

## Supporting Information

### The deep eutectic melt of sorbitol and metformin hydrochloride: Synthesis of 3-substituted 2-aminonaphtho[2,3-*b*]furan-4,9-diones and their photophysical properties

Kurosh Rad-Moghadam\*, Seyyed Ali Reza Mousazadeh Hassani and Saeedeh Toorchis Roudsari

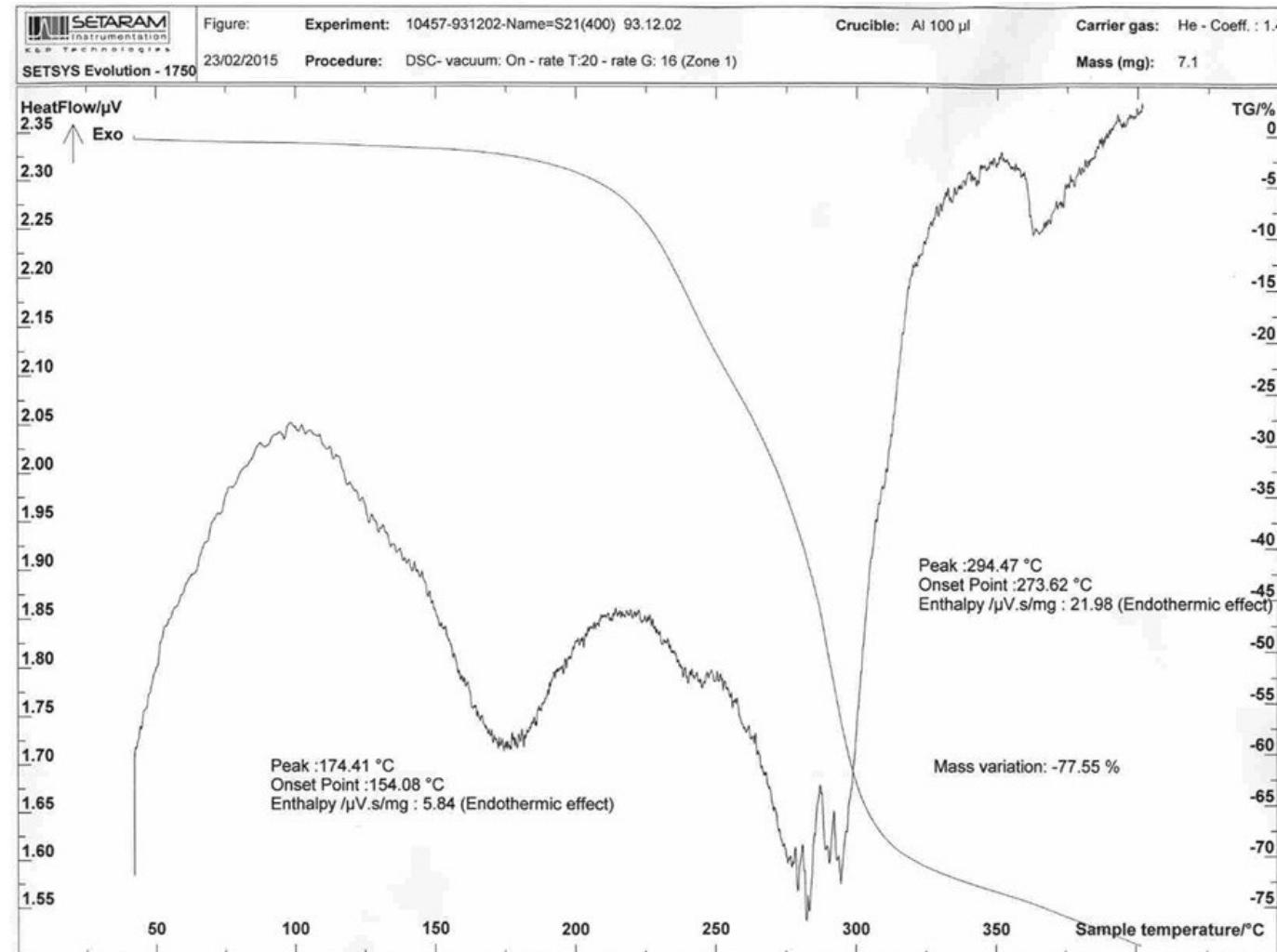
Chemistry department, Univrsity of Guilan, Rasht 41335-1914; [radmm@guiilan.ac.ir](mailto:radmm@guiilan.ac.ir)

#### Contents

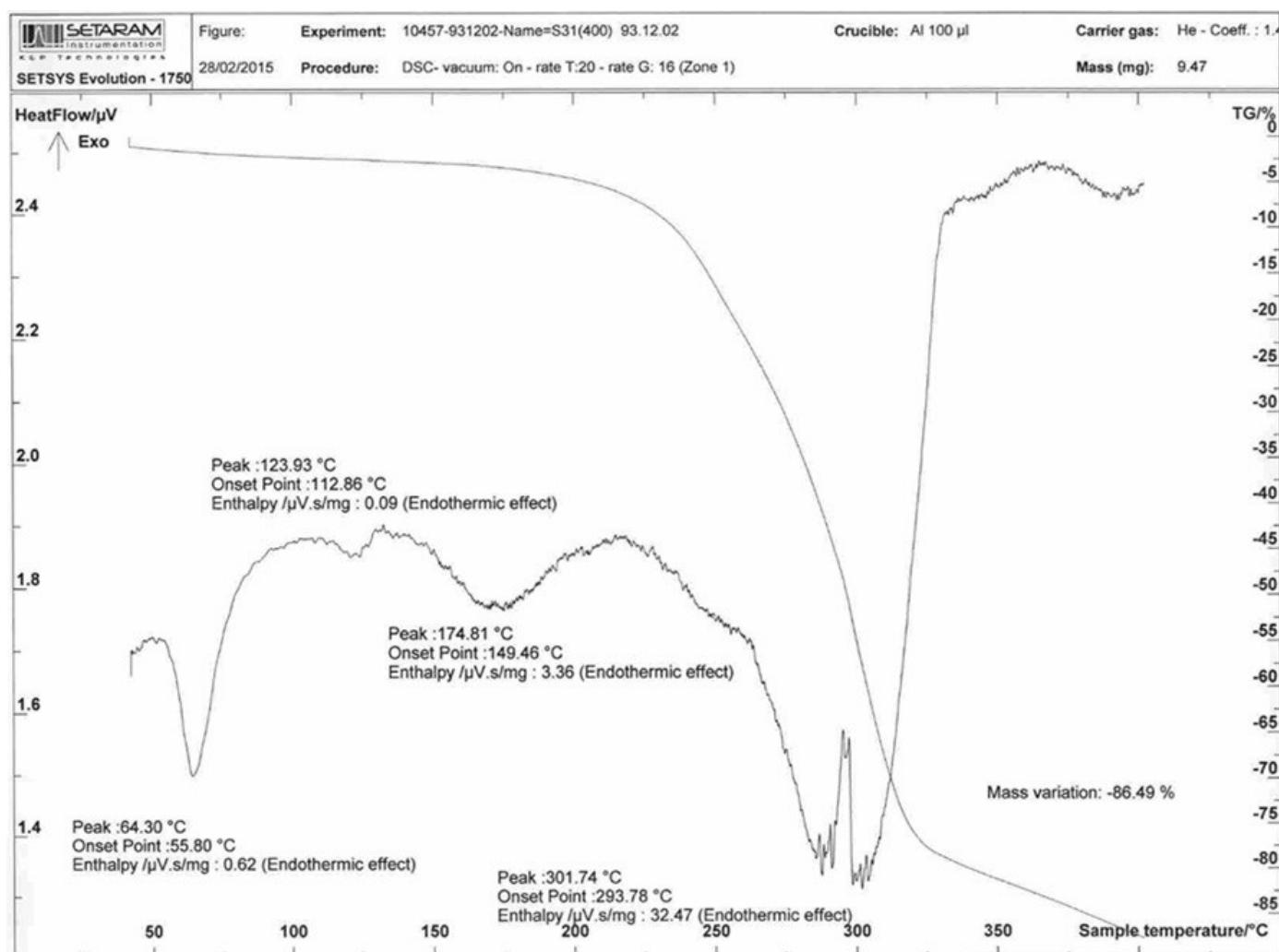
- S<sub>1</sub> Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) of Sorbitol:MetHCl (2:1)
- S<sub>2</sub> Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) of Sorbitol:MetHCl (3:1)
- S<sub>3</sub> Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) of Sorbitol:MetHCl (4:1)
- S<sub>4</sub> The IR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4d**)
- S<sub>5</sub> The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione in DMSO-d<sub>6</sub> + D<sub>2</sub>O (**4d**)
- S<sub>6</sub> The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione in DMSO-d<sub>6</sub> (**4d**)
- S<sub>7</sub> The <sup>13</sup>C NMR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4d**)
- S<sub>8</sub> The Mass spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4d**)
- S<sub>9</sub> The IR spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4g**)
- S<sub>10</sub> The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4g**)
- S<sub>11</sub> The <sup>13</sup>C NMR spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4g**)

- S<sub>12</sub>** The Mass spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4g**)
- S<sub>13</sub>** The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl
- S<sub>13</sub>** The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl
- S<sub>13</sub>** The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl
- S<sub>13</sub>** The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl
- S<sub>14</sub>** The <sup>13</sup>C NMR spectrum of 3:1 S:MetHCl
- S<sub>14</sub>** The <sup>13</sup>C NMR spectrum of 3:1 S:MetHCl
- S<sub>15</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4b**)
- S<sub>16</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4c**)
- S<sub>17</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4d**)
- S<sub>18</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4e**)
- S<sub>19</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4f**)
- S<sub>20</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4g**)
- S<sub>21</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4h**)
- S<sub>22</sub>** The absorption (dashed) and emission (solid) spectra for compound (**4i**)

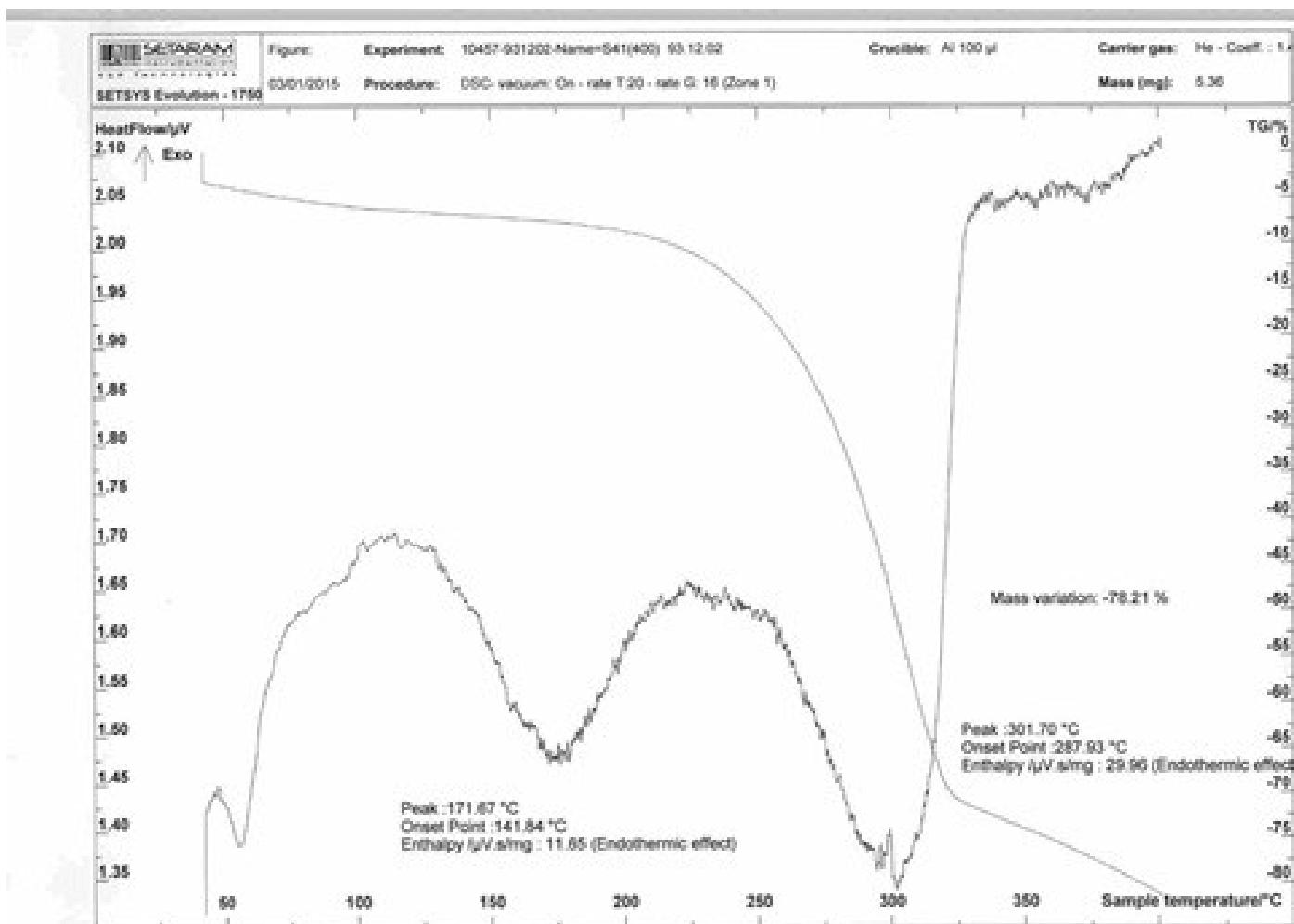
**S<sub>1</sub>** Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) of Sorbitol:MetHCl (2:1)



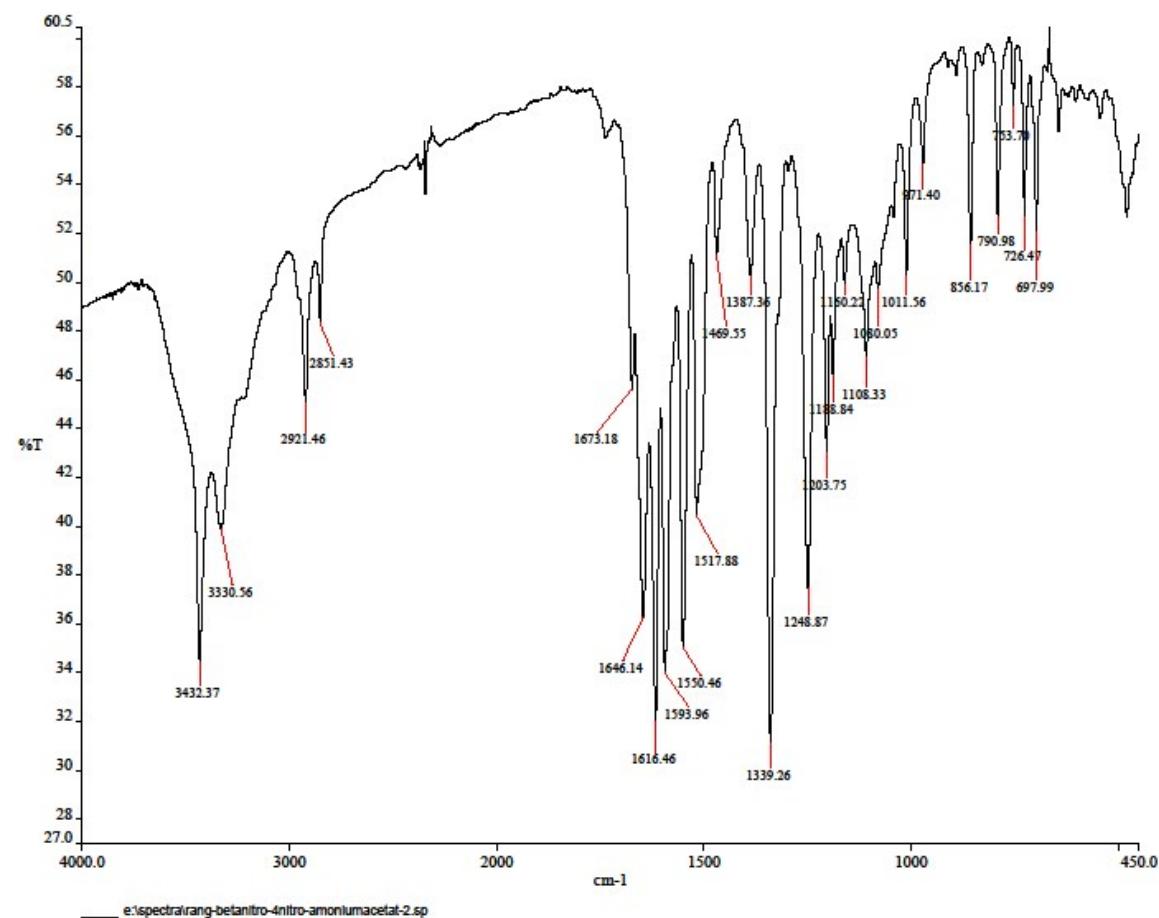
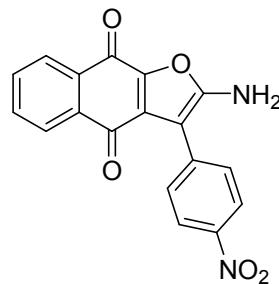
**S<sub>2</sub>** Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) of Sorbitol:MetHCl (3:1)



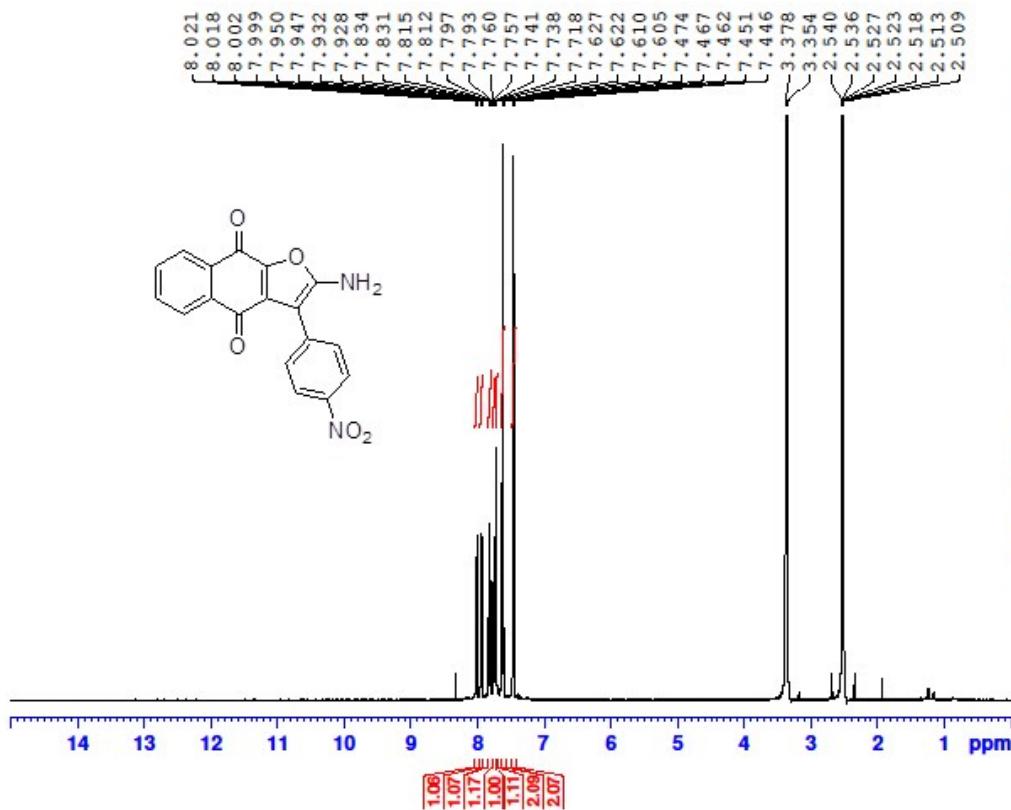
S<sub>3</sub> Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) of Sorbitol:MetHCl (4:1)



S<sub>4</sub> The IR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4d**)



S<sub>5</sub> The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione in DMSO-d<sub>6</sub> (**4d**)



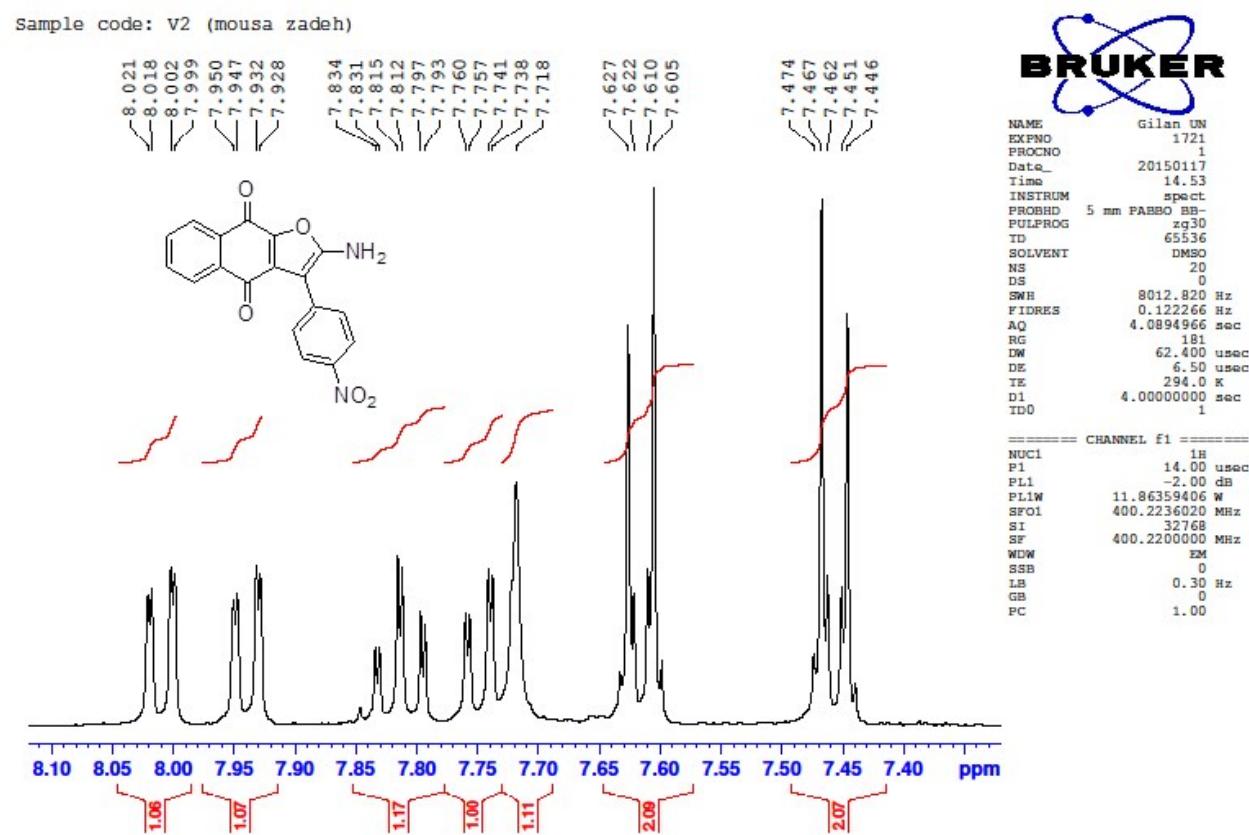
```

NAME          Gilan UN
EXPNO         1721
PROCNO        1
Date_        20150117
Time         14.53
INSTRUM       spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD            65536
SOLVENT      DMSO
NS             20
DS              0
SWH           8012.820 Hz
FIDRES       0.122266 Hz
AQ            4.0894966 sec
RG             1B1
DW            62.400 usec
DE            6.50 usec
TE            294.0 K
D1           4.0000000 sec
TDO            1

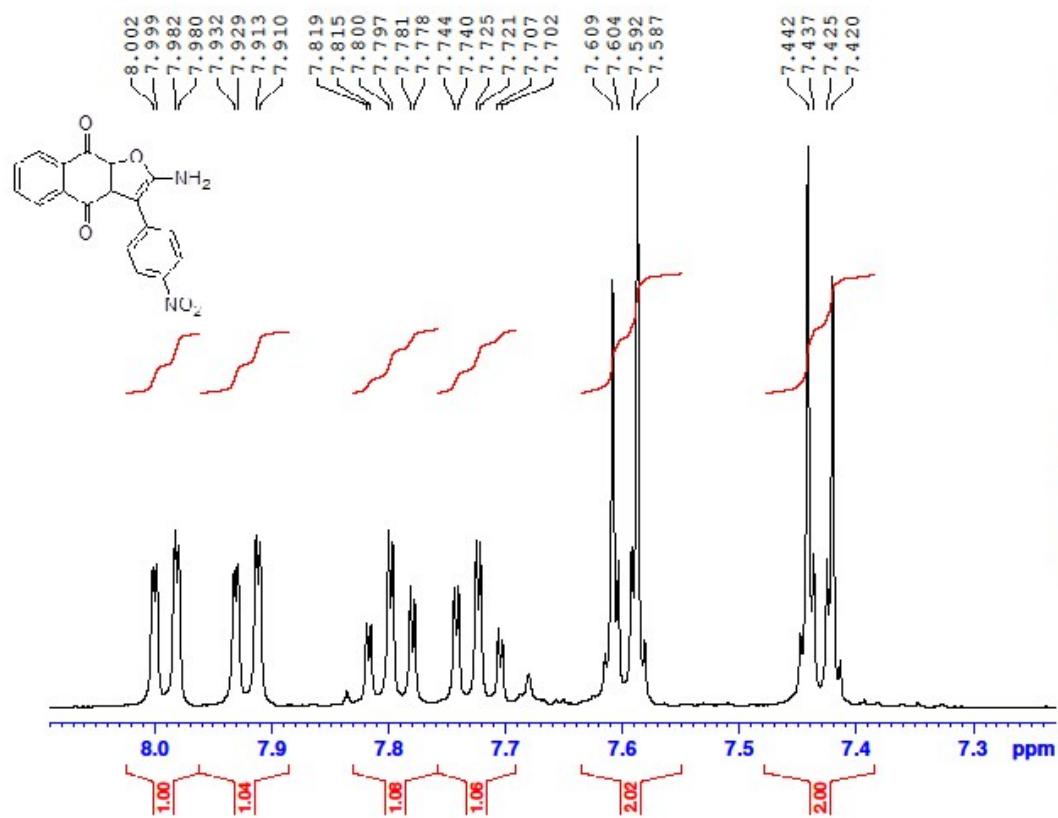
===== CHANNEL f1 =====
NUC1           1H
P1            14.00 usec
PL1           -2.00 dB
PL1W        11.86359406 W
SF01        400.2236020 MHz
SI             32768
SF           400.2200000 MHz
WDW            EM
SSB             0
LB            0.30 Hz
GB             0
PC            1.00

```

S<sub>5</sub> The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione in DMSO-d<sub>6</sub> (**4d**)



S<sub>6</sub> The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione in DMSO-d<sub>6</sub> + D<sub>2</sub>O (4d)



```

NAME Gilan UN
EXPNO 174B
PROCNO 1
Date_ 20150121
Time 16.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 293.9 K
D1 4.0000000 sec
TD0 1

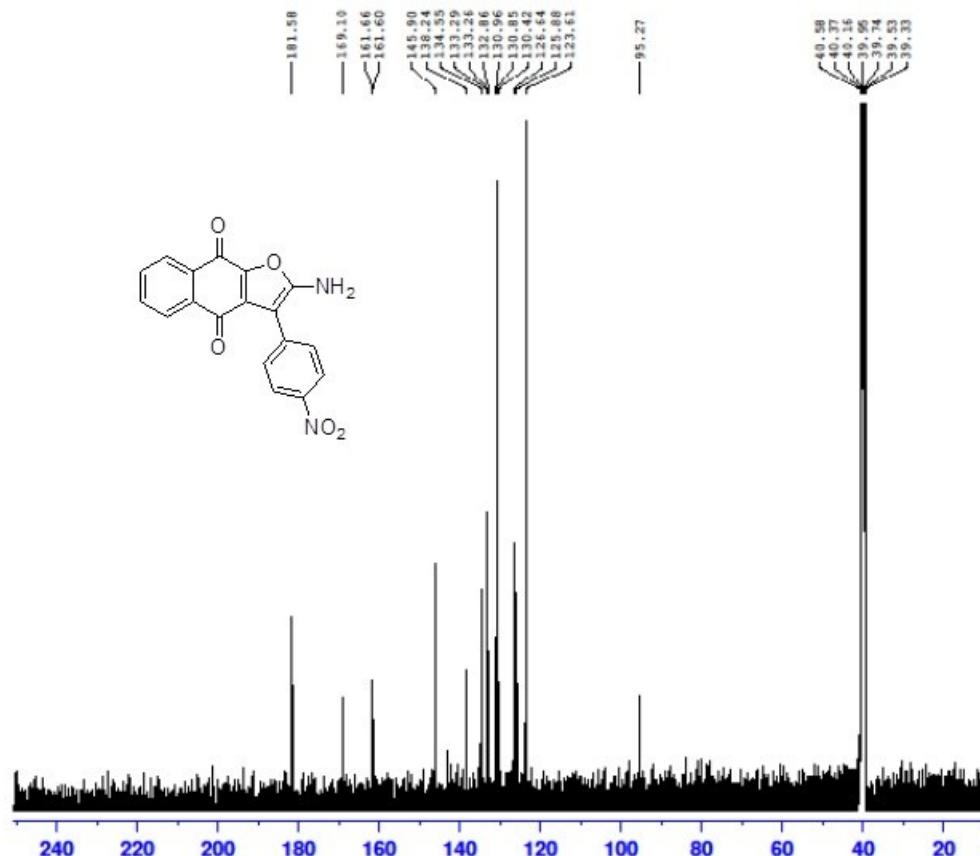
```

```

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SF01 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

S<sub>7</sub> The <sup>13</sup>C NMR spectrum of  
2-amino-3-(4-nitrophenyl)  
naphtho[2,3-*b*]furan-4,9-  
dione (**4d**)



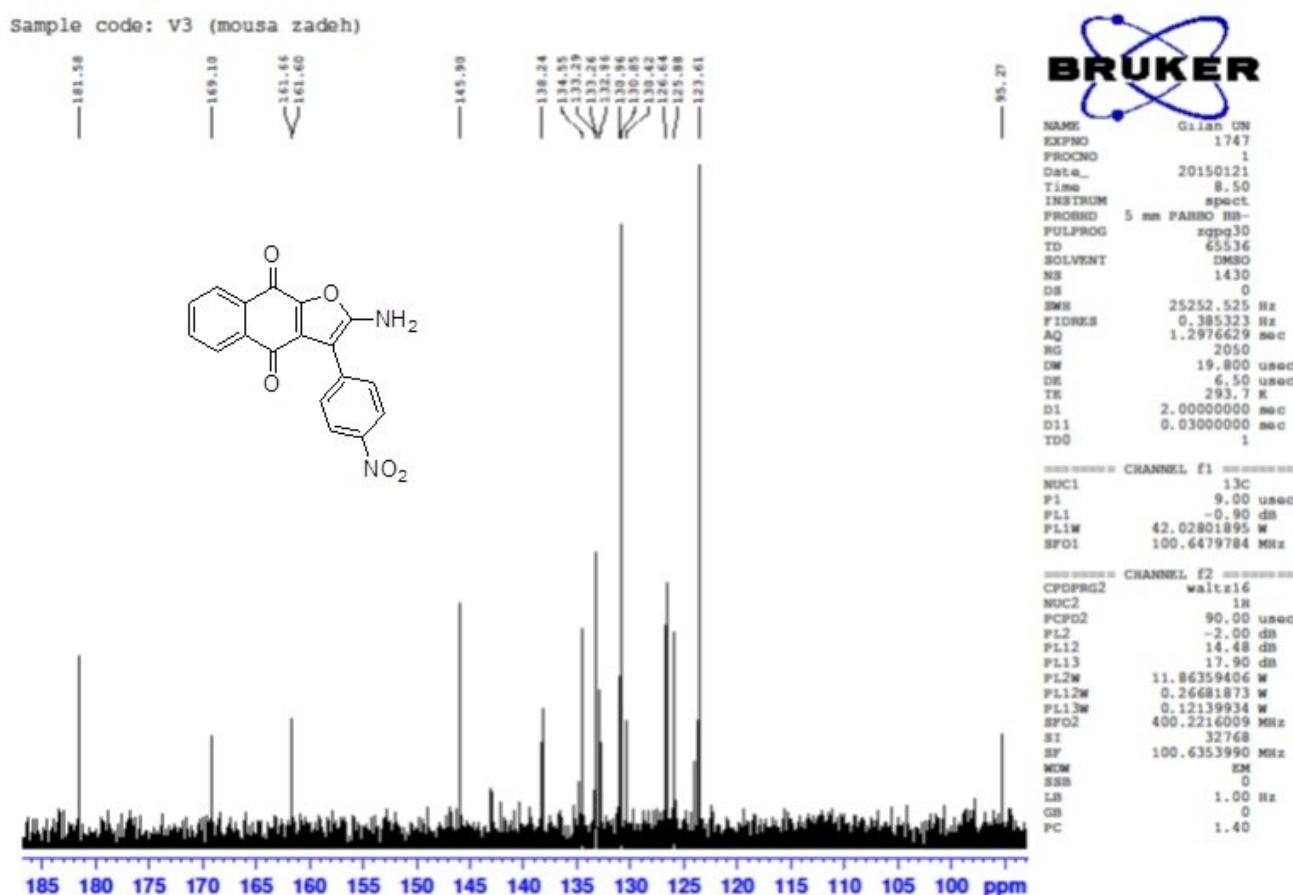
**BRUKER**

NAME Gilan UN  
EXPNO 1747  
PROCNO 1  
Date\_ 20150121  
Time 8.50  
INSTRUM spec  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
ID 65536  
SOLVENT DMSO  
NS 1430  
DS 0  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 2050  
DW 19.800 usec  
DE 6.50 usec  
TE 293.7 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

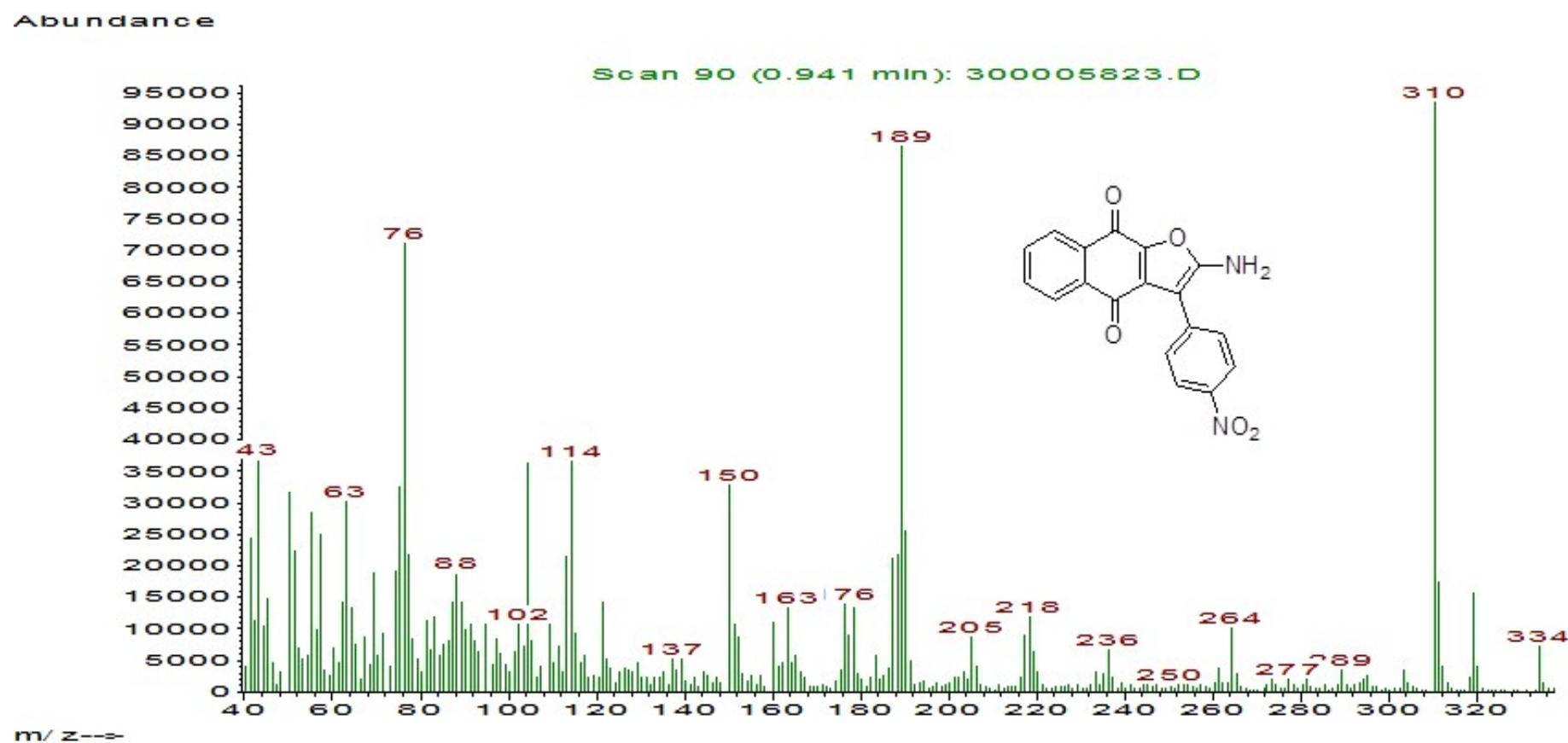
===== CHANNEL f1 =====  
NUC1 <sup>13</sup>C  
PI 9.00 usec  
PL1 -0.90 dB  
PL1W 42.02801895 MHz  
SFO1 100.6479784 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 <sup>1</sup>H  
PCPD2 90.00 usec  
PL2 -2.00 dB  
PL12 14.48 dB  
PL13 17.90 dB  
PL2W 11.86359406 MHz  
PL12W 0.26681873 MHz  
PL13W 0.12139934 MHz  
SFO2 400.2216009 MHz  
SI 32768  
SF 100.6353990 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

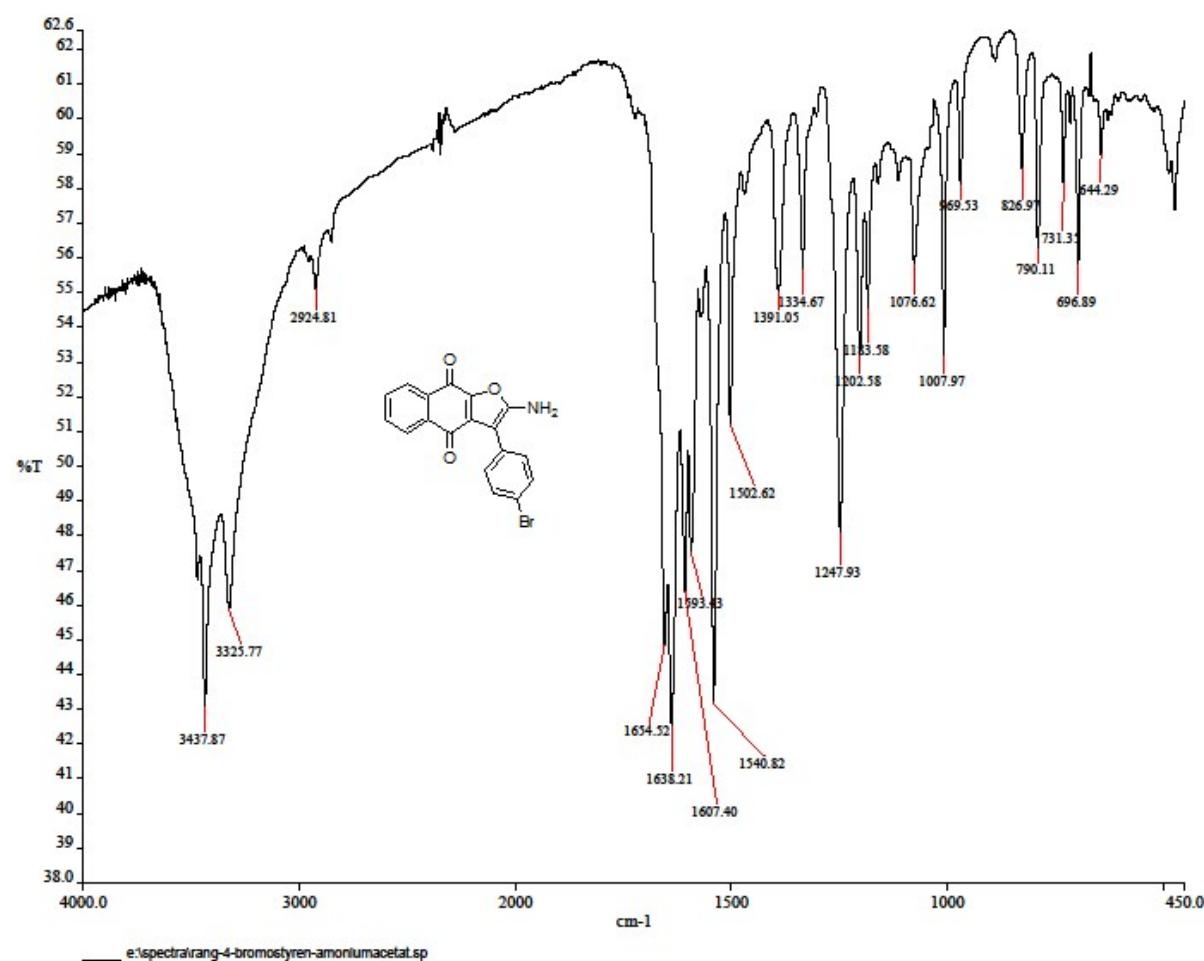
S<sub>7</sub> The <sup>13</sup>C NMR spectrum of  
2-amino-3-(4-nitrophenyl)  
naphtho[2,3-*b*]furan-4,9-  
dione (**4d**)



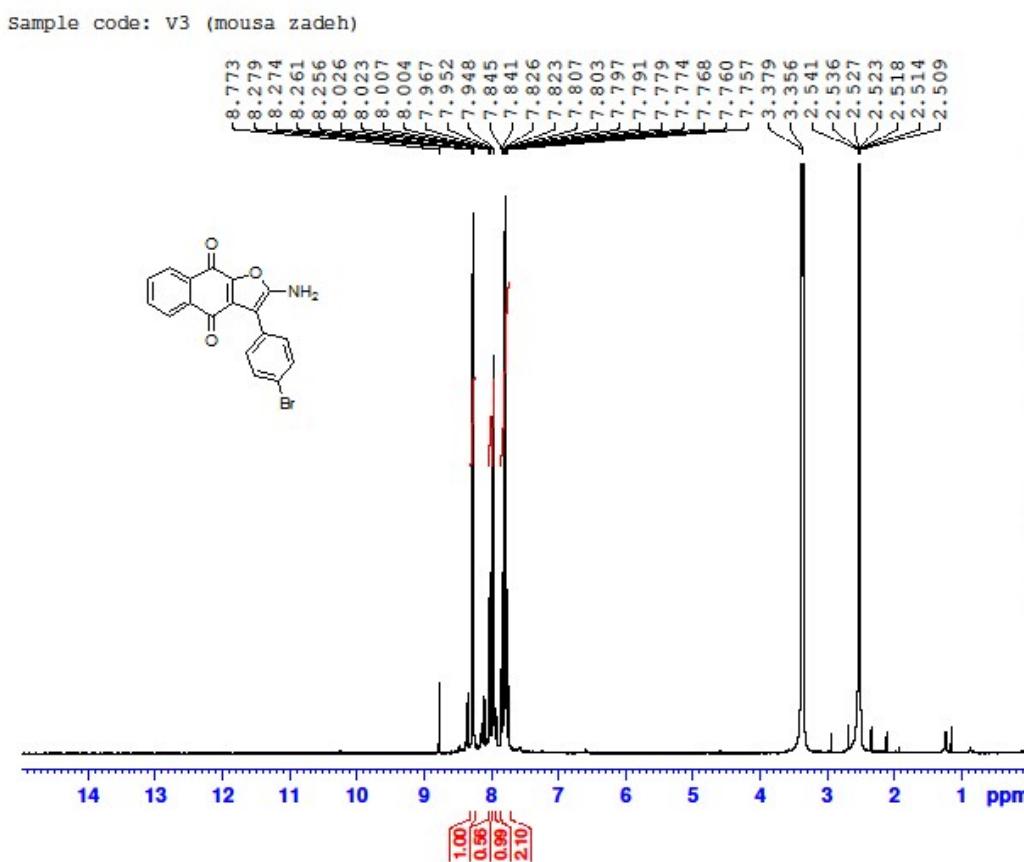
S<sub>8</sub> The Mass spectrum of 2-amino-3-(4-nitrophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4d**)



**S<sub>9</sub>** The IR spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (**4g**)



**S<sub>10</sub>** The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (4g)



**BRUKER**

```

NAME      Gilan UN
EXPNO     1720
PROCNO    1
Date_     20150117
Time      14.43
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT   DMSO
NS        20
DS        0
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ        4.089496 sec
RG        181
DW        62.400 usec
DE        6.50 usec
TE        294.0 K
D1        4.00000000 sec
TDO      1

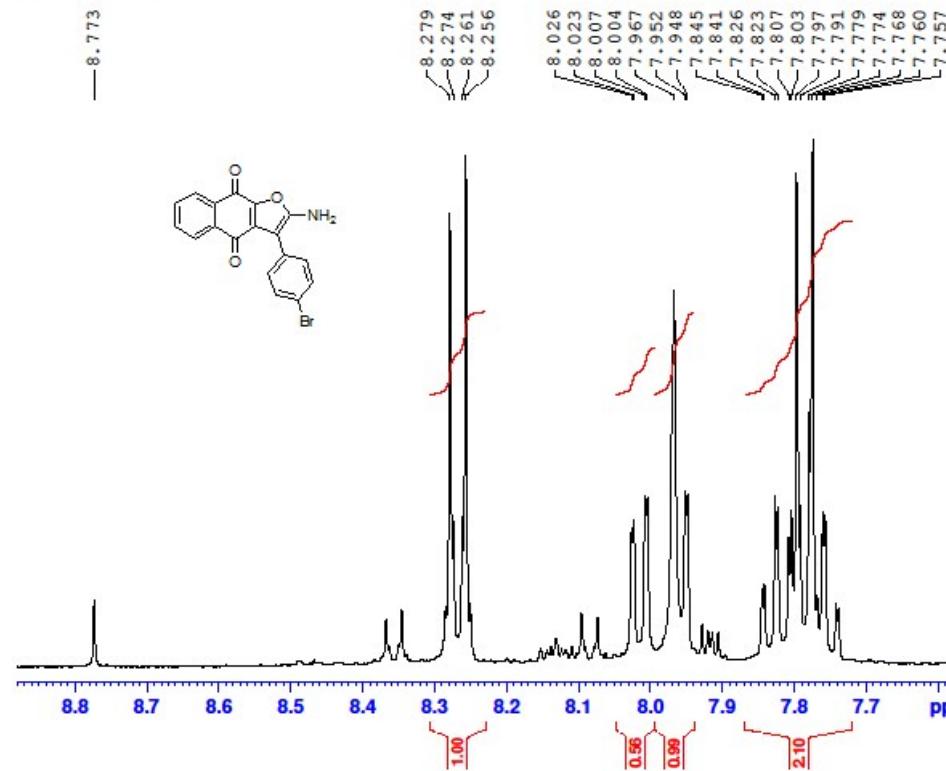
===== CHANNEL f1 =====

NUC1      1H
P1        14.00 usec
PL1      -2.00 dB
PL1W    11.86359406 W
SFO1    400.2236020 MHz
SI        32768
SF        400.2200000 MHz
WDW      EM
SSB      0
LB        0.30 Hz
GB      0
PC        1.00

```

**S<sub>10</sub>** The <sup>1</sup>H NMR spectrum of 2-amino-3-(4-bromophenyl)naphtho[2,3-*b*]furan-4,9-dione (4g)

Sample code: v3 (mousa zadeh)



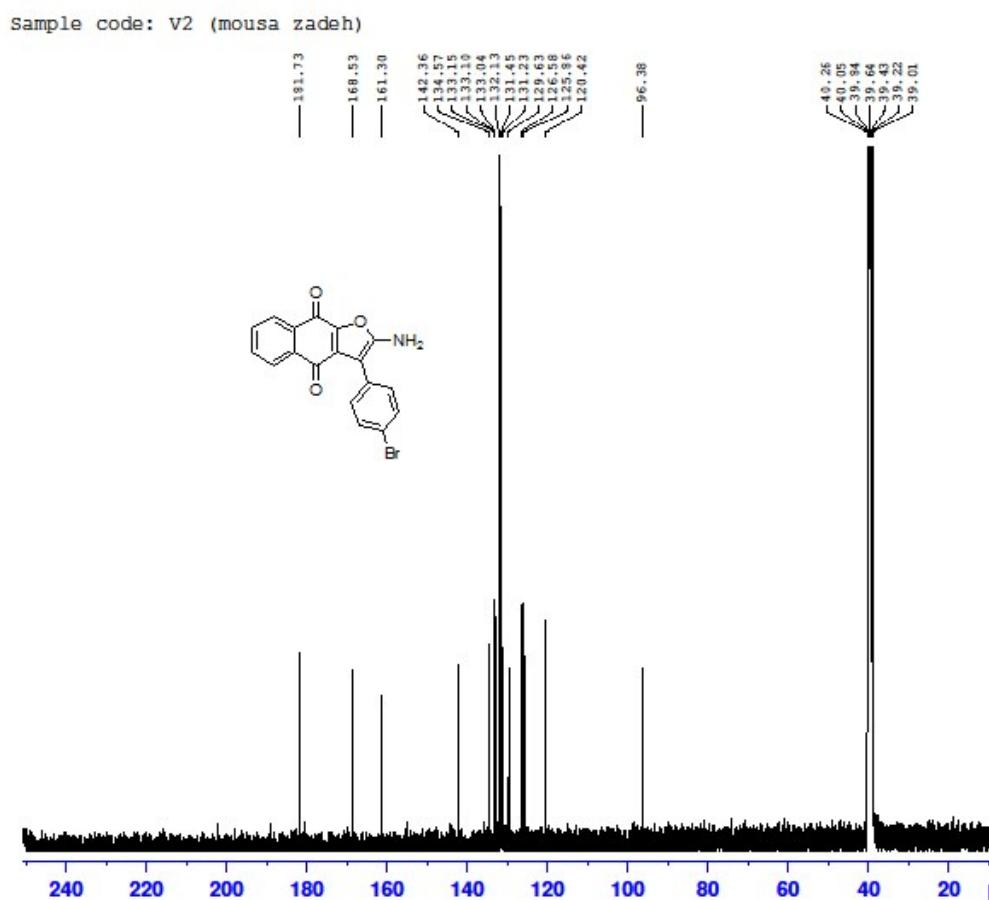
```

NAME Gilan UN
EXPNO 1720
PROCNO 1
Date_ 20150117
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 4.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SF01 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

S<sub>11</sub> The <sup>13</sup>C NMR spectrum of  
2-amino-3-(4-bromophenyl)  
naphtha[2,3-*b*]furan-4,9-dione  
(4g)

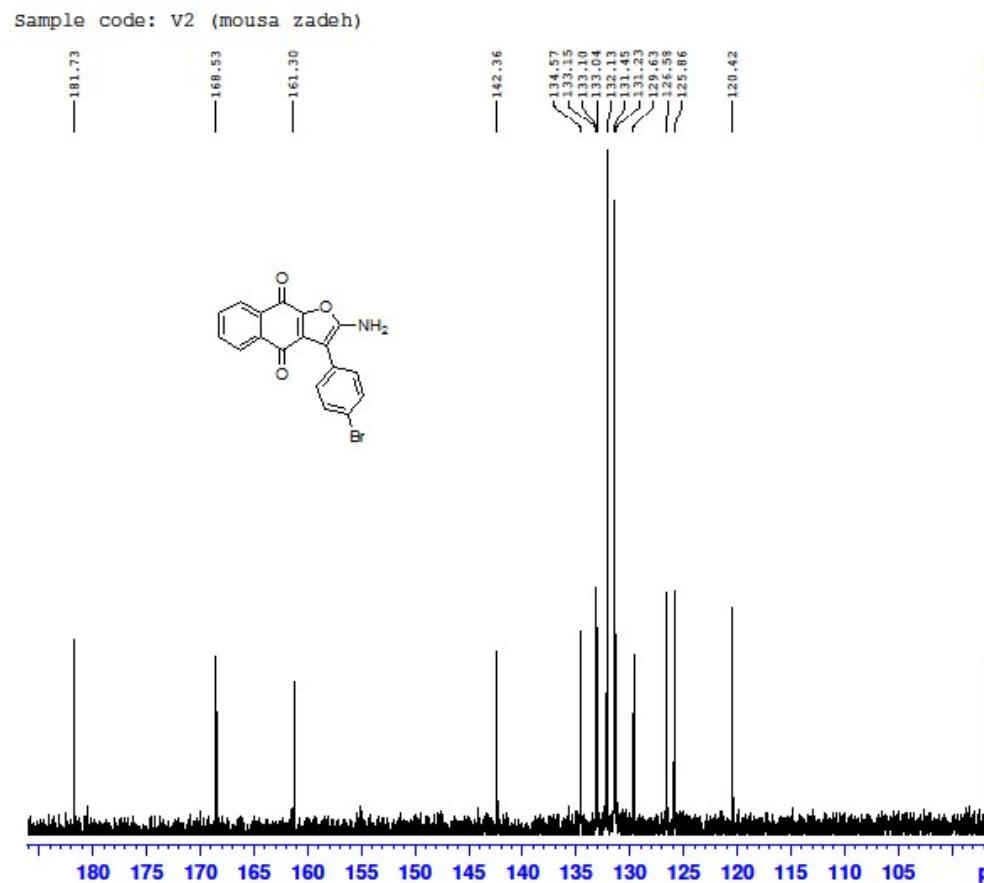


NAME Gilan UN  
EXPNO 1749  
PROCNO 1  
Date 20150121  
Time 16.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8192  
DS 0  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 2050  
DW 19.800 usec  
DE 6.50 usec  
TE 294.3 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 <sup>13</sup>C  
P1 9.00 usec  
PL1 -0.90 dB  
PL1W 42.02801895 W  
SFO1 100.6479784 MHz

===== CHANNEL f2 =====  
CPDPGR2 waltz16  
NUC2 <sup>1</sup>H  
PCPD2 90.00 usec  
PL2 -2.00 dB  
PL12 14.48 dB  
PL13 17.90 dB  
PL2W 11.86359406 W  
PL12W 0.26681873 W  
PL13W 0.12139934 W  
SFO2 400.2216009 MHz  
SI 32768  
SF 100.6353990 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

**S<sub>11</sub>** The <sup>13</sup>C NMR spectrum of  
2-amino-3-(4-bromophenyl)  
naphtha[2,3-*b*]furan-4,9-dione  
(4g)



**BRUKER**

NAME Gilan UN  
 EXPNO 1749  
 PROCNO 1  
 Date\_ 20150121  
 Time 16.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpp3D  
 TD 65536  
 SOLVENT DMSO  
 NS 8192  
 DS 0  
 SWH 25252.525 Hz  
 FIDRES 0.385323 Hz  
 AQ 1.2976629 sec  
 RG 2050  
 DW 19.800 usec  
 DE 6.50 usec  
 TE 294.3 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 T0 0

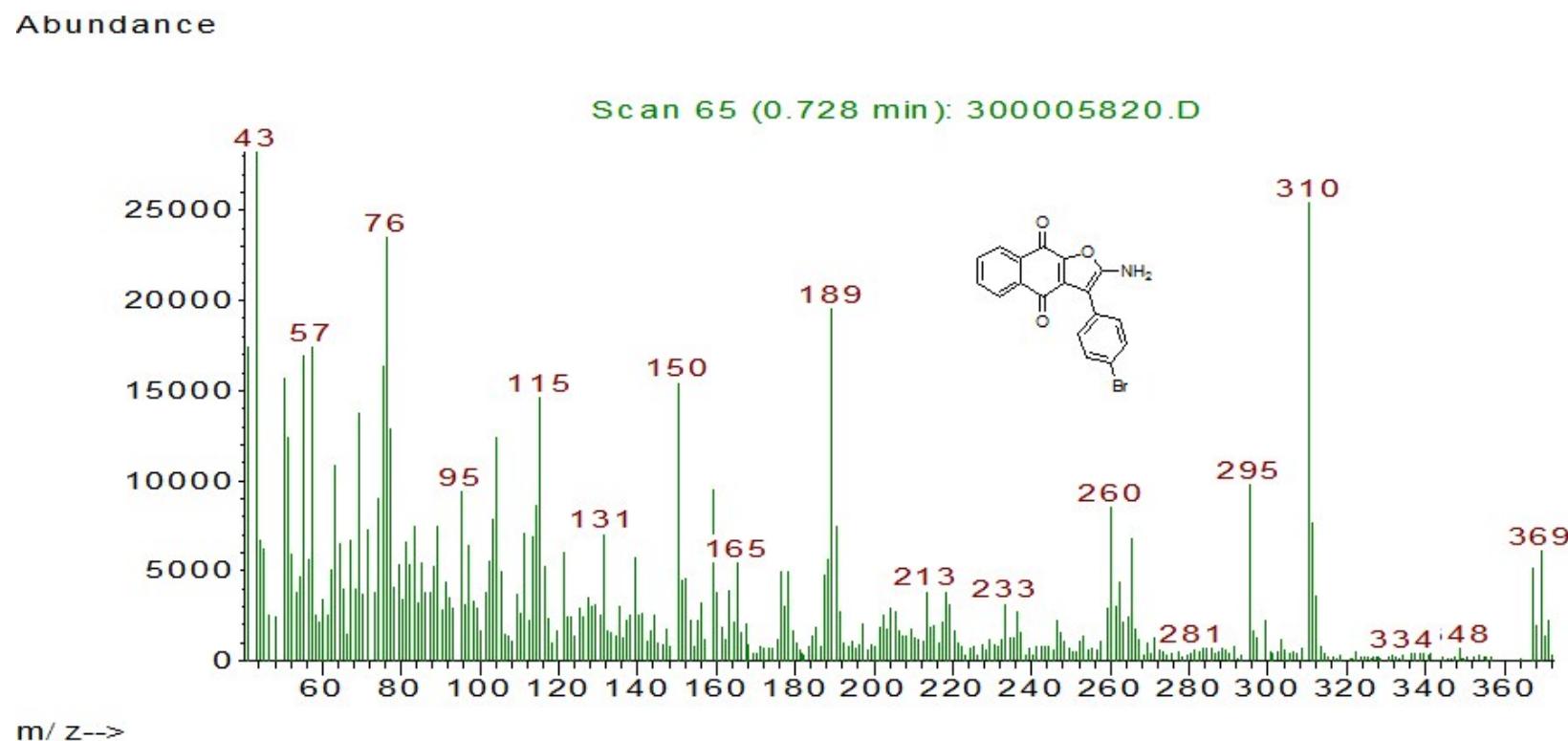
===== CHANNEL f1 =====

NUC1 <sup>13</sup>C  
 P1 9.00 usec  
 PL1 -0.90 dB  
 PL1W 42.02801895 W  
 SFO1 100.6479784 MHz

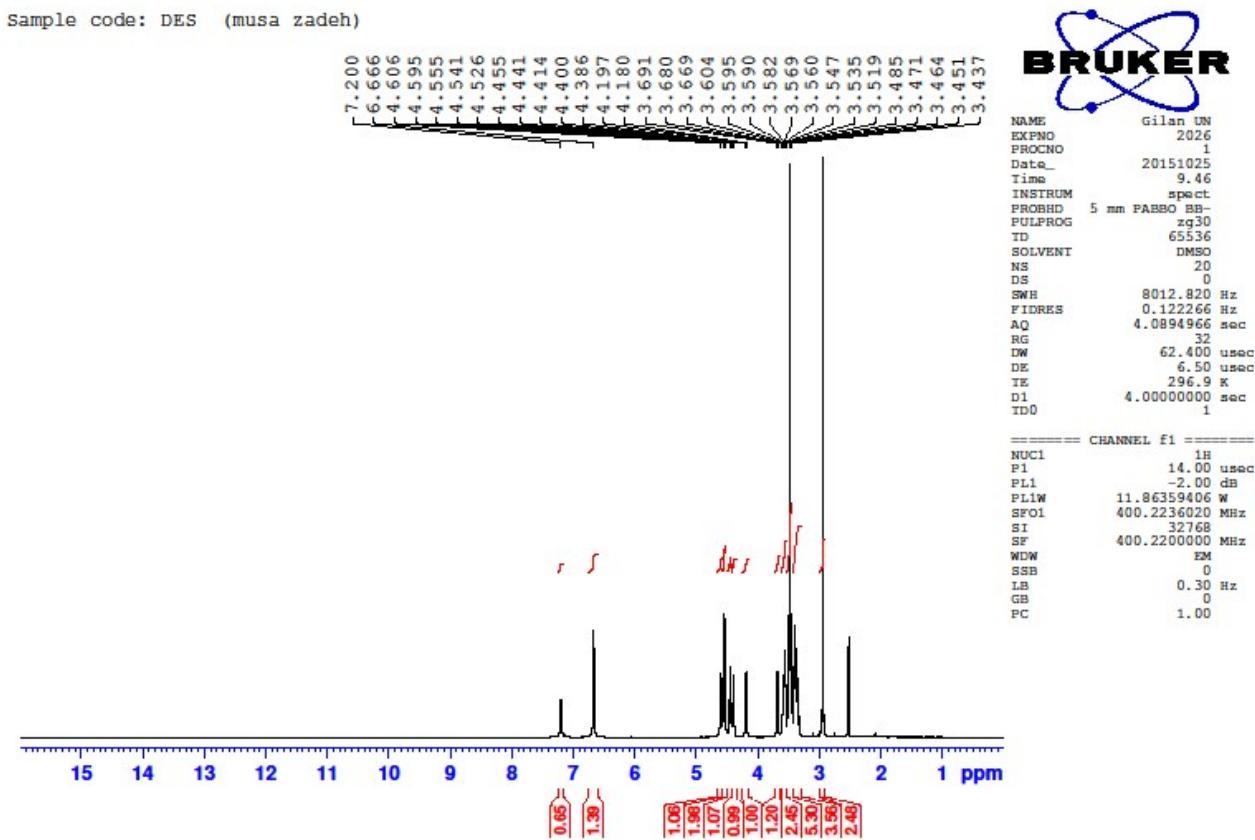
===== CHANNEL f2 =====

CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 90.00 usec  
 PL2 -2.00 dB  
 PL12 14.48 dB  
 PL13 17.90 dB  
 PL2W 11.86359406 W  
 PL12W 0.26681873 W  
 PL13W 0.12139934 W  
 SFO2 400.2216009 MHz  
 SI 32768  
 SF 100.6353990 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

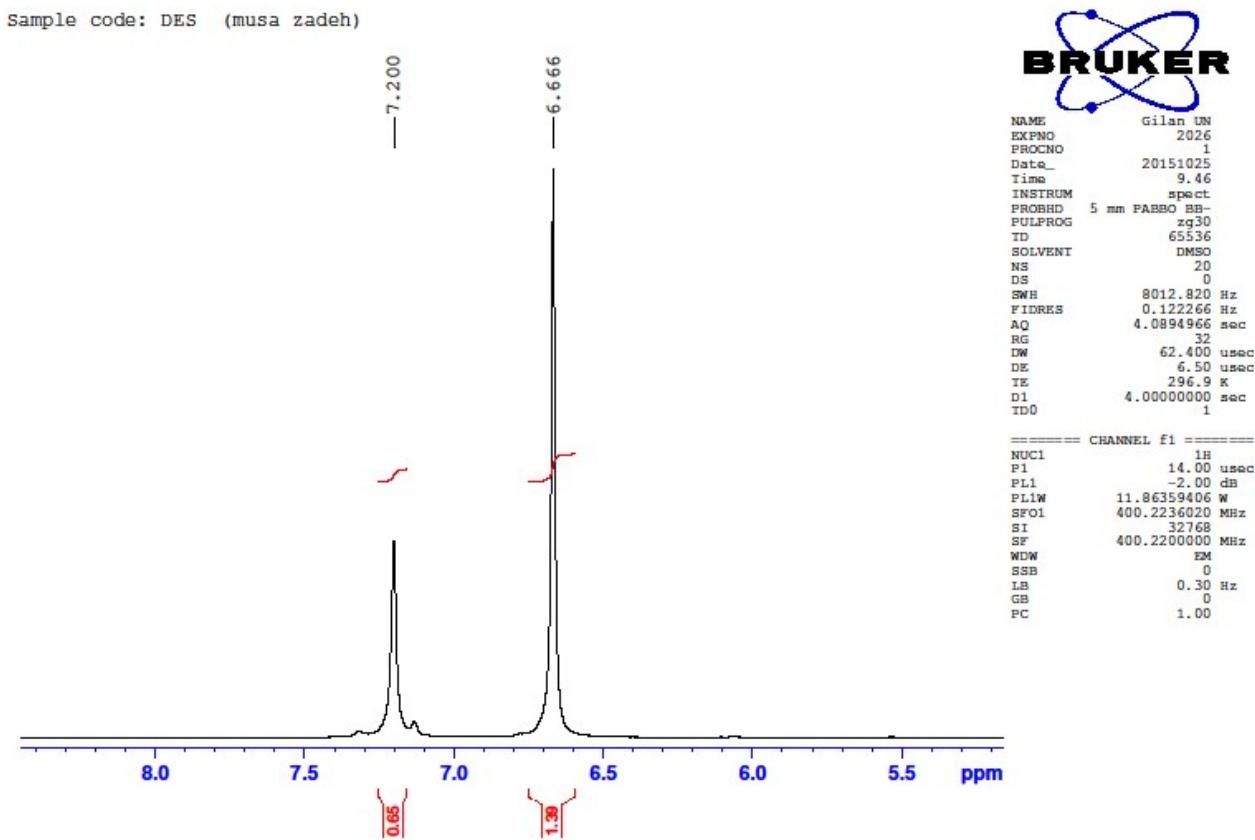
S<sub>12</sub> The Mass spectrum of 2-amino-3-(4-bromophenyl) naphtha [2,3-*b*]furan-4,9-dione (**4g**)



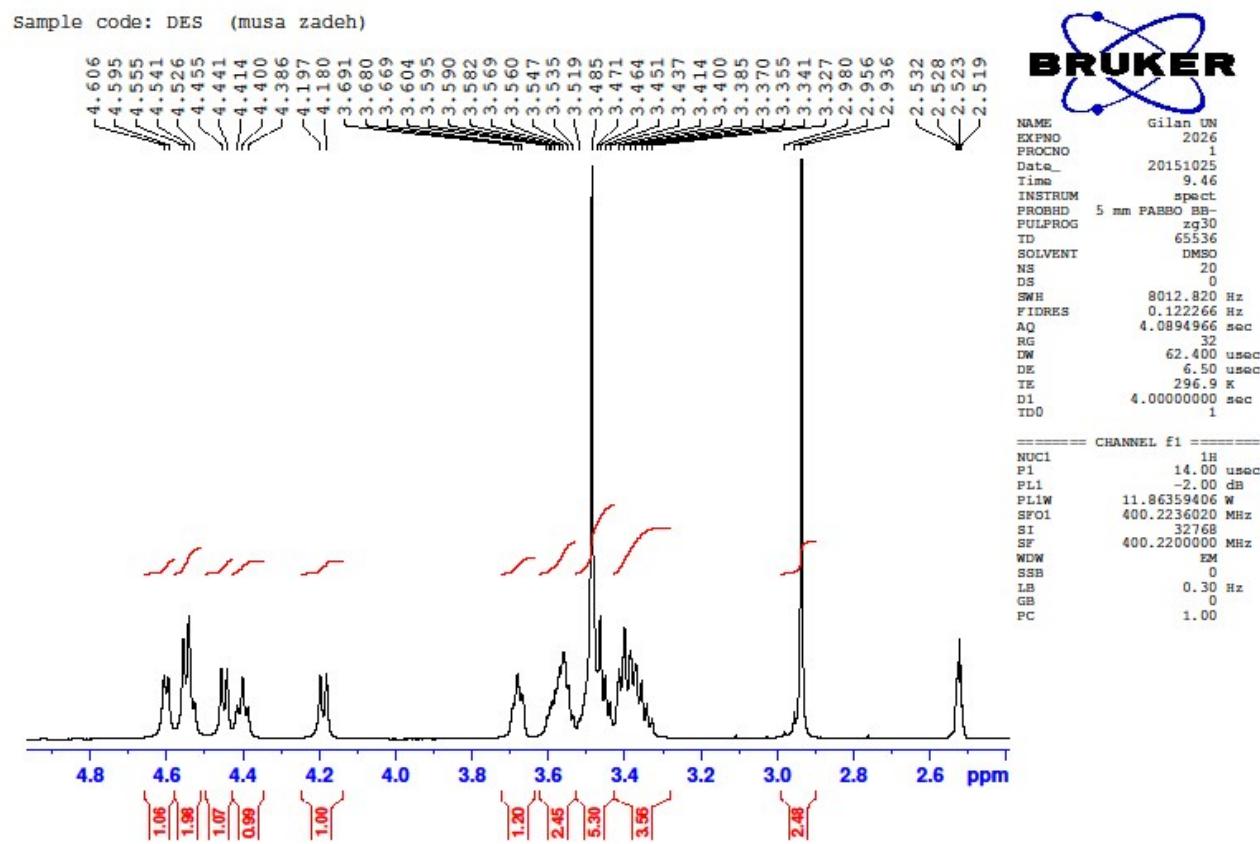
S<sub>13</sub> The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl



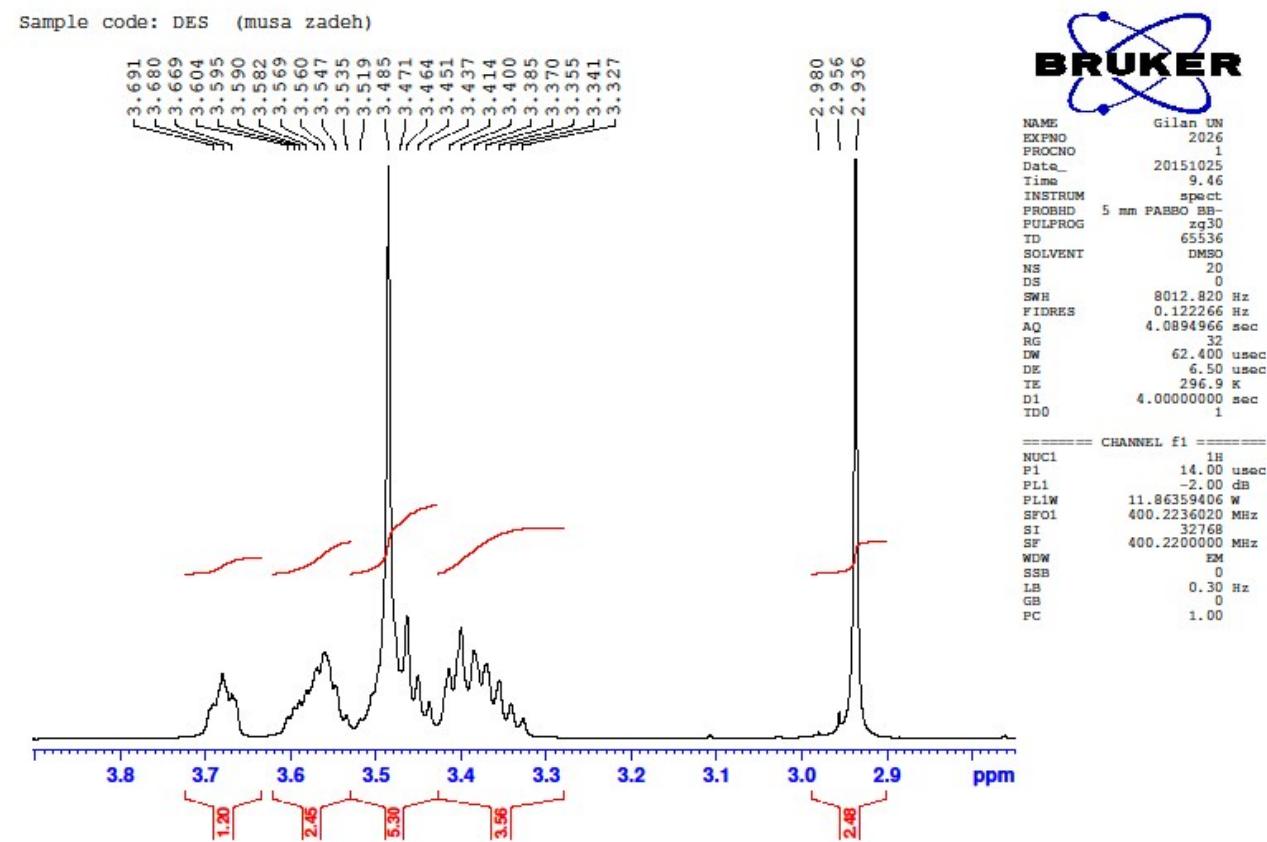
S<sub>13</sub> The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl



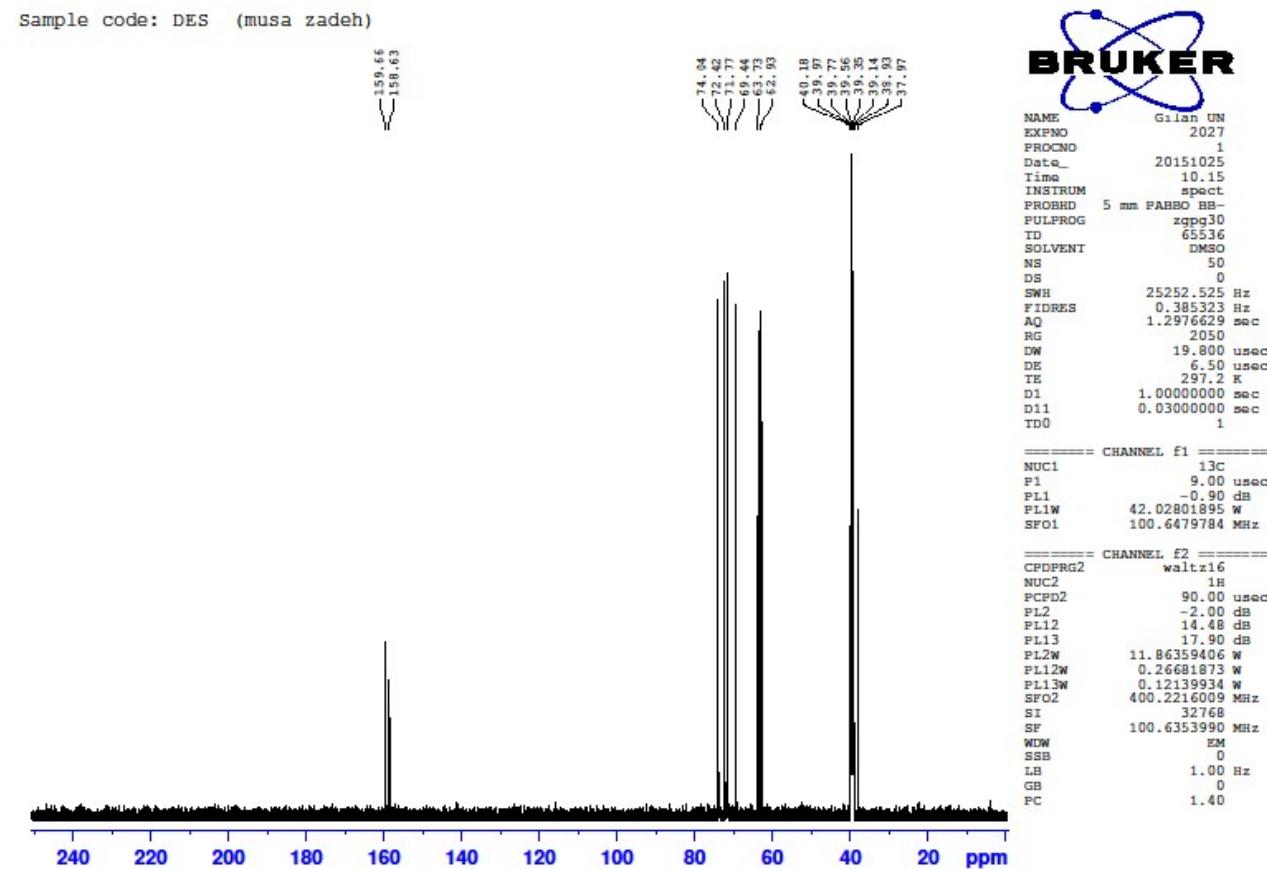
S<sub>13</sub> The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl



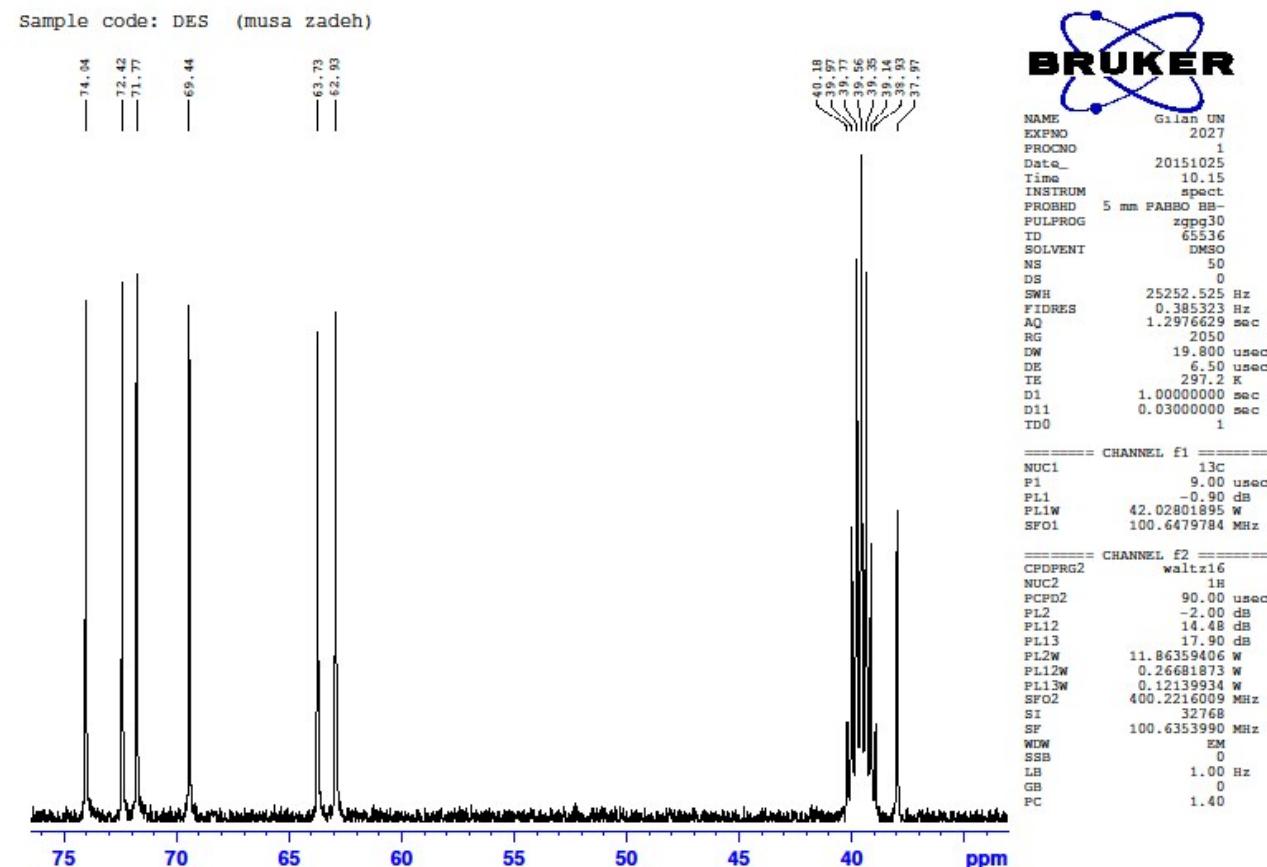
S<sub>13</sub> The <sup>1</sup>H NMR spectrum of 3:1 S:MetHCl



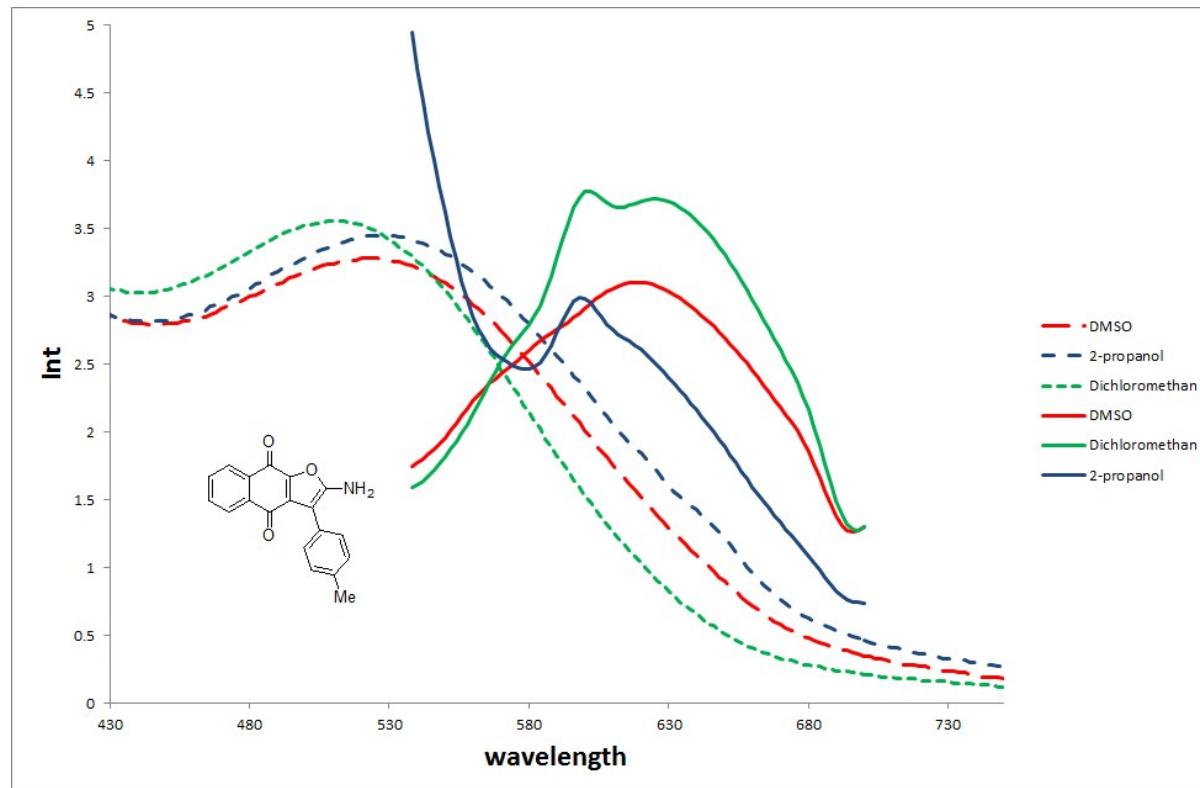
S<sub>14</sub> The <sup>13</sup>C NMR spectrum of 3:1 S:MetHCl



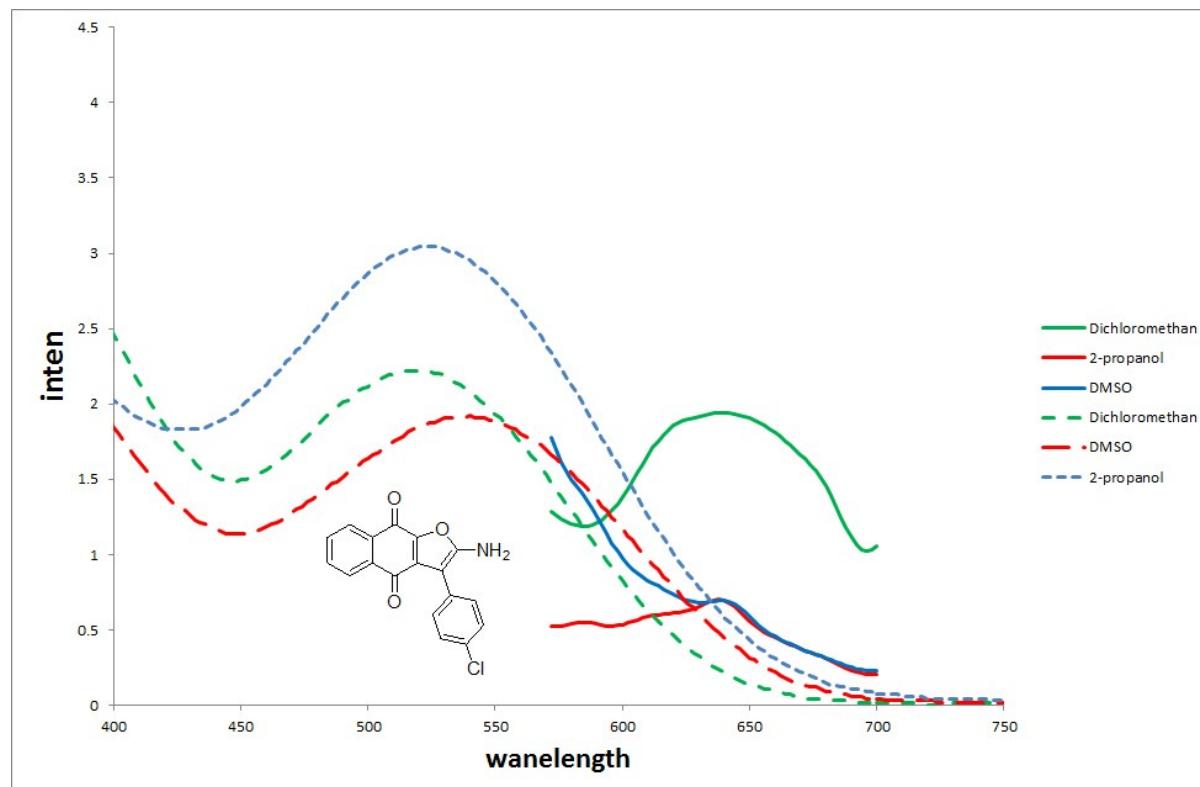
S<sub>14</sub> The <sup>13</sup>C NMR spectrum of 3:1 S:MetHCl



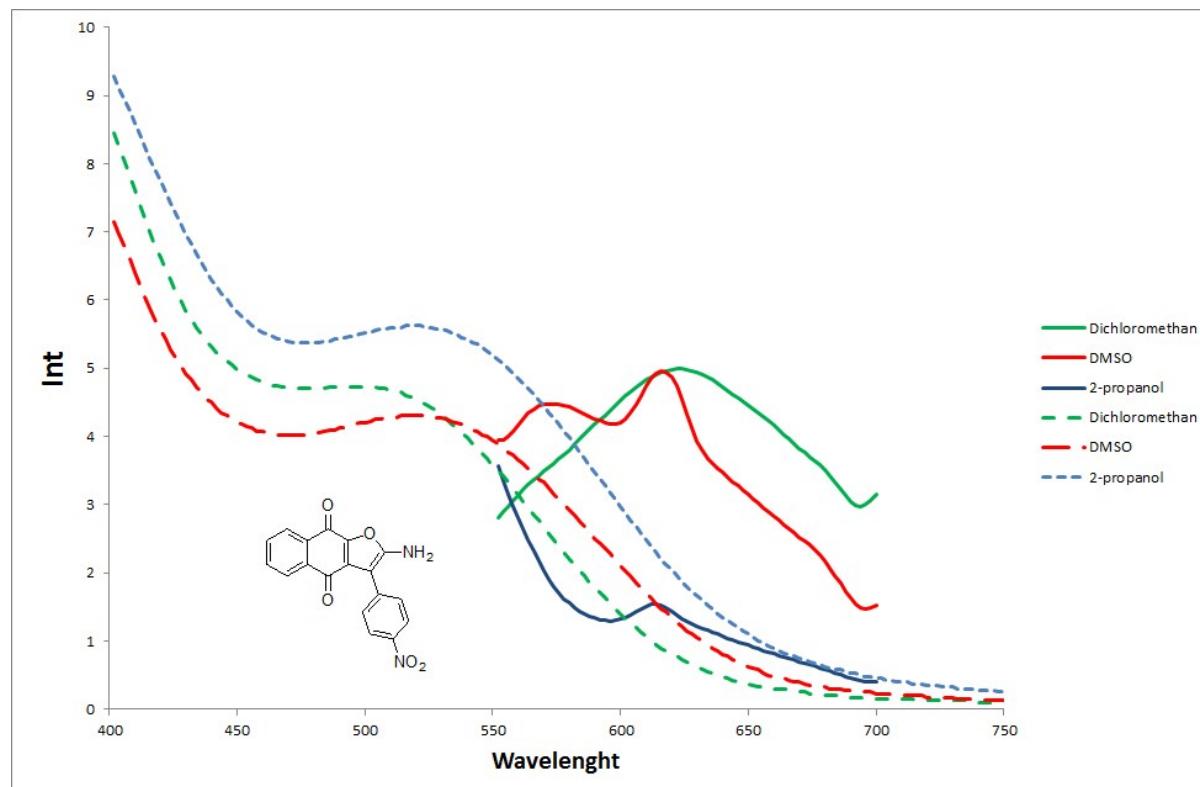
S<sub>15</sub> The absorption (dashed) and emission (solid) spectra for compound 4b



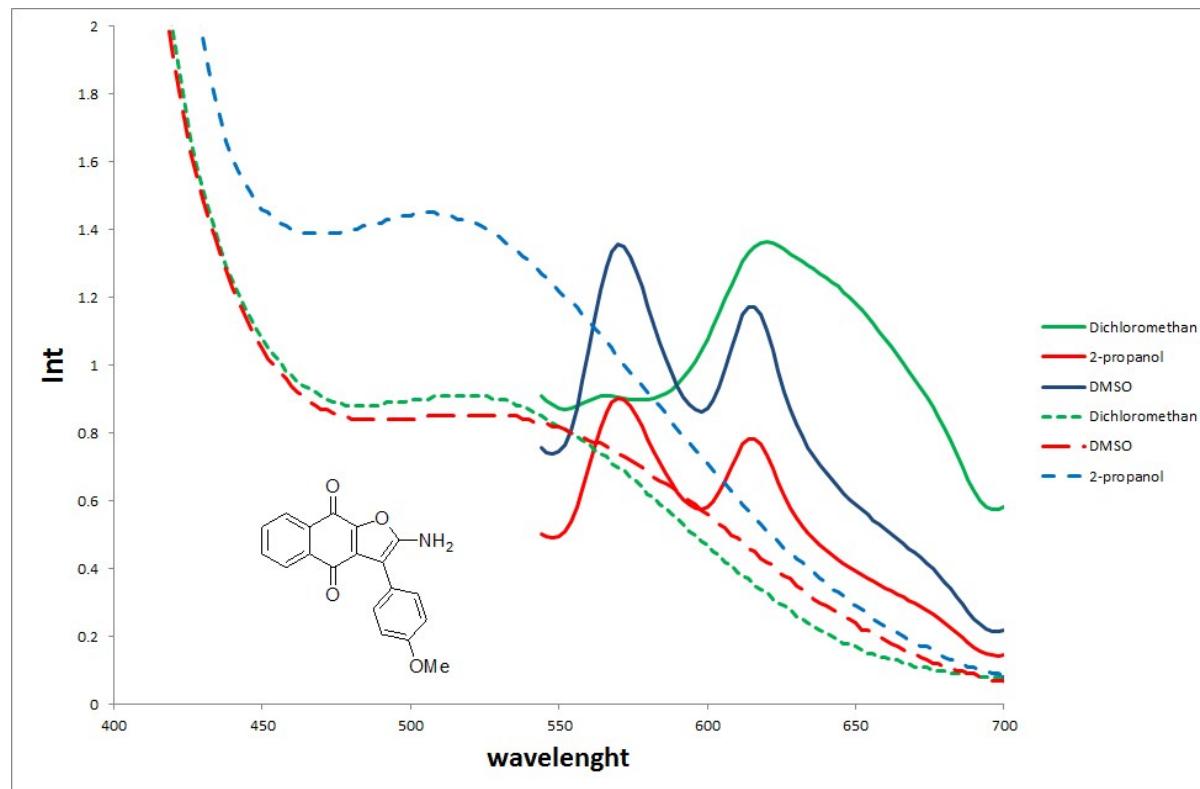
S<sub>16</sub> The absorption (dashed) and emission (solid) spectra for compound 4c



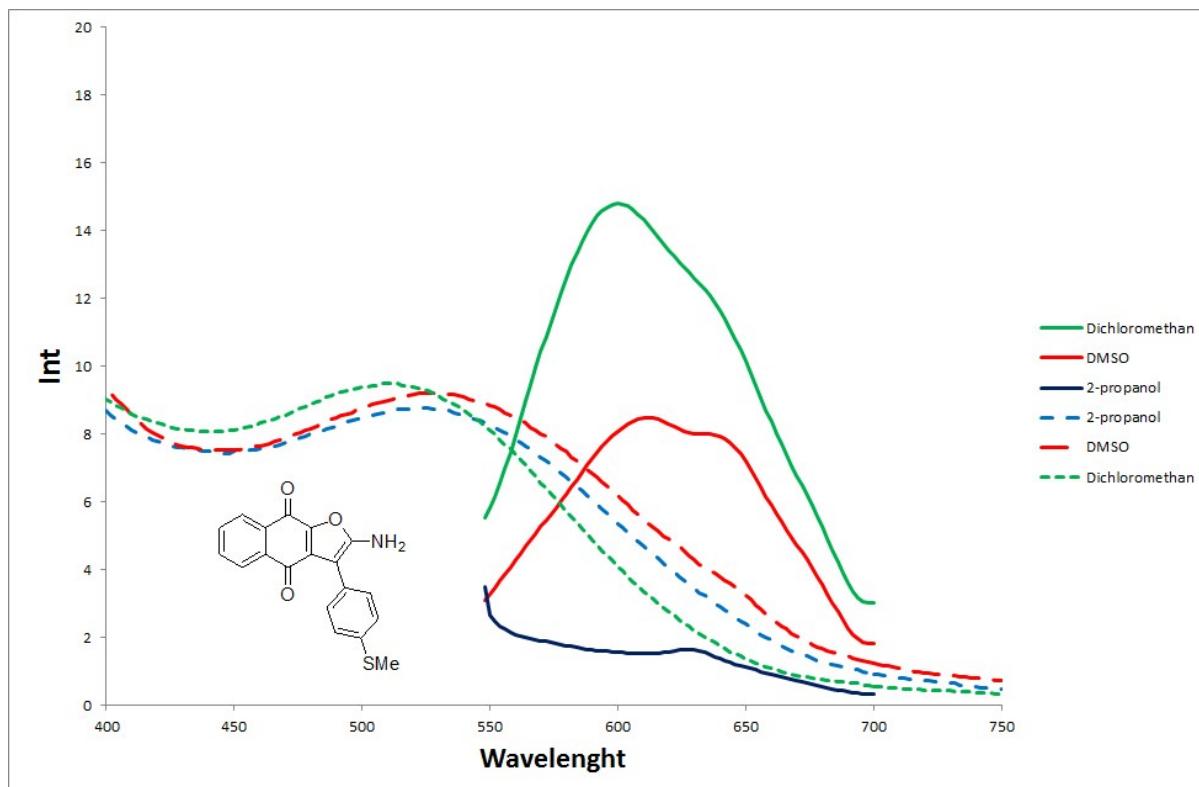
S<sub>17</sub> The absorption (dashed) and emission (solid) spectra for compound 4d



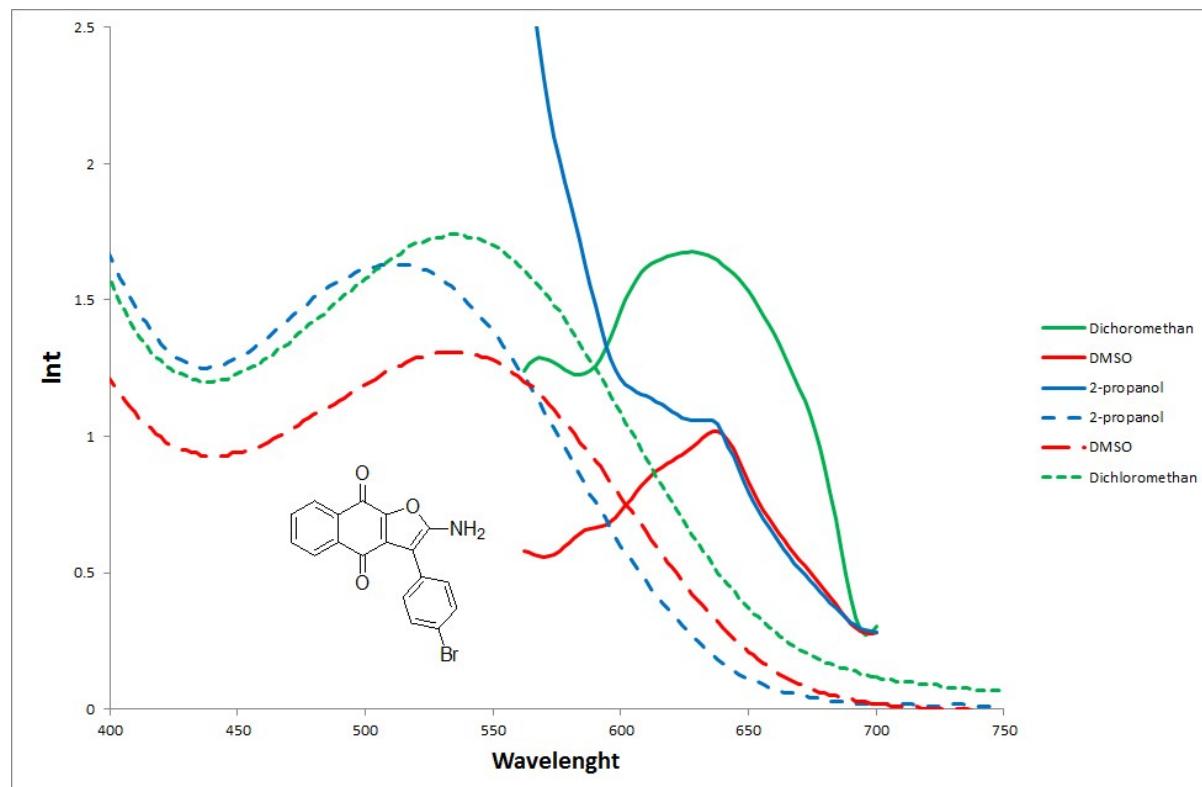
S<sub>18</sub> The absorption (dashed) and emission (solid) spectra for compound 4e



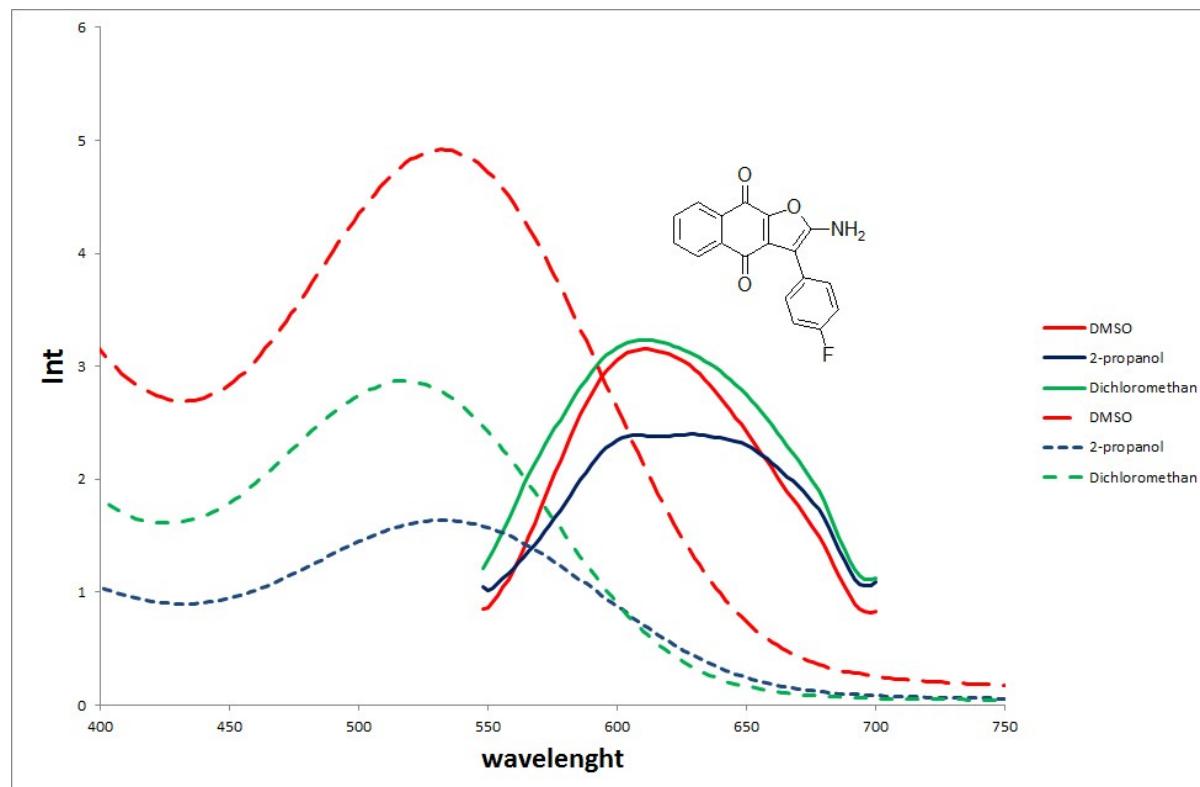
S<sub>19</sub> The absorption (dashed) and emission (solid) spectra for compound 4f



S<sub>20</sub> The absorption (dashed) and emission (solid) spectra for compound 4g



S<sub>21</sub> The absorption (dashed) and emission (solid) spectra for compound 4h



S<sub>22</sub> The absorption (dashed) and emission (solid) spectra for compound 4i

