

Electronic Supplementary Information

An efficient and rapid intramolecular cyclization of quadruple Mannich reaction for the one-pot synthesis of pentaazaphenalenenes and their antimicrobial activities

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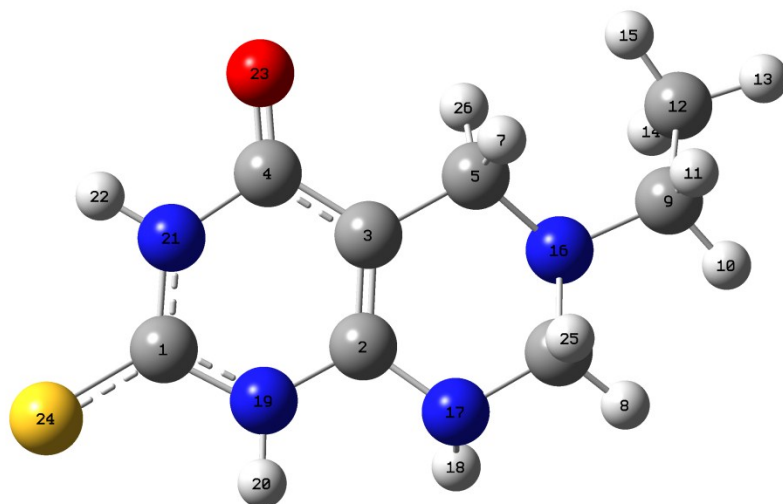
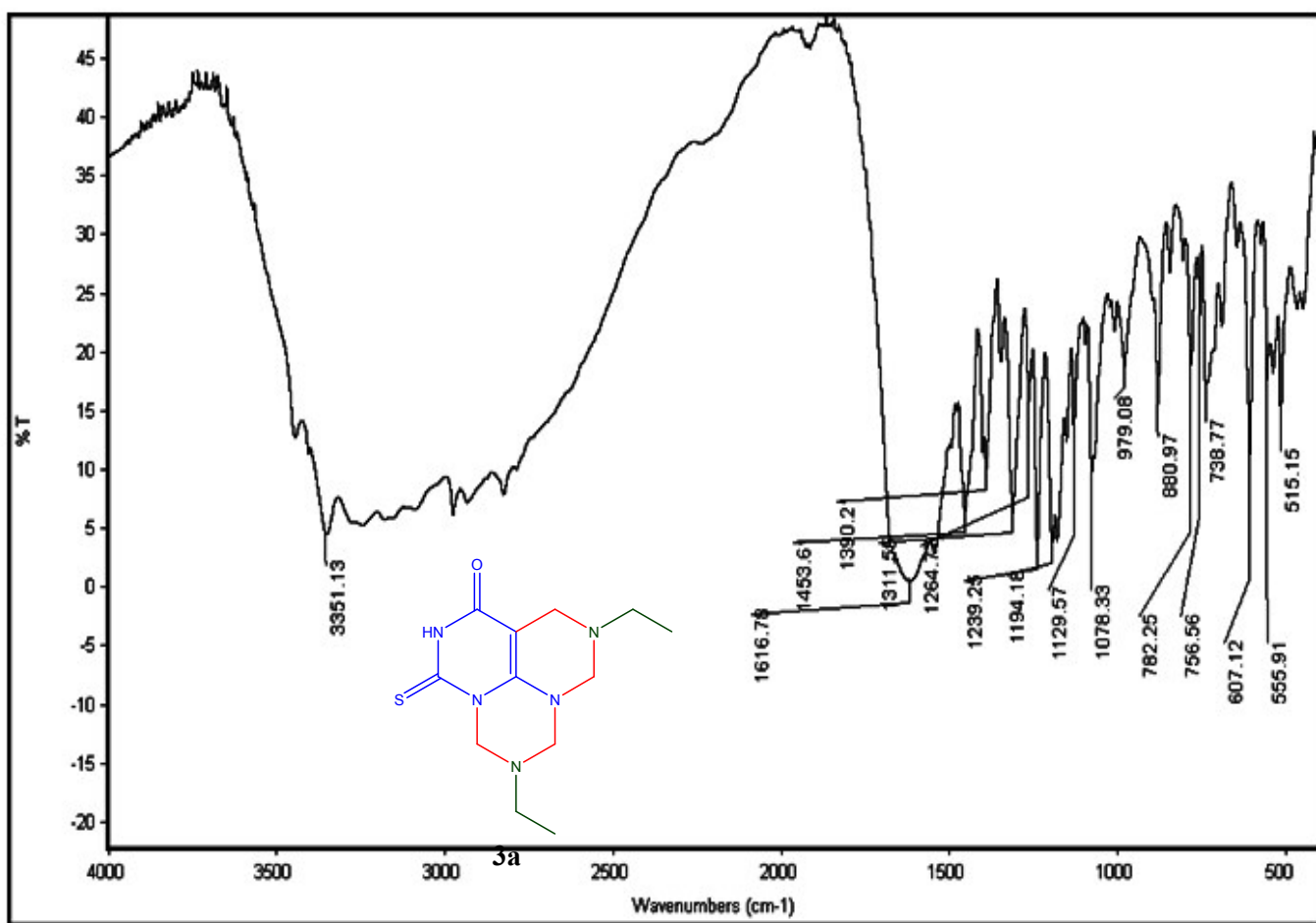


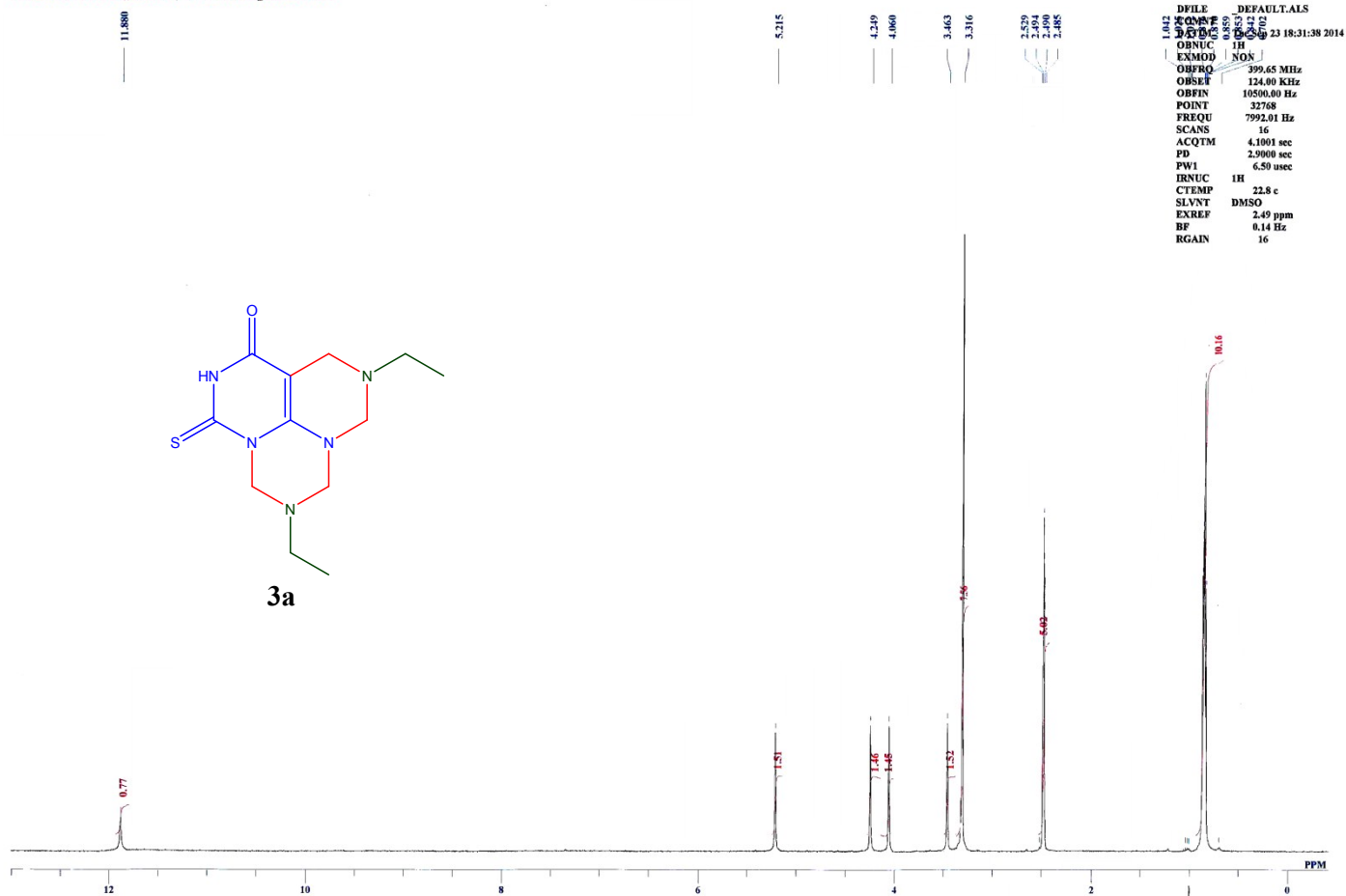
Figure S1. The geometry structure of intermediate tautomer **6a**. Atom color code: Carbon (gray), nitrogen (blue), oxygen (red), sulfur (yellow), bromine (orange) and hydrogen (white).

Table S1. Values of atomic charge of intermediate tautomer **6a**.

Atom	Number	Charge
C	1	0.24198
C	2	0.42319
C	3	- 0.23840
C	4	0.65682
C	5	- 0.26874
C	6	- 0.08130
H	7	0.22825
H	8	0.25065
C	9	- 0.27104
H	10	0.23901
H	11	0.21085
C	12	- 0.70967
H	13	0.24841
H	14	0.24718
H	15	0.24192
N	16	- 0.55760
N	17	- 0.67056
H	18	0.42809
N	19	- 0.61320
H	20	0.46452
N	21	- 0.64060
H	22	0.47049
O	23	- 0.61361
S	24	- 0.18107
H	25	0.21903
H	26	0.27539



FTIR spectrum of compound 3a.

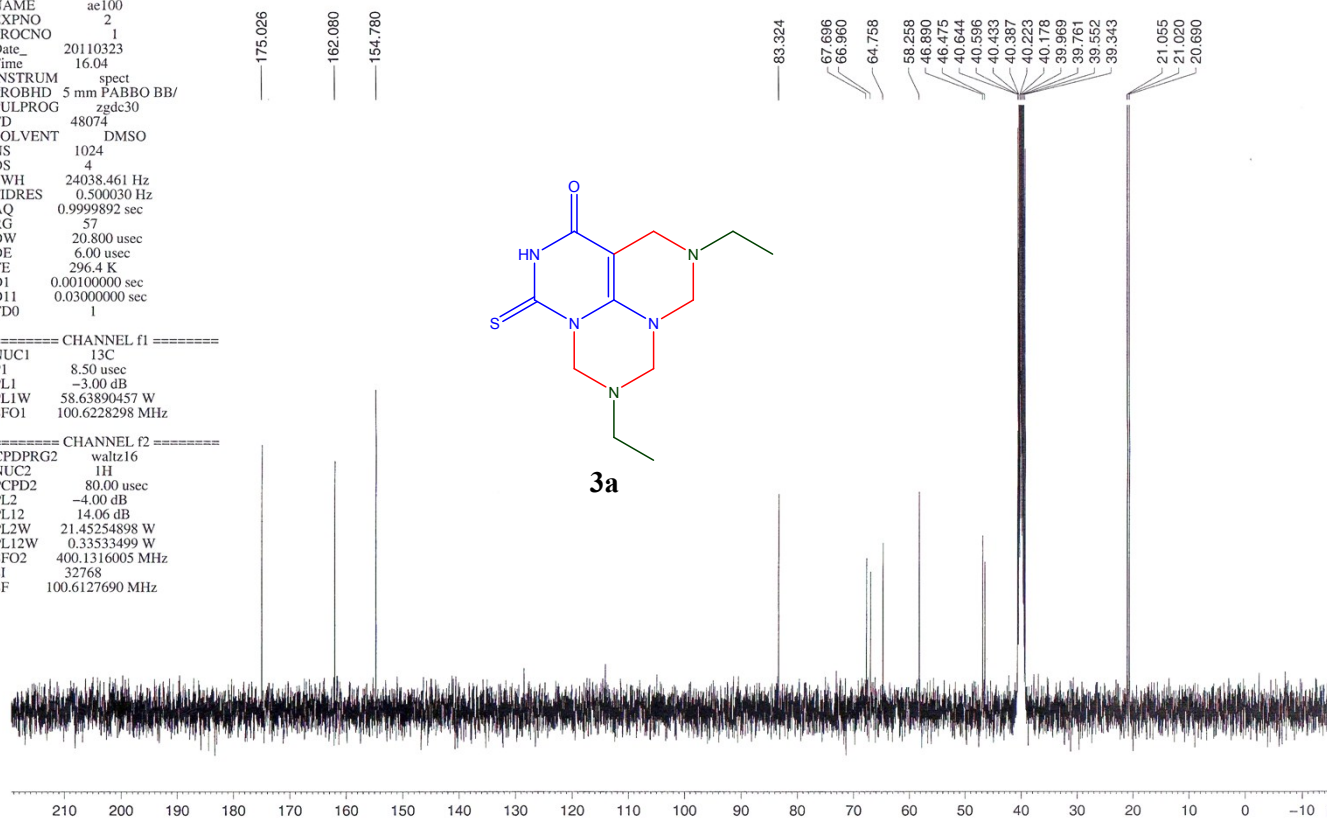
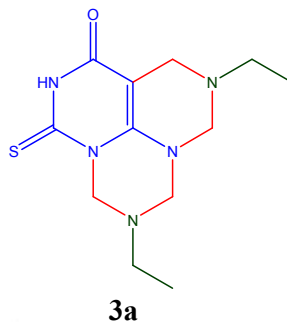


¹H-NMR spectrum of compound **3a** (400 MHz, DMSO-*d*₆).

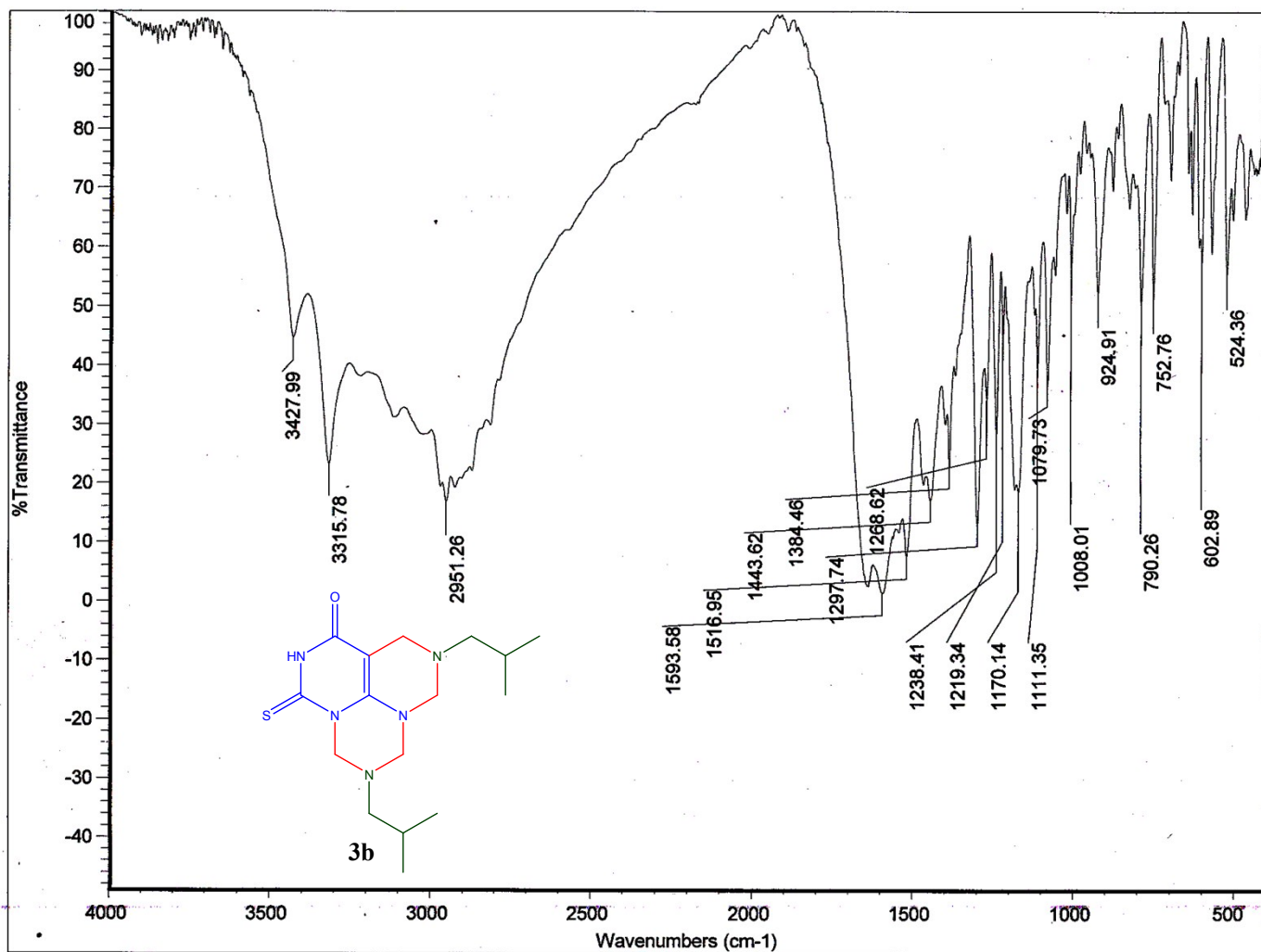
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 EXPNO 2
 PROCNO 1
 Date_ 20110323
 Time 16.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgdc30
 TD 48074
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999892 sec
 RG 57
 DW 20.800 usec
 DE 6.00 usec
 TE 296.4 K
 D1 0.00100000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -3.00 dB
 PL1W 58.63890457 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 14.06 dB
 PL2W 21.45254898 W
 PL12W 0.33533499 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz



^{13}C -NMR spectrum of compound **3a** (400 MHz, $\text{DMSO-}d_6$).



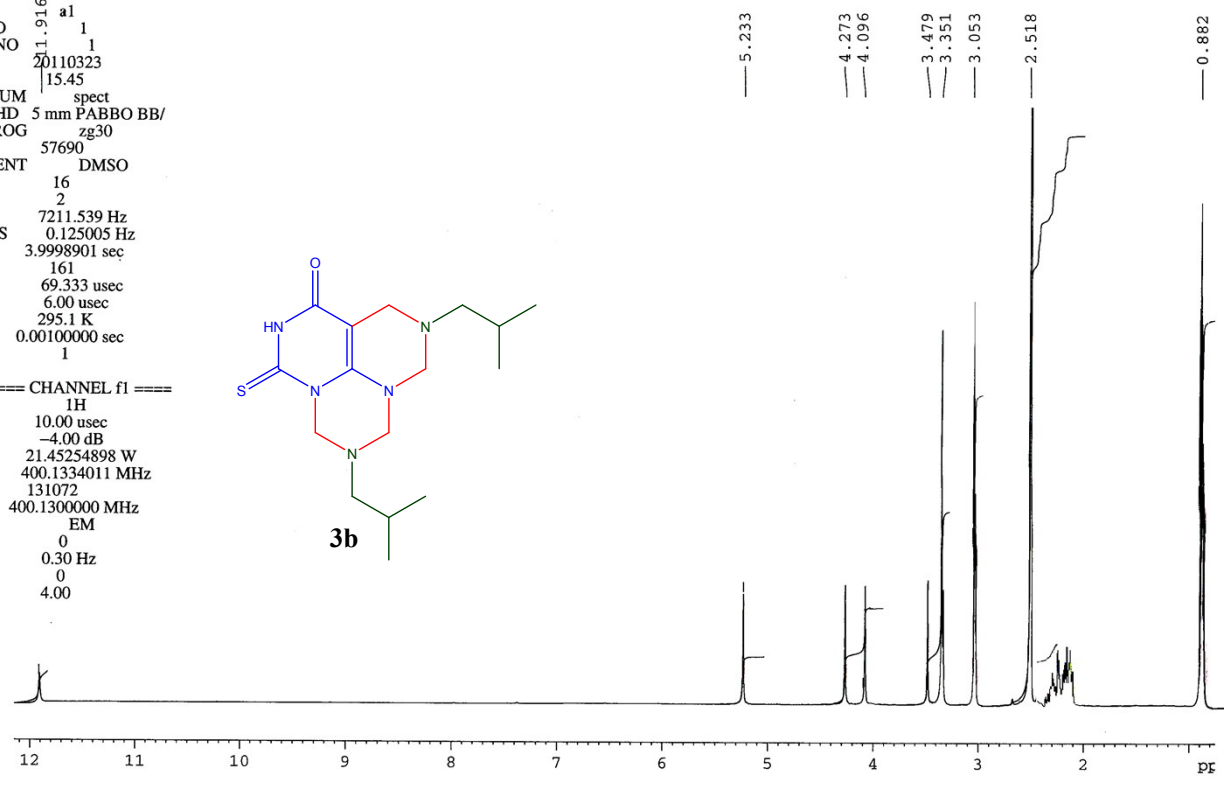
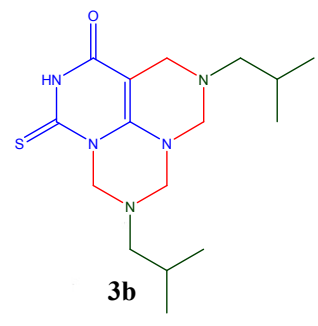
FTIR spectrum of compound **3b**

```

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PROCNO 1
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INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 57690
SOLVENT DMSO
NS 16
DS 2
SWH 7211.539 Hz
FIDRES 0.125005 Hz
AQ 3.9998901 sec
RG 161
DW 69.333 usec
DE 6.00 usec
TE 295.1 K
D1 0.00100000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
PL1W 21.45254898 W
SFO1 400.1334011 MHz
SI 131072
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

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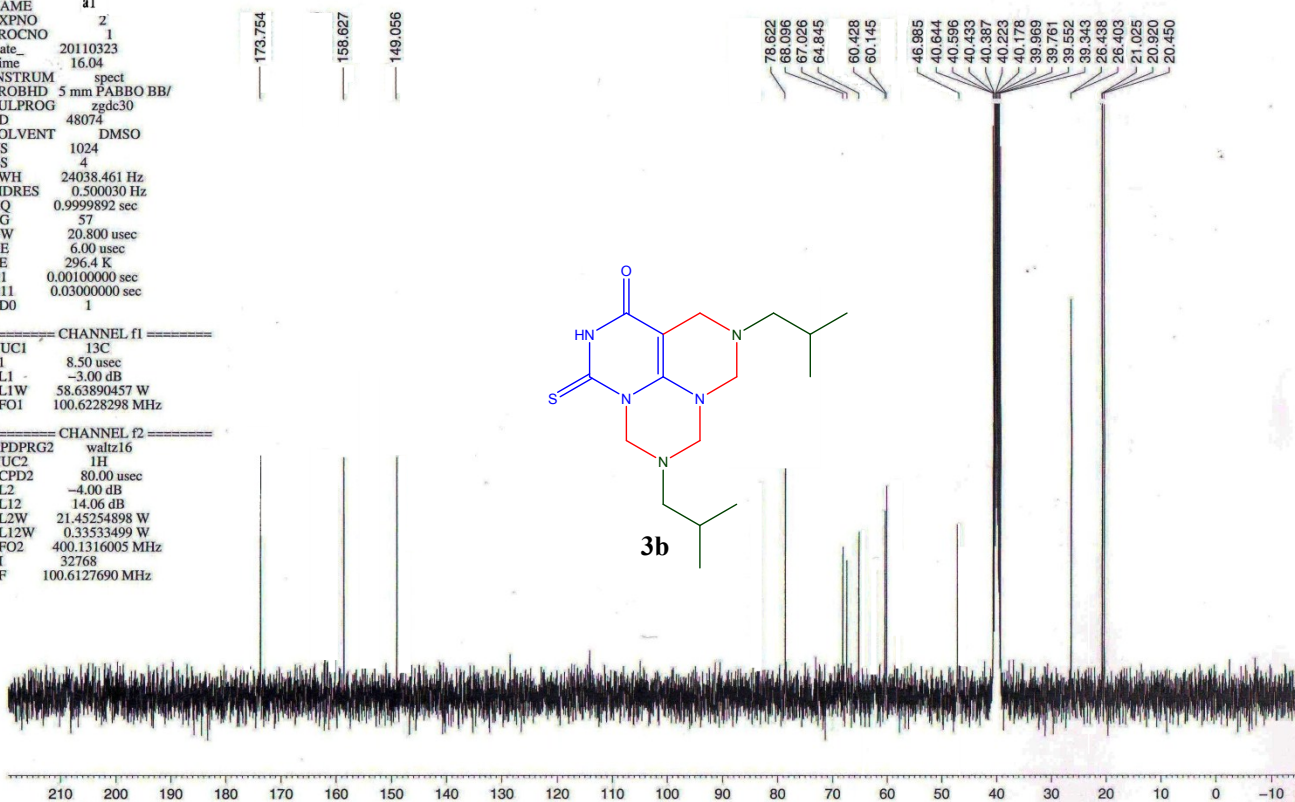


H-NMR spectrum of compound **3b** (400 MHz, DMSO-*d*₆).

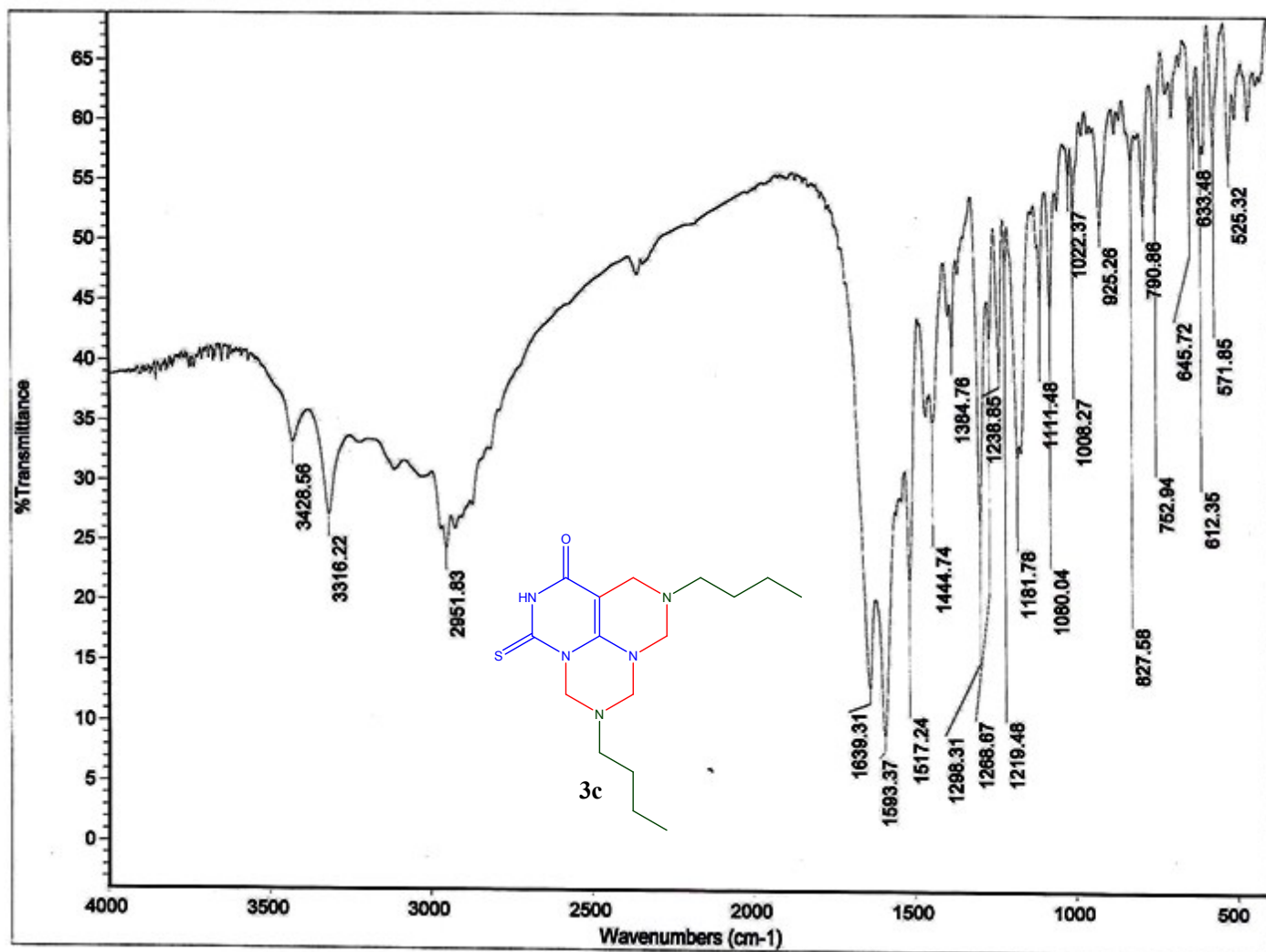
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 PROCNO 1
 Date 20110323
 Time 16.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgdc30
 TD 48074
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999892 sec
 RG 57
 DW 20.800 usec
 DE 6.00 usec
 TE 296.4 K
 D1 0.00100000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -3.00 dB
 PL1W 58.63890457 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 14.06 dB
 PL2W 21.45254898 W
 PL12W 0.33533499 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz



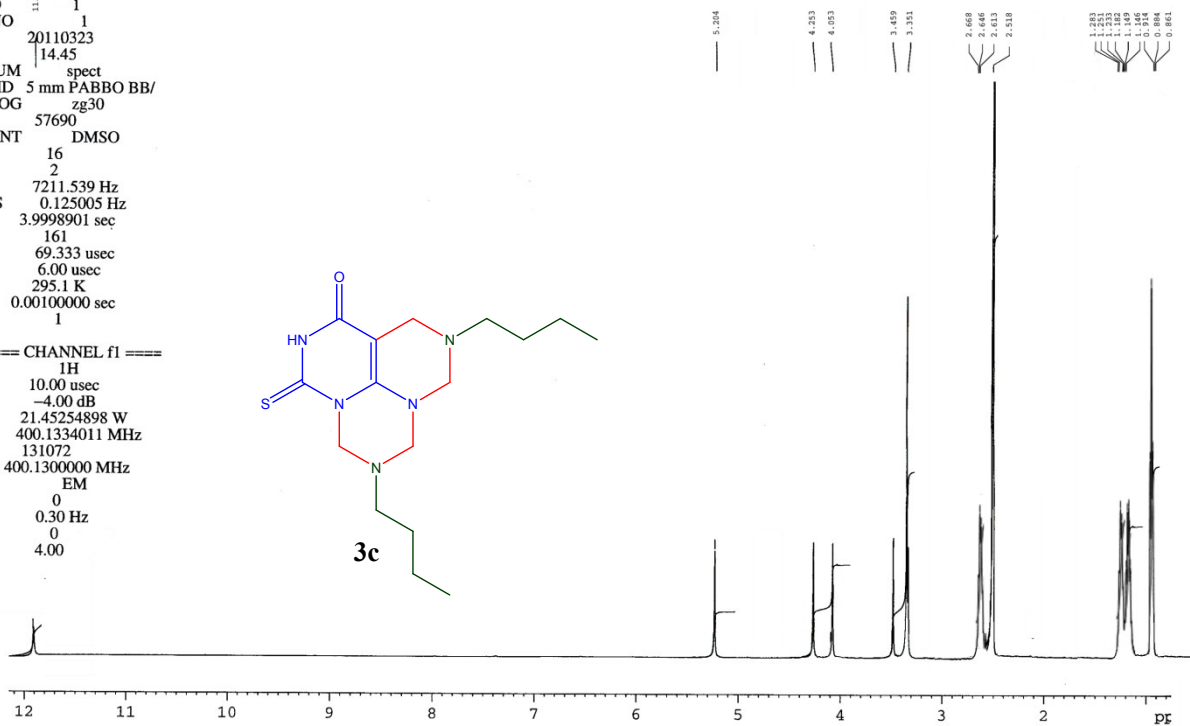
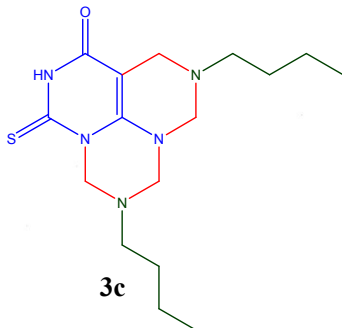
¹³C-NMR spectrum of compound **3b** (400 MHz, DMSO-*d*₆).



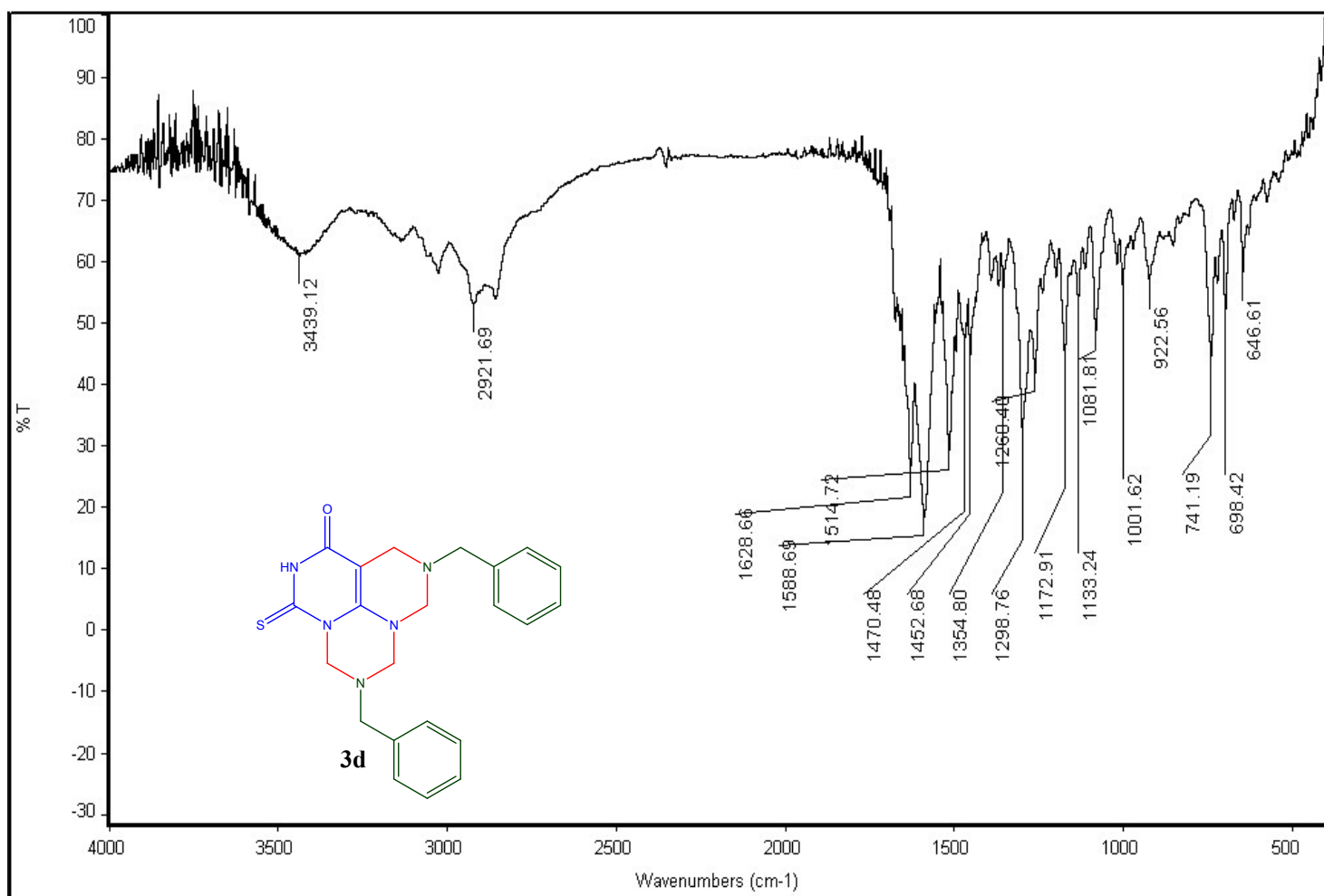
FTIR spectrum of compound 3c

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 PROCNO 1
 Date_ 20110323
 Time 14.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 57690
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 7211.539 Hz
 FIDRES 0.125005 Hz
 AQ 3.9998901 sec
 RG 161
 DW 69.333 usec
 DE 6.00 usec
 TE 295.1 K
 DI 0.00100000 sec
 TDO 1

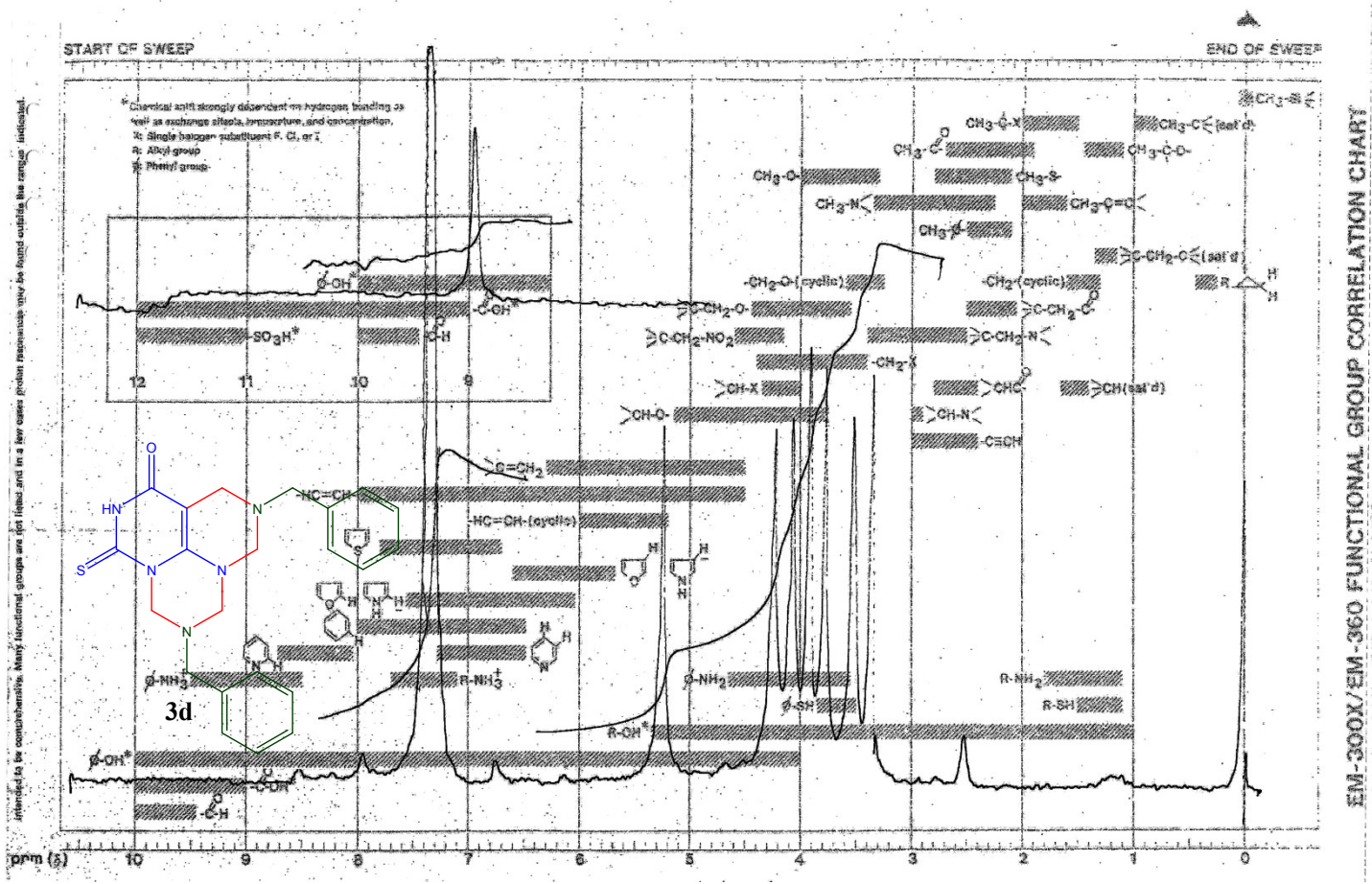
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 P1 10.00 usec
 PL1 -4.00 dB
 PL1W 21.45254898 W
 SFO1 400.1334011 MHz
 SI 131072
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00



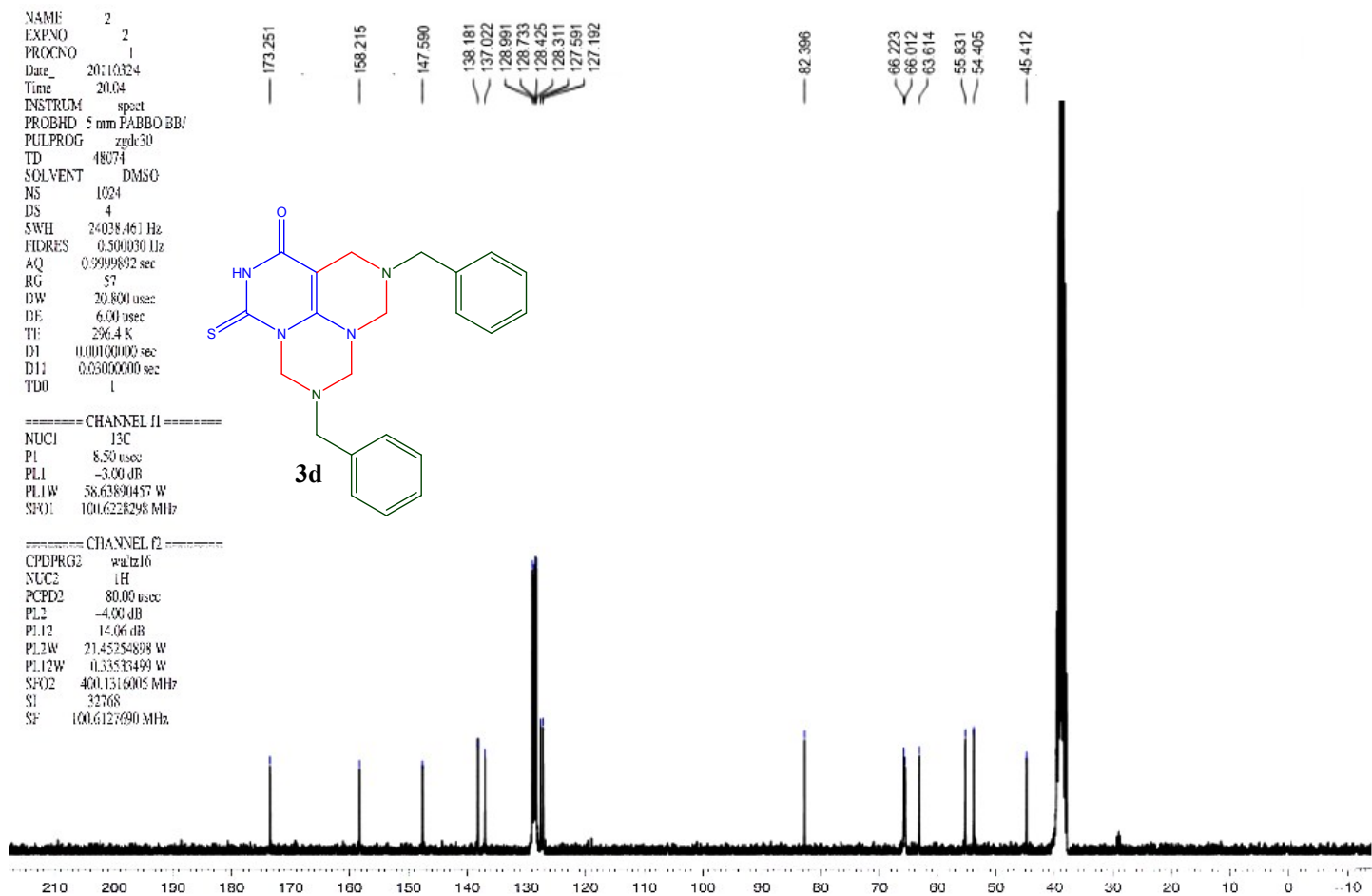
¹H-NMR spectrum of compound **3c** (400 MHz, DMSO-*d*₆).



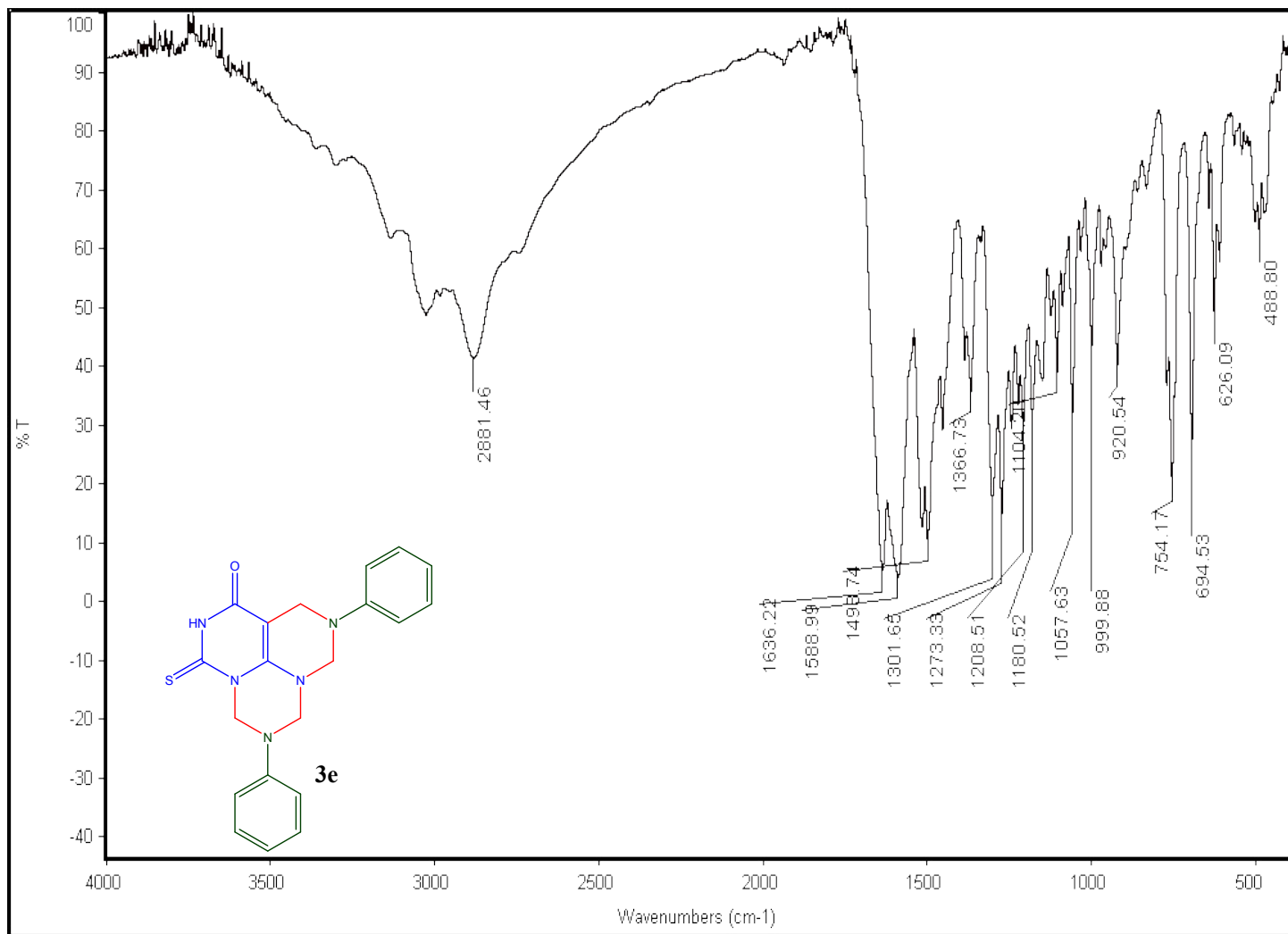
FTIR spectrum of compound **3d**.



¹H-NMR spectrum of compound **3d** (90 MHz, DMSO-*d*₆).



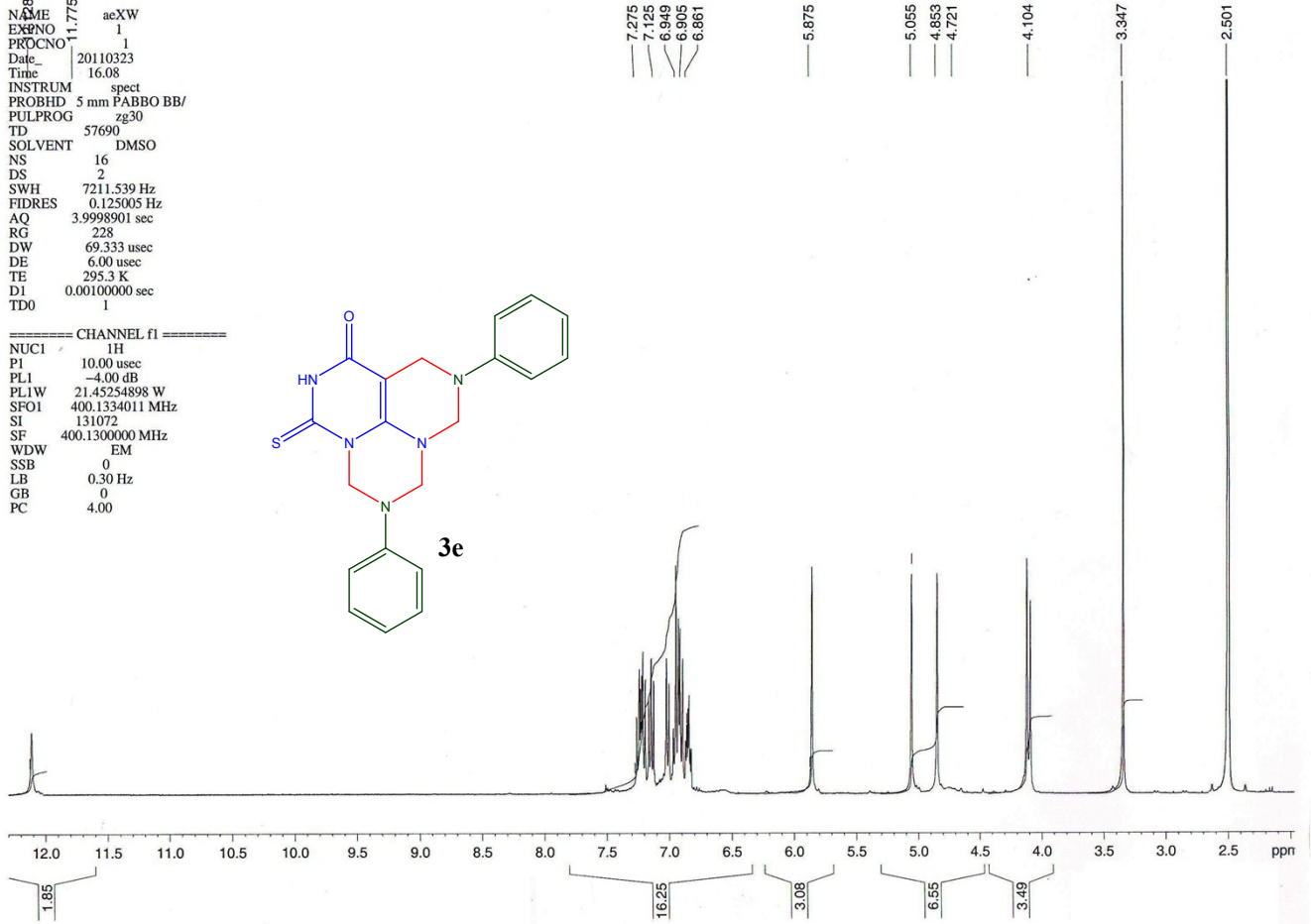
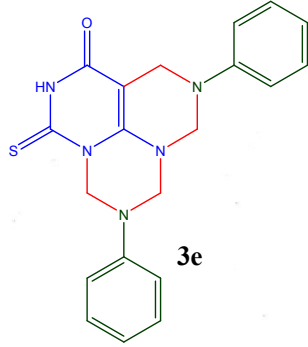
^{13}C -NMR spectrum of compound **3d** (400 MHz, $\text{DMSO-}d_6$).



FTIR spectrum of compound 3e

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 PROCNO 1
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 Time 16.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 57690
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 7211.539 Hz
 FIDRES 0.125005 Hz
 AQ 3.9998901 sec
 RG 228
 DW 69.333 usec
 DE 6.00 usec
 TE 295.3 K
 D1 0.00100000 sec
 TD0 1

CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -4.00 dB
 PL1W 21.45254898 W
 SFO1 400.1334011 MHz
 SI 131072
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

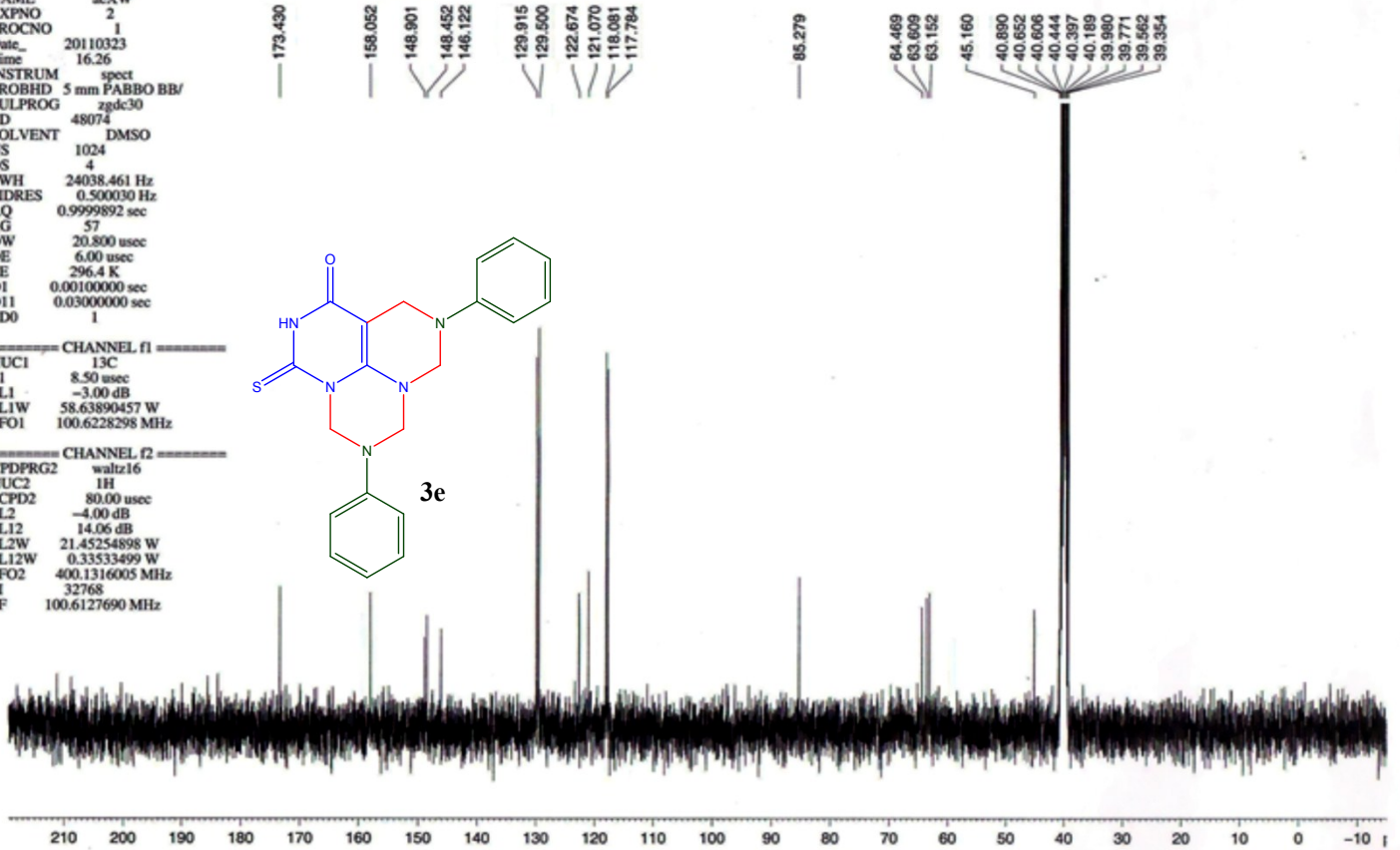
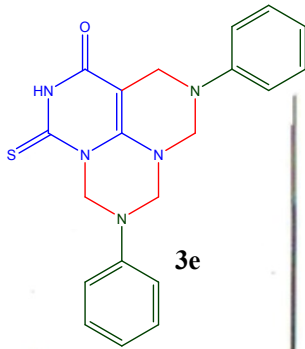


¹H-NMR spectrum of compound **3e** (400 MHz, DMSO-*d*₆).

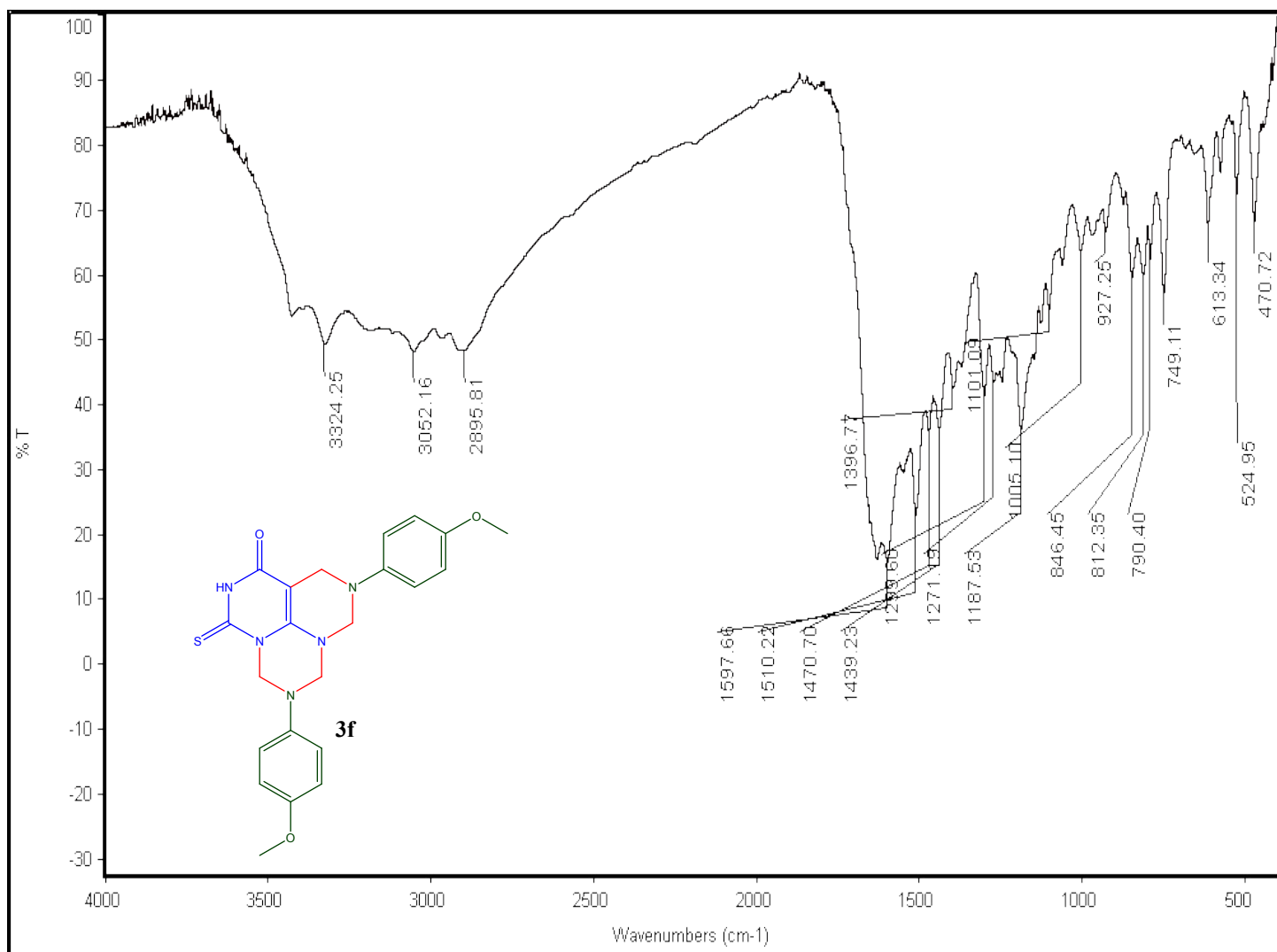
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 PROCNO 1
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 Time 16.25
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 PULPROG zgdc30
 TD 48074
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999892 sec
 RG 57
 DW 20.800 usec
 DE 6.00 usec
 TE 296.4 K
 D1 0.00100000 sec
 D11 0.03000000 sec
 TD0 1

CHANNEL f1
 NUC1 13C
 P1 8.50 usec
 PL1 -3.00 dB
 PL1W 58.63890457 W
 SFO1 100.6228298 MHz

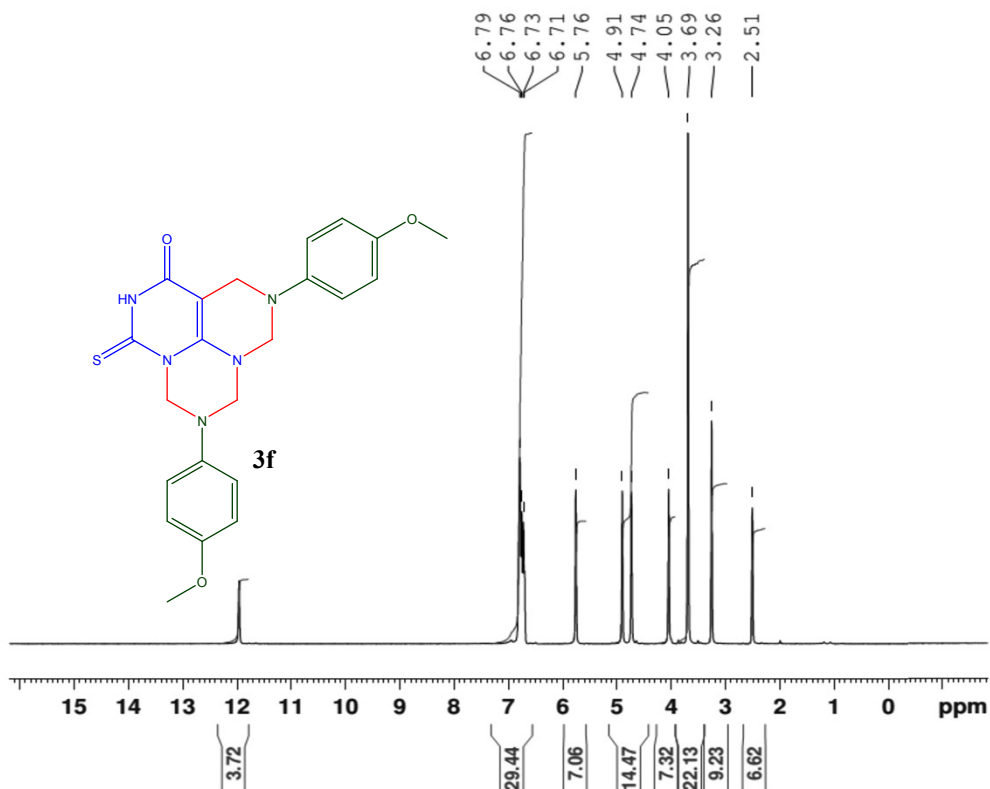
CHANNEL f2
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 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 14.06 dB
 PL2W 21.45254898 W
 PL12W 0.33533499 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz



^{13}C -NMR spectrum of compound **3e** (400 MHz, $\text{DMSO-}d_6$).



FTIR spectrum of compound **3f**



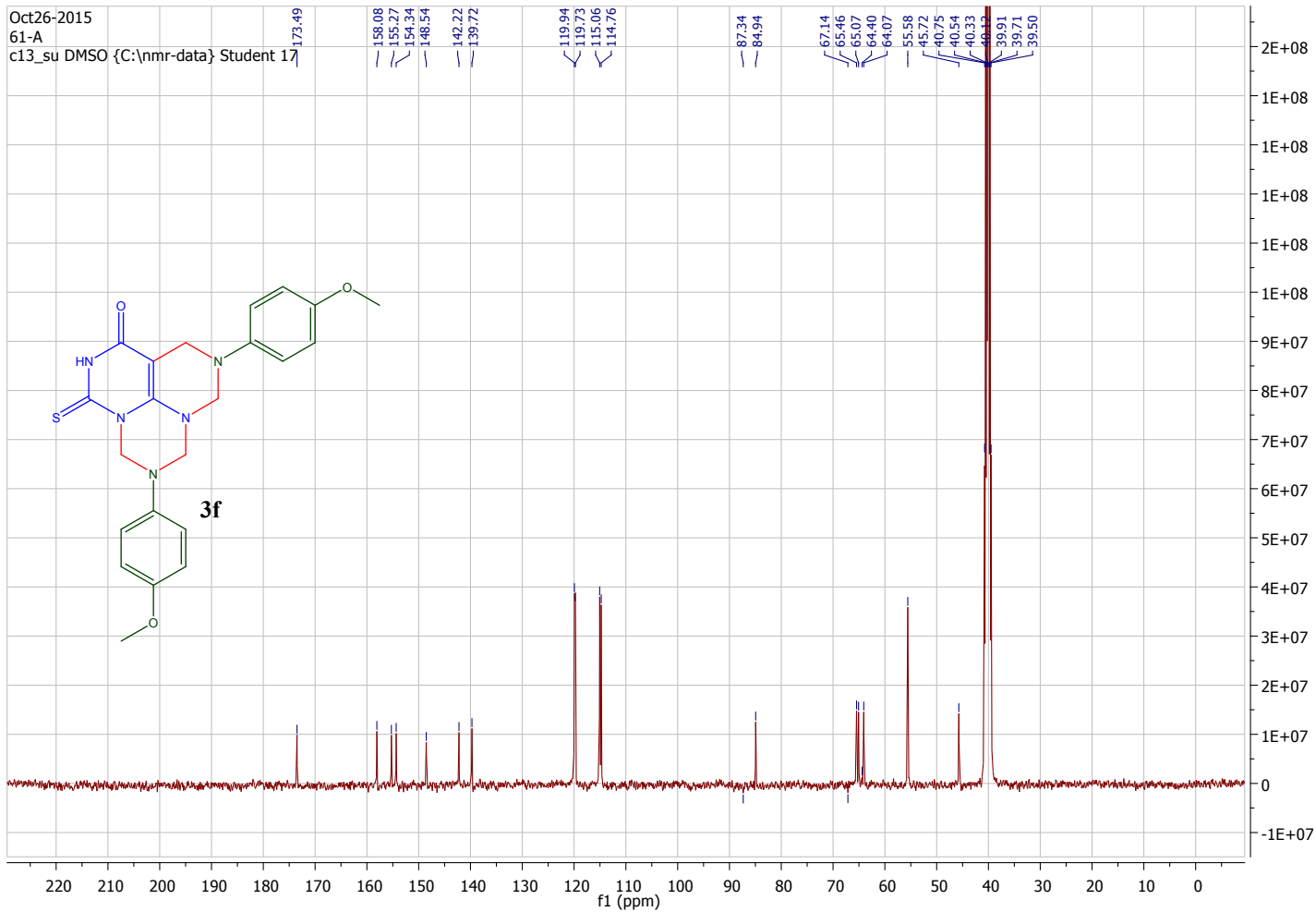
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PROCNO   1

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PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       20
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       199.04
DW       62.400 usec
DE       6.50 usec
TE       313.2 K
D1       1.00000000 sec
TD0      1

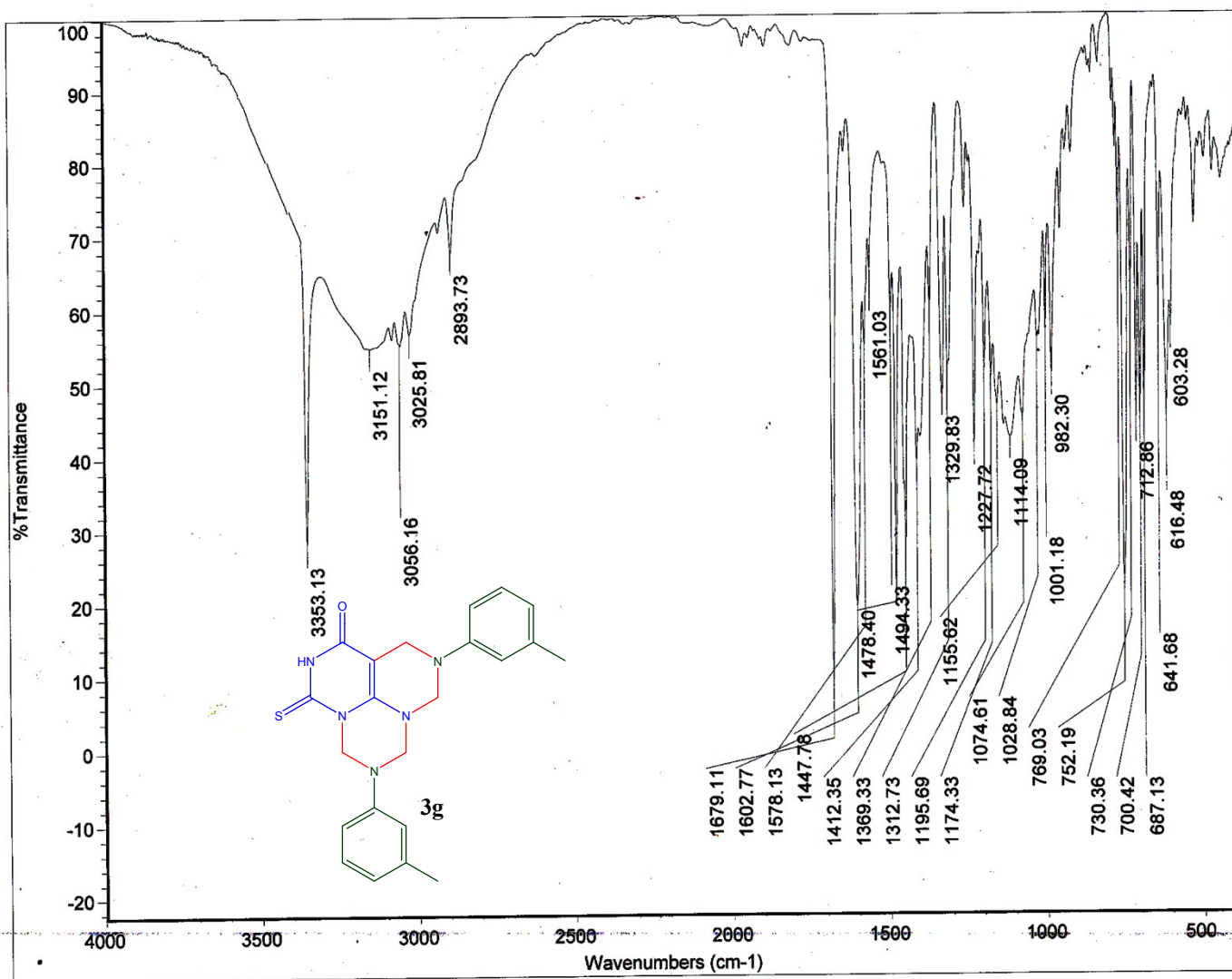
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NUC1     1H
P1       12.00 usec
PLW1     22.00000000 W

F2 - Processing parameters
SI       65536
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WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
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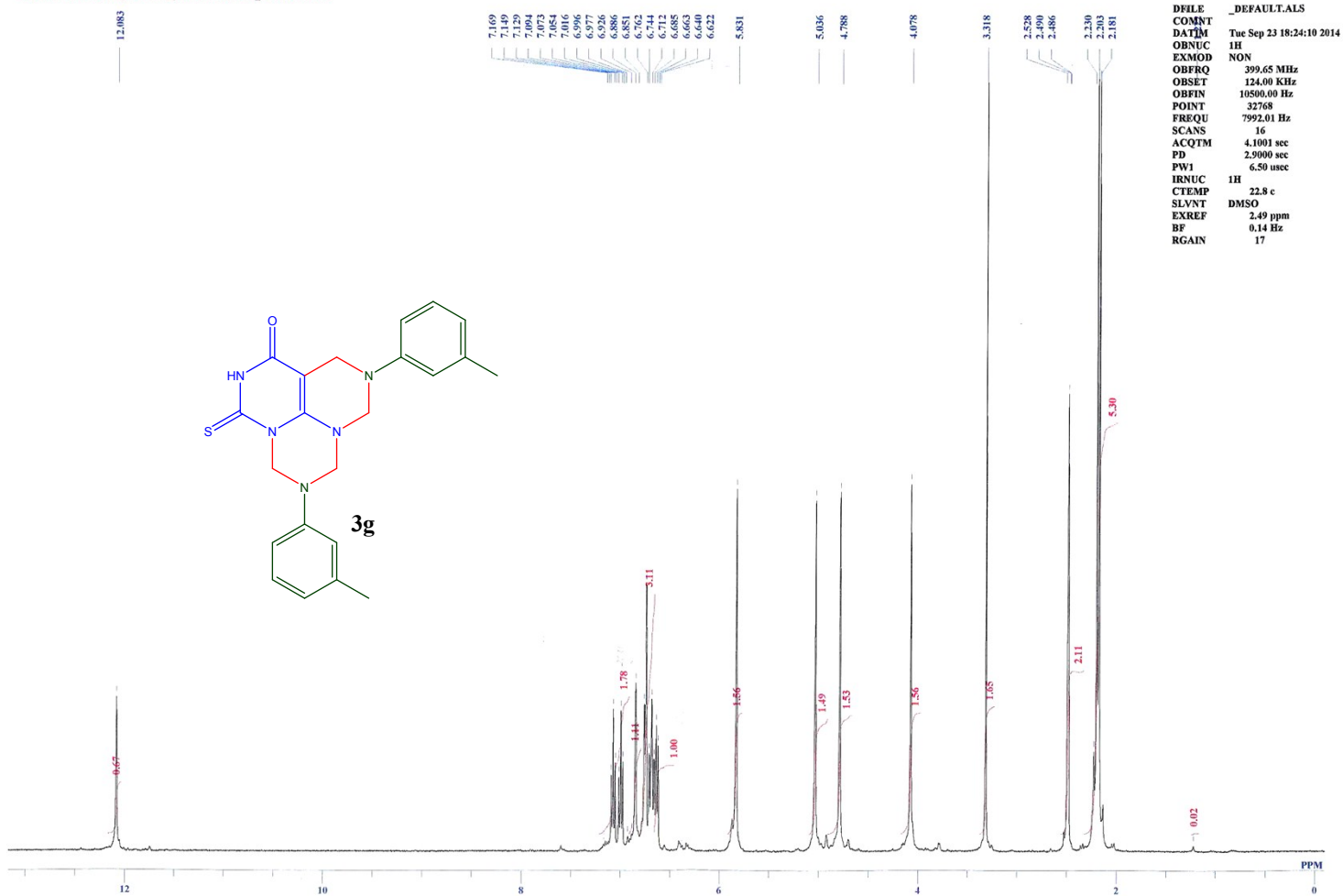
$^1\text{H-NMR}$ spectrum of compound **3f** (400 MHz, $\text{DMSO-}d_6$).



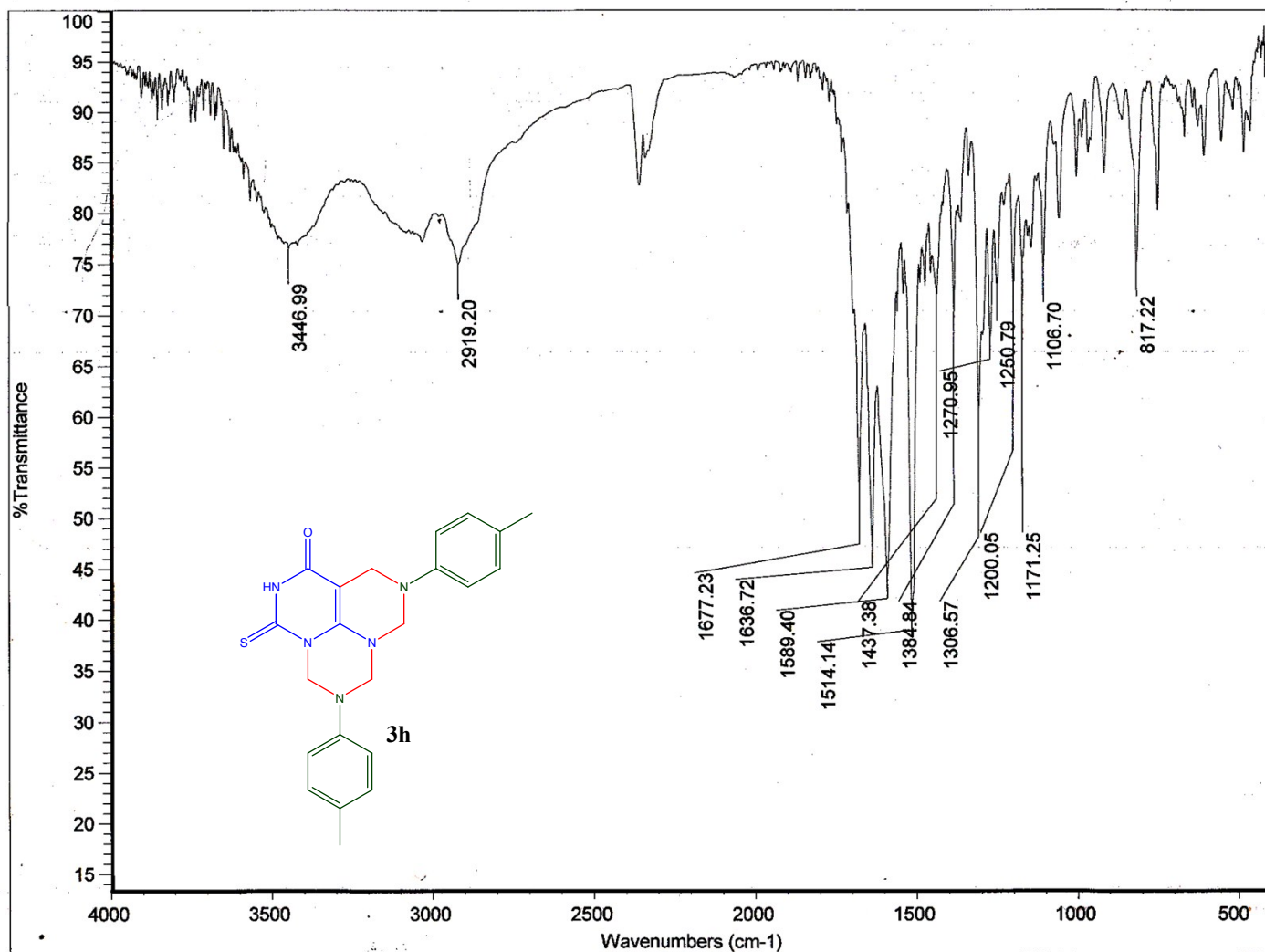
^{13}C -NMR spectrum of compound **3f** (400 MHz, $\text{DMSO}-d_6$).



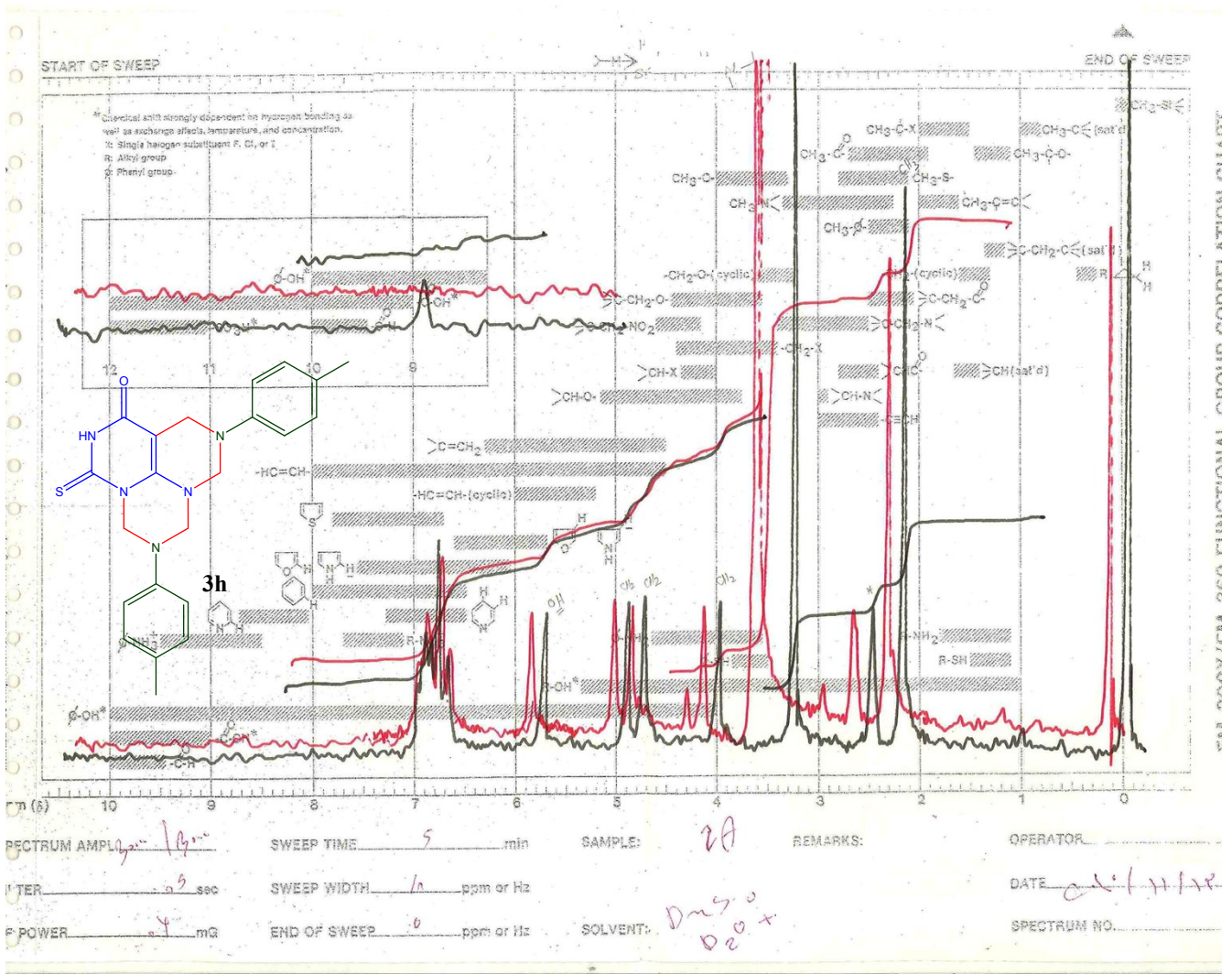
FTIR spectrum of compound **3g**



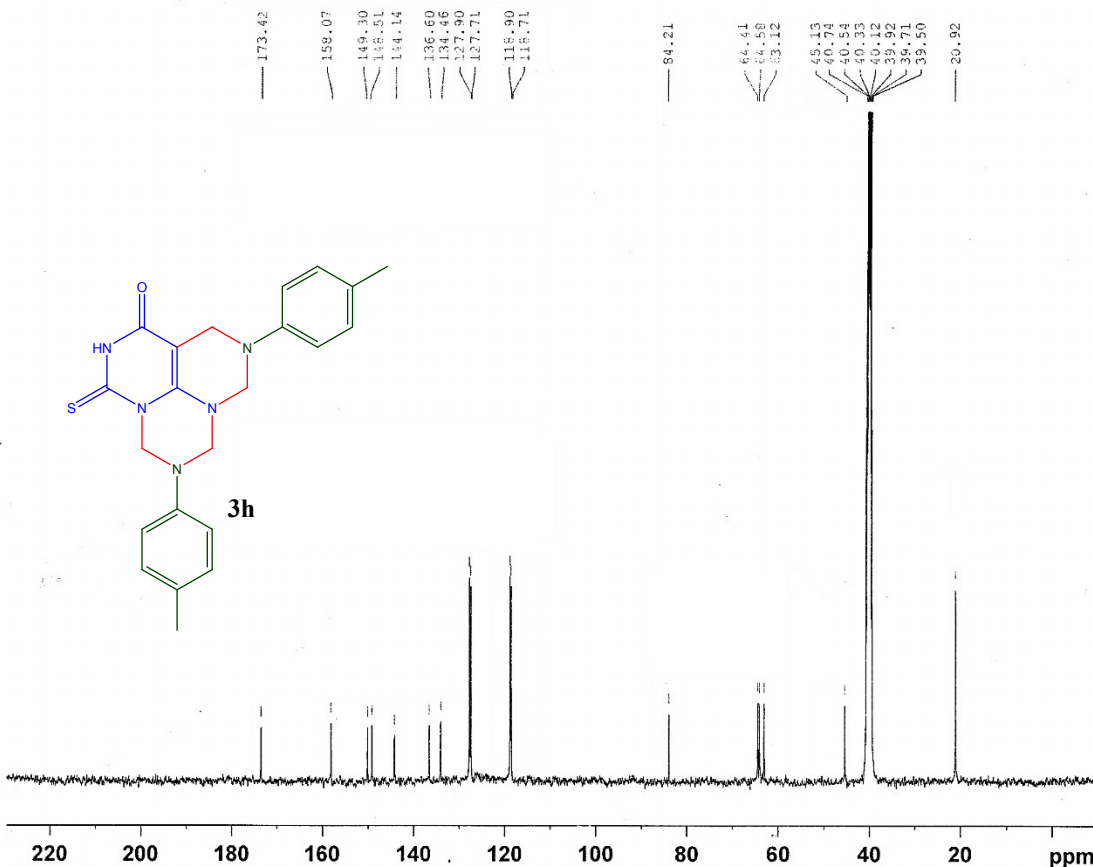
¹H-NMR spectrum of compound **3g** (400 MHz, DMSO-*d*₆).



FTIR spectrum of compound **3h**



¹H-NMR spectrum of compound **3h** (90 MHz, DMSO-d₆).



```

Current Data Parameters
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PROCNO    1

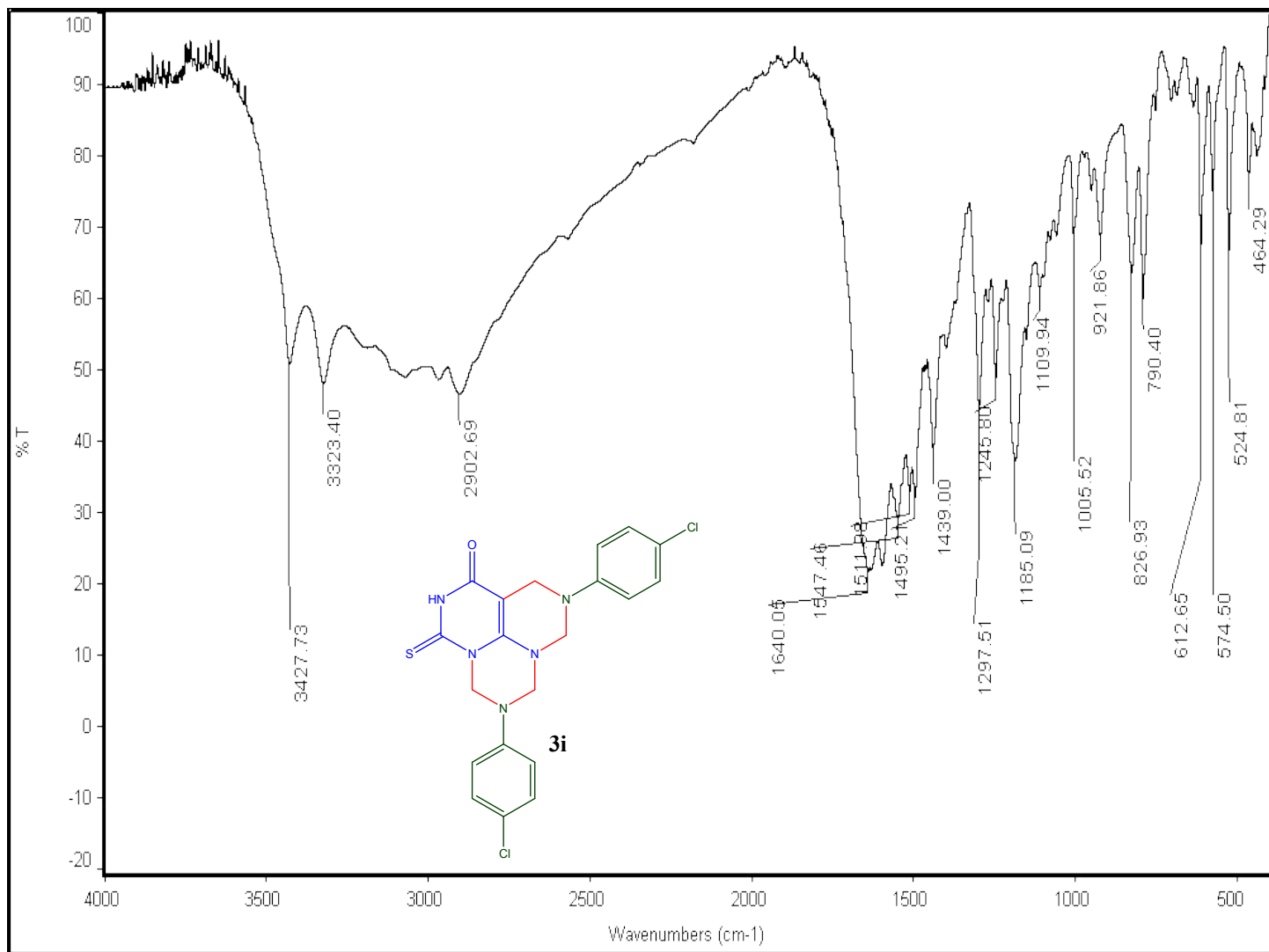
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Time      20.15
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PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         1200
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         100.43
DW         20.800 usec
DE         6.50 usec
TE         313.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      100.6238364 MHz
NUC1       13C
P1         9.50 usec
PLW1       56.0000000 W

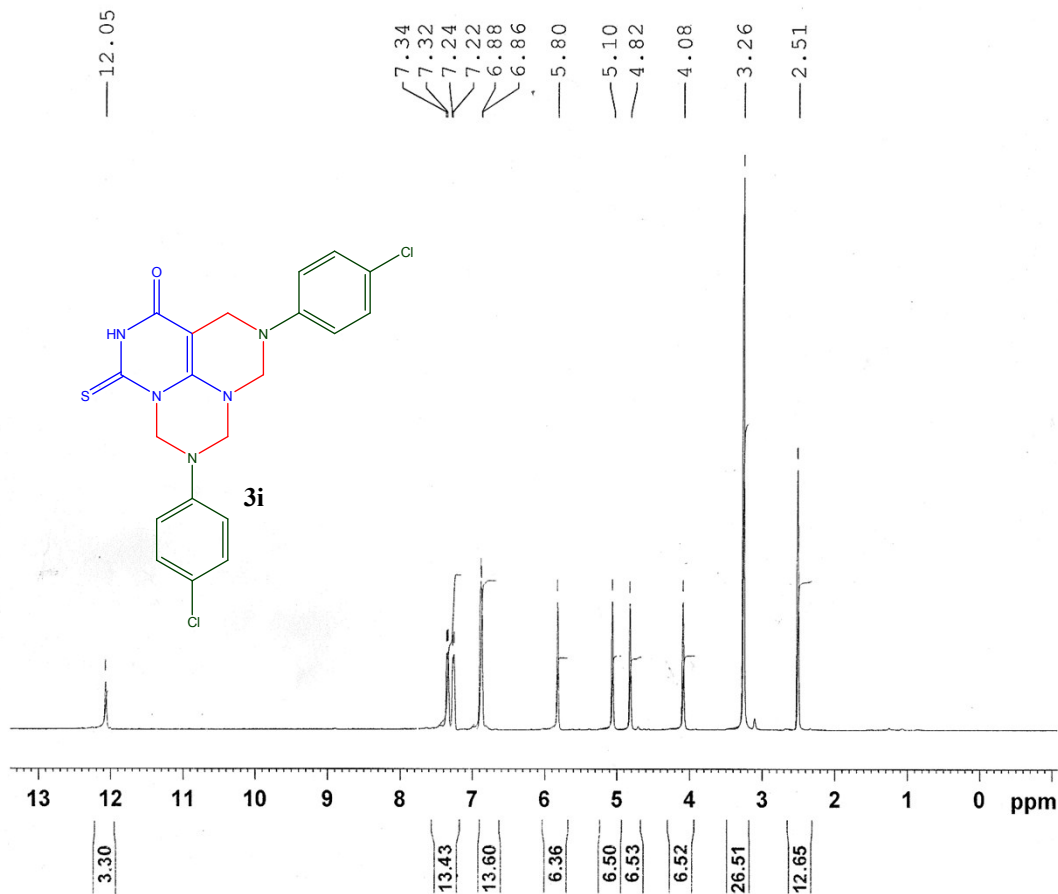
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SFO2      400.1316005 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      22.0000000 W
PLW12     0.41091001 W
PLW13     0.33284000 W

F2 - Processing parameters
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         6.00 Hz
GB         0
PC         1.40
    
```

^{13}C -NMR spectrum of compound **3h** (400 MHz, $\text{DMSO-}d_6$).



FTIR spectrum of compound **3i**



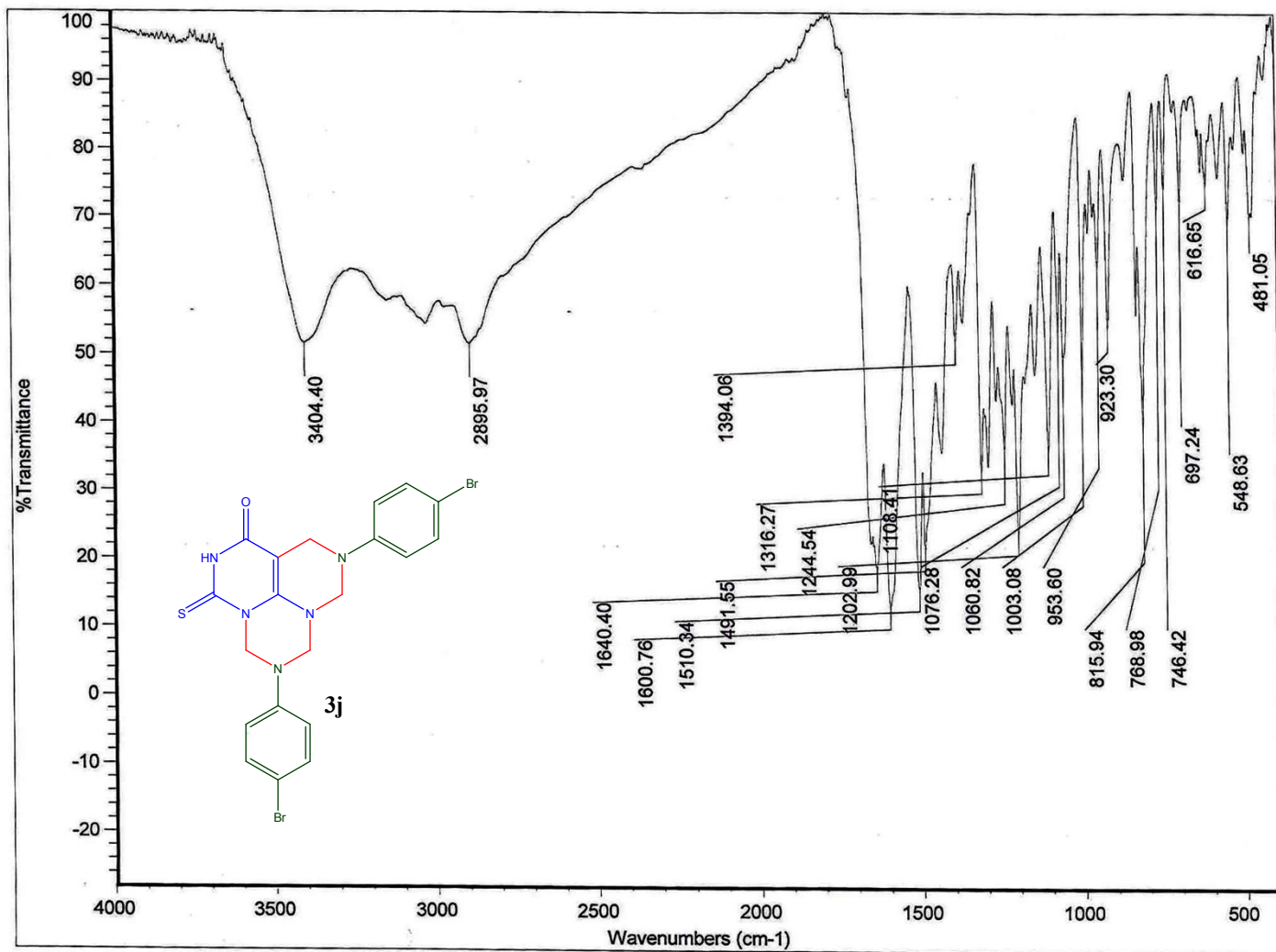
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NAME Oct26-2015
EXNO 160
PROCNO 1

F2 - Acquisition Parameters
Date 20151026
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TDO 1

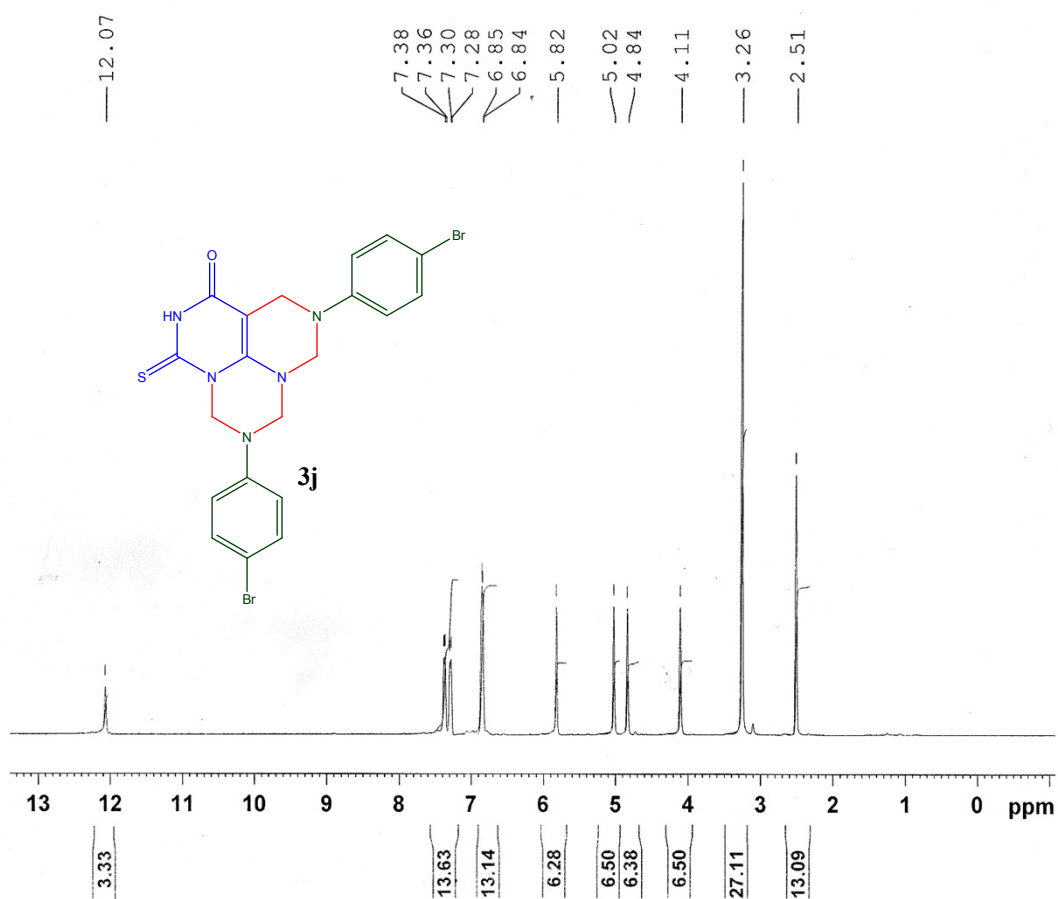
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SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR spectrum of compound **3i** (400 MHz, DMSO-*d*₆).



FTIR spectrum of compound **3j**



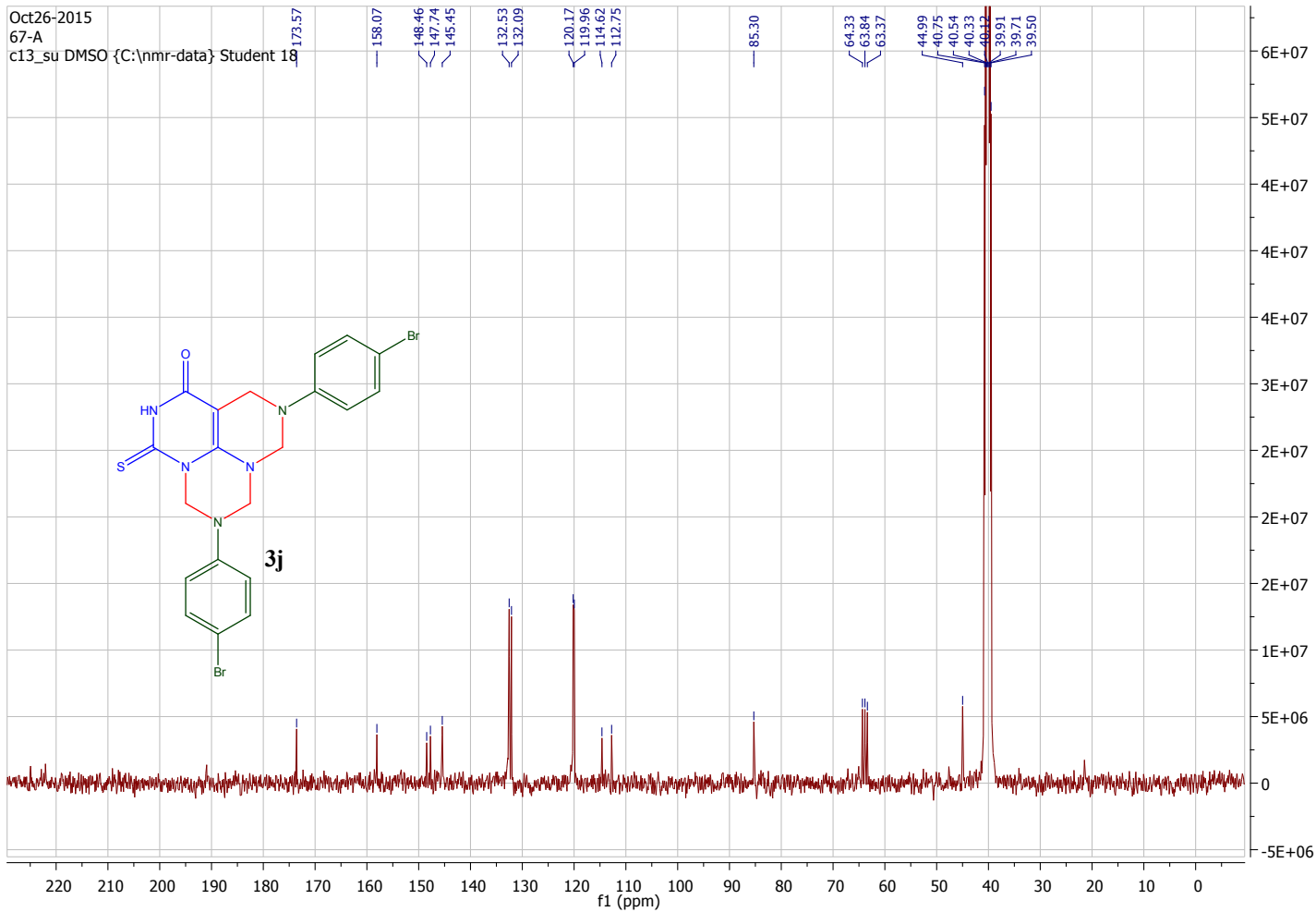
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NAME Oct26-2015
EXPNO 160
PROCNO 1

F2 - Acquisition Parameters
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Time 23.08
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PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.0000000 sec
TDO 1

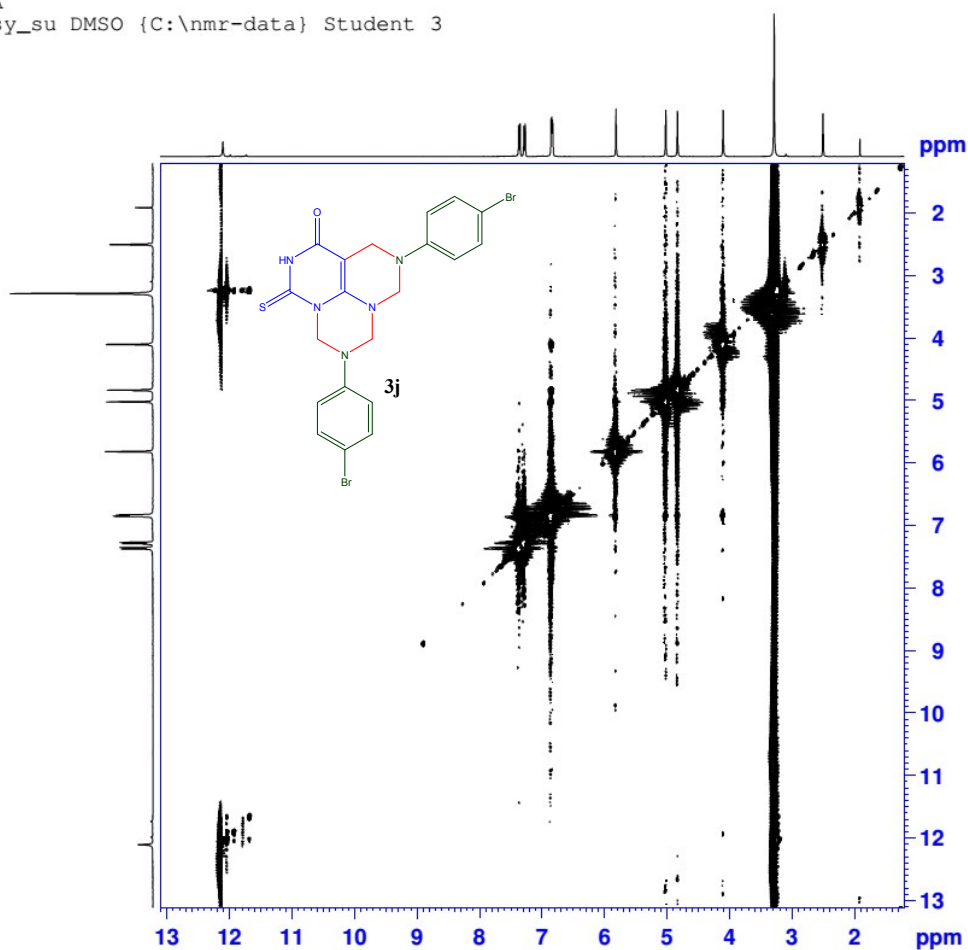
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SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR spectrum of compound **3j** (400 MHz, DMSO-*d*₆).



^{13}C -NMR spectrum of compound **3j** (400 MHz, $\text{DMSO-}d_6$).



Current Data Parameters
NAME Sep01-2016
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160901
Time 17.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG roesyppp-2
TD 2048
SOLVENT DMSO
NS 60
DS 128
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150400 sec
RG 120.97
DW 105.000 usec
DE 6.50 usec
TE 318.2 K
DO 0.00009336 sec
D11 0.99795198 sec
D12 0.03000000 sec
D1 0.00002000 sec
IN0 0.00021000 sec
L4 794
P15 200000.00 usec

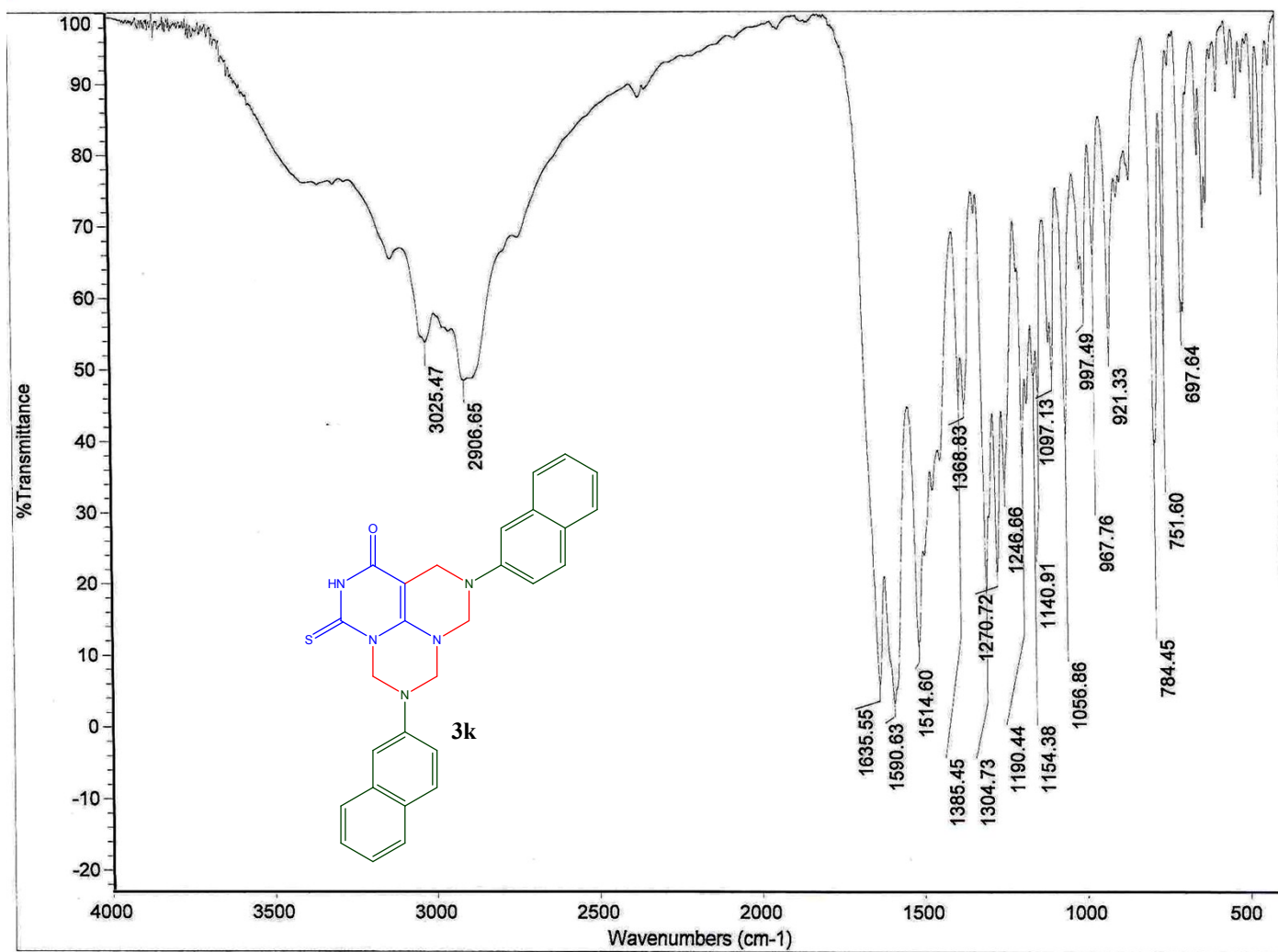
CHANNEL f1
SF01 400.1328648 MHz
NUC1 1H
P1 12.00 usec
P17 2500.00 usec
P25 126.00 usec
PLW1 22.00000000 W
PLW10 4.68639994 W
PLW27 0.79819000 W

F1 - Acquisition parameters
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SF01 400.1329 MHz
FIDRES 18.601191 Hz
SW 11.901 ppm
FnMODE States-TPI1

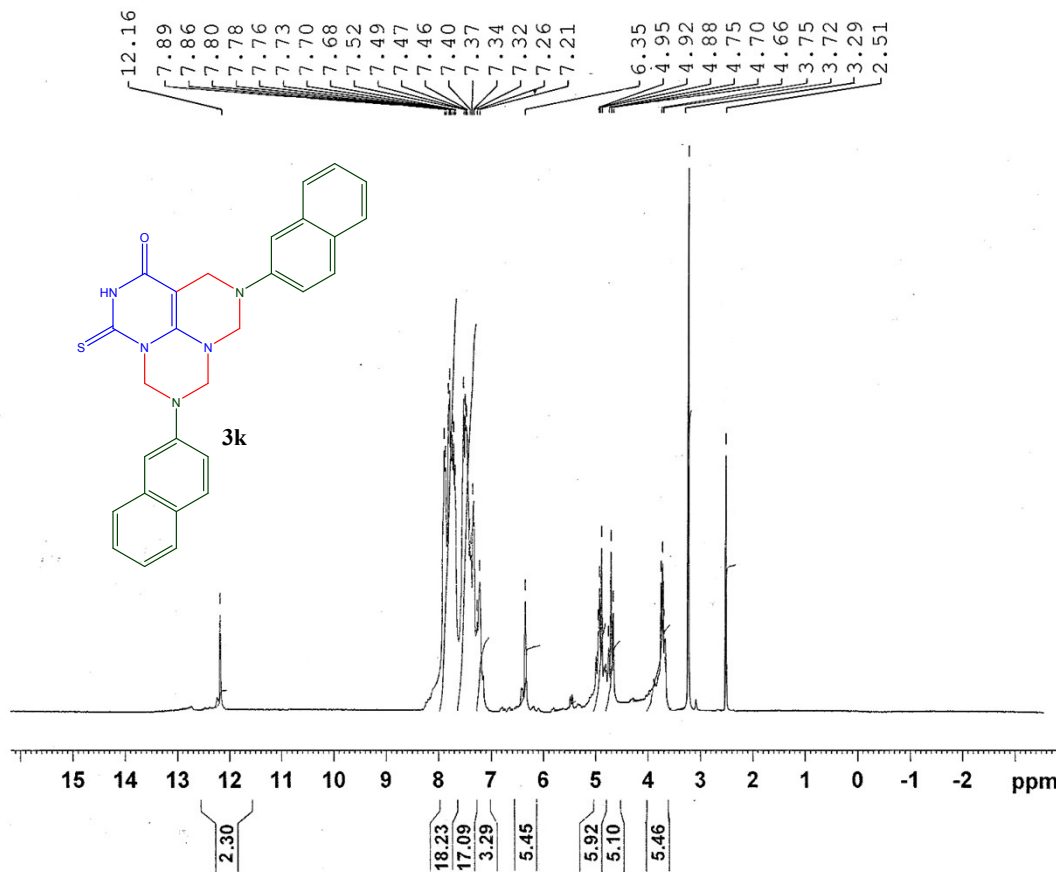
F2 - Processing parameters
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SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPI1
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

ROESY-NMR spectrum of compound **3j** (400 MHz, DMSO-*d*₆).



FTIR spectrum of compound 3k



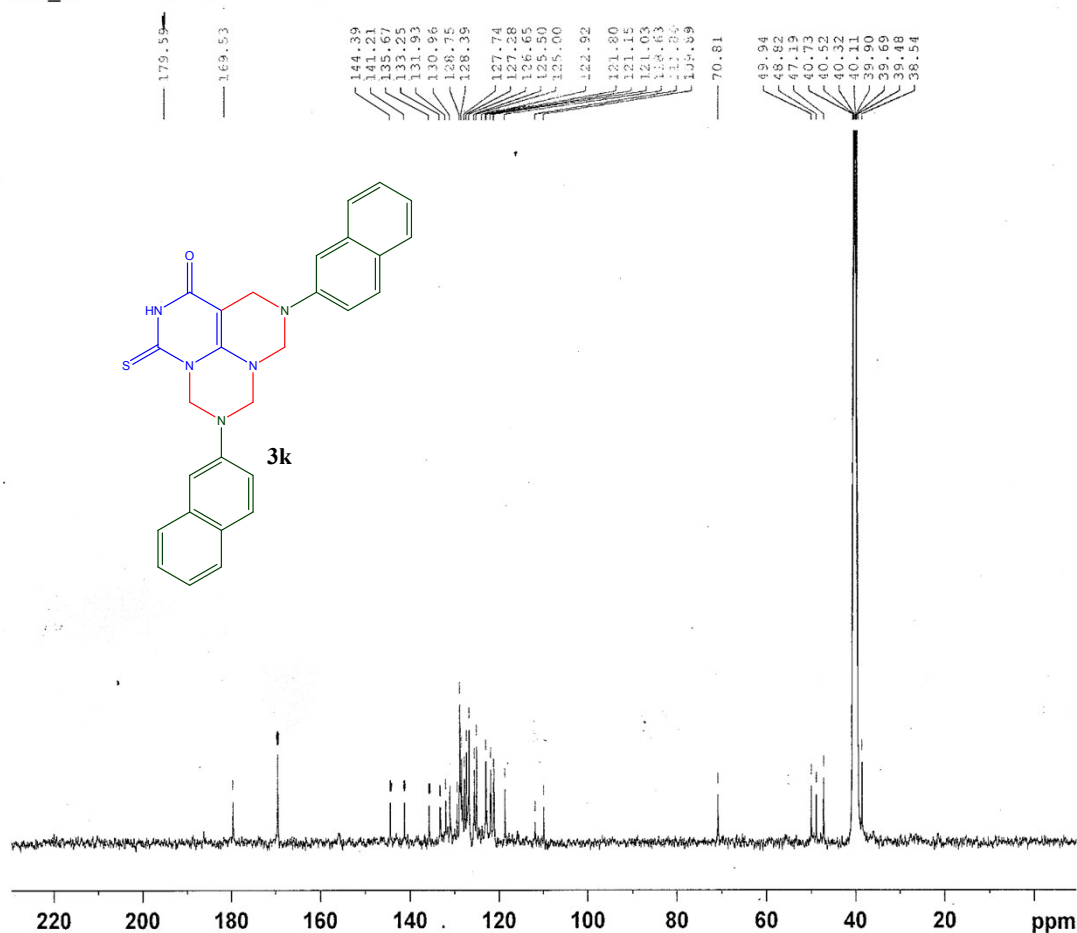
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NAME Oct26-2015
EXPNO 170
PROCNO 1

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Date_ 20151027
Time 0.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 135
DW 62.400 usec
DE 6.50 usec
TE 313.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR spectrum of compound **3k** (400 MHz, DMSO-*d*₆).



Current Data Parameters
 NAME Oct26-2015
 EXPNO 171
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151027
 Time_ 1.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 175.84
 DW 20.800 usec
 DE 6.50 usec
 TE 313.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6238364 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 56.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 22.00000000 W
 PLW12 0.41091001 W
 PLW13 0.33284000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 1.40

¹³C-NMR spectrum of compound **3k** (400 MHz, DMSO-*d*₆).