

## Supporting Information

### **Bimetallic Copper and Zinc -Catalyzed Oxidative Cycloaddition of 3-Aminopyridazines and Nitriles: A Direct Synthesis of 1,2,4-Triazolo[1,5-b]pyridazines via C-N and N-N Bond-forming Process**

Qiu-Chao Mu<sup>a,b</sup>, Ji-Yuan Lv<sup>b</sup>, Mu-Yi Chen<sup>b</sup>, Xing-Feng Bai<sup>a,b</sup>, Jing Chen<sup>\*a</sup>, Chun-Gu Xia<sup>a</sup>,  
and Li-Wen Xu<sup>\*a,b</sup>

<sup>a</sup> State Key Laboratory for Oxo Synthesis and Selective Oxidation Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, and University of the Chinese Academy of Sciences, P. R. China. E-mail: [liwenxu@hznu.edu.cn](mailto:liwenxu@hznu.edu.cn).

<sup>b</sup> Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, Hangzhou Normal University, Hangzhou 311121, P. R. China. Fax: 862886 5135; Tel: 86 2886 5135

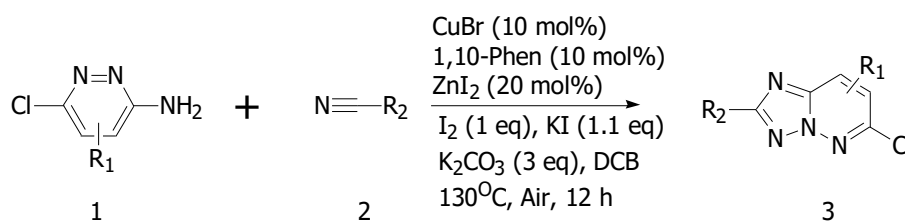
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## S-1. General Information

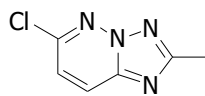
Reagents were purchased from commercial sources and were used as received unless mentioned otherwise. Reactions were monitored by thin layer chromatography using silica gel.  $^1\text{H}$  NMR was recorded at 300 MHz and 400 MHz: chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard (DMSO- $d_6$  at 2.50).  $^{13}\text{C}$  NMR was recorded at 75 MHz and 100 MHz: chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard (DMSO- $d_6$  at 39.52). High-resolution mass spectra (HRMS) were recorded by an Agilent instrument with ESI-MS technique. LC-MS was recorded by Shimadzu LCMS-2020, equipped with an ESI ion source in the positive ionization mode.

## S-2. General Procedure



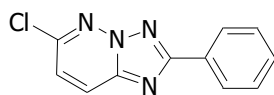
To a dried vial was added 1 (0.77 mmol), 2 (1.93 mmol), CuBr (11.05 mg, 0.077 mmol), 1,10-phenanthroline (13.9mg, 0.077 mmol), ZnI<sub>2</sub> (49.2 mg, 0.154 mmol), I<sub>2</sub> (195.6 mg, 0.77 mmol), KI (141.1 mg, 0.85 mmol) and K<sub>2</sub>CO<sub>3</sub> (319.2 mg, 2.31 mmol). 1,2-Dichlorobenzene (5 ml) was then added. The reaction mixture was stirred at 130 °C for 12 h in pre-heated oil bath. After cooling to room temperature, the reaction was diluted with EtOAc and filtered over glass filter. The filtrate was concentrated and purified by column chromatography on silica gel.

### Characterization of 3a-3n:



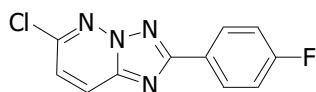
3a

6-Chloro-2-methyl-[1,2,4]triazolo[1,5-b]pyridazine (3a): light yellow solid; 63% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta$  = 8.42 (d,  $J$  = 9.0 Hz, 1H), 7.80 (d,  $J$  = 9.0 Hz, 1H), 2.54 (s, 3H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta$  = 162.8, 146.3, 144.3, 127.2, 125.1, 14.9. LC/MS: 100% purity,  $[\text{M}+\text{H}]^+$  = 169. HR-MS calcd for  $\text{C}_6\text{H}_6\text{ClN}_4$   $[\text{M}+\text{H}]^+$ : 169.0279. found: 169.0281.



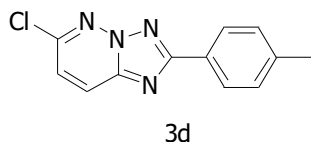
3b

6-Chloro-2-phenyl-[1,2,4]triazolo[1,5-b]pyridazine (3b): light yellow solid; 63% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta$  = 8.55 (d,  $J$  = 9.0 Hz, 1H), 8.23-8.20 (m, 2H), 7.86 (d,  $J$  = 9.0 Hz, 1H), 7.61-7.55 (m, 3H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta$  = 162.3, 146.9, 145.1, 131.1, 130.2, 129.5, 127.8, 127.2, 125.7. LC/MS: 99.2% purity,  $[\text{M}+\text{H}]^+$  = 231. HR-MS calcd for  $\text{C}_{11}\text{H}_8\text{ClN}_4$   $[\text{M}+\text{H}]^+$ : 231.0438. found: 231.0437.

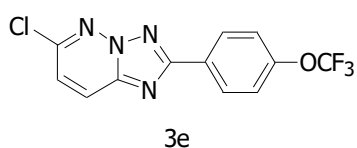


3c

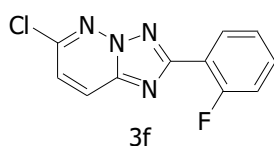
6-Chloro-2-(4-fluoro-phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3c): light yellow solid; 52% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta$  = 8.54 (d,  $J$  = 9.0 Hz, 1H), 8.26-8.20 (m, 2H), 7.87 (d,  $J$  = 12.0 Hz, 1H), 7.43-7.37 (m, 2H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta$  = 165.7, 162.4, 161.4, 147.0, 145.2, 129.6 (d,  $J$  = 9.0 Hz), 127.8, 126.8 (d,  $J$  = 3.0 Hz), 125.8, 116.7 (d,  $J$  = 21.7 Hz).  $^{19}\text{F}$  (282 MHz, DMSO- $d_6$ )  $\delta$  = -109.9. LC/MS: 99.4% purity,  $[\text{M}+\text{H}]^+$  = 249. HR-MS calcd for  $\text{C}_{11}\text{H}_7\text{ClFN}_4$   $[\text{M}+\text{H}]^+$ : 249.0345. found: 249.0343.



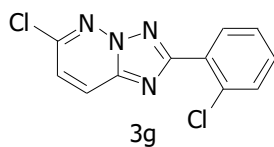
6-Chloro-2-p-tolyl-[1,2,4]triazolo[1,5-b]pyridazine (3d): light yellow solid; 36% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 8.56-8.53 (m, 1H), 8.15-8.12 (m, 2H), 7.89-7.83 (m, 1H), 7.40 (d,  $J$  = 8.0 Hz, 2H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$  = 162.4, 146.7, 145.1, 141.0, 130.1, 127.7, 127.4, 127.1, 125.6, 117.5, 21.5. LC/MS: 99.1% purity,  $[\text{M}+\text{H}]^+$  = 245. HR-MS calcd for  $\text{C}_{12}\text{H}_{10}\text{ClN}_4$   $[\text{M}+\text{H}]^+$ : 245.0601. found: 245.0594.



6-Chloro-2-(4-trifluoromethoxy-phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3e): light yellow solid; 18% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 8.62-8.59 (m, 1H), 8.25-8.21 (m, 1H), 7.93-7.90 (m, 1H), 7.67-7.61 (m, 1H), 7.49-7.42 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$  = 161.07, 150.39, 147.2, 145.3, 129.4 (d,  $J$  = 11.0 Hz), 128.0, 126.0, 122.0. LC/MS: 98.1% purity,  $[\text{M}+\text{H}]^+$  = 315. HR-MS calcd for  $\text{C}_{12}\text{H}_7\text{ClF}_3\text{N}_4\text{O}$   $[\text{M}+\text{H}]^+$ : 315.0268. found: 315.026.

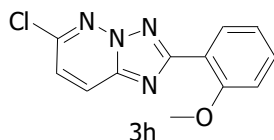


6-Chloro-2-(2-fluoro-phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3f): light yellow solid; 34% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 8.61-8.58 (m, 1H), 8.38-8.35 (m, 2H), 7.93-7.90 (m, 1H), 7.60 (d,  $J$  = 8.0 Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$  = 161.7, 159.1-158.9 (t,  $J$  = 19.0 Hz, 5.0 Hz), 147.3, 144.5, 133.0 (d,  $J$  = 8.0 Hz), 130.8 (d,  $J$  = 2.0 Hz), 128.0, 126.0, 125.4 (d,  $J$  = 4.0 Hz), 118.1 (d,  $J$  = 11.0 Hz), 117.3 (d,  $J$  = 21.0 Hz). LC/MS: 97.5% purity,  $[\text{M}+\text{H}]^+$  = 249. HR-MS calcd for  $\text{C}_{11}\text{H}_7\text{ClFN}_4$   $[\text{M}+\text{H}]^+$ : 249.0346. found: 249.0343.

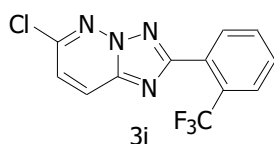


6-Chloro-2-(2-chloro-phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3g):

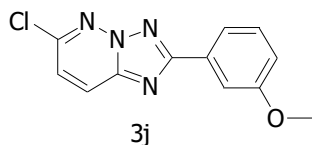
light yellow solid; 22% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 8.65-8.62 (m, 1H), 8.07 (d,  $J$  = 4.0 Hz, 2H), 8.04 (d,  $J$  = 8.0 Hz, 1H), 7.95-7.92 (m, 1H), 7.71-7.55 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$  = 160.9, 147.5, 144.6, 132.4 (d,  $J$  = 7.0 Hz), 132.1, 131.4, 129.2, 128.0 (d,  $J$  = 16.0 Hz), 126.1. LC/MS: 99.2% purity,  $[\text{M}+\text{H}]^+$  = 265.1. HR-MS calcd for  $\text{C}_{11}\text{H}_7\text{Cl}_2\text{N}_4$   $[\text{M}+\text{H}]^+$ : 265.0049. found: 265.0048.



6-Chloro-2-(2-methoxy-phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3h): light yellow solid; 22% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta$  = 8.52-8.49 (t,  $J$  = 6.0 Hz, 3.0 Hz, 1H), 7.97-7.90 (m, 1H), 7.83 (d,  $J$  = 9.0 Hz, 1H), 7.53-7.47 (m, 1H), 7.22-7.12 (t,  $J$  = 9.0 Hz, 21 Hz, 1H), 7.09-7.07 (t,  $J$  = 6.0 Hz, 1H), 3.85 (s, 3H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta$  = 161.3, 158.1, 146.7, 144.0, 132.2, 131.3, 127.6, 125.4, 120.9, 119.3, 112.9, 56.2. LC/MS: 90.2% purity,  $[\text{M}+\text{H}]^+$  = 261. HR-MS calcd for  $\text{C}_{12}\text{H}_{10}\text{ClN}_4\text{O}$   $[\text{M}+\text{H}]^+$ : 261.0548. found: 261.0543.

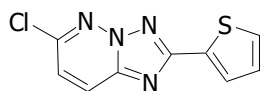


6-Chloro-2-(2-(trifluoromethyl)phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3i): light yellow solid; 39% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 8.61-8.59 (m, 1H), 7.98-7.94 (m, 2H), 7.93 (d,  $J$  = 12.0 Hz, 1H), 7.88-7.80 (m, 1H), 7.79-7.75 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$  = 161.4, 147.7, 144.4, 133.1 (d,  $J$  = 23.0 Hz), 131.1, 129.5 (d,  $J$  = 3.0 Hz), 128.2, 127.9, 127.4-127.2 (m), 126.2, 125.5, 122.8.  $^{19}\text{F}$  (376 MHz, DMSO- $d_6$ )  $\delta$  = -56.9. LC/MS: 97.5% purity,  $[\text{M}+\text{H}]^+$  = 299. HR-MS calcd for  $\text{C}_{12}\text{H}_7\text{ClF}_3\text{N}_4$   $[\text{M}+\text{H}]^+$ : 299.0315. found: 299.0311.



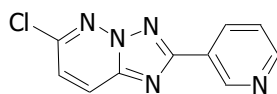
6-Chloro-2-(3-methoxy-phenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3j): light yellow solid; 27% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 8.46 (d,  $J$  = 8.0 Hz, 1H), 7.79-7.73 (m, 2H),

7.66-7.64 (m, 1H), 7.44 (d,  $J = 8.0$  Hz, 1H), 7.09-7.06 (m, 1H), 3.83 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta = 162.1, 160.0, 147.0, 145.0, 131.4, 130.7, 127.7, 125.7, 119.5, 117.0, 112.0, 55.6$ . LC/MS: 98.9% purity,  $[\text{M}+\text{H}]^+ = 261$ . HR-MS calcd for  $\text{C}_{12}\text{H}_{10}\text{ClN}_4\text{O}$   $[\text{M}+\text{H}]^+$ : 261.0551. found: 261.0543.



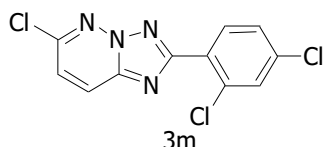
3k

6-Chloro-2-(Thiophen-2-yl)-[1,2,4]triazolo[1,5-b]pyridazine (3k): light yellow solid; 30% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta = 8.48$  (d,  $J = 12.0$  Hz, 1H), 7.86-7.79 (m, 3H), 7.25-7.22 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta = 158.6, 146.8, 145.0, 132.9, 130.1, 129.0$  (d,  $J = 26.0$  Hz), 127.4, 125.9. LC/MS: 89.7% purity,  $[\text{M}+\text{H}]^+ = 237.1$ . HR-MS calcd for  $\text{C}_9\text{H}_6\text{ClN}_4\text{S}$   $[\text{M}+\text{H}]^+$ : 237.0014. found: 237.0002.



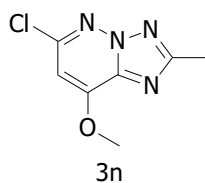
3l

6-Chloro-2-(Pyridin-4-yl)-[1,2,4]triazolo[1,5-b]pyridazine (3l): light yellow solid; 39% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta = 9.33$  (s, 1H), 8.73-8.72 (m, 1H), 8.57-8.48 (m, 2H), 7.89 (d,  $J = 12.0$  Hz, 1H), 7.62-7.57 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta = 160.2, 151.9, 148.1, 147.4, 145.2, 134.6, 128.0, 126.2$  (d,  $J = 8.4$  Hz), 124.6. LC/MS: 99.3% purity,  $[\text{M}+\text{H}]^+ = 232$ . HR-MS calcd for  $\text{C}_{10}\text{H}_7\text{ClN}_5$   $[\text{M}+\text{H}]^+$ : 232.0389. found: 232.039.



3m

6-Chloro-2-(2,4-dichlorophenyl)-[1,2,4]triazolo[1,5-b]pyridazine (3m): light yellow solid; 22% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta = 8.59$  (d,  $J = 9.0$  Hz, 1H), 8.08 (d,  $J = 9.0$  Hz, 1H), 7.89-7.81 (m, 2H), 7.62-7.59 (m, 1H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta = 160.0, 147.6, 144.3, 136.0, 133.5$  (d,  $J = 6.7$  Hz), 130.9, 128.2 (t,  $J = 8.2$  Hz, 2.2 Hz), 126.1. LC/MS: 87.8% purity,  $[\text{M}+\text{H}]^+ = 299$ . HR-MS calcd for  $\text{C}_{11}\text{H}_6\text{Cl}_3\text{N}_4$   $[\text{M}+\text{H}]^+$ : 298.9655. found: 298.9655.



6-Chloro-8-methoxy-2-methyl-[1,2,4]triazolo[1,5-b]pyridazine (**3n**): light yellow solid; 33% yield;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  = 7.28 (s, 1H), 4.09 (s, 3H), 2.46 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$  = 161.1, 155.5, 147.2, 139.8, 103.5, 58.4, 14.7. LC/MS: 100% purity,  $[\text{M}+\text{H}]^+ = 199$ . HR-MS calcd for  $\text{C}_7\text{H}_8\text{ClN}_4\text{O}$   $[\text{M}+\text{H}]^+$ : 199.0387. found: 199.0387.

### S-3. Gram-Scale Preparation of **3a**

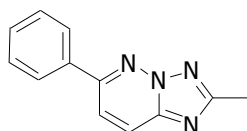
6-Chloro-2-methyl-[1,2,4]triazolo[1,5-b]pyridazine (**3a**): under the standard conditions described above, **1a** (2.0 g, 15.4 mmol), **2a** (100 ml), CuBr (220.9 mg, 1.54 mmol), 1,10-phenanthroline (277.5 mg, 1.54 mmol),  $\text{ZnI}_2$  (983.1 mg, 3.08 mmol),  $\text{I}_2$  (3.9 g, 15.4 mmol), KI (2.8 g, 16.9 mmol) and  $\text{K}_2\text{CO}_3$  (6.4 g, 46.2 mmol), in 1,2-Dichlorobenzene (20 ml), afforded **3a** (1.95 g, 75% yield) as a light yellow solid.

### S-4. Procedure and analytical data for the derivatives of **3a**

#### 1. Synthesis of **4a**

To a 25 ml round bottom Schlenk was added **3a** (100 mg, 0.59 mmol), phenylboronic acid (108.3 mg, 0.89 mmol),  $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$  (41.4 mg, 0.059 mmol),  $\text{Na}_2\text{CO}_3$  (187.6 mg, 1.77 mmol), dioxane (8 ml),  $\text{H}_2\text{O}$  (2 ml). The reaction vessel was vacuumed and backfilled with  $\text{N}_2$  (3 times). The reaction mixture was heated at 80  $^\circ\text{C}$  overnight. The reaction was cooled to r.t., diluted with  $\text{H}_2\text{O}$  and extracted with EtOAc. The combined organic layers were dried over sodium sulfate, filtered and concentrated. The residue was purified by silica gel flash chromatography.



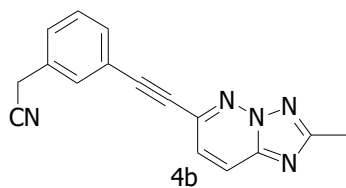


4a

2-Methyl-6-phenyl-[1,2,4]triazolo[1,5-b]pyridazine (4a): light yellow solid; 68% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta$  = 8.36 (d,  $J$  = 12.0 Hz, 1H), 8.16-8.13 (t,  $J$  = 6.0 Hz, 3.0 Hz, 1H), 8.08-8.03 (m, 2H), 7.57-7.53 (m, 3H), 2.52 (s, 3H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta$  = 162.6, 151.4, 144.3, 134.7, 131.9 (d,  $J$  = 9.7 Hz), 130.8, 129.5, 129.2 (d,  $J$  = 11.2 Hz), 127.4, 125.4, 121.8, 14.9. LC/MS: 98.7% purity,  $[\text{M}+\text{H}]^+$  = 211. HR-MS calcd for  $\text{C}_{12}\text{H}_{11}\text{N}_4$   $[\text{M}+\text{H}]^+$ : 211.0988. found: 211.0984.

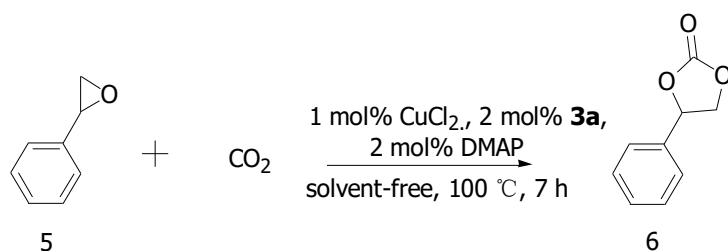
## 2. Synthesis of 4b

To a 25 ml round bottom Schlenk was added **3a** (100 mg, 0.59 mmol), arylethyne (125.6 mg, 0.89 mmol), Pd(OAc) $_2$  (13.2 mg, 0.059 mmol), RuPhos (55.0 mg, 0.118 mmol), Et $_3$ N (179.1 mg, 1.77 mmol), CH $_3$ CN (10 ml). The reaction vessel was vacuumed and backfilled with N $_2$  (3 times). The reaction mixture was heated at 80 °C overnight. The reaction was cooled to r.t., diluted with H $_2$ O and extracted with EtOAc. The combined organic layers were dried over sodium sulfate, filtered and concentrated. The residue was purified by silica gel flash chromatography.



[3-(2-Methyl-[1,2,4]triazolo[1,5-b]pyridazin-6-ylethynyl)-phenyl]-acetonitrile (4b): light yellow solid; 59% yield;  $^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ )  $\delta$  = 8.35 (d,  $J$  = 9.0 Hz, 1H), 7.82-7.76 (t,  $J$  = 9.0 Hz, 9.0 Hz, 1H), 7.66-7.62 (m, 2H), 7.54-7.47 (m, 2H), 4.10 (s, 2H), 2.53 (s, 3H).  $^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ )  $\delta$  = 163.4, 144.4, 137.7, 132.8, 131.9 (d,  $J$  = 21.0 Hz), 130.4 (d,  $J$  = 26.2 Hz), 126.4, 125.3, 121.2, 119.2, 92.1, 85.3, 22.5, 14.9. LC/MS: 99.6% purity,  $[\text{M}+\text{H}]^+$  = 274. HR-MS calcd for  $\text{C}_{16}\text{H}_{12}\text{N}_5$   $[\text{M}+\text{H}]^+$ : 274.1093. found: 274.1093.

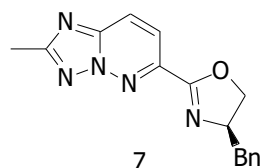
## S-5. Procedure for 6



$\text{CO}_2$  (g) from a gas balloon was allowed to react with **5** (500mg, 4.16 mmol),  $\text{CuCl}_2$  (5.6 mg, 0.04 mmol), **3a** (13.5 mg, 0.08 mmol), DMAP (9.8 mg, 0.08 mmol) at 100 °C for 7 h in pre-heated oil bath. GC-MS of the crude reaction mixture in EtOAc showed 82% conversion of the starting epoxide to the desired product **6**.

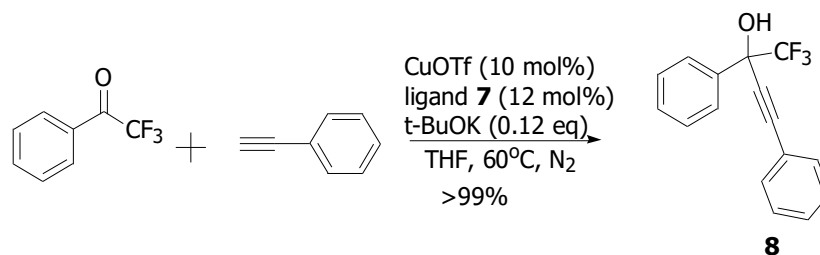
## S-6. Procedure for 7

To an oven dried Schlenk tube were added oxazoline (389 mg, 2.4 mmol),  $\text{Pd}(\text{OAc})_2$  (44.5 mg, 0.2 mmol), dppe (96 mg, 0.24 mmol) and  $\text{LiOtBu}$  (320 mg, 4.0 mmol) under  $\text{N}_2$ . The tube was degassed with  $\text{N}_2$  three times and addition of **3a** (340 mg, 2 mmol) to the reaction vessel was followed by the addition of anhydrous Dioxane (5 ml). The reaction mixture was stirred in an oil bath at 100 °C for 12h, and then cooled to room temperature, diluted with  $\text{H}_2\text{O}$  and extracted with EtOAc. The combined organic layers were dried over sodium sulfate, filtered and concentrated. The residue was purified by silica gel flash chromatography.



6-(4-Benzyl-4,5-dihydro-oxazol-2-yl)-2-methyl-1,2,4-triazolo[1,5-b]pyridazine (**7**): light yellow solid; 70% yield;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  = 8.06 (d,  $J$  = 12.0 Hz, 1H), 7.99 (d,  $J$  = 12.0 Hz, 1H), 7.21-7.18 (m, 5H), 4.65-4.61 (m, 1H), 4.50-4.45 (t,  $J$  = 12.0 Hz, 8 Hz, 1H), 4.26-4.22 (t,  $J$  = 8.0 Hz, 8 Hz, 1H), 3.19-3.14 (m, 1H), 2.78-2.73 (m, 1H), 2.62 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  = 164.6, 160.4, 145.2, 141.5, 137.2, 129.2, 128.6, 126.7, 124.0, 122.2, 73.0, 68.1, 41.4, 15.0. HR-MS calcd for  $\text{C}_{16}\text{H}_{15}\text{N}_5\text{NaO}$   $[\text{M}+\text{Na}]^+$ : 316.1169. found: 316.1160.

## S-7. Procedure for 8

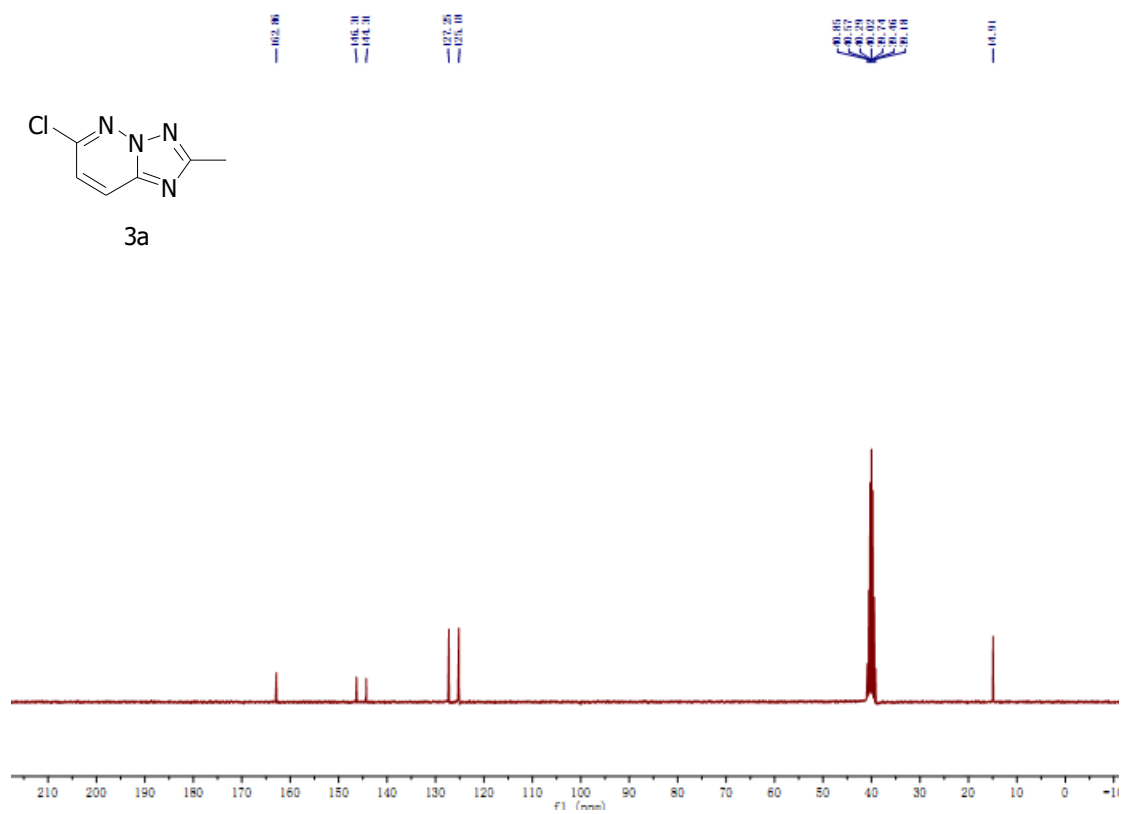
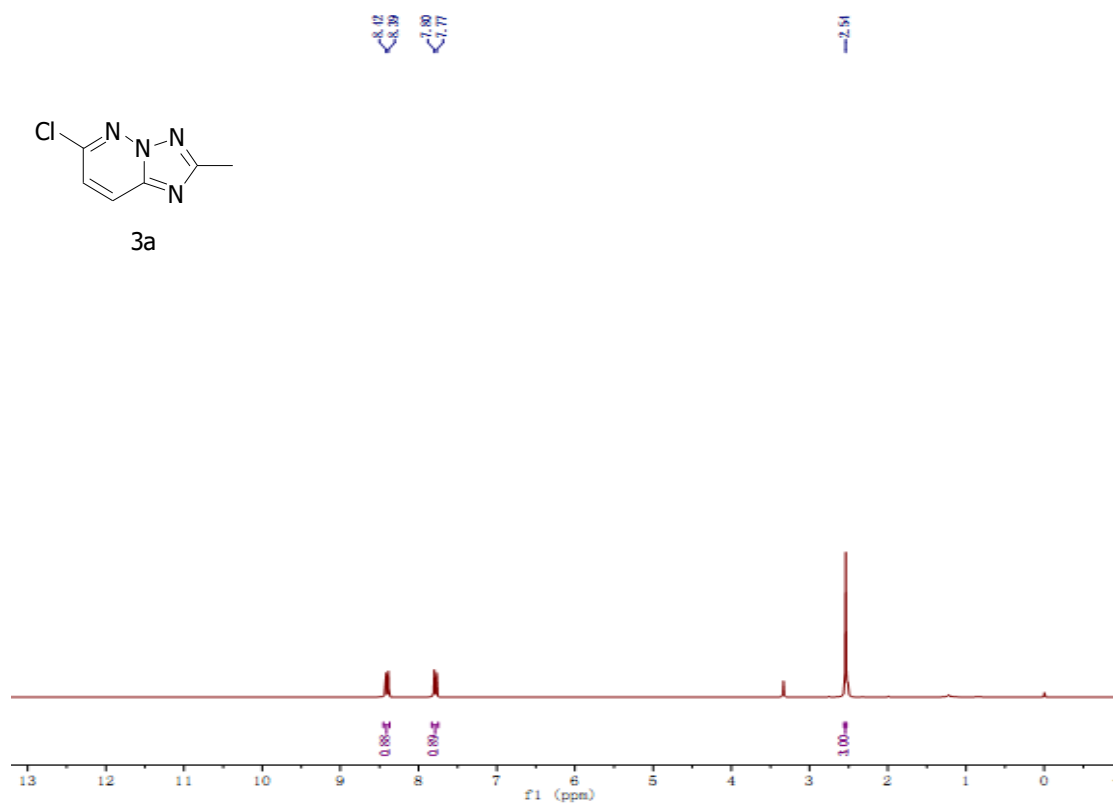


To a CuOTf • 1/2benzene (10 mol%), KOtBu (0.12 eq) and ligand **7** (12 mol%) in THF (2 ml) under N<sub>2</sub>, trifluoroacetophenone (1 eq) and alkyne (2 eq) were added at room temperature. The mixture was warmed up to 60 °C. After 12 h, the reaction mixture was diluted with AcOEt, and SiO<sub>2</sub> was added. Filtration, removal of the solvent gave crude product as brown oil. GC-MS of the crude reaction mixture in EtOAc showed 99% conversion of the starting trifluoroacetophenone to the desired product **8**.

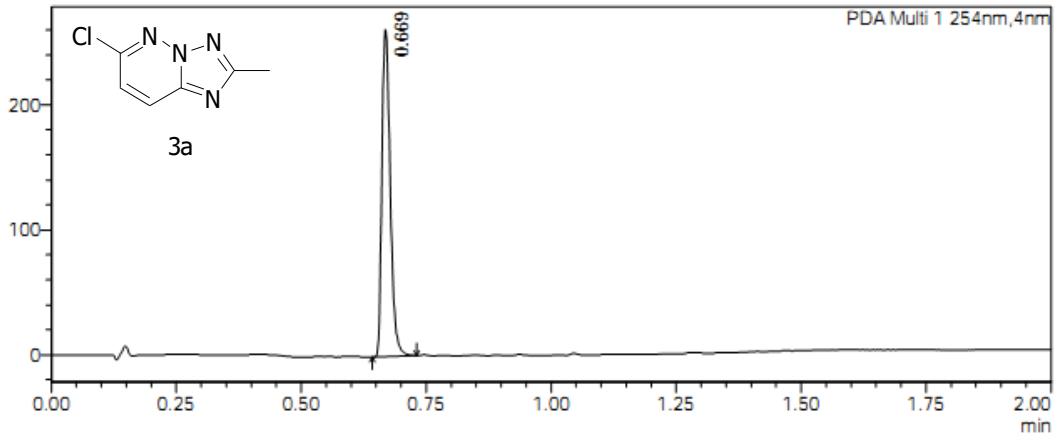
## S-8. References

1. For synthesis of 3a, 3b, please see: Y. Tamura, J. H. Kim, M. Ikeda, *J. Heterocyclic. Chem.* **1975**, 12, 107-108.
2. For synthesis of 6, please see: A. Kilic, A. A. Palali, M. Durgun, Z. Tasci, M. Ulusoy, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*. **2013**, 113, 432-438.

## S-9. NMR Spectra



mAU



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.669	261613	100.000	303476	100.000
Total		261613	100.000	303476	100.000

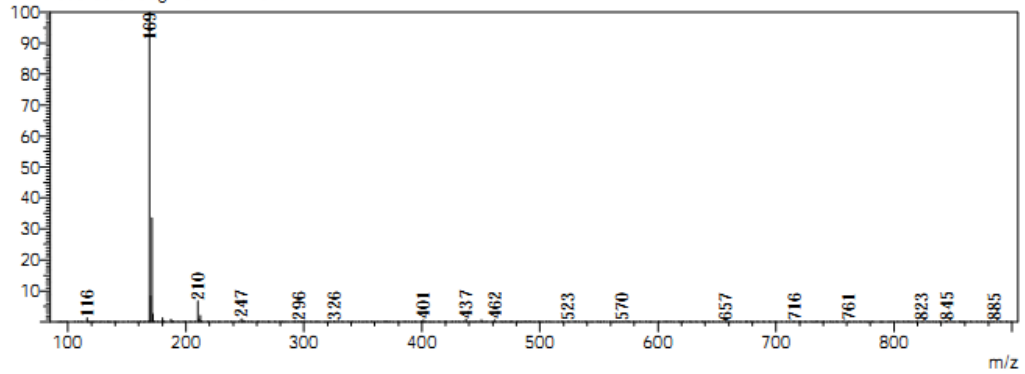
Mass Spectrum

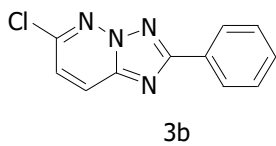
Line#:1 R.Time:0.665(Scan#:90)

MassPeaks:394

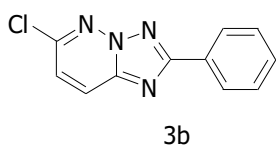
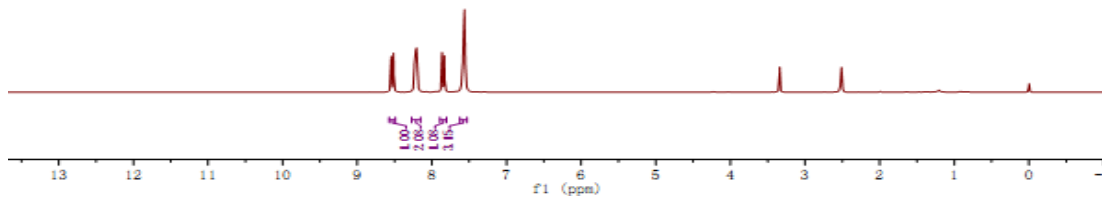
Spectrum Mode:Averaged 0.656-0.673(89-91) BasePeak:169(753680)

BG Mode:Calc Segment 1 - Event 1



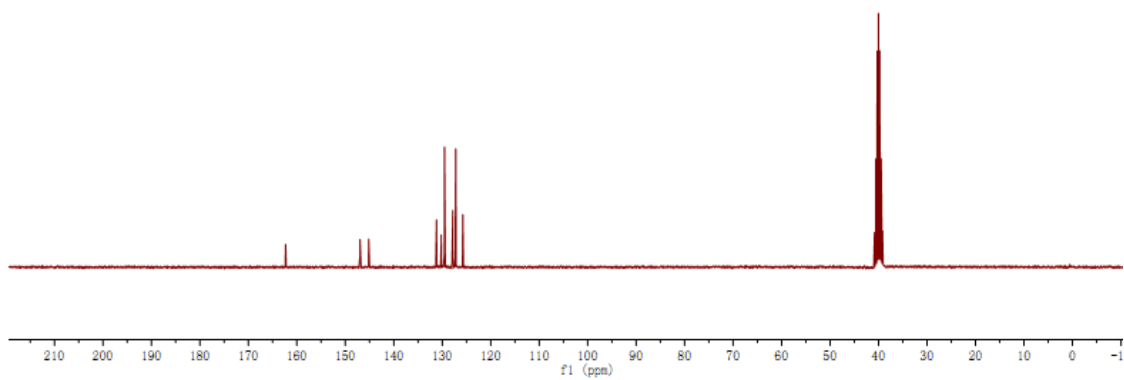


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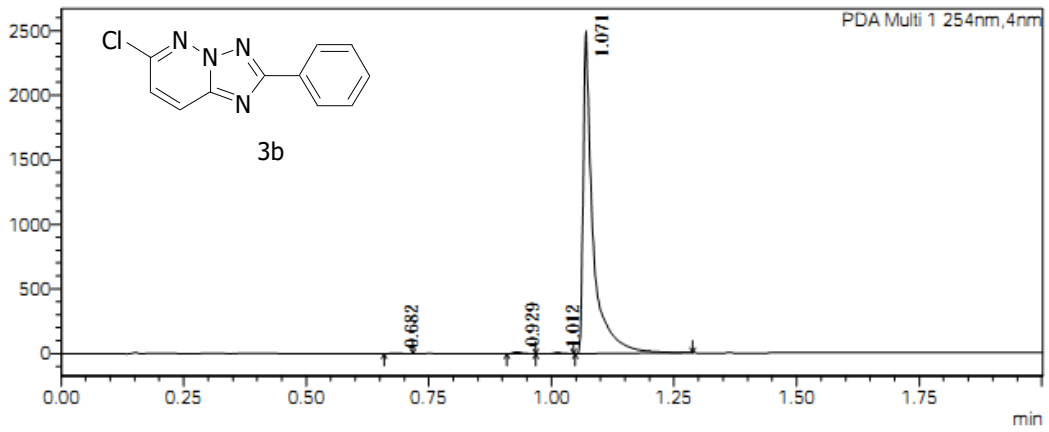


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Peak Table

PDA Ch1 254nm

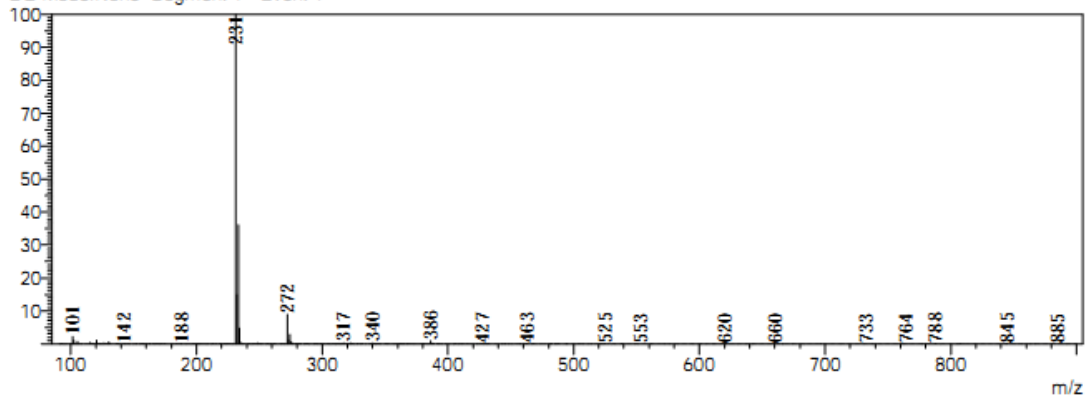
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.682	4363	0.178	6757	0.194
2	0.929	12435	0.508	13806	0.397
3	1.012	6764	0.277	7095	0.204
4	1.071	2421983	99.037	3450859	99.205
Total		2445545	100.000	3478517	100.000

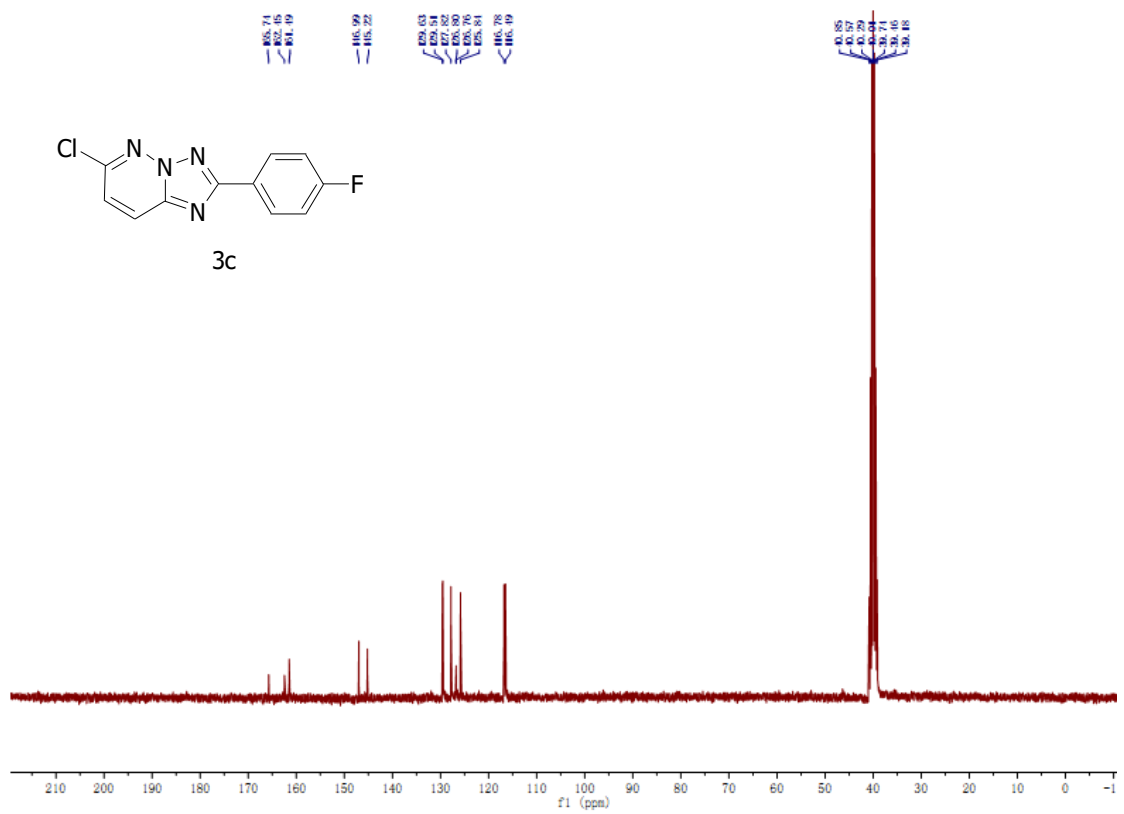
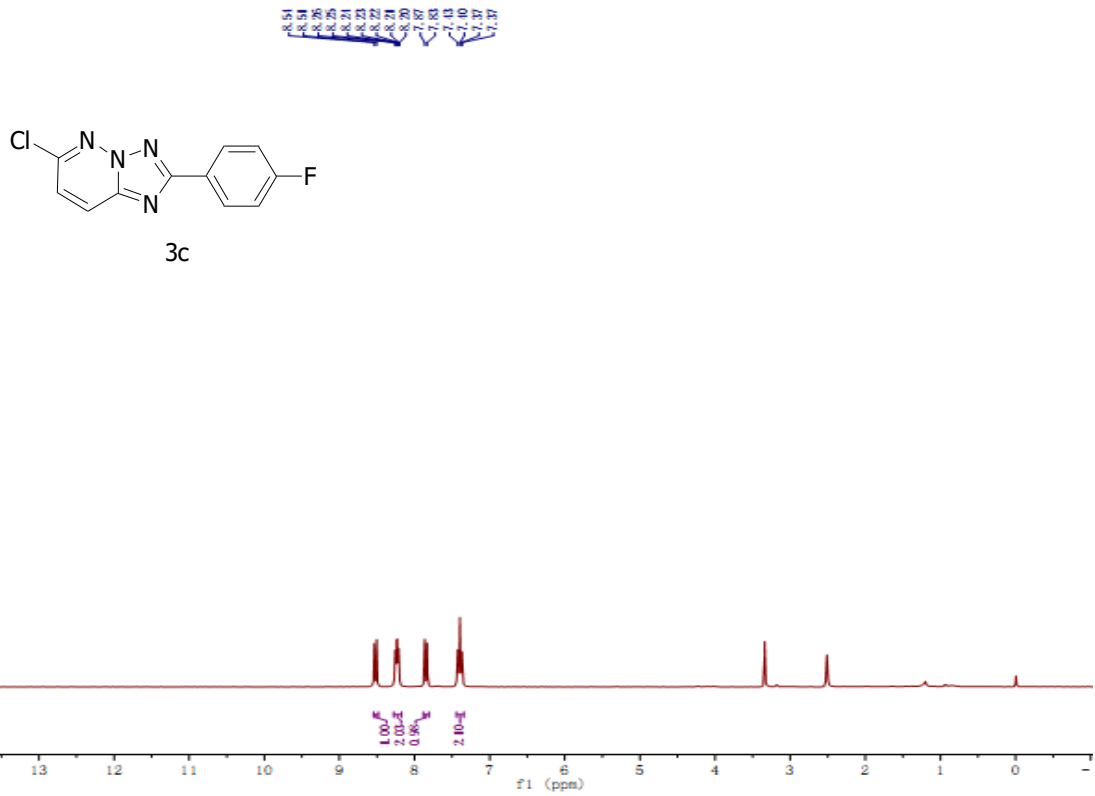
Line#:2 R.Time:1.081(Scan#:140)

MassPeaks:630

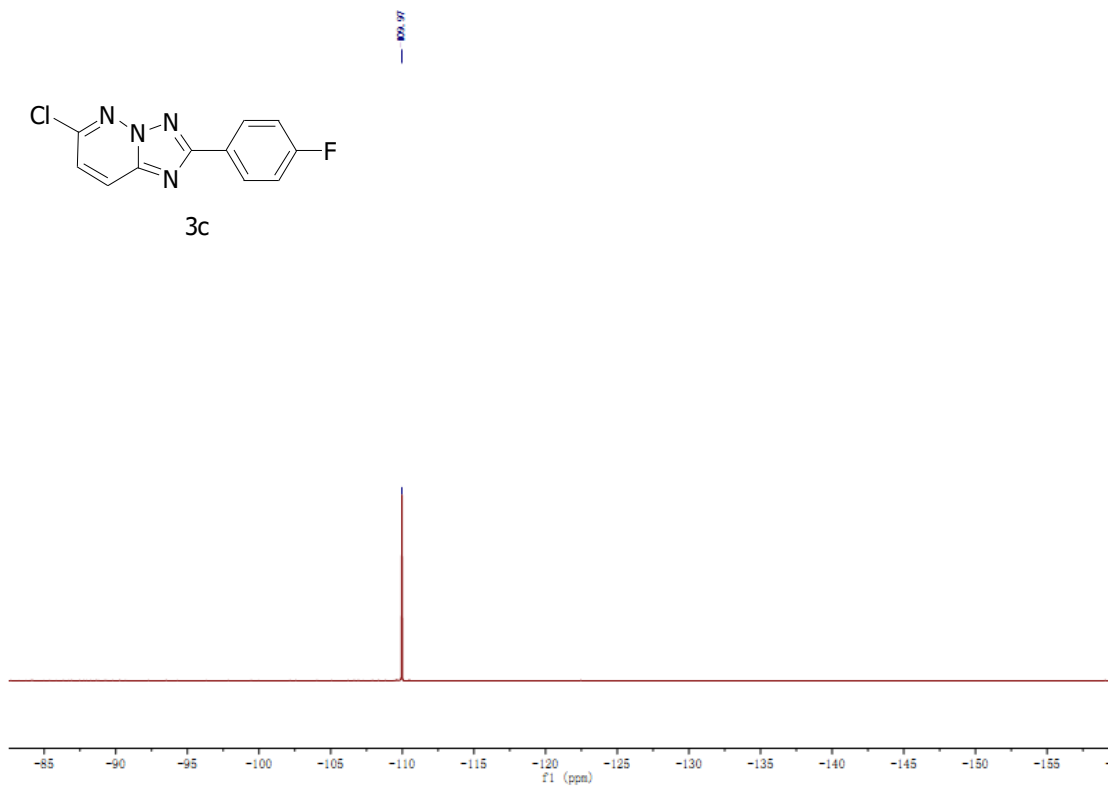
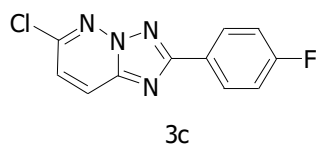
Spectrum Mode:Single 1.081(140) BasePeak:231(1674587)

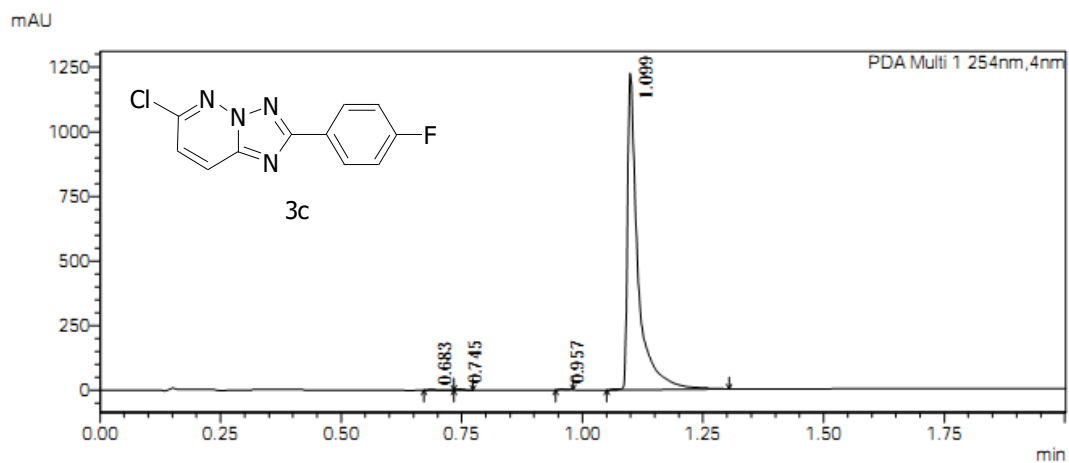
BG Mode:None Segment 1 - Event 1







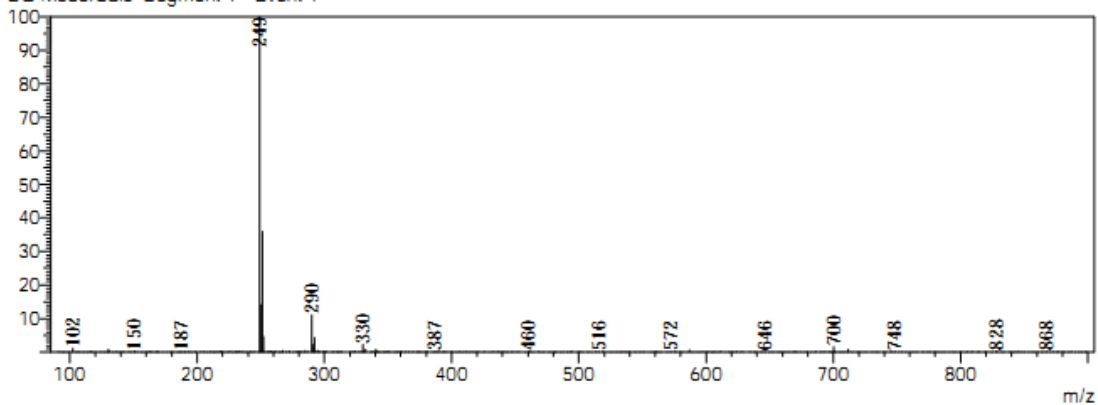


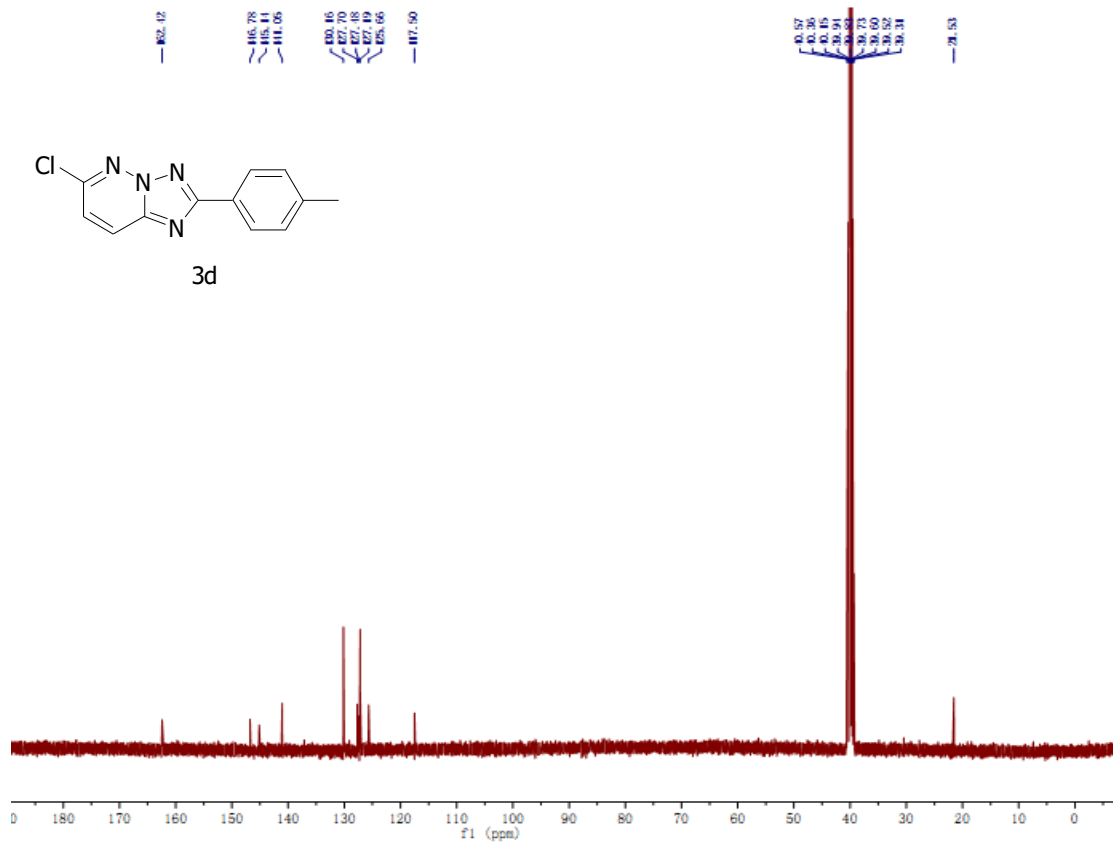
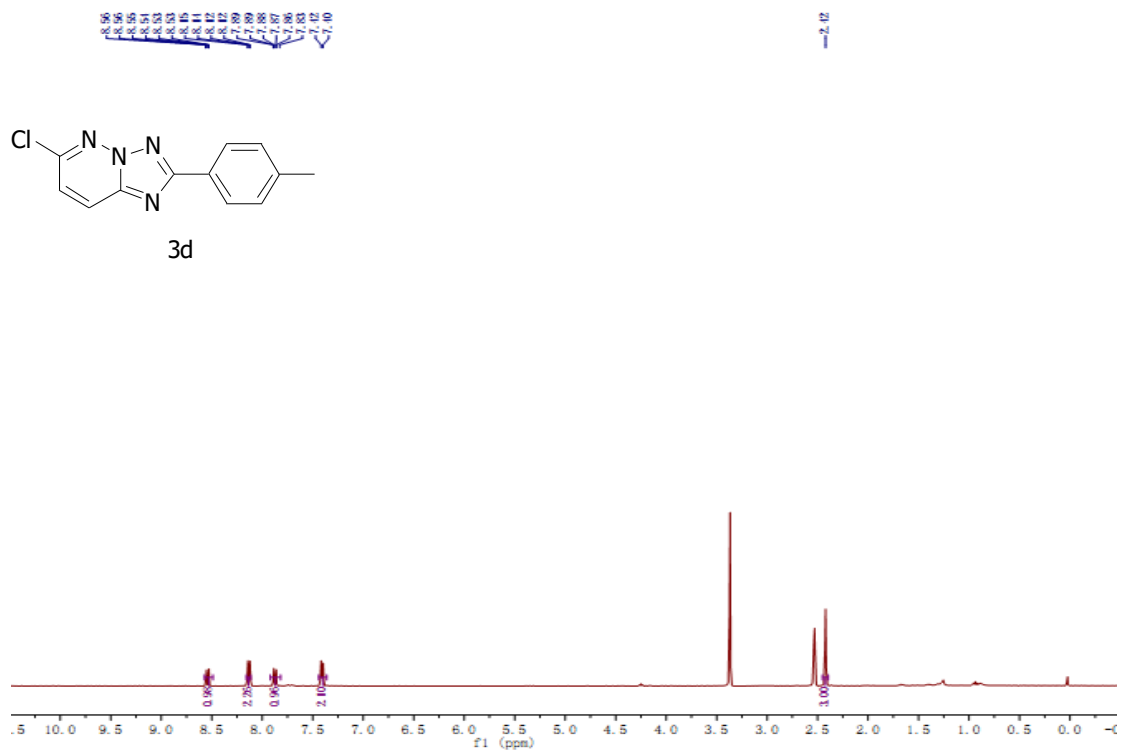


Peak Table

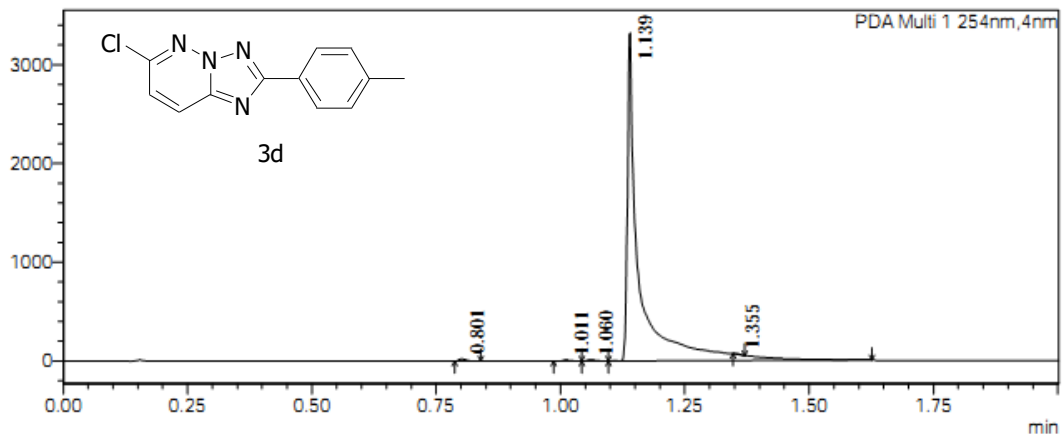
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.683	2180	0.180	3309	0.178
2	0.745	4976	0.411	4806	0.258
3	0.957	2713	0.224	2547	0.137
4	1.099	1200069	99.184	1849859	99.427
Total		1209937	100.000	1860521	100.000

Line#:1 R.Time:1.098(Scan#:142)  
 MassPeaks:434  
 Spectrum Mode:Averaged 1.090-1.106(141-143) BasePeak:249(620070)  
 BG Mode:Calc Segment 1 - Event 1





mAU



Peak Table

PDA Ch1 254nm

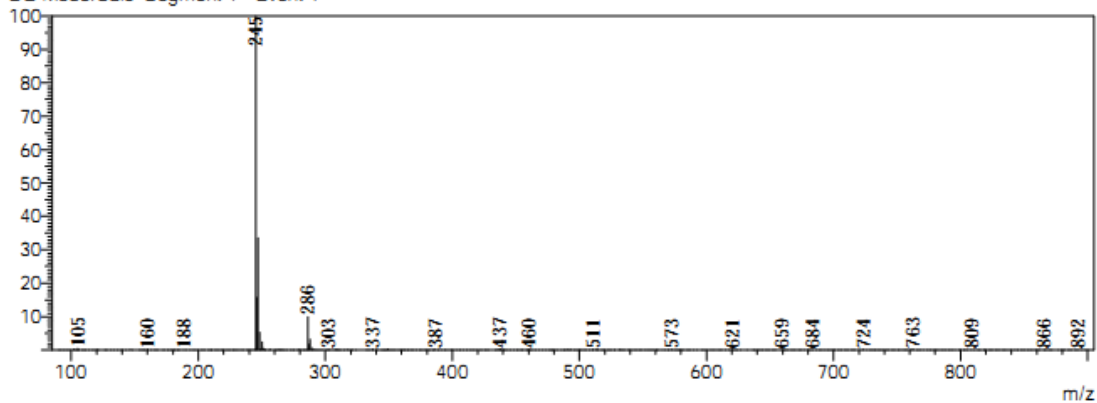
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.801	21350	0.671	20146	0.365
2	1.011	9224	0.290	9805	0.178
3	1.060	11386	0.358	12799	0.232
4	1.139	3131172	98.371	5468693	99.129
5	1.355	9901	0.311	5292	0.096
Total		3183033	100.000	5516735	100.000

Line#:1 R.Time:1.140(Scan#:147)

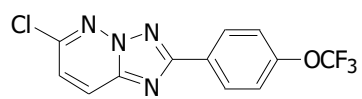
MassPeaks:470

Spectrum Mode:Averged 1.131-1.148(146-148) BasePeak:245(1650455)

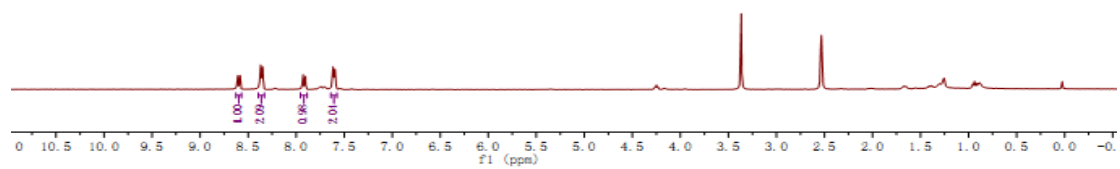
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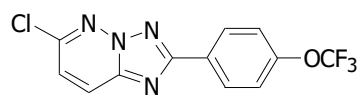
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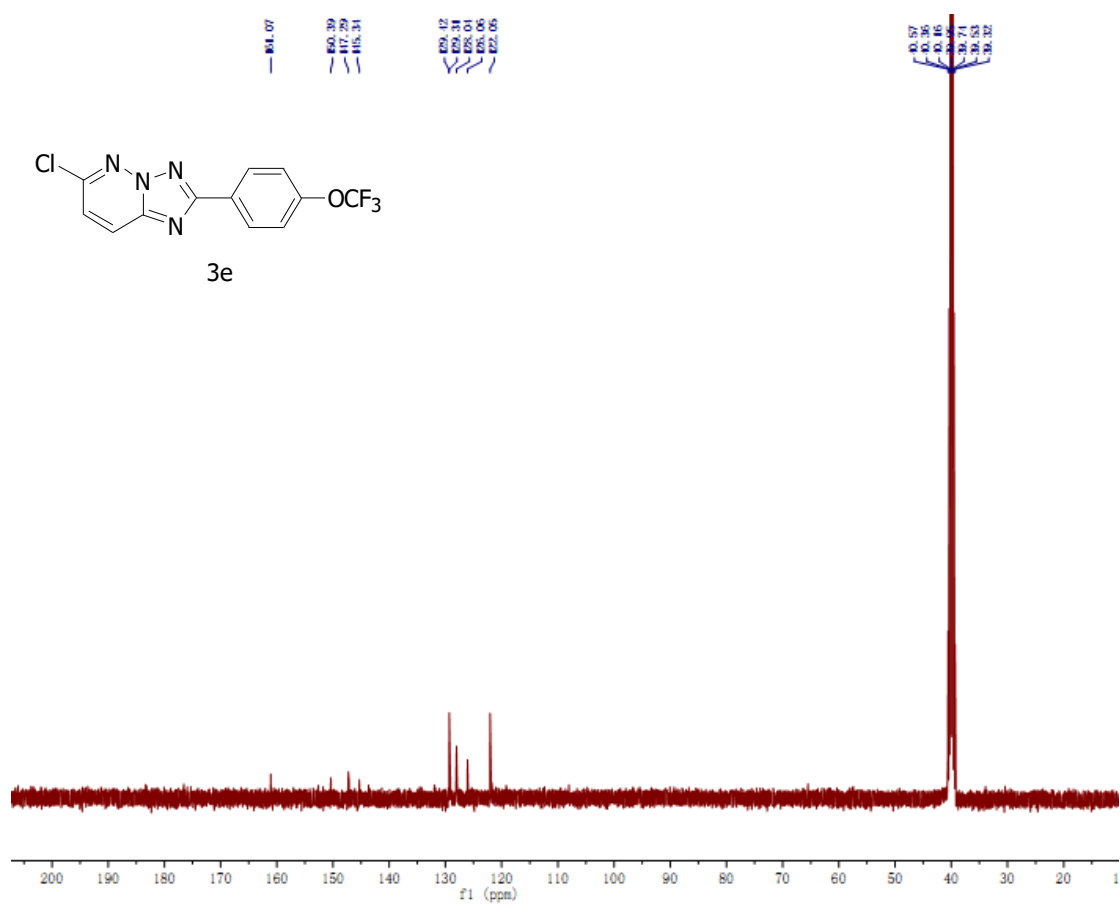
3e

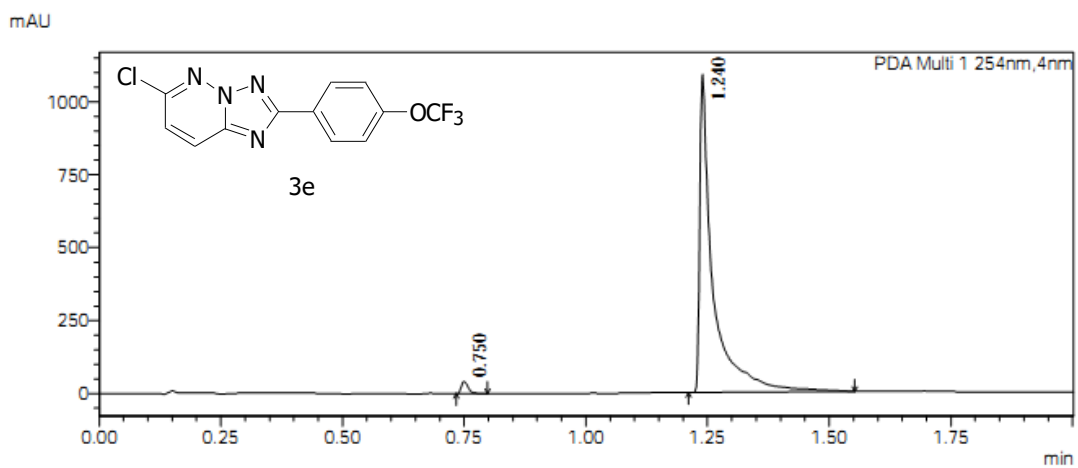


161.07  
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149.39  
148.31  
129.12  
128.11  
127.01  
125.05  
124.05



3e

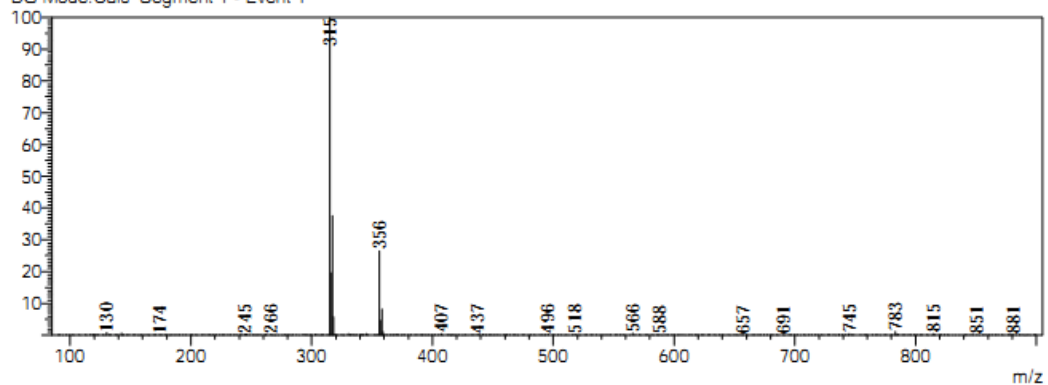




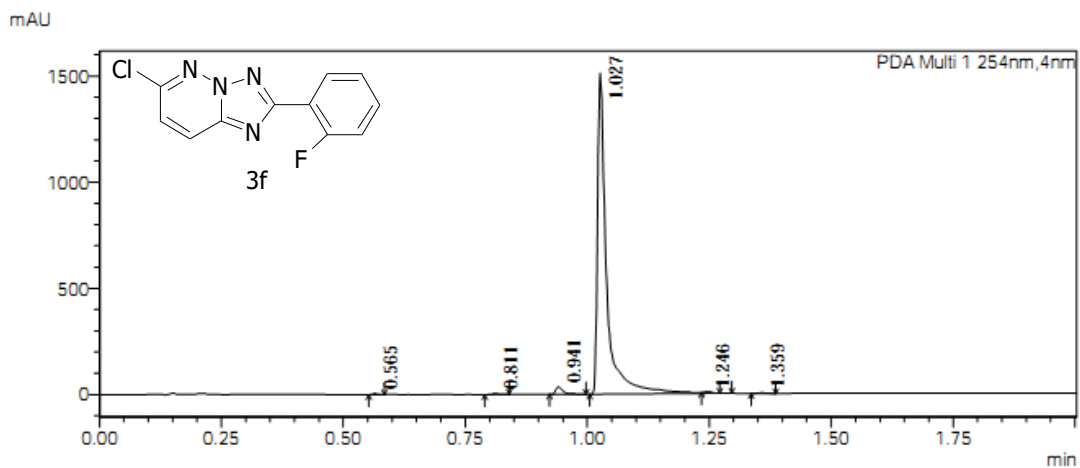
Peak Table

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.750	40047	3.561	40127	1.897
2	1.240	1084424	96.439	2075182	98.103
Total		1124471	100.000	2115309	100.000

Line#:1 R.Time:1.240(Scan#:159)  
 MassPeaks:382  
 Spectrum Mode:Averaged 1.231-1.248(158-160) BasePeak:315(611193)  
 BG Mode:Calc Segment 1 - Event 1





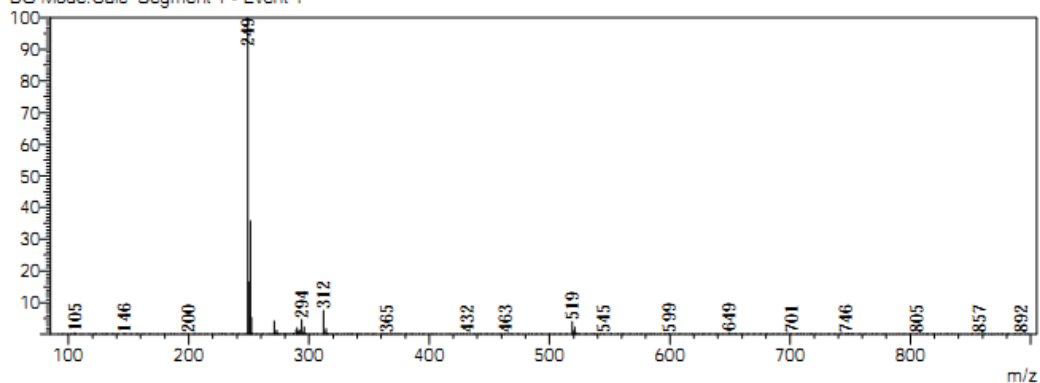


PDA Ch1 254nm

Peak Table

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.565	3651	0.237	2870	0.142
2	0.811	3054	0.198	3095	0.154
3	0.941	34292	2.227	36707	1.821
4	1.027	1491056	96.844	1965868	97.516
5	1.246	4132	0.268	3799	0.188
6	1.359	3465	0.225	3605	0.179
Total		1539650	100.000	2015945	100.000

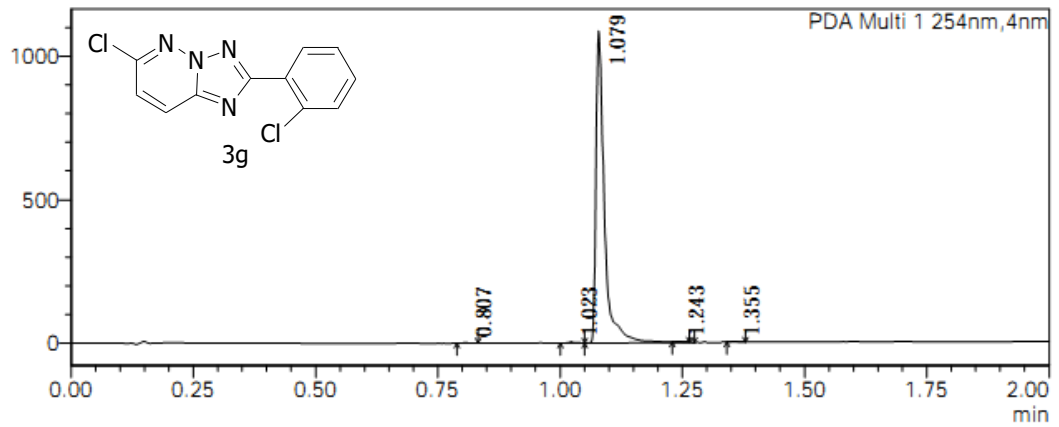
Line#:1 R.Time:1.023(Scan#:133)  
 MassPeaks:353  
 Spectrum Mode:Averaged 1.015-1.031(132-134) BasePeak:249(896040)  
 BG Mode:Calc Segment 1 - Event 1







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Peak Table

PDA Ch1 254nm

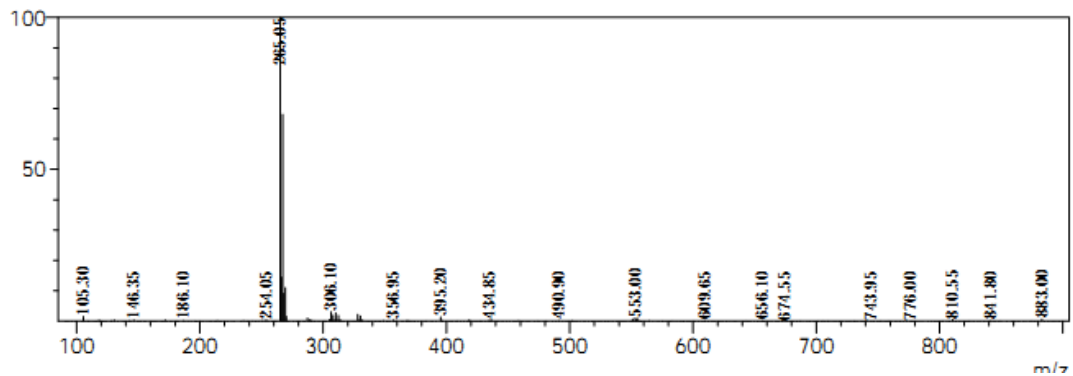
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.807	2307	0.211	2312	0.175
2	1.023	2929	0.268	3530	0.268
3	1.079	1082494	99.036	1308083	99.201
4	1.243	2311	0.211	2119	0.161
5	1.355	2989	0.274	2578	0.195
Total		1093030	100.000	1318622	100.000

Line#:1 R.Time:1.081(Scan#:140)

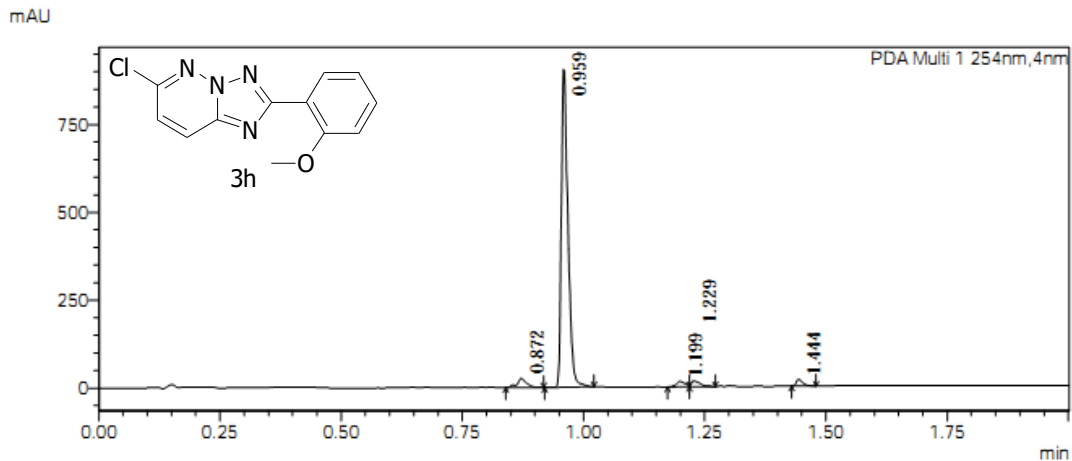
MassPeaks:439

Spectrum Mode:Averaged 1.073-1.090(139-141) BasePeak:265.05(1096597)

BG Mode:Calc Segment 1 - Event 1



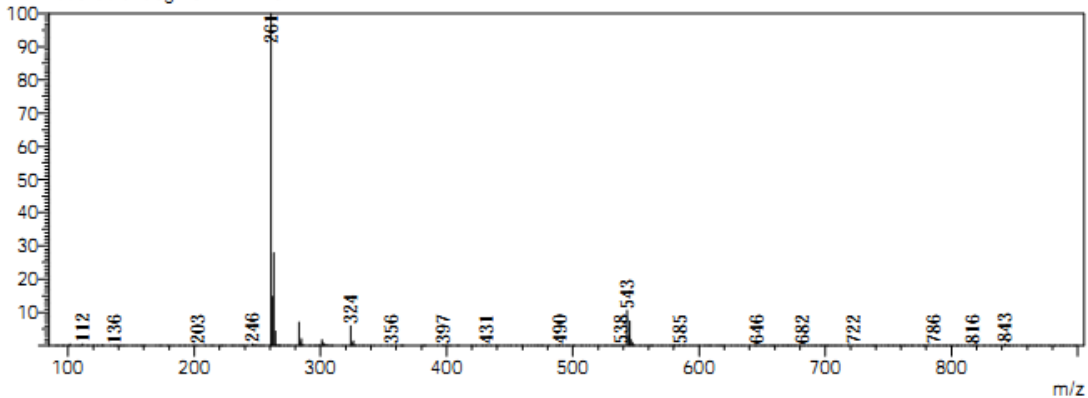


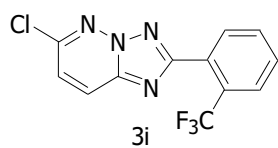


Peak Table

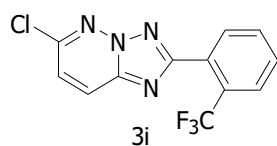
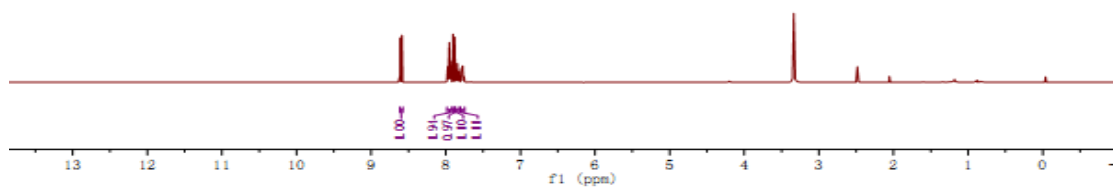
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.872	25920	2.648	35617	3.693
2	0.959	901845	92.118	870550	90.261
3	1.199	15870	1.621	19899	2.063
4	1.229	16122	1.647	19952	2.069
5	1.444	19252	1.966	18467	1.915
Total		979009	100.000	964484	100.000

Line#:1 R.Time:0.956(Scan#:125)  
 MassPeaks:397  
 Spectrum Mode:Averaged 0.948-0.965(124-126) BasePeak:261(534678)  
 BG Mode:Calc Segment 1 - Event 1

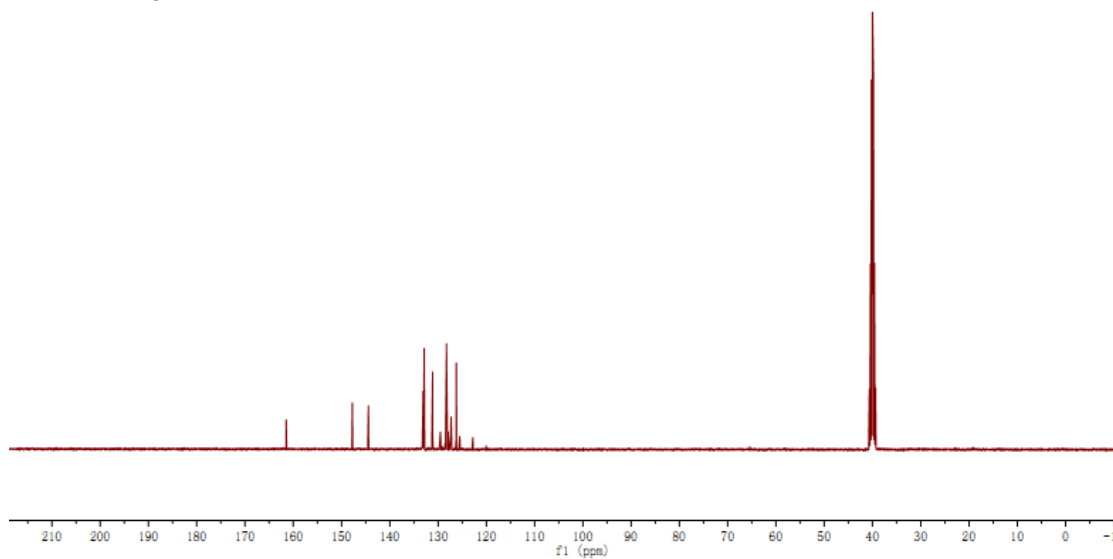


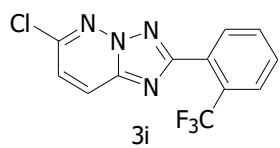


8.61  
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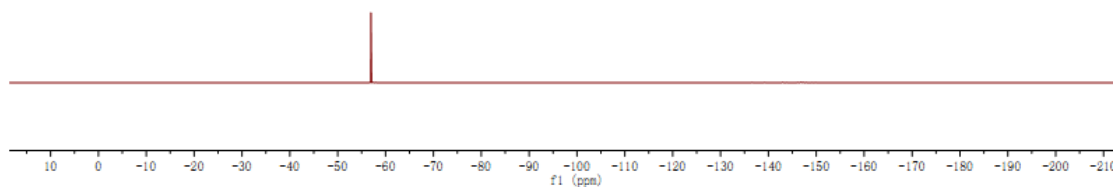


161.18  
147.77  
145.43  
142.88  
141.43  
139.51  
138.26  
137.03  
137.35  
137.29  
137.21  
135.52  
132.80

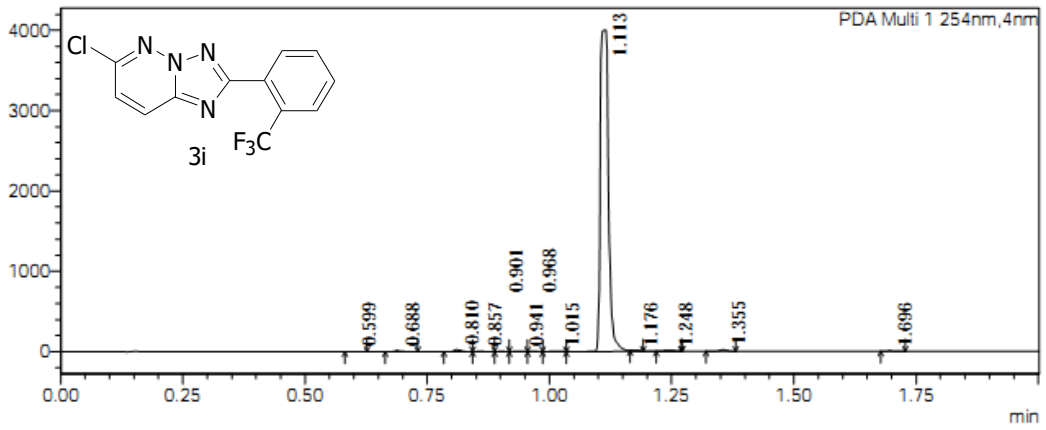




163.91



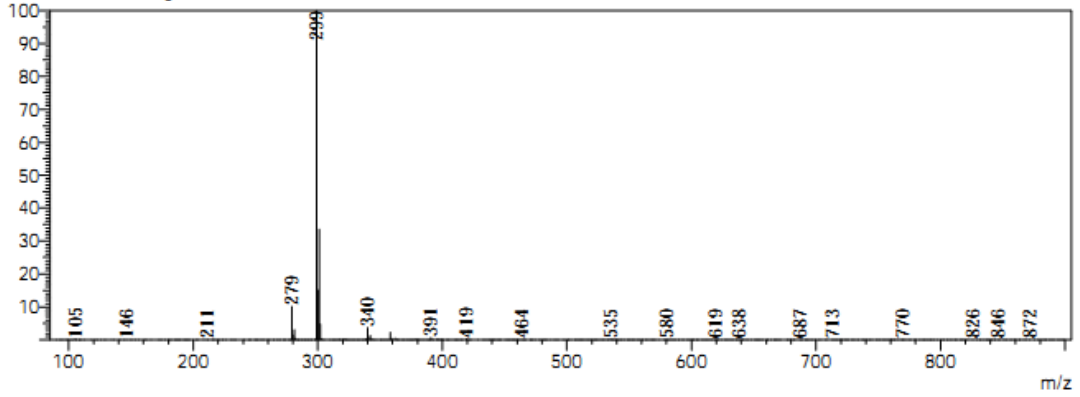
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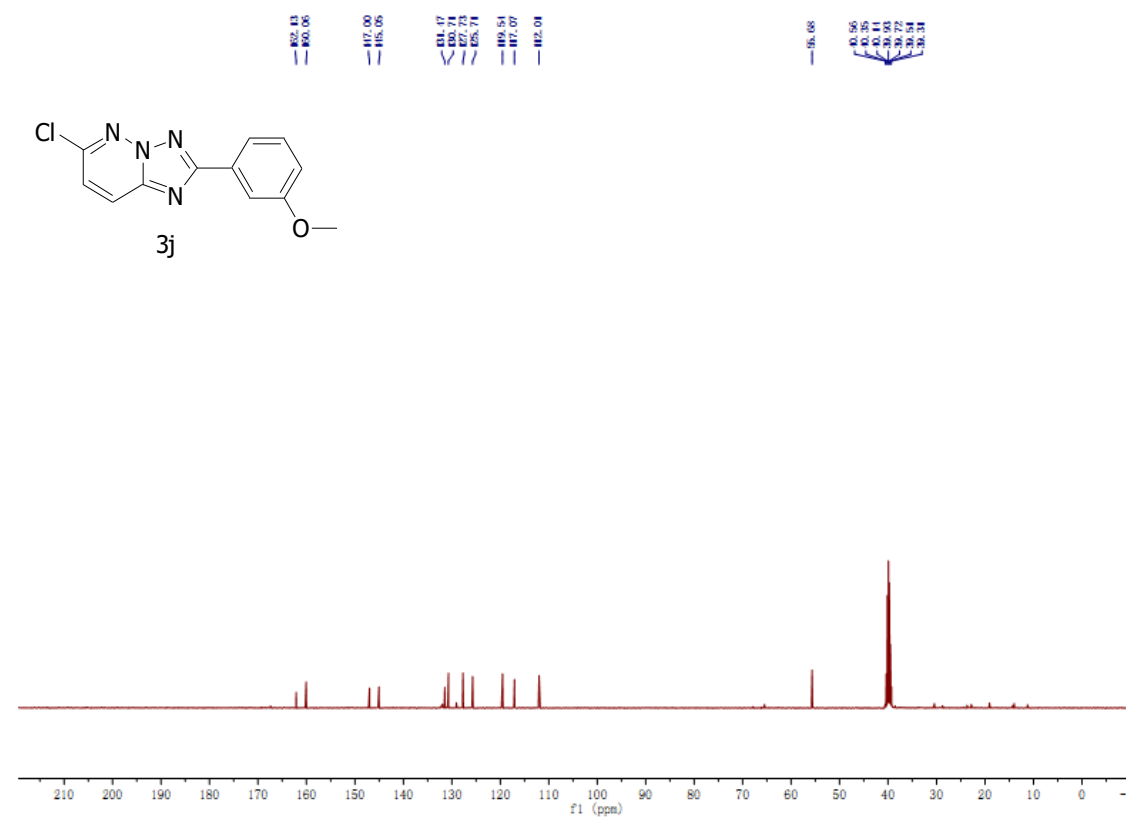
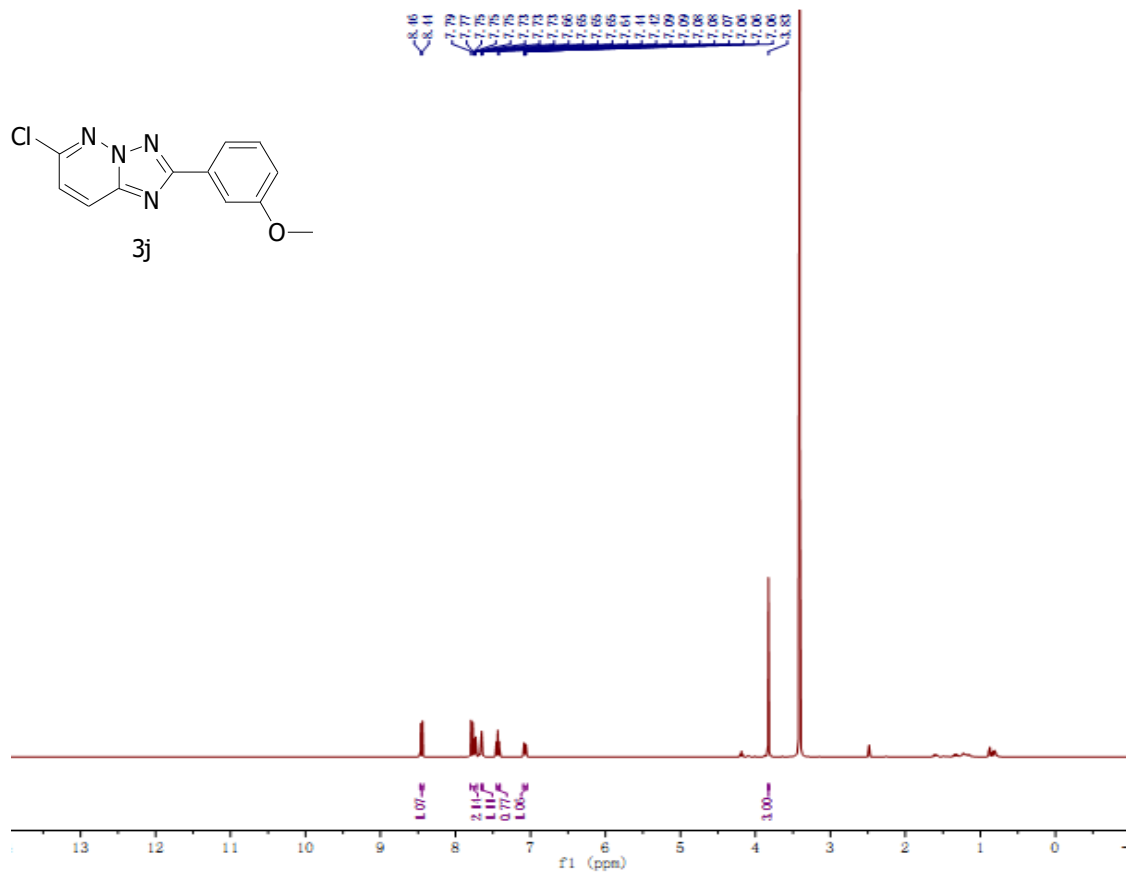


Peak Table

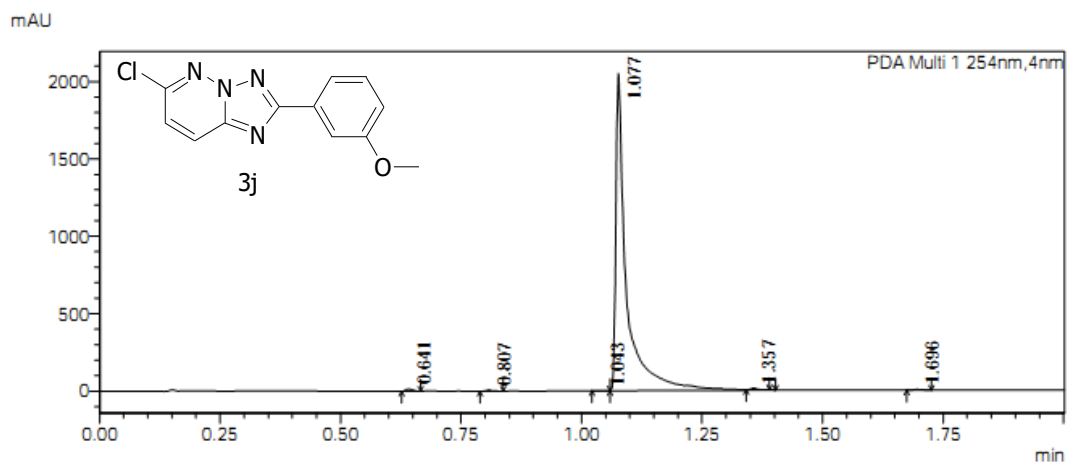
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.599	2930	0.071	2872	0.060
2	0.688	11775	0.287	15061	0.314
3	0.810	24850	0.606	24568	0.512
4	0.857	5716	0.139	6831	0.142
5	0.901	4300	0.105	3973	0.083
6	0.941	5131	0.125	6322	0.132
7	0.968	3478	0.085	4105	0.085
8	1.015	6753	0.165	8671	0.181
9	1.113	3995370	97.417	4685202	97.579
10	1.176	3796	0.093	2521	0.053
11	1.248	11373	0.277	14735	0.307
12	1.355	20114	0.490	20874	0.435
13	1.696	5711	0.139	5706	0.119
Total		4101296	100.000	4801441	100.000

Line#:1 R.Time:1.115(Scan#:144)  
 MassPeaks:528  
 Spectrum Mode:Averaged 1.106-1.123(143-145) BasePeak:299(4724019)  
 BG Mode:Calc Segment 1 - Event 1







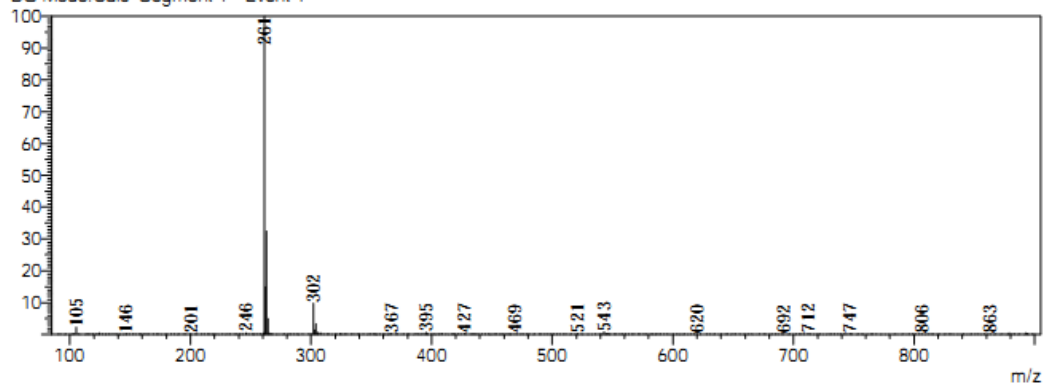


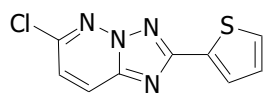
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.641	14245	0.686	13471	0.422
2	0.807	4907	0.236	4912	0.154
3	1.043	2117	0.102	1945	0.061
4	1.077	2042714	98.333	3160285	98.983
5	1.357	8955	0.431	7747	0.243
6	1.696	4409	0.212	4407	0.138
Total		2077347	100.000	3192767	100.000

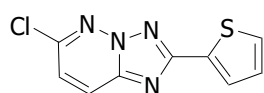
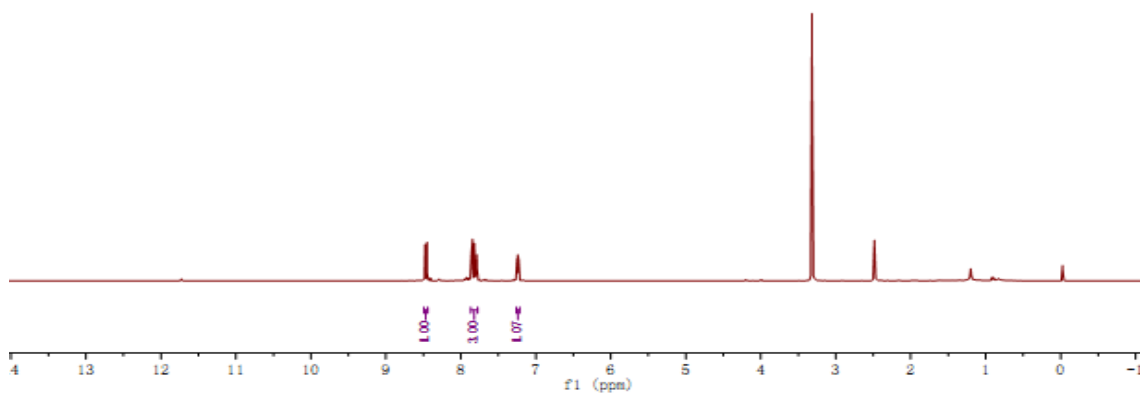
Line#:1 R.Time:1.073(Scan#:139)  
 MassPeaks:367  
 Spectrum Mode:Averaged 1.065-1.081(138-140) BasePeak:261(817785)  
 BG Mode:Calc Segment 1 - Event 1





3k

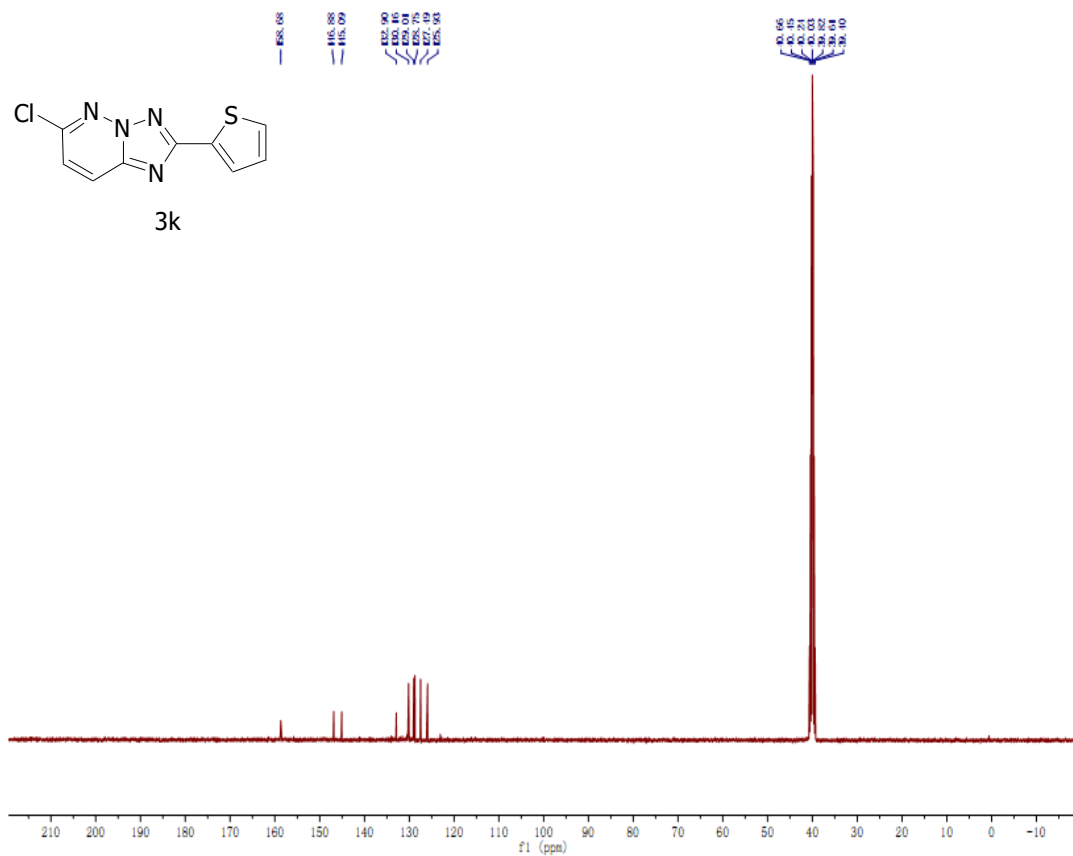
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7.80  
7.79  
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7.71  
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7.72  
7.72

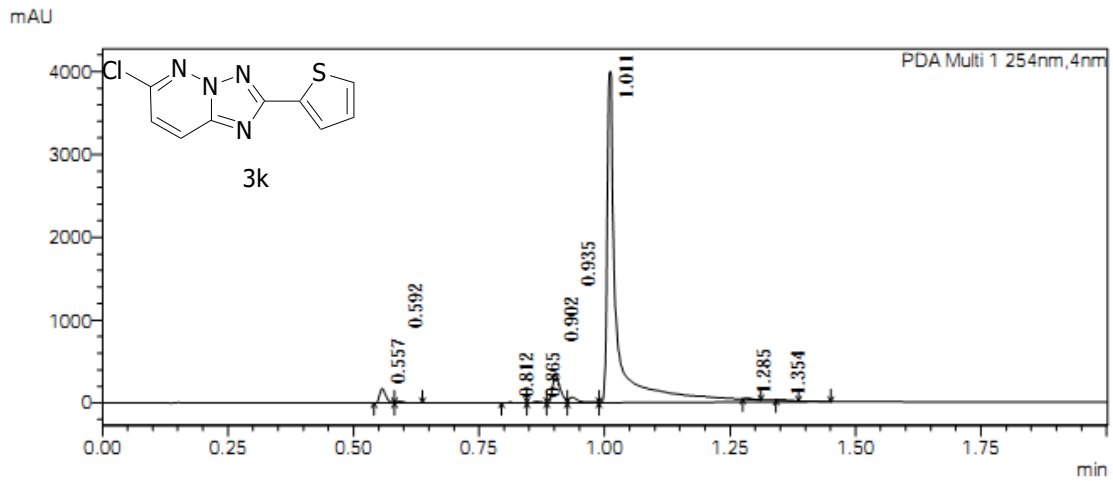


3k

158.08  
145.88  
145.09  
127.90  
127.16  
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125.95  
125.95

40.66  
40.15  
40.03  
39.82  
39.10

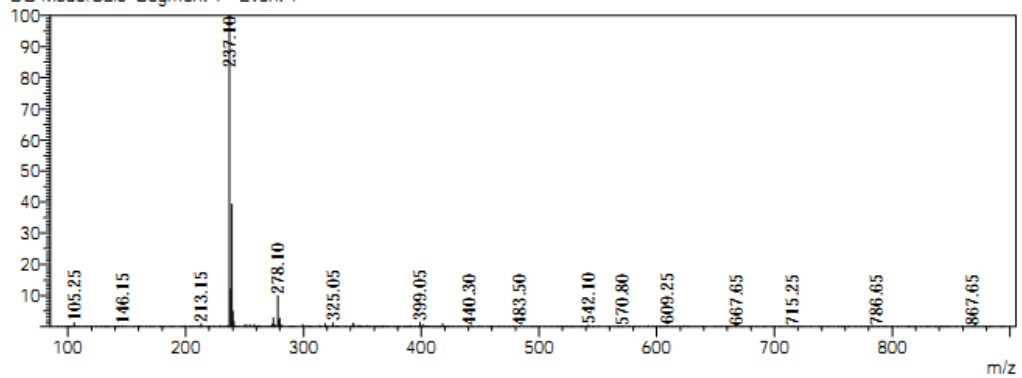


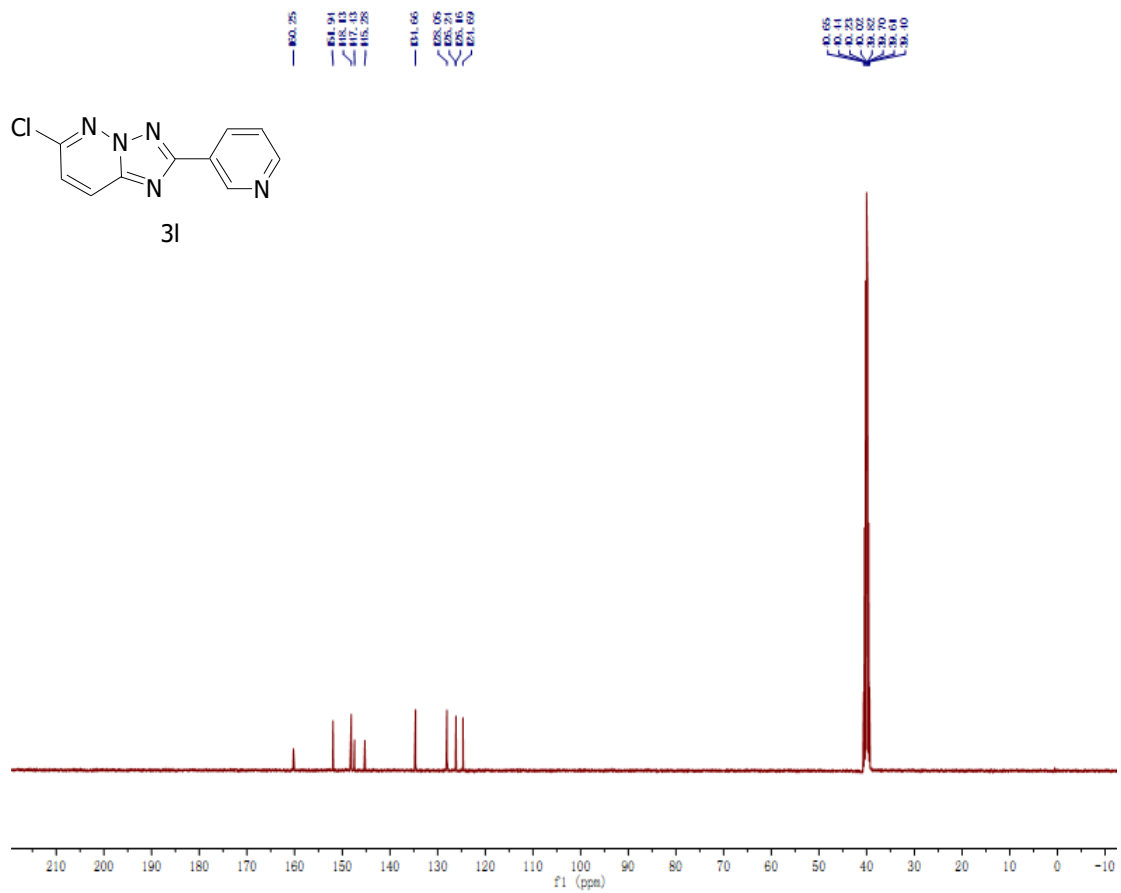
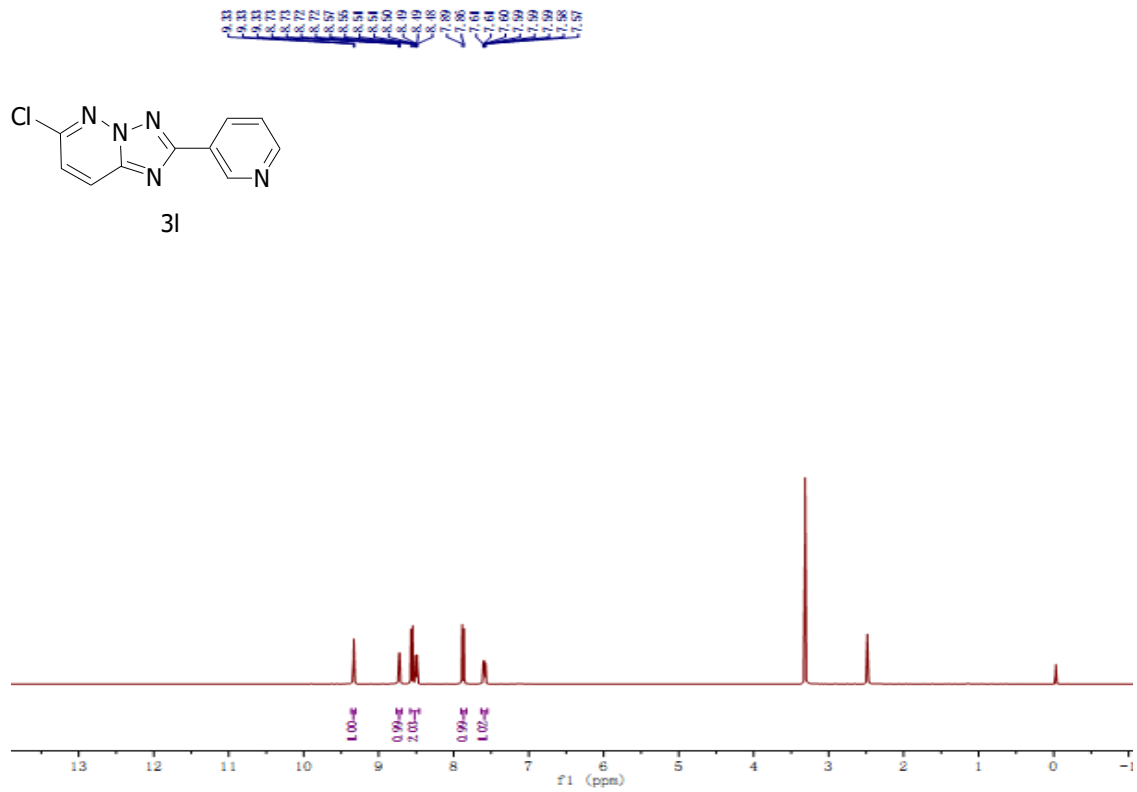


Peak Table  
PDA Ch1 254nm

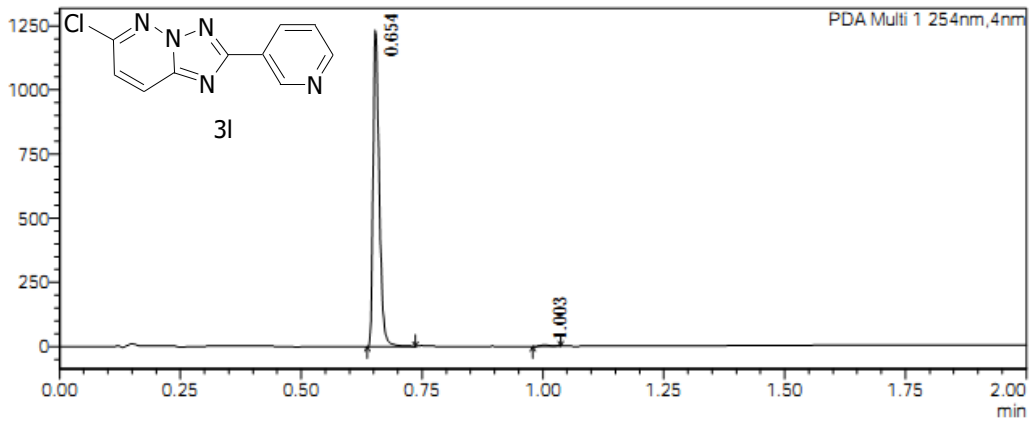
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.557	173905	3.783	149008	2.419
2	0.592	18952	0.412	19246	0.312
3	0.812	4786	0.104	5591	0.091
4	0.865	12224	0.266	13102	0.213
5	0.902	332530	7.234	349727	5.678
6	0.935	64412	1.401	78248	1.270
7	1.011	3973098	86.432	5528420	89.764
8	1.285	11455	0.249	10199	0.166
9	1.354	5407	0.118	5330	0.087
Total		4596769	100.000	6158870	100.000

Line#:2 R.Time:1.015(Scan#:132)  
MassPeaks:439  
Spectrum Mode:Averaged 1.006-1.023(131-133) BasePeak:237.10(371976)  
BG Mode:Calc Segment 1 - Event 1





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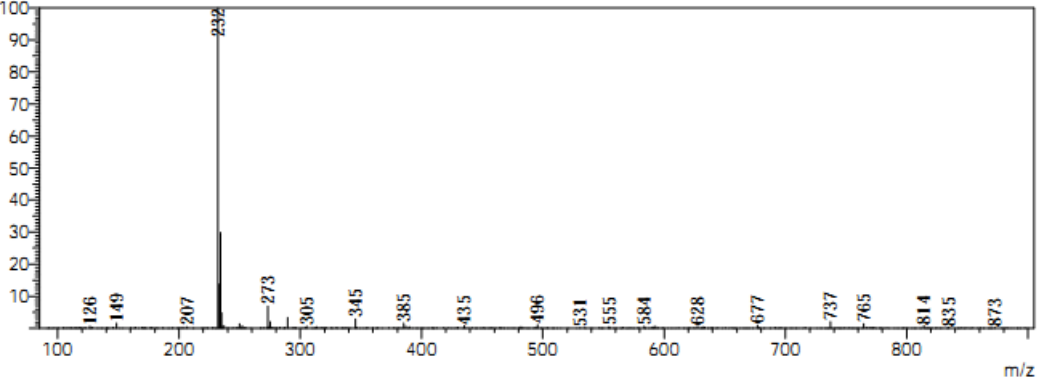


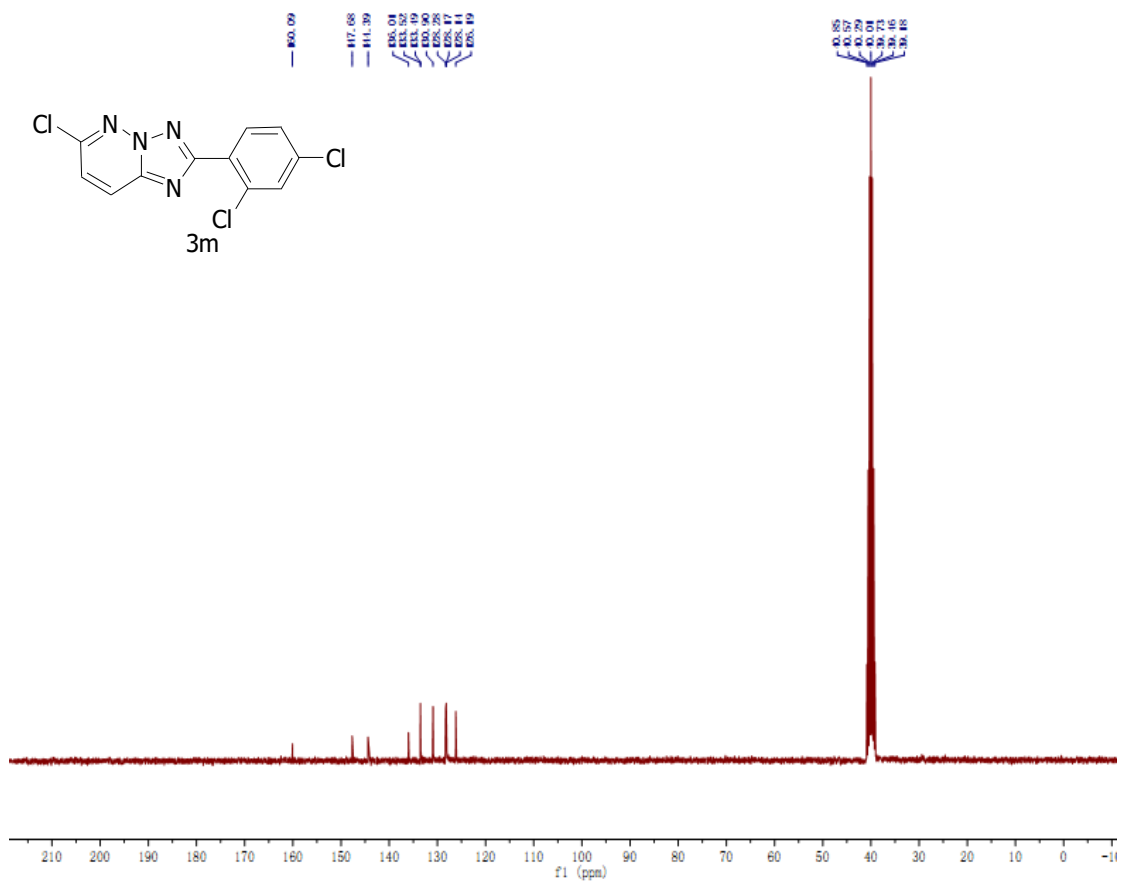
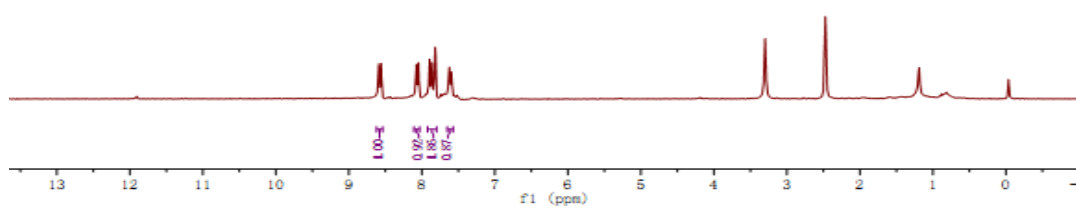
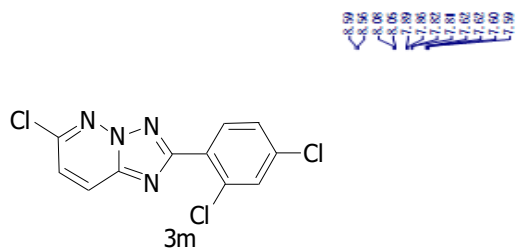
Peak Table

PDA Ch1 254nm

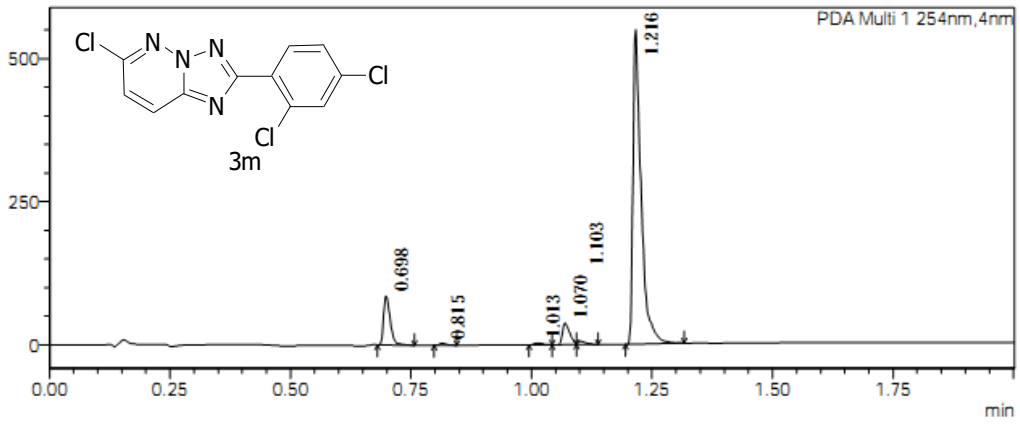
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.654	1202826	99.531	1089144	99.390
2	1.003	5669	0.469	6687	0.610
Total		1208495	100.000	1095830	100.000

Line#:1 R.Time:0.656(Scan#:89)  
MassPeaks:424  
Spectrum Mode:Averaged 0.648-0.665(88-90) BasePeak:232(138229)  
BG Mode:Calc Segment 1 - Event 1





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Peak Table

PDA Ch1 254nm

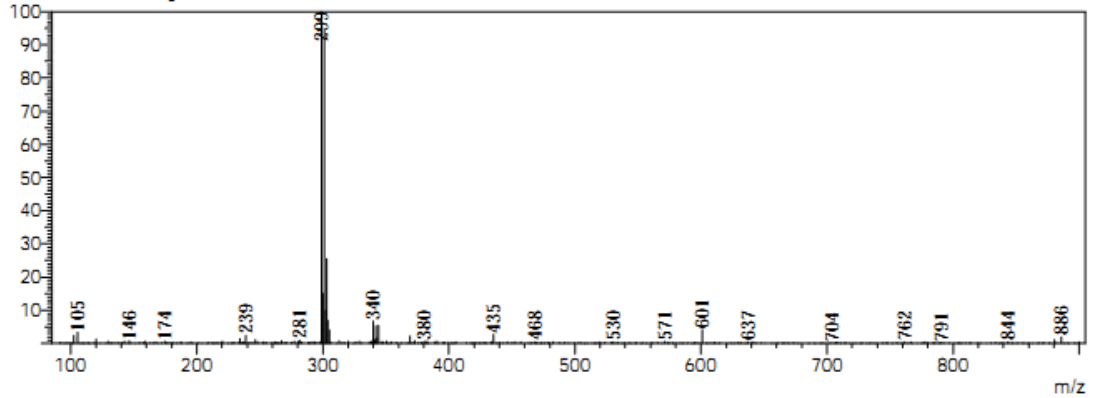
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.698	84727	12.518	81089	10.448
2	0.815	3632	0.537	3625	0.467
3	1.013	2985	0.441	3524	0.454
4	1.070	37501	5.540	39071	5.034
5	1.103	5701	0.842	6552	0.844
6	1.216	542319	80.122	642285	82.753
Total		676864	100.000	776146	100.000

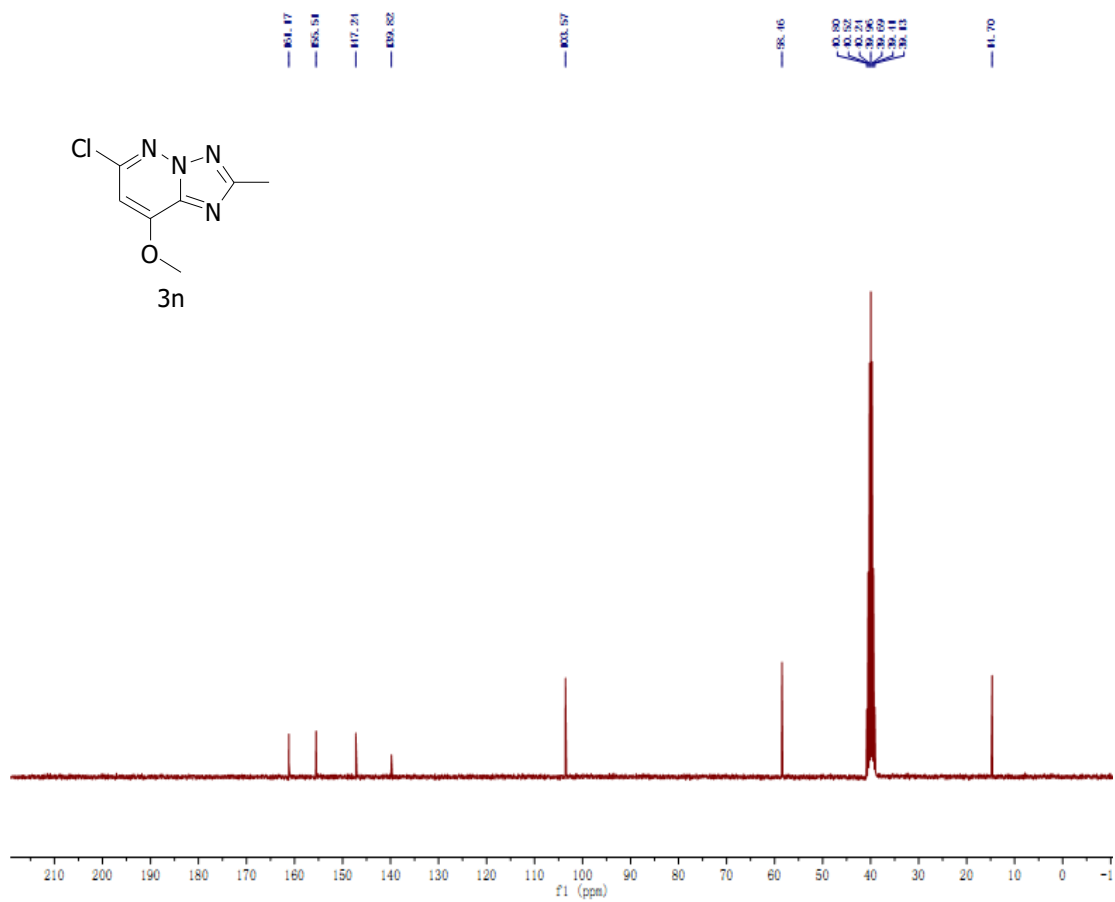
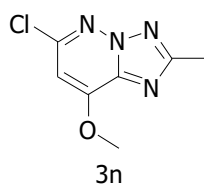
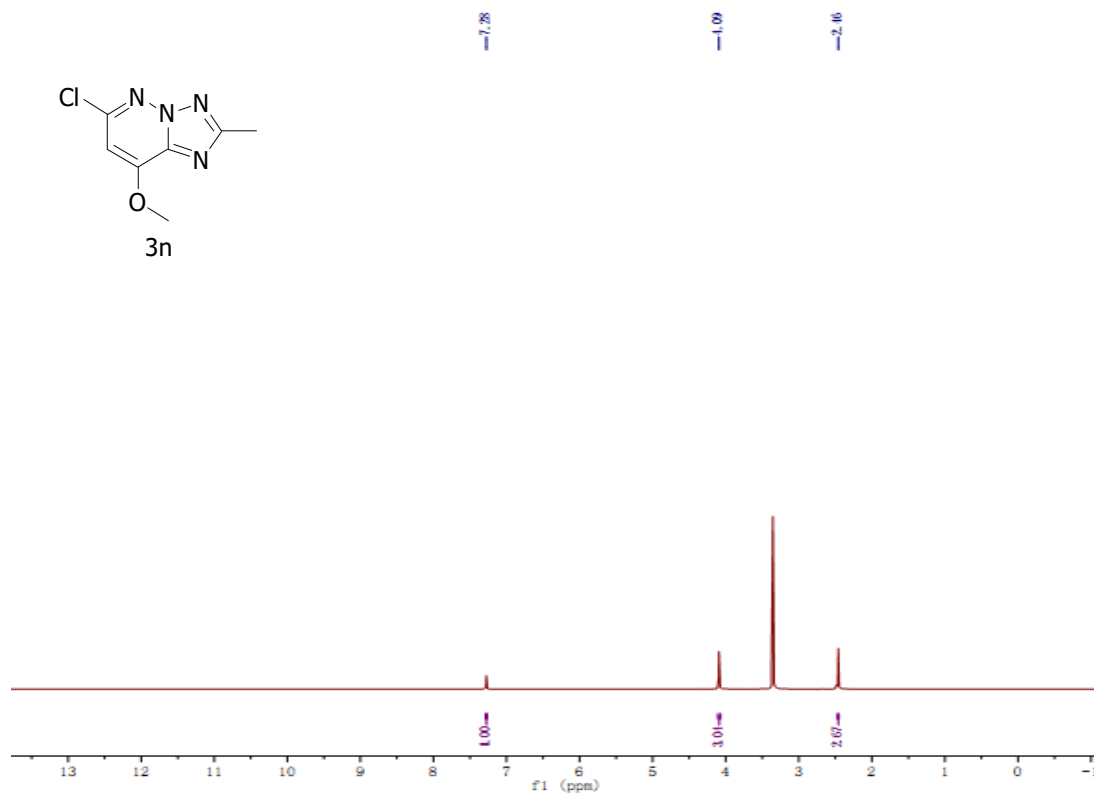
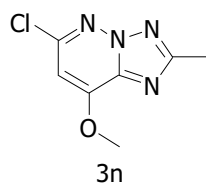
Line#:3 R.Time:1.215(Scan#:156)

MassPeaks:388

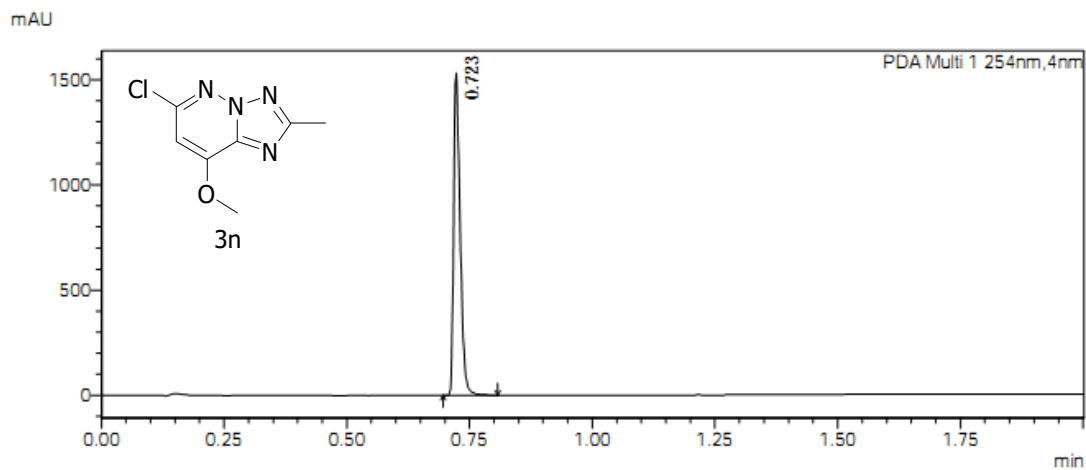
Spectrum Mode:Averaged 1.206-1.223(155-157) BasePeak:299(54822)

BG Mode:Calc Segment 1 - Event 1





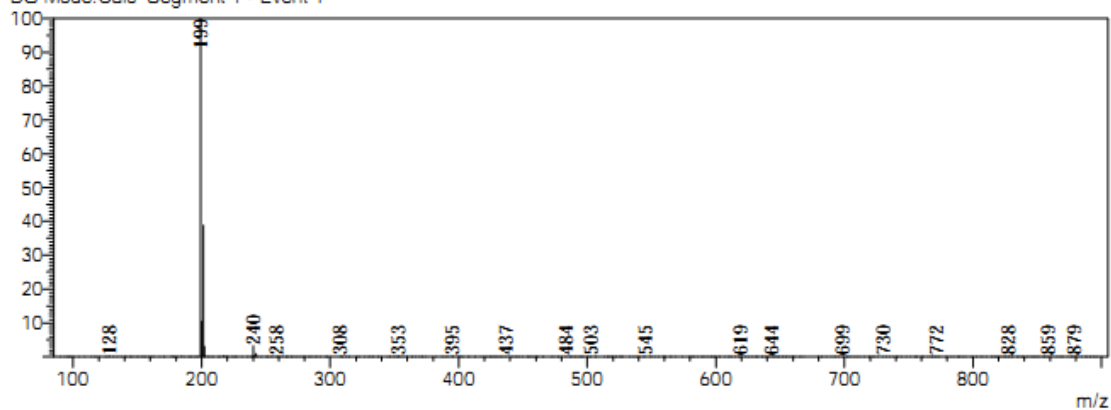




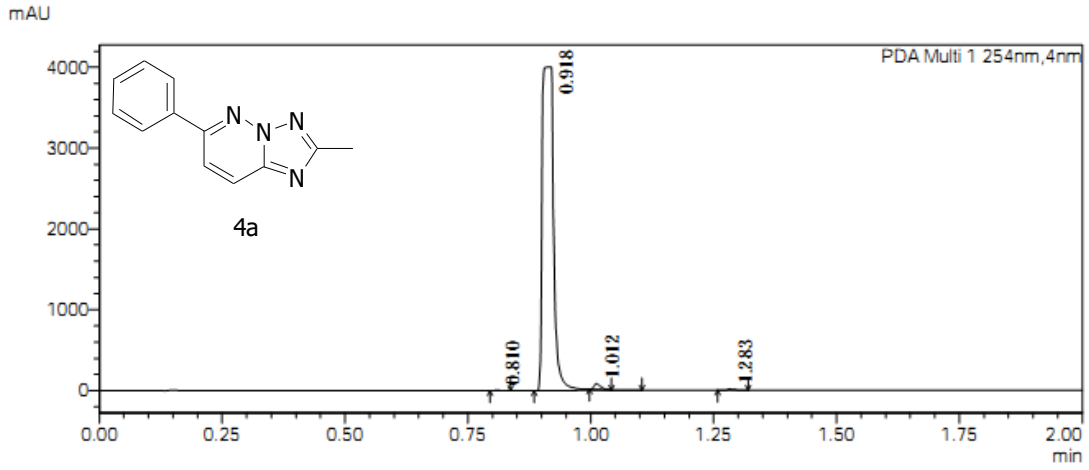
PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.723	1507282	100.000	1418910	100.000
Total		1507282	100.000	1418910	100.000

Line#:1 R.Time:0.723(Scan#:97)  
 MassPeaks:372  
 Spectrum Mode:Averaged 0.715-0.731(96-98) BasePeak:199(734375)  
 BG Mode:Calc Segment 1 - Event 1



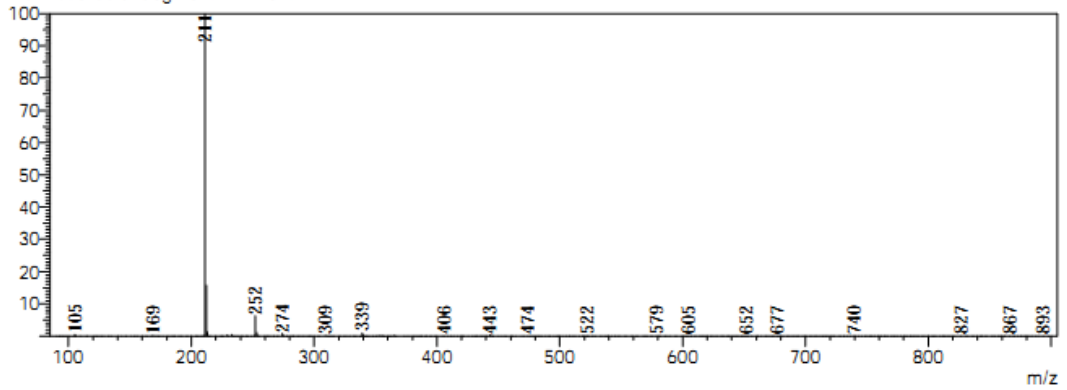




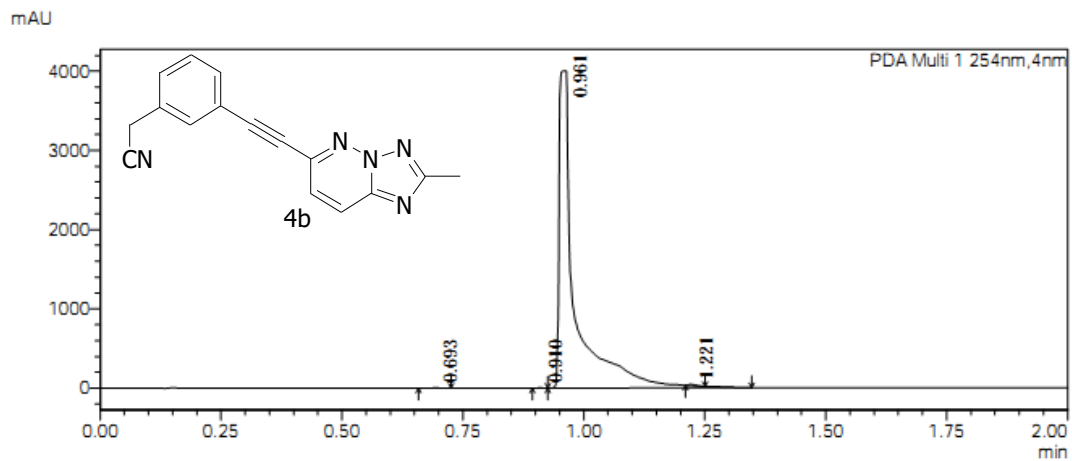
Peak Table

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.810	4355	0.107	4107	0.063
2	0.918	3997883	97.881	6427469	98.715
3	1.012	69984	1.713	67356	1.034
4	1.283	12212	0.299	12188	0.187
Total		4084434	100.000	6511120	100.000

Line#:1 R.Time:0.915(Scan#:120)  
 MassPeaks:443  
 Spectrum Mode:Averaged 0.906-0.923(119-121) BasePeak:211(2360958)  
 BG Mode:Calc Segment 1 - Event 1







PDA Ch1 254nm

Peak Table

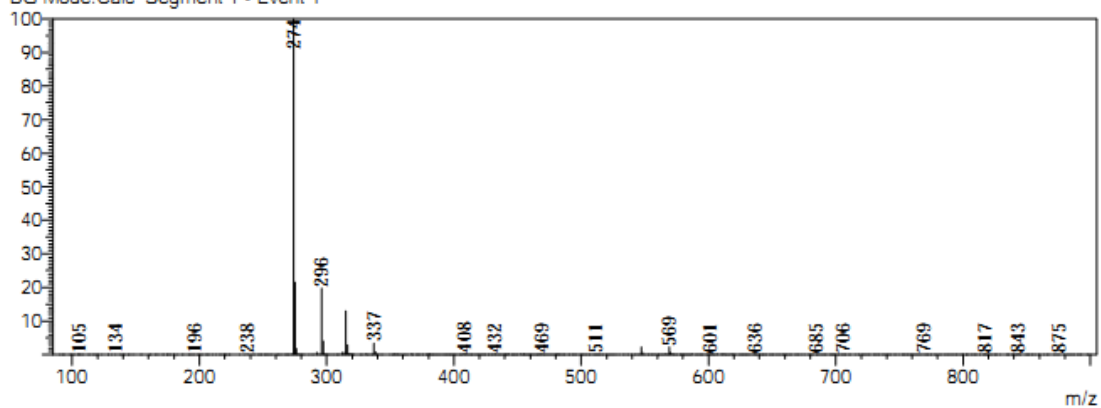
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.693	7139	0.177	8108	0.089
2	0.910	2411	0.060	2020	0.022
3	0.961	3996101	99.265	9071081	99.695
4	1.221	20042	0.498	17649	0.194
Total		4025694	100.000	9098858	100.000

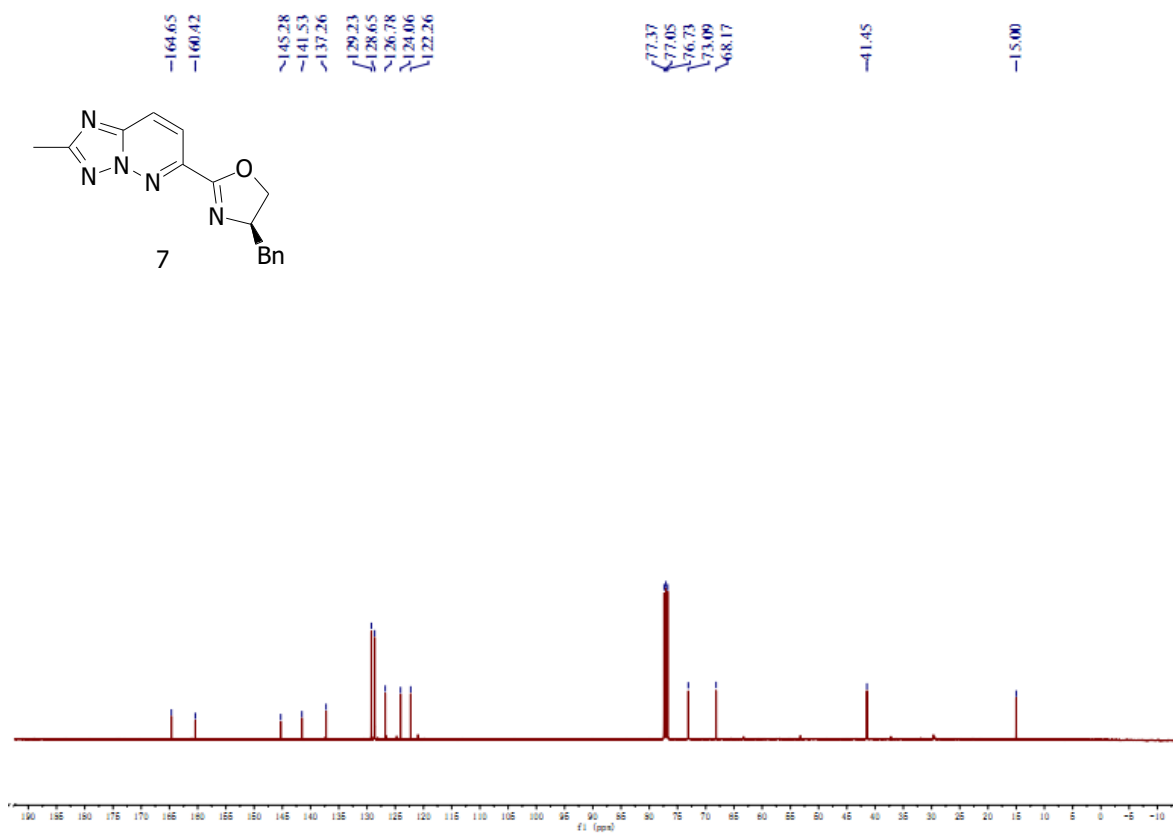
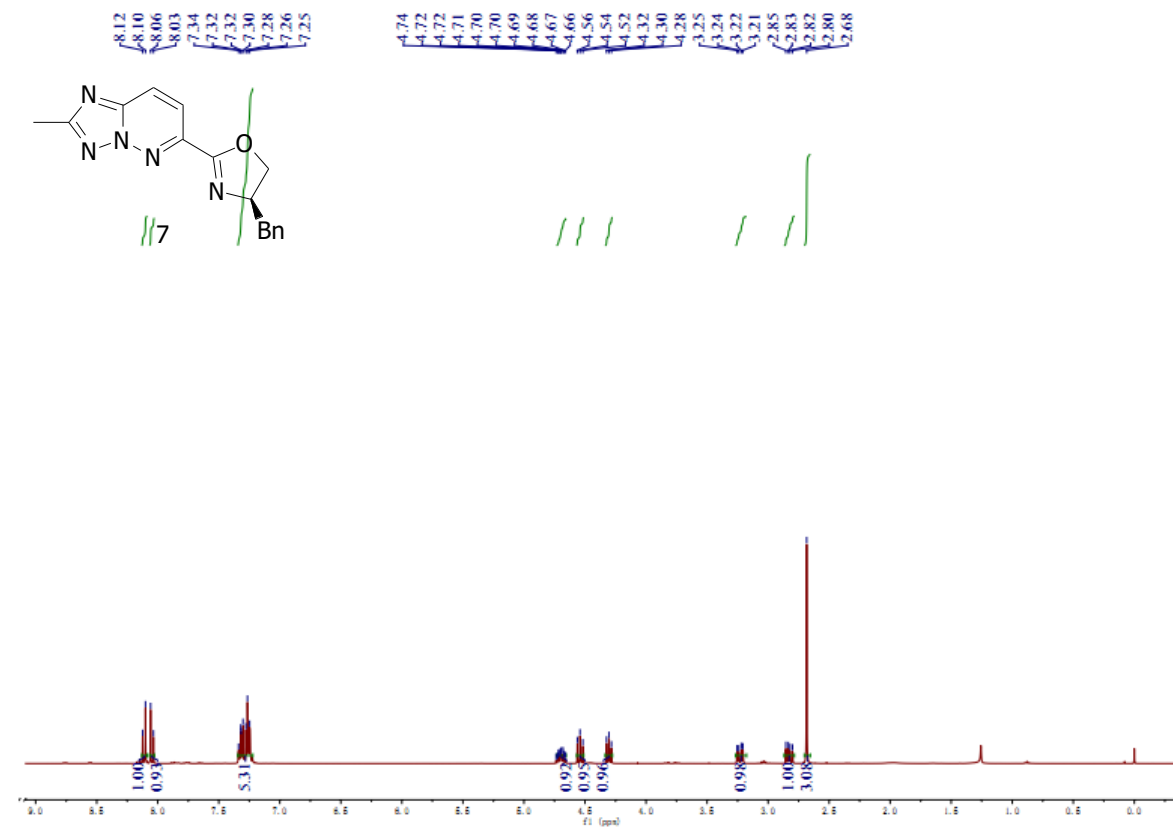
Line#:1 R.Time:0.965(Scan#:126)

MassPeaks:550

Spectrum Mode:Averaged 0.956-0.973(125-127) BasePeak:274(1577027)

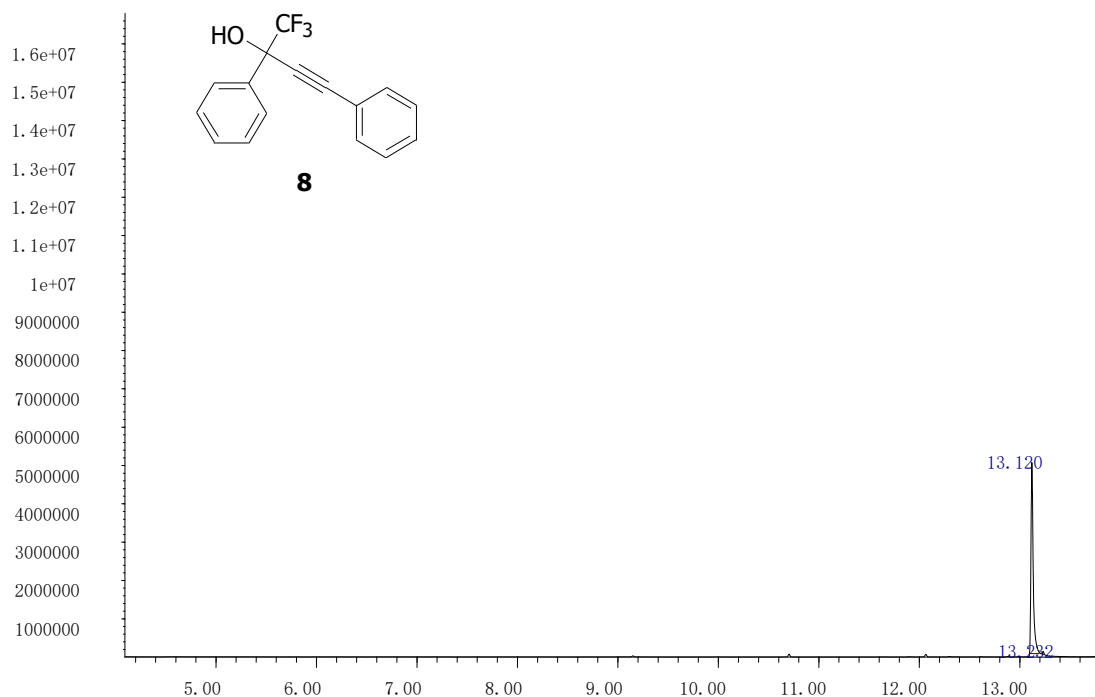
BG Mode:Calc Segment 1 - Event 1





# GC-MS spectrum of product 8

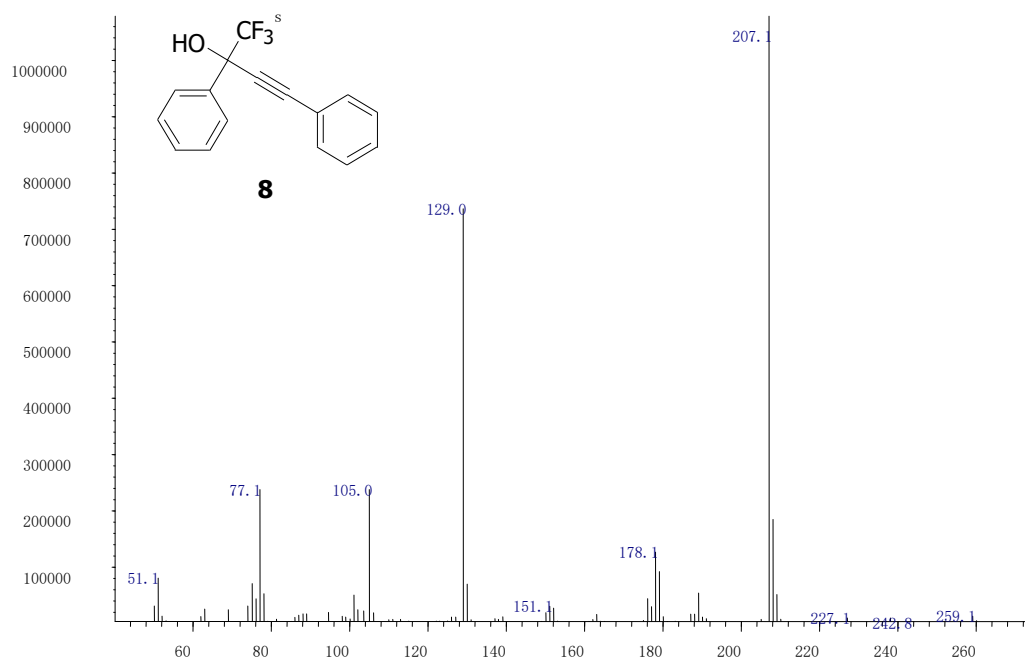
丰度



时间-->

#	Time	Height	Area	Area %
1	13.120	4992043	76776930	99.177%
2	13.232	79946	636887	0.823%

丰度

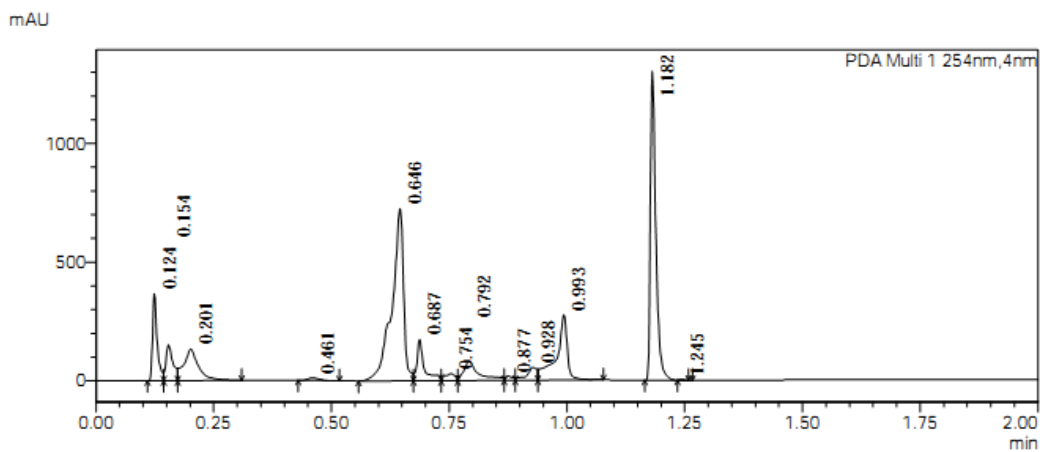


m/z-->

# S-10. LC-MS spectra of formation of 3a

t=1 h

<Chromatogram>



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.124	357211	10.913	250065	6.285
2	0.154	150568	4.600	156152	3.925
3	0.201	131738	4.025	290622	7.305
4	0.461	10258	0.313	19005	0.478
5	0.646	718677	21.957	1253845	31.515
6	0.687	172735	5.277	184702	4.642
7	0.754	29178	0.891	47511	1.194
8	0.792	83979	2.566	178313	4.482
9	0.877	16567	0.506	18747	0.471
10	0.928	53462	1.633	81057	2.037
11	0.993	272116	8.314	442314	11.117
12	1.182	1273983	38.922	1054600	26.507
13	1.245	2689	0.082	1660	0.042
Total		3273160	100.000	3978592	100.000

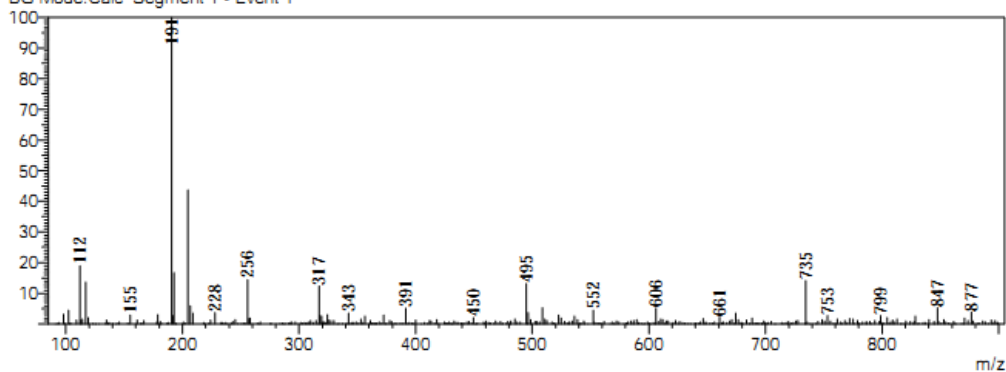
Mass Spectrum

Line#:1 R.Time:0.128(Scan#:21)

MassPeaks:388

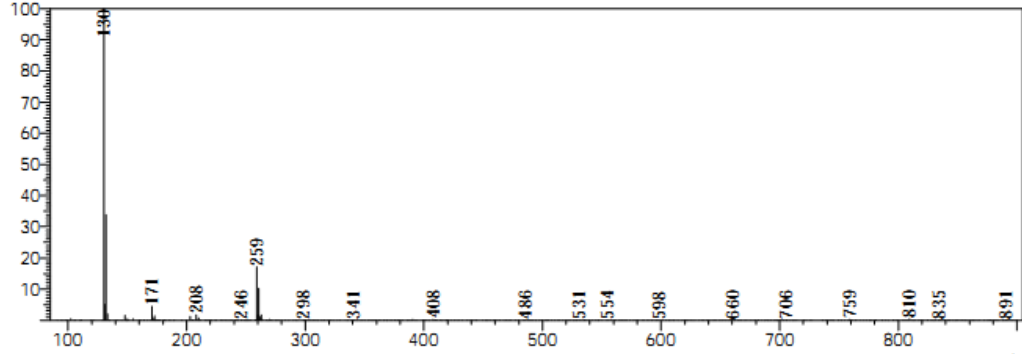
Spectrum Mode:Averaged 0.119-0.136(20-22) BasePeak:191(31740)

BG Mode:Calc Segment 1 - Event 1

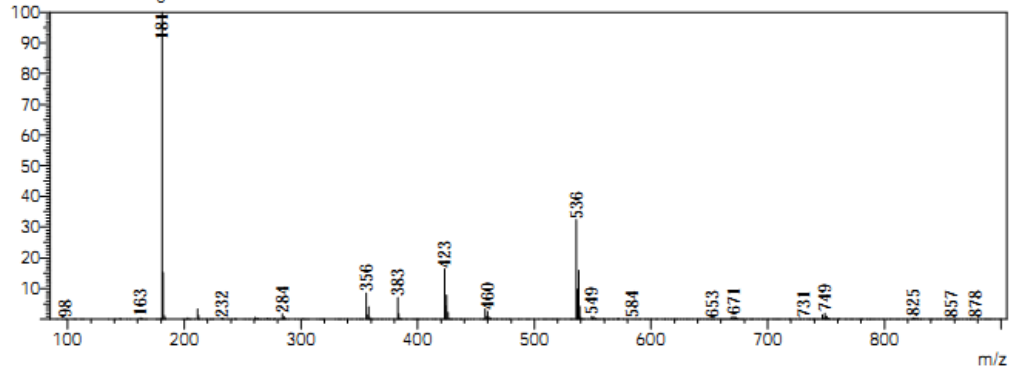




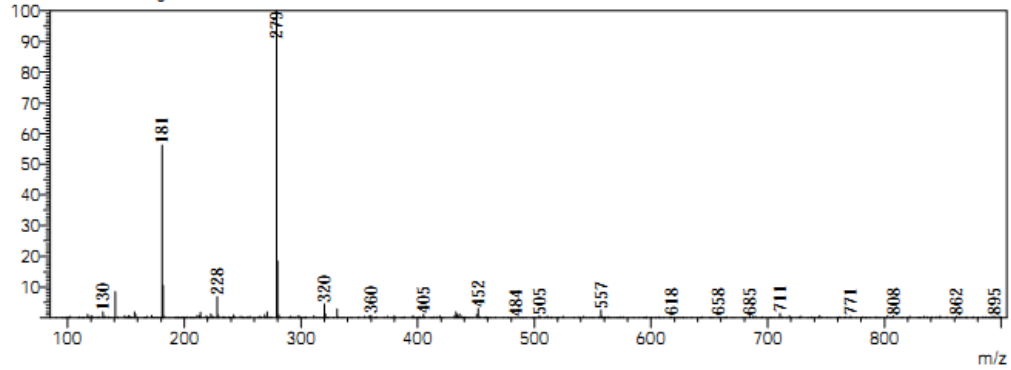
Line#:2 R.Time:0.203(Scan#:30)  
MassPeaks:404  
Spectrum Mode:Averaged 0.194-0.211(29-31) BasePeak:130(576714)  
BG Mode:Calc Segment 1 - Event 1



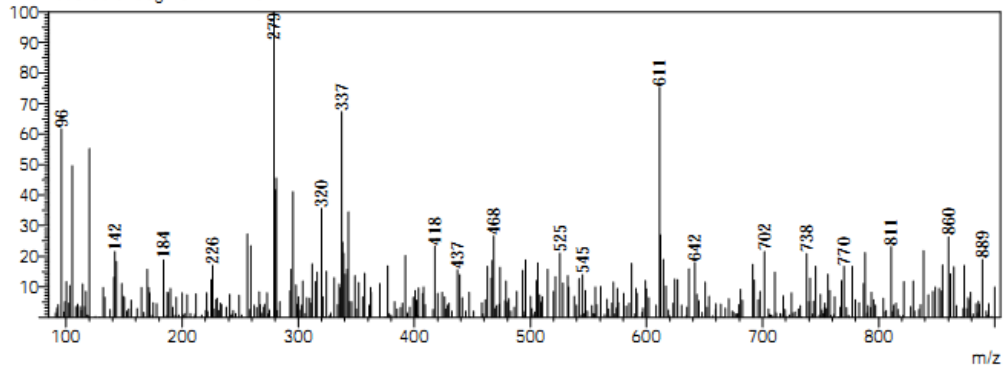
Line#:3 R.Time:0.644(Scan#:83)  
MassPeaks:412  
Spectrum Mode:Averaged 0.636-0.653(82-84) BasePeak:181(1215288)  
BG Mode:Calc Segment 1 - Event 1



Line#:4 R.Time:0.994(Scan#:125)  
MassPeaks:347  
Spectrum Mode:Averaged 0.986-1.003(124-126) BasePeak:279(98412)  
BG Mode:Calc Segment 1 - Event 1

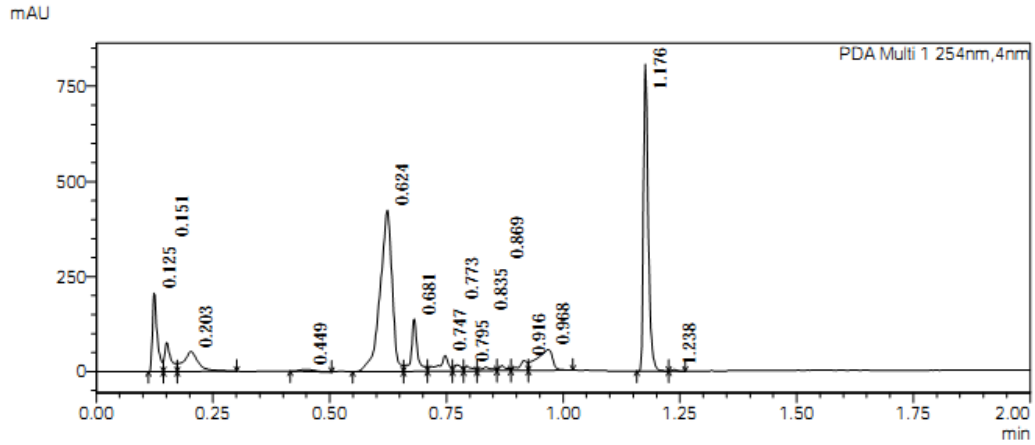


Line#:5 R.Time:1.178(Scan#:147)  
MassPeaks:396  
Spectrum Mode:Averaged 1.169-1.186(146-148) BasePeak:279(2318)  
BG Mode:Calc Segment 1 - Event 1



t=2 h

<Chromatogram>



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.125	203841	11.008	150370	7.215
2	0.151	75819	4.094	71607	3.436
3	0.203	52467	2.833	117651	5.645
4	0.449	5322	0.287	11117	0.533
5	0.624	423414	22.866	761325	36.528
6	0.681	132132	7.136	122513	5.878
7	0.747	39879	2.154	56498	2.711
8	0.773	15392	0.831	18119	0.869
9	0.795	12486	0.674	13949	0.669
10	0.835	9678	0.523	14397	0.691
11	0.869	13178	0.712	13390	0.642
12	0.916	26212	1.416	32760	1.572
13	0.968	55271	2.985	128917	6.185
14	1.176	782900	42.279	568810	27.291
15	1.238	3760	0.203	2791	0.134
Total		1851751	100.000	2084213	100.000

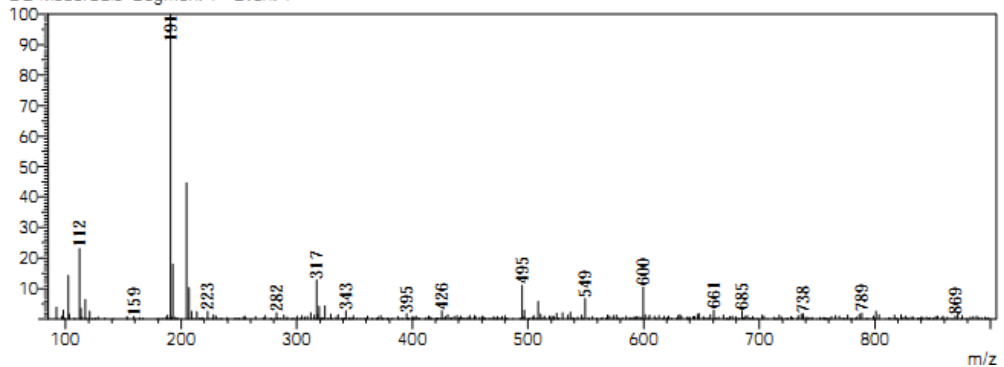
Mass Spectrum

Line#:1 R.Time:0.128(Scan#:21)

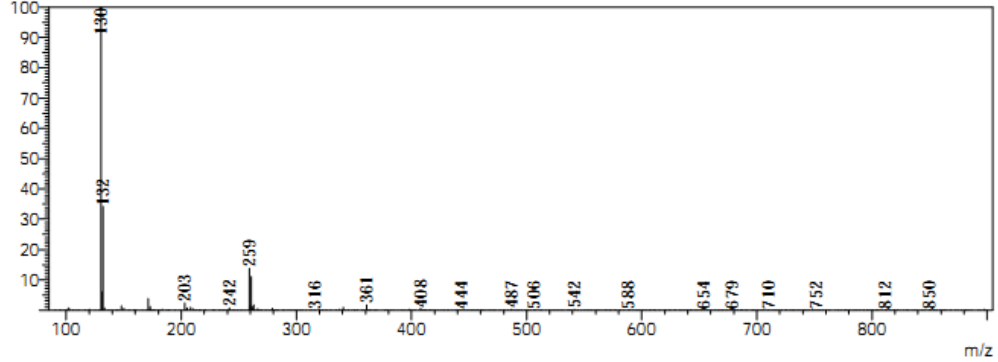
MassPeaks:373

Spectrum Mode:Averaged 0.119-0.136(20-22) BasePeak:191(24141)

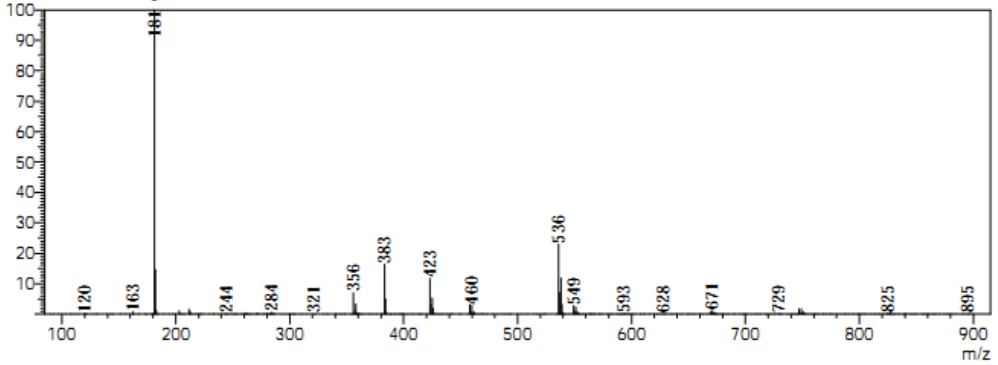
BG Mode:Calc Segment 1 - Event 1



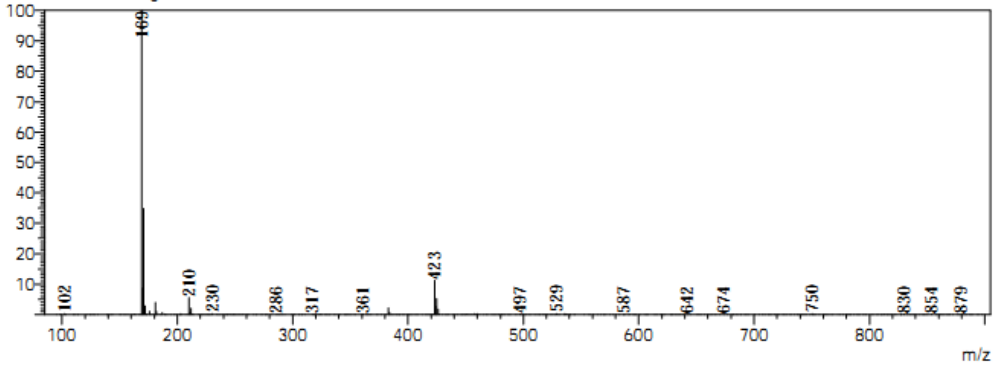
Line#:2 R.Time:0.203(Scan#:30)  
MassPeaks:429  
Spectrum Mode:Averaged 0.194-0.211(29-31) BasePeak:130(279290)  
BG Mode:Calc Segment 1 - Event 1



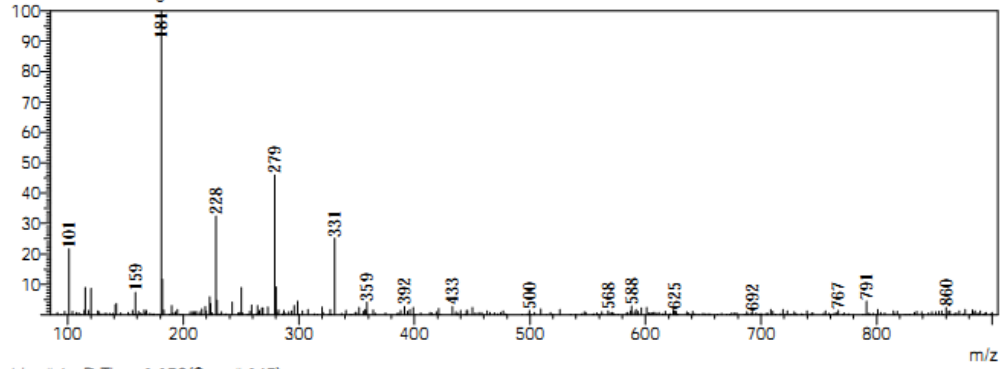
Line#:3 R.Time:0.619(Scan#:80)  
MassPeaks:395  
Spectrum Mode:Averaged 0.611-0.628(79-81) BasePeak:181(980147)  
BG Mode:Calc Segment 1 - Event 1



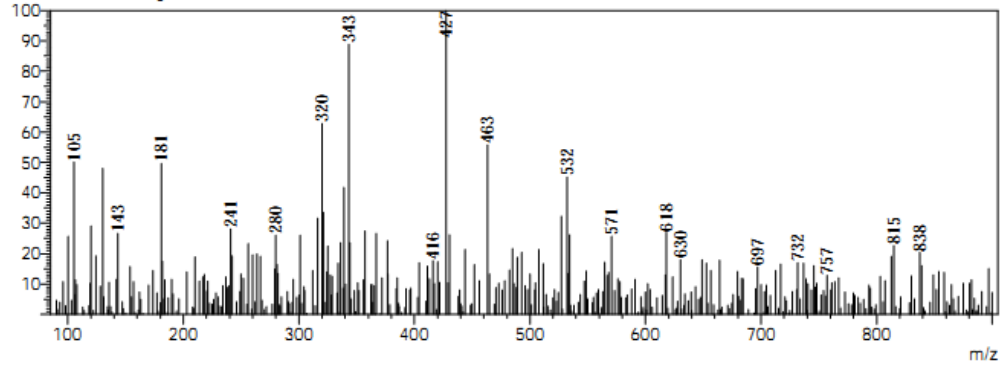
Line#:4 R.Time:0.678(Scan#:87)  
MassPeaks:424  
Spectrum Mode:Averaged 0.669-0.686(86-88) BasePeak:169(635992)  
BG Mode:Calc Segment 1 - Event 1



Line#:5 R.Time:0.969(Scan#:122)  
MassPeaks:319  
Spectrum Mode:Averaged 0.961-0.978(121-123) BasePeak:181(23695)  
BG Mode:Calc Segment 1 - Event 1

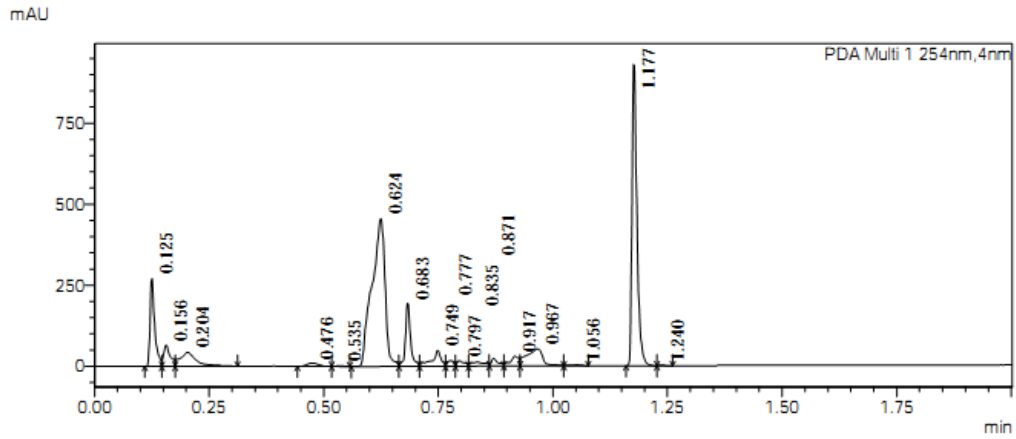


Line#:6 R.Time:1.178(Scan#:147)  
MassPeaks:389  
Spectrum Mode:Averaged 1.169-1.186(146-148) BasePeak:427(2406)  
BG Mode:Calc Segment 1 - Event 1



t=3 h

<Chromatogram>



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.125	267286	12.632	191625	7.786
2	0.156	64133	3.031	65649	2.668
3	0.204	42700	2.018	103855	4.220
4	0.476	9417	0.445	16208	0.659
5	0.535	2677	0.127	3001	0.122
6	0.624	452399	21.380	907021	36.855
7	0.683	184691	8.729	150544	6.117
8	0.749	48553	2.295	66385	2.697
9	0.777	17172	0.812	18397	0.748
10	0.797	16209	0.766	20748	0.843
11	0.835	12135	0.573	25906	1.053
12	0.871	22738	1.075	24550	0.998
13	0.917	29862	1.411	39530	1.606
14	0.967	52284	2.471	127048	5.162
15	1.056	2273	0.107	3859	0.157
16	1.177	889142	42.021	694728	28.229
17	1.240	2285	0.108	1972	0.080
Total		2115955	100.000	2461024	100.000

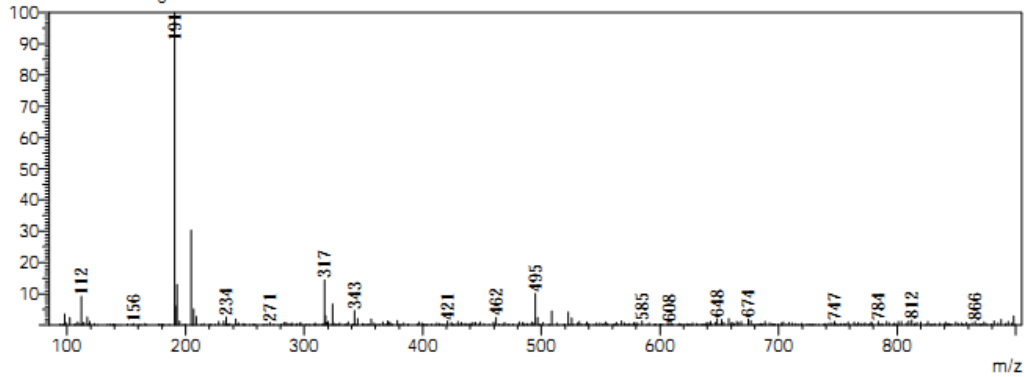
Mass Spectrum

Line#:1 R.Time:0.128(Scan#:21)

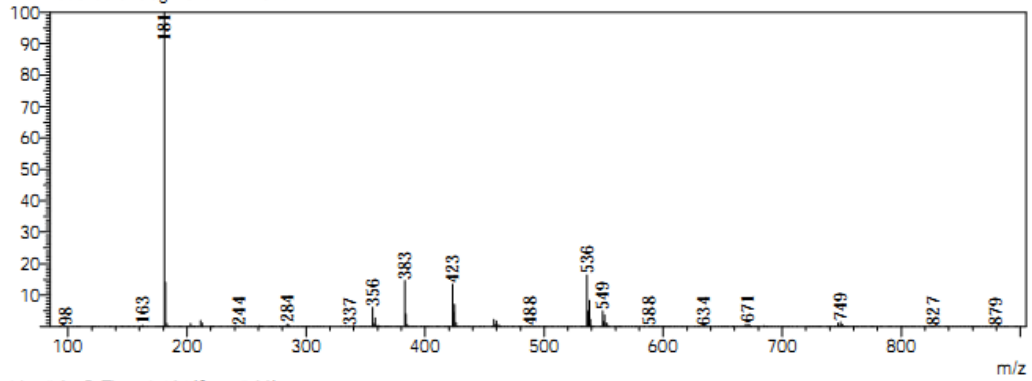
MassPeaks:393

Spectrum Mode:Averaged 0.119-0.136(20-22) BasePeak:191(33234)

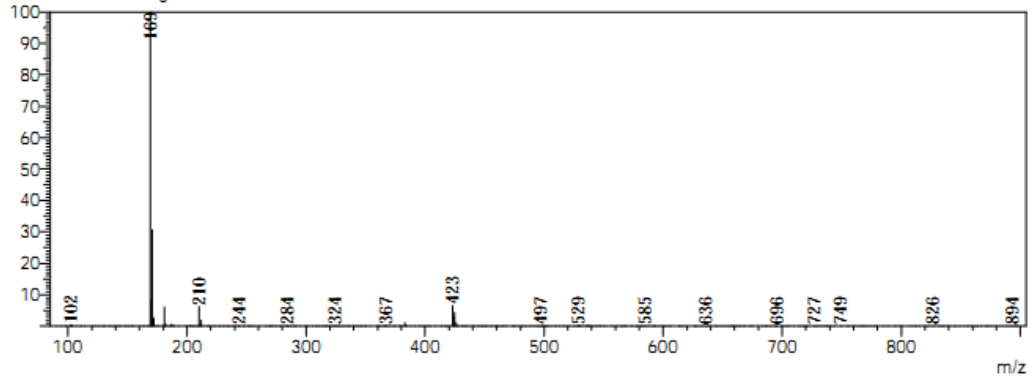
BG Mode:Calc Segment 1 - Event 1



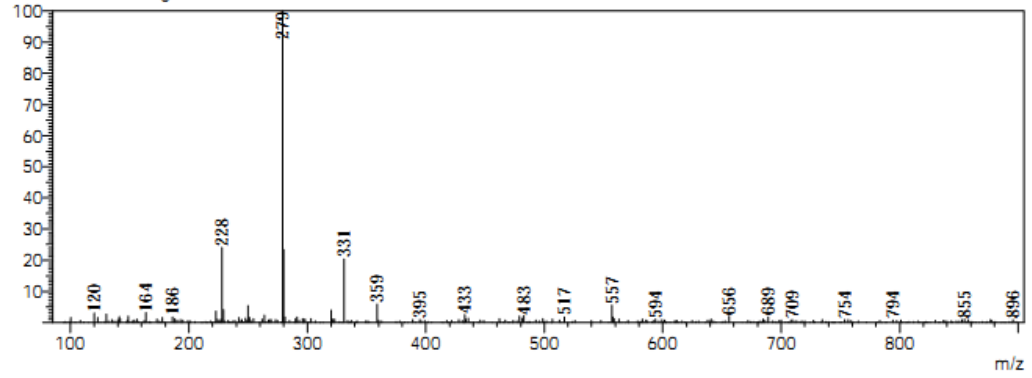
Line#:2 R.Time:0.628(Scan#:81)  
MassPeaks:400  
Spectrum Mode:Averaged 0.619-0.636(80-82) BasePeak:181(1192670)  
BG Mode:Calc Segment 1 - Event 1



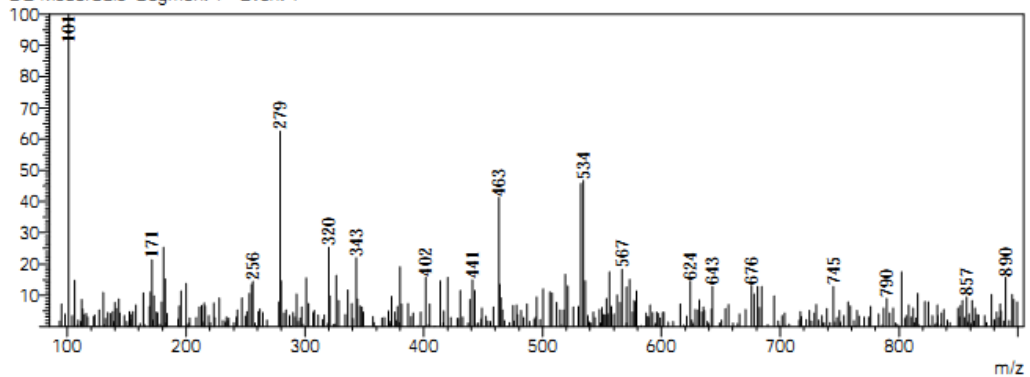
Line#:3 R.Time:0.686(Scan#:88)  
MassPeaks:426  
Spectrum Mode:Averaged 0.678-0.694(87-89) BasePeak:169(1144405)  
BG Mode:Calc Segment 1 - Event 1



Line#:4 R.Time:0.969(Scan#:122)  
MassPeaks:329  
Spectrum Mode:Averaged 0.961-0.978(121-123) BasePeak:279(37482)  
BG Mode:Calc Segment 1 - Event 1

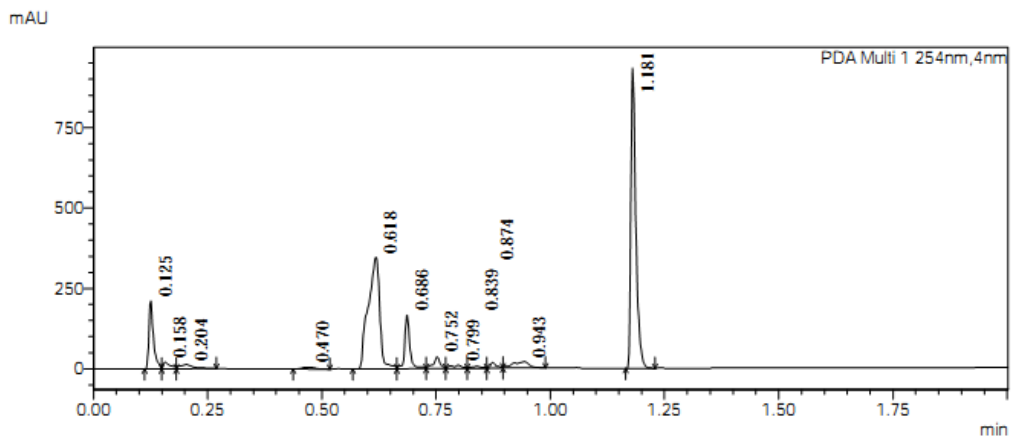


Line#:5 R.Time:1.178(Scan#:147)  
MassPeaks:375  
Spectrum Mode:Averaged 1.169-1.186(146-148) BasePeak:101(4130)  
BG Mode:Calc Segment 1 - Event 1



t=4 h

<Chromatogram>



Peak Table

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.125	206054	11.707	147533	8.319
2	0.158	19853	1.128	23294	1.313
3	0.204	12495	0.710	24714	1.394
4	0.470	5238	0.298	9921	0.559
5	0.618	345985	19.657	607651	34.263
6	0.686	160763	9.134	129348	7.293
7	0.752	35901	2.040	36198	2.041
8	0.799	10626	0.604	16895	0.953
9	0.839	5621	0.319	9163	0.517
10	0.874	18235	1.036	16230	0.915
11	0.943	19743	1.122	48488	2.734
12	1.181	919568	52.246	704056	39.699
Total		1760081	100.000	1773492	100.000

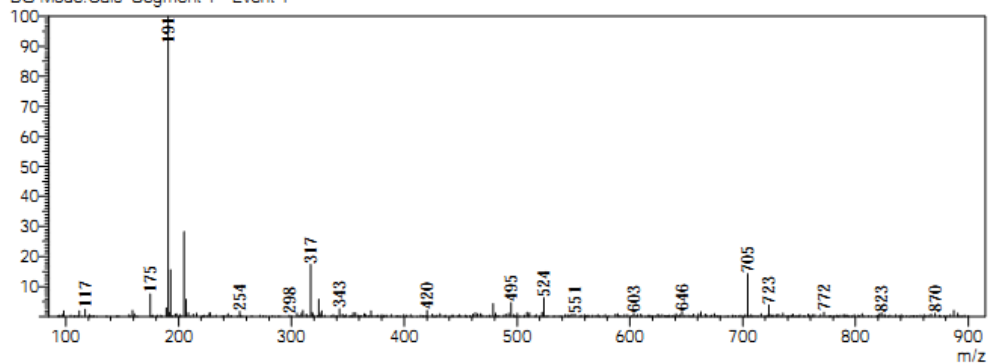
Mass Spectrum

Line#:1 R.Time:0.128(Scan#:21)

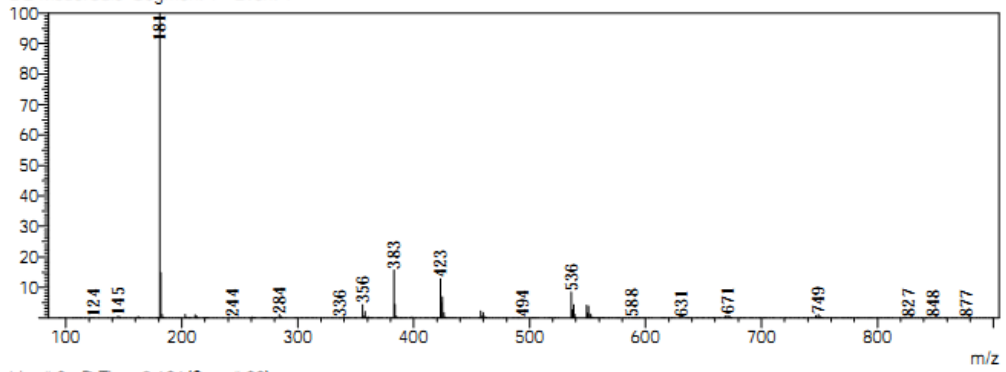
MassPeaks:396

Spectrum Mode:Averaged 0.119-0.136(20-22) BasePeak:191(42131)

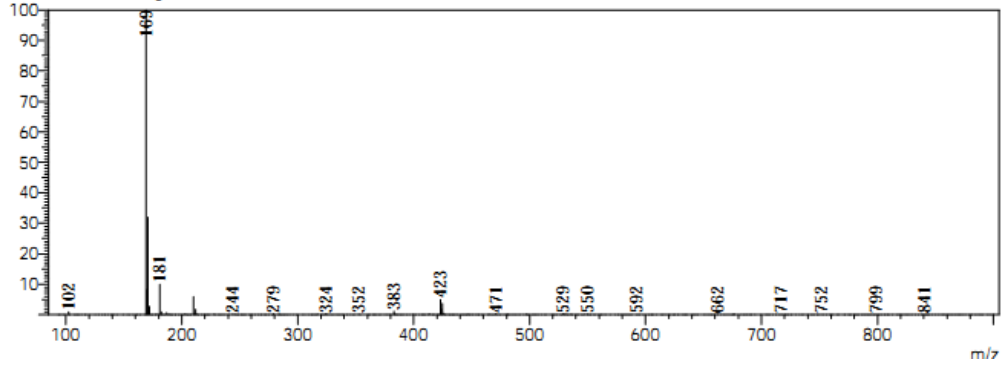
BG Mode:Calc Segment 1 - Event 1



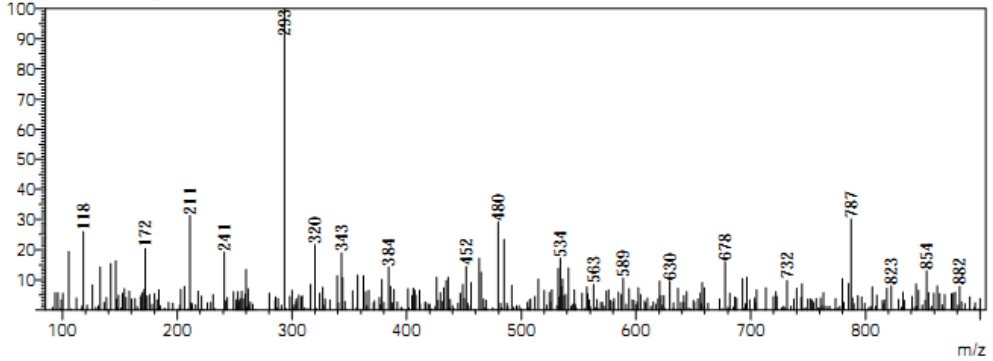
Line#:2 R.Time:0.619(Scan#:80)  
MassPeaks:404  
Spectrum Mode:Averaged 0.611-0.628(79-81) BasePeak:181(1154377)  
BG Mode:Calc Segment 1 - Event 1



Line#:3 R.Time:0.686(Scan#:88)  
MassPeaks:441  
Spectrum Mode:Averaged 0.678-0.694(87-89) BasePeak:169(1056608)  
BG Mode:Calc Segment 1 - Event 1



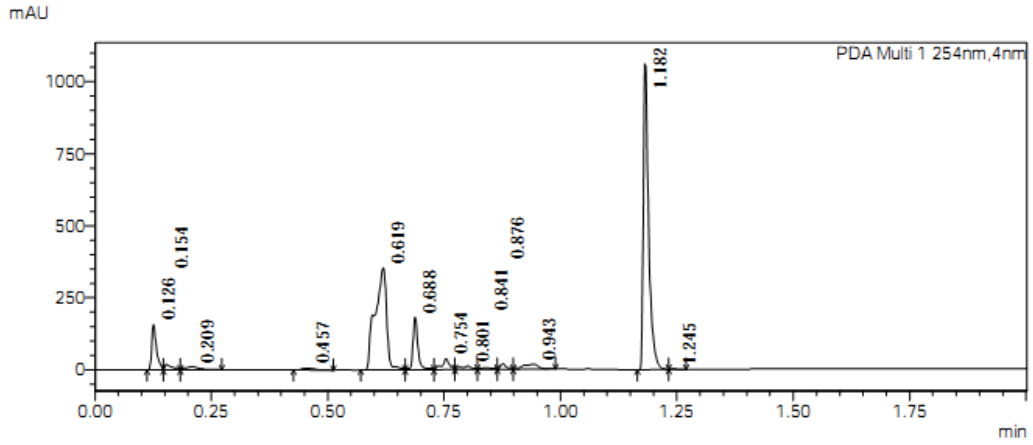
Line#:4 R.Time:1.178(Scan#:147)  
MassPeaks:389  
Spectrum Mode:Averaged 1.169-1.186(146-148) BasePeak:293(3561)  
BG Mode:Calc Segment 1 - Event 1





t=5 h

<Chromatogram>



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.126	149048	8.179	111871	5.928
2	0.154	18547	1.018	23678	1.255
3	0.209	9826	0.539	21178	1.122
4	0.457	5513	0.302	10858	0.575
5	0.619	350658	19.241	607135	32.169
6	0.688	181479	9.958	135167	7.162
7	0.754	37388	2.052	40719	2.158
8	0.801	12316	0.676	20425	1.082
9	0.841	5830	0.320	10605	0.562
10	0.876	19265	1.057	17523	0.928
11	0.943	17490	0.960	41298	2.188
12	1.182	1012725	55.570	844559	44.750
13	1.245	2334	0.128	2285	0.121
Total		1822418	100.000	1887302	100.000

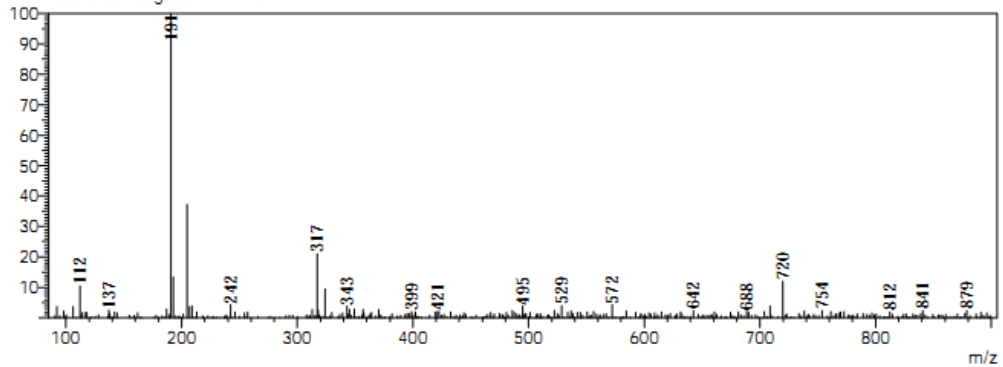
Mass Spectrum

Line#:1 R.Time:0.126(Scan#:21)

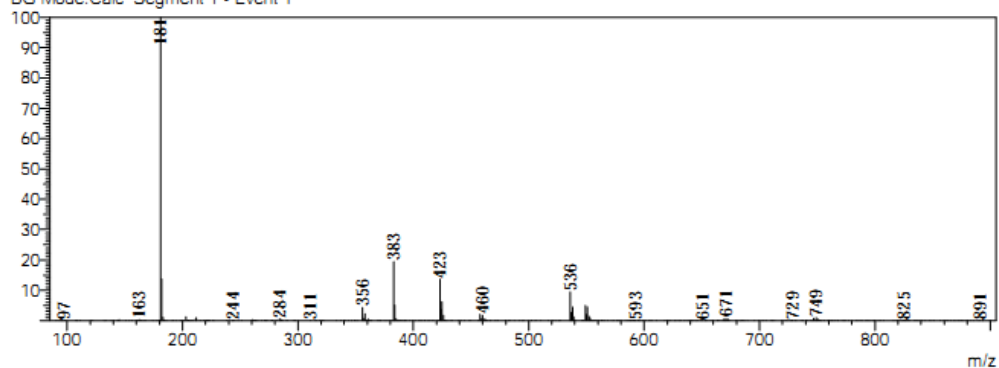
MassPeaks:384

Spectrum Mode:Averaged 0.119-0.136(20-22) BasePeak:191(20480)

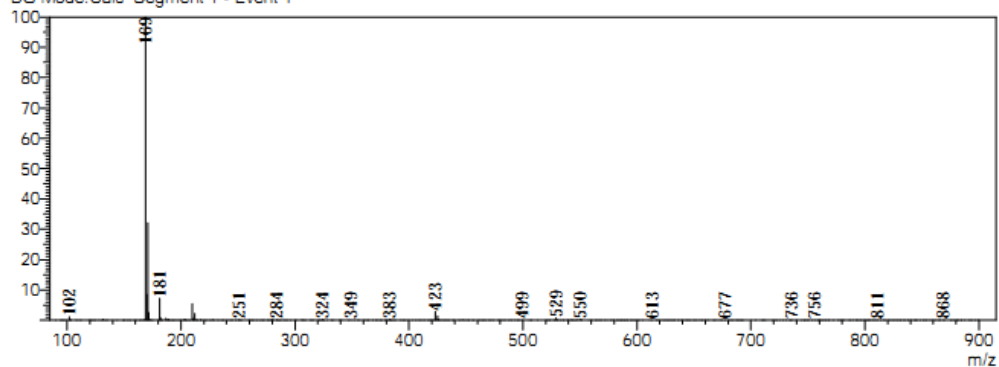
BG Mode:Calc Segment 1 - Event 1



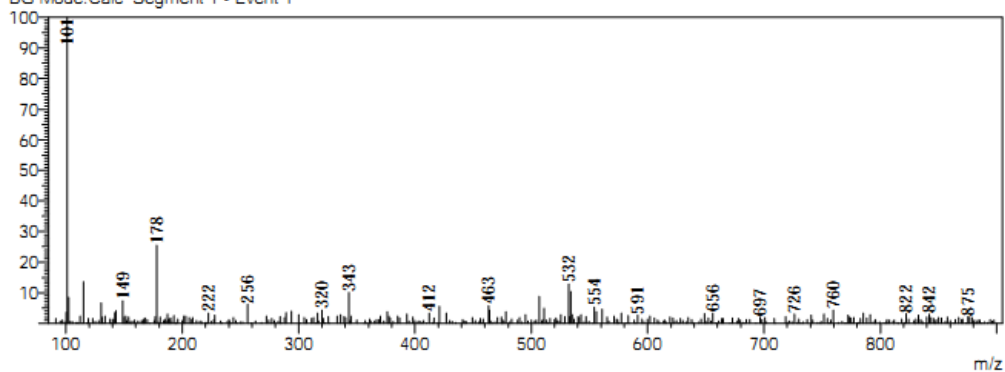
Line#:2 R.Time:0.619(Scan#:80)  
MassPeaks:373  
Spectrum Mode:Averaged 0.611-0.628(79-81) BasePeak:181(1101305)  
BG Mode:Calc Segment 1 - Event 1



Line#:3 R.Time:0.686(Scan#:88)  
MassPeaks:421  
Spectrum Mode:Averaged 0.678-0.694(87-89) BasePeak:169(981361)  
BG Mode:Calc Segment 1 - Event 1

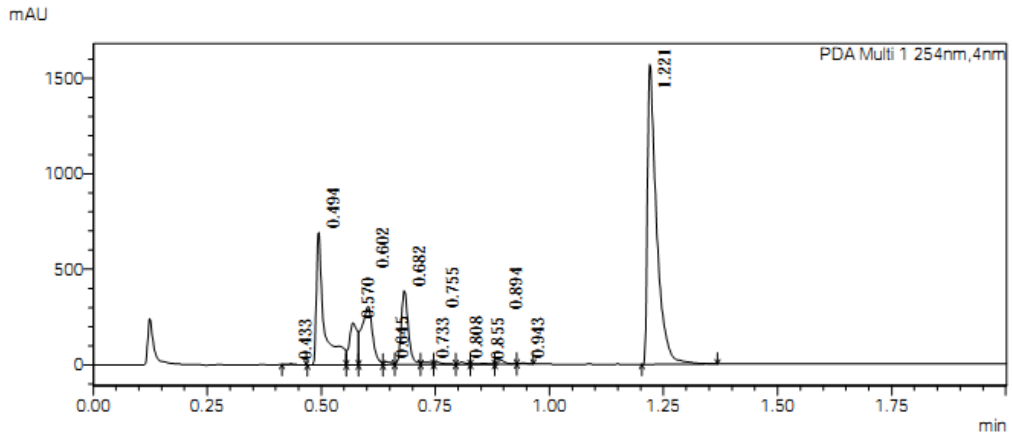


Line#:4 R.Time:1.186(Scan#:148)  
MassPeaks:379  
Spectrum Mode:Averaged 1.178-1.194(147-149) BasePeak:101(15900)  
BG Mode:Calc Segment 1 - Event 1



t=12 h

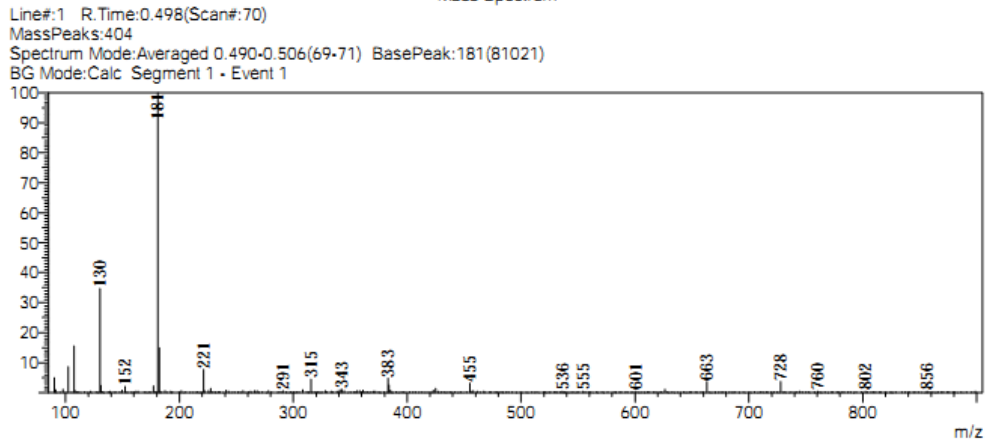
<Chromatogram>

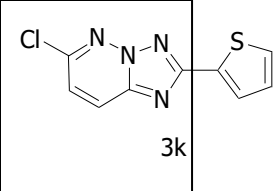


Peak Table

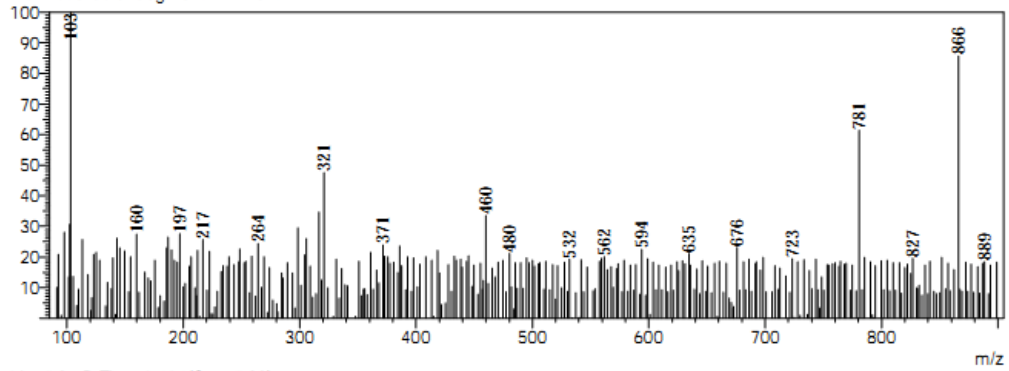
Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.433	3253	0.101	3313	0.077
2	0.494	671849	20.836	839896	19.509
3	0.570	218048	6.762	265948	6.177
4	0.602	303498	9.412	499546	11.603
5	0.645	13275	0.412	16741	0.389
6	0.682	386589	11.989	415124	9.642
7	0.733	10864	0.337	17187	0.399
8	0.755	11269	0.349	13854	0.322
9	0.808	11534	0.358	11511	0.267
10	0.855	5226	0.162	8414	0.195
11	0.894	21315	0.661	21684	0.504
12	0.943	6429	0.199	5902	0.137
13	1.221	1561384	48.422	2186074	50.778
Total		3224534	100.000	4305195	100.000

Mass Spectrum

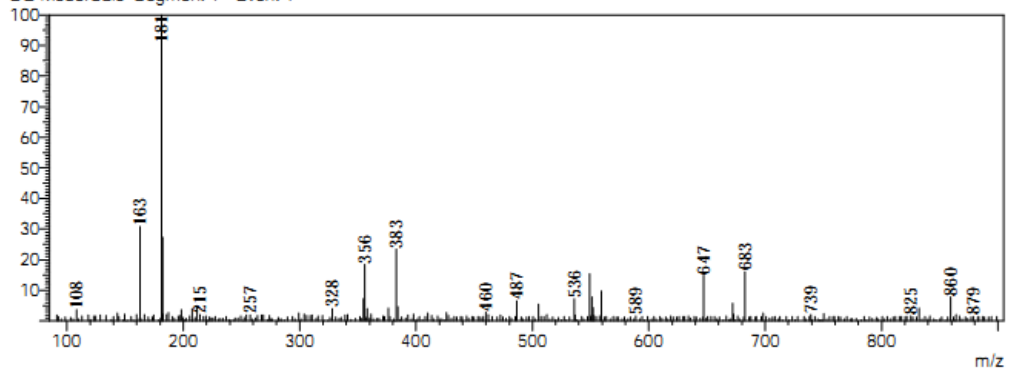




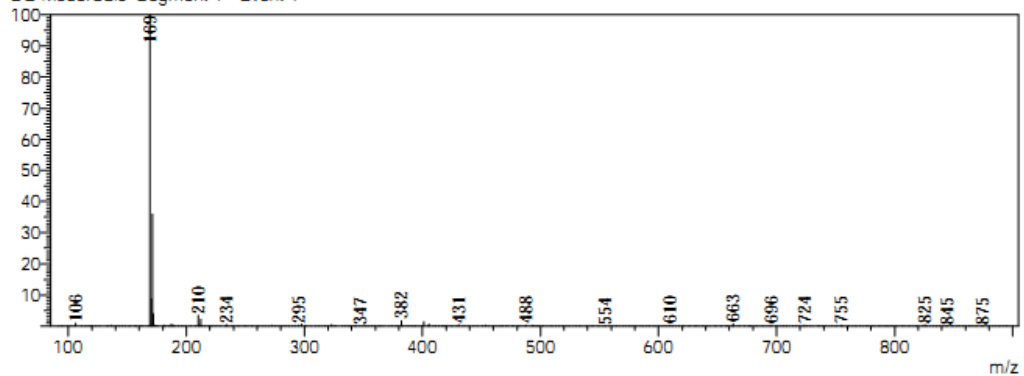
Line#:2 R.Time:0.573(Scan#:79)  
 MassPeaks:323  
 Spectrum Mode:Averaged 0.565-0.581(78-80) BasePeak:103(2108)  
 BG Mode:Calc Segment 1 - Event 1



Line#:3 R.Time:0.606(Scan#:83)  
 MassPeaks:352  
 Spectrum Mode:Averaged 0.598-0.615(82-84) BasePeak:181(27190)  
 BG Mode:Calc Segment 1 - Event 1



Line#:4 R.Time:0.681(Scan#:92)  
 MassPeaks:350  
 Spectrum Mode:Averaged 0.673-0.690(91-93) BasePeak:169(279411)  
 BG Mode:Calc Segment 1 - Event 1



Line#:5 R.Time:1.223(Scan#:157)  
 MassPeaks:410  
 Spectrum Mode:Averaged 1.215-1.231(156-158) BasePeak:386(8559)  
 BG Mode:Calc Segment 1 - Event 1

