

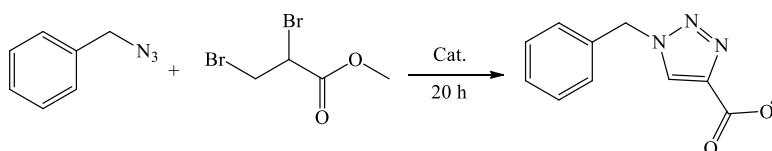
**CATALYTIC CYCLIZATION OF 2,3-DIBROMOPROPIONATES WITH BENZYL AZIDES TO AFFORD 1-BENZYL-1,2,3-TRIAZOLE-4-CARBOXYLATE: THE USE OF A NONTOXIC BISMUTH CATALYST**

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Table S1. The full version of experimental conditions of synthesis of methyl (1-benzyl-1, 2, 3-triazole-4-yl) carboxylate via the cyclization of benzyl azide with methyl 2, 3 -dibromopropionate



Entry	Catalyst	Amount	Temp(°C)	Solvent	Additive	Yield(%)
1	—	—	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	49
2	p-TSA	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	57
3	CuCl	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	40
4	BiCl <sub>3</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	78
5	FeCl <sub>3</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	48
6	AlCl <sub>3</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	43
7	ZnSO <sub>4</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	71
8	ZrOCl <sub>2</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	72
9	SrCl <sub>2</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	52
10	CoSO <sub>4</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	55
11	InCl <sub>3</sub>	5%	80	DMSO	K <sub>2</sub> CO <sub>3</sub>	46
12	BiCl <sub>3</sub>	5%	80	DMSO	—	34
13	BiCl <sub>3</sub>	5%	80	DMSO	Et <sub>3</sub> N	68
14	BiCl <sub>3</sub>	5%	80	DMSO	NaOAc	74

15	BiCl <sub>3</sub>	5%	80	DMF	NaOAc	80
16	BiCl <sub>3</sub>	5%	80	Chlorobenzene	NaOAc	31
17	BiCl <sub>3</sub>	5%	80	Toluene	NaOAc	31
18	BiCl <sub>3</sub>	5%	80	Acetonitrile	NaOAc	63
19	BiCl <sub>3</sub>	5%	80	THF	NaOAc	46
20	BiCl <sub>3</sub>	5%	80	NMP	NaOAc	78
21	BiCl <sub>3</sub>	5%	30	DMF	NaOAc	0
22	BiCl <sub>3</sub>	5%	60	DMF	NaOAc	68
23	BiCl <sub>3</sub>	5%	70	DMF	NaOAc	71
24	BiCl <sub>3</sub>	5%	90	DMF	NaOAc	70
25	BiCl <sub>3</sub>	5%	100	DMF	NaOAc	70
26	BiCl <sub>3</sub>	5%	115	DMF	NaOAc	2
27	BiCl <sub>3</sub>	10%	80	DMF	NaOAc	83
28	BiCl <sub>3</sub>	15%	80	DMF	NaOAc	78

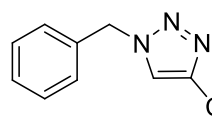
The general synthesis of azides: the synthetic procedure of benzyl azide (**1a**). 5 mmol of benzyl chloride is stirred with 6.5 mmol of sodium azide in 5 mL DMSO at room temperature overnight, then the resulting mixture is poured into water and extracted with ethyl acetate. The benzyl azide is purified on flash chromatography and obtained as a colorless oil.

The general synthesis of 2,3-dibromopropionate: the synthetic procedure of methyl 2, 3-dibromopropionate (**2a**). In a solution of 8.6 g methyl acrylate with 100 mL CCl<sub>4</sub>, the mixture that made of 17.6 g bromine with 40 mL CCl<sub>4</sub> is added dropwise in 12 hours maintaining the temperature in 4~6 °C. The reaction is proceeded for another 12 hours at room temperature and detected by GC. On completion of the reaction, the CCl<sub>4</sub> is removed by rotate evaporator and the desired product is obtained as a pale yellow oil with 96% yield. It is used in the cyclization without further purification.

The general procedure for the determination of LC yield of the 1, 2, 3-triazole: On completion of the reaction, about 10 mg (accurate to 0.2 mg as m<sub>x</sub>) of the reaction mixture is sampled and diluted to 5.0 mL with methanol. The sample is injected to the LC through a 20.0 μL loop and the peak area is recorded as A<sub>x</sub>. The rest of the reaction mixture is worked up, then the desired product purified on column chromatography is identified as the standard sample. About 10 mg (accurate to 0.2 mg as m<sub>s</sub>) of standard sample is dissolved with methanol then constant volume to 50 mL and injected to the LC through a 20.0 μL loop. The peak area is recorded as A<sub>s</sub>. The quantity of product in the reaction sample is calculated through the following equation:  $n = m_s \times (A_x / A_s)$ . The yield is calculated from  $n \times m / m_x$ , while m means the

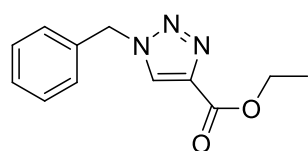
total quality of the reaction mixture.

#### Identification data and Copies of $^1\text{H}$ charts of **3a-3v**



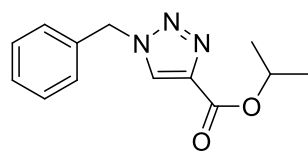
**3a** (Borukhova, Svetlana et al, ChemSusChem, 8(3), 504-512; 2015)

Methyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3a**). m.p. 105.1~107.0 °C  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.973 (s, 1H, NCH=C),  $\delta$  7.409-7.292 (m, 5H, Ar-H),  $\delta$  5.584 (s, 2H, N- $\text{CH}_2$ ),  $\delta$  3.933 (s, 3H,  $\text{OCH}_3$ ).  $^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ )  $\delta$  161.01, 140.25, 133.56, 129.27, 129.12, 128.22, 127.28, 54.43, 52.12; Ft-IR (KBr):  $\nu$  = 1725, 1230 ( $\text{CO}_2\text{Me}$ ). MS (ESI) m/z: 218( $[\text{M}+\text{H}]^+$ ).



**3b** (Ozkal, Erhan et al, Advanced Synthesis & Catalysis, 356(4), 857-869; 2014)

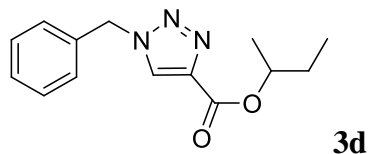
Ethyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3b**). m.p. 90.0~90.5 °C  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.966 (s, 1H, NCH=C),  $\delta$  7.413-7.290 (m, 5H, Ar-H),  $\delta$  5.582 (s, 2H, N- $\text{CH}_2$ ),  $\delta$  4.405 (q,  $J$  = 7.2 Hz, 2H,  $\text{OCH}_2$ ),  $\delta$  1.391 (t,  $J$  = 7.2 Hz, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  160.69, 140.62, 133.80, 129.30, 129.11, 128.26, 127.35, 61.28, 54.44, 14.30. Ft-IR (KBr):  $\nu$  = 1717, 1228 ( $\text{CO}_2$   $\text{CH}_2$ ). MS (ESI) m/z: 232( $[\text{M}+\text{H}]^+$ ).



**3c** (1205237-17-7)

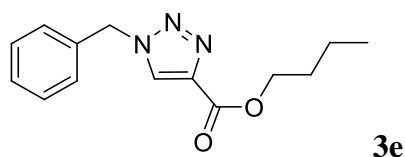
Isopropyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3c**). m.p. 119.0~120.9 °C  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.945 (s, 1H, NCH=C),  $\delta$  7.406-7.289 (m, 5H, Ar-H),  $\delta$  5.577 (s, 2H, N- $\text{CH}_2$ ),  $\delta$  5.282 (heptet,  $J$  = 6.6 Hz, 1H, OCH),  $\delta$  1.370 (d,  $J$  = 6.6 Hz, 6H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  160.29, 141.04, 133.79, 129.33, 129.14, 128.27, 127.17, 69.03, 54.46, 21.87. Ft-IR (KBr):  $\nu$  = 1722, 1216 ( $\text{CO}_2\text{CH}$ ). MS (ESI)

m/z: 246([M+H]<sup>+</sup>).



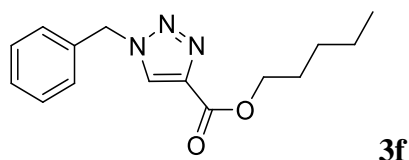
sec-Butyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3d**). m.p. 76.8~77.9 °C

<sup>1</sup>H-NMR(600 MHz, CDCl<sub>3</sub>): δ 7.948 (s, 1H, NCH=C), δ 7.408-7.294 (m, 5H, Ar-H), δ 5.579 (s, 2H, N-CH<sub>2</sub>), δ 5.144-5.092 (m, 1H, OCH), δ 1.800-1.612 (m, 2H, CH<sub>2</sub>), δ 1.334 (d, *J*= 6.6, 3H, CH-CH<sub>3</sub>), δ 0.946 (t, *J*= 6.6, 3H, CH<sub>2</sub>-CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 160.45, 140.98, 133.83, 129.31, 129.11, 128.26, 127.18, 73.54, 54.44, 28.82, 19.54, 9.84. Ft-IR (KBr): ν = 1717, 1211 (CO<sub>2</sub>CH). MS(ESI) m/z: 260 ([M+H]<sup>+</sup>); HRMS: calcd. for C<sub>14</sub>H<sub>18</sub>N<sub>3</sub>O<sub>2</sub> (M+H<sup>+</sup>) 260.1394; found 260.1390



Butyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3e**). m.p. 106.0~107.5 °C

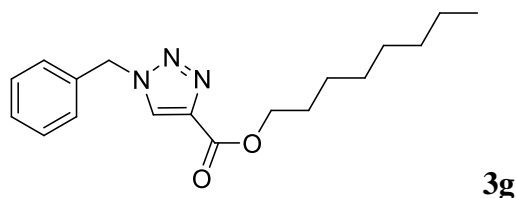
<sup>1</sup>H-NMR(600 MHz, CDCl<sub>3</sub>): δ 7.961 (s, 1H, NCH=C), δ 7.421-7.291 (m, 5H, Ar-H), δ 5.581 (s, 2H, N-CH<sub>2</sub>), δ 4.342 (t, *J*= 7.2, 2H, OCH<sub>2</sub>), δ 1.768-1.720 (m, 2H, CH<sub>2</sub>), δ 1.455-1.417 (m, 2H, CH<sub>2</sub>), δ 0.961-0.936 (t, *J*= 7.8 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 160.81, 140.67, 133.76, 129.33, 129.15, 128.27, 127.25, 65.16, 54.48, 30.67, 19.11, 13.71. Ft-IR (KBr): ν = 1722, 1217 (CO<sub>2</sub>CH<sub>2</sub>). MS (ESI) m/z: 260([M+H]<sup>+</sup>); HRMS: calcd. for C<sub>14</sub>H<sub>18</sub>N<sub>3</sub>O<sub>2</sub> (M+H<sup>+</sup>) 260.1394; found 260.1388



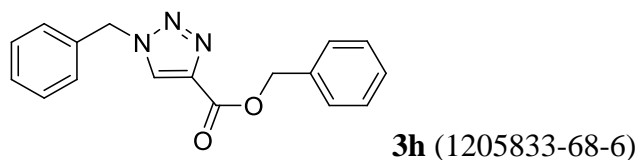
Pentyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3f**). m.p. 63.3~64.1 °C

<sup>1</sup>H-NMR(600 MHz, CDCl<sub>3</sub>): δ 7.961 (s, 1H, NCH=C), δ 7.406-7.291 (m, 5H, Ar-H), δ 5.582 (s, 2H, N-CH<sub>2</sub>), δ 4.331 (t, *J*= 7.2 Hz, 2H, OCH<sub>2</sub>), δ 1.786-1.739 (m, 2H, CH<sub>2</sub>), δ 1.409-1.325 (m, 4H, CH<sub>2</sub>-CH<sub>2</sub>), δ 0.903 (t, *J*= 6.6 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150

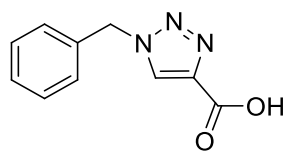
MHz, CDCl<sub>3</sub>)  $\delta$  160.80, 140.73, 133.75, 129.33, 129.16, 128.27, 127.25, 65.45, 54.48, 28.35, 27.99, 22.32, 13.94. Ft-IR (KBr):  $\nu$  = 1722, 1231 (CO<sub>2</sub>CH<sub>2</sub>). MS (ESI) m/z: 274([M+H]<sup>+</sup>); HRMS: calcd. for C<sub>15</sub>H<sub>20</sub>N<sub>3</sub>O<sub>2</sub> (M+H<sup>+</sup>) 274.1550; found 274.1556



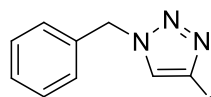
n-Octyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3g**). m.p. 86.4~87.2 °C  
<sup>1</sup>H-NMR(600 MHz, CDCl<sub>3</sub>):  $\delta$  7.959 (s, 1H, NCH=C),  $\delta$  7.412-7.291 (m, 5H, Ar-H),  $\delta$  5.581 (s, 2H, N-CH<sub>2</sub>),  $\delta$  4.328 (t,  $J$  = 7.2 Hz, 2H, OCH<sub>2</sub>),  $\delta$  1.778-1.730 (m, 2H, CH<sub>2</sub>),  $\delta$  1.390-1.257 (m, 10H, CH<sub>2</sub>),  $\delta$  0.872 (t,  $J$  = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  160.81, 140.69, 133.74, 129.34, 129.17, 128.28, 127.23, 65.49, 54.49, 31.77, 29.21, 29.15, 28.65, 25.87, 22.63, 14.08. Ft-IR (KBr):  $\nu$  = 1722, 1208 (CO<sub>2</sub>CH<sub>2</sub>). MS(ESI) m/z: 316([M+H]<sup>+</sup>); HRMS: calcd. for C<sub>18</sub>H<sub>26</sub>N<sub>3</sub>O<sub>2</sub> (M+H<sup>+</sup>) 316.2020; found 316.2025



Benzyl 1-benzyl-1H-1, 2, 3-triazole-4-carboxylate (**3h**). m.p. 136.6~137.7 °C  
<sup>1</sup>H-NMR(600 MHz, CDCl<sub>3</sub>):  $\delta$  7.958 (s, 1H, NCH=C),  $\delta$  7.438-7.273 (m, 10H, Ar-H),  $\delta$  5.564 (s, 2H, N-CH<sub>2</sub>),  $\delta$  5.371 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  160.48, 140.31, 135.42, 133.64, 129.34, 129.19, 128.61, 128.60, 128.46, 128.28, 127.41, 66.88, 54.51. Ft-IR (KBr):  $\nu$  = 1716, 1217 (CO<sub>2</sub>CH<sub>2</sub>). MS(ESI) m/z: 294([M+H]<sup>+</sup>)

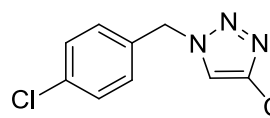


1-Benzyl-1H-1, 2, 3-triazole-4-carboxylic acid (**3i**). m.p. 176.3~180.1 °C  
<sup>1</sup>H-NMR(600 MHz, CDCl<sub>3</sub>): δ 8.035 (s, 1H, NCH=C), δ 7.421-7.308 (m, 5H, Ar-H),  
δ 5.598 (s, 2H, N-CH<sub>2</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 161.99, 140.28, 135.97,  
129.40, 129.20, 128.67, 128.39, 53.40. Ft-IR (KBr): ν = 1684, 946 (CO<sub>2</sub>H). MS (ESI)  
m/z: 204([M+H]<sup>+</sup>).



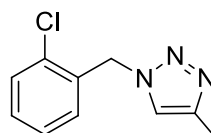
**3j** (Roque, Dario R. et al, Synthesis, (15), 2497-2502; 2005)

1-Benzyl-1H-1, 2, 3-triazole-4-carbonitrile (**3j**). m.p. 80.0~81.2 °C <sup>1</sup>H-NMR (600  
MHz, CDCl<sub>3</sub>): δ 7.852 (s, 1H, NCH=C), δ 7.347-7.192 (m, 5H, Ar-H), δ 5.527 (s, 2H,  
N-CH<sub>2</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 132.92, 129.52, 129.50, 129.32, 128.40,  
121.48, 111.37, 54.87. Ft-IR (KBr): ν = 2240 (CN), MS (ESI) m/z: 185([M+H]<sup>+</sup>)



**3k** (Abu-Orabi, Sultan T. et al, Gazzetta Chimica Italiana,  
122(1), 29-33; 1992)

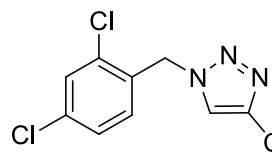
Methyl 1-(4-chlorobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3k**), m.p. 130.0~131.9  
°C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.995 (s, 1H, NCH=C), 7.377 (d, *J*=8.4 Hz, 2H),  
7.237 (d, *J*= 8.4 Hz, 2H), 5.558 (s, 2H, N-CH<sub>2</sub>), 3.935 (s, 3H, OCH<sub>3</sub>). Ft-IR (KBr):  
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 160.89, 140.40, 135.25, 132.08, 129.50, 129.49,  
127.22, 53.67, 52.18. ν = 1724, 1216 (CO<sub>2</sub>CH<sub>3</sub>). MS (ESI) m/z: 252 ([M+H]<sup>+</sup>)



**3l** (Abu-Orabi, Sultan T. et al, Gazzetta Chimica Italiana,  
122(1), 29-33; 1992)

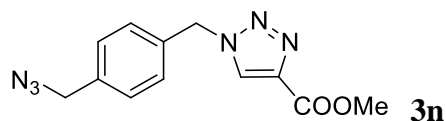
Methyl 1-(2-chlorobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3l**), m.p. 100.8~101.6  
°C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.075 (s, 1H, NCH=C), 7.468 –7.294 (m,4H),  
5.718 (s, 2H, N-CH<sub>2</sub>), 3.938 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 161.07, 140.16,

133.81, 131.49, 130.82, 130.79, 130.17, 127.79, 127.67, 52.23, 51.84. Ft-IR (KBr):  $\nu = 1720, 1220$  (CO<sub>2</sub>CH<sub>3</sub>). MS (ESI) m/z: 252 ([M+H]<sup>+</sup>).

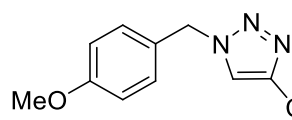


**3m** (Abu-Orabi, Sultan T. et al, Jordan Journal of Chemistry, 3(4), 337-347; 2008)

Methyl 1-(2,4-dichlorobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3m**), m.p. 120.5~121.1 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.084 (s, 1H, NHC=C), 7.485 (d,  $J=2.4$  Hz, 1H, Ar-H), 7.295 (dd,  $J = 8.4$  Hz, 1.8 Hz, 1H, Ar-H), 7.230 (d,  $J = 8.4$  Hz, 1H, Ar-H), 5.681 (s, 2H, CH<sub>2</sub>), 3.944 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  160.96, 140.34, 136.21, 134.47, 131.57, 130.13, 130.05, 128.16, 127.61, 52.29, 51.20. Ft-IR (KBr):  $\nu = 1725, 1224$  (CO<sub>2</sub>CH<sub>3</sub>). MS (ESI) m/z: 286 ([M+H]<sup>+</sup>)



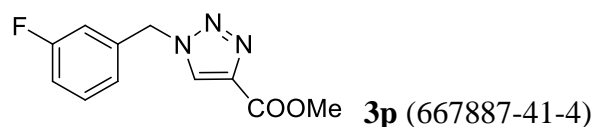
Methyl 1-(4-(azidomethyl)benzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3n**), m.p. 94.3~95.8 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.994 (s, 1H; NHC=C), 7.358 (d,  $J = 7.8$  Hz, 2H; Ar-H), 7.313 (d,  $J = 8.4$  Hz, 2H; Ar-H), 5.539 (s, 2H; N-CH<sub>2</sub>), 4.369 (s, 2H; N<sub>3</sub>-CH<sub>2</sub>), 3.934 (s, 3H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  160.95, 140.32, 136.59, 133.66, 128.96, 128.64, 127.27, 54.11, 54.01, 52.16. Ft-IR (KBr):  $\nu = 2098$  (N<sub>3</sub>), 1727, 1236, (CO<sub>2</sub>Me). MS (ESI) m/z: 295 ([M+Na]<sup>+</sup>); HRMS: calcd. for C<sub>12</sub>H<sub>13</sub>N<sub>6</sub>O<sub>2</sub> (M+H<sup>+</sup>) 273.1095; found 273.1097



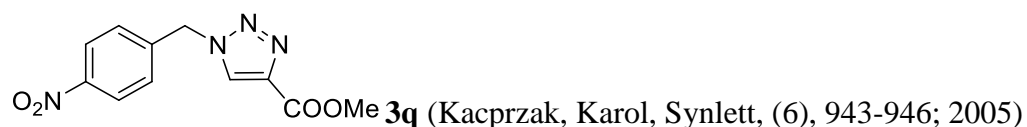
**3o** (Abu-Orabi, Sultan T. et al, Gazzetta Chimica Italiana, 122(1), 29-33; 1992)

Methyl 1-(4-methoxybenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3o**), m.p. 136.2~137.3 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.938 (s, 1H; NHC=C), 7.264 (d,  $J = 8.4$  Hz, 2H; Ar-H), 6.916 (d,  $J = 8.4$  Hz, 2H; Ar-H), 5.510 (s, 2H; CH<sub>2</sub>), 3.921 (s, 3H;

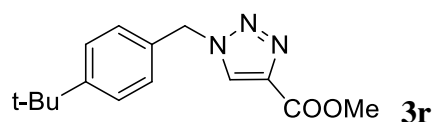
CH<sub>3</sub>), 3.817 (s, 3H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 161.04, 160.15, 140.11, 129.85, 127.07, 125.46, 114.61, 55.29, 53.98, 52.09. Ft-IR (KBr): ν = 1722, 1209, (CO<sub>2</sub>Me). MS (ESI) m/z: 270 ([M+Na]<sup>+</sup>).



Methyl 1-(3-fluorobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3p**), m.p. 112.4~113.5 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.022 (s, 1H; NHC=C), 7.378 (m, 1H; Ar-H), 7.084 (m, 2H; Ar-H), 6.988 (d, *J* = 9 Hz, 1H; Ar-H), 5.582 (s, 2H; CH<sub>2</sub>), 3.942 (s, 3H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 163.06 (d, *J* = 247.5 Hz), 162.23 (s), 160.99 (s), 140.53 (s), 136.00 (d, *J* = 7.3 Hz), 131.06 (d, *J* = 8.3 Hz), 127.43 (s), 123.77 (s), 116.27 (d, *J* = 20.7 Hz), 115.25 (d, *J* = 22.2 Hz), 53.84 (s), 52.27 (s). Ft-IR (KBr): ν = 1712, 1232, (CO<sub>2</sub>Me). MS (ESI) m/z: 258 ([M+Na]<sup>+</sup>).

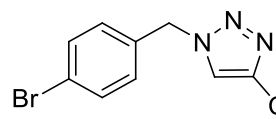


Methyl 1-(4-nitrobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3q**), m.p. 170.5~172.9 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.078 (s, 1H; NHC=C), 8.263 (d, *J* = 8.4 Hz, 2H; Ar-H), 7.442 (d, *J* = 8.4 Hz, 2H; Ar-H), 5.708 (d, 2H; CH<sub>2</sub>), 3.957 (s, 3H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 159.77, 147.34, 139.84, 139.56, 127.77, 125.54, 123.51, 52.41, 51.36. Ft-IR (KBr): ν = 1720, 1186, (CO<sub>2</sub>Me), 1515, 1353 (NO<sub>2</sub>), MS (ESI) m/z: 263 ([M+H]<sup>+</sup>).



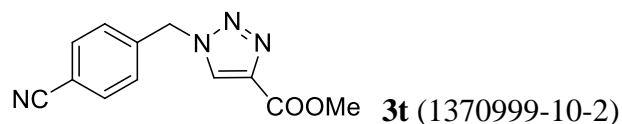
Methyl 1-(4-tert-butylbenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3r**), m.p. 122.8~124.2 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.965 (s, 1H; NHC=C), 7.414 (d, *J* = 8.4 Hz, 2H; Ar-H), 7.232 (d, *J* = 8.4 Hz, 2H; Ar-H), 5.541 (s, 2H; CH<sub>2</sub>), 3.928 (s, 3H; CH<sub>3</sub>), 1.318 (s, 9H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 161.17, 152.45, 140.25, 130.54, 128.18, 127.33, 126.29, 54.24, 52.20, 34.71, 31.23. Ft-IR (KBr): ν = 1727, 1209

(CO<sub>2</sub>Me). MS (ESI) m/z: 569 ([2M+Na]). HRMS: calcd. for C<sub>15</sub>H<sub>20</sub>N<sub>3</sub>O<sub>2</sub> (M+H<sup>+</sup>) 274.1550; found 274.1545



**3s** (Abu-Orabi, Sultan T. et al, *Gazzetta Chimica Italiana*, 122(1), 29-33; 1992)

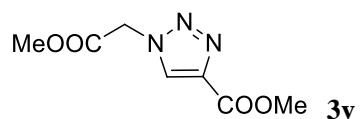
Methyl 1-(4-bromobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3s**). m.p. 141.7~143.2 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.002 (s, 1H; NHC=C), 7.531 (d, *J* = 8.4 Hz, 2H; Ar-H), 7.174 (d, *J* = 8.4 Hz, 2H; Ar-H), 5.544 (s, 2H; CH<sub>2</sub>), 3.933 (s, 3H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 160.88, 140.42, 132.59, 132.46, 129.76, 127.22, 123.37, 53.72, 52.18. Ft-IR (KBr): ν = 1720, 1216 (CO<sub>2</sub>Me). MS (ESI) m/z: 615 ([2M+Na]<sup>+</sup>).



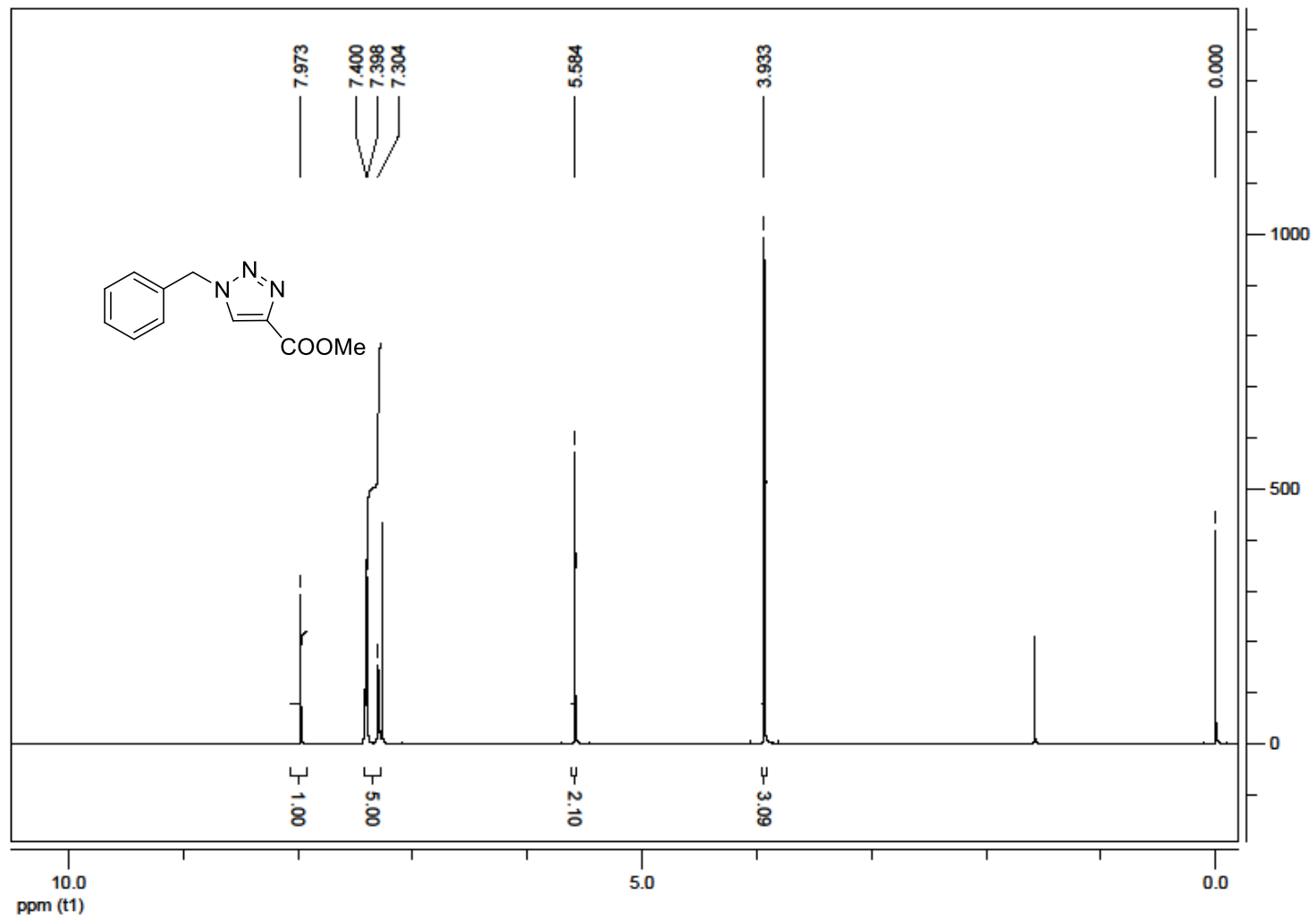
Methyl 1-(4-cyanobenzyl)-1H-1, 2, 3-triazole-4-carboxylate (**3t**). m.p. 80.0~81.2 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.07 (s, 1 H, NHC=C), δ 7.70 (d, 2 H, Ar-H), δ 7.39 (d, 2 H, Ar-H), δ 5.67 (s, 2 H; CH<sub>2</sub>), δ 3.95 (s, 3 H; CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO) δ 160.97, 141.18, 139.28, 133.16, 130.05, 129.19, 118.85, 111.51, 52.89, 52.20. Ft-IR (KBr): ν = 2226 (CN), 1718, 1233 (CO<sub>2</sub>Me). MS (ESI) m/z: 252 ([M+Na]<sup>+</sup>)



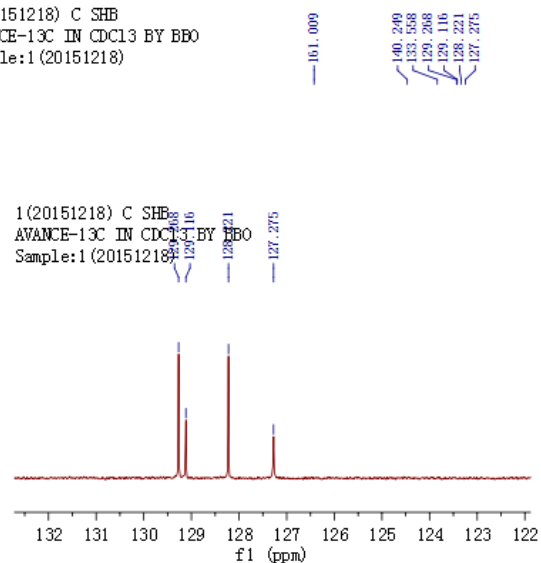
Methyl 1-(pyridin-2-ylmethyl)-1H-1,2,3-triazole-4-carboxylate (**3u**). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.54-8.55 (m, 1 H), δ 8.28 (s, 1 H), δ 8.22-7.27 (m, 3 H), δ 5.66 (s, 2 H), δ 3.88 (s, 3 H). <sup>13</sup>C NMR (150 MHz, DMSO) δ 160.72, 154.33, 149.47, 138.61, 137.39, 130.12, 123.35, 122.21, 54.41, 51.79. Ft-IR (KBr): ν = 1731, 1234 (CO<sub>2</sub>Me), MS (ESI) m/z: 219 ([M+H]<sup>+</sup>)



Methyl 1-(2-methoxy-2-oxoethyl)-1H-1,2,3-triazole-4-carboxylate (**3v**). m.p. 102.4-104.8 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>), δ 8.26 (s, 1 H), δ 5.25 (s, 2 H), δ 3.97 (s, 3 H), δ 3.84 (s, 3 H). <sup>13</sup>C NMR (150 MHz, DMSO) δ 167.69, 160.97, 139.04, 130.88, 53.06, 52.24, 50.95. Ft-IR (KBr): ν = 1750, 1219 (CO<sub>2</sub>Me). HRMS: calcd. for C<sub>7</sub>H<sub>9</sub>N<sub>3</sub>O<sub>4</sub> (M+H<sup>+</sup>) 200.0666; found 200.0667



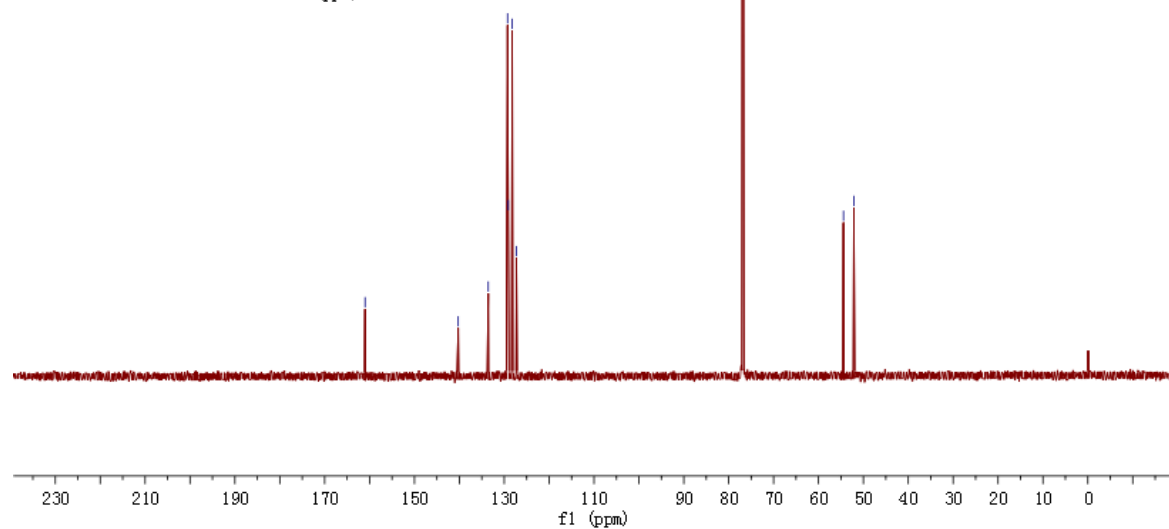
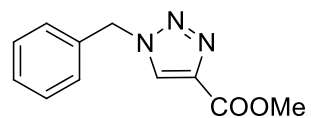
1 (20151218) C SHB  
 AVANCE-13C IN CDCl3 BY BBO  
 Sample:1 (20151218)



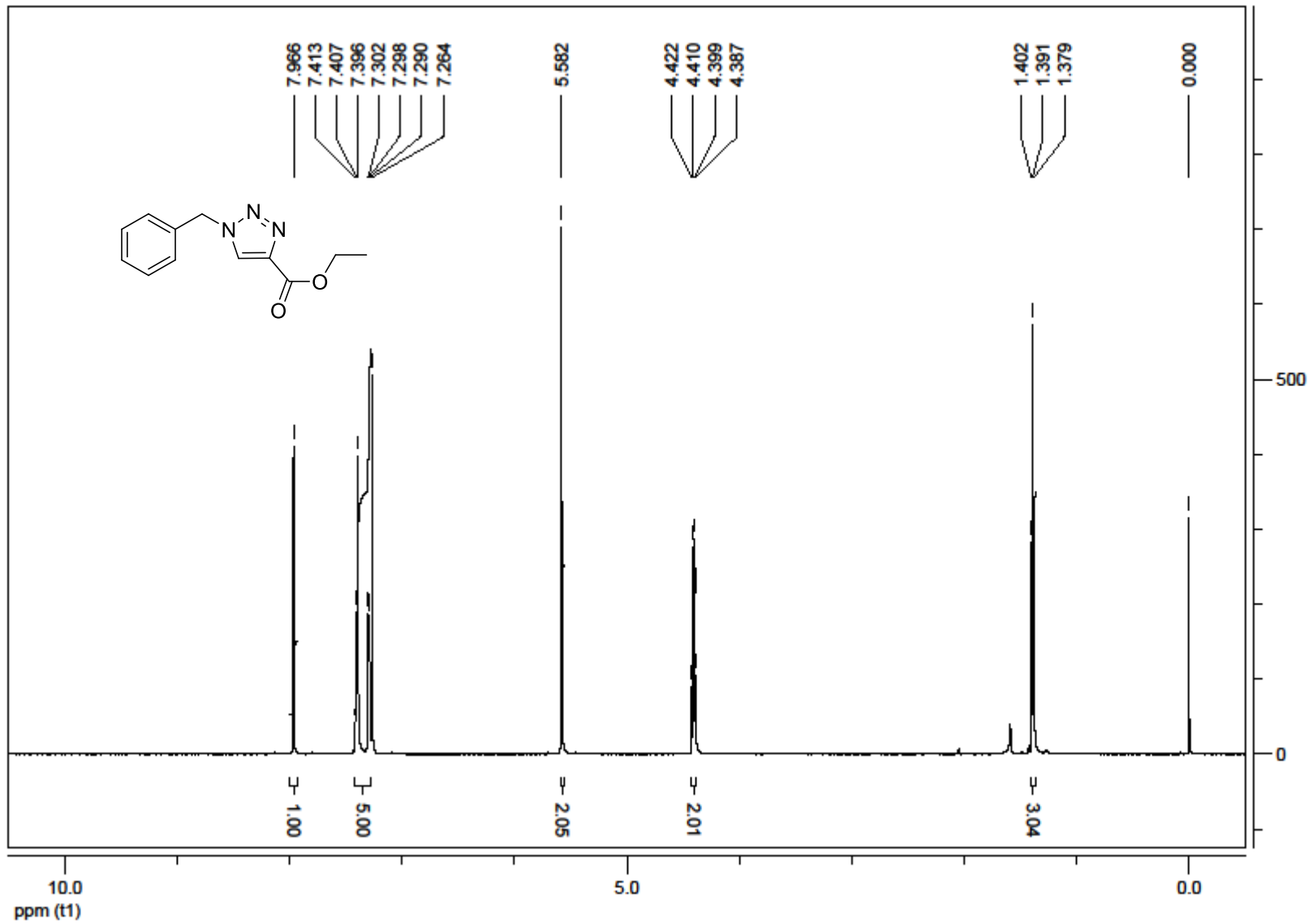
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	275
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-18T14:11:19
19 Modification Date	2015-12-18T14:24:24
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



2 (20151218) C  
 AVANCE-13C IN CDC13 BY BBO  
 Sample:2 (20151218)

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140.615  
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 129.113  
 128.260  
 127.354

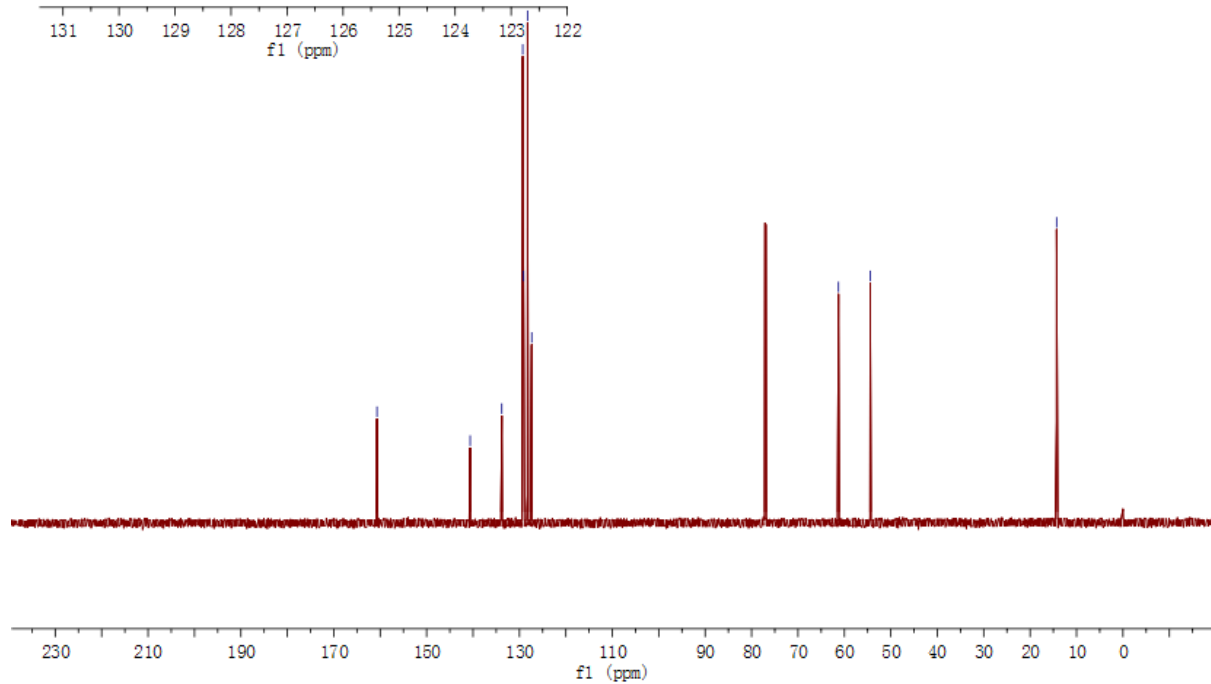
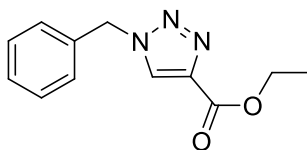
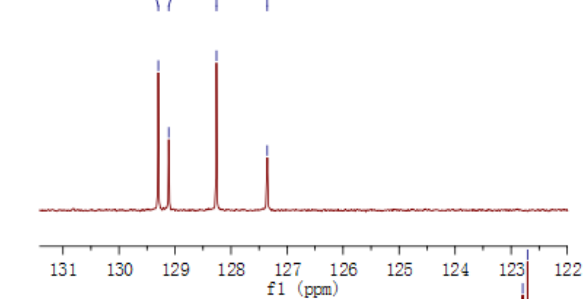
61.277

54.445

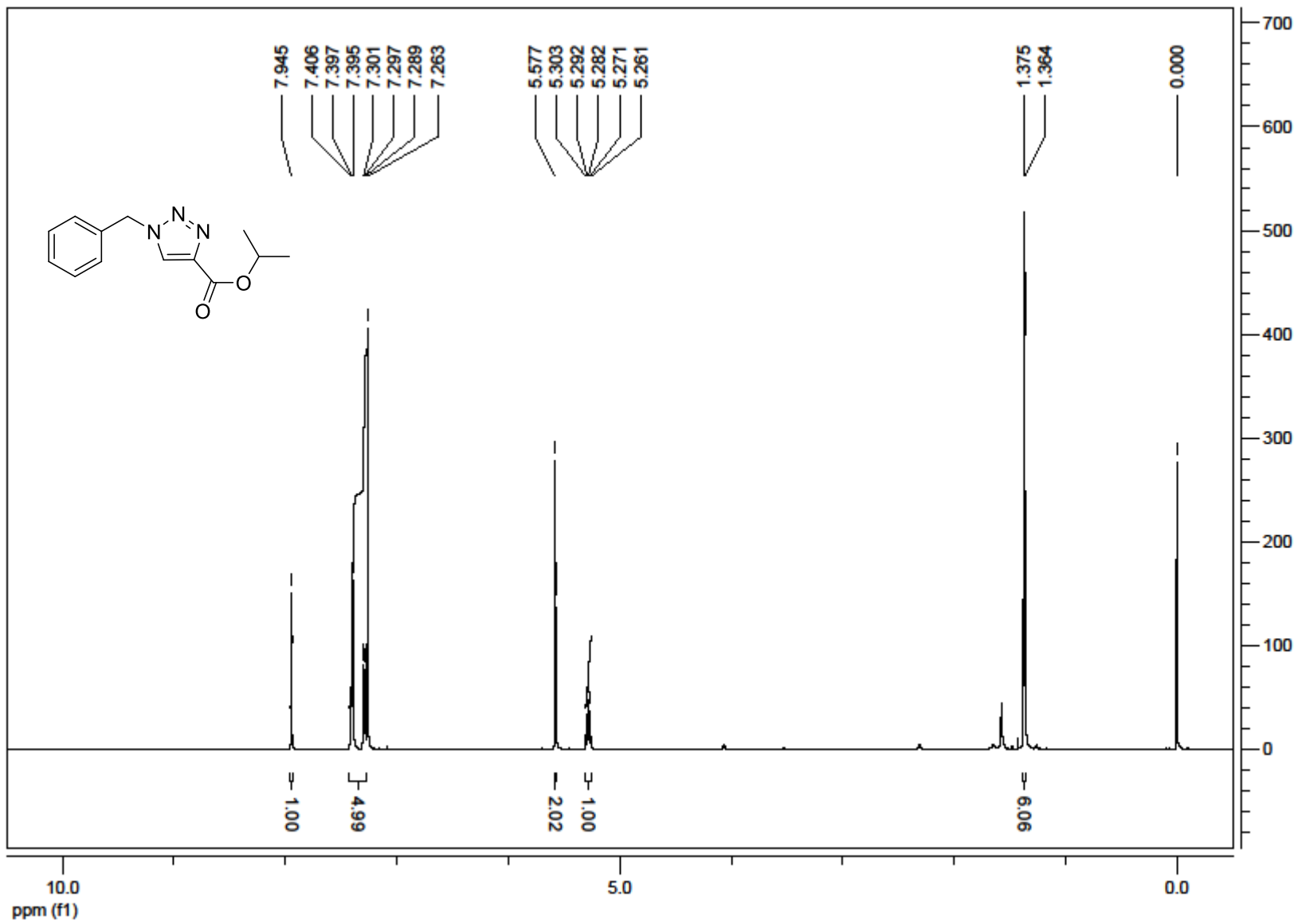
14.295

2 (20151218)  
 AVANCE-13C IN CDC13 BY BBO  
 Sample:2 (20151218)

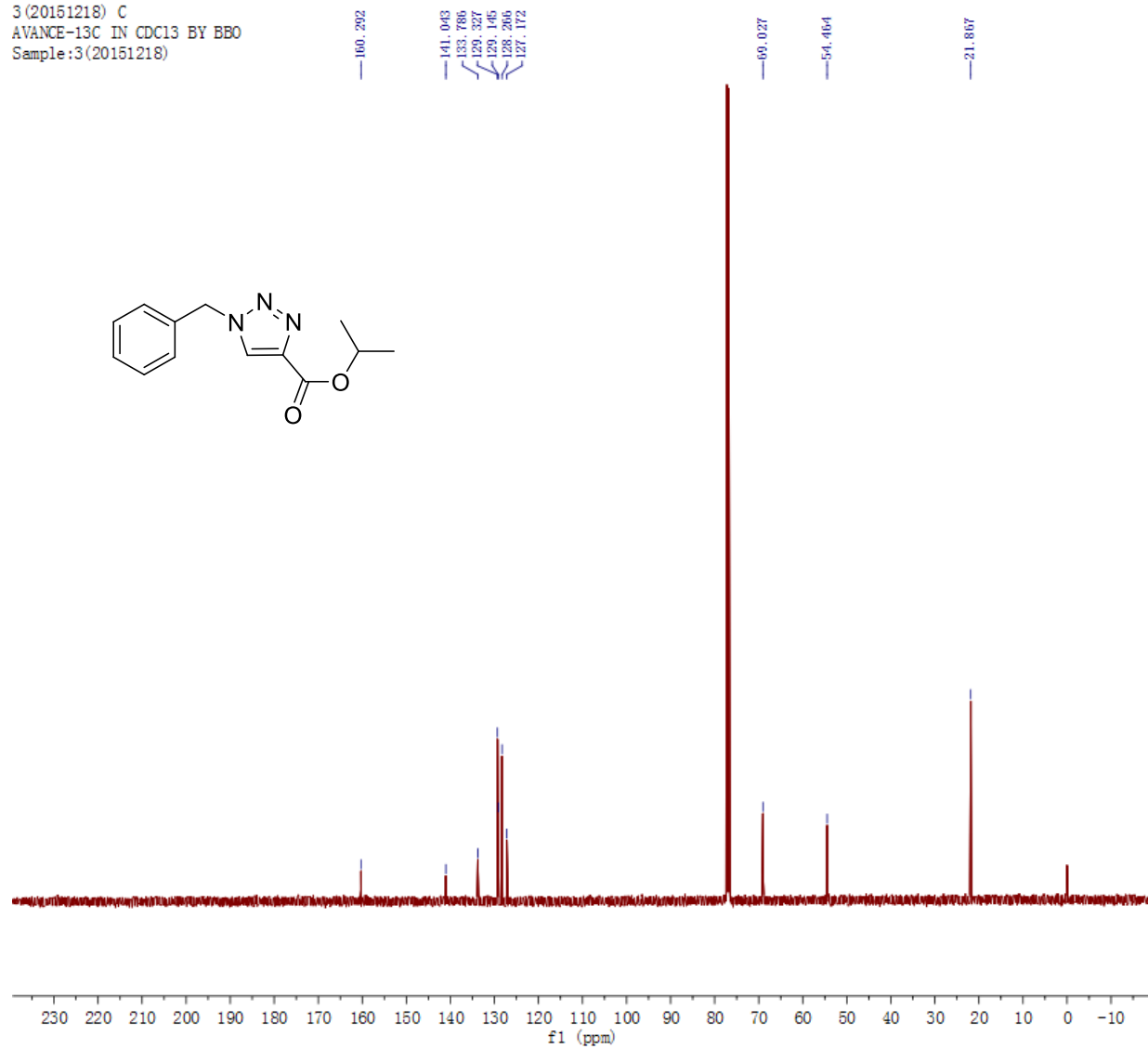
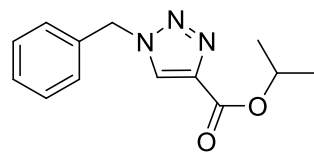
140.615  
 133.802  
 128.260  
 127.354



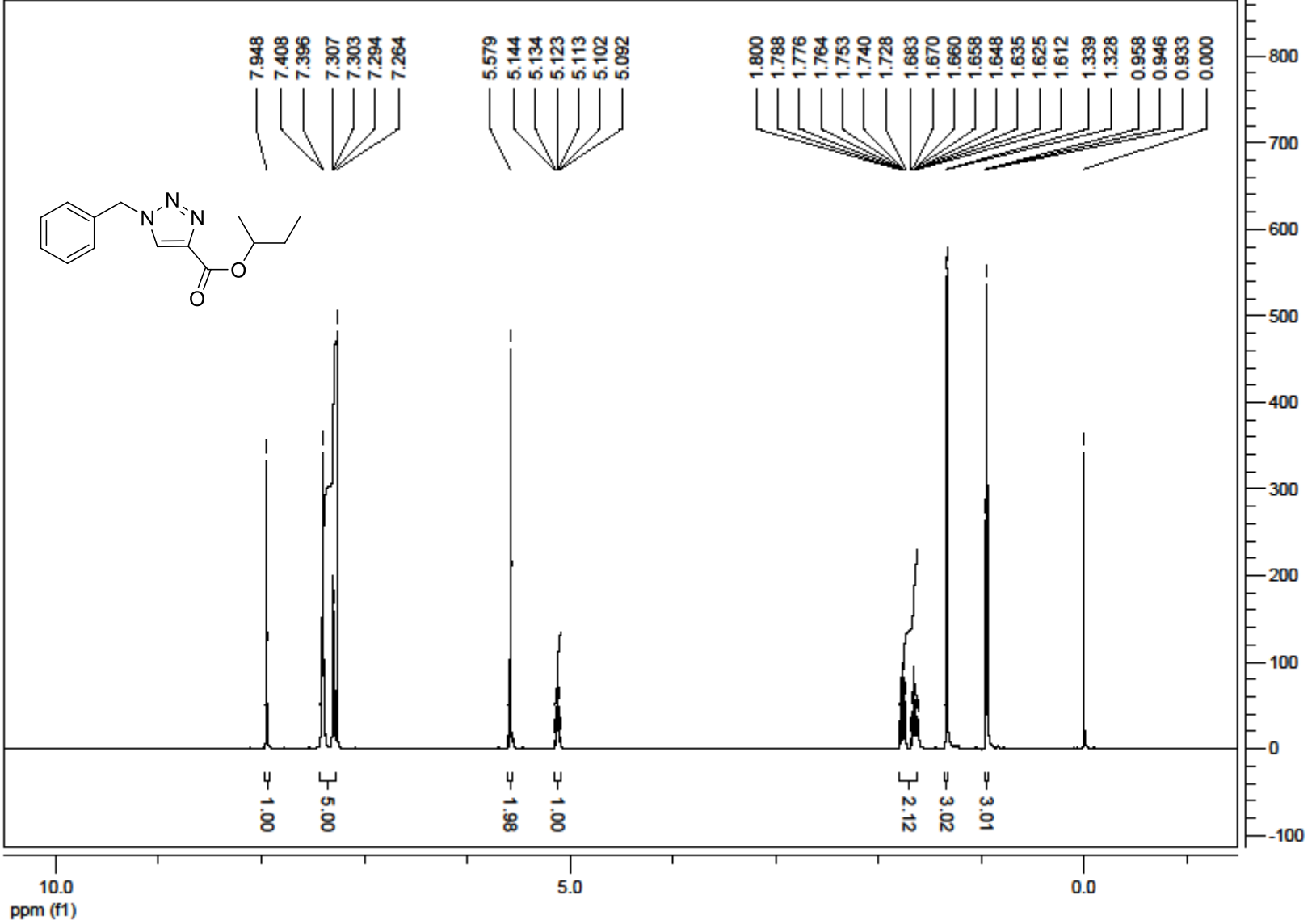
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2 Title	2(20151218) C
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	51
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-18T15:23:37
19 Modification Date	2015-12-18T15:24:56
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2931.9
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



3 (20151218) C  
AVANCE-13C IN CDCl3 BY BBO  
Sample:3 (20151218)



Parameter	Value
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3 Comment	AVANCE-13C IN CDCl3 BY BBO Sample:3 (20151218)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	268
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-18T15:28:27
19 Modification Date	2015-12-18T15:41:12
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21 Spectral Width	39062.5
22 Lowest Frequency	-2933.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

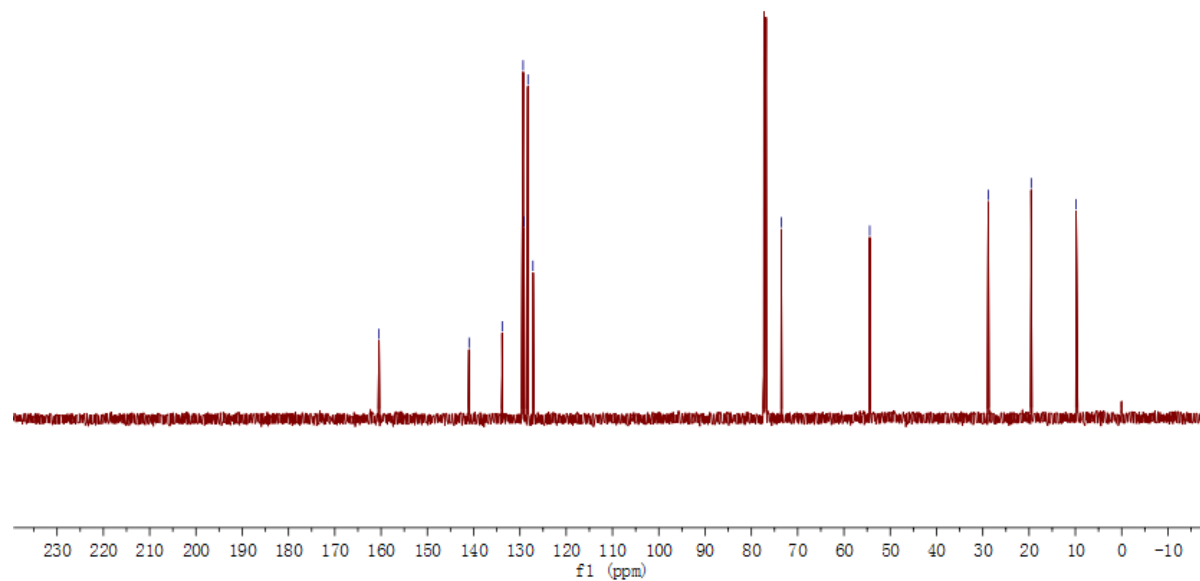
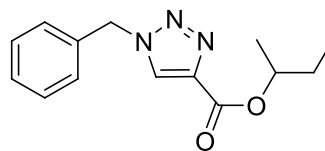
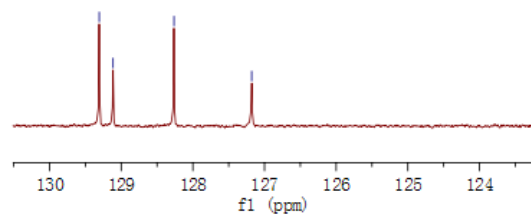


4 (20151218) C  
 AVANCE-13C IN CDC13 BY BBO  
 Sample:4 (20151218)

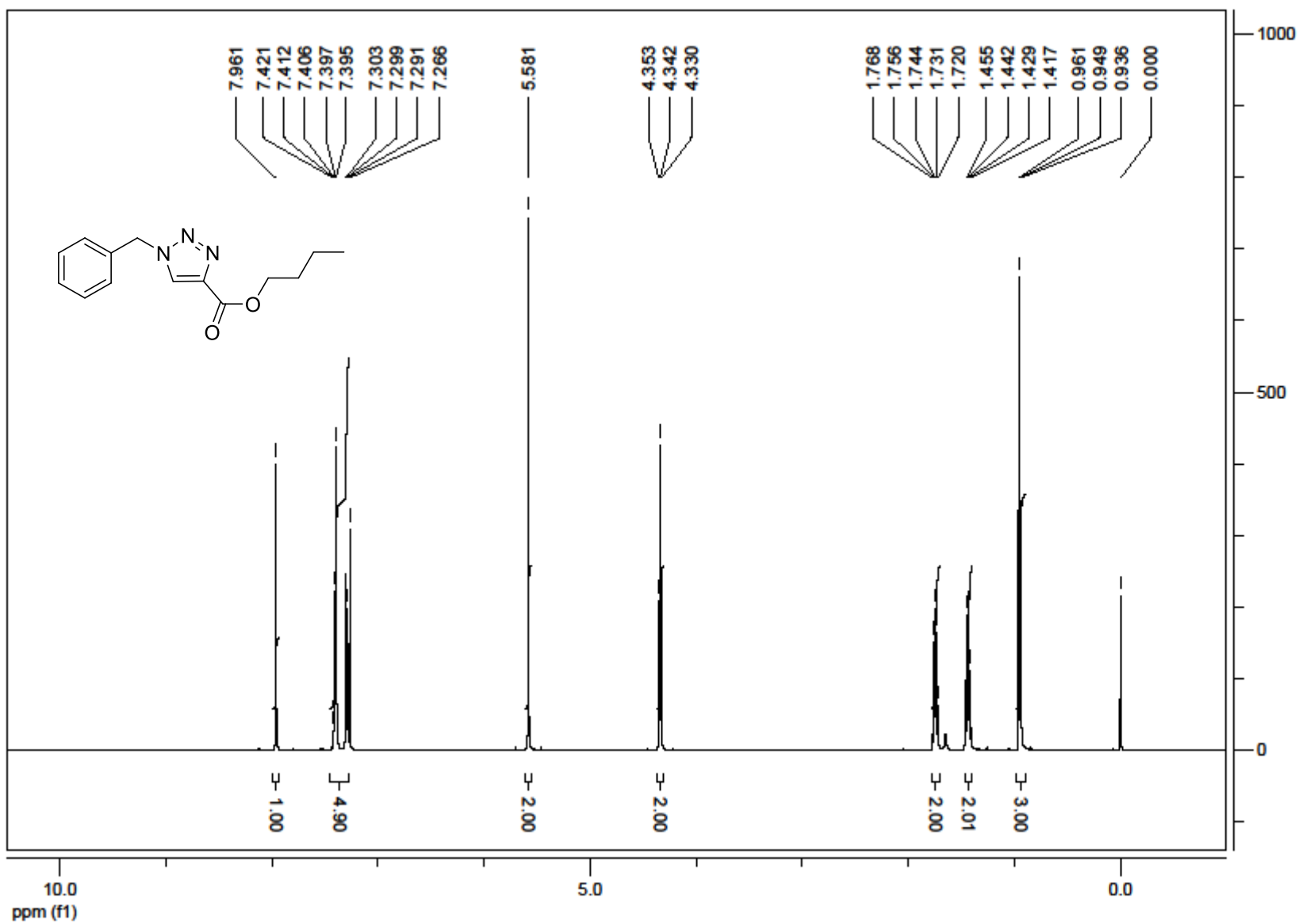
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 129.306  
 129.113  
 128.263  
 127.179  
 73.536  
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 19.544  
 -0.838

4 (20151218) C  
 AVANCE-13C IN CDC13 BY BBO  
 Sample:4 (20151218)

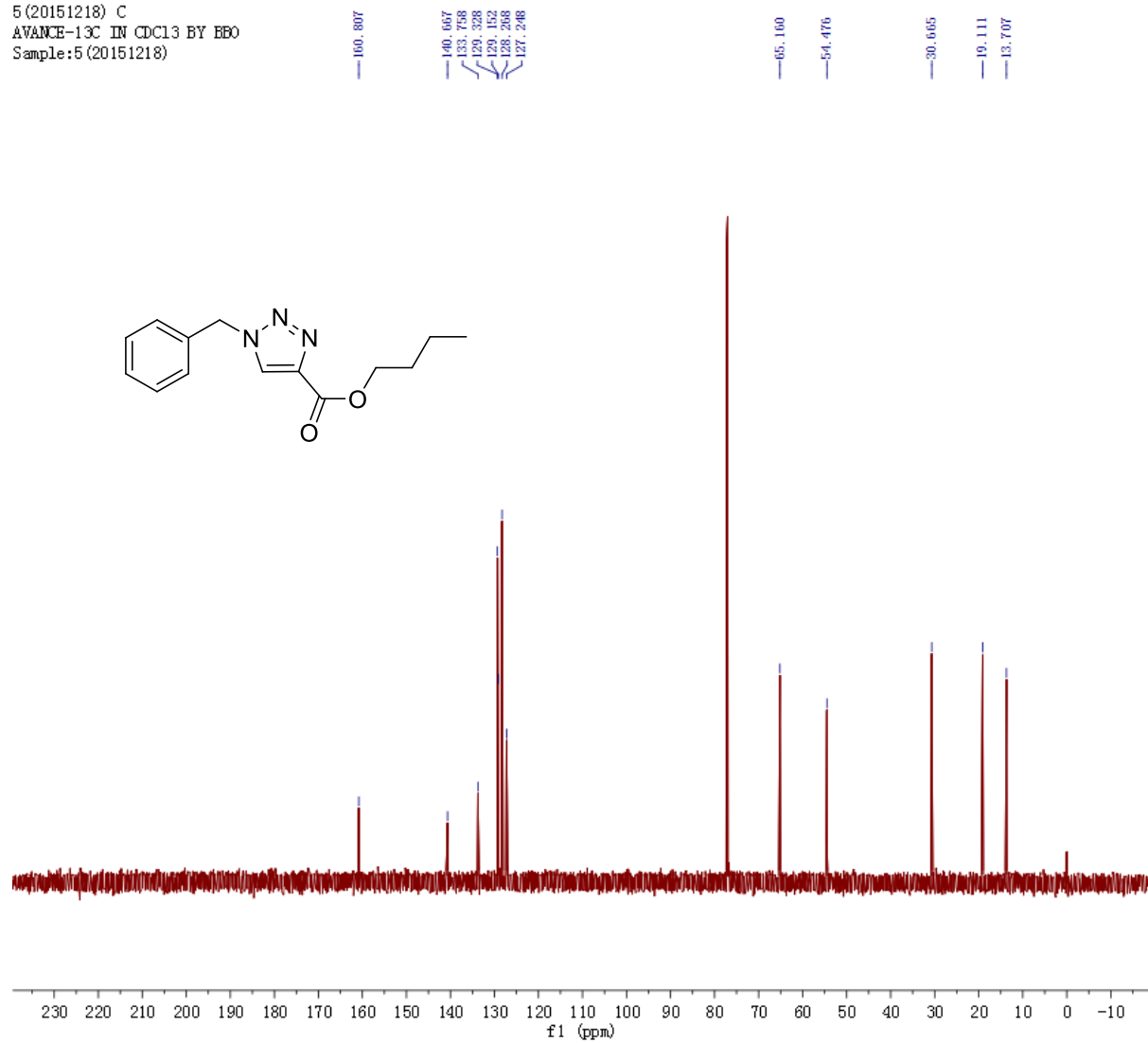
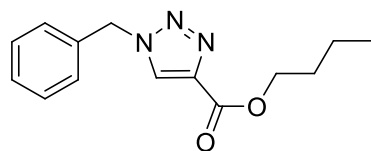
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 140.983  
 133.832  
 129.306  
 129.113  
 128.263  
 127.179



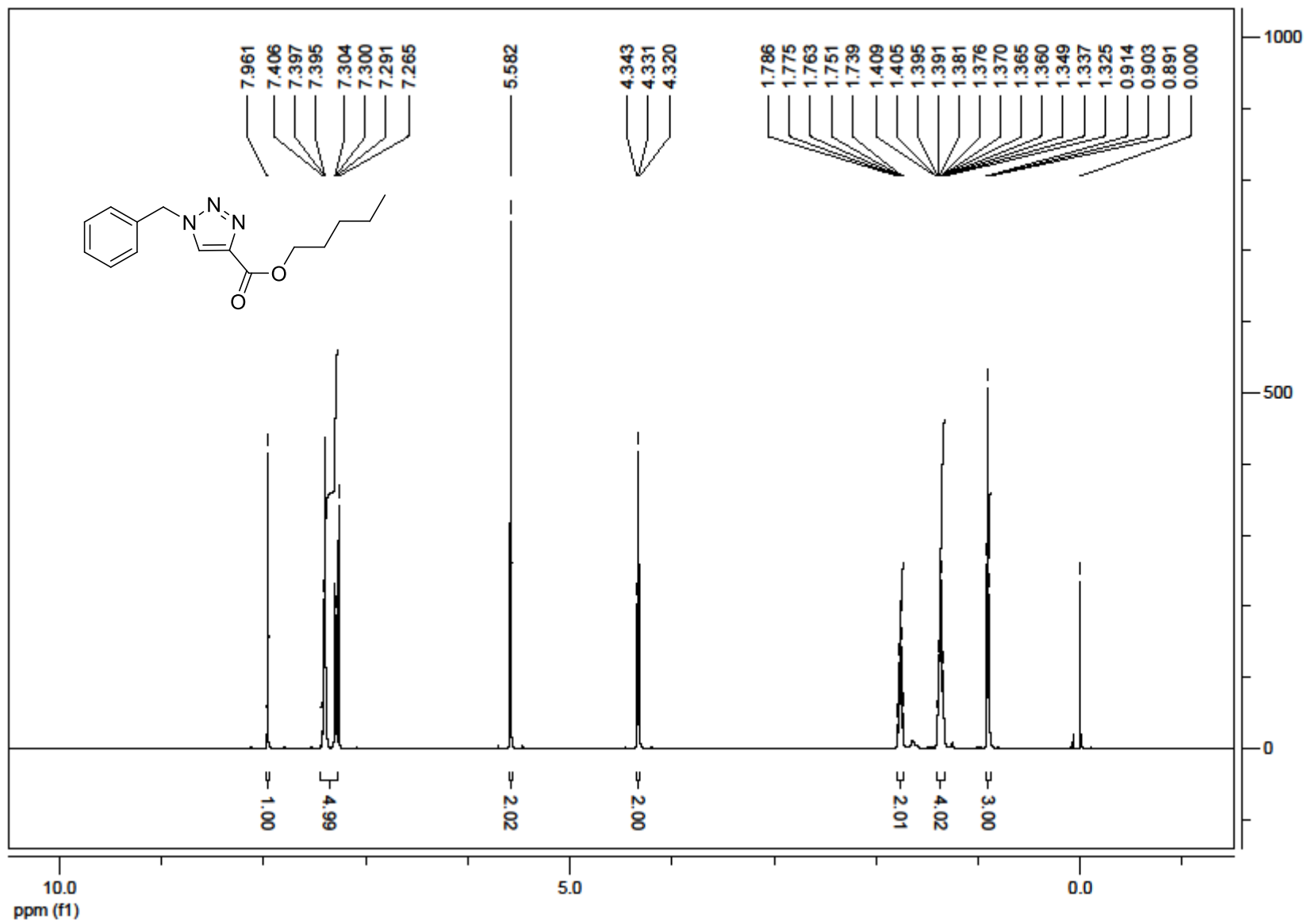
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	60
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-18T15:44:42
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22 Lowest Frequency	-2932.5
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



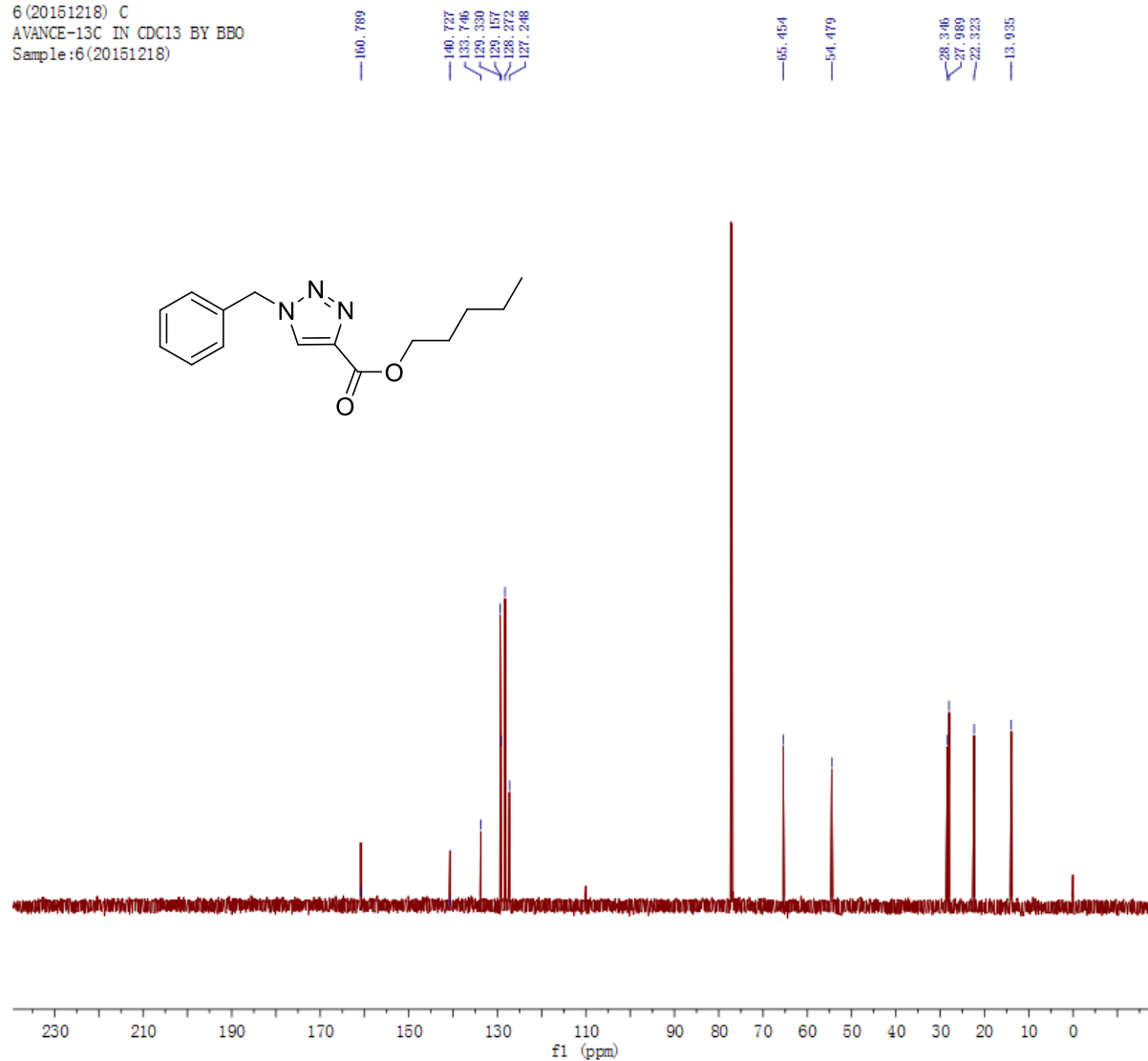
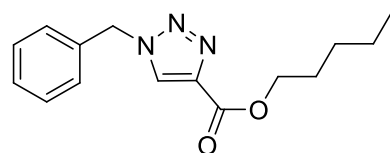
5 (20151218) C  
AVANCE-13C IN CDCl3 BY BBO  
Sample:5 (20151218)



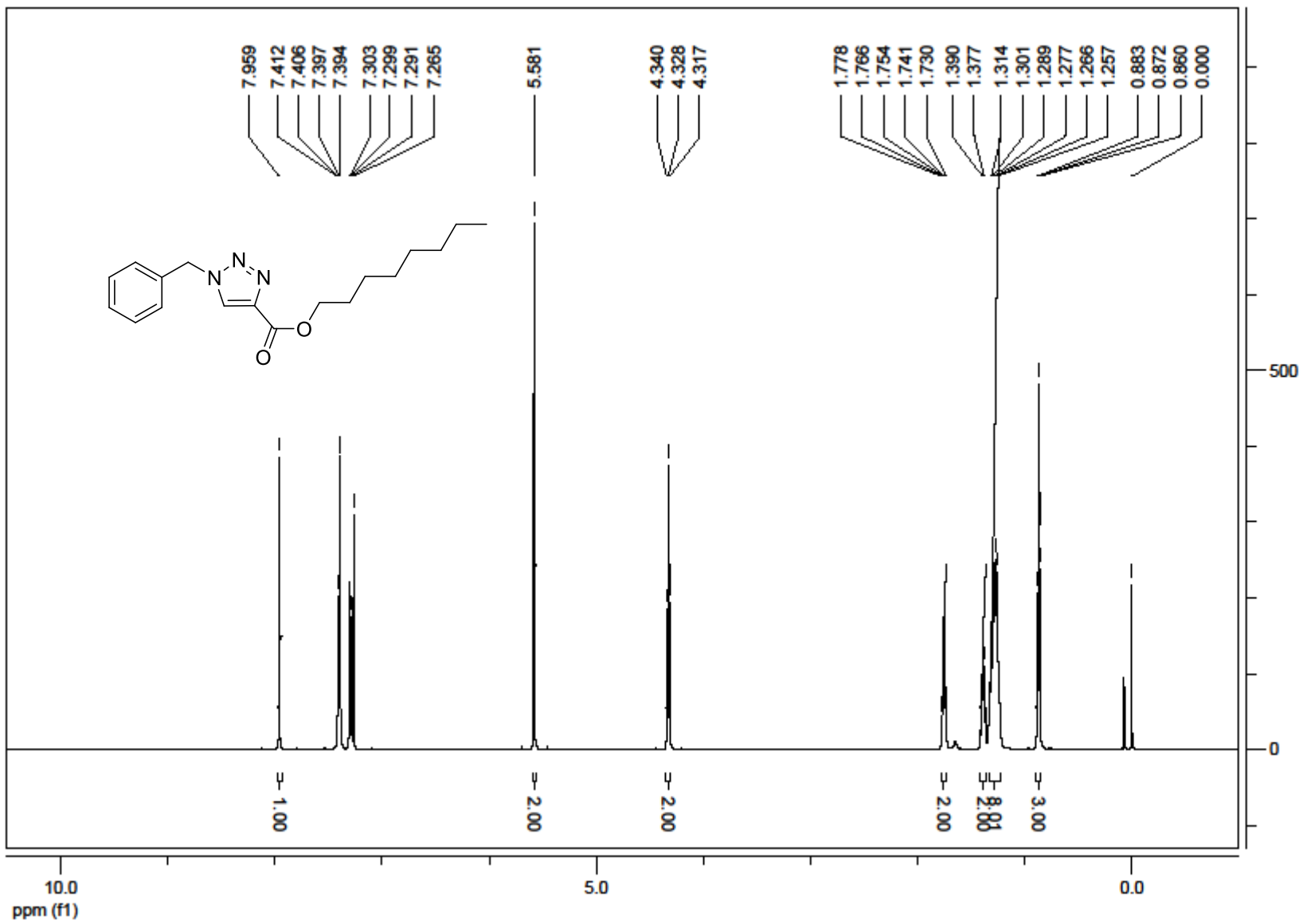
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	48
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-21T09:24:59
19 Modification Date	2015-12-21T09:25:54
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2932.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



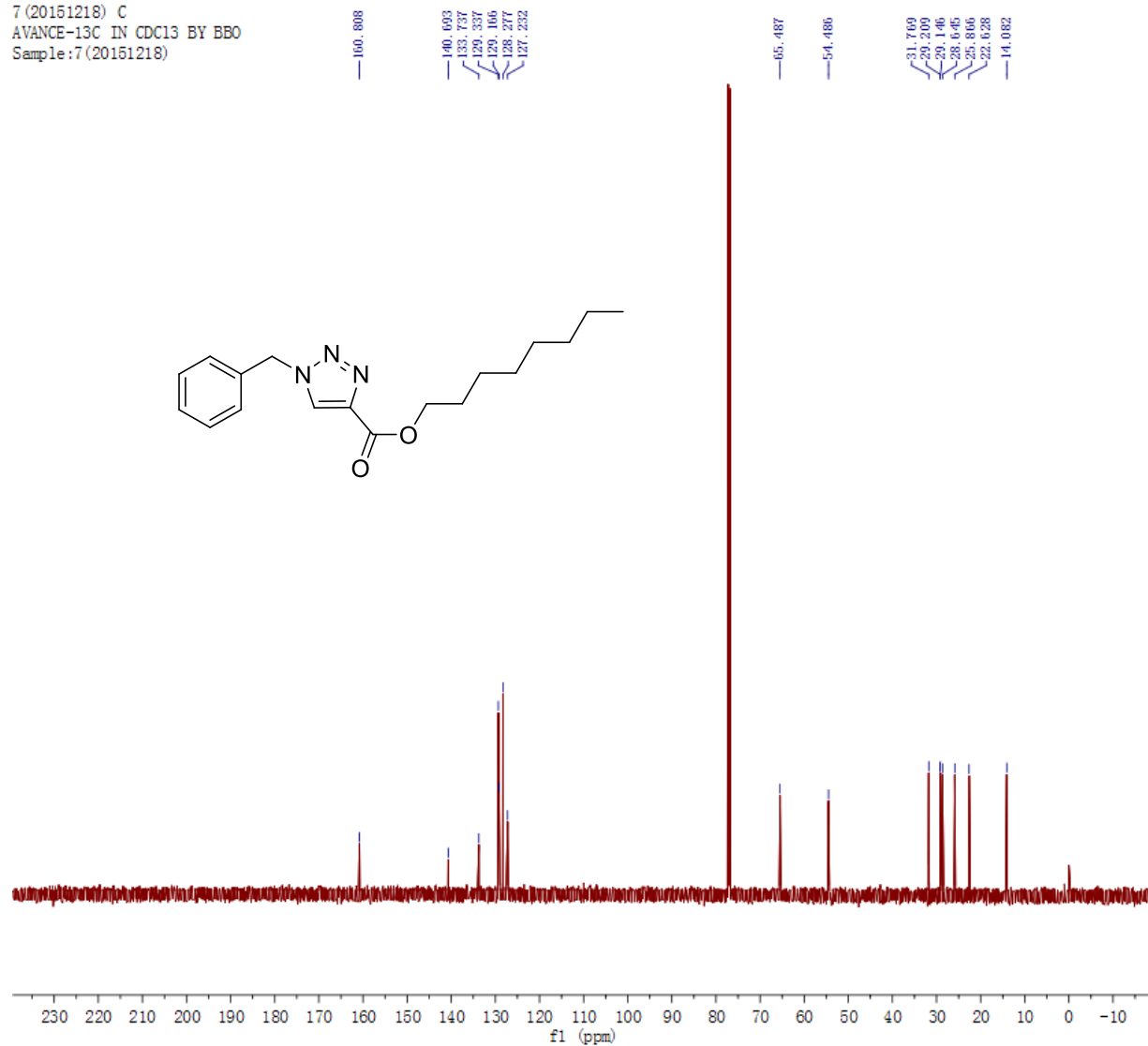
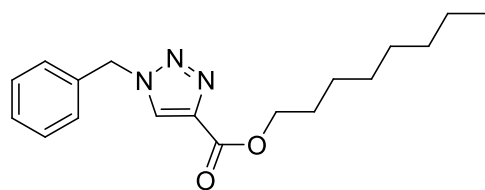
6 (20151218) C  
AVANCE-13C IN CDCl3 BY BBO  
Sample:6(20151218)



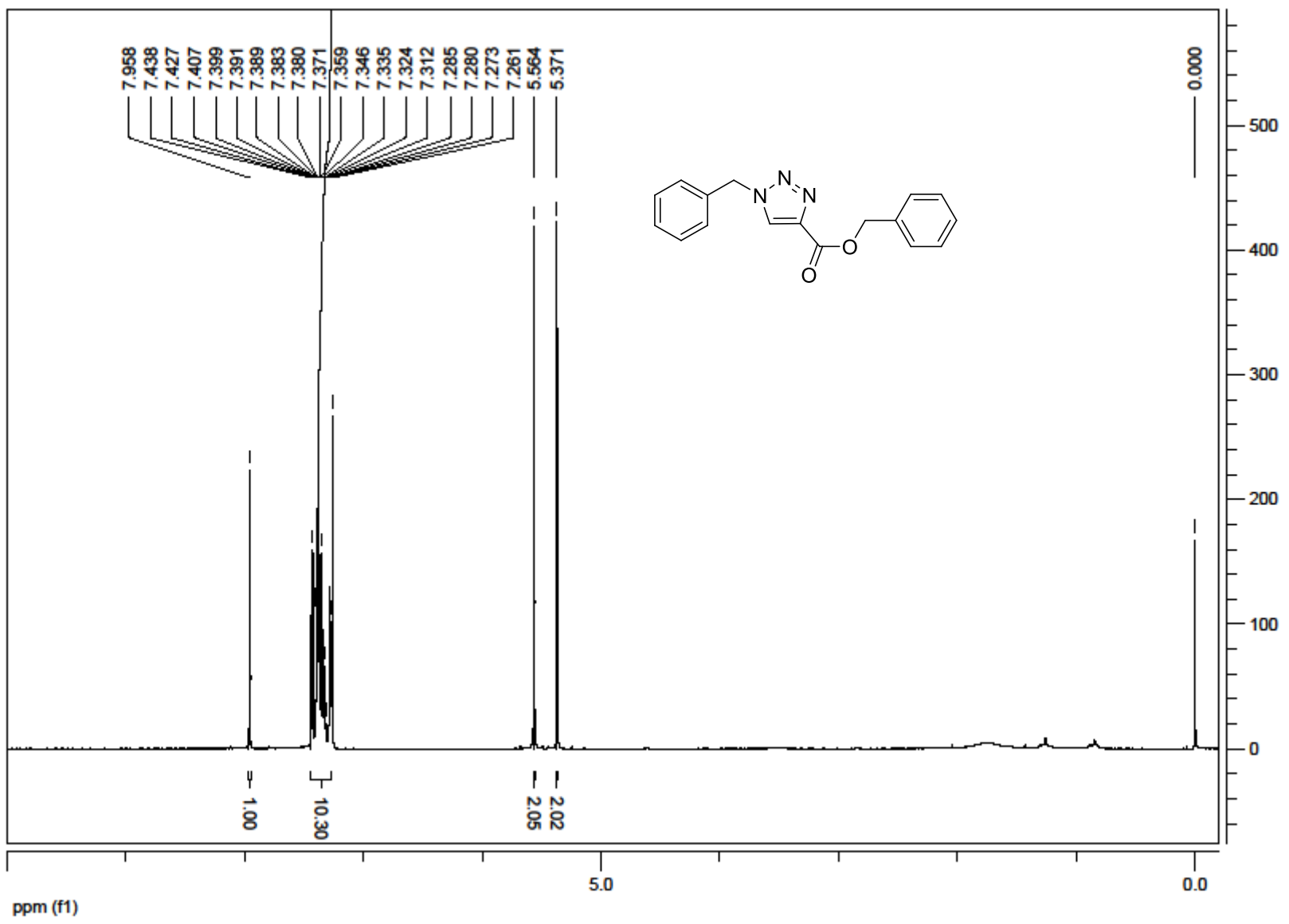
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	96
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
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22 Lowest Frequency	-2933.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



7 (20151218) C  
AVANCE-13C IN CDCl3 BY BBO  
Sample:7 (20151218)



Parameter	Value
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3 Comment	AVANCE-13C IN CDCl3 BY BBO Sample:7 (20151218)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	121
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
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25 Spectral Size	65536

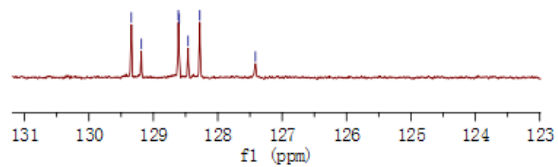


8 (20151222) sunhongbin C  
 AVANCE-13C IN CDC13 BY BBO  
 Sample:8(20151222)

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 127.415

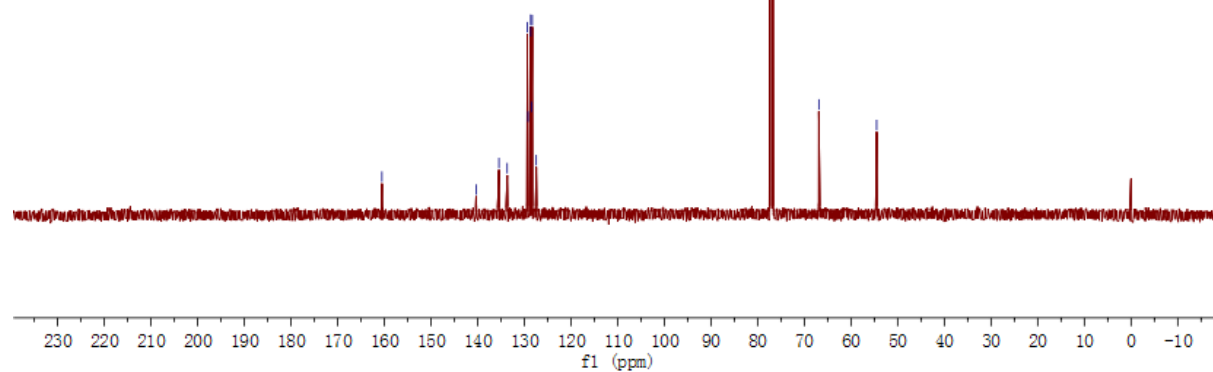
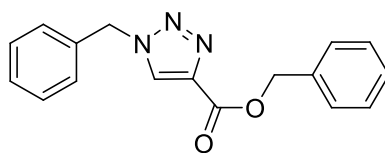
8 (20151222) sunhongbin C  
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 Sample:8(20151222)

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 128.126  
 128.126  
 128.126

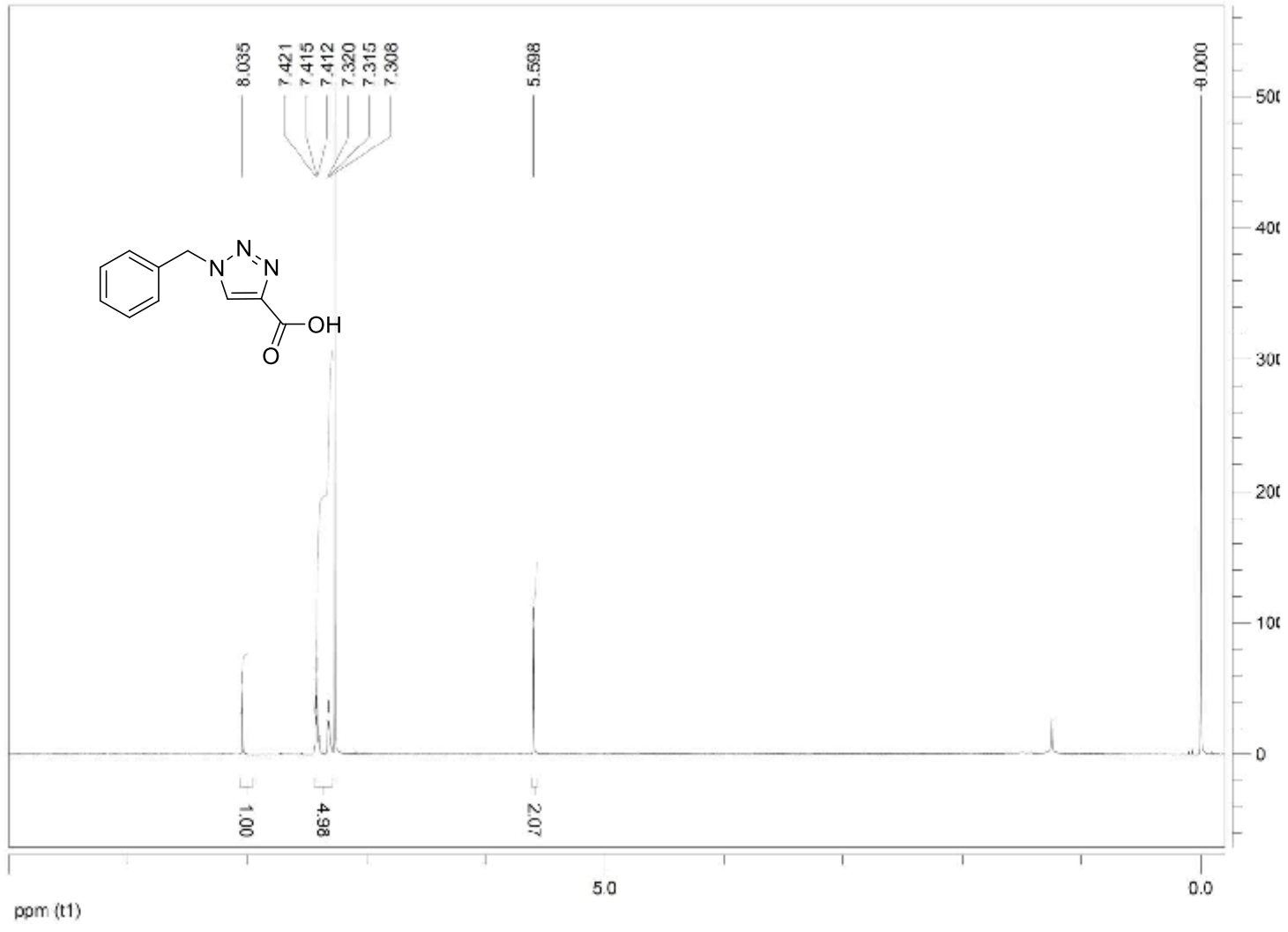


66.880

54.507



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1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/ lidong/ 新建文件夹 (2)/
2 Title	8 (20151222) sunhongbin C/ 2/ fid
3 Comment	8 (20151222) sunhongbin C AVANCE-13C IN CDC13 BY BBO Sample:8 (20151222)
4 Origin	Brucker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	266
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-22T08:32:13
19 Modification Date	2015-12-22T08:33:50
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2934.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



24hao C  
AVANCE-13C IN DMSO BY EBO  
Sample:24hao

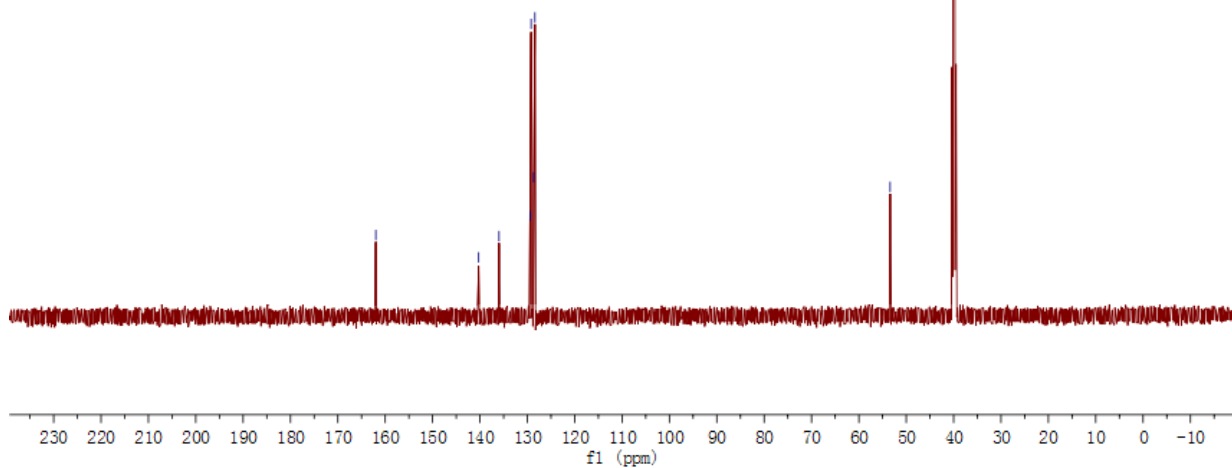
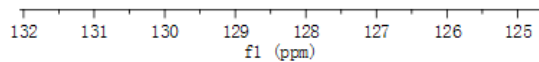
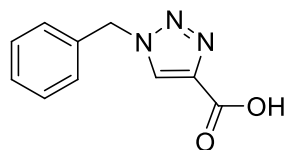
161.989

140.275  
135.971  
129.398  
129.202  
128.668  
128.391

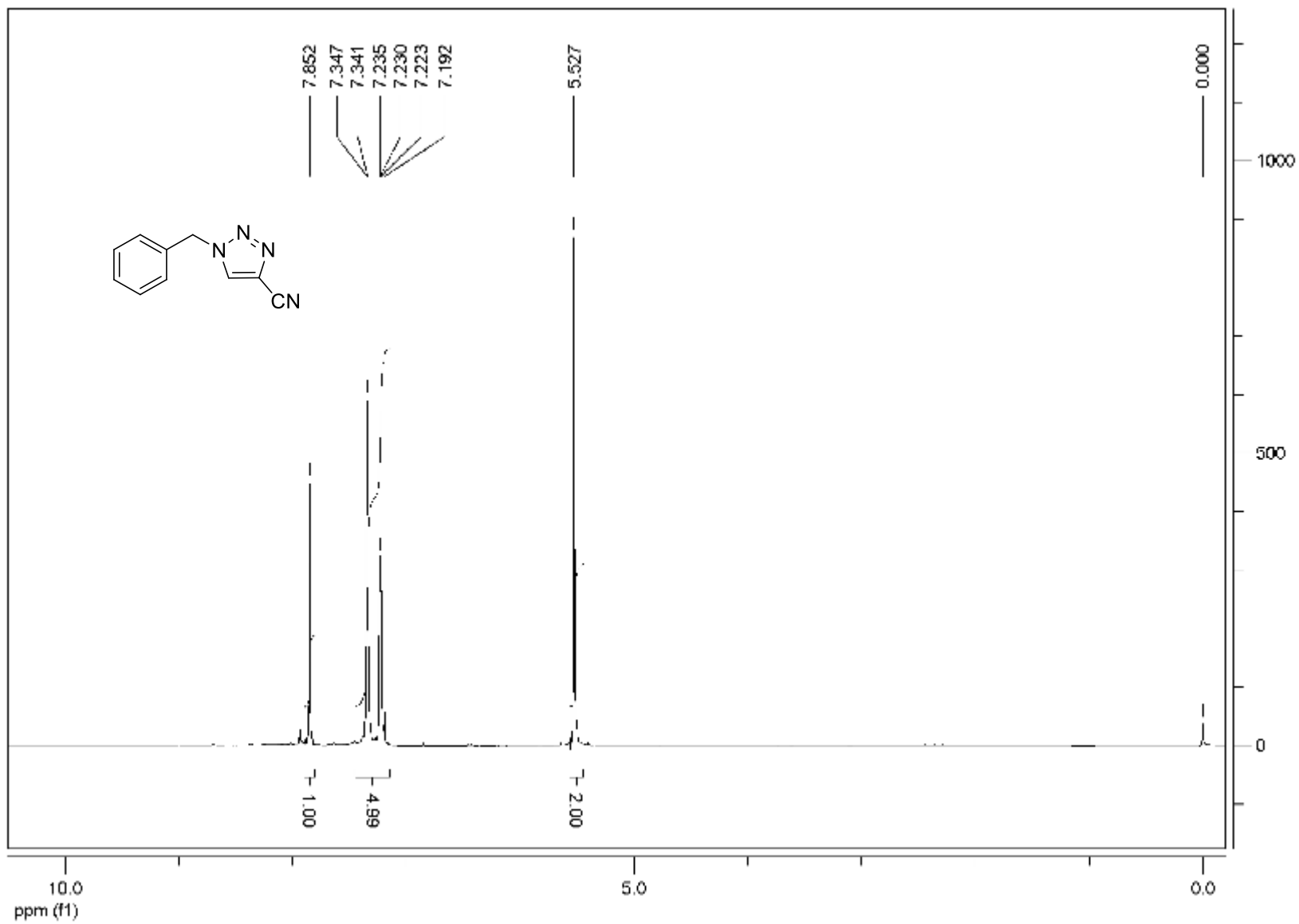
53.403

24hao C  
AVANCE-13C IN DMSO BY EBO  
Sample:24hao

129.398  
129.202  
128.668  
128.391



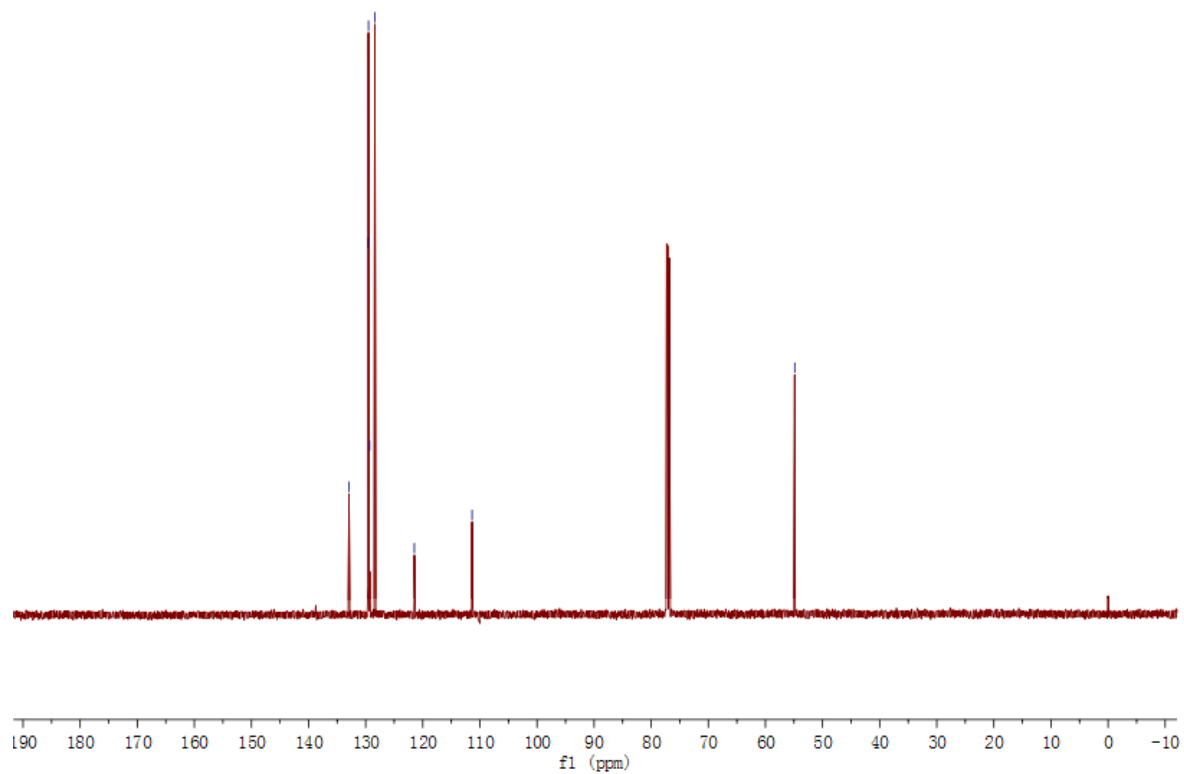
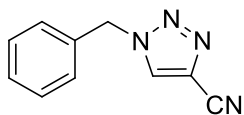
Parameter	Value
1 Data File Name	E:/ lidong/ 李栋/ 新建文件夹 (2)/ 24hao C/ 2/ fid
2 Title	24hao C
3 Comment	AVANCE-13C IN DMSO BY EBO Sample:24hao
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	142
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2016-01-05T11:01:16
19 Modification Date	2016-01-05T11:07:46
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



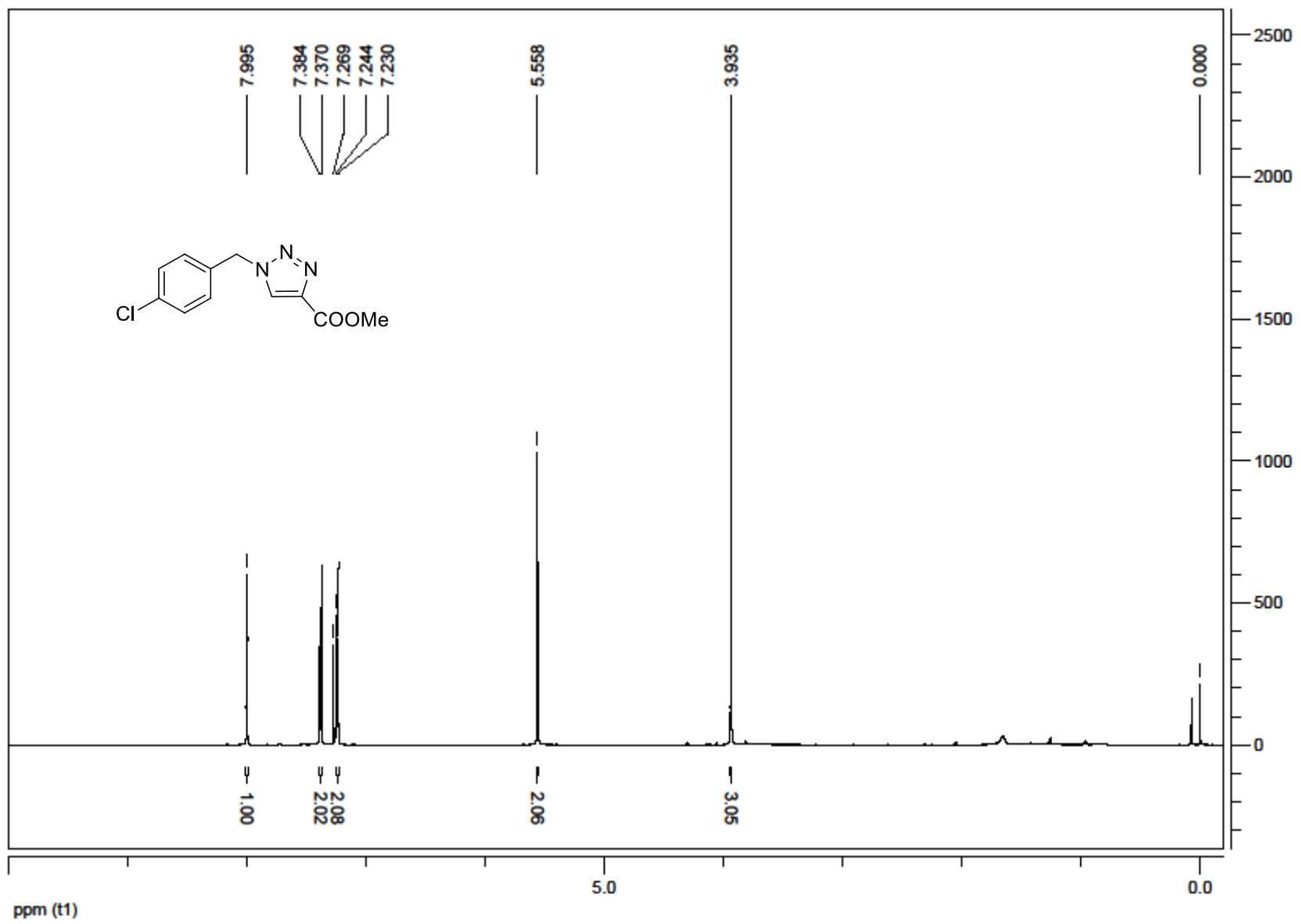
10(20151223) C  
AVANCE-13C IN CDC13 BY BBO  
Sample:10(20151223)

132.918  
129.524  
129.503  
129.315  
128.397  
121.475  
111.367

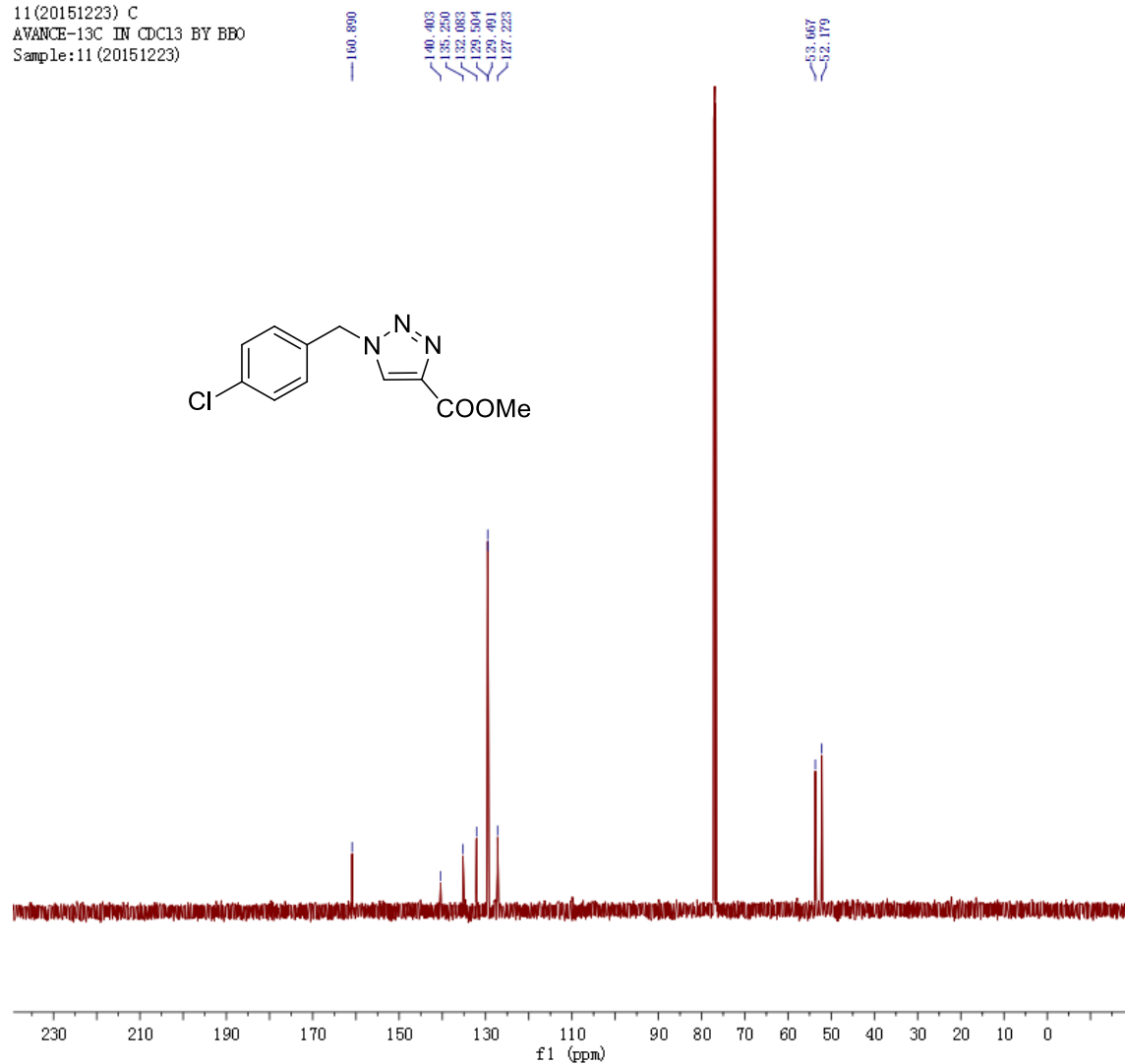
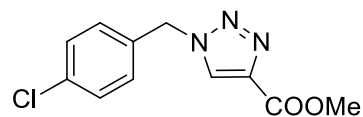
54.869



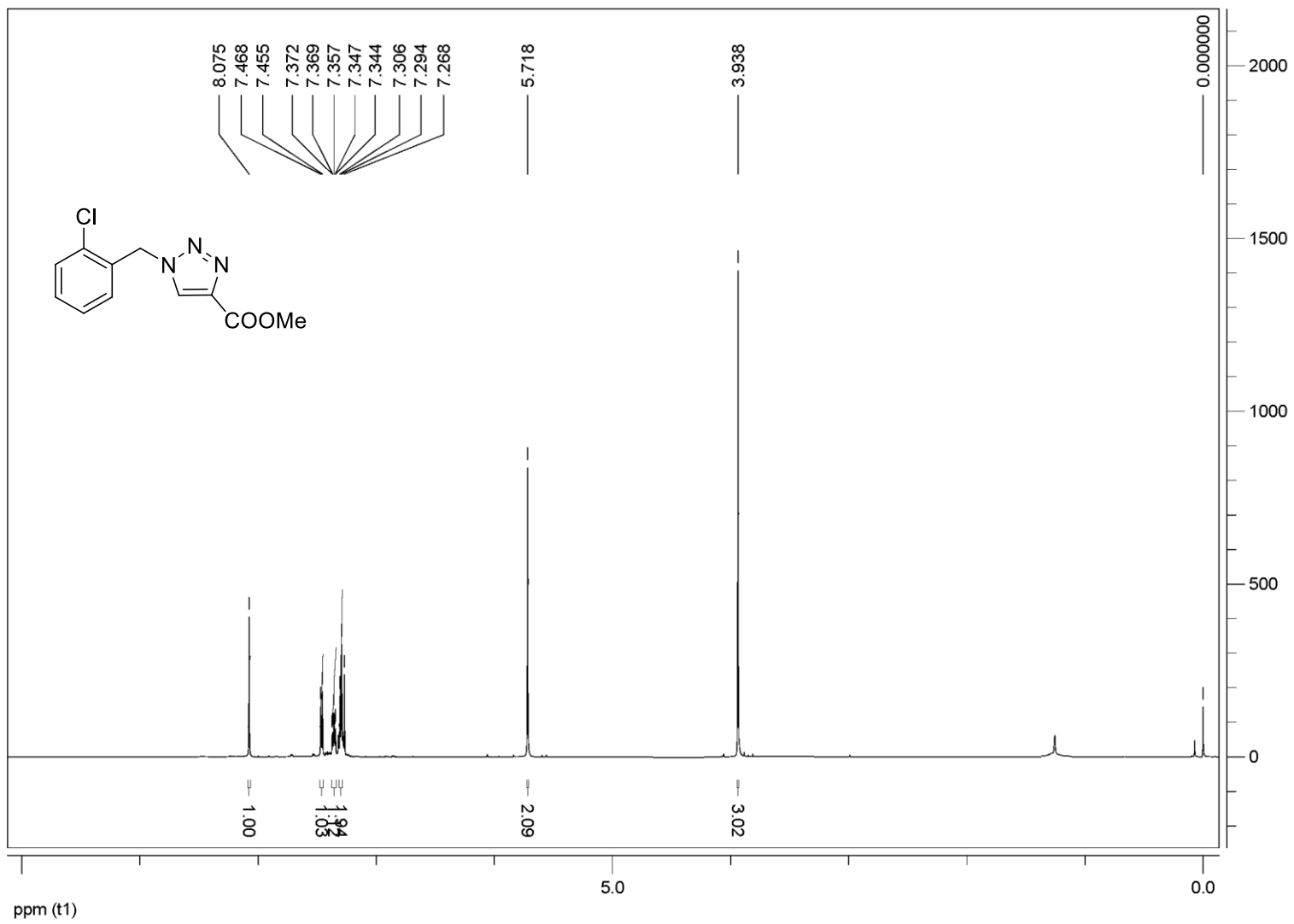
Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/lidong/ 新建文件夹(2)/ 10(20151223) C/ 2/ fid
2 Title	10(20151223) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:10(20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	106
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T08:22:11
19 Modification Date	2015-12-23T08:23:38
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2936.2
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



11 (20151223) C  
AVANCE-13C IN CDCl3 BY BBO  
Sample: 11 (20151223)

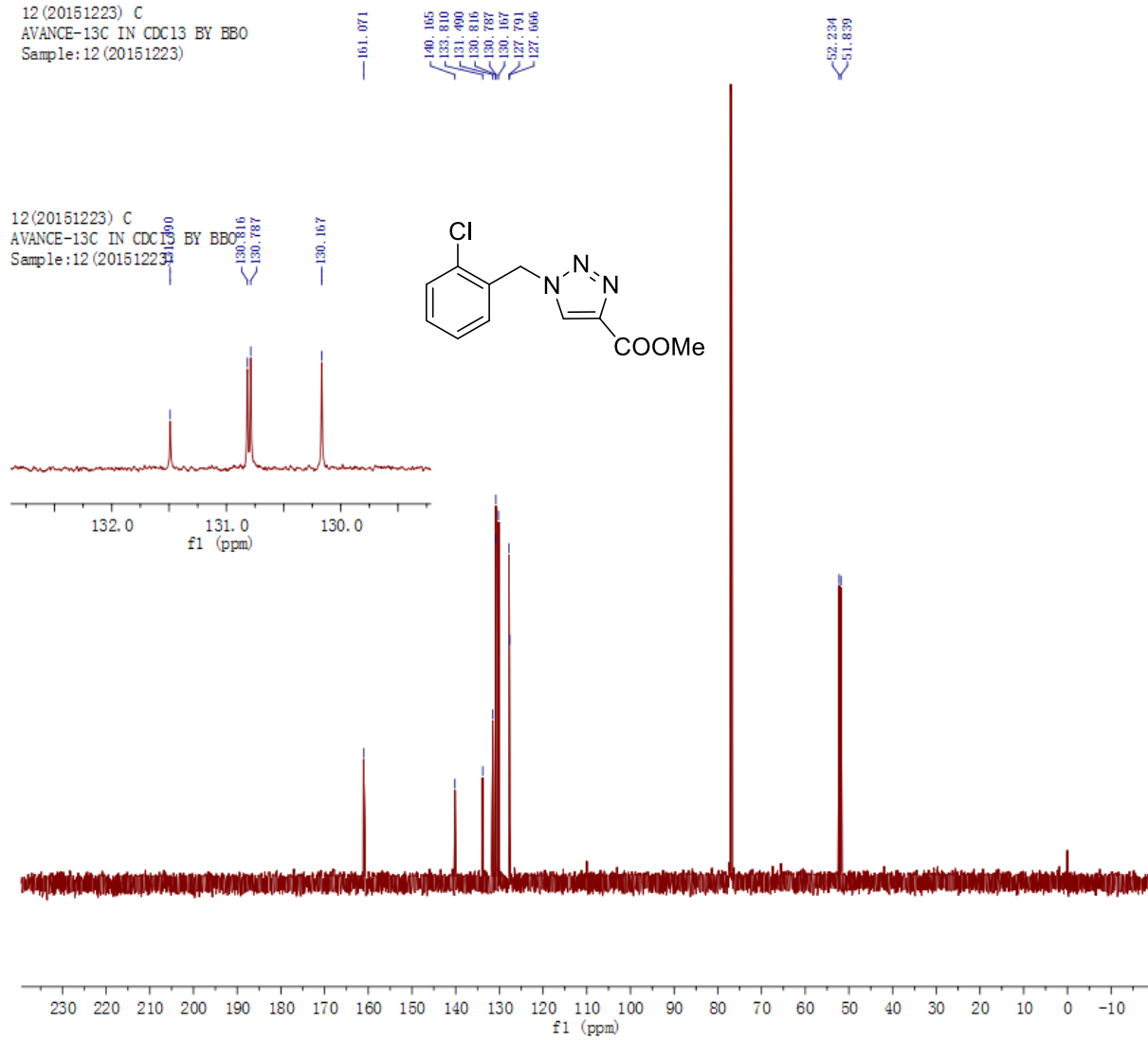
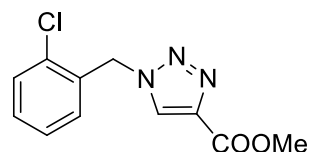


Parameter	Value
1 Data File Name	C:/ Documents and Settings/ Administrator/ 桌面/ lidong/ 新建文件夹 (2)/ 11 (20151223) C/ 2/ fid
2 Title	11 (20151223) C
3 Comment	AVANCE-13C IN CDCl3 BY BBO Sample: 11 (20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	103
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T08:32:01
19 Modification Date	2015-12-23T08:36:00
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

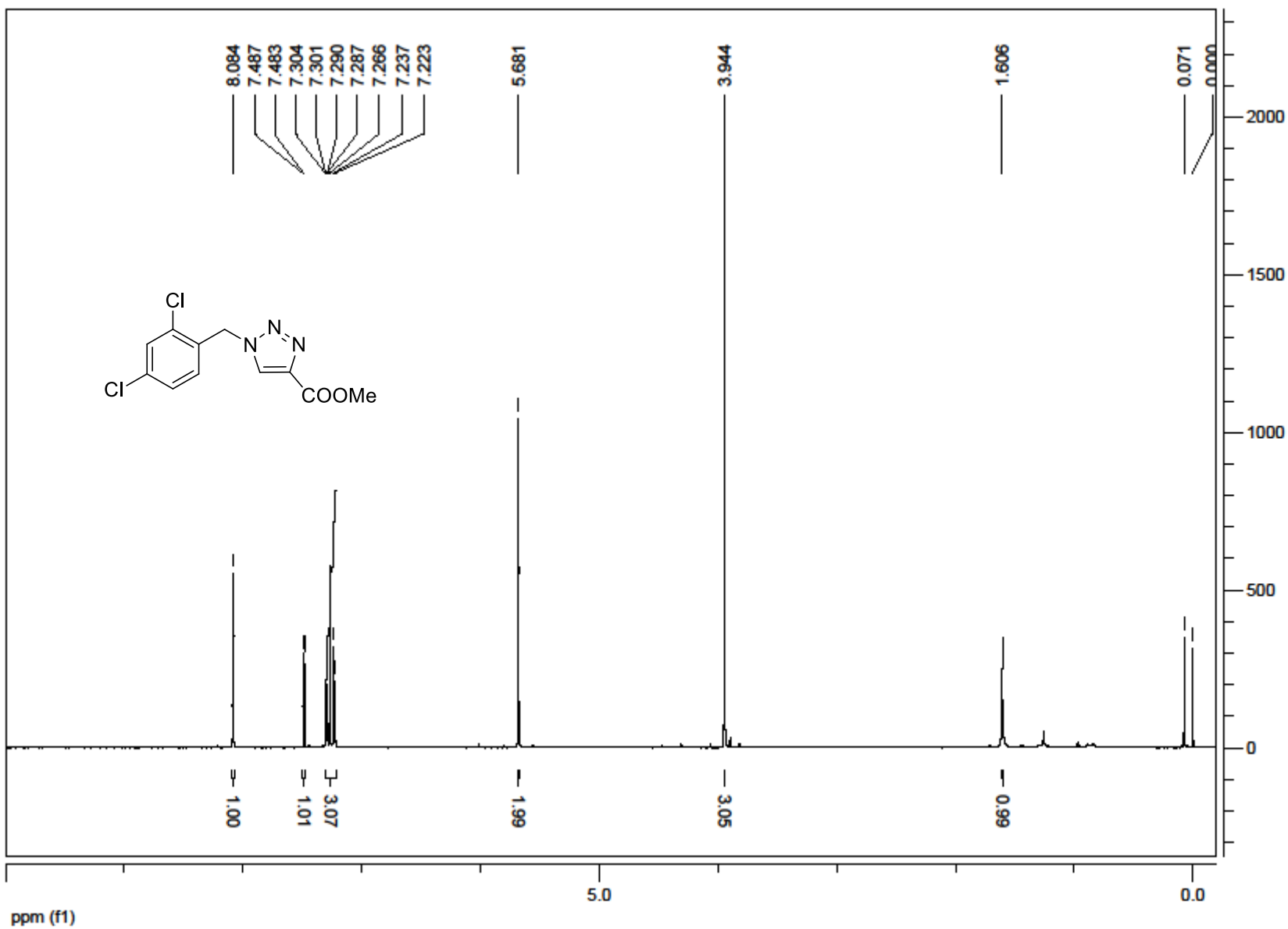


12 (20151223) C  
 AVANCE-13C IN CDC13 BY BBO  
 Sample: 12 (20151223)

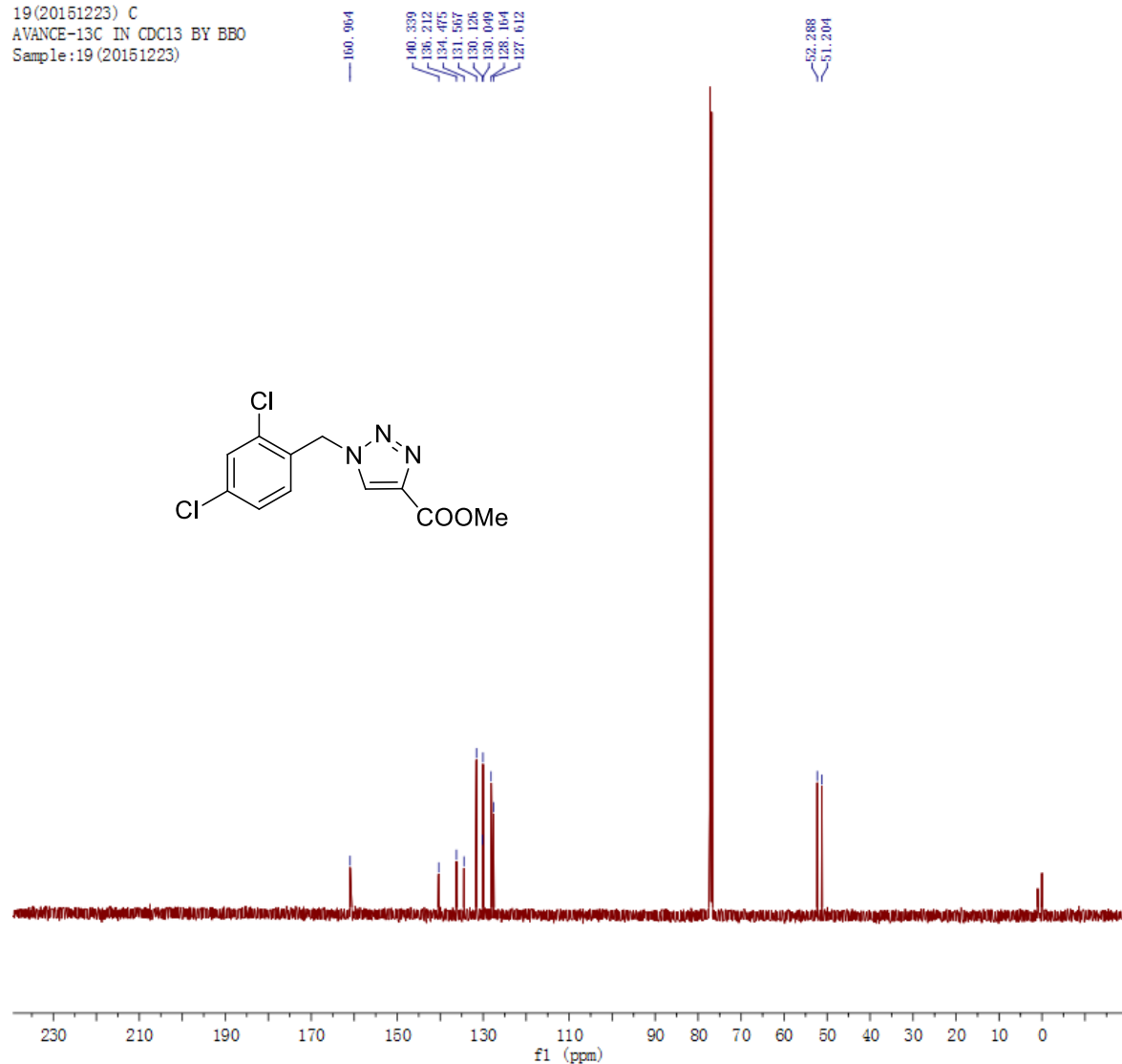
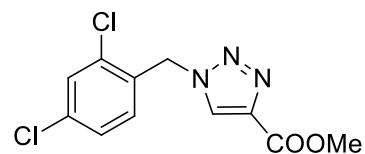
12 (20151223) C  
 AVANCE-13C IN CDC13 BY BBO  
 Sample: 12 (20151223)



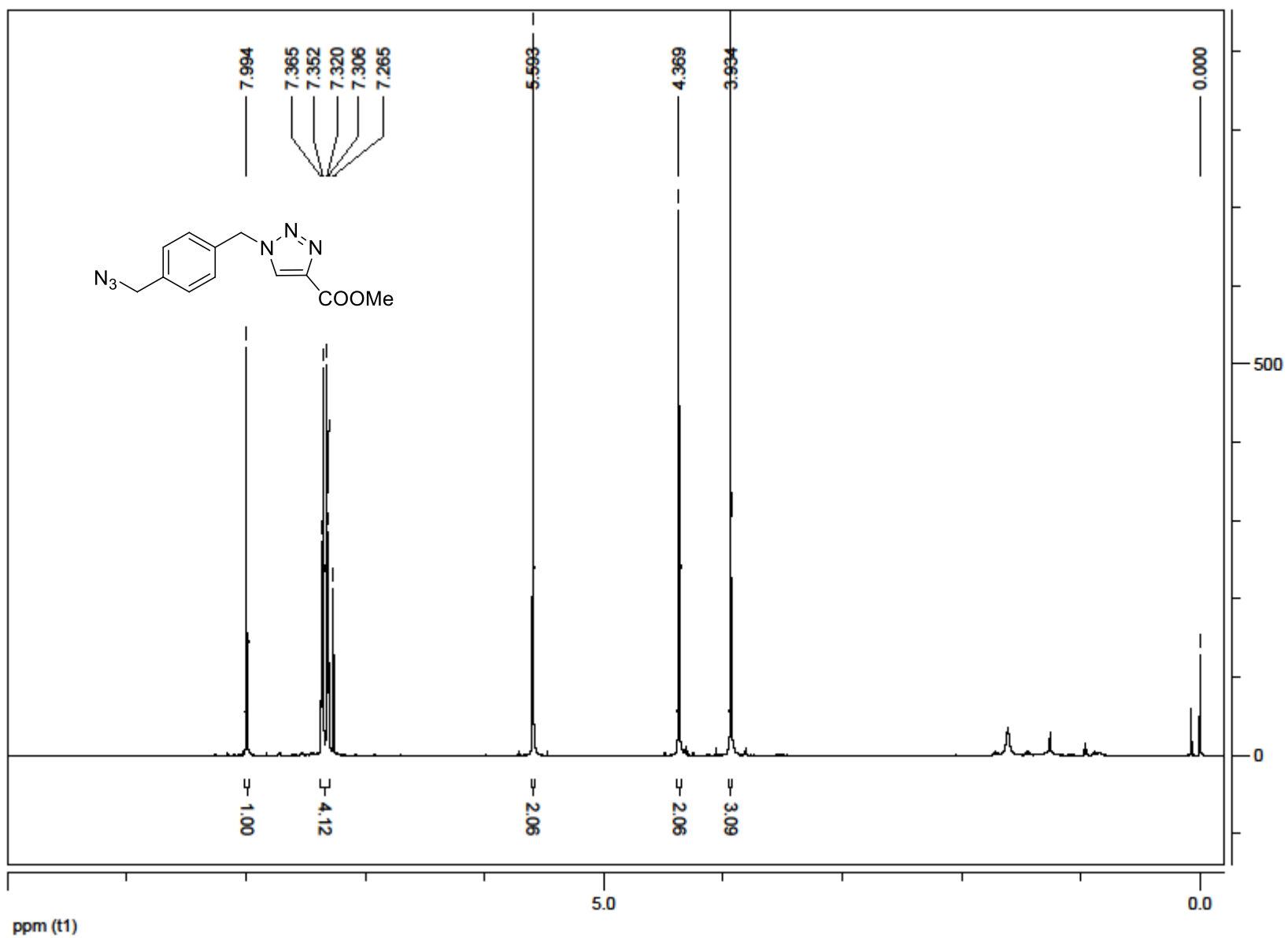
Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/ lidong/ 新建文件夹 (2)/ 12 (20151223) C/ 2/ fid
2 Title	12 (20151223) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample: 12 (20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	58
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T08:39:53
19 Modification Date	2015-12-23T08:42:24
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2932.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



19(20151223) C  
AVANCE-13C IN CDC13 BY BBO  
Sample:19(20151223)



Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/ lidong/ 新建文件夹 (2)/ 19(20151223) C/ 2/ fid
2 Title	19(20151223) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:19(20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	268
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T09:54:58
19 Modification Date	2015-12-23T10:07:14
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2933.0
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

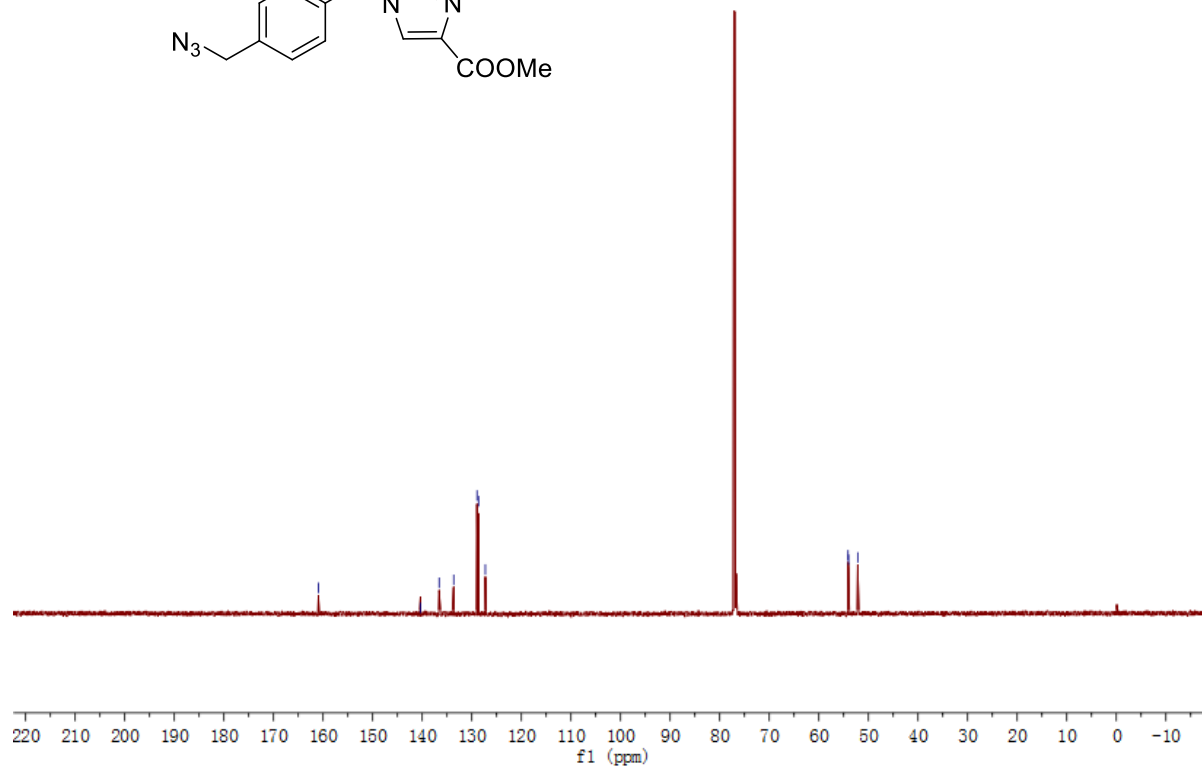
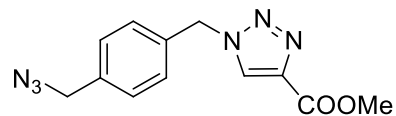


16(20151223)  
AVANCE-13C IN CDC13 BY BBO  
Sample:16(20151223)

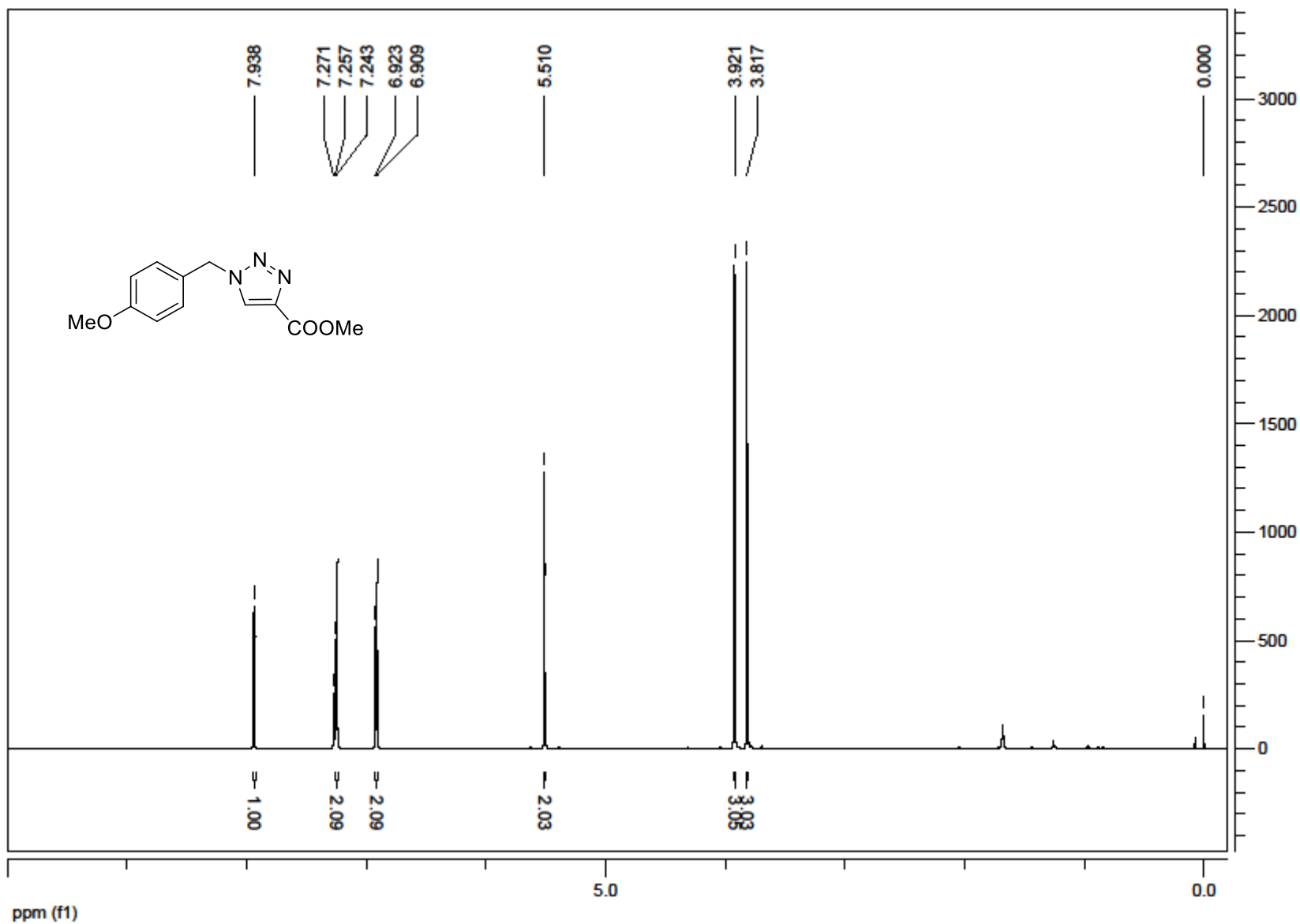
160.951

140.319  
136.594  
133.657  
128.957  
128.643  
127.270

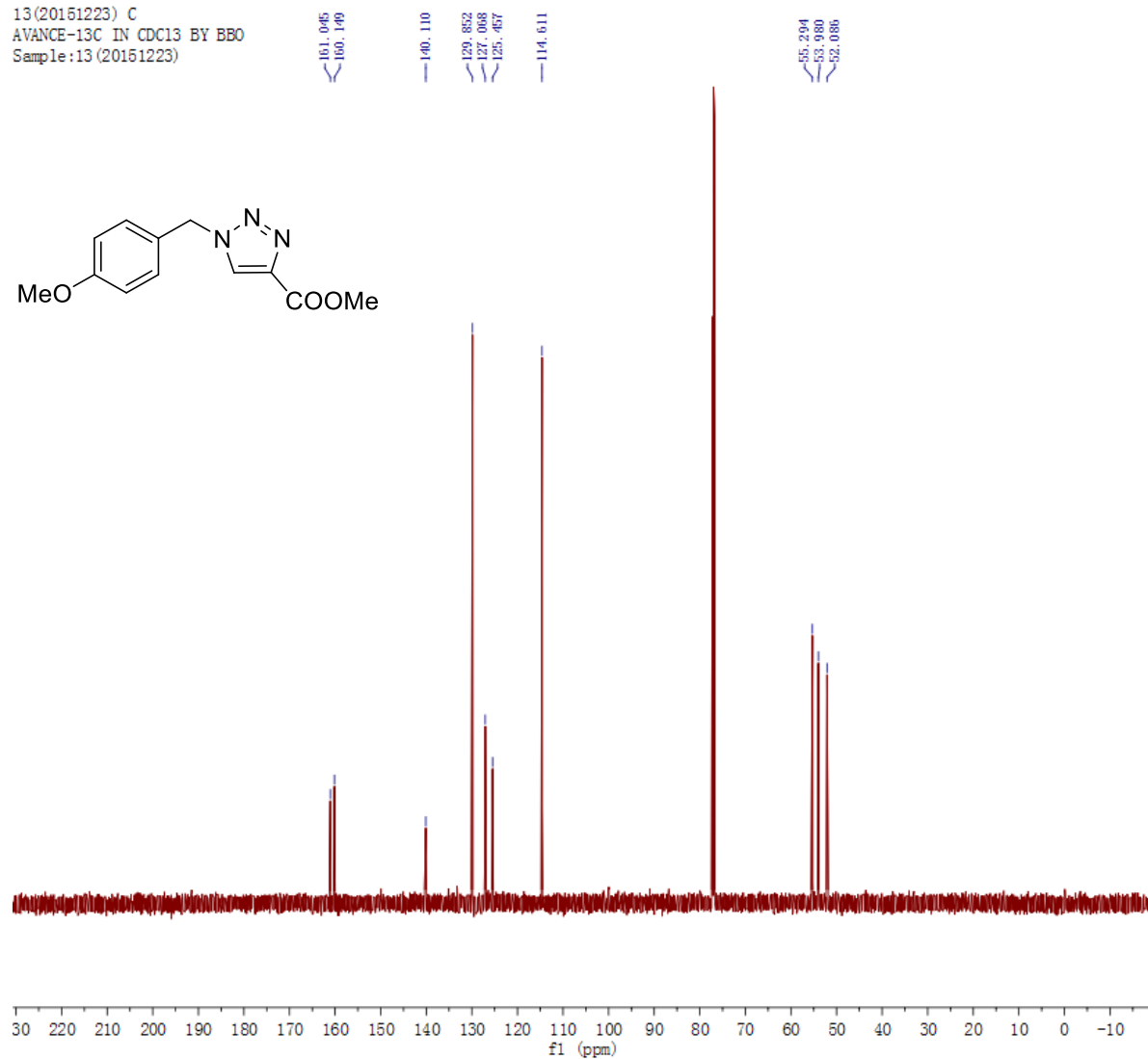
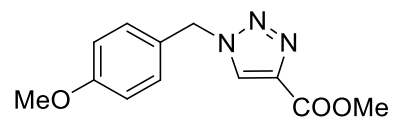
54.114  
54.013  
52.163



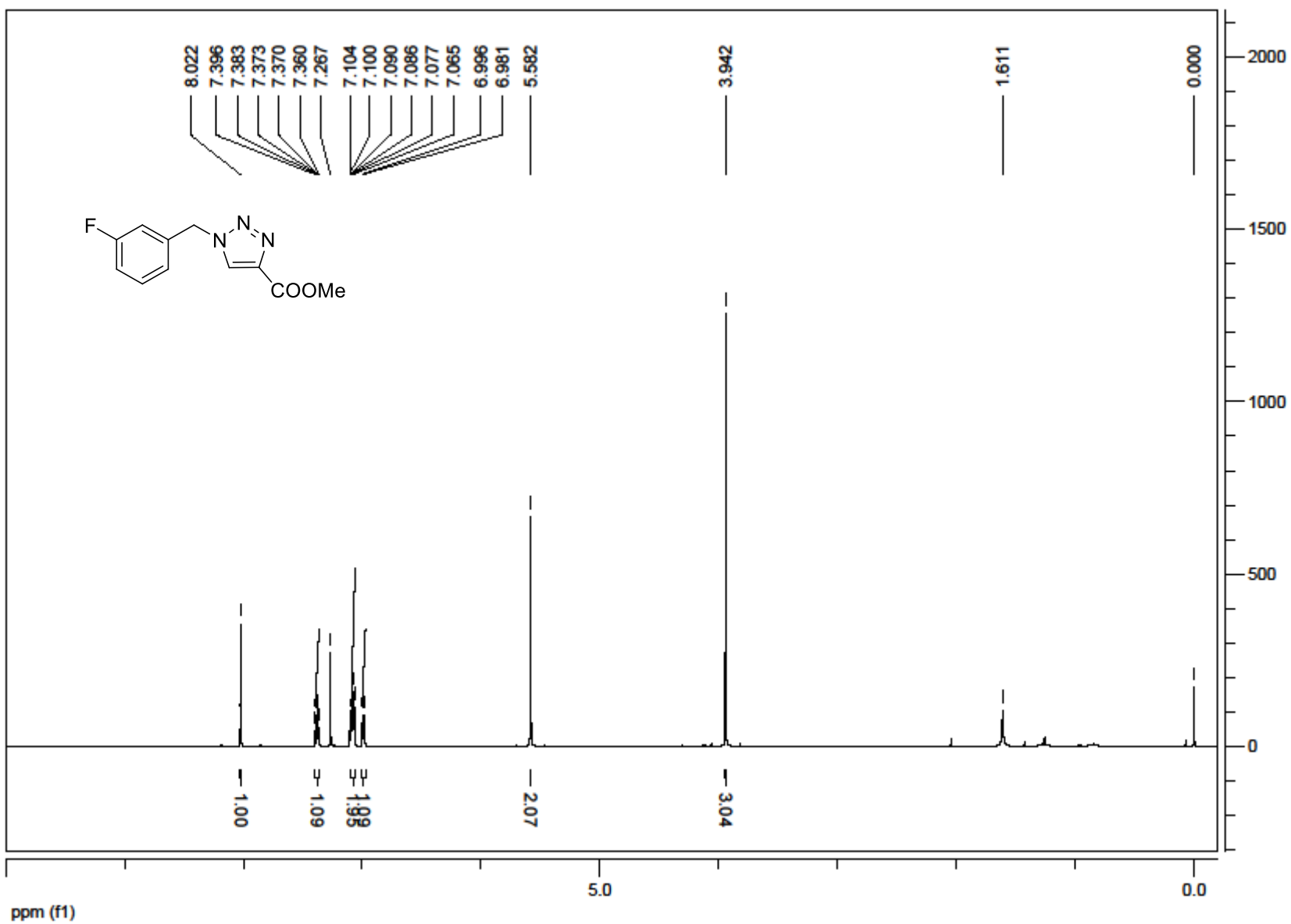
Parameter	Value
1 Data File Name	C:/Users/Administrator.ZG/C-20110924WDR/Desktop/16(20151223) C/2/ fid
2 Title	16(20151223)
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:16(20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	687
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-24T09:30:00
19 Modification Date	2015-12-24T09:32:26
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



13(20151223) C  
AVANCE-13C IN CDCl3 BY BBO  
Sample:13(20151223)



Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/ lidong/ 新建文件夹 (2)/ 13(20151223) C/ 2/ fid
2 Title	13(20151223) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:13(20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	70
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T08:46:00
19 Modification Date	2015-12-23T08:49:10
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

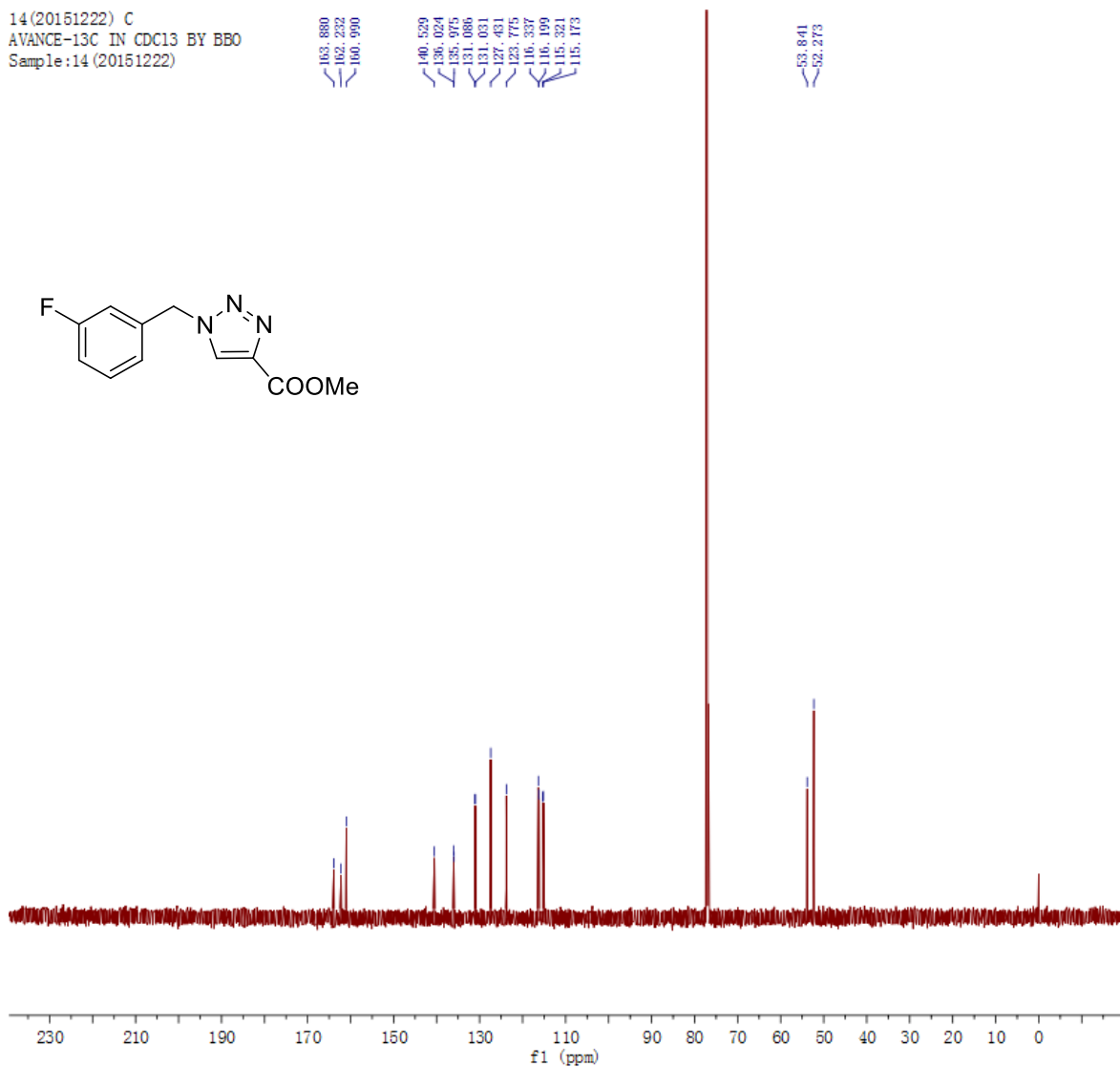
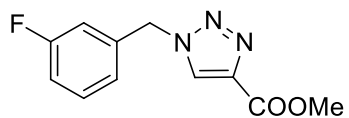


14(20151222) C  
AVANCE-13C IN CDC13 BY BBO  
Sample:14(20151222)

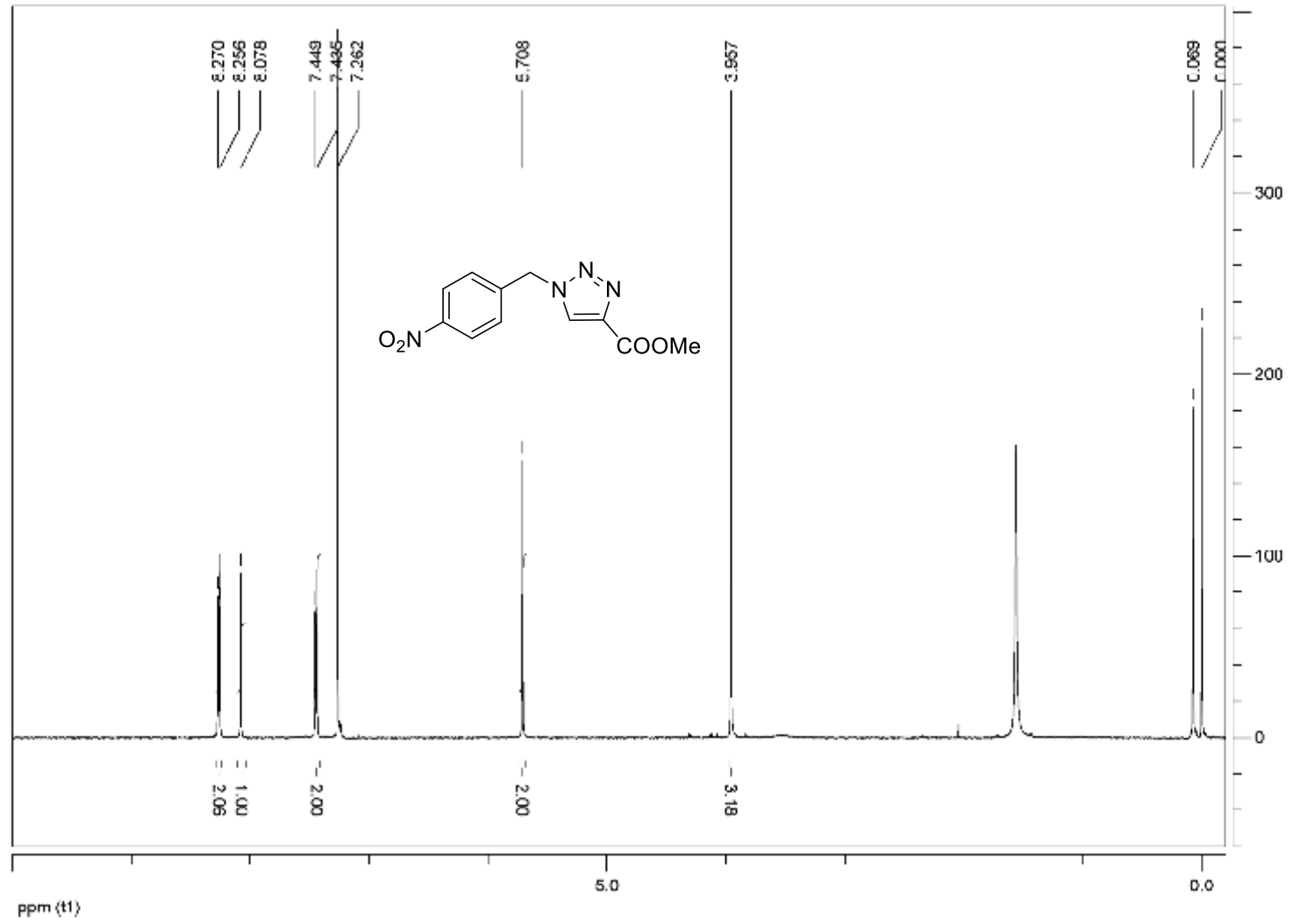
163.880  
162.232  
100.990

140.529  
136.024  
134.375  
131.086  
131.081  
127.431  
123.775  
116.337  
116.109  
115.321  
115.173

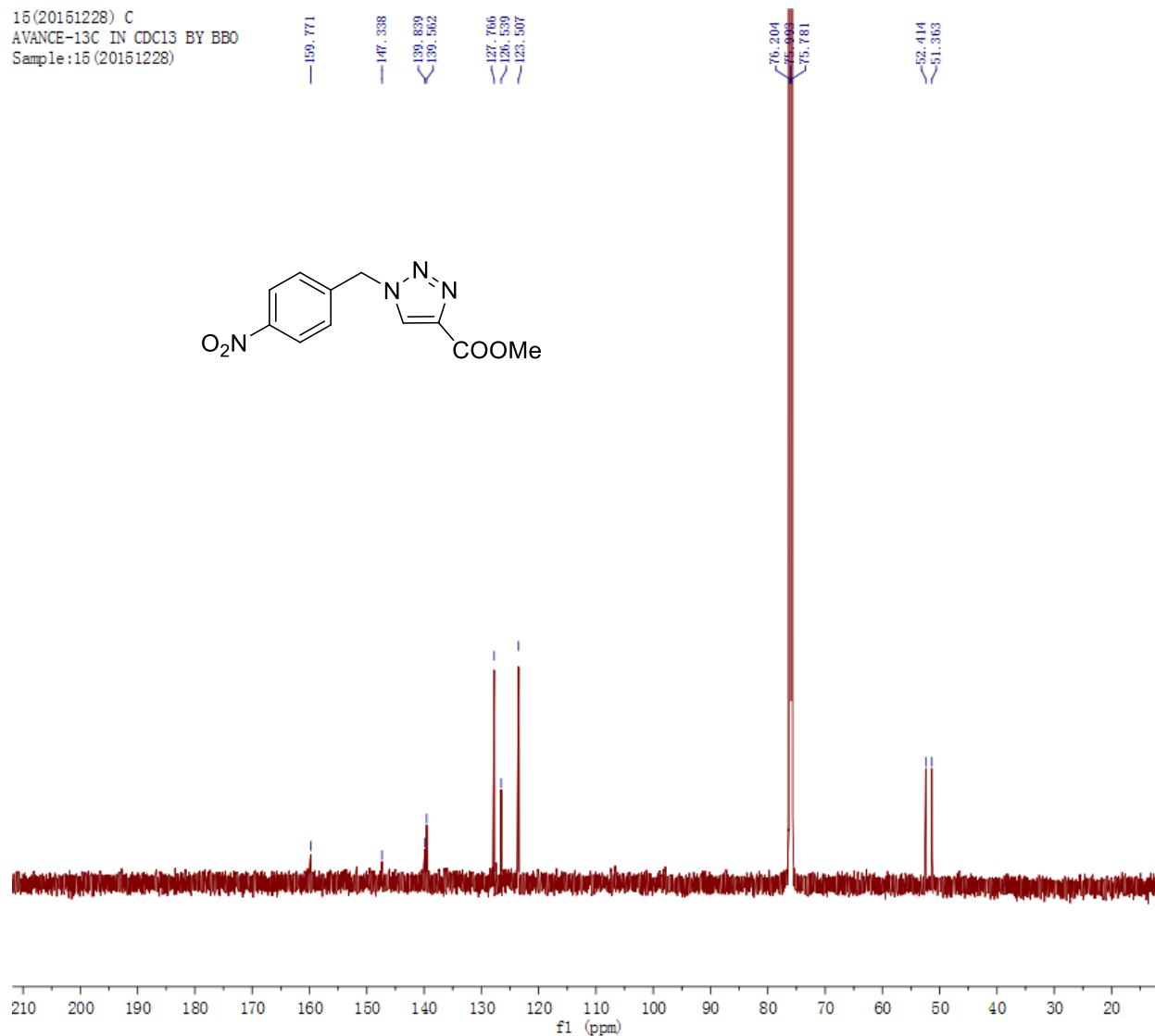
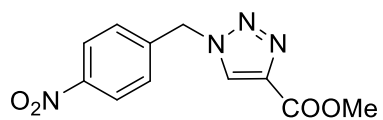
53.841  
52.273



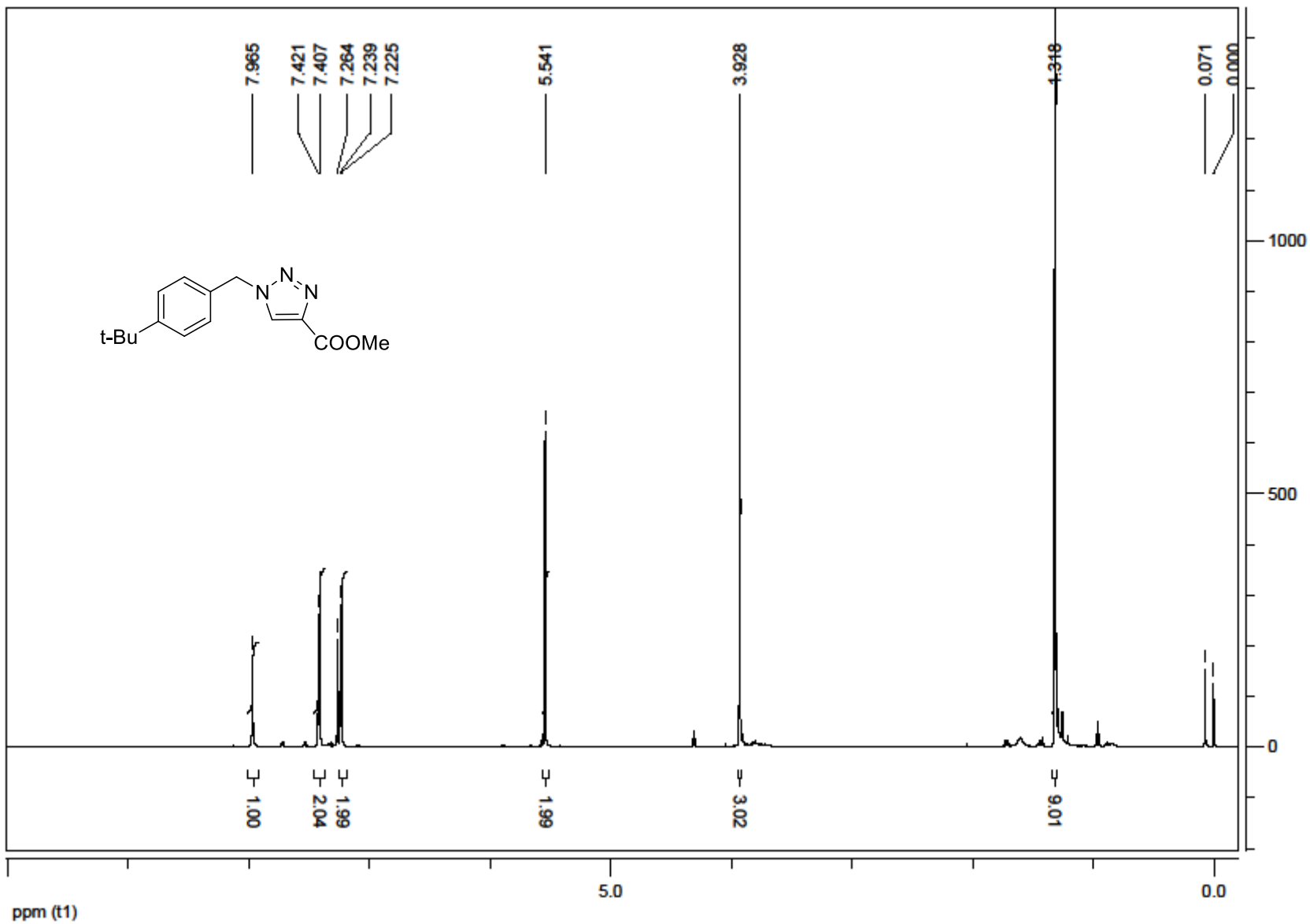
Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/ lidong/ 新建文件夹 (2)/ 14(20151222) C/ 2/ fid
2 Title	14(20151222) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:14(20151222)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	176
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-22T10:58:50
19 Modification Date	2015-12-22T11:05:36
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2932.2
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



15(20151228) C  
AVANCE-13C IN CDC13 BY BBO  
Sample:15(20151228)



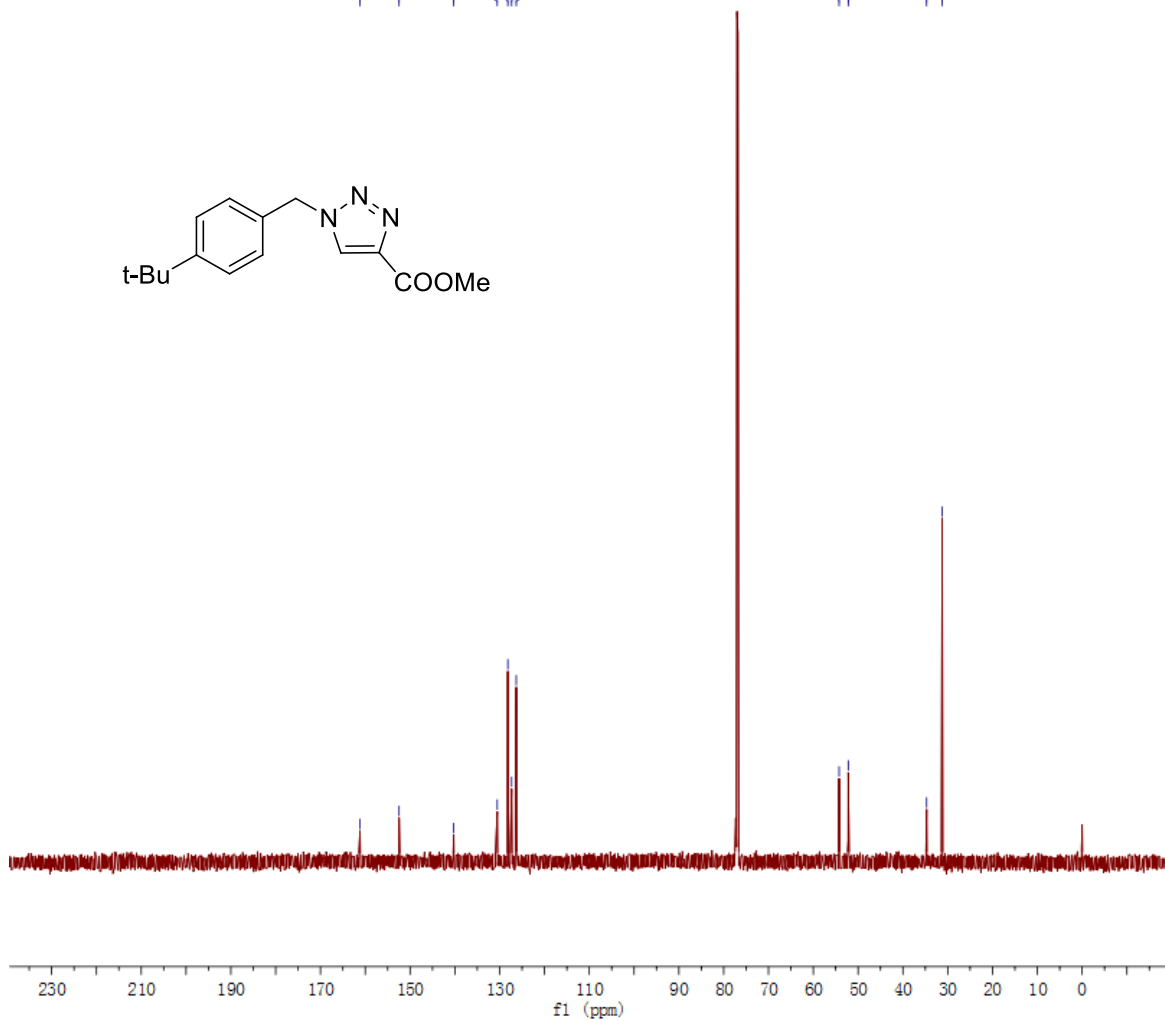
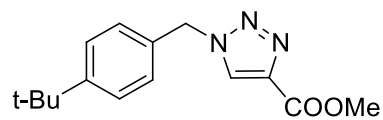
Parameter	Value
1 Data File Name	E:/ lidong/ 新建文件夹 (2)/ 15(20151228) C/ 2/ fid
2 Title	15(20151228) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:15(20151228)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	CDC13
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	19645
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-28T16:25:05
19 Modification Date	2015-12-29T08:15:06
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-3087.4
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



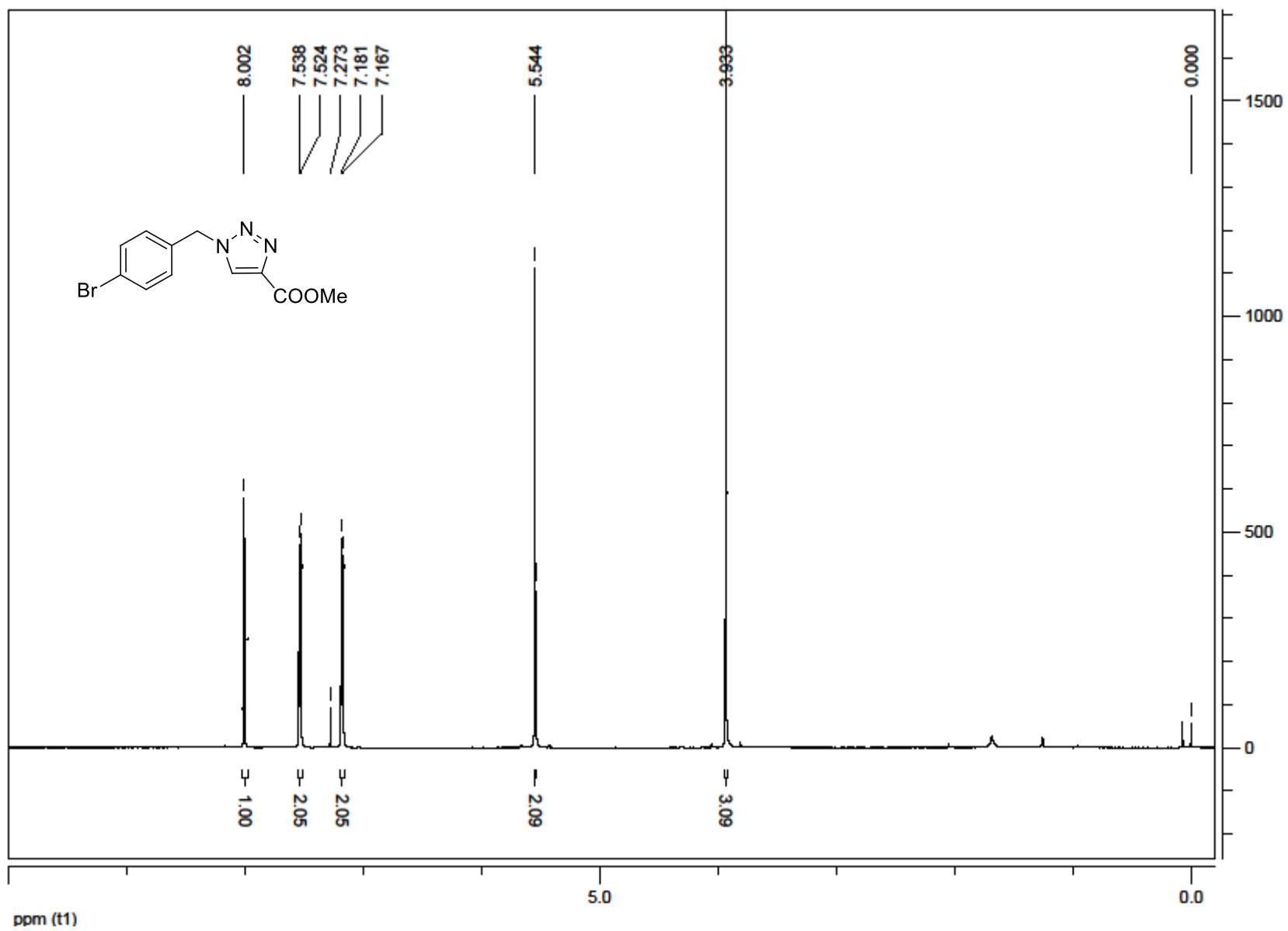
18(20151223) C  
AVANCE-13C IN CDC13 BY BBO  
Sample:18(20151223)

161.173  
152.462  
140.248  
130.542  
128.179  
127.333  
126.294

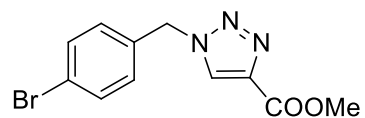
54.240  
52.202  
34.707  
31.232



Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/桌面/lidong/新建文件夹 (2)/18(20151223) C/ 2/ fid
2 Title	18(20151223) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:18(20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	157
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T08:53:56
19 Modification Date	2015-12-23T09:00:10
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2933.3
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

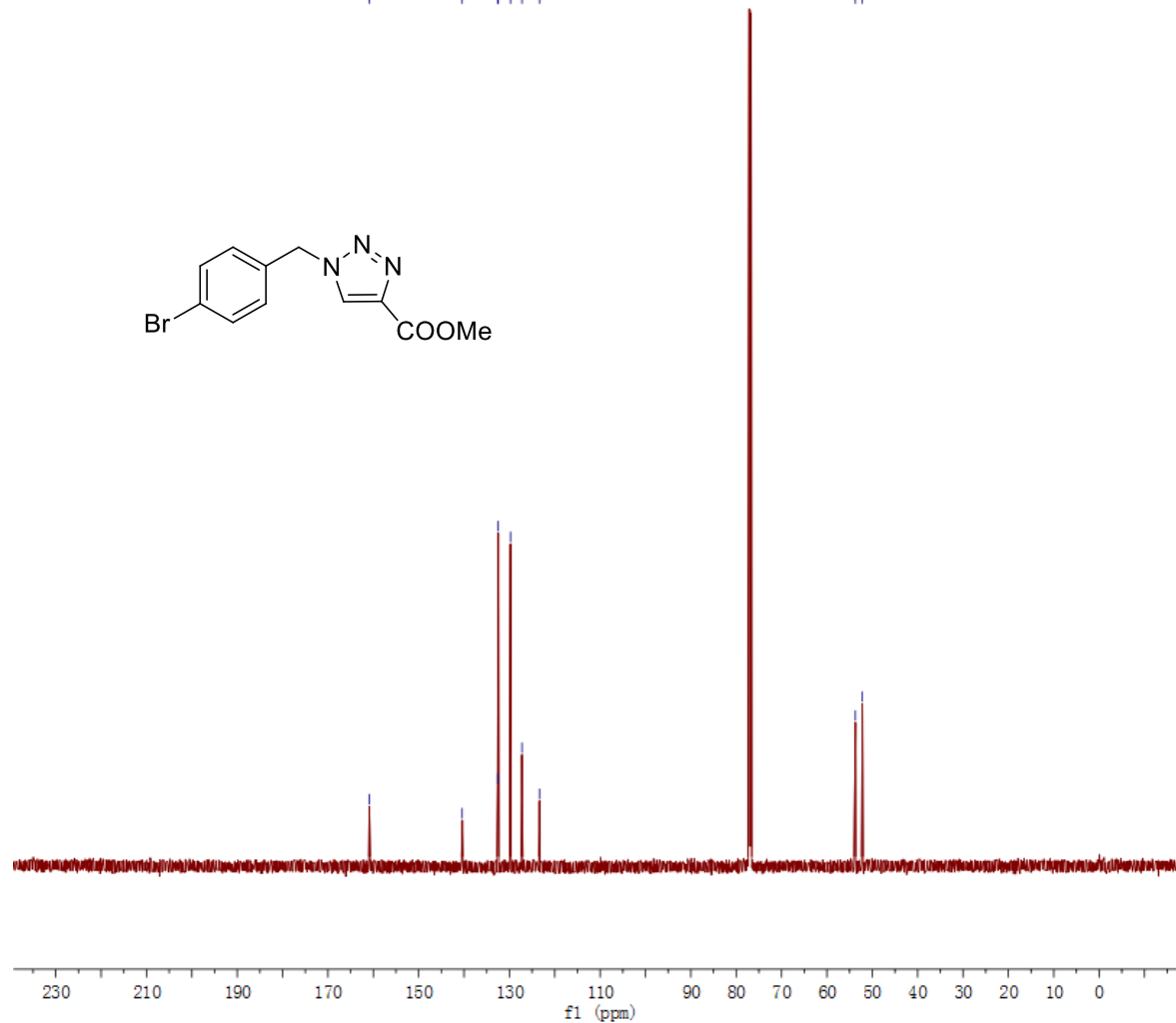


17 (20151223) C  
AVANCE-13C IN CDC13 BY BBO  
Sample:17 (20151223)



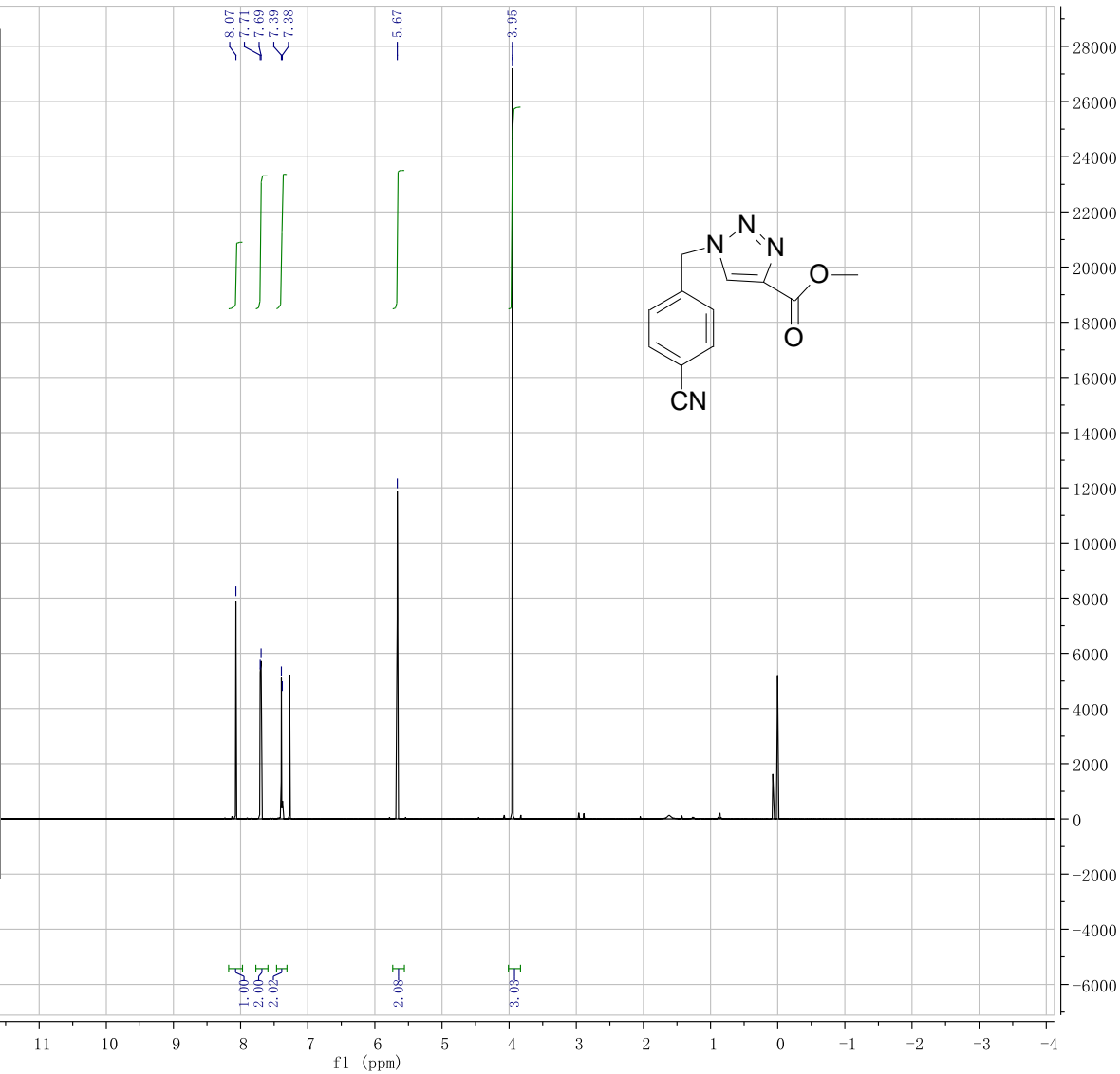
160.879  
140.420  
132.590  
132.464  
129.762  
127.222  
123.367

53.723  
52.183

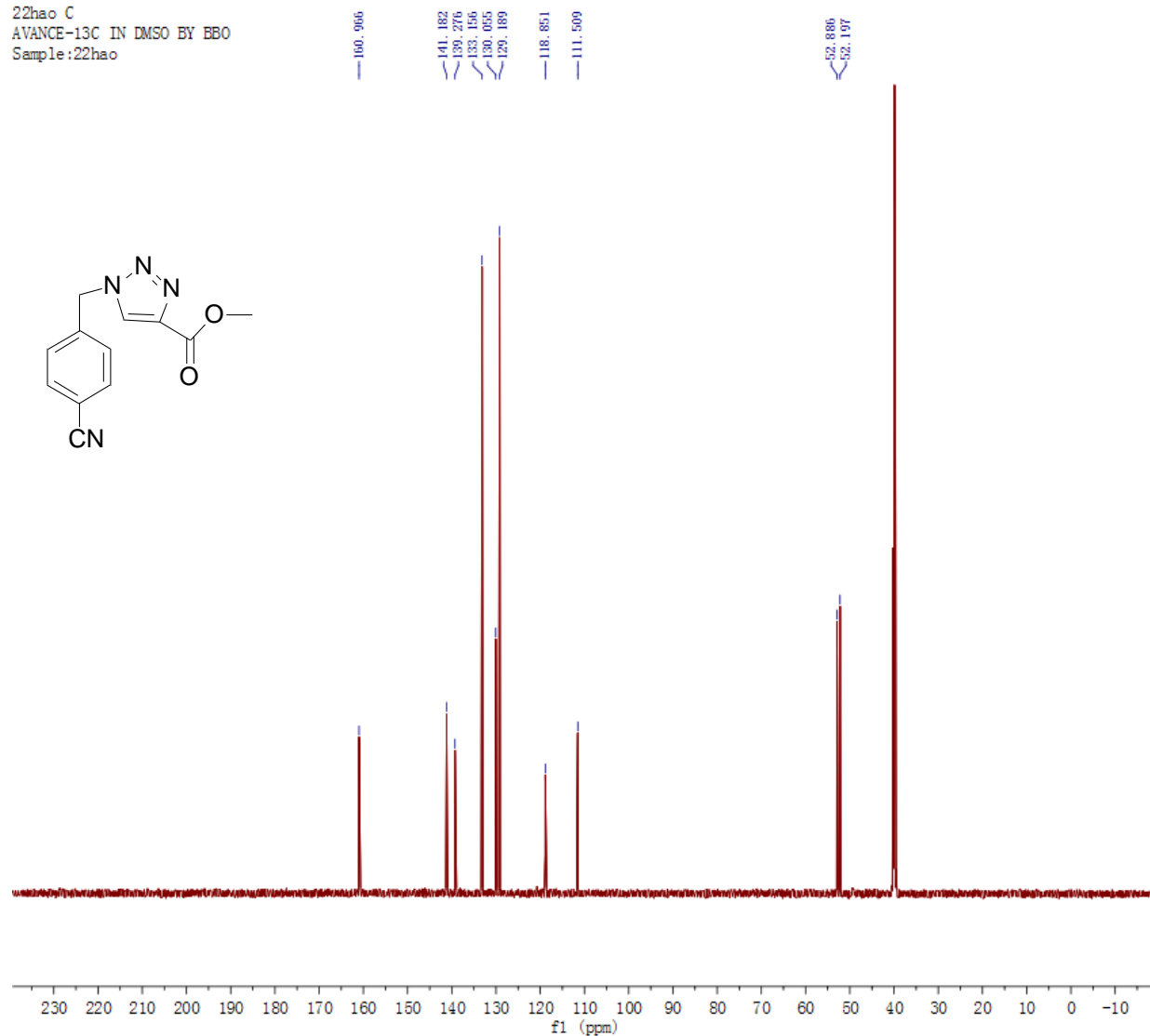
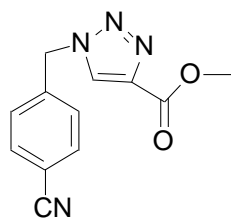


Parameter	Value
1 Data File Name	C:/ Documents and Settings/Administrator/ 桌面/ lidong/ 新建文件夹 (2)/ 17 (20151223) C/ 2/ fid
2 Title	17 (20151223) C
3 Comment	AVANCE-13C IN CDC13 BY BBO Sample:17 (20151223)
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDC13
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	318
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-23T15:38:14
19 Modification Date	2015-12-23T15:39:18
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

AVANCE-1H IN CDCL3 By BBO	
Parameter	Value
1 Data File Name	C:\Users\Administrator.ZGC-20110924\DRY\Desktop\lidong\yang5(san dan zuo)\1\fid
2 Title	AVANCE-1H IN CDCL3 By BBO Sample:yang5(san dan zuo)
3 Comment	
4 Origin	
5 Owner	
6 Site	
7 Spectrometer	
8 Author	
9 Solvent	
10 Temperature	297.9
11 Pulse Sequence	ZG30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	
15 Relaxation Delay	
16 Pulse Width	
17 Acquisition Time	
18 Acquisition Date	
19 Modification Date	
20 Spectrometer Frequency	600.13
21 Spectral Width	12335.5
22 Lowest Frequency	-2472.7
23 Nucleus	
24 Acquired Size	
25 Spectral Size	65536



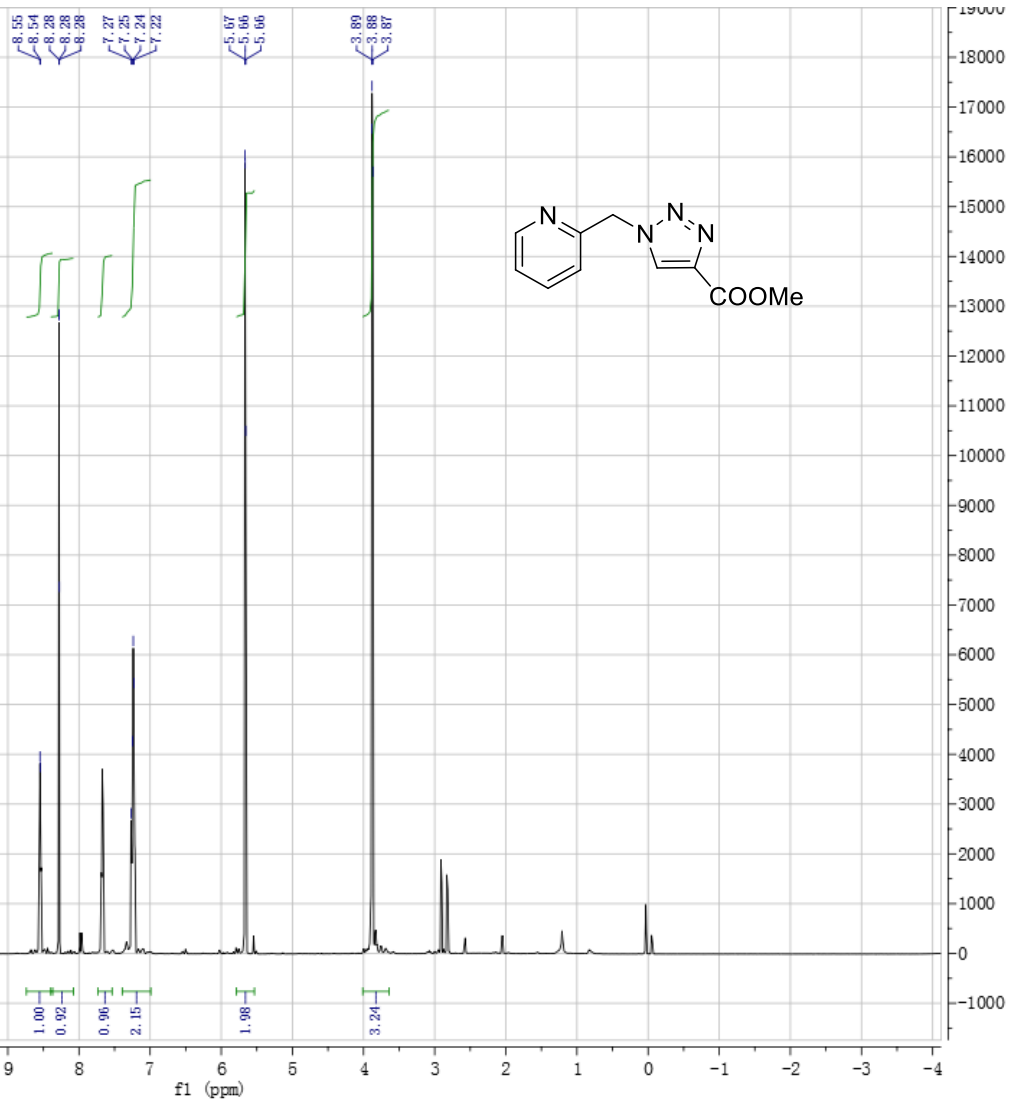
22hao C  
AVANCE-13C IN DMSO BY BBO  
Sample:22hao



Parameter	Value
1 Data File Name	E:/ lidong/ 新建文件夹 (2)/ 22hao C/ 2/ fid
2 Title	22hao C
3 Comment	AVANCE-13C IN DMSO BY BBO Sample:22hao
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	148
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-28T14:08:58
19 Modification Date	2015-12-28T14:09:30
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

yang Shao  
 AVANCE-1H-IN-CDCL3 By EBO  
 Sample: yang 3

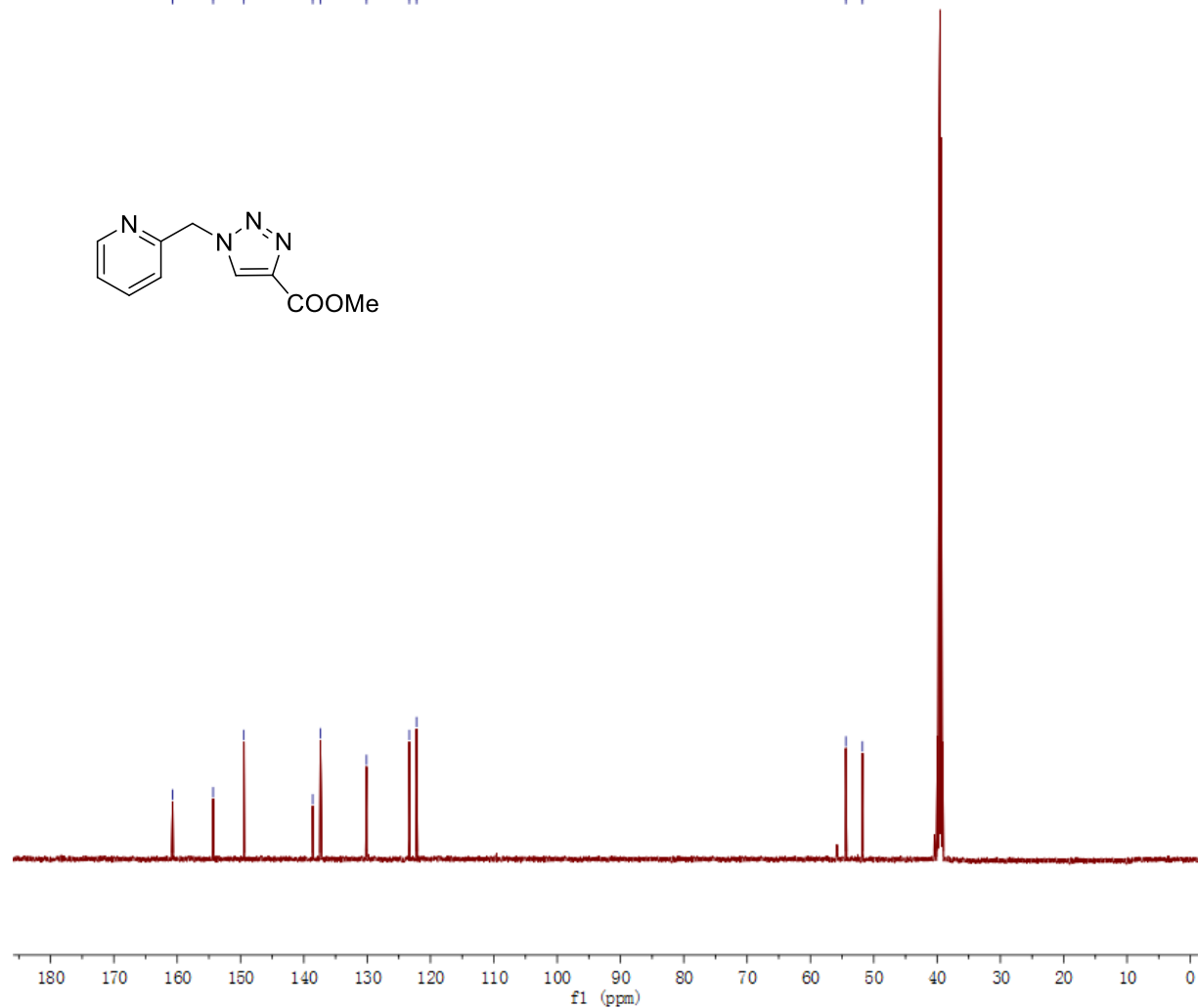
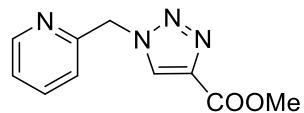
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1 Data File Name	C:/Users/Administrator.ZG/C-20110924WDR/Desktop/20150406/ yang Shao/ 1/ fid
2 Title	yang Shao
3 Comment	AVANCE-1H IN CDCL3 By EBO Sample: yang 3
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCL3
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	88
15 Relaxation Delay	1.0000
16 Pulse Width	12.8500
17 Acquisition Time	2.6564
18 Acquisition Date	2015-03-26T14:55:28
19 Modification Date	2015-03-26T14:55:30
20 Spectrometer Frequency	600.13
21 Spectral Width	12335.5
22 Lowest Frequency	-2472.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



23hao C  
AVANCE-13C IN DMSO BY BBO  
Sample:23hao

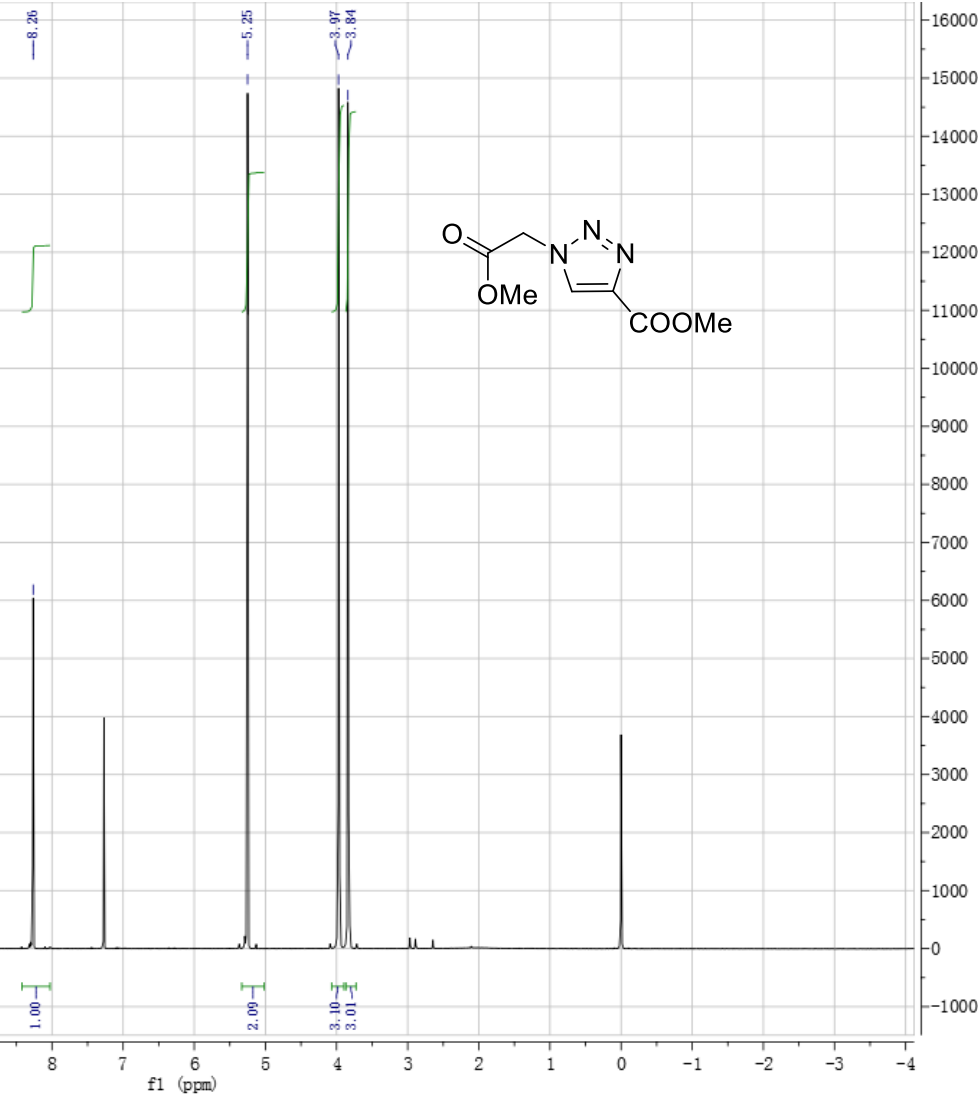
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140.473  
138.608  
137.387  
130.117  
123.353  
122.209

54.412  
51.792

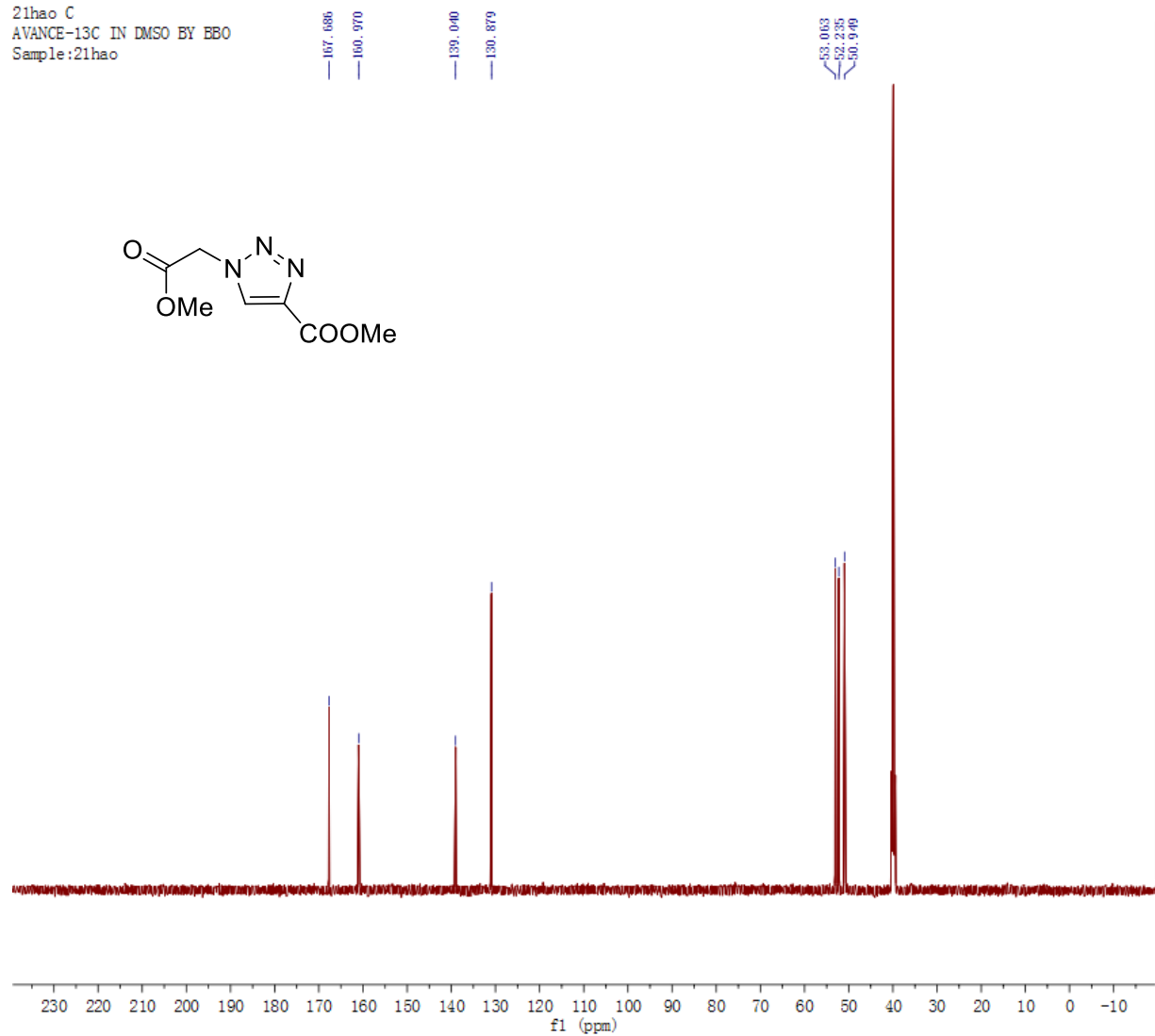
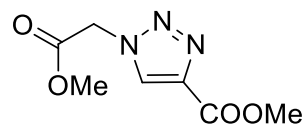


Parameter	Value
1 Data File Name	E:/ lidong/ 新建文件夹 (2)/ 23hao C/ 2/ fid
2 Title	23hao C
3 Comment	AVANCE-13C IN DMSO BY BBO Sample:23hao
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	307
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-28T14:16:33
19 Modification Date	2015-12-28T14:31:18
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-3003.0
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

Parameter	Value
1 Data File Name	C:/Users/Administrator.ZGC-20110924WDR/Desktop/lidong/新建文件夹/yanglhao/1/ fid
2 Title	yang lhao
3 Comment	AVANCE-1H IN CDCL3 By EBO Sample:yang 1
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCL3
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	175
15 Relaxation Delay	1.0000
16 Pulse Width	12.8500
17 Acquisition Time	2.6564
18 Acquisition Date	2015-03-26T14:38:41
19 Modification Date	2015-03-26T14:38:42
20 Spectrometer Frequency	600.13
21 Spectral Width	12335.5
22 Lowest Frequency	-2472.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



21hao C  
AVANCE-13C IN DMSO BY BBO  
Sample:21hao



Parameter	Value
1 Data File Name	E:/ lidong/ 新建文件 夹 (2)/ 21hao C/ 2/ fid
2 Title	21hao C
3 Comment	AVANCE-13C IN DMSO BY BBO Sample:21hao
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	149
14 Receiver Gain	175
15 Relaxation Delay	2.0000
16 Pulse Width	11.5500
17 Acquisition Time	0.8389
18 Acquisition Date	2015-12-28T13:53:53
19 Modification Date	2015-12-28T13:59:20
20 Spectrometer Frequency	150.90
21 Spectral Width	39062.5
22 Lowest Frequency	-2946.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536