Supporting Information to

Direct access to 2-amino-5-azidomethylfurans through palladium-catalyzed azidative cycloisomerization of homoallenyl amides

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Department of Chemistry, Zhejiang Normal University, 688 Yingbin Road, Jinhua 321004, PR China. luofang19@zjnu.cn and gangguo@zjnu.cn


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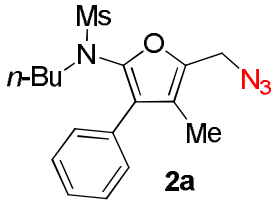
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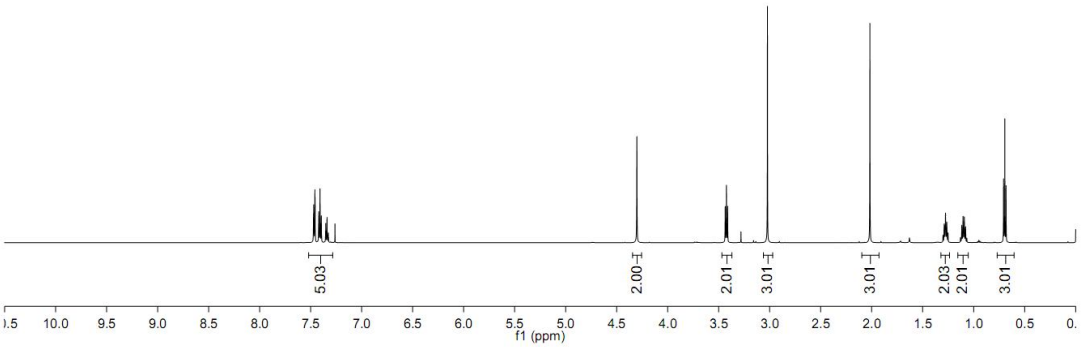
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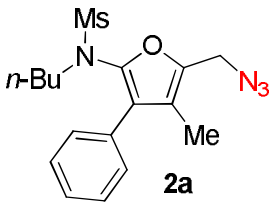
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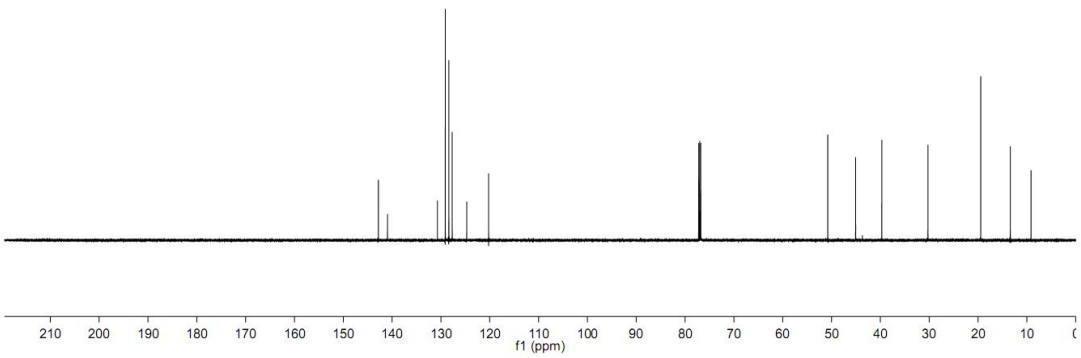
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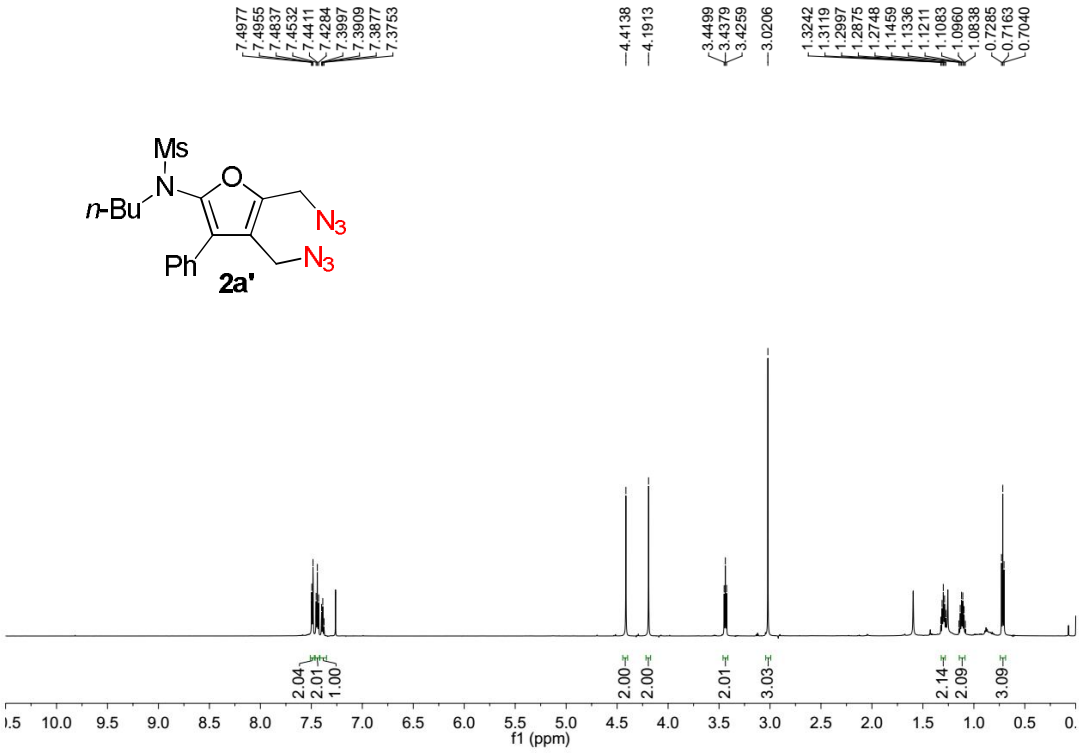
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N3
Ph
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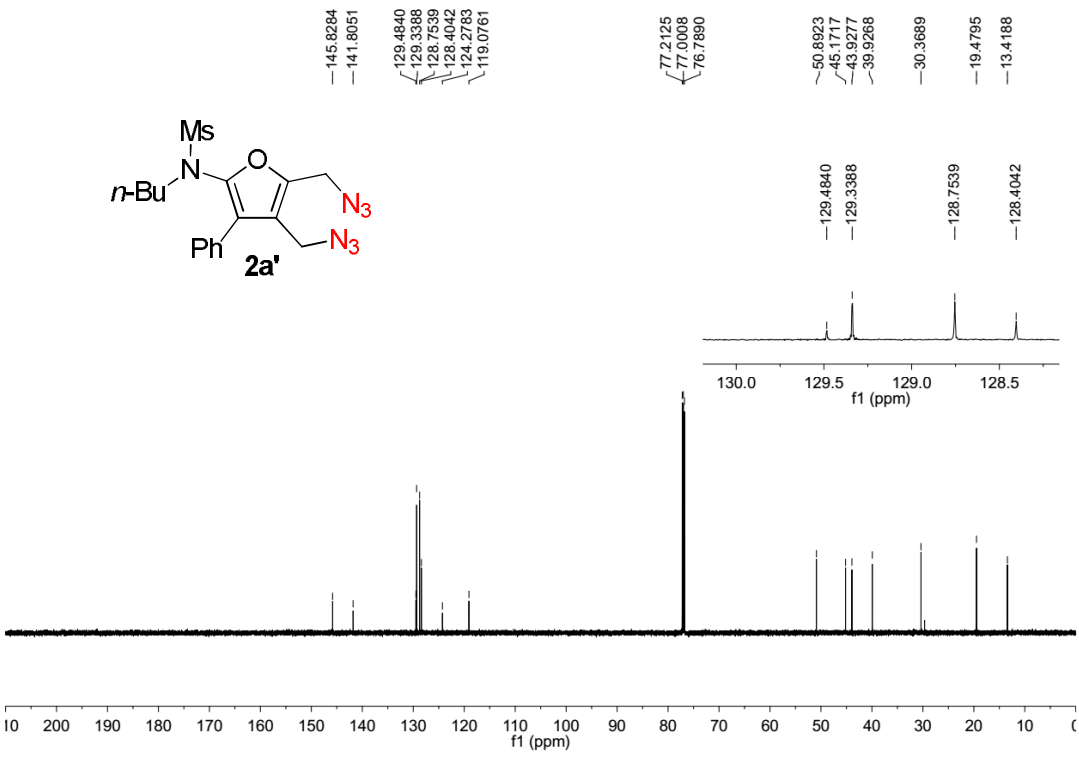
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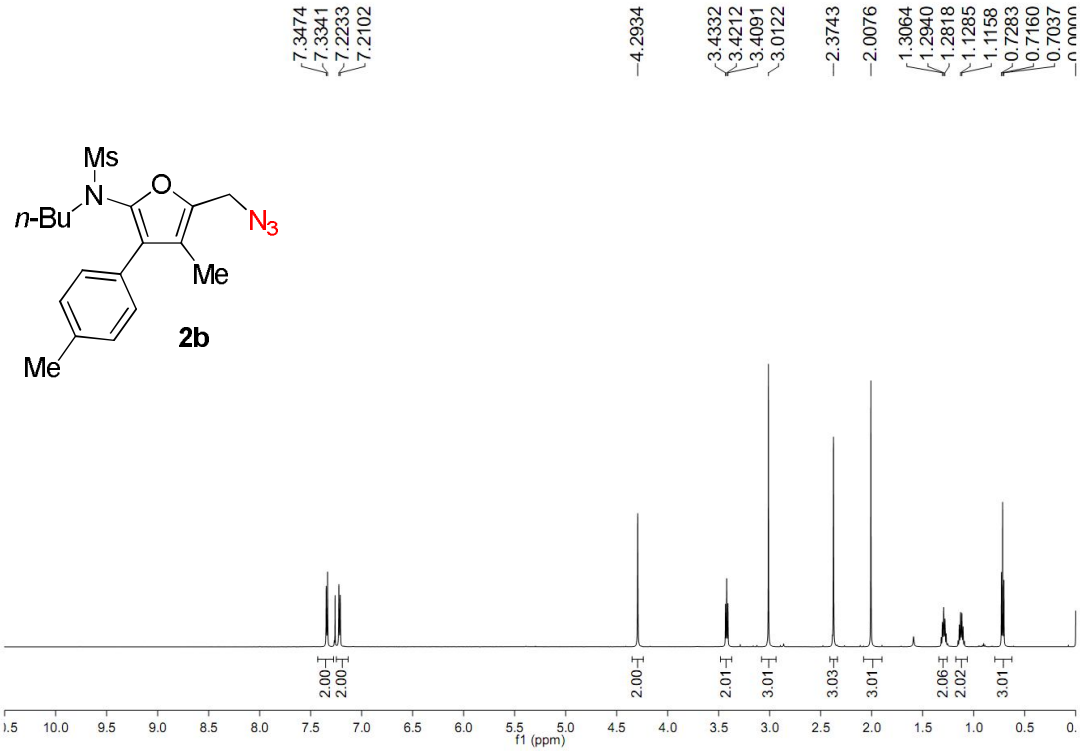
f1 (ppm)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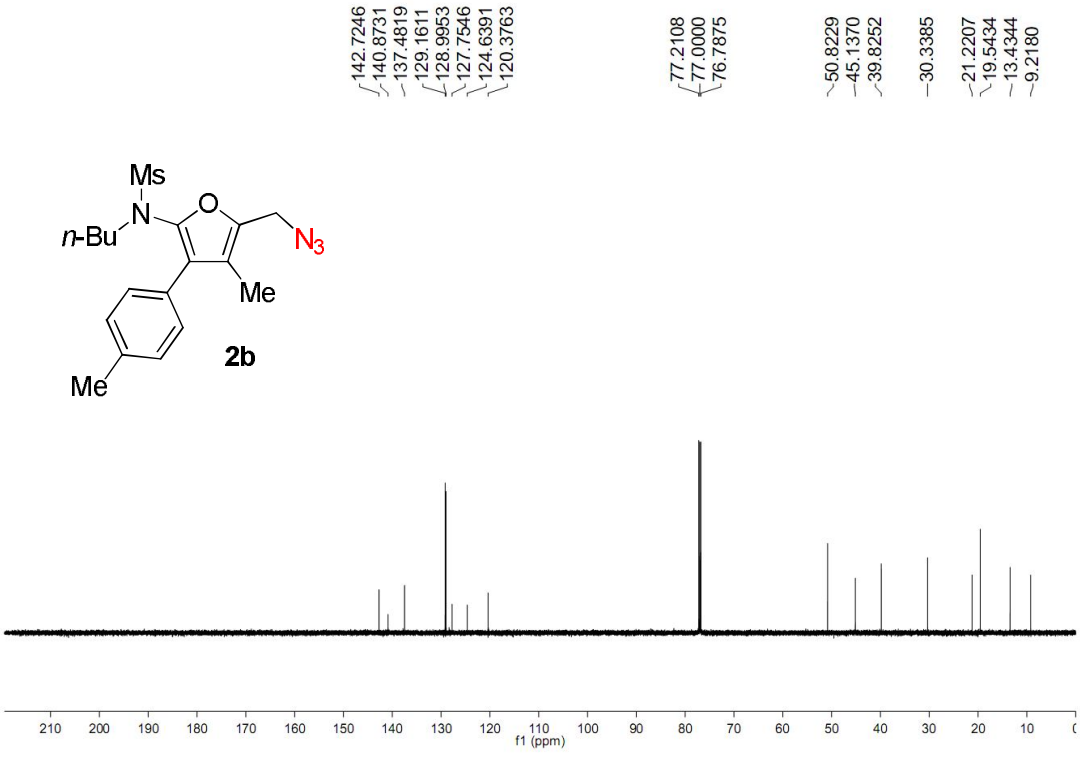
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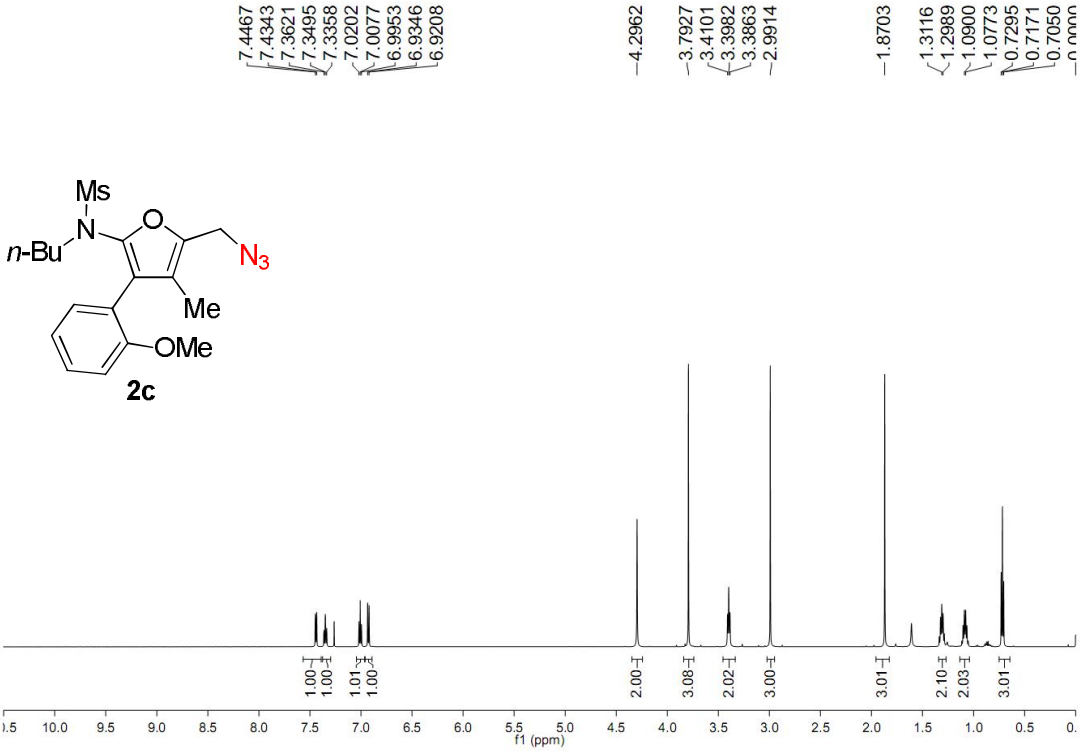
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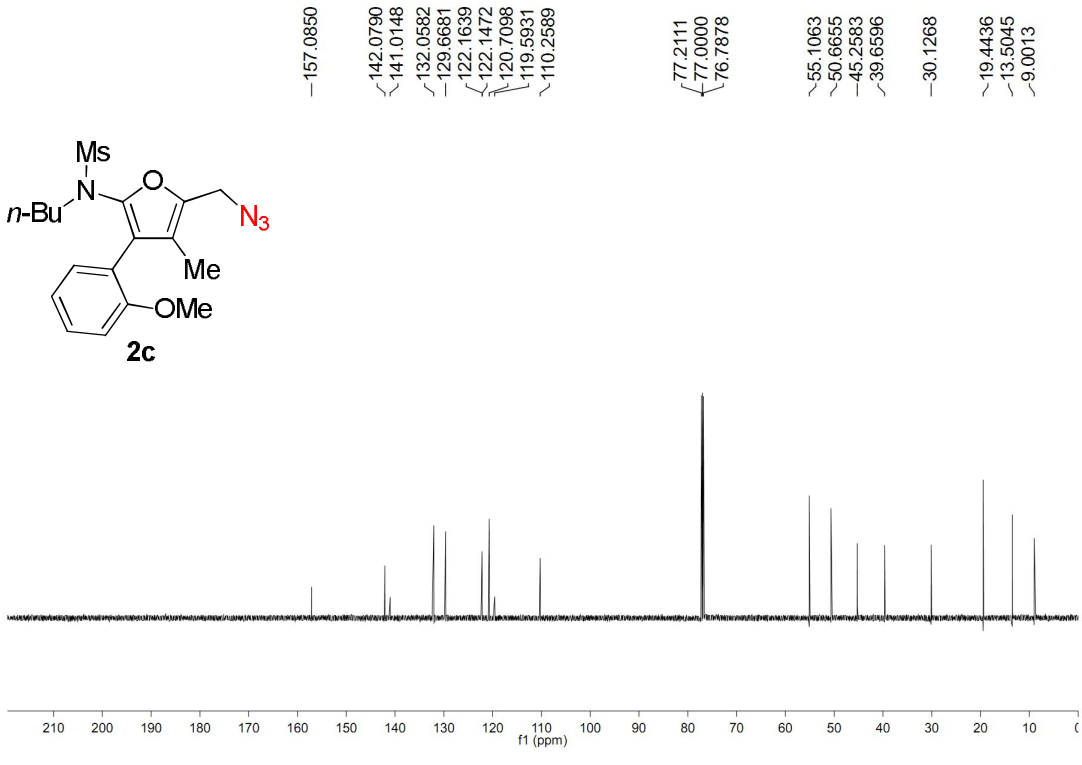
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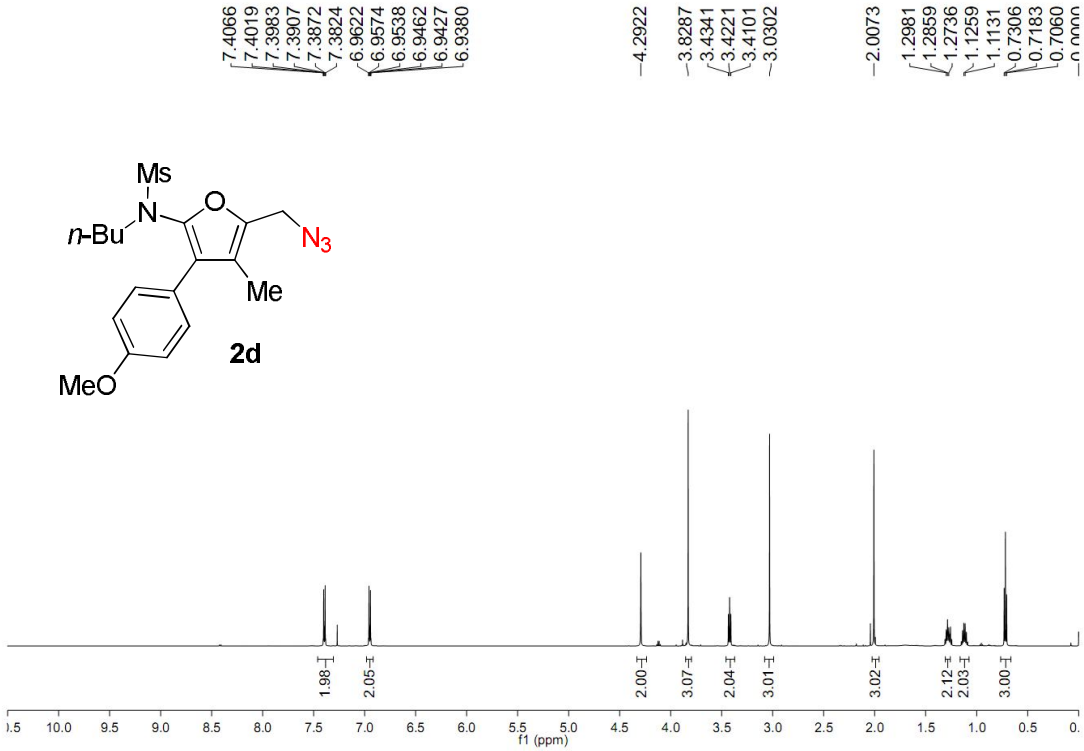
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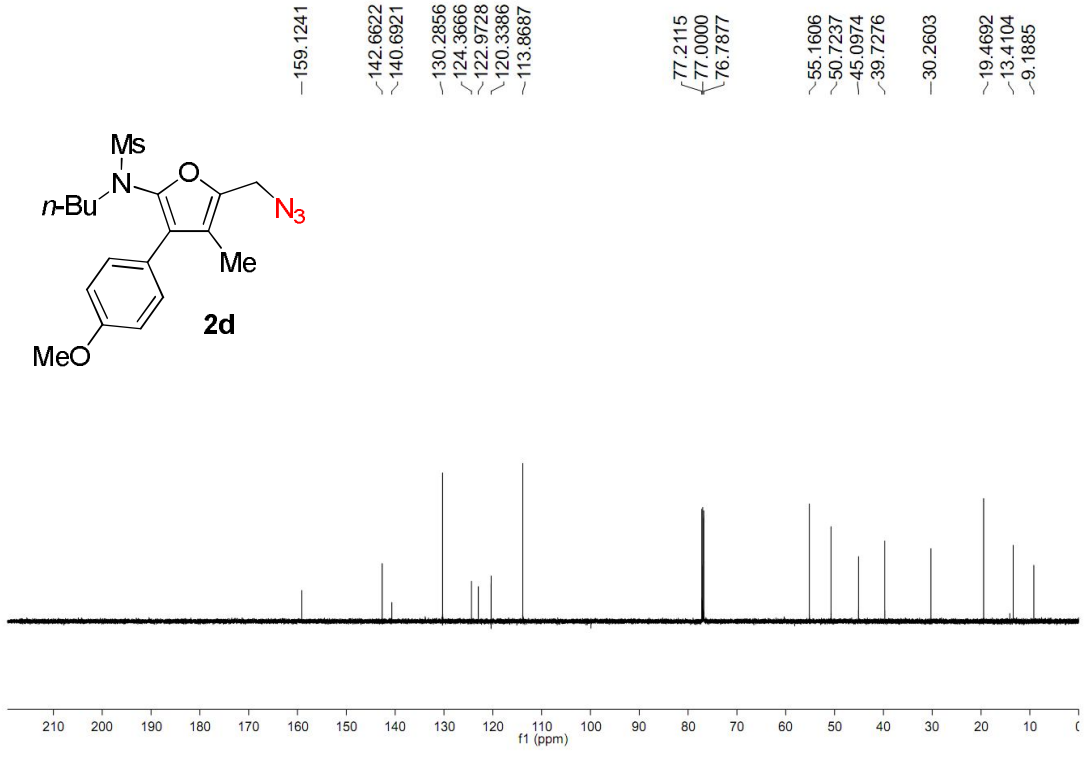
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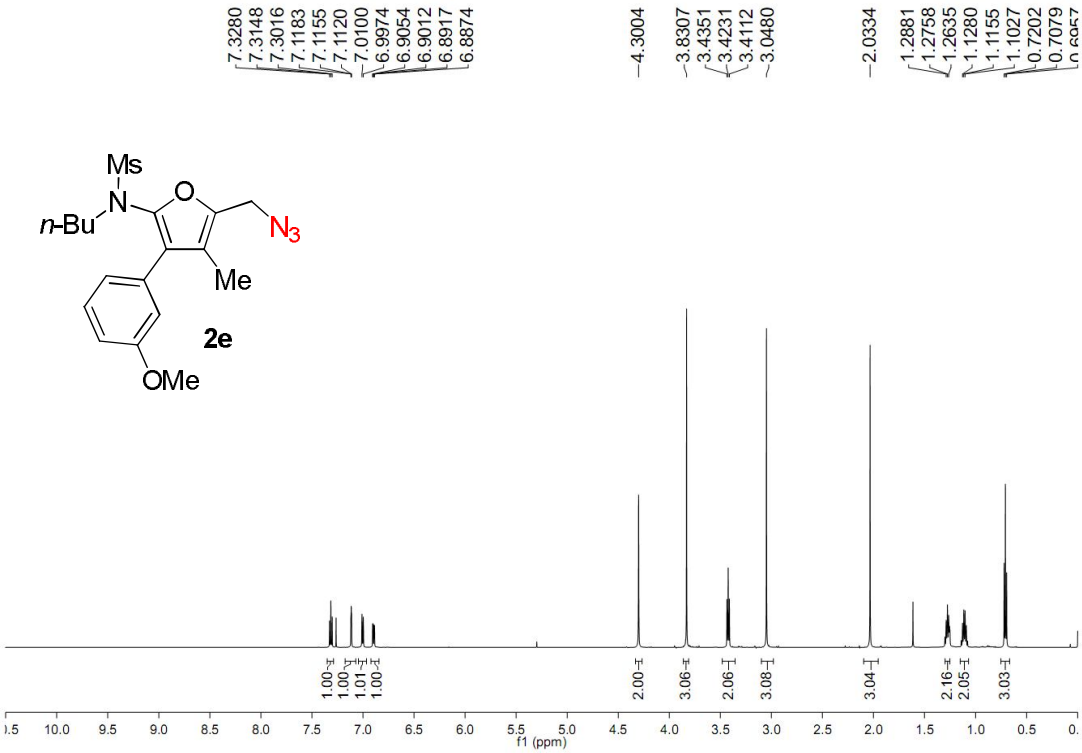
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OMe
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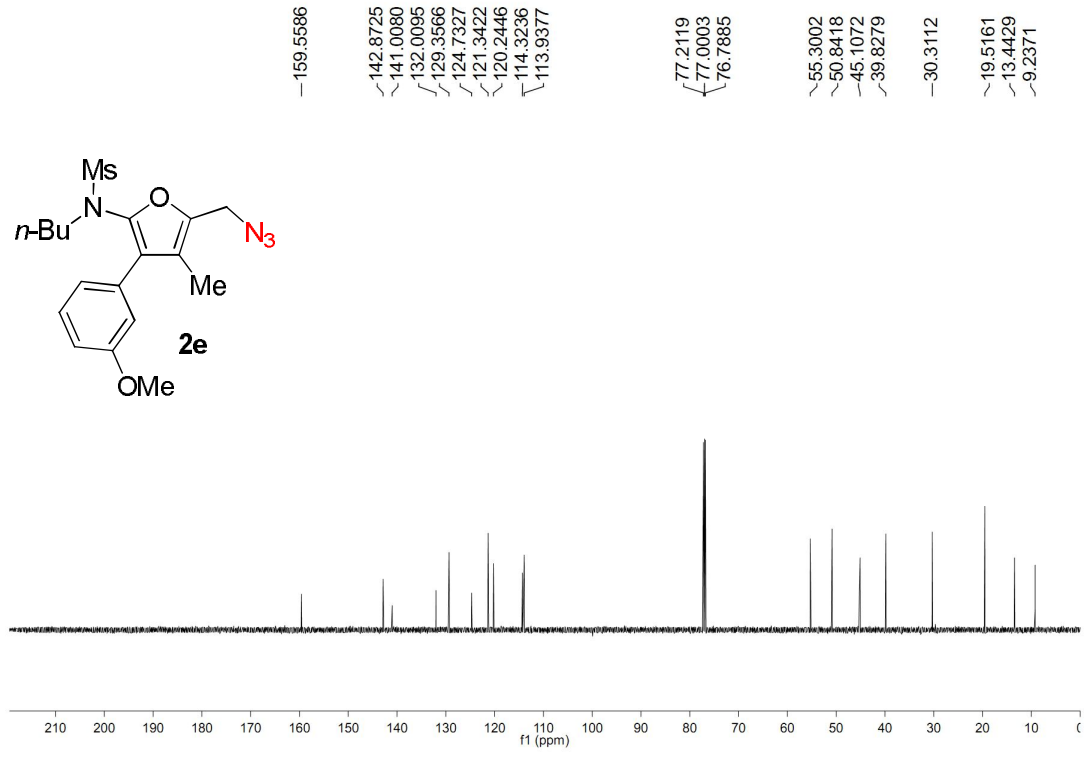
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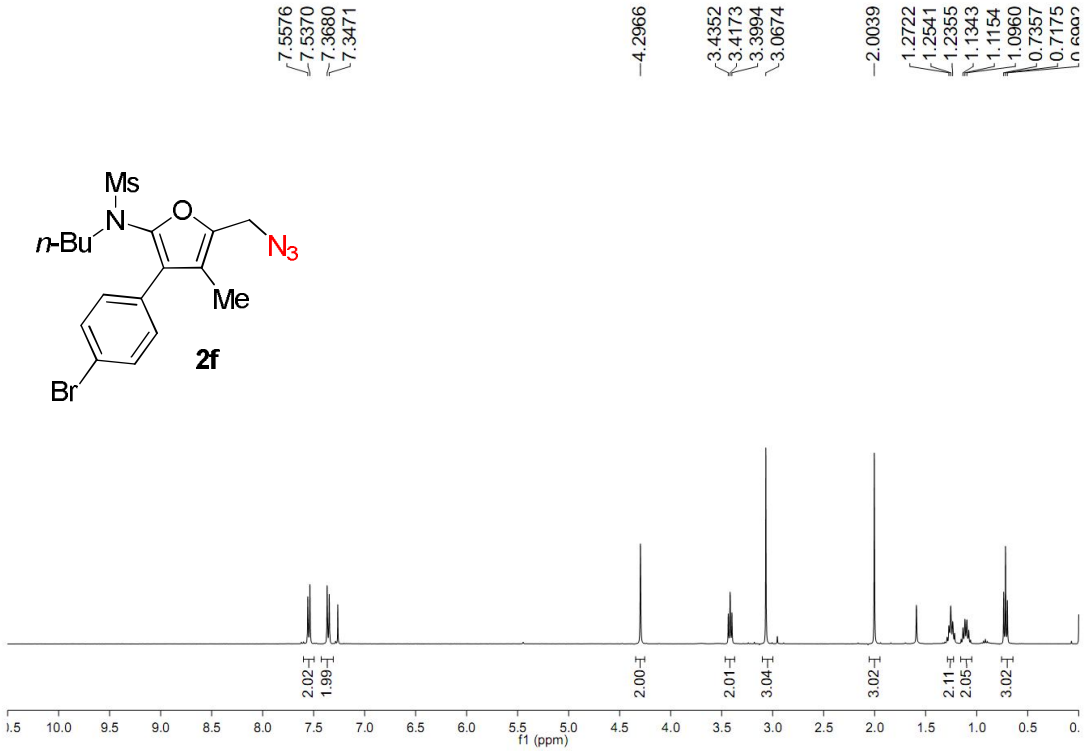
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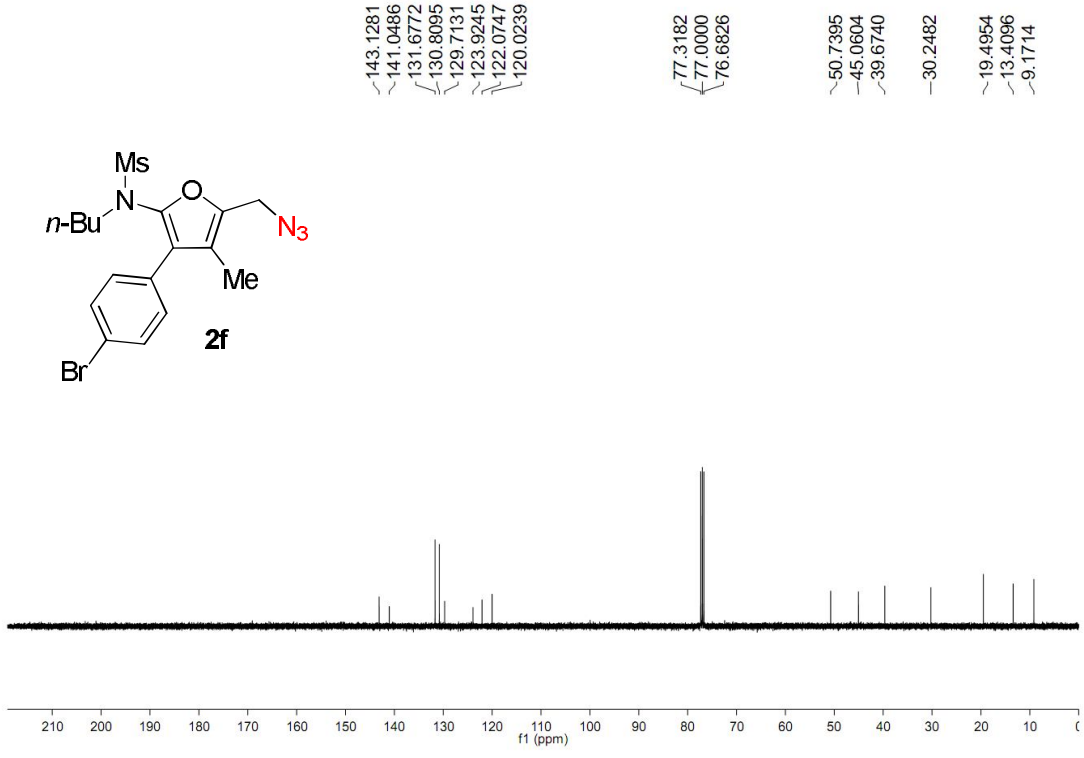
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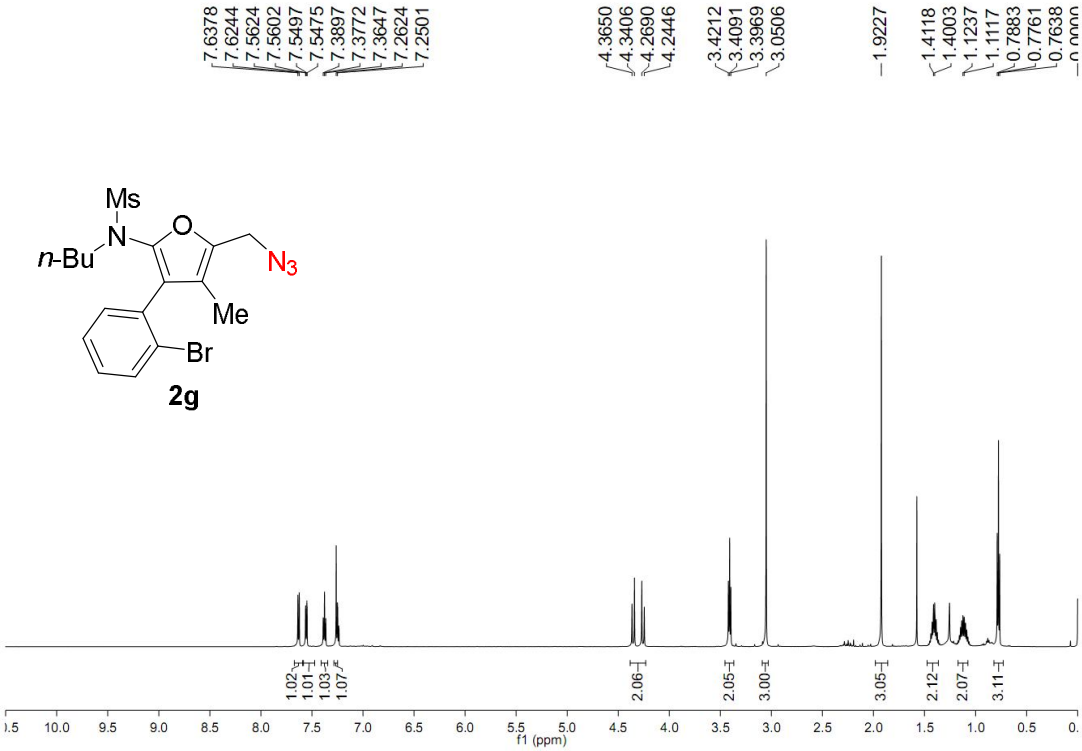
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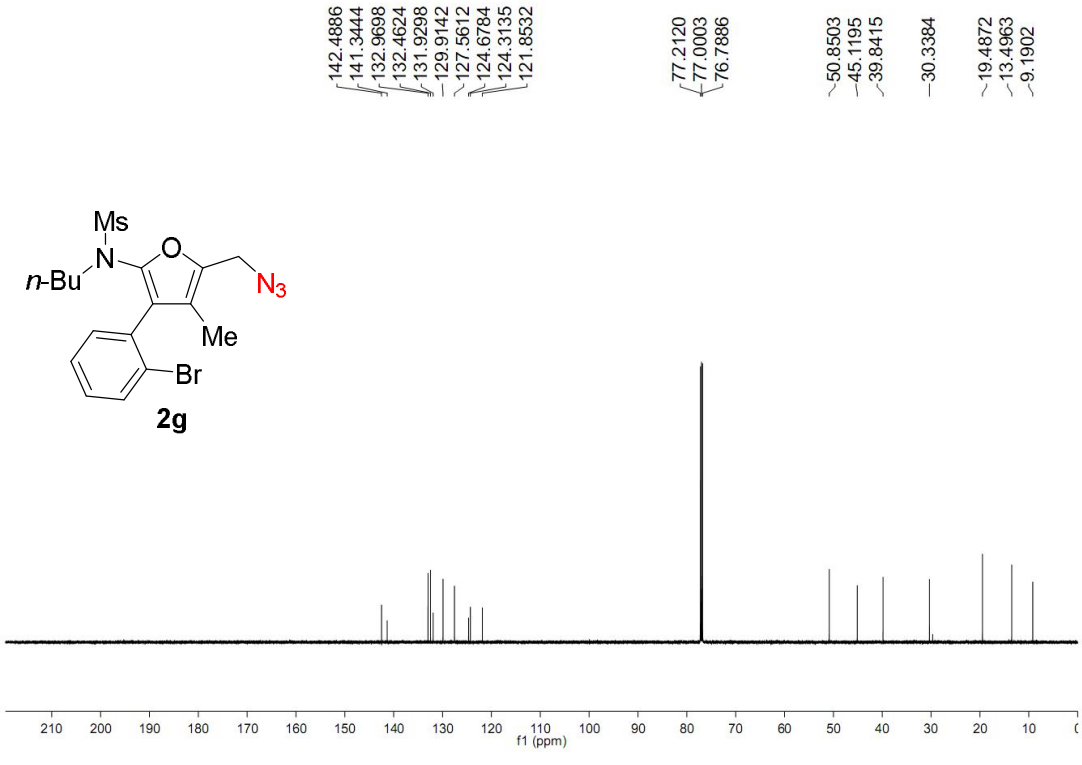
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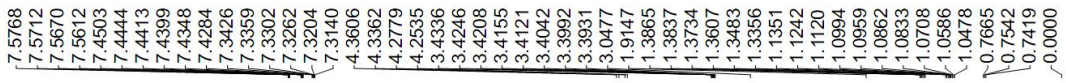
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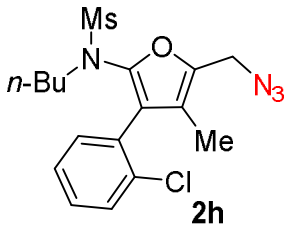
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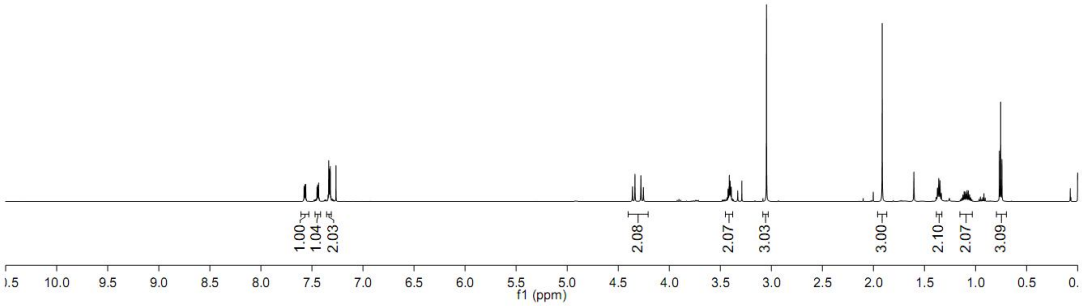
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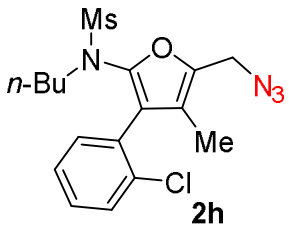
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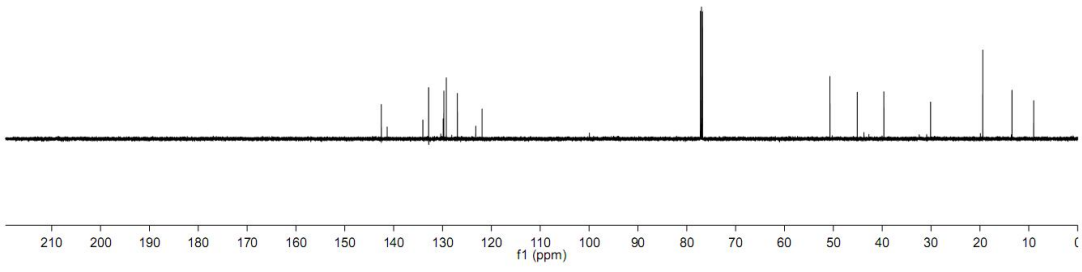
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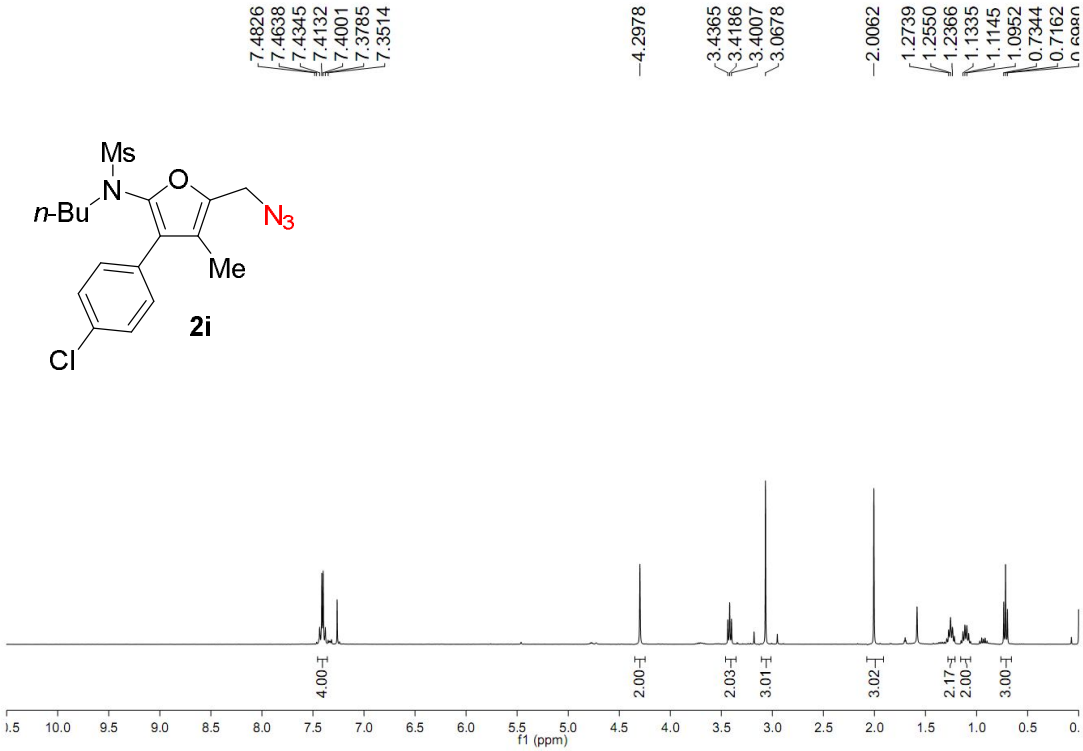
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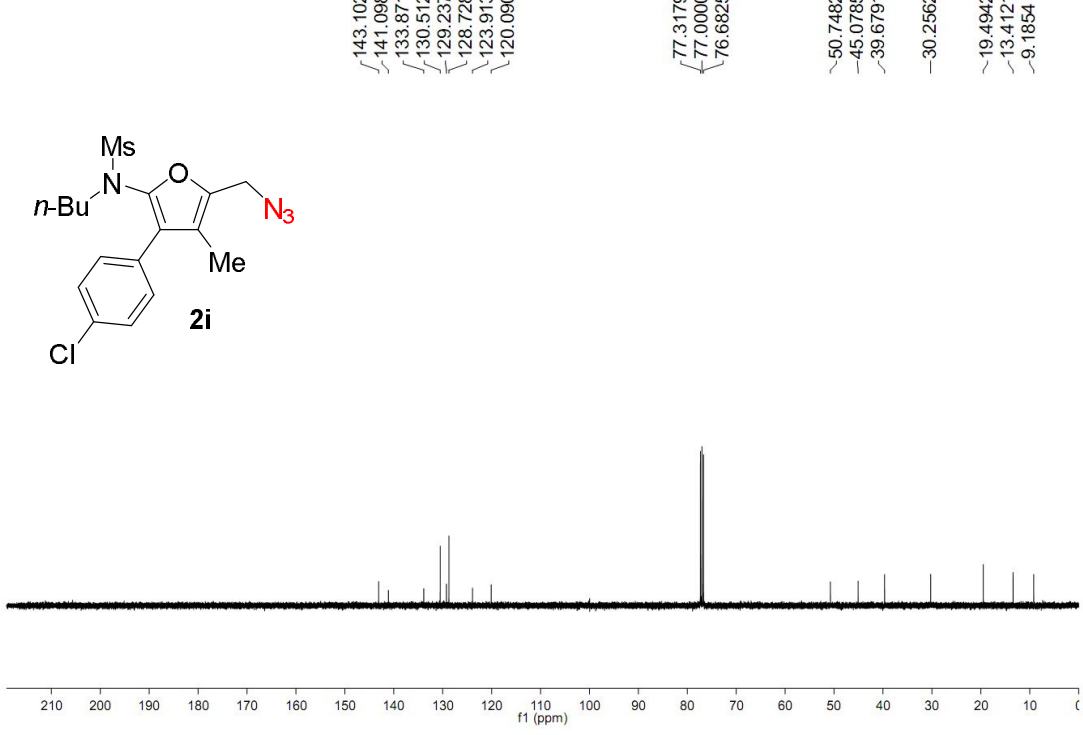
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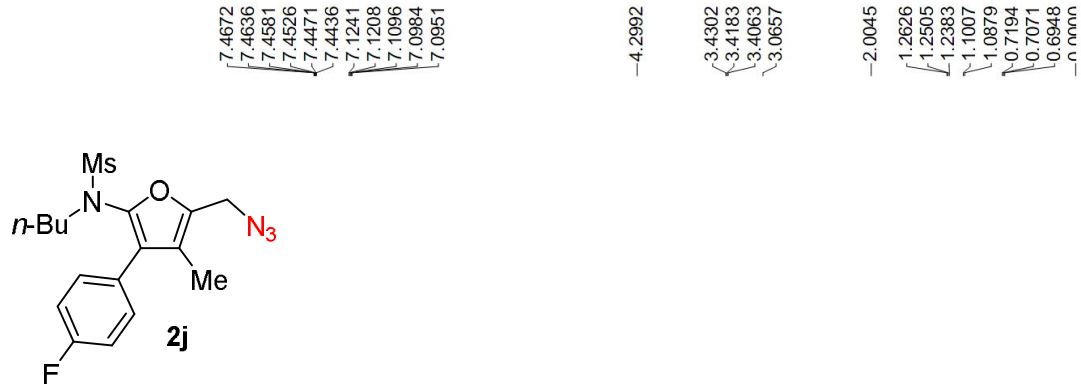
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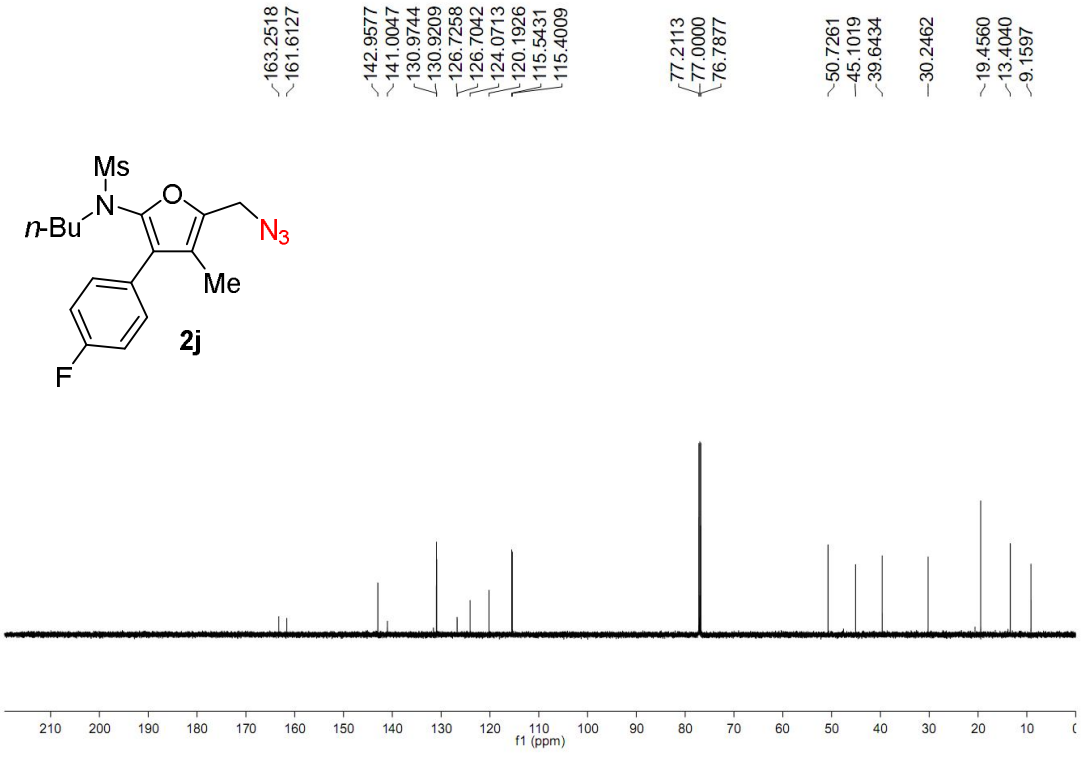
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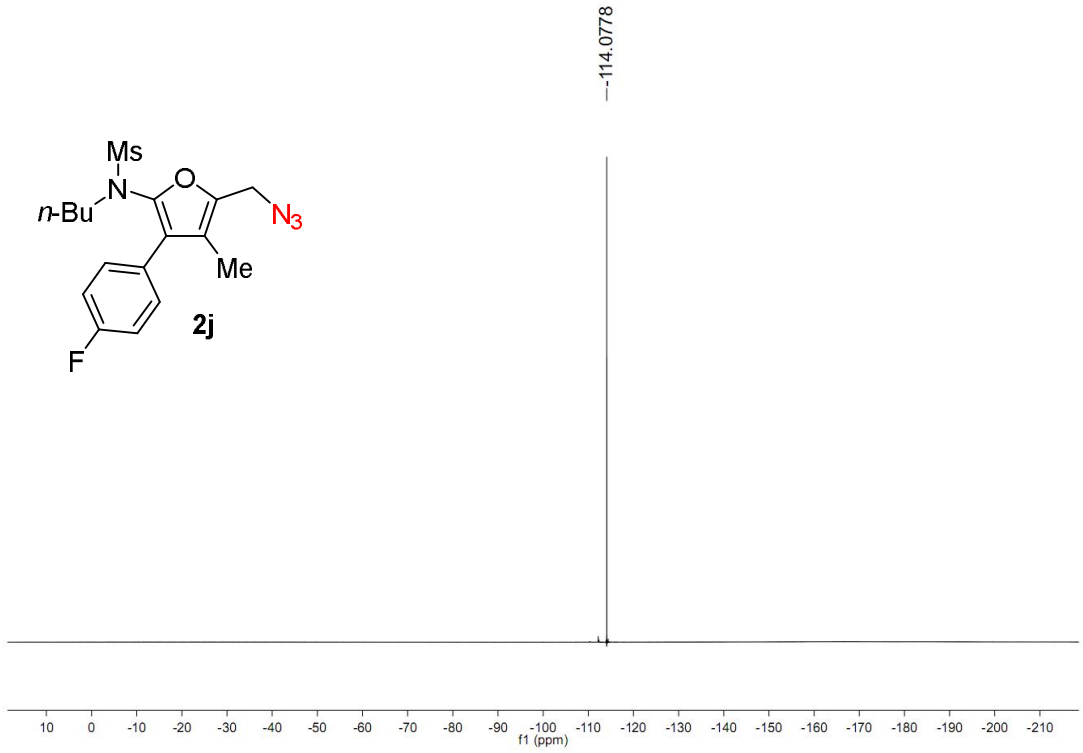
2j
f1 (ppm)


-114.0778
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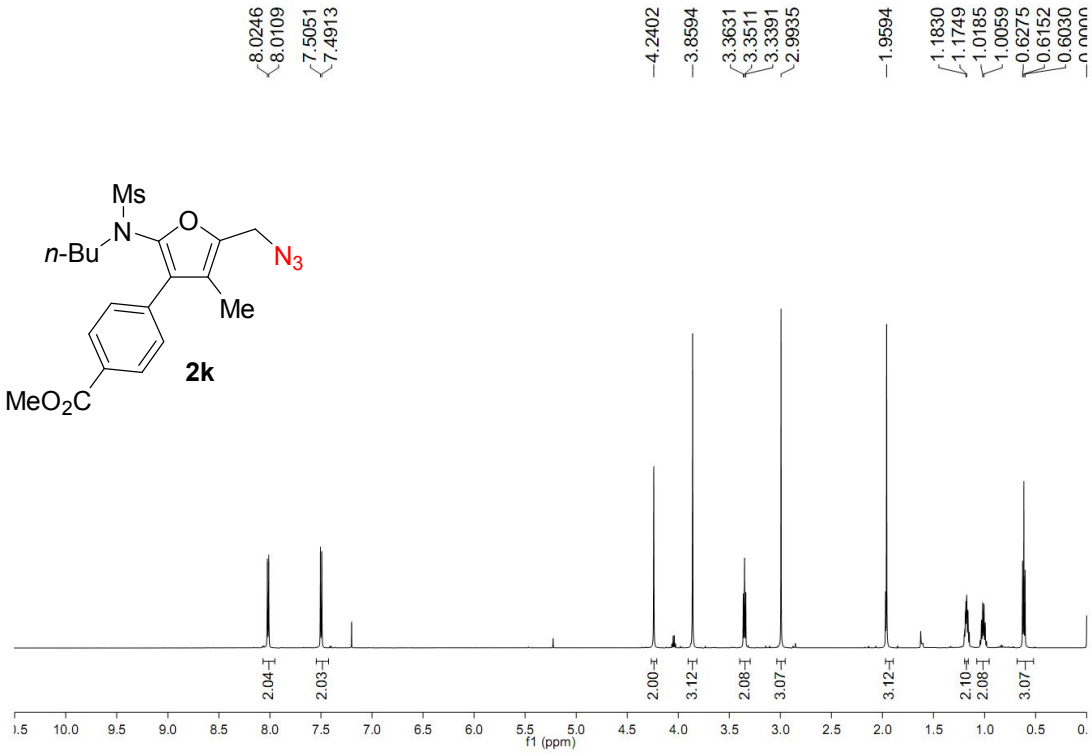
N
O
n-Bu
N3
Me
F
2j
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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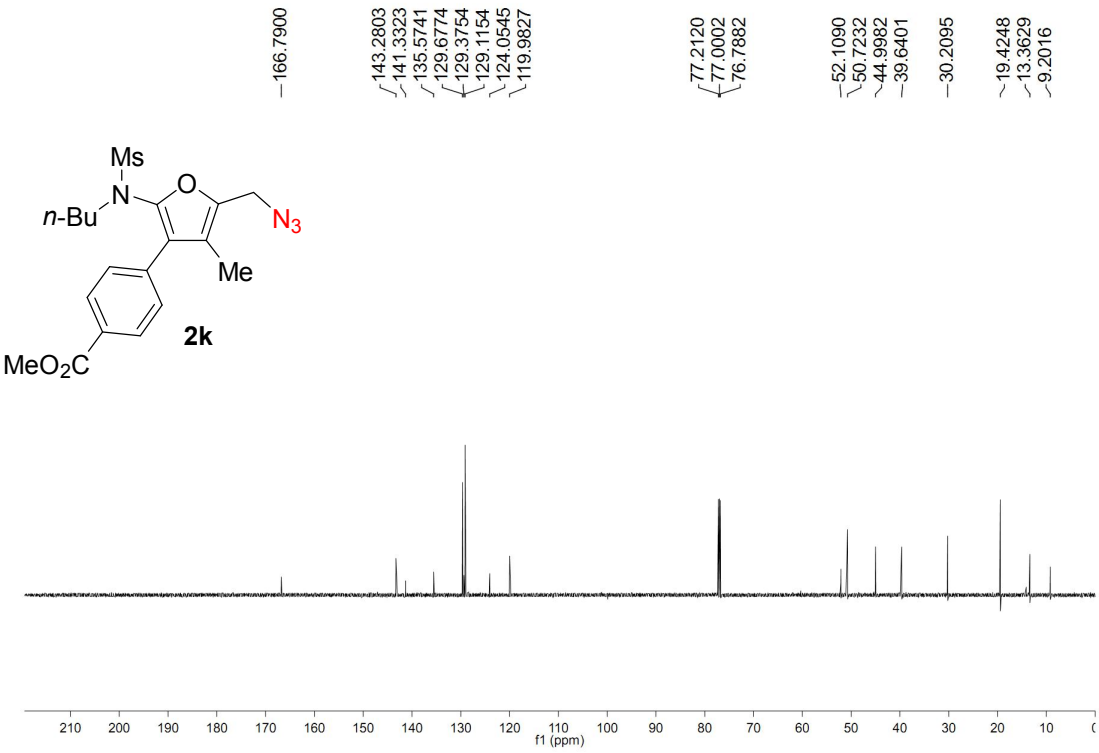
7.5051
7.4913
4.2402
3.8594
3.3631
3.3511
3.3391
2.9935
1.9594
1.1830
1.1749
1.0185
1.0059
0.6275
0.6152
0.6030
Ms
N
O
n-Bu
N3
Me
2k
MeO2C
2.04
2.03
2.00
3.12
2.08
3.07
3.12
2.10
2.08
3.07
f1 (ppm)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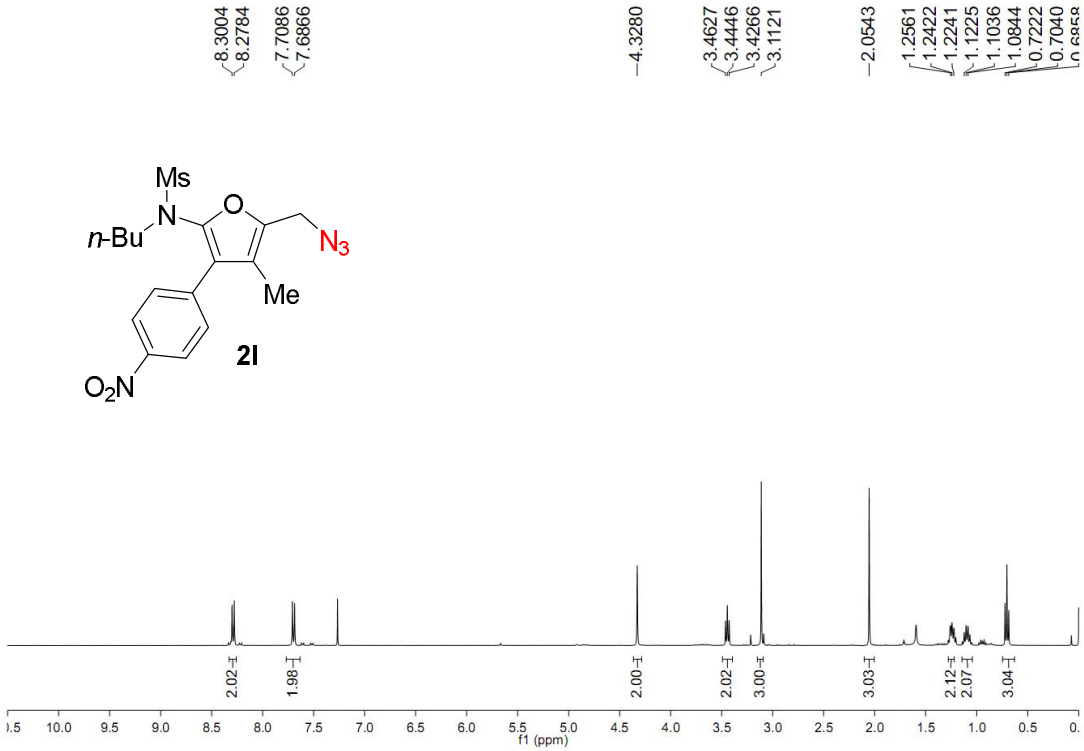
141.3323
135.5741
129.6774
129.3754
129.1154
124.0545
119.9827
77.2120
77.0002
76.7882
52.1090
50.7232
44.9982
39.6401
30.2095
19.4248
13.3629
9.2016
Ms
N
O
n-Bu
N3
Me
2k
MeO2C
f1 (ppm)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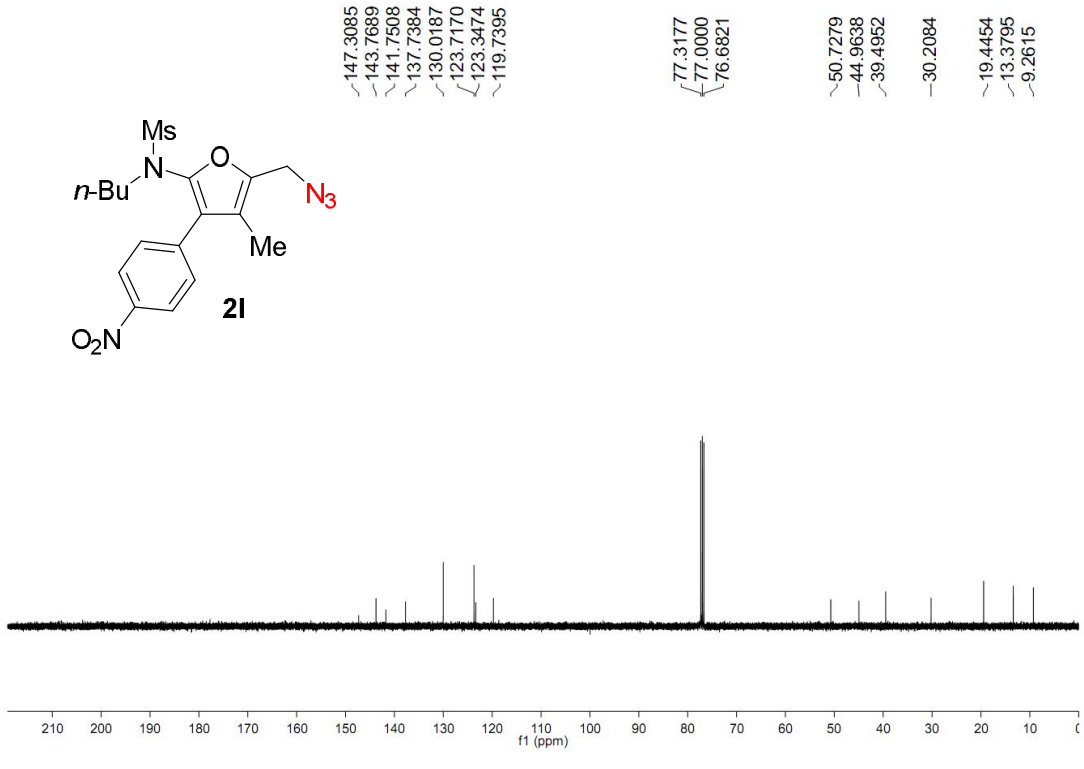
8.2784
7.7086
7.6866
4.3280
3.4627
3.4446
3.4266
3.1121
2.0543
1.2561
1.2422
1.2241
1.1225
1.1036
1.0844
0.7222
0.7040
Ms
N
O
n-Bu
N3
Me
O2N
2l
2.02
1.98
2.00
2.02
3.00
3.03
2.12
2.07
3.04
f1 (ppm)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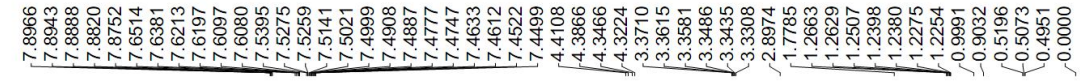
137.7384
130.0187
123.7170
123.3474
119.7395
77.3177
77.0000
76.6821
50.7279
44.9638
39.4952
30.2084
19.4454
13.3795
9.2615
Ms
N
O
n-Bu
N3
Me
O2N
2l
f1 (ppm)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7.8943
7.8888
7.8820
7.8752
7.6514
7.6381
7.6213
7.6197
7.6097
7.6080
7.5395
7.5275
7.5259
7.5141
7.5021
7.4999
7.4908
7.4887
7.4777
7.4747
7.4633
7.4612
7.4522
7.4499
4.4108
4.3866
4.3466
4.3224
3.3710
3.3615
3.3581
3.3486
3.3435
3.3308
2.8974
1.7785
1.2663
1.2629
1.2507
1.2398
1.2380
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1.2254
0.9991
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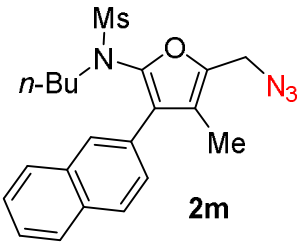
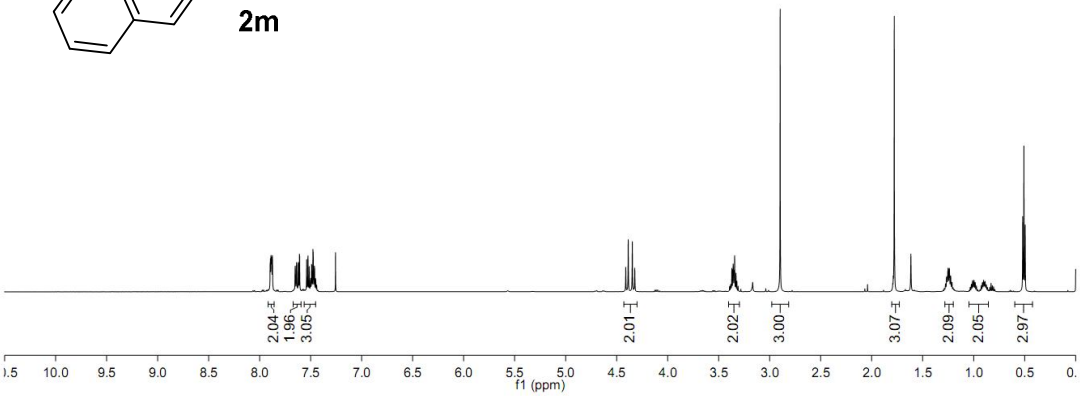
0.5196
0.5073
0.4951
0.0000


Ms
N
O
n-Bu
N3
Me

2m


2.04
1.96
3.05
2.01
2.02
3.00
3.07
2.09
2.05
2.97
f1 (ppm)


142.5413
141.8928
133.4837
132.0662
128.6785
128.6332
128.4281
128.0666
126.2714
125.8498
125.5074
125.3254
123.3708
122.2093
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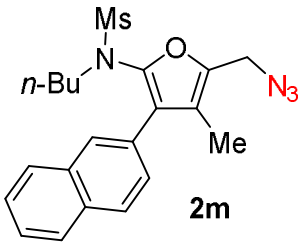
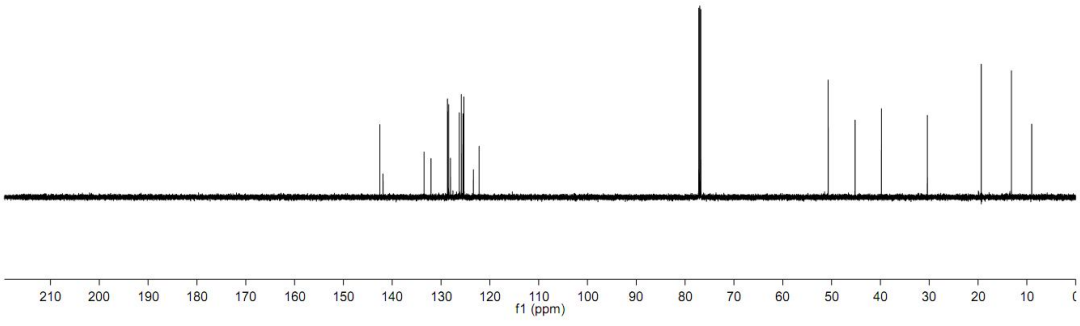
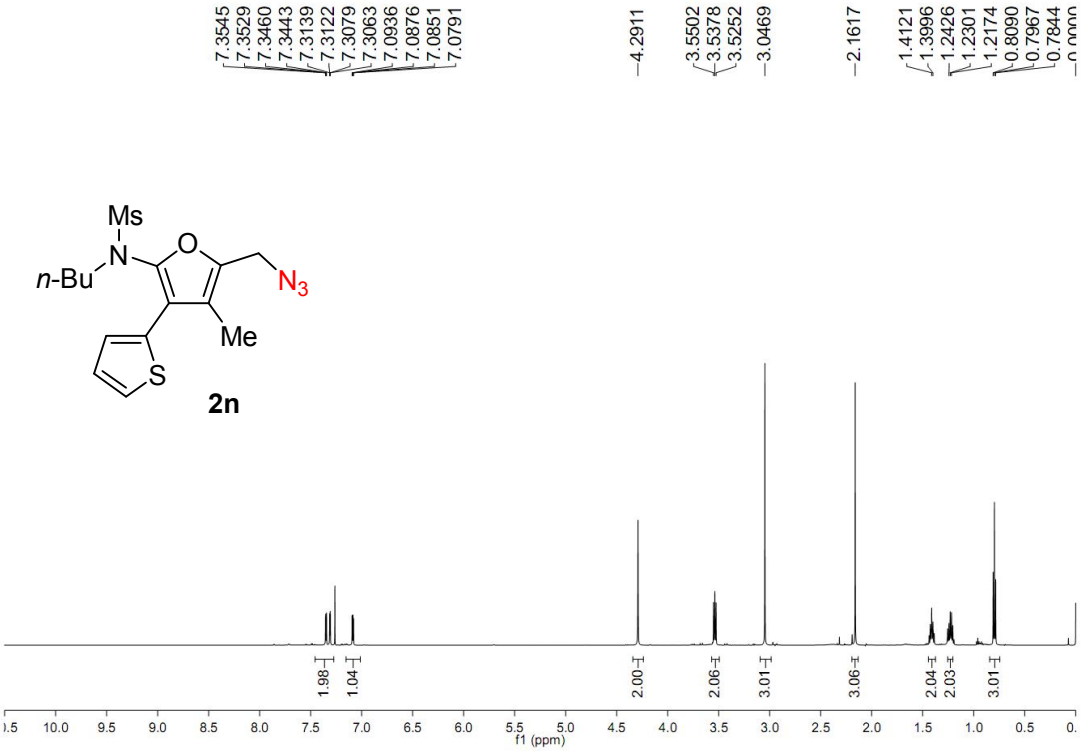
50.7082
45.1906
39.7958
30.3852
19.3442
13.1620
9.0061


Ms
N
O
n-Bu
N3
Me

2m


f1 (ppm)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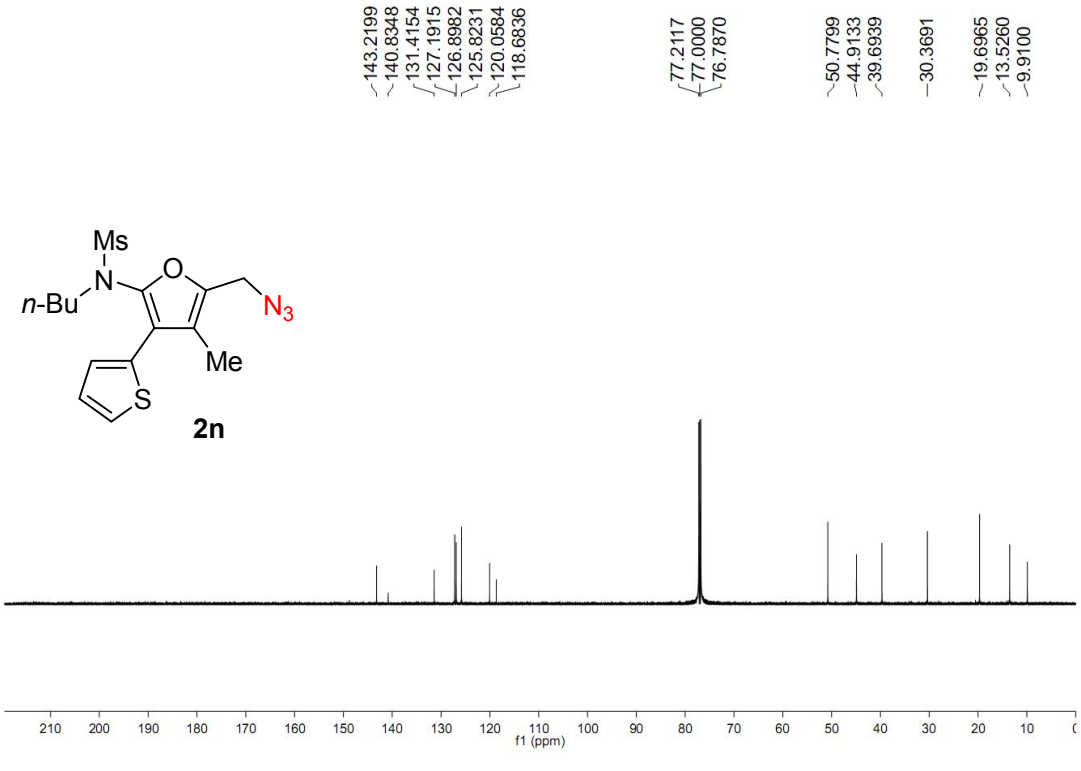
7.3529
7.3460
7.3443
7.3139
7.3122
7.3079
7.3063
7.0936
7.0876
7.0851
7.0791
4.2911
3.5502
3.5378
3.5252
3.0469
2.1617
1.4121
1.3996
1.2426
1.2301
1.2174
0.8090
0.7967
0.7844
Ms
N
O
n-Bu
N3
Me
S
2n
1.98
1.04
2.00
2.06
3.01
3.06
2.04
2.03
3.01
f1 (ppm)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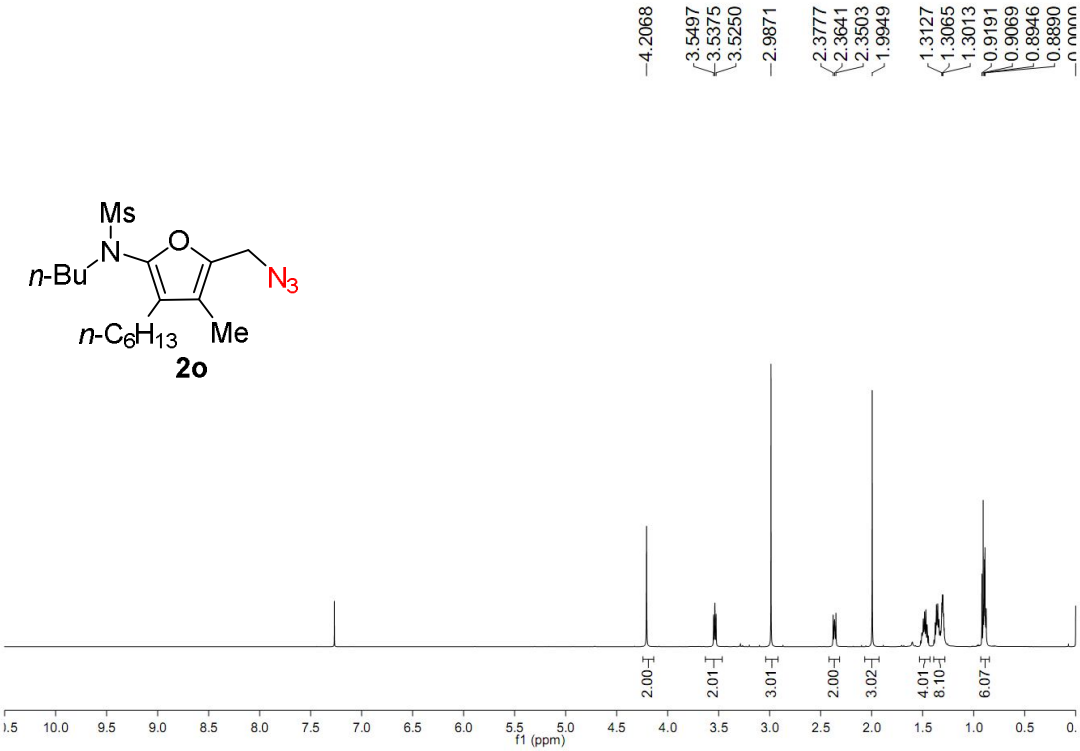
140.8348
131.4154
127.1915
126.8982
125.8231
120.0584
118.6836
77.2117
77.0000
76.7870
50.7799
44.9133
39.6939
30.3691
19.6965
13.5260
9.9100
Ms
N
O
n-Bu
N3
Me
S
2n
f1 (ppm)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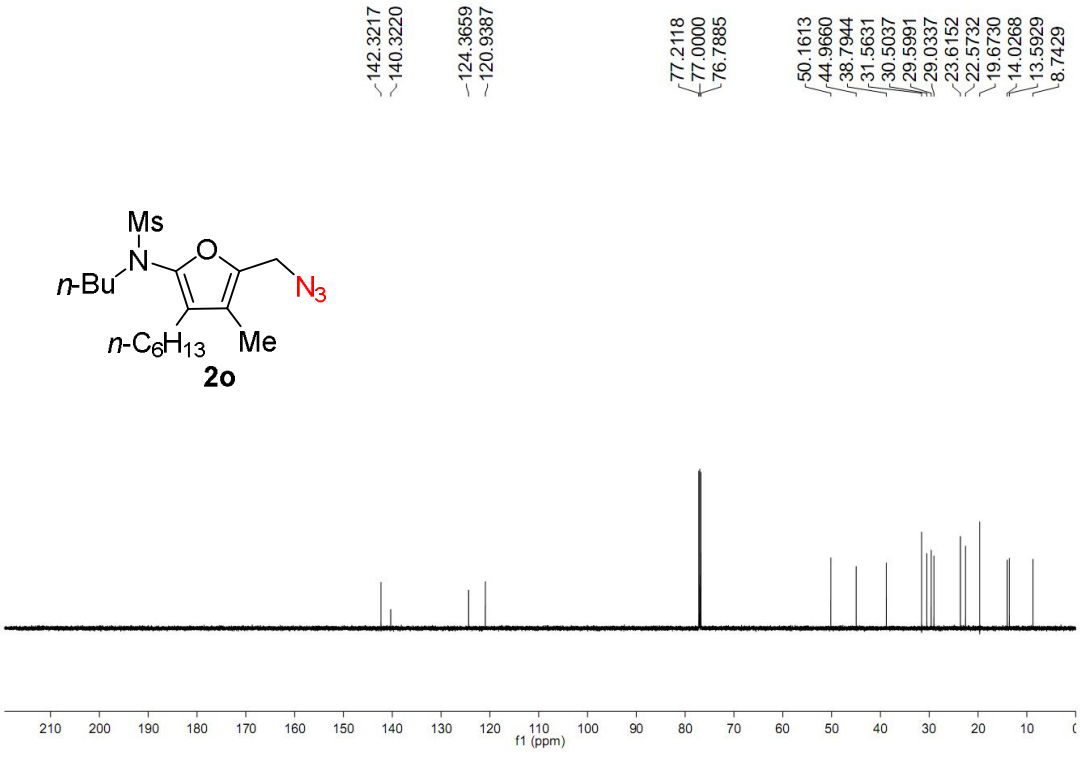
3.5497
3.5375
3.5250
2.9871
2.3777
2.3641
2.3503
1.9949
1.3127
1.3065
1.3013
0.9191
0.9069
0.8946
0.8890
Ms
N
O
n-Bu
N3
n-C6H13
Me
2o
2.00
2.01
3.01
2.00
3.02
4.01
8.10
6.07
f1 (ppm)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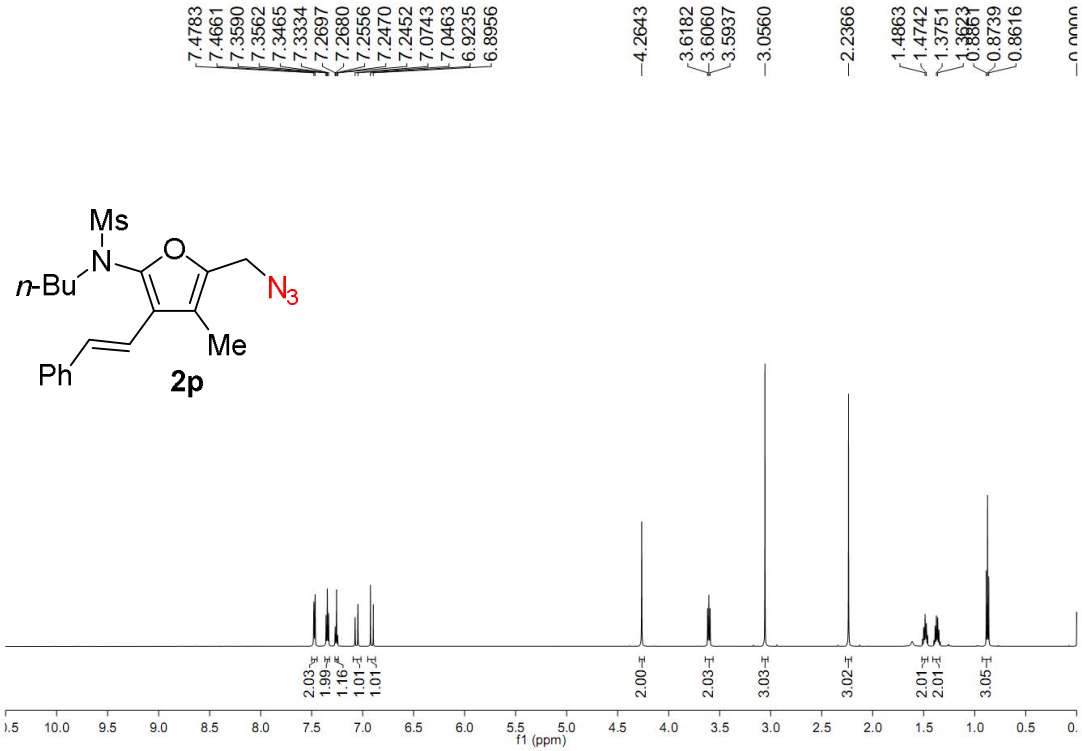
140.3220
124.3659
120.9387
77.2118
77.0000
76.7885
50.1613
44.9660
38.7944
31.5631
30.5037
29.5991
29.0337
23.6152
22.5732
19.6730
14.0268
13.5929
8.7429
Ms
N
O
n-Bu
N3
n-C6H13
Me
2o
f1 (ppm)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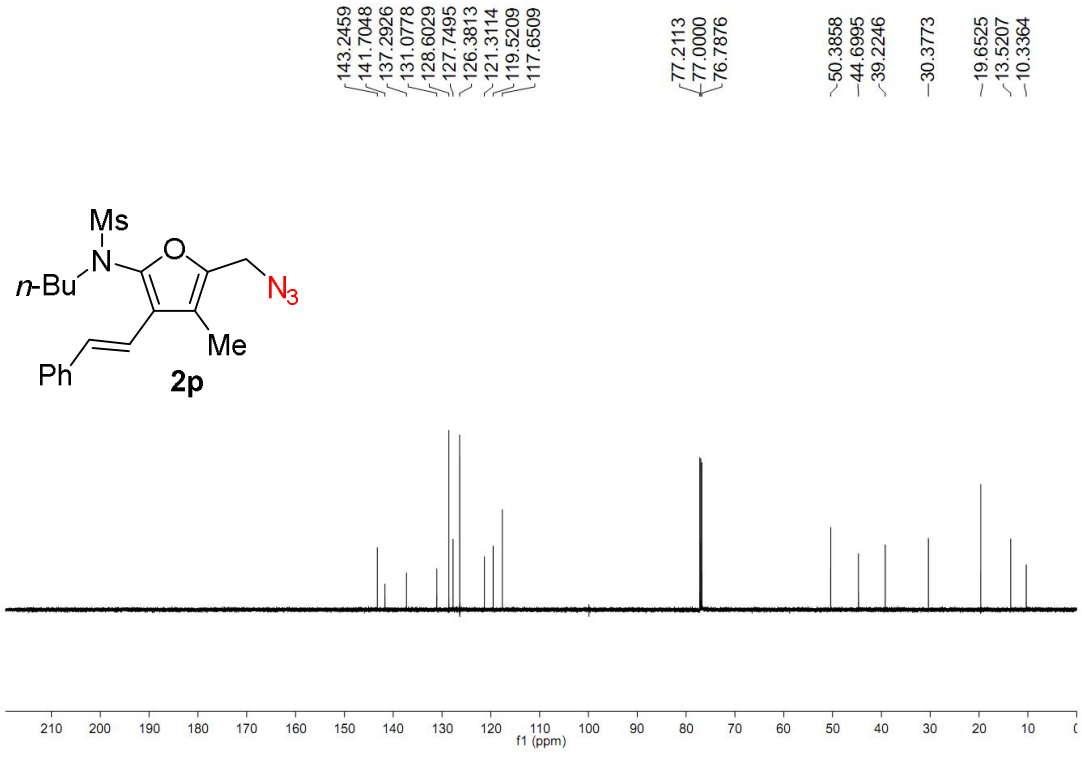
7.3590
7.3562
7.3465
7.3334
7.2697
7.2680
7.2556
7.2470
7.2452
7.0743
7.0463
6.9235
6.8956
4.2643
3.6182
3.6060
3.5937
3.0560
2.2366
1.4863
1.4742
1.3751
1.3623
0.8861
0.8739
0.8616
0.0000
Ms
N
O
n-Bu
N3
Me
Ph
2p
2.03
1.99
1.16
1.01
1.01
2.00
2.03
3.03
3.02
2.01
2.01
3.05
f1 (ppm)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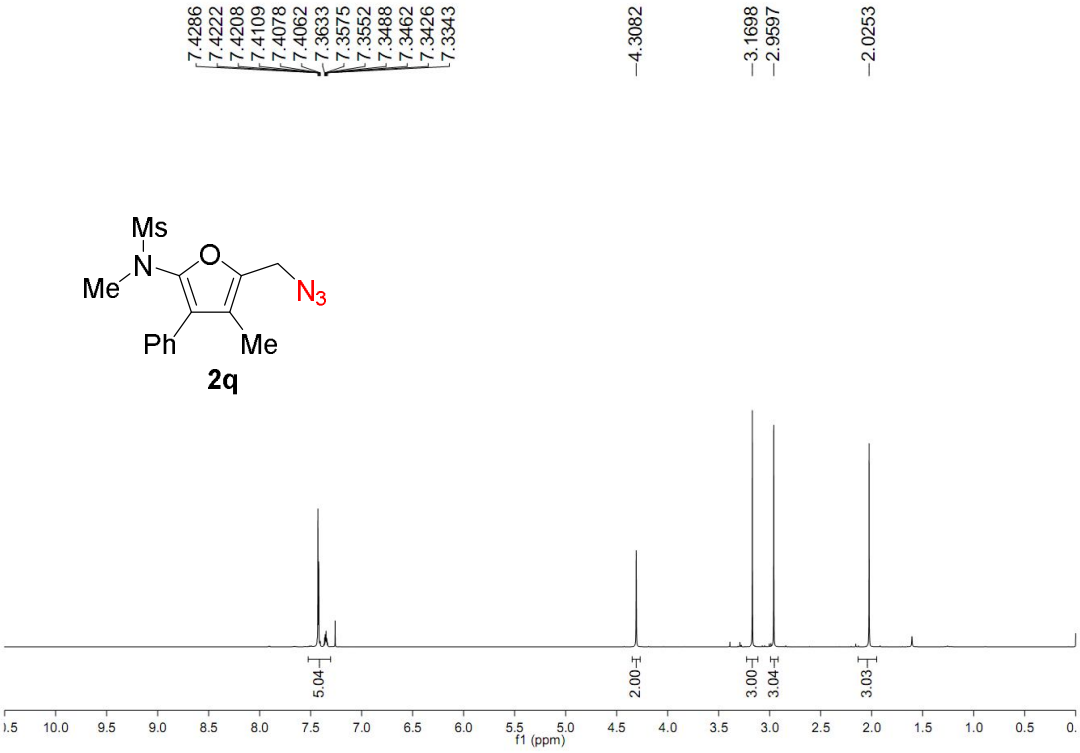
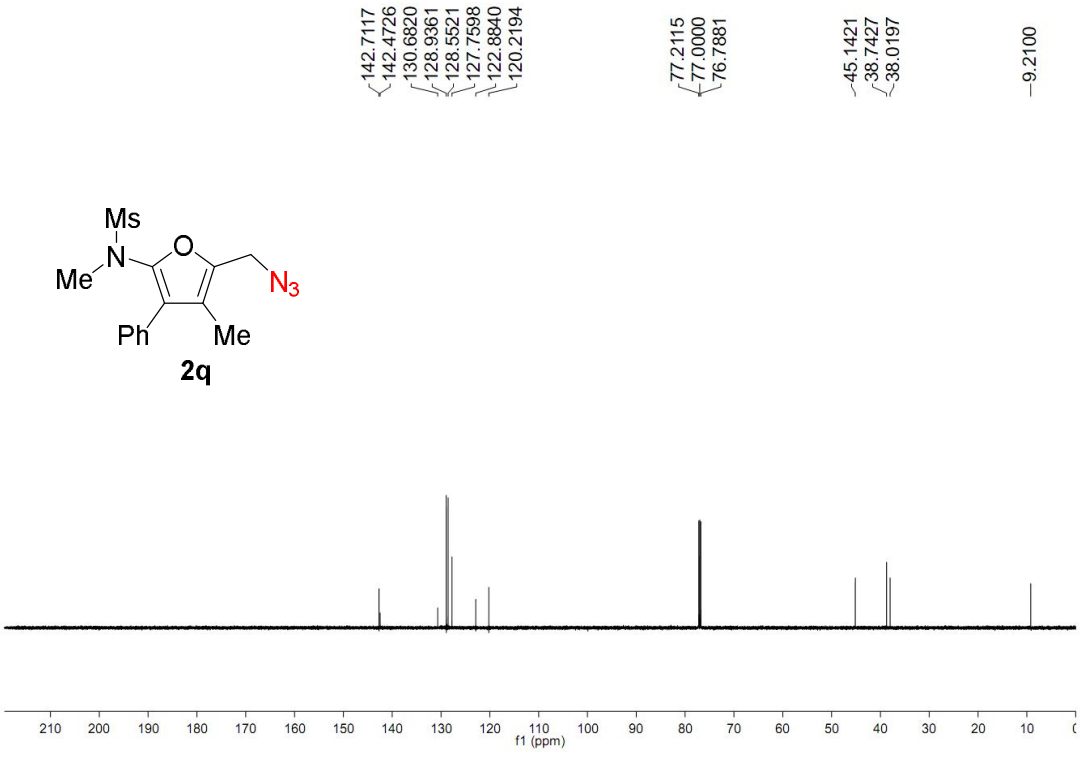
137.2926
131.0778
128.6029
127.7495
126.3813
121.3114
119.5209
117.6509
77.2113
77.0000
76.7876
50.3858
44.6995
39.2246
30.3773
19.6525
13.5207
10.3364
Ms
N
O
n-Bu
N3
Me
Ph
2p
f1 (ppm)


7.4286
7.4222
7.4208
7.4109
7.4078
7.4062
7.3633
7.3575
7.3552
7.3488
7.3462
7.3426
7.3343
4.3082
3.1698
2.9597
2.0253
Ms
N
Me
O
N3
Ph
Me
2q
5.04
2.00
3.00
3.04
3.03
f1 (ppm)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130.6820
128.9361
128.5521
127.7598
122.8840
120.2194
77.2115
77.0000
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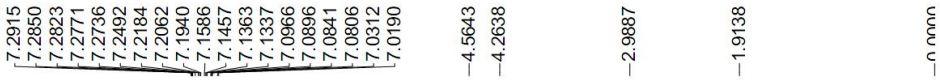
45.1421
38.7427
38.0197
9.2100
Ms
N
Me
O
N3
Ph
Me
2q
f1 (ppm)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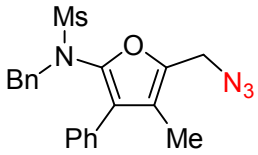
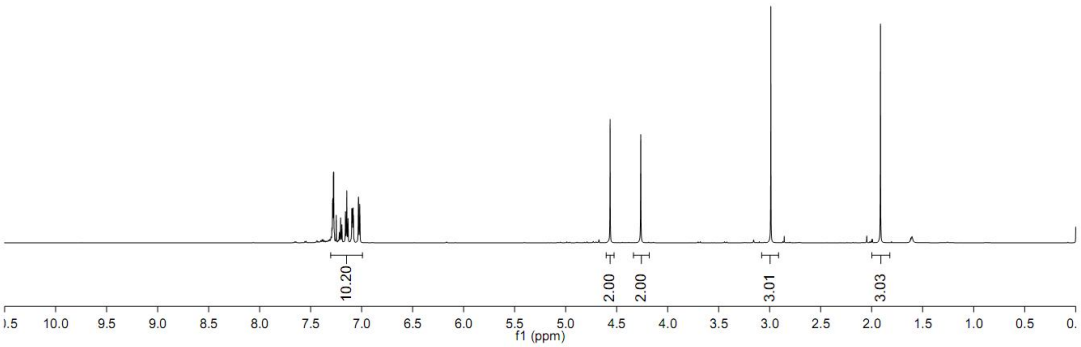
7.2771
7.2736
7.2492
7.2184
7.2062
7.1940
7.1586
7.1457
7.1363
7.1337
7.0966
7.0896
7.0841
7.0806
7.0312
7.0190
4.5643
4.2638
2.9887
1.9138


Ms
N
Bn
O
N3
Ph
Me

2r


10.20
2.00
2.00
3.01
3.03
f1 (ppm)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130.4084
129.0229
128.9871
128.3466
128.1665
128.0755
127.5067
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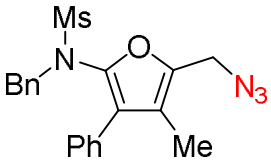
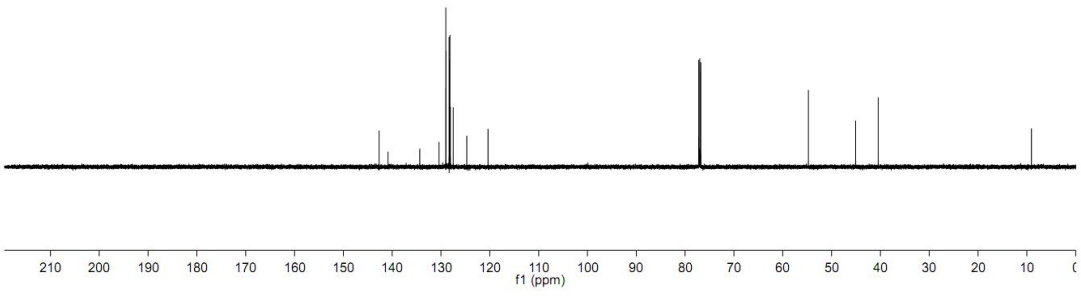
120.3662
77.2119
77.0000
76.7885
54.7527
45.0674
40.4485
9.0646


Ms
N
Bn
O
N3
Ph
Me

2r


f1 (ppm)


7.5023
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7.4885
7.4099
7.3976
7.3846
7.3383
7.3259
7.3154
7.3136
4.2898
3.7472
3.7411
3.7350
3.7211
3.7150
3.7074
3.7012
3.6951
3.0907
2.0158
1.7390
1.7341
1.7289
1.6648
1.6384
1.6187
1.4993
1.4777
1.2570
1.2529
1.2278
1.2223
1.2058
1.1837
1.1671
1.1616
0.9694
0.9582
0.9308
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0.8998
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0.8838
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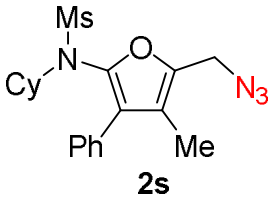
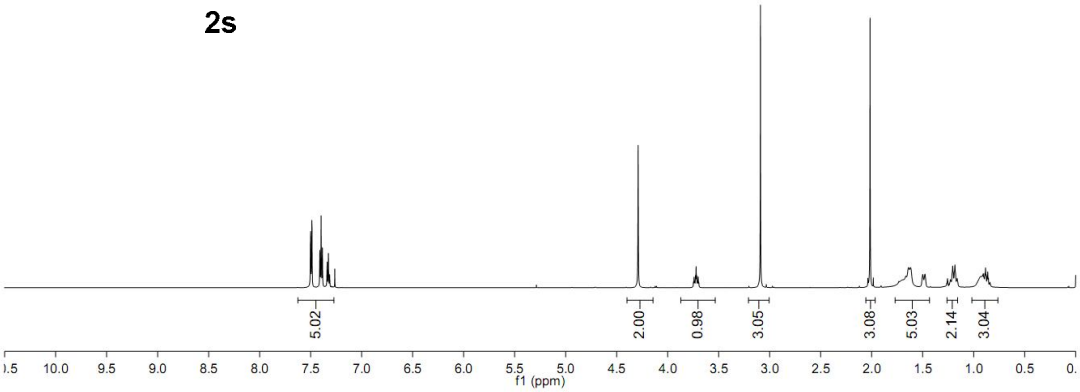
0.8680
0.8621
0.8560
0.8402


Ms
N
Cy
O
N3
Ph
Me

2s


5.02
2.00
0.98
3.05
3.08
5.03
2.14
3.04
f1 (ppm)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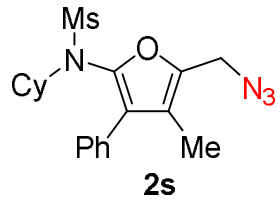
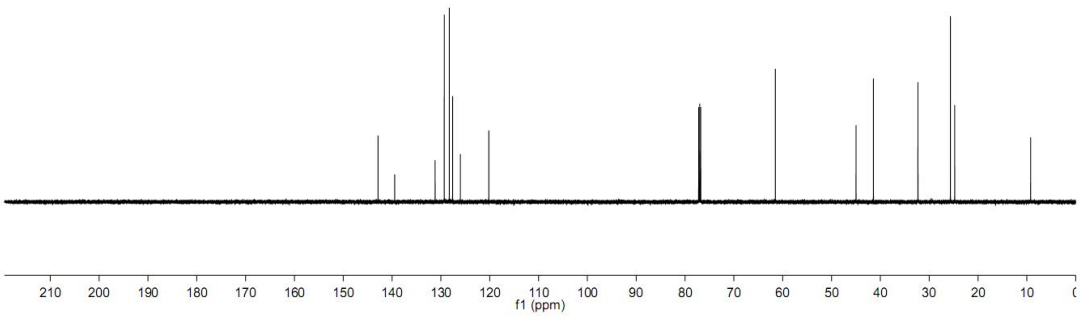
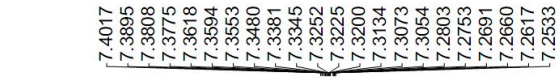
131.1918
129.3132
128.2852
127.6002
126.0201
120.1841
77.2117
77.0000
76.7878
61.5048
44.9842
41.4264
32.3071
25.6584
24.7789
9.2214


Ms
N
Cy
O
N3
Ph
Me

2s


f1 (ppm)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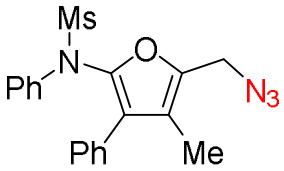
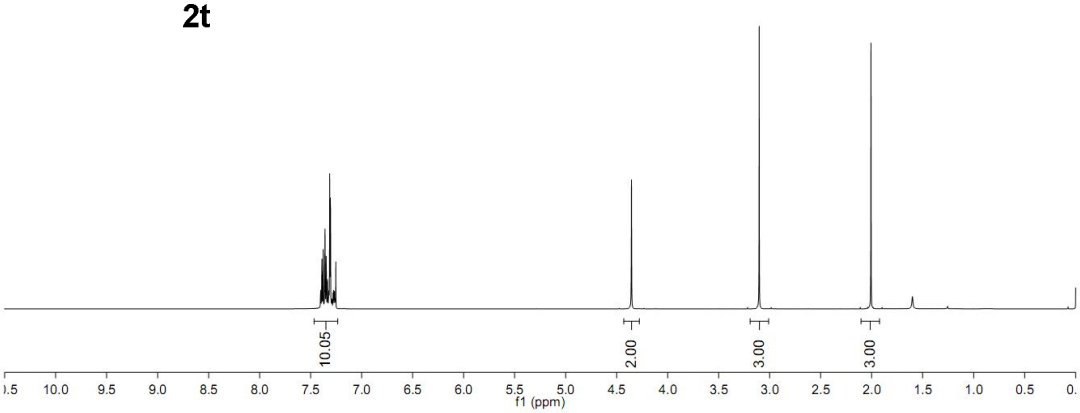
7.3808
7.3775
7.3618
7.3594
7.3553
7.3480
7.3381
7.3345
7.3252
7.3225
7.3200
7.3134
7.3073
7.3054
7.2803
7.2753
7.2691
7.2660
7.2617
7.2533
4.3549
3.1026
2.0066


Ms
N
Ph
O
N3
Ph
Me

2t


10.05
2.00
3.00
3.00
f1 (ppm)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139.7831
130.5230
129.4277
129.0818
128.3992
127.9986
127.7761
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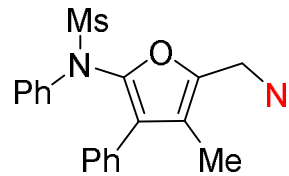
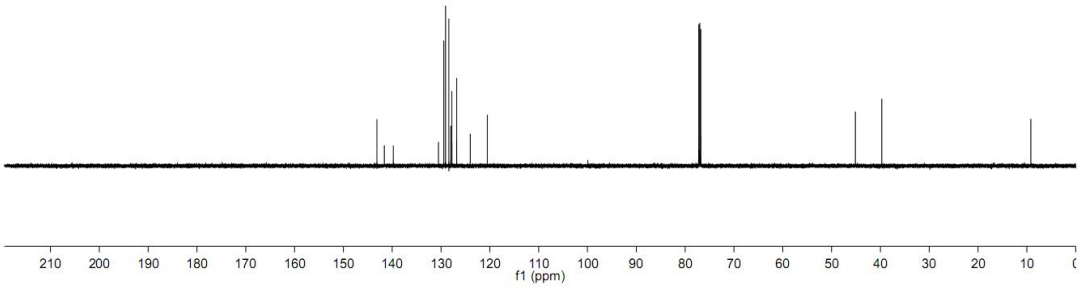
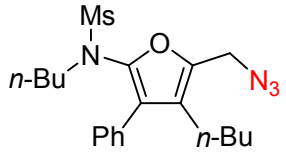
124.0206
120.5237
77.2119
77.0000
76.7885
45.1247
39.7217
9.1876


Ms
N
Ph
O
N3
Ph
Me

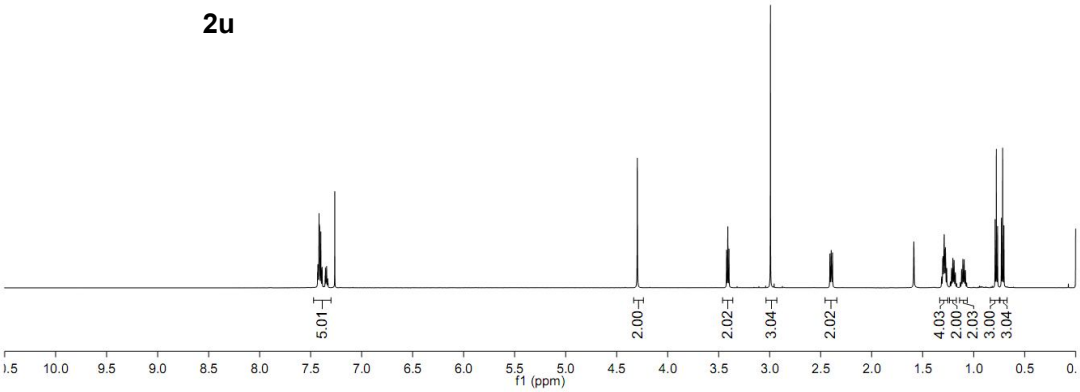
2t


f1 (ppm)

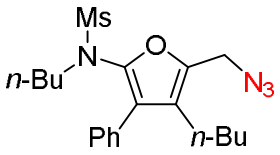

7.4318
7.4289
7.4253
7.4178
7.4152
7.4125
7.4084
7.4002
7.3974
7.3898
7.3872
7.3580
7.3551
7.3519
7.3475
7.3435
7.3392
7.3346
7.3319
4.2974
3.4225
3.4106
3.3986
2.9924
2.4097
2.3970
2.3838
1.3136
1.3032
1.3008
1.2892
1.2851
1.2773
1.2643
1.2287
1.2167
1.2042
1.1917
1.1797
1.1311
1.1188
1.1063
1.0935
1.0811
0.7899
0.7777
0.7656
0.7282
0.7160
0.7037


Ms
N
O
n-Bu
N3
Ph
n-Bu

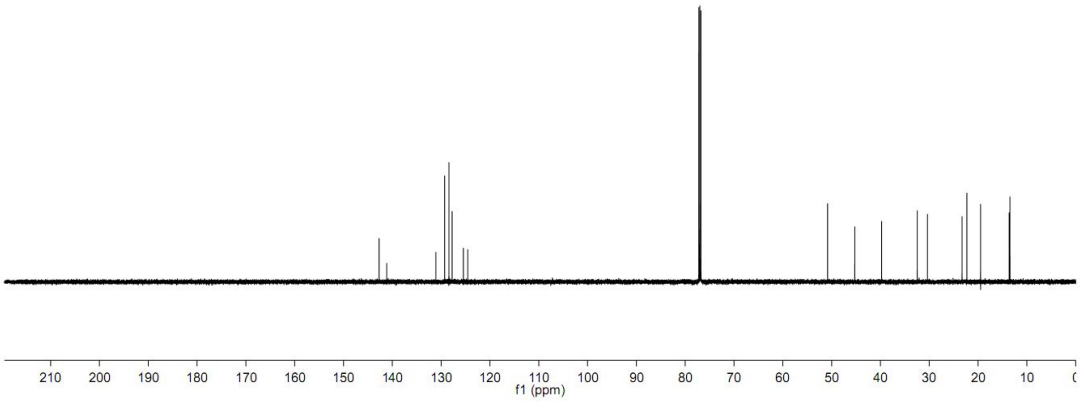
2u


5.01
2.00
2.02
3.04
2.02
4.03
2.00
2.03
3.00
3.04
f1 (ppm)


142.7119
141.1492
131.0743
129.2820
128.4076
127.7489
125.4498
124.5445
77.2112
77.0000
76.7879
50.8324
45.2467
39.7643
32.4626
30.3679
23.2767
22.2910
19.4925
13.6291
13.4639


Ms
N
O
n-Bu
N3
Ph
n-Bu

2u


f1 (ppm)


7.4127
7.4005
7.3986
7.3925
7.3886
7.3679
7.3562
7.3535
7.3406
7.3389
4.3662
3.3979
3.3859
3.3739
2.9401
2.3967
1.8014
1.7815
1.7261
1.7040
1.6456
1.6246
1.6060
1.3587
1.3536
1.3375
1.3325
1.3210
1.3162
1.3092
1.2966
1.2926
1.2846
1.2715
1.2546
1.1981
1.1929
1.1876
1.1765
1.1713
1.1663
1.1199
1.1163
1.1039
1.0912
1.0785
0.7485
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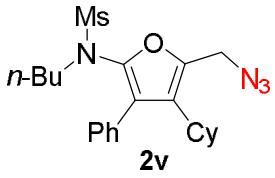
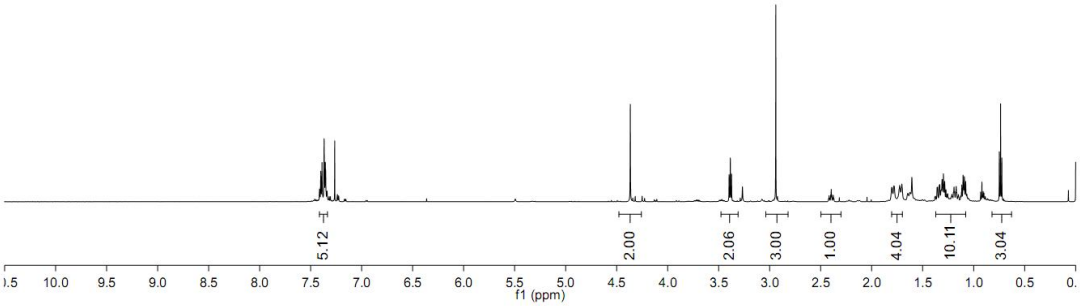
0.7239
0.0000


Ms
N
O
n-Bu
N3
Ph
Cy

2v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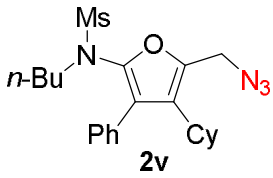
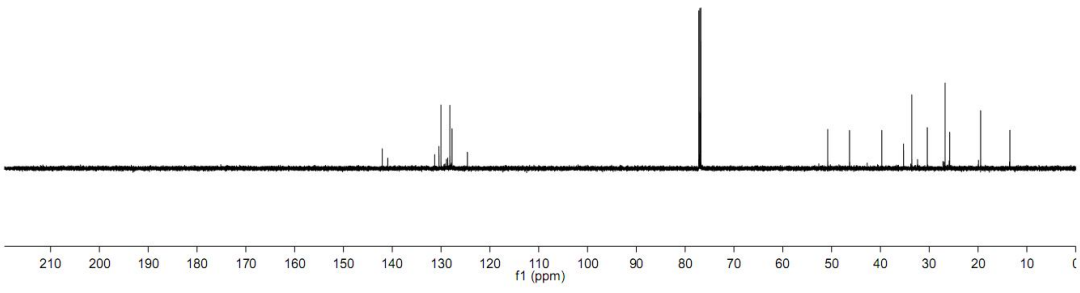
2.00
2.06
3.00
1.00
4.04
10.11
3.04
f1 (ppm)


142.0545
140.9258
131.3179
130.4385
130.0289
128.2089
127.7632
124.6095
77.2119
77.0000
76.7884
50.7965
46.3329
39.7180
35.2666
33.5735
30.3929
26.7577
25.8189
19.4715
13.4814


Ms
N
O
n-Bu
N3
Ph
Cy

2v


f1 (ppm)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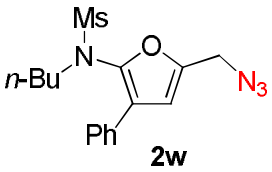
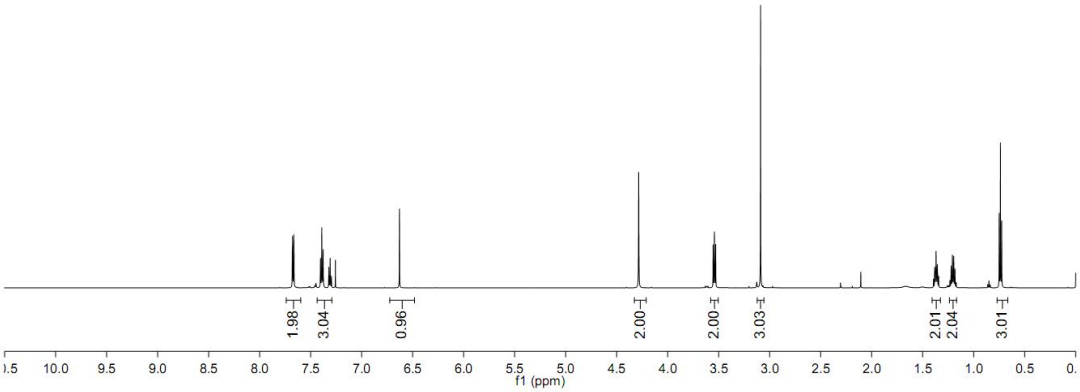
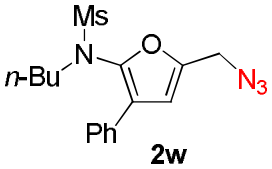
7.6775
7.6744
7.6656
7.6643
7.4035
7.4005
7.3910
7.3801
7.3779
7.3231
7.3212
7.3193
7.3115
7.3089
7.3061
7.2984
4.2840
3.5542
3.5419
3.5295
3.0893
1.3815
1.3689
1.3647
1.3565
1.3438
1.2209
1.2084
1.1957
0.7377
0.7254


Ms
N
O
n-Bu
N3
Ph

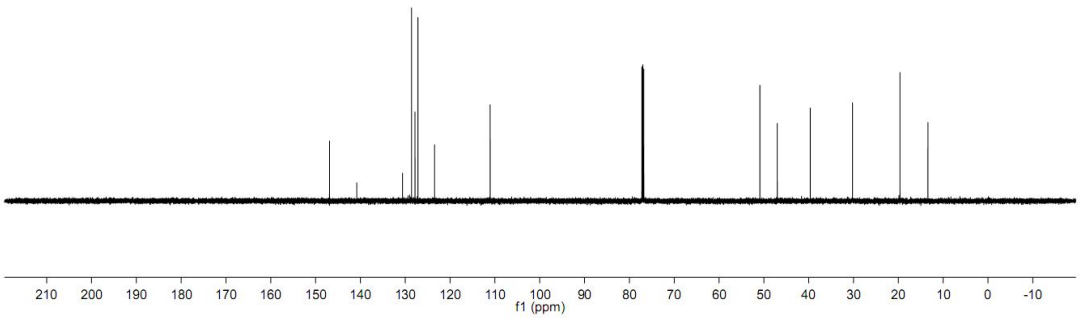
2w

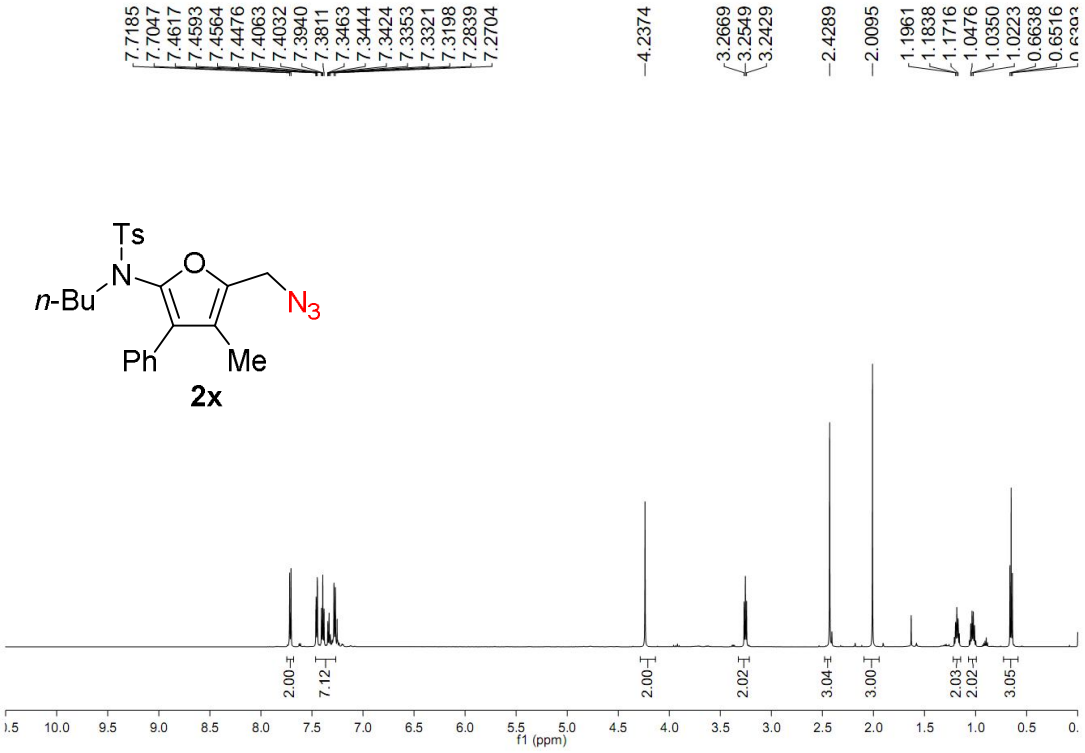

1.98
3.04
0.96
2.00
2.00
3.03
2.01
2.04
3.01
f1 (ppm)

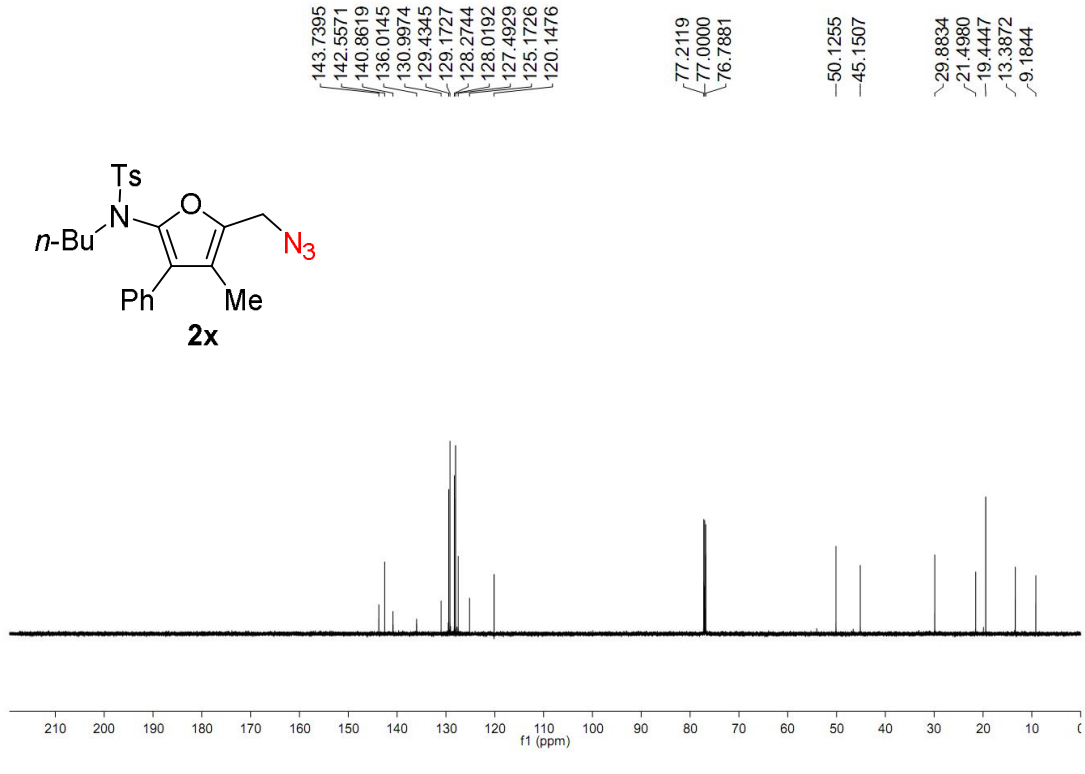

146.8943
140.8253
130.6212
128.6113
127.8373
127.1825
123.4589
111.0687
77.2119
77.0000
76.7885
50.8913
47.0105
39.6543
30.2250
19.6384
13.3964

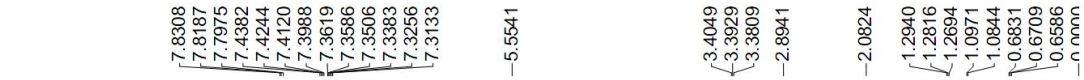

Ms
N
O
n-Bu
N3
Ph

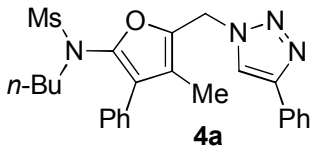
2w


f1 (ppm)

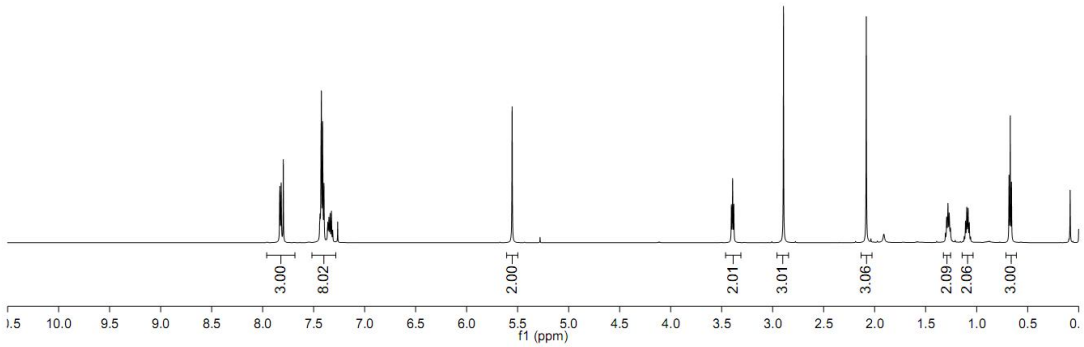

7.7185
7.7047
7.4617
7.4593
7.4564
7.4476
7.4063
7.4032
7.3940
7.3811
7.3463
7.3444
7.3424
7.3353
7.3321
7.3198
7.2839
7.2704
4.2374
3.2669
3.2549
3.2429
2.4289
2.0095
1.1961
1.1838
1.1716
1.0476
1.0350
1.0223
0.6638
0.6516
Ts
N
O
n-Bu
N3
Ph
Me
2x
2.00
7.12
2.00
2.02
3.04
3.00
2.03
2.02
3.05
f1 (ppm)


143.7395
142.5571
140.8619
136.0145
130.9974
129.4345
129.1727
128.2744
128.0192
127.4929
125.1726
120.1476
77.2119
77.0000
76.7881
50.1255
45.1507
29.8834
21.4980
19.4447
13.3872
9.1844
Ts
N
O
n-Bu
N3
Ph
Me
2x
f1 (ppm)

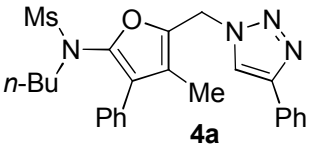

7.8308
7.8187
7.7975
7.4382
7.4244
7.4120
7.3988
7.3619
7.3586
7.3506
7.3383
7.3256
7.3133
5.5541
3.4049
3.3929
3.3809
2.8941
2.0824
1.2940
1.2816
1.2694
1.0971
1.0844
0.6831
0.6709
0.6586


Ms
N
O
N
N
N
n-Bu
Me
Ph
Ph

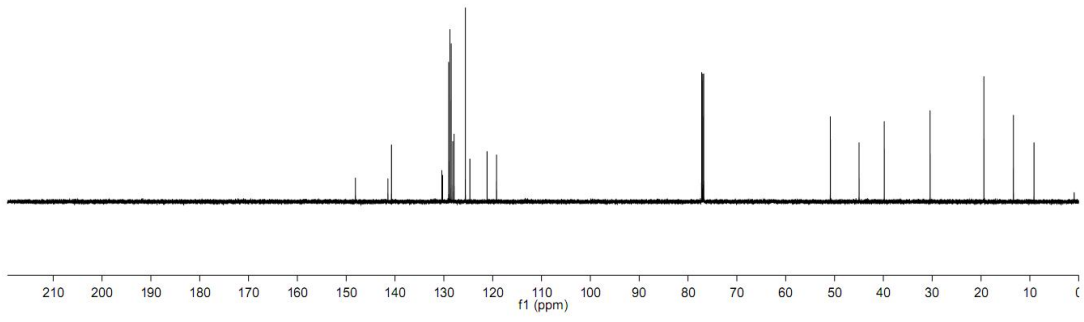
4a

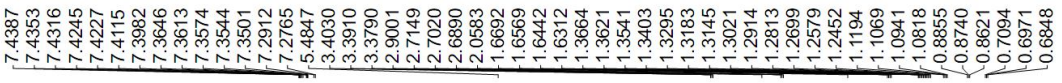

3.00
8.02
2.00
2.01
3.01
3.06
2.09
2.06
3.00
f1 (ppm)


148.1147
141.4636
140.7355
130.4243
130.2644
129.0321
128.7646
128.4986
128.1824
127.9067
125.5991
124.6739
121.1507
119.2102
77.2120
77.0000
76.7877
50.8588
44.9736
39.8156
30.4340
19.4084
13.3671
9.1539


Ms
N
O
N
N
N
n-Bu
Me
Ph
Ph

4a


f1 (ppm)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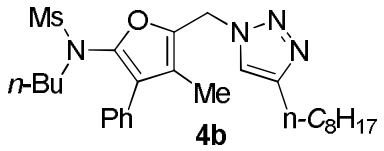
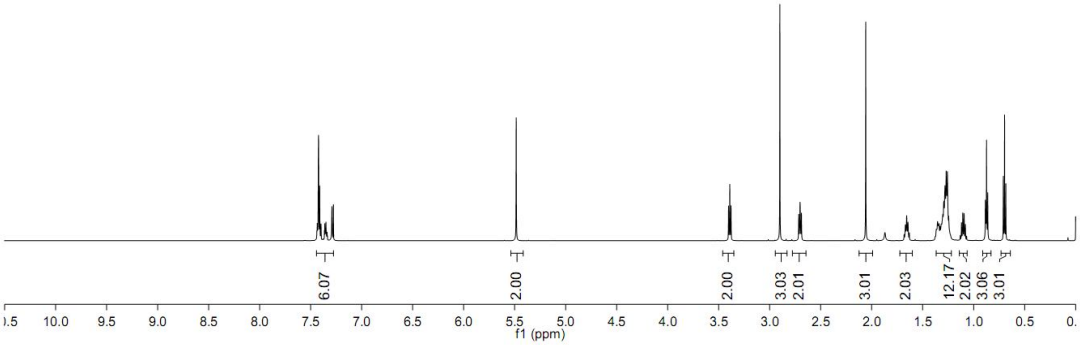
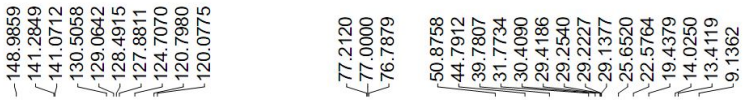
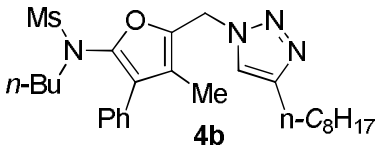
7.4353
7.4316
7.4245
7.4227
7.4115
7.3982
7.3646
7.3613
7.3574
7.3544
7.3501
7.2912
7.2765
5.4847
3.4030
3.3910
3.3790
2.9001
2.7149
2.7020
2.6890
2.0583
1.6692
1.6569
1.6442
1.6312
1.3664
1.3621
1.3541
1.3403
1.3295
1.3183
1.3145
1.3021
1.2914
1.2813
1.2699
1.2579
1.2452
1.1194
1.1069
1.0941
1.0818
0.8855
0.8740
0.8621
0.7094
0.6971
0.6848


Ms
N
n-Bu
O
N
N
N
Me
Ph
n-C8H17

4b


6.07
2.00
2.00
3.03
2.01
3.01
2.03
12.17
2.02
3.06
3.01
f1 (ppm)


148.9859
141.2849
141.0712
130.5058
129.0642
128.4915
127.8811
124.7070
120.7980
120.0775
77.2120
77.0000
76.7879
50.8758
44.7912
39.7807
31.7734
30.4090
29.4186
29.2540
29.2227
29.1377
25.6520
22.5764
19.4379
14.0250
13.4119
9.1362


Ms
N
n-Bu
O
N
N
N
Me
Ph
n-C8H17

4b

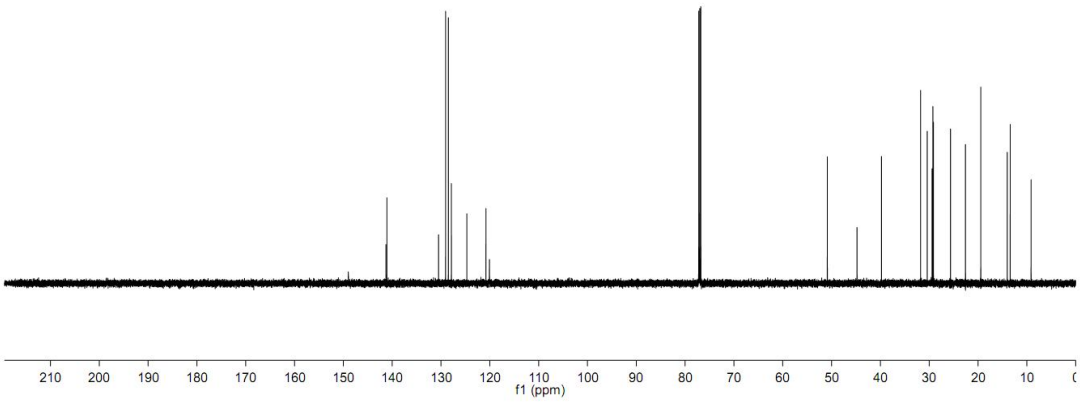
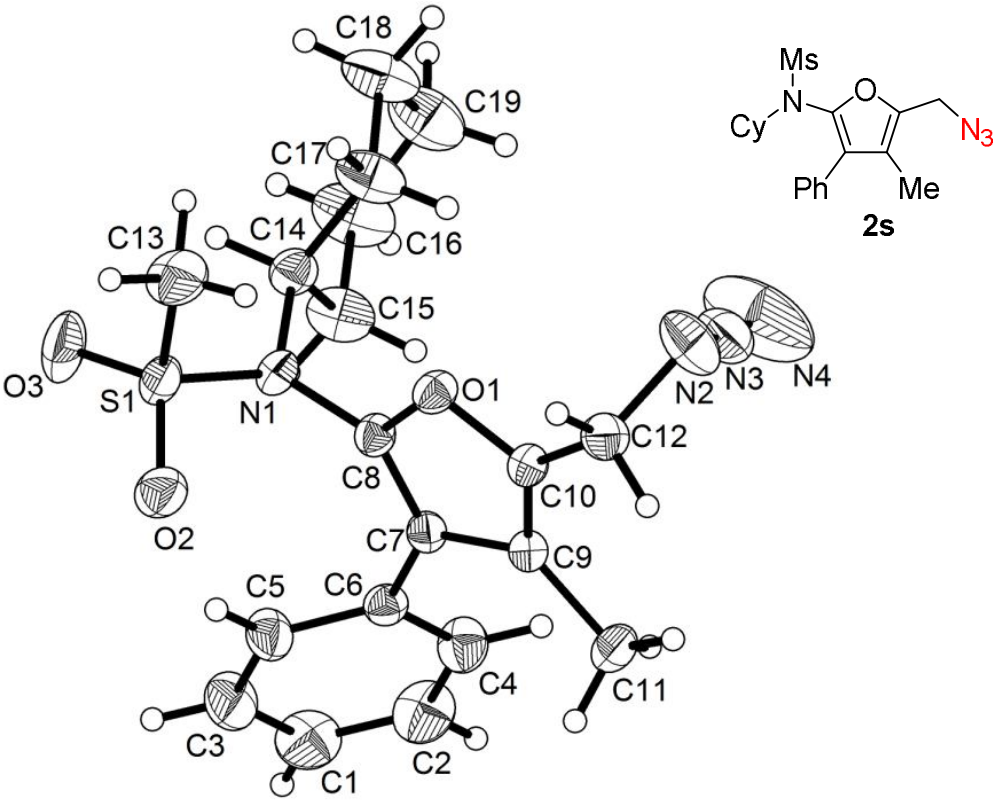

f1 (ppm)

Figure S1. ORTEP Drawing of 2s Showing the Atom-labeling Scheme and Displacement Ellipsoids Drawn at the 50% Probability Level



Checkcif Report of 2s

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: a

```
Bond precision:  C-C = 0.0033 A          Wavelength=0.71073

Cell:          a=11.8249(4)      b=13.3798(4)      c=13.3981(5)
               alpha=79.783(2)   beta=77.825(2)    gamma=78.013(2)
Temperature:   296 K
```

	Calculated	Reported
Volume	2007.04(12)	2007.04(12)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C19 H24 N4 O3 S	?
Sum formula	C19 H24 N4 O3 S	C19 H24 N4 O3 S
Mr	388.48	388.48
Dx,g cm-3	1.286	1.286
Z	4	4
Mu (mm-1)	0.188	0.188
F000	824.0	824.0
F000'	824.81	
h,k,lmax	15,17,17	15,17,17
Nref	9302	9234
Tmin,Tmax	0.956,0.963	0.956,0.963
Tmin'	0.945	

```
Correction method= # Reported T Limits: Tmin=0.956 Tmax=0.963
AbsCorr = EMPIRICAL

Data completeness= 0.993          Theta(max)= 27.570

R(reflections)= 0.0475( 7050)     wR2(reflections)= 0.1427( 9234)

S = 1.020                  Npar= 487
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of          N7 Check
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as EMPIRICAL
PLAT220_ALERT_2_C Non-Solvent Resd 1    N    Ueq(max)/Ueq(min) Range         4.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2    N    Ueq(max)/Ueq(min) Range         5.6 Ratio
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of          N6 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of          N3 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of          S2 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of         C31 Check
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...           3 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF      Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical           ? Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as       mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.002 Degree
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C11 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C29 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          84 Do !
           C12  -N2   -N3   -N4    159.00  3.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         100 Do !
           C31 -N6   -N7   -N8    135.00  4.00   1.555   1.555   1.555   1.555
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          15 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/05/2016; check.def file version of 05/05/2016

Datablock a - ellipsoid plot