Supporting Information

New Journal of Chemistry

An efficient synthesis of novel spiroindenopyridazine-4*H*-pyran derivatives

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The Table of Contents

Experimental Section

General remarks:

Melting points were measured on an Electrothermal 9100 apparatus. Mass spectra were recorded with an Agilent 5975C VL MSD with Triple-Axis Detector operating at an ionization potential of 70 eV. ^{1}H and ^{13}C NMR spectra were measured (DMSO) with a Bruker DRX-300 AVANCE spectrometer at 300 and 75 MHz, respectively. IR spectra were recorded on a Bruker Tensor 27, ῡ in cm^{-1}. All NMR spectra at room temperature were determined in DMSO-d_6. Chemical shifts are reported in parts per million (δ) downfield from an internal tetramethylsilane reference. Coupling constants (J values) are reported in hertz (Hz), and spin multiplicities are indicated by the following symbols: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). All chemicals were purchased from Merck or Aldrich and were used without further purification.

* Signals related to DMSO and residual ethanol, are indicated on the spectra.

* Some products are poorly soluble in DMSO, for example compounds 5b, 5c, 5d, 5f and 5h.

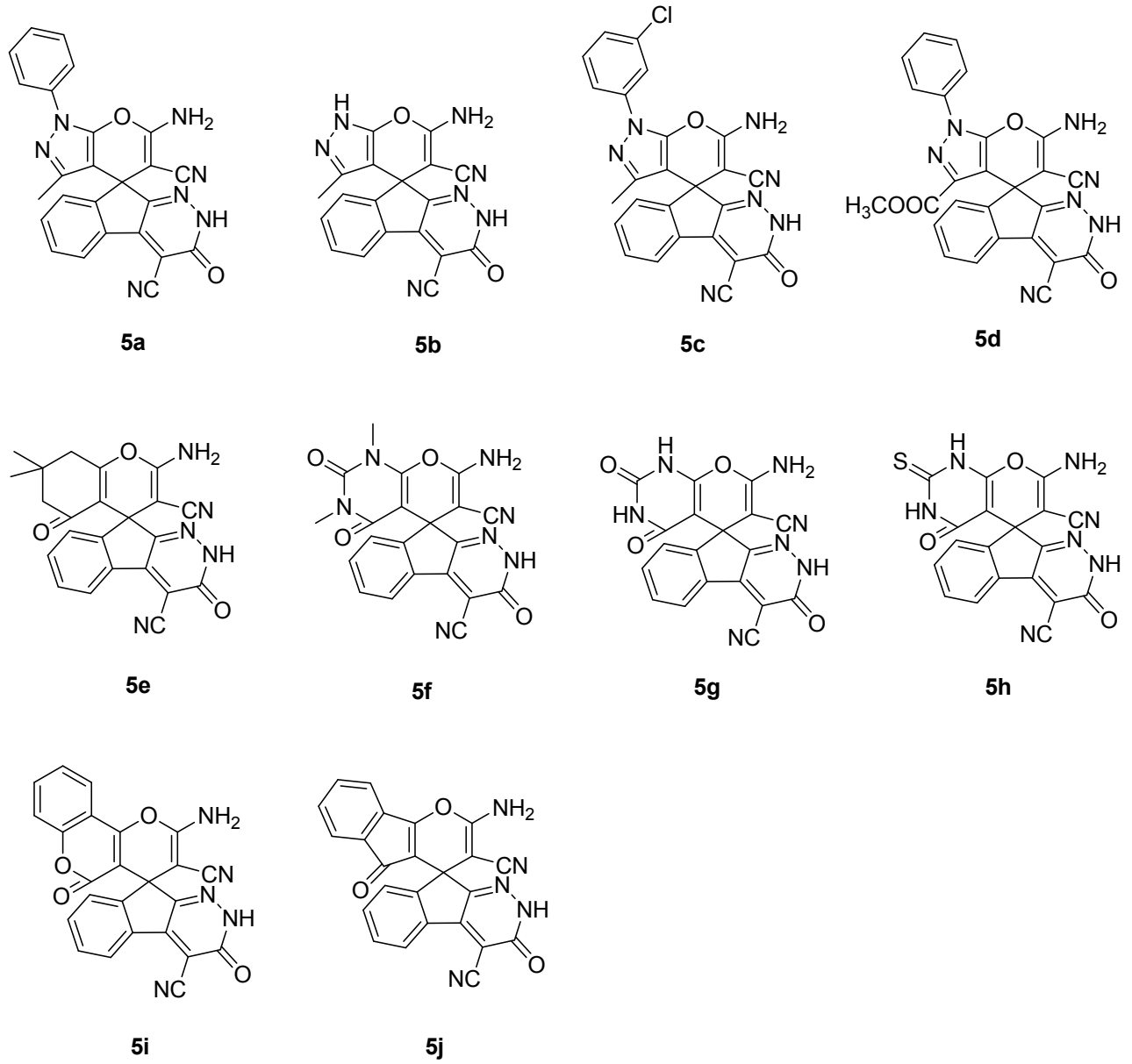
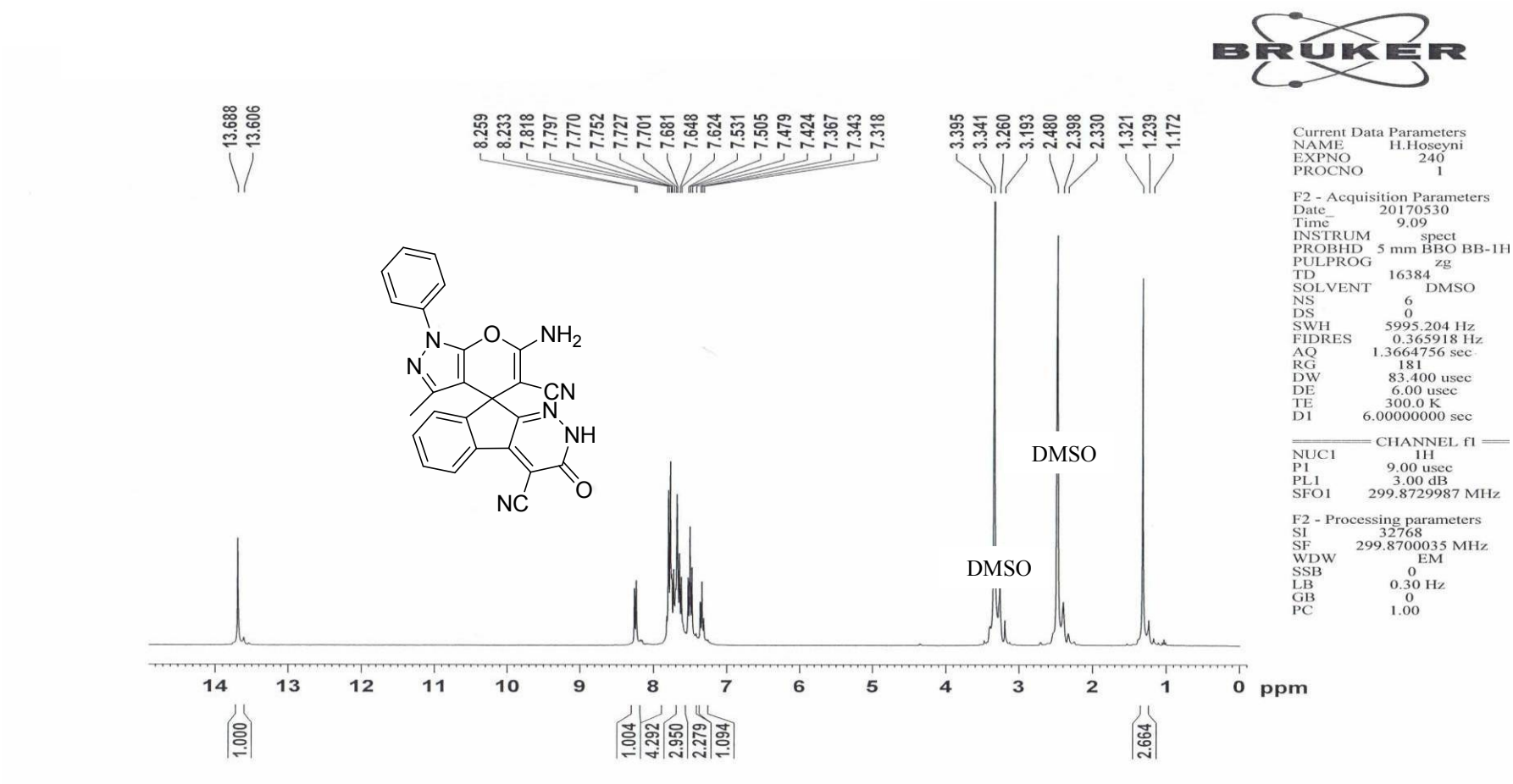


Figure 1. Structure of all products **5**

The structures of all products **5a-j** were deduced from their IR, mass, ^{1}H NMR, and ^{13}C NMR spectra.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7.624
7.531
7.505
7.479
7.424
7.367
7.343
7.318
3.395
3.341
3.260
3.193
2.480
2.398
2.330
1.321
1.239
1.172
DMSO
DMSO
NH2
CN
NH
NC
O
N
N
O
14
13
12
11
10
9
8
7
6
5
4
3
2
1
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PL1 3.00 dB
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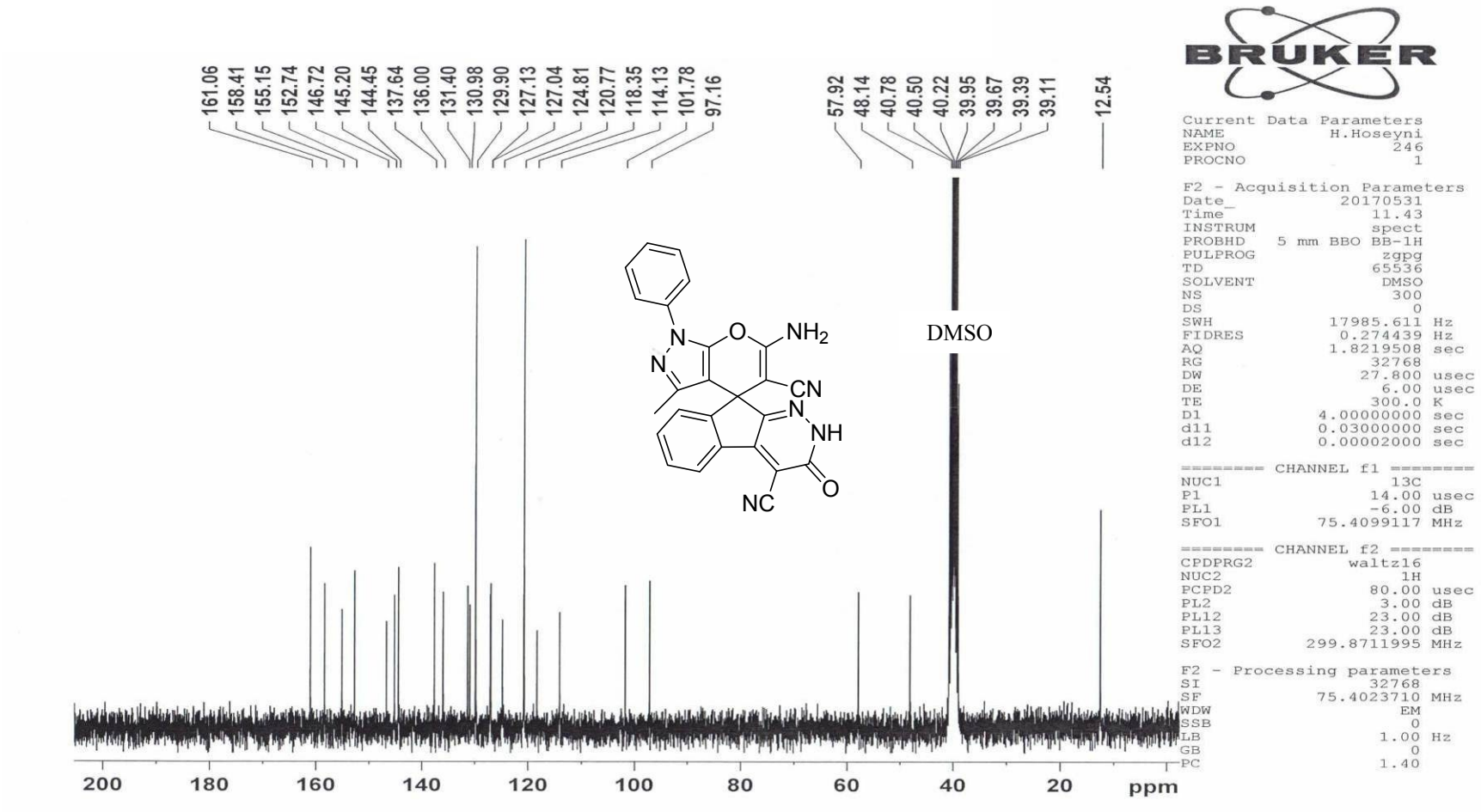
^{1}H NMR of 5a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127.13
127.04
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118.35
114.13
101.78
97.16
57.92
48.14
40.78
40.50
40.22
39.95
39.67
39.39
39.11
12.54
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NH
NC
O
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140
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100
80
60
40
20
ppm
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FIDRES 0.274439 Hz
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RG 32768
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DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
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PL1 -6.00 dB
SFO1 75.4099117 MHz
CHANNEL f2
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PL12 23.00 dB
PL13 23.00 dB
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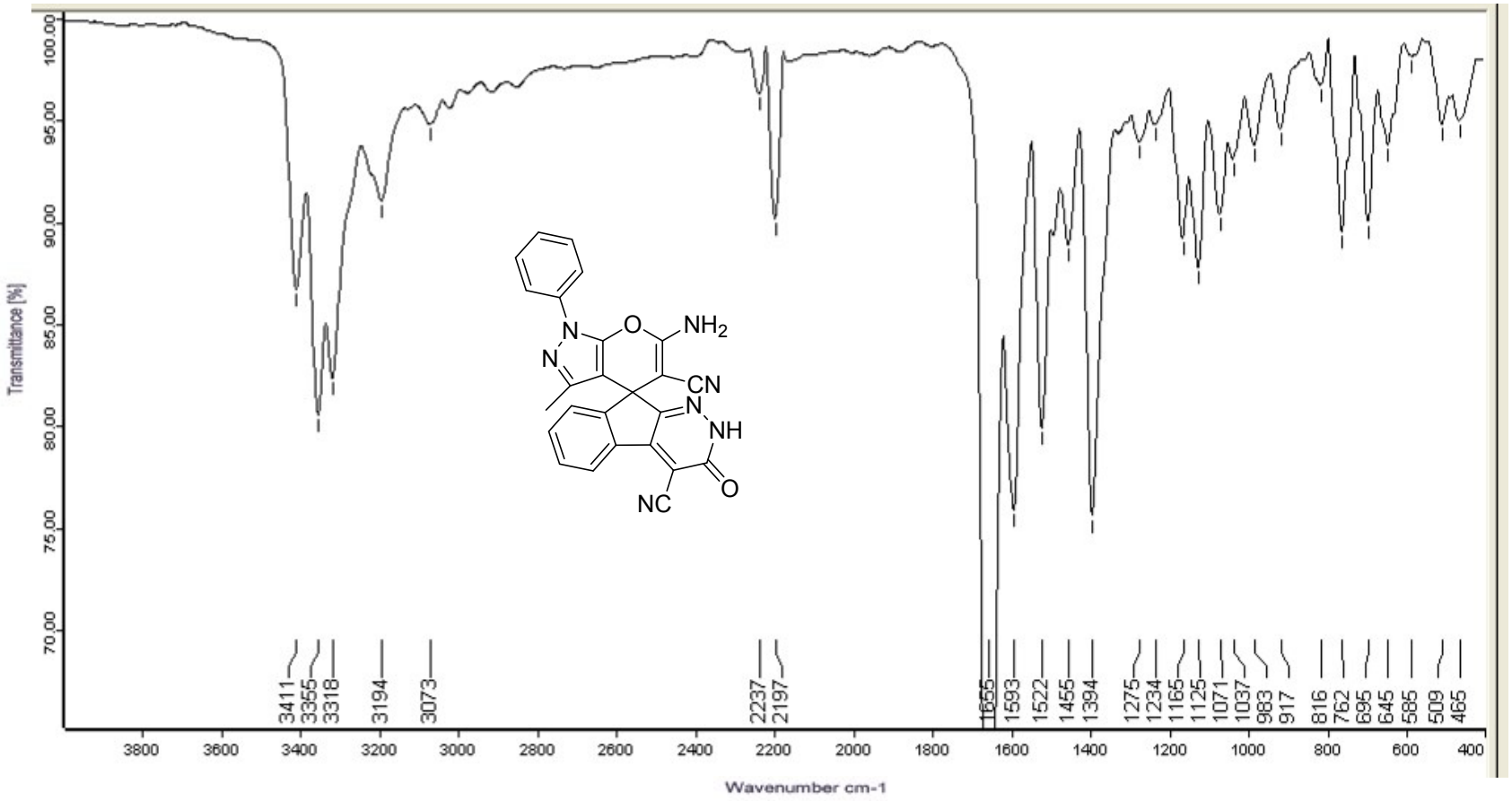
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1037
983
917
816
762
695
645
585
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3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
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800
600
400
Wavenumber cm-1
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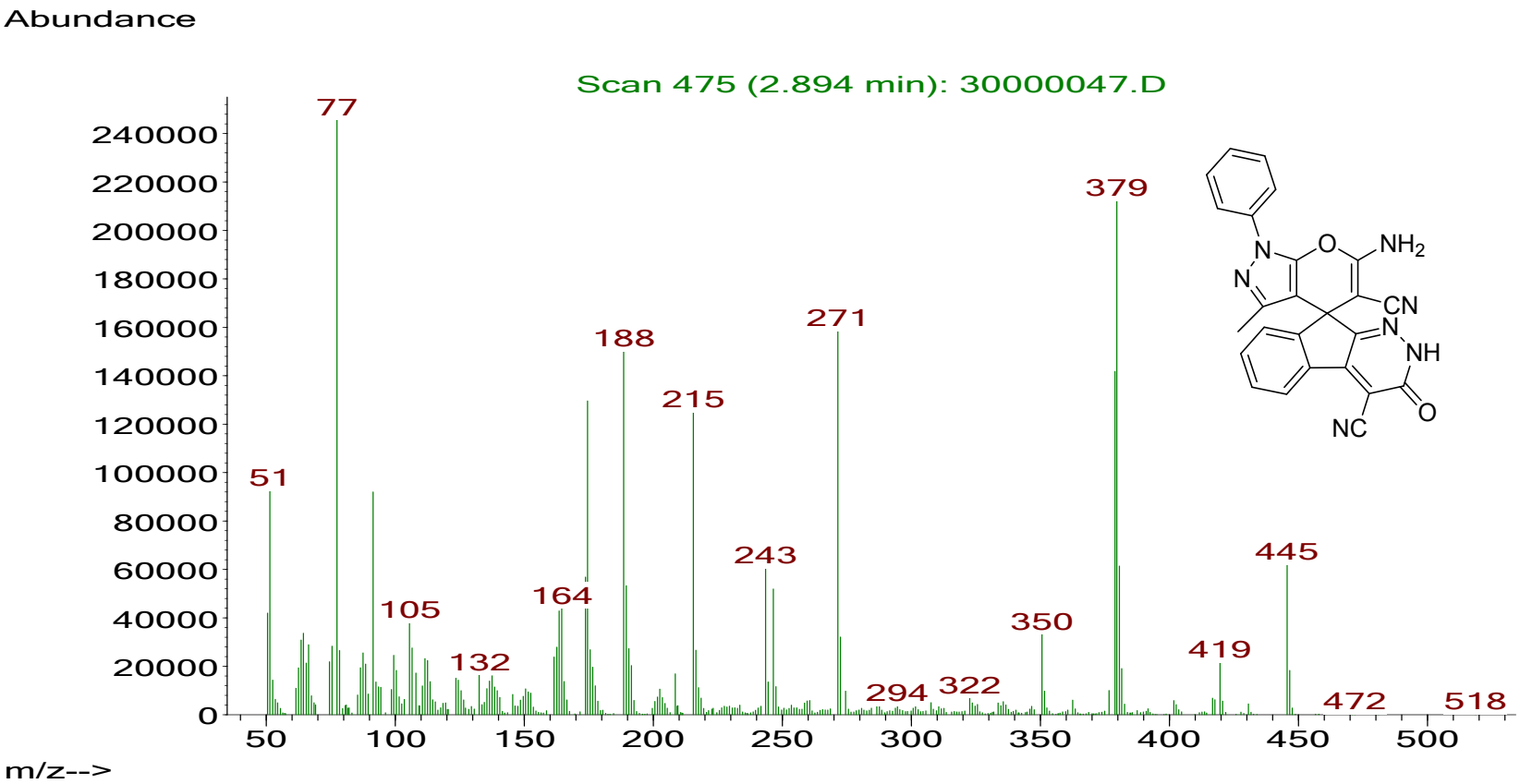
CN
NH
O
NC

IR of 5a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271
215
51
243
445
164
105
350
419
132
294
322
472
518
50
100
150
200
250
300
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400
450
500
m/z-->
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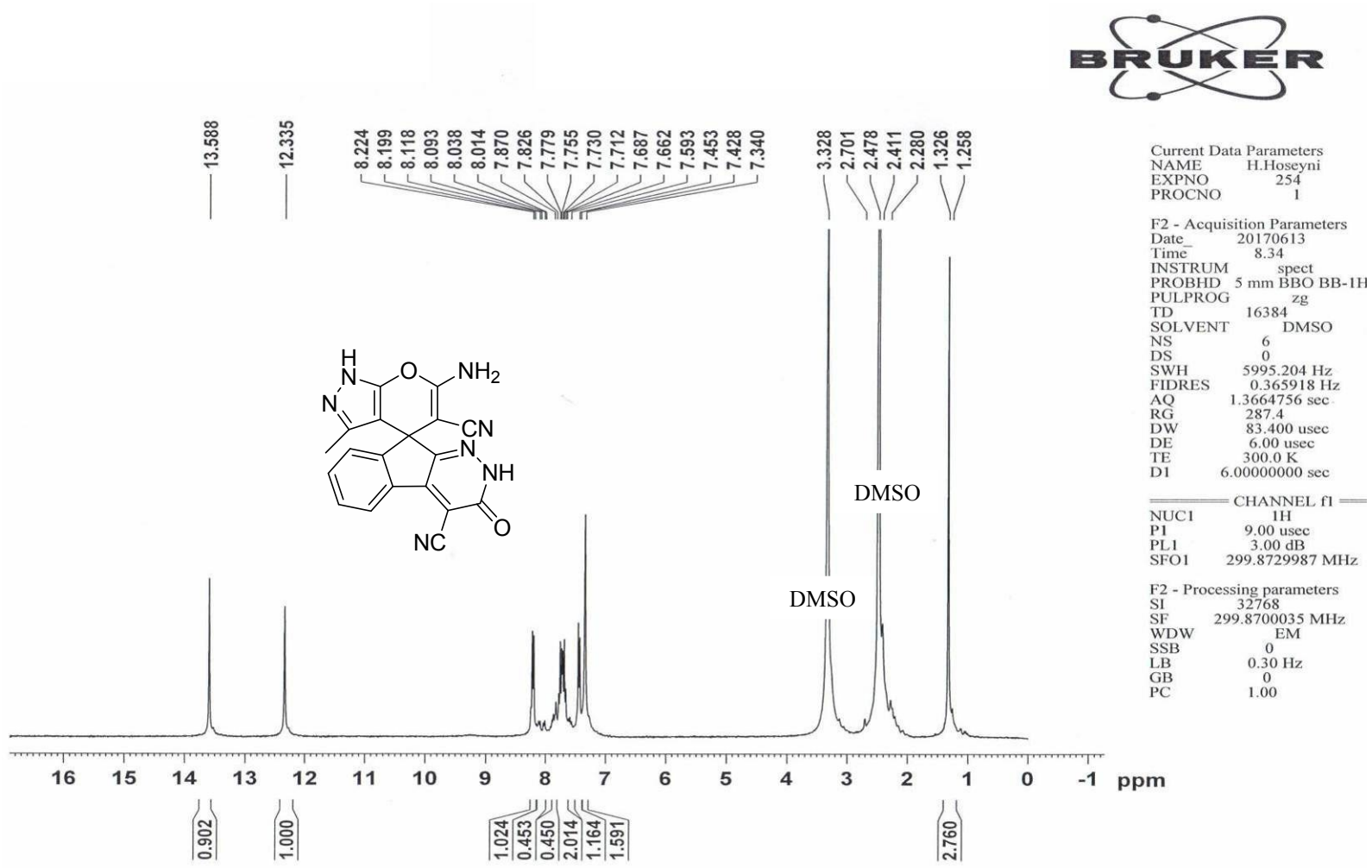
N
O
NH2
CN
N
NH
O
NC

MS of 5a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7.712
7.687
7.662
7.593
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2.478
2.411
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1.258
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DMSO
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0.450
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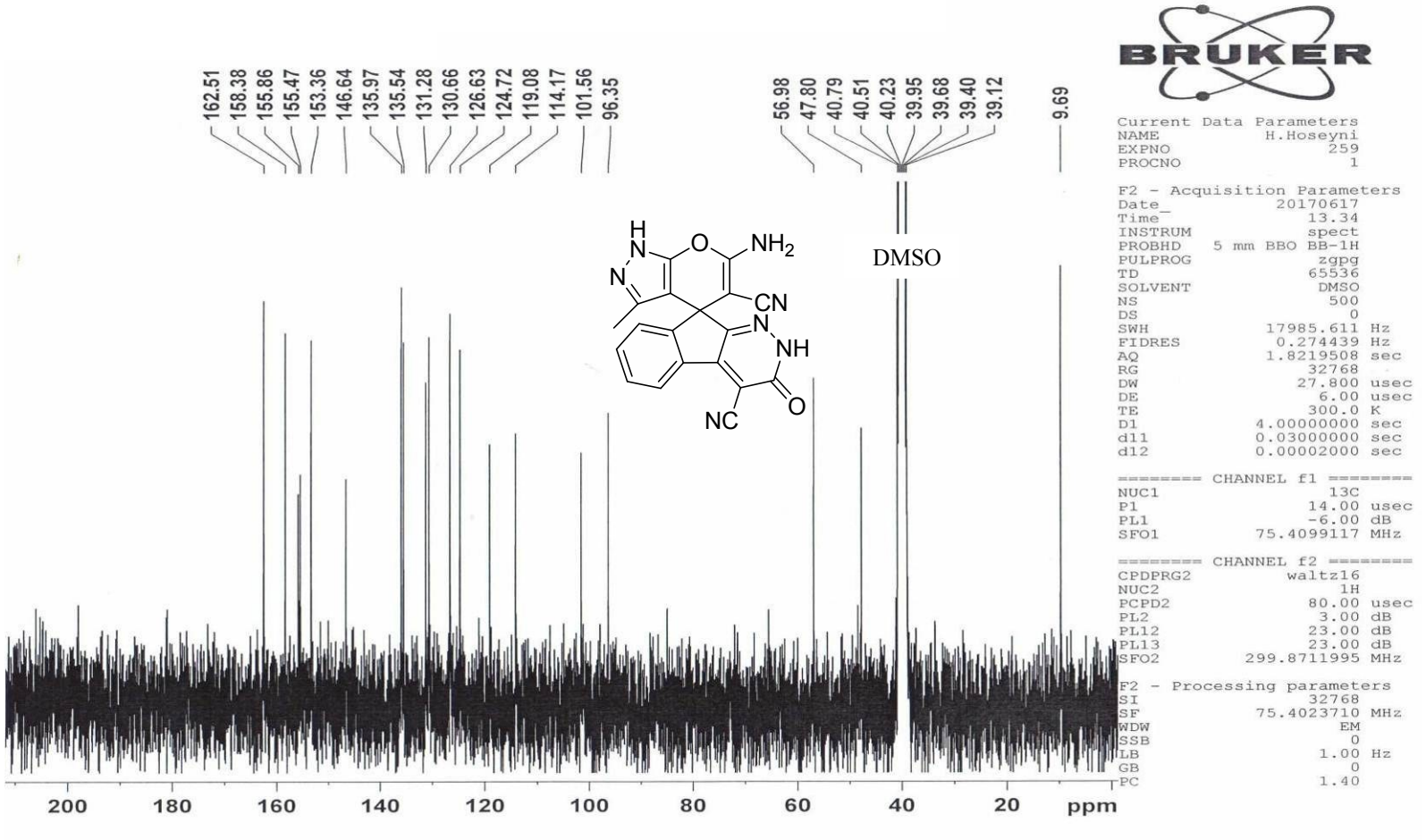
^{1}H NMR of 5b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119.08
114.17
101.56
96.35
56.98
47.80
40.79
40.51
40.23
39.95
39.68
39.40
39.12
9.69
DMSO
H
N
N
O
NH2
CN
N
NH
O
NC
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
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SFO1 75.4099117 MHz
======== CHANNEL f2 ========
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PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
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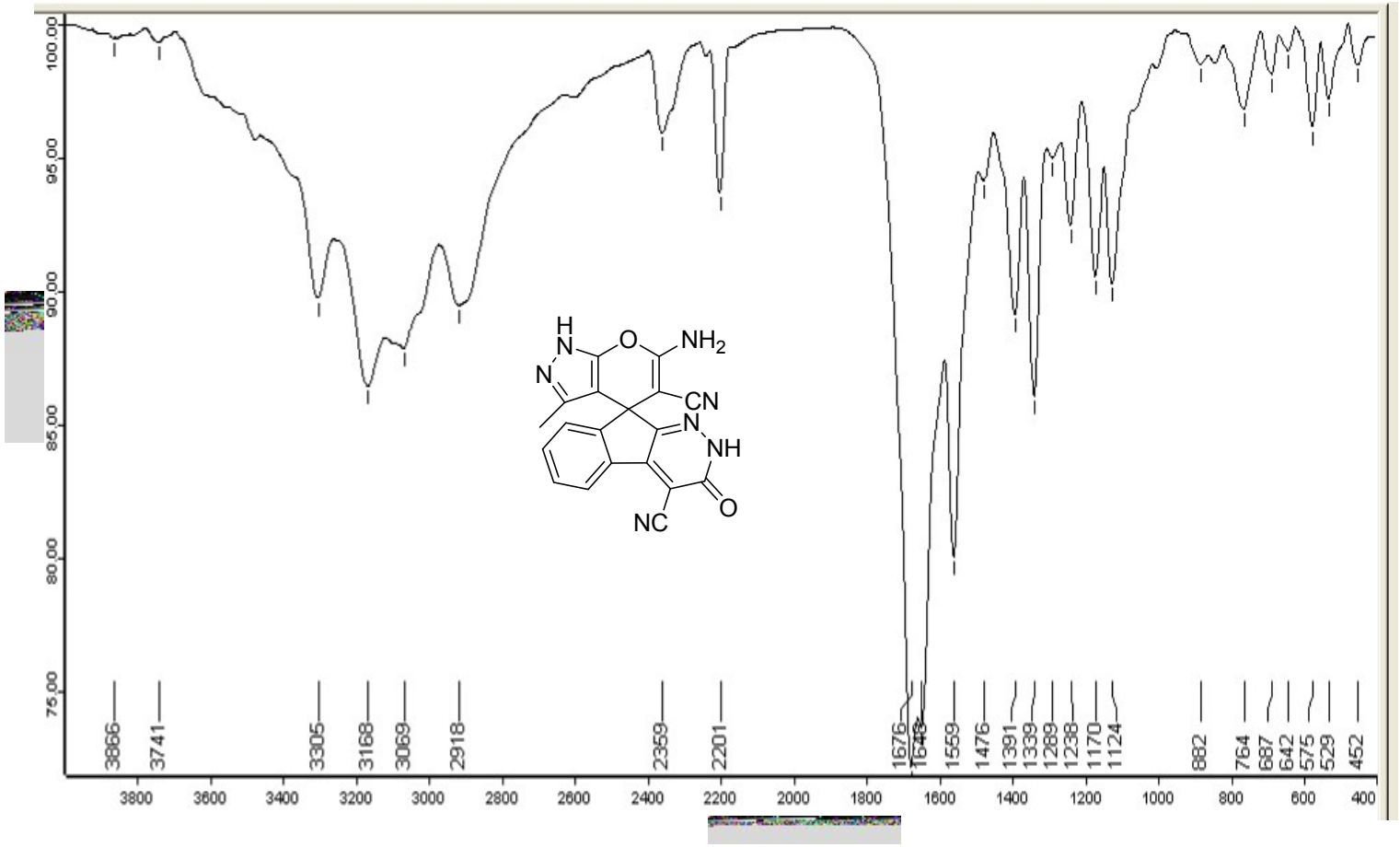
^{13}C NMR of 5b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1476
1391
1339
1289
1238
1170
1124
882
764
687
642
575
529
452
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
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800
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H
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NH2
CN
N
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O
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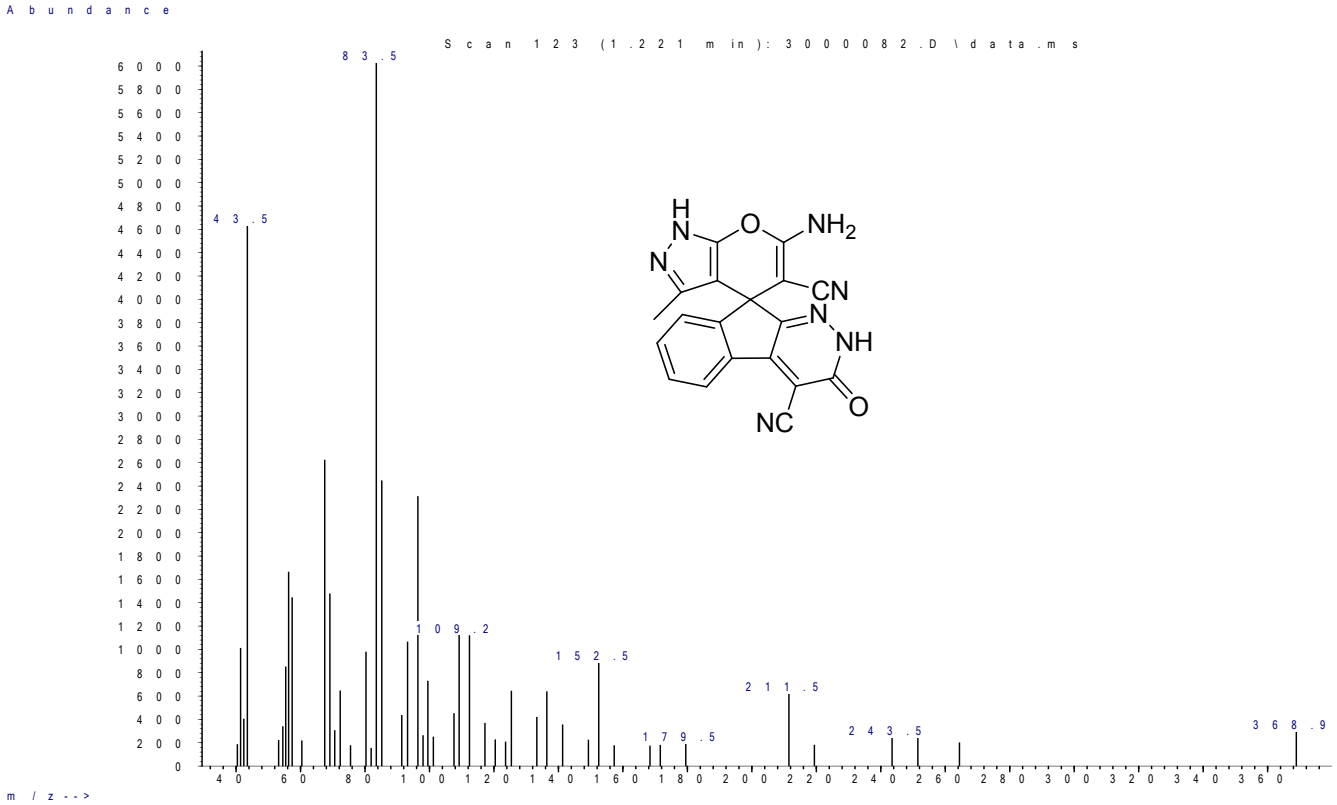
IR of 5b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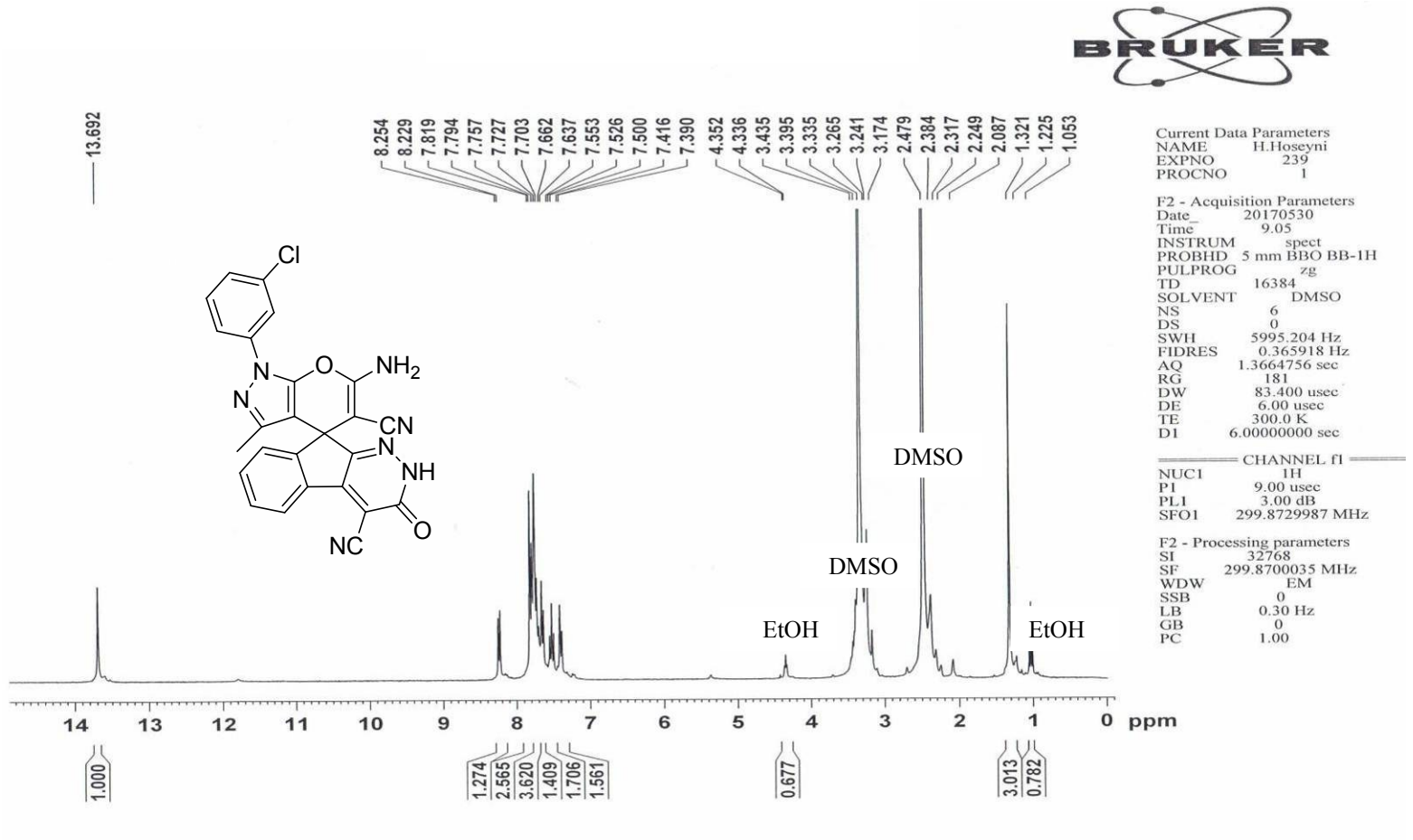
MS of 5b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7.637
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7.526
7.500
7.416
7.390
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4.336
3.435
3.395
3.335
3.265
3.241
3.174
2.479
2.384
2.317
2.249
2.087
1.321
1.225
1.053
Cl
N
O
NH2
N
CN
N
NH
O
NC
DMSO
DMSO
EtOH
EtOH
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12
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10
9
8
7
6
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4
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RG 181
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DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
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LB 0.30 Hz
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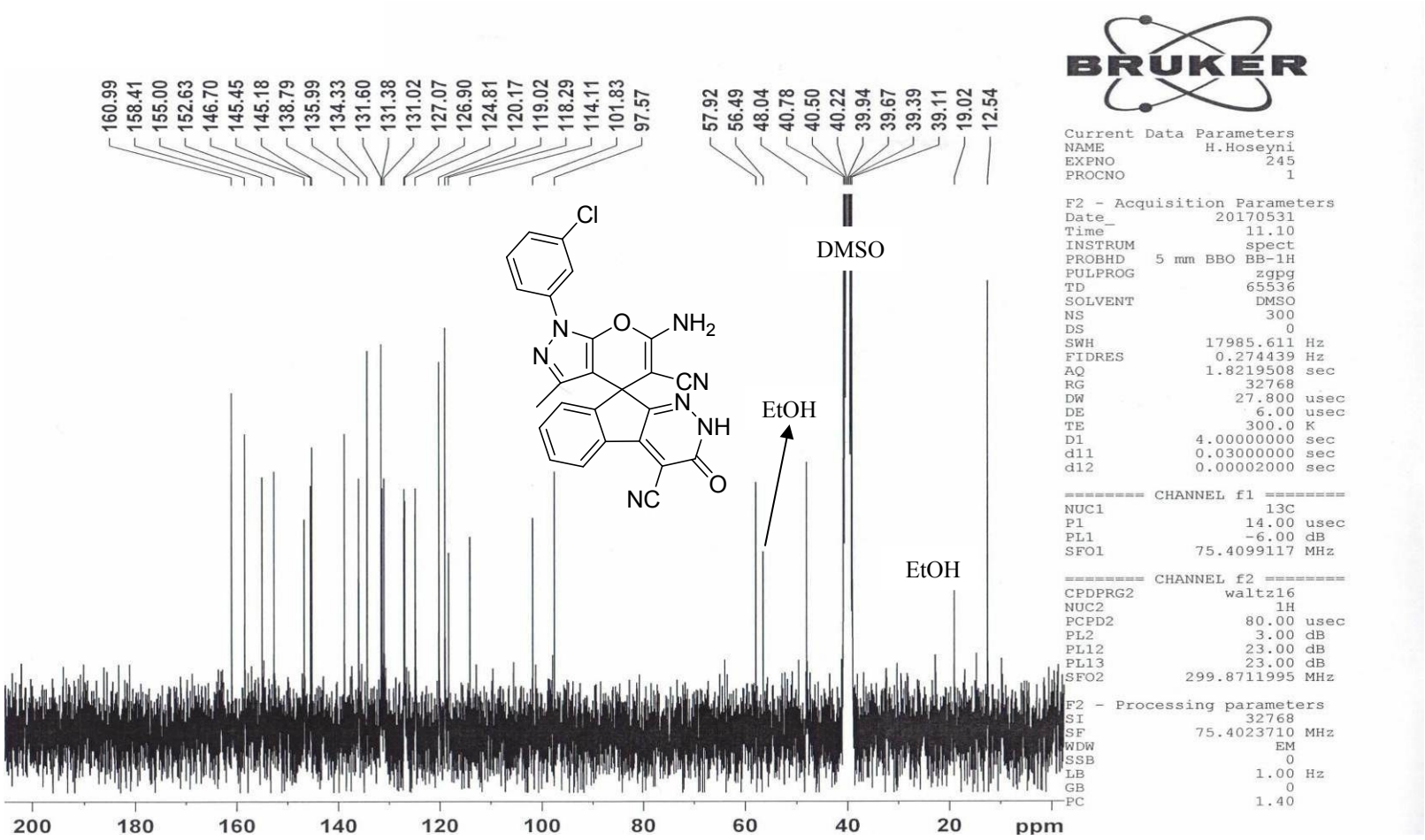
PC 1.00

^{1}H NMR of 5c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126.90
124.81
120.17
119.02
118.29
114.11
101.83
97.57
57.92
56.49
48.04
40.78
40.50
40.22
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39.39
39.11
19.02
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80
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ppm
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RG 32768
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DE 6.00 usec
TE 300.0 K
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d11 0.03000000 sec
d12 0.00002000 sec
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PL1 -6.00 dB
SFO1 75.4099117 MHz
CHANNEL f2
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PL12 23.00 dB
PL13 23.00 dB
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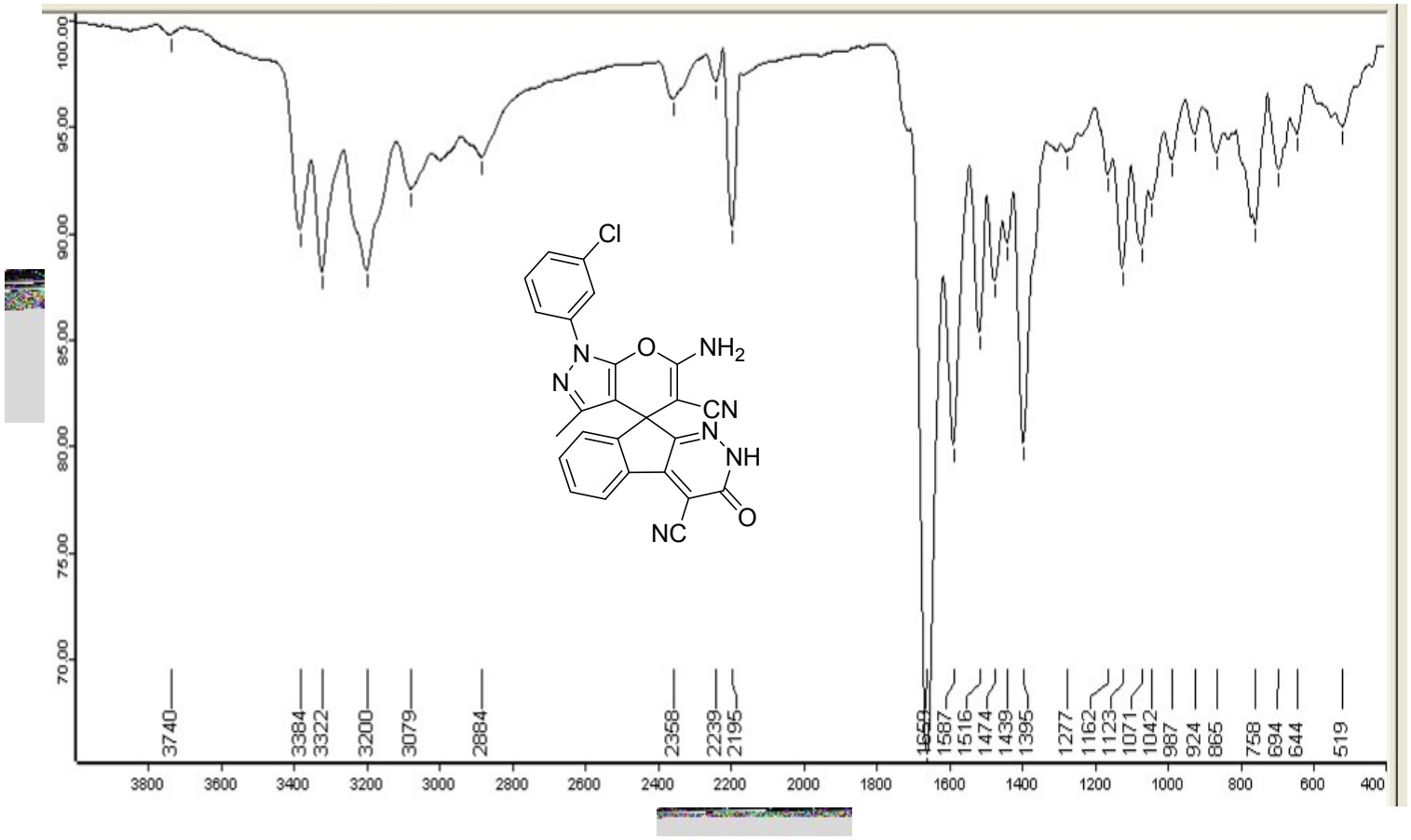
^{13}C NMR of 5c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1587
1516
1474
1439
1395
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1162
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1071
1042
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924
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758
694
644
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3800
3600
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2600
2400
2200
2000
1800
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N
NH
O
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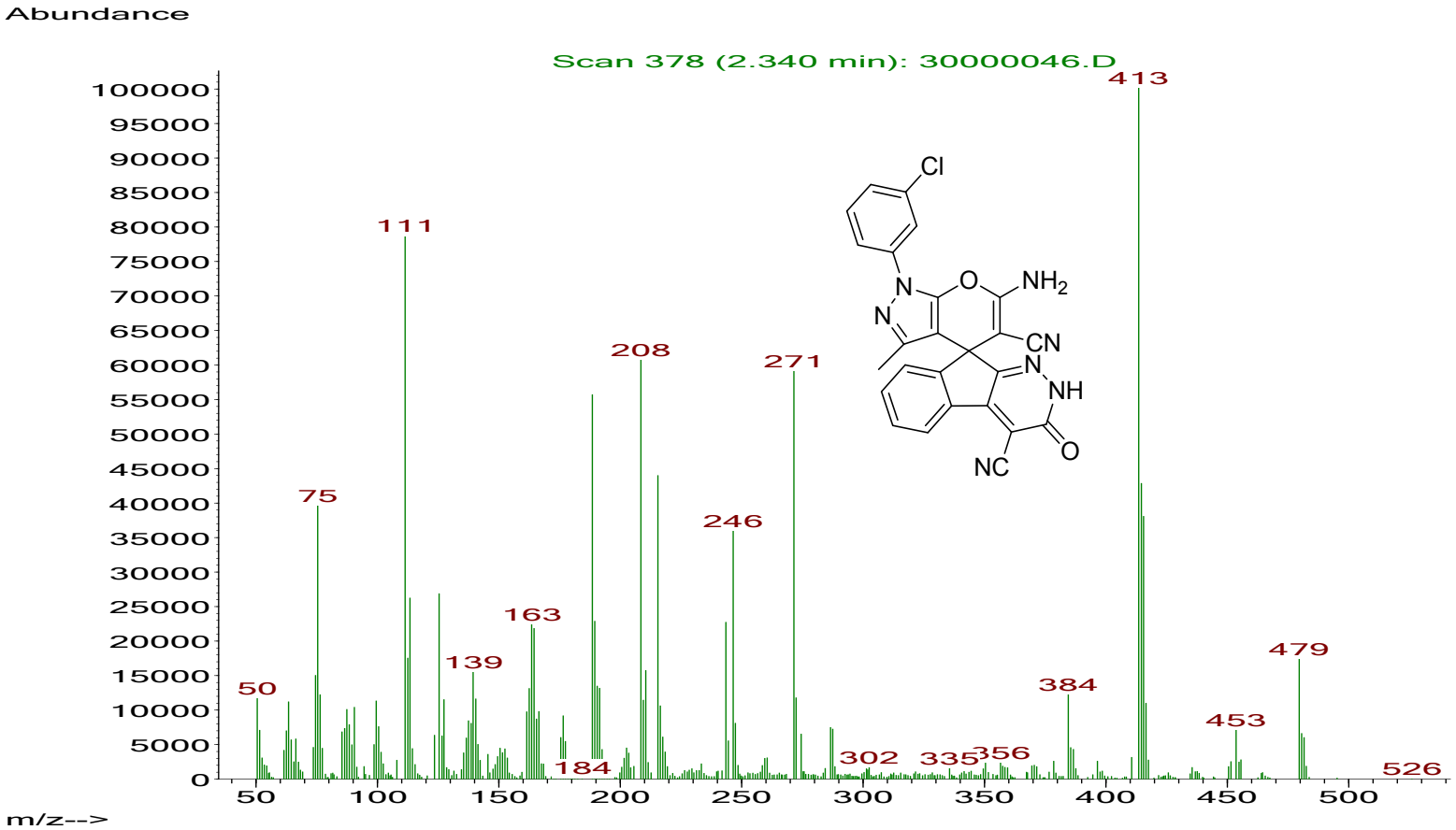
IR of 5c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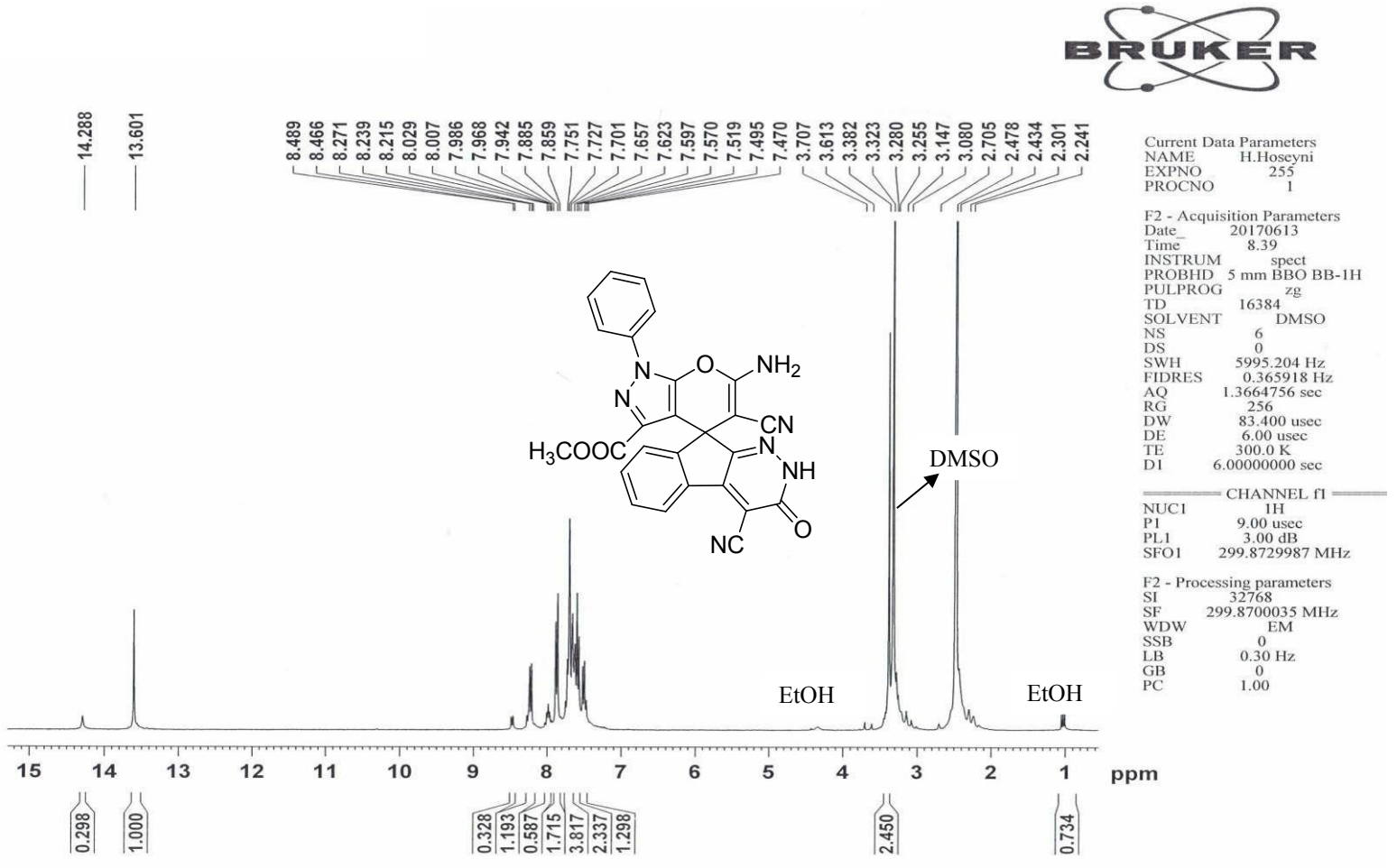
MS of 5c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7.885
7.859
7.751
7.727
7.701
7.657
7.623
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7.519
7.495
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3.080
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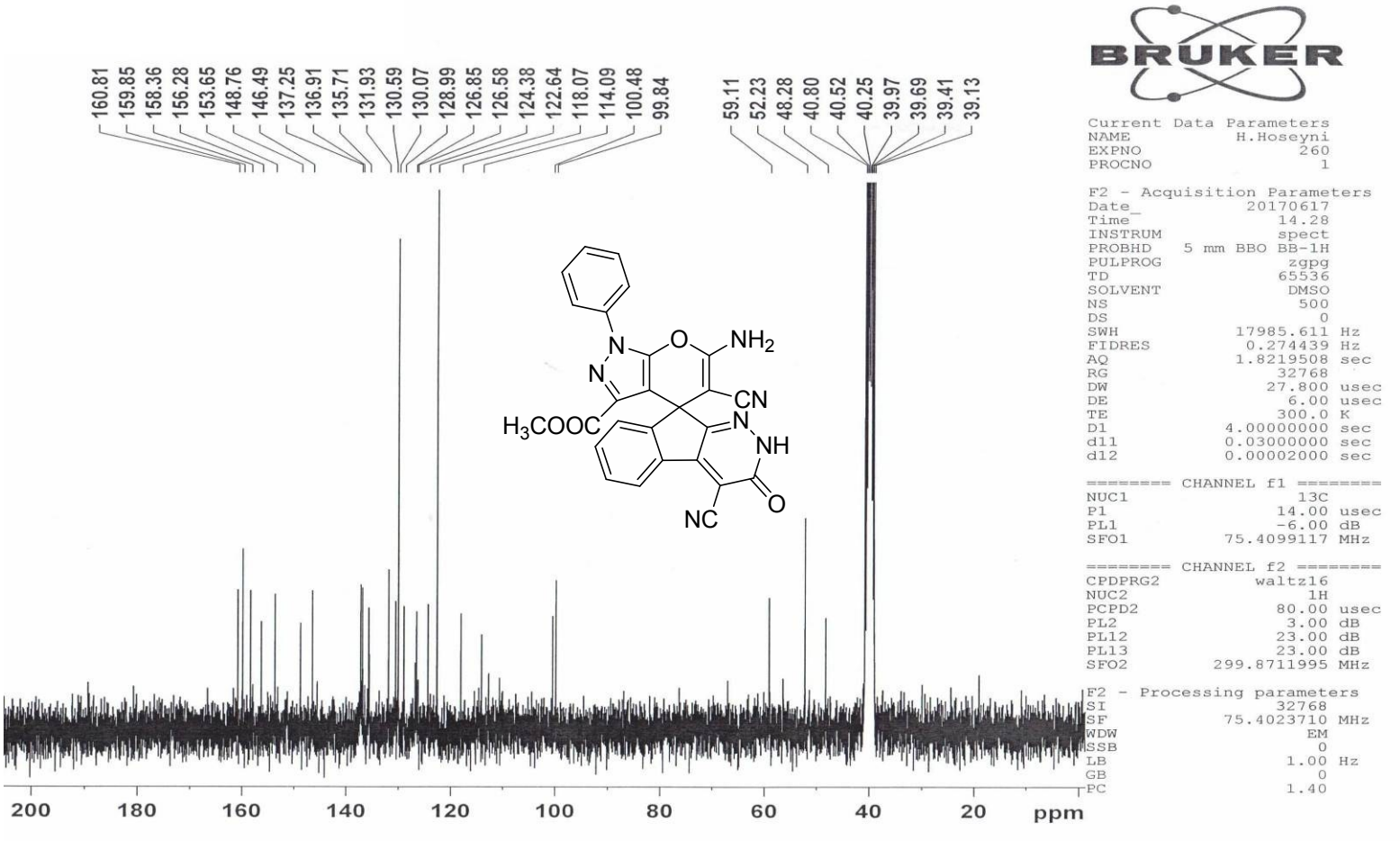
^{1}H NMR of 5d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126.85
126.58
124.38
122.64
118.07
114.09
100.48
99.84
59.11
52.23
48.28
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40.52
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39.41
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ppm
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SOLVENT DMSO
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SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
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NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
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NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
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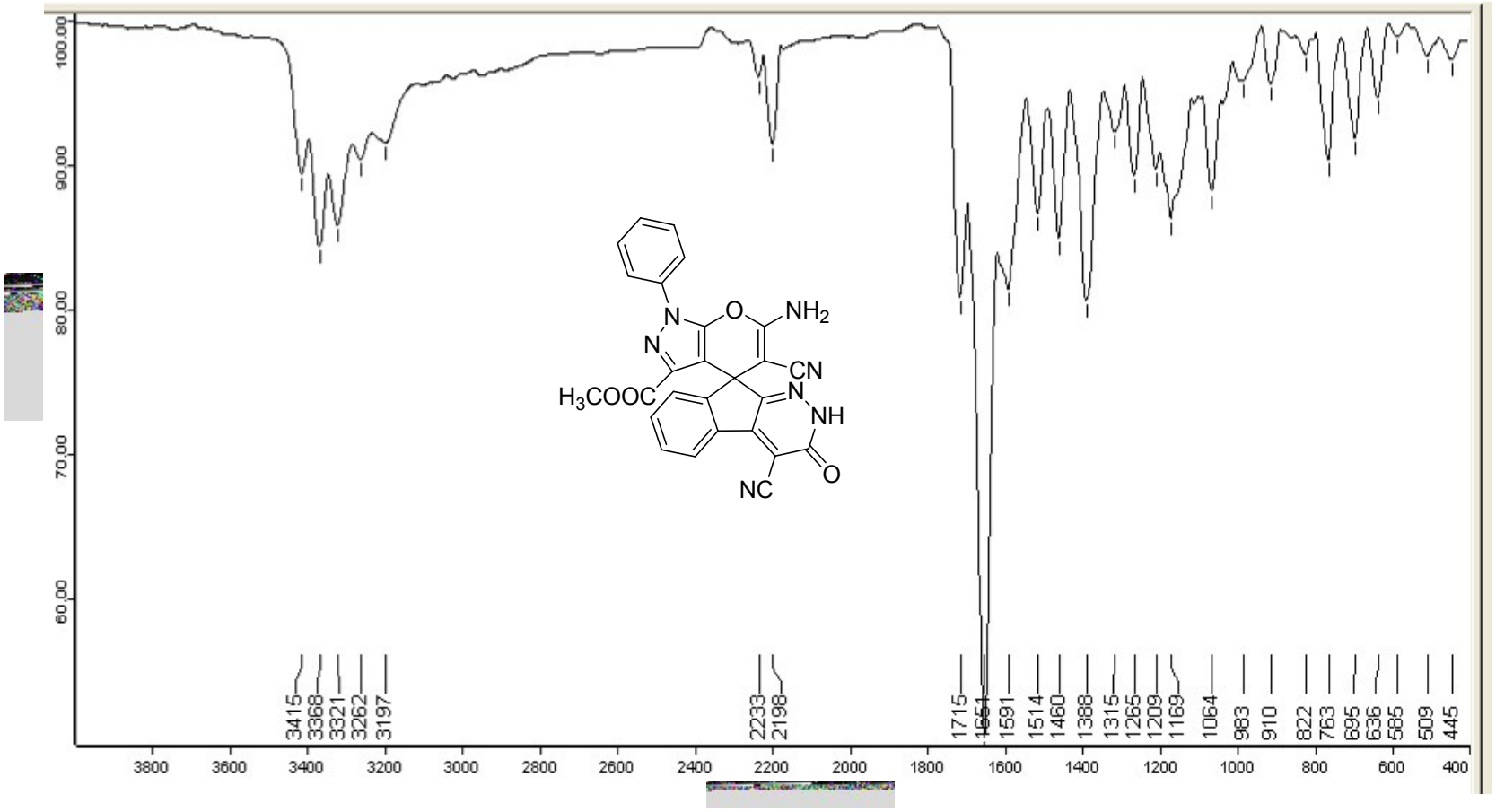
^{13}C NMR of 5d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2200
2000
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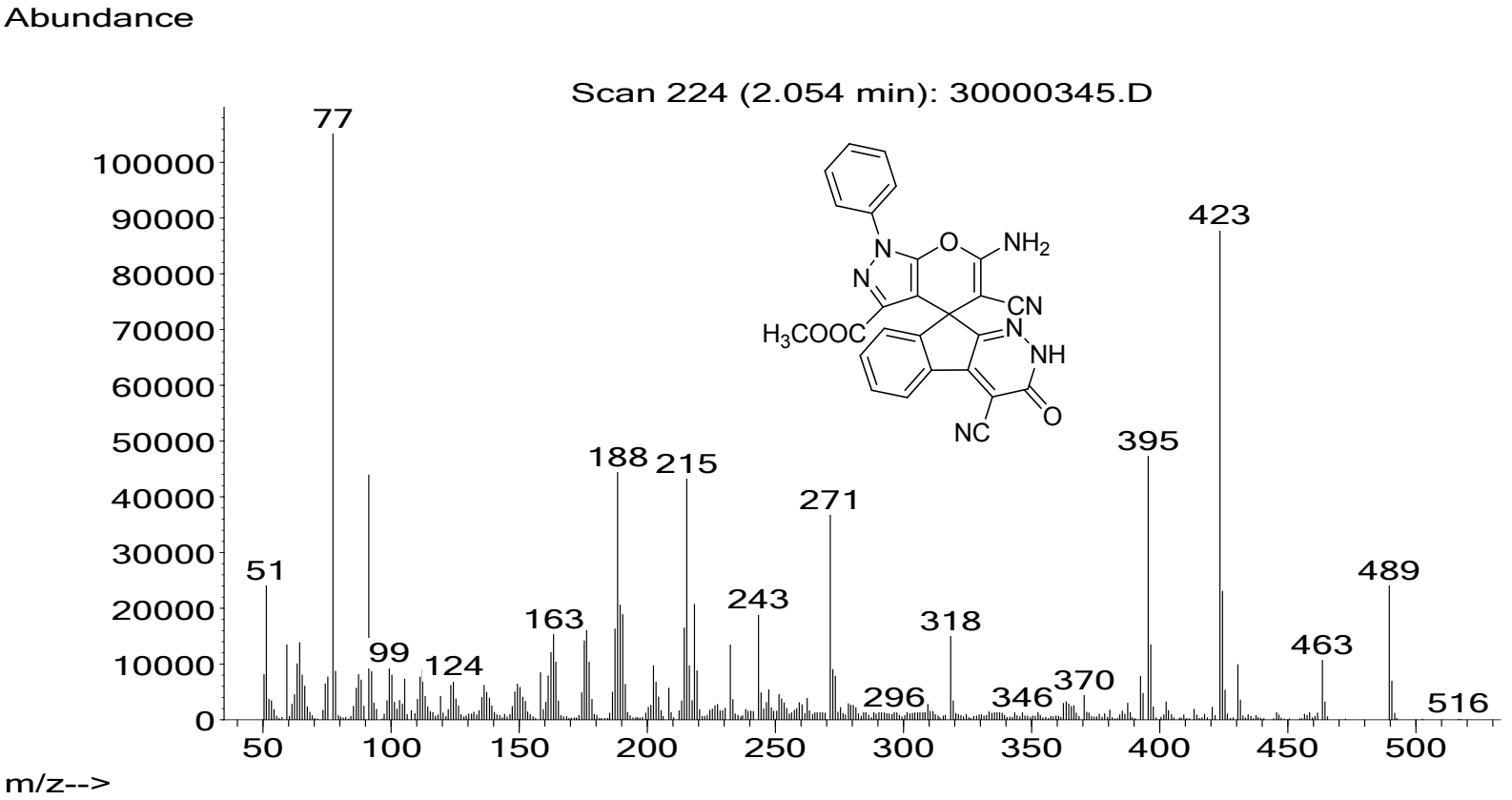
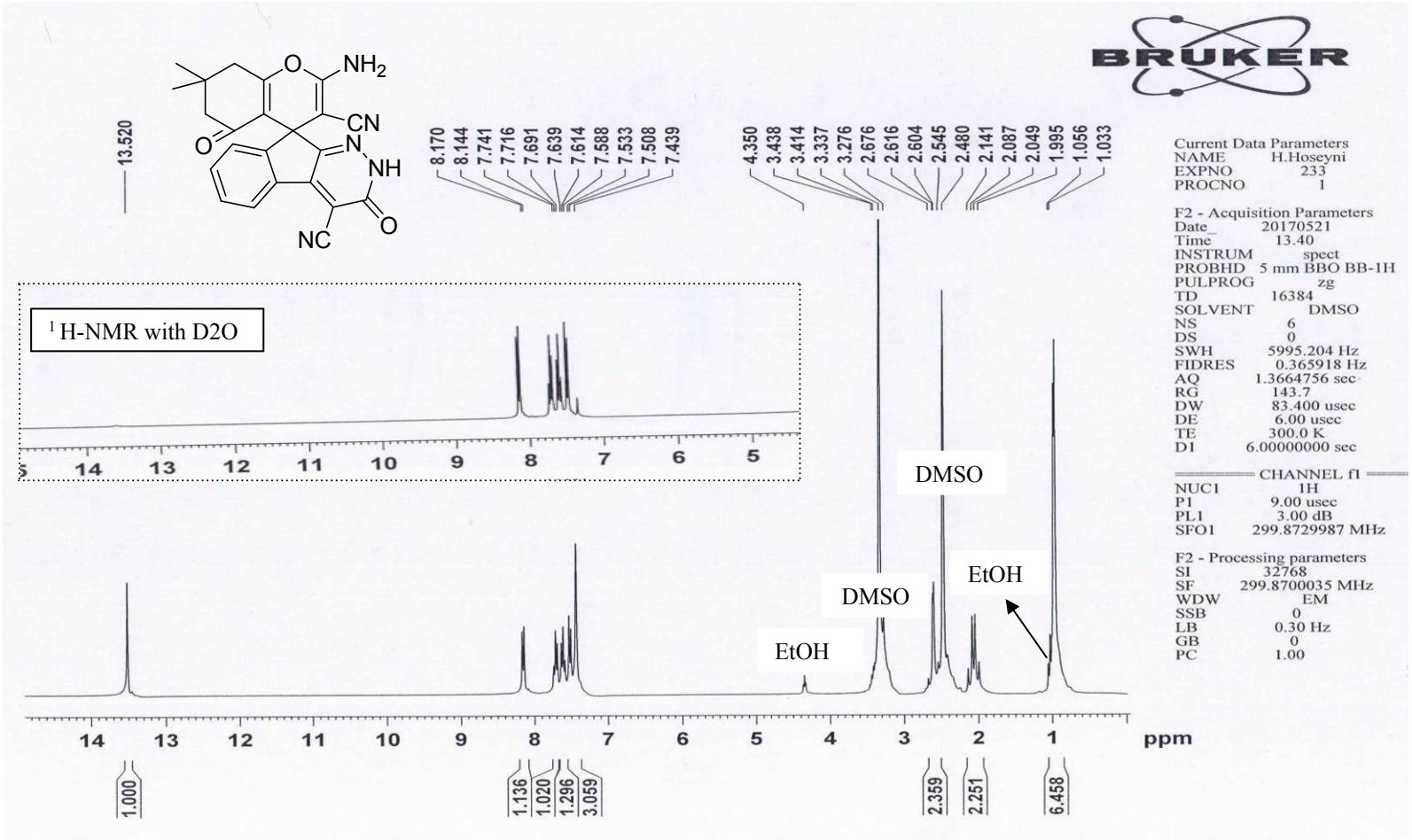
1400
1200
1000
800
600
400
N
N
O
NH2
CN
H3COOC
N
NH
O
NC

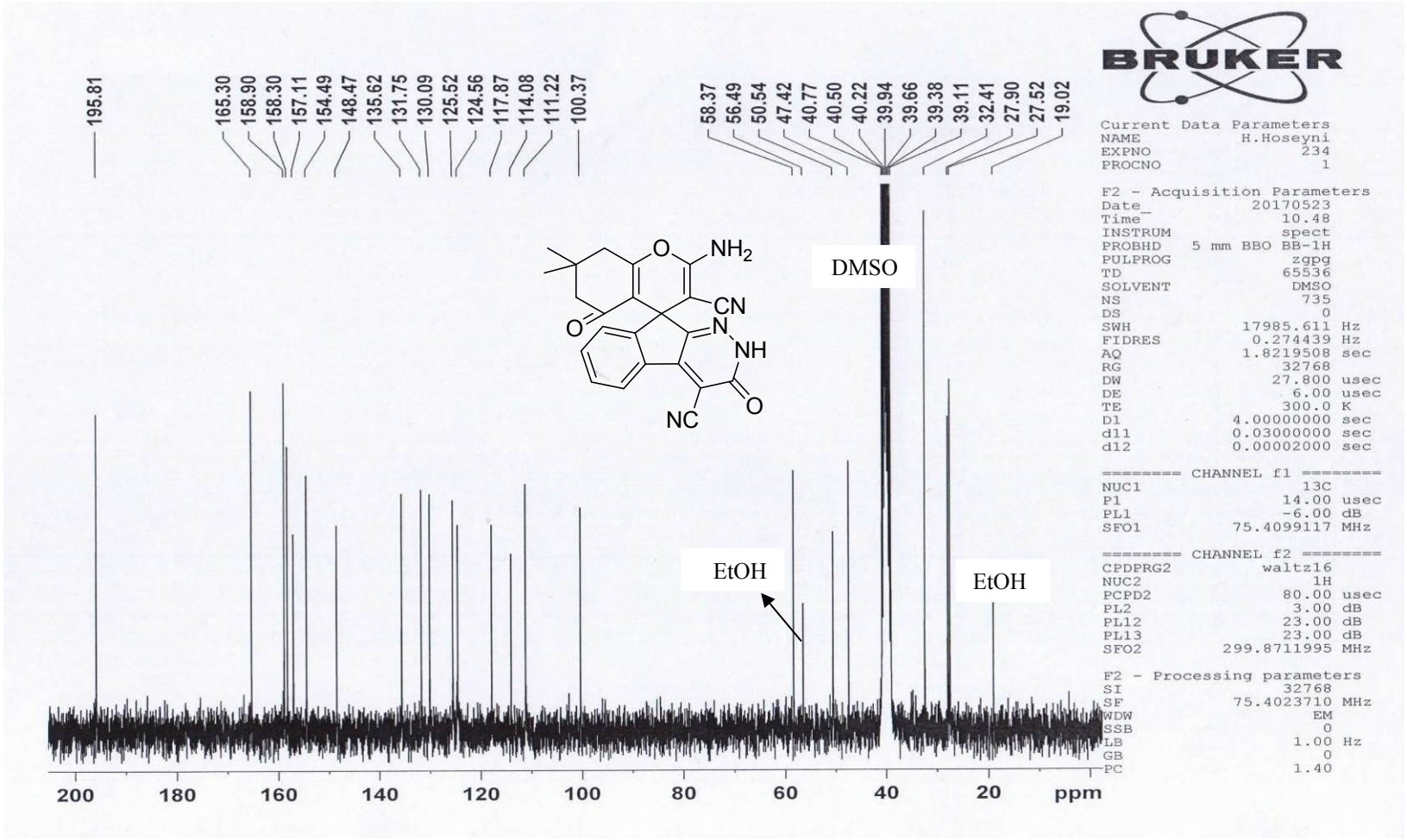
IR of 5d


Abundance
Scan 224 (2.054 min): 30000345.D
77
423
188
215
271
395
51
489
243
163
318
463
99
124
296
346
370
516
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
50
100
150
200
250
300
350
400
450
500
m/z-->

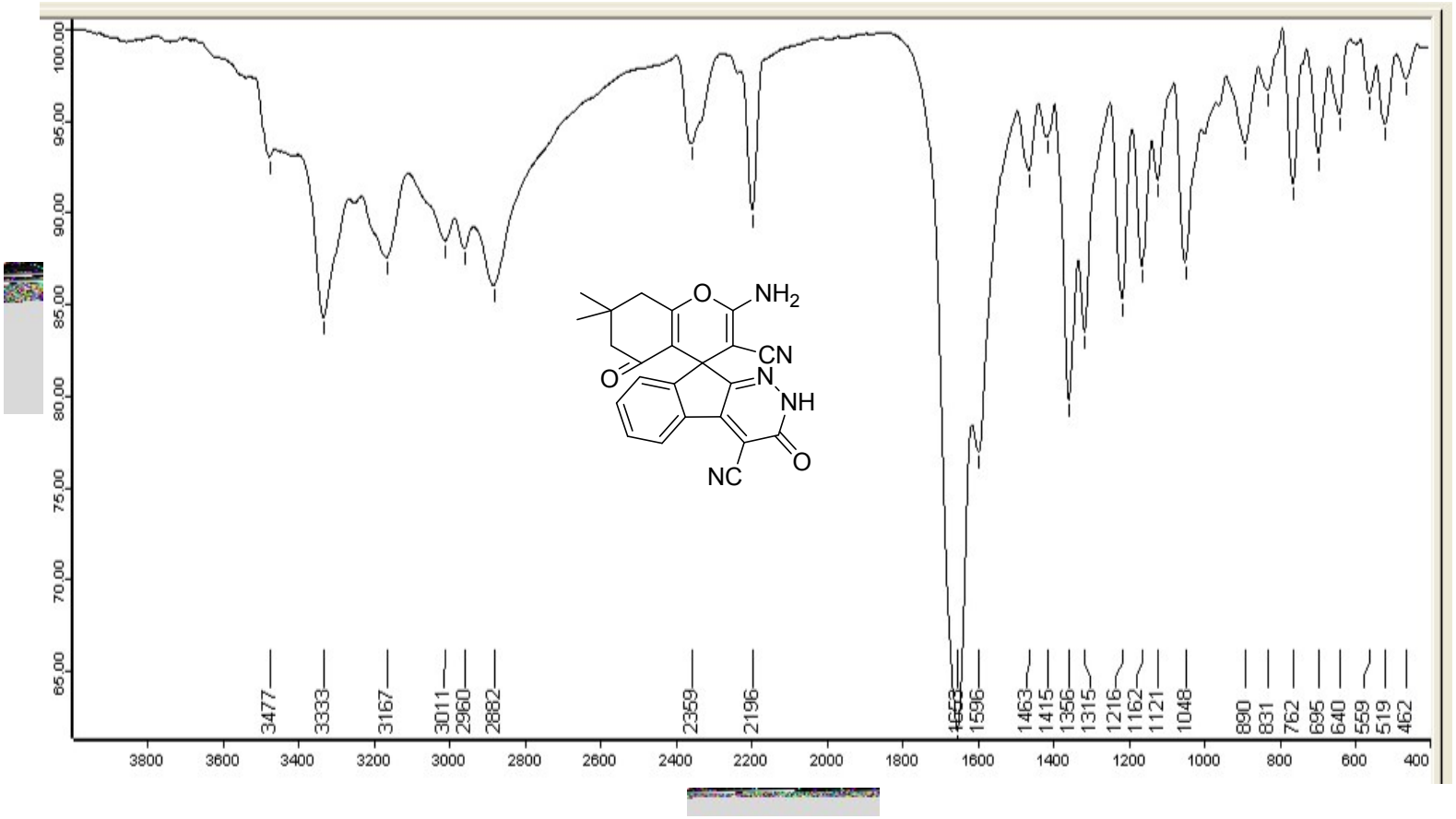
MS of 5d


BRUKER
13.520
8.170
8.144
7.741
7.716
7.691
7.639
7.614
7.588
7.533
7.508
7.439
4.350
3.438
3.414
3.337
3.276
2.676
2.616
2.604
2.545
2.480
2.141
2.087
2.049
1.995
1.056
1.033
[1] H-NMR with D2O
DMSO
DMSO
EtOH
EtOH
ppm
1.000
1.136
1.020
1.296
3.059
2.359
2.251
6.458
Current Data Parameters
NAME H.Hoseyni
EXPNO 233
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170521
Time 13.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 6
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 143.7
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
SI 32768
SF 299.8700035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

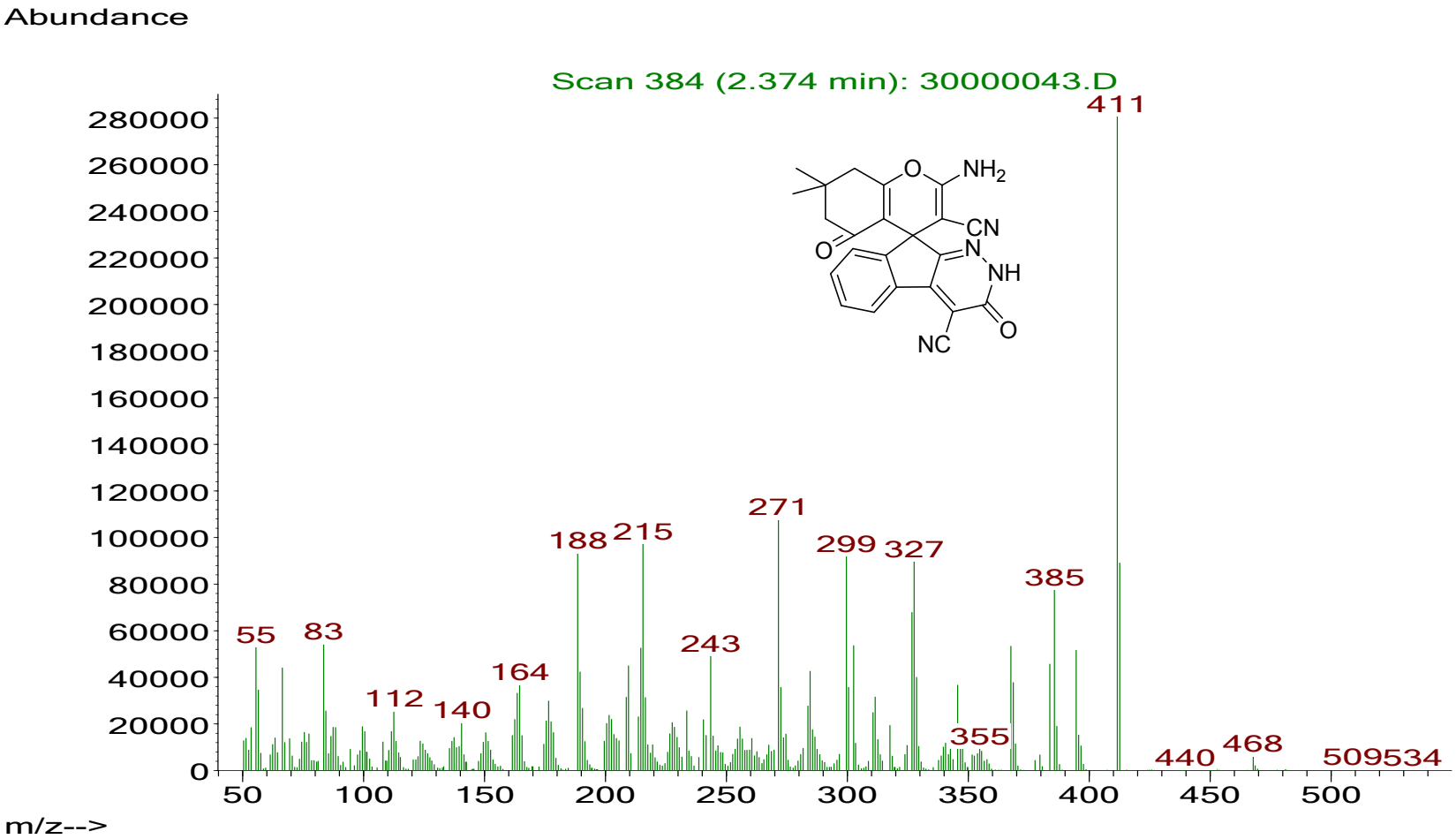
[1]H NMR of 5e


195.81
165.30
158.90
158.30
157.11
154.49
148.47
135.62
131.75
130.09
125.52
124.56
117.87
114.08
111.22
100.37
58.37
56.49
50.54
47.42
40.77
40.50
40.22
39.94
39.66
39.38
39.11
32.41
27.90
27.52
19.02
DMSO
EtOH
EtOH
O
NH2
CN
N
NH
O
O
NC
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 234
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170523
Time 10.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 735
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

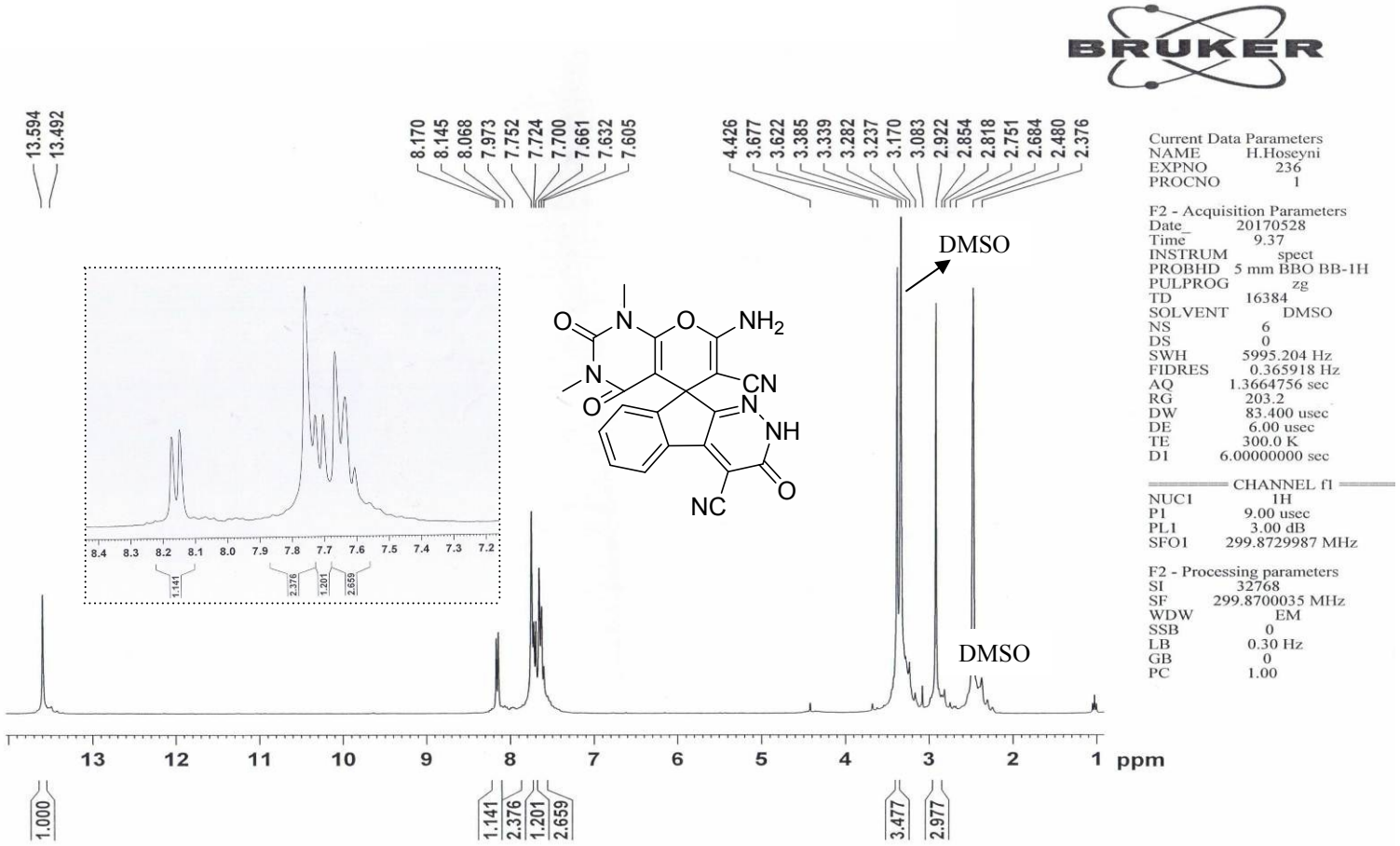
^{13}C NMR of 5e


100.00
95.00
90.00
85.00
80.00
75.00
70.00
65.00
3477
3333
3167
3011
2960
2882
2359
2196
1653
1596
1463
1415
1356
1315
1216
1162
1121
1048
890
831
762
695
640
559
519
462
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
O
NH2
CN
N
NH
O
O
NC

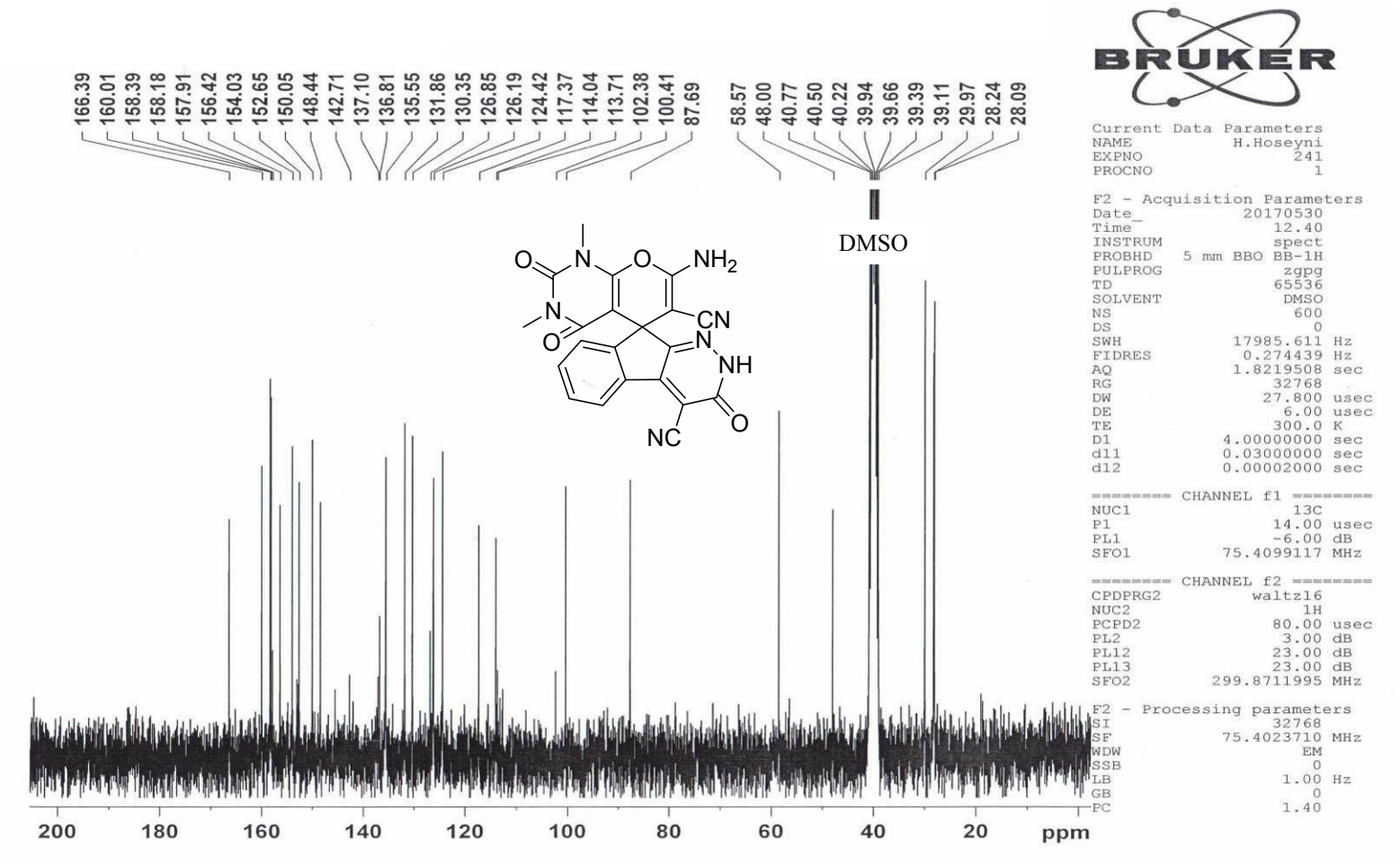
IR of 5e


Abundance
Scan 384 (2.374 min): 30000043.D
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
411
271
188
215
299
327
385
55
83
243
164
112
140
355
440
468
509534
50
100
150
200
250
300
350
400
450
500
m/z-->

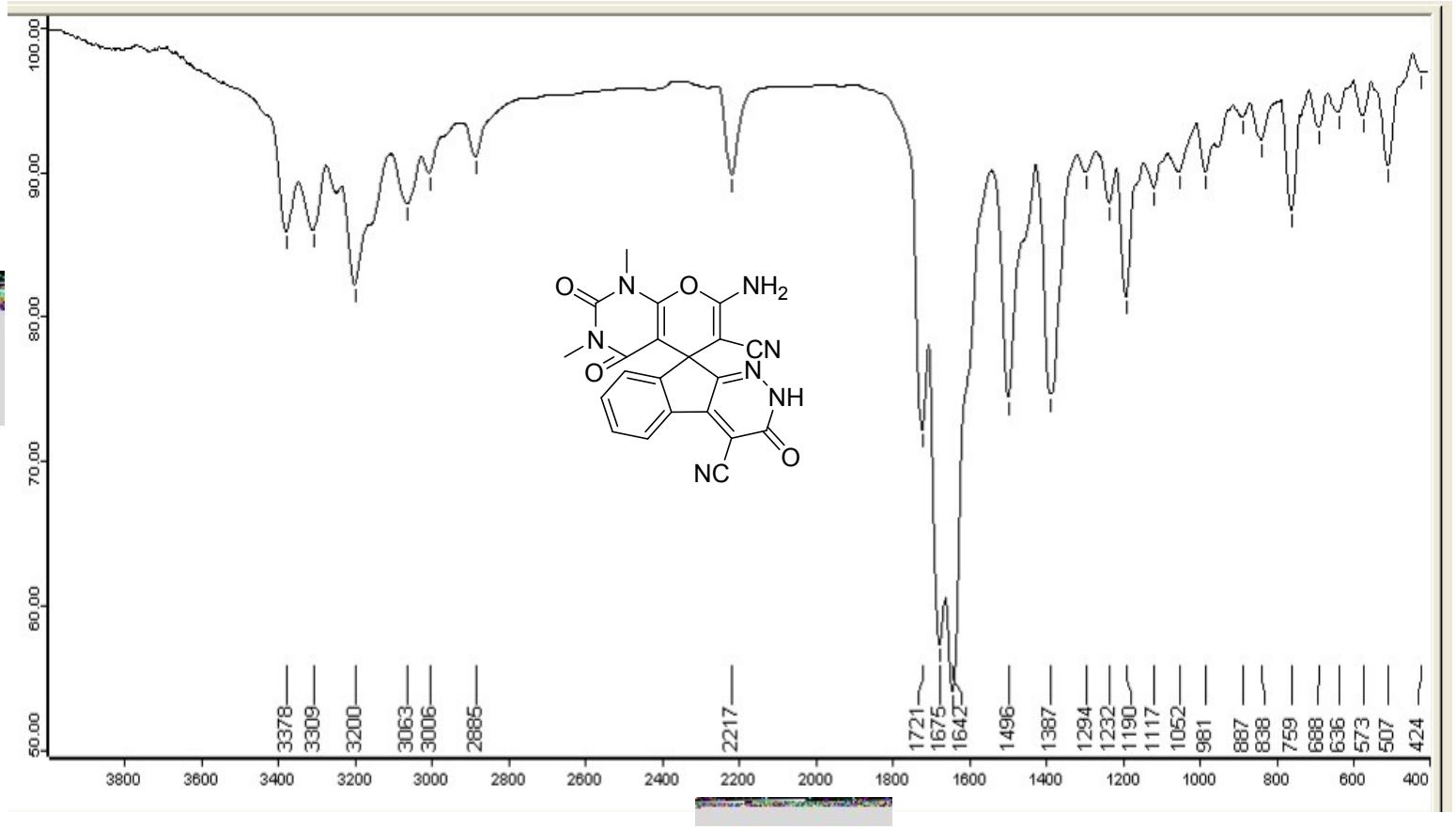
MS of 5e


BRUKER
13.594
13.492
8.170
8.145
8.068
7.973
7.752
7.724
7.700
7.661
7.632
7.605
4.426
3.677
3.622
3.385
3.339
3.282
3.237
3.170
3.083
2.922
2.854
2.818
2.751
2.684
2.480
2.376
DMSO
DMSO
NH2
CN
NH
NC
Current Data Parameters
NAME H.Hoseyni
EXPNO 236
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170528
Time 9.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 6
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 203.2
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
SI 32768
SF 299.8700035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
1.000
1.141
2.376
1.201
2.659
3.477
2.977

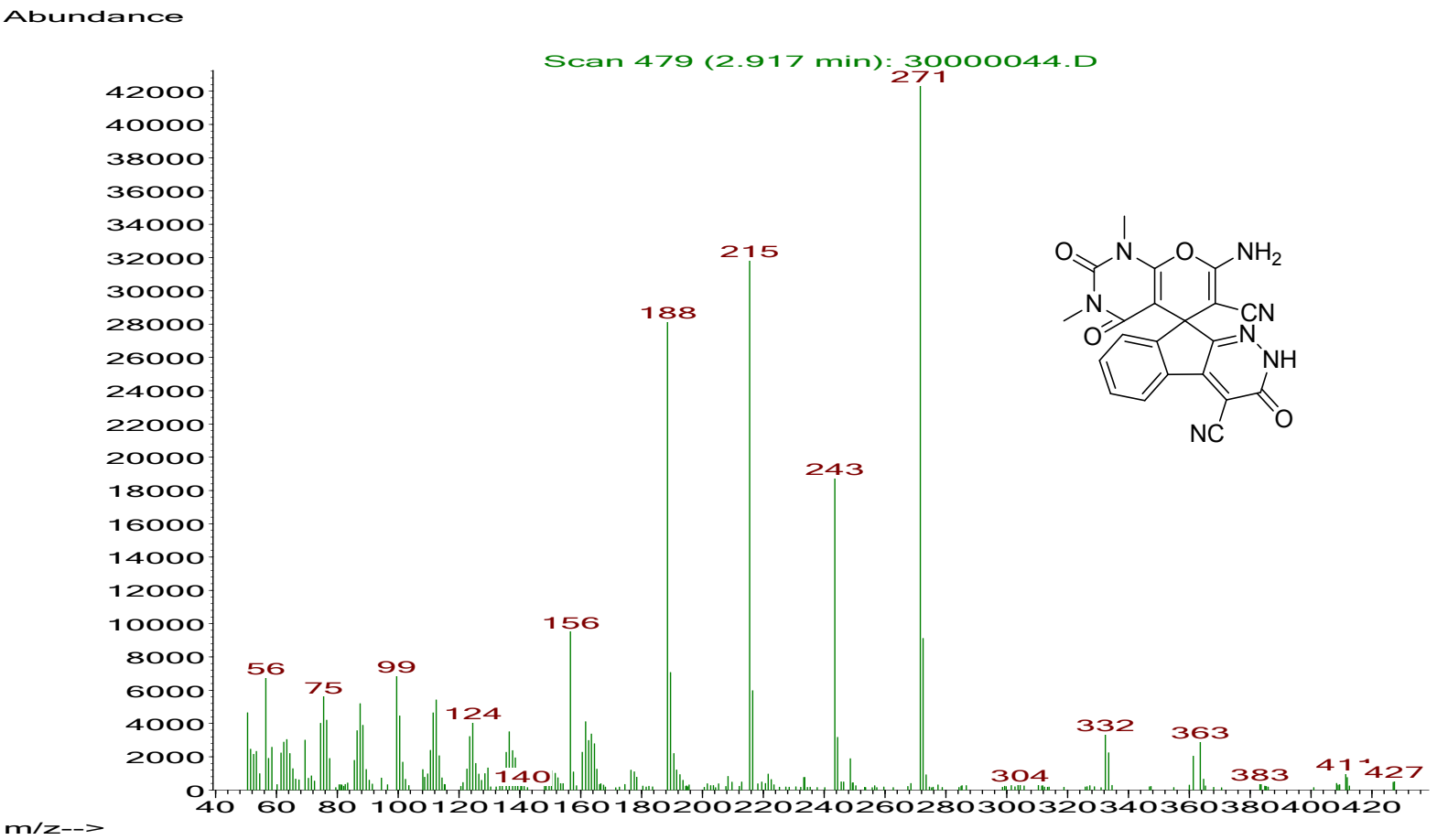
^{1}H NMR of 5f


166.39
160.01
158.39
158.18
157.91
156.42
154.03
152.65
150.05
148.44
142.71
137.10
136.81
135.55
131.86
130.35
126.85
126.19
124.42
117.37
114.04
113.71
102.38
100.41
87.69
58.57
48.00
40.77
40.50
40.22
39.94
39.66
39.39
39.11
29.97
28.24
28.09
DMSO
O
N
O
NH2
N
CN
O
N
NH
O
NC
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 241
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170530
Time 12.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 600
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

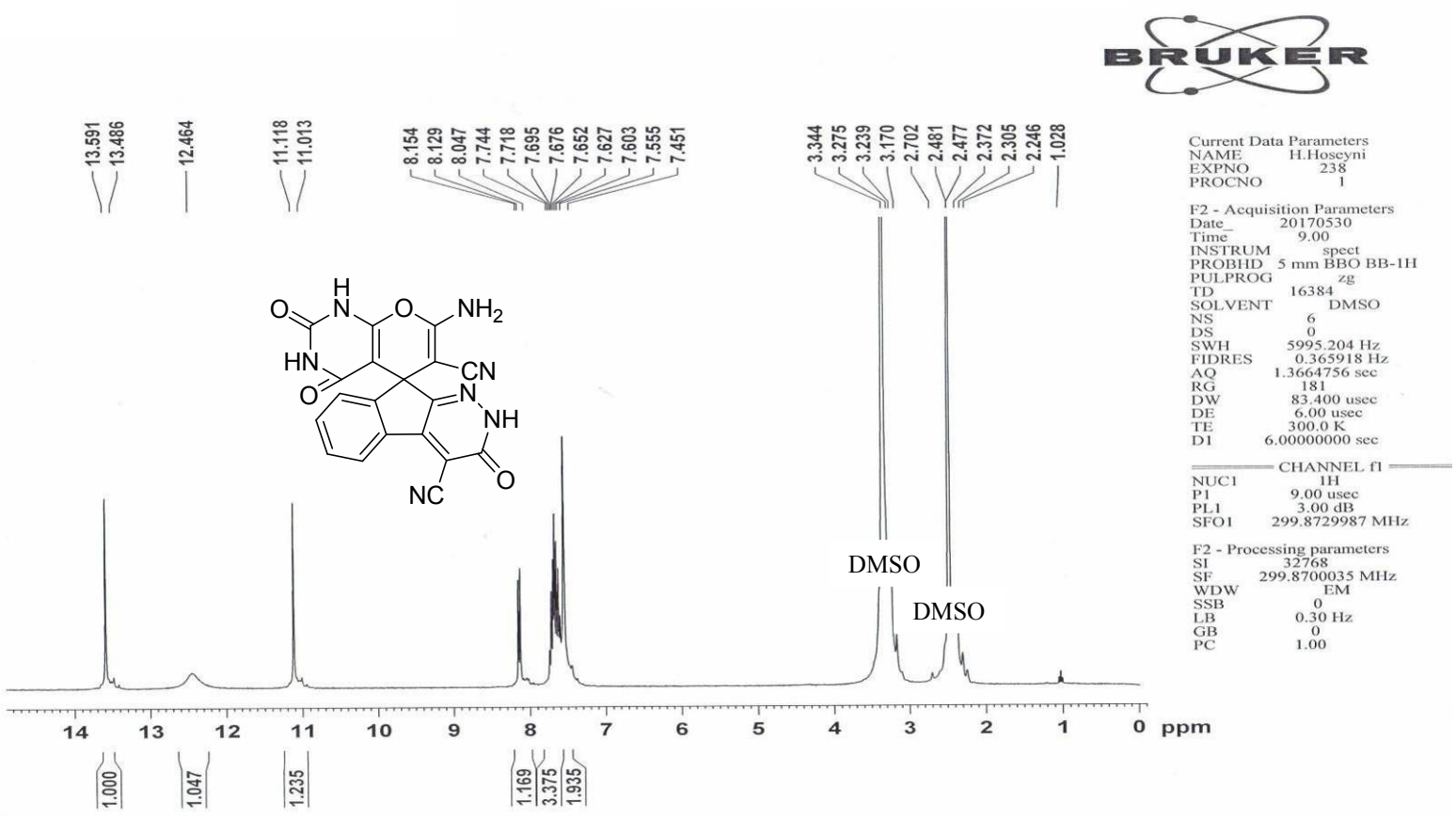
^{13}C NMR of 5f


100.00
90.00
80.00
70.00
60.00
50.00
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
3378
3309
3200
3063
3006
2885
2217
1721
1675
1642
1496
1387
1294
1232
1190
1117
1052
981
887
838
759
688
636
573
507
424
O
N
O
NH2
N
CN
O
N
NH
O
NC

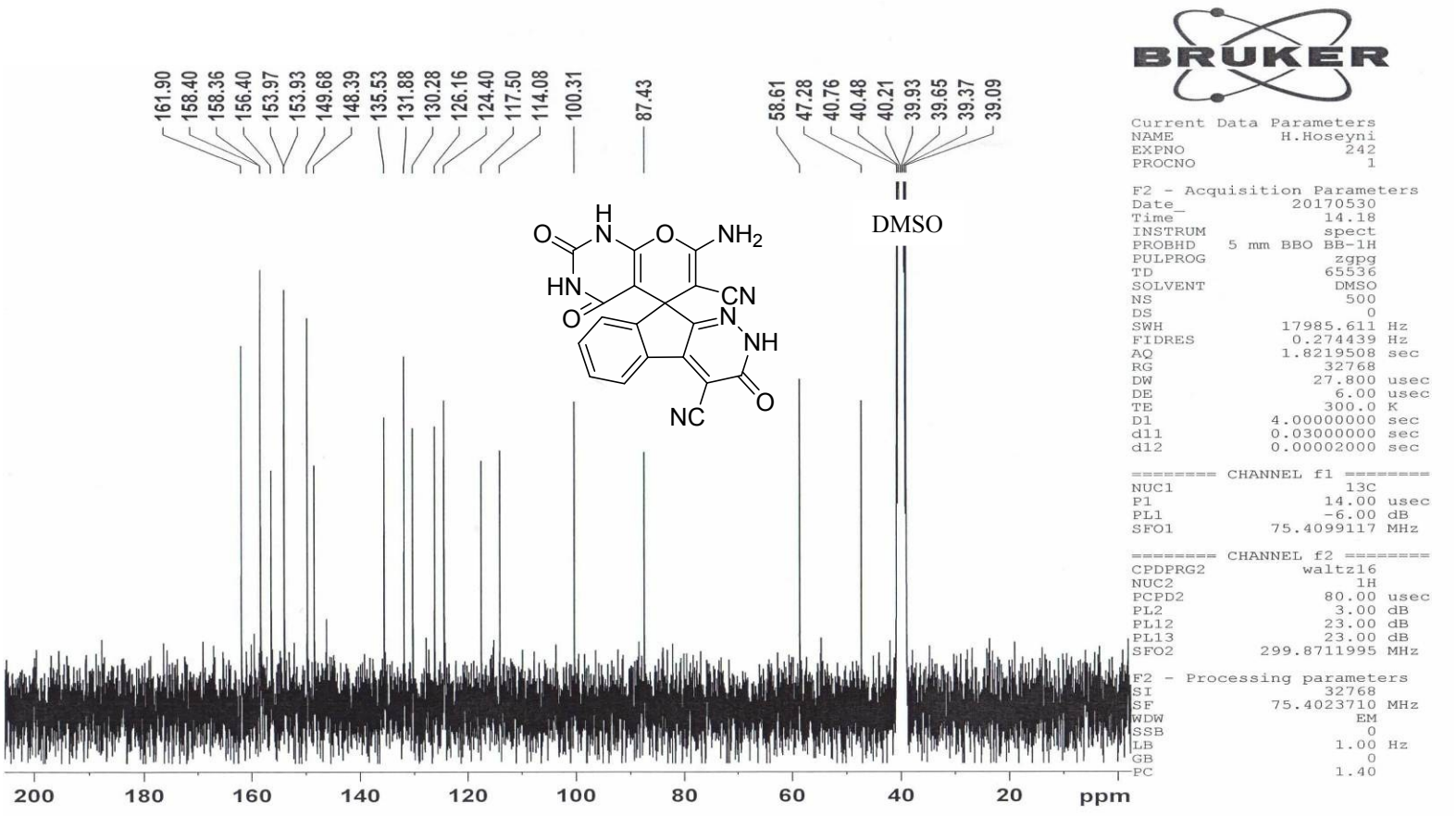
IR of 5f


Abundance
Scan 479 (2.917 min): 30000044.D
271
215
188
243
156
56
75
99
124
140
304
332
363
383
427
m/z-->

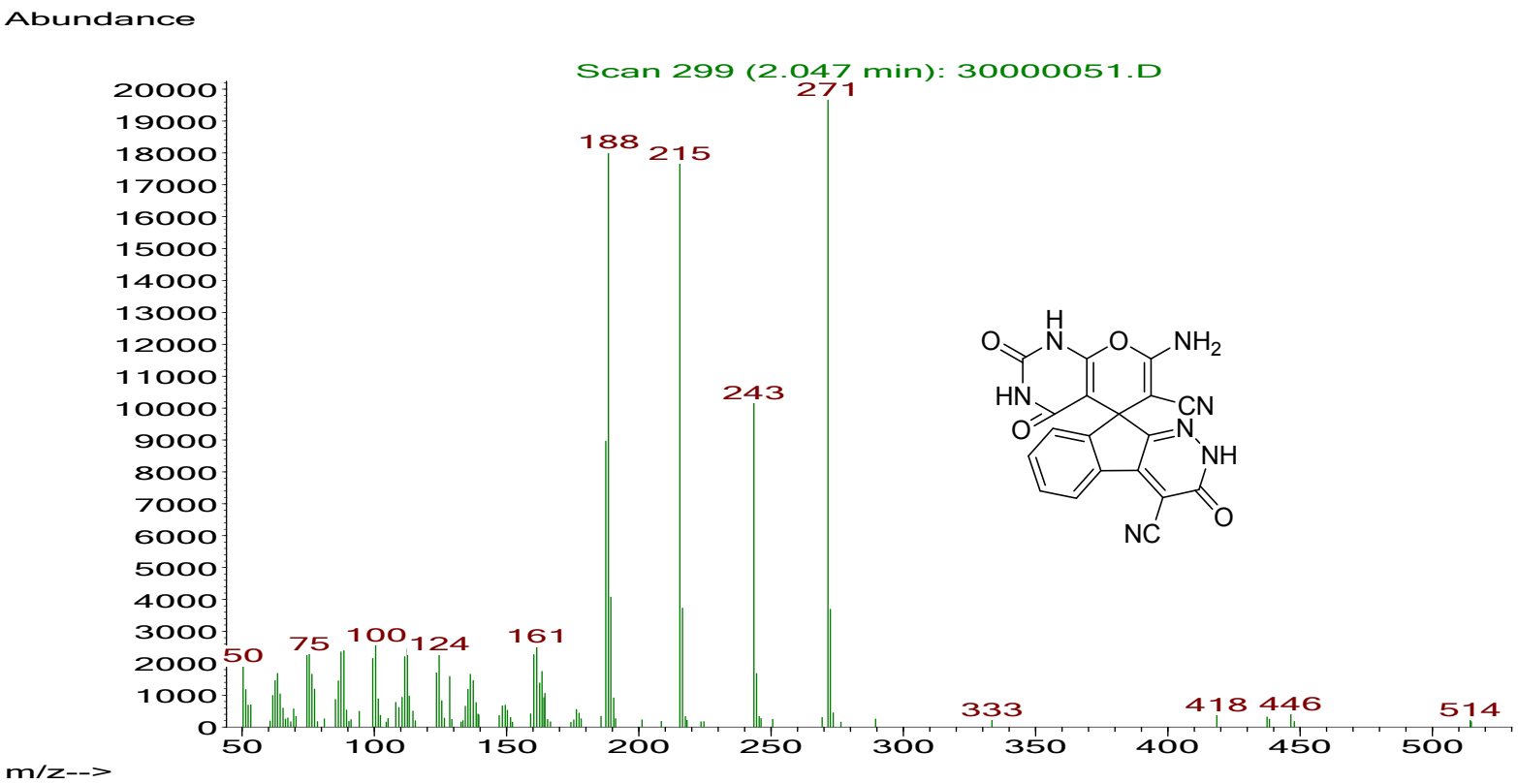
MS of 5f


BRUKER
13.591
13.486
12.464
11.118
11.013
8.154
8.129
8.047
7.744
7.718
7.695
7.676
7.652
7.627
7.603
7.555
7.451
3.344
3.275
3.239
3.170
2.702
2.481
2.477
2.372
2.305
2.246
1.028
DMSO
DMSO
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.047
1.235
1.169
3.375
1.935
Current Data Parameters
NAME H.Hoscyni
EXPNO 238
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170530
Time 9.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 6
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 181
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
SI 32768
SF 299.8700035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

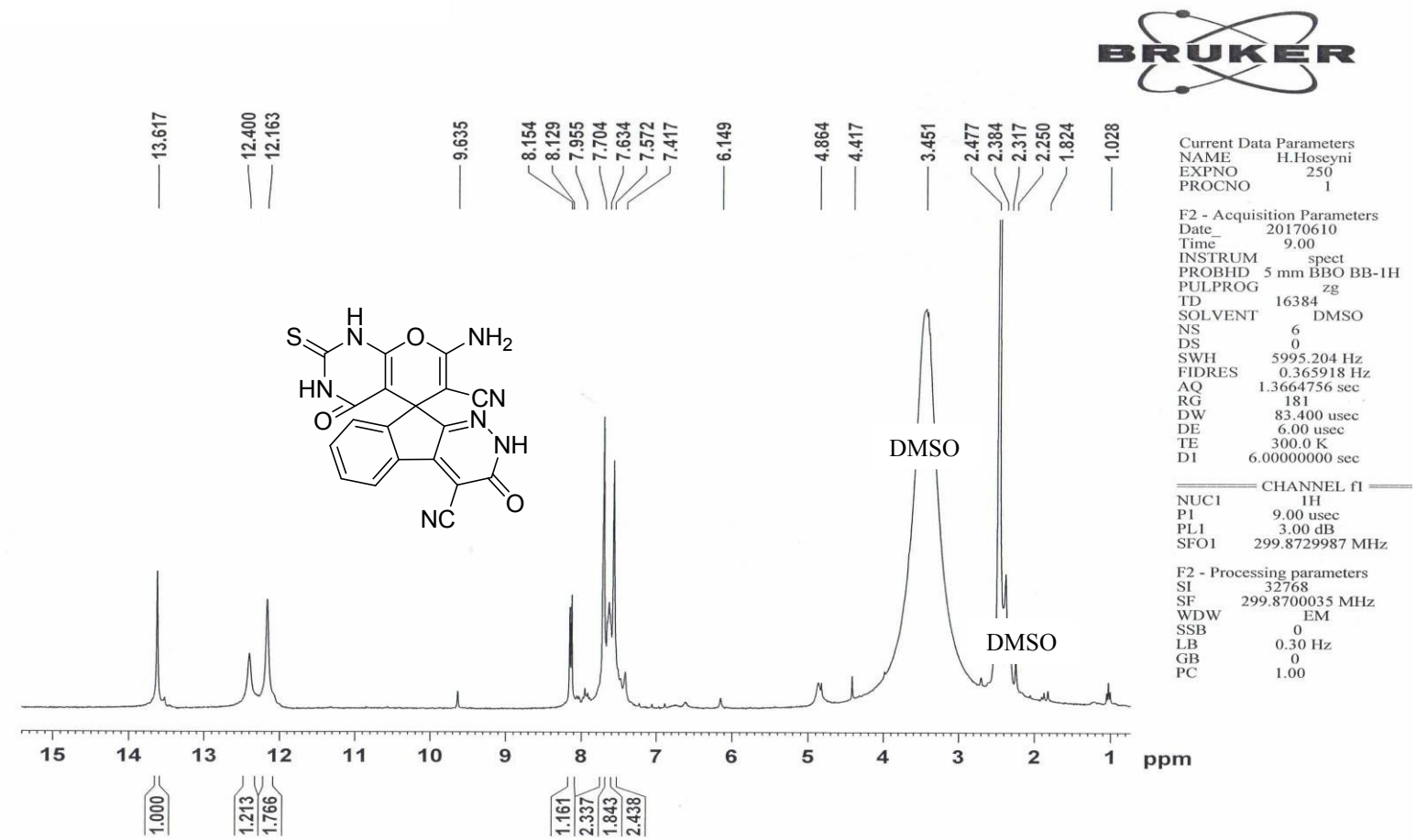
^{1}H NMR of 5g


161.90
158.40
158.36
156.40
153.97
153.93
149.68
148.39
135.53
131.88
130.28
126.16
124.40
117.50
114.08
100.31
87.43
58.61
47.28
40.76
40.48
40.21
39.93
39.65
39.37
39.09
DMSO
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 242
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170530
Time 14.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 500
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

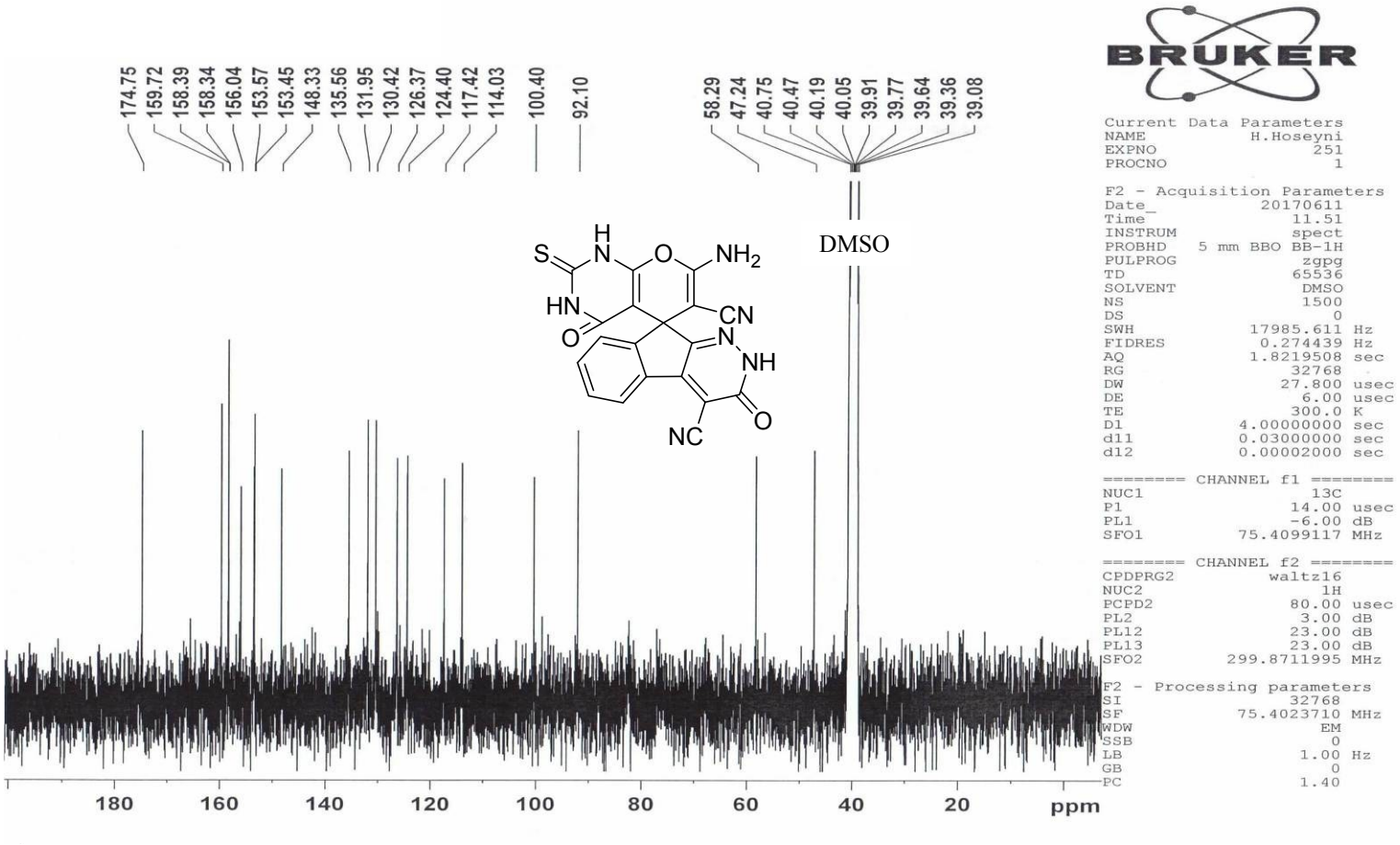
^{13}C NMR of 5g


Abundance
Scan 299 (2.047 min): 30000051.D
271
188
215
243
50
75
100
124
161
333
418
446
514
m/z-->

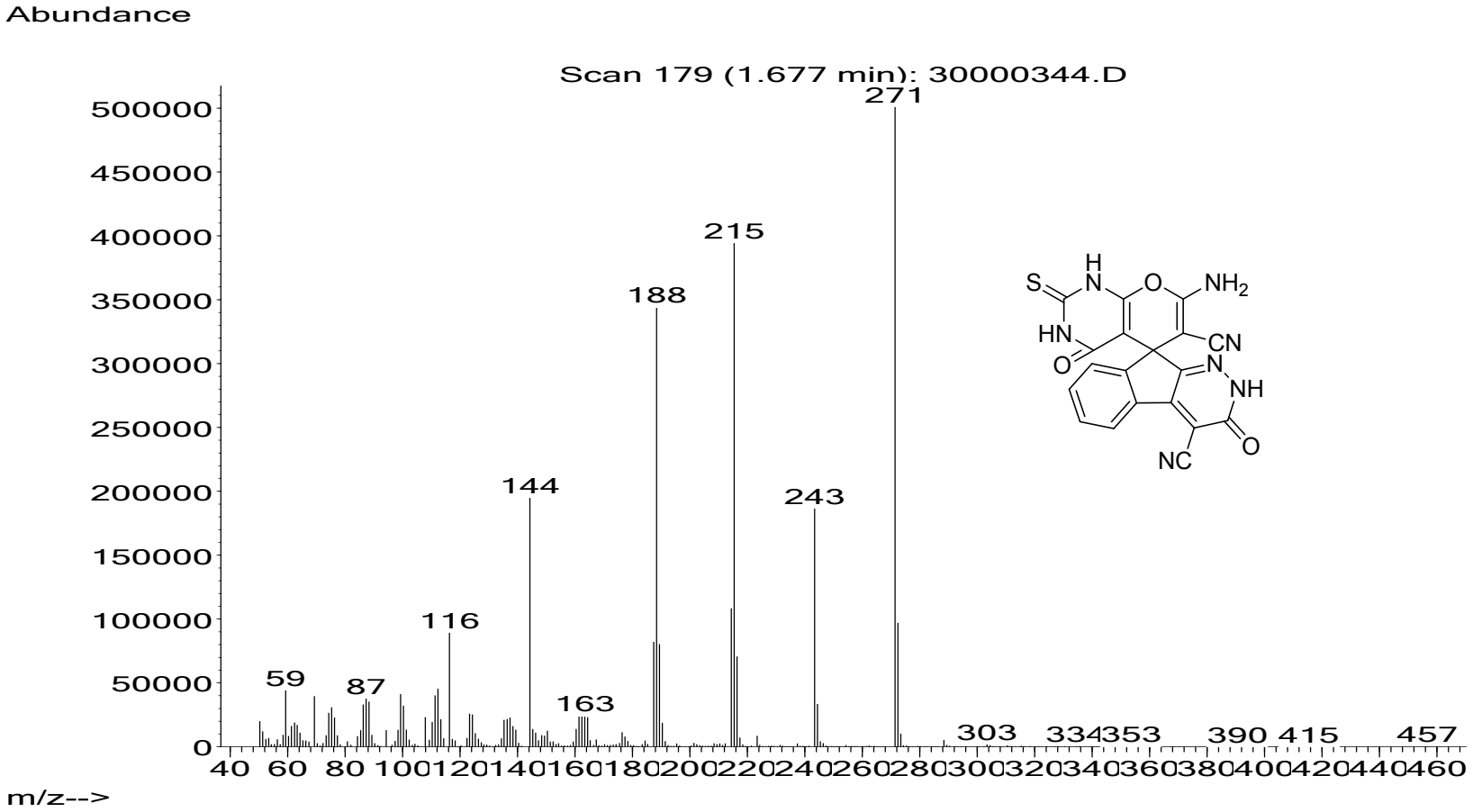
MS of 5g


BRUKER
13.617
12.400
12.163
9.635
8.154
8.129
7.955
7.704
7.634
7.572
7.417
6.149
4.864
4.417
3.451
2.477
2.384
2.317
2.250
1.824
1.028
DMSO
DMSO
Current Data Parameters
NAME H.Hoseyni
EXPNO 250
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170610
Time 9.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 6
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 181
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
SI 32768
SF 299.8700035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.213
1.766
1.161
2.337
1.843
2.438

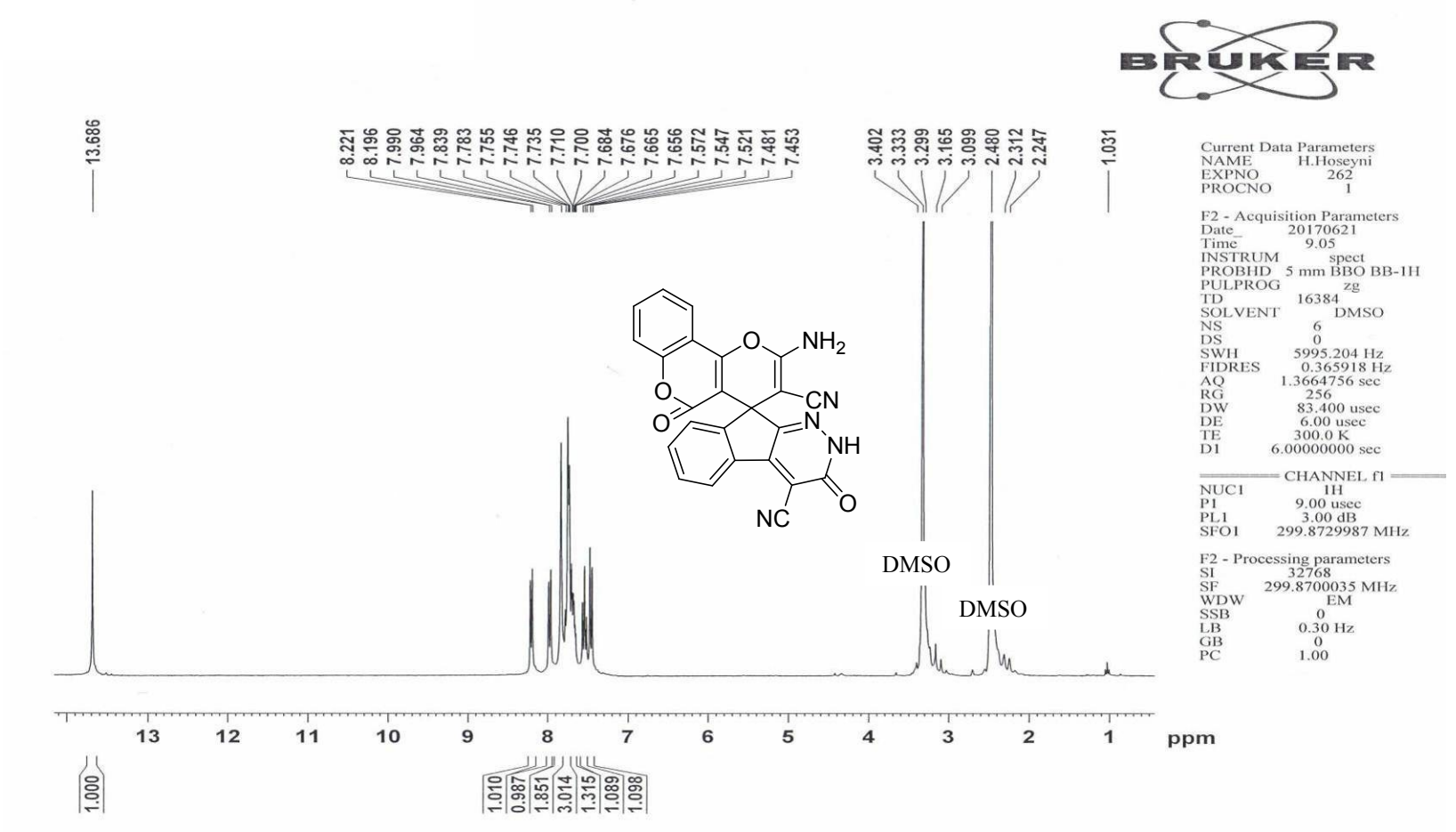
^{1}H NMR of 5h


174.75
159.72
158.39
158.34
156.04
153.57
153.45
148.33
135.56
131.95
130.42
126.37
124.40
117.42
114.03
100.40
92.10
58.29
47.24
40.75
40.47
40.19
40.05
39.91
39.77
39.64
39.36
39.08
DMSO
H
S
N
O
NH2
HN
O
CN
N
NH
O
NC
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 251
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170611
Time 11.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 1500
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

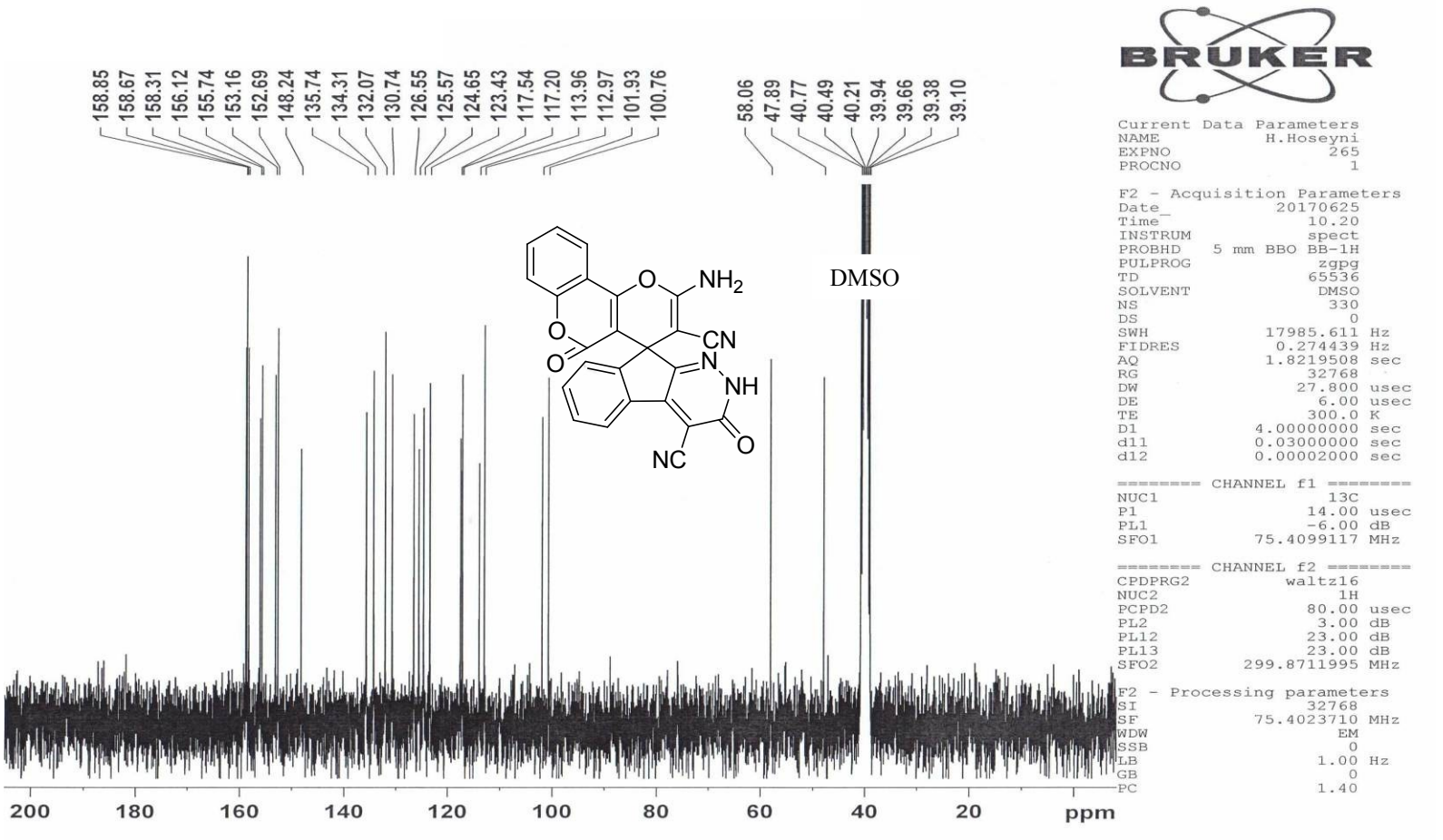
^{13}C NMR of 5h


Abundance
Scan 179 (1.677 min): 30000344.D
271
215
188
144
243
116
59
87
163
303
334
353
390
415
457
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460
m/z-->

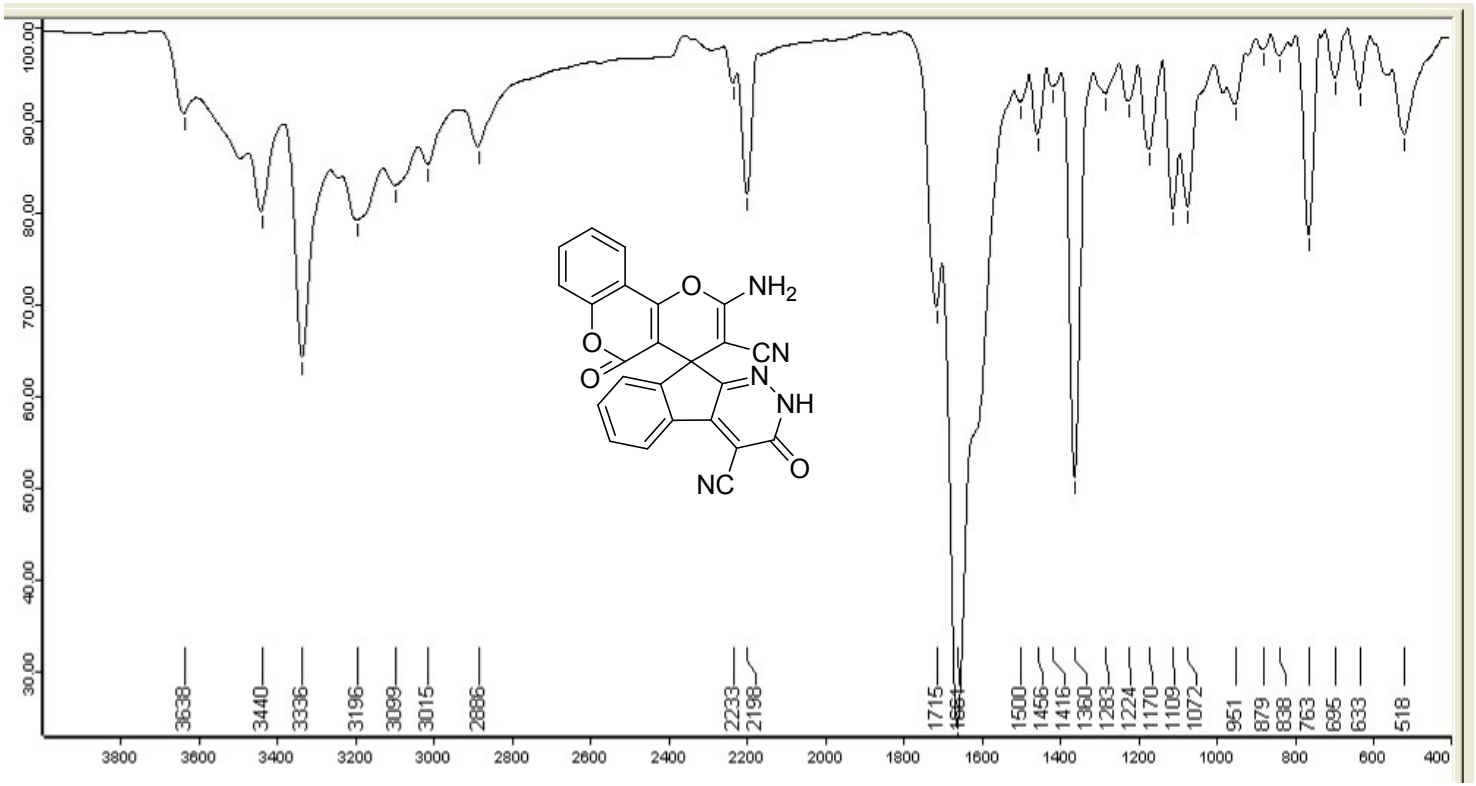
MS of 5h


BRUKER
13.686
8.221
8.196
7.990
7.964
7.839
7.783
7.755
7.746
7.735
7.710
7.700
7.684
7.676
7.665
7.656
7.572
7.547
7.521
7.481
7.453
3.402
3.333
3.299
3.165
3.099
2.480
2.312
2.247
1.031
DMSO
DMSO
NH2
CN
NH
NC
O
O
O
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.010
0.987
1.851
3.014
1.315
1.089
1.098
Current Data Parameters
NAME H.Hoseyni
EXPNO 262
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170621
Time 9.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 6
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 256
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
SI 32768
SF 299.8700035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

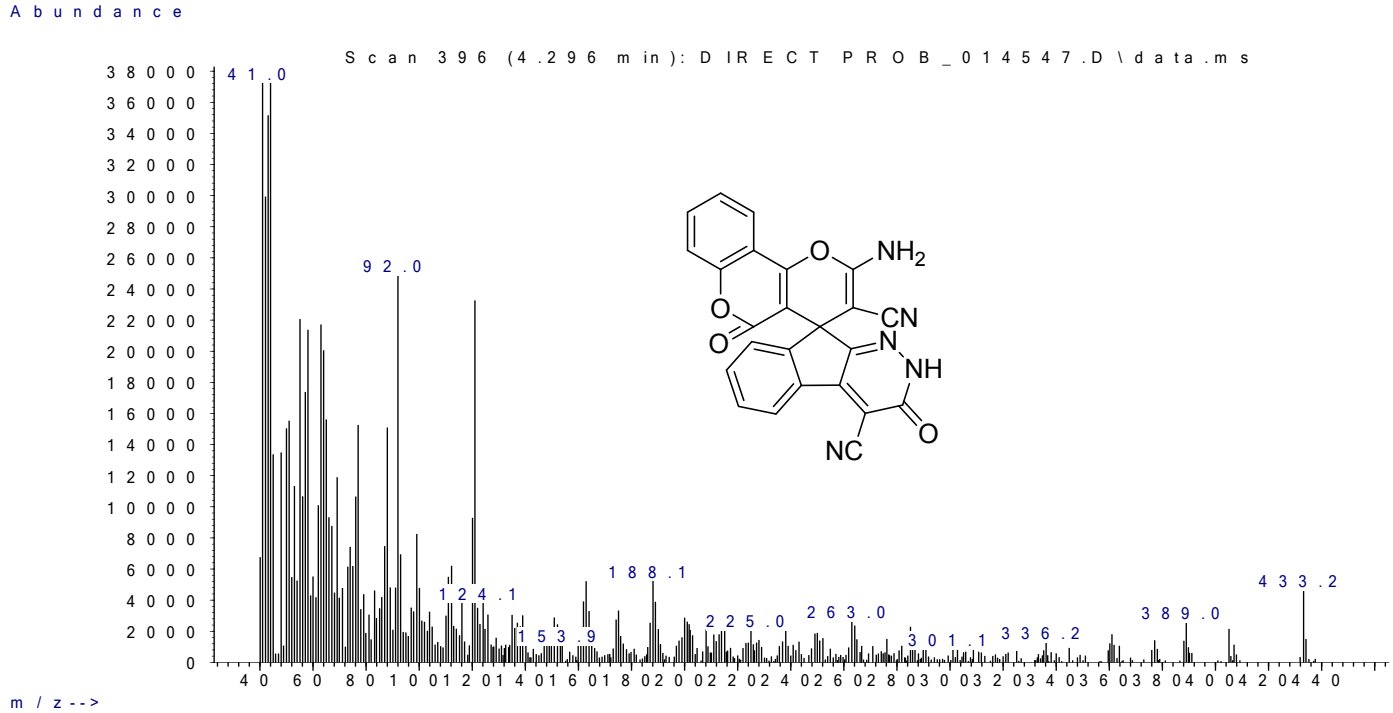
^{1}H NMR of 5i


158.85
158.67
158.31
156.12
155.74
153.16
152.69
148.24
135.74
134.31
132.07
130.74
126.55
125.57
124.65
123.43
117.54
117.20
113.96
112.97
101.93
100.76
58.06
47.89
40.77
40.49
40.21
39.94
39.66
39.38
39.10
DMSO
O
NH2
CN
N
NH
O
O
NC
O
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 265
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170625
Time 10.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 330
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

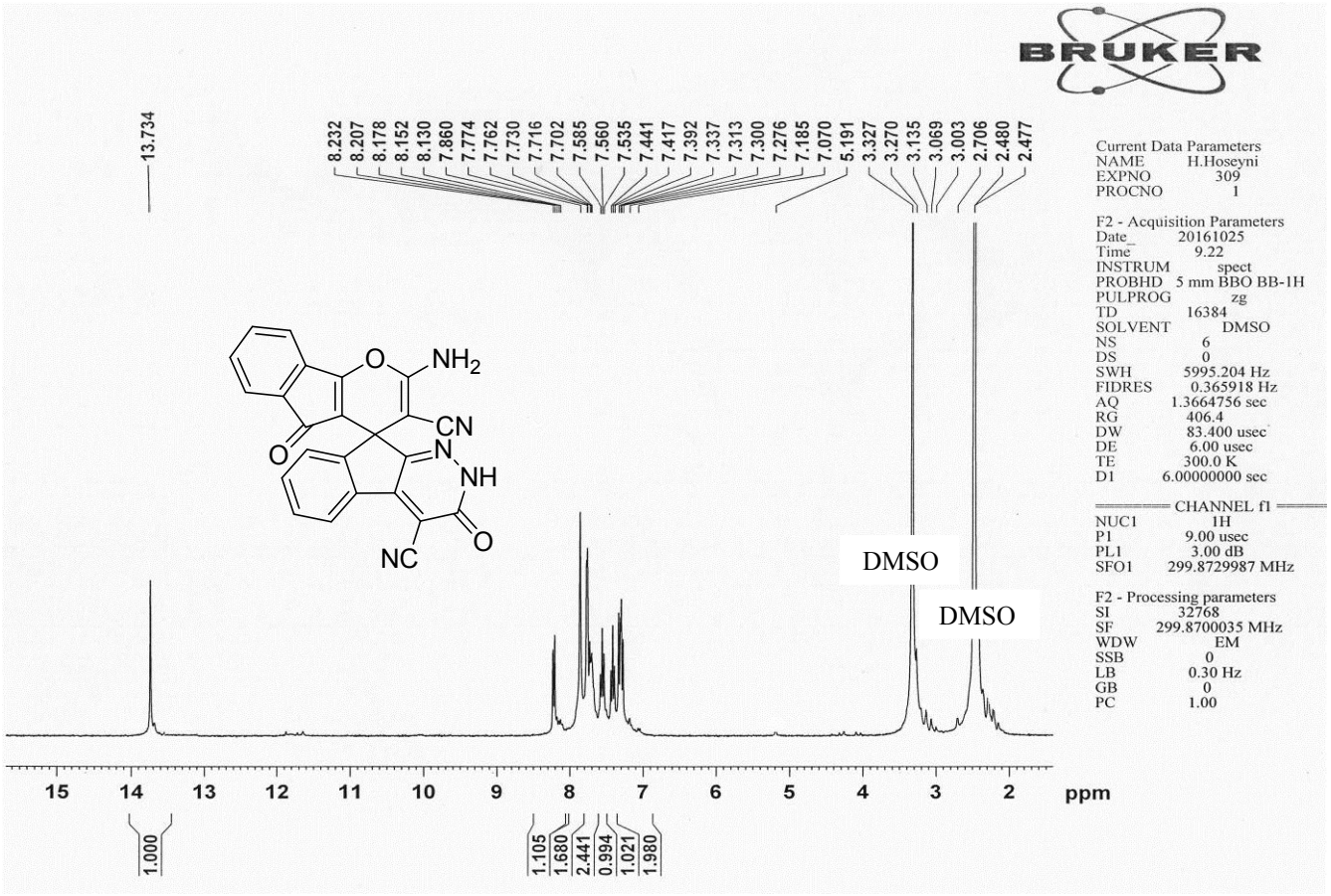
^{13}C NMR of 5i


100.00
90.00
80.00
70.00
60.00
50.00
40.00
30.00
3638
3440
3336
3196
3099
3015
2886
2233
2198
1715
1661
1500
1456
1416
1360
1283
1224
1170
1109
1072
951
879
838
763
695
633
518
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
O
NH2
O
O
CN
N
NH
NC
O

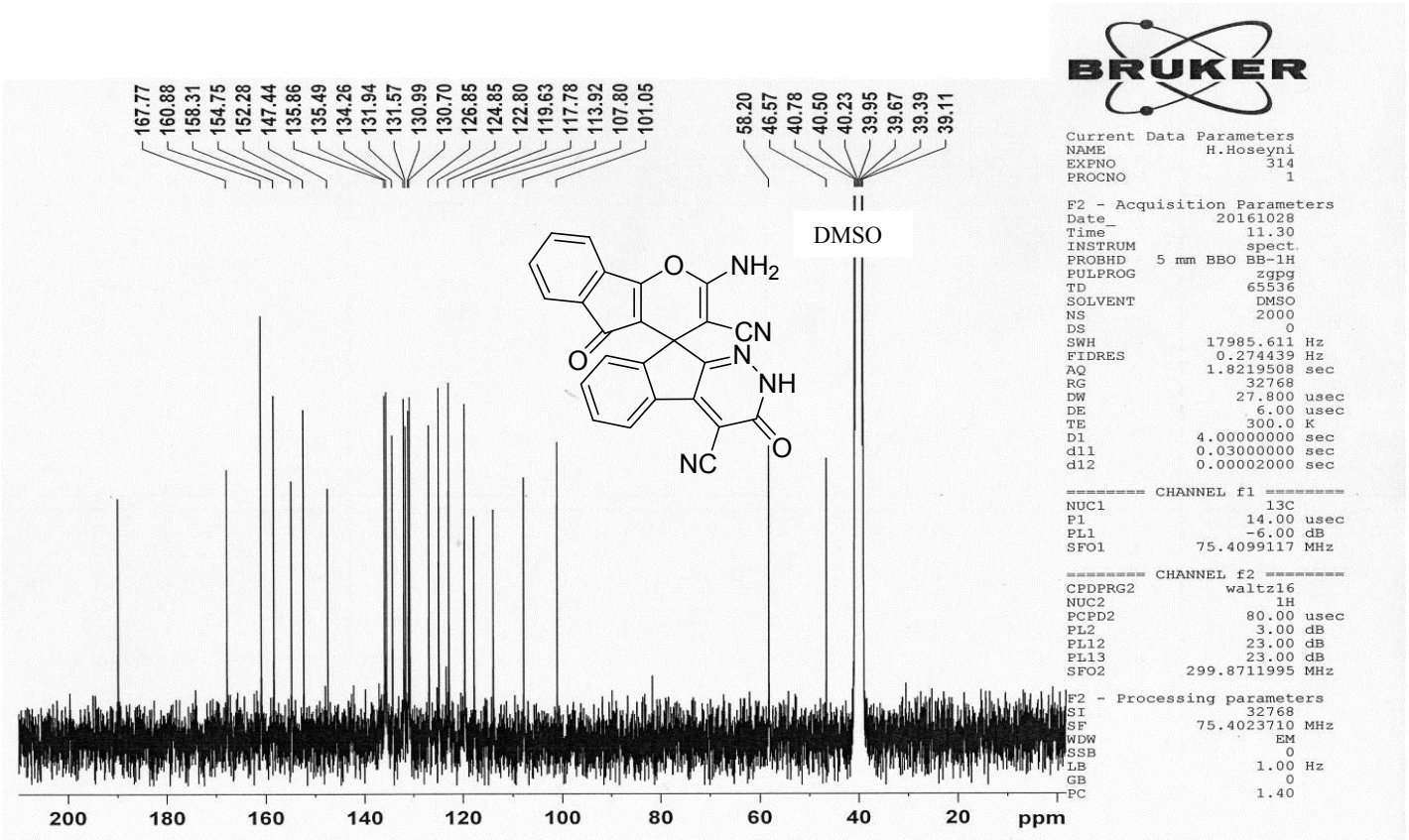
IR of 5i


Abundance
Scan 396 (4.296 min): DIRECT PROB_014547.D\data.ms
41.0
92.0
124.1
153.9
188.1
225.0
263.0
301.1
336.2
389.0
433.2
m/z-->

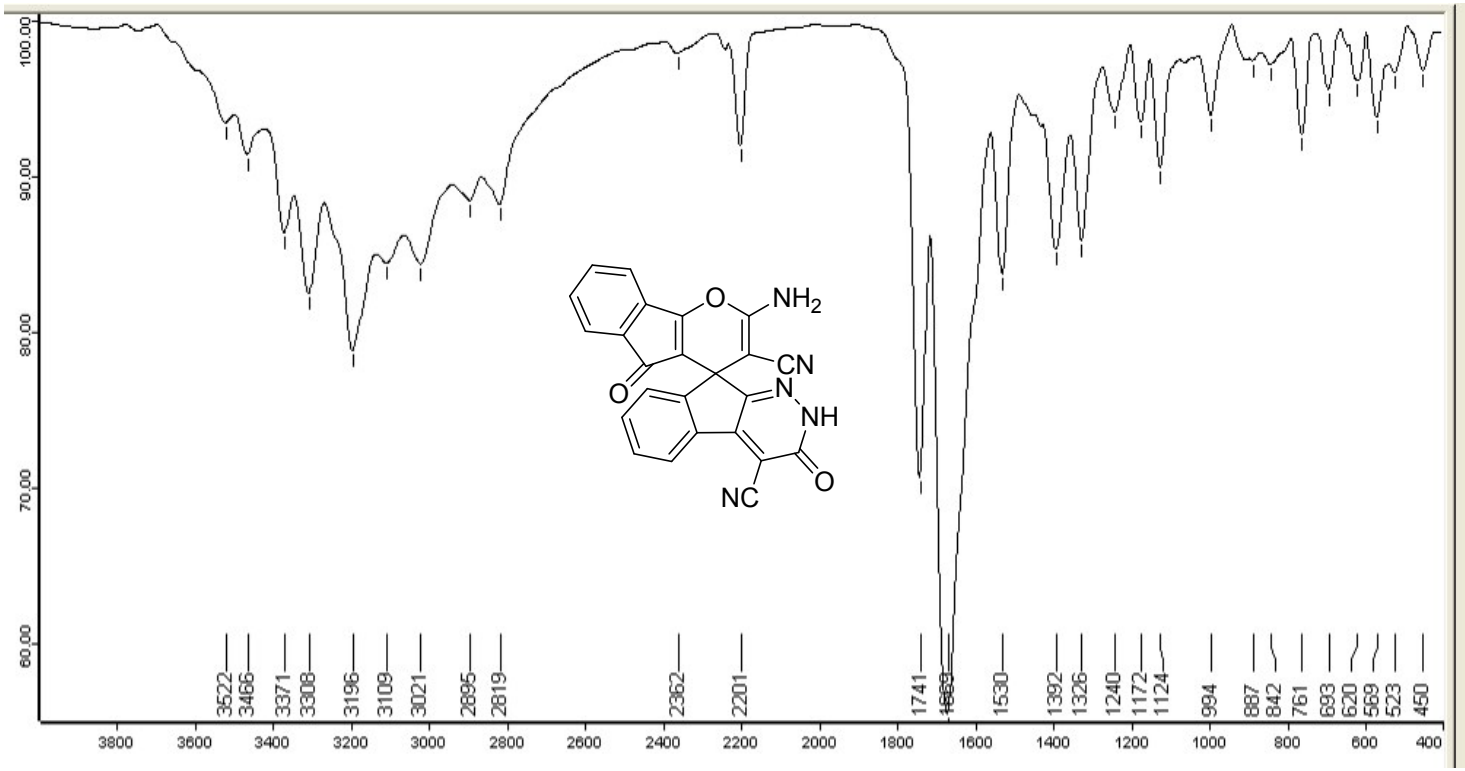
MS of 5i


BRUKER
13.734
8.232
8.207
8.178
8.152
8.130
7.860
7.774
7.762
7.730
7.716
7.702
7.585
7.560
7.535
7.441
7.417
7.392
7.337
7.313
7.300
7.276
7.185
7.070
5.191
3.327
3.270
3.135
3.069
3.003
2.706
2.480
2.477
DMSO
DMSO
15
14
13
12
11
10
9
8
7
6
5
4
3
2
ppm
1.000
1.105
1.680
2.441
0.994
1.021
1.980
Current Data Parameters
NAME H.Hoseyni
EXPNO 309
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 9.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 6
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 406.4
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 299.8729987 MHz
F2 - Processing parameters
SI 32768
SF 299.8700035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR of 5j


167.77
160.88
158.31
154.75
152.28
147.44
135.86
135.49
134.26
131.94
131.57
130.99
130.70
126.85
124.85
122.80
119.63
117.78
113.92
107.80
101.05
58.20
46.57
40.78
40.50
40.23
39.95
39.67
39.39
39.11
DMSO
O
NH2
CN
N
NH
O
O
NC
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 314
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161028
Time 11.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 2000
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 75.4099117 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C NMR of 5j


100.00
90.00
80.00
70.00
60.00
3522
3466
3371
3308
3196
3109
3021
2895
2819
2362
2201
1741
1663
1530
1392
1326
1240
1172
1124
994
887
842
761
693
620
569
523
450
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
O
NH2
CN
N
NH
O
O
NC

IR of 5j