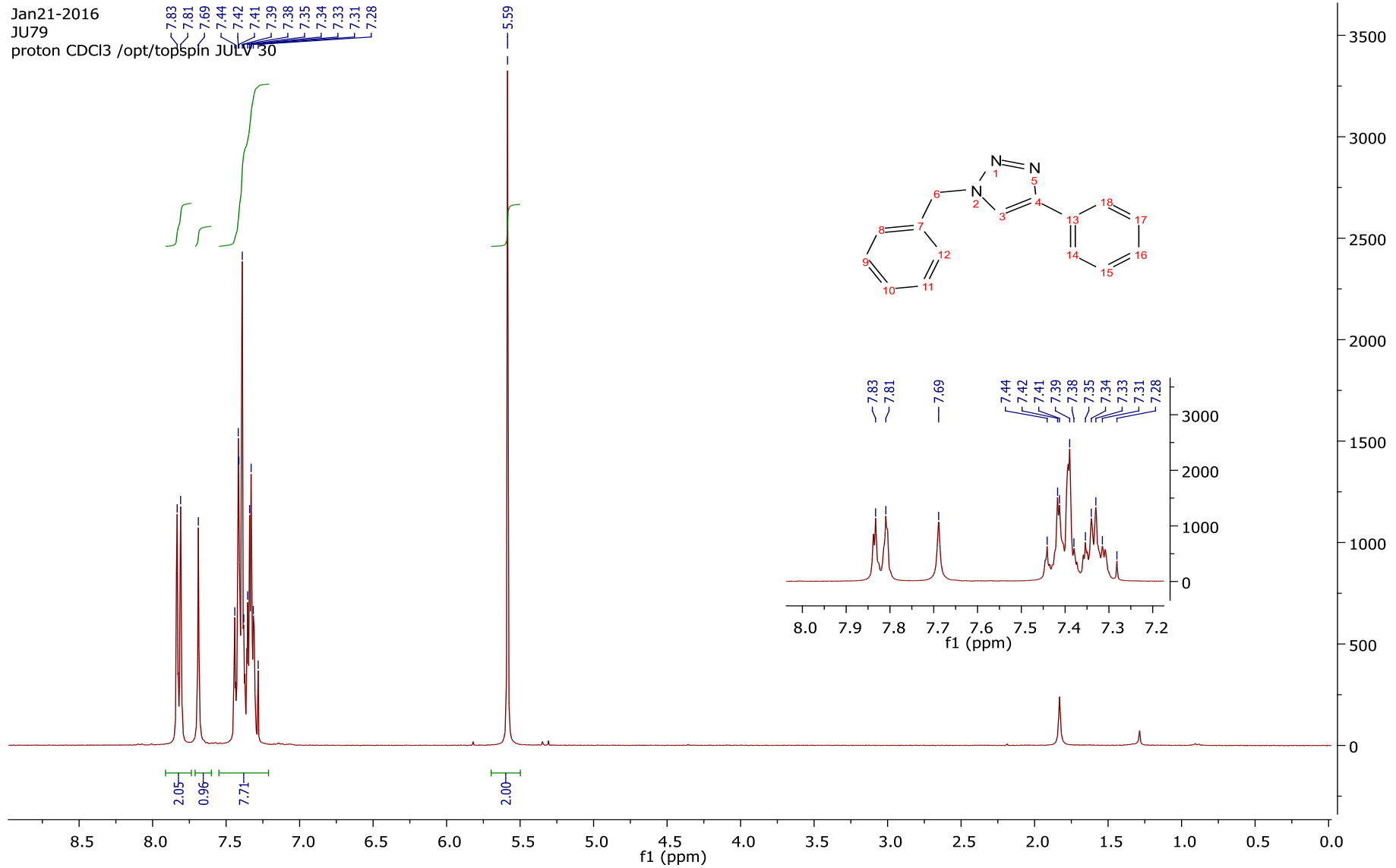
Supplementary Materials for: *Catalysts* (MPDI)

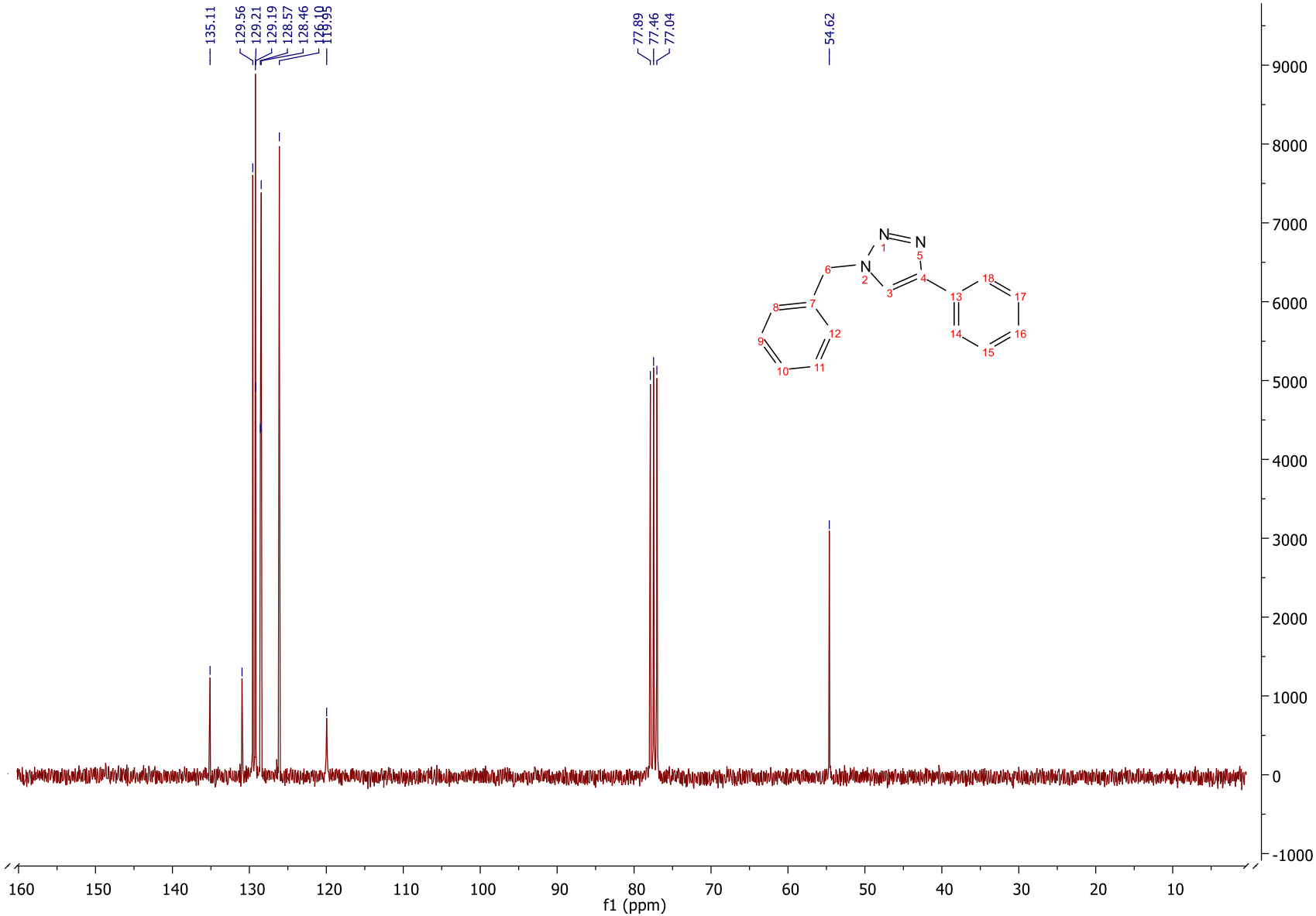
2-Aminobenzothiazole-Containing Copper(II) Complex as Catalyst in Click Chemistry: An Experimental and Theoretical Study

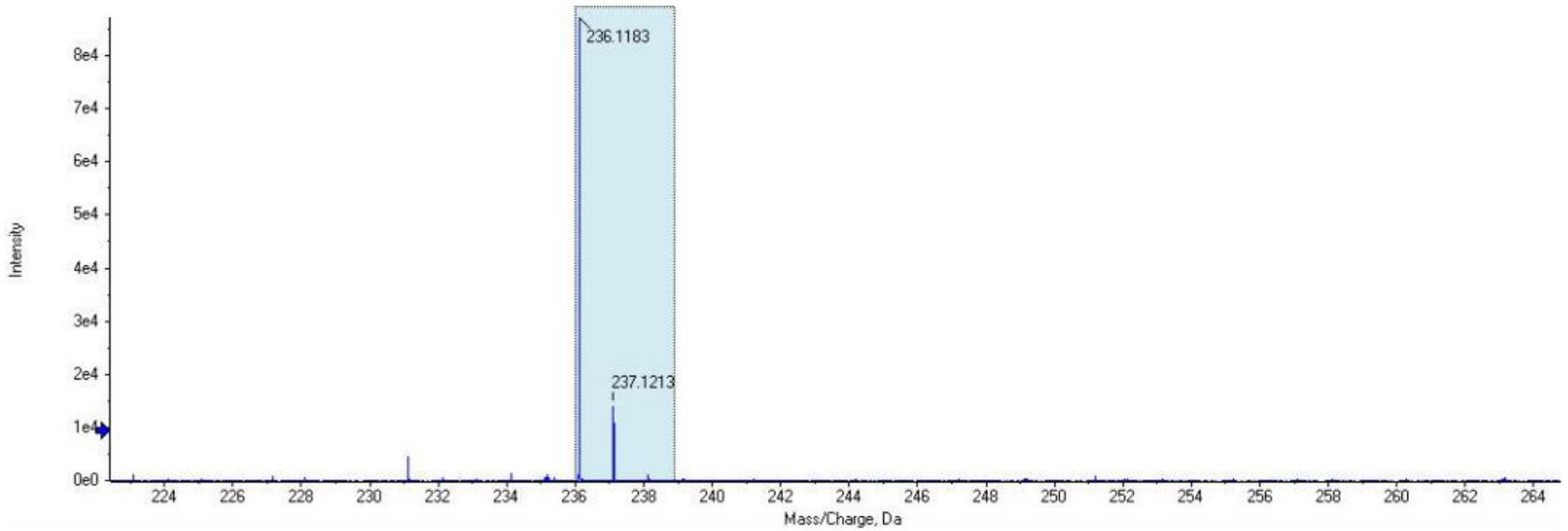
Lahoucine Bahsis [1,2,*], Meryem Hrimla [2], Hicham Ben El Ayouchia [2], Hafid Anane [2], Miguel Julve [3] and Salah-Eddine Stiriba [2,3,*]

[1] Département de Chimie, Faculté des Sciences d'El Jadida, Université Chouaïb Doukkali, B.P.:20, El Jadida 24000, Morocco
[2] Laboratoire de Chimie Analytique et Moléculaire/*LCAM*, Faculté Polydisciplinaire de Safi, Université Cadi Ayyad, Safi 46030, Morocco; meryemhrimla.uca@gmail.com (M.H.); belayou@gmail.com (H.B.); ananehafid@gmail.com (H.A.)
[3] Instituto de Ciencia Molecular/*ICMol*, Universidad de Valencia, C/Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain; miguel.julve@uv.es
* Correspondence: bahsis.lahoucine@gmail.com (L.B.); stiriba@uv.es (S.-E.S.)

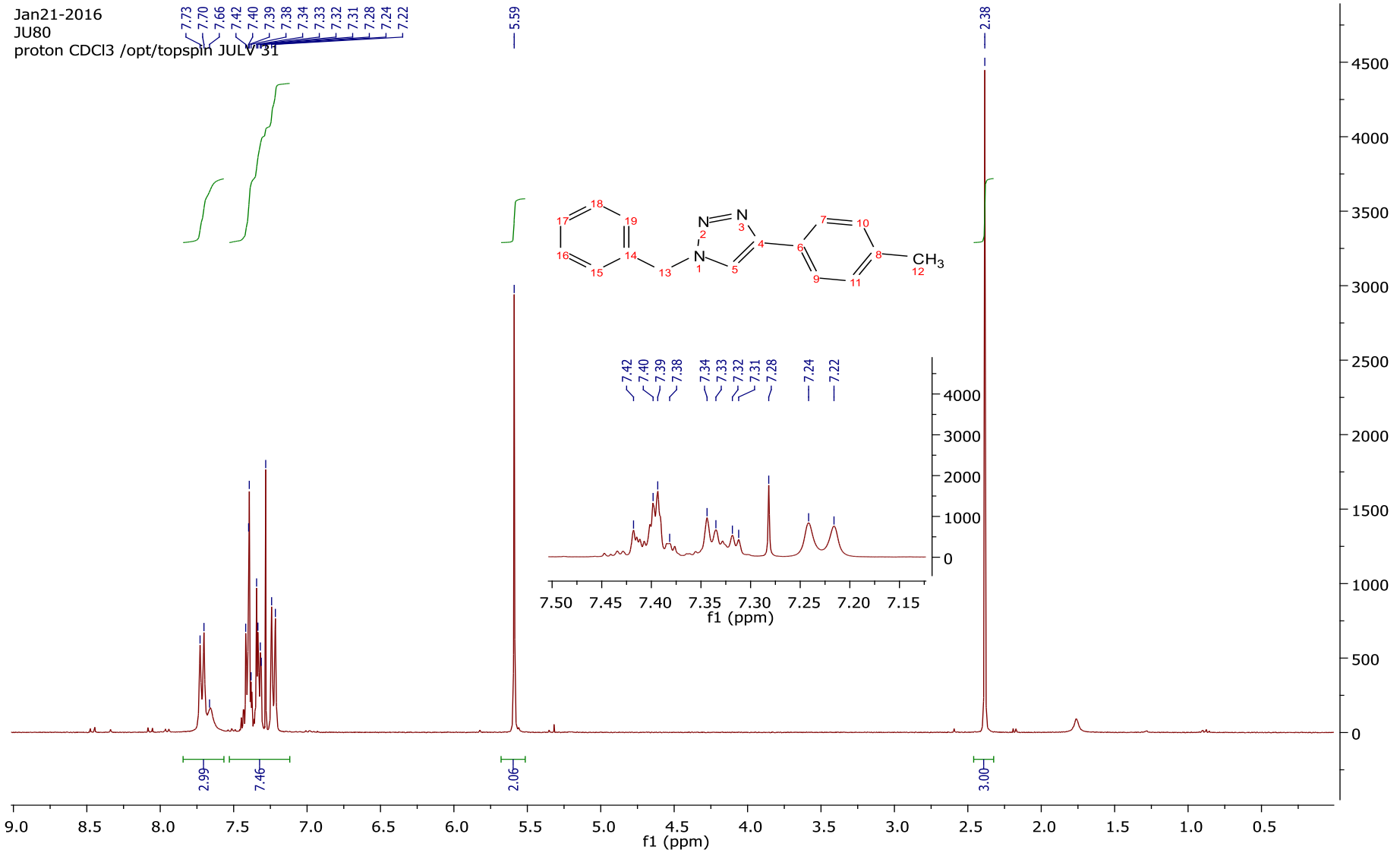
1-Benzyl-4-phenyl-1H-1,2,3-triazole (3a)

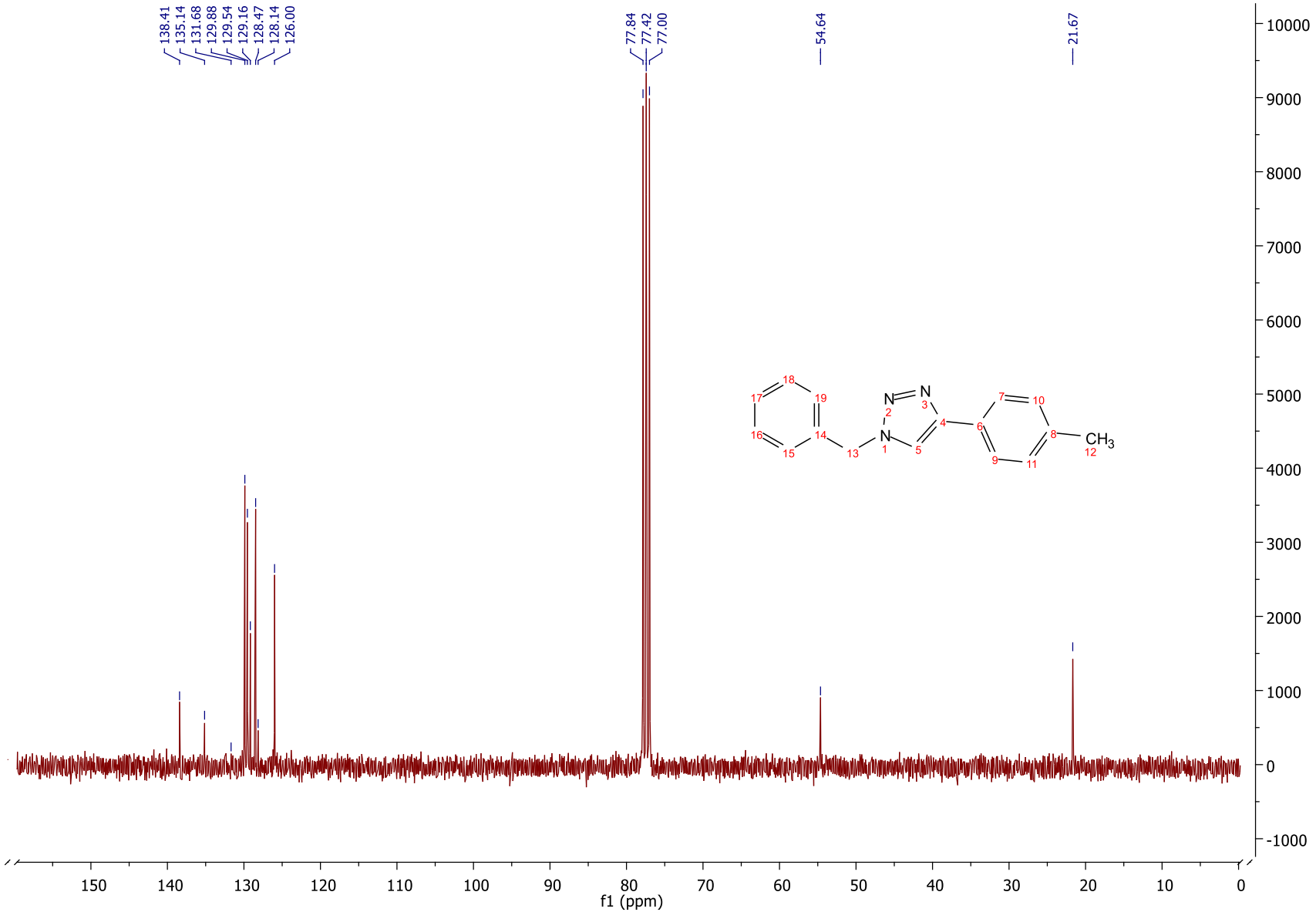


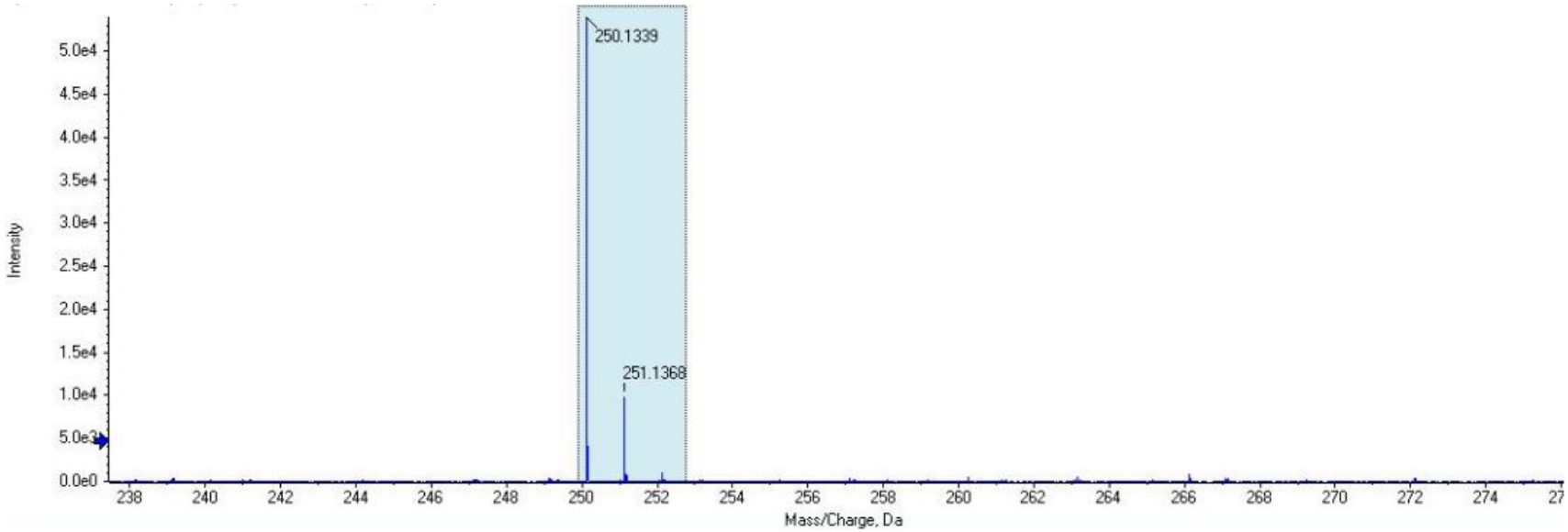

135.11
129.56
129.21
129.19
128.57
128.46
126.10
119.95
77.89
77.46
77.04
54.62
N
N
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


236.1183
237.1213
Intensity
8e4
7e4
6e4
5e4
4e4
3e4
2e4
1e4
0e0
224
226
228
230
232
234
236
238
240
242
244
246
248
250
252
254
256
258
260
262
264
Mass/Charge, Da

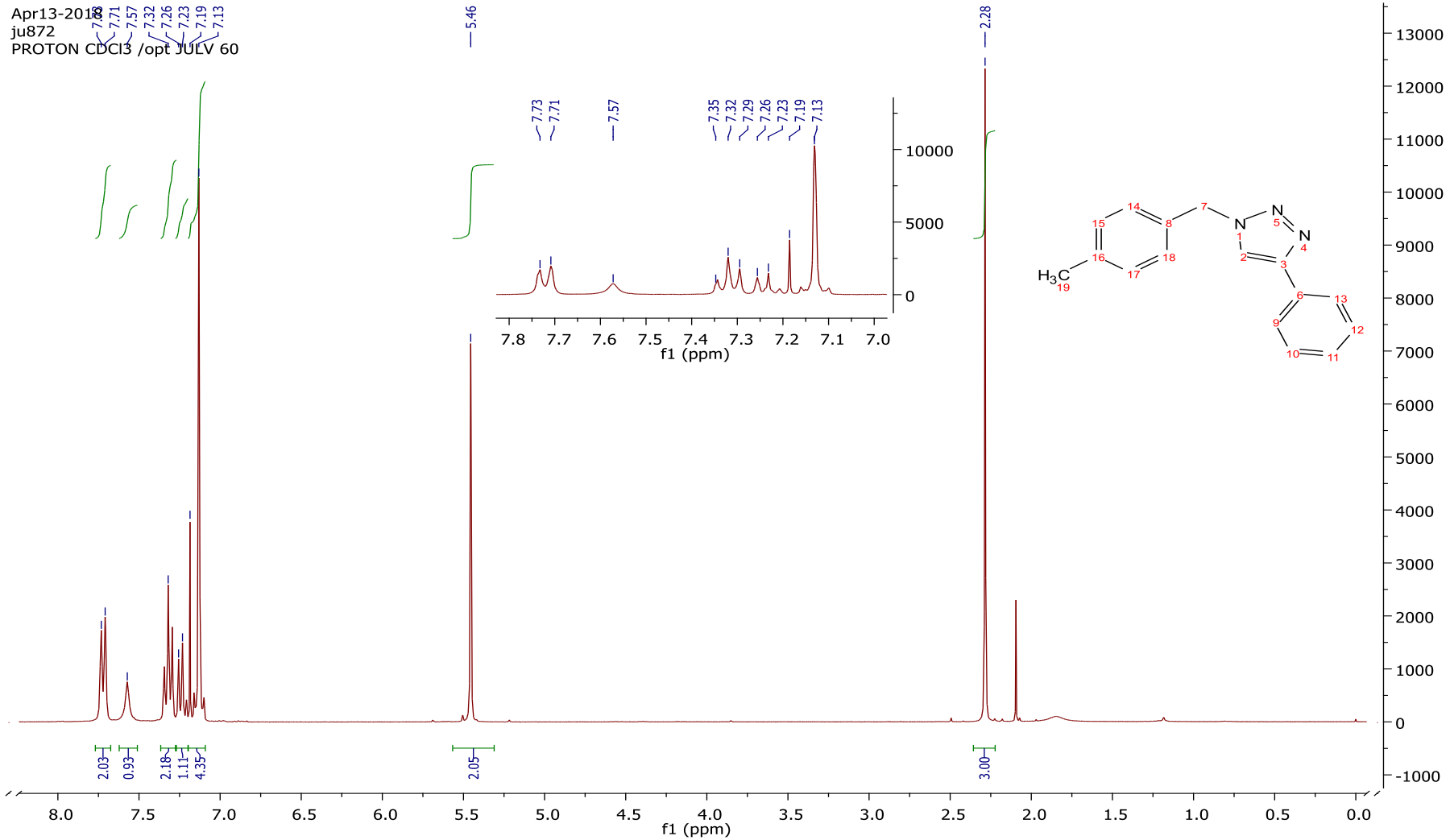
1- Benzyl-4-p-tolyl-1H-1,2,3-triazole (3b)

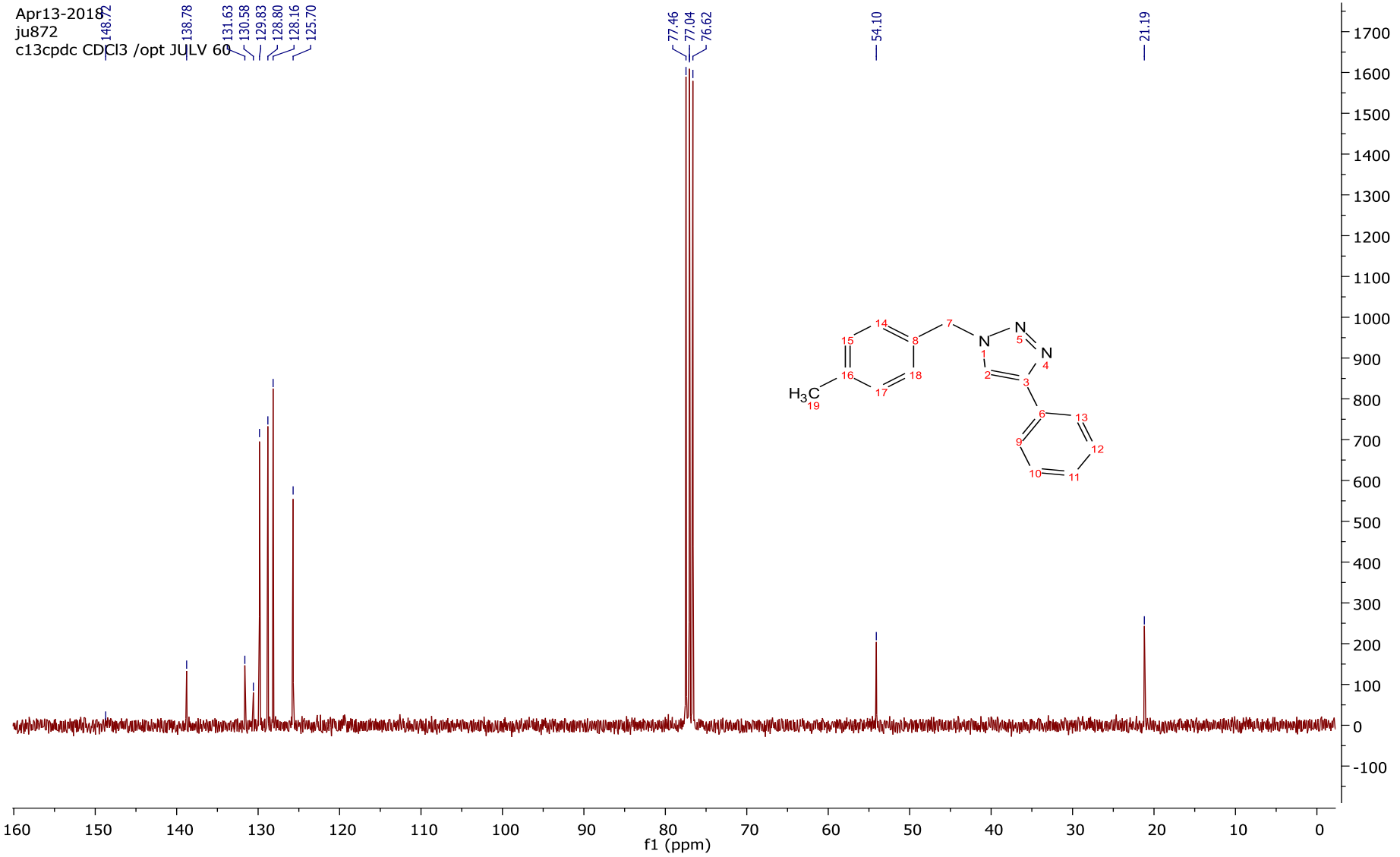


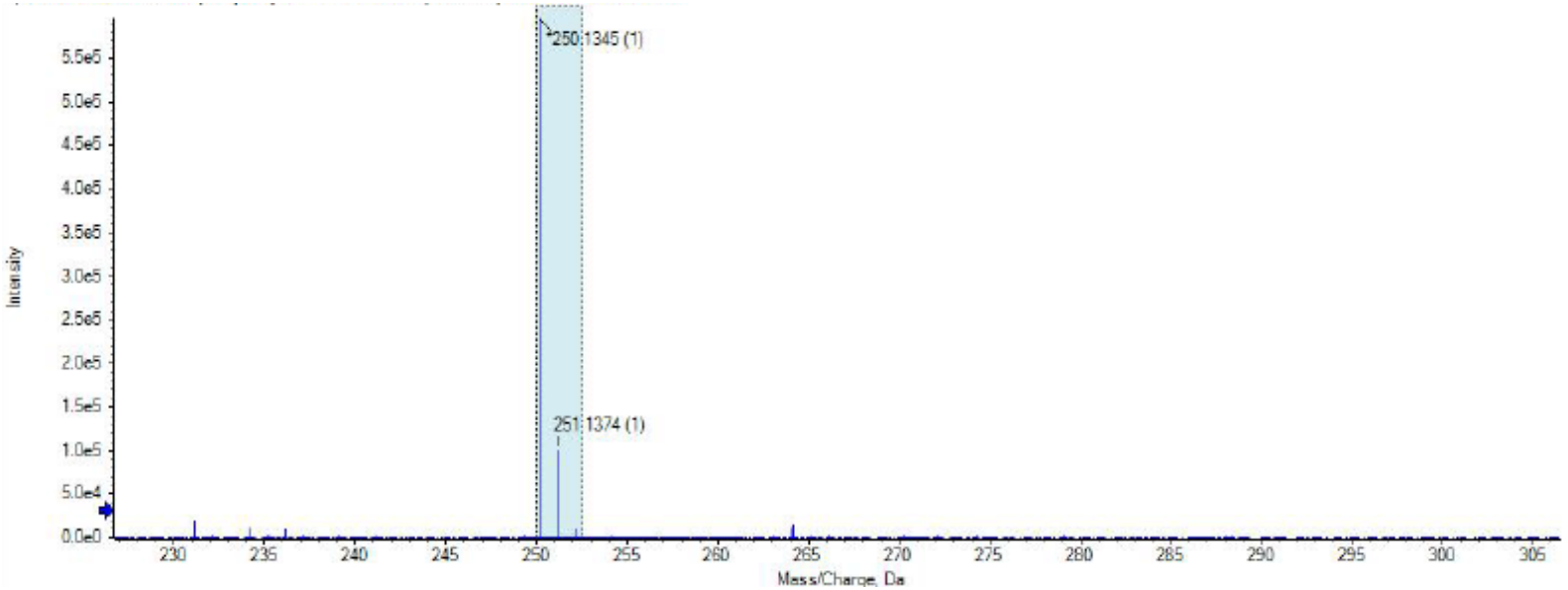

138.41
135.14
131.68
129.88
129.54
129.16
128.47
128.14
126.00
77.84
77.42
77.00
54.64
21.67
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
N
N
N
CH3
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19


250.1339
251.1368
Intensity
5.0e4
4.5e4
4.0e4
3.5e4
3.0e4
2.5e4
2.0e4
1.5e4
1.0e4
5.0e3
0.0e0
238
240
242
244
246
248
250
252
254
256
258
260
262
264
266
268
270
272
274
Mass/Charge, Da

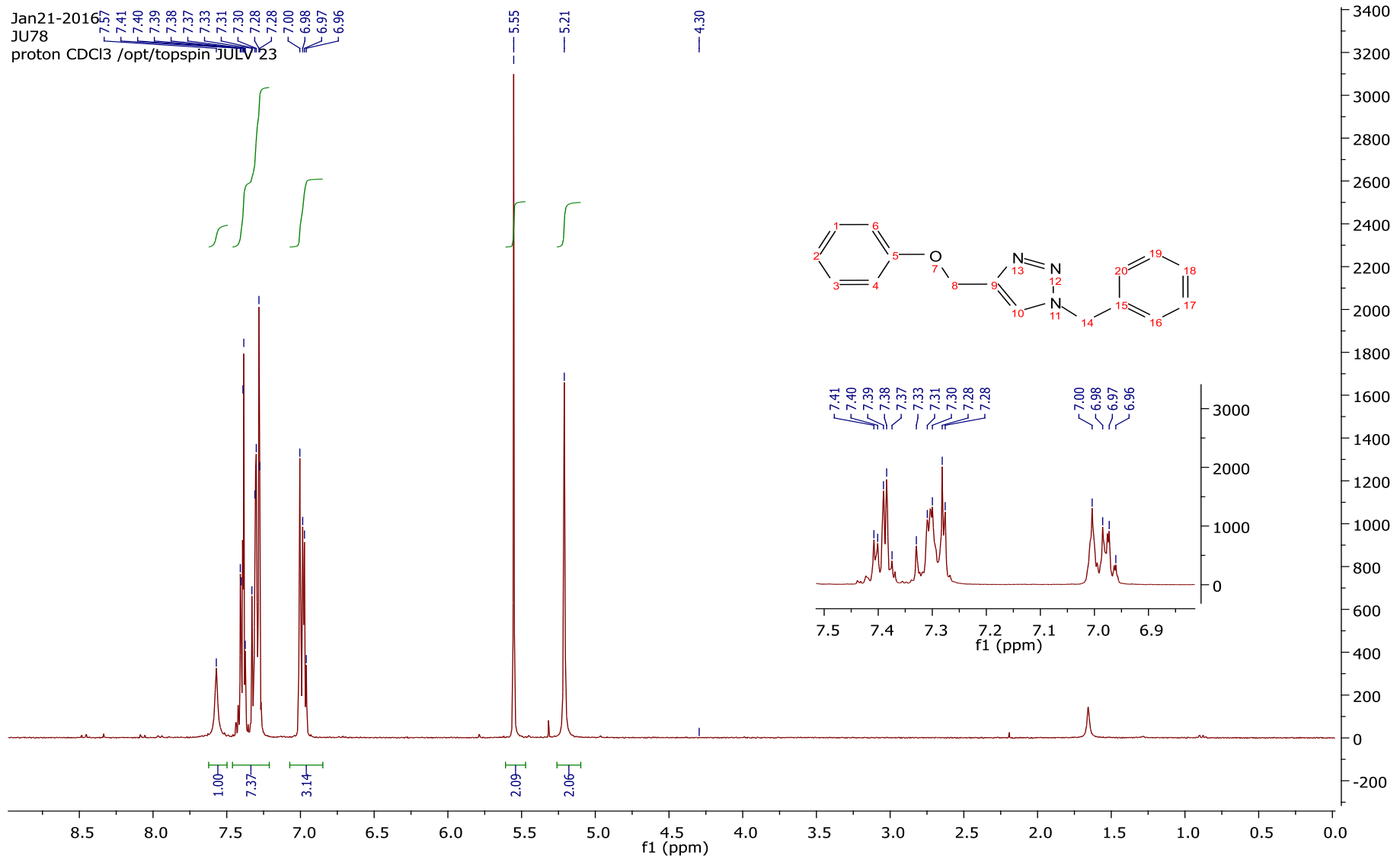
1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole (3c)

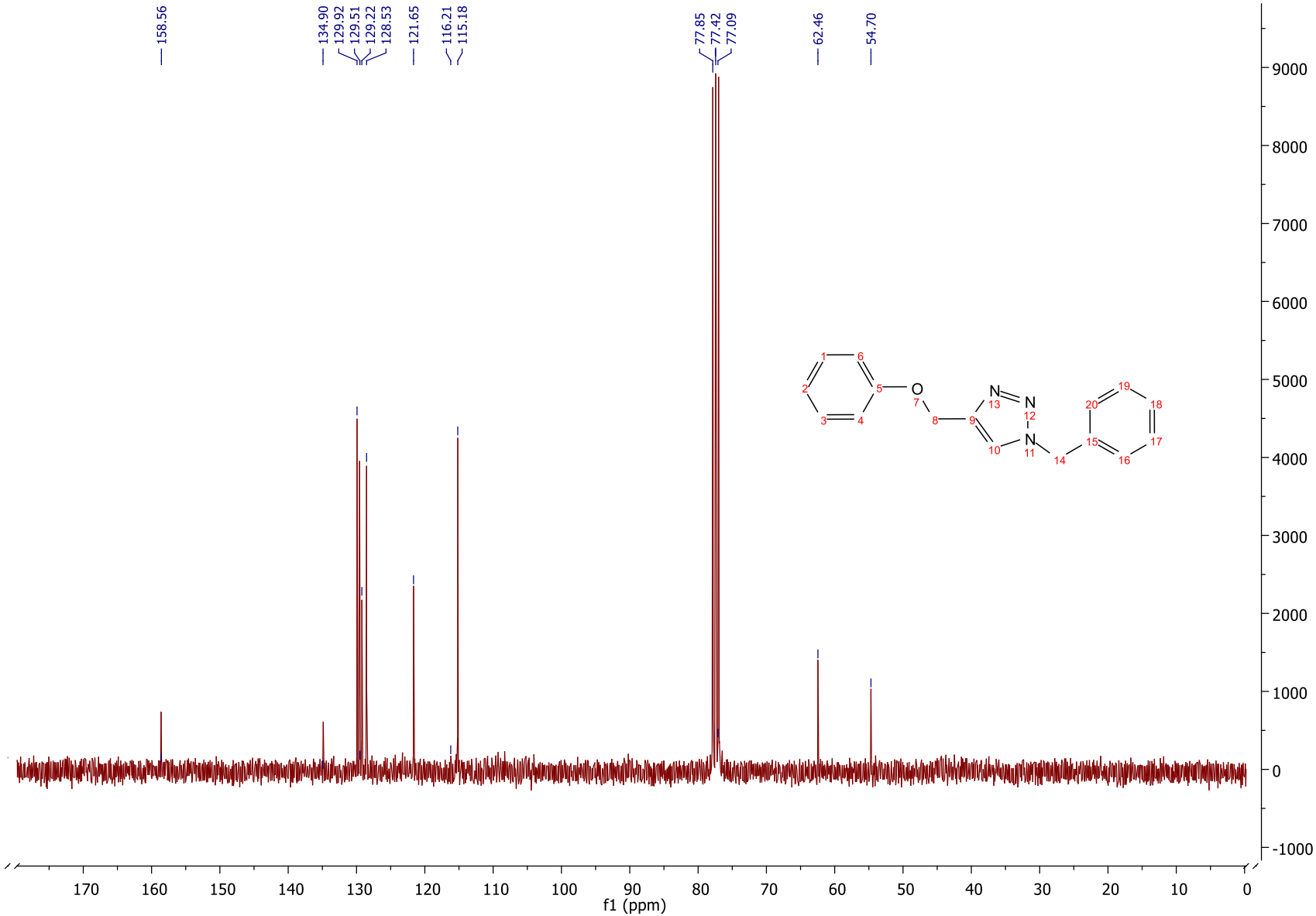


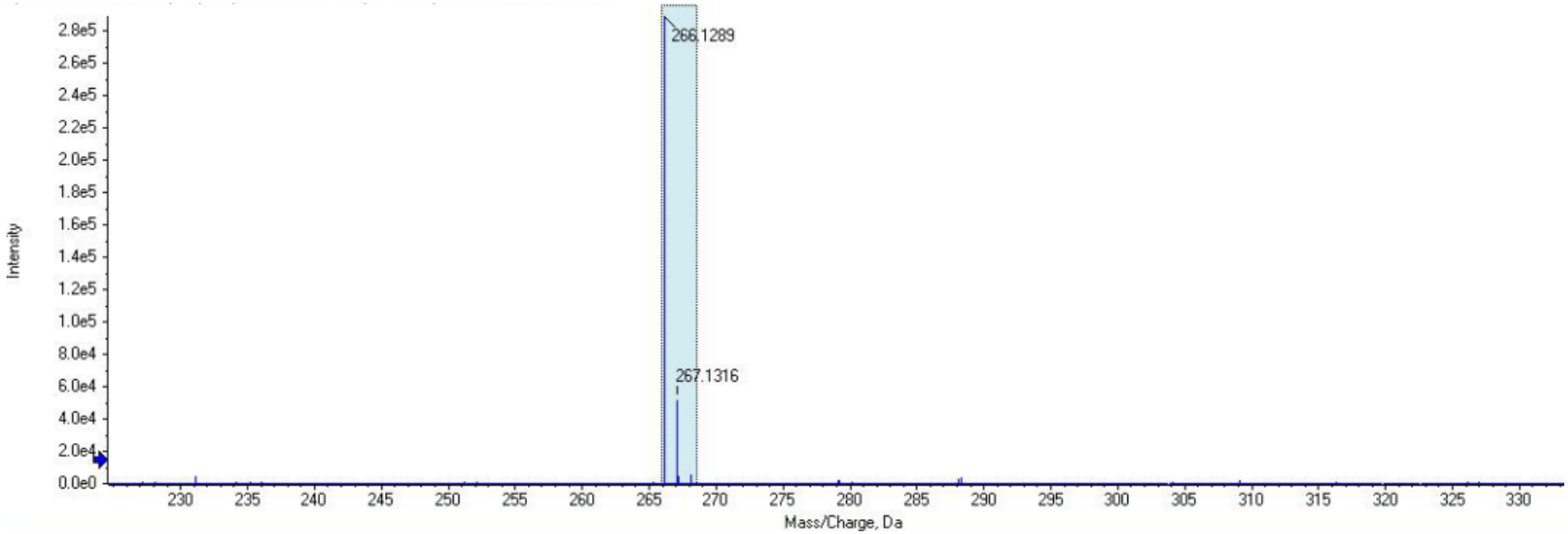

Apr13-2018
ju872
c13cpdc CDCl3 /opt JULV 60
148.72
138.78
131.63
130.58
129.83
128.80
128.16
125.70
77.46
77.04
76.62
54.10
21.19
f1 (ppm)


250.1345 (1)
251.1374 (1)
Intensity
5.5e5
5.0e5
4.5e5
4.0e5
3.5e5
3.0e5
2.5e5
2.0e5
1.5e5
1.0e5
5.0e4
0.0e0
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
Mass/Charge, Da

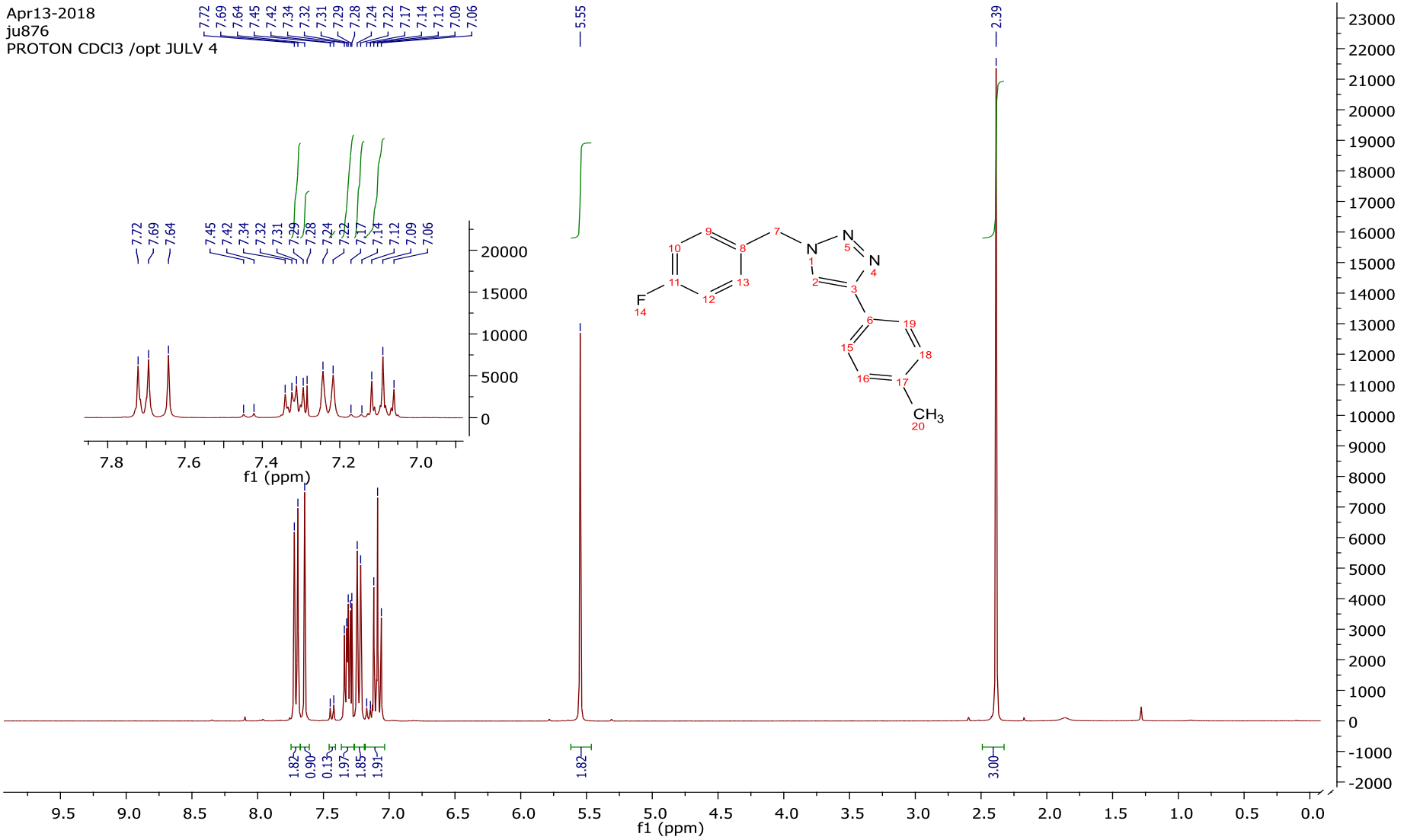
1-benzyl-4-(phenoxymethyl)-1H-1,2,3-triazole (3d)

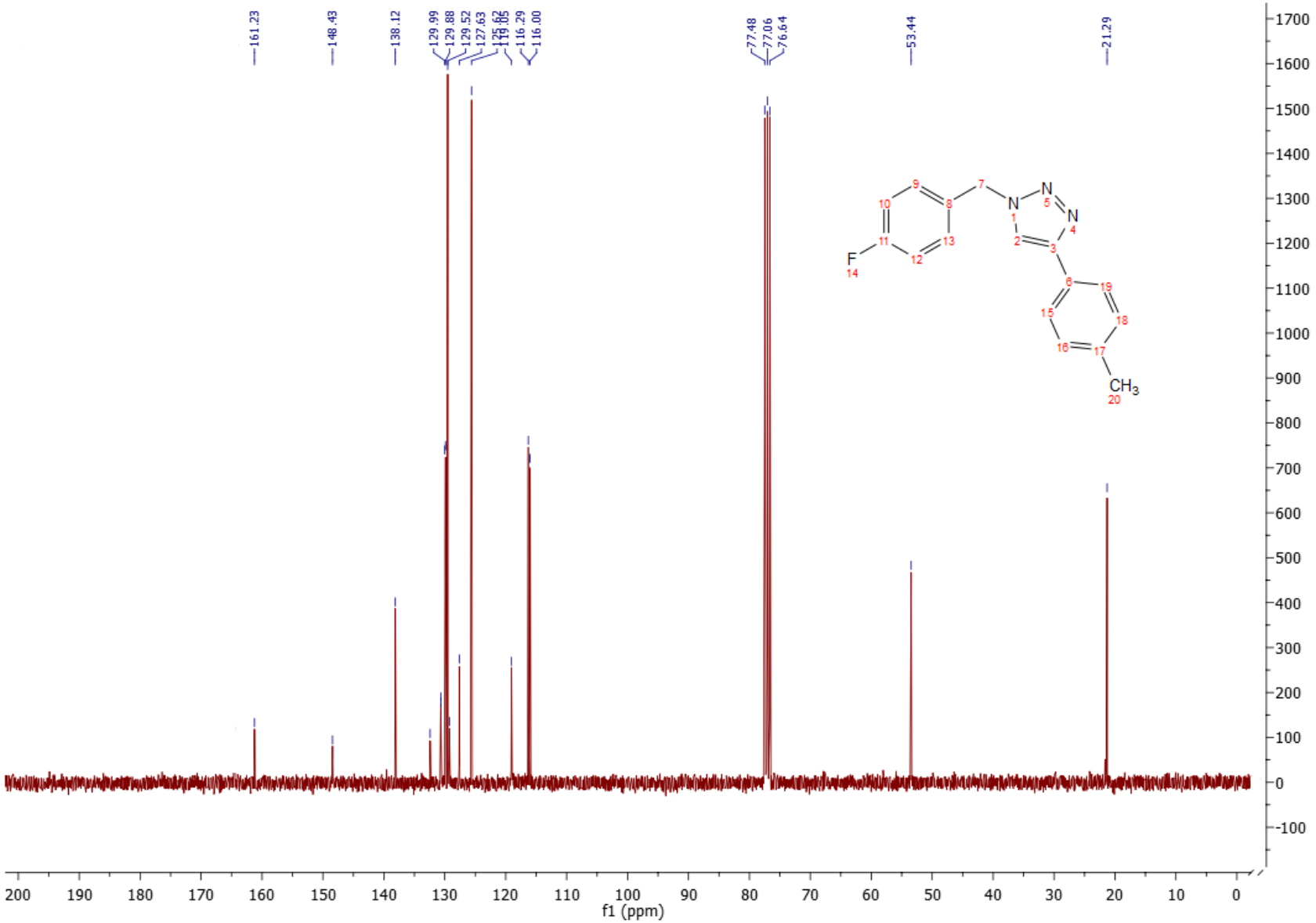


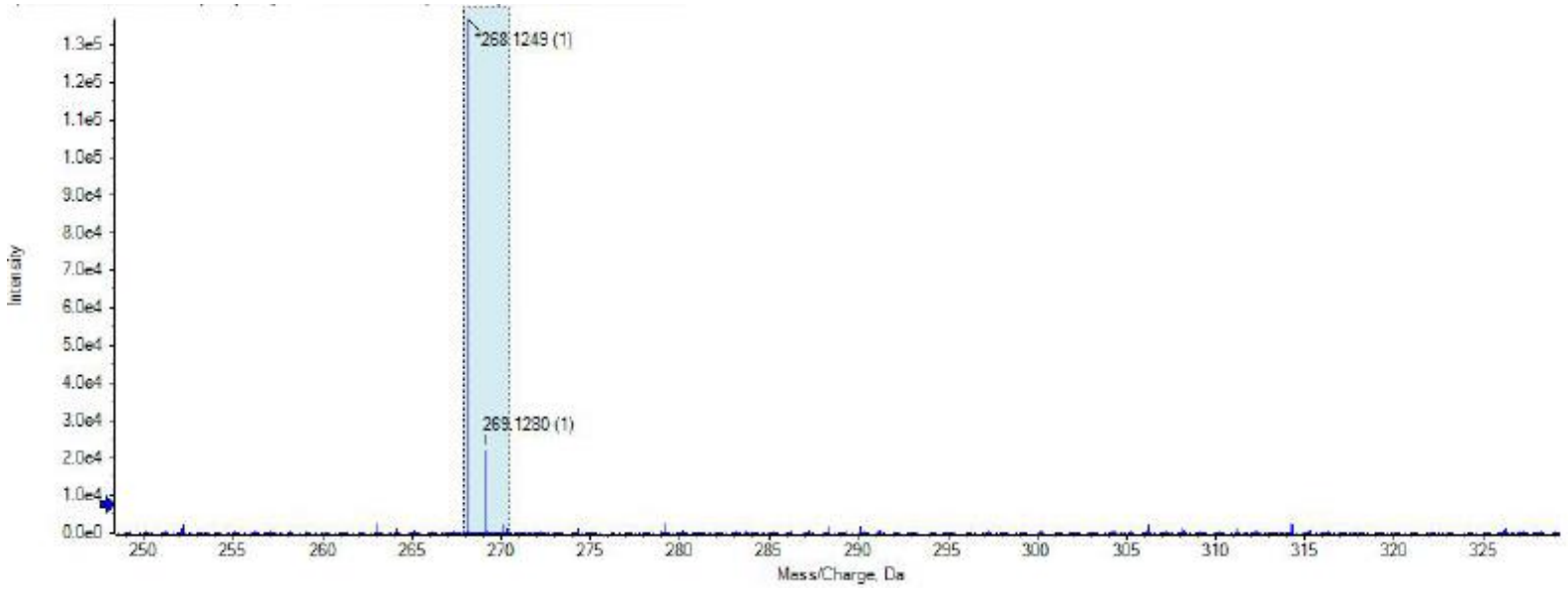

158.56
134.90
129.92
129.51
129.22
128.53
121.65
116.21
115.18
77.85
77.42
77.09
62.46
54.70
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
N
N
N


266.1289
267.1316
Intensity
Mass/Charge, Da
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
230
235
240
245
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
330

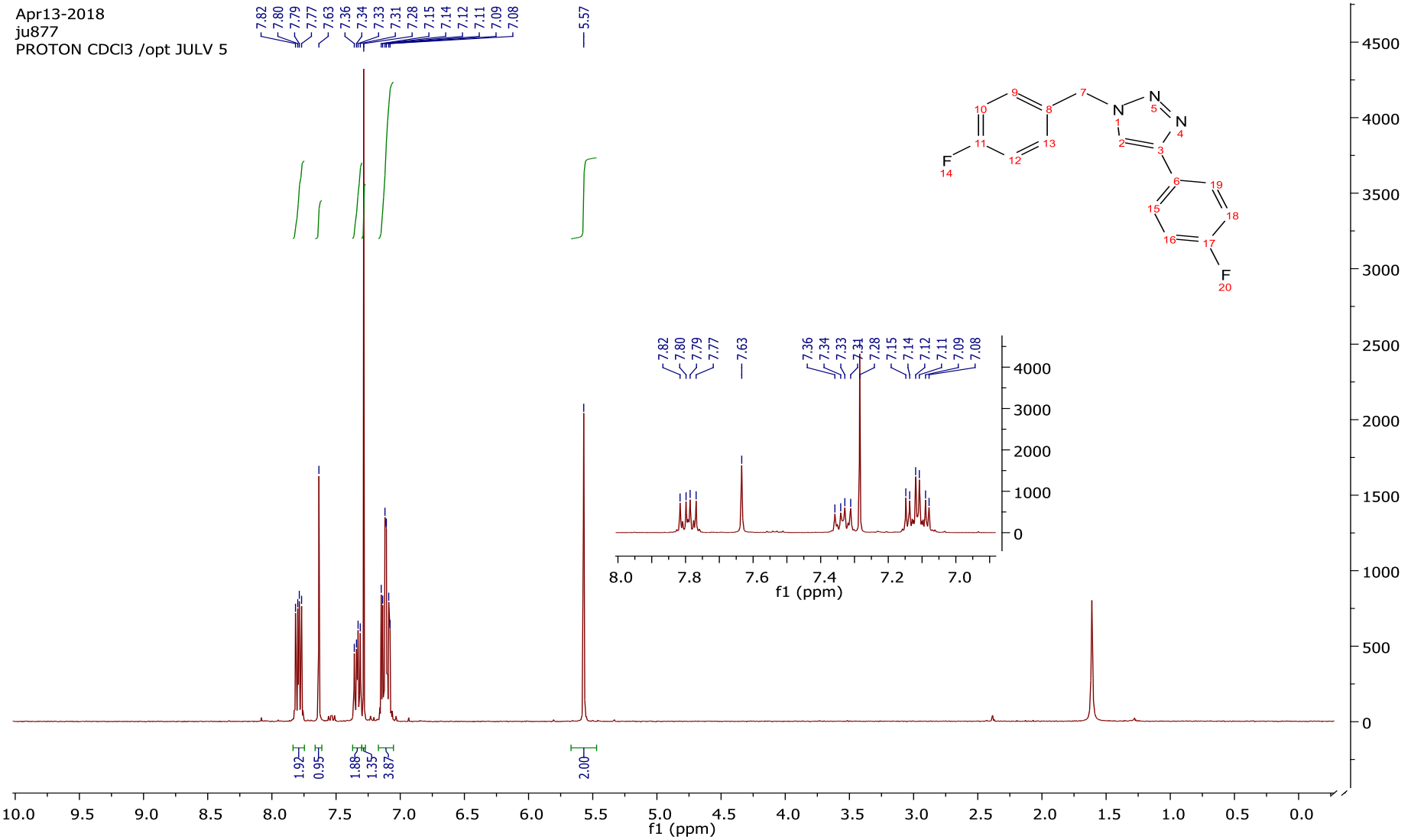
1-(4-Fluoro-benzyl)-4-p-tolyl-1H-[1,2,3]triazole (3e)

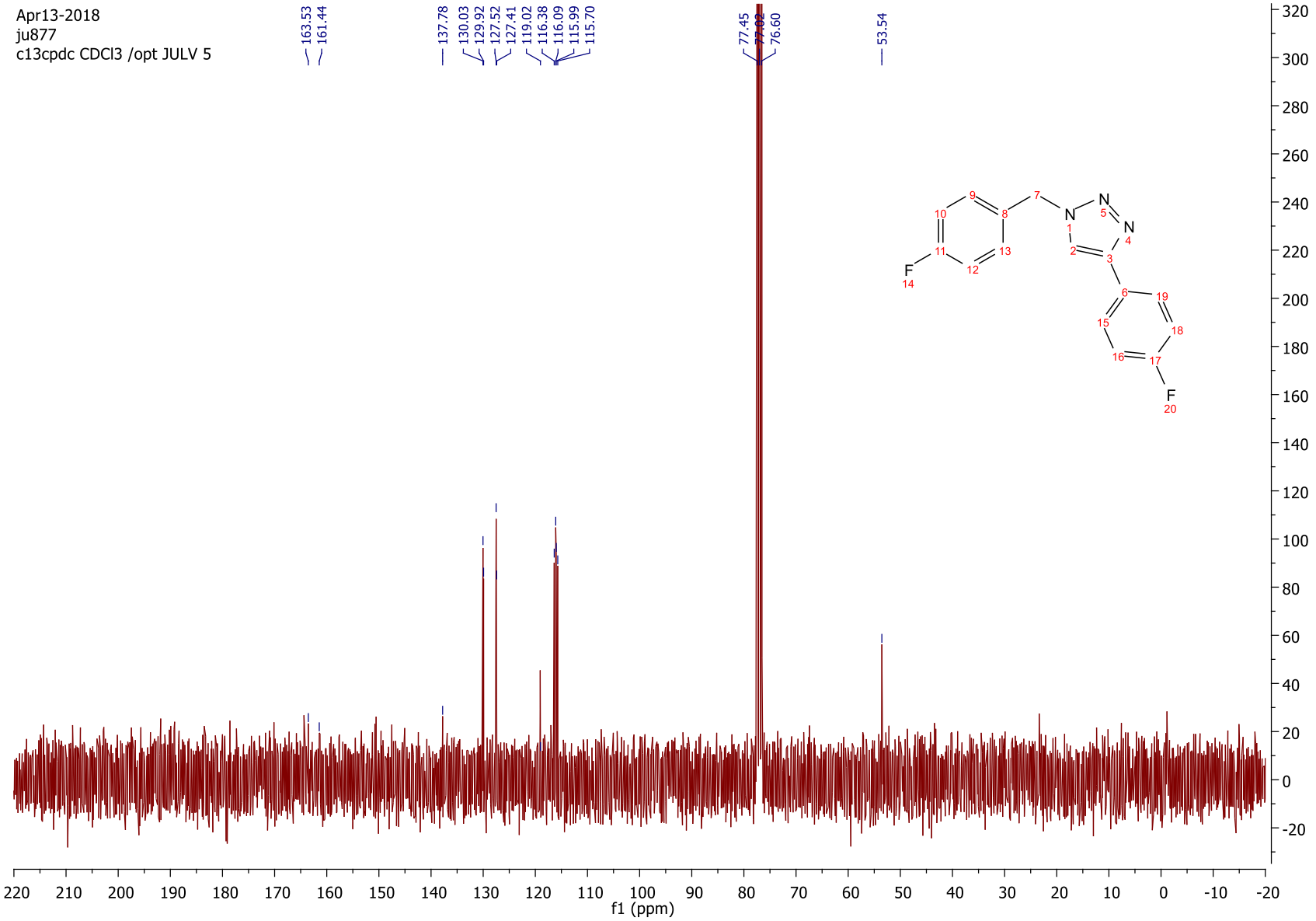


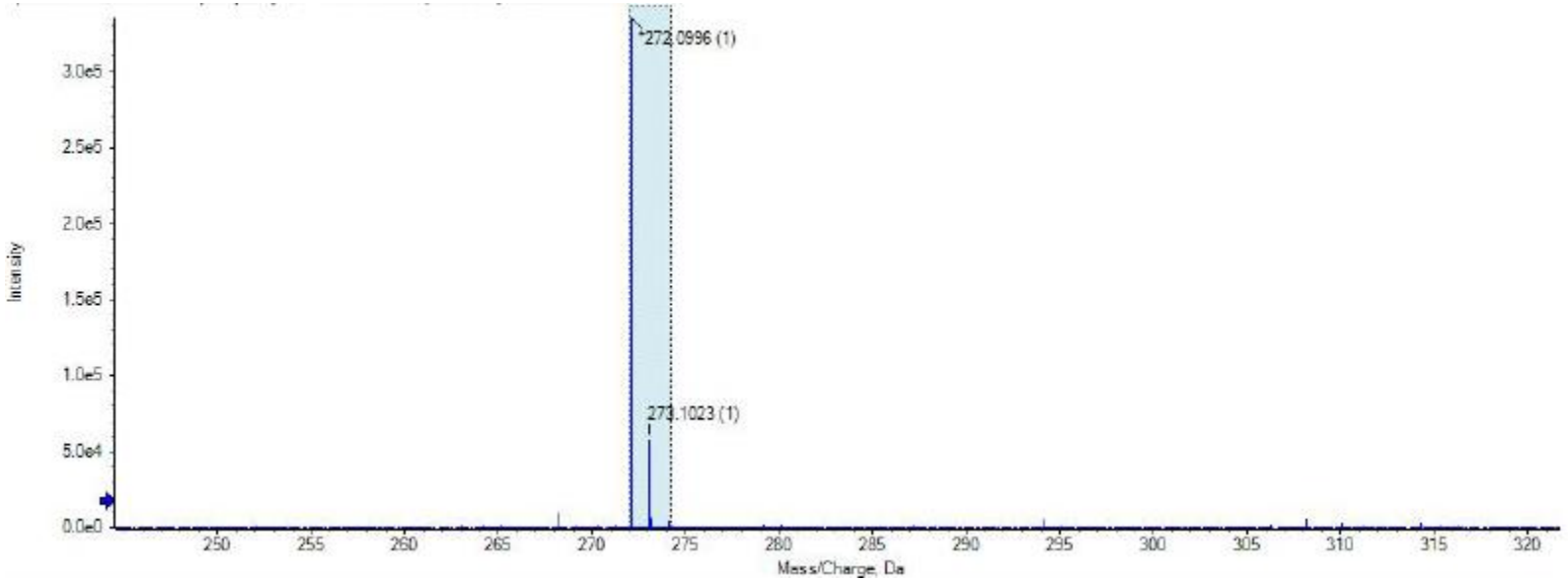

161.23
148.43
138.12
129.99
129.88
129.52
127.63
116.29
116.00
77.48
77.06
76.64
53.44
21.29
f1 (ppm)


268.1249 (1)
269.1280 (1)
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
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
Mass/Charge, Da

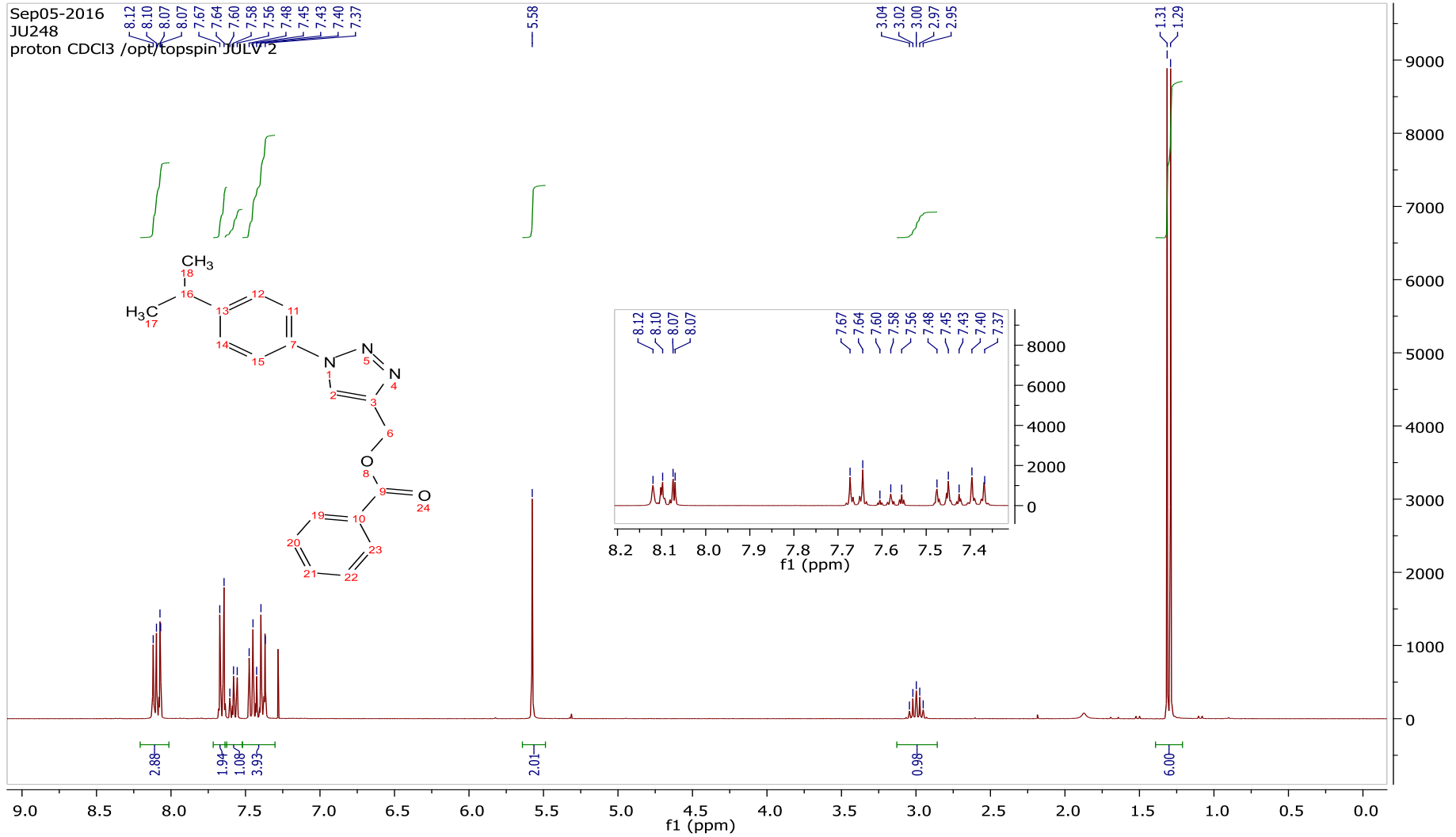
1-(4-fluorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3f)

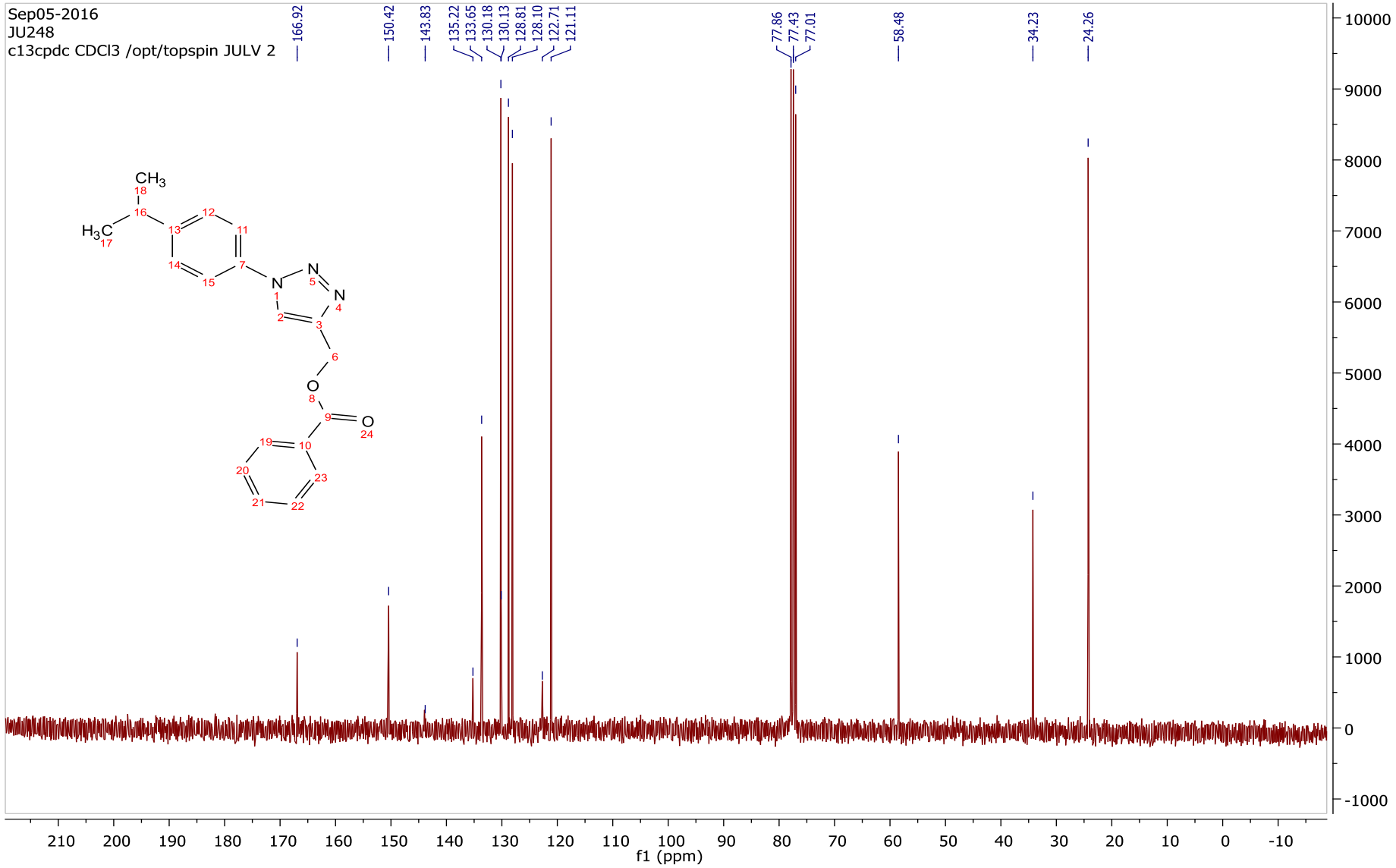


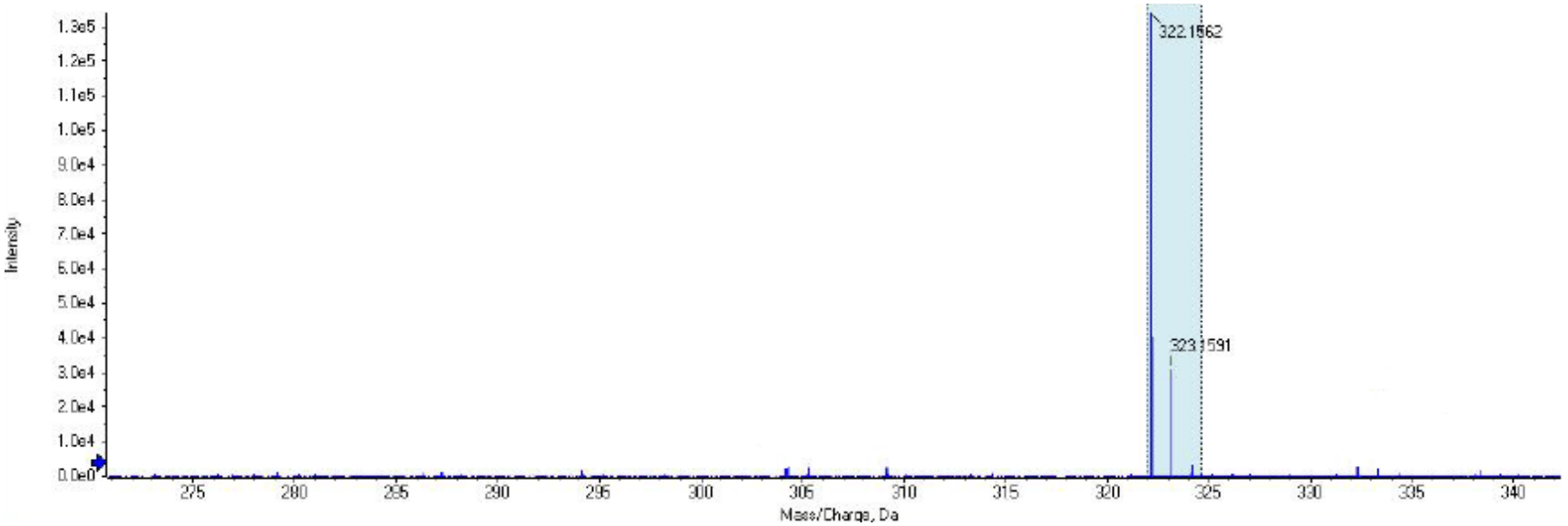

Apr13-2018
ju877
c13cpdc CDCl3 /opt JULV 5
163.53
161.44
137.78
130.03
129.92
127.52
127.41
119.02
116.38
116.09
115.99
115.70
77.45
77.02
76.60
53.54
f1 (ppm)


272.0996 (1)
271.1023 (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

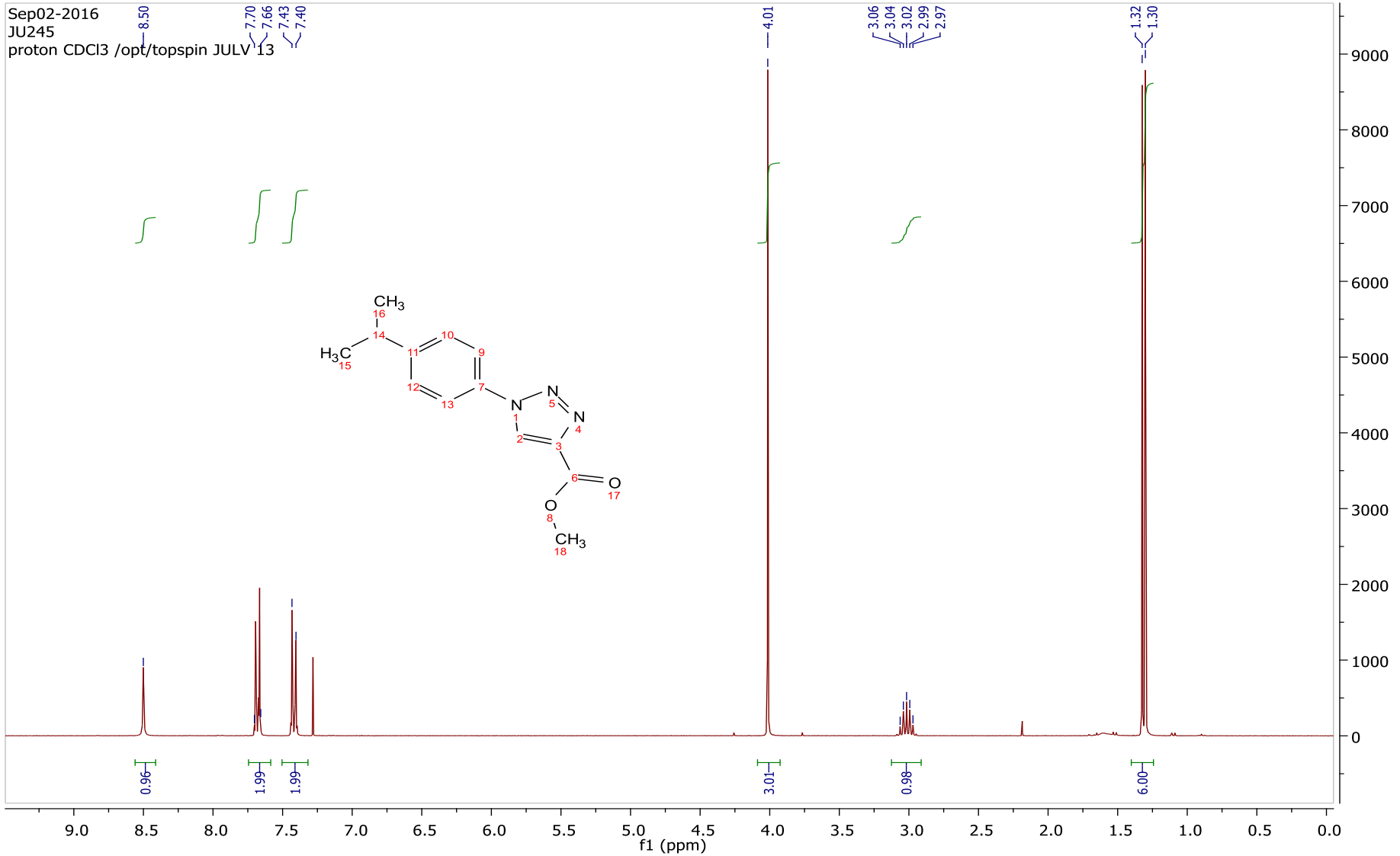
(1-(4-isopropylphenyl)-1H-1,2,3-triazol-4-yl)methyl benzoate (3g)

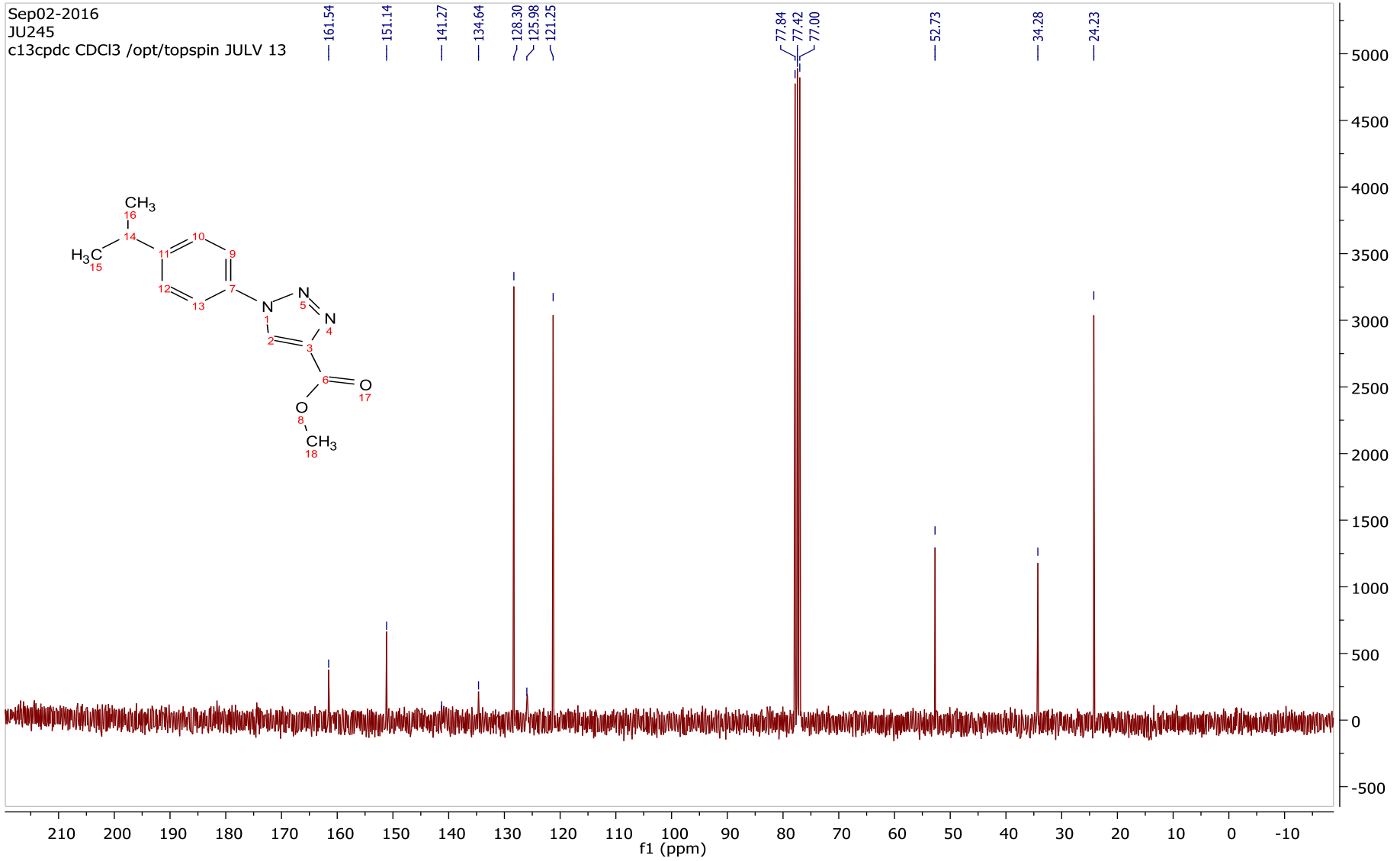


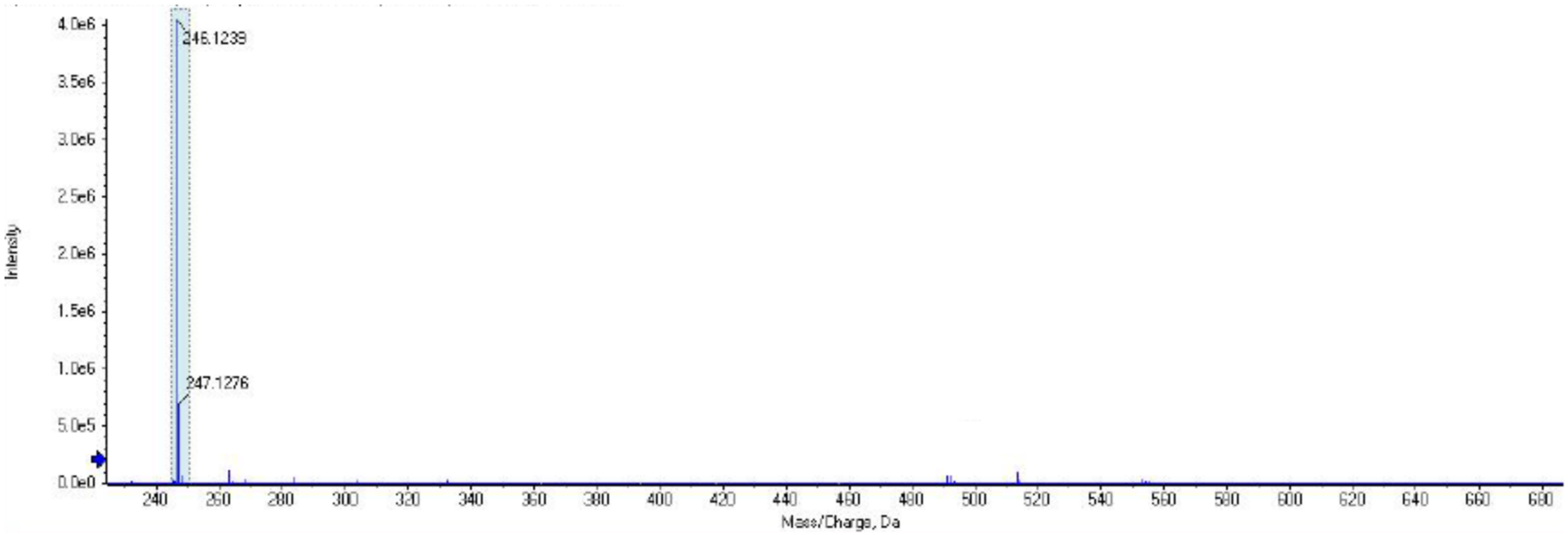

Sep05-2016
JU248
c13cpdc CDCl3 /opt/topspin JULV 2
166.92
150.42
143.83
135.22
133.65
130.18
130.13
128.81
128.10
122.71
121.11
77.86
77.43
77.01
58.48
34.23
24.26
f1 (ppm)


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
Intensity
322.1562
323.1591
275
280
285
290
295
300
305
310
315
320
325
330
335
340
Mass/Charge, Da

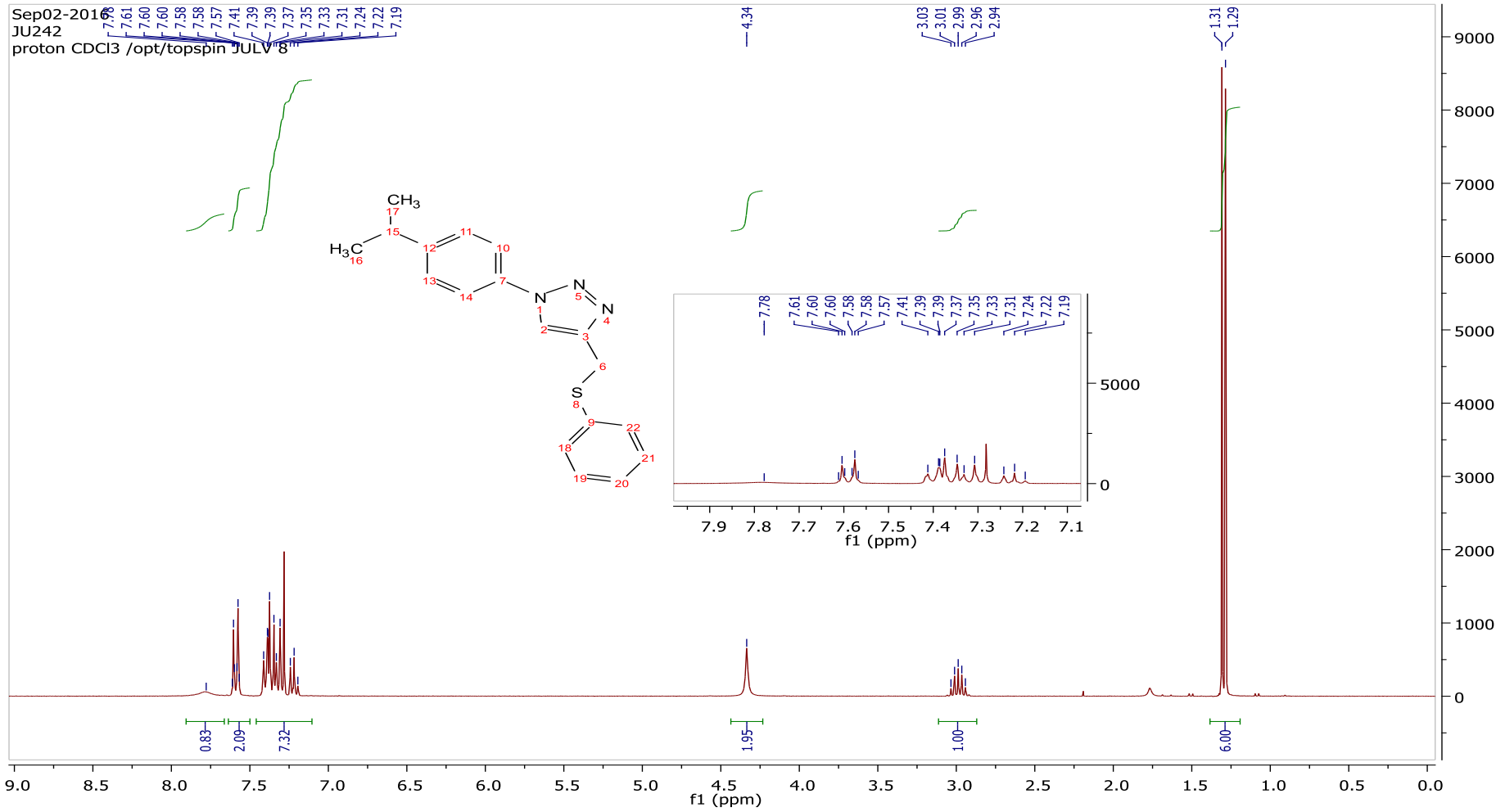
Methyl 1-(4-isopropylphenyl)-1H-1,2,3-triazole-4-carboxylate (3h)

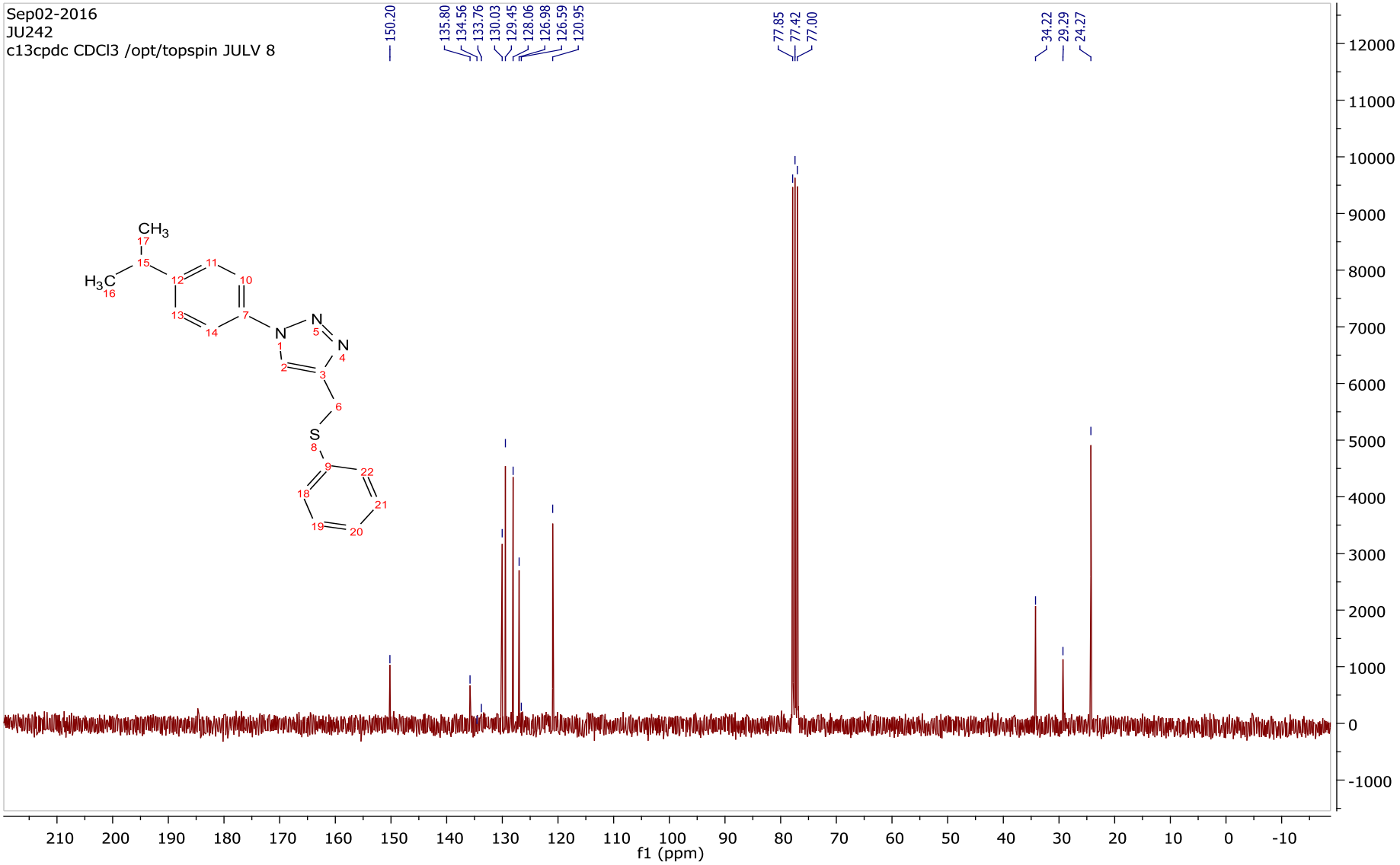


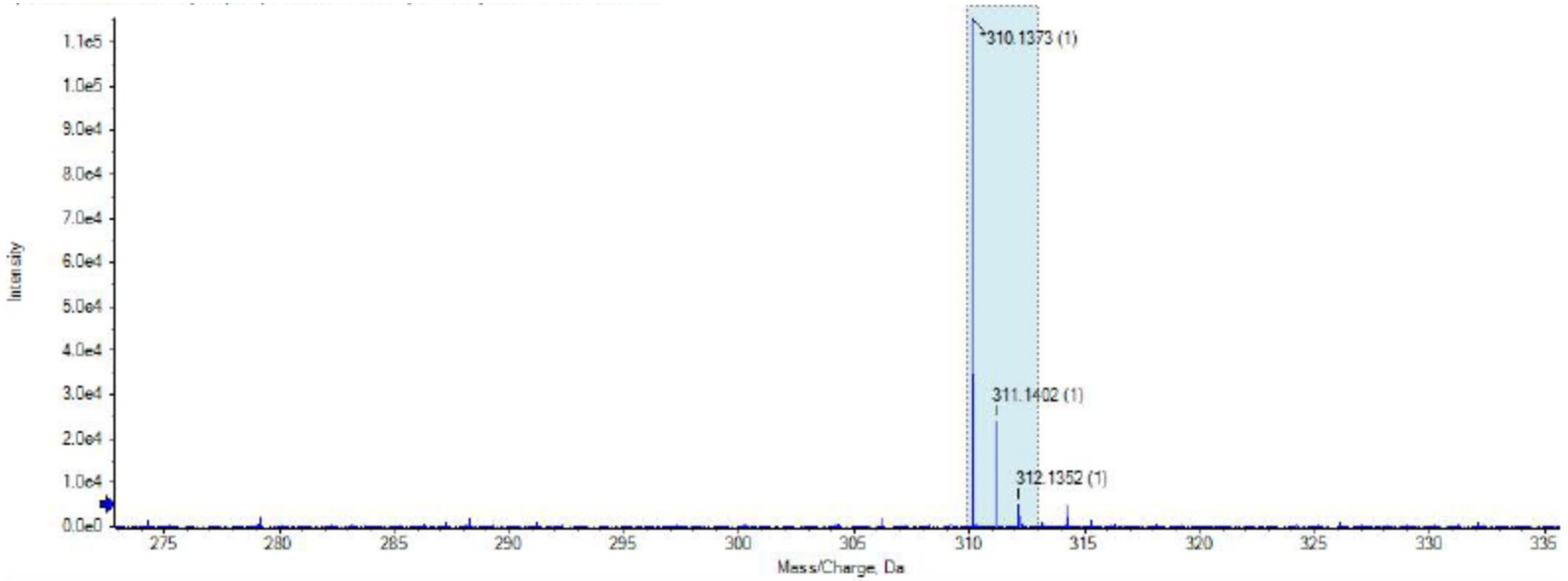

Sep02-2016
JU245
c13cpdc CDCl3 /opt/topspin JULV 13
161.54
151.14
141.27
134.64
128.30
125.98
121.25
77.84
77.42
77.00
52.73
34.28
24.23
CH3
16
14
H3C
15
11
10
9
12
13
7
N
1
N
5
N
4
2
3
6
O
17
O
8
CH3
18
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


246.1239
247.1276
Intensity
Mass/Charge, Da

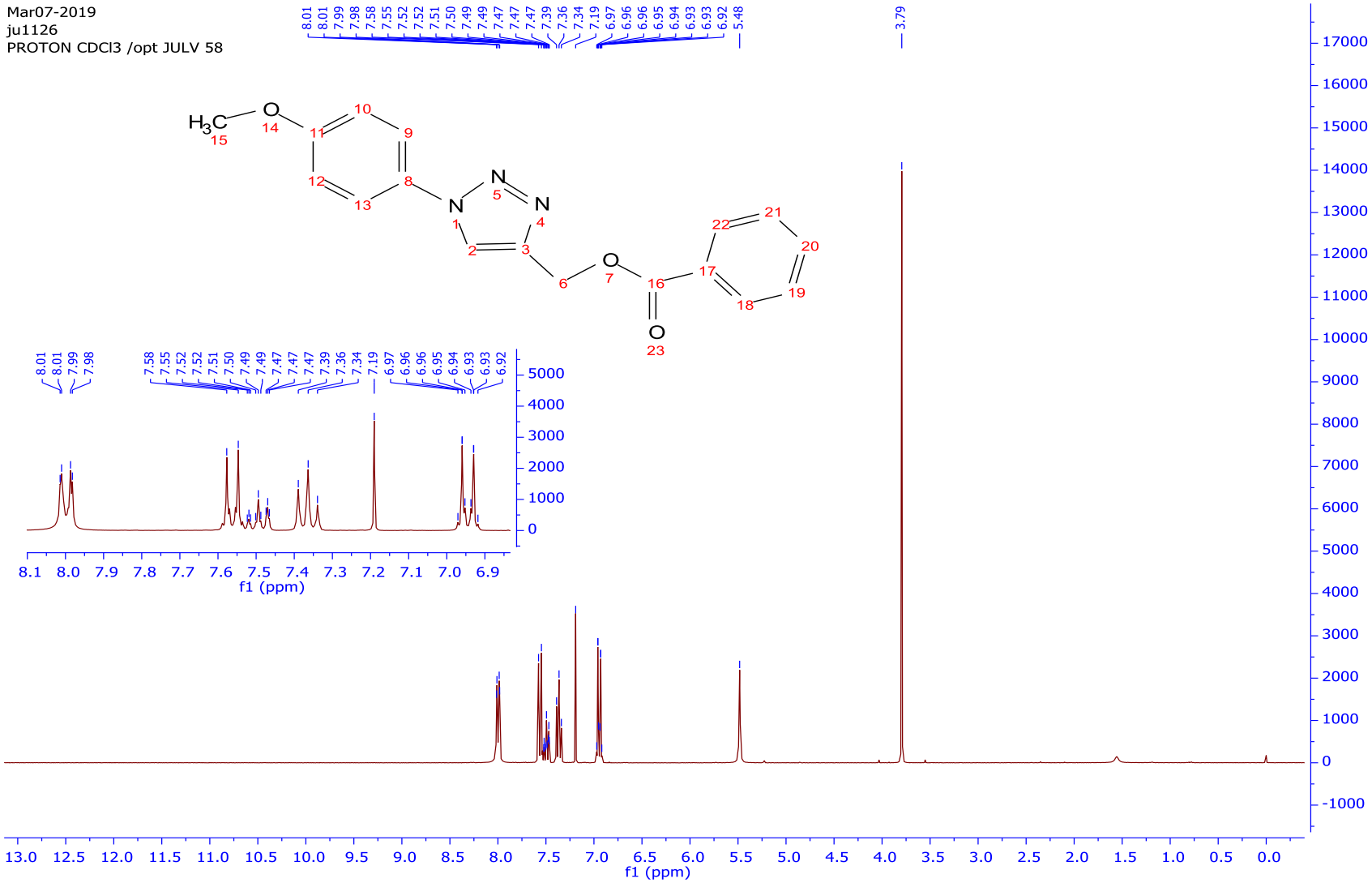
1-(4-isopropylphenyl)-4-(phenylthiomethyl)-1H-1,2,3-triazole (3i)

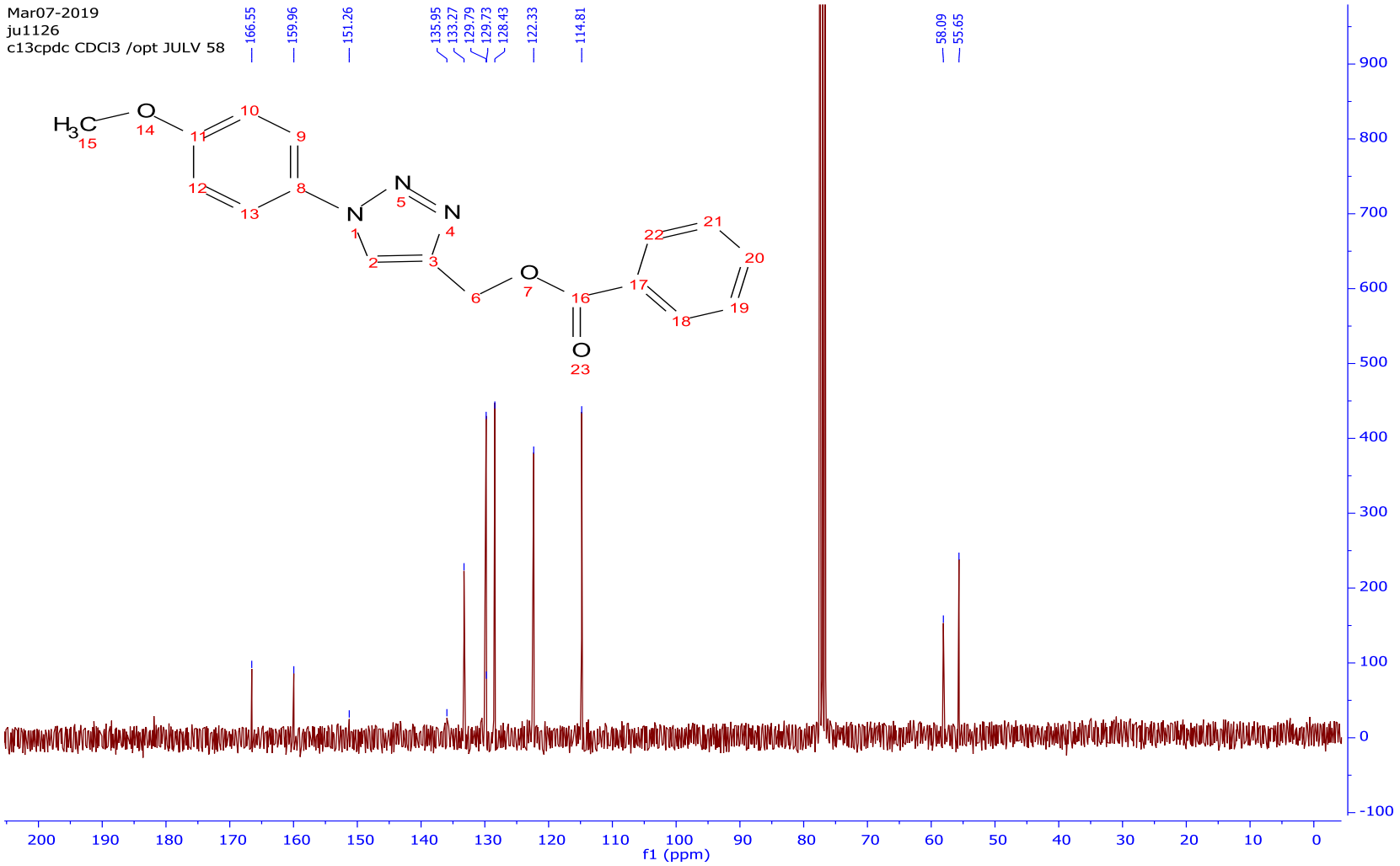


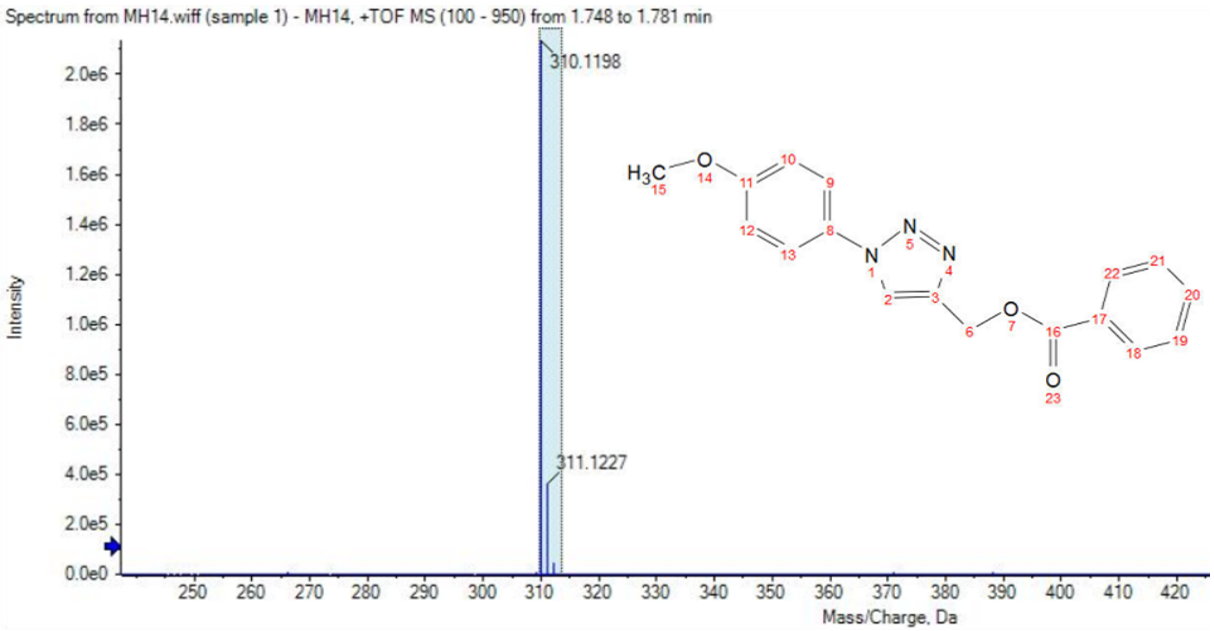

Sep02-2016
JU242
c13cpdc CDCl3 /opt/topspin JULV 8
150.20
135.80
134.56
133.76
130.03
129.45
128.06
126.98
126.59
120.95
77.85
77.42
77.00
34.22
29.29
24.27
CH3
H3C
N
S
f1 (ppm)


310.1373 (1)
311.1402 (1)
312.1352 (1)
Intensity
Mass/Charge, Da
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
275
280
285
290
295
300
305
310
315
320
325
330
335

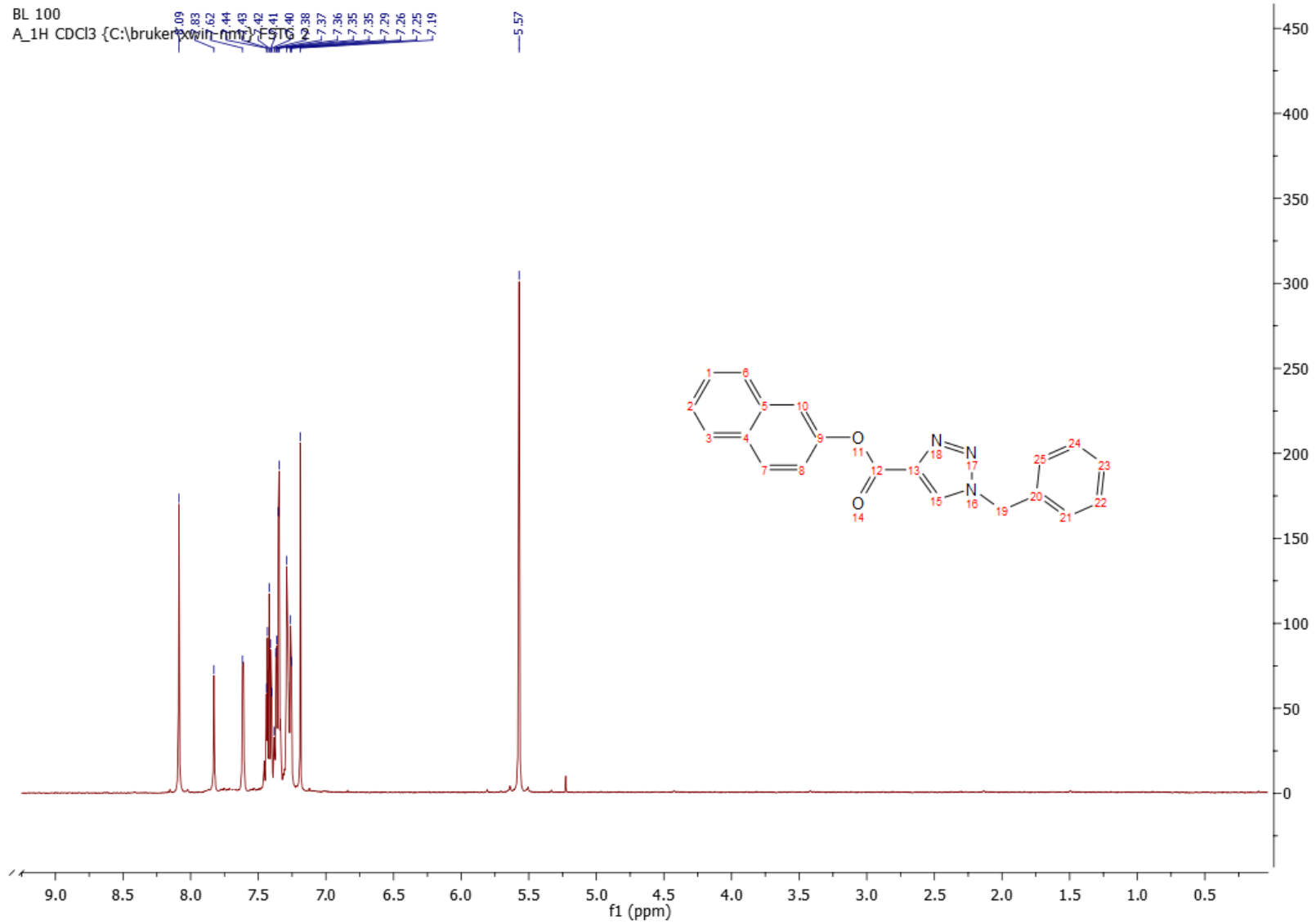
(1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl benzoate (3j)

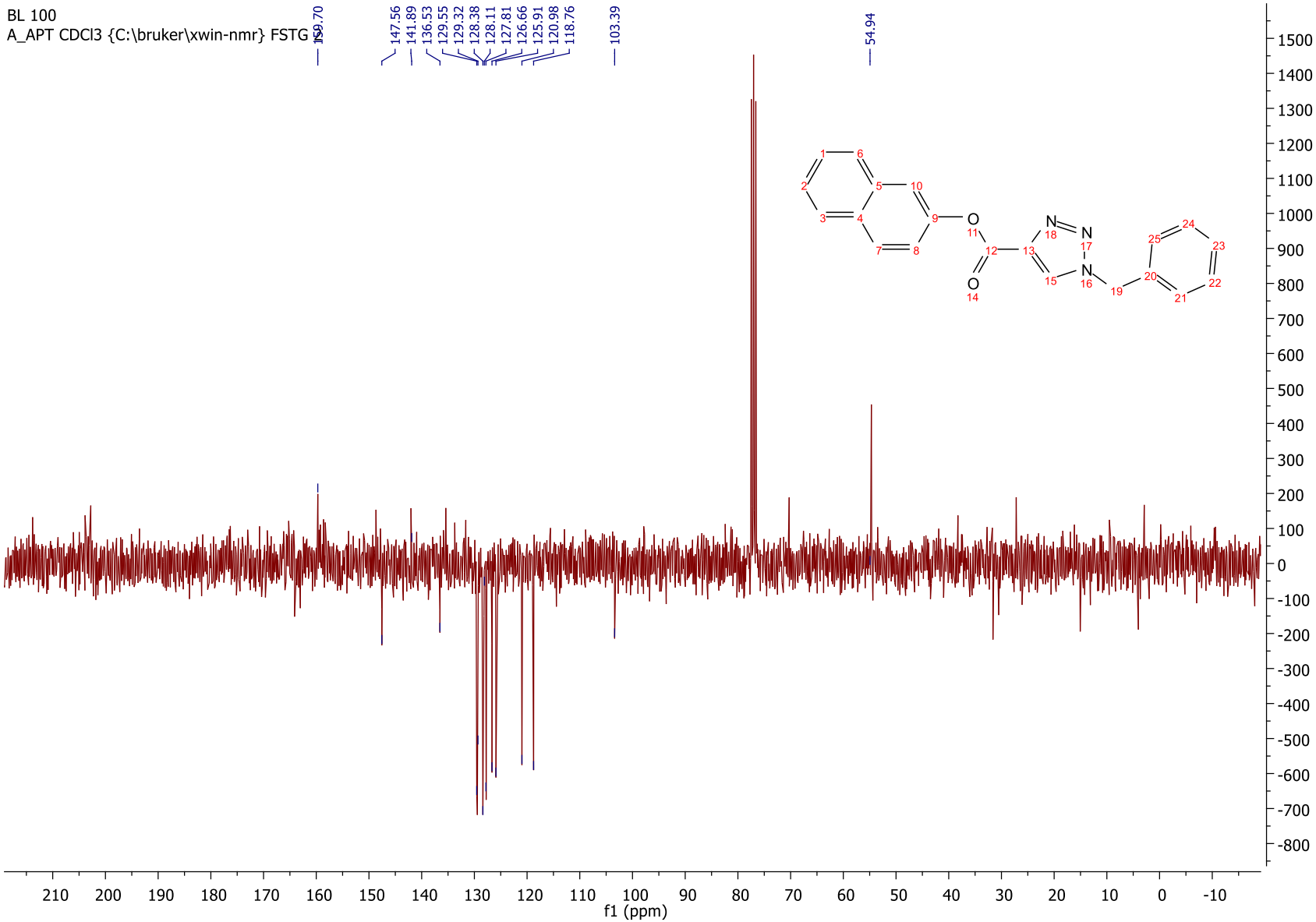


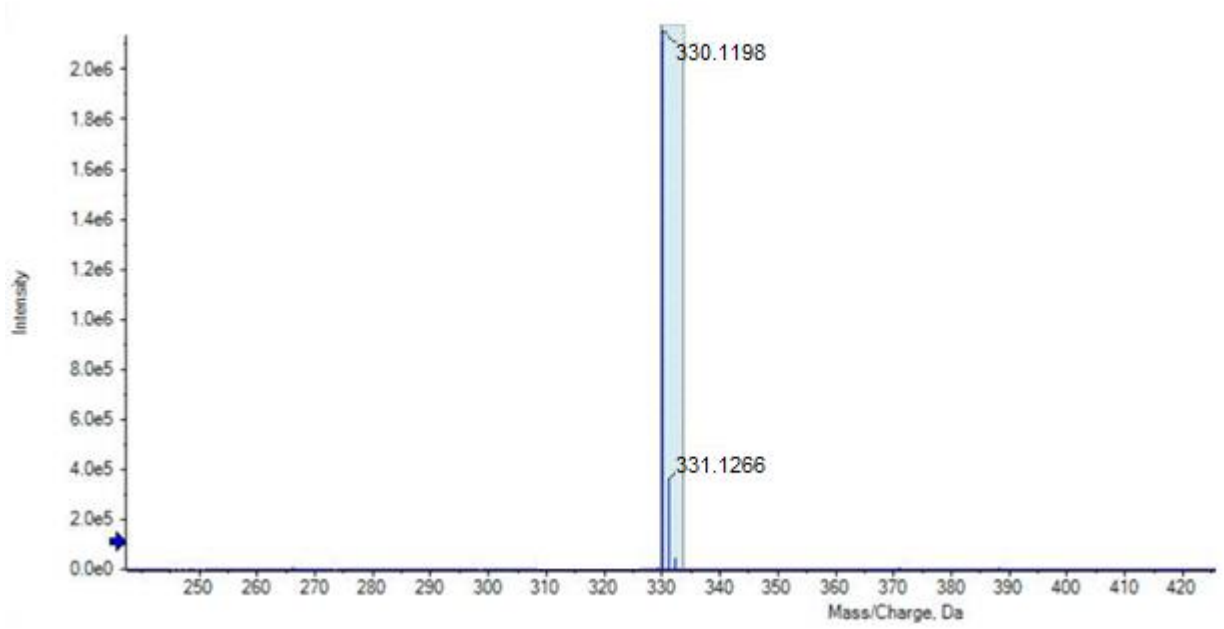

Mar07-2019
ju1126
c13cpdc CDCl3 /opt JULV 58
166.55
159.96
151.26
135.95
133.27
129.79
129.73
128.43
122.33
114.81
58.09
55.65
f1 (ppm)


Spectrum from MH14.wiff (sample 1) - MH14, +TOF MS (100 - 950) from 1.748 to 1.781 min
310.1198
311.1227
Intensity
2.0e6
1.8e6
1.6e6
1.4e6
1.2e6
1.0e6
8.0e5
6.0e5
4.0e5
2.0e5
0.0e0
250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420
Mass/Charge, Da

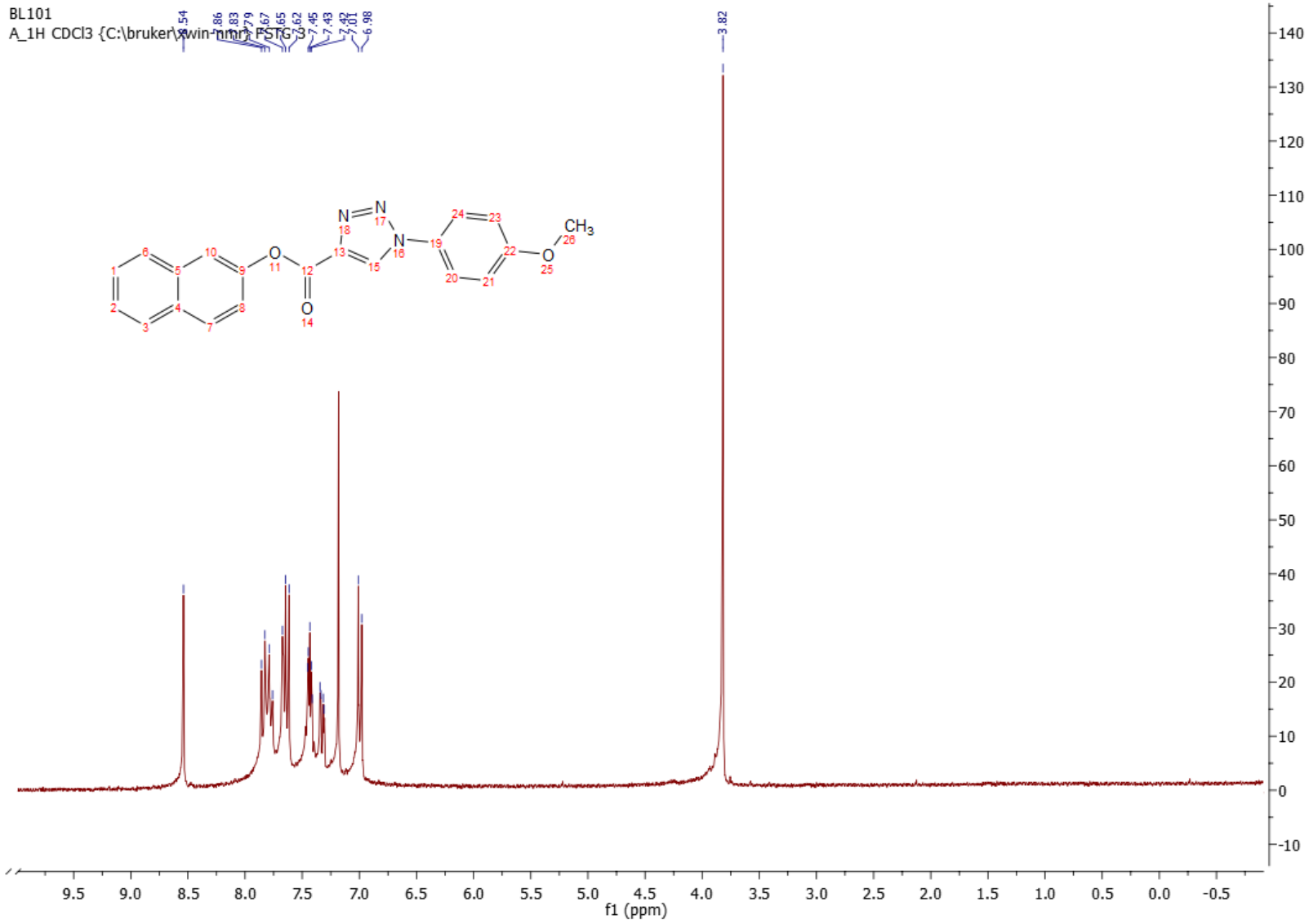
Naphthalen-2-yl 1-benzyl-1H-1,2,3-triazole-4-carboxylate (3k)

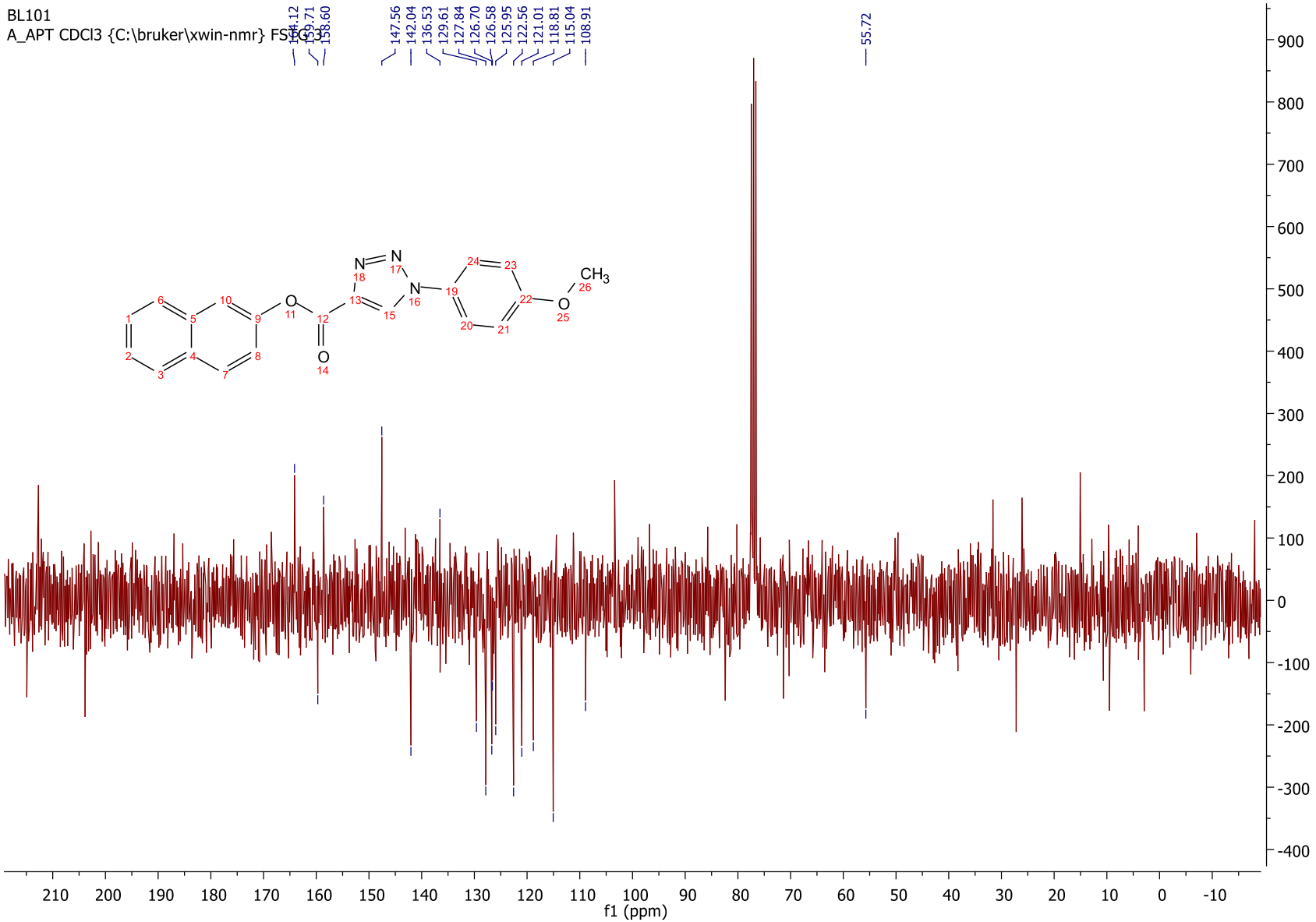


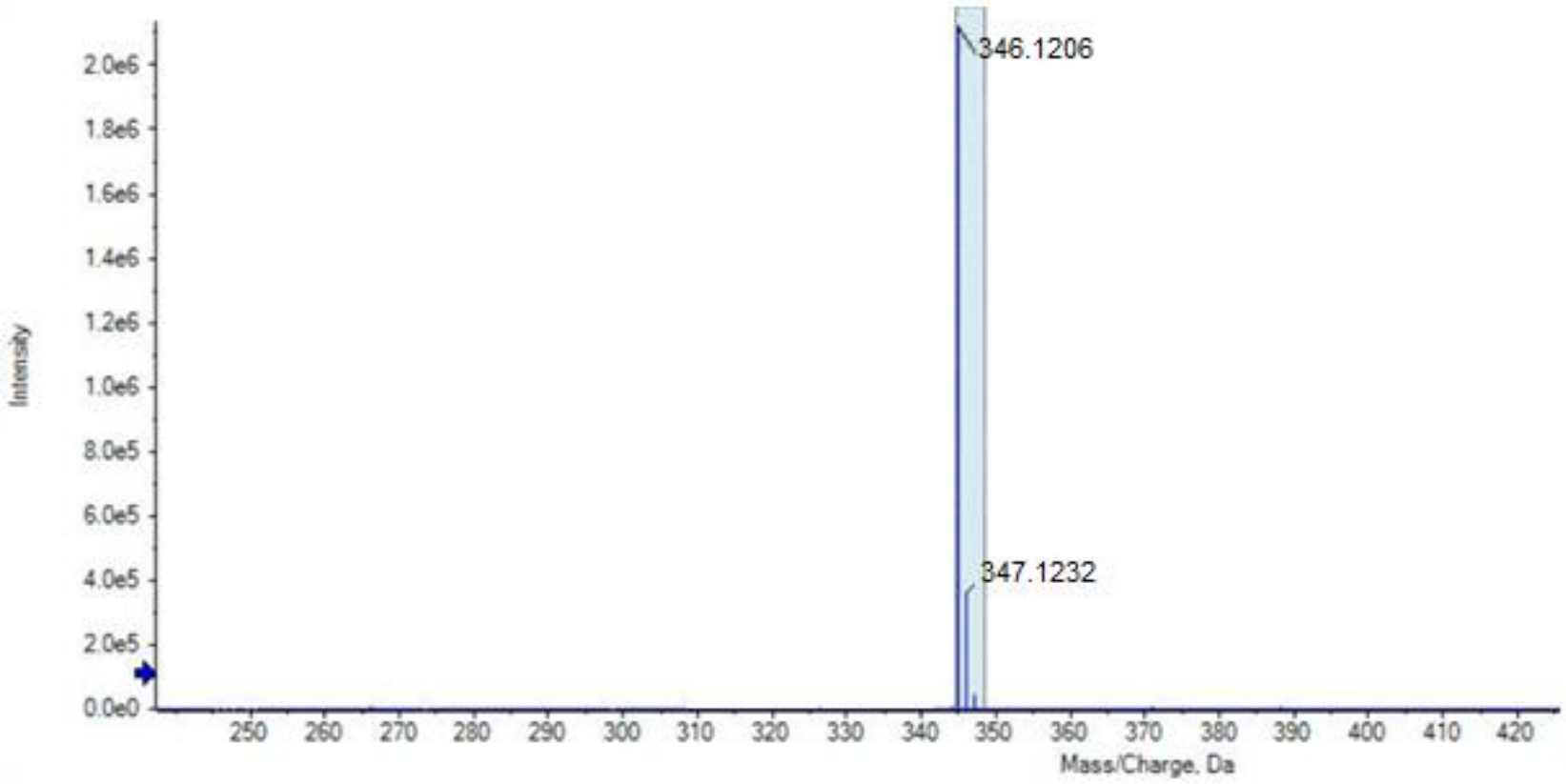

BL 100
A_APT CDCl3 {C:\bruker\xwin-nmr} FSTG
159.70
147.56
141.89
136.53
129.55
129.32
128.38
128.11
127.81
126.66
125.91
120.98
118.76
103.39
54.94
f1 (ppm)


330.1198
331.1266
Intensity
2.0e6
1.8e6
1.6e6
1.4e6
1.2e6
1.0e6
8.0e5
6.0e5
4.0e5
2.0e5
0.0e0
250
260
270
280
290
300
310
320
330
340
350
360
370
380
390
400
410
420
Mass/Charge, Da

Naphthalen-2-yl 1-(4-methoxyphenyl)-1H-1,2,3-triazole-4-carboxylate (3l)




BL101
A_APT CDCl3 {C:\bruker\xwin-nmr} FSEC3
154.12
149.71
138.60
147.56
142.04
136.53
129.61
127.84
126.70
126.58
125.95
122.56
121.01
118.81
115.04
108.91
55.72
f1 (ppm)


346.1206
347.1232
Intensity
2.0e6
1.8e6
1.6e6
1.4e6
1.2e6
1.0e6
8.0e5
6.0e5
4.0e5
2.0e5
0.0e0
250
260
270
280
290
300
310
320
330
340
350
360
370
380
390
400
410
420
Mass/Charge, Da