

Transformation of 3-(4-methoxybenzylidene)-5-(*p*-tolyl)-2(3*H*)-Furanone into New Nitrogen Heterocyclic Candidates as Insecticidal Agents with *In-Silico* Studies

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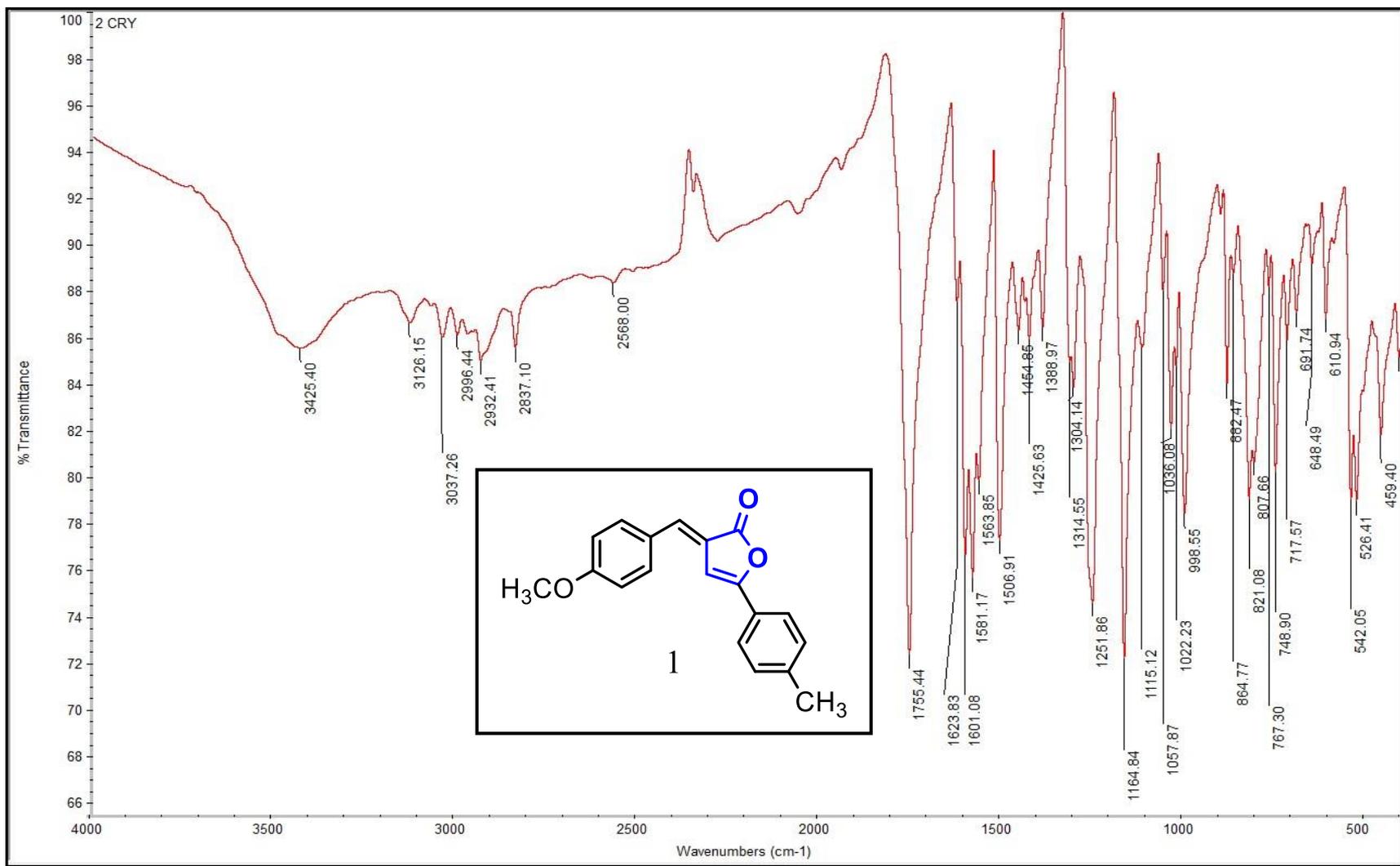
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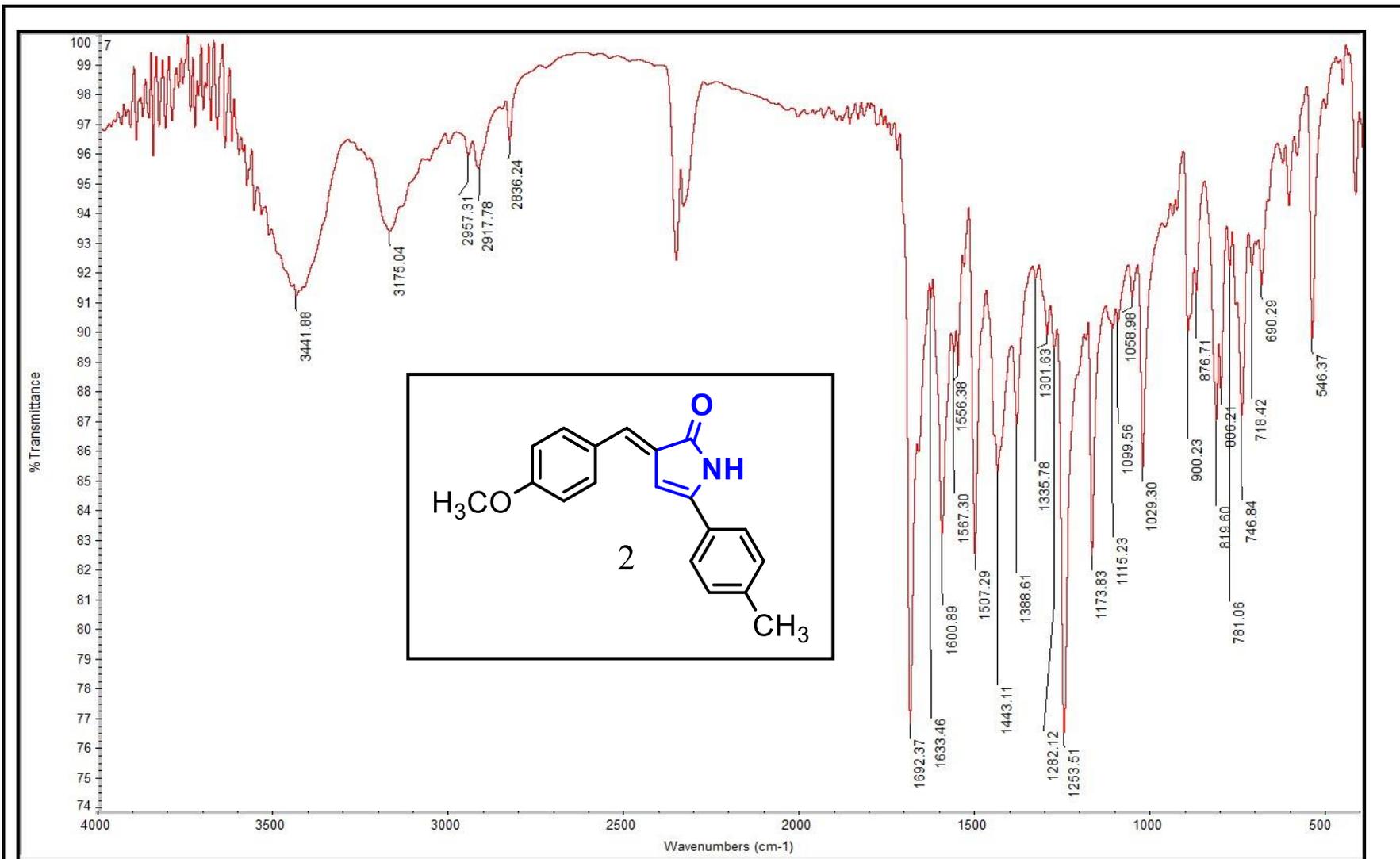
*E-mail: david.shoukry@sci.asu.edu.eg (DSAH); sayed.karam2008@sci.asu.edu.eg (SKR)

Supporting information:

Spectral Data:



IR spectrum of compound 1



IR spectrum of compound 2

NorhanMahmoud-7-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz

9 repetitions
OBSERVE H1, 300.0687870 MHz

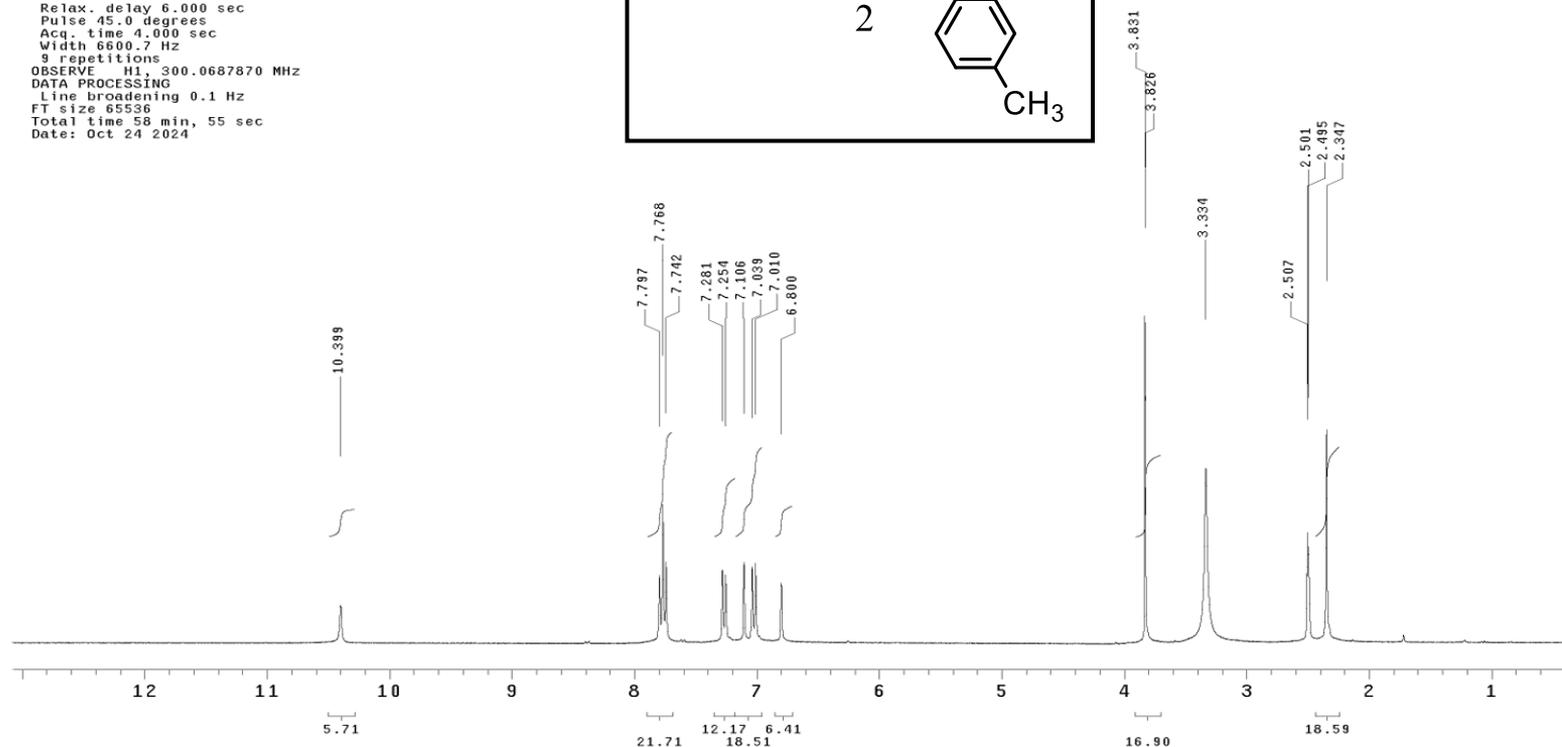
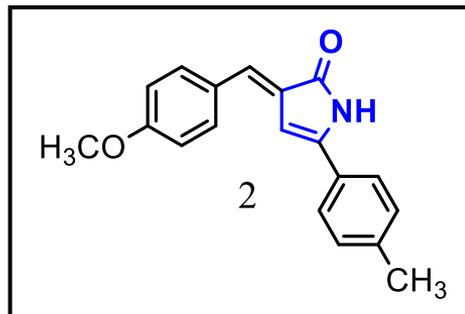
DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 58 min, 55 sec

Date: Oct 24 2024



^1H NMR spectrum (DMSO- d_6) of compound 2

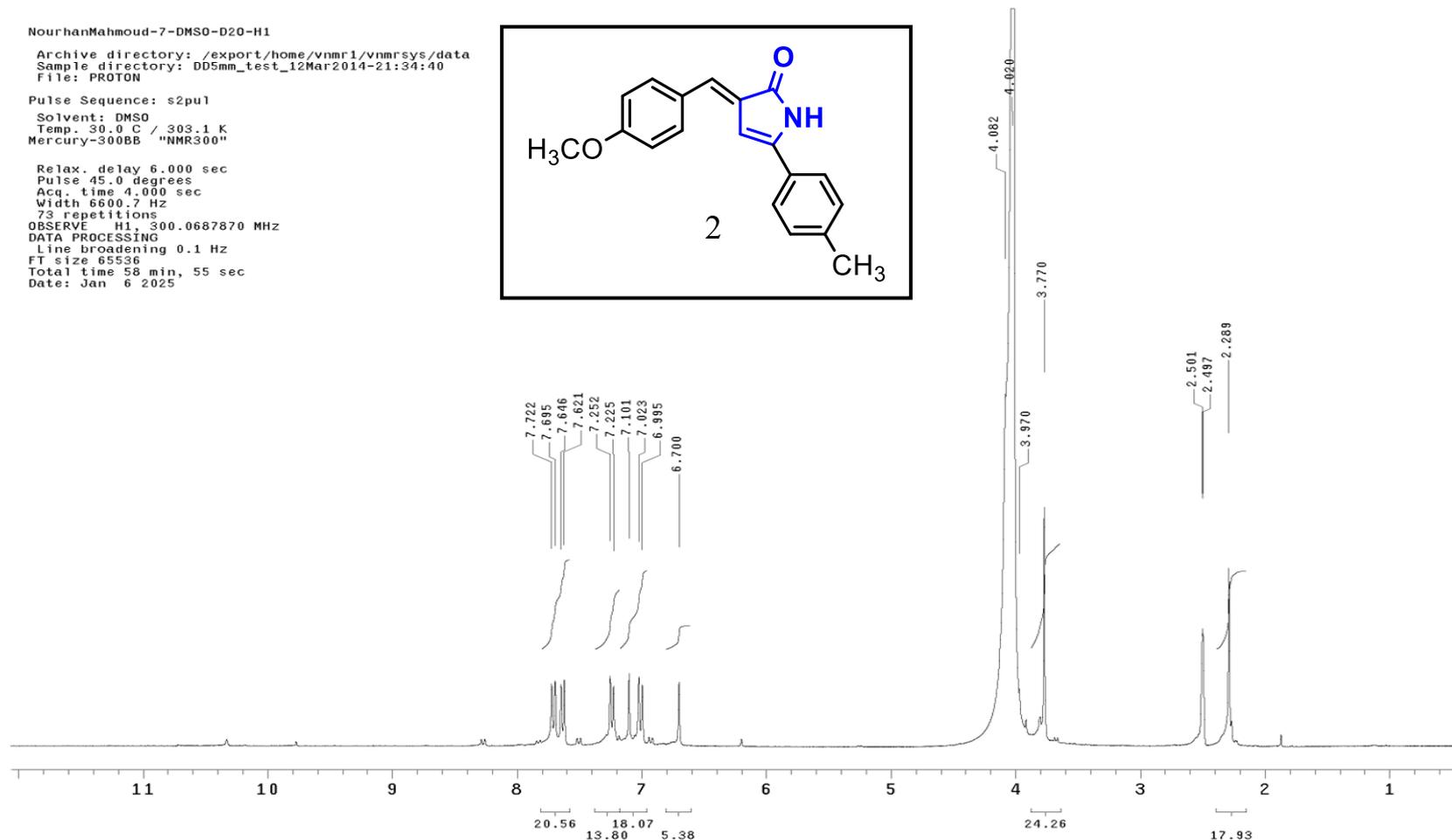
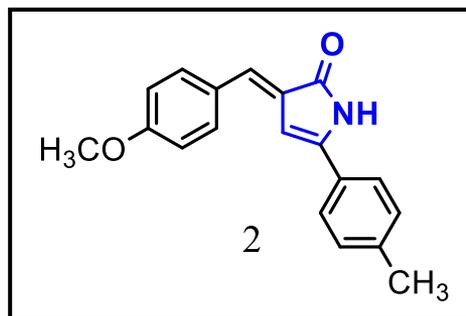
NourhanMahmoud-7-DMSO-D2O-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
73 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Jan 6 2025



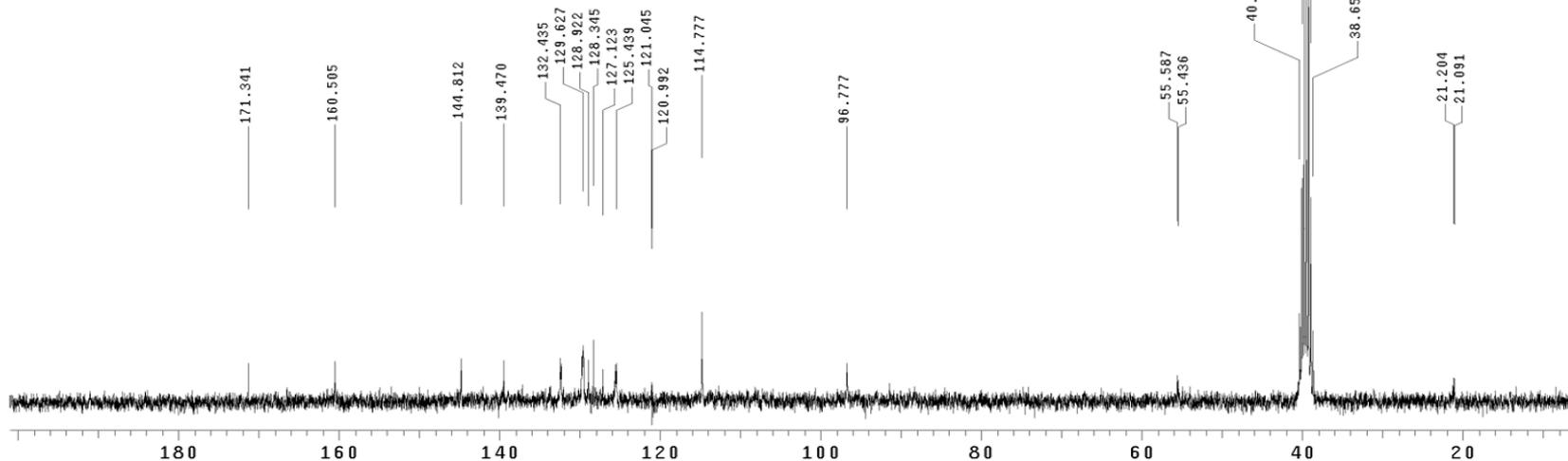
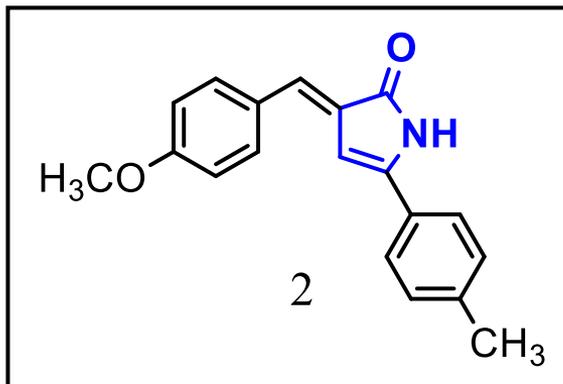
¹H NMR spectrum (DMSO-*d*₆ + D₂O) of compound 2

NourhanMahmoud-7-DMSO-C13

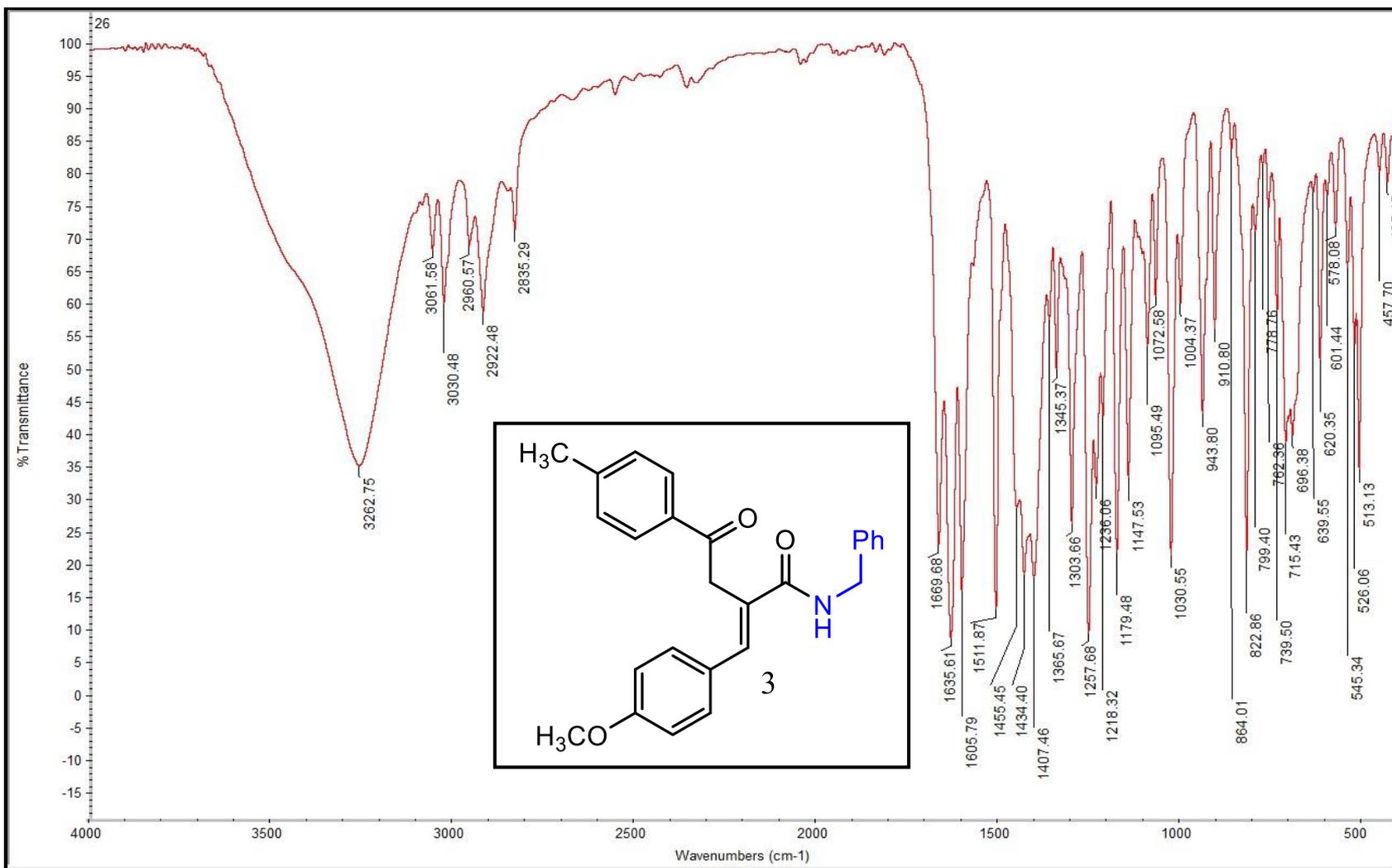
Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
3072 repetitions
OBSERVE C13, 75.4523771 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 311 hr, 12 min, 6 sec
Date: Dec 30 2024



¹³C NMR spectrum of compound 2.



IR spectrum of compound 3

NourhanMahmoud-26-DMSO-H1

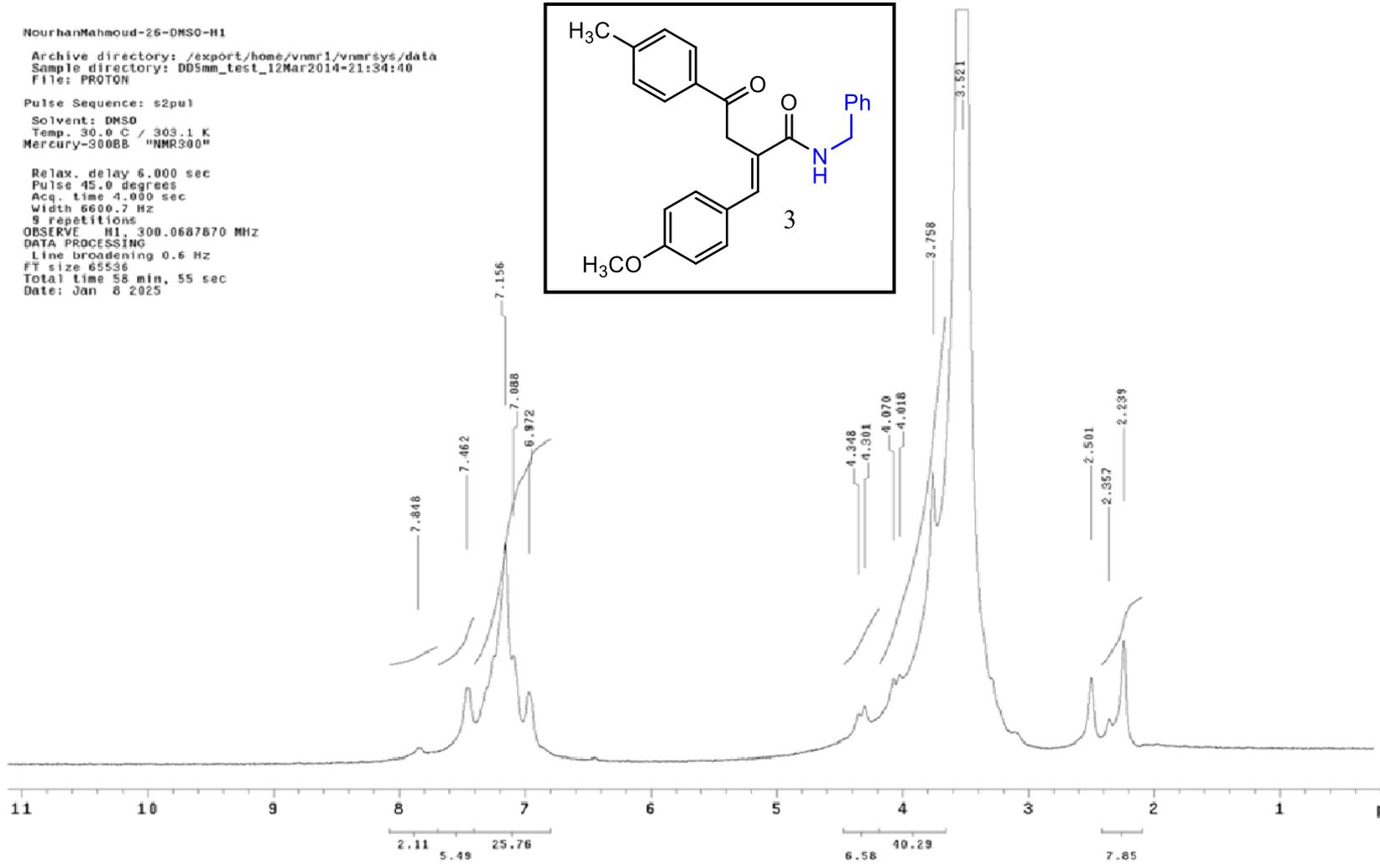
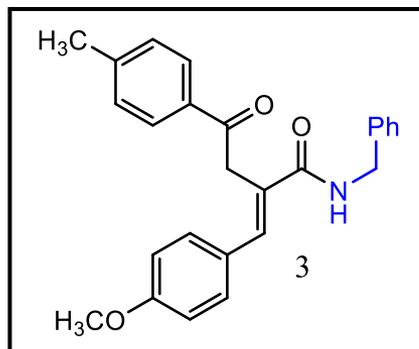
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

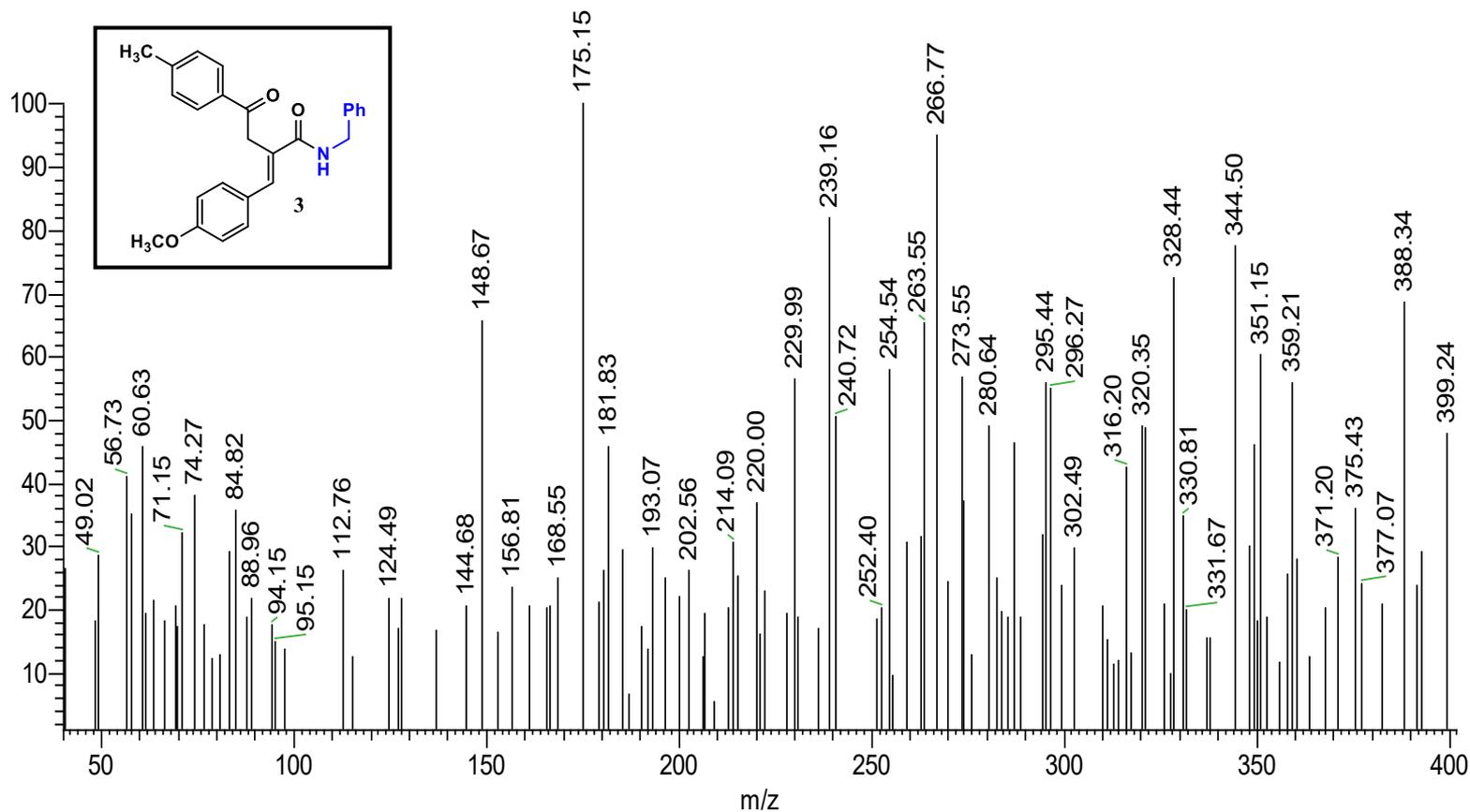
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
9 repetitions

OBSERVE H1, 300.0687670 MHz
DATA PROCESSING
Line broadening 0.6 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Jan 8 2025



¹H NMR spectrum (DMSO-*d*₆) of compound 3

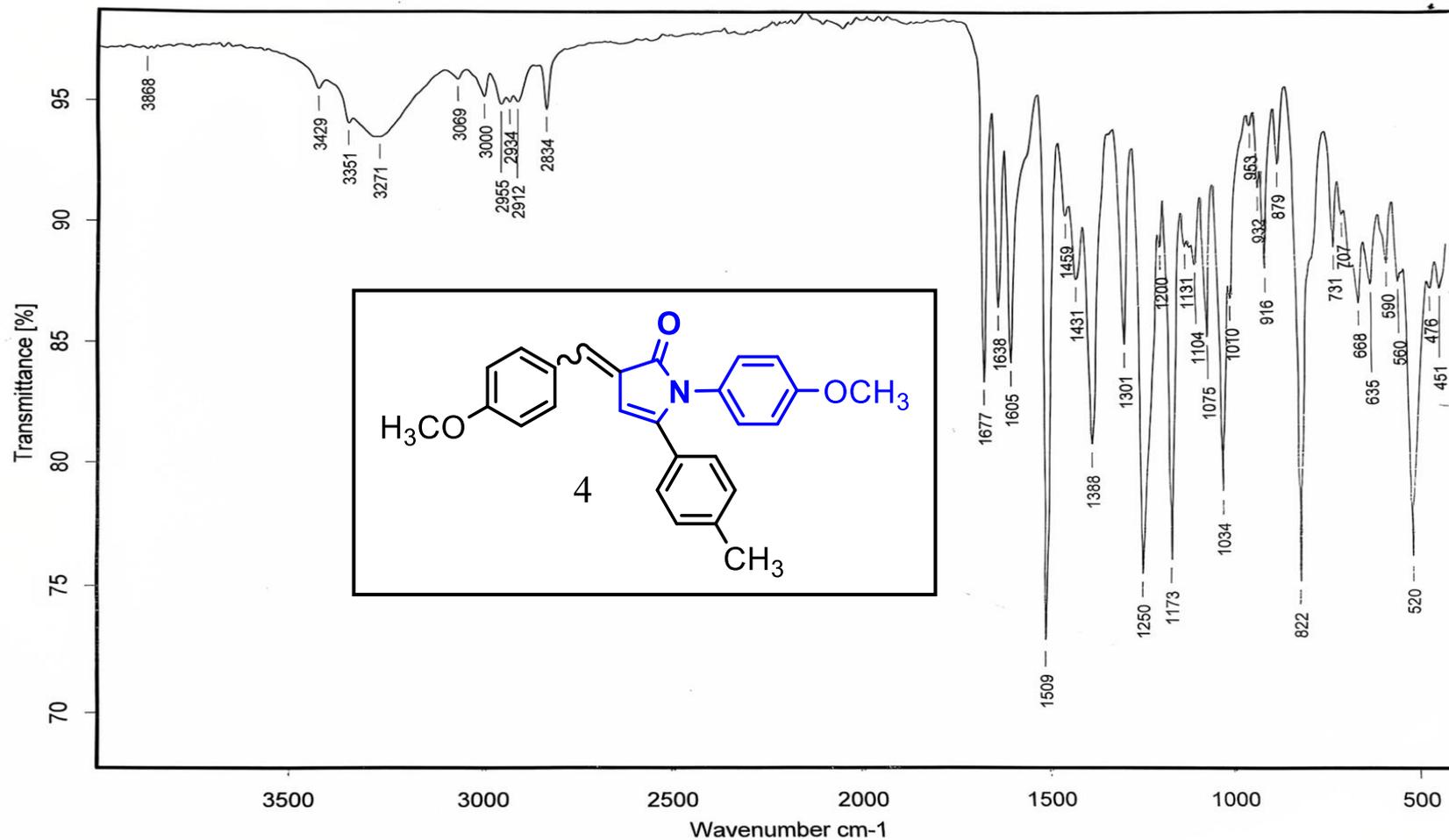
26 #16 RT: 0.28 P: + NL: 4.87E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS of compound 3

9-NH.0

9/12/2024



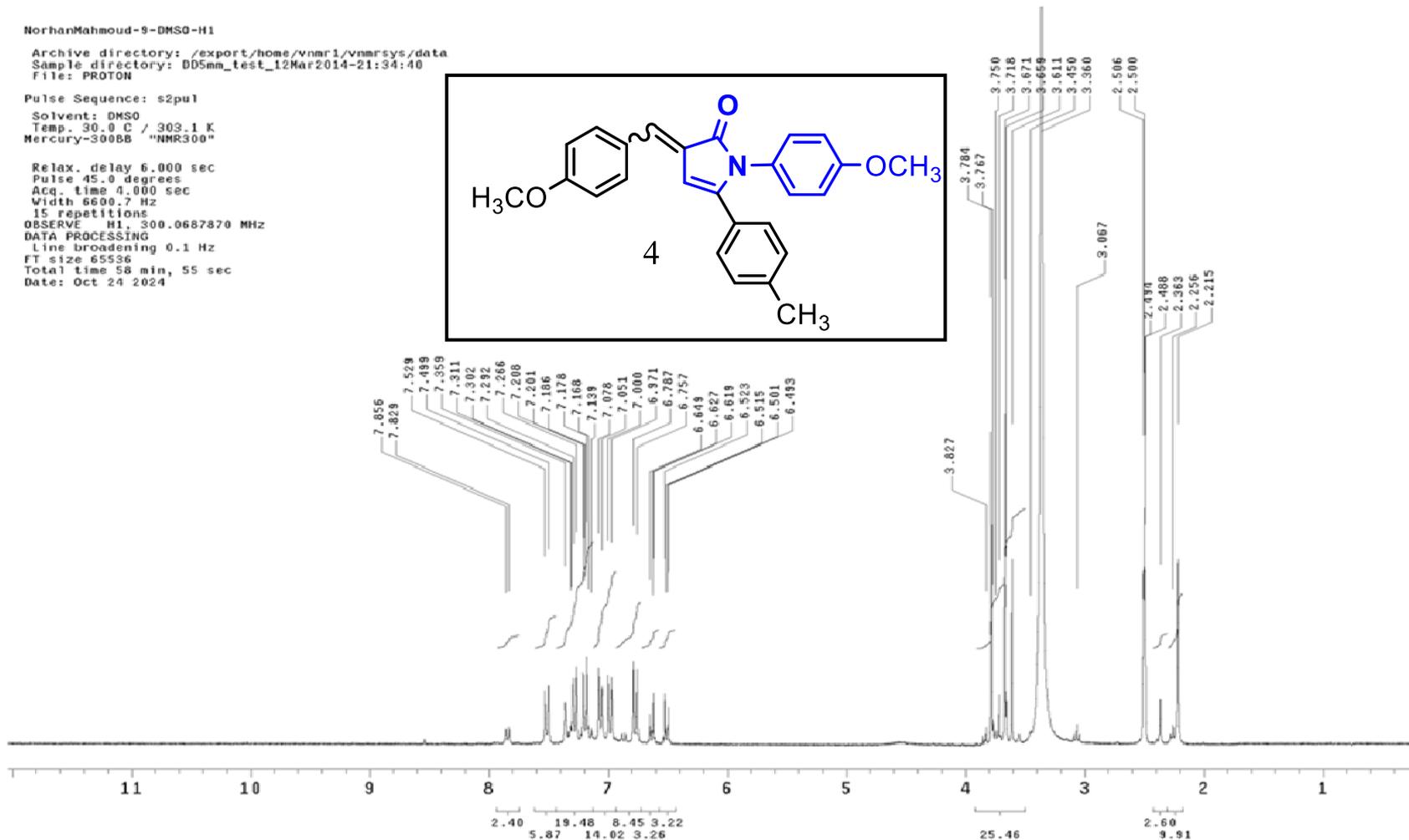
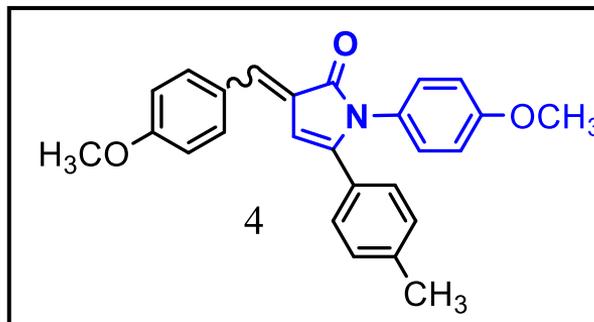
IR spectrum of compound 4

NorhanMahmoud-9-DMSO-H1

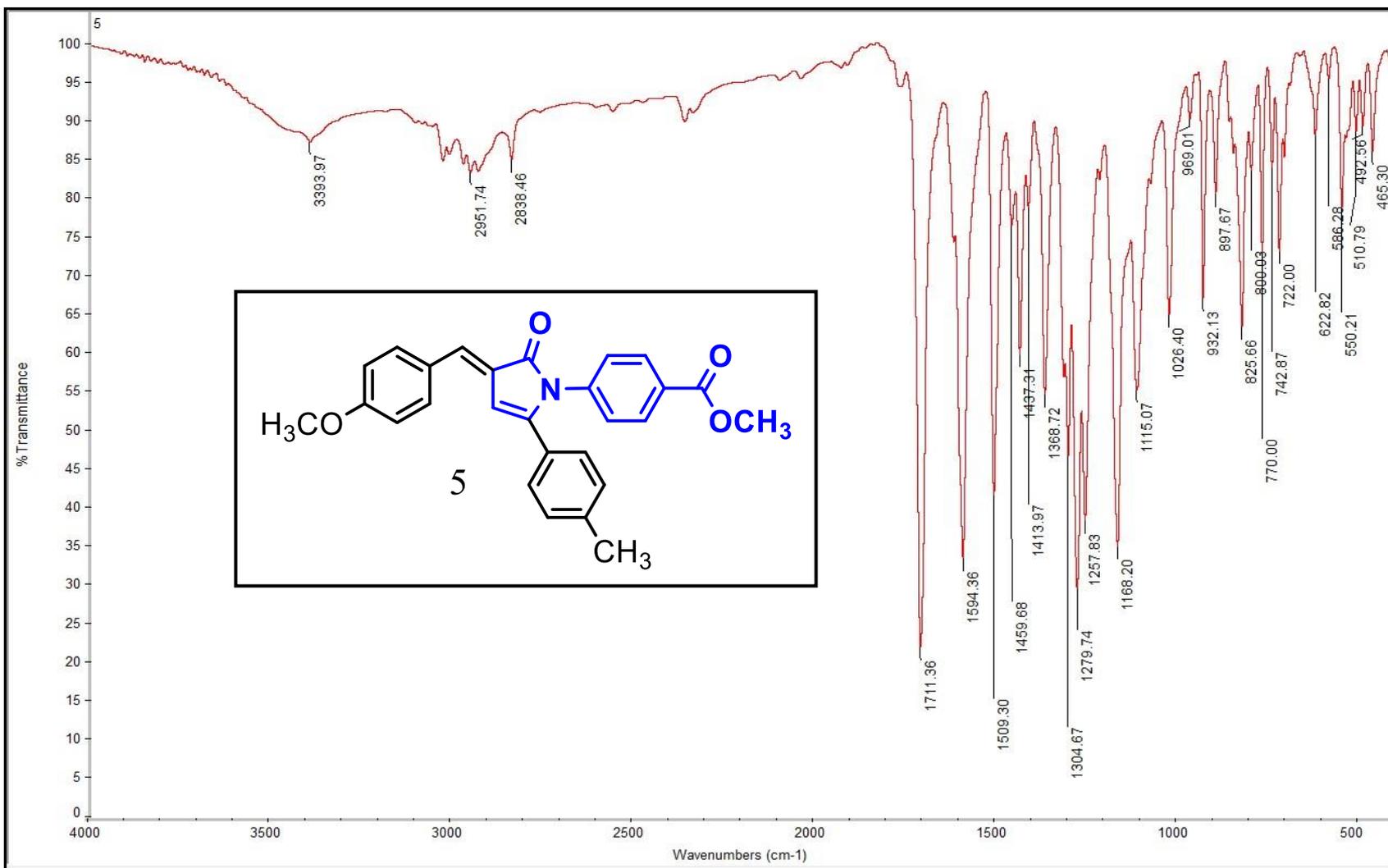
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 0.000 sec
Width 6600.7 Hz
15 repetitions
OBSERVE H1, 300.0687370 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Oct 24 2024



¹H NMR spectrum (DMSO-*d*₆) of compound 4



IR spectrum of compound 5

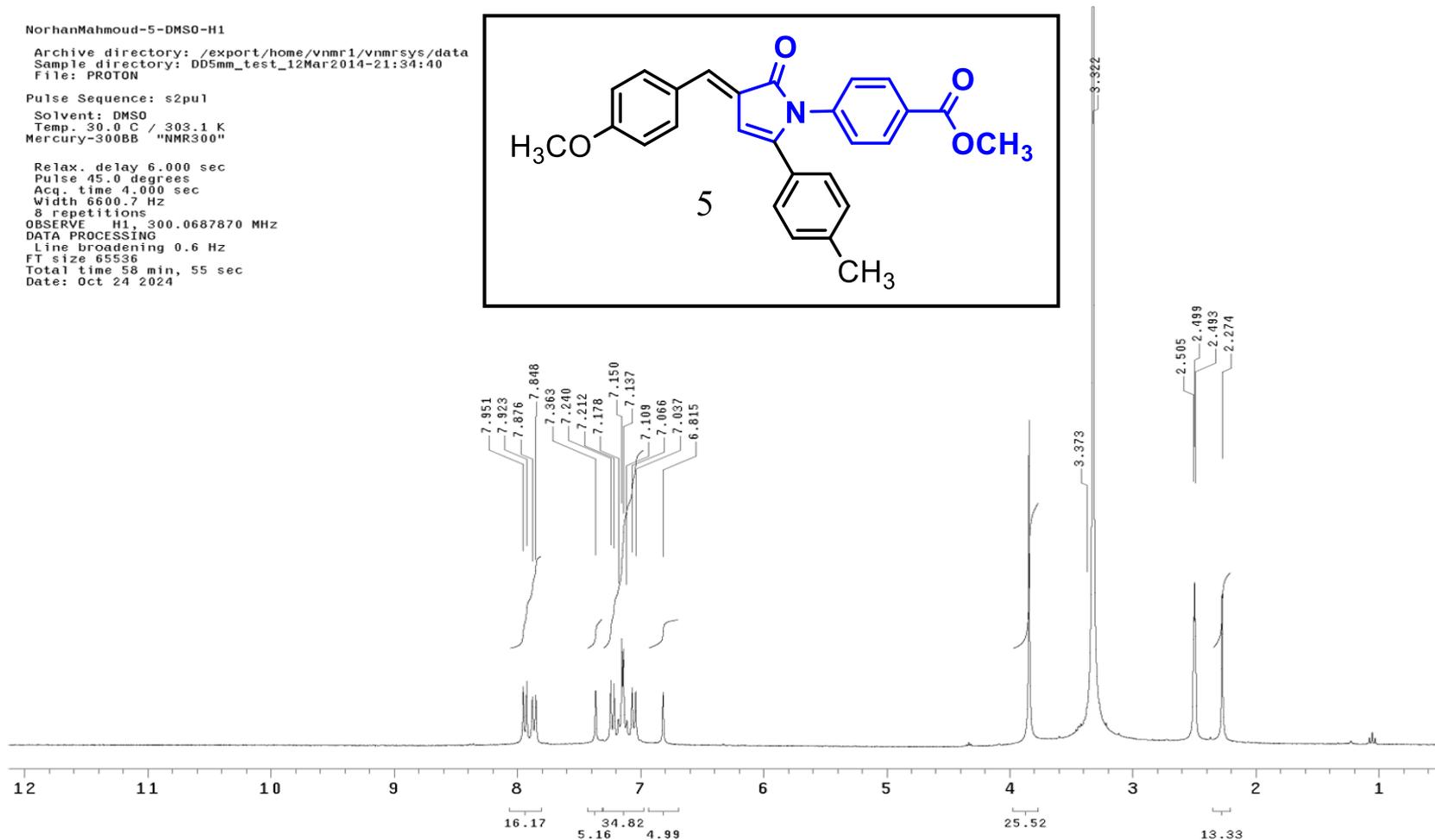
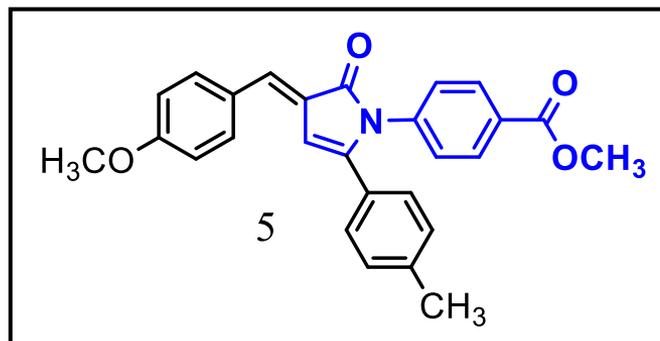
NorhanMahmoud-5-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
8 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.6 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Oct 24 2024



¹H NMR spectrum (DMSO-*d*₆) of compound 5



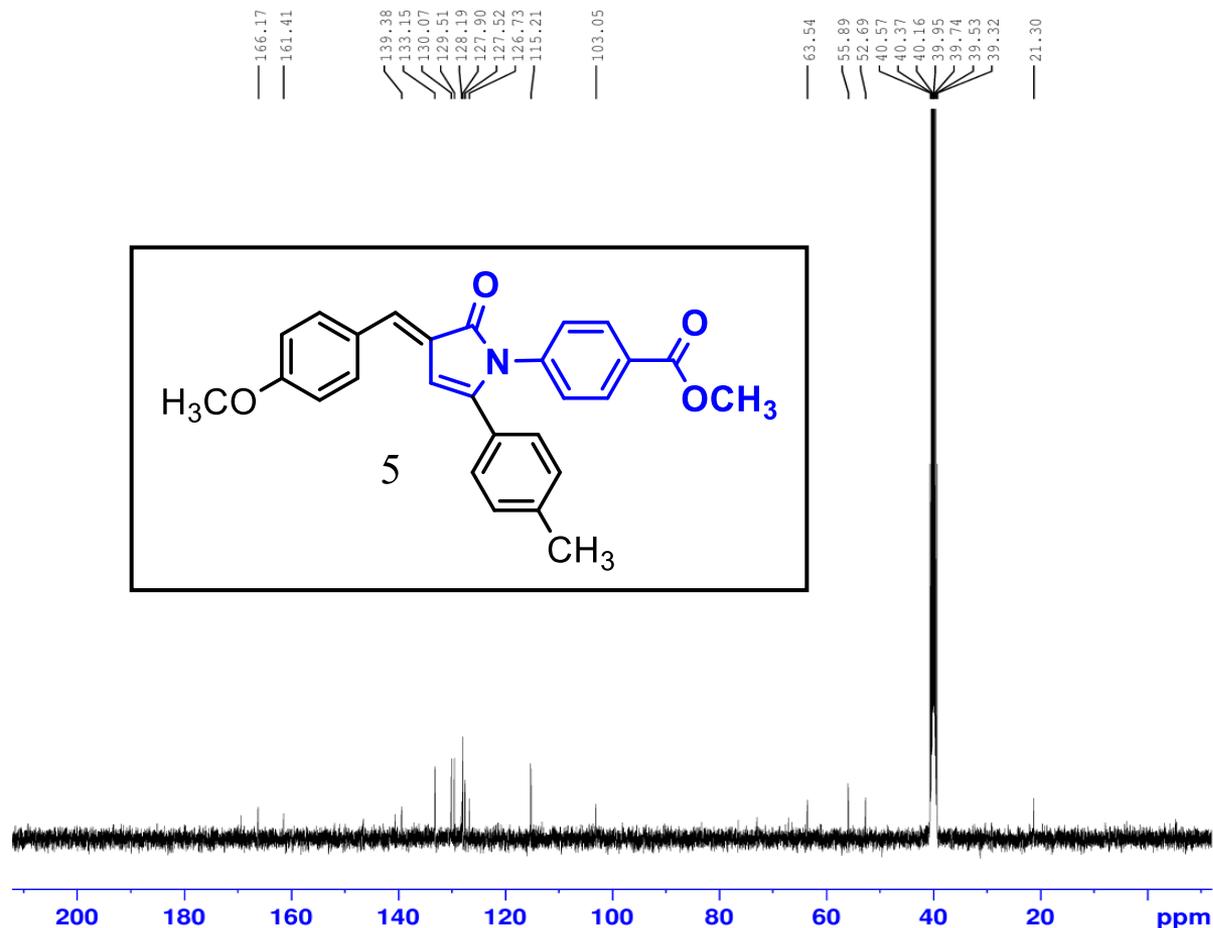
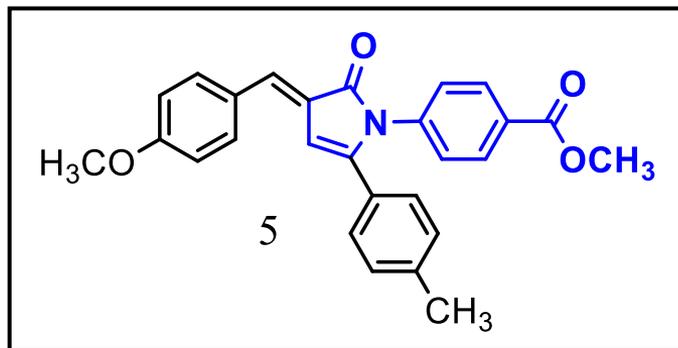
Current Data Parameters
NAME nourhan-mahmoud-cpd-5
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250618
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65336
SOLVENT DMSO
NS 3618
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

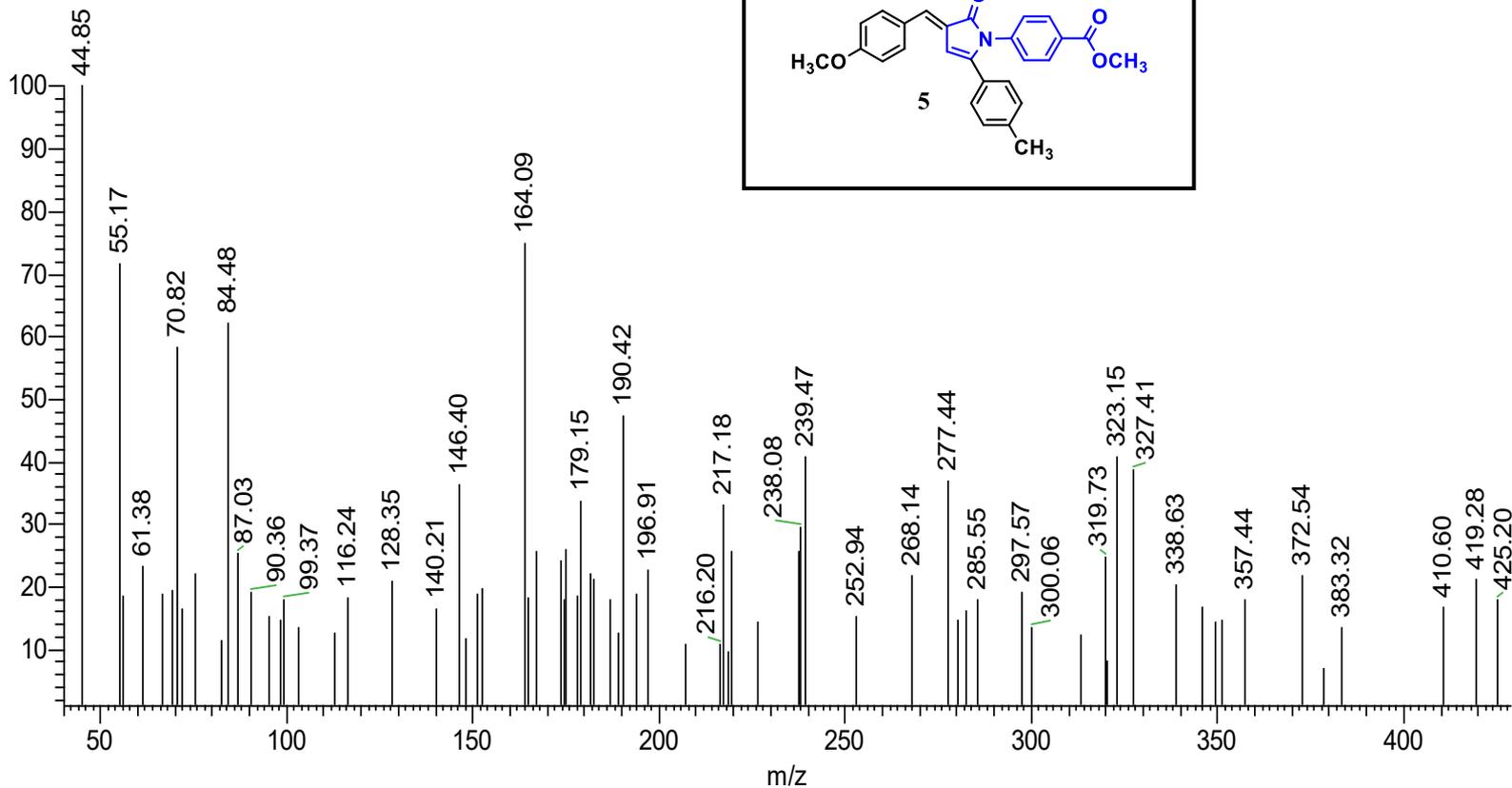
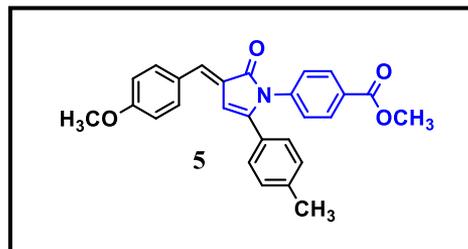
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

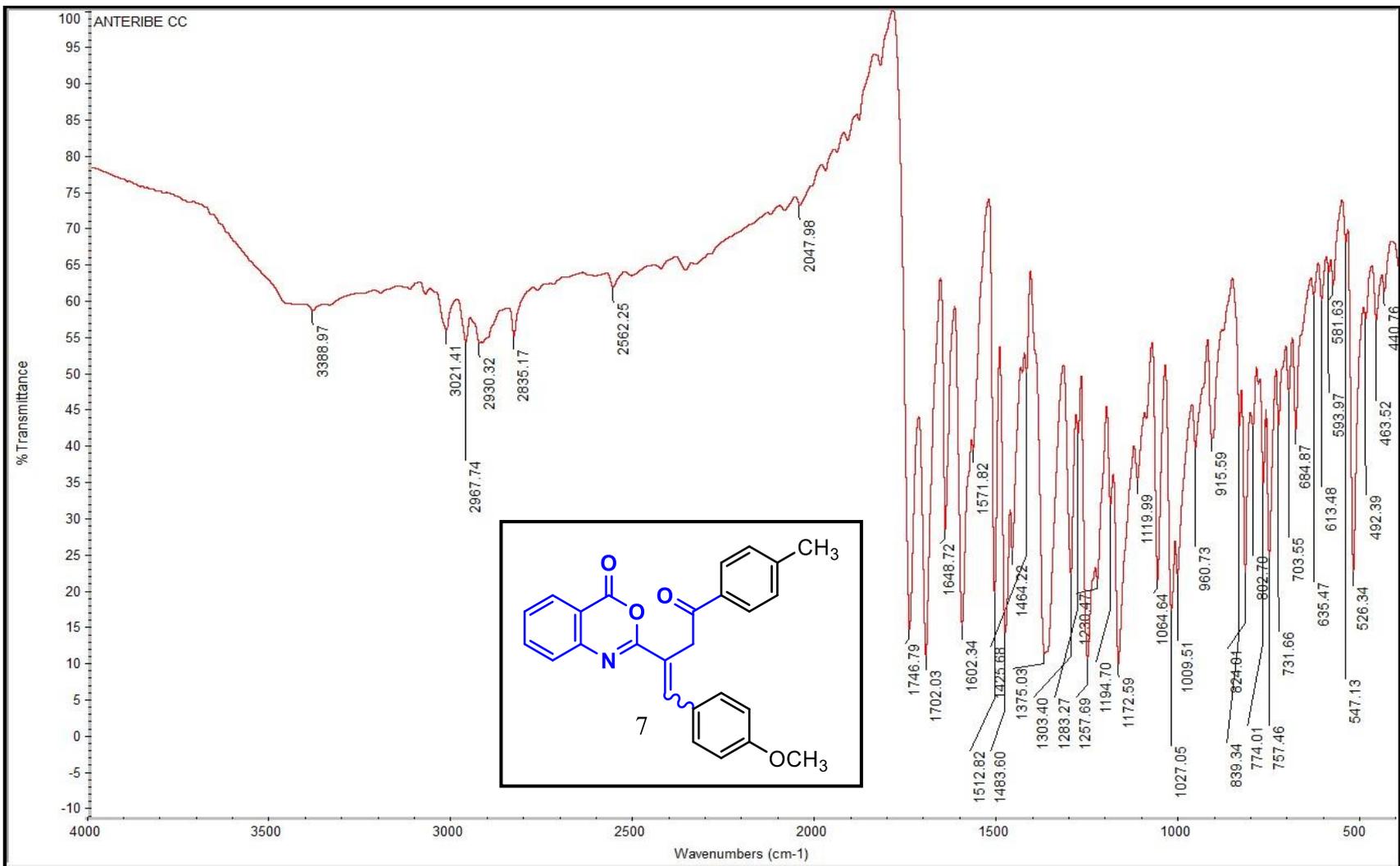


¹³C NMR spectrum of compound 5

5 #66 RT: 1.12 P: + NL: 6.17E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS of compound 5



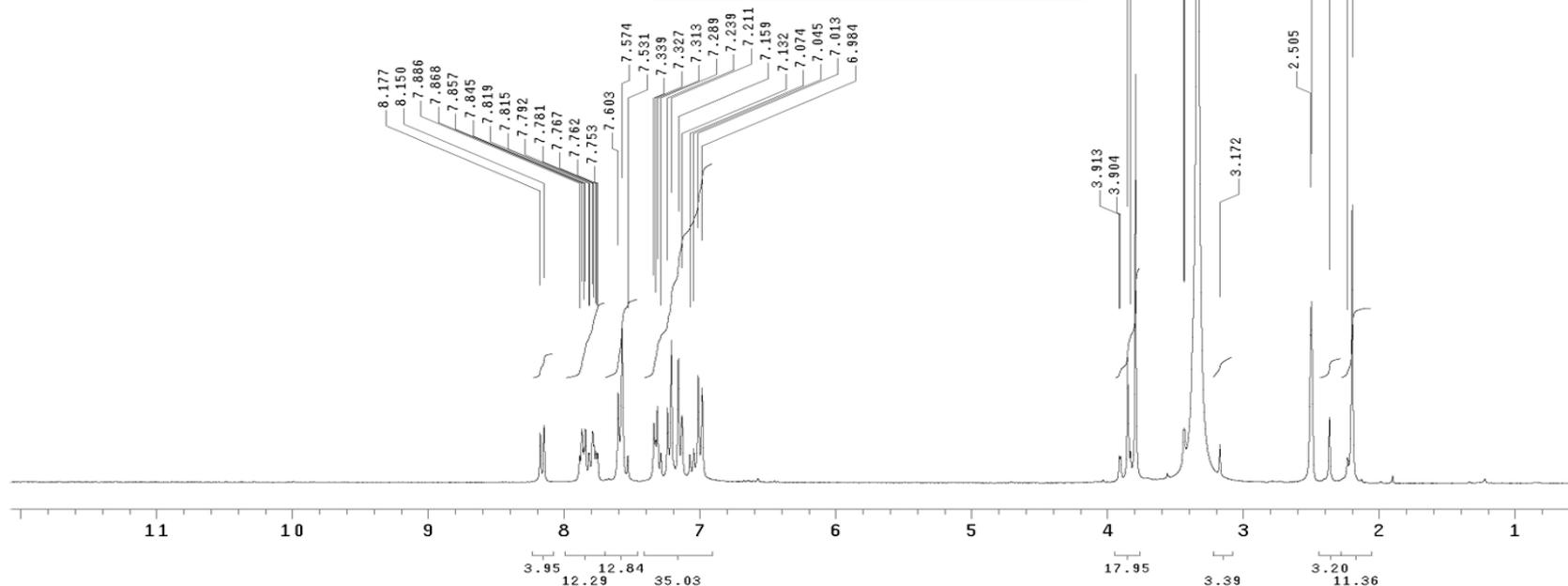
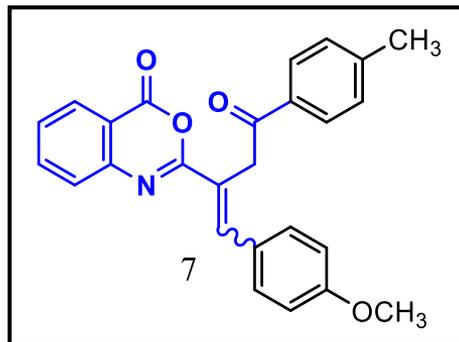
IR spectrum of compound 7

NorhanMahmoud-3-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
8 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.6 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Oct 24 2024



¹H NMR spectrum (DMSO-*d*₆) of compound 7

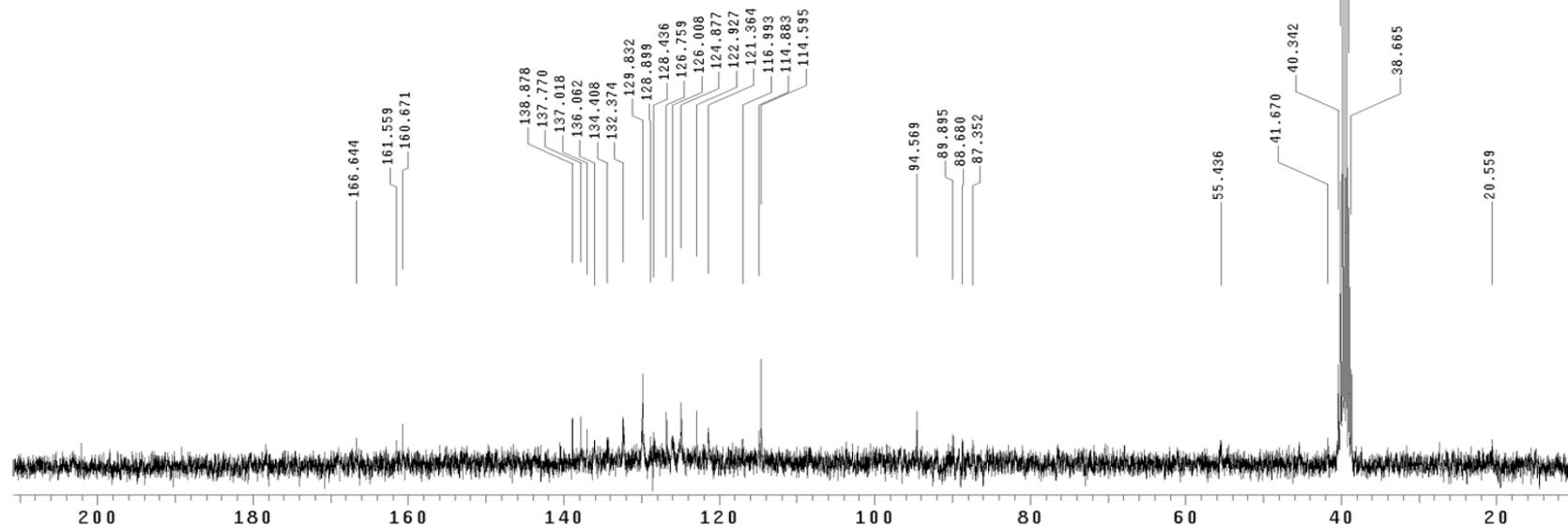
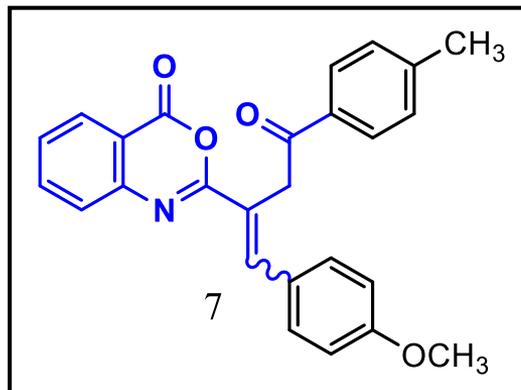
NourhanMahmoud-3-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

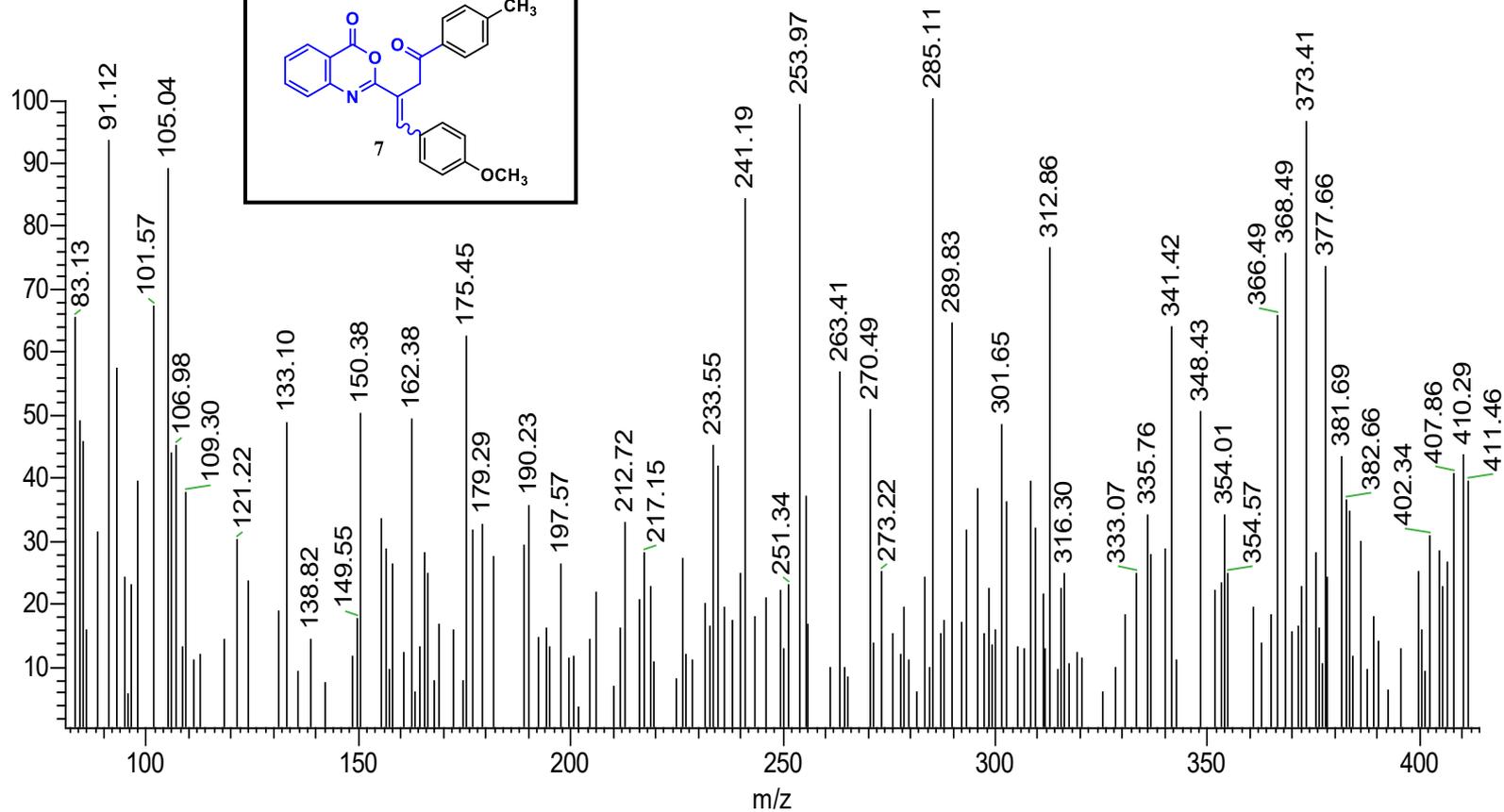
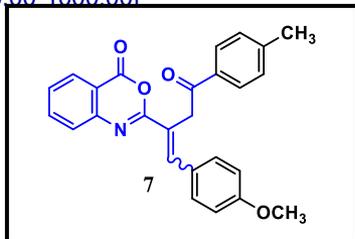
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2200 repetitions
OBSERVE C13, 75.4523822 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 311 hr, 12 min, 6 sec
Date: Jan 2 2025

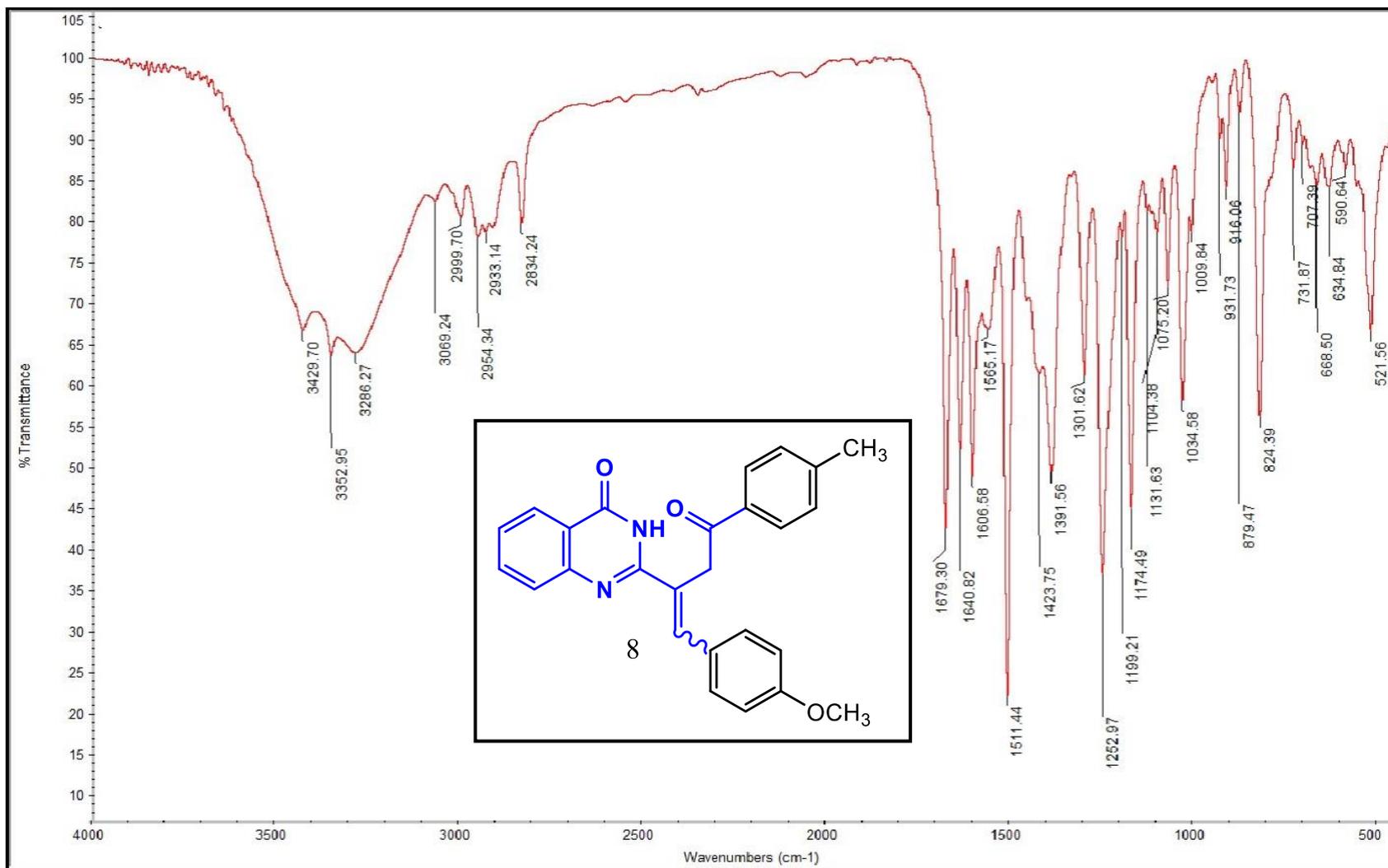


¹³C NMR spectrum of compound 7

3#102 RT: 1.72 P: + NL: 7.94E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS of compound 7



IR spectrum of compound 8

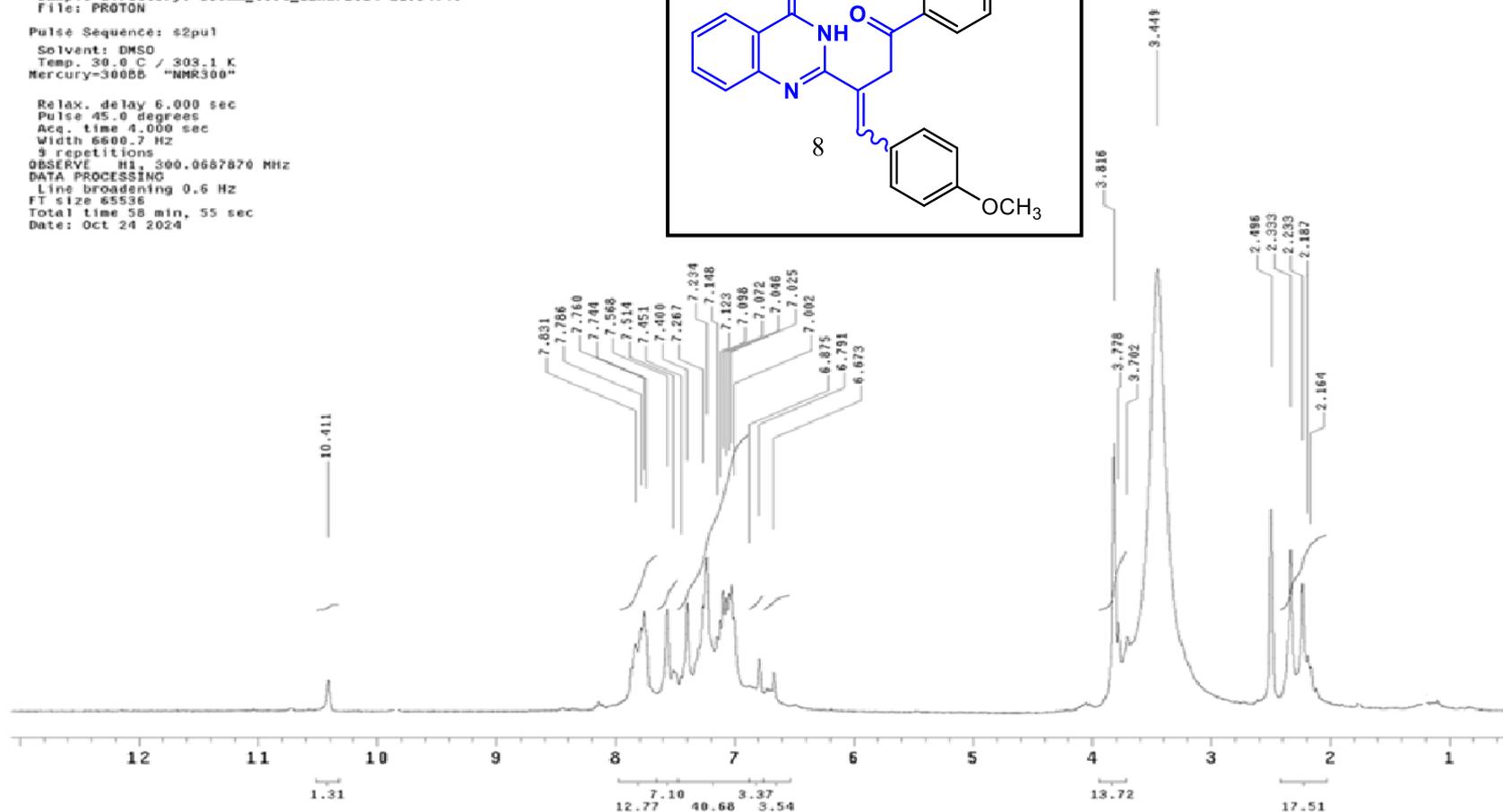
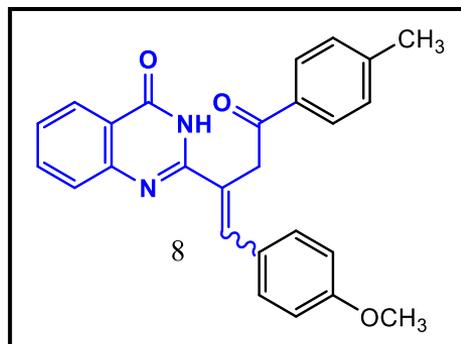
NorhanMahmoud-16cy-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: 005mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury=30005 "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
3 repetitions
OBSERVE H1, 300.0667870 MHz
DATA PROCESSING
Line broadening 0.6 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Oct 24 2024



¹H NMR spectrum (DMSO-d₆) of compound 8

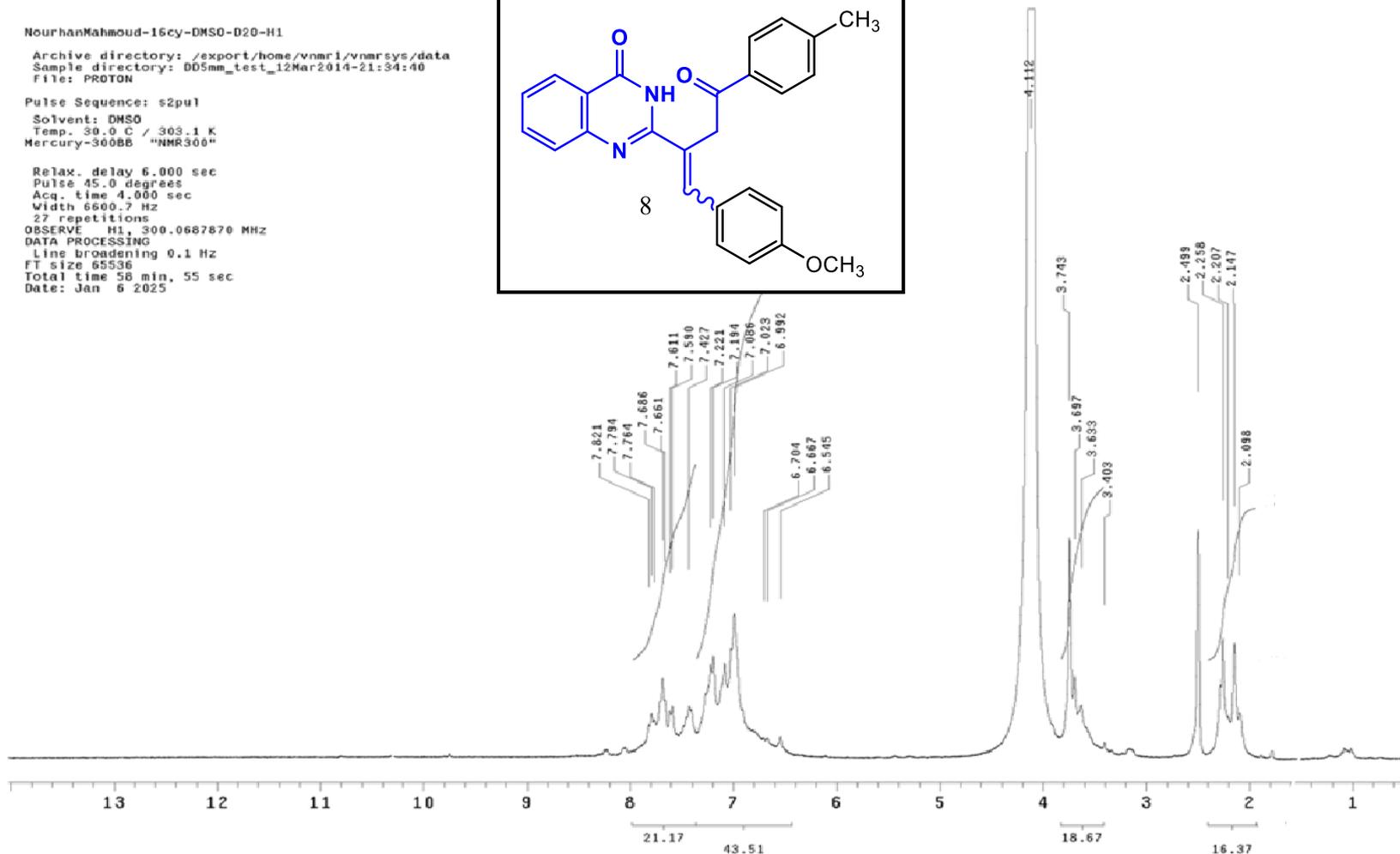
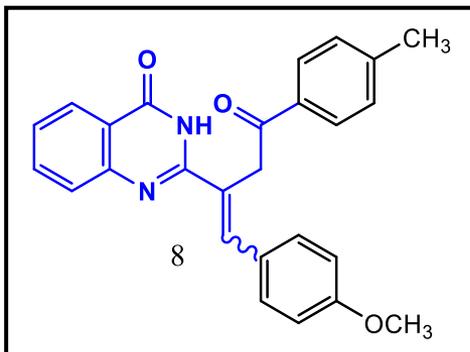
NourhanMahmoud-16cy-DMSO-D20-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6500.7 Hz
27 repetitions
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DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Jan 6 2025



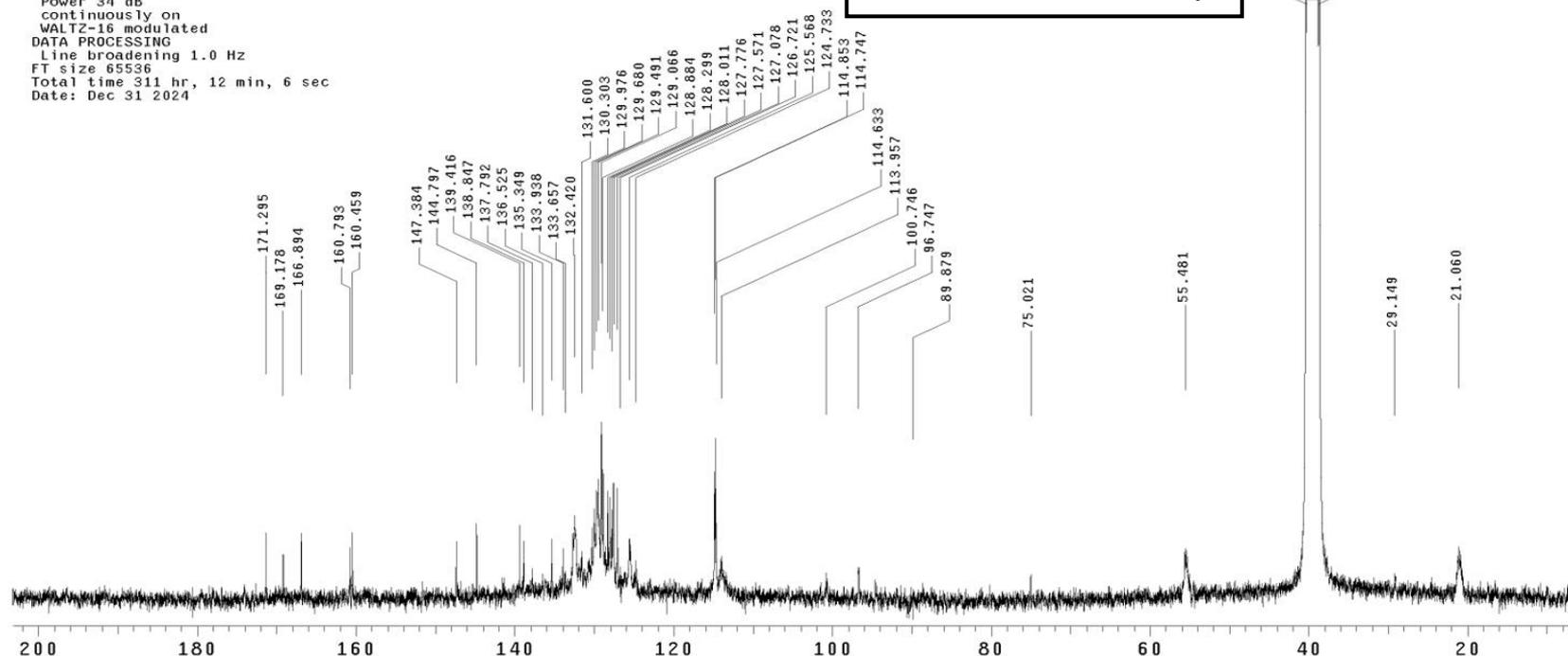
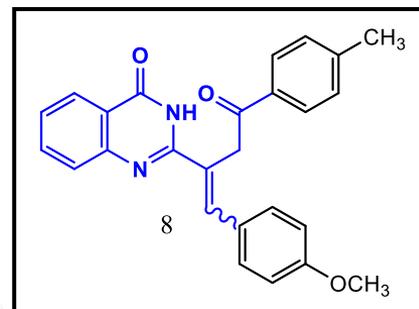
¹H NMR spectrum (DMSO-d₆ + D₂O) of compound 8

NourhanMahmoud-16cy-DMSO-C13

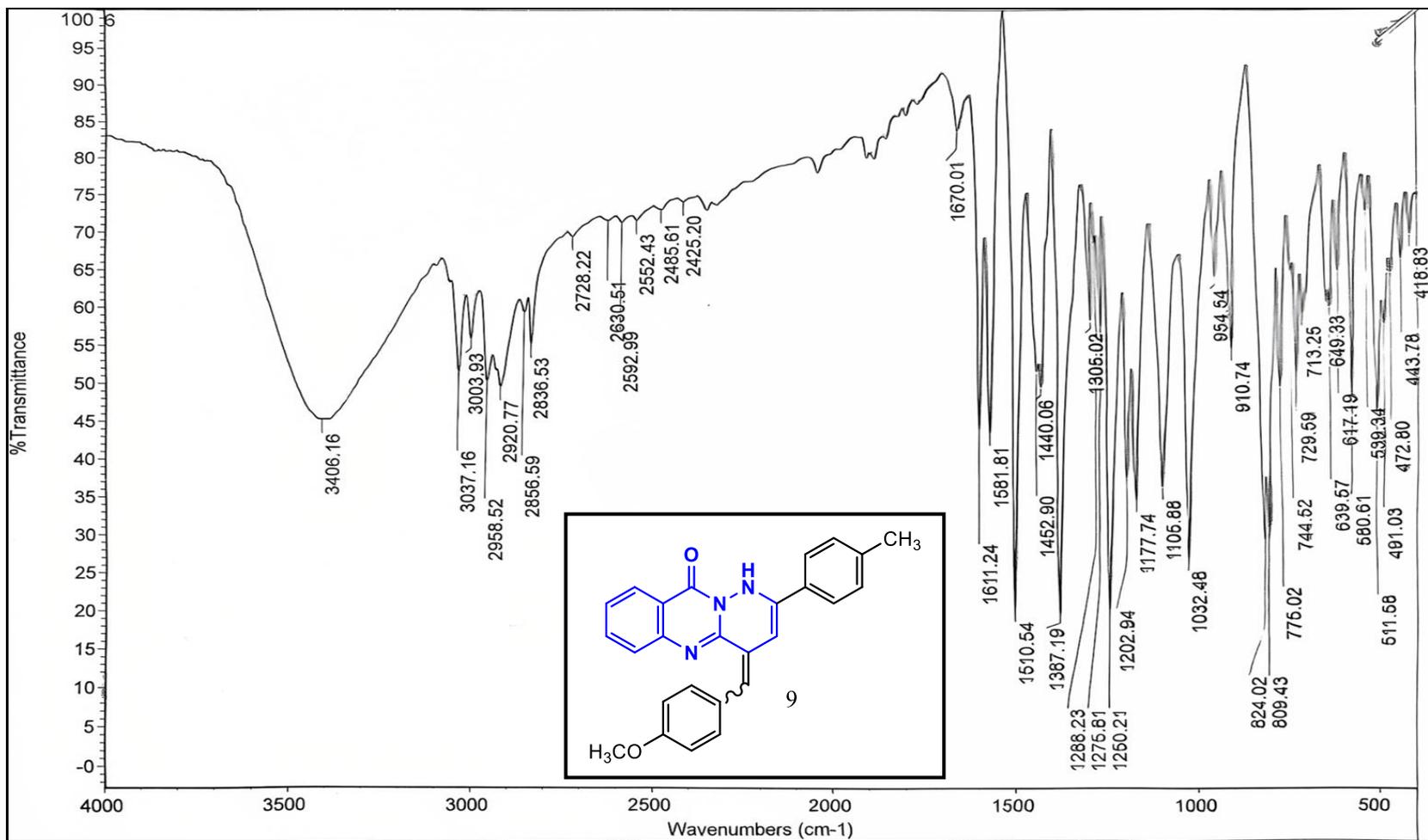
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Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
43520 repetitions
OBSERVE C13, 75.4523794 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 311 hr, 12 min, 6 sec
Date: Dec 31 2024



¹³C NMR spectrum of compound 8



IR spectrum of compound 9

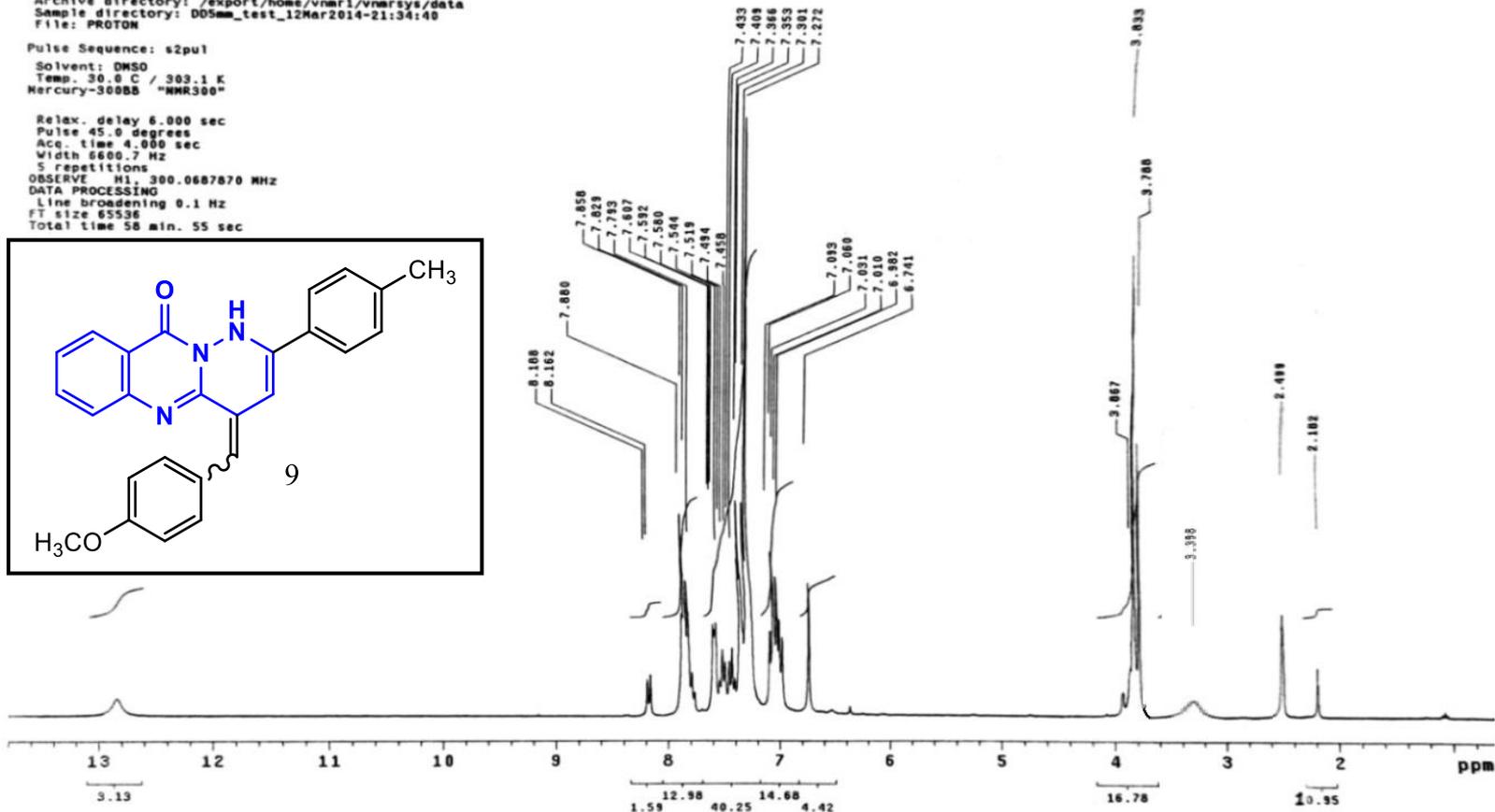
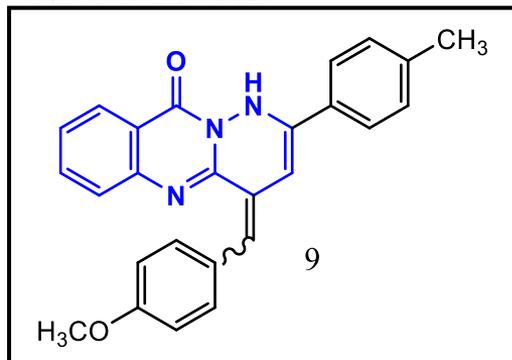
NourhanMahmoud-A2-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:48
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp: 30.6 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
5 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65528
Total time 58 min. 55 sec



¹H NMR spectrum (DMSO-*d*₆) of compound 9

HourhanMahmoud-A2-DMSO-D2O-H1

Archive directory: /expofit/home/vnari/vnarsys/data
Sample directory: D05nm_test_12Mar2014-21134:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 30.0 C / 303.1 K

Mercury-300BB "NMR300"

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 4.000 sec

Width 6500.7 Hz

41 repetitions

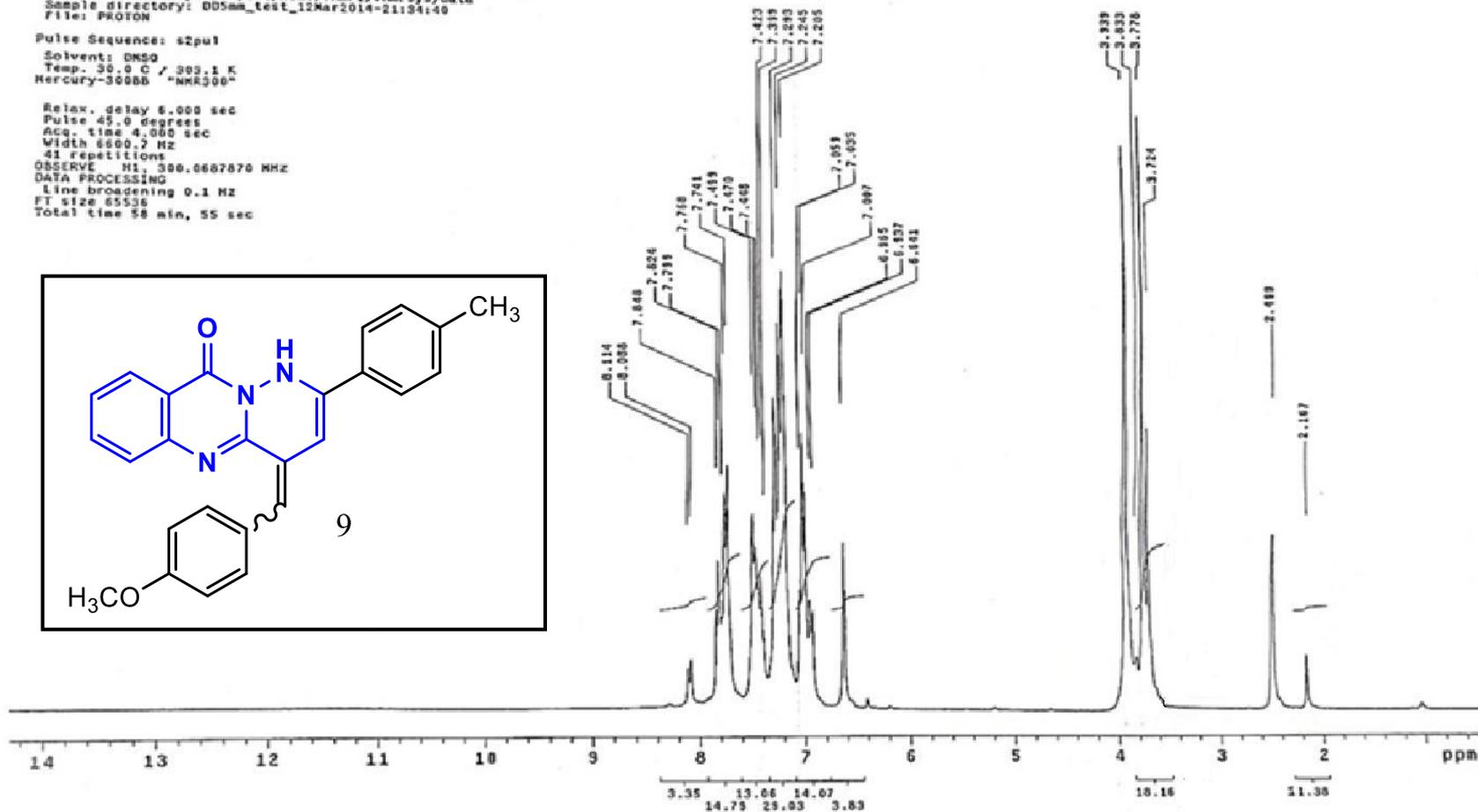
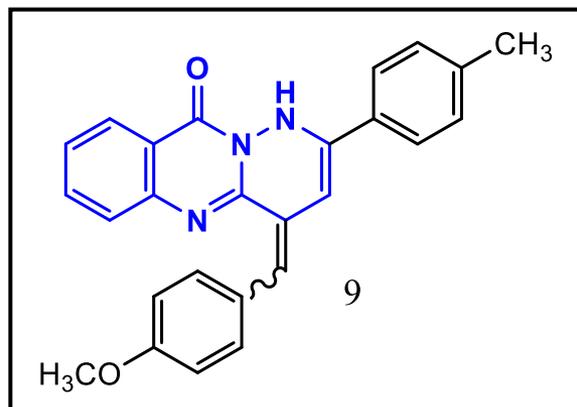
OBSERVE H1, 300.6607870 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 58 min, 55 sec



¹H NMR spectrum (DMSO-*d*₆+ D₂O) of compound 9

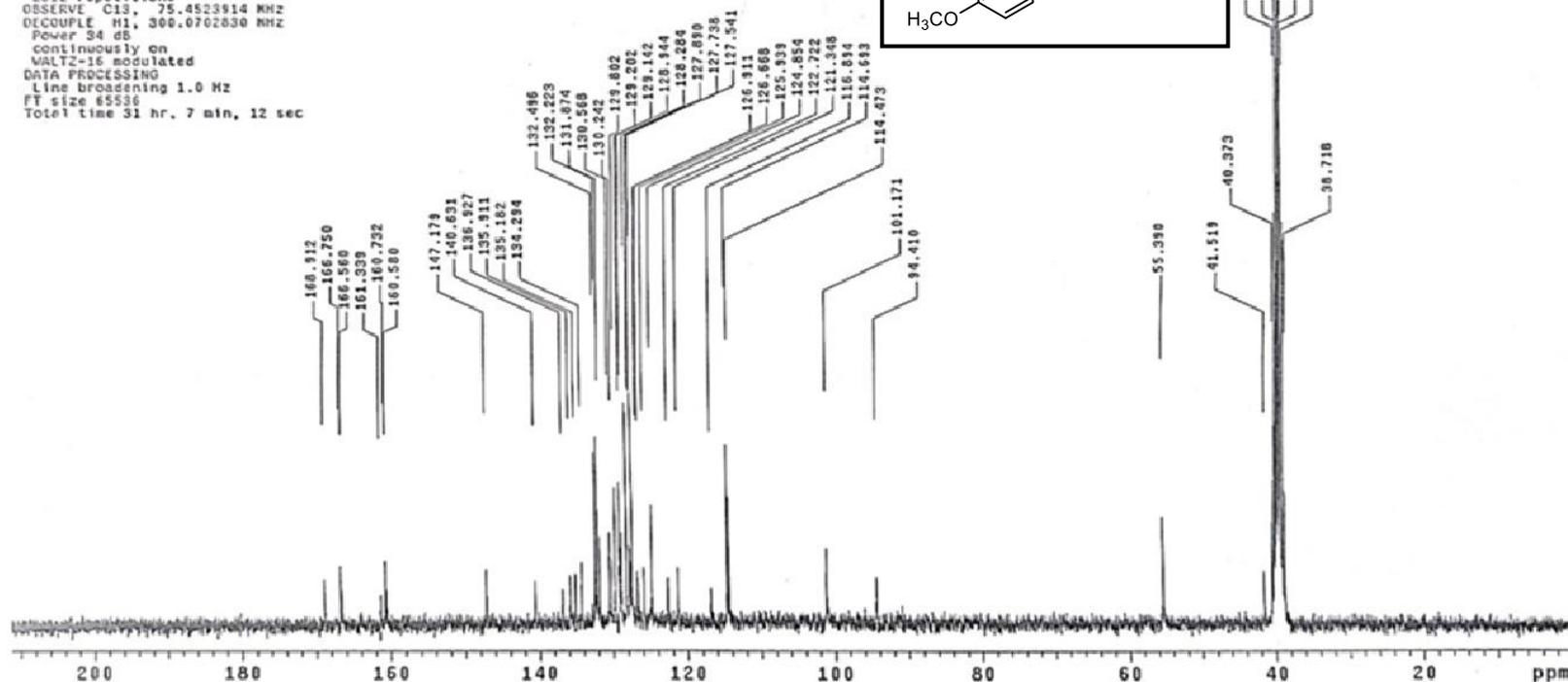
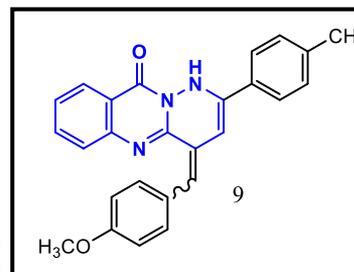
KourhanMahmoud-A2-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul

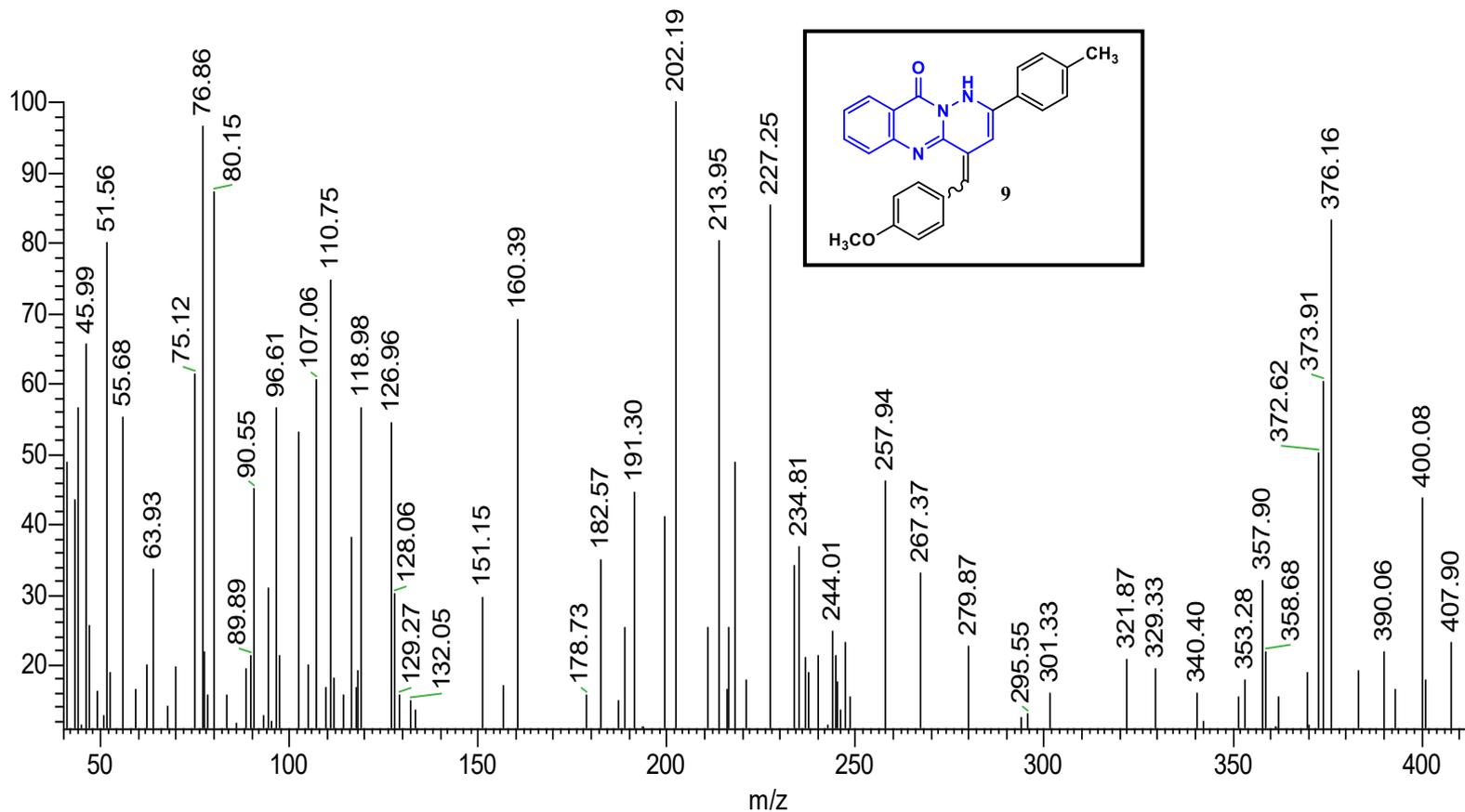
Solvent: DMSO
Ambient temperature
Mercury-300DS *NMR300*

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 16761.7 Hz
2312 repetitions
OBSERVE C13, 75.4523914 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr. 7 min, 12 sec

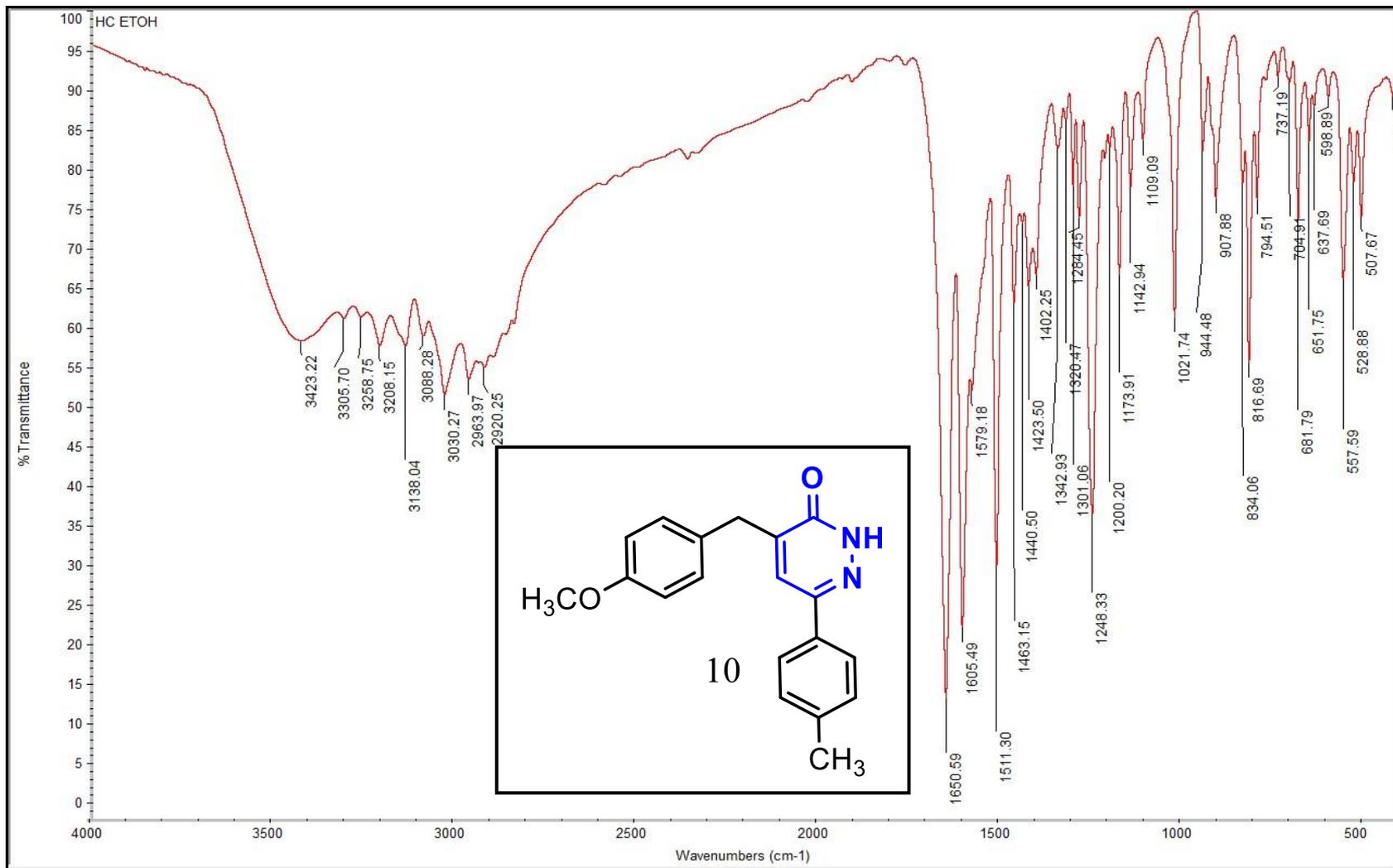


¹³C NMR spectrum of compound 9

6 #289 RT: 4.85 P: + NL: 5.26E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS of compound 9



IR spectrum of compound 10

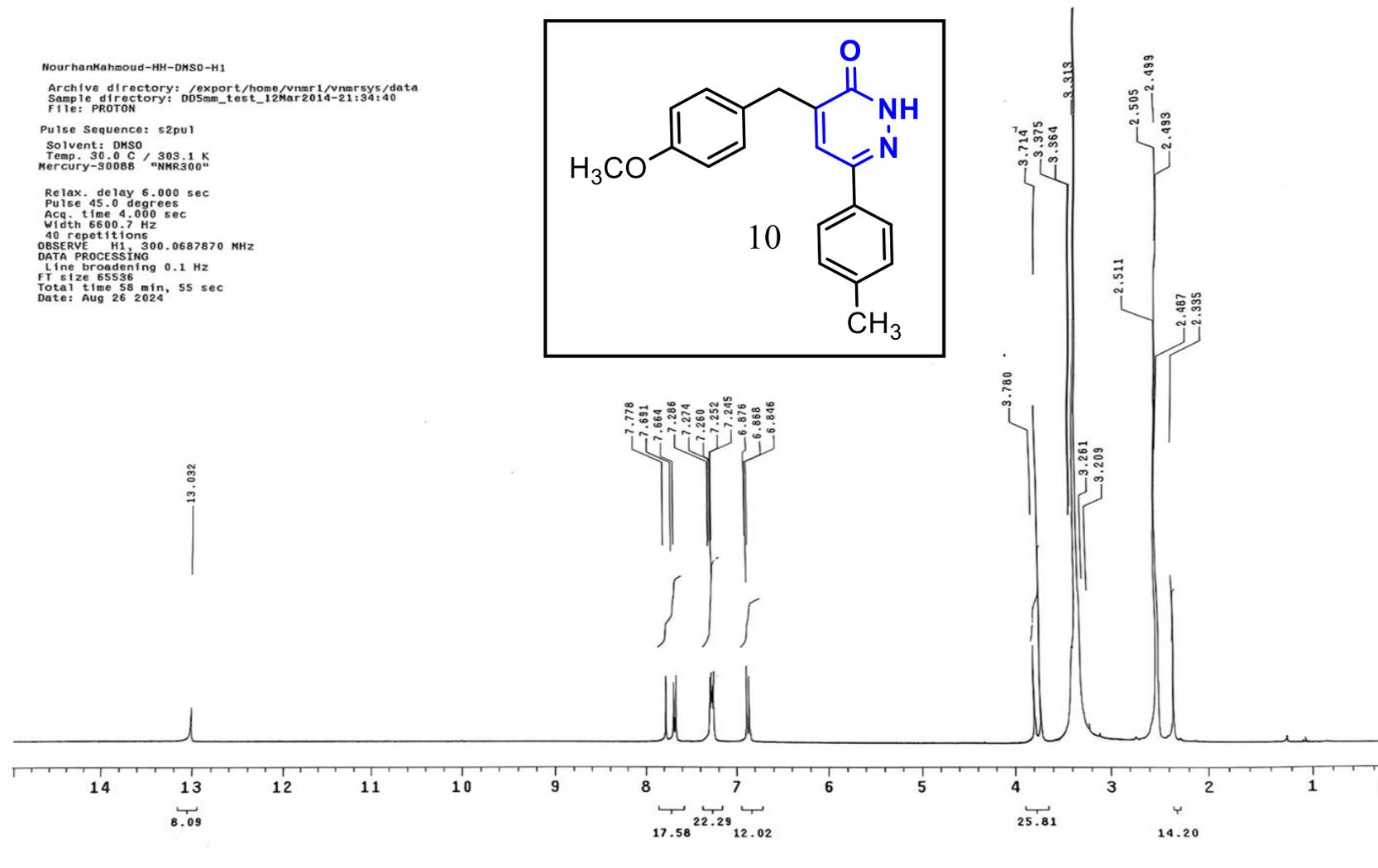
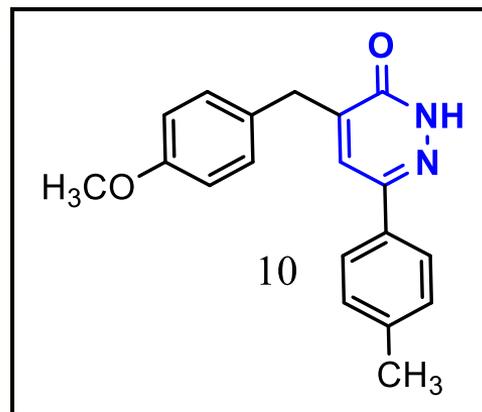
NourhanMahmoud-HH-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
40 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Aug 26 2024



¹H NMR spectrum (DMSO-*d*₆) of compound 10

NourhanMahmoud-HH-DMSO-D2O-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-3006B "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz

17 repetitions
OBSERVE H1 300.0687870 MHz

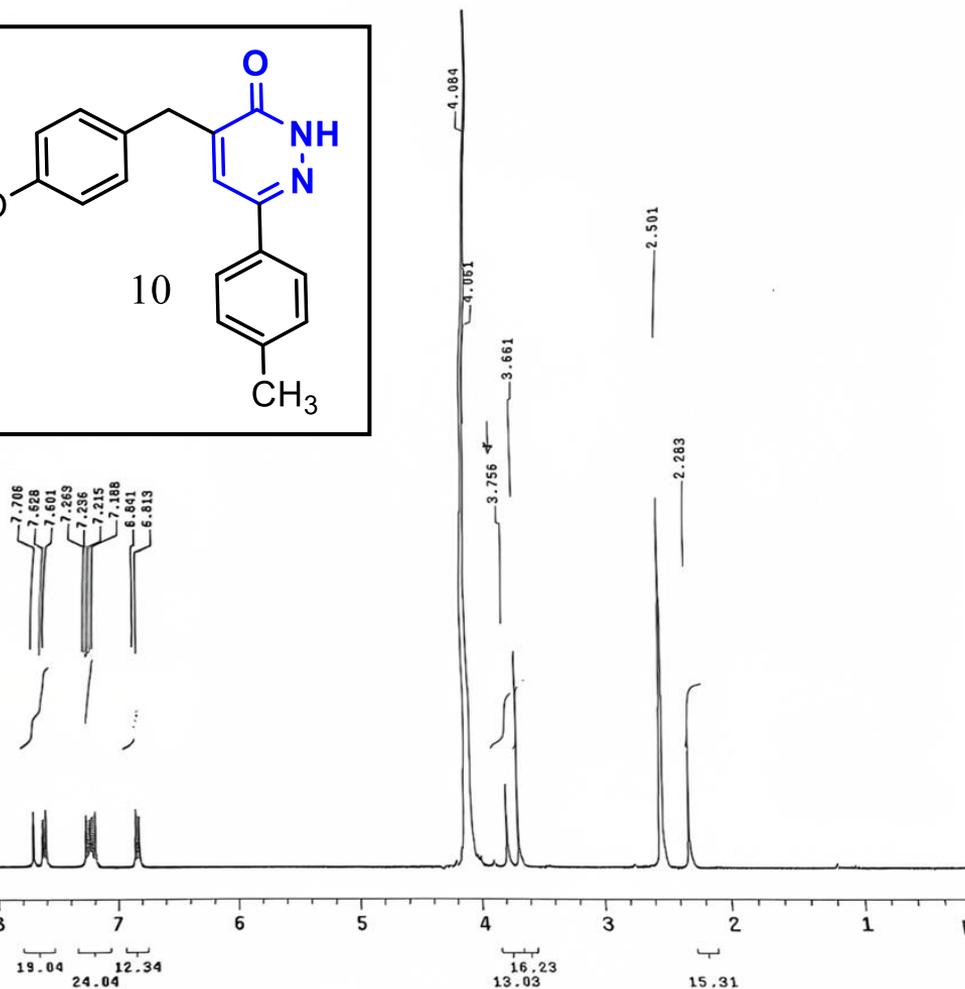
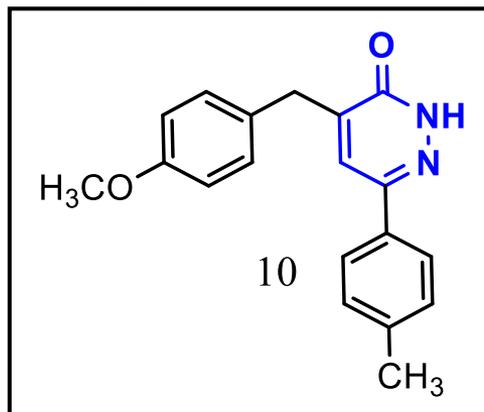
DATA PROCESSING

Line broadening 0.1 Hz

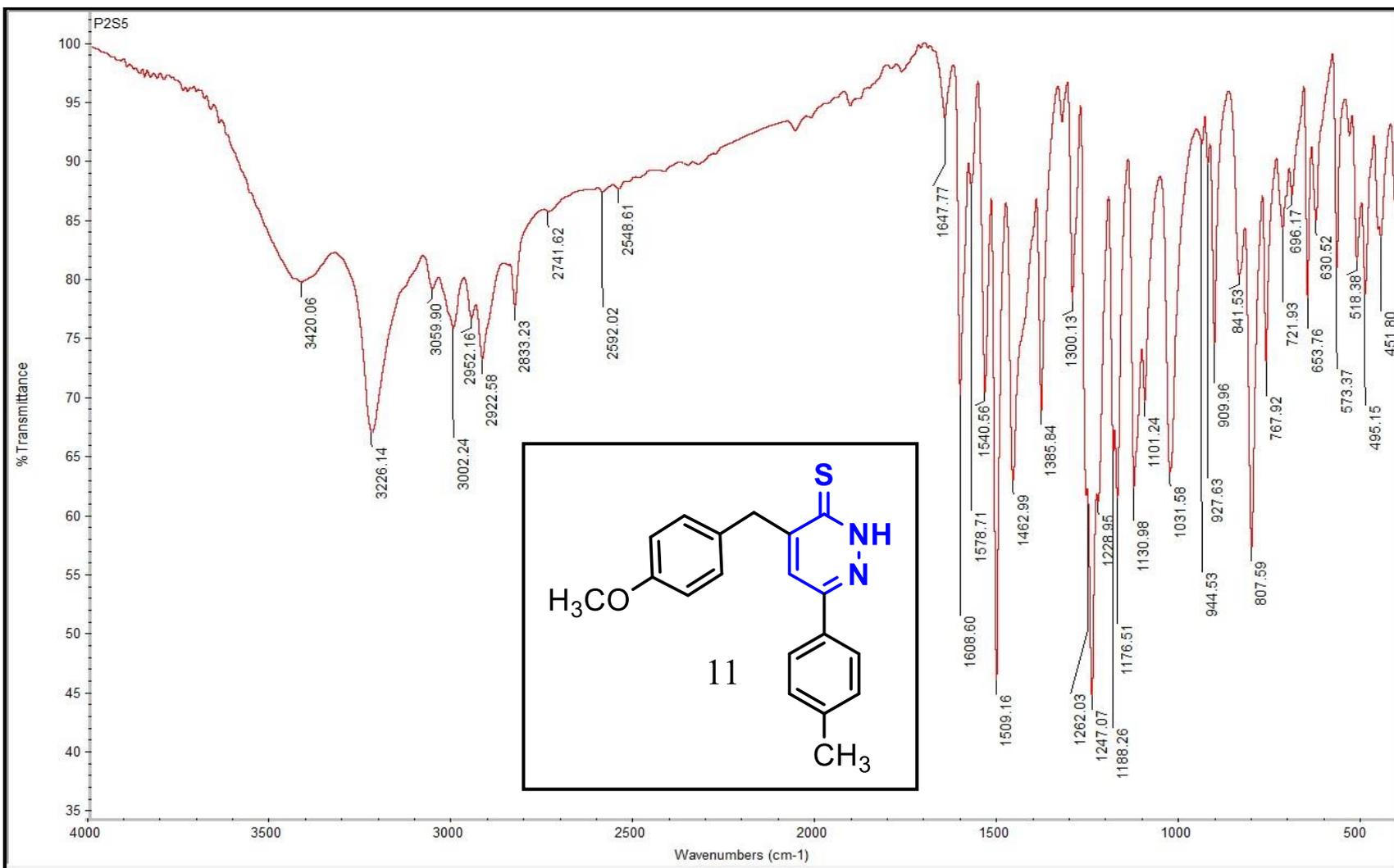
FT size 65536

Total time 58 min, 55 sec

Date: Aug 26 2024



¹H NMR spectrum (DMSO-*d*₆ + D₂O) of compound 10



IR spectrum of compound 11

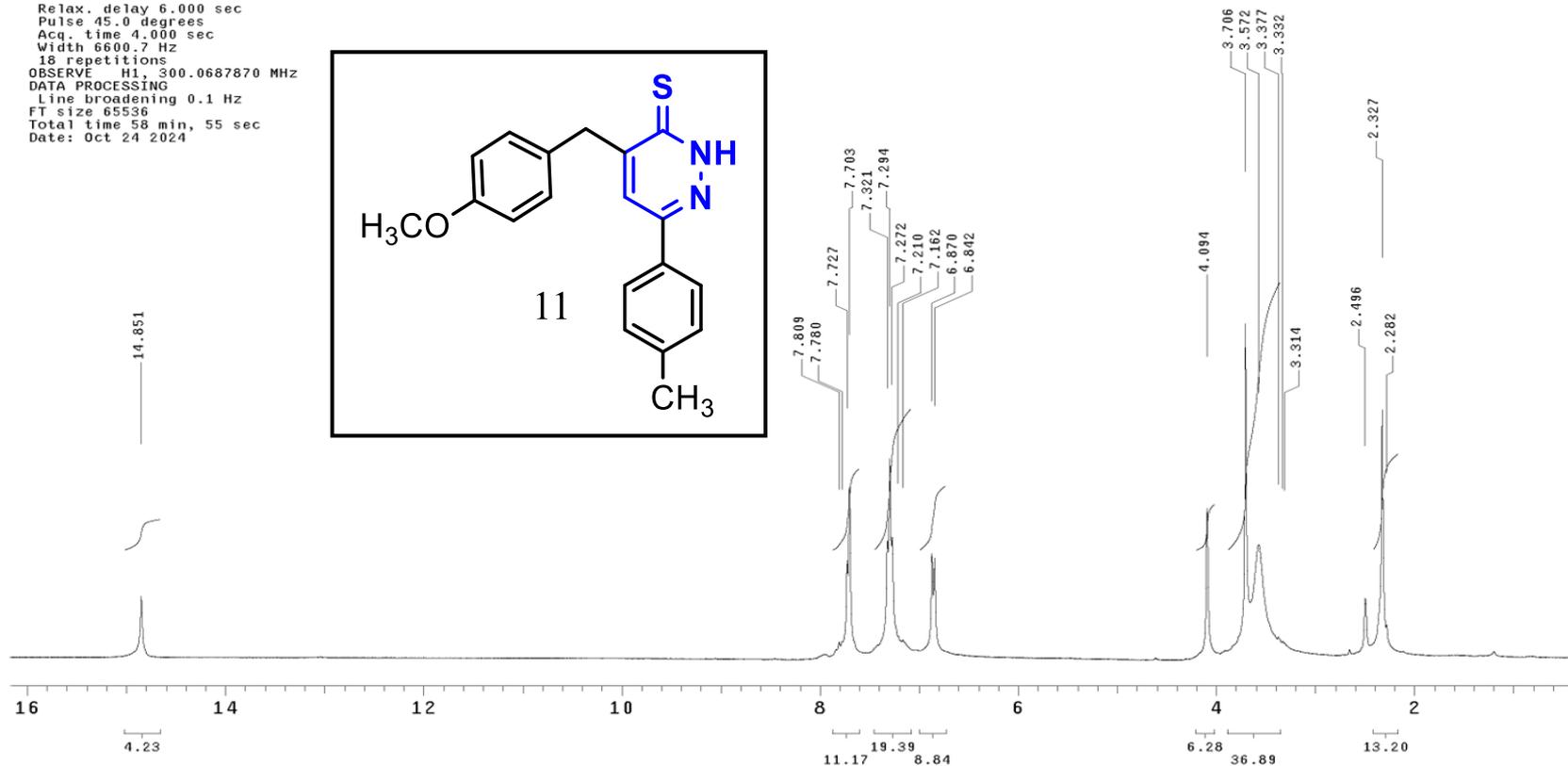
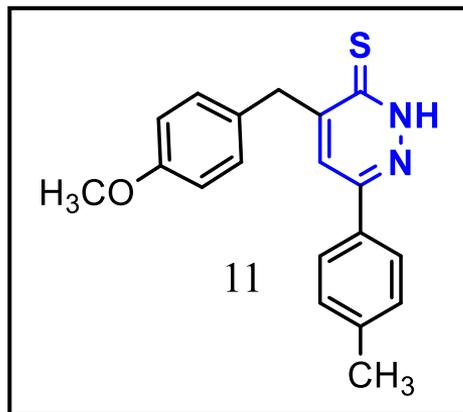
NourhanMahmoud-P2S5-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pu1

Solvent: DMSO
Temp: 30.0 C / 303.1 K
File: NorhanMahmoud-P2S5-DMSO-H1
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
18 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Oct 24 2024



¹H NMR spectrum (DMSO-d₆) of compound 11

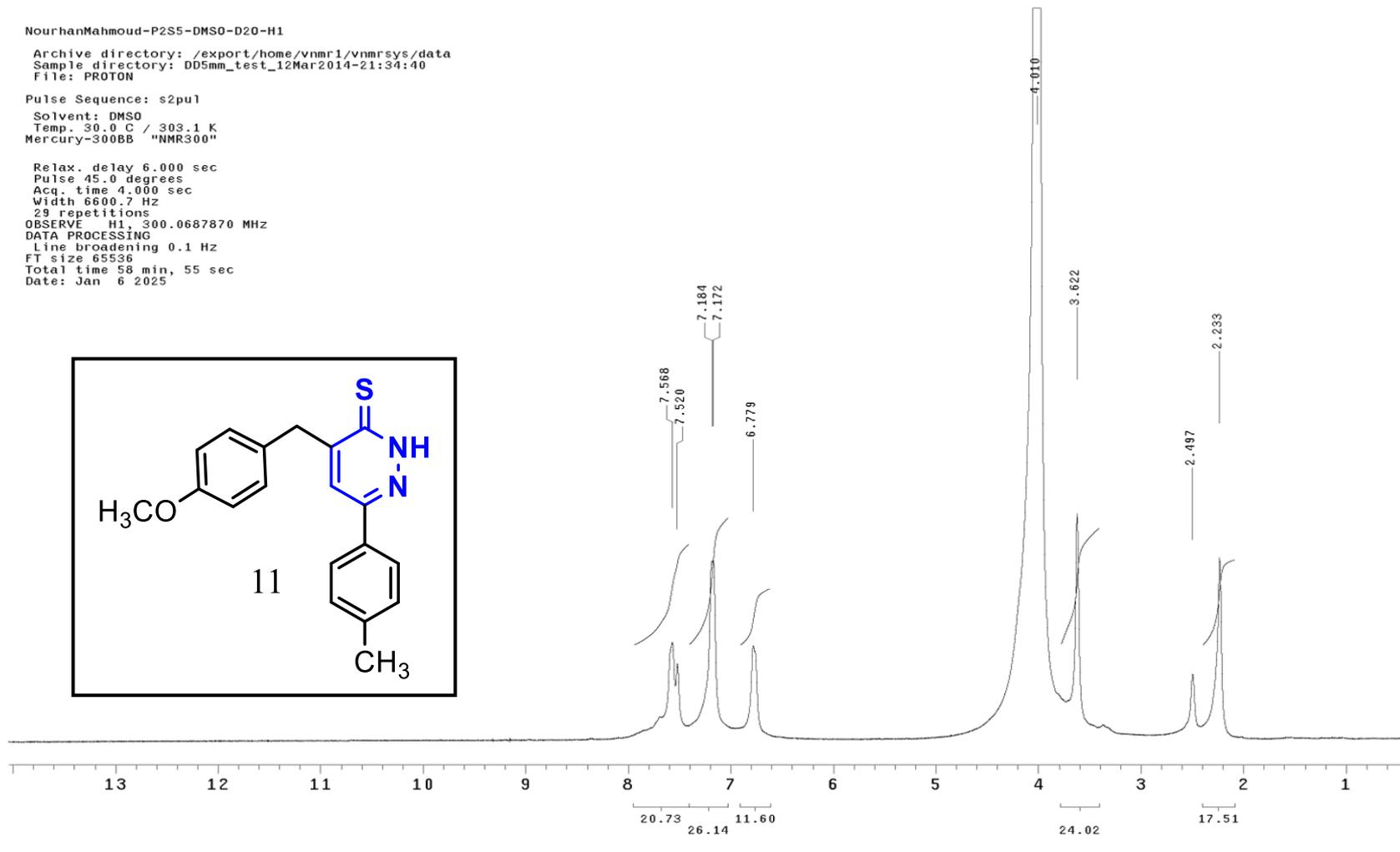
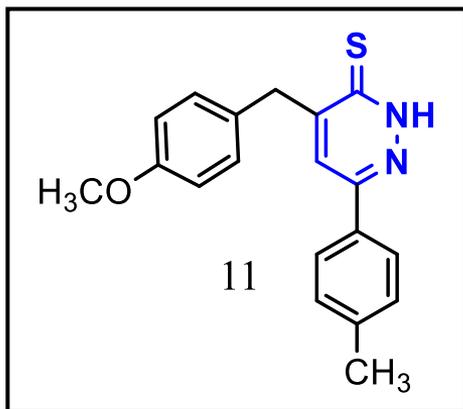
NourhanMahmoud-P2S5-DMSO-D20-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
29 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Jan 6 2025



¹H NMR spectrum (DMSO-d₆ + D₂O) of compound 11

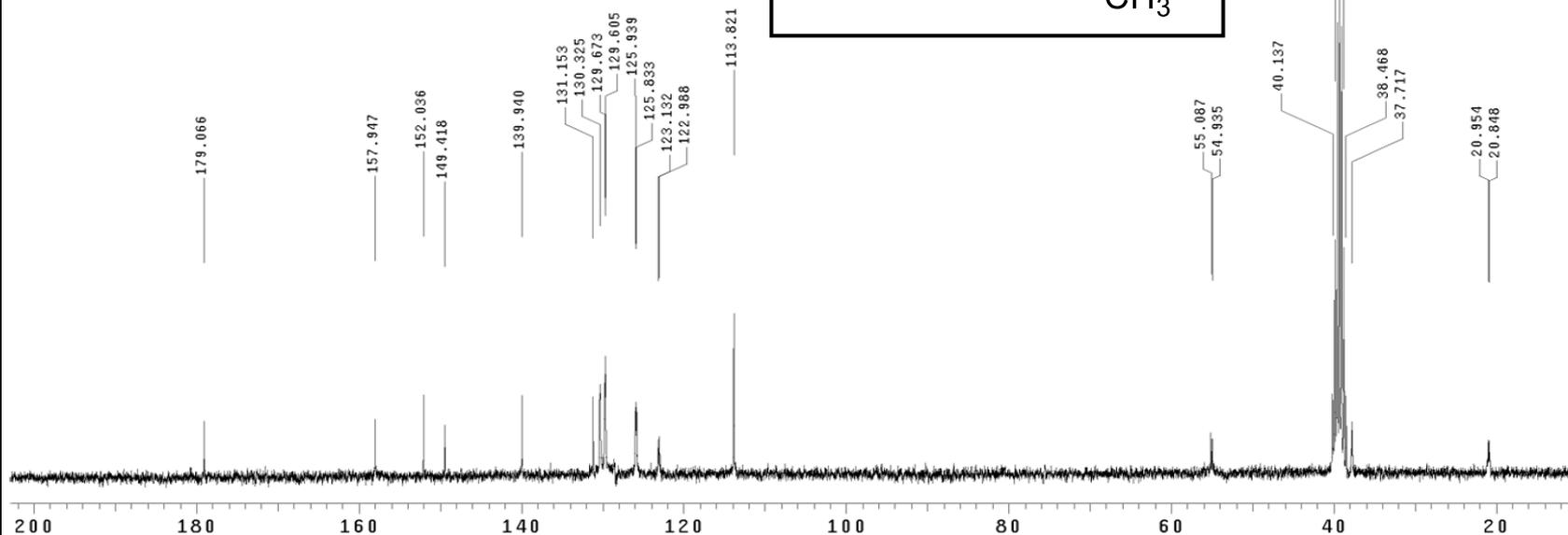
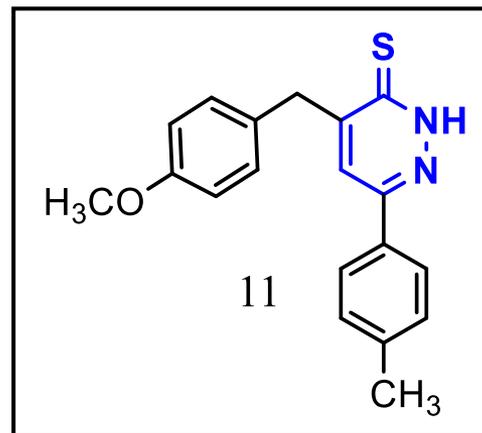
NourhanMahmoud-P2S5-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

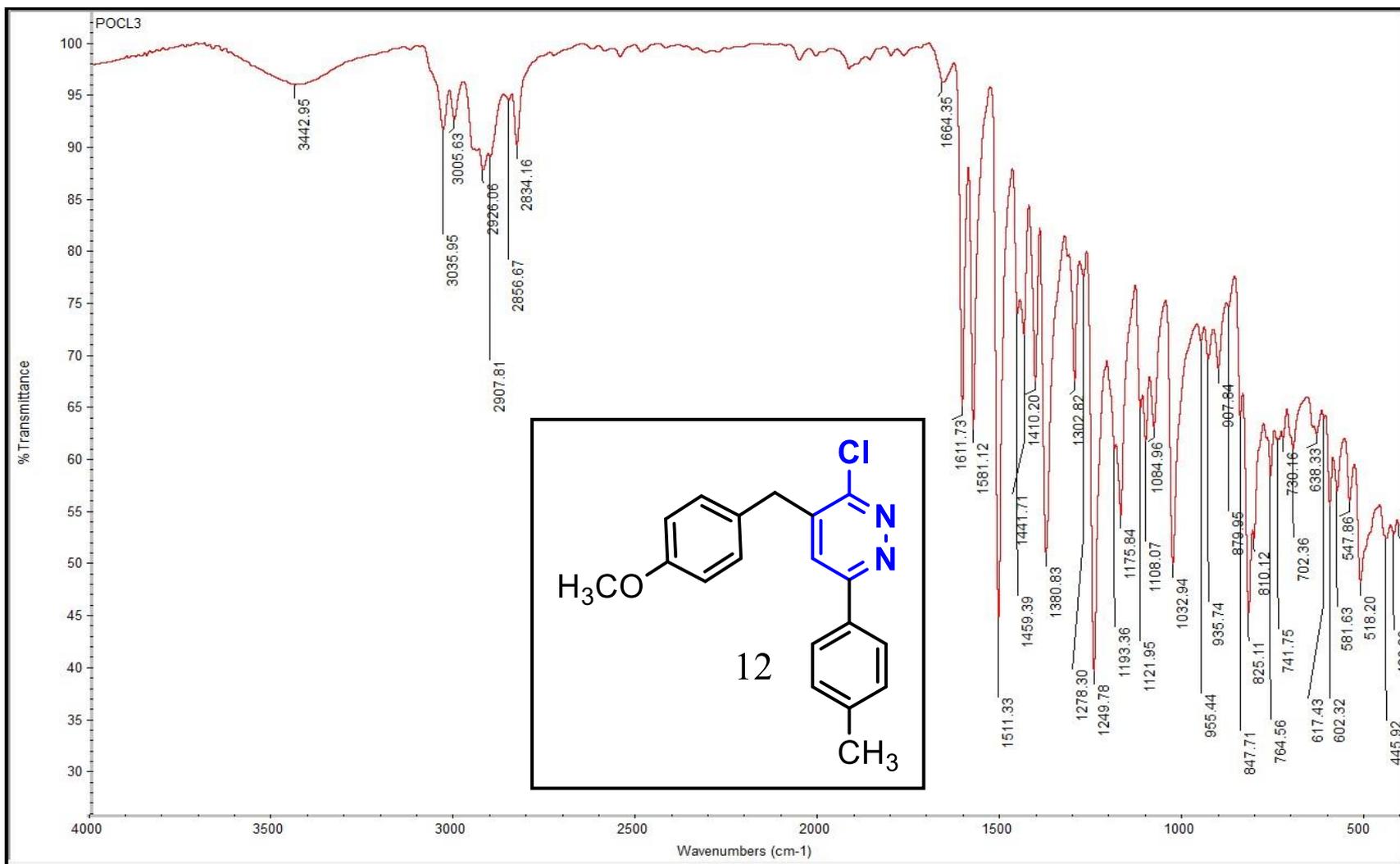
Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2088 repetitions
OBSERVE C13, 75.4523868 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 311 hr, 12 min, 6 sec
Date: Dec 31 2024



¹³C NMR spectrum (DMSO-*d*₆) of compound 11



IR spectrum of compound 12

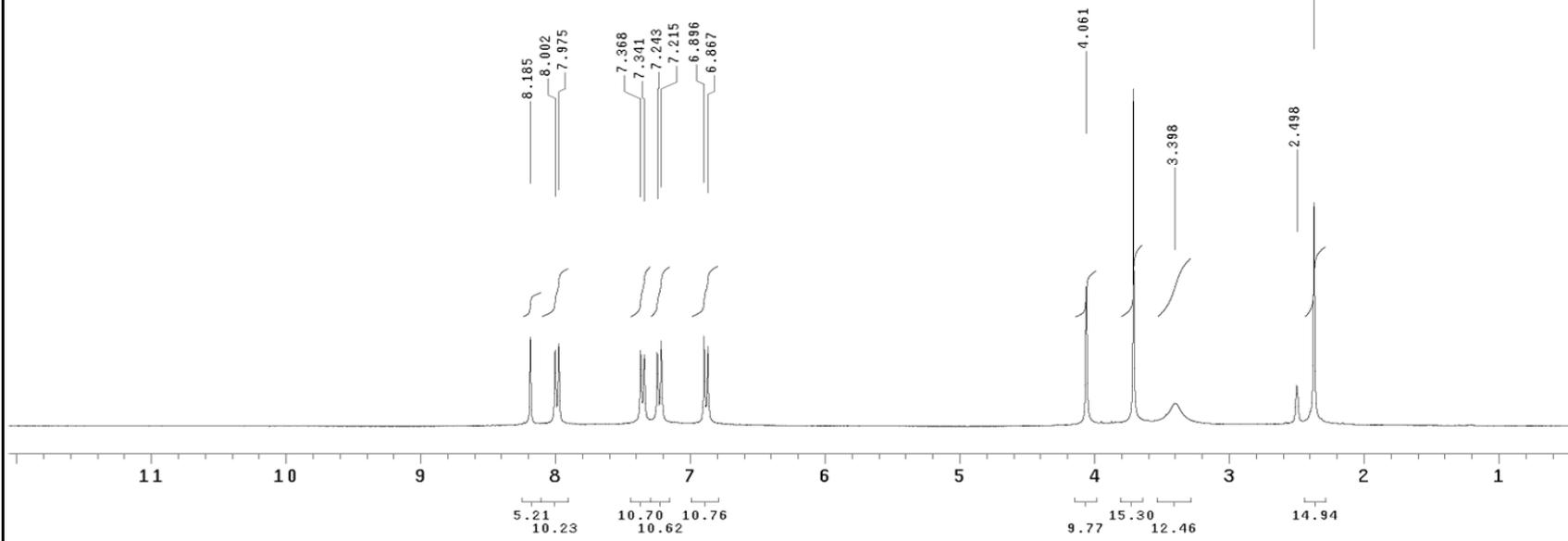
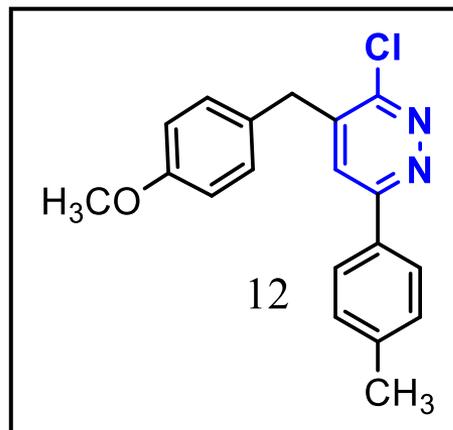
NorhanMahmoud-POC13-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
11 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Oct 24 2024



¹H NMR spectrum (DMSO-*d*₆) of compound 12

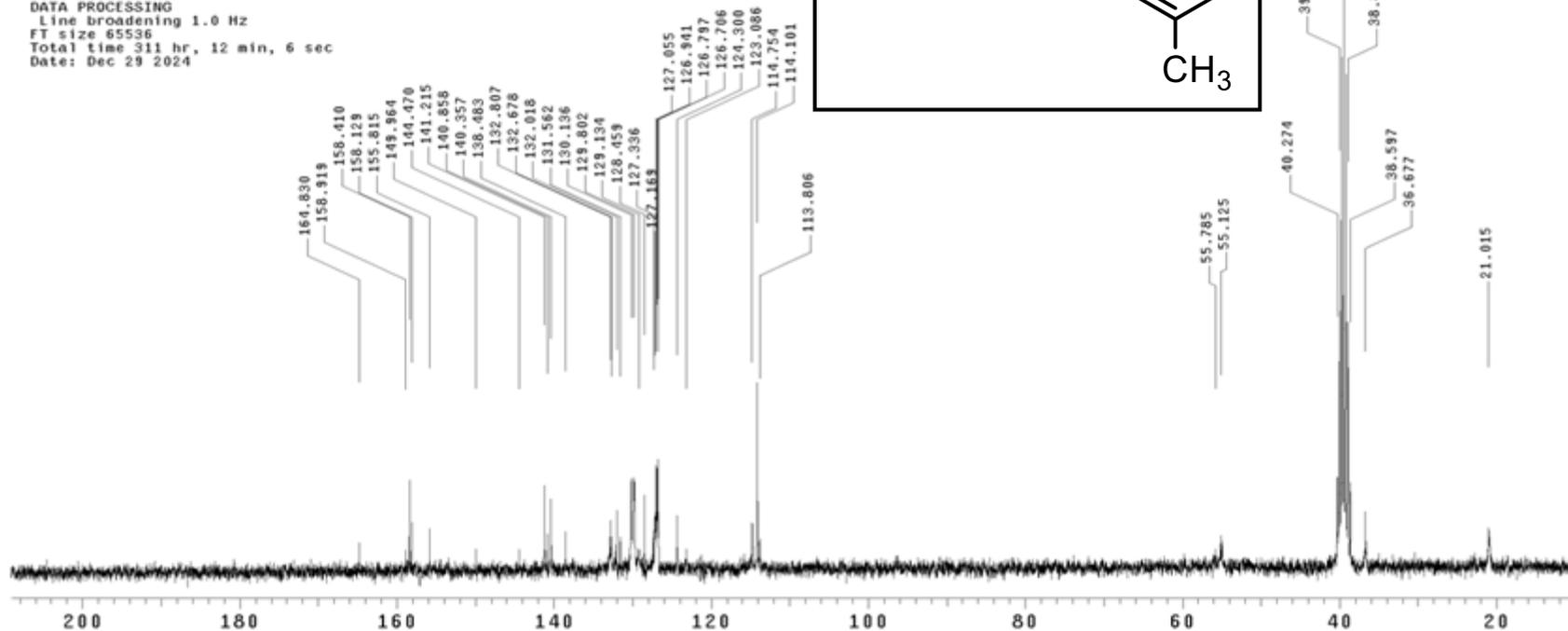
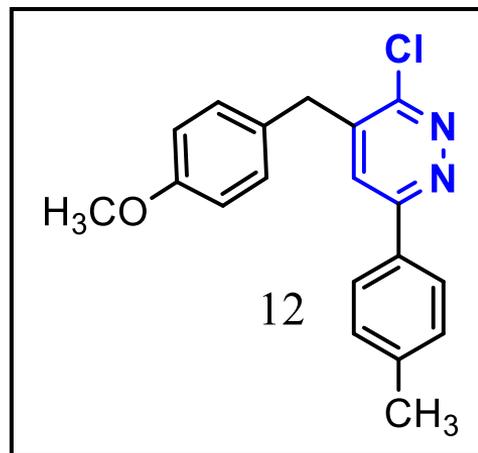
NourhanMahmoud-POC13-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

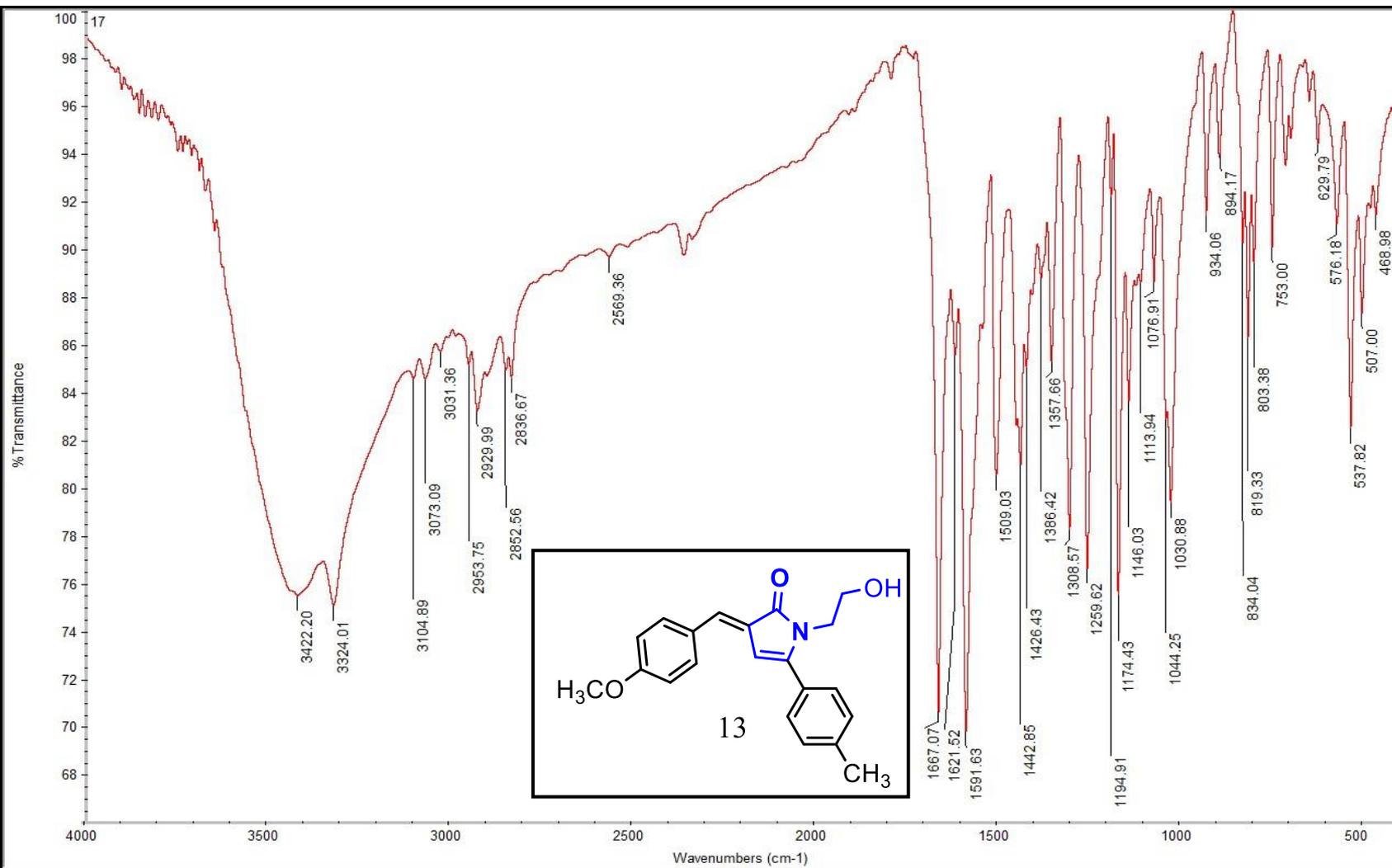
Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2320 repetitions
OBSERVE C13, 75.4523885 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 311 hr, 12 min, 6 sec
Date: Dec 29 2024



¹³C NMR spectrum of compound 12



IR spectrum of compound 13

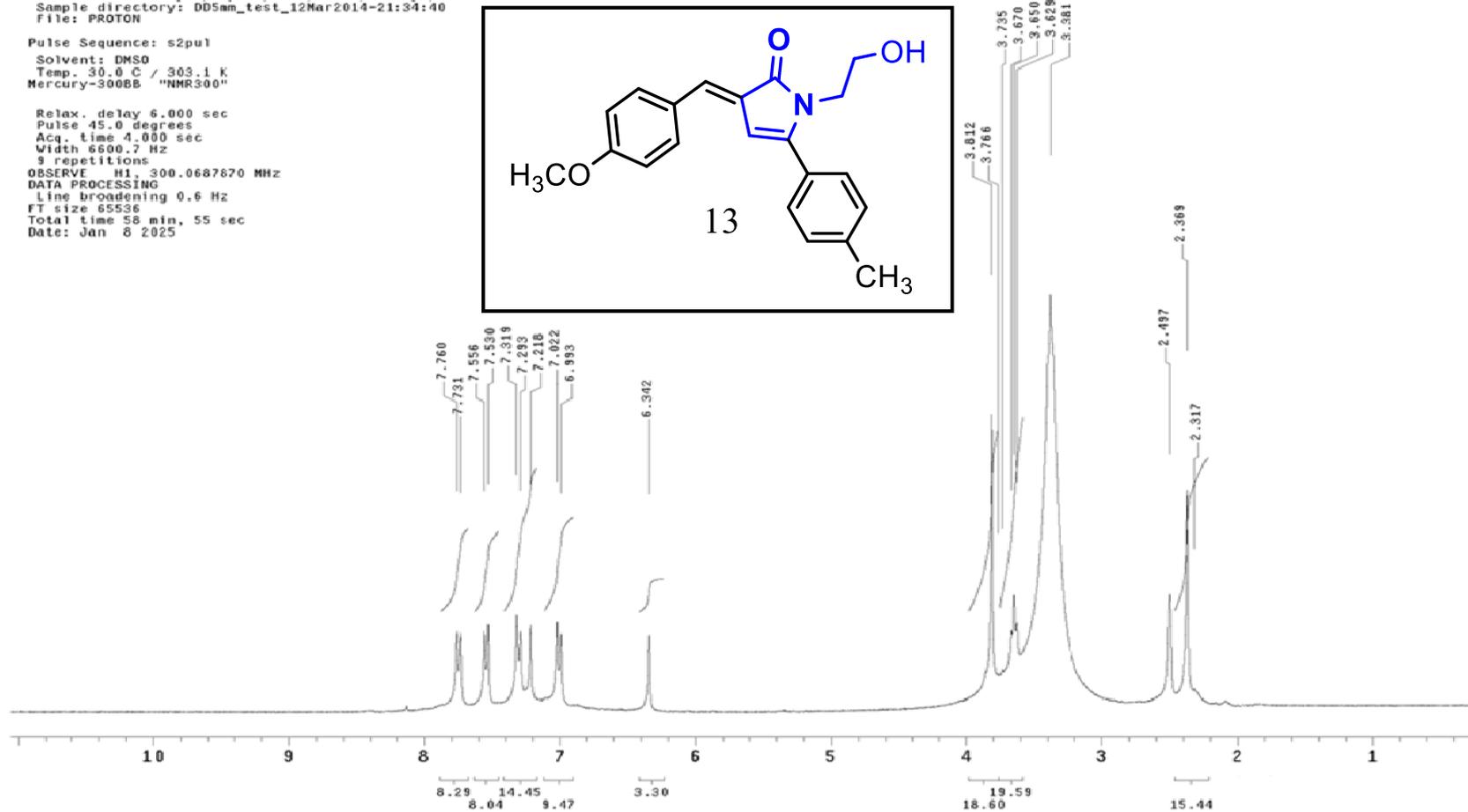
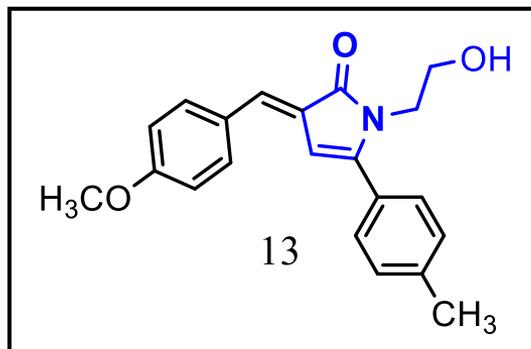
NourhanMahmoud-17-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5am_test_12Mar2014-21:34:40
File: PROTON

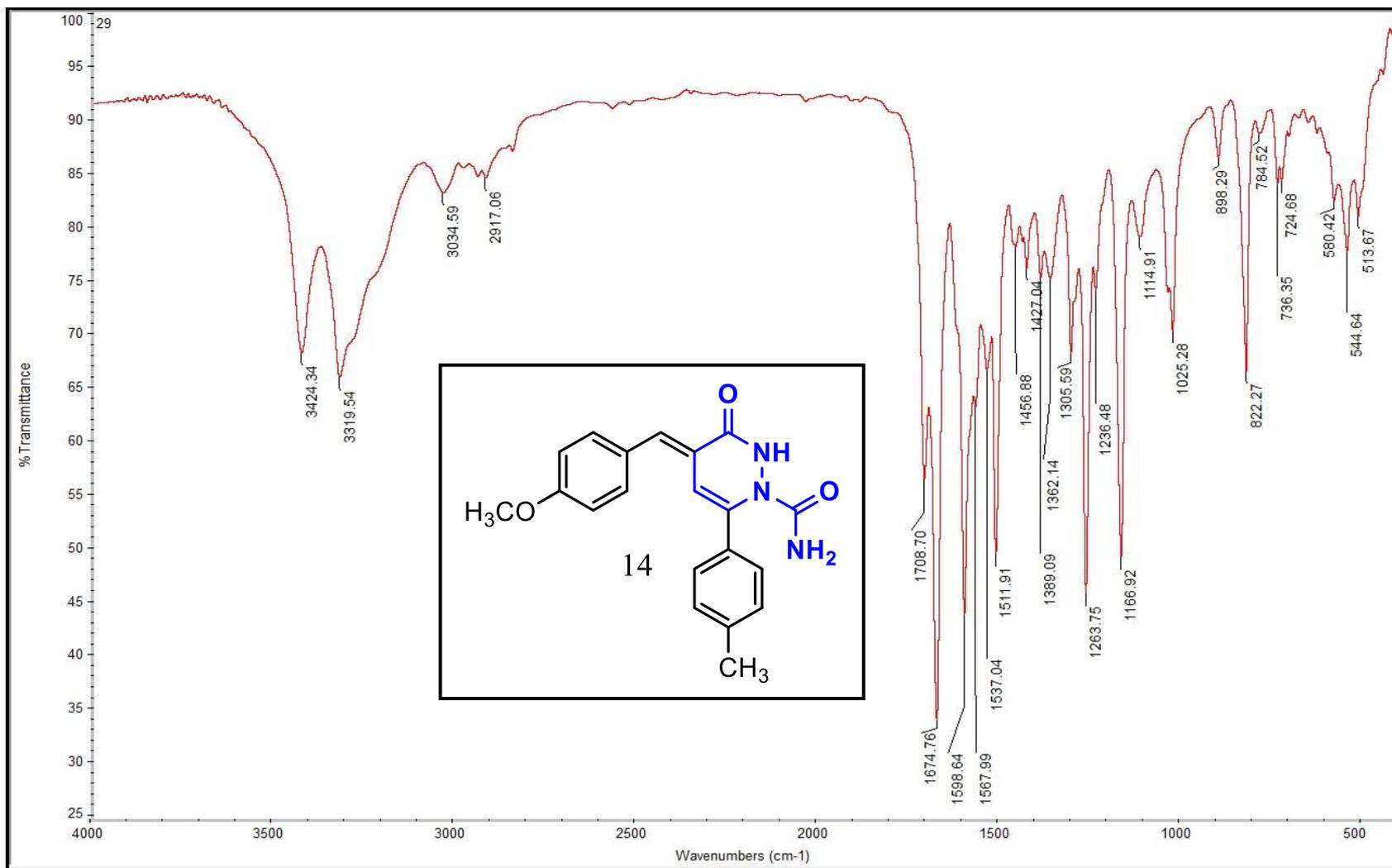
Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
9 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.6 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Jan 8 2025



¹H NMR spectrum (DMSO-d₆) of compound 13



IR spectrum of compound 14

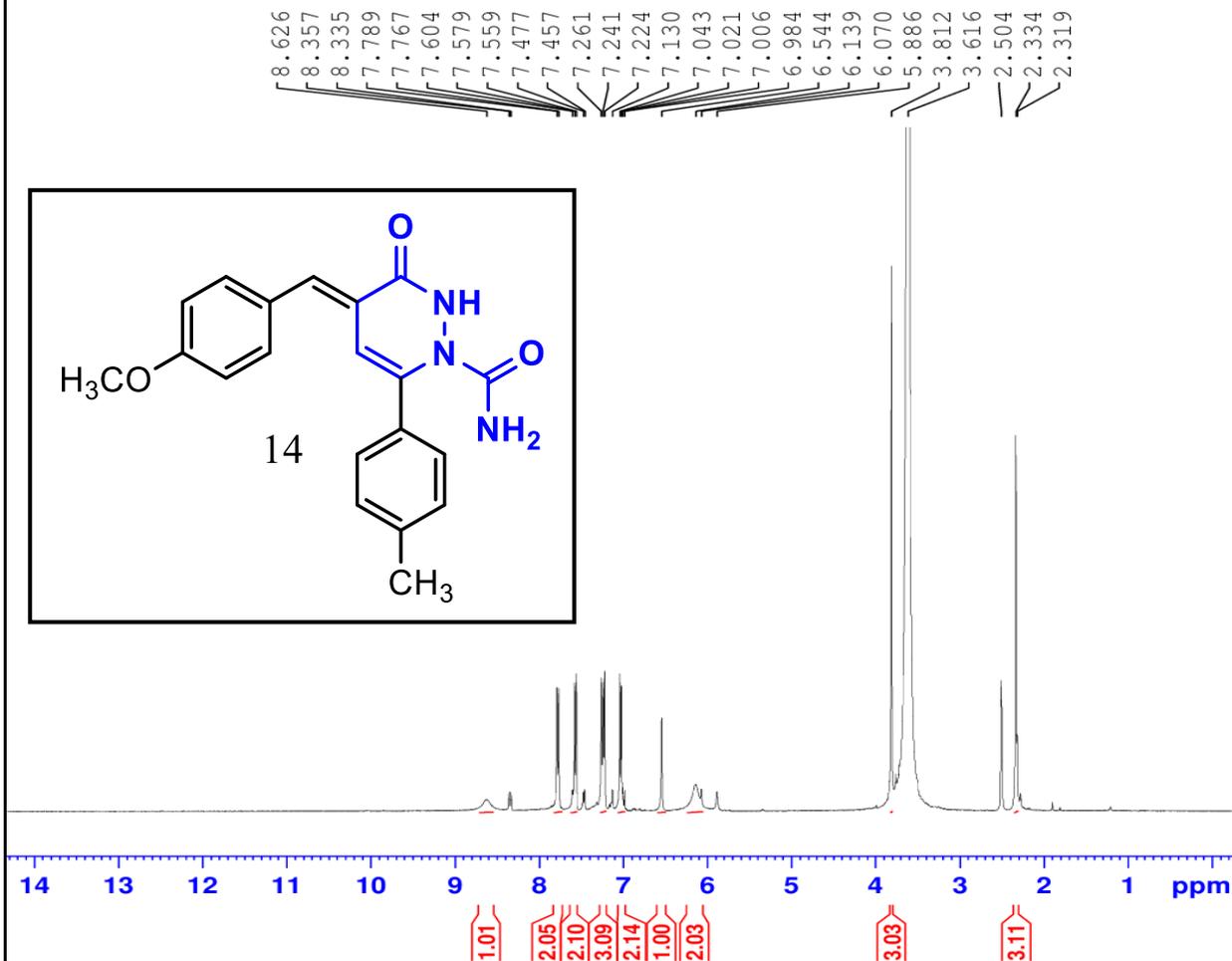


Current Data Parameters
NAME nourhan-mahmoud-29
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250616
Time 10.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 51
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 117.48
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR spectrum (DMSO-*d*₆) of compound 14

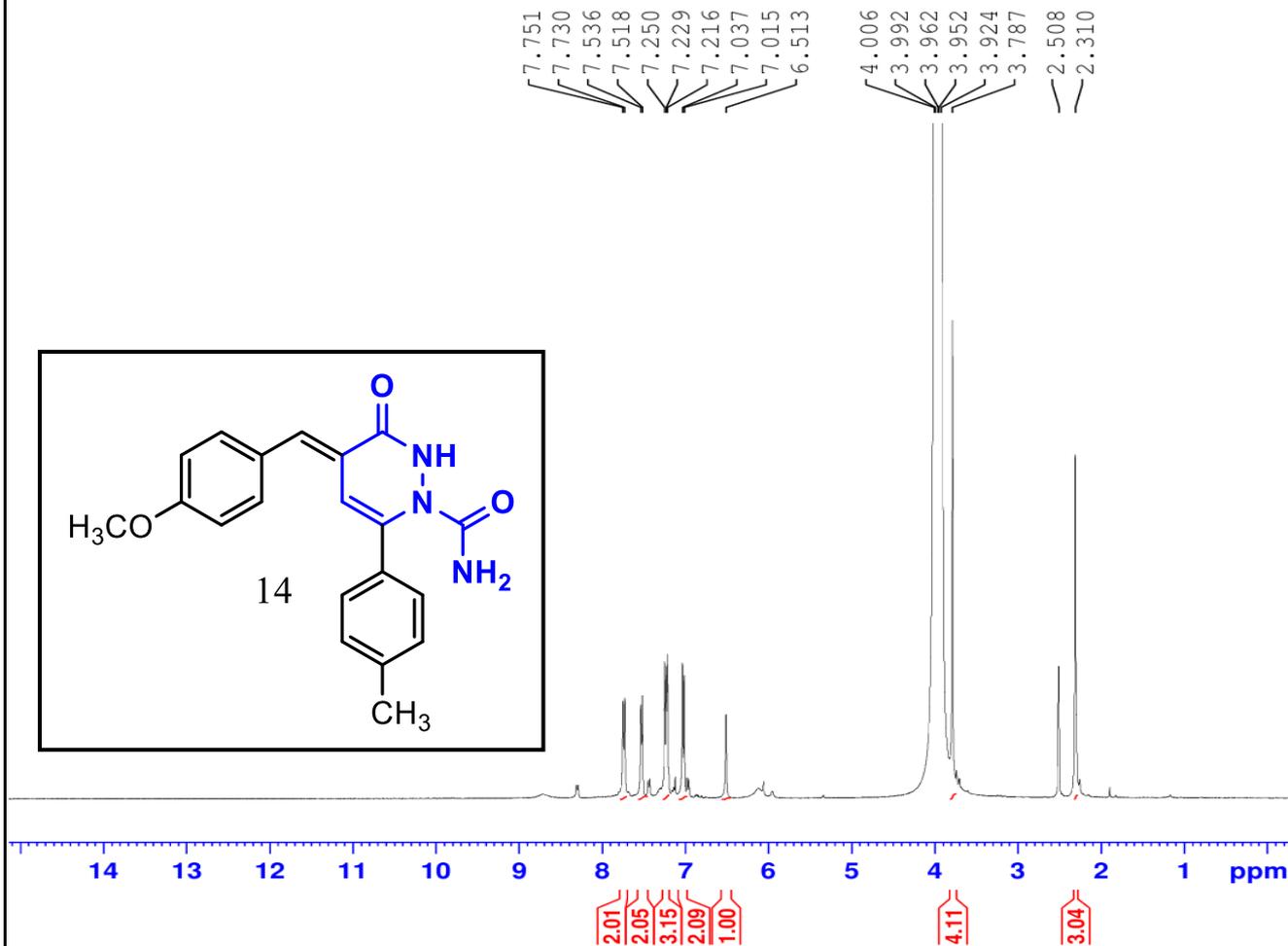
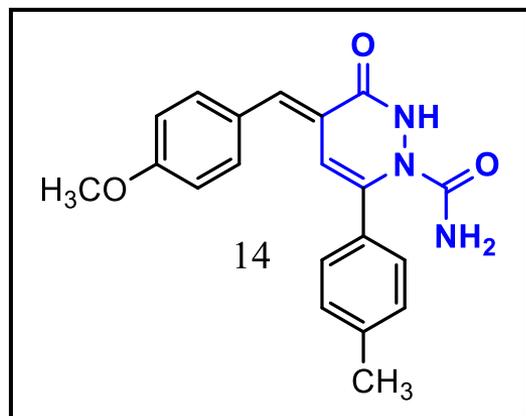


Current Data Parameters
NAME nourhan-mahmoud-29-d2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250624
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 91
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 126.31
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR spectrum (DMSO-*d*₆ + D₂O) of compound 14



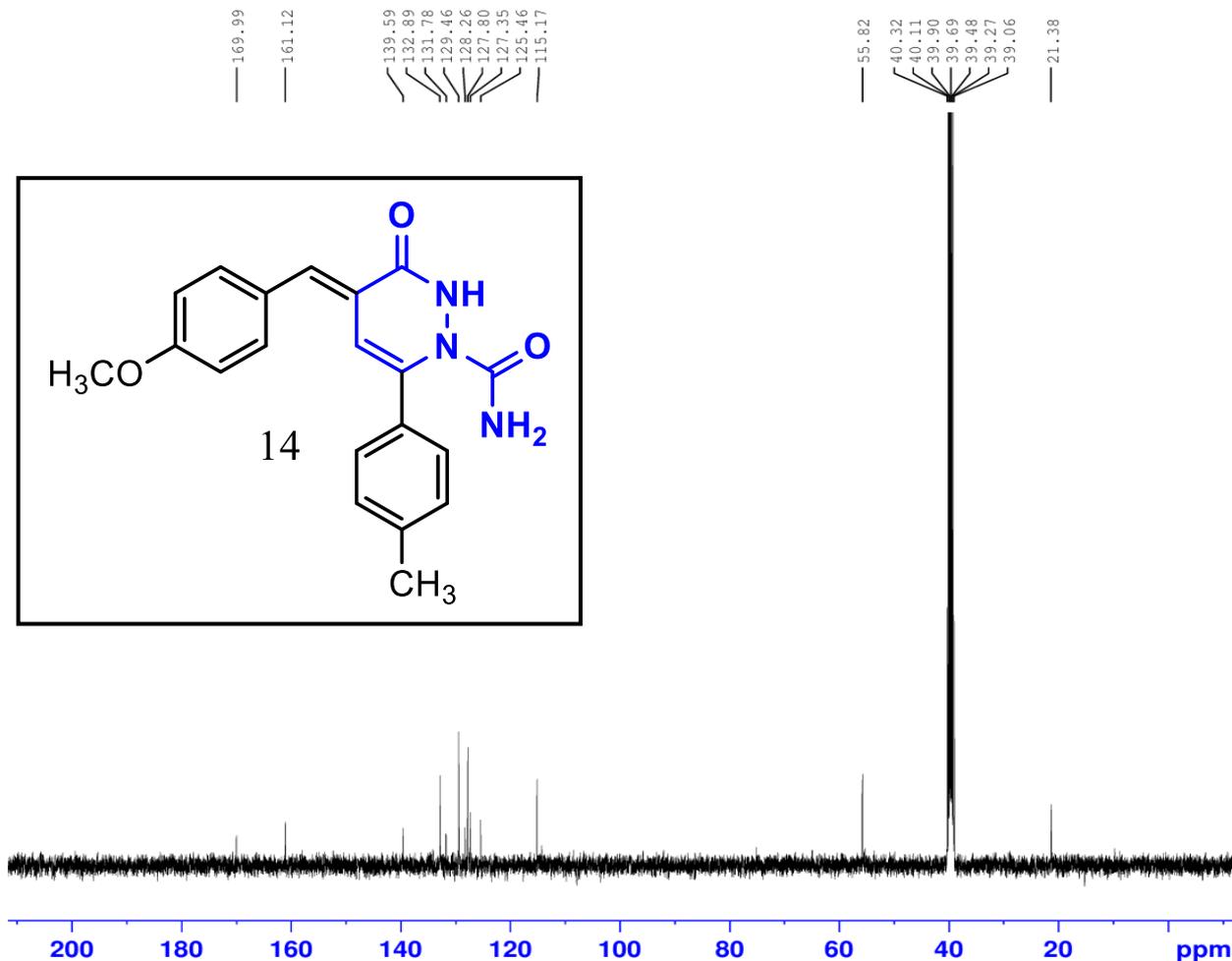
Current Data Parameters
NAME nourhan-mahmoud-29
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 13.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1201
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

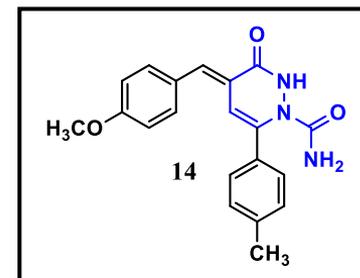
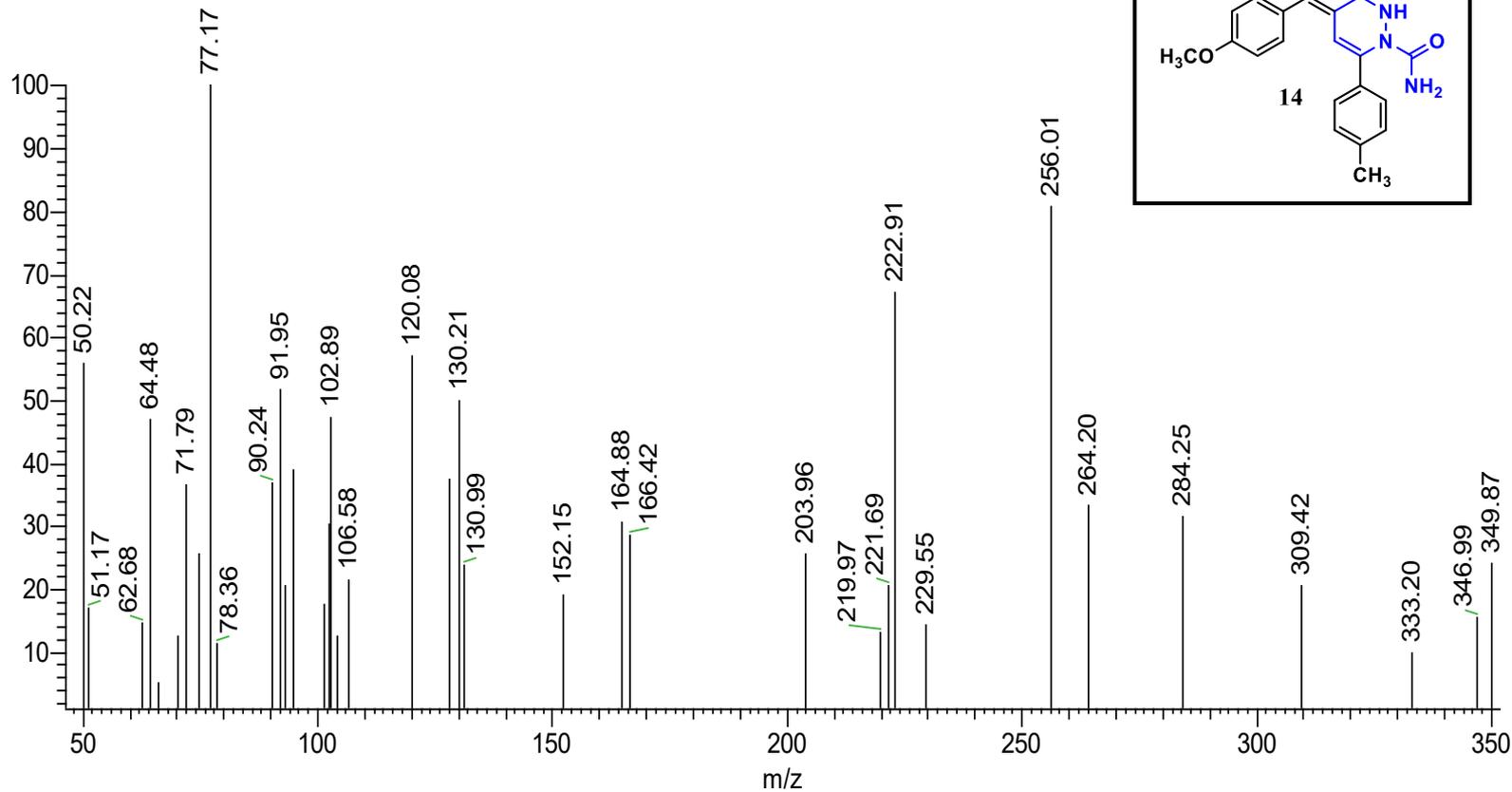
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SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹³C NMR spectrum of compound 14

29 #31 RT: 0.54 P: + NL: 7.51E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS of compound 14