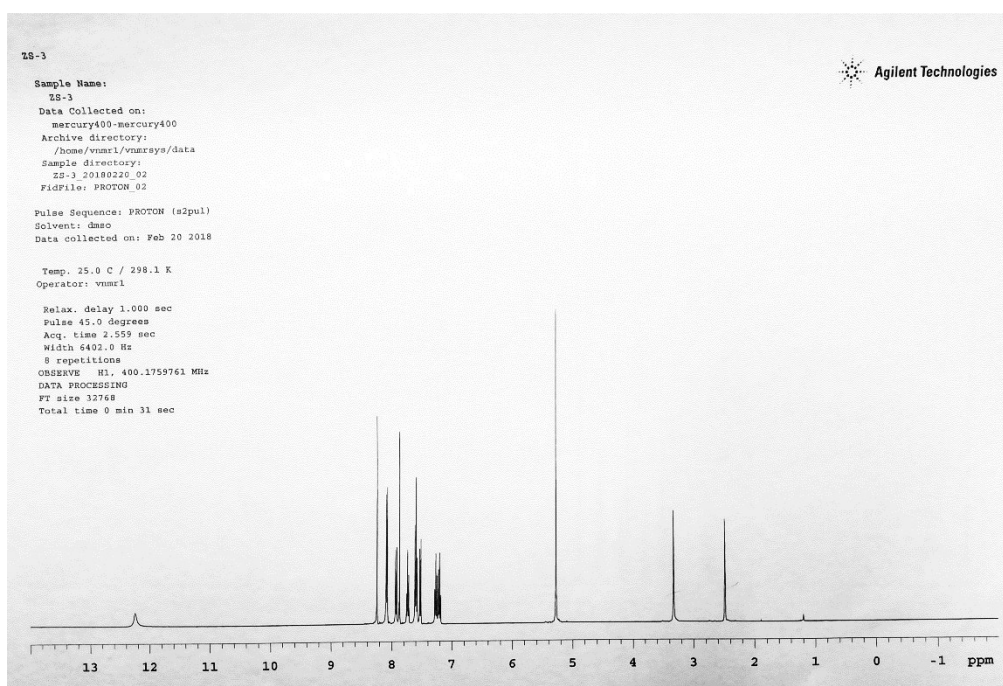


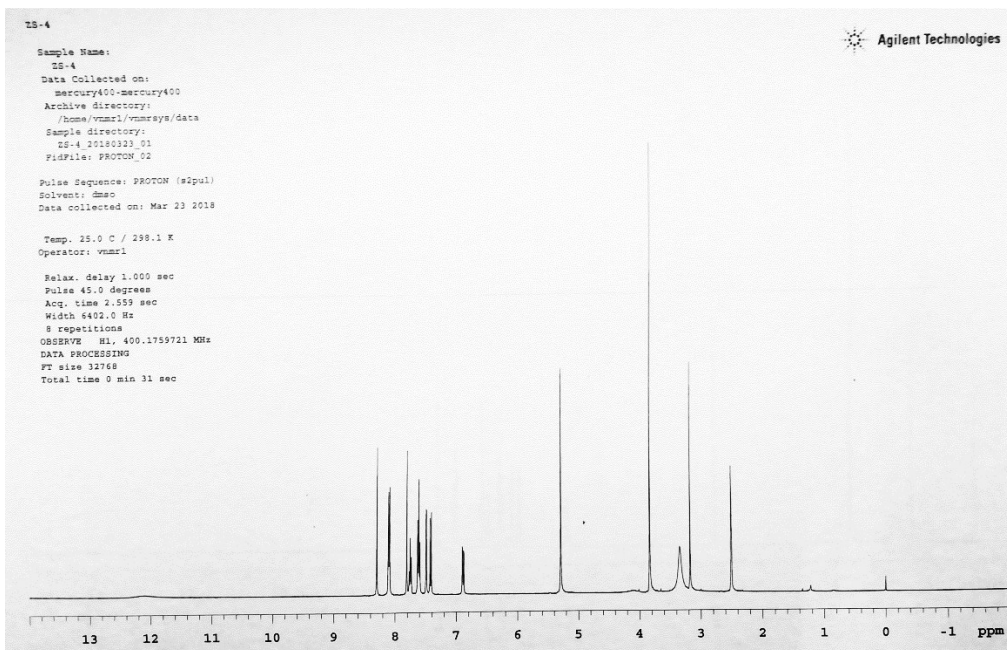
Design, Synthesis, Molecular Docking and ADME Studies of Novel Indole-Thiazolidinedione Derivatives and their Antineoplastic Activity as CDK6 Inhibitors

Supplementary Data

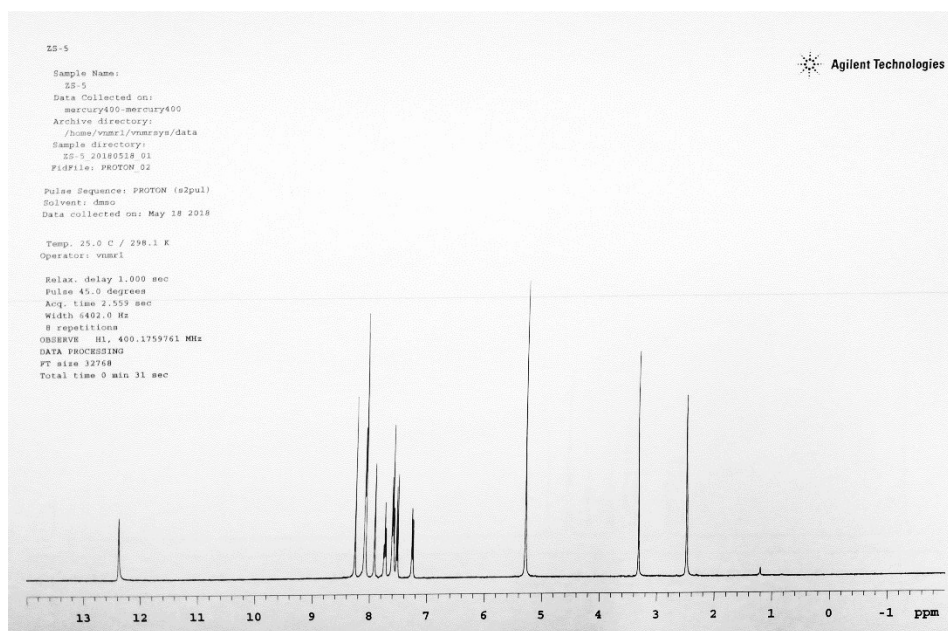
Suppl. Figure 1. ^1H NMR spectrum of compound **9**.



Suppl. Figure 2. ^1H NMR spectrum of compound **10**.



Suppl. Figure 3. ^1H NMR spectrum of compound 11.



Suppl. Figure 4. ^1H NMR spectrum of compound **12**.

ZS-9

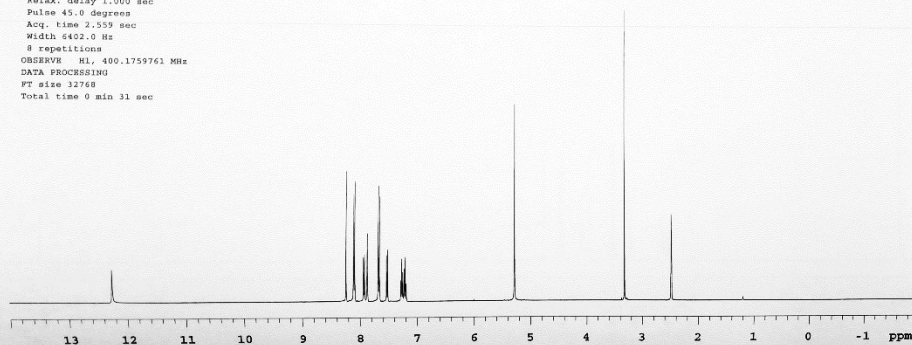
Sample Name:
ZS-9
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
ZS-9_20180406_01
FIDFile: PROTON_02



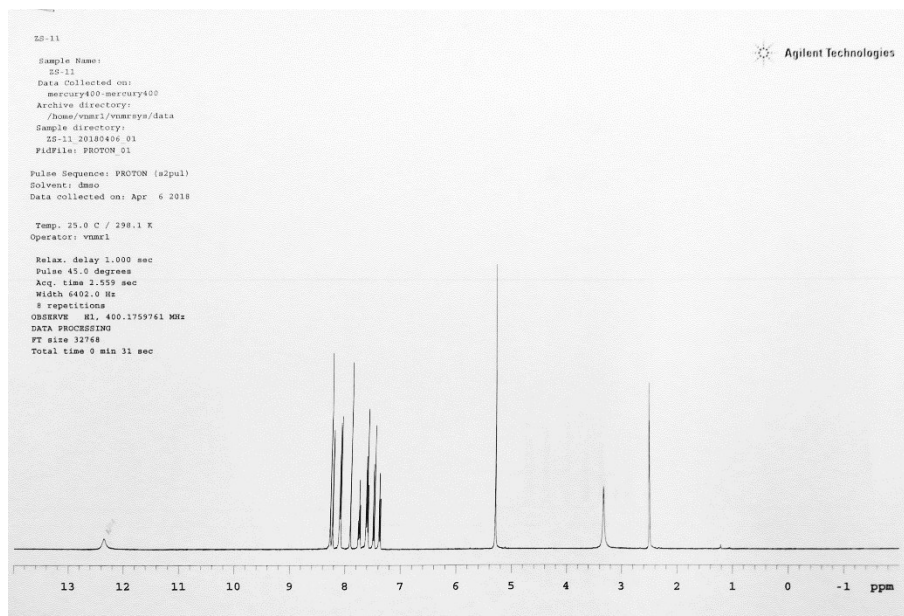
Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: Apr 6 2018

Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 4422.0 Hz
8 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 12768
Total time 0 min 31 sec



Suppl. Figure 5. ^1H NMR spectrum of compound 13.



Suppl. Figure 6. ^1H NMR spectrum of compound 14.

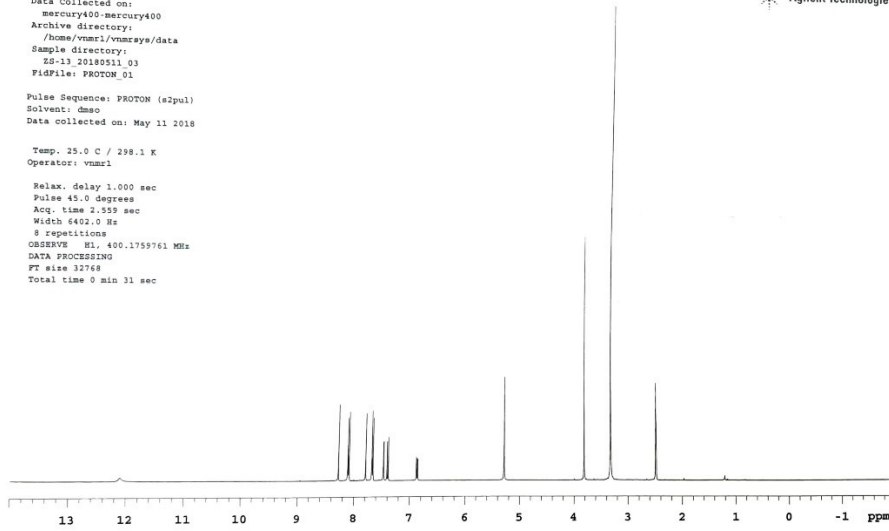
ZS-13

Sample Name:
ZS-13
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vmrc1/vmrcays/data
Sample directory:
ZS-13_20180511_03
FidFile: PROTON_01

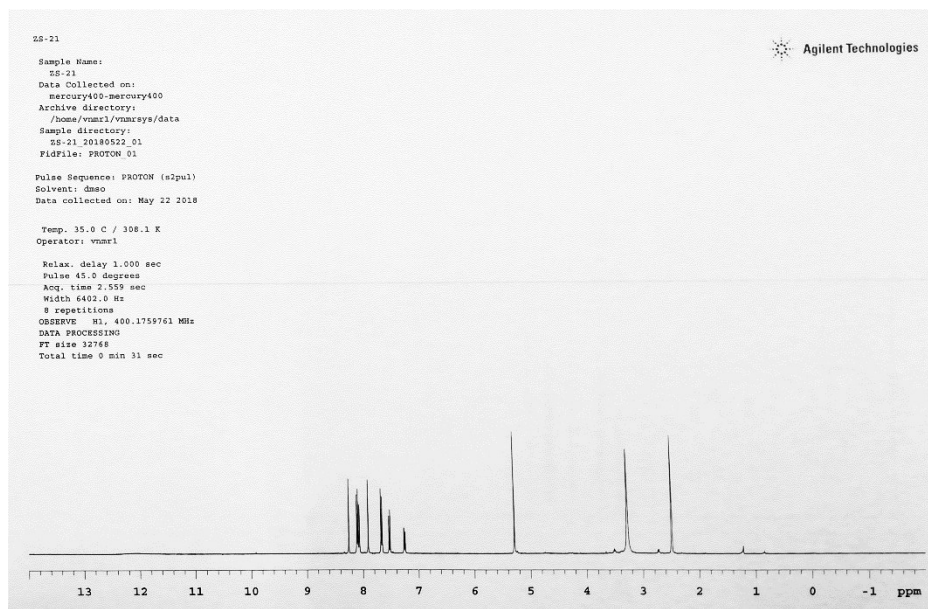
Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: May 11 2018

Temp. 25.0 C / 298.1 K
Operator: vmrc1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
8 repetitions
OBSERVE F1: 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 31 sec



Suppl. Figure 7. ^1H NMR spectrum of compound 15



Suppl. Figure 8. ^1H NMR spectrum of compound 16

ZS-22

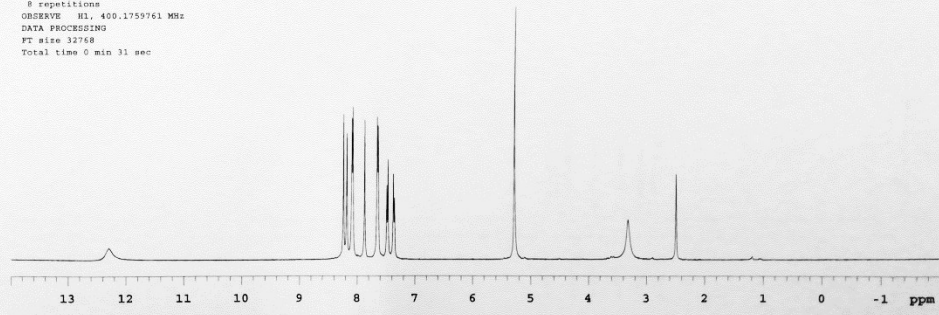


Sample Name:
ZS-22
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
ZS-22_20180522_01
Fidfile: PROTON_04

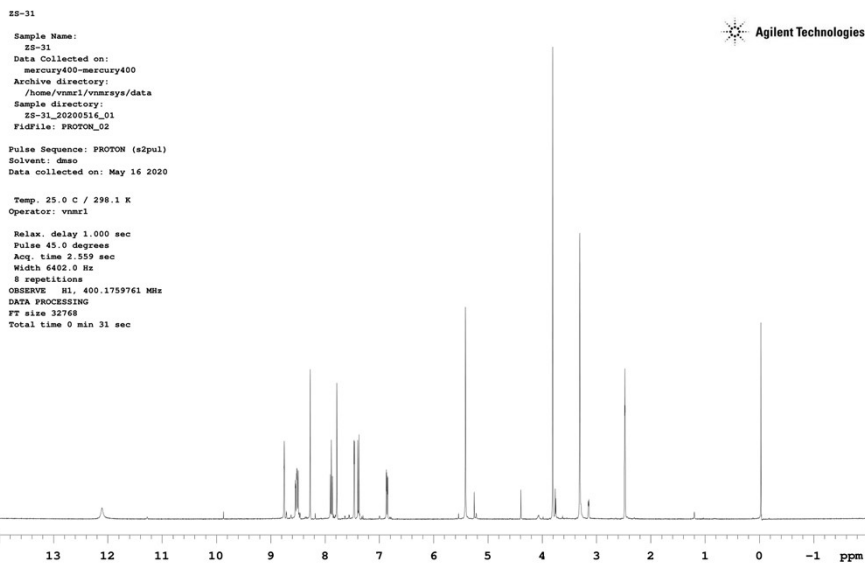
Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: May 22 2018

Temp. 35.0 C / 308.1 K
Operator: vnmr1

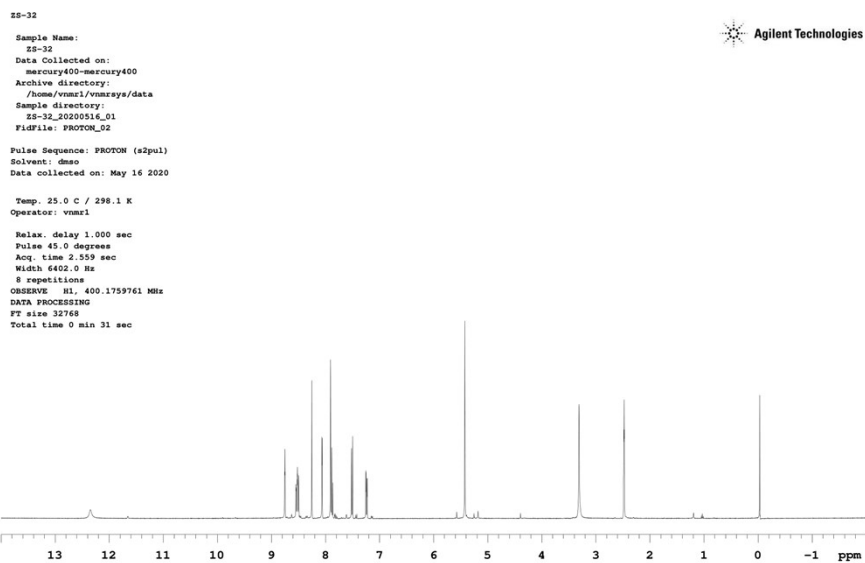
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2:55 sec
Width 6402.0 Hz
8 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 31 sec



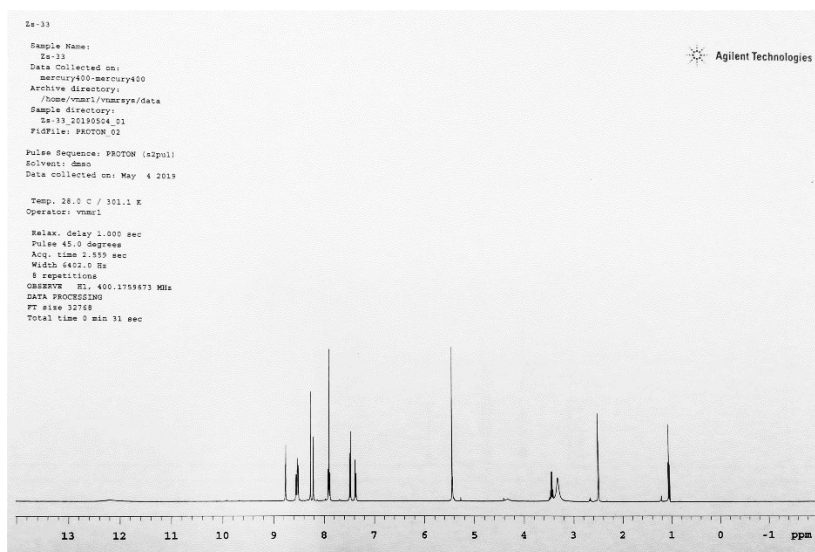
Suppl. Figure 9. ^1H NMR spectrum of compound 17



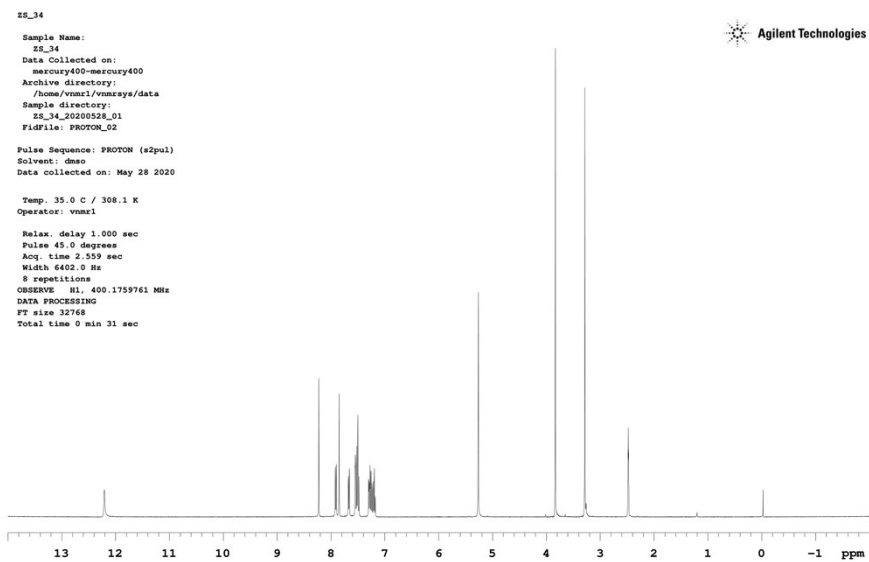
Suppl. Figure 10. ^1H NMR spectrum of compound 18



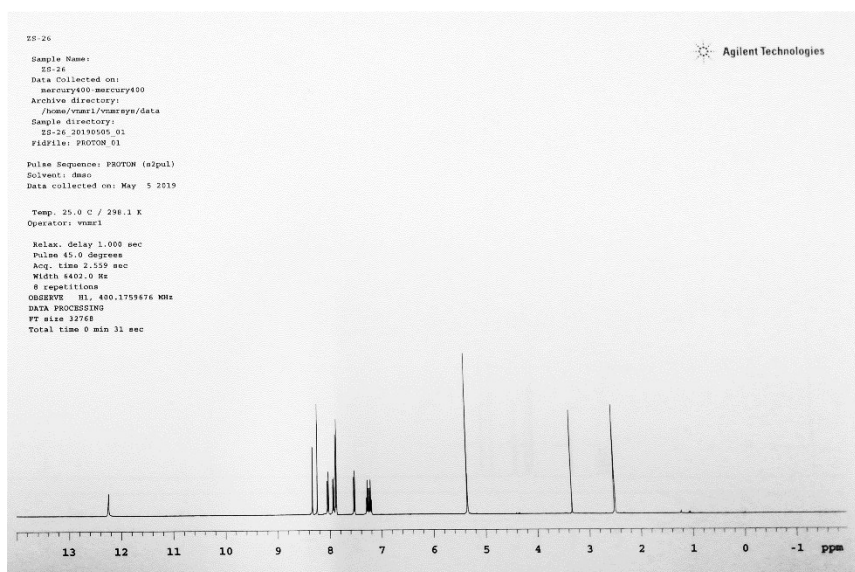
Suppl. Figure 11. ^1H NMR spectrum of compound 19



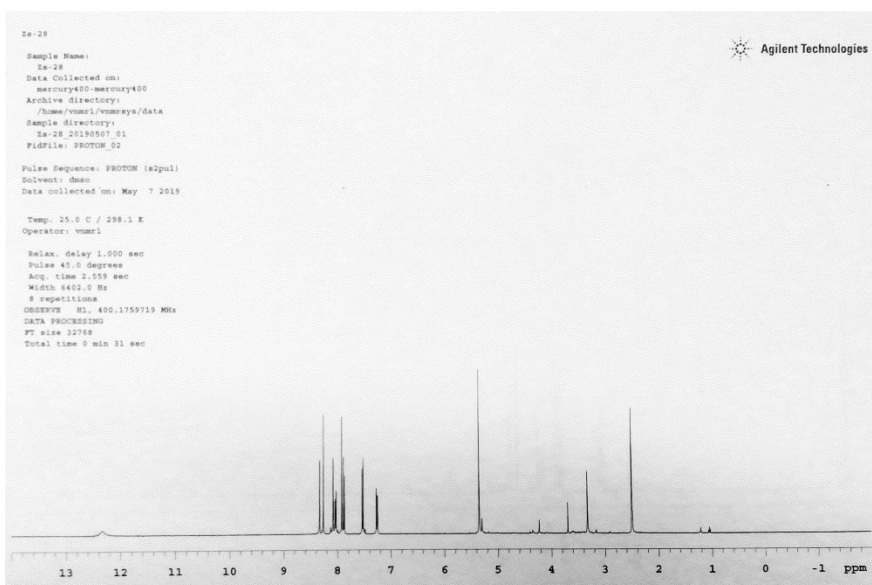
Suppl. Figure 12. ^1H NMR spectrum of compound 20



Suppl. Figure 13. ^1H NMR spectrum of compound 21

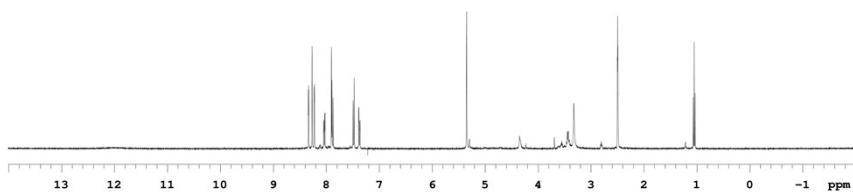


Suppl. Figure 14. ^1H NMR spectrum of compound 22



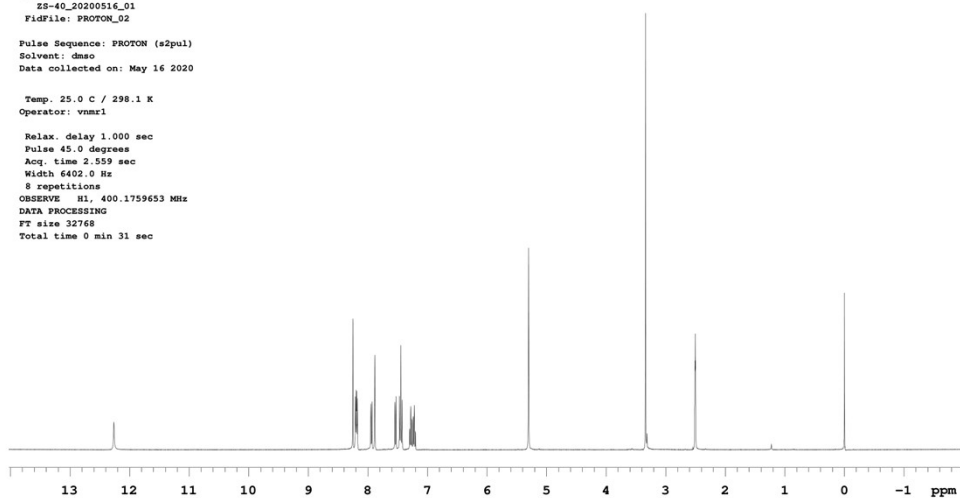
Suppl. Figure 15. ^1H NMR spectrum of compound **23**.

Zs-29
Sample Name:
Zs-29
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
Zs-29_20190507_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: May 7 2019
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
8 repetitions
OBSERVE H1, 400.1759722 MHz
DATA PROCESSING
F2 size 32768
Total time 0 min 31 sec

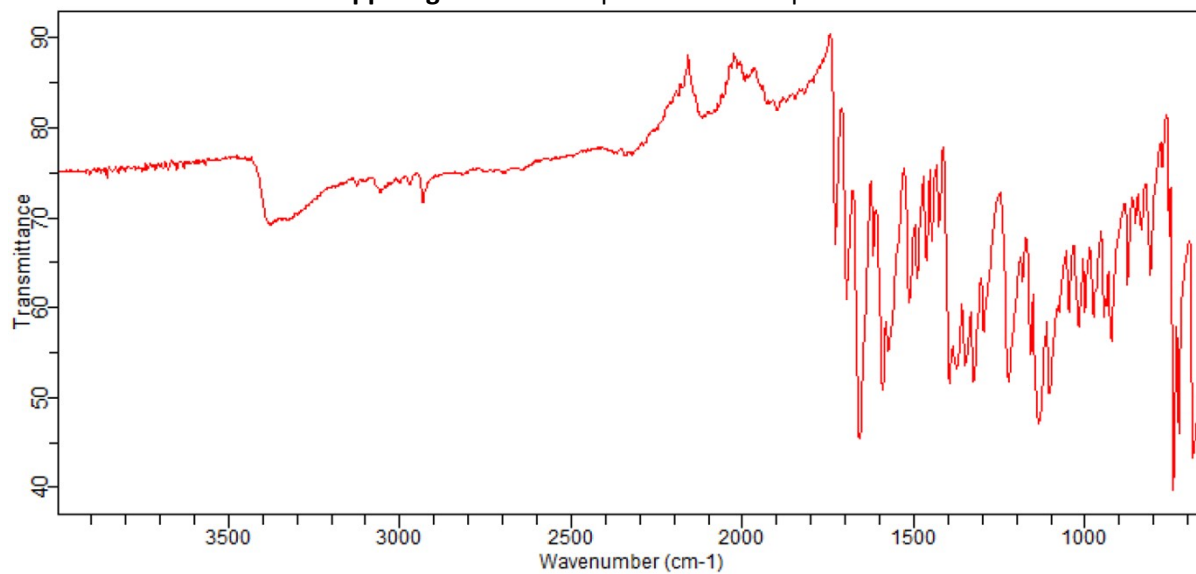


Suppl. Figure 16. ¹H NMR spectrum of compound 24.

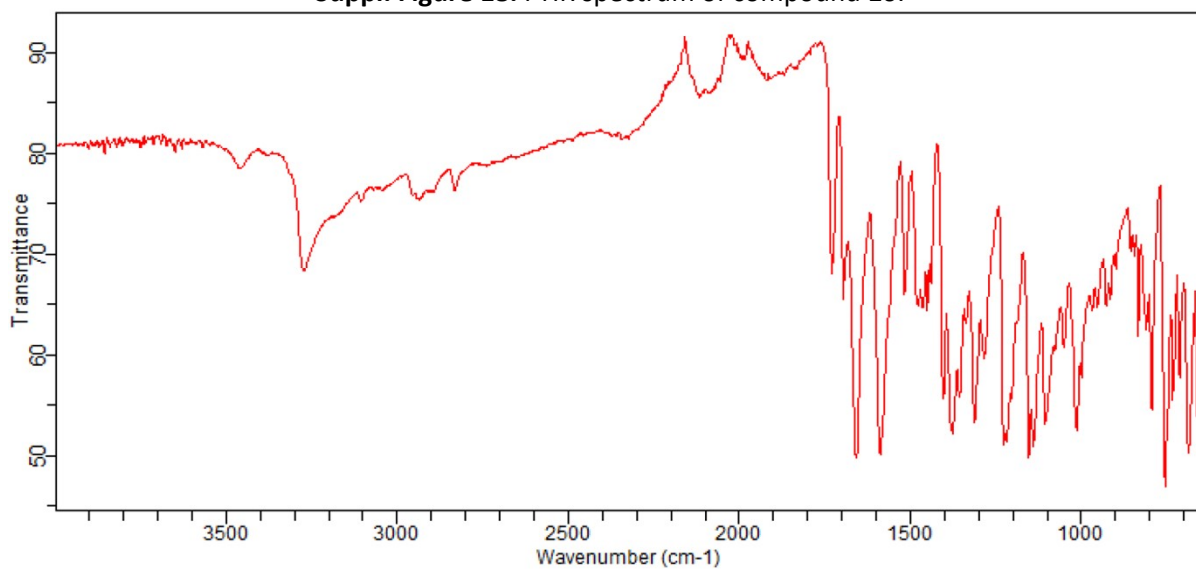
ZS-40
Sample Name:
ZS-40
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
ZS-40_20200516_01
FidFile: PROTON_02
Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: May 16 2020
Temp. 25.0 C / 298.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
8 repetitions
OBSERVE H1, 400.1759653 MHz
DATA PROCESSING
F2 size 32768
Total time 0 min 31 sec



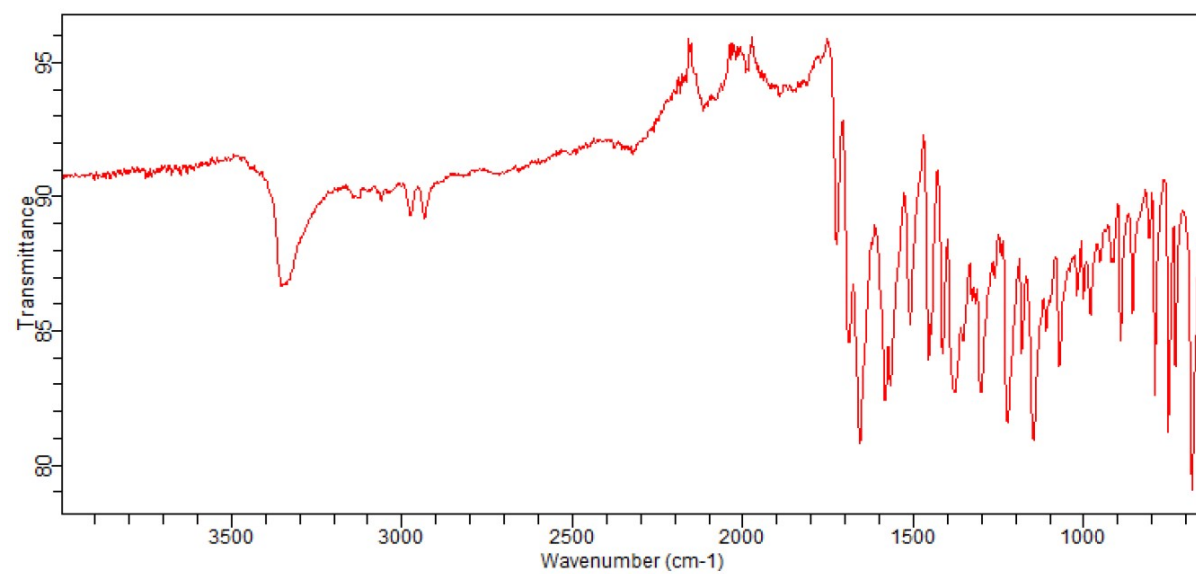
Suppl. Figure 17. FTIR spectrum of compound 9.



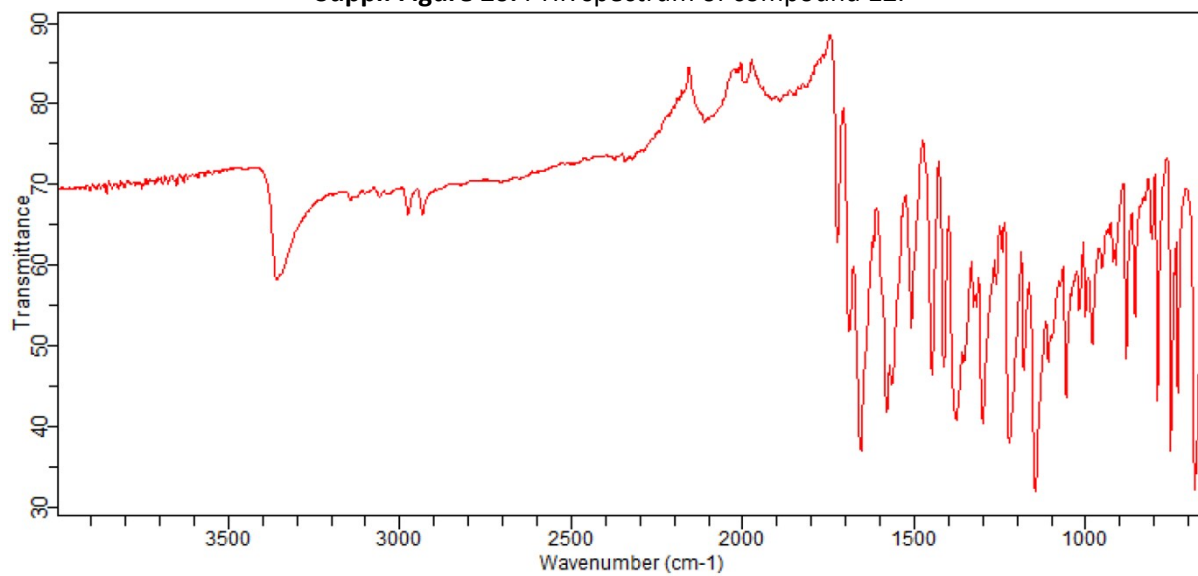
Suppl. Figure 18. FTIR spectrum of compound 10.



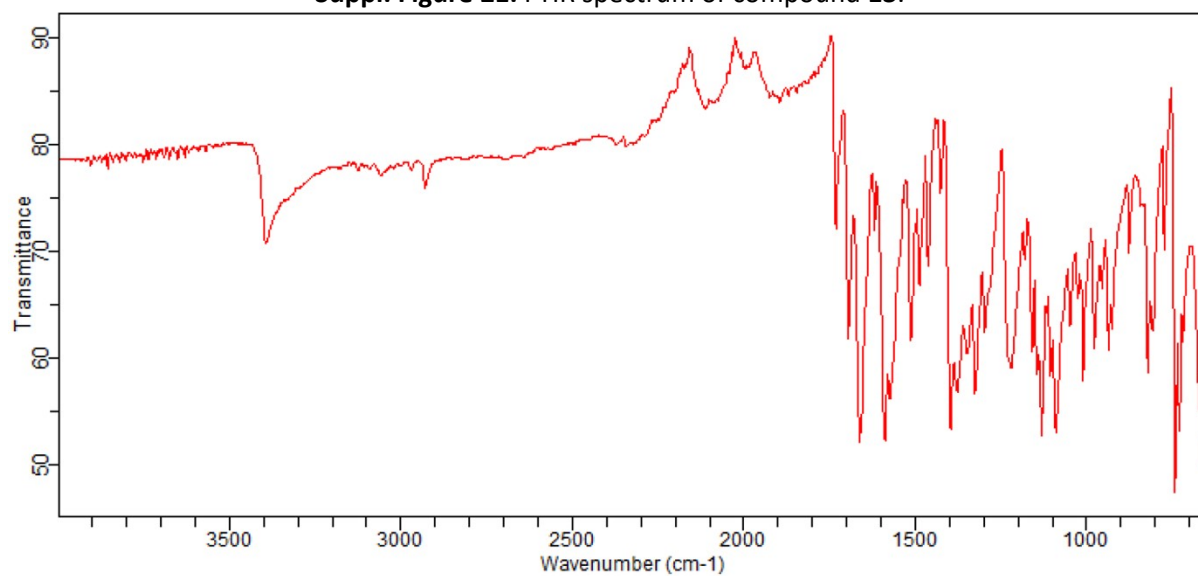
Suppl. Figure 19. FTIR spectrum of compound 11.



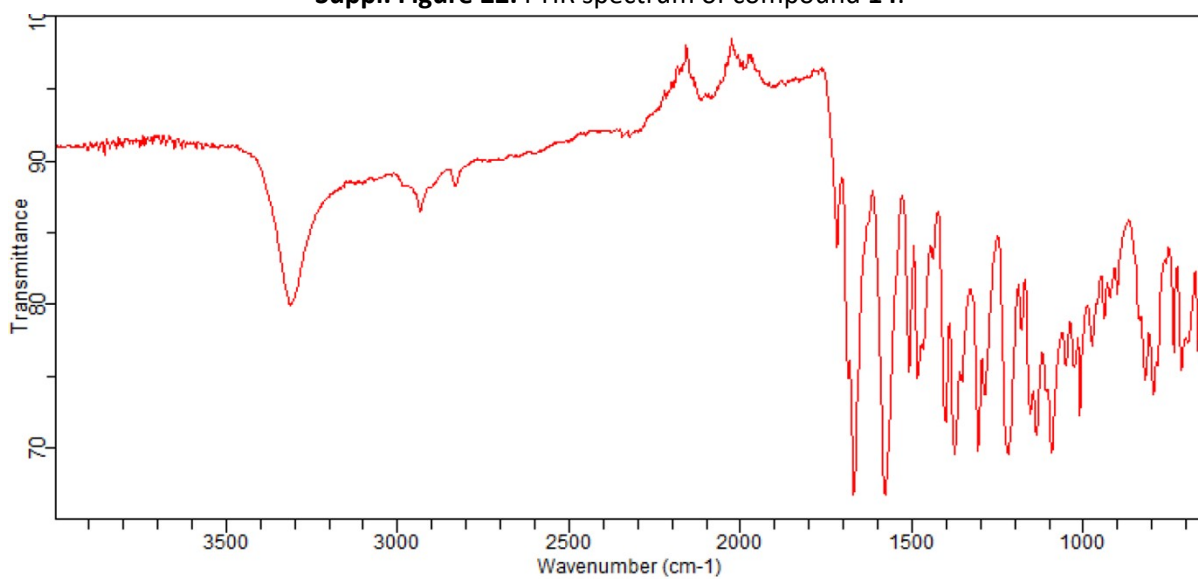
Suppl. Figure 20. FTIR spectrum of compound **12**.



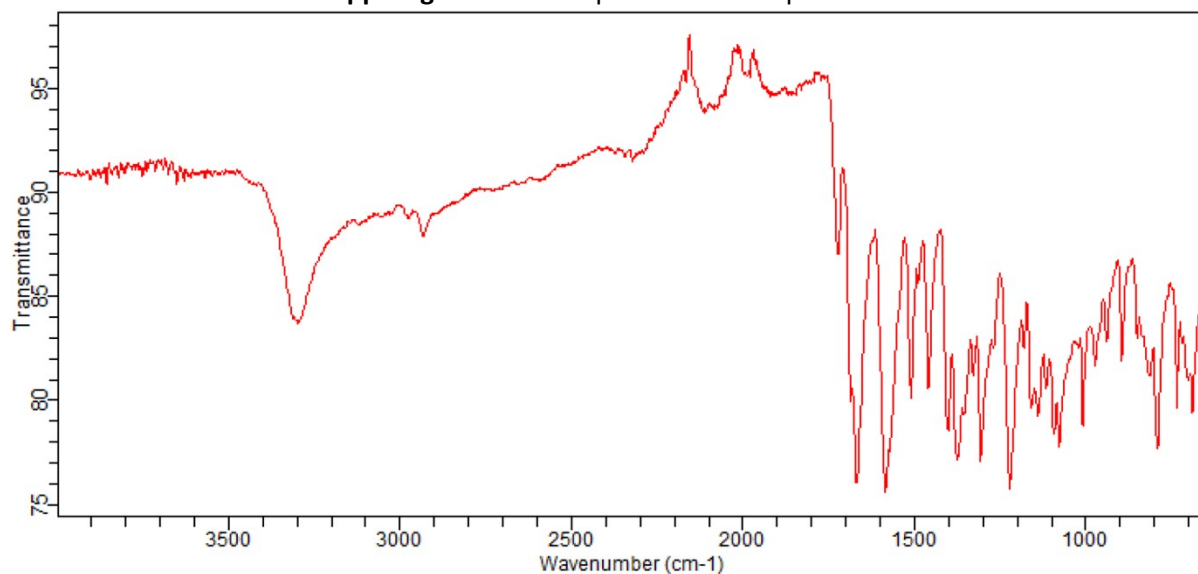
Suppl. Figure 21. FTIR spectrum of compound **13**.



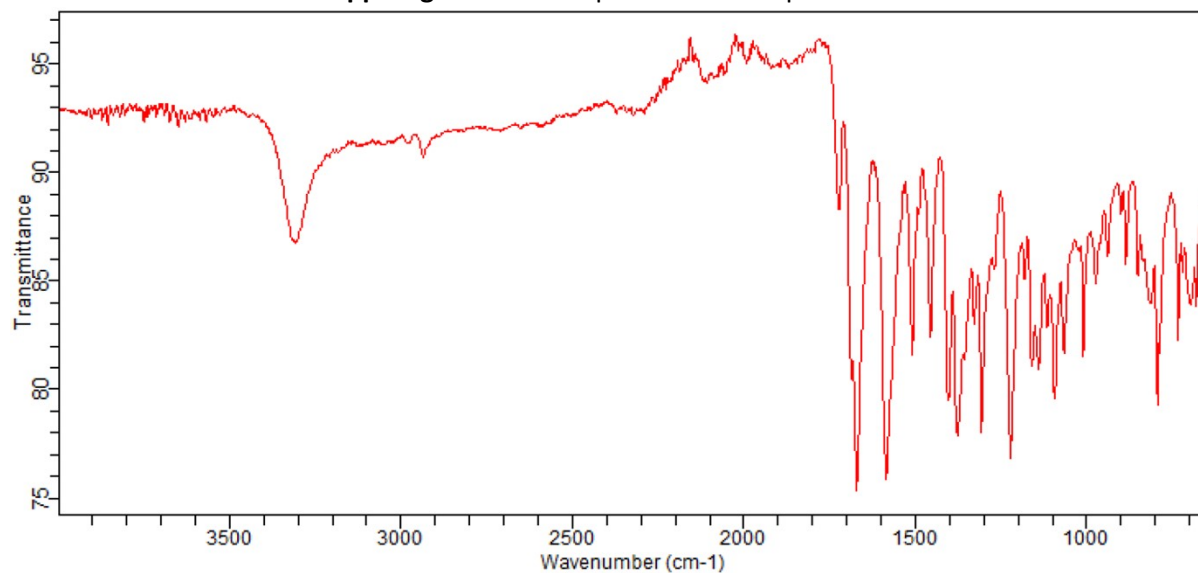
Suppl. Figure 22. FTIR spectrum of compound **14**.



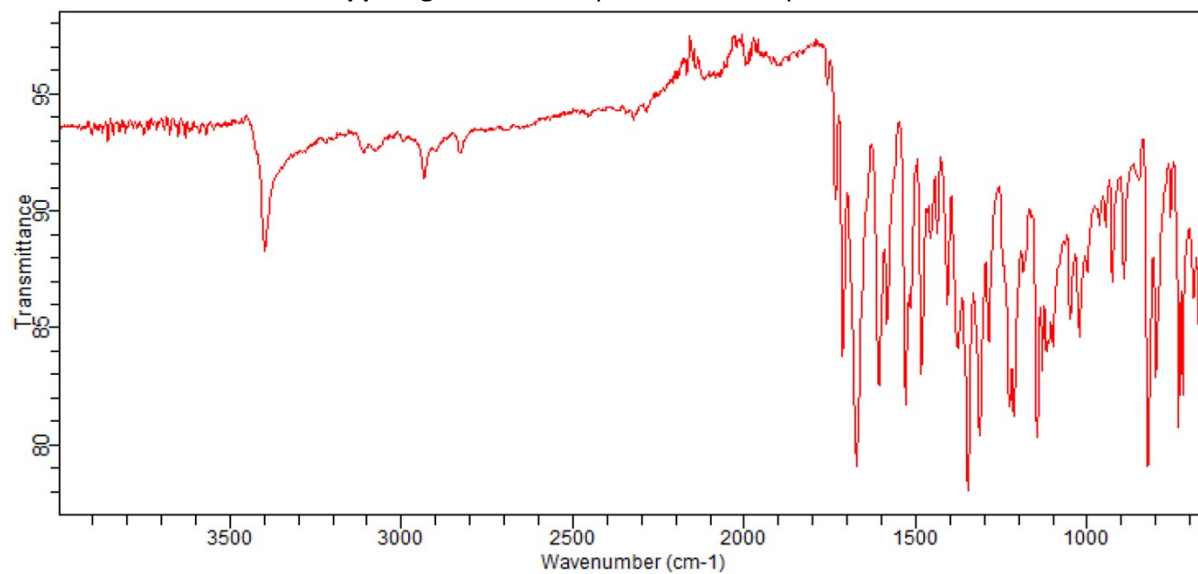
Suppl. Figure 23. FTIR spectrum of compound 15.



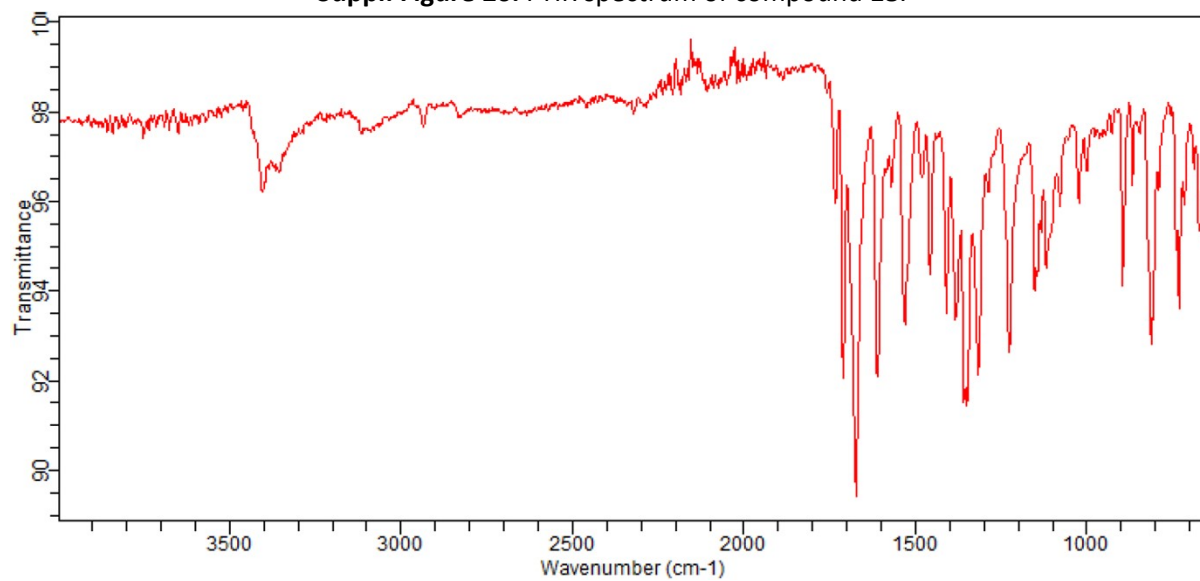
Suppl. Figure 24. FTIR spectrum of compound 16.



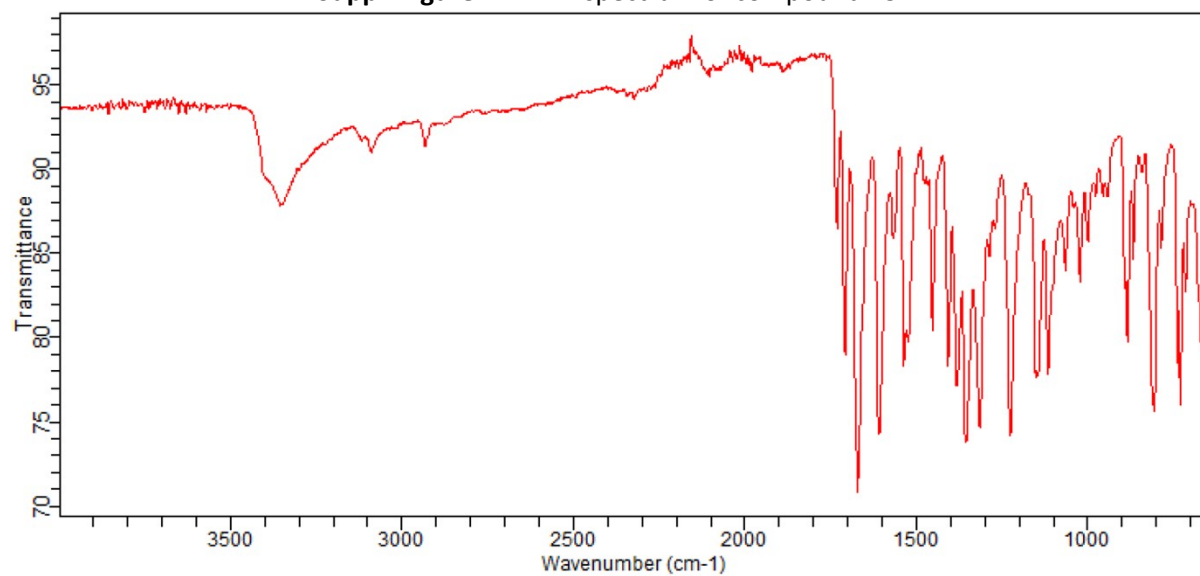
Suppl. Figure 25. FTIR spectrum of compound 17.



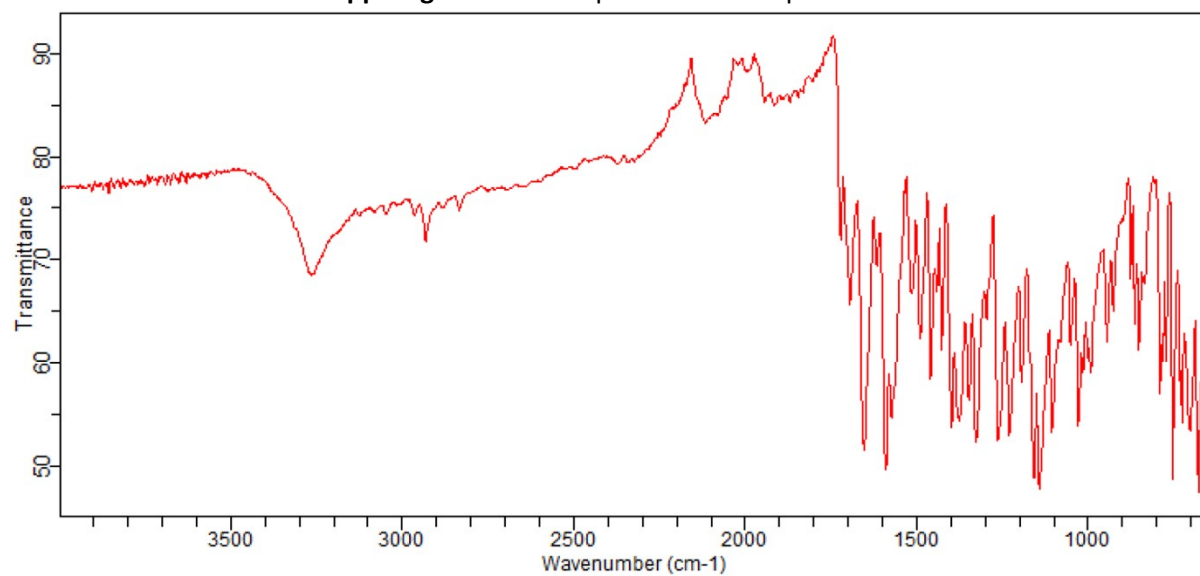
Suppl. Figure 26. FTIR spectrum of compound 18.



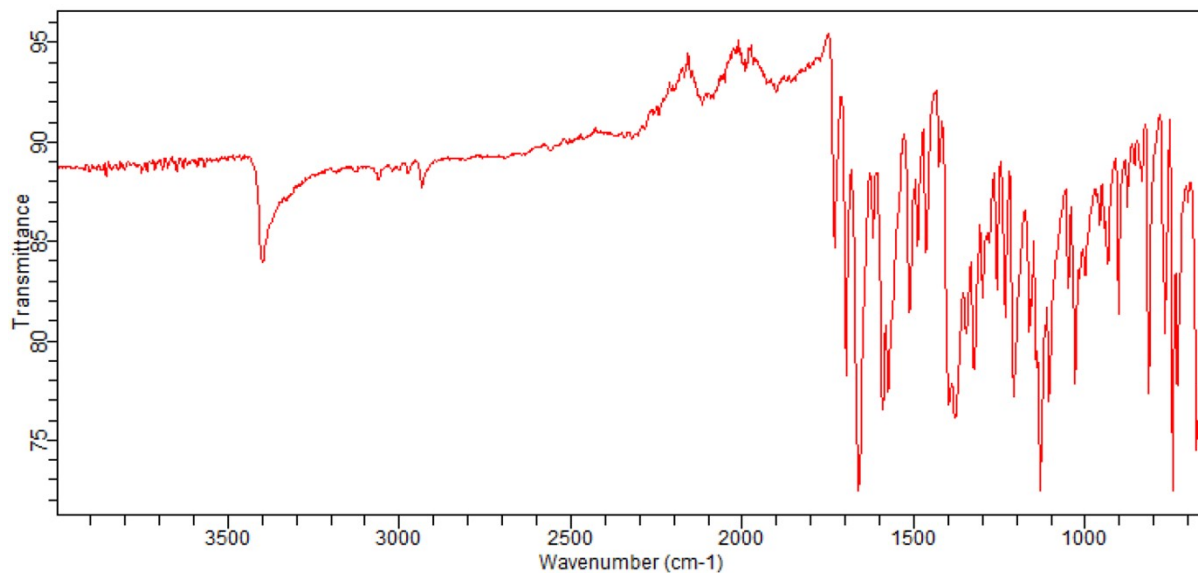
Suppl. Figure 27. FTIR spectrum of compound 19.



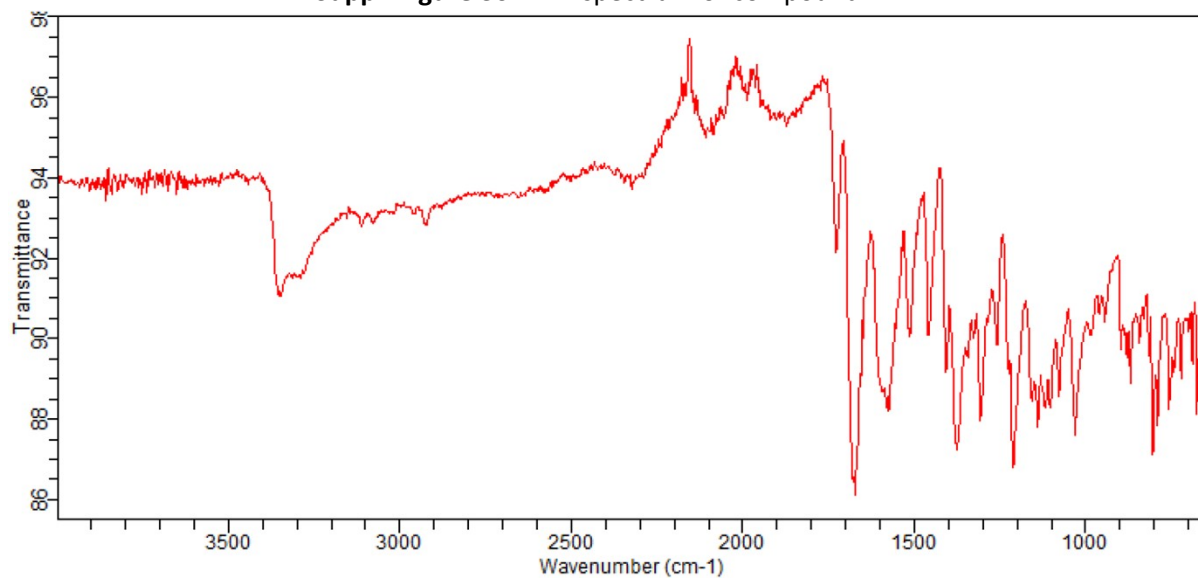
Suppl. Figure 28. FTIR spectrum of compound 20.



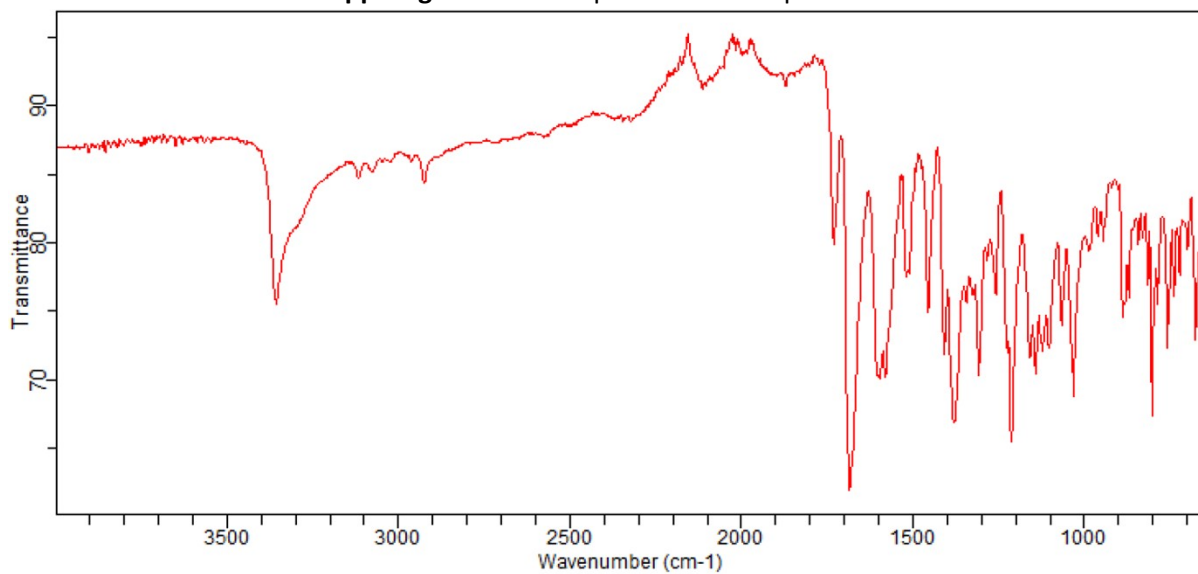
Suppl. Figure 29. FTIR spectrum of compound **21**.



Suppl. Figure 30. FTIR spectrum of compound **22**.



Suppl. Figure 31. FTIR spectrum of compound **23**.



Suppl. Figure 32. FTIR spectrum of compound 24.

