Electronic Supporting Information (ESI)

Deciphering the Mechanism of Silver Catalysis of "Click" Chemistry in Water by Combining Experimental and MEDT Studies †

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Figure S1

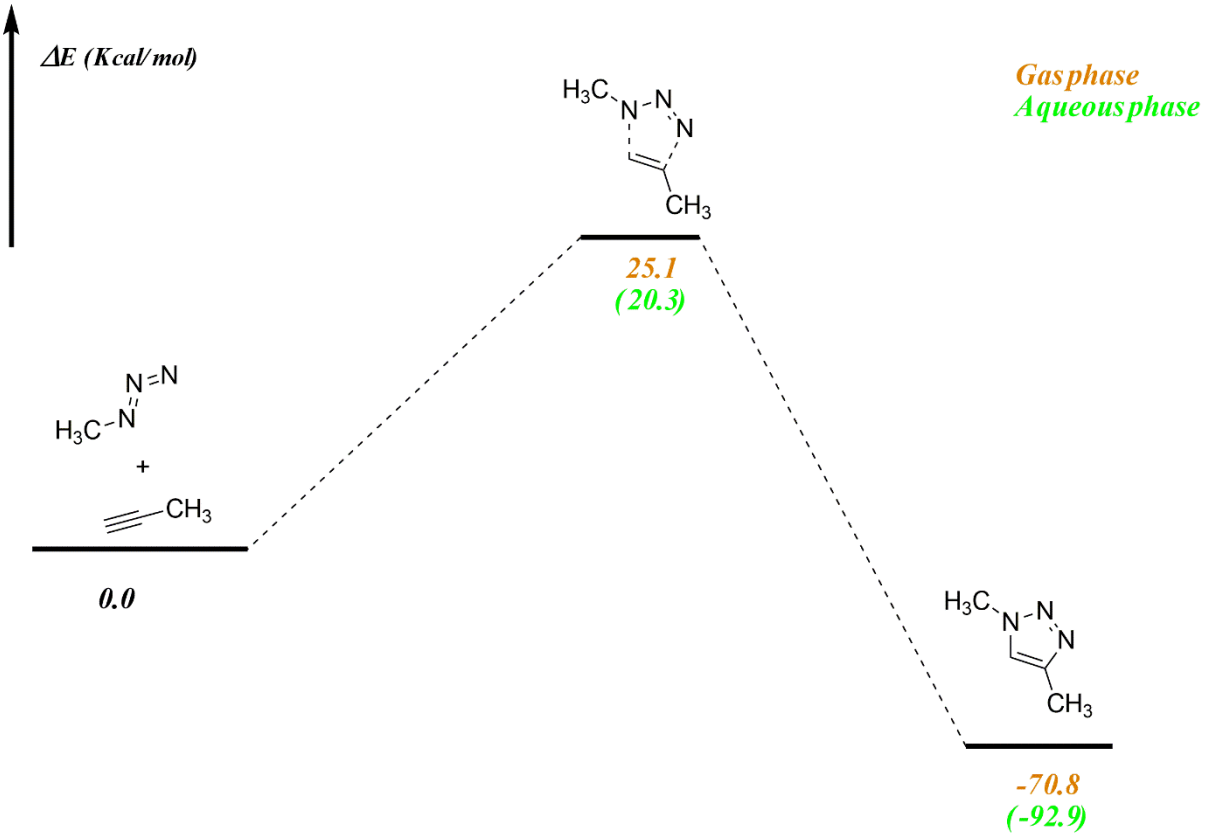


Figure S1. Energy profile for the non-catalyzed azide-alkyne cycloaddition reaction between methyl alkyne and methyl azide

1. Characterization of 1,2,3 triazoles products

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

Yield: 92%. White solid. M.P.: 128.8 ºC. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 5.59 (s, 2H, CH_2), 7.31-7.44 (m, 8H, CH_{Ar}), 7.69 (s, 1H, $CH_{Triazole}$), 7.81-7.83(s, 2H, CH_{Ar}). ^{13}C NMR (75MHz, $CDCl_3$, δ ppm): 54.62 (CH_2), 119.95 (CH_{Ar}), 126.10 (CH_{Ar}), 128.46 ($2CH_{Ar}$), 128.57 ($2CH_{Ar}$), 129.21 (C_{Ar}), 129.56 ($CH_{Triazole}$), 130.95 (C_{Ar}), 135.11 (C_{Ar}). HRMS (ESI) $[M + H]^+$ found m/z = 236.1183. Calcd value for $C_{15}H_{13}N_3$ = 236.1182.

1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole (3b)

Yield: 93%. White solid. M.P.: 106.5°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 2.28 (s, 3H, CH_3); 5.46 (s, 2H, CH_2); 7.13-7.35 (m, 7H, CH_{Ar}); 7.57 (s, 1H, $CH_{Triazole}$); 7.71-7.73 (d, 2H, CH_{Ar}). ^{13}C NMR (100MHz, $CDCl_3$, δ ppm): 21.19 (CH_3); 54.10 (CH_2); 125.70 ($2CH_{Ar}$); 128.16 ($3CH_{Ar}$); 129.80 ($4CH_{Ar}$); 129.83 (C_{Ar}); 130.58 ($CH_{Triazole}$); 131.63 (C_{Ar}); 138.78

(C_{Ar}); 148.72 ($C_{Triazole}$). HRMS (ESI) [M + H] $^{+}$ found m/z = 250.1344. Calcd value for $C_{16}H_{15}N_3$ = 250.1345.

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

Yield: 94%. White solid. ^{1}H NMR (300MHz, $CDCl_3$, 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 (75MHz, $CDCl_3$, 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 ($C_{Triazole}$). HRMS (ESI) [M + H] $^{+}$ found m/z = 250.1339. Calcd value for $C_{16}H_{15}N_3$ = 250.1339.

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

Yield: 92%. White solid. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 5.21 (s, 2H,CH_2); 5.55 (s,2H,OCH_2); 6.96-7.00 (m, 3H,CH_{Ar}); 7.28-7.41 (m, 7H,CH_{Ar}); 7.57 (s, 1H,$CH_{Triazole}$). ^{13}C NMR (75MHz, $CDCl_3$, δ ppm): 54.7 (CH_2); 62.46 (CH_2); 115.18 ($2CH_{Ar}$); 116.56 (CH_{Ar}); 121.65 ($CH_{Triazole}$) ; 128.53 (CH_{Ar}); 129.22 ($2CH_{Ar}$) ; 129.51 ($4CH_{Ar}$) ; 129.92 (C_{Ar}); 134,90 ($C_{Triazole}$); 158.56 (C_{Ar}). HRMS (ESI) [M + H] $^{+}$ found m/z =266.1289. Calcd value for $C_{16}H_{15}N_3O$ = 266.1288.

1-(4-Fluoro-benzyl)-4-p-tolyl-1H-[1,2,3]triazole (3e)

Yield: 86%. White solid. M.P.: 149°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 2.39 (s, 3H, CH_3); 5.55 (s, 2H, CH_2); 7.06-7.17 (m, 2H, CH_{Ar}); 7.22-7.29 (m, 2H, CH_{Ar}); 7.39-7.45 (m, 2H, CH_{Ar}); 7.64 (s, 1H, $CH_{Triazole}$); 7.69-7.72 (m, 2H, CH_{Ar}). ^{13}C NMR (100MHz, $CDCl_3$, δ ppm): 21.29 (CH_3); 53.44 (CH_2); 116.29 ($2CH_{Ar}$); 125.62 ($2CH_{Ar}$); 127.63 (C_{Ar}); 129.24 ($2CH_{Ar}$); 129.88 ($2CH_{Ar}$); 130.66 ($CH_{Triazole}$); 131.80 ($2CH_{Ar}$); 132.74 ($2C_{Ar}$); 148.43 ($C_{Triazole}$); 161.23 (C_{Ar}-F). HRMS (ESI) [M + H] $^{+}$ found m/z = 268.1249. Calcd value for $C_{16}H_{14}FN_3$ = 268.1245.

1-(4-fluorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3f)

Yield: 79%. White solid. M.P.: 128.2°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 5.55 (s, 2H, CH_2); 7.08-7.15 (m, 4H, CH_{Ar}); 7.31-7.36 (m, 2H, CH_{Ar}); 7.63 (s, 1H, $CH_{Triazole}$); 7.77-7.82 (m, 2H, CH_{Ar}). ^{13}C NMR (100MHz, $CDCl_3$, δ ppm): 53.54 (CH_2); 115.70 ($2CH_{Ar}$); 116.38 ($2CH_{Ar}$); 119.06 ($C_{Triazole}$); 127.41 (C_{Ar}); 127.52 ($2CH_{Ar}$); 129.92 ($2CH_{Ar}$); 130.03 (C_{Ar});

137.78 ($CH_{Triazole}$); 161.29 (C_{Ar}-F); 163.53 (C_{Ar}-F). HRMS (ESI) [M + H] $^{+}$ found m/z = 272.0996. Calcd value for $C_{15}H_{11}F_2N_3$ = 272.0994.

1-(4-isopropylphenyl)-4-phenyl-1H-1,2,3-triazole (3g)

Yield: 82%. White solid. M.P.: 127.5°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 1.31 (s, 3H, CH_3); 1.34 (s, 3H, CH_3); 2.98-3.07 (m, 1H, CH); 7.36-7.40 (t, 1H, CH_{Ar}); 7.43-7.51 (d, 2H, CH_{Ar}); 7.71-7.74 (d, 2H, CH_{Ar}); 7.93-7.95 (d, 2H, CH_{Ar}); 7.94-7.96 (d, 2H, CH_{Ar}); 8.13 (s, 1H, $CH_{Triazole}$). ^{13}C NMR (100MHz, $CDCl_3$, δ ppm): 23.92 ($2CH_3$); 33.87 (CH); 117.62 (C_{Ar}); 120.62 ($2CH_{Ar}$); 125.86 ($2CH_{Ar}$); 127.73 (CH_{Ar}); 128.37 ($2CH_{Ar}$); 128.92 ($2CH_{Ar}$); 130.73 ($CH_{Triazole}$); 135.01 (C_{Ar}); 148.16 ($C_{Triazole}$); 149.87 (C_{Ar}). HRMS (ESI) [M + H] $^{+}$ found m/z = 264.1498. Calcd value for $C_{15}H_{11}F_2N_3$ = 264.1495.

(1-(4-isopropylphenyl)-1H-1,2,3-triazol-4-yl)methyl benzoate (3h)

Yield: 84%.White solid. MP= 117.2°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm) : 1.29 (s, 3H, CH_3); 1.31 (s, 3H, CH_3); 2.95-3.04 (m, 1H, CH); 5.58 (s, 2H, CH_2); 7.37-7.40 (d, 2H, CH_{Ar}); 7.43-7.48 (t, 2H, CH_{Ar}); 7.56-7.60 (d, 1H, CH_{Ar}); 7.64-7.67 (d, 2H, CH_{Ar}); 8.07-8.10 (d, 2H, CH_{Ar}); 8.12 (s, 1H,$CH_{Triazole}$). ^{13}C NMR (75MHz, $CDCl_3$, δ ppm): 24.26 ($2CH_3$); 34.23 (CH); 58.48 (CH_2); 121.11 ($CH_{Triazole}$); 122.71 (C_{Ar}); 128.10 ($2CH_{Ar}$); 128.81 ($2CH_{Ar}$); 130.13 ($2CH_{Ar}$); 130.18 ($2CH_{Ar}$); 133.65 (C_{Ar}); 135.22 (CH_{Ar}); 143.83 ($C_{Triazole}$); 150.42 (C_{Ar}); 166.92 (C_{Ester}). HRMS (ESI) [M + H] $^{+}$ found m/z = 322.1562. Calcd value for $C_{19}H_{19}N_3O_2$ = 322.1550.

Methyl 1-(4-isopropylphenyl)-1H-1,2,3-triazole-4-carboxylate (3i)

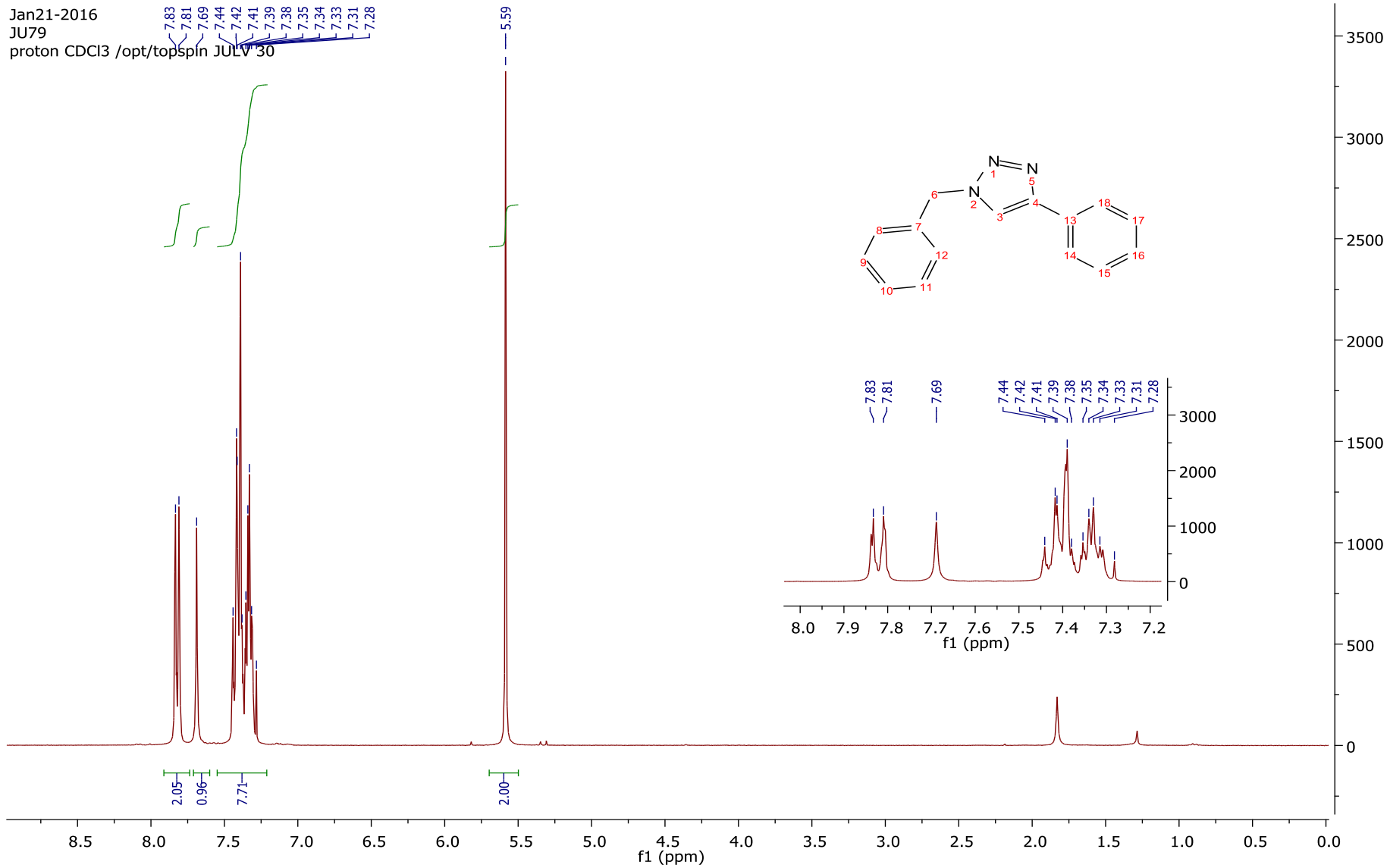
Yield: 78%. White solid. MP= 71.5°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 1.30 (s, 3H, CH_3); 1.32 (s, 3H, CH_3); 2.97-3.06 (m, 1H, CH); 4.01 (s, 3H, OCH_3); 7.40-7.43 (d, 2H, CH_{Ar}); 7.66-7.70 (d, 2H, CH_{Ar}); 8.50 (s, 1H, $CH_{Triazole}$). ^{13}C NMR (75MHz, $CDCl_3$, δ ppm): 24.23 ($2CH_3$); 34.28 (CH); 52.73 (OCH_3); 121.25 (C_{Ar}); 125.98 ($2CH_{Ar}$); 128.30 ($CH_{Triazole}$); 134.64 ($2CH_{Ar}$); 141.27 ($C_{Triazole}$); 151.14 (C_{Ar}); 161.54 (C_{Ester}). HRMS (ESI) [M + H] $^{+}$ found m/z = 246.1239. Calcd value for $C_{13}H_{15}N_3O_2$ = 246.1237.

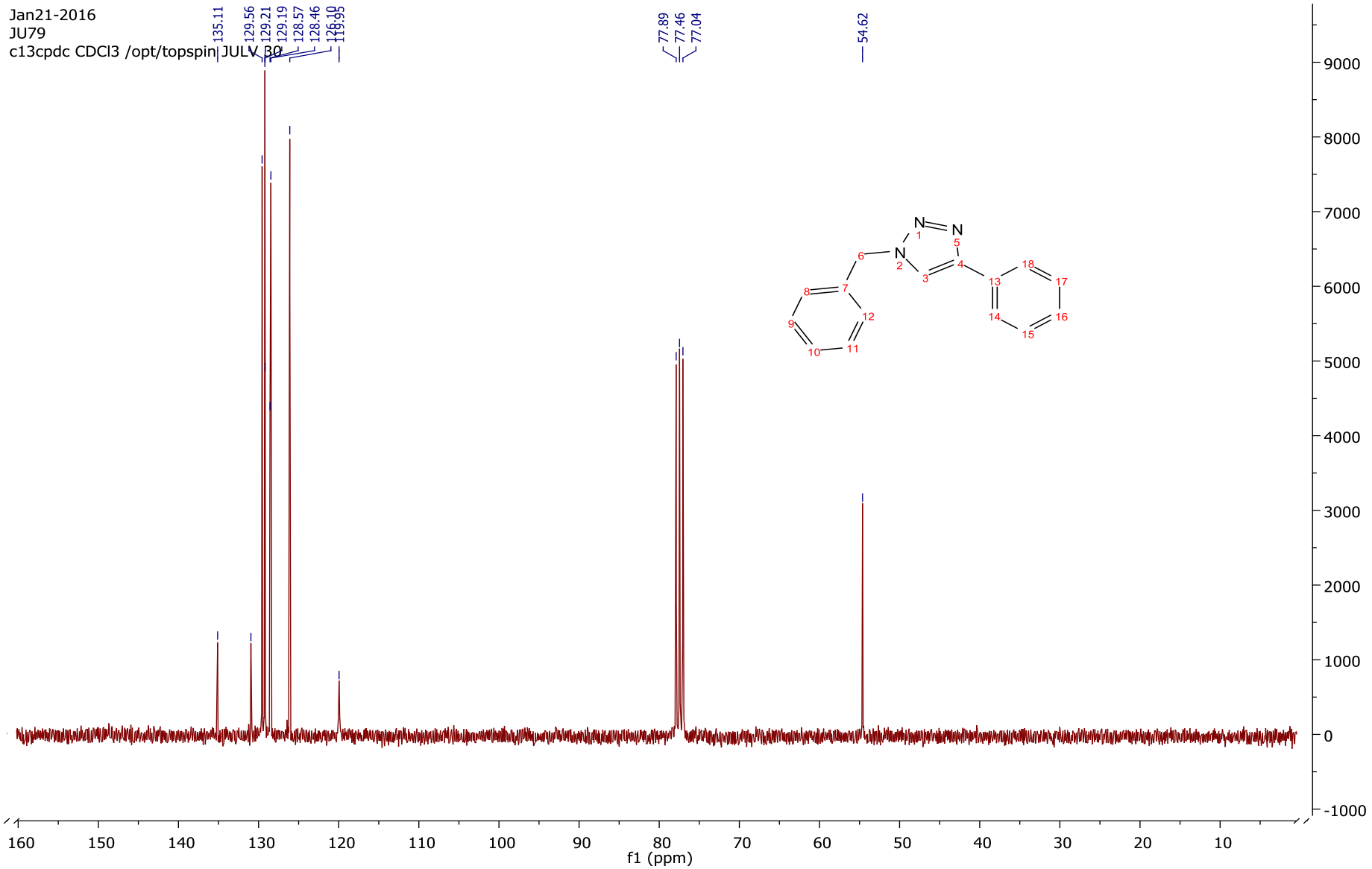
1-(4-isopropylphenyl)-4-(phenylthiomethyl)-1H-1,2,3-triazole (3j)

Yield: 81%.White solid. MP= 138.6°C. ^{1}H NMR (300MHz, $CDCl_3$, δ ppm): 1.29 (s, 3H, CH_3); 1.31 (s, 3H, CH_3); 2.94-3.03 (m, 1H, CH); 4.34 (s, 2H, CH_2); 7.19-7.24 (d, 1H, CH_{Ar});

7.31-7.41 (m, 6H, CH_{Ar}); 7.57-7.61 (d, 2H, CH_{Ar}); 7.78 (s, 1H, $CH_{Triazole}$). ^{13}C NMR (75MHz, $CDCl_3$, δ ppm): 24.27 ($2CH_3$); 29.29 (CH); 34.22 (CH_2); 120.95 ($CH_{Triazole}$); 126.59 (CH_{Ar}); 126.98 ($2CH_{Ar}$); 128.06 ($2CH_{Ar}$); 129.45 ($2CH_{Ar}$); 130.03 ($C_{Triazole}$); 133.76 (C_{Ar}); 134.56 ($2CH_{Ar}$); 135.80 (C_{Ar}); 150.20 (C_{Ar}). HRMS (ESI) $[M + H]^+$ found m/z = 310.1373. Calcd value for $C_{18}H_{19}N_3S$ = 310.1372.

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

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77.46
77.04
54.62
N
N
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
9000
8000
7000
6000
5000
4000
3000
2000
1000
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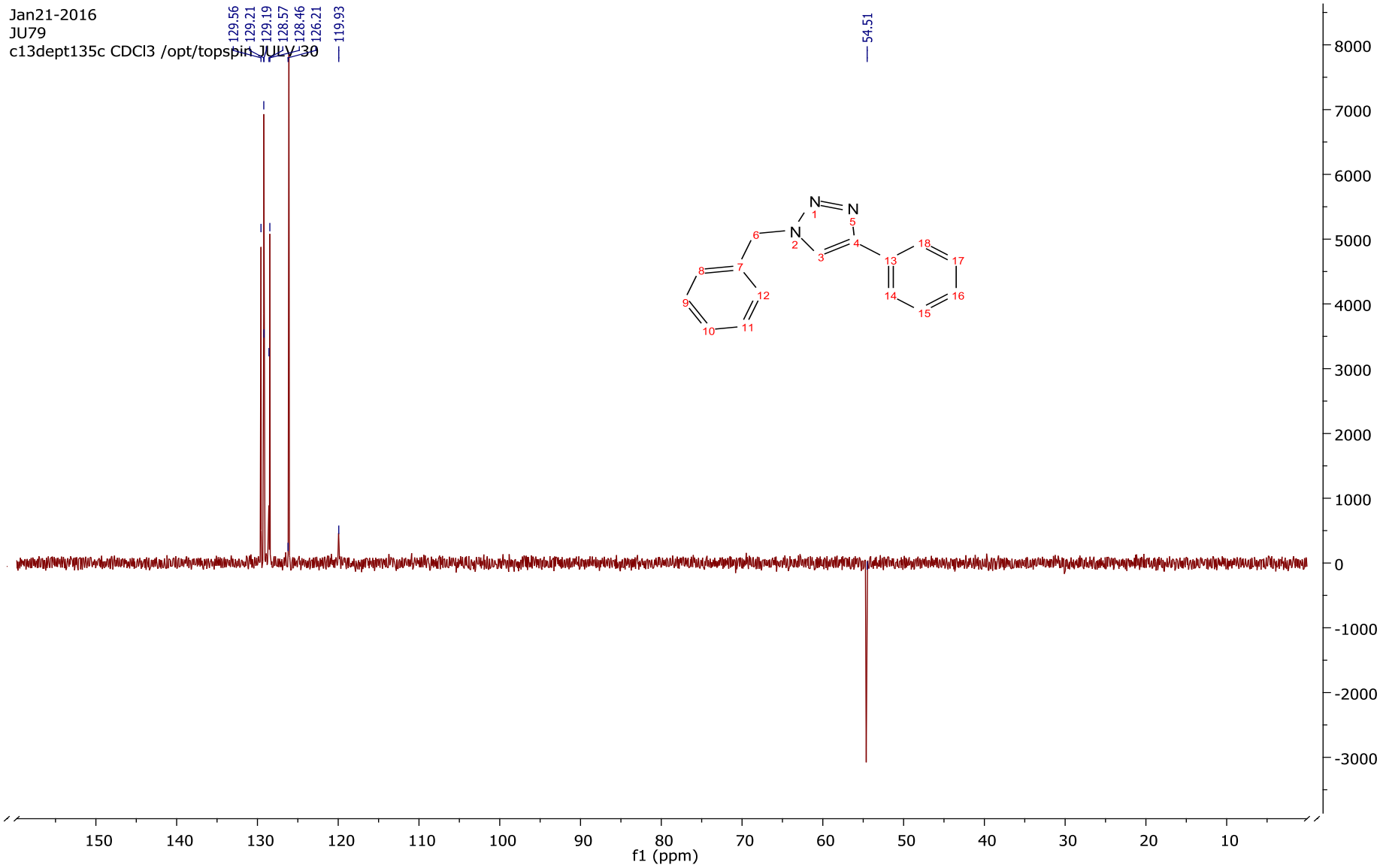
f1 (ppm)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129.19
128.57
128.46
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119.93
54.51
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
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50
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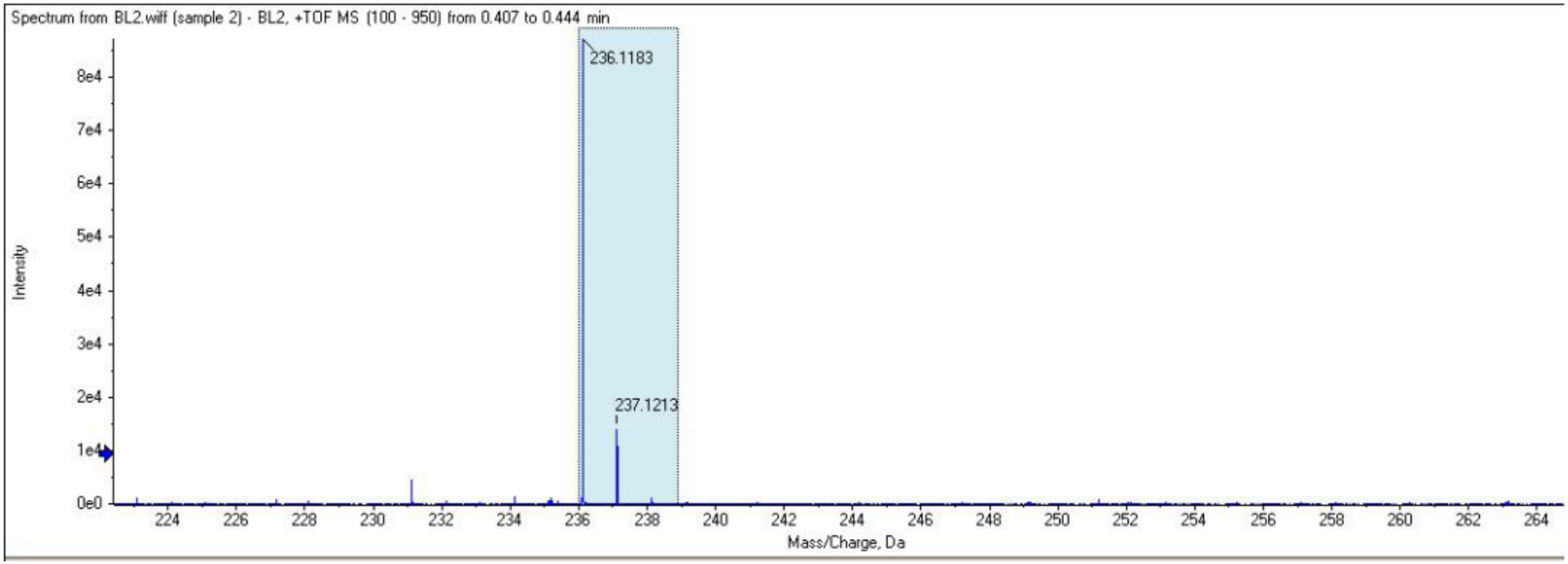
30
20
10
f1 (ppm)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4e4
3e4
2e4
1e4
0e0
224
226
228
230
232
234
236
238
240
242
244
246
248
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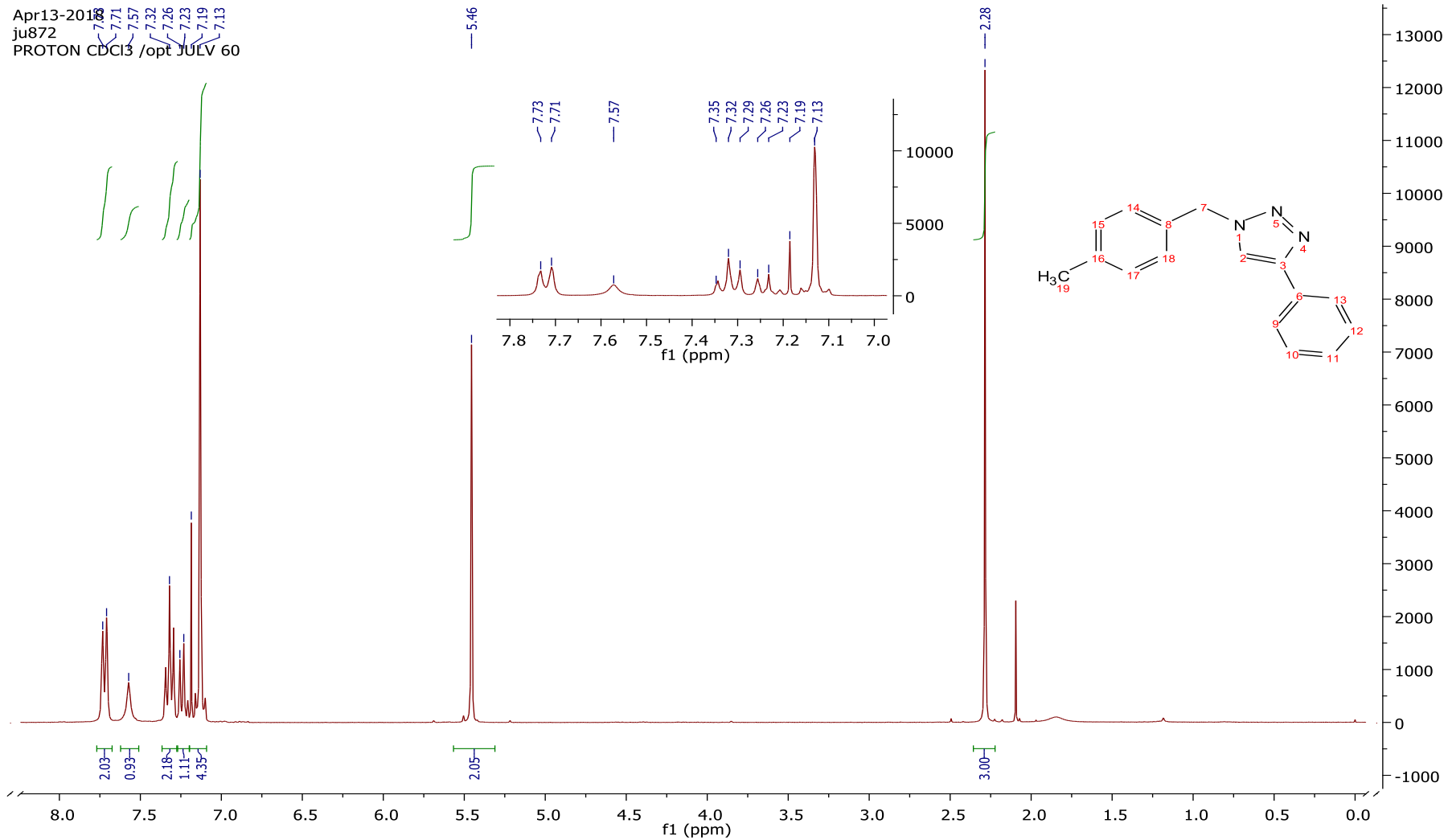
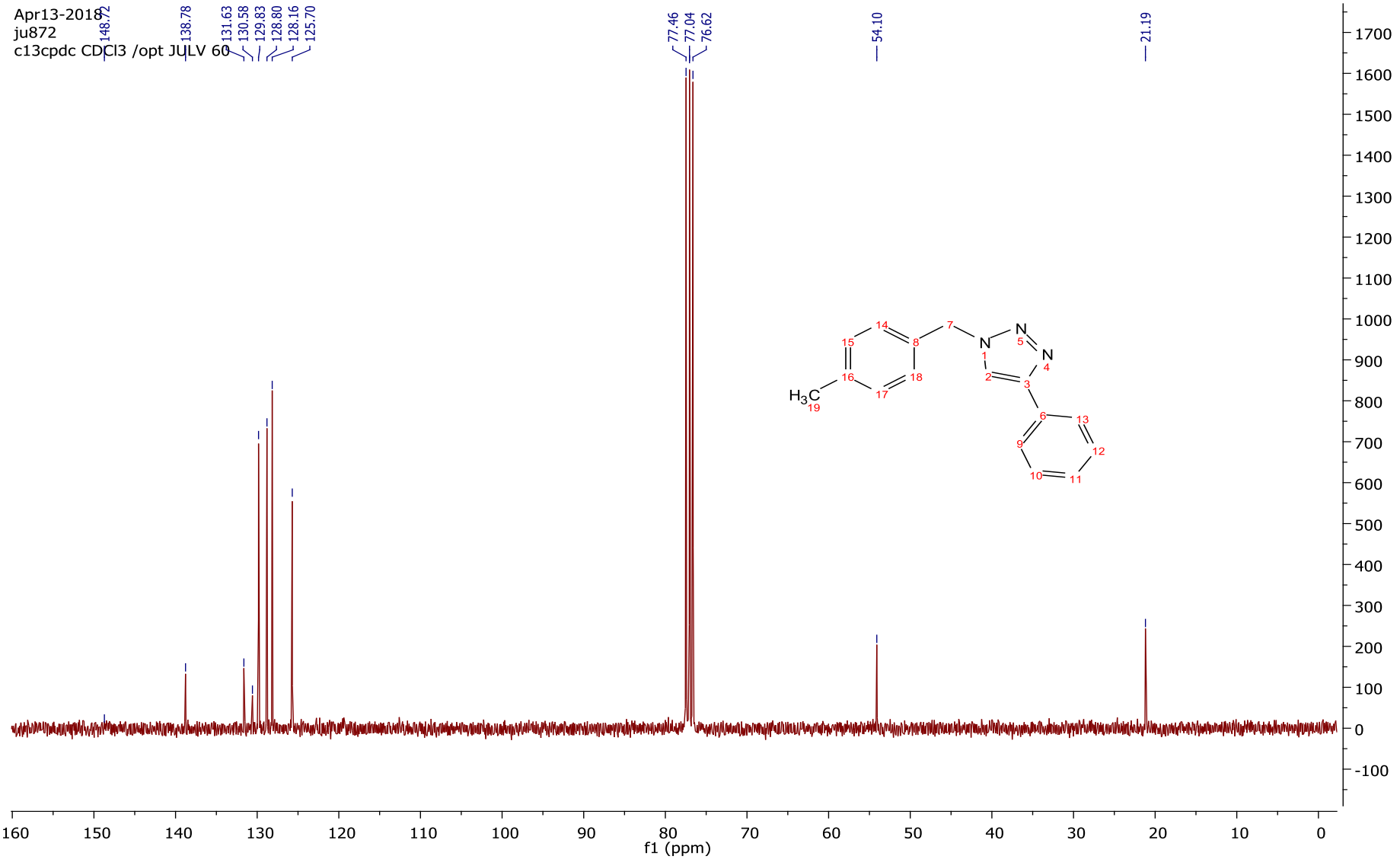
264
Mass/Charge, Da

1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole (3b)

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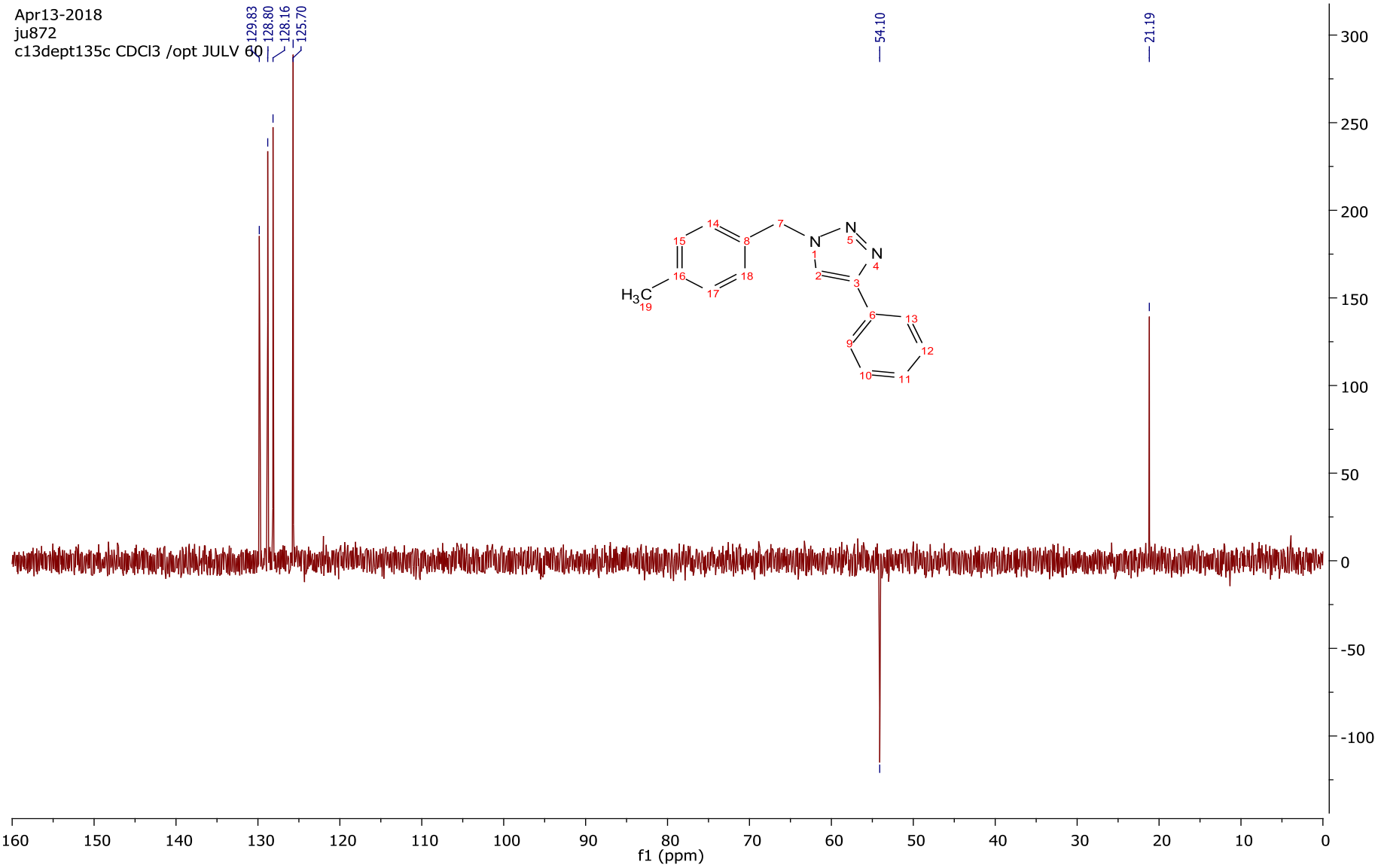
f1 (ppm)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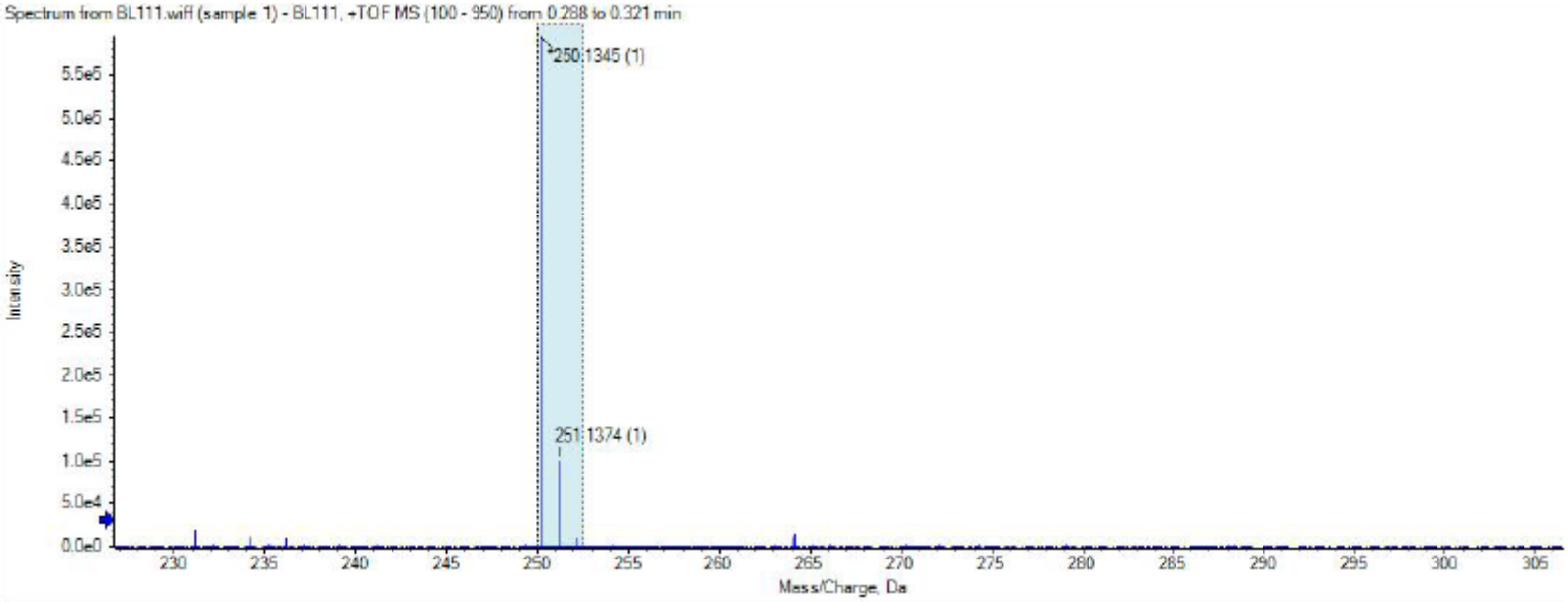
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1.0e5
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245
250
255
260
265
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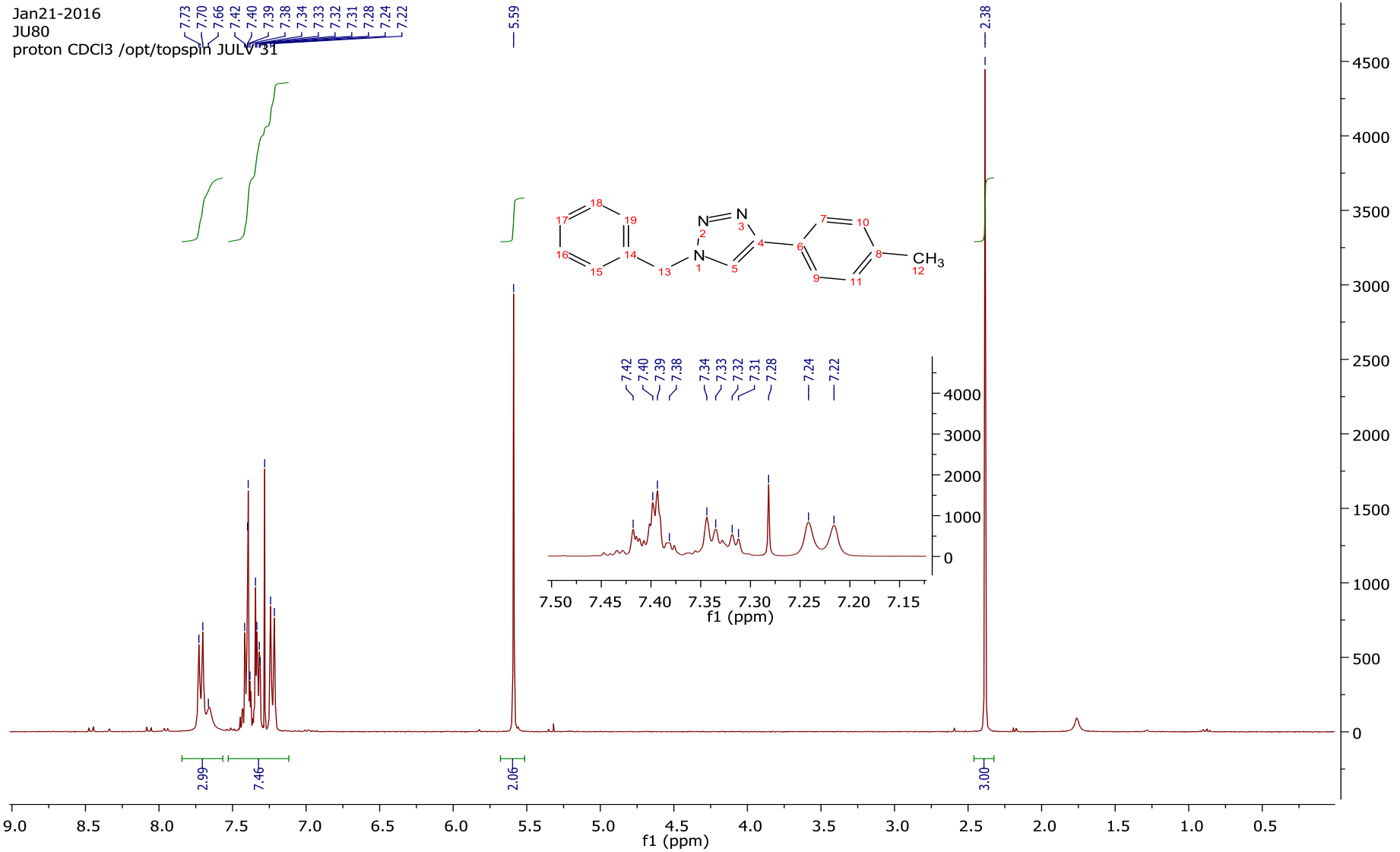
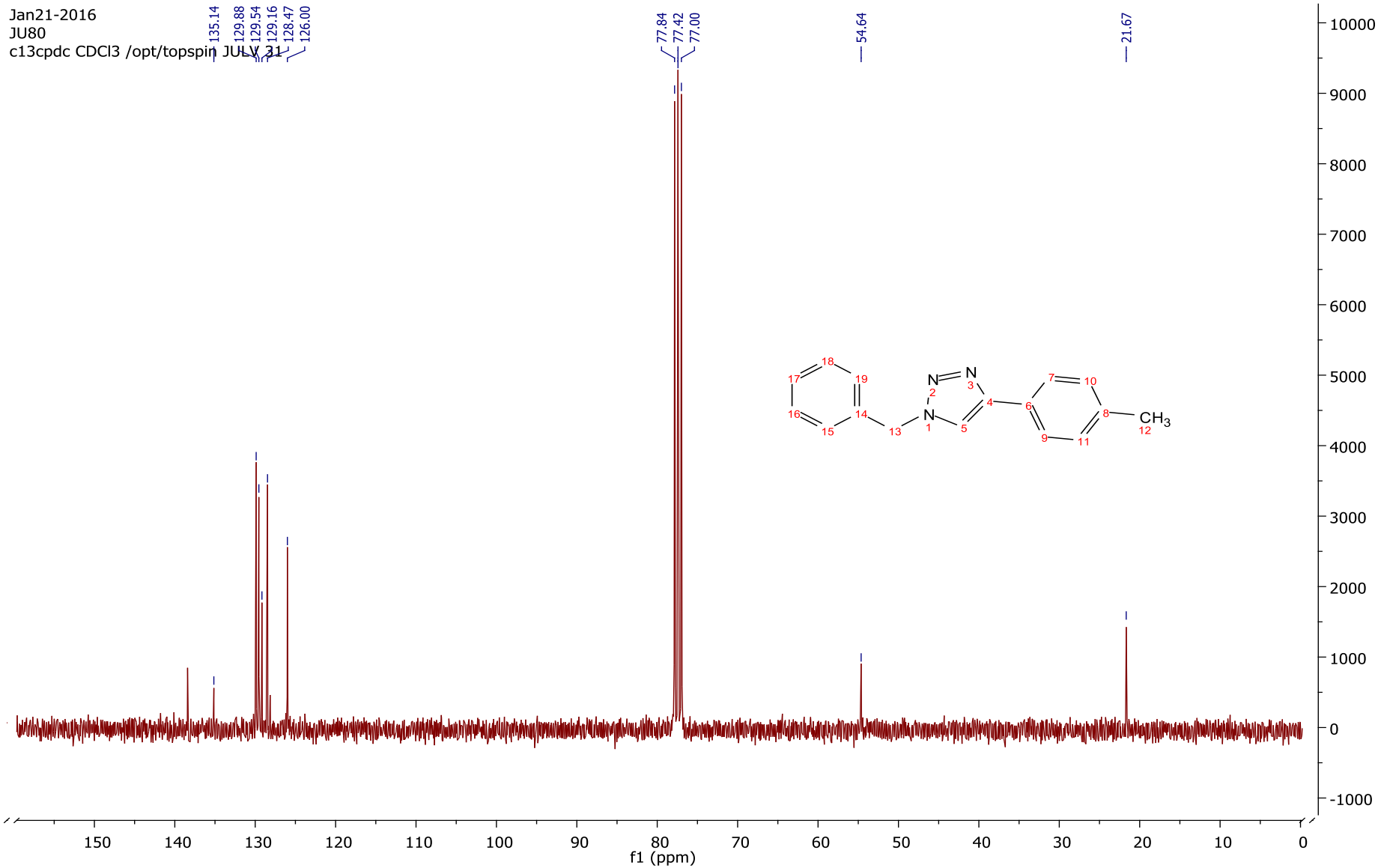
305
Mass/Charge, Da

1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole (3c)

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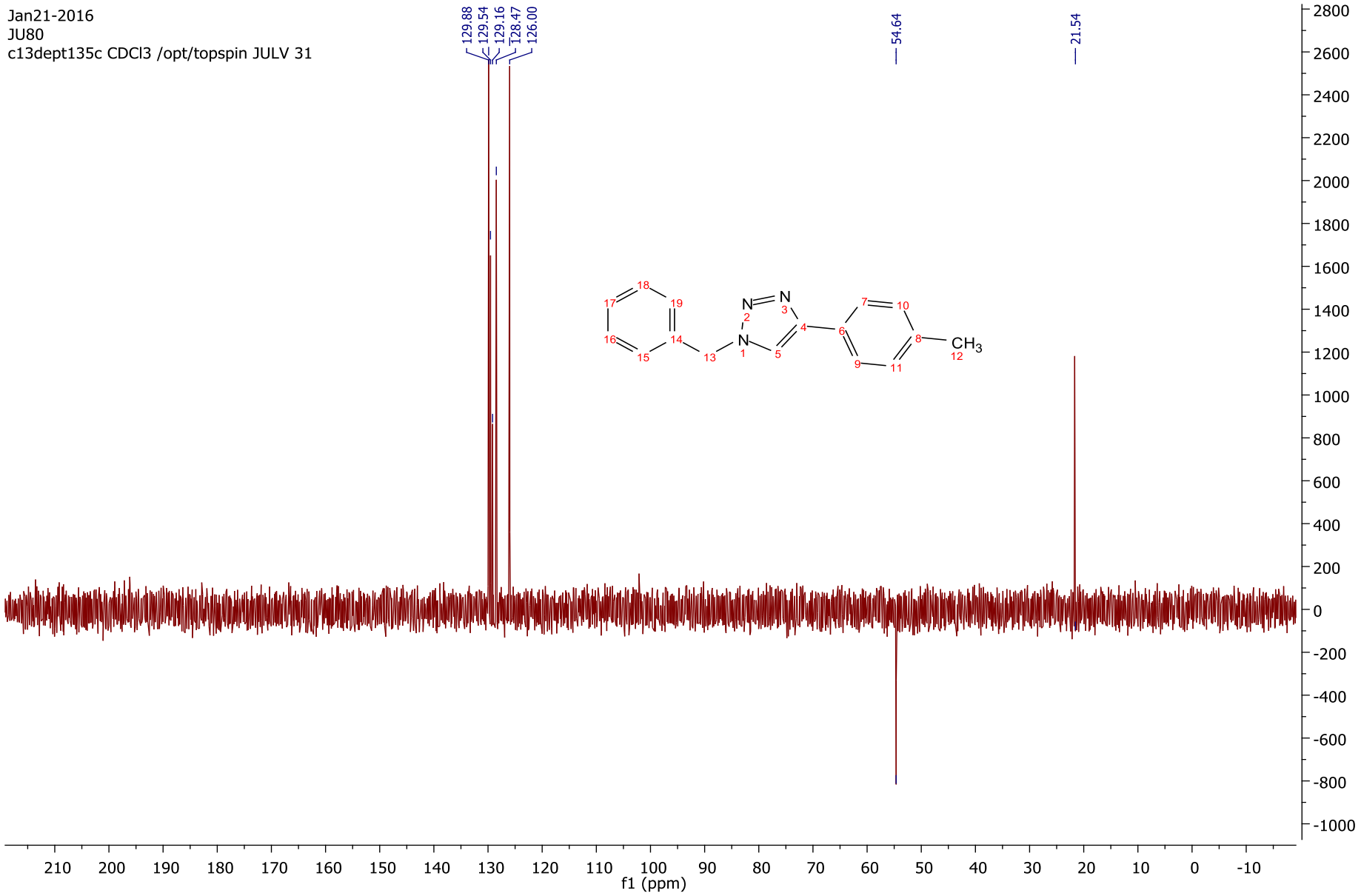
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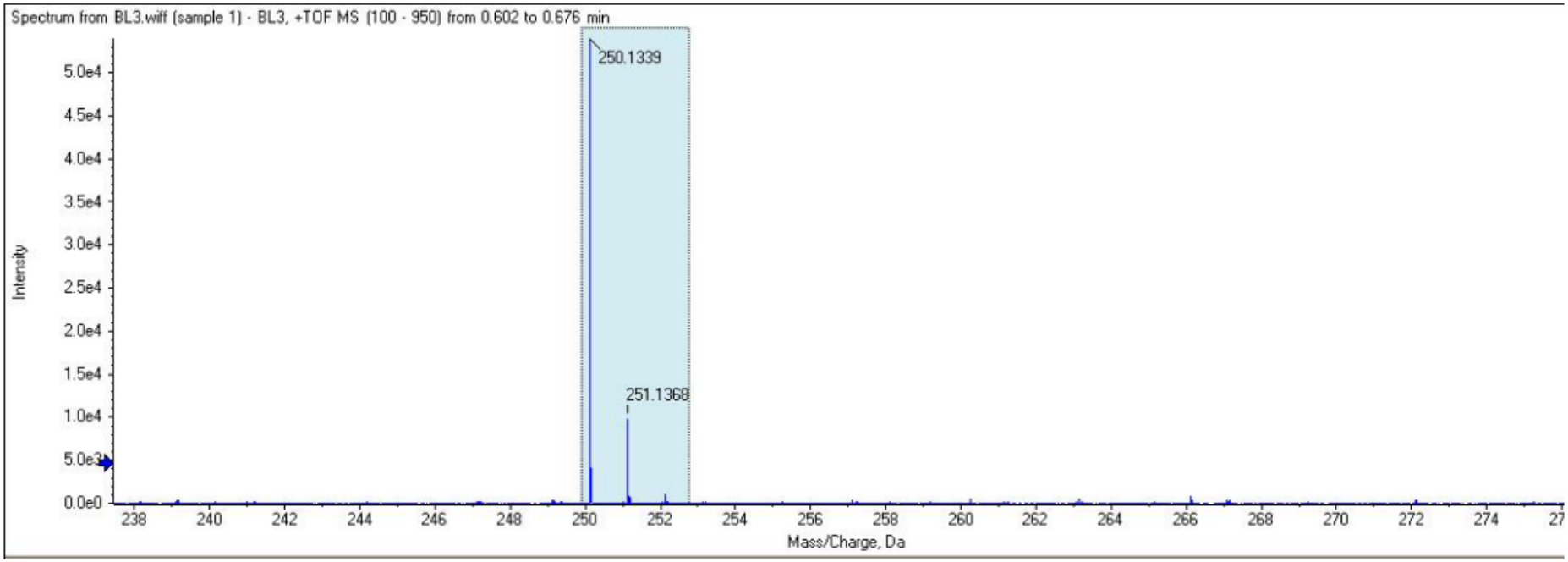
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0.0e0
238
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242
244
246
248
250
252
254
256
258
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268
270
272
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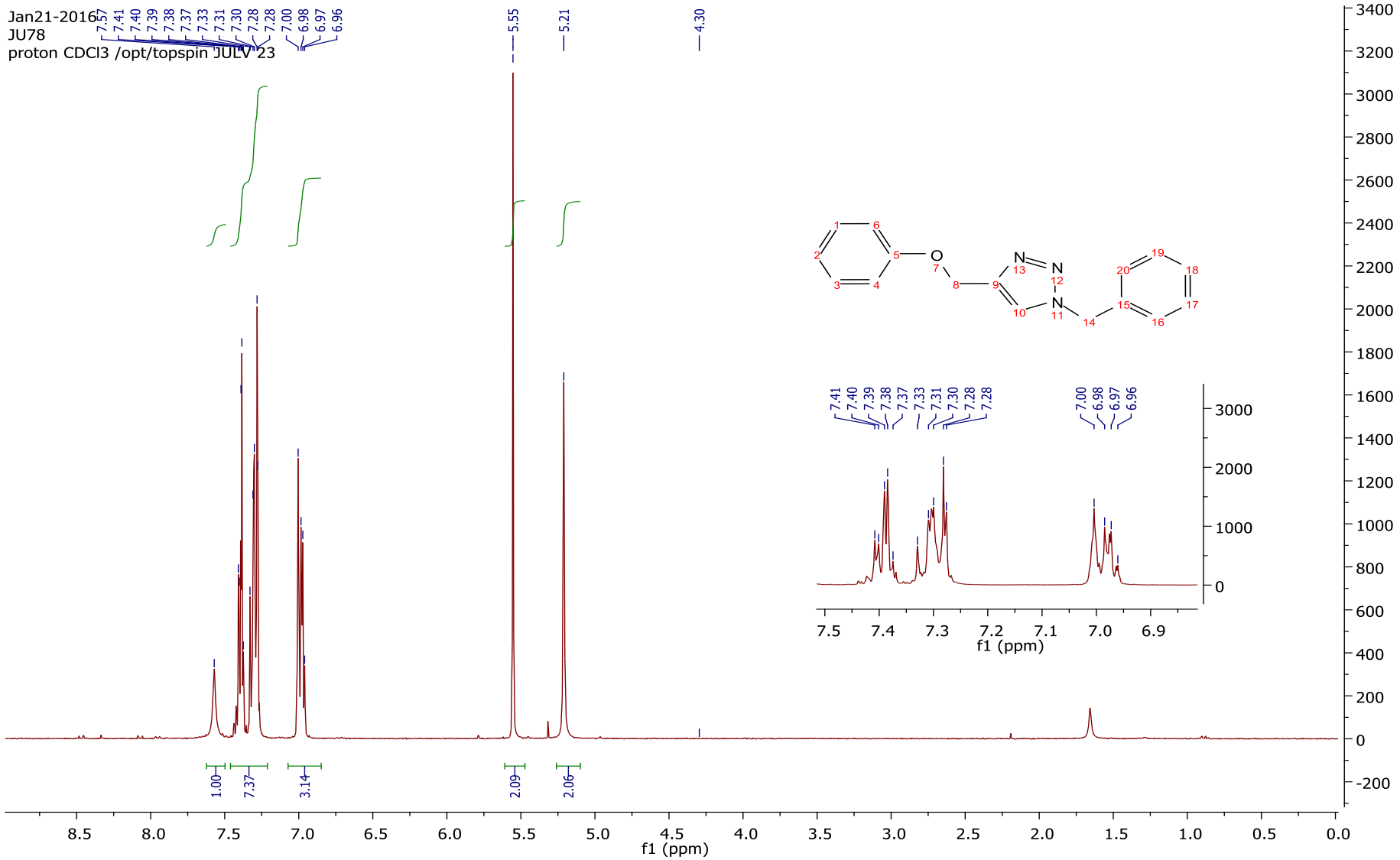
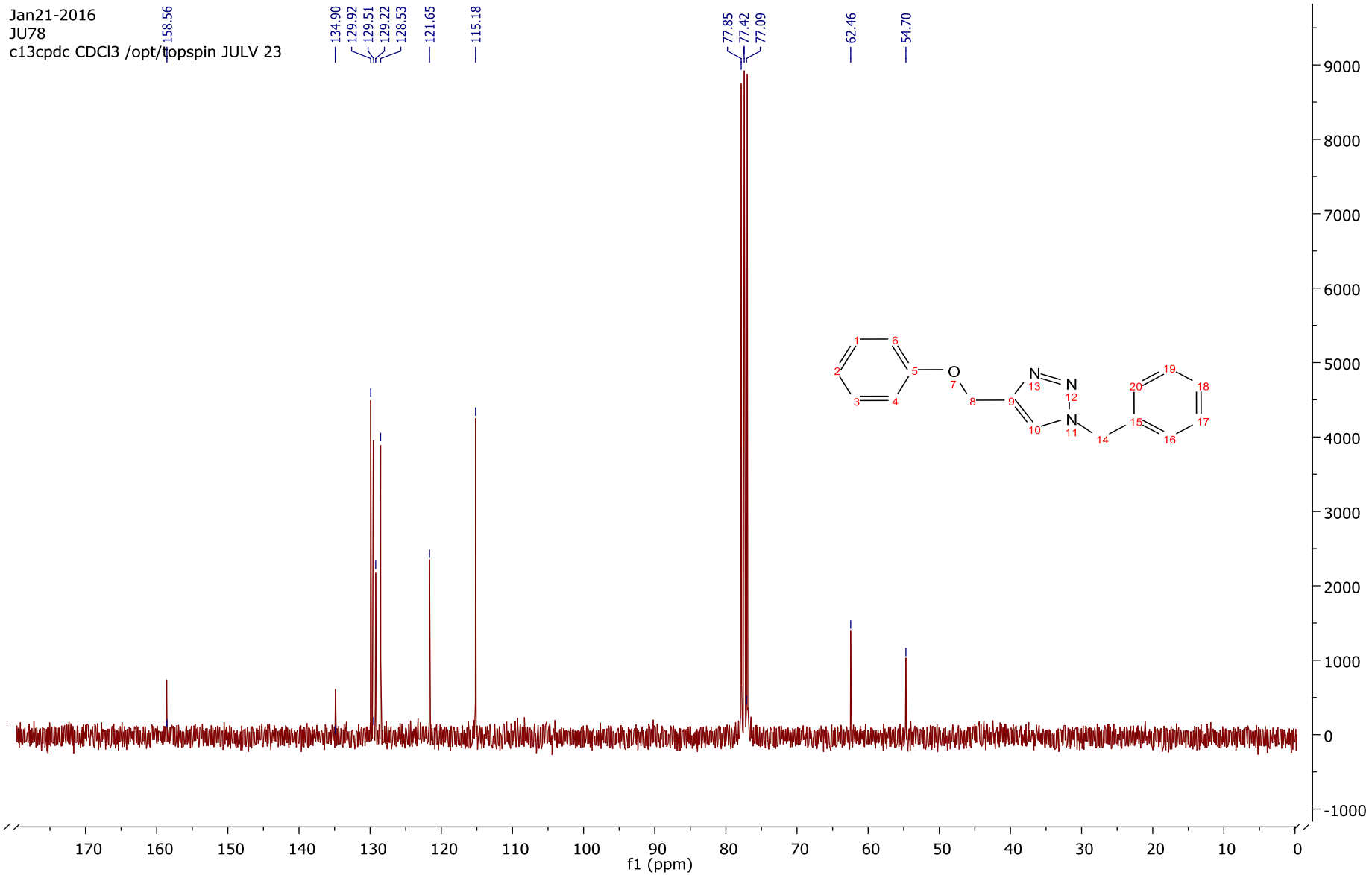
Mass/Charge, Da

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

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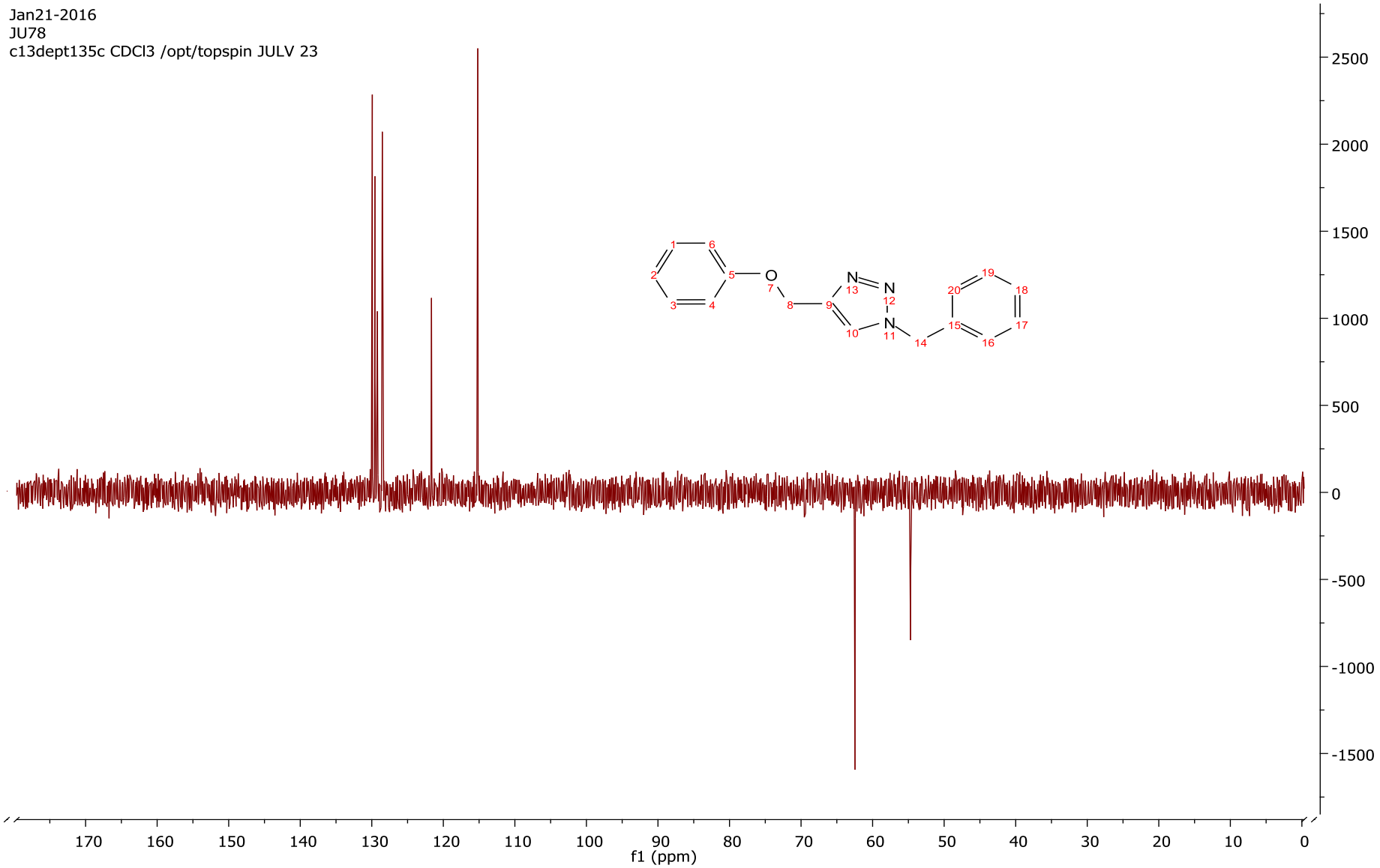
54.70
f1 (ppm)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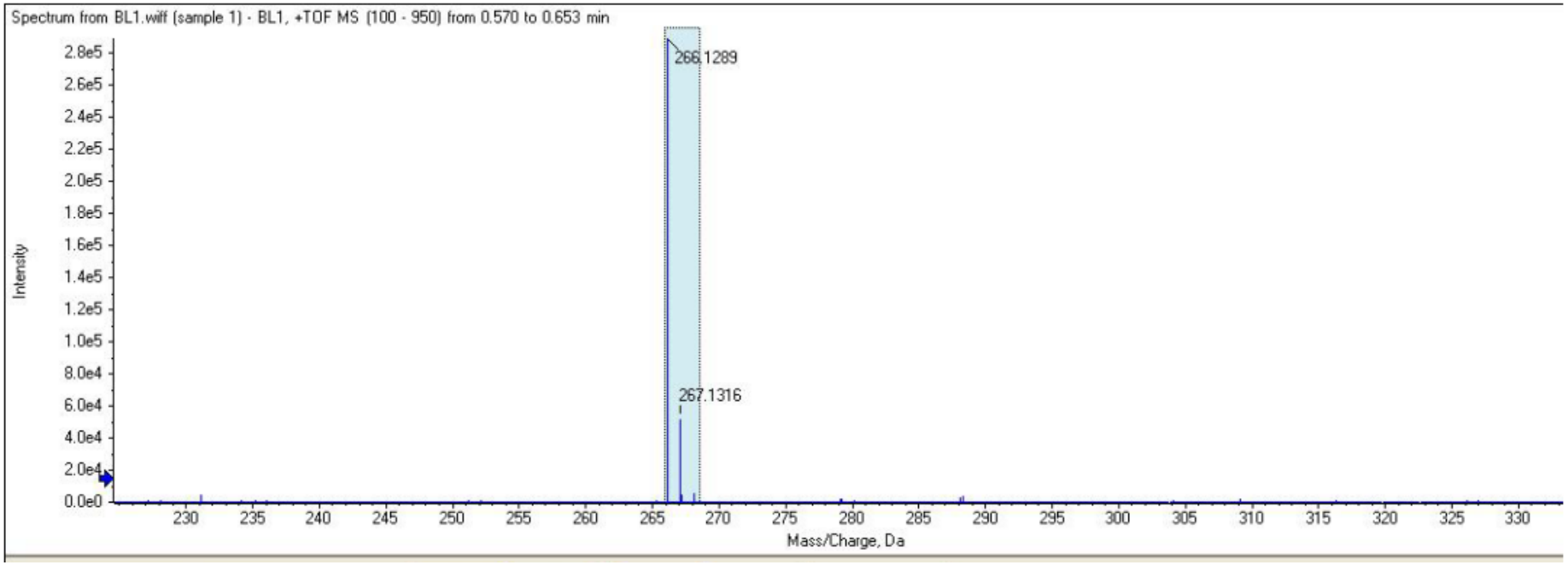
0
f1 (ppm)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6.0e4
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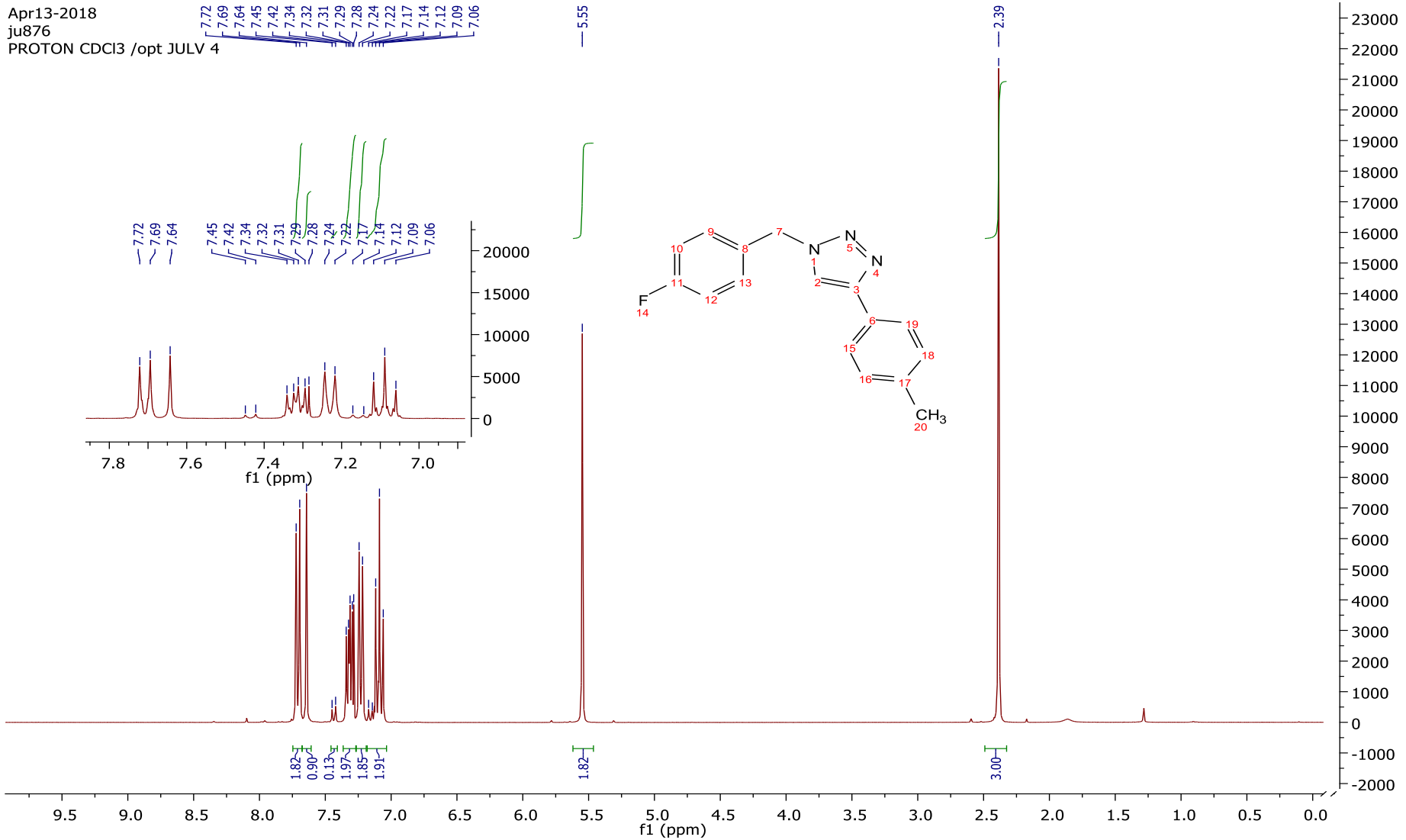
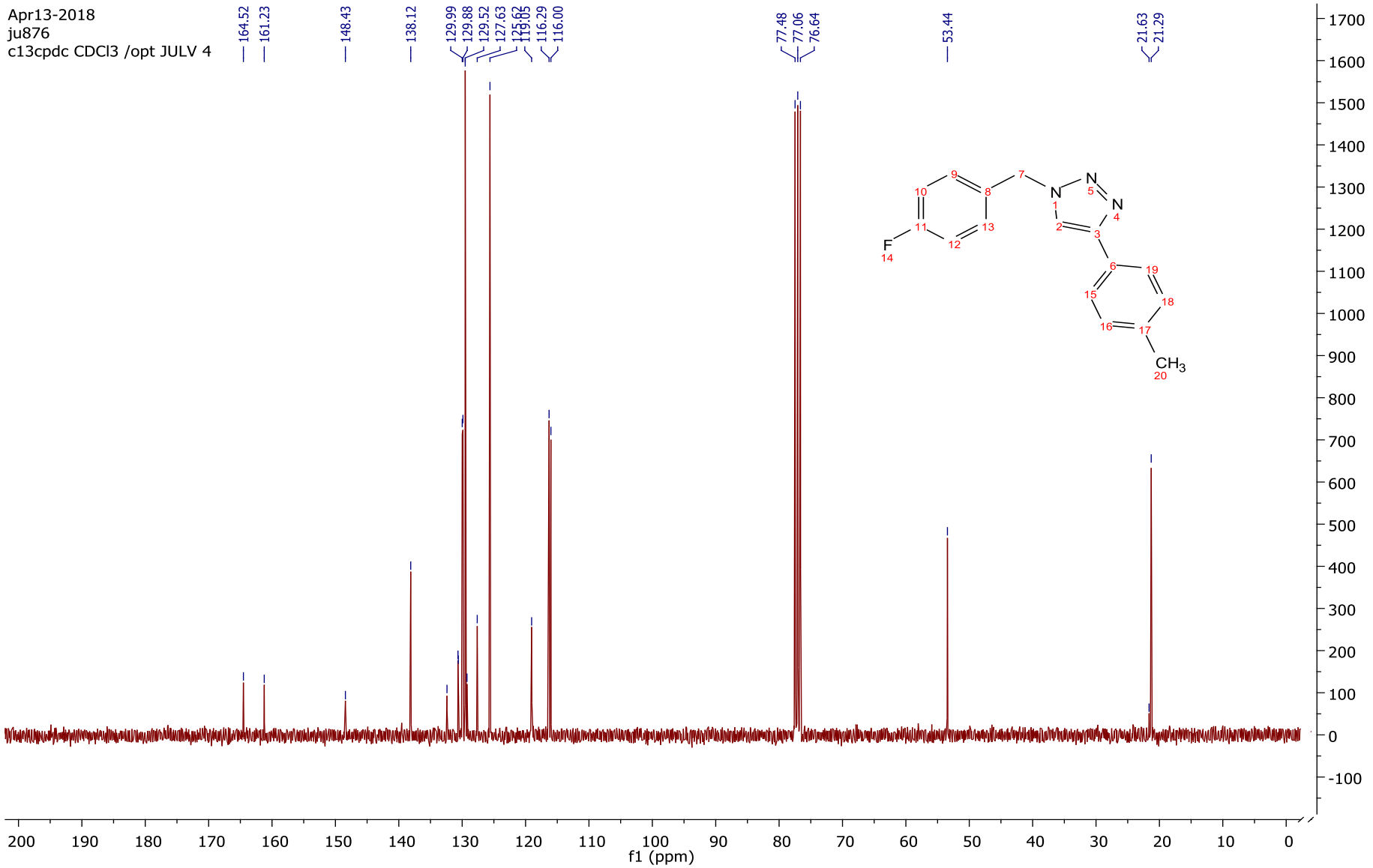
1-(4-Fluoro-benzyl)-4-p-tolyl-1H-[1,2,3]triazole (3e)




Apr13-2018
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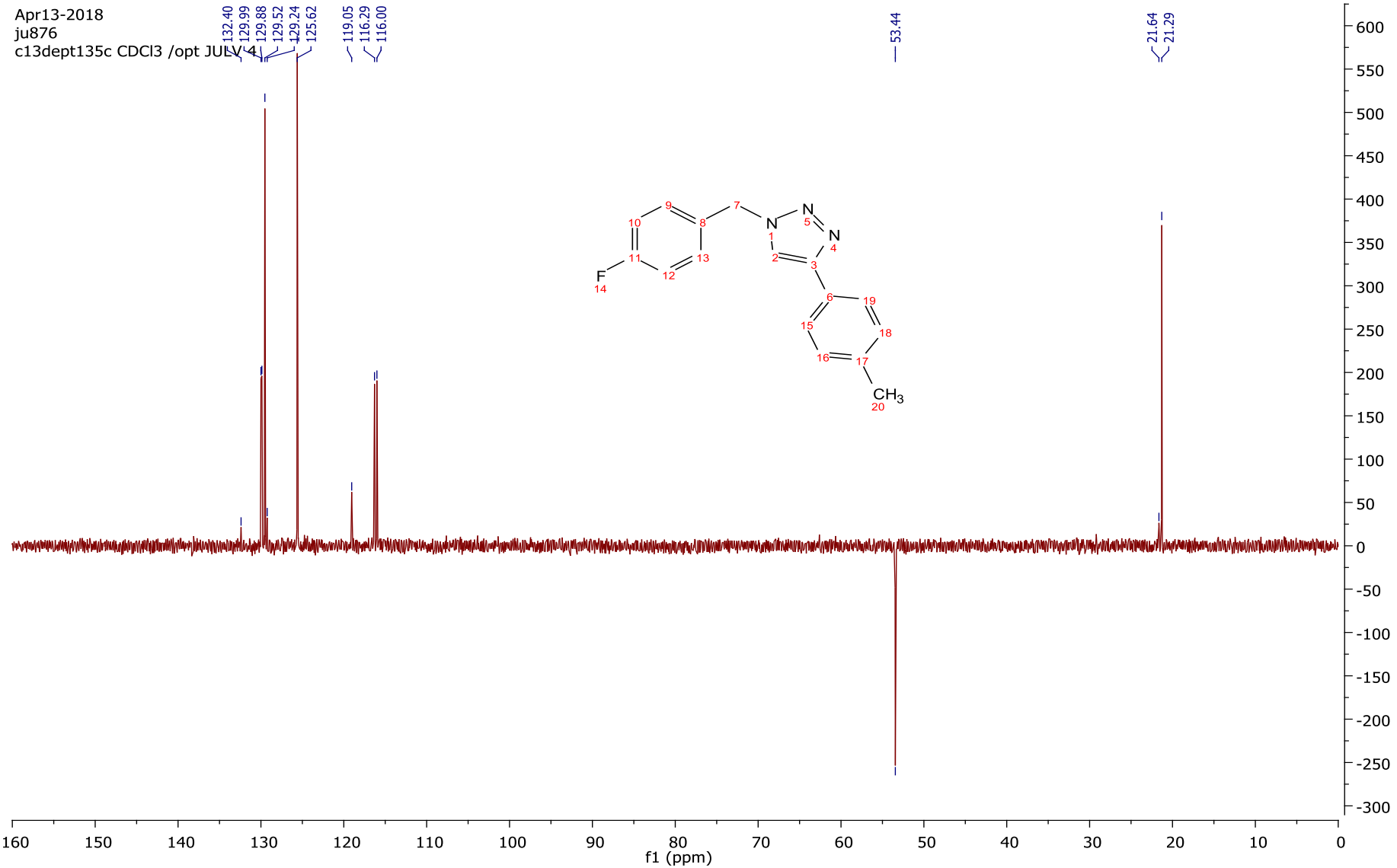
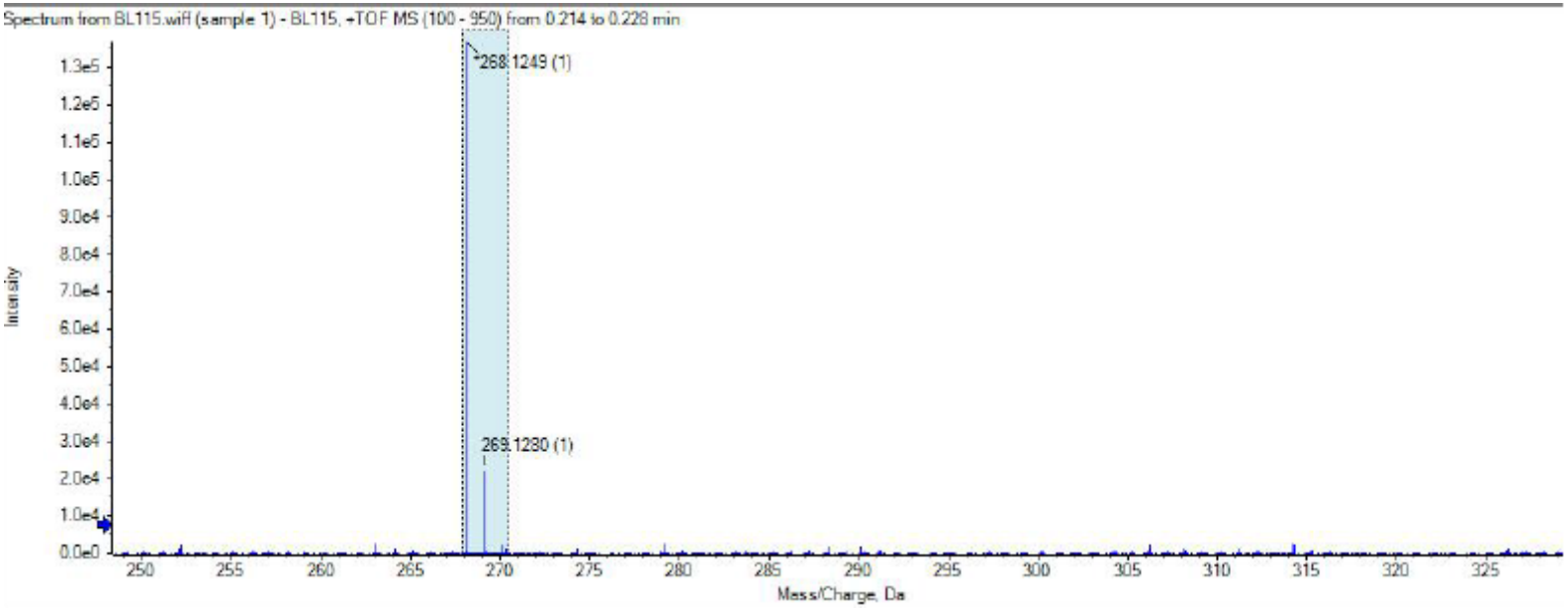
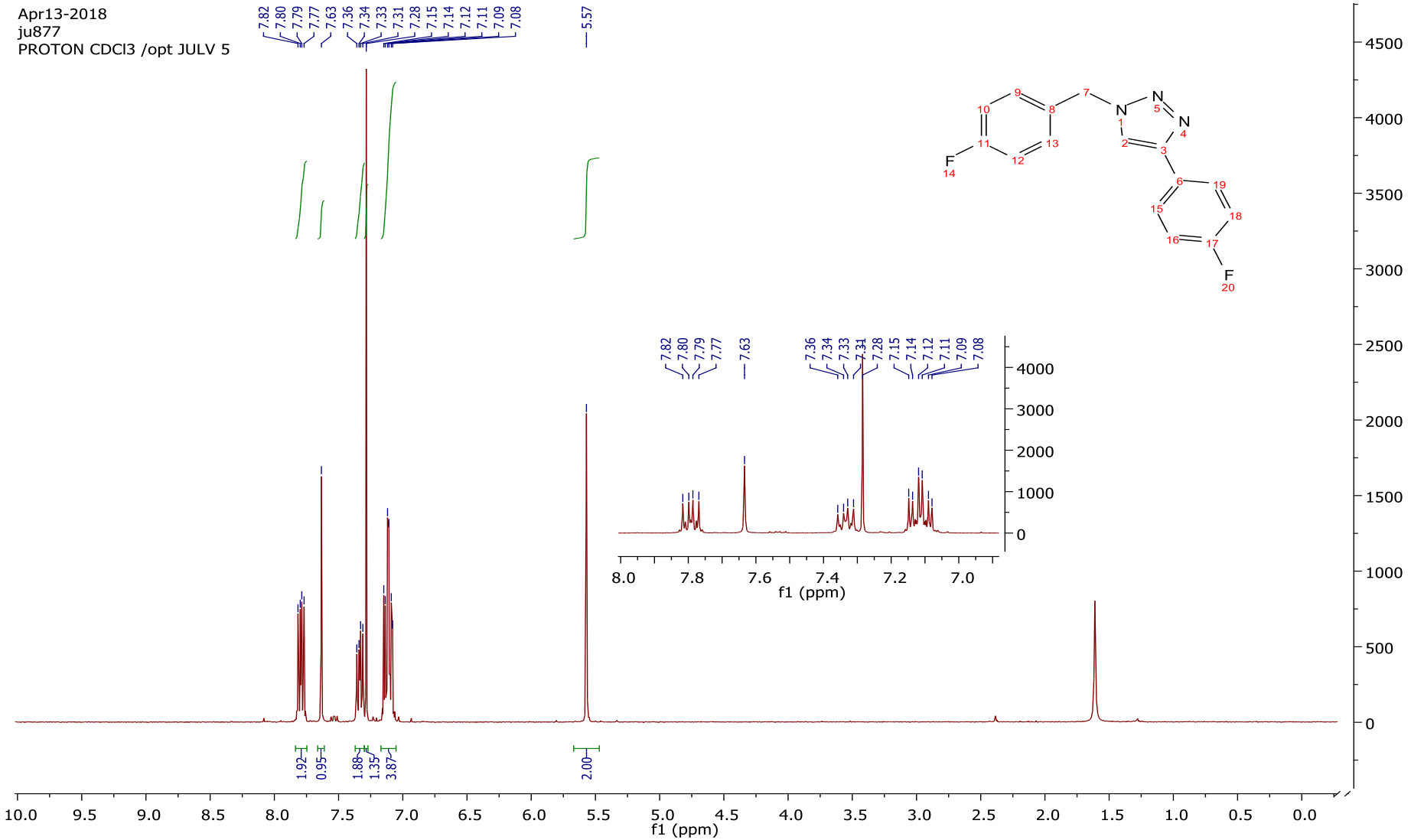
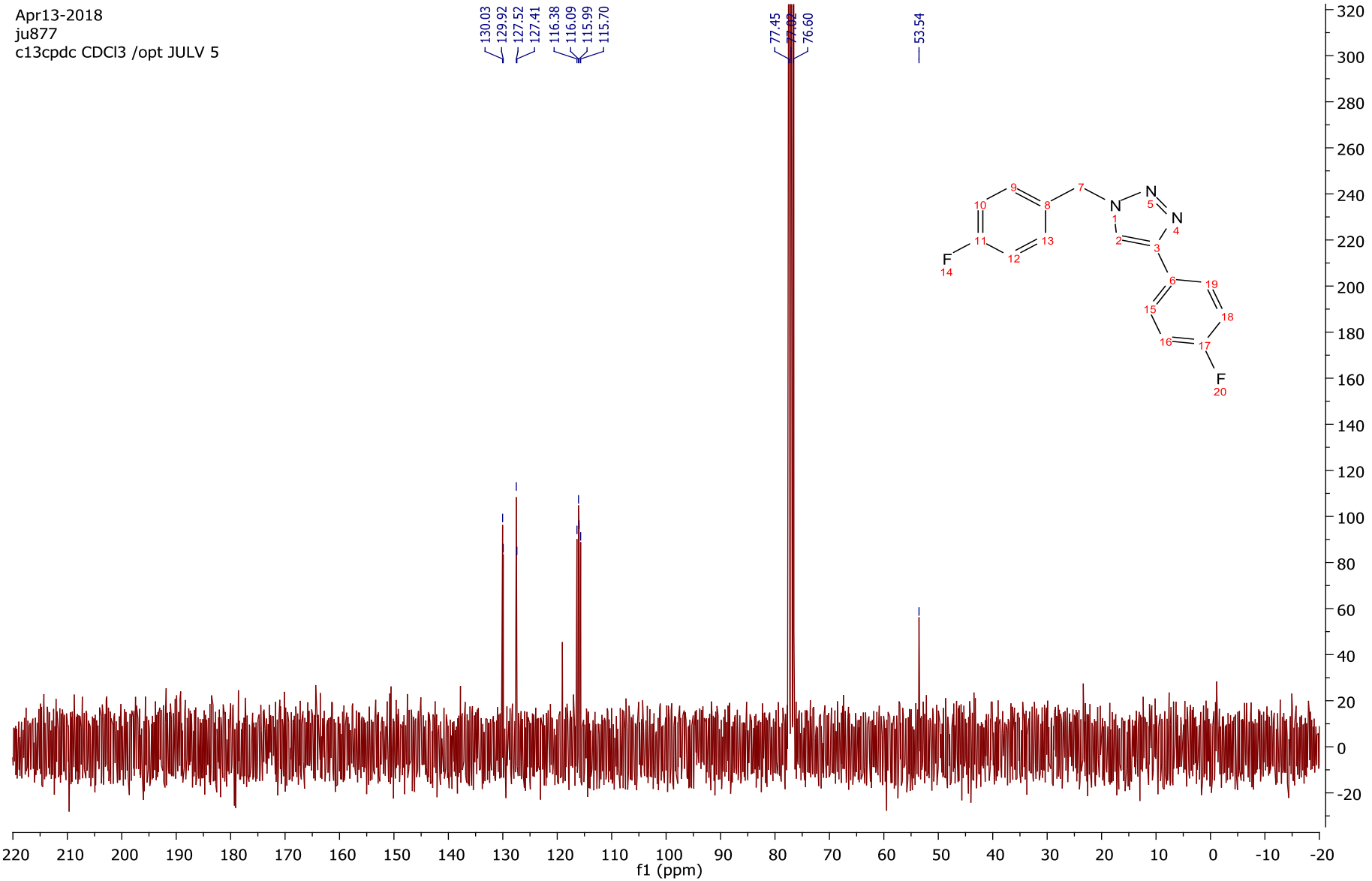
164.52
161.23
148.43
138.12
129.99
129.88
129.52
127.63
125.62
119.05
116.29
116.00
77.48
77.06
76.64
53.44
21.63
21.29
F
CH3
f1 (ppm)

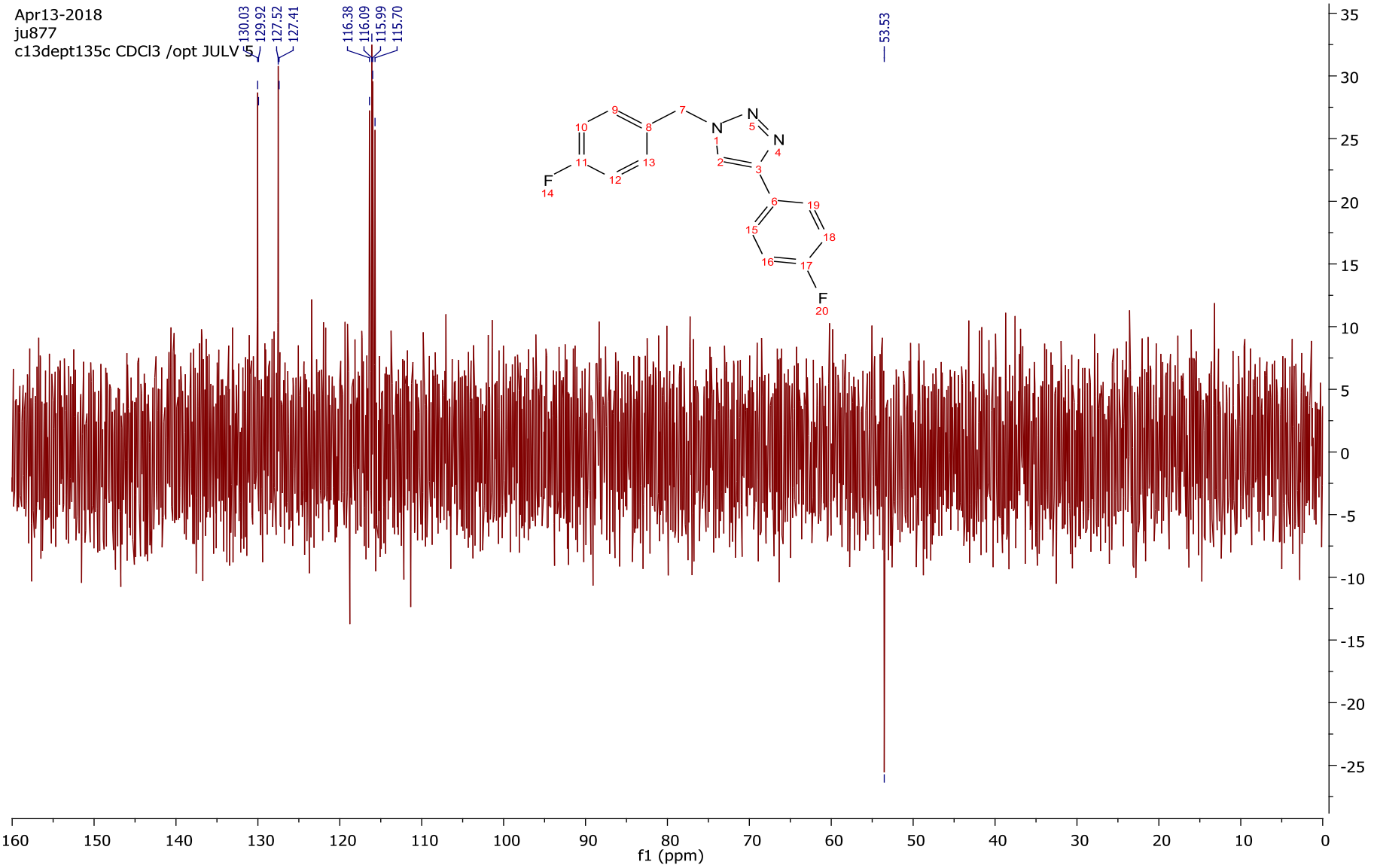

Apr13-2018
ju876
c13dept135c CDCl3 /opt JULY 4
132.40
129.99
129.88
129.52
129.24
125.62
119.05
116.29
116.00
53.44
21.64
21.29
F
CH3
f1 (ppm)

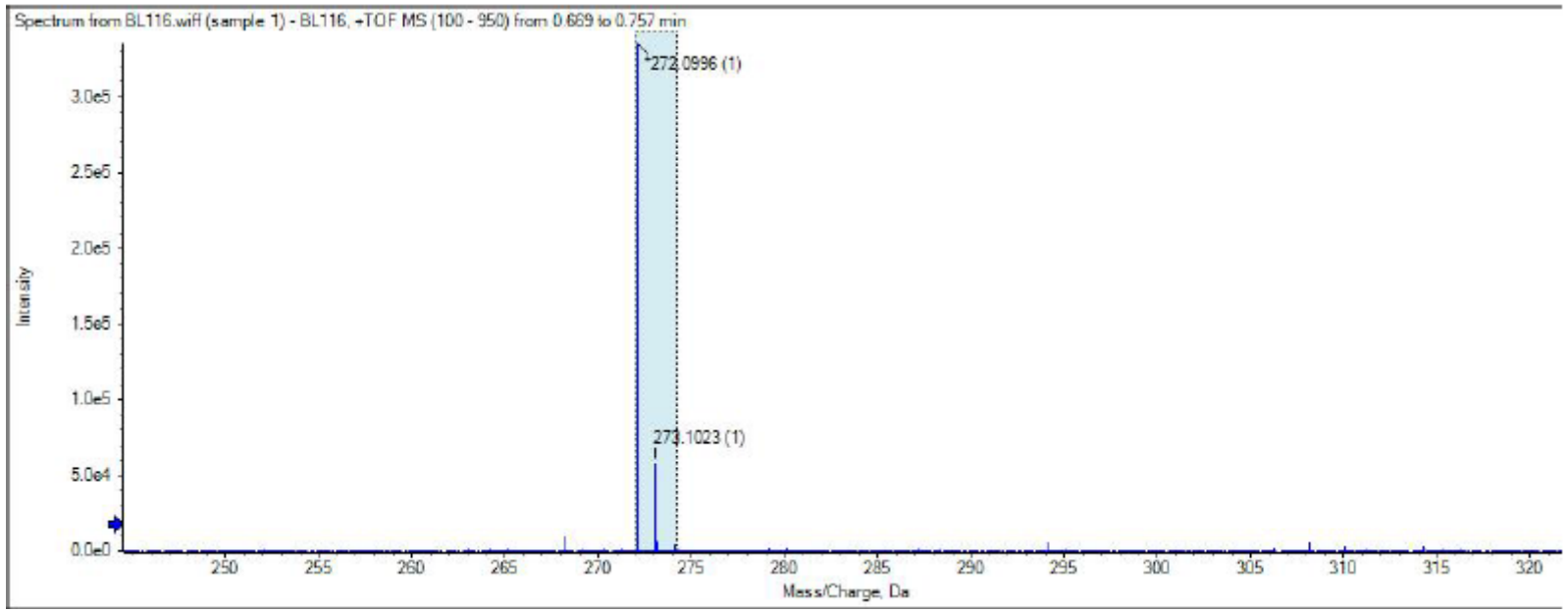

Spectrum from BL115.wiff (sample 1) - BL115, +TOF MS (100 - 950) from 0.214 to 0.228 min
268.1249 (1)
269.1230 (1)
Intensity
Mass/Charge, Da

1-(4-fluorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3f)

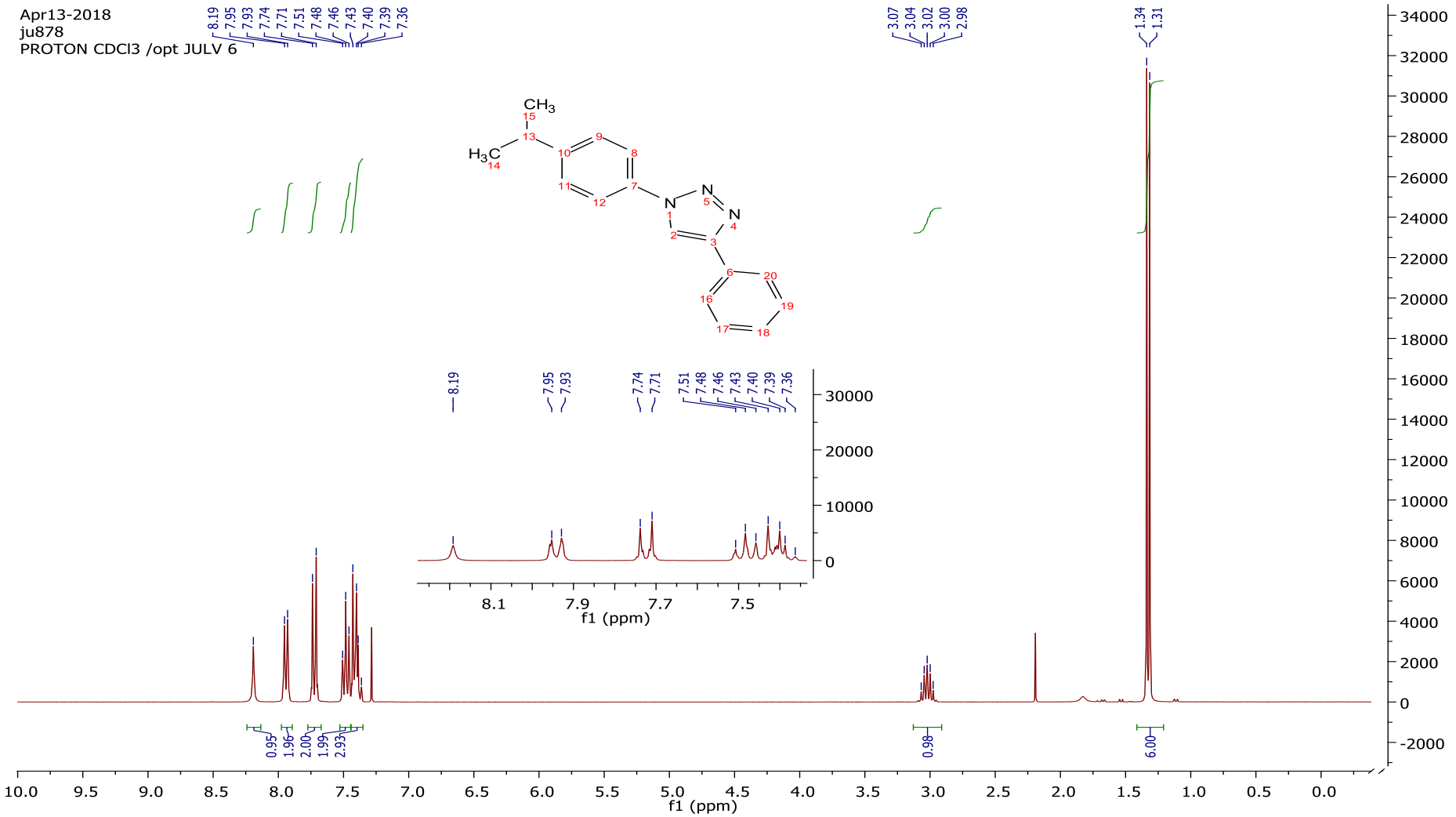


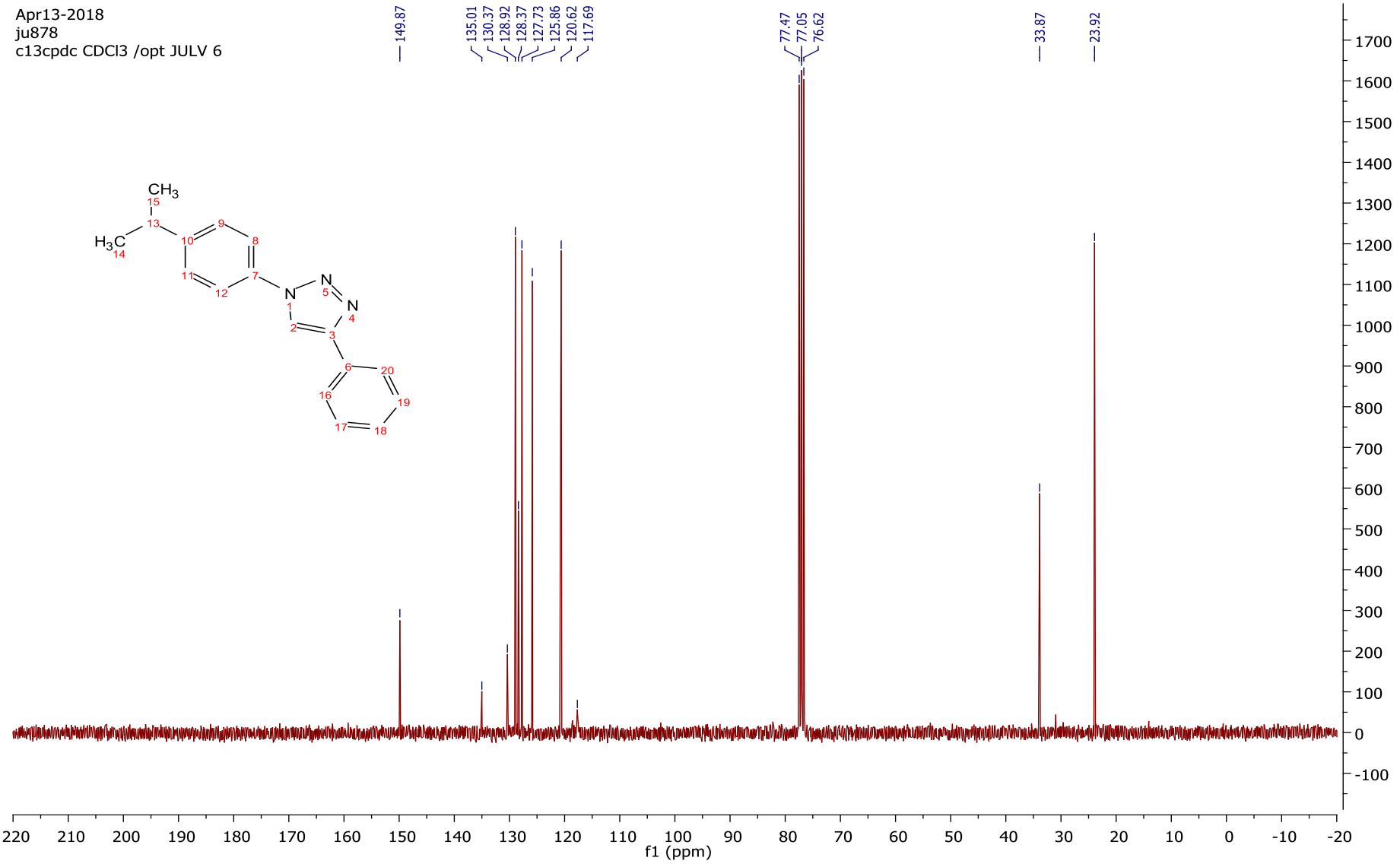

Apr13-2018
ju877
c13cpdc CDCl3 /opt JULV 5
130.03
129.92
127.52
127.41
116.38
116.09
115.99
115.70
77.45
77.02
76.60
53.54
f1 (ppm)

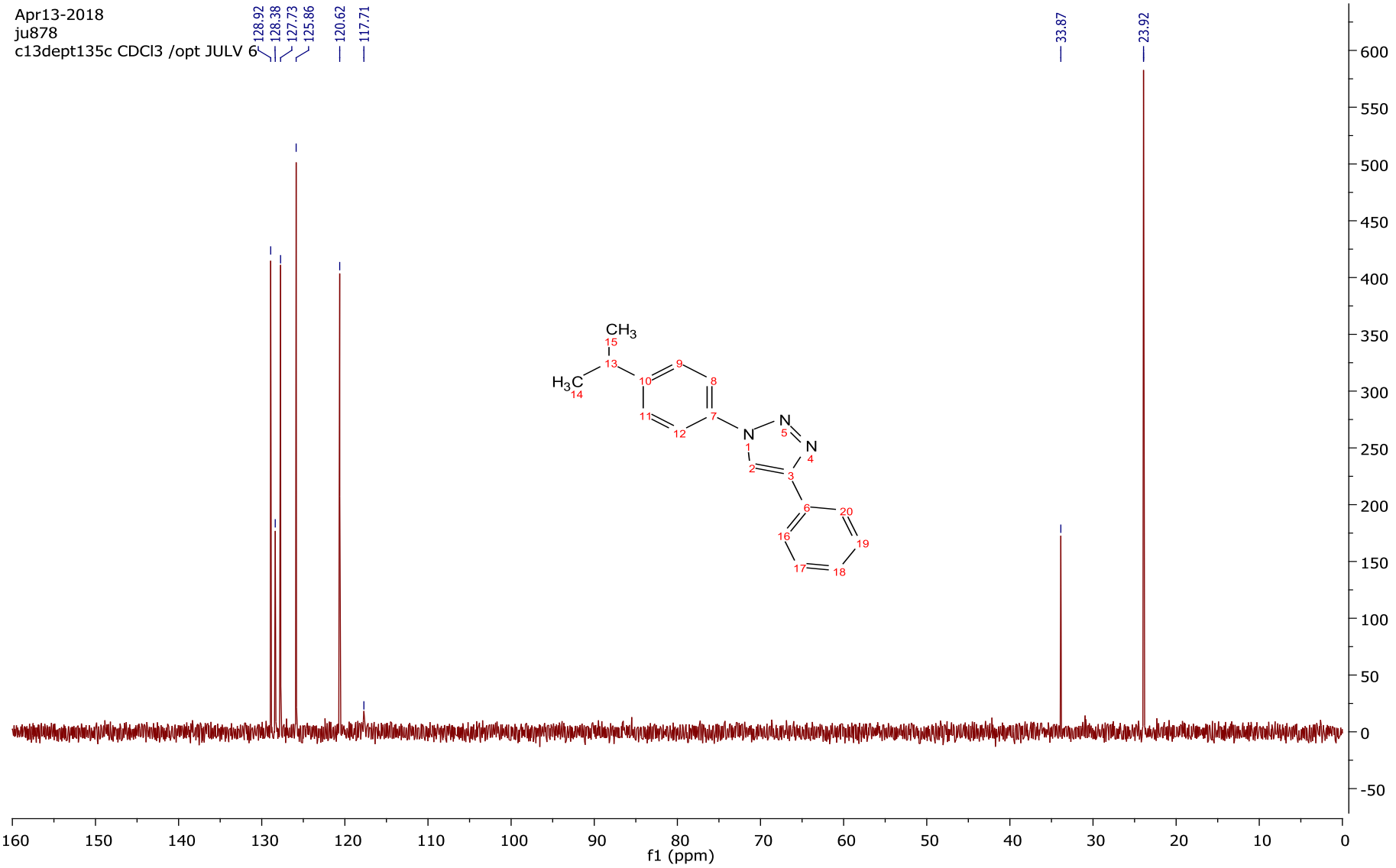

Apr13-2018
ju877
c13dept135c CDCl3 /opt JULV 5
130.03
129.92
127.52
127.41
116.38
116.09
115.99
115.70
53.53
f1 (ppm)

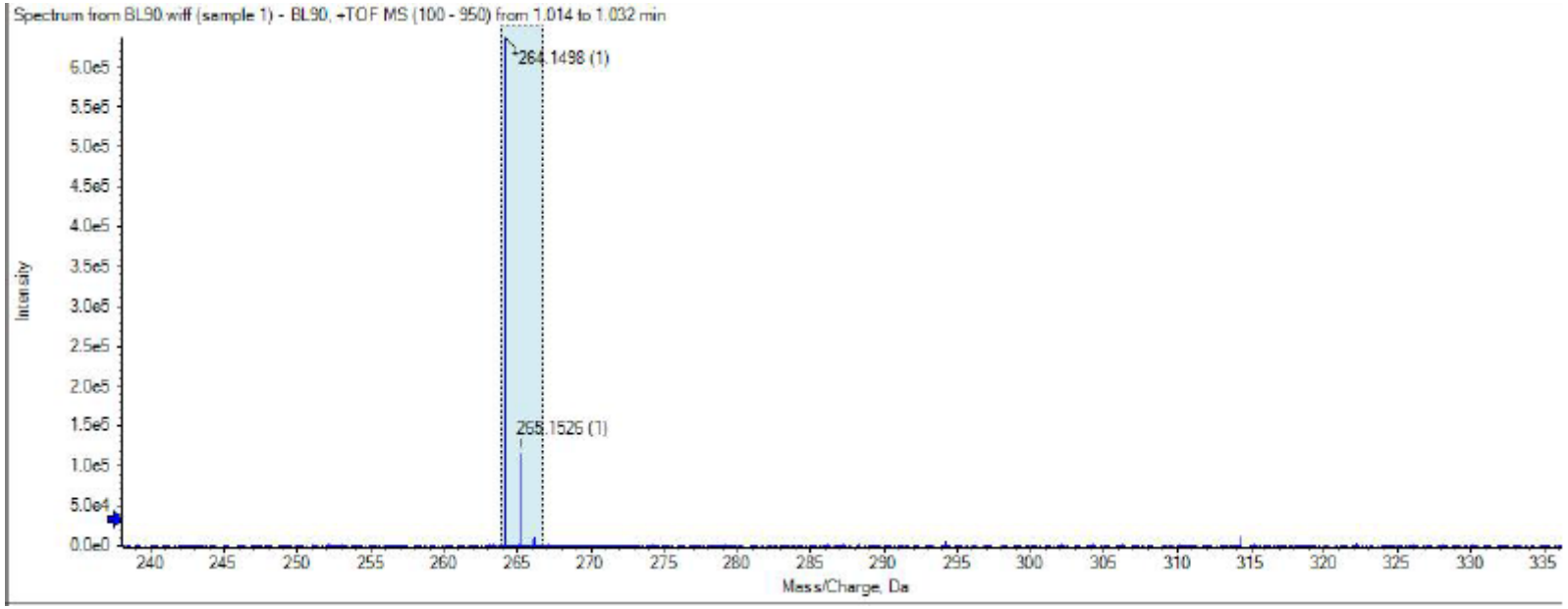

Spectrum from BL116.wiff (sample 1) - BL116, +TOF MS (100 - 950) from 0.669 to 0.757 min
272.0996 (1)
273.1023 (1)
Intensity
3.0e5
2.5e5
2.0e5
1.5e5
1.0e5
5.0e4
0.0e0
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
Mass/Charge, Da

1-(4-isopropylphenyl)-4-phenyl-1H-1,2,3-triazole (3g)

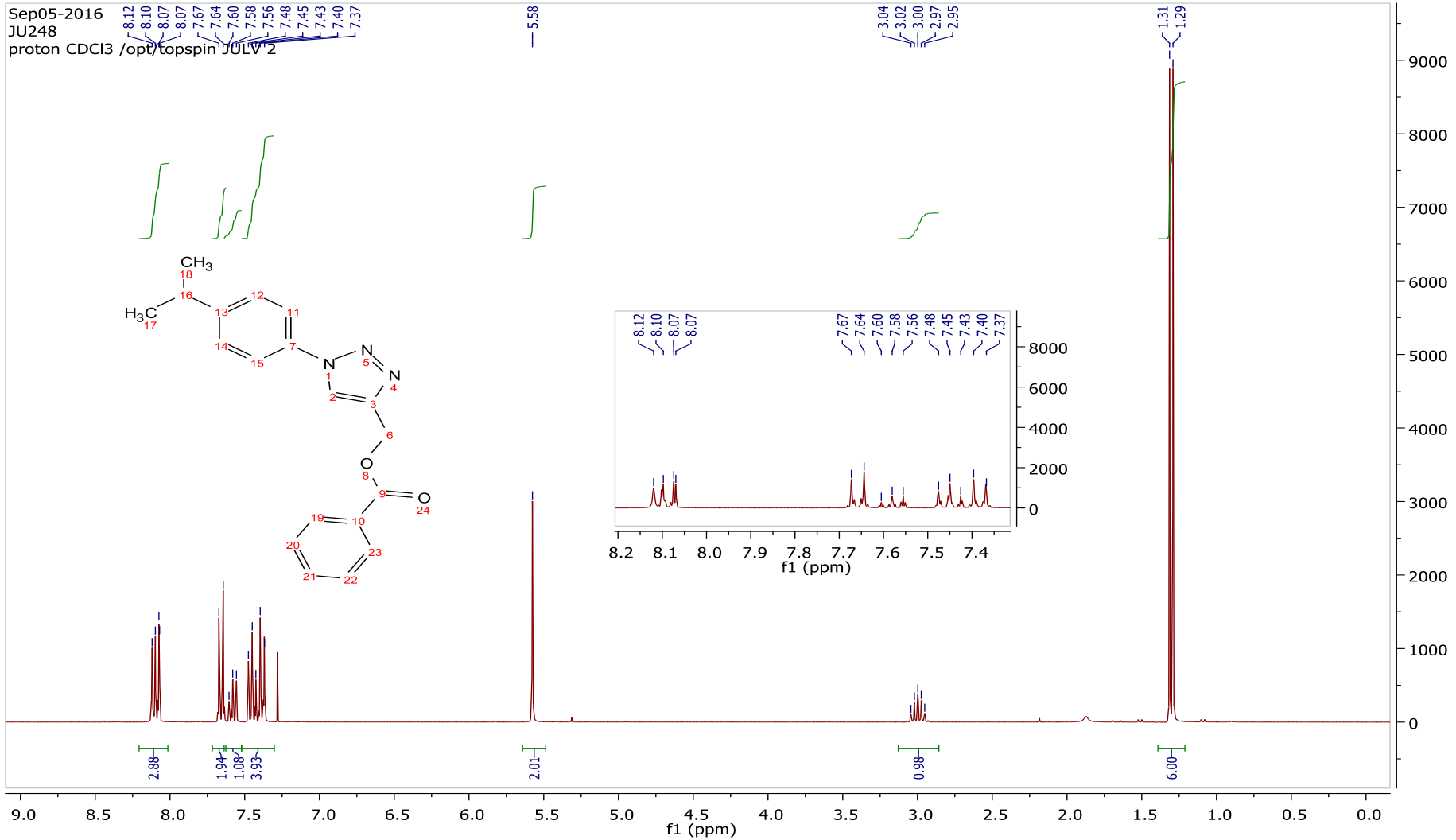


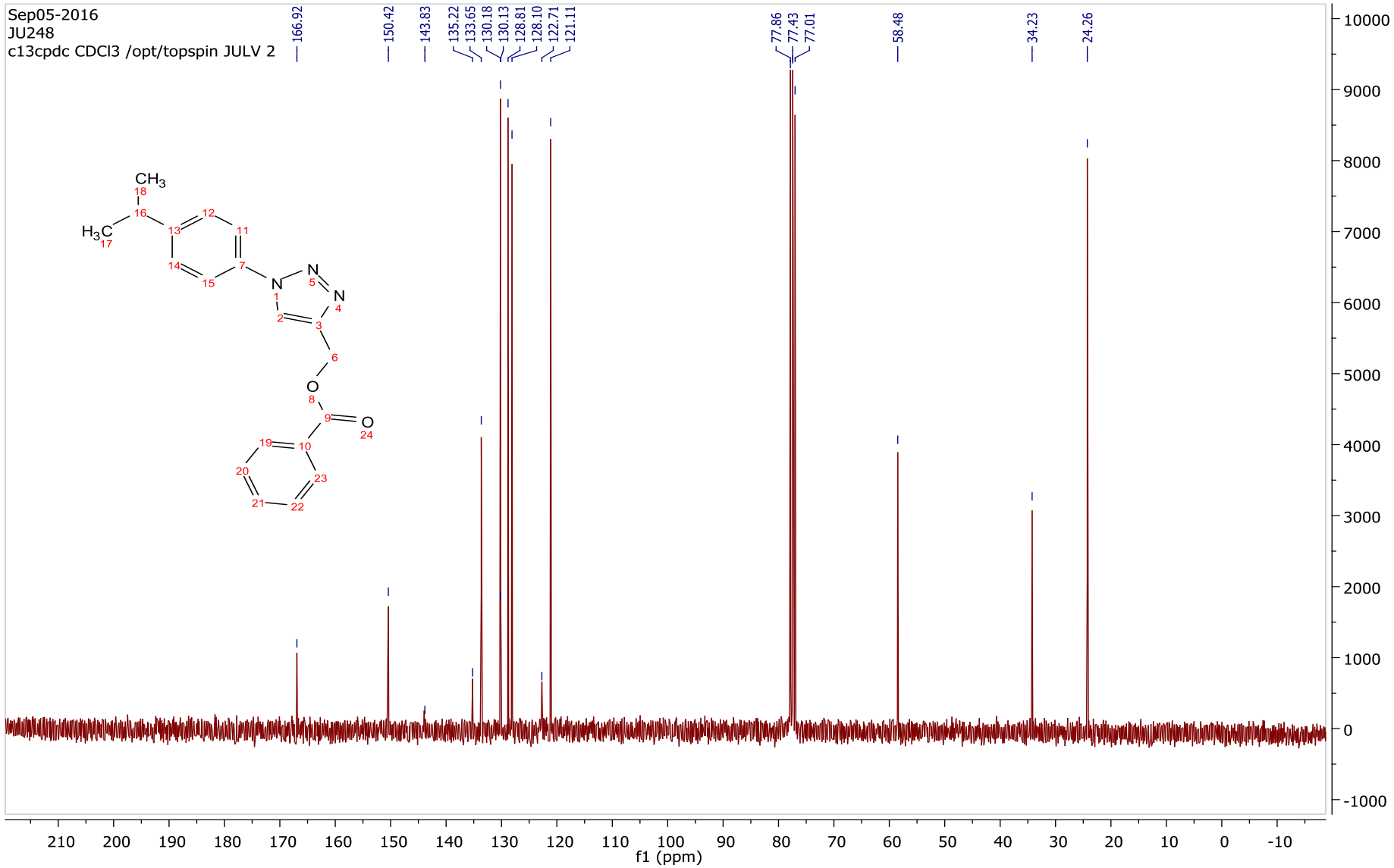

Apr13-2018
ju878
c13cpdc CDCl3 /opt JULV 6
149.87
135.01
130.37
128.92
128.37
127.73
125.86
120.62
117.69
77.47
77.05
76.62
33.87
23.92
f1 (ppm)

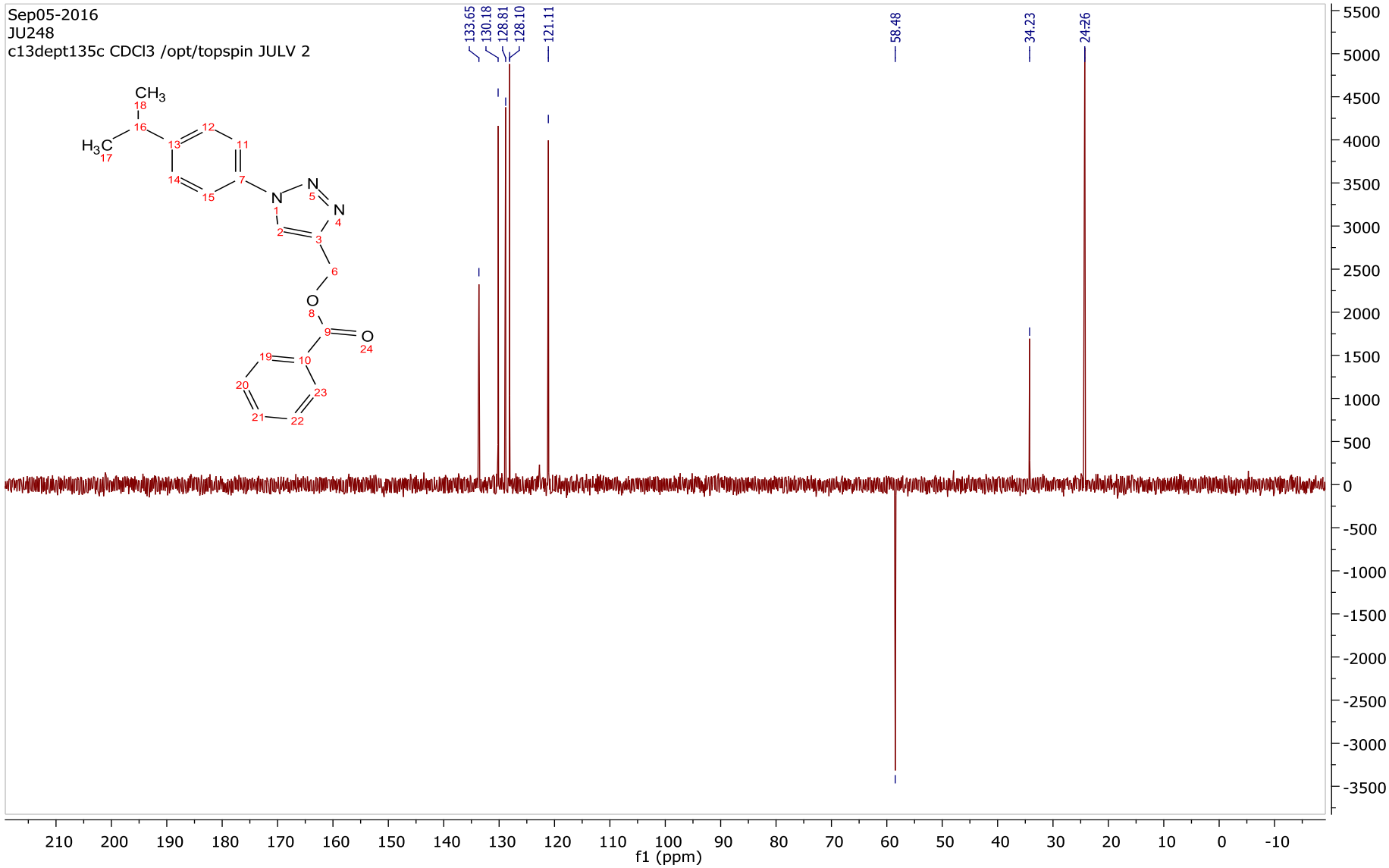

Apr13-2018
ju878
c13dept135c CDCl3 /opt JULV 6
128.92
128.38
127.73
125.86
120.62
117.71
33.87
23.92
CH3
15
H3C
14
13
10
9
8
11
12
7
N
1
N
5
N
4
2
3
6
20
16
19
17
18
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

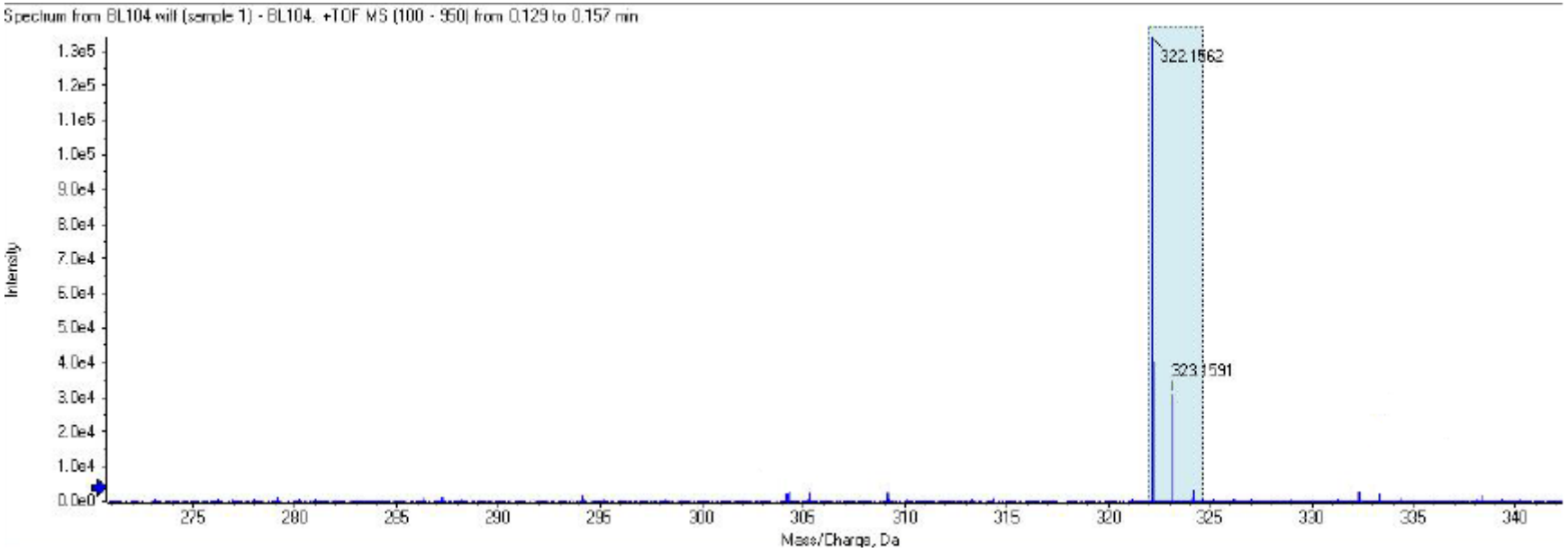

Spectrum from BL90.wiff (sample 1) - BL90, +TOF MS (100 - 950) from 1.014 to 1.032 min
264.1498 (1)
265.1525 (1)
Intensity
6.0e5
5.5e5
5.0e5
4.5e5
4.0e5
3.5e5
3.0e5
2.5e5
2.0e5
1.5e5
1.0e5
5.0e4
0.0e0
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
330
335
Mass/Charge, Da

(1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl benzoate (3h)

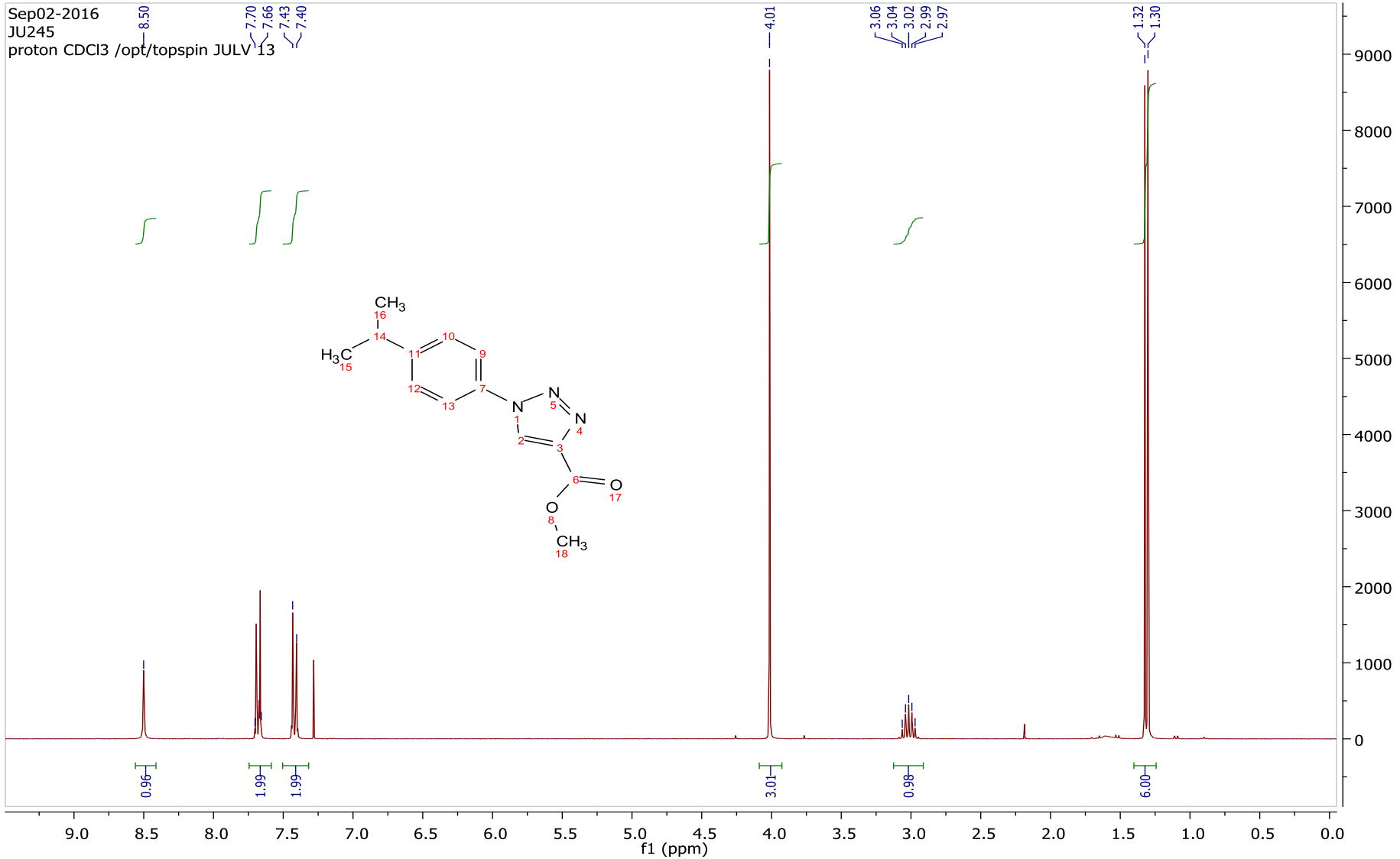


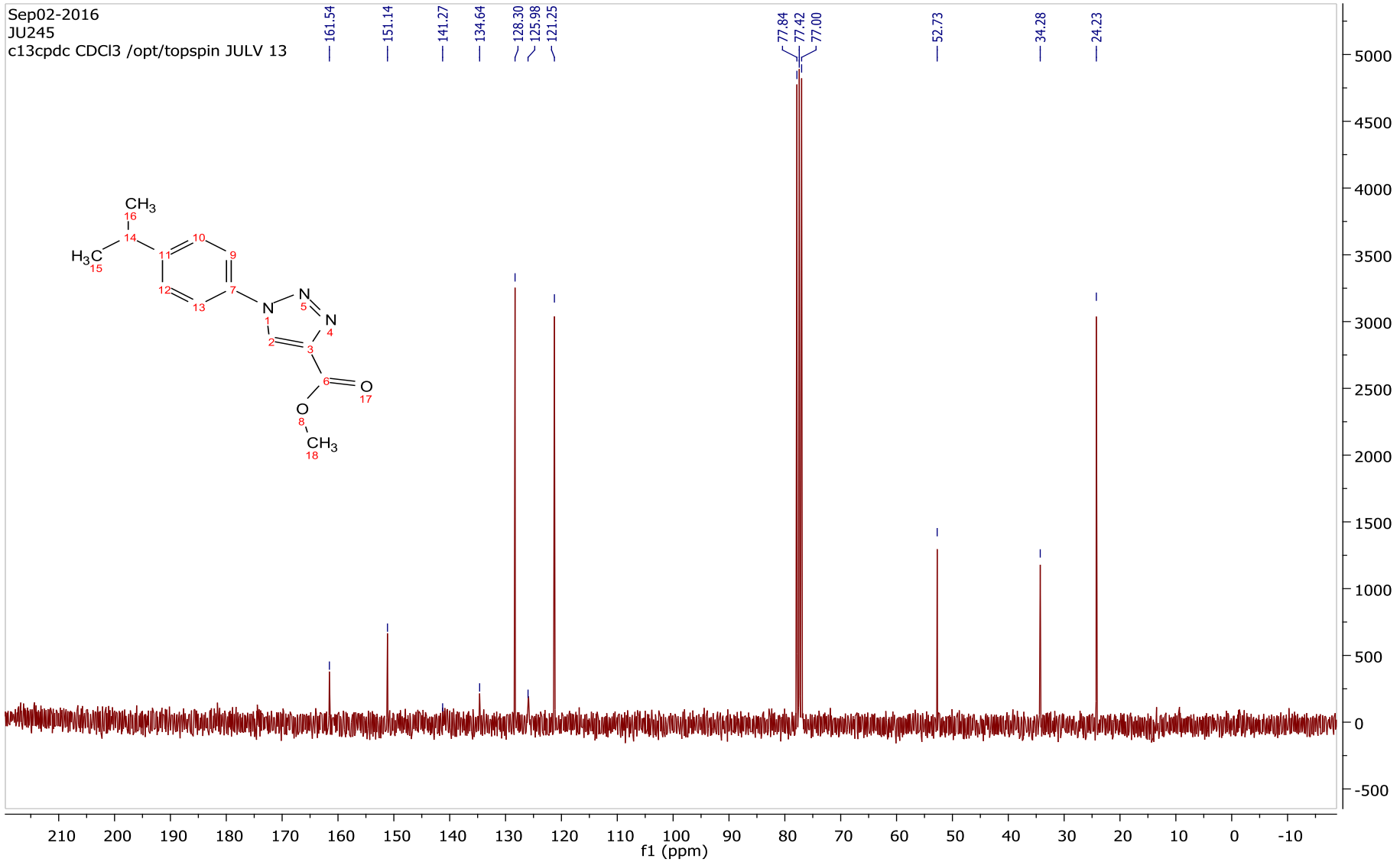

Sep05-2016
JU248
c13cpdc CDCl3 /opt/topspin JULV 2
166.92
150.42
143.83
135.22
133.65
130.18
130.13
128.81
128.10
122.71
121.11
77.86
77.43
77.01
58.48
34.23
24.26
f1 (ppm)

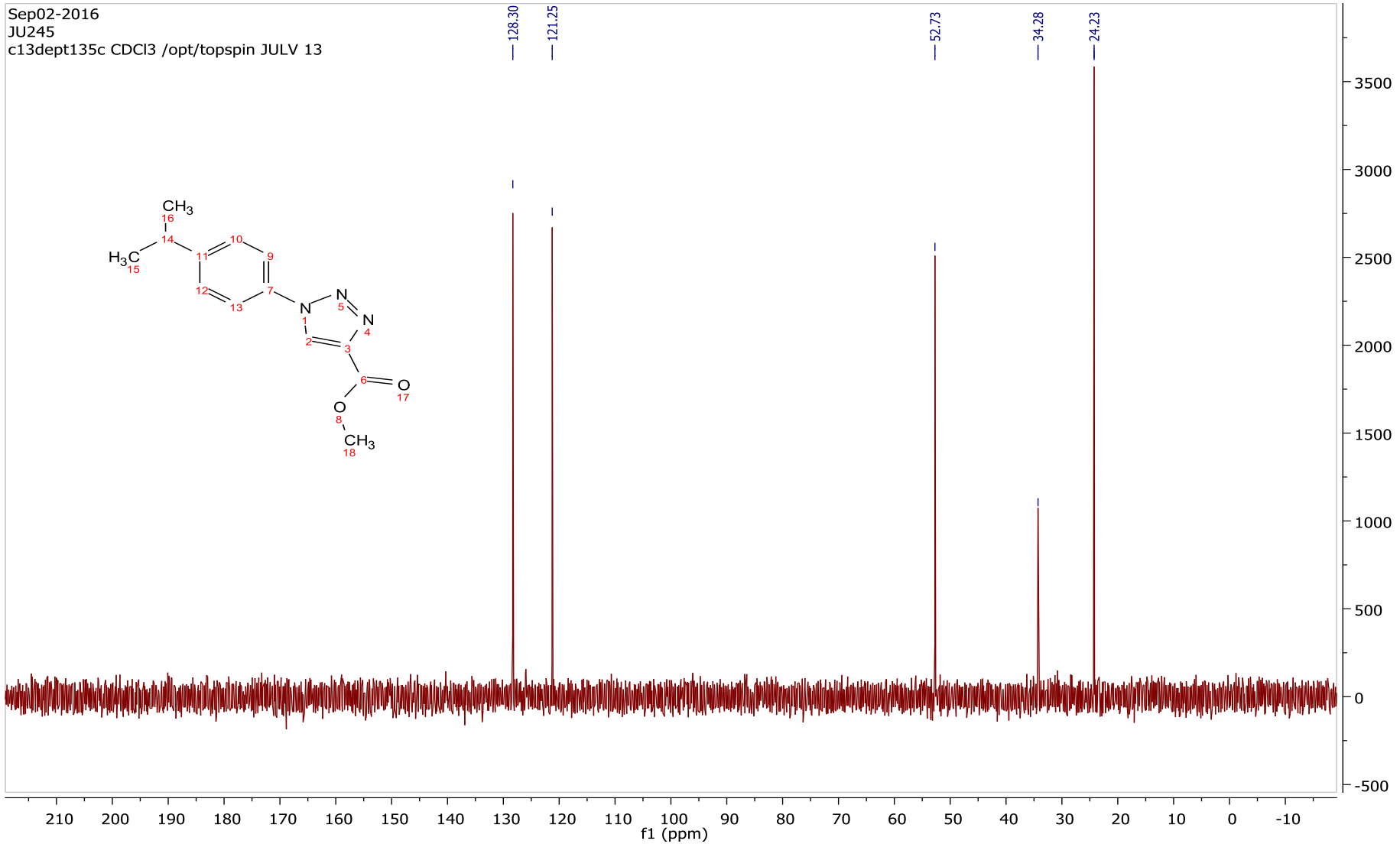

Sep05-2016
JU248
c13dept135c CDCl3 /opt/topspin JULV 2
133.65
130.18
128.81
128.10
121.11
58.48
34.23
24.26
f1 (ppm)

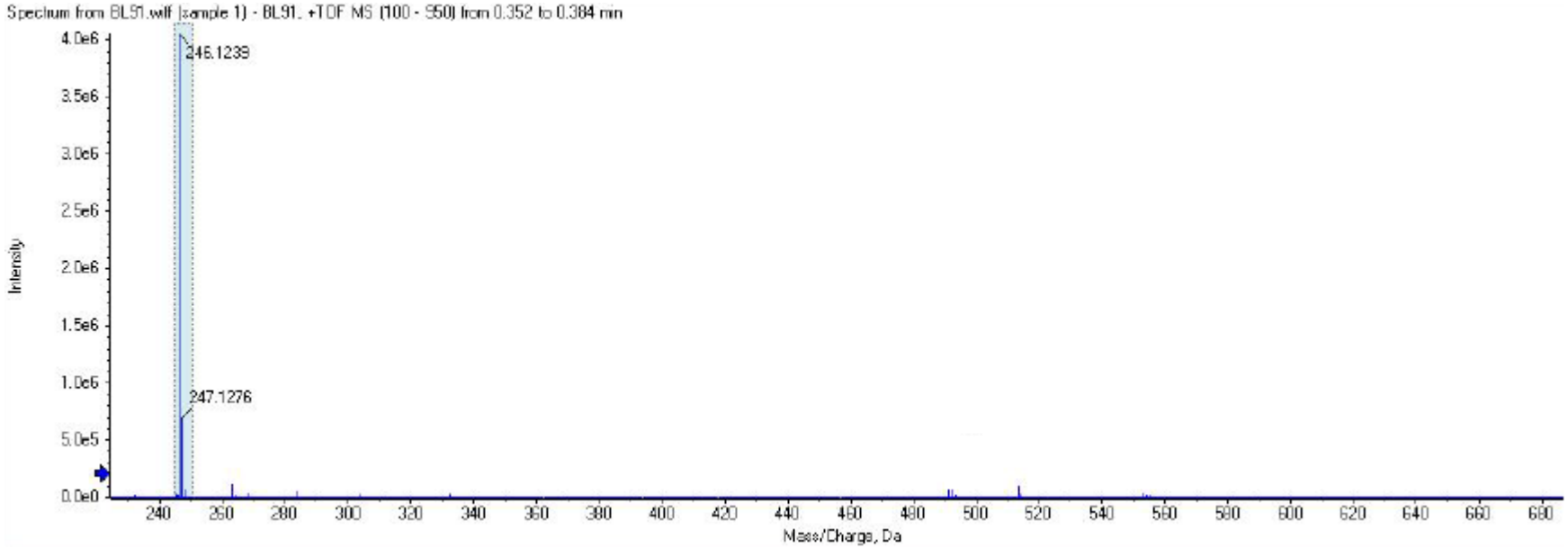

Spectrum from BL104.wiff (sample 1) - BL104, +TOF MS (100 - 950) from 0.129 to 0.157 min
Intensity
1.3e5
1.2e5
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
322.1562
323.1591
275
280
285
290
295
300
305
310
315
320
325
330
335
340
Mass/Charge, Da

Methyl 1-(4-isopropylphenyl)-1H-1,2,3-triazole-4-carboxylate (3i)

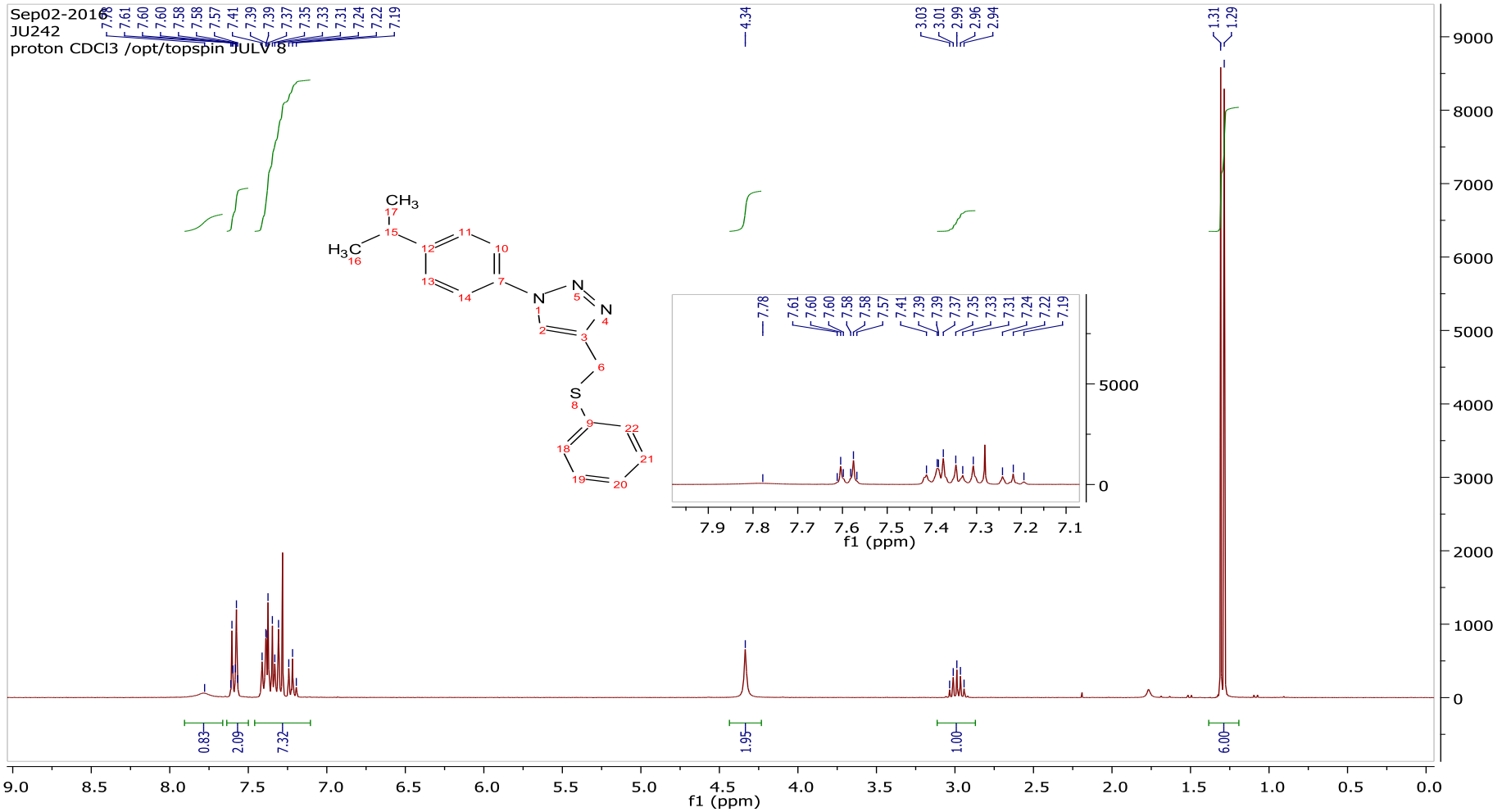


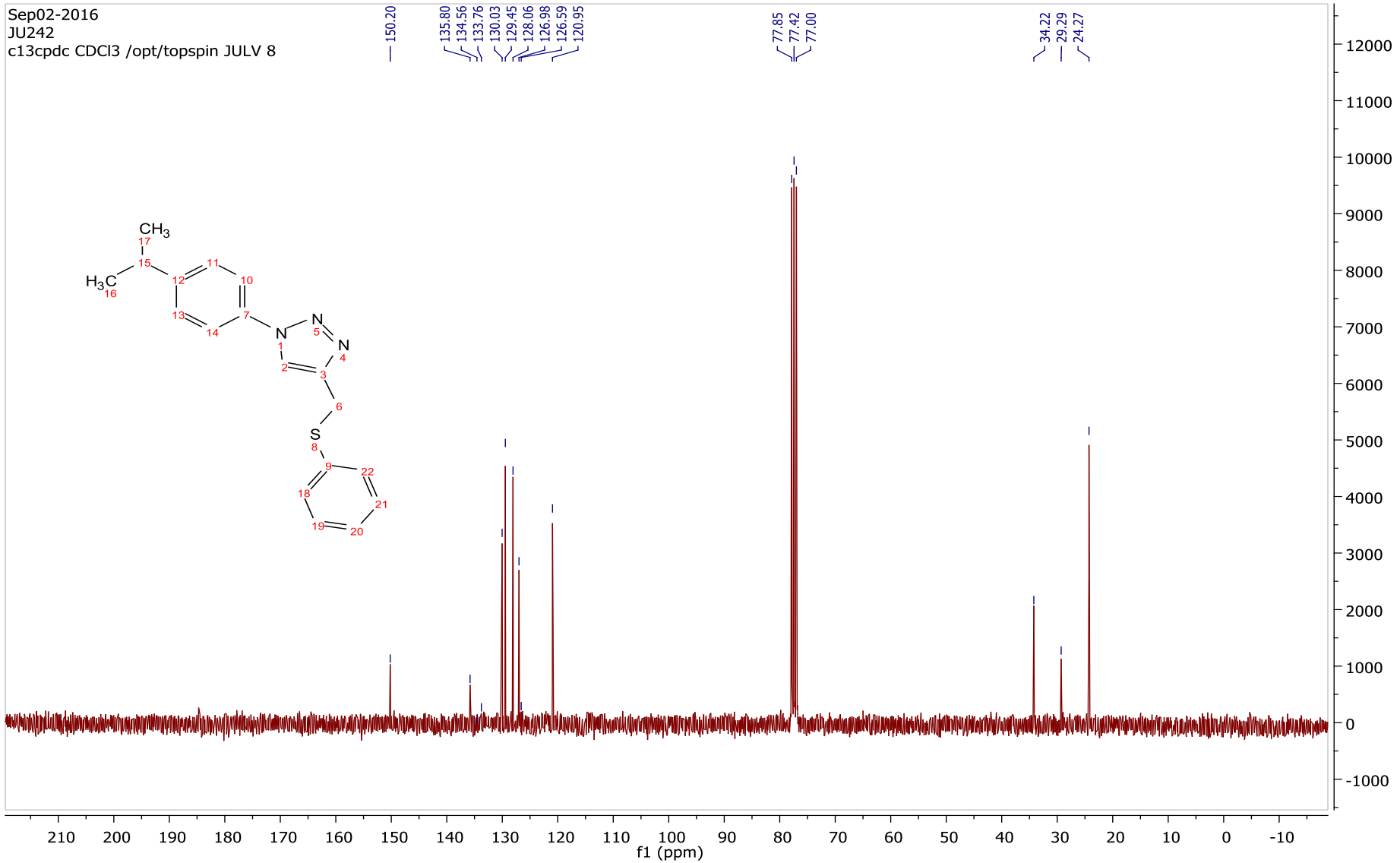

Sep02-2016
JU245
c13cpdc CDCl3 /opt/topspin JULV 13
161.54
151.14
141.27
134.64
128.30
125.98
121.25
77.84
77.42
77.00
52.73
34.28
24.23
f1 (ppm)

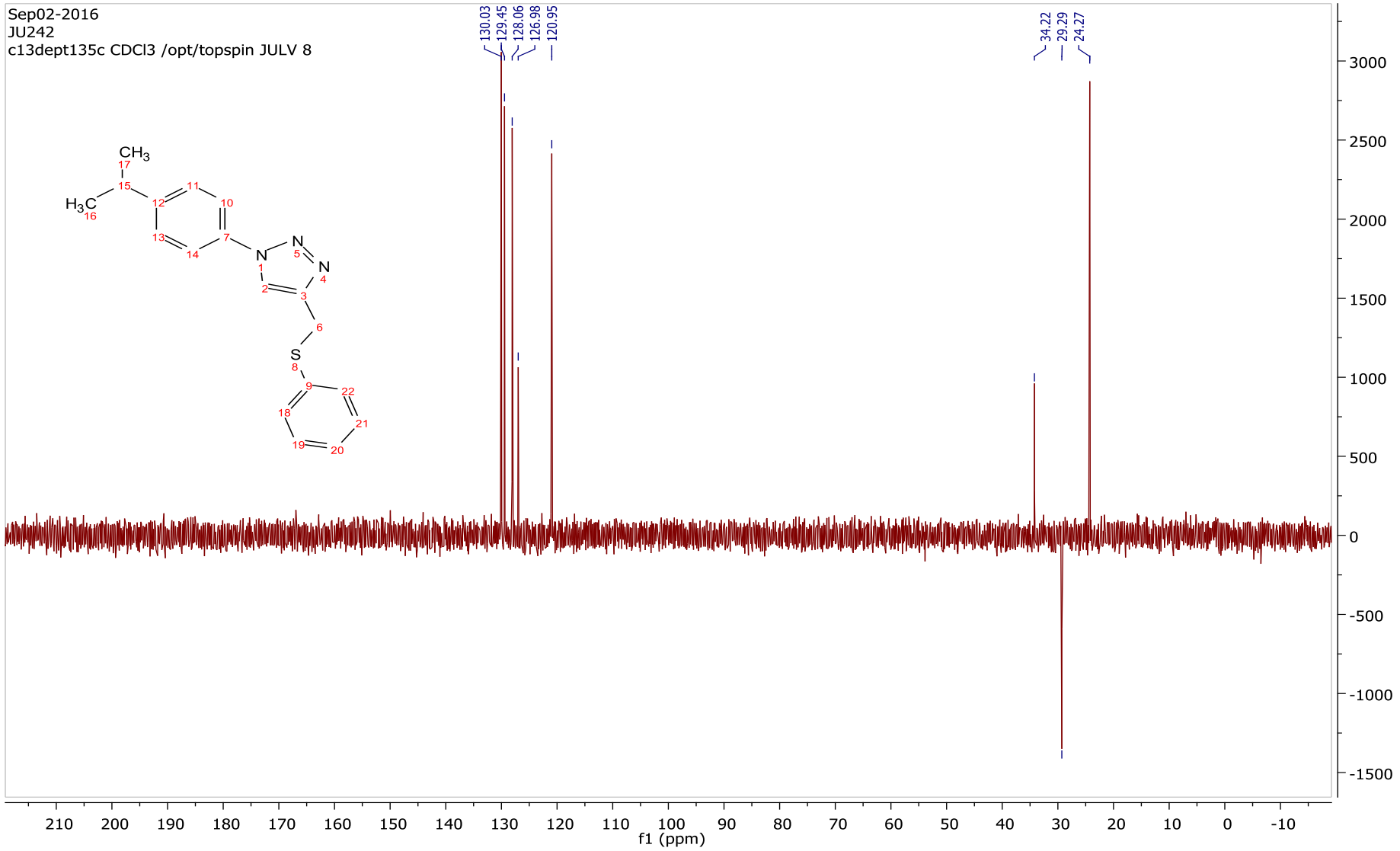

Sep02-2016
JU245
c13dept135c CDCl3 /opt/topspin JULV 13
128.30
121.25
52.73
34.28
24.23
f1 (ppm)

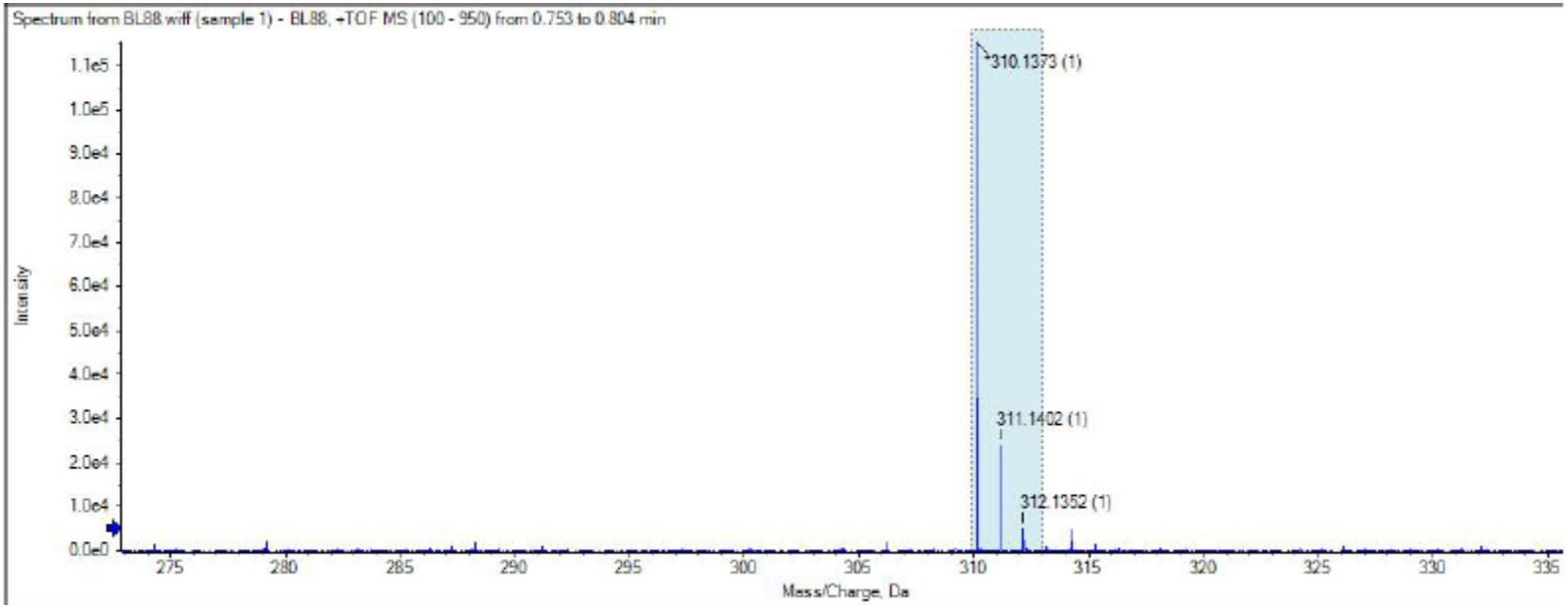

Spectrum from BL91.wiff (sample 1) - BL91, +TOF MS (100 - 950) from 0.352 to 0.384 min
4.0e6
3.5e6
3.0e6
2.5e6
2.0e6
1.5e6
1.0e6
5.0e5
0.0e0
Intensity
246.1239
247.1276
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
Mass/Charge, Da

1-(4-isopropylphenyl)-4-(phenylthiomethyl)-1H-1,2,3-triazole (3j)




Sep02-2016
JU242
c13cpdc CDCl3 /opt/topspin JULV 8
150.20
135.80
134.56
133.76
130.03
129.45
128.06
126.98
126.59
120.95
77.85
77.42
77.00
34.22
29.29
24.27
f1 (ppm)


Sep02-2016
JU242
c13dept135c CDCl3 /opt/topspin JULV 8
130.03
129.45
128.06
126.98
120.95
34.22
29.29
24.27
CH3
H3C
N
S
f1 (ppm)


Spectrum from BL88.wiff (sample 1) - BL88, +TOF MS (100 - 950) from 0.753 to 0.804 min
Intensity
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
310.1373 (1)
311.1402 (1)
312.1352 (1)
275
280
285
290
295
300
305
310
315
320
325
330
335
Mass/Charge, Da