

## Supplementary Material

### Synthesis of novel star-shaped molecules based on 1,3,5-triazine core linked to different heterocyclic systems as novel hybrid molecules

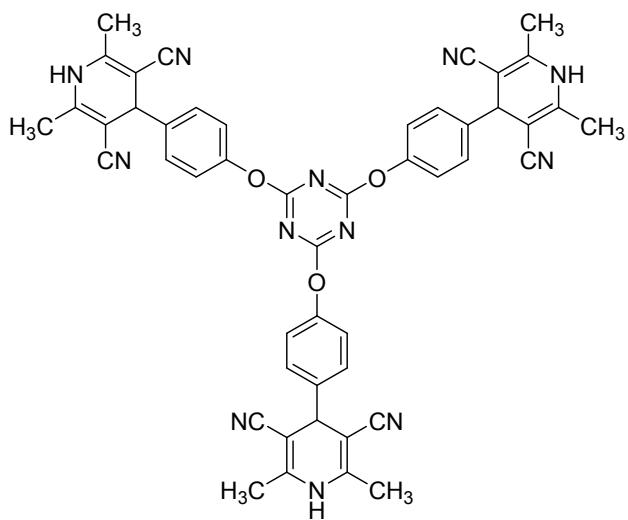
Hadeer M. Diab, Mostafa E. Salem, Ismail A. Abdelhamid\* and Ahmed H. M. Elwahy\*

*Department of Chemistry, Faculty of Science, Cairo University, Giza 12613, Egypt*

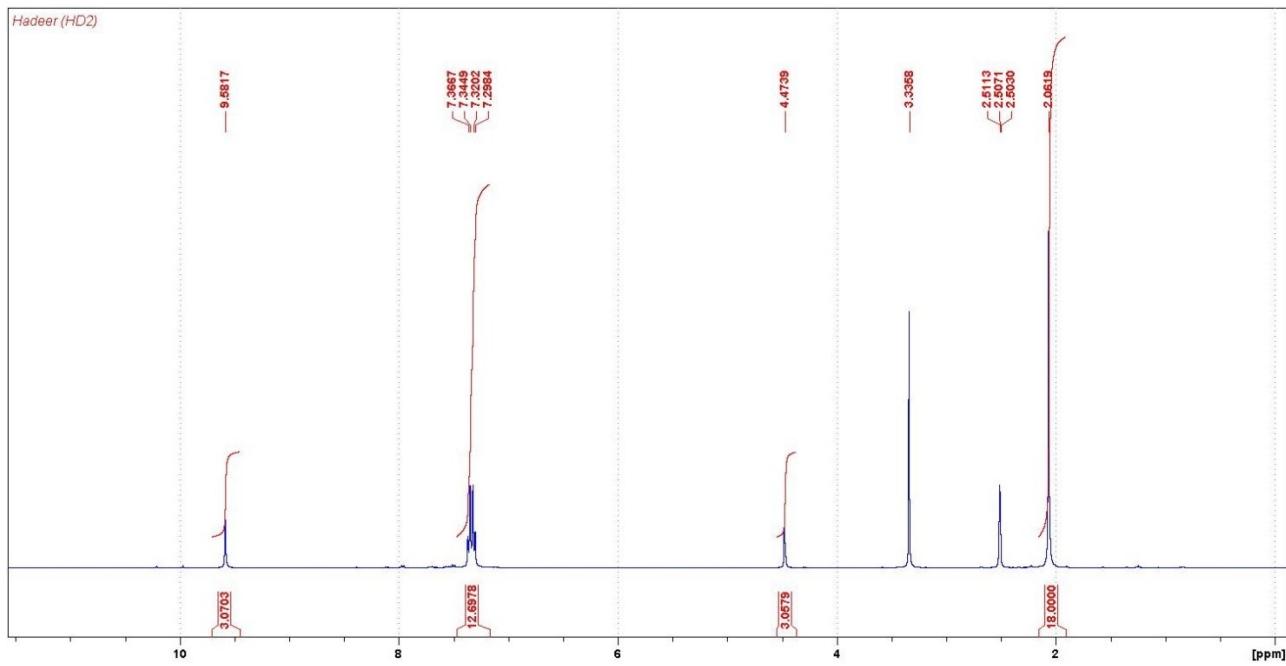
*Email: [ismail\\_shafy@yahoo.com](mailto:ismail_shafy@yahoo.com), [aelwahy@hotmail.com](mailto:aelwahy@hotmail.com)*

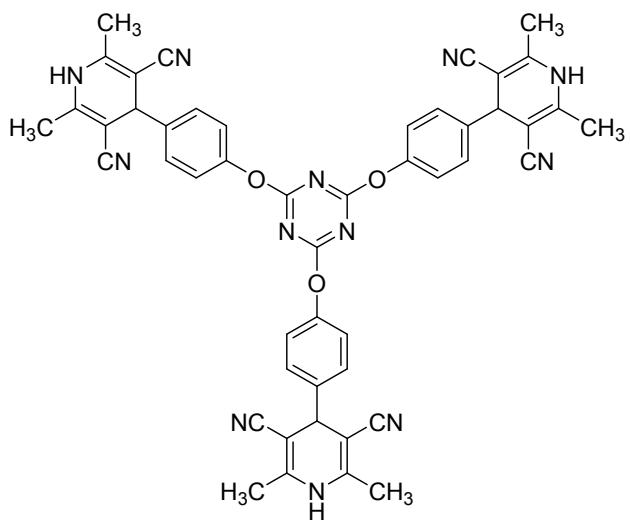
### Table of Contents

1. IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for synthesized compounds

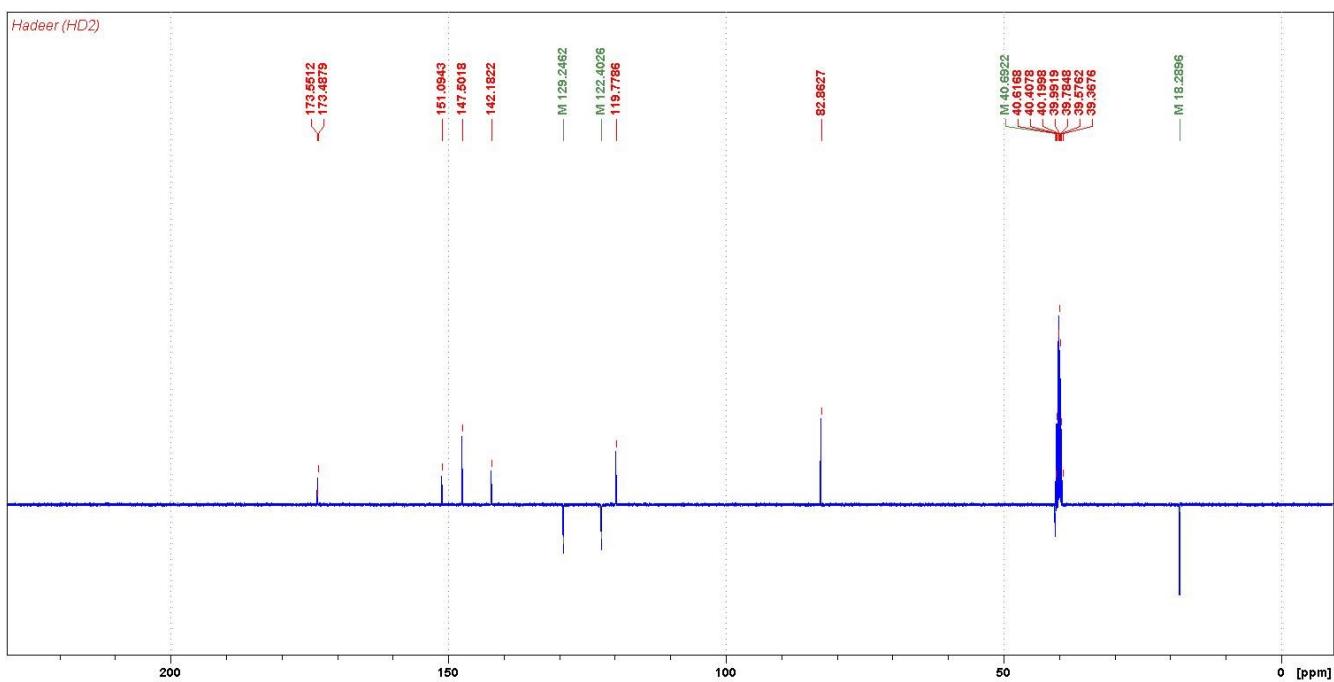


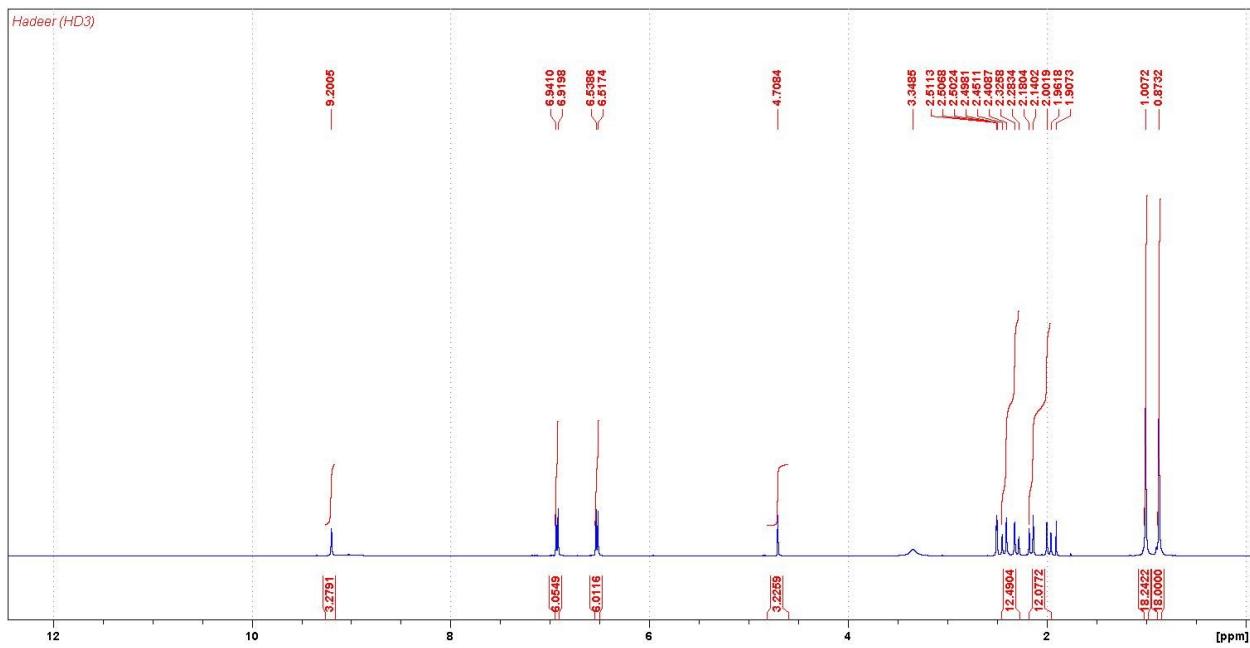
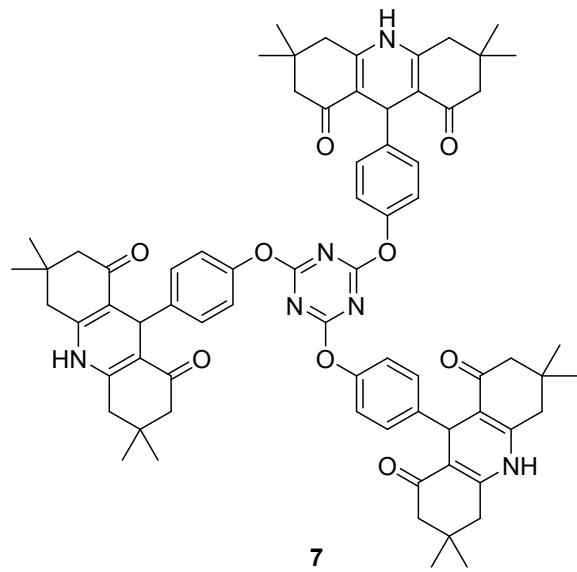
The  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) of compound 5



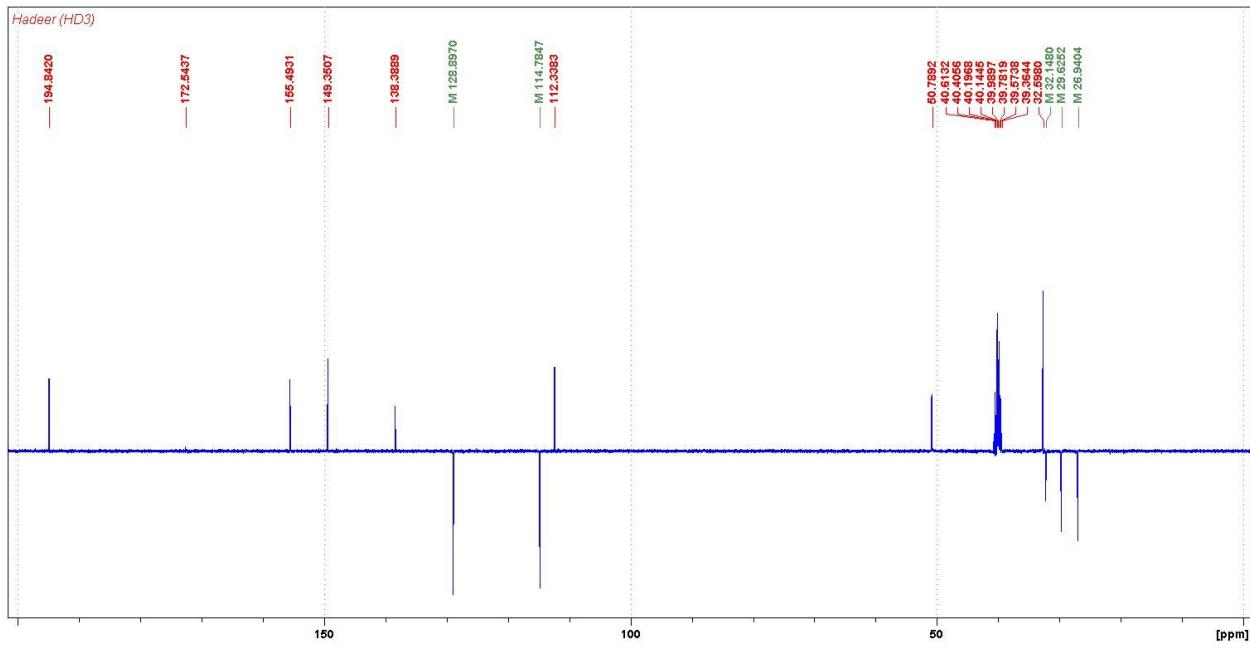
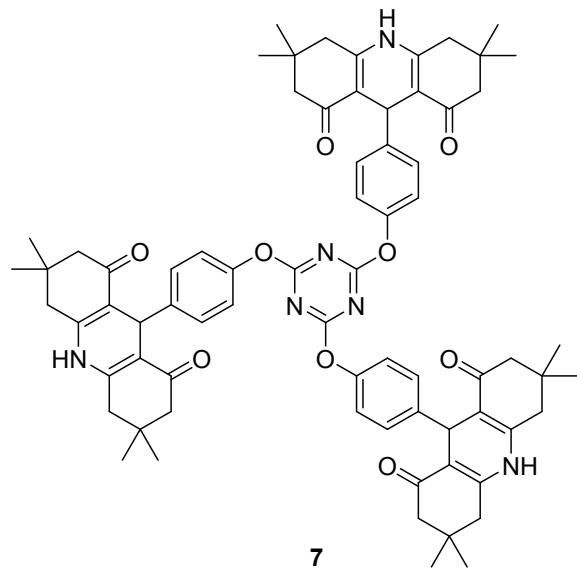


<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) of compound 5

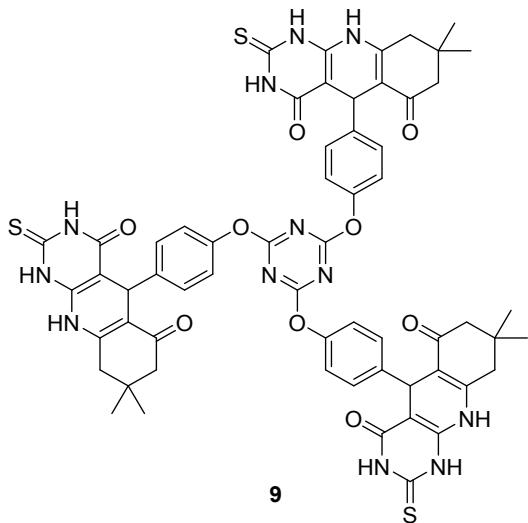




The  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) of compound 7



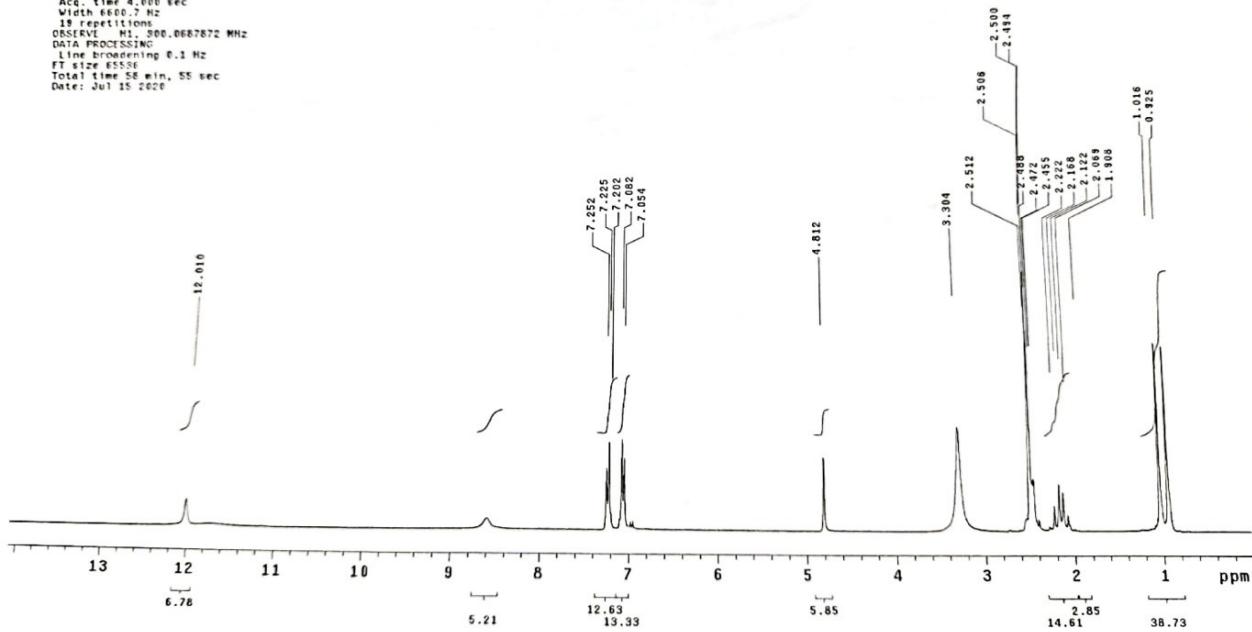
$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ ) of compound 7



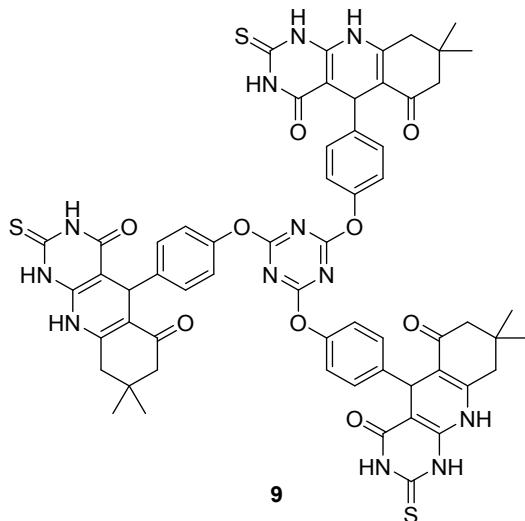
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Sample directory: D05mm_test_12Mar2014-21:34:40
Pulse Sequence: s2pul
Solvent: DMSO
Temp: 30.0 C / 303.1 K
File: HadeerDiab-HD86-DMSO-H1
Mercury-30088 "NNR300"
Relax, delay 6.000 sec
Pulse 45.0 degrees
Acc. time 4.000 sec
Width 6600.7 Hz
16 repetitions
OBSERVE F1: 300.00087872 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size: EST
Total time: 55 min, 55 sec
Date: Jul 15 2006

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The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 9



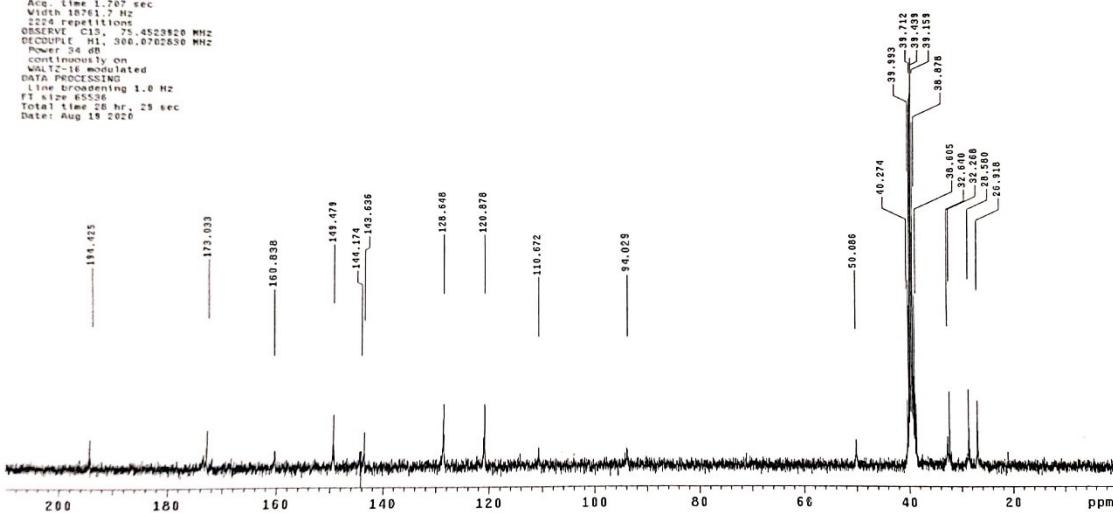
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HareerDiab-HD88-DMSO-C13
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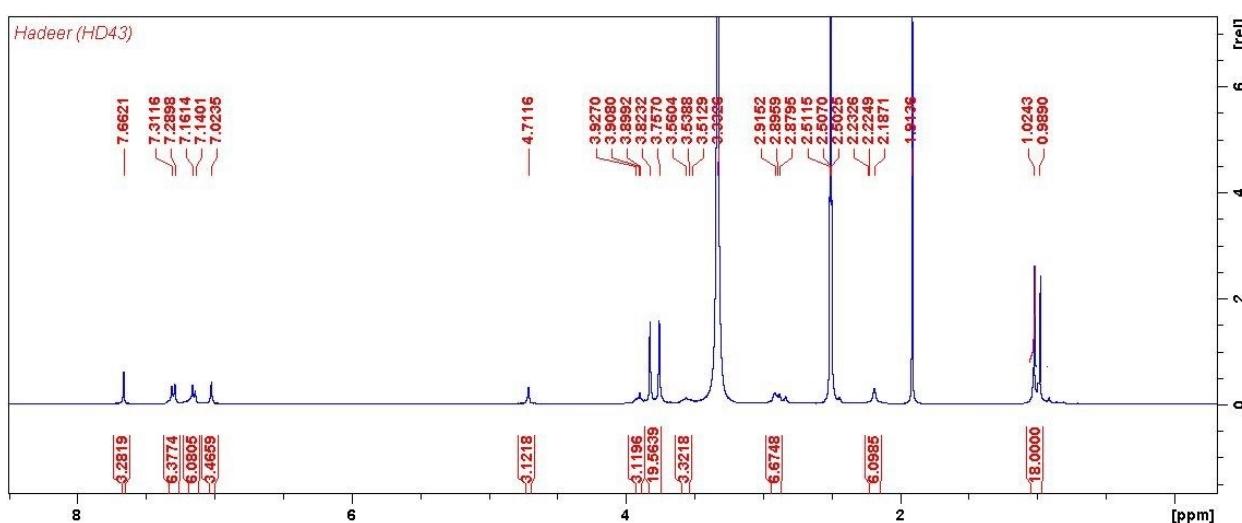
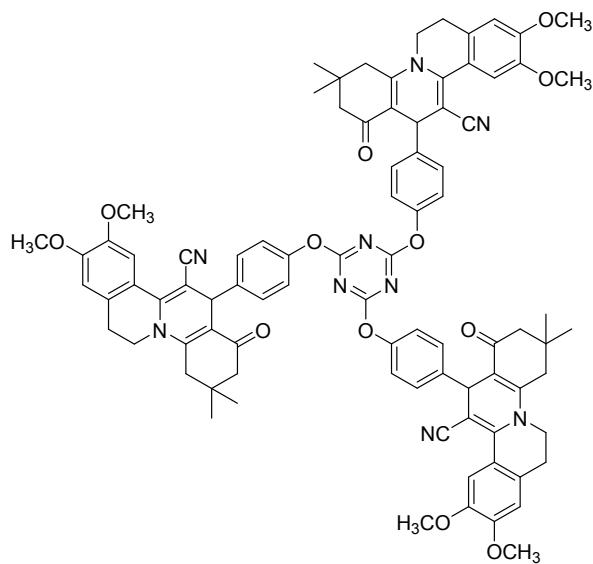
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Solvent: DMSO
Ambient temperature
Mercury-3600B "NMR30B"

Pulse 45.0 degrees
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2224 repetitions
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DECOUPLE: 13C, 360.0702830 MHz
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Convoluted only on
WALTZ-16 magnetized
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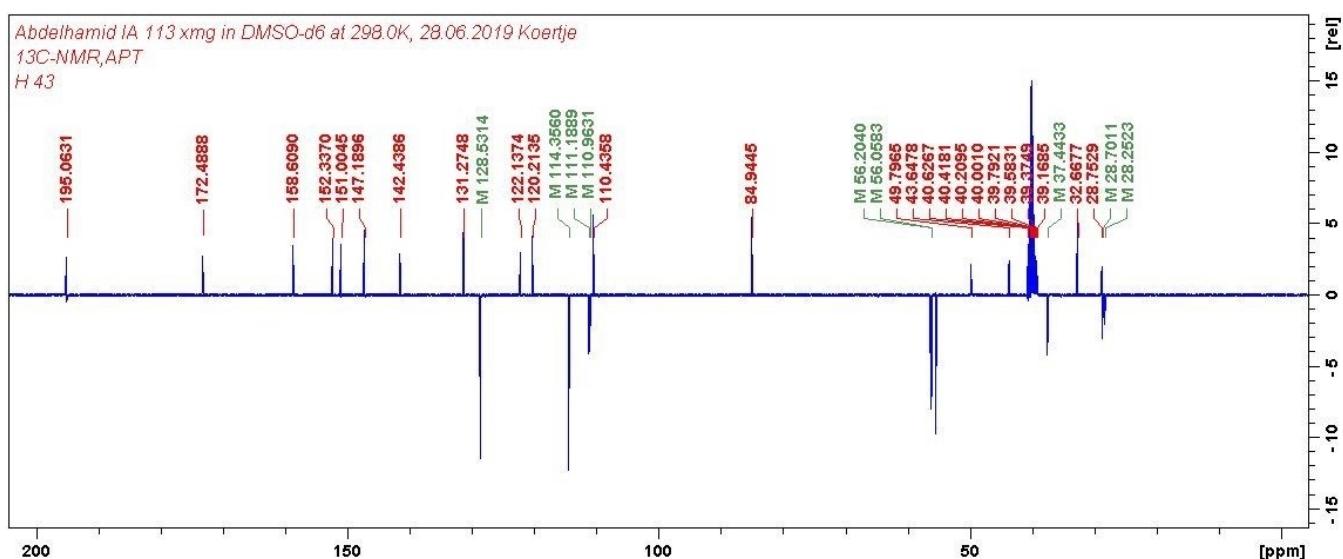
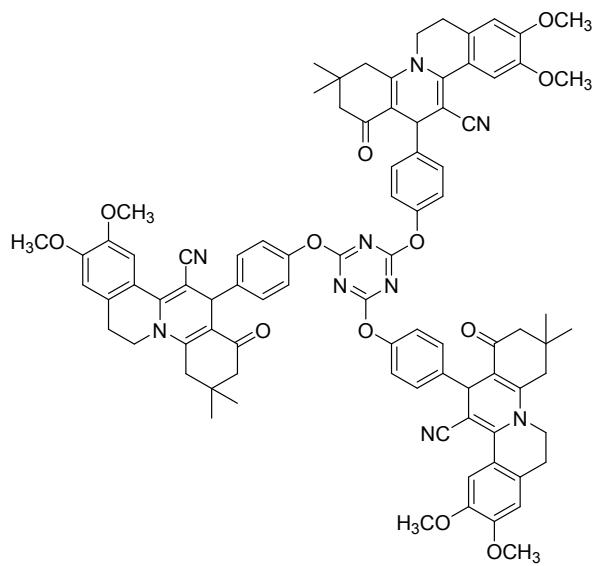
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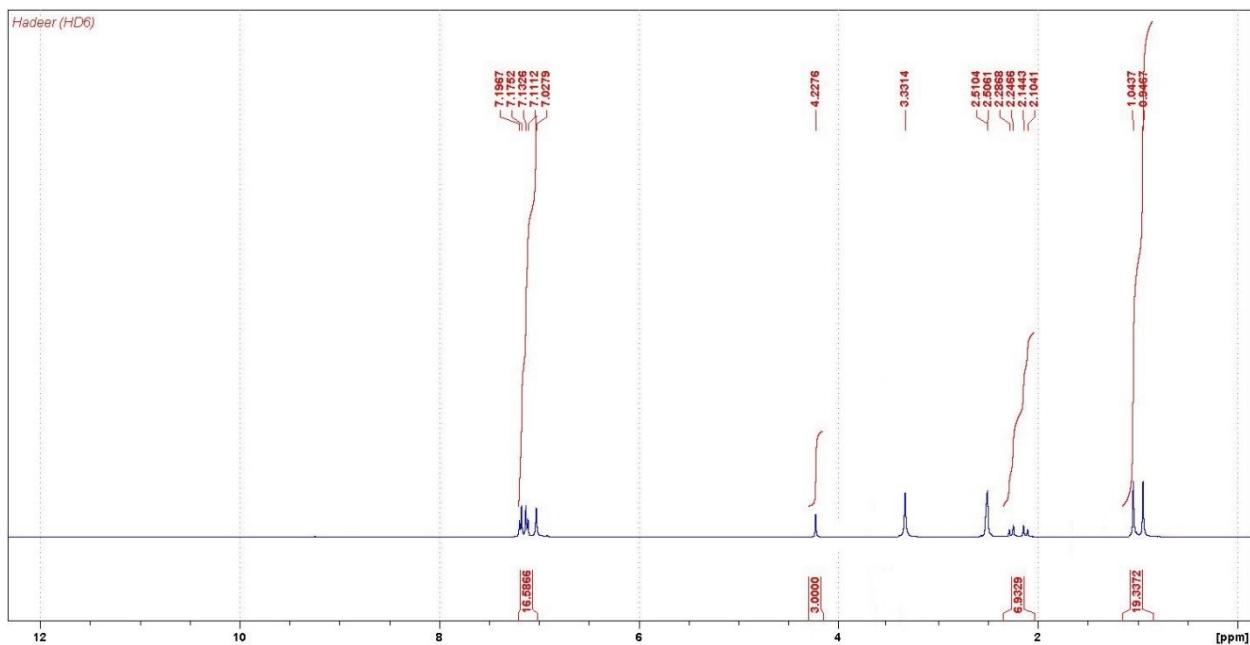
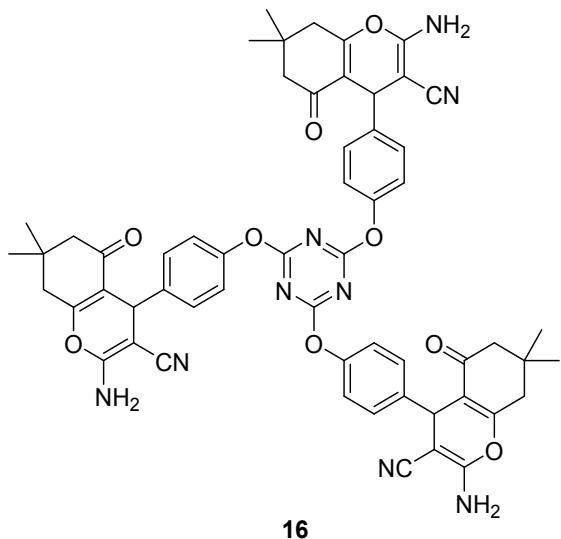
$^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}-d_6$ ) of compound 9



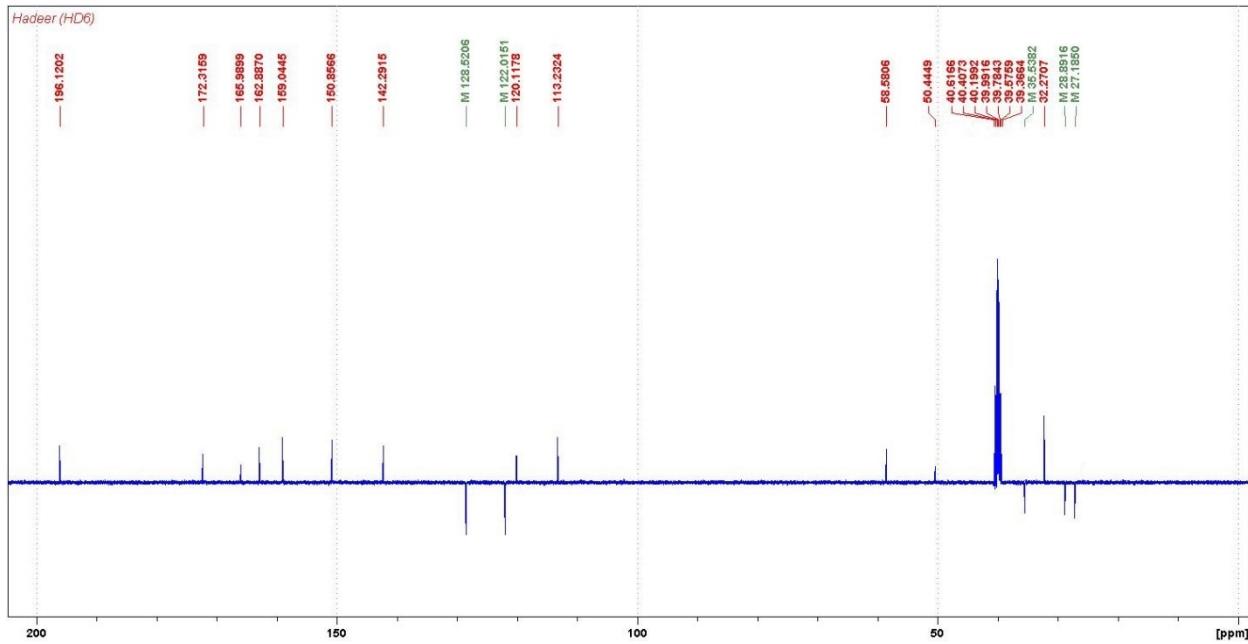
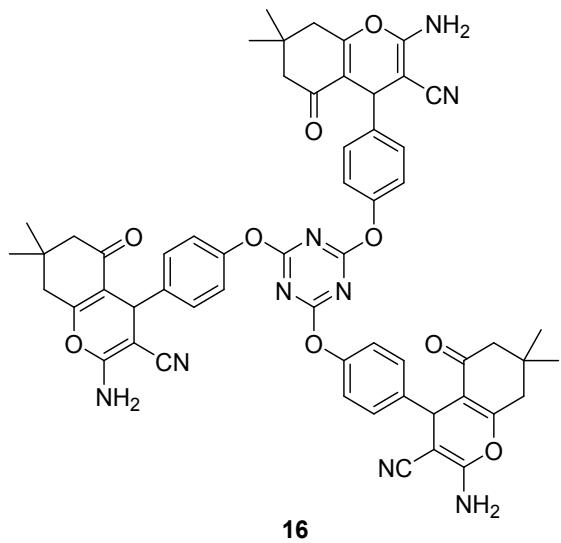
The  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) of compound 12



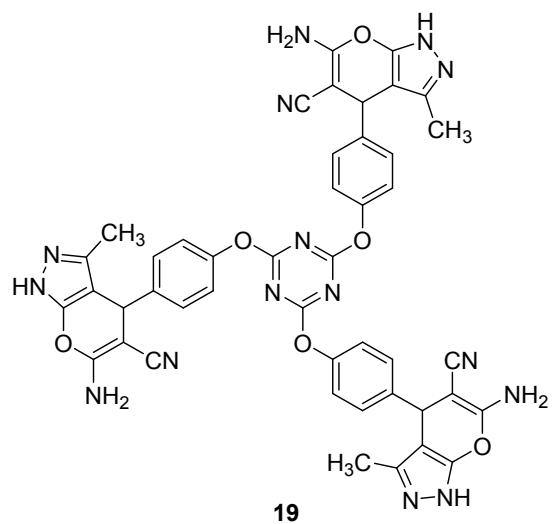
<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) of compound 12



The  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) of compound 16



$^{13}\text{C}$  NMR (100 MHz, DMSO-*d*<sub>6</sub>) of compound 16



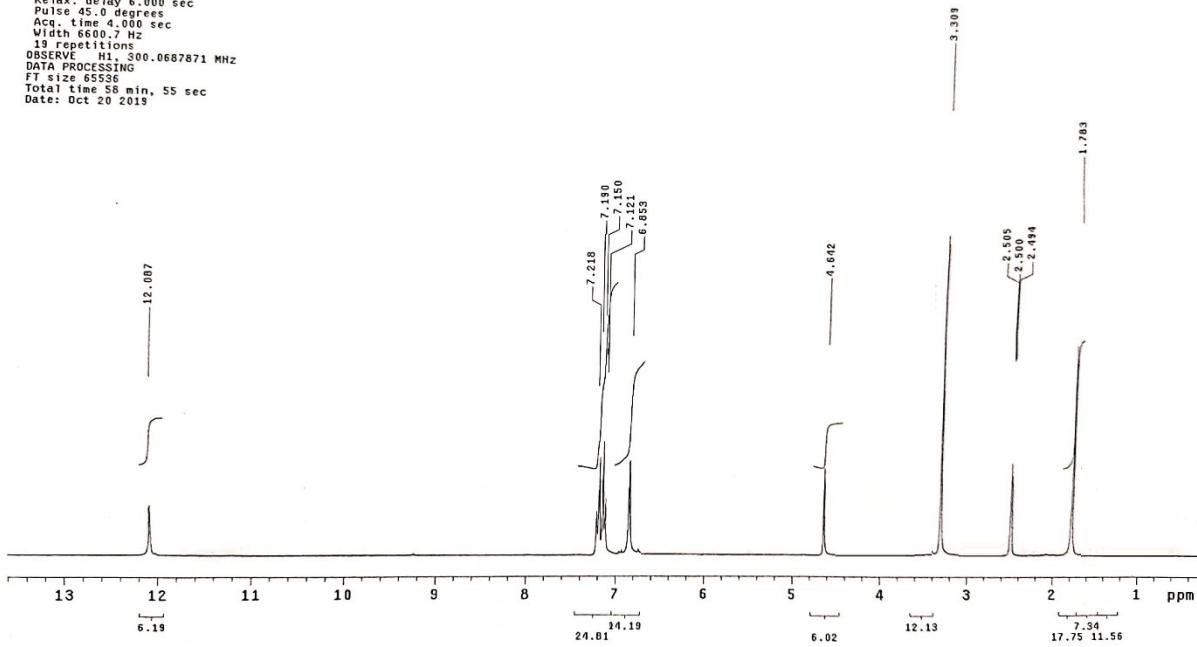
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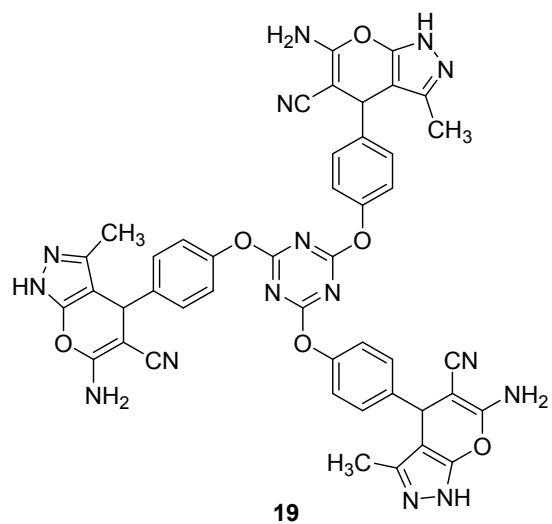
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Sample directory: D5mmm_test_12Mar2014-21:34:40
File: PROTON

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

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
112 repetitions
OBSERVE FREQ 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Oct 20 2019

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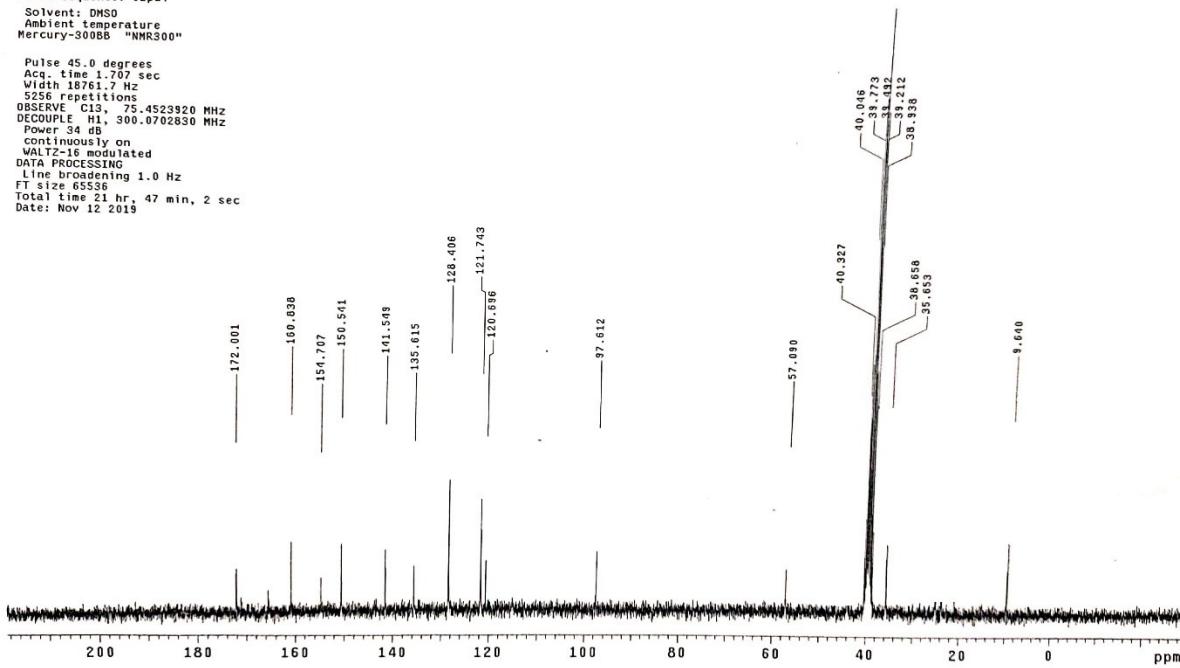


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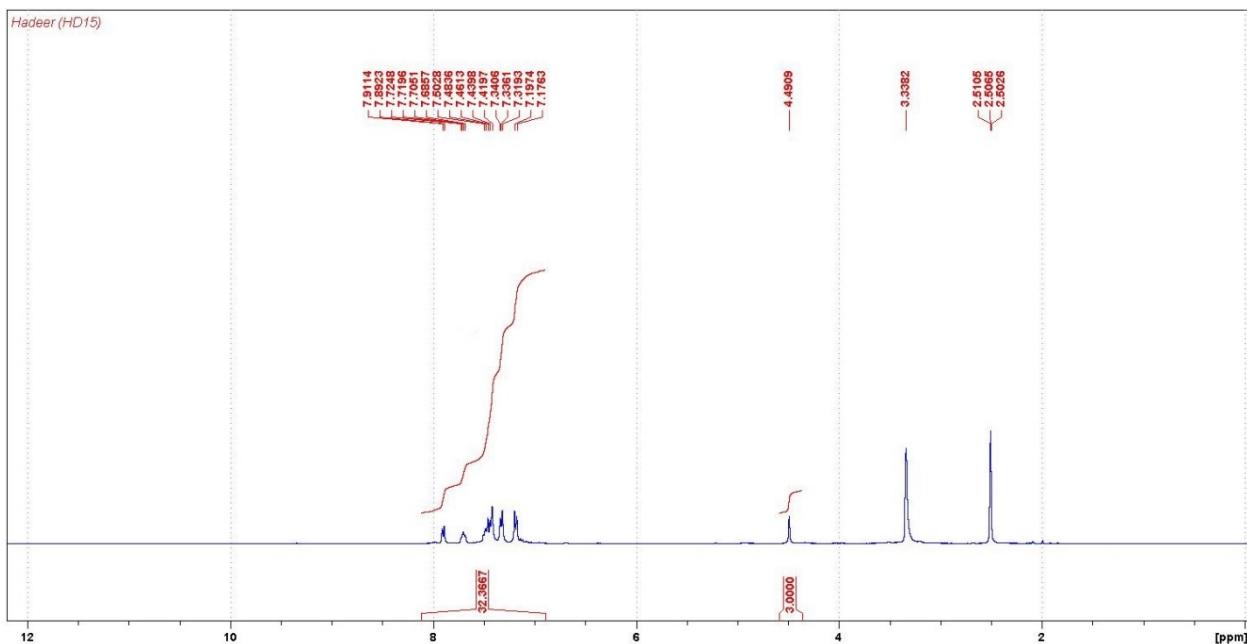
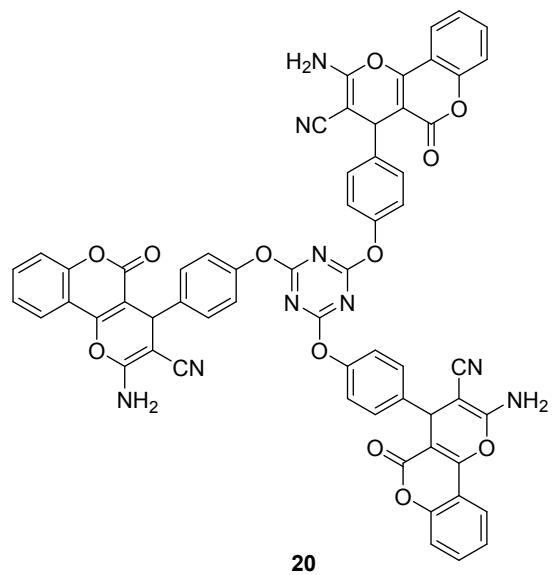
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File: PROTON

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"
Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
3256 repetitions
DS500E 75.4523920 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 21 hr, 47 min, 2 sec
Date: Nov 12 2019

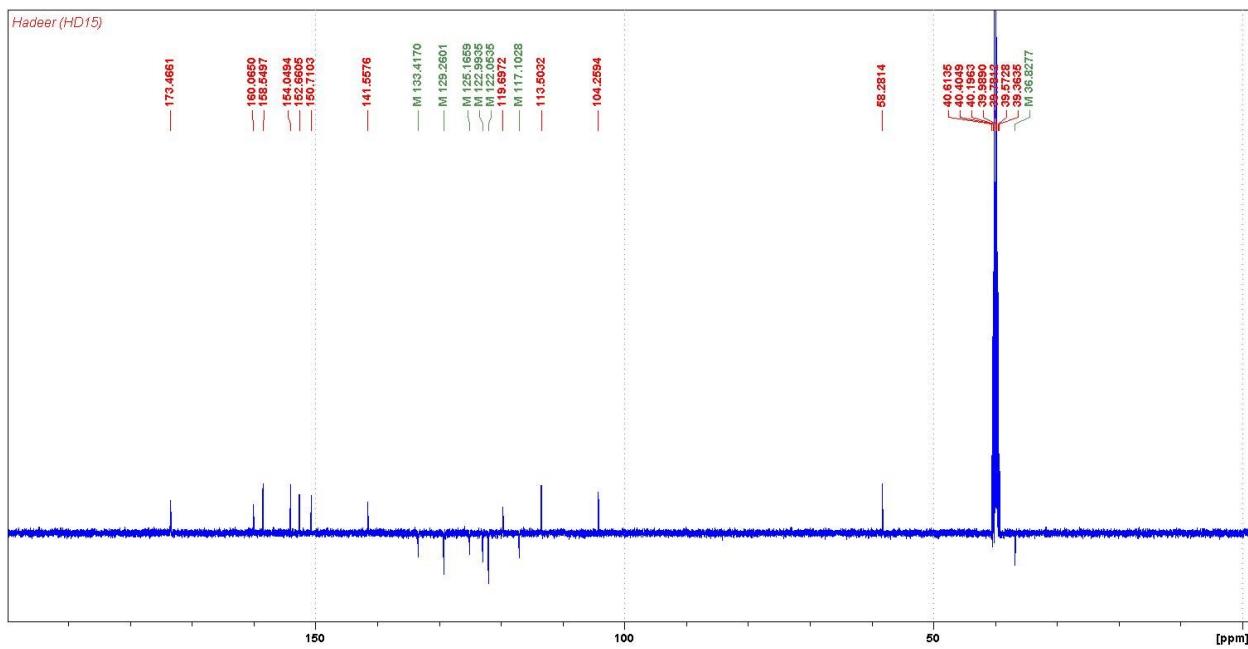
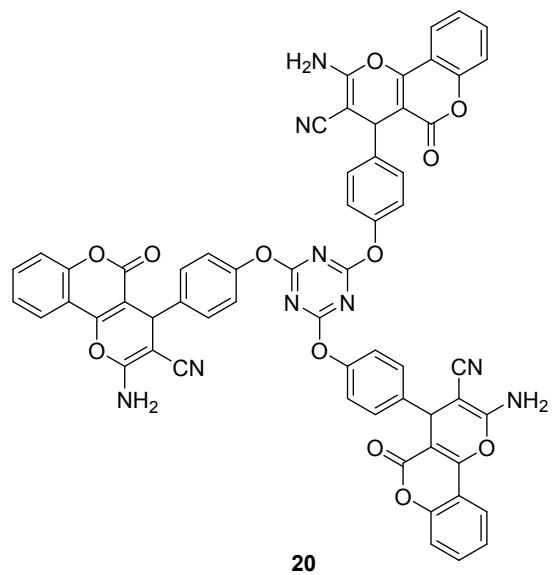
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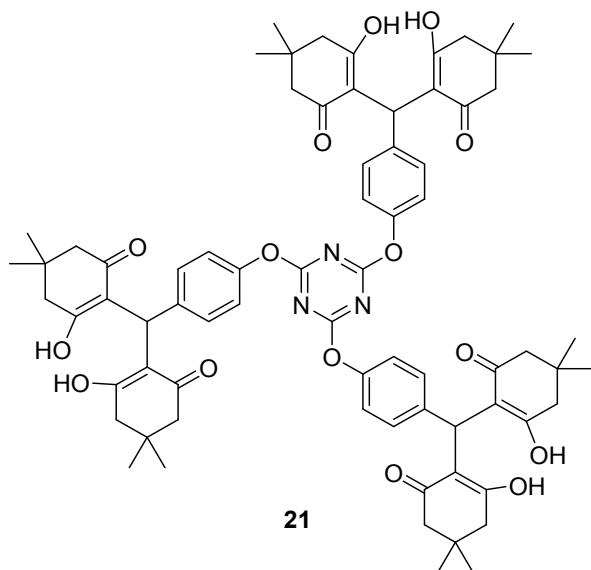
<sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>) of compound 19



The  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) of compound 20



<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) of compound 20



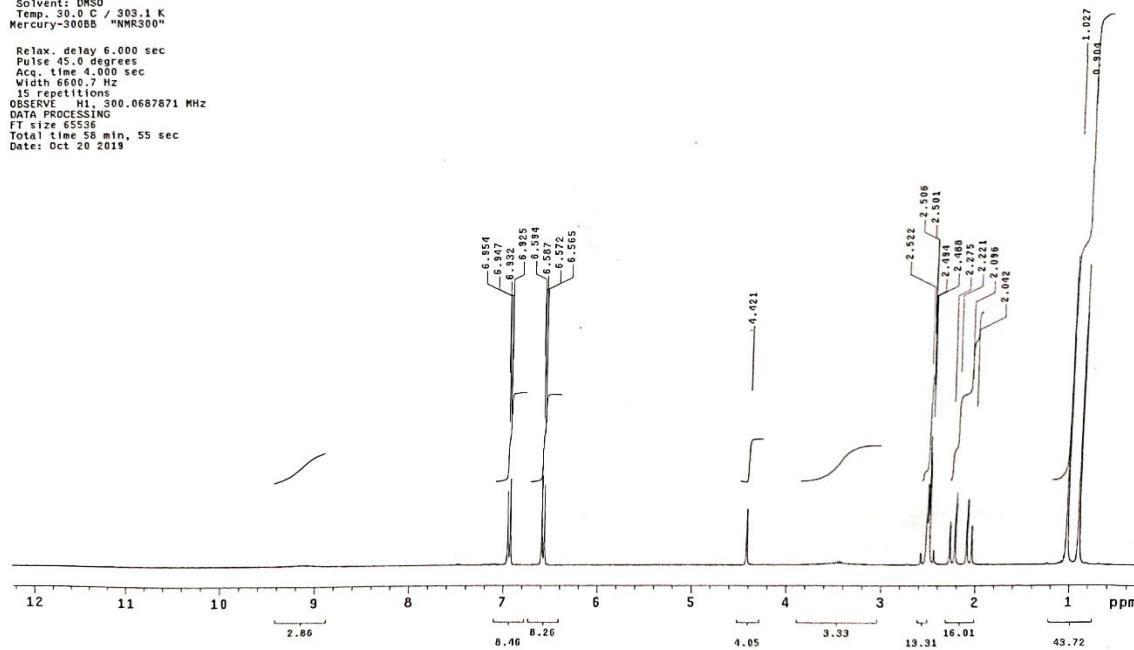
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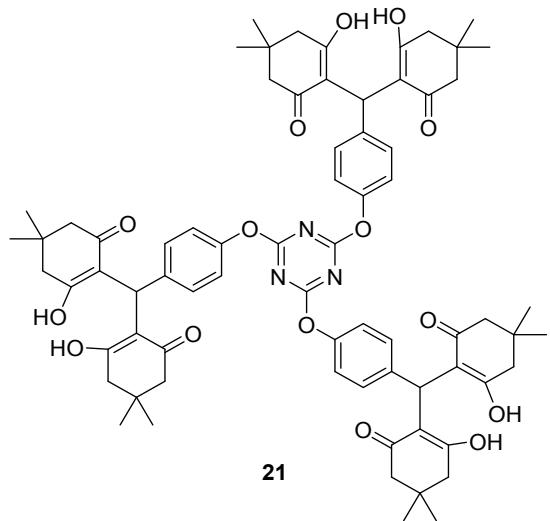
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax delay 6.000 sec
Pulse 90 degrees
Acc. time 4.000 sec
Width 6600.7 Hz
15 repetitions
Data points 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Oct 20 2019

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The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 21



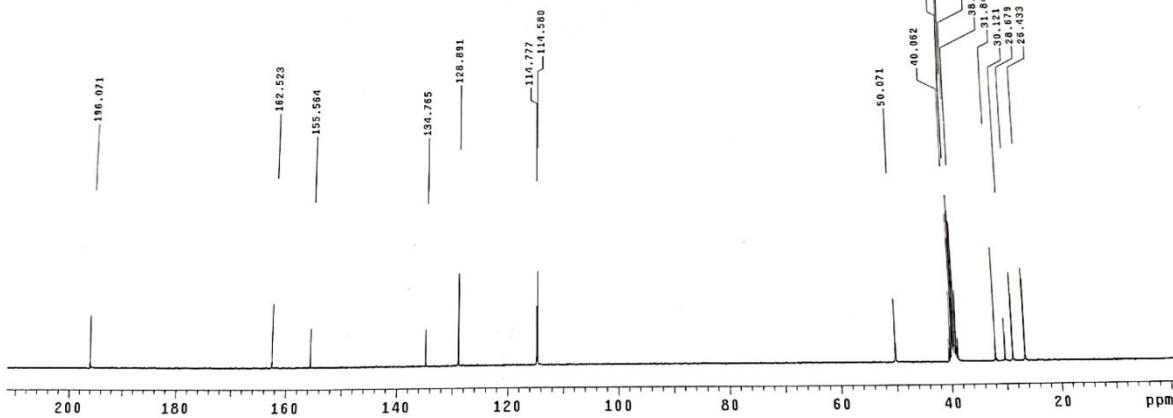
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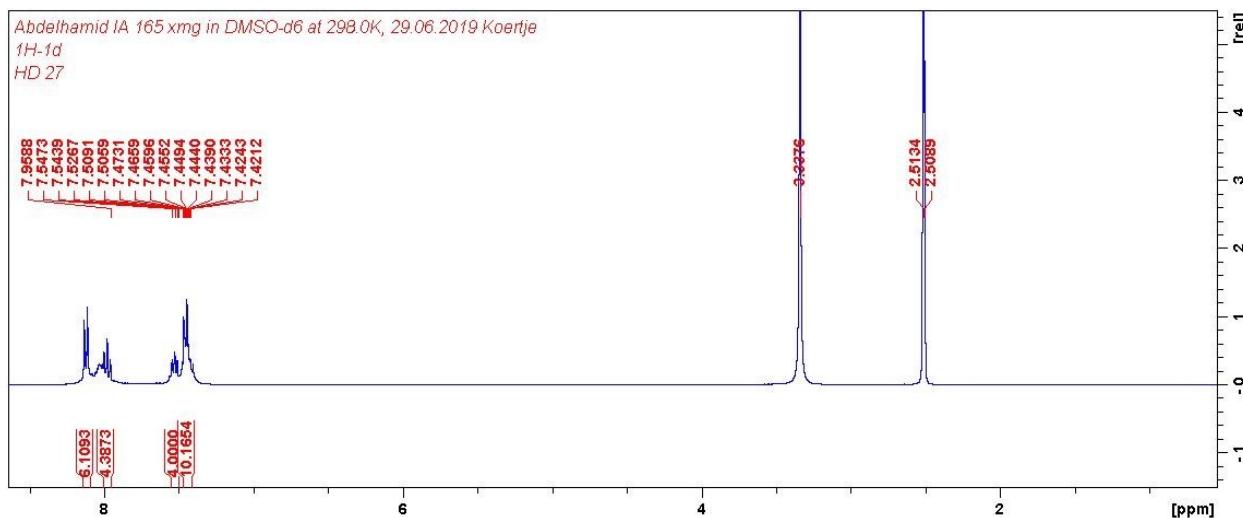
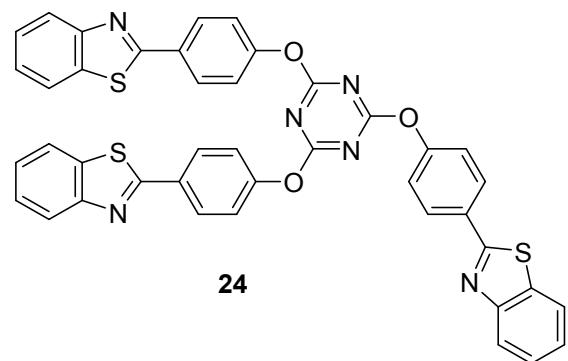
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Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR500"

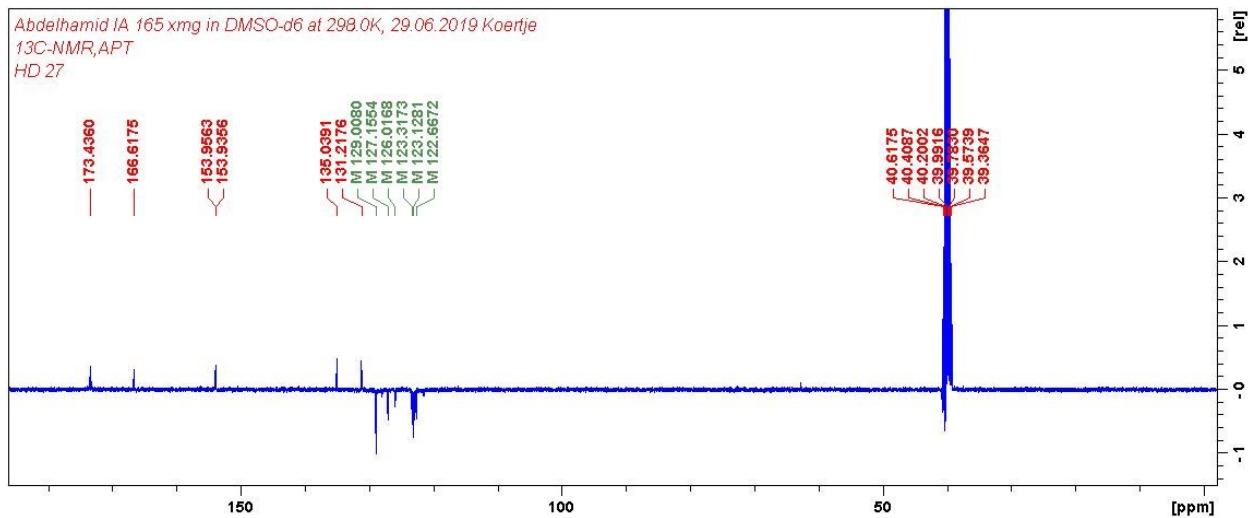
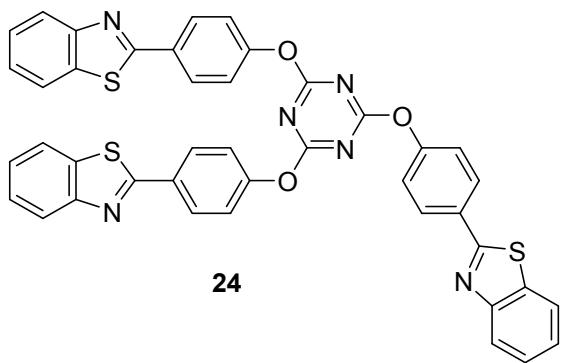
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Pulse 45.0 degrees  
Aq. time 1.707 sec  
Width 18761.7 Hz  
35000 FID points  
OBSERVE\_C13, 75.4525825 MHz  
DECOUPLE\_H1, 300.0702830 MHz  
Power 34 dB  
Continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 21 hr, 47 min, 2 sec  
Date: Oct 30 2013

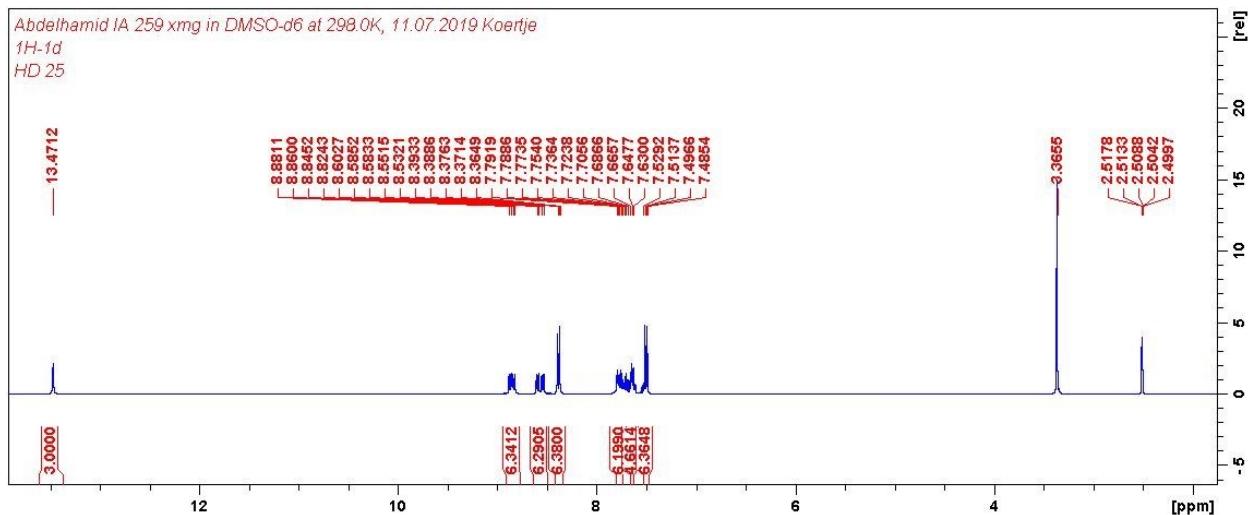
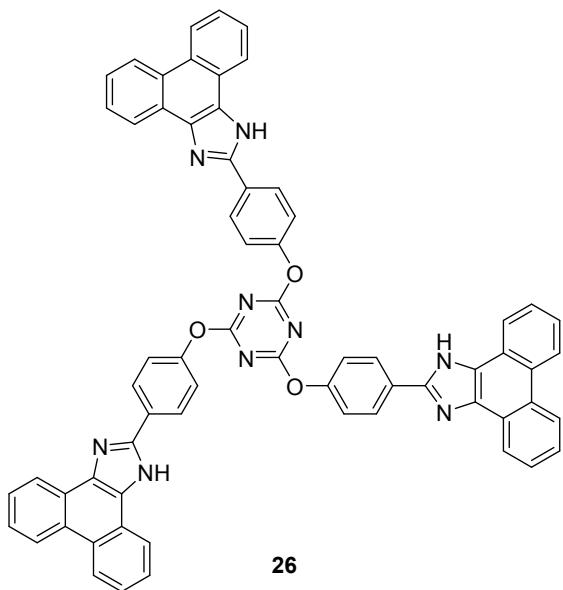




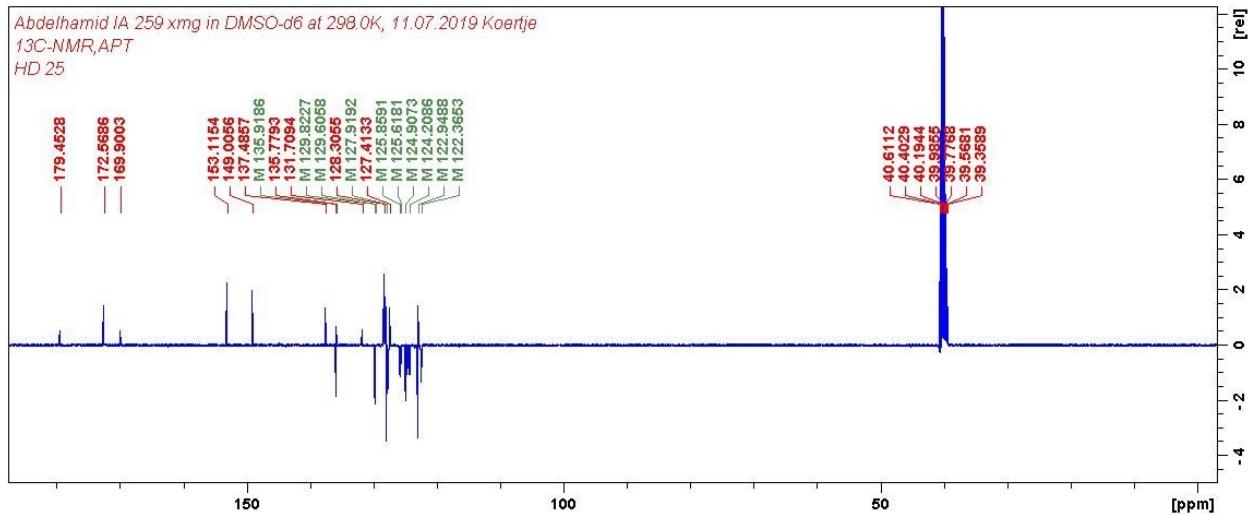
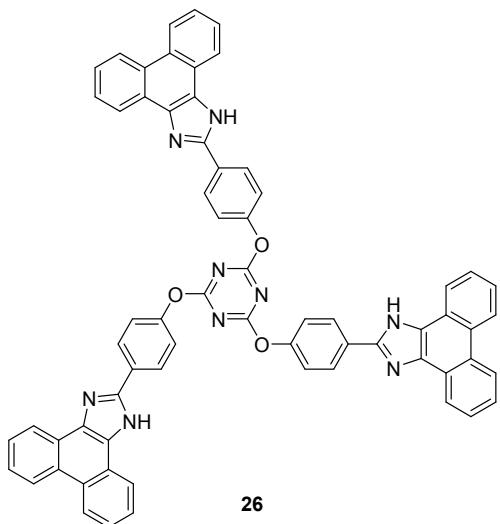
The <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) of compound 24



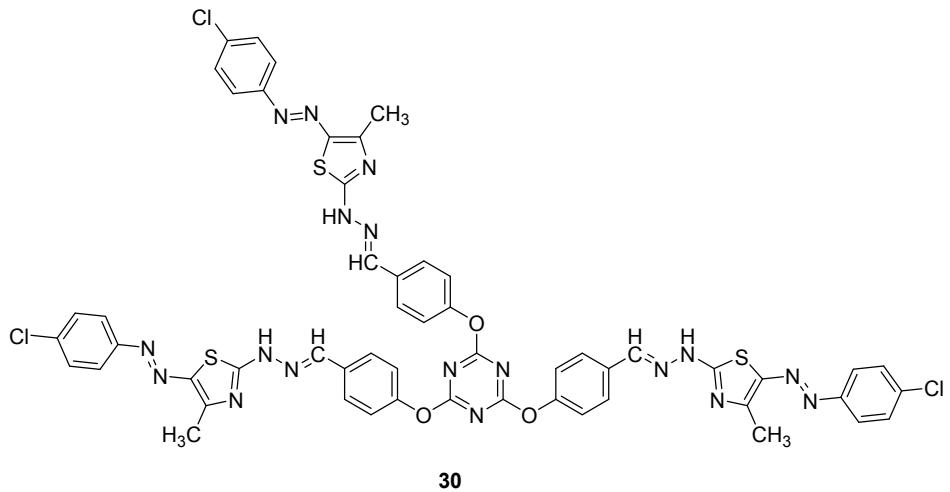
<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) of compound 24



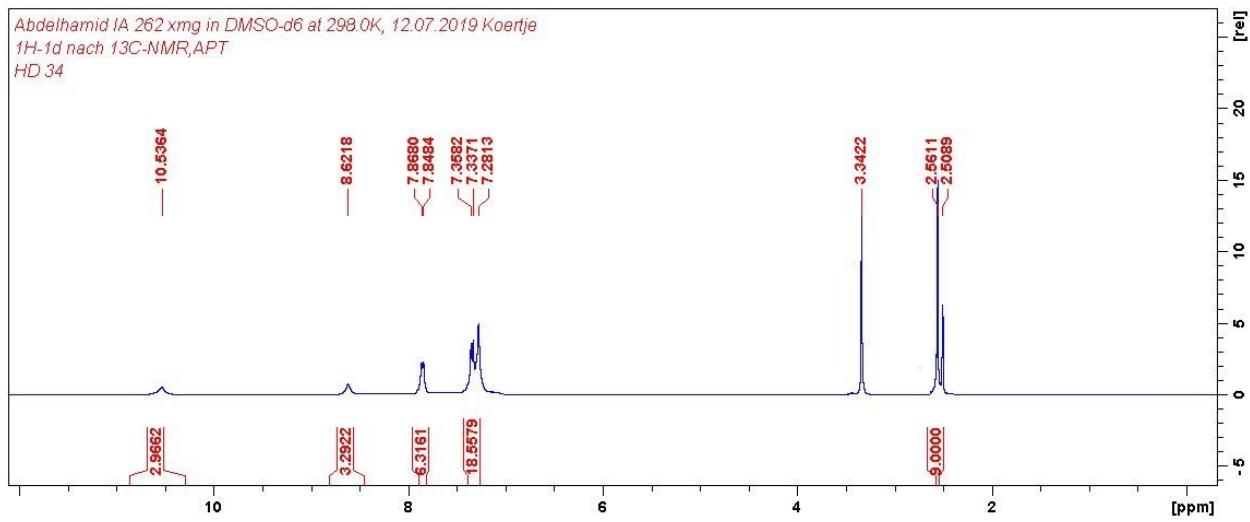
The <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) of compound 26



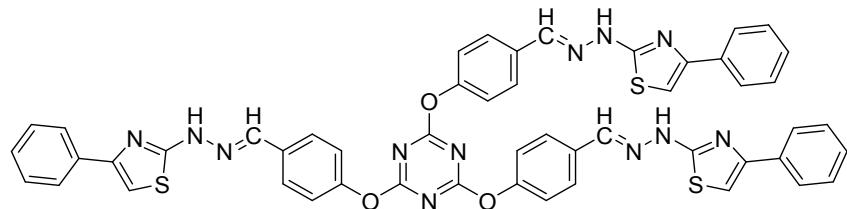
<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) of compound 26



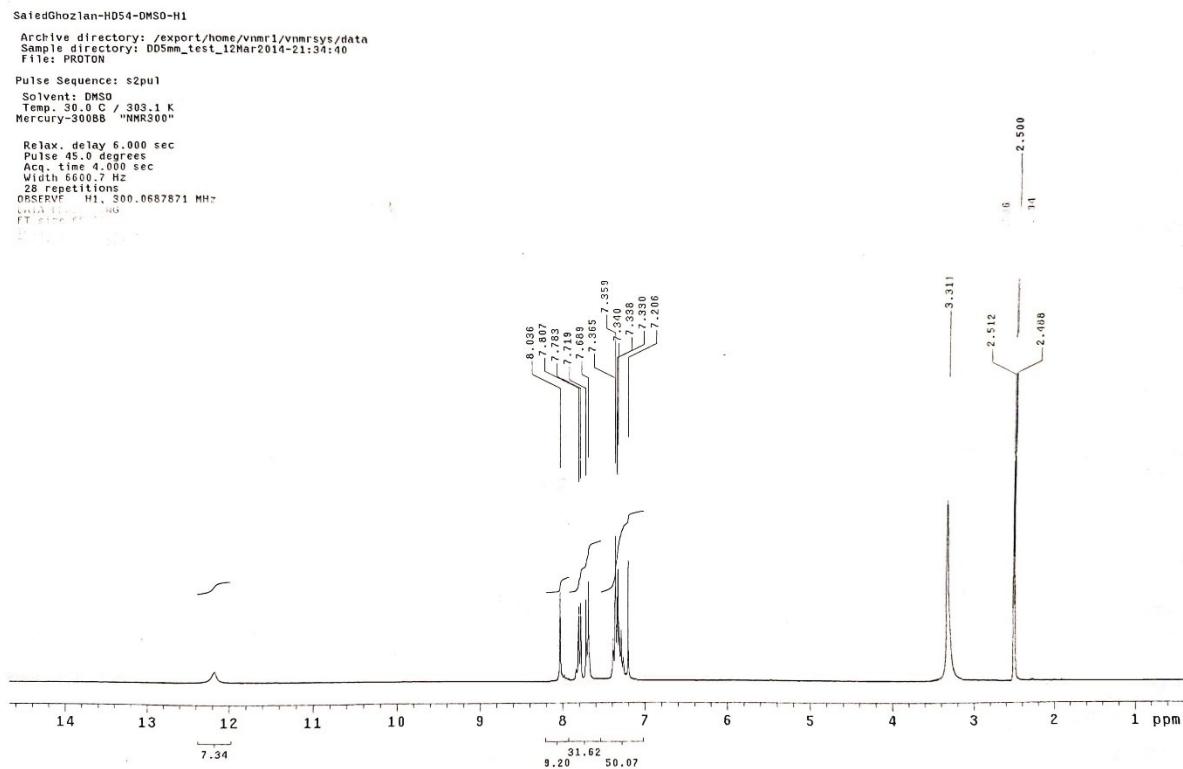
*Abdelhamid IA 262 xmg in DMSO-d<sub>6</sub> at 298.0K, 12.07.2019 Koertje*  
*1H-1d nach 13C-NMR, APT*  
*HD 34*



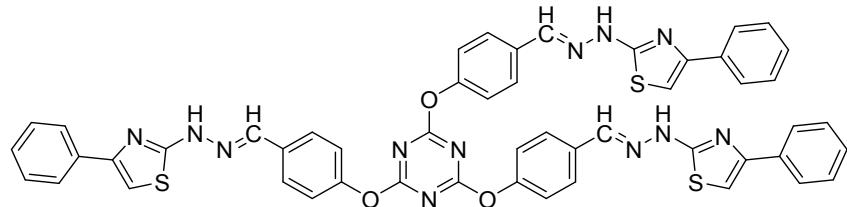
The <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) of compound 30



**33**



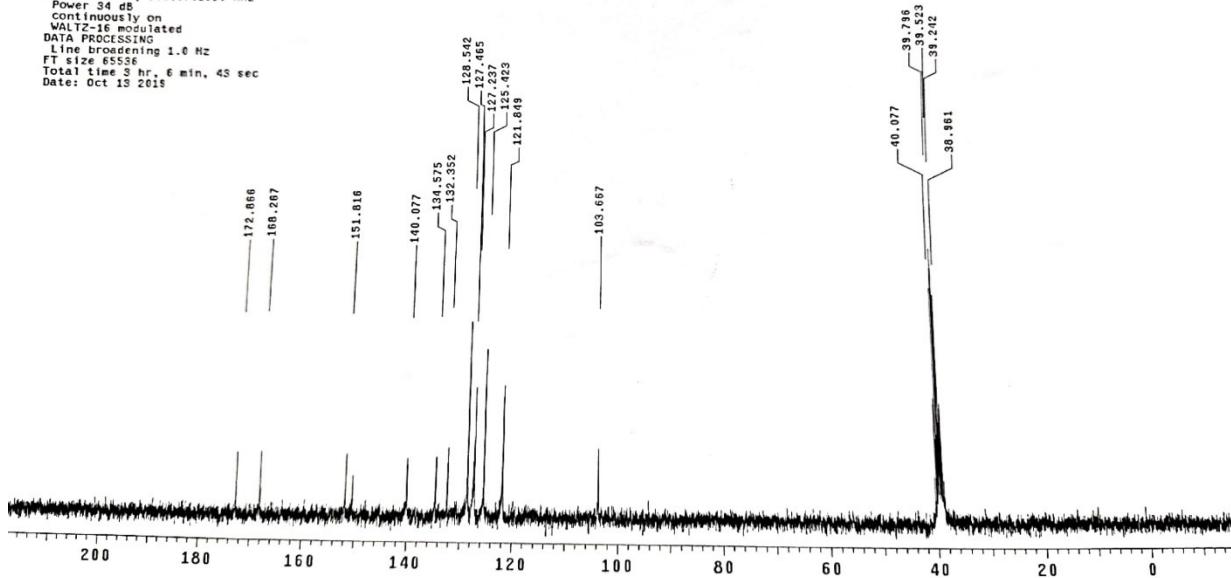
The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 33



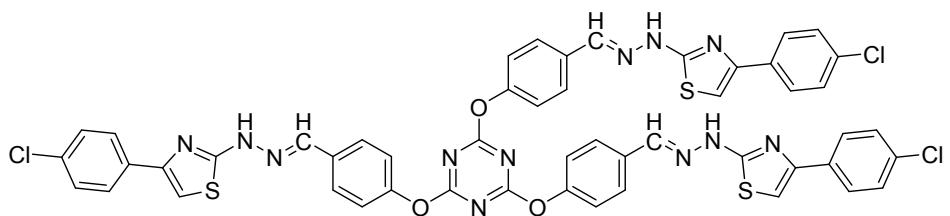
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Sample directory: DD5mm_test_12Mar2014-21:54:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300B "NMR300"
Pulse 45.0 degrees
AcqTime 1.74 sec
Width 1876.0 Hz
1576 repetitions
OBSERVE C13, 75.4522846 MHz
DECOUPLE H1, 300.0702850 MHz
Power 54
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT Size 4552
Total time 3 hr, 6 min, 43 sec
Date: Oct 13 2015

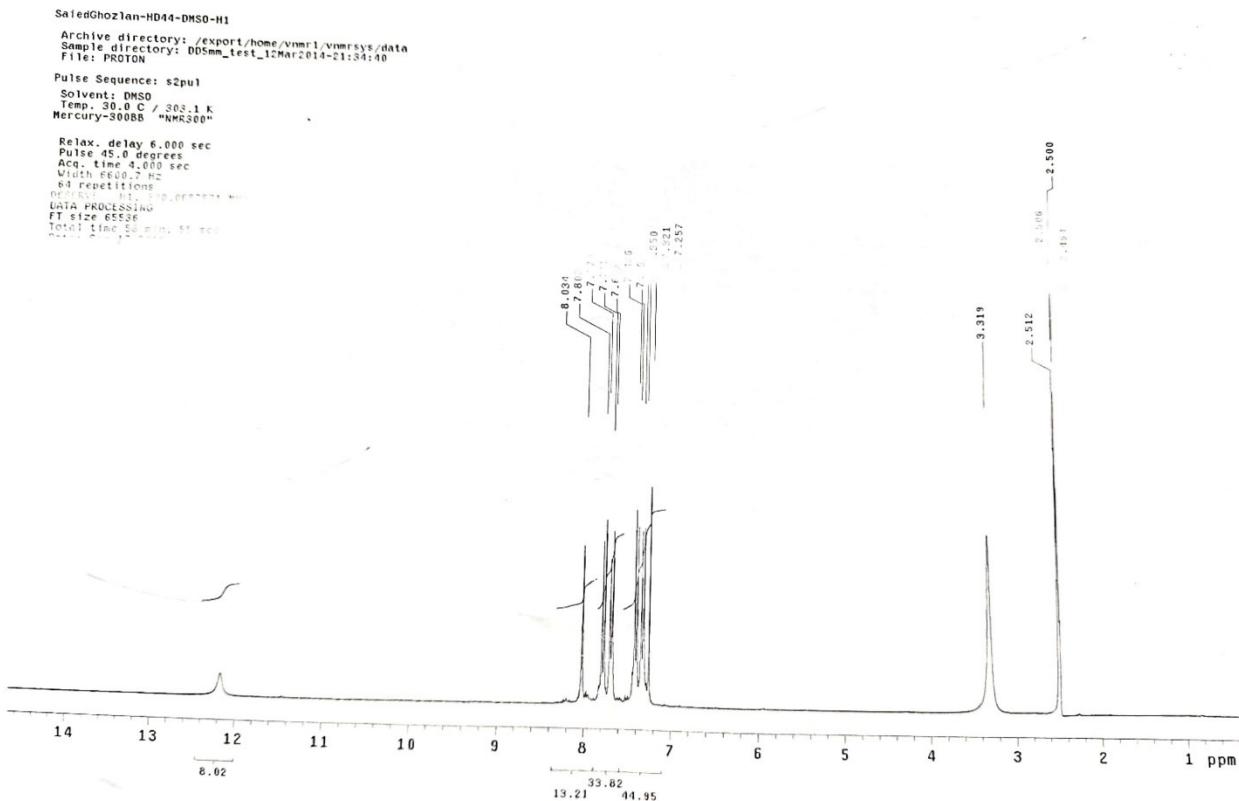
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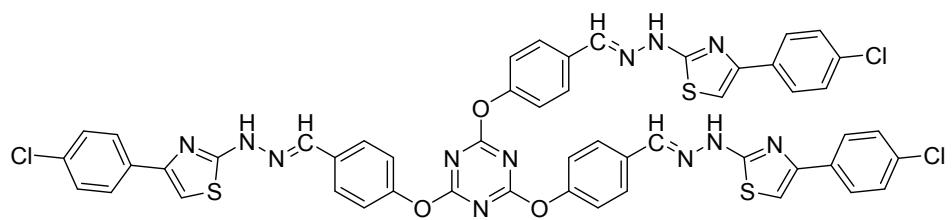
$^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ) of compound 33



**34**



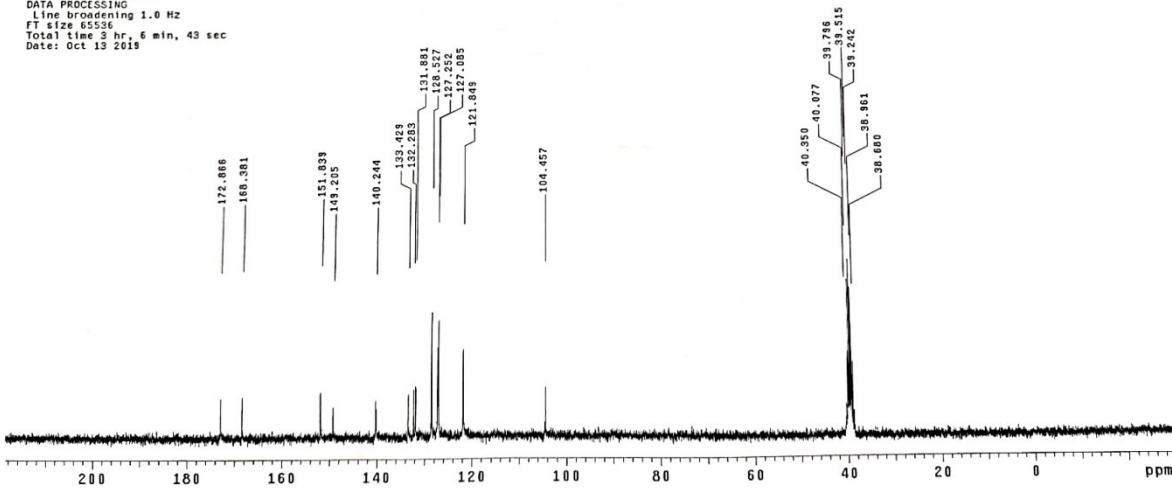
The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 34



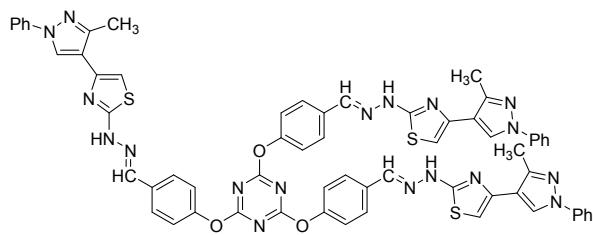
**34**

IbrahimZaky-HD44-DMSO-C13  
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Sample directory: D05mm\_test\_12Mar2014-21:34:40  
File: PROTON

Pulse Sequence: s2pul1  
Solvent: DMSO  
Temp. 30.0 C / 303.1 K  
Mercury-300BB "NMR300"  
Pulse 45.0 degrees  
Acq. time 1.767 sec  
Width 16761.7 Hz  
2768 repetitions  
OSDPWR 1000, 75.4522848 MHz  
DECOUPLE 13C 300.0702830 MHz  
Power 34 dB  
Coil Inv 1  
WALT 16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 1 hr, 6 min, 49 sec  
Date: Oct 13 2019



<sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>) of compound 34



**36**

SaledGhozlan-HD57-DMSO-H1  
Archive directory: /export/home/vnmr1/vnmrssys/data  
Sample directory: 005mm\_test\_12Mar2014-21:34:40  
File: PROTON

Pulse Sequence: s2pul

Solvent: DMSO

Temp: 30.0 C / 303.1 K

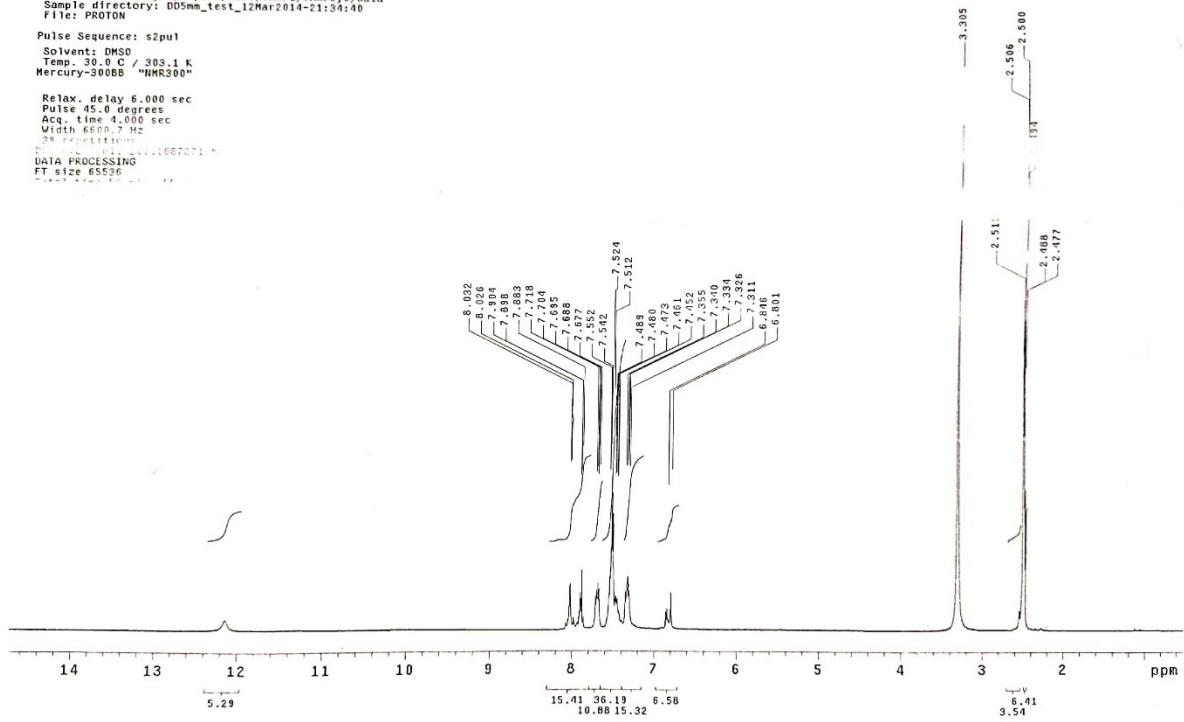
Width 6600.7 Hz

32 repetitions

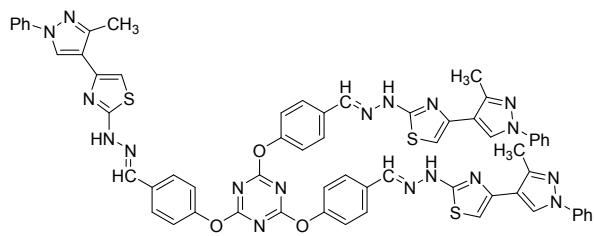
Scan time: 1.000 sec, 0.687071 sec

DATA PROCESSING

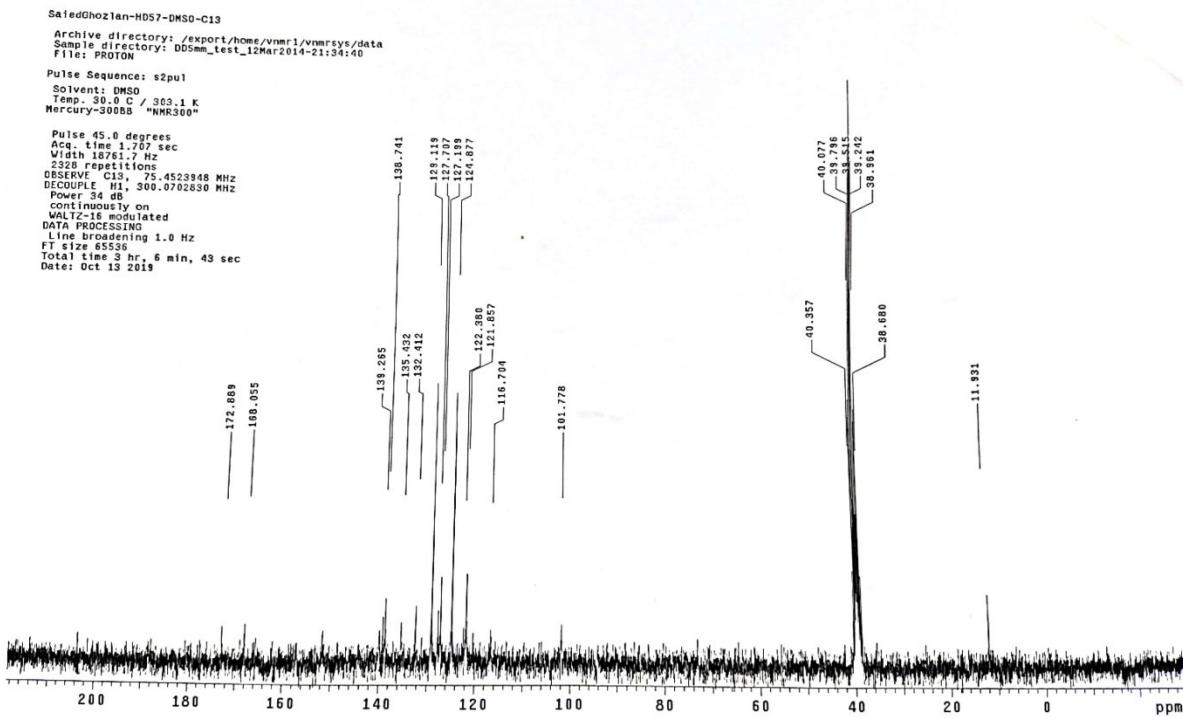
FT size 65536

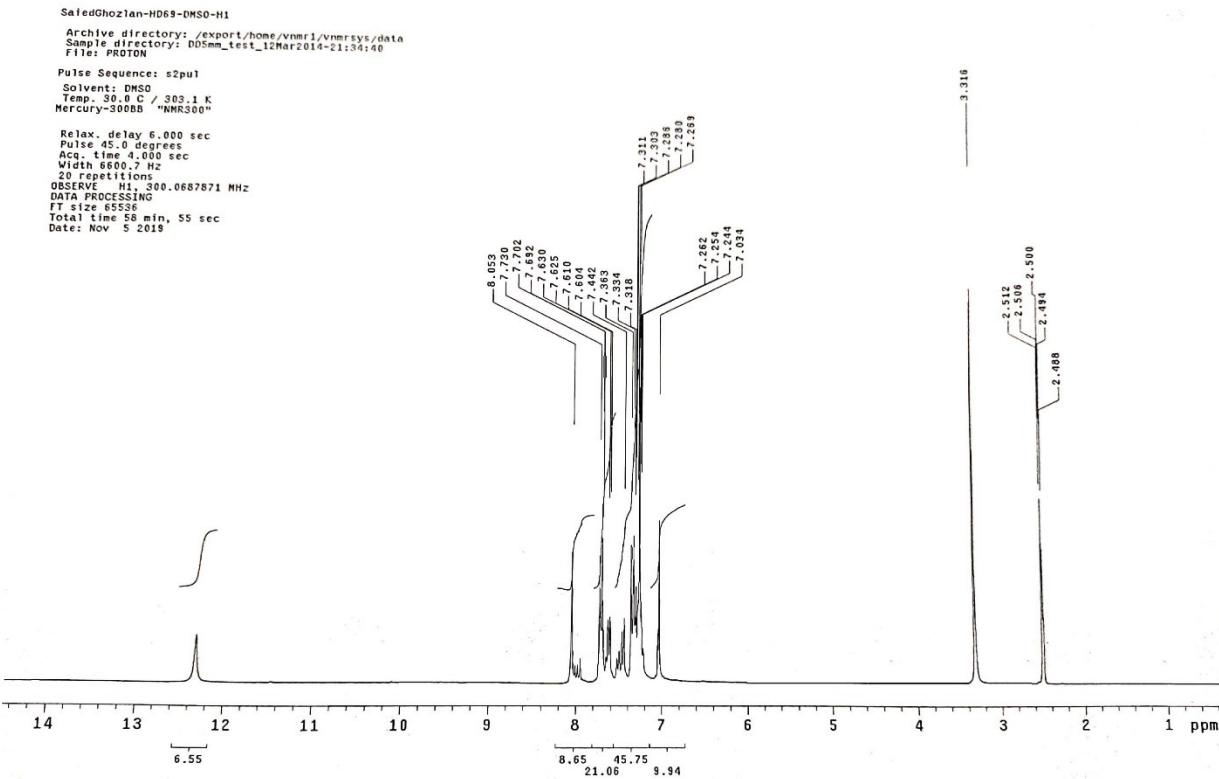
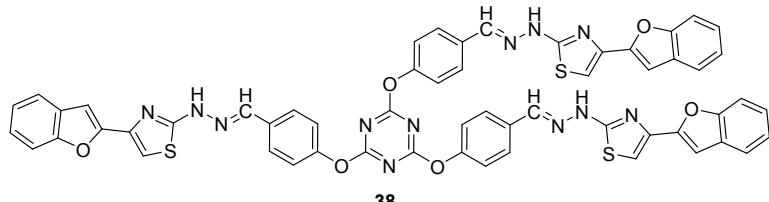


The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 36

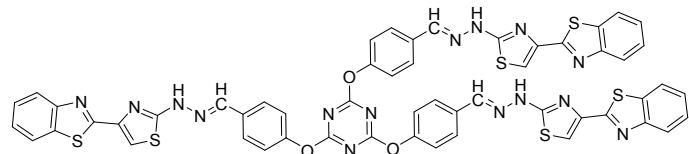


36





The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 38



40

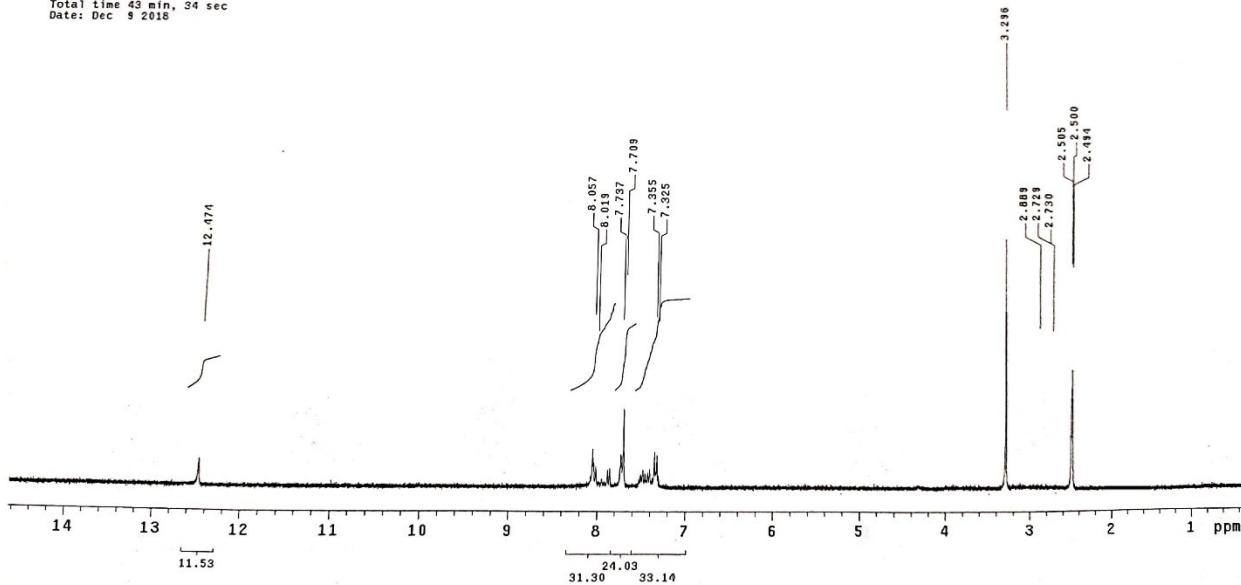
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MustafaAlSayed-HA1-DMSO-1H
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Sample directory: 005mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NNR300"

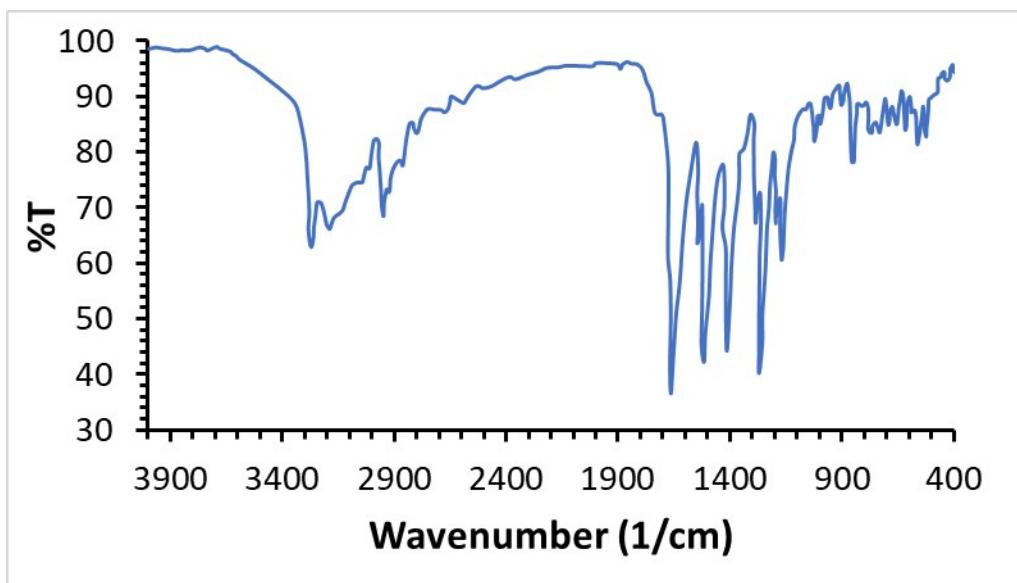
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.855 sec
Width 6600.7 Hz
36 repetitions
Data points 16384
0.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 43 min, 34 sec
Date: Dec 9 2018

```

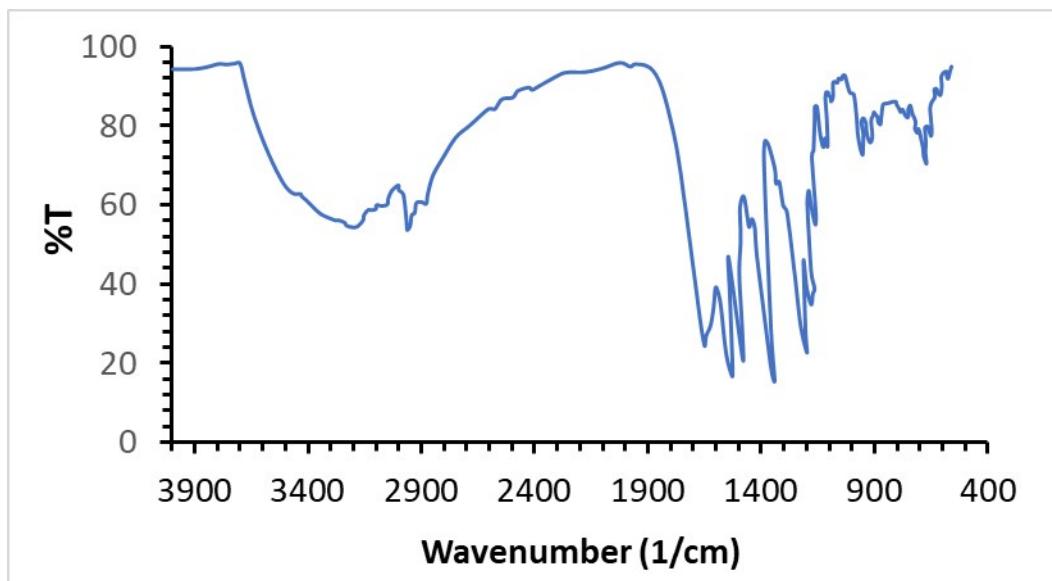


The  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ) of compound 40

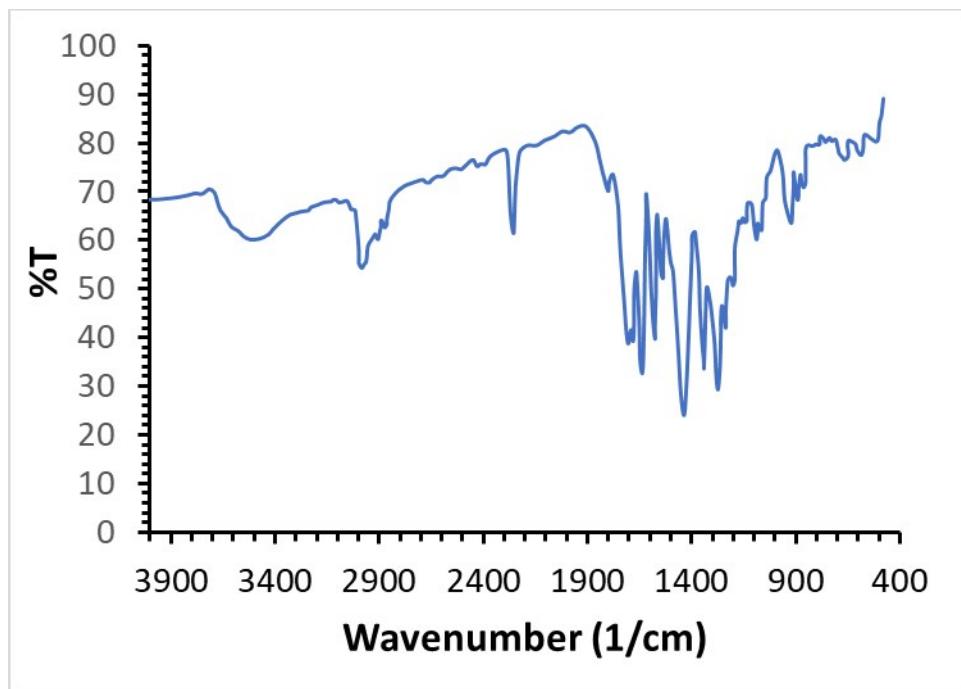
## IR Spectra



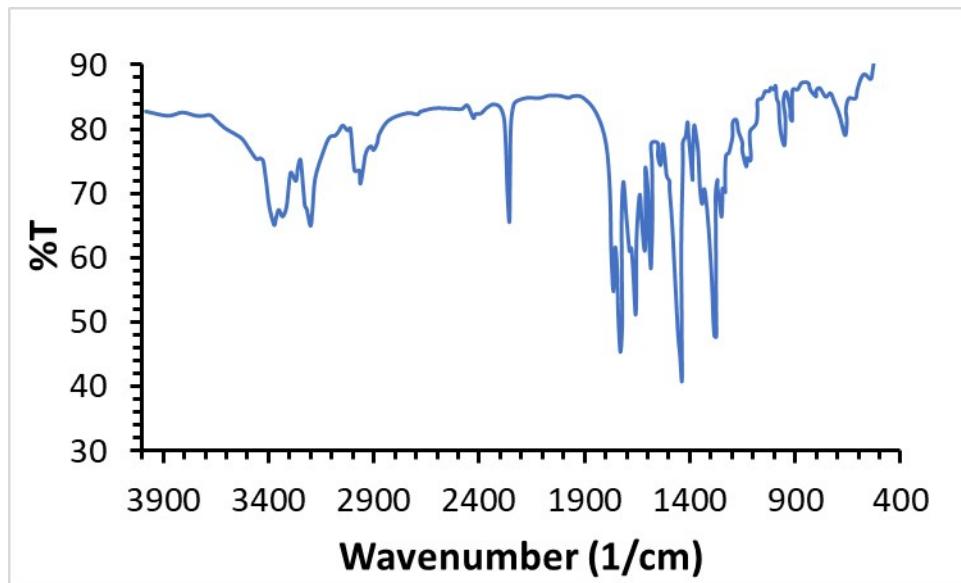
**Figure 1.** IR spectrum of compound 7



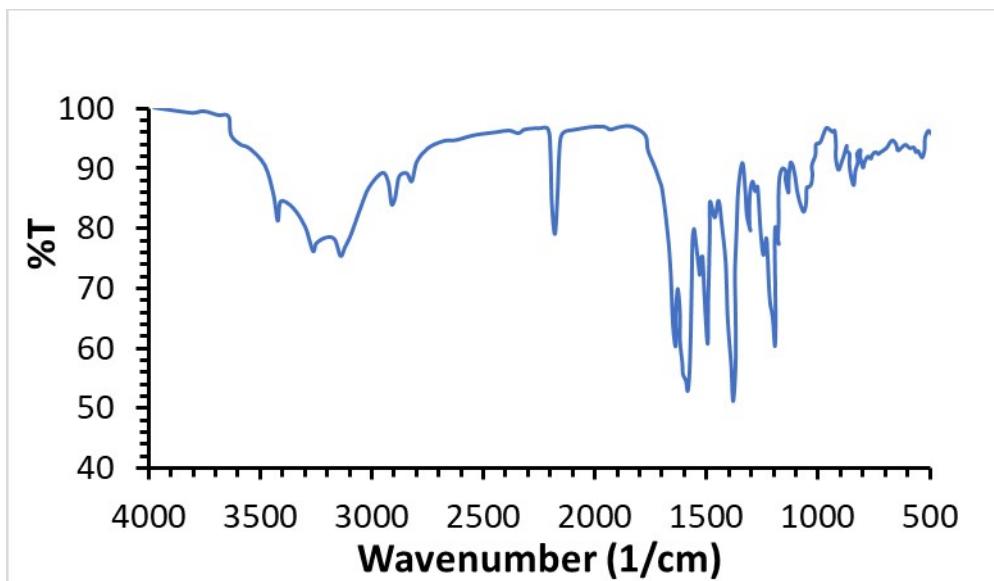
**Figure 2.** IR spectrum of compound 9



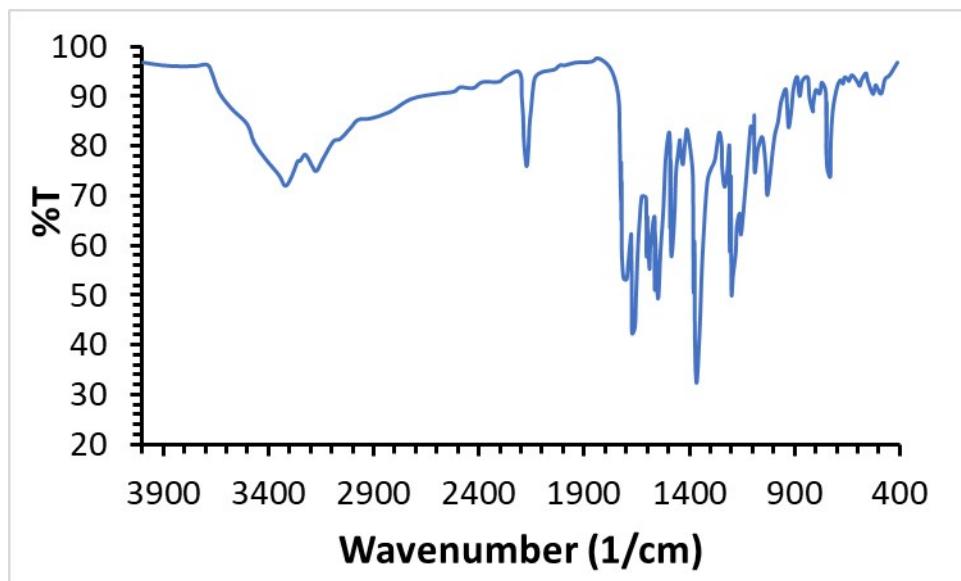
**Figure 3.** IR spectrum of compound **12**



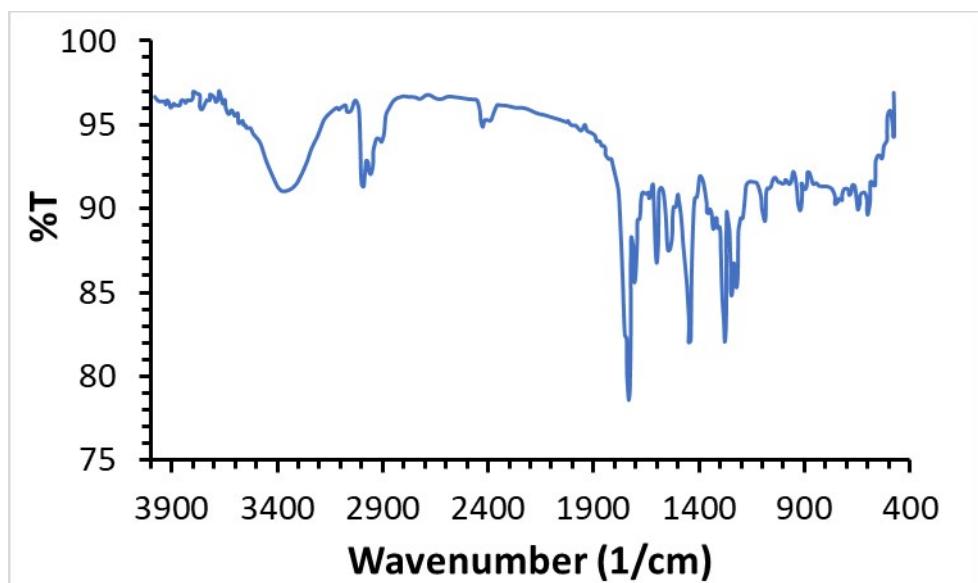
**Figure 4.** IR spectrum of compound **16**



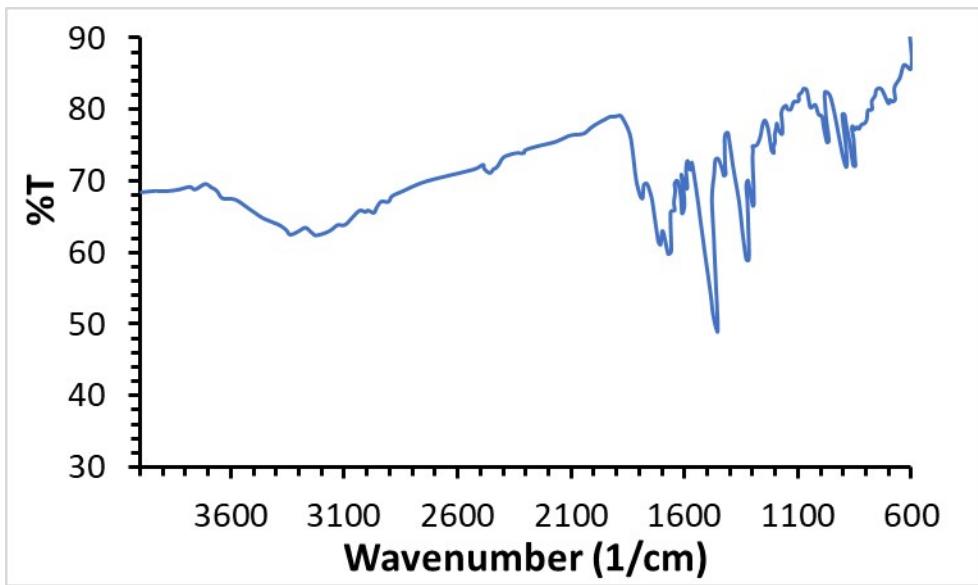
**Figure 5.** IR spectrum of compound **19**



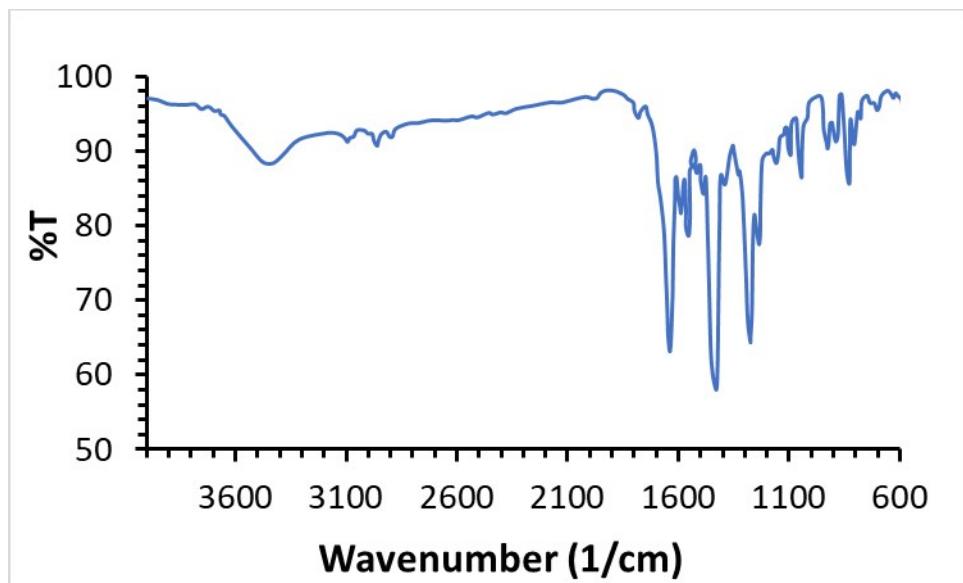
**Figure 6.** IR spectrum of compound **20**



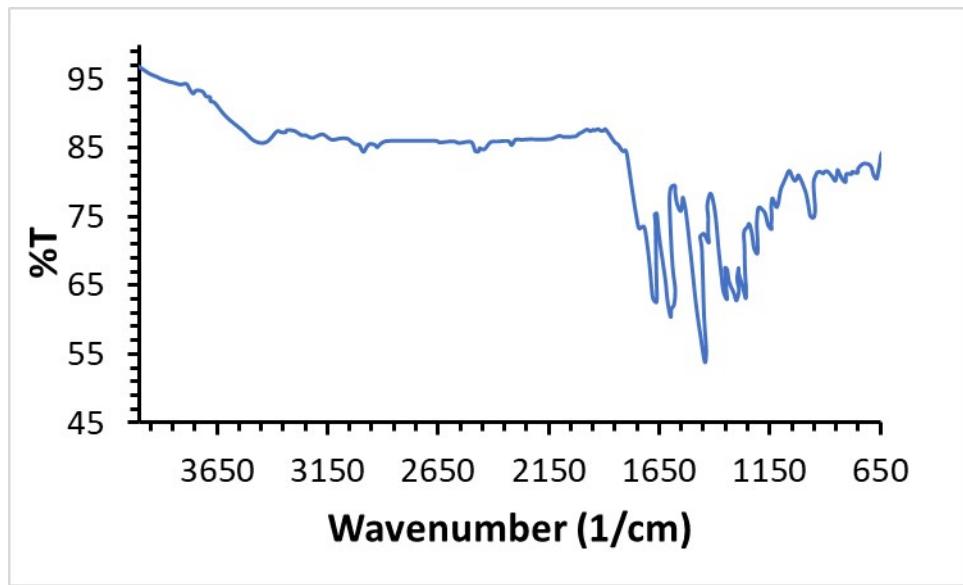
**Figure 7.** IR spectrum of compound **21**



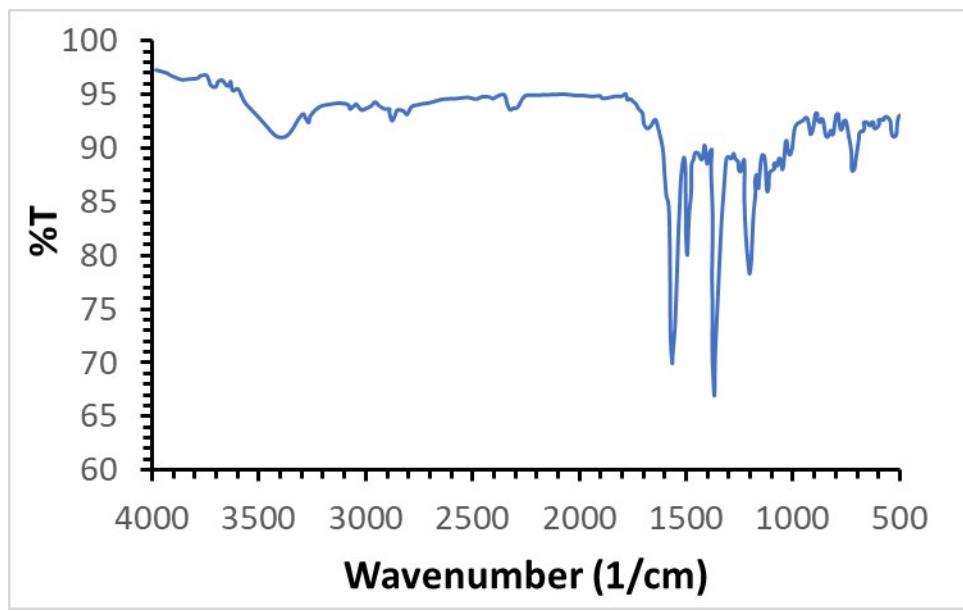
**Figure 8.** IR spectrum of compound **24**



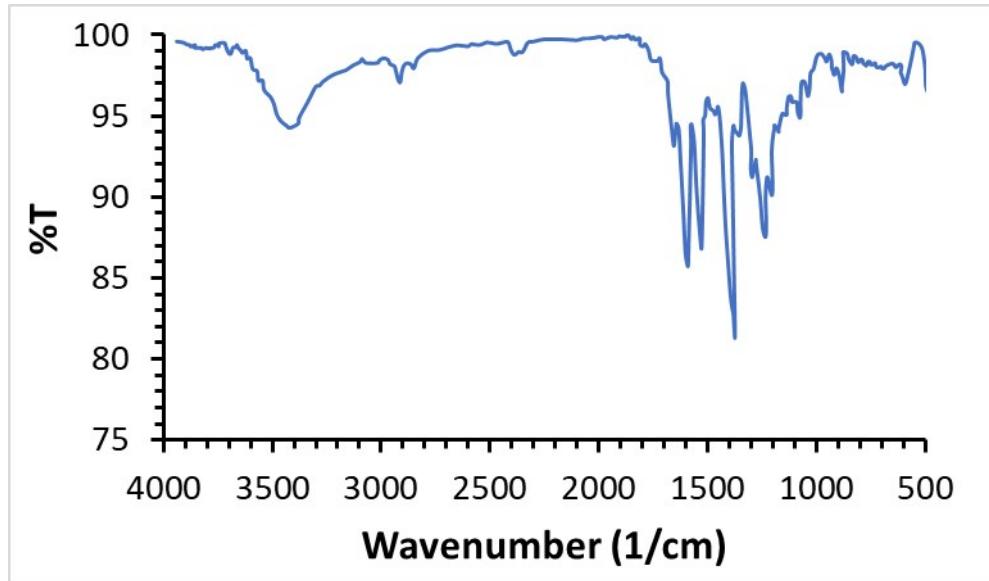
**Figure 9.** IR spectrum of compound **26**



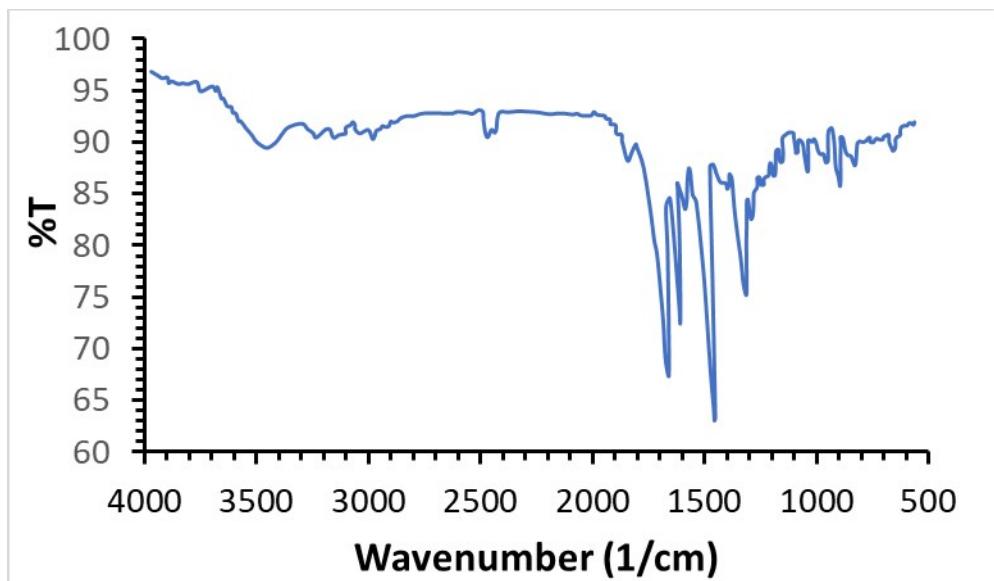
**Figure 10.** IR spectrum of compound **30**



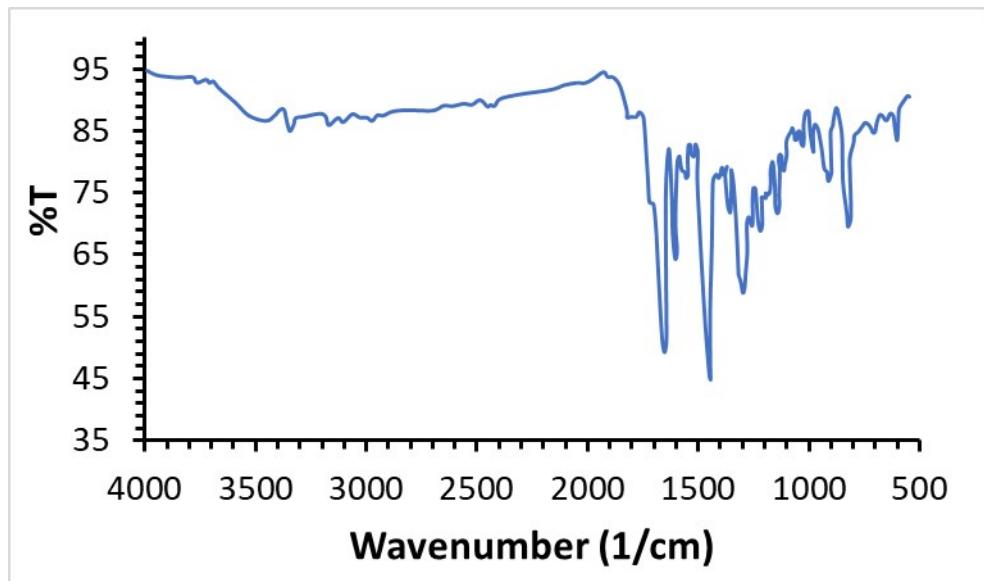
**Figure 11.** IR spectrum of compound 33



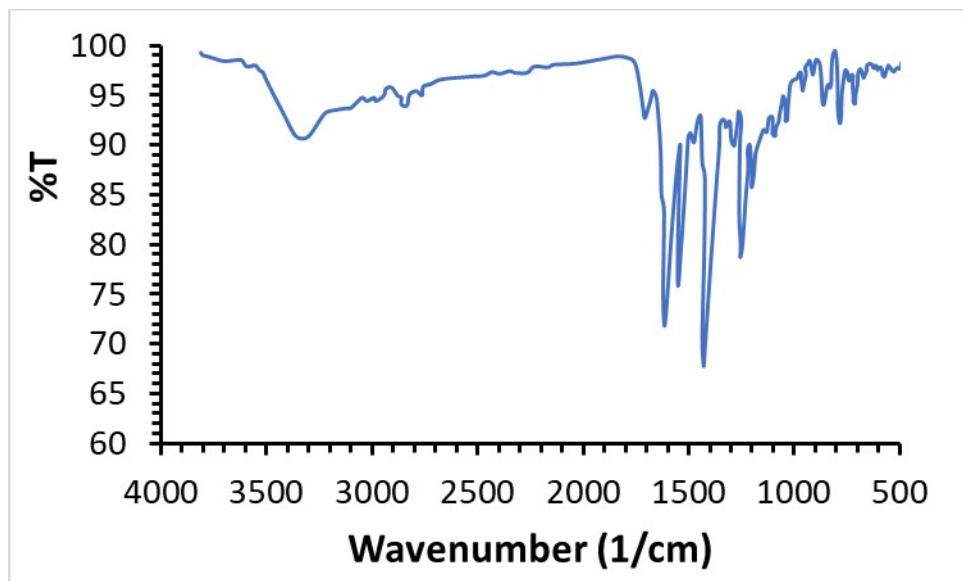
**Figure 12.** IR spectrum of compound 34



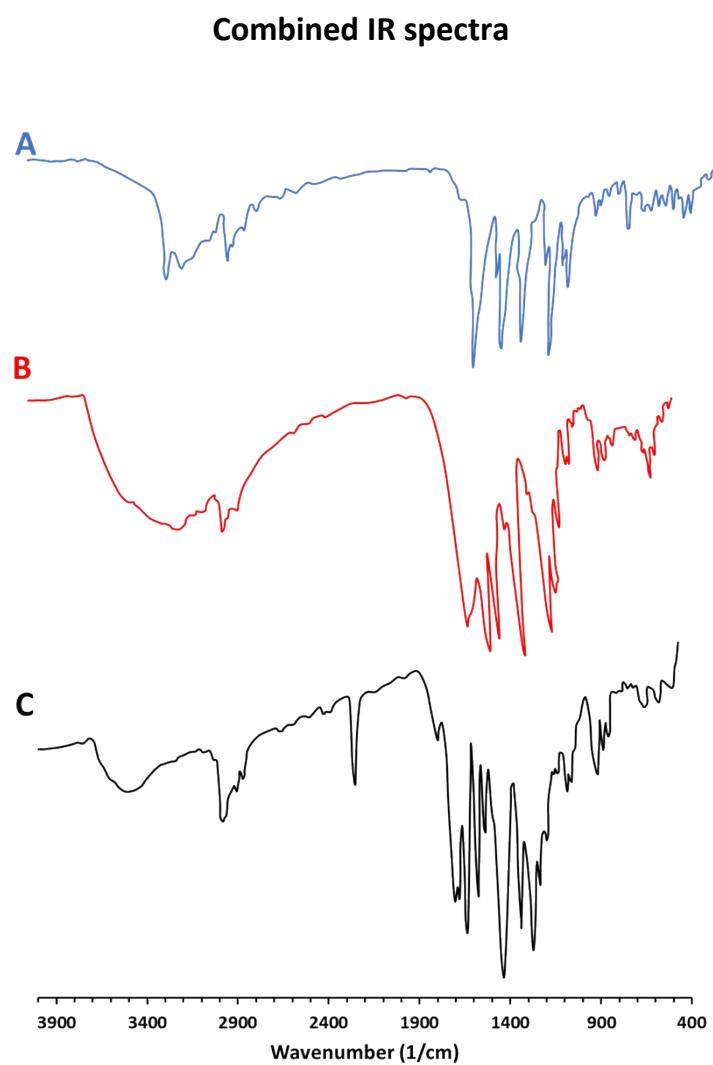
**Figure 13.** IR spectrum of compound **36**



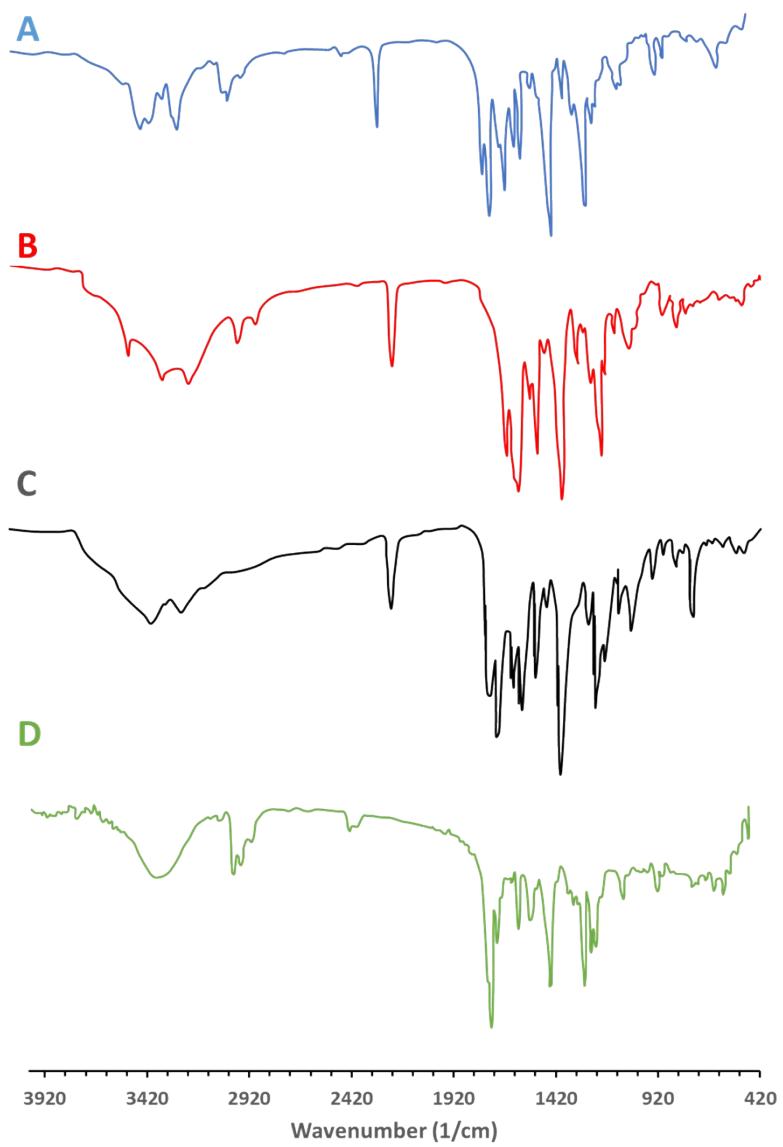
**Figure 14.** IR spectrum of compound **38**



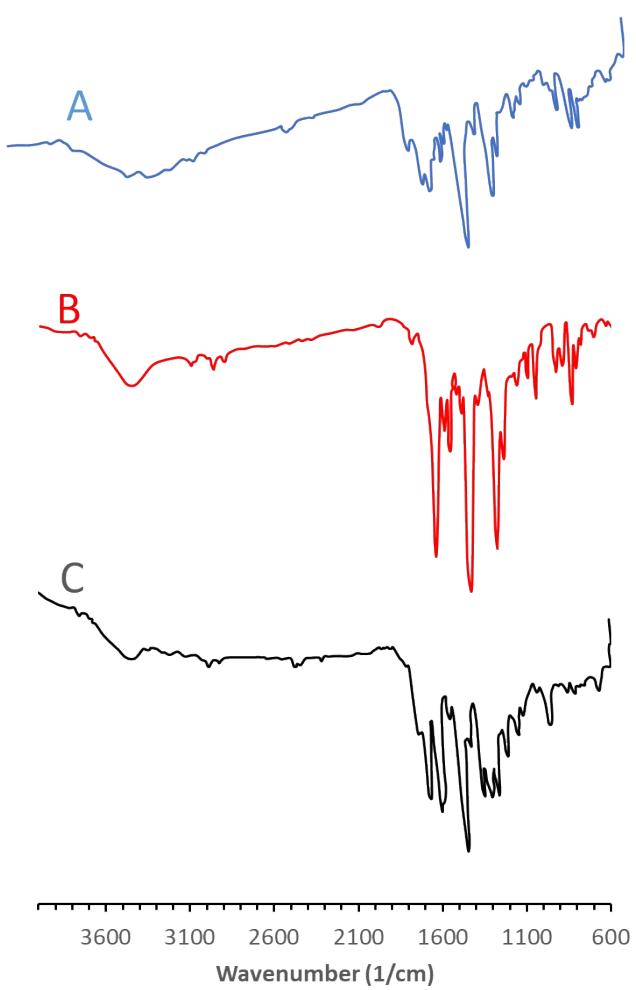
**Figure 15.** IR spectrum of compound **40**



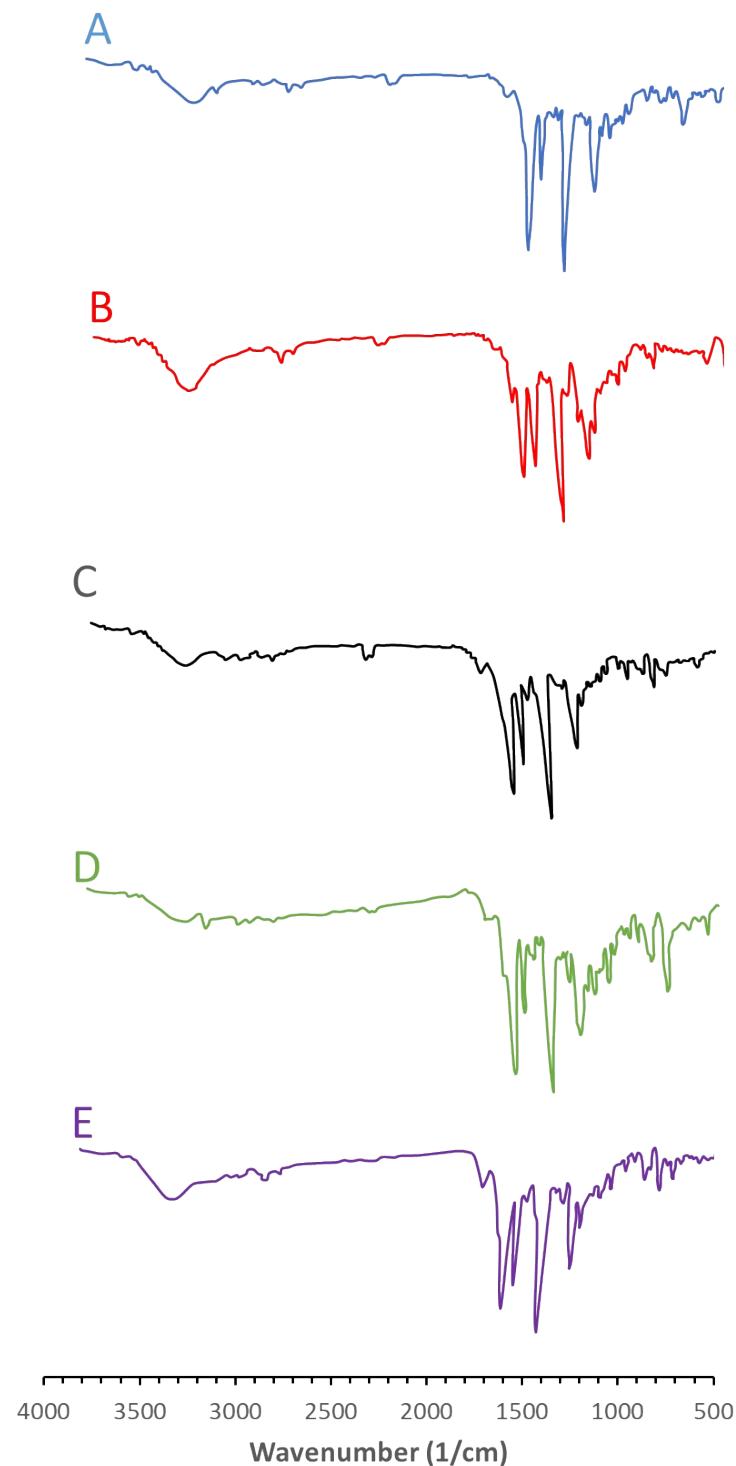
**Figure 1.** IR spectra of compounds **7 (A)** , **12 (B)** and **9 (C)**



**Figure 2.** IR spectra of compounds **16** (**A**), **19** (**B**), **20** (**C**) and **9** (**D**)



**Figure 3.** IR spectra of compounds **26** (**A**), **24** (**B**), and **30** (**C**)



**Figure 4.** IR spectra of compounds **33** (A), **34** (B), **36** (C), **38** (D) and **9** (E)