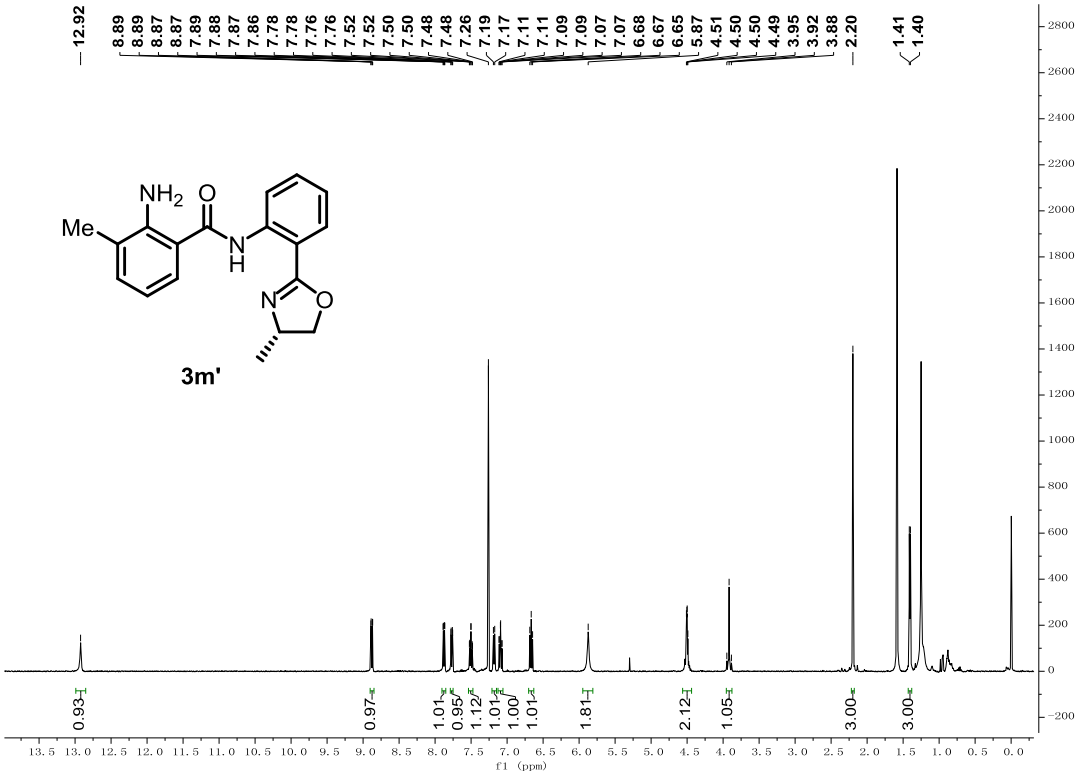
N
H
N
O
Me
3m
f1 (ppm)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7.52
7.50
7.50
7.48
7.48
7.26
7.19
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7.11
7.11
7.09
7.09
7.07
7.07
6.68
6.67
6.65
5.87
4.51
4.50
4.50
4.49
3.95
3.92
3.88
2.20
1.41
1.40
NH2
O
Me
N
H
N
O
3m'
0.93
0.97
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1.00
1.01
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1.05
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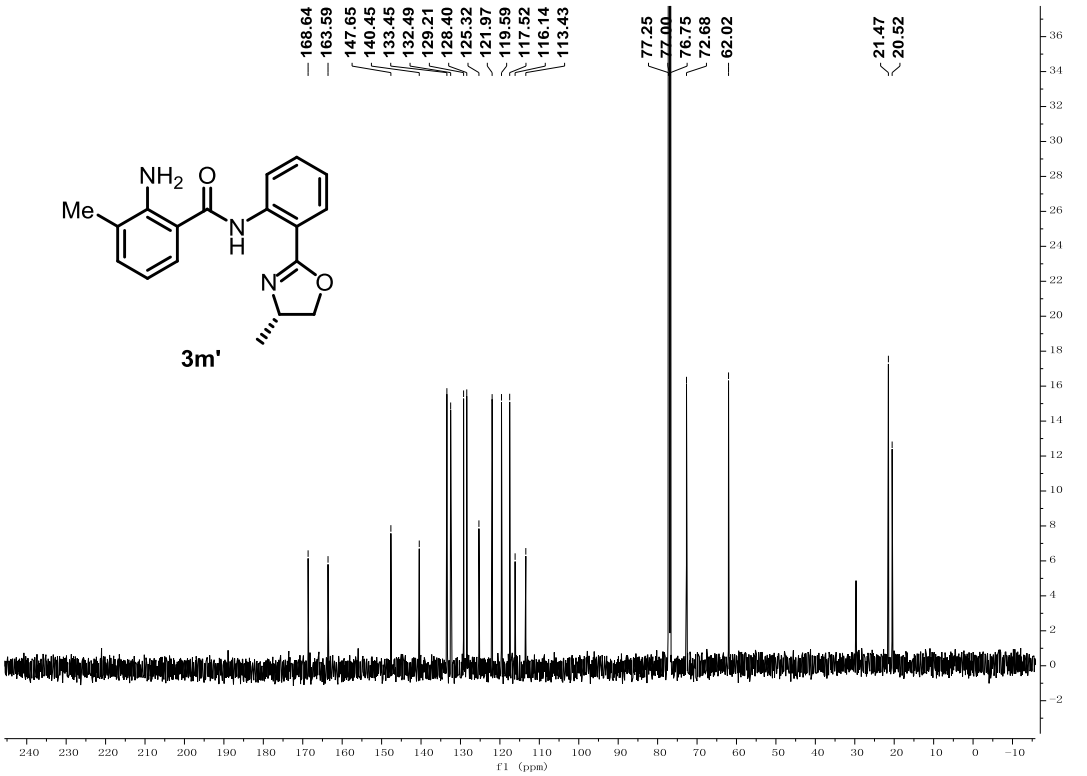
3.00
f1 (ppm)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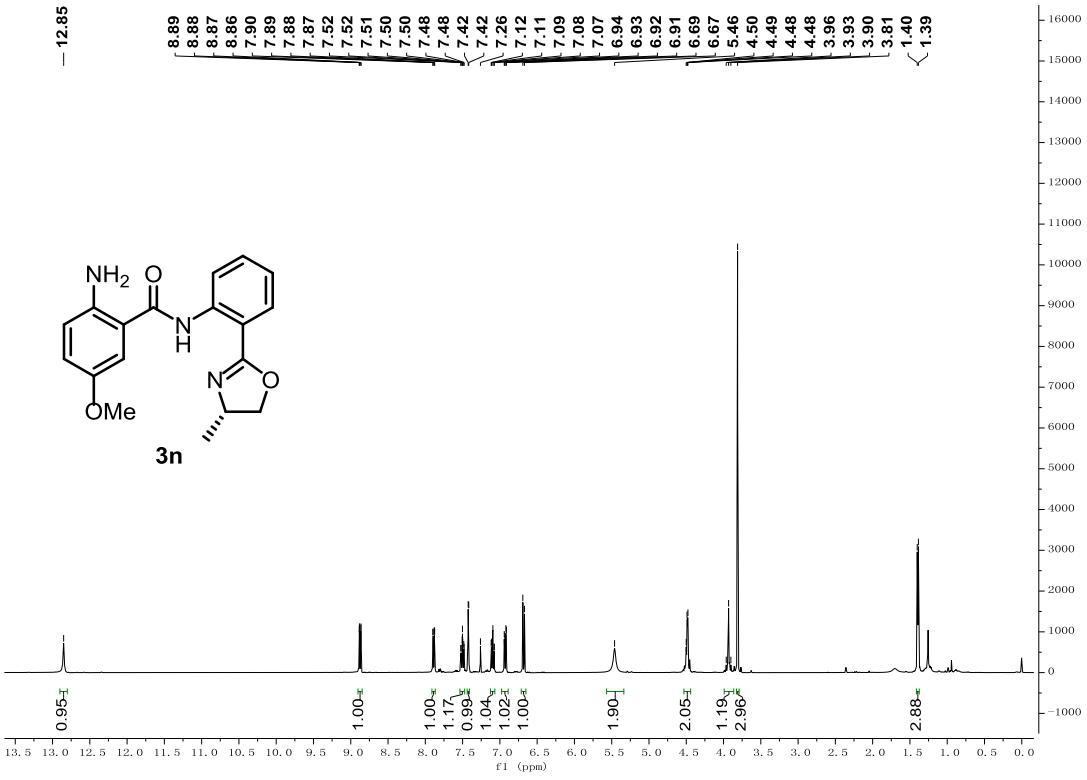
125.32
121.97
119.59
117.52
116.14
113.43
77.25
77.00
76.75
72.68
62.02
21.47
20.52
NH2
O
Me
N
H
N
O
3m'
f1 (ppm)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7.08
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4.48
4.48
3.96
3.93
3.90
3.81
1.40
1.39
NH2
O
N
H
N
O
OMe
3n
0.95
1.00
1.00
1.17
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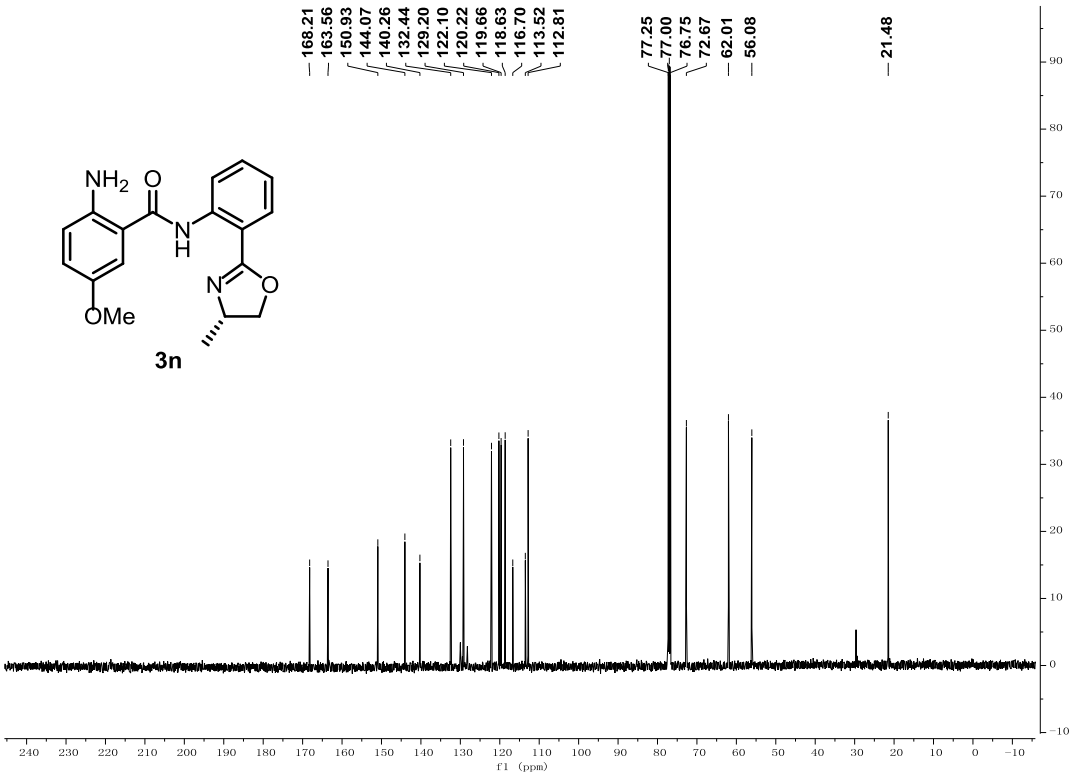
1.04
1.02
1.00
1.90
2.05
1.19
2.96
2.88
f1 (ppm)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118.63
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113.52
112.81
77.25
77.00
76.75
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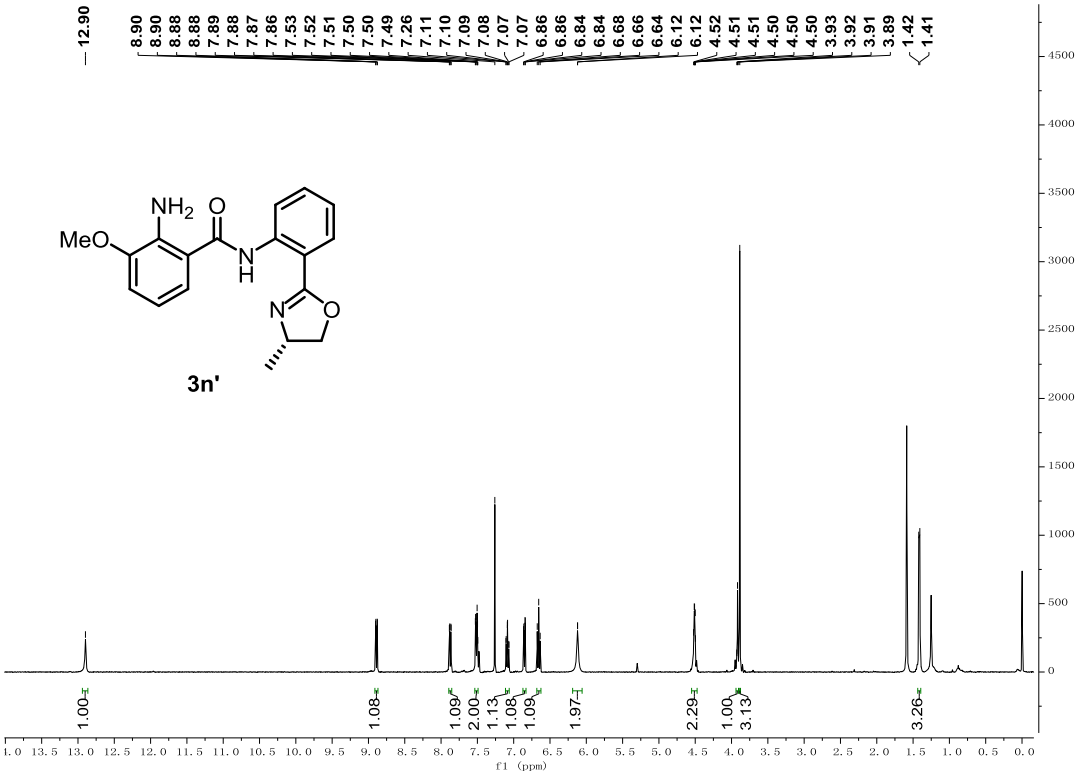
62.01
56.08
21.48
NH2
O
N
H
N
O
OMe
3n
f1 (ppm)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4.51
4.50
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4.50
3.93
3.92
3.91
3.89
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1.41
NH2
O
MeO
N
H
N
O
3n'
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1.09
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1.13
1.08
1.09
1.97
2.29
1.00
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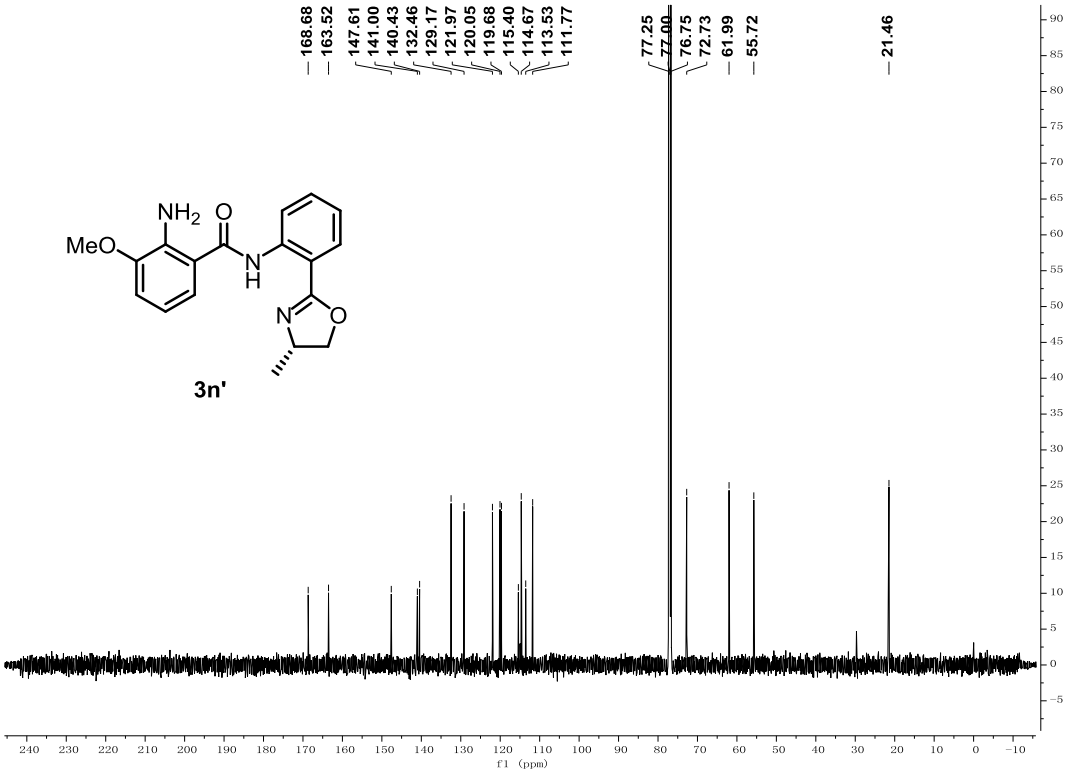
3.26
f1 (ppm)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115.40
114.67
113.53
111.77
77.25
77.00
76.75
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55.72
21.46
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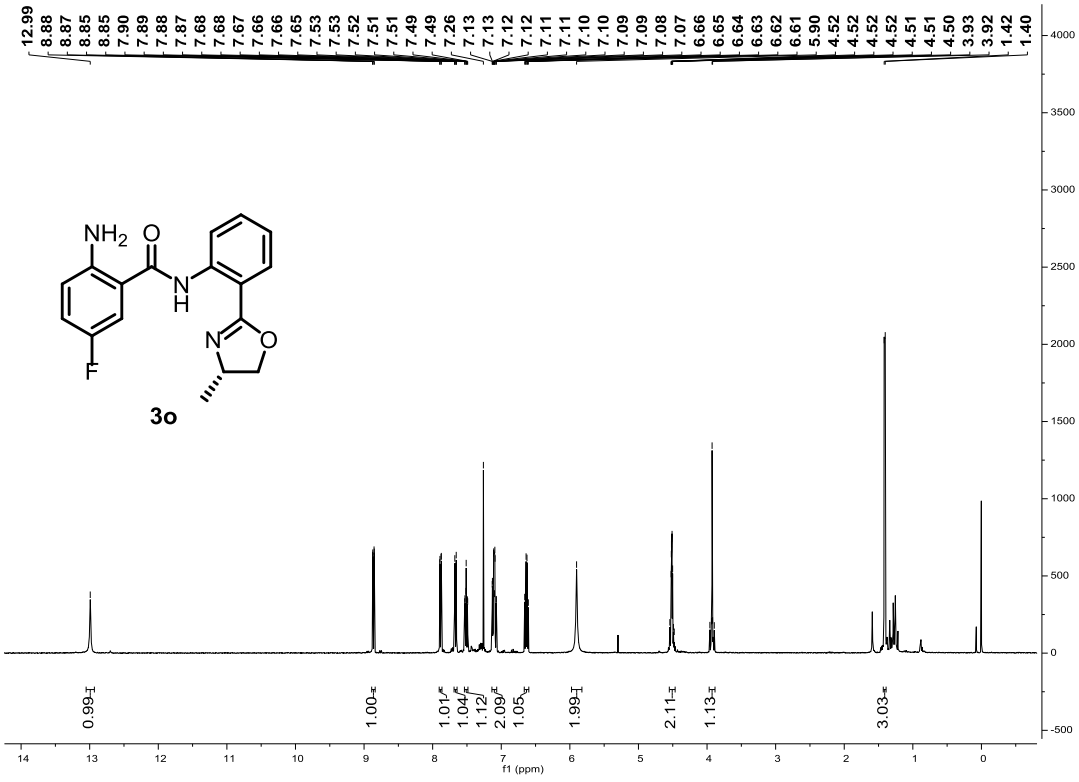
O
MeO
N
H
N
O
3n'
f1 (ppm)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4.51
4.51
4.50
3.93
3.92
1.42
1.40
NH2
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N
H
N
O
F
3o
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1.00
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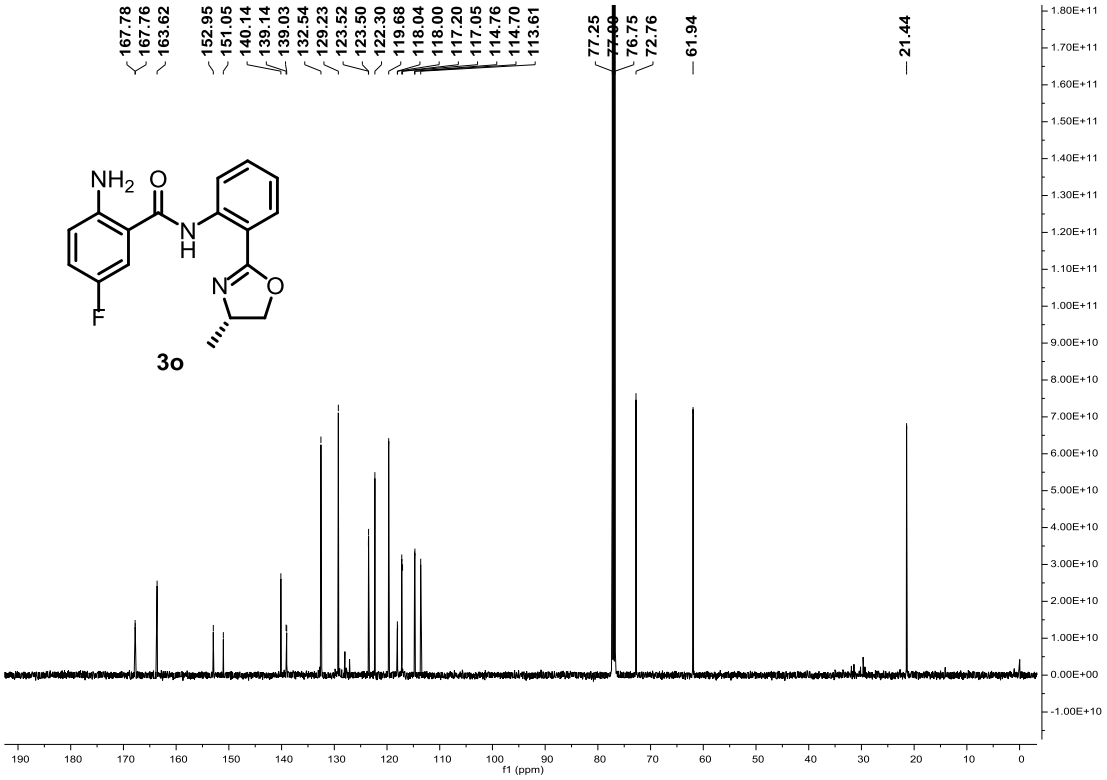
1.04
1.12
2.09
1.05
1.99
2.11
1.13
3.03
f1 (ppm)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119.68
118.04
118.00
117.20
117.05
114.76
114.70
113.61
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72.76
61.94
21.44
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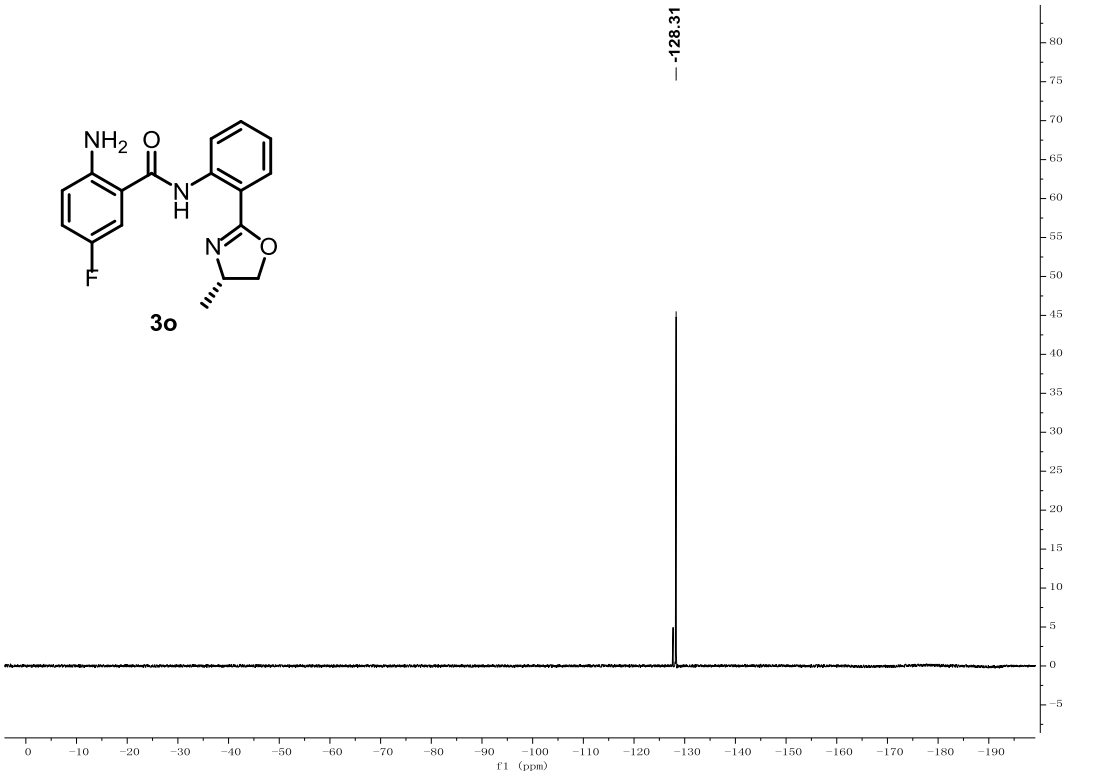
H
N
O
F
3o
f1 (ppm)


-128.31
NH2
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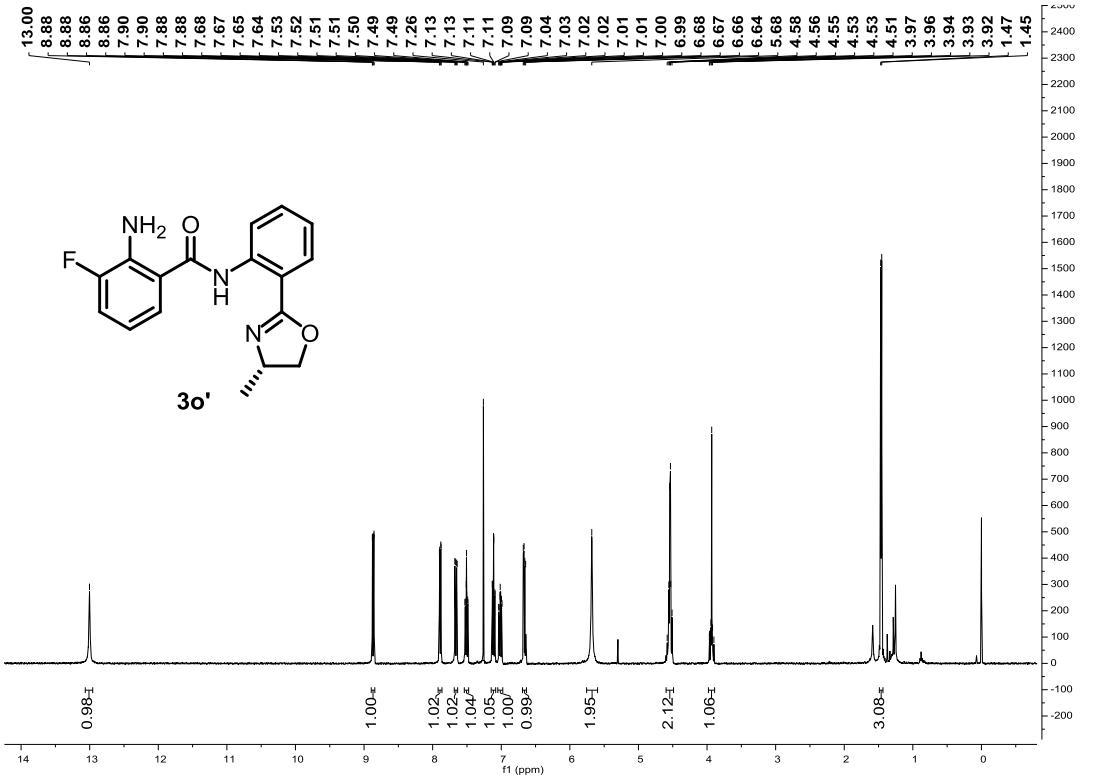
O
F
3o
f1 (ppm)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7.67
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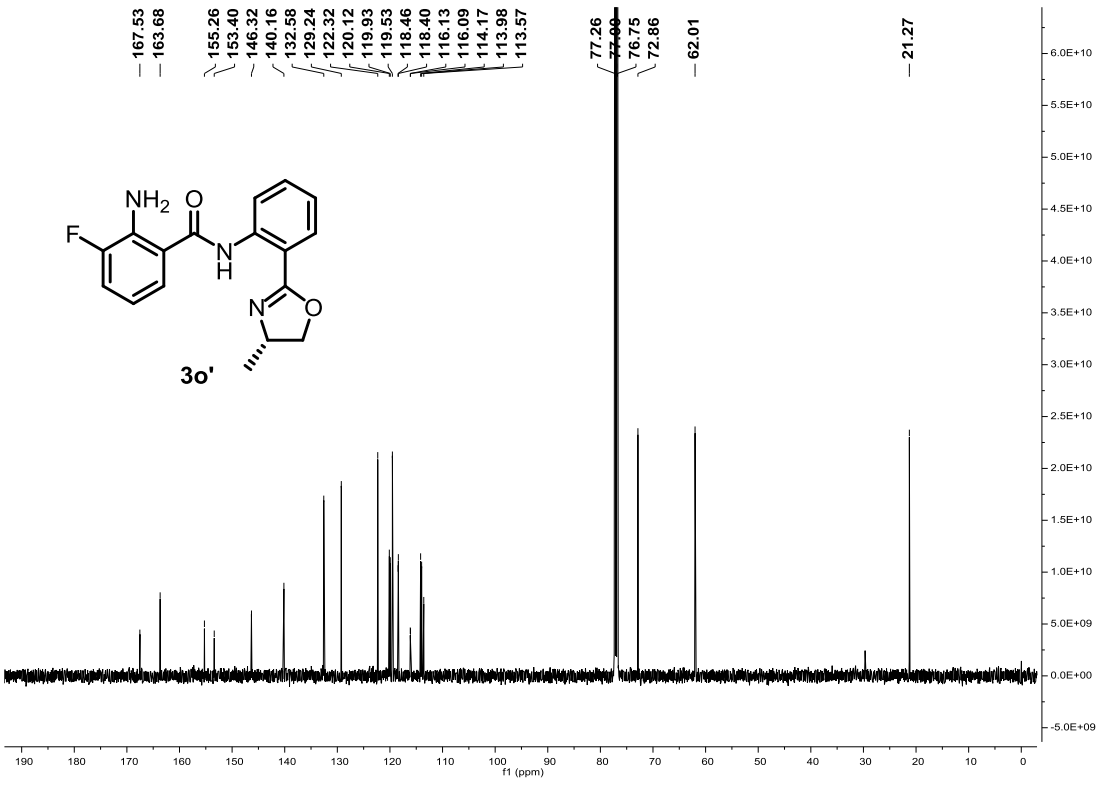
7.64
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.26
7.13
7.13
7.11
7.11
7.09
7.04
7.03
7.02
7.02
7.01
7.01
7.00
6.99
6.68
6.67
6.66
6.64
5.68
4.58
4.56
4.55
4.53
4.53
4.51
3.97
3.96
3.94
3.93
3.92
1.47
1.45
NH2
O
F
N
H
N
O
3o'
0.98
1.00
1.02
1.02
1.04
1.05
1.00
0.99
1.95
2.12
1.06
3.08
f1 (ppm)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129.24
122.32
120.12
119.93
119.53
118.46
118.40
116.13
116.09
114.17
113.98
113.57
77.26
77.00
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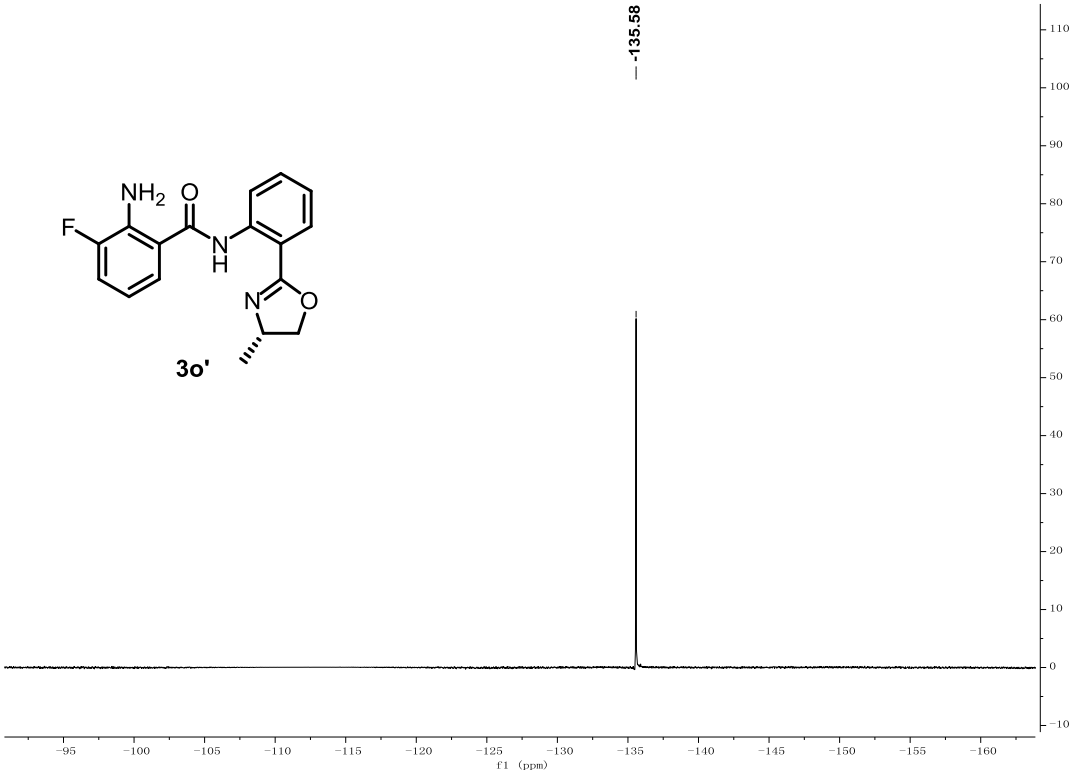
72.86
62.01
21.27
NH2
O
F
N
H
N
O
3o'
f1 (ppm)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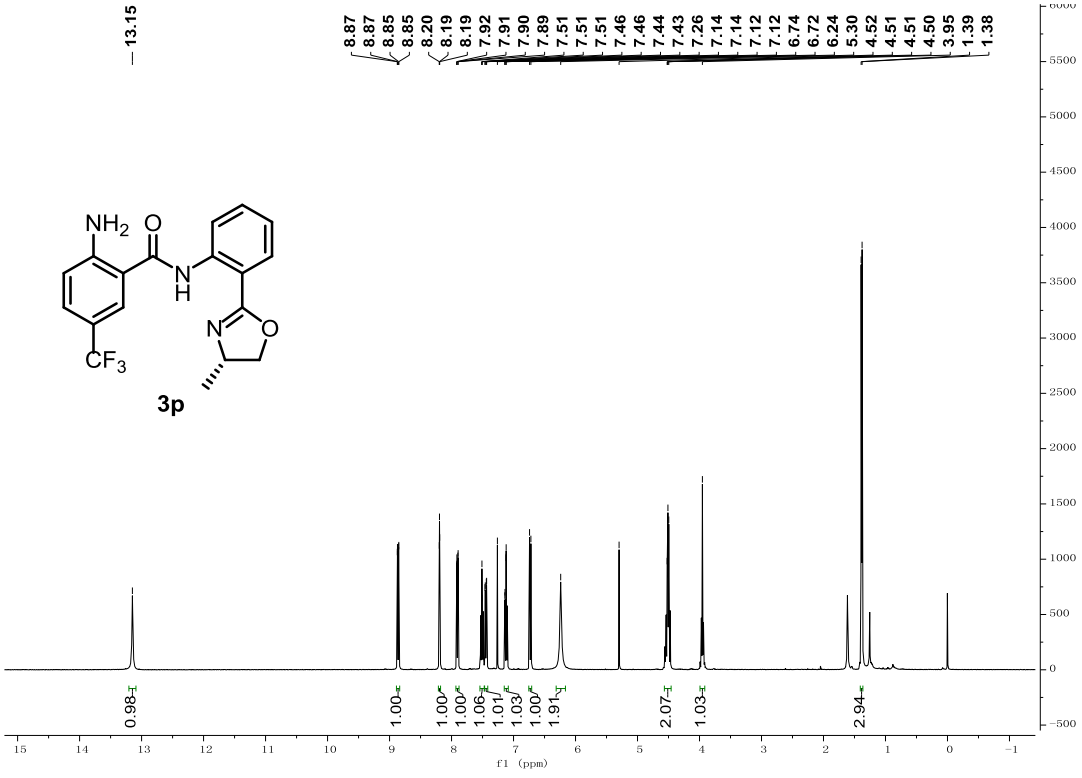
N
O
3o'
f1 (ppm)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8.19
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7.91
7.90
7.89
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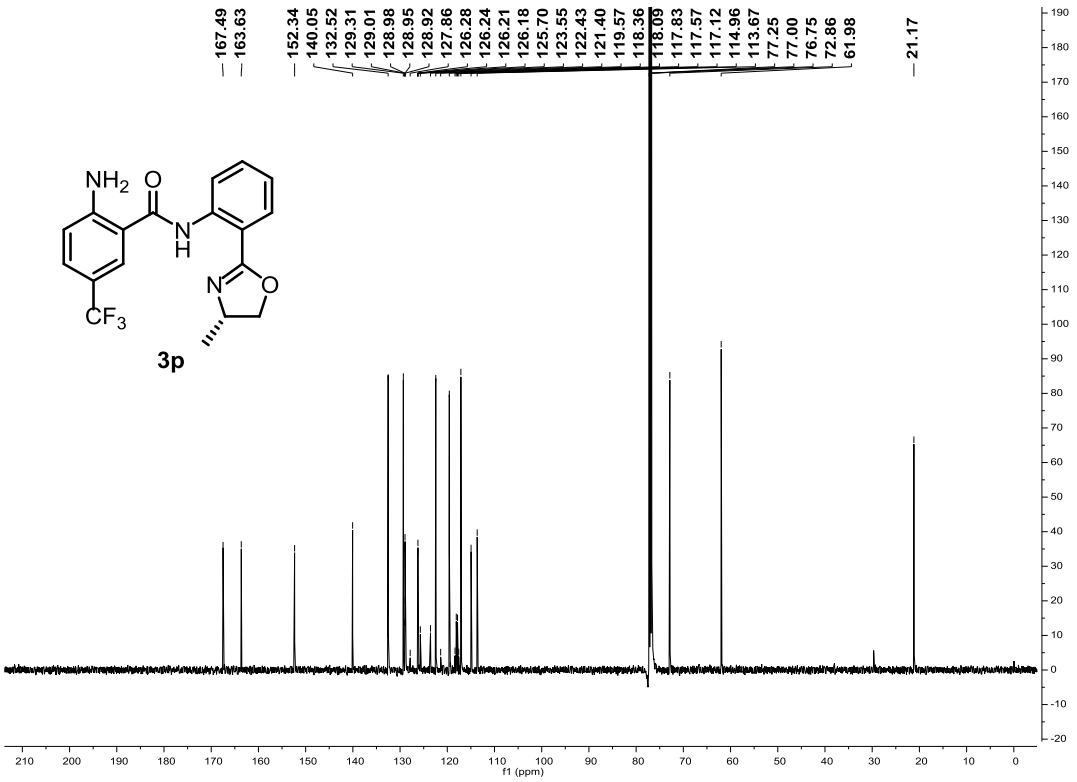
7.51
7.51
7.46
7.46
7.44
7.43
7.26
7.14
7.14
7.12
7.12
6.74
6.72
6.24
5.30
4.52
4.51
4.51
4.50
3.95
1.39
1.38
NH2
O
N
H
N
O
CF3
3p
0.98
1.00
1.00
1.00
1.06
1.01
1.03
1.00
1.91
2.07
1.03
2.94
f1 (ppm)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126.21
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121.40
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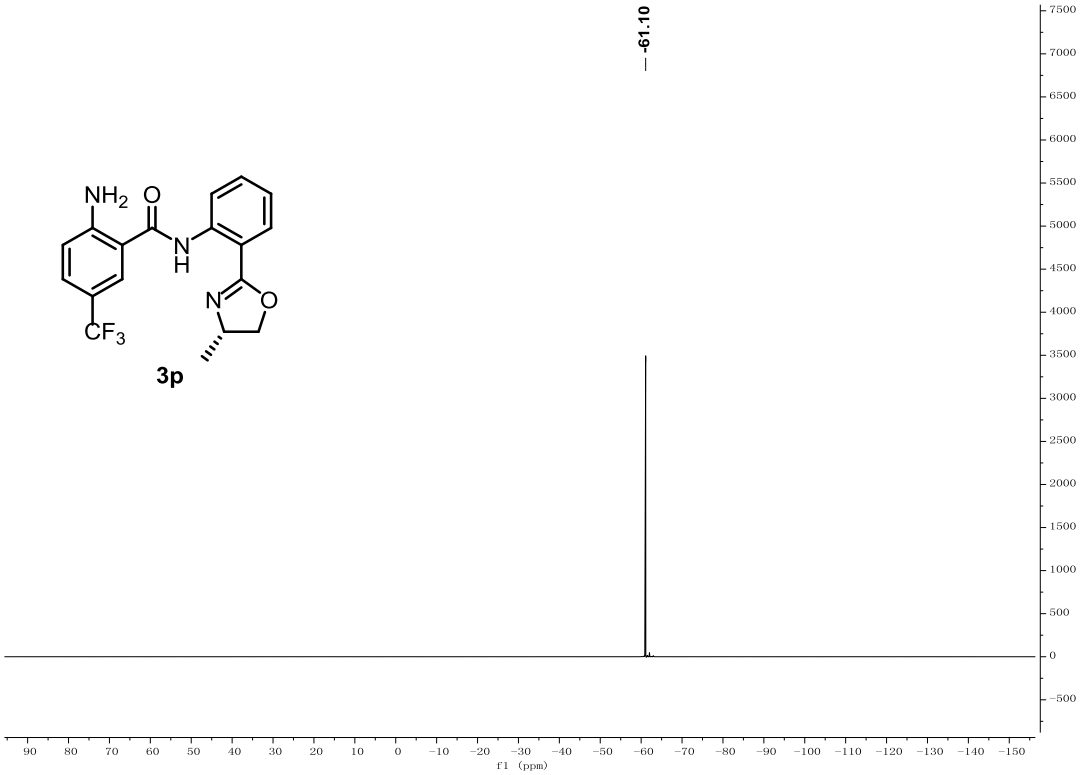
118.36
118.09
117.83
117.57
117.12
114.96
113.67
77.25
77.00
76.75
72.86
61.98
21.17
NH2
O
N
H
N
O
CF3
3p
f1 (ppm)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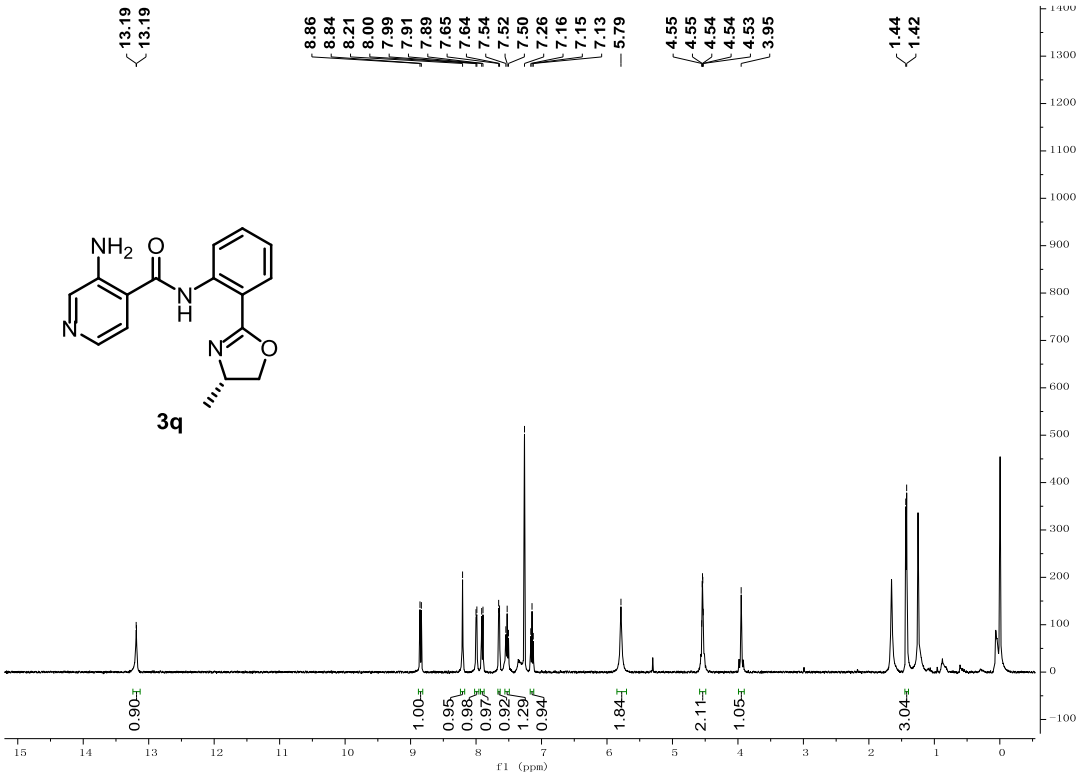
f1 (ppm)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7.91
7.89
7.65
7.64
7.54
7.52
7.50
7.26
7.16
7.15
7.13
5.79
4.55
4.55
4.54
4.54
4.53
3.95
1.44
1.42
NH2
O
N
H
N
O
3q
0.90
1.00
0.95
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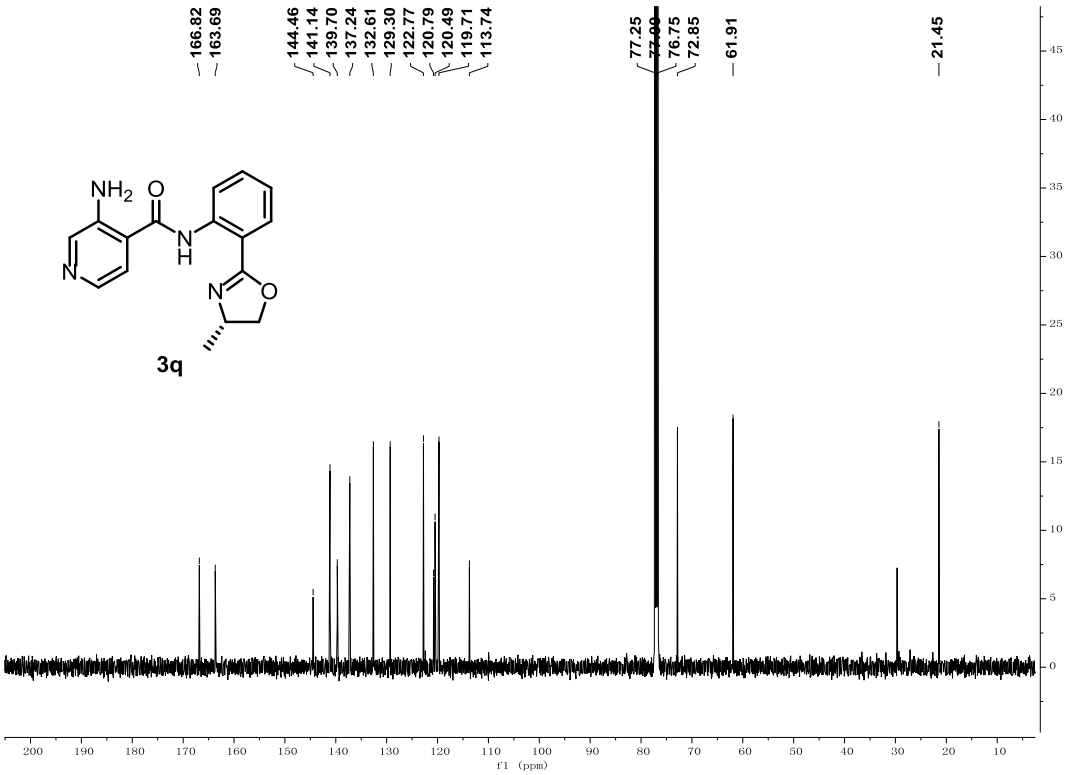
0.97
0.92
1.29
0.94
1.84
2.11
1.05
3.04
f1 (ppm)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120.79
120.49
119.71
113.74
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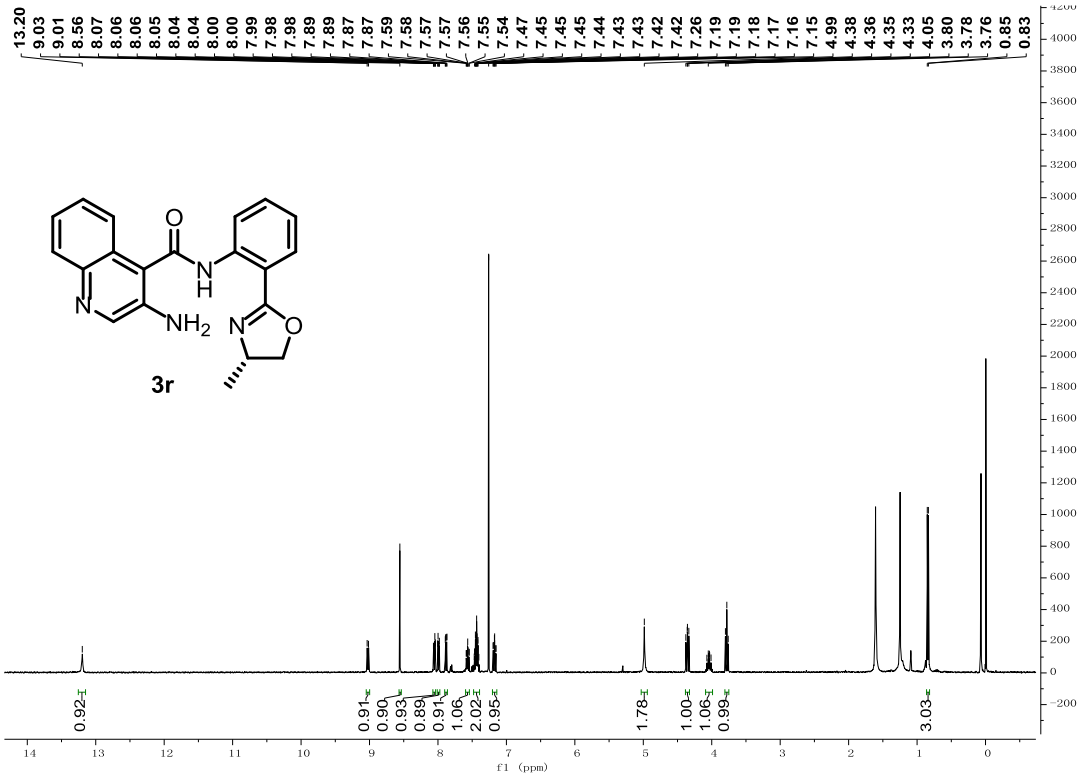
76.75
72.85
61.91
21.45
NH2
O
N
H
N
O
3q
f1 (ppm)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8.06
8.05
8.04
8.04
8.00
8.00
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7.17
7.16
7.15
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4.38
4.36
4.35
4.33
4.05
3.80
3.78
3.76
0.85
0.83
O
N
H
N
NH2
N
O
3r
0.92
0.91
0.90
0.93
0.89
0.91
1.06
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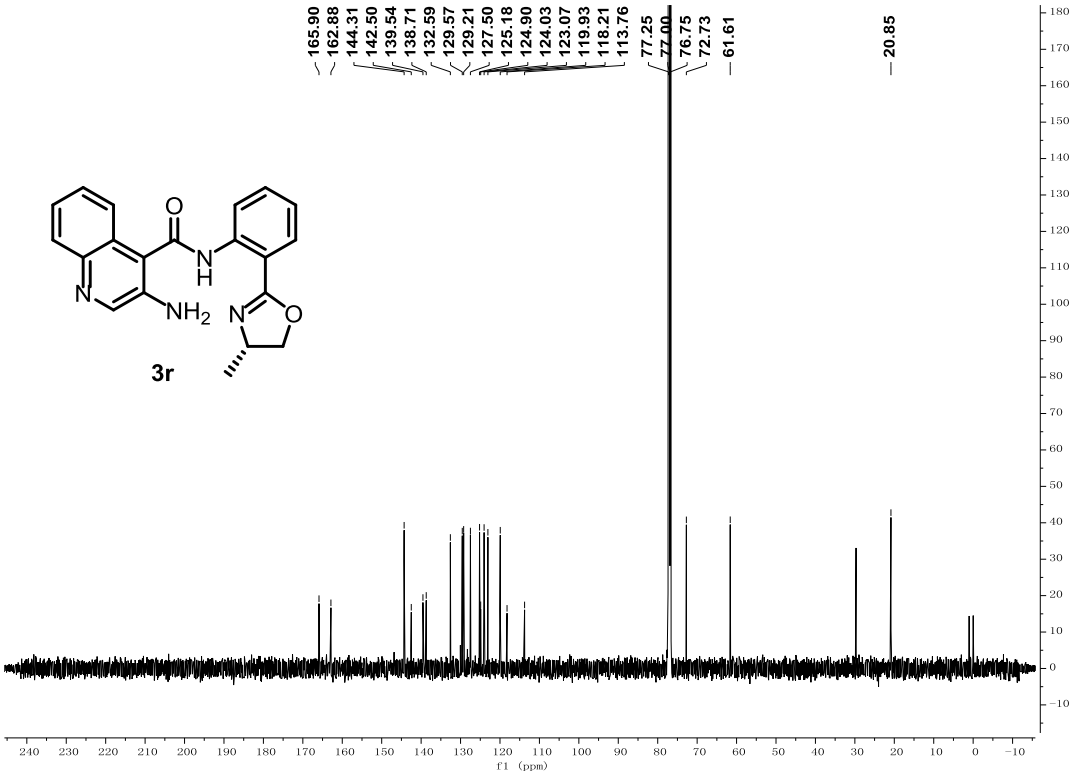
0.95
1.78
1.00
1.06
0.99
3.03
f1 (ppm)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124.90
124.03
123.07
119.93
118.21
113.76
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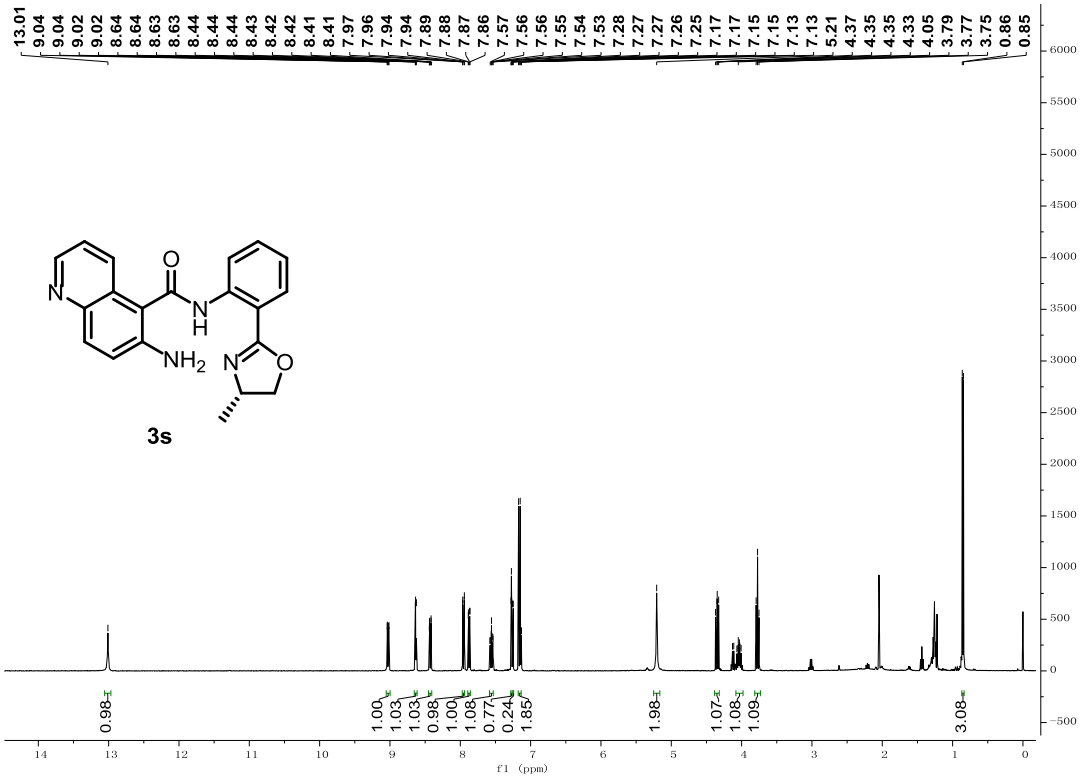
72.73
61.61
20.85
O
N
H
N
NH2
N
O
3r
f1 (ppm)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9.04
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8.44
8.43
8.42
8.42
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8.41
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7.96
7.94
7.94
7.89
7.88
7.87
7.86
7.57
7.56
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7.26
7.25
7.17
7.17
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7.15
7.13
7.13
5.21
4.37
4.35
4.35
4.33
4.05
3.79
3.77
3.75
0.86
0.85
O
N
H
N
NH2
N
O
3s
0.98
1.00
1.03
1.03
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1.00
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0.77
0.24
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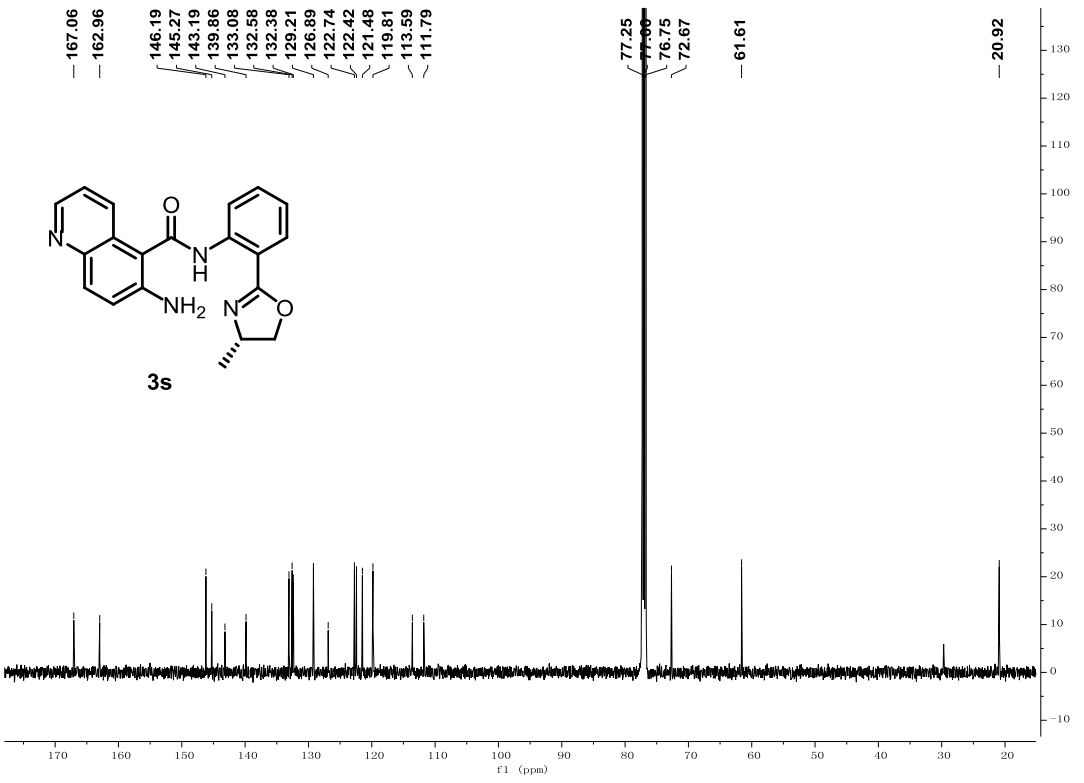
1.98
1.07
1.08
1.09
3.08
f1 (ppm)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121.48
119.81
113.59
111.79
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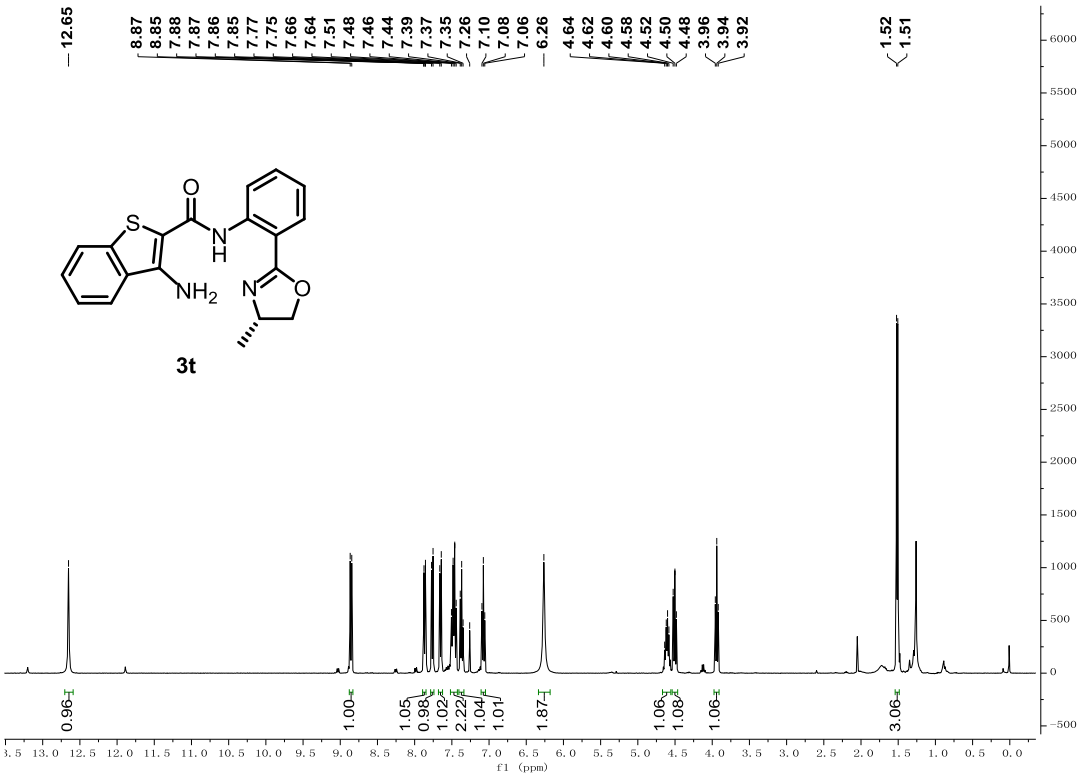
72.67
61.61
20.92
O
N
H
N
NH2
N
O
3s
f1 (ppm)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7.48
7.46
7.44
7.39
7.37
7.35
7.26
7.10
7.08
7.06
6.26
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4.62
4.60
4.58
4.52
4.50
4.48
3.96
3.94
3.92
1.52
1.51
O
S
N
H
NH2
N
O
3t
0.96
1.00
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1.06
1.08
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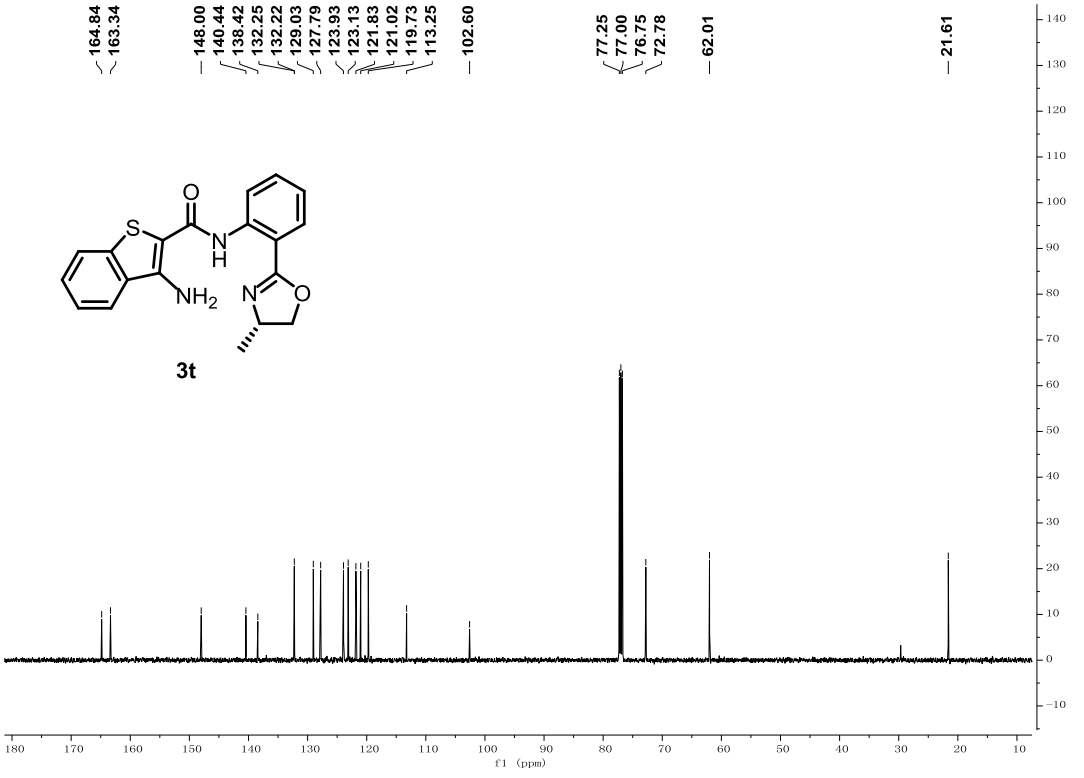
3.06
f1 (ppm)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123.93
123.13
121.83
121.02
119.73
113.25
102.60
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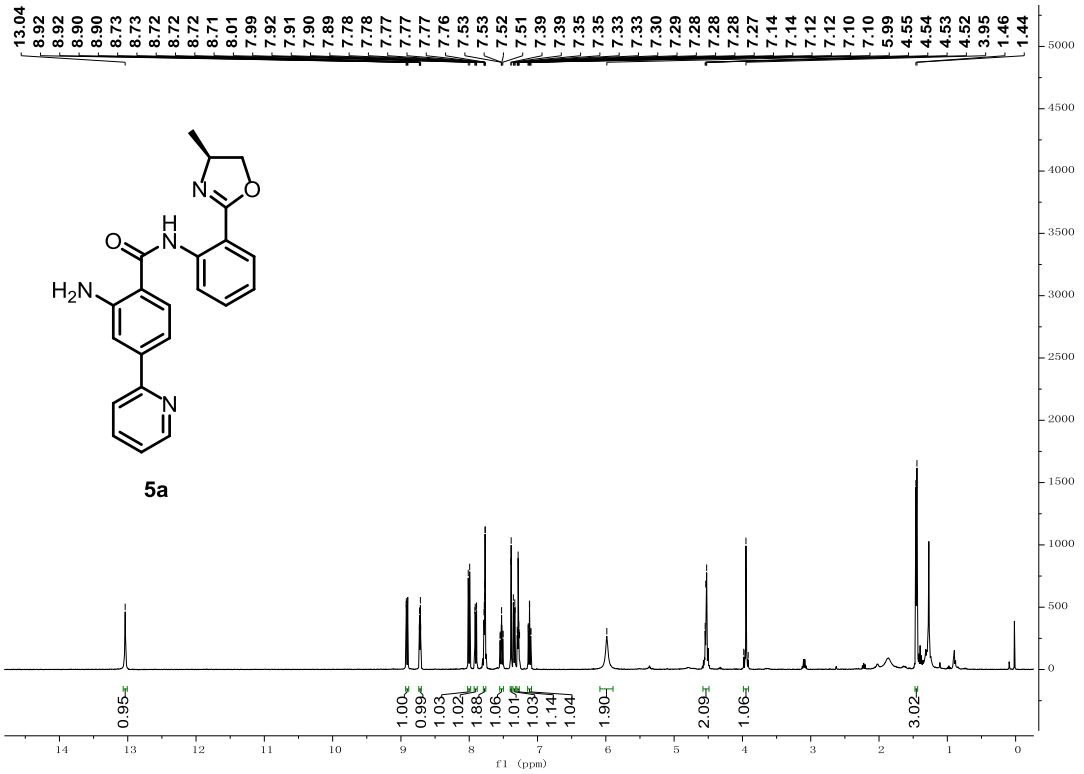
72.78
62.01
21.61
O
S
N
H
NH2
N
O
3t
f1 (ppm)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8.72
8.71
8.01
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7.92
7.91
7.90
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7.78
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7.76
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7.53
7.52
7.51
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7.35
7.35
7.33
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7.30
7.29
7.28
7.28
7.28
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7.10
7.10
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4.55
4.54
4.53
4.52
3.95
1.46
1.44
H2N
O
H
N
N
O
N
5a
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1.00
0.99
1.03
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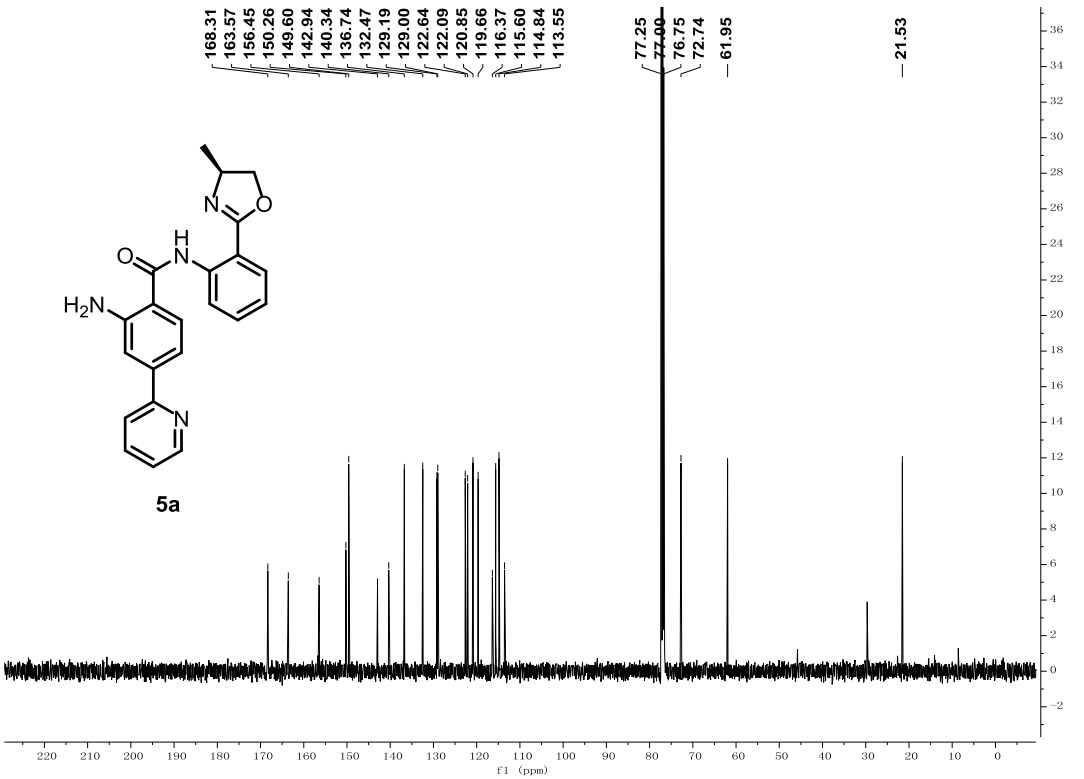
1.01
1.03
1.14
1.04
1.90
2.09
1.06
3.02
f1 (ppm)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122.09
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119.66
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114.84
113.55
77.25
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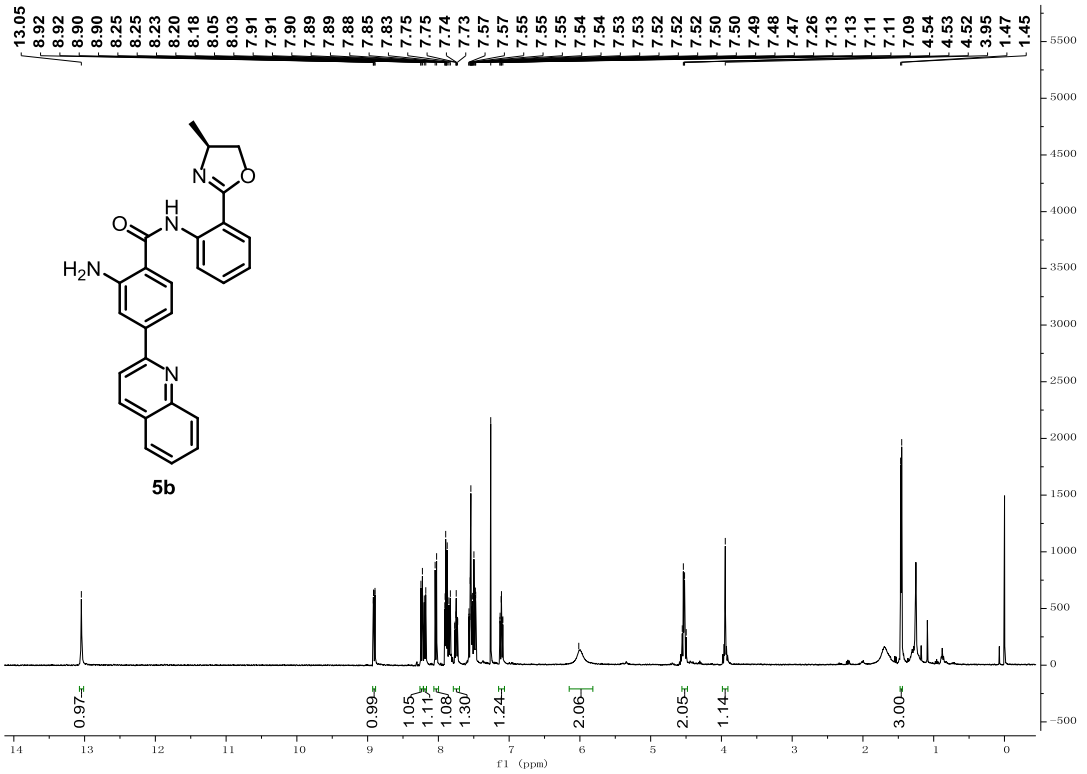
72.74
61.95
21.53
H2N
O
H
N
N
O
N
5a
f1 (ppm)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8.05
8.03
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7.91
7.90
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7.89
7.88
7.85
7.83
7.75
7.75
7.74
7.73
7.57
7.57
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7.55
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7.13
7.11
7.11
7.09
4.54
4.53
4.52
3.95
1.47
1.45
5b
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0.99
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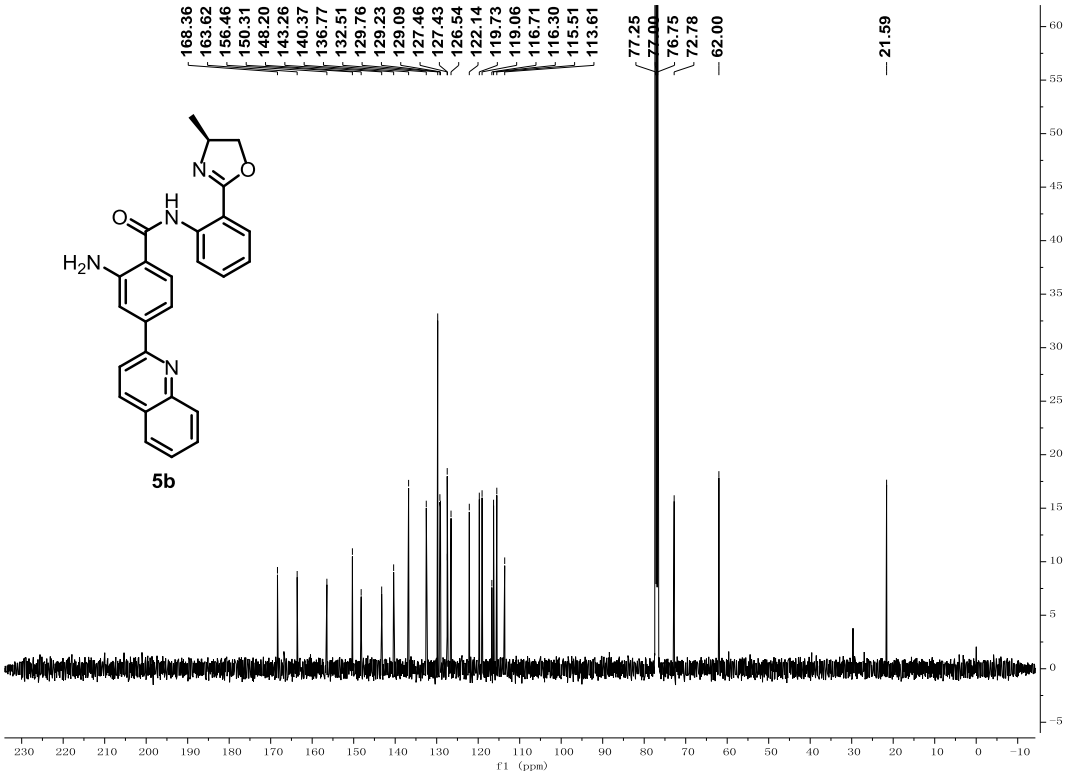
1.11
1.08
1.30
1.24
2.06
2.05
1.14
3.00
f1 (ppm)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129.23
129.09
127.46
127.43
126.54
122.14
119.73
119.06
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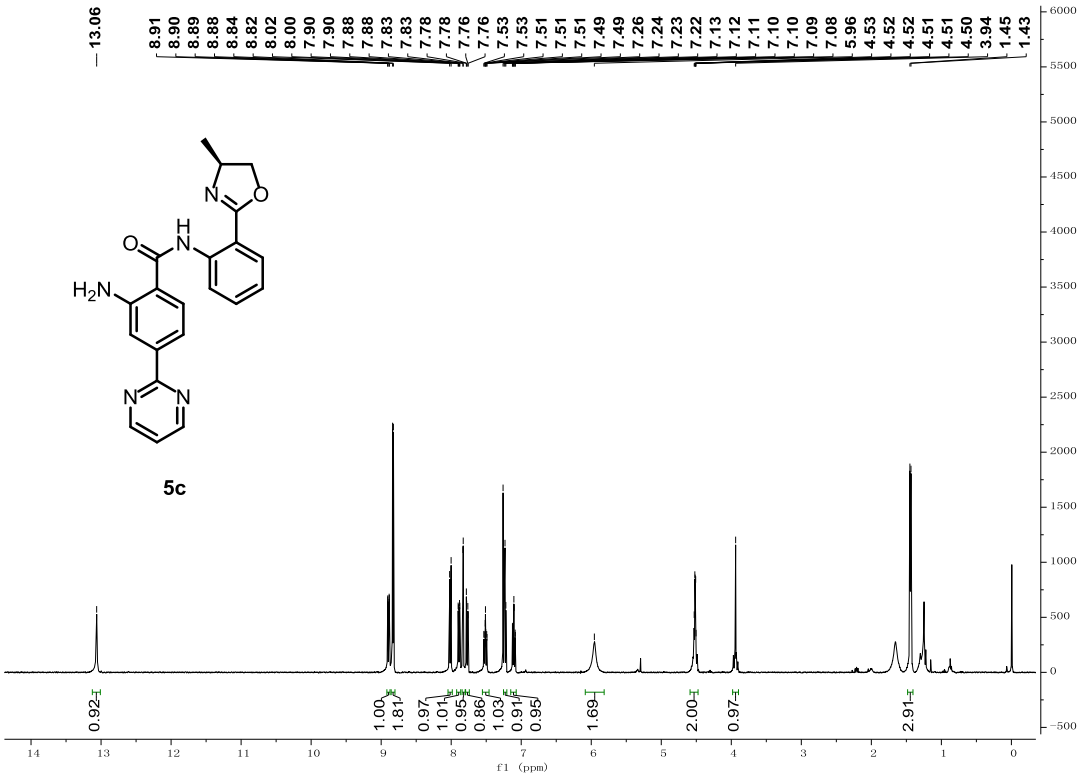
116.30
115.51
113.61
77.25
77.00
76.75
72.78
62.00
21.59
5b
f1 (ppm)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7.78
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7.24
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7.22
7.13
7.12
7.11
7.10
7.10
7.09
7.08
5.96
4.53
4.52
4.52
4.51
4.51
4.50
3.94
1.45
1.43
O
N
H
N
O
H2N
N
N
5c
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1.01
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0.86
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0.91
0.95
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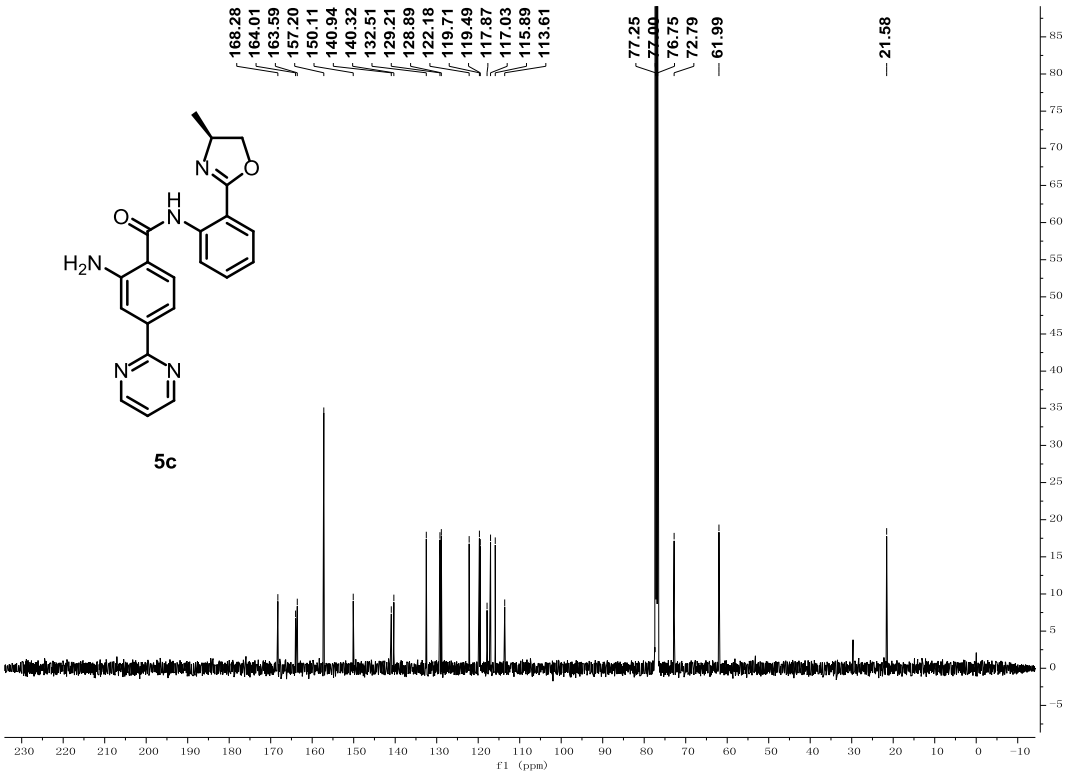
0.97
2.91
f1 (ppm)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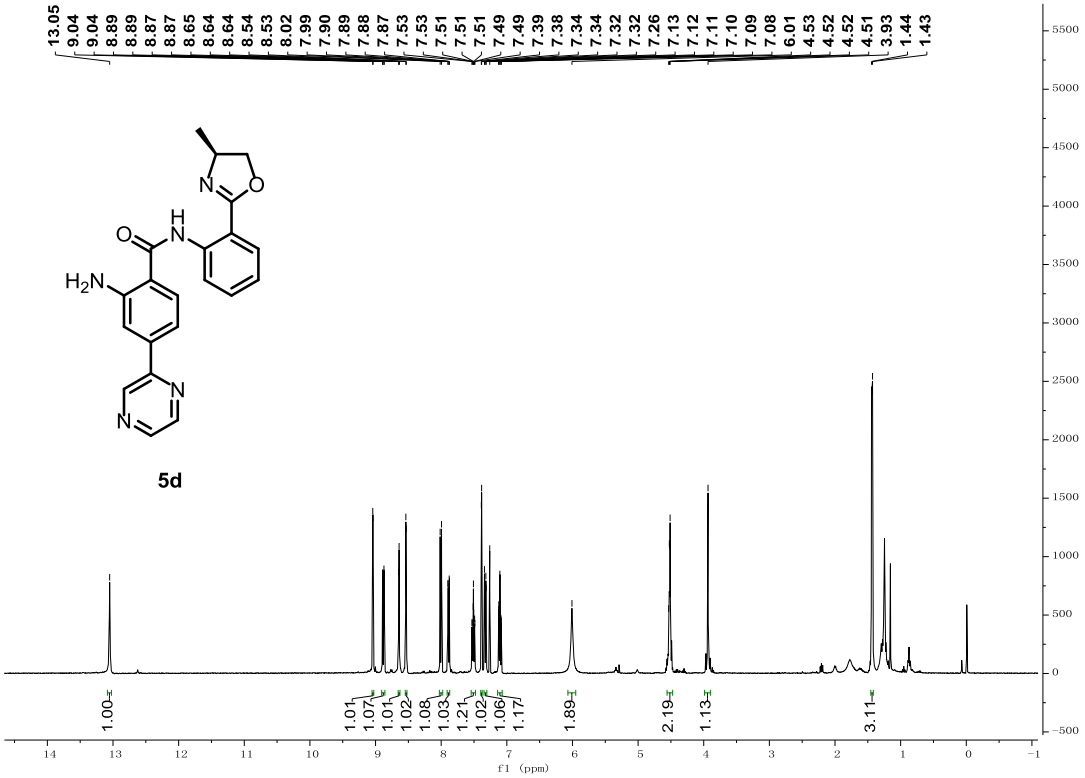
119.49
117.87
117.03
115.89
113.61
77.25
77.00
76.75
72.79
61.99
21.58
O
N
H
N
O
H2N
N
N
5c
f1 (ppm)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7.49
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7.34
7.32
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7.26
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7.12
7.11
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7.09
7.08
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4.52
4.51
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1.44
1.43
5d
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1.01
1.07
1.01
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1.08
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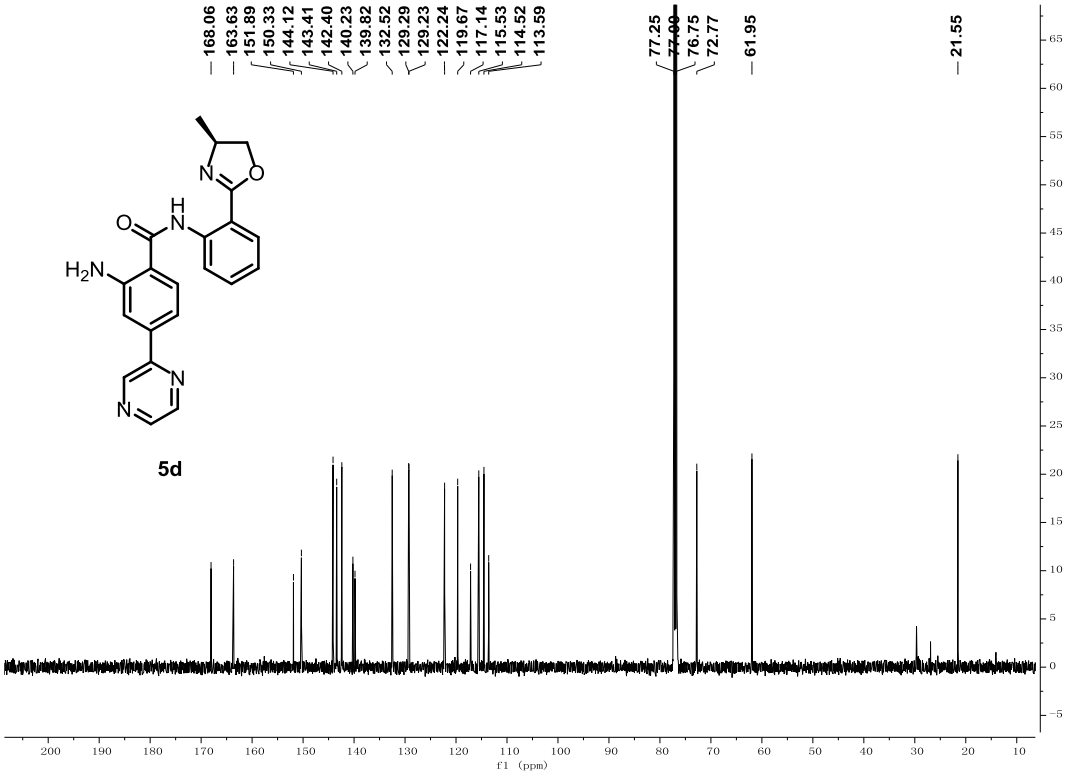
1.21
1.02
1.06
1.17
1.89
2.19
1.13
3.11
f1 (ppm)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150.33
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122.24
119.67
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115.53
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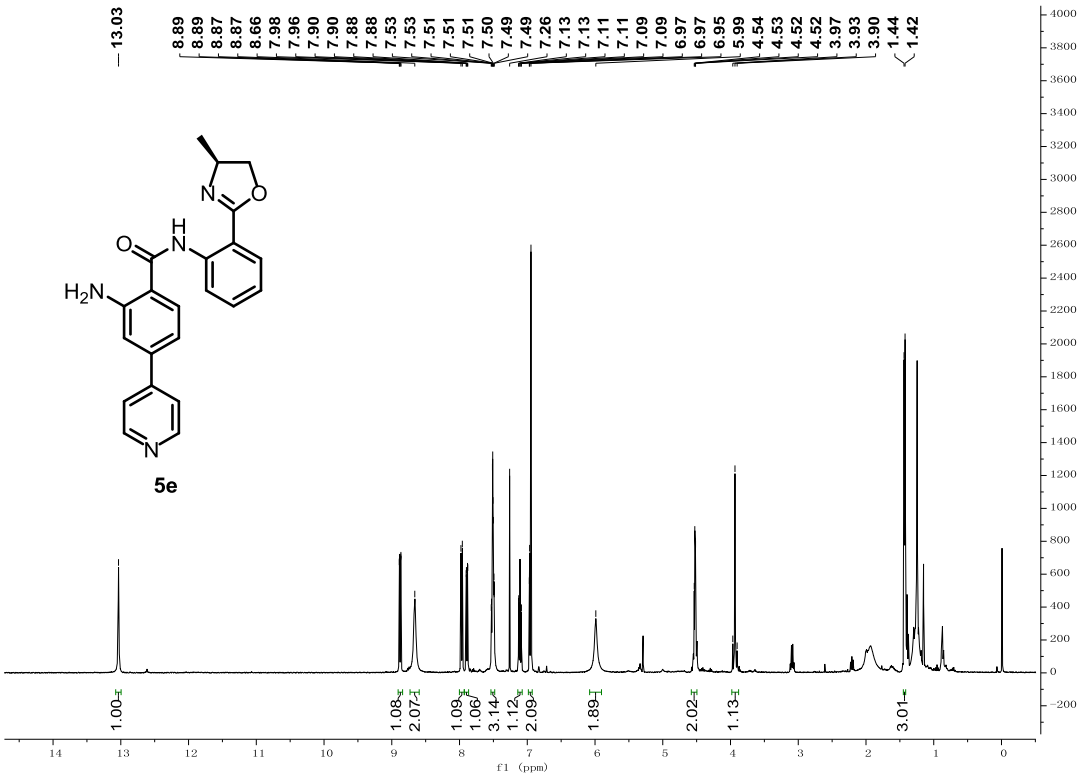
77.25
77.00
76.75
72.77
61.95
21.55
5d
f1 (ppm)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1.42
5e
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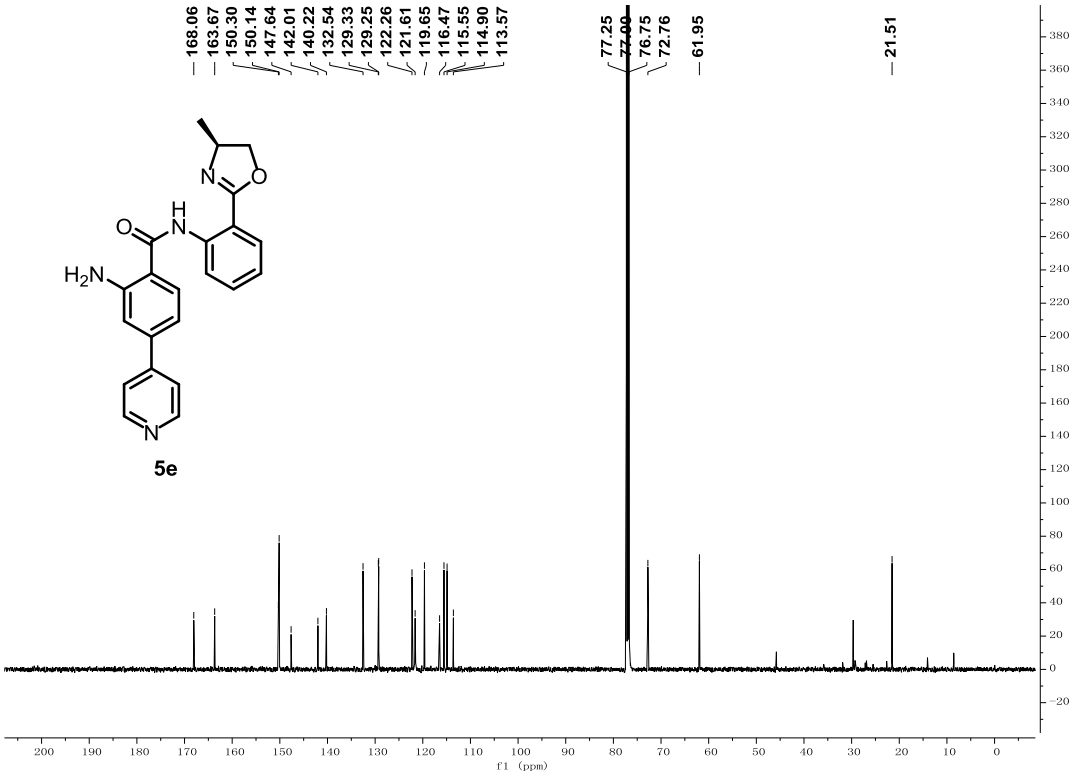
1.06
3.14
1.12
2.09
1.89
2.02
1.13
3.01
f1 (ppm)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119.65
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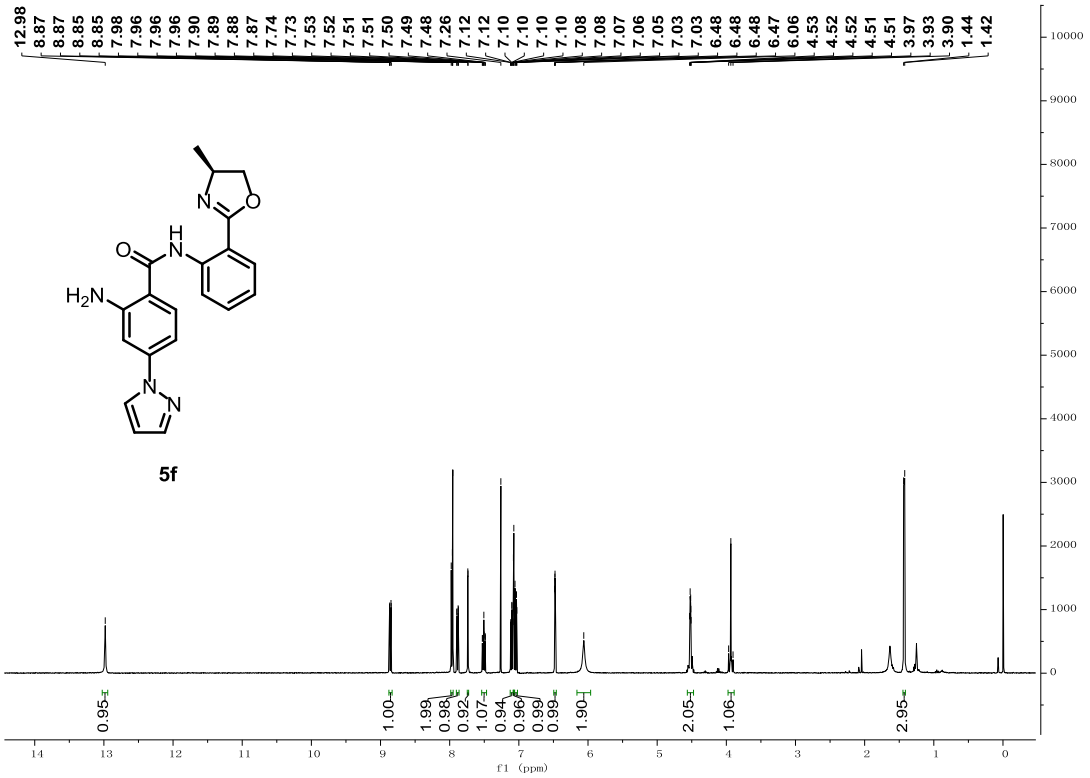
113.57
77.25
77.00
76.75
72.76
61.95
21.51
5e
f1 (ppm)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7.87
7.74
7.73
7.53
7.52
7.51
7.51
7.50
7.49
7.48
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7.12
7.12
7.10
7.10
7.10
7.10
7.08
7.08
7.07
7.06
7.05
7.03
7.03
6.48
6.48
6.48
6.47
6.06
4.53
4.52
4.52
4.51
4.51
3.97
3.93
3.90
1.44
1.42
5f
0.95
1.00
1.99
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0.94
0.96
0.99
0.99
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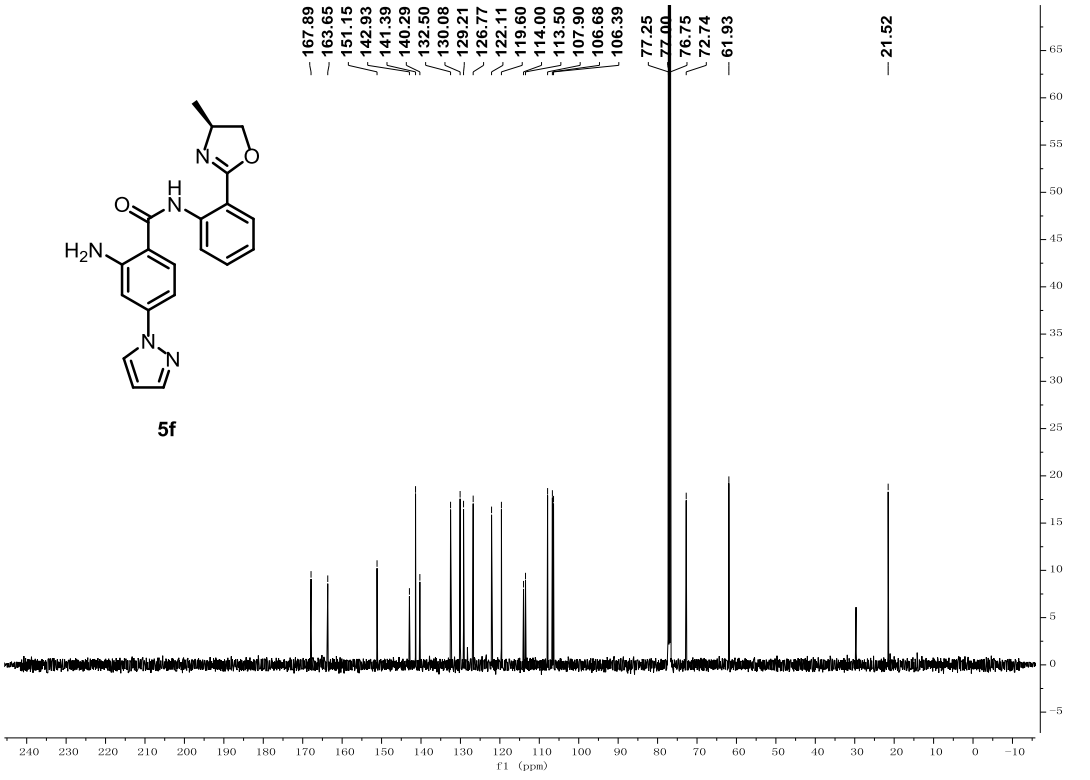
2.05
1.06
2.95
f1 (ppm)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114.00
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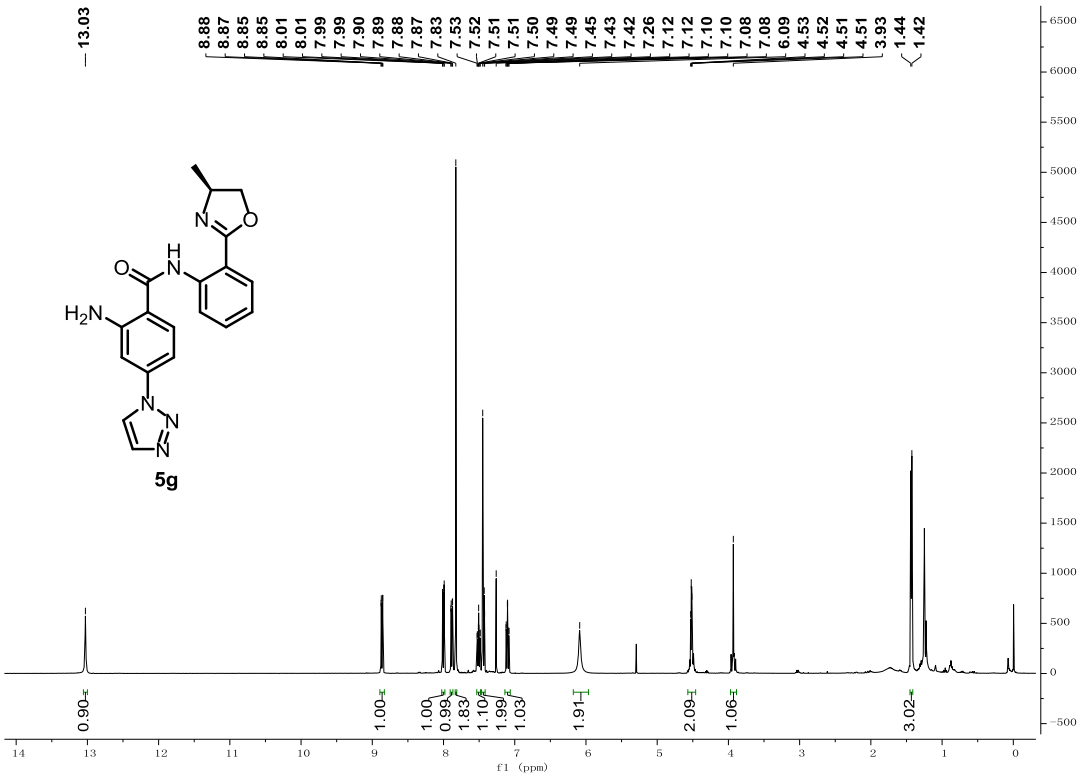
77.00
76.75
72.74
61.93
21.52
5f
f1 (ppm)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7.87
7.83
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.45
7.43
7.42
7.26
7.12
7.12
7.10
7.10
7.08
7.08
6.09
4.53
4.52
4.51
4.51
3.93
1.44
1.42
5g
0.90
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1.00
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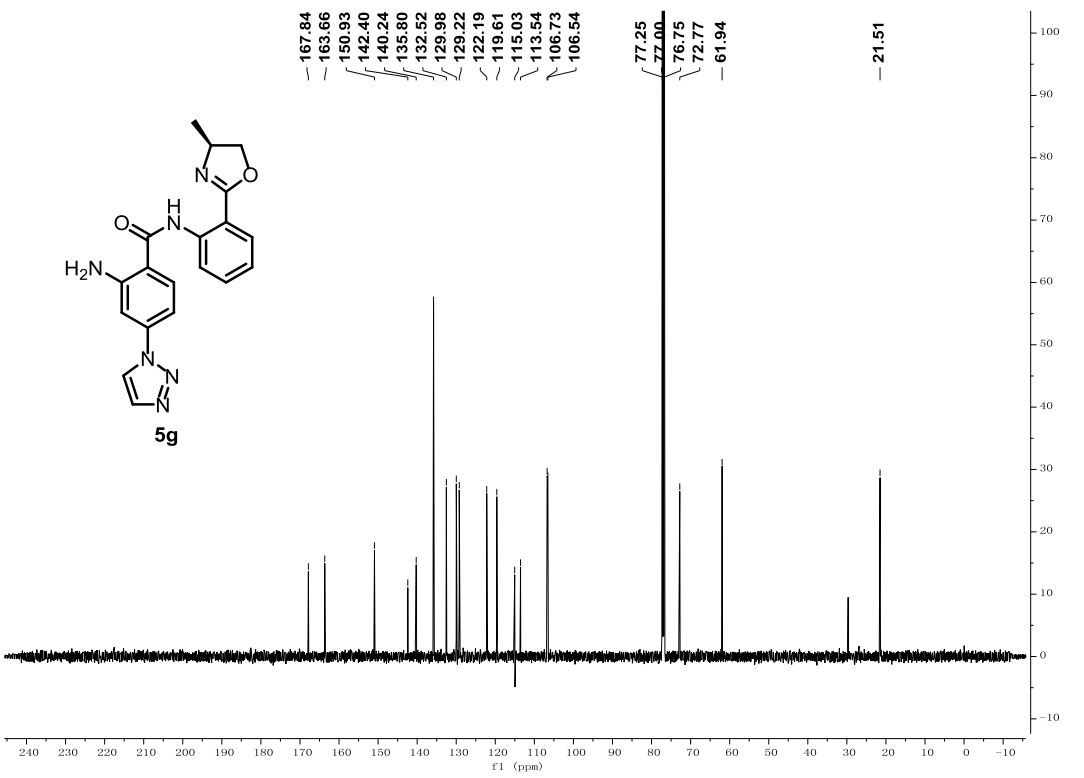
1.99
1.03
1.91
2.09
1.06
3.02
f1 (ppm)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72.77
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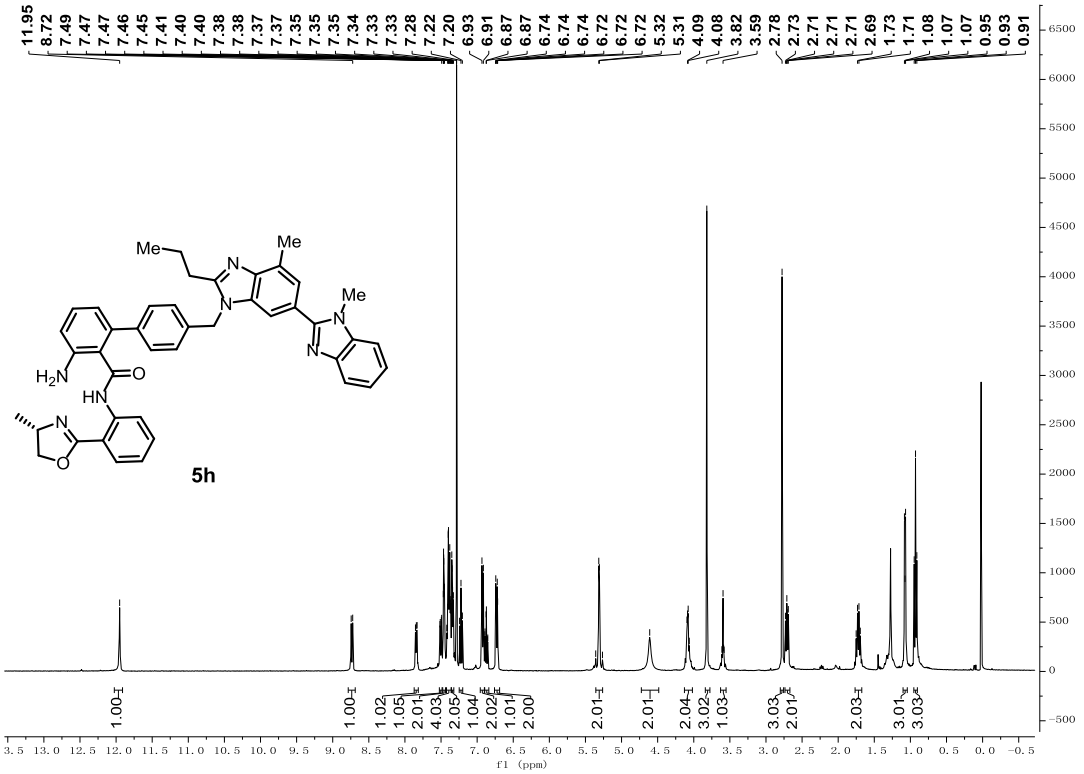
5g
f1 (ppm)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7.35
7.35
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7.28
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6.91
6.87
6.74
6.74
6.74
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6.72
6.72
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5.31
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4.08
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3.59
2.78
2.73
2.71
2.71
2.71
2.69
1.73
1.71
1.08
1.07
1.07
0.95
0.93
0.91
Me
Me
Me
N
N
N
N
H2N
O
HN
O
5h
1.00
1.00
1.02
1.05
2.01
4.03
2.05
1.04
2.02
1.01
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1.03
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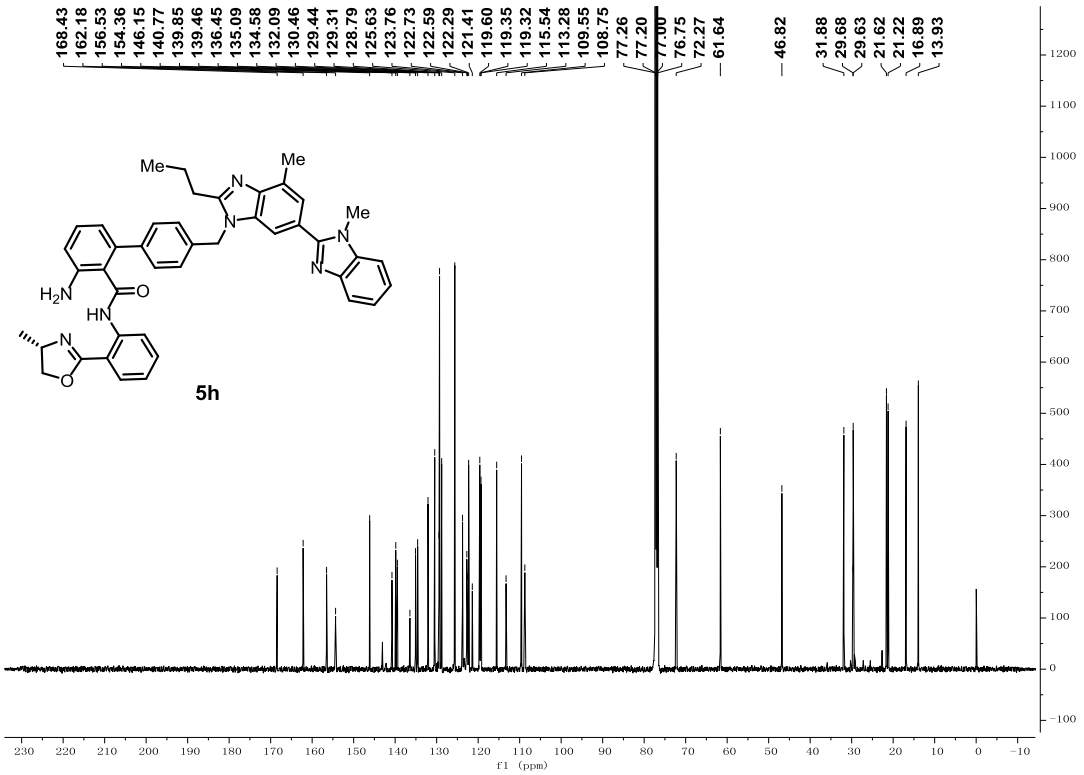
2.03
3.01
3.03
f1 (ppm)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77.00
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72.27
61.64
46.82
31.88
29.68
29.63
21.62
21.22
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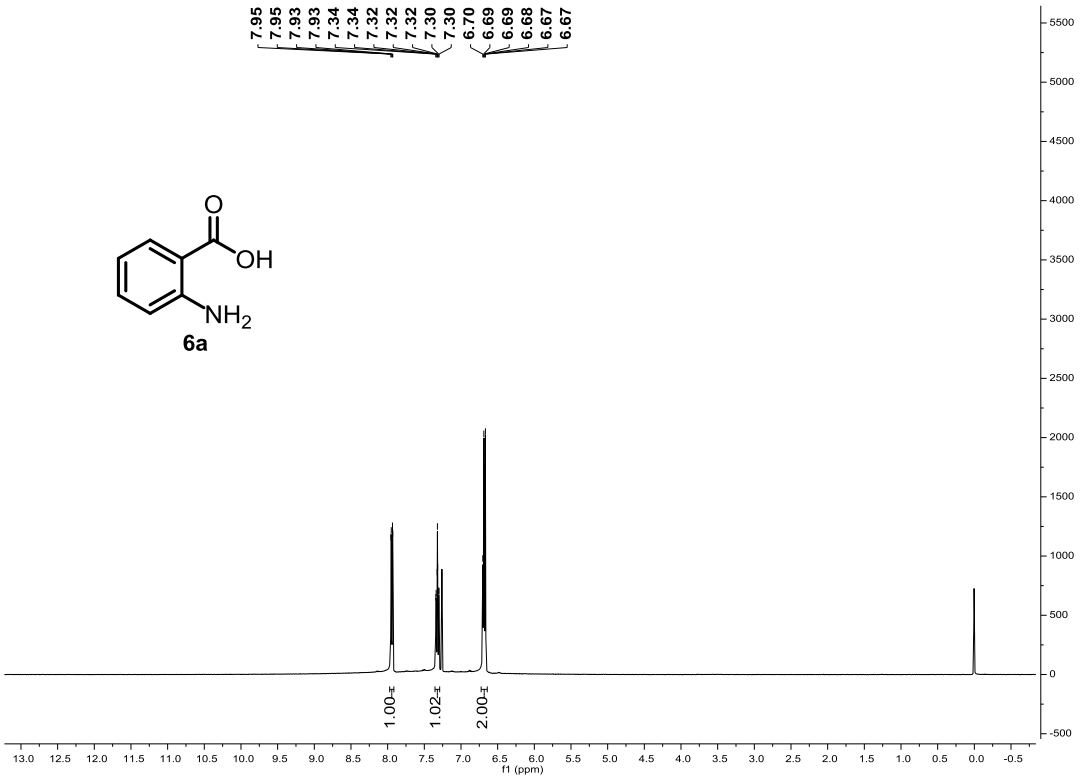
13.93
Me
Me
Me
N
N
N
N
H2N
O
HN
O
5h
f1 (ppm)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7.93
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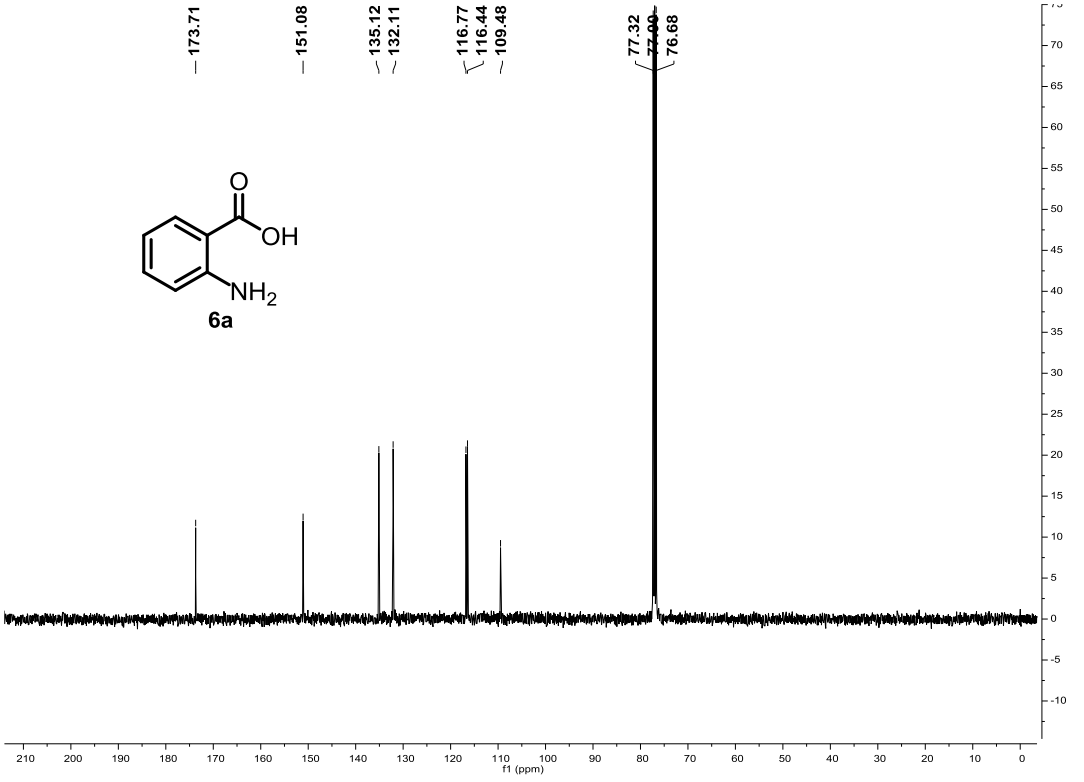
7.34
7.32
7.32
7.32
7.30
7.30
6.70
6.69
6.69
6.68
6.67
6.67
O
OH
NH2
6a
1.00
1.02
2.00
f1 (ppm)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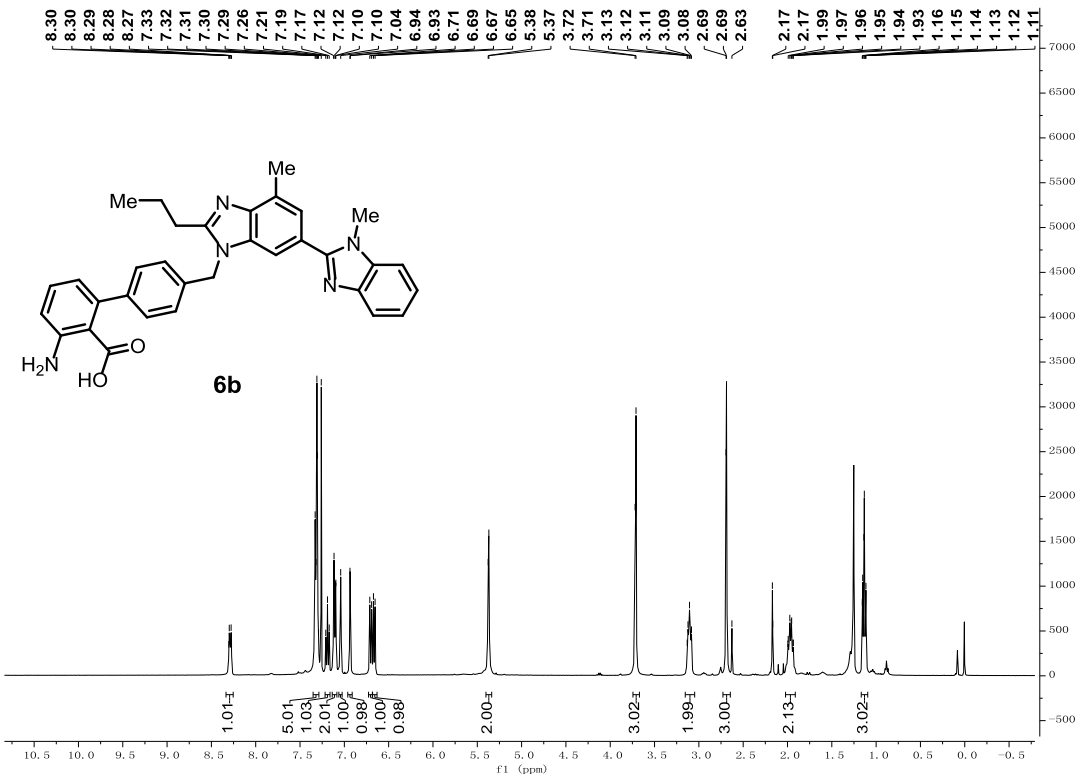
77.32
77.00
76.68
O
OH
NH2
6a
f1 (ppm)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7.12
7.12
7.10
7.10
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3.13
3.12
3.11
3.09
3.08
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2.69
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2.17
2.17
1.99
1.97
1.96
1.95
1.94
1.93
1.16
1.15
1.14
1.13
1.12
1.11
Me
Me
N
N
Me
N
N
H2N
O
HO
6b
1.01
5.01
1.03
2.01
1.00
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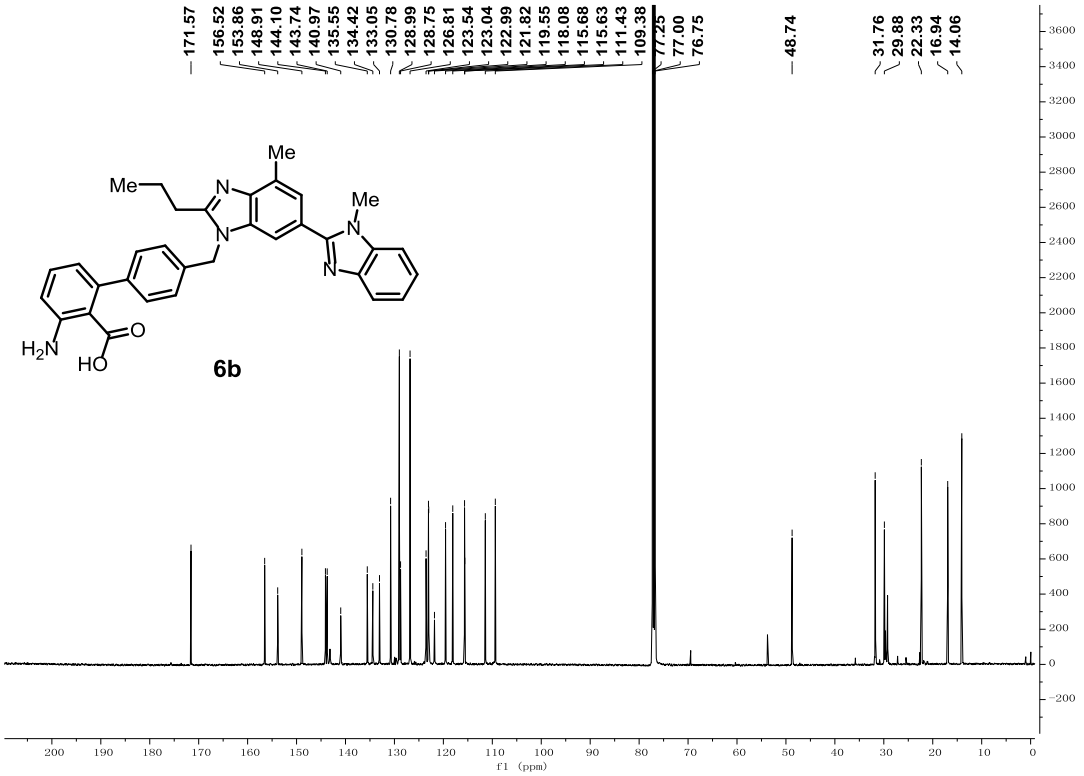
1.00
0.98
2.00
3.02
1.99
3.00
2.13
3.02
f1 (ppm)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130.78
128.99
128.75
126.81
123.54
123.04
122.99
121.82
119.55
118.08
115.68
115.63
111.43
109.38
77.25
77.00
76.75
48.74
31.76
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14.06
Me
Me
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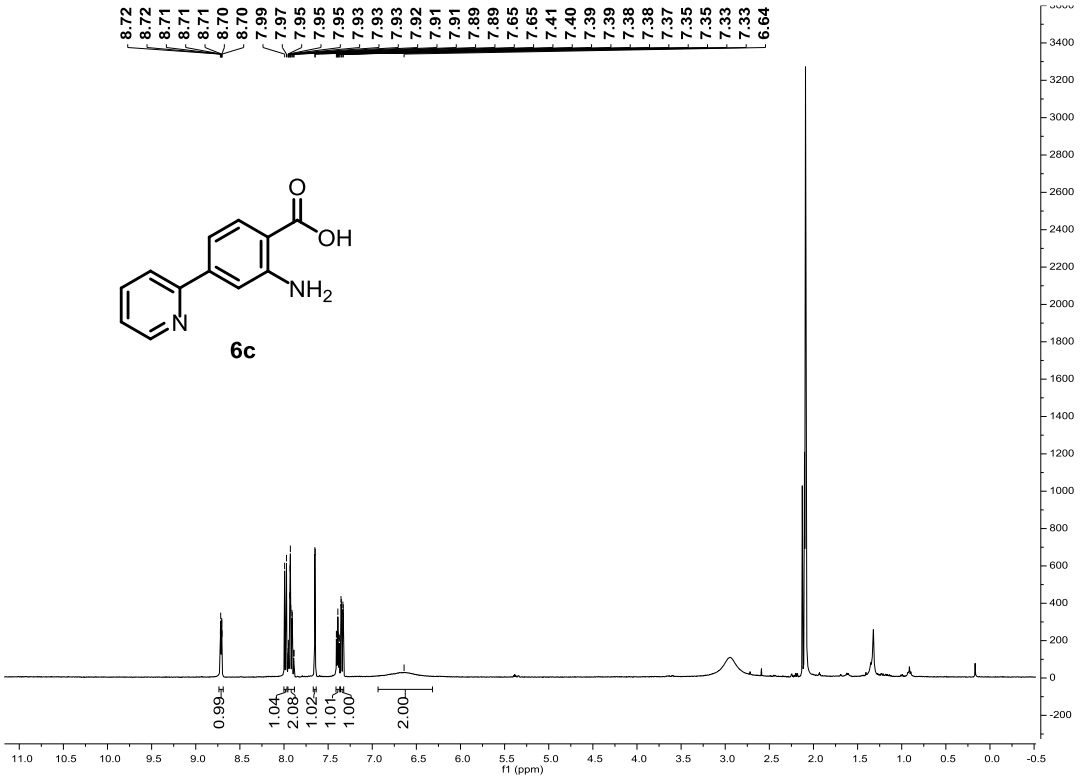
Me
N
N
H2N
O
HO
6b
f1 (ppm)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7.39
7.39
7.38
7.38
7.37
7.35
7.35
7.33
7.33
6.64
O
OH
NH2
N
6c
0.99
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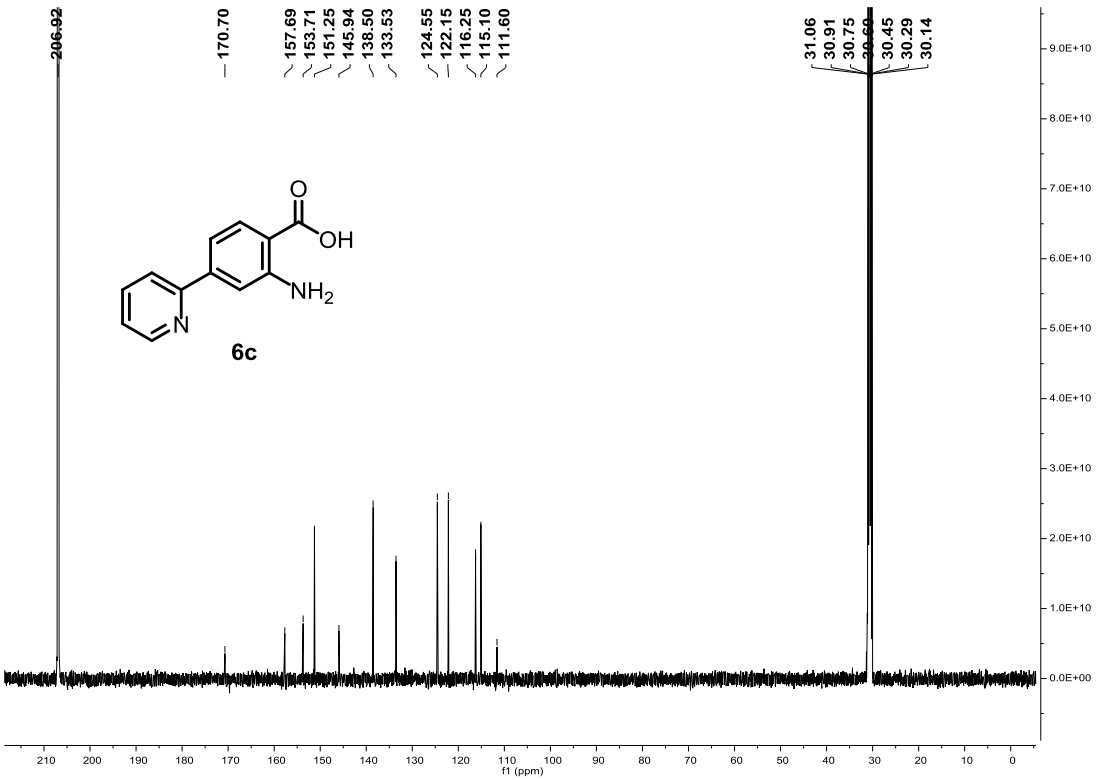
2.08
1.02
1.01
1.00
2.00
f1 (ppm)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145.94
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124.55
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116.25
115.10
111.60
31.06
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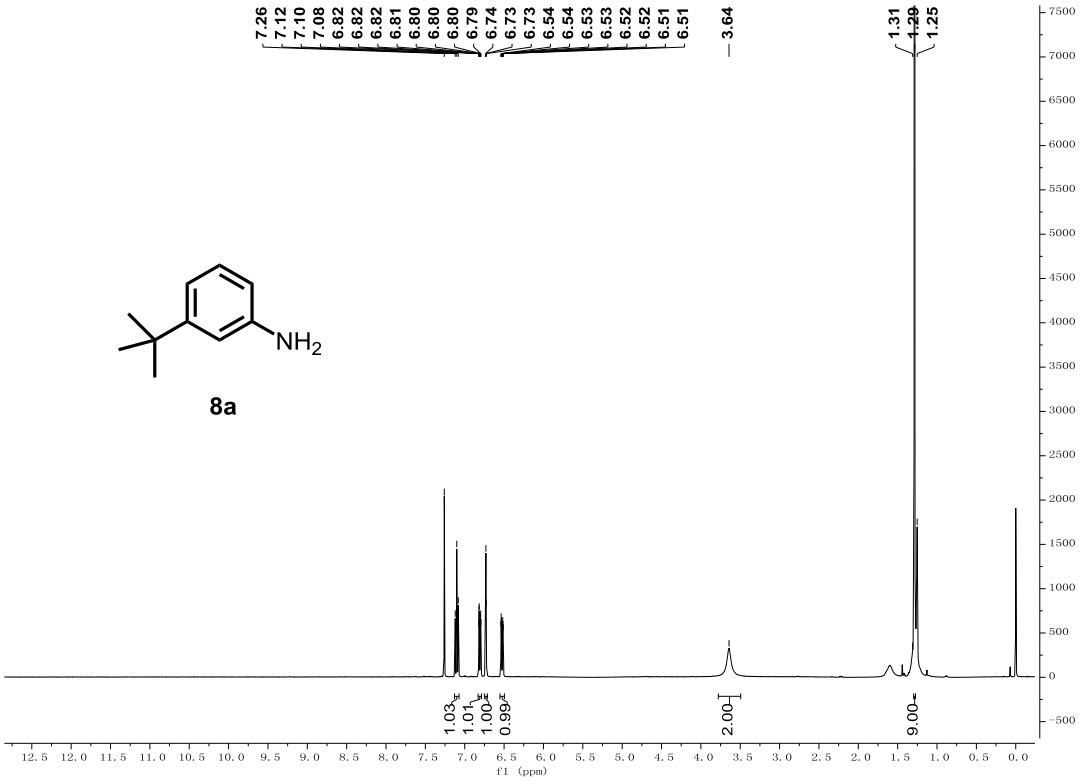
30.75
30.60
30.45
30.29
30.14
O
OH
NH2
N
6c
f1 (ppm)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6.73
6.73
6.54
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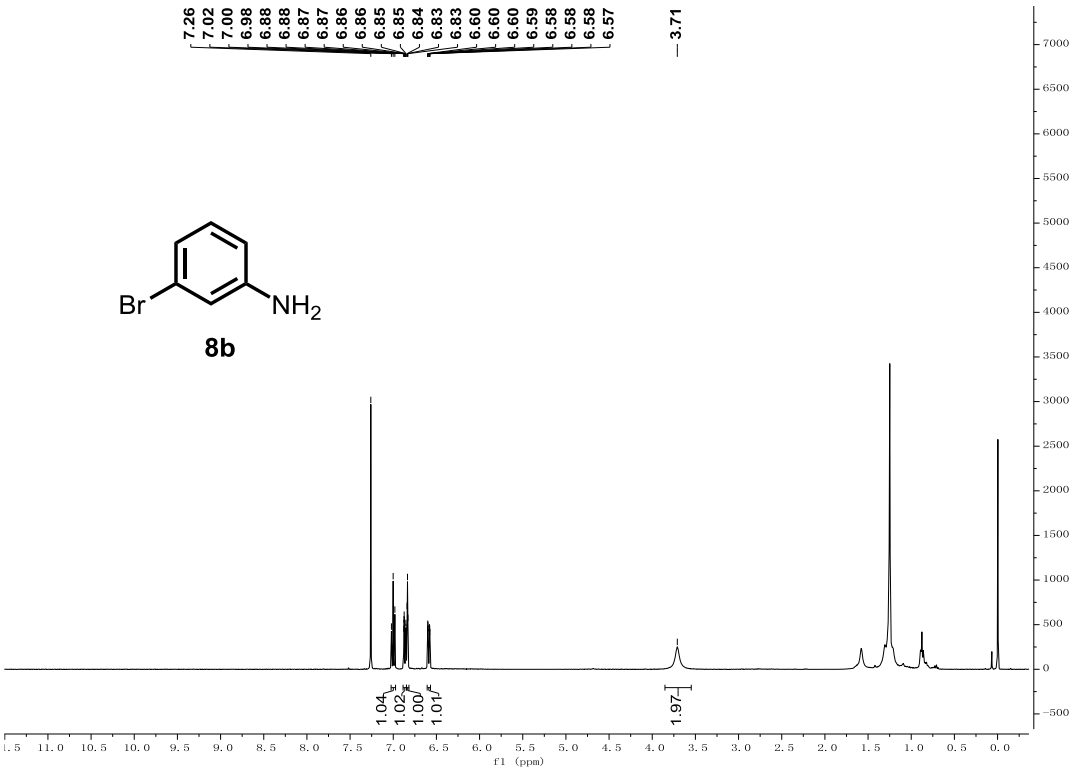
6.53
6.53
6.52
6.52
6.51
6.51
3.64
1.31
1.29
1.25
NH2
1.03
1.01
1.00
0.99
2.00
9.00
f1 (ppm)

8a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6.86
6.85
6.85
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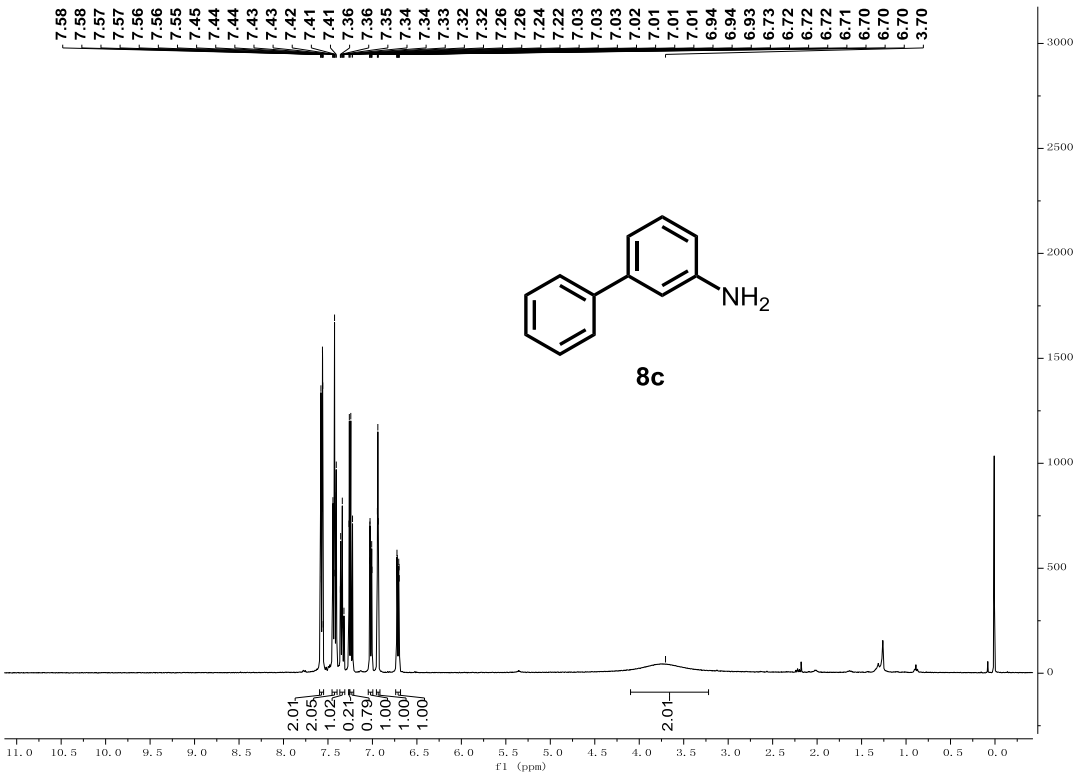
6.60
6.60
6.59
6.58
6.58
6.57
3.71
Br
NH2
1.04
1.02
1.00
1.01
1.97
f1 (ppm)

8b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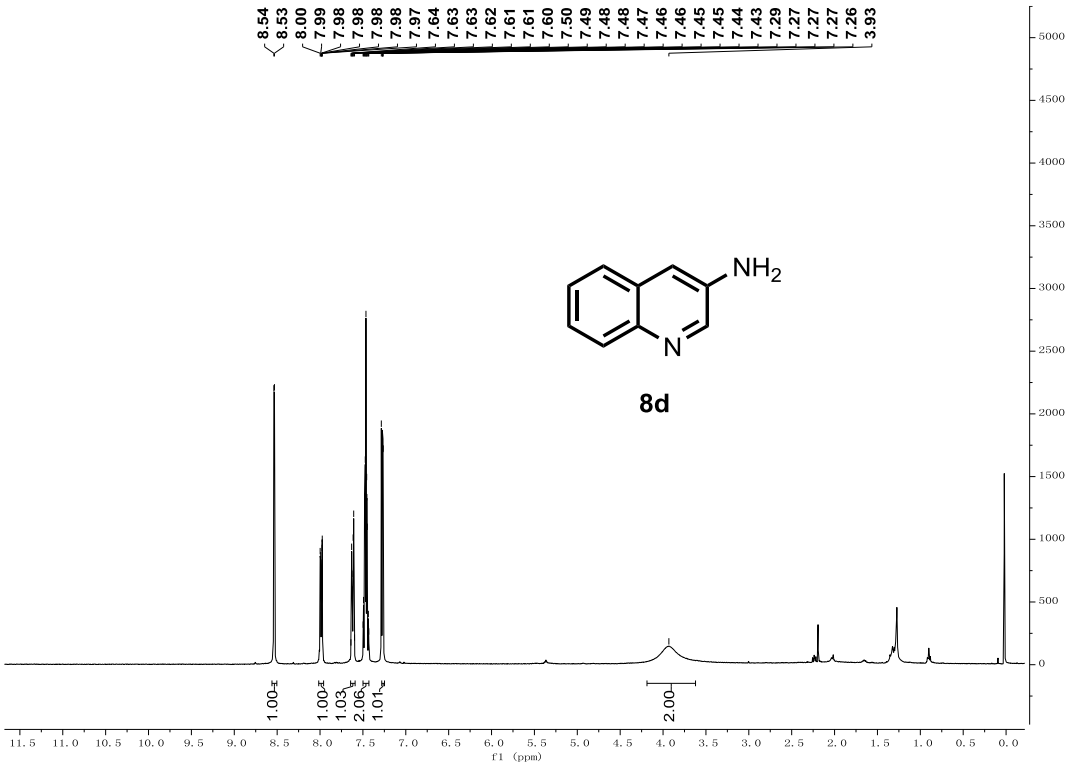
NH2
8c
2.01 2.05 1.02 0.21 0.79 1.00 1.00 1.00 2.01
f1 (ppm)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NH2
N
8d
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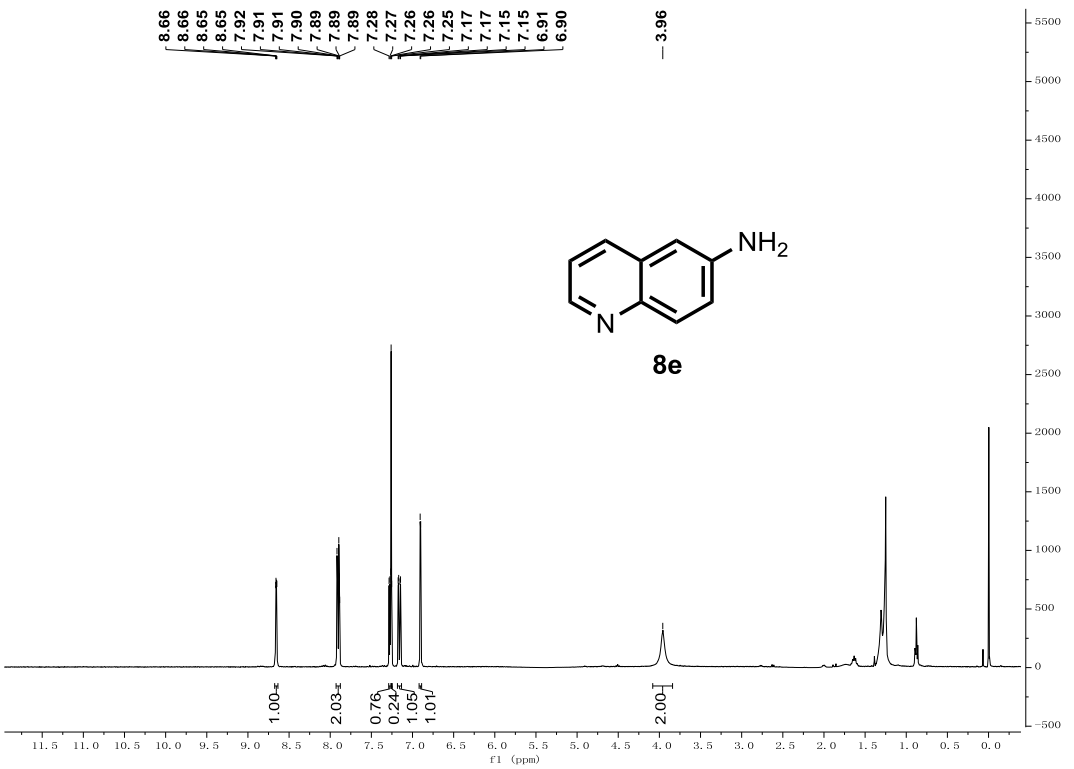
f1 (ppm)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7.27
7.26
7.26
7.25
7.17
7.17
7.15
6.91
6.90
3.96
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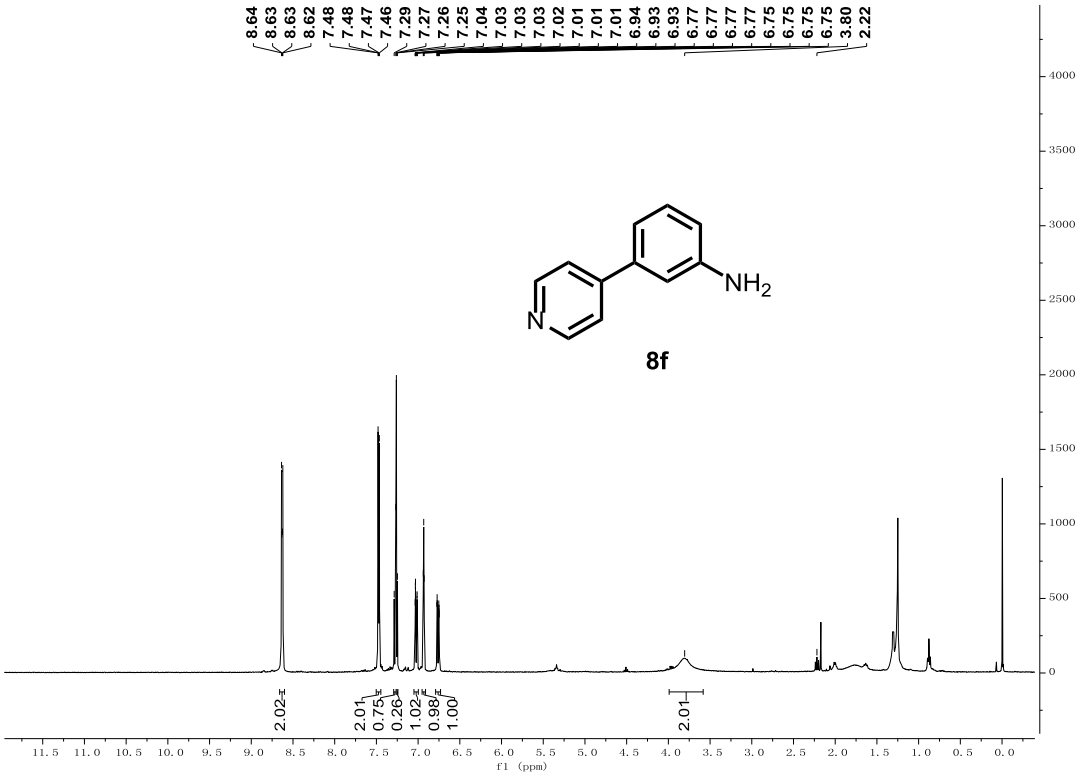
N
8e
1.00
2.03
0.76
0.24
1.05
1.01
2.00
f1 (ppm)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7.03
7.03
7.03
7.02
7.01
7.01
7.01
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6.93
6.77
6.77
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6.75
6.75
6.75
3.80
2.22
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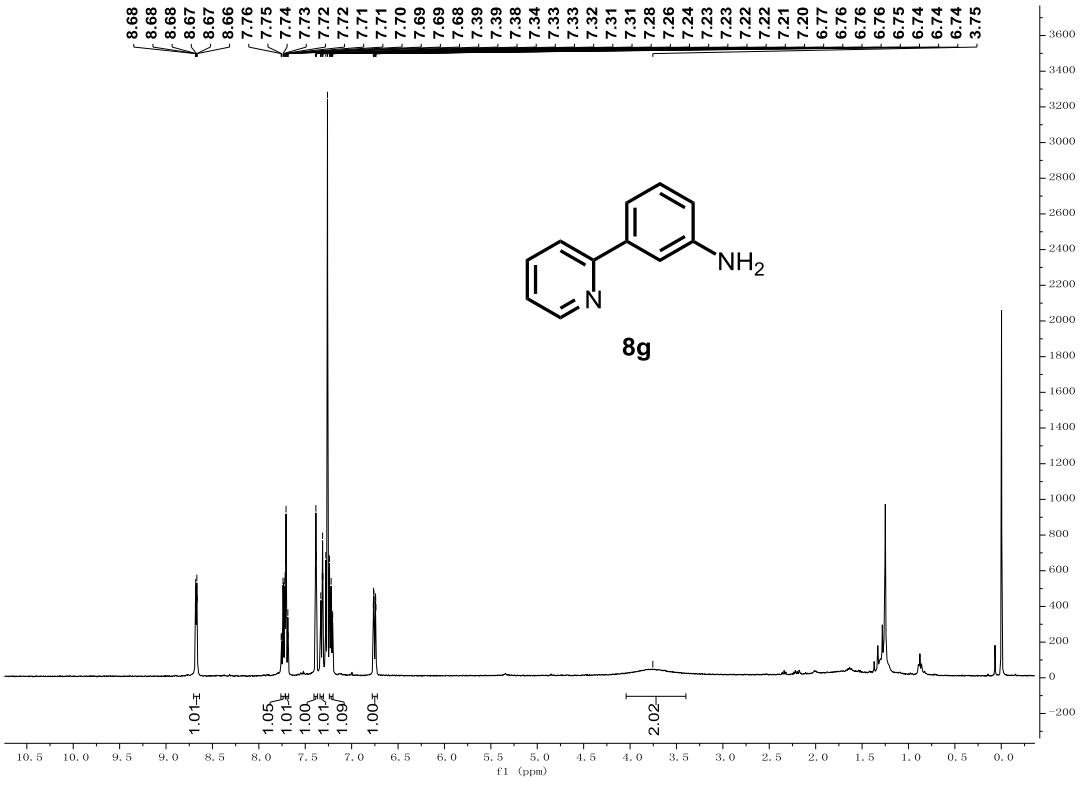
0.75
0.26
1.02
0.98
1.00
2.01
f1 (ppm)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NH2
N
8g
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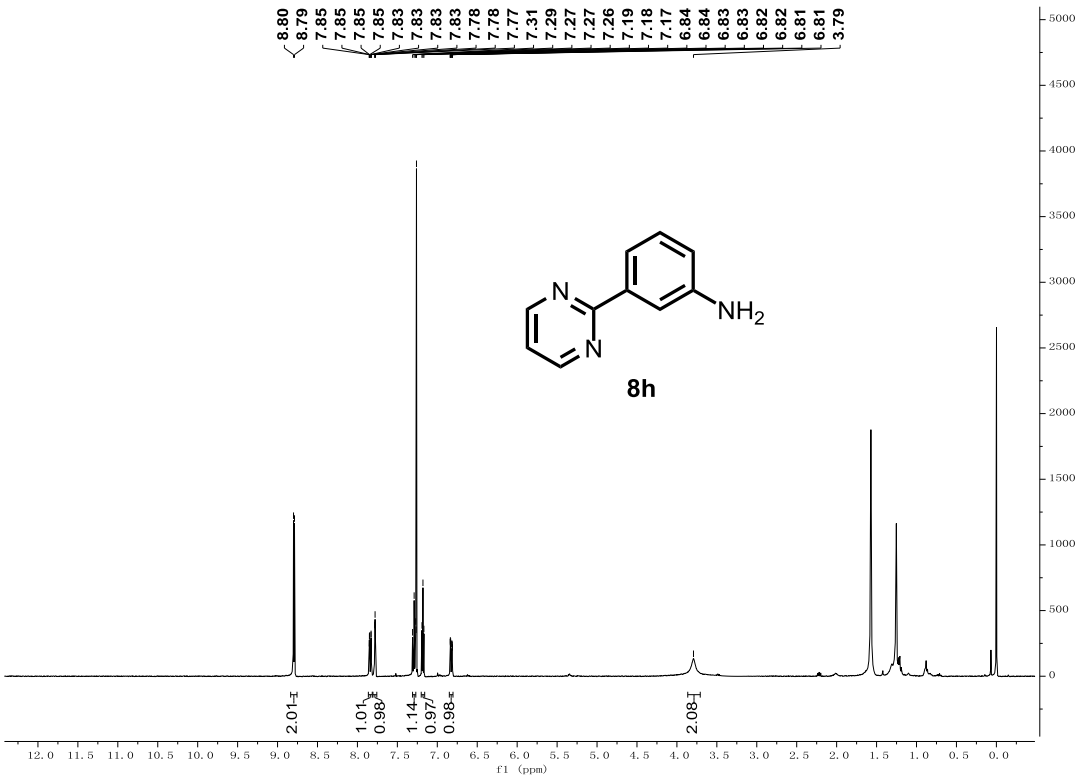
f1 (ppm)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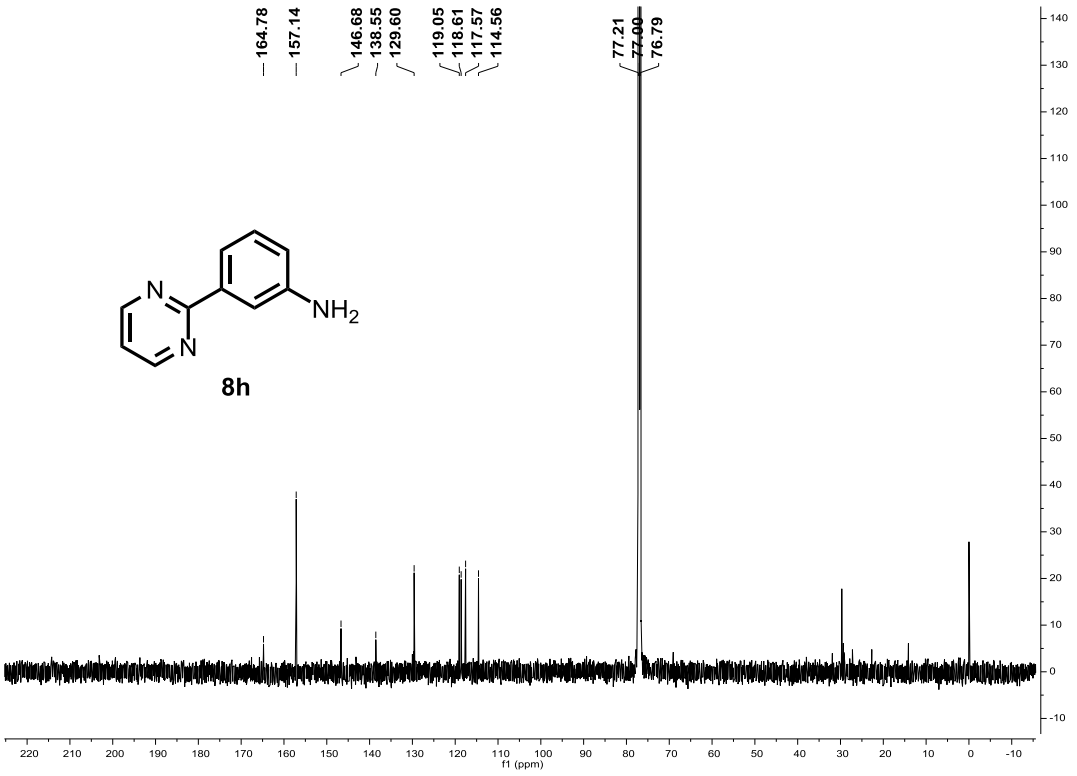
N
N
NH2
8h
2.01 1.01 0.98 1.14 0.97 0.98 2.08
f1 (ppm)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129.60
119.05
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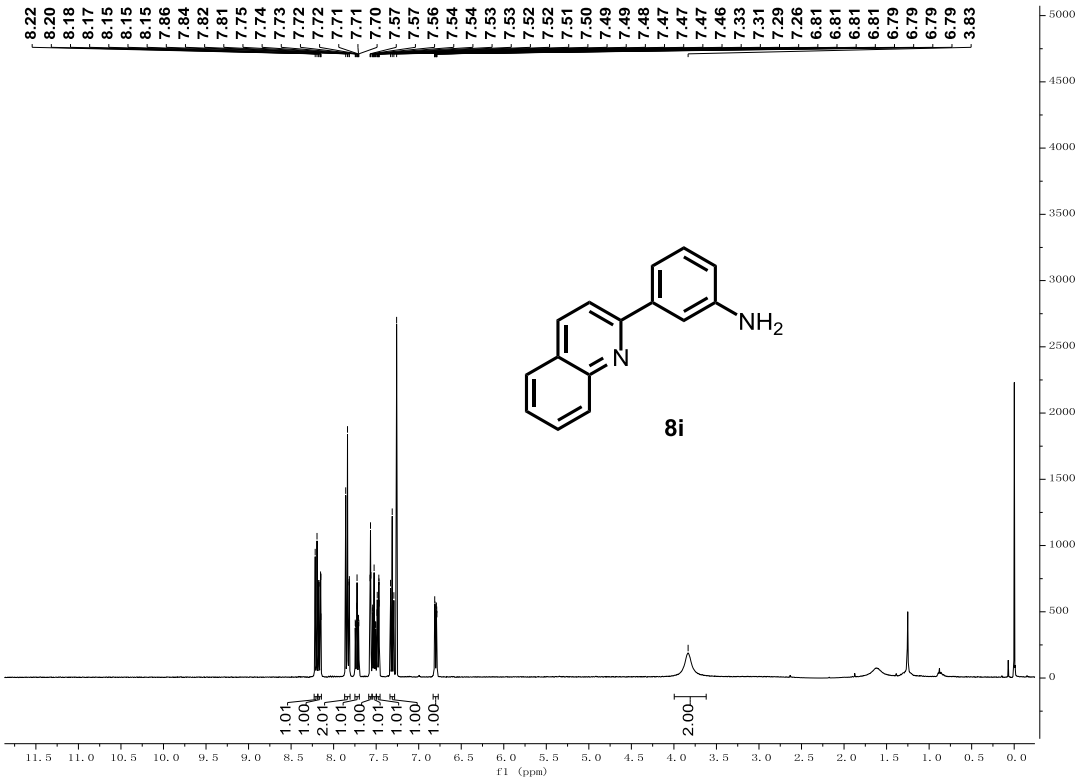
117.57
114.56
77.21
77.00
76.79
N
N
NH2
8h
f1 (ppm)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6.79
6.79
3.83
N
NH2
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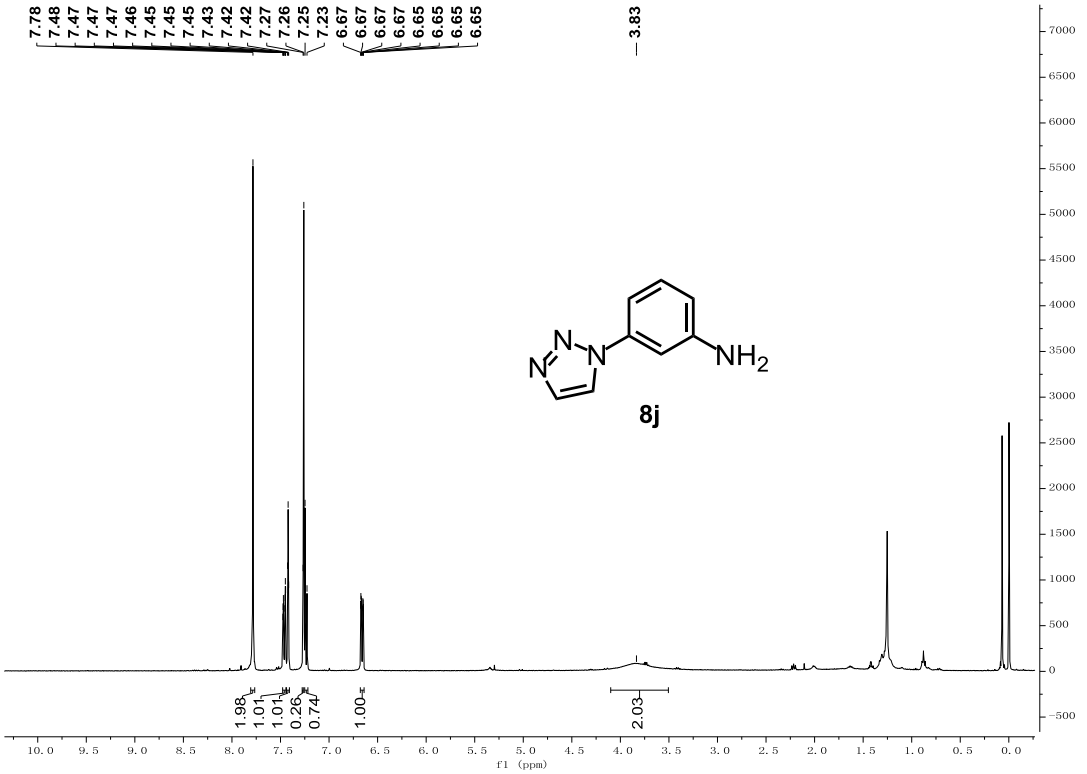
1.01
1.01
1.00
1.00
2.00
f1 (ppm)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6.67
6.67
6.65
6.65
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NH2
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1.01
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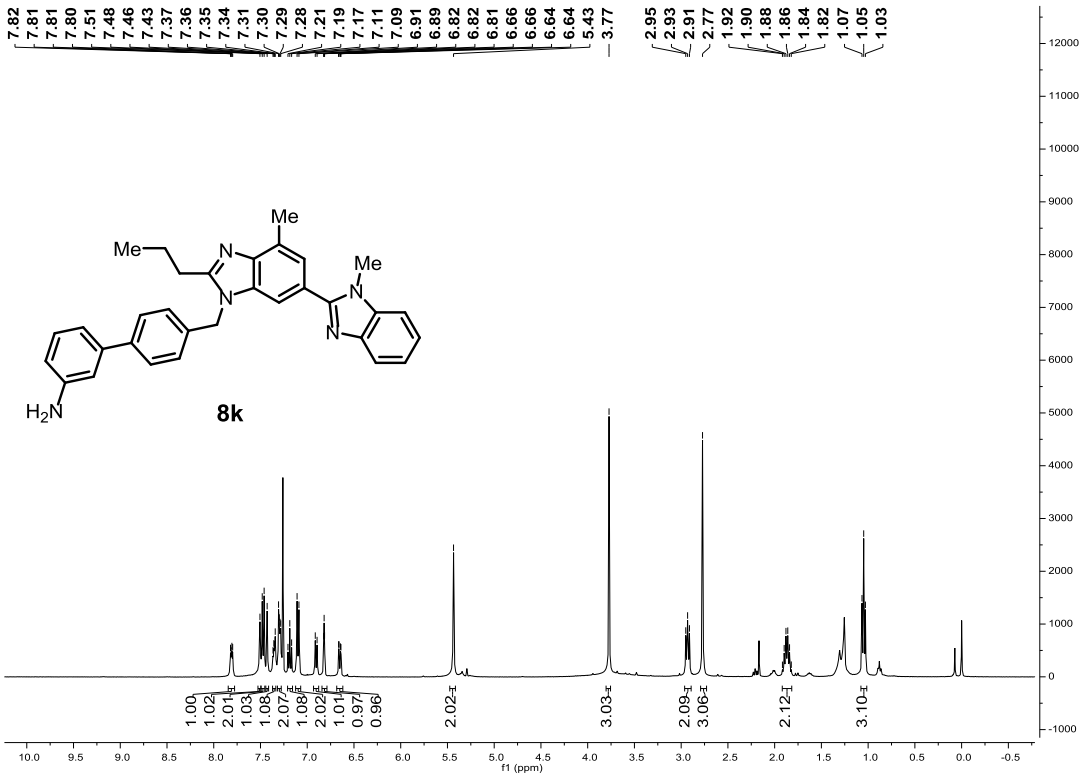
0.74
1.00
2.03
f1 (ppm)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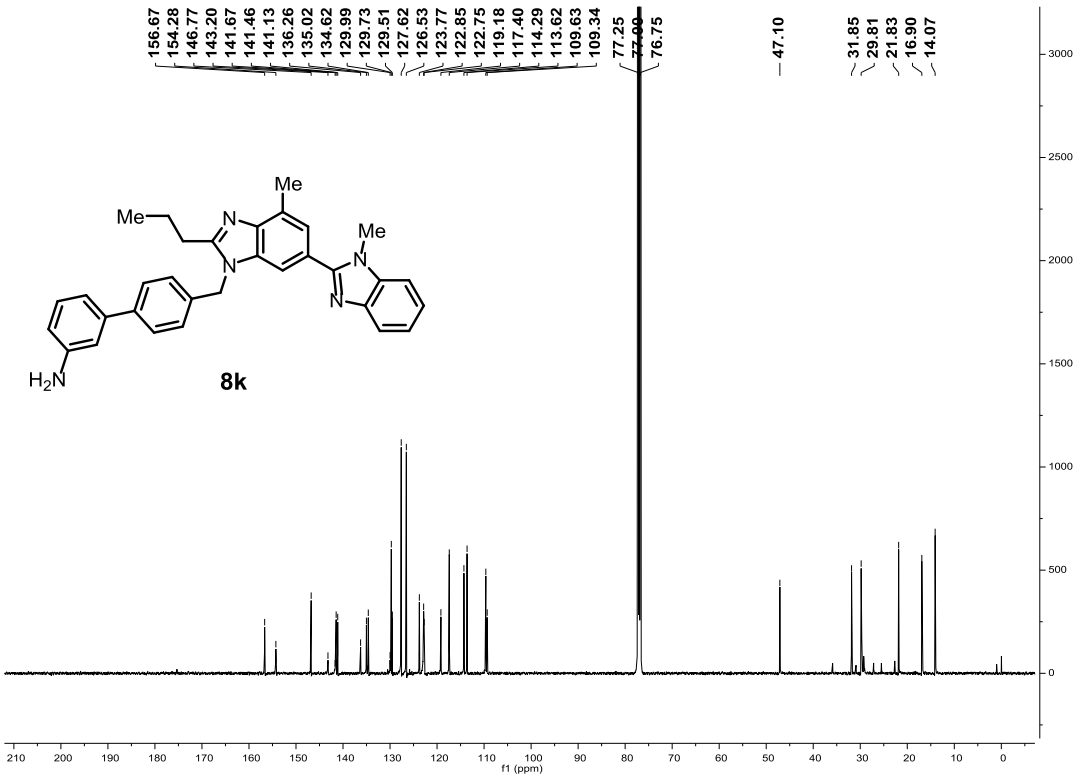
1.88
1.86
1.84
1.82
1.07
1.05
1.03
Me
Me
Me
N
N
N
N
H2N
8k
1.00
1.02
2.01
1.03
1.08
2.07
1.08
2.02
1.01
0.97
0.96
2.02
3.03
2.09
3.06
2.12
3.10
f1 (ppm)


156.67
154.28
146.77
143.20
141.67
141.46
141.13
136.26
135.02
134.62
129.99
129.73
129.51
127.62
126.53
123.77
122.85
122.75
119.18
117.40
114.29
113.62
109.63
109.34
77.25
77.00
76.75
47.10
31.85
29.81
21.83
16.90
14.07
Me
Me
N
N
Me
N
N
H2N
8k
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)