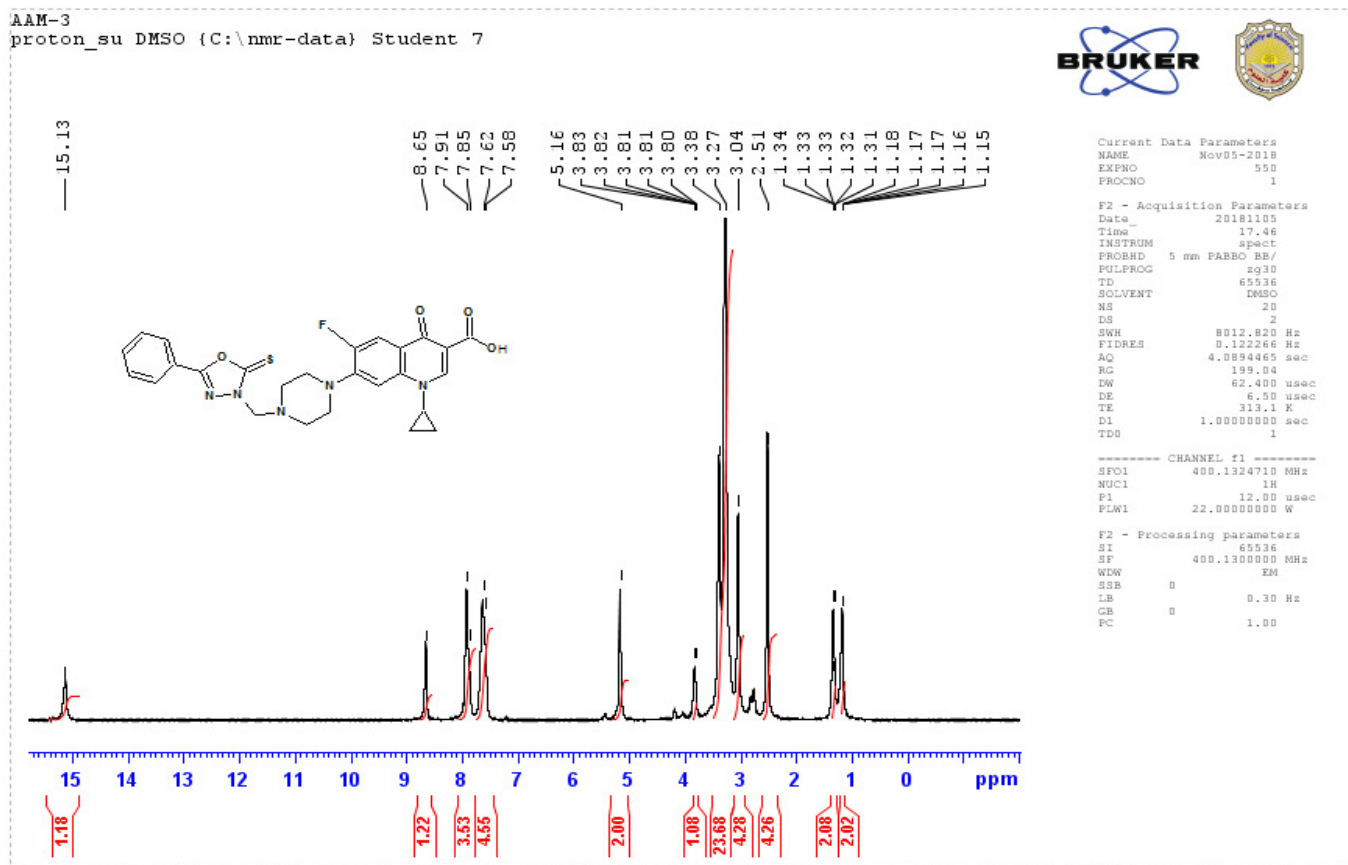
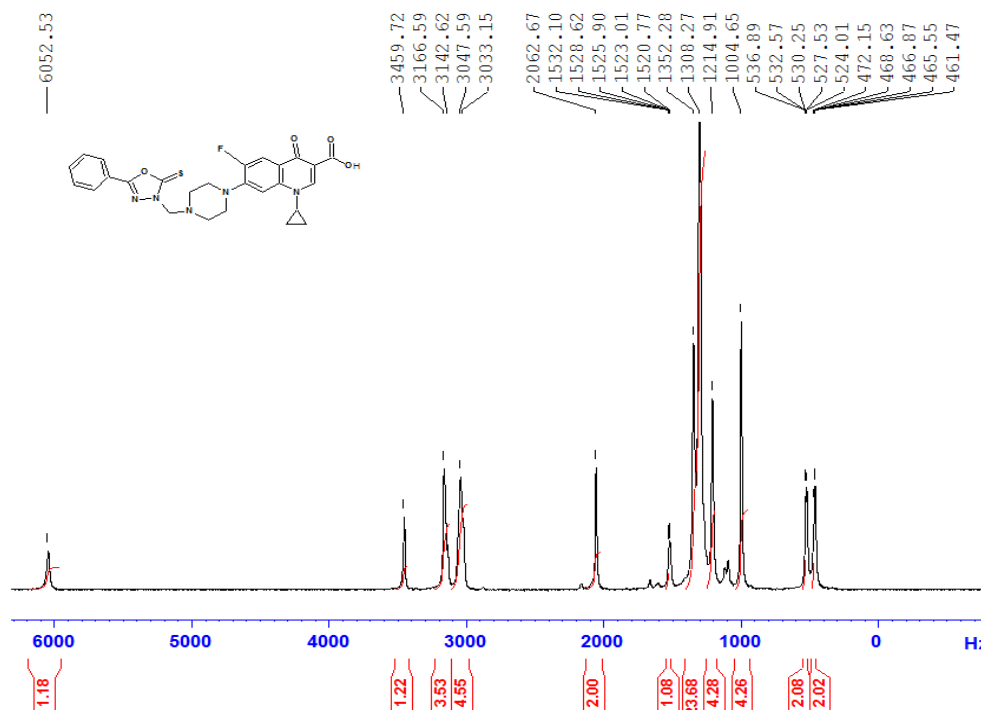


Supporting Information

Figure S1- ^1H , ^{13}C NMR and dept-135 Spectra of 1:



AAM-3
proton_su DMSO {C:\nmr-data} Student 7



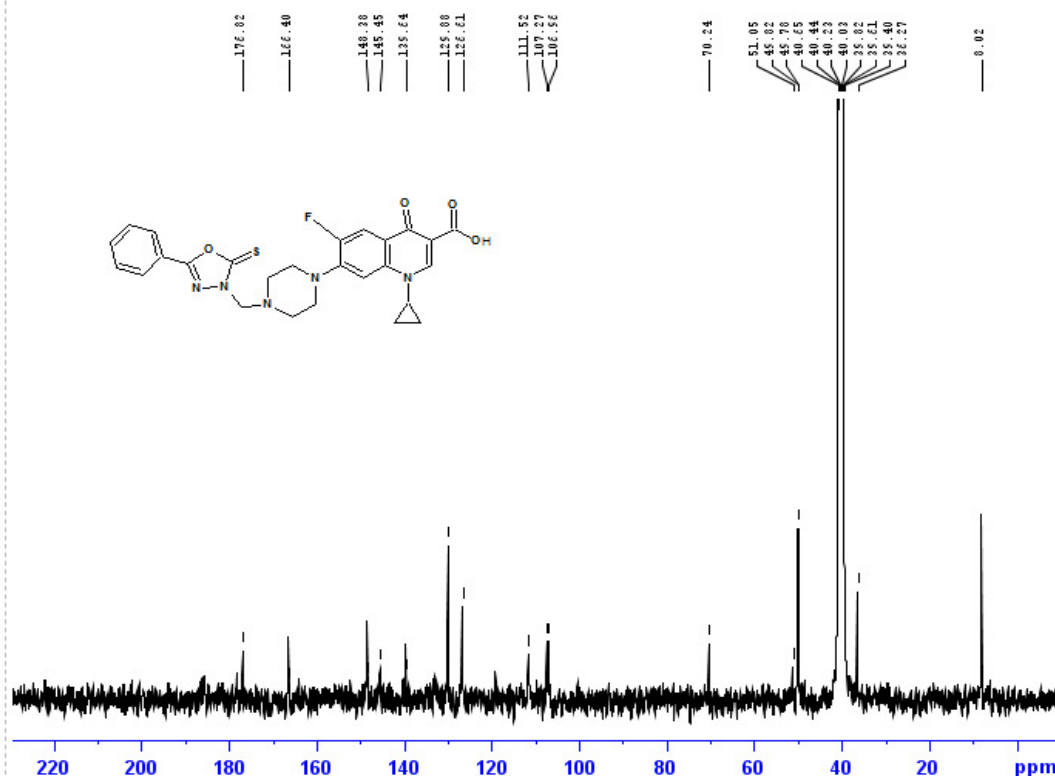
Current Data Parameters
NAME Nov05-2018
EXPNO 550
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181105
Time 17.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 313.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-3
c13_su DMSO {C:\nmr-data} Student 12



Current Data Parameters
NAME Dec25-2018
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181225
Time 11.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG waltz16
TD 65536
SOLVENT DMSO
NS 1100
DS 4
SWH 24030.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 175.84
DW 20.800 usec
DE 6.50 usec
TE 313.2 K
D1 2.0000000 sec
D11 0.02000000 sec
TD0 1

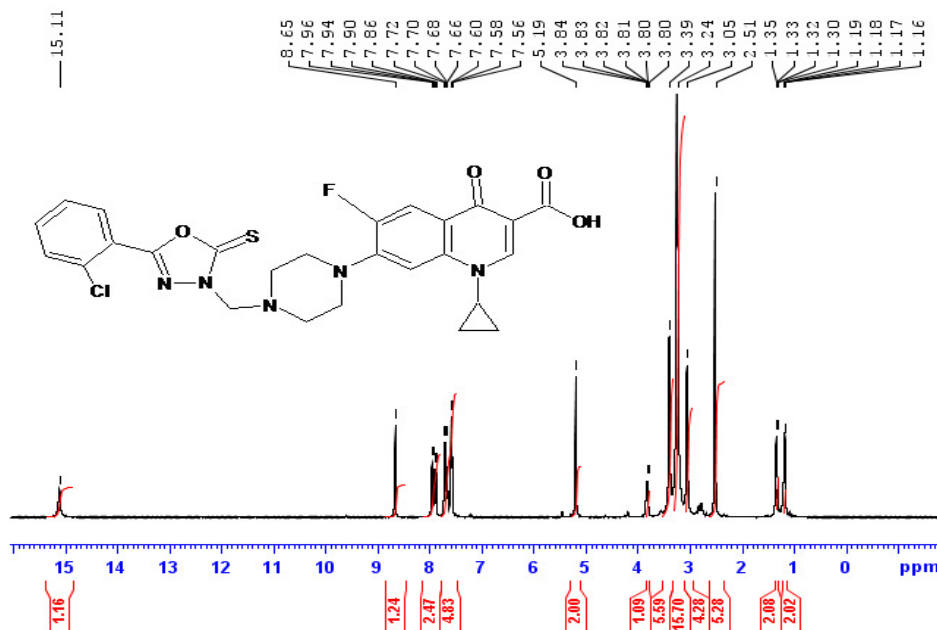
===== CHANNEL f1 =====
SF01 100.6230364 MHz
NUC1 13C
P1 5.50 usec
PLW1 56.00000000 W

===== CHANNEL f2 =====
SF02 400.1316005 MHz
NUC2 1H
CPDPRG12 waltz16
P2PC2 50.00 usec
PLW2 22.00000000 W
PLW12 0.41051001 W
PLW13 0.23204000 W

F2 - Processing parameters
SI 32768
SF 100.6127650 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S2- ^1H , ^{13}C NMR and dept-135 Spectra of 2

AAM-19
proton_su DMSO (C:\nmr-data) Student 22



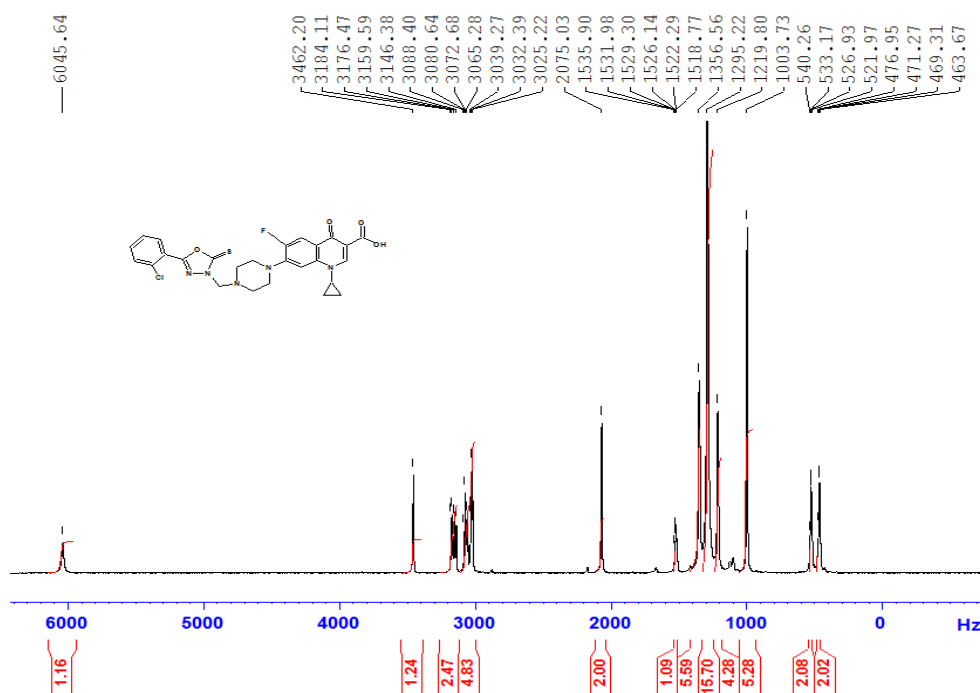
Current Data Parameters
NAME Jan03-2019
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190103
Time 12.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 318.1 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-19
proton_su DMSO (C:\nmr-data) Student 22



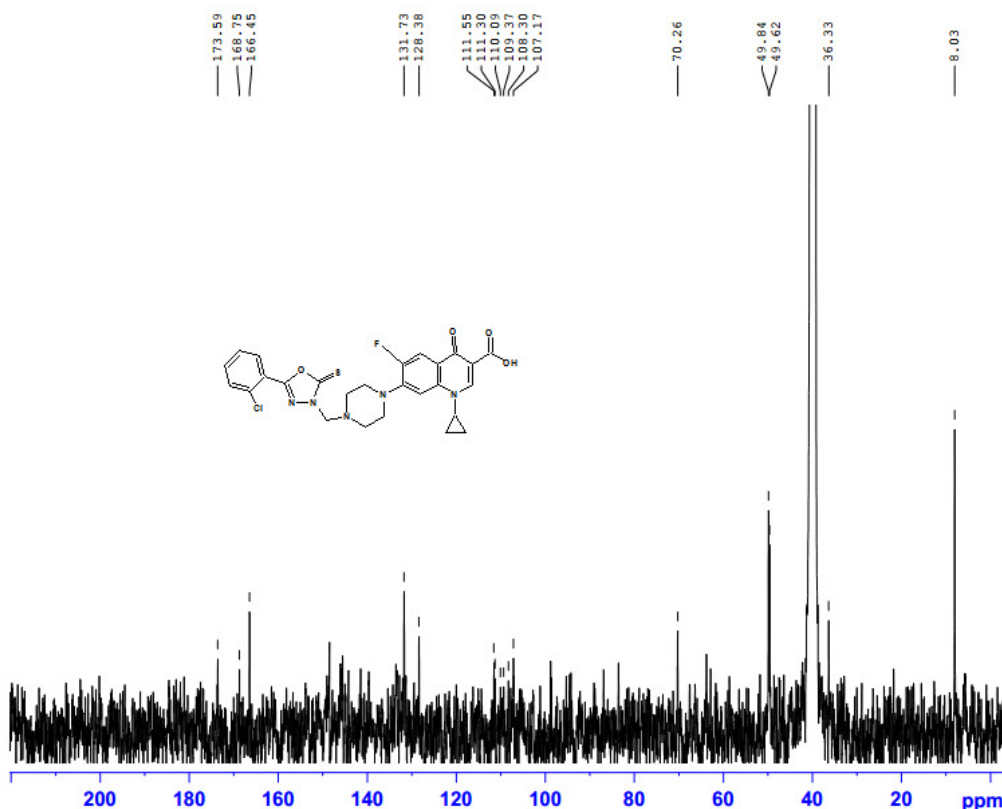
Current Data Parameters
NAME Jan03-2019
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190103
Time 12.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 318.1 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 13C
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-19
c13_su DMSO {C:\nmr-data} Student 2



Current Data Parameters
NAME Jan15-2019
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190116
Time_ 12.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 100.43
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

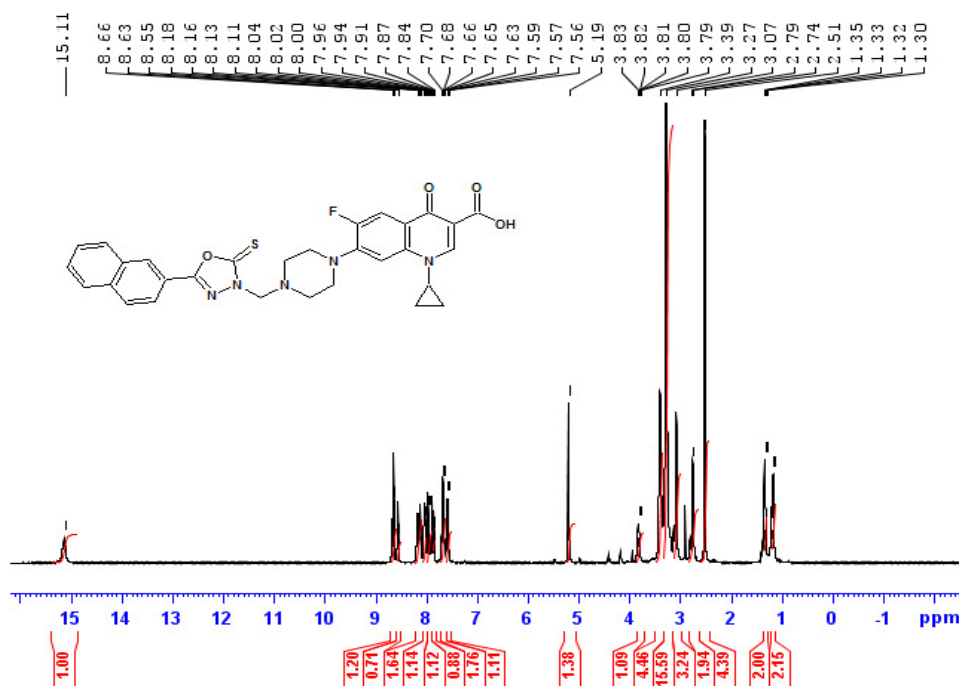
CHANNEL f1
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
PLW1 56.00000000 W

CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPOPRG2 waltz16
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W
PLW13 0.33284000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S3-¹H, ¹³C NMR and dept-135 Spectra of 3

AAM-22
proton_su DMSO {C:\nmr-data} Student 11

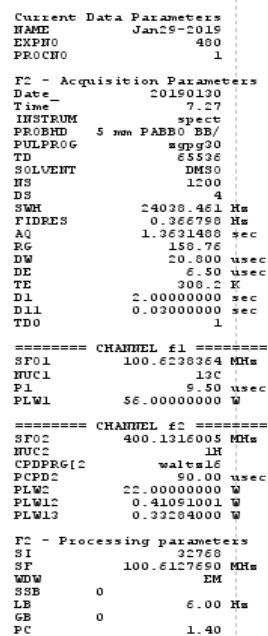
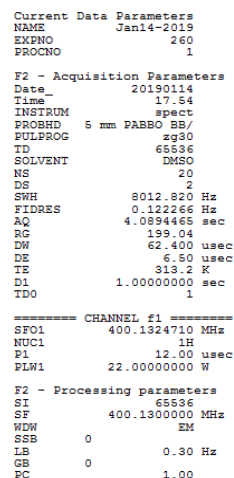


Current Data Parameters
NAME Jan14-2019
EXPNO 268
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190114
Time_ 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TD0 1

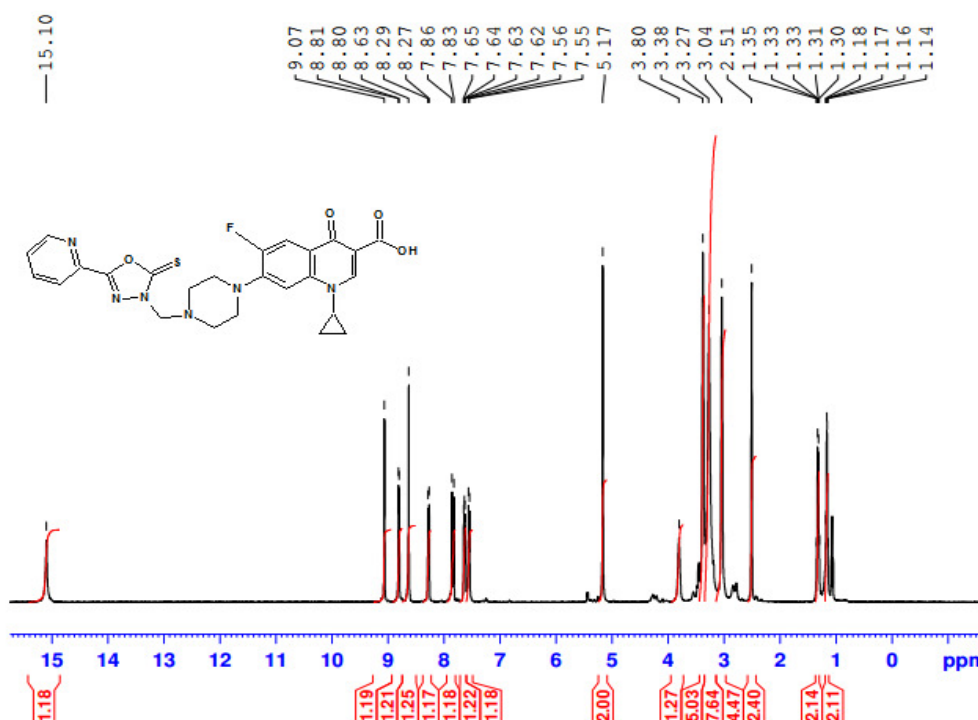
CHANNEL f1
SFO1 400.1324718 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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



S4- ^1H , ^{13}C NMR and dept-135 Spectra of 4

AAM-11
proton_su DMSO {C:\nmr-data} Student 9



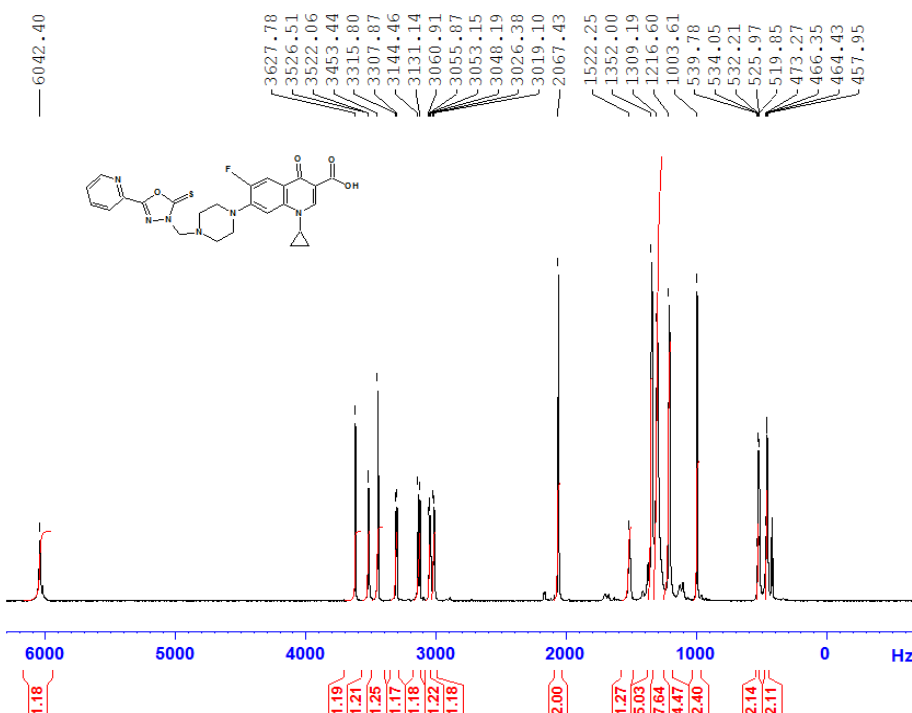
Current Data Parameters
NAME Jan14-2019
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190114
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 175.84
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-11
proton_su DMSO {C:\nmr-data} Student 9

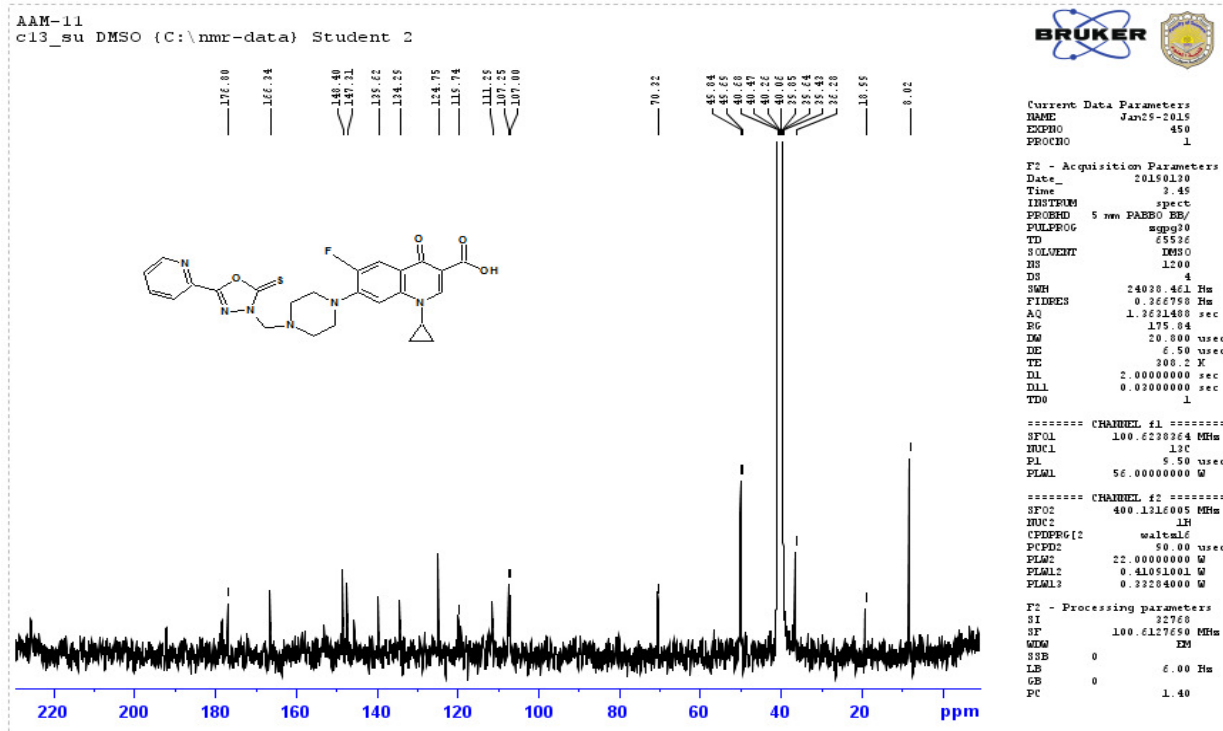


Current Data Parameters
NAME Jan14-2019
EXPNO 110
PROCNO 1

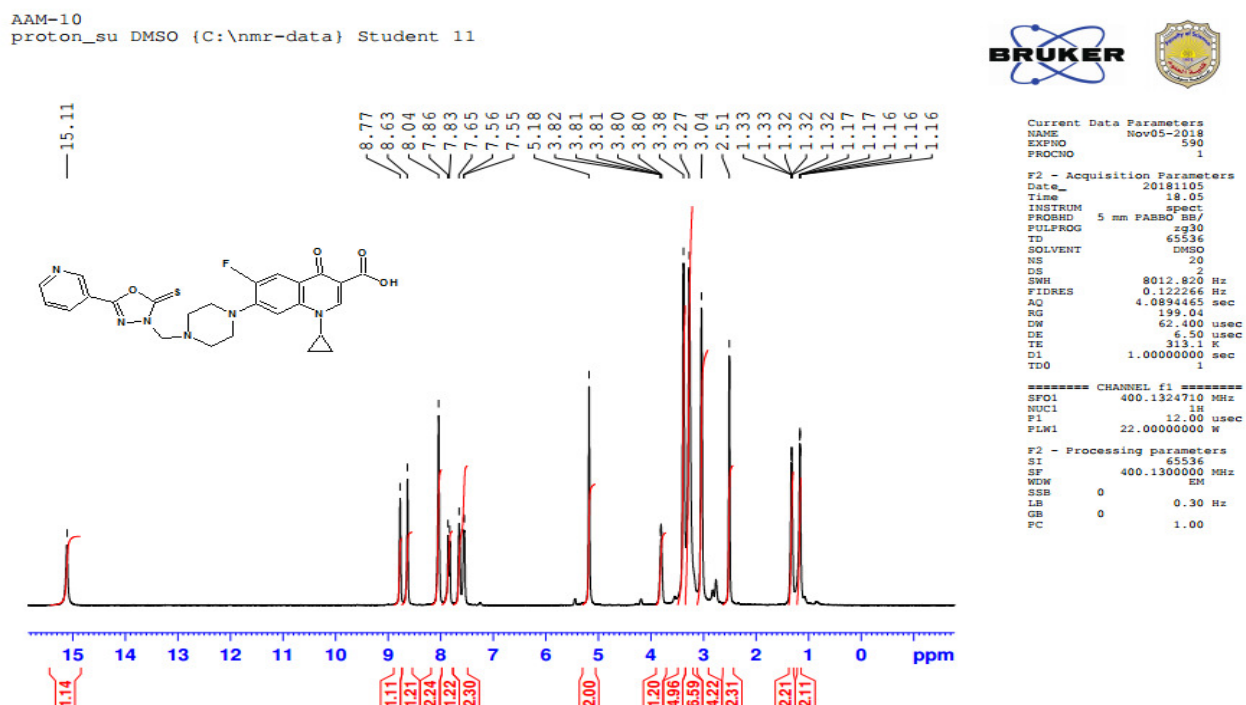
F2 - Acquisition Parameters
Date_ 20190114
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 175.84
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

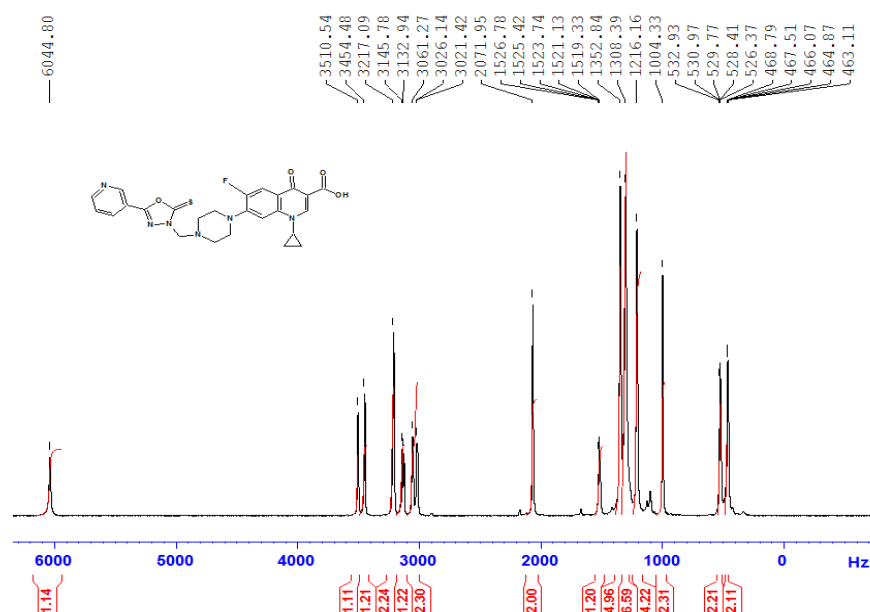
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S5- ^1H , ^{13}C NMR and dept-135 Spectra of 5



AAM-10
proton_su DMSO (C:\nmr-data) Student 11



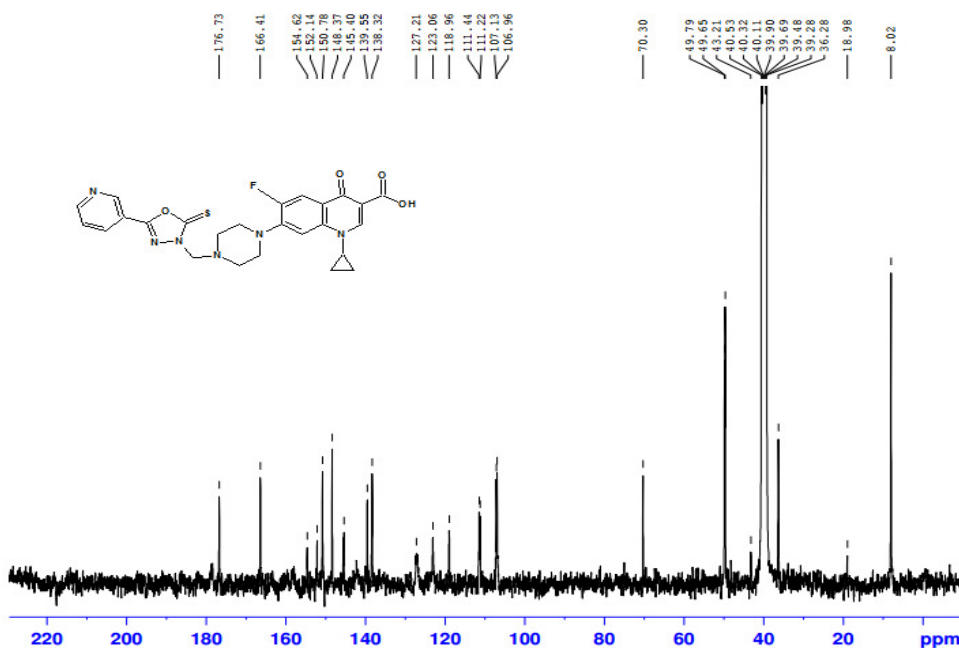
Current Data Parameters
NAME Nov05-2018
EXPNO 590
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181105
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DM 62.400 usec
DE 6.50 usec
TE 313.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.90 Hz
GB 0
PC 1.00

AAM-10
c13_su DMSO (C:\nmr-data) Student 2



Current Data Parameters
NAME Nov26-2018
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181126
Time 15.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1100
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 158.76
DM 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

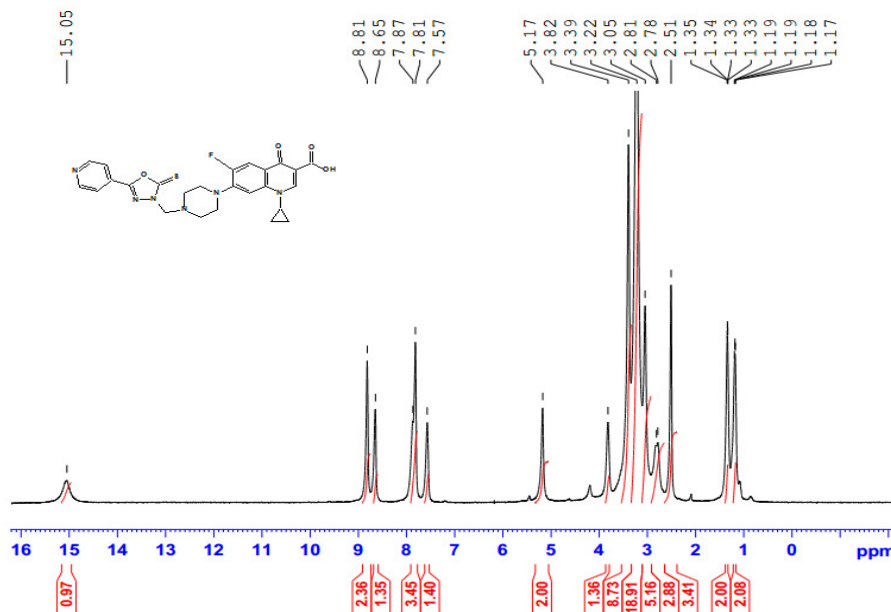
===== CHANNEL f1 =====
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
PLW1 56.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W
PLW13 0.33284000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S6- ^1H , ^{13}C NMR and dept-135 Spectra of 6

AAM-6
proton_su DMSO {C:\nmr-data} Student 17



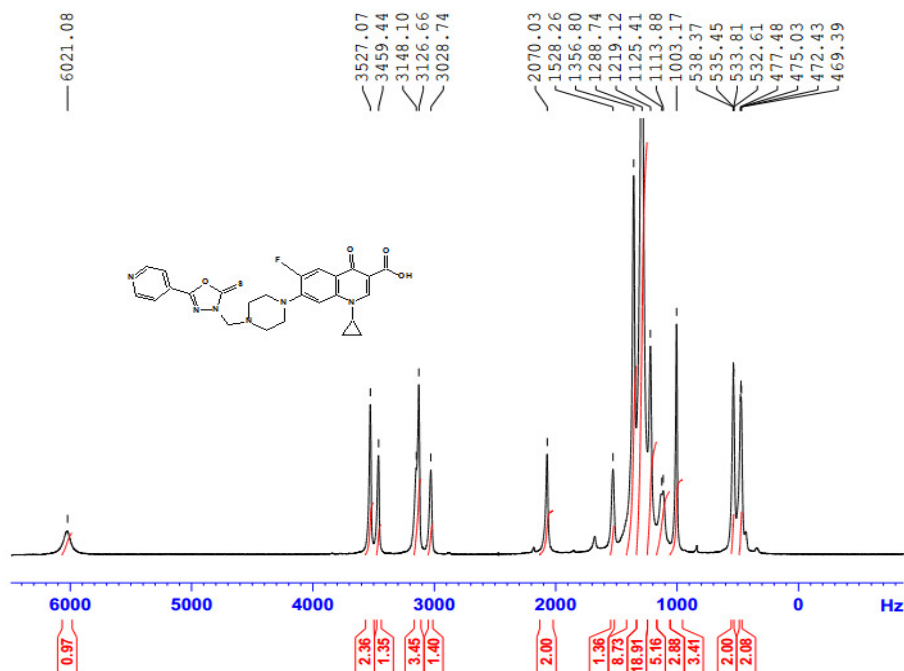
Current Data Parameters
NAME Jan27-2019
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190127
Time 13.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 30
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 328.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-6
proton_su DMSO {C:\nmr-data} Student 17

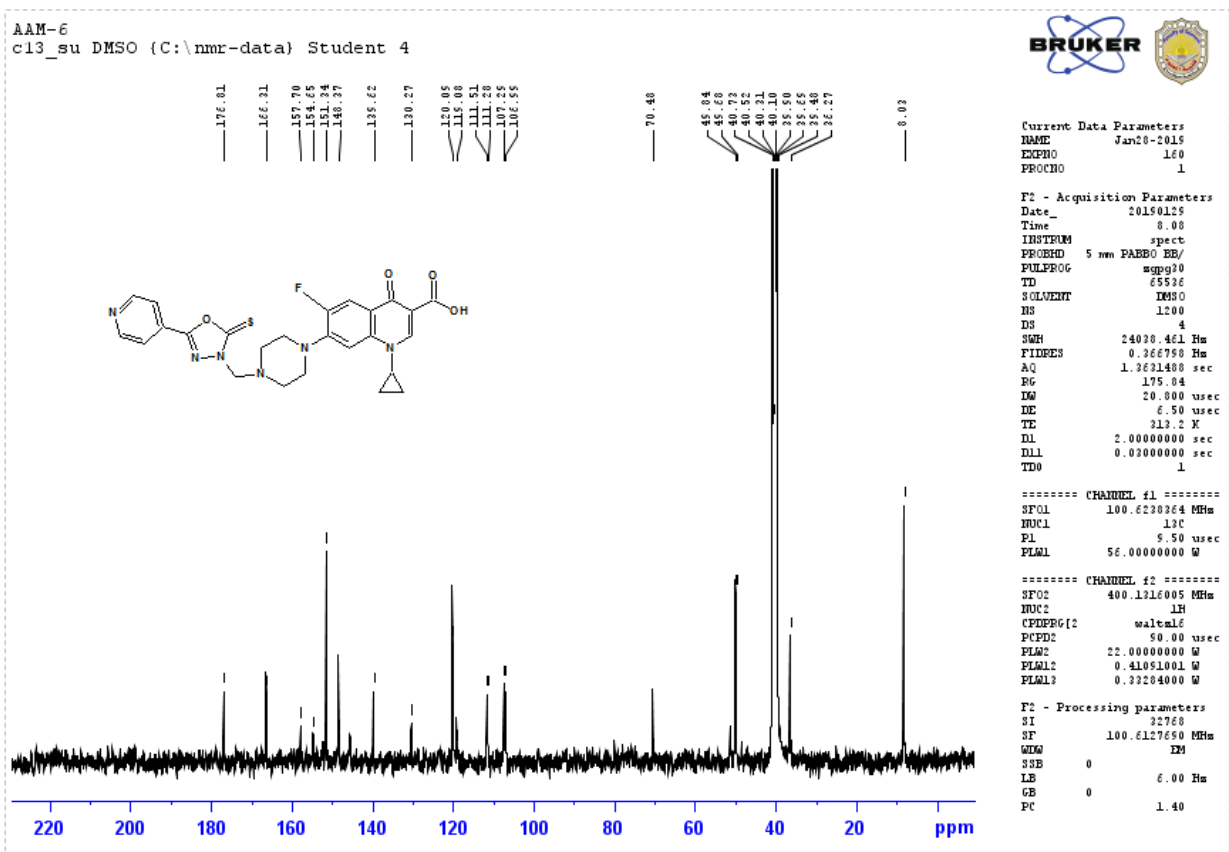


Current Data Parameters
NAME Jan27-2019
EXPNO 30
PROCNO 1

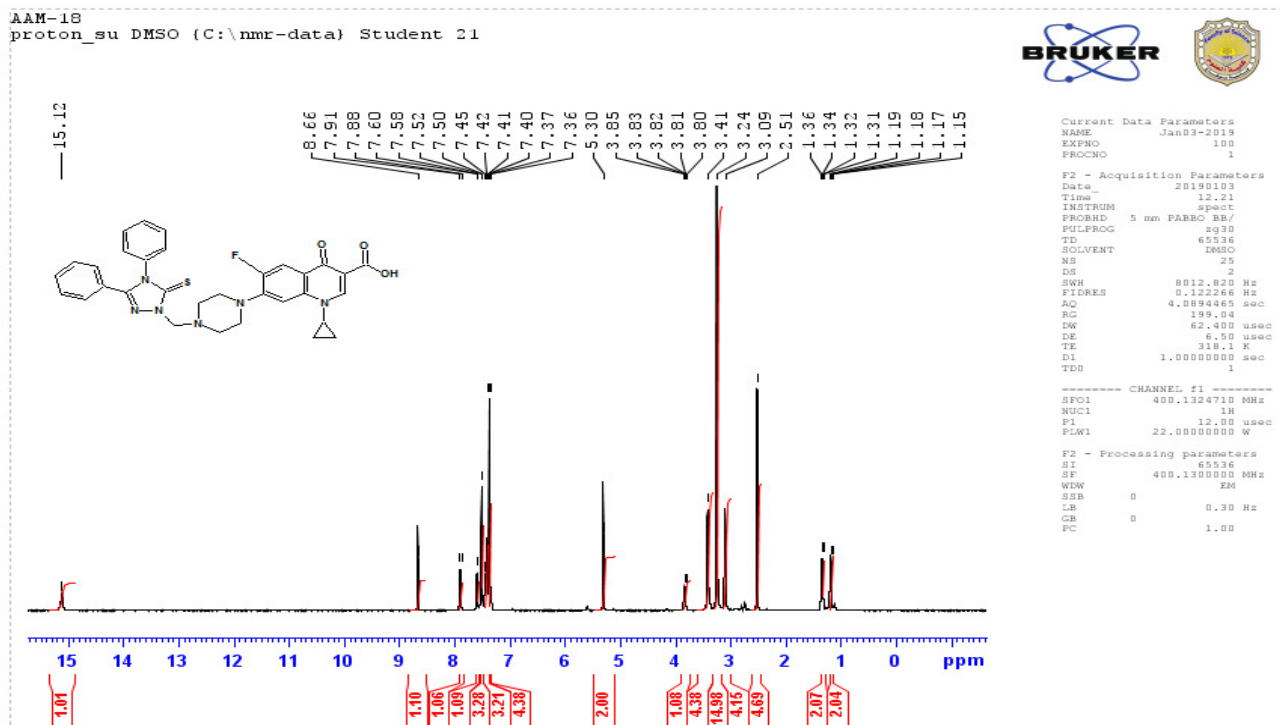
F2 - Acquisition Parameters
Date_ 20190127
Time 13.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 30
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 328.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

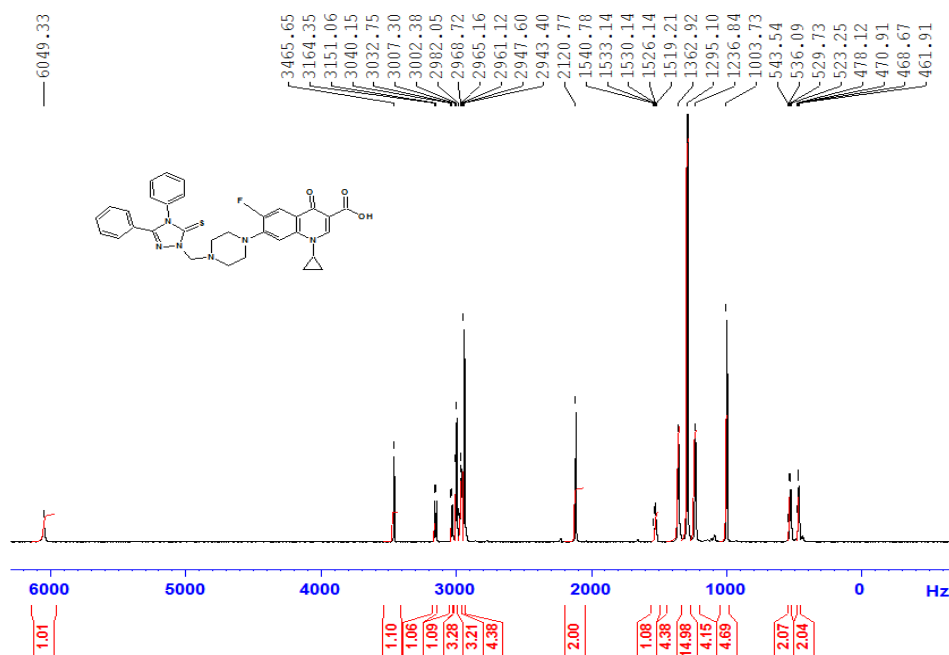
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S7- ^1H , ^{13}C NMR and dept-135 Spectra of 7



AAM-18
proton_su DMSO {C:\nmr-data} Student 21



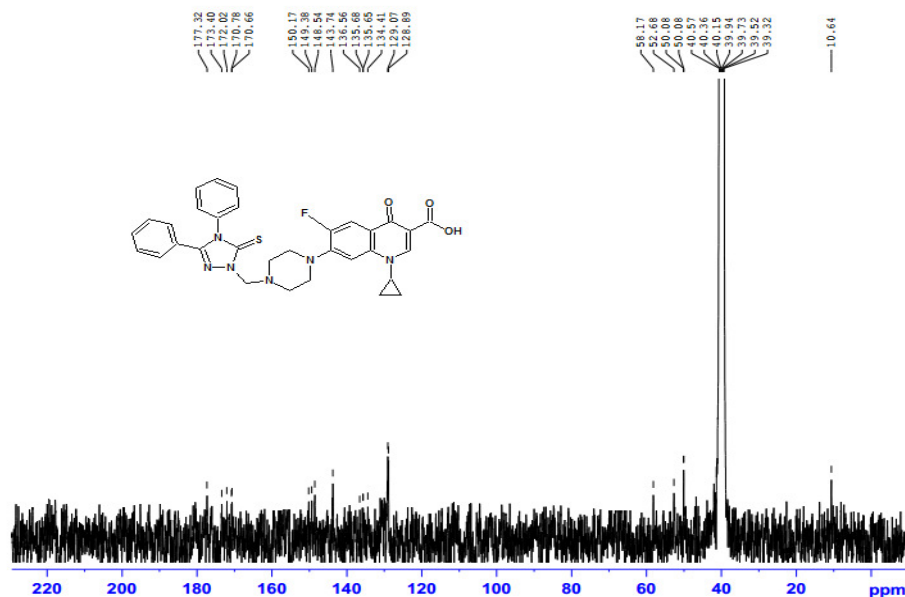
Current Data Parameters
NAME Jan03-2019
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date 20190103
Time 12.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 318.1 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-18
c13_su DMSO {C:\nmr-data} Student 24



Current Data Parameters
NAME Jan15-2019
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date 20190116
Time 10.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 100.43
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

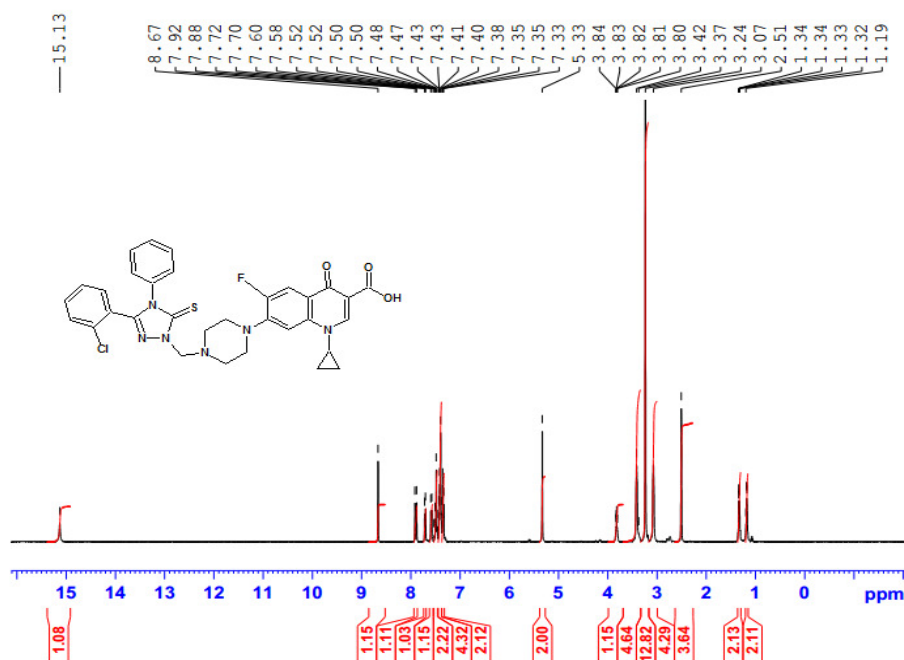
CHANNEL f1
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
PLW1 56.00000000 W

CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W
PLW13 0.33284000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S8- ^1H , ^{13}C NMR and dept-135 Spectra of 8

AAM-20
proton_su DMSO {C:\nmr-data} Student 17



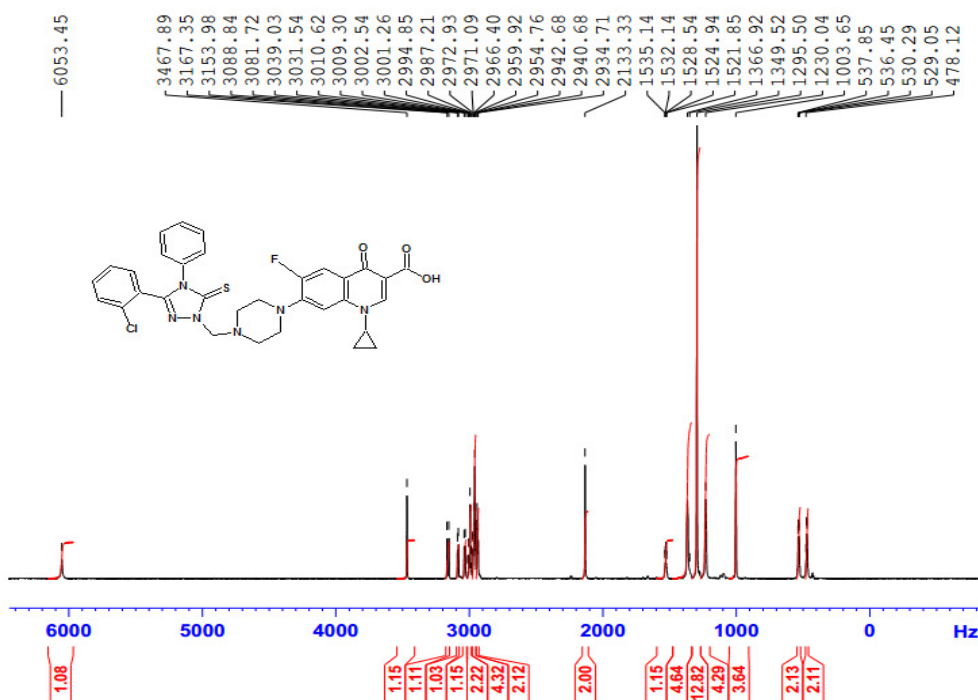
Current Data Parameters
NAME Jan03-2019
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190103
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 318.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-20
proton_su DMSO {C:\nmr-data} Student 17

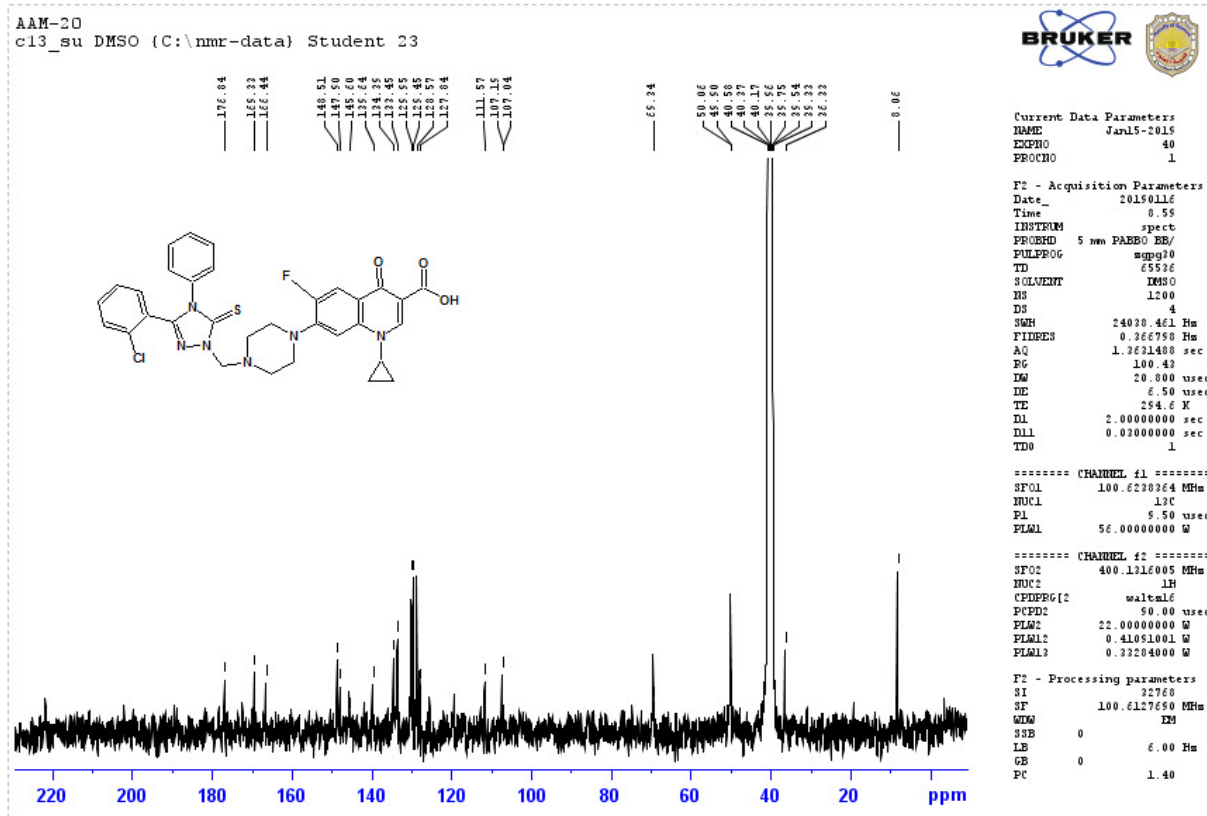


Current Data Parameters
NAME Jan03-2019
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190103
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 318.2 K
D1 1.00000000 sec
TDO 1

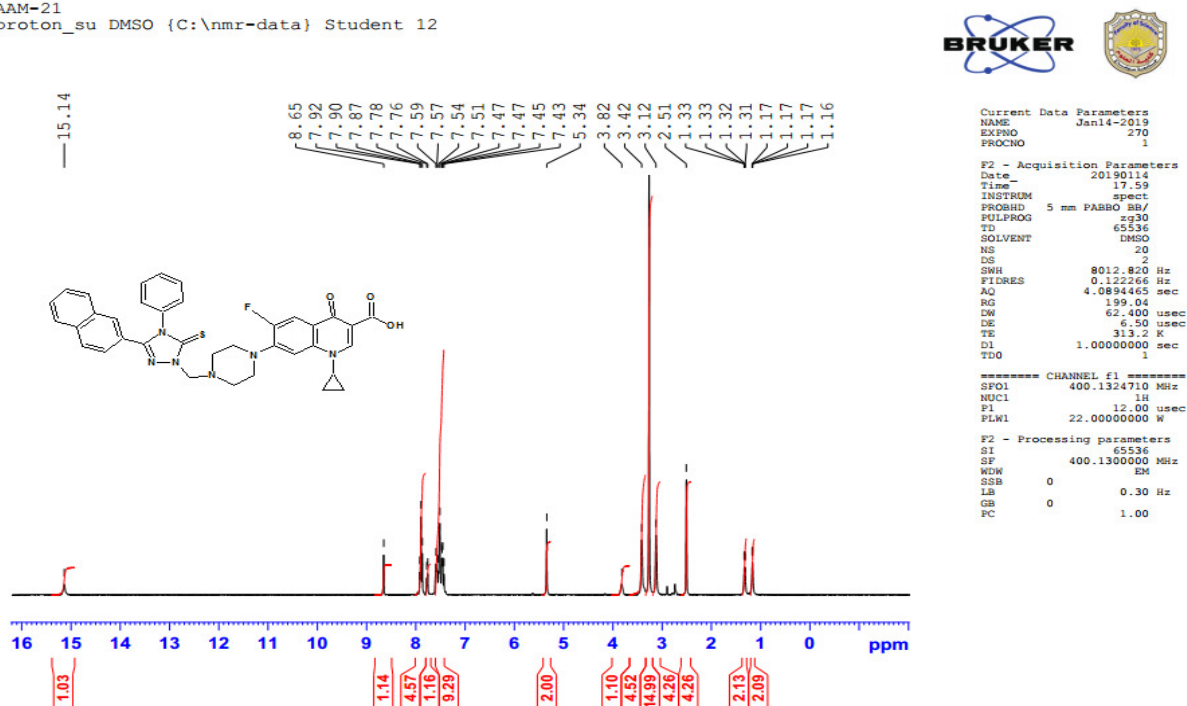
===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

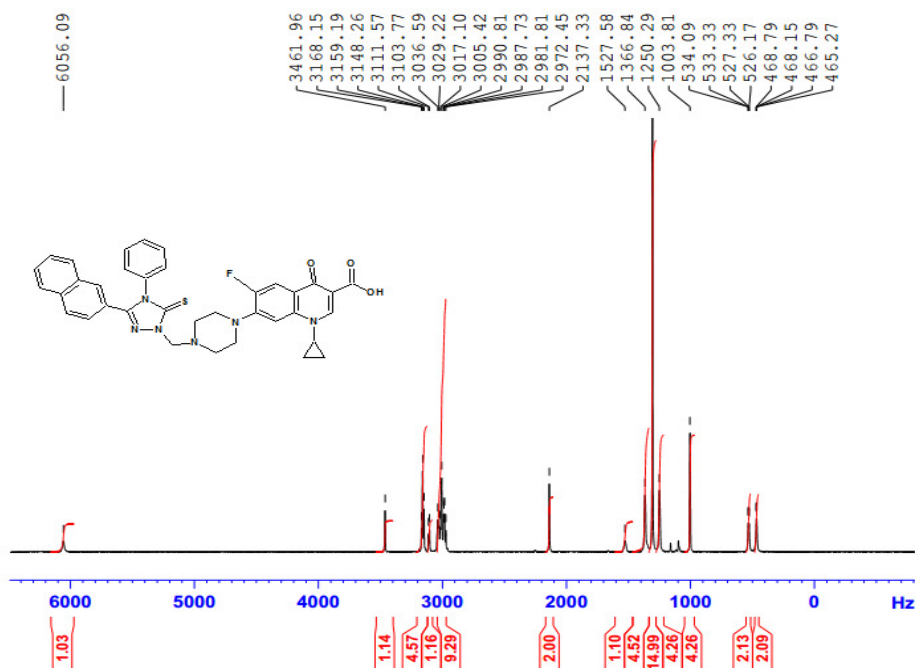


S9- ^1H , ^{13}C NMR and dept-135 Spectra of 9

AAM-21
proton_su DMSO (C:\nmr-data) Student 12



AAM-21
proton_su DMSO {C:\nmr-data} Student 12



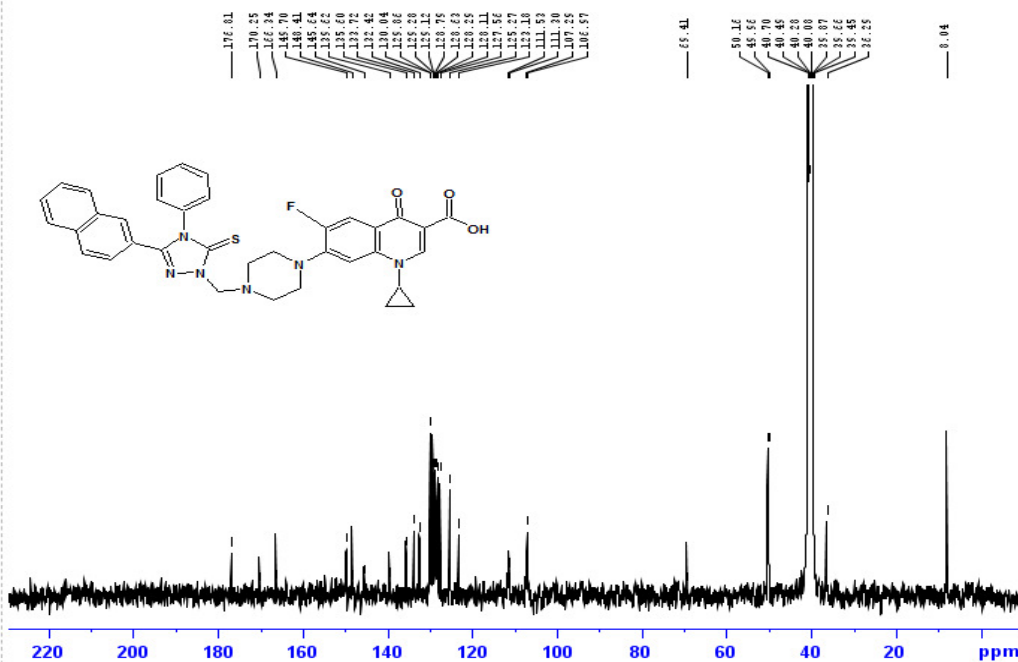
Current Data Parameters
NAME Jan14-2019
EXPNO 270
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190114
Time 17.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-21
c13_su DMSO {C:\nmr-data} Student 24



Current Data Parameters
NAME Jan15-2019
EXPNO 430
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190120
Time 1.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1280
DS 4
SWH 24020.461 Hz
FIDRES 0.266750 Hz
AQ 1.3611400 sec
RG 175.04
DW 20.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.02000000 sec
TDO 1

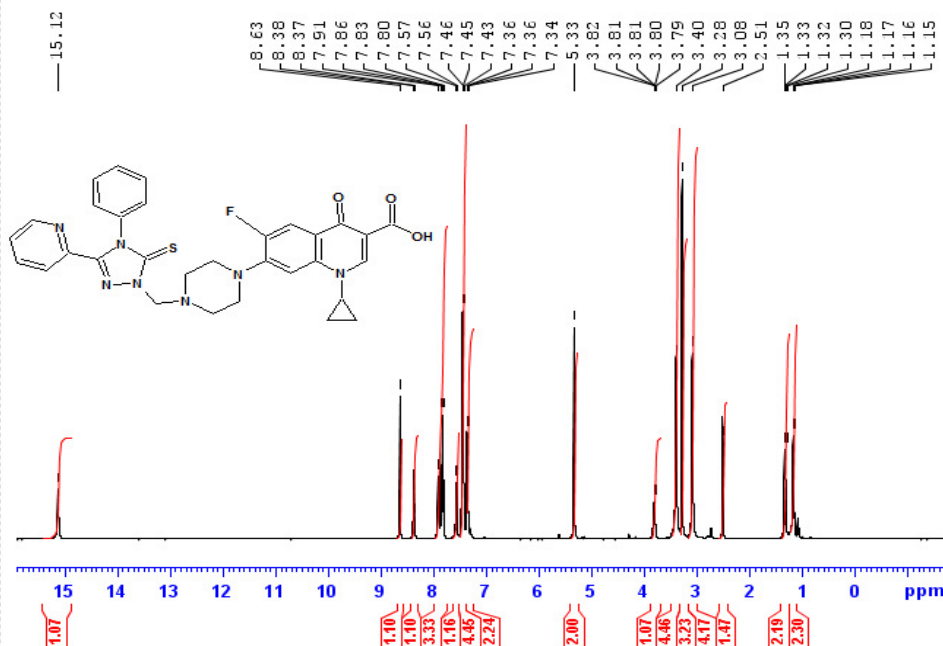
===== CHANNEL f1 =====
SFO1 100.6238264 MHz
NUC1 13C
P1 5.50 usec
PLW1 56.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 50.00 usec
PLW2 22.00000000 W
PLW12 0.41951001 W
PLW13 0.32254000 W

F2 - Processing parameters
SI 32768
SF 100.6127650 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S10- ^1H , ^{13}C NMR and dept-135 Spectra of 10

AAM-7
proton_su DMSO (C:\nmr-data) Student 21



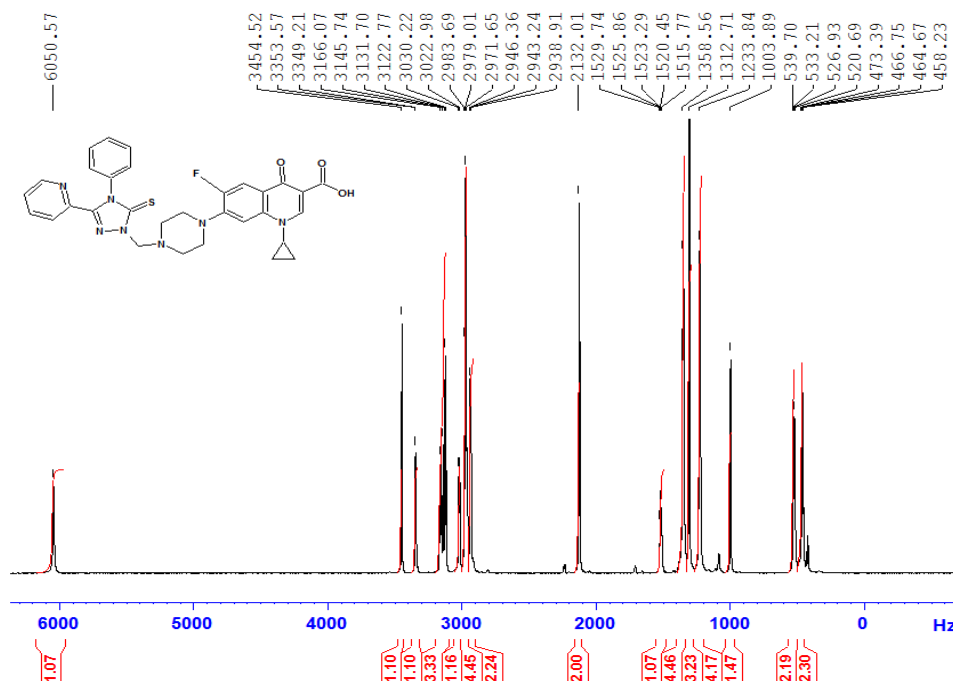
Current Data Parameters
NAME Sep29-2018
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180929
Time 12.09
INSTRUM spect
PROCBD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 135
DW 62.400 usec
DE 6.50 usec
TE 310.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-7
proton_su DMSO (C:\nmr-data) Student 21

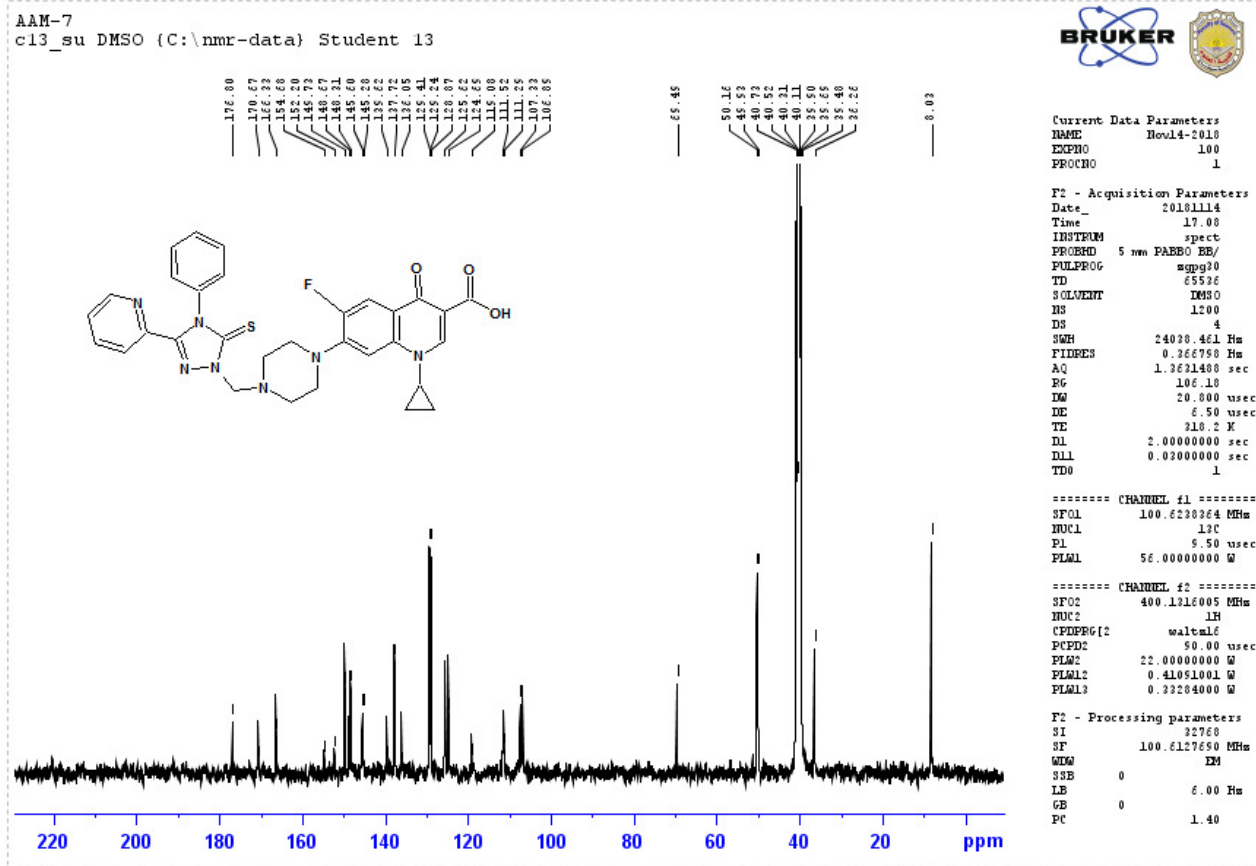


Current Data Parameters
NAME Sep29-2018
EXPNO 40
PROCNO 1

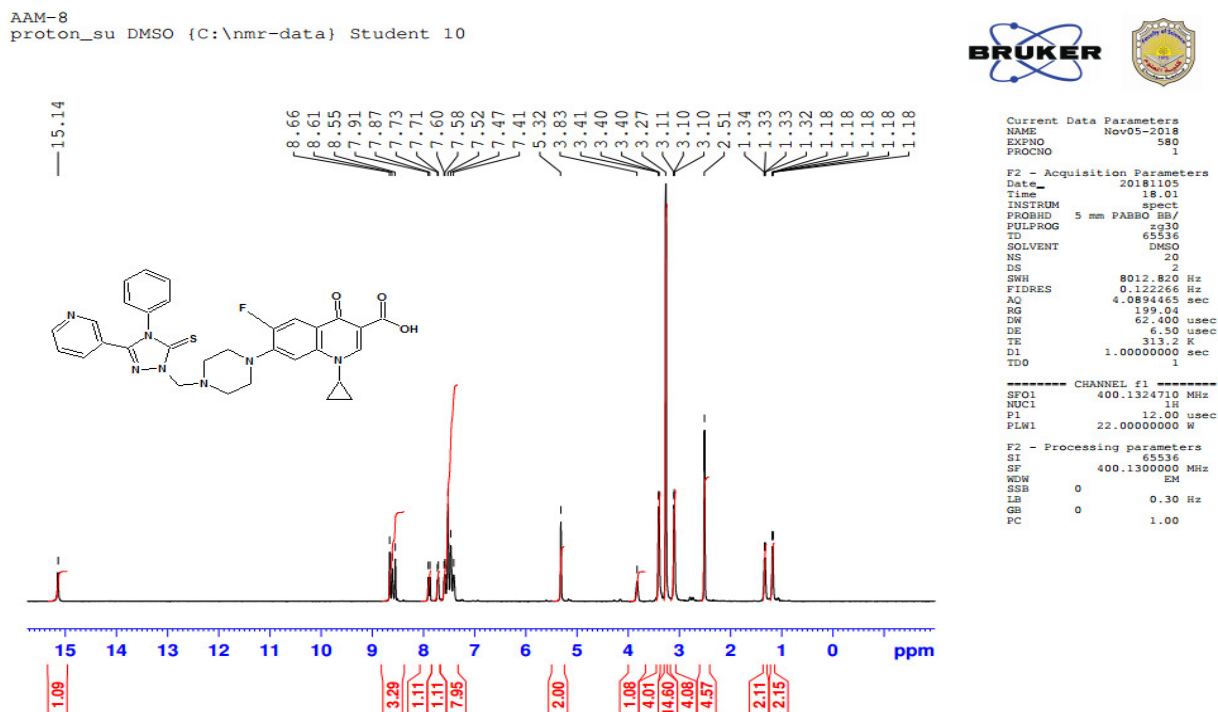
F2 - Acquisition Parameters
Date_ 20180929
Time 12.09
INSTRUM spect
PROCBD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 135
DW 62.400 usec
DE 6.50 usec
TE 310.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

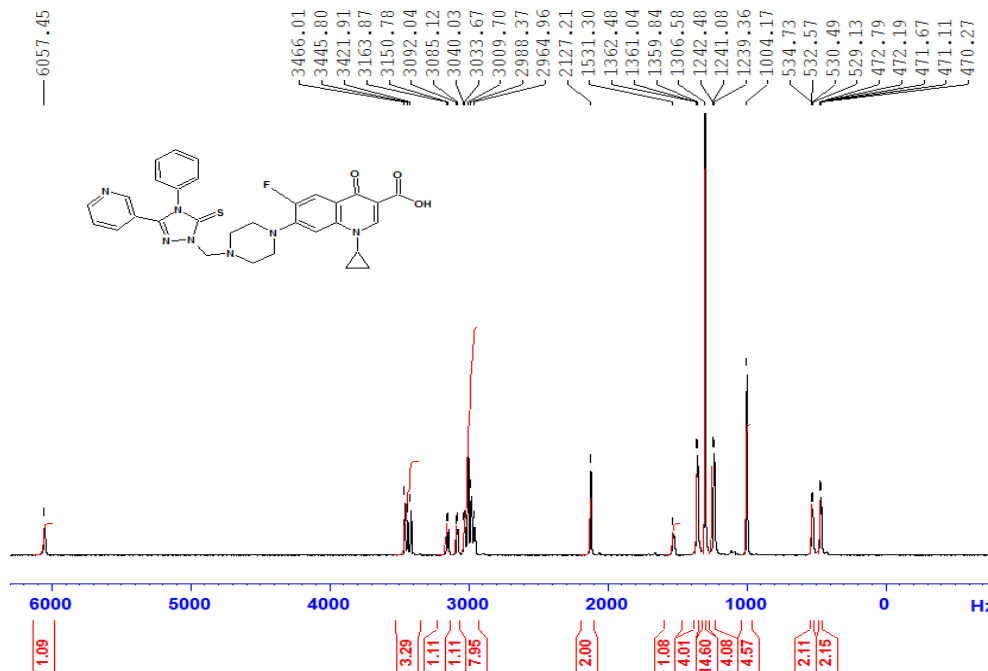
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S11-¹H, ¹³C NMR and dept-135 Spectra of 11



AAM-8
proton_su DMSO {C:\nmr-data} Student 10



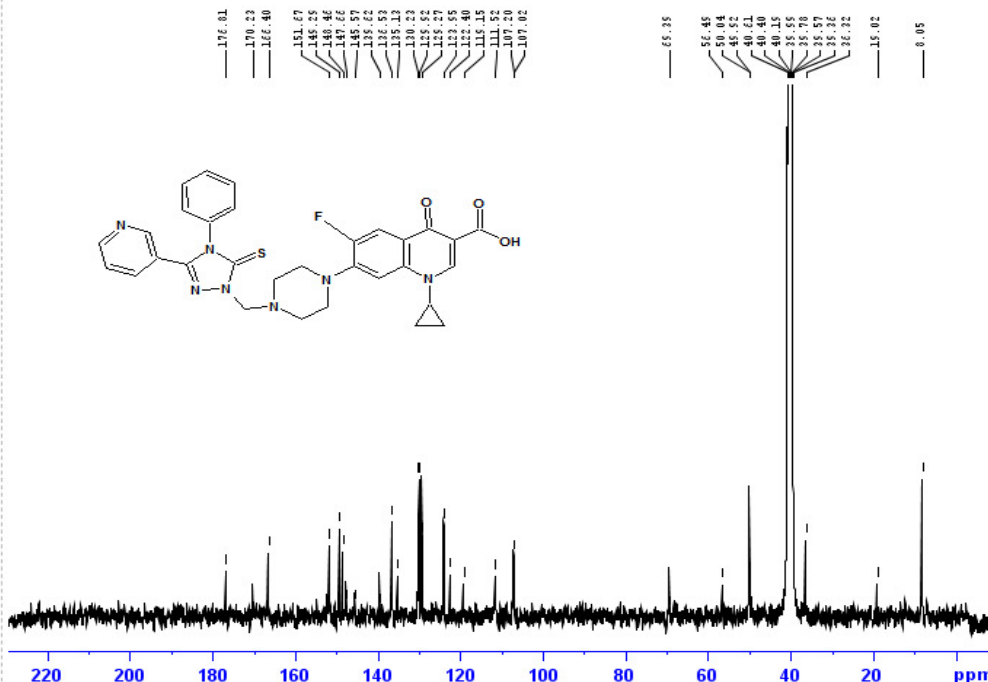
Current Data Parameters
NAME Nov05-2018
EXPNO 580
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181105
Time 18.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894466 sec
RG 139.04
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-8
c13_su DMSO {C:\nmr-data} Student 1



Current Data Parameters
NAME Nov05-2018
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181126
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4
DS 4
SWH 24038.461 Hz
FIDRES 0.266758 Hz
AQ 1.3621400 sec
RG 100.42
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

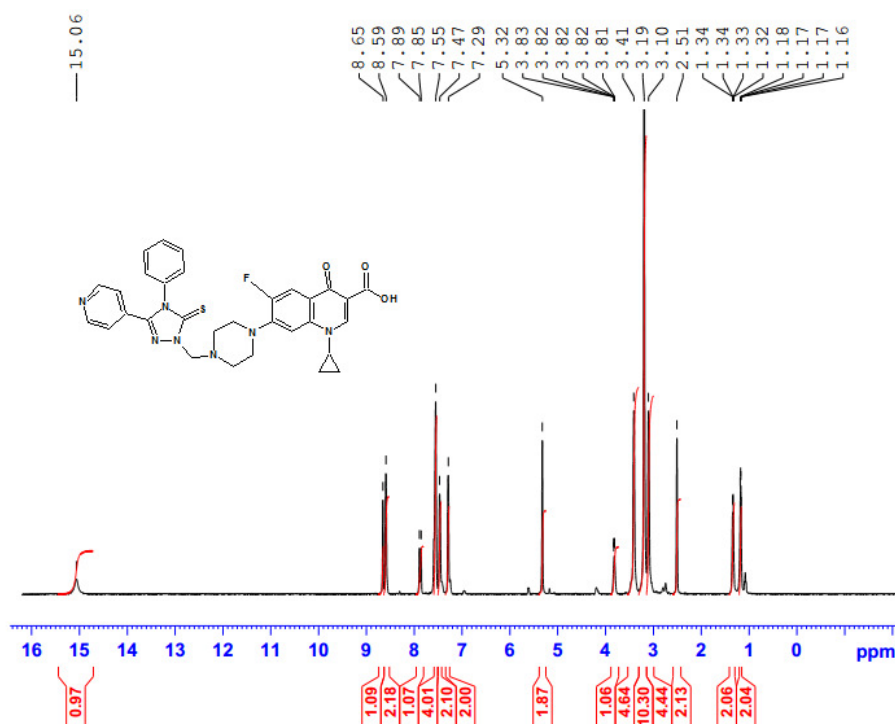
===== CHANNEL f1 =====
SFO1 100.6230264 MHz
NUC1 13C
P1 5.50 usec
PLW1 56.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 50.00 usec
PLW2 22.00000000 W
PLW2 0.41051001 W
PLW2 0.32284000 W

F2 - Processing parameters
SI 22768
SF 100.6127650 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S12- ¹H, ¹³C NMR and dept-135 Spectra of 12

AAM-23
proton_su DMSO {C:\nmr-data} Student 21



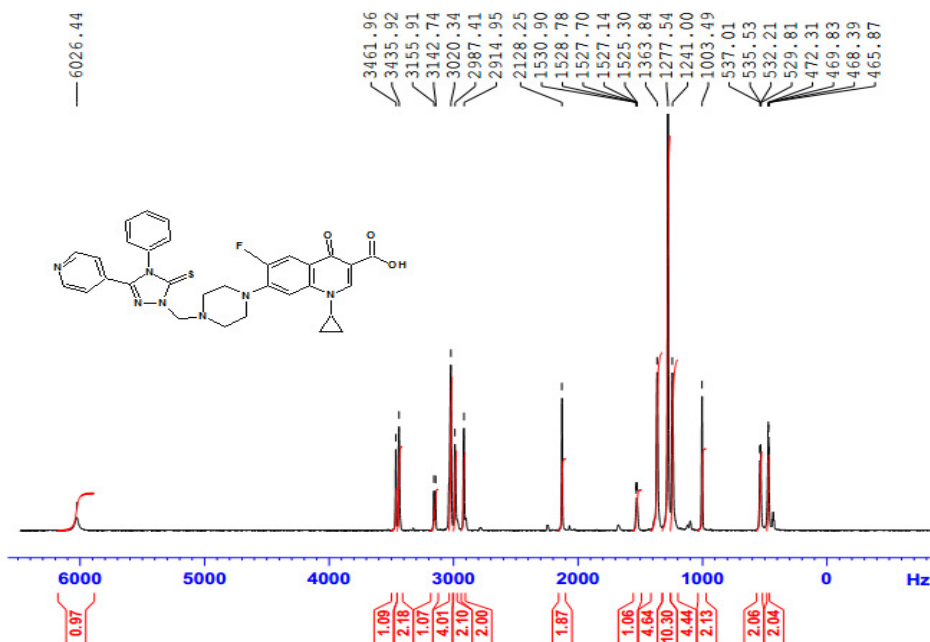
Current Data Parameters
NAME Jan27-2019
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190127
Time 13.35
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 158.76
DW 62.400 usec
DE 6.50 usec
TE 328.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

AAM-23
proton_su DMSO {C:\nmr-data} Student 21

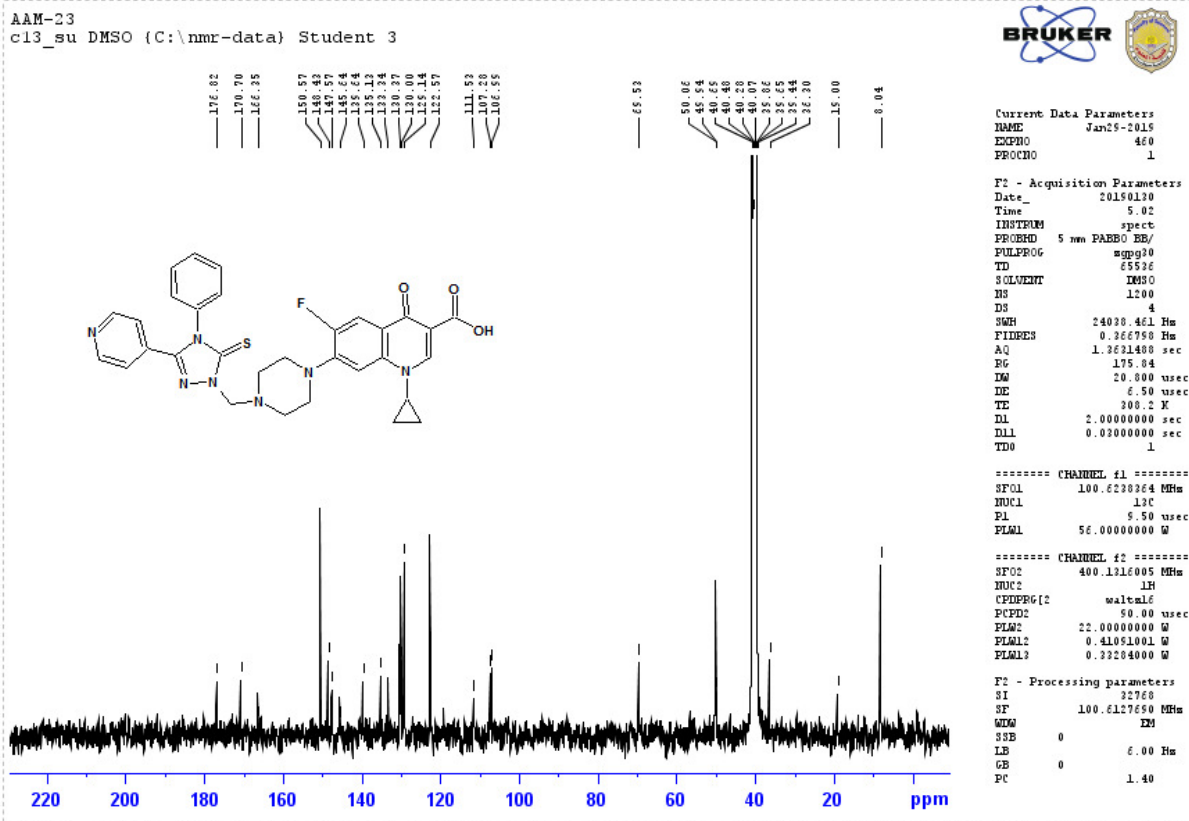


Current Data Parameters
NAME Jan27-2019
EXPNO 70
PROCNO 1

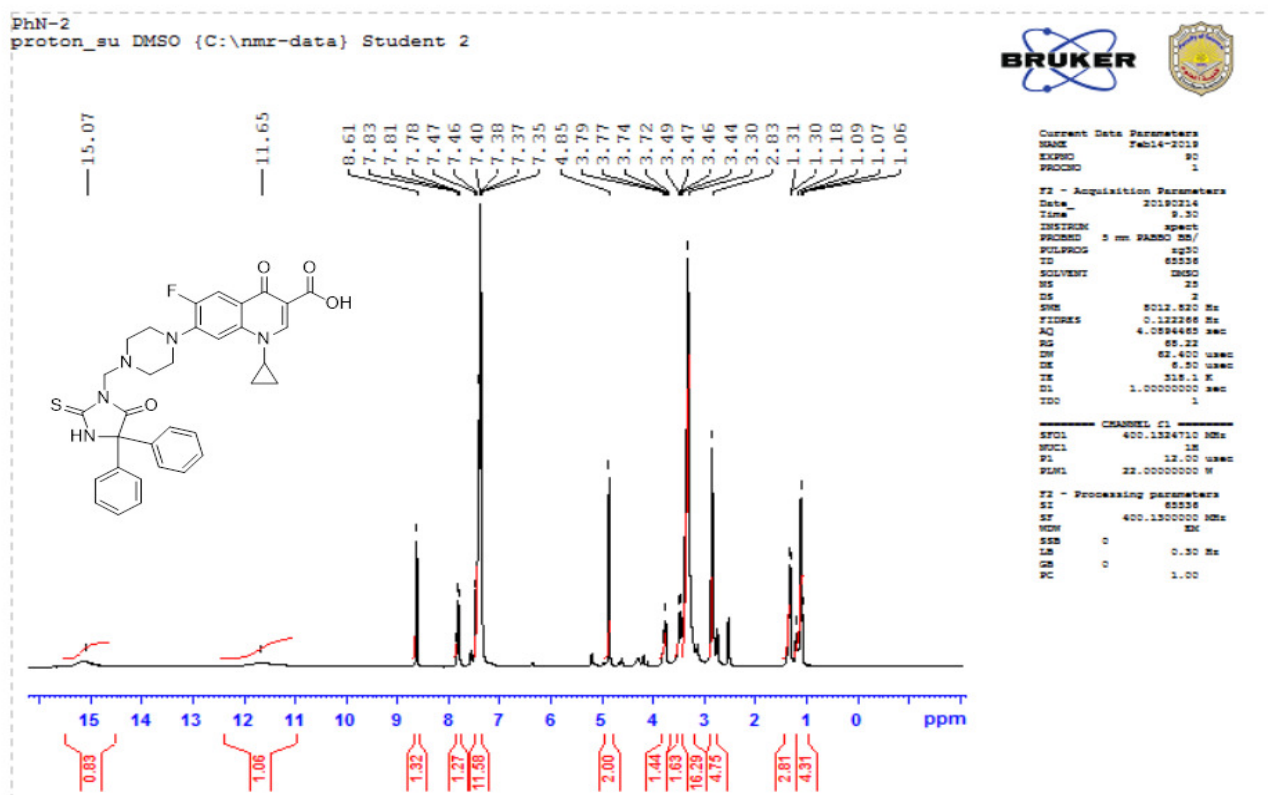
F2 - Acquisition Parameters
Date_ 20190127
Time 13.35
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 25
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 158.76
DW 62.400 usec
DE 6.50 usec
TE 328.1 K
D1 1.00000000 sec
TD0 1

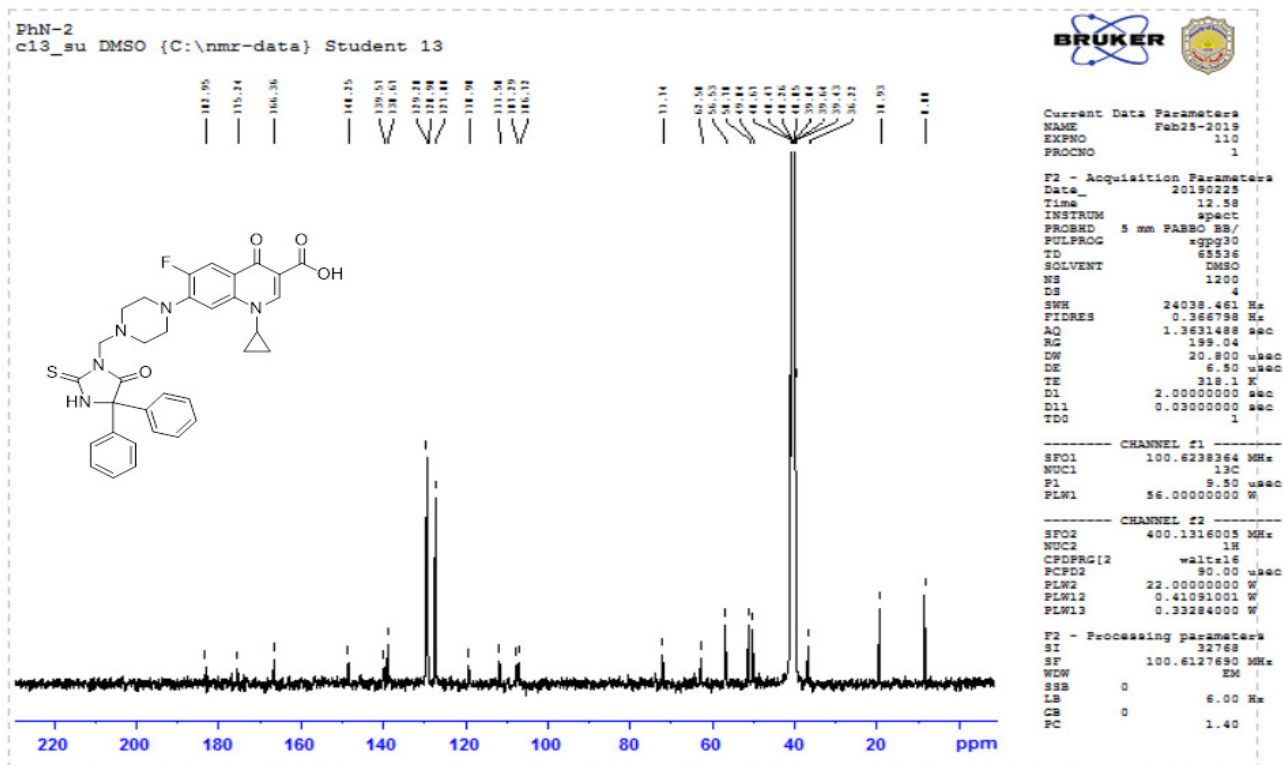
===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

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

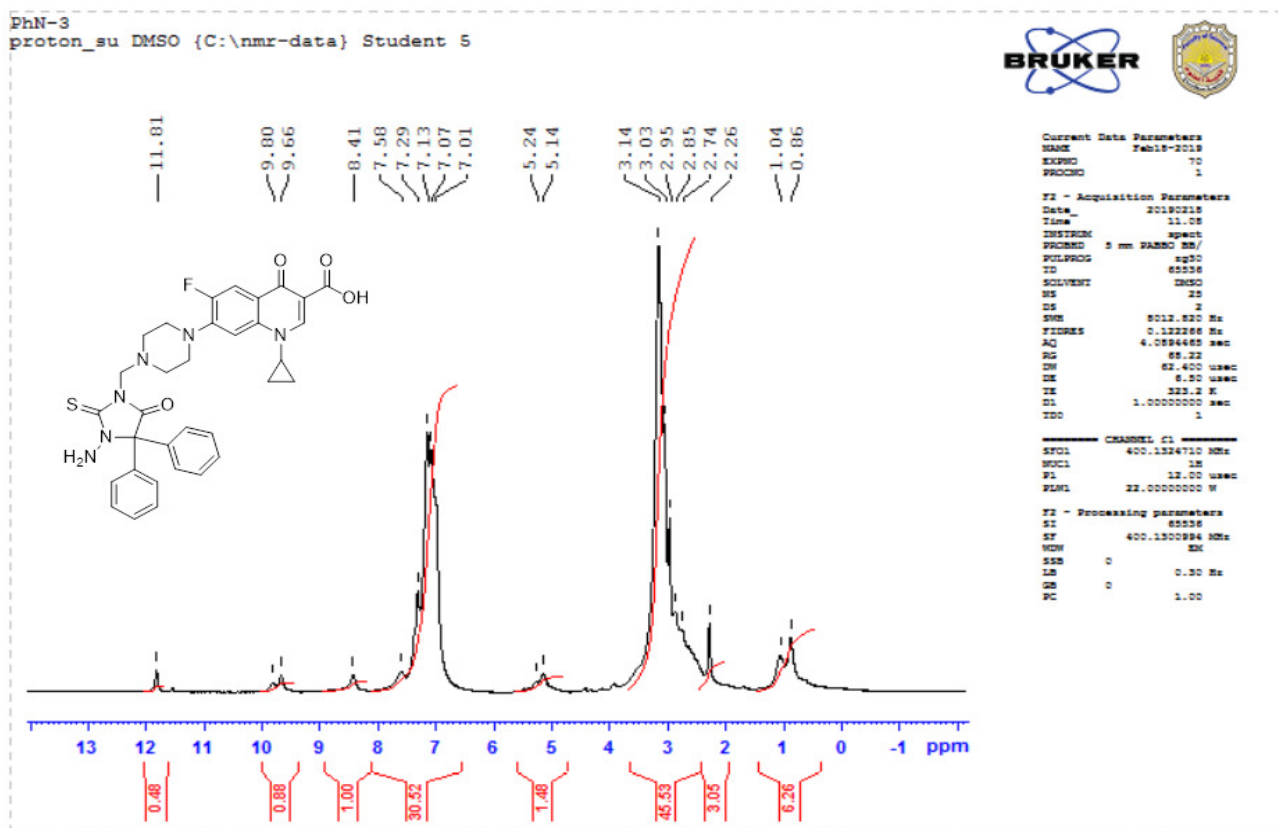


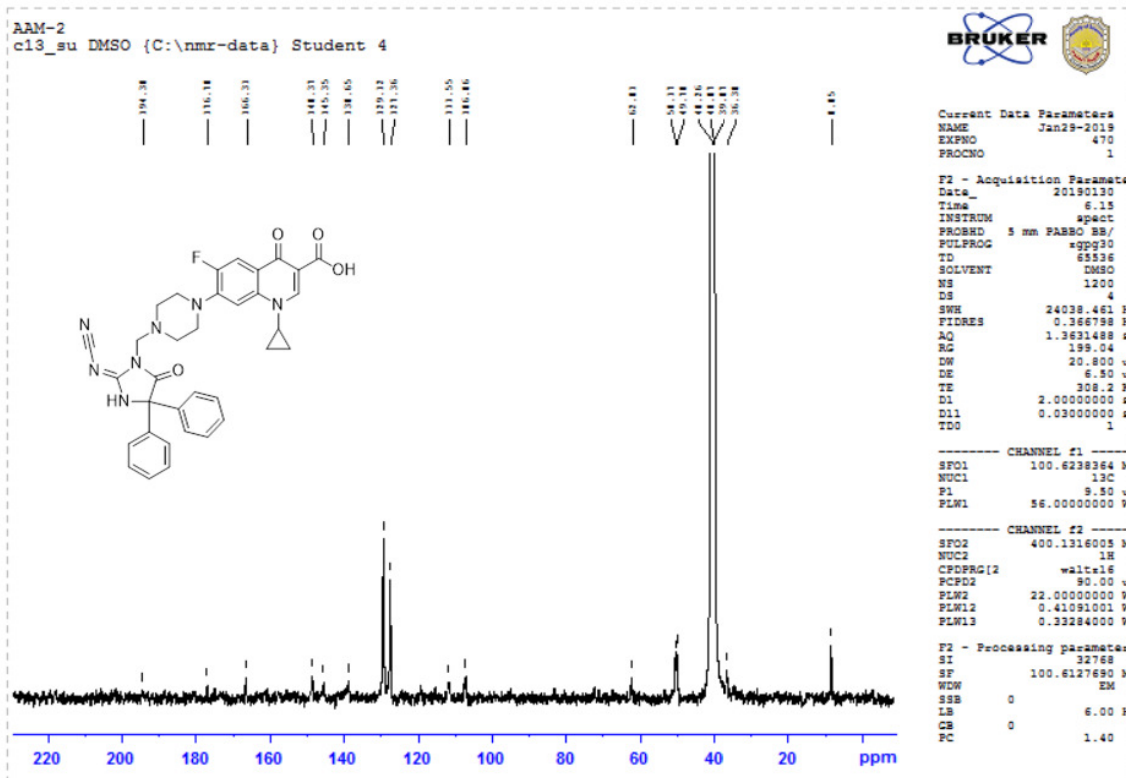
S13- ^1H , ^{13}C NMR and dept-135 Spectra of 13



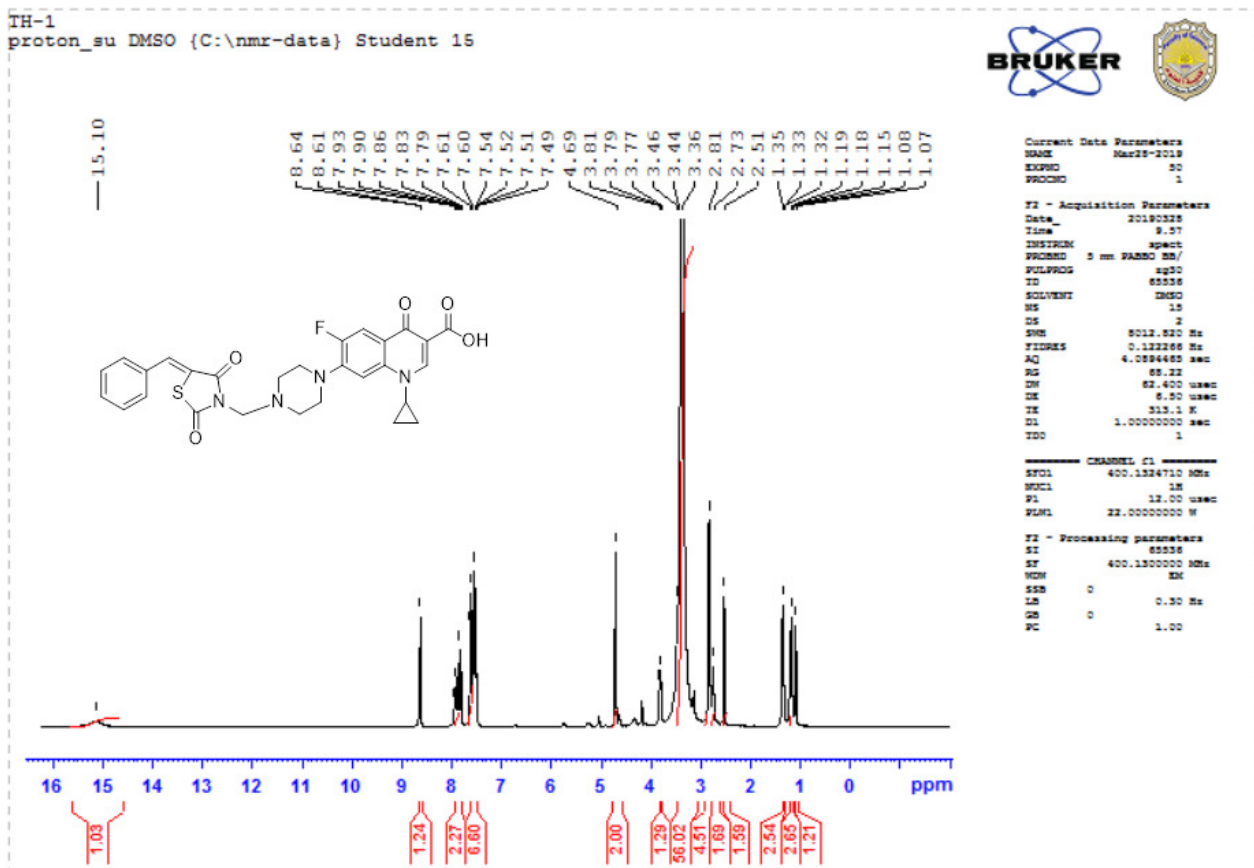


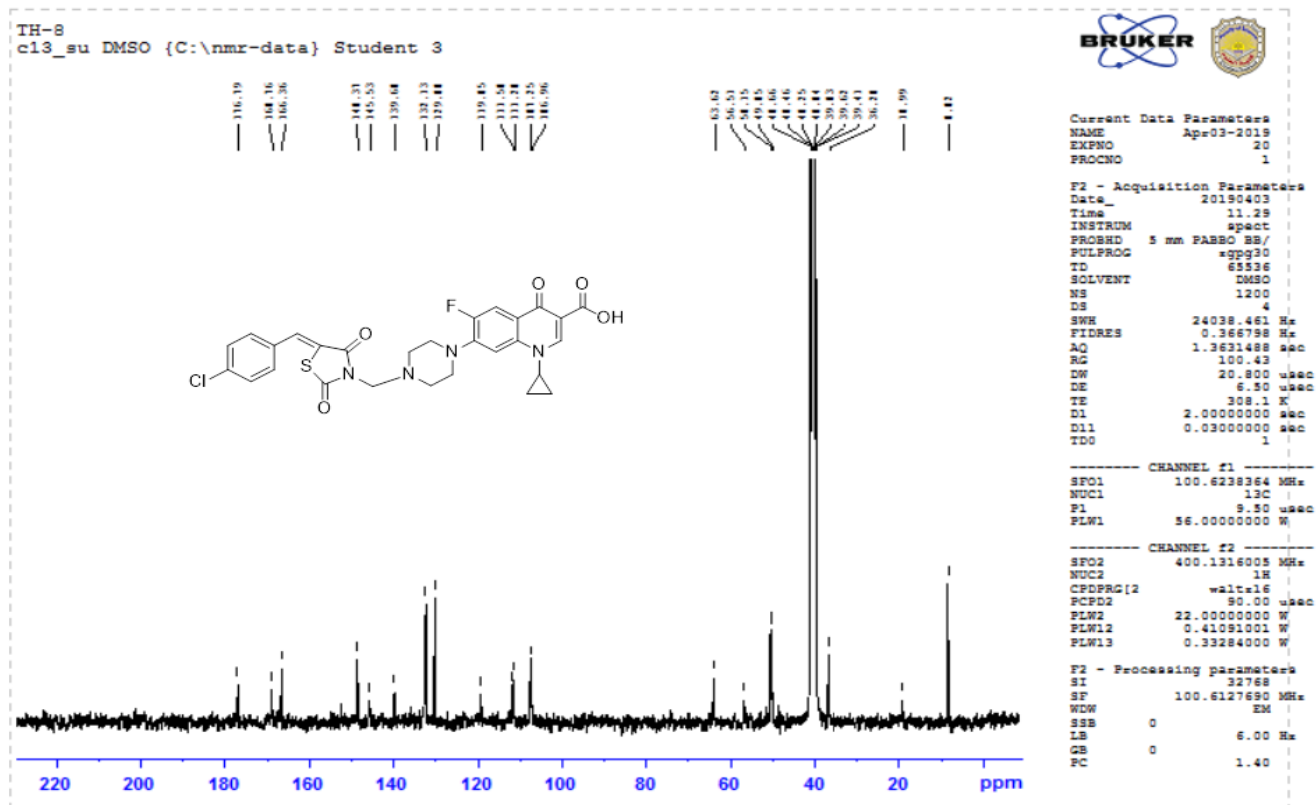
S14- ^1H , ^{13}C NMR and dept-135 Spectra of 14



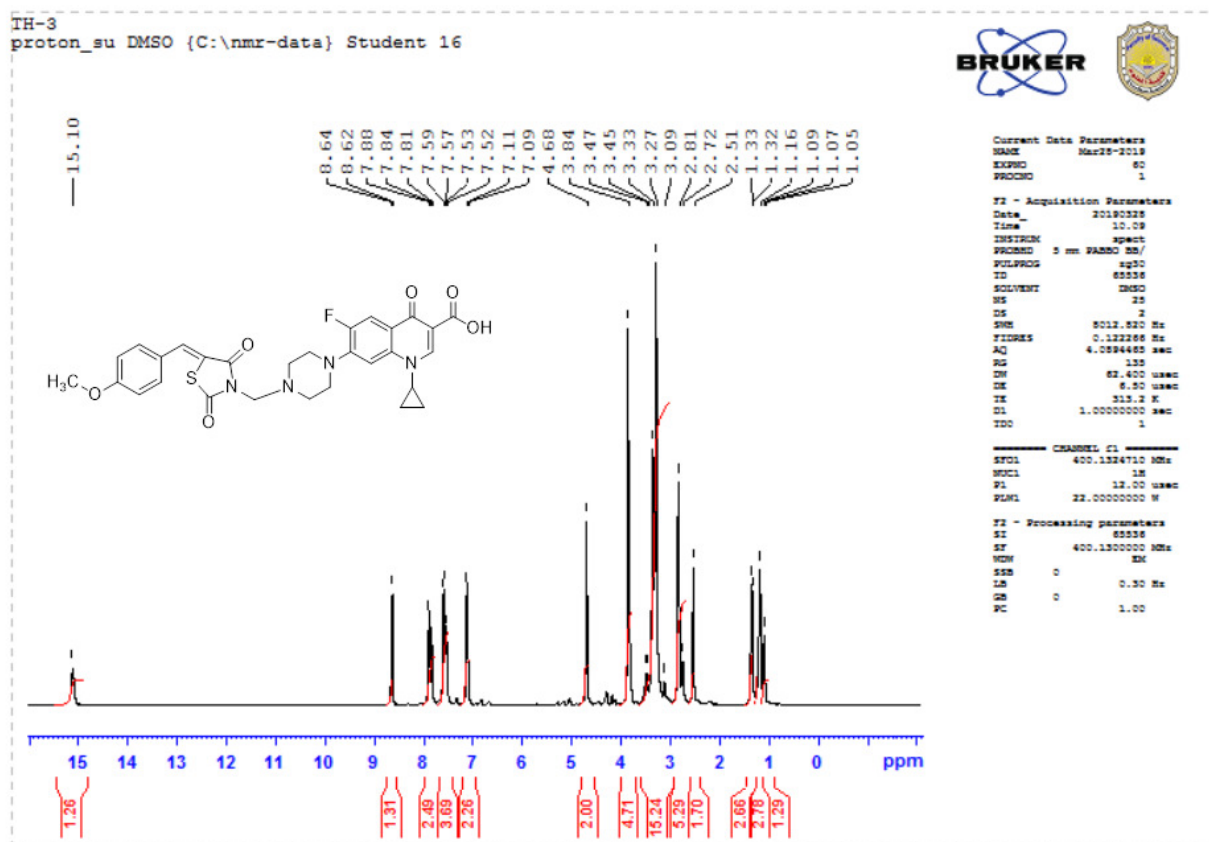


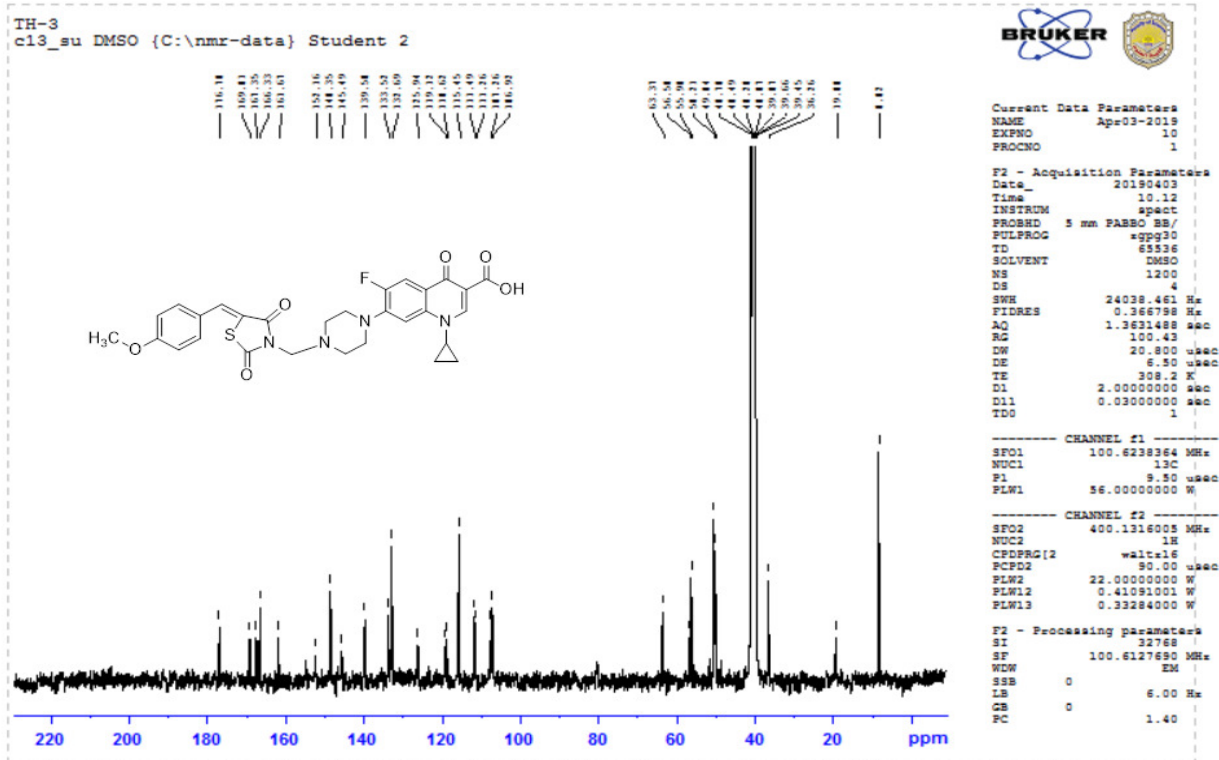
S16- ^1H , ^{13}C NMR and dept-135 Spectra of 16



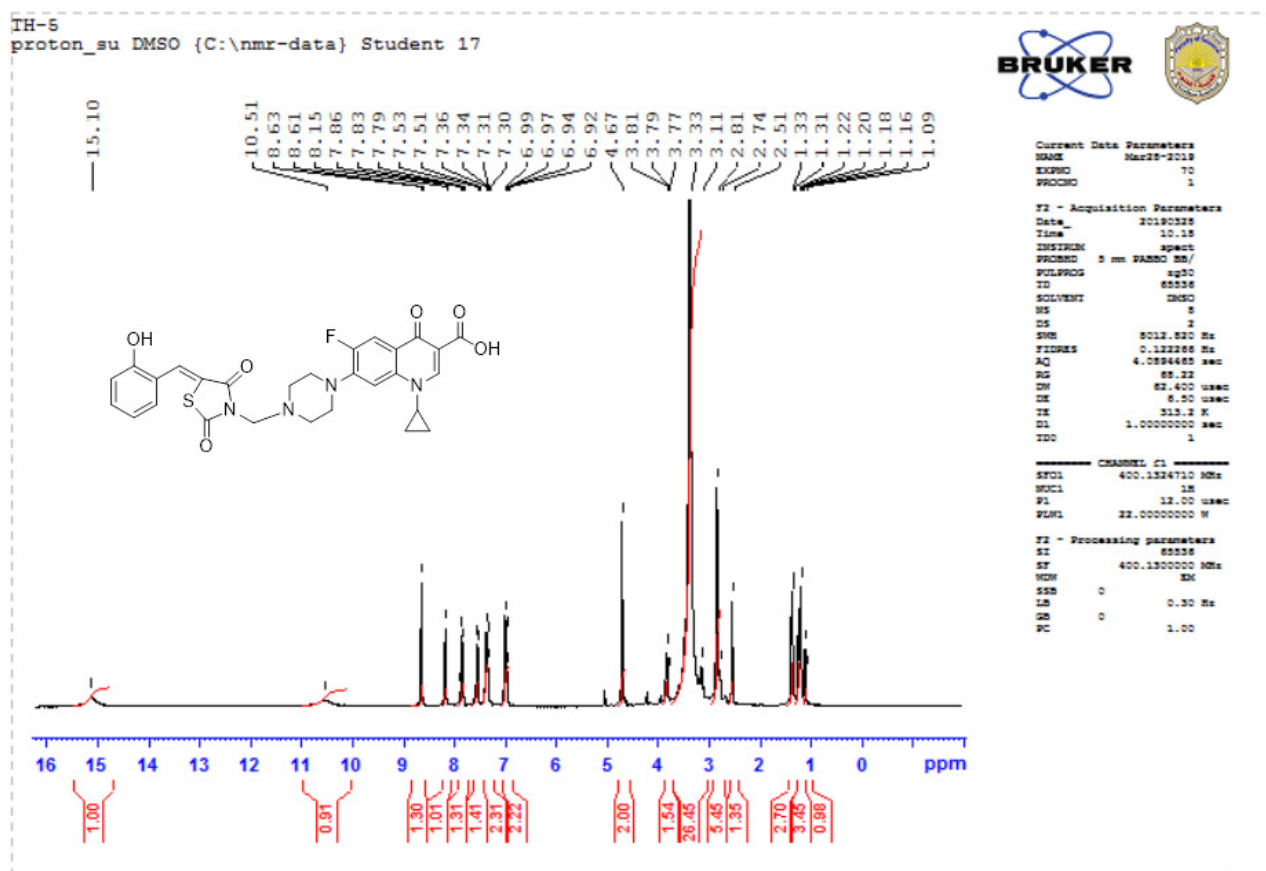


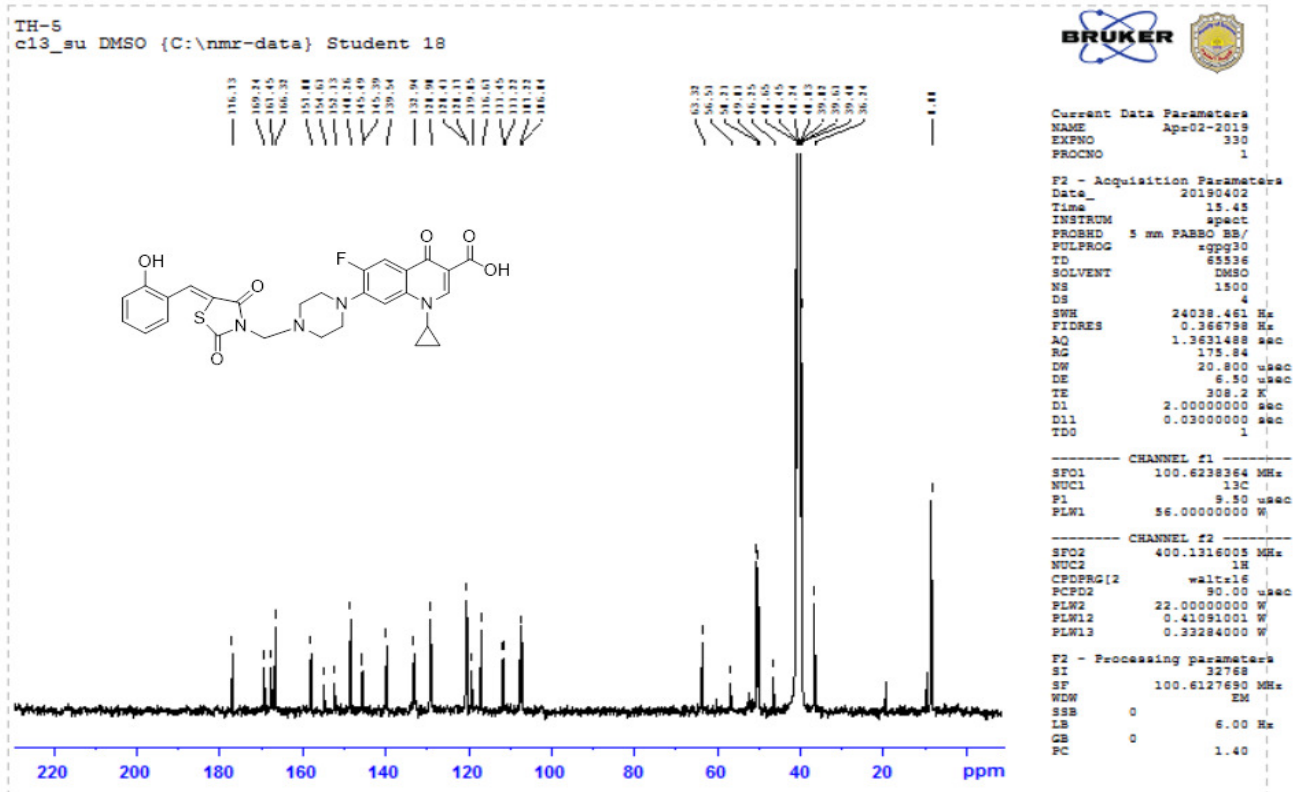
S18- ^1H , ^{13}C NMR and dept-135 Spectra of



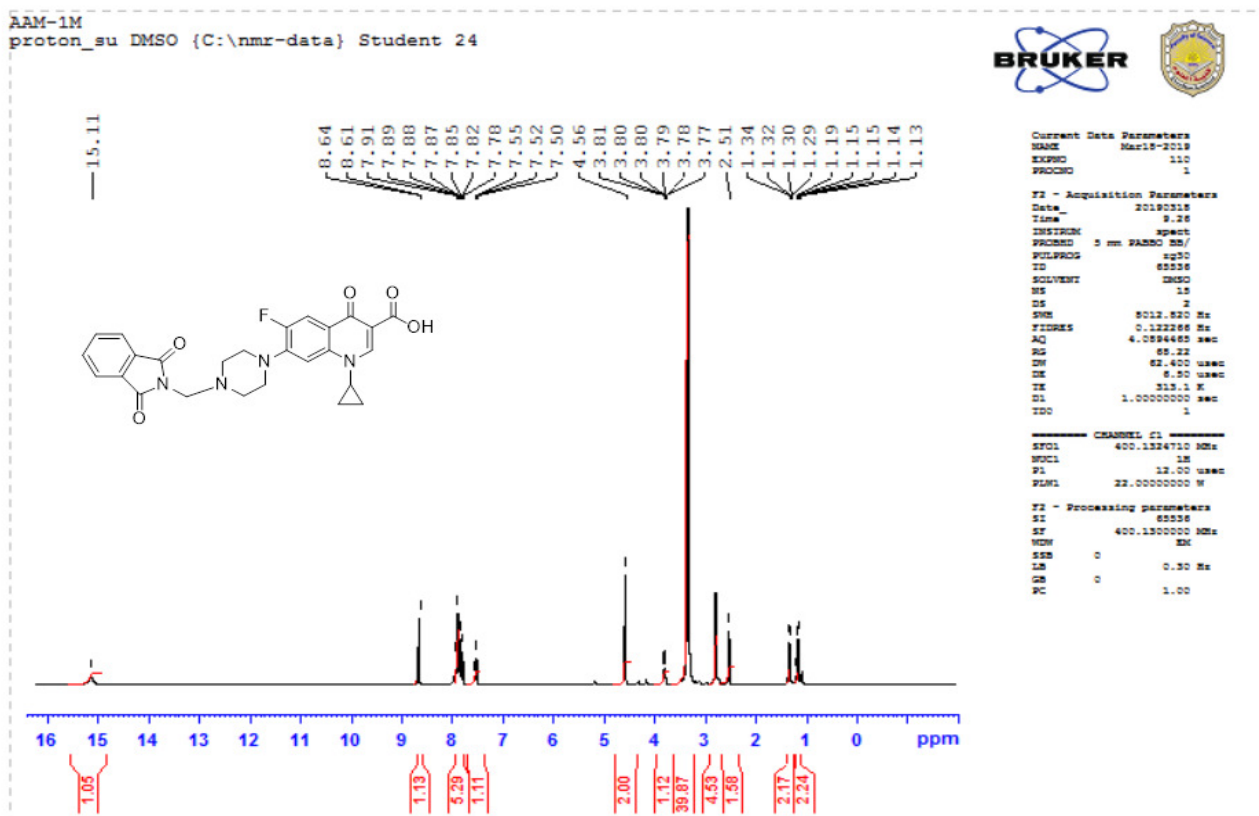


S19- ^1H , ^{13}C NMR and dept-135 Spectra of 19

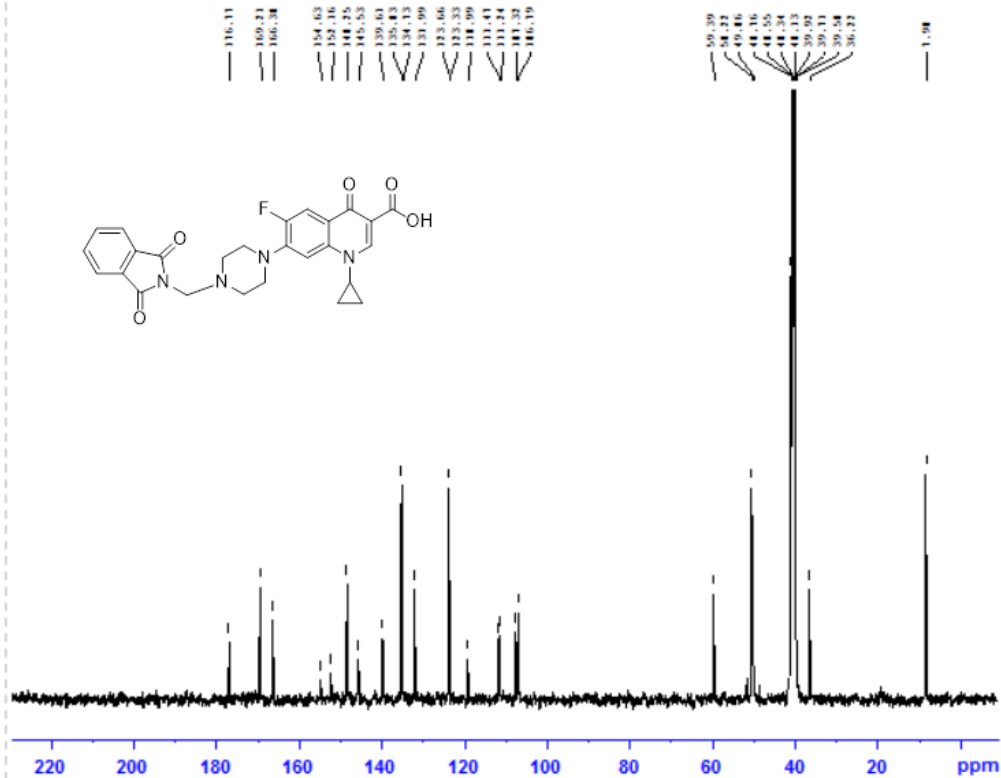




S20- ^1H , ^{13}C NMR and dept-135 Spectra of 20



AAM-1-M
c13_su DMSO {C:\nmr-data} Student 20



Current Data Parameters
NAME Mar26-2019
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190326
Time 11.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.04
DW 20.800 usec
DE 6.50 usec
TE 323.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

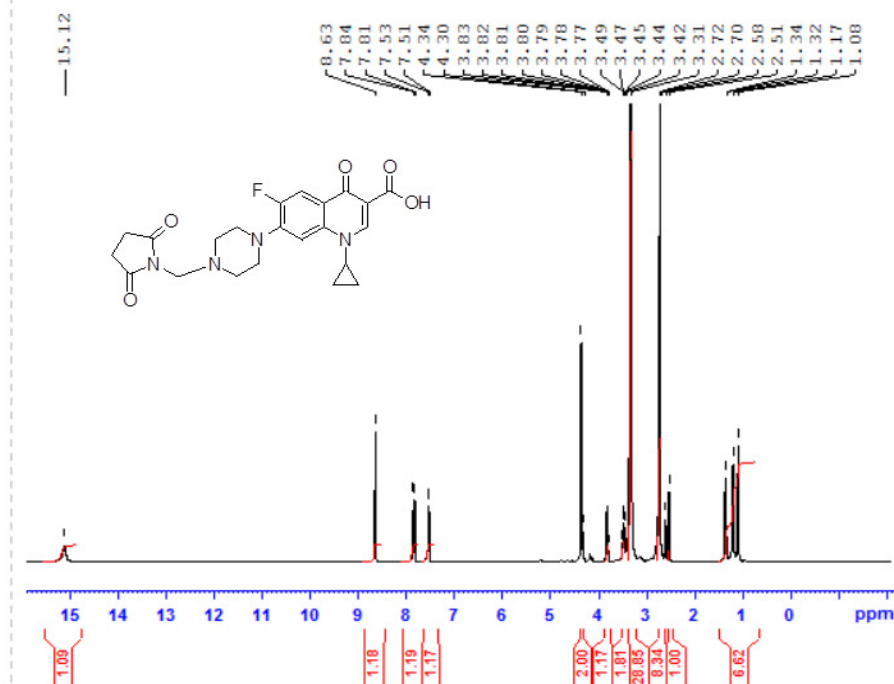
CHANNEL f1
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
PLW1 56.00000000 W

CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPOPRG[2] waltz16
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41081001 W
PLW13 0.33284000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S21- ^1H , ^{13}C NMR and dept-135 Spectra of 21

AAM-2M
proton_su DMSO {C:\nmr-data} Student 1

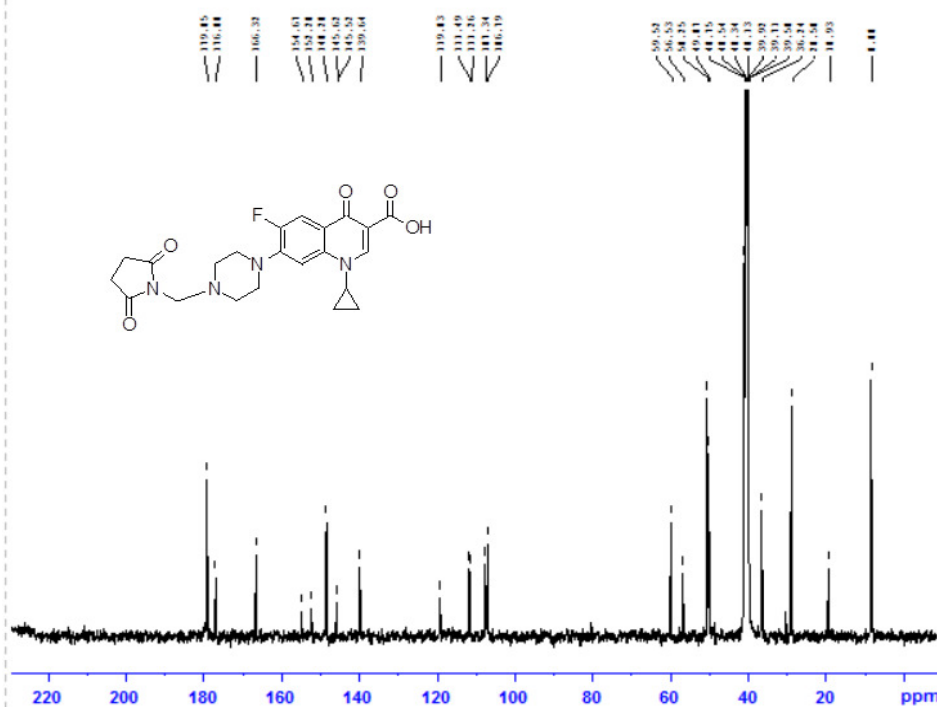


Current Data Parameters
NAME Mar26-2019
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190316
Time 9.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15
DS 2
SWH 5012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0584465 sec
RG 65.22
DW 62.400 usec
DE 6.50 usec
TE 313.1 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00



```

Current Data Parameters
NAME           Mar26-2019
EXPNO         110
PROCNO        1

F2 - Acquisition Parameters
Data_         20190326
Time_         13.41
INSTRUM       spect
PROBHD        5 mm F4BBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            1200
DS            4
SWH           24038.451
FIDRES        0.366789 Hz
AQ            1.3631488 sec
RG            199.04
DE            20.800      usec
CE            6.50      usec
TE            323.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

----- CHANNEL f1 -----
SF01          100.6238364 MHz
NUC1          13C
P1            9.50      usec
PLW1          56.00000000 W

----- CHANNEL f2 -----
SF02          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         30.00      usec
PLW2          22.0000000 W
PLW12         0.41091001 W
PLW13         0.33284000 W

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            0.600 Hz
GB            0
PC            1.40

```


Table S1**Molecular properties of compounds 1-21 predicted using Swiss ADME website.**

Molecule	Comp 1	Comp 2	Comp 3	Comp 4	Comp 5	Comp 6	Comp 7
MW	521.56	556.01	571.62	522.55	522.55	522.55	596.67
Heavy atoms	37	38	41	37	37	37	43
Aromatic heavy atoms	21	21	25	21	21	21	27
Fraction Csp3	0.31	0.31	0.27	0.32	0.32	0.32	0.25
Rotatable bonds	6	6	6	6	6	6	7
H-bond acceptors	7	7	7	8	8	8	6
H-bond donors	1	1	1	1	1	1	1
MR	145.25	150.26	162.76	143.05	143.05	143.05	172.31
TPSA	128.83	128.83	128.83	141.72	141.72	141.72	120.62
iLOGP	3.26	3.37	4.21	2.81	2.81	2.81	4.02
XLOGP3	1.47	2.1	2.72	0.73	0.73	0.73	2.63
WLOGP	3.58	4.24	4.74	2.98	2.98	2.98	4.78
MLOGP	2.43	2.9	3.05	1.46	1.46	1.46	3.66
Silicos-IT Log P	3.58	4.23	4.58	3.02	3.02	3.02	4.19
Consensus Log P	2.87	3.37	3.86	2.2	2.2	2.2	3.86
ESOL Log S	-4.02	-4.62	-5.15	-3.56	-3.56	-3.56	-5.2
ESOL Solubility (mg/ml)	4.94E-02	1.32E-02	4.02E-03	1.43E-01	1.43E-01	1.43E-01	3.77E-03
ESOL Solubility (mol/l)	9.47E-05	2.38E-05	7.03E-06	2.73E-04	2.73E-04	2.73E-04	6.33E-06
ESOL Class	Moderately soluble	Moderately soluble	Moderately soluble	Soluble	Soluble	Soluble	Moderately soluble
Ali Log S	-3.78	-4.44	-5.08	-3.28	-3.28	-3.28	-4.81
Ali Solubility (mg/ml)	8.62E-02	2.04E-02	4.76E-03	2.71E-01	2.71E-01	2.71E-01	9.17E-03
Ali Solubility (mol/l)	1.65E-04	3.67E-05	8.33E-06	5.19E-04	5.19E-04	5.19E-04	1.54E-05
Ali Class	Soluble	Moderately soluble	Moderately soluble	Soluble	Soluble	Soluble	Moderately soluble
Silicos-IT LogSw	-5.81	-6.38	-7.42	-5.43	-5.43	-5.43	-7.4
Silicos-IT Solubility (mg/ml)	8.13E-04	2.31E-04	2.17E-05	1.93E-03	1.93E-03	1.93E-03	2.38E-05
Silicos-IT Solubility (mol/l)	1.56E-06	4.16E-07	3.80E-08	3.69E-06	3.69E-06	3.69E-06	3.98E-08
Silicos-IT class	Moderately soluble	Poorly soluble	Poorly soluble	Moderately soluble	Moderately soluble	Moderately soluble	Poorly soluble
GI absorption	High	Low	Low	Low	Low	Low	Low
BBB permeant	No	No	No	No	No	No	No
Pgp substrate	Yes	Yes	Yes	Yes	Yes	Yes	Yes
CYP1A2 inhibitor	No	No	No	No	No	No	No
CYP2C19 inhibitor	Yes	Yes	Yes	No	No	No	Yes
CYP2C9 inhibitor	Yes	Yes	Yes	Yes	Yes	Yes	Yes
CYP2D6 inhibitor	No	No	Yes	No	No	No	Yes
CYP3A4 inhibitor	No	Yes	No	Yes	Yes	Yes	No
log Kp (cm/s)	-8.44	-8.2	-7.86	-8.97	-8.97	-8.97	-8.07
Lipinski #violations	1	1	1	1	1	1	1

Ghose #violations	2	2	2	2	2	2	3
Veber #violations	0	0	0	1	1	1	0
Egan #violations	0	0	0	1	1	1	0
Muegge #violations	0	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	0	0	0
Brenk #alerts	1	1	1		1	1	1
Leadlikeness #violations	1	1	1		1	1	1
Synthetic Accessibility	3.88	3.93	4.12		3.92	3.92	4.28

Table S2

Molecule	Comp 8	Comp 9	Comp 10	Comp 11	Comp 12	Comp 13	Comp 14
MW	631.12	646.73	646.73	597.66	597.66	611.69	626.7
Heavy atoms	44	47	47	43	43	44	45
Aromatic heavy atoms	27	31	31	27	27	22	22
Fraction Csp3	0.25	0.22	0.22	0.26	0.26	0.27	0.27
Rotatable bonds	7	7	7	7	7	7	7
H-bond acceptors	6	6	6	7	7	6	7
H-bond donors	1	1	1	1	1	2	2
MR	177.32	189.82	189.82	170.11	170.11	182.83	185.63
TPSA	120.62	120.62	120.62	133.51	133.51	130.21	147.44
iLOGP	3.88	4.01	4.01	3.66	3.45	4.17	4.05
XLOGP3	4.17	4.79	4.79	2.47	1.56	2.17	1.61
WLOGP	5.43	5.93	5.93	4.18	4.18	2.64	2.23
MLOGP	4.11	4.22	4.22	2.7	2.7	2.46	2.5
Silicos-IT Log P	4.84	5.19	5.19	3.62	3.62	4.51	3.22
Consensus Log P	4.49	4.83	4.83	3.33	3.1	3.19	2.72
ESOL Log S	-6.37	-6.89	-6.89	-5.1	-4.53	-4.91	-4.64
ESOL Solubility (mg/ml)	2.68E-04	8.26E-05	8.26E-05	4.70E-03	1.76E-02	7.57E-03	1.44E-02
ESOL Solubility (mol/l)	4.24E-07	1.28E-07	1.28E-07	7.87E-06	2.94E-05	1.24E-05	2.29E-05
ESOL Class	Poorly soluble	Poorly soluble	Poorly soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble
Ali Log S	-6.41	-7.05	-7.05	-4.92	-3.97	-4.54	-4.32
Ali Solubility (mg/ml)	2.45E-04	5.70E-05	5.70E-05	7.22E-03	6.35E-02	1.77E-02	3.01E-02
Ali Solubility (mol/l)	3.88E-07	8.81E-08	8.81E-08	1.21E-05	1.06E-04	2.90E-05	4.81E-05
Ali Class	Poorly soluble	Poorly soluble	Poorly soluble	Moderately soluble	Soluble	Moderately soluble	Moderately soluble
Silicos-IT LogSw	-7.97	-9.01	-9.01	-7.03	-7.03	-8.12	-7.03
Silicos-IT Solubility (mg/ml)	6.76E-06	6.36E-07	6.36E-07	5.62E-05	5.62E-05	4.59E-06	5.84E-05
Silicos-IT Solubility (mol/l)	1.07E-08	9.84E-10	9.84E-10	9.40E-08	9.40E-08	7.50E-09	9.31E-08
Silicos-IT class	Poorly soluble	Poorly soluble	Poorly soluble	Poorly soluble	Poorly soluble	Poorly soluble	Poorly soluble
GI absorption	Low	Low	Low	Low	Low	High	Low
BBB permeant	No	No	No	No	No	No	No
Pgp substrate	Yes	No	No	Yes	Yes	Yes	Yes
CYP1A2 inhibitor	No	No	No	No	No	No	No
CYP2C19 inhibitor	Yes	Yes	Yes	Yes	Yes	Yes	No
CYP2C9 inhibitor	Yes	Yes	Yes	Yes	Yes	Yes	Yes
CYP2D6 inhibitor	No	No	No	Yes	Yes	Yes	Yes

CYP3A4 inhibitor	Yes	No	No	Yes	Yes	Yes	Yes
log Kp (cm/s)	-7.19	-6.84	-6.84	-8.19	-8.84	-8.49	-8.98
Lipinski #violations	1	2	2	1	1	1	1
Ghose #violations	3	4	4	3	3	3	3
Veber #violations	0	0	0	0	0	0	1
Egan #violations	0	1	1	1	1	0	1
Muegge #violations	1	2	2	0	0	1	1
Bioavailability Score	0.55	0.17	0.17	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	0	0	0
Brenk #alerts	1	1	1	1	1	1	2
Leadlikeness #violations	2	2	2	1	1	1	1
Synthetic Accessibility	4.32	4.52	4.52	4.29	4.23	4.55	4.73

Table S3

Molecule	Comp 15	Comp 16	Comp 17	Comp 18	Comp 19	Comp 20	Comp 21
MW	626.7	548.59	583.03	578.61	564.58	490.48	442.44
Heavy atoms	45	39	40	41	40	36	32
Aromatic heavy atoms	22	16	16	16	16	16	10
Fraction Csp3	0.27	0.29	0.29	0.31	0.29	0.31	0.45
Rotatable bonds	7	6	6	7	6	5	5
H-bond acceptors	7	7	7	8	8	7	7
H-bond donors	2	1	1	1	2	1	1
MR	185.63	157.26	162.27	163.75	159.28	139.95	124.47
TPSA	147.44	128.46	128.46	137.69	148.69	103.16	103.16
iLOGP	4.05	3.74	4.07	3.94	3.31	2.81	2.36
XLOGP3	1.61	1.64	2.26	1.61	1.28	0.16	-1.6
WLOGP	2.23	3.1	3.75	3.1	2.8	1.76	0.62
MLOGP	2.5	2.05	2.51	1.48	1.55	1.72	1.11
Silicos-IT Log P	3.22	2.92	3.57	3	2.45	2.22	1.39
Consensus Log P	2.72	2.69	3.23	2.63	2.28	1.74	0.78
ESOL Log S	-4.64	-4.18	-4.78	-4.27	-4.05	-2.98	-1.48
ESOL Solubility (mg/ml)	1.44E-02	3.61E-02	9.71E-03	3.12E-02	5.07E-02	5.13E-01	1.48E+01
ESOL Solubility (mol/l)	2.29E-05	6.58E-05	1.66E-05	5.39E-05	8.98E-05	1.05E-03	3.34E-02
ESOL Class	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Soluble	Very soluble
Ali Log S	-4.32	-3.95	-4.59	-4.11	-4	-1.88	-0.06
Ali Solubility (mg/ml)	3.01E-02	6.15E-02	1.48E-02	4.46E-02	5.62E-02	6.41E+00	3.88E+02
Ali Solubility (mol/l)	4.81E-05	1.12E-04	2.55E-05	7.70E-05	9.96E-05	1.31E-02	8.77E-01
Ali Class	Moderately soluble	Soluble	Moderately soluble	Moderately soluble	Moderately soluble	Very soluble	Very soluble
Silicos-IT LogSw	-7.03	-5.59	-6.16	-5.68	-4.99	-5.24	-3.33
Silicos-IT Solubility (mg/ml)	5.84E-05	1.42E-03	4.03E-04	1.22E-03	5.74E-03	2.85E-03	2.08E-01
Silicos-IT Solubility (mol/l)	9.31E-08	2.59E-06	6.92E-07	2.10E-06	1.02E-05	5.81E-06	4.70E-04
Silicos-IT class	Poorly soluble	Moderately soluble	Poorly soluble	Moderately soluble	Moderately soluble	Moderately soluble	Soluble
GI absorption	Low	High	High	Low	Low	High	High
BBB permeant	No	No	No	No	No	No	No
Pgp substrate	Yes	Yes	Yes	Yes	Yes	Yes	Yes
CYP1A2 inhibitor	No	No	No	No	No	No	No
CYP2C19 inhibitor	No	Yes	Yes	No	No	No	No
CYP2C9 inhibitor	Yes	Yes	Yes	Yes	Yes	Yes	No
CYP2D6 inhibitor	Yes	No	No	No	No	No	No
CYP3A4 inhibitor	Yes	Yes	Yes	Yes	Yes	No	No
log Kp (cm/s)	-8.98	-8.48	-8.25	-8.69	-8.84	-9.18	-10.13

Lipinski #violations	1	1	1	1	1	0	0
Ghose #violations	3	2	2	2	2	2	0
Veber #violations	1	0	0	0	1	0	0
Egan #violations	1	0	0	1	1	0	0
Muegge #violations	1	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	0	0	0
Brenk #alerts	2	2	2	2	2	1	1
Leadlikeness #violations	1	1	1	1	1	1	1
Synthetic Accessibility	4.73	4.13	4.12	4.24	4.2	3.3	3.1