

Supplementary material of 2-aminothiazole derivatives

4.1. Analysis of the physicochemical properties

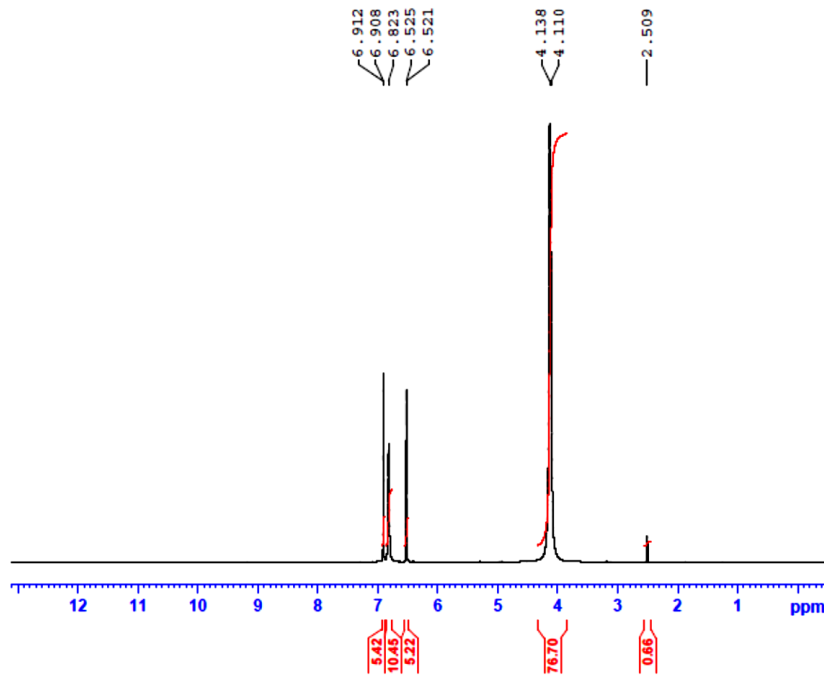
In order to estimate drug-like properties of compounds **(1, 2)** and **(6-18)**, Lipinski's rule of five was evaluated for these compounds. Data Warrior was used to estimate molecular weight (MW), CLogP, hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD) for each molecule and the values are presented in Table 2. Data in the table showed that all of the compounds satisfied Lipinski's rule, i.e. each compound has: a MW <500, CLogP <5, HBAs <10 and HBDs <5. In addition, the low MW as well as CLogP values of the compounds offer an opportunity for further optimization without leading to "molecular obesity".

Table 2. Data Warrior values of 2-aminothiazoles derivatives

Compound	MW	CLogP	HBA	HBD
(1)	100.145	0.6076	2	1
(2)	147.589	-0.0641	3	0
(6)	209.233	0.7842	6	1
(7)	210.221	-0.6482	7	2
(8)	207.26	3.0044	5	0
(9)	188.254	2.6587	2	0
(10)	222.699	3.2647	2	0
(11)	233.251	1.7371	5	0
(12)	204.253	2.313	3	1
(13)	204.253	2.313	3	1
(14)	218.279	2.5887	3	0
(15)	218.279	2.5887	3	0
(16)	248.305	2.5187	4	0
(17)	248.305	2.5187	4	0
(18)	241.317	3.096	3	1

Sample 1 = compound 1

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Sample : 1 DMSO



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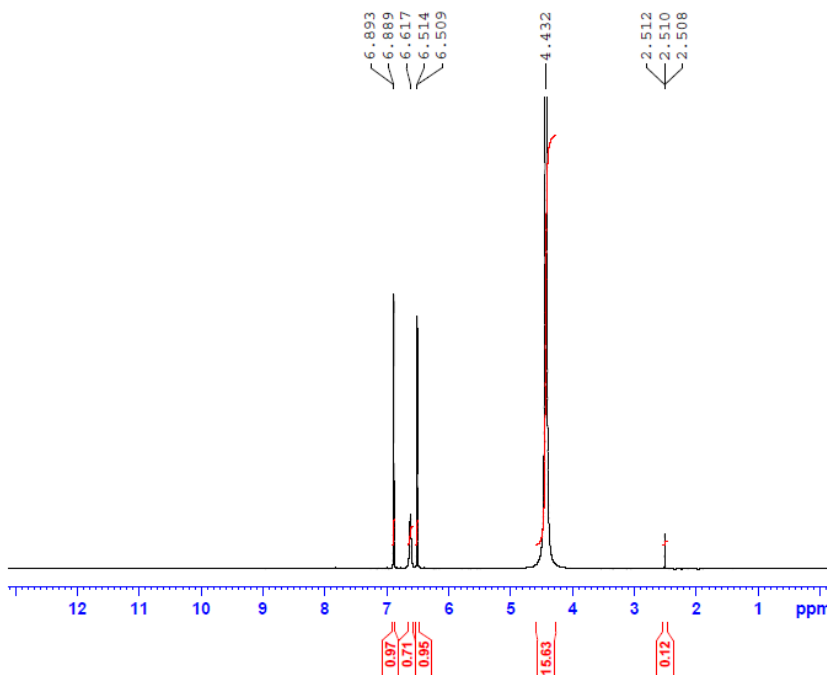
Current data parameters
NAME SAMARAHU 1 10-06-2019
EXPNO 10
PROCNO 1

F2 - Acquisition parameters
DATE_ 20190610
TIME 14.24
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 17006.803 Hz
FIDRES 0.2099503 Hz
AQ 1.9267584 sec
RG 2.53
DM 29.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 850.1452500 MHz
NUC1 1H
P1 8.00 usec
PLW1 15.89999962 W

F2 - processing parameters
SI 65536
SF 850.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

Samar Abusahit
Sample : 1 DMSO:D2O



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Current Data Parameters
NAME SAMARAHU 1 17-06-2019
EXPNO 10
PROCNO 1

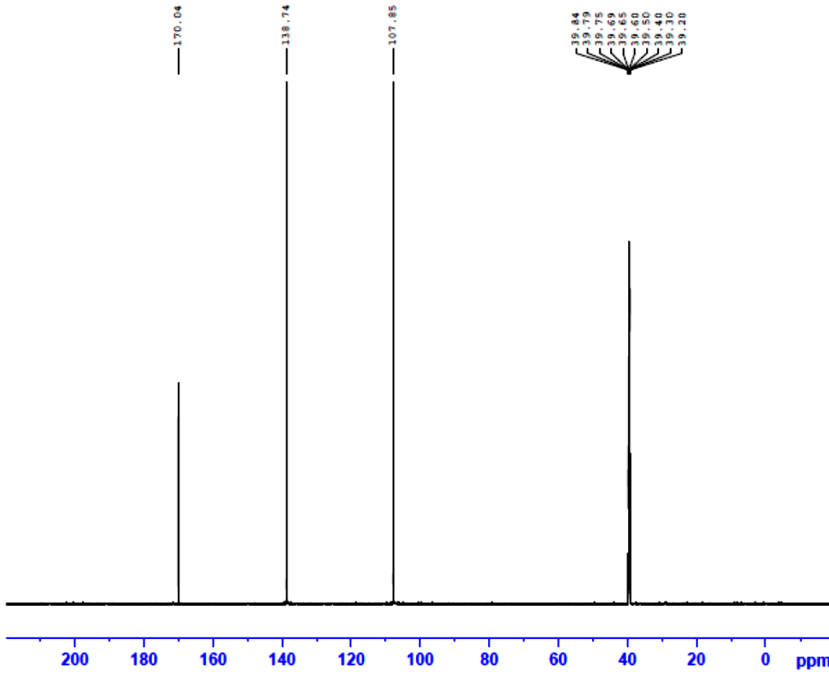
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Date_ 20190617
Time 9.57
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 17006.803 Hz
FIDRES 0.2099503 Hz
AQ 1.9267584 sec
RG 2.04
DM 29.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 850.1452500 MHz
NUC1 1H
P1 8.00 usec
PLW1 15.89999962 W

F2 - Processing parameters
SI 65536
SF 850.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

Samar Abusahit
Sample : 1

DMSO



Current Data Parameters
NAME SAMARASU 1 10-06-2019
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
DATE_ 20190610
TIME 14.20
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 21
DS 4
SWH 51020.406 HZ
FIDRES 0.778510 HZ
AQ 0.6422328 SEC
RG 186.93
CW 9.800 USEC
DE 18.00 USEC
TE 298.0 K
D1 2.0000000 SEC
D11 0.0300000 SEC
TDO 1

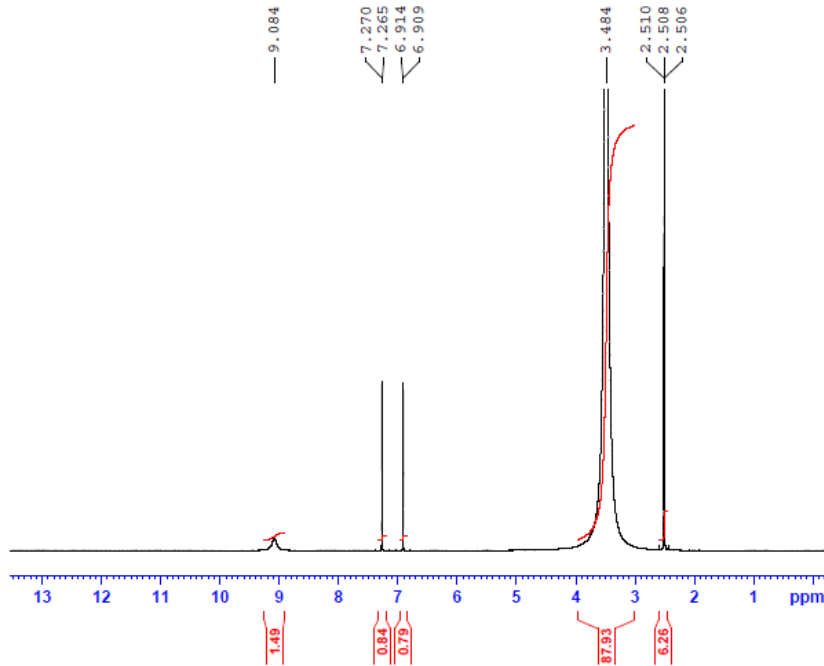
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NUC1 13C
P1 12.00 USEC
PLW1 140.0000000 W

===== CHANNEL f2 =====
NUC2 1H
CPROG2 waltz16
PCPD2 80.00 USEC
PLW2 15.89999962 W
PLW3 0.10000000 W
PLW13 0.10176000 W

F2 - Processing parameters
SI 32768
SF 213.7678126 MHz
WDW EM
SSB 0
LB 1.50 HZ
GB 0
PC 2.00

Sample 2 = compound 2

Samar Abusahit
Sample : 2 DMSO



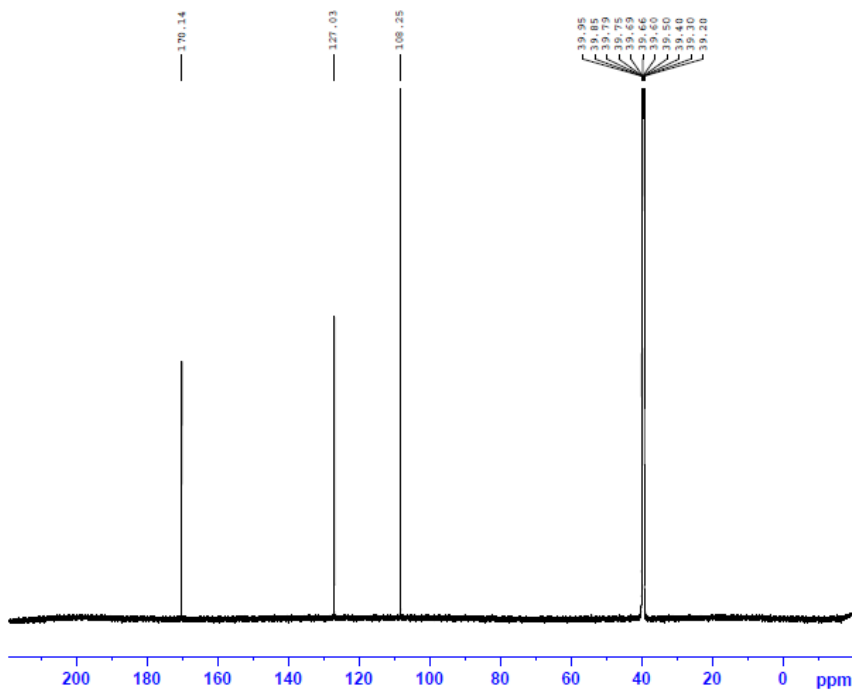
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Current data parameters
NAME SAMAHIT 2 10-06-2019
EXPNO 20
PROCNO 1

F2 - Acquisition parameters
Date_ 20190619
Time 17.11
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 17006.803 HZ
FIDRES 0.255003 HZ
AQ 1.5267584 SEC
RG 7.85
DM 29.400 USRC
DE 10.00 USRC
TE 298.2 K
D1 1.00000000 SEC
TD0 1

===== CHANNEL f1 =====
SFO1 850.1434006 MHZ
NUC1 1H
P1 8.00 USRC
PLW1 15.89999962 W

F2 - processing parameters
SI 65536
SF 850.1400000 MHZ
WDW EM
SSB 0
LB 0.30 HZ
GB 0
PC 2.00
```

Samar Abusahit
Sample : 2 DMSO



```
Current data parameters
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EXPNO 22
PROCNO 1

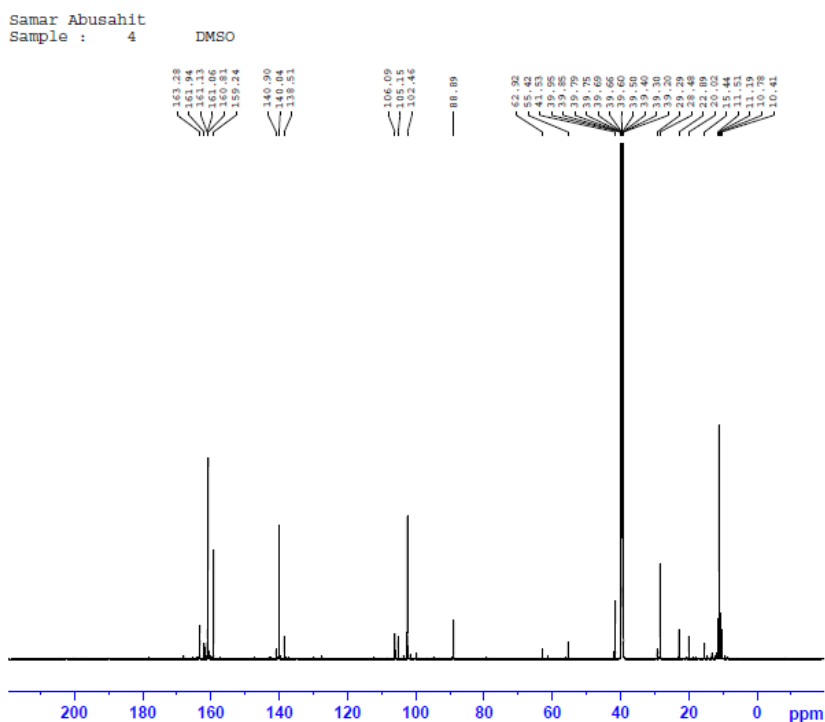
F2 - Acquisition parameters
Date_ 20190619
Time 18.45
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 51020.400 HZ
FIDRES 0.778510 HZ
AQ 0.6422520 SEC
RG 186.93
DM 9.800 USRC
DE 10.00 USRC
TE 298.2 K
D1 2.00000000 SEC
D11 0.03000000 SEC
TD0 1

===== CHANNEL f1 =====
SFO1 213.7692488 MHZ
NUC1 13C
P1 12.00 USRC
PLW1 140.00000000 W

===== CHANNEL f2 =====
SFO2 850.1434006 MHZ
NUC2 1H
CPCPRG[2] waltz16
PCPD2 80.00 USRC
PLW2 15.89999962 W
PLW12 0.15899999 W
PLW13 0.10176000 W

F2 - processing parameters
SI 32768
SF 213.7679506 MHZ
WDW EM
SSB 0
LB 1.50 HZ
GB 0
PC 2.00
```

Sample 4 = compound 7



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Current Data Parameters
NAME SAMARAHU 4 11-06-2019
EXPNO 71
PROCNO 1

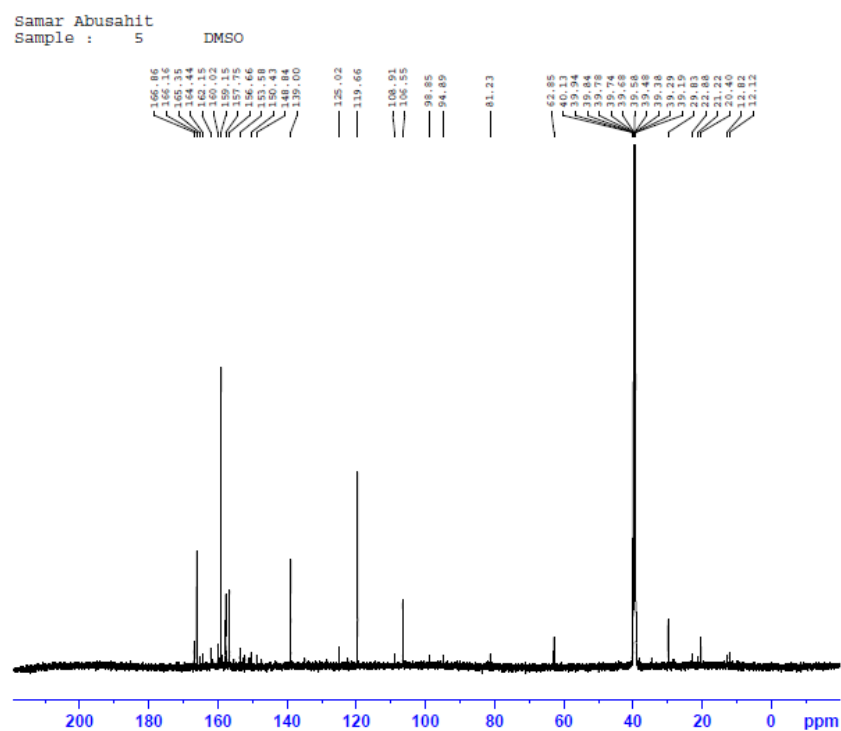
F2 - Acquisition Parameters
Date_ 20190612
Time 9.01
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2912
DS 4
SWH 51020.406 Hz
FIDRES 0.778510 Hz
AQ 0.6422528 sec
RG 186.93
DW 9.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1

==== CHANNEL f1 =====
SFO1 213.7802488 MHz
NUC1 13C
P1 12.00 usec
PLW1 140.0000000 W

==== CHANNEL f2 =====
SFO2 850.1434006 MHz
NUC2 1H
CQDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.89999962 W
PLW12 0.15899999 W
PLW13 0.10176000 W

F2 - Processing parameters
SI 32768
SF 213.7679316 MHz
WUM RM
SGB 0
LB 1.50 Hz
GB 0
PC 2.00

Sample 5= compound 6



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Current Data Parameters
NAME SAMARAHU 5 11-06-2019
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190611
Time 14.46
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 51020.406 Hz
FIDRES 0.778510 Hz
AQ 0.6422528 sec
RG 186.93
DW 9.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1

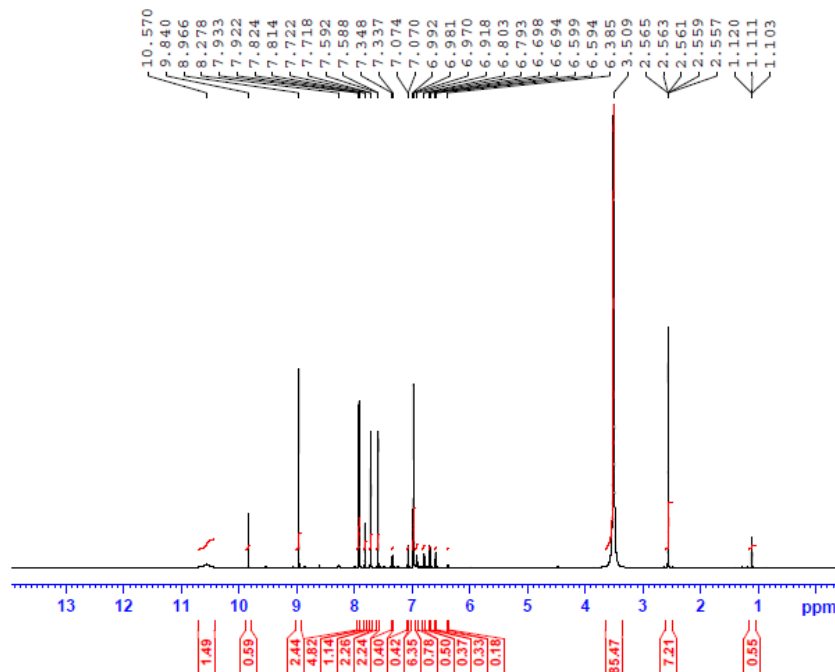
==== CHANNEL f1 =====
SFO1 213.7802488 MHz
NUC1 13C
P1 12.00 usec
PLW1 140.0000000 W

==== CHANNEL f2 =====
SFO2 850.1434006 MHz
NUC2 1H
CQDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.89999962 W
PLW12 0.15899999 W
PLW13 0.10176000 W

F2 - Processing parameters
SI 32768
SF 213.7679512 MHz
WUM RM
SGB 0
LB 1.50 Hz
GB 0
PC 2.00

Sample 7 = compound 12

Samar Abusahit
Sample : 7 DMSO



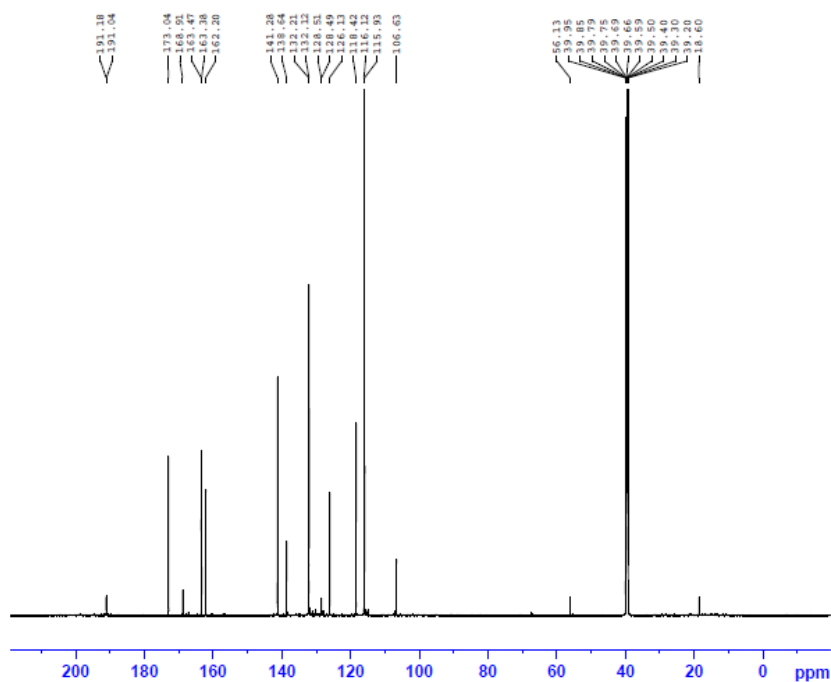
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Current data parameters
NAME      SAMARAHIT 7 10-06-2019
EXPNO    30
PROCNO   1

F2 - Acquisition parameters
DATE_    20190610
TIME     23.07
INSTRUM  spect
PROBHD   5 mm CPQCI 1H-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
RG        32
DS        2
SWH       17006.803 HZ
FIRWGSS  0.209903 HZ
AQ        1.9267304 SEC
RG         7.85
DM        29.400 USBC
DE        16.00 USBC
TE        298.0 K
D1        1.0000000 SEC
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1         8.00 USBC
PLW1      15.89999962 W

F2 - processing parameters
SI         65536
SF         850.1399947 MHz
WDW        RM
SSB         0
LB          0.30 HZ
GB          0
PC          2.00
```

Samar Abusahit
Sample : 7 DMSO



```
Current data parameters
NAME      SAMARAHIT 7 10-06-2019
EXPNO    32
PROCNO   1

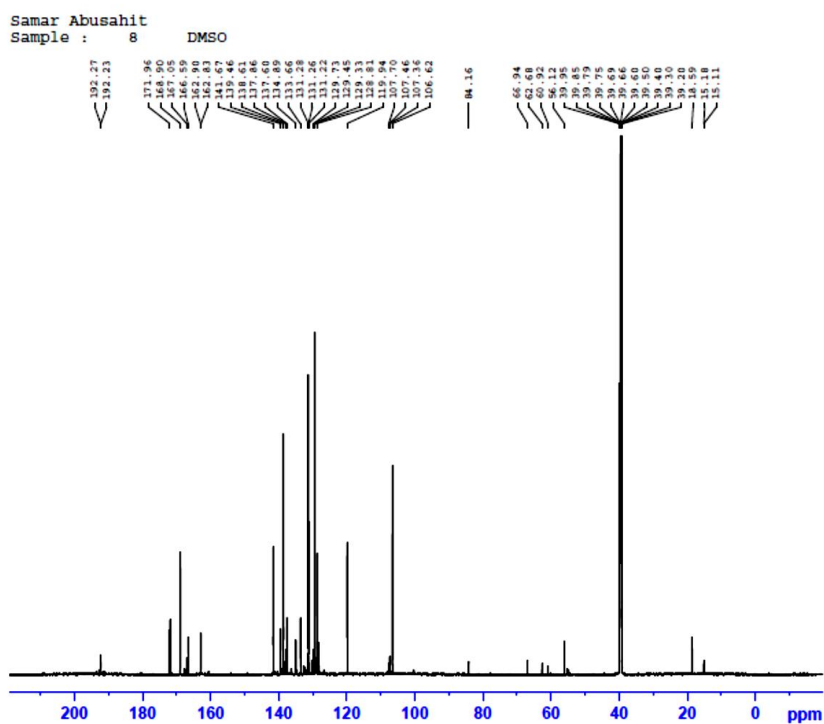
F2 - Acquisition parameters
DATE_    20190610
TIME     23.16
INSTRUM  spect
PROBHD   5 mm CPQCI 1H-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
RG        32
DS        4
SWH       51020.406 HZ
FIRWGSS  0.778510 HZ
AQ        0.6422528 SEC
RG         186.93
DM        3.800 USBC
DE        18.00 USBC
TE        298.0 K
D1        2.0000000 SEC
D11       0.0300000 SEC
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        12.00 USBC
PLW1     140.00000000 W

===== CHANNEL f2 =====
NUC2      1H
CPDPRG2  waltz16
PCPD2    80.00 USBC
PLW2     15.89999962 W
PLW12    0.158999999 W
PLW13    0.101760000 W

F2 - processing parameters
SI         65536
SF         213.7679561 MHz
WDW        RM
SSB         0
LB          1.50 HZ
GB          0
PC          2.00
```

Sample 8 = compound 10



Current Data Parameters
NAME SAMARASU 8 10-06-2019
EXPNO 41
PROCNO 1

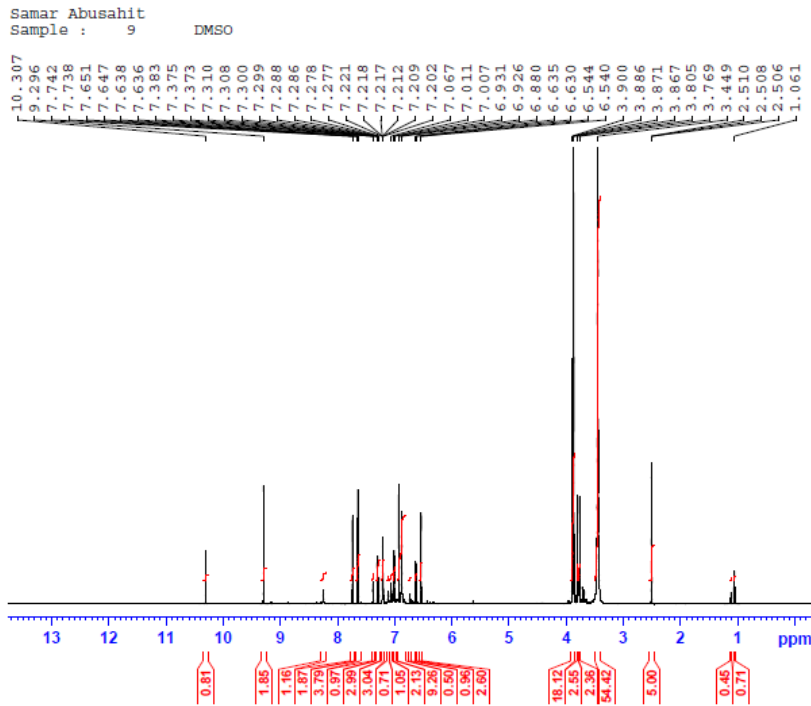
F2 - Acquisition Parameters
Date_ 20190611
Time 8.56
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SFO 51020.406 Hz
FIDRES 0.778510 Hz
AQ 0.6422528 sec
RG 186.93
DM 9.800 usec
DE 18.00 usec
TE 298.0 K
TR 2.0000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 213.7892488 Mhz
NUC1 13C
P1 12.00 usec
PLW1 140.0000000 W

===== CHANNEL f2 =====
SFO2 850.1434006 Mhz
NUC2 1H
CPOPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.89999962 W
PLW12 0.15899999 W
PLW13 0.10176000 W

F2 - Processing parameters
SI 32768
SF 213.7679581 Mhz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 2.00

Sample 9 = compound 17

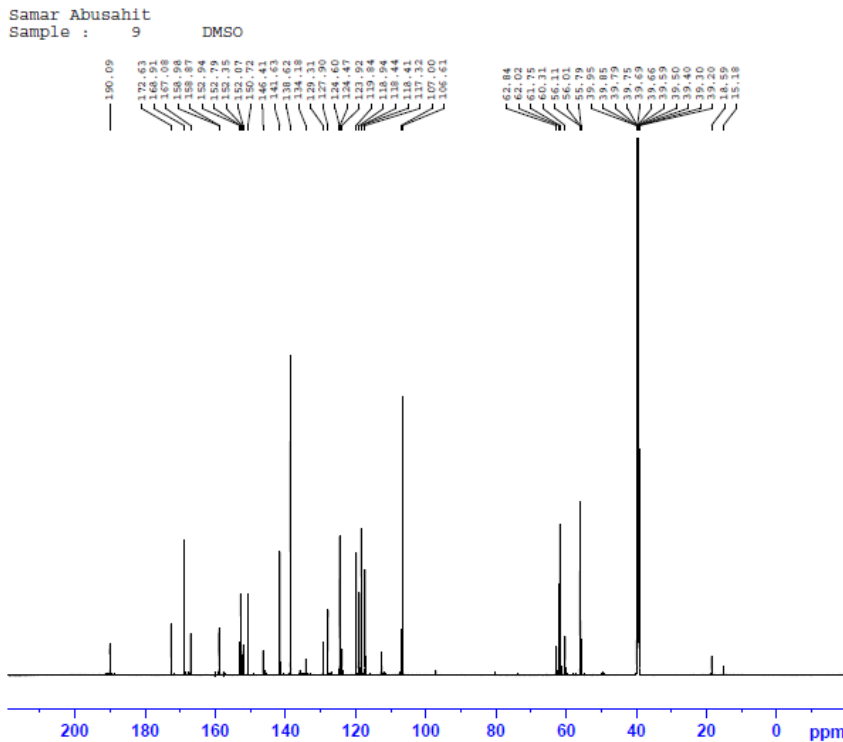


Current Data Parameters
NAME SAMARAHU 9 11-06-2019
EXPRNO 60
PROCNO 1

F2 - Acquisition Parameters
Date 20190611
Time 21.35
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 17006.803 Hz
FIDREC 0.259503 Hz
AQ 1.9267584 sec
RG 7.13
DW 29.400 usec
DE 18.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 850.1432500 MHz
NUC1 1H
PI 12.00 usec
PLM1 15.89999962 W

F2 - Processing parameters
SI 65536
SF 850.1400000 MHz
RGW DM
SGB 0
LB 0.30 Hz
GB 0
PC 2.00



Current Data Parameters
NAME SAMARAHU 9 11-06-2019
EXPRNO 61
PROCNO 1

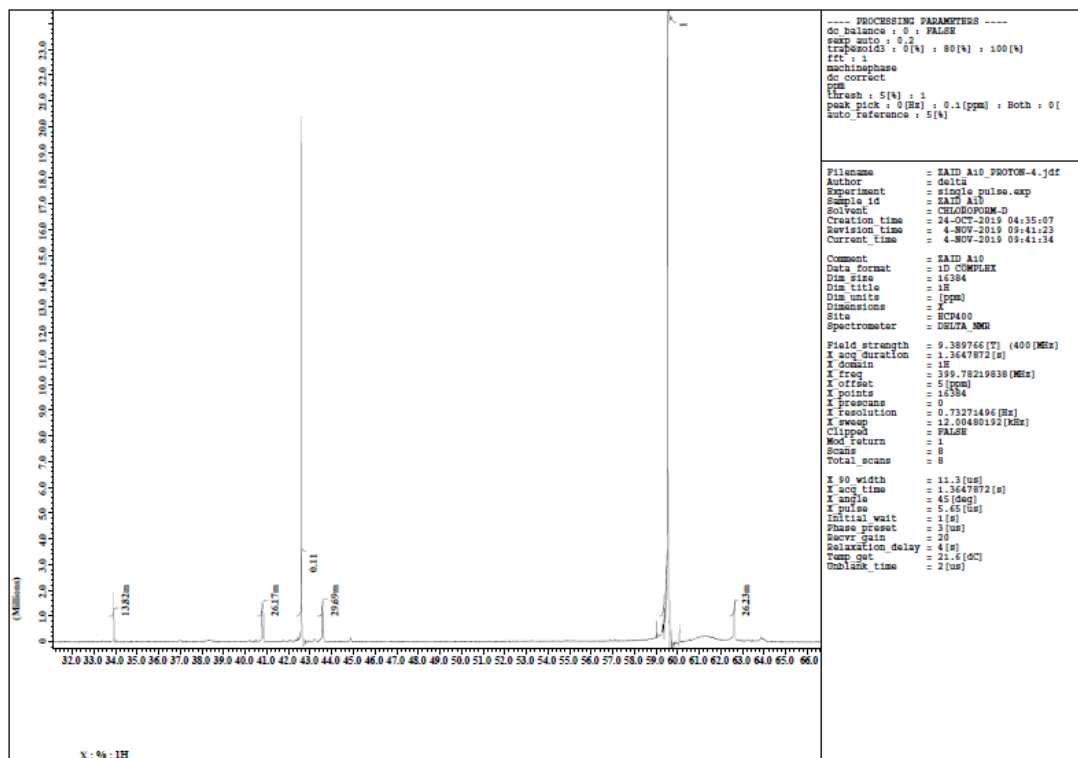
F2 - Acquisition Parameters
Date 20190612
Time 1.28
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5120
DS 4
SWH 51020.406 Hz
FIDREC 0.778510 Hz
AQ 0.6422328 sec
RG 186.93
DW 9.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 213.7892488 MHz
NUC1 13C
PI 12.00 usec
PLM1 140.0000000 W

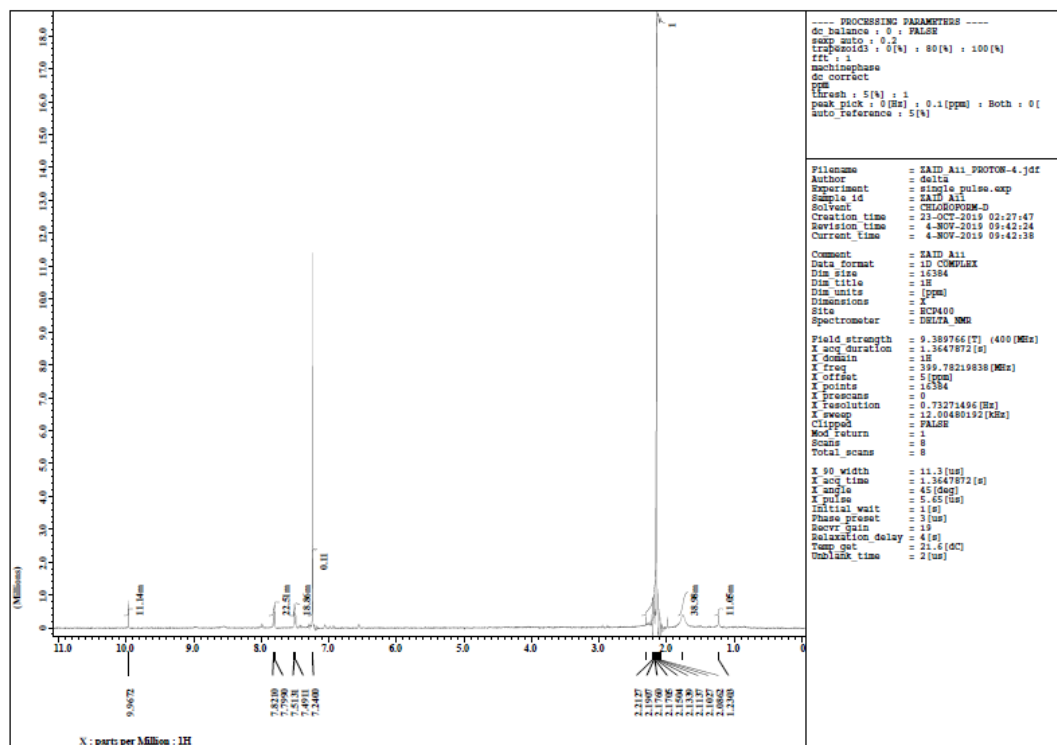
==== CHANNEL f2 =====
SFO2 850.1434006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLM2 15.89999962 W
PLM3 0.15899999 W
PLM3 0.10176000 W

F2 - Processing parameters
SI 32768
SF 213.7679581 MHz
RGW BM
SGB 0
LB 1.50 Hz
GB 0
PC 2.00

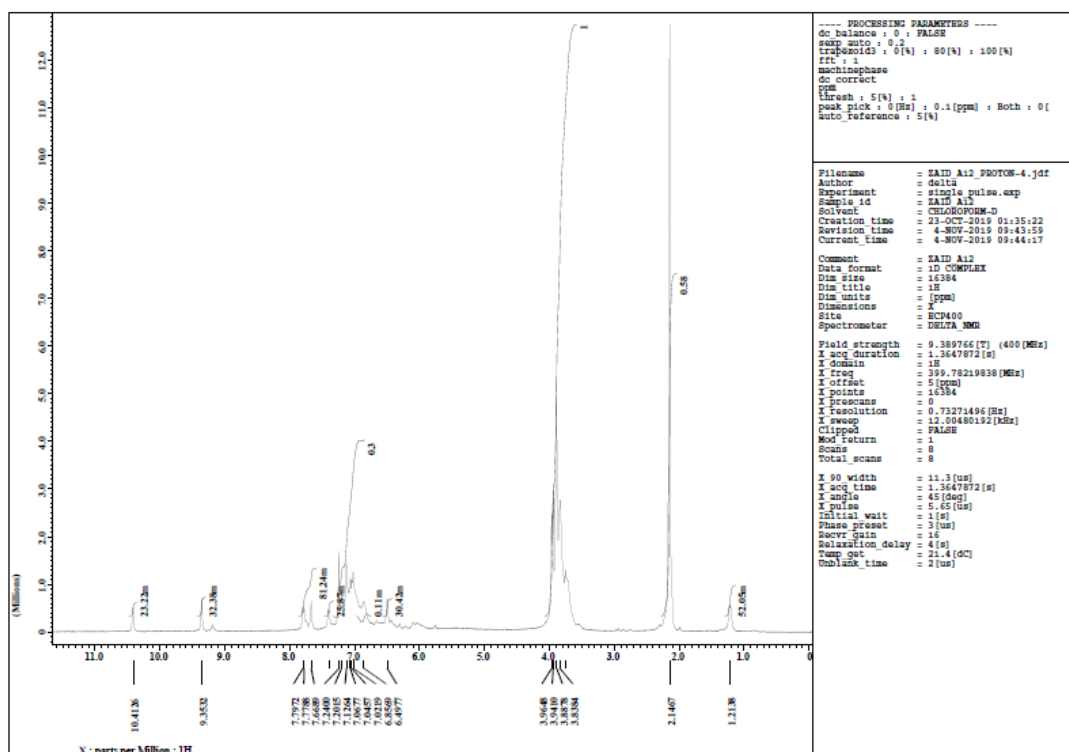
Sample 10 = compound 12



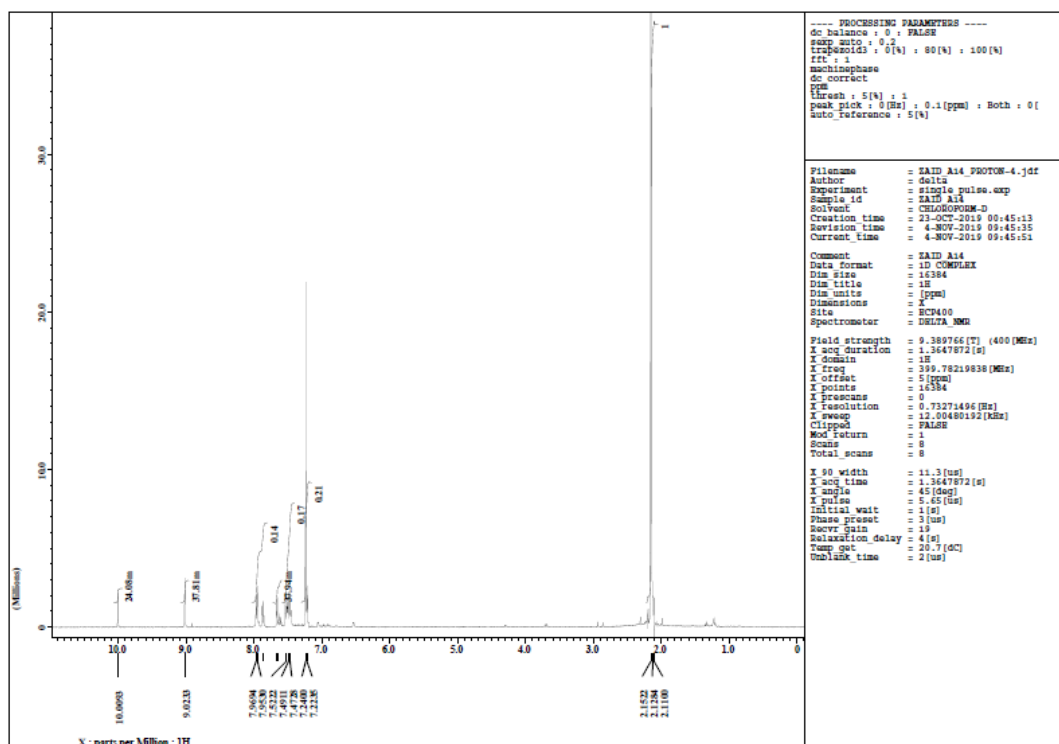
Sample 11 = compound 10



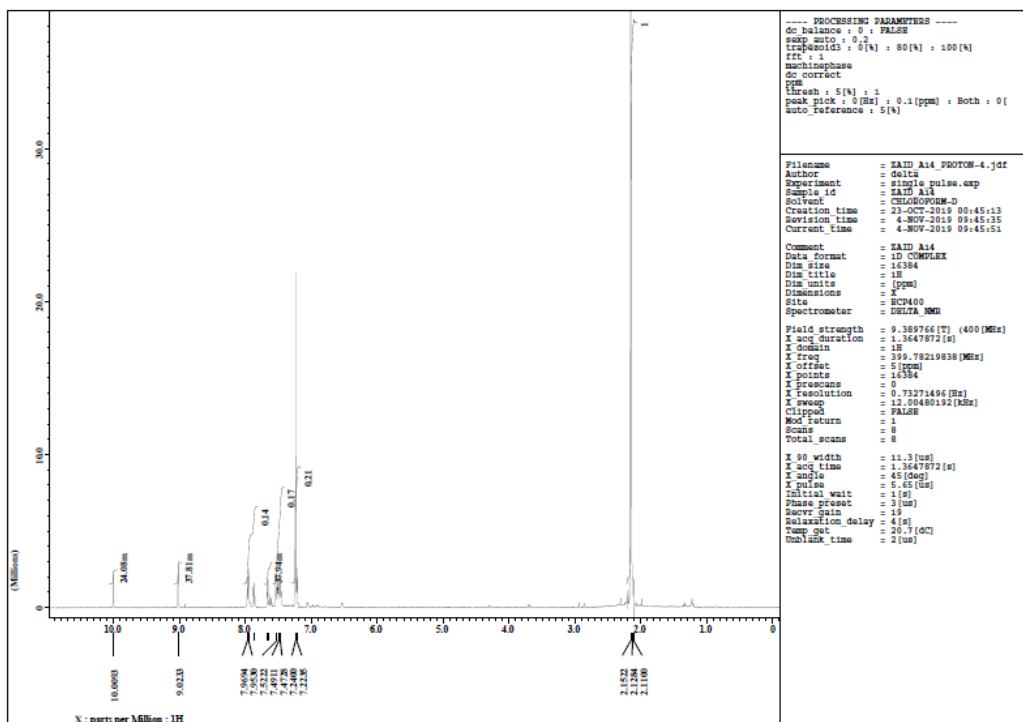
Sample 12 = compound 17



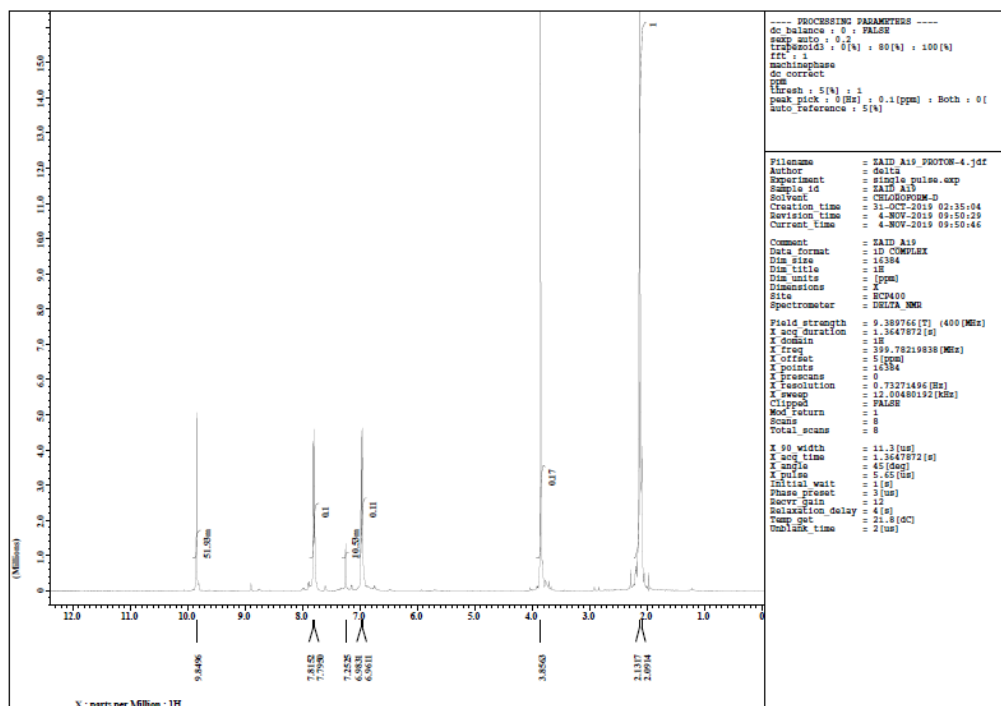
Sample 14 = compound 9



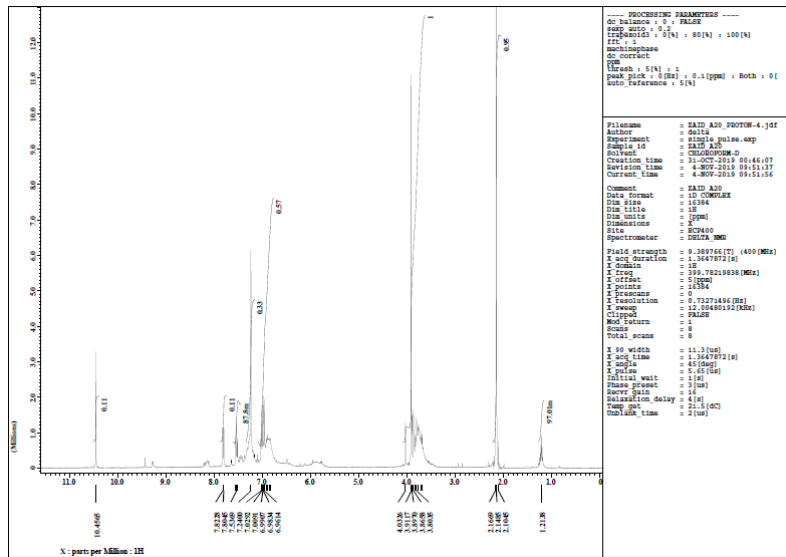
Sample 14 = compound 9



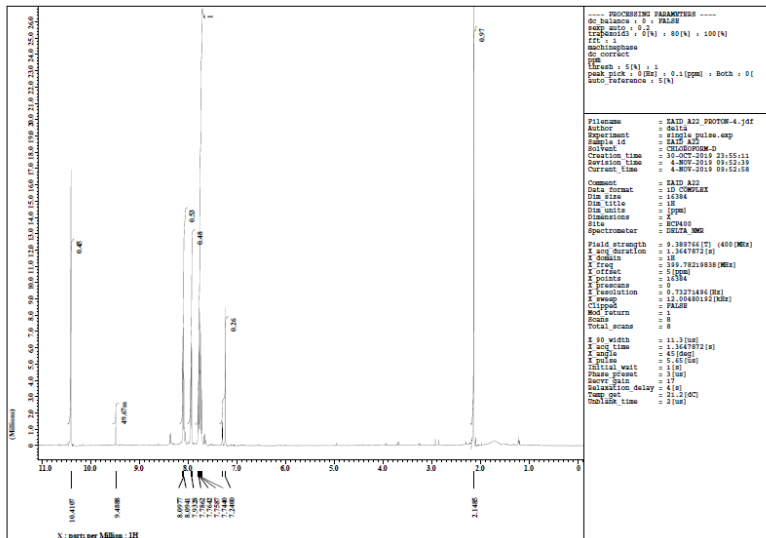
Sample 19 = compound 14



Sample 20 = compound 15



Sample 22 = compound 11



Sample 23 = compound 13

