

*Electronic supplementary information (ESI)*

**Marine Natural Products for Drug Discovery: First Discovery of Kealiinines A-C and Their Derivatives as Novel Antiviral and Antiphytopathogenic Fungus Agents**

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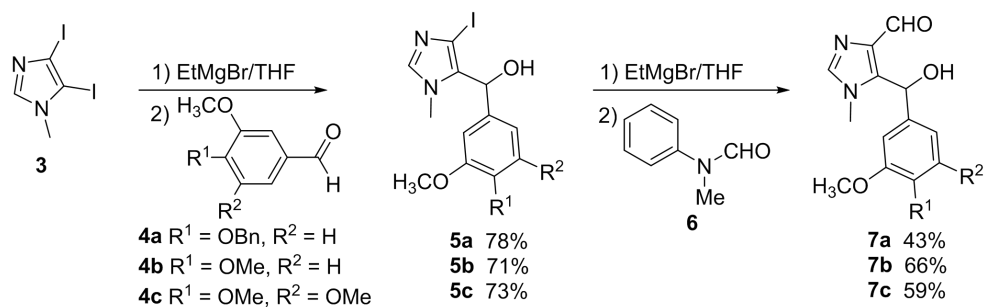
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## General Procedures for the Preparation of (substituted phenyl)(4-iodo-1-methyl-1H-imidazol-5-yl)methanols (**5**).

To a solution of 4,5-diiodo-1-methyl-1H-imidazole (**3**) (10 mmol) in anhydrous tetrahydrofuran (THF) (100 mL) was added C<sub>2</sub>H<sub>5</sub>MgBr (3 M in ether, 3.5 mL, 10.5 mmol) dropwise under argon at 0 °C. After completing addition of C<sub>2</sub>H<sub>5</sub>MgBr, the reaction mixture was allowed to be stirred at room temperature for 2 h. Then a solution of substituted benzaldehyde (**4**) (11 mmol) in anhydrous THF (7 mL) was added. The reaction mixture was stirred at room temperature for 16 h and quenched with aqueous saturated ammonium chloride (80 mL). After separation, the aqueous phase was extracted with ethyl acetate (EA) (100 mL×3). The combined organic phase was washed with brine (150 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated. The residue was washed with a little ethyl acetate and filtered to give **5** as a pale yellow or white solid.

For **5a**: pale yellow solid; mp. 161–163 °C; yield 78%; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.59 (s, 1H), 7.44–7.31 (m, 5H), 7.00 (d, *J* = 8.4 Hz), 6.98 (d, *J* = 1.6 Hz, 1H), 6.66–6.63 (m, 1H), 6.24 (d, *J* = 4.0 Hz, 1H), 5.80 (d, *J* = 4.0 Hz, 1H), 5.04 (s, 2H), 3.74 (s, 3H), 3.41 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 149.4, 147.2, 141.8, 137.5, 135.3, 135.2, 128.8, 128.3, 117.7, 113.9, 109.8, 85.6, 70.4, 66.5, 55.9, 33.1.

For **5b**: white solid; mp. 189–191 °C; yield 71%; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.59 (s, 1H), 6.95 (d, *J* = 1.6 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.67 (d, *J* = 8.4 Hz, 1H), 6.23 (d, *J* = 4.0 Hz, 1H), 5.79 (d, *J* = 4.0 Hz, 1H), 3.72 (s, 3H), 3.71 (s, 3H), 3.40 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 148.5, 147.7, 141.3, 134.8, 134.3, 117.2, 111.6, 109.0, 85.1, 66.0, 55.4, 55.3, 32.6.

For **5c**: pale yellow solid; mp. 178–179 °C; yield 73%; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.59 (s, 1H), 6.58 (s, 2H), 6.32 (s, 1H), 5.79 (s, 1H), 3.72 (s, 6H), 3.63 (s, 3H), 3.45 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 152.7, 141.3, 137.6, 136.3, 134.5, 102.4, 85.2, 66.2, 60.0, 55.7, 32.7.

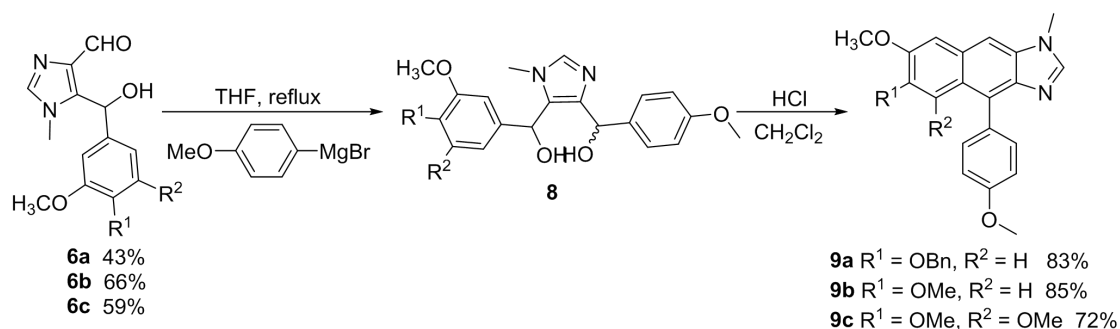


**General Procedures for the Preparation of 5-((substituted phenyl)(hydroxy)methyl)-1-methyl-1H-imidazole-4-carbaldehydes (7).** To a solution of (substituted phenyl)(4-iodo-1-methyl-1H-imidazol-5-yl)methanol (**5**) (6.7 mmol) in anhydrous tetrahydrofuran (THF) (120 mL) was added  $\text{C}_2\text{H}_5\text{MgBr}$  (3 M in ether, 5.6 mL, 16.8 mmol) dropwise under argon at 0 °C. After completing addition of  $\text{C}_2\text{H}_5\text{MgBr}$ , the reaction mixture was warmed slowly to room temperature and stirred for 3–4 h. The anhydrous *N*-methyl-*N*-phenylformamide (**6**) (1.36 g, 10.0 mmol) was added by syringe and stirred at room temperature for 16 h. The mixture was quenched with aqueous saturated  $\text{NH}_4\text{Cl}$  (80 mL) and extracted with ethyl acetate (100 mL $\times$ 3). The combined organic phase was washed with brine (150 mL), dried over anhydrous  $\text{Na}_2\text{SO}_4$  and concentrated. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to give **7** as a yellow solid.

For **7a**: yellow solid; mp. 145–147 °C; yield 43%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.88 (s, 1H), 7.43 (s, 1H), 7.42–7.28 (m, 5H), 6.97 (d,  $J$  = 1.6 Hz, 1H), 6.77 (d,  $J$  = 8.0 Hz, 1H), 6.58 (dd,  $J$  = 8.0, 1.6 Hz, 1H), 6.01 (s, 2H), 5.12 (s, 2H), 3.84 (s, 3H), 3.53 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  189.3, 150.0, 148.2, 142.0, 139.2, 138.2, 136.9, 133.4, 128.6, 127.9, 127.2, 118.2, 113.6, 110.1, 71.0, 67.5, 56.0, 32.7.

For **7b**: yellow solid; mp. 141–143 °C; yield 66%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.91 (s, 1H), 7.48 (s, 1H), 6.95 (d,  $J$  = 2.0 Hz, 1H), 6.77 (d,  $J$  = 8.0 Hz, 1H), 6.64 (dd,  $J$  = 8.0, 2.0 Hz, 1H), 5.94 (s, 2H), 3.86 (s, 3H), 3.85 (s, 3H), 3.58 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  189.5, 149.6, 149.2, 142.2, 139.2, 138.5, 133.1, 118.4, 111.1, 109.7, 67.8, 56.0, 32.5.

For **7c**: yellow solid; mp. 149–151 °C; yield 59%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.92 (s, 1H), 7.48 (s, 1H), 6.51 (s, 2H), 6.02 (s, 1H), 5.87 (s, 1H), 3.82 (s, 3H), 3.80 (s, 6H), 3.60 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  189.5, 153.6, 141.6, 139.2, 138.4, 138.0, 136.0, 103.3, 68.0, 60.8, 56.2, 32.8.



**General Procedures for the Preparation of Intermediates (8).** To a suspension of magnesium chips (18 mmol) and anhydrous THF (80 mL) was added 1-bromo-4-methoxybenzene (12 mmol) dropwise over ca. 30 mins under argon to maintain a controlled reflux. Then, the reaction mixture was refluxed for another 2–3 h and cooled to room temperature. A solution of 5-((substituted phenyl)(hydroxy)methyl)-1-methyl-1H-imidazole-4-carbaldehydes (**7**) (2 mmol) in anhydrous THF (18 mL) was added, followed by heating the reaction mixture at reflux for 16 h. The reaction was quenched with aqueous saturated  $\text{NH}_4\text{Cl}$  (80 mL), filtered and the filtrate was extracted with ethyl acetate (80 mL $\times$ 3). The combined organic phase was washed with brine (100 mL), dried over anhydrous  $\text{Na}_2\text{SO}_4$  and concentrated. The residue was used for next step without further purification.

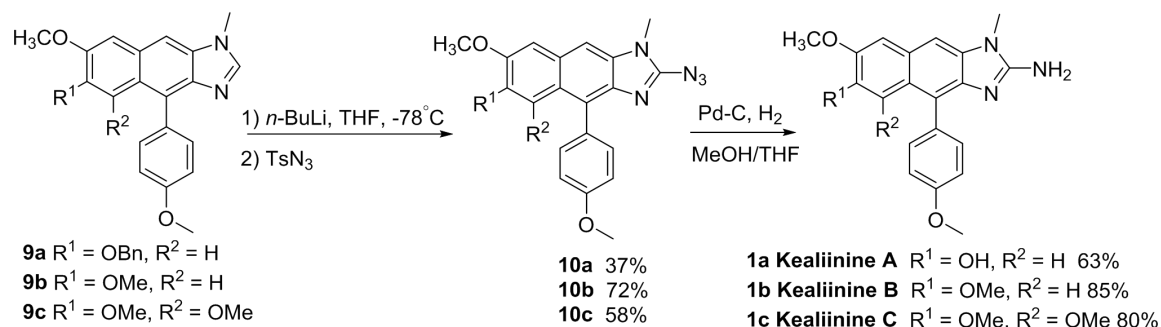
**General Procedures for the Preparation of 4-(4-methoxyphenyl)-1-methyl-1H-naphtho[2,3-d]imidazole (9).** To a solution of the crude product (**8**) (nearly 2 mmol) in  $\text{CH}_2\text{Cl}_2$  (30 mL) was added concentrated  $\text{HCl}$  (2 mL, 24 mmol) dropwise and stirred at room temperature for 3–4 h. To the mixture was added water (30 mL) and aqueous saturated  $\text{NaHCO}_3$  to pH 7, and the resulting mixture was extracted with  $\text{CH}_2\text{Cl}_2$  (50 mL $\times$ 3). The combined organic phase was washed with brine (50 mL), dried over anhydrous  $\text{Na}_2\text{SO}_4$  and concentrated. The residue was purified by column chromatography on silica gel with  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  as eluent to give **9** as a light brown solid.

For **9a**: light brown solid; mp. 221–223 °C; yield 83%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (s, 1H), 7.64 (s, 1H), 7.42 (d,  $J$  = 8.4 Hz, 2H), 7.41–7.30 (m, 6H), 7.08 (d,  $J$  = 8.4 Hz, 2H), 5.16 (s, 2H), 4.07 (s, 3H), 3.95 (s, 3H), 3.88 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 149.2, 146.8, 146.0, 141.1, 136.9, 133.8, 132.0, 129.1, 128.5, 127.9, 127.8, 127.5, 127.3, 123.9, 114.0, 107.1, 105.8, 103.0, 70.4, 55.9, 55.4, 31.1.

For **9b**: light brown solid; mp. 212–214 °C; yield 85%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (s, 1H), 7.64 (s, 1H), 7.58 (d,  $J$  = 8.8 Hz, 2H), 7.34 (s, 1H), 7.25 (s, 1H), 7.12 (d,  $J$  = 8.8 Hz, 2H), 4.04 (s, 3H), 3.91 (s, 3H,  $\text{OCH}_3$ ), 3.89 (s, 3H), 3.84 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.9, 148.9, 148.1, 146.0, 141.3, 133.8, 132.0, 129.2, 128.0, 127.2, 124.0, 114.0, 105.6, 104.4, 103.2, 55.8, 55.7, 55.4, 31.1.

For **9c**: light brown solid; mp. 224–226 °C; yield 72%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (s, 1H), 7.65 (s, 1H), 7.40 (d,  $J$  = 8.8 Hz, 2H), 7.10 (s, 1H), 7.02 (d,  $J$  = 8.8 Hz, 2H), 4.01 (s, 3H), 3.92 (s, 3H), 3.89 (s, 3H), 3.87 (s, 3H), 3.33 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.1, 151.9, 150.1,

146.4, 142.7, 140.8, 134.3, 132.3, 130.6, 129.4, 127.9, 119.6, 112.6, 103.8, 102.0, 61.2, 60.6, 55.7, 55.3, 31.1.



## General Procedures for the Preparation of

**2-Azido-4-(4-methoxyphenyl)-1-methyl-1H-naphtho[2,3-d]imidazole (10).** To a solution of 4-(4-methoxyphenyl)-1-methyl-1H-naphtho[2,3-d]imidazole (**9**) (0.47 mmol) in anhydrous THF (10 mL) was added *n*-BuLi (1.6 M in hexane, 0.59 mL, 0.90 mmol) dropwise at -78 °C under argon and was stirred at -78 °C for 3 h. The tosyl azide ( $\text{TsN}_3$ ) (0.71 mmol) was added by syringe and the resulting mixture was stirred at room temperature for 2 h. The reaction mixture was quenched with aqueous saturated  $\text{NH}_4\text{Cl}$  (4 mL) and extracted with ethyl acetate (20 mL $\times$ 3). The combined organic phase was washed with brine (20 mL), dried over anhydrous  $\text{Na}_2\text{SO}_4$  and concentrated. The crude product was purified quickly by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to give **10** as a yellow solid. (The products were not stable!)

For **10a**: yellow solid; yield 37%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43–7.27 (m, 9H), 7.20 (s, 1H), 7.03 (d,  $J = 8.8$  Hz, 2H), 5.12 (s, 2H), 4.02 (s, 3H), 3.92 (s, 3H), 3.57 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.7, 149.9, 148.9, 146.7, 138.8, 136.9, 134.8, 132.2, 128.8, 128.5, 127.7, 127.4, 126.5, 125.6, 124.2, 113.8, 107.2, 105.9, 102.6, 70.4, 55.8, 55.3, 29.0.

For **10b**: yellow solid; yield 72%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (d,  $J = 8.8$  Hz, 2H), 7.44 (s, 1H), 7.31 (s, 1H), 7.21 (s, 1H), 7.10 (d,  $J = 8.8$  Hz, 2H), 4.02 (s, 3H), 3.92 (s, 3H), 3.83 (s, 3H), 3.63 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.9, 150.0, 148.6, 148.1, 139.1, 134.9, 132.4, 129.0, 126.5, 125.9, 124.4, 113.9, 105.8, 104.7, 102.8, 55.9, 55.7, 55.4, 29.1.

For **10c**: yellow solid; yield 58%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 (s, 1H), 7.40 (d,  $J = 8.8$  Hz, 2H), 7.04 (s, 1H), 7.00 (d,  $J = 8.8$  Hz, 2H), 3.99 (s, 3H), 3.91 (s, 3H), 3.90 (s, 3H), 3.59 (s, 3H), 3.29 (s, 3H,  $\text{NCH}_3$ );  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 151.6, 150.4, 150.1, 140.8, 140.4, 135.3, 131.8, 131.1, 128.7, 125.6, 119.7, 112.4, 103.3, 102.2, 61.2, 60.6, 55.7, 55.3, 29.0.

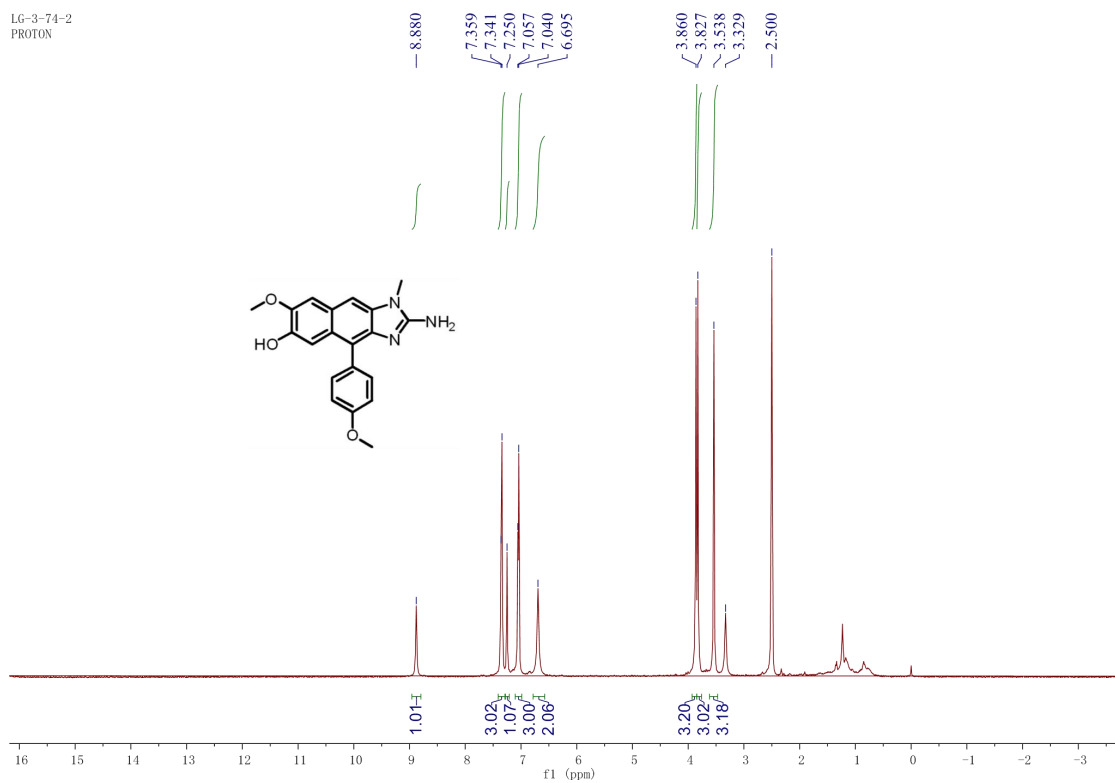
**General Procedures for the Preparation of Kealiinines A-C (1).** To a solution of 2-azido-4-(4-methoxyphenyl)-1-methyl-1H-naphtho[2,3-d]imidazole (**10**) (0.32 mmol) in THF (20 mL) and MeOH (20 mL) was added 10% Pd/C (50 mg). A balloon containing hydrogen was connected with the reaction vessel and the reaction mixture was stirred under hydrogen atmosphere at room temperature for 10 h. The mixture was filtered through celite and the filter cake was washed with MeOH (10 mL×3), and the filtrate was concentrated to give a grey-green or pale brown solid which could be further purified by column chromatography on silica gel with CH<sub>2</sub>Cl<sub>2</sub>/MeOH as eluent.

For **kealiinine A**: grey-green solid; mp. 277–278 °C; yield 63%; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.88 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.34 (s, 1H), 7.25 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 2H), 7.04 (s, 1H), 6.70 (s, 2H), 3.86 (s, 3H), 3.83 (s, 3H), 3.54 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 158.4, 157.4, 147.1, 145.1, 134.8, 132.6, 130.6, 124.4, 124.2, 120.3, 113.8, 107.6, 107.1, 101.6, 55.8, 55.6, 28.9.

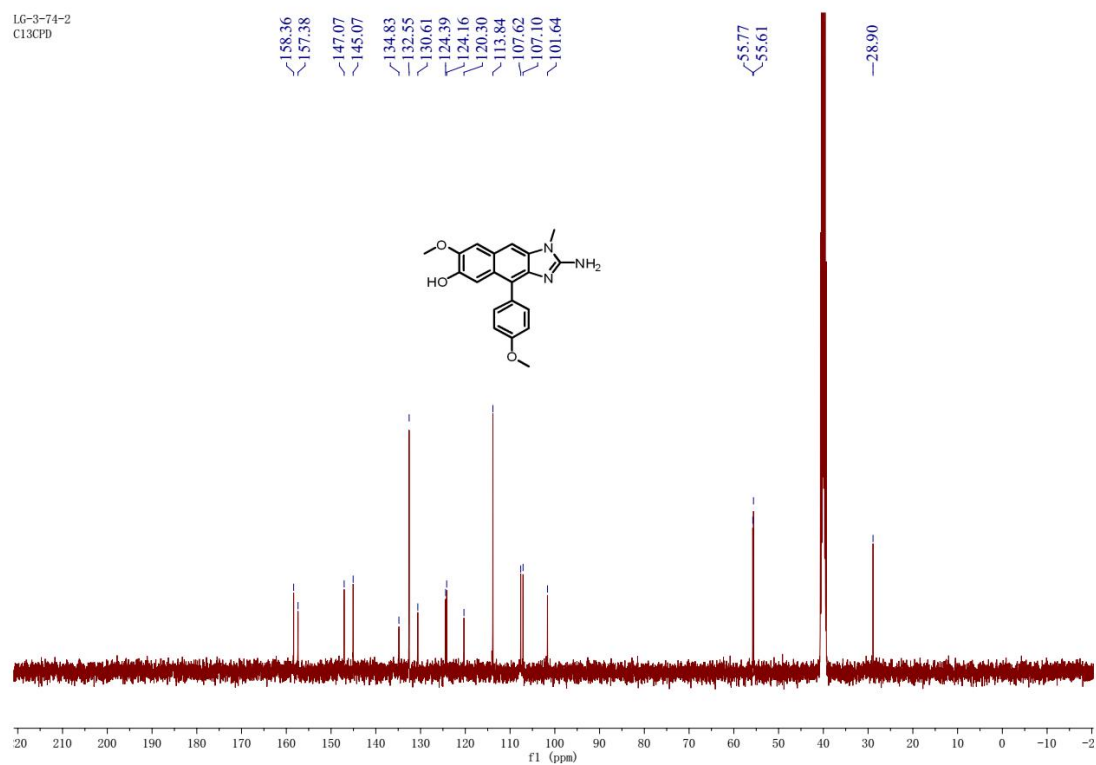
For **kealiinine B**: pale brown solid; mp. 278–280 °C; yield 85%; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.43 (d, *J* = 8.0 Hz, 2H), 7.38 (s, 1H), 7.29 (s, 1H), 7.11 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.69 (s, 2H), 3.86 (s, 3H), 3.83 (s, 3H), 3.63 (s, 3H), 3.55 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 157.8, 157.2, 146.9, 146.8, 140.4, 135.0, 132.1, 129.8, 124.0, 123.0, 120.6, 113.3, 106.7, 104.0, 101.1, 55.2, 55.0, 55.0, 28.4.

For **kealiinine C**: pale brown solid; mp. 302–304 °C; yield 80%; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.40 (s, 1H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.15 (s, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.72 (s, 2H), 3.88 (s, 3H), 3.80 (s, 3H), 3.72 (s, 3H), 3.53 (s, 3H), 3.10 (s, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 157.3, 157.0, 149.5, 148.9, 139.4, 135.7, 133.2, 130.9, 126.4, 120.1, 118.3, 111.8, 102.9, 101.6, 60.5, 60.0, 55.4, 55.0, 28.4.

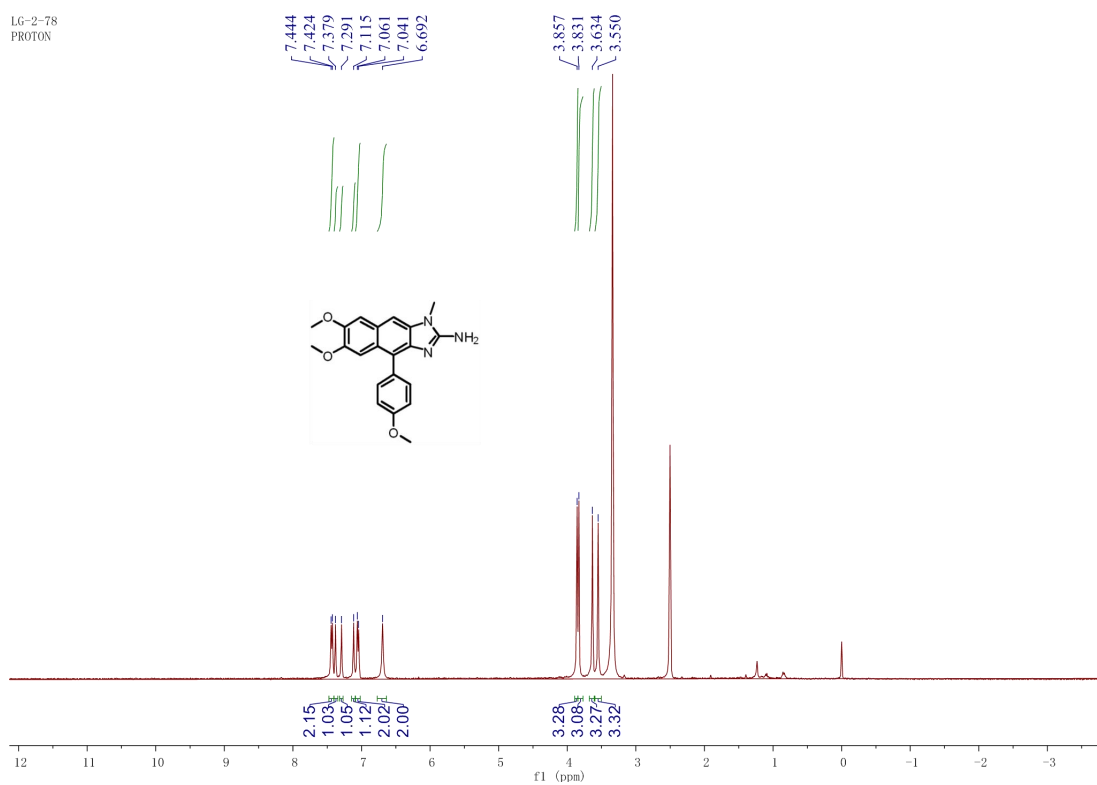
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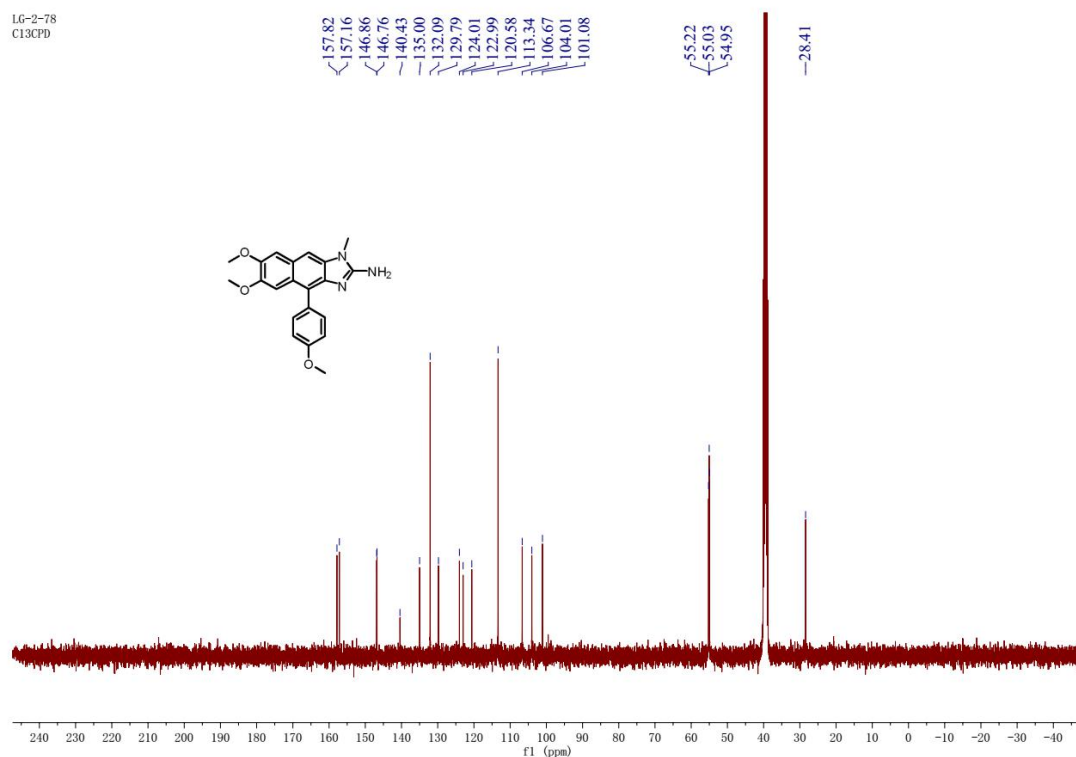
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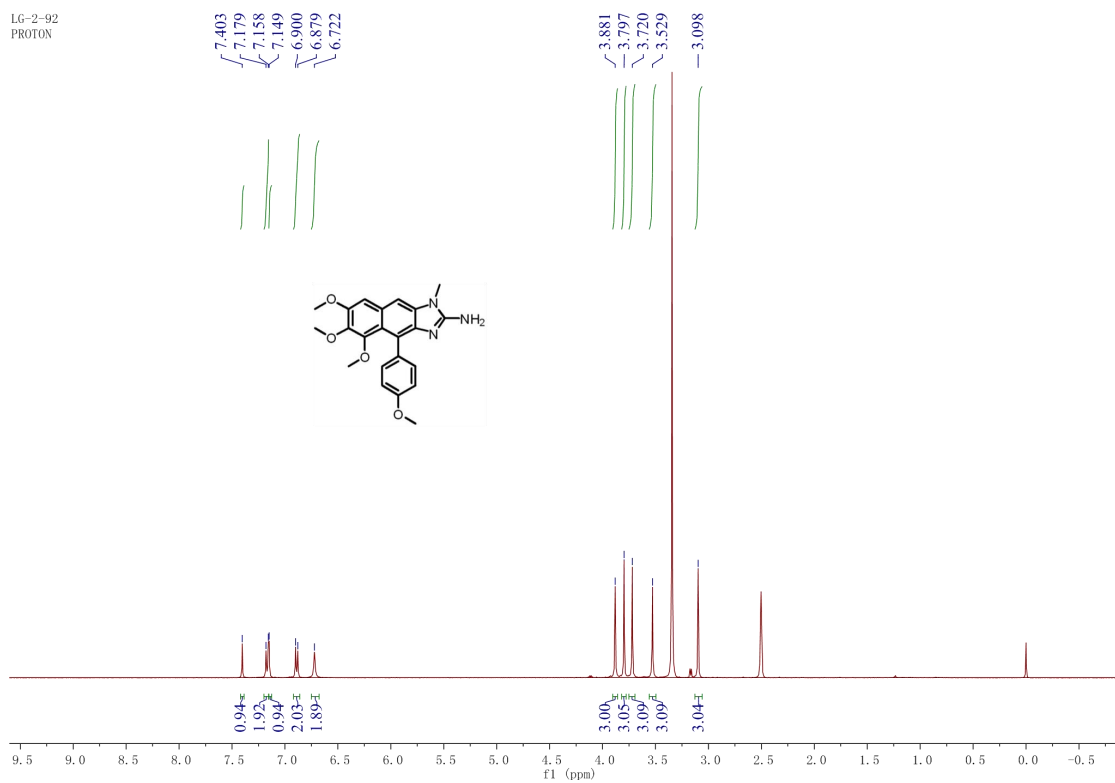
LG-2-78  
PROTON



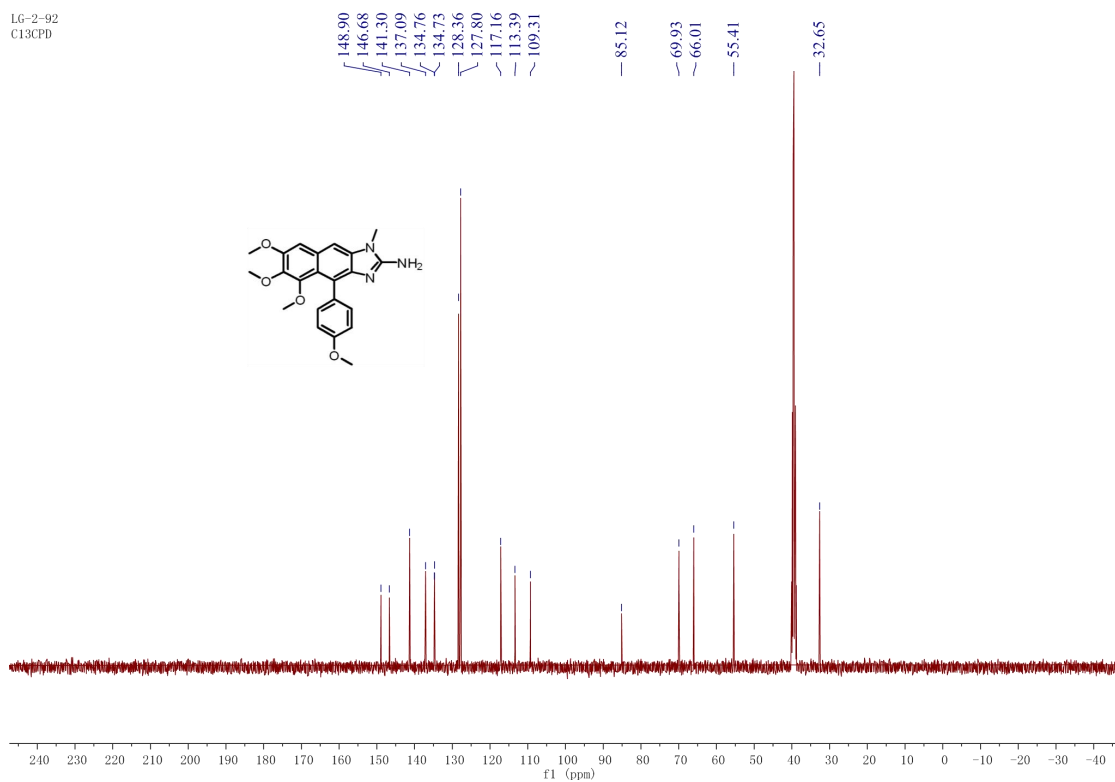
LG-2-78  
C13CPD



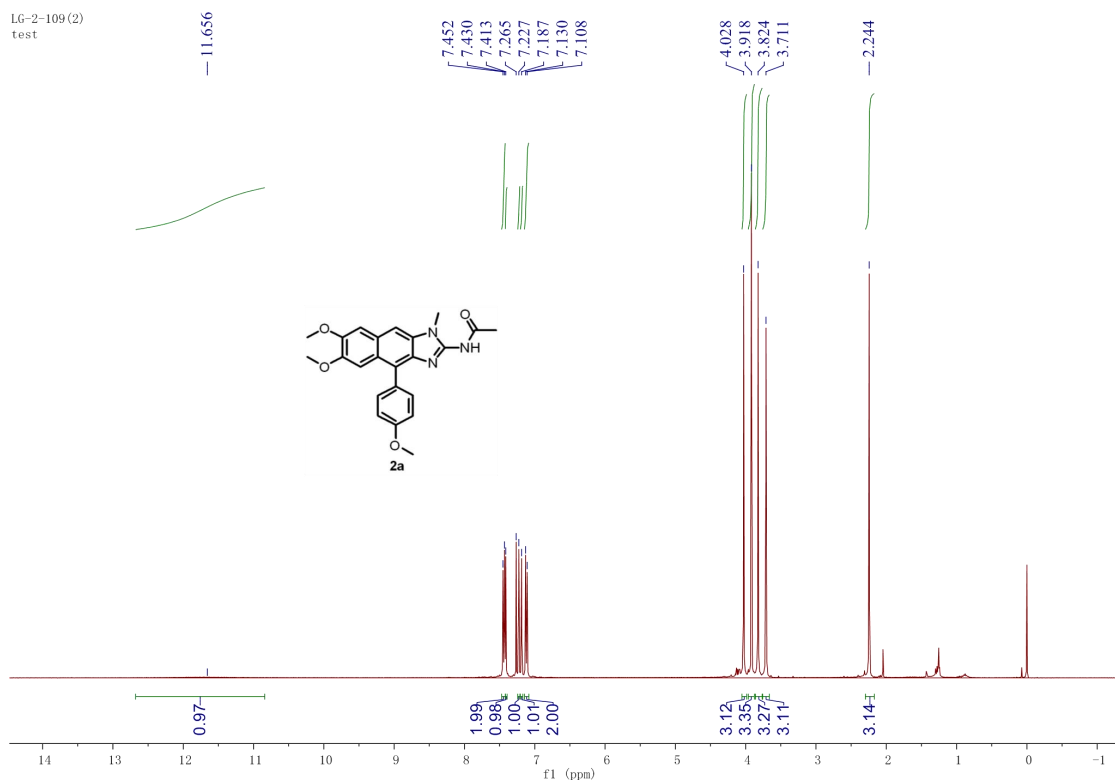
LG-2-92  
PROTON



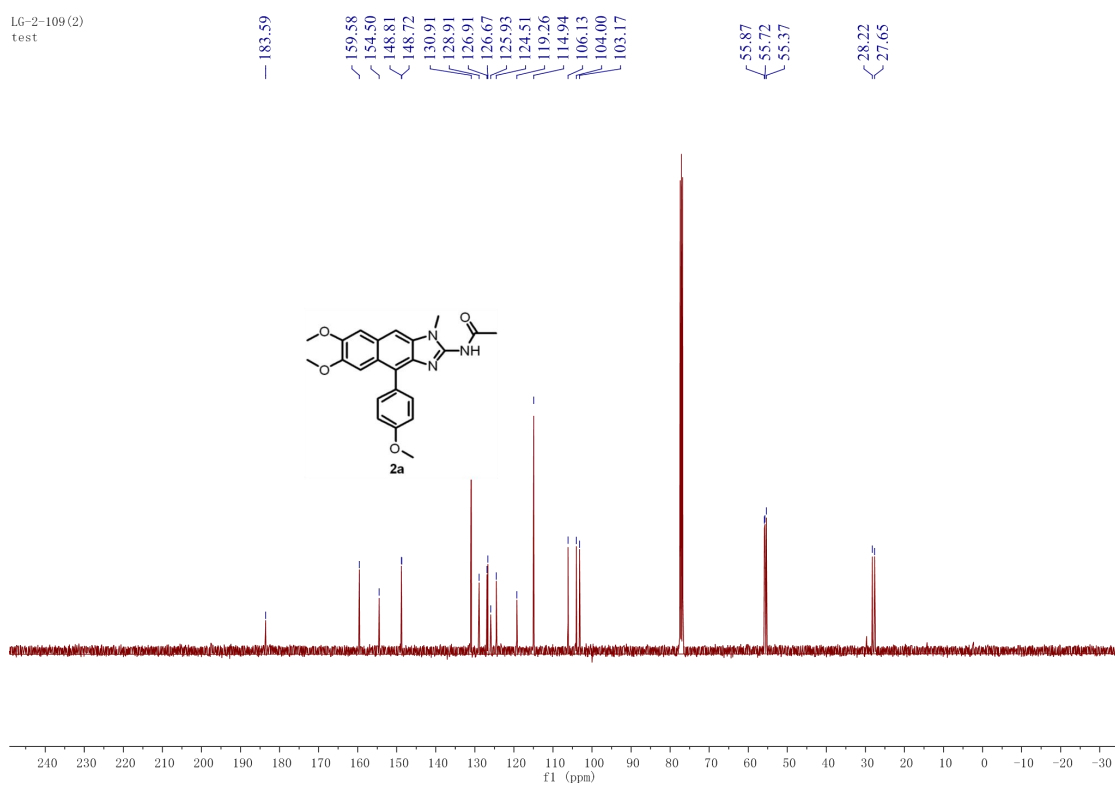
LG-2-92  
C13CPD



LG-2-109 (2)  
test

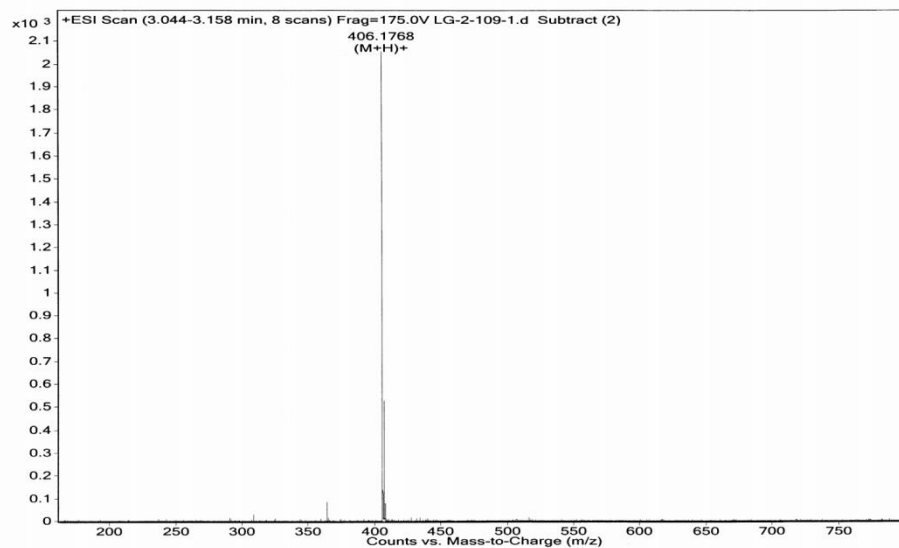


LG-2-109 (2)  
test

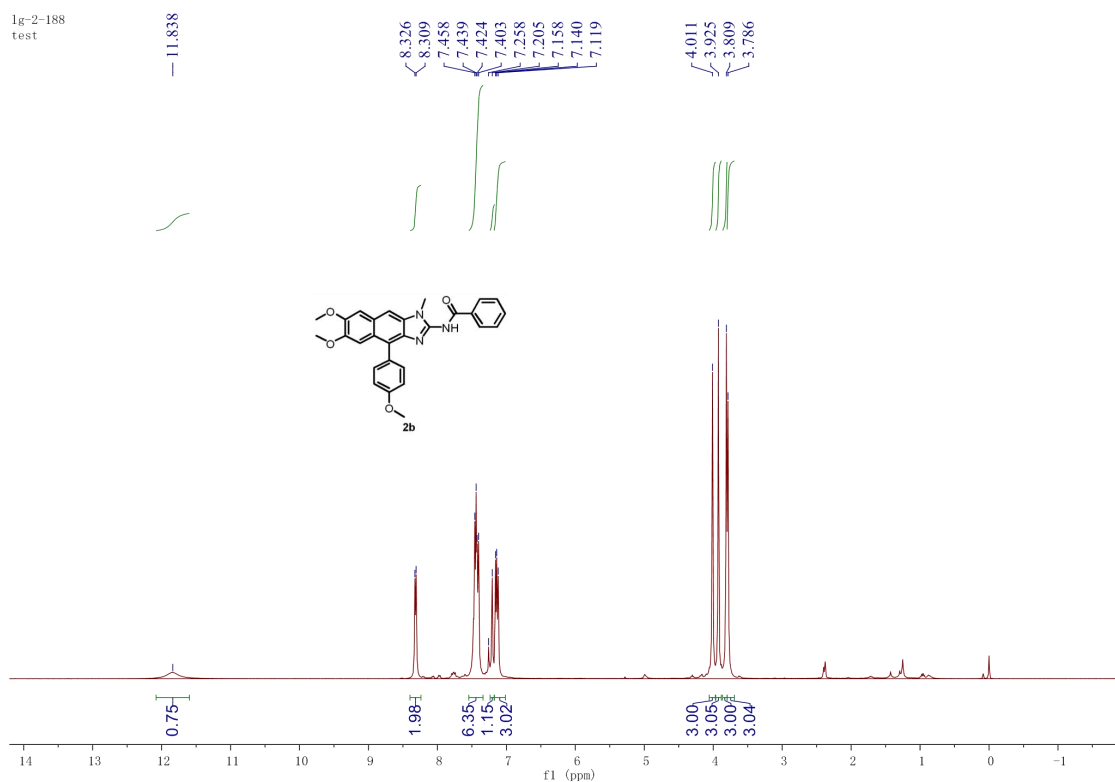




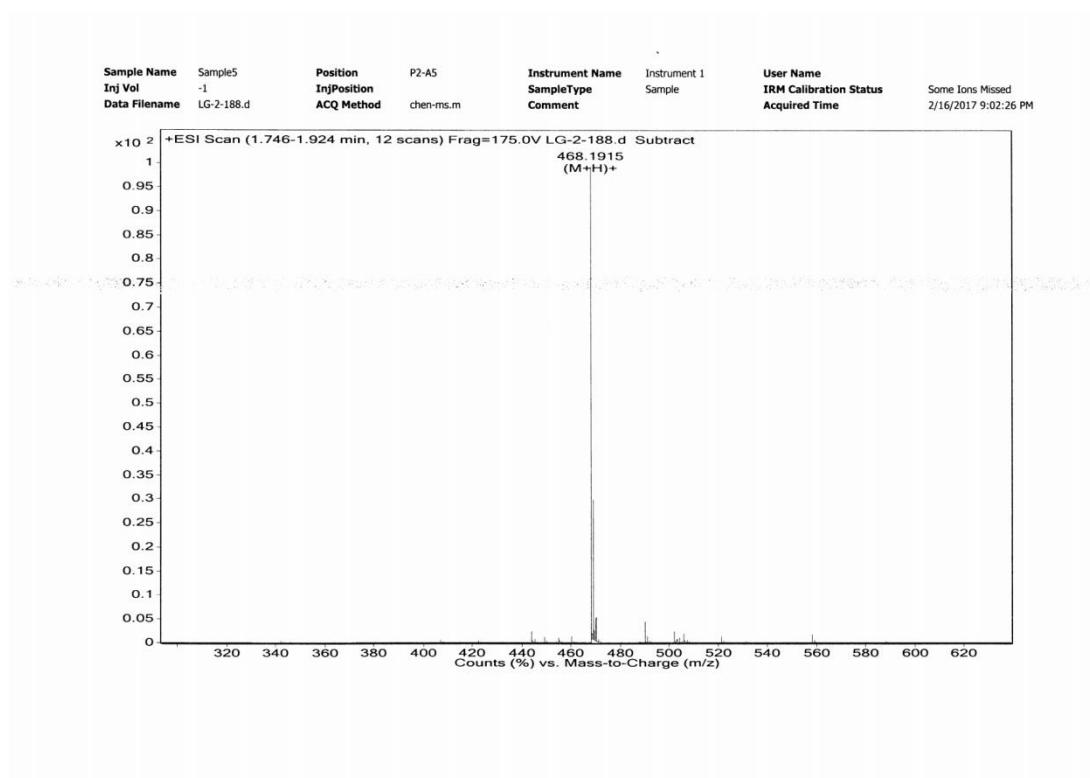
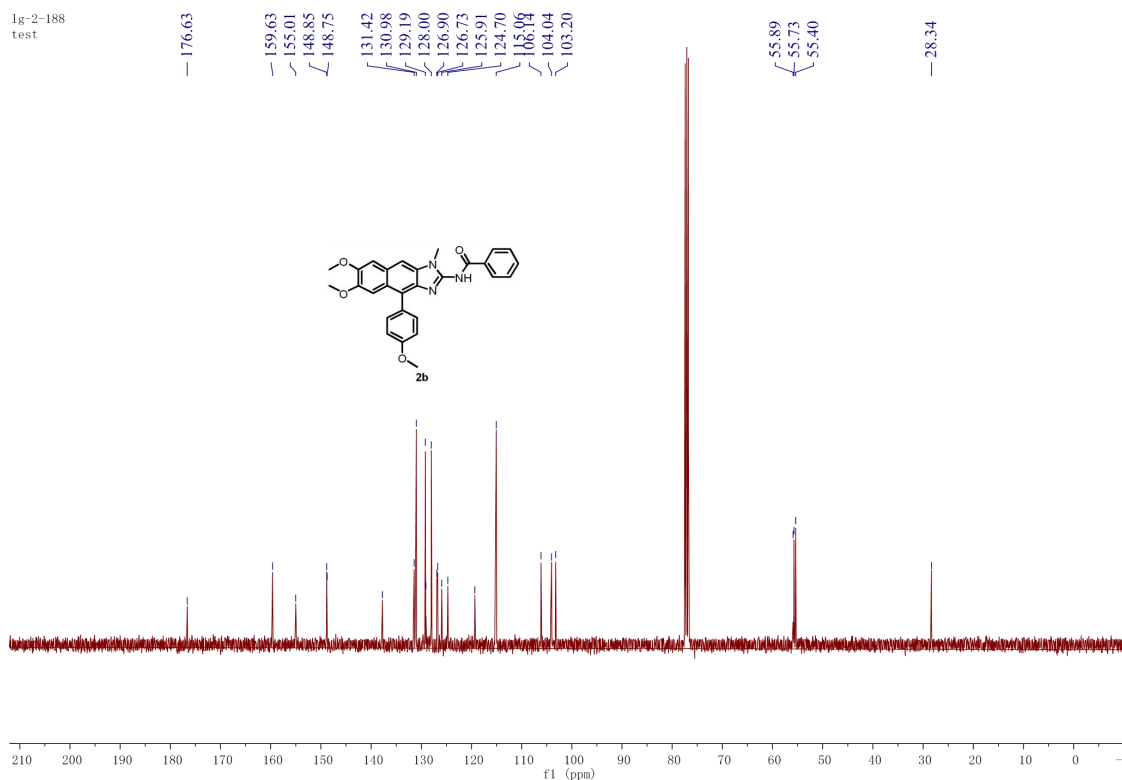
Sample Name	Sample37	Position	P2-E1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	LG-2-109-1.d	ACQ Method	chen-ms.m	Comment		Acquired Time	9/14/2016 7:46:05 AM



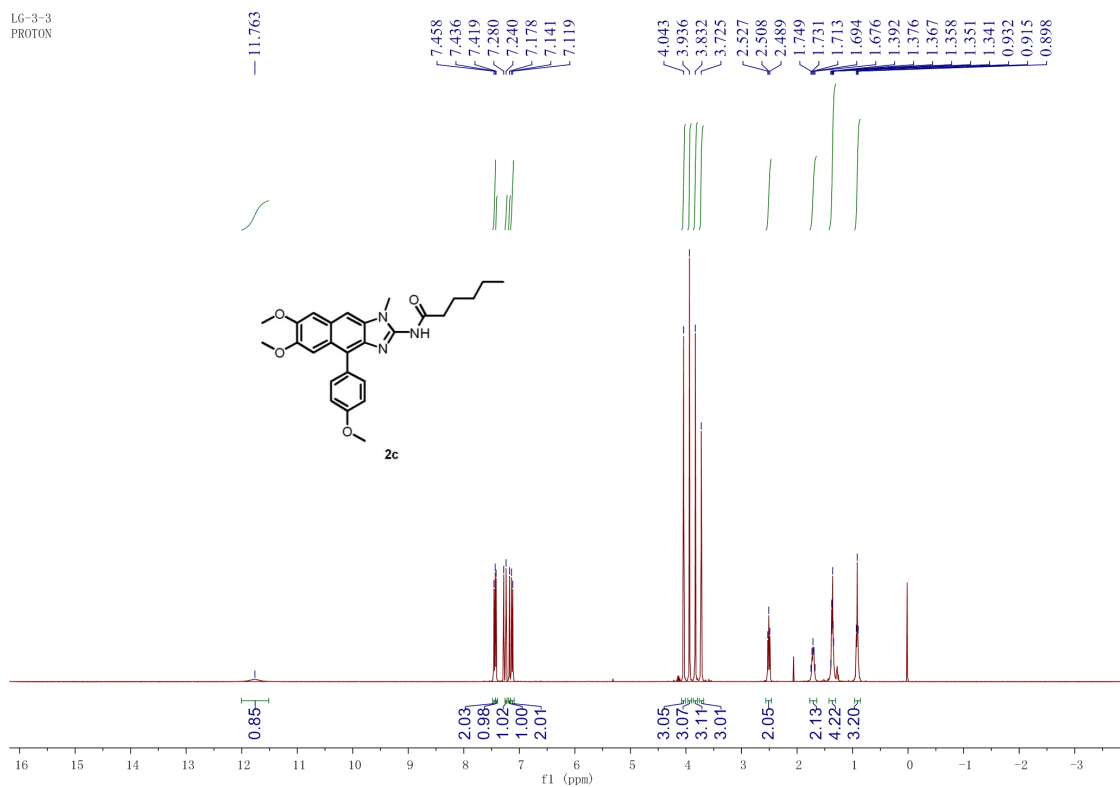
lg-2-188  
test



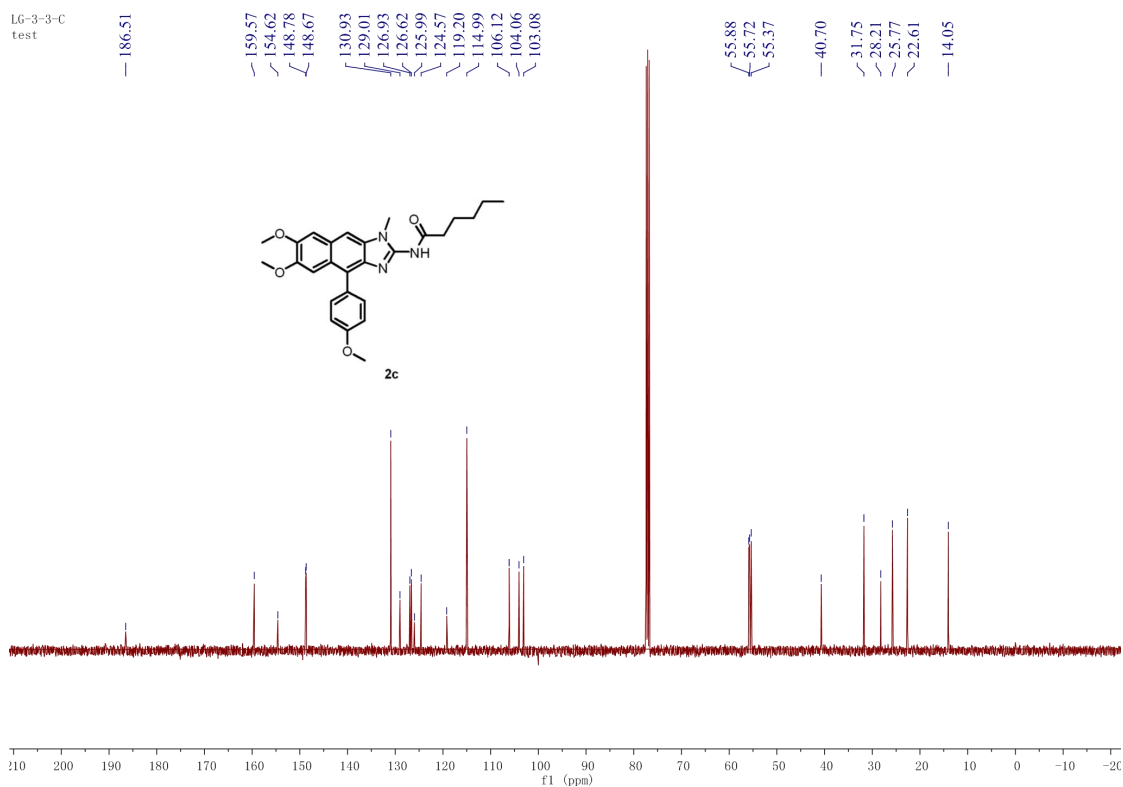
lg-2-188  
test



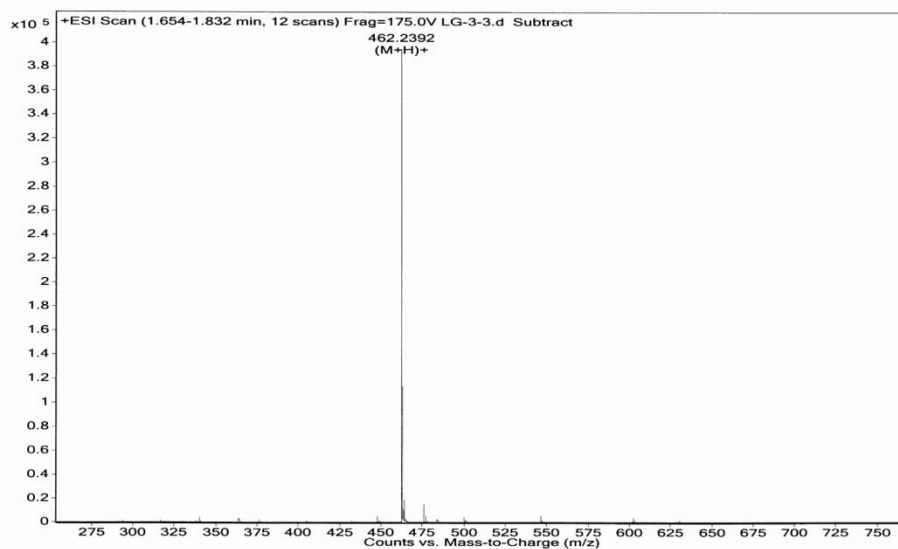
LG-3-3  
PROTON



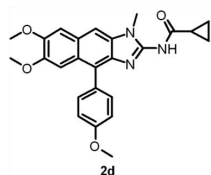
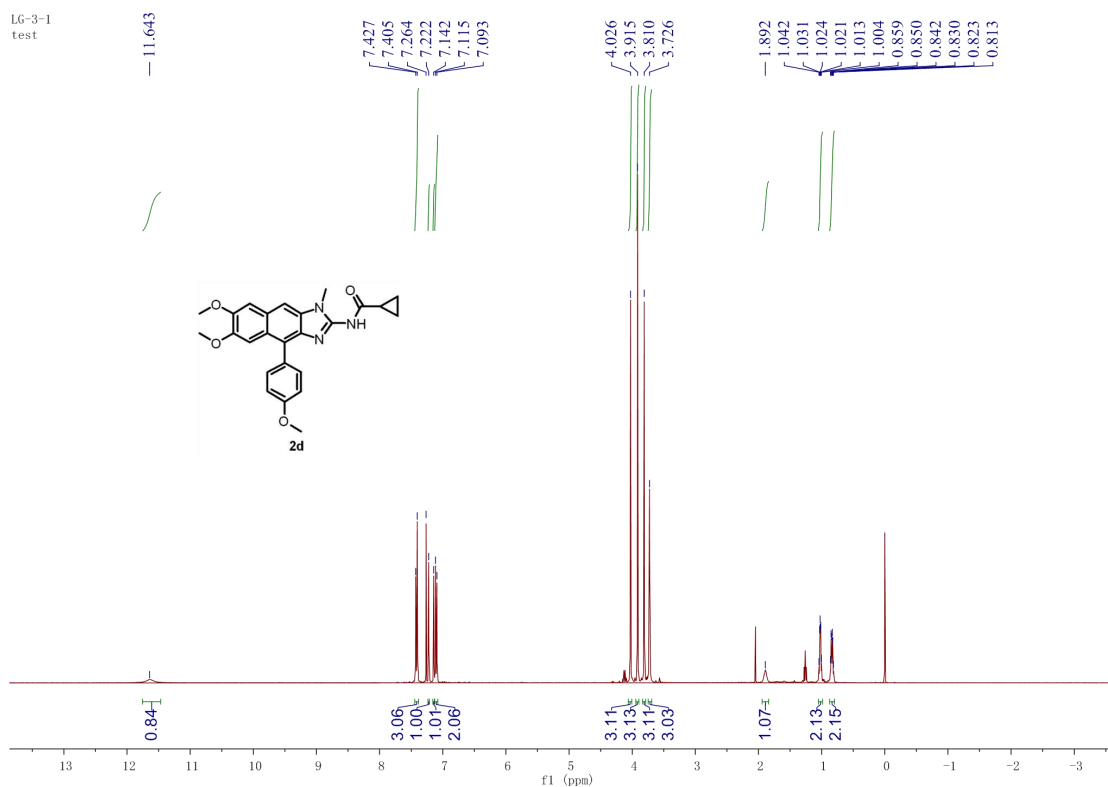
LG-3-3-C  
test



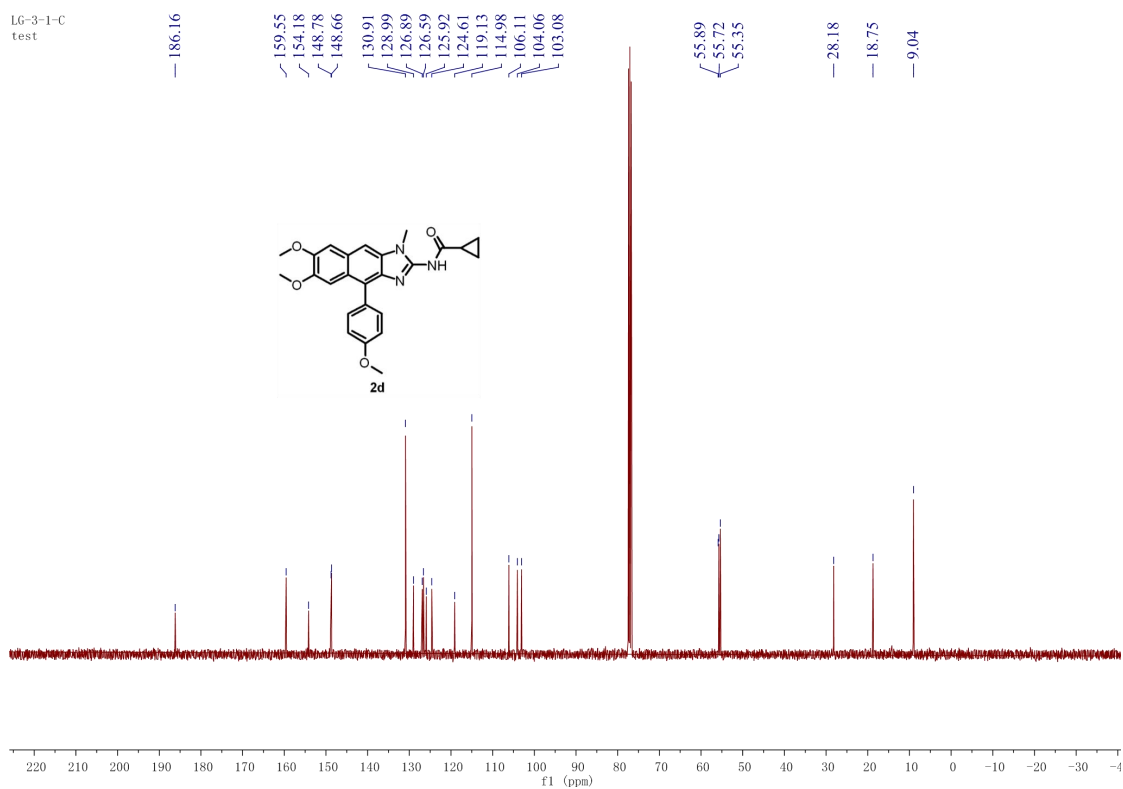
Sample Name	Sample13	Position	P1-B4	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	LG-3-3.d	ACQ Method	chen-ms.m	Comment		Acquired Time	11/16/2016 5:54:29 PM



LG-3-1  
test

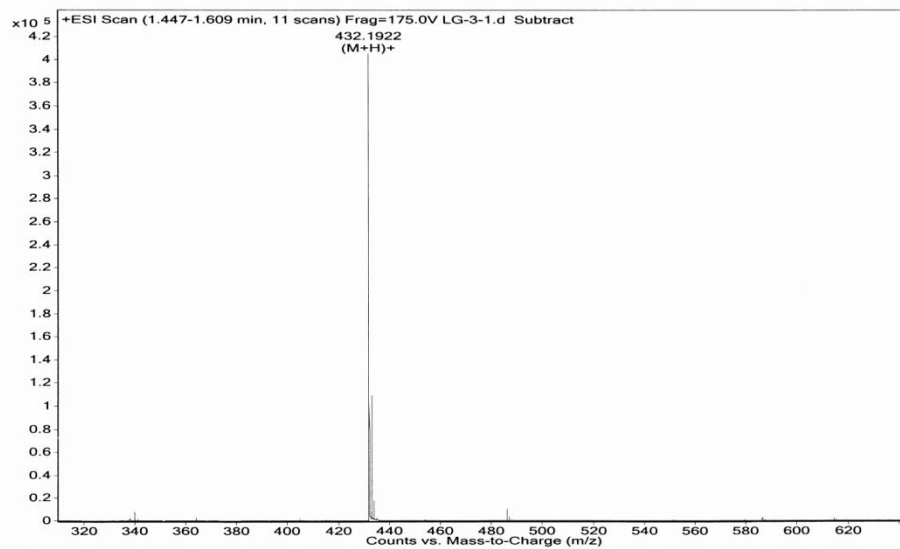


LG-3-1-C  
test

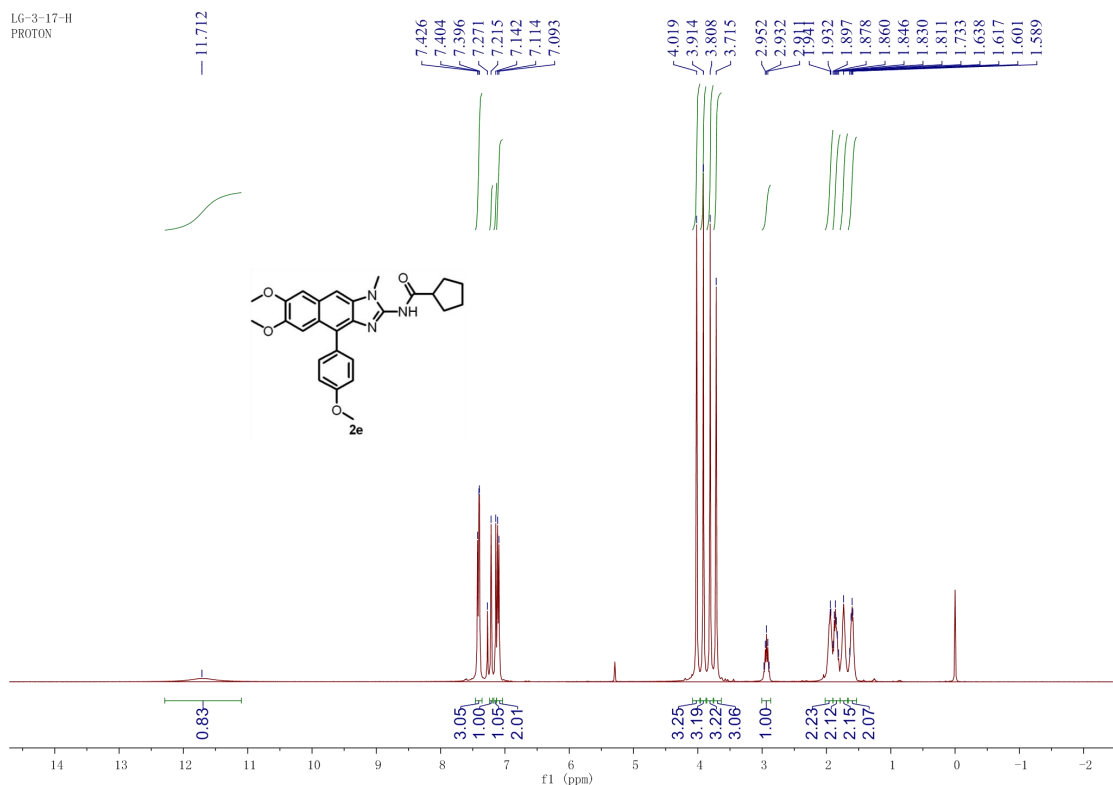


Sample Name	Sample12	Position	P1-B3	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	LG-3-1.d	ACQ Method	chen-ms.m	Comment		Acquired Time

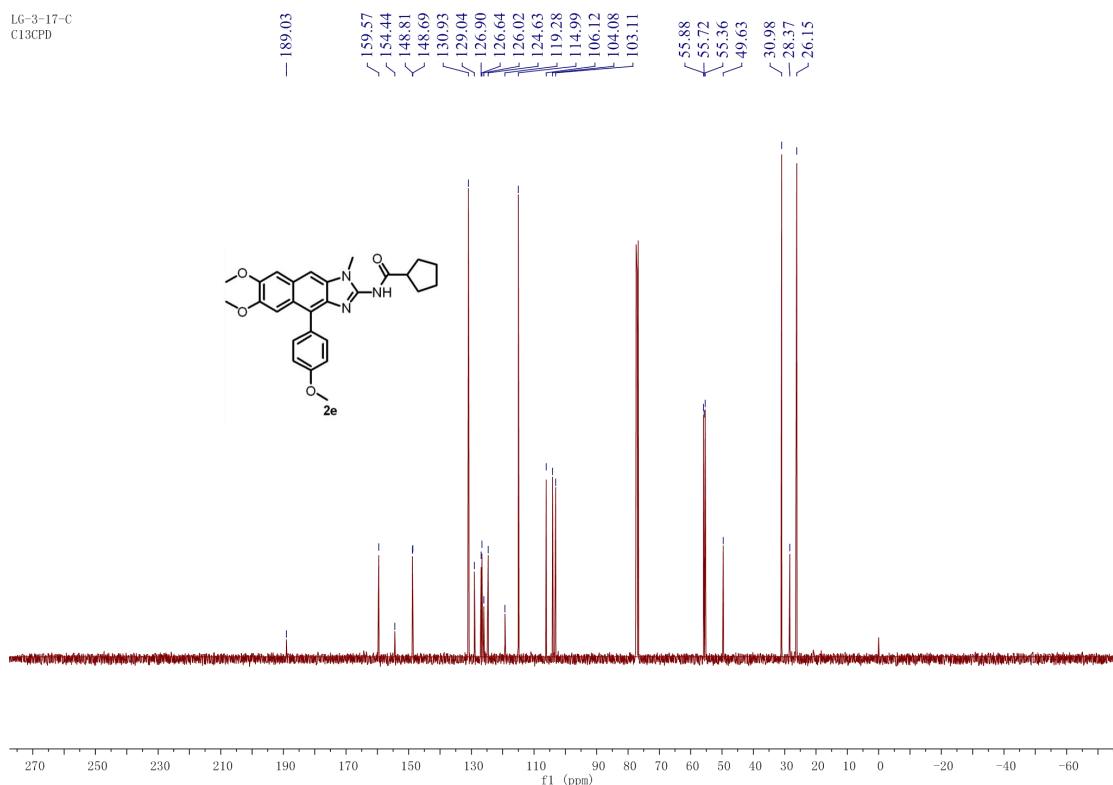
Some Ions Missed  
11/16/2016 5:48:47 PM



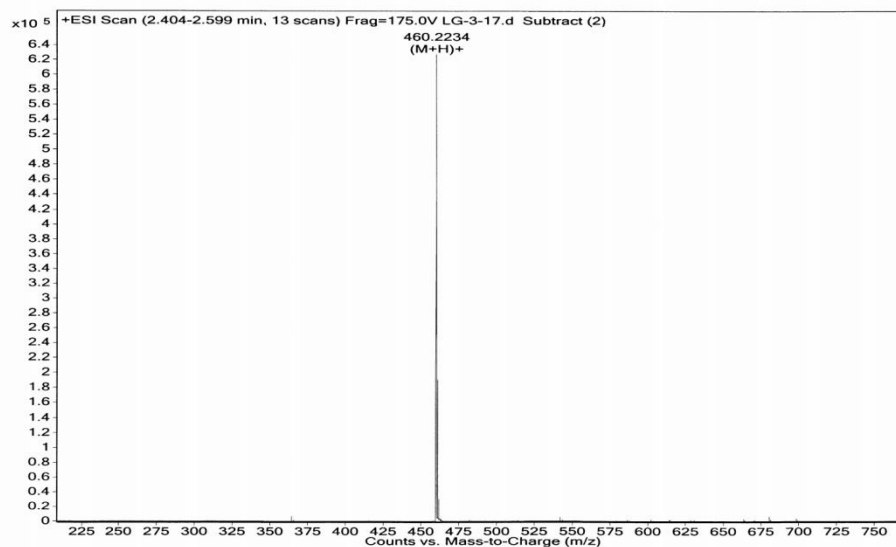
LG-3-17-H  
PROTON



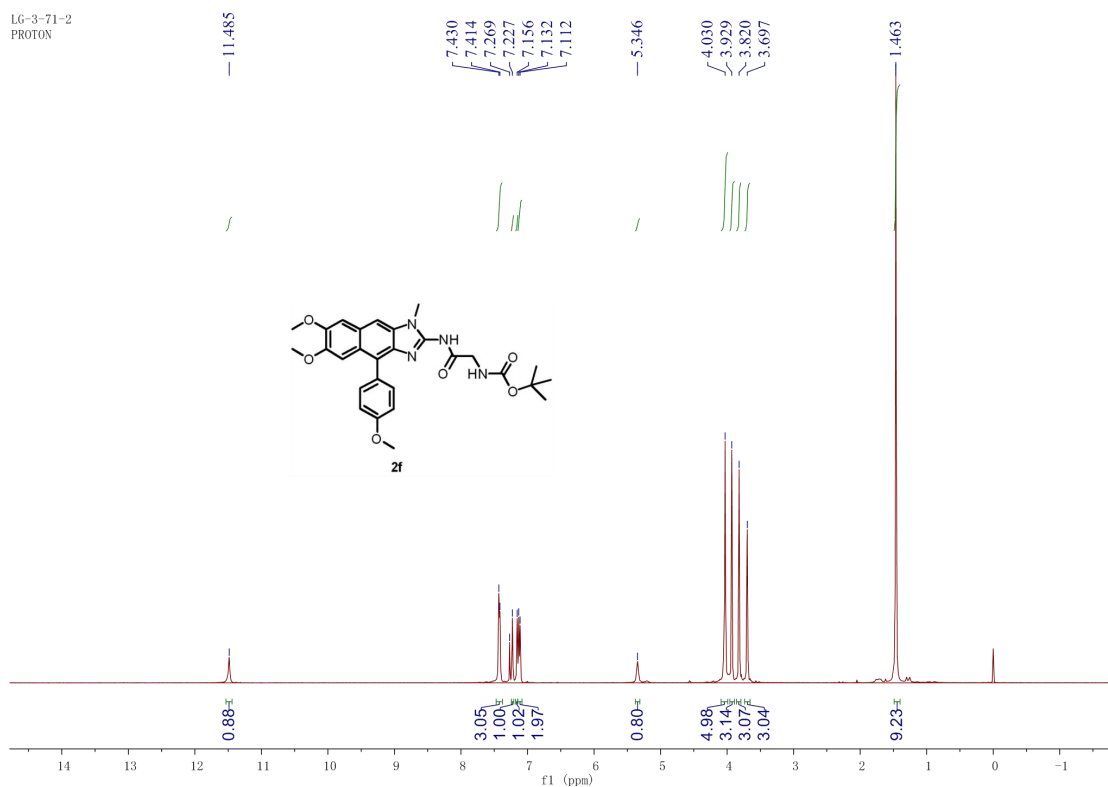
LG-3-17-C  
C13CPD



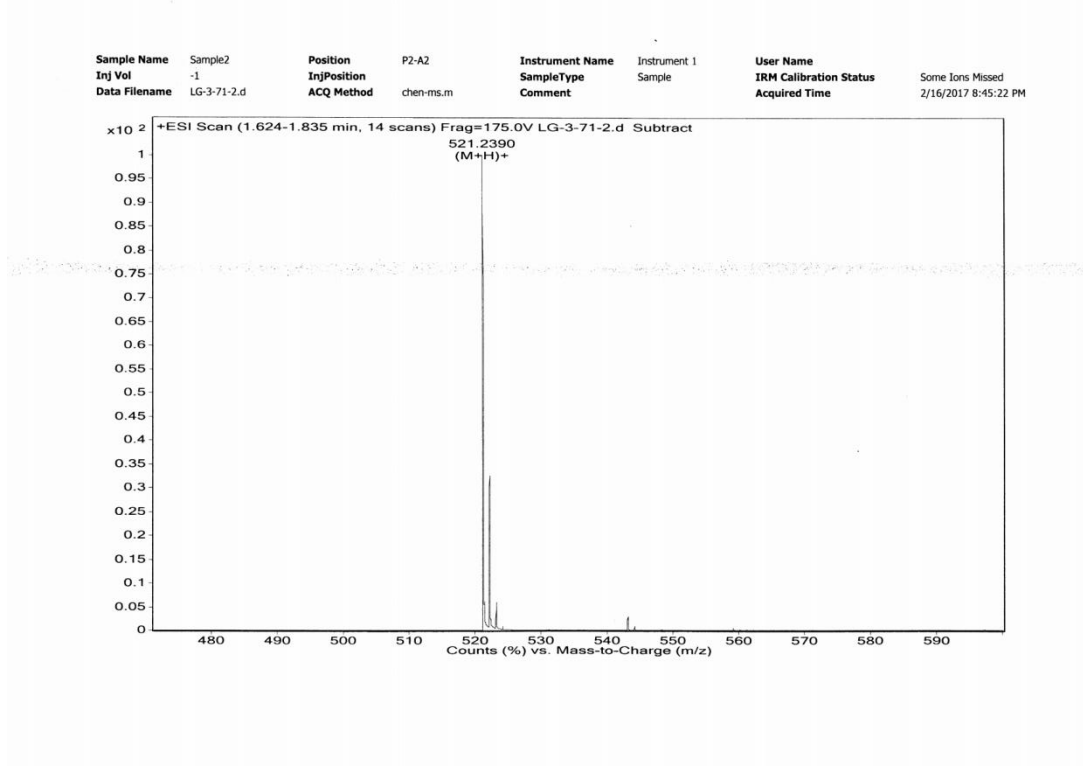
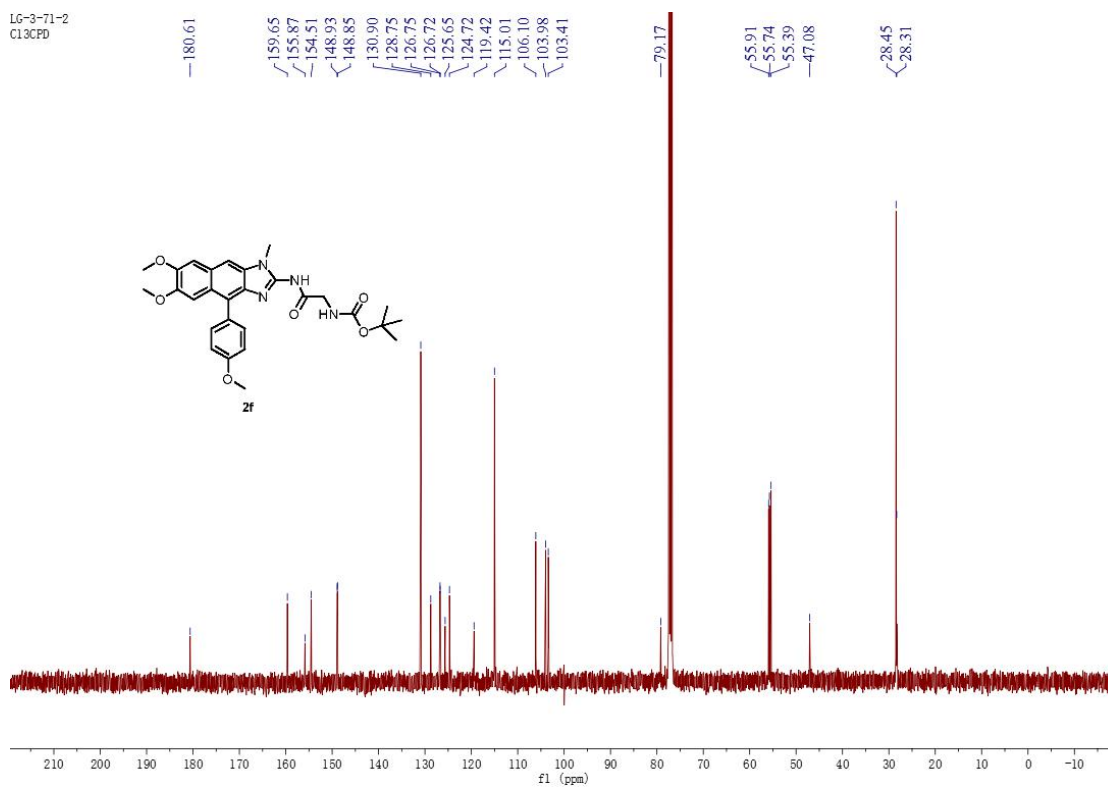
Sample Name	Sample16	Position	P1-B7	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	LG-3-17.d	ACQ Method	chen-ms.m	Comment		Acquired Time	11/16/2016 6:11:33 PM



LG-3-71-2  
PROTON

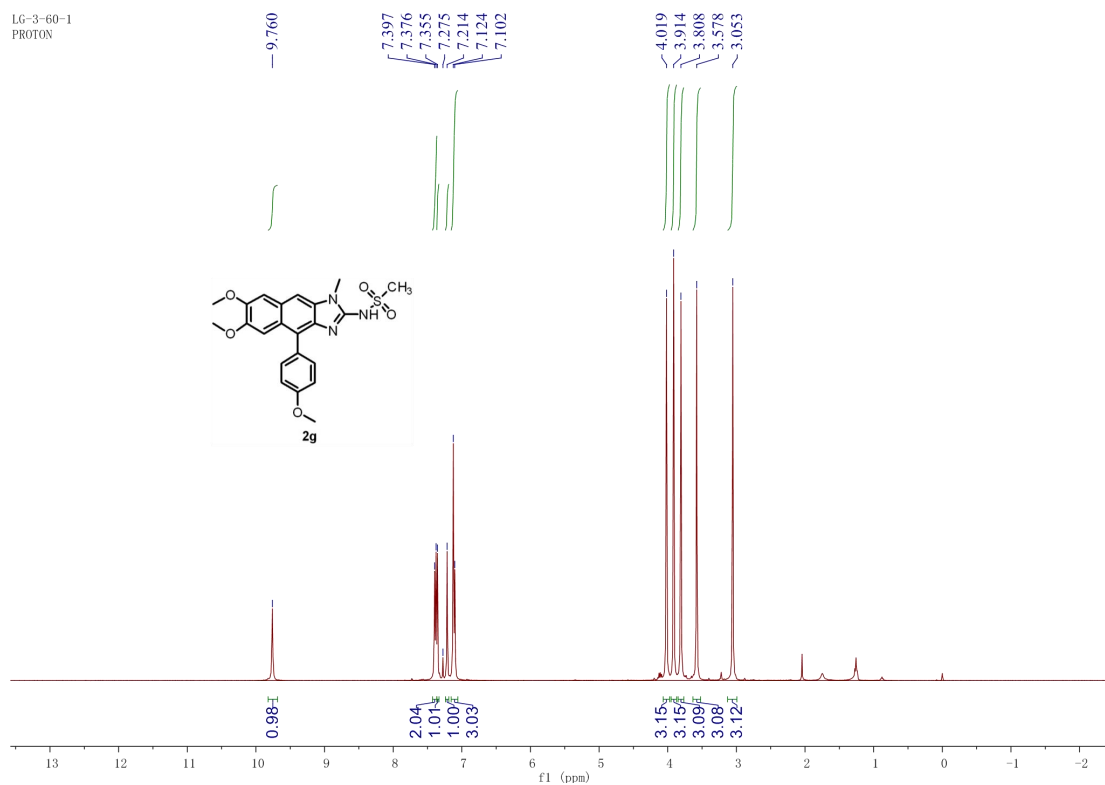


LG-3-71-2  
C13CPD

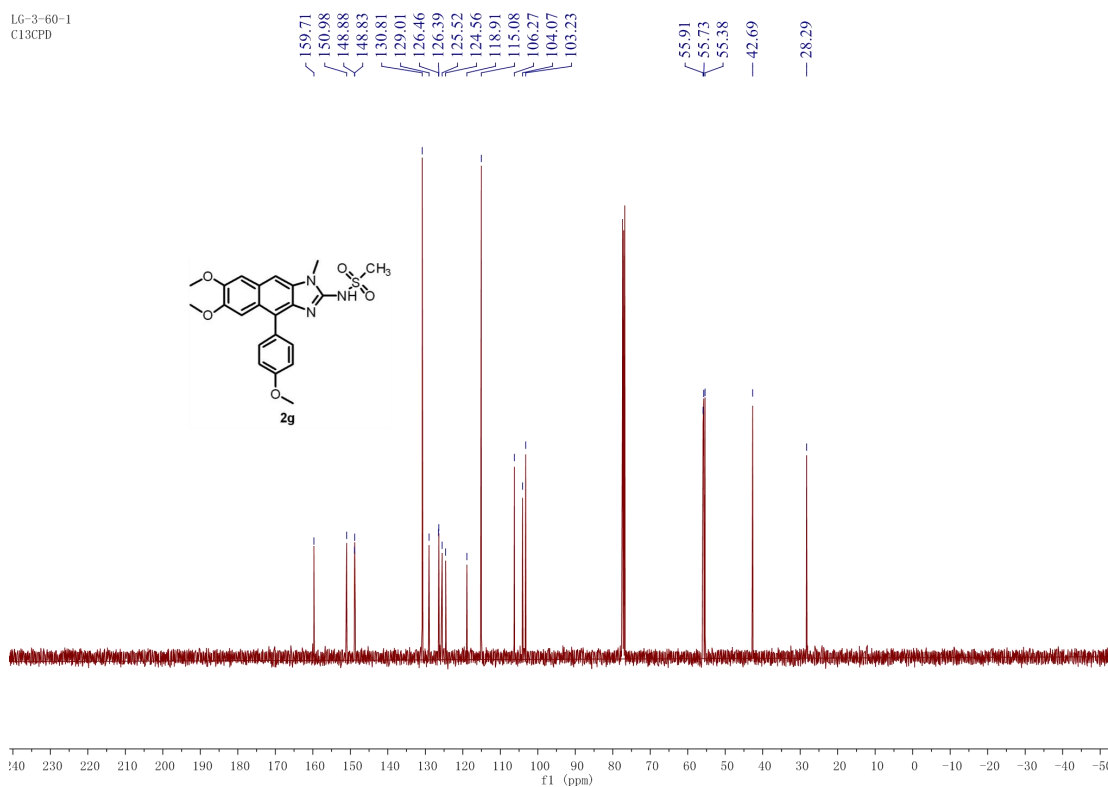




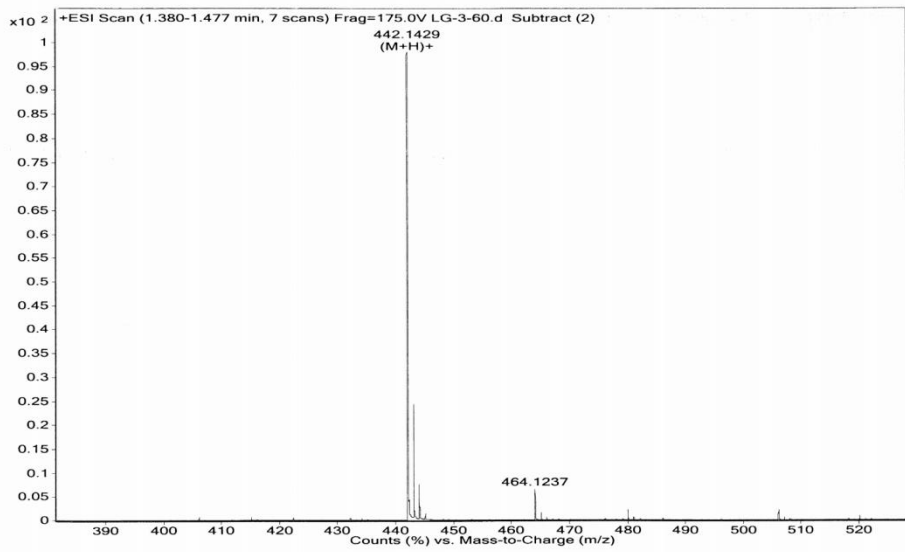
LG-3-60-1  
PROTON



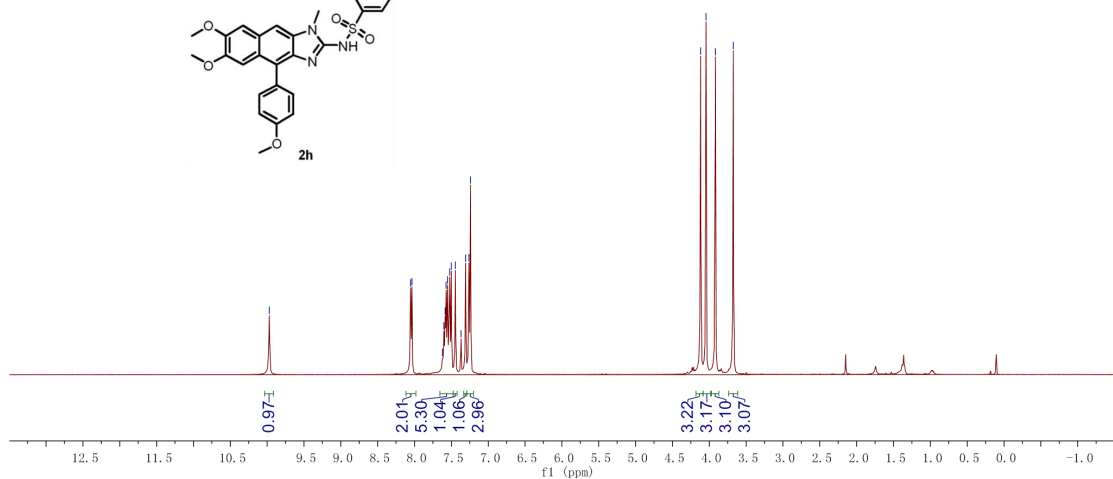
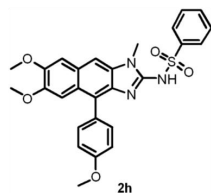
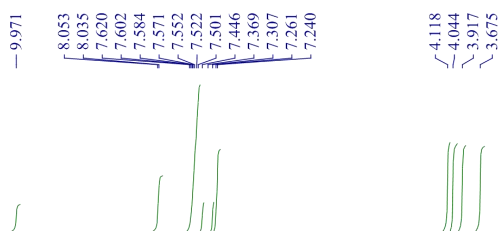
LG-3-60-1  
C13CPD



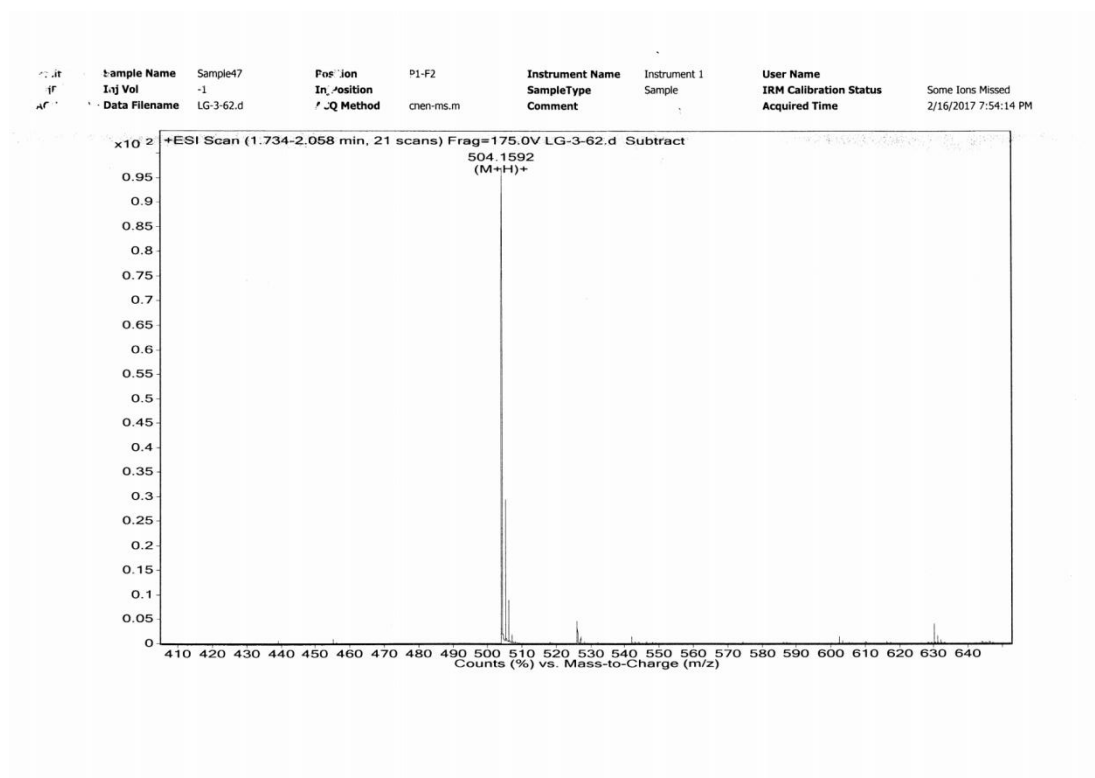
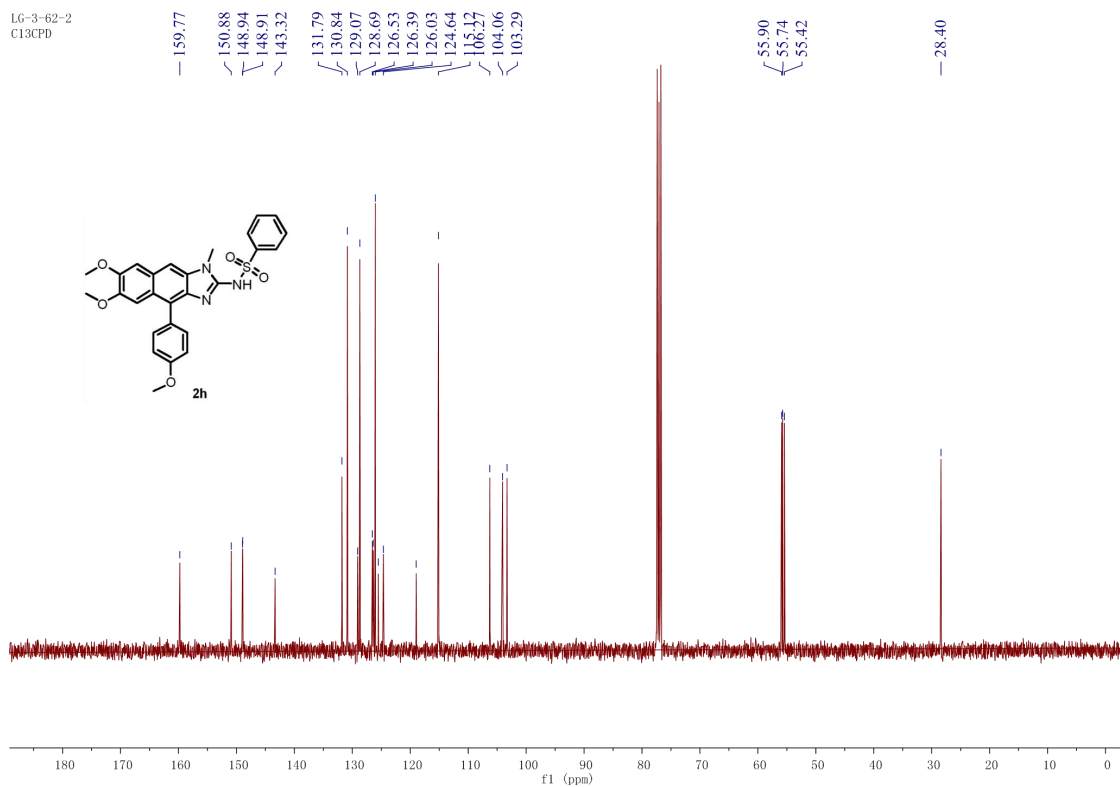
Sample Name	Position	Instrument Name	User Name
Sample46	P1-F1-	Instrument 1	
Inj Vol	InjPosition	SampleType	Calibration Status
-1		Sample	
Data File	ACQ Method	Comment	Acquired Time
LG-3-60.d	chen-ms.f1		2/16/2017 7:48:34 PM



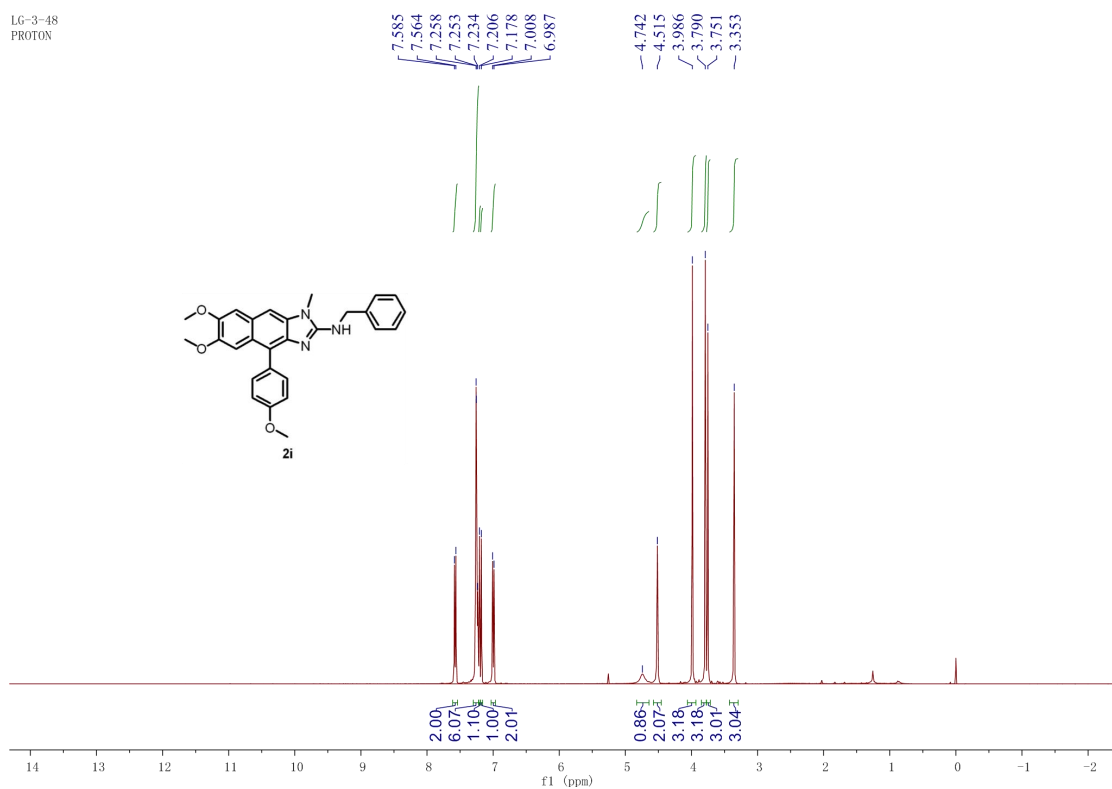
LG-3-62-2  
PROTON



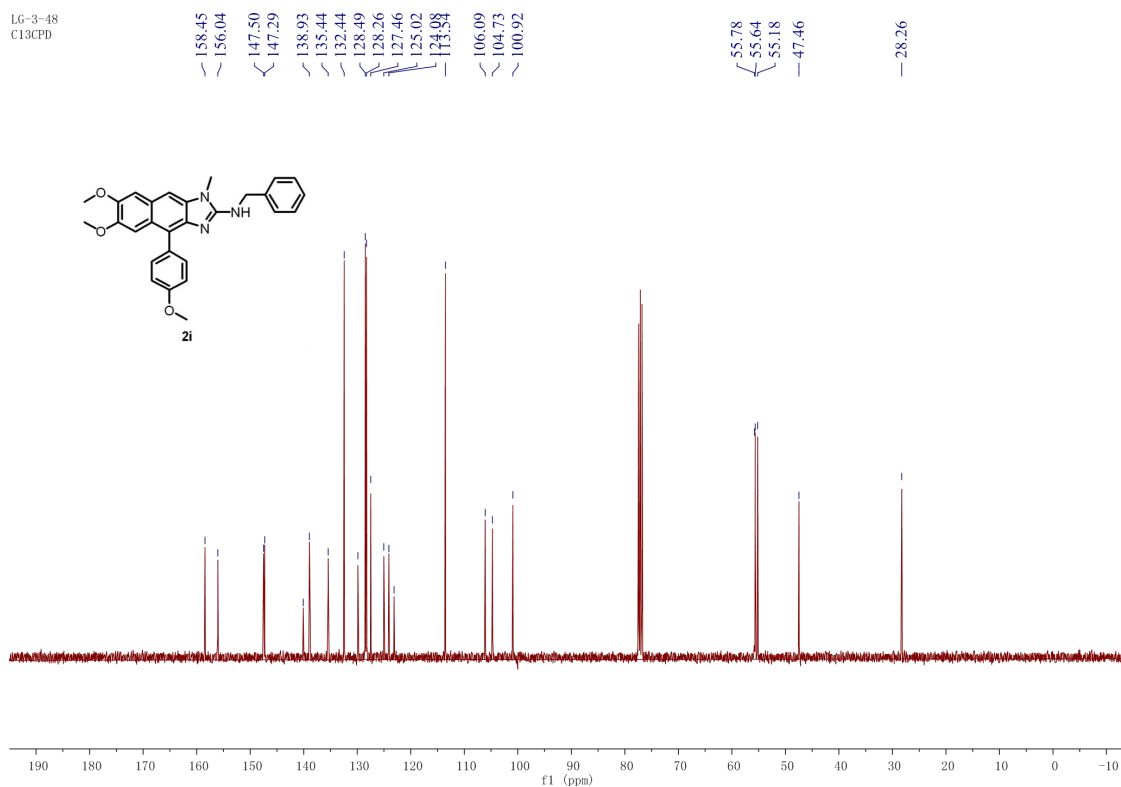
LG-3-62-2  
C13CPD



LG-3-48  
PROTON

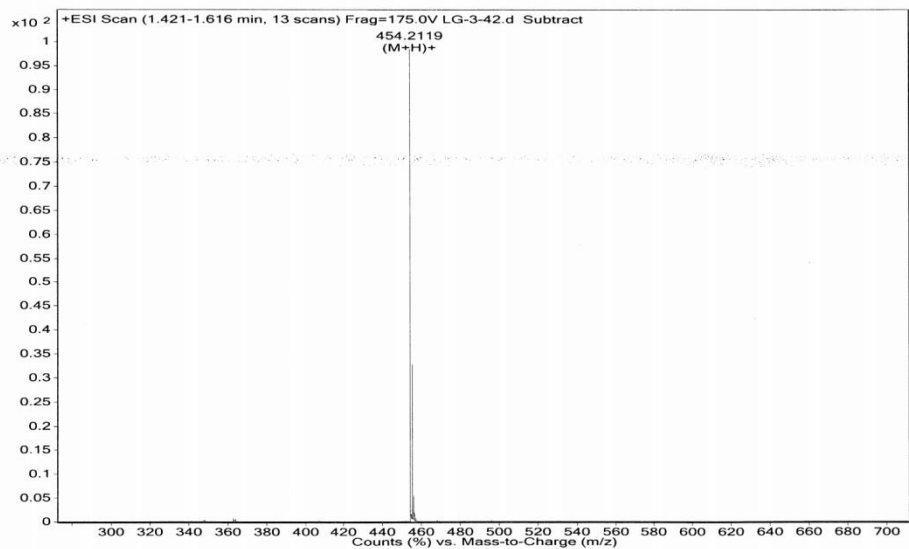


LG-3-48  
C13CPD

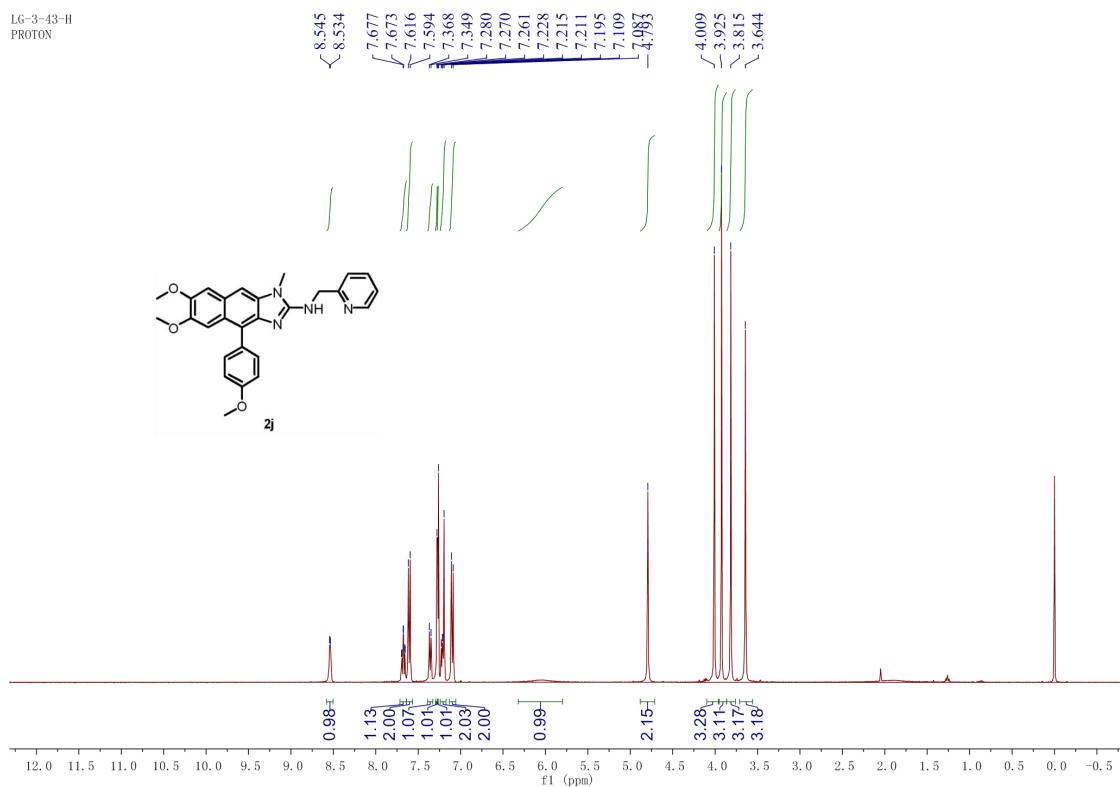


Sample Name	Sample53	Position	P1-F8	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	LG-3-42.d	ACQ Method	chen-ms.m	Comment		Acquired Time

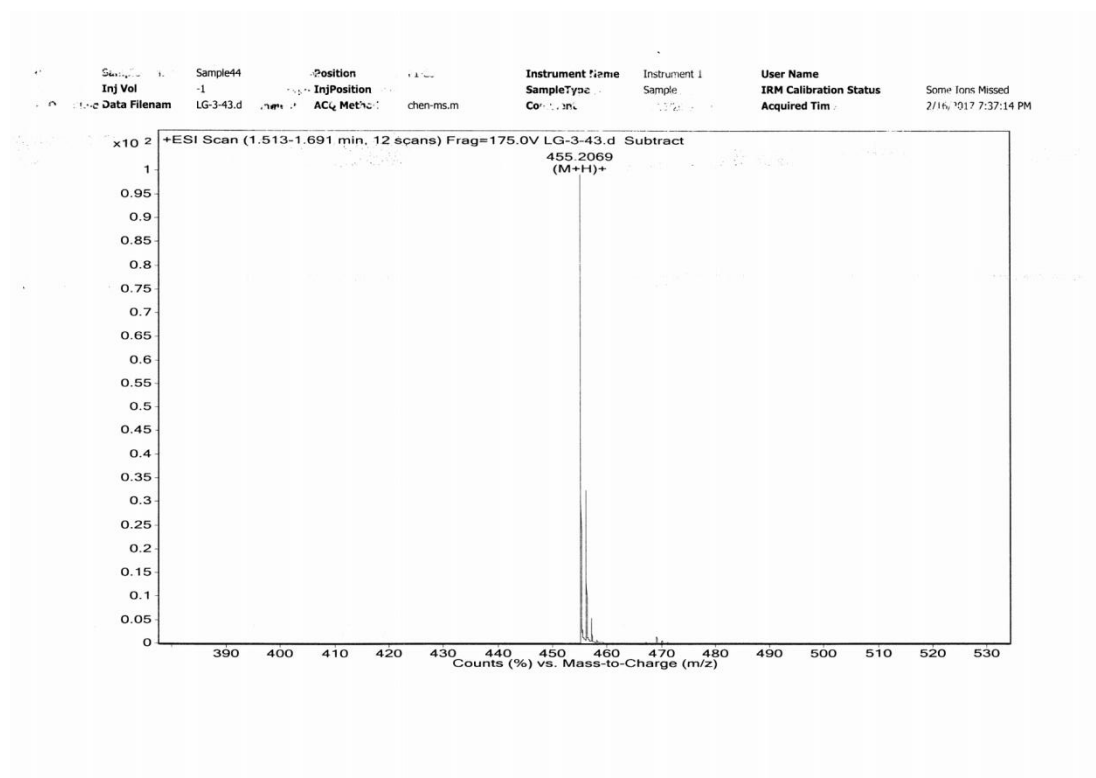
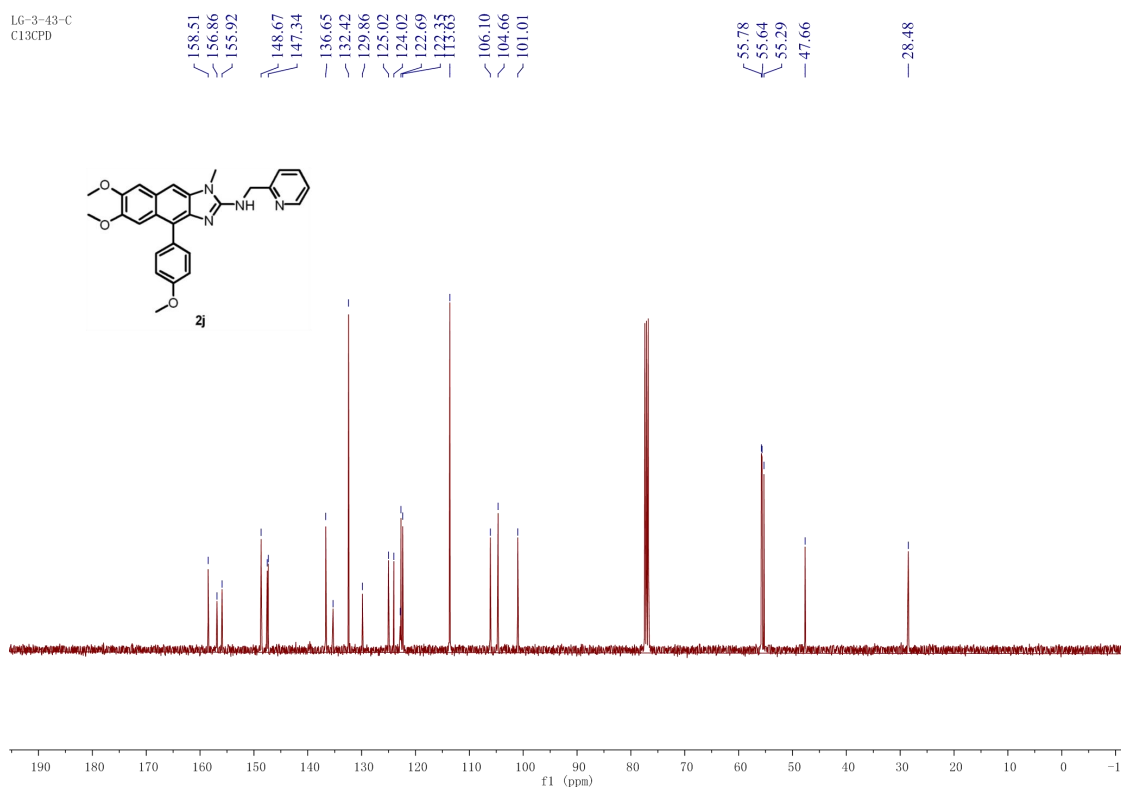
Some Ions Missed  
2/16/2017 8:28:18 PM



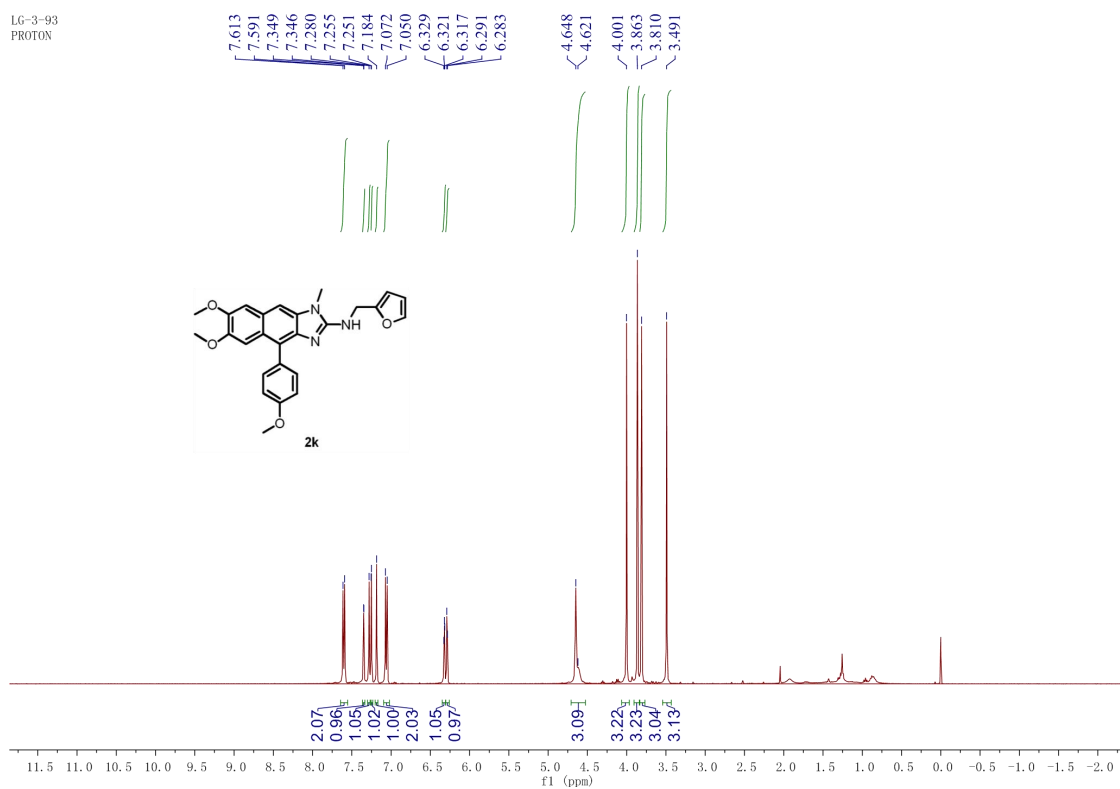
LG-3-43-H  
PROTON



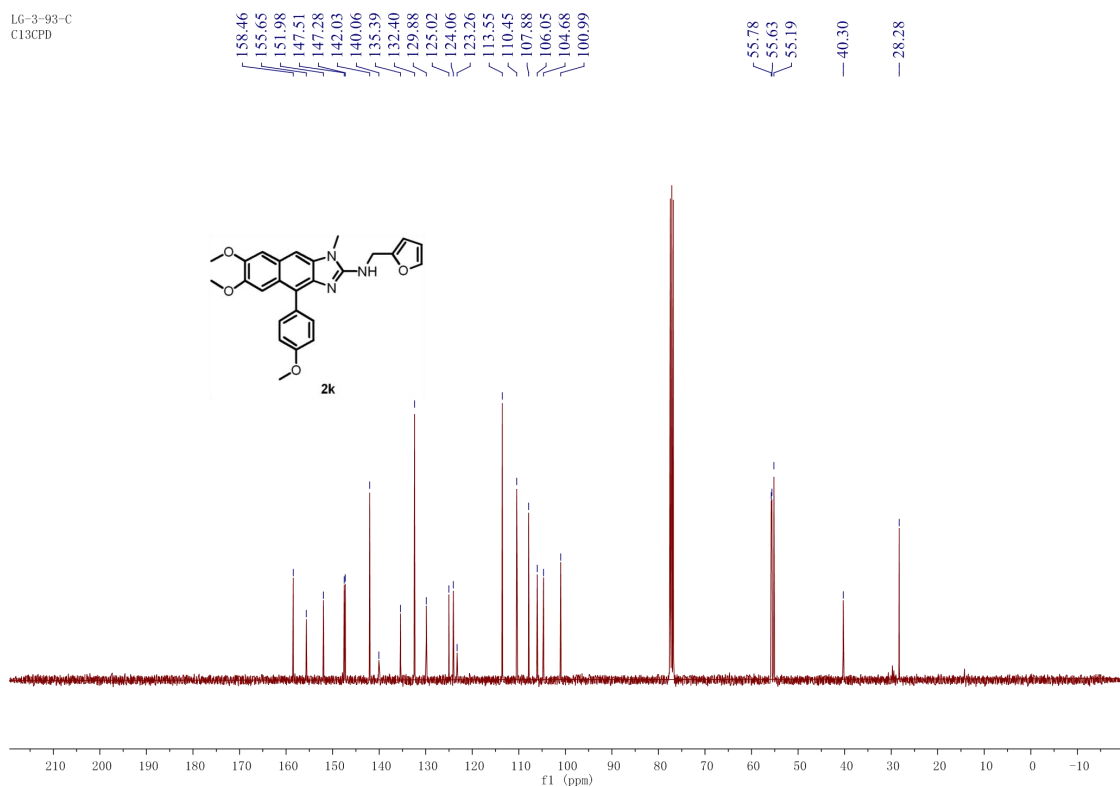
LG-3-43-C  
C13CPD



LG-3-93  
PROTON



LG-3-93-C  
C13CPD

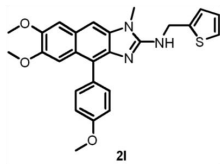


+ESI Scan (1.580-1.727 min, 10 scans) Frag=175.0V LG-3-93.d Subtract

444.1913  
(M+H)<sup>+</sup>

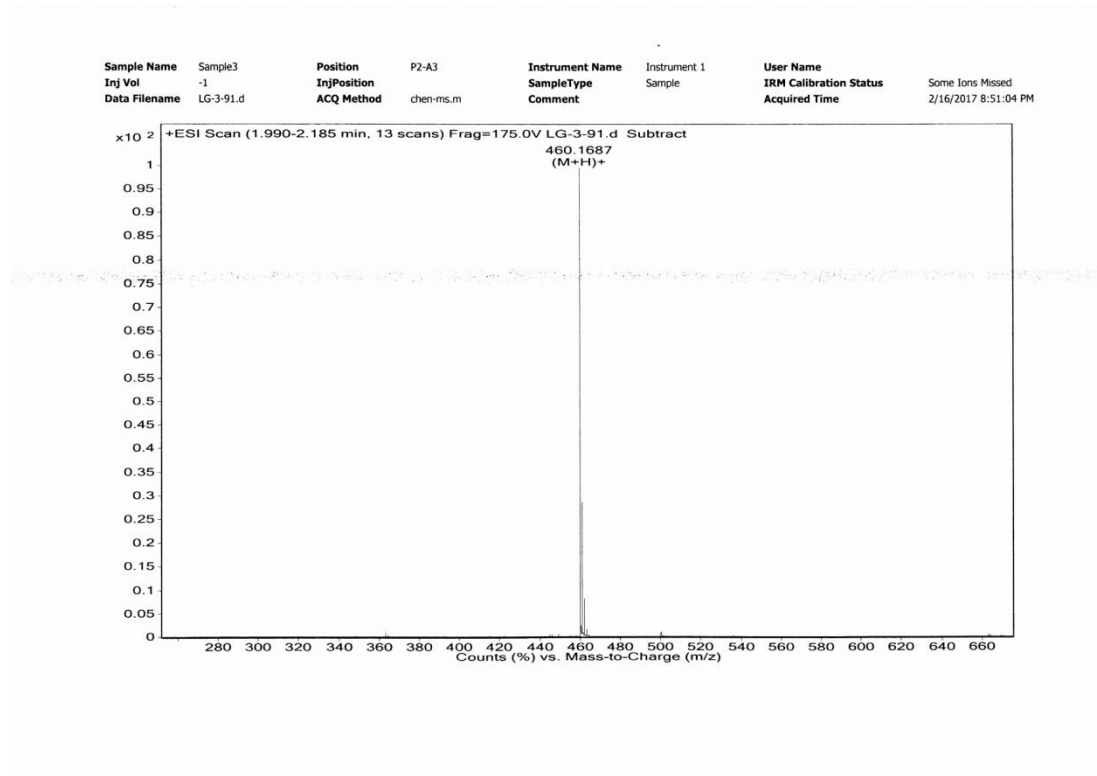
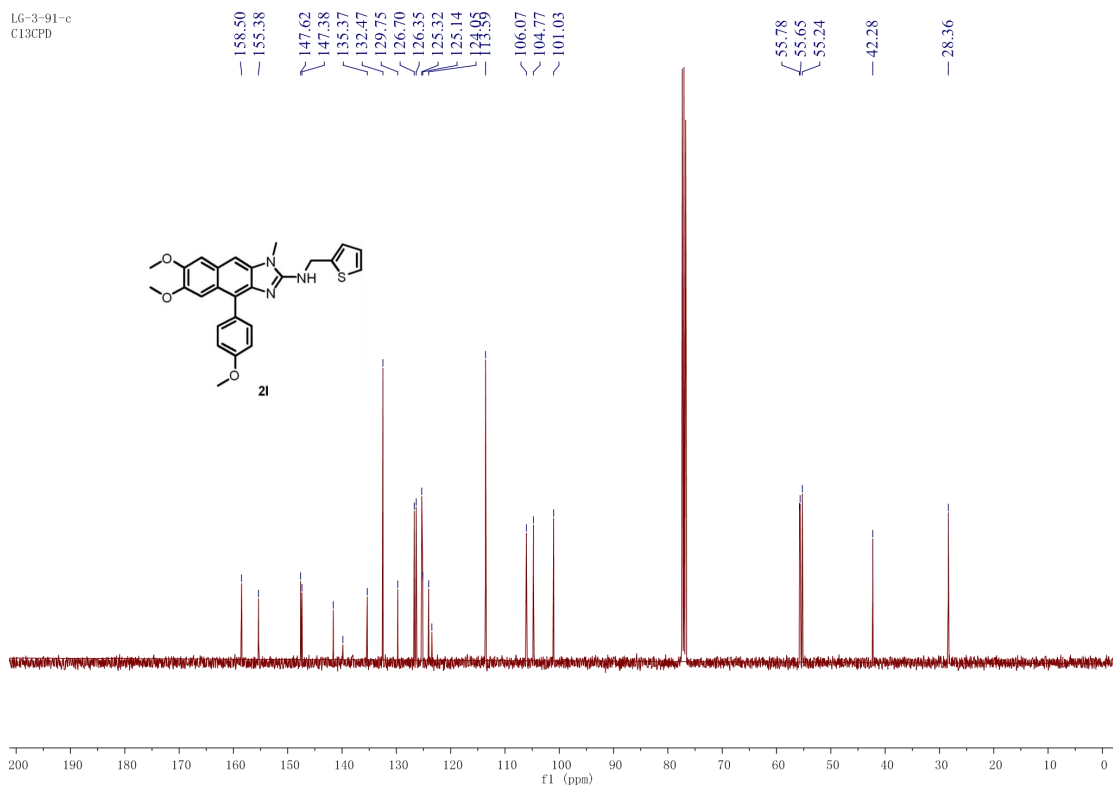
Counts (%) vs. Mass-to-Charge (m/z)

7.645  
7.623  
7.308  
7.261  
7.255  
7.229  
7.217  
7.191  
7.072  
7.050  
7.018  
7.011  
6.955  
6.946  
6.943  
6.934

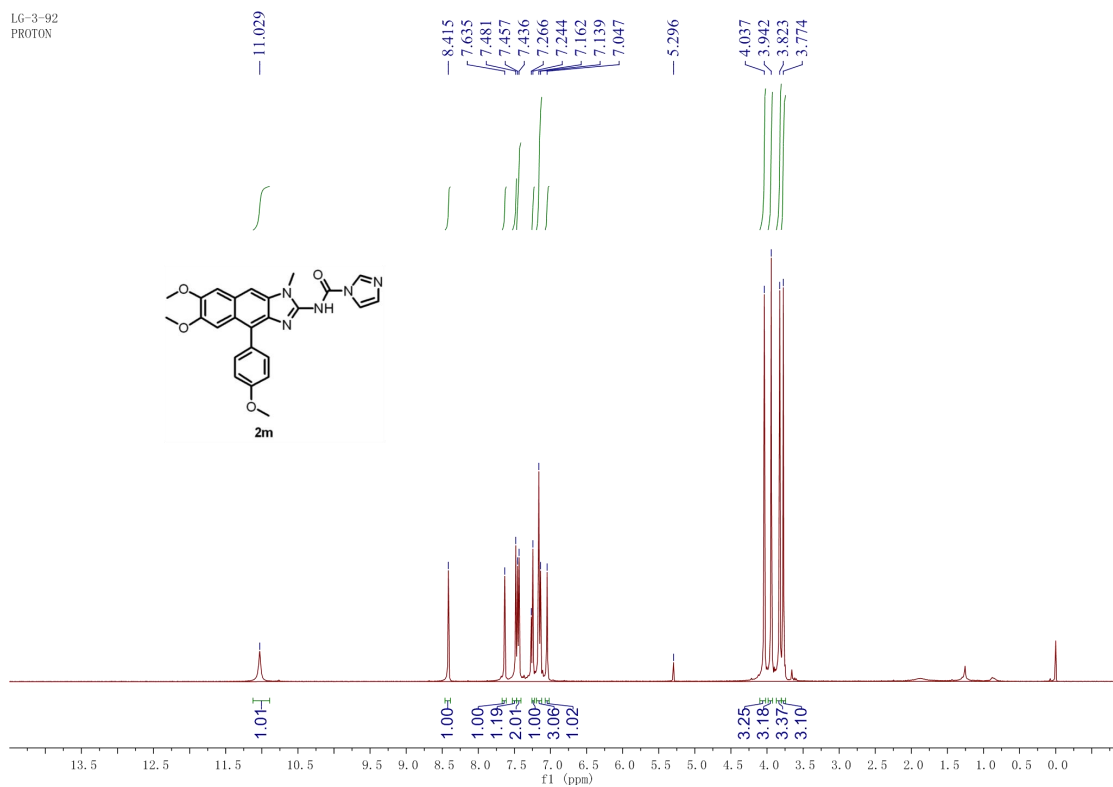




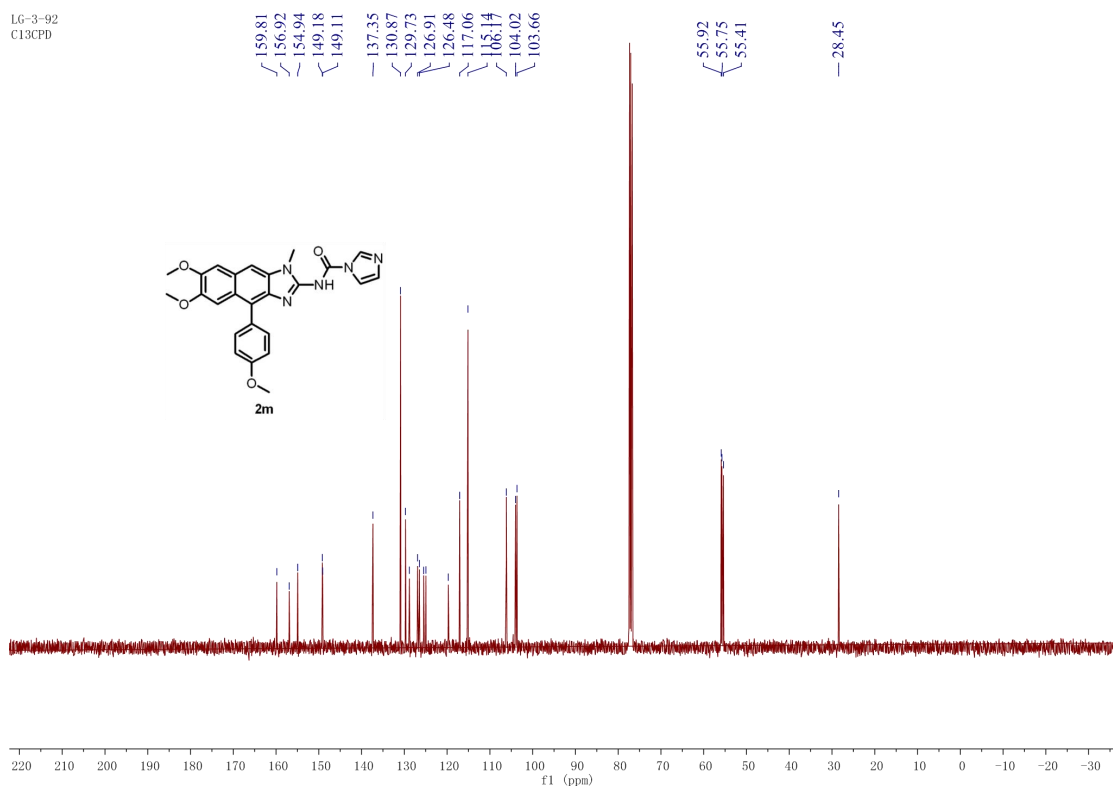
LG-3-91-c  
C13CPD



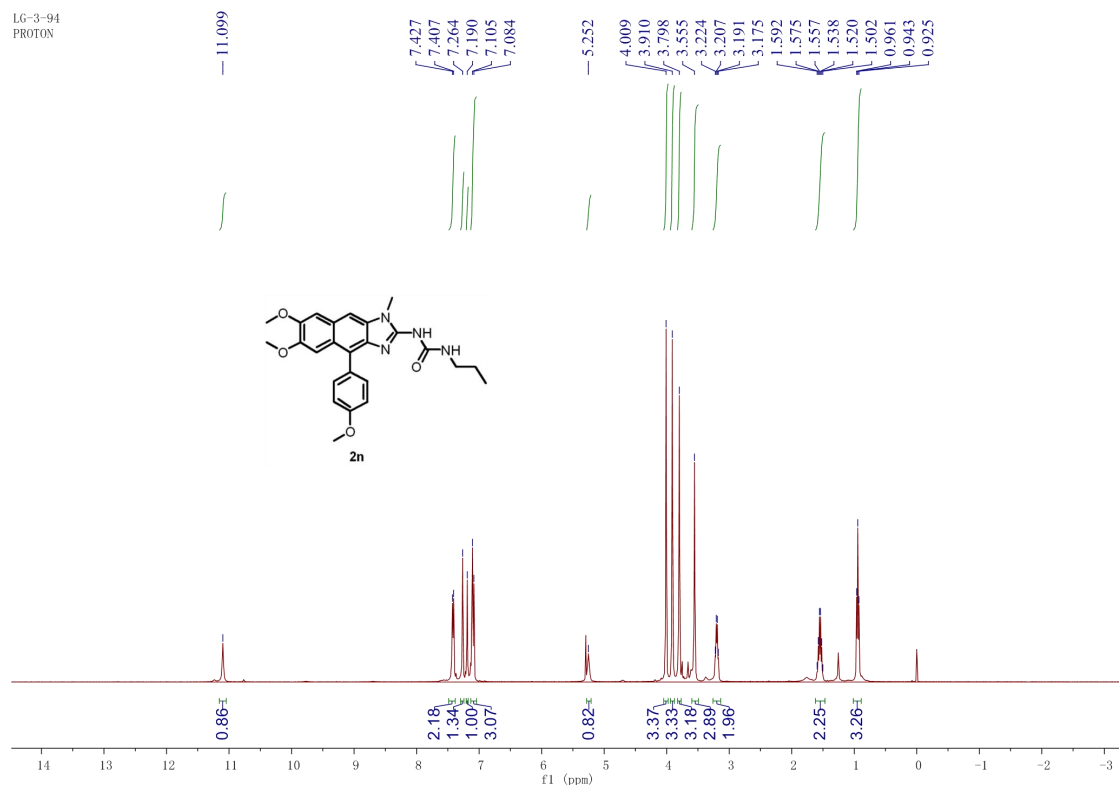
LG-3-92  
PROTON



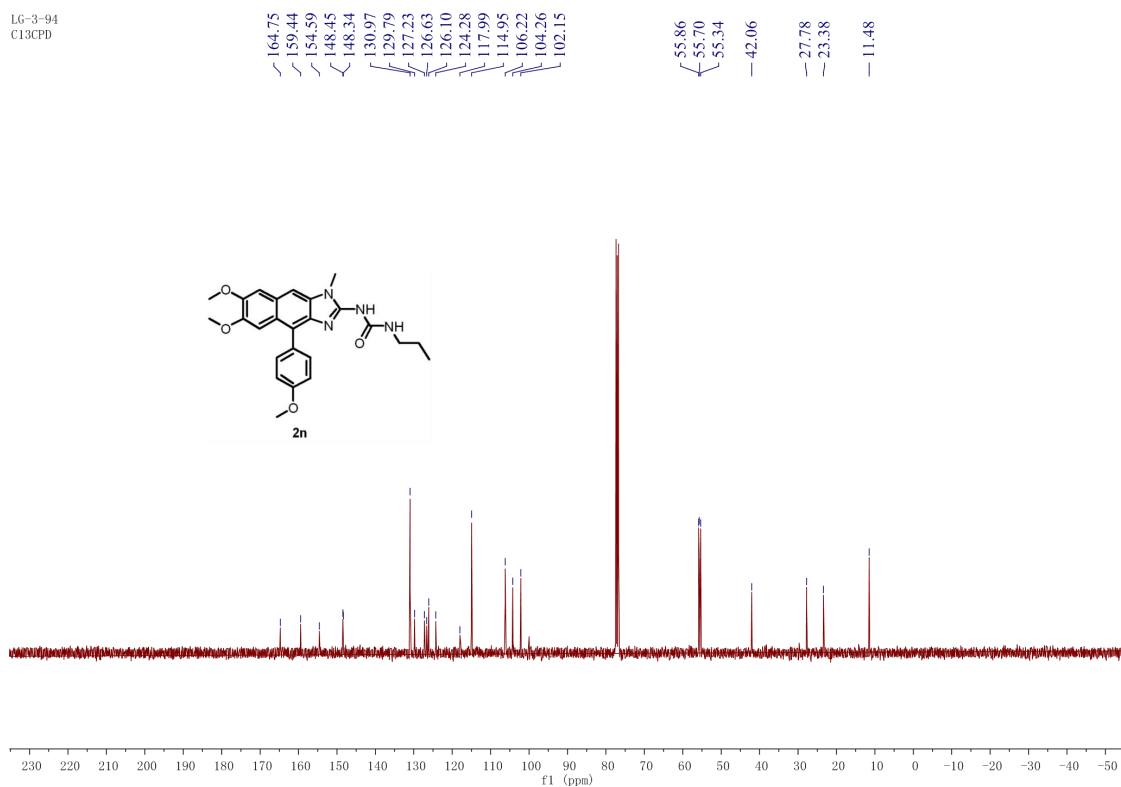
LG-3-92  
C13CPD



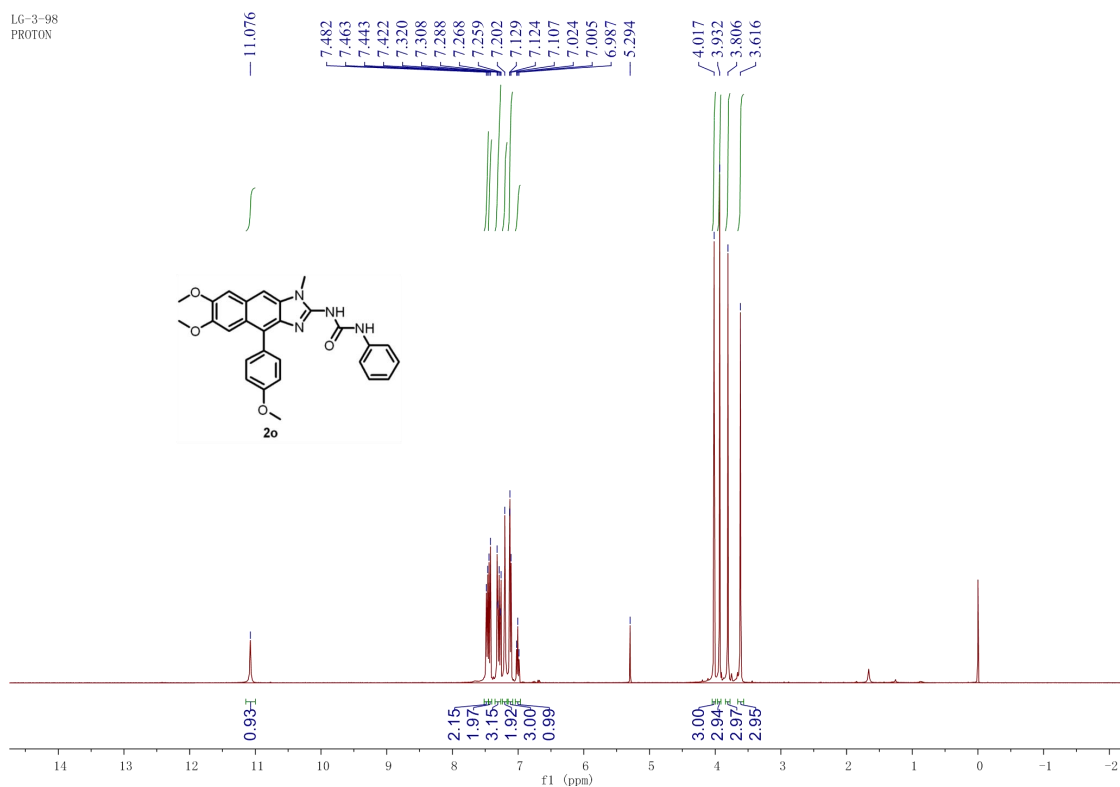
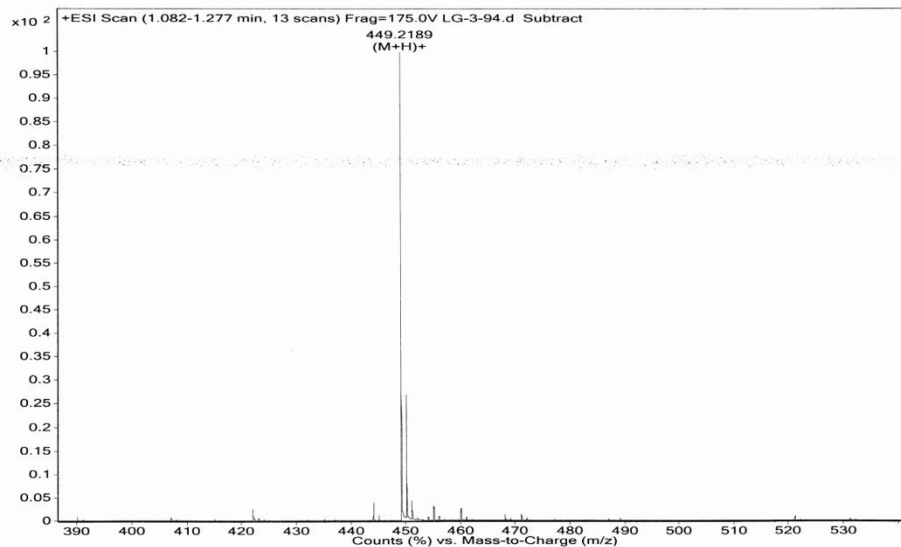
LG-3-94  
PROTON



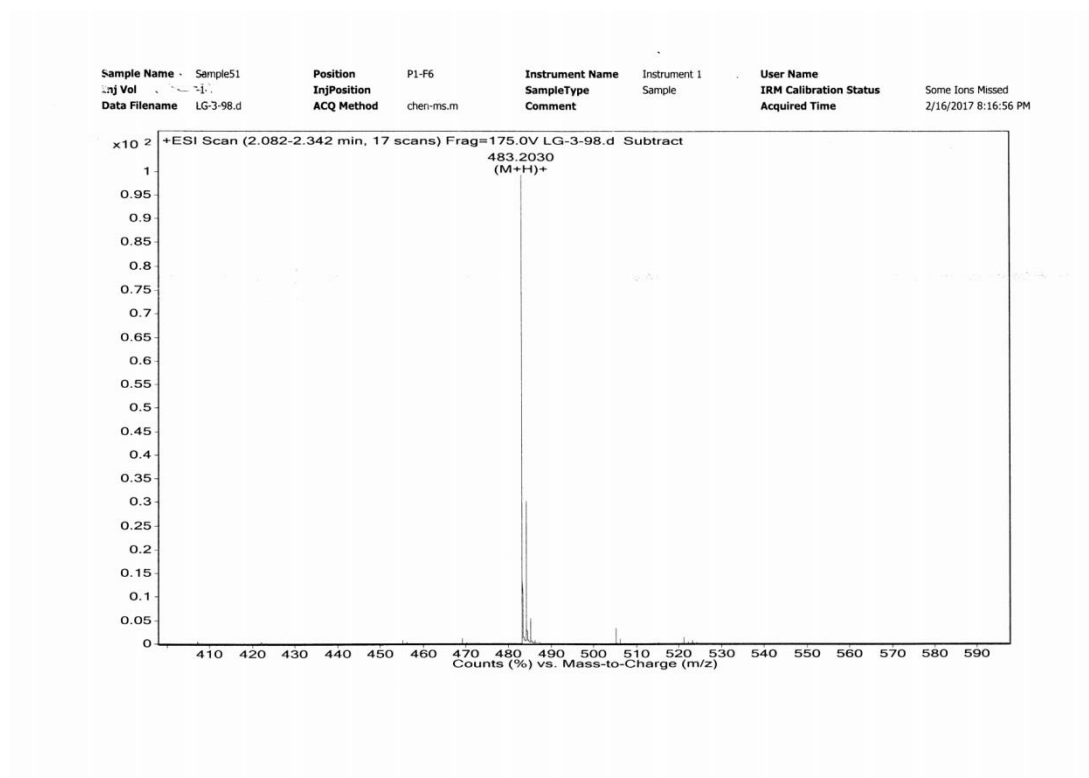
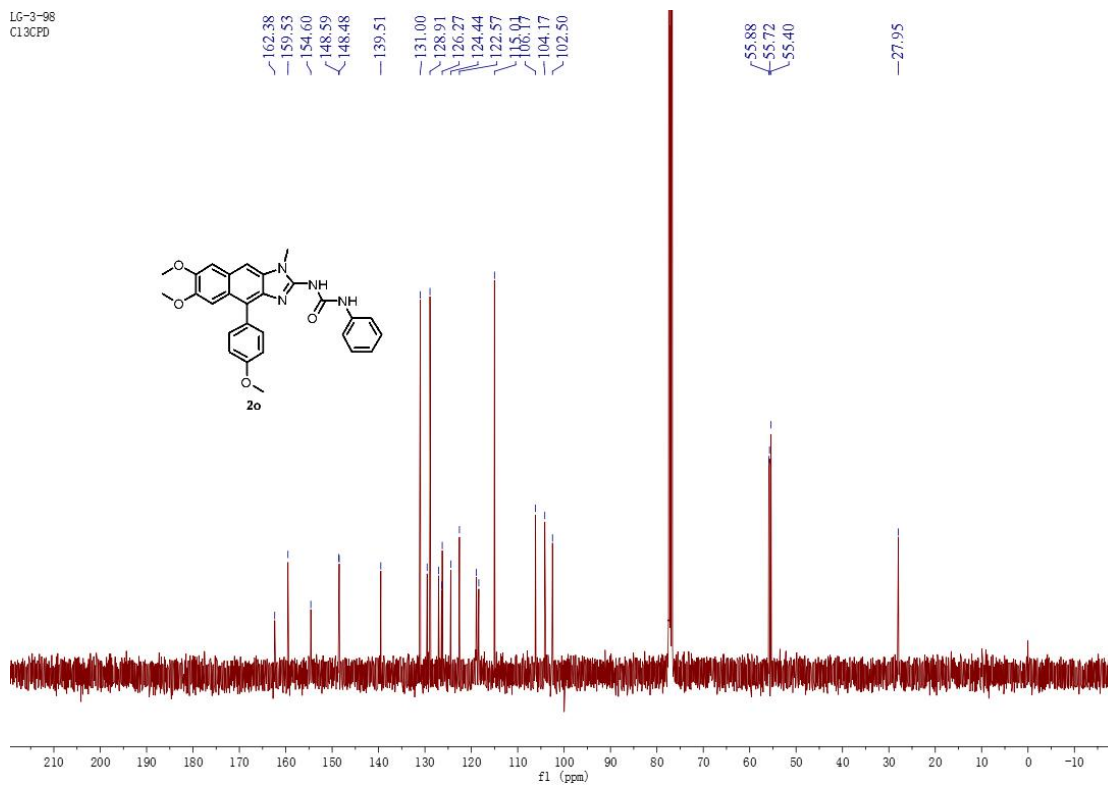
LG-3-94  
C13CPD



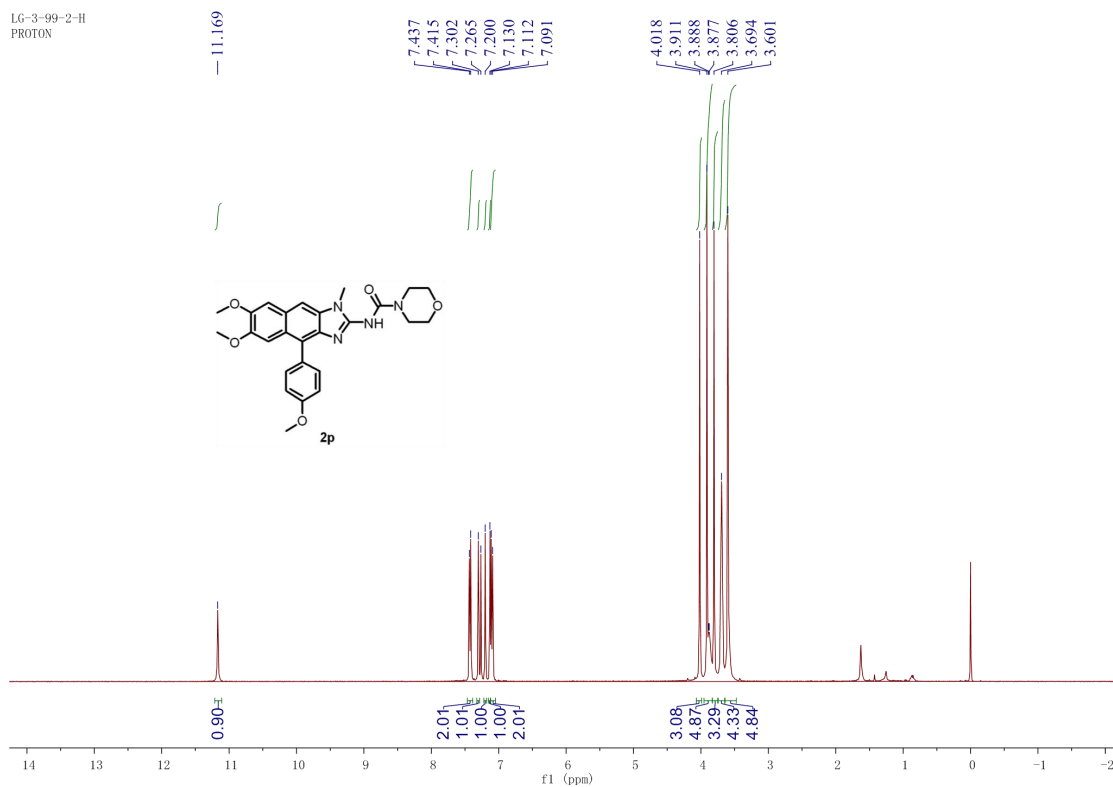
LG-3-98  
PROTON



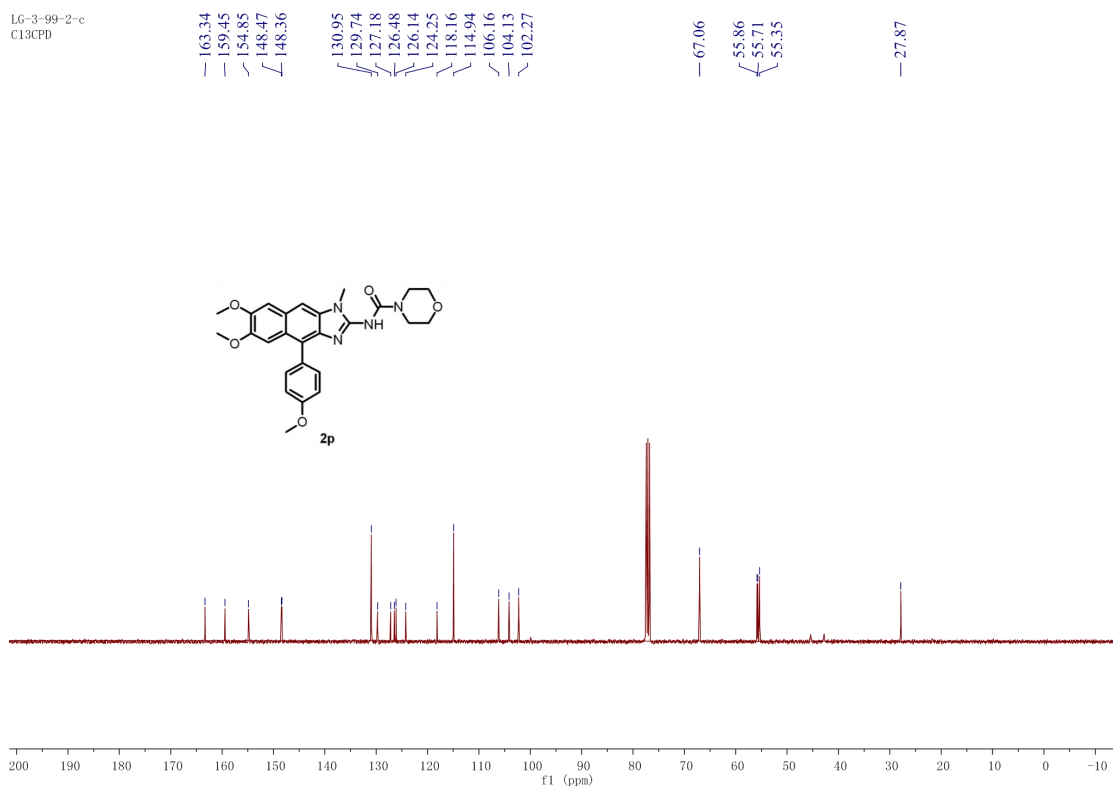
LG-3-98  
C13CPD



LG-3-99-2-H  
PROTON

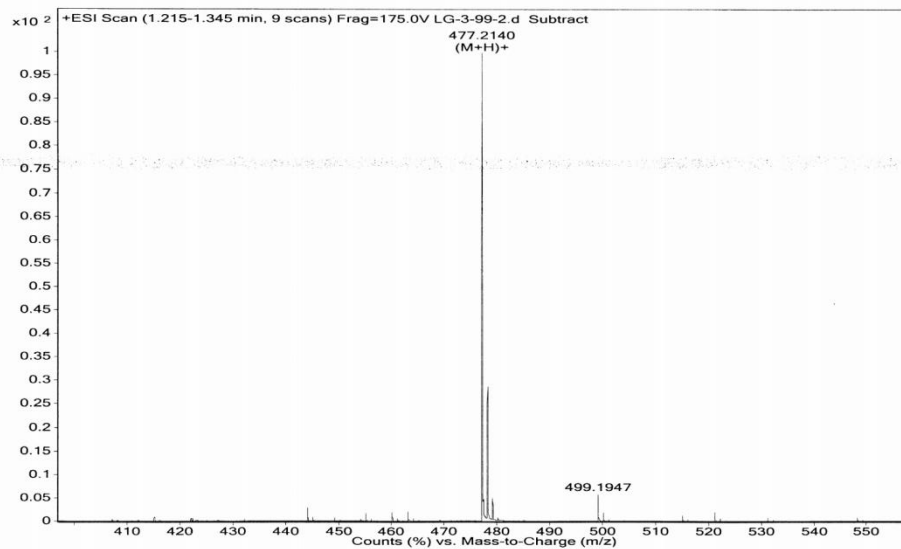


LG-3-99-2-c  
C13CPD



Sample Name	Sample4	Position	P2-A4	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	LG-3-99-2.d	ACQ Method	chen-ms.m	Comment		Acquired Time

Some Ions Missed  
2/16/2017 8:56:43 PM



LG-3-102-H

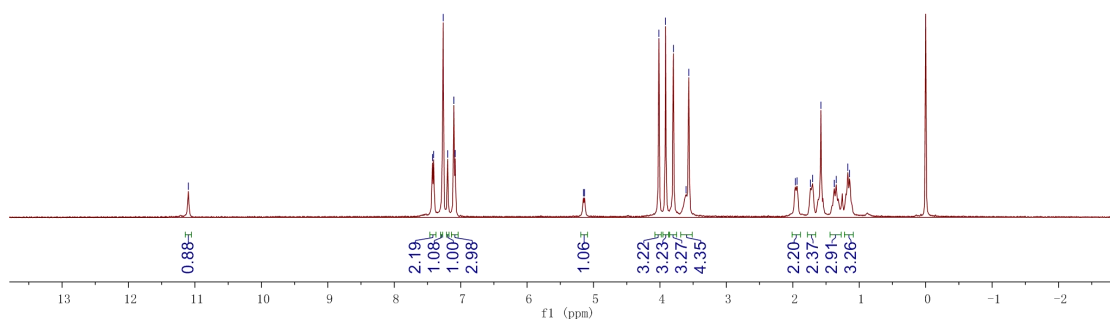
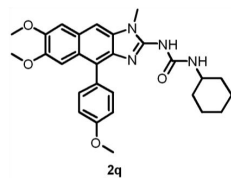
11.099

7.425, 7.406, 7.263, 7.196, 7.102, 7.083

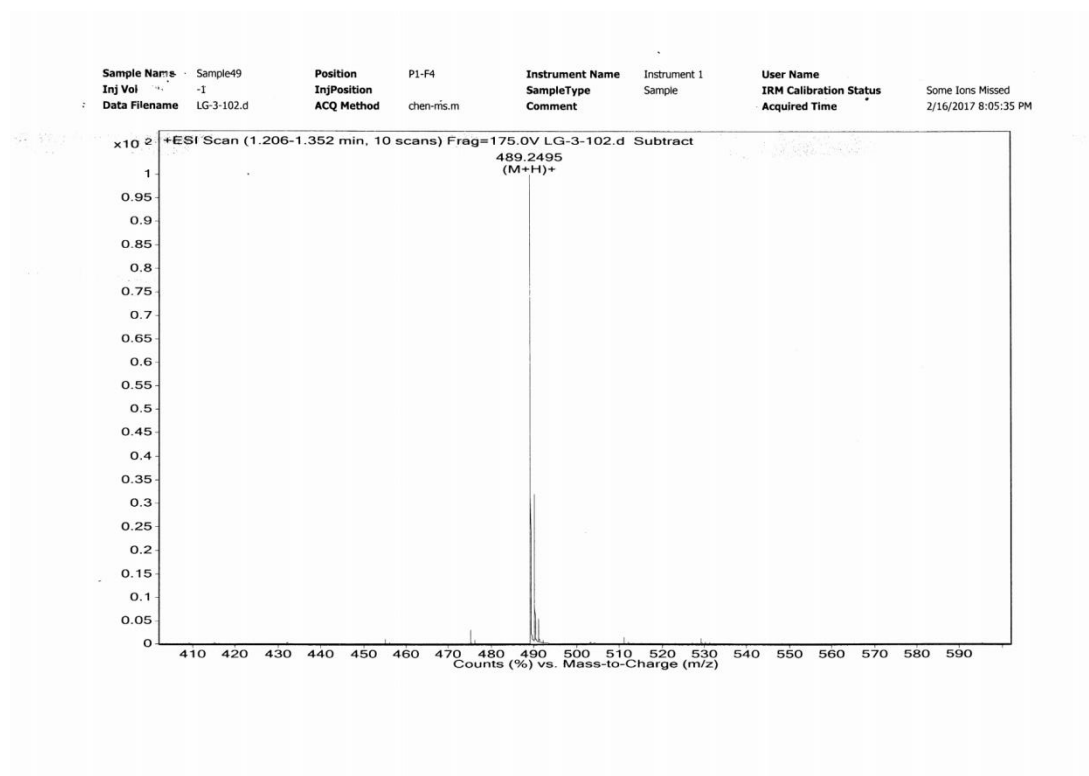
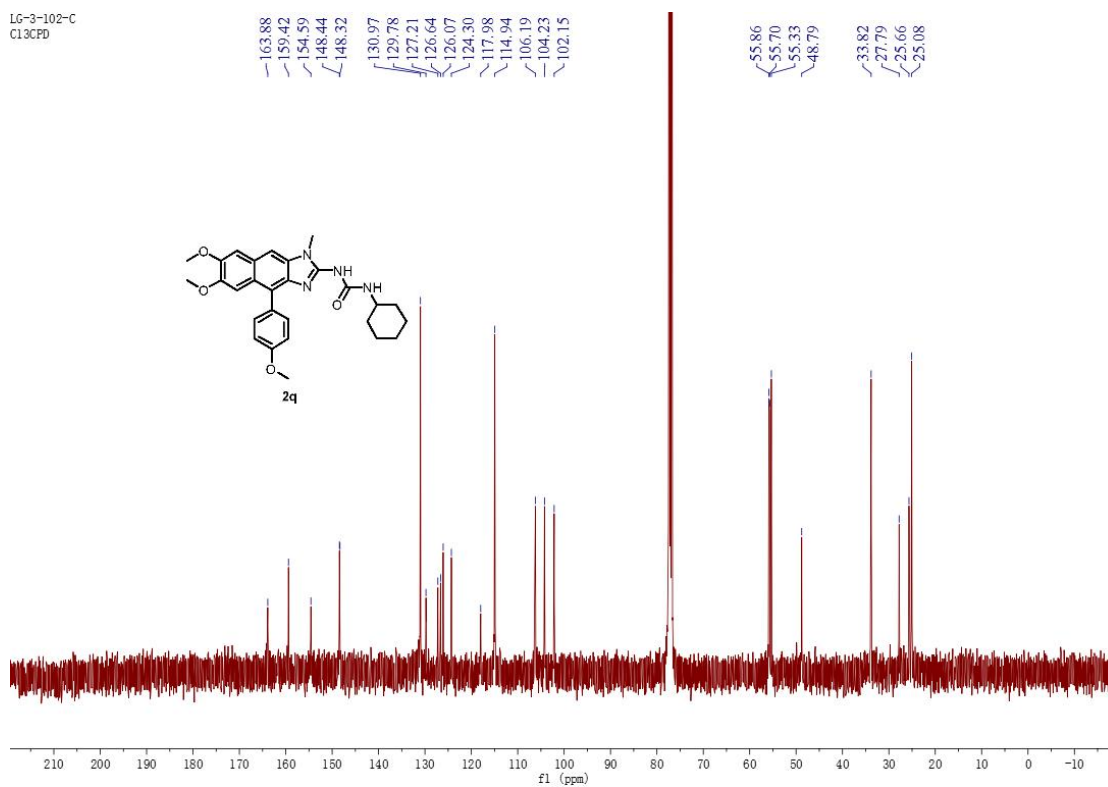
5.153, 5.134

4.016, 3.915, 3.798, 3.606, 3.566

1.961, 1.936, 1.735, 1.702, 1.577, 1.377, 1.347, 1.173, 1.146

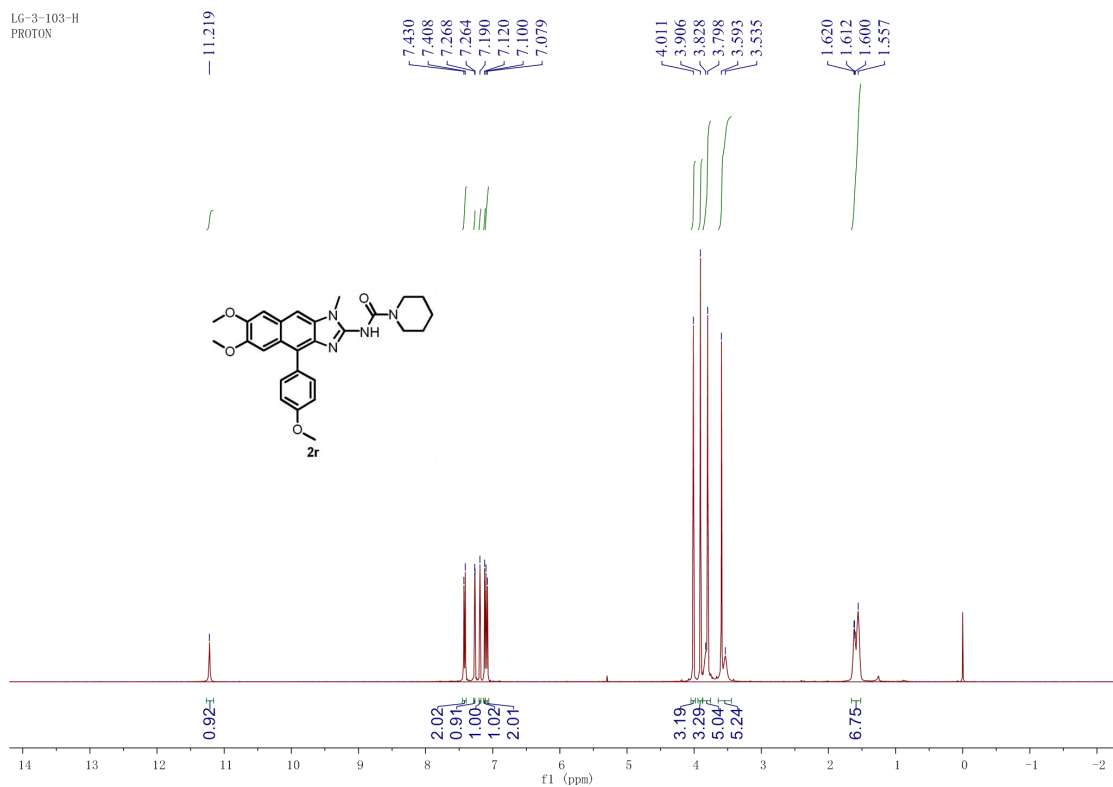


LG-3-102-C  
C13CPD

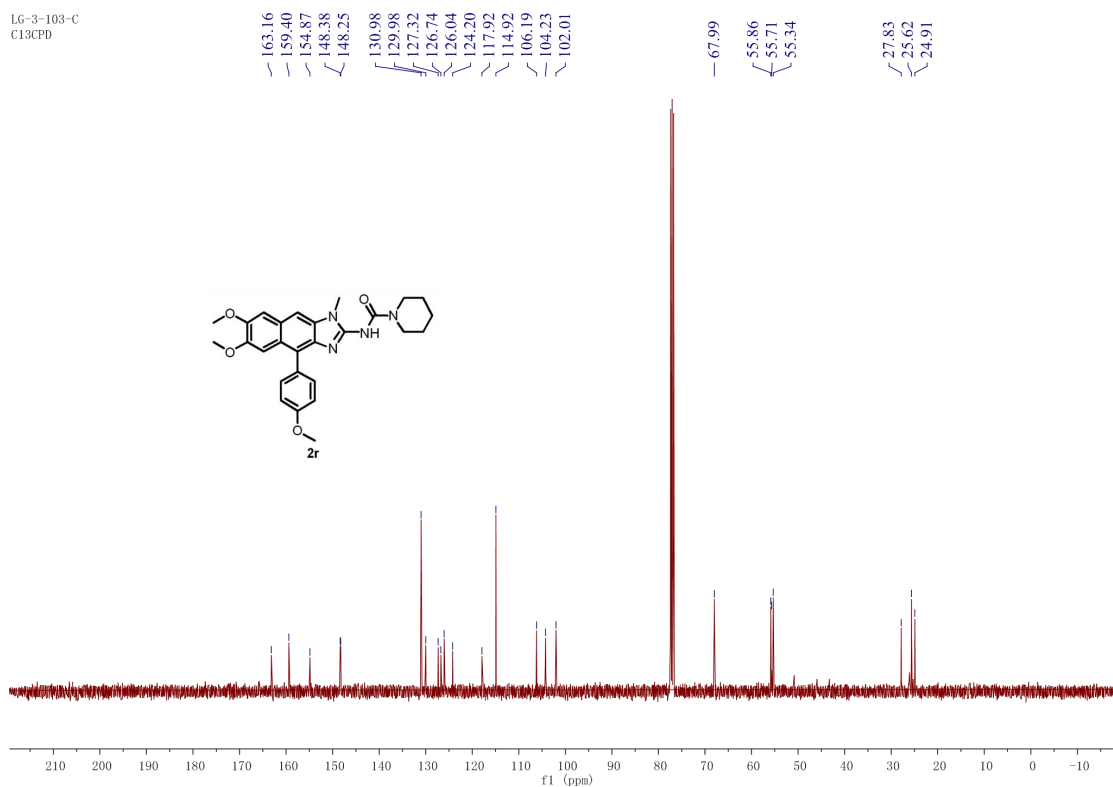


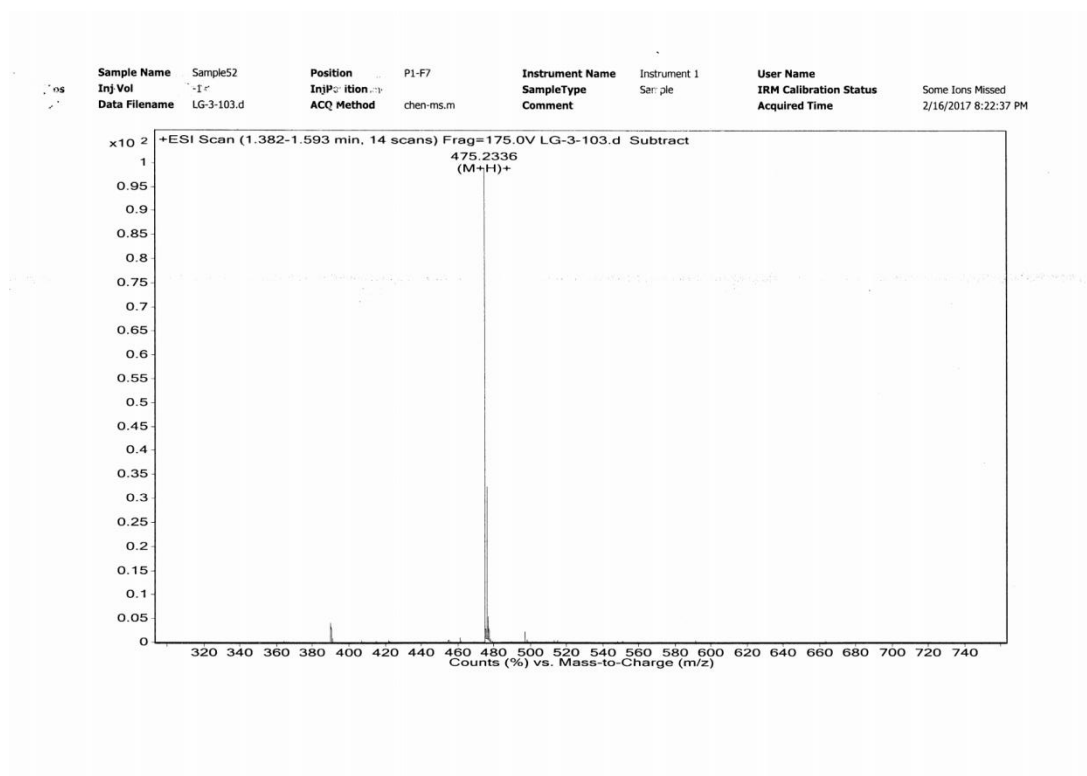


LG-3-103-H  
PROTON

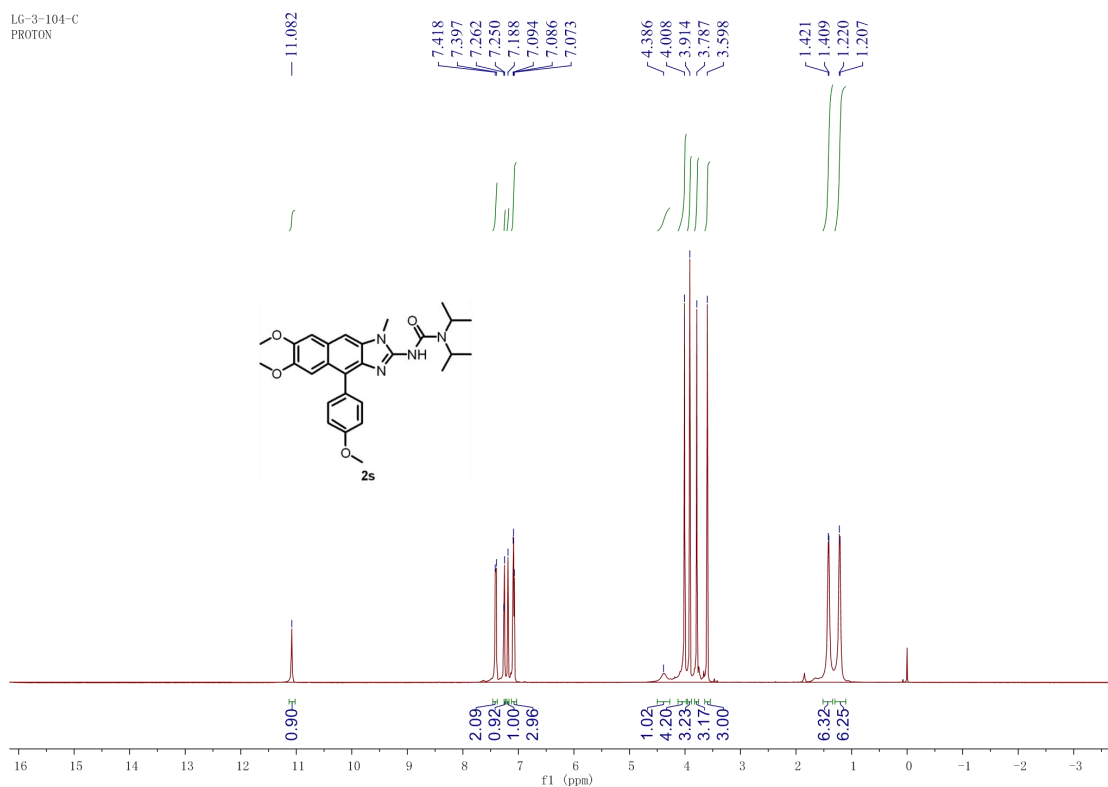


LG-3-103-C  
C13CPD

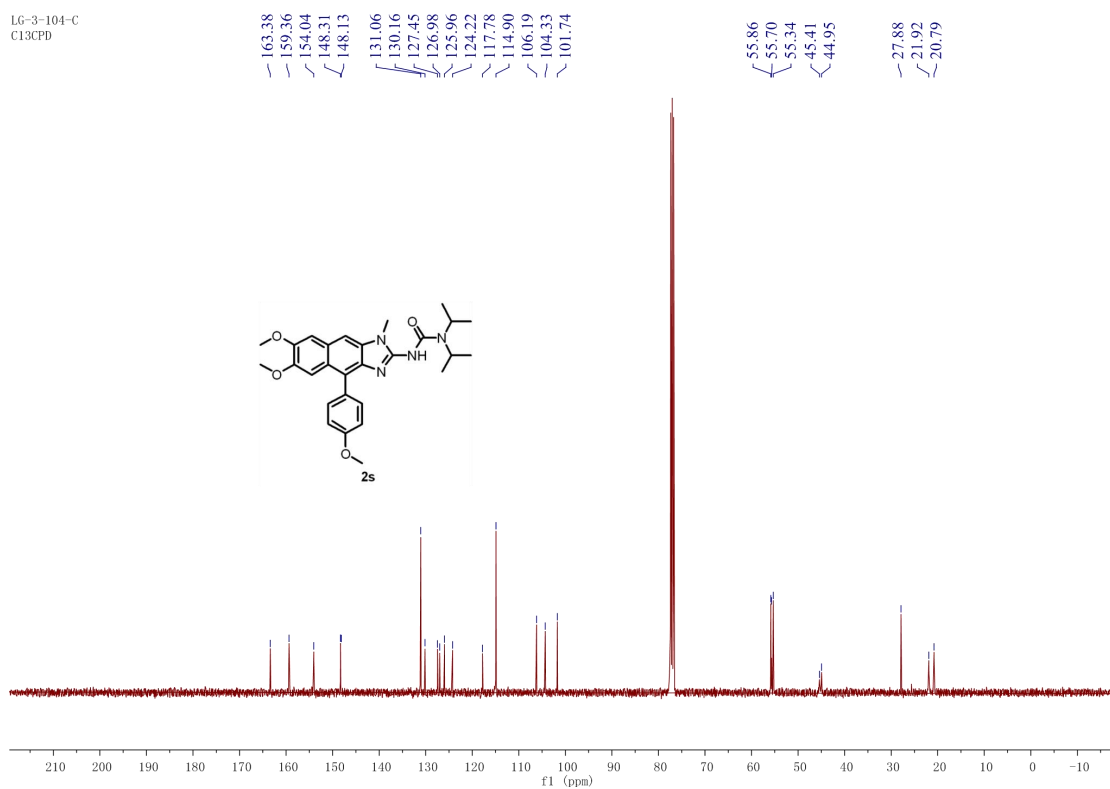




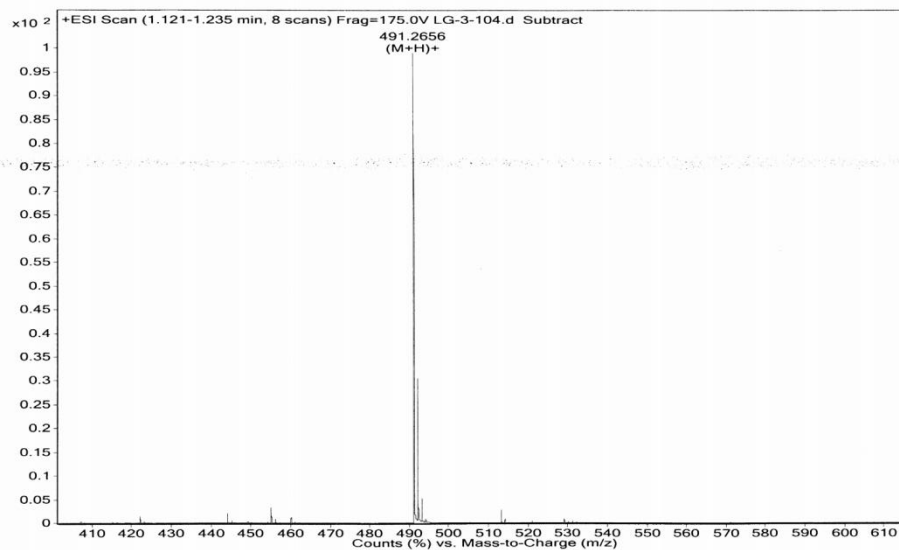
LG-3-104-C  
PROTON



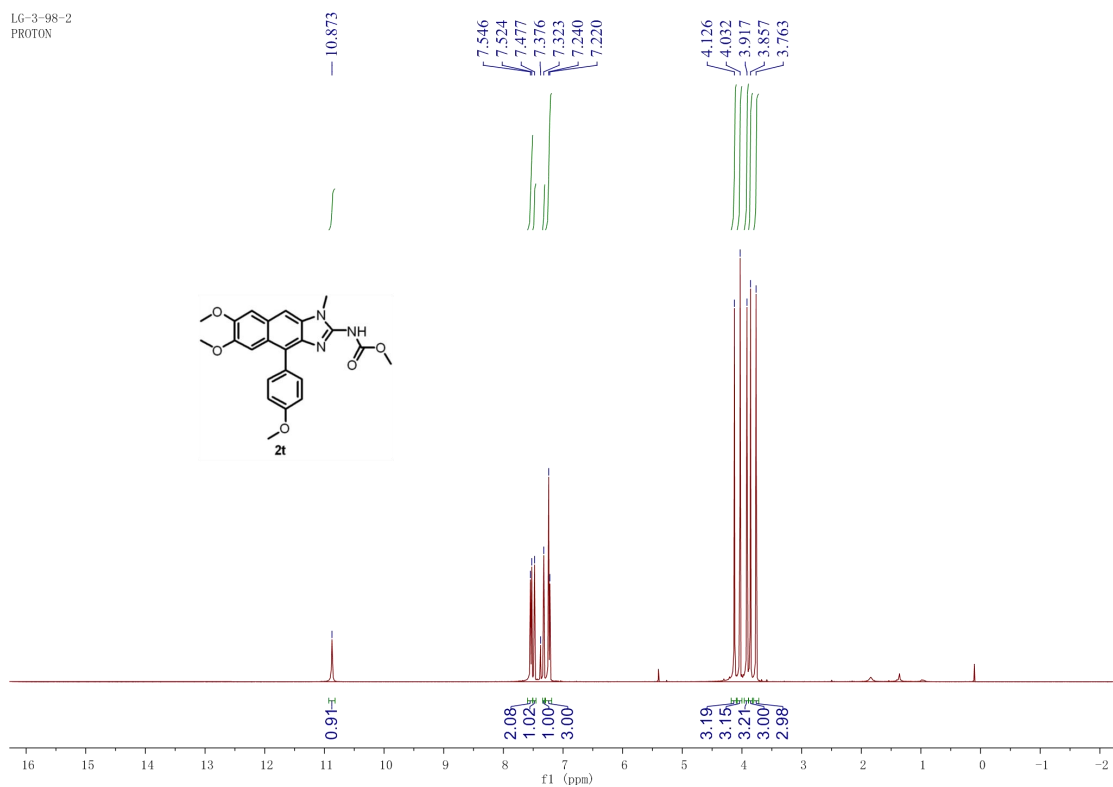
LG-3-104-C  
C13CPD



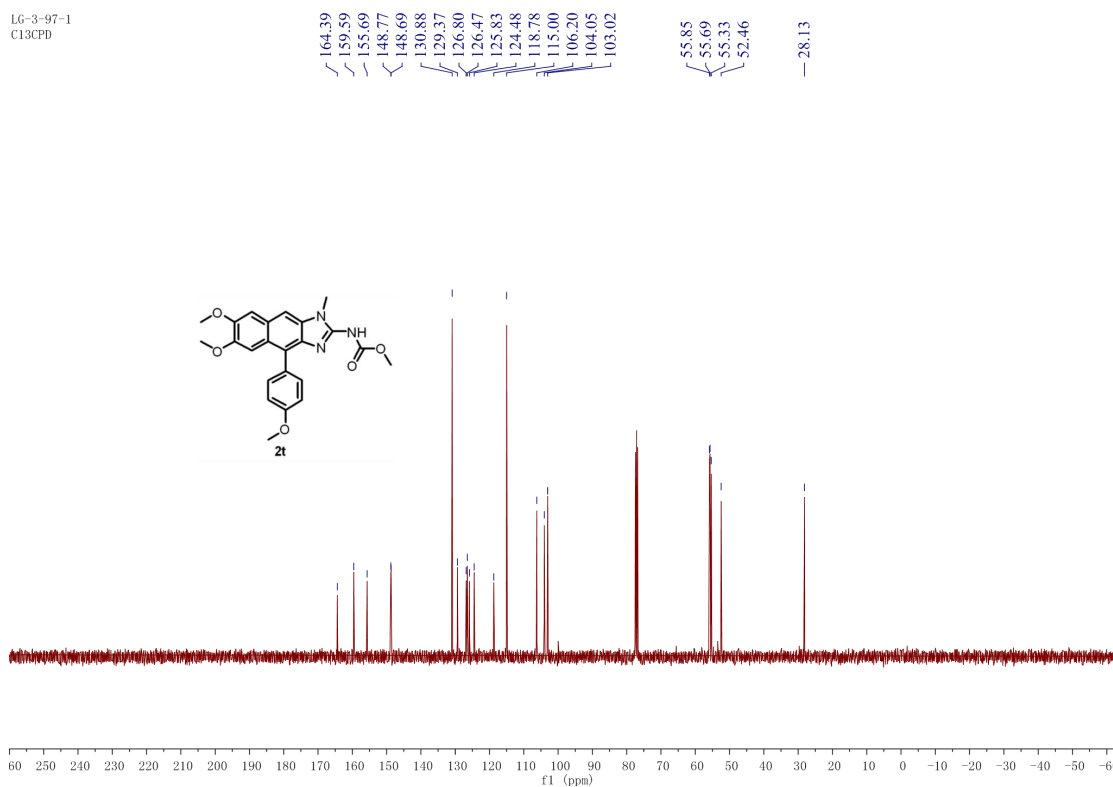
Sample Name	Sample7	Position	P2-A7	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	LG-3-104.d	ACQ Method	chen-ms.m	Comment		Acquired Time



LG-3-98-2  
PROTON

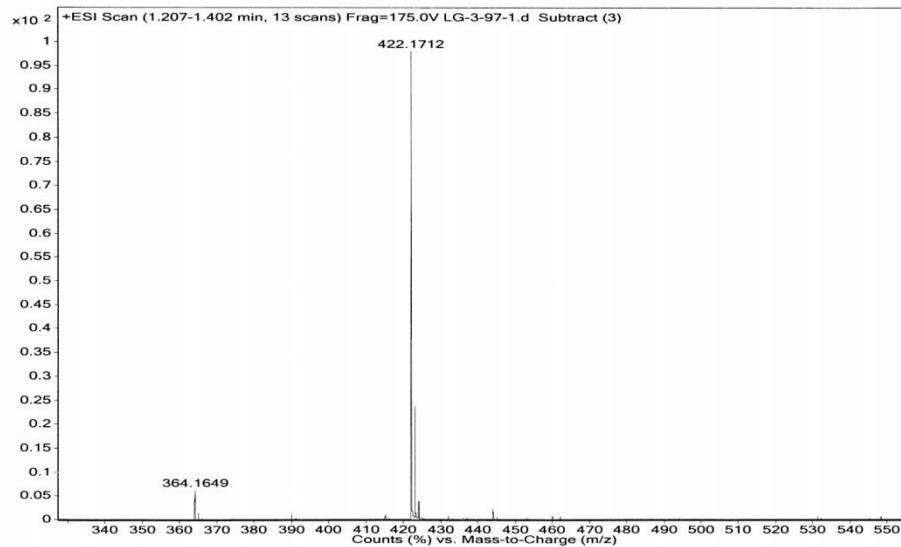


LG-3-97-1  
C13CPD

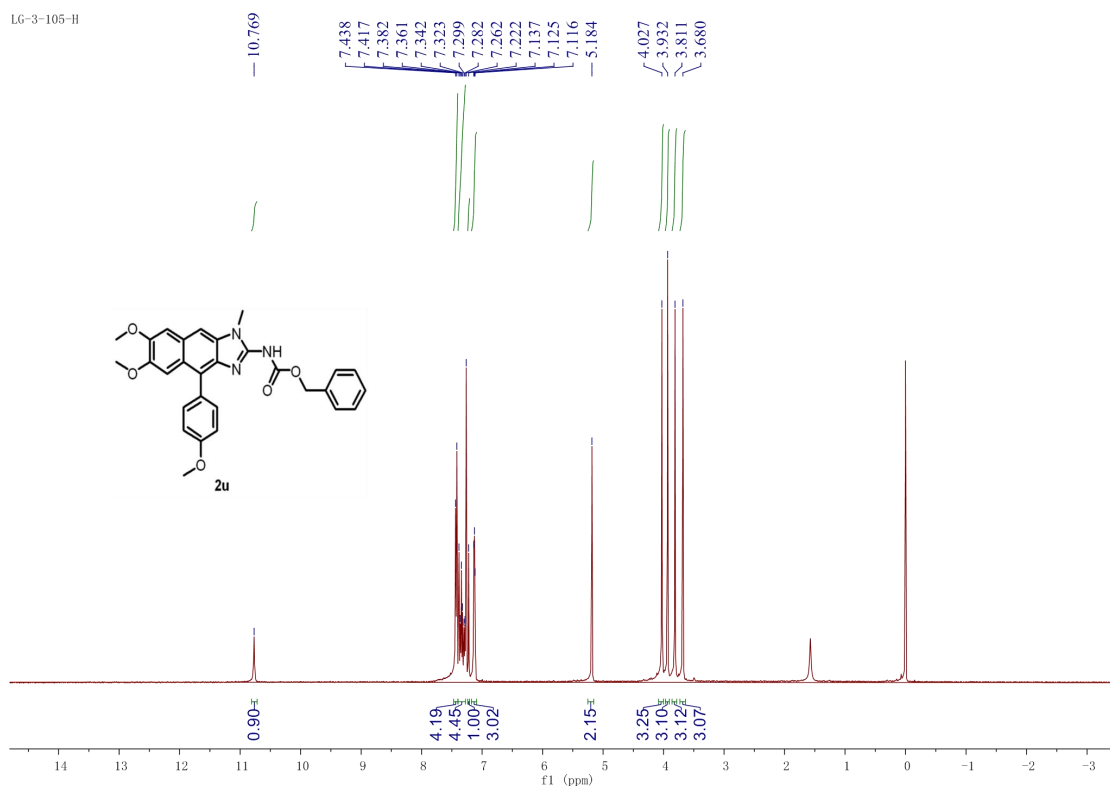


Sample Name	Sample11	Position	P1-B2	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	LG-3-97-1.d	ACQ Method	chen-ms.m	Comment		Acquired Time

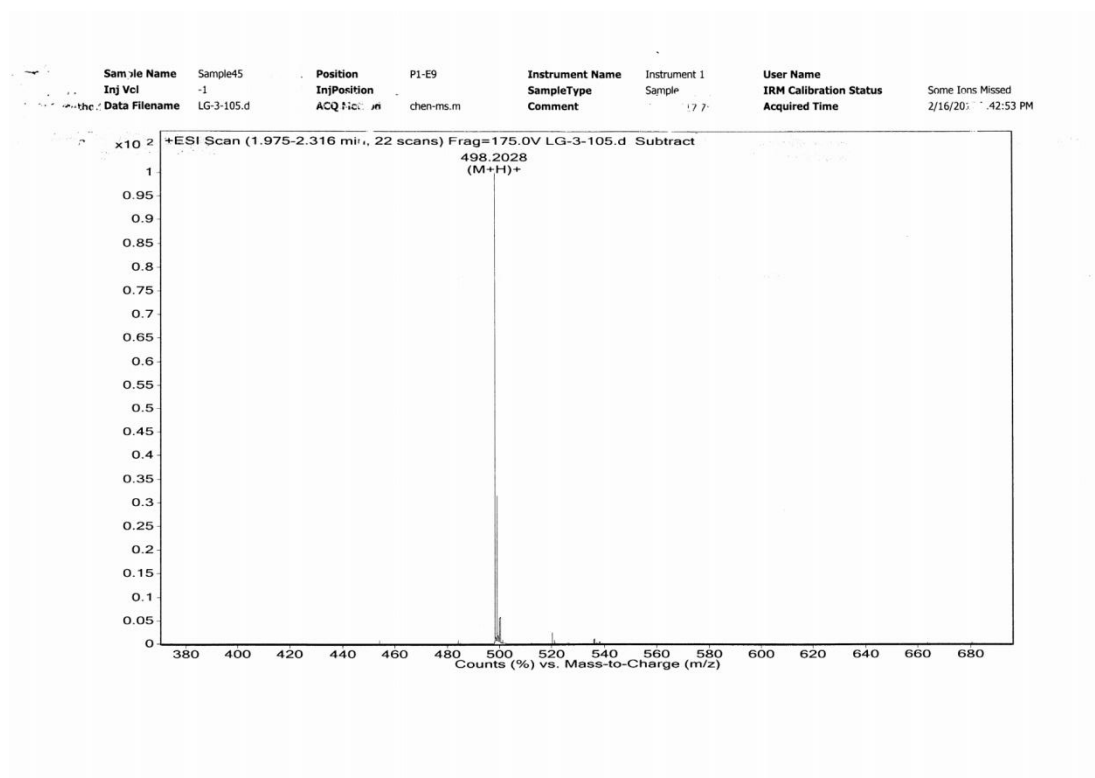
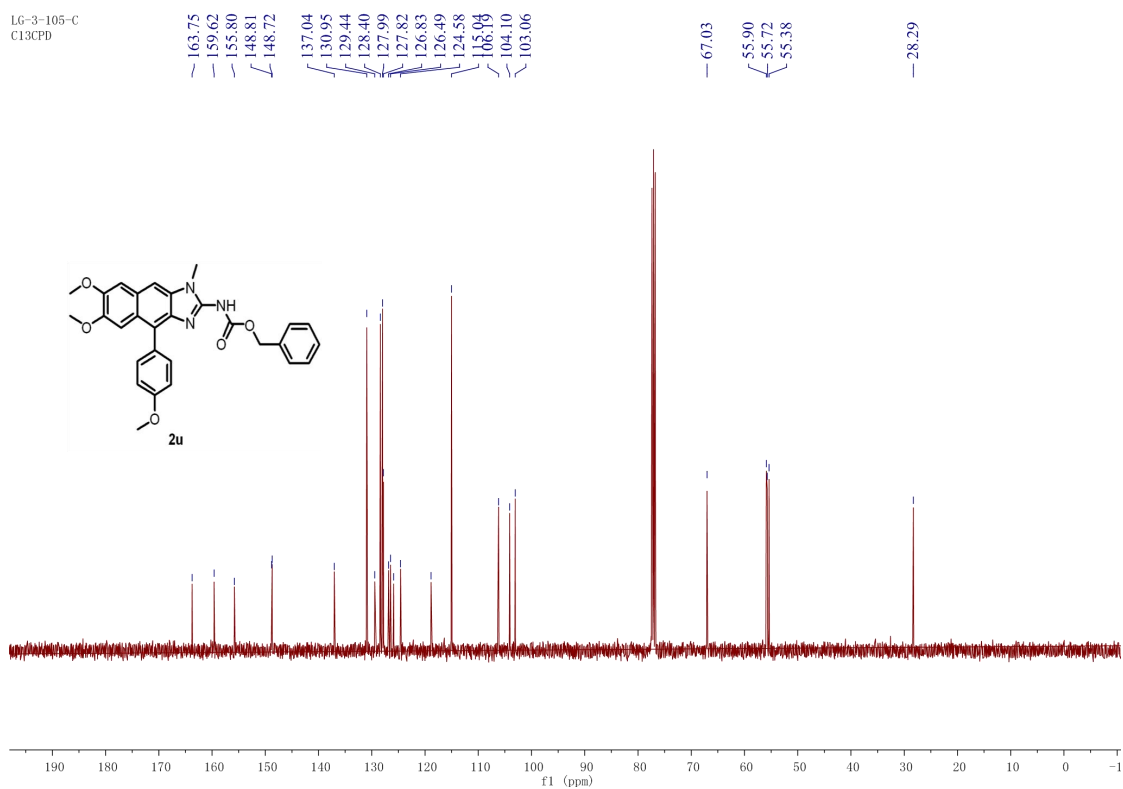
Some Ions Missed  
1/5/2017 10:04:58 AM



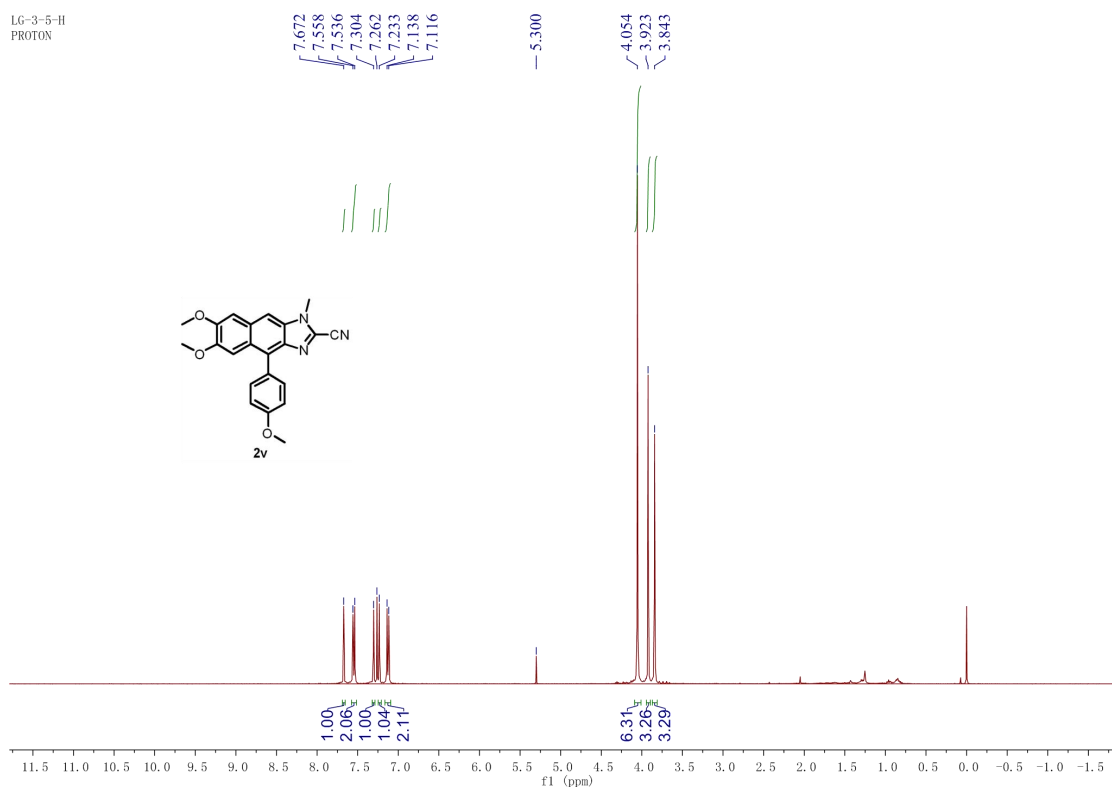
LG-3-105-H



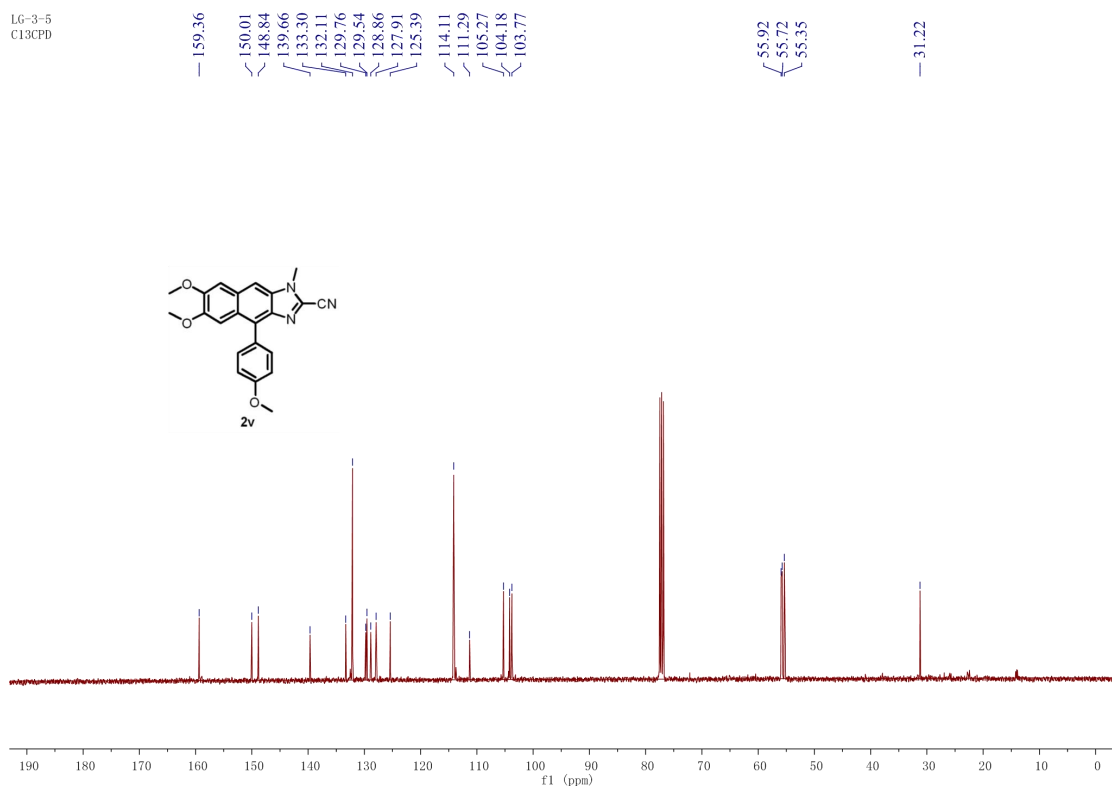
LG-3-105-C  
C13CPD



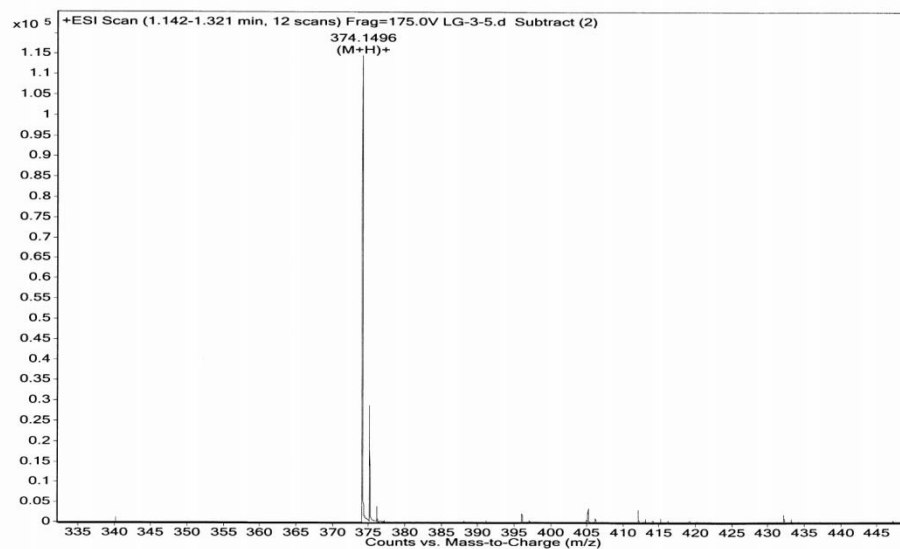
LG-3-5-H  
PROTON



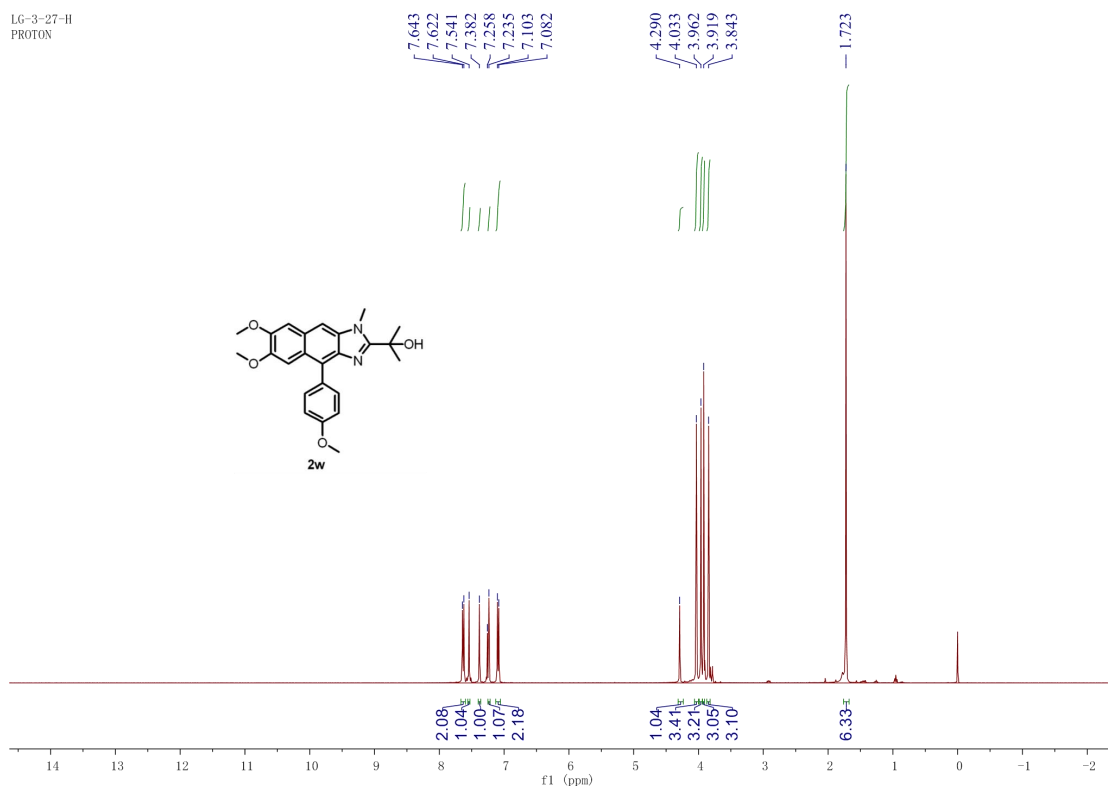
LG-3-5  
C13CPD



Sample Name	Sample14	Position	PI-85	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	LG-3-5.d	ACQ Method	chen-ms.m	Comment		Acquired Time	11/16/2016 6:00:11 PM

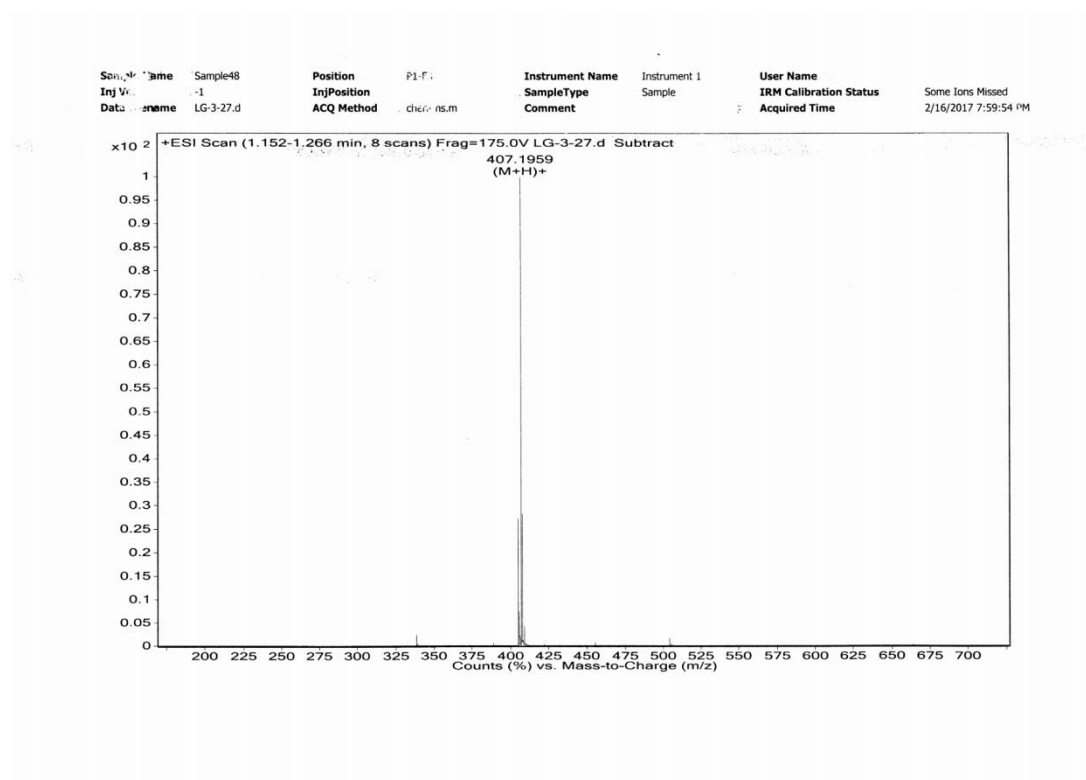
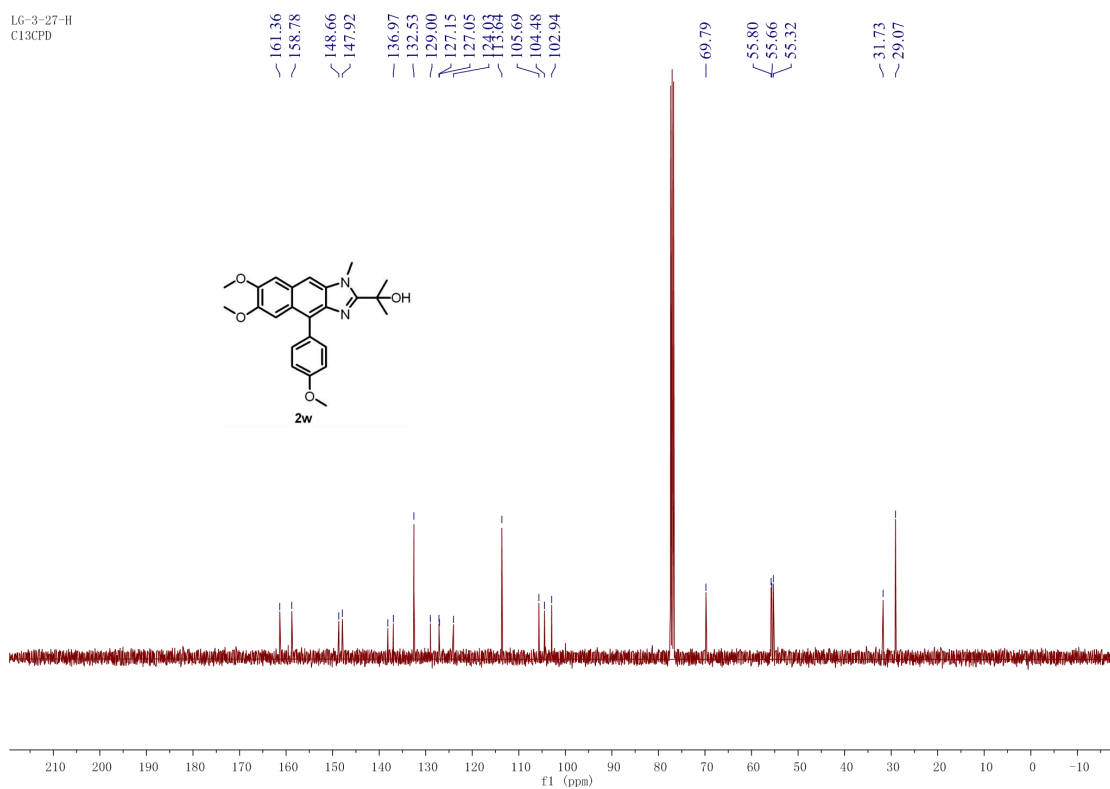


LG-3-27-H  
PROTON

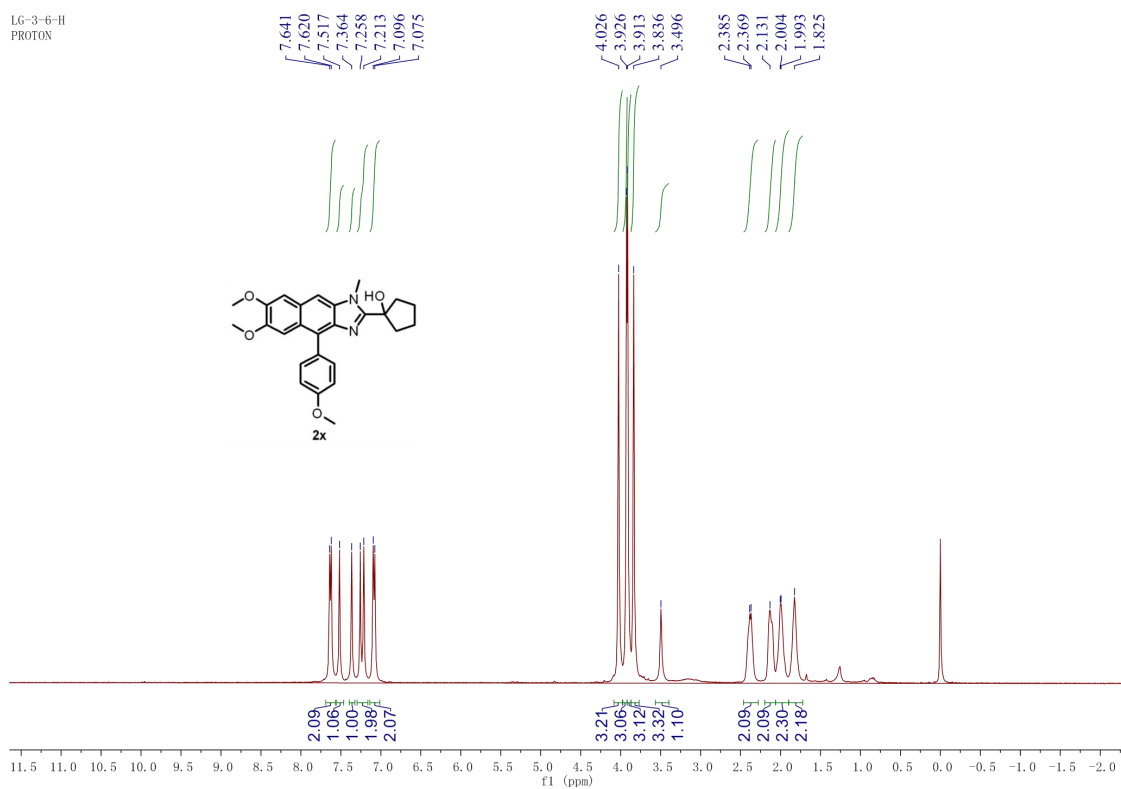




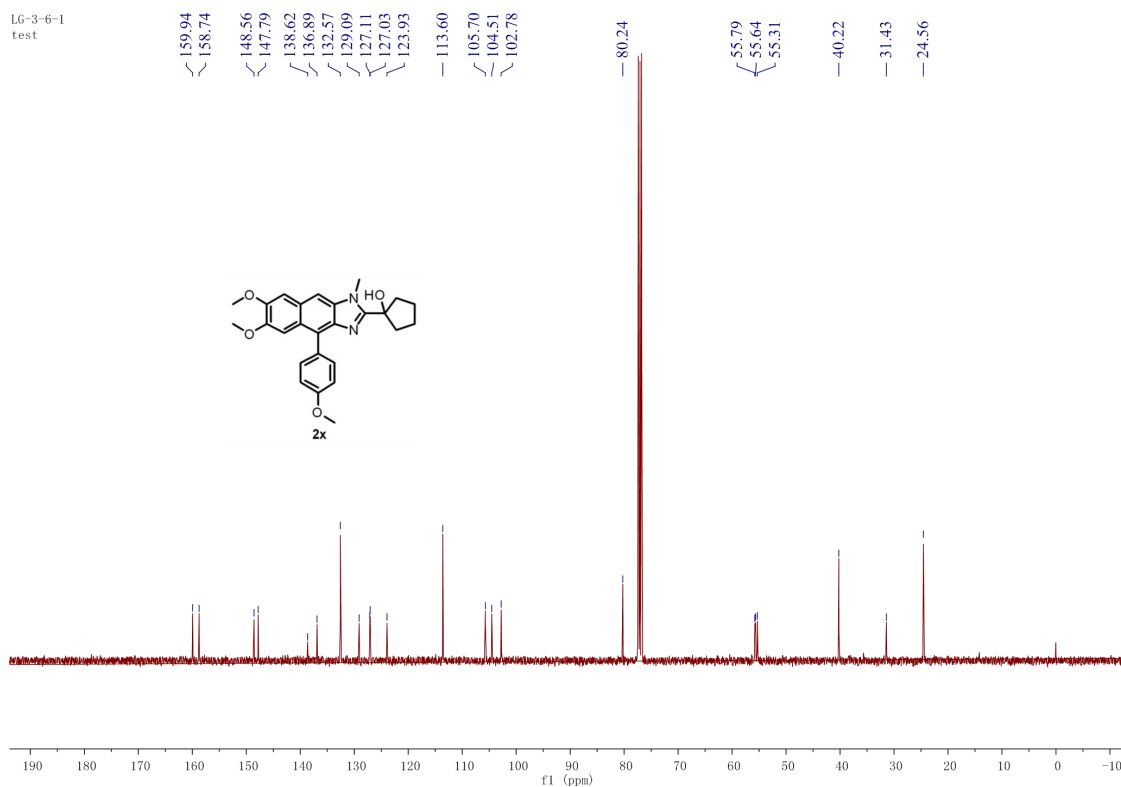
LG-3-27-H  
C13CPD



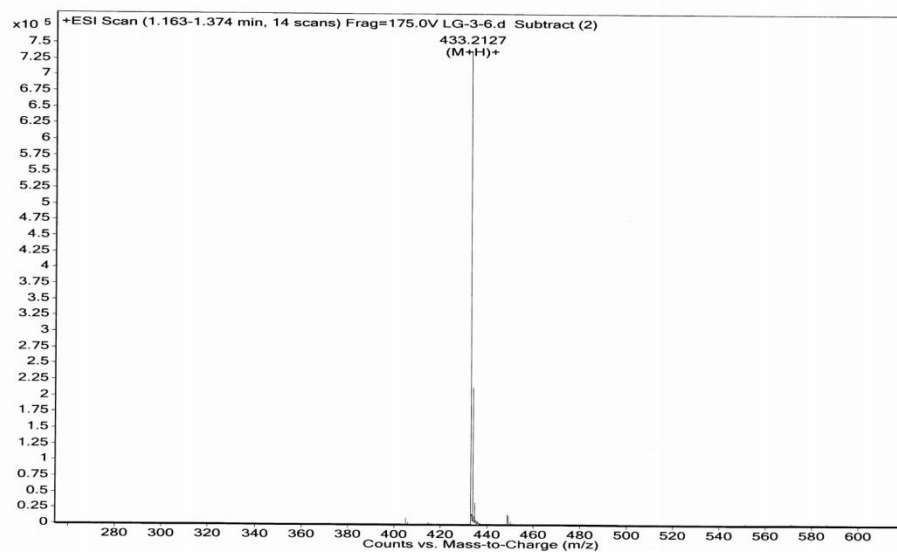
LG-3-6-H  
PROTON



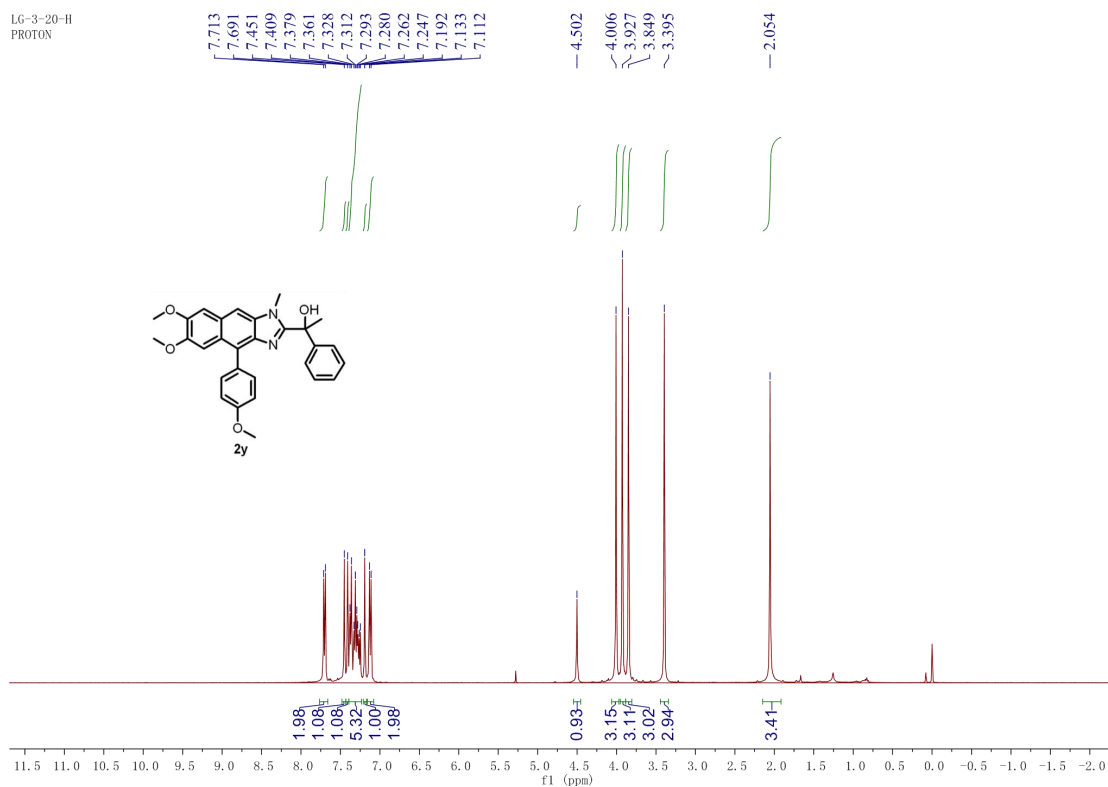
LG-3-6-1  
test



Sample Name	Sample15	Position	P1-B6	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	LG-3-6.d	ACQ Method	chen-ms.m	Comment		Acquired Time	11/16/2016 6:05:52 PM

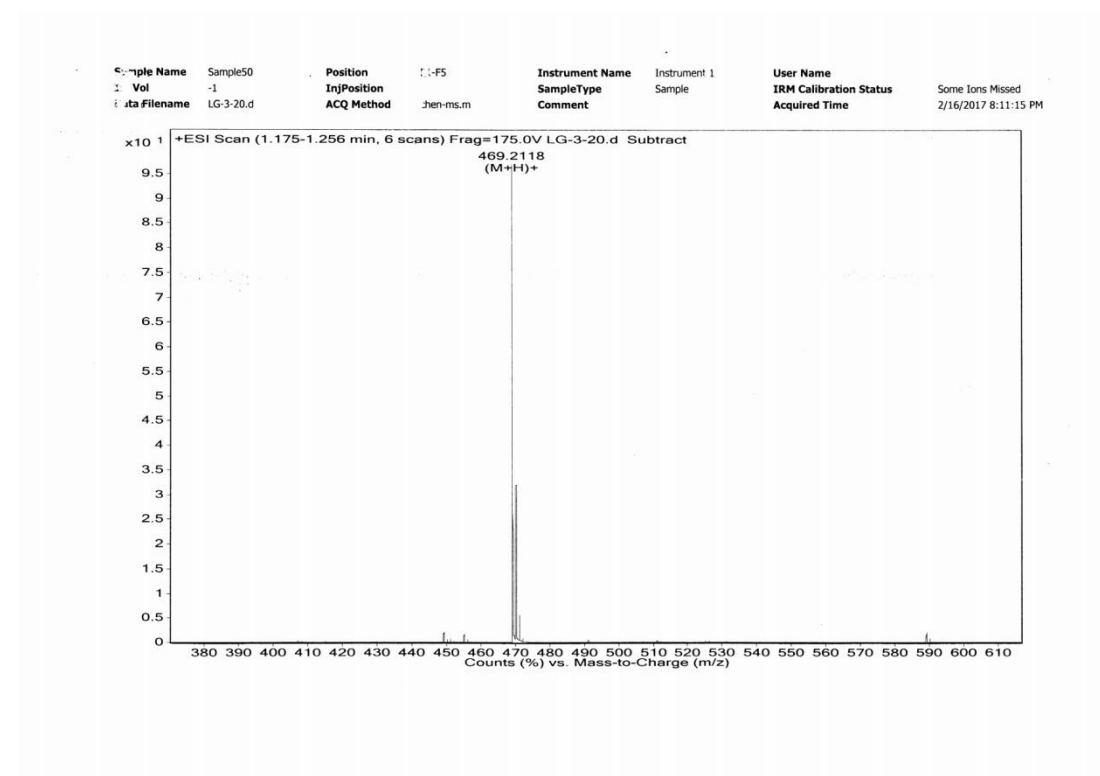
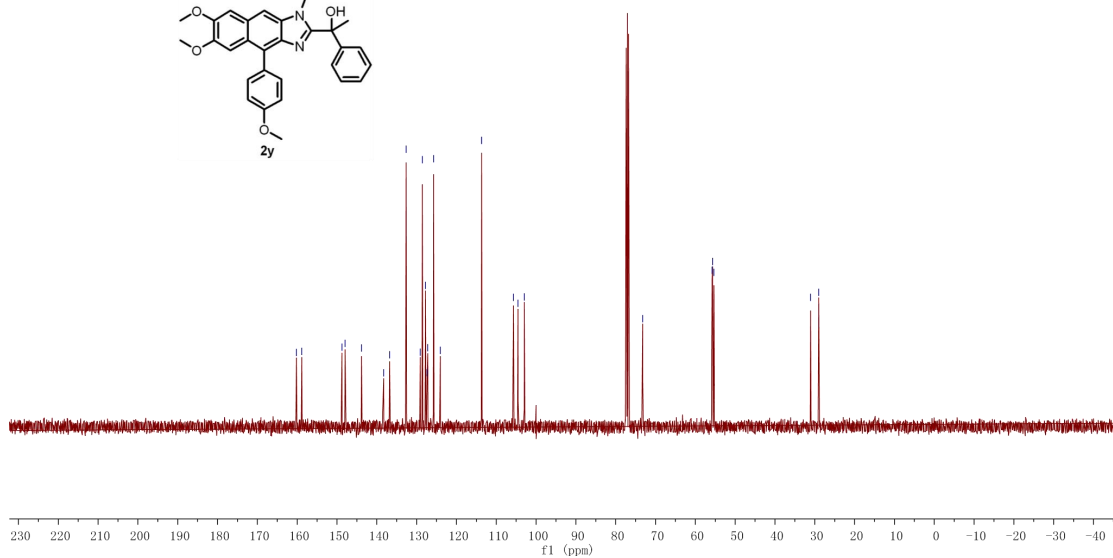
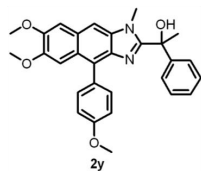


LG-3-20-H  
PROTON

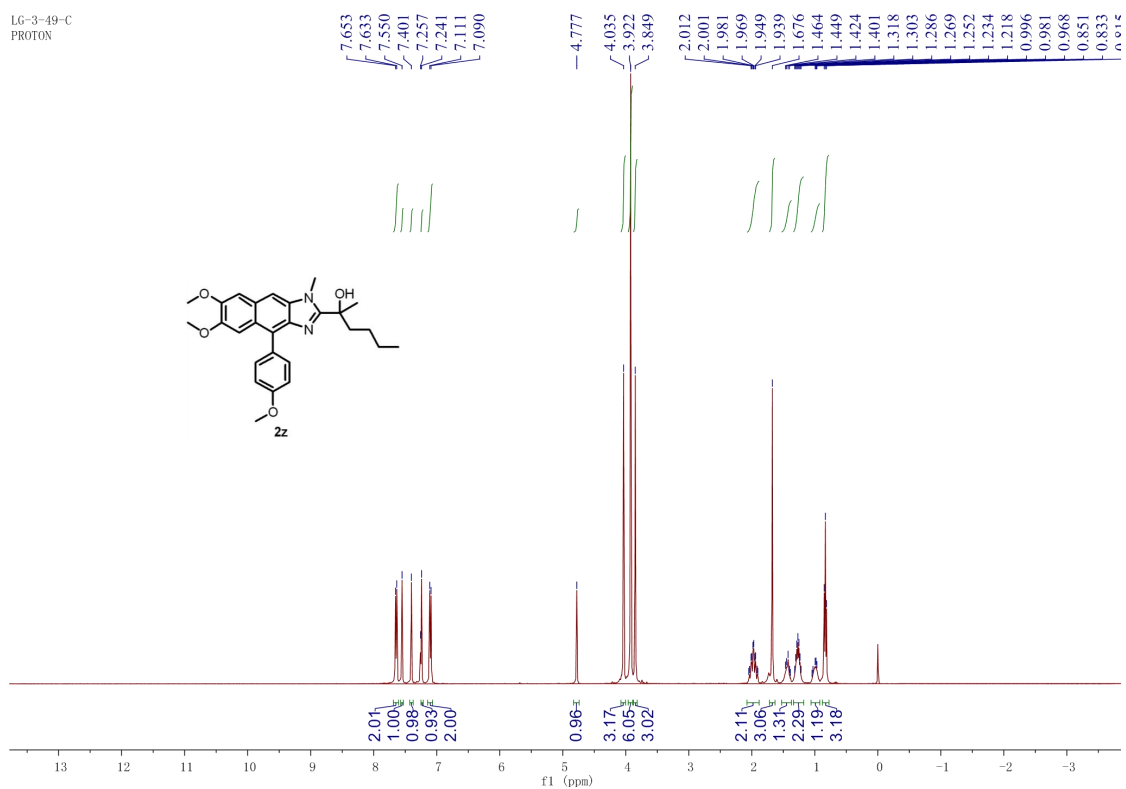


LG-3-20-H  
C13CPD

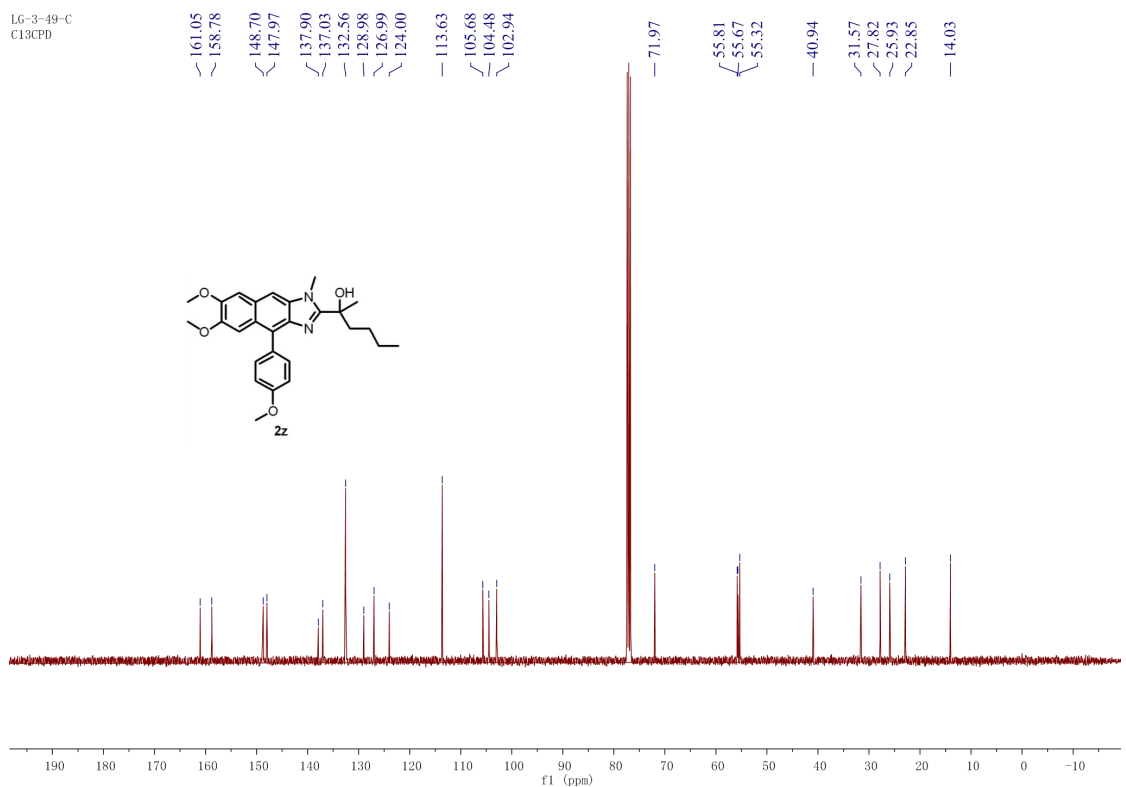
160.18  
158.84  
148.75  
147.96  
132.64  
128.55  
127.77  
127.19  
123.73  
105.66  
104.54  
102.95  
73.21  
55.80  
55.67  
55.33  
31.04  
29.00



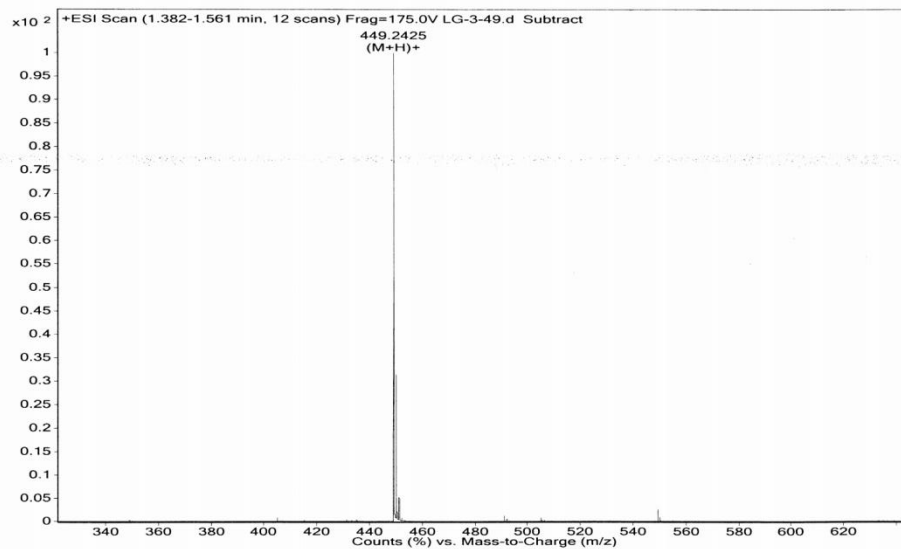
LG-3-49-C  
PROTON



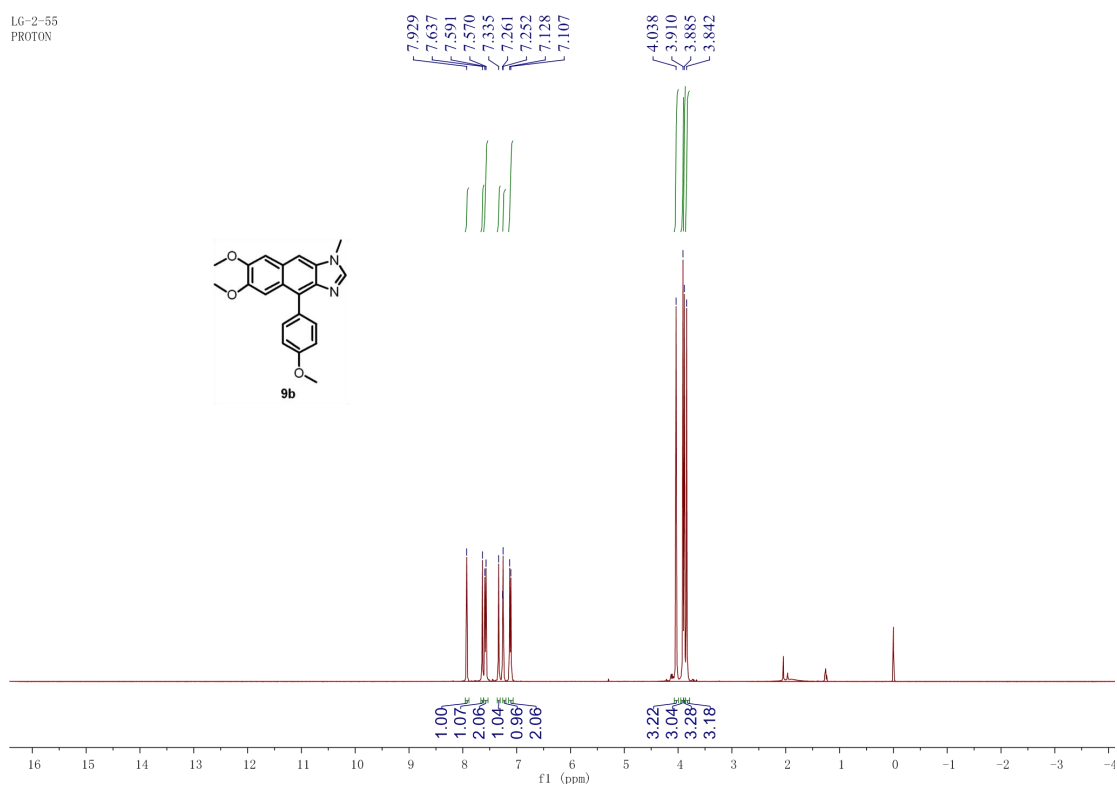
LG-3-49-C  
C13CPD



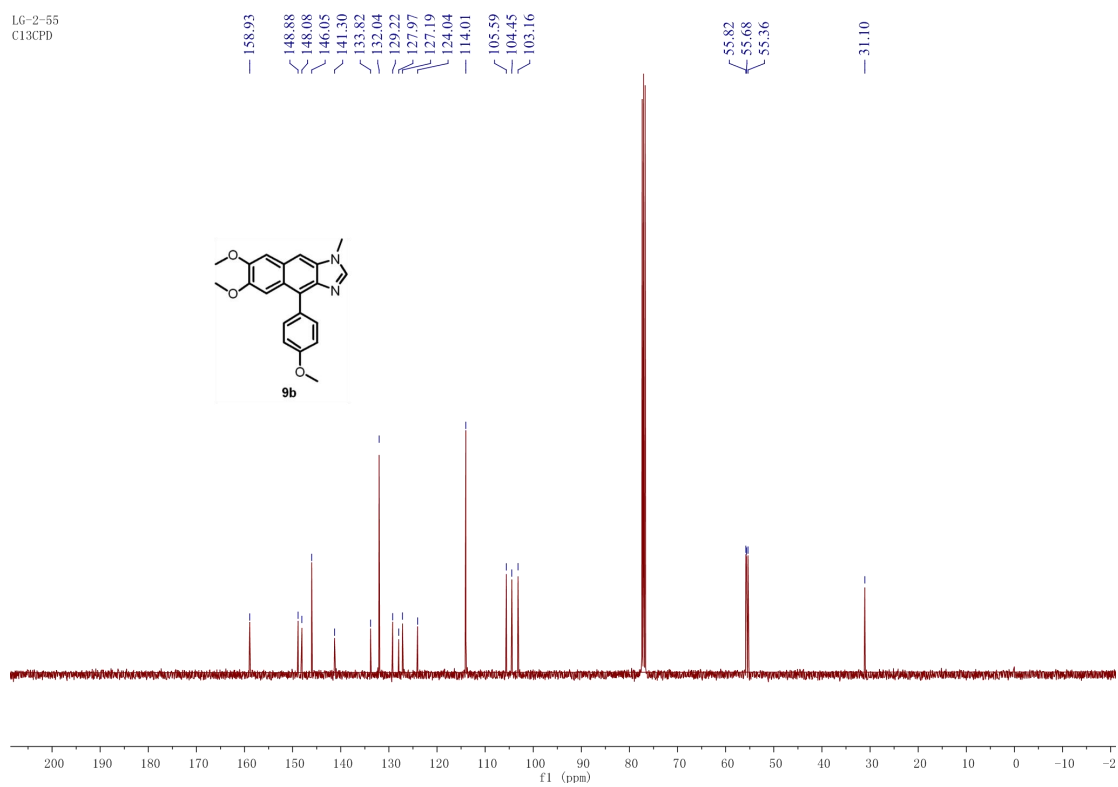
Sample Name	Position	Instrument Name	User Name
Sample54	P1-F9	Instrument 1	
Inj Vol	InjPosition	SampleType	IRM Calibration Status
-1			2/16/2017 8:33:58 PM
Data Filename	ACQ Method	Comment	Acquired Time
LG-3-49.d	chen-ms.m		



LG-2-55  
PROTON



LG-2-55  
C13CPD



Crystal data and structure refinement for **2d**.

Identification code	<b>2d</b>
Empirical formula	C <sub>25</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>
Formula weight	431.48
Temperature	113(2) K
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 10.901(2) Å    alpha = 90 deg. b = 18.268(3) Å    beta = 100.519(5) deg. c = 10.756(2) Å    gamma = 90 deg.
Volume	2106.0(7) Å <sup>3</sup>
Z, Calculated density	4, 1.361 Mg/m <sup>3</sup>
Absorption coefficient	0.093 mm <sup>-1</sup>
F(000)	912
Crystal size	0.20×0.18 ×0.12 mm
Theta range for data collection	3.15 to 27.54 deg.
Limiting indices	-13≤h≤14, -23≤k≤23, -13≤l≤13
Reflections collected / unique	26655 / 4813 [R(int) = 0.0327]
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)
Data / restraints / parameters	4813 / 1 / 296
Goodness-of-fit on F <sup>2</sup>	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0890
R indices (all data)	R1 = 0.0455, wR2 = 0.0951
Largest diff. peak and hole	0.289 and -0.265 e. Å <sup>-3</sup>
CCDC numbers	1827519