SUPPLEMENTARY MATERIAL

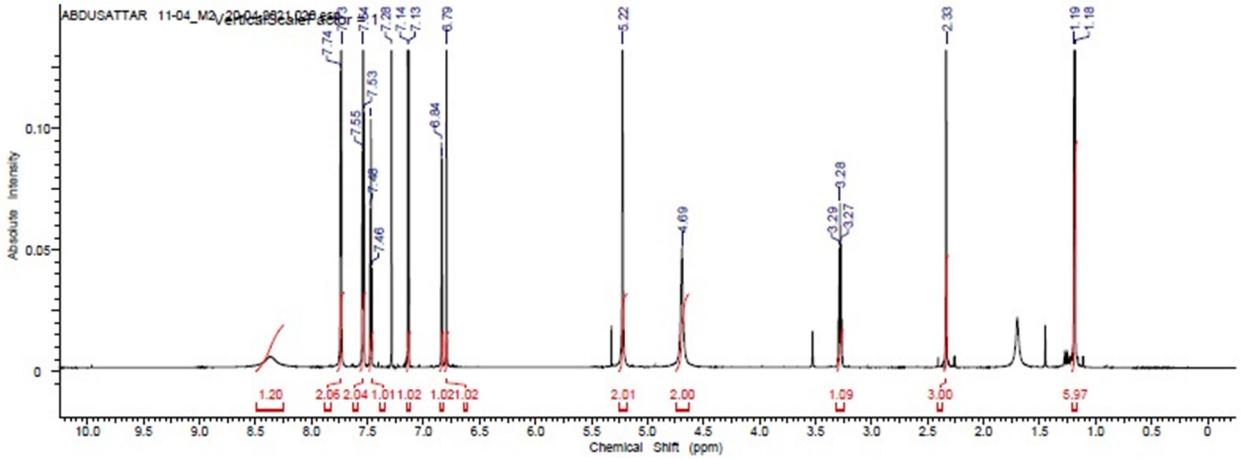
Synthesis and Biological evaluation of 1,2,3-triazole tethered thymol-1,3,4-oxadiazole derivatives as anticancer and antimicrobial agents

Figure S1-S9: ^{1}H NMR of final compounds

Compound 6

4/23/2021 9:41:27 PM

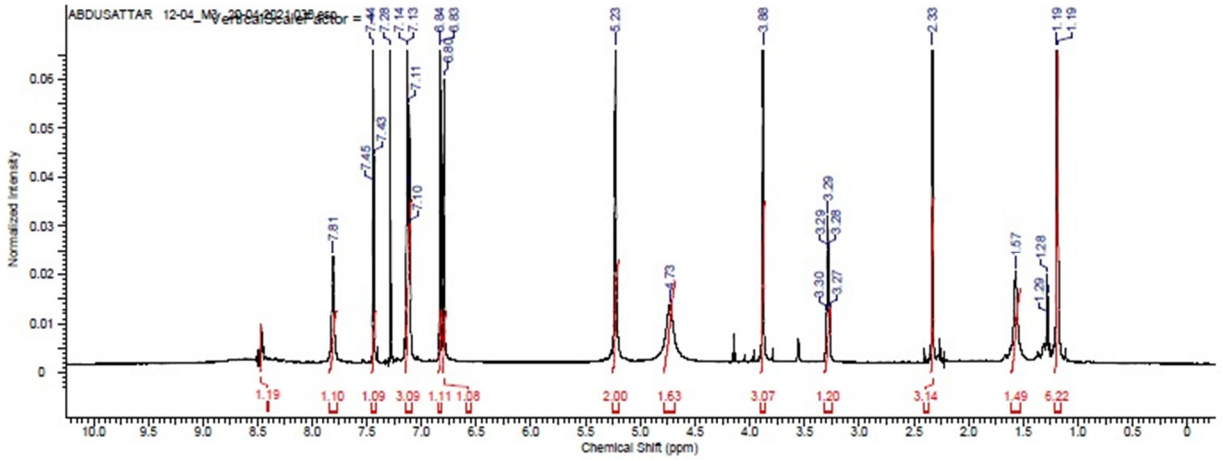
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Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	11.37
SW(cyclical) (Hz)	17006.80	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	5250.0283
Spectrum Type	STANDARD	Sweep Width (Hz)	17006.28	Temperature (degree C)	24.999		



Compound 7

4/24/2021 9:31:50 PM

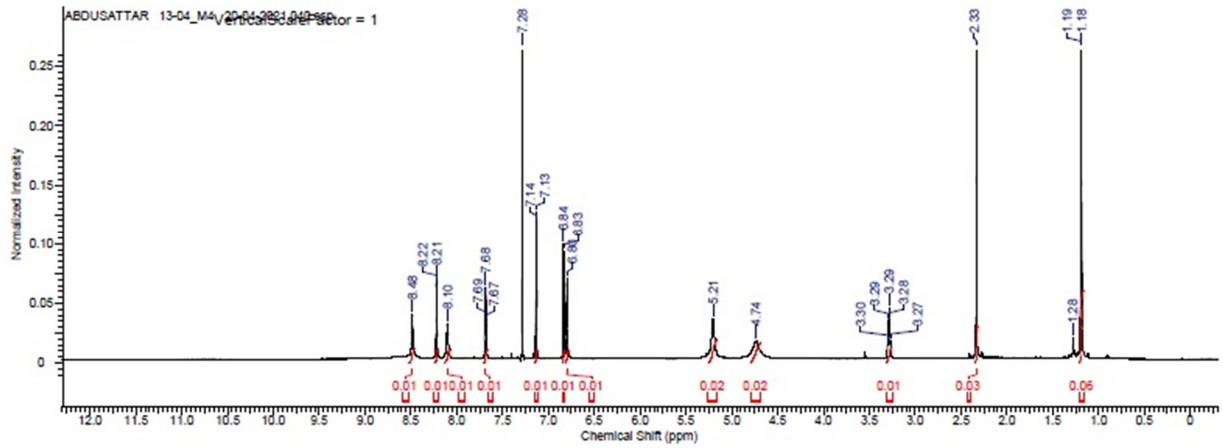
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Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	12.46
SW(cyclical) (Hz)	17006.80	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	5250.0283
Spectrum Type	STANDARD	Sweep Width (Hz)	17006.28	Temperature (degree C)	25.000		



Compound 8

4/24/2021 9:45:03 PM

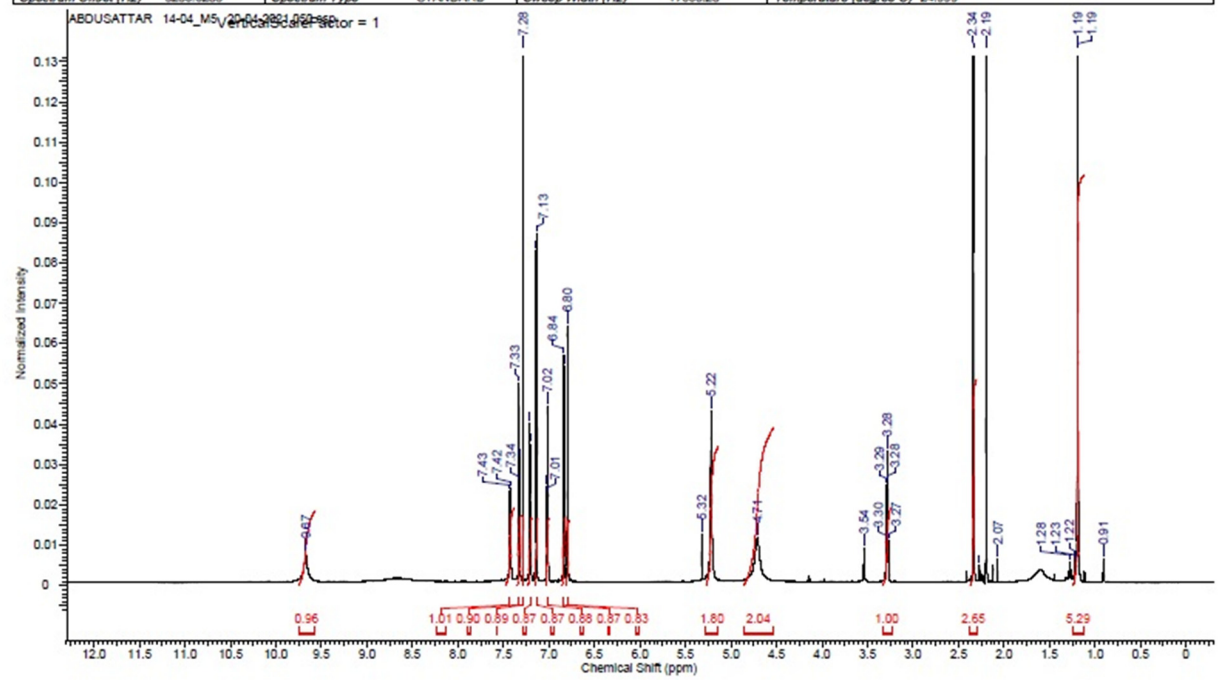
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Date Stamp	20 Apr 2021 17:26:08						
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Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	12.46
SW(cyclical) (Hz)	17006.80	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	5250.0283
Spectrum Type	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	25.000		



Compound 9

7/31/2021 2:14:02 PM

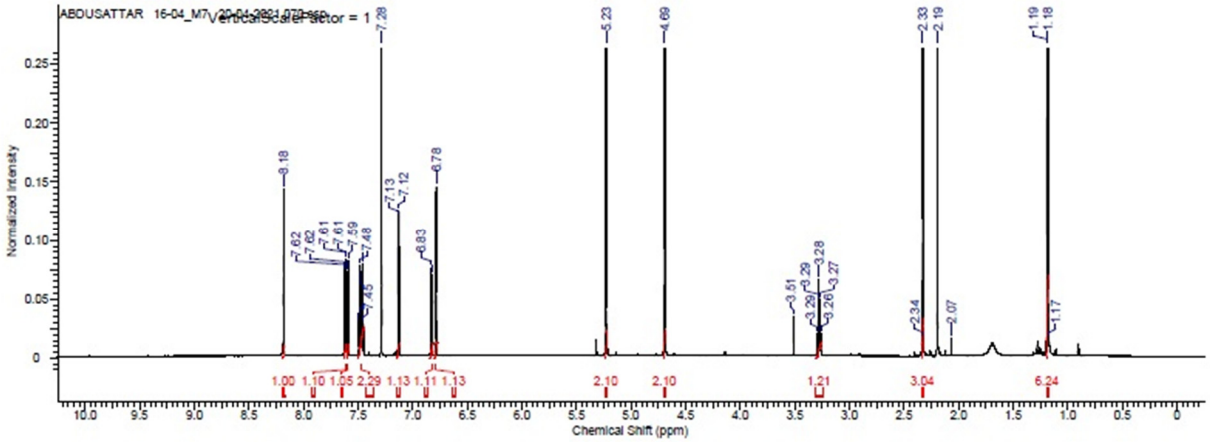
Acquisition Time (sec)	1.9268	*Comment*	Dr. Abdusattar Sampe 14-04 CDCL3			*Date*	20 Apr 2021 18:17:20
Date Stamp	20 Apr 2021 18:17:20			*File Name*	C:\Users\hp\Desktop\Azizah 20210422\ABDUSATTAR 14-04 M5 20-04-2021\50\fid		
Frequency (MHz)	850.15	*Nucleus*	1H	*Number of Transients*	32	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	12.46	*SW(cyclical) (Hz)*	17006.80	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	5250.0283	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	24.999



Compound 11

4/24/2021 10:56:08 PM

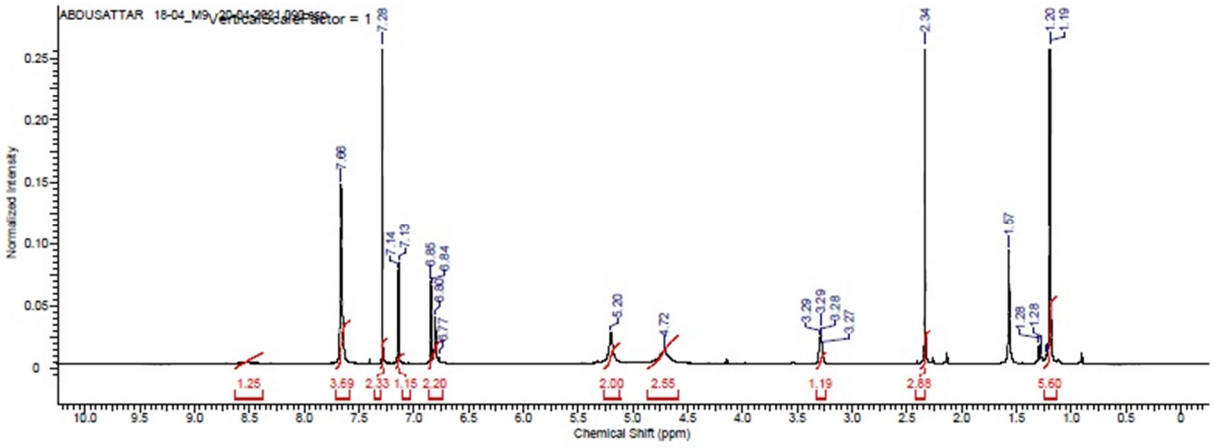
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Date Stamp	20 Apr 2021 20:04:00				
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Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	12.46
SW(cyclical) (Hz)	17006.80	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	5250.0283
Spectrum Type	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	25.000		



Compound 13

4/24/2021 11:13:54 PM

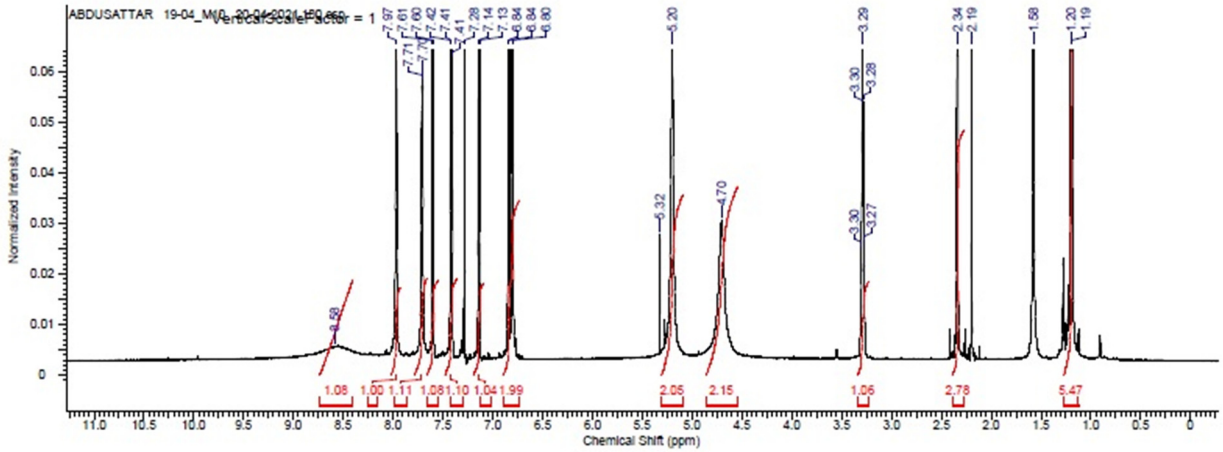
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Date Stamp	20 Apr 2021 21:12:16				
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Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	12.46
SW(cyclical) (Hz)	17006.80	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	5250.0283
Spectrum Type	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	25.000		



Compound 14

4/25/2021 12:35:16 AM

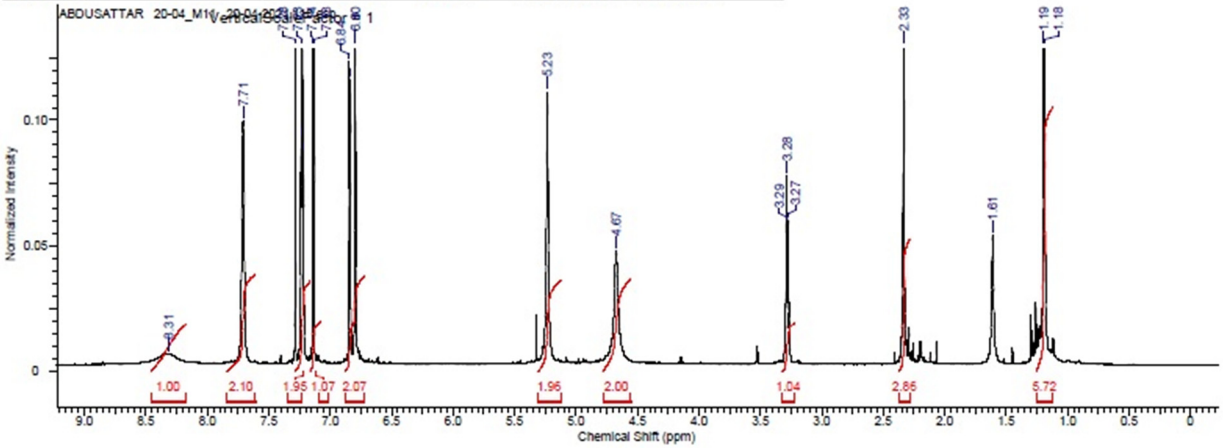
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Date Stamp	20 Apr 2021 22:05:36				
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Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	12.46
SW(cyclical) (Hz)	17006.80	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	5250.0283
Spectrum Type	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	24.998		



Compound 15

4/25/2021 12:42:29 AM

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Date Stamp	20 Apr 2021 22:58:56				
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Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	12.46
SW(cyclical) (Hz)	17006.80	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	5250.0283
Spectrum Type	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	25.000		



Compound 16

4/25/2021 12:48:47 AM

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Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	12.46
SW(cyclical) (Hz)	17006.80	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	5250.0283
Spectrum Type	STANDARD	*Sweep Width (Hz)*	17006.28	*Temperature (degree C)*	25.000		

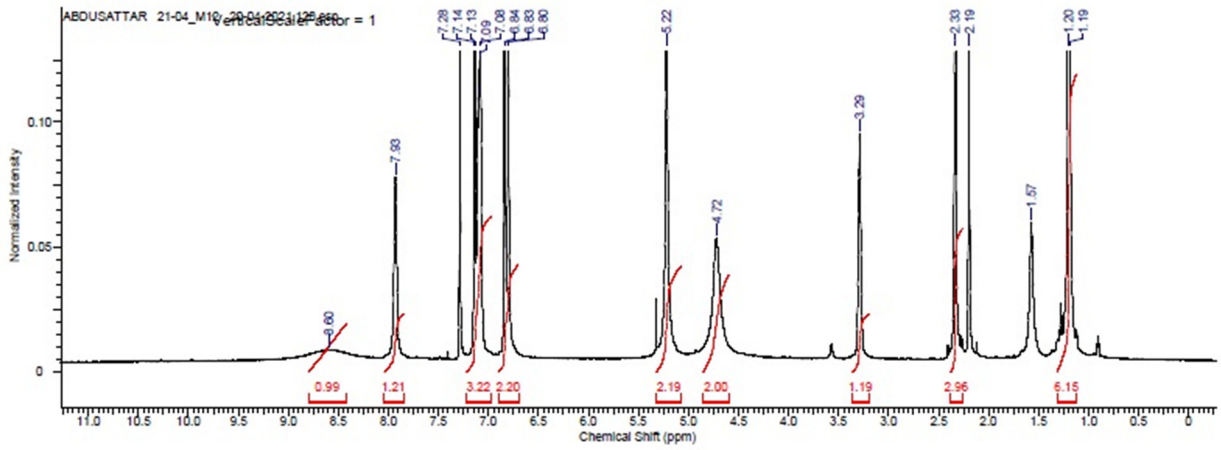
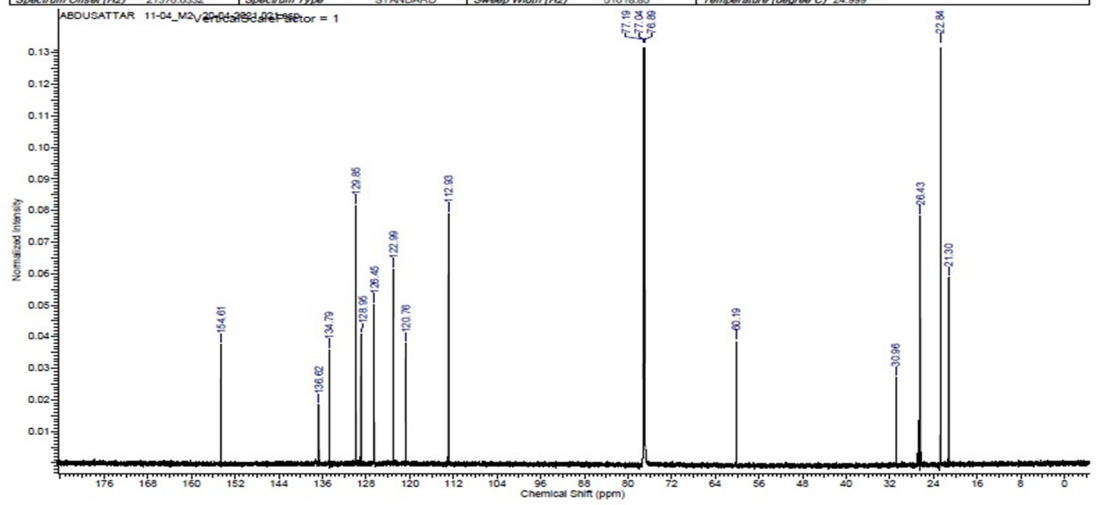


Figure S10-S18: ^{13}C NMR of final compounds

Compound 6

7/31/2021 2:20:56 PM

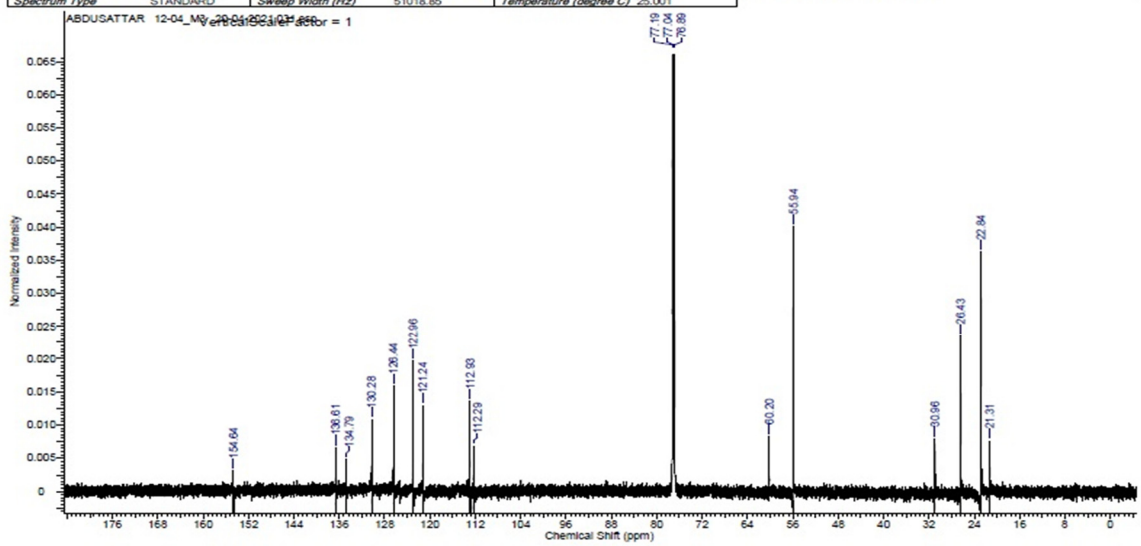
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Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	21376.0332	Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999



Compound 7

4/25/2021 1:02:28 AM

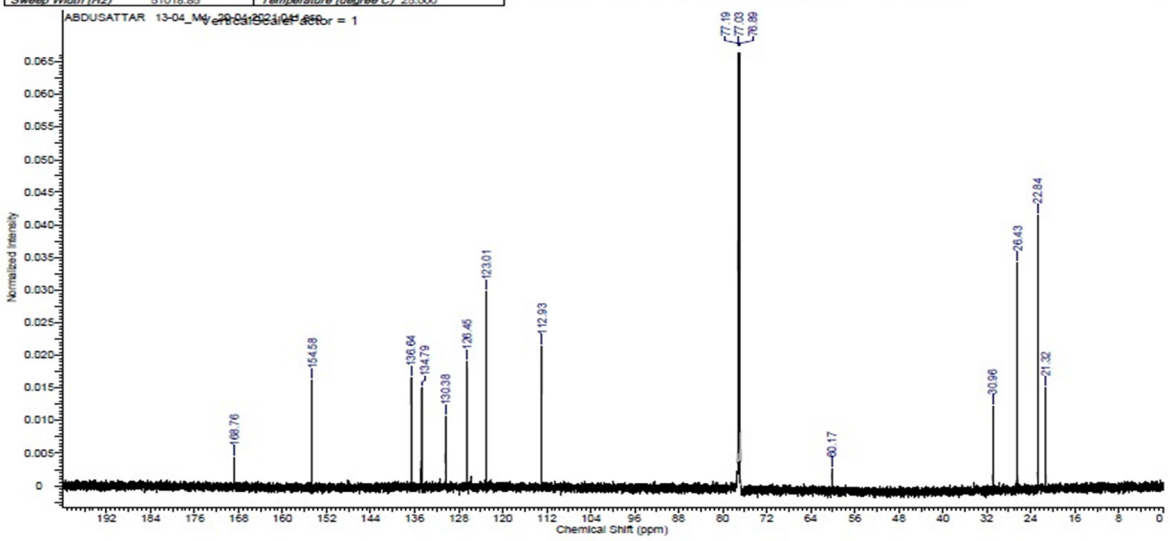
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Nucleus	13C	Number of Transients	500	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	186.93
SW(cyclical) (Hz)	51020.41	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	21376.0332
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.001		



Compound 8

4/25/2021 1:20:18 AM

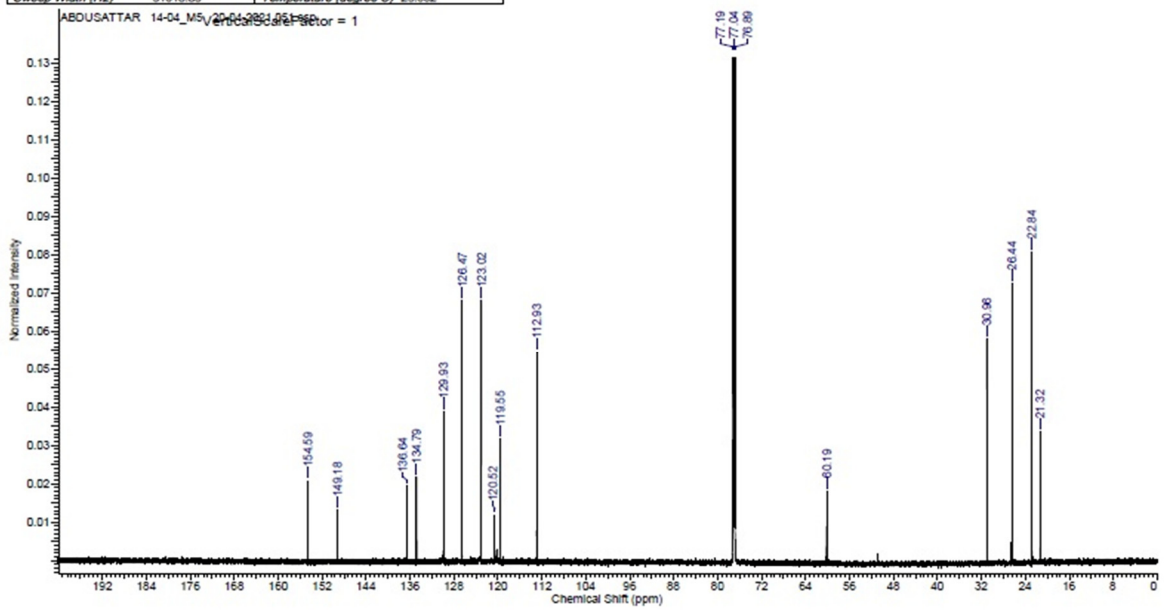
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Date Stamp	20 Apr 2021 18:13:04						
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Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	186.93
SW(cyclical) (Hz)	51020.41	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	21376.0332	*Spectrum Type*	STANDARD
Sweep Width (Hz)	51018.85	*Temperature (degree C)*	25.000				



Compound 9

4/25/2021 1:23:18 AM

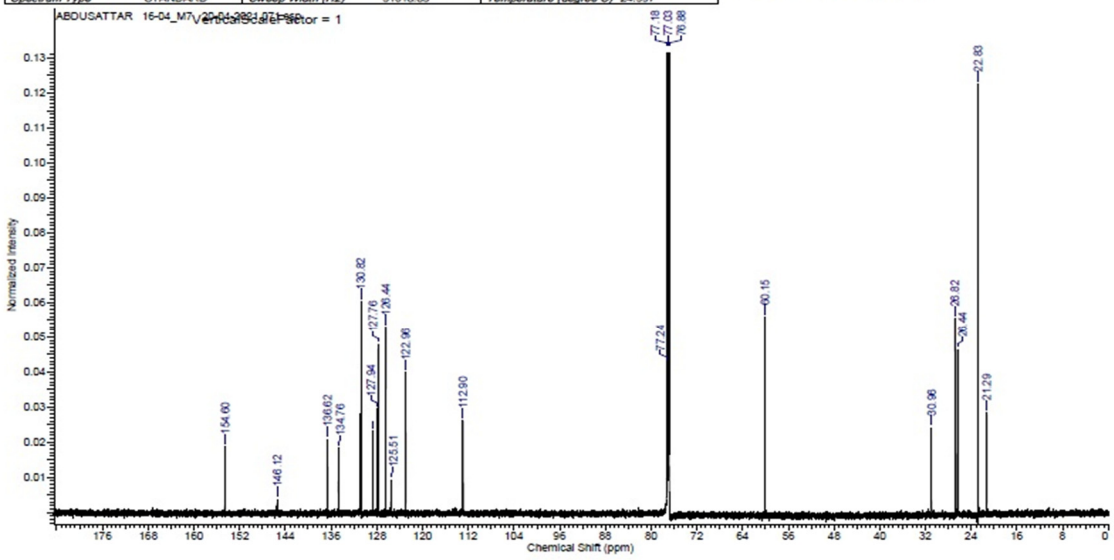
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Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	186.93
SW(cyclical) (Hz)	51020.41	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	21376.0332	*Spectrum Type*	STANDARD
Sweep Width (Hz)	51018.85	*Temperature (degree C)*	25.002				



Compound 11

4/25/2021 1:34:06 AM

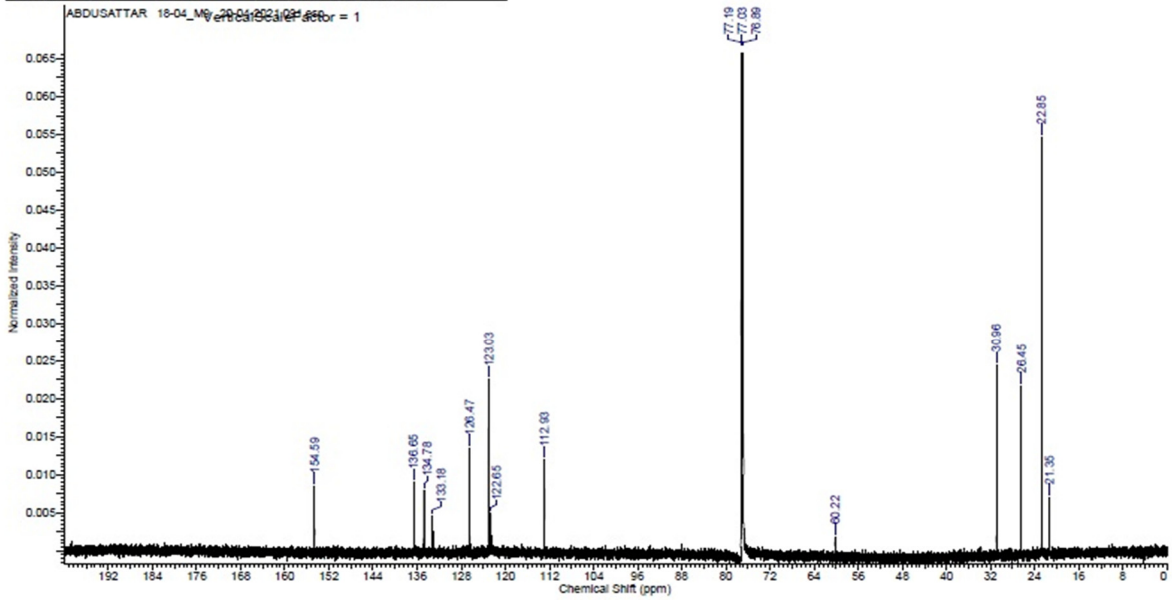
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Nucleus	13C	Number of Transients	700	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	186.93
SW(cyclical) (Hz)	51020.41	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	21376.0332
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.997		



Compound 13

4/25/2021 1:42:00 AM

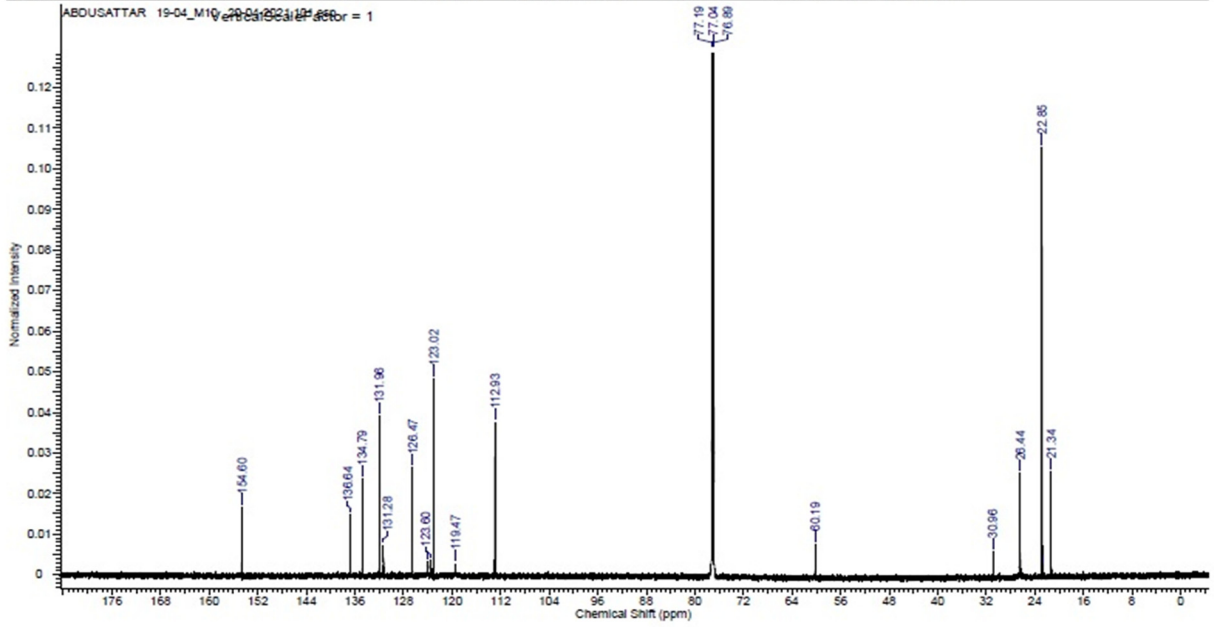
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Nucleus	13C	Number of Transients	1024	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	186.93
SW(cyclical) (Hz)	51020.41	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	21376.0332	Spectrum Type	STANDARD
Sweep Width (Hz)	51018.85	Temperature (degree C)	25.001				



Compound 14

7/31/2021 3:53:41 PM

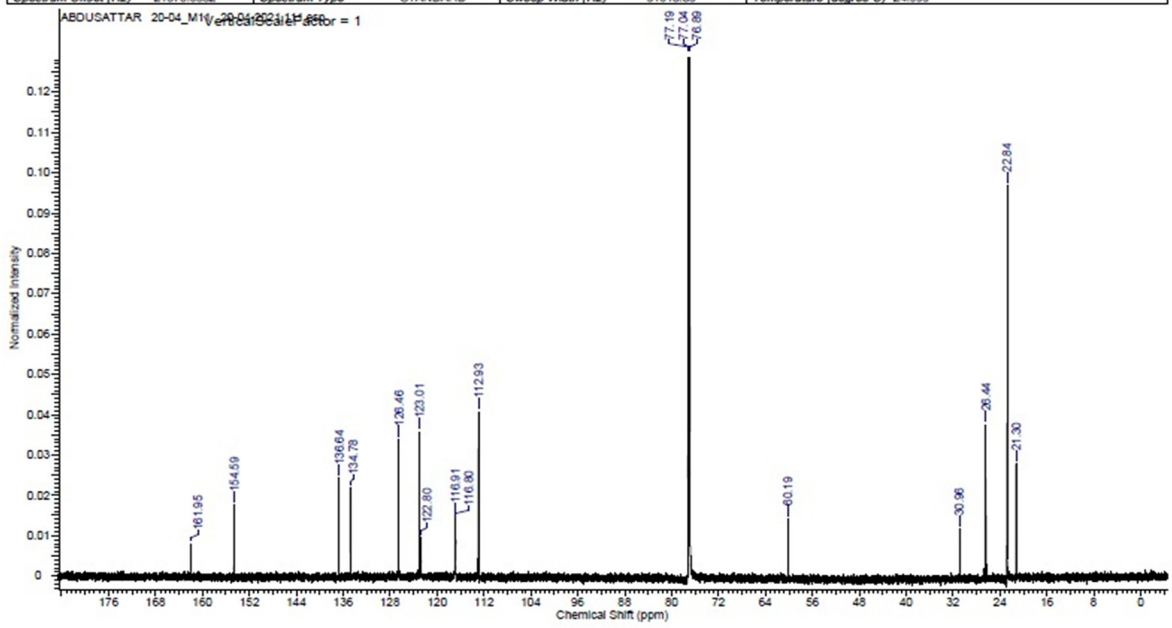
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Date Stamp	20 Apr 2021 22:52:32			*File Name*	C:\Users\hp\Desktop\Azizah_20210422\ABDUSATTAR_19-04_M10_20-04-2021\101\fid		
Frequency (MHz)	213.77	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	186.93	*SW(cyclical) (Hz)*	51020.41	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	21376.0332	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	51018.85	*Temperature (degree C)*	25.001



Compound 15

7/31/2021 3:55:32 PM

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Frequency (MHz)	213.77	*Nucleus*	13C	*Number of Transients*	500	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	186.93	*SW(cyclical) (Hz)*	51020.41	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	21376.0332	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	51018.85	*Temperature (degree C)*	24.999



Compound 16

4/25/2021 1:52:43 AM

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Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	186.93
SW(cyclical) (Hz)	51020.41	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	21376.0332	*Spectrum Type*	STANDARD
Sweep Width (Hz)	51018.85	*Temperature (degree C)*	25.001				

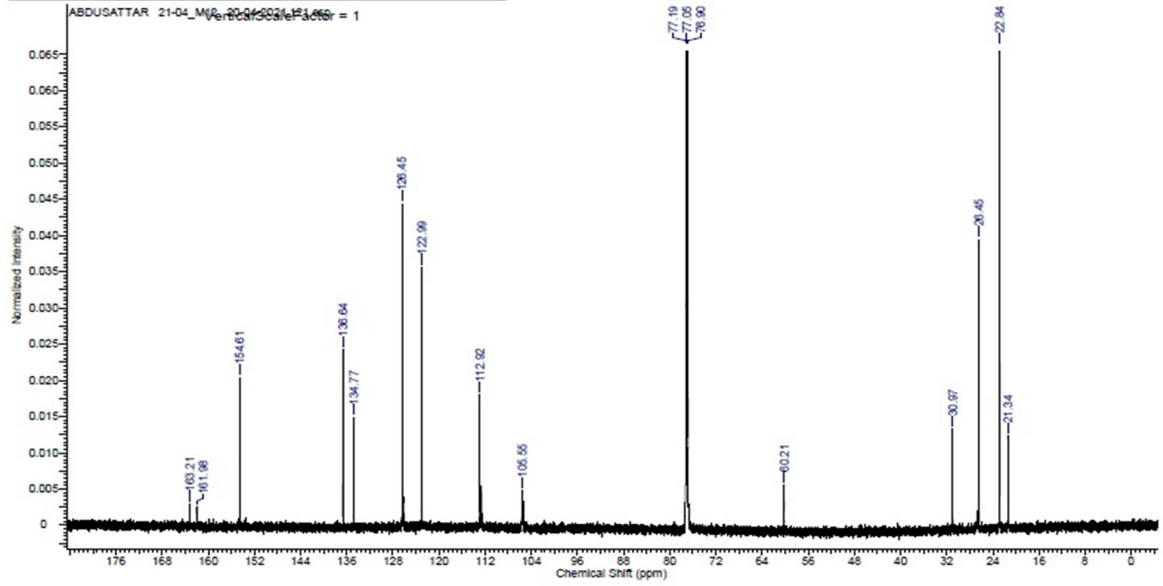
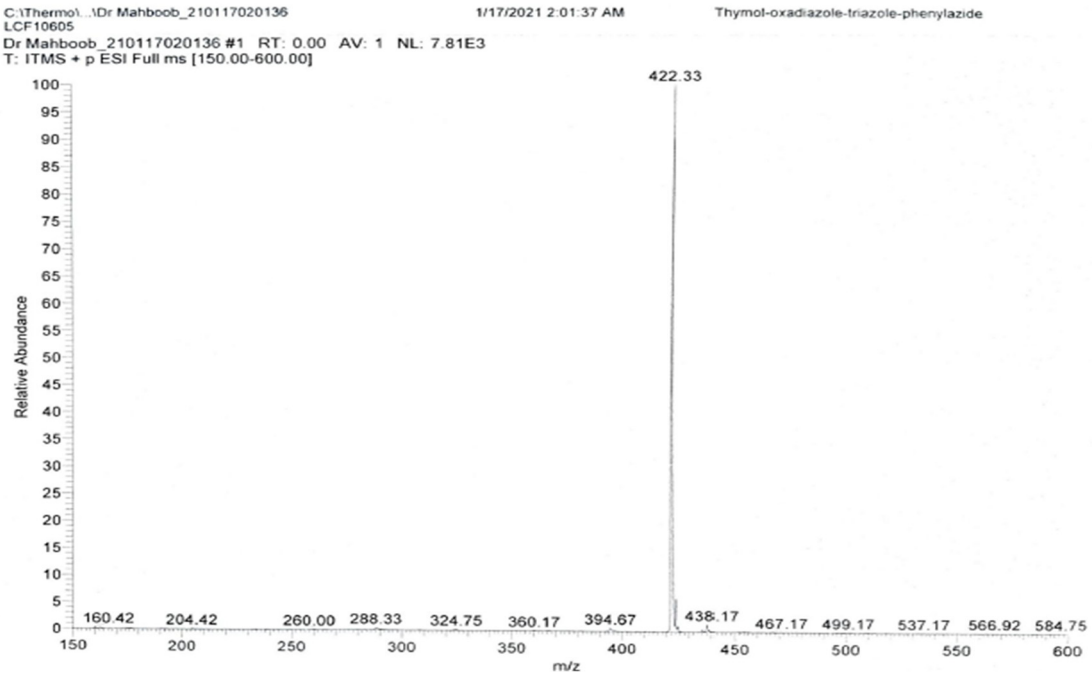
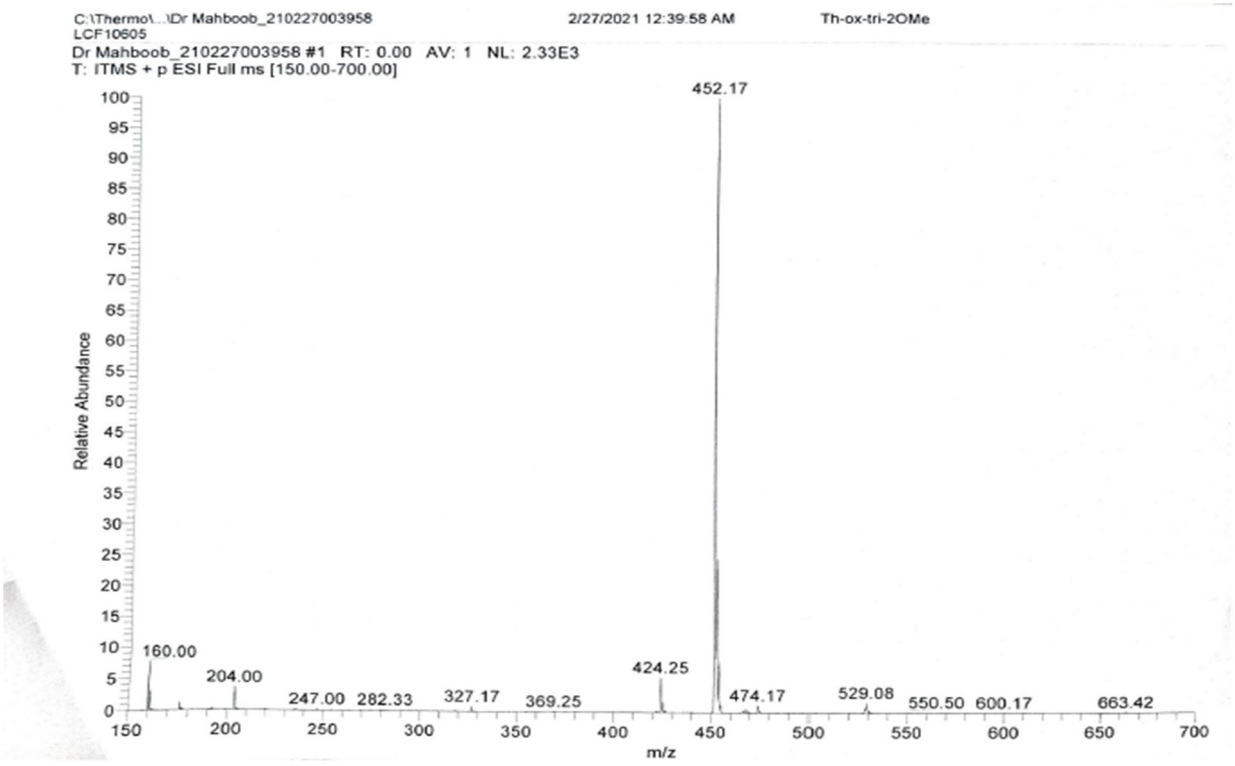


Figure S19-S29: Mass of final compounds

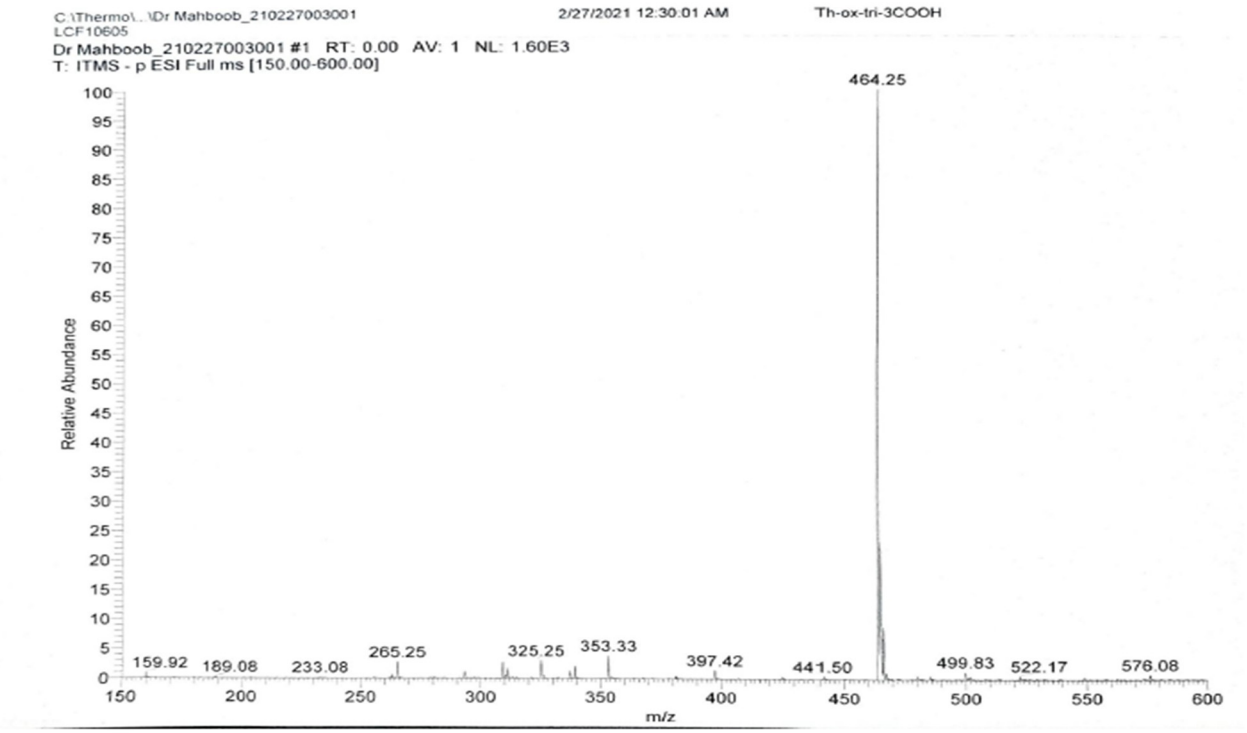
Compound 6



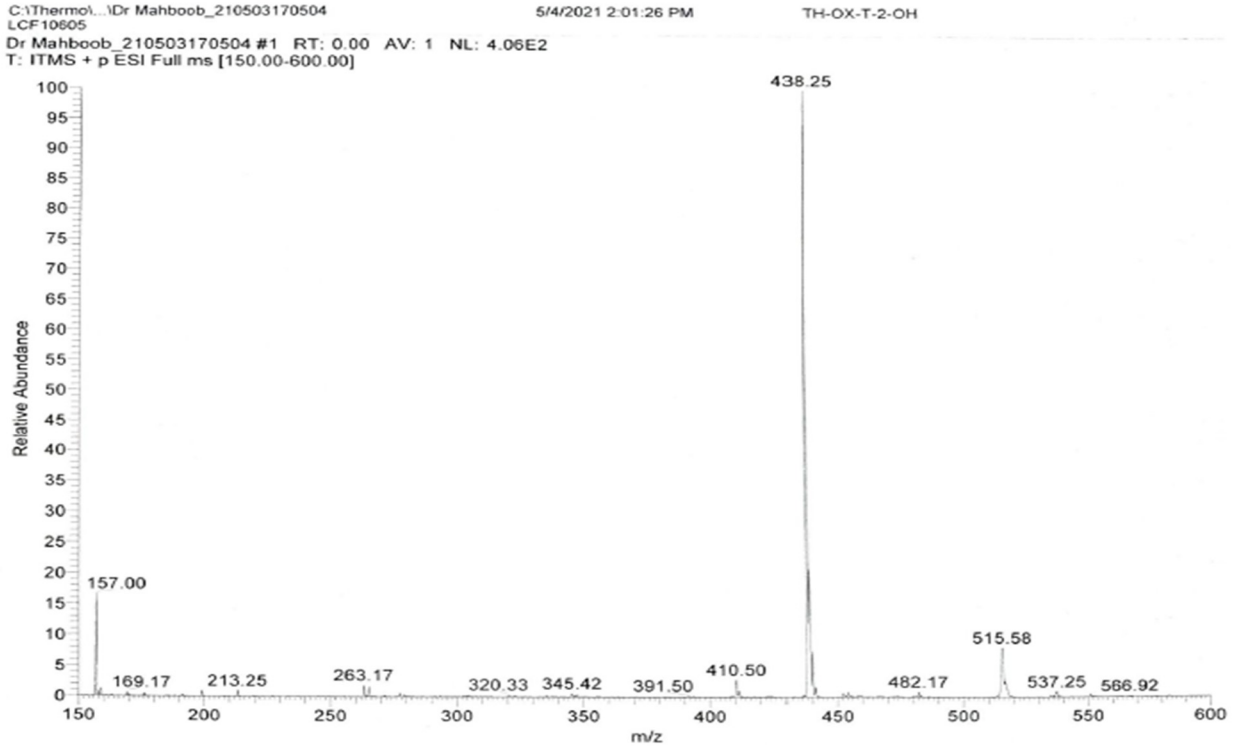
Compound 7



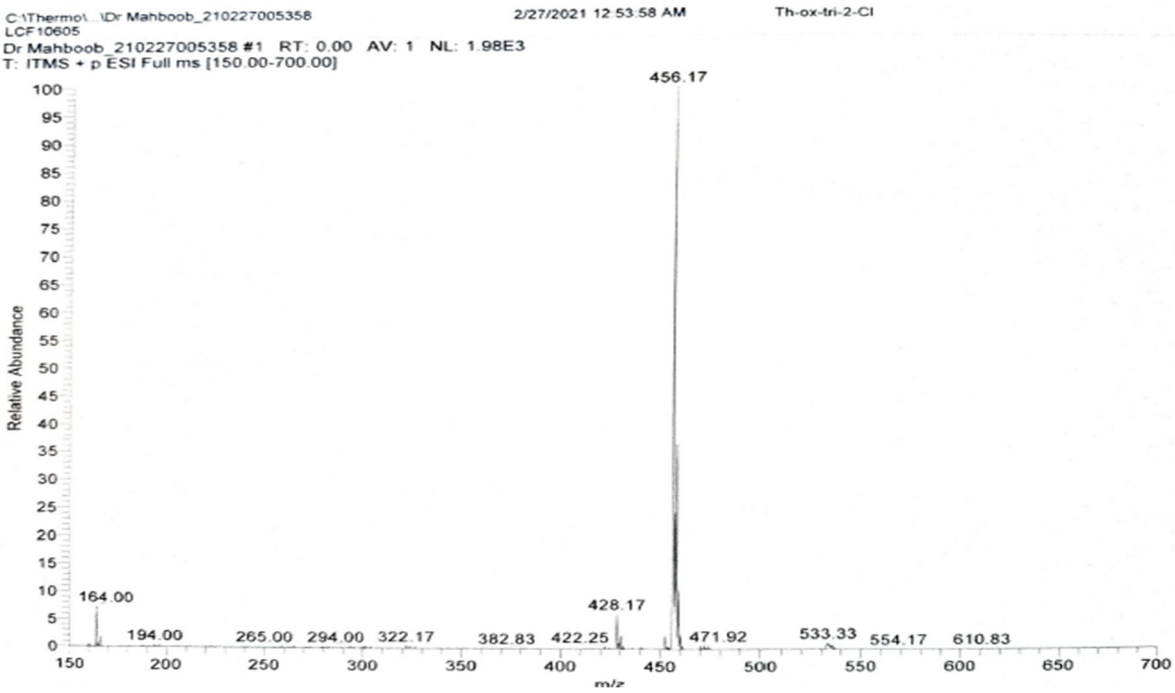
Compound 8



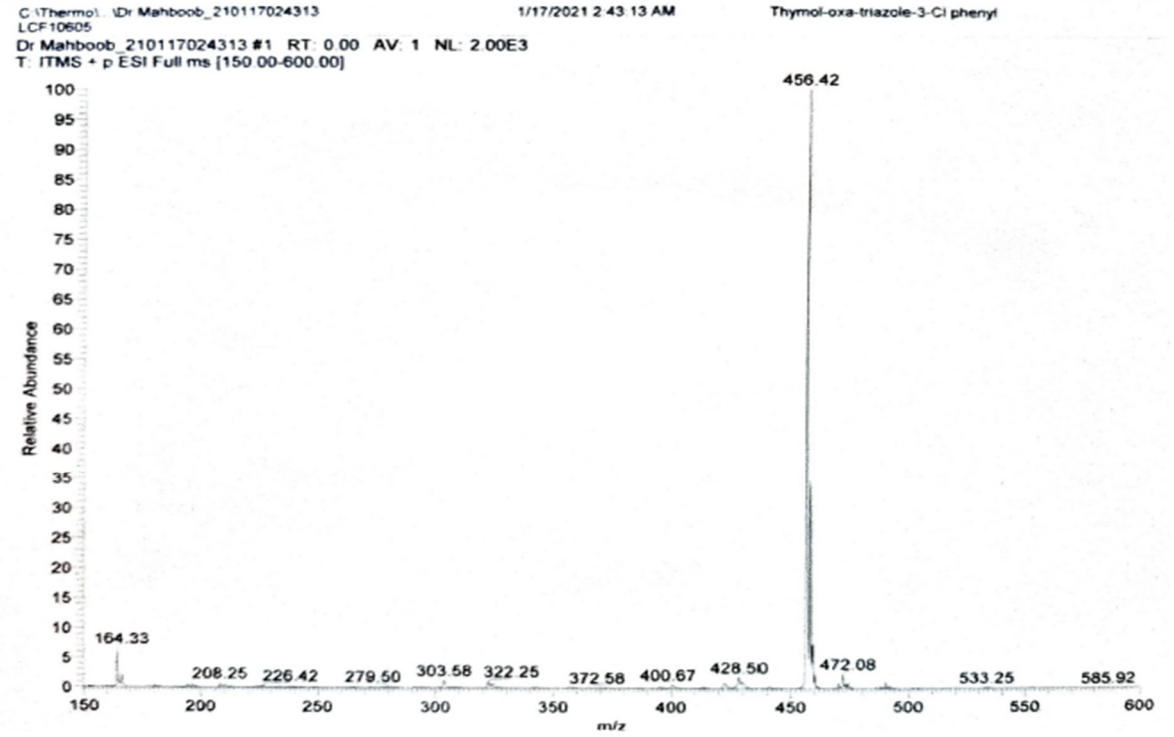
Compound 9



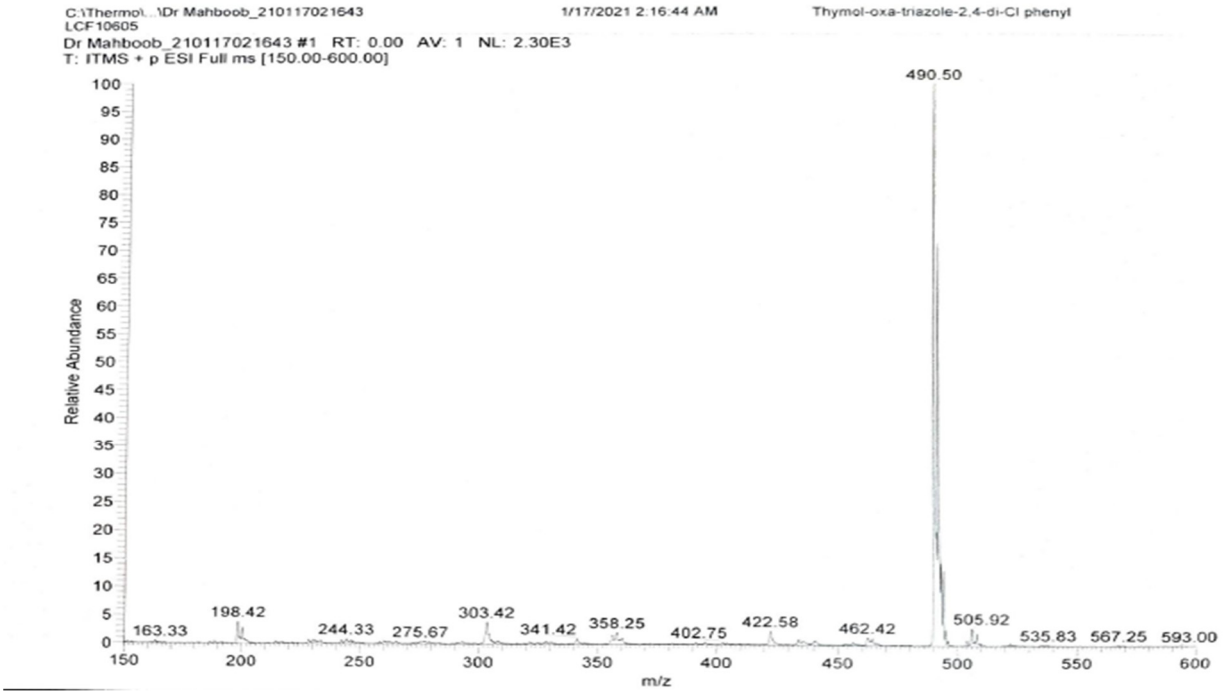
Compound 10



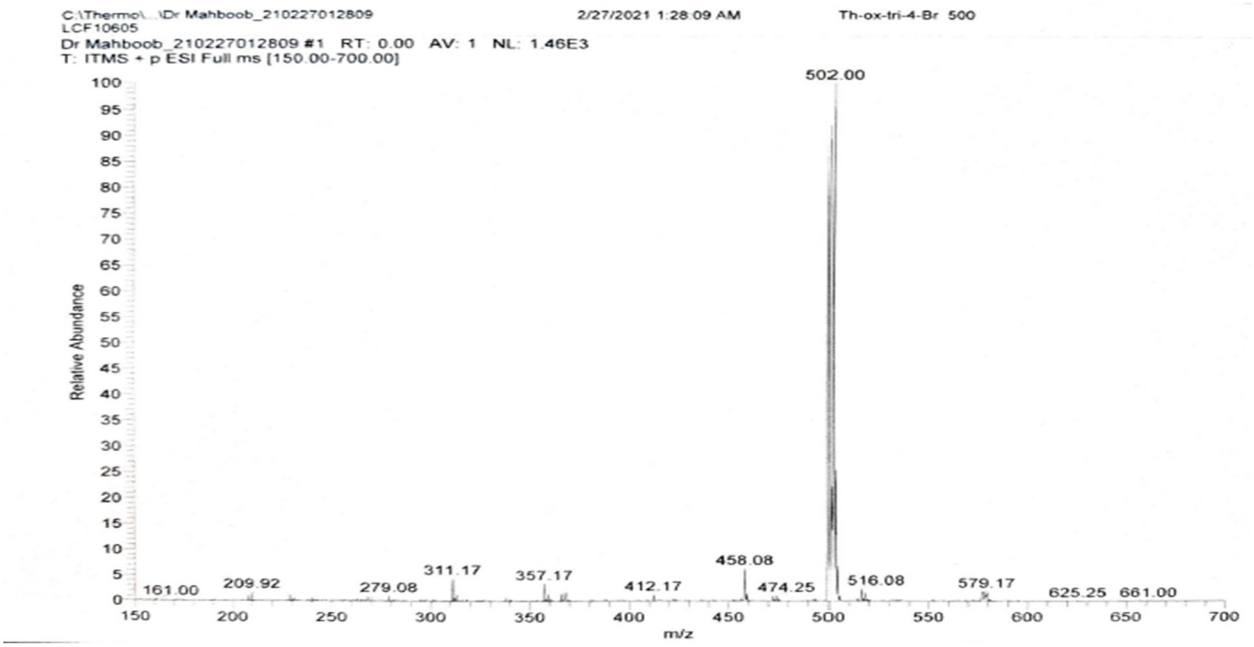
Compound 11



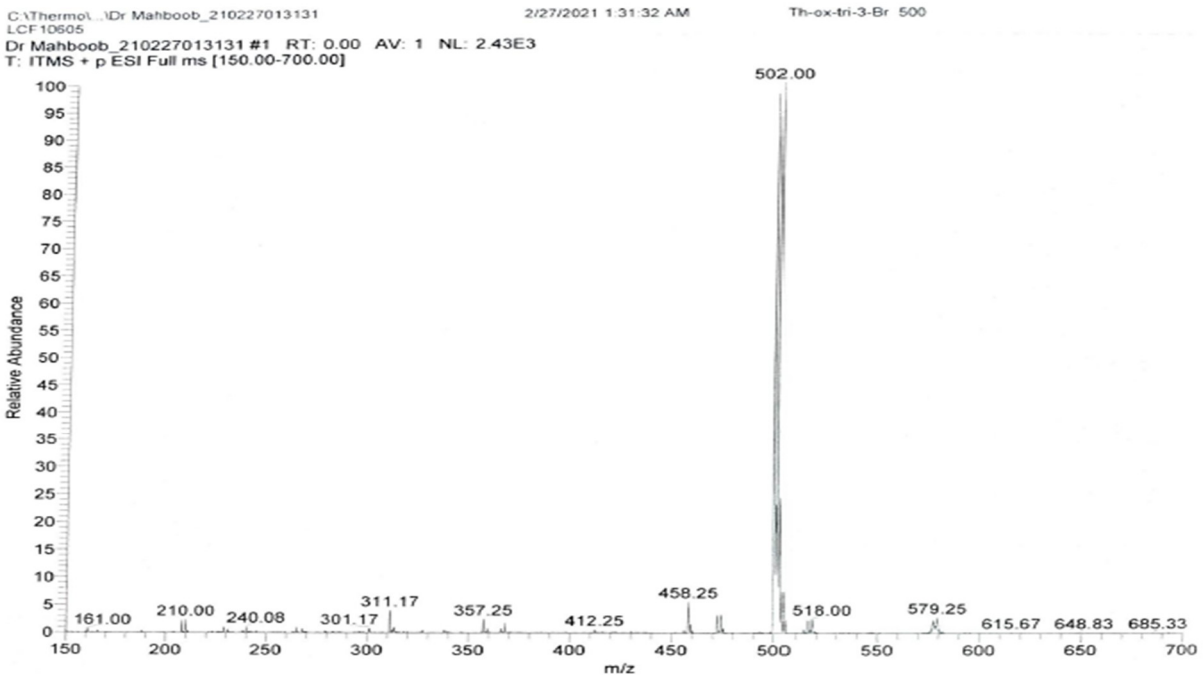
Compound 12



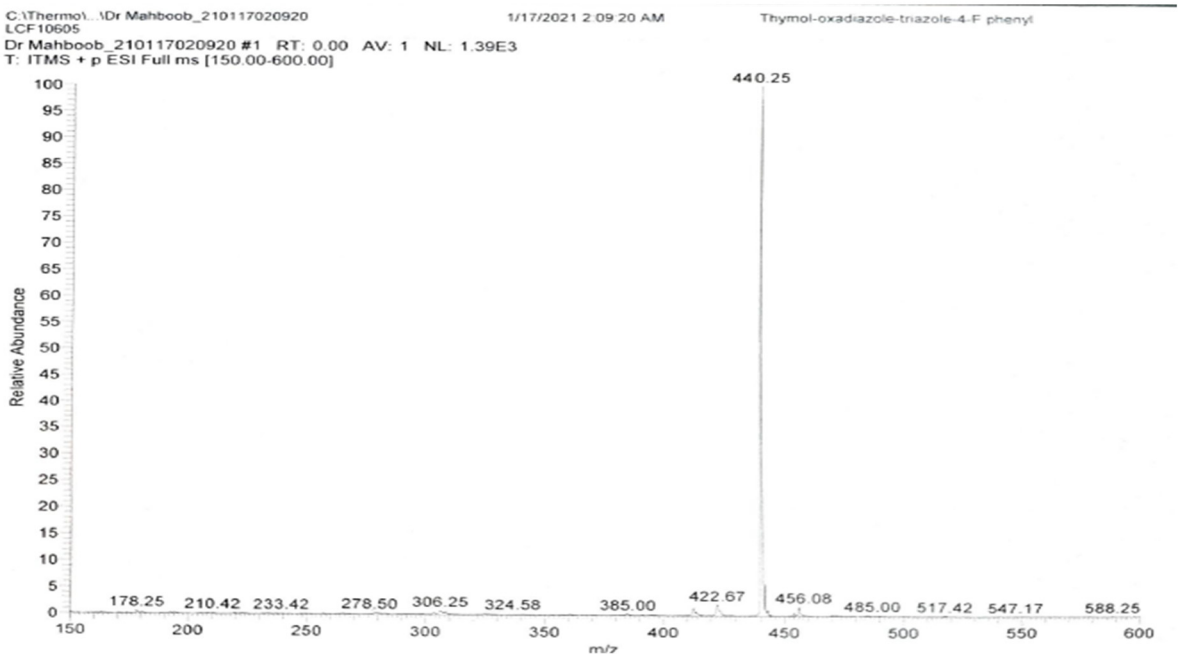
Compound 13



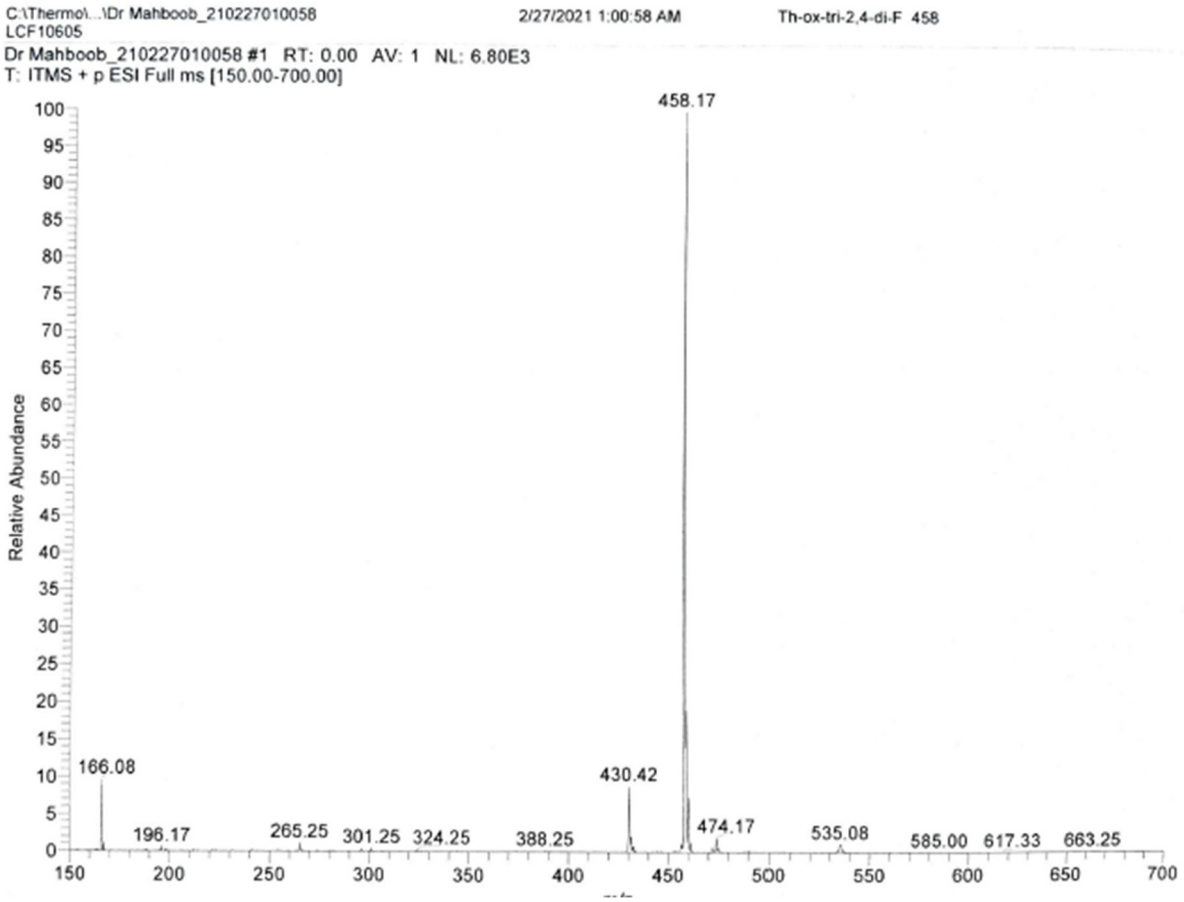
Compound 14

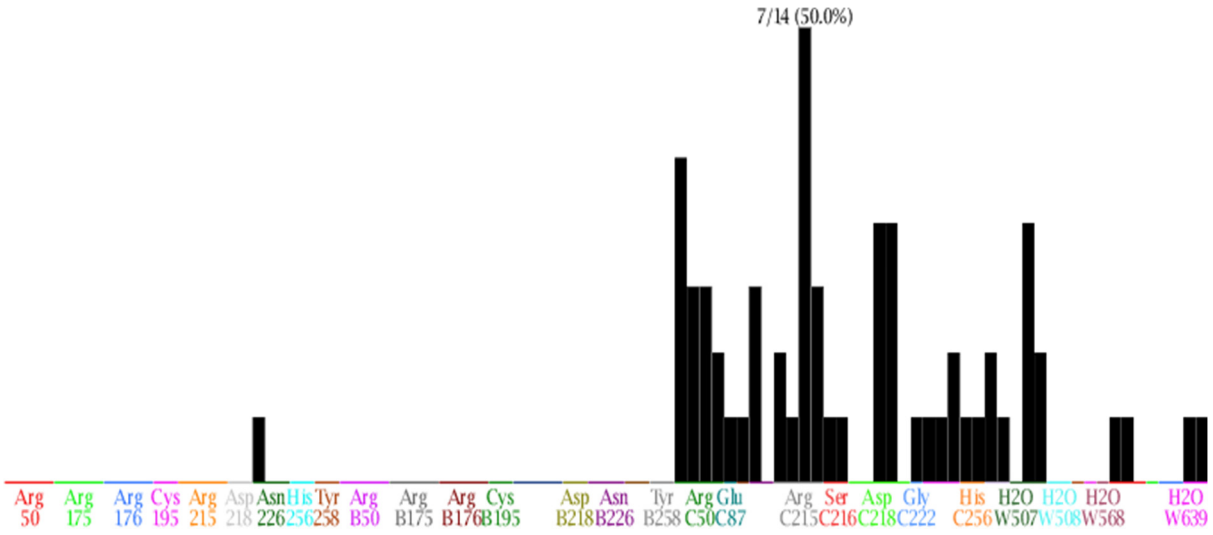


Compound 15

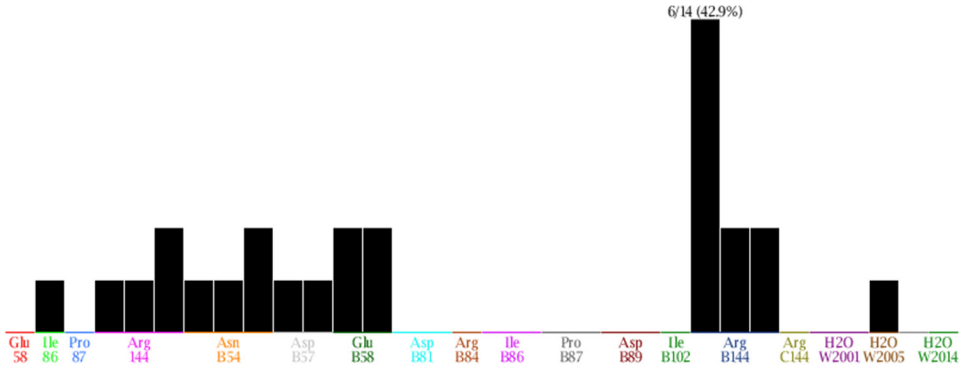


Compound 16


C:\Thermo\...\Dr Mahboob_210227010058
LCF10605
2/27/2021 1:00:58 AM
Th-ox-tri-2,4-di-F 458
Dr Mahboob_210227010058 #1 RT: 0.00 AV: 1 NL: 6.80E3
T: ITMS + p ESI Full ms [150.00-700.00]
Relative Abundance
458.17
166.08
430.42
474.17
196.17
265.25
301.25
324.25
388.25
535.08
585.00
617.33
663.25



FigureS30. PLIF histogram which represented the interacted docked compounds with residues of thymidylate synthase.



FigureS31. PLIF histogram which represented the interacted docked compounds with residues of DNA gyrase (4uro).