1 # Supplementary Material

2 **Thiadiazole–azetidinone sulfonamide hybrids with antimycobacterial activity supported by**

3 **structure-based analysis**

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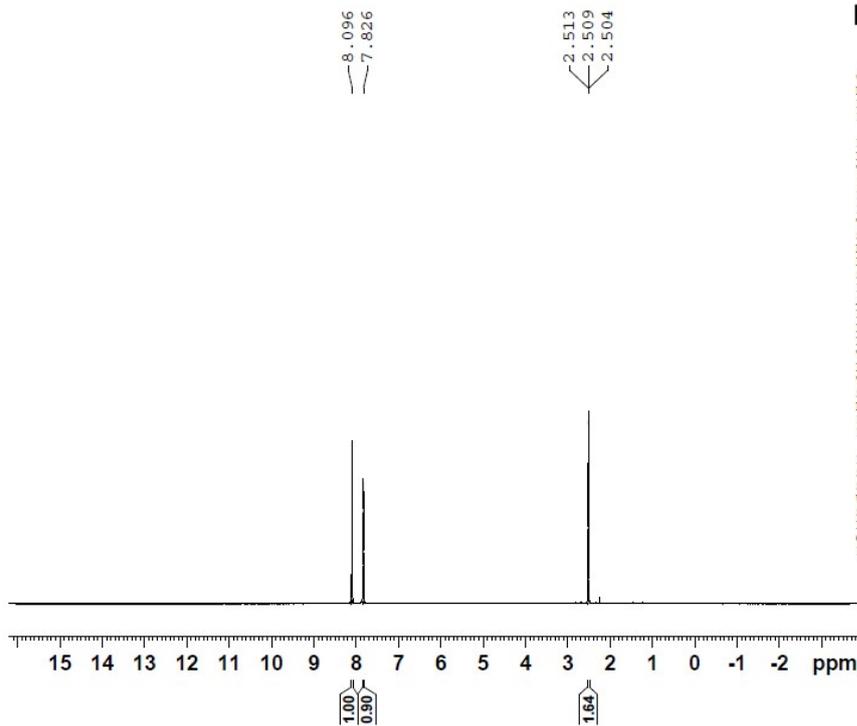19 Visakhapatnam-530045, (A.P.), India.

Description of the Spectral Analysis
1. Spectral data of ATS

¹H NMR

ATS-PROTON

8.096
7.826

2.513
2.509
2.504

BRUKER
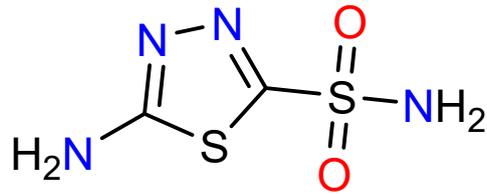
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EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
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PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   32
DS   2
SWH   8012.820 Hz
FIDRES   0.244532 Hz
AQ   4.0894465 sec
RG   115.78
DW   62.400 usec
DE   6.50 usec
TE   295.3 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P1   15.00 usec
PLW1   10.21100044 W

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

15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

1.00 0.90   1.64

^{13}C NMR

Current Data Parameters
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PROCNO   1
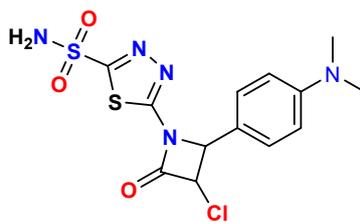
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PULPROG   zgpg
TD   32768
SOLVENT   DMSO
NS   2048
DS   4
SWH   24414.062 Hz
FIDRES   0.745058 Hz
AQ   0.6710886 sec
RG   501.187
DW   20.480 usec
DE   6.50 usec
TE   298.2 K
D1   1.00000000 sec
D11   0.03000000 sec
D31   0.00001500 sec
D32   0.89999998 sec
D40   0.00093990 sec
L4   23
L5   26
P32   90.00 usec
TD0   1

======== CHANNEL f1 ========
SFO1   75.4878687 MHz
NUC1   13C
P1   15.00 usec
PLW1   15.00000000 W

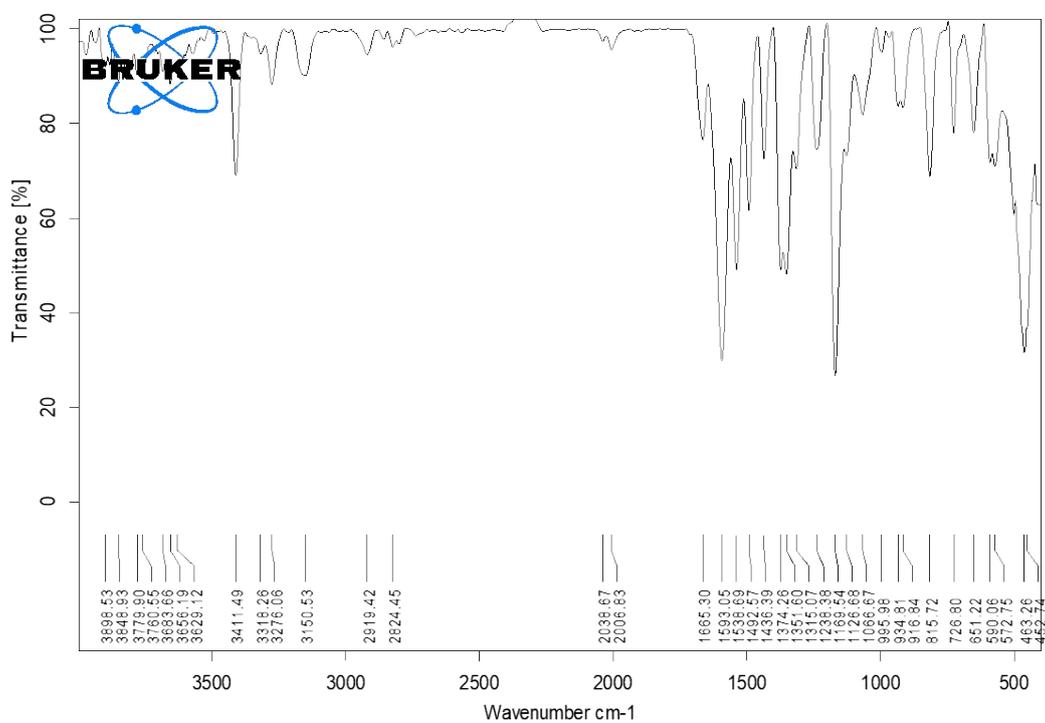======== CHANNEL f2 ========
SFO2   300.1812007 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   10.00000000 W
PLW12   0.20863999 W
PLW13   0.10495000 W

F2 - Processing parameters
SI   32768
SF   75.4803210 MHz
WDW   EM
SSB   0
LB   1.00 Hz
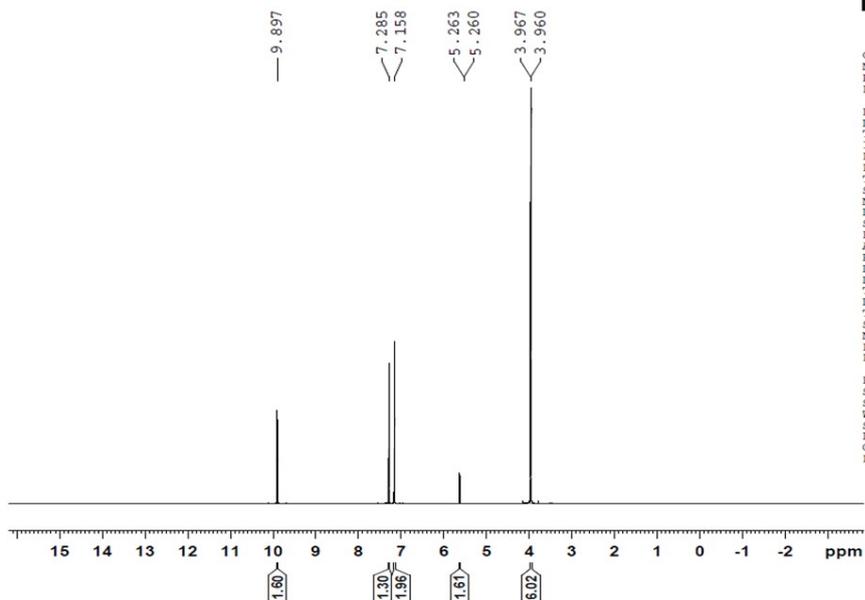GB   0
PC   1.40
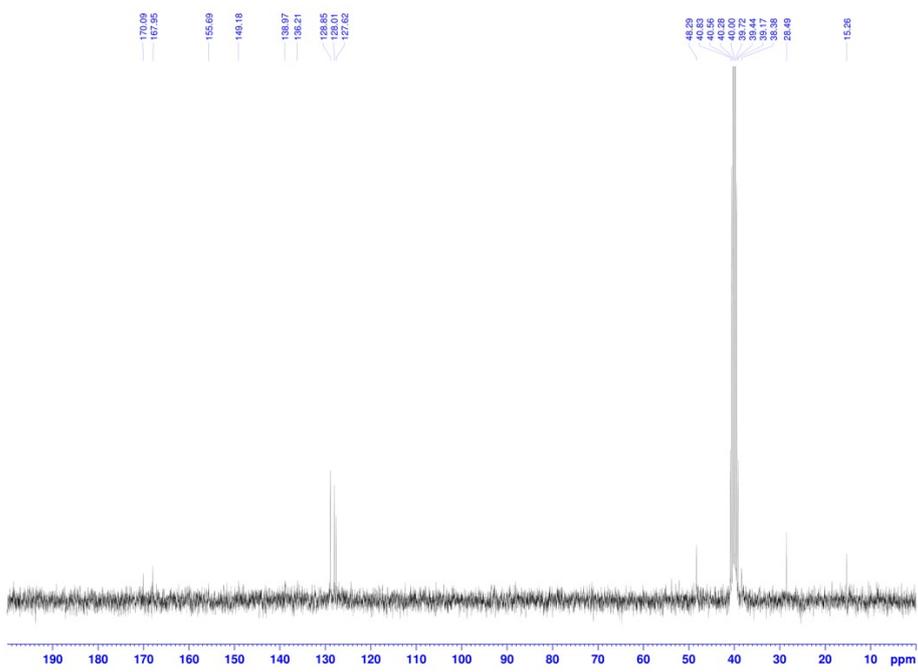
2. Spectral data of AZTDS-1

IR spectra

¹H NMR

AZTDS-1N-PROTON

9.897
7.285
7.158
5.263
5.260
3.967
3.960

15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

1.60   1.30 1.96   1.61   6.02

¹³C NMR

170.09
167.95
155.69
149.18
138.97
136.21
128.85
128.01
127.62
48.29
40.83
40.56
40.28
40.00
39.72
39.44
39.17
38.38
28.49
15.26

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

BRUKER

Current Data Parameters
NAME   S-1
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20220206
Time   4.39
INSTRUM   FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG   zgpg
TD   32768
SOLVENT   DMSO
NS   2048
DS   4
SWH   24414.062 Hz
FIDRES   0.745058 Hz
AQ   0.6710886 sec
RG   501.187
DW   20.480 usec
DE   6.50 usec
TE   298.2 K
D1   1.00000000 sec
D11   0.03000000 sec
D31   0.00001500 sec
D32   0.89999998 sec
D40   0.00093990 sec
L4   23
L5   26
P32   90.00 usec
TD0   1

======== CHANNEL f1 ========
SFO1   75.4878687 MHz
NUC1   13C
P1   15.00 usec
PLW1   15.00000000 W

======== CHANNEL f2 ========
SFO2   300.1812007 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   10.00000000 W
PLW12   0.20863999 W
PLW13   0.10495000 W
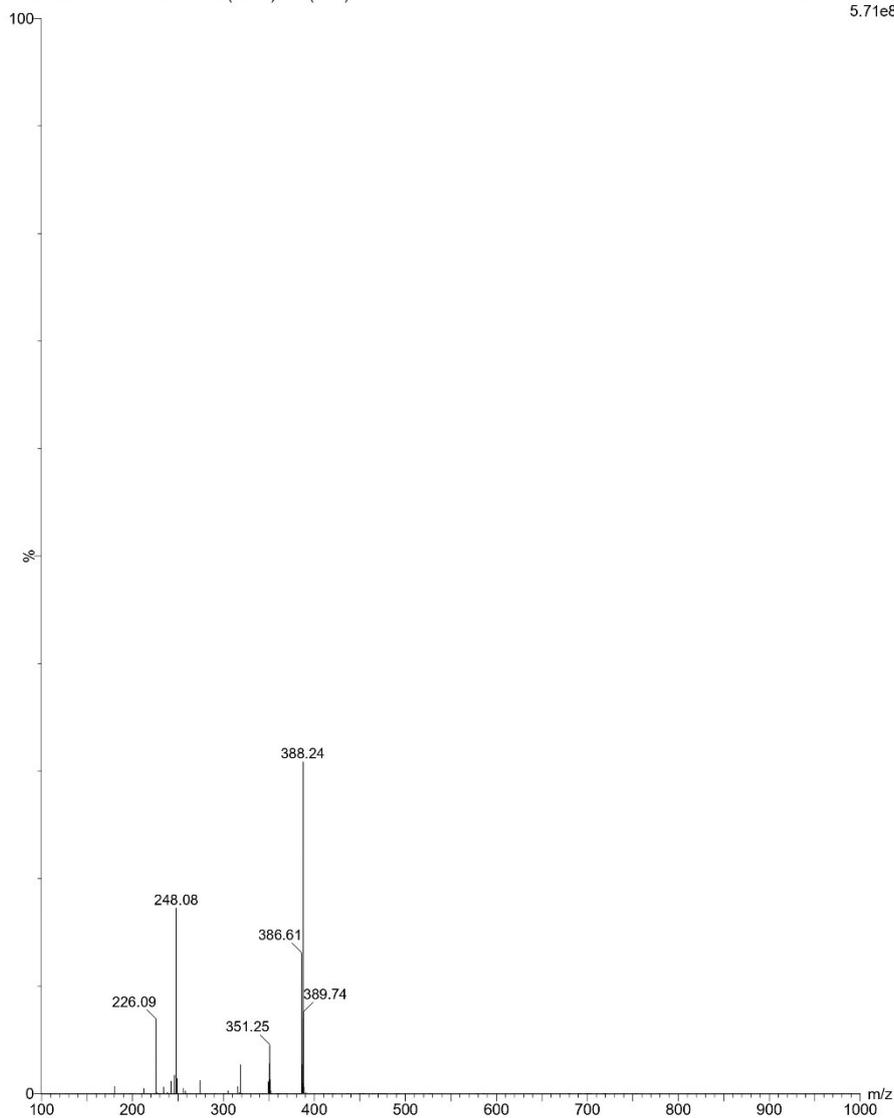
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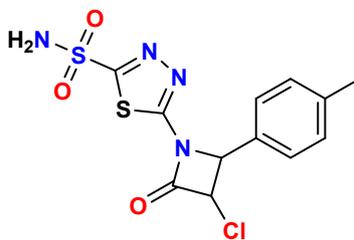WDW   EM
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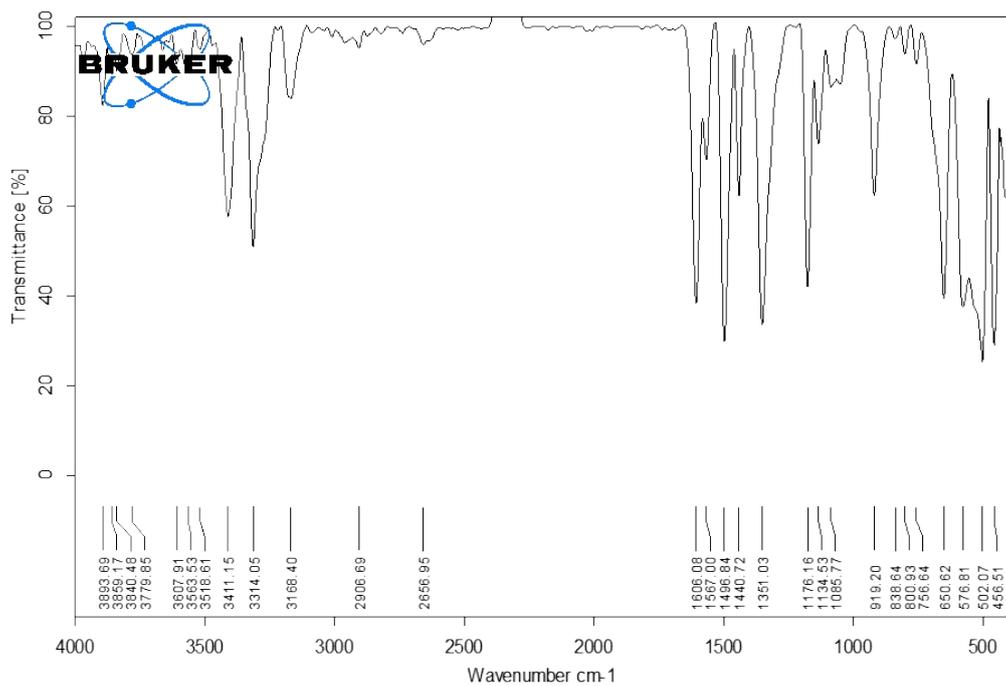GB   0
PC   1.40

HRMS

3. Spectral data of AZTDS-2

IR spectra

^{1}H NMR

AZTDS-2-PROTON

Peak labels: 8.040, 7.807, 7.431, 7.083, 7.064, 5.240, 5.222, 5.195, 5.177, 2.237, 2.229, 2.159, 2.107, 1.993, 1.874, 1.473, 1.382, 1.240, 1.116

Integrations: 1.86, 1.00, 0.93, 3.11, 1.88, 0.30, 0.57, 0.11, 0.38, 0.78, 1.47, 0.51
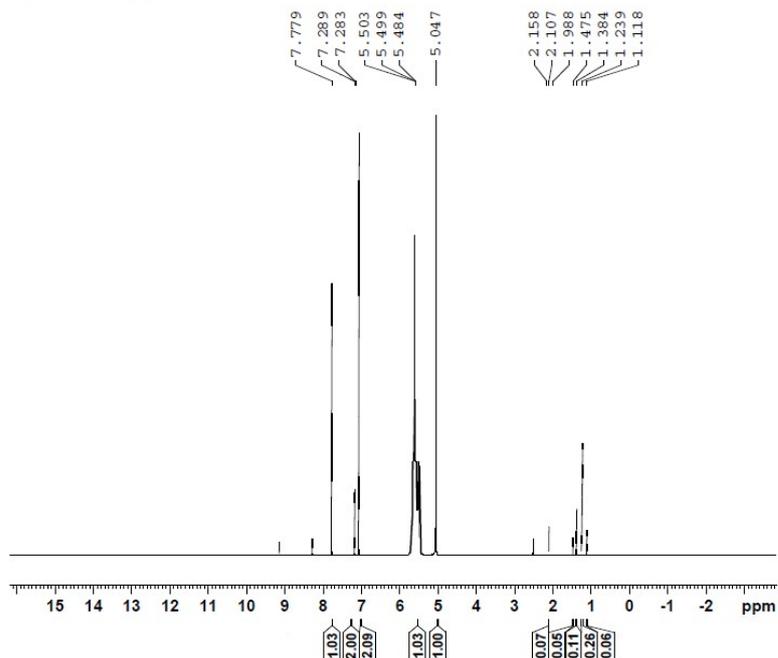
Curre
NAME   25022022
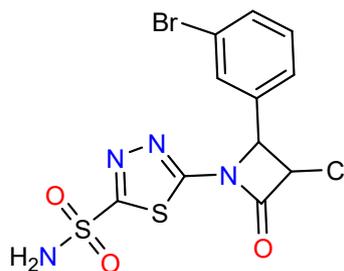EXPNO   7
PROCNO   1

F2 - Acquisition Parameters
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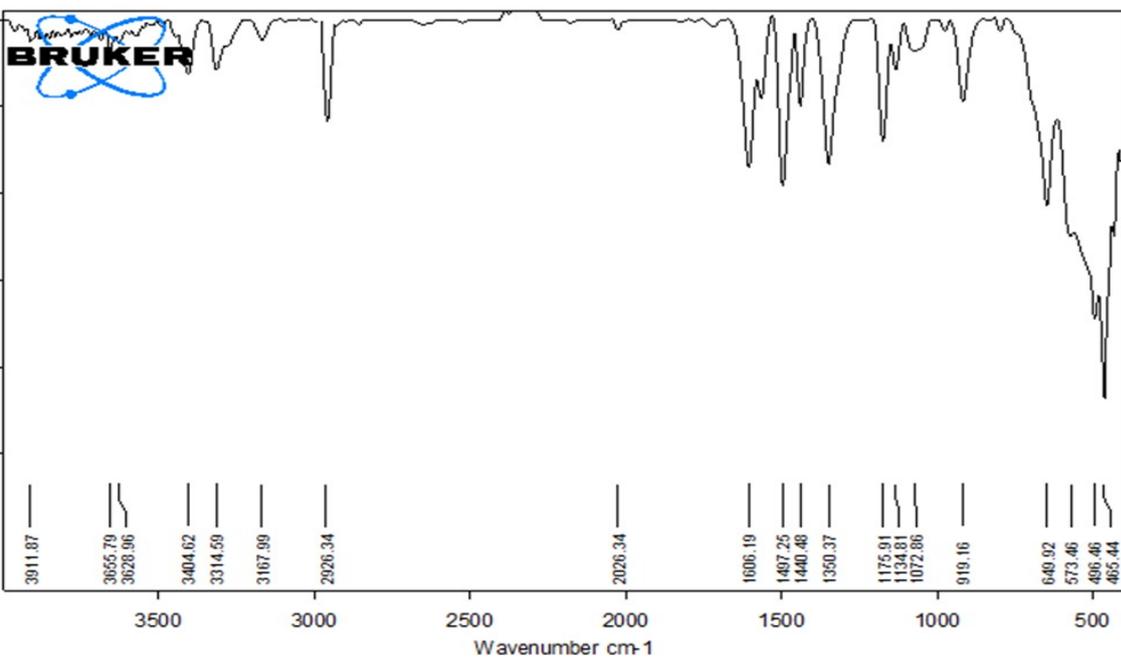INSTRUM   spect
PROBHD   Z108618_0646 (
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   0
SWH   8012.820 Hz
FIDRES   0.244532 Hz
AQ   4.0894465 sec
RG   132.41
DW   62.400 usec
DE   6.50 usec
TE   298.2 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P1   15.00 usec
PLW1   10.21100044 W

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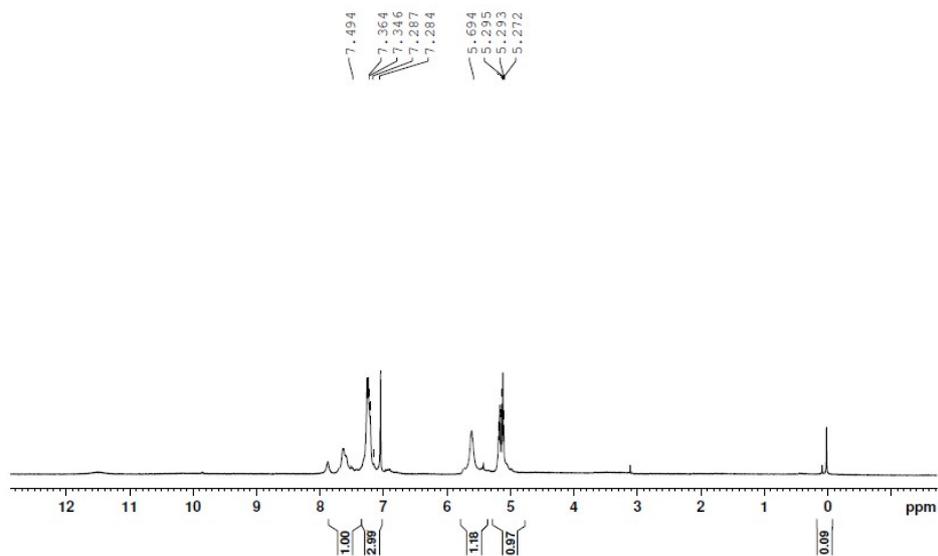SSB   0
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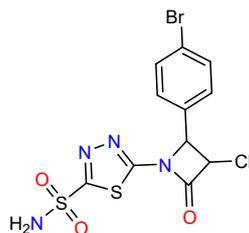GB   0
PC   1.00

4. Spectral data of AZTDS-3

IR spectra

¹H NMR

7.779
7.289
7.283
5.503
5.499
5.484
5.047
2.158
2.107
1.988
1.475
1.384
1.239
1.118

15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

1.03 2.00 2.09 1.03 1.00 0.07 0.05 0.11 0.26 0.06

5. Spectral data of AZTDS-4

IR Spectra

IR spectrum peaks: 3911.87, 3655.79, 3628.96, 3404.62, 3314.59, 3167.99, 2926.34, 2026.34, 1606.19, 1497.25, 1440.48, 1350.37, 1175.91, 1134.81, 1072.86, 919.16, 649.92, 573.46, 496.46, 465.44

Wavenumber cm-1

¹H NMR

7.494
7.364
7.346
7.287
7.284
5.694
5.295
5.293
5.272

12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00 2.99   1.18 0.97   0.09

6. Spectral data of AZTDS-5

IR spectra

¹H NMR

AZTDS-5-PROTON

7.889
7.868
7.585
7.269
7.262
5.690
5.669
5.297
3.969
3.962

Current Data Parameters
NAME   17122021
EXPNO   7
PROCNO   1

F2 - Acquisition Parameters
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Time   11.26 h
INSTRUM   spect
PROBHD   Z108618_0646 (
PULPROG   zg30
TD   65536
SOLVENT   CDC13
NS   32
DS   2
SWH   8012.820 Hz
FIDRES   0.244532 Hz
AQ   4.0894465 sec
RG   204
DW   62.400 usec
DE   6.50 usec
TE   298.2 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P1   15.00 usec
PLW1   10.21100044 W

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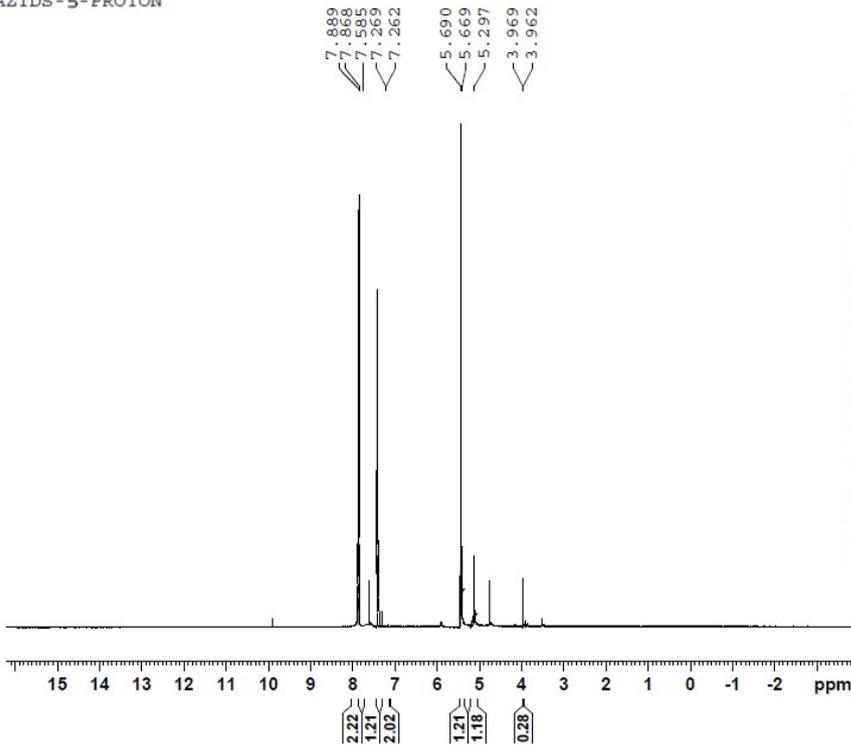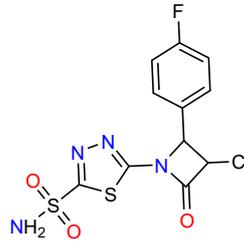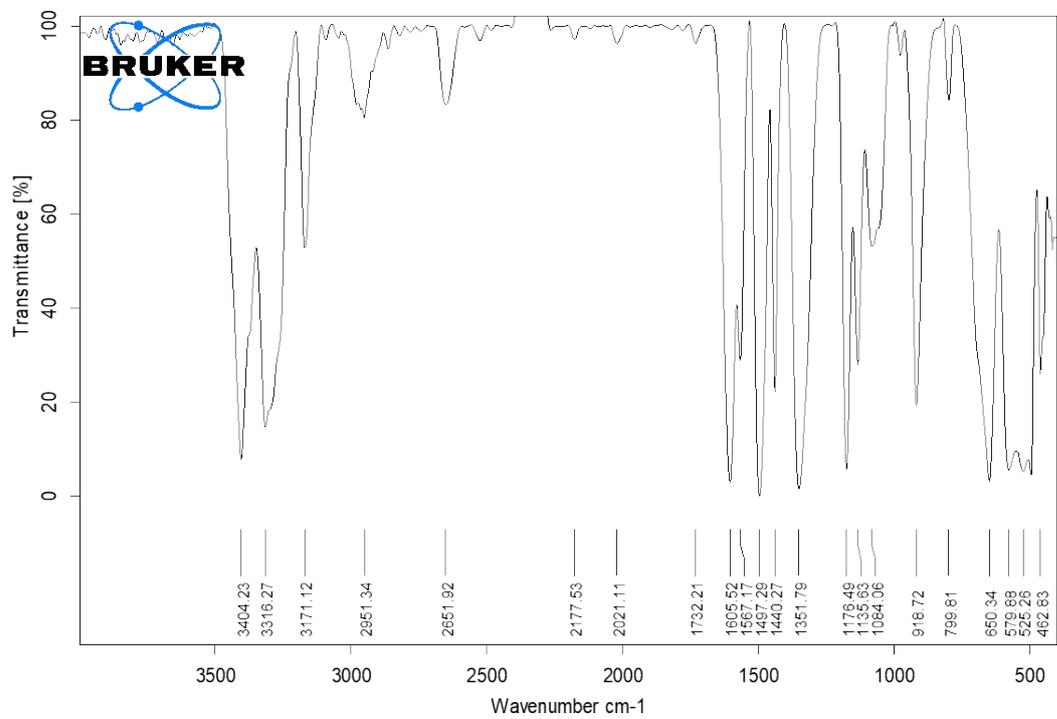LB   0.30 Hz
GB   0
PC   1.00

2.22 1.21 2.02   1.21 1.18   0.28

7. Spectral data of AZTDS-8

IR Spectra

¹H NMR

AZTDS-8-PROTON

7.813
7.645
7.641
7.060
5.645
5.641
5.244
5.224
5.218
2.508

Current Data Parameters
NAME   25022022
EXPNO   11
PROCNO   1

F2 - Acquisition Parameters
Date_   20220225
Time   17.19 h
INSTRUM   spect
PROBHD   Z108618_0646 (
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   0
SWH   8012.820 Hz
FIDRES   0.244532 Hz
AQ   4.0894465 sec
RG   132.41
DW   62.400 usec
DE   6.50 usec
TE   298.2 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P1   15.00 usec
PLW1   10.21100044 W

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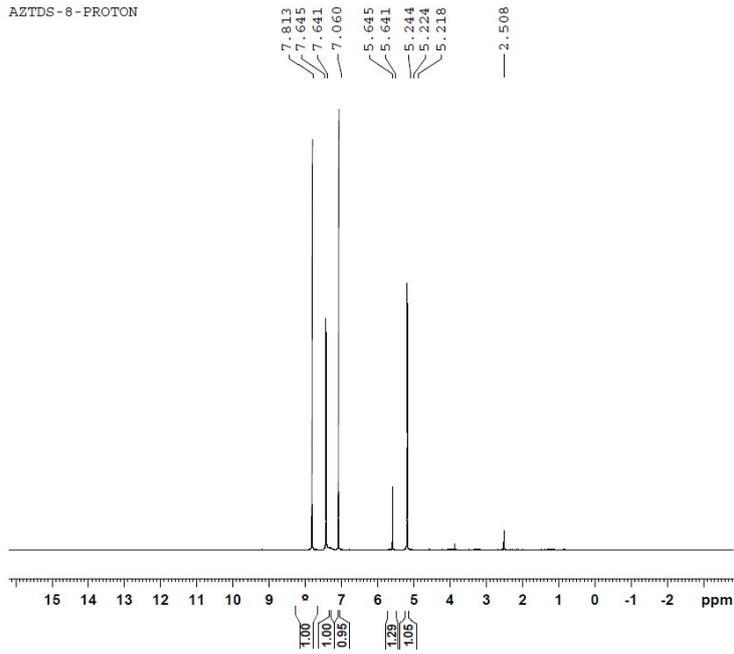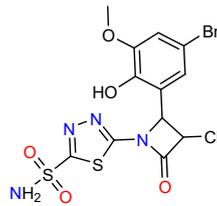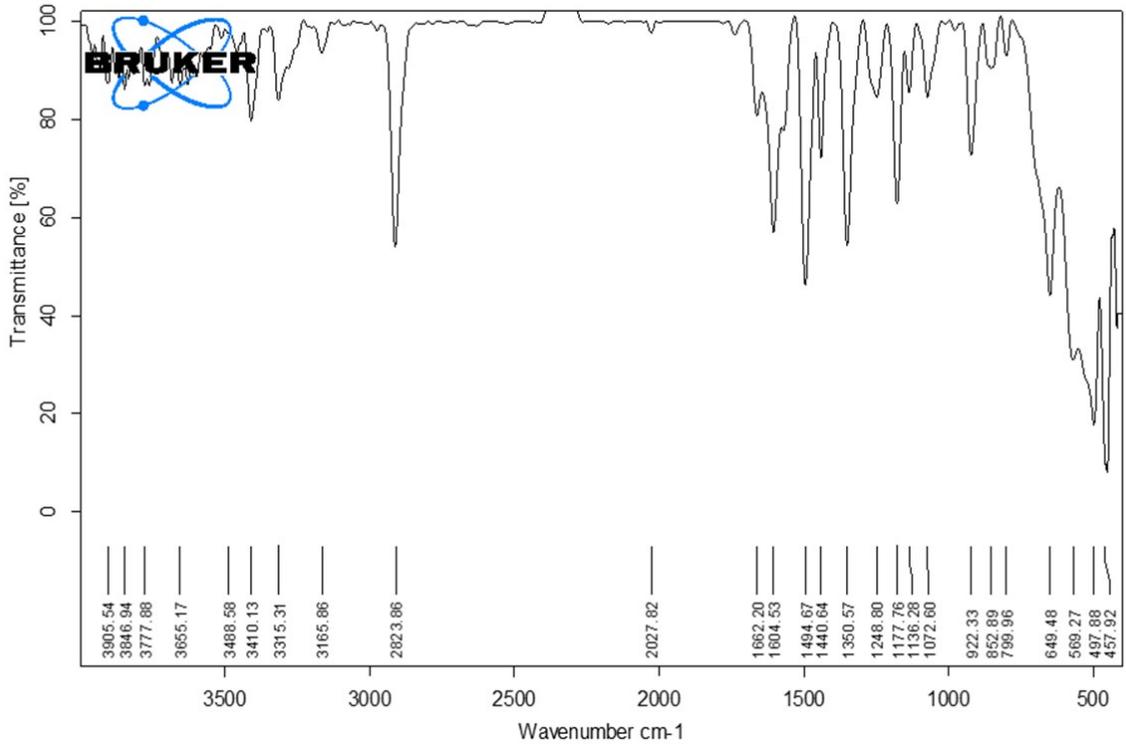SSB   0
LB   0.30 Hz
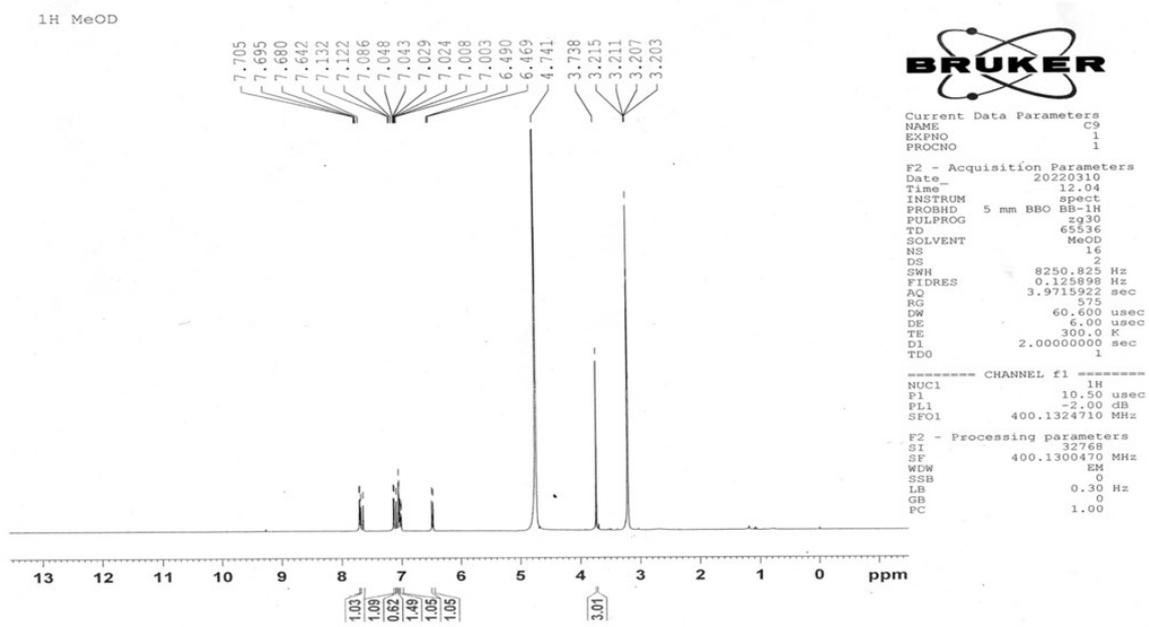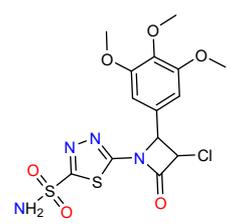GB   0
PC   1.00

15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

1.00 1.00 0.95 1.29 1.05

8. Spectral data of AZTDS-12

IR spectra

¹H NMR

9. Spectral data of AZTDS-14

IR spectra

Transmittance [%]

Wavenumber cm-1

3350.93
3176.92
3012.75
2971.48
2946.68
2842.94
2801.97
2752.30
2715.11
2654.67
2563.90
2276.72
2246.97
2109.23
1957.29
1685.99
1588.09
1505.45
1462.96
1427.39
1390.55
1329.47
1237.69
1188.30
1126.79
990.57
846.06
783.99
757.57
729.04
626.36
591.57
462.87
423.66

¹H NMR

AZTDS-14-PROTON

Current Data Parameters
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PROCNO   1

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Date_   20220218
Time   11.59 h
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PROBHD   Z108618_0646 (
PULPROG   zg30
TD   65536
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NS   32
DS   2
SWH   8012.820 Hz
FIDRES   0.244532 Hz
AQ   4.0894465 sec
RG   162.09
DW   62.400 usec
DE   6.50 usec
TE   293.4 K
D1   2.00000000 sec
TD0   1
SPO1   400.1324708 MHz
NUC1   1H
P1   15.00 usec
PLW1   10.21100044 W

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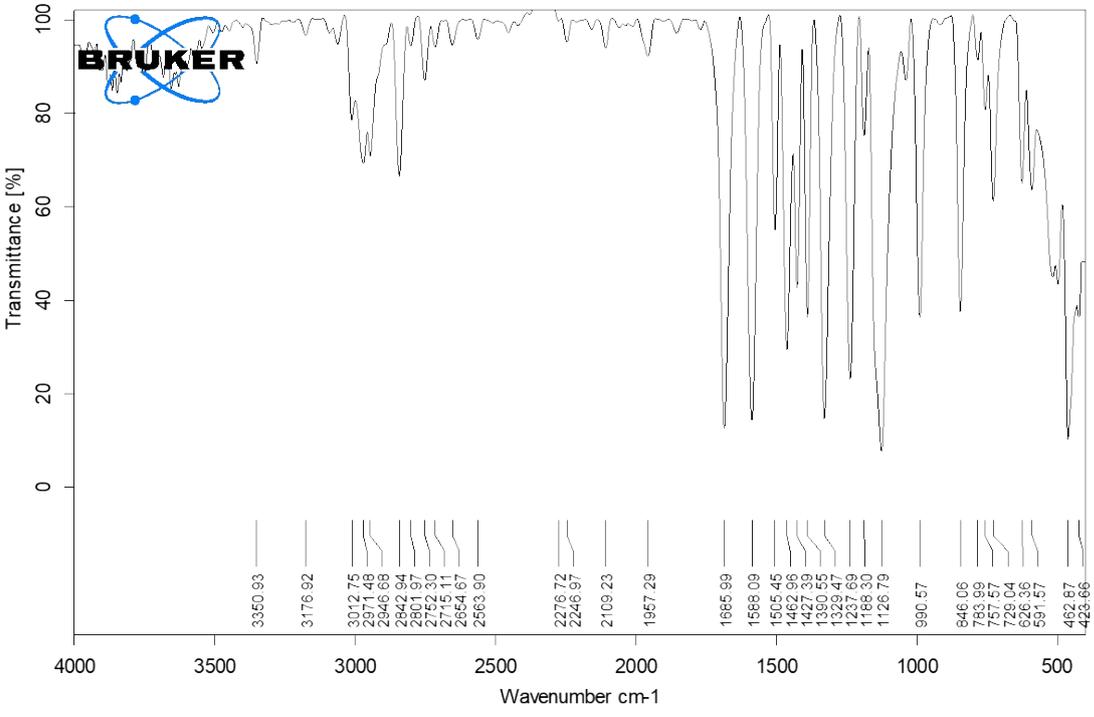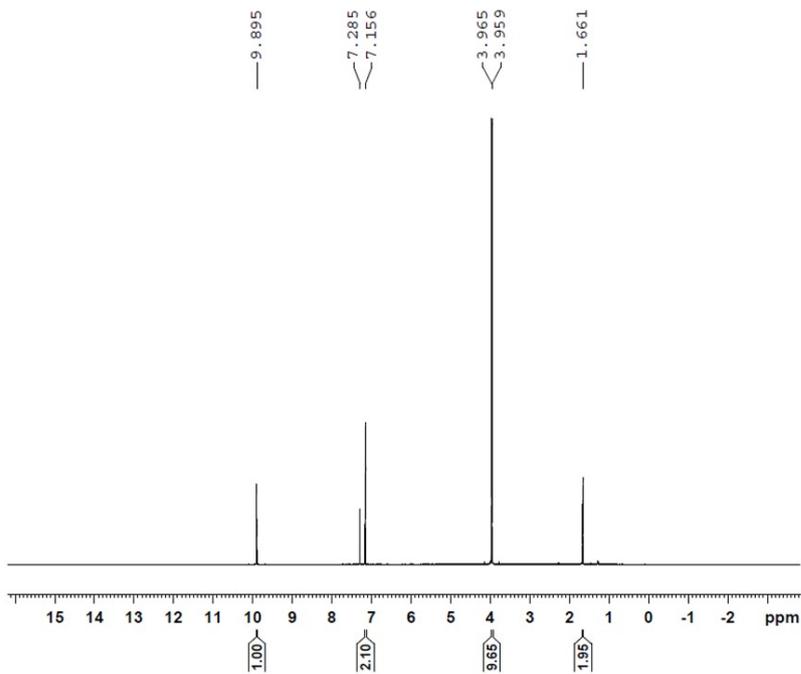LB   0.30 Hz
GB   0
PC   1.00