Supplementary material of 2-aminothiazole derivatives

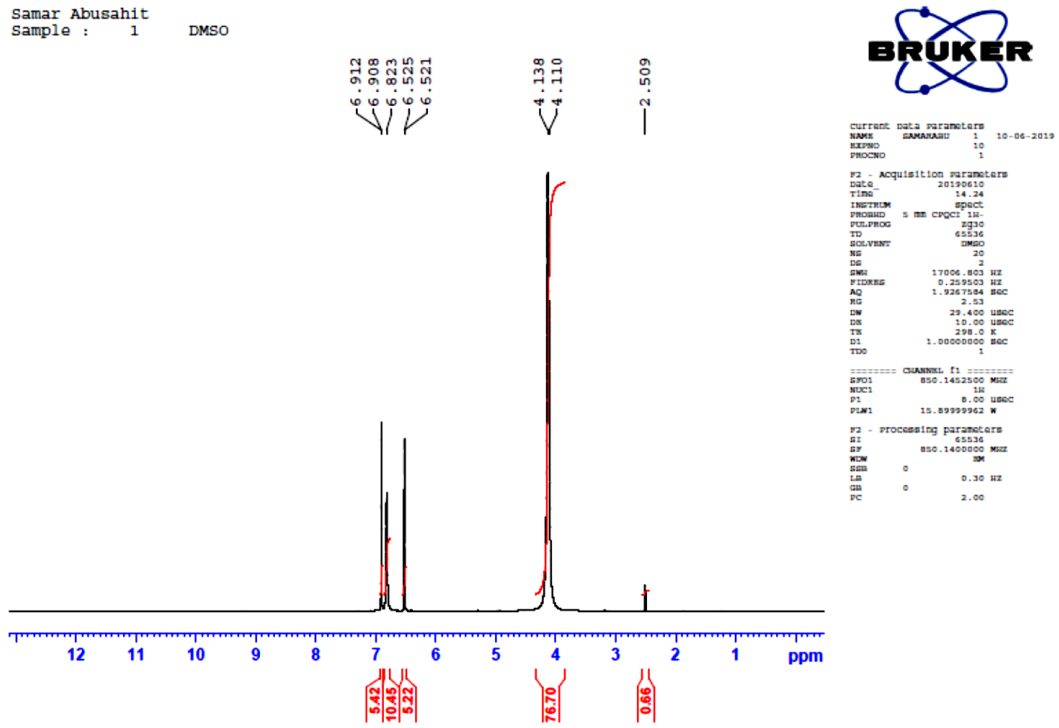
4.1. Analysis of the physicochemical properties

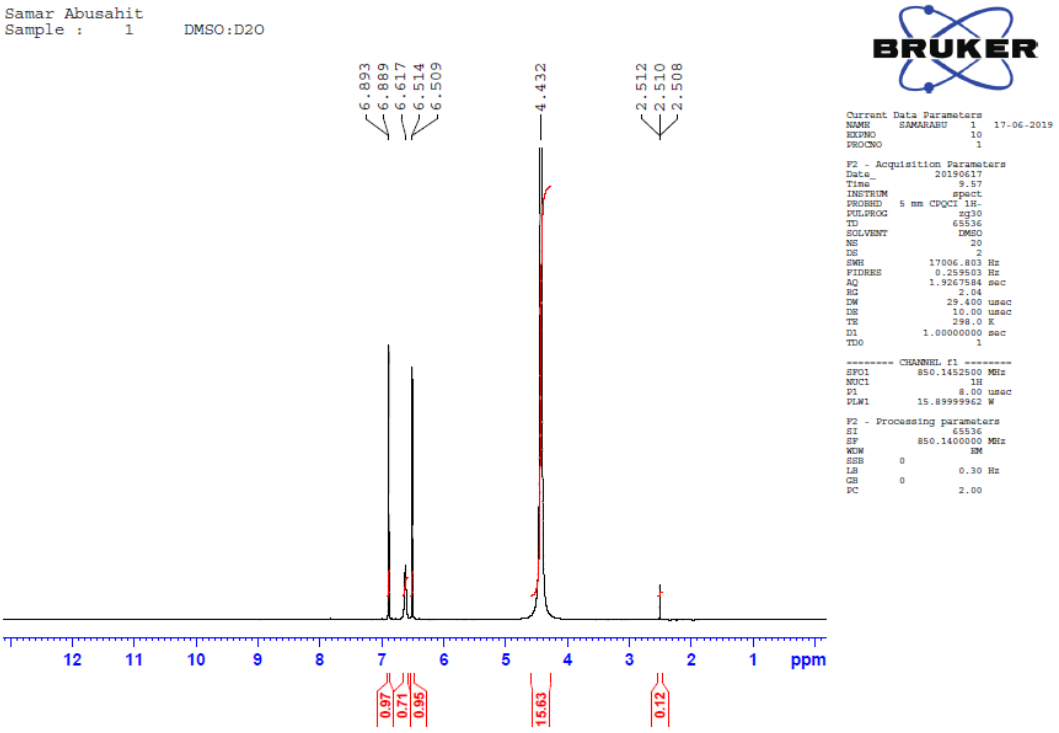
In order to estimate drug-like properties of compounds **(1**, **2)** and (**6-18**), Lipinski's rule of five was evaluated for these compounds. Data Warrior was used to estimate molecular weight (MW), CLogP, hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD) for each molecule and the values 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

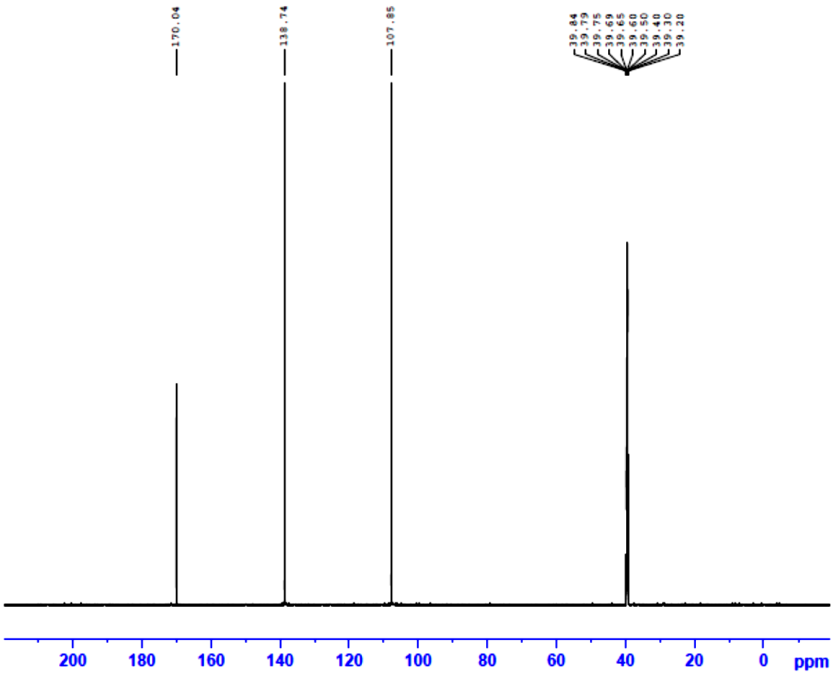
Compound	MW	CLogP	HBA	HBD
(1)	100.145	0.6076	2	1
(2)	147.589	-0.0641	3	0
(6)	209.233	0.7842	6	1
(7)	210.221	-0.6482	7	2
(8)	207.26	3.0044	5	0
(9)	188.254	2.6587	2	0
(10)	222.699	3.2647	2	0
(11)	233.251	1.7371	5	0
(12)	204.253	2.313	3	1
(13)	204.253	2.313	3	1
(14)	218.279	2.5887	3	0
(15)	218.279	2.5887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





Samar Abusahit
Sample : 1 DMSO

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PROCNO                      1

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TD                65536
SOLVENT             DMSO
NS                    21
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               2.00000000 sec
D11              0.03000000 sec
TD0                    1

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NUC1                    13C
P1                    12.00 usec
PLW1          140.00000000 W

======== CHANNEL f2 ========
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NUC2                    1H
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PCPD2                 80.00 usec
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PLW12          0.15899999 W
PLW13          0.10176000 W

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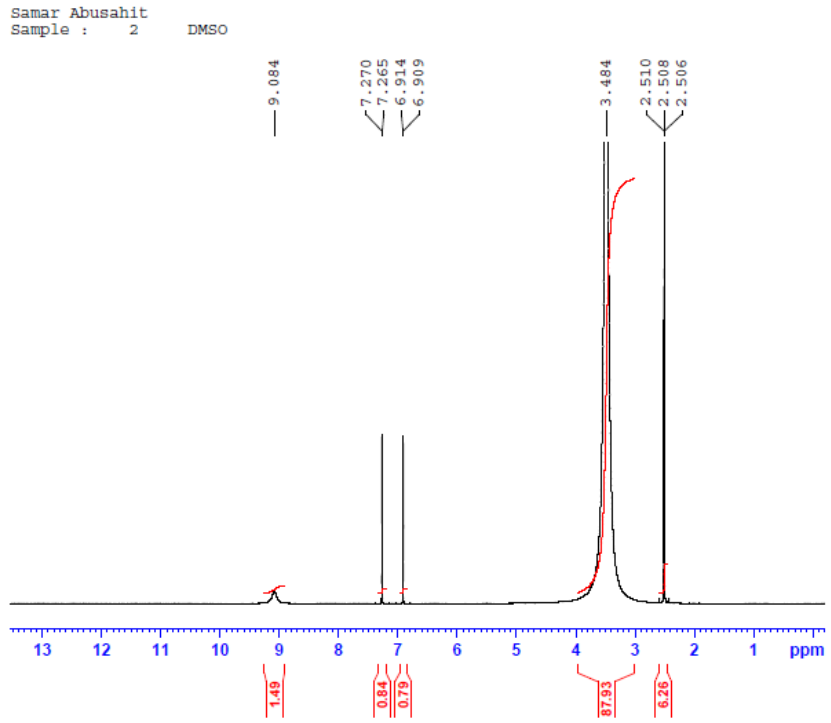

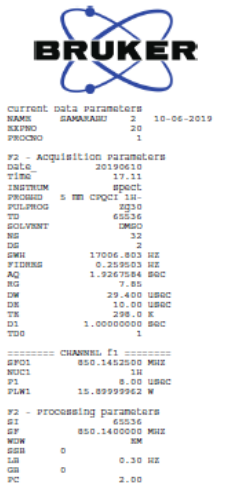

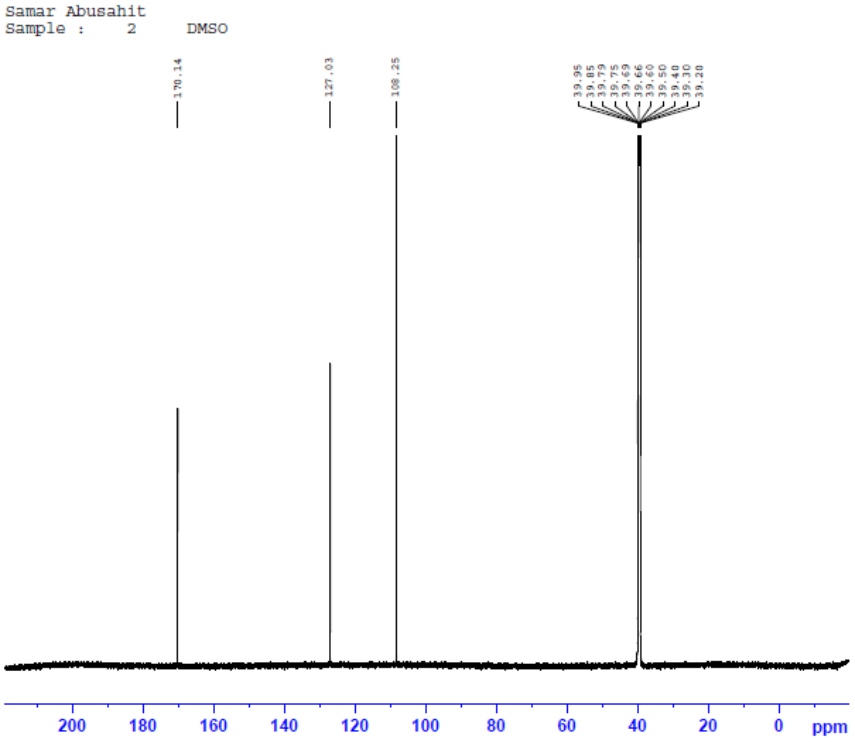

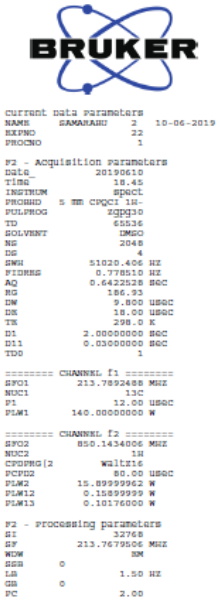

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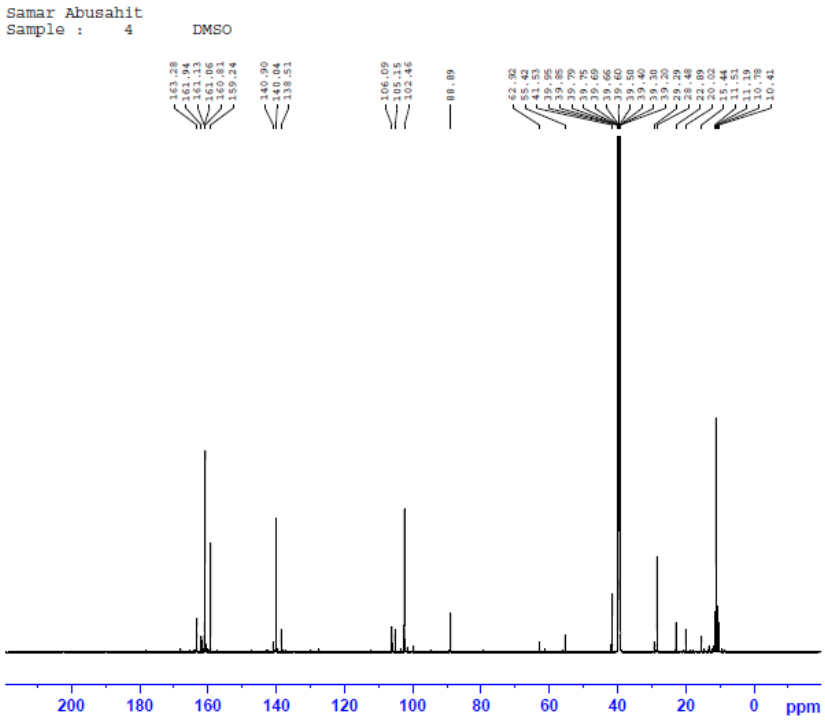

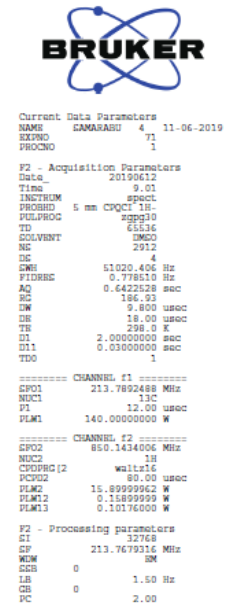

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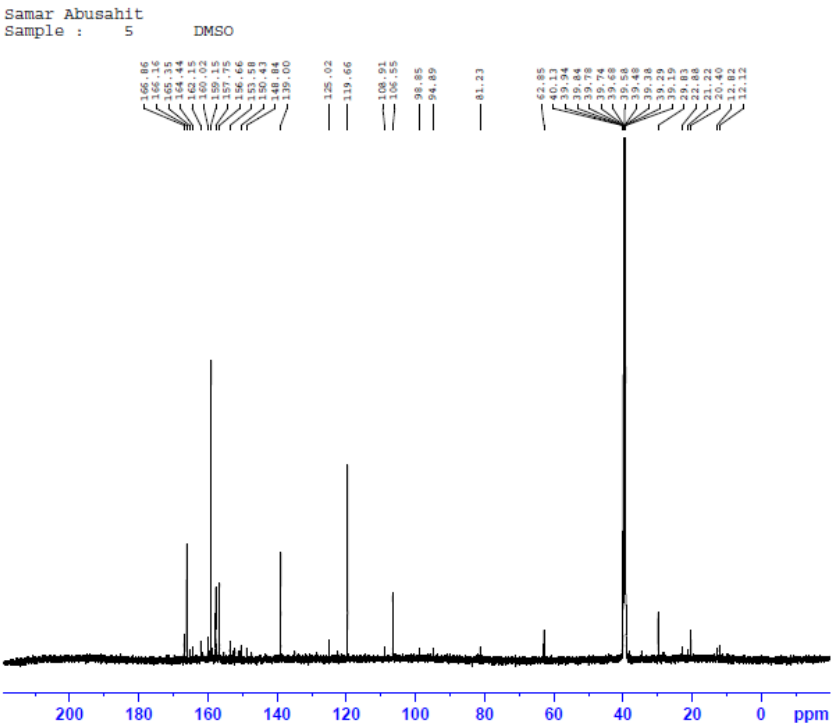

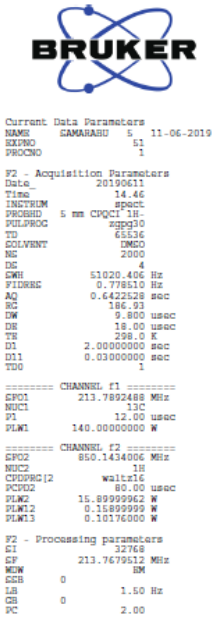

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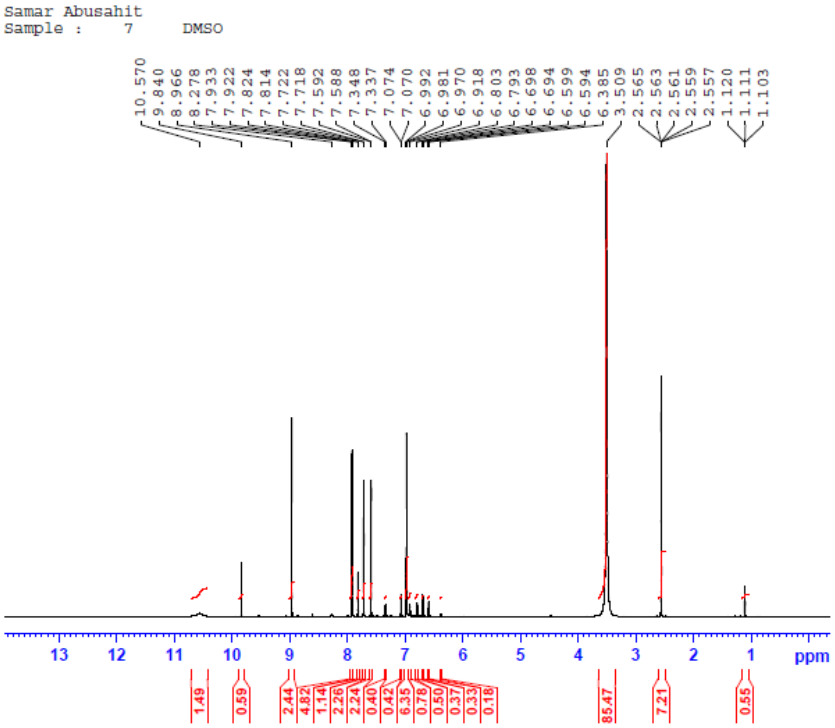

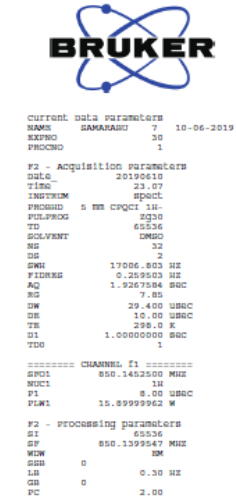

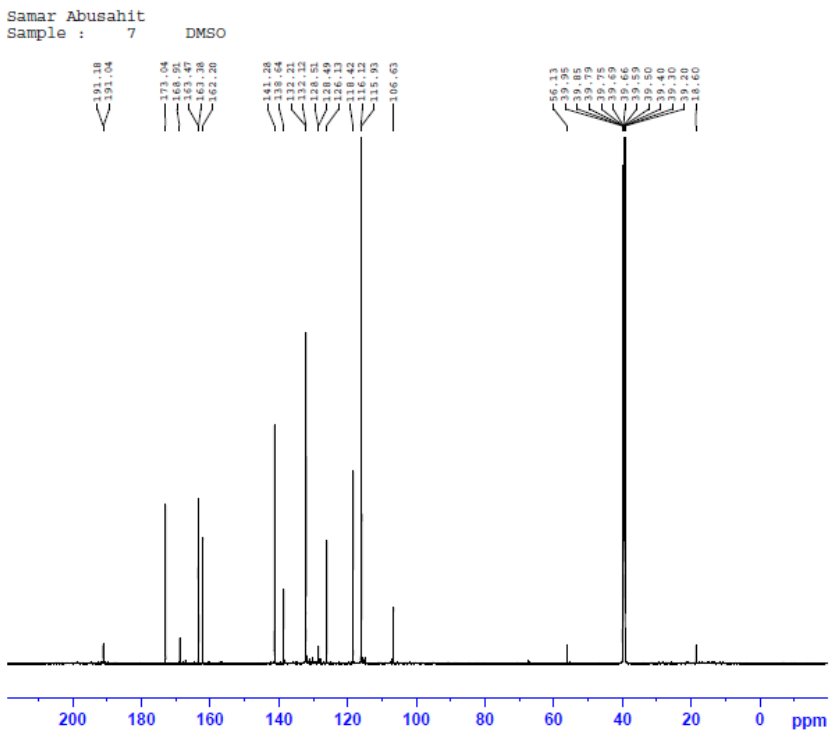

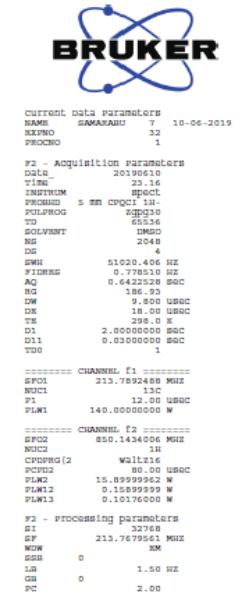

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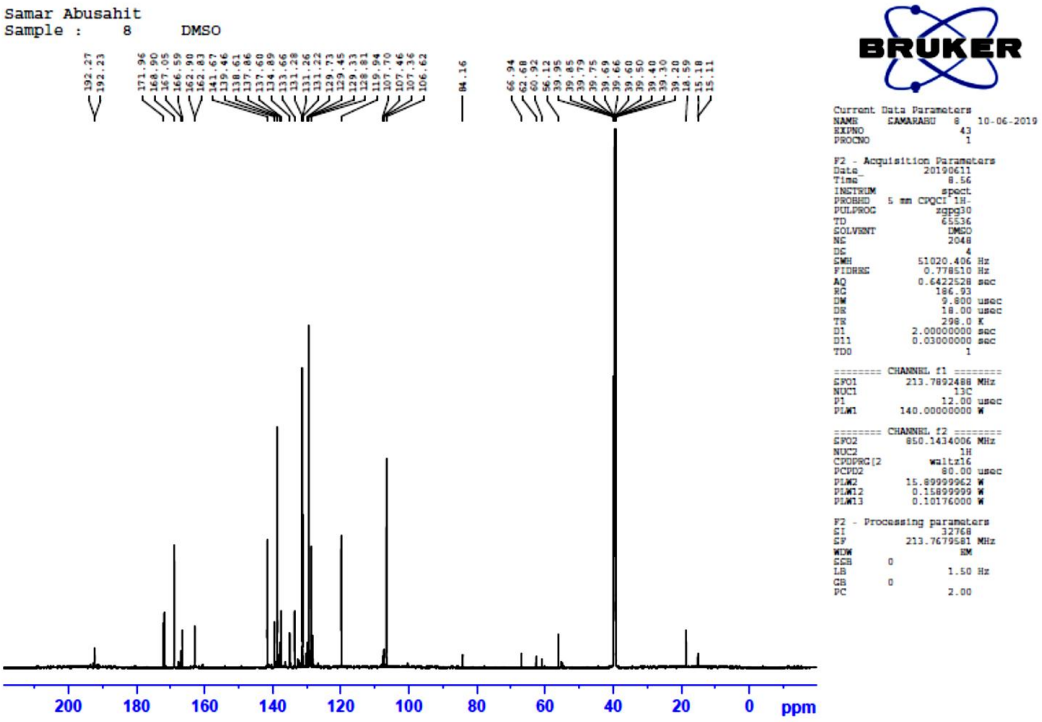

BRUKER

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PROCNO                1

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NS                2048
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            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         213.7892488 MHz
NUC1                 13C
P1                 12.00 usec
PLW1       140.00000000 W

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

F2 - Processing parameters
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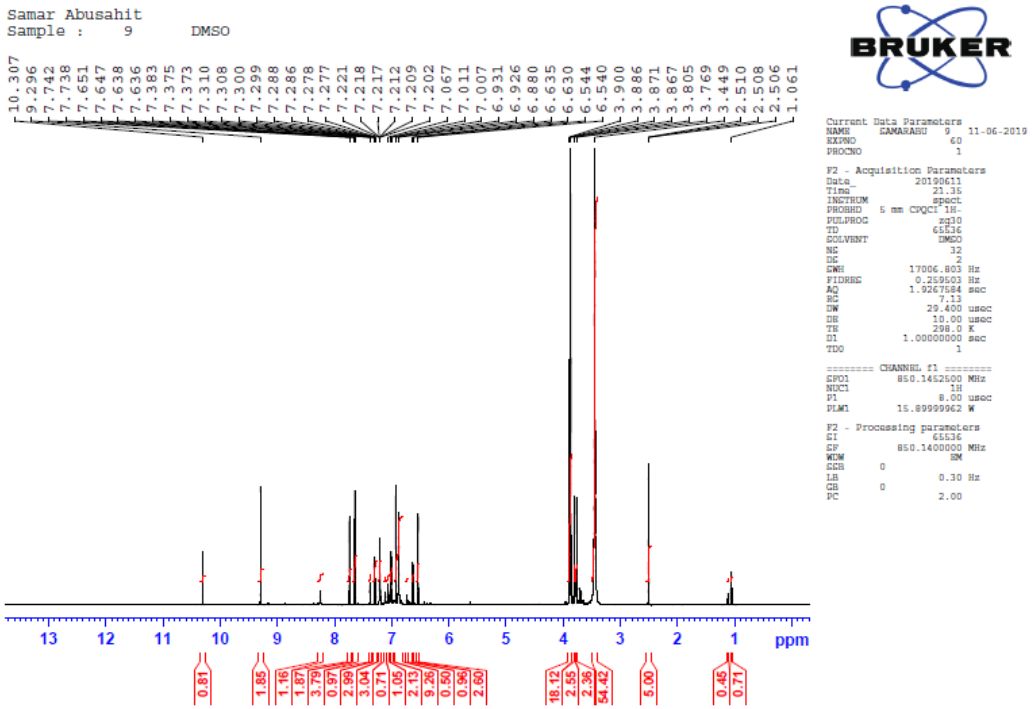

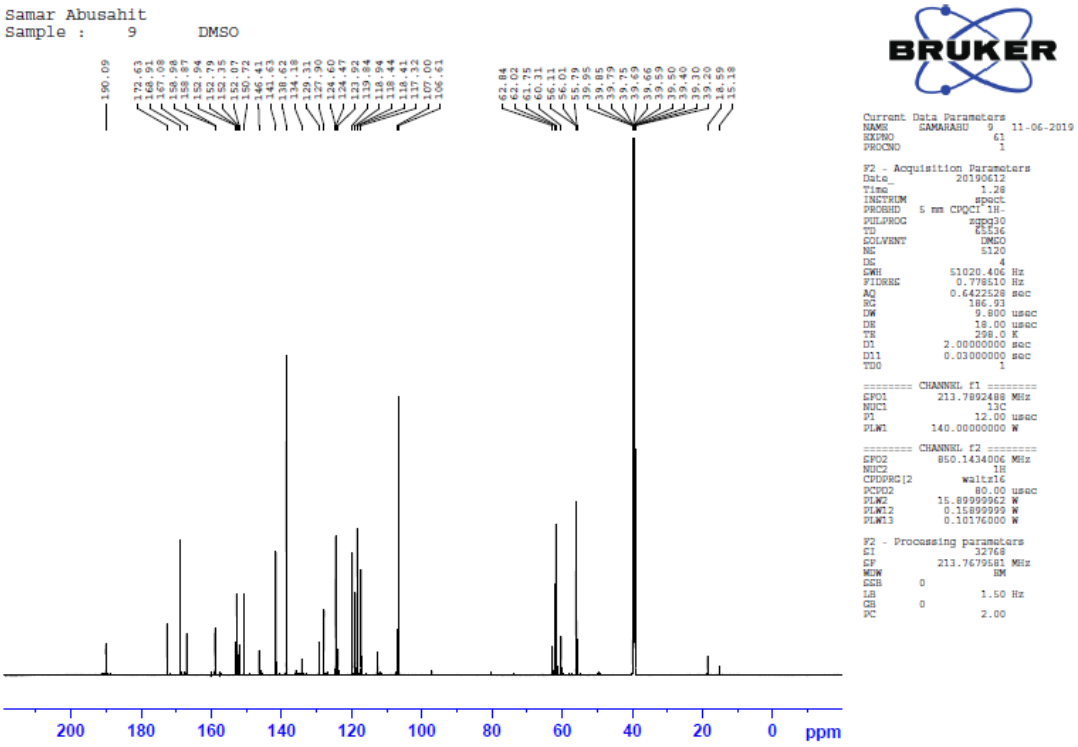

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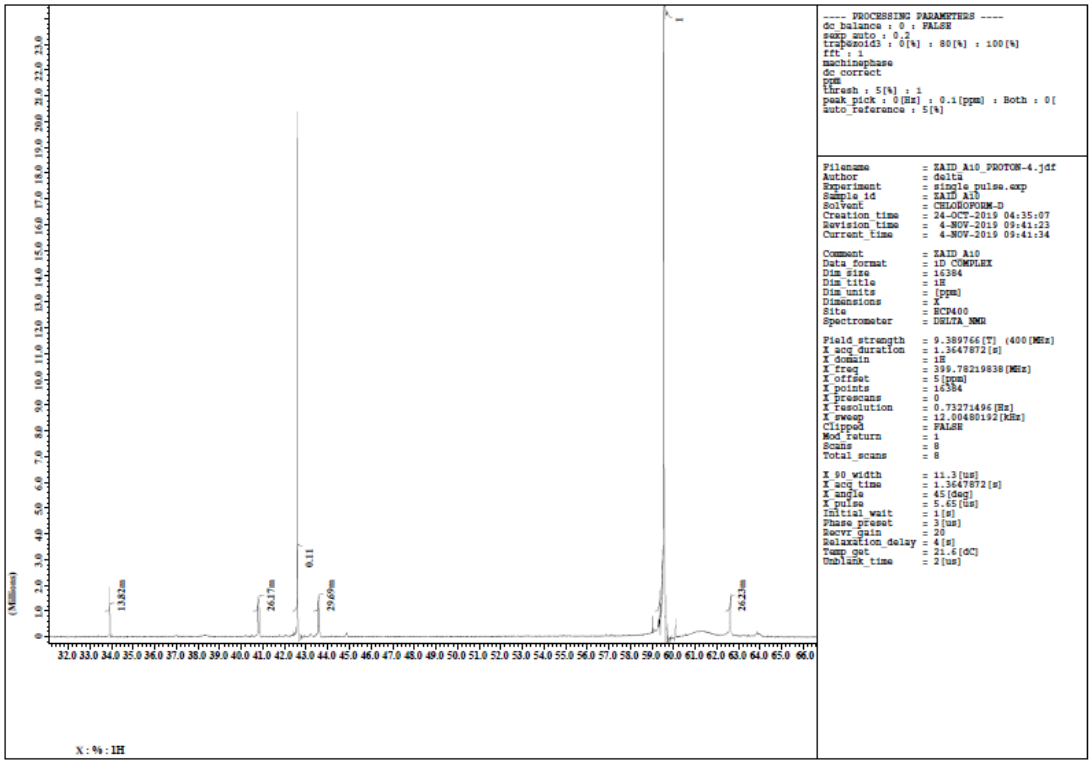

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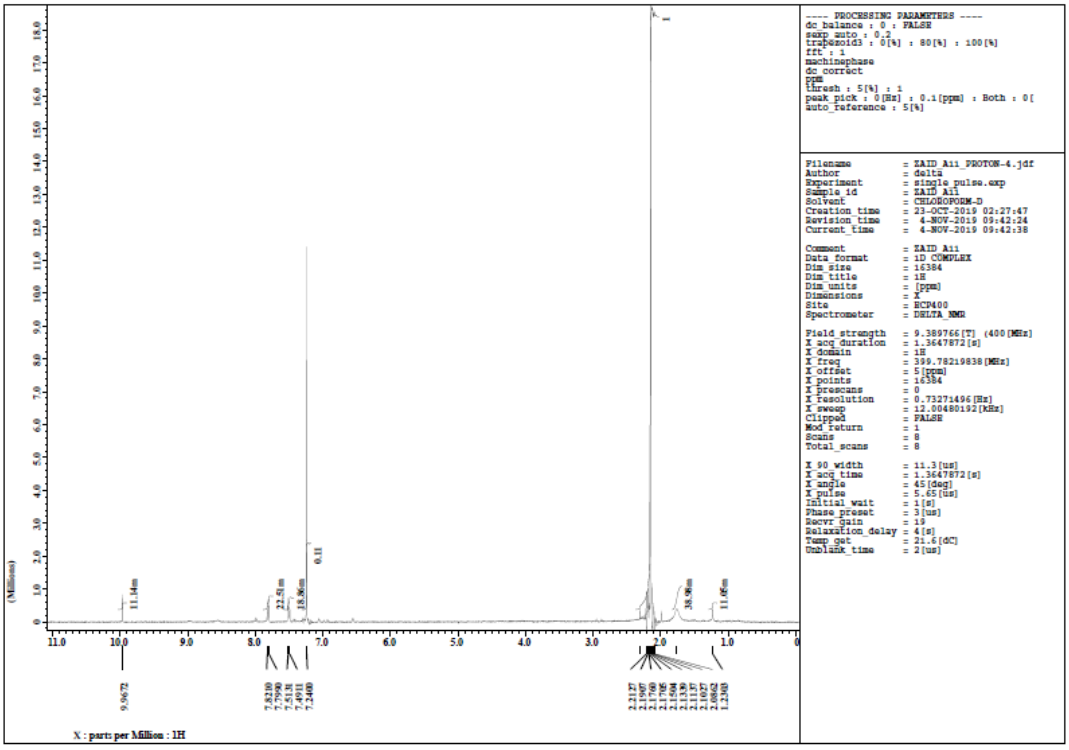

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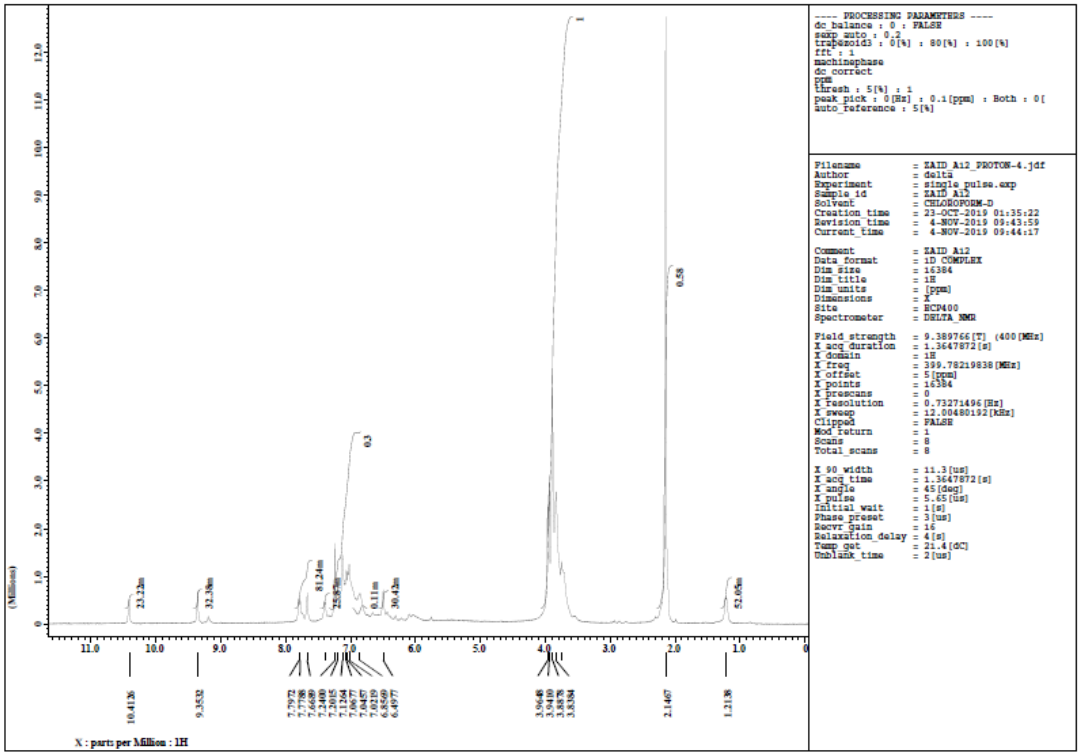

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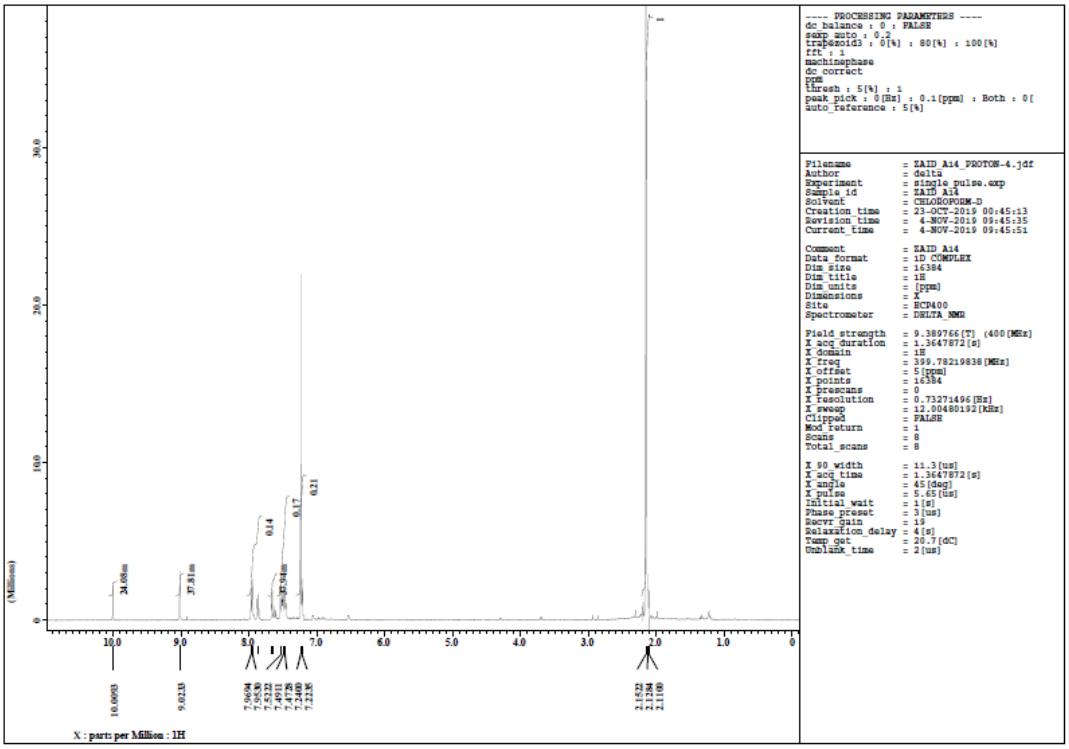

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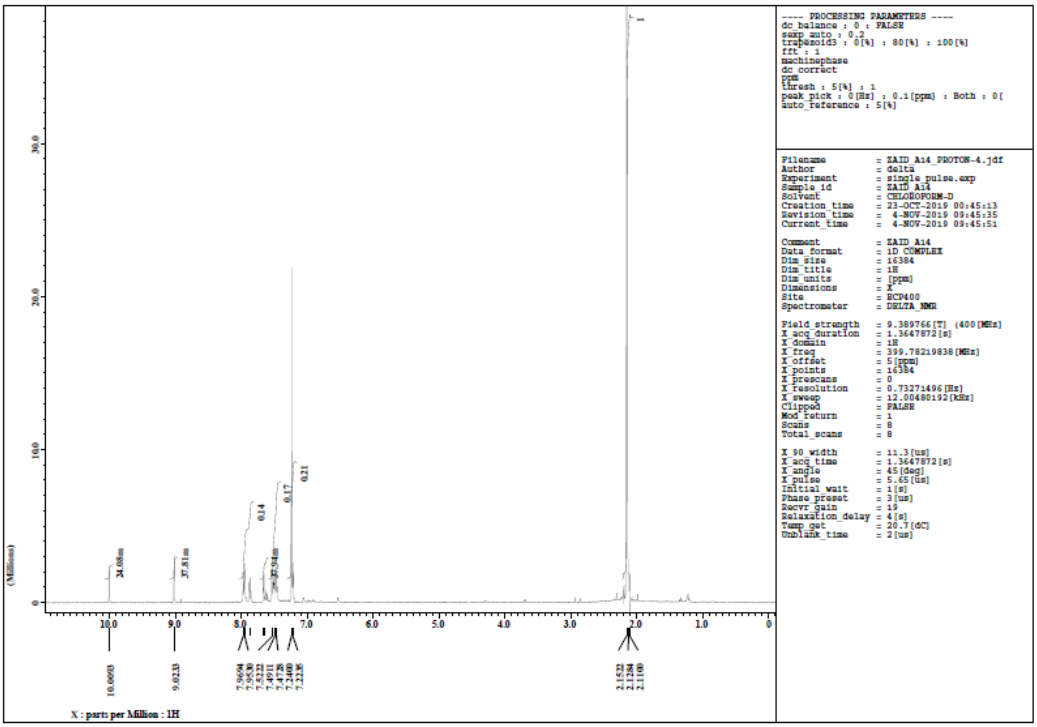

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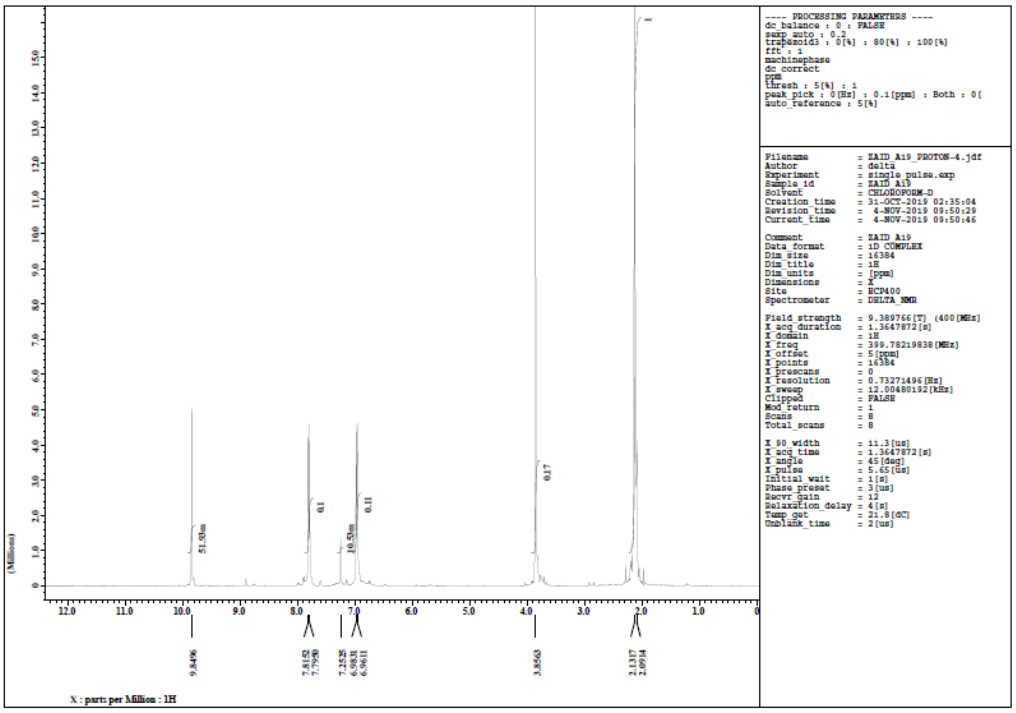

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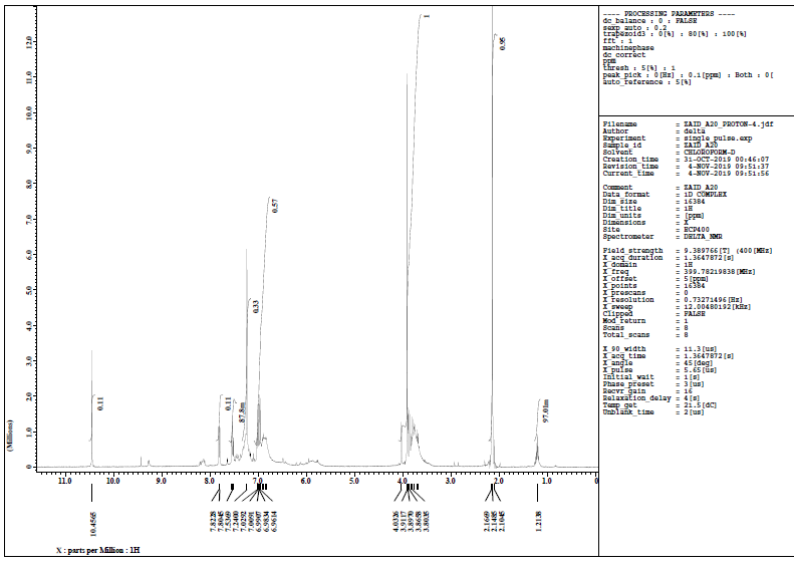

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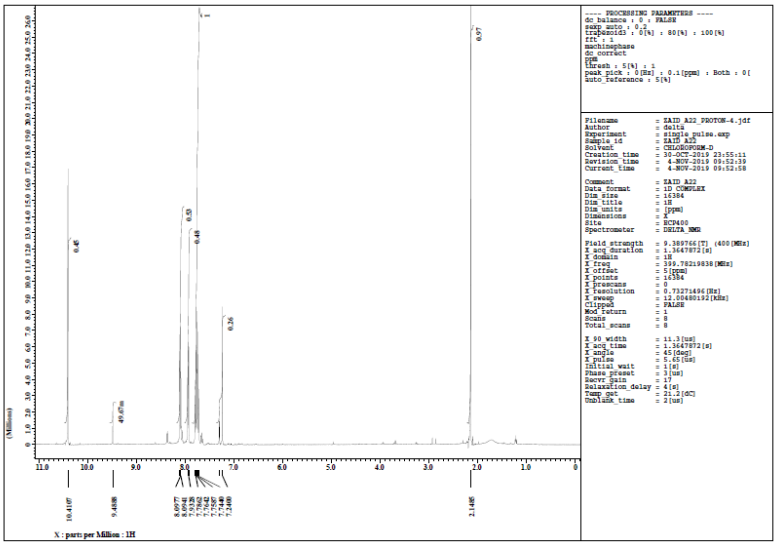

Sample 23 = compound 13