

Supplementary Material

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

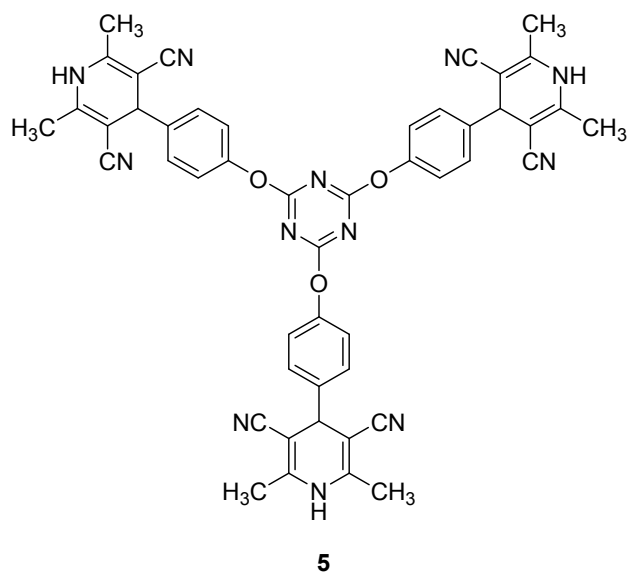
Hadeer M. Diab, Mostafa E. Salem, Ismail A. Abdelhamid* and Ahmed H. M. Elwahy*

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

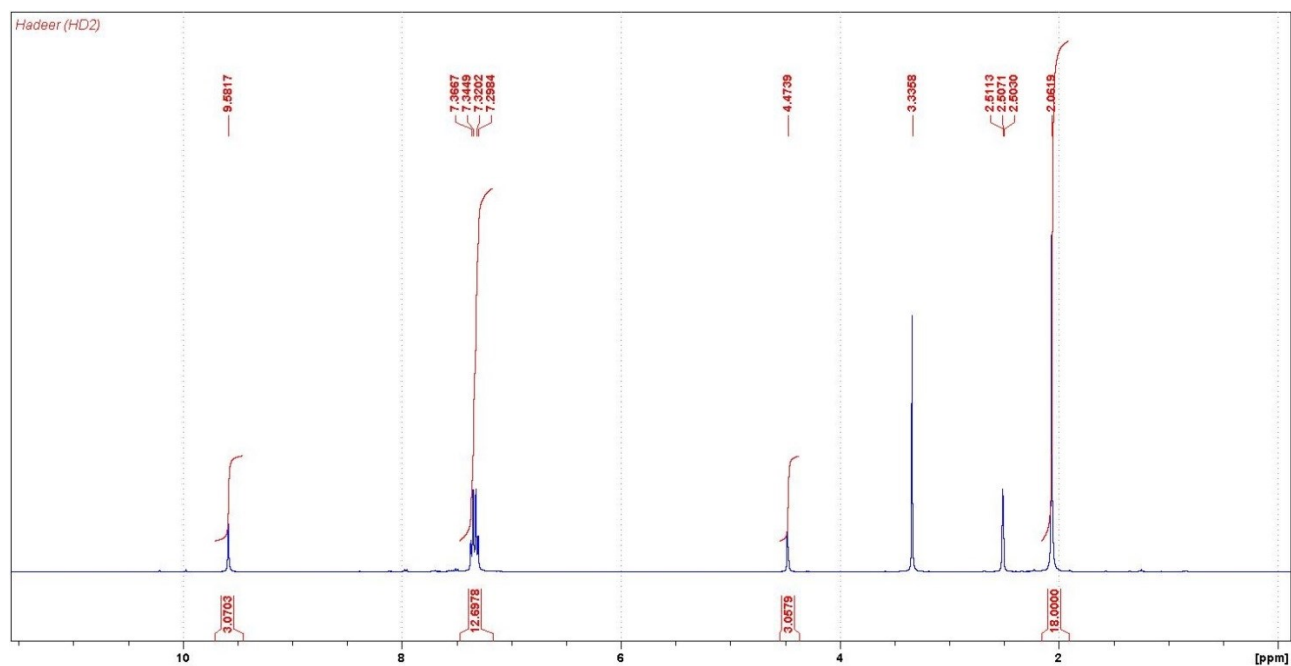
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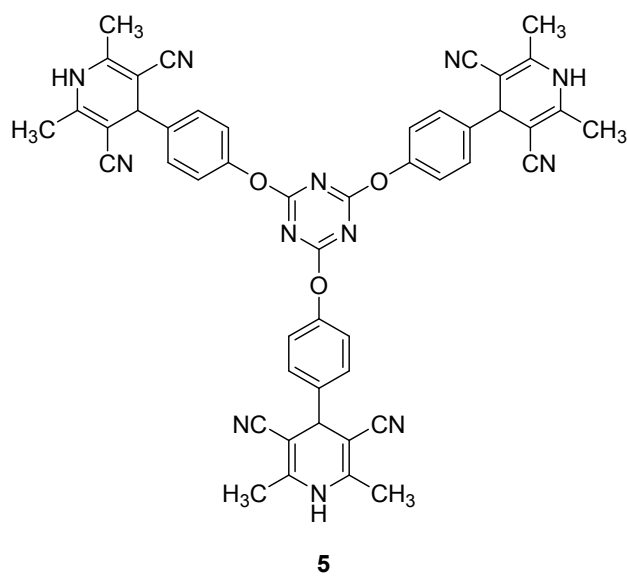
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1. IR, ^1H and ^{13}C NMR spectra for synthesized compounds

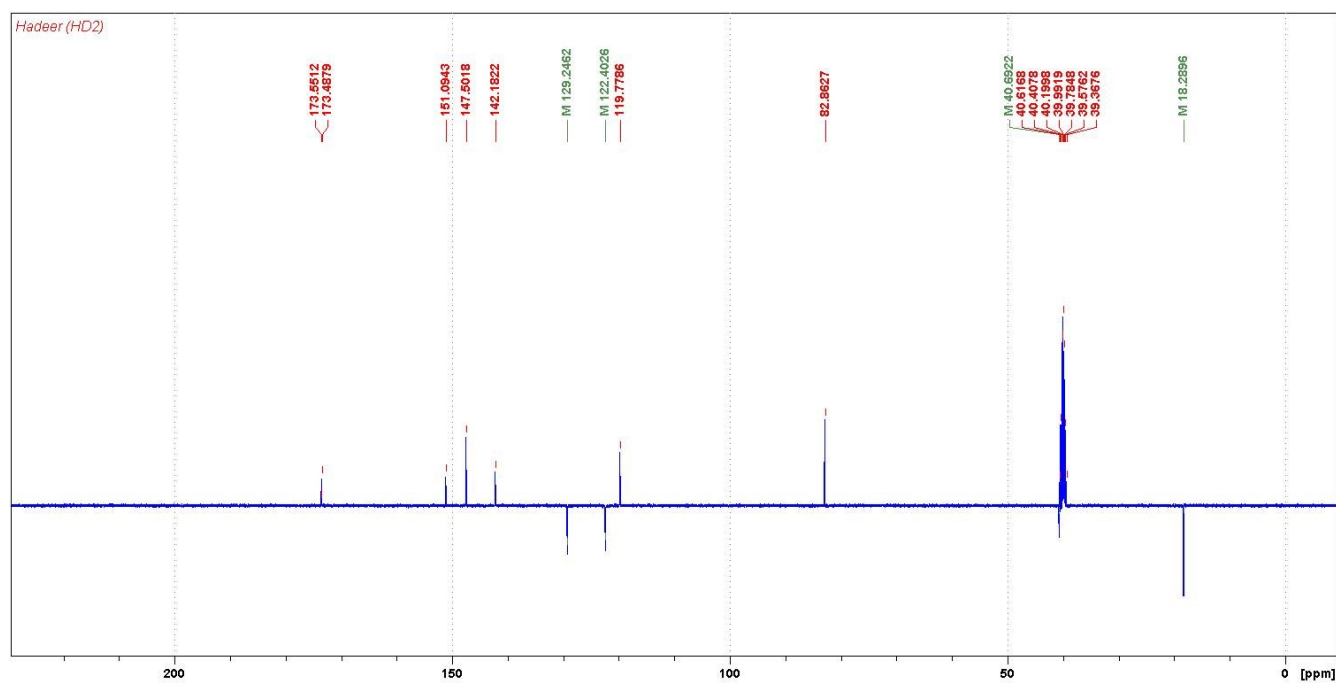


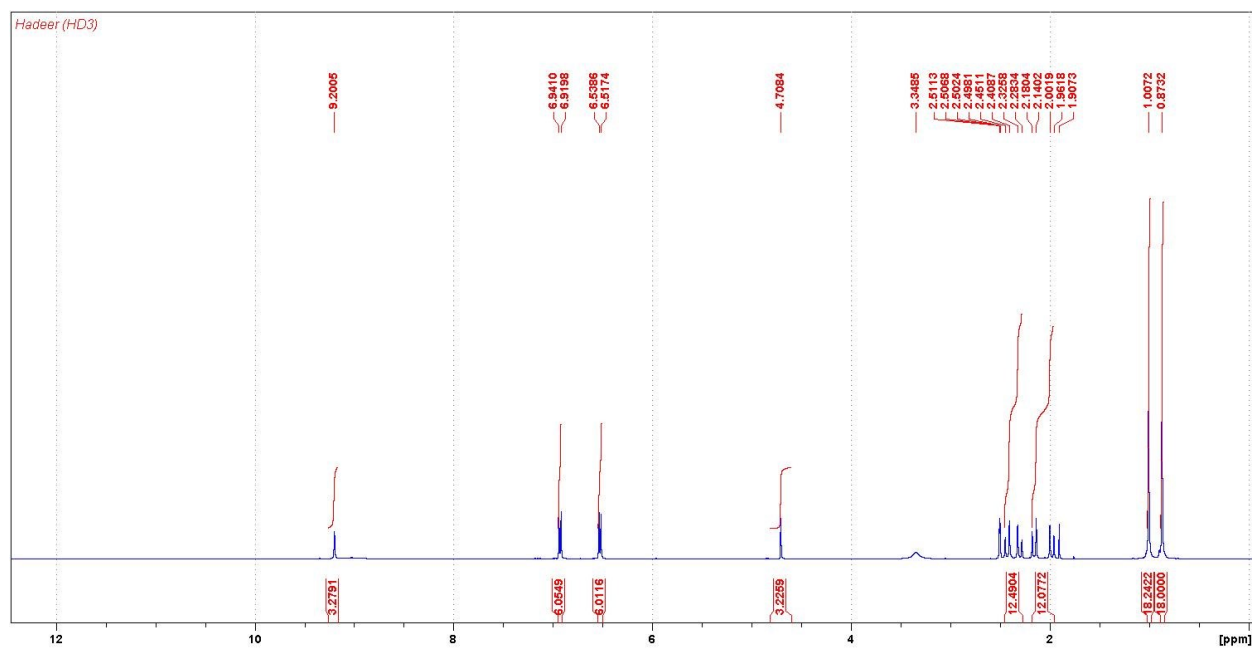
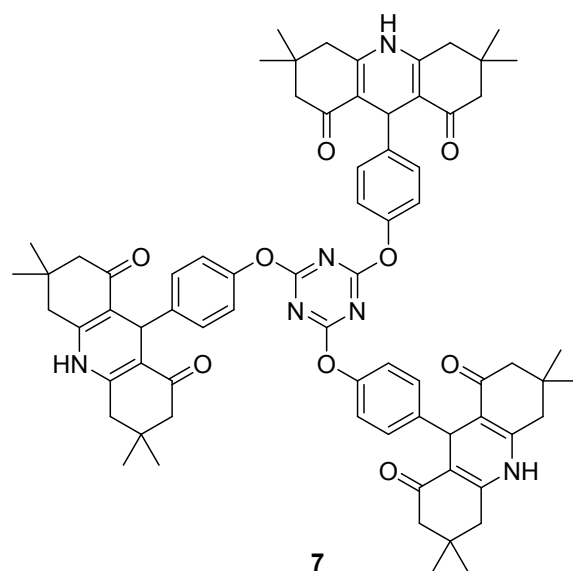
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) of compound 5



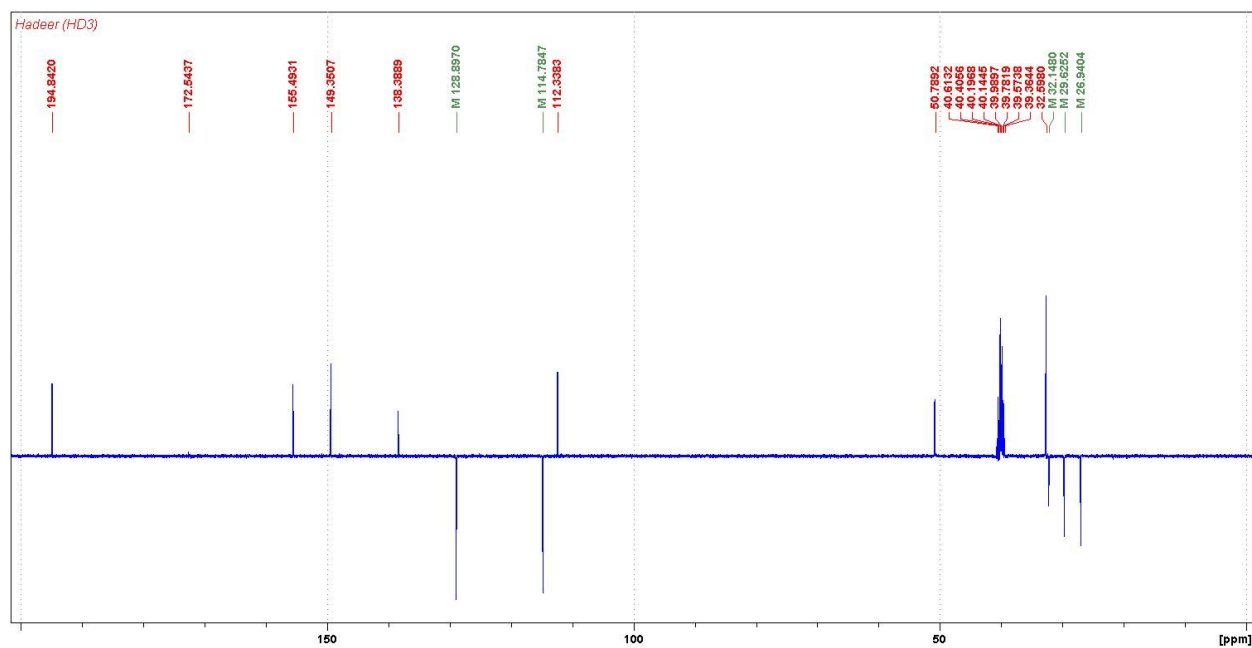
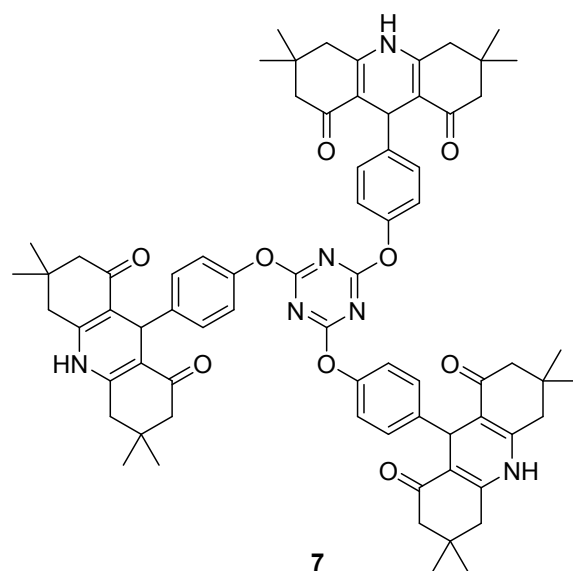


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of compound 5

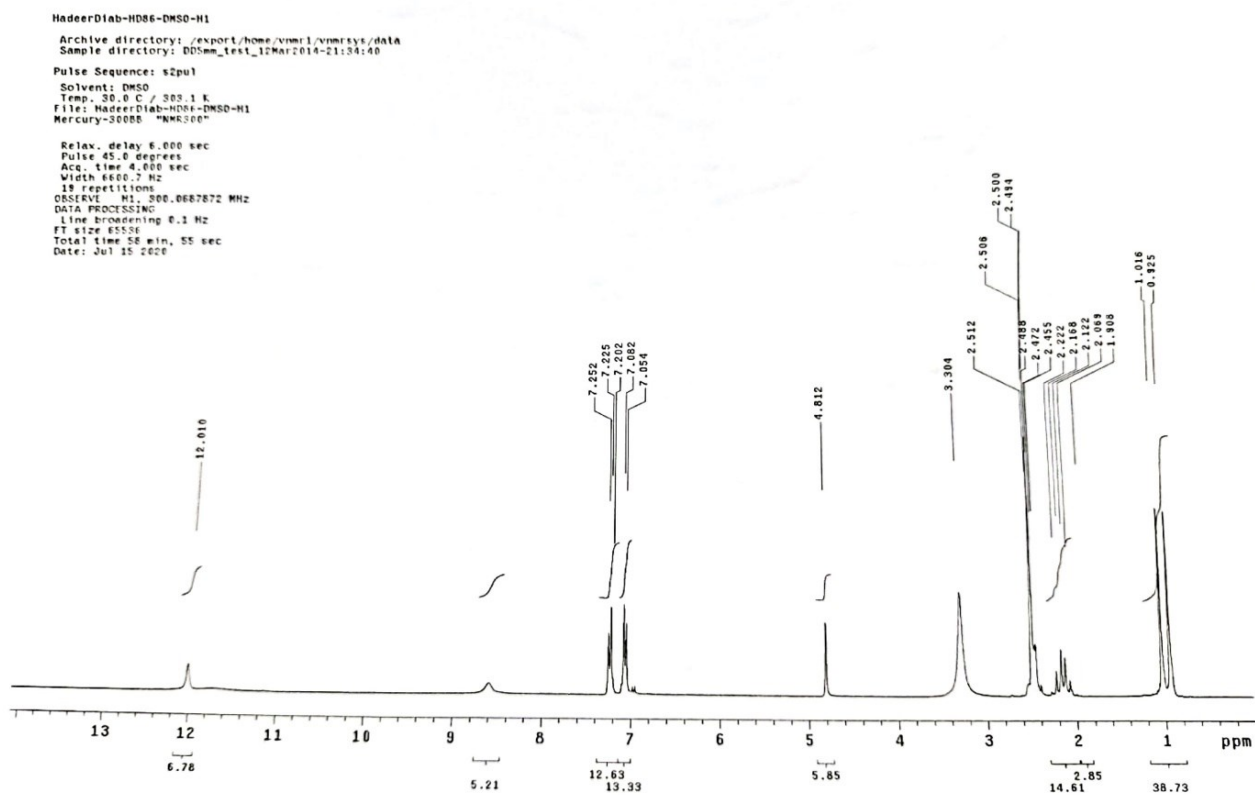
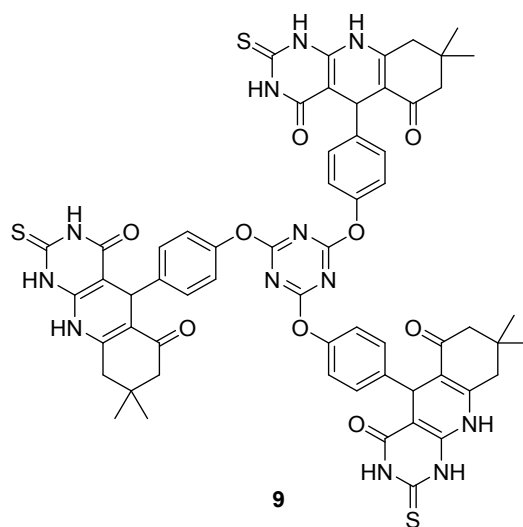




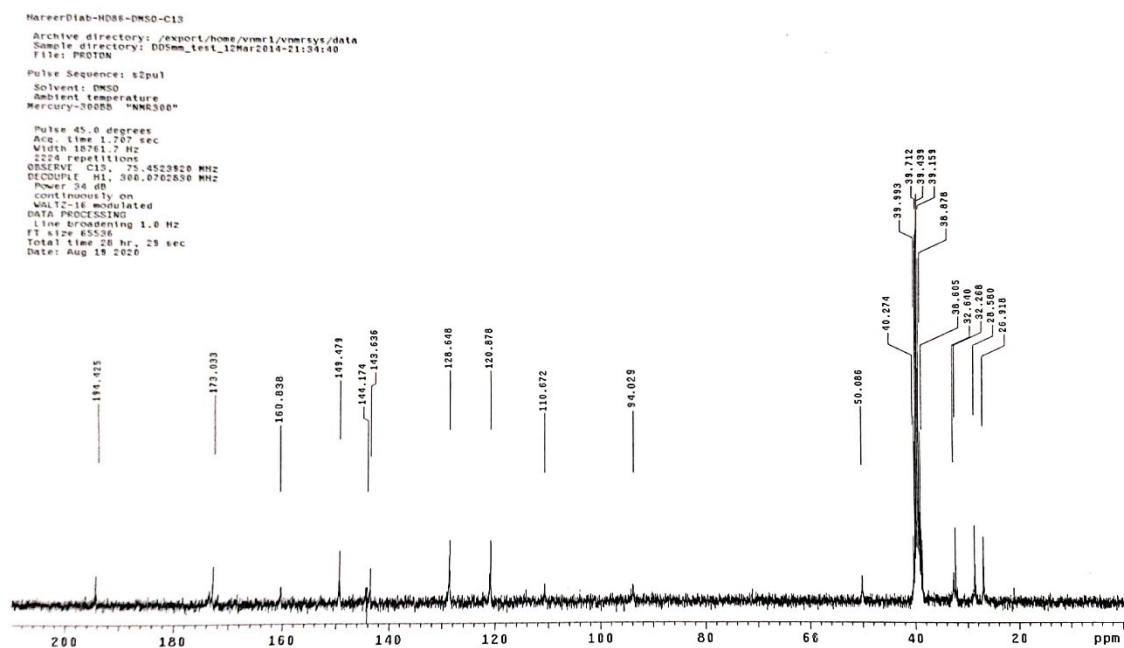
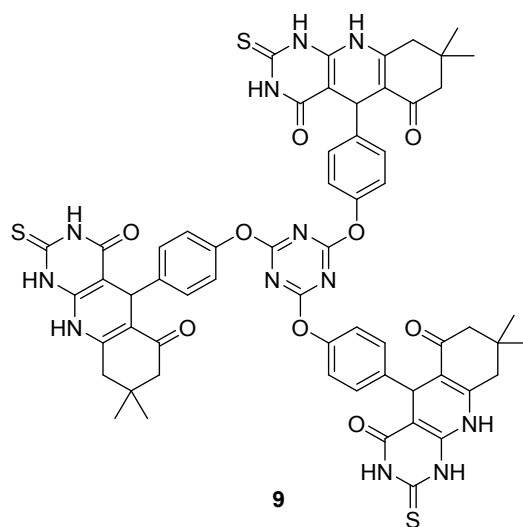
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) of compound 7



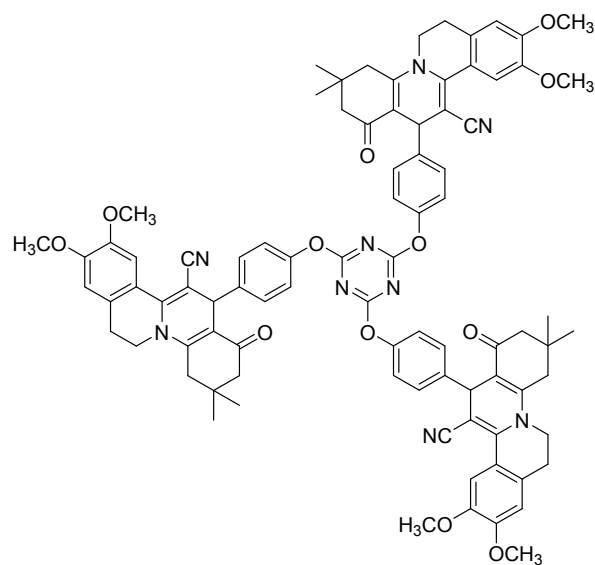
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of compound 7



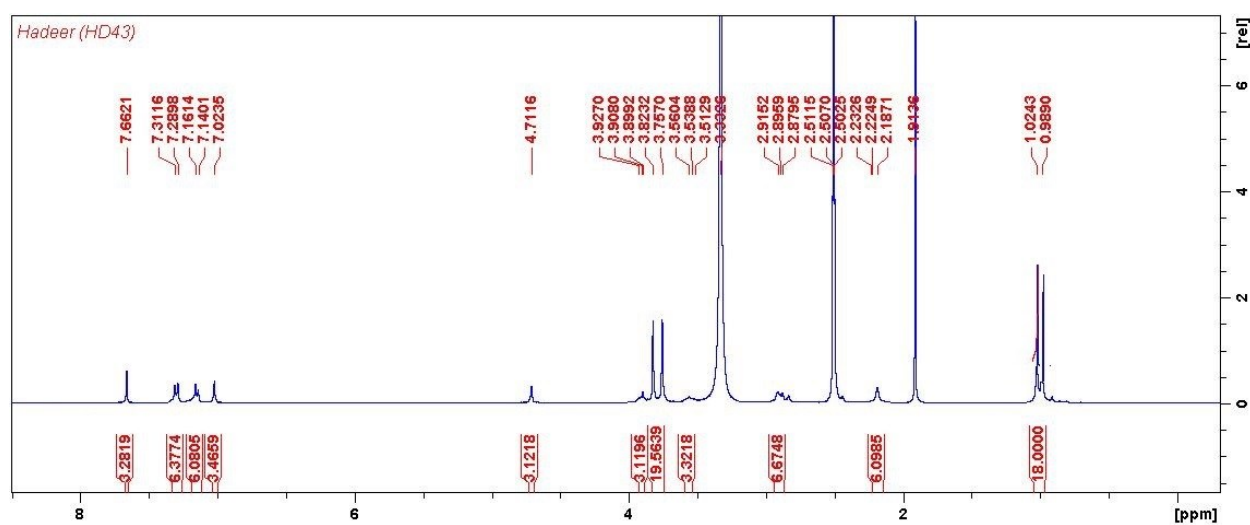
The ^1H NMR (300 MHz, $\text{DMSO}-d_6$) of compound 9



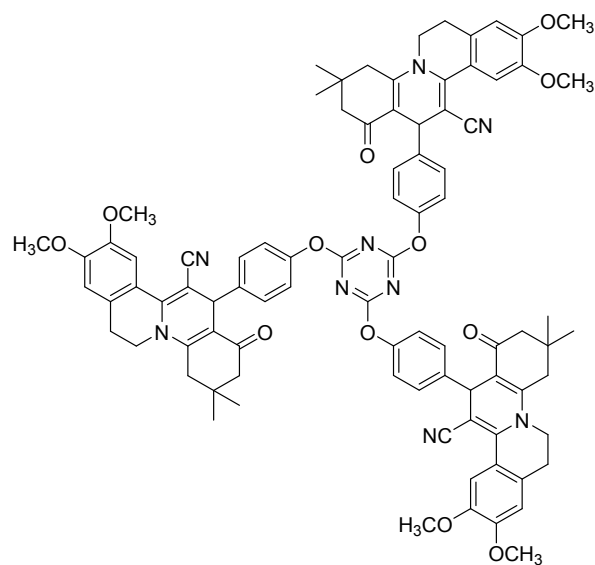
^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of compound 9



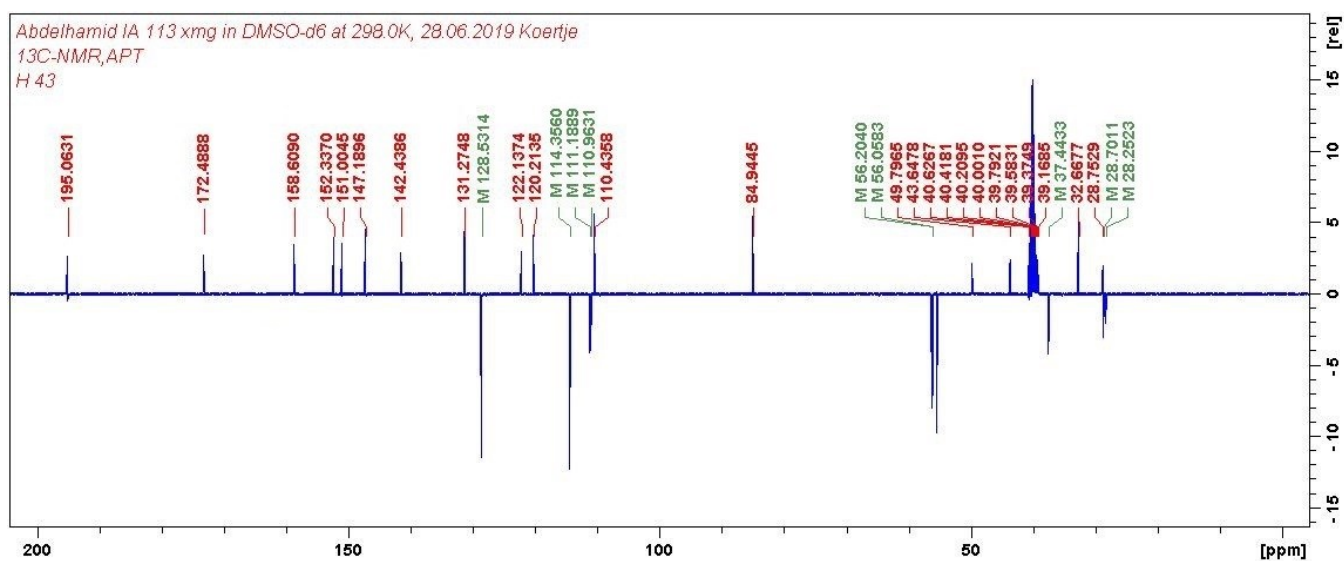
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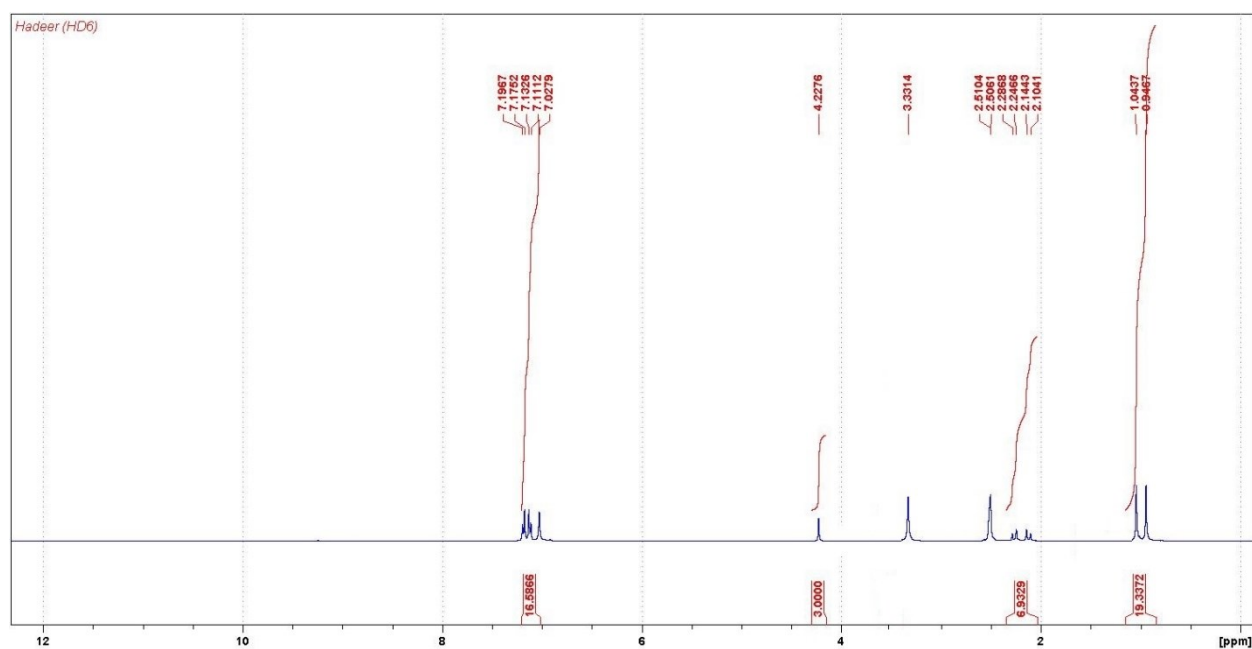
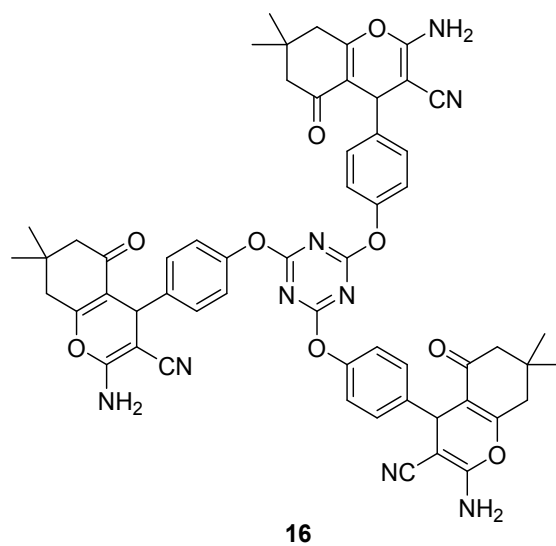
The ¹H NMR (400 MHz, DMSO-*d*₆) of compound 12



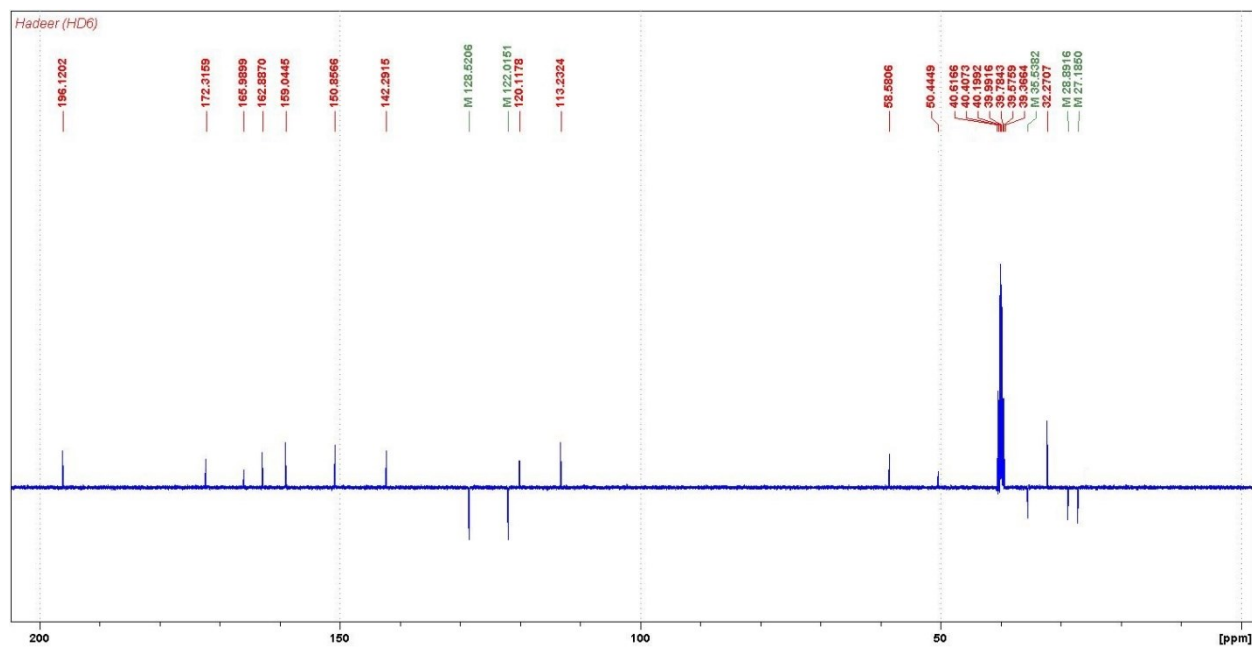
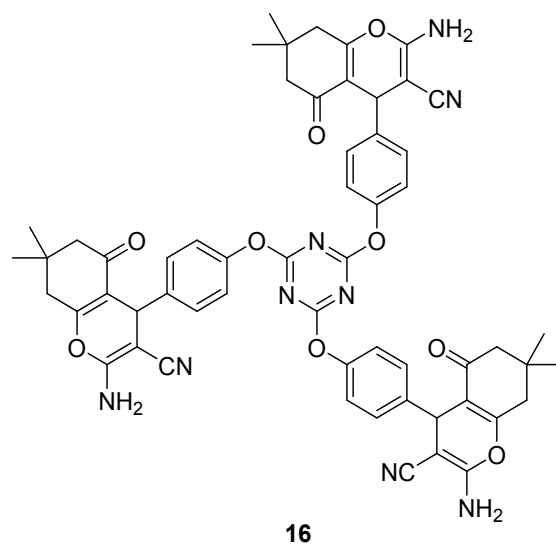
12



¹³C NMR (100 MHz, DMSO-d₆) of compound 12

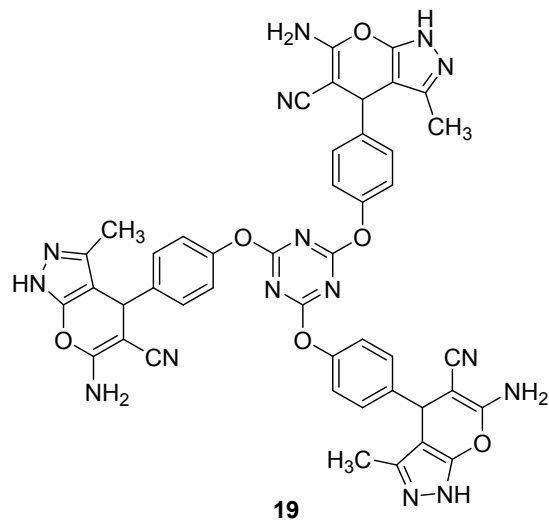


The ¹H NMR (400 MHz, DMSO-*d*₆) of compound 16



^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of compound 16





HadeerDiab-HD14-DMSO-C13

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 File: PROTON

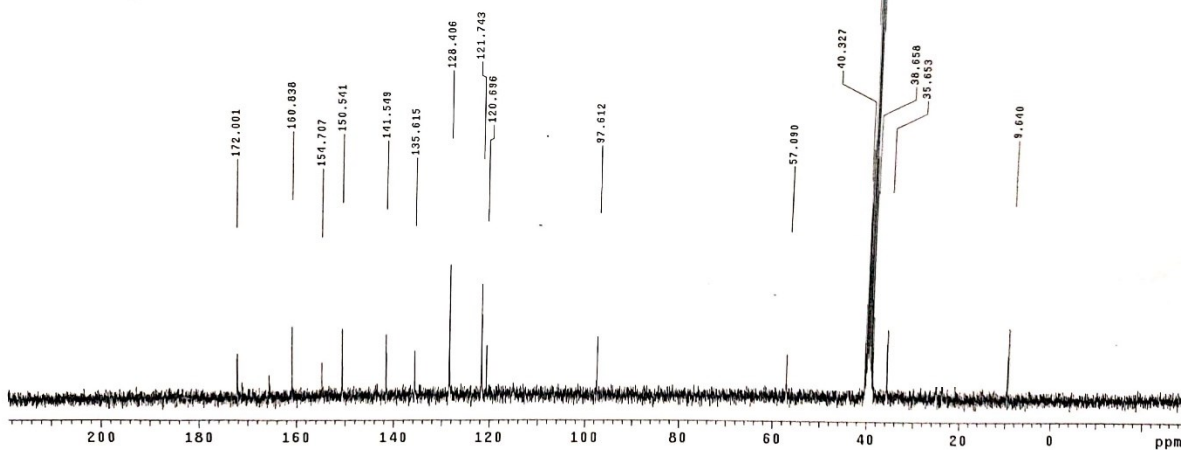
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Solvent: DMSO

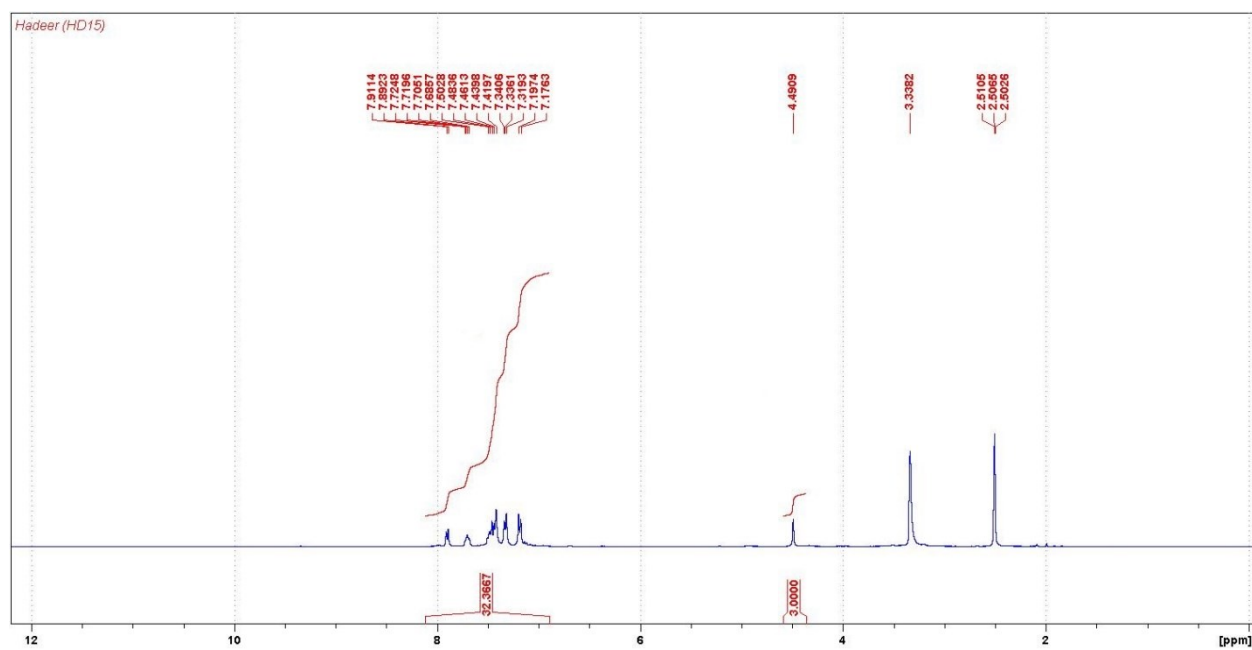
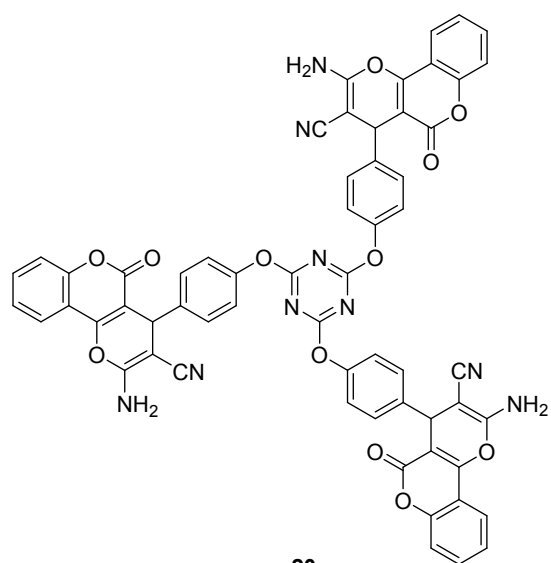
Ambient temperature

Mercury-3000B "NMR300"

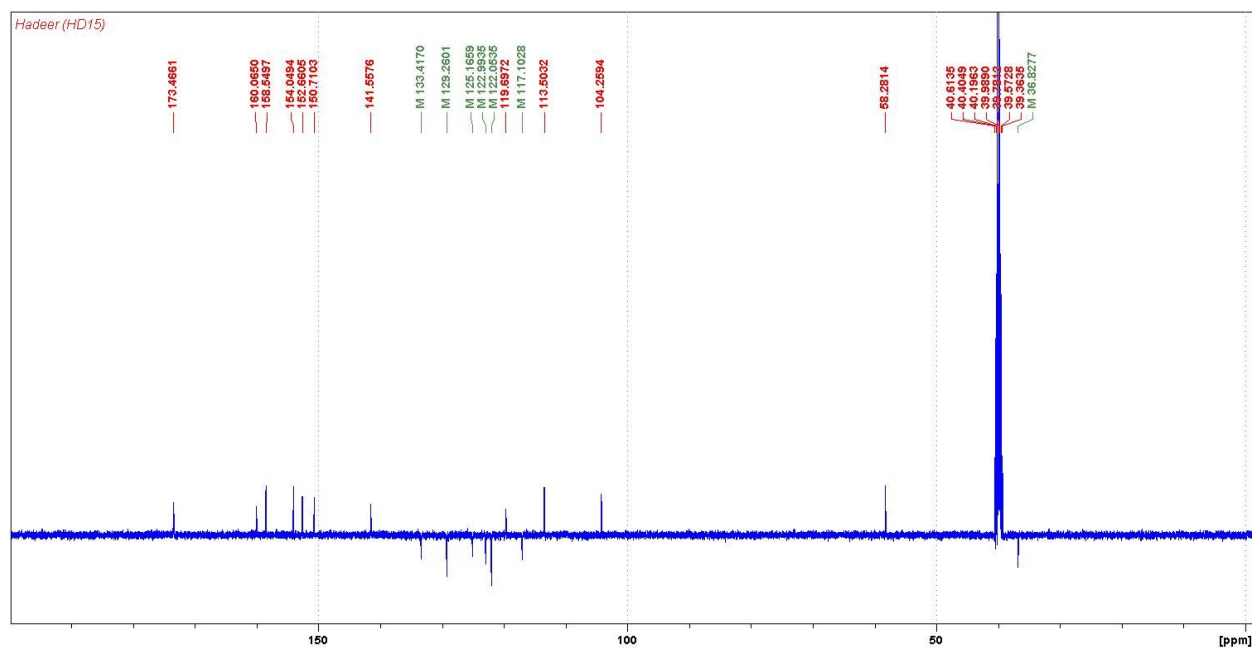
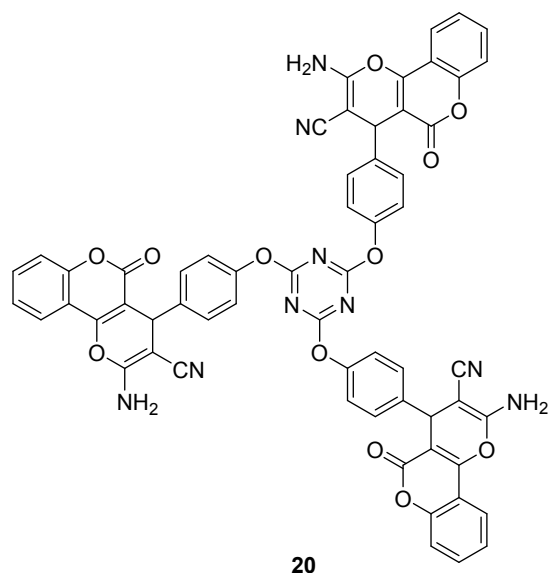
Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 5256 repetitions
 OBSERVE C13, 75.4523920 MHz
 DECOUPLE H1, 300.0702830 MHz
 Power 34 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 21 hr, 47 min, 2 sec
 Date: Nov 12 2013



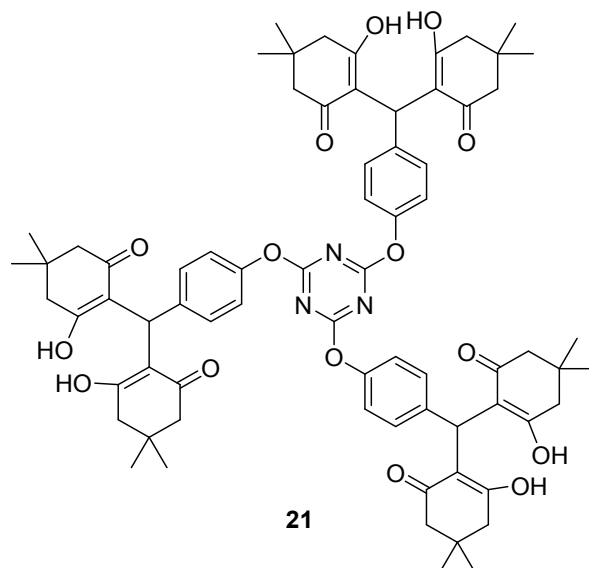
^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of compound 19



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



^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of compound 20

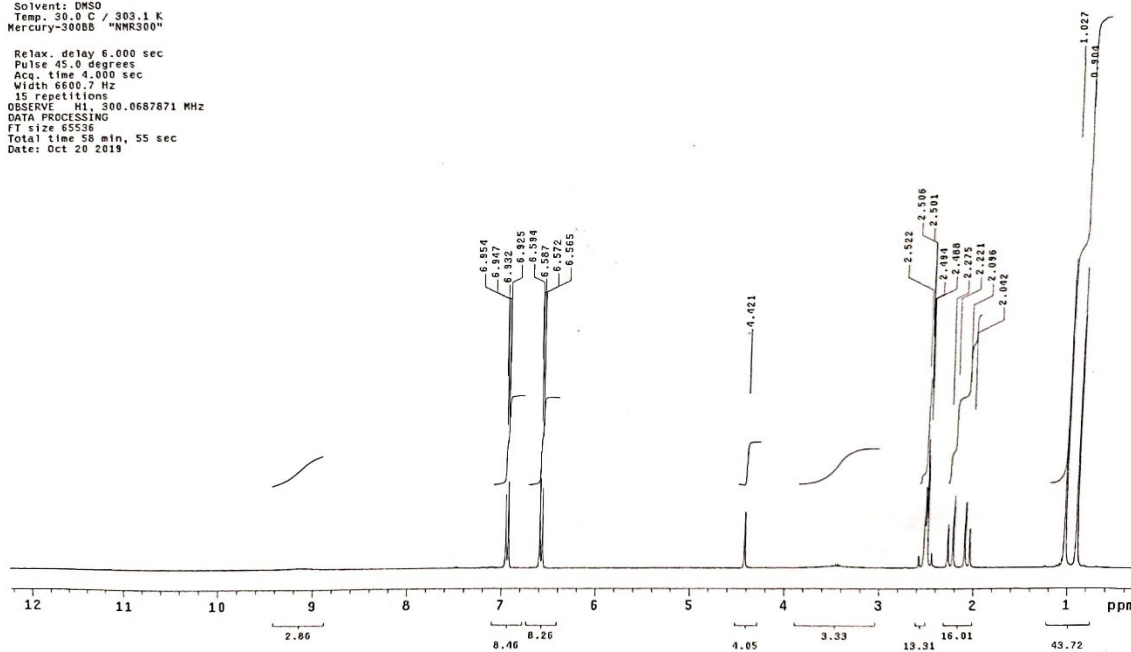


HadeerDiab-HD60-DMSO-H1

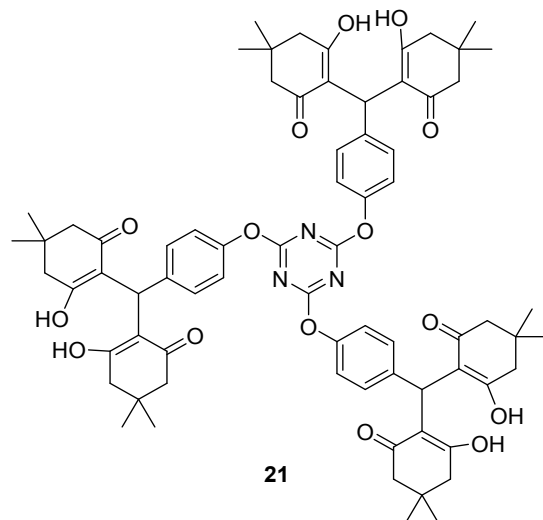
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Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

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

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Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
15 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Oct 20 2019



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



HsdeerDiab-HD60-DMSO-C13

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

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

Mercury-3000B "NMR300"

Pulse 45.0 degrees

Acq. time 1.707 sec

Width 10761.7 Hz

35000 repetitions

OBSERVE C13, 75.4528825 MHz

DECOUPLE H1, 300.6702030 MHz

Power 34 dB

continuously on

WALTZ-16 modulated

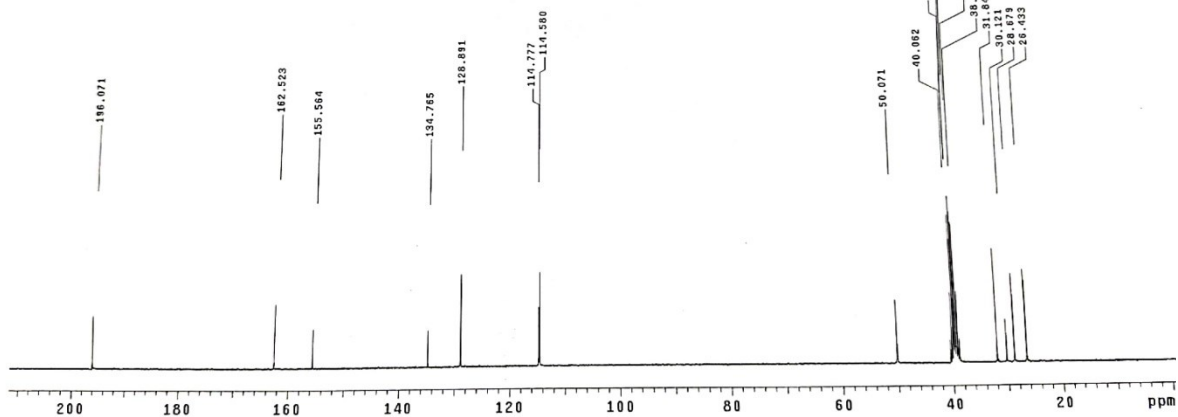
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Line broadening 1.0 Hz

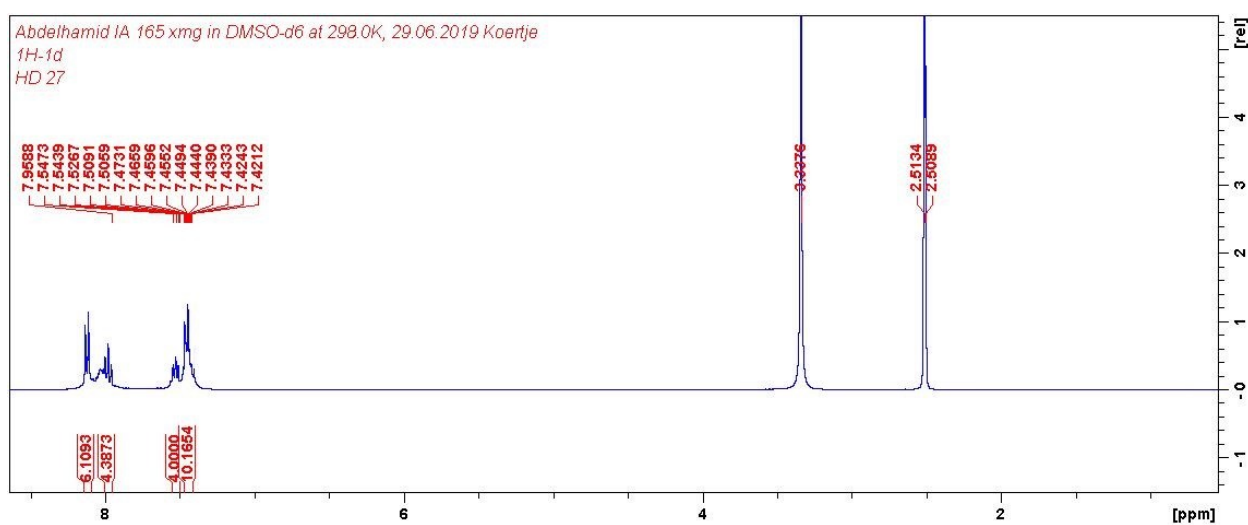
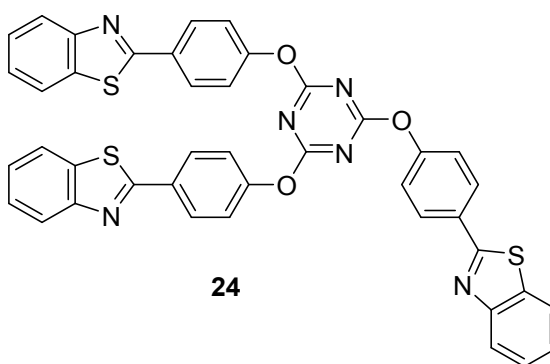
FT size 65536

Total time 21 hr, 47 min, 2 sec

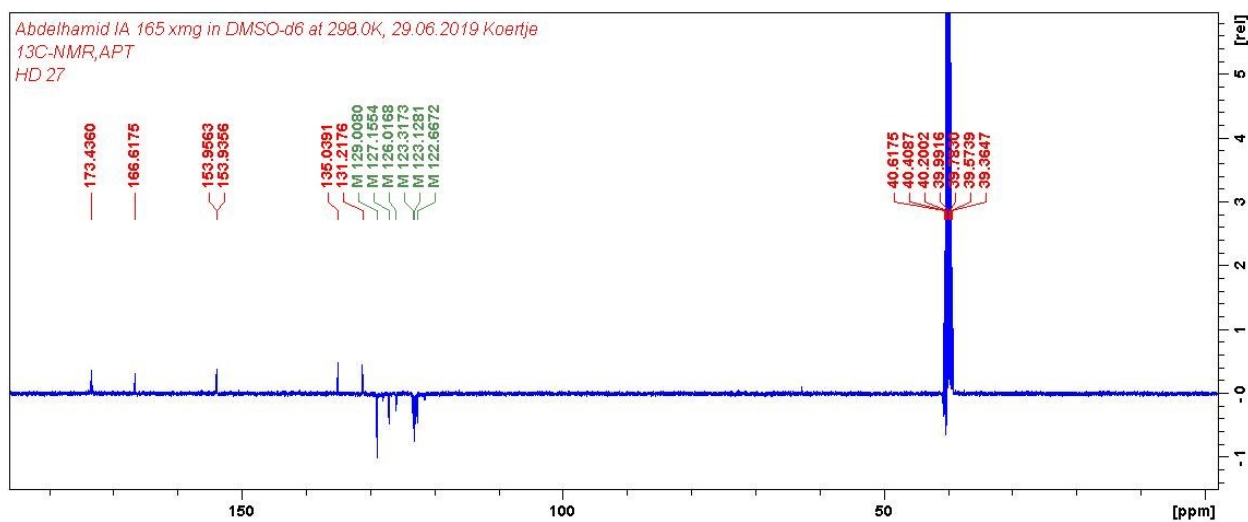
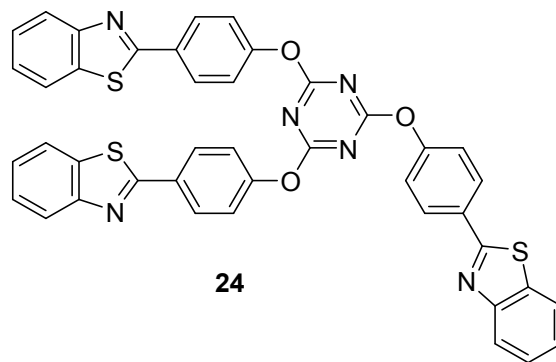
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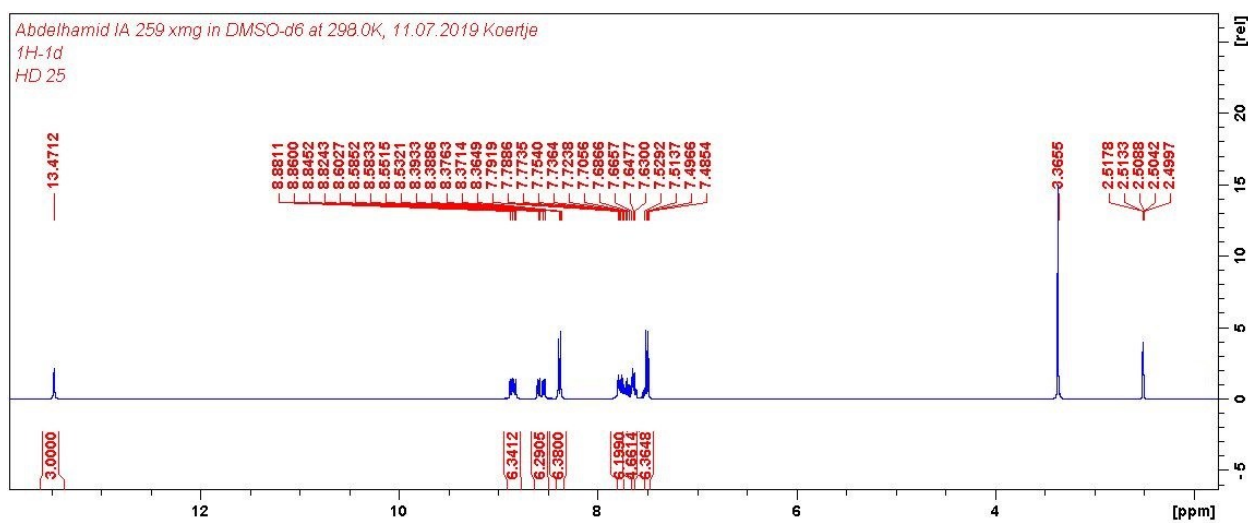
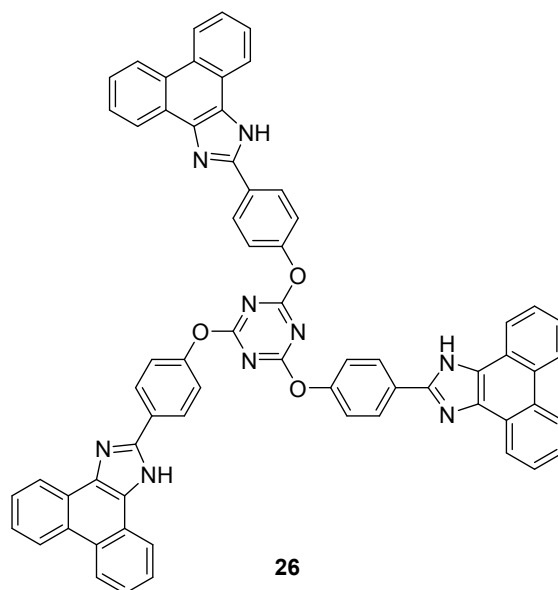
^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of compound 21



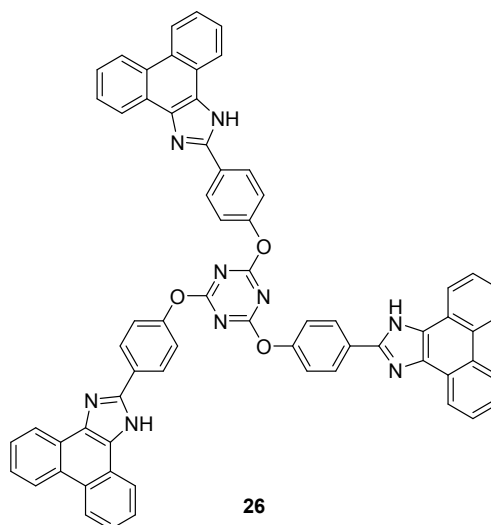
The ¹H NMR (400 MHz, DMSO-*d*₆) of compound 24



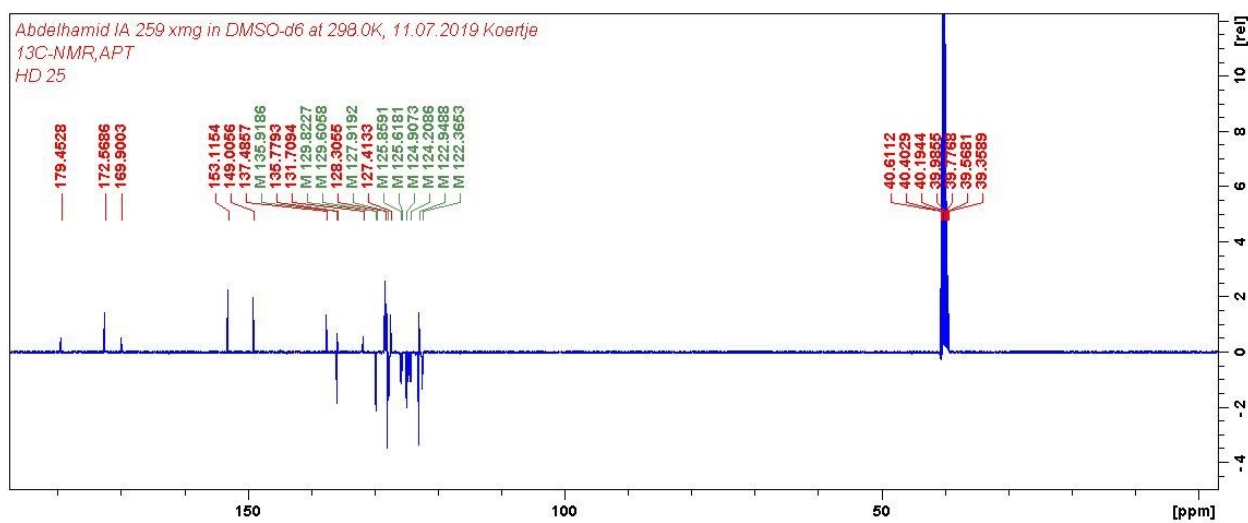
¹³C NMR (100 MHz, DMSO-*d*₆) of compound 24



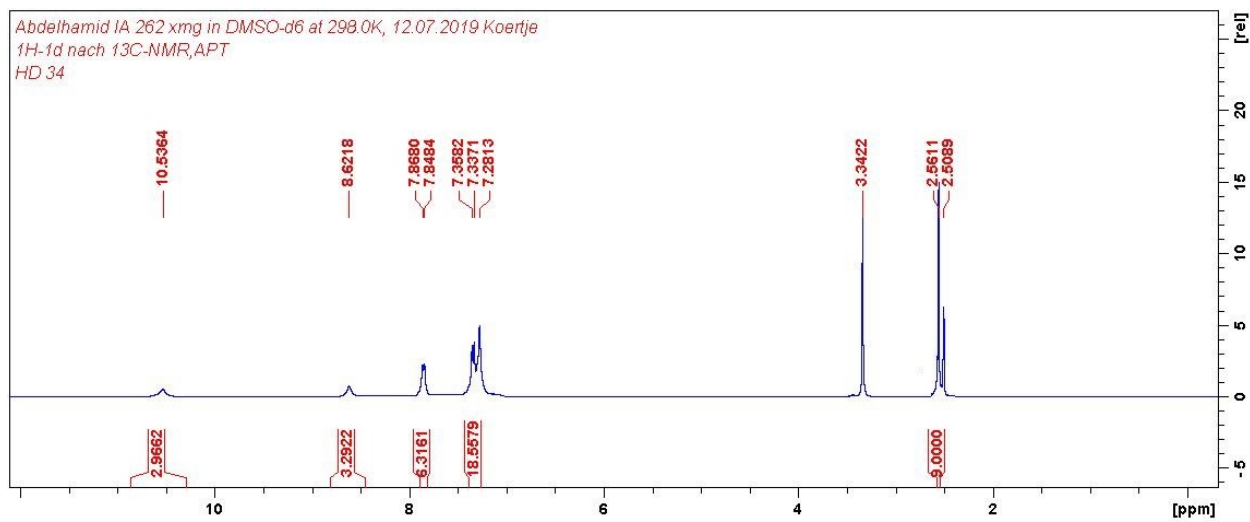
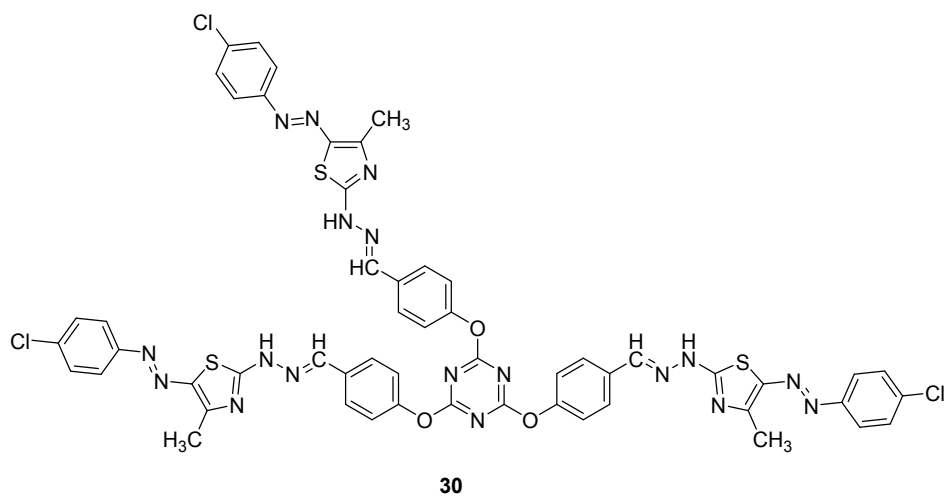
The ¹H NMR (400 MHz, DMSO-*d*₆) of compound 26



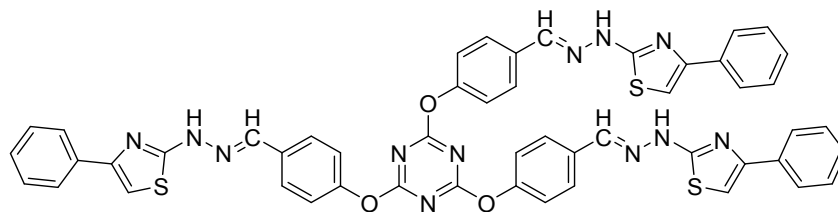
26



¹³C NMR (100 MHz, DMSO-*d*₆) of compound 26



The ¹H NMR (400 MHz, DMSO-*d*₆) of compound 30



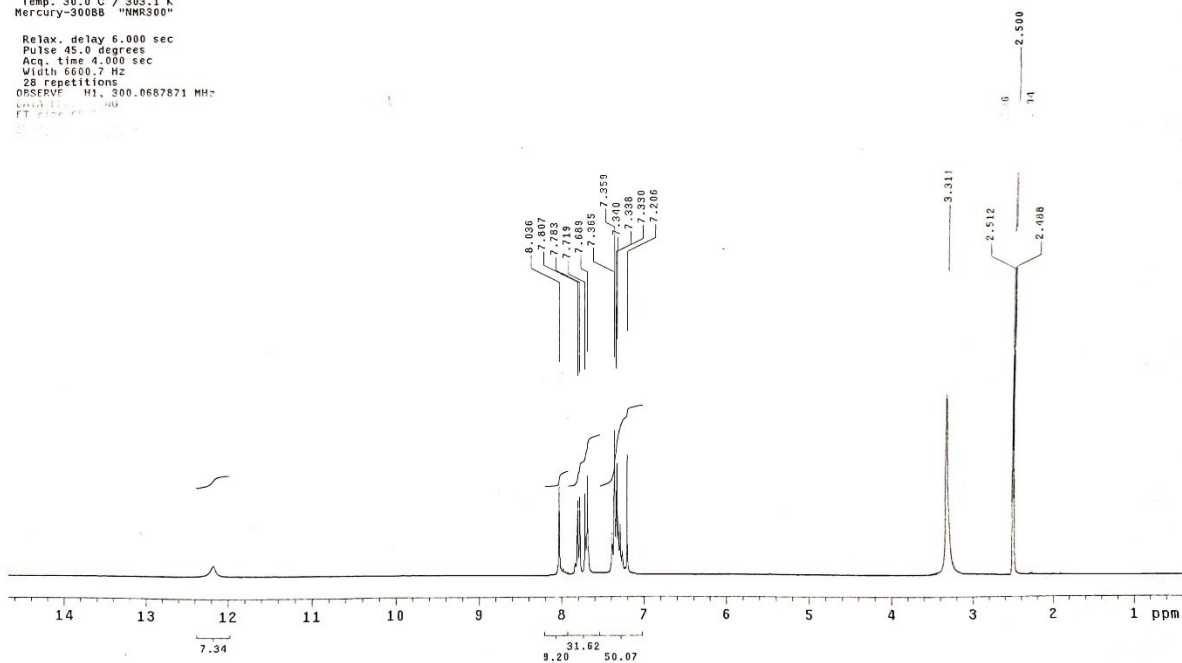
33

SaiedGhozlan-HD54-DMSO-H1

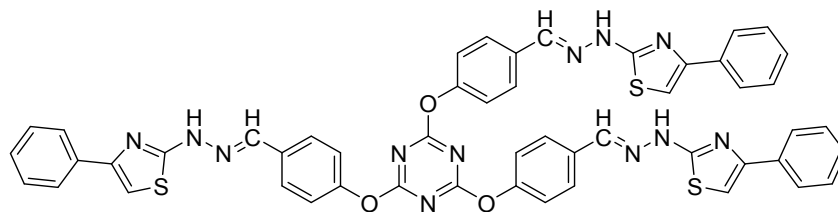
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Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

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
28 repetitions
OBSERVE H1: 300.0687871 MHz
UNIT 1: 100
FT 0.00000000



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



33

SafedGhozlan-HD54-DMSO-C13

Archive directory: /export/home/vmr1/vnmr/sys/data
Sample directory: D05mm_test_12Mar2014-21:54:40
File: PROTON

Pulse Sequence: s2pul

Solvent: DMSO

Temp. 30.0 C / 303.1 K

Mercury-300BS "NMR300"

Pulse 45.0 degrees

Acq. time 1.707 sec

Width 18761.7 Hz

1576 repetitions

OBSERVE C13, 75.4523648 MHz

DECOUPLE H1, 300.0702630 MHz

Power 34 dB

Continuously on

WALTZ-16 modulated

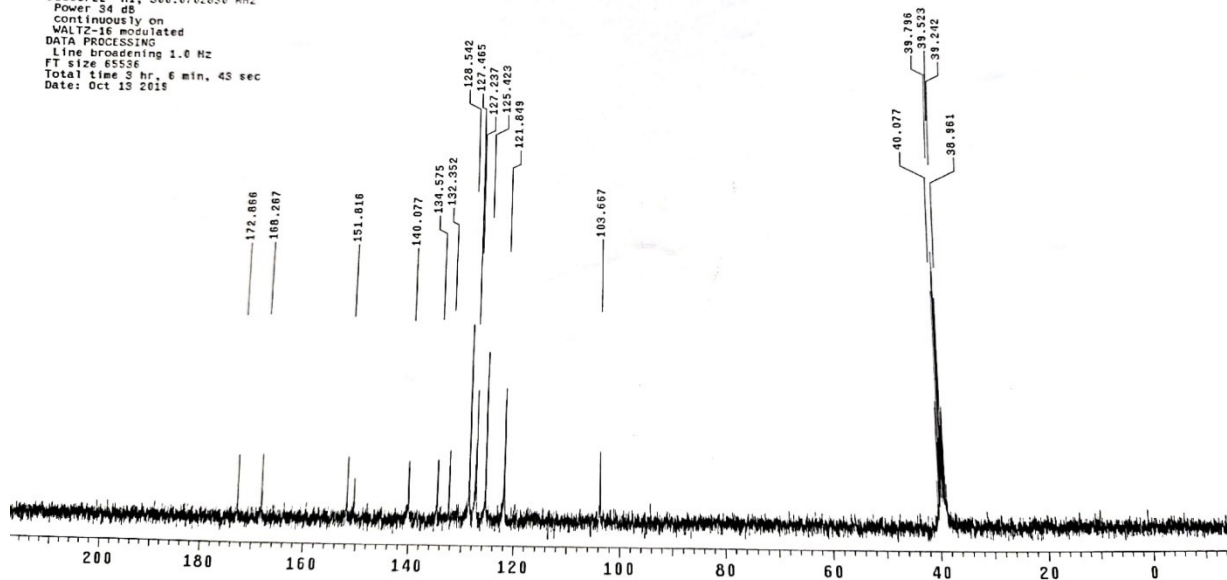
DATA PROCESSING

Line broadening 1.0 Hz

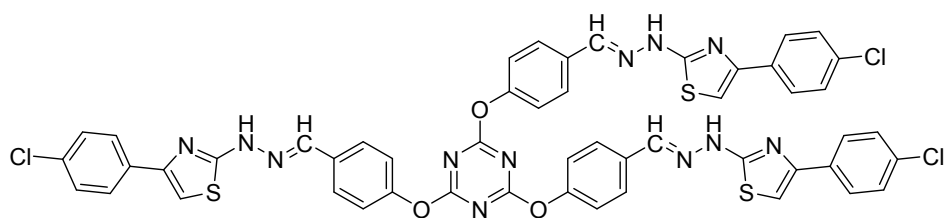
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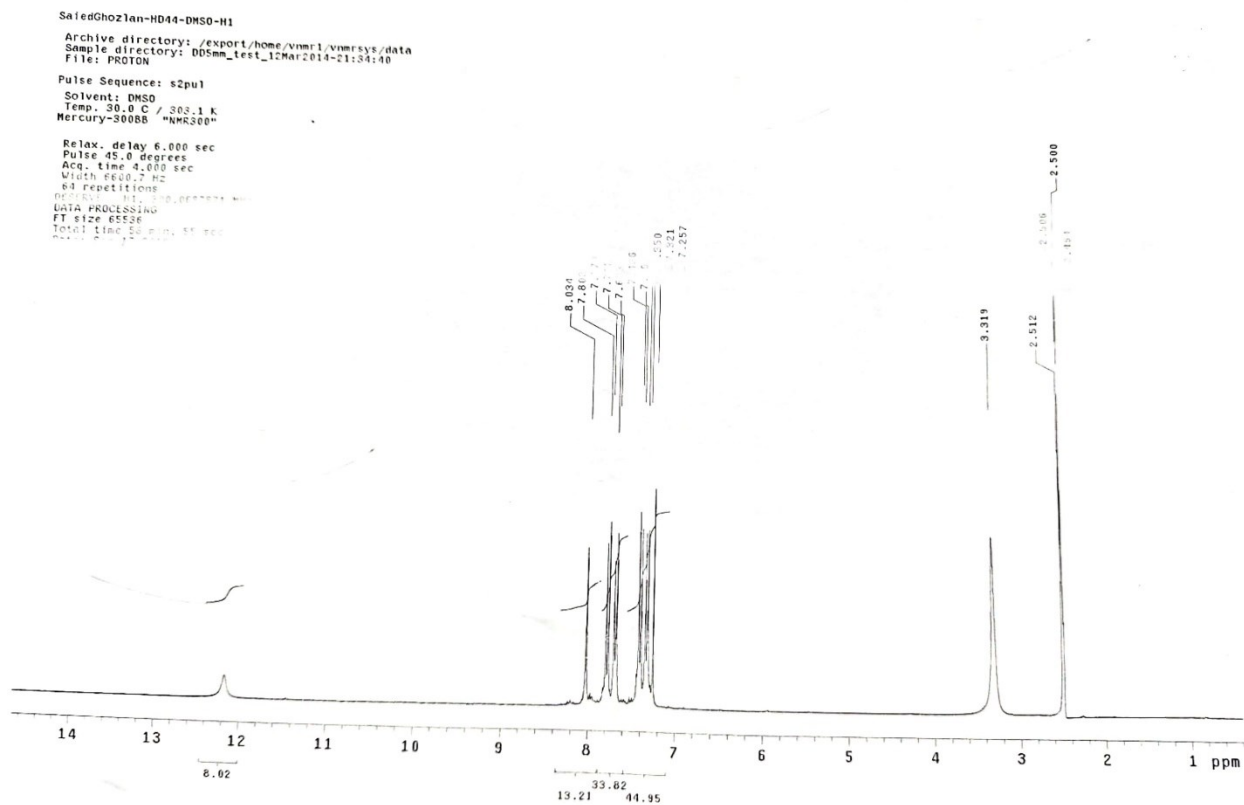
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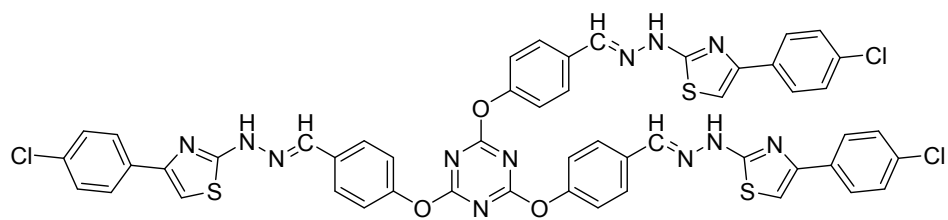
^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of compound 33



34



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



34

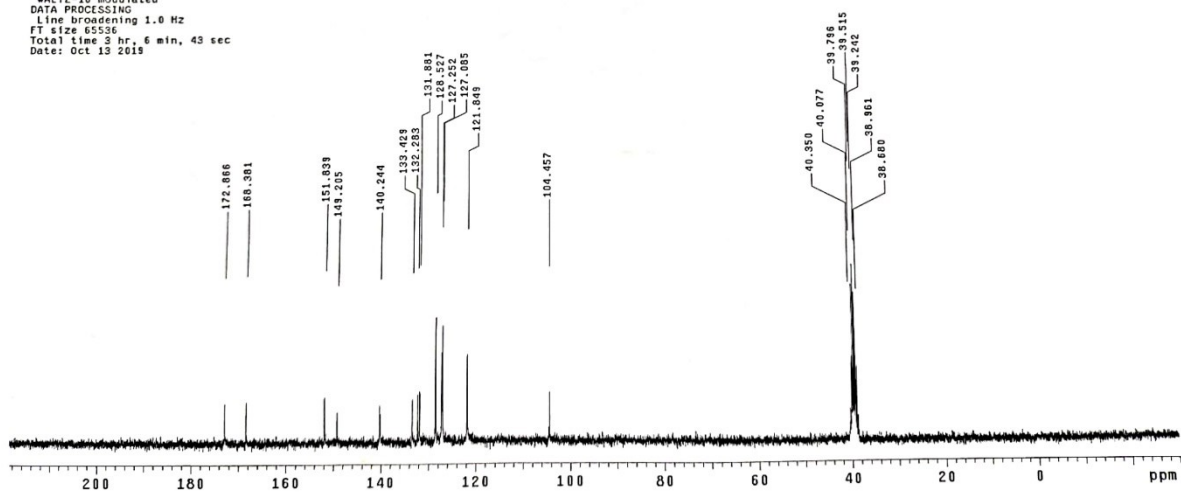
IbrahimZaky-HD44-DMSO-C13

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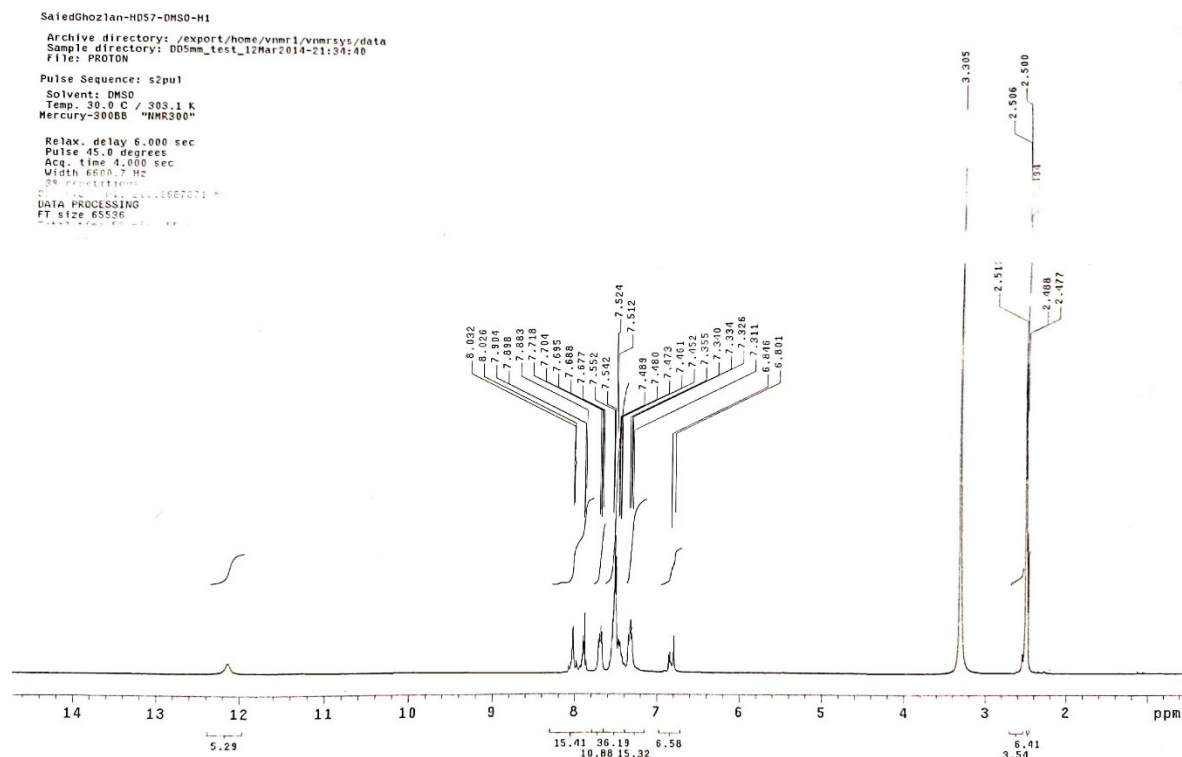
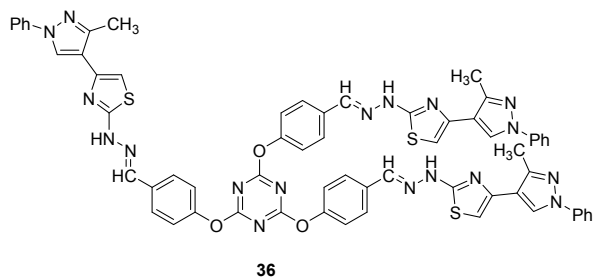
Pulse Sequence: s2pul

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

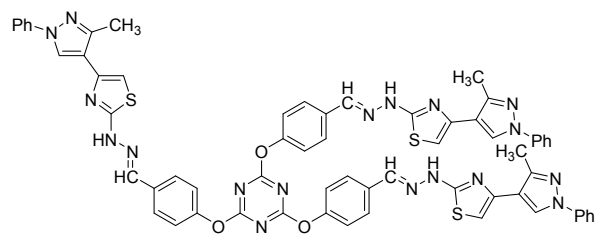
Pulse 45.0 degrees
Acq. time 1.707 sec
Width 16761.7 Hz
2768 repetitions
OBSERVE C13, 75.4523948 MHz
DECOUPLE H1, 300.0702850 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 3 hr, 6 min, 43 sec
Date: Oct 13 2019



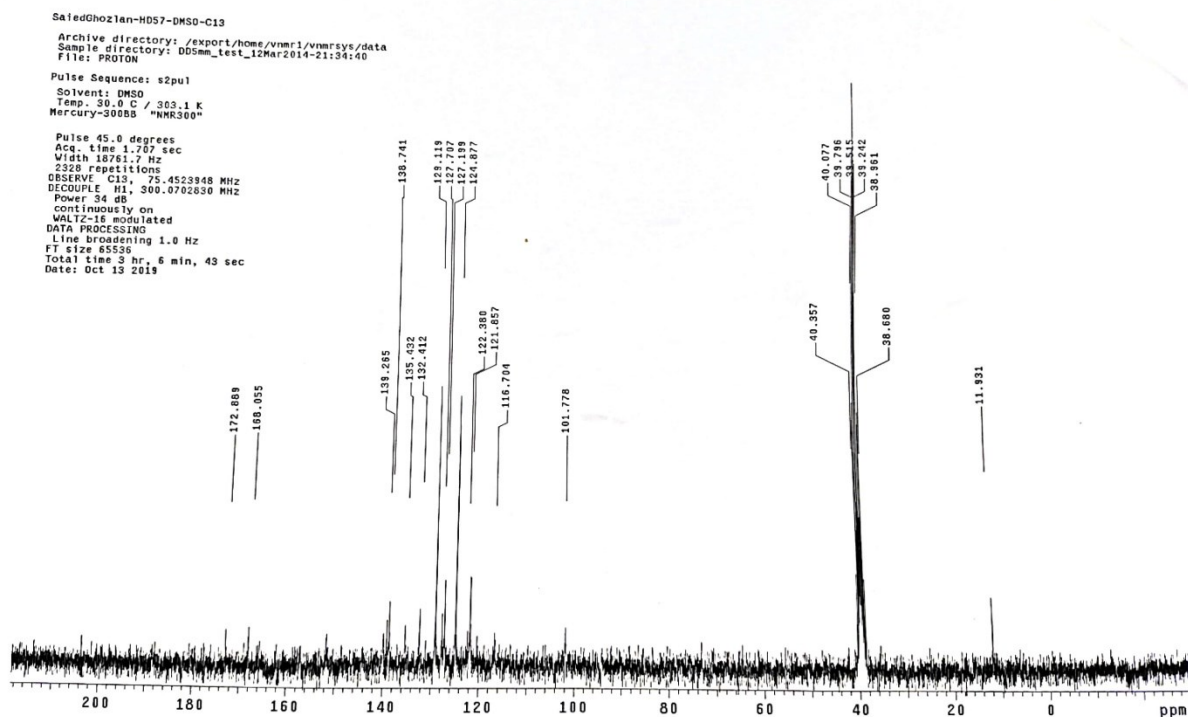
¹³C NMR (75 MHz, DMSO-*d*₆) of compound 34



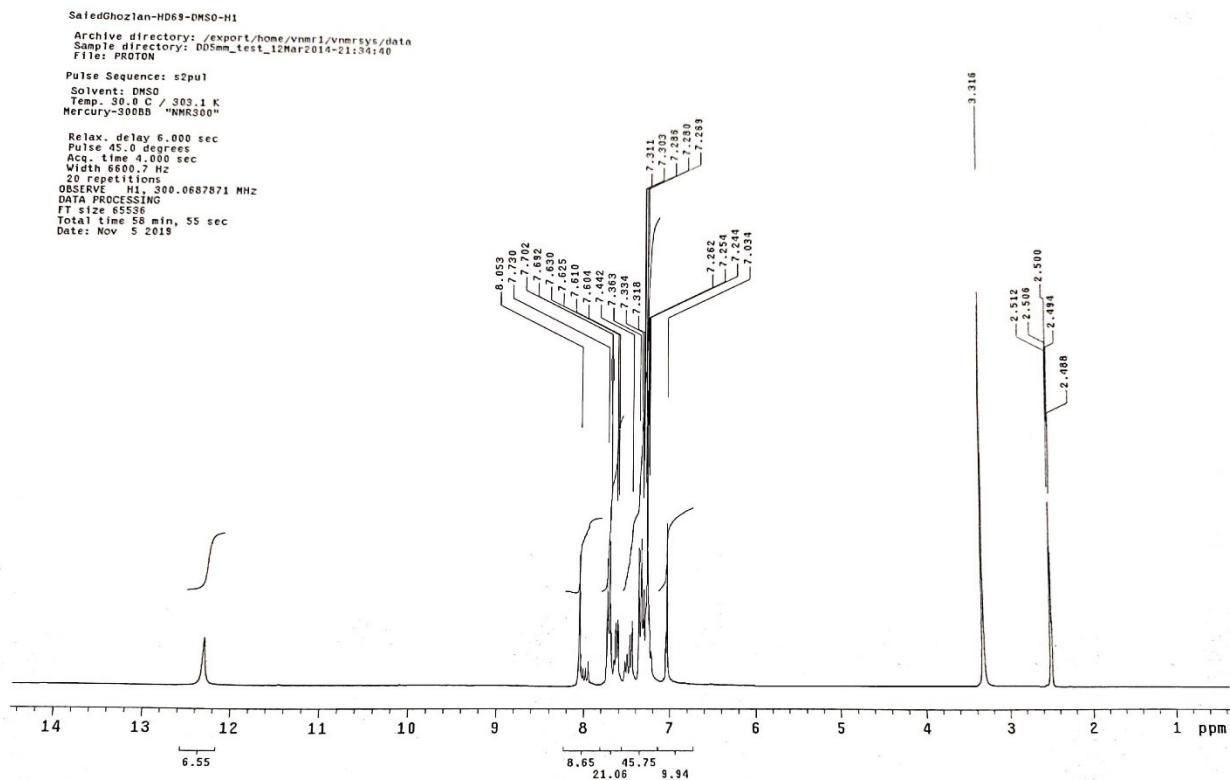
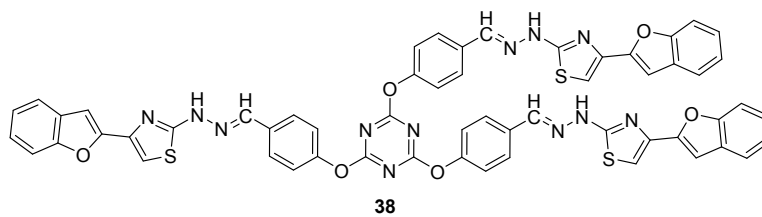
The ^1H NMR (300 MHz, $\text{DMSO}-d_6$) of compound 36



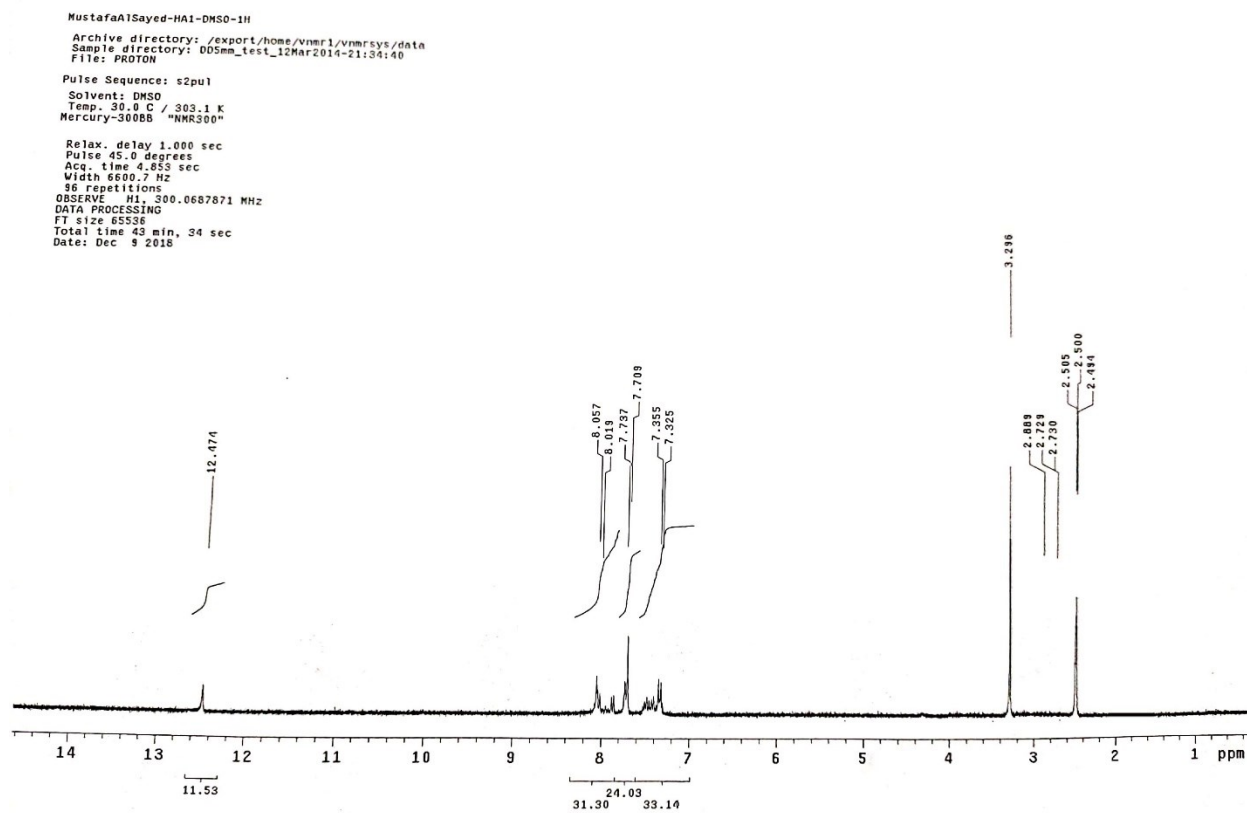
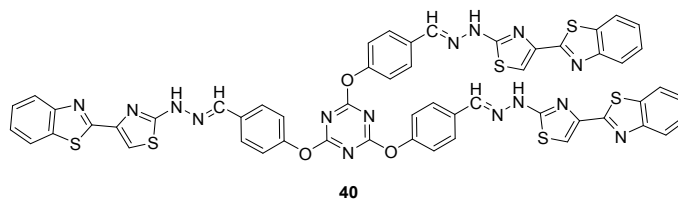
36



^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of compound 36



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



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

IR Spectra

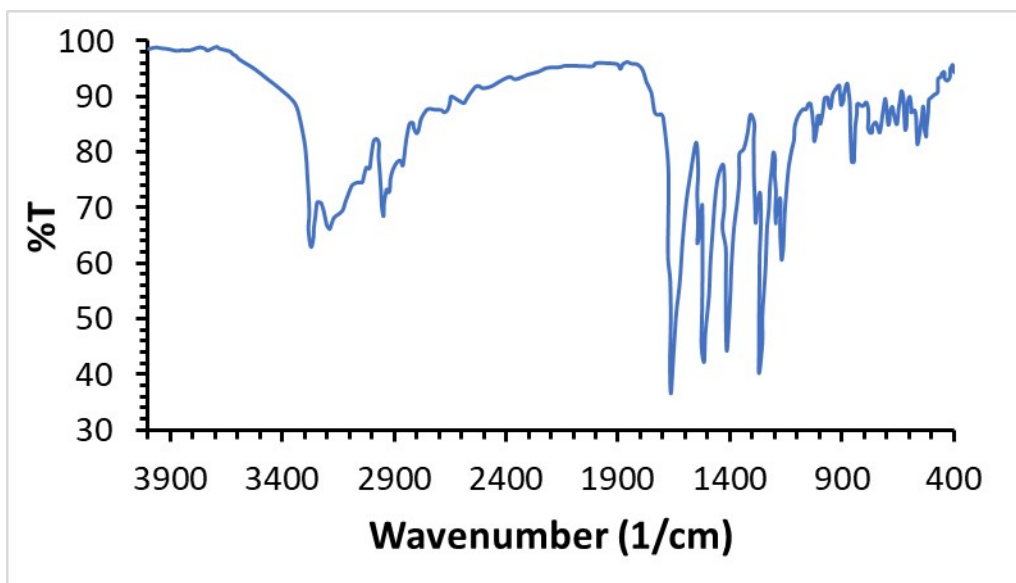


Figure 1. IR spectrum of compound 7

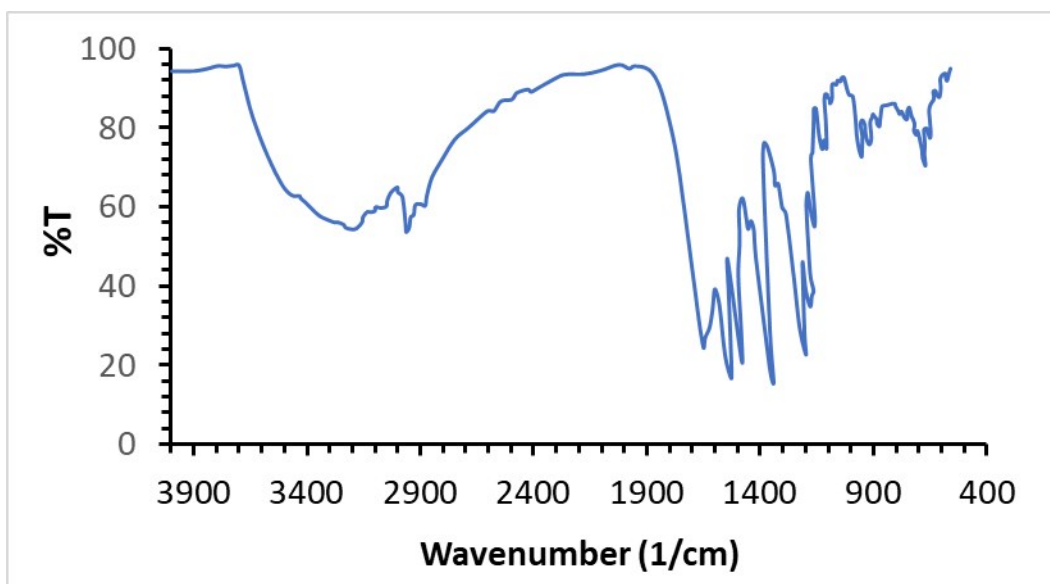


Figure 2. IR spectrum of compound 9

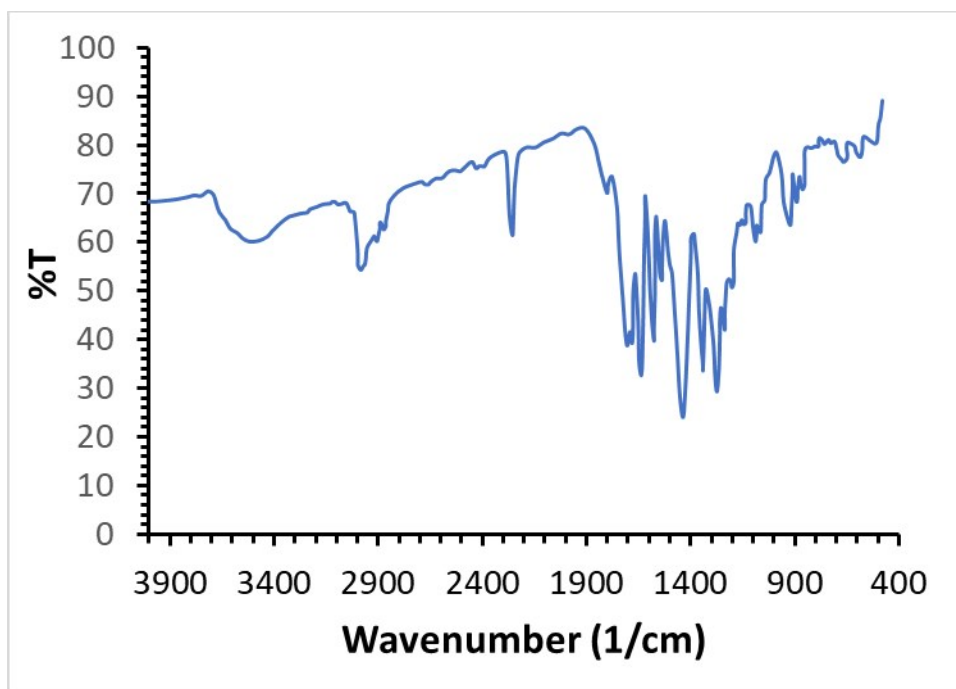


Figure 3. IR spectrum of compound **12**

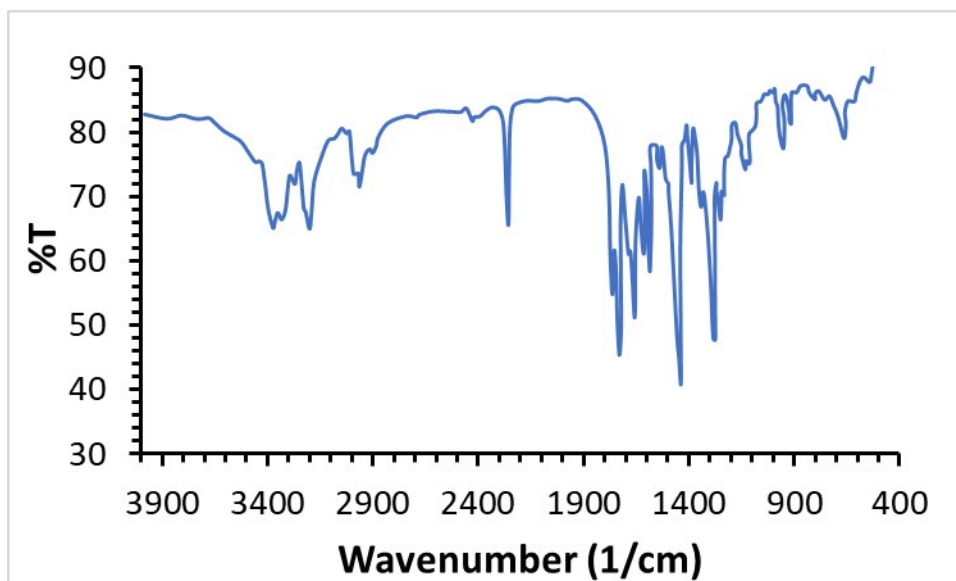


Figure 4. IR spectrum of compound **16**

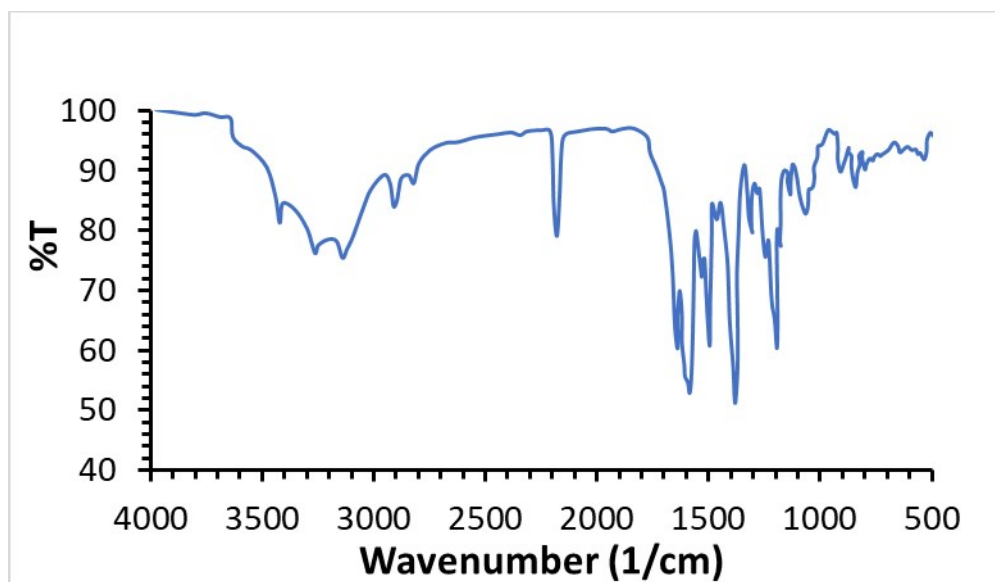


Figure 5. IR spectrum of compound **19**

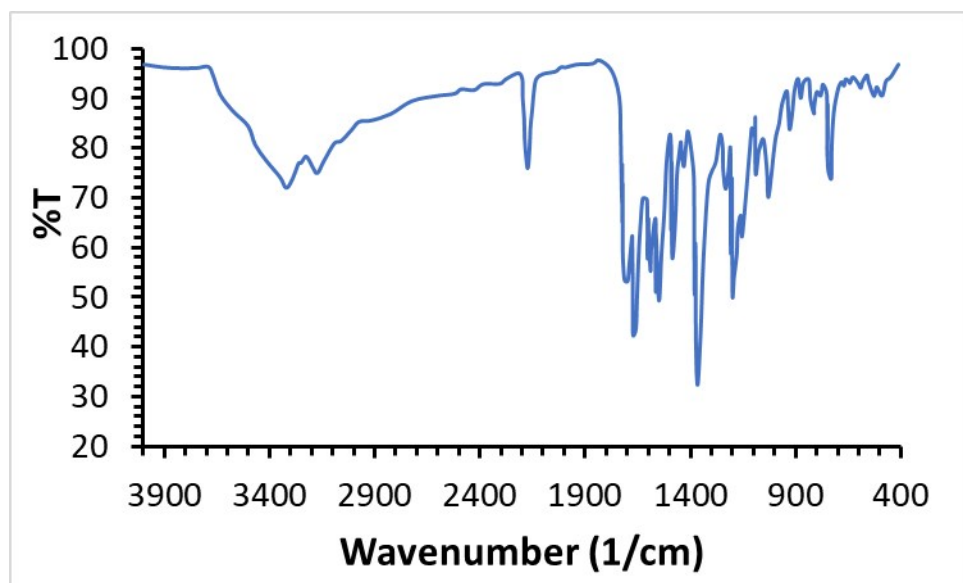


Figure 6. IR spectrum of compound **20**

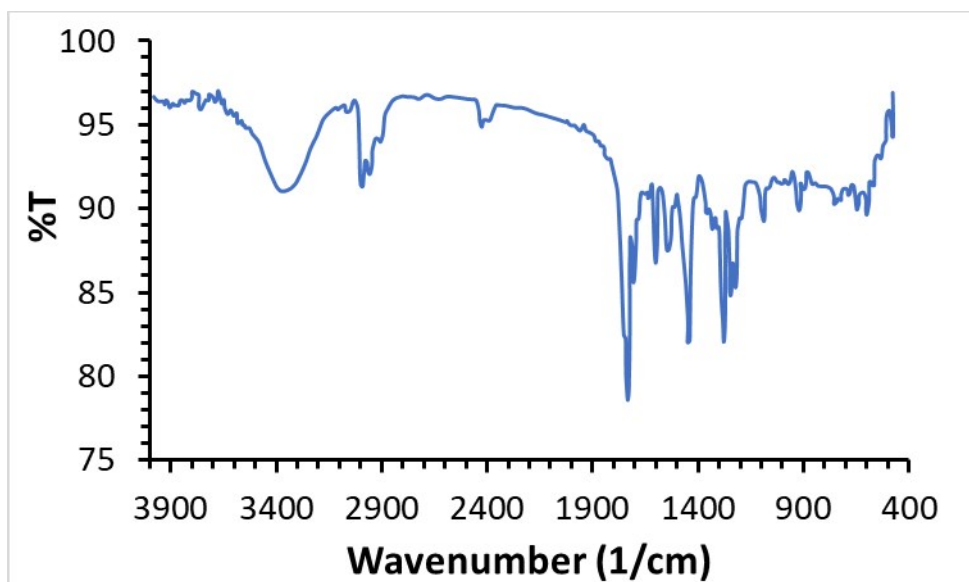


Figure 7. IR spectrum of compound **21**

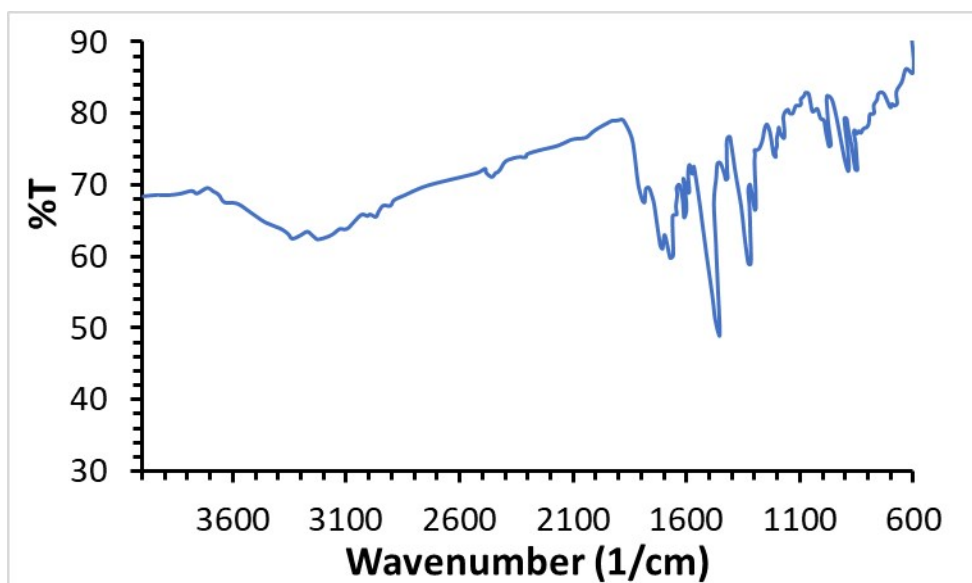


Figure 8. IR spectrum of compound **24**

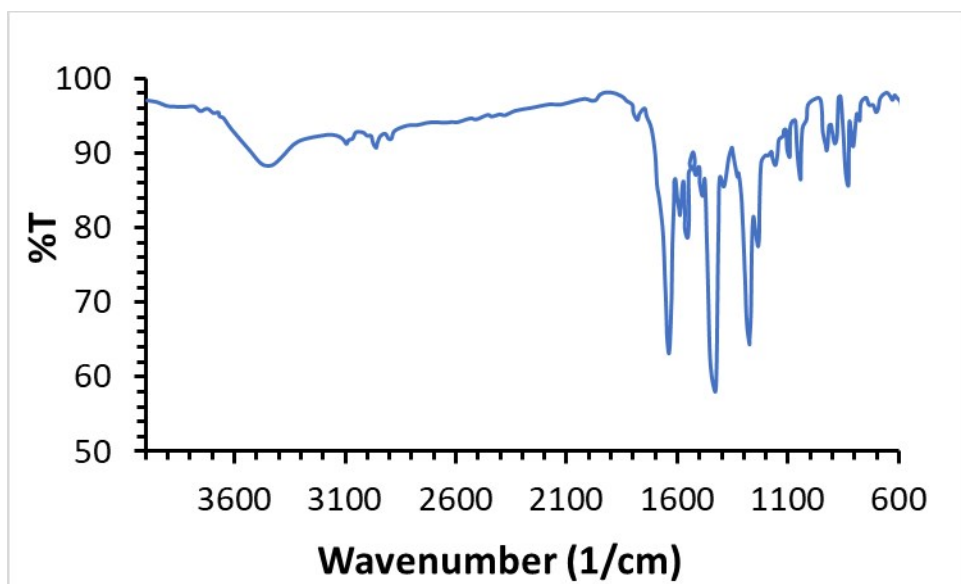


Figure 9. IR spectrum of compound **26**

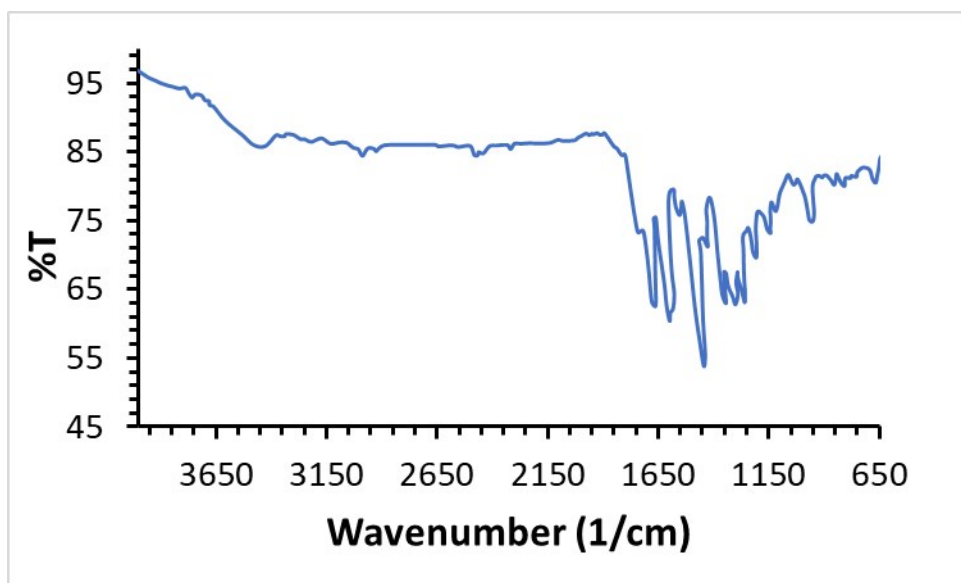


Figure 10. IR spectrum of compound **30**

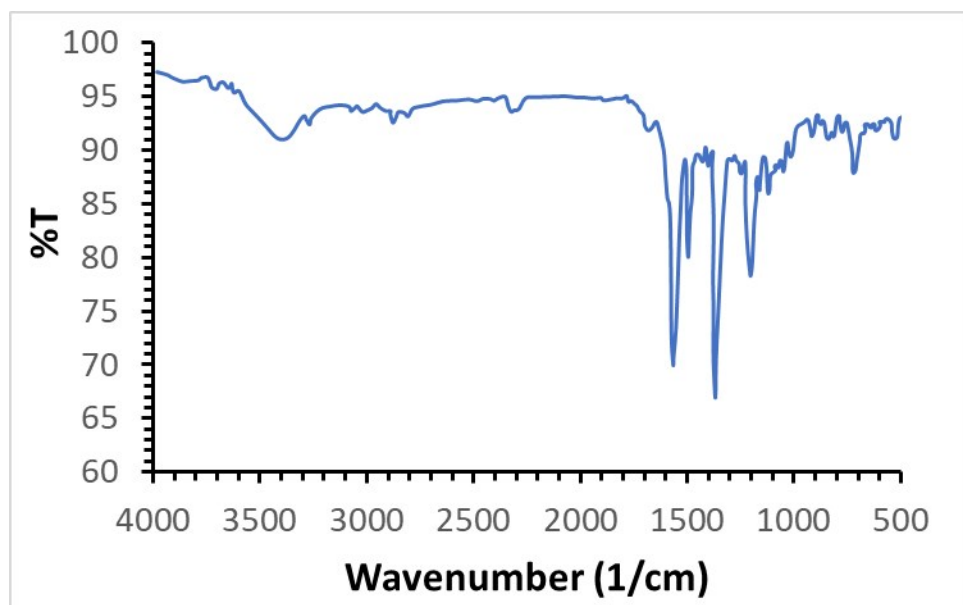


Figure 11. IR spectrum of compound **33**

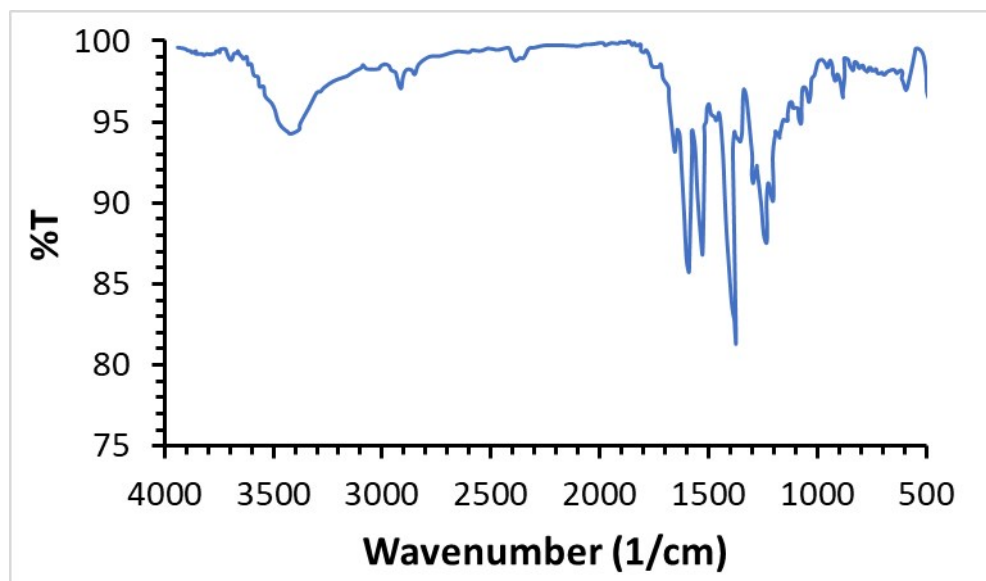


Figure 12. IR spectrum of compound **34**

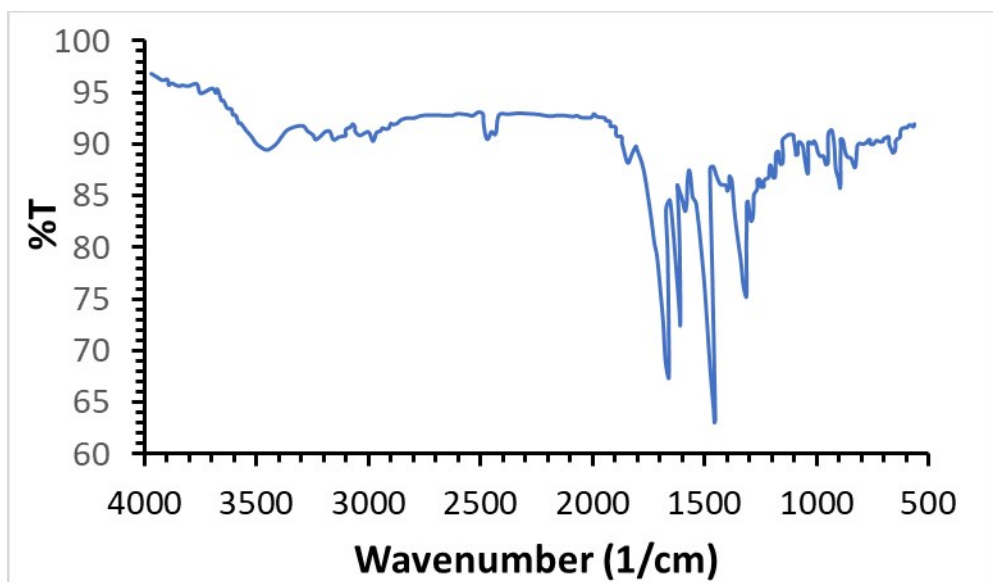


Figure 13. IR spectrum of compound **36**

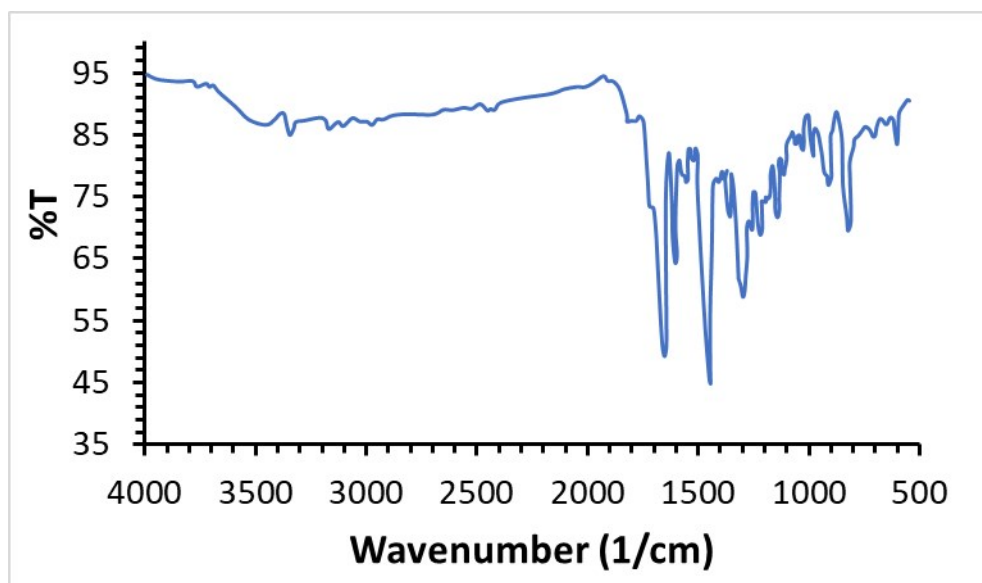


Figure 14. IR spectrum of compound **38**

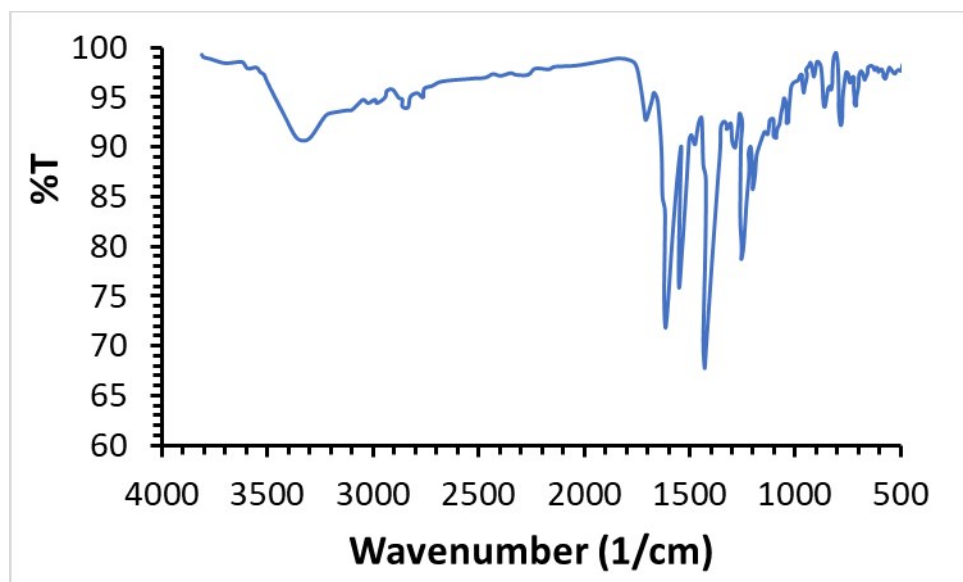


Figure 15. IR spectrum of compound **40**

Combined IR spectra

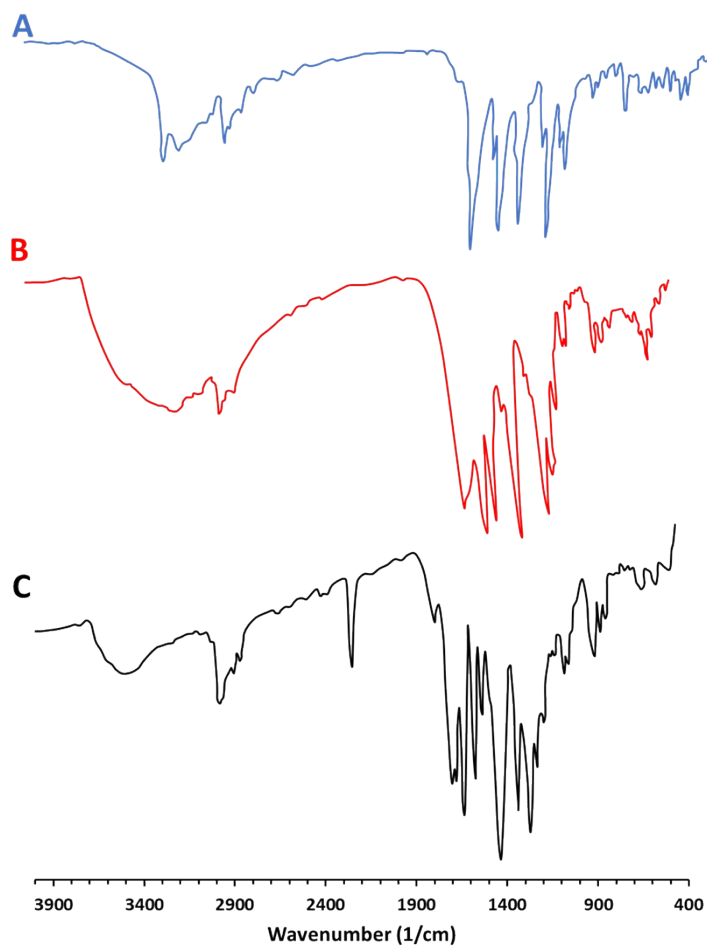


Figure 1. IR spectra of compounds **7 (A)** , **12 (B)** and **9 (C)**

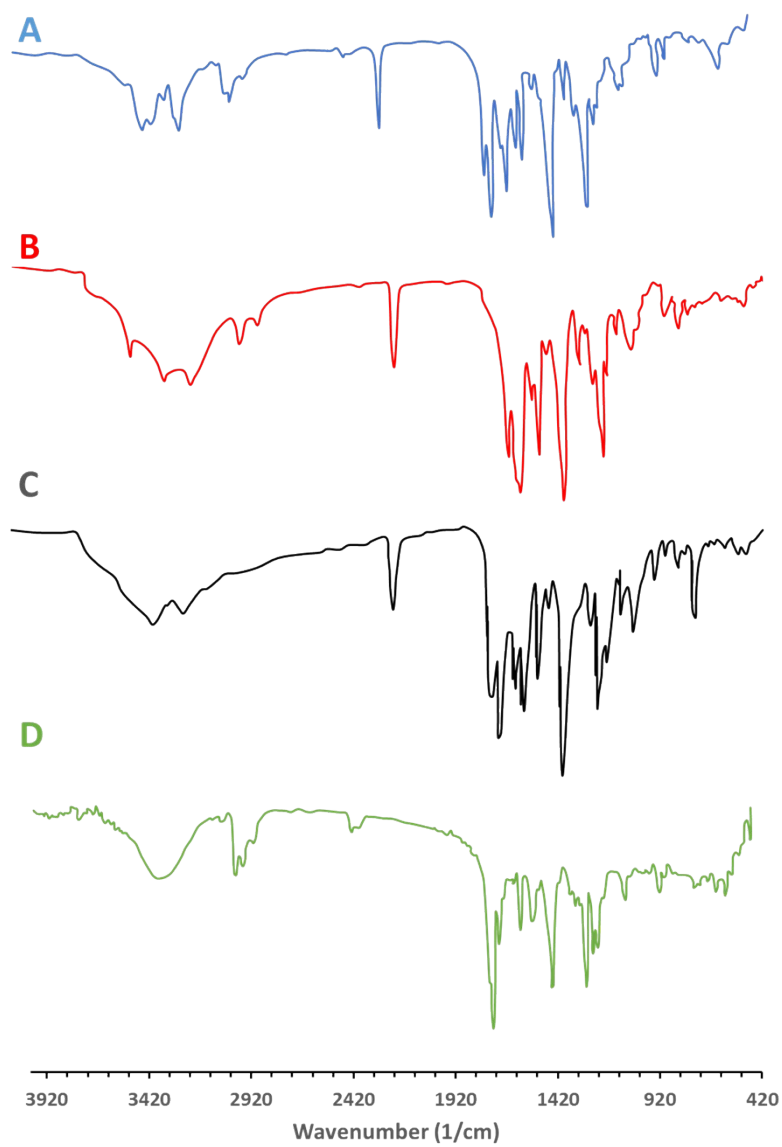


Figure 2. IR spectra of compounds **16 (A)**, **19 (B)**, **20 (C)** and **9 (D)**

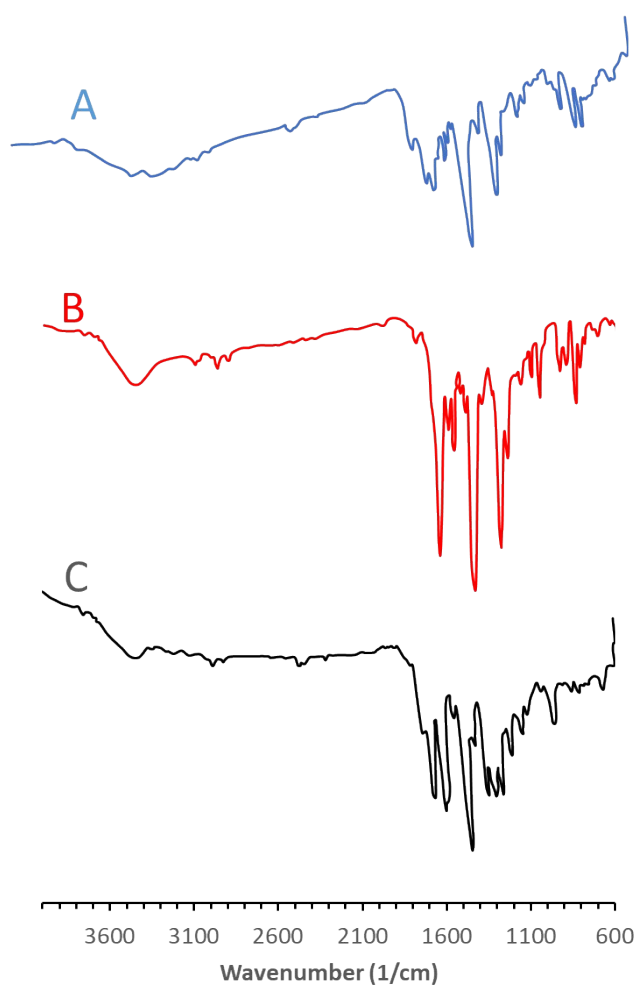


Figure 3. IR spectra of compounds **26 (A)**, **24 (B)**, and **30 (C)**

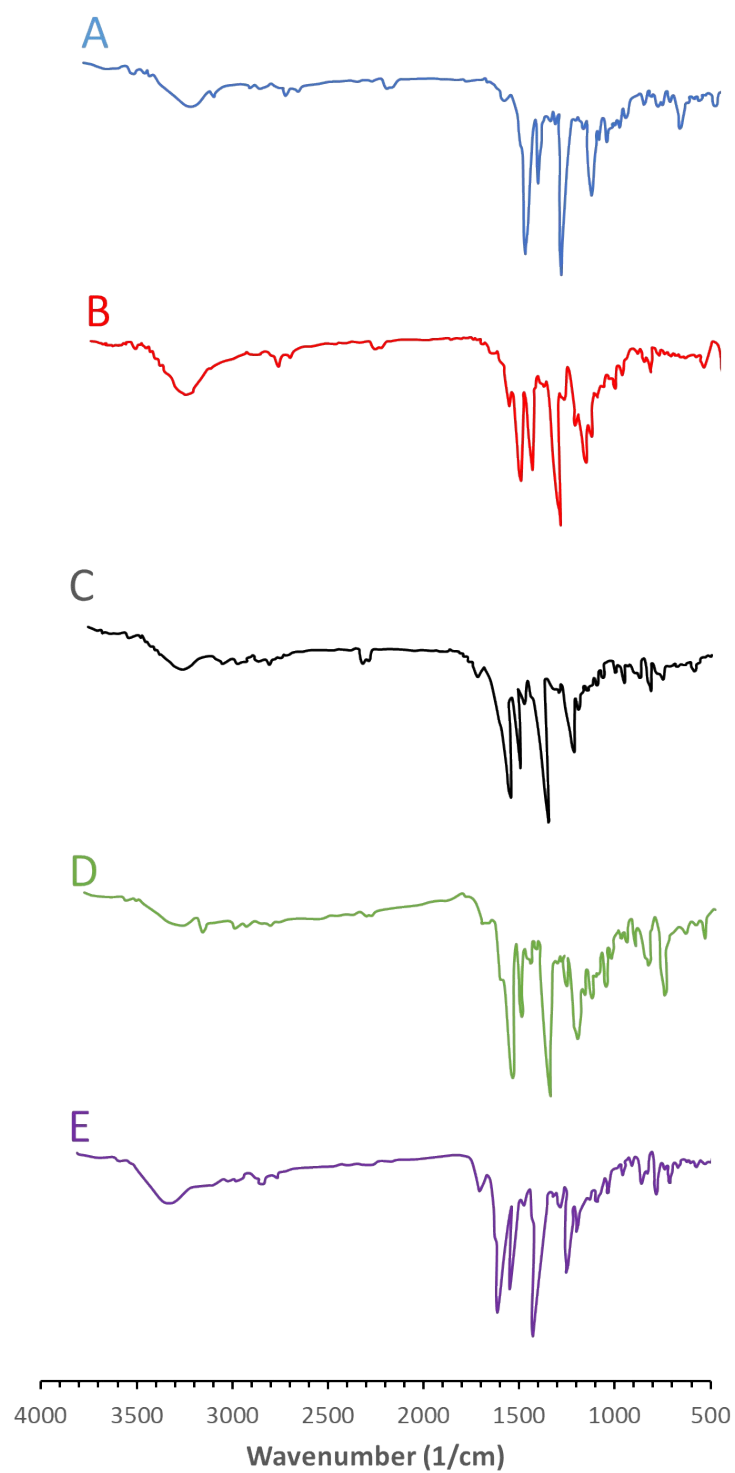


Figure 4. IR spectra of compounds **33** (A), **34** (B), **36** (C), **38** (D) and **9** (E)