

NEW JOURNAL OF CHEMISTRY

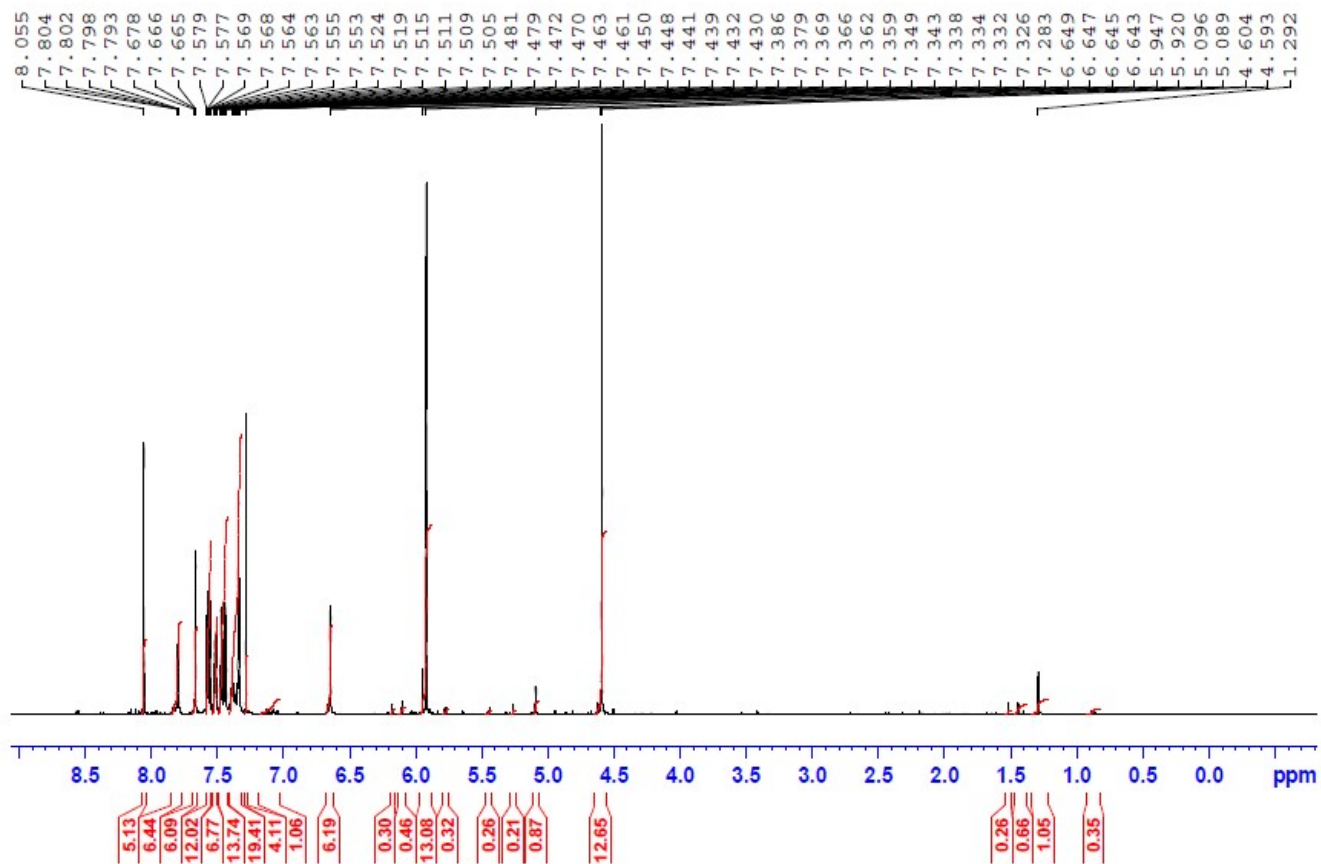
SUPPLEMENTARY MATERIAL

Design, synthesis, anticancer activity and molecular docking studies of new benzimidazole derivatives bearing 1,3,4-oxadiazole moiety as potential thymidylate synthase inhibitors

Abdulraheem SA Almalki^a, Syed Nazreen^{* , b}, Serag Eldin I. Elbehairi^{c,d}, Mohammad Asad^{e,f}, Ali A Shati^c, Mohammad Y. Alfaifi^c, Abdulrahman Alhadhrami^a, Ahmed A. Elhenawy^{b,g}, Ali Q. Alorabi^b, Abdullah M. Asiri^{e,f}, Mohammad Mahboob Alam^{* , b}

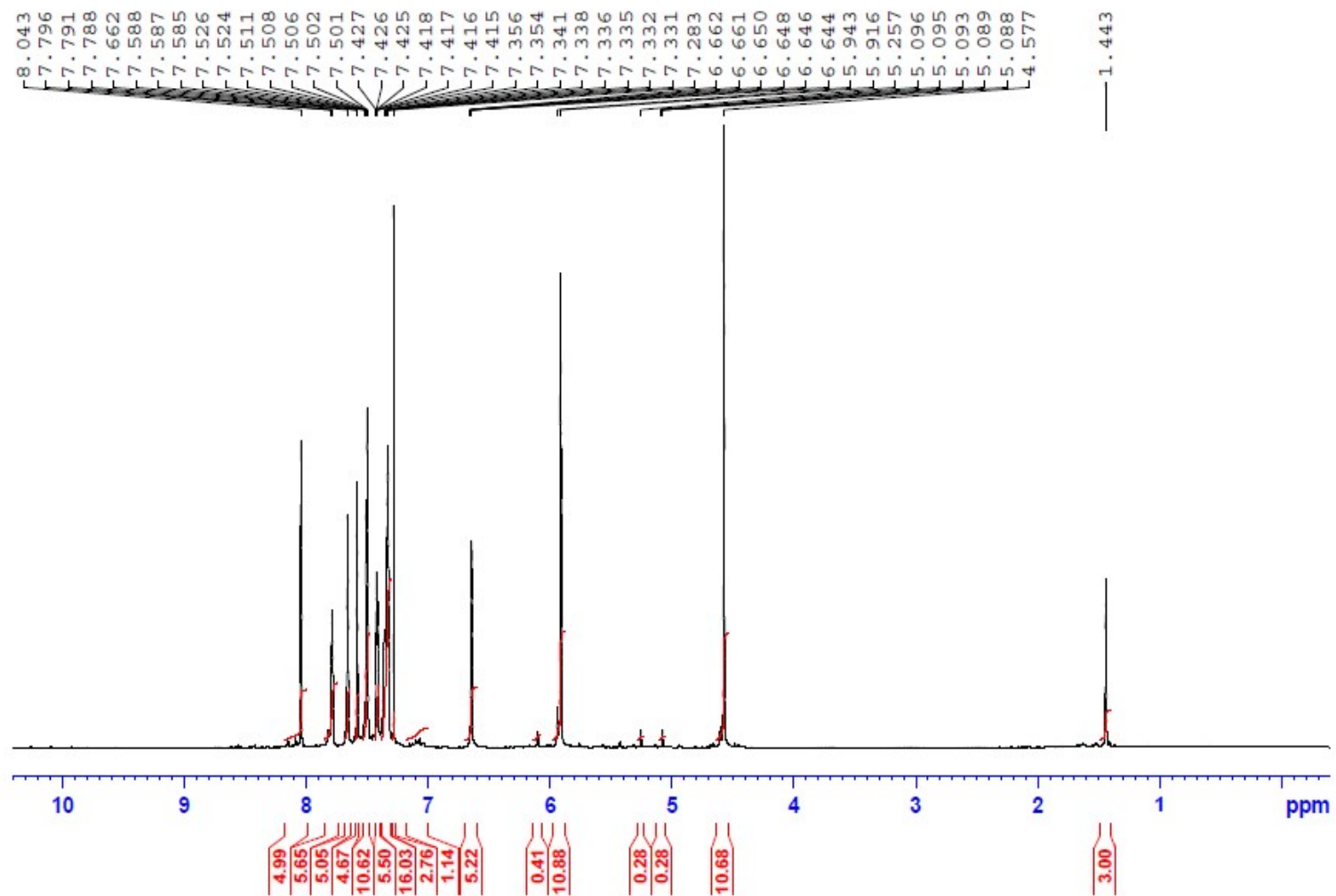
¹H NMR of compound 7

Mahboob
Sample 12 CDCL₃



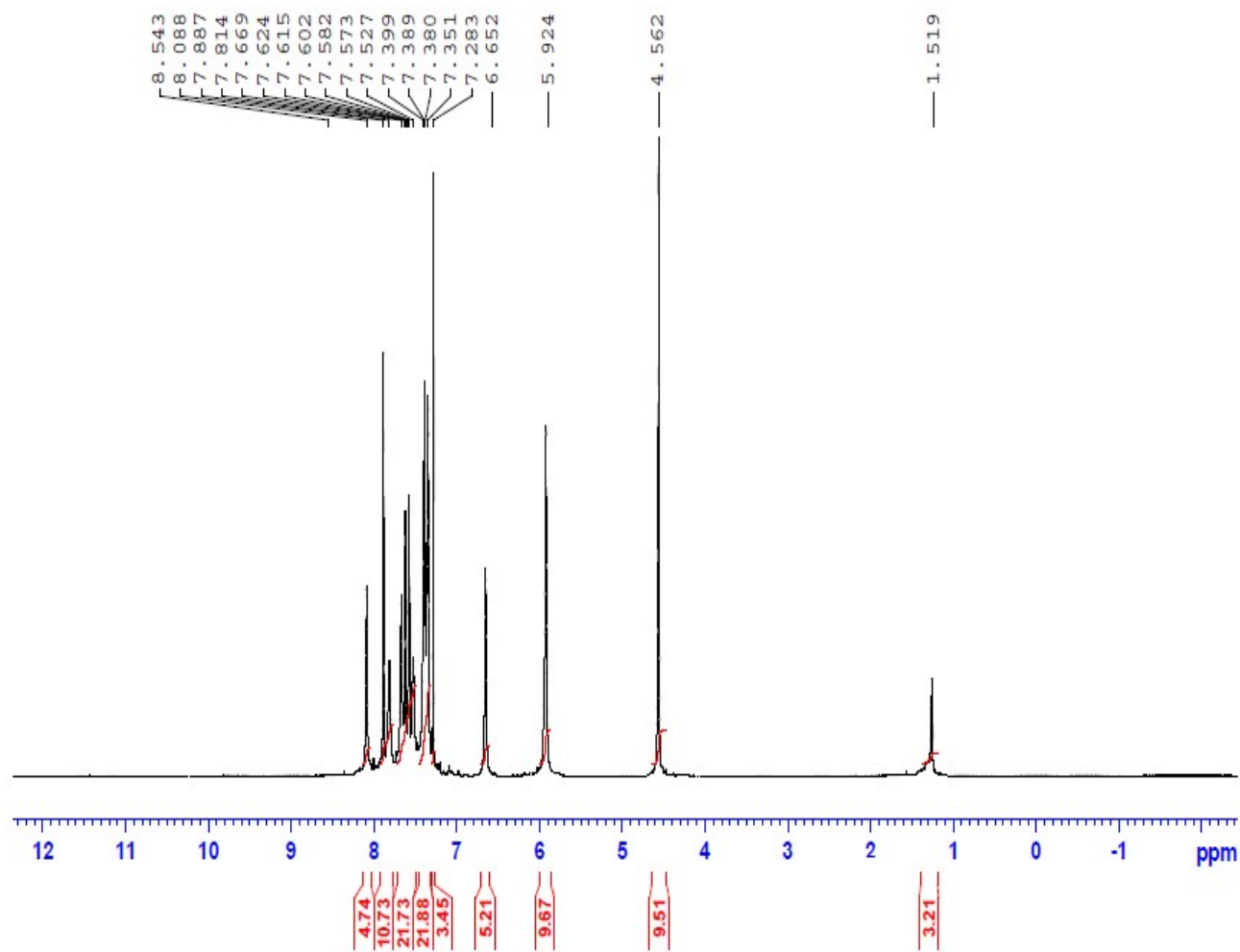
¹H NMR of compound 8

Mahboob
Sample 14 CDCL₃



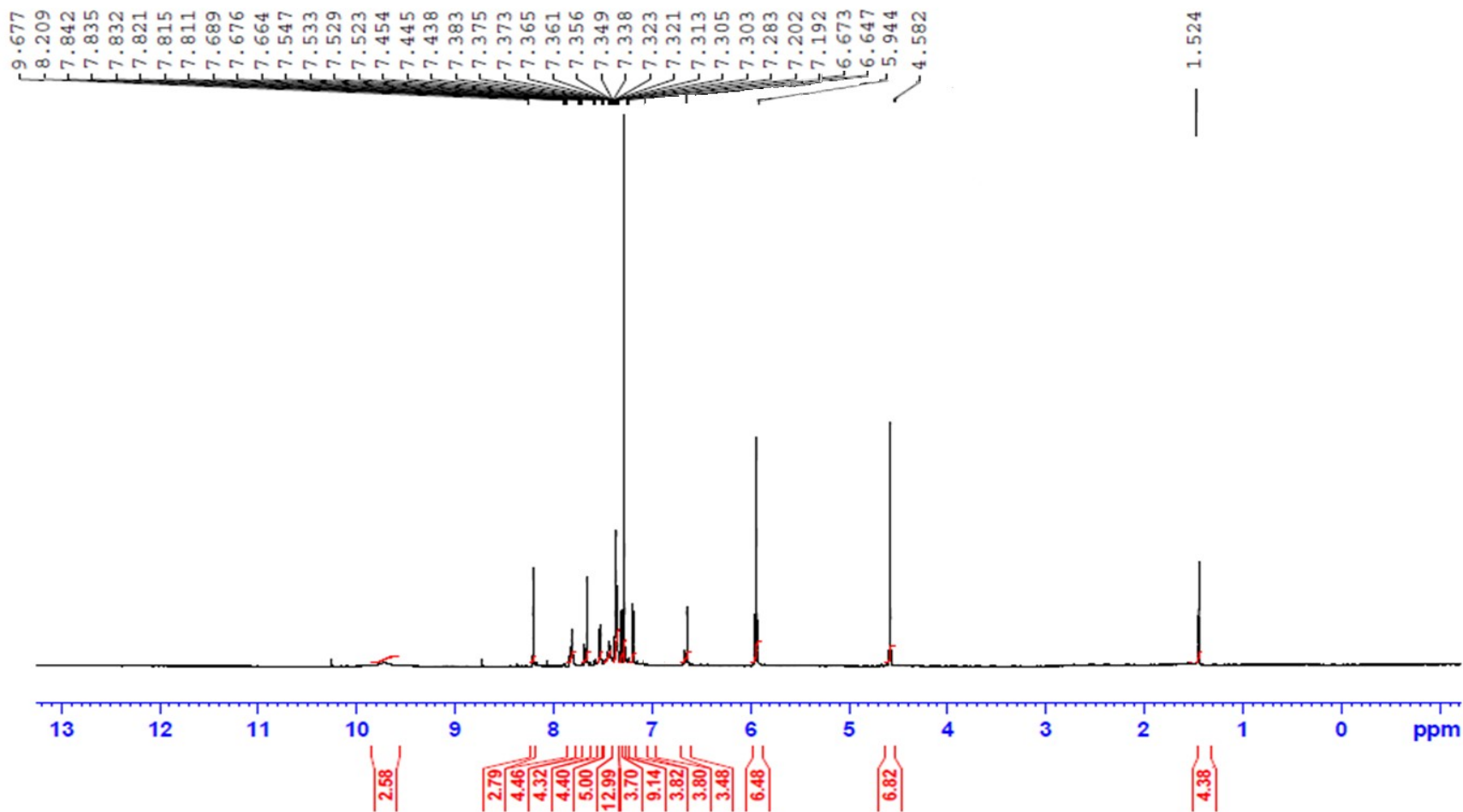
¹H NMR of compound 9

Mahboob
Sample 10 CDCL₃

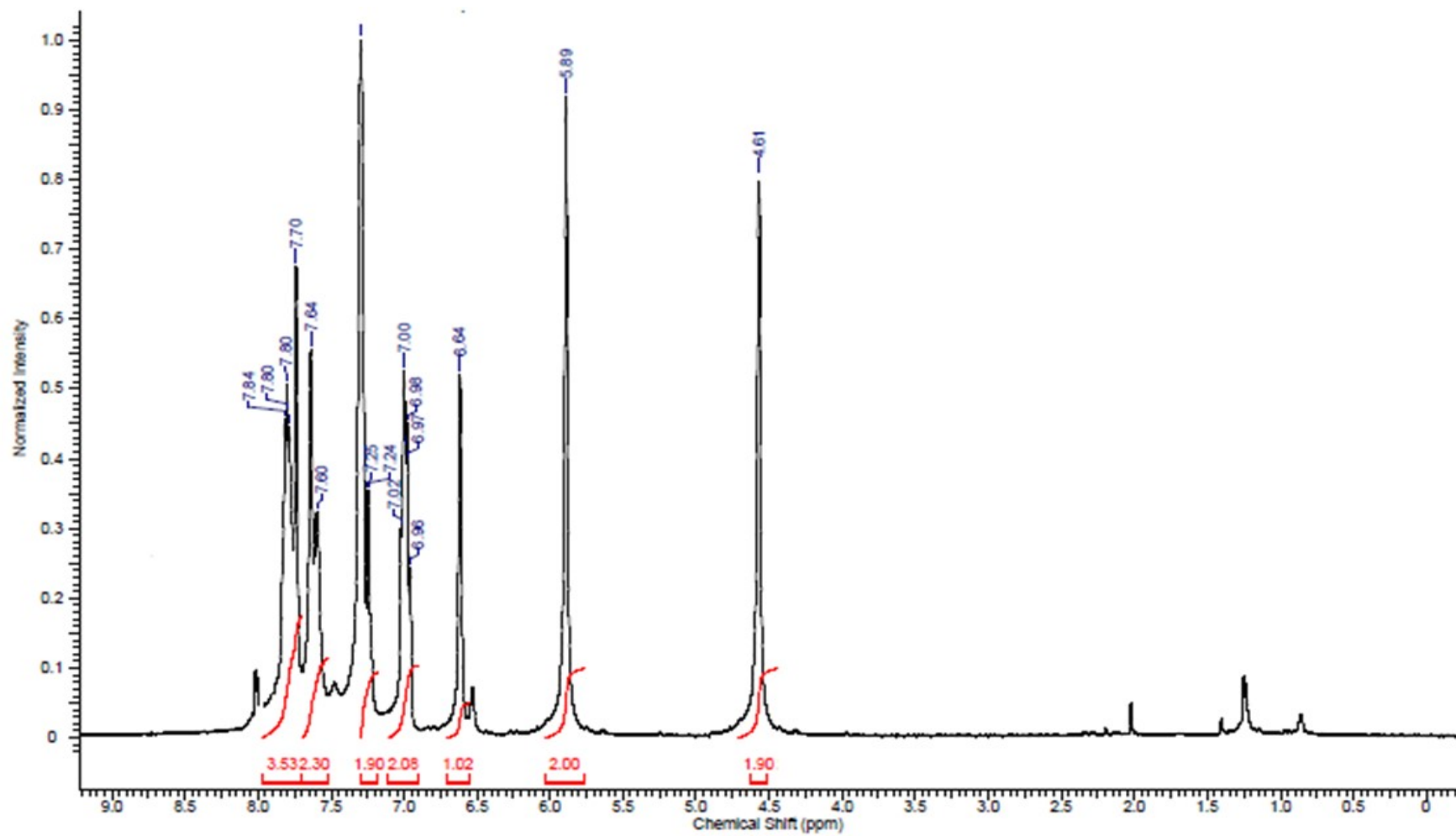


¹H NMR of compound 10

Mahboob
Sample 11 CDCL₃

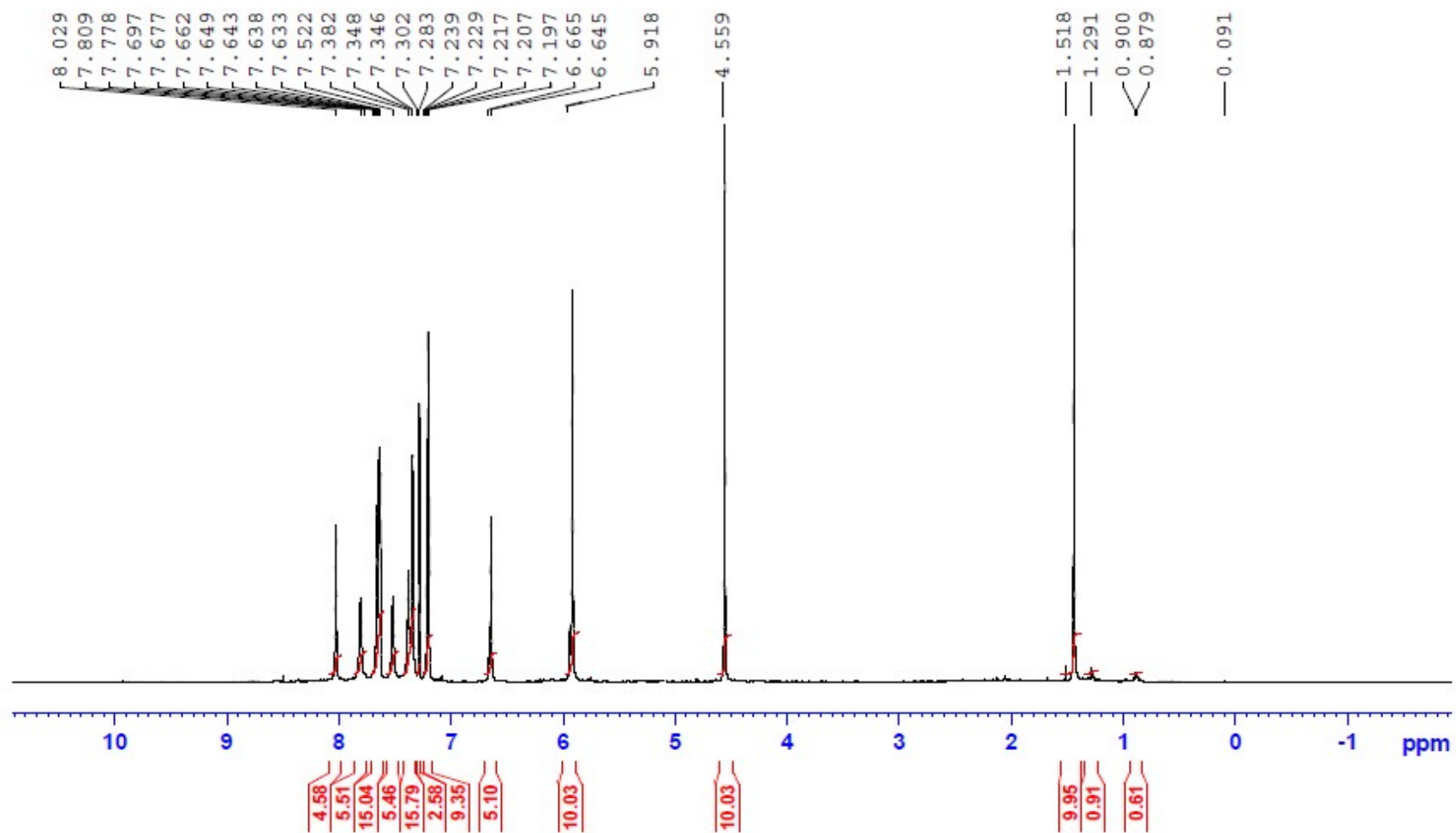


¹H NMR of compound 11



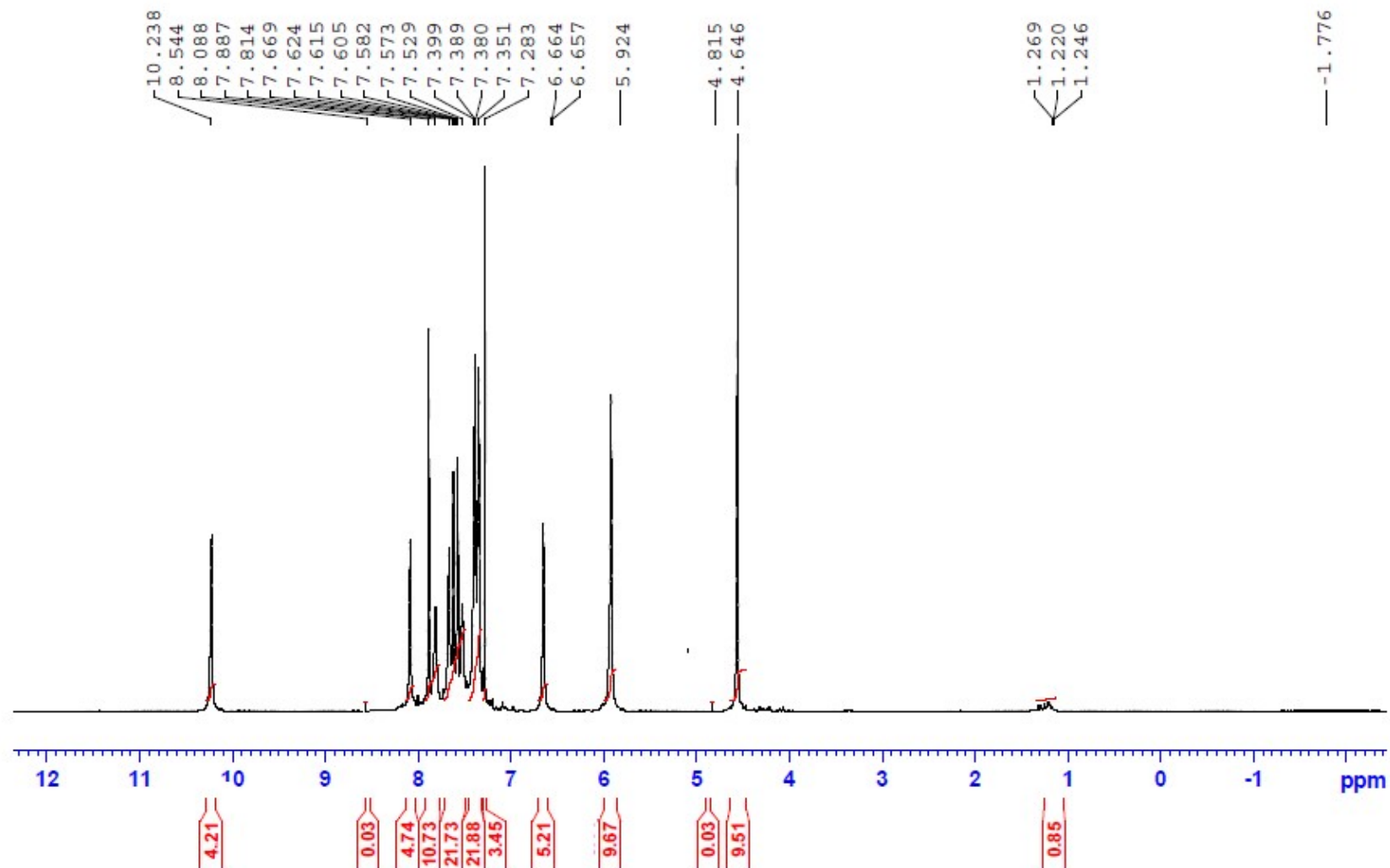
¹H NMR of compound 12

Mahboob
Sample 13 CDCL₃



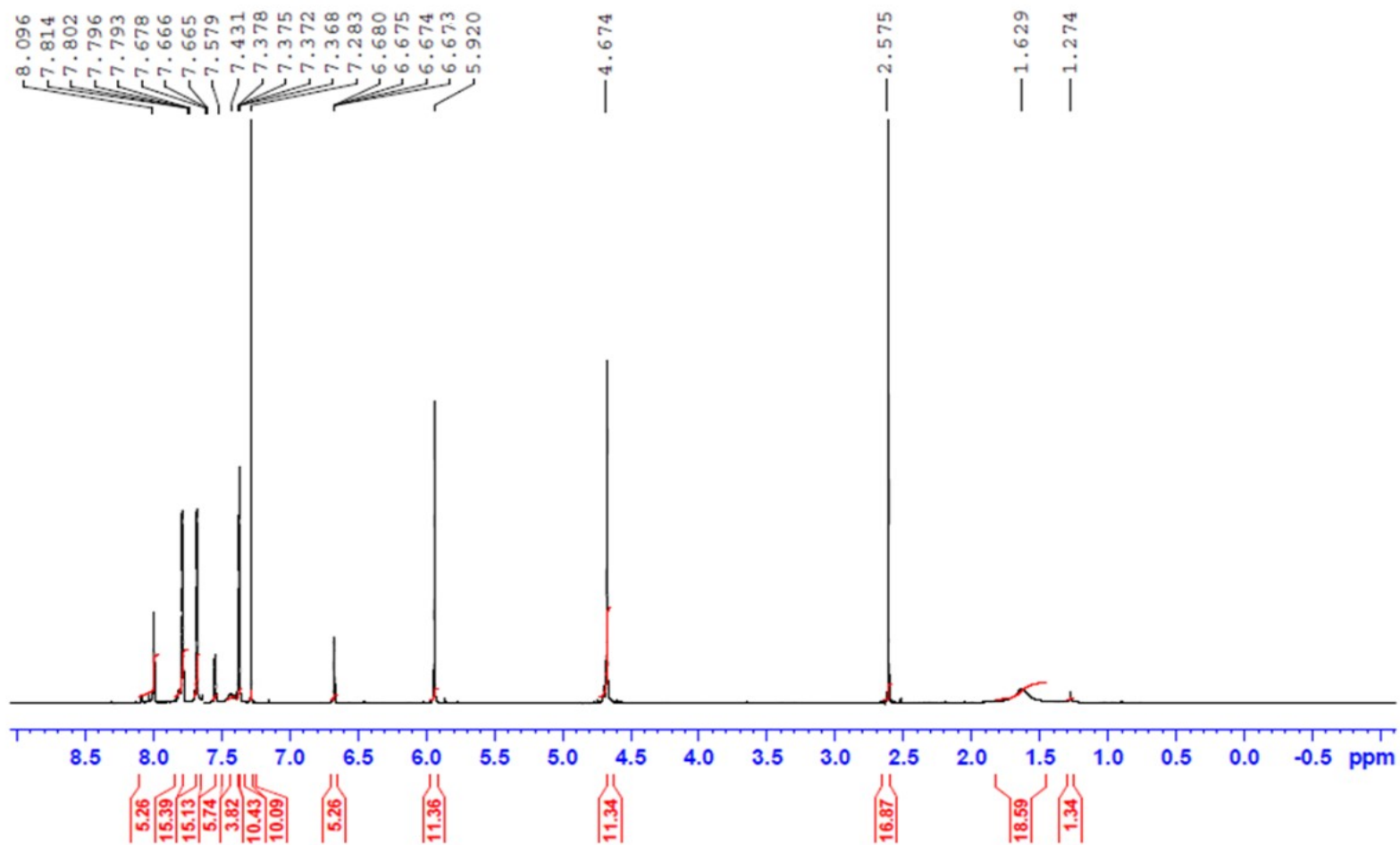
¹H NMR of compound 13

Mahboob
Sample 21 CDCL₃

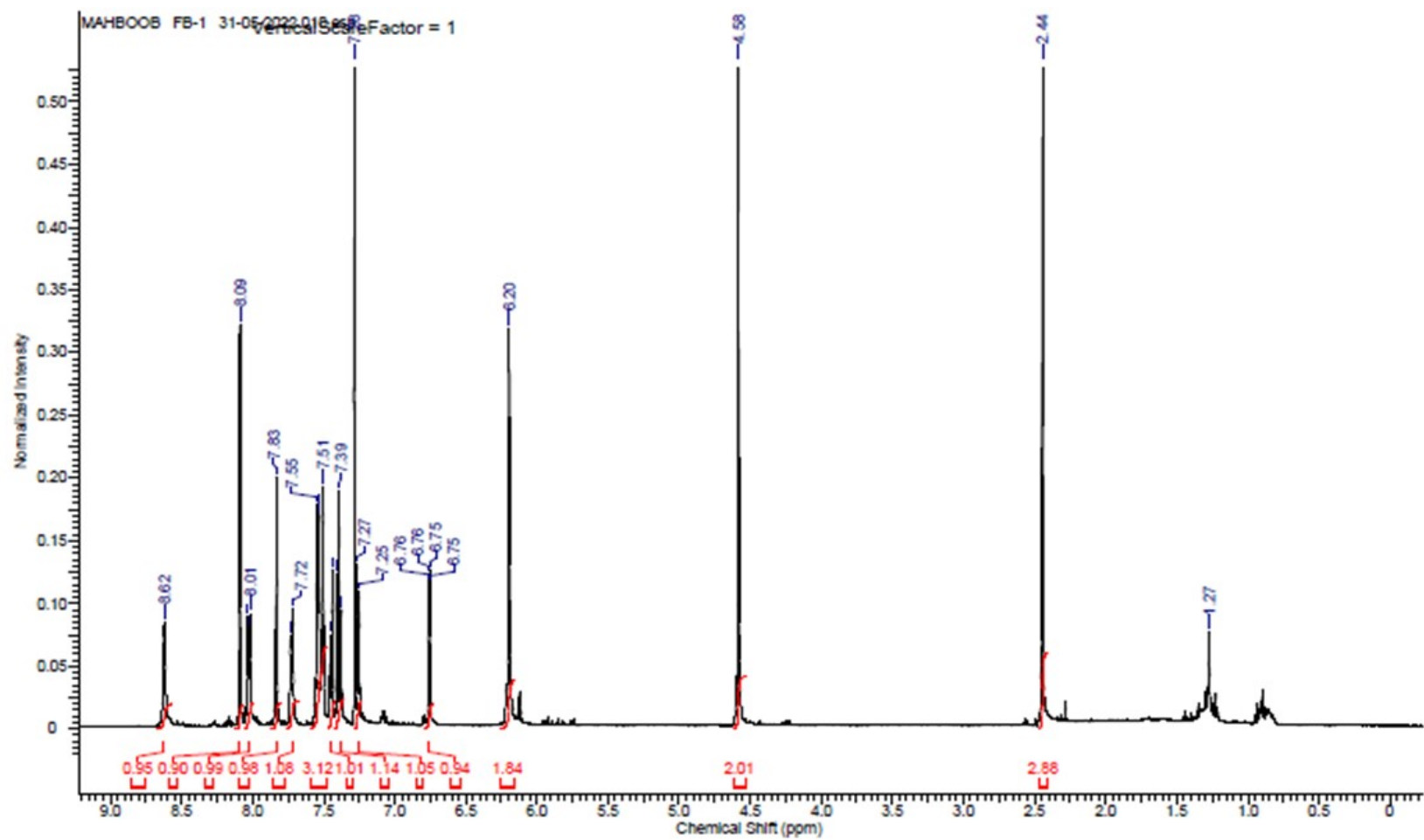


¹H NMR of compound 14

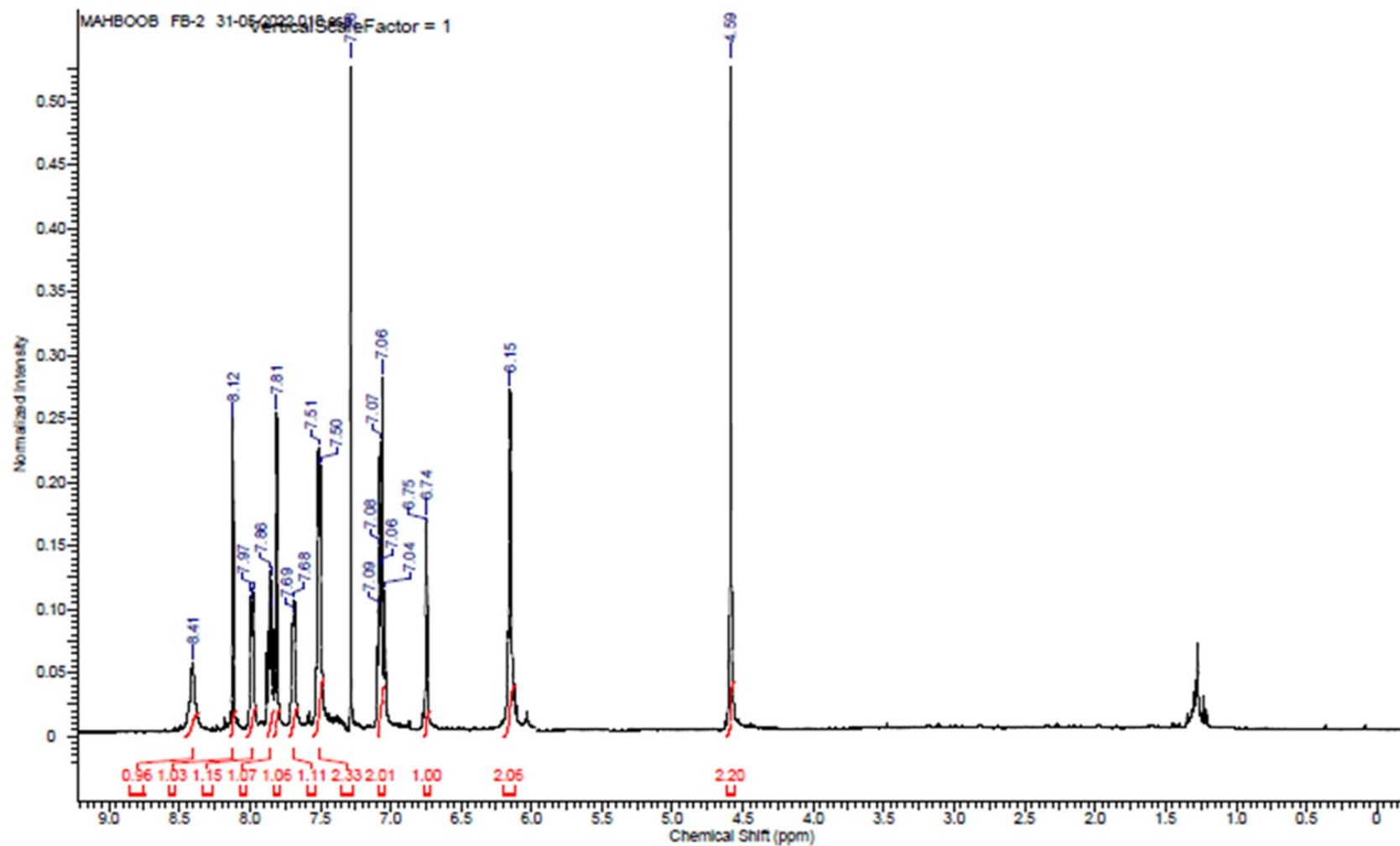
Mahboob
Sample 25 CDCL₃



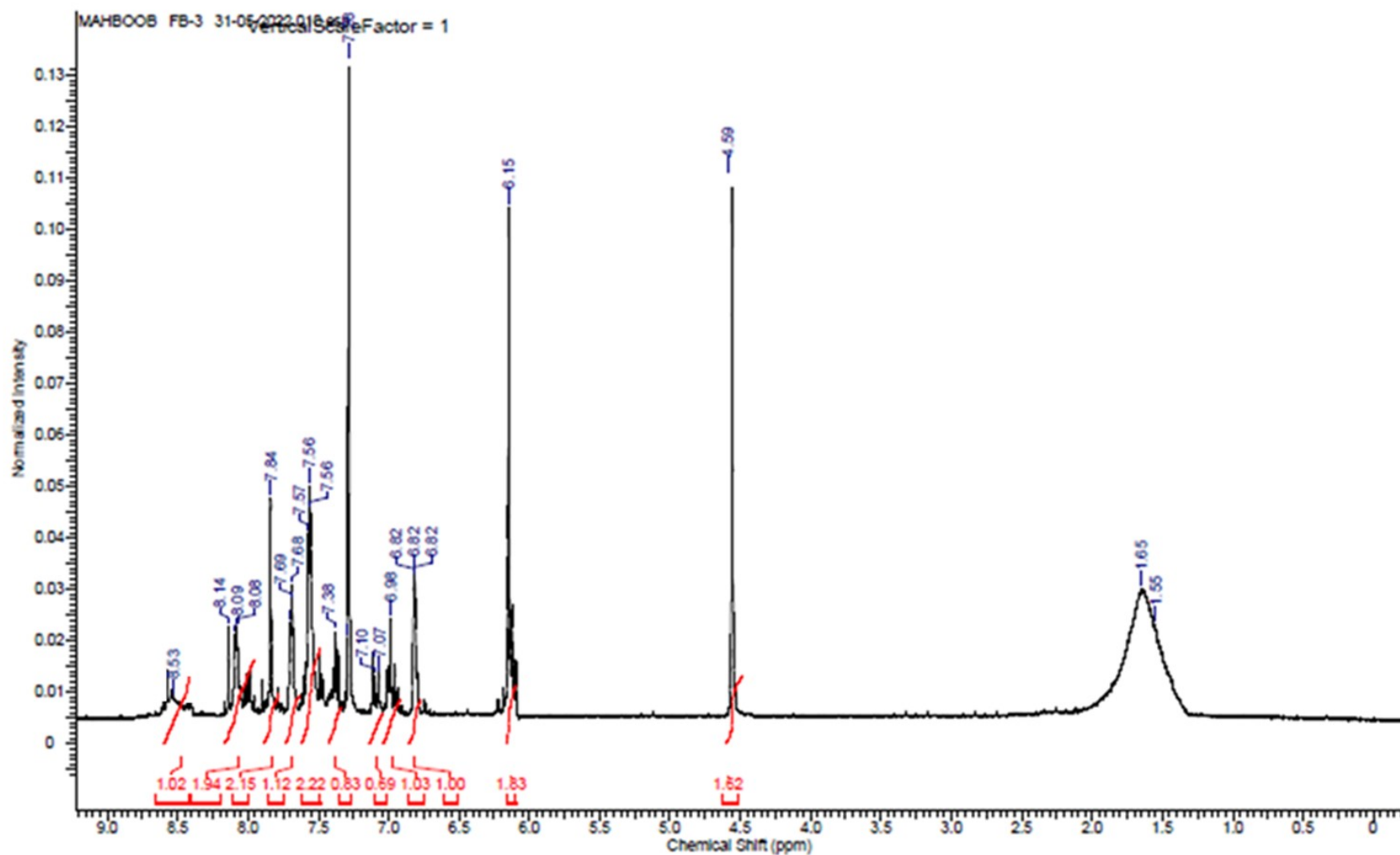
¹H NMR of compound 15



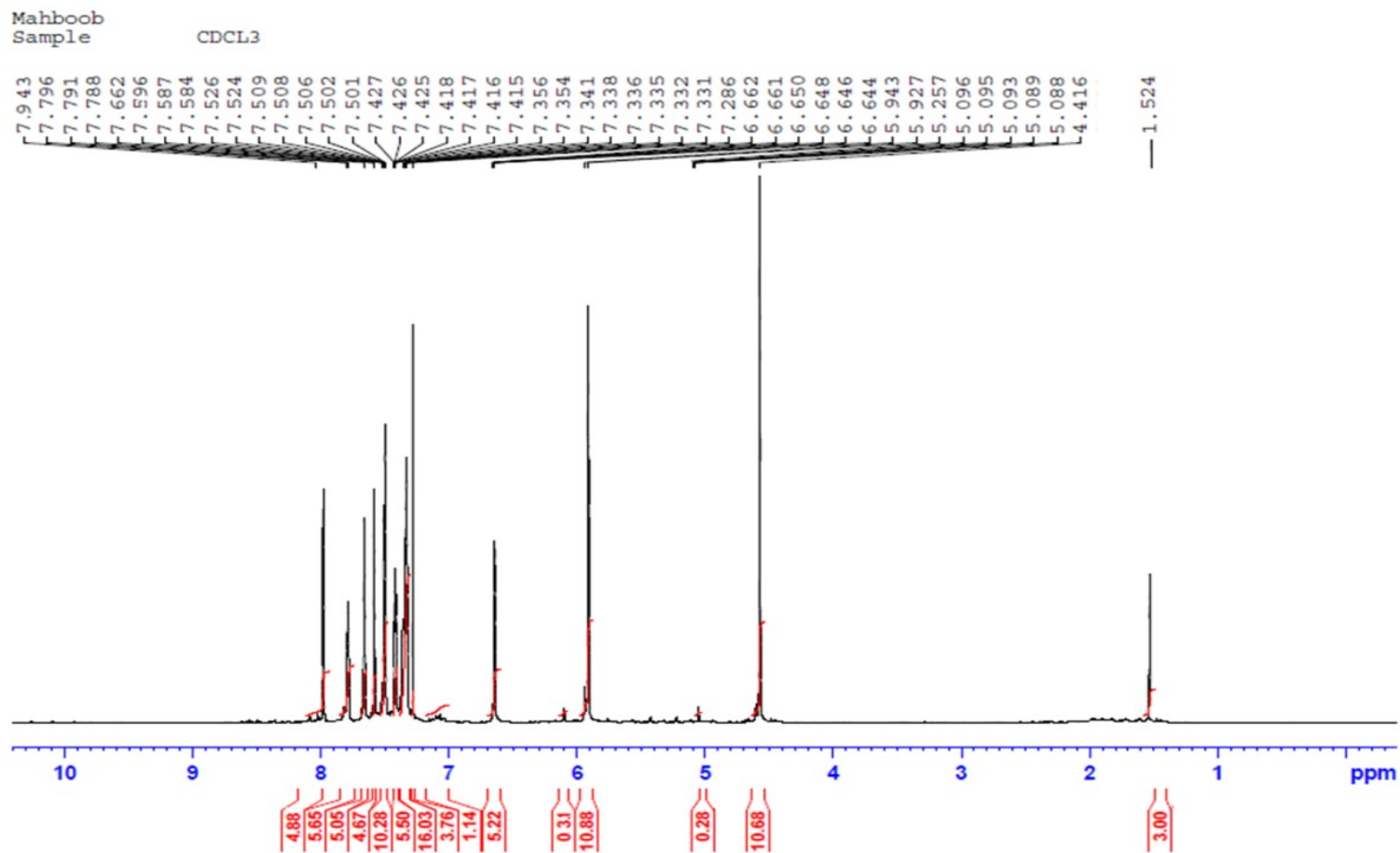
¹H NMR of compound 16



¹H NMR of compound 17

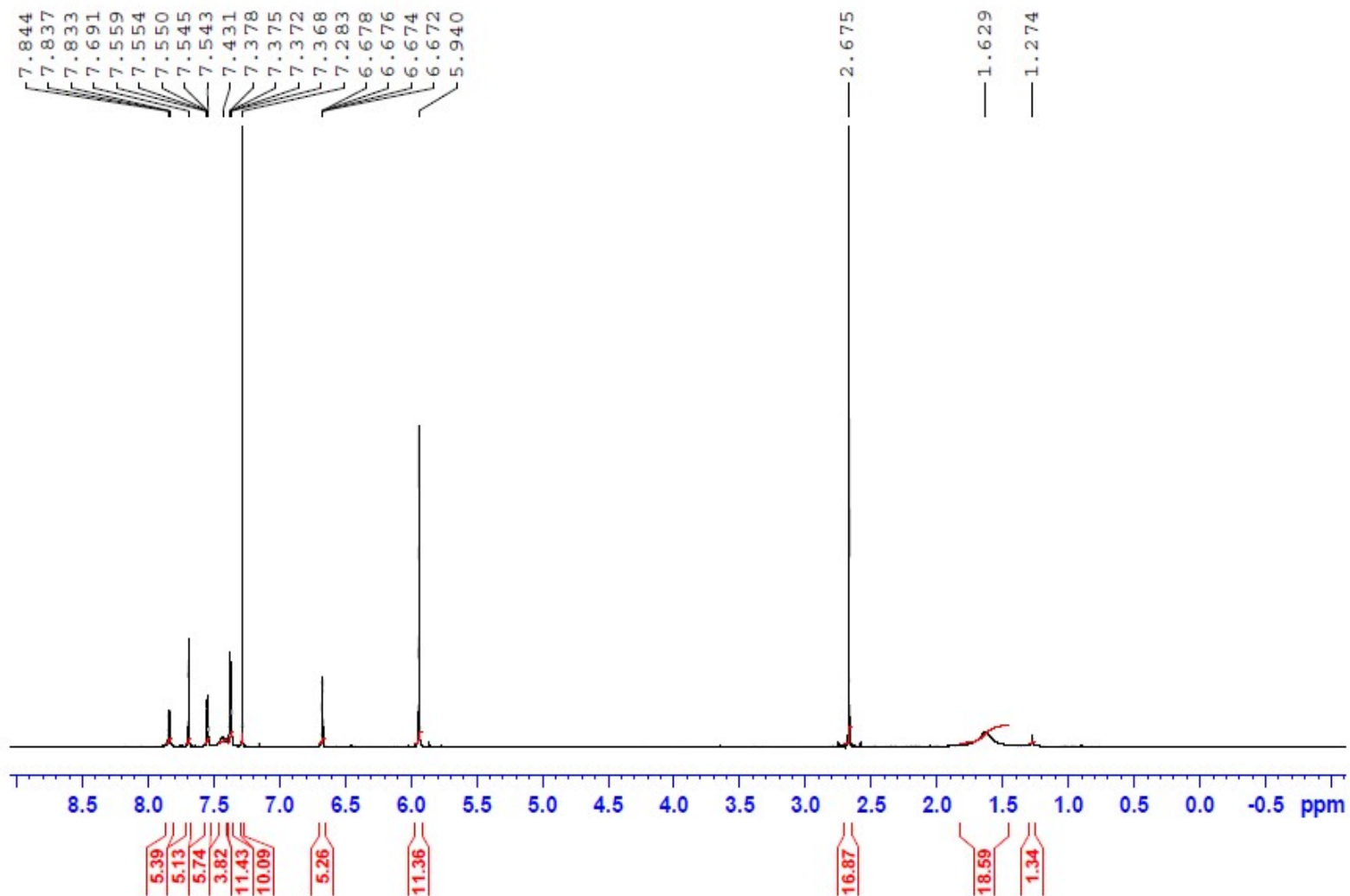


¹H NMR of compound 18



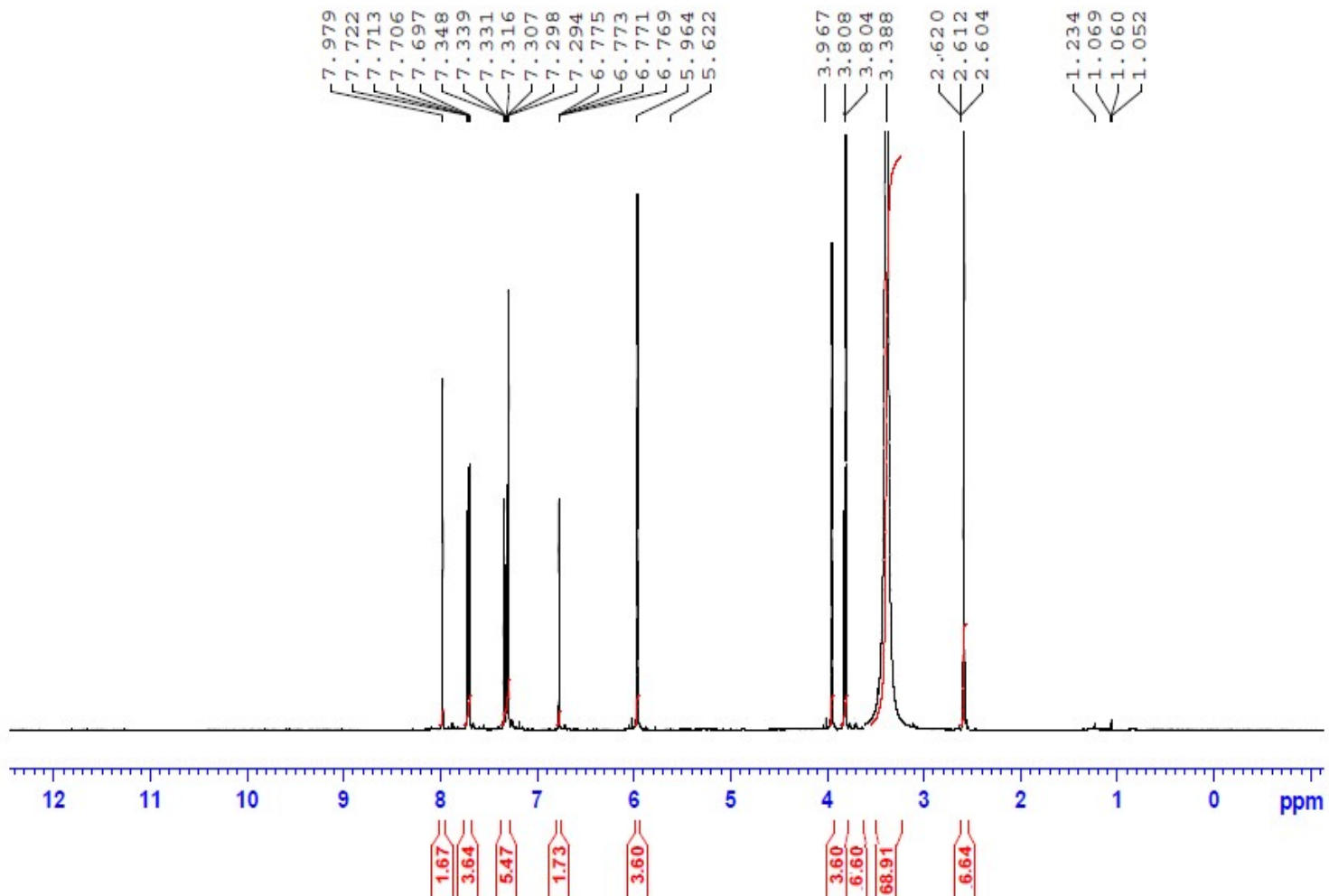
¹H NMR of compound 19

Mahboob
Sample 15 CDCL₃



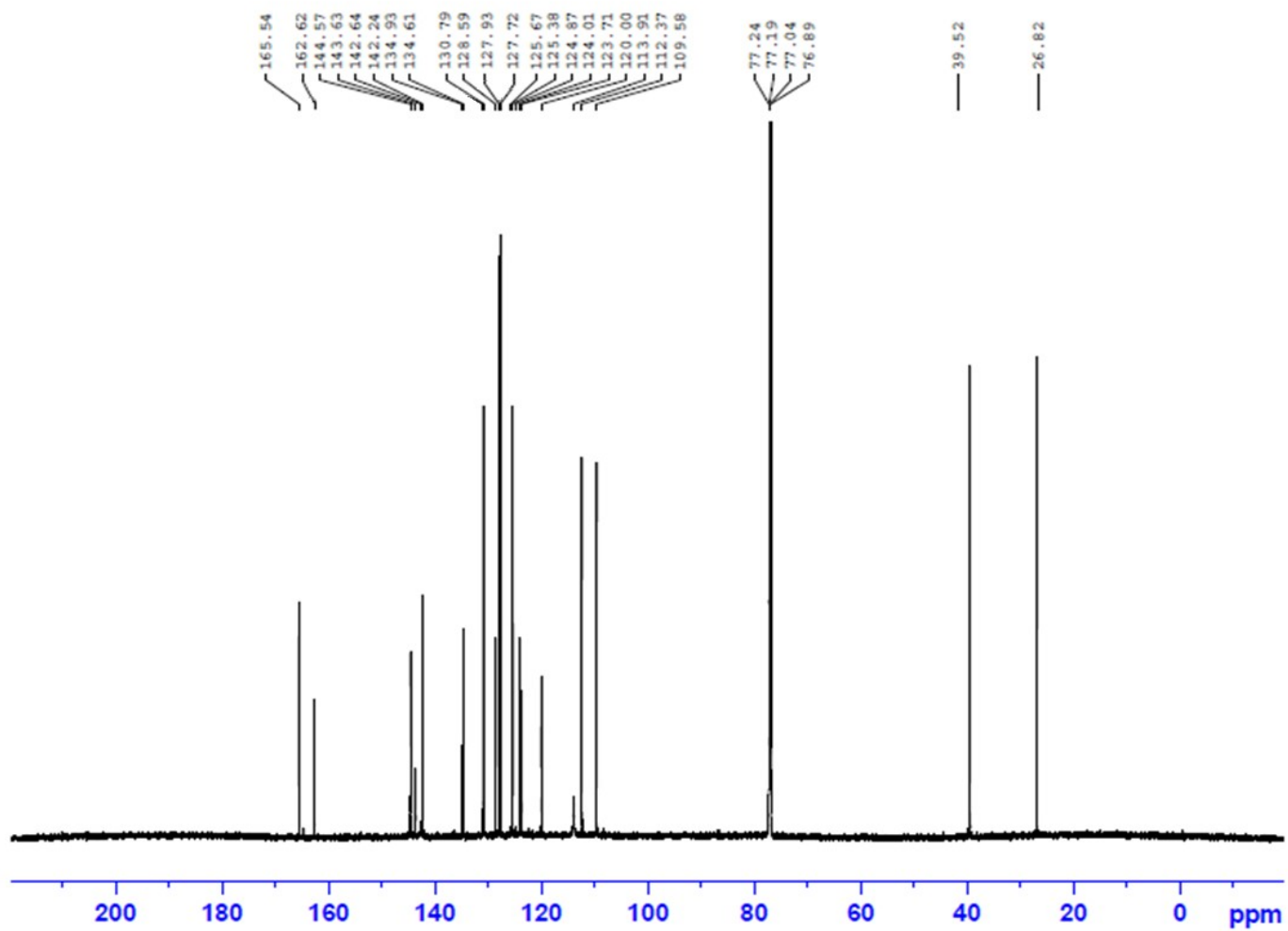
¹H NMR of compound 20

Mahboob
Sample 16 DMSO



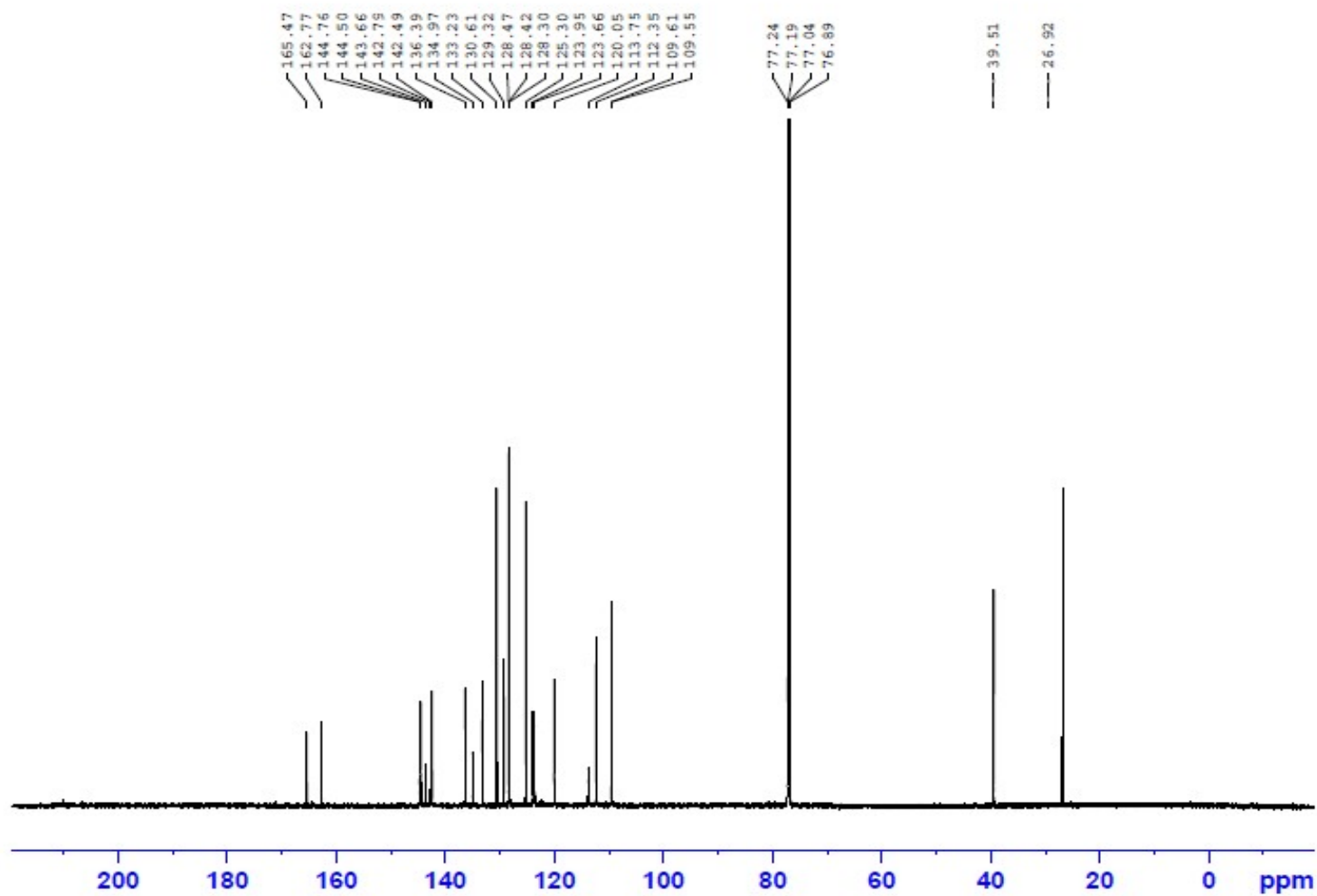
¹³C NMR of compound 7

Mahboob
Sample 12 CDCL₃



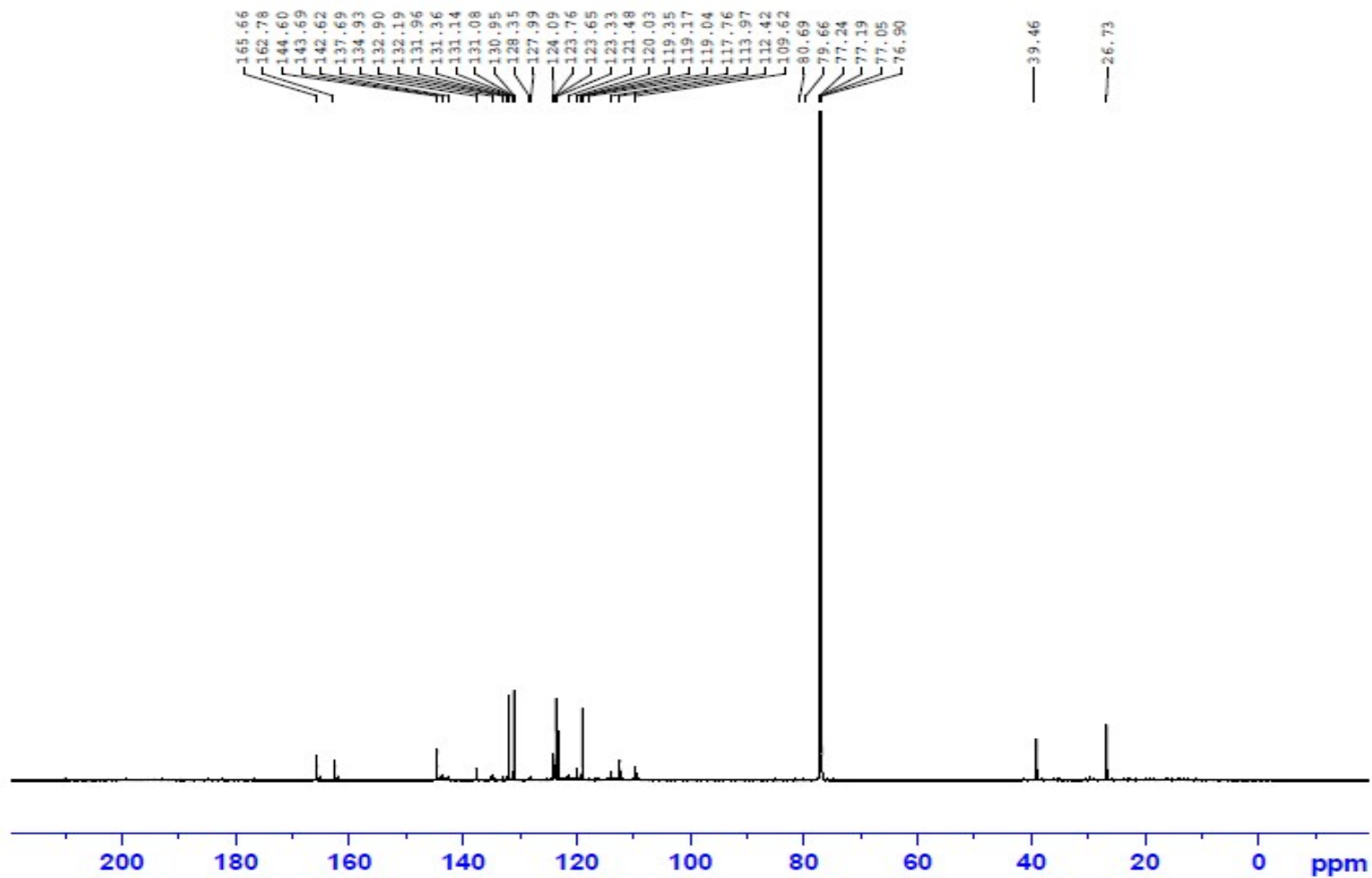
¹³C NMR of compound 8

Mahboob
Sample 14 CDCL₃



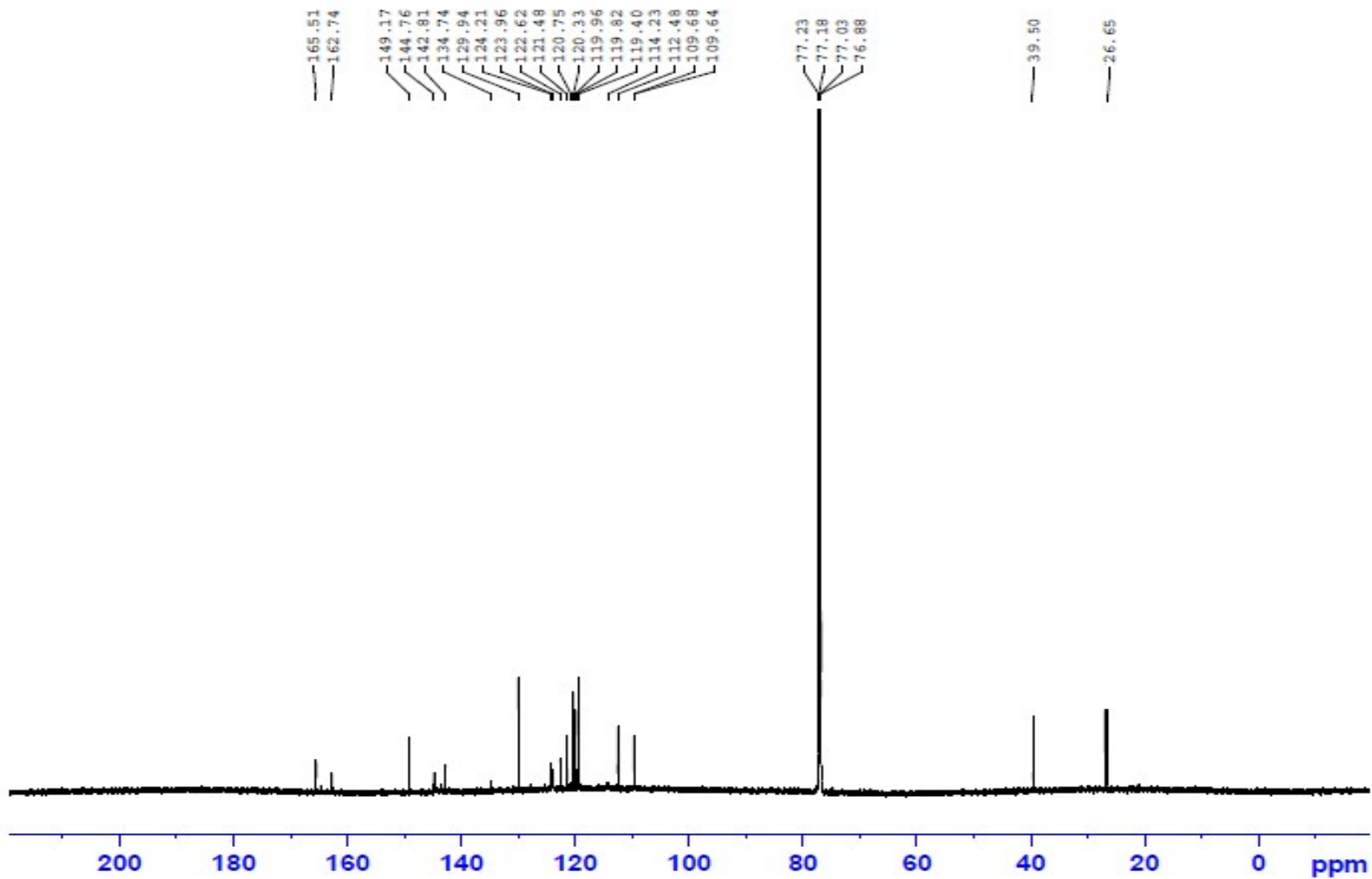
¹³C NMR of compound 9

Mahboob
Sample 10 CDCL₃

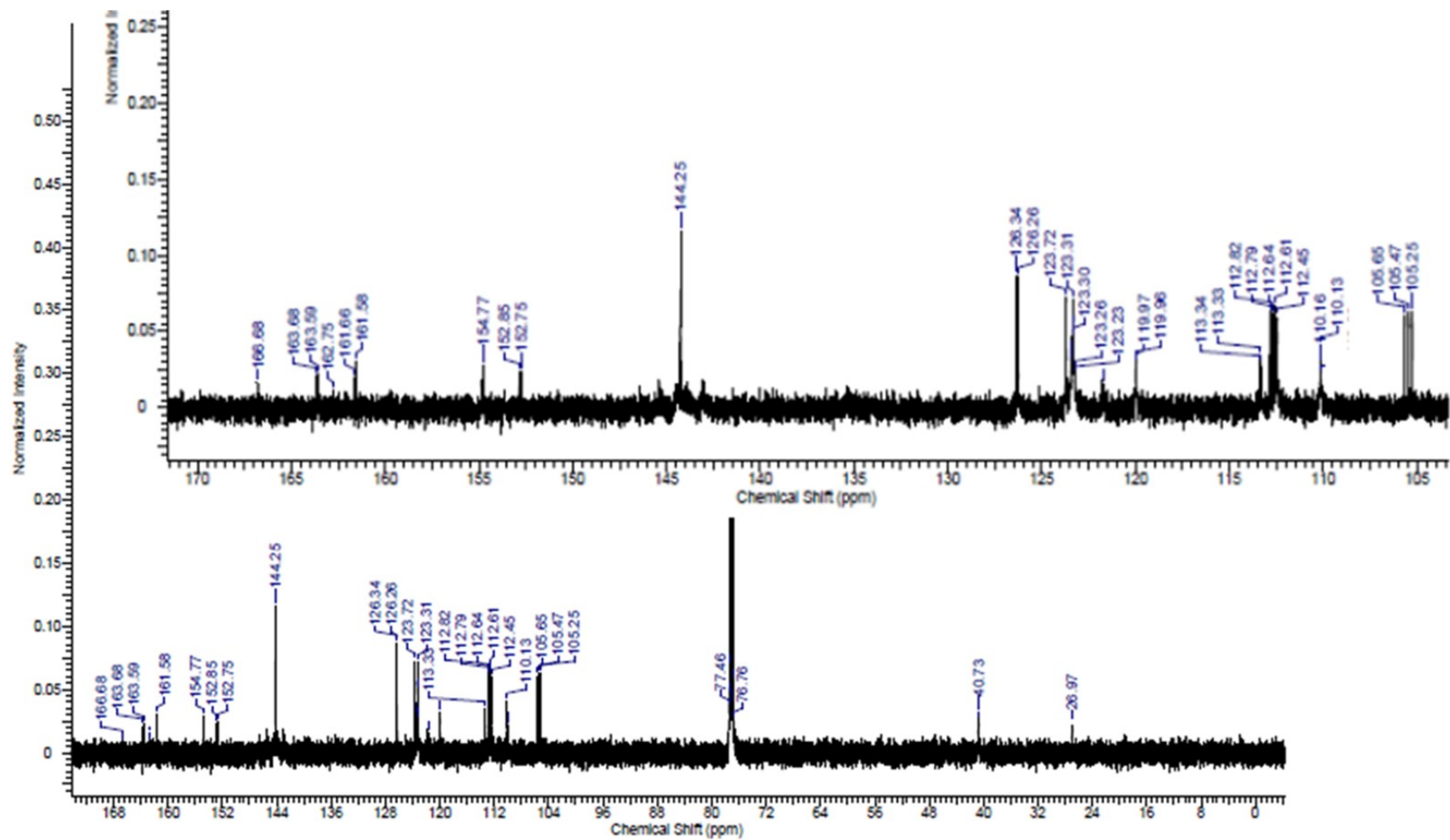


¹³C NMR of compound 10

Mahboob
Sample 11 CDCL₃



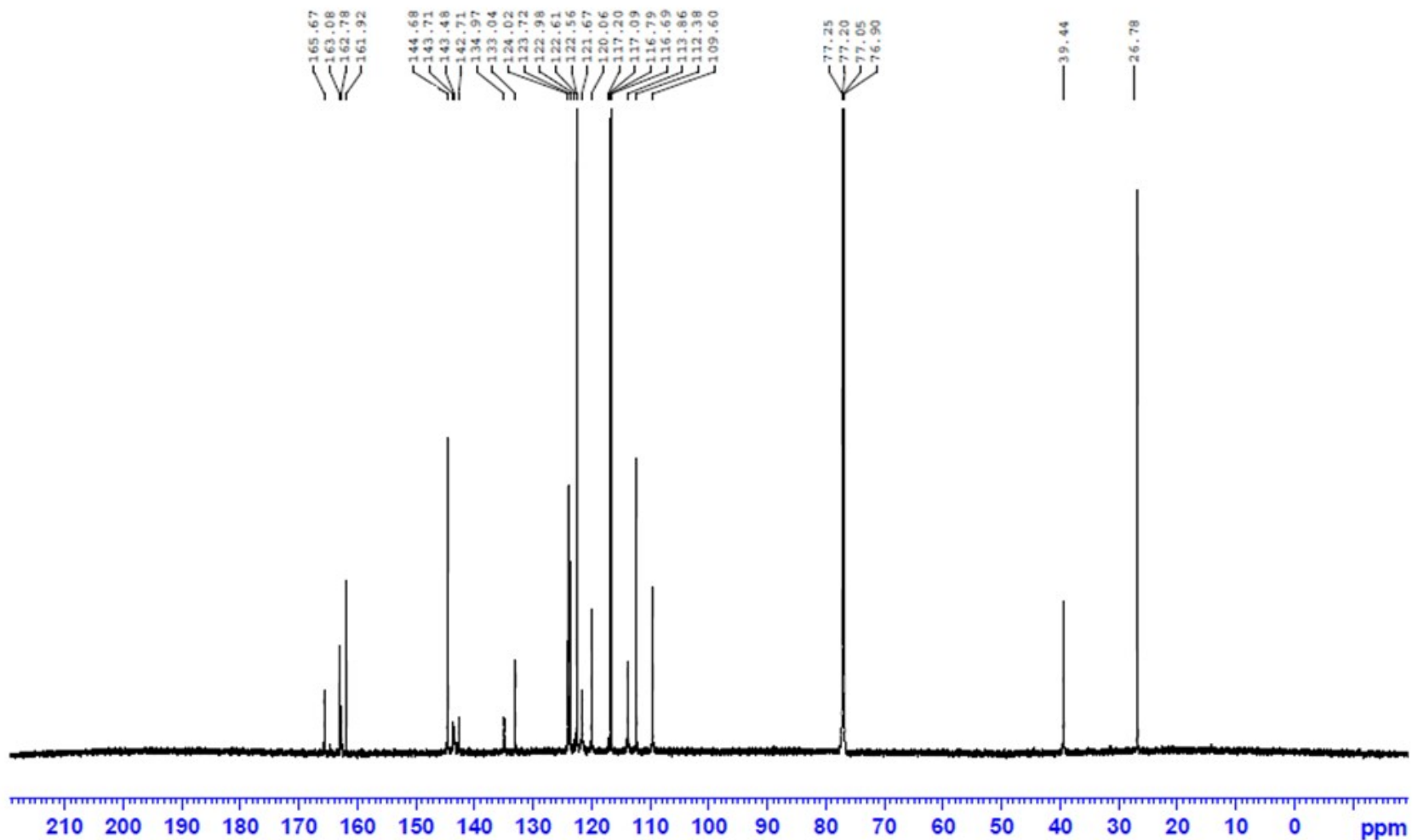
¹³C NMR of compound 11



¹³C NMR of compound 12

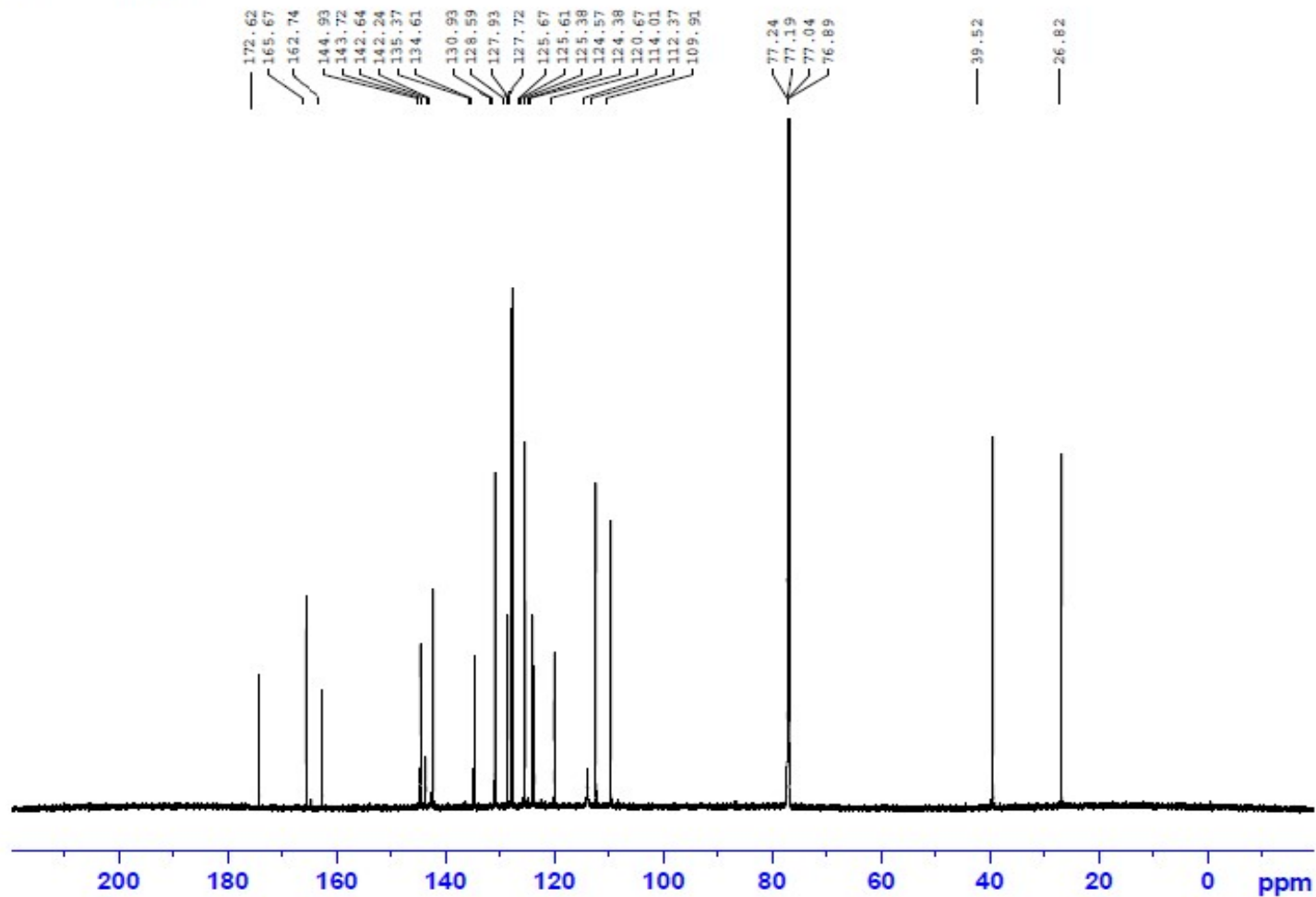
Mahboob
Sample

CDCL₃



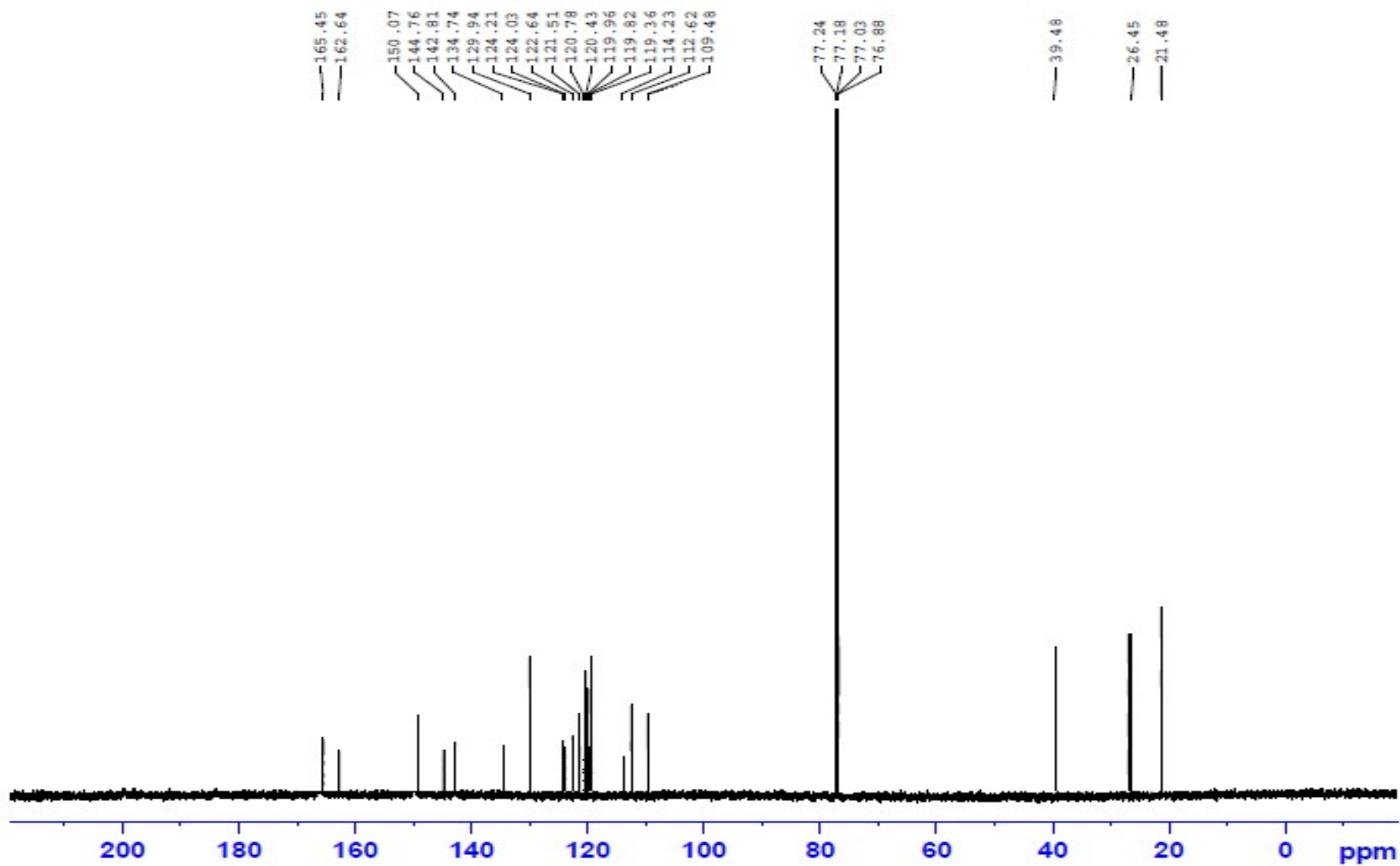
¹³C NMR of compound 13

Mahboob
Sample 21 CDCL₃



¹³C NMR of compound 14

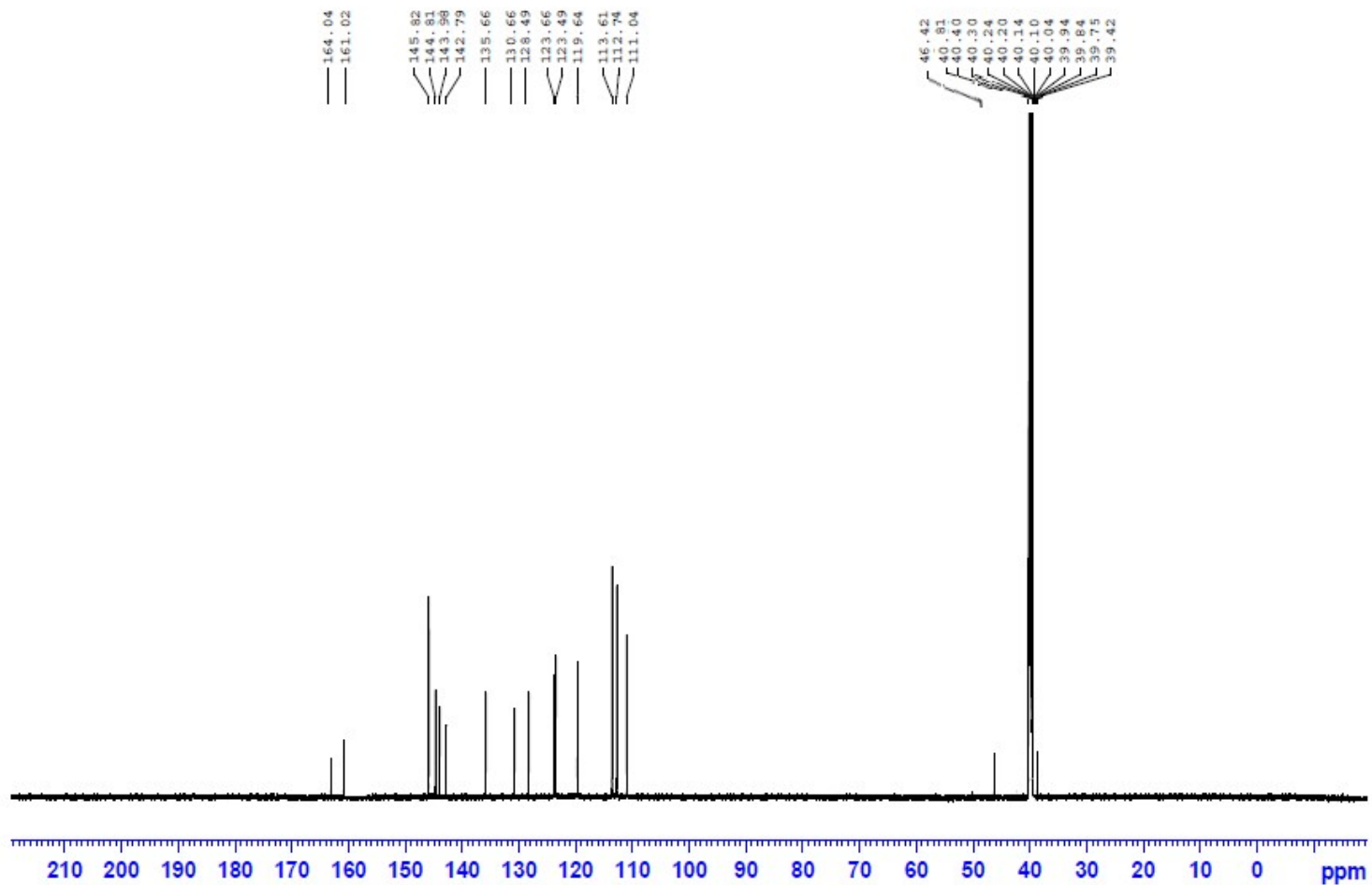
Mahboob
Sample 25 CDCL₃



¹³C NMR of compound 18

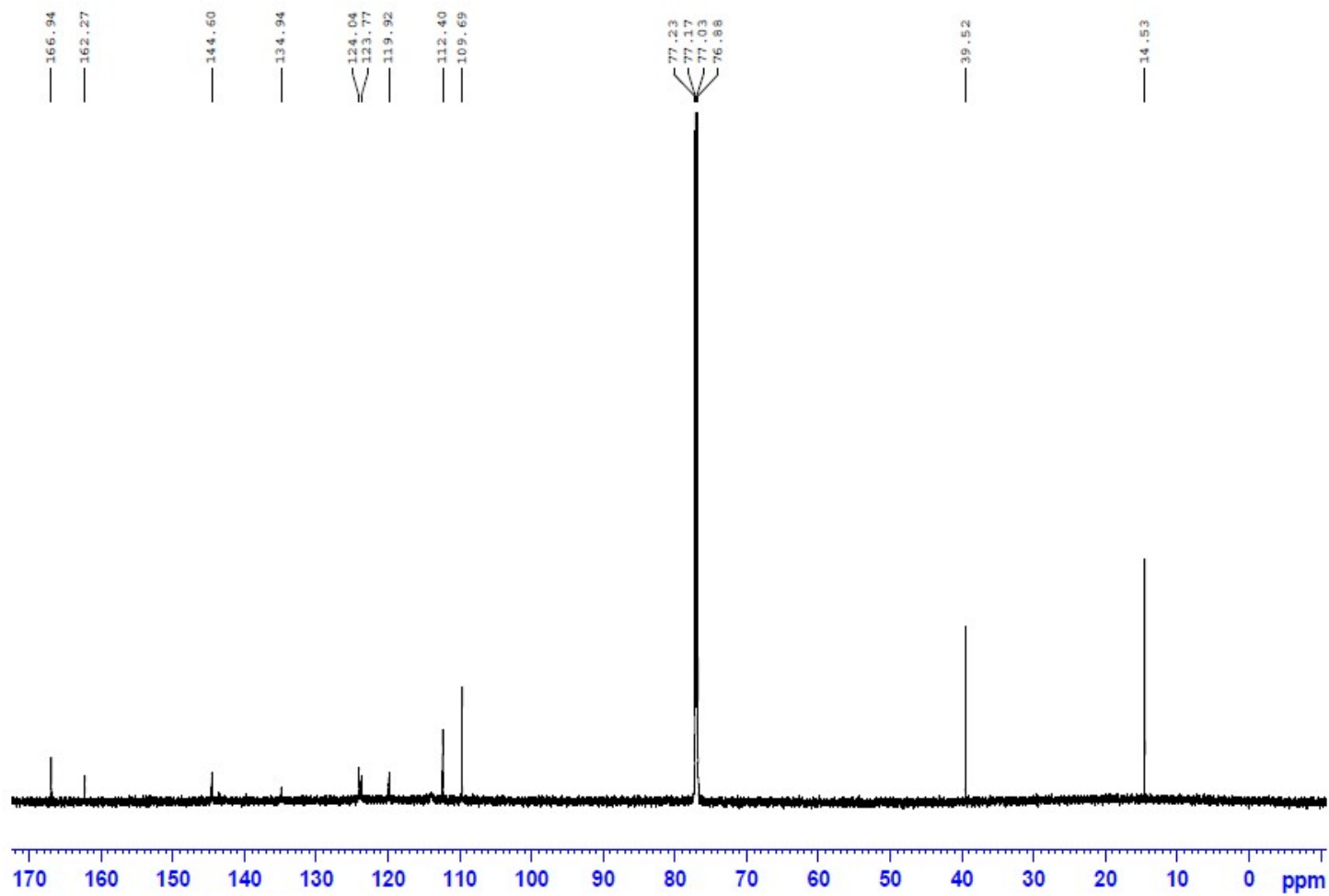
Mahboob
Sample

DMSO



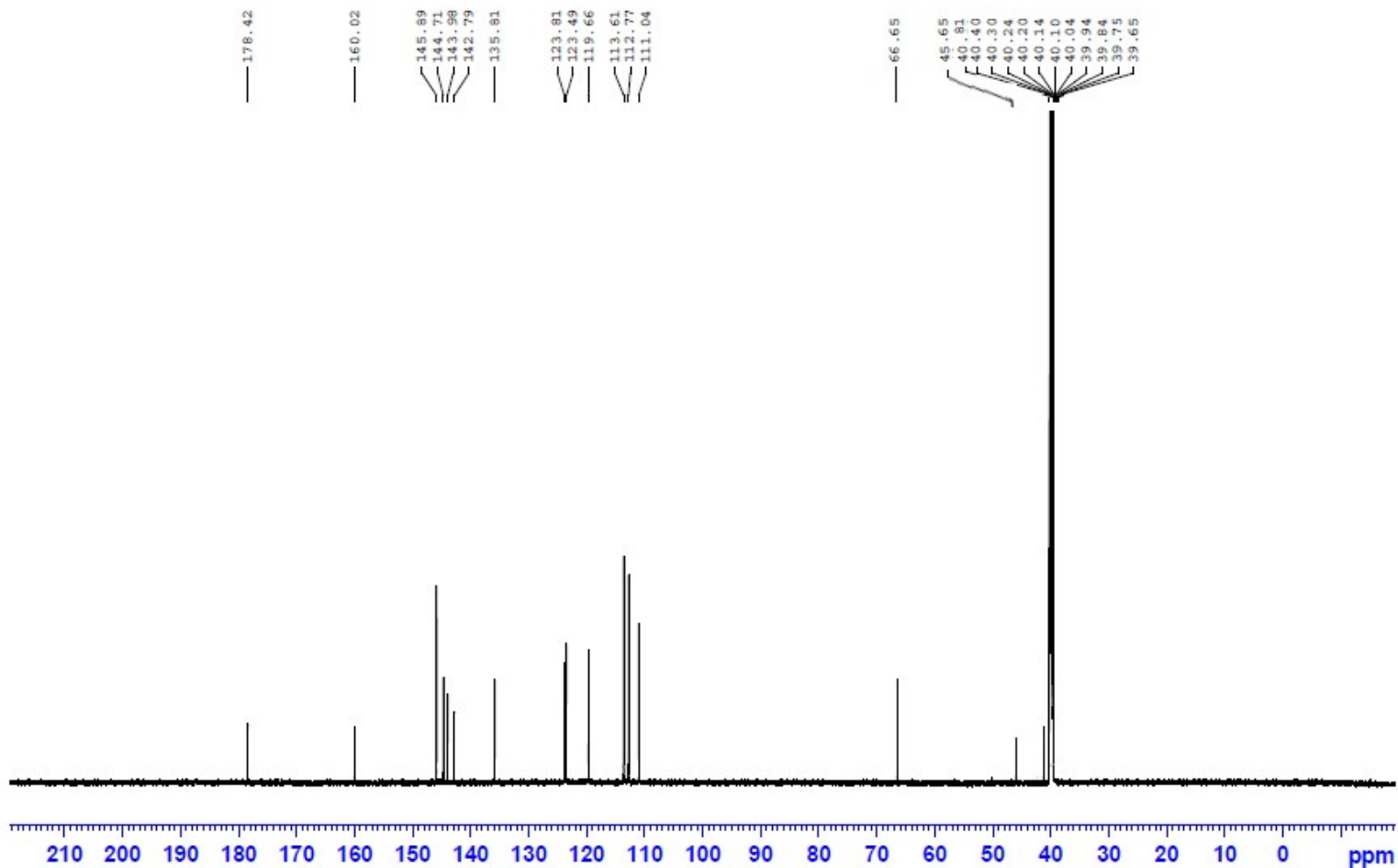
¹³C NMR of compound 19

Mahboob
Sample 15 CDCL₃



¹³C NMR of compound 20

Mahboob
Sample 16 DMSO



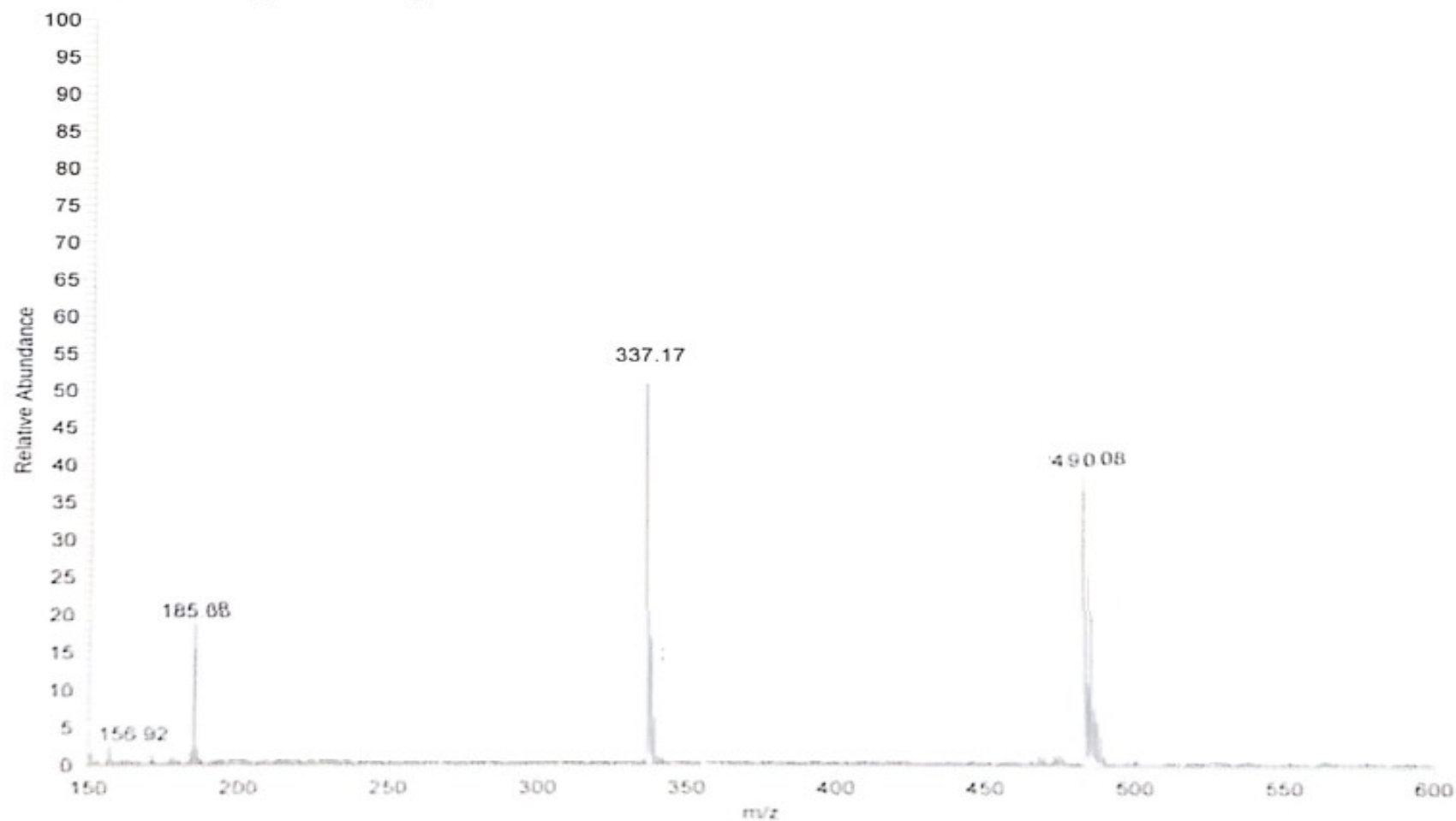
Mass of compound 7

Dr Mohammad Mahboob_210405132615
LCF10605

4/5/2021 2:35:09 PM

BIOXT- 3-Cl 489

Dr Mohammad Mahboob_210405132615 #1 RT: 0.00 AV: 1 NL: 1.46E2
T: ITMS + p ESI Full ms [150.00-600.00]



Mass of compound 8

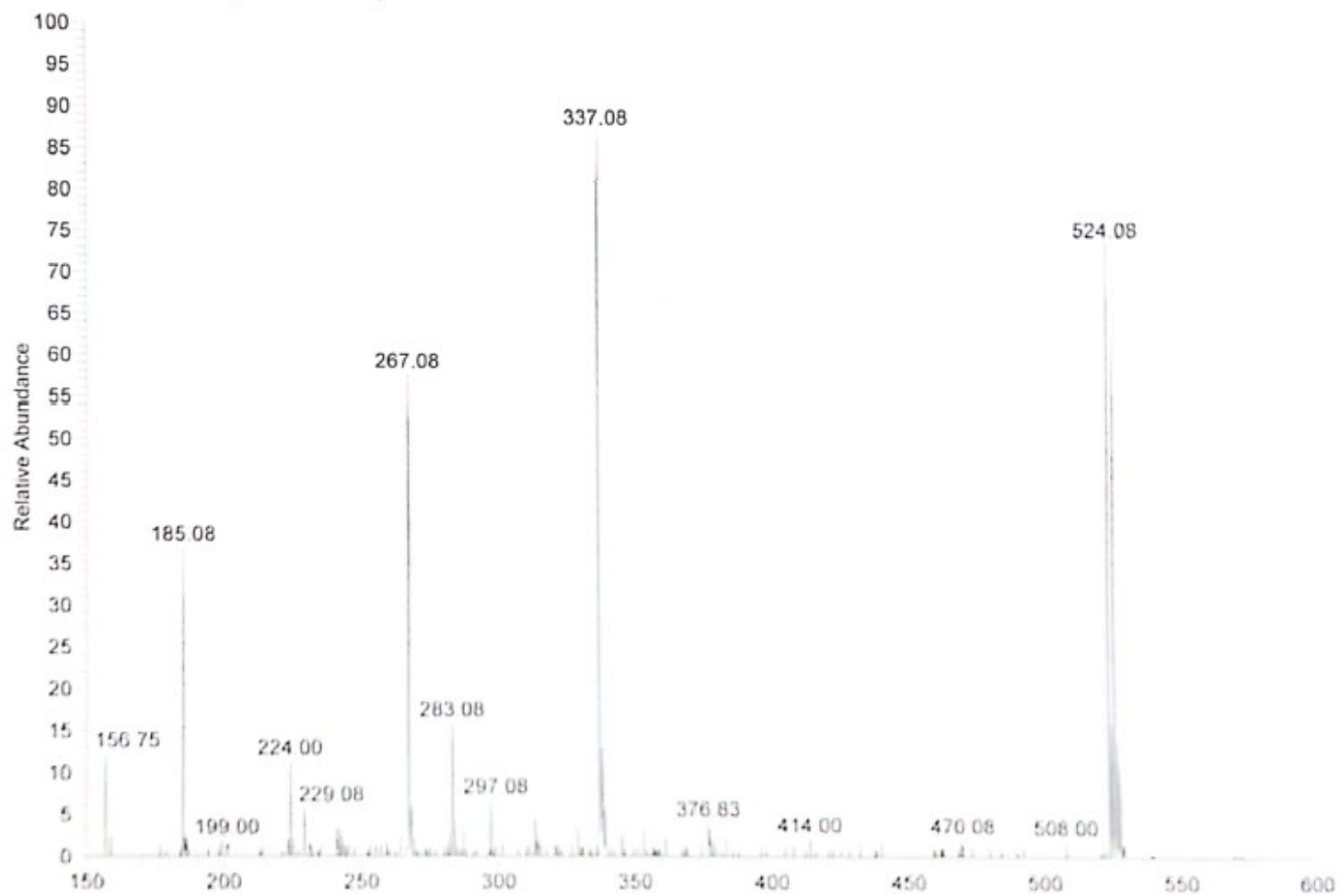
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LCF10605

3/31/2021 2:29:17 PM

BIOXt-2.2-di-Cl

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T: ITMS + p ESI Full ms [150.00-600.00]



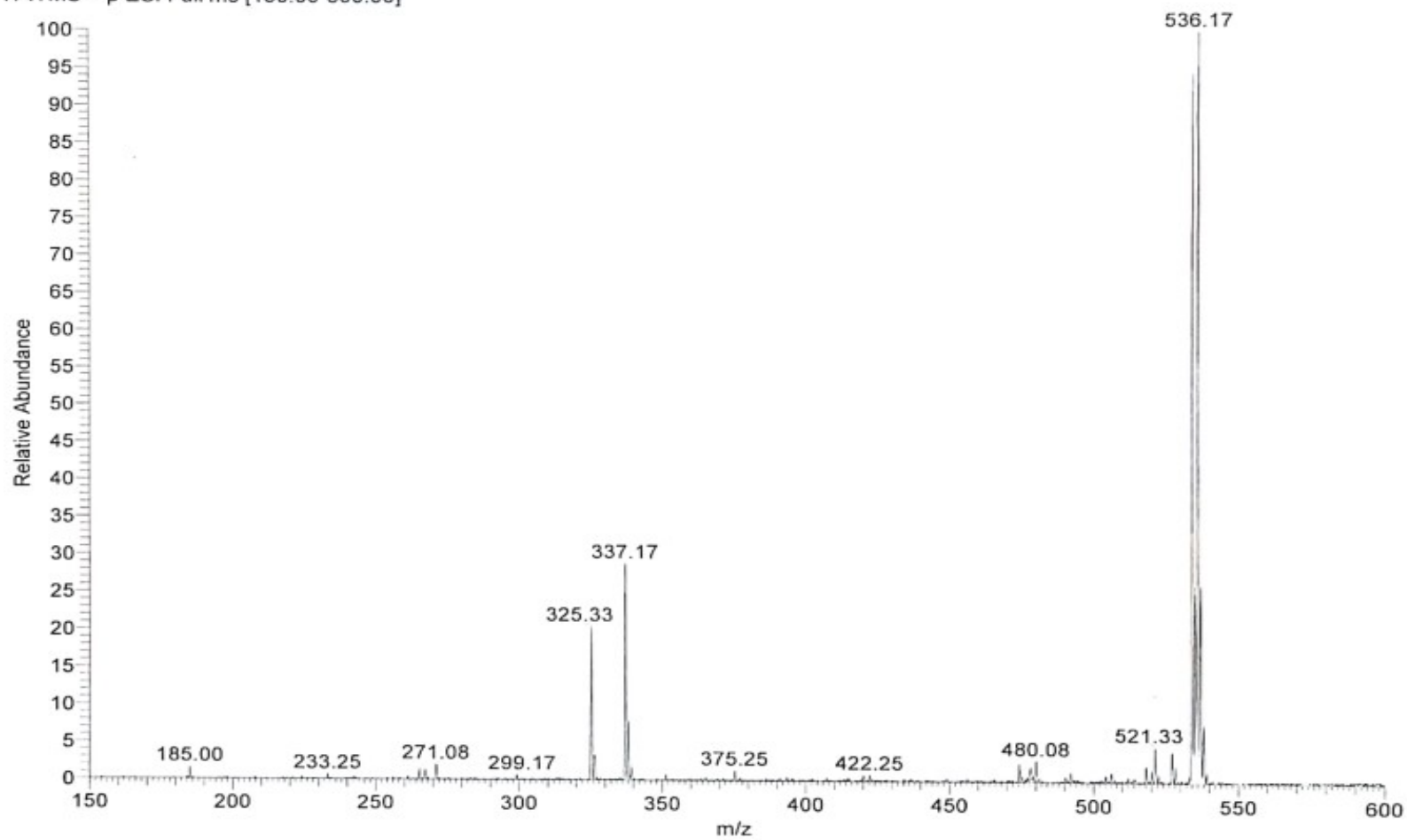
Mass of compound 9

C:\Thermo\...Dr Mahboob_210501164917
LCF10605

5/1/2021 5:05:59 PM

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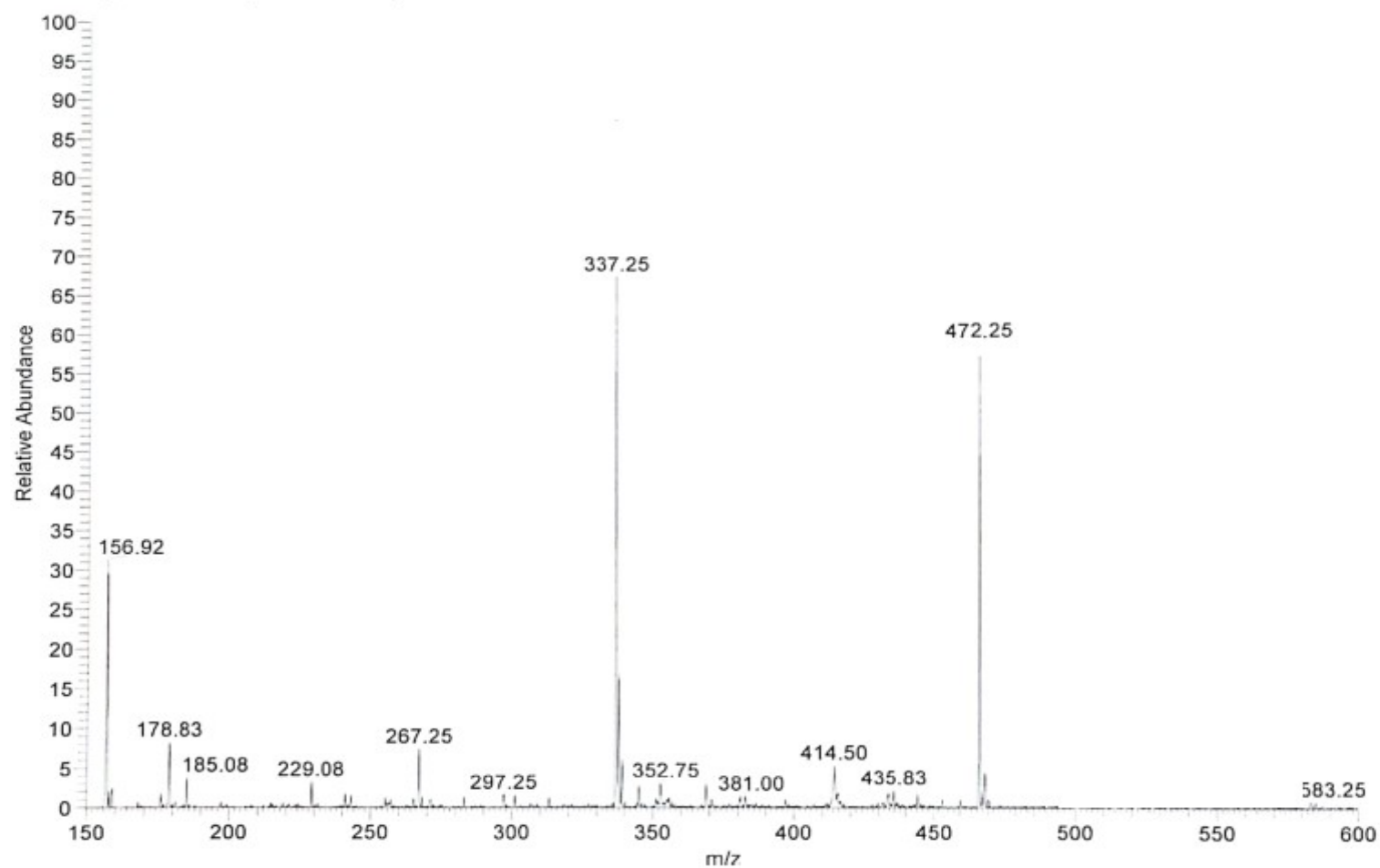
Mass of compound 10

C:\ThermoL... \Dr Mahboob_210331143765
LCF10605

3/31/2021 5:37:25 PM

BIOXt-2OH

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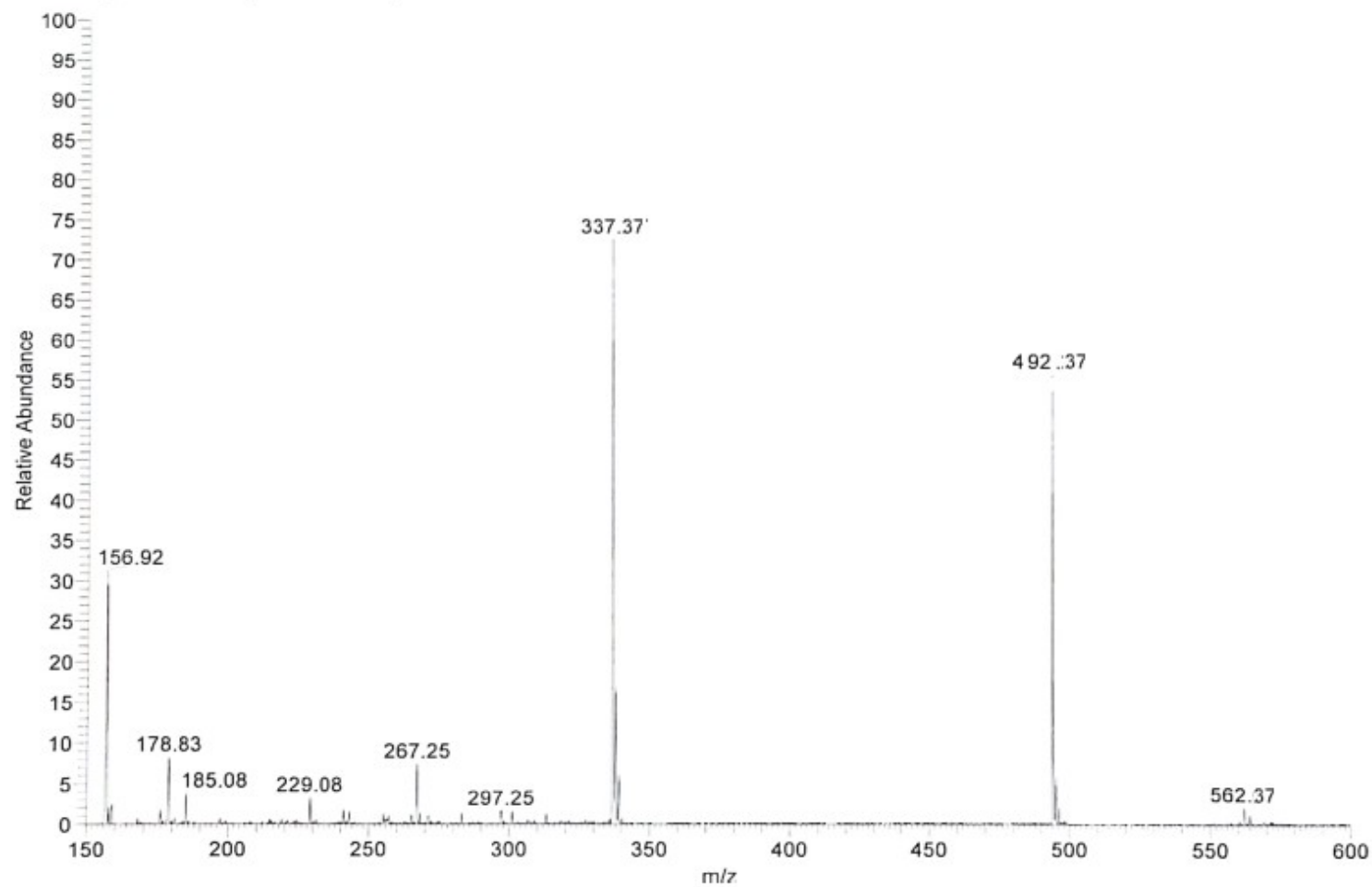


Mass of compound 11

C:\ThermoL...Dr Mahboob_210331143737
LCF10605

3/31/2021 3:37:31 PM

Dr Mahboob_210331143737 #1 RT: 0.00 AV: 1 NL: 1.96E3
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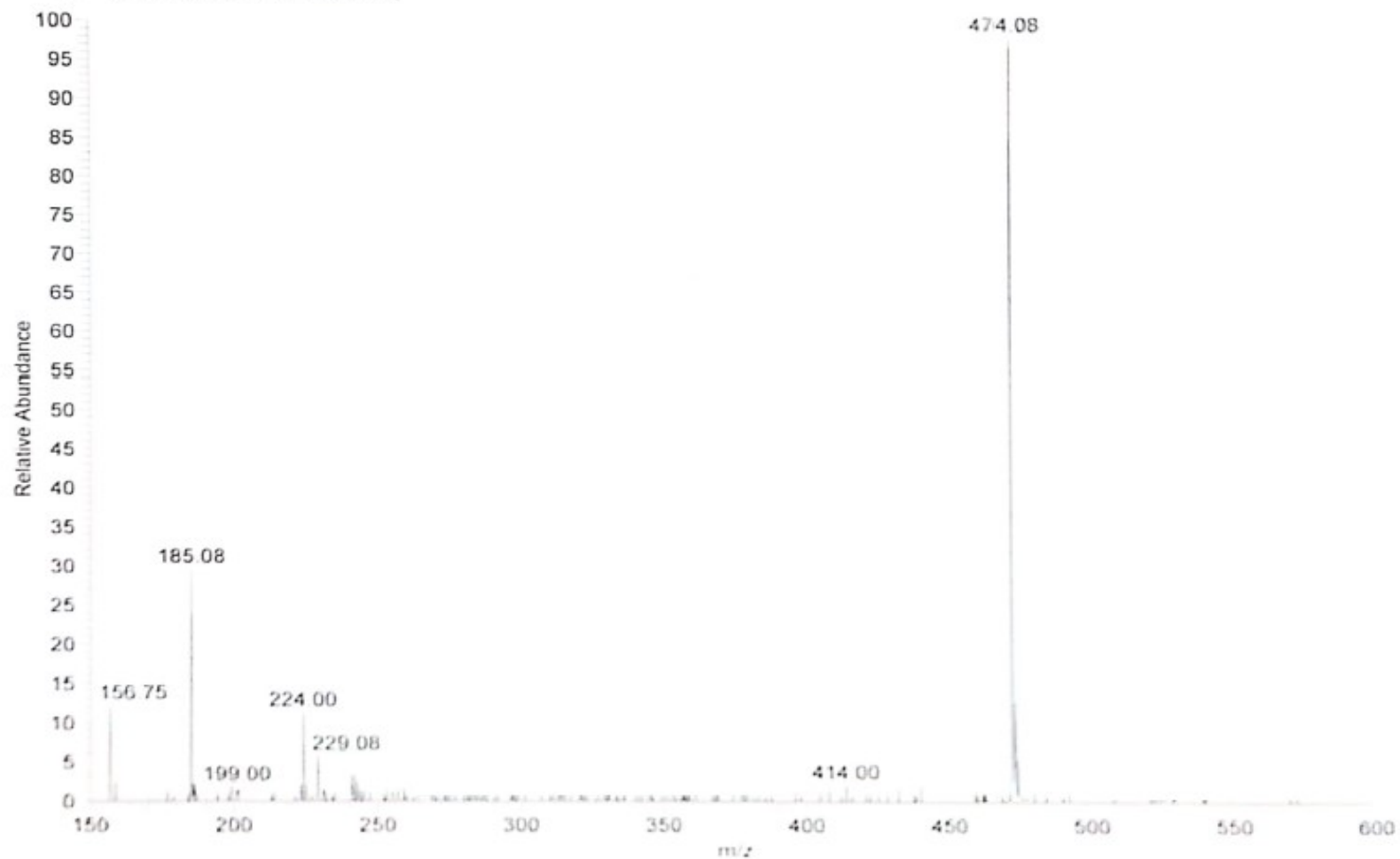


Mass of compound 12

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LCF10605

3/31/2021 4:26:17 PM

Dr Mahboob_2103241437\37.#1 RT: 0.00 AV: 1 NL: 1.92E2
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Mass of compound 13

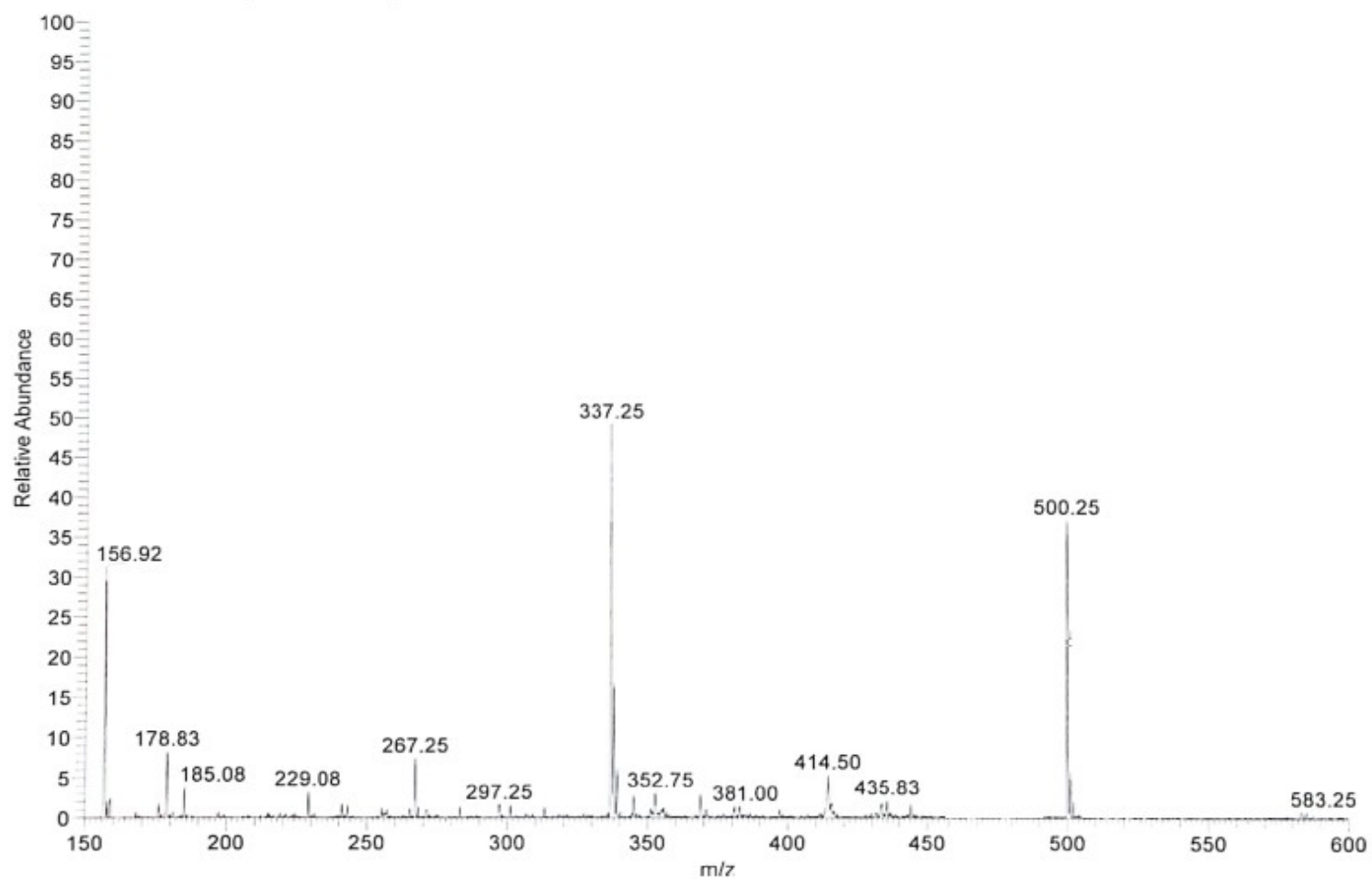
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3/31/2021 2:37:26 PM

BIOXI-3COOH 599

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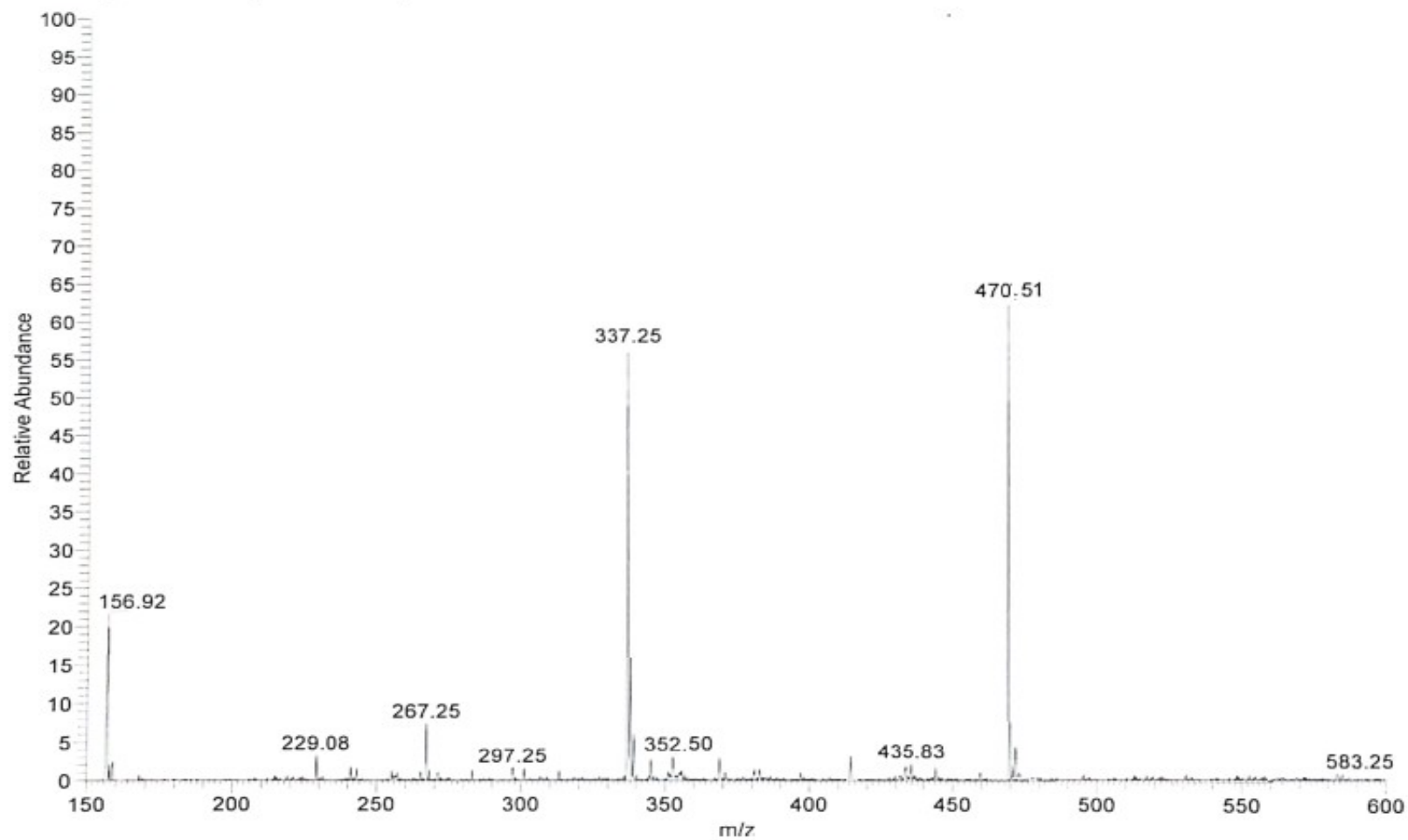
Mass of compound 14

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LCF10605

3/31/2021 5:37:25 PM

BIOXt-2 Me

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T: ITMS + p ESI Full ms [150.00-600.00]



Mass of compound 15

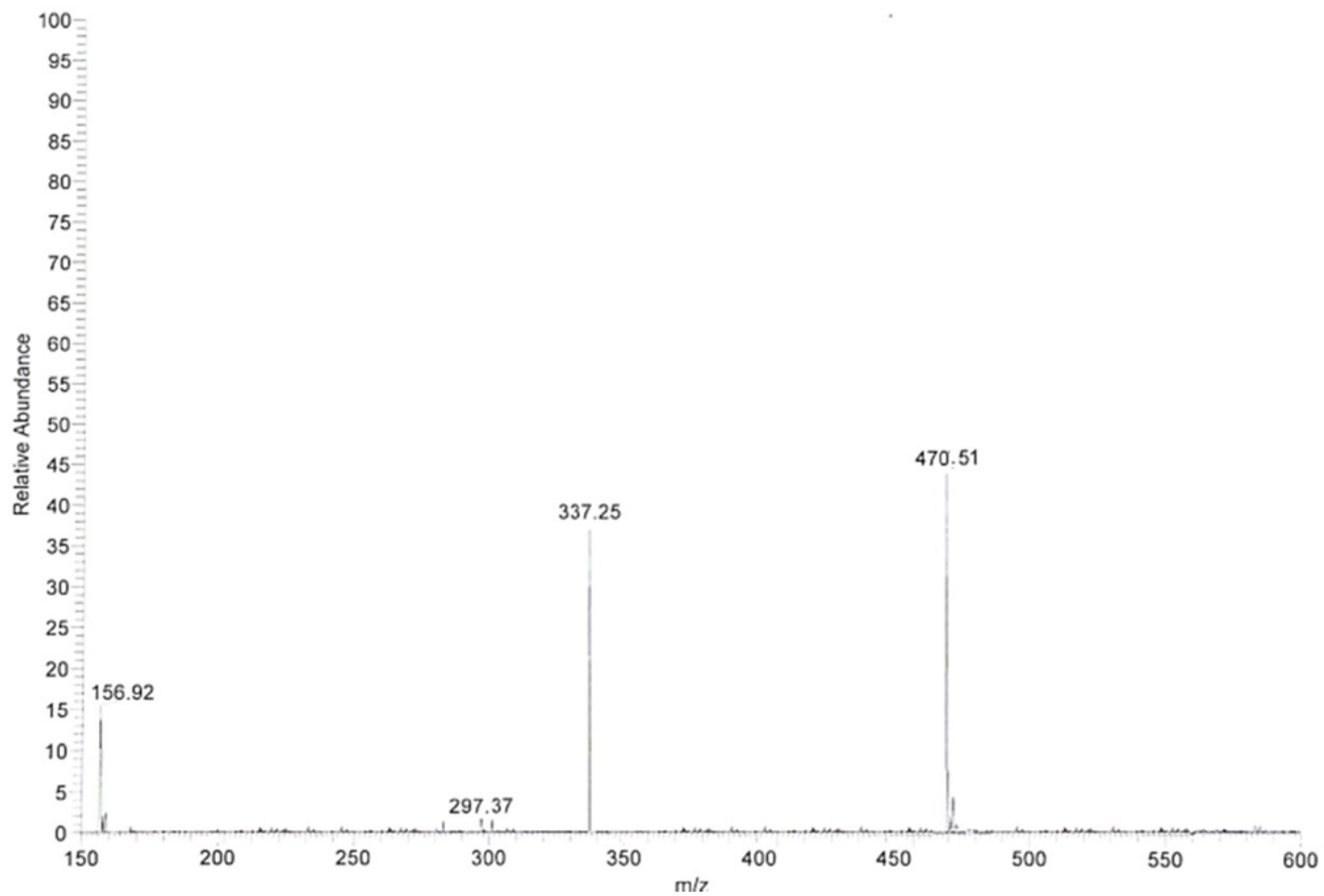
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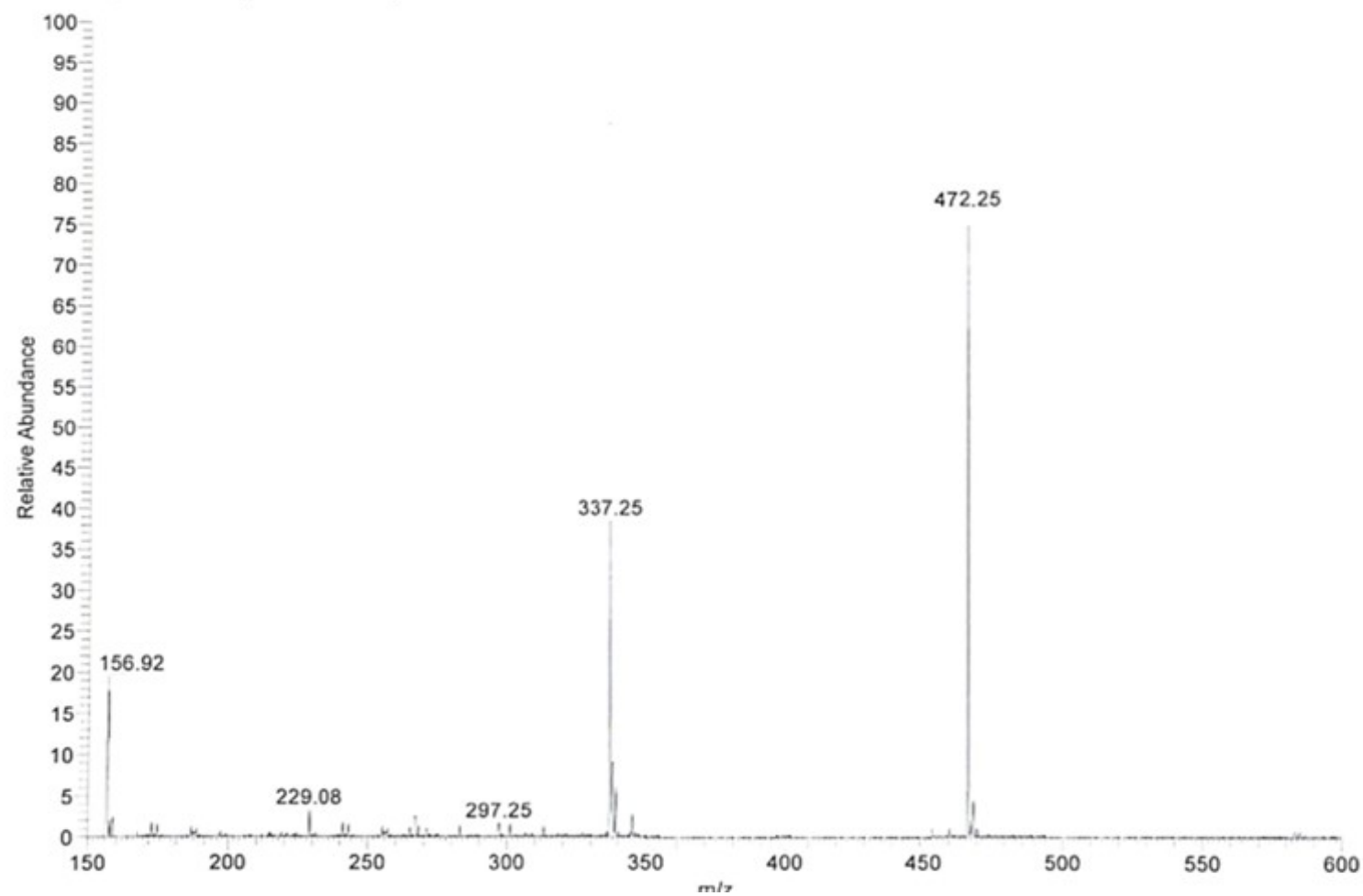
Mass of compound 16

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LCF10605

5/21/2022 6:37:22 PM

BIOXI-3OH

Dr Mahboob_210331143767 #1 RT: 0.00 AV: 1 NL: 1.96E3
T: ITMS + p ESI Full ms [150.00-600.00]



Mass of compound 17

C:\Thermo\...Dr Mahboob_210331143767

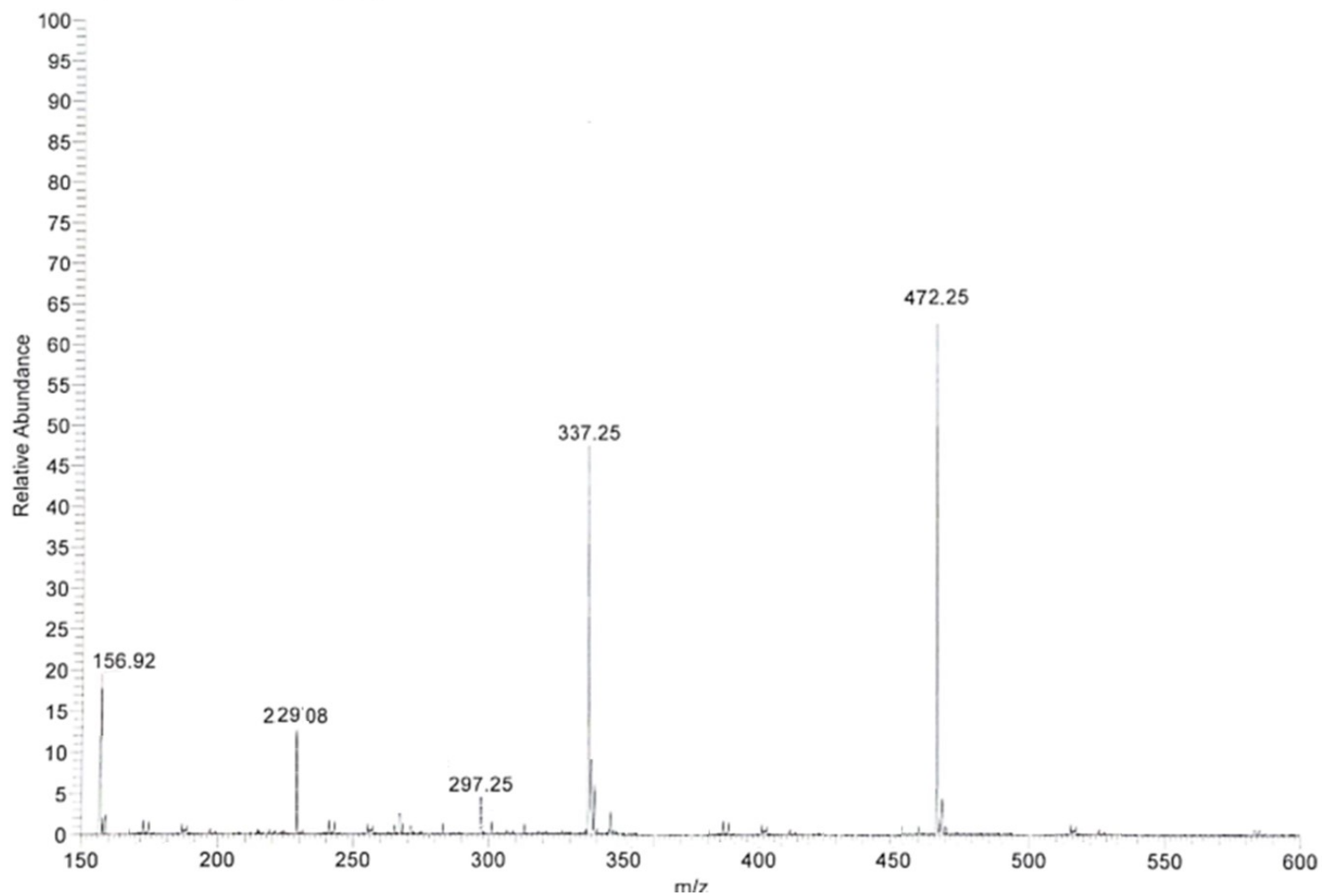
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BIOXI-4OH

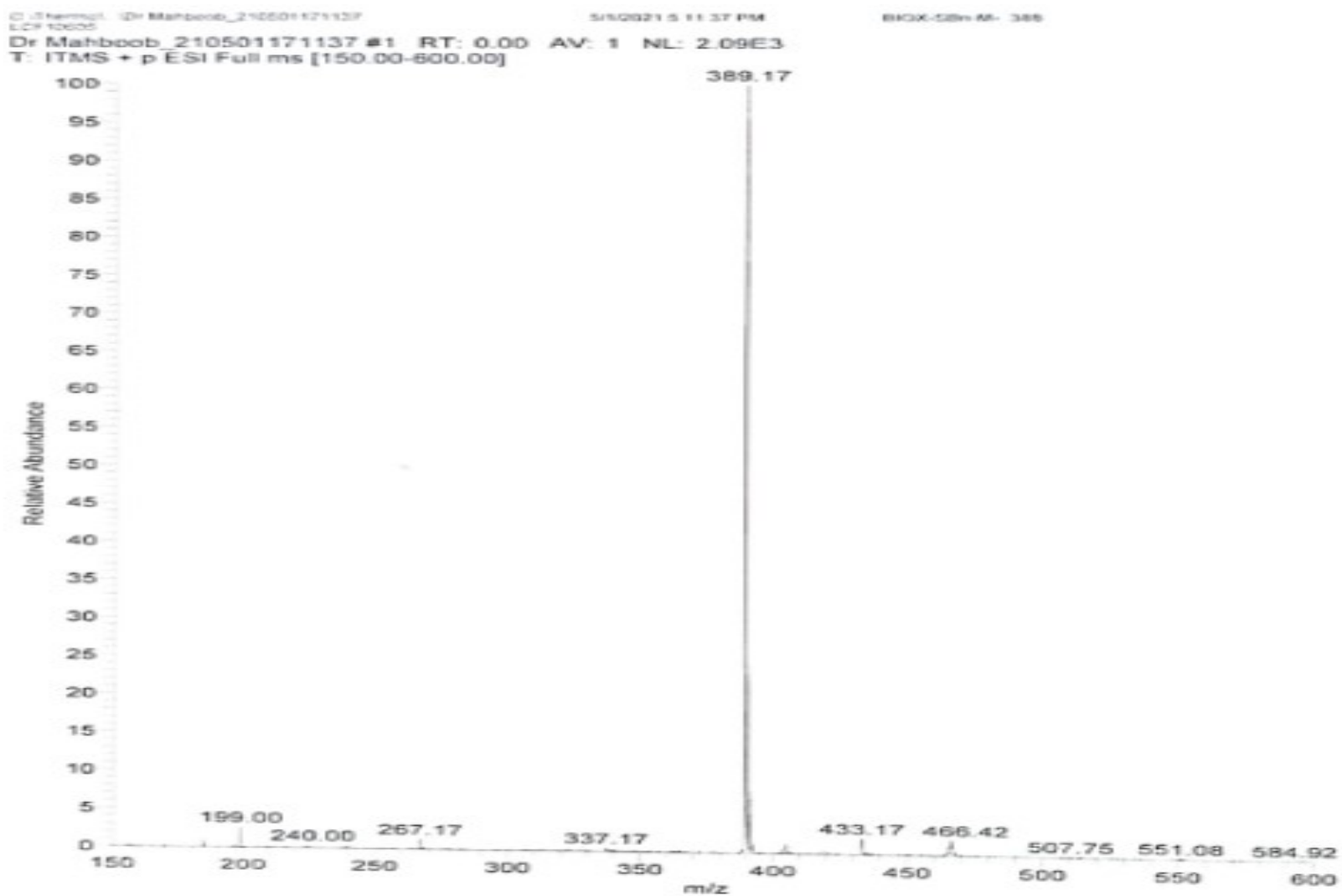
LCF10605

Dr Mahboob_210331143767 #1 RT: 0.00 AV: 1 NL: 1.96E3

T: ITMS + p ESI Full ms [150.00-600.00]



Mass of compound 18



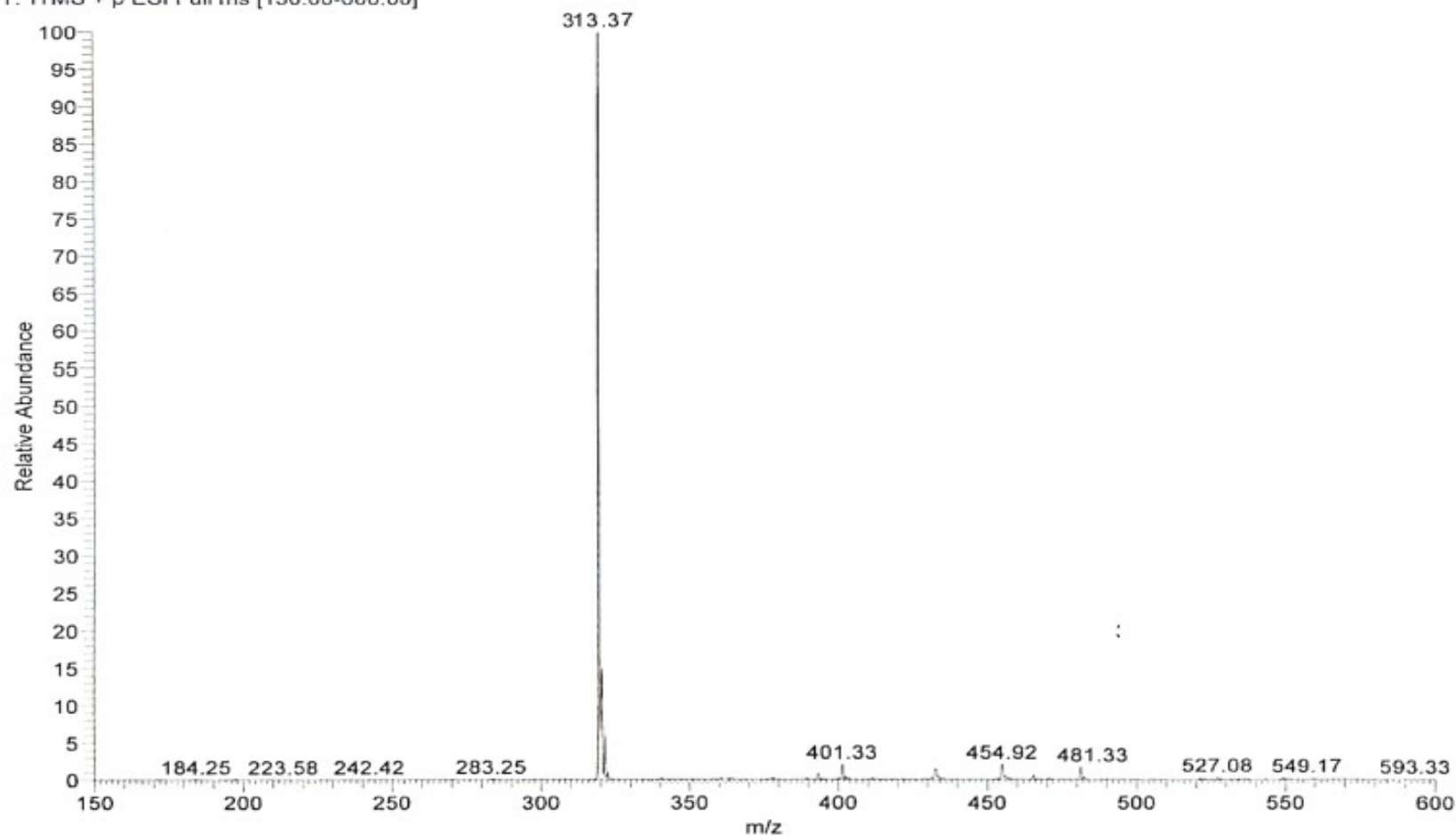
Mass of compound 19

C:\ThermoL...Dr Mahboob_210501172054
LCF10605

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BIOX-S-M-313

Dr Mahboob_210501172054 #1 RT: 0.00 AV: 1 NL: 2.39E4
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Mass of compound 20

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LCF10605

5/1/2021 5:31:45 PM

BIOX-SB-Morpholine

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