# Magnetic Polyvinylpolypyrrolidone Polymer Composite-Supported Copper(I) Catalyst: An Efficient and Easily Reusable Catalyst for Sustainable Synthesis of 1,2,3-Triazoles in Water

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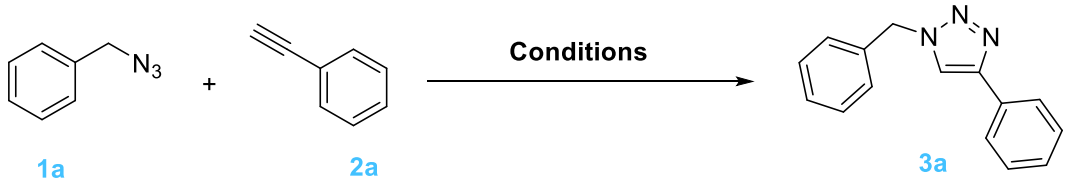
## SUPPORTING INFORMATION

**Table S1.** Comparison of the prepared catalyst with other literature procedures concerning the click reaction between benzyl azide and phenylacetylene.




1a 2a 3a

| Entry | Catalyst[a] (Copper loading) | Solvent/*T* (°C) | Time | Yield (%) | Ref. |
|---|---|---|---|---|---|
| 1 | CPF-1 (2 mol%) | Methanol/80 °C | 8 h | 97 | 1 |
| 2 | CuI-$Fe_3O_4$@$SiO_2$ (TMS-EDTA) (5 mol%) | Ethanol/r.t. | 120 min | 97 | 2 |
| 3 | Cu(II)/GQDs/$NiFe_2O_4$ (0.947 mol%) | $H_2O$/60 °C | 20 min | 98 | 3 |
| 4 | $MnFe_2O_4$@GO@CS/Cu (5 mol%) | $H_2O$/EtOH/50 °C | 30 min | 95 | 4 |
| 5 | CuNPs-PVPP (1 mol%) | $H_2O$/r.t. | 8 h | 96 | 5 |
| 7 | Cu(I)/PVPP-$Fe_3O_4$ (0.2 mol%) | $H_2O$/r.t. | 6 h | 92 | **This work** |

Abbreviations: CPF= copper-containing polyoxomolybdates-based framework; CS= chitosan; GQDs = graphene quantum dots; GO= graphene oxide.

**Table S2.** Concentration of phenylacetylene in the reactions studied at the optimized reaction

| | Concentration of phenylacetylene (in ppm) | | |
|---|---|---|---|
| **Time (h)** | **Reaction 1[a]** | **Reaction 2[b]** | **Reaction 3[c]** |
| 0 | 5645.3358 | 5610.8334 | 6427.9766 |
| 0.5 | 4097.9068 | 5115.1649 | 5937.12708 |
| 1 | 2461.85808 | 3099.18947 | 3879.78262 |
| 2 | 1223.44668 | 1930.91836 | 2042.3204 |
| 3 | 815.09916 | 1266.66467 | 1226.81721 |
| 4 | 407.51849 | 787.260782 | 858.016992 |
| 6 | 0 | 118.475623 | 158.932211 |

[a]CuAAC reaction between benzyl azide and phenylacetylene catalyzed by fresh catalyst. [b]CuAAC reaction between benzyl azide and phenylacetylene catalyzed by the first reused catalyst. [c]CuAAC reaction between phenylacetylene and the *in situ* formed benzyl azide from benzyl bromide and sodium azide.

**Table S3.** Concentration of phenylacetylene in the studied hot filtration test at 60 °C (Reaction 4: Reaction 5).

| | Concentration of phenylacetylene (in ppm) | |
|---|---|---|
| **Time (min)** | **Reaction 4[a]** | **Reaction 5[b]** |
| 0 | 4846.8126 | 4436.495 |
| 15 | 2856.95599 | 2867.90245 |
| 30 | 1222.84725 | 2777.5076 |
| 60 | 0 | 2614.1248 |

[a]The model reaction was carried out at 60 °C. [b]Hot filtration test of the model reaction by removal of the Cu(I)/PVPP-$Fe_3O_4$ catalyst at 15 min.

**1. Characterization of the 1,2,3 triazole products (3a-3k)**

**1-benzyl-4-phenyl-1*H*-1,2,3-triazole (3a)**

White solid. Yield: 92%. m.p.: 130-132 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.60 (s, 2H, $CH_2$); 7.28-7.44 (m, 8H, $CH_{ar}$); 7.68 (s,1H, $CH_{triazole}$); 7.81-7.83 (d, 2H, $CH_{ar}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 54.4 ($CH_2$); 119.5 ($CH_{ar}$); 125.9 ($3CH_{ar}$); 127.8 ($2CH_{ar}$); 128.2 ($2CH_{ar}$); 129.2 ($CH_{triazole}$); 131,5 ($C_{ar}$); 135.0 ($C_{ar}$); 148.3 ($C_{triazole}$). HR-MS (FAB+) *m/z*: Calcd for $C_{15}H_{14}N_3$: 236.1188; Found: 236.1177. NMR data are in accordance with those reported for this compound[6].

**1-Benzyl-4-p-tolyl-1*H*-1,2,3-triazole (3b)**

White solid. Yield: 83%. m.p.: 154-155 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 2.38 (s, 3H, $CH_3$), 5.59 (s, 2H, $CH_2$), 7.22-7.42 (m, 7H, $CH_{ar}$), 7.66 (s, 1H, $CH_{triazole}$), 7.70-7.73 (d, 2H, $CH_{ar}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 21.67 ($CH_3$), 54.64 ($CH_2$), 126.00 ($CH_{ar}$), 128.14 ($2CH_{ar}$), 128.47 ($2CH_{ar}$), 129.16 ($2CH_{ar}$), 129.54 ($2CH_{ar}$), 129.88 ($C_{ar}$), 131.68 ($CH_{triazole}$), 135.14 ($2C_{ar}$), 138.41 ($C_{triazole}$). HR-MS (FAB+) *m/z*: Calcd for $C_{16}H_{15}N_3$: 250.1339; Found: 250.1339. NMR data agree with those reported for this compound[7].

**(1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl benzoate (3c)**

White solid. Yield: 99%. m.p.: 122-123 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.47 (s, 2H, $CH_2$), 5.54 (s, 2H, $CH_2$), 7.31-7.38 (m, 5H, $CH_{ar}$), 7.40-7.46 (dd, 1H, $CH_{ar}$), 7.57 (t, 1H, $CH_{ar}$), 7.70 (s, 1H, $CH_{triazole}$), 8.03-8.05 (d, 2H, $CH_{ar}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 54.76 ($CH_2$), 58.45 ($CH_2$), 128.57 ($CH_{triazole}$), 128.77 ($2CH_{ar}$), 129.26 ($2CH_{ar}$), 129.56 ($2CH_{ar}$), 130.14 ($4CH_{ar}$), 133.59 ($C_{ar}$), 134.75 ($C_{triazole}$), 153.18 ($C_{ar}$), 166.84 ($C_{carbonyl}$). HR-MS (FAB+) m/z:

Calcd for $C_{17}H_{15}N_3O_2$: 294.1237; Found: 294.1241. The NMR data align with the previously reported data for this compound[8].

**1-benzyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole (3d)**

White solid. Yield: 99%. m.p.: 122-123 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.21 (s, 2H, $CH_2$), 5.55 (s, 2H, $OCH_2$), 6.96-7.00 (q, 3H, $CH_{ar}$), 7.28-7.33 (q, 4H, $CH_{ar}$), 7.37-7.41 (m, 3H, $CH_{ar}$), 7.57 (s, 1H, $CH_{triazole}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 54.70 ($CH_2$), 62.46 ($CH_2$), 115.18 ($2CH_{ar}$), 121.65 ($CH_{triazole}$), 128.53 ($2CH_{ar}$), 129.22 ($2CH_{ar}$), 129.55 ($4CH_{ar}$), 129.92 ($C_{ar}$), 134.87 ($C_{triazole}$), 158.60 ($C_{ar}$). HR-MS (FAB+) *m/z*: Calcd for $C_{16}H_{15}N_3O$: 266.1288; Found: 266.1289. The NMR data align with the previously reported data for this compound[8].

**4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzaldehyde (3e)**

White solid. Yield: 99%. m.p.: 134-135 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.62 (s, 2H, $CH_2$); 7.28-7.43 (m, 5H, $CH_{ar}$); 7.8 (s, 1H, $CH_{triazole}$); 7.92-7.94 ( d , 2H, $CH_{ar}$); 7.98-8.00 ( d , 2H, $CH_{ar}$) ; 10,02 (s, 1H, CHO). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 54.4 ($CH_2$); 120.7 ($CH_{ar}$); 126.0 ($2CH_{ar}$); 128.2 ($2CH_{ar}$); 129.0 ($2CH_{ar}$); 129.3 ($2CH_{ar}$); 130,4 ($CH_{triazole}$); 134.3 ($CH_{ar}$); 135.8 ($CH_{ar}$); 136.3 ($CH_{ar}$); 146.9 ($C_{triazole}$); 191.7 (CHO). HR-MS (FAB+) *m/z*: Calcd for $C_{16}H_{14}N_3O$: 264.1137; Found: 264,1134. NMR data agree with those reported for this compound[8].

**Methyl 4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzoate (3f)**

White solid. Yield: 75%. m.p.: 176-177 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 3.94 (s, 3H, $CH_3$), 5.61 (s, 2H, $CH_2$), 7.33-7.36 (m, 2H, $CH_{ar}$), 7.40-7.43 (m, 3H, $CH_{ar}$), 7.76 (s, 1H, $CH_{triazole}$), 7.88-7.91 (d, 2H, $CH_{ar}$), 8.08-8.11 (d, 2H, $CH_{ar}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 52.54 ($CH_2$), 54.78 ($CH_2$), 120.73 ($CH_{ar}$), 125.87 ($CH_{ar}$), 128.55 ($2CH_{ar}$), 129.35 ($2CH_{ar}$), 129.65 ($2CH_{ar}$), 130.01 ($CH_{ar}$), 130.59 ($CH_{triazole}$), 134.80 ($C_{ar}$), 135.22 ($C_{ar}$), 148.06 ($C_{triazole}$), 156.25 ($C_{ar}$), 167.16 ($C_{carbonyl}$). HR-MS (FAB+) *m/z*: Calcd for $C_{17}H_{15}N_3O_2$: 294.1237; Found: 294.1242. NMR data are in accordance with those reported for this compound[8].

**Ethyl 1-benzyl-1*H*-1,2,3-triazole-4-carboxylate (3g)**

White solid. Yield: 53%. m.p.: 89-90 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 1.35-1.40 (t, 3H, $CH_3$); 4.35-4.42 (q, 4H, $OCH_2$); 5.57 (s, 2H, $CH_2$); 7.26-7.29 (m, 3H, $CH_{ar}$); 7.37-7.4 (m, 3H, $CH_{ar}$); 7.96 (s, 1H, $CH_{triazol}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 14.4 ($CH_3$); 54.6 ($CH_2$); 61.4 ($CH_2$); 127.4 ($CH_{ar}$); 128.4 ($2CH_{ar}$); 129.3 ($CH_{ar}$); 129.4 ($CH_{ar}$); 133.8 ($CH_{triazolic}$); 140.7

($C_{triazolic}$); 160.8 (CO). HR-MS (FAB+) *m/z*: Calcd for $C_{12}H_{14}N_3O_2$: 232.1086; Found: 232.1087. NMR data agree with those reported for this compound[6].

**4-((4-phenyl-1*H*-1,2,3-triazol-1-yl)methyl)pyridine (3h)**

White solid. Yield: 95%. m.p.: 81.3 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.73 (s, 2H, $CH_2$); 7.25-7.36 (m, 2H, $CH_{ar}$); 7.41-7.46 (m, 3H, $CH_{ar}$); 7.69-7.75 (m, 1H, $CH_{ar}$); 7.83-7.87 (m, 1H, $CH_{ar}$); 7.96 (s, 1H, $CH_{Triazole}$); 8.64 (s, 2H, $CH_{ar}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 56.11 ($CH_2$); 120.57 (2 $CH_{ar}$); 124.00 (2 $CH_{ar}$); 126.13 ($CH_{ar}$); 128.58 (2 $CH_{ar}$); 129.21 ($C_{ar}$); 130.93 ($CH_{Triazole}$); 137.84 ($C_{ar}$); 150.13 ($C_{Triazole}$); 154.91 (2 $CH_{ar}$). HR-MS MS (FAB+) *m/z*: Calcd for $C_{14}H_{12}N_4$: 236.1062; Found: 237.1132. The NMR data align with the previously reported data for this compound[8].

**1,4-diphenyl-1*H*-1,2,3-triazole (3i)**

White solid. Yield: 72%. m.p.: 183–184 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.33–7.4 (m, 2H, $CH_{ar}$); 7.44–7.49 (t, 2H, $CH_{ar}$); 7.53–7.58 (t, 2H, $CH_{ar}$); 7.79–7.81 (d, 2H, $CH_{ar}$); 7.92–7.94 (d, 2H, $CH_{ar}$); 8.22 (s, 1H, $CH_{triazole}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 118.07 ($2CH_{ar}$); 120.98 ($C_{ar}$); 126.34 (2 $CH_{ar}$); 128,98 ($CH_{ar}$); 129,31 ($CH_{ar}$); 129,37 ($2CH_{ar}$); 130,23 ($2CH_{ar}$); 130.34 ($CH_{triazolic}$); 130.73 ($C_{ar}$); 137.47 ($C_{triazolic}$). HR-MS (FAB+) *m/z*: Calcd for $C_{14}H_{12}N_3$: 222.1031; Found: 222.1029. The NMR data align with the previously reported data for this compound[6].

**4-(phenoxymethyl)-1-phenyl-1*H*-1,2,3-triazole (3j)**

White solid. Yield: 93%. m.p.: 87-88 °C. $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.23 (s, 2H, $CH_2$), 6.89-6.97 (m, 3H, $CH_{ar}$ ), 7.18-7.27 (d, 2H, $CH_{ar}$ ), 7.37-7.45 (m, 3H, $CH_{ar}$ ), 7.65-7.68 (d, 2H, $CH_{ar}$ ), 7.98 (s, 1H, $CH_{Triazole}$ ). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 62.40 ($CH_2$), 115.18 ($2CH_{ar}$), 121.03 ($CH_{Triazole}$), 121.28 ($CH_{ar}$), 121.77 ($2CH_{ar}$), 129.28 ($C_{ar}$), 130.01 ($CH_{ar}$), 130.18 ($2CH_{ar}$), 137.40 ($2CH_{ar}$), 145.49 ($C_{Triazole}$), 158.58 ($C_{ar}$). HR-MS (FAB+) *m/z*: Calcd for $C_{15}H_{13}N_3O$: 252.1130; Found: 252.1129. The NMR data agree with the previously reported data for this compound[8].

**(1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl benzoate (3k)**

White solid. Yield: 82%. m.p.: 110-111 °C. $^{1}$H NMR (400 MHz, $CDCl_3$, δ ppm): 5.59 (s, 2H, $CH_2$), 7.46-7.59 (m, 5H, $CH_{ar}$ ), 7.75-7.77 (d, 2H, $CH_{ar}$), 8.07-8.11 (d, 2H, $CH_{ar}$), 8.16 (s, 1H, $CH_{Triazole}$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm)**:** 58.45 ($CH_2$), 118.65 ($CH_{Triazole}$), 121.07 ($C_{ar}$), 122.69 ($2CH_{ar}$), 124.12 ($2CH_{ar}$), 128.83 ($CH_{ar}$), 129.34 (2 $CH_{ar}$), 130.18 ($C_{ar}$), 133.67 ($C_{ar}$), 137.32 ($CH_{ar}$), 144.09 ($C_{Triazole}$), 166.93 ($C_{Carbonyle}$). HR-MS (FAB+) *m/z*: Calcd for $C_{16}H_{13}N_3O_2$: 280.1080; Found: 280.1080. The NMR data align with the previously reported data for this compound[8].

## 2. References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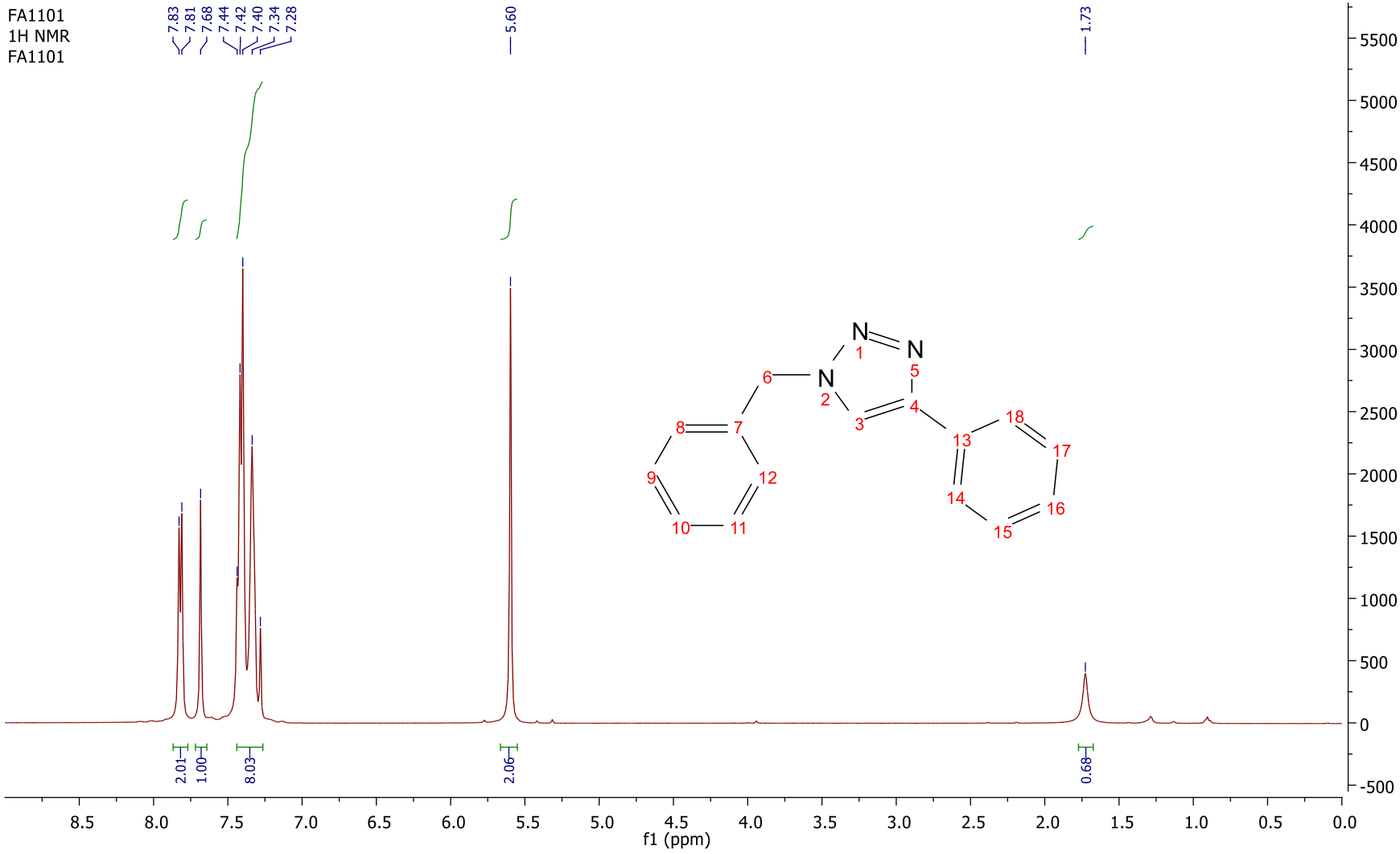
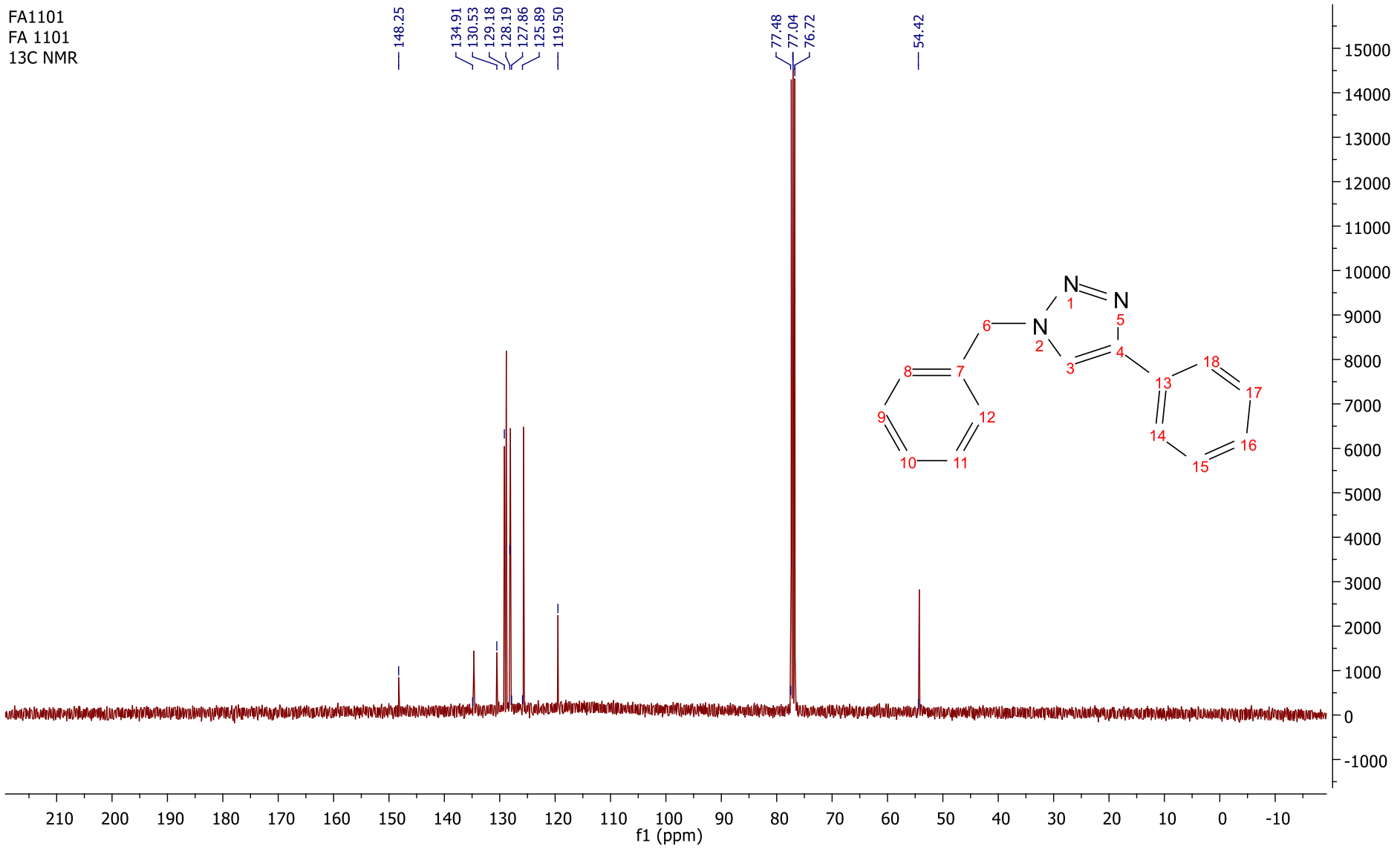
**1-benzyl-4-phenyl-1*H*-1,2,3-triazole (3a)**

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54.42
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N
N
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2
3
4
5
6
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8
9
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11
12
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14
15
16
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9000
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6000
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200
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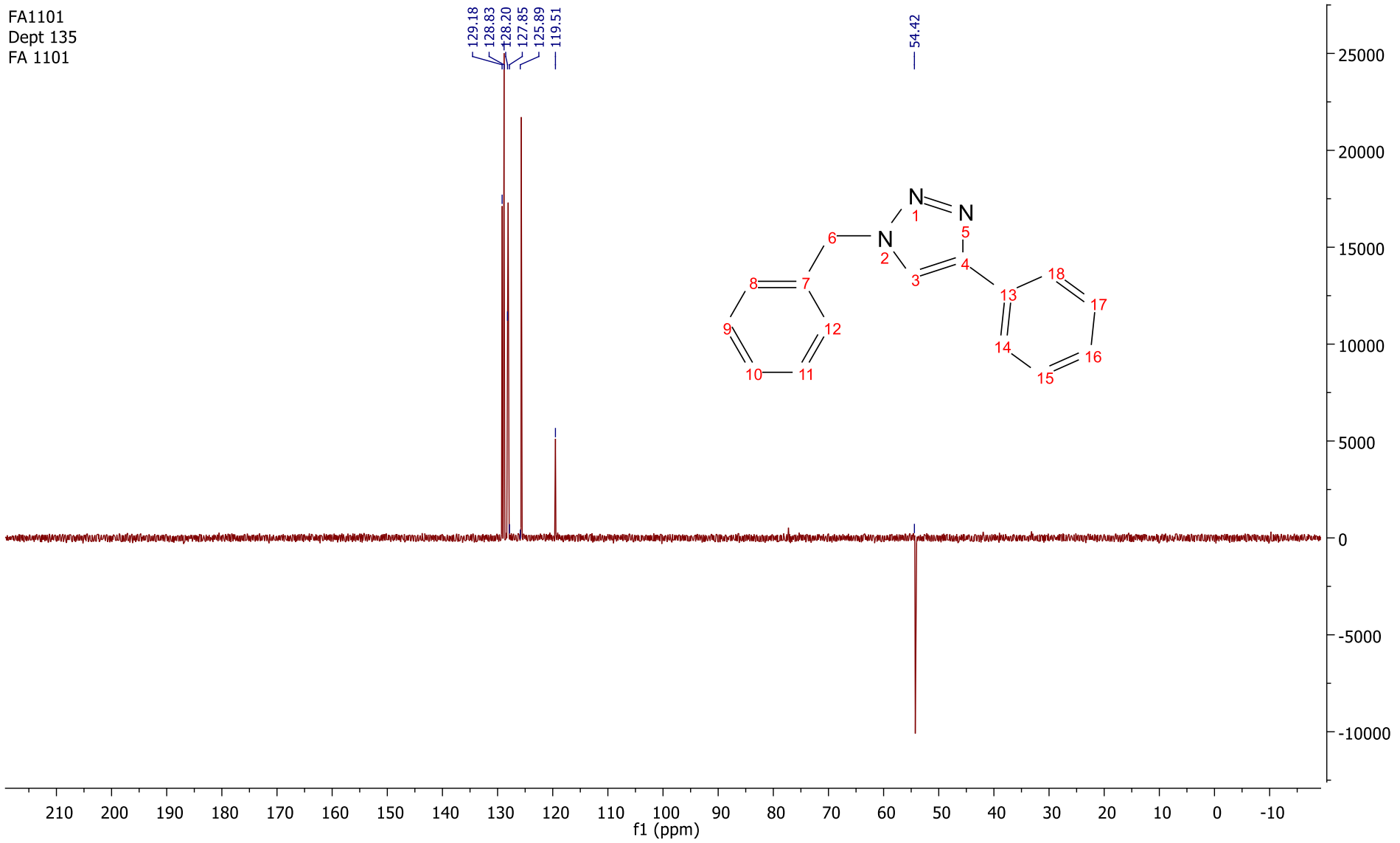
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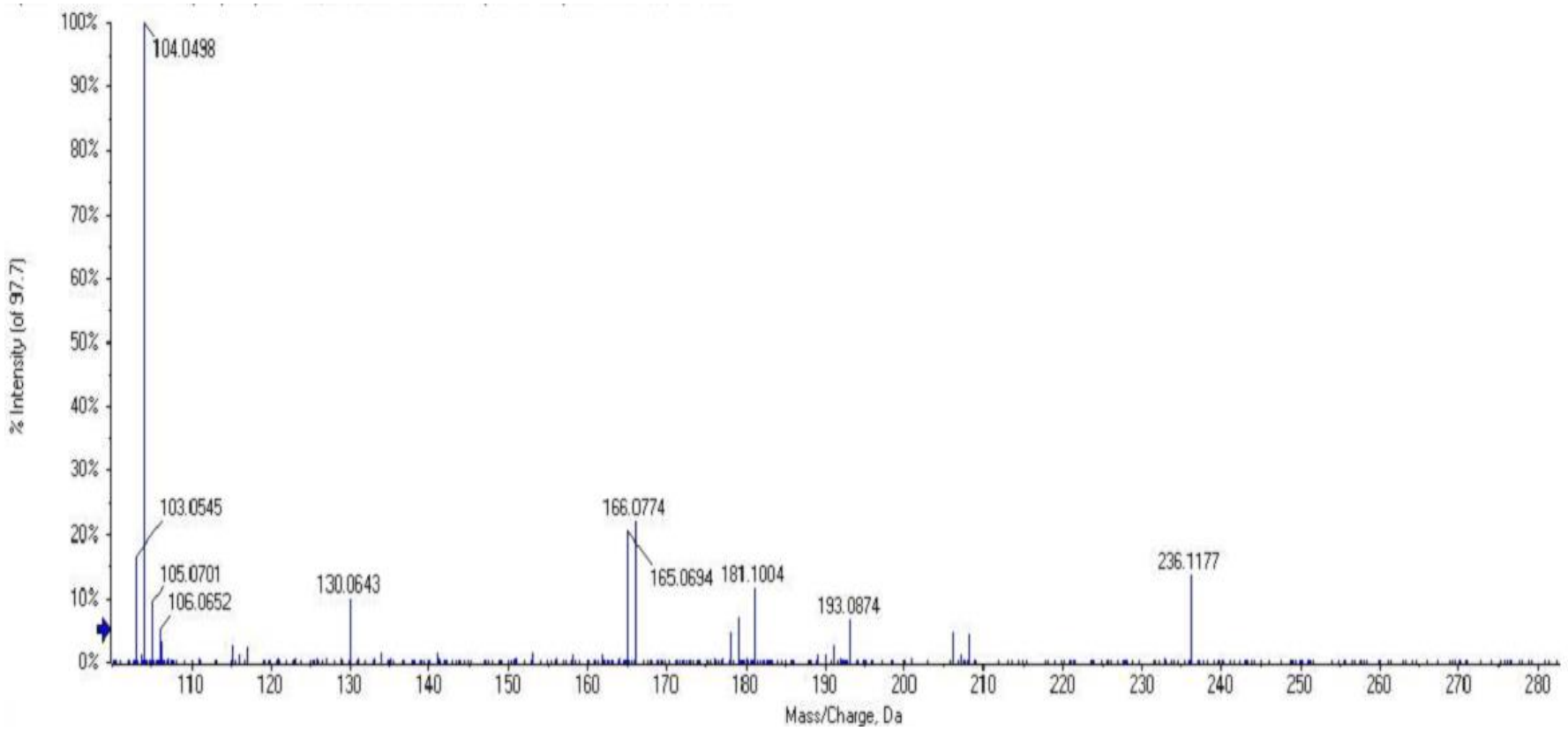
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% Intensity (of 97.7)
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236.1177
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120
130
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190
200
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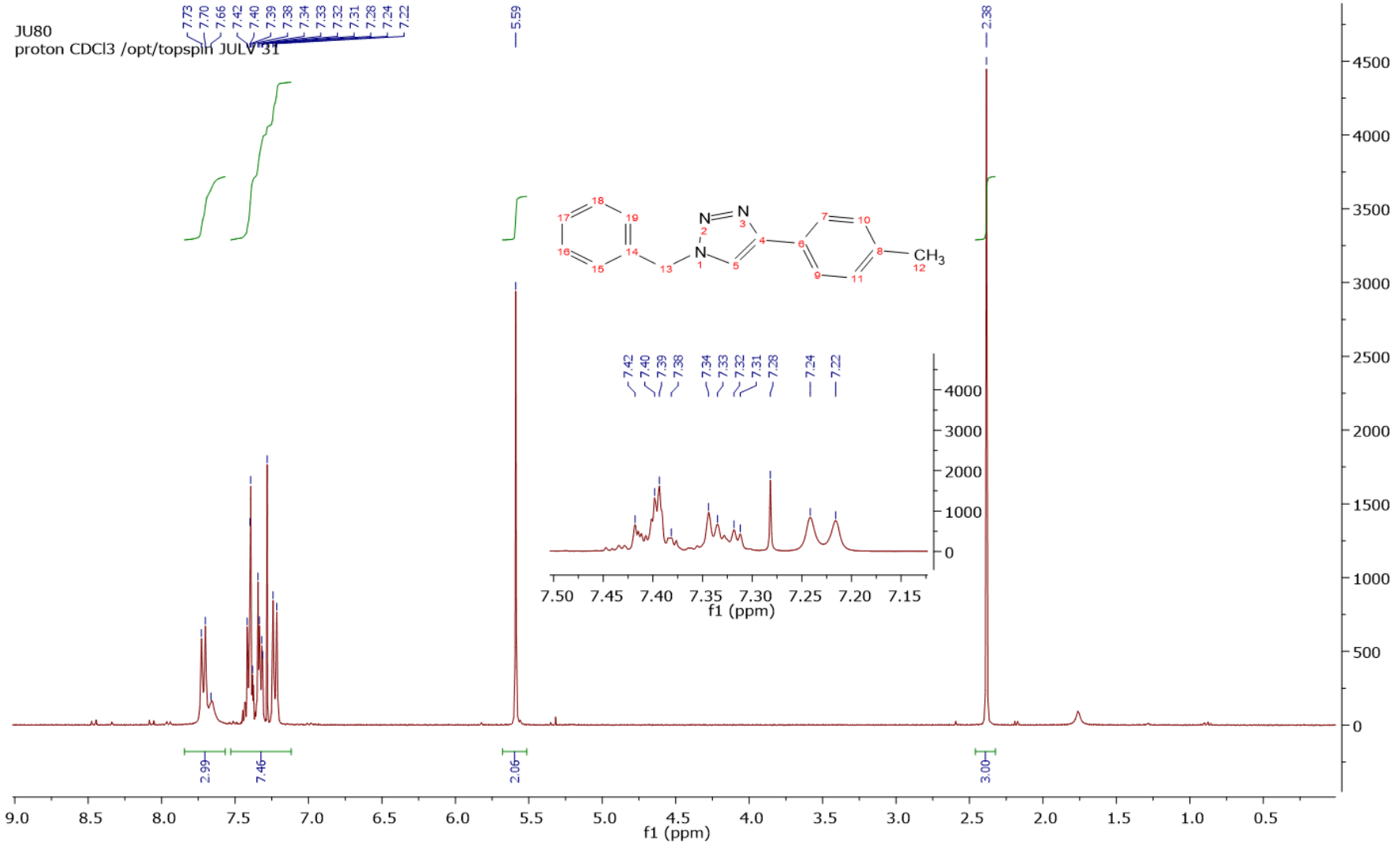
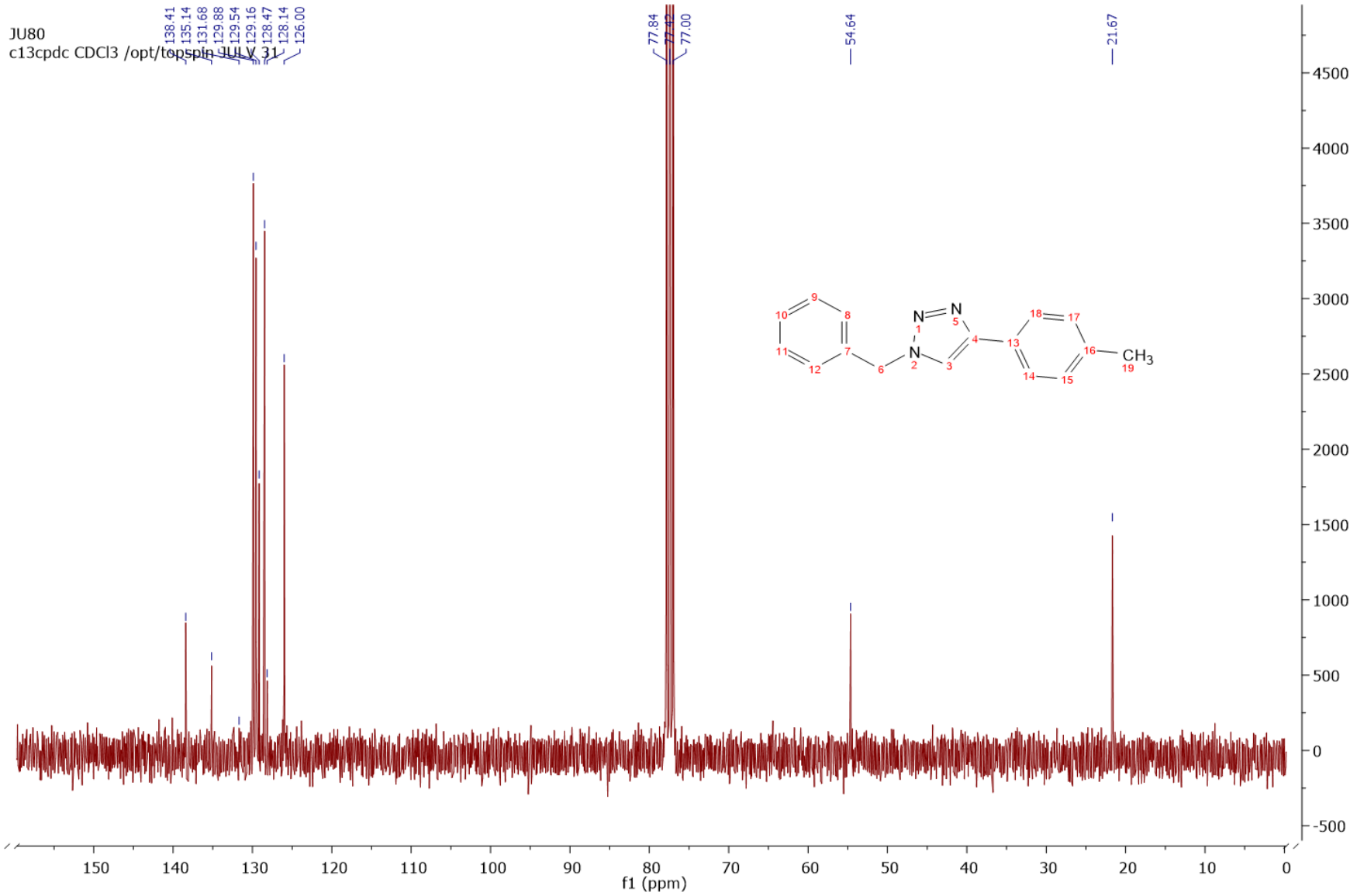
Mass/Charge, Da

**1- Benzyl-4-p-tolyl-1H-1,2,3-triazole (3b)**

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131.68
129.88
129.54
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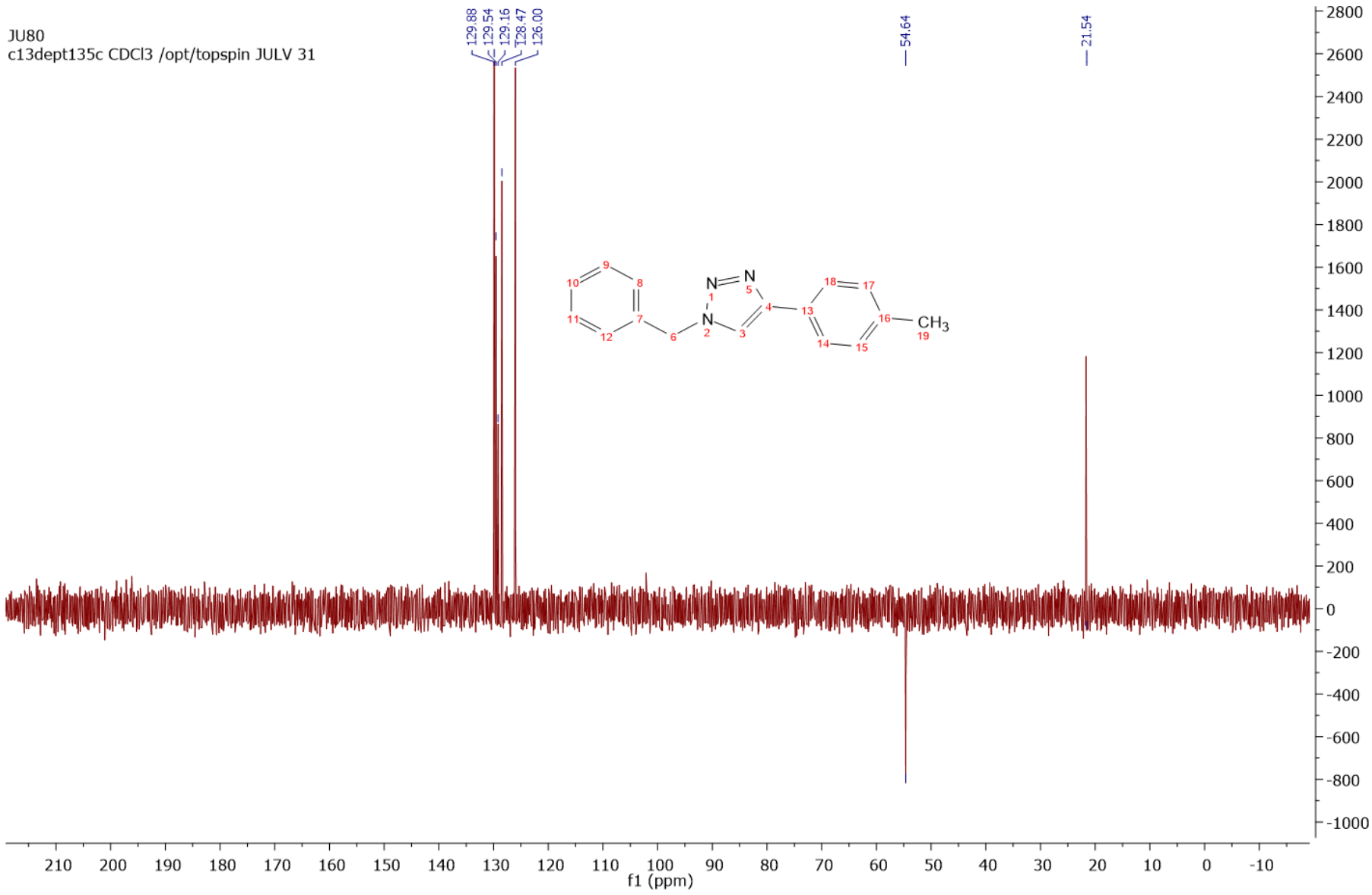
77.00
54.64
21.67
f1 (ppm)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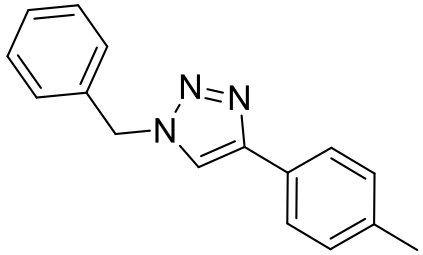
f1 (ppm)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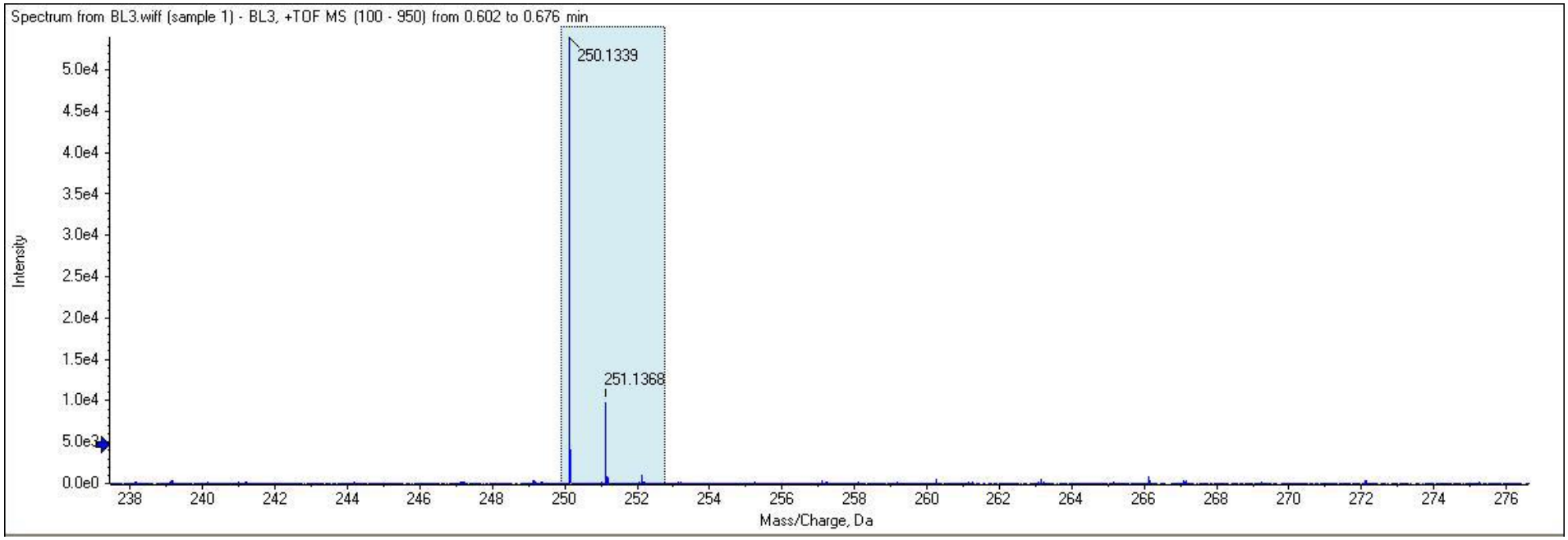
N
N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5.0e3
0.0e0
238
240
242
244
246
248
250
252
254
256
258
260
262
264
266
268
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272
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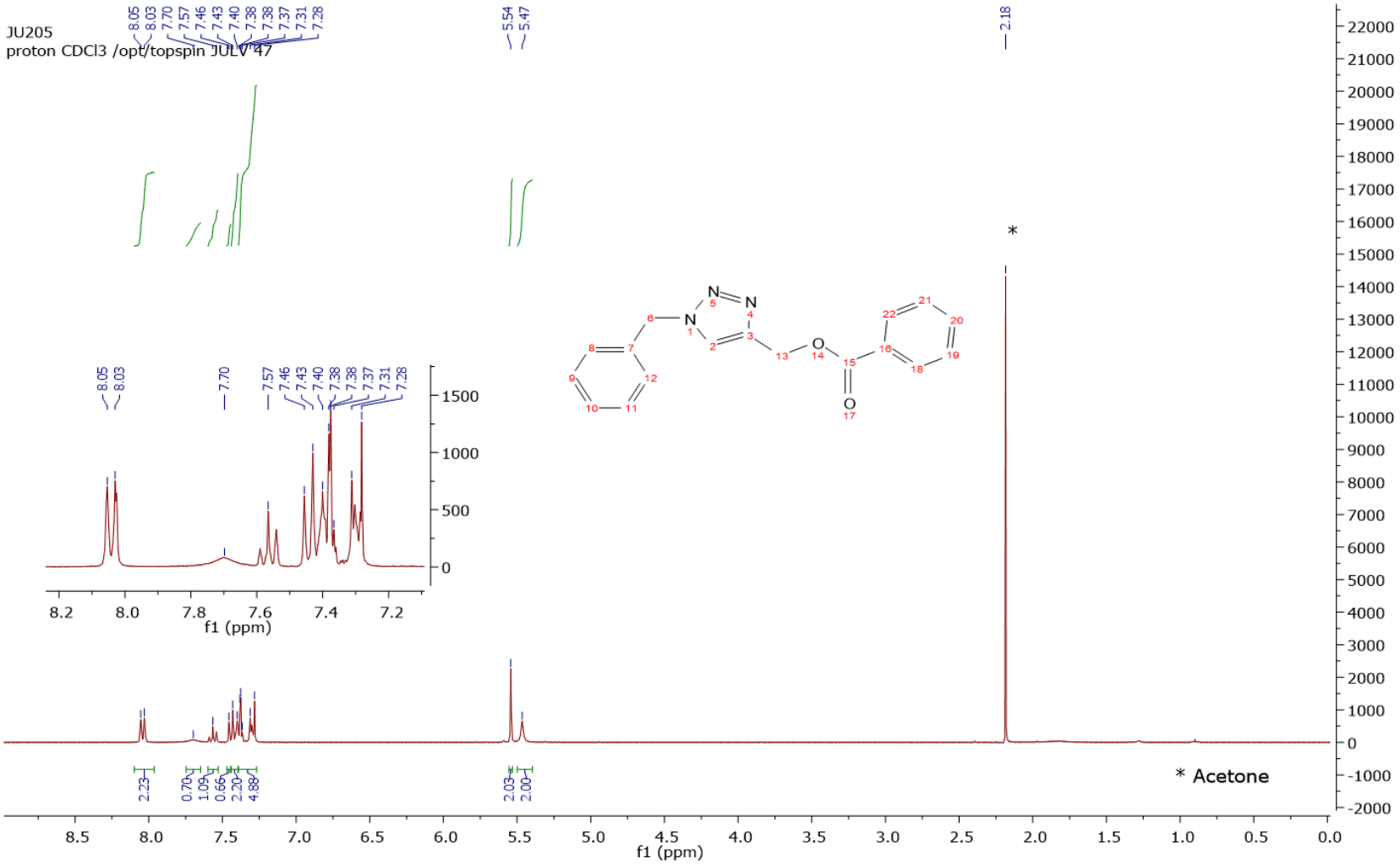
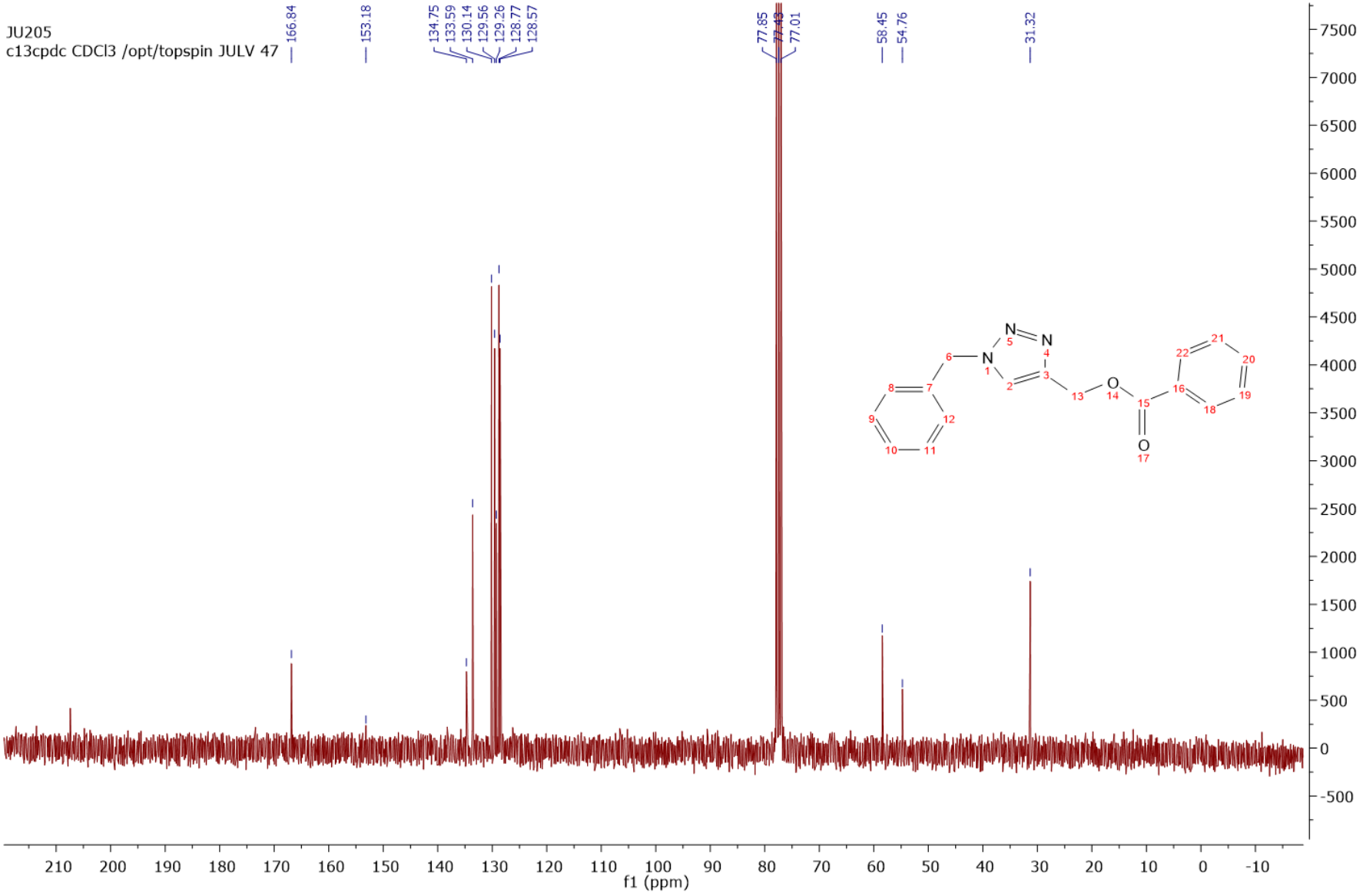
276
Mass/Charge, Da

**(1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl benzoate (3c)**

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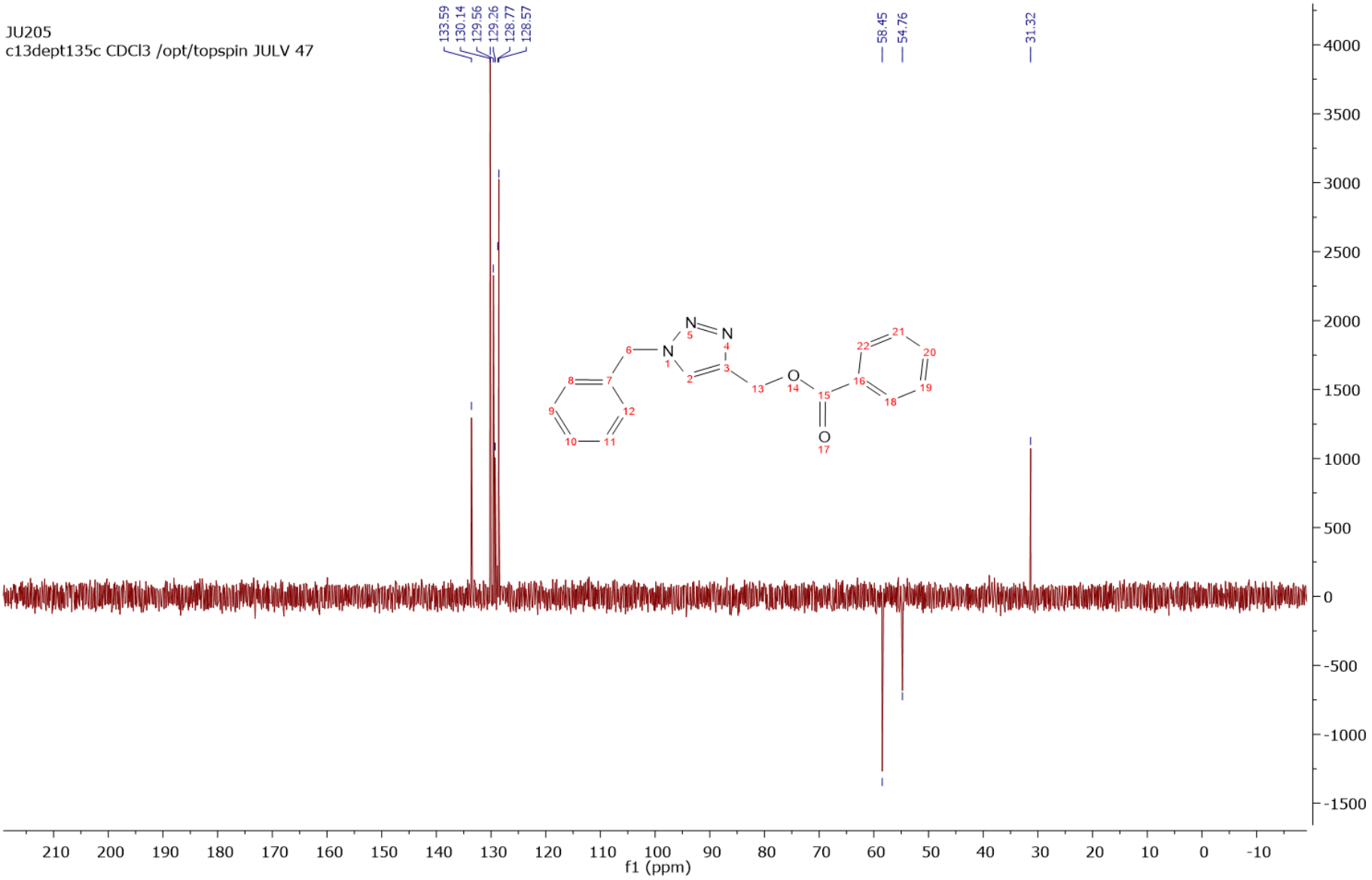
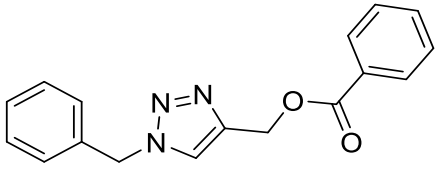
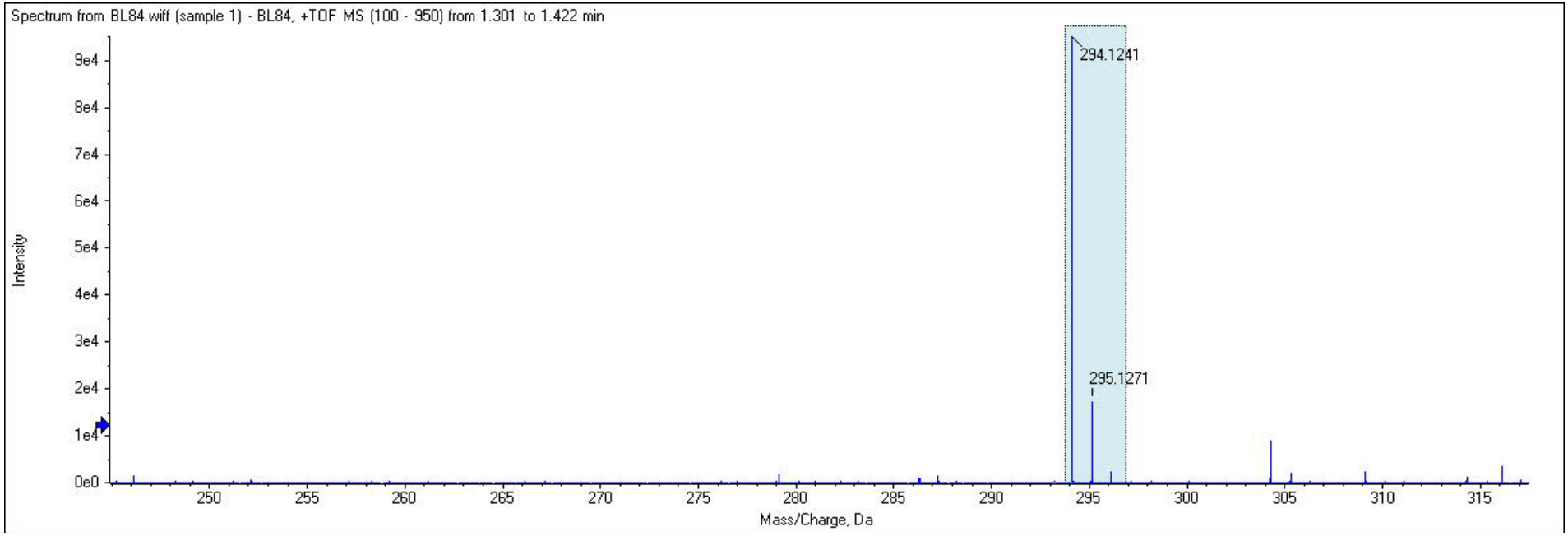
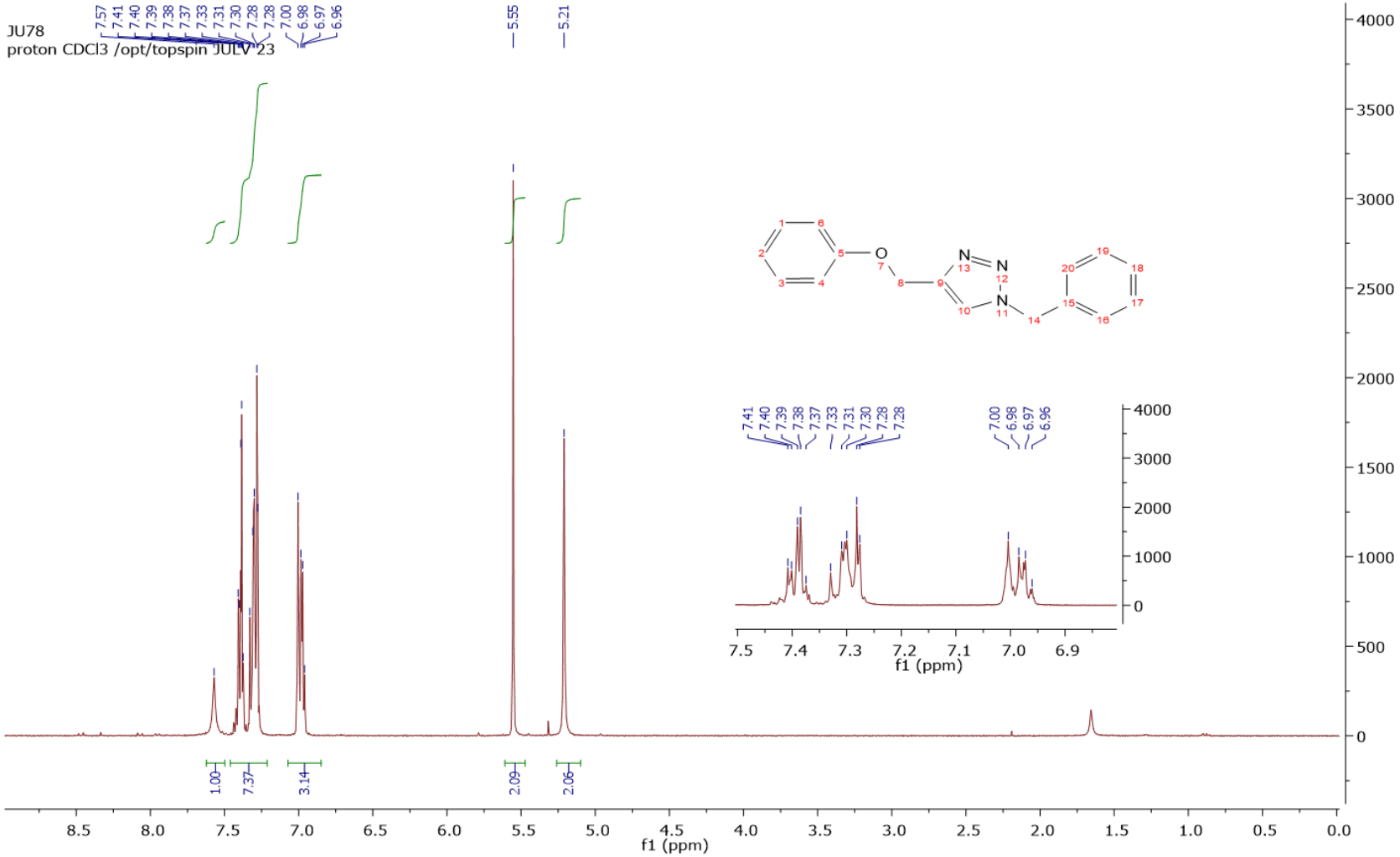
129.26
128.77
128.57
77.85
77.43
77.01
58.45
54.76
31.32
f1 (ppm)

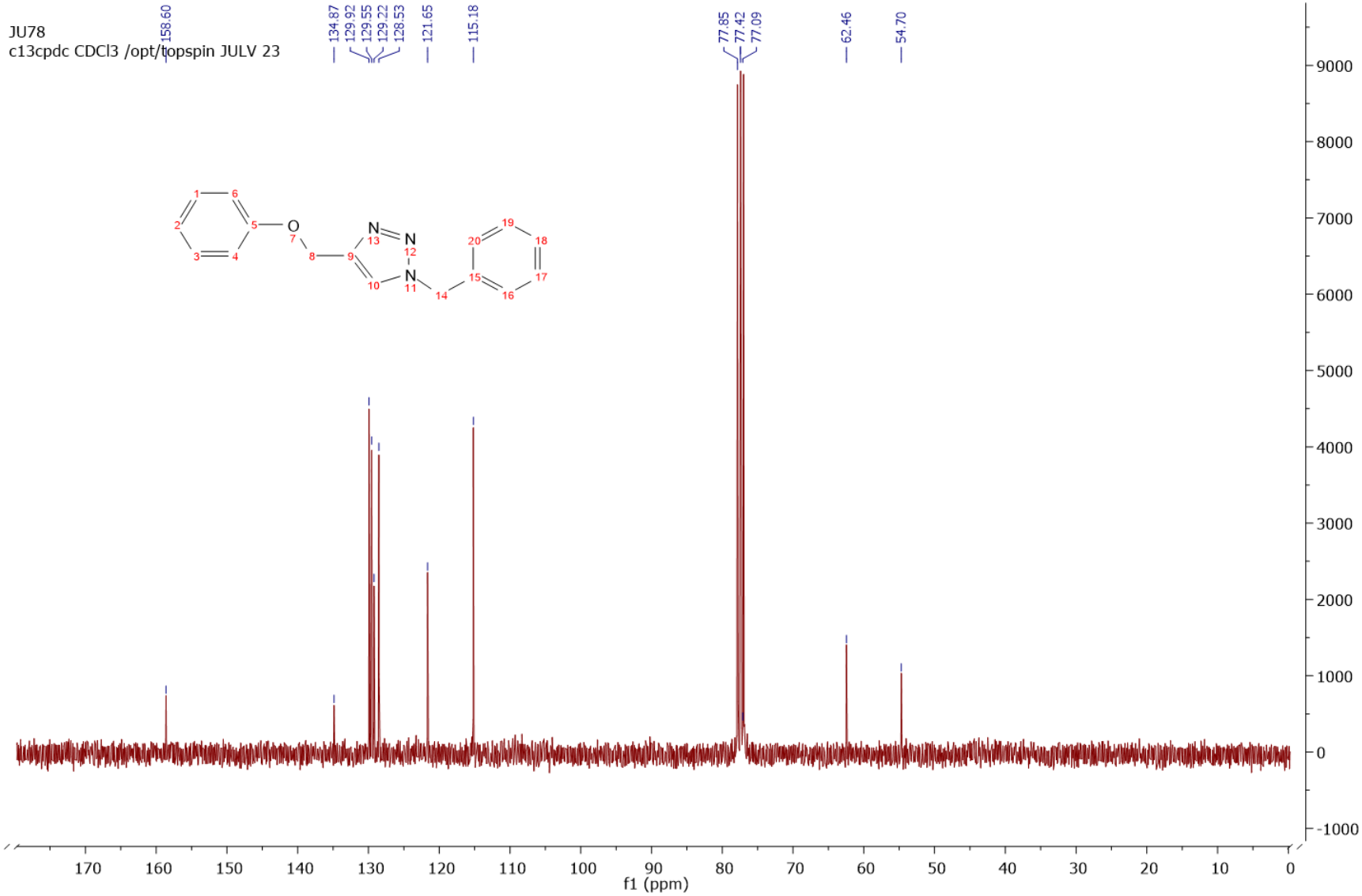

JU205
c13dept135c CDCl3 /opt/topspin JULV 47
133.59
130.14
129.56
129.26
128.77
128.57
58.45
54.76
31.32
f1 (ppm)

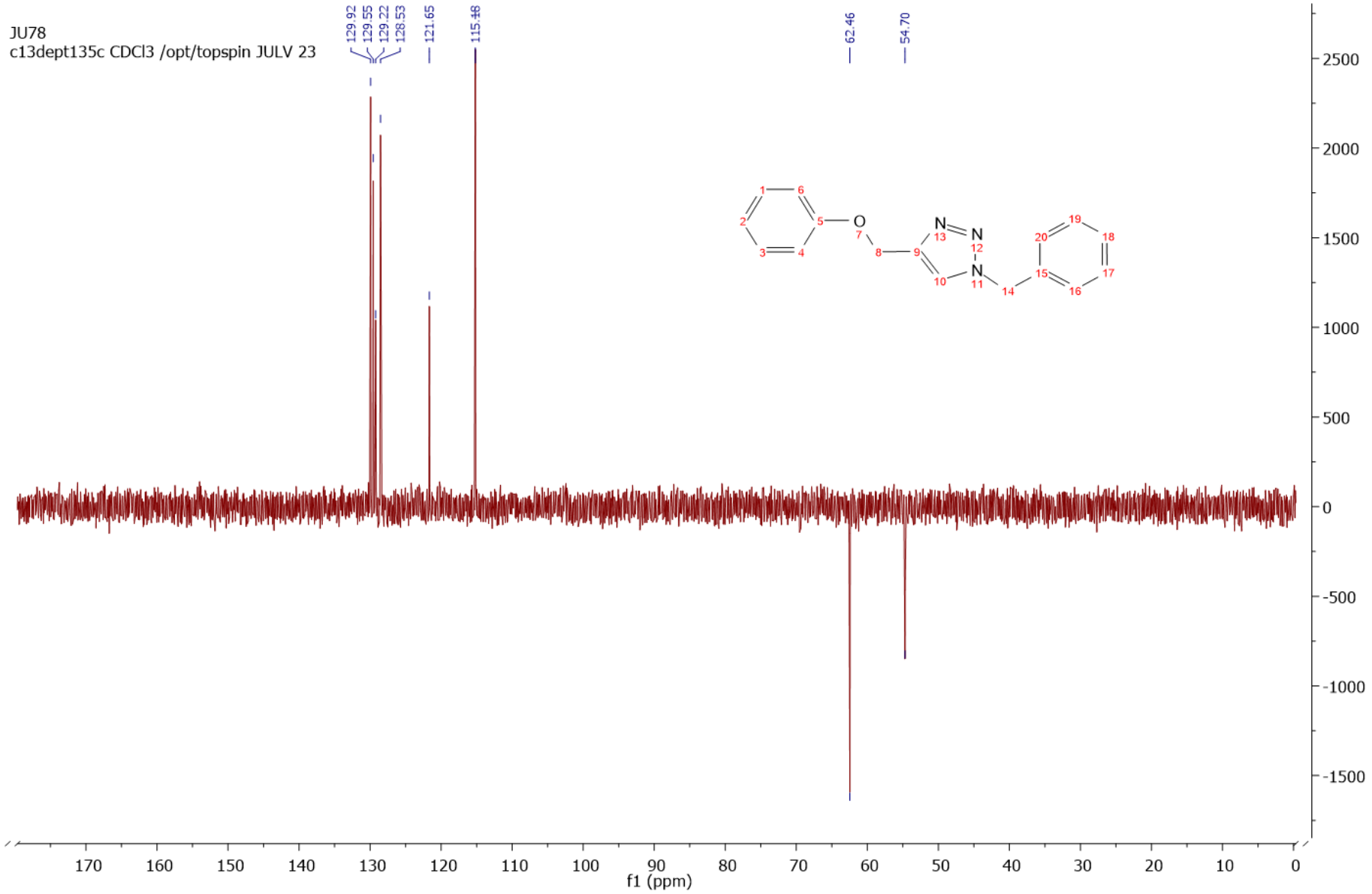


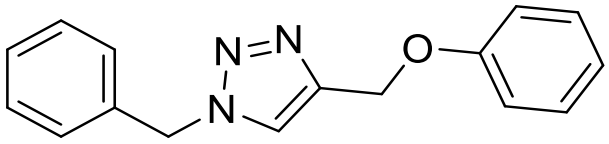

Spectrum from BL84.wiff (sample 1) - BL84, +TOF MS (100 - 950) from 1.301 to 1.422 min
294.1241
295.1271
Intensity
9e4
8e4
7e4
6e4
5e4
4e4
3e4
2e4
1e4
0e0
250
255
260
265
270
275
280
285
290
295
300
305
310
315
Mass/Charge, Da

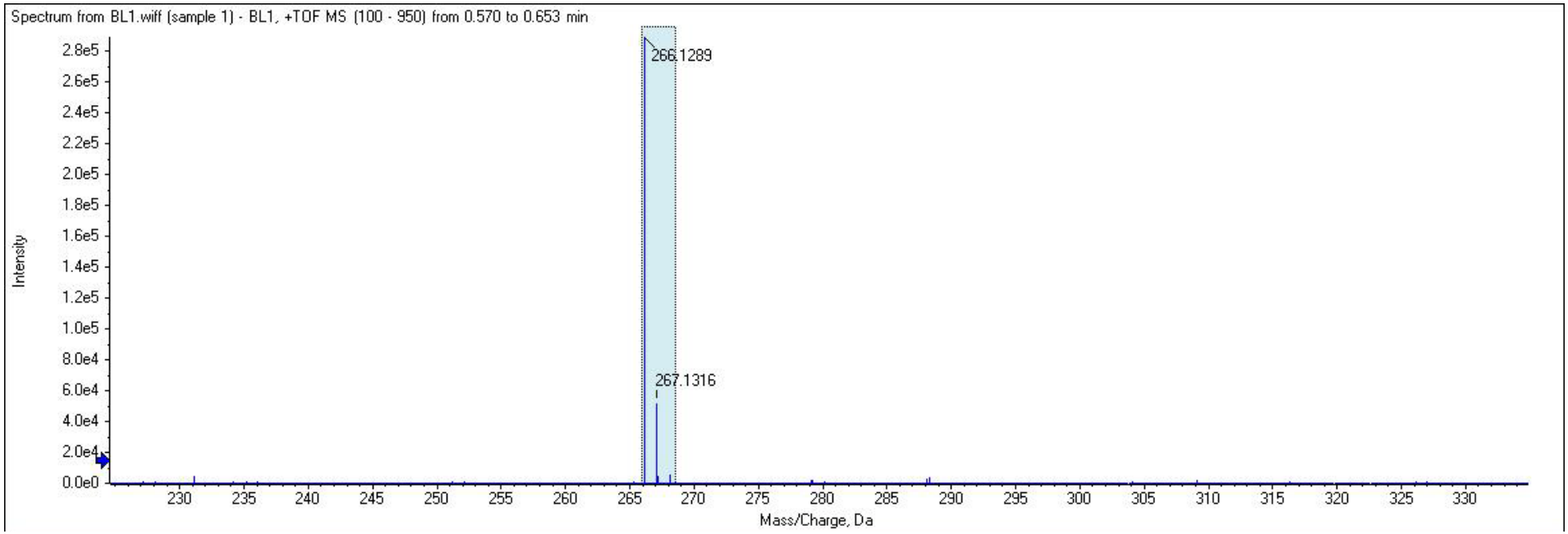
**1-benzyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole (3d)**



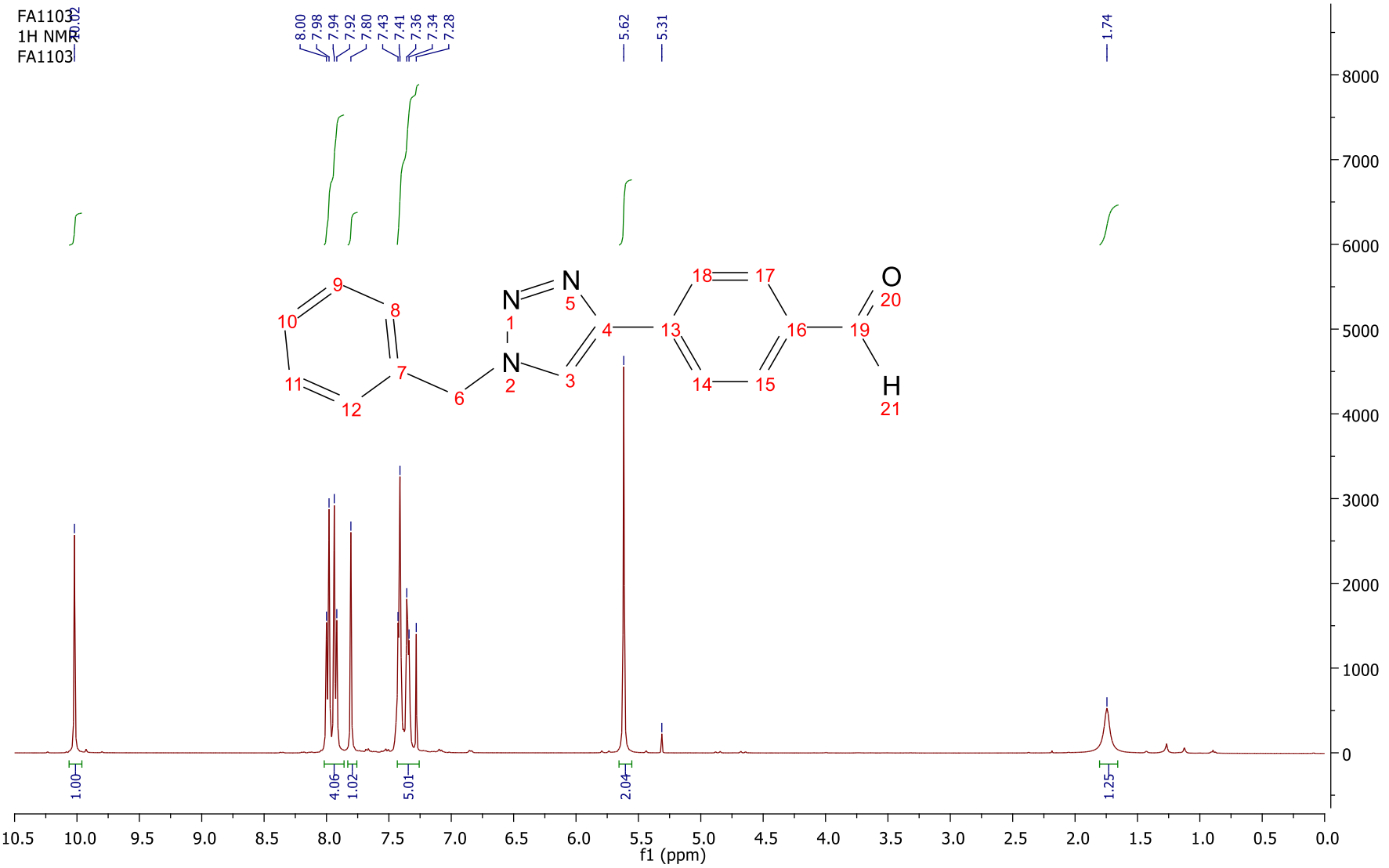

JU78
c13cpdc CDCl3 /opt/topspin JULV 23
158.60
134.87
129.92
129.55
129.22
128.53
121.65
115.18
77.85
77.42
77.09
62.46
54.70
f1 (ppm)

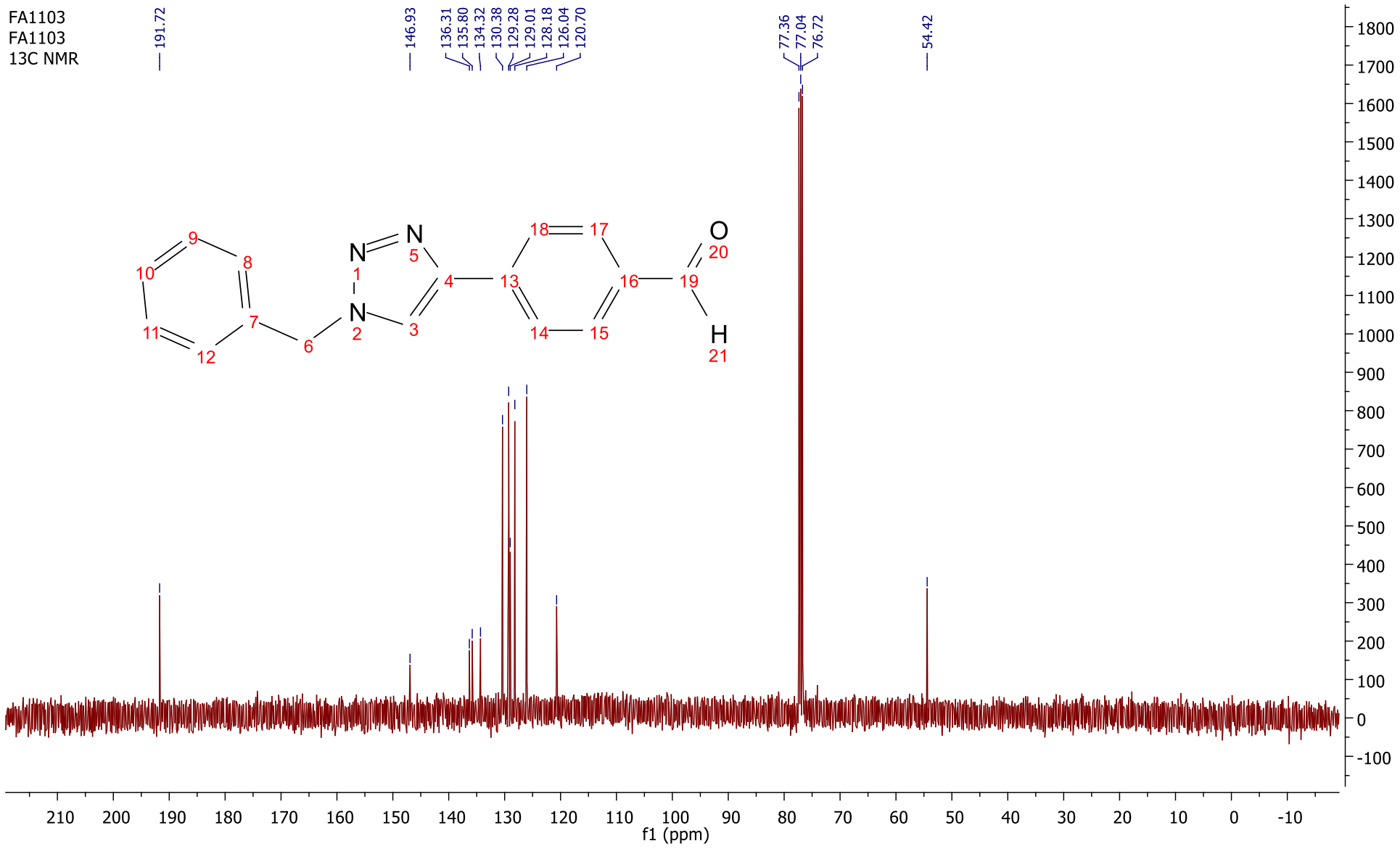

JU78
c13dept135c CDCl3 /opt/topspin JULV 23
129.92
129.55
129.22
128.53
121.65
115.48
62.46
54.70
2500
2000
1500
1000
500
0
-500
-1000
-1500
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

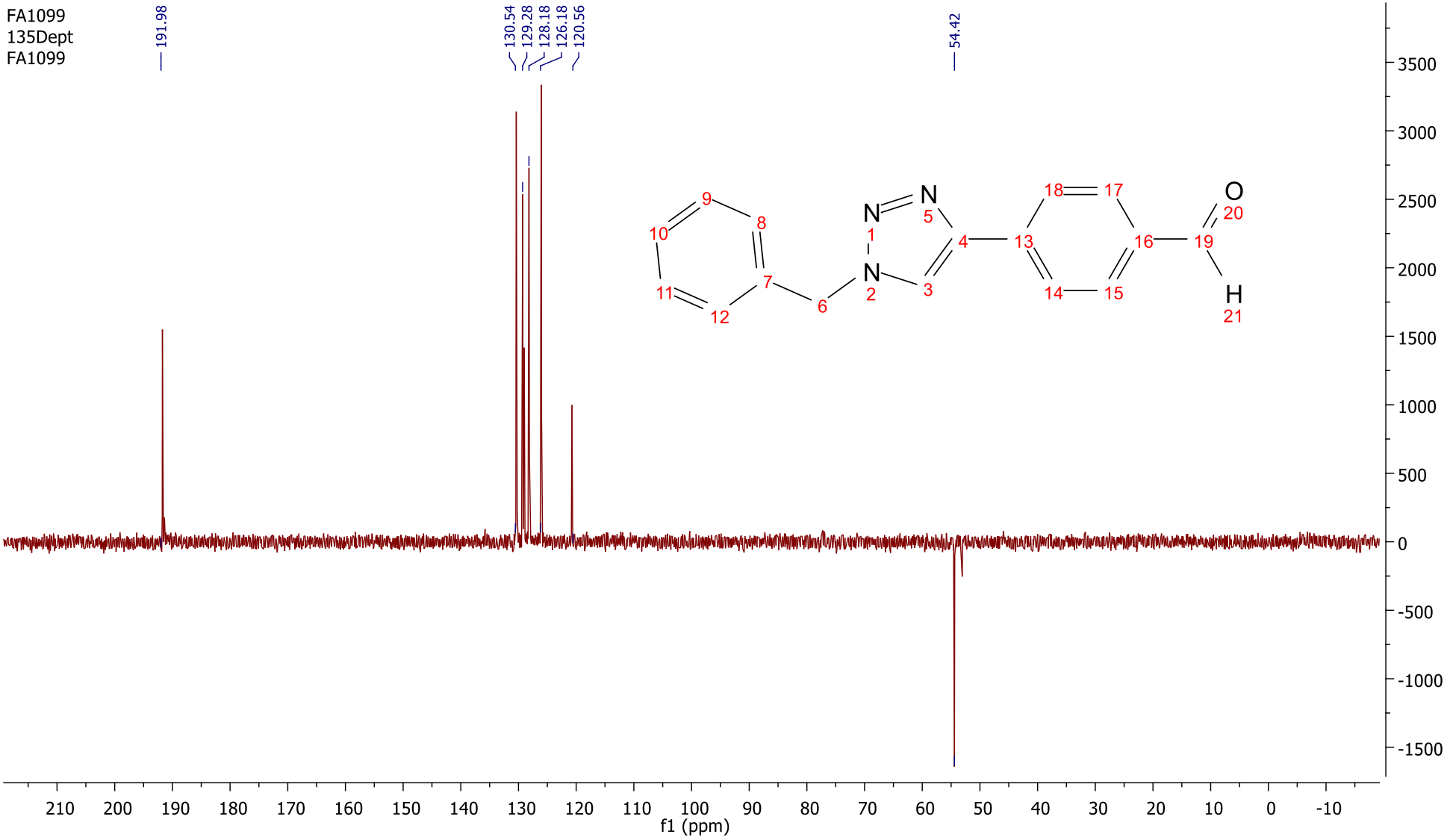

N
N
N
O

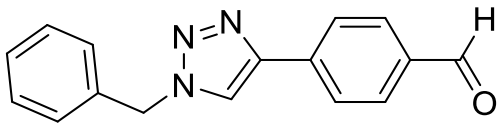

Spectrum from BL1.wiff (sample 1) - BL1, +TOF MS (100 - 950) from 0.570 to 0.653 min
Intensity
2.8e5
2.6e5
2.4e5
2.2e5
2.0e5
1.8e5
1.6e5
1.4e5
1.2e5
1.0e5
8.0e4
6.0e4
4.0e4
2.0e4
0.0e0
266.1289
267.1316
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
330
Mass/Charge, Da

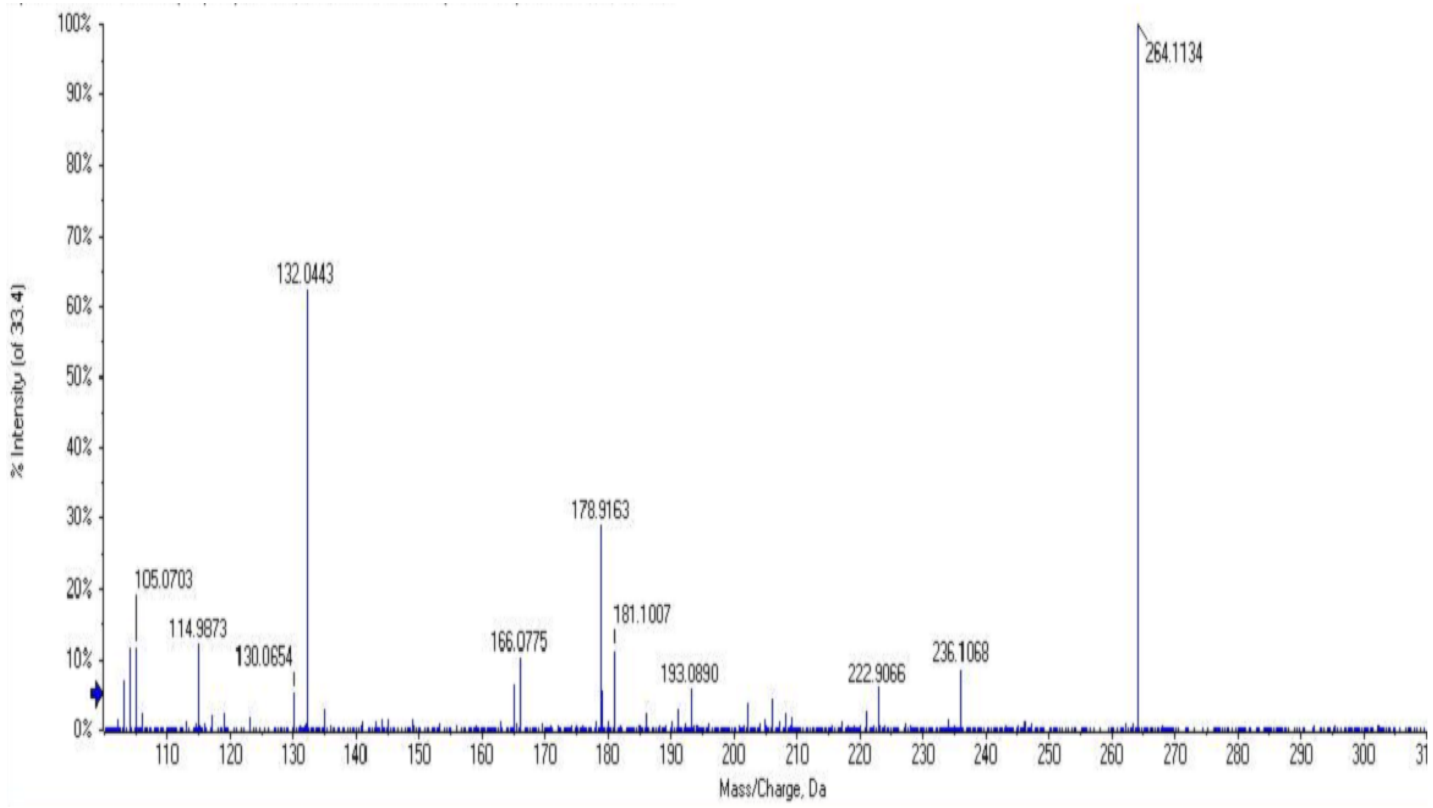
**4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzaldehyde (3e)**



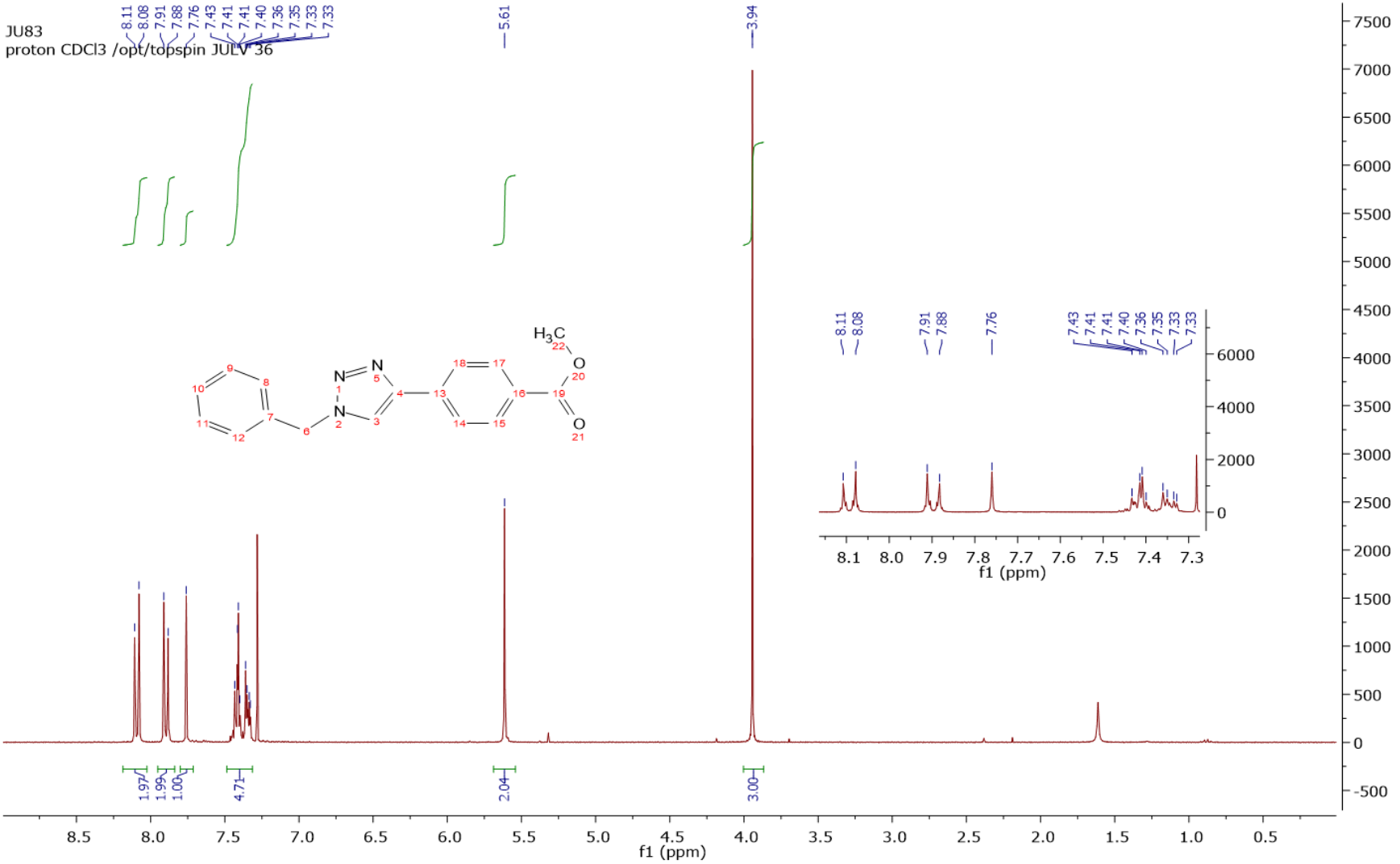

FA1103
FA1103
13C NMR
191.72
146.93
136.31
135.80
134.32
130.38
129.28
129.01
128.18
126.04
120.70
77.36
77.04
76.72
54.42
f1 (ppm)

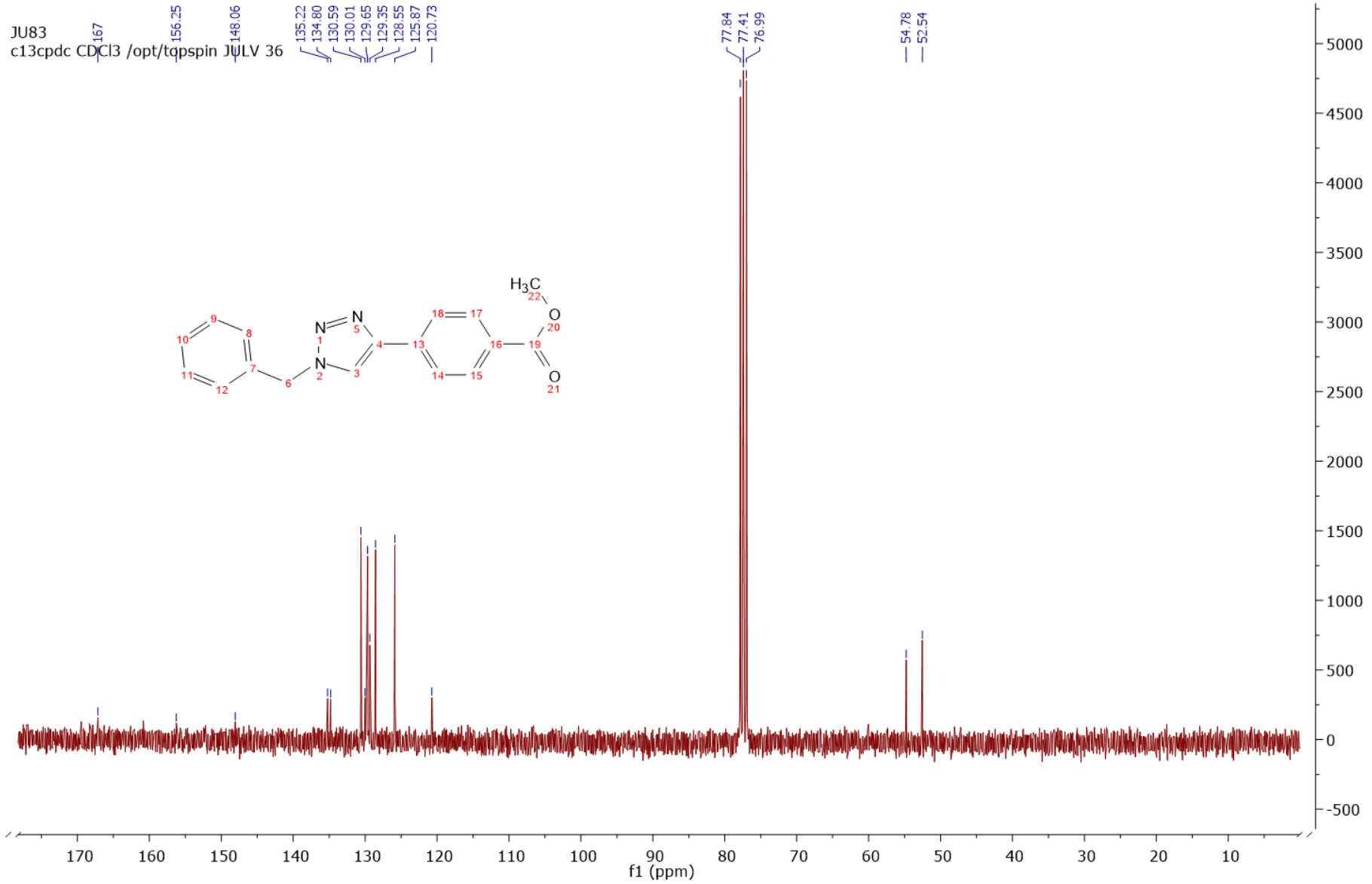

FA1099
135Dept
FA1099
191.98
130.54
129.28
128.18
126.18
120.56
54.42
f1 (ppm)

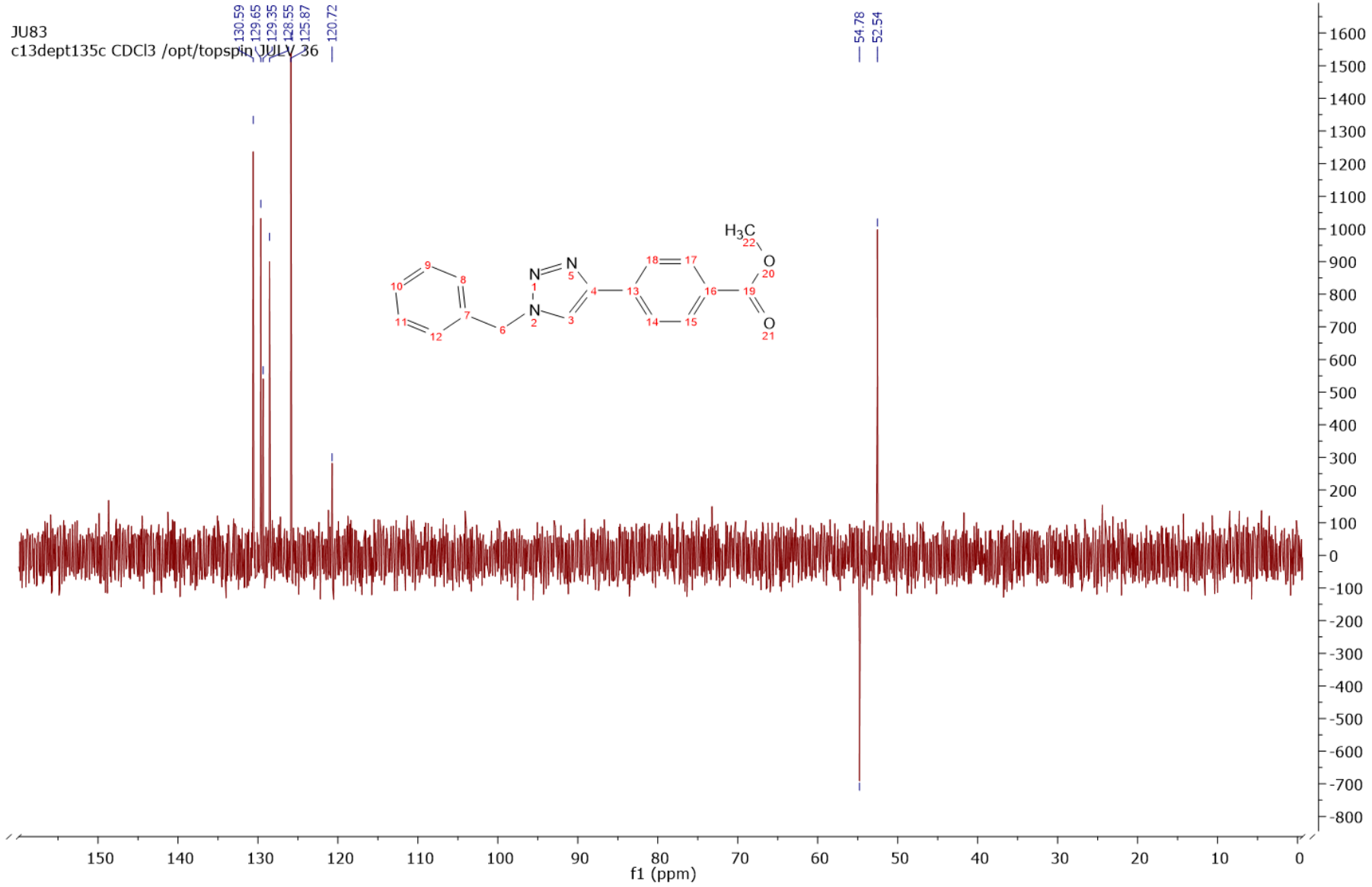

N
N
N
H
O

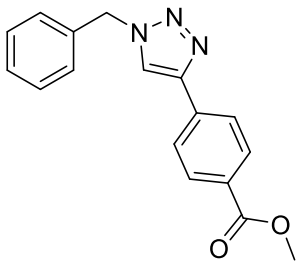

% Intensity (of 33.4)
Mass/Charge, Da
264.1134
132.0443
178.9163
105.0703
114.9873
130.0654
166.0775
181.1007
193.0890
222.9066
236.1068

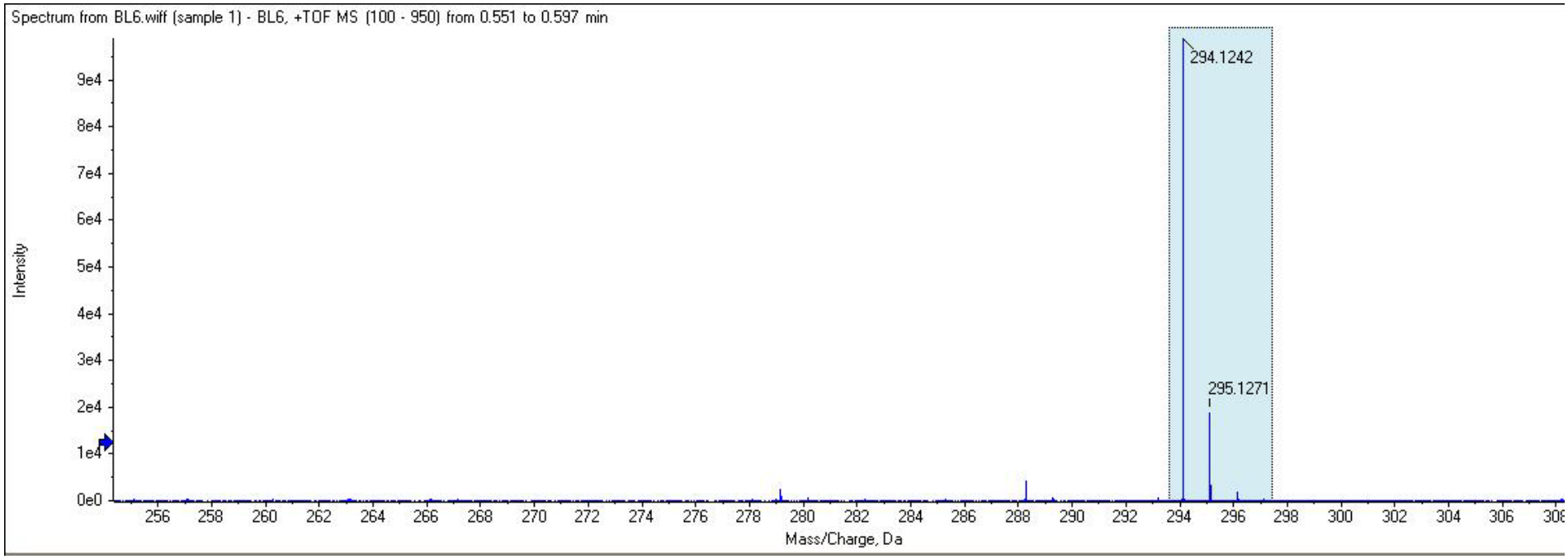
**Methyl 4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzoate (3f)**



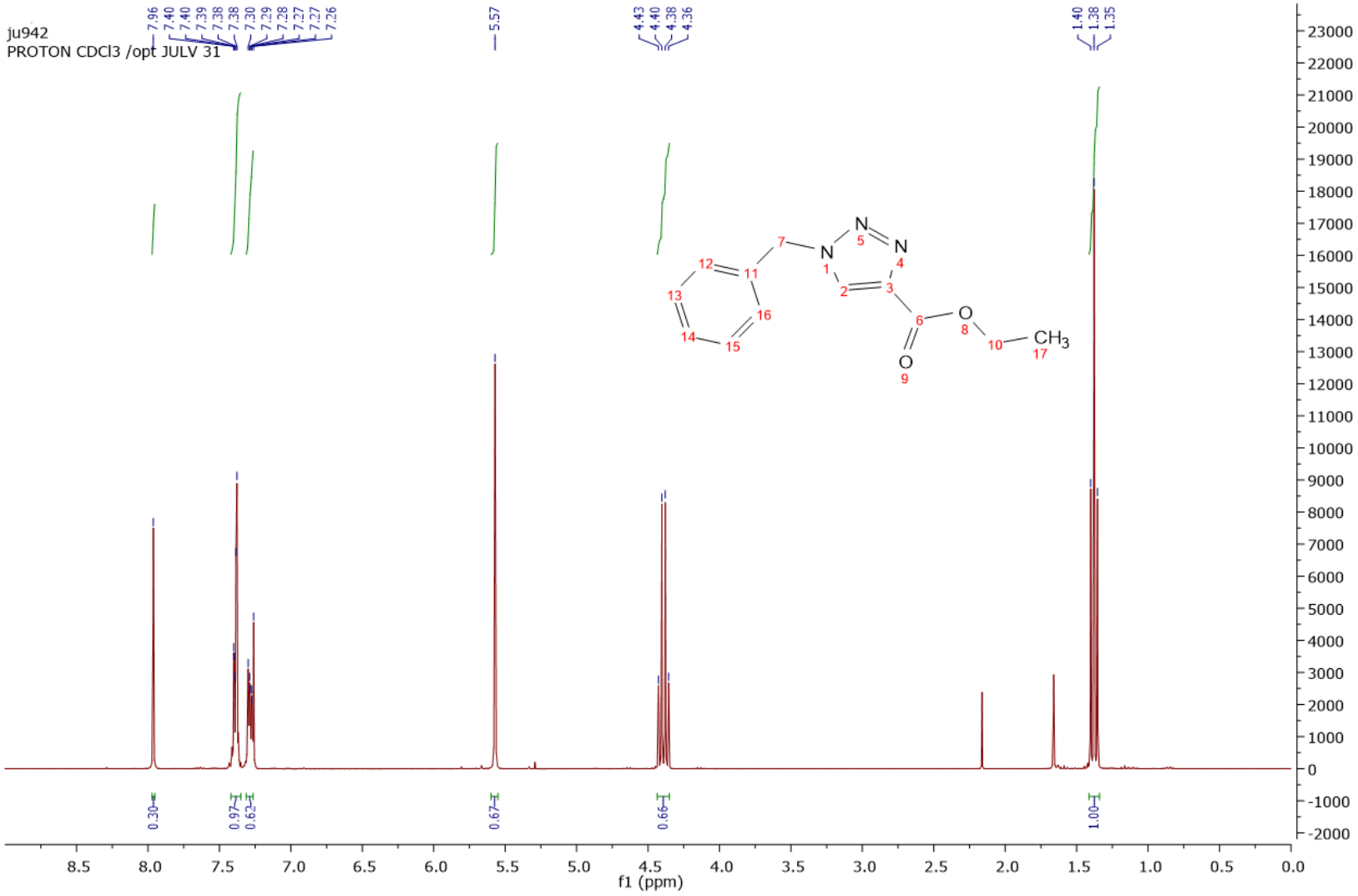

JU83
c13cpdc CDCl3 /opt/topspin JULV 36
167
156.25
148.06
135.22
134.80
130.59
130.01
129.65
129.35
128.55
125.87
120.73
77.84
77.41
76.99
54.78
52.54
H3C
22
O
20
O
21
N
1
N
2
N
5
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

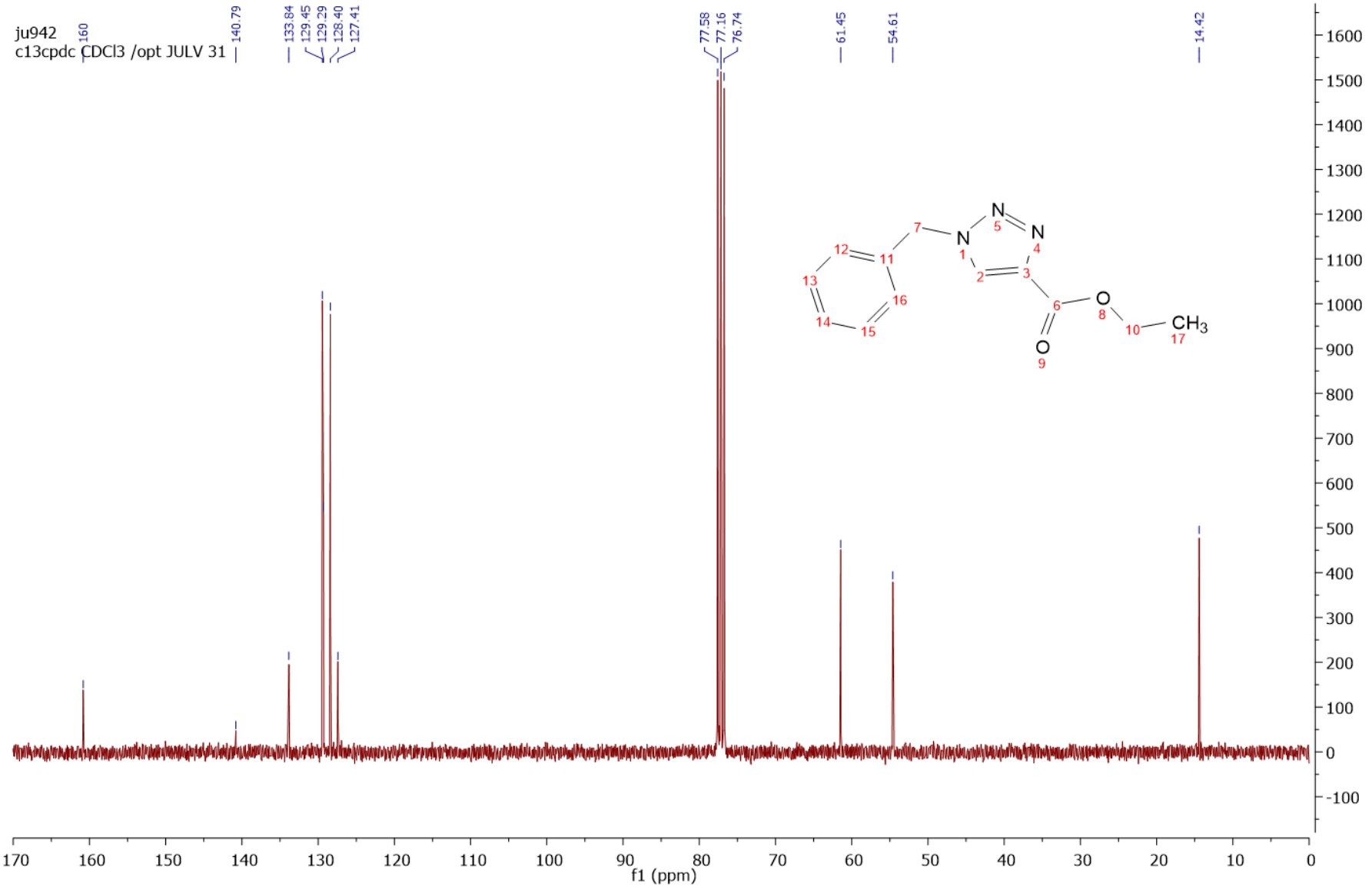

JU83
c13dept135c CDCl3 /opt/topspin JULY 36
130.59
129.65
129.35
128.55
125.87
120.72
54.78
52.54
f1 (ppm)

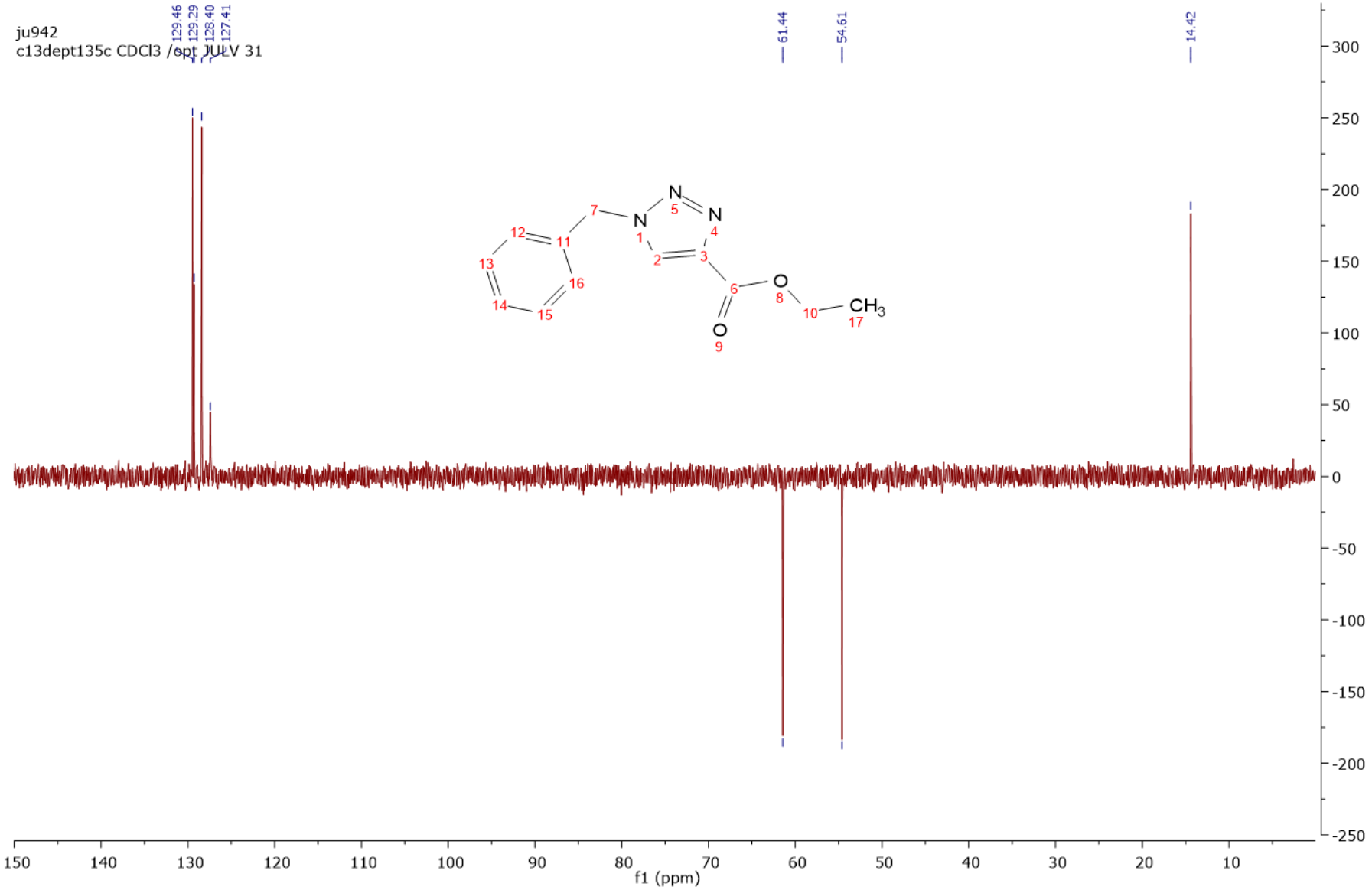


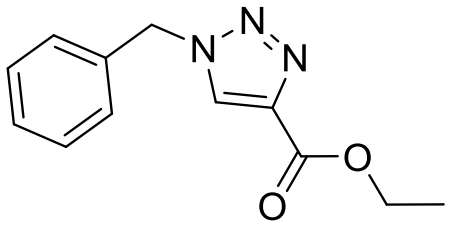

Spectrum from BL6.wiff (sample 1) - BL6, +TOF MS (100 - 950) from 0.551 to 0.597 min
294.1242
295.1271
Intensity
9e4
8e4
7e4
6e4
5e4
4e4
3e4
2e4
1e4
0e0
256 258 260 262 264 266 268 270 272 274 276 278 280 282 284 286 288 290 292 294 296 298 300 302 304 306
Mass/Charge, Da

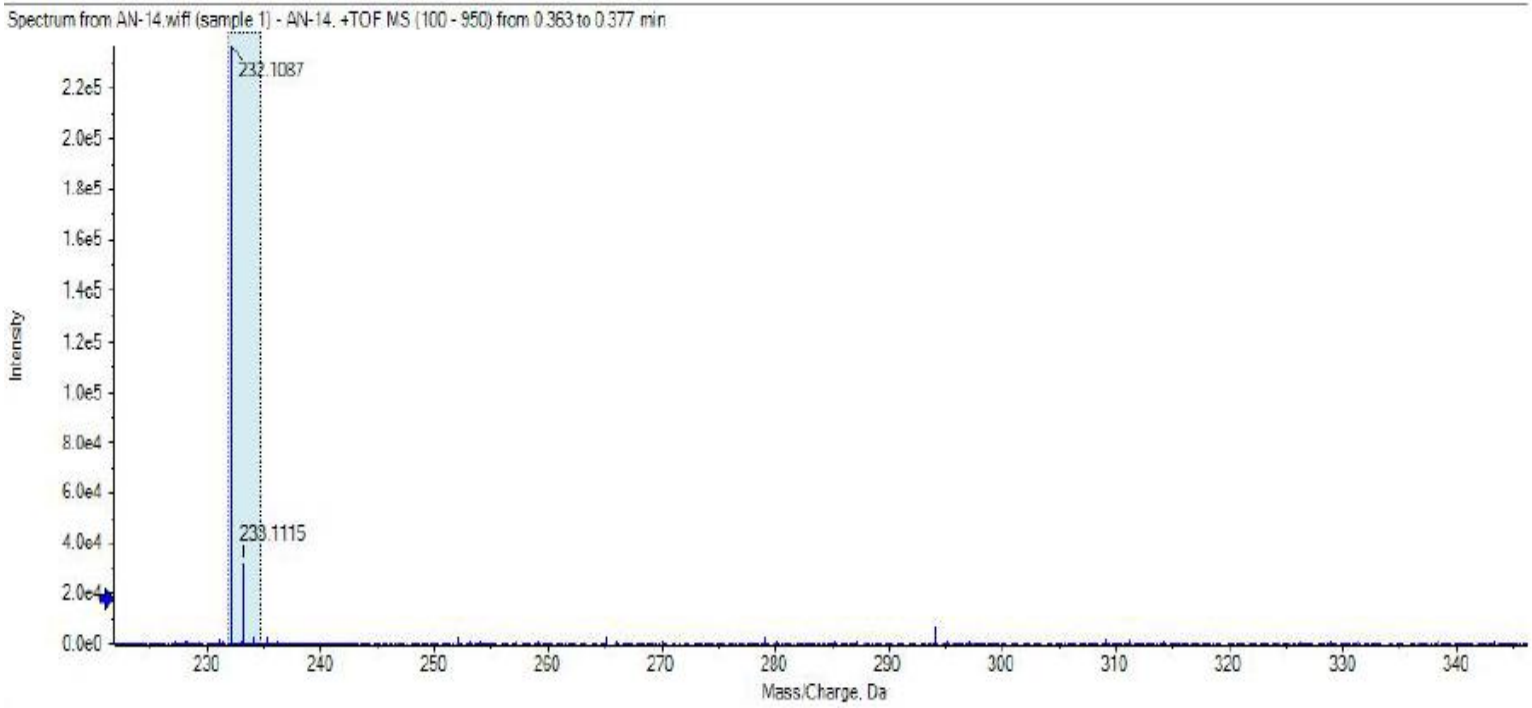
**Ethyl 1-phenyl-1*H*-1,2,3-triazole-4-carboxylate (3g)**



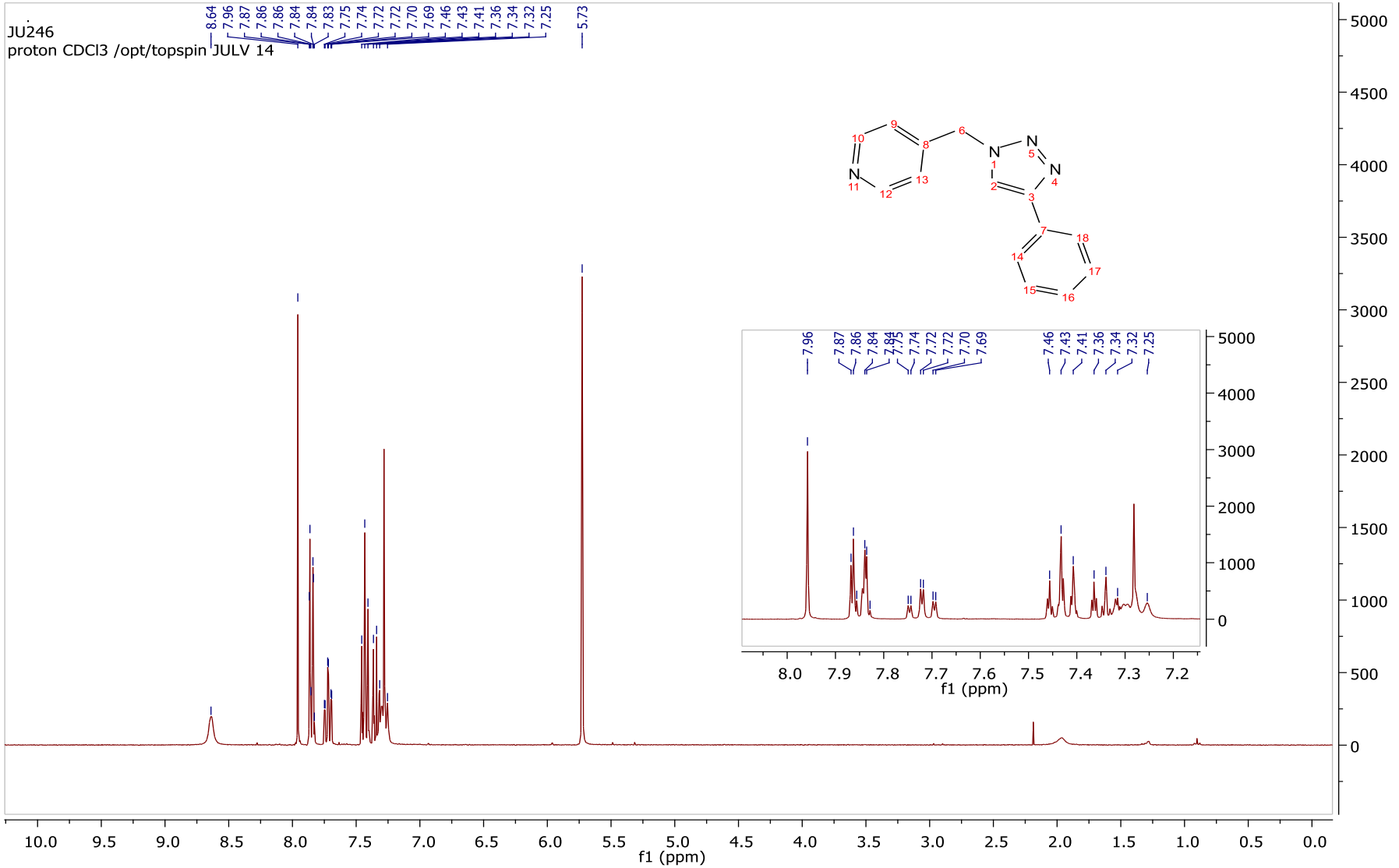

ju942
c13cpdc CDCl3 /opt JULV 31
160
140.79
133.84
129.45
129.29
128.40
127.41
77.58
77.16
76.74
61.45
54.61
14.42
f1 (ppm)

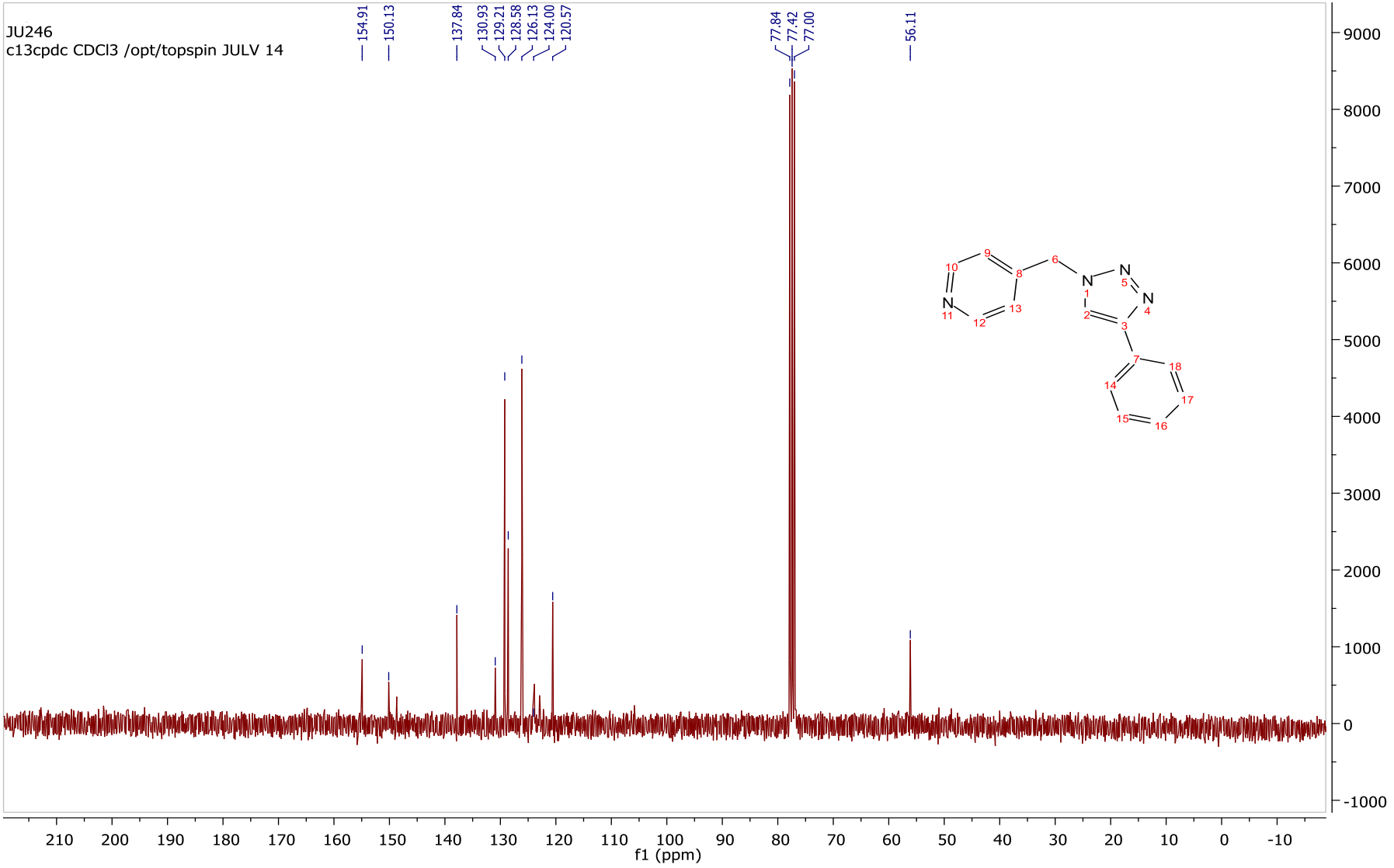

ju942
c13dept135c CDCl3 /opt JULV 31
129.46
129.29
128.40
127.41
61.44
54.61
14.42
f1 (ppm)

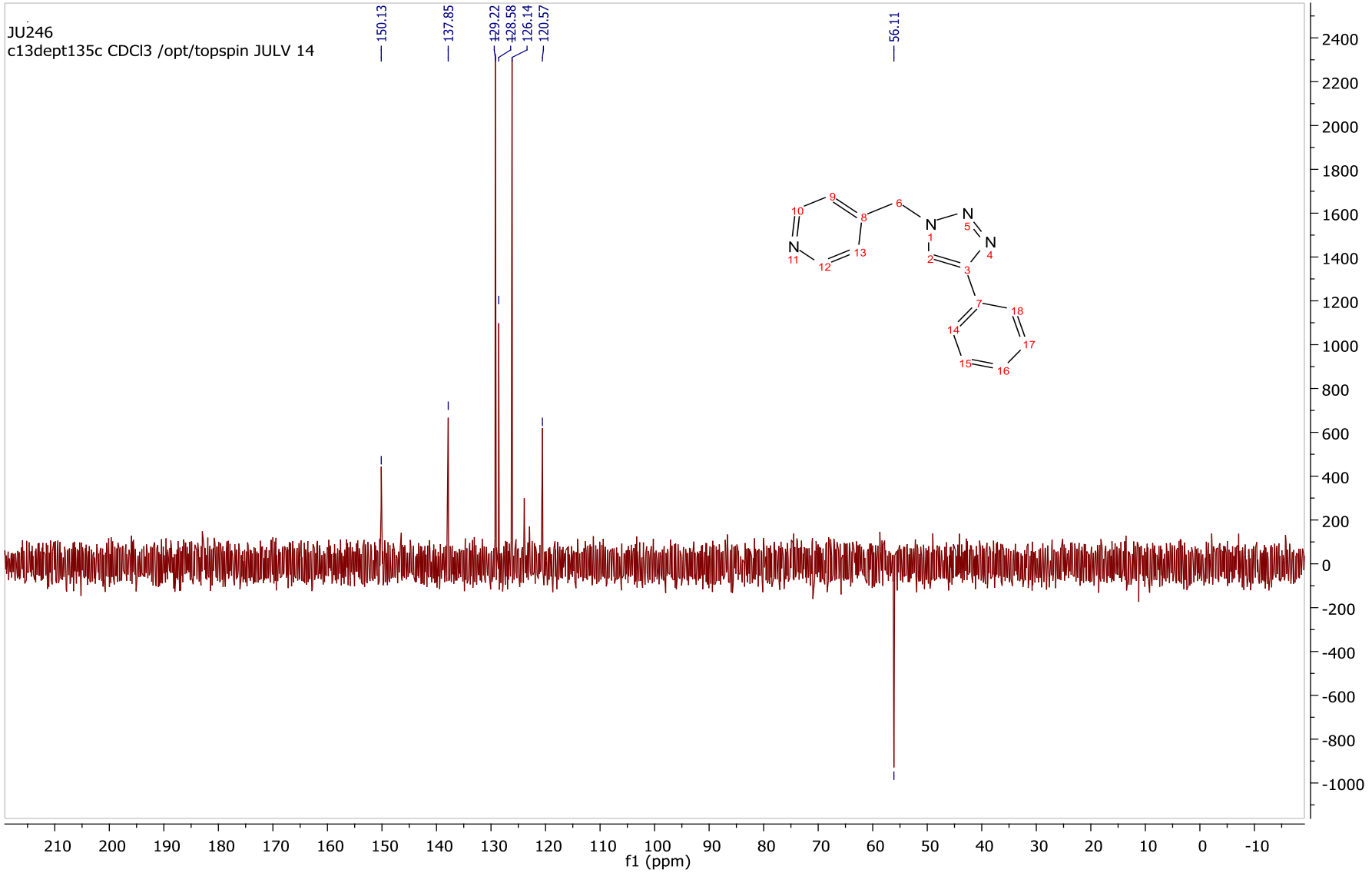

N
N
N
O
O

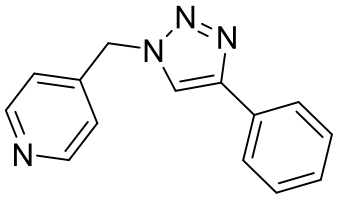

Spectrum from AN-14.wiff (sample 1) - AN-14, +TOF MS (100 - 950) from 0.363 to 0.377 min
232.1087
239.1115
Intensity
2.2e5
2.0e5
1.8e5
1.6e5
1.4e5
1.2e5
1.0e5
8.0e4
6.0e4
4.0e4
2.0e4
0.0e0
230
240
250
260
270
280
290
300
310
320
330
340
Mass/Charge, Da

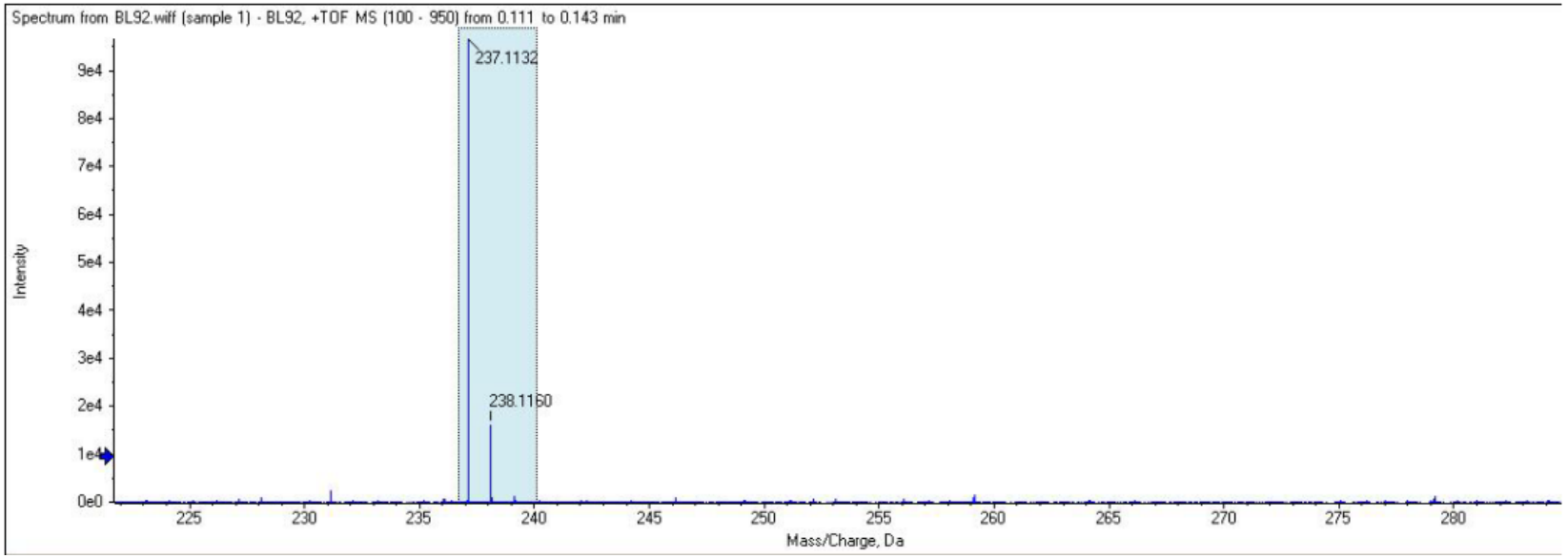
**4-((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)pyridine (3h)**



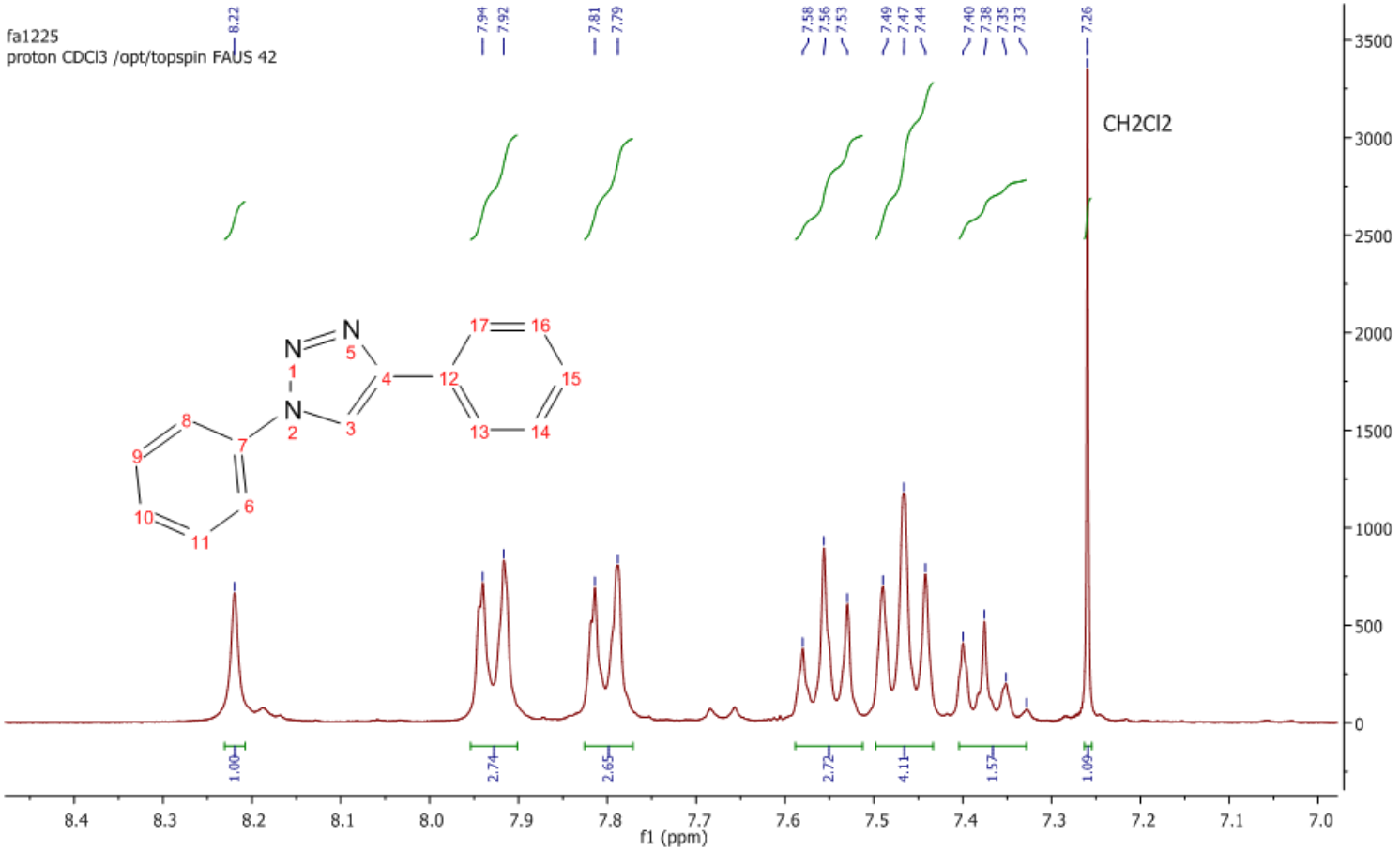

JU246
c13cpdc CDCl3 /opt/topspin JULV 14
154.91
150.13
137.84
130.93
129.21
128.58
126.13
124.00
120.57
77.84
77.42
77.00
56.11
f1 (ppm)

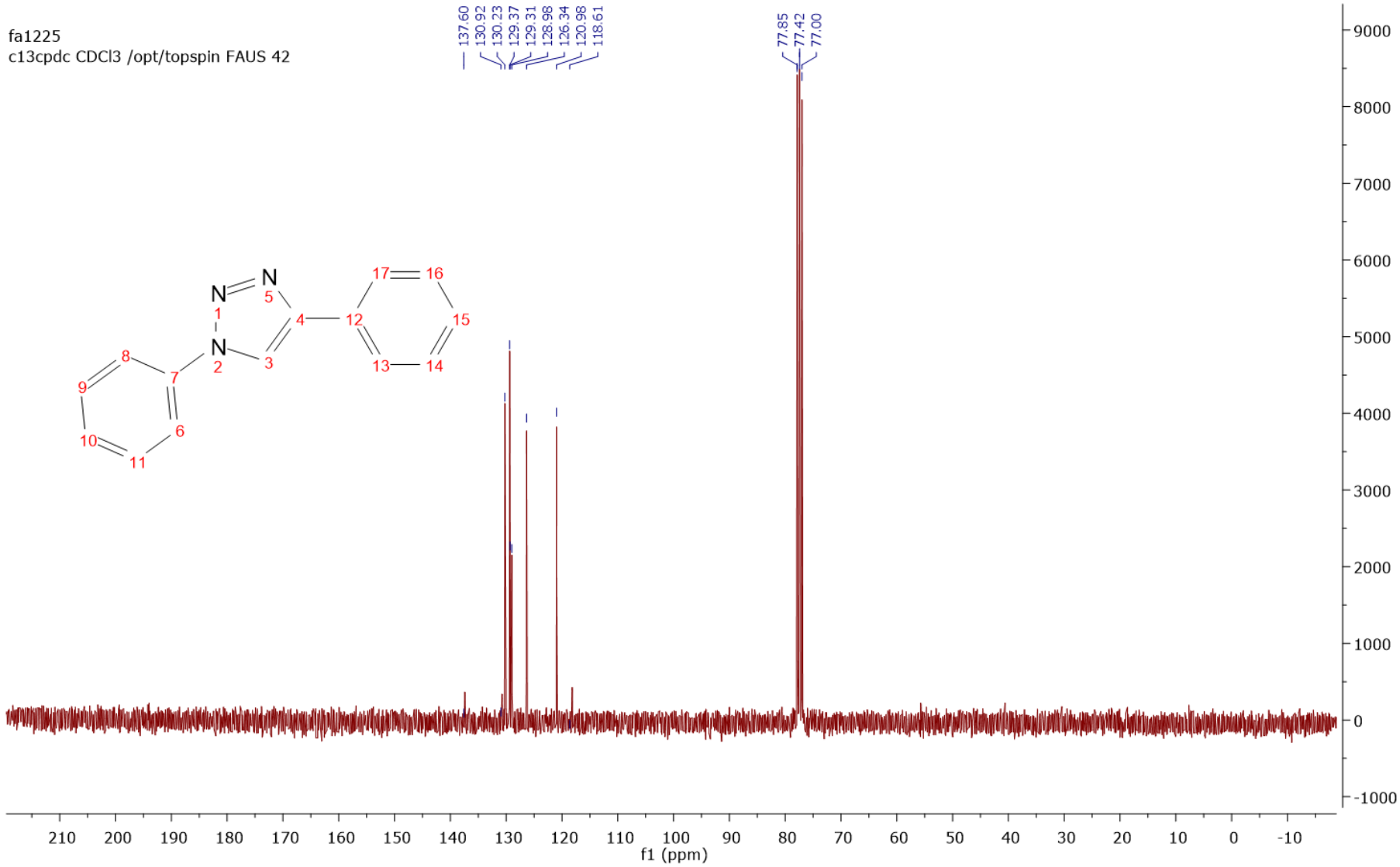

JU246
c13dept135c CDCl3 /opt/topspin JULV 14
150.13
137.85
129.22
128.58
126.14
120.57
56.11
f1 (ppm)

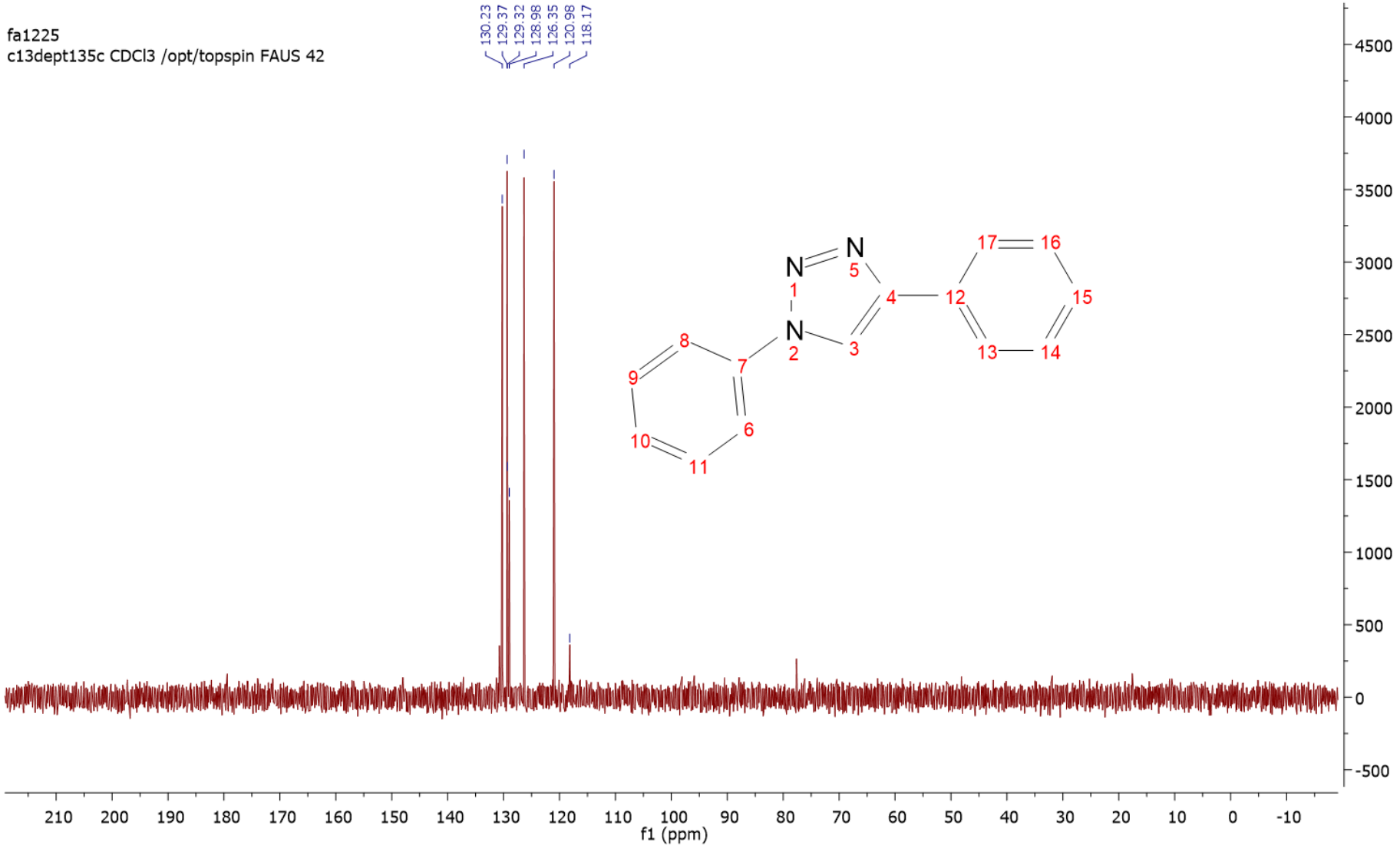

N
N
N
N

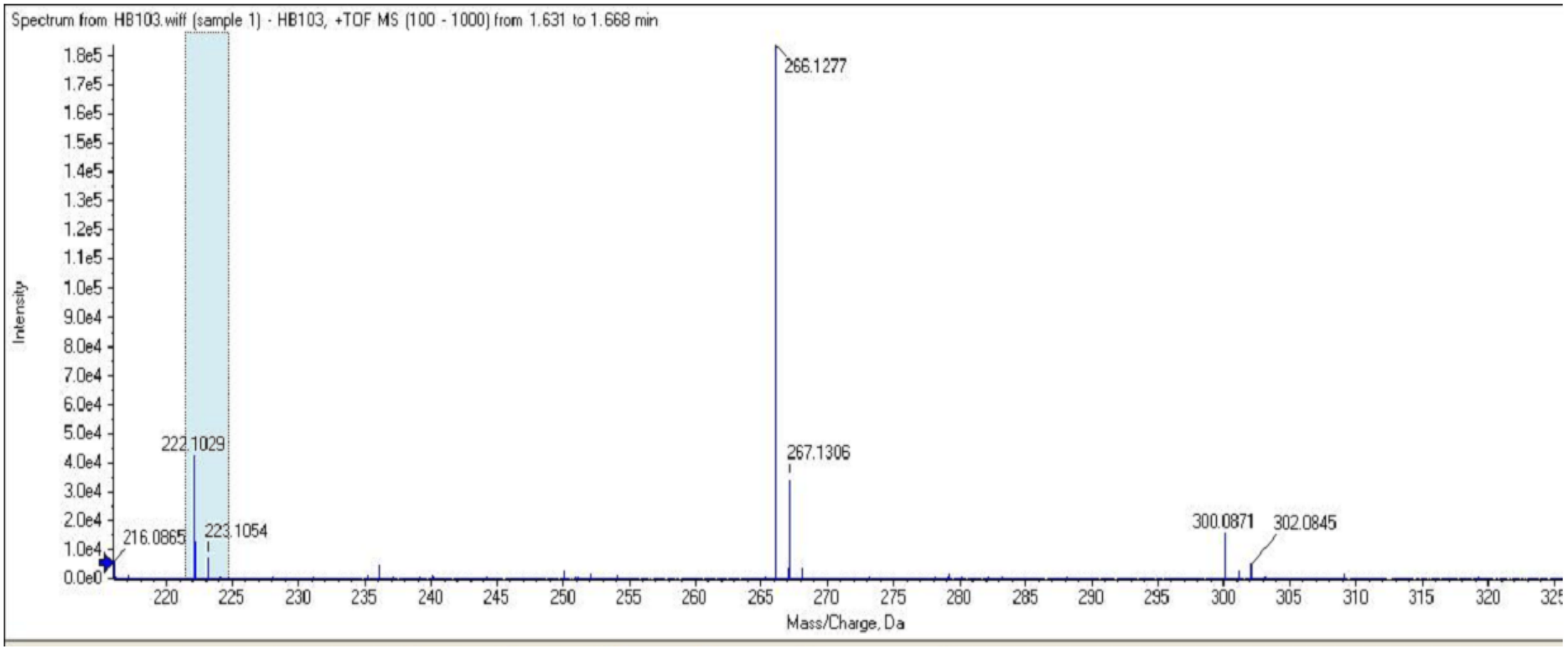

Spectrum from BL92.wiff (sample 1) - BL92, +TOF MS (100 - 950) from 0.111 to 0.143 min
237.1132
238.1160
Intensity
9e4
8e4
7e4
6e4
5e4
4e4
3e4
2e4
1e4
0e0
225
230
235
240
245
250
255
260
265
270
275
280
Mass/Charge, Da

**1,4-diphenyl-1*H*-1,2,3-triazole (3i)**

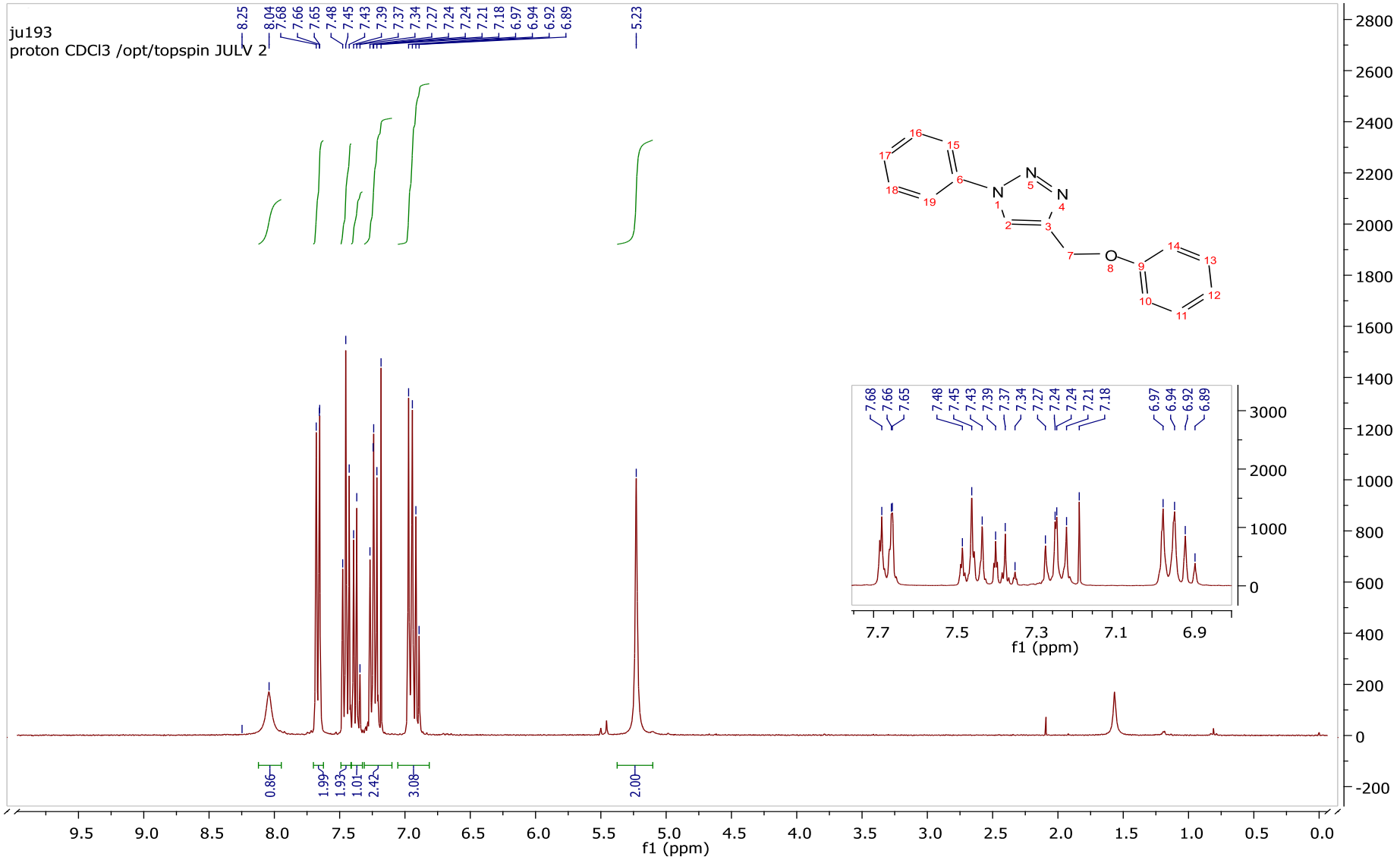


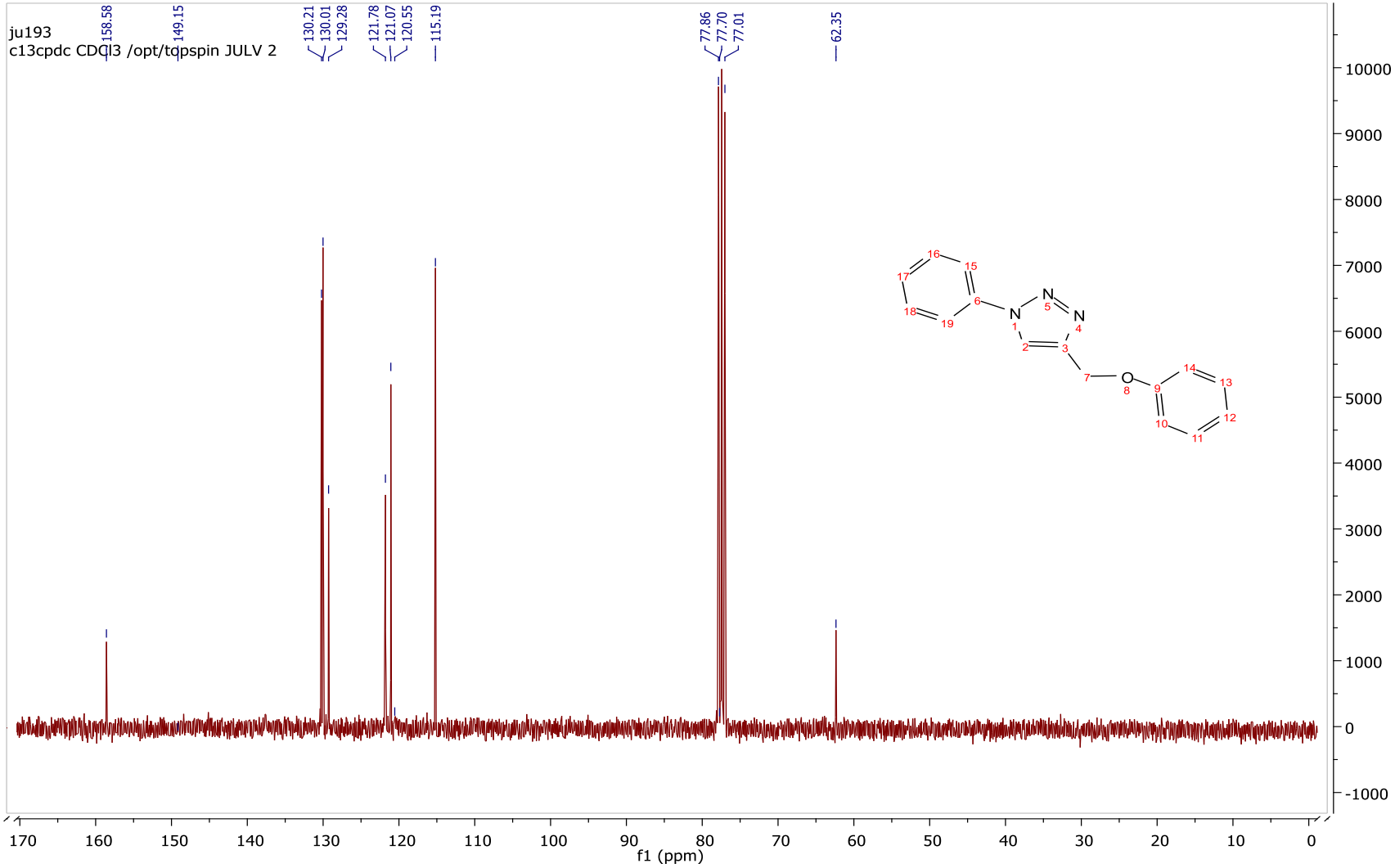

fa1225
c13cpdc CDCl3 /opt/topspin FAUS 42
137.60
130.92
130.23
129.37
129.31
128.98
126.34
120.98
118.61
77.85
77.42
77.00
N
N
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

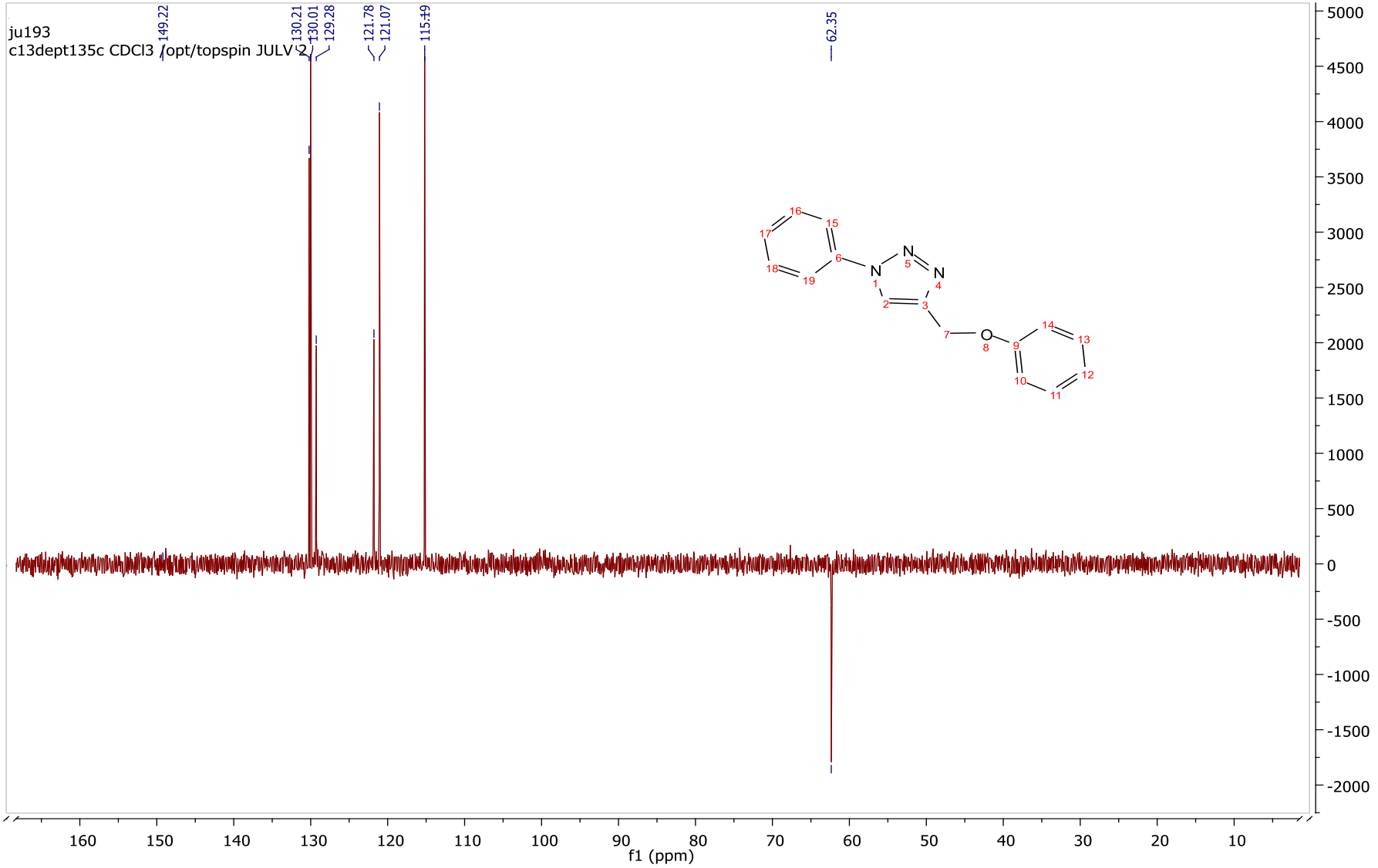

fa1225
c13dept135c CDCl3 /opt/topspin FAUS 42
130.23
129.37
129.32
128.98
126.35
120.98
118.17
N
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

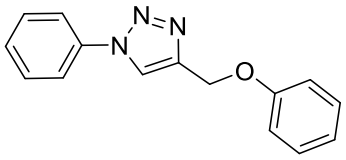

Spectrum from HB103.wiff (sample 1) - HB103, +TOF MS (100 - 1000) from 1.631 to 1.668 min
Intensity
1.8e5
1.7e5
1.6e5
1.5e5
1.4e5
1.3e5
1.2e5
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
266.1277
222.1029
267.1306
216.0865
223.1054
300.0871
302.0845
220
225
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
Mass/Charge, Da

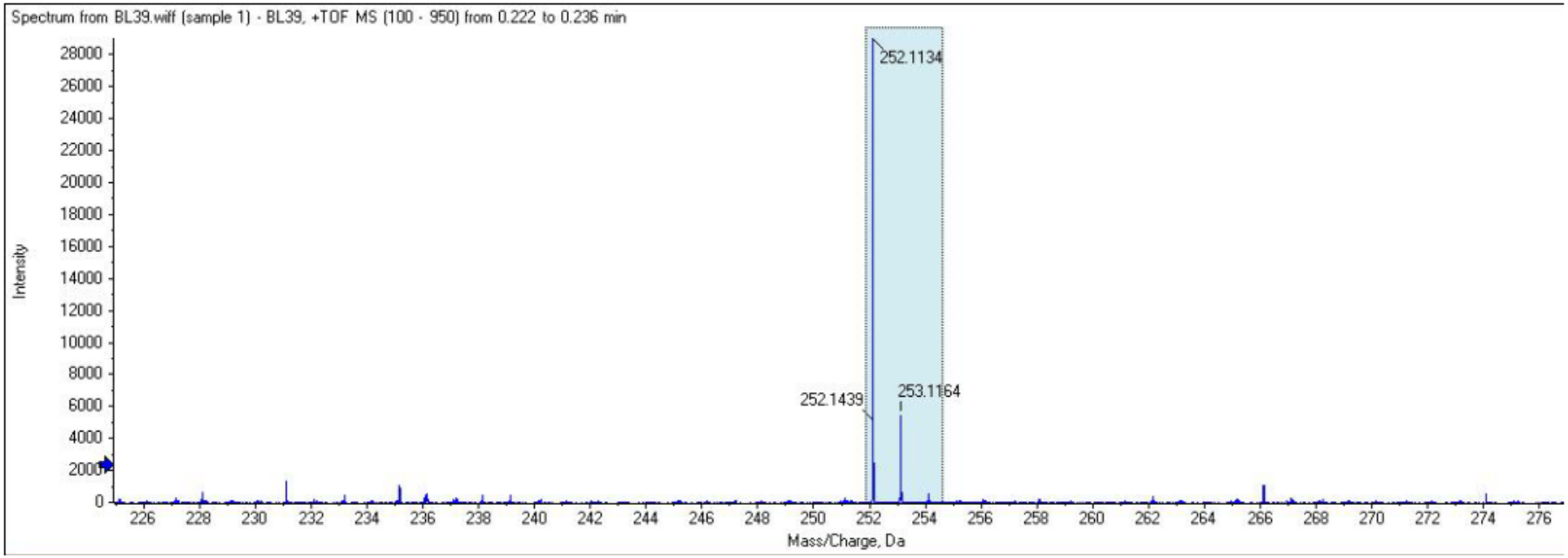
**4-(phenoxymethyl)-1-phenyl-1H-1,2,3-triazole (3j)**



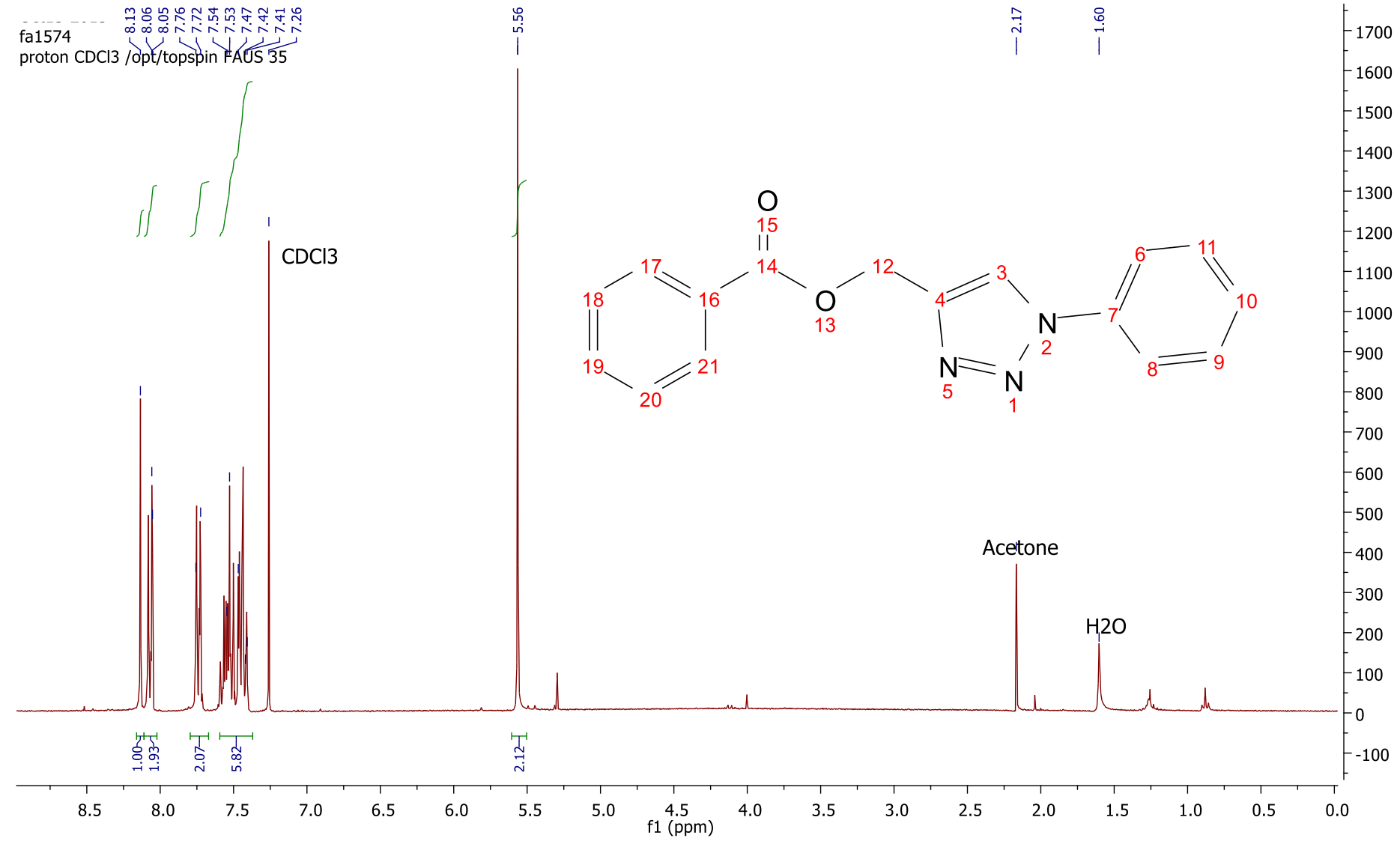

ju193
c13cpdc CDCl3 /opt/topspin JULV 2
158.58
149.15
130.21
130.01
129.28
121.78
121.07
120.55
115.19
77.86
77.70
77.01
62.35
f1 (ppm)

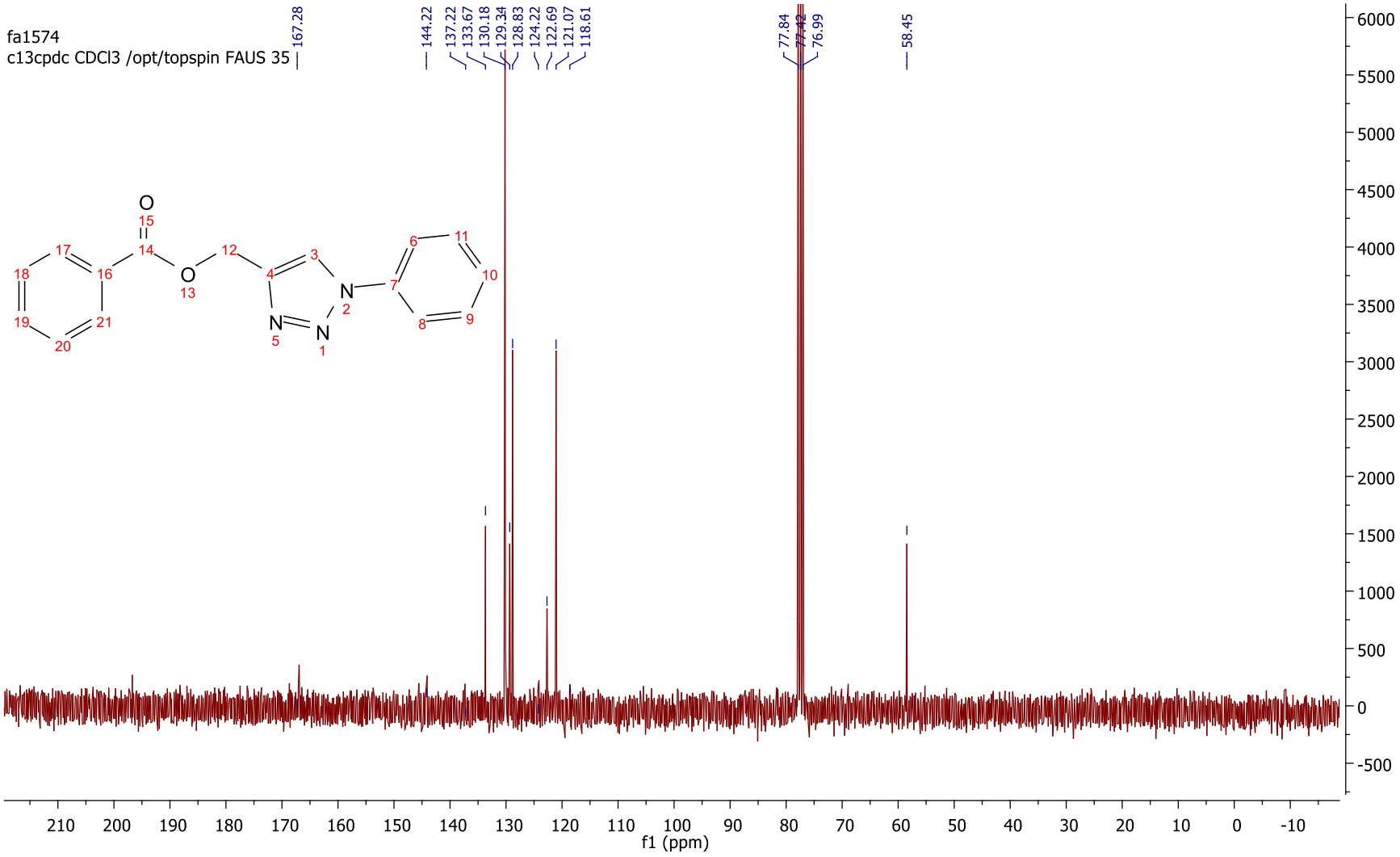

ju193
c13dept135c CDCl3 /opt/topspin JULV 2
149.22
130.21
130.01
129.28
121.78
121.07
115.49
62.35
f1 (ppm)

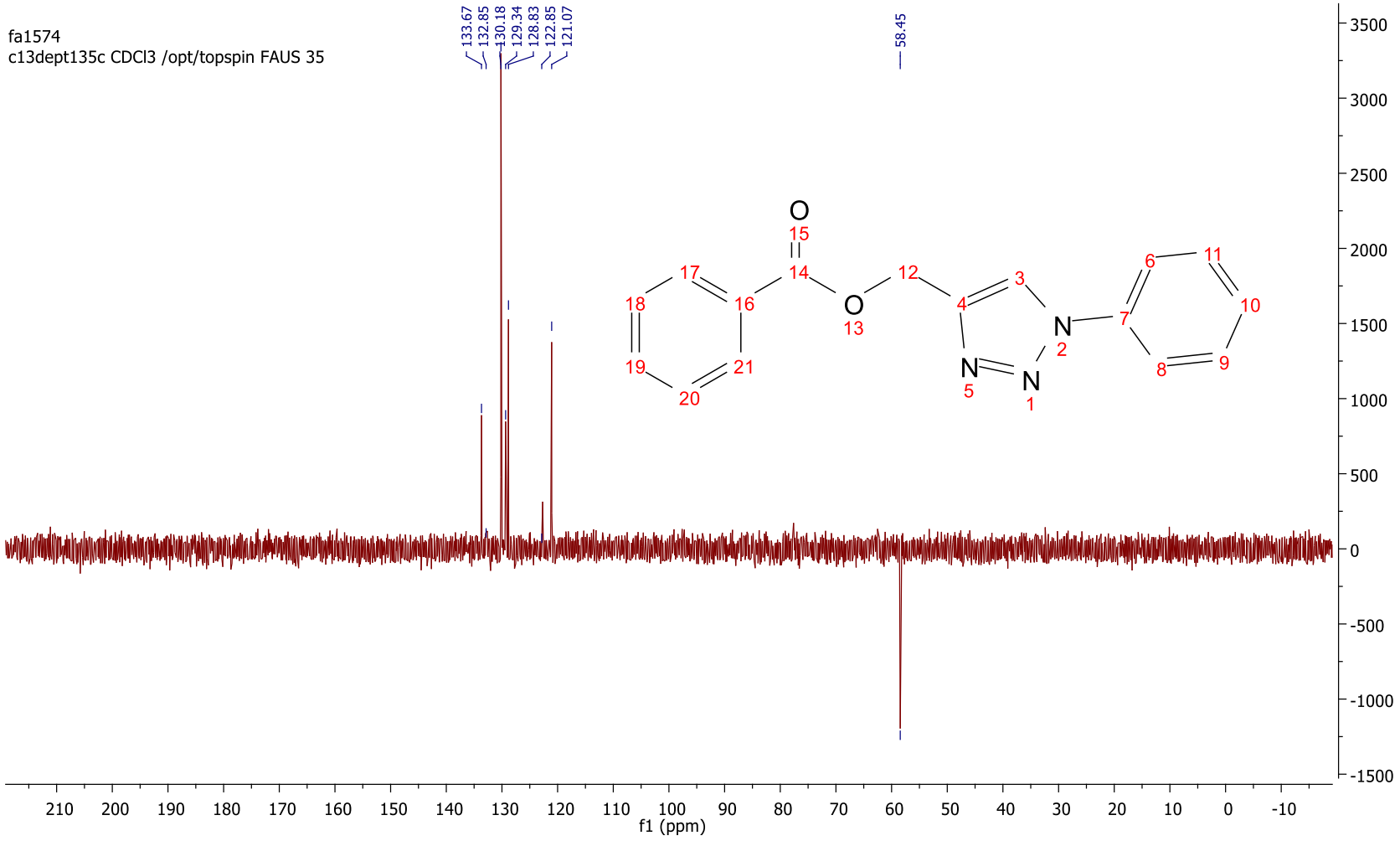

N
N
N
O

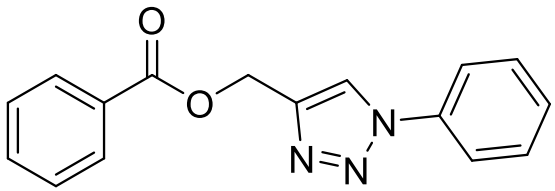

Spectrum from BL39.wiff (sample 1) - BL39, +TOF MS (100 - 950) from 0.222 to 0.236 min
Intensity
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
252.1134
252.1439
253.1164
226
228
230
232
234
236
238
240
242
244
246
248
250
252
254
256
258
260
262
264
266
268
270
272
274
276
Mass/Charge, Da

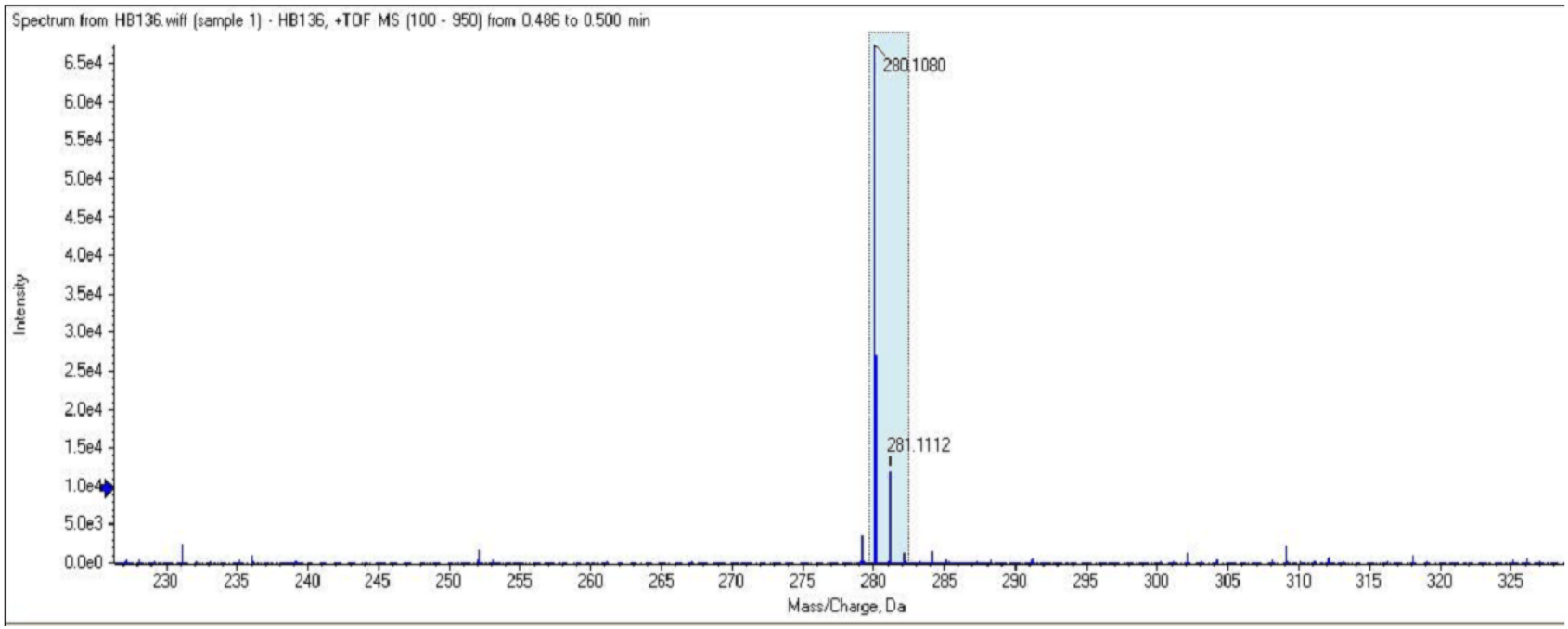
**(1-phenyl-1H-1,2,3-triazol-4-yl)methyl benzoate (3k)**




fa1574
c13cpdc CDCl3 /opt/topspin FAUS 35
167.28
144.22
137.22
133.67
130.18
129.34
128.83
124.22
122.69
121.07
118.61
77.84
77.42
76.99
58.45
O
15
14
O
13
12
4
3
N
2
7
6
11
10
9
8
N
5
N
1
17
16
18
19
21
20
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


fa1574
c13dept135c CDCl3 /opt/topspin FAUS 35
133.67
132.85
130.18
129.34
128.83
122.85
121.07
58.45
O
15
14
O
13
12
17
16
18
19
20
21
3
4
N
2
N
5
N
1
6
11
7
10
8
9
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
N
N=N


Spectrum from HB136.wiff (sample 1) - HB136, +TOF MS (100 - 950) from 0.486 to 0.500 min
280.1080
281.1112
Intensity
6.5e4
6.0e4
5.5e4
5.0e4
4.5e4
4.0e4
3.5e4
3.0e4
2.5e4
2.0e4
1.5e4
1.0e4
5.0e3
0.0e0
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
Mass/Charge, Da