

Synthesis, Characterization, *In silico* Molecular Docking, and Antibacterial Activities of Some New Nitrogen-heterocyclic Analogues Based *p*-Phenolic Unit

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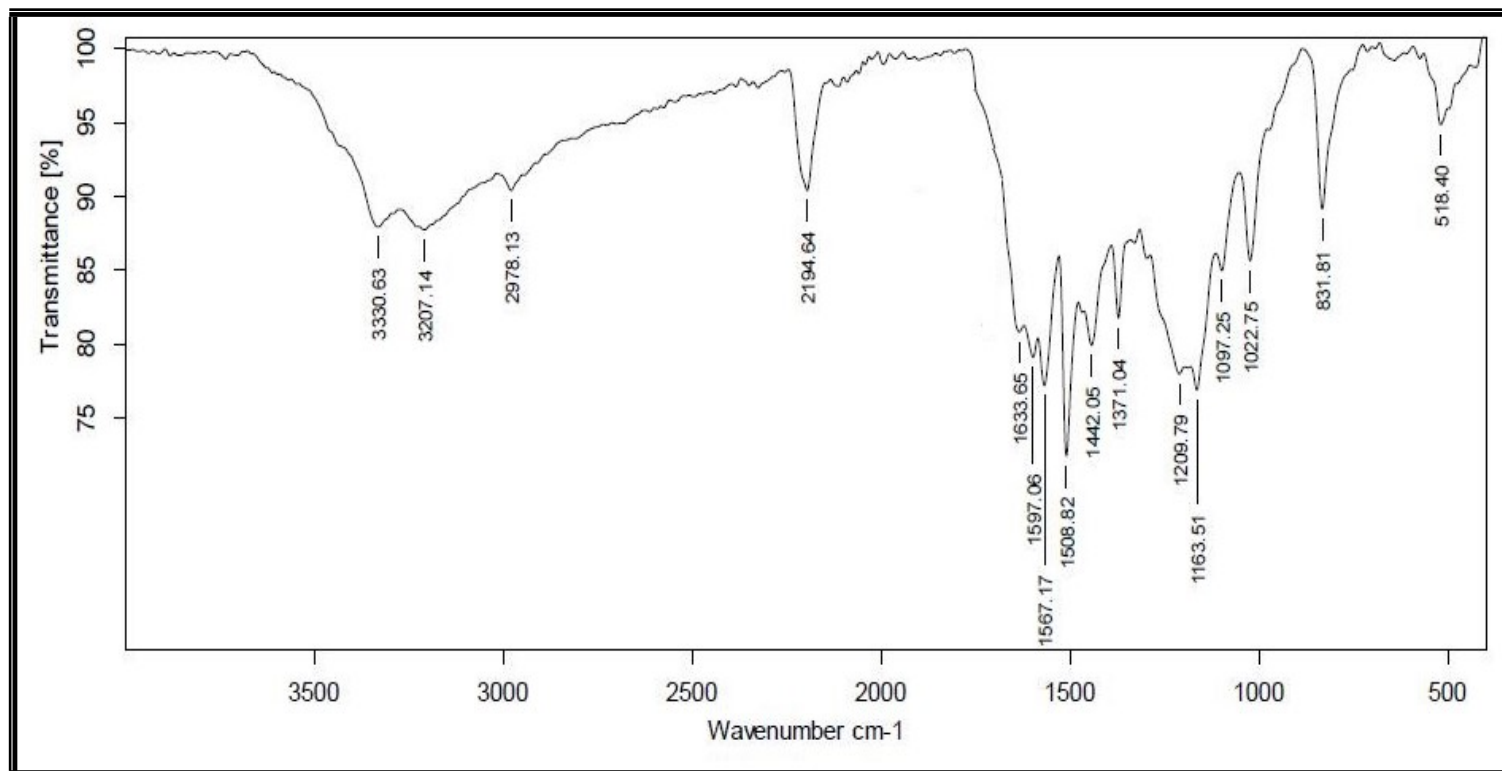


Figure S1. IR Spectrum of Compound (2a)

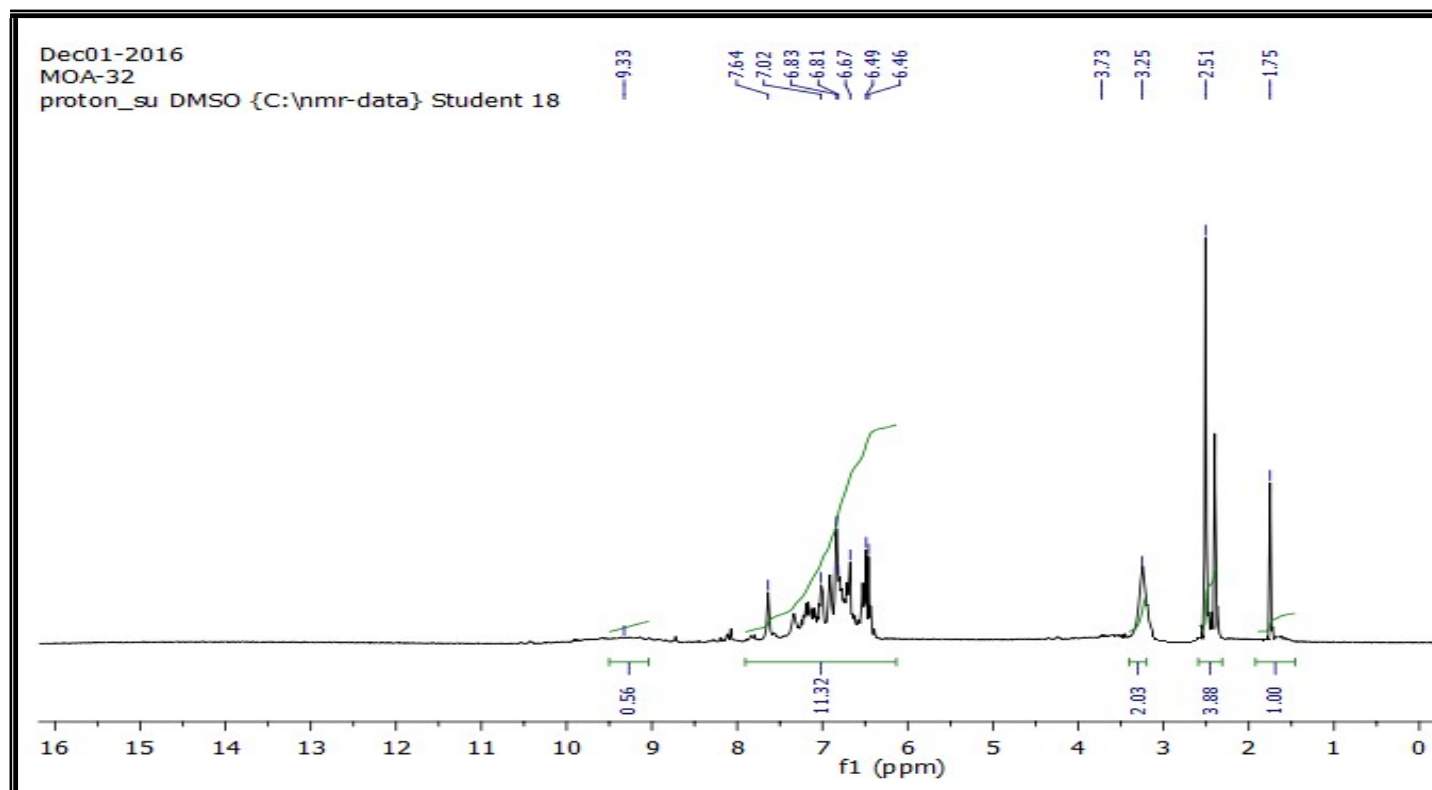


Figure S2. ^1H NMR Spectrum of Compound (2a)

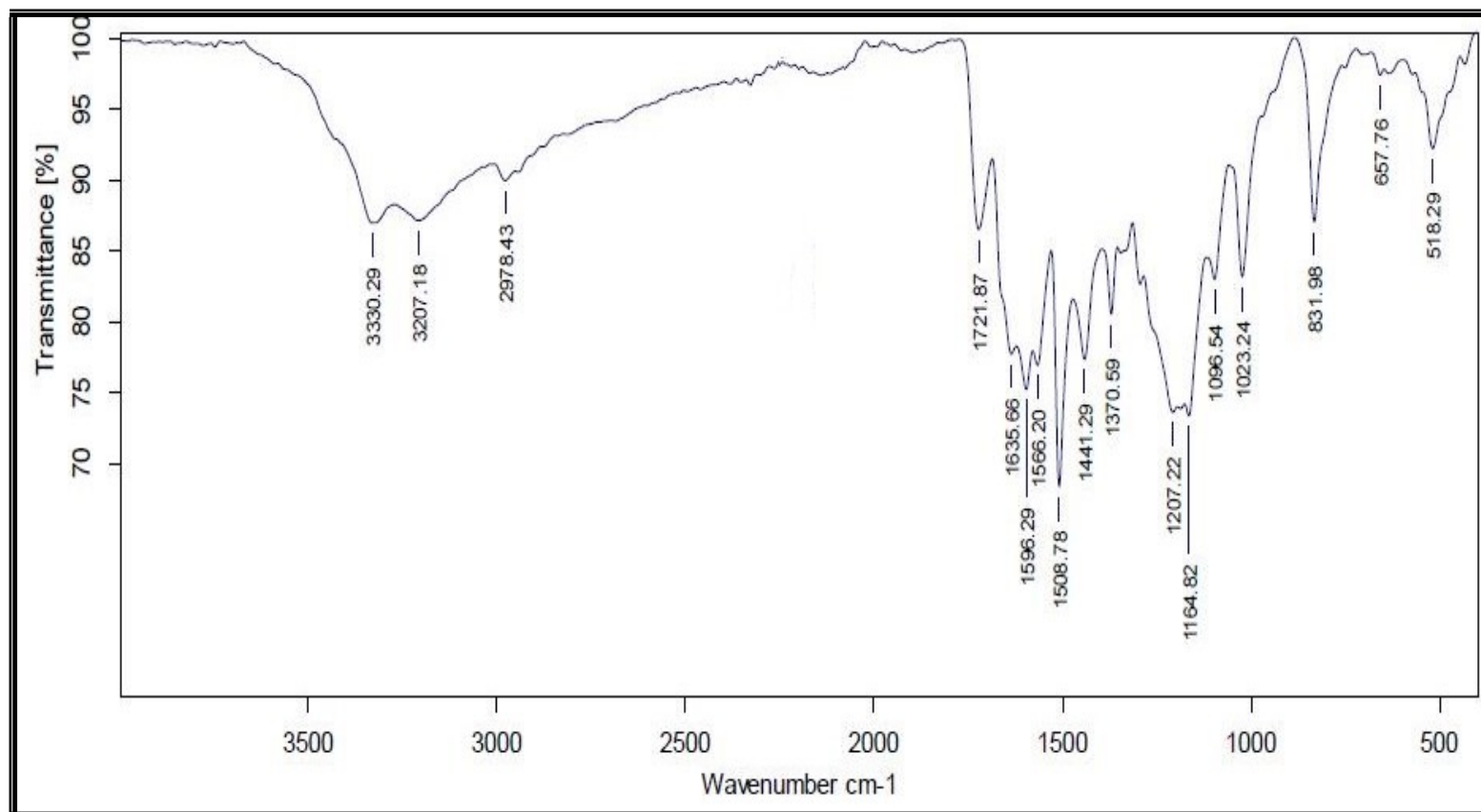


Figure S3. IR Spectrum of Compound (2b)

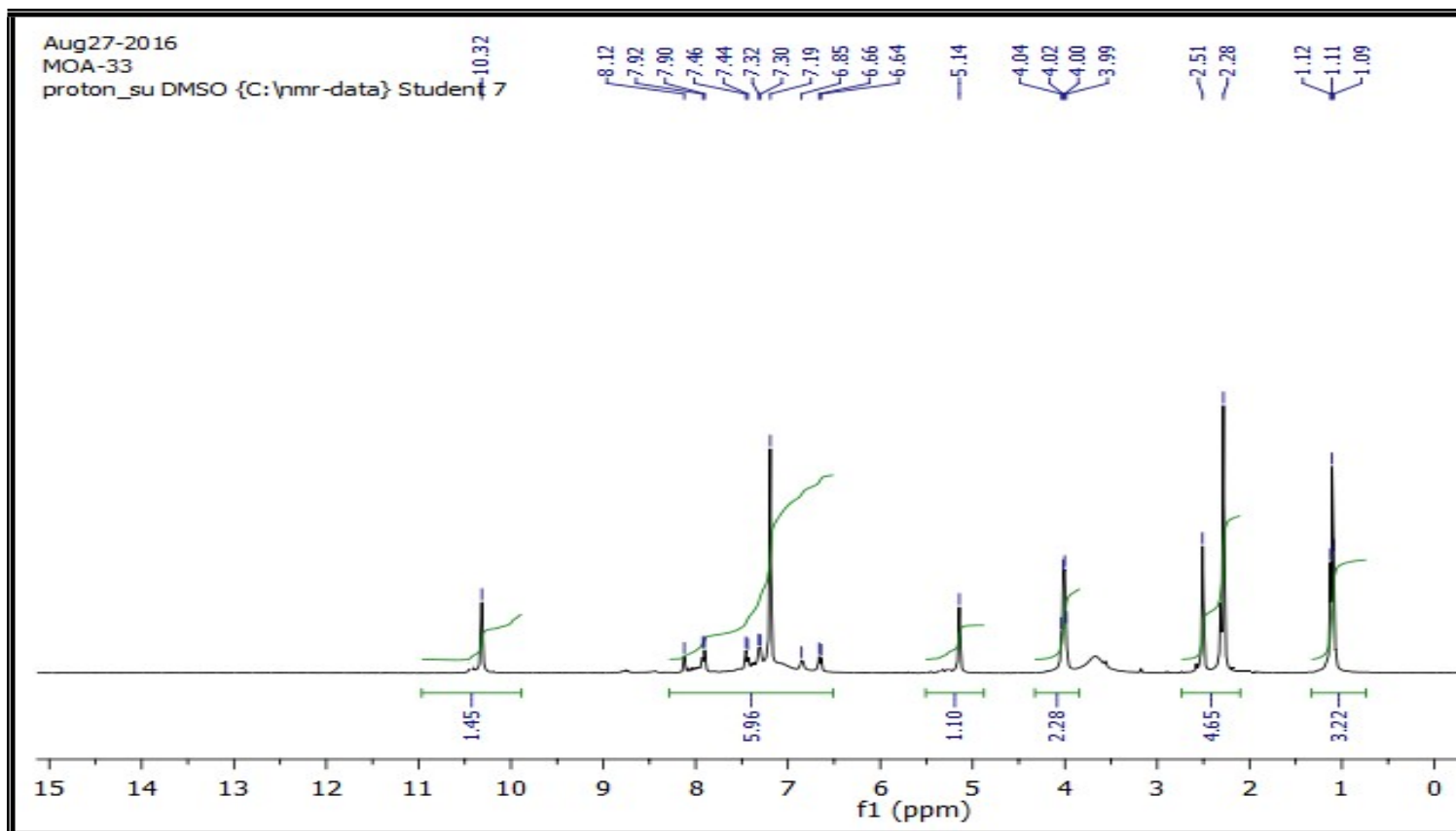


Figure S4. ^1H NMR Spectrum of Compound (2b)

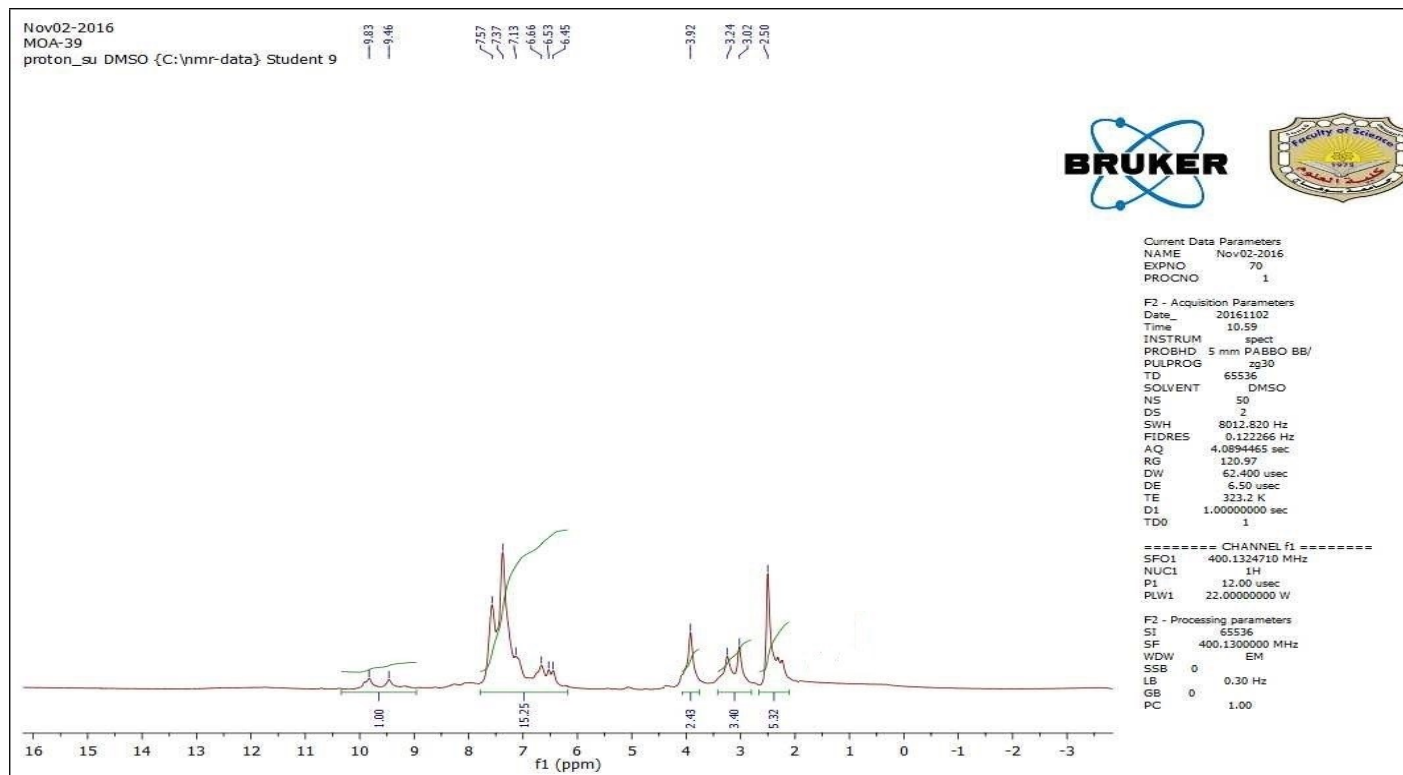


Figure S5. ^1H NMR Spectrum of Compound (3)

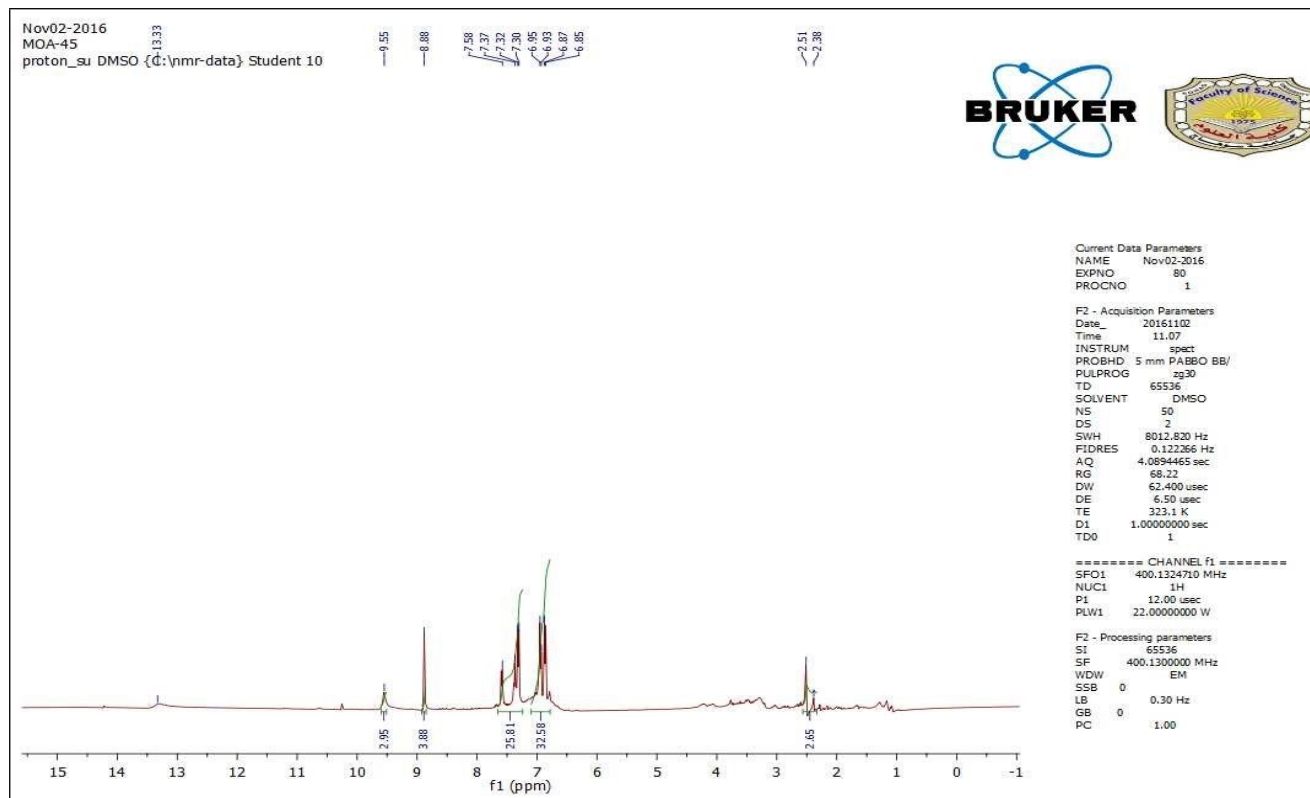


Figure S6. ^1H NMR Spectrum of Compound (4)

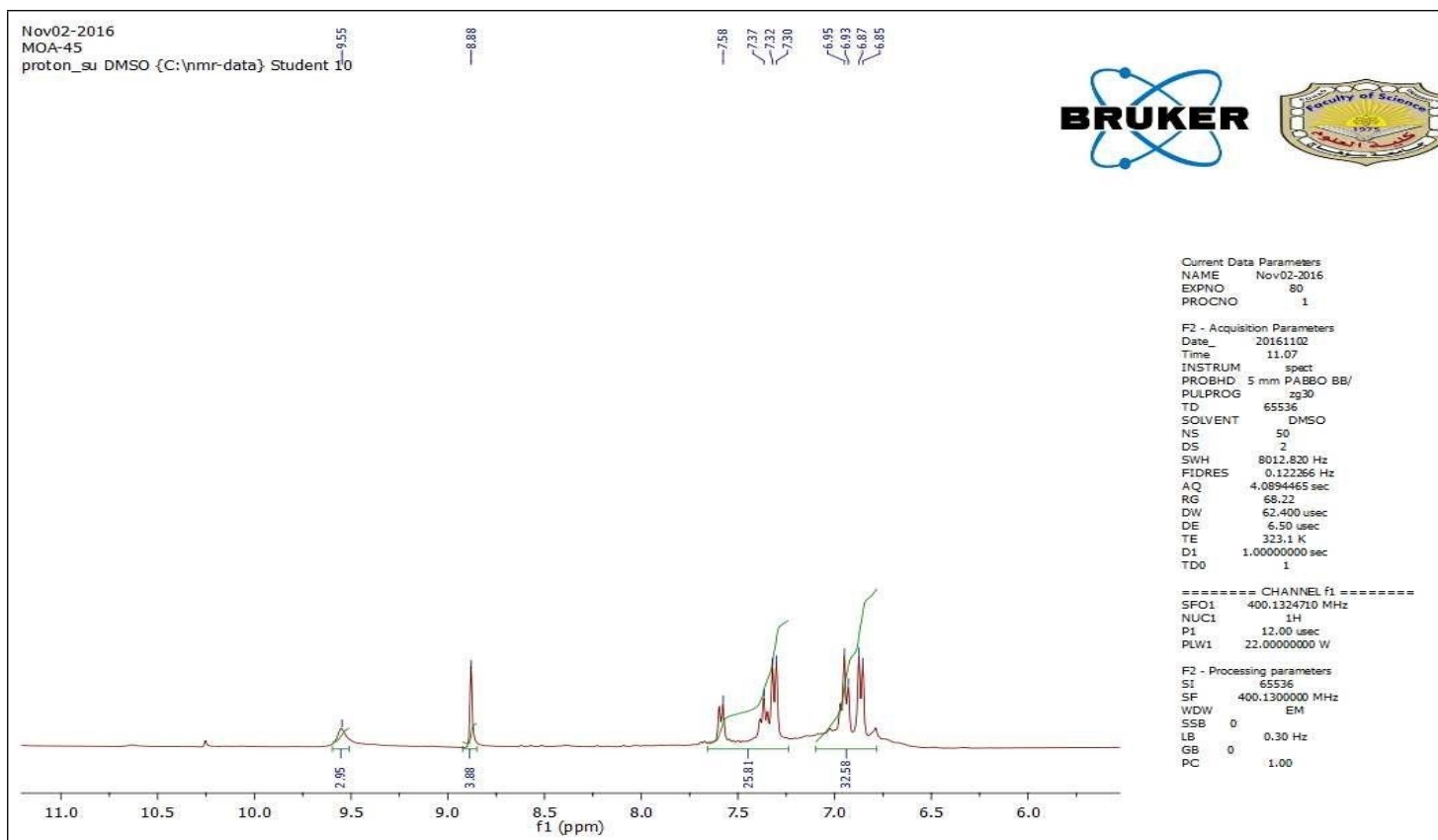


Figure S7. ^1H NMR Spectrum of Compound (4)

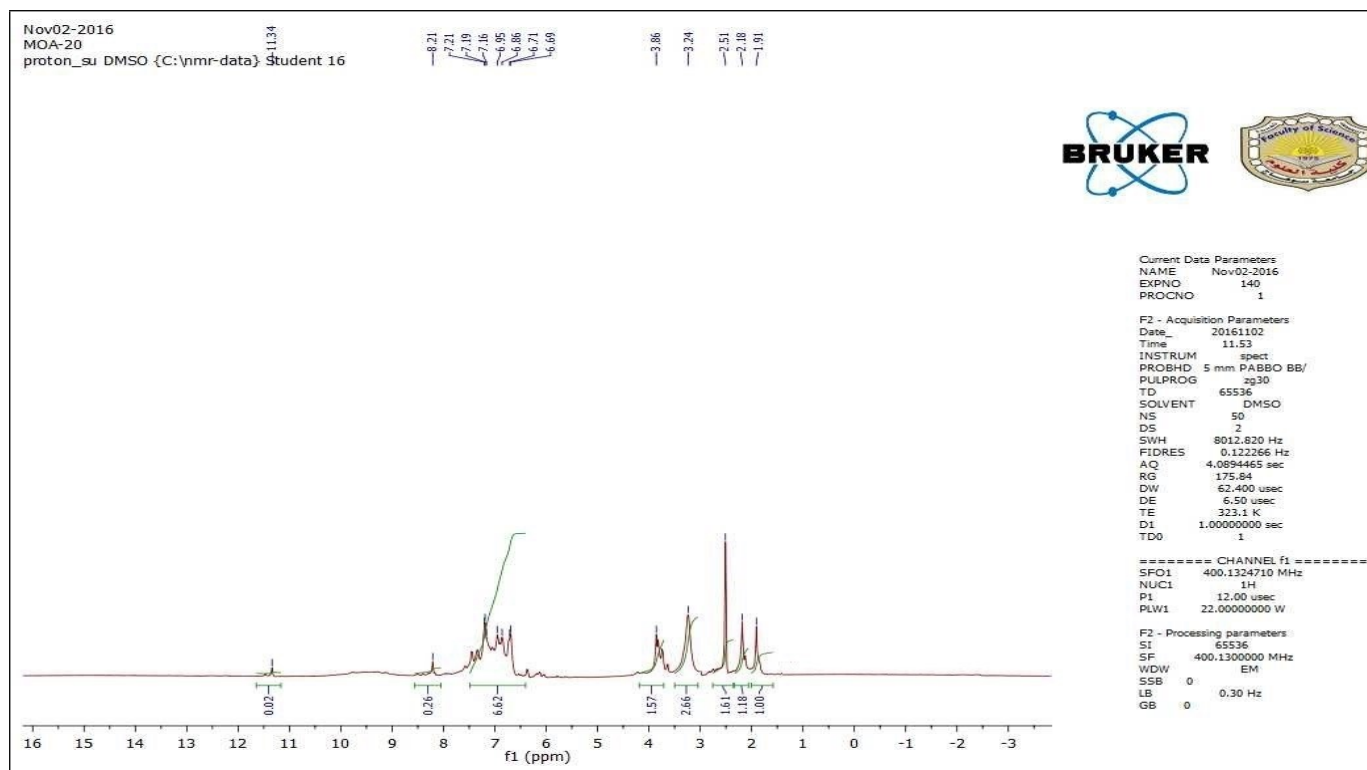


Figure S8. ^1H NMR Spectrum of Compound (5)

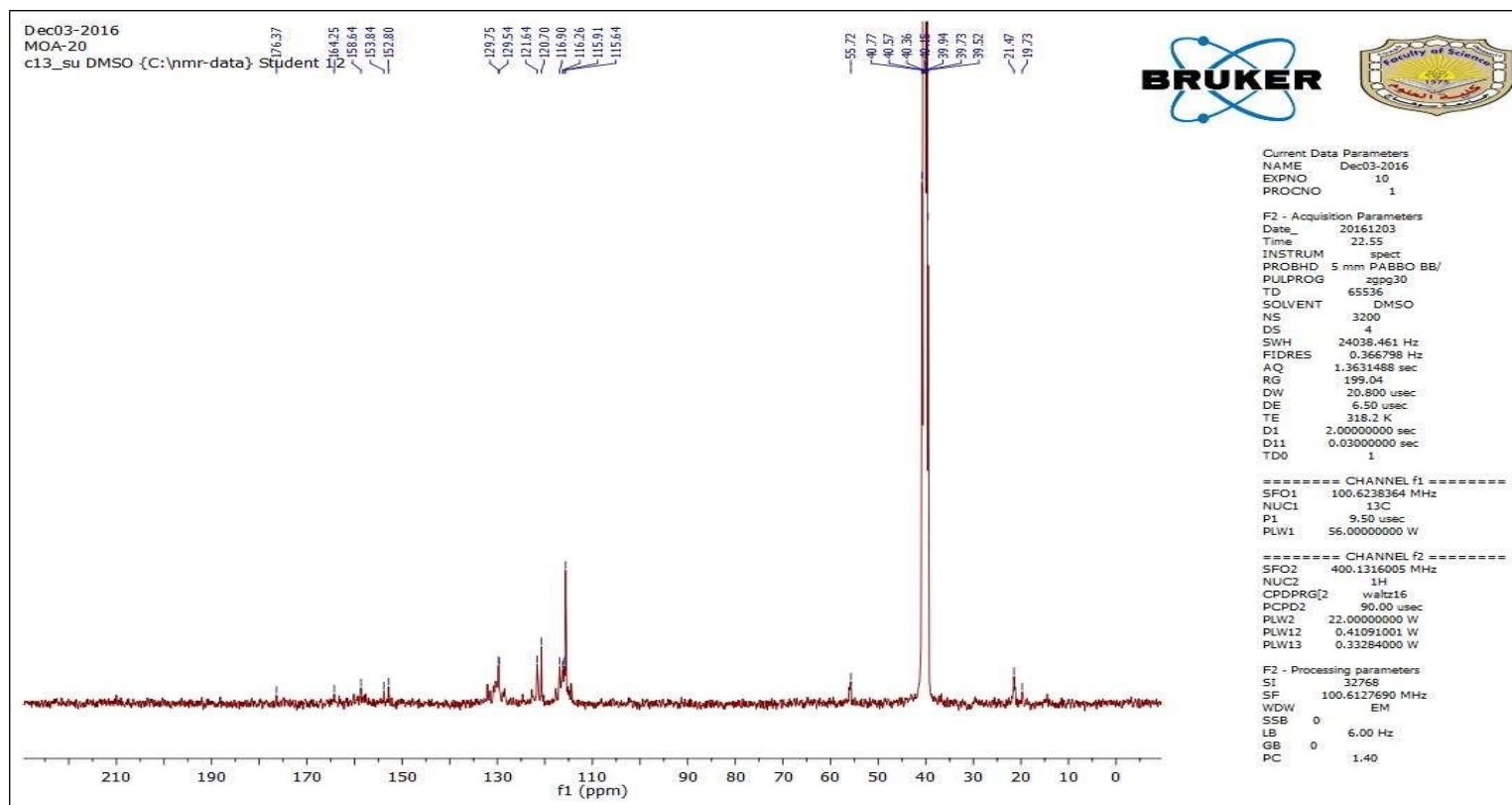


Figure S9. ¹³C NMR Spectrum of Compound (5)

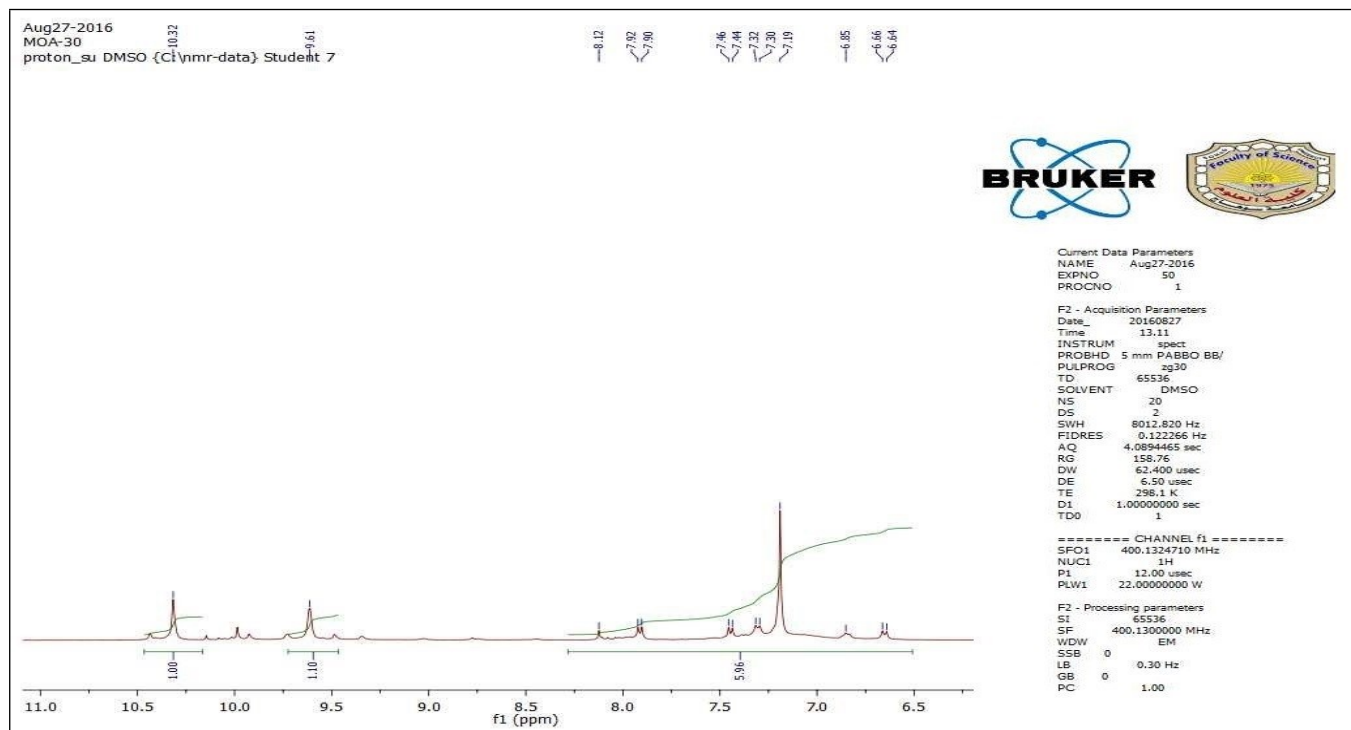


Figure S10. ^1H NMR Spectrum of Compound (6a)

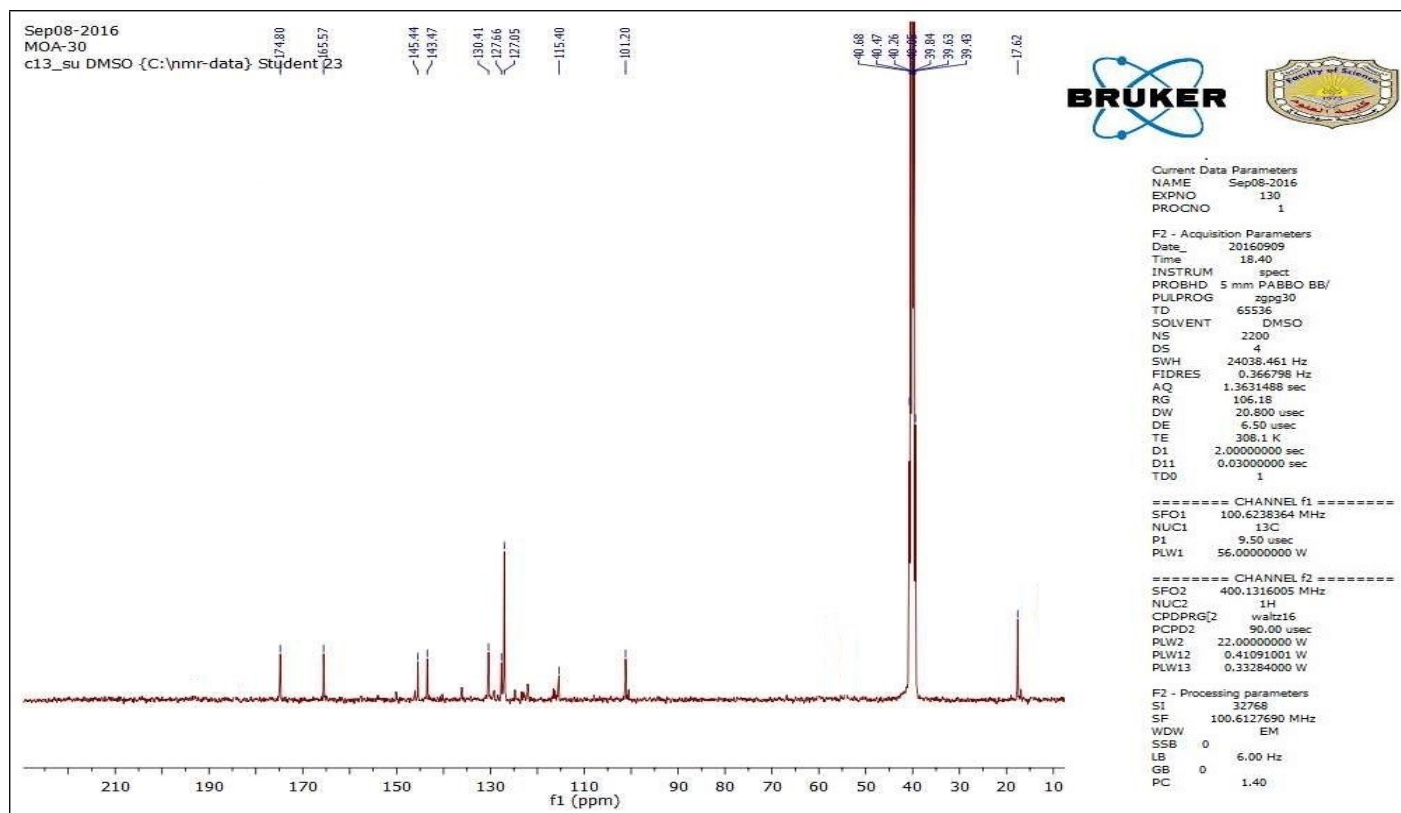


Figure S11. ^{13}C NMR Spectrum of Compound (6a)

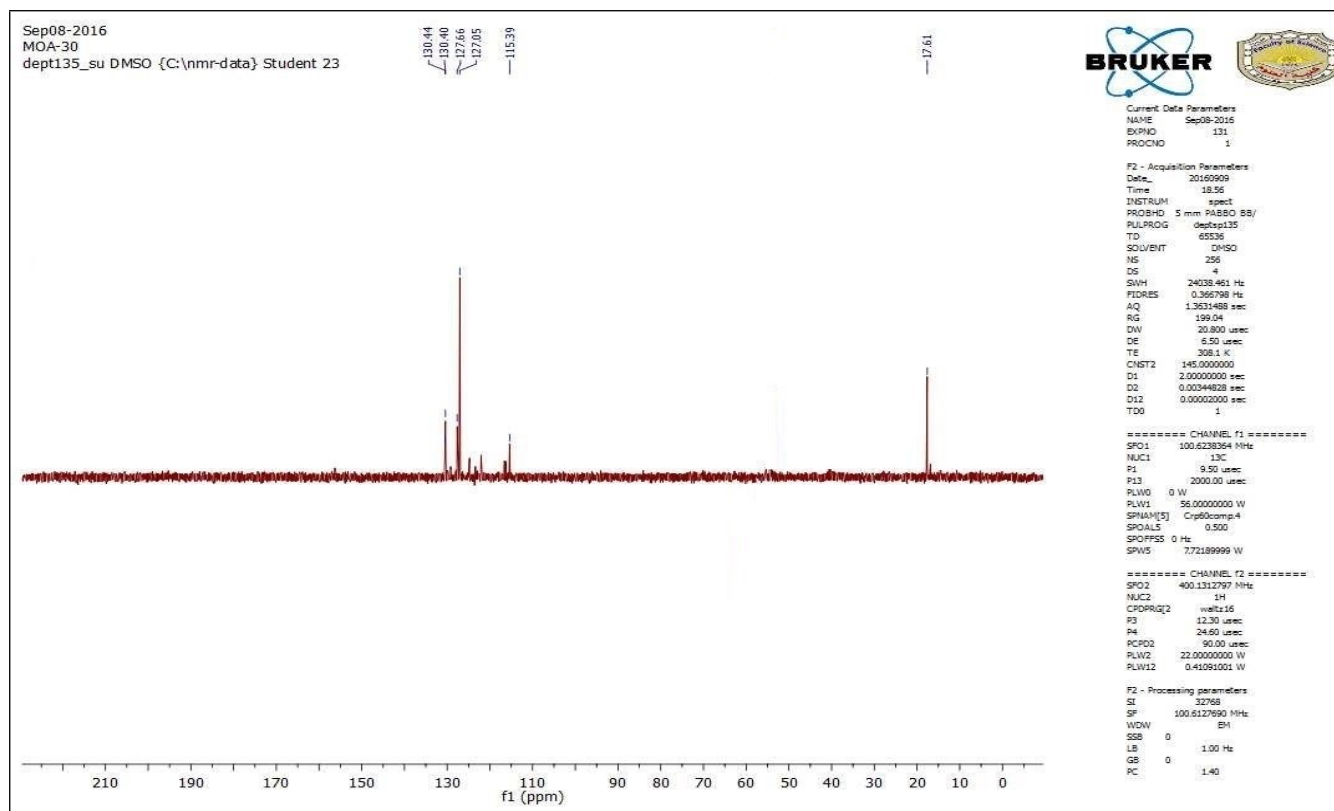


Figure S12. DEPT 135 ^{13}C NMR Spectrum of Compound (6a)

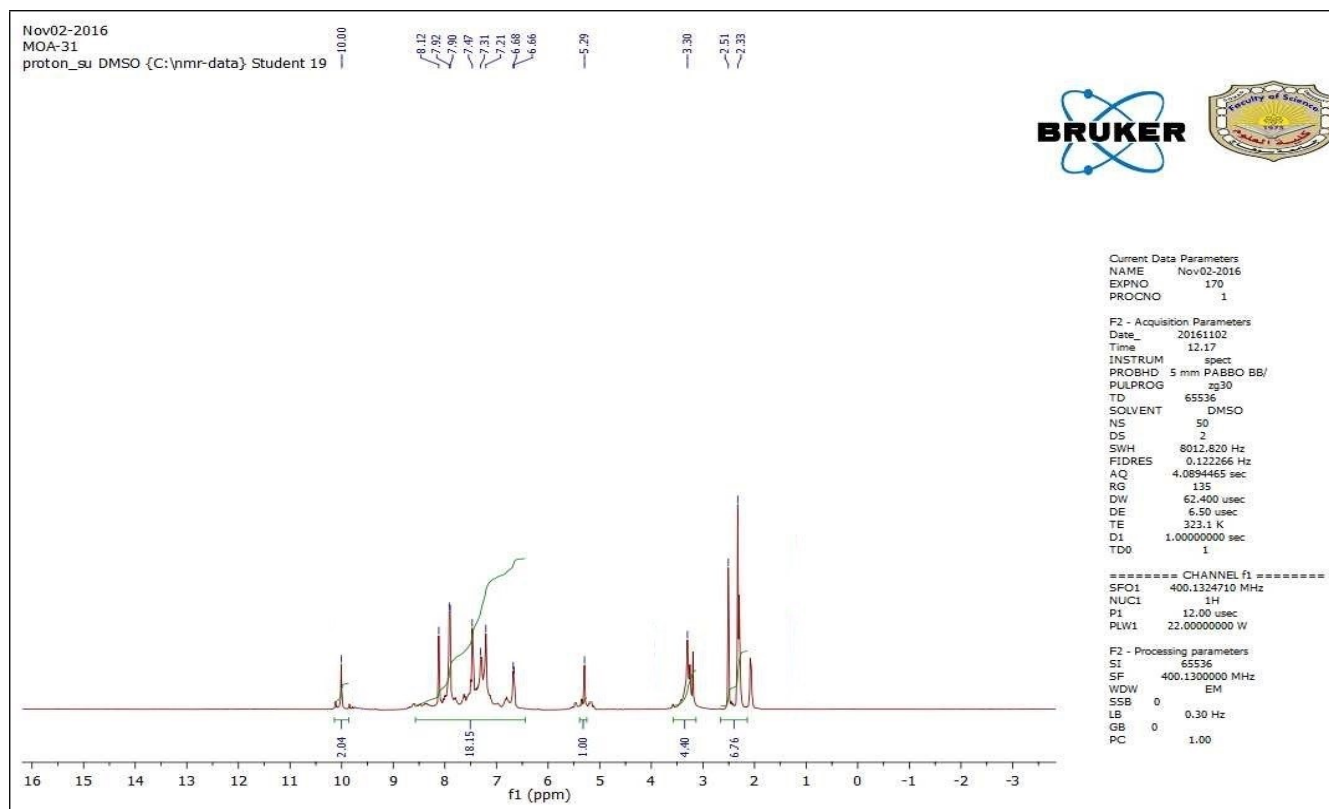


Figure S13. ^1H NMR Spectrum of Compound (6b)

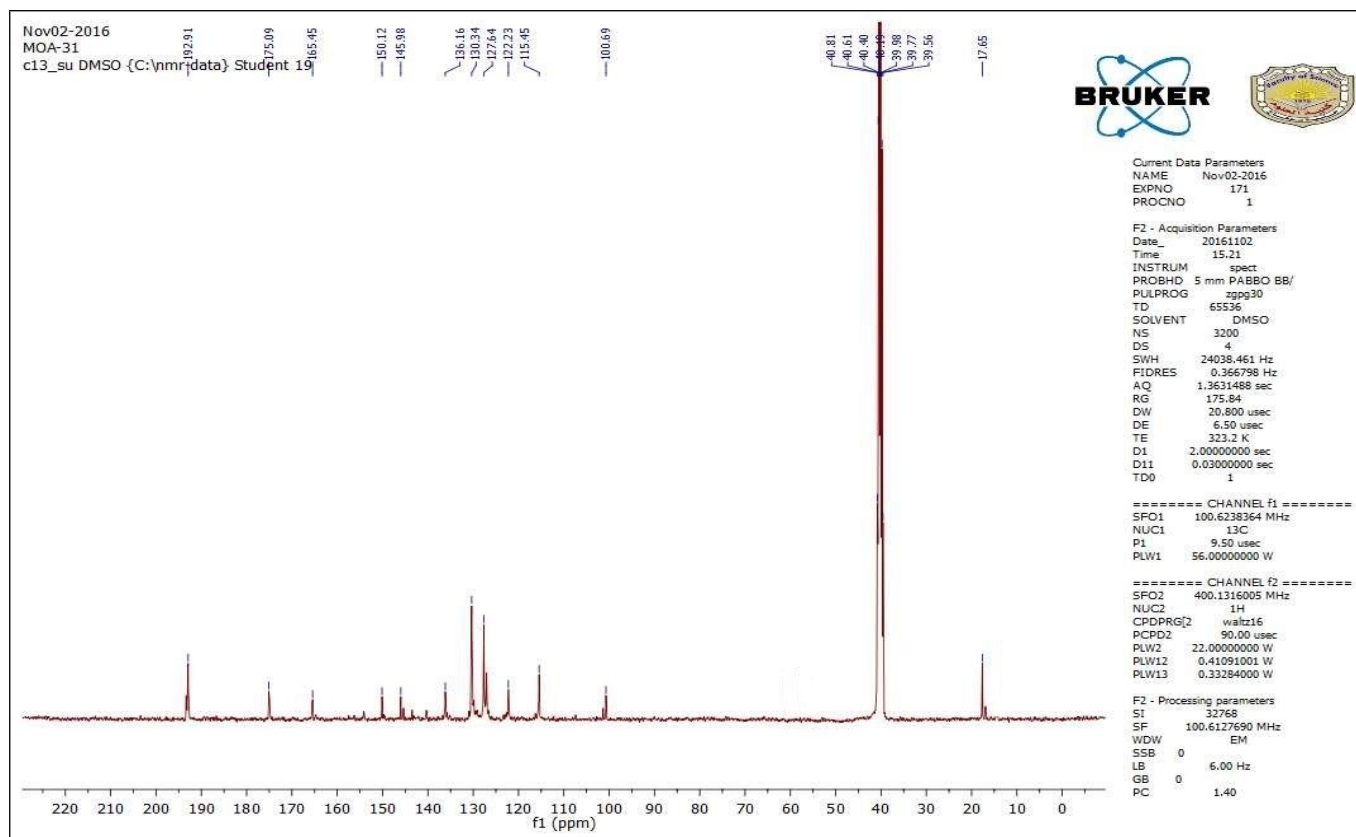


Figure S14. ^{13}C NMR Spectrum of Compound (6b)

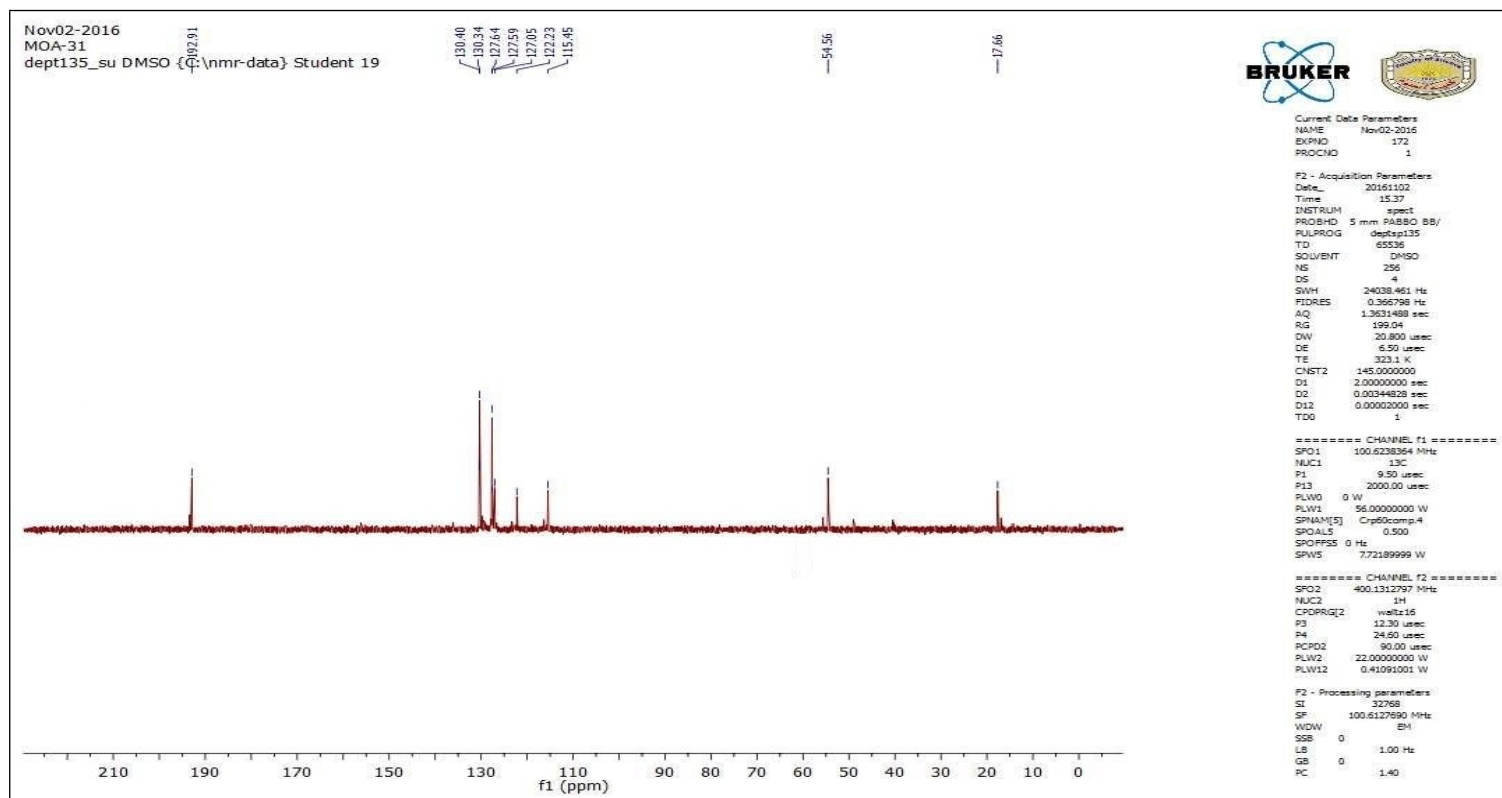


Figure S15. DEPT 135 ^{13}C NMR Spectrum of Compound (6b)

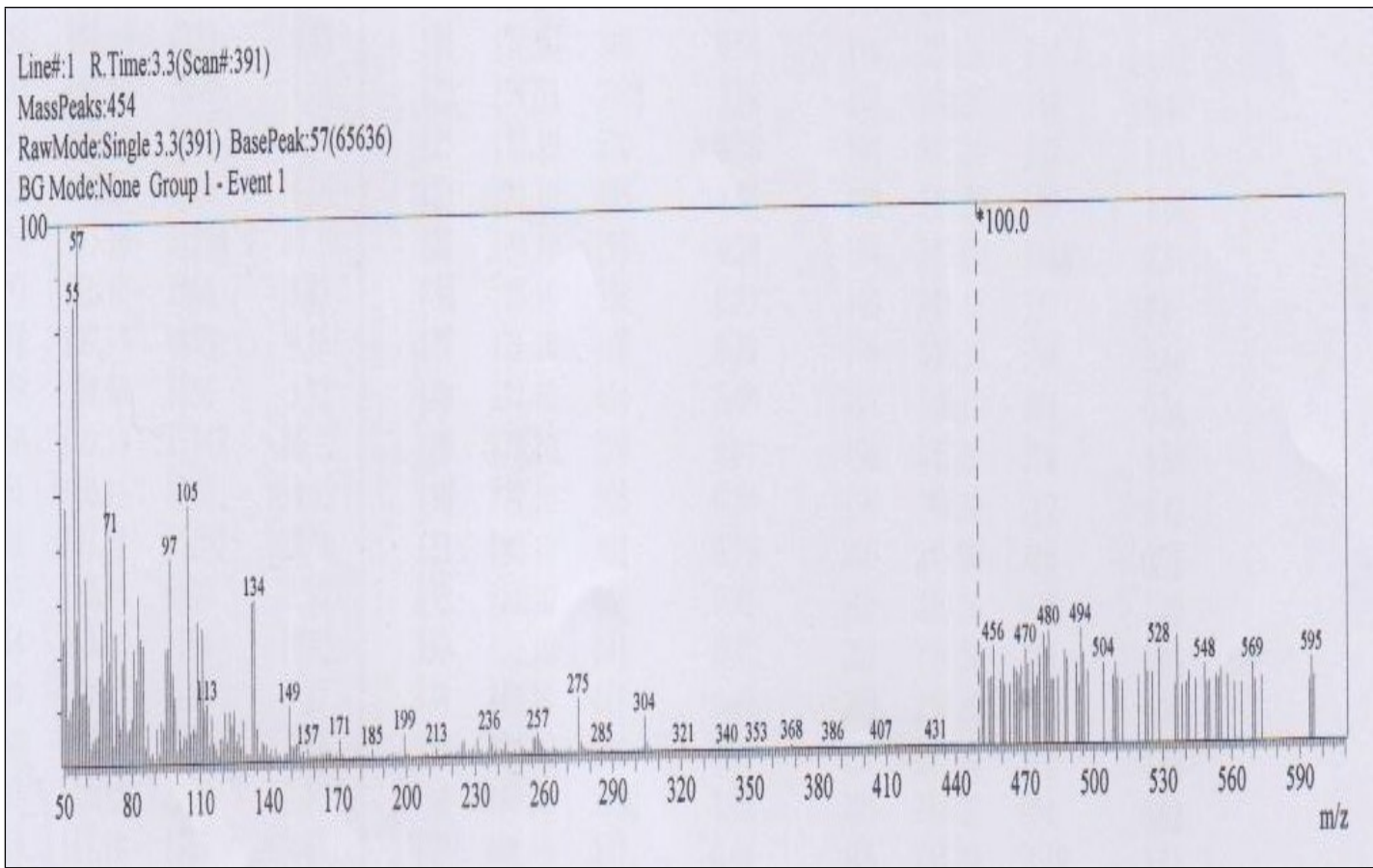


Figure S16. Mass Spectrum of Compound (6b)

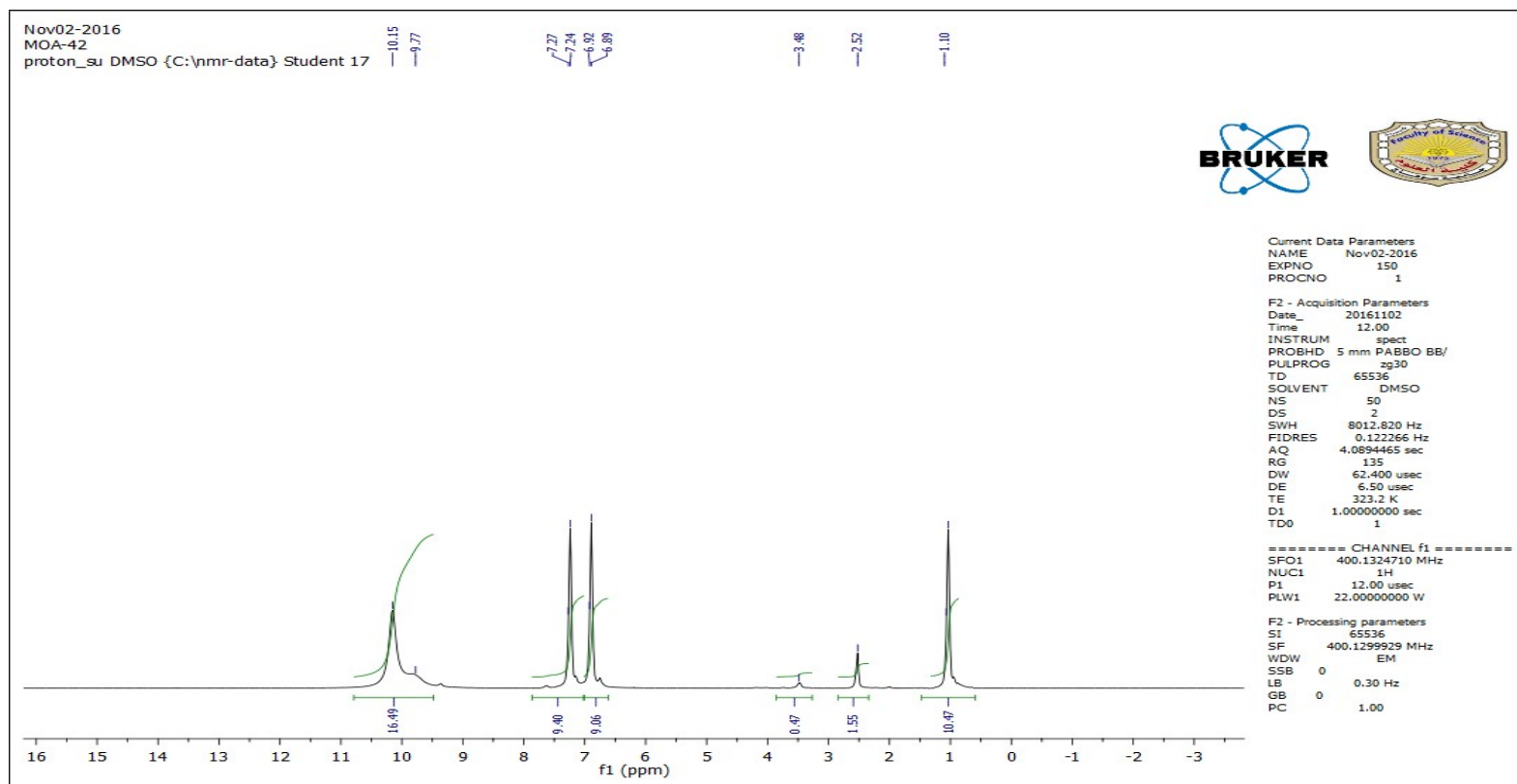


Figure S17. ^1H NMR Spectrum of Compound (7)

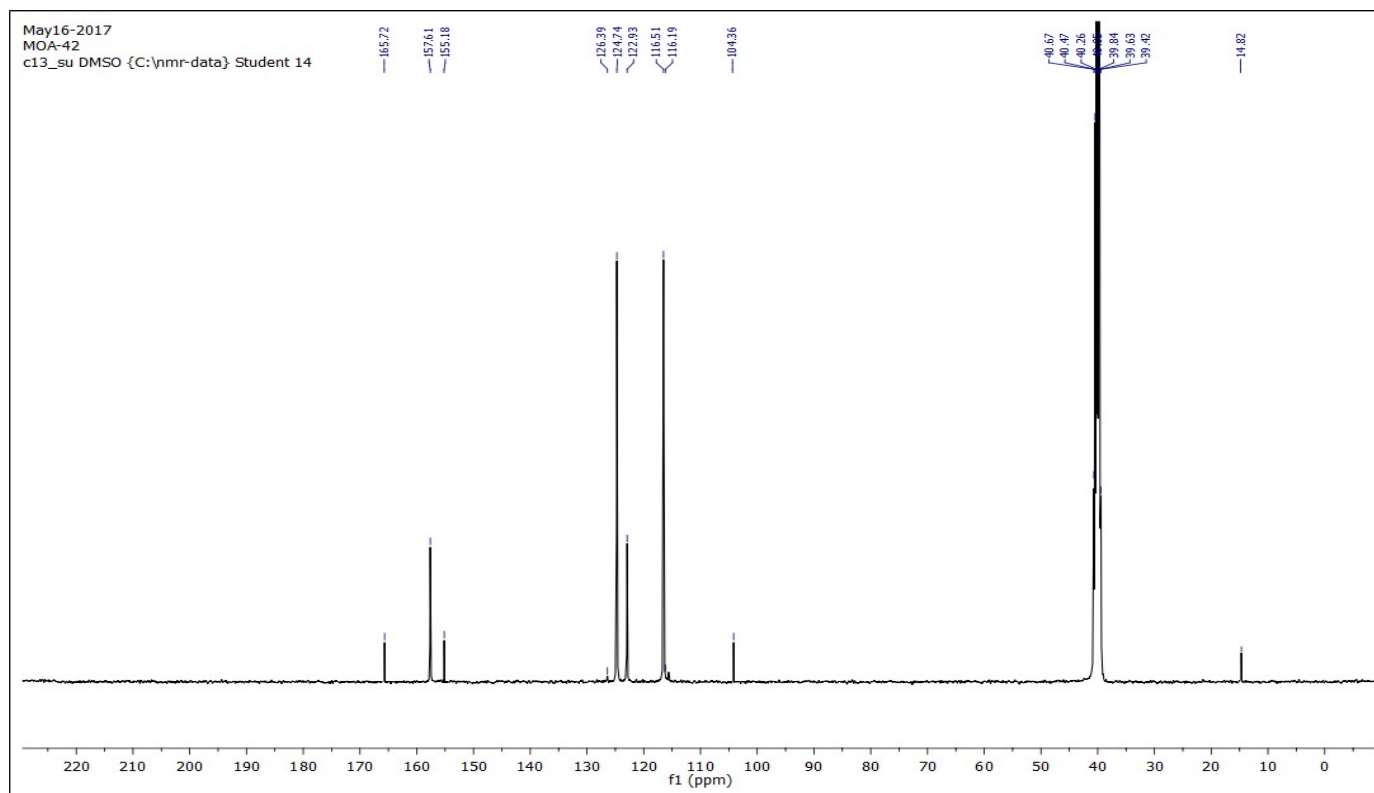


Figure S18. ^{13}C NMR Spectrum of Compound (7)

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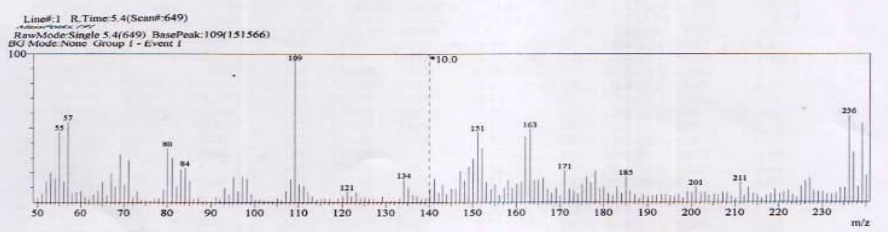
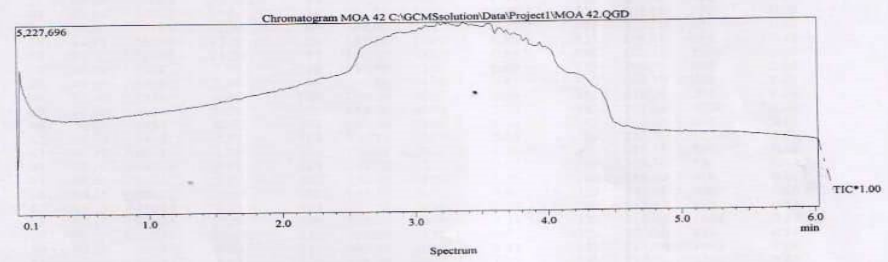


DI Analysis Shimadzu Qp-2010 Plus

Sample Information
 Analyzed by : Noha Bagato.
 Analyzed : 23/05/2017 05:13:03 م
 Sample Name : MOA 42
 Sample ID :
 Customer Name : علوم القاهرة - د. جهاد جادوي - نسمة
 Data File : C:\GCMSolution\Data\Project1\MOA 42.QGD
 Org Data File : C:\GCMSolution\Data\Project1\MOA 42.QGD
 Method File : C:\GCMSolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSolution\System\Tune1_default.qgt
 Report File :
 Tuning File : C:\GCMSolution\System\Tune1_default.qgt
 SEndTSModified by : Noha Bagato.
 Modified : 23/05/2017 05:19:08 م

Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1428
 Start m/z : 50.00
 End m/z : 700.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSolution\Data\Project1\MOA 42.QGD



Mass Table
 Line#1 R.Time:5.4(Scan#:649)
 MassPeaks:191
 RawMode:Single 5.4(649) BasePeak:109(151566)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	4220	2.78	4	53.05	30180	19.91	7	56.05	21125	13.94
2	51.00	9295	6.13	5	54.05	23974	15.82	8	57.05	81868	54.01
3	52.05	20728	13.68	6	55.05	71625	47.26	9	58.05	9073	5.99

Figure S19. Mass Spectrum of Compound (7)

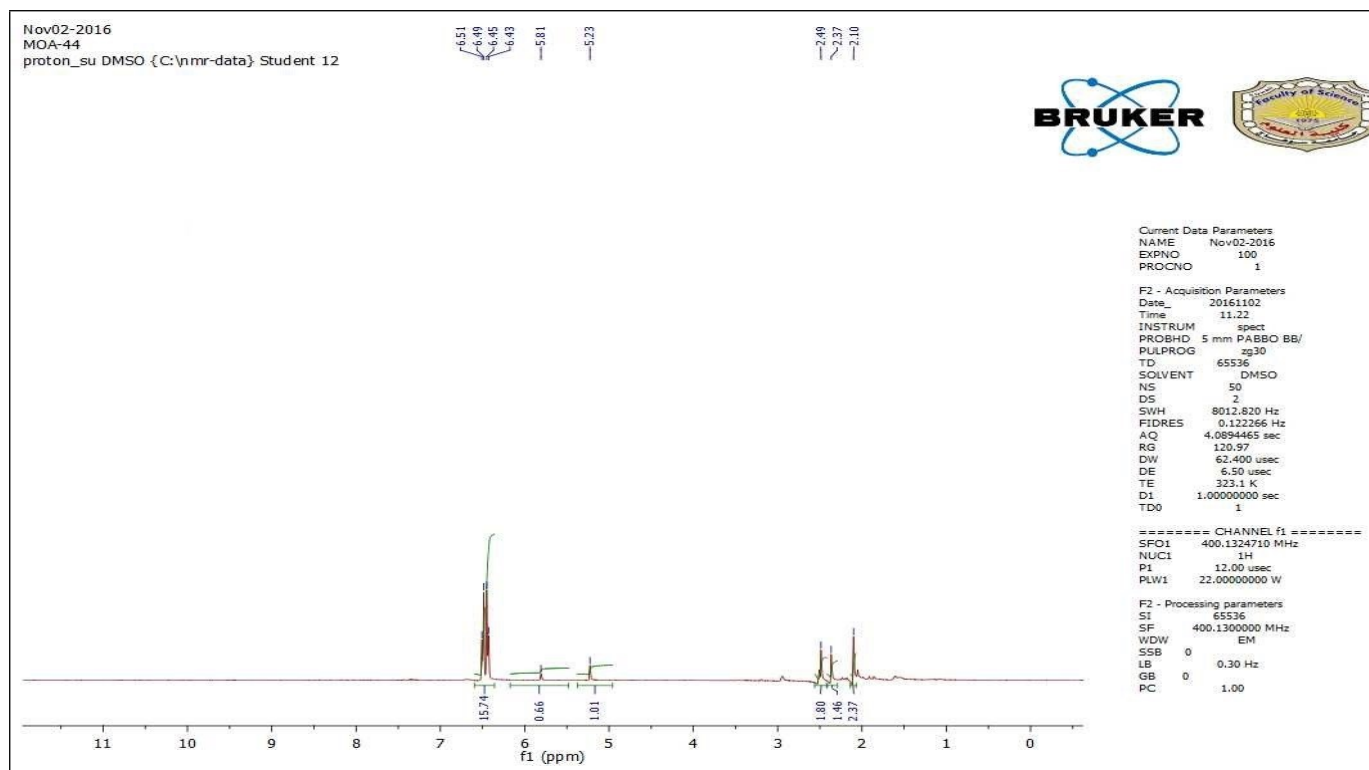


Figure S20. ^1H NMR Spectrum of Compound (8)

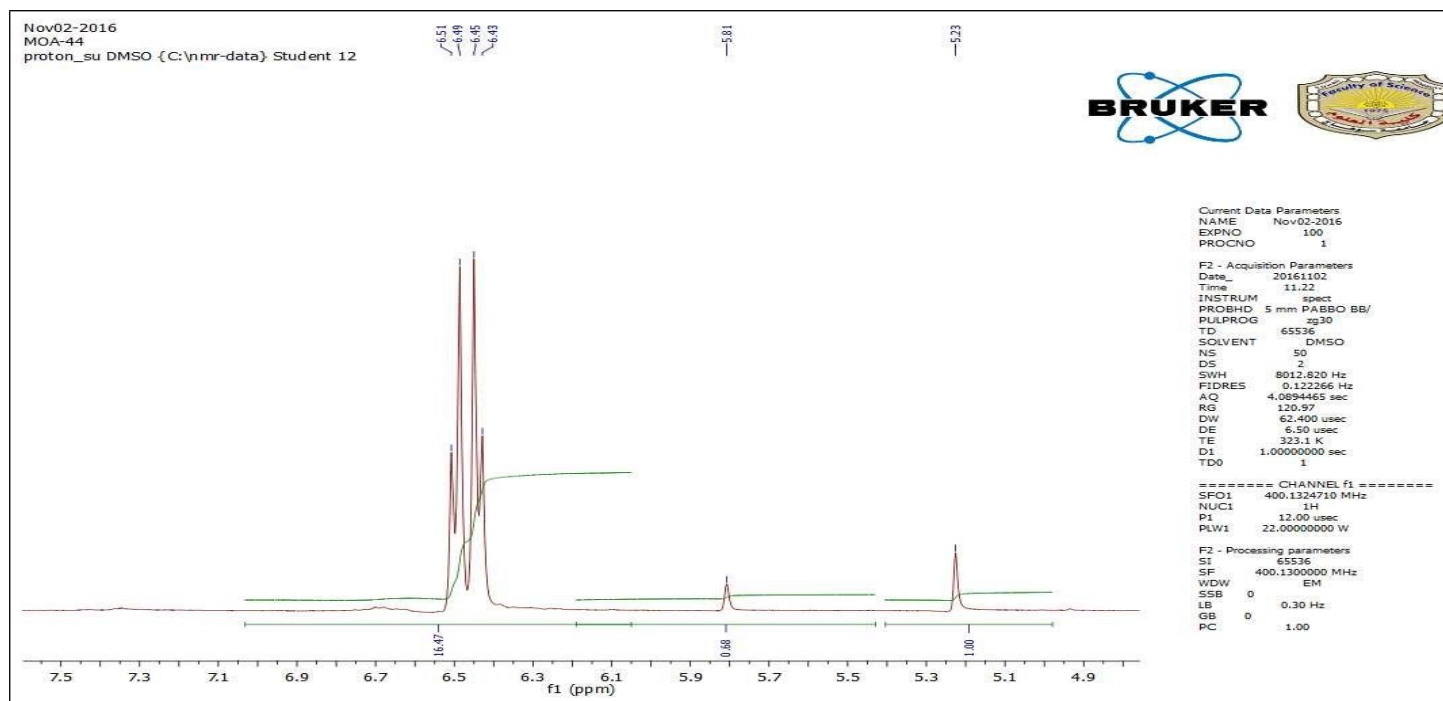
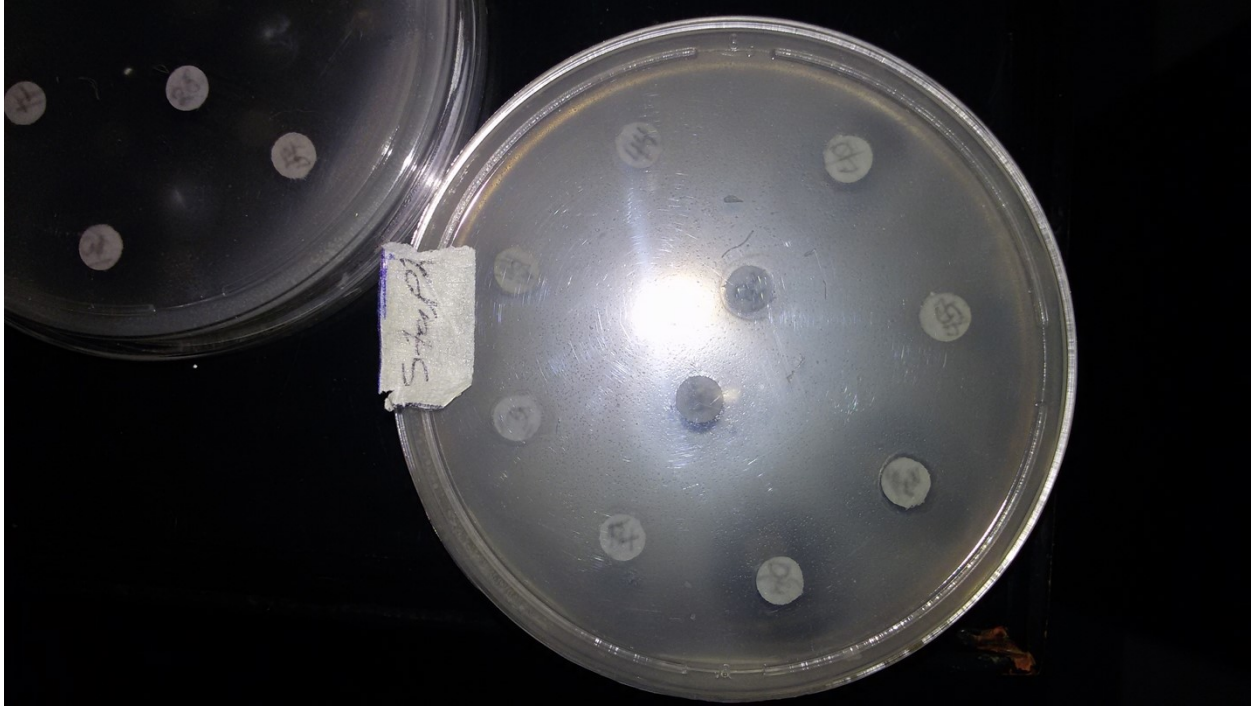
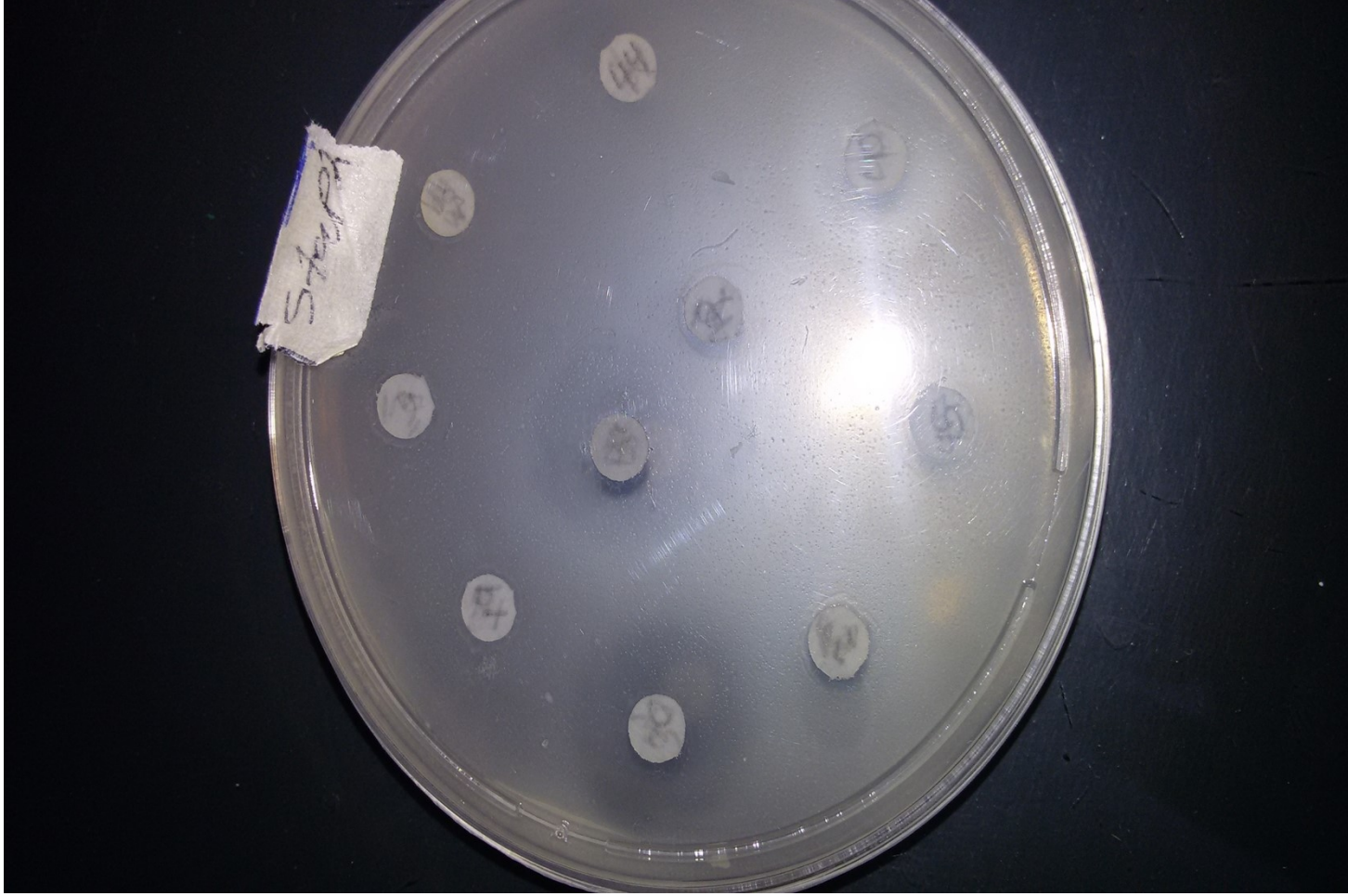
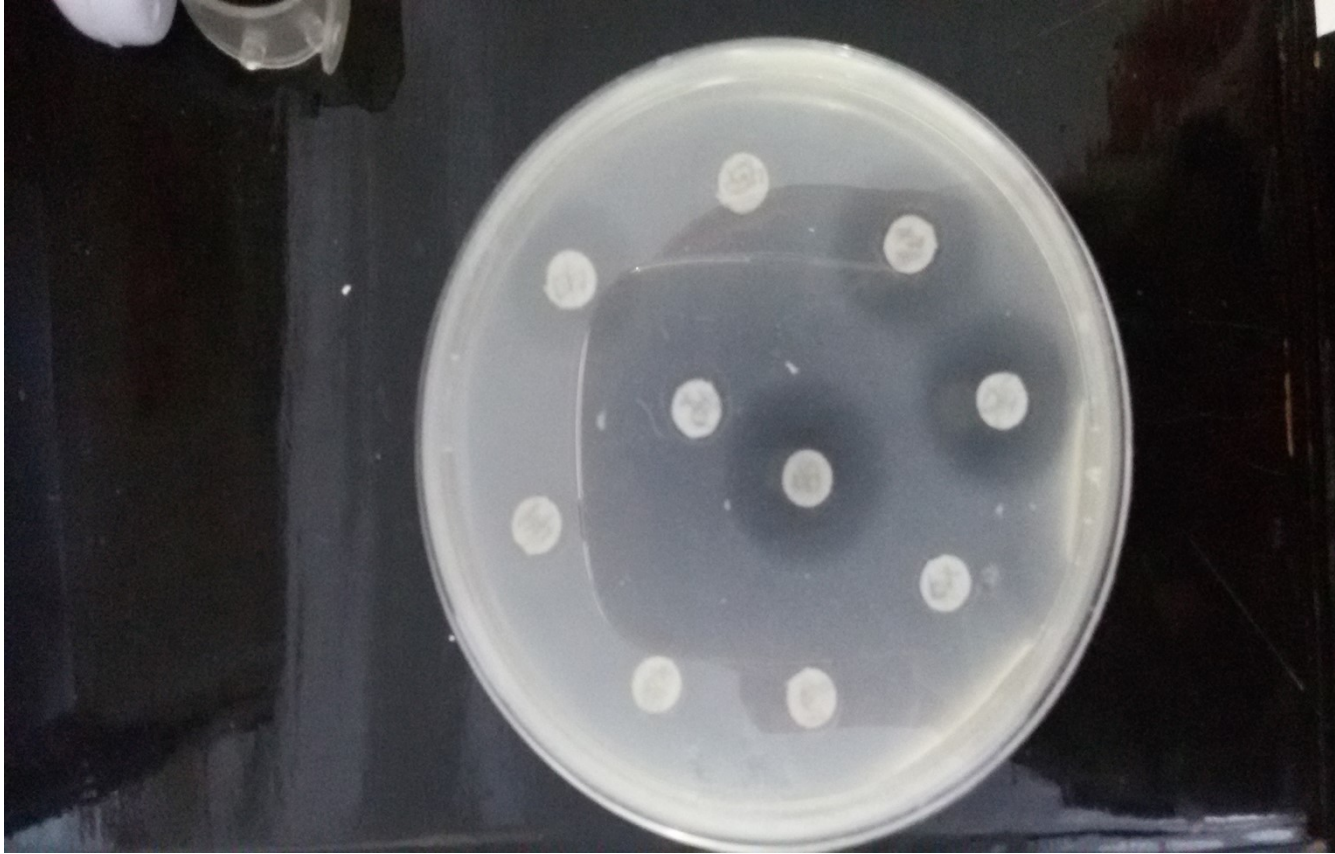


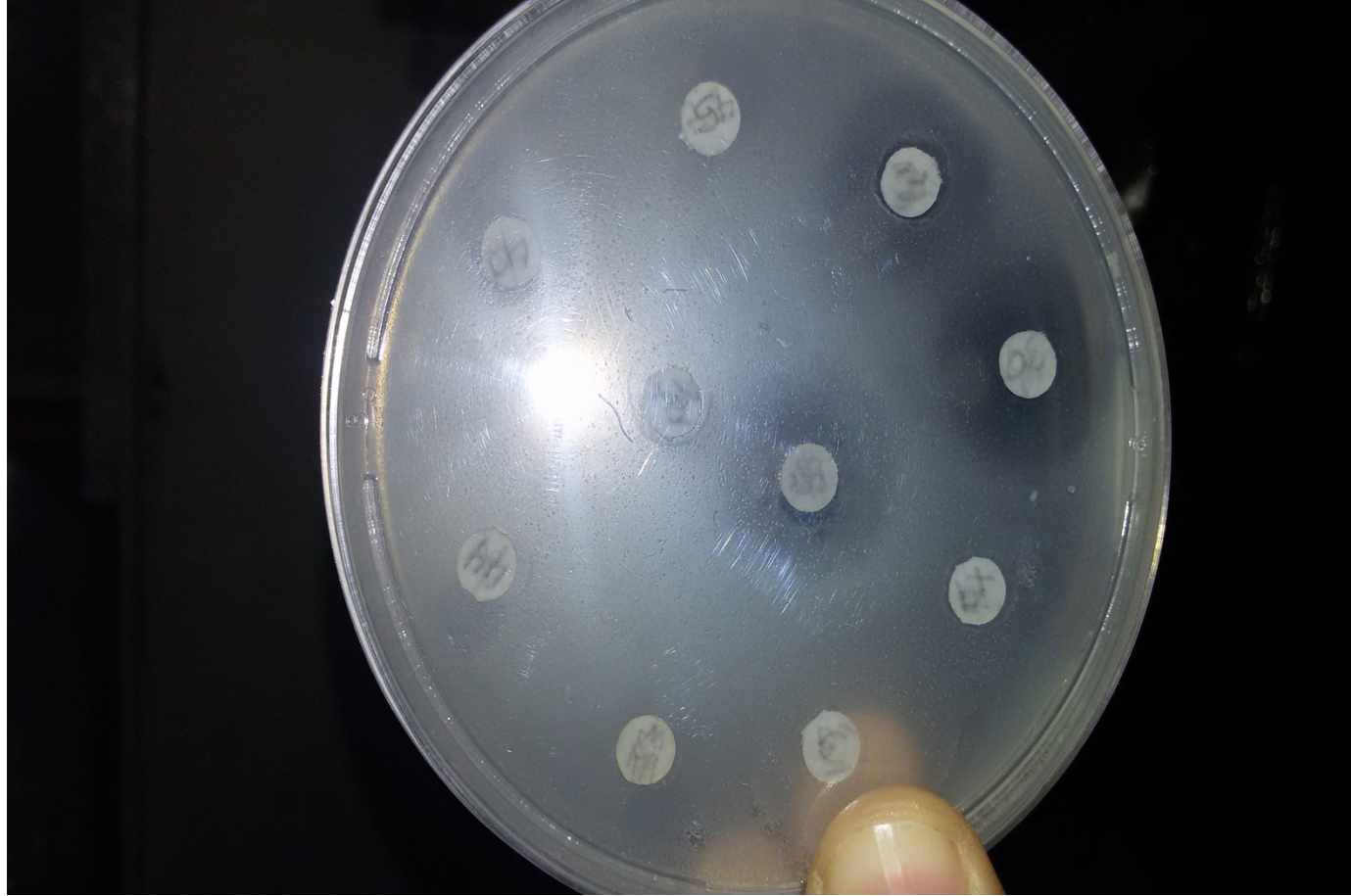
Figure S21. ^1H NMR Spectrum of Compound (8)

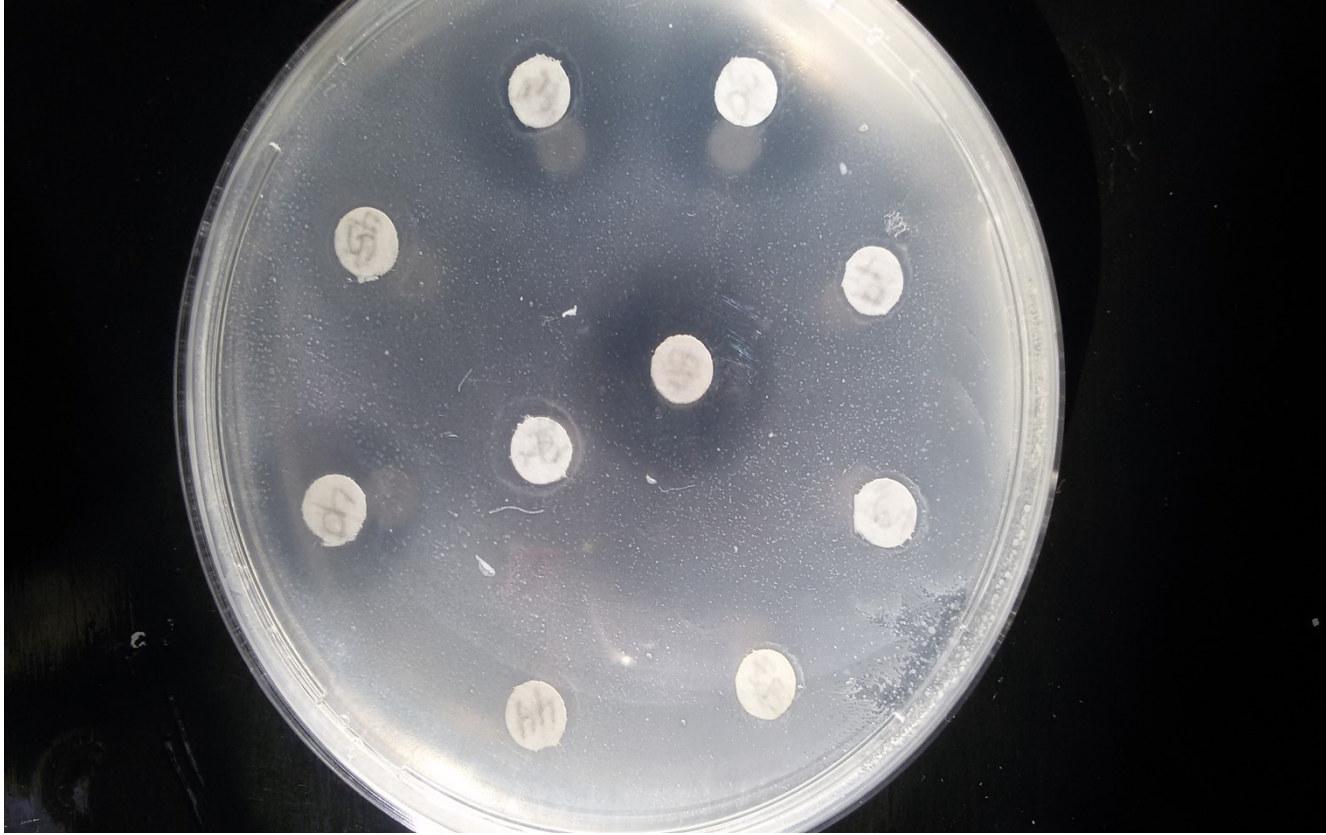


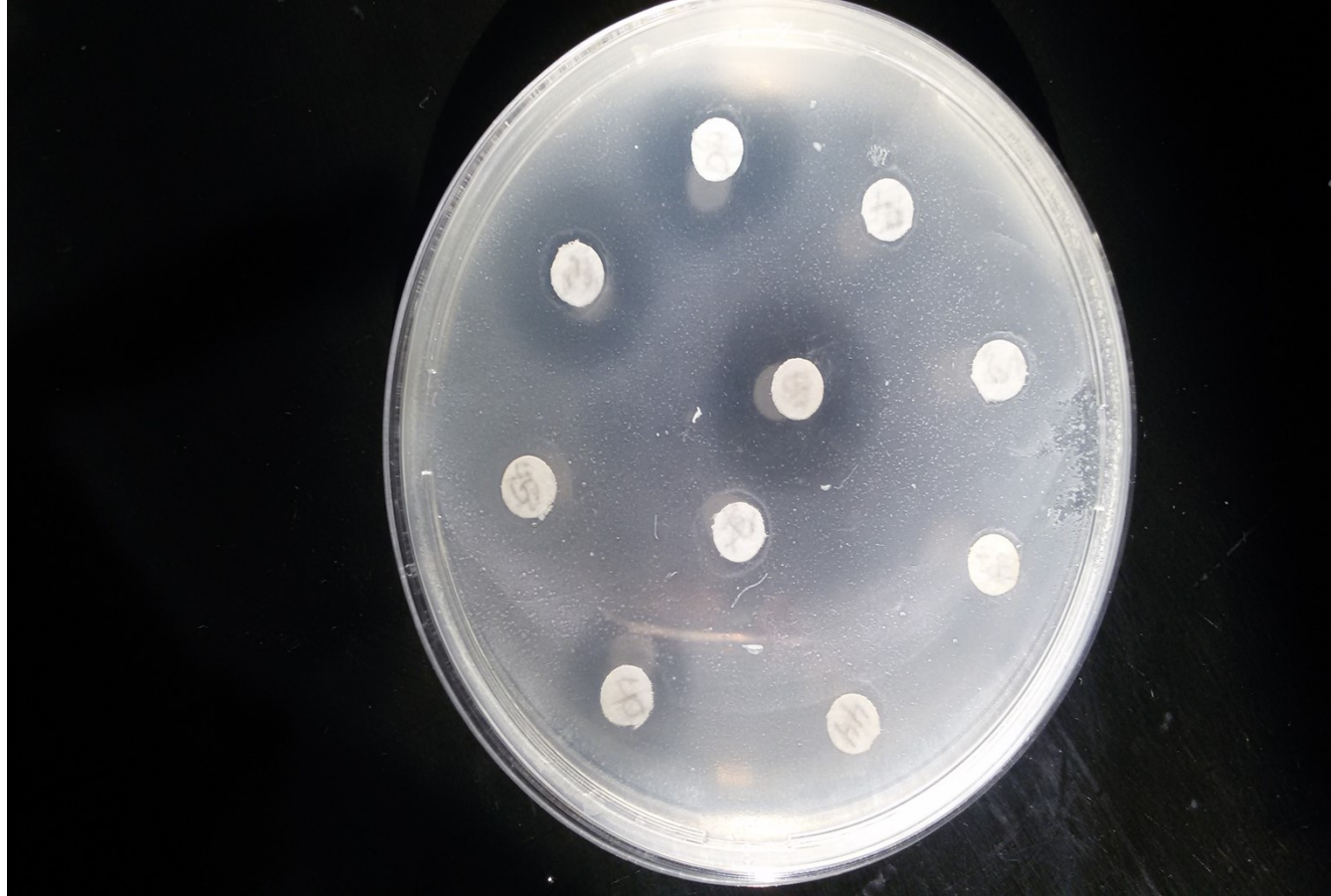
S-101/21

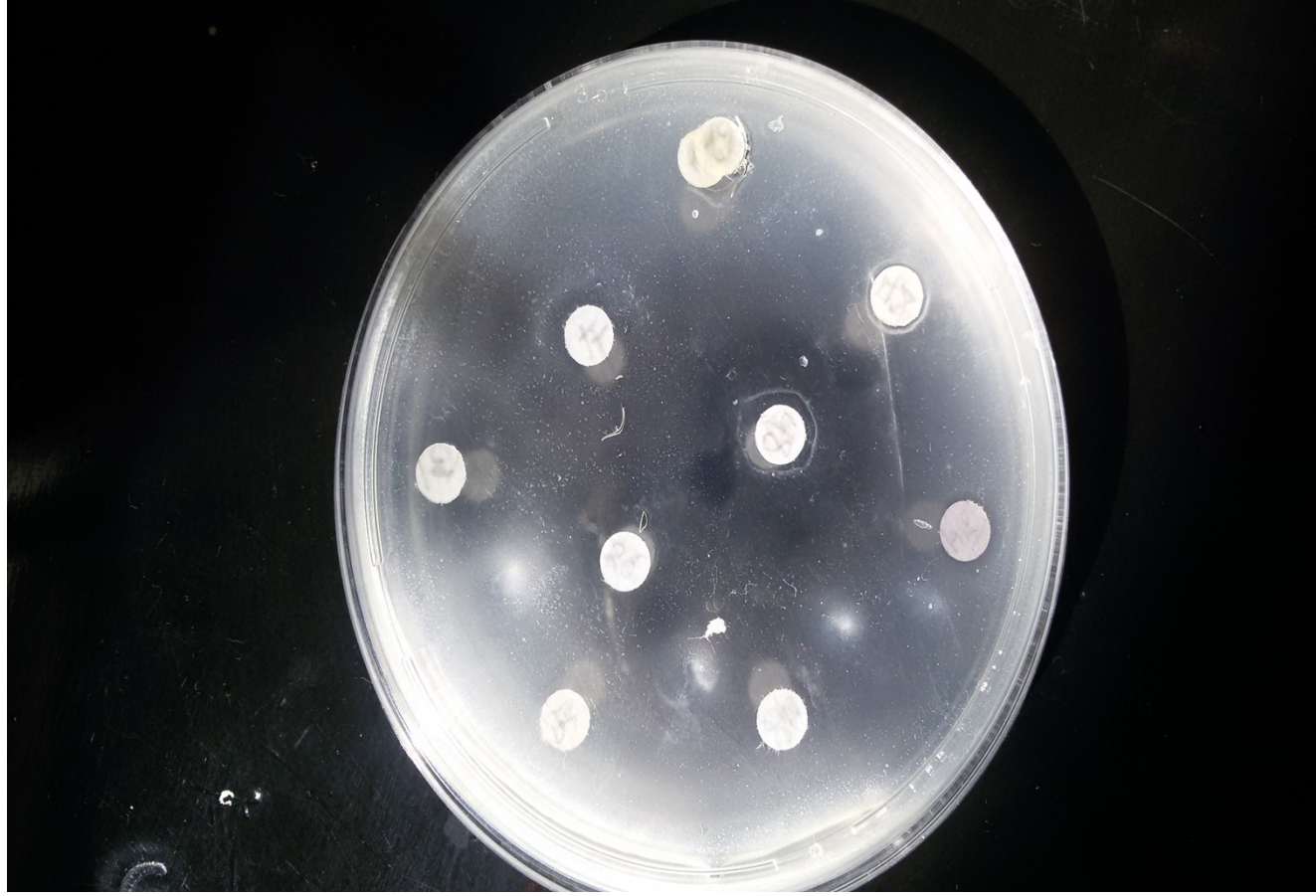


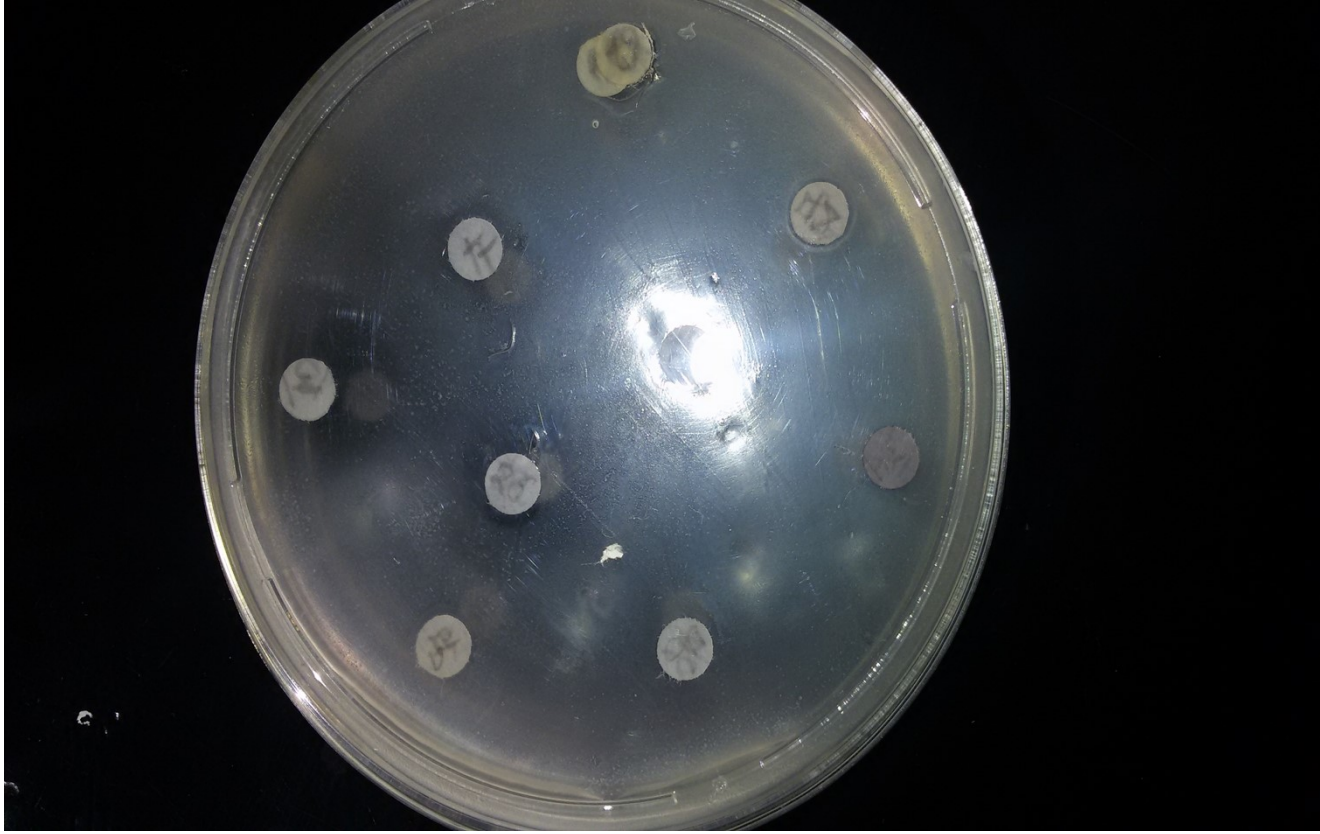


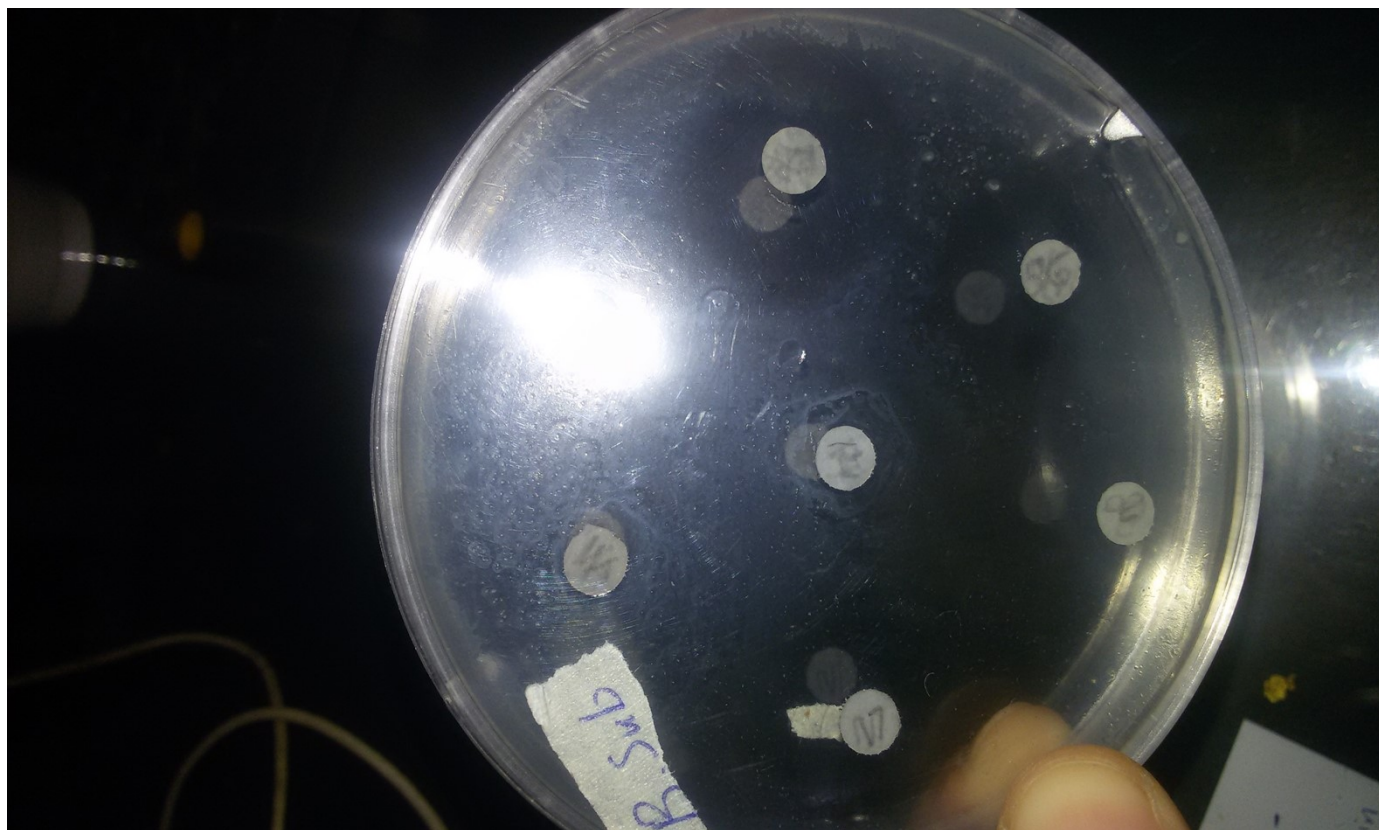












Figures S22. Antibacterial activity of compounds against pathogenic bacterial strains *Escherichia coli*, *Staphylococcus haemolyticus*, *Kocuria kristinae*, *Enterococcus casseliflavus*, and *Bacillus cereus*.

Card Type: GP Testing Instrument: VITEK 2

Bionumber: 050402123720221

Organism Quantity:

Comments:

Identification Information	Card: GP	Lot Number: 242381940	Expires: May 29, 2017 12:00 EEST
	Completed: Mar 16, 2017 14:12 EET	Status: Final	Analysis Time: 7.00 hours
Selected Organism	86% Probability Bionumber: 050402123720221		Staphylococcus haemolyticus Confidence: Acceptable Identification
SRF Organism			
Analysis Organisms and Tests to Separate:			
Analysis Messages:			
Contraindicating Typical Biopattern(s) Staphylococcus haemolyticus SAC(57),AlaA(7),dGAL(77),POLYB(1).			

2	AMY	-	4	PIPLC	-	5	dXYL	-	8	AOH1	+	9	BGAL	-	11	AGLU	+
13	APPA	-	14	COEX	-	15	AspA	-	16	BGAR	-	17	AMAN	-	19	PHOS	+
20	LeuA	-	23	ProA	-	24	BQUPr	-	25	AGAL	-	26	PyrA	+	27	BGUR	-
28	AlaA	+	29	TyrA	-	30	dSOR	-	31	URE	-	32	POLYB	+	37	dGAL	-
38	dRIB	+	39	LATk	+	42	LAC	-	44	NAG	+	45	dMAL	+	46	BAC	-
47	NOVO	-	50	NCE5	+	52	dMAN	-	53	dBINE	-	54	MBUG	-	56	PUL	-
57	dRAF	-	58	O129R	+	59	SAL	-	60	SAC	-	62	dTRE	-	63	ADH2a	-
64	OPTD	+															

Figure (8): Identification report of bacterial isolate (*Staphylococcus haemolyticus*) using VITEK 2 system.

BiNumber: 120200601563571
Organism Quantity:

Comments:

Identification Information	Card: GP	Lot Number: 242381940	Expires: May 29, 2017 13:00 EEST
	Completed: Mar 18, 2017 15:59 EET	Status: Final	Analysis Time: 3.75 hours
Selected Organism	96% Probability BiNumber: 120200601563571		Enterococcus casseliflavus Confidence: Excellent identification
SRF Organism			
Analysis Organisms and Tests to Separate:			
Analysis Messages:			
Contraindicating Typical Biopattern(s) Enterococcus casseliflavus AMAN(24).			

2	AMY	+	4	PIPLC	-	5	dXYL	-	8	ADH1	-	9	BGAL	+	11	AGLU	-
13	APPA	-	14	CDEX	-	15	AspA	-	16	BGAR	-	17	AMAN	+	19	PHOS	-
20	LeuA	-	23	ProA	-	24	BGUPr	-	25	AGAL	-	26	PyrA	-	27	BGUR	-
28	AlaA	-	29	TyrA	+	30	dSOR	+	31	URE	-	32	POLYB	-	37	dGAL	-
38	dRIB	+	39	ILATk	-	42	LAC	-	44	NAG	+	45	dMAL	-	46	BACI	-
47	NOVO	-	50	NC6.5	+	52	dMAN	+	53	dMNE	+	54	MBdG	+	56	PUL	-
57	dRAF	+	58	O129R	-	59	SAL	+	60	SAC	+	62	dTRE	+	63	ADH2s	-
64	OPTO	+															

Figure (6): Identification report of bacterial isolate (*Enterococcus casseliflavus*) using VITEK 2 system.

Card:	GP	Lot Number:	242381940	Expires:	May 29, 2017 19:00 EEST											
Completed:	Mar 16, 2017 12:43 EET	Status:	Final	Analysis Time:	5:50 hours											
95% Probability	Kocuria kristinae															
Bionumber:	050032102000201		Confidence: Very good identification													
Organisms and Tests to Separate:																
Special Messages:																
Identifying Typical Biopattern(s): -																
Kocuria kristinae TyrA(79), O129R(7).																
Biochemical Details																
ADP	-	4	PIPLC	-	5	dXYL	-	8	ADH1	+	9	BGAL	-	11	AGLU	+
ALP	-	14	CDEX	-	15	AspA	-	16	BGAR	-	17	AMAN	-	19	PHOS	-
ALAL	+	23	ProA	+	24	BGURr	-	25	AGAL	-	26	PyrA	+	27	BGUR	-
AKF	+	29	TyrA	-	30	dSOR	-	31	URE	-	32	POLYB	-	37	dGAL	-
ARF	-	39	ILATx	+	42	LAC	-	44	NAG	-	45	dMAL	-	46	BACI	-
ND10	-	50	NC6.5	-	52	dMAN	-	53	dMNE	-	54	MBdG	-	56	PLL	-
RF	-	58	O129R	+	59	SAL	-	60	SAC	-	62	dTRE	-	63	ADH2s	-
PTD	-															

(7): Identification report of bacterial isolate (*Kocuria kristinae*)
VITEK 2 system.

Figure S23. BIOMERIEUX VITEK2 SYSTEM-bio number analysis