

## Supporting Information

### Efficient trifluoromethylation of C(sp<sup>2</sup>)-H functionalized $\alpha$ -oxoketene dithioacetals : route to regioselective synthesis of trifluoromethylated pyrazoles

Nutan Sharma,<sup>a</sup> Neelam Kumari,<sup>b</sup> Tejpal Singh Chundawat,<sup>c</sup> Sushil Kumar<sup>d</sup> and Sunita Bhagat<sup>a\*</sup>

<sup>a</sup>Organic Synthesis Research Laboratory, Department of Chemistry, A.R.S.D. College, University of Delhi, New Delhi-110021, India.

<sup>b</sup>Institute of Nuclear Medicine & Allied Sciences, Defence Research & Development Organization, Brig. SK Mazumdar Marg, Delhi-110054, India

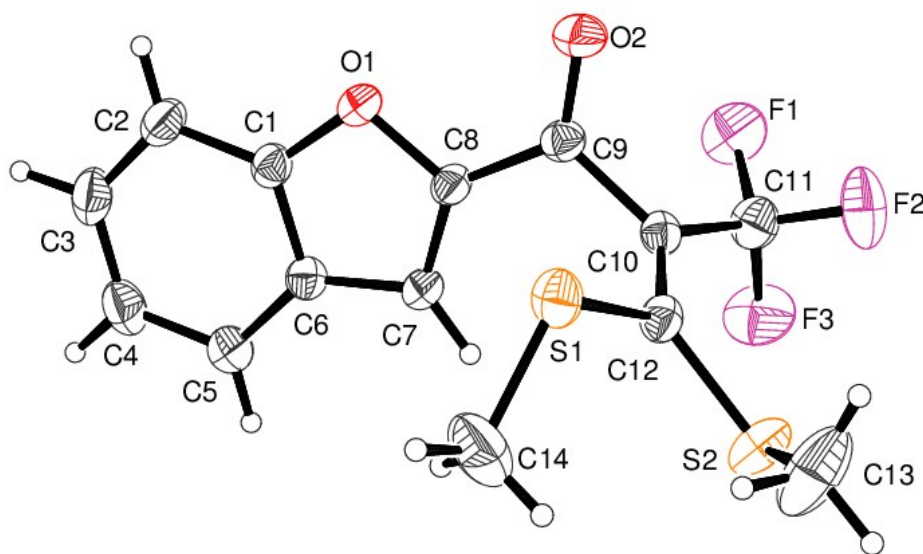
<sup>c</sup>Department of Applied Sciences, THE NORTHCAP UNIVERSITY (formerly ITM University), Gurgaon-122001, Haryana, India

<sup>d</sup>Physical Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India

Email id: sunitabhagat28@gmail.com

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# X-ray Crystallographic Studies



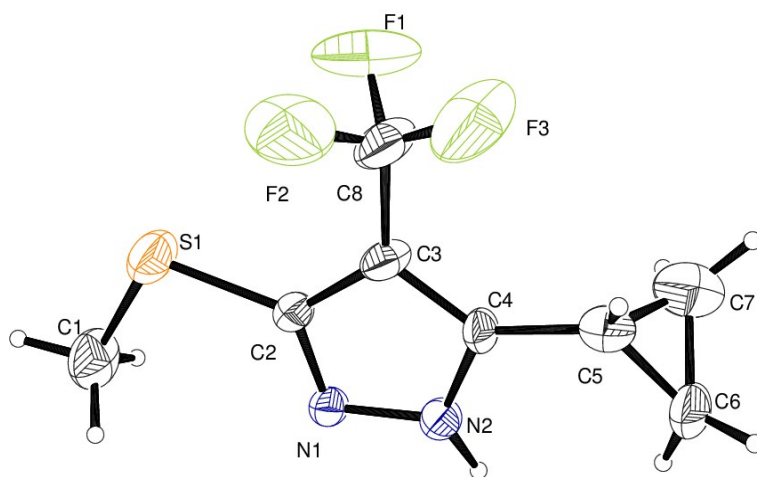
**Figure 1. ORTEP Structure of compound 31**

The intensity data for 31 was collected on an Oxford Xcalibur CCD diffractometer equipped with graphite monochromatic Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293(2) K<sup>1</sup>. A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on  $F^2$  using SHELXL97<sup>2</sup>. The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package<sup>3</sup>.

**Table 1.** Crystal data and structure refinement for compound **3I**

Empirical formula	C <sub>14</sub> H <sub>11</sub> F <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Formula weight	332.35
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	<i>P b c a</i>
<i>a</i>	13.456(5) Å
<i>b</i>	10.034(5) Å
<i>c</i>	22.429(5) Å
$\alpha$	90(5)°
$\beta$	90(5)°
$\gamma$	90(5)°
Volume	3028(2) Å <sup>3</sup>
<i>Z</i>	8
Density (calculated)	1.458 Mg/m <sup>3</sup>
Absorption coefficient	0.383 mm <sup>-1</sup>
<i>F</i> (000)	1360
Crystal size	0.22 x 0.20 x 0.18 mm <sup>3</sup>
Theta range for data collection	3.12 to 25.00°
Index ranges	-16 ≤ <i>h</i> ≤ 15, -11 ≤ <i>k</i> ≤ 11, -21 ≤ <i>l</i> ≤ 26
Reflections collected	9837
Independent reflections	2653 [ <i>R</i> (int) = 0.0226]
Completeness to theta = 25.00°	99.8 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9342 and 0.9204
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>
Data / restraints / parameters	2653 / 0 / 190
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.087
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )] <sup>a, b</sup>	<i>R</i> <sub>1</sub> = 0.0470, <i>wR</i> <sub>2</sub> = 0.1121
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.0583, <i>wR</i> <sub>2</sub> = 0.1175
Largest diff. peak and hole	0.205 and -0.180 e.Å <sup>-3</sup>

$$^a R = \sum(|F_o| - |F_c|) / \sum |F_o|; \quad ^b wR = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)] \}^{1/2}$$



**Figure 2. ORTEP drawings of compound 4i**

The intensity data for was collected on an Oxford CCD diffractometer equipped with Xcalibur Sapphire diffraction measurement device graphite monochromatic Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293(2) K<sup>1</sup>. A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on  $F^2$  using SHELXL97<sup>2</sup>. The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package<sup>3</sup>.

**Table 2.** Crystallographic data and structure refinement for compounds **4i**

Empirical formula	C <sub>8</sub> H <sub>9</sub> N <sub>2</sub> F <sub>3</sub> S
Formula weight	222.23
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2/c
<i>a</i>	19.392(5) Å
<i>b</i>	12.369(5) Å
<i>c</i>	18.099(5) Å
$\alpha$	90(5)°
$\beta$	110.204(5)°
$\gamma$	90(5)°
Volume	4074(2) Å <sup>3</sup>
<i>Z</i>	16
Density (calculated)	1.449 Mg/m <sup>3</sup>
Absorption coefficient	0.323 mm <sup>-1</sup>
<i>F</i> (000)	1824
Crystal size	0.22 x 0.21 x 0.20 mm <sup>3</sup>
Theta range for data collection	2.98 to 25.00°
Index ranges	-21 ≤ <i>h</i> ≤ 23, -14 ≤ <i>k</i> ≤ 14, -21 ≤ <i>l</i> ≤ 21
Reflections collected	24995
Independent reflections	6891 [ <i>R</i> (int) = 0.0832]
Completeness to theta = 25.00°	95.9 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9382 and 0.9323
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>
Data / restraints / parameters	6891 / 2 / 523
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.041
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )] <sup>a, b</sup>	<i>R</i> <sub>1</sub> = 0.1116, <i>wR</i> <sub>2</sub> = 0.2682
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.2134, <i>wR</i> <sub>2</sub> = 0.3318
Largest diff. peak and hole	0.417 and -0.278 e.Å <sup>-3</sup>

$${}^a R = \sum (\|F_o\| - |F_c|) / \sum |F_o|; {}^b wR = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$$

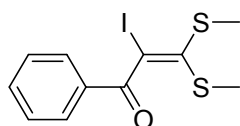
## References :

1. CrysAlispro, *Agilent Technologies*, Version 1.171.34.49 (2011).
2. Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112-122.
3. Farrugia, L.J. WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data*; Department of Chemistry, University of Glasgow (1997-2009).

### General procedure for the synthesis of $\alpha$ -iodo substituted oxoketene dithioacetals (2a-l)

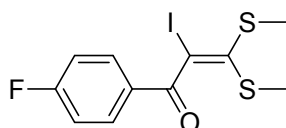
To a stirred solution of substituted oxoketene dithioacetal (1equiv.) in  $\text{CHCl}_3$ , N-iodosuccinimide (1.2equiv.) was added portionwise at rt. Colour of the reaction mixture changes to dark brown. Reaction mixture was stirred at rt for 1hr. Progress of reaction was monitored by TLC. After consumption of starting material, solvent was evaporated and crude compound was directly purified by column chromatography using silica gel (100: 200 mesh) in n-Hexane to afford **2a-l** as pure compound.

#### Analytical data of $\alpha$ -iodo substituted oxoketene dithioacetals (2a-l)



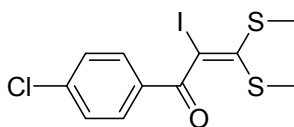
#### **2-iodo-3,3-bis(methylthio)-1-phenylprop-2-en-1-one (2a)** :

The compound was obtained as a yellow viscous material, yield : (718 mg, 92%) ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.84 (d,  $J = 7.93$  Hz, 1H), 7.79 (d,  $J = 7.93$  Hz, 1H), 7.26 (d,  $J = 7.93$  Hz, 3H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.13 (s, 3H, -SCH<sub>3</sub>);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 185.3, 165.3, 142.2, 136.5, 129.0, 127.7, 95.2 (vinylic CI), 17.2 (-SCH<sub>3</sub>), 14.9 (-SCH<sub>3</sub>).



#### **1-(4-fluorophenyl)-2-iodo-3,3-bis(methylthio)prop-2-en-1-one (2b)** :

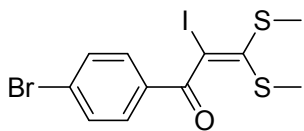
The compound was obtained as a pale yellow liquid, yield : (706 mg, 93%) ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.86 (dd,  $J = 8.24, 2.75$  Hz, 2H), 7.08 (t,  $J = 8.24$ , 2H), 2.41 (s, 3H, -SCH<sub>3</sub>), 2.07 (s, 3H, -SCH<sub>3</sub>);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 189.0, 167.2, 164.6, 142.5, 132.4, 130.3, 116.0, 115.8, 96.7 (vinylic C-I), 19.3 (-SCH<sub>3</sub>), 17.3 (-SCH<sub>3</sub>).



#### **1-(4-chlorophenyl)-2-iodo-3,3-bis(methylthio)prop-2-en-1-one (2c)** :

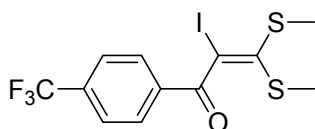
The compound was obtained as a yellow liquid, yield : (698 mg, 94%) ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.81 (d,  $J = 8.70$  Hz, 2H), 7.42 (d,  $J = 8.70$  Hz, 2H),

2.45 (s, 3H, -SCH<sub>3</sub>), 2.11 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 189.2, 142.9, 140.1, 132.4, 131.0, 129.1, 96.4 (vinylic C-I), 19.3 (-SCH<sub>3</sub>), 17.3 (-SCH<sub>3</sub>).



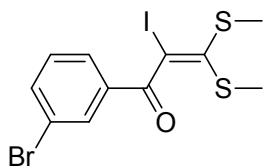
**1-(4-bromophenyl)-2-iodo-3,3-bis(methylthio)prop-2-en-1-**

**one (2d)** : The compound was obtained as a brown solid, yield : (643 mg, 91%) ; mp 50-52°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.74 (d, *J* = 8.70, 2H), 7.59 (d, *J* = 8.70, 2H), 2.46 (s, 3H, -SCH<sub>3</sub>), 2.12 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 189.4, 142.9, 132.8, 132.1, 131.1, 128.9, 96.4 (vinylic C-I), 19.3 (-SCH<sub>3</sub>), 17.3 (-SCH<sub>3</sub>).



**2-iodo-3,3-bis(methylthio)-1-(4-**

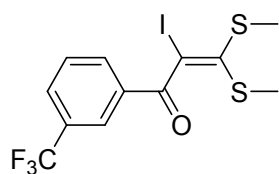
**(trifluoromethyl)phenyl)prop-2-en-1-one (2e)** : The compound was obtained as a pale yellow liquid, yield : (665 mg, 93%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.98 (d, *J* = 8.24, 2H), 7.72 (d, *J* = 8.24, 2H), 2.47 (s, 3H, -SCH<sub>3</sub>), 2.10 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 189.2, 143.8, 137.1, 134.8, 134.5, 129.9, 125.7, 124.8, 122.2, 95.8 (vinylic C-I), 19.3 (-SCH<sub>3</sub>), 17.4 (-SCH<sub>3</sub>).



**1-(3-bromophenyl)-2-iodo-3,3-bis(methylthio)prop-2-en-1-one**

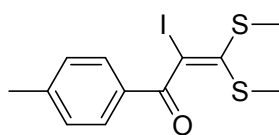
**(2f)** : The compound was obtained as a light yellow solid, yield : (665 mg, 94%) ; mp 54-56°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.91 (t, *J* = 1.83 Hz, 1H), 7.67 (dt, *J* = 7.79, 2.75, 1H), 7.57 (dq, *J* = 7.79, 2.75, 1H), 7.24 (t, *J* = 7.79, 1H), 2.37 (s, 3H, -SCH<sub>3</sub>), 2.05 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 188.9, 143.5, 136.3, 136.0, 132.3, 130.2, 128.2, 122.9, 96.0 (vinylic C-I), 19.3 (-SCH<sub>3</sub>), 17.3 (-SCH<sub>3</sub>).





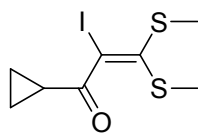
**2-iodo-3,3-bis(methylthio)-1-(3-(trifluoromethyl)phenyl)prop-**

**2-en-1-one (2g)** : The compound was obtained as yellow liquid, yield : (644 mg, 90%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.14 (s, 1H), 8.04 (d, *J* = 8.39, 1H), 7.81 (d, *J* = 7.63, 1H), 7.61 (t, *J* = 7.63, 1H), 2.48 (s, 3H, -SCH<sub>3</sub>), 2.10 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 189.0, 143.9, 134.8, 132.8, 131.5, 129.9, 129.3, 126.2, 124.9, 95.6 (vinylic C-I), 19.2 (-SCH<sub>3</sub>), 17.4 (-SCH<sub>3</sub>).



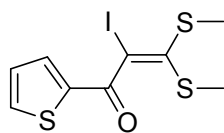
**2-iodo-3,3-bis(methylthio)-1-(p-tolyl)prop-2-en-1-one (2h)** :

The compound was obtained as a yellow liquid, yield : (687 mg, 90%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.78 (d, *J* = 8.24, 2H), 7.25 (d, *J* = 8.24, 2H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.40 (s, 3H, Ar-CH<sub>3</sub>), 2.11 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 190.1, 144.7, 141.7, 131.3, 129.9, 129.4, 97.8 (vinylic C-I), 21.7 (Ar-CH<sub>3</sub>), 19.3 (-SCH<sub>3</sub>), 17.3 (-SCH<sub>3</sub>).



**1-cyclopropyl-2-iodo-3,3-bis(methylthio)prop-2-en-1-one (2i)** :

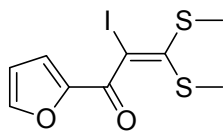
The compound was obtained as a yellow liquid, yield : (792 mg, 95%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 2.39 (s, 3H, SCH<sub>3</sub>), 2.25 (s, 3H, SCH<sub>3</sub>), 2.16-2.12 (m, 1H, cyclopropyl CH), 1.20-1.16 (m, 2H, cyclopropyl CH<sub>2</sub>), 1.01-0.96 (s, 2H, cyclopropyl CH<sub>2</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 206.9, 200.4, 100.5 (vinylic C-I), 30.8 (cyclopropyl CH), 19.7 (-SCH<sub>3</sub>), 17.6 (-SCH<sub>3</sub>), 13.1 (cyclopropyl CH<sub>2</sub>).



**2-iodo-3,3-bis(methylthio)-1-(thiophen-2-yl)prop-2-en-1-one (2j)**

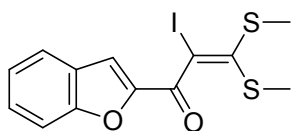
: The compound was obtained as a yellow liquid, yield : (711 mg, 92%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.68 (d, *J* = 5.04 Hz, 1H), 7.61 (d, *J* = 4.58, 1H), 7.11(t, *J* =

4.58, 1H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.17 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 183.4, 143.2, 140.9, 135.2, 134.4, 128.3, 95.8 (vinylic C-I), 19.6 (-SCH<sub>3</sub>), 17.4 (-SCH<sub>3</sub>).



**1-(furan-2-yl)-2-iodo-3,3-bis(methylthio)prop-2-en-1-one (2k) :**

The compound was obtained as a yellow liquid, yield : (722 mg, 91%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.63 (t, *J* = 1.83 Hz, 1H), 7.14 (d, *J* = 3.66 Hz, 1H), 6.54 (dd, *J* = 3.66, 1.83 Hz, 1H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.18 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 178.7, 149.7, 147.7, 144.2, 120.2, 112.6, 94.8 (vinylic C-I), 19.6 (-SCH<sub>3</sub>), 17.4 (-SCH<sub>3</sub>).



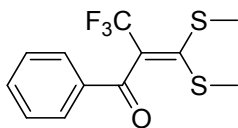
**1-(benzofuran-2-yl)-2-iodo-3,3-bis(methylthio)prop-2-en-1-**

**one (2l) :** The compound was obtained as a yellow viscous material, yield : (686 mg, 93%) ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.68 (d, *J* = 7.79 Hz, 1H), 7.57 (d, *J* = 8.70 Hz, 1H), 7.48-7.44 (m, 2H), 7.29 (t, *J* = 7.79 Hz, 1H), 2.48 (s, 3H, -SCH<sub>3</sub>), 2.18 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 180.5, 156.2, 149.9, 145.2, 128.6, 126.9, 124.0, 123.4, 115.9, 112.5, 94.2 (vinylic C-I), 19.7 (-SCH<sub>3</sub>), 17.4 (-SCH<sub>3</sub>).

### **General procedure for synthesis of trifluoromethylated $\alpha$ -oxoketene dithioacetals (3a-l)**

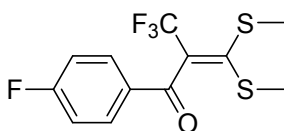
To a solution of compound **2** (1equiv.) in DMF, CuI (1.2equiv.) was added portionwise. After stirring for 5 minutes, FSO<sub>2</sub>CF<sub>2</sub>COOMe (1.5equiv.) was added dropwise at rt and reaction mass was heated to 90°C and stirred for 2-3hrs. Progress of reaction was monitored by TLC. After consumption of starting material **2**, crude was quenched with NH<sub>4</sub>OAc and extracted with EtOAc. Organic layer was washed with water. Combined organic layers were concentrated and crude was purified by column chromatography using 5% EtOAc: Hexane in silica gel(100:200) mesh to afford **3a-l** as pure compound.

### Analytical data of trifluoromethylated $\alpha$ -oxoketene dithioacetals (3a-l)



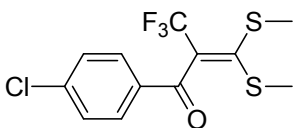
**3,3-bis(methylthio)-1-phenyl-2-(trifluoromethyl)prop-2-en-1-one (3a)**

: The compound was obtained as a light yellow solid, yield : (434 mg, 80%) ; mp 77-79°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2927, 1672 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.89 (d,  $J$  = 8.54, 2H), 7.59 (t,  $J$  = 7.32 Hz, 1H), 7.48 (t,  $J$  = 7.32, 2H), 2.44 (s, 3H, -SCH<sub>3</sub>), 2.16 (s, 3H, -SCH<sub>3</sub>) ; **<sup>13</sup>C NMR** (100 MHz, DMSO-d<sub>6</sub>)  $\delta$ : 188.2, 151.2, 135.0, 132.2, 130.5, 129.2, 125.9, 122.2 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 17.2 (-SCH<sub>3</sub>), 16.9 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>11</sub>F<sub>3</sub>OS<sub>2</sub>: 293.0281, found 293.0282.



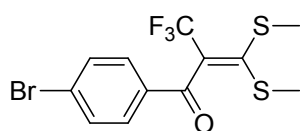
**1-(4-fluorophenyl)-3,3-bis(methylthio)-2-(trifluoromethyl)prop-2-en-1-one (3b)**

: The compound was obtained as a pale yellow viscous material, yield : (465 mg, 85%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2925, 1671 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.92 (dd,  $J$  = 8.24, 2.75 Hz, 2H), 7.15 (t,  $J$  = 8.24, 2H), 2.44 (s, 3H, -SCH<sub>3</sub>), 2.18 (s, 3H, -SCH<sub>3</sub>) ; **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 187.8, 167.5, 164.9, 150.8, 132.6, 131.8, 122.2 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 116.2, 116.0, 17.2 (-SCH<sub>3</sub>), 16.9 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>F<sub>4</sub>OS<sub>2</sub>: 311.0187, found 311.0177.



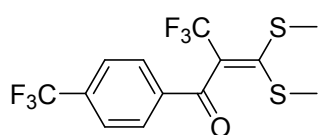
**1-(4-chlorophenyl)-3,3-bis(methylthio)-2-(trifluoromethyl)prop-2-en-1-one (3c)**

: The compound was obtained as a yellow solid, yield : (463 mg, 84%) ; mp 50-52°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2927, 1685 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.83 (d,  $J$  = 8.24 Hz, 2H), 7.45 (d,  $J$  = 8.70 Hz, 2H), 2.44 (s, 3H, -SCH<sub>3</sub>), 2.17 (s, 3H, -SCH<sub>3</sub>) ; **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 181.1, 151.0, 140.4, 134.6, 130.4, 129.2, 122.0 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 17.2 (-SCH<sub>3</sub>), 17.0 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>ClF<sub>3</sub>OS<sub>2</sub>: 326.9892, found 326.9898.



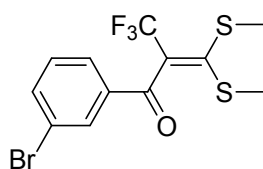
**1-(4-bromophenyl)-3,3-bis(methylthio)-2-(trifluoromethyl)prop-**

**2-en-1-one (3d)** : The compound was obtained as a light yellow viscous material, yield : (446 mg, 86%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2927, 1672 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.75 (d,  $J$  = 8.70, 2H), 7.62 (d,  $J$  = 8.70, 2H), 2.43 (s, 3H, -SCH<sub>3</sub>), 2.17 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 188.2, 151.2, 135.0, 132.2, 130.5, 129.2, 125.9, 122.2 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 17.2 (-SCH<sub>3</sub>), 16.9 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>ClF<sub>3</sub>OS<sub>2</sub>: 370.9387, found 370.9381.



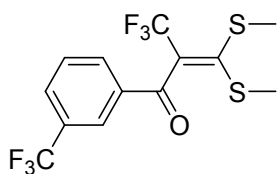
**3,3-bis(methylthio)-2-(trifluoromethyl)-1-(4-**

**(trifluoromethyl)phenyl)prop-2-en-1-one (3e)** : The compound was obtained as a yellow solid, yield : (444 mg, 86%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2826, 1685 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.99 (d,  $J$  = 8.24, 2H), 7.74 (d,  $J$  = 8.24, 2H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.16 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 188.1, 152.0, 139.0, 135.1, 134.7, 131.0, 130.7, 129.2, 125.9, 124.8, 122.2, 122.0 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 17.2 (-SCH<sub>3</sub>), 17.0 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>13</sub>H<sub>10</sub>F<sub>6</sub>OS<sub>2</sub>: 361.0155, found 361.0156.

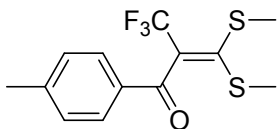


**1-(3-bromophenyl)-3,3-bis(methylthio)-2-(trifluoromethyl)prop-2-**

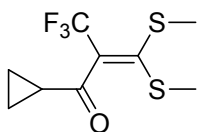
**en-1-one (3f)** : The compound was obtained as a light yellow viscous material, yield : (441 mg, 85%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2925, 1670 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.04 (d,  $J$  = 1.53 Hz, 1H), 7.77 (d,  $J$  = 7.63, 1H), 7.71 (d,  $J$  = 7.63, 1H), 7.36 (t,  $J$  = 7.63, 1H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.17 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 187.8, 151.6, 138.0, 136.6, 131.8, 130.3, 127.6, 123.1, 122.2 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 17.2 (-SCH<sub>3</sub>), 16.9 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>BrF<sub>3</sub>OS<sub>2</sub>: 370.9387, found 370.9389.



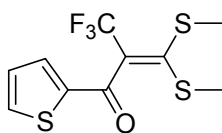
**3,3-bis(methylthio)-2-(trifluoromethyl)-1-(3-(trifluoromethyl)phenyl)prop-2-en-1-one (3g)** : The compound was obtained as a pale yellow solid, yield : (429 mg, 83%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2925, 1680 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.15 (s, 1H), 8.04 (d,  $J = 7.63$ , 1H), 7.84 (d,  $J = 7.63$ , 1H), 7.63 (t,  $J = 8.01$ , 1H), 2.45 (s, 3H, -SCH<sub>3</sub>), 2.16 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 187.8, 152.2, 136.8, 132.1, 131.7, 131.4, 130.8, 130.5, 130.1, 129.5, 125.6, 122.1 (vinylic C-CF<sub>3</sub>), 119.6 (vinylic CF<sub>3</sub>), 17.1 (-SCH<sub>3</sub>), 17.0 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>13</sub>H<sub>10</sub>F<sub>6</sub>OS<sub>2</sub>: 361.0155, found 361.0156.



**3,3-bis(methylthio)-1-(p-tolyl)-2-(trifluoromethyl)prop-2-en-1-one (3h)**: The compound was obtained as a yellow liquid, yield : (413 mg, 82%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2928, 1665 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.74 (d,  $J = 8.39$ , 2H), 7.21 (d,  $J = 7.63$ , 2H), 2.40 (s, 3H, -SCH<sub>3</sub>), 2.35 (s, 3H, Ar-CH<sub>3</sub>), 2.06 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 190.1, 144.7, 141.7, 131.3, 129.9, 129.4, 125.9, 122.4 (vinylic C-CF<sub>3</sub>), 119.4 (-CF<sub>3</sub>), 21.7 (Ar-CH<sub>3</sub>), 19.3 (-SCH<sub>3</sub>), 17.3 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>13</sub>H<sub>13</sub>F<sub>3</sub>OS<sub>2</sub>: 307.0438, found 307.0457.

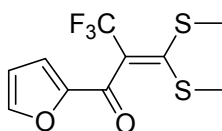


**1-cyclopropyl-3,3-bis(methylthio)-2-(trifluoromethyl)prop-2-en-1-one (3i)** : The compound was obtained as a yellow liquid, yield : (491 mg, 86%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2884, 1692 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 2.36 (s, 6H, 2 x SCH<sub>3</sub>), 2.12-2.07 (m, 1H, cyclopropyl CH), 1.22-1.18 (m, 2H, cyclopropyl CH<sub>2</sub>), 1.05-1.00 (m, 2H, cyclopropyl CH<sub>2</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 198.9, 150.3, 122.4 (vinylic C-CF<sub>3</sub>), 119.7 (vinylic CF<sub>3</sub>), 22.5 (cyclopropyl CH), 17.3 (-SCH<sub>3</sub>), 12.7 (cyclopropyl CH<sub>2</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>9</sub>H<sub>11</sub>F<sub>3</sub>OS<sub>2</sub>: 257.0281, found 257.0280.



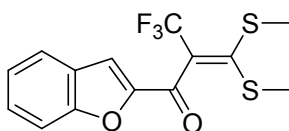
**3,3-bis(methylthio)-1-(thiophen-2-yl)-2-(trifluoromethyl)prop-2-en-1-**

**one (3j)** : The compound was obtained as a yellow liquid, yield : (462 mg, 85%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2885, 1665 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.71 (d,  $J$  = 5.34 Hz, 1H), 7.60 (d,  $J$  = 3.81, 1H), 7.12 (t,  $J$  = 3.81, 1H), 2.43 (s, 3H, -SCH<sub>3</sub>), 2.22 (s, 3H, -SCH<sub>3</sub>) ; **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 181.4, 151.5, 143.4, 135.6, 134.1, 128.3, 122.2 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 17.4 (-SCH<sub>3</sub>), 16.9 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>10</sub>H<sub>9</sub>F<sub>3</sub>OS<sub>2</sub>: 298.9846, found 298.9839.



**1-(furan-2-yl)-3,3-bis(methylthio)-2-(trifluoromethyl)prop-2-en-1-one**

**(3k)** : The compound was obtained as a yellow liquid, yield : (453 mg, 84%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2878, 1655 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.64 (t,  $J$  = 1.83 Hz, 1H), 7.15 (d,  $J$  = 3.66 Hz, 1H), 6.55 (q,  $J$  = 3.66, 1.83 Hz, 1H), 2.42 (s, 3H), 2.23 (s, 3H) ; **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 176.5, 152.6, 151.9, 147.9, 130.8, 130.4, 122.3 (vinylic C-CF<sub>3</sub>), 119.9 (-CF<sub>3</sub>), 112.7, 17.5 (-SCH<sub>3</sub>), 16.9 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>10</sub>H<sub>9</sub>F<sub>3</sub>O<sub>2</sub>S<sub>2</sub>: 283.0074, found 283.0072.



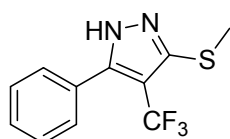
**1-(benzofuran-2-yl)-3,3-bis(methylthio)-2-(trifluoromethyl)prop-2-**

**en-1-one (3l)** : The compound was obtained as a yellow solid, yield : (475 mg, 93%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 2925, 1656 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.70 (d,  $J$  = 8.24 Hz, 1H), 7.57 (d,  $J$  = 8.24 Hz, 1H), 7.48 (t,  $J$  = 8.24 Hz, 2H) 7.30 (t,  $J$  = 7.79 Hz, 1H), 2.46 (s, 3H), 2.23 (s, 3H) ; **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 178.3, , 156.3, 153.5, 152.0, 128.9, 126.9, 124.1, 123.5, 122.4 (vinylic C-CF<sub>3</sub>), 119.5 (-CF<sub>3</sub>), 115.6, 112.5, 17.7 (-SCH<sub>3</sub>), 17.0 (-SCH<sub>3</sub>) ; **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>14</sub>H<sub>11</sub>F<sub>3</sub>O<sub>2</sub>S<sub>2</sub>: 333.0231, found 333.0230.

## General procedure for the synthesis of trifluoromethylated 1*H*-pyrazoles (4a-l)

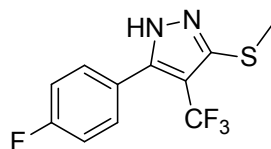
In an oven-dried RBF, hydrazine hydrate (1.5equiv.) was added to a solution of compound **3** (1equiv.) in EtOH and reaction mass was heated at 90°C for 2-3hrs. Progress of reaction was monitored by TLC. The reaction mixture was then cooled and solvent was evaporated. After that crude was purified by column chromatography using 20% ethyl acetate/hexane as eluent to afford the corresponding products **4a-l**.

### 5.7.4.1 Analytical data of 3,4-dihydro-1*H*-quinazolin-2-ylidenes (4a-l)



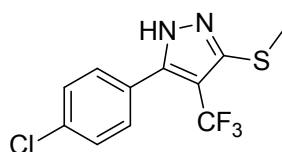
#### 3-(methylthio)-5-phenyl-4-(trifluoromethyl)-1*H*-pyrazole (4a) :

The compound was obtained as light yellow solid, yield : (247 mg, 80%) ;mp 122-124°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3221, 2924 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.45 (s, 5H), 2.54 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 146.3, 146.1, 129.8, 128.7, 128.4, 128.1, 124.2, 121.5(C-CF<sub>3</sub>), 114.0, 108.7 (q,  $J$  = 32.5Hz, -CF<sub>3</sub>), 15.4 (-SCH<sub>3</sub>) ; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>)  $\delta$ : -54.22 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>11</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>S: 259.0517, found 259.0515.



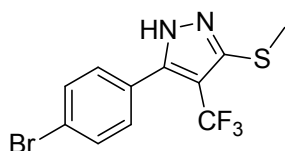
#### 5-(4-fluorophenyl)-3-(methylthio)-4-(trifluoromethyl)-1*H*-pyrazole (4b) :

The compound was obtained as light yellow solid, yield : (252 mg, 81%) ; mp 112-114°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3218, 2926 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.45 (dd,  $J$  = 8.70, 3.21 Hz, 2H), 7.12 (t,  $J$  = 8.70 Hz, 2H), 2.53 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 164.8, 162.3, 146.0, 145.4, 130.5, 124.4, 124.0, 121.3 (C-CF<sub>3</sub>), 116.0, 115.7, 109.0 (-CF<sub>3</sub>), 15.7 (-SCH<sub>3</sub>) ; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>)  $\delta$ : -54.92 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>11</sub>H<sub>8</sub>F<sub>4</sub>N<sub>2</sub>S: 277.0422, found 277.0417.

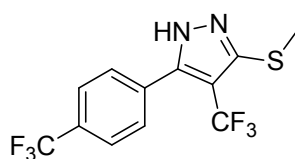


**5-(4-chlorophenyl)-3-(methylthio)-4-(trifluoromethyl)-1*H*-pyrazole (4c) :** The compound was obtained as light yellow solid, yield : (257 mg, 82%) ;

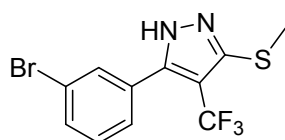
mp 120-122°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3216, 2925 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.20 (bs, 1H, NH), 7.36 (s, 4H), 2.50 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 146.1, 145.0, 136.0, 129.7, 128.9, 126.9, 124.0, 121.3(C-CF<sub>3</sub>), 118.7, 113.6, 109.1(-CF<sub>3</sub>), 15.9 (-SCH<sub>3</sub>) ; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>)  $\delta$ : -53.91 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>11</sub>H<sub>8</sub>ClF<sub>3</sub>N<sub>2</sub>S: 293.0127, found 293.0126.



**5-(4-bromophenyl)-3-(methylthio)-4-(trifluoromethyl)-1H-pyrazole (4d)** : The compound was obtained as light yellow viscous material, yield : (254 mg, 80%) ; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3219, 2925 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.41 (bs, 1H, NH), 7.53 (d, J = 7.79 Hz, 2H), 7.30 (d, J = 8.24 Hz, 2H), 2.50 (s, 3H, -SCH<sub>3</sub>); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 131.9, 130.0, 128.9, 127.4, 125.5, 124.3, 15.9 (-SCH<sub>3</sub>) ; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>)  $\delta$ : -53.22 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>11</sub>H<sub>8</sub>BrF<sub>3</sub>N<sub>2</sub>S: 336.9622, found 336.9620.



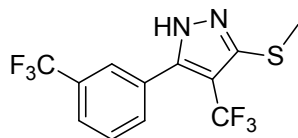
**3-(methylthio)-4-(trifluoromethyl)-5-(4-(trifluoromethyl)phenyl)-1H-pyrazole (4e)** : The compound was obtained as light yellow solid, yield : (253 mg, 80%) ; mp 76-78°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3226, 2926 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.19 (bs, 1H, NH), 7.67 (d, J = 8.24 Hz, 2H), 7.59 (d, J = 7.33 Hz, 2H), 2.54 (s, 3H); **<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 146.5, 144.4, 132.4, 131.8, 131.4, 128.9, 125.6, 124.1, 122.3, 121.3 (C-CF<sub>3</sub>), 109.2 (-CF<sub>3</sub>), 16.2 (-SCH<sub>3</sub>) ; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>)  $\delta$ : -53.93 (s, 3F), -62.82 (s, 3F, Ar-CF<sub>3</sub>); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>8</sub>F<sub>6</sub>N<sub>2</sub>S: 327.0390, found 327.0385.



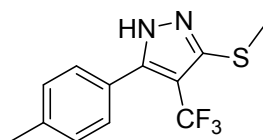
**5-(3-bromophenyl)-3-(methylthio)-4-(trifluoromethyl)-1H-pyrazole (4f)** : The compound was obtained as light yellow viscous material, yield : (257 mg, 81%) ; mp 104-106°C; **IR** ( $\nu_{\max}$ cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3219, 2925; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.84 (bs, 1H, NH), 7.58-7.52 (m, 2H), 7.37 (d, J = 7.33 Hz, 1H), 7.25 (d, J = 8.24 Hz, 1H), 2.49 (s,



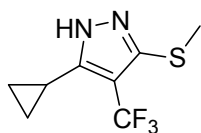
3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 145.8, 144.7, 132.7, 131.3, 130.7, 130.1, 127.2, 124.0, 122.5, 121.3(C-CF<sub>3</sub>), 18.7, 109.6 (-CF<sub>3</sub>), 16.0 (-SCH<sub>3</sub>); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ: -53.25 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>11</sub>H<sub>8</sub>BrF<sub>3</sub>N<sub>2</sub>S: 336.9622, found 336.9621.



**3-(methylthio)-4-(trifluoromethyl)-5-(3-(trifluoromethyl)phenyl)-1H-pyrazole (4g)** : The compound was obtained as light yellow solid, yield : (263 mg, 83%) ; mp 92-94°C; **IR** (ν<sub>max</sub>cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3219, 2925 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ: 7.74 (s, 1H), 7.67 (t, *J* = 8.39 Hz, 2H), 7.54 (d, *J* = 8.39 Hz, 1H), 2.52 (s, 3H, -SCH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 146.4, 144.2, 131.9, 131.3, 130.0, 129.9, 129.2, 126.3, 125.3, 122.2, 121.3(C-CF<sub>3</sub>), 114.0, 109.7(-CF<sub>3</sub>), 16.1 (-SCH<sub>3</sub>); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ: -53.81 (s, 3F), 62.84 (s, 3F, Ar-CF<sub>3</sub>); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>8</sub>F<sub>6</sub>N<sub>2</sub>S: 327.0390, found 327.0382.

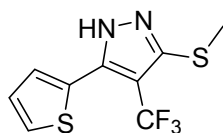


**3-(methylthio)-5-(p-tolyl)-4-(trifluoromethyl)-1H-pyrazole (4h)** : The compound was obtained as light yellow solid, yield : (223 mg, 72%) ; mp 128-130°C; **IR** (ν<sub>max</sub>cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3233, 2927 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ: 7.87 (bs, 1H, NH), 7.32(d, *J* = 8.24 Hz, 2H), 7.21 (d, *J* = 8.24 Hz, 2H), 2.51 (s, 3H,-SCH<sub>3</sub>), 2.37 (s, 3H, Ar-CH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 146.4, 146.2, 140.1, 129.4, 128.3, 125.0, 124.2, 121.5(C-CF<sub>3</sub>), 108.1(-CF<sub>3</sub>), 21.3 (Ar-CH<sub>3</sub>), 15.2 (-SCH<sub>3</sub>) ; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ: -53.95 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>12</sub>H<sub>11</sub>F<sub>3</sub>N<sub>2</sub>S: 273.0673, found 273.0664.



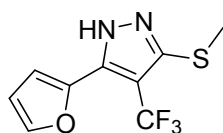
**5-cyclopropyl-3-(methylthio)-4-(trifluoromethyl)-1H-pyrazole (4i)** : The compound was obtained as a off white crystalline solid, yield : (230 mg, 76%) ; mp 116-118°C; **IR** (ν<sub>max</sub>cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3174, 2920 ; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ: 9.30 (bs, 1H, NH), 2.46 (s, 3H,-SCH<sub>3</sub>), 2.01-1.93 (m, 1H,cyclopropyl CH), 1.02-0.97 (q, 2H, cyclopropyl CH<sub>2</sub>), 0.81-0.76 (q, 2H, cyclopropyl CH<sub>2</sub>) ; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 148.5, 144.7,

121.8 (C-CF<sub>3</sub>), 110.2 (q, *J* = 37.3 Hz, -CF<sub>3</sub>), 15.9 (-SCH<sub>3</sub>), 6.9 (cyclopropyl CH), 6.2 (cyclopropyl CH<sub>2</sub>); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ: -54.95 (s, 3F); HRMS (ESI) (M+H)<sup>+</sup> Calcd for C<sub>8</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>S: 223.0517, found 223.0521.



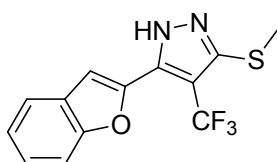
**3-(methylthio)-5-(thiophen-2-yl)-4-(trifluoromethyl)-1H-pyrazole (4j)**

: The compound was obtained as a viscous brown material, yield : (244 mg, 79%) ; IR (ν<sub>max</sub>cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3459, 2923 ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 9.38 (bs, 1H, NH), 7.28 (d, *J* = 5.04 Hz, 1H), 7.24 (d, *J* = 3.66 Hz, 1H), 6.98 (t, *J* = 4.58 Hz, 1H), 2.39 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 144.1, 141.7, 129.2, 128.5, 127.8, 127.4, 124.1, 121.4(C-CF<sub>3</sub>), 108.4 (-CF<sub>3</sub>), 15.9(-SCH<sub>3</sub>) ; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ: -54.40 (s, 3F); HRMS (ESI) (M+H)<sup>+</sup> Calcd for C<sub>9</sub>H<sub>7</sub>F<sub>3</sub>N<sub>2</sub>S<sub>2</sub>: 265.0081, found 265.0082.



**5-(furan-2-yl)-3-(methylthio)-4-(trifluoromethyl)-1H-pyrazole (4k) :**

The compound was obtained as a off white crystalline solid, yield : (240 mg, 78%) ; mp 146-148°C; IR (ν<sub>max</sub>cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3440, 2926 ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 9.05 (bs, 1H, NH), 7.45 (d, *J* = 1.83 Hz, 1H), 6.83 (d, *J* = 3.21 Hz, 1H), 6.50 (dd, *J* = 3.66, 1.83 Hz, 1H), 2.55 (s, 3H, -SCH<sub>3</sub>) ; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 146.5, 143.3, 141.8, 136.3, 124.1, 121.5 (C-CF<sub>3</sub>), 112.1, 111.4, 105.8 (q, *J* = 38.3 Hz, -CF<sub>3</sub>), 15.0 (-SCH<sub>3</sub>) ; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ: -54.60 (s, 3F); HRMS (ESI) (M+H)<sup>+</sup> Calcd for C<sub>9</sub>H<sub>7</sub>F<sub>3</sub>N<sub>2</sub>OS: 249.0309, found 249.0306.

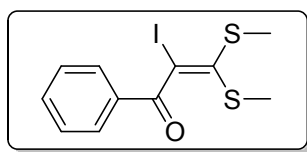


**5-(benzofuran-2-yl)-3-(methylthio)-4-(trifluoromethyl)-1H-pyrazole (4l) :**

The compound was obtained as a off white crystalline solid, yield : (241 mg, 77%) ; mp 178-180°C; IR (ν<sub>max</sub>cm<sup>-1</sup>) (CHCl<sub>3</sub>): 3420, 2924 ; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 7.67 (d, *J* = 7.79 Hz, 1H), 7.56 (d, *J* = 8.24 Hz, 1H), 7.31 (t, *J* = 8.24 Hz, 1H) 7.24-7.21 (m, 2H), 2.49 (s, 3H, -SCH<sub>3</sub>) ; <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) δ: 154.2, 127.6,

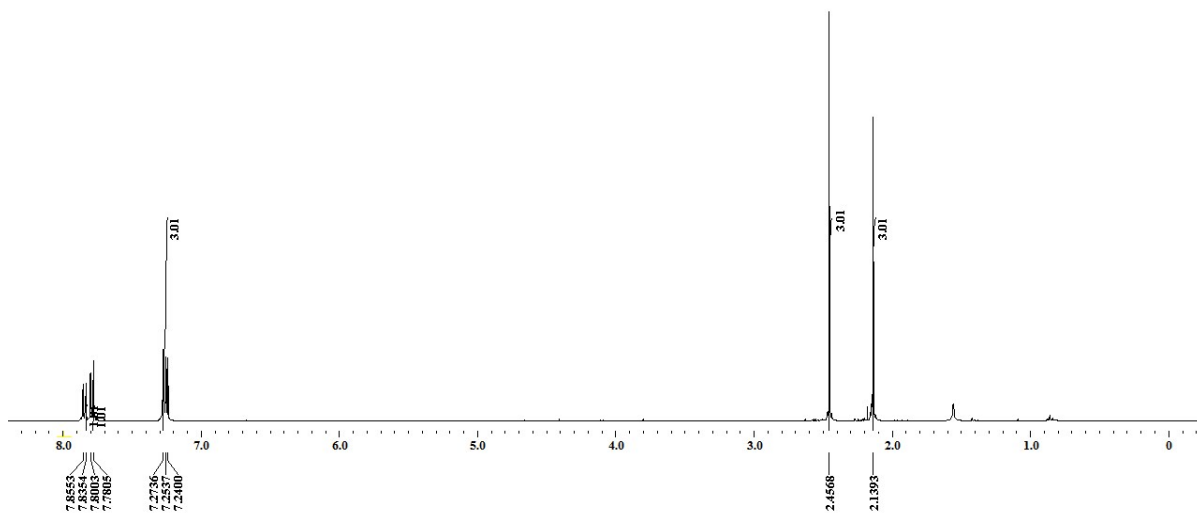
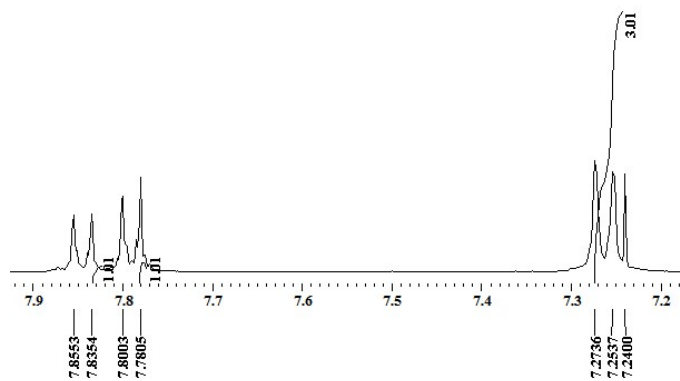
125.8, 124.4, 123.6, 121.9 (C-CF<sub>3</sub>), 111.3, 106.7(-CF<sub>3</sub>), 14.7 (-SCH<sub>3</sub>) ; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>) δ: -55.20 (s, 3F); **HRMS** (ESI) (M+H)<sup>+</sup> Calcd for C<sub>13</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>OS: 299.0466, found 299.0466.

***COPIES OF  $^1\text{H}$ ,  $^{13}\text{C}$ NMR & HRMS  
DATA***

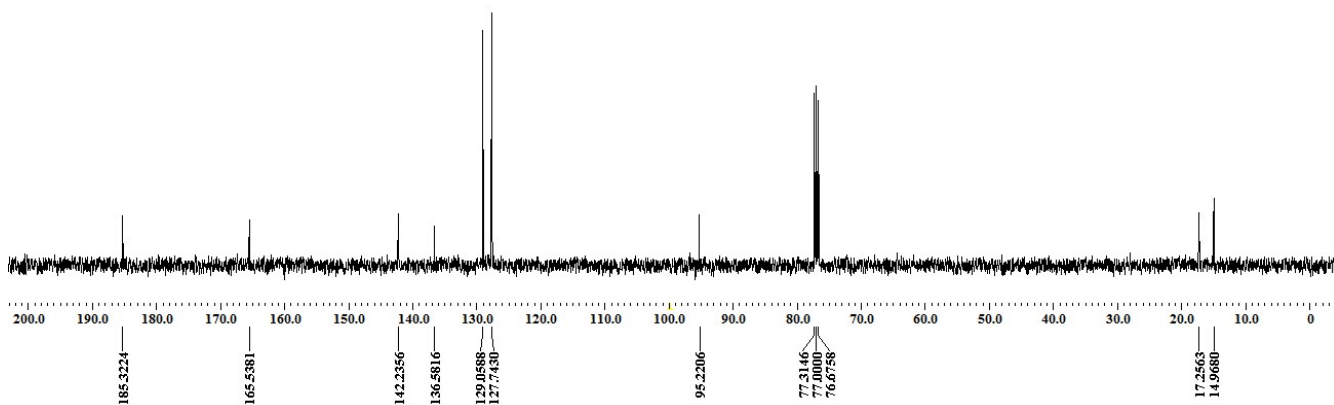


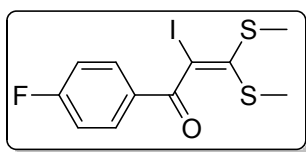
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$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



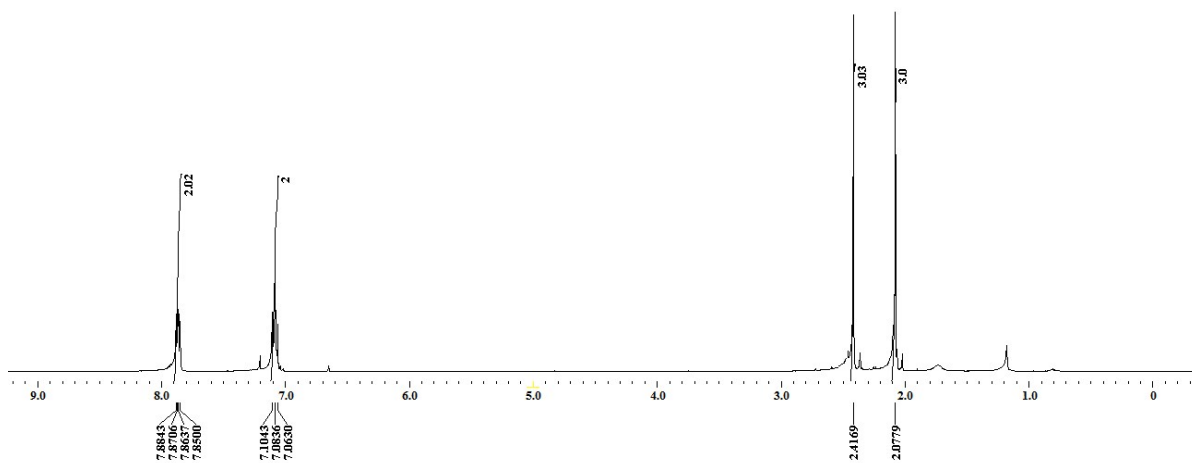
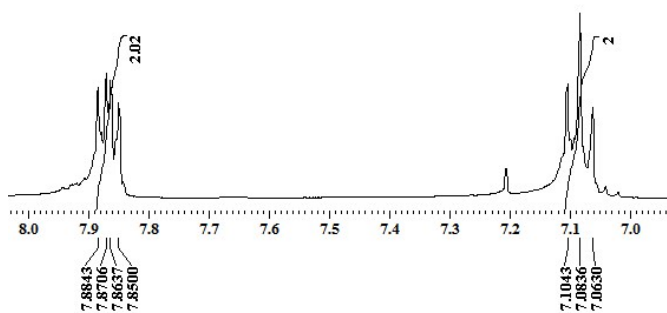
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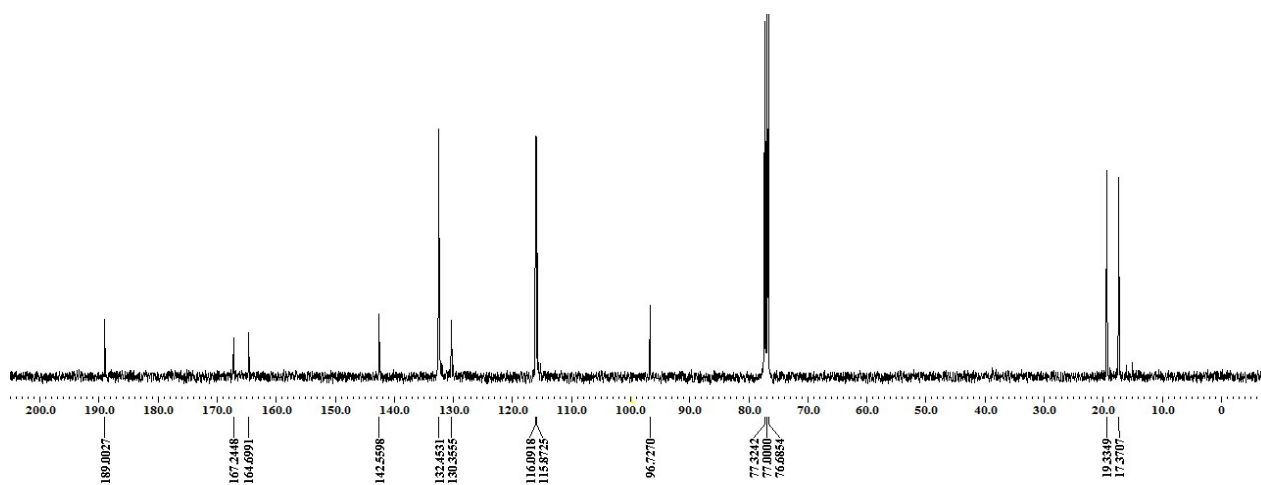


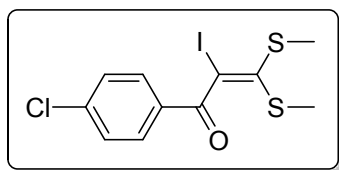
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$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



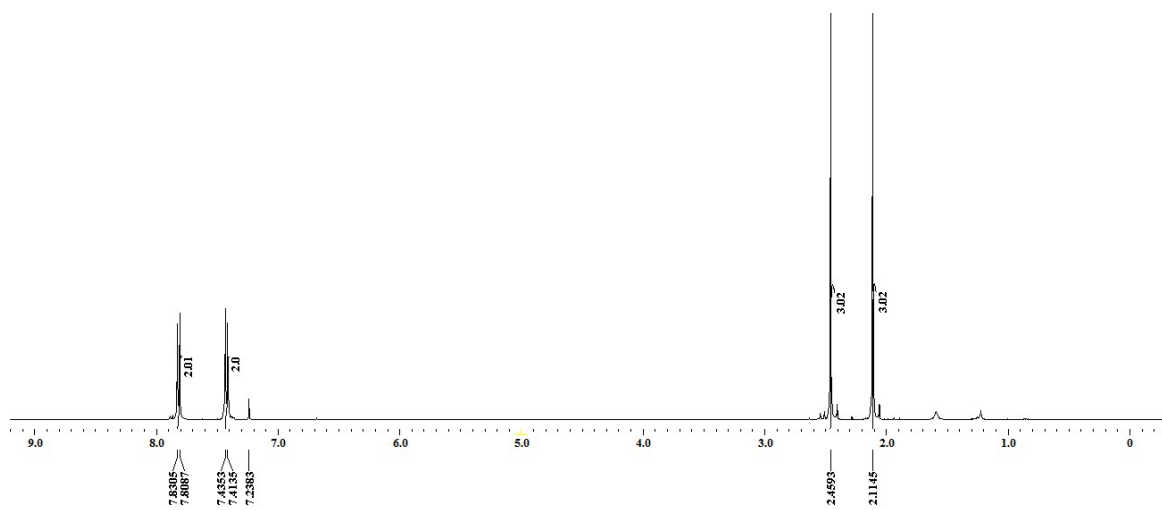
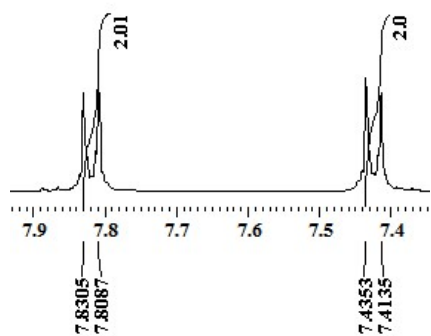
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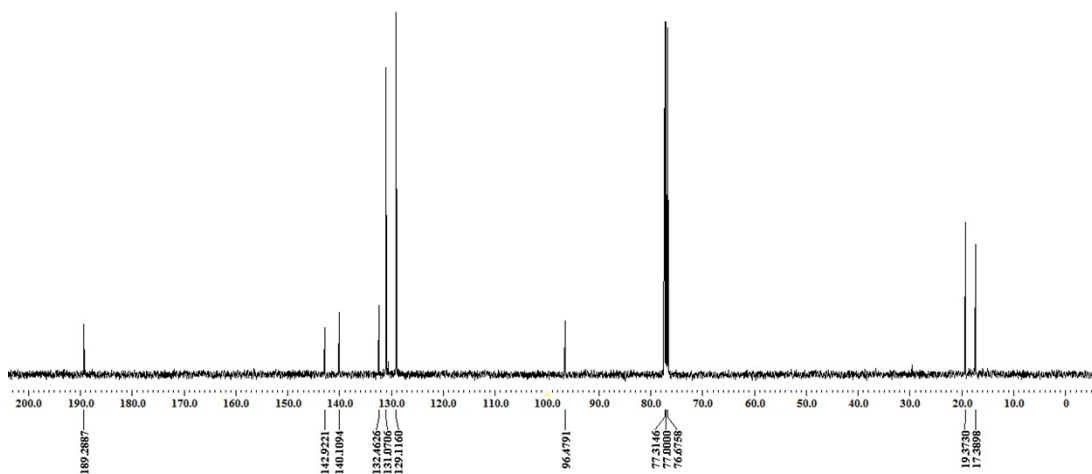


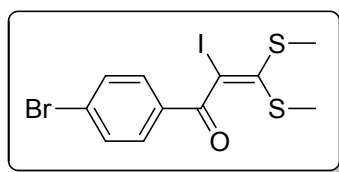
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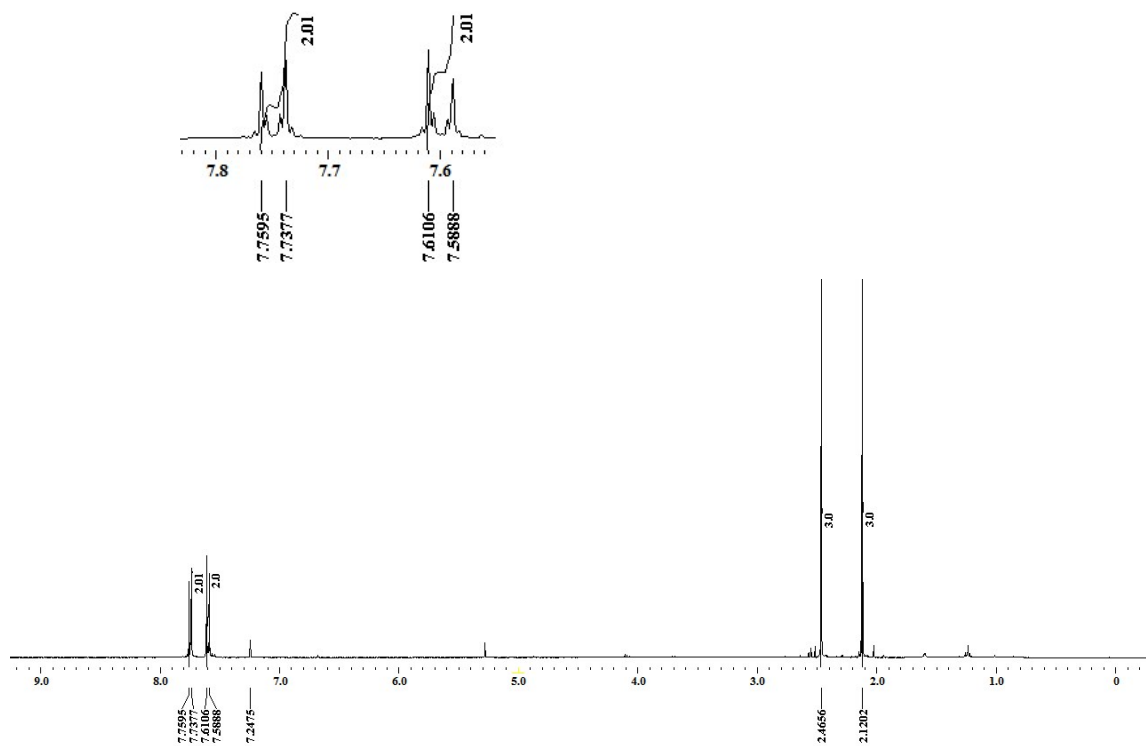
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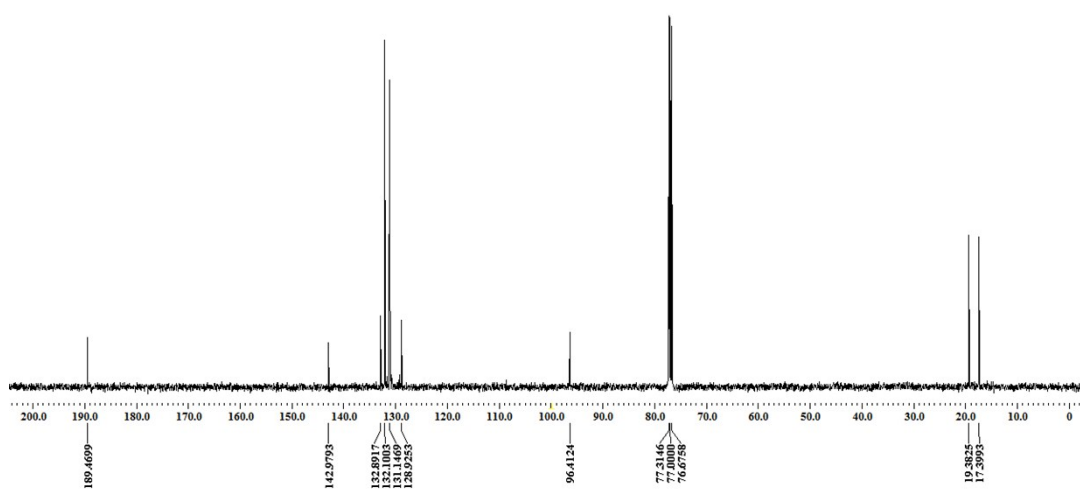


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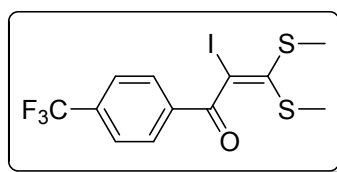
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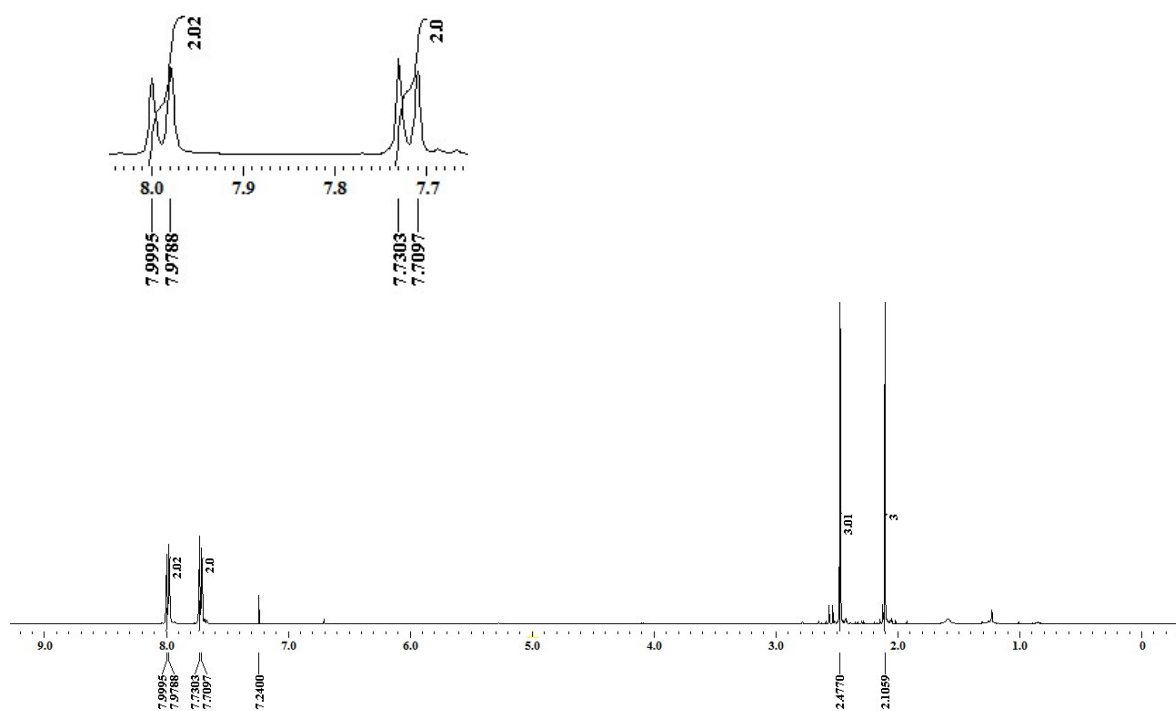




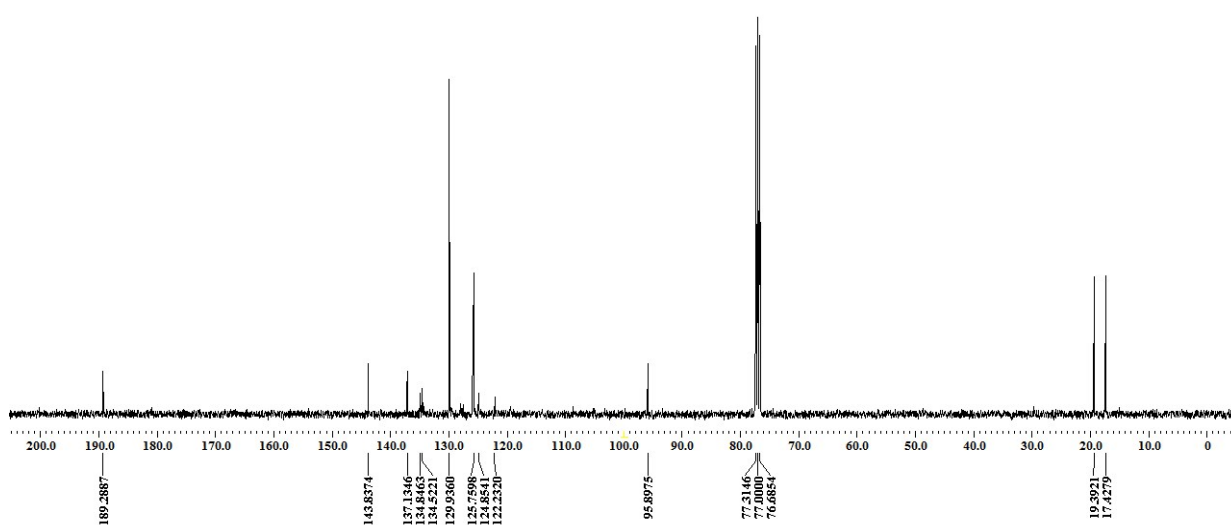


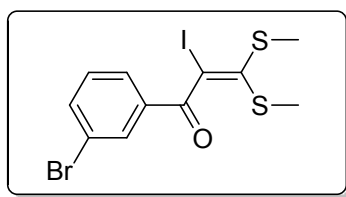
2e

$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



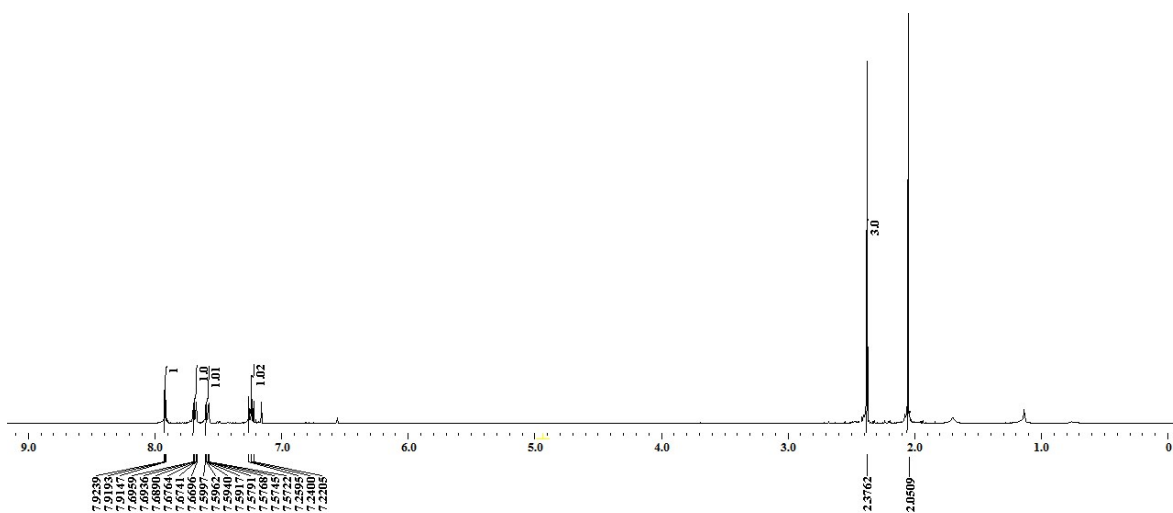
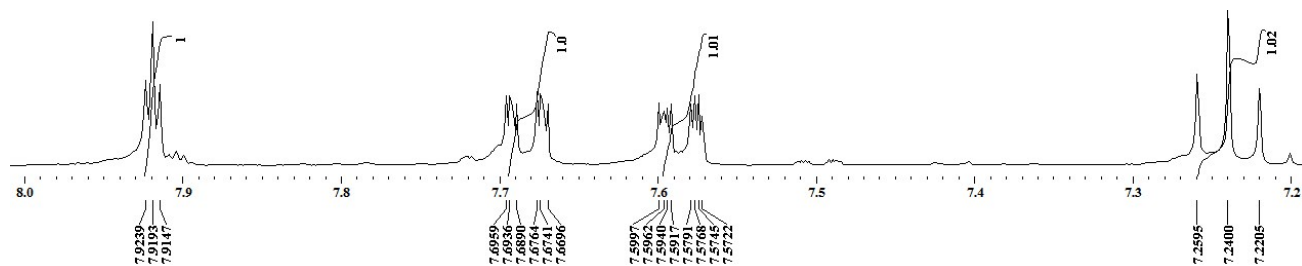
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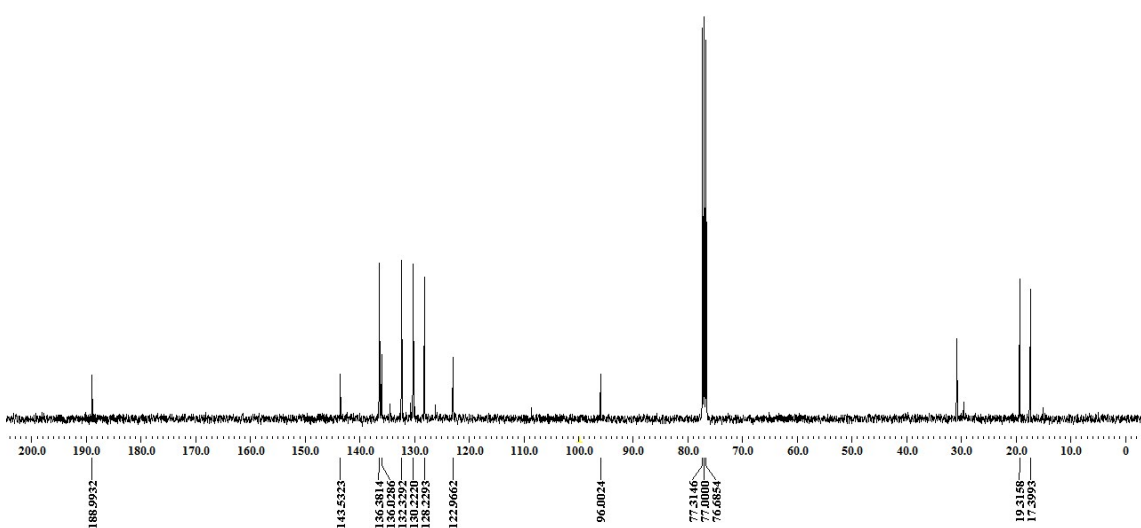


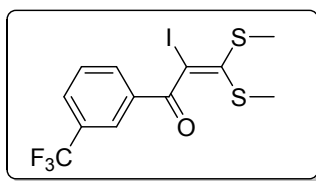
2f

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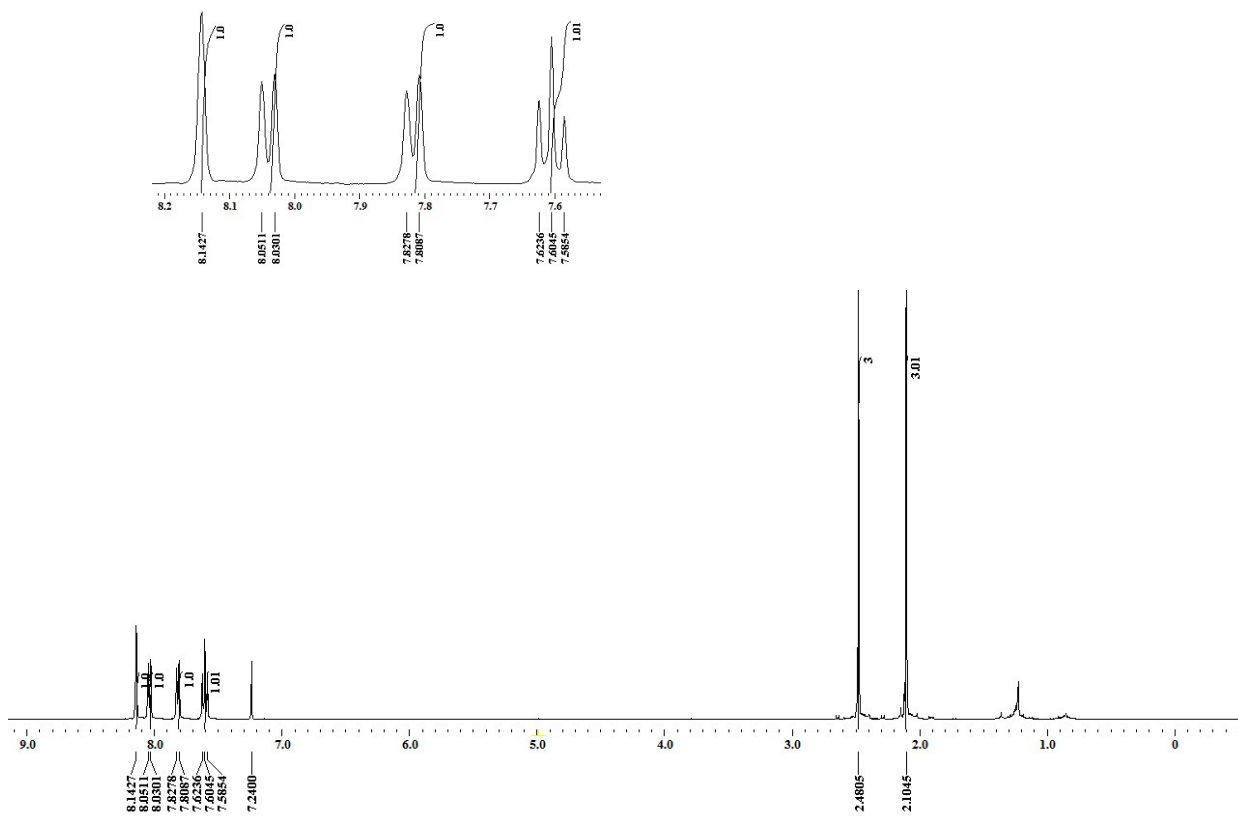
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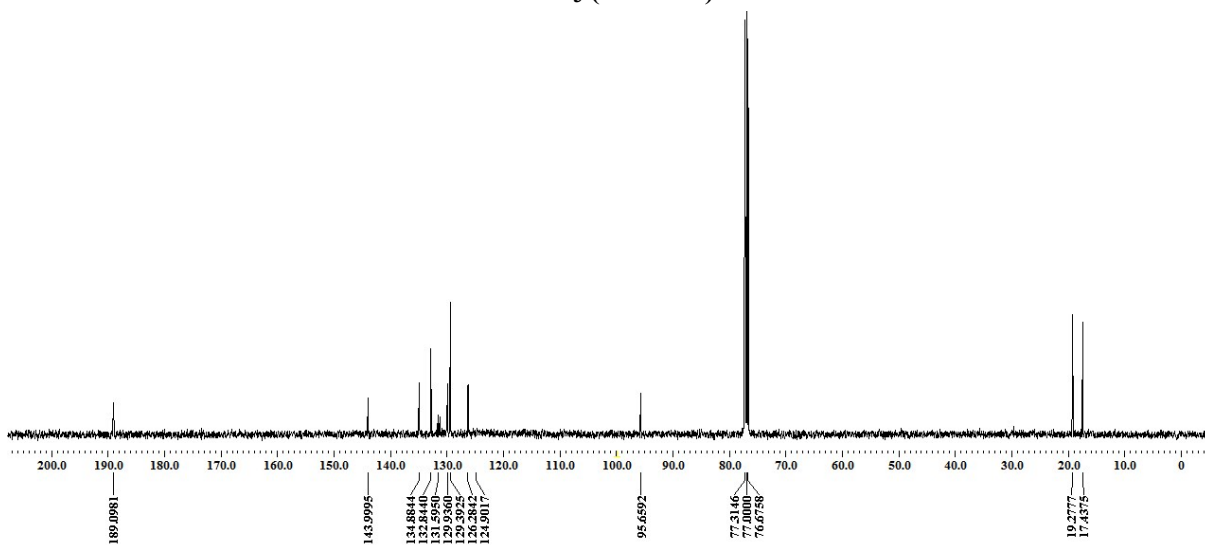


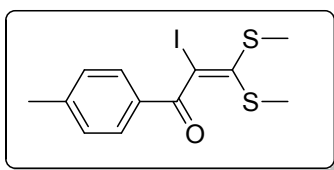
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<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



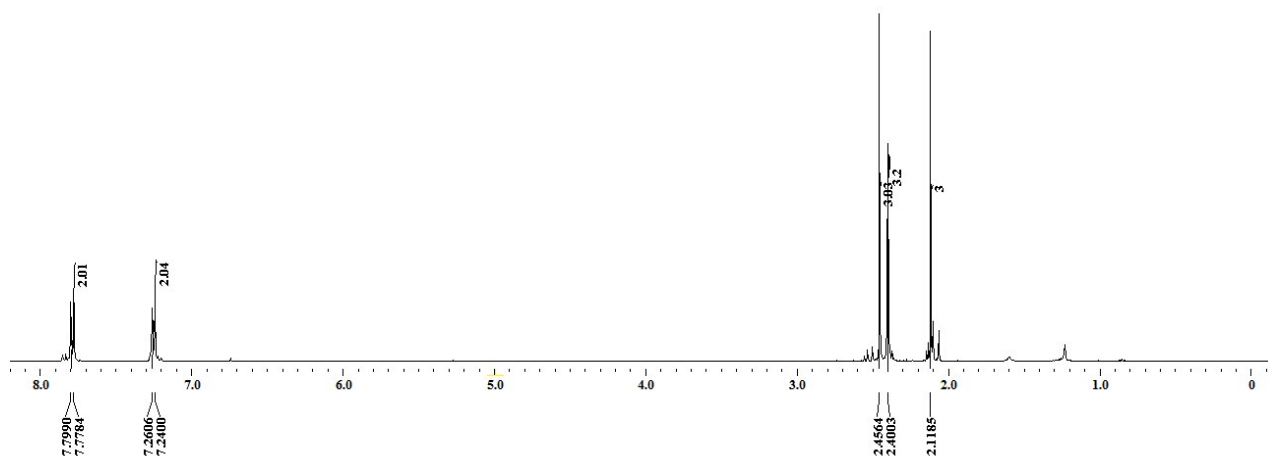
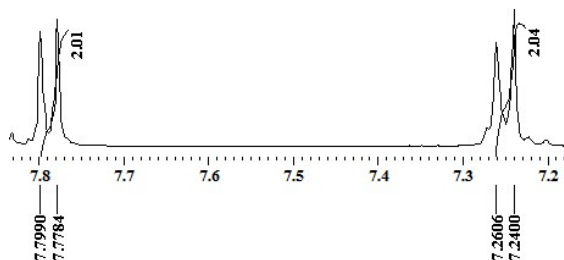
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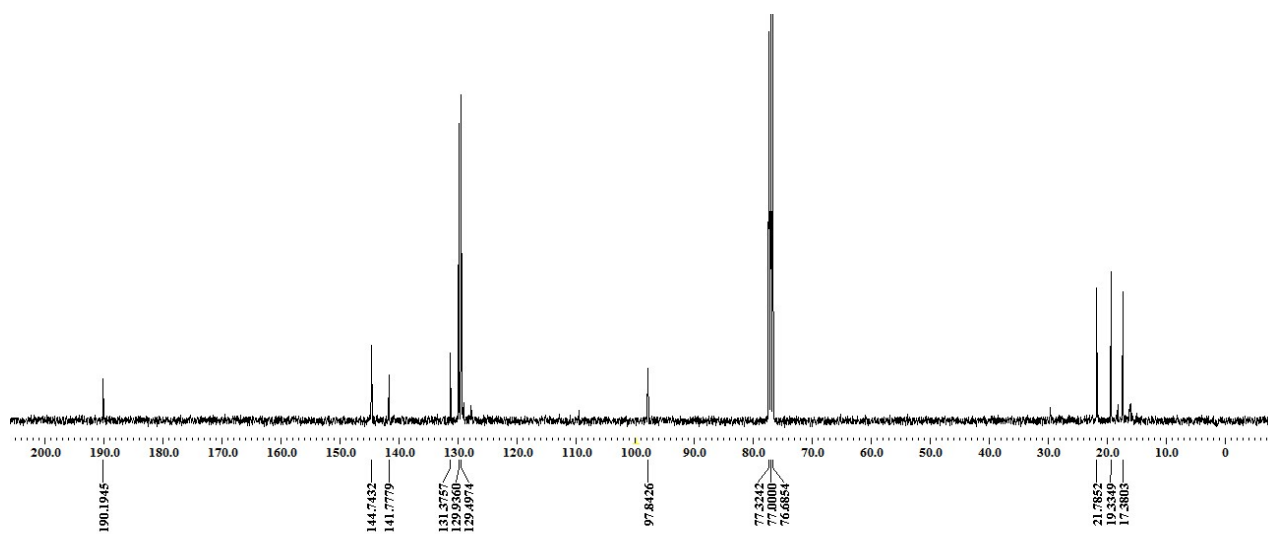


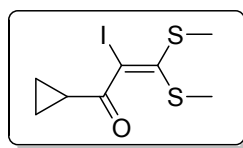
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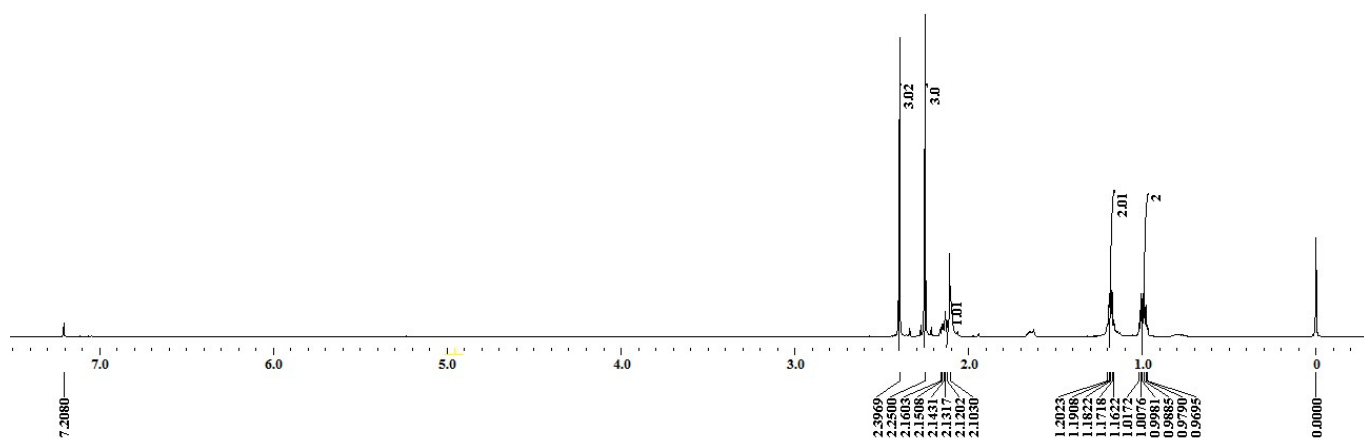
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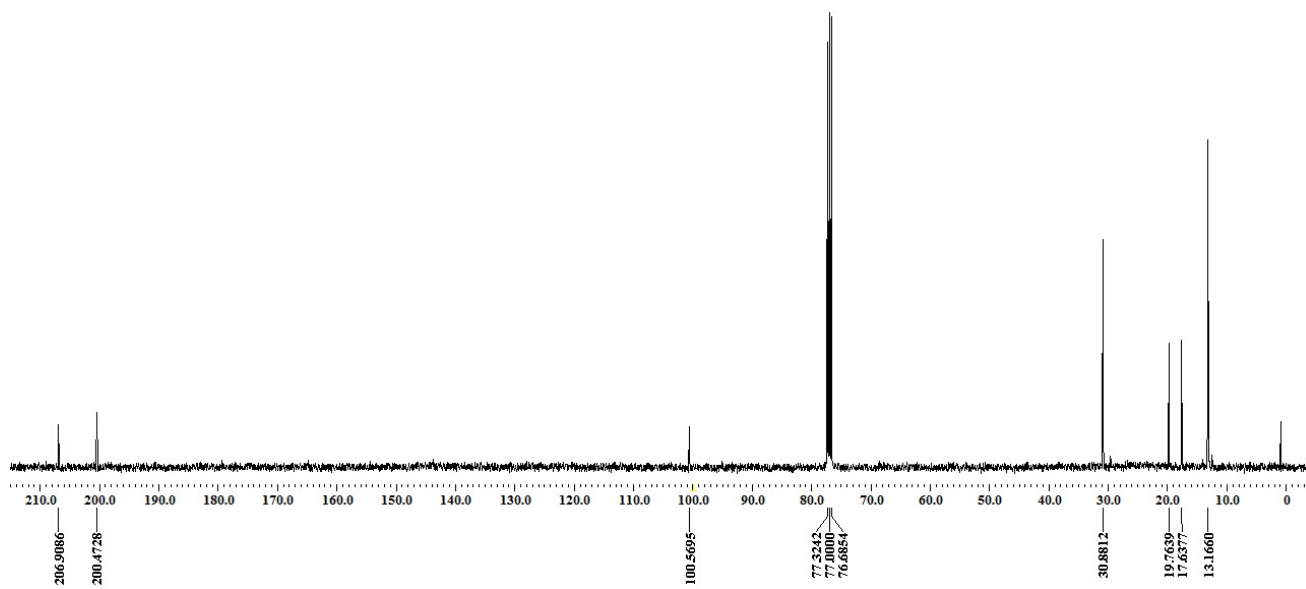


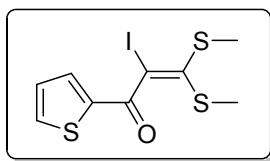
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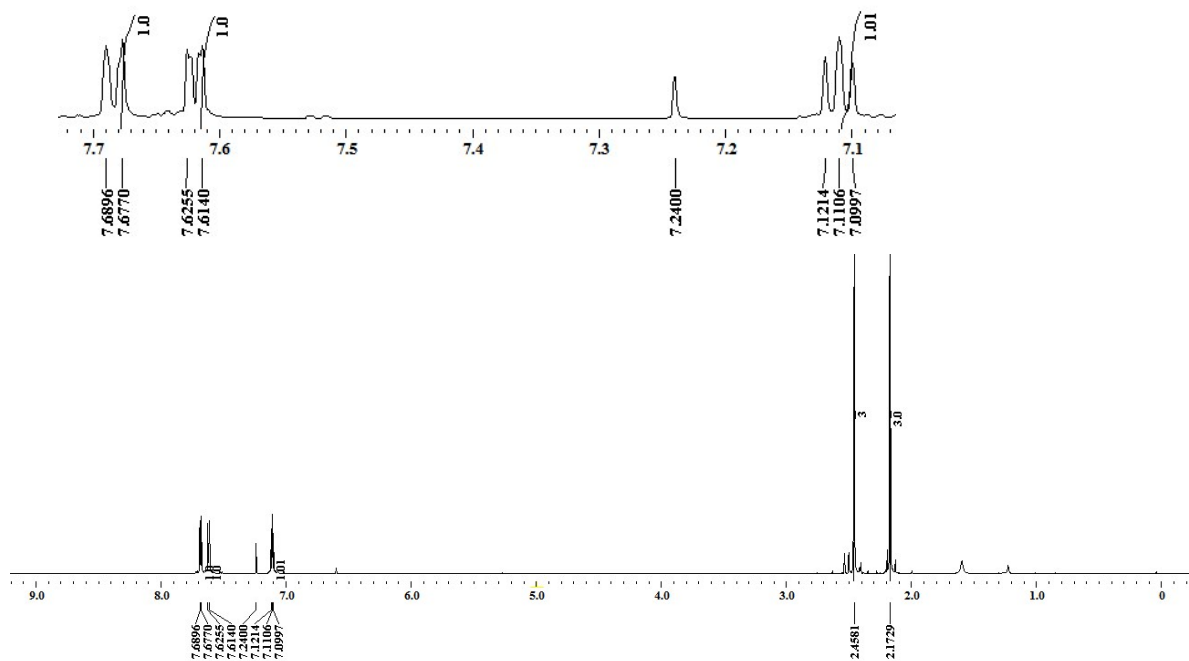
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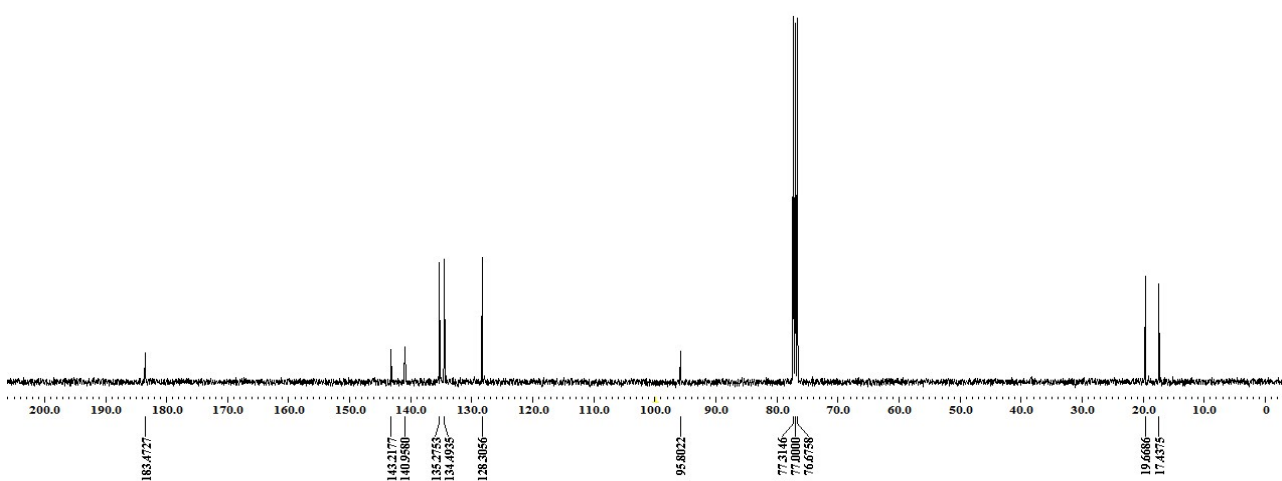


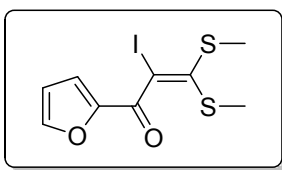
2j

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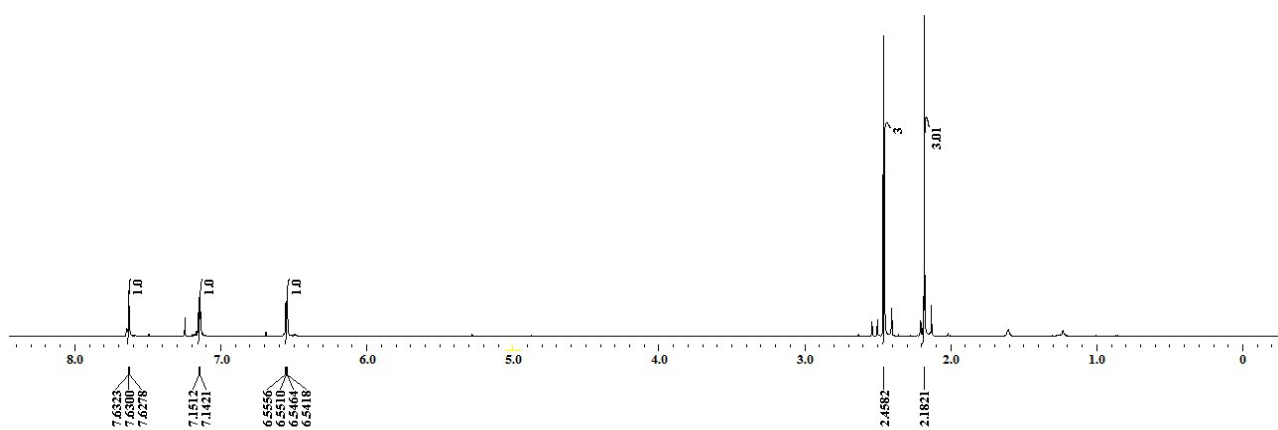
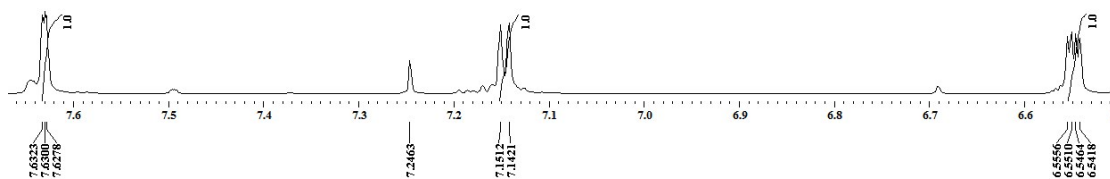
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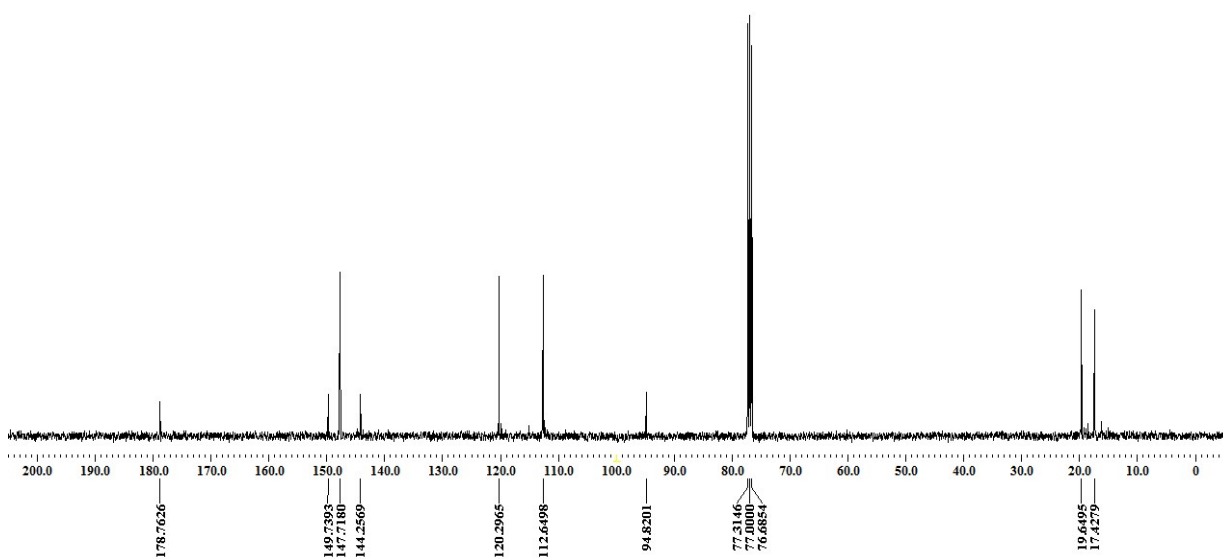


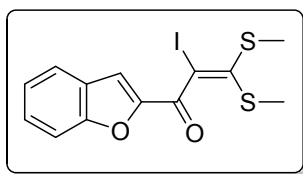
2k

$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



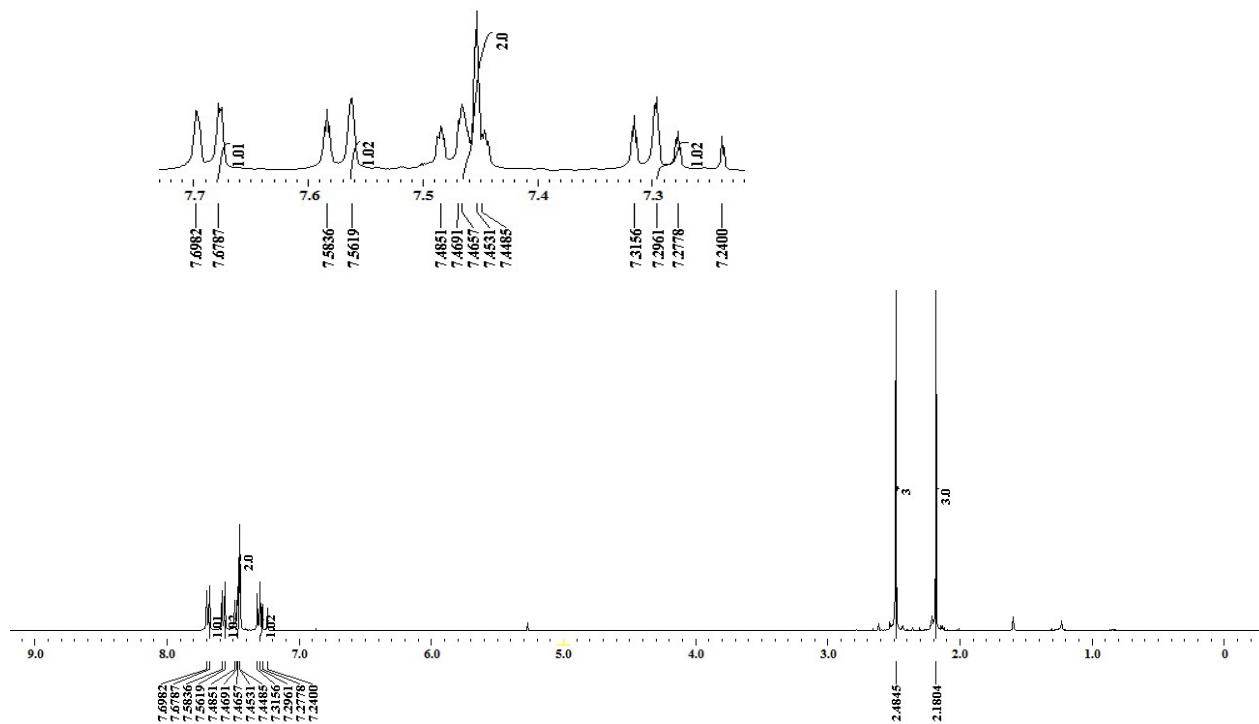
$^{13}\text{C-NMR}$  in  $\text{CDCl}_3$  (100MHz)



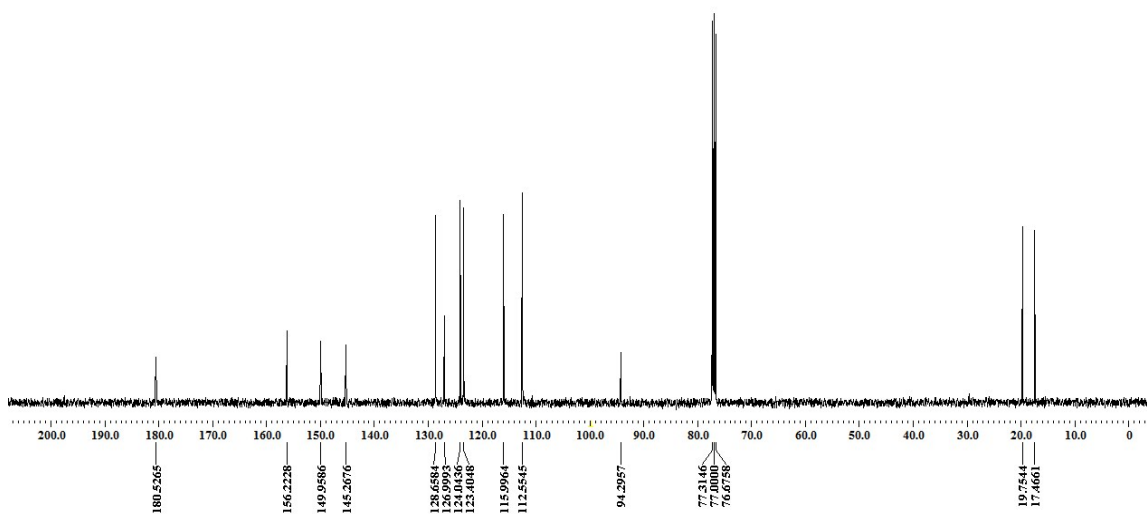


21

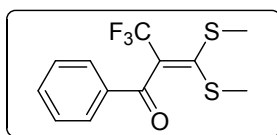
$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



$^{13}\text{C-NMR}$  in  $\text{CDCl}_3$  (100MHz)

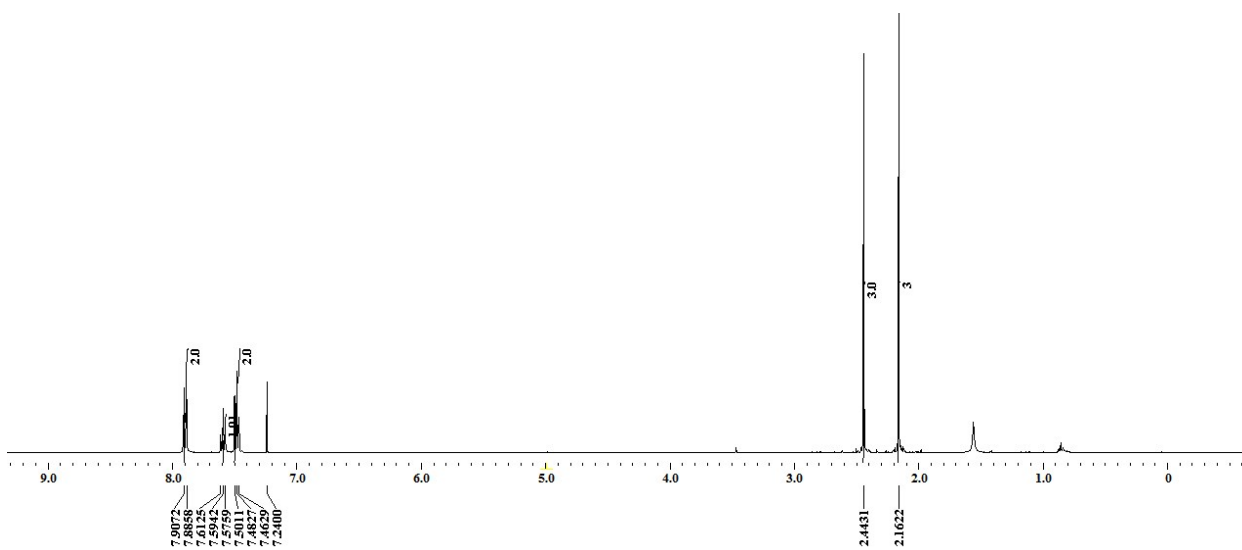
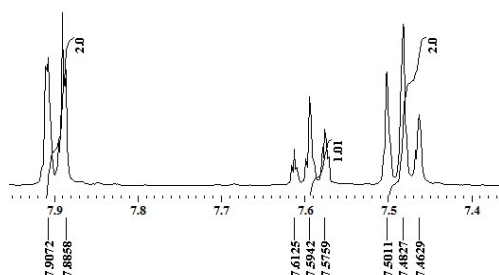




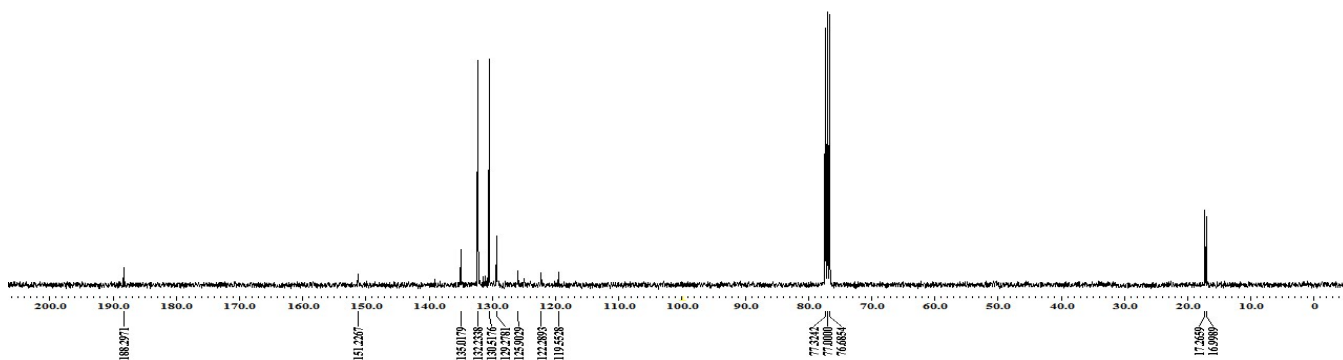


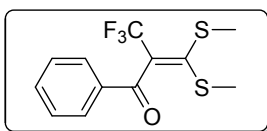
**3a**

**<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)**



**<sup>13</sup>C-NMR in CDCl<sub>3</sub> (400MHz)**





3a

Data File SBNS318.d Sample Name SBNS318  
 Sample Type Sample Position P2A3  
 Instrument Name Instrument 1 User Name lcmsdu-PC\admin  
 IRM Calibration Status Success DA Method Default.m  
 Comment

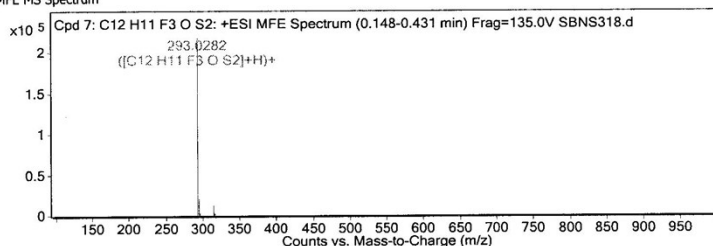
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

Compound Table

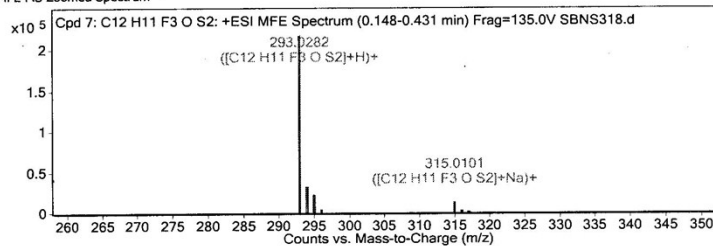
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C12 H11 F3 O S2	0.204	292.0209	C12 H11 F3 O S2	C12 H11 F3 O S2	-1.85	C12 H11 F3 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 7: C12 H11 F3 O S2	293.0282	0.204	Find by Molecular Feature	292.0209

MFE MS Spectrum



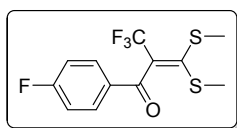
MFE MS Zoomed Spectrum



MS Spectrum Peak List

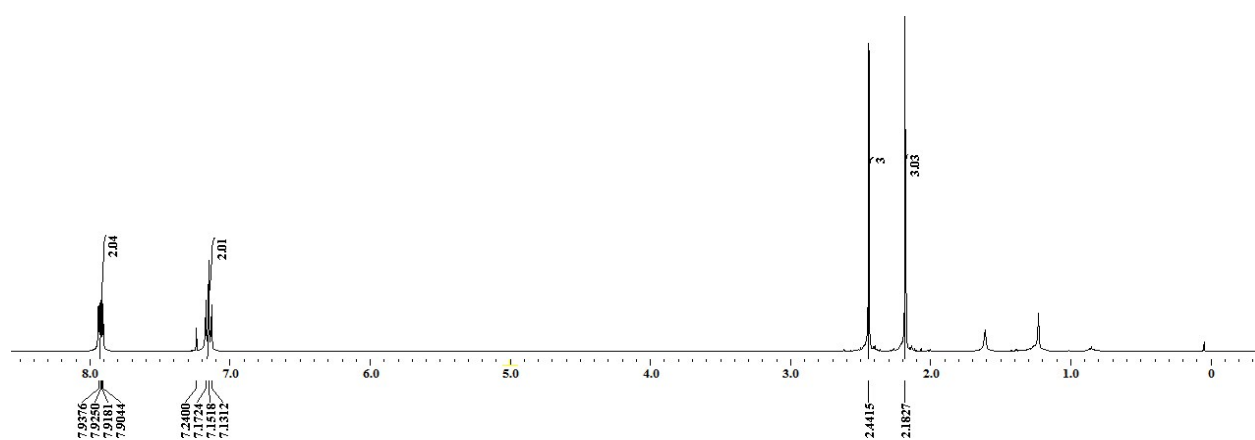
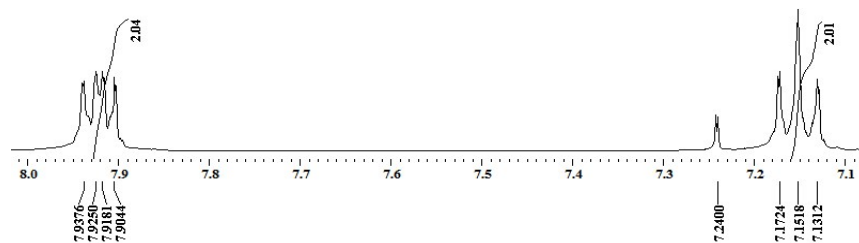
m/z	z	Abund	Formula	Ion
293.0282	1	218569.19	C12 H11 F3 O S2	(M+H)+
294.0312	1	31013.34	C12 H11 F3 O S2	(M+H)+
295.025	1	20199.12	C12 H11 F3 O S2	(M+H)+
296.0267	1	2891.79	C12 H11 F3 O S2	(M+H)+
315.0101	1	12451.48	C12 H11 F3 O S2	(M+Na)+
316.0135	1	1928.45	C12 H11 F3 O S2	(M+Na)+
317.0083	1	1555.29	C12 H11 F3 O S2	(M+Na)+
318.009	1	155.1	C12 H11 F3 O S2	(M+Na)+

--- End Of Report ---

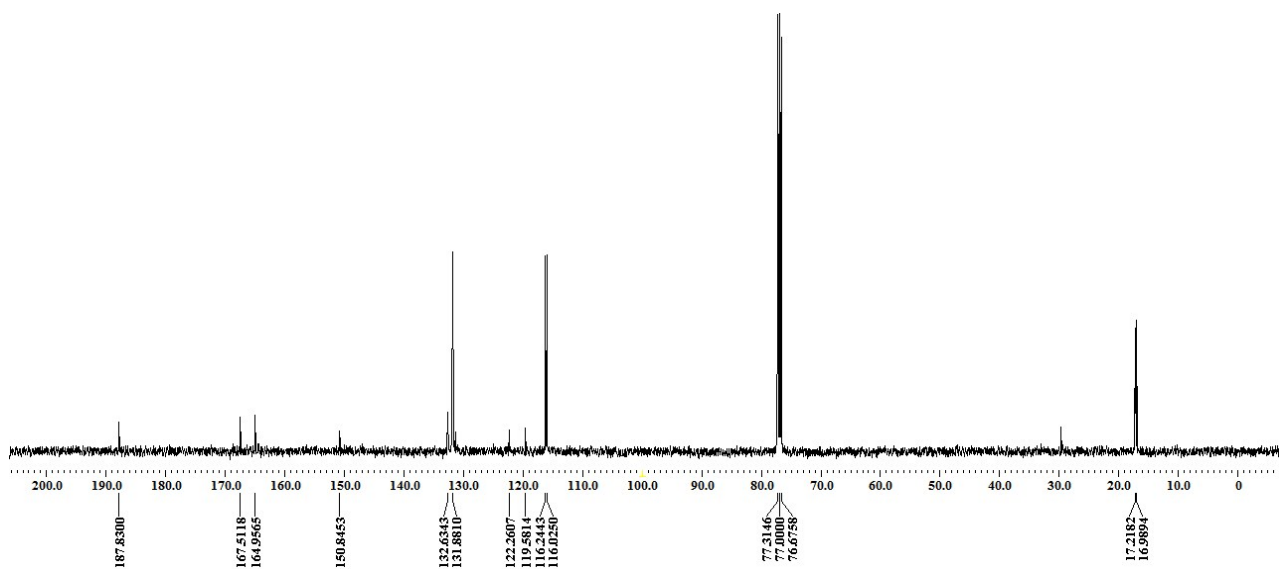


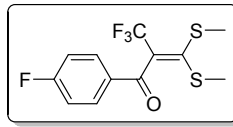
**3b**

$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



$^{13}\text{C-NMR}$  in  $\text{CDCl}_3$  (100MHz)





### 3b

**Data File** SB-NS-348.d      **Sample Name** SB-NS-348  
**Sample Type** Sample      **Position** P2E8  
**Instrument Name** Instrument 1      **User Name** lcmsdu-PC\admin

**IRM Calibration Status** Success      **DA Method** Default.m  
**Comment**

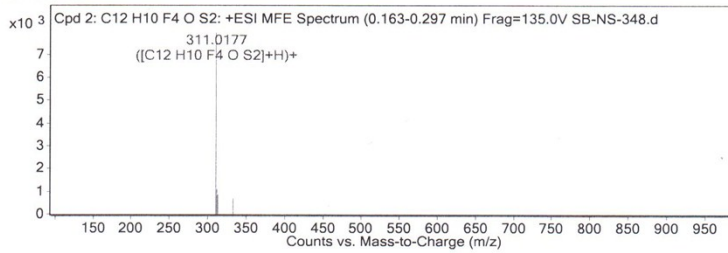
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

#### Compound Table

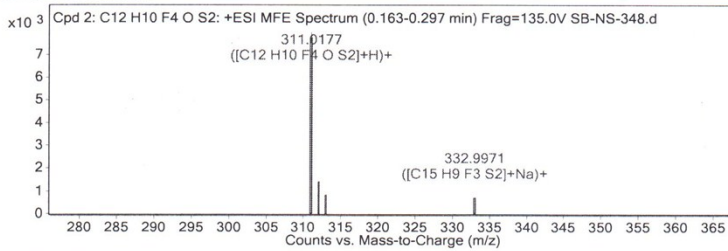
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C12 H10 F4 O S2	0.202	310.0105	C12 H10 F4 O S2	C12 H10 F4 O S2	1.25	C12 H10 F4 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C12 H10 F4 O S2	311.0177	0.202	Find by Molecular Feature	310.0105

#### MFE MS Spectrum



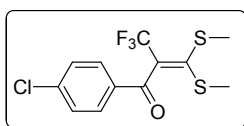
#### MFE MS Zoomed Spectrum



#### MS Spectrum Peak List

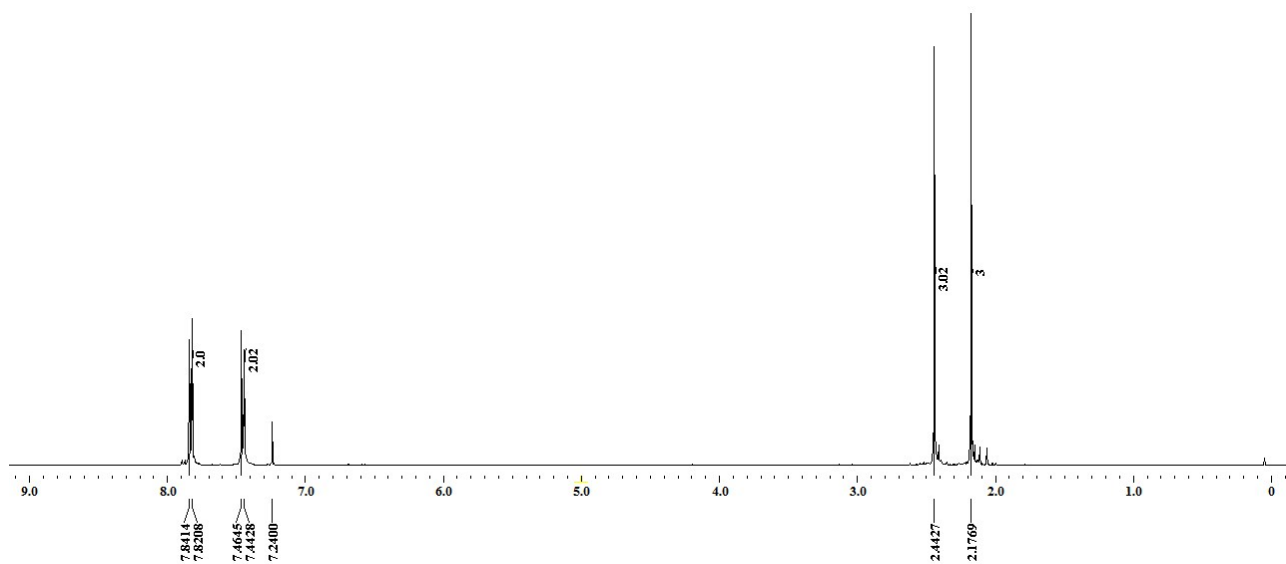
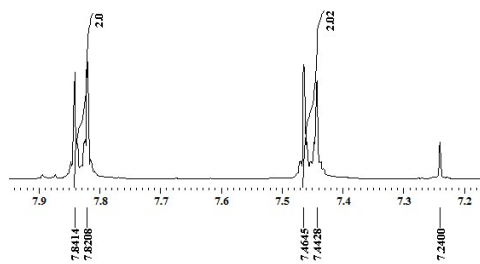
m/z	z	Abund	Formula	Ion
311.0177	1	7975.05	C12 H10 F4 O S2	(M+H)+
312.0213	1	1119.29	C12 H10 F4 O S2	(M+H)+
313.0155	1	843.83	C12 H10 F4 O S2	(M+H)+
332.9971	1	700.81	C15 H9 F3 S2	(M+Na)+

--- End Of Report ---

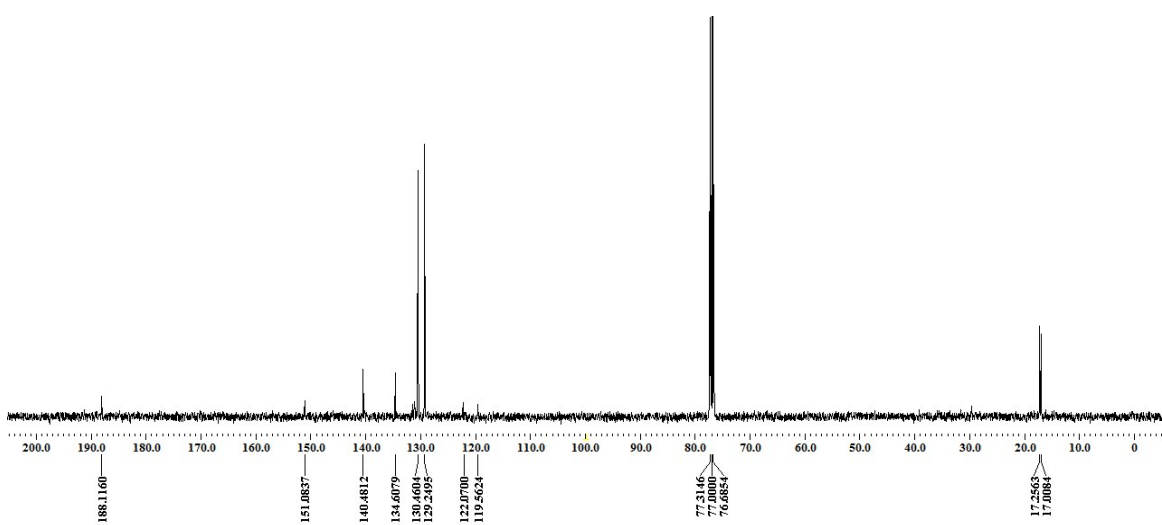


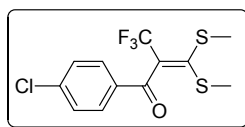
3c

$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



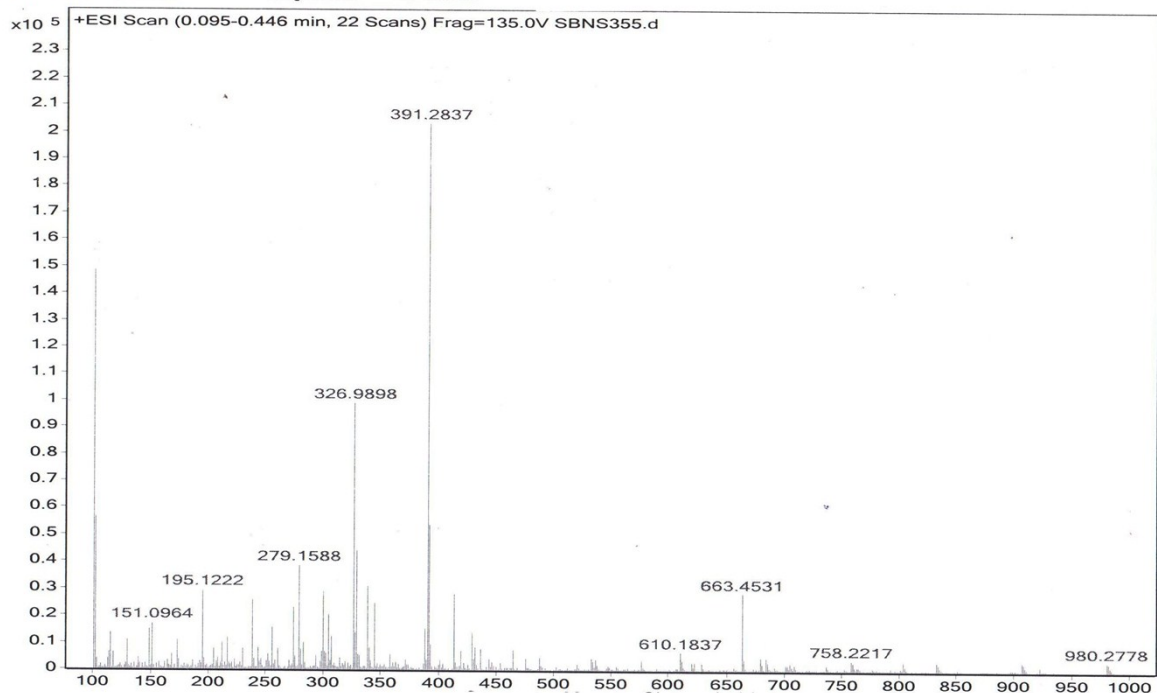
$^{13}\text{C-NMR}$  in  $\text{CDCl}_3$  (100MHz)

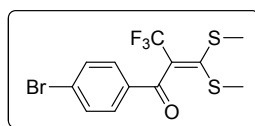




3c

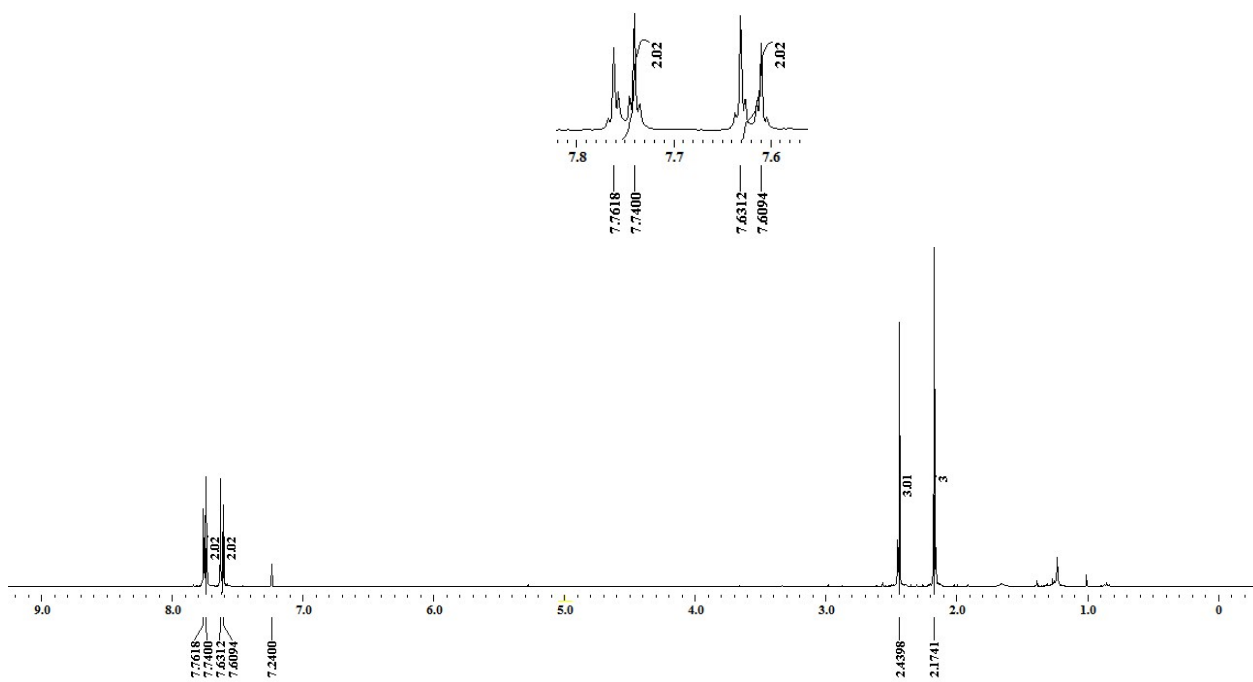
Sample Name	SBNS355	Position	P2F8	Instrument Name	6530 QTOF LCMS	User Name	lcmsdu-PC\admin
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SBNS355.d						



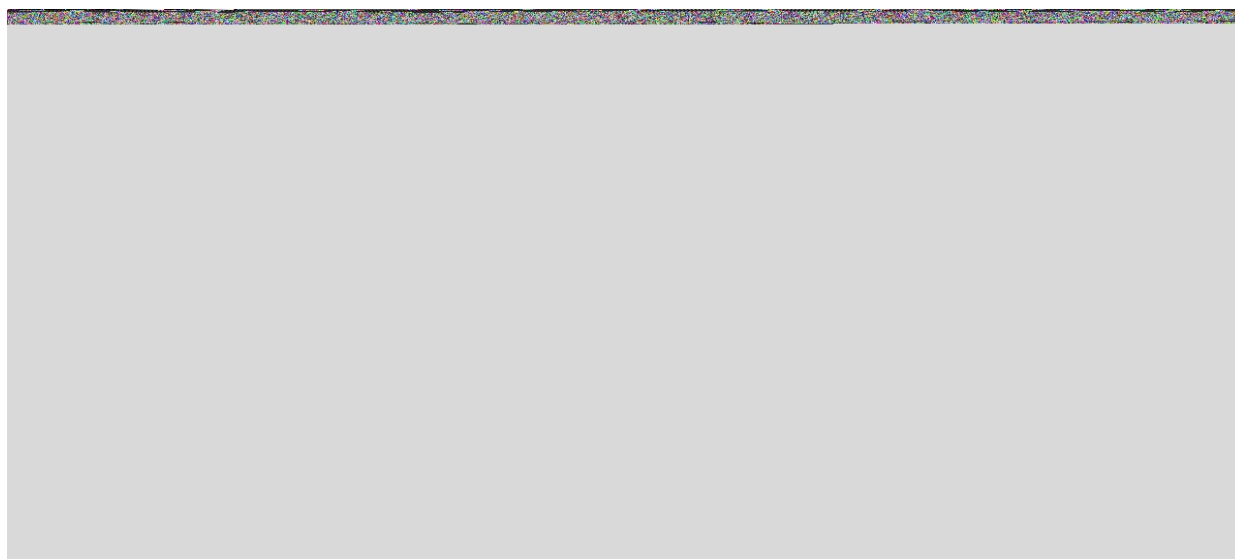


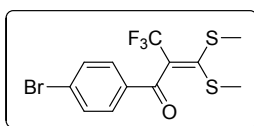
3d

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





### 3d

<b>Data File</b>	SB-NS-392.d	<b>Sample Name</b>	SB-NS-392
<b>Sample Type</b>	Sample	<b>Position</b>	P1-B4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	29.10.2014.m	<b>Acquired Time</b>	09-06-2016 14:23:54
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

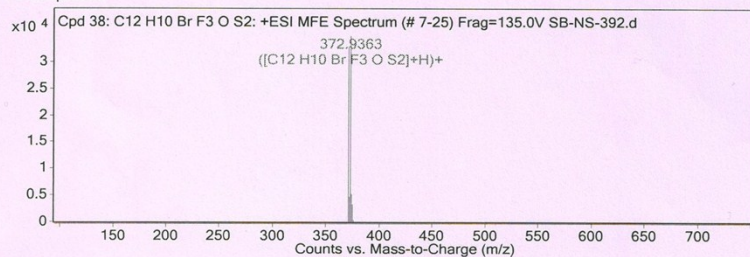
<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125)	

#### Compound Table

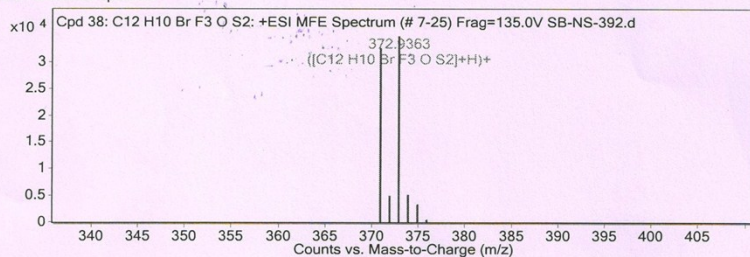
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 38: C12 H10 Br F3 O S2	12	369.9311	C12 H10 Br F3 O S2	C12 H10 Br F3 O S2	-0.73	C12 H10 Br F3 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 38: C12 H10 Br F3 O S2	370.9381	12	Find by Molecular Feature	369.9311

#### MFE MS Spectrum



#### MFE MS Zoomed Spectrum

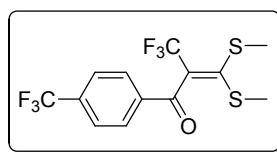


#### MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
370.9381	1	32896.02	C12 H10 Br F3 O S2	(M+H)+
371.9421	1	4643.4	C12 H10 Br F3 O S2	(M+H)+
372.9363	1	34831.87	C12 H10 Br F3 O S2	(M+H)+
373.9398	1	5186.56	C12 H10 Br F3 O S2	(M+H)+
374.9332	1	3230.62	C12 H10 Br F3 O S2	(M+H)+
375.9368	1	295.27	C12 H10 Br F3 O S2	(M+H)+

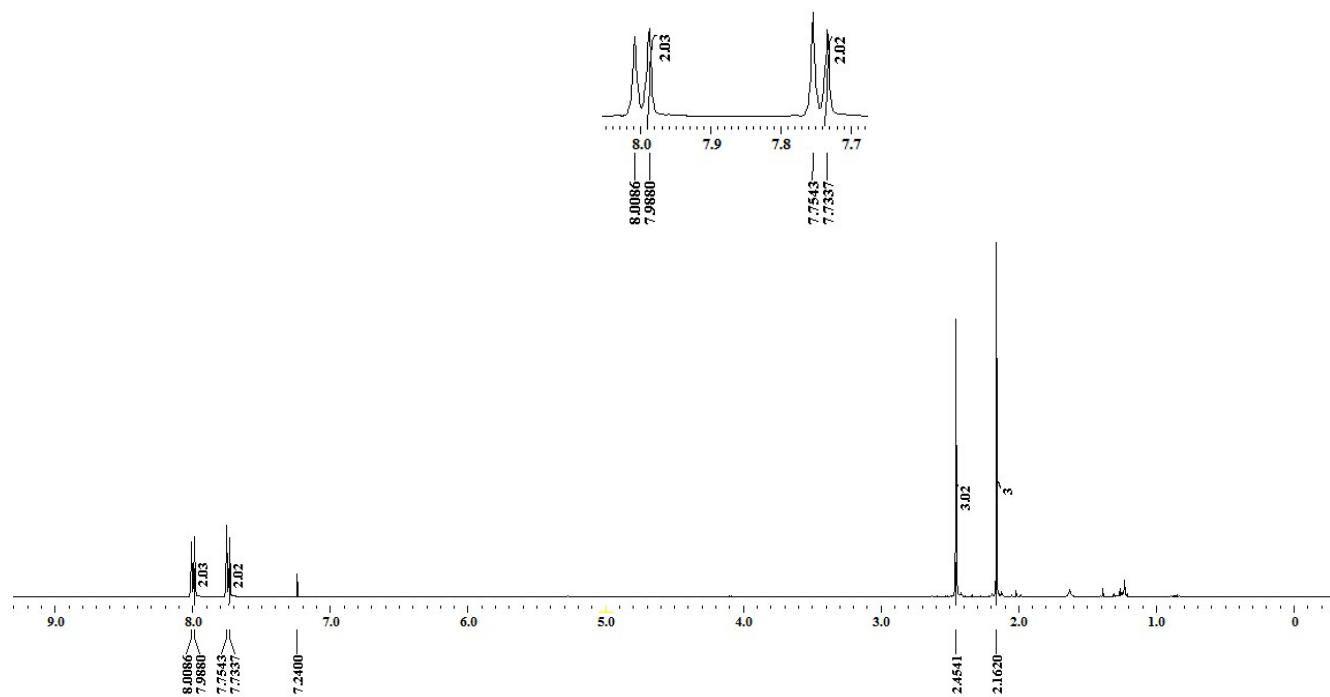
--- End Of Report ---



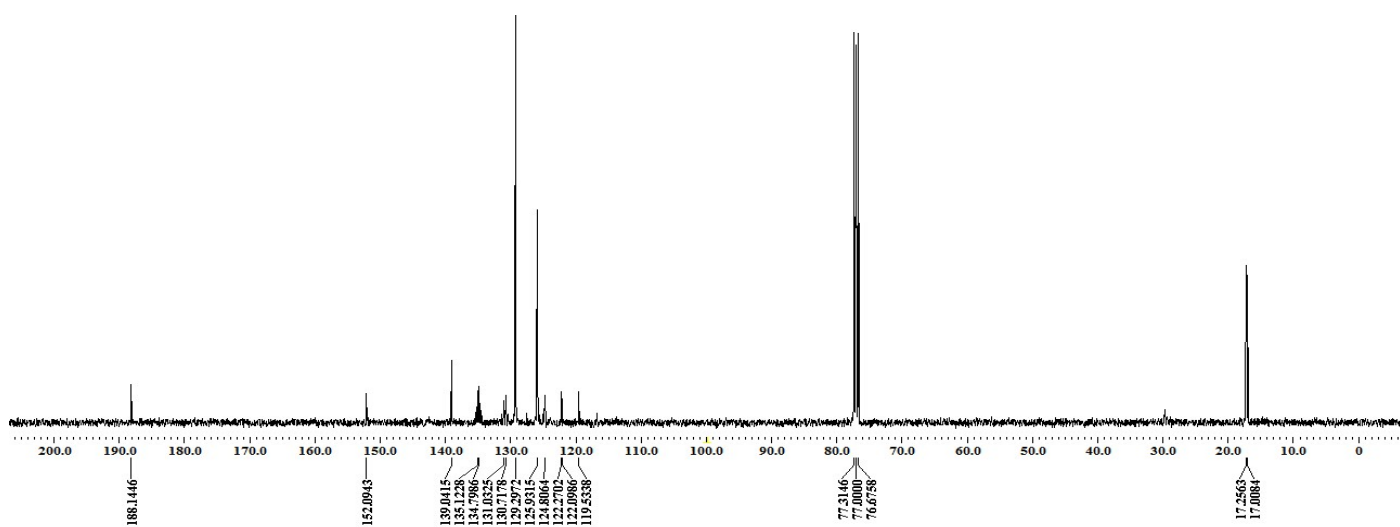


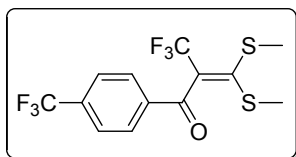
3e

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





3e

Data File SB-NS-380.d Sample Name SB-NS-380  
 Sample Type Sample Position P1F3  
 Instrument Name Instrument 1 User Name lcmsdu-PC\admin  
 Acq Method 29.10.2014.m  
 IRM Calibration Status Success DA Method Default.m  
 Comment

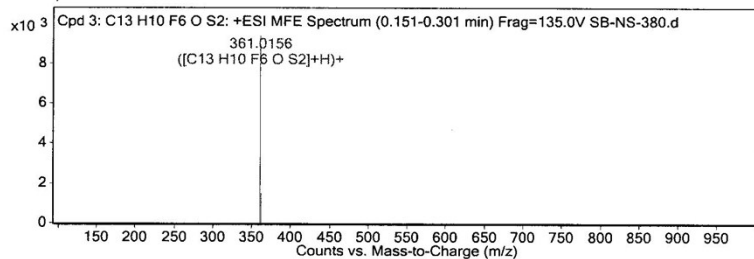
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

Compound Table

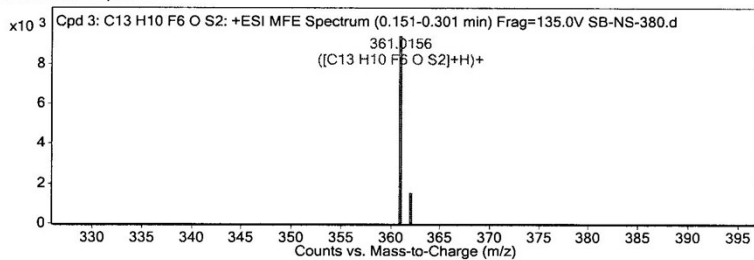
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C13 H10 F6 O S2	0.199	360.0083	C13 H10 F6 O S2	C13 H10 F6 O S2	-1.6	C13 H10 F6 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C13 H10 F6 O S2	361.0156	0.199	Find by Molecular Feature	360.0083

MFE MS Spectrum



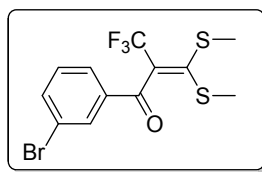
MFE MS Zoomed Spectrum



MS Spectrum Peak List

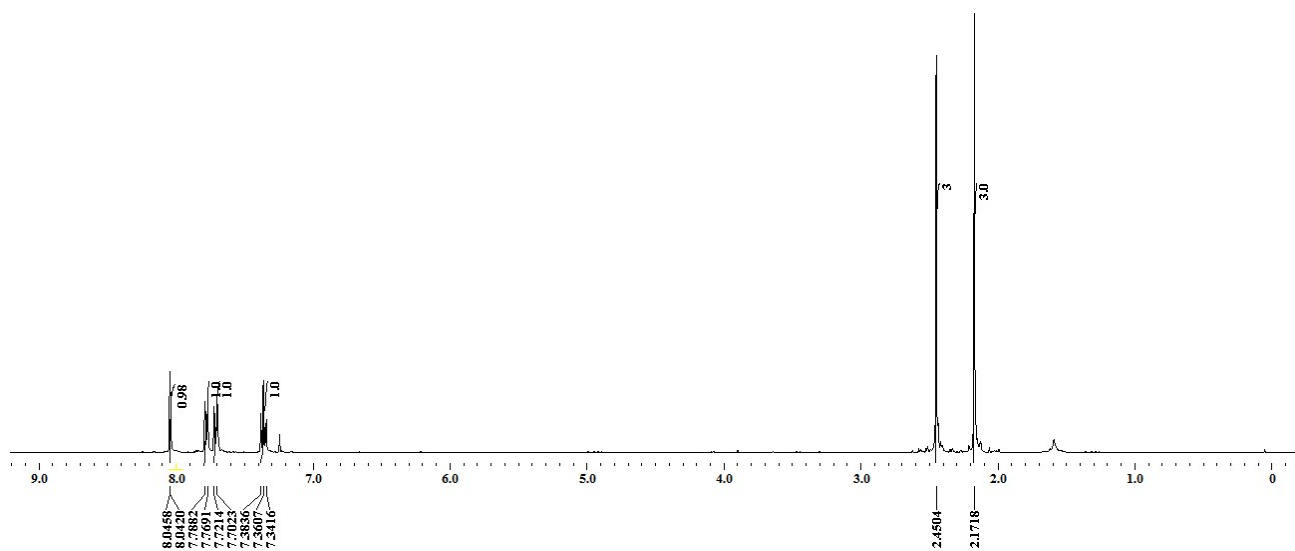
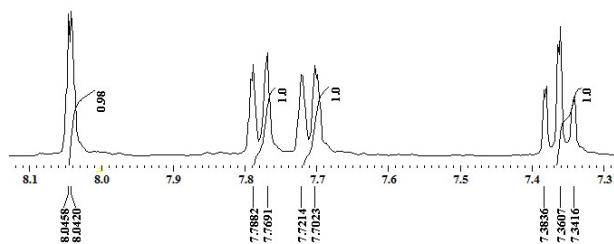
m/z	z	Abund	Formula	Ion
361.0156	1	9403.09	C13 H10 F6 O S2	(M+H)+
362.0182	1	1485.17	C13 H10 F6 O S2	(M+H)+

--- End Of Report ---

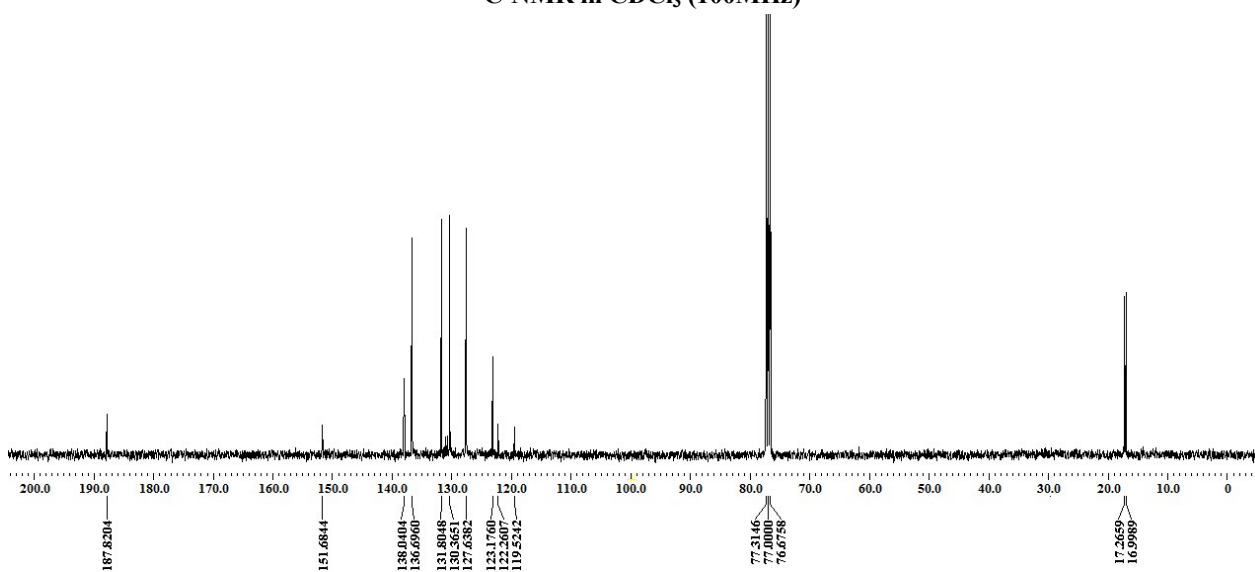


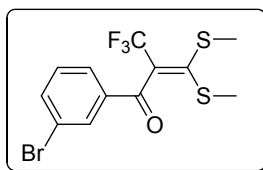
3f

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





3f

**Data File** EXP-408.d **Sample Name** EXP-408  
**Sample Type** Sample **Position** P2E1  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**

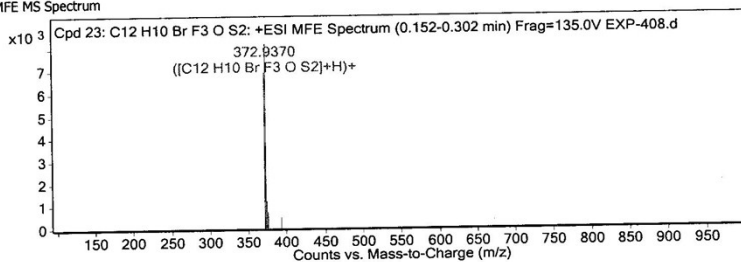
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

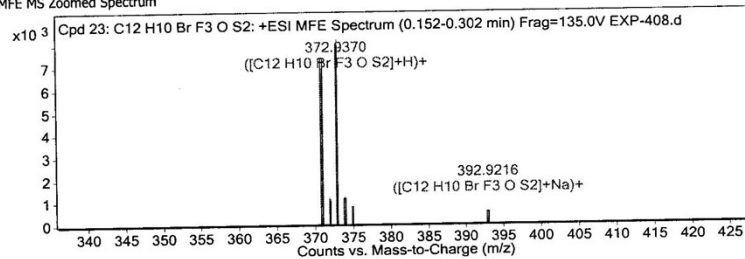
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C12 H10 Br F3 O S2	0.196	369.9318	C12 H10 Br F3 O S2	C12 H10 Br F3 O S2	-2.5	C12 H10 Br F3 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 23: C12 H10 Br F3 O S2	370.9389	0.196	Find by Molecular Feature	369.9318

**MFE MS Spectrum**



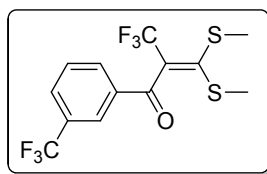
**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

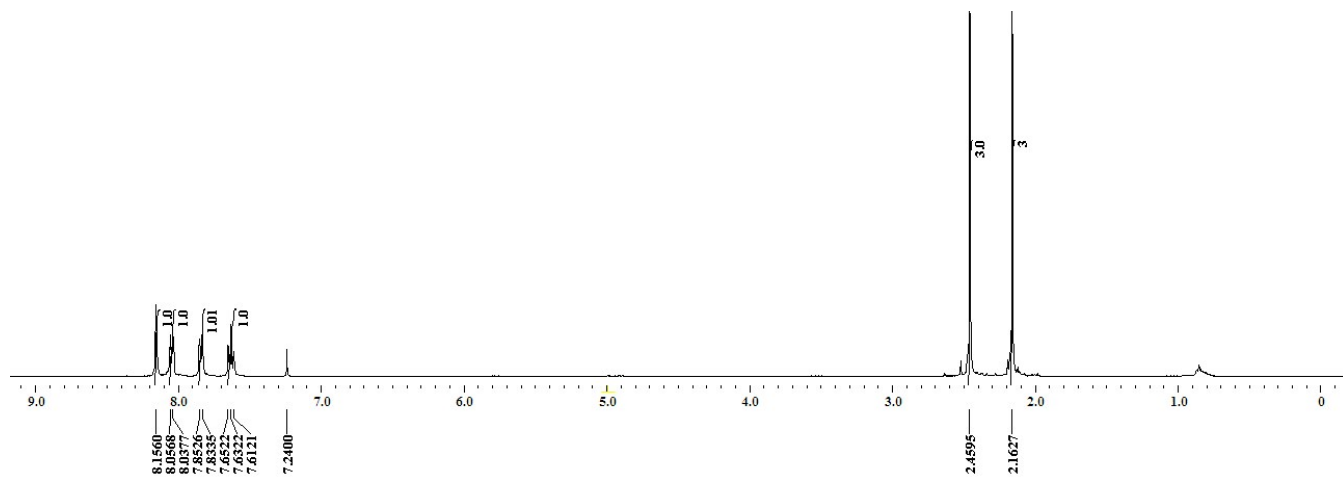
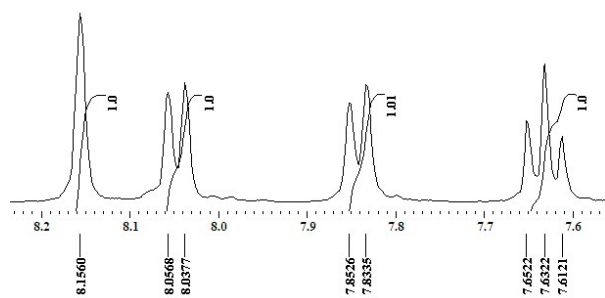
m/z	z	Abund	Formula	Ion
370.9389	1	6933.57	C12 H10 Br F3 O S2	(M+H)+
371.9424	1	1170.93	C12 H10 Br F3 O S2	(M+H)+
372.937	1	8203.74	C12 H10 Br F3 O S2	(M+H)+
373.9384	1	1207.36	C12 H10 Br F3 O S2	(M+H)+
374.936	1	739.39	C12 H10 Br F3 O S2	(M+H)+
392.9216	1	508.03	C12 H10 Br F3 O S2	(M+Na)+

--- End Of Report ---

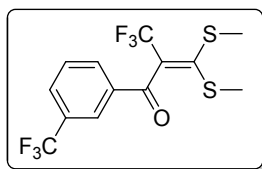
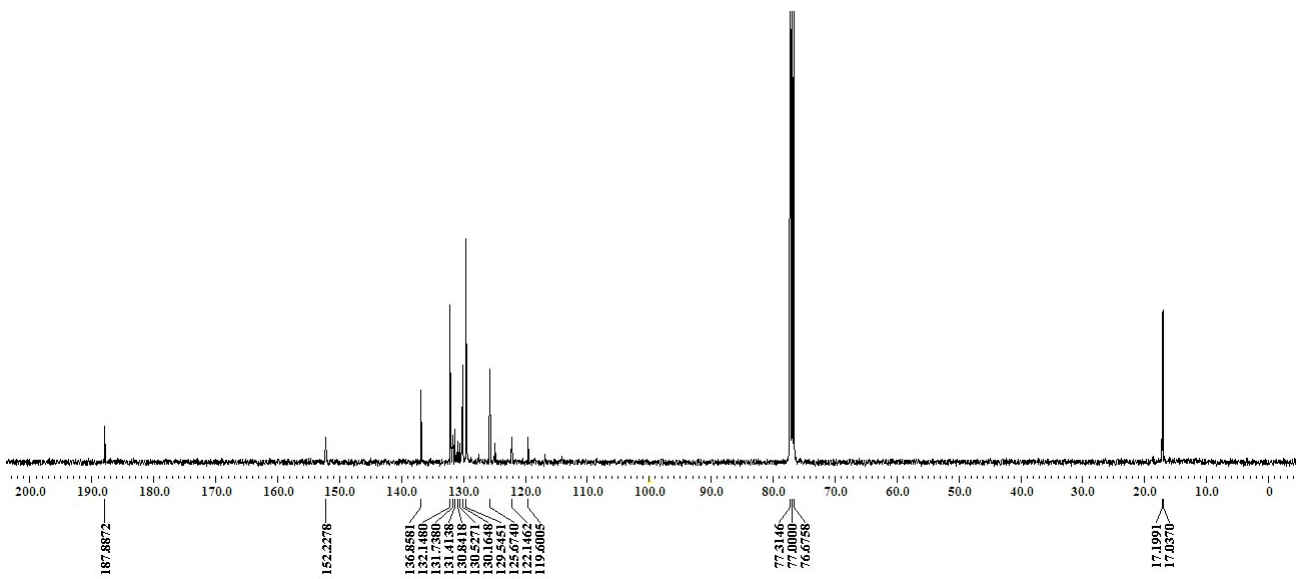


**3g**

**<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)**



**<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)**



**3g**

**Data File** SB-NS-383.d      **Sample Name** SB-NS-380  
**Sample Type** Sample      **Position** P1F3  
**Instrument Name** Instrument 1      **User Name** lcmsdu-PC\admin  
**Acq Method** 29.10.2014.m  
**IRM Calibration Status** Success      **DA Method** Default.m  
**Comment**

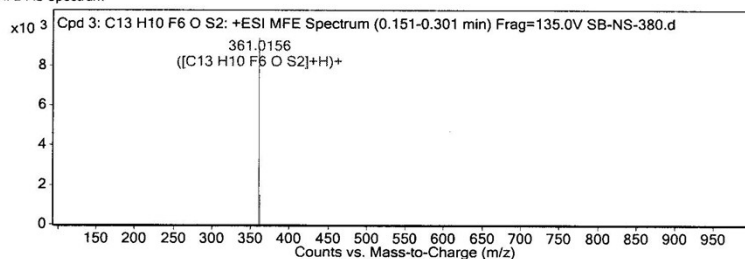
**Sample Group**      **Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

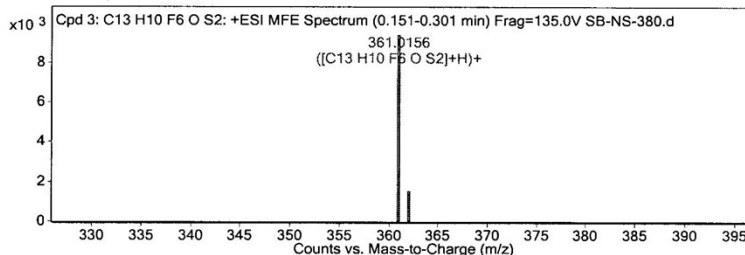
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C13 H10 F6 O S2	0.199	360.0083	C13 H10 F6 O S2	C13 H10 F6 O S2	-1.6	C13 H10 F6 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C13 H10 F6 O S2	361.0156	0.199	Find by Molecular Feature	360.0083

**MFE MS Spectrum**



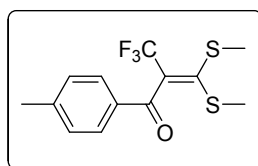
**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

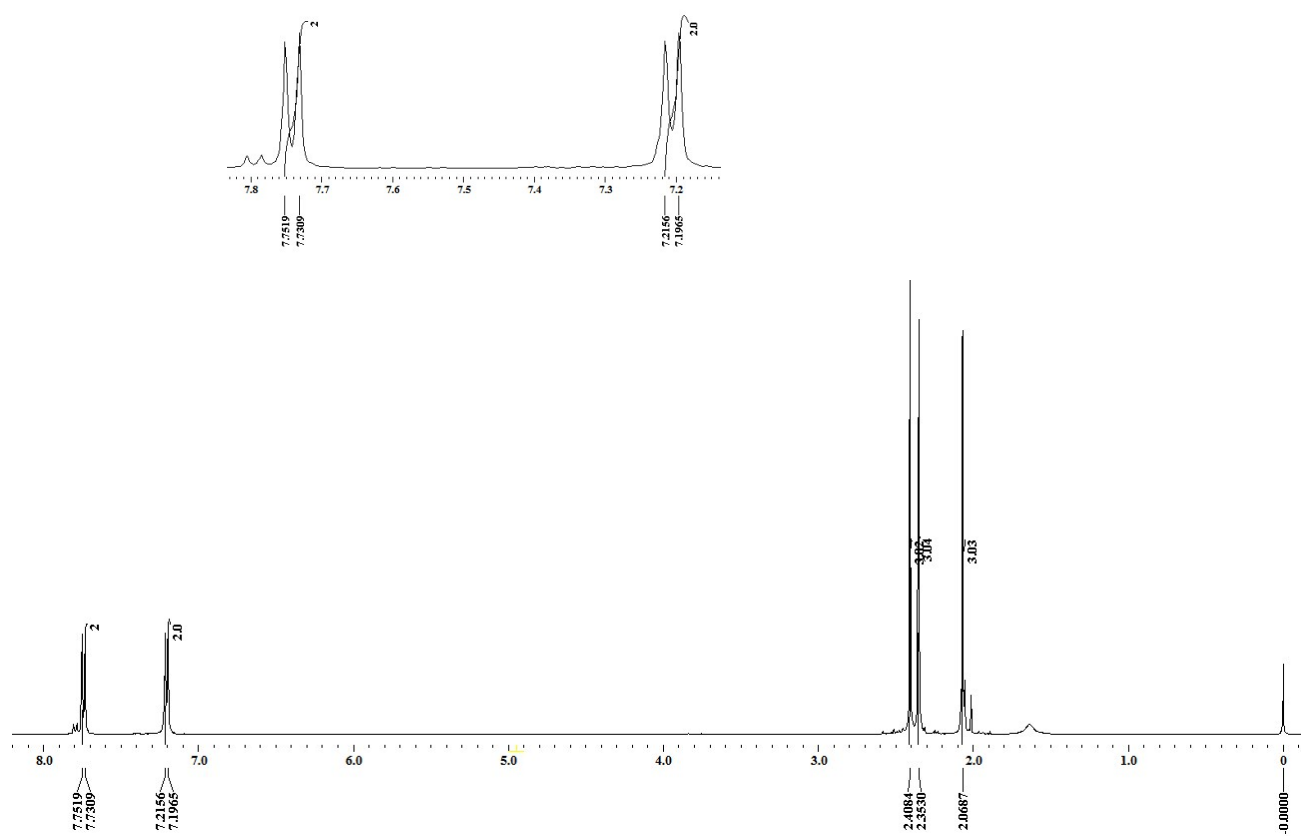
m/z	z	Abund	Formula	Ion
361.0156	1	9403.09	C13 H10 F6 O S2	(M+H)+
362.0182	1	1485.17	C13 H10 F6 O S2	(M+H)+

--- End Of Report ---

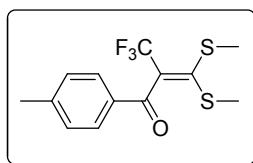
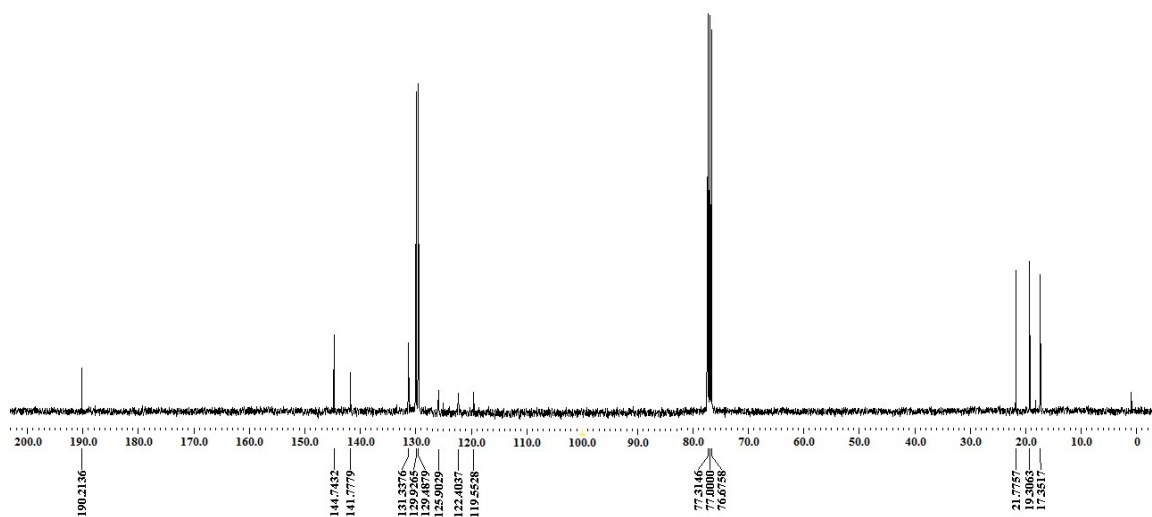


**3h**

**<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)**



$^{13}\text{C}$ -NMR in  $\text{CDCl}_3$  (100MHz)



**3h**



Data File EXP346.d Sample Name EXP346  
 Sample Type Sample Position P1F6  
 Instrument Name Instrument 1 User Name lcmsdu-PC\admin

IRM Calibration Status Success DA Method Default.m  
 Comment

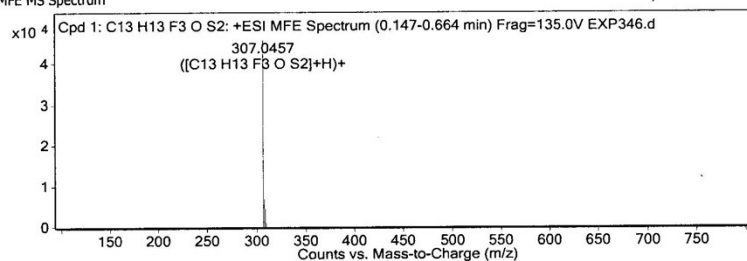
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

**Compound Table**

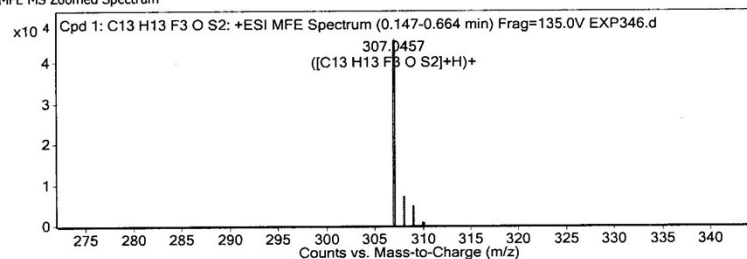
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C13 H13 F3 O S2	0.215	306.0384	C13 H13 F3 O S2	C13 H13 F3 O S2	-7.94	C13 H13 F3 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C13 H13 F3 O S2	307.0457	0.215	Find by Molecular Feature	306.0384

MFE MS Spectrum



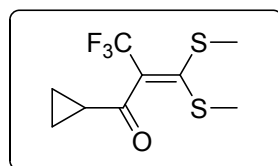
MFE MS Zoomed Spectrum



MS Spectrum Peak List

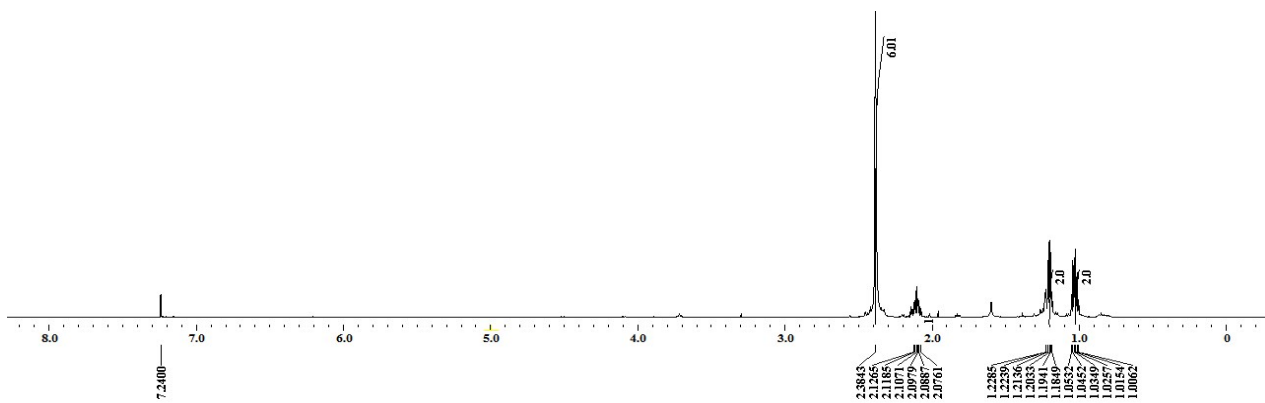
m/z	z	Abund	Formula	Ion
307.0457	1	45739.2	C13 H13 F3 O S2	(M+H)+
308.0496	1	6862.78	C13 H13 F3 O S2	(M+H)+
309.0411	1	4587.63	C13 H13 F3 O S2	(M+H)+
310.046	1	596.13	C13 H13 F3 O S2	(M+H)+

--- End Of Report ---

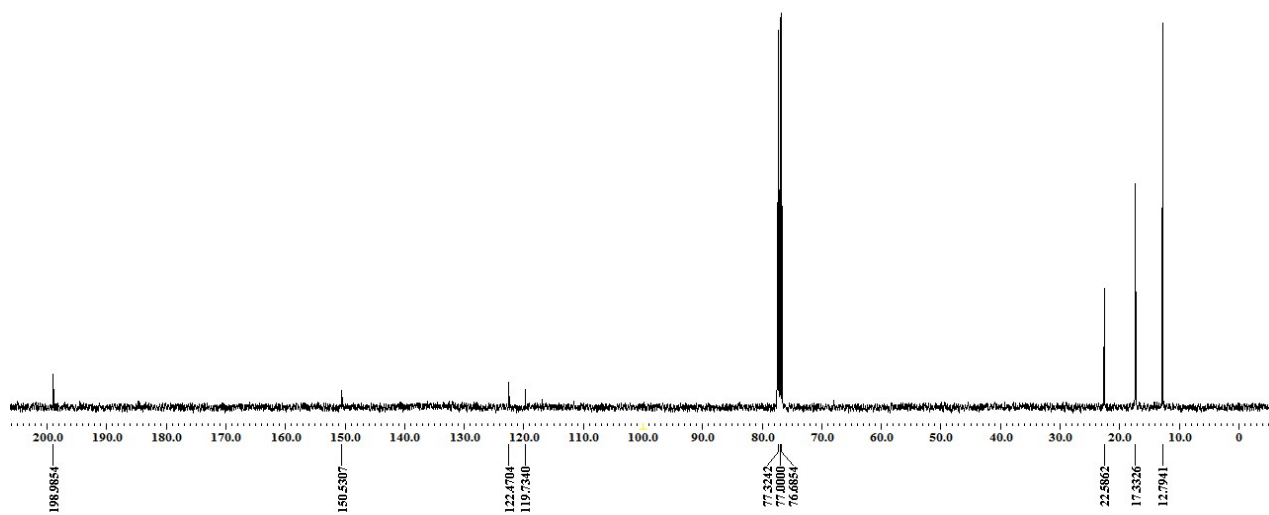


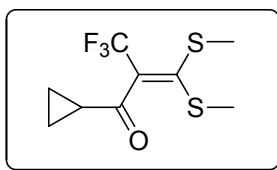
3i

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



**<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)**





3i

**Data File** SBNS368.d **Sample Name** SBNS368  
**Sample Type** Sample **Position** P2D4  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin

**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**

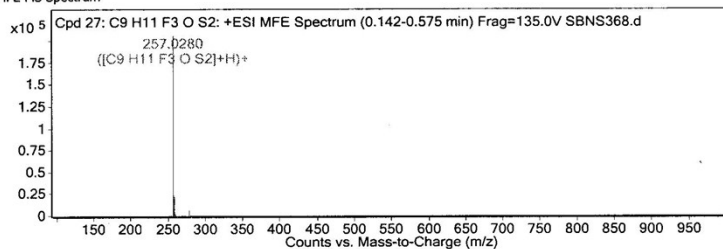
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

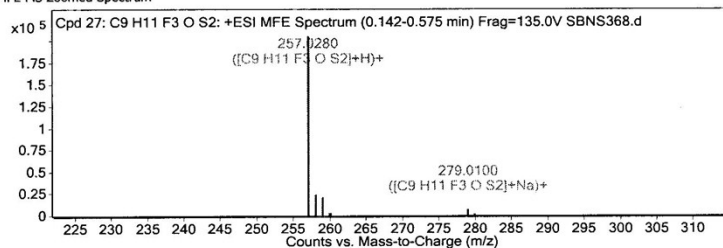
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 27: C9 H11 F3 O S2	0.196	256.0207	C9 H11 F3 O S2	C9 H11 F3 O S2	-1.26	C9 H11 F3 O S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 27: C9 H11 F3 O S2	257.028	0.196	Find by Molecular Feature	256.0207

**MFE MS Spectrum**



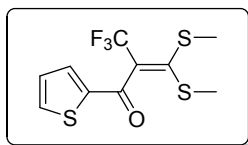
**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

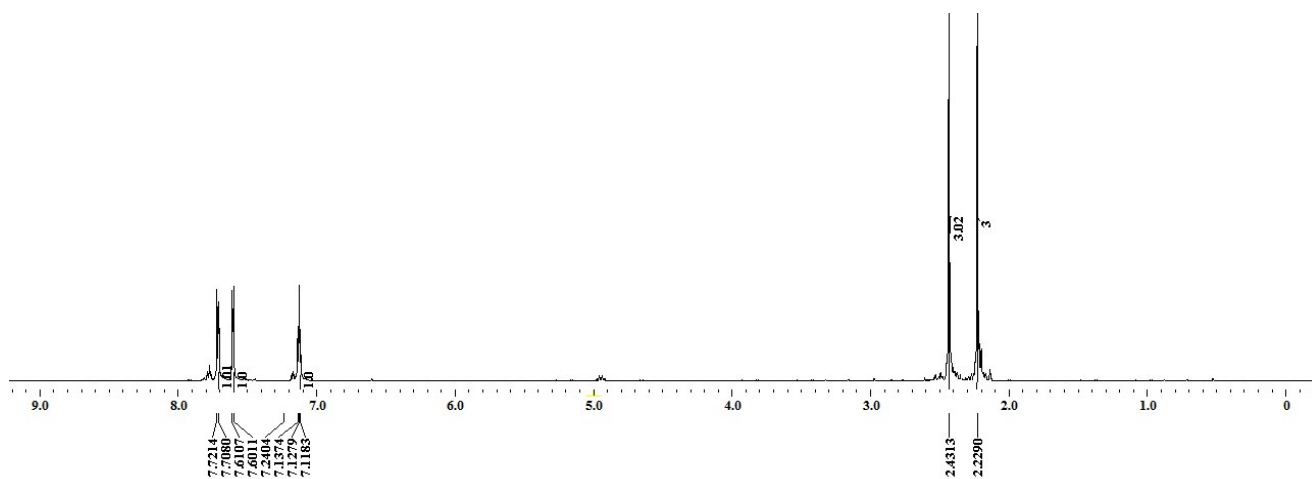
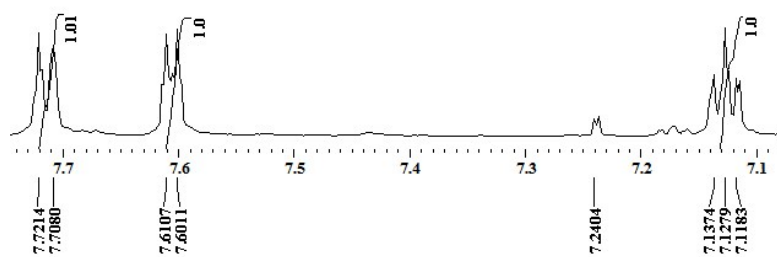
m/z	z	Abund	Formula	Ion
257.028	1	205398.03	C9 H11 F3 O S2	(M+H)+
258.0309	1	22227.01	C9 H11 F3 O S2	(M+H)+
259.0239	1	20336.6	C9 H11 F3 O S2	(M+H)+
260.0284	1	2383.76	C9 H11 F3 O S2	(M+H)+
279.01	1	6269.26	C9 H11 F3 O S2	(M+Na)+
280.0143	1	768.19	C9 H11 F3 O S2	(M+Na)+

--- End Of Report ---

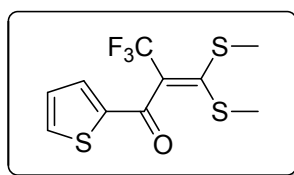
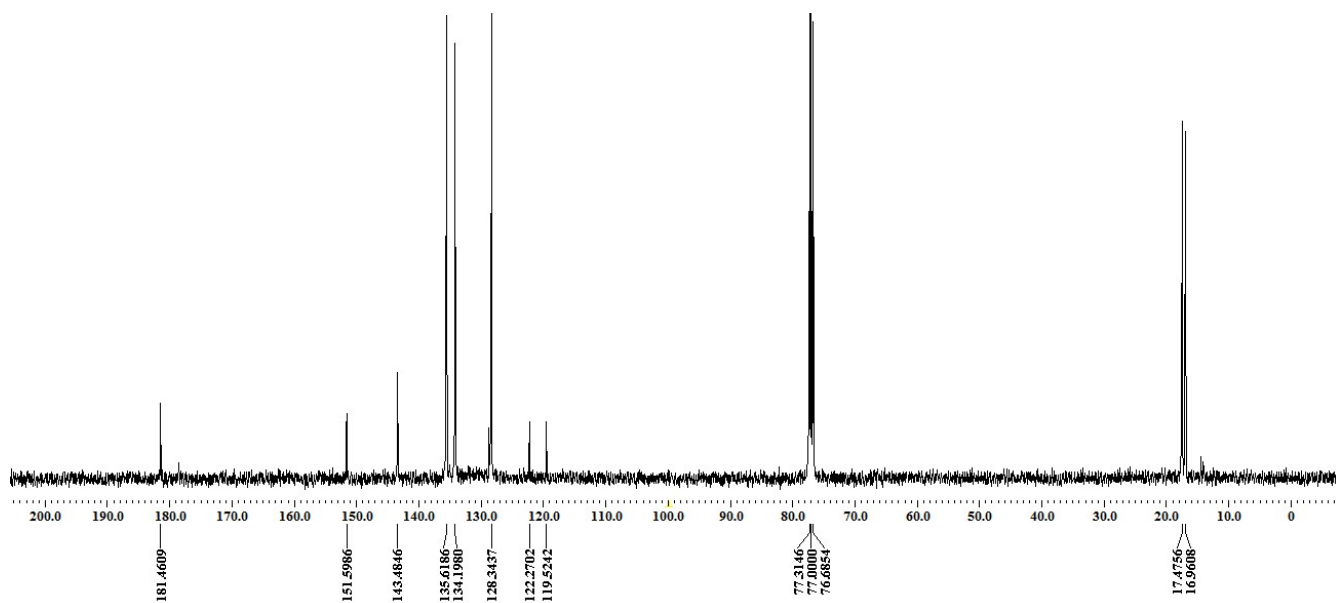


3j


<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)



3j

**Data File** EXP361.d **Sample Name** EXP361  
**Sample Type** Sample **Position** P1E2  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status**  **DA Method** Default.m  
**Comment**

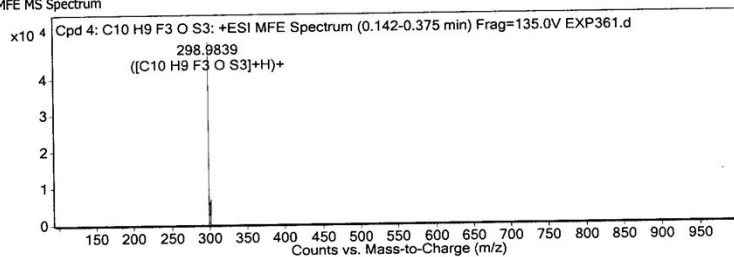
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

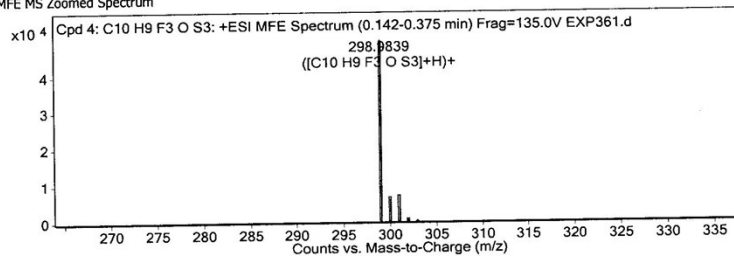
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C10 H9 F3 O S3	0.197	297.9767	C10 H9 F3 O S3	C10 H9 F3 O S3	0.17	C10 H9 F3 O S3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 4: C10 H9 F3 O S3	298.9839	0.197	Find by Molecular Feature	297.9767

**MFE MS Spectrum**



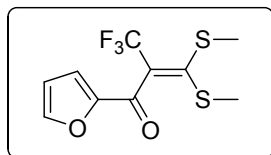
**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

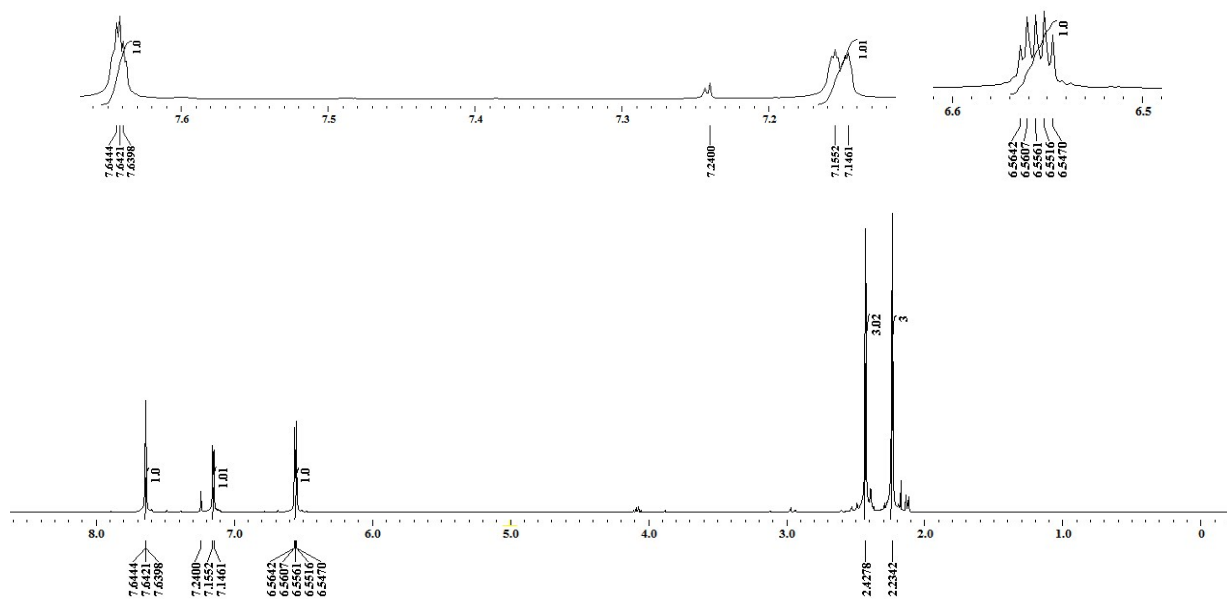
m/z	z	Abund	Formula	Ion
298.9839	1	49916.02	C10 H9 F3 O S3	(M+H)+
299.9868	1	6201.3	C10 H9 F3 O S3	(M+H)+
300.9804	1	6972.59	C10 H9 F3 O S3	(M+H)+
301.9835	1	1003.5	C10 H9 F3 O S3	(M+H)+
302.9815	1	287.83	C10 H9 F3 O S3	(M+H)+

--- End Of Report ---

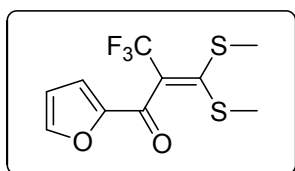
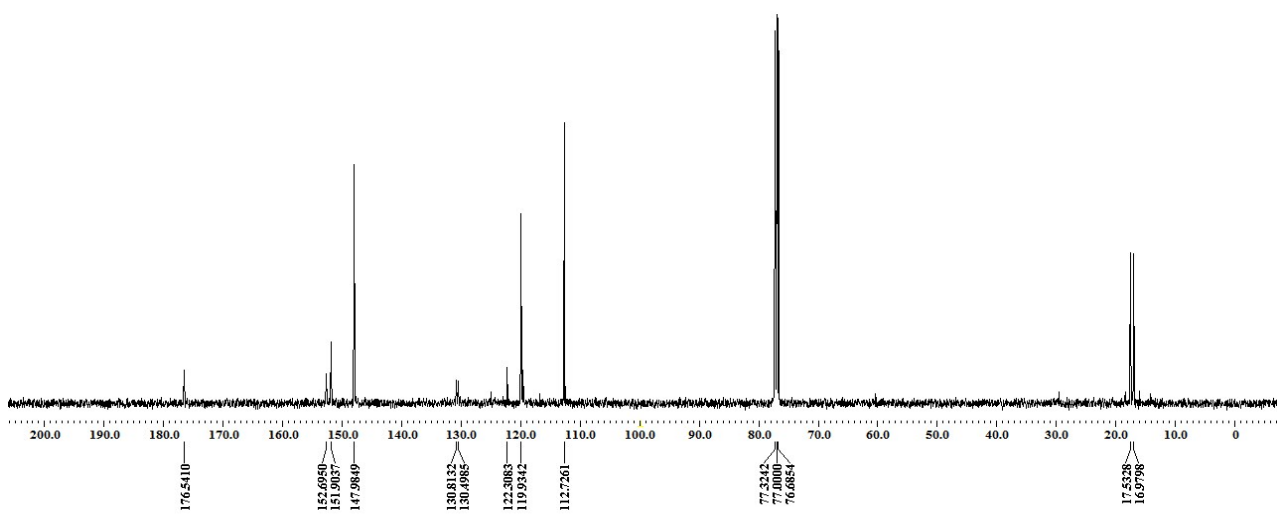


3k

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)



**3k**

Data File SBNS 377.d Sample Name SBNS 377  
 Sample Type Sample Position P2-B6  
 Instrument Name Instrument 1 User Name

IRM Calibration Status Success DA Method Default.m  
 Comment

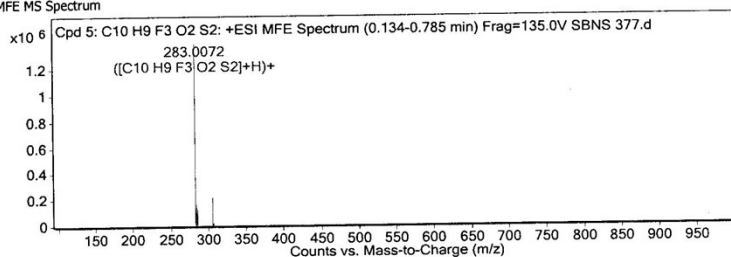
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

Compound Table

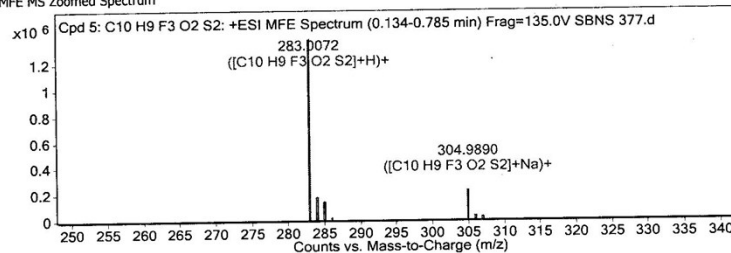
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C10 H9 F3 O2 S2	0.226	281.9999	C10 H9 F3 O2 S2	C10 H9 F3 O2 S2	-1.12	C10 H9 F3 O2 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 5: C10 H9 F3 O2 S2	283.0072	0.226	Find by Molecular Feature	281.9999

MFE MS Spectrum



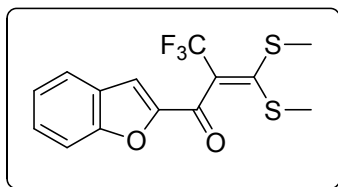
MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
283.0072	1	1395088.25	C10 H9 F3 O2 S2	(M+H)+
284.0099	1	168605.67	C10 H9 F3 O2 S2	(M+H)+
285.004	1	132272.56	C10 H9 F3 O2 S2	(M+H)+
286.0064	1	14895.13	C10 H9 F3 O2 S2	(M+H)+
304.989	1	220674	C10 H9 F3 O2 S2	(M+Na)+
305.9918	1	26229.04	C10 H9 F3 O2 S2	(M+Na)+
306.9865	1	23123.41	C10 H9 F3 O2 S2	(M+Na)+
307.9901	1	2765.94	C10 H9 F3 O2 S2	(M+Na)+

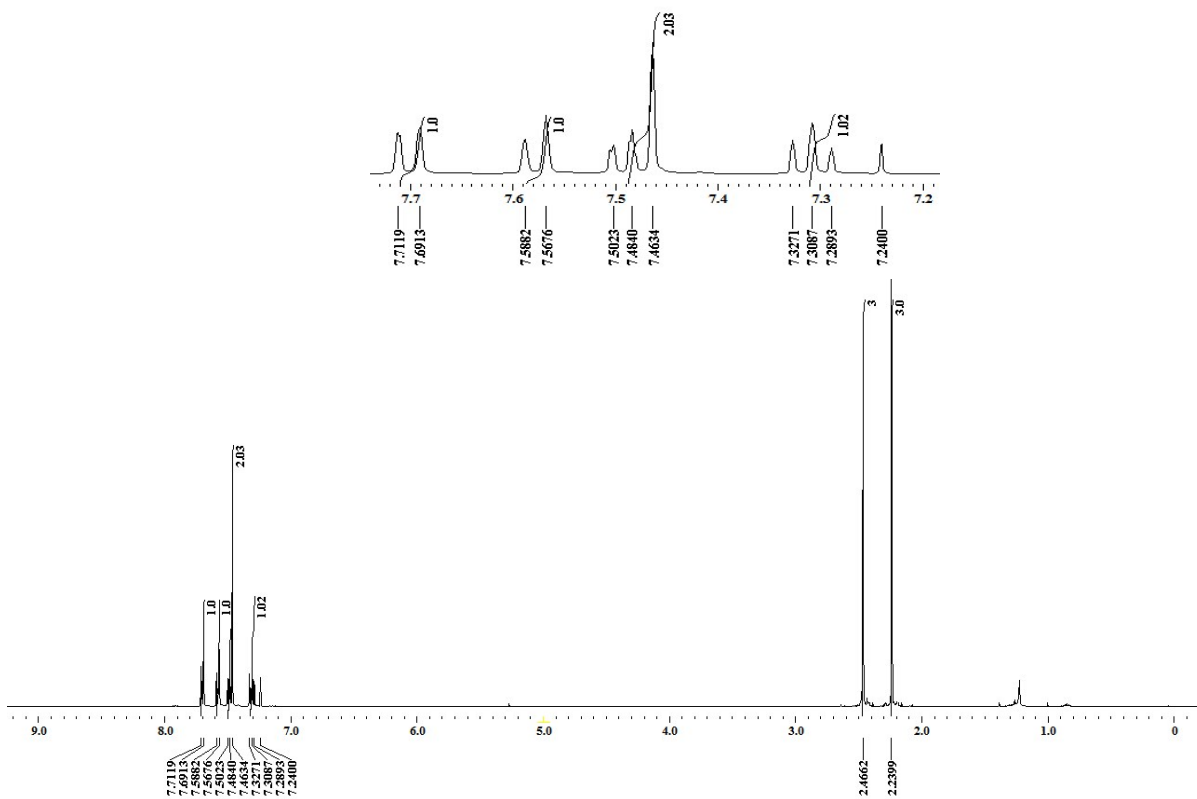
--- End Of Report ---



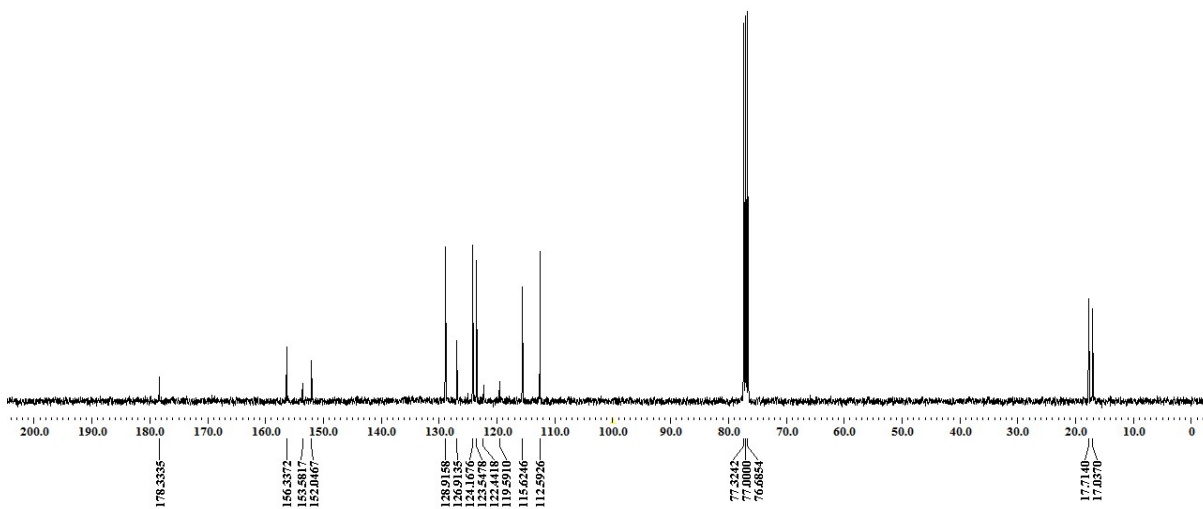
31

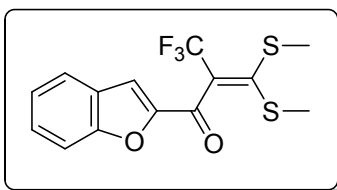
<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)





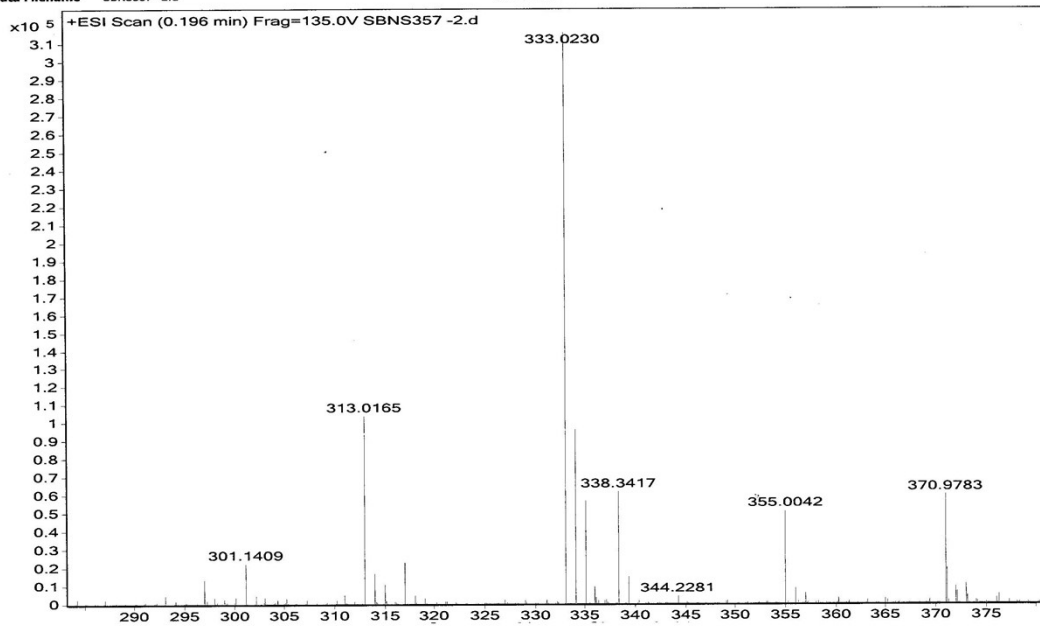
<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)

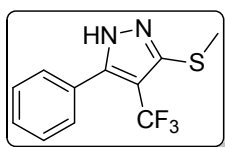




31

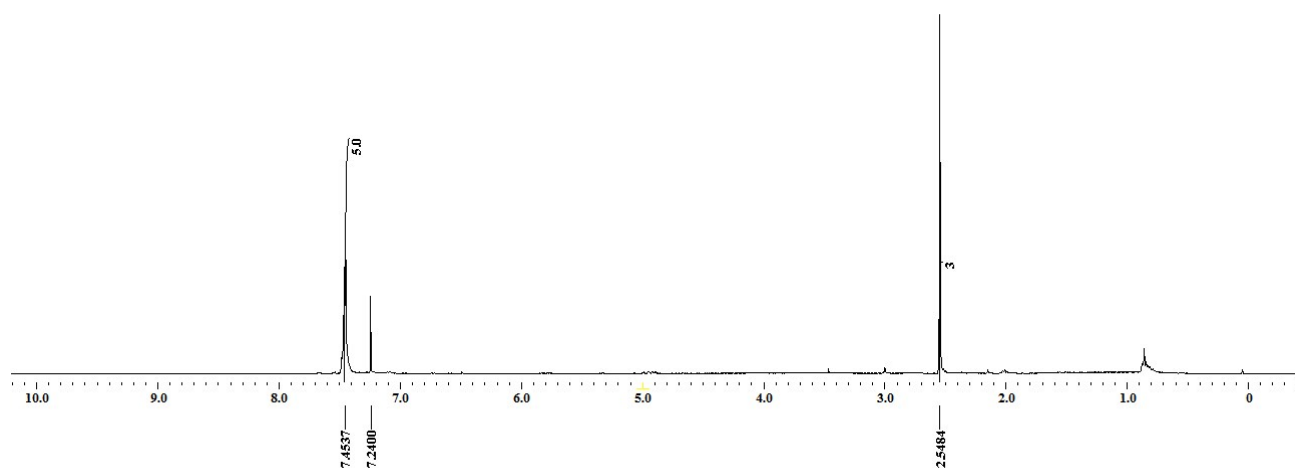
Sample Name	SBNS357 -2	Position	P2-E4	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SBNS357 -2.d			Comment			



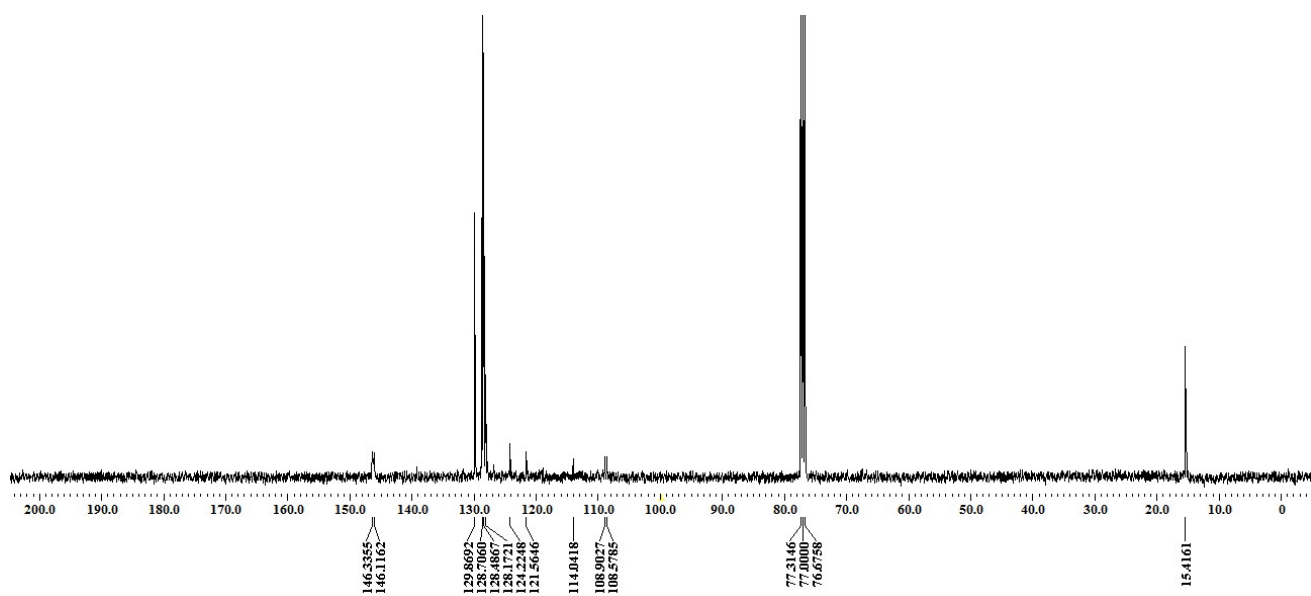


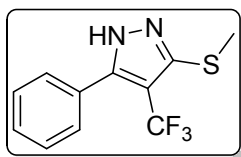
4a

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





4a

Data File SB-NS-328.d Sample Name SB-NS-328  
 Sample Type Sample Position P2C8  
 Instrument Name Instrument 1 User Name lcmsdu-PC\admin

IRM Calibration Status XXXXXXXXXX DA Method Default.m  
 Comment

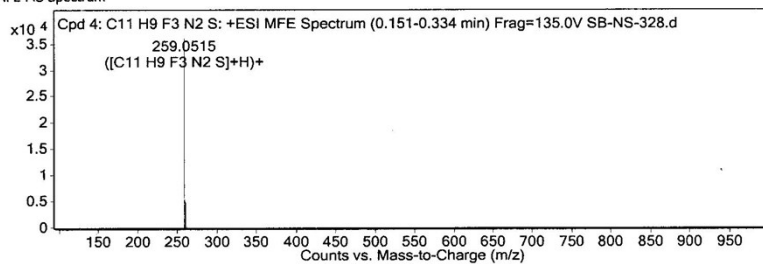
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

Compound Table

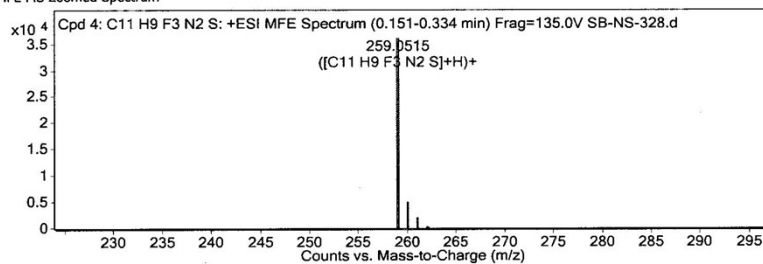
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C11 H9 F3 N2 S	0.204	258.0442	C11 H9 F3 N2 S	C11 H9 F3 N2 S	-1.25	C11 H9 F3 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 4: C11 H9 F3 N2 S	259.0515	0.204	Find by Molecular Feature	258.0442

MFE MS Spectrum



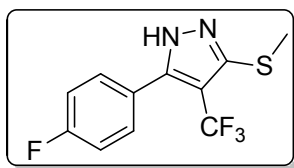
MFE MS Zoomed Spectrum



MS Spectrum Peak List

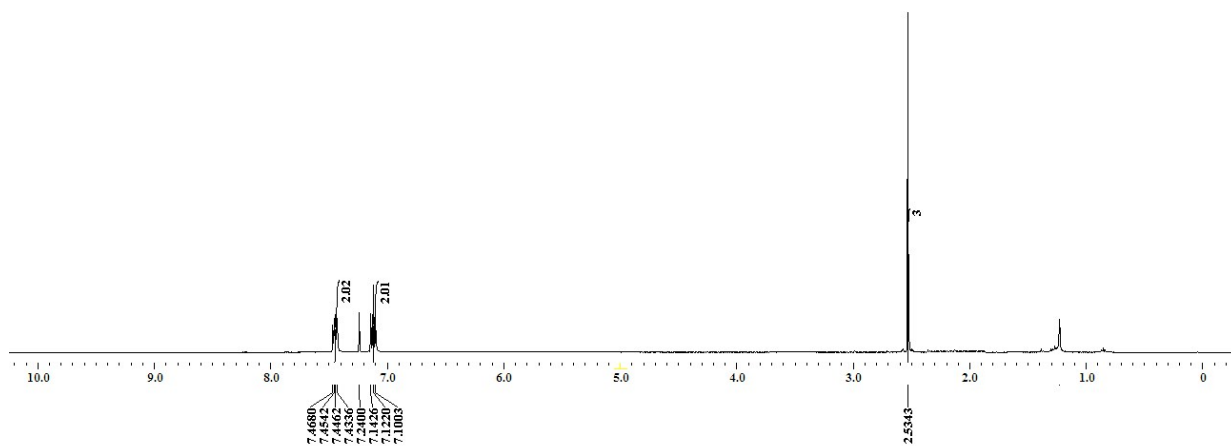
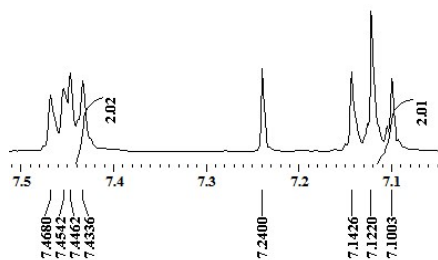
m/z	z	Abund	Formula	Ion
259.0515	1	36040.07	C11 H9 F3 N2 S	(M+H)+
260.0543	1	4999.66	C11 H9 F3 N2 S	(M+H)+
261.0484	1	1928.92	C11 H9 F3 N2 S	(M+H)+
262.0542	1	204.75	C11 H9 F3 N2 S	(M+H)+

--- End Of Report ---

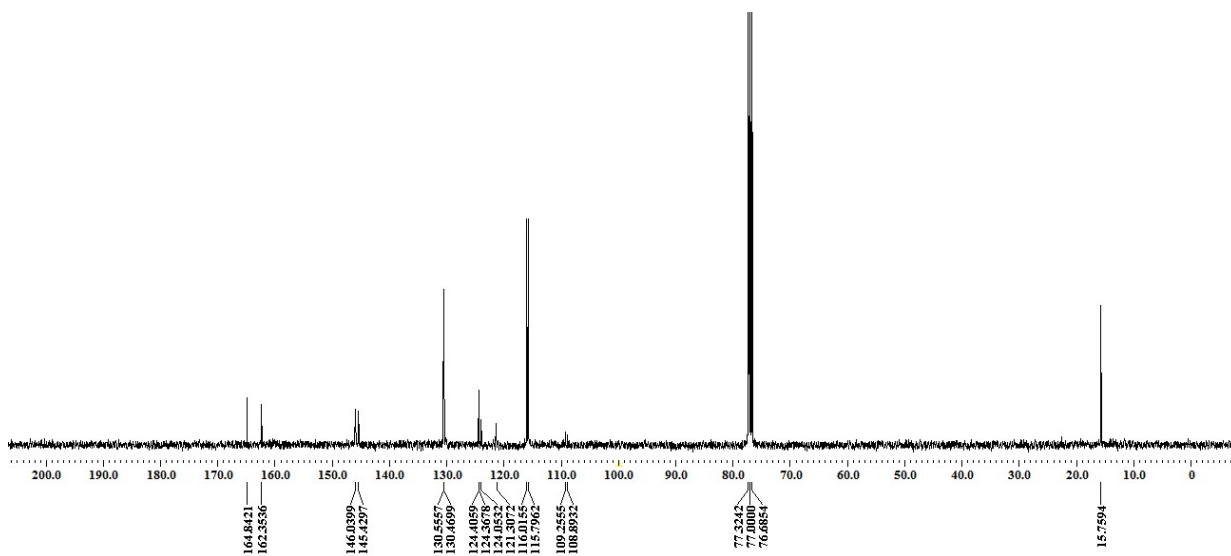


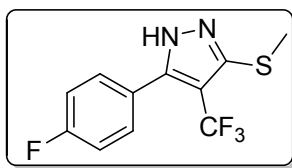
4b

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





**4b**

**Data File** SB-NS-360.d **Sample Name** SB-NS-360  
**Sample Type** Sample **Position** P2C3  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin

**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**

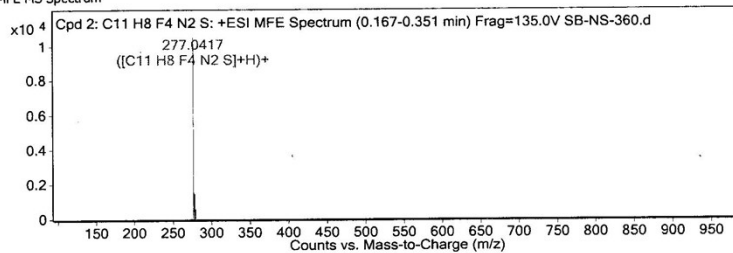
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

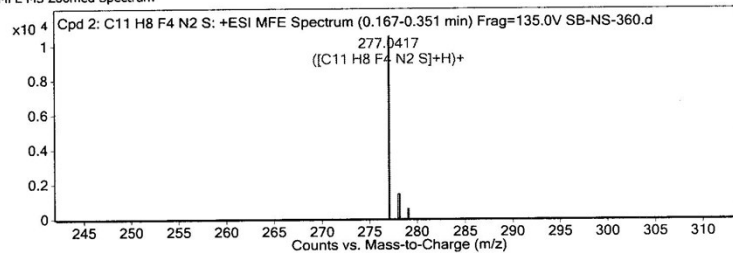
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C11 H8 F4 N2 S	0.219	276.0345	C11 H8 F4 N2 S	C11 H8 F4 N2 S	-0.31	C11 H8 F4 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C11 H8 F4 N2 S	277.0417	0.219	Find by Molecular Feature	276.0345

**MFE MS Spectrum**



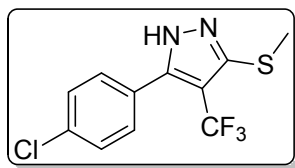
**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

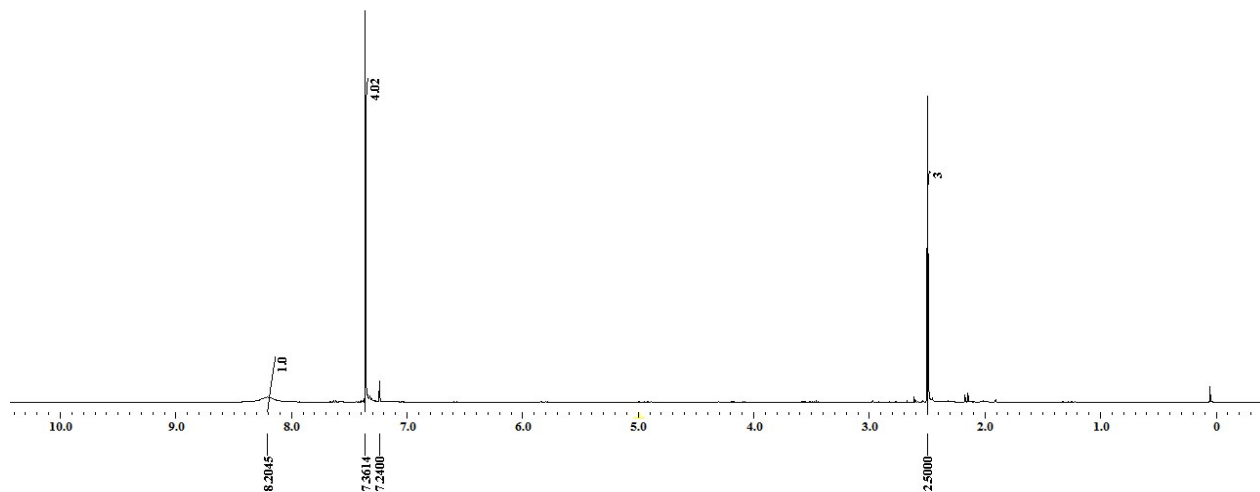
m/z	z	Abund	Formula	Ion
277.0417	1	10519.26	C11 H8 F4 N2 S	(M+H)+
278.0453	1	1480.11	C11 H8 F4 N2 S	(M+H)+
279.0394	1	601.3	C11 H8 F4 N2 S	(M+H)+

--- End Of Report ---

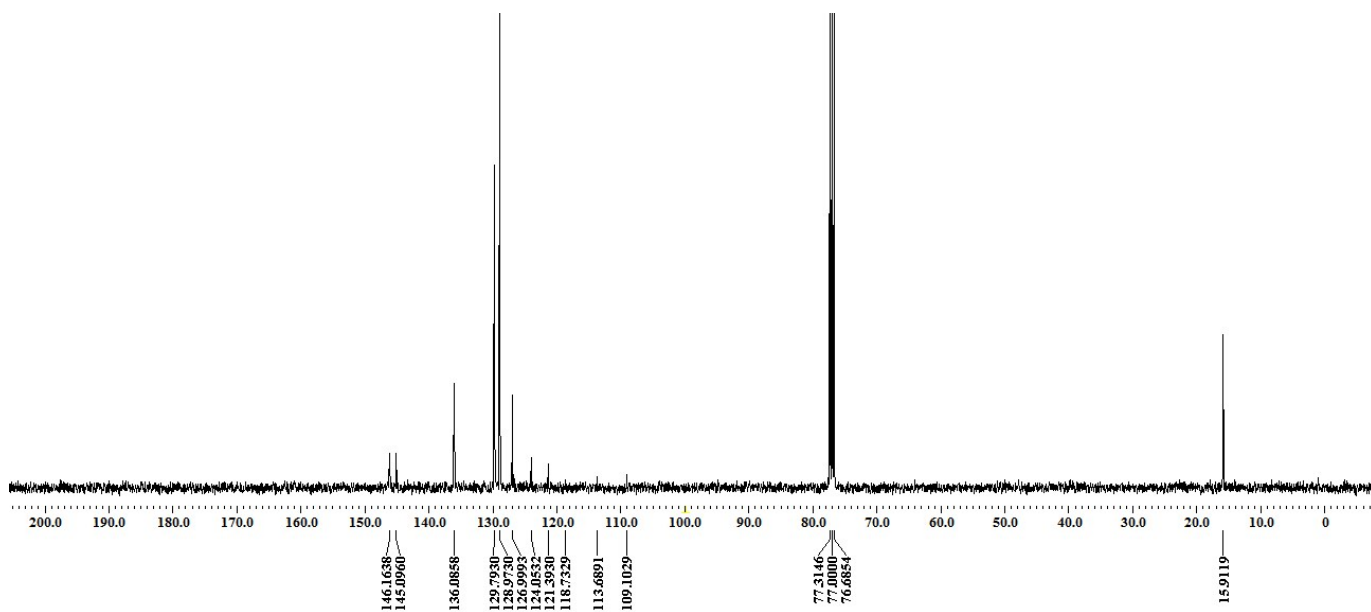


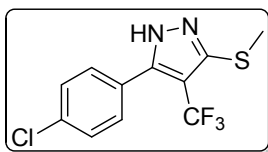
4c

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





4c

Data File SBNS-372.d Sample Name SBNS-372  
 Sample Type Sample Position P2F2  
 Instrument Name Instrument 1 User Name icmsdu-PC\admin  
 IRM Calibration Status Success DA Method Default.m  
 Comment

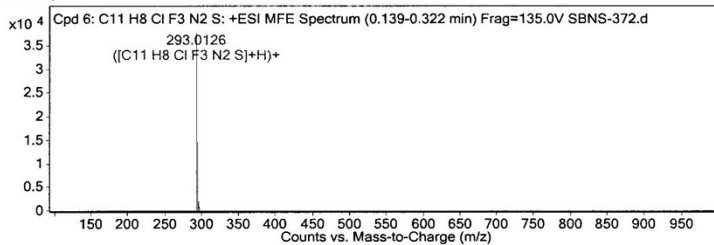
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

Compound Table

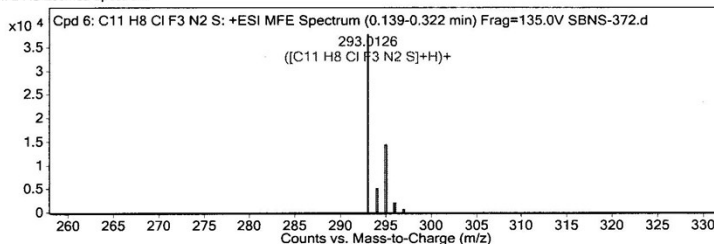
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C11 H8 Cl F3 N2 S	0.204	292.0055	C11 H8 Cl F3 N2 S	C11 H8 Cl F3 N2 S	-2.14	C11 H8 Cl F3 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C11 H8 Cl F3 N2 S	293.0126	0.204	Find by Molecular Feature	292.0055

MFE MS Spectrum



MFE MS Zoomed Spectrum

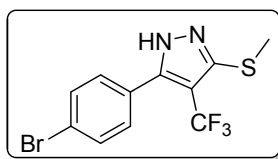


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
293.0126	1	37672.71	C11 H8 Cl F3 N2 S	(M+H)+
294.0166	1	4994.9	C11 H8 Cl F3 N2 S	(M+H)+
295.0096	1	14469.53	C11 H8 Cl F3 N2 S	(M+H)+
296.0128	1	1875.03	C11 H8 Cl F3 N2 S	(M+H)+
297.0116	1	729.36	C11 H8 Cl F3 N2 S	(M+H)+

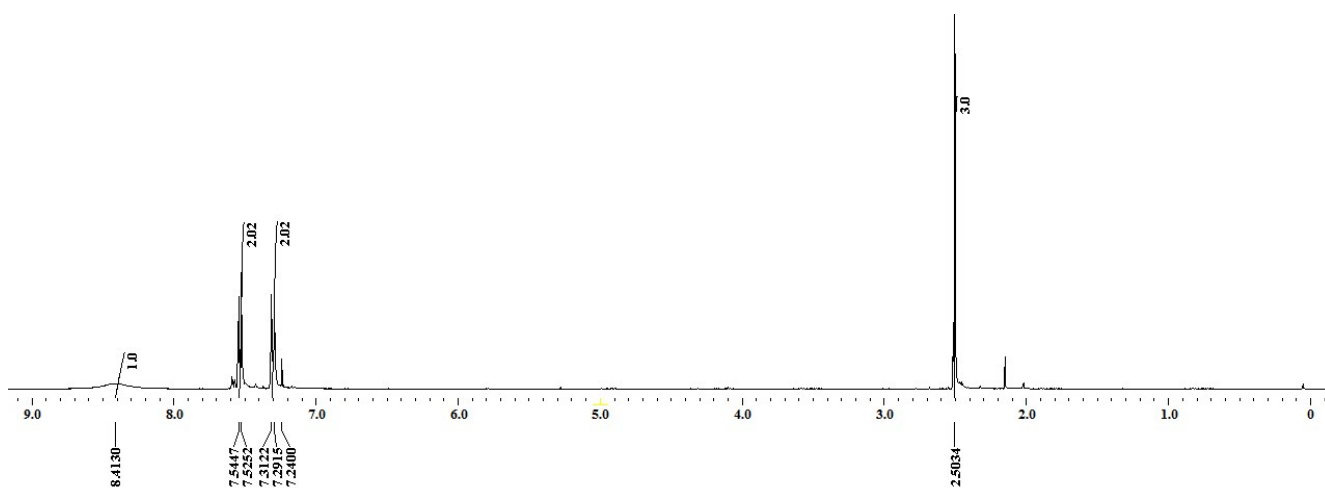
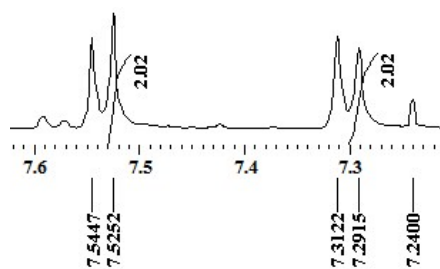
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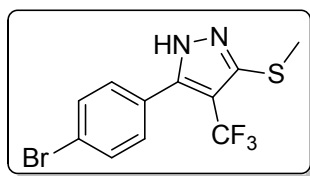
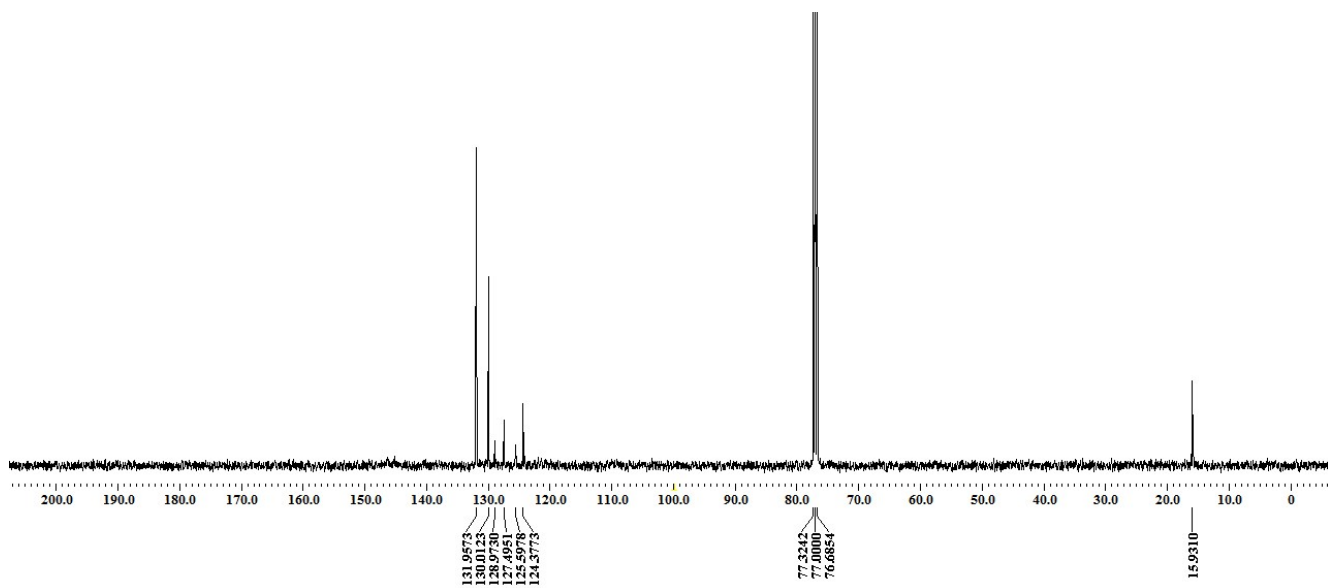


4d

$^1\text{H-NMR}$  in  $\text{CDCl}_3$  (400MHz)



$^{13}\text{C-NMR}$  in  $\text{CDCl}_3$  (100MHz)



4d

<b>Data File</b>	SB-NS-383	<b>Sample Name</b>	SB-NS-409
<b>Sample Type</b>	Sample	<b>Position</b>	P2A3
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	lcmsdu-PC\admin
<b>Acq Method</b>	29.10.2014.m	<b>Acquired Time</b>	26-02-2015 15:20:07
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

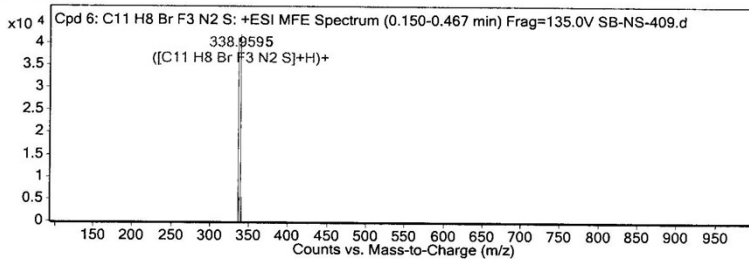
<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125)	

#### Compound Table

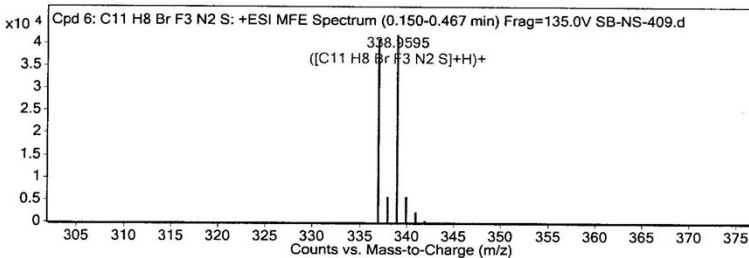
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C11 H8 Br F3 N2 S	0.207	335.9547	C11 H8 Br F3 N2 S	C11 H8 Br F3 N2 S	-0.92	C11 H8 Br F3 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C11 H8 Br F3 N2 S	336.9621	0.207	Find by Molecular Feature	335.9547

#### MFE MS Spectrum

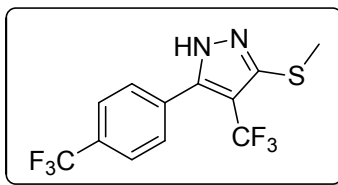


#### MFE MS Zoomed Spectrum



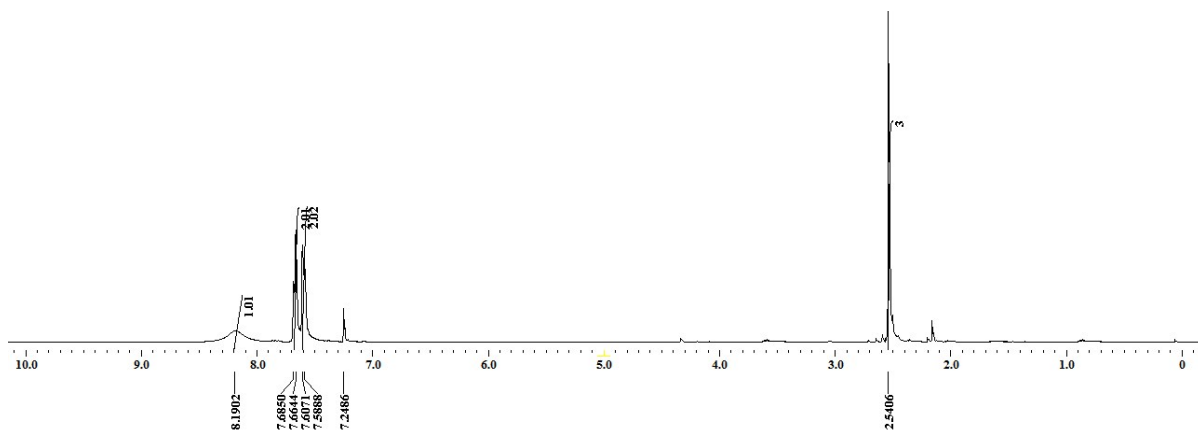
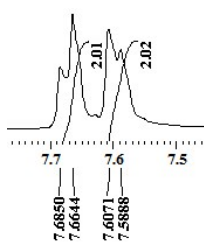
#### MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
336.9620	1	41064.77	C11 H8 Br F3 N2 S	(M+H)+
337.9652	1	5446.67	C11 H8 Br F3 N2 S	(M+H)+
338.9595	1	41900.1	C11 H8 Br F3 N2 S	(M+H)+
339.9625	1	5446.27	C11 H8 Br F3 N2 S	(M+H)+
340.9577	1	2330.67	C11 H8 Br F3 N2 S	(M+H)+
341.9549	1	188.9	C11 H8 Br F3 N2 S	(M+H)+

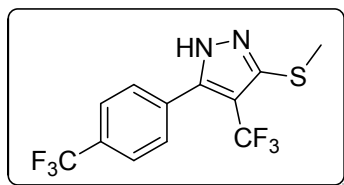
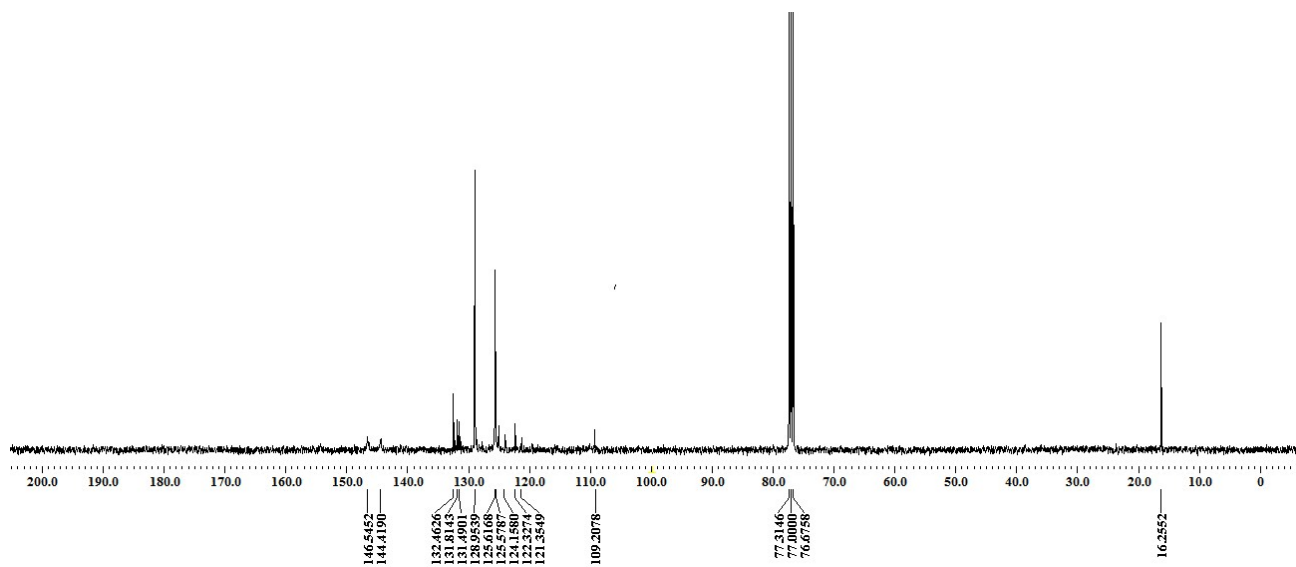


4e

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



**<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)**



4e

<b>Data File</b>	SB-NS-386.d	<b>Sample Name</b>	SB-NS-386
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A9
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	29.10.2014.m	<b>Acquired Time</b>	06-06-2016 15:03:31
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

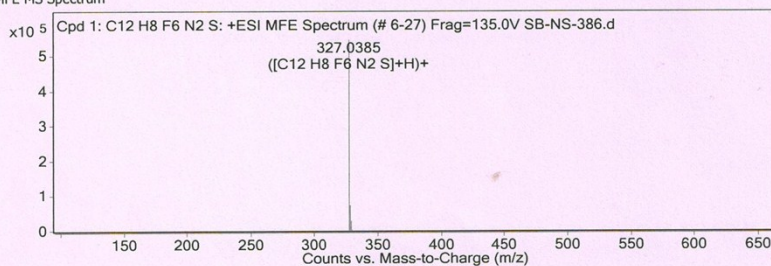
<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125)	

#### Compound Table

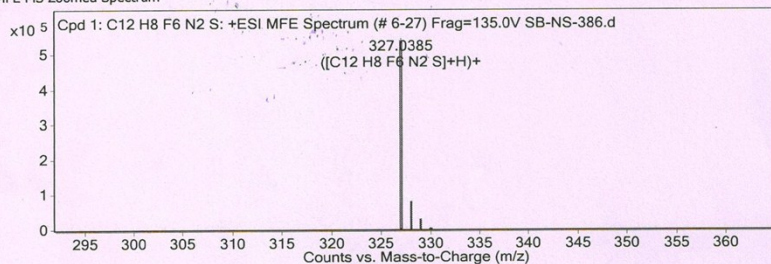
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C12 H8 F6 N2 S	11	326.0312	C12 H8 F6 N2 S	C12 H8 F6 N2 S	0.16	C12 H8 F6 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C12 H8 F6 N2 S	327.0385	11	Find by Molecular Feature	326.0312

#### MFE MS Spectrum



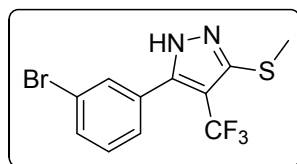
#### MFE MS Zoomed Spectrum



#### MS Spectrum Peak List

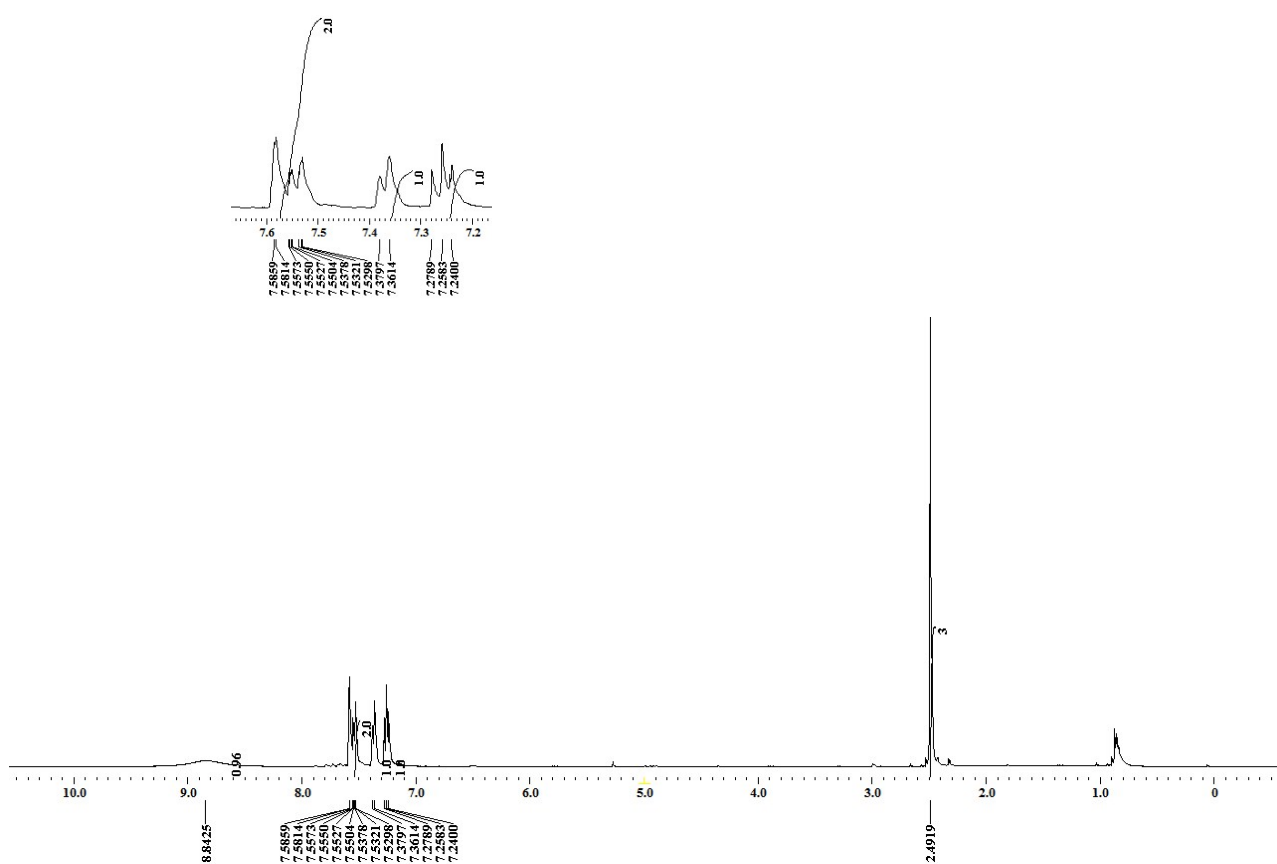
m/z	z	Abund	Formula	Ion
327.0385	1	546059.94	C12 H8 F6 N2 S	(M+H)+
328.0412	1	73402.99	C12 H8 F6 N2 S	(M+H)+
329.0355	1	26823.88	C12 H8 F6 N2 S	(M+H)+
330.0383	1	3189.78	C12 H8 F6 N2 S	(M+H)+

--- End Of Report ---

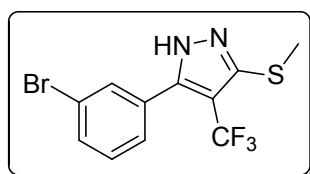
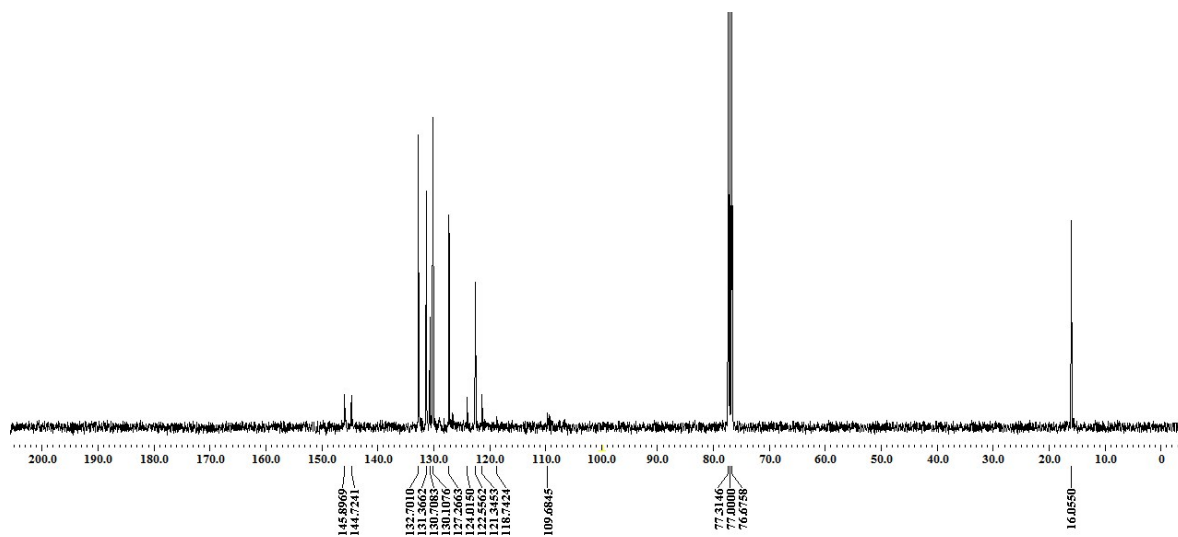


4f

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



**<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)**



## 4f

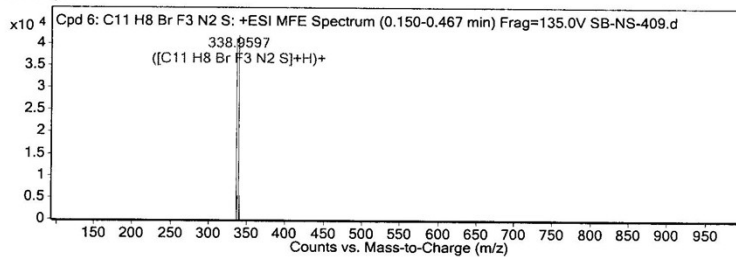
**Data File** SB-NS-409.d **Sample Name** SB-NS-409  
**Sample Type** Sample **Position** P2A3  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status** XXXXXXXXXX **DA Method** Default.m  
**Comment**  
**Sample Group** **Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

## Compound Table

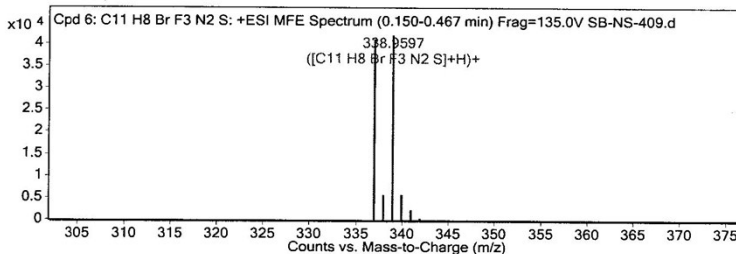
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C11 H8 Br F3 N2 S	0.207	335.9547	C11 H8 Br F3 N2 S	C11 H8 Br F3 N2 S	-0.92	C11 H8 Br F3 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C11 H8 Br F3 N2 S	336.9621	0.207	Find by Molecular Feature	335.9547

## MFE MS Spectrum



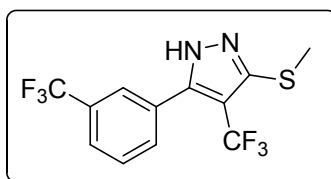
## MFE MS Zoomed Spectrum



## MS Spectrum Peak List

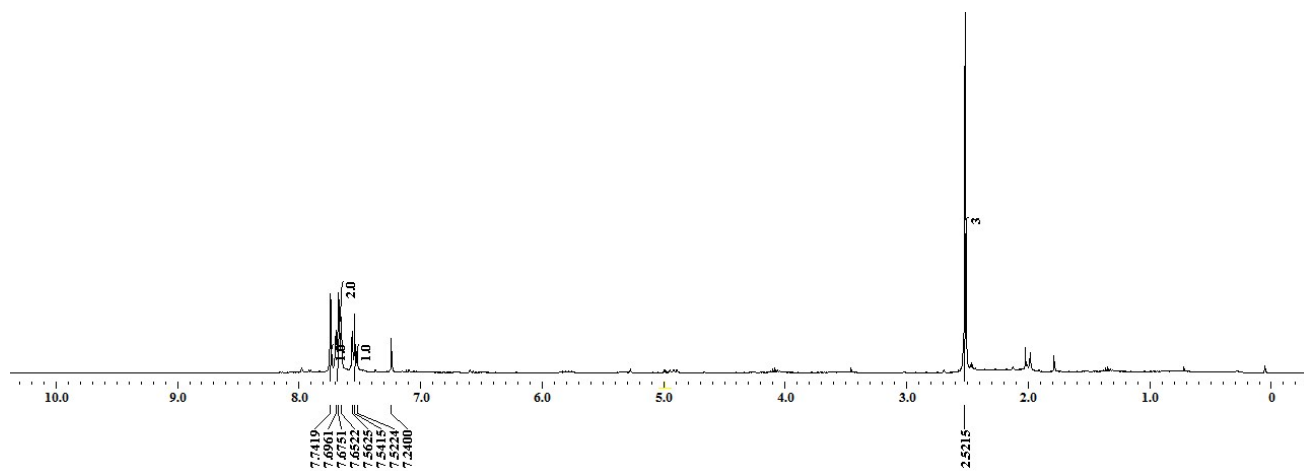
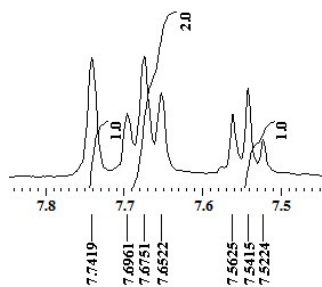
m/z	z	Abund	Formula	Ion
336.9621	1	41064.77	C11 H8 Br F3 N2 S	(M+H)+
337.9652	1	5446.67	C11 H8 Br F3 N2 S	(M+H)+
338.9597	1	41900.1	C11 H8 Br F3 N2 S	(M+H)+
339.9625	1	5446.27	C11 H8 Br F3 N2 S	(M+H)+
340.9577	1	2330.67	C11 H8 Br F3 N2 S	(M+H)+
341.9549	1	188.9	C11 H8 Br F3 N2 S	(M+H)+

--- End Of Report ---

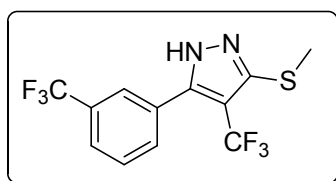
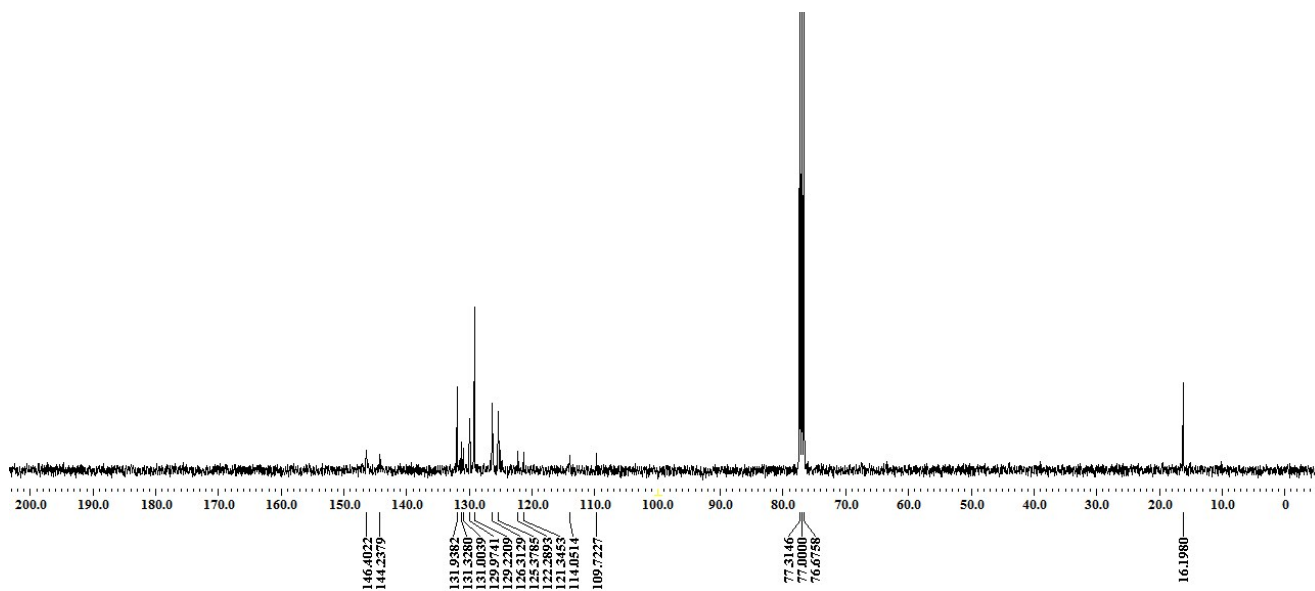


4g

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





4g

Data File SB-NS-416.d Sample Name SB-NS-416  
 Sample Type Sample Position P1-A9  
 Instrument Name Instrument 1 User Name  
 Acq Method 29.10.2014.m Acquired Time 06-06-2016 15:06:14  
 IRM Calibration Status Success DA Method Default.m  
 Comment

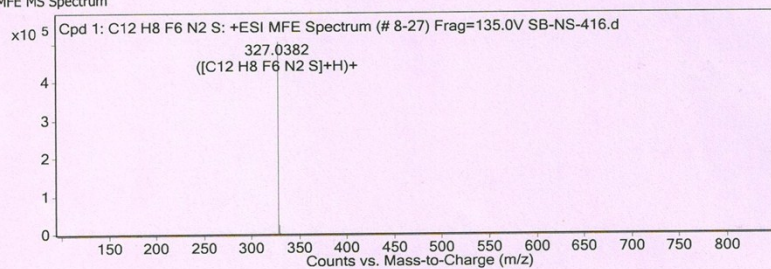
Sample Group Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.05.01 (B5125)

Compound Table

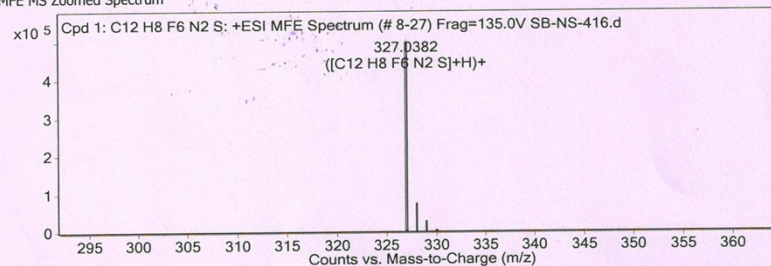
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C12 H8 F6 N2 S	11	326.0308	C12 H8 F6 N2 S	C12 H8 F6 N2 S	1.22	C12 H8 F6 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C12 H8 F6 N2 S	327.0382	11	Find by Molecular Feature	326.0308

MFE MS Spectrum



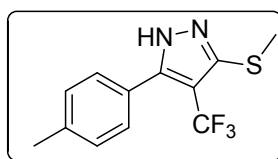
MFE MS Zoomed Spectrum



MS Spectrum Peak List

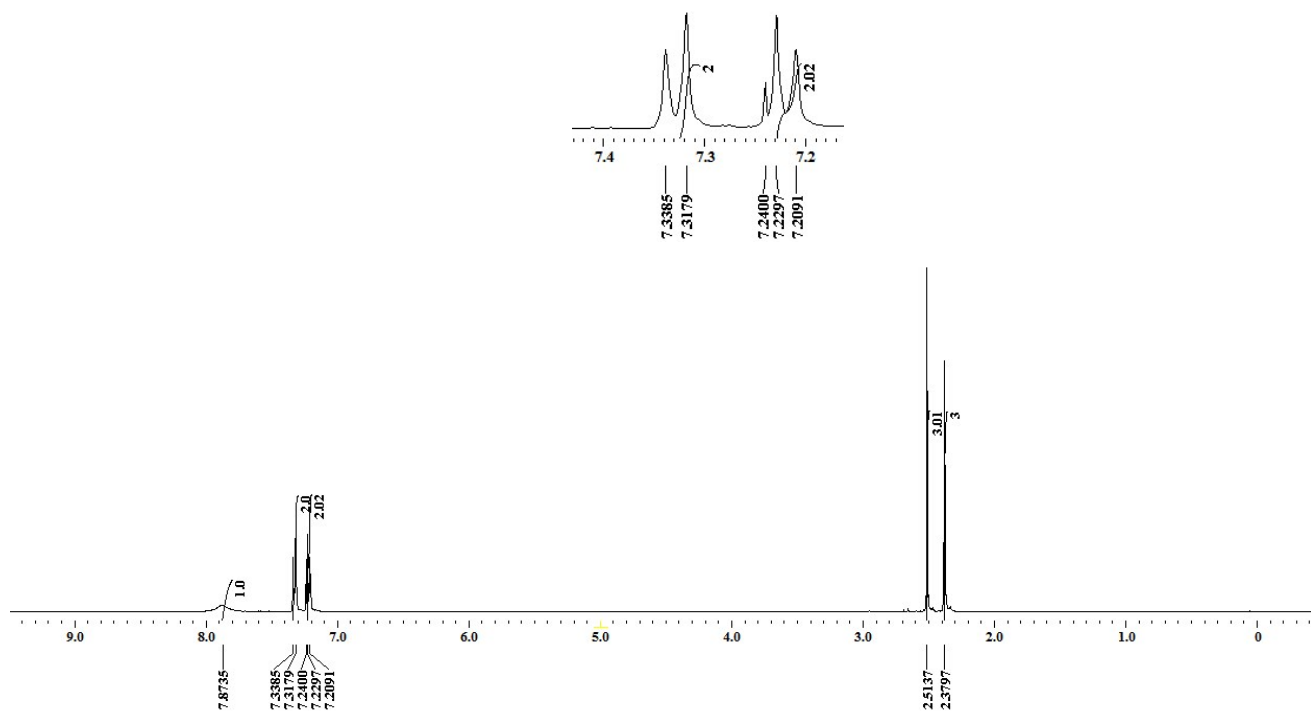
m/z	z	Abund	Formula	Ion
327.0382	1	504488.09	C12 H8 F6 N2 S	(M+H)+
328.0408	1	68466.58	C12 H8 F6 N2 S	(M+H)+
329.0354	1	24271.75	C12 H8 F6 N2 S	(M+H)+
330.0367	1	3050.17	C12 H8 F6 N2 S	(M+H)+

--- End Of Report ---

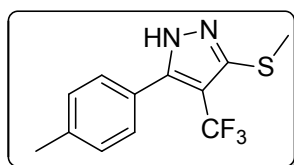
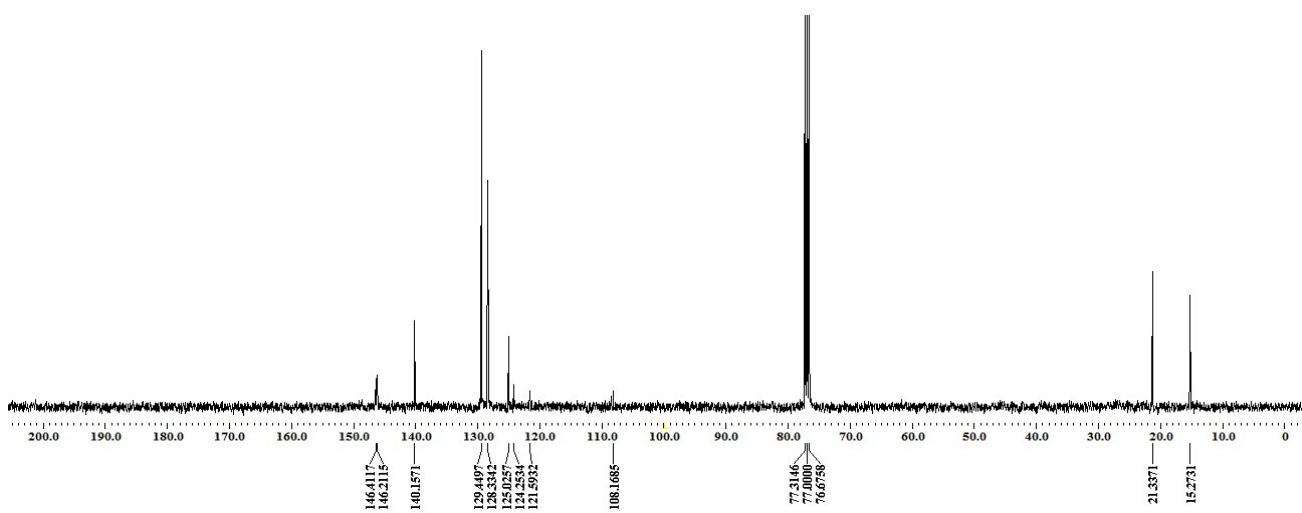


4h

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)



4h

**Data File** SB-NS-362.d      **Sample Name** SB-NS-362  
**Sample Type** Sample      **Position** P2D7  
**Instrument Name** Instrument 1      **User Name** lcmsdu-PC\admin

**IRM Calibration Status** Success      **DA Method** Default.m  
**Comment**

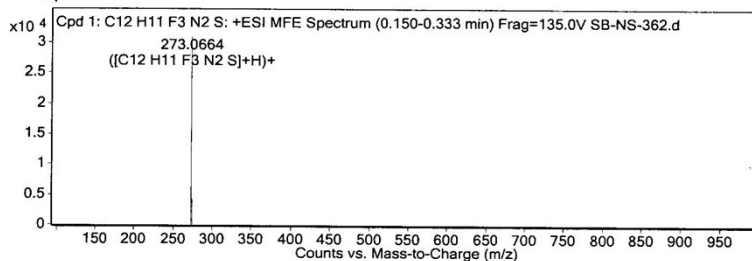
**Sample Group**      **Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

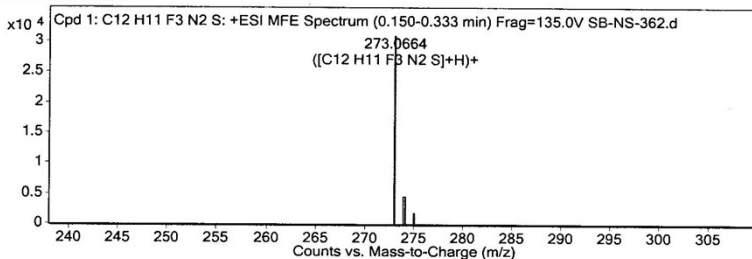
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C12 H11 F3 N2 S	0.203	272.0592	C12 H11 F3 N2 S	C12 H11 F3 N2 S	1.18	C12 H11 F3 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C12 H11 F3 N2 S	273.0664	0.203	Find by Molecular Feature	272.0592

MFE MS Spectrum



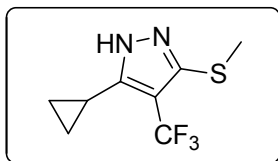
MFE MS Zoomed Spectrum



MS Spectrum Peak List

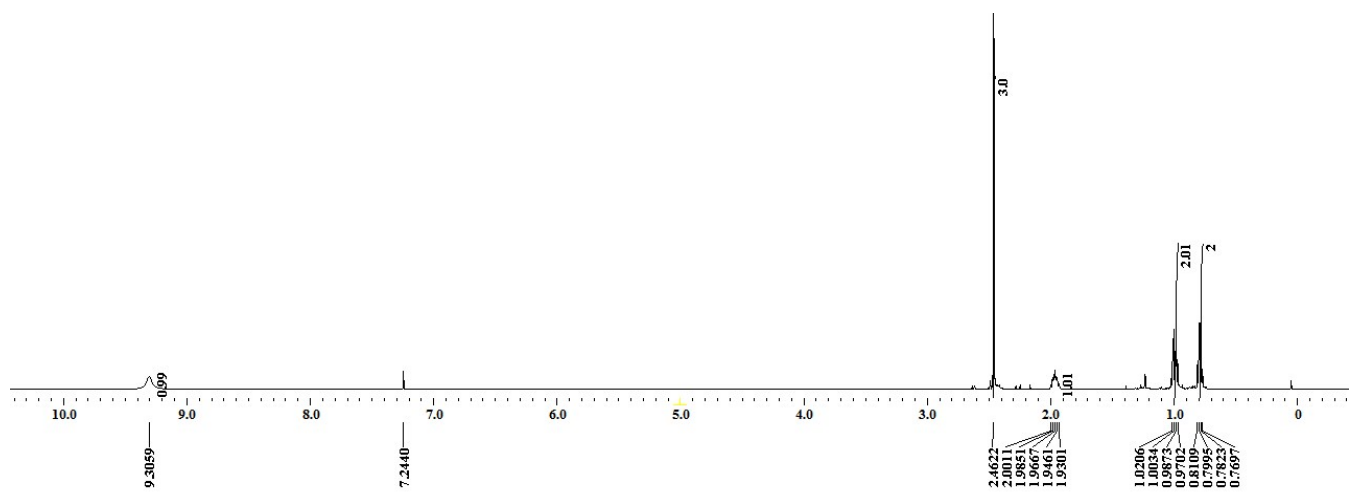
m/z	z	Abund	Formula	Ion
273.0664	1	30955.35	C12 H11 F3 N2 S	(M+H)+
274.0699	1	4273.48	C12 H11 F3 N2 S	(M+H)+
275.0642	1	1961.88	C12 H11 F3 N2 S	(M+H)+

--- End Of Report ---

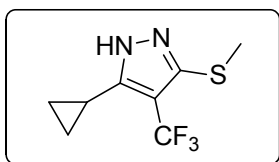
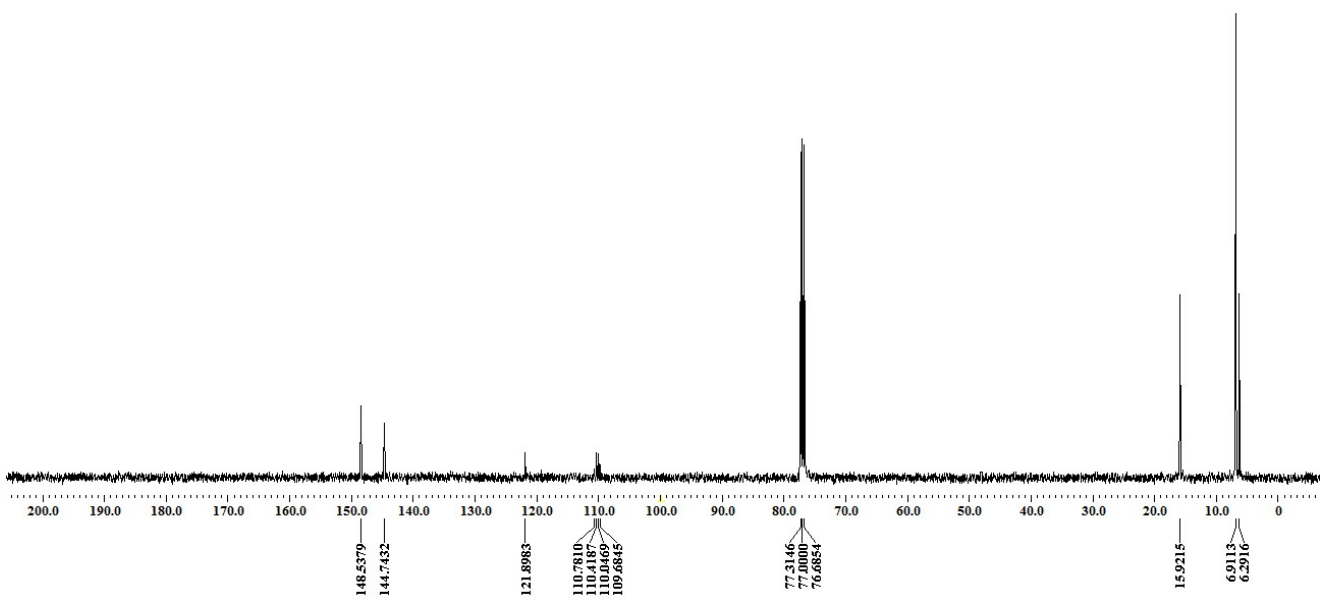


4i

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



**<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)**



**4i**

**Data File** SB NS 371.d **Sample Name** SB NS 371  
**Sample Type** Sample **Position** P2E9  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status** SUCCESS **DA Method** Default.m  
**Comment**

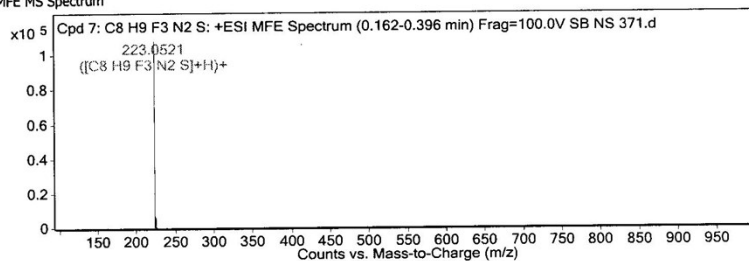
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

#### Compound Table

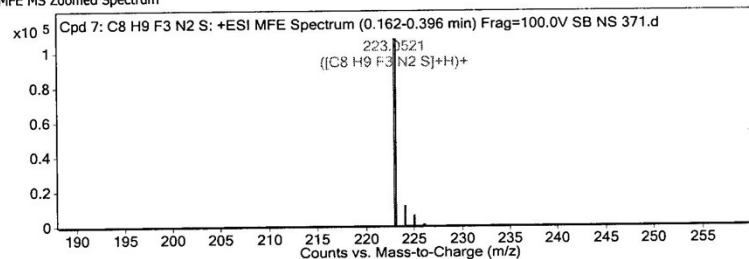
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C8 H9 F3 N2 S	0.219	222.0449	C8 H9 F3 N2 S	C8 H9 F3 N2 S	-4.82	C8 H9 F3 N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 7: C8 H9 F3 N2 S	223.0521	0.219	Find by Molecular Feature	222.0449

#### MFE MS Spectrum



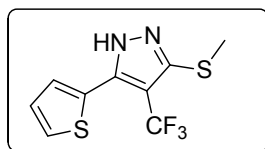
#### MFE MS Zoomed Spectrum



#### MS Spectrum Peak List

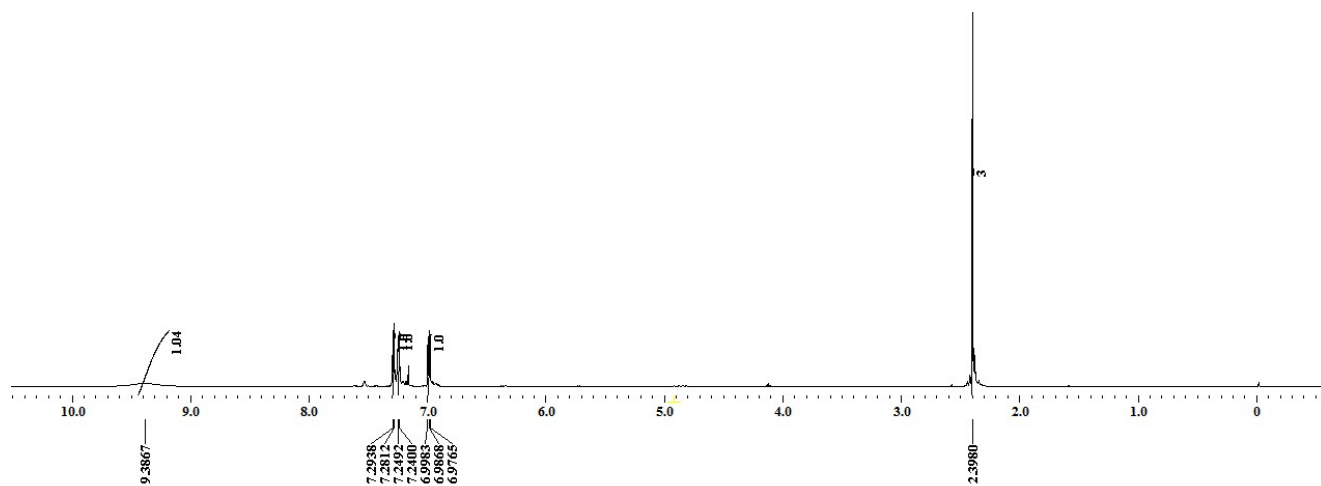
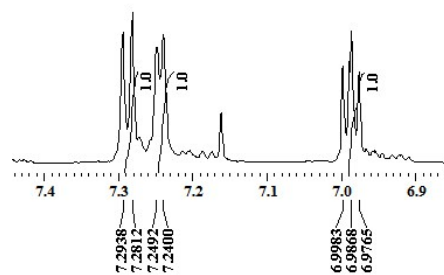
m/z	z	Abund	Formula	Ion
223.0521	1	107913.52	C8 H9 F3 N2 S	(M+H)+
224.0553	1	11598.36	C8 H9 F3 N2 S	(M+H)+
225.0498	1	5874.66	C8 H9 F3 N2 S	(M+H)+
226.0537	1	636.85	C8 H9 F3 N2 S	(M+H)+

--- End Of Report ---

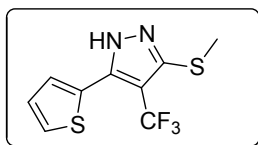
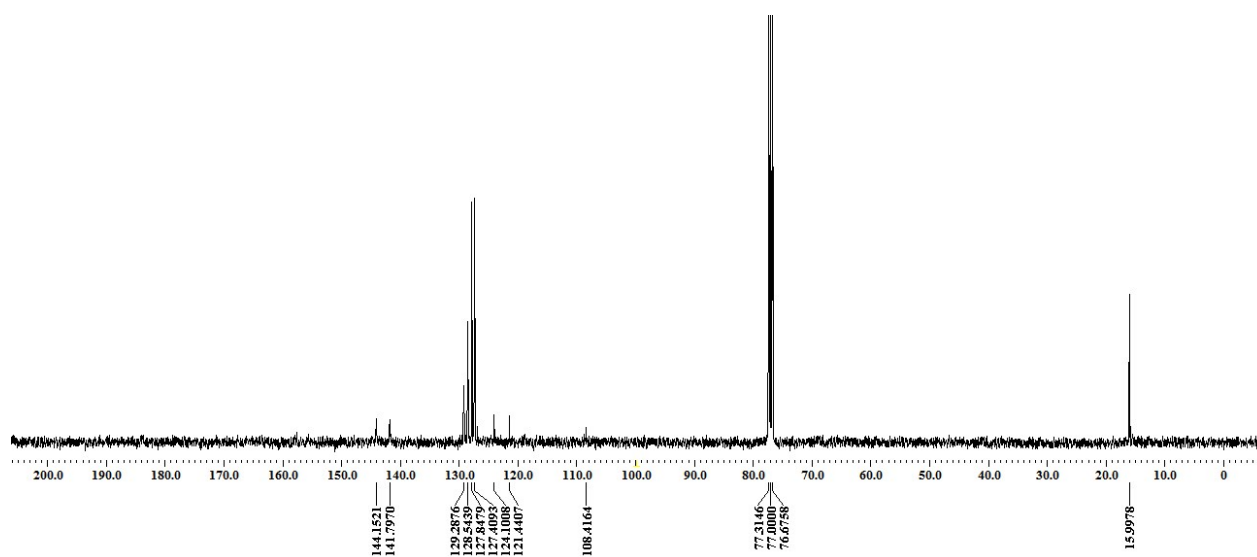


4j

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)



4j

**Data File** SB-NS370.d **Sample Name** SB-NS370  
**Sample Type** Sample **Position** P1B6  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**

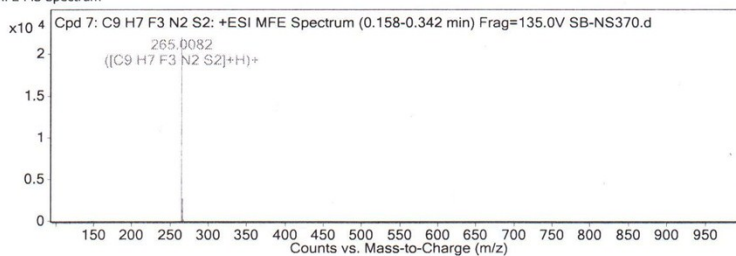
**Sample Group** **Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

## Compound Table

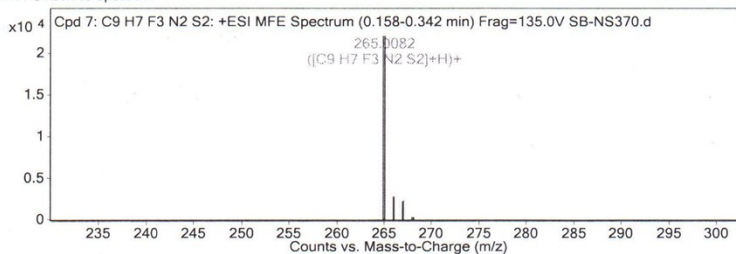
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C9 H7 F3 N2 S2	0.205	264.001	C9 H7 F3 N2 S2	C9 H7 F3 N2 S2	-2.91	C9 H7 F3 N2 S2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 7: C9 H7 F3 N2 S2	265.0082	0.205	Find by Molecular Feature	264.001

## MFE MS Spectrum



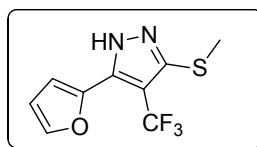
## MFE MS Zoomed Spectrum



## MS Spectrum Peak List

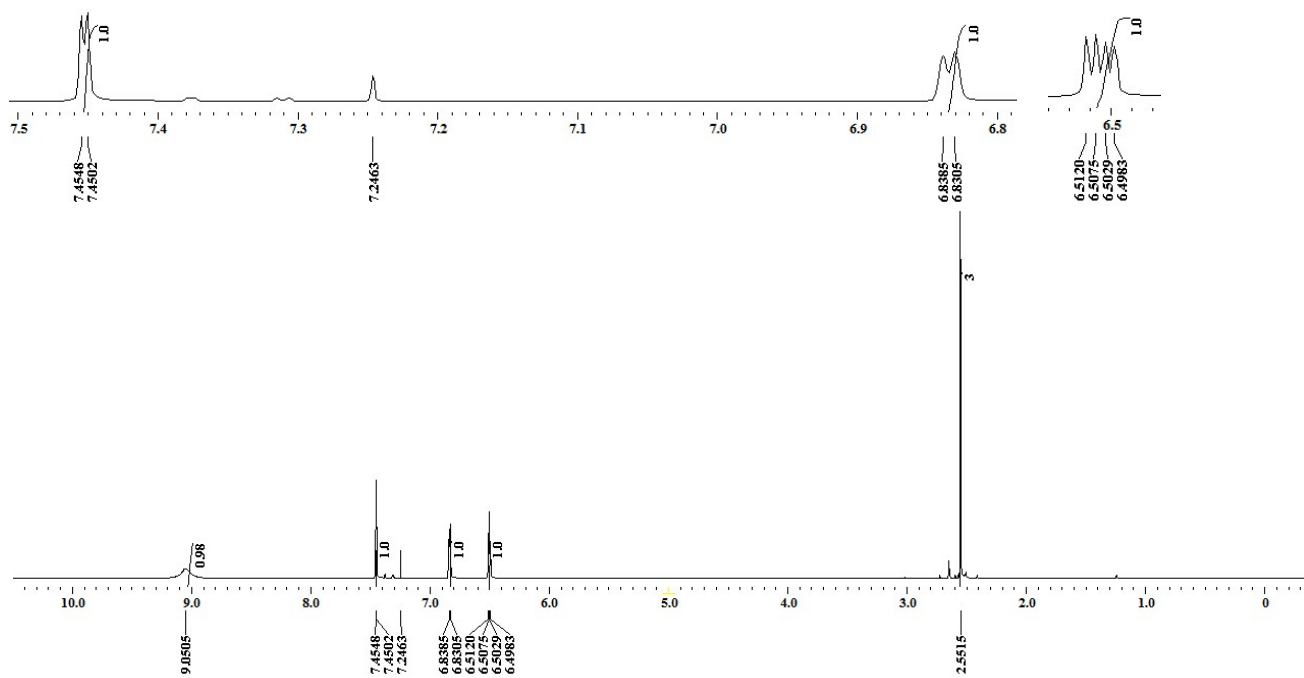
m/z	z	Abund	Formula	Ion
265.0082	1	22043.51	C9 H7 F3 N2 S2	(M+H)+
266.0107	1	2720.37	C9 H7 F3 N2 S2	(M+H)+
267.0055	1	2392.42	C9 H7 F3 N2 S2	(M+H)+
268.0078	1	207.89	C9 H7 F3 N2 S2	(M+H)+

--- End Of Report ---

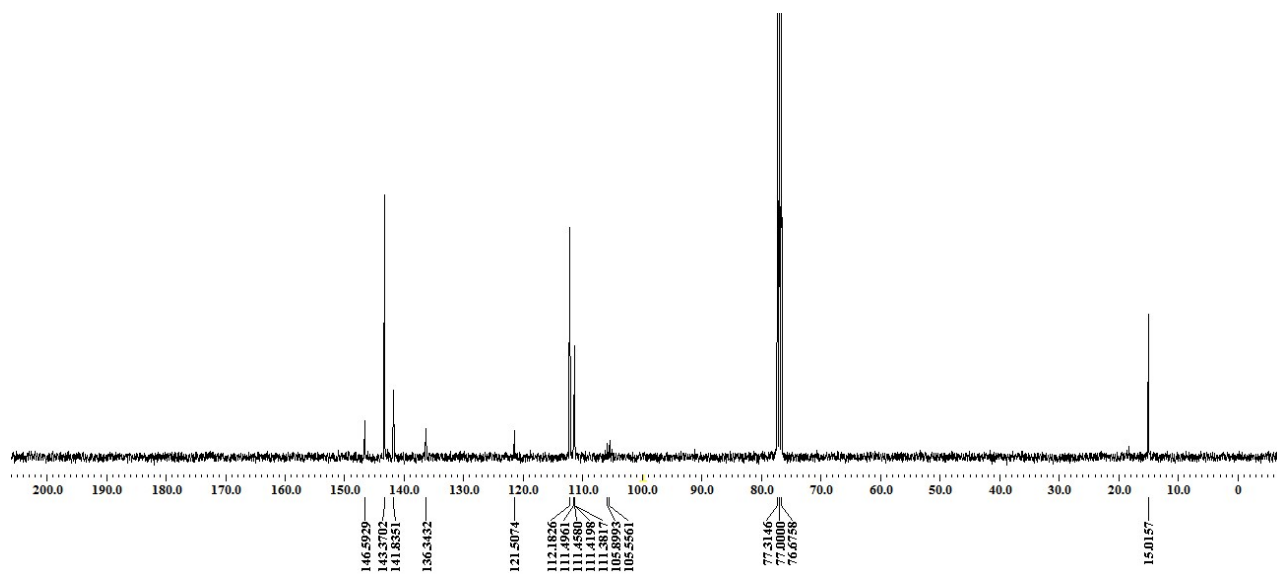


4k

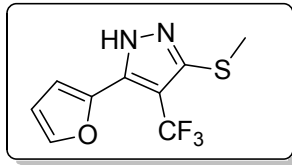
<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)







4k

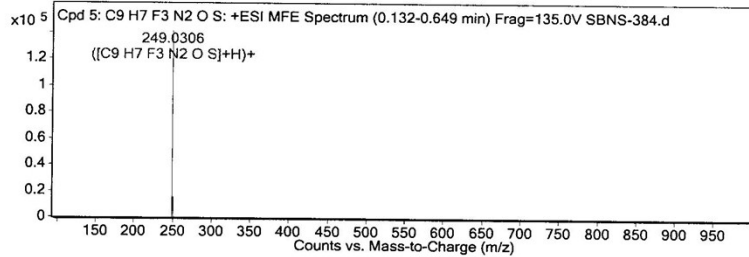
**Data File** SBNS-384.d **Sample Name** SBNS-384  
**Sample Type** Sample **Position** P2F9  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**  
**Sample Group** **Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

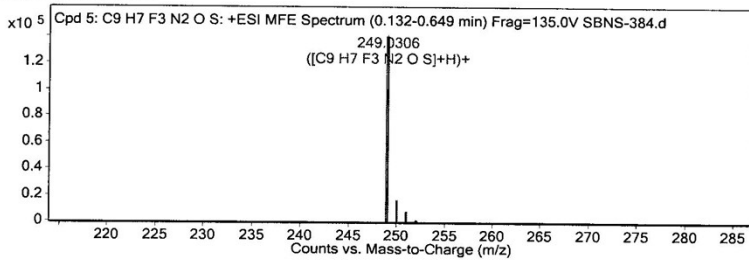
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C9 H7 F3 N2 O S	0.202	248.0233	C9 H7 F3 N2 O S	C9 H7 F3 N2 O S	-0.9	C9 H7 F3 N2 O S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 5: C9 H7 F3 N2 O S	249.0306	0.202	Find by Molecular Feature	248.0233

**MFE MS Spectrum**



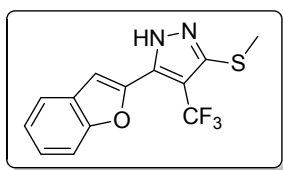
**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

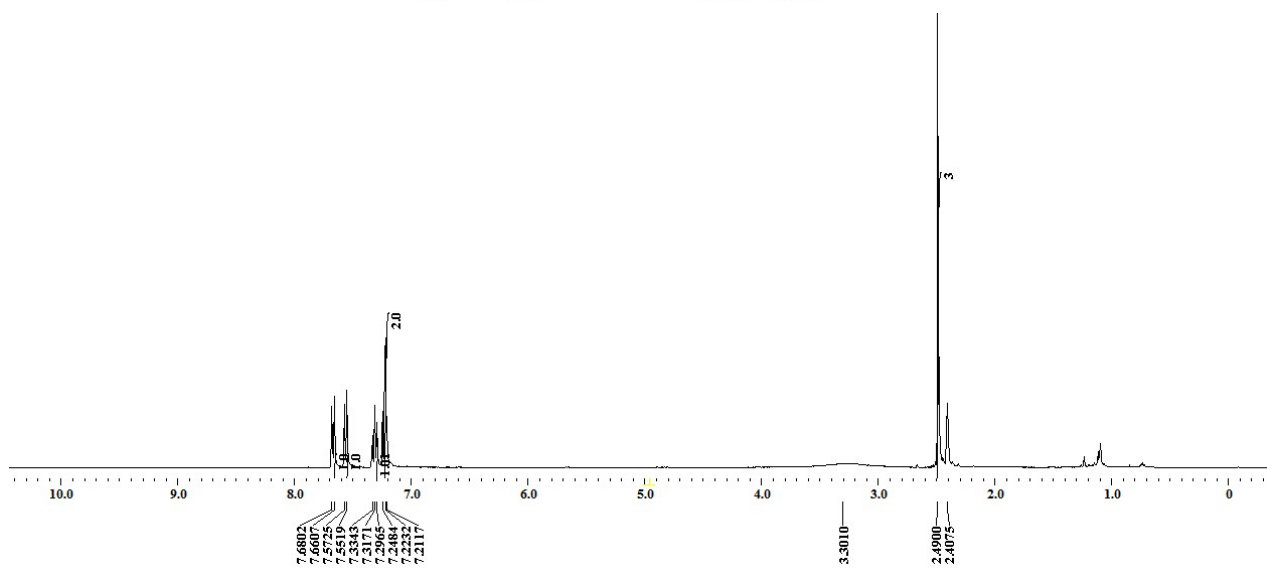
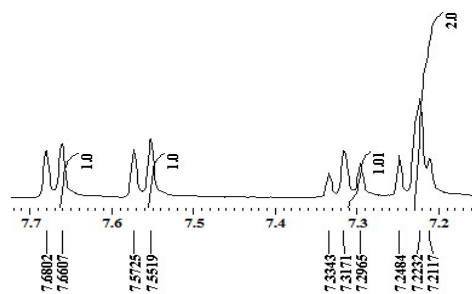
m/z	z	Abund	Formula	Ion
249.0306	1	141447.28	C9 H7 F3 N2 O S	(M+H)+
250.0334	1	15580.35	C9 H7 F3 N2 O S	(M+H)+
251.028	1	6658.76	C9 H7 F3 N2 O S	(M+H)+
252.0311	1	666.46	C9 H7 F3 N2 O S	(M+H)+

--- End Of Report ---

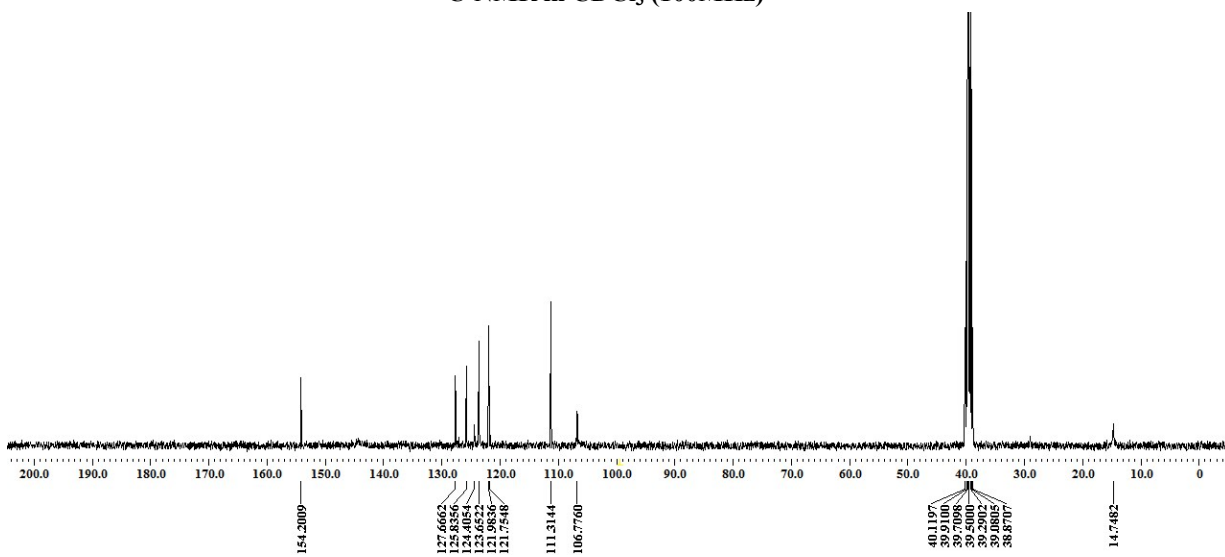


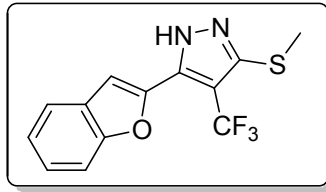
4l

<sup>1</sup>H-NMR in CDCl<sub>3</sub> (400MHz)



<sup>13</sup>C-NMR in CDCl<sub>3</sub> (100MHz)





4I

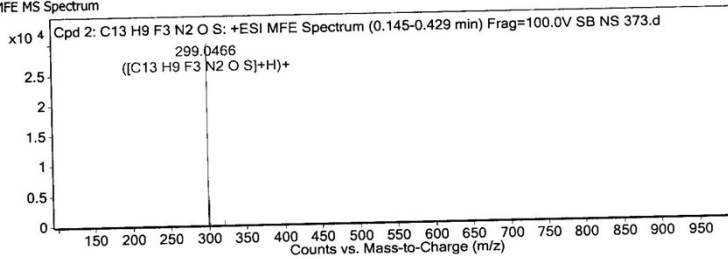
**Data File** SB NS 373.d **Sample Name** SB NS 373  
**Sample Type** Sample **Position** P1E8  
**Instrument Name** Instrument 1 **User Name** lcmsdu-PC\admin  
**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**  
**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125)

**Compound Table**

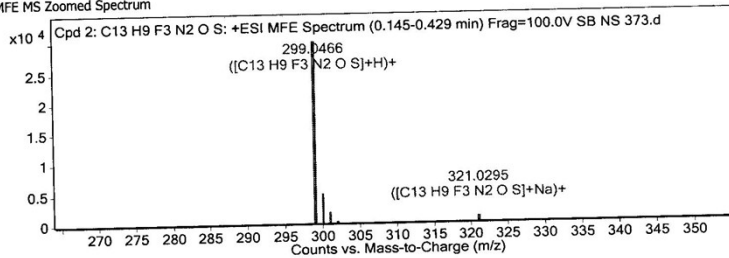
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C13 H9 F3 N2 O S	0.208	298.0394	C13 H9 F3 N2 O S	C13 H9 F3 N2 O S	-2.07	C13 H9 F3 N2 O S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C13 H9 F3 N2 O S	299.0466	0.208	Find by Molecular Feature	298.0394

**MFE MS Spectrum**



**MFE MS Zoomed Spectrum**



**MS Spectrum Peak List**

m/z	z	Abund	Formula	Ion
299.0466	1	30043.73	C13 H9 F3 N2 O S	(M+H)+
300.0498	1	4814.03	C13 H9 F3 N2 O S	(M+H)+
301.0446	1	1909.71	C13 H9 F3 N2 O S	(M+H)+
302.051	1	301.89	C13 H9 F3 N2 O S	(M+H)+
321.0295	1	755.68	C13 H9 F3 N2 O S	(M+Na)+

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