Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis, solid state self-assembly driven by antiparallel π···π stacking and {···H–C–C–F}$_2$ dimer synthons, and *in vitro* acetyl cholinesterase inhibition activity of phenoxy pendant isatins

Saba Mehreen[a], Aman Ullah[b], Humaira Nadeem[c], Necmi Dege[d], Muhammad Moazzam Naseer[a,*]

[a] *Department of Chemistry, Quaid-i- Azam University, Islamabad, 45320, Pakistan*
[b] *Department of Agricultural, Food and Nutritional Science, 4-10 Agriculture/Forestry Centre, University of Alberta, Edmonton, AB, T6G 2P5, Canada*
[c]*Department of Pharmaceutical Chemistry, Riphah Institute of Pharmaceutical Sciences, Riphah International University, G-7/4, Islamabad, Pakistan*
[d]*Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139, Kurupelit, Samsun, Turkey.*

*Corresponding author: moazzam@qau.edu.pk (M. M. N.)

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1)- Experimental

1.1 General Information

Anhydrous Na_2SO_4 and anhydrous K_2CO_3 were purchased from Fluka (Switzerland). Isatin, 5-chloro isatin, 5-bromo isatin, phenol, 4-chloro phenol, 4-bromo phenol, 4-floro phenol and 1,2-dibromo ethane were products of Aldrich (Canada). Acetonitrile and dimethyl formamide were obtained from Lab-Scan (Poland). All enzymes were purchased from Sigma-aldrich and used without further purification. These are AChE*Electric eel* (Sigma-Aldrich GmbH, USA), BChE equine serum lyophilized (Sigma-Aldrich GmbH, USA), substrates: acetylthiocholine iodide (Sigma-Aldrich, U.K.), butyrylthiocholineiodide (Sigma-Aldrich, Switzerland), DTNB (5,5-dithio-bis-nitrobenzoic acid) (Sigma-Aldrich, Germany). Disodium hydrogenphosphate (Na_2HPO_4) was of extra pure analytical grade from Merck Group (Darmstadt, Germany) were used. All the reagents used were of analytical reagent grade, while commercial solvents were distilled before use. Monitoring of reactions was carried out using precoated silica gel-60 F_{254} TLC plates, purchased from Merck (Germany). Melting points of reported compounds were recorded in open capillaries on Gallenkamp (MP-D) melting point apparatus and are reported as such. Bruker Avance (300 MHz) NMR spectrometer was engaged to record ^1H and ^{13}C-NMR spectra using $CDCl_3$ as solvent and TMS as internal reference. 96 well plate microplate photometer (Thermoscientific, multiskan FC, China) was employed for measuring absorbances for acetylcholinesterase assay.

1.2 Single crystal X-ray analysis

X-ray single crystal data was collected by using MoKa (l = 0.71073 Å) radiation on a STOE IPDS 2 diffractometer equipped with an STOE image plate (34 cm diameter) area detector, and a 2-circle goniometer. Data collection, data reduction, and structure solution/refinement were carried out using the software package X-RED32; Stoe & Cie, 2002. The structure was solved by direct method and refined in a routine manner (SHELXL)[1, 2]. The details of the X-ray crystal data and the structure solution as well as the refinement are given in Table S1.

1.3 Acetylcholinesterase Assay

The AChE inhibition activity was performed with a slight modification of the Ellman's method.[3] Total volume of the reaction mixture was 100 µL. It contained 60 µL Na_2HPO_4 buffer with

concentration of 50 mM having pH 7.7. 10 µL test compound (0.5 mM/well) was added, followed by the addition of 10 µL (0.005 unit/well) enzyme. The contents were mixed and pre-read at 405 nm. Then, contents were preincubated for 10 min at 37 °C. The reaction was initiated by the addition of 10 µL of 0.5 mM/well substrate (acetylthiocholine iodide), followed by the addition of 10 µL DTNB (0.5 mM/well). After 30 min of incubation at 37 °C, absorbance was measured at 405 nm using 96 well plate microplate photometer (Thermoscientific, multiskan FC, China). All experiments were carried out with their respective controls in triplicate. Donepezil (0.5 mM/well) was used as a positive control. Percentage inhibition was calculated as follows:

$$Inhibition\ (\%) = \frac{Control\ - Test}{Control} \times 100$$

Where, Control is the total enzyme activity without inhibitor and Test is the enzyme activity in the presence of test compound. IC_{50} values (concentration at which there is 50 % enzyme catalyzed reaction) were calculated using EZ–Fit Enzyme kinetics software (Perrella Scientific Inc. Amherst, USA).

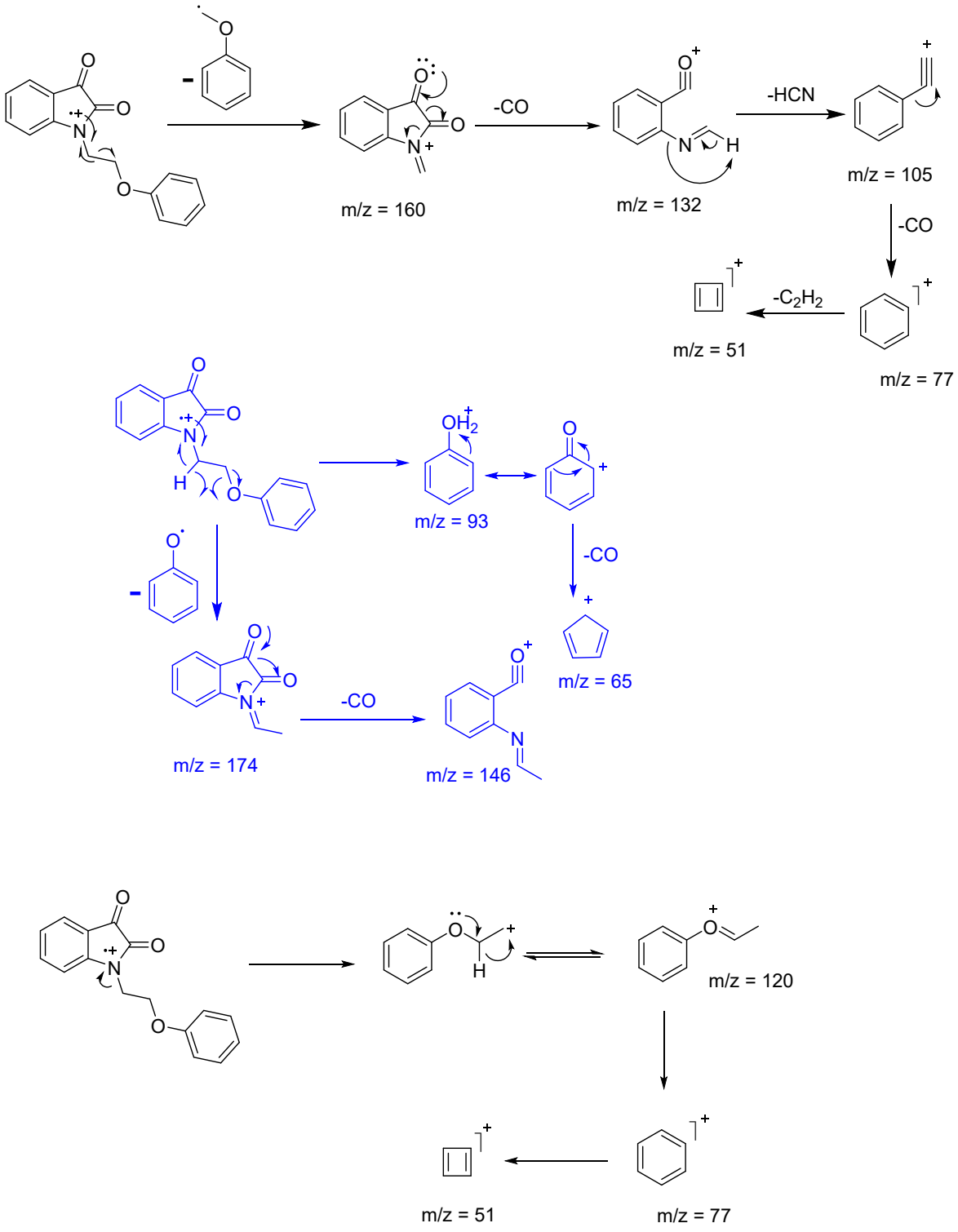


Figure S1: Representative fragmentation patterns of compound **PI1**

Table S1. X-ray crystallographic data of of phenoxy pendant isatin **PI4**

Crystal data	**PI4**
CCDC	2090877
Chemical formula	$C_{16}H_{12}FNO_3$
M_r	285.27
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	296
a, b, c (Å)	6.7305 (9), 8.9170 (12), 11.7682 (15)
β (°)	82.956 (11), 78.846 (11), 88.804 (11)
V (Å^3)	687.70 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.69 × 0.59 × 0.42
Data collection	
Diffractometer	STOE *IPDS* 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.922, 0.972
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6252, 2687, 2030
R_{int}	0.044
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.104, 1.00
No. of reflections	2687
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.16, -0.21

2)- **Table S2:** Acetyl cholinesterase inhibition (%) of phenoxy pendant isatin **PI1-12**

Compd. no.	Concentration	% Inhibition
P1-1	10µL	79.48
	5µL	69.65
	2.5µL	46.76
P1-2	10µL	83.75
	5µL	53.24
	2.5µL	27.13
P1-4	10µL	78.41
	5µL	57.65
	2.5µL	26.93
P1-6	10µL	81.40
	5µL	35.67
	2.5µL	14
P1-9	10µL	60.51
	5µL	36.83
	2.5µL	22.85
P1-10	10µL	64.68
	5µL	49.27
	2.5µL	39.73
P1-11	10µL	78.30
	5µL	34.88
	2.5µL	19.38
P1-12	10µL	55.67
	5µL	40.78
	2.5µL	18.21
Positive control	10µL	100
	5µL	70.27
	2.5µL	44.71

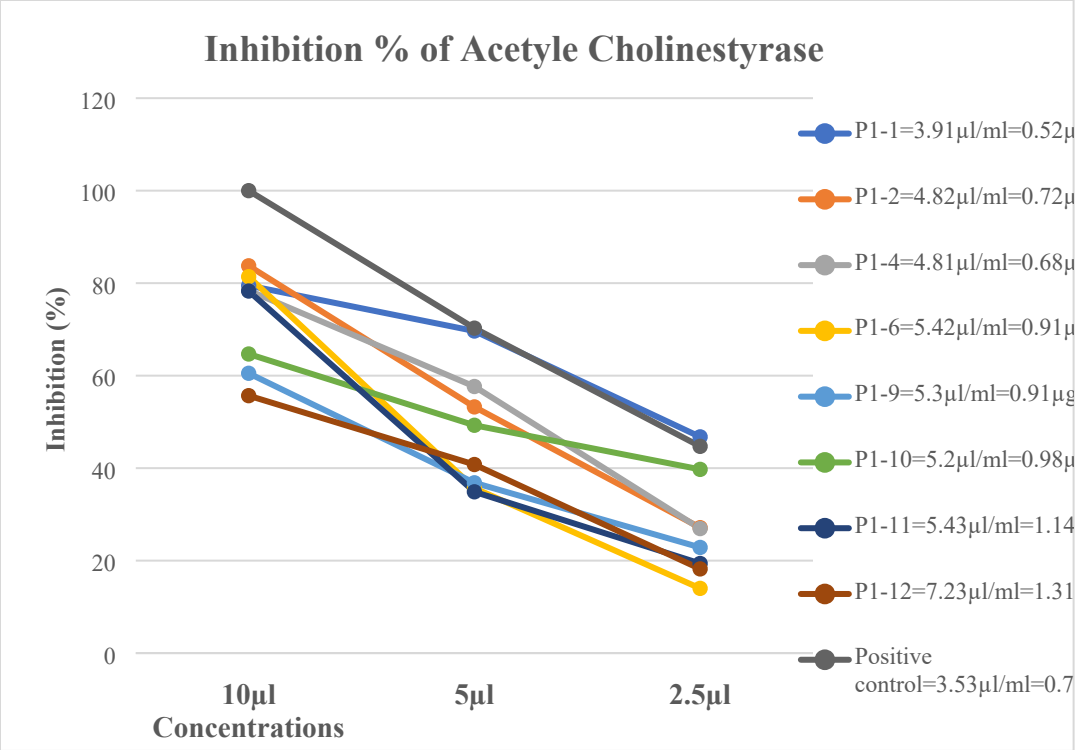


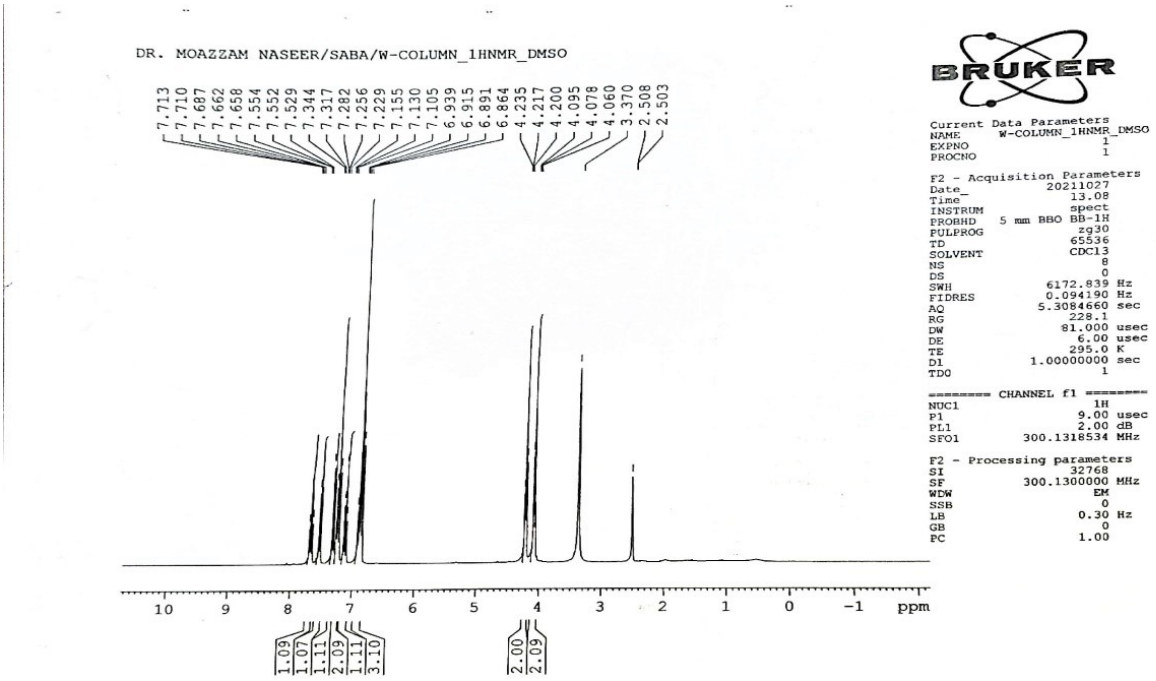
Figure S2: Graph between concentration (µg/mL) verses % inhibition

References

1. G. M. Sheldrick, *Acta Crystallographica Section C: Structural Chemistry*, 2015, **71**, 3-8.
2. C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. Streek, *Journal of Applied Crystallography*, 2006, **39**, 453-457.
3. I. Silman and J. L. Sussman, *Current opinion in pharmacology*, 2005, **5**, 293-302.

Copies of ^{1}H-NMR,^{13}C-NMR and MS spectra of compounds (PI1-12)

^{1}H-NMR of PI1



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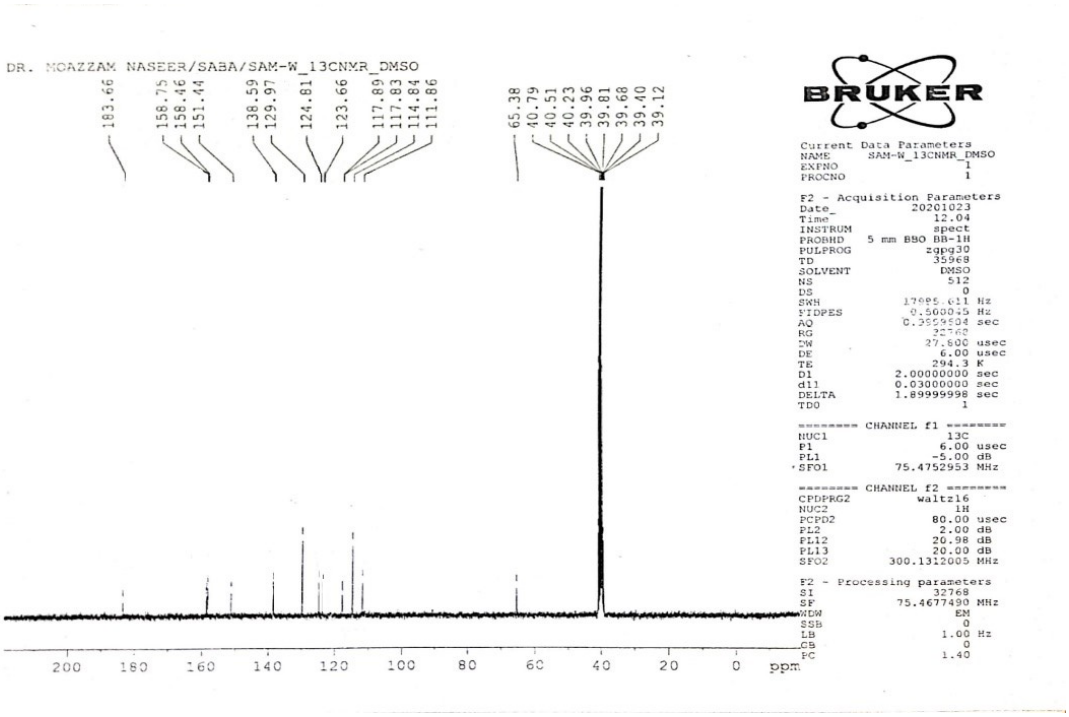
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117.89
117.83
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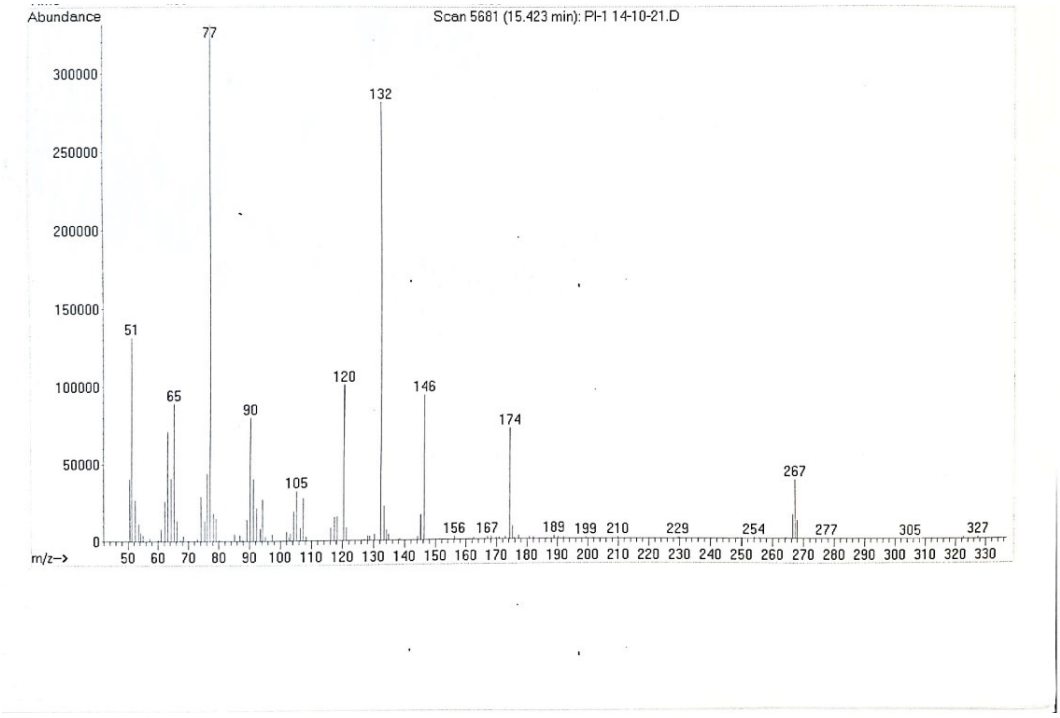
GC-MS of PI1



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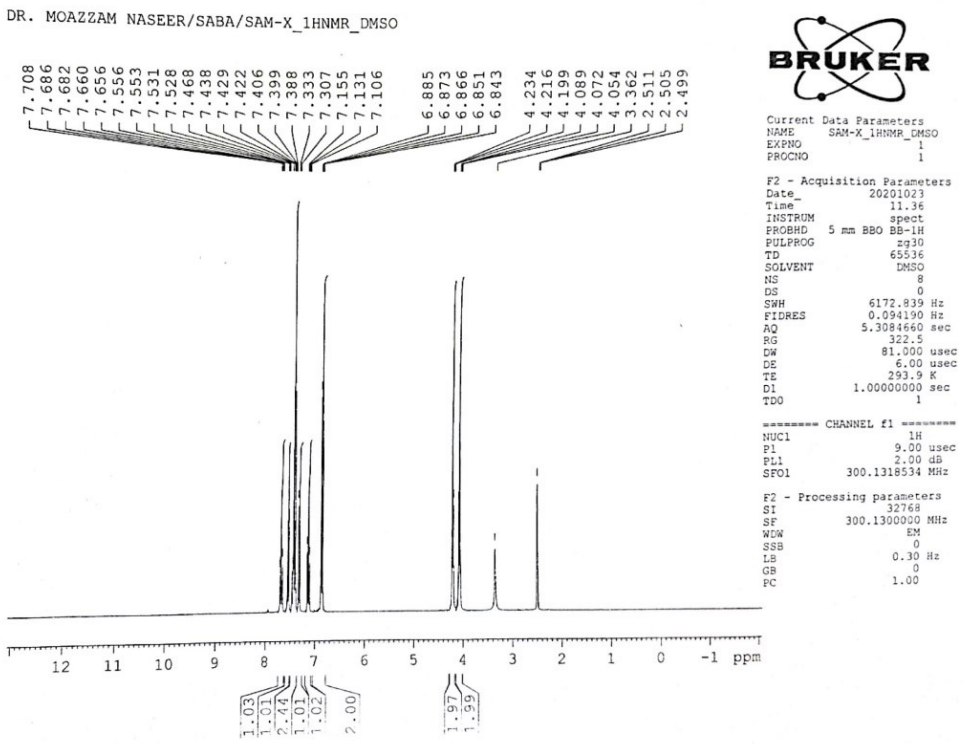

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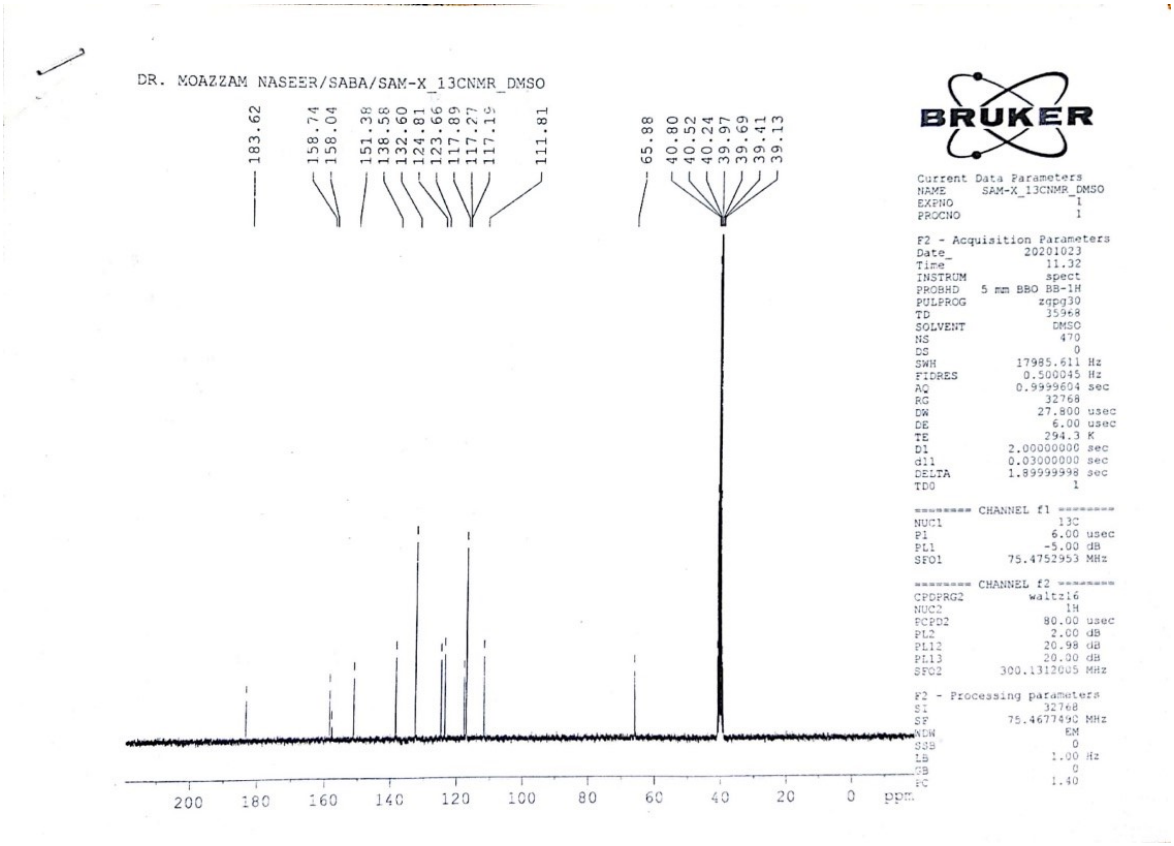
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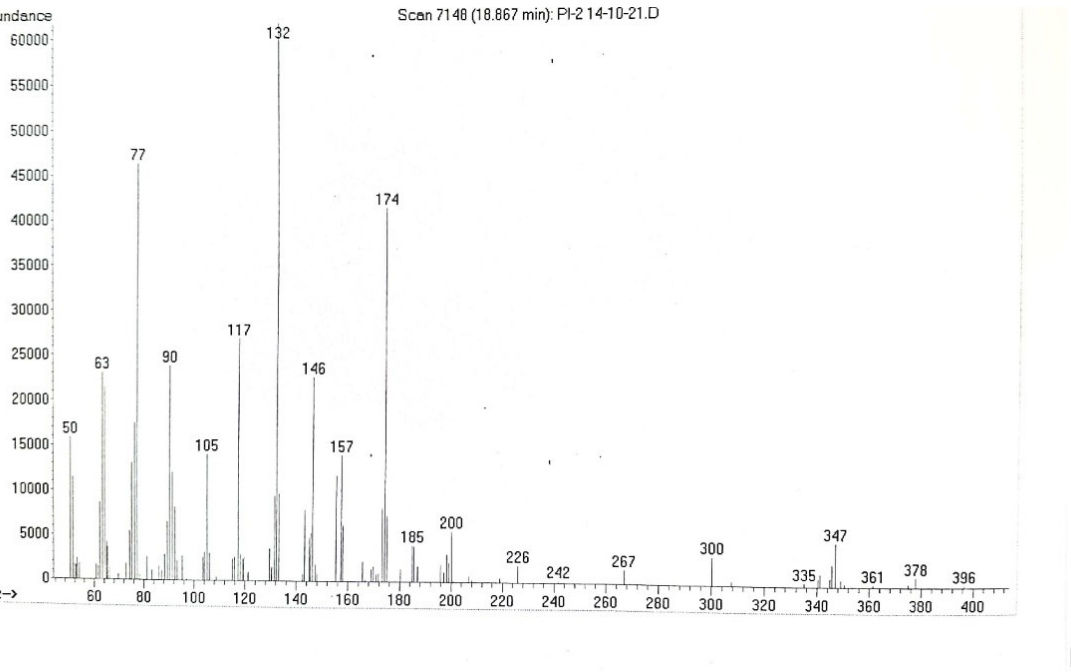

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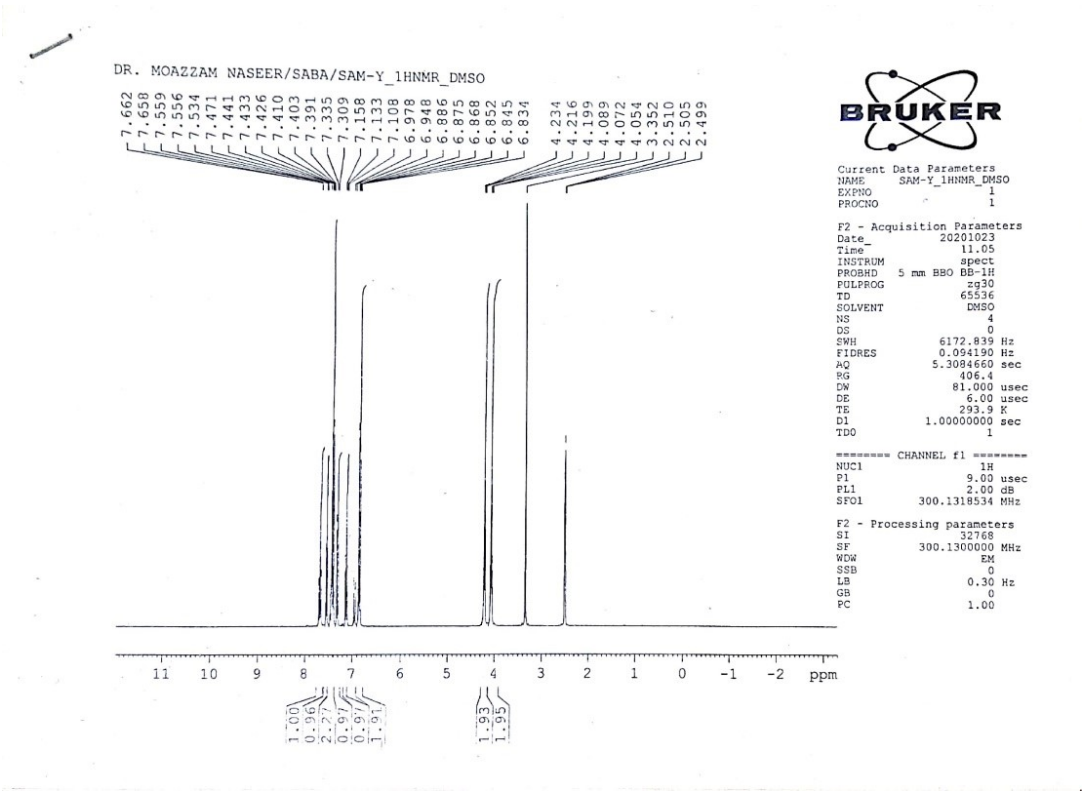

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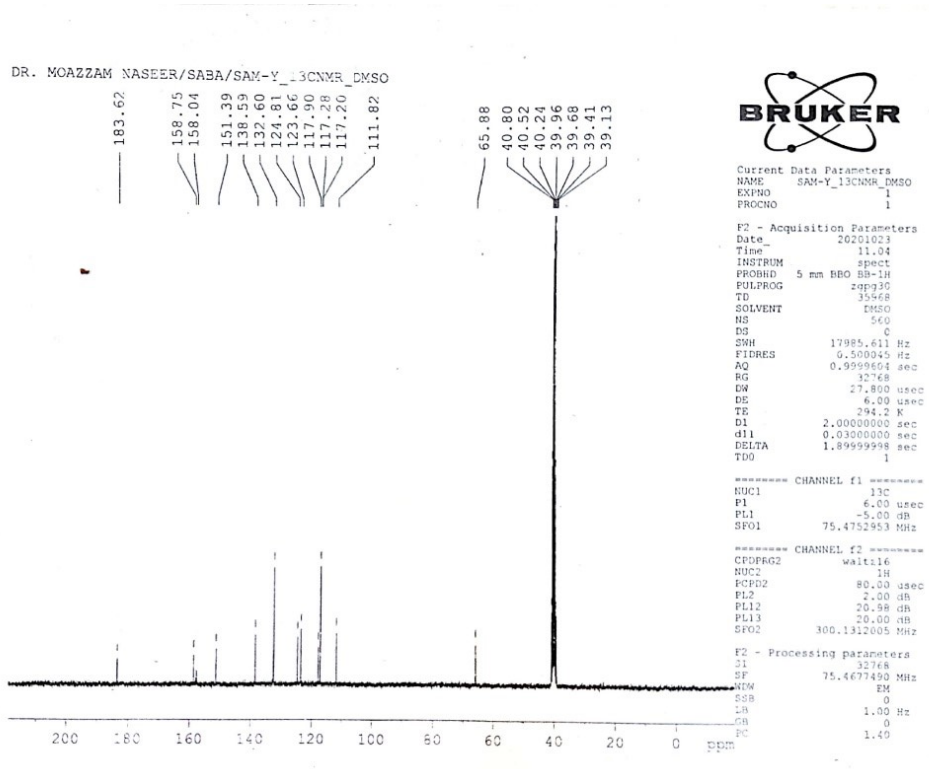
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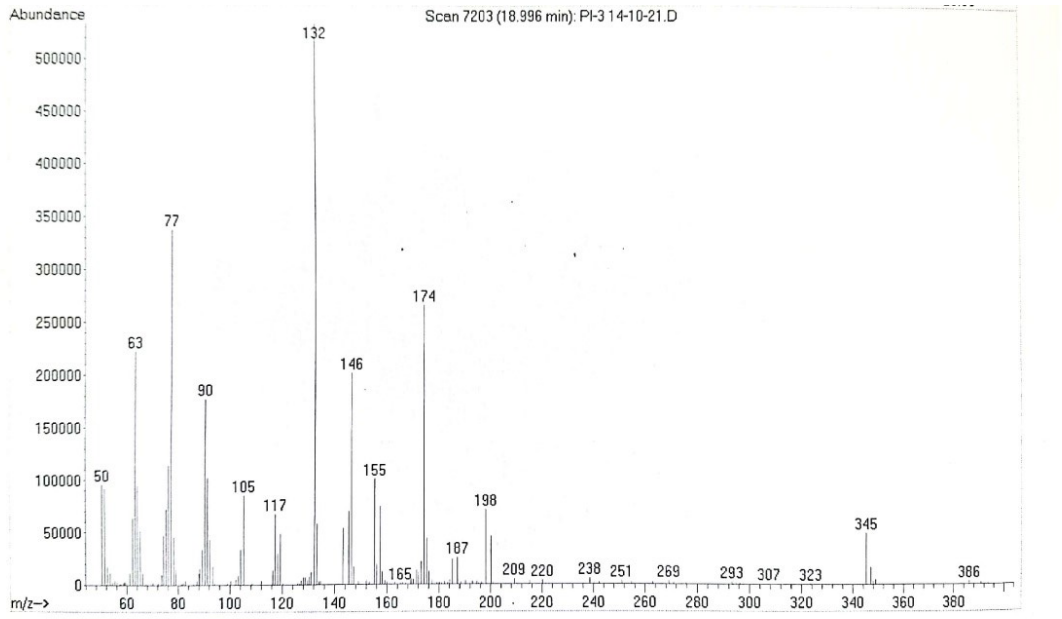

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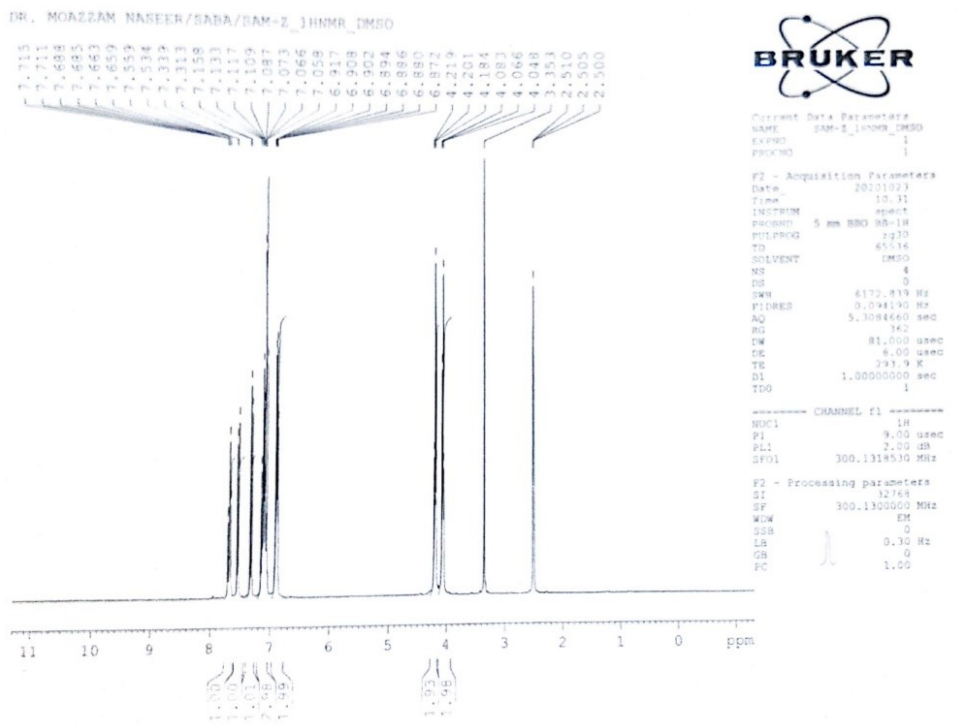

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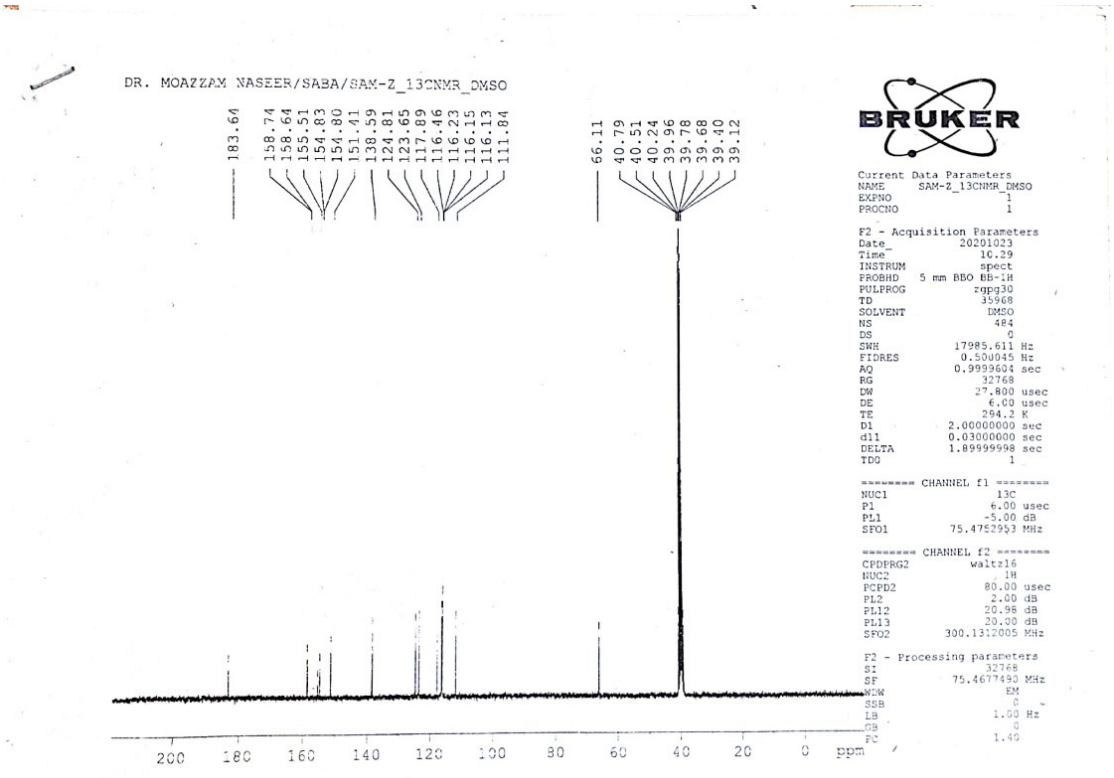
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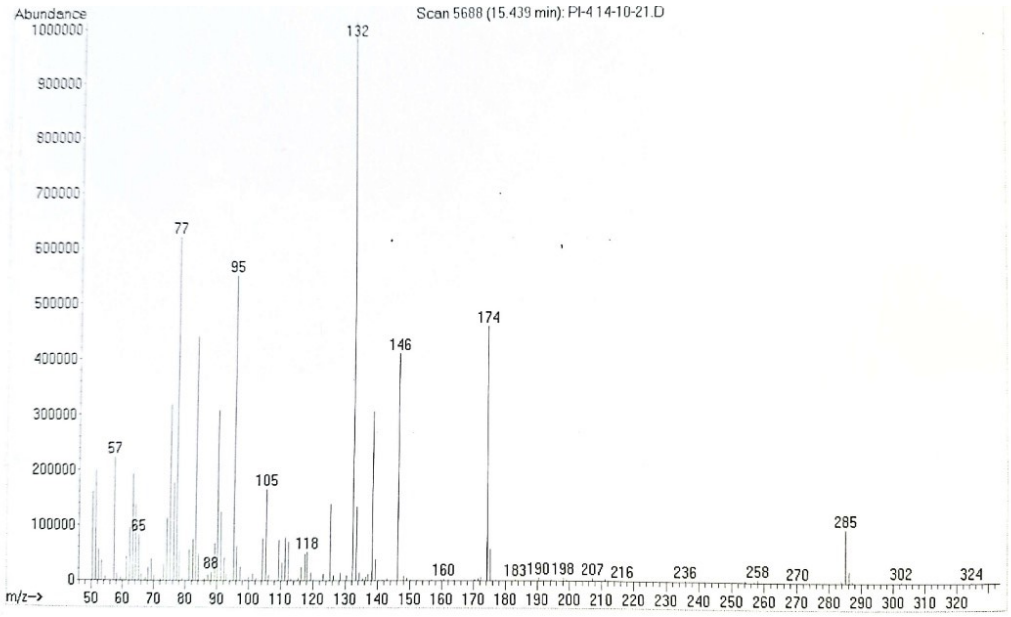

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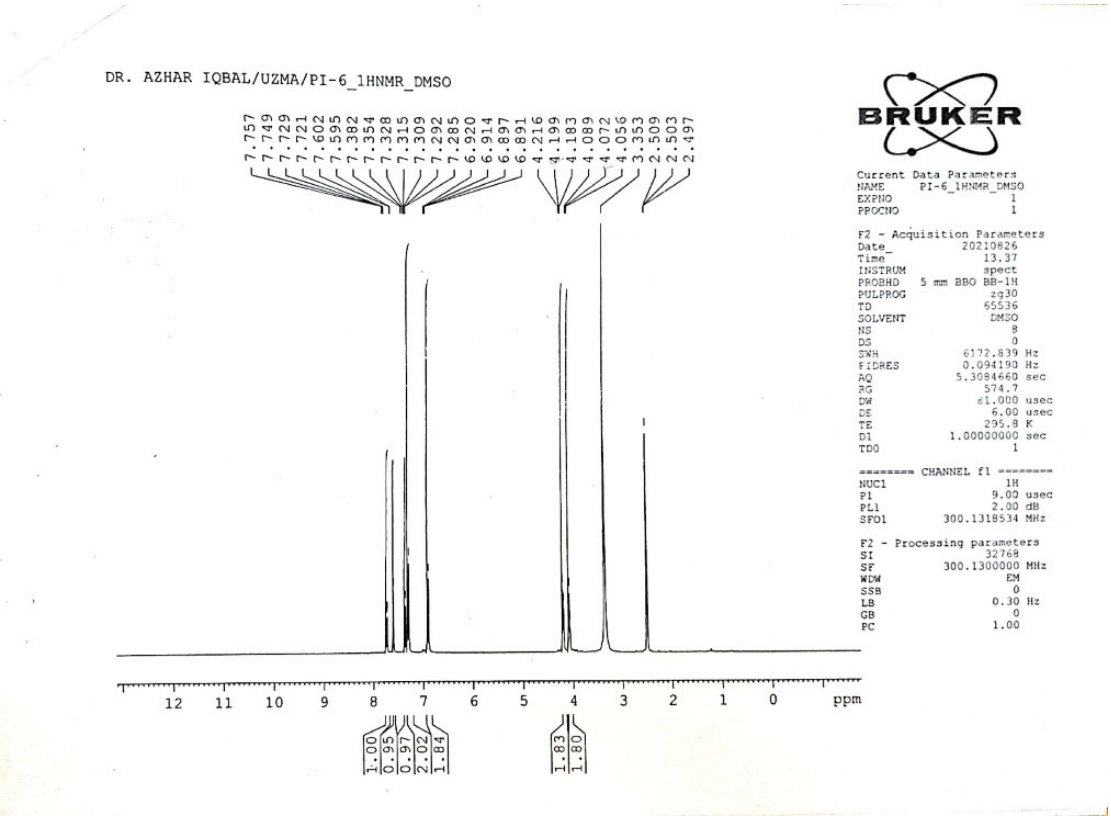

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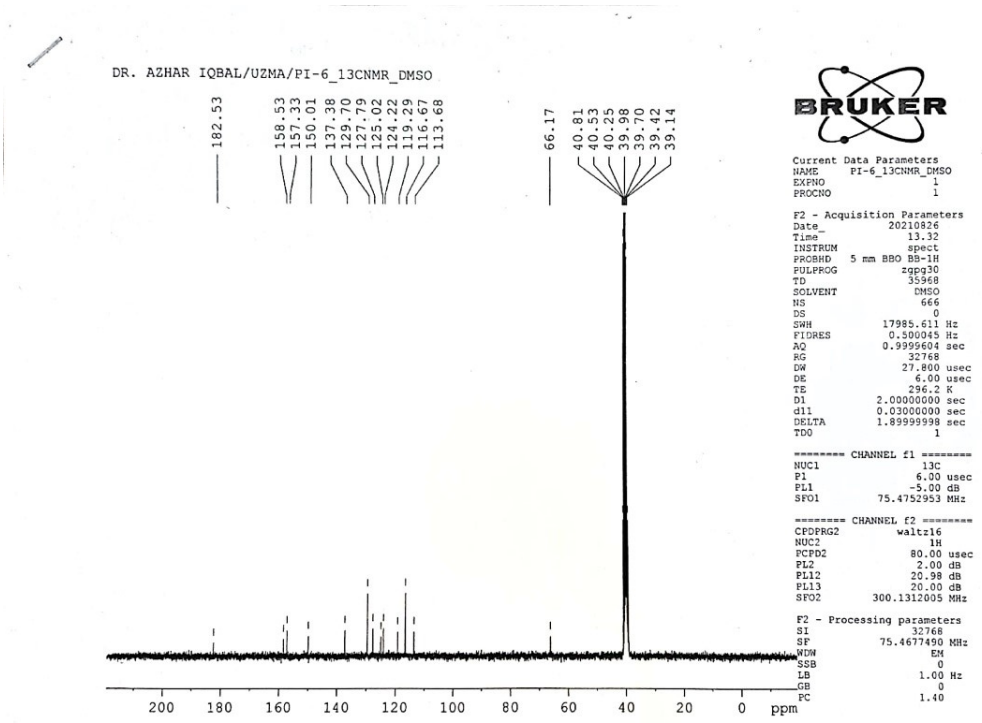
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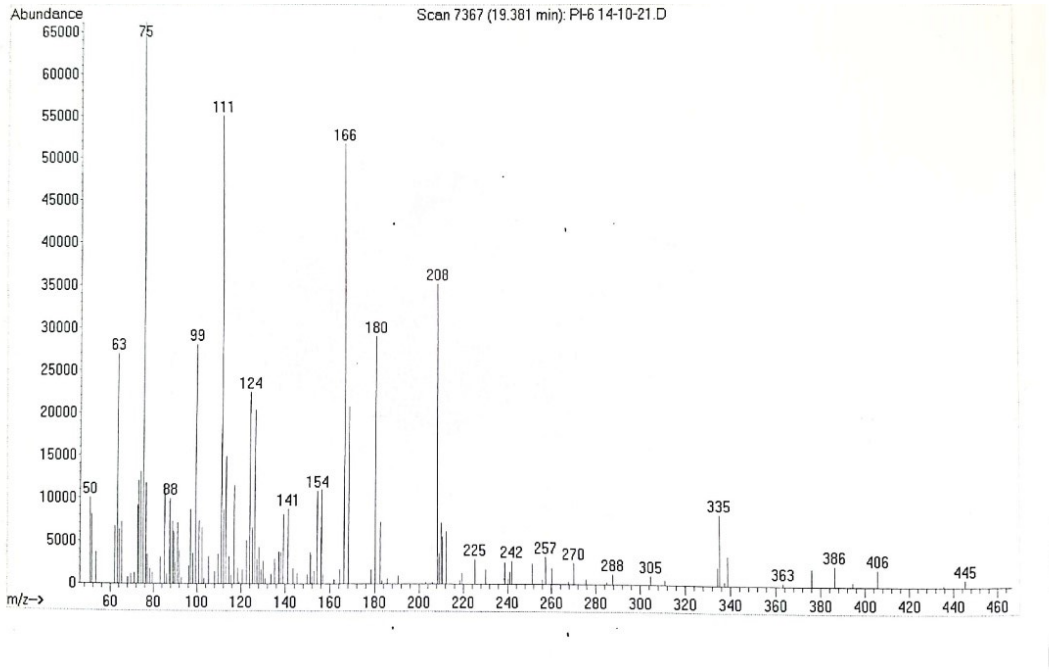

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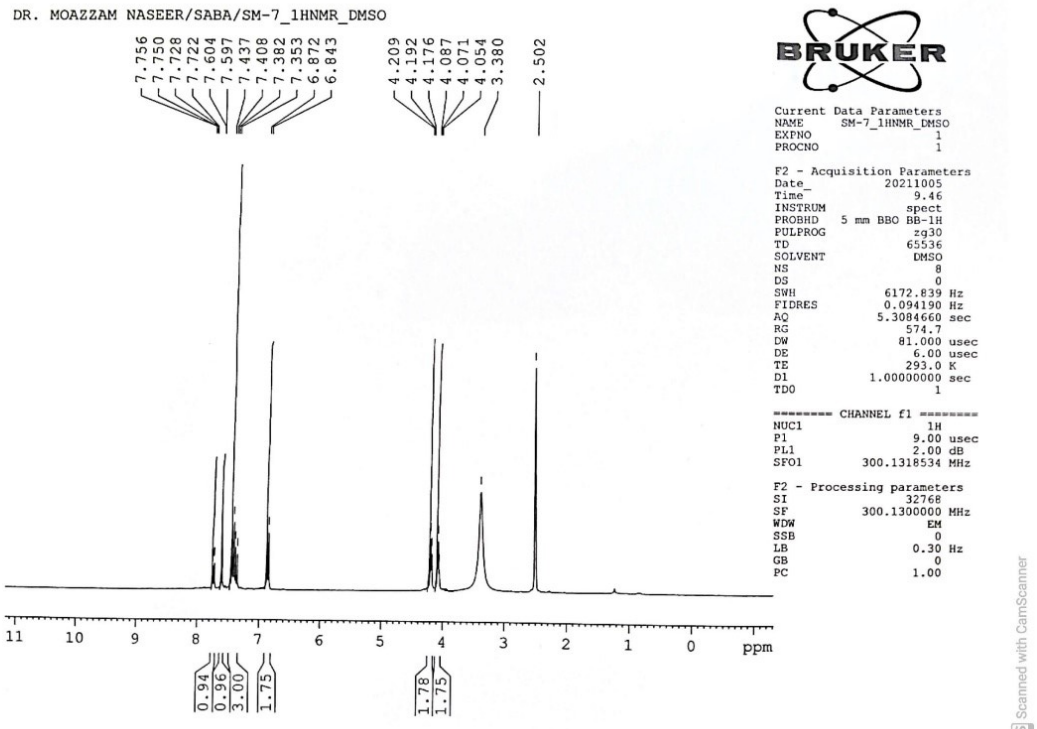

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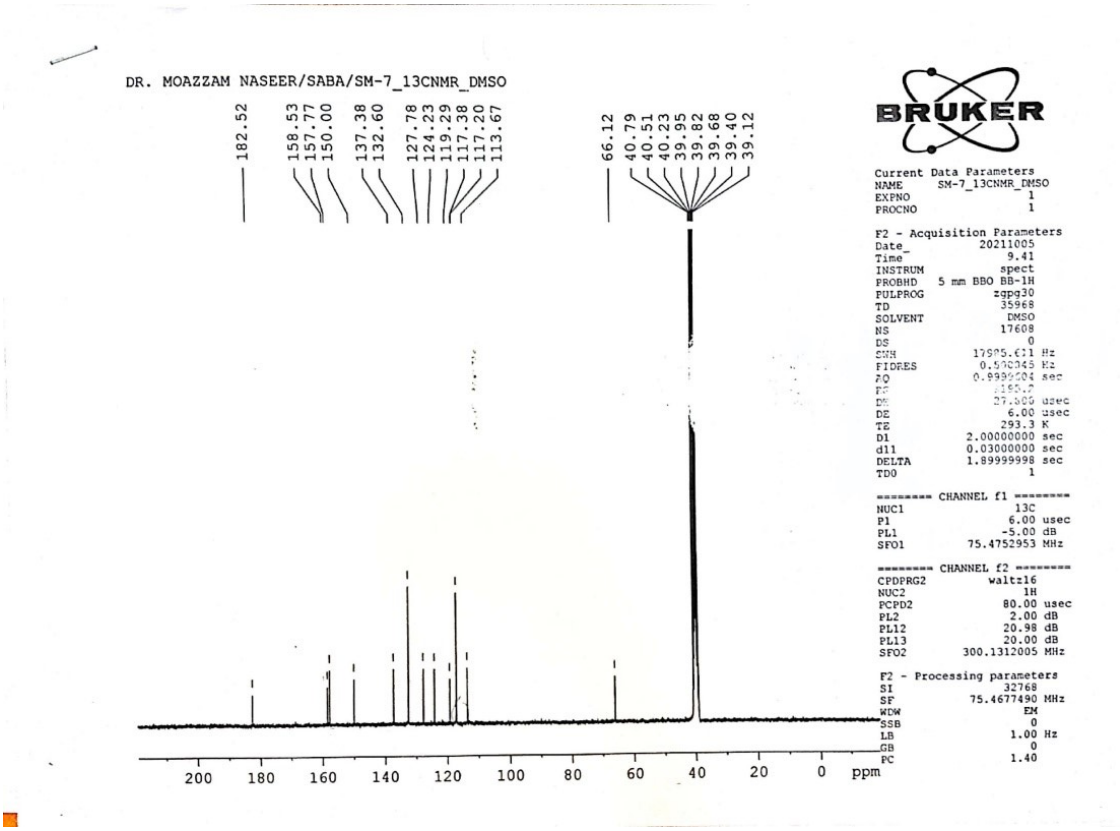
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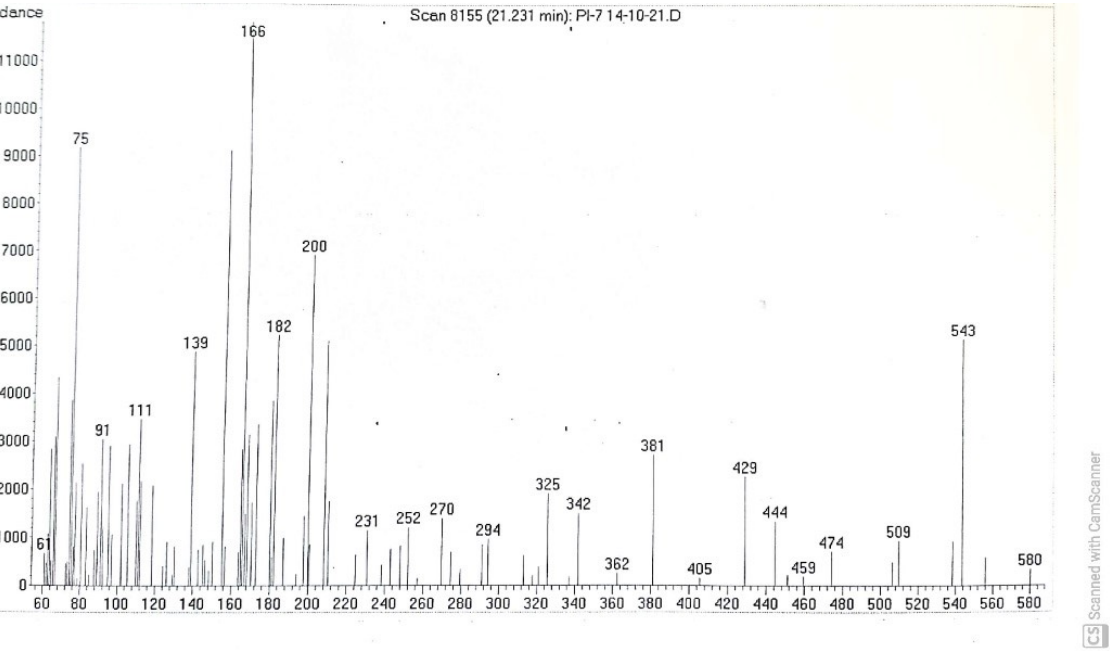
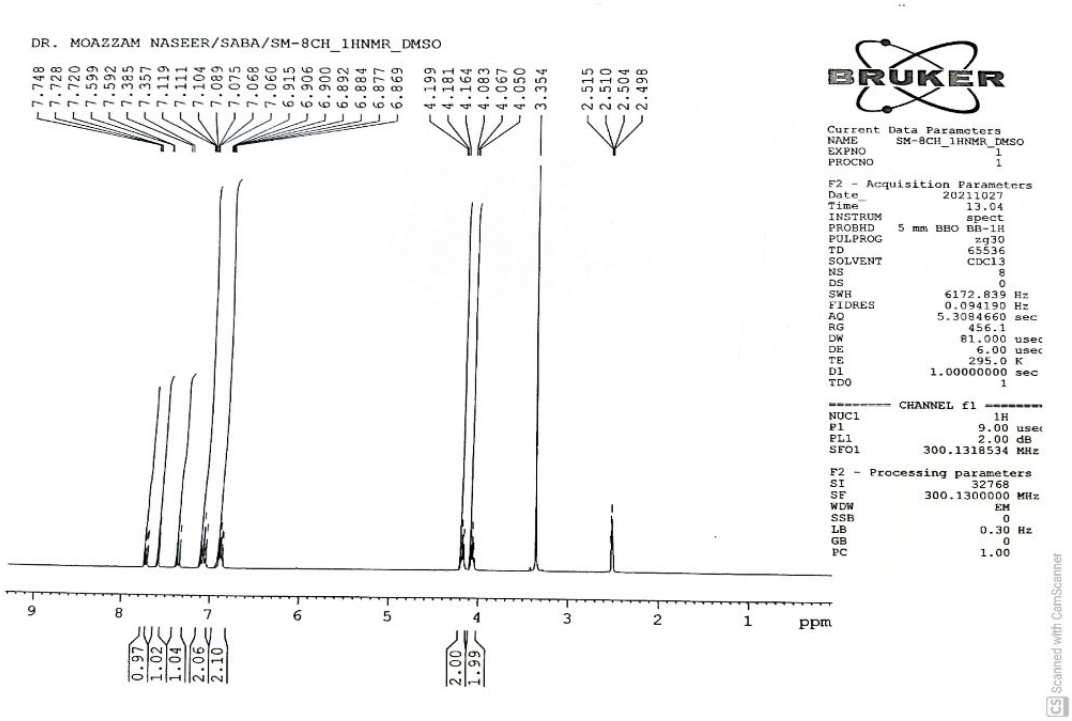
0
ppm
BRUKER
Current Data Parameters
NAME SM-7_13CNMR_DMSO
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211005
Time 9.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 35968
SOLVENT DMSO
NS 17608
DS 0
SWH 17985.611 Hz
FIDRES 0.500345 Hz
AQ 0.9999504 sec
RG 165.2
DW 27.809 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

GC-MS of PI7


Scan 8155 (21.231 min): PI-7 14-10-21.D
166
75
200
182
139
543
111
91
381
429
325
342
444
231
252
270
294
474
509
61
362
405
459
580

^{1}H-NMR of PI8



BRUKER

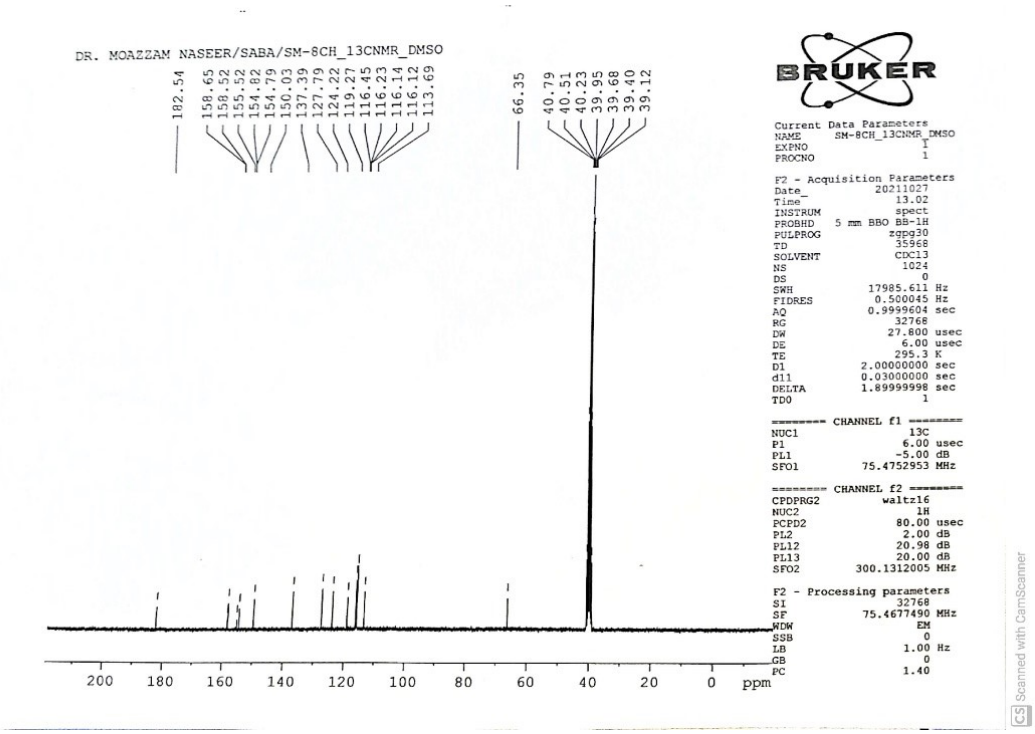
Current Data Parameters
NAME SM-8CH_1HNMR_DMSO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211027
Time 13.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

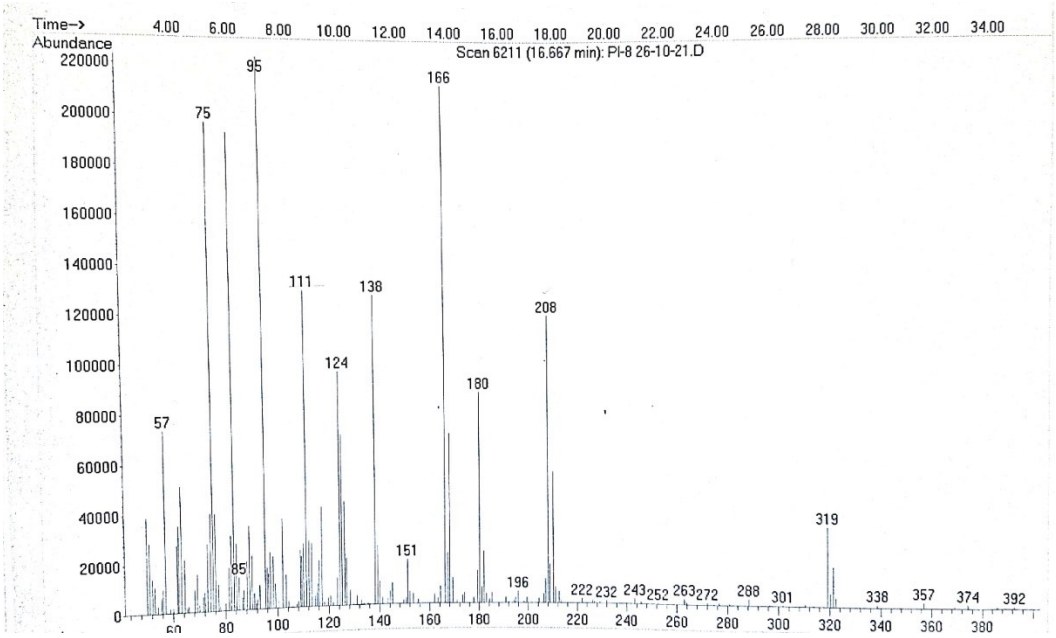
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

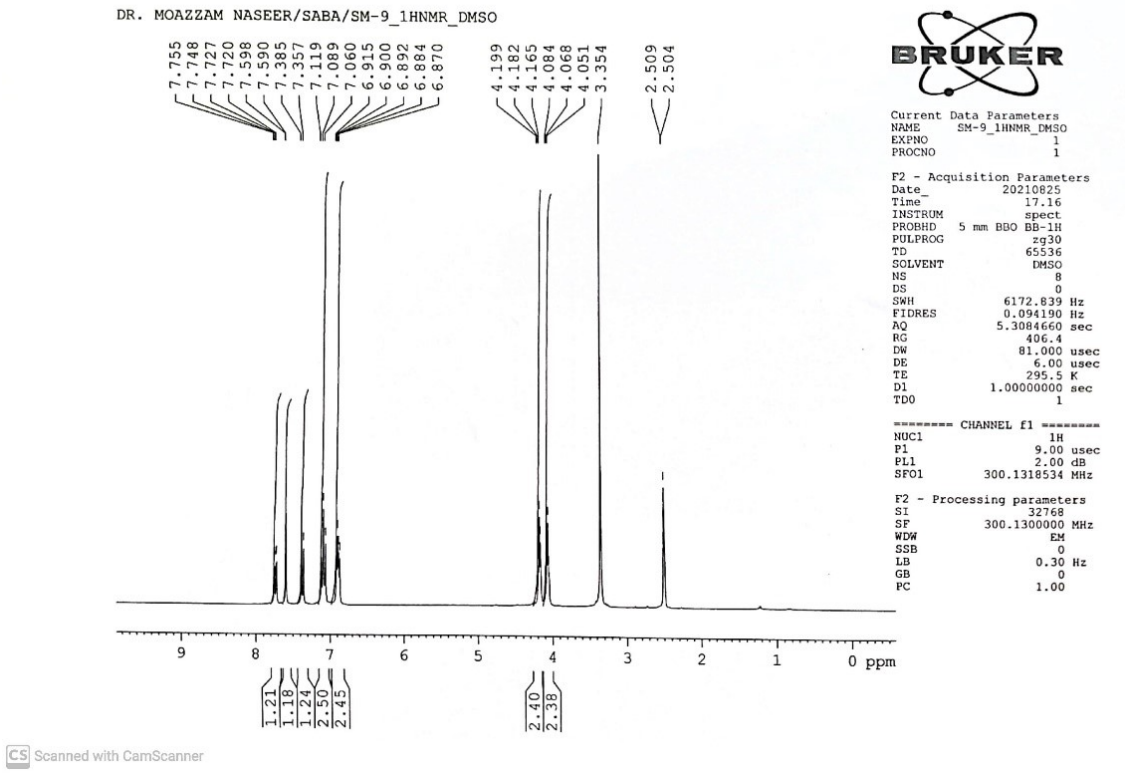
^{13}C-NMR of PI8



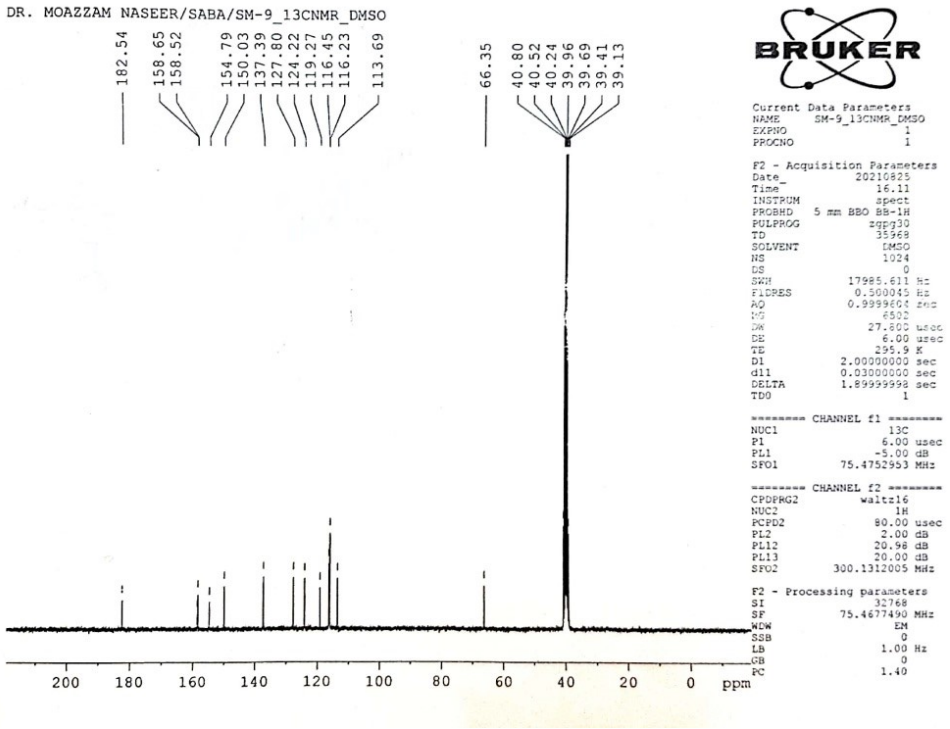
GC-MS of PI8



^{1}H-NMR of PI9



^{13}C-NMR of PI9



BRUKER

Current Data Parameters
NAME SM-9_13CNMR_DMSO
EXPNO 1
PROCNO 1

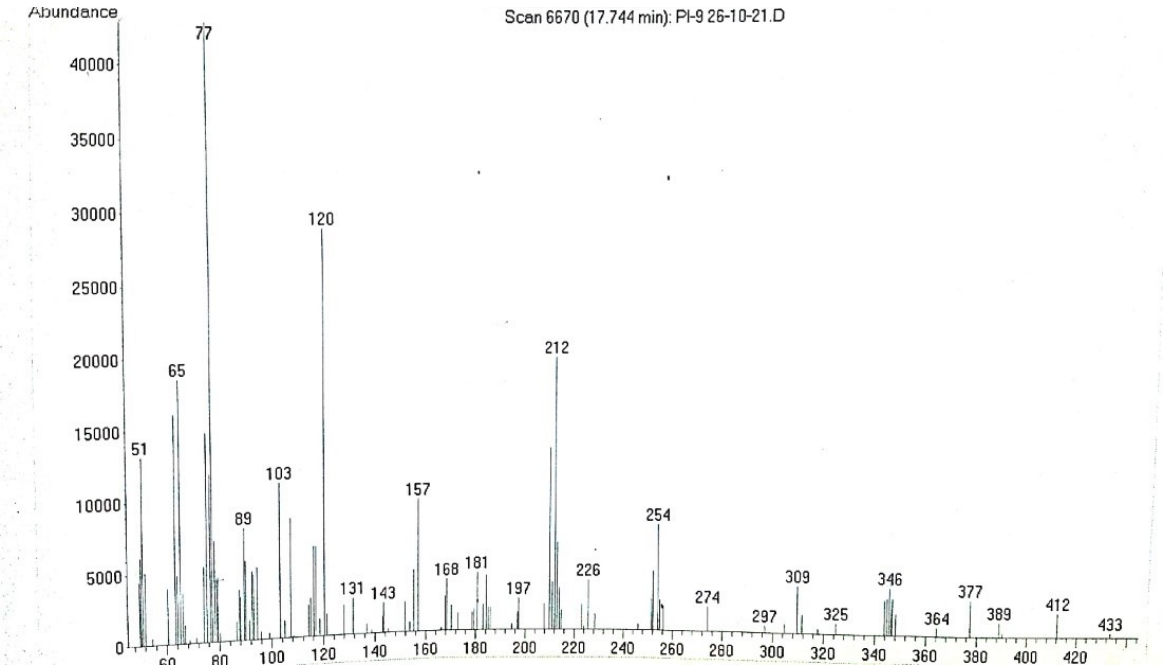
F2 - Acquisition Parameters
Date_ 20210825
Time 16.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 35968
SOLVENT DMSO
NS 1024
DS 0
SWH 17985.611 Hz
FIDRES 0.500045 Hz
AQ 0.9999607 sec
RG 4502
DW 27.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

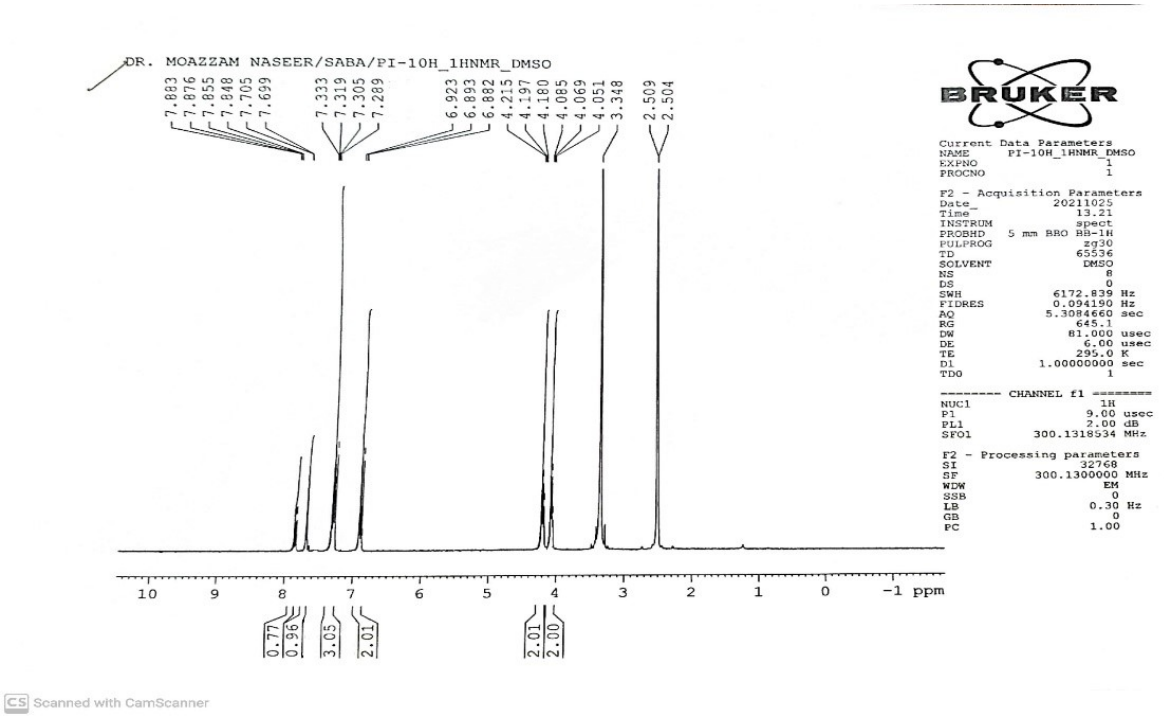
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

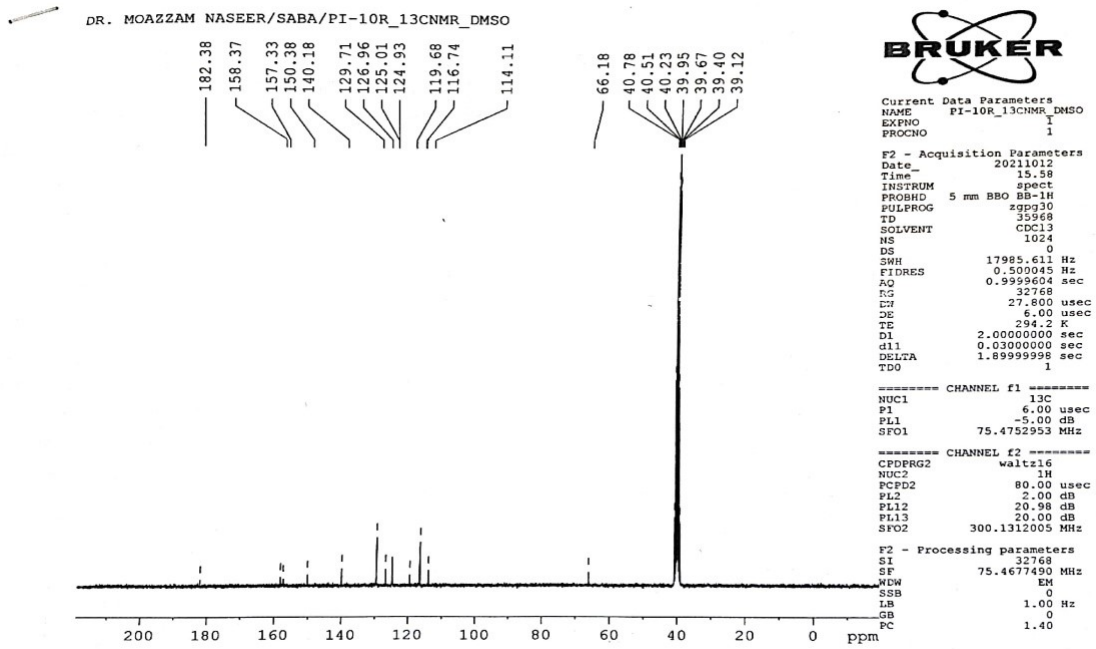
GC-MS of PI9



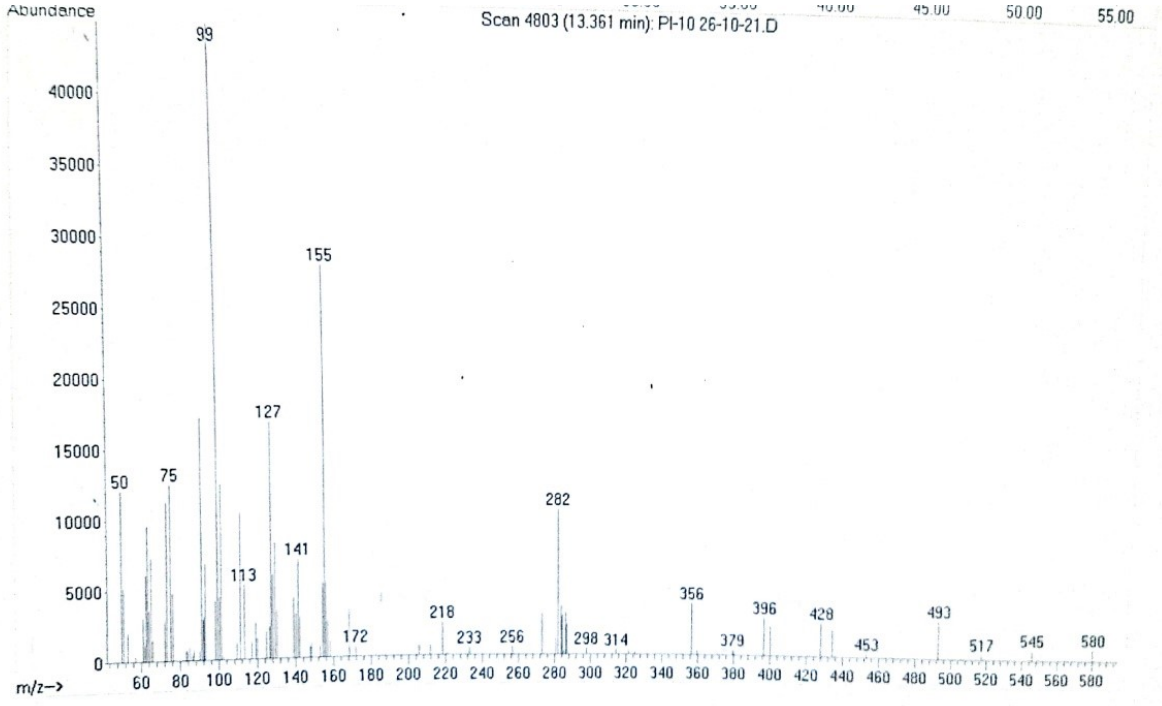
^{1}H-NMR of PI10



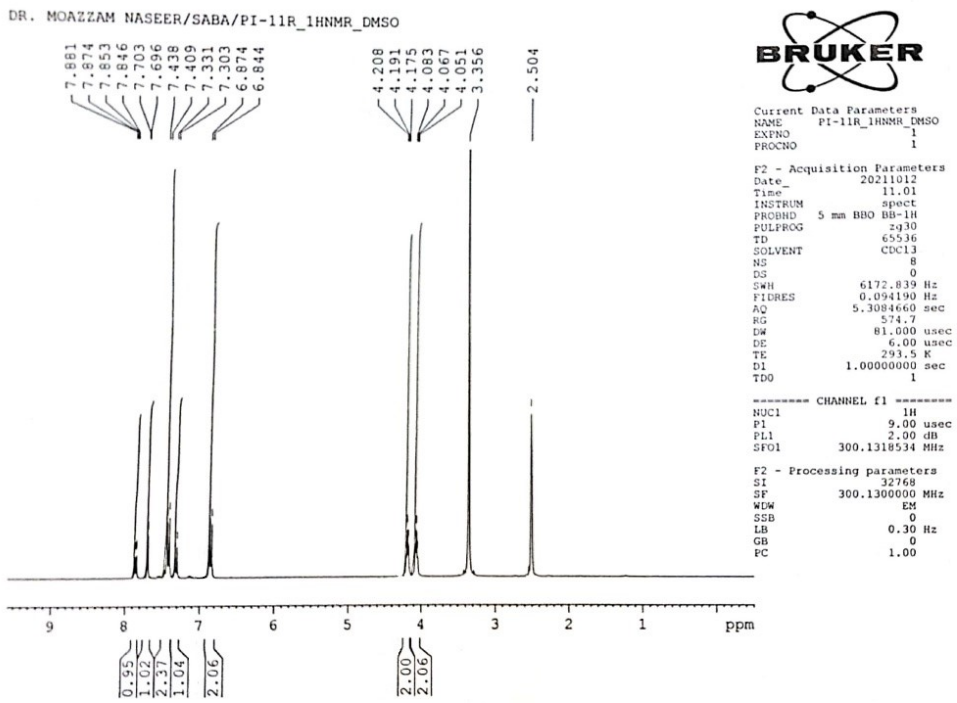
^{13}C-NMR of PI10



GC-MS of PI10



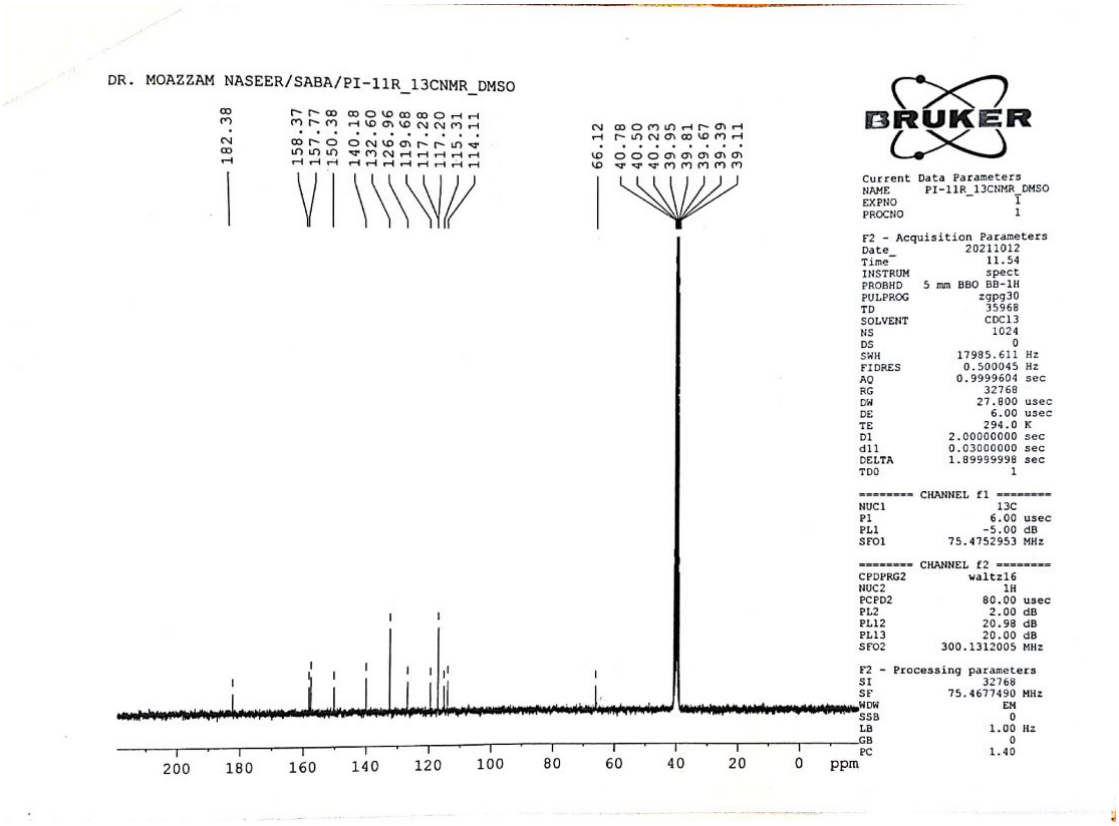
^{1}H-NMR of PI11



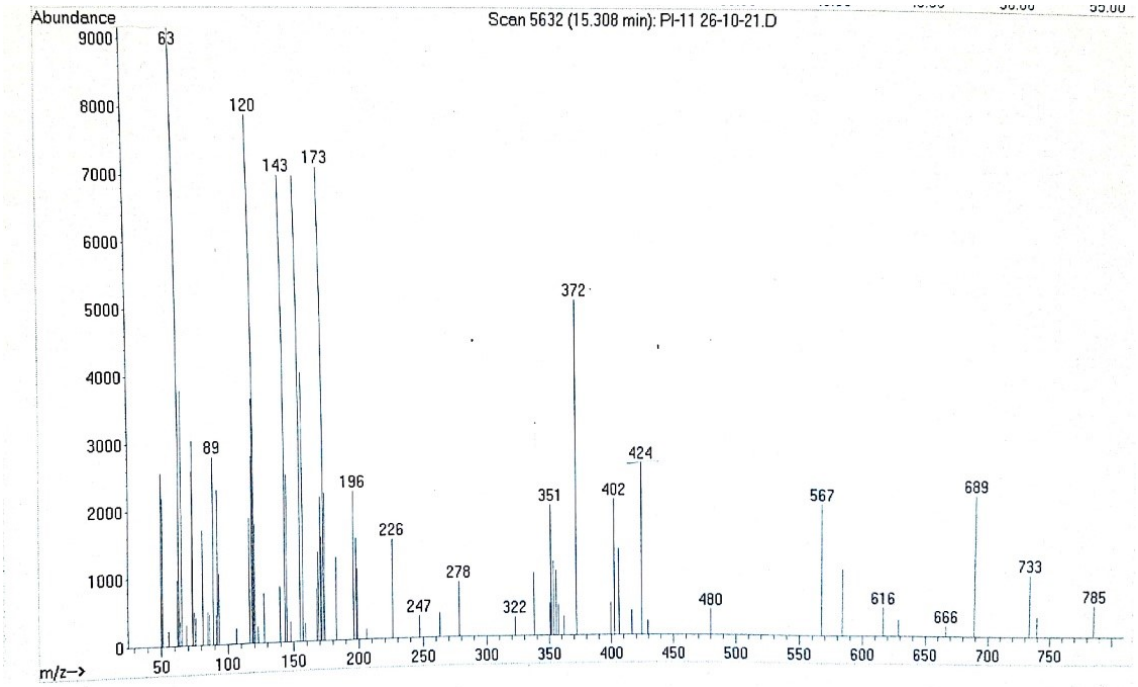
BRUKER

```
Current Data Parameters
NAME      PI-11R_1HNMR_DMSO
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211012
Time                 11.01
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                  574.7
DW                 81.000 usec
DE                  6.00 usec
TE                293.5 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  9.00 usec
PL1                 2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

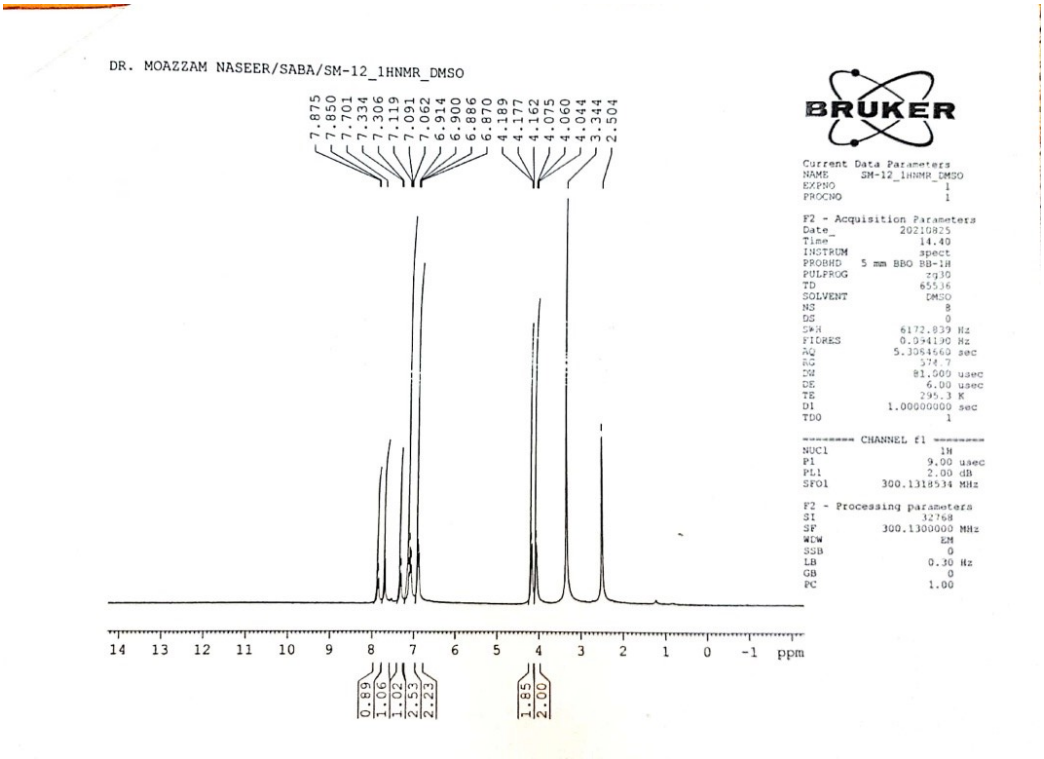
^{13}C-NMR of PI11


DR. MOAZZAM NASEER/SABA/PI-11R_13CNMR_DMSO
182.38
158.37
157.77
150.38
140.18
132.60
126.96
119.68
117.28
117.20
115.31
114.11
66.12
40.78
40.50
40.23
39.95
39.81
39.67
39.39
39.11
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME PI-11R_13CNMR_DMSO
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211012
Time 11.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 35968
SOLVENT CDCl3
NS 1024
DS 0
SWH 17985.611 Hz
FIDRES 0.500045 Hz
AQ 0.9999604 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 294.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

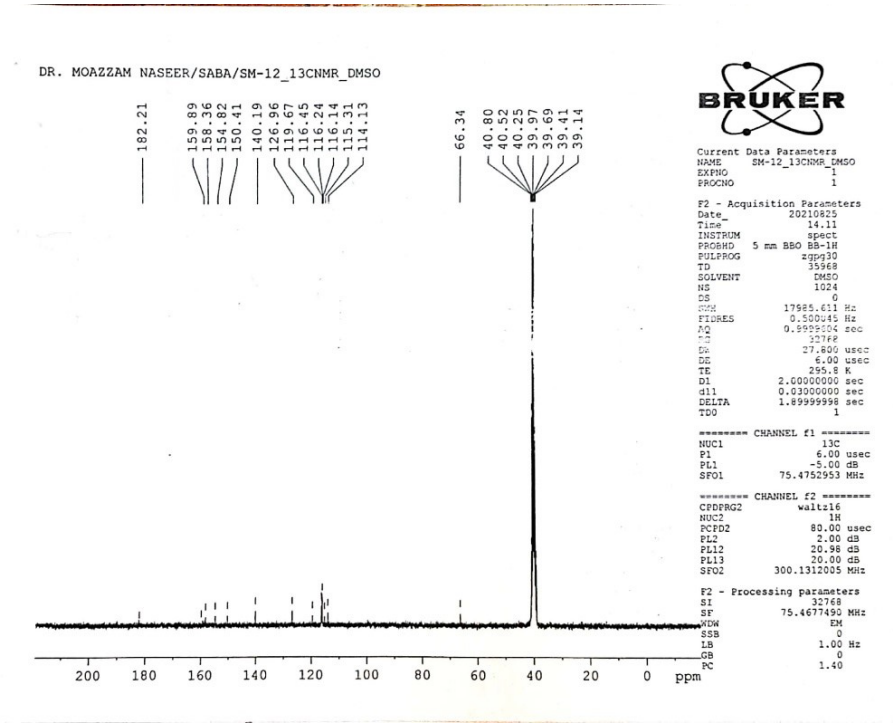
GC-MS of PI11



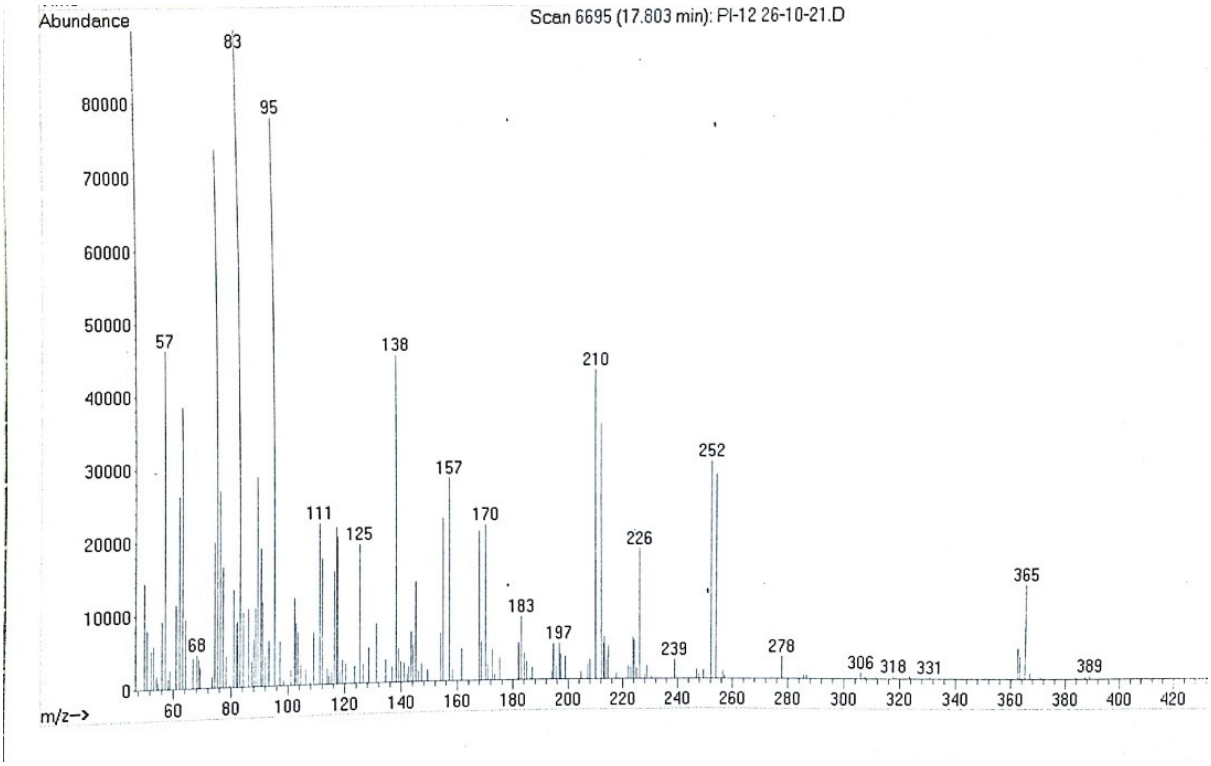
^{1}H-NMR of PI12



^{13}C-NMR of PI12


DR. MOAZZAM NASEER/SABA/SM-12_13CNMR_DMSO
182.21
159.89
158.36
154.82
150.41
140.19
126.96
119.67
116.45
116.24
116.14
115.31
114.13
66.34
40.80
40.52
40.25
39.97
39.69
39.41
39.14
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME SM-12_13CNMR_DMSO
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210825
Time 14.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 35968
SOLVENT DMSO
NS 1024
DS 0
SWH 17985.611 Hz
FIDRES 0.500045 Hz
AQ 0.9999004 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

GC-MS of PI12


Abundance
Scan 6695 (17.803 min): PI-12 26-10-21.D
83
95
57
138
210
252
157
111
170
125
226
365
183
197
68
239
278
306
318
331
389
80000
70000
60000
50000
40000
30000
20000
10000
0
m/z-->
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420