Supporting Information

Synthesis of 5-amino-*N*'-(9*H*-fluoren-9-ylidene)-8-nitro-7-aryl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbohydrazide derivatives based on heterocyclic ketene aminals

Hajar Hosseini, Mohammad Bayat

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.

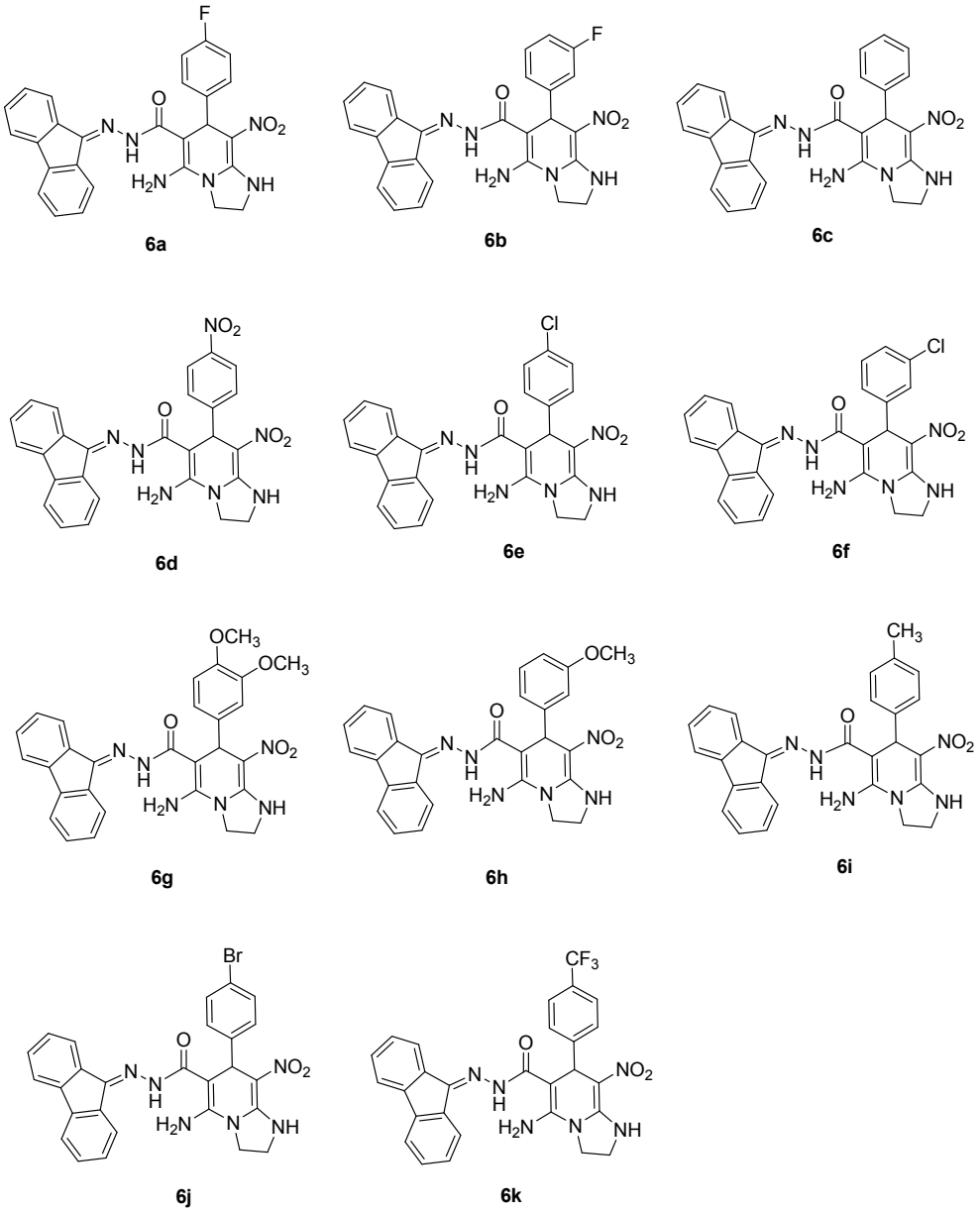
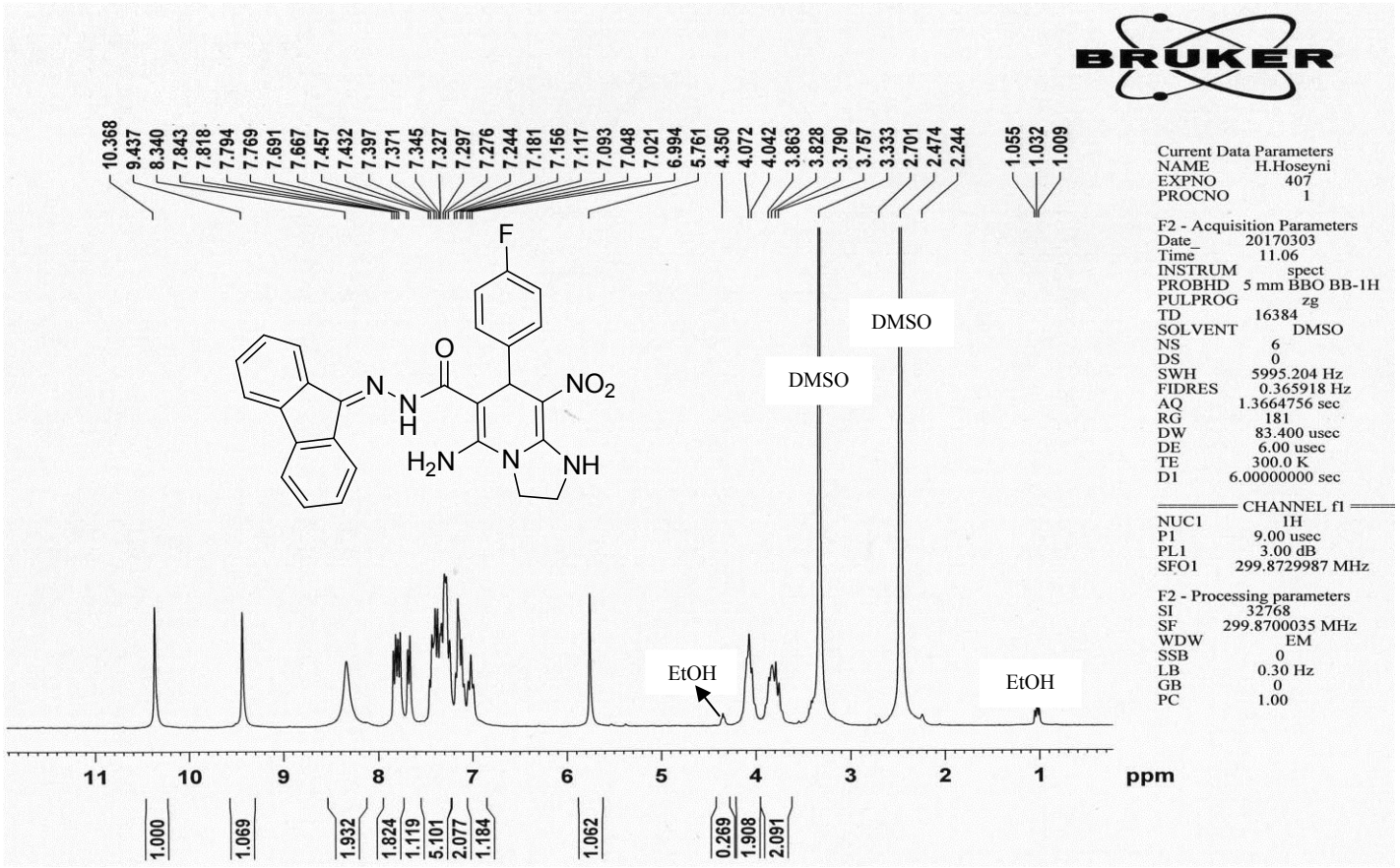


Figure 1. Structure of all products **6a-k.**

The structures of all products **6a-k** were deduced from their IR, mass, ^{1}H NMR, and ^{13}C NMR spectra (see the following images).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7.397
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2.474
2.244
1.055
1.032
1.009
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DMSO
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EtOH
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8
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6
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4
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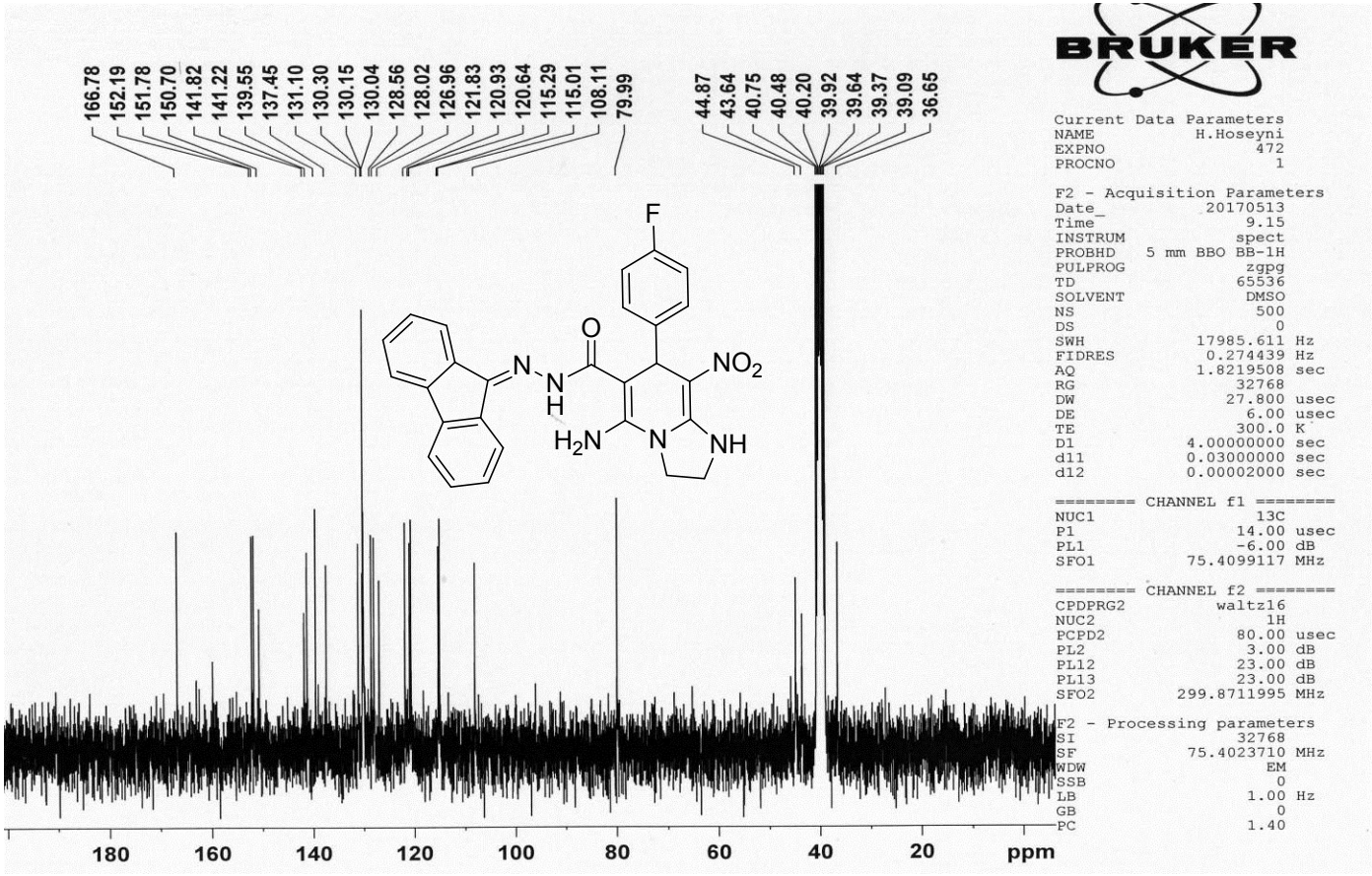
^{1}H NMR of 6a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39.92
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39.37
39.09
36.65
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N
H
NO2
H2N
N
NH
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SFO1 75.4099117 MHz
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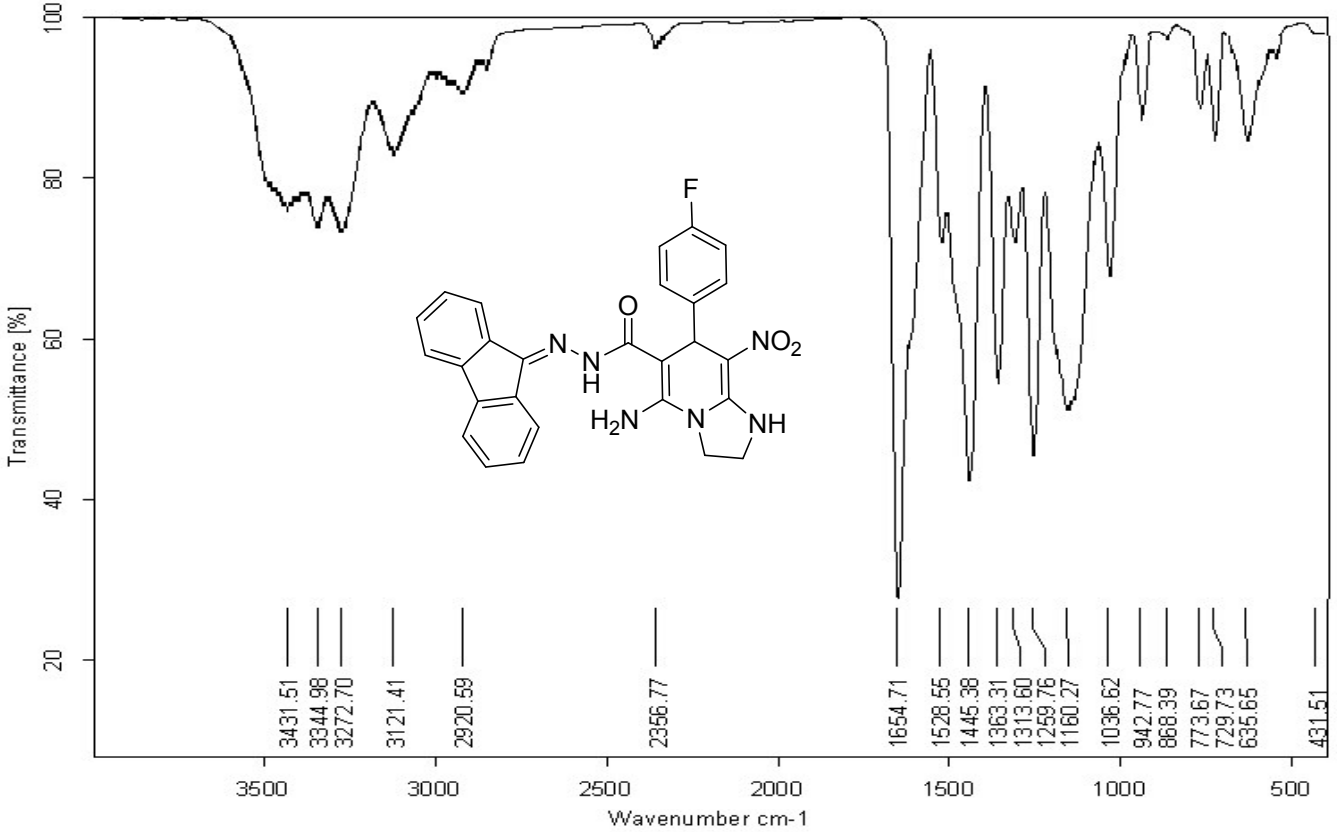
^{13}C NMR of 6a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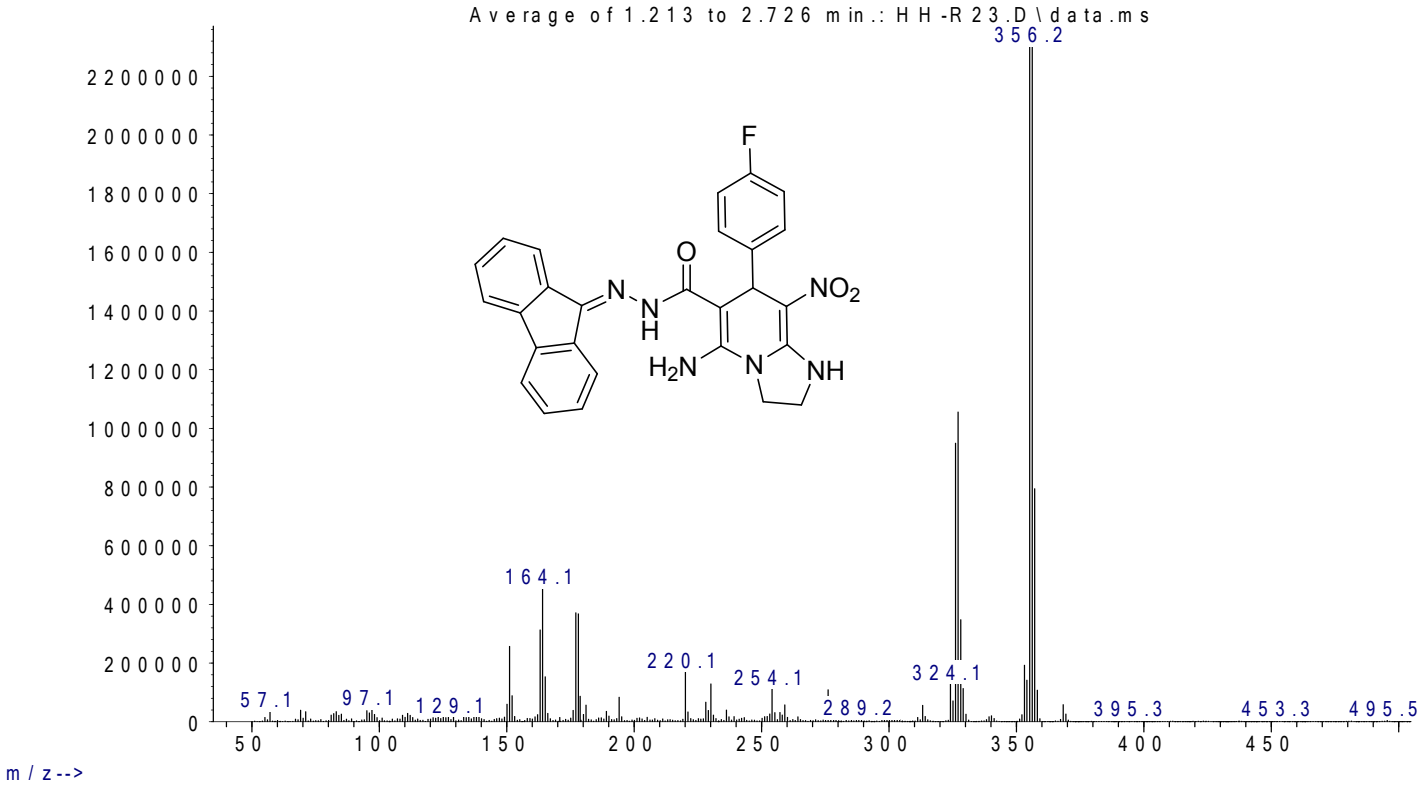
NH

IR of 6a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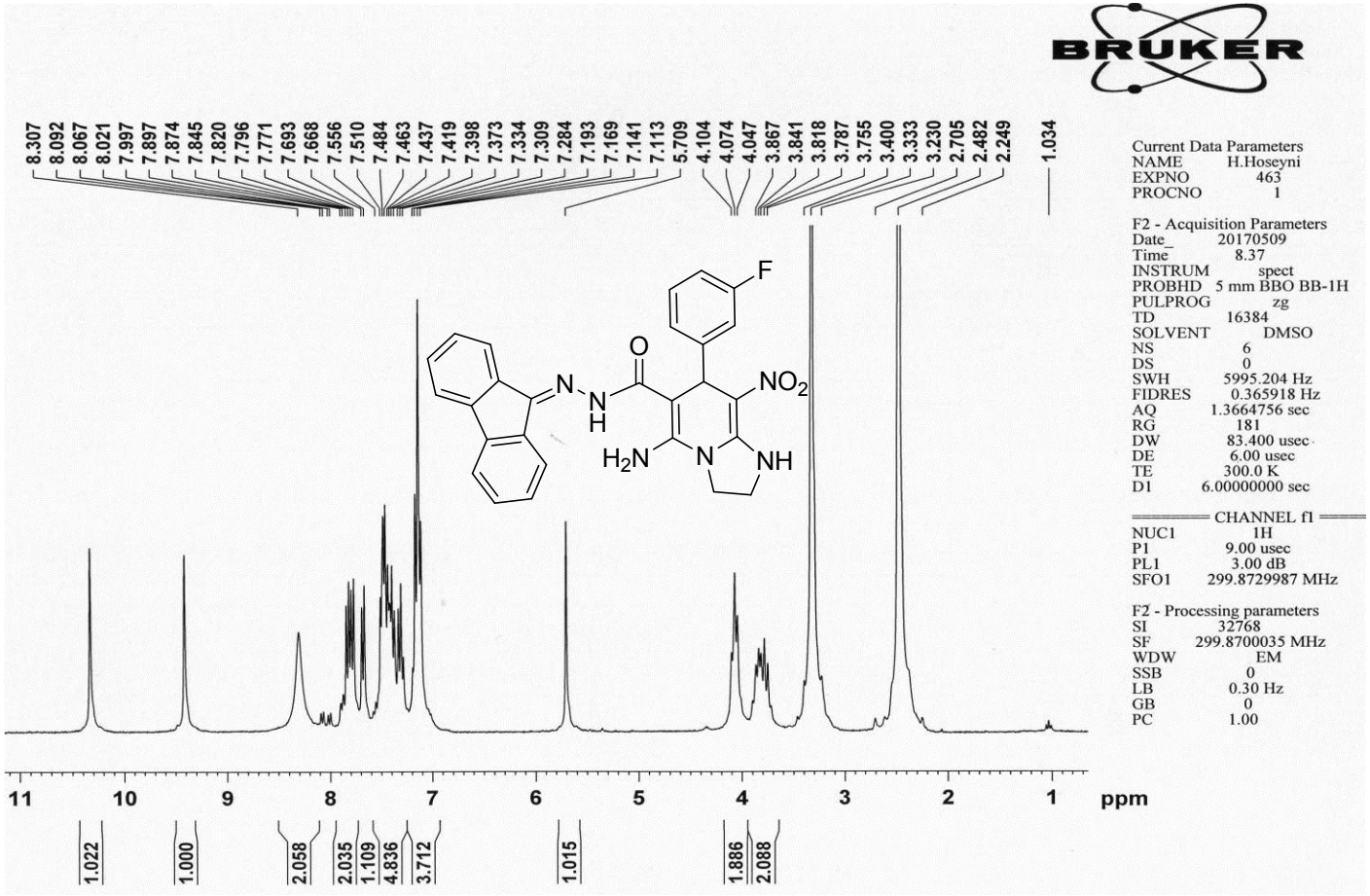
MS of 6a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O
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N
H
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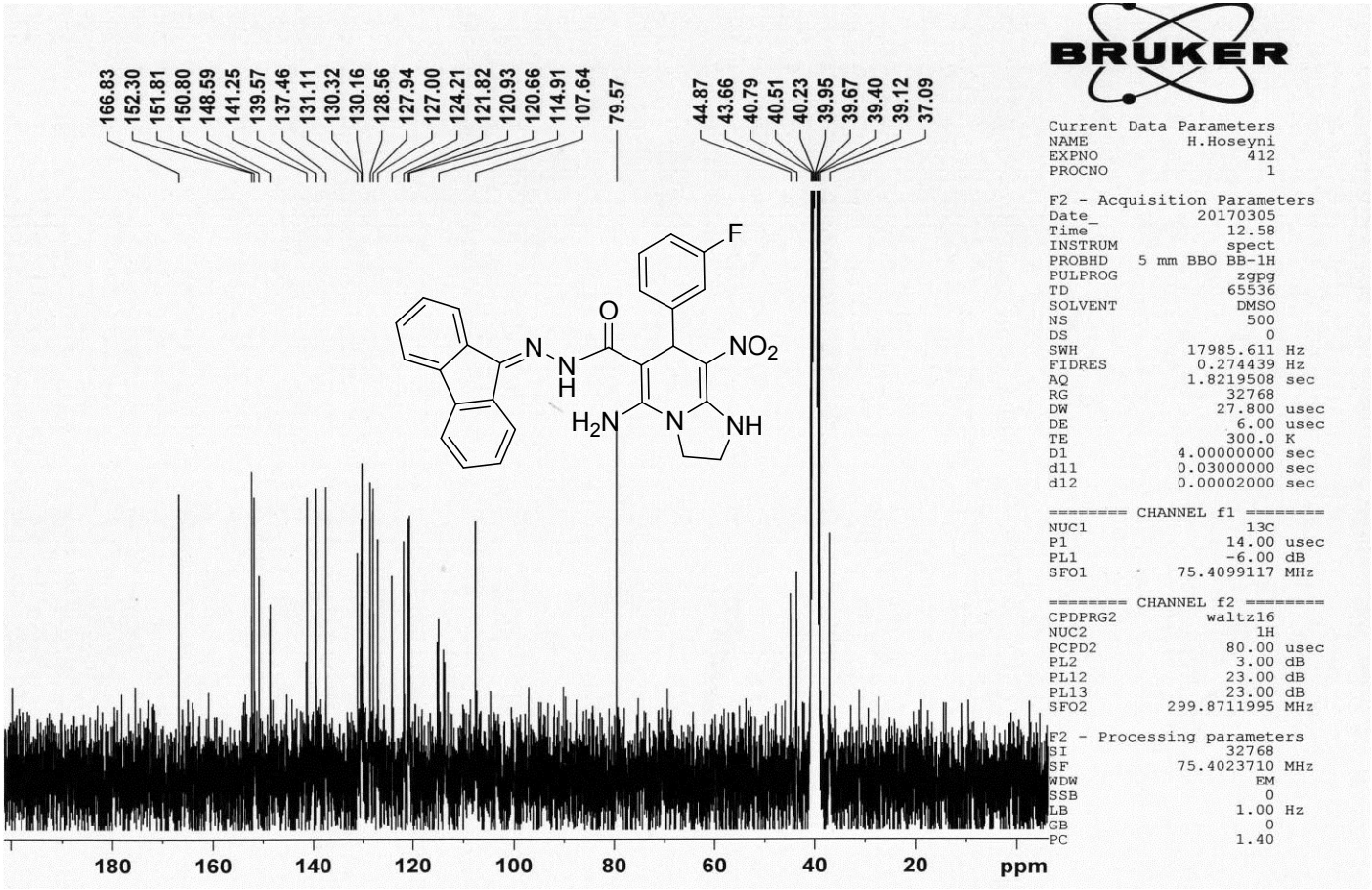
^{1}H NMR of 6b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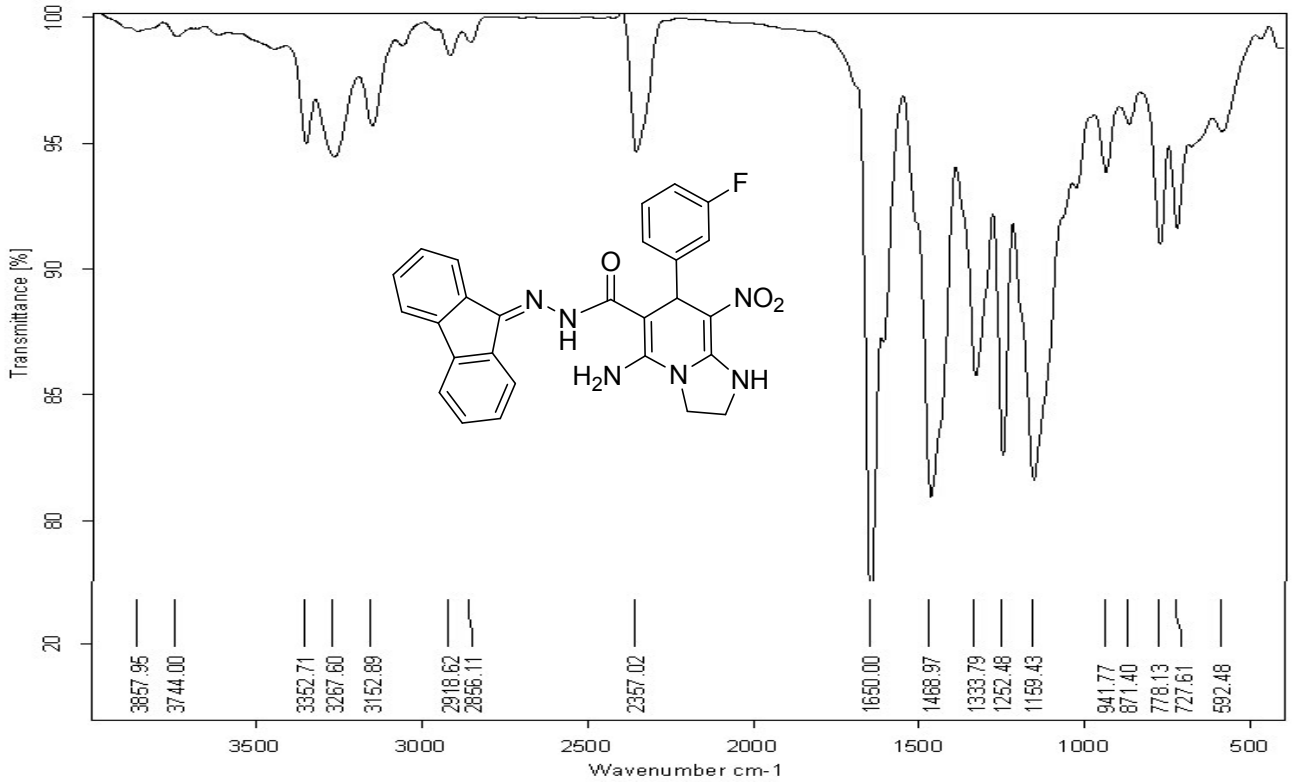
^{13}C NMR of 6b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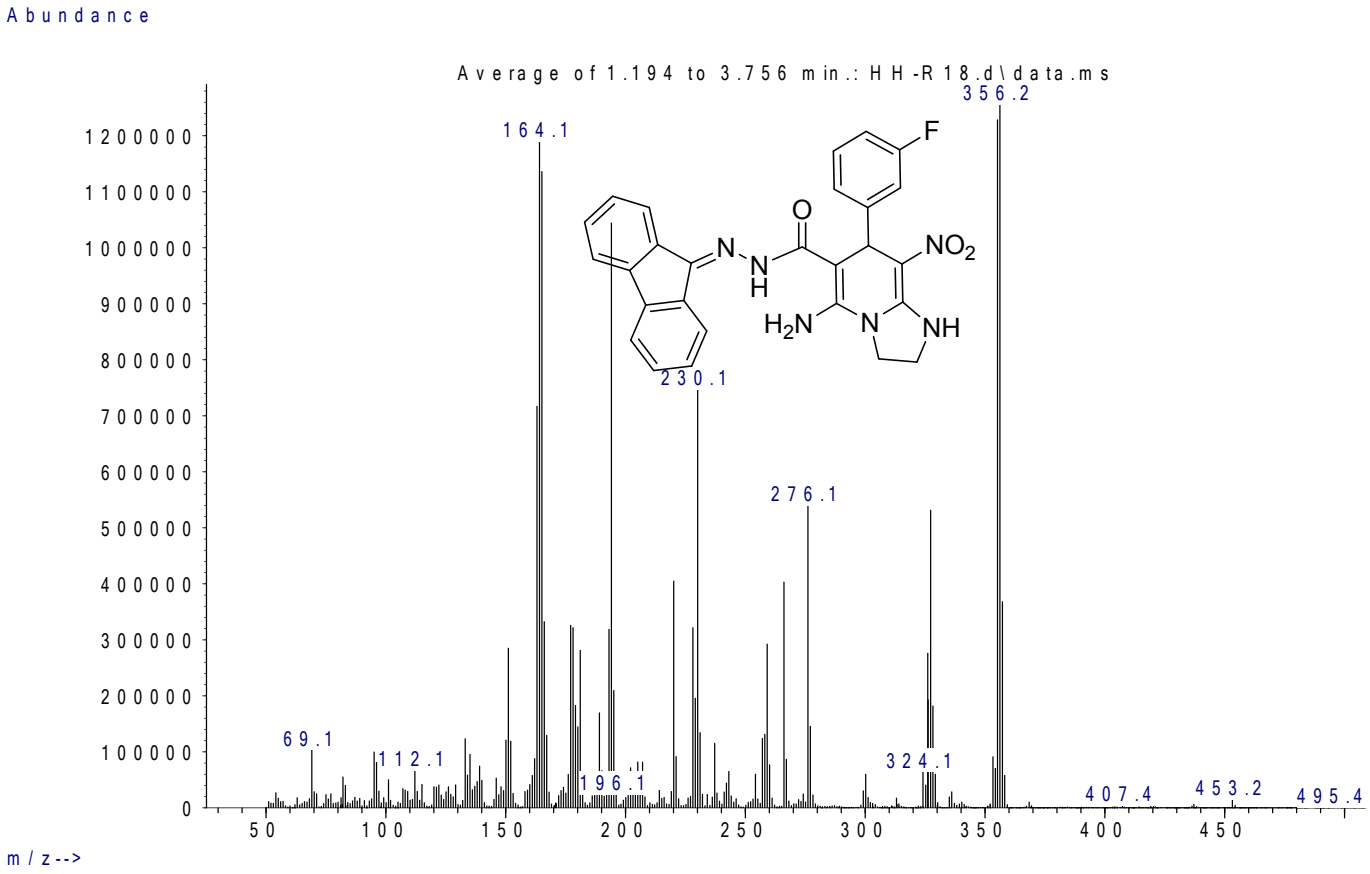
IR of 6b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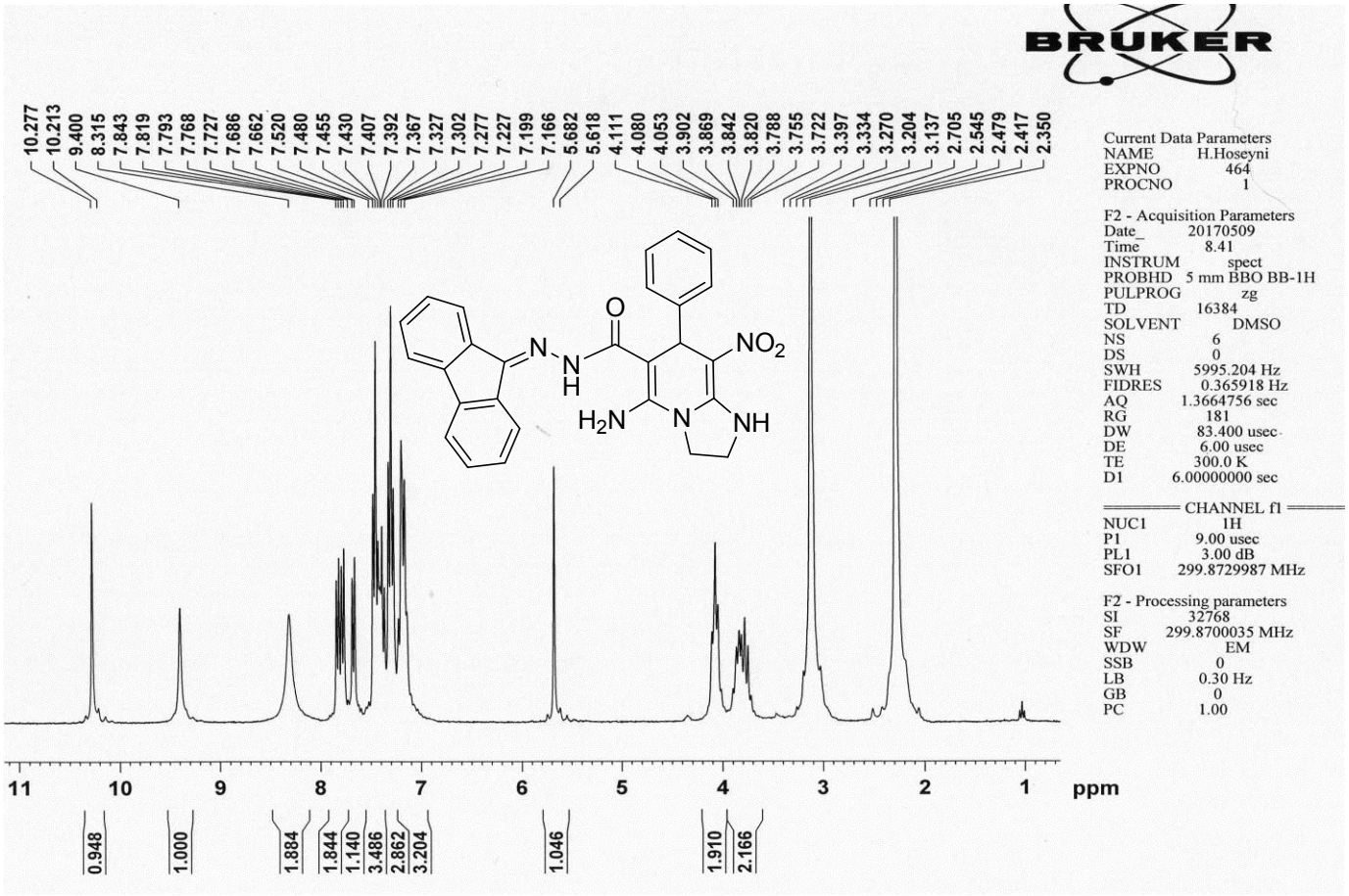
m/z-->

MS of 6b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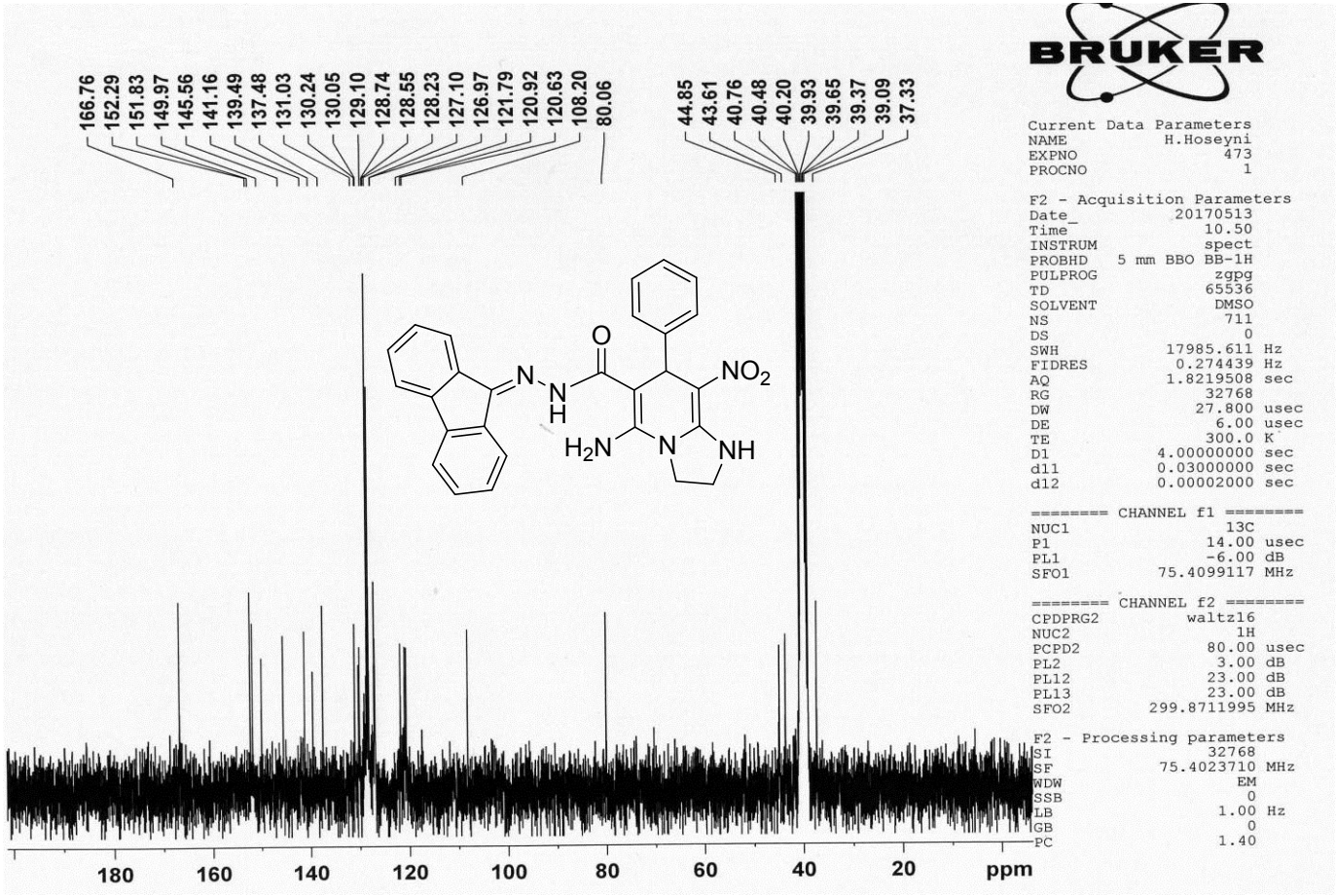
^{1}H NMR of 6c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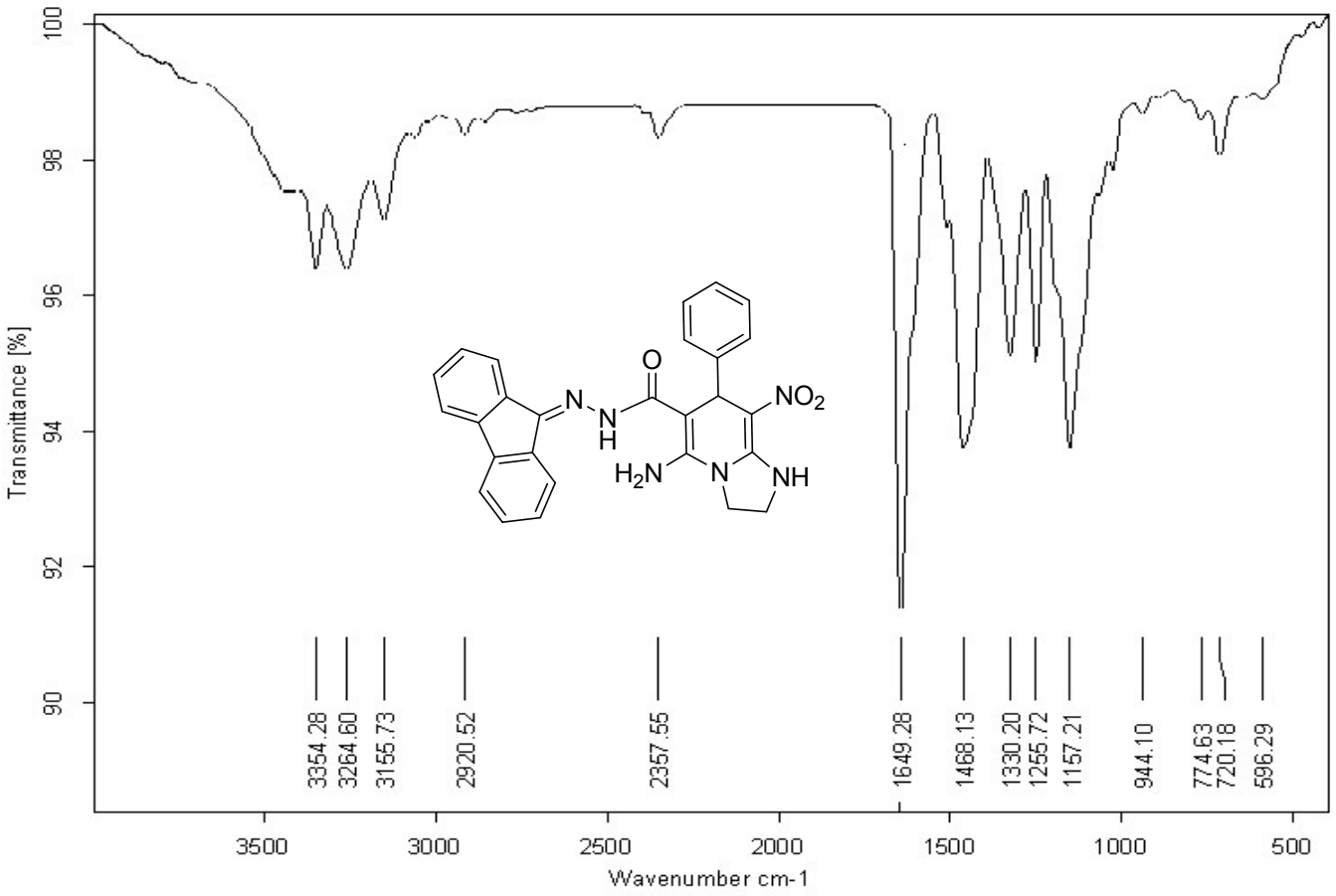
^{13}C NMR of 6c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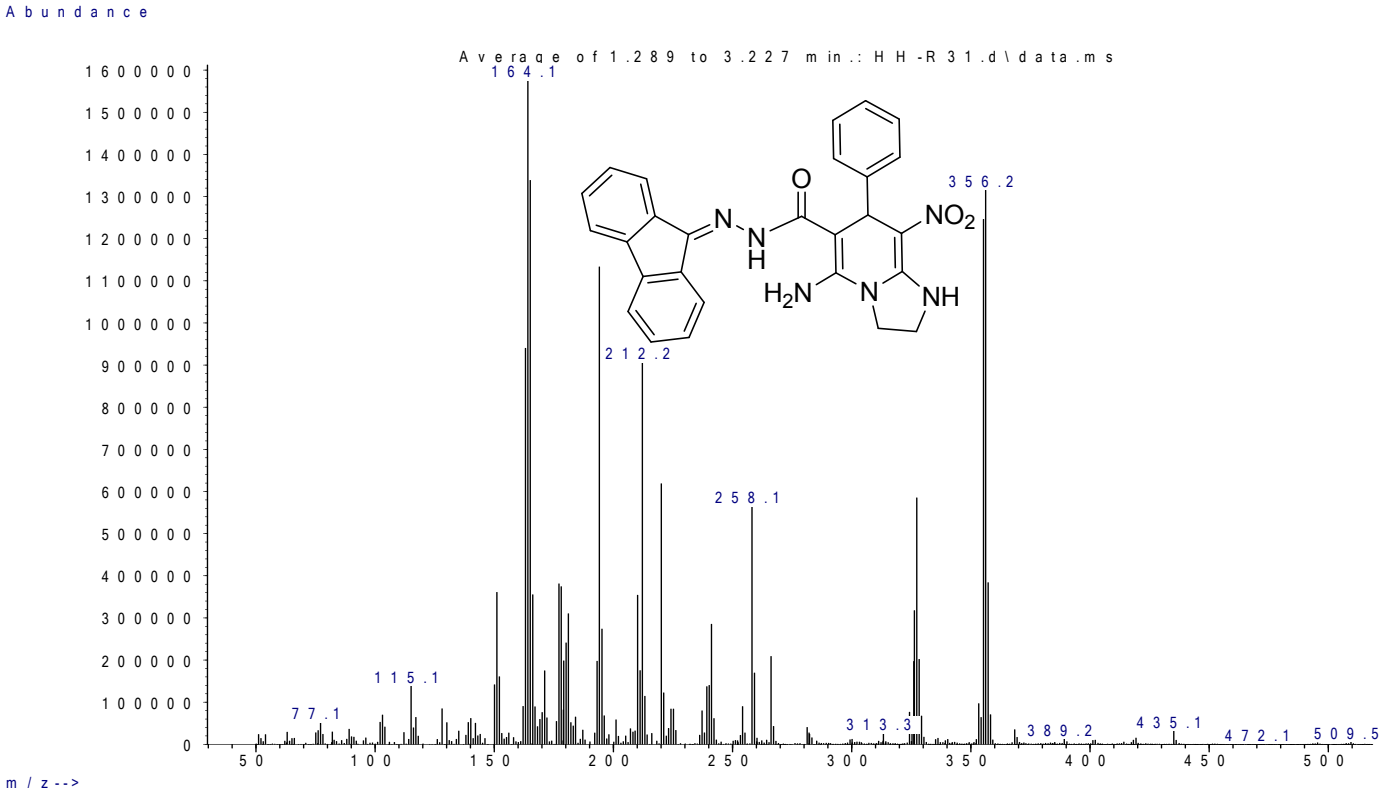
IR of 6c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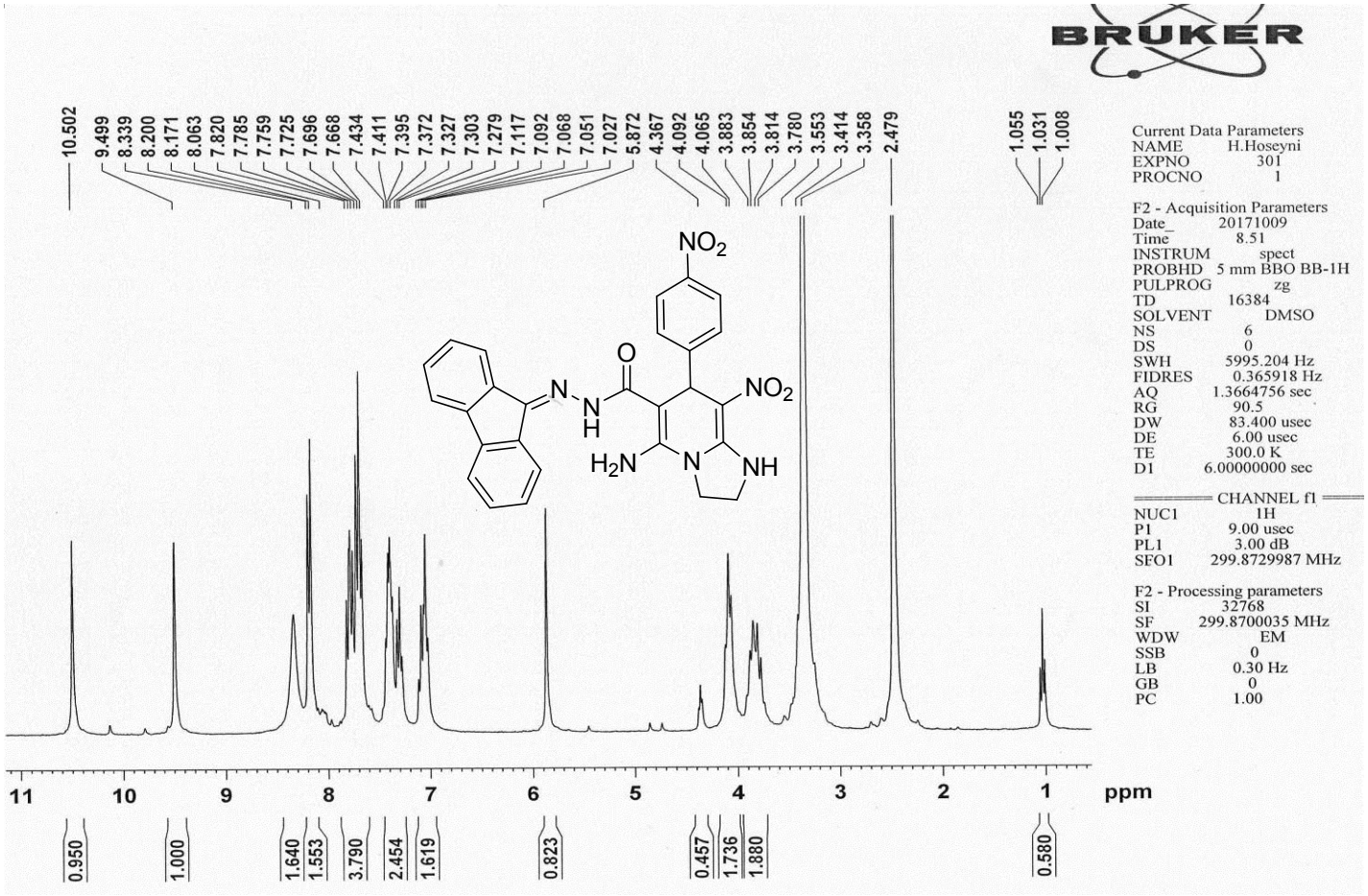
m/z-->

MS of 6c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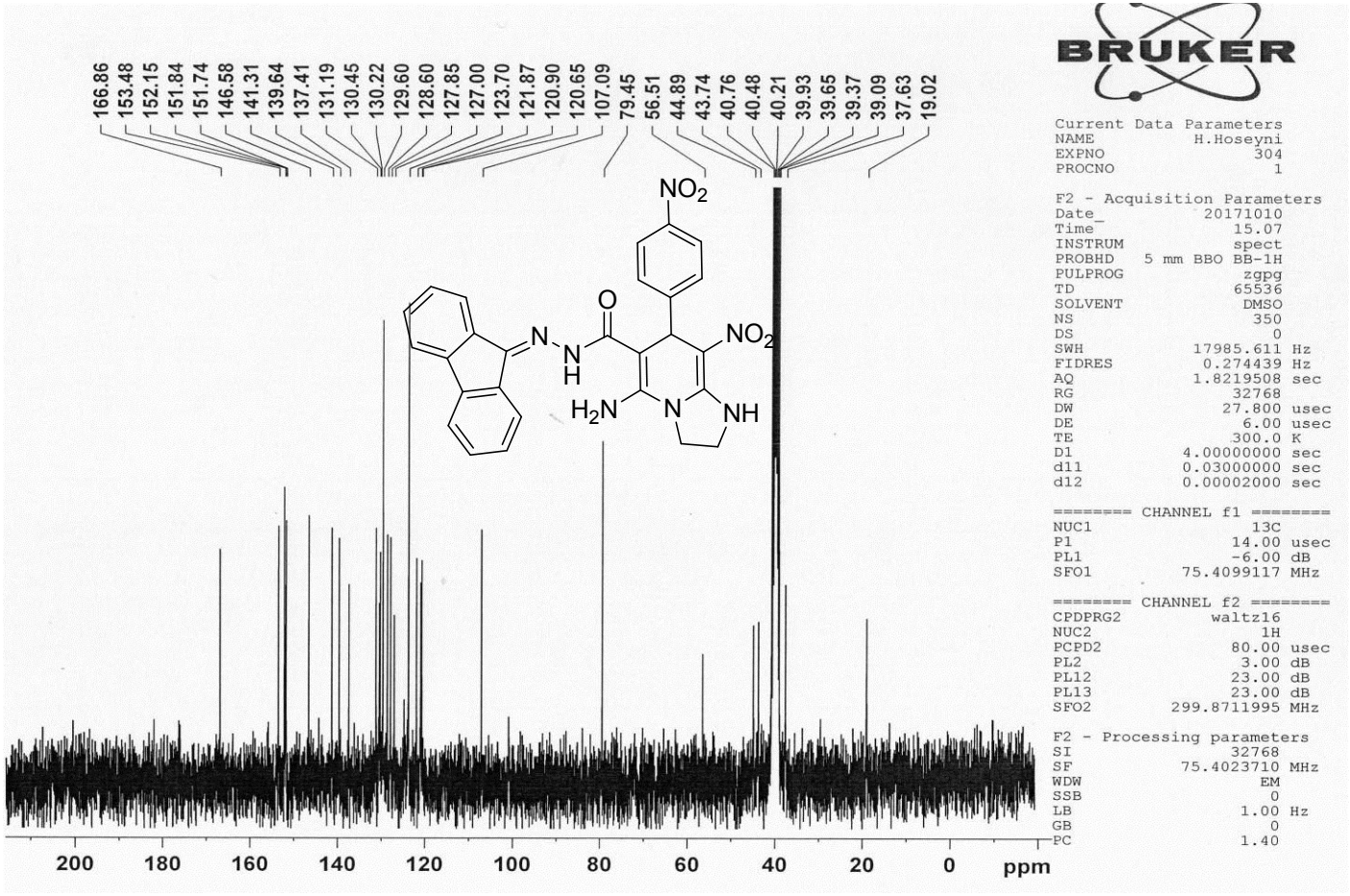
^{1}H NMR of 6d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CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
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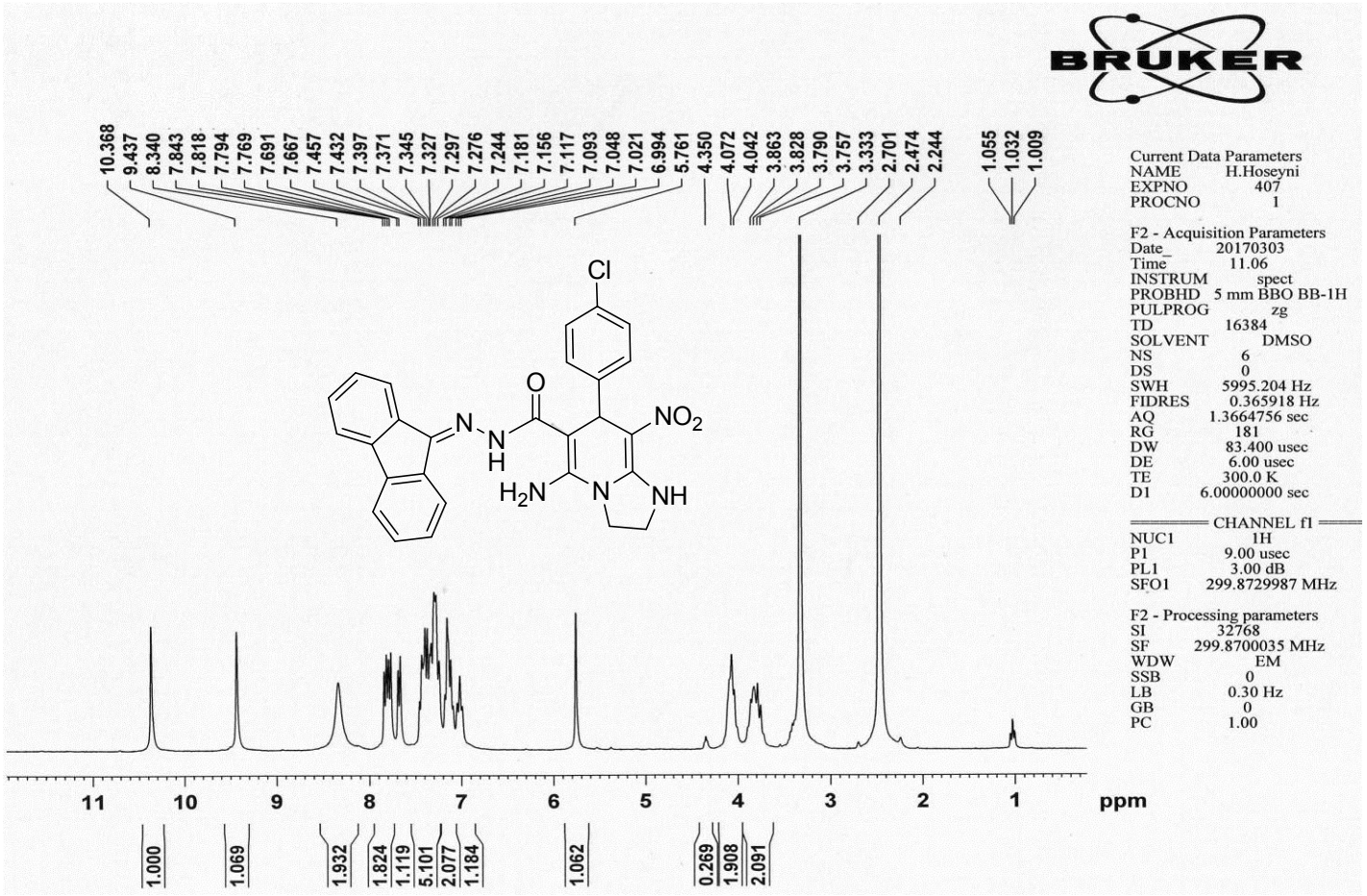
^{13}C NMR of 6d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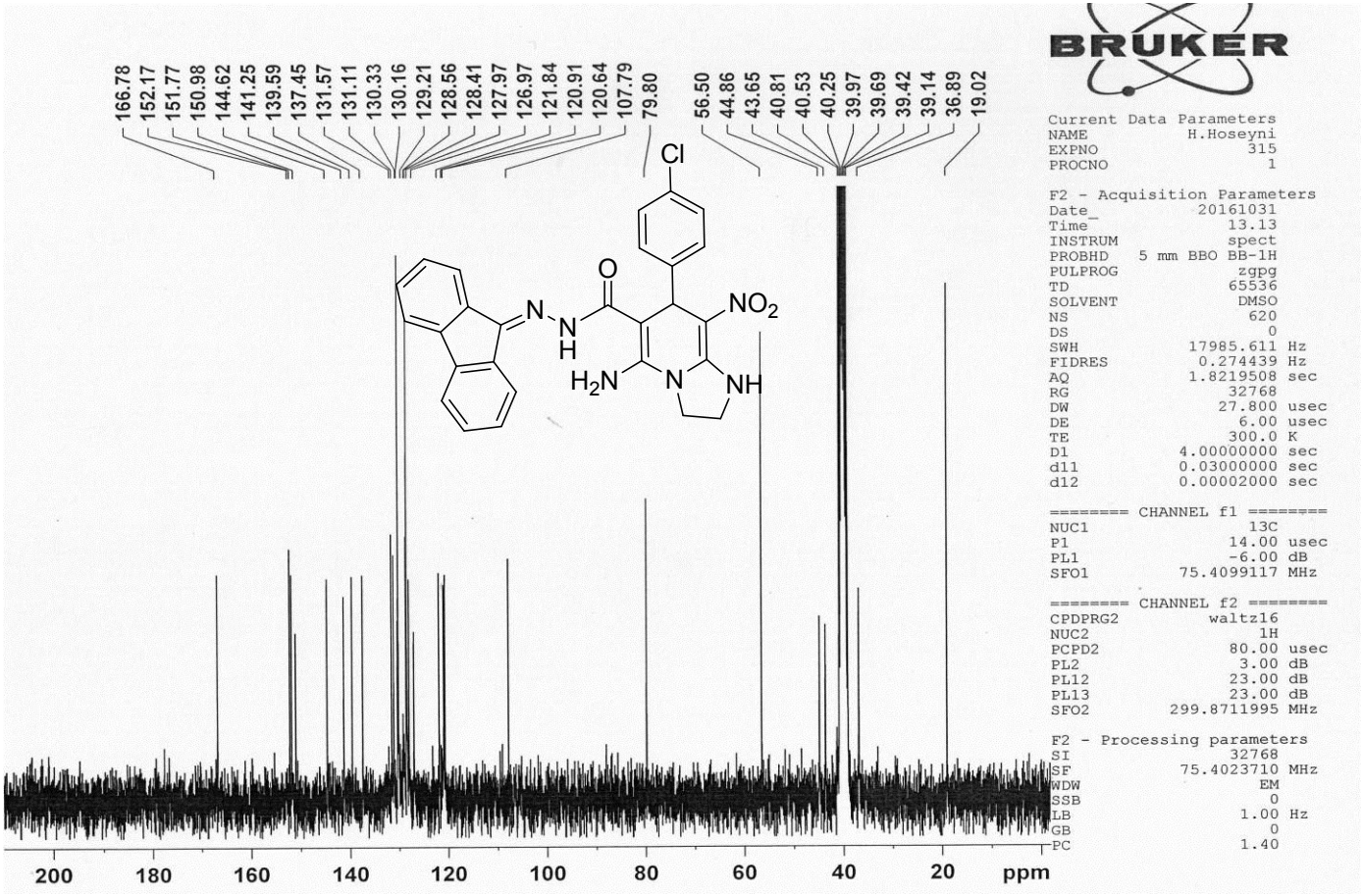
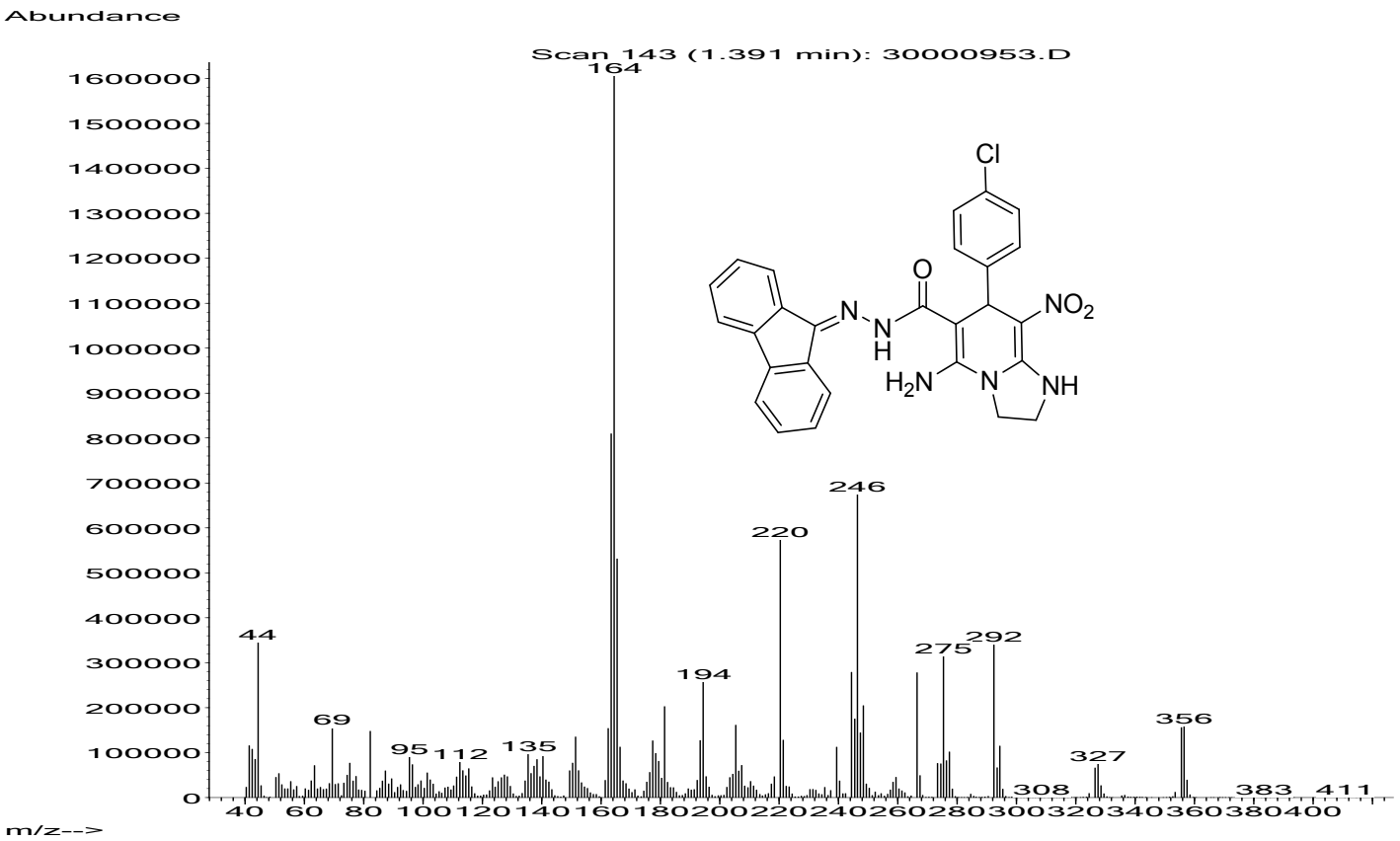
7.244
7.181
7.156
7.117
7.093
7.048
7.021
6.994
5.761
4.350
4.072
4.042
3.863
3.828
3.790
3.757
3.333
2.701
2.474
2.244
1.055
1.032
1.009
Cl
O
N
N
H
NO2
H2N
N
NH
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.069
1.932
1.824
1.119
5.101
2.077
1.184
1.062
0.269
1.908
2.091
Current Data Parameters
NAME H.Hoseyni
EXPNO 407
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170303
Time 11.06
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

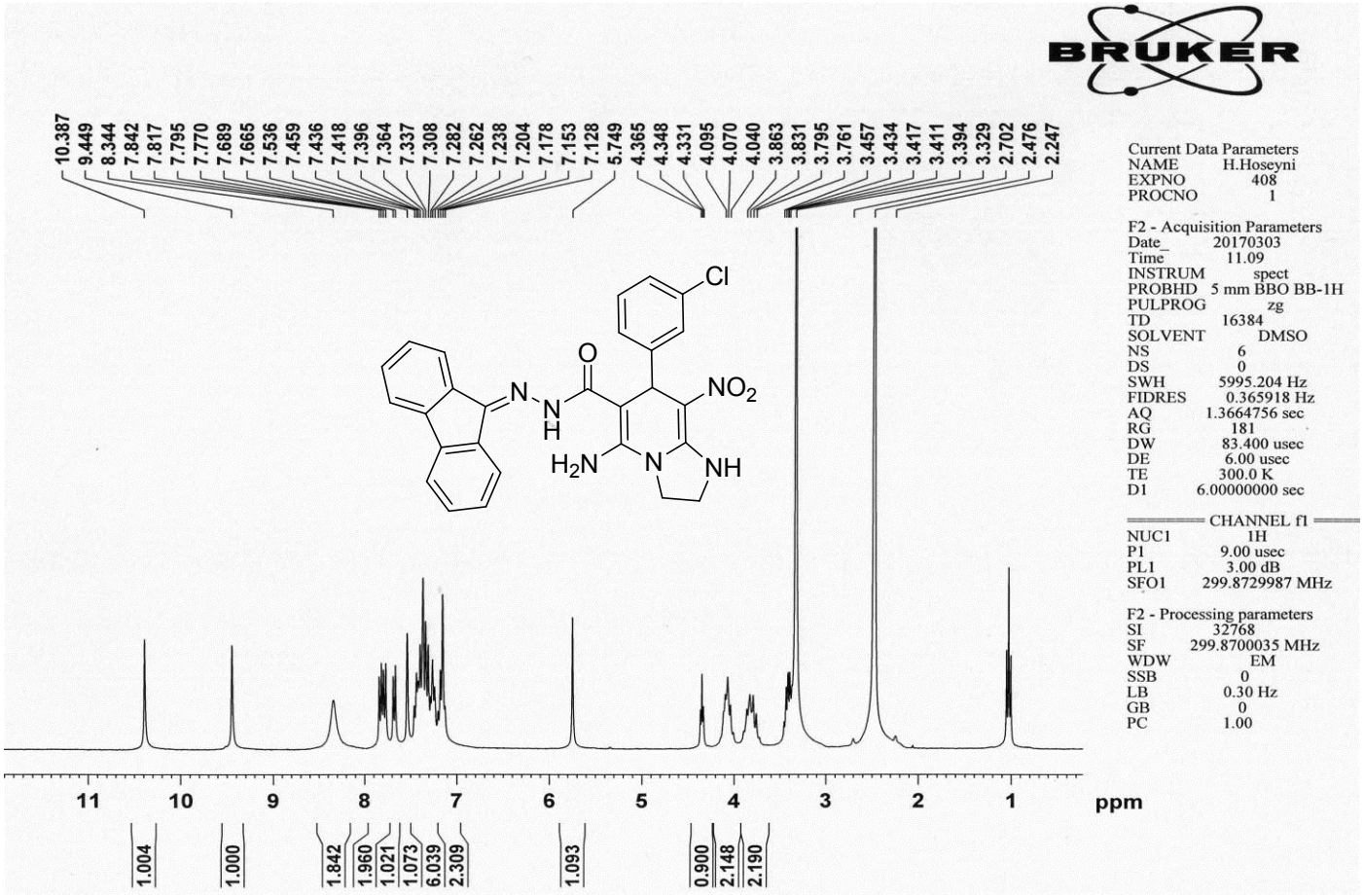
^{1}H NMR of 6e


166.78
152.17
151.77
150.98
144.62
141.25
139.59
137.45
131.57
131.11
130.33
130.16
129.21
128.56
128.41
127.97
126.97
121.84
120.91
120.64
107.79
79.80
56.50
44.86
43.65
40.81
40.53
40.25
39.97
39.69
39.42
39.14
36.89
19.02
Cl
O
N
N
H
NO2
H2N
N
NH
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 315
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161031
Time 13.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 620
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

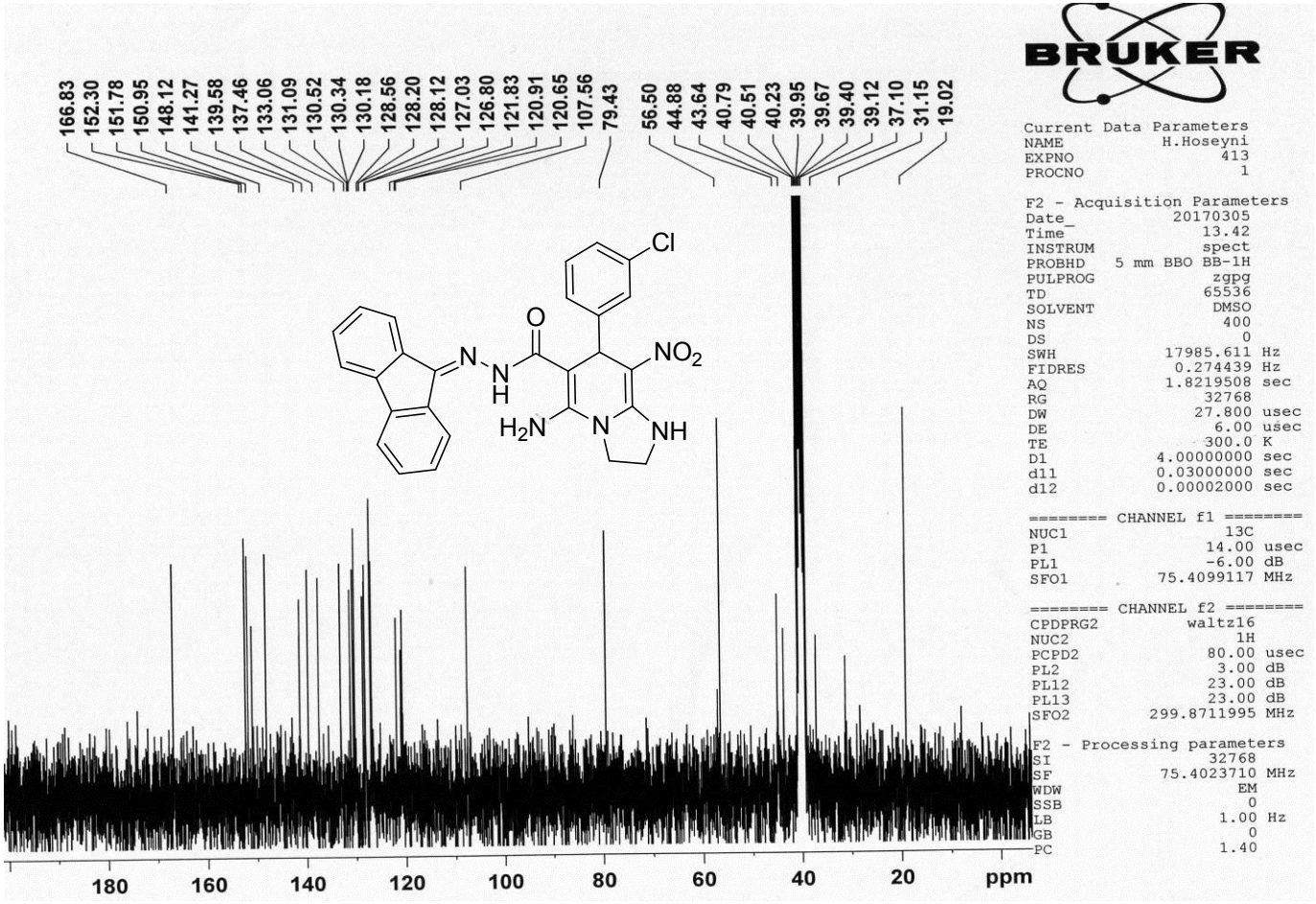
^{13}C NMR of 6e


Abundance
Scan 143 (1.391 min): 30000953.D
164
246
220
44
194
275
292
69
95
112
135
356
327
308
383
411
m/z-->

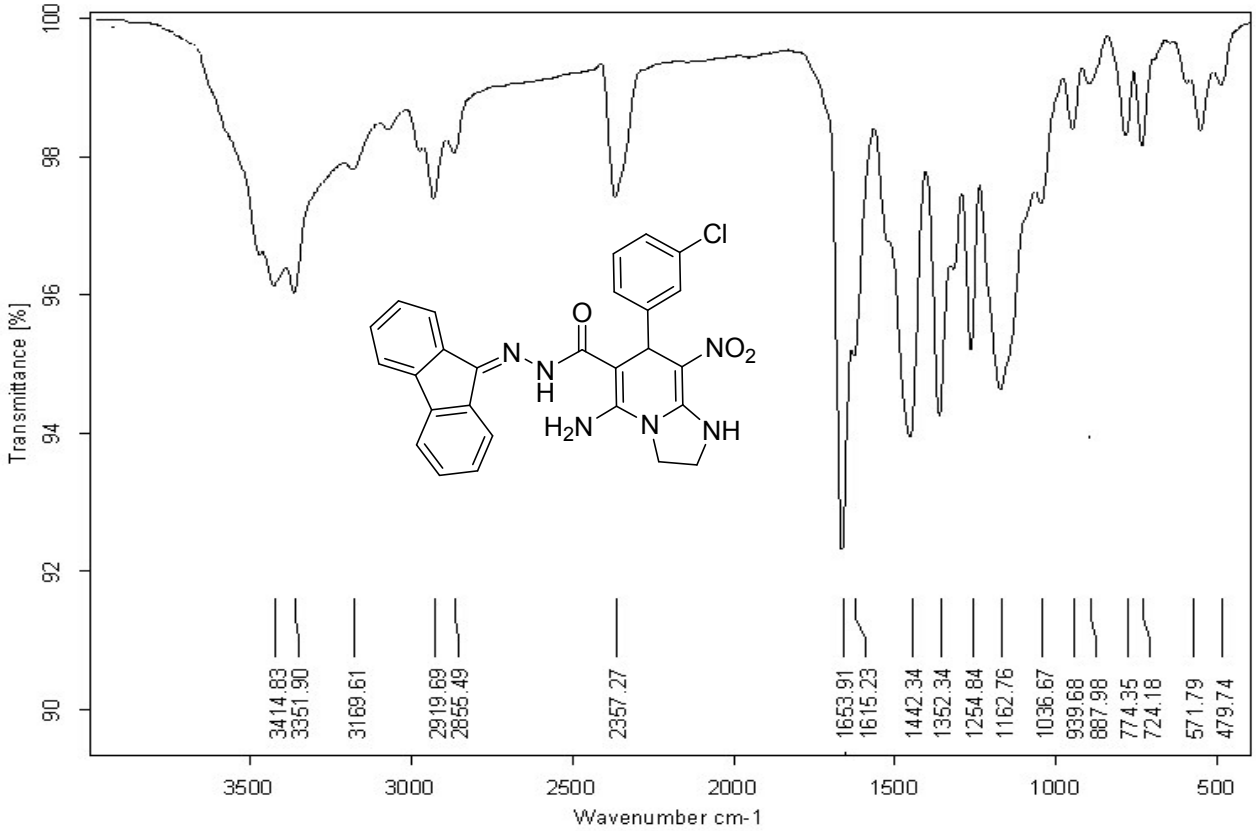
MS of 6e


BRUKER
10.387
9.449
8.344
7.842
7.817
7.795
7.770
7.689
7.665
7.536
7.459
7.436
7.418
7.396
7.364
7.337
7.308
7.282
7.262
7.238
7.204
7.178
7.153
7.128
5.749
4.365
4.348
4.331
4.095
4.070
4.040
3.863
3.831
3.795
3.761
3.457
3.434
3.417
3.411
3.394
3.329
2.702
2.476
2.247
Cl
O
N
N
H
NO2
H2N
N
NH
Current Data Parameters
NAME H.Hoseyni
EXPNO 408
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170303
Time 11.09
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
11
10
9
8
7
6
5
4
3
2
1
ppm
1.004
1.000
1.842
1.960
1.021
1.073
6.039
2.309
1.093
0.900
2.148
2.190

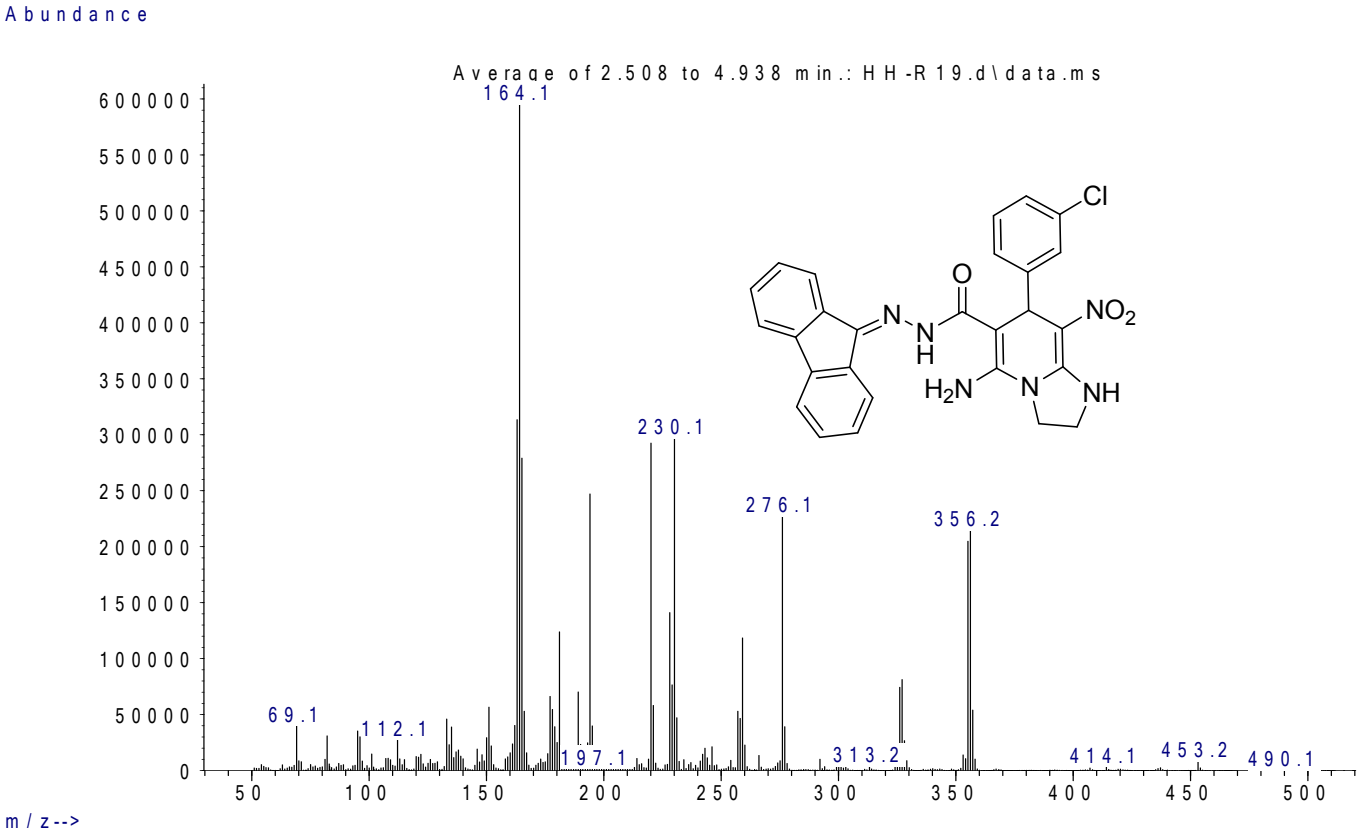
^{1}H NMR of 6f


166.83
152.30
151.78
150.95
148.12
141.27
139.58
137.46
133.06
131.09
130.52
130.34
130.18
128.56
128.20
128.12
127.03
126.80
121.83
120.91
120.65
107.56
79.43
56.50
44.88
43.64
40.79
40.51
40.23
39.95
39.67
39.40
39.12
37.10
31.15
19.02
Cl
O
N
N
H
NO2
H2N
N
NH
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 413
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170305
Time 13.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 400
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

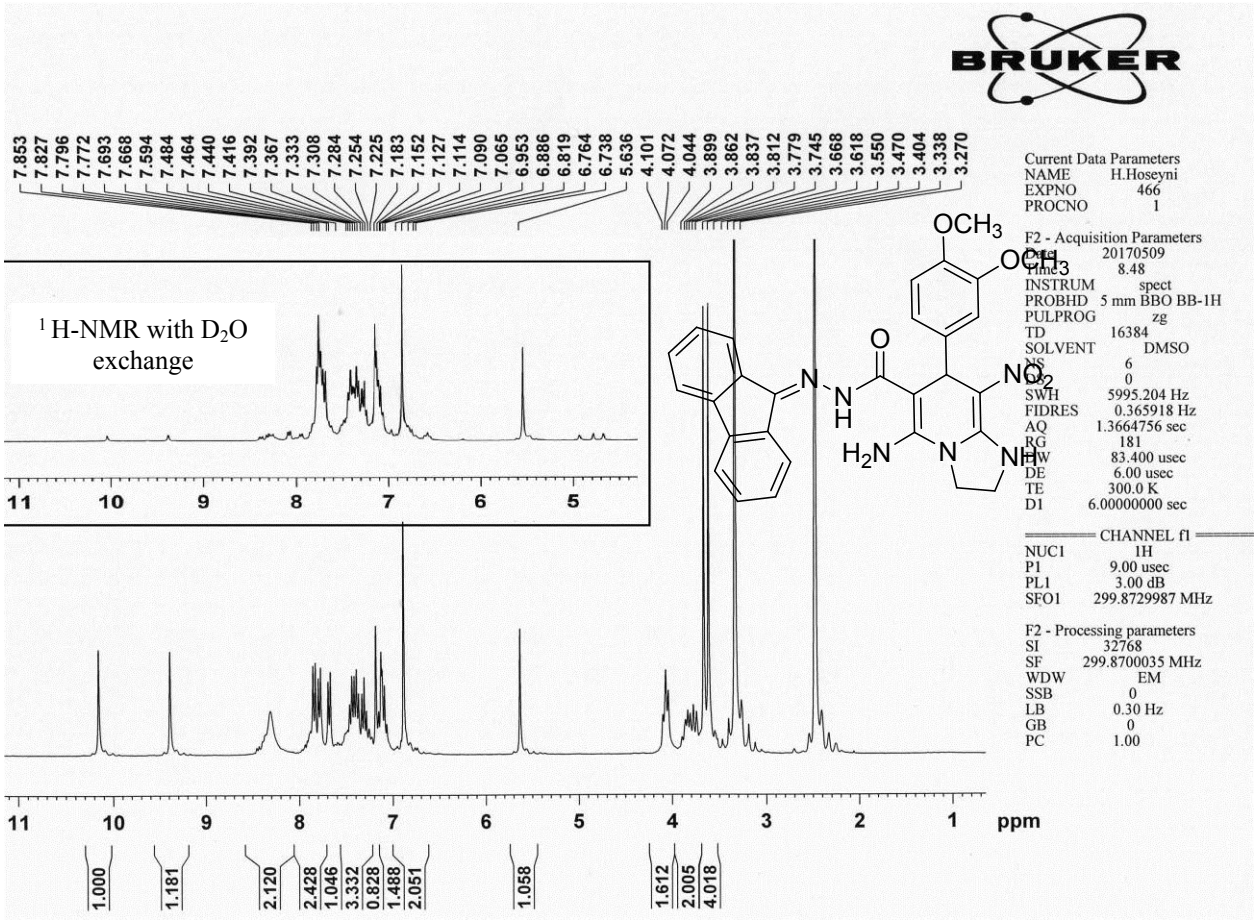
^{13}C NMR of 6f


Transmittance [%]
100
98
96
94
92
90
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3414.83
3351.90
3169.61
2919.69
2855.49
2357.27
1653.91
1615.23
1442.34
1352.34
1254.84
1162.76
1036.67
939.68
887.98
774.35
724.18
571.79
479.74
Cl
O
N
N
H
NO2
H2N
N
NH

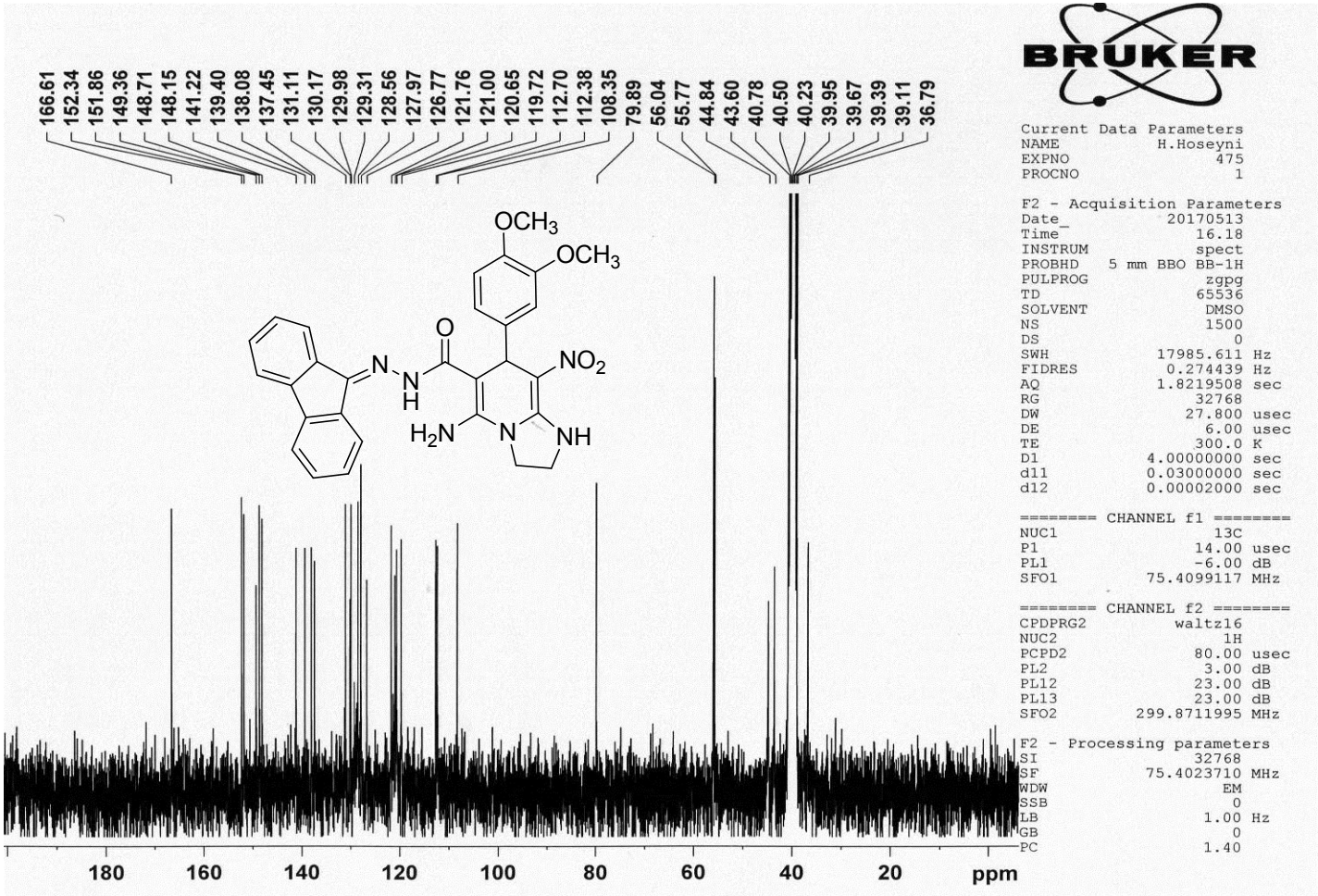
IR of 6f


Abundance
Average of 2.508 to 4.938 min.: HH-R19.d\data.ms
164.1
230.1
276.1
356.2
69.1
112.1
197.1
313.2
414.1
453.2
490.1
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
50
100
150
200
250
300
350
400
450
500
m/z-->

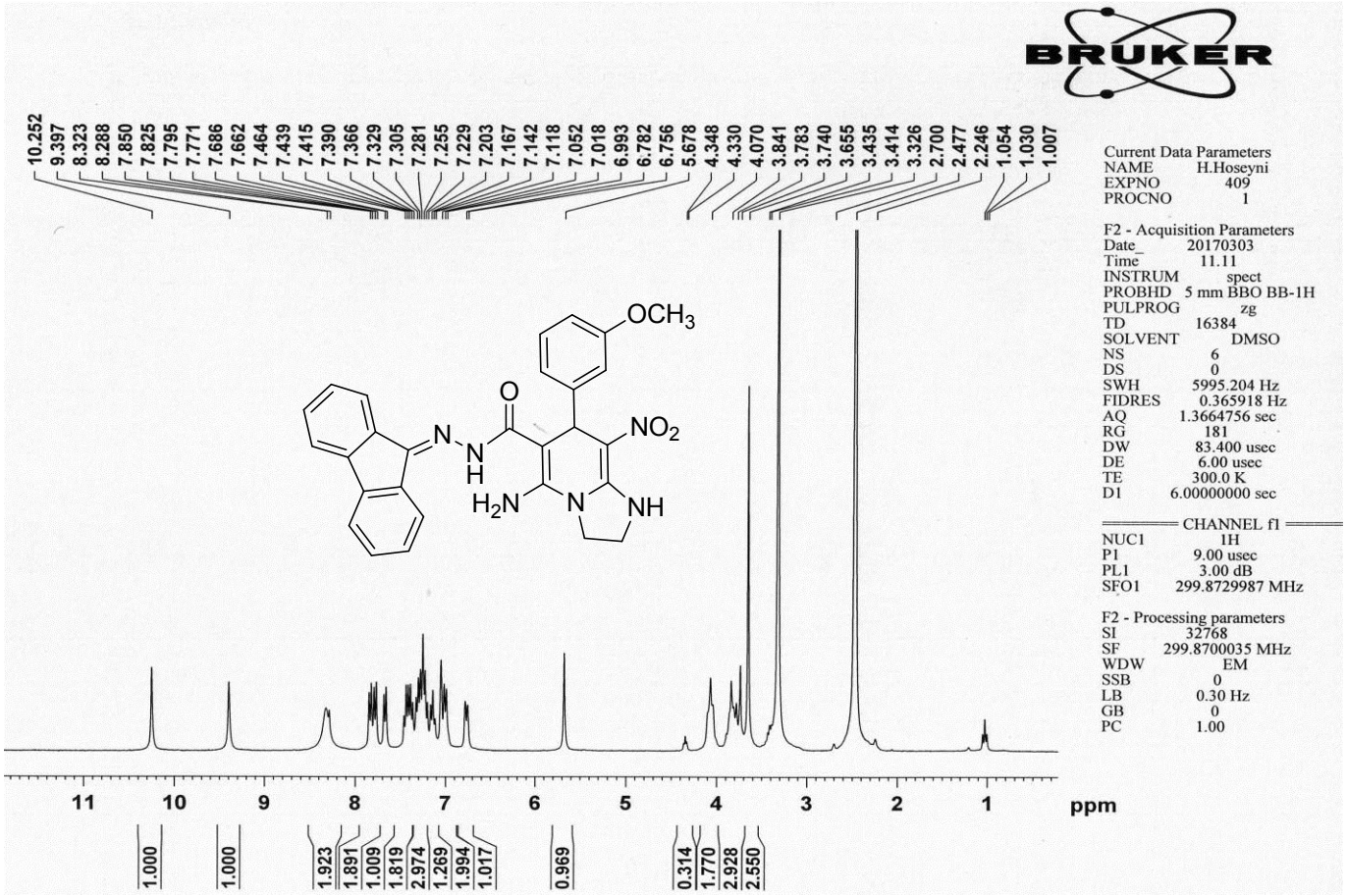
MS of 6f


BRUKER
7.853 7.827 7.796 7.772 7.693 7.668 7.594 7.484 7.464 7.440 7.416 7.392 7.367 7.333 7.308 7.284 7.254 7.225 7.183 7.152 7.127 7.114 7.090 7.065 6.953 6.886 6.819 6.764 6.738 5.636 4.101 4.072 4.044 3.899 3.862 3.837 3.812 3.779 3.745 3.668 3.618 3.550 3.470 3.404 3.338 3.270
^{1}H-NMR with D_2O exchange
OCH3
OCH3
NO2
O
N
N
H
H2N
N
NH
Current Data Parameters
NAME H.Hoseyni
EXPNO 466
PROCNO 1
F2 - Acquisition Parameters
Date 20170509
Time 8.48
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
11 10 9 8 7 6 5 4 3 2 1 ppm
1.000 1.181 2.120 2.428 1.046 3.332 0.828 1.488 2.051 1.058 1.612 2.005 4.018

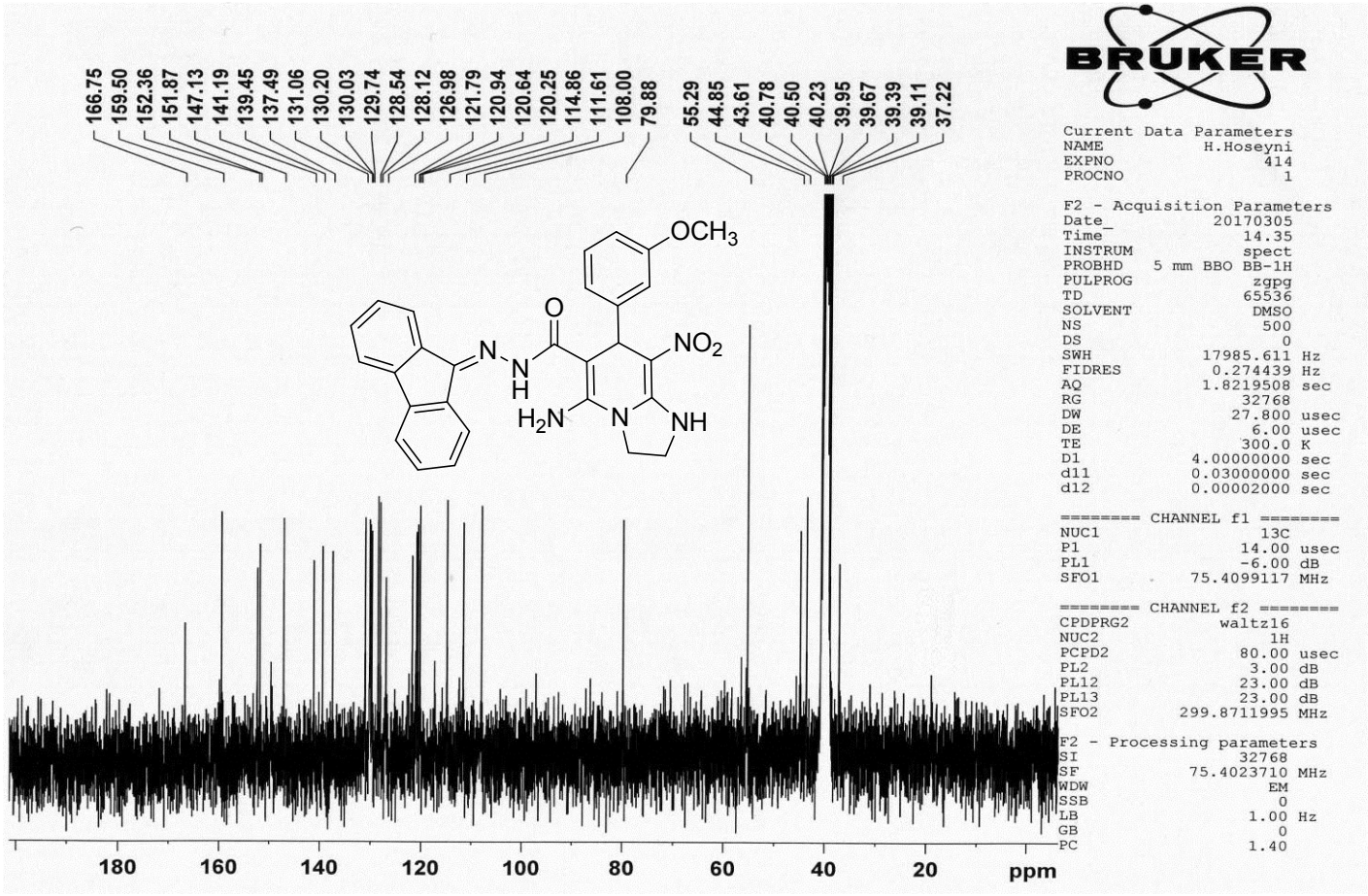
^{1}H NMR of 6g


166.61
152.34
151.86
149.36
148.71
148.15
141.22
139.40
138.08
137.45
131.11
130.17
129.98
129.31
128.56
127.97
126.77
121.76
121.00
120.65
119.72
112.70
112.38
108.35
79.89
56.04
55.77
44.84
43.60
40.78
40.50
40.23
39.95
39.67
39.39
39.11
36.79
OCH3
OCH3
O
N
N
H
NO2
H2N
N
NH
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 475
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170513
Time 16.18
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

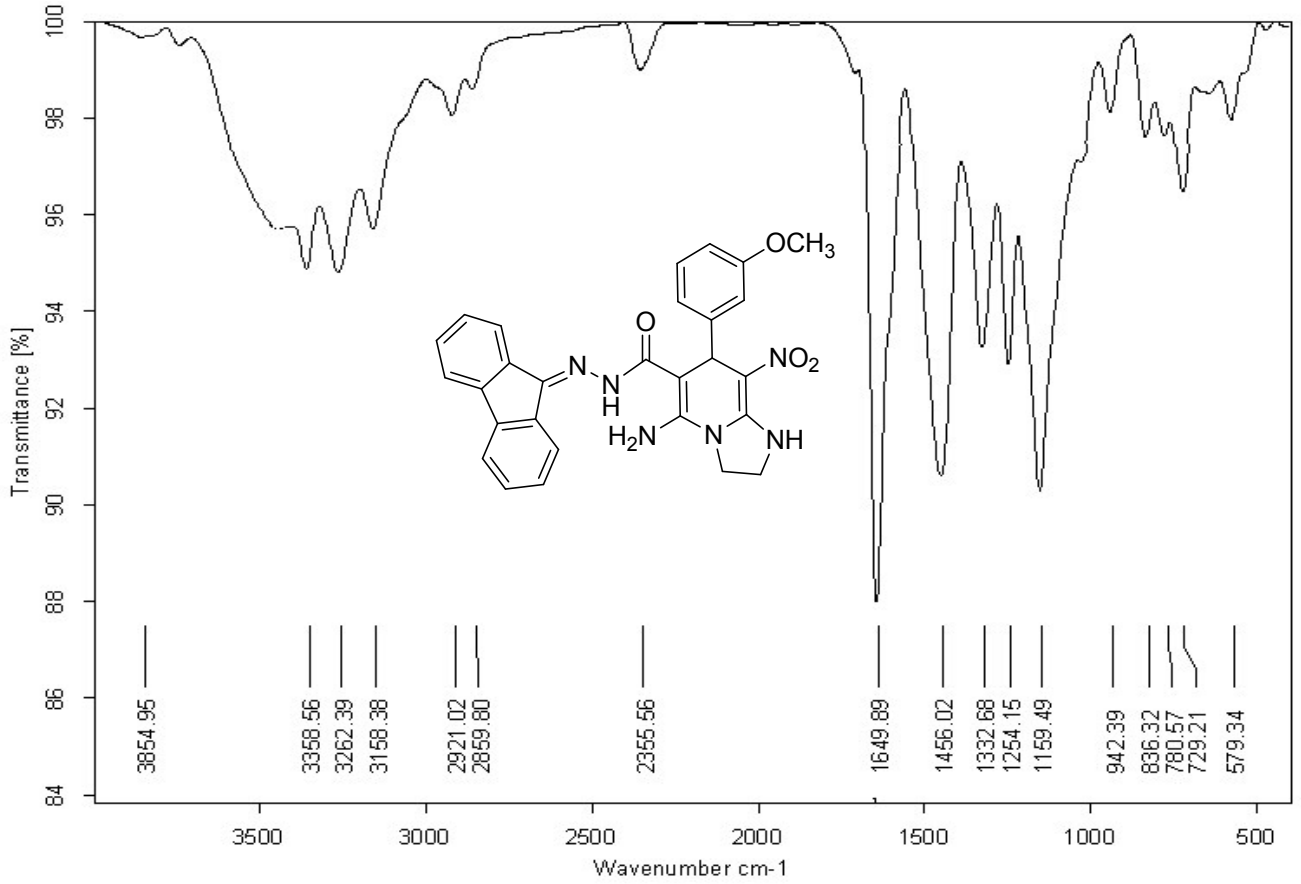
^{13}C NMR of 6g


BRUKER
10.252
9.397
8.323
8.288
7.850
7.825
7.795
7.771
7.686
7.662
7.464
7.439
7.415
7.390
7.366
7.329
7.305
7.281
7.255
7.229
7.203
7.167
7.142
7.118
7.052
7.018
6.993
6.782
6.756
5.678
4.348
4.330
4.070
3.841
3.783
3.740
3.655
3.435
3.414
3.326
2.700
2.477
2.246
1.054
1.030
1.007
OCH3
O
N
N
H
NO2
H2N
N
NH
Current Data Parameters
NAME H.Hoseyni
EXPNO 409
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170303
Time 11.11
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
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.000
1.923
1.891
1.009
1.819
2.974
1.269
1.994
1.017
0.969
0.314
1.770
2.928
2.550

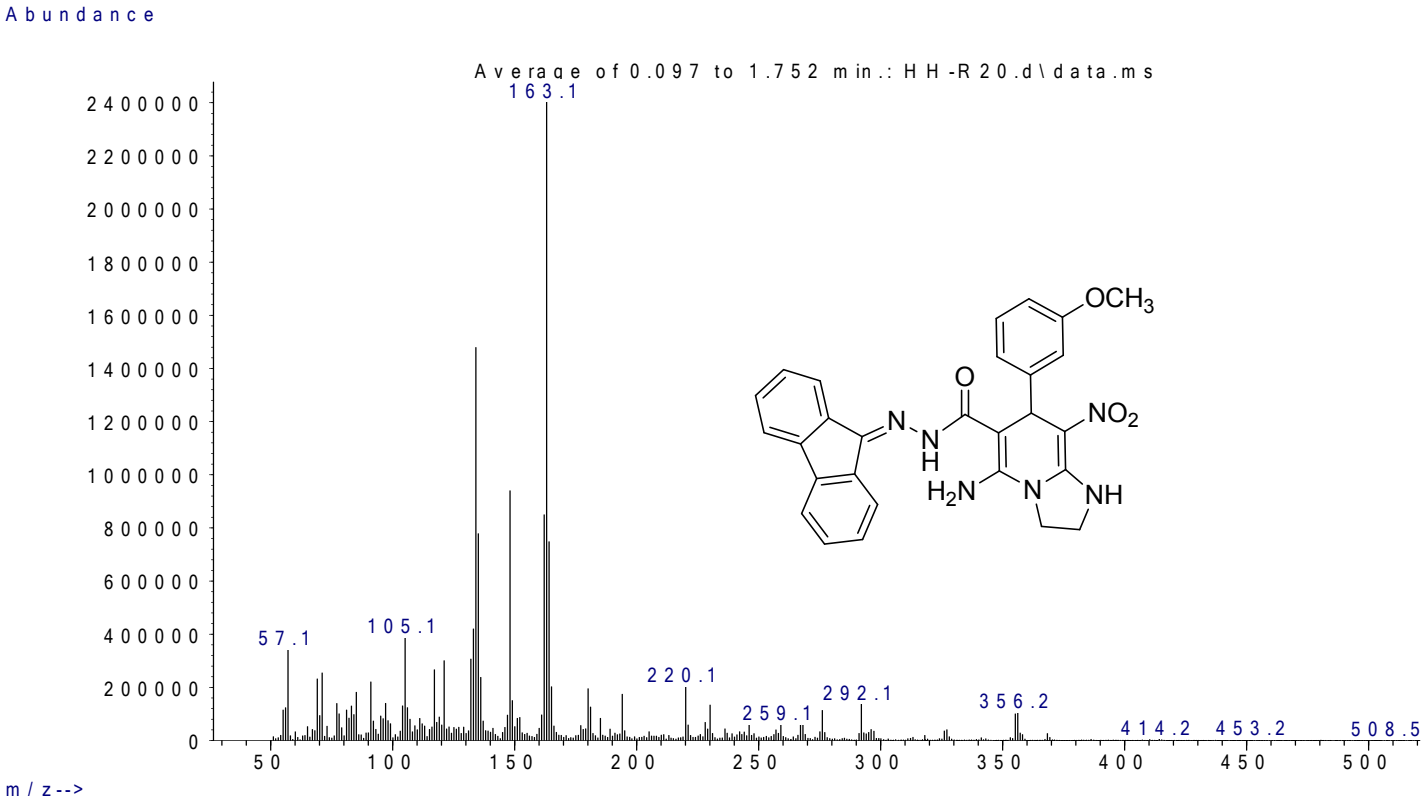
^{1}H NMR of 6h


166.75
159.50
152.36
151.87
147.13
141.19
139.45
137.49
131.06
130.20
130.03
129.74
128.54
128.12
126.98
121.79
120.94
120.64
120.25
114.86
111.61
108.00
79.88
55.29
44.85
43.61
40.78
40.50
40.23
39.95
39.67
39.39
39.11
37.22
OCH3
O
N
N
H
NO2
H2N
N
NH
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 414
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170305
Time 14.35
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

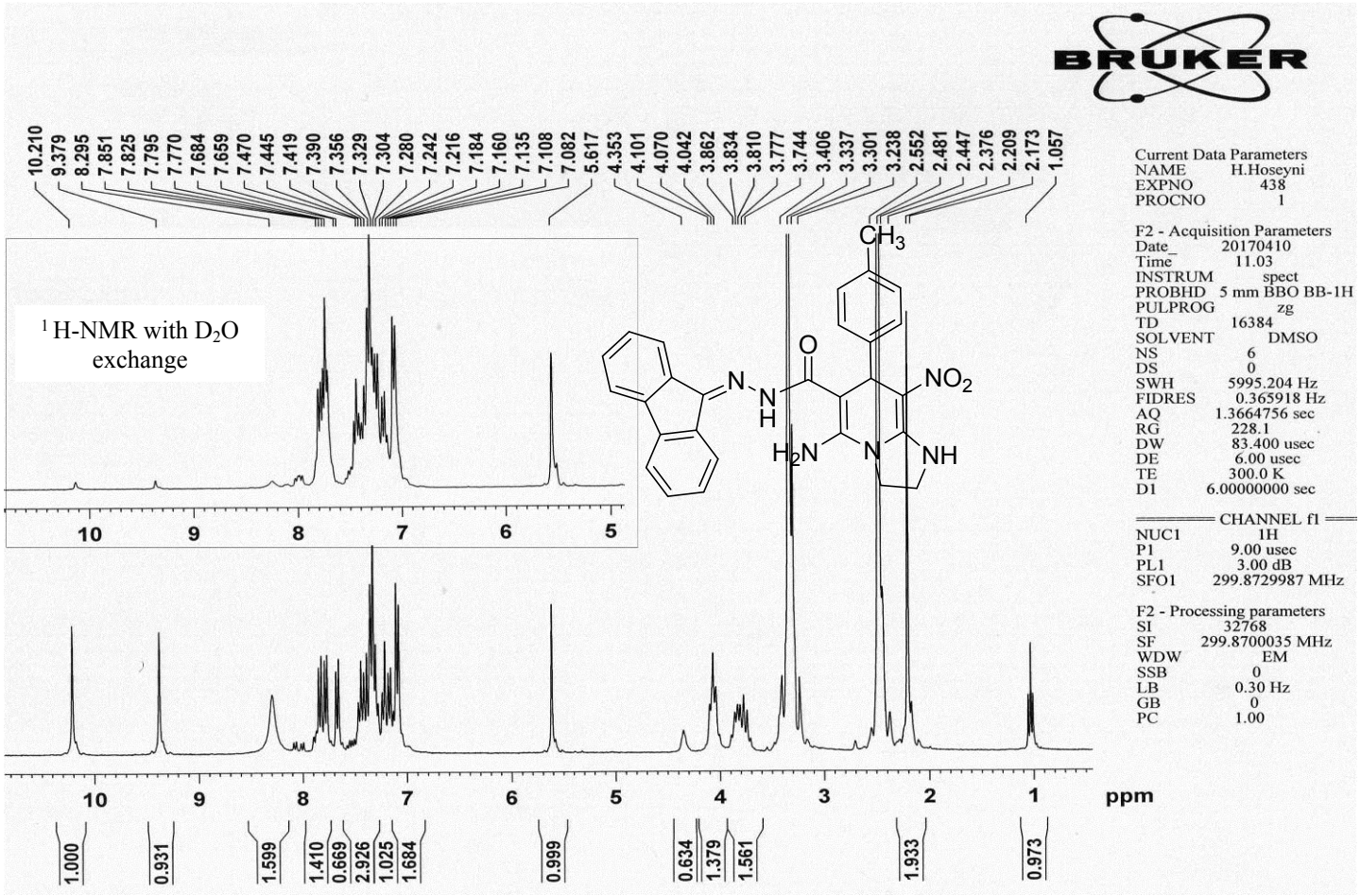
^{13}C NMR of 6h


Transmittance [%]
100
98
96
94
92
90
88
86
84
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3854.95
3358.56
3262.39
3158.38
2921.02
2859.80
2355.56
1649.89
1456.02
1332.68
1254.15
1159.49
942.39
836.32
780.57
729.21
579.34
OCH3
O
NO2
N
N
H
H2N
N
NH

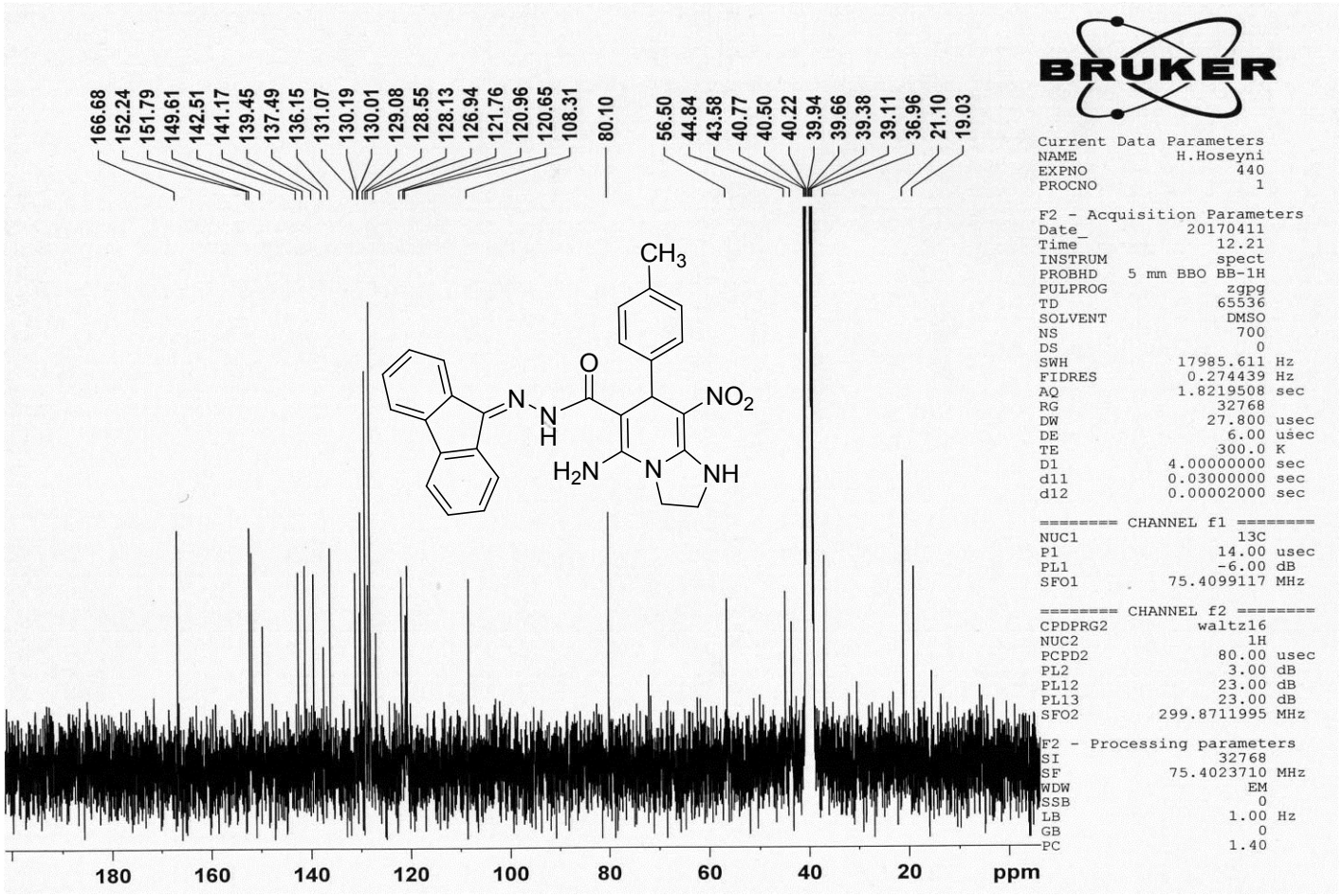
IR of 6h


Abundance
Average of 0.097 to 1.752 min.: HH-R20.d\data.ms
163.1
57.1
105.1
220.1
259.1
292.1
356.2
414.2
453.2
508.5
m/z-->

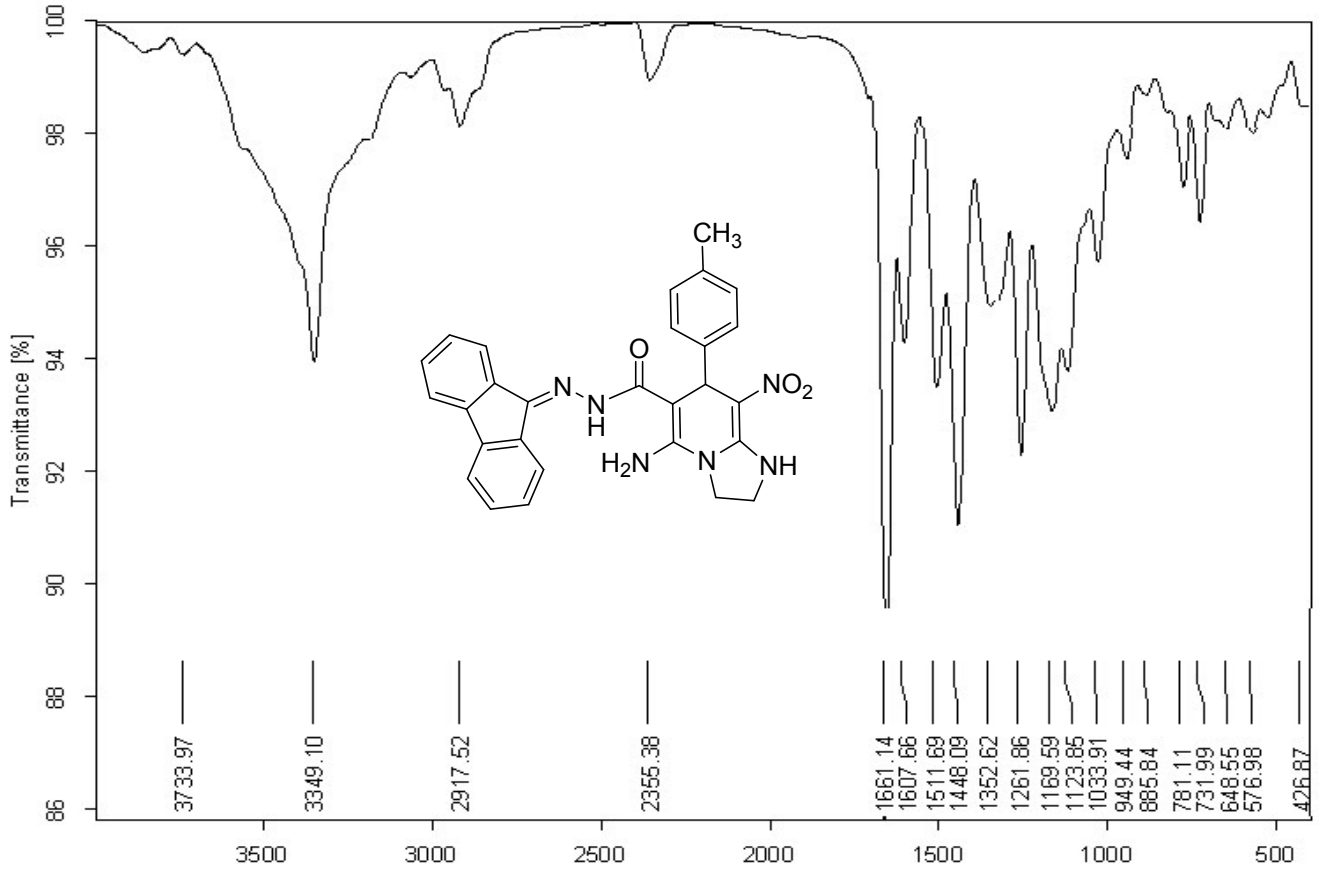
MS of 6h


BRUKER
10.210
9.379
8.295
7.851
7.825
7.795
7.770
7.684
7.659
7.470
7.445
7.419
7.390
7.356
7.329
7.304
7.280
7.242
7.216
7.184
7.160
7.135
7.108
7.082
5.617
4.353
4.101
4.070
4.042
3.862
3.834
3.810
3.777
3.744
3.406
3.337
3.301
3.238
2.552
2.481
2.447
2.376
2.209
2.173
1.057
[1] H-NMR with D2O exchange
CH3
NO2
O
N
N
H
H2N
N
NH
Current Data Parameters
NAME H.Hoseyni
EXPNO 438
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170410
Time 11.03
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 228.1
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
0.931
1.599
1.410
0.669
2.926
1.025
1.684
0.999
0.634
1.379
1.561
1.933
0.973

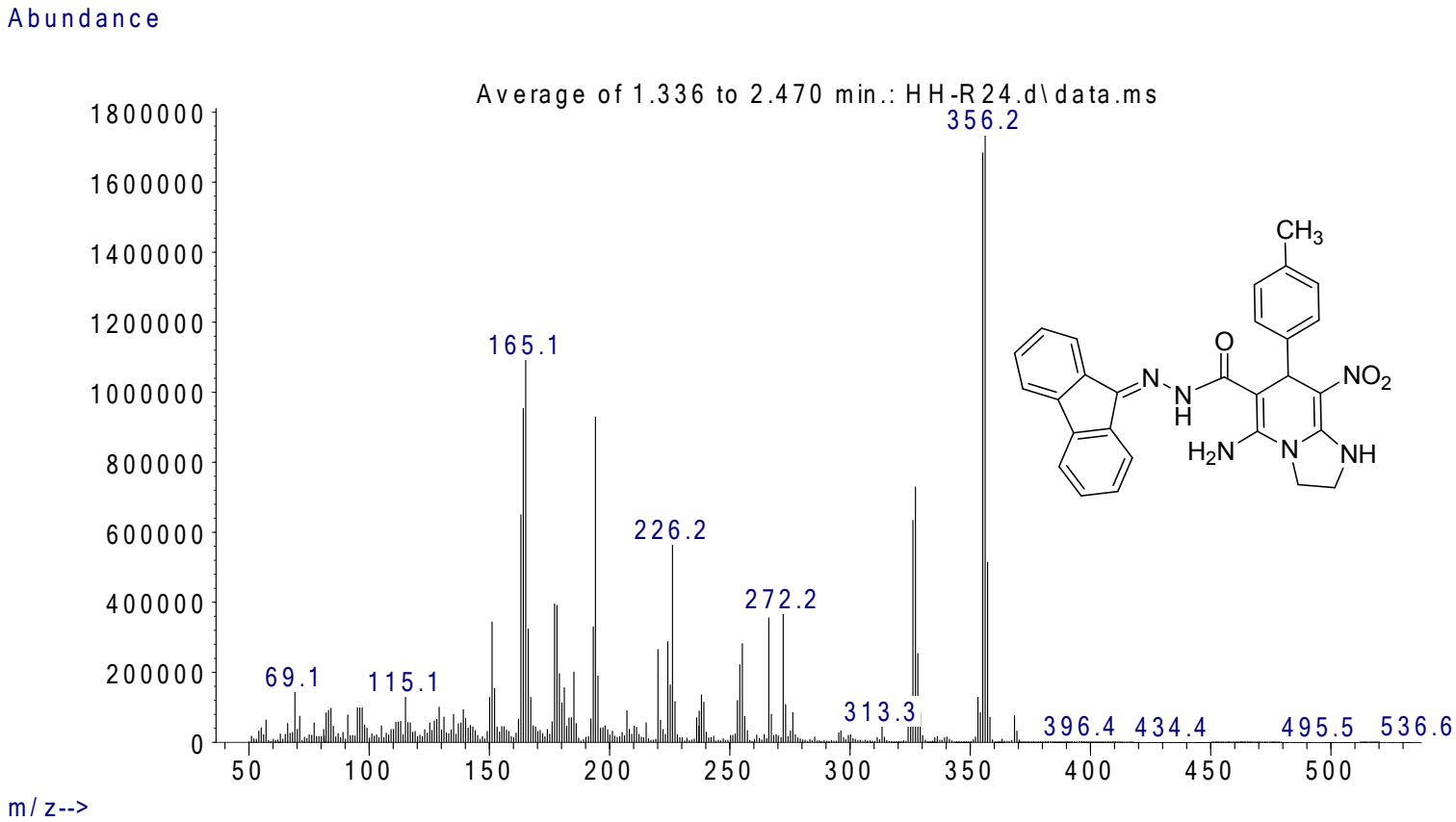
[1]H NMR of 6i


166.68
152.24
151.79
149.61
142.51
141.17
139.45
137.49
136.15
131.07
130.19
130.01
129.08
128.55
128.13
126.94
121.76
120.96
120.65
108.31
80.10
56.50
44.84
43.58
40.77
40.50
40.22
39.94
39.66
39.38
39.11
36.96
21.10
19.03
CH3
O
N
N
H
NO2
H2N
N
NH
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 440
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170411
Time 12.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 700
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

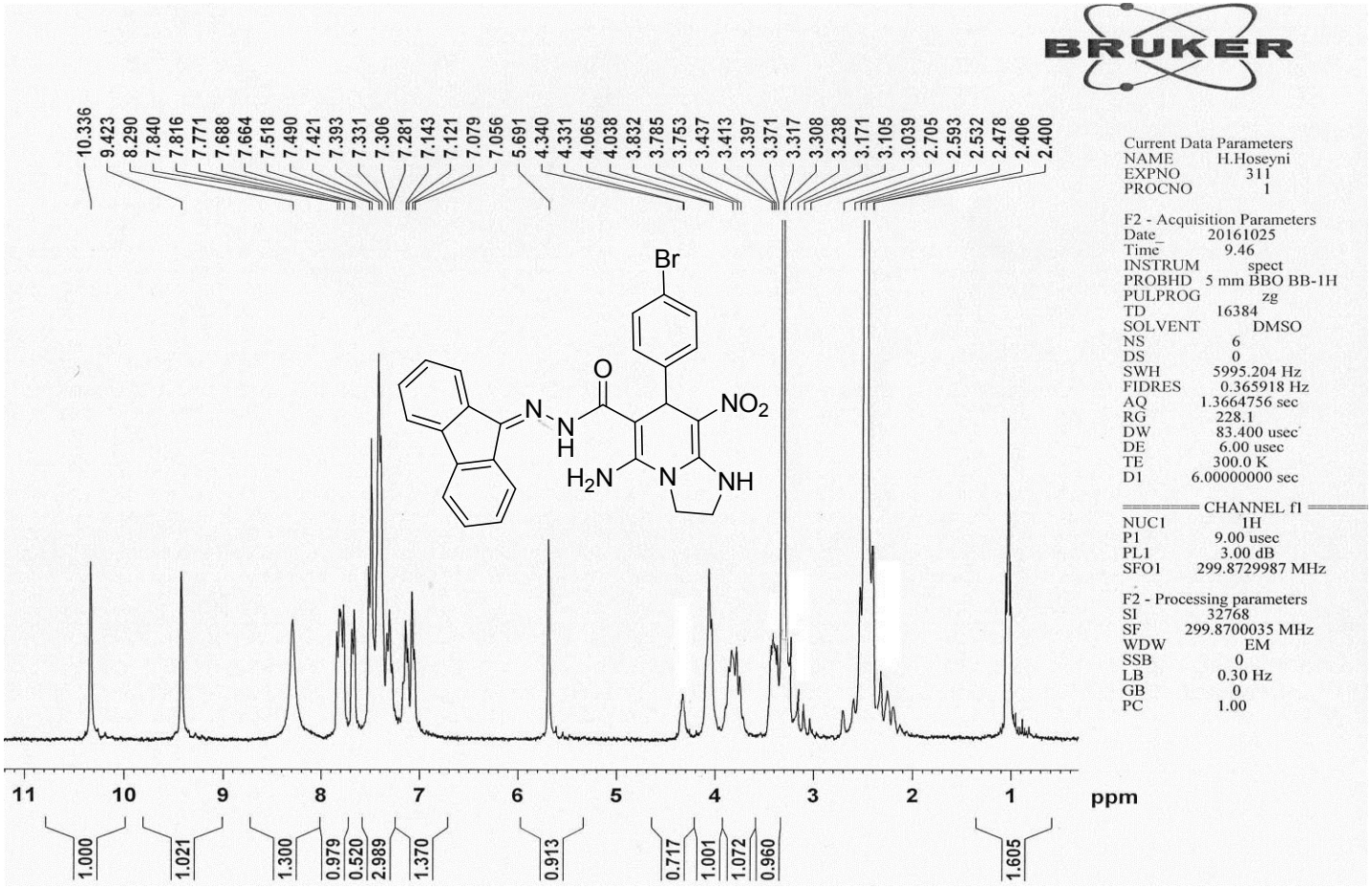
^{13}C NMR of 6i


Transmittance [%]
100
98
96
94
92
90
88
86
3500
3000
2500
2000
1500
1000
500
3733.97
3349.10
2917.52
2355.38
1661.14
1607.66
1511.69
1448.09
1352.62
1261.86
1169.59
1123.85
1033.91
949.44
885.84
781.11
731.99
648.55
576.98
426.87
CH3
O
N
N
H
NO2
H2N
N
NH

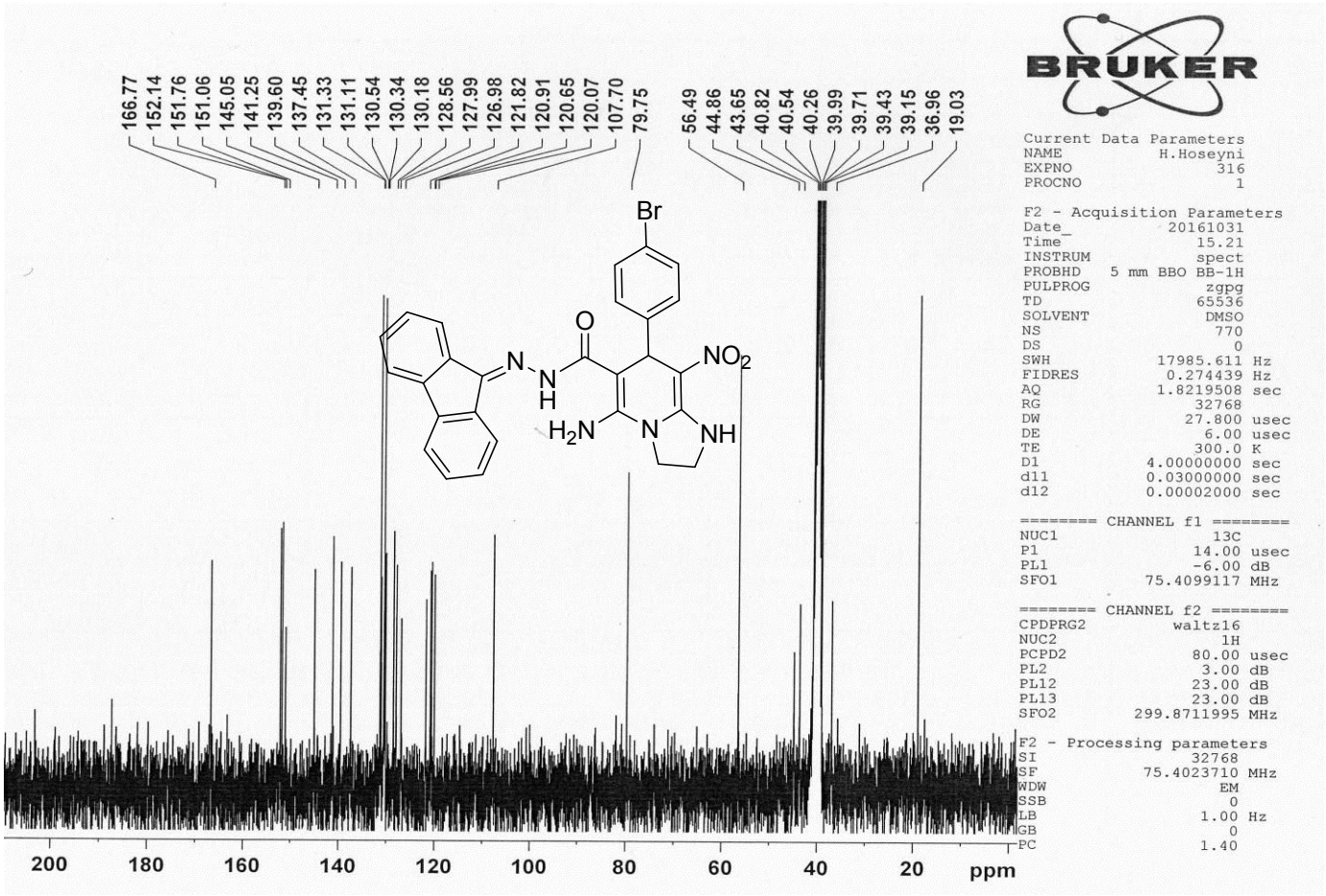
IR of 6i


Abundance
Average of 1.336 to 2.470 min.: HH-R24.d\data.ms
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
356.2
165.1
226.2
272.2
69.1
115.1
313.3
396.4
434.4
495.5
536.6
50
100
150
200
250
300
350
400
450
500
m/z-->

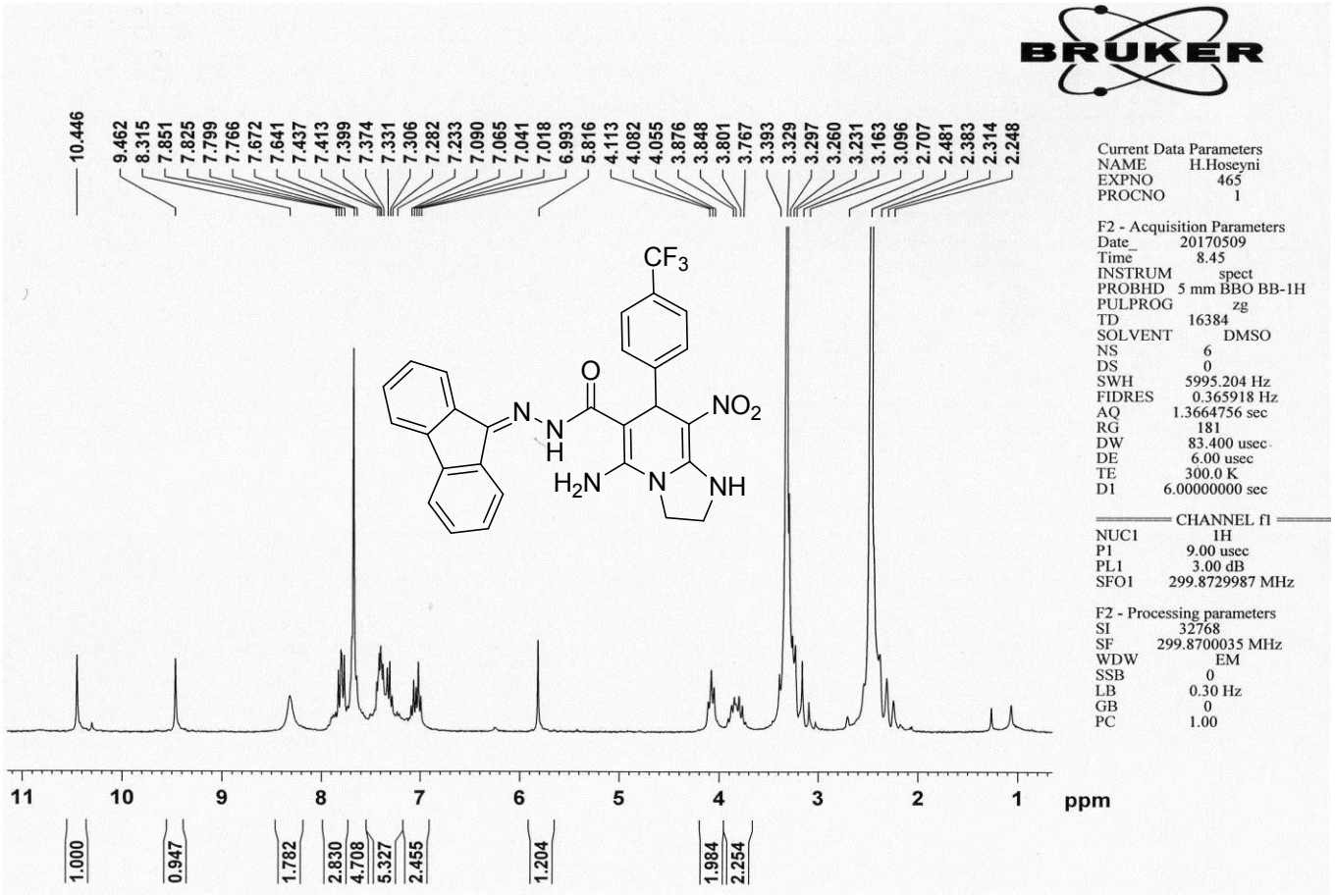
MS of 6i


BRUKER
10.336
9.423
8.290
7.840
7.816
7.771
7.688
7.664
7.518
7.490
7.421
7.393
7.331
7.306
7.281
7.143
7.121
7.079
7.056
5.691
4.340
4.331
4.065
4.038
3.832
3.785
3.753
3.437
3.413
3.397
3.371
3.317
3.308
3.238
3.171
3.105
3.039
2.705
2.593
2.532
2.478
2.406
2.400
Br
O
N
N
H
NO2
H2N
N
NH
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.021
1.300
0.979
0.520
2.989
1.370
0.913
0.717
1.001
1.072
0.960
1.605
Current Data Parameters
NAME H.Hoseyni
EXPNO 311
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 9.46
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 228.1
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

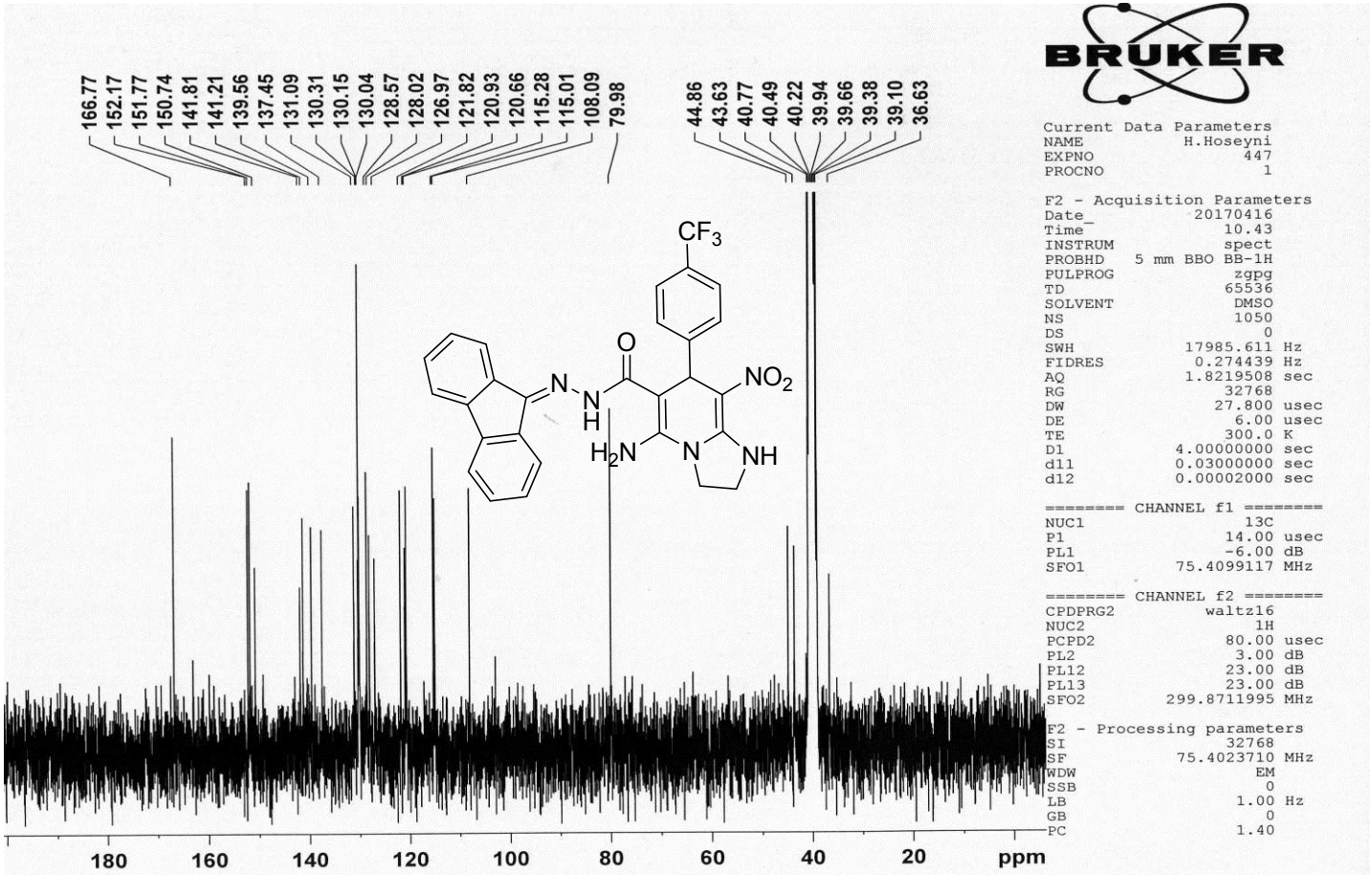
^{1}H NMR of 6j


166.77
152.14
151.76
151.06
145.05
141.25
139.60
137.45
131.33
131.11
130.54
130.34
130.18
128.56
127.99
126.98
121.82
120.91
120.65
120.07
107.70
79.75
56.49
44.86
43.65
40.82
40.54
40.26
39.99
39.71
39.43
39.15
36.96
19.03
Br
O
N
N
H
NO2
H2N
N
NH
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 316
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161031
Time 15.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 770
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 6j


BRUKER
10.446
9.462
8.315
7.851
7.825
7.799
7.766
7.672
7.641
7.437
7.413
7.399
7.374
7.331
7.306
7.282
7.233
7.090
7.065
7.041
7.018
6.993
5.816
4.113
4.082
4.055
3.876
3.848
3.801
3.767
3.393
3.329
3.297
3.260
3.231
3.163
3.096
2.707
2.481
2.383
2.314
2.248
CF3
O
N
N
H
NO2
H2N
N
NH
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
0.947
1.782
2.830
4.708
5.327
2.455
1.204
1.984
2.254
Current Data Parameters
NAME H.Hoseyni
EXPNO 465
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170509
Time 8.45
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 6k


166.77
152.17
151.77
150.74
141.81
141.21
139.56
137.45
131.09
130.31
130.15
130.04
128.57
128.02
126.97
121.82
120.93
120.66
115.28
115.01
108.09
79.98
44.86
43.63
40.77
40.49
40.22
39.94
39.66
39.38
39.10
36.63
CF3
O
NO2
N
N
H
H2N
N
NH
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME H.Hoseyni
EXPNO 447
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170416
Time 10.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 1050
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 6k