

Supporting Information

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A New Diterpene: Abietane Glycoside from the Roots of *Isodon rugosus* Wall Ex Benth.

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Table S1. α -Glucosidase Inhibitory Potential IC_{50} (mg/mL) of rugosodon 1 and oridonin 2

S. No.	Sample	IC_{50} (mg/mL)
1	Rugosodon	0.438
2	Oridonin	0.998
3	Acarbose (standard)	0.921

Table S2. Anticancer Activity, LC_{50} (μ M/mL) of rugosodon 1 and oridonin 2

S.No.	Sample	LC_{50} (μ M/mL) ^a		
		NCI-H460	HeLa	MCF-7
1	Rugosodon	>50	>50	>50
2	Oridonin	>50	>50	>50
3	Doxorubicin	0.50	0.35	0.40

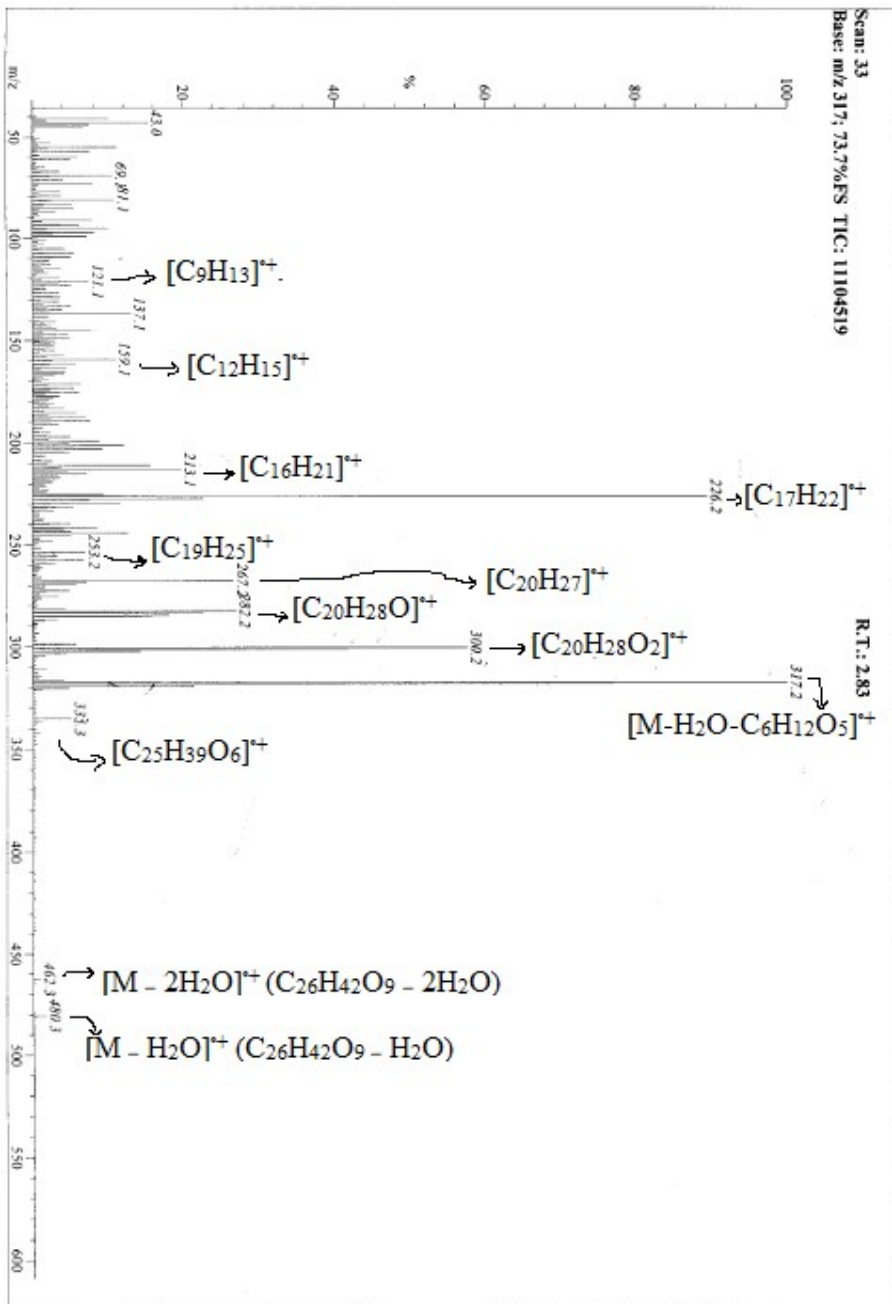
^aIncubation: 72 hours, values obtained are average of three days, $n = 2$ each day

HEJ MASS SECTION
9/8/2015 1:09:53 PM

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Sample: ARIFULLAH /DR. BINA
Instrument: JEOL MS 600H-1

Date Run: 09-08-2015 (Time Run: 12:57:47)

Ionization mode: EI+



S1: EIMS Spectrum of Compound 1 (rugosodon)

HE1 MASS SECTION
9/8/2015 1:10:21 PM

File: ARF-15M
Sample: ARIFULLAH /DR. BINA
Instrument: JEOL MS 600H-1

Date Run: 09-08-2015 (Time Run: 12:57:47)

Ionization mode: EI+

Scan: 33

R.T.: 2.83

Base: m/z 317; 73.7%FS TIC: 11104519

Displayed TIC: 11104519

Threshold: 1% of Base

Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base	Mass %Base
41.0	10.1	87.0	3.1	121.1	7.4	150.1	2.0	179.1	2.1	208.1	1.1	240.2	2.2	273.2	1.8			
42.0	1.9	89.0	1.1	122.1	3.5	151.1	3.0	180.1	1.9	209.1	2.6	241.2	8.7	275.2	3.5			
43.0	15.4	91.0	7.9	123.1	5.1	152.1	2.6	181.1	2.9	210.1	2.0	242.2	4.2	276.2	1.2			
44.0	7.5	92.0	1.4	124.1	1.7	153.1	2.9	182.1	2.1	211.1	15.6	243.1	5.1	281.2	4.3			
45.0	6.7	93.1	3.7	125.1	1.8	154.1	1.6	183.1	4.1	212.1	3.9	244.2	12.8	282.2	27.0			
51.0	1.1	94.0	6.1	126.1	1.1	155.1	2.9	184.1	1.6	213.1	19.7	245.2	5.0	283.2	22.7			
53.0	2.5	95.1	10.1	127.1	3.5	156.1	4.1	185.1	5.8	214.1	4.7	246.2	1.1	284.2	18.1			
55.0	11.2	96.1	2.1	128.1	2.7	157.1	1.8	186.1	2.1	215.1	7.1	247.1	1.0	285.2	15.8			
56.0	2.2	97.1	8.2	129.1	3.7	158.1	11.0	187.1	7.0	216.1	21.6	248.2	2.7	286.2	3.3			
57.0	7.6	98.0	2.7	130.1	3.7	159.1	2.5	188.1	2.5	217.2	3.7	251.2	1.1	287.2	1.6			
60.0	6.0	99.1	7.2	131.1	3.5	161.1	5.7	189.1	7.6	218.2	21.9	252.2	7.0	298.2	5.7			
61.0	5.2	101.0	1.9	132.1	1.4	162.1	2.3	190.1	2.5	219.1	2.6	253.2	2.6	299.2	5.7			
65.1	1.7	103.0	1.5	133.1	5.0	163.1	4.4	191.1	3.4	220.1	1.6	254.2	3.1	300.2	57.6			
67.1	3.7	105.0	4.3	134.1	1.9	164.1	1.1	192.1	1.5	221.1	1.8	255.2	3.3	301.2	41.8			
68.1	1.2	106.1	1.0	135.1	3.9	165.1	4.3	193.1	1.3	223.1	2.1	256.3	1.8	302.2	14.2			
69.1	10.6	107.1	5.5	136.1	2.3	166.1	4.1	195.1	2.3	224.1	1.9	257.2	6.7	303.2	4.5			
70.1	2.3	108.1	1.6	137.1	13.0	167.1	2.9	196.1	1.8	225.1	9.5	258.2	2.0	304.2	1.6			
71.1	4.2	109.1	5.1	138.1	2.2	168.0	1.4	197.1	4.9	226.2	89.5	259.2	3.0	311.1	1.8			
72.1	1.2	110.1	2.7	139.1	2.0	169.1	2.1	198.1	2.1	227.2	22.7	260.2	1.0	314.2	1.2			
73.1	8.0	111.1	2.2	141.1	3.0	170.1	1.1	199.1	8.9	228.2	7.5	261.2	1.3	316.2	4.1			
74.1	1.0	112.1	1.7	142.1	1.8	171.1	6.3	200.2	4.7	229.2	11.7	262.2	1.3	317.2	100.0			
77.1	3.8	113.1	2.4	143.1	2.4	172.1	2.0	201.2	12.1	230.2	2.5	266.2	1.1	318.2	77.1			
79.1	3.8	114.1	1.1	144.1	3.1	173.1	5.4	202.1	6.5	231.2	5.3	267.2	26.7	319.3	21.4			
81.1	10.9	115.0	3.8	145.1	7.8	174.1	2.3	203.1	9.2	232.2	1.9	268.3	7.1	320.3	4.8			
82.1	2.6	116.1	1.5	146.1	1.4	175.1	6.2	204.2	4.2	233.1	2.8	269.2	5.8	321.3	1.2			
83.1	5.2	117.1	2.1	147.1	4.7	176.1	1.7	205.1	4.8	237.2	1.6	270.2	1.7	335.3	5.0			
84.1	1.6	119.1	3.6	148.1	1.3	177.1	3.5	206.1	1.5	238.2	1.4	271.3	1.6	336.3	1.3			
85.1	5.5	120.1	1.3	149.1	4.9	178.1	2.8	207.1	1.8	239.2	5.0	272.2	4.9	480.3	1.7			

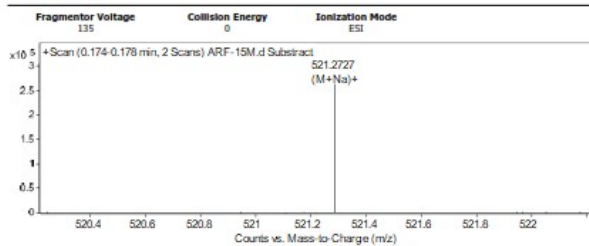
S2: Expansion of the EIMS Spectrum of Compound 1 (rugosodon)

Qualitative Analysis Report

Data Filename	ARF-15M.d	Sample Name	ARF-15M
Sample Type	E-S	Position	P1-C4
Instrument Name	SIP	User Name	Tech # 4
Acq Method	SIBU.m	Acquired Time	10/03/2018 11:18:40 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group	Info.	
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
228.942	2	32067		
338.8867	1	103730.38		
374.4414	1	108102.18		
521.2727	1	272501.27	C ₂₆ H ₄₂ O ₉	(M+Na) ⁺
522.3172	1	51978.05	C ₂₆ H ₄₂ O ₉	(M+Na) ⁺
695.5471	1	1790048.19		
696.7823	1	41878.68		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	10

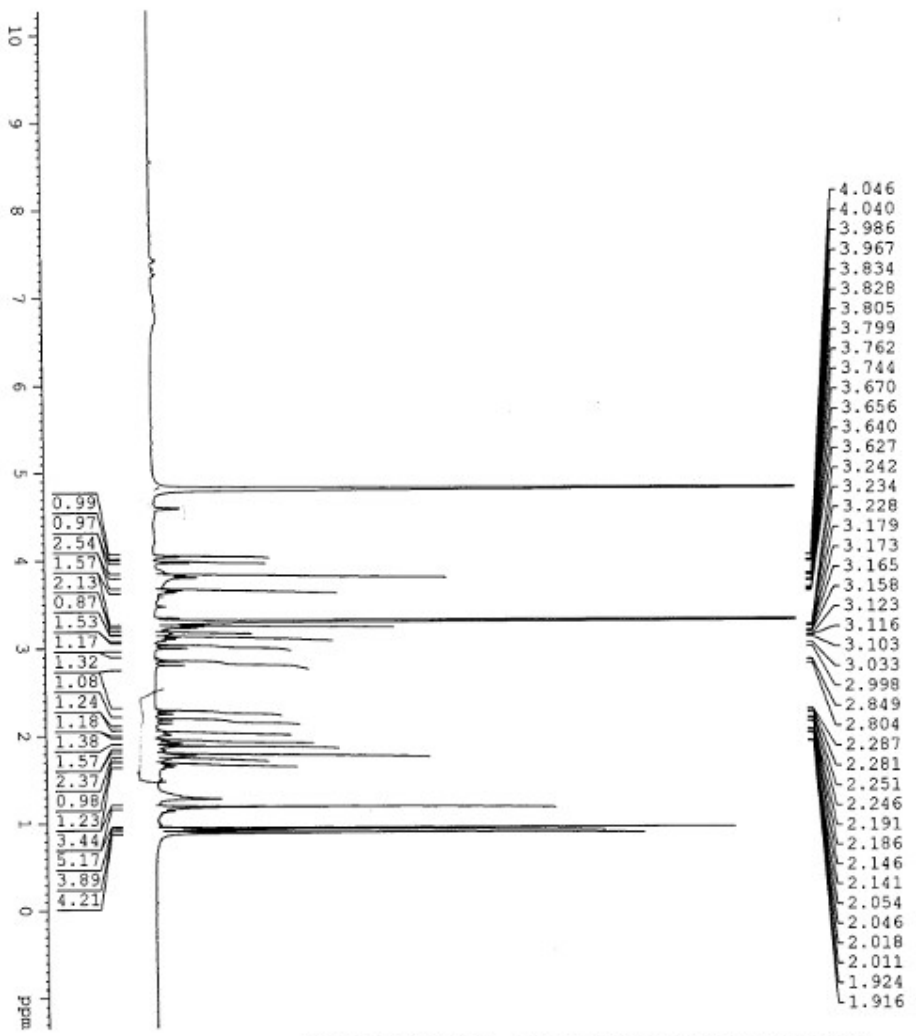
Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₆ H ₄₂ O ₉	498.2629	521.2723	521.2727	-0.4	-1.2	6.0000

--- End Of Report ---

S3: ESIMS Spectrum of Compound 1 (rugosodon)

ARI FUJIIAH/DR, BINA/ARF-ISM/
ICCBS, U.O.K/



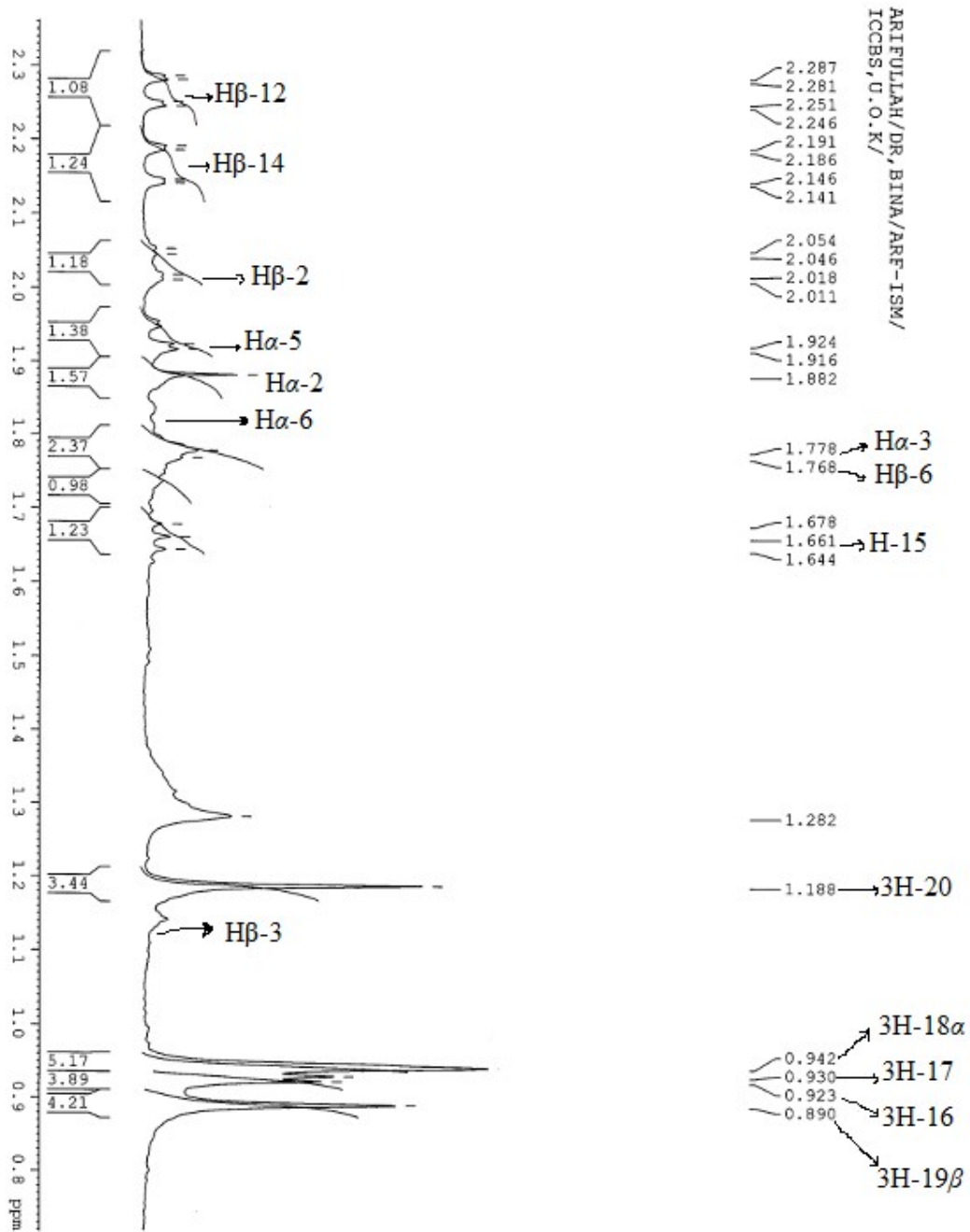
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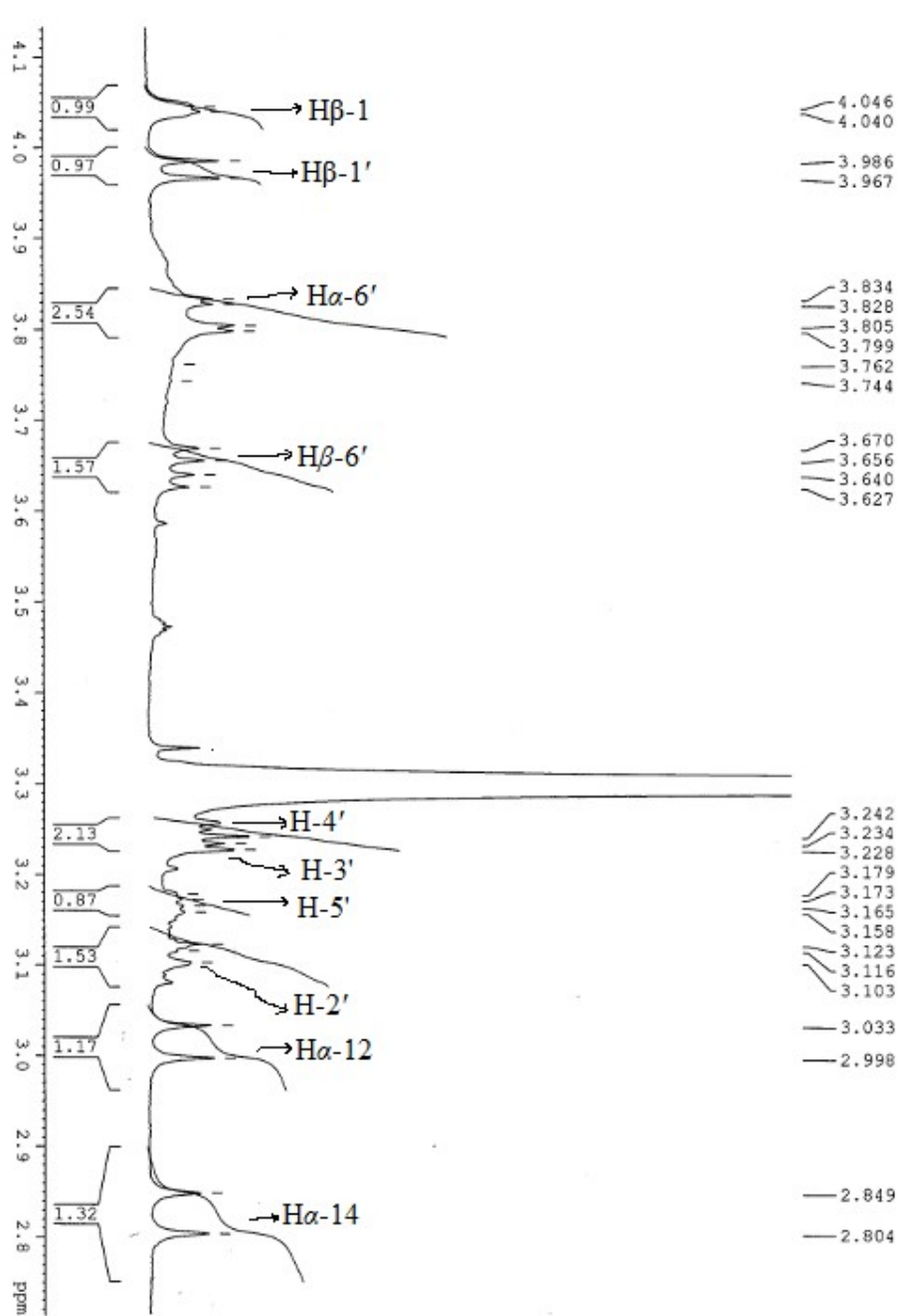
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SOLVENT   DMSO
NS         64
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FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         456.1
DE         62.400 usec
TE         300.0 K
D1         2.000000000 sec
TD0        1

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P1         10.20 usec
PL         0.00 dB
SFO1       400.1332010 MHz
SI         16384
SF         400.1300111 MHz
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LB         0.30 Hz
GB         0
PC         1.00
  
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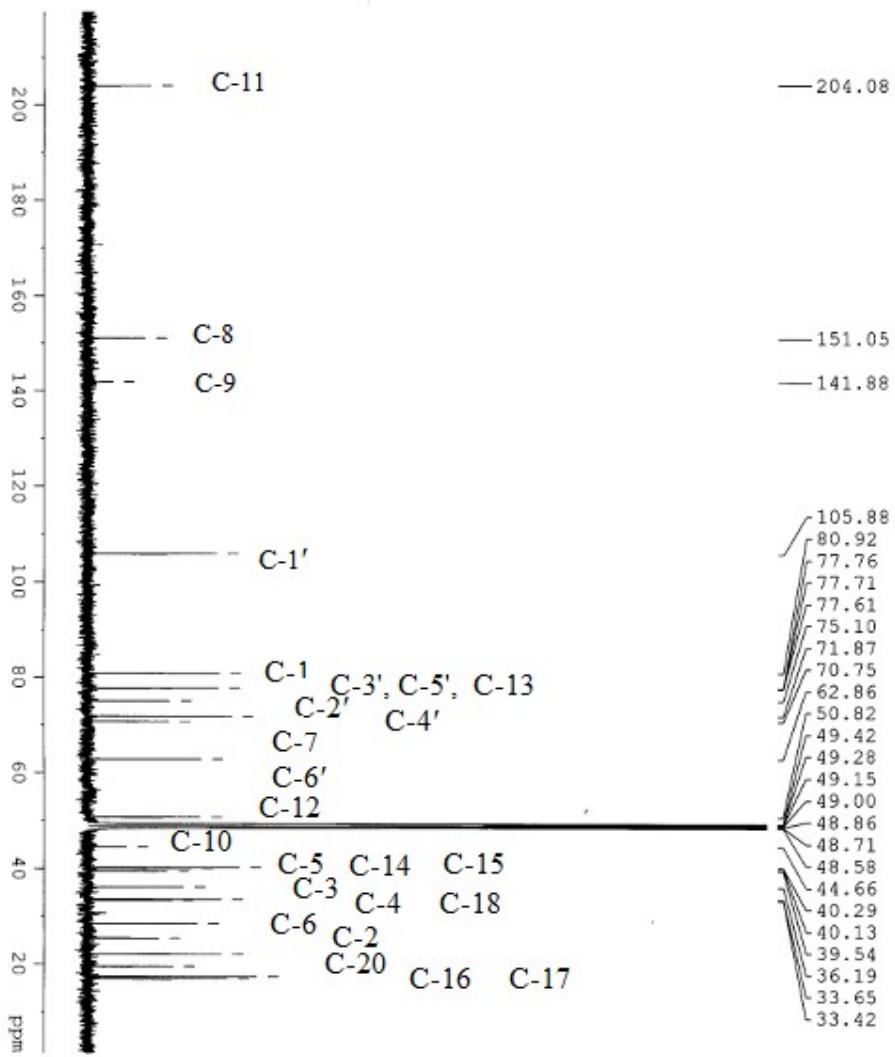
S4: ¹H-NMR (400 MHz, CD₃OD) Spectrum of Compound 1 (rugosodon)



S5: Expansion of the ¹H-NMR Spectrum of Compound 1 (rugosodon)



S6: Expansion of the ¹H-NMR Spectrum of Compound 1 (rugosodon)

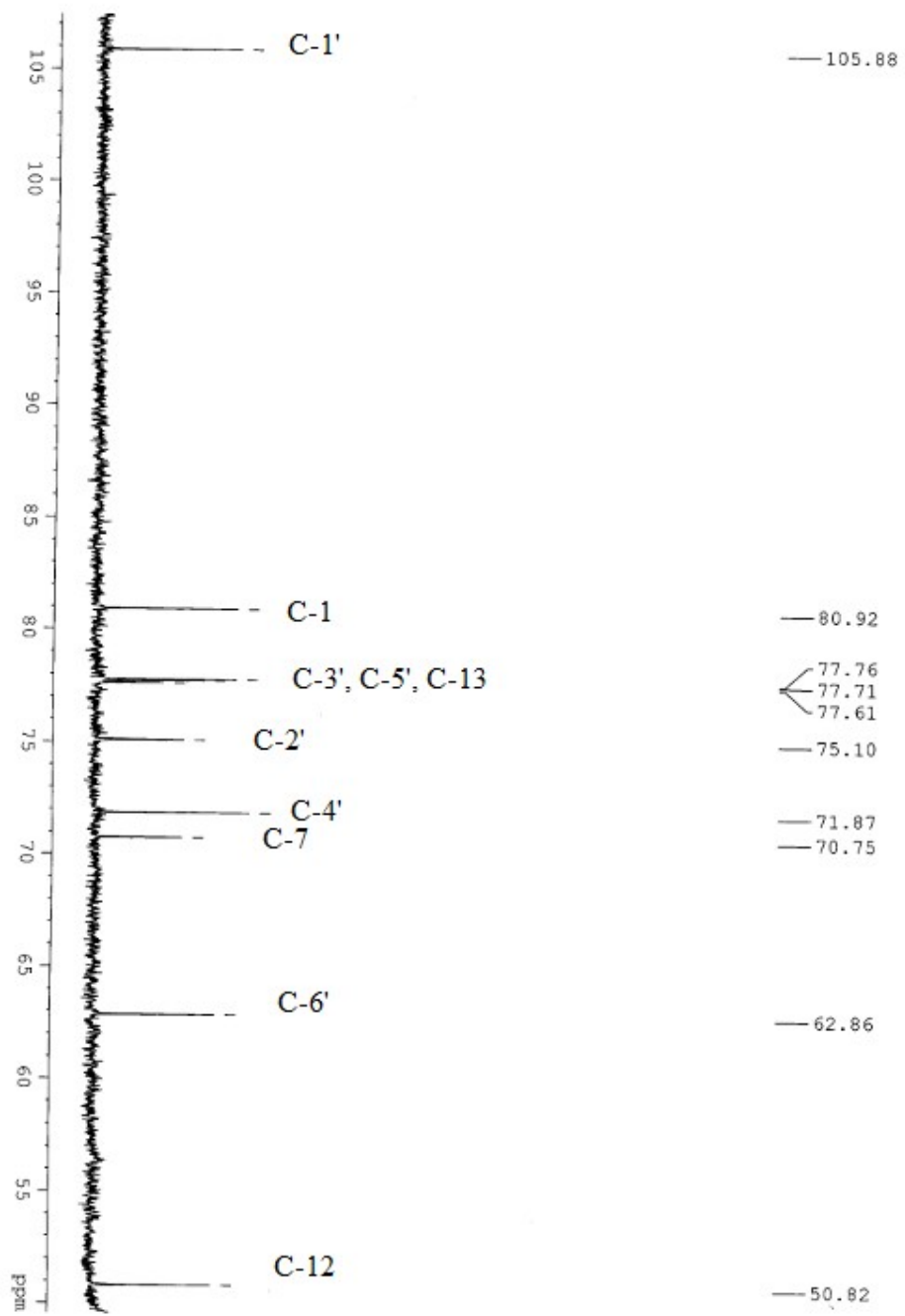


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 SOLVENT: MeOD
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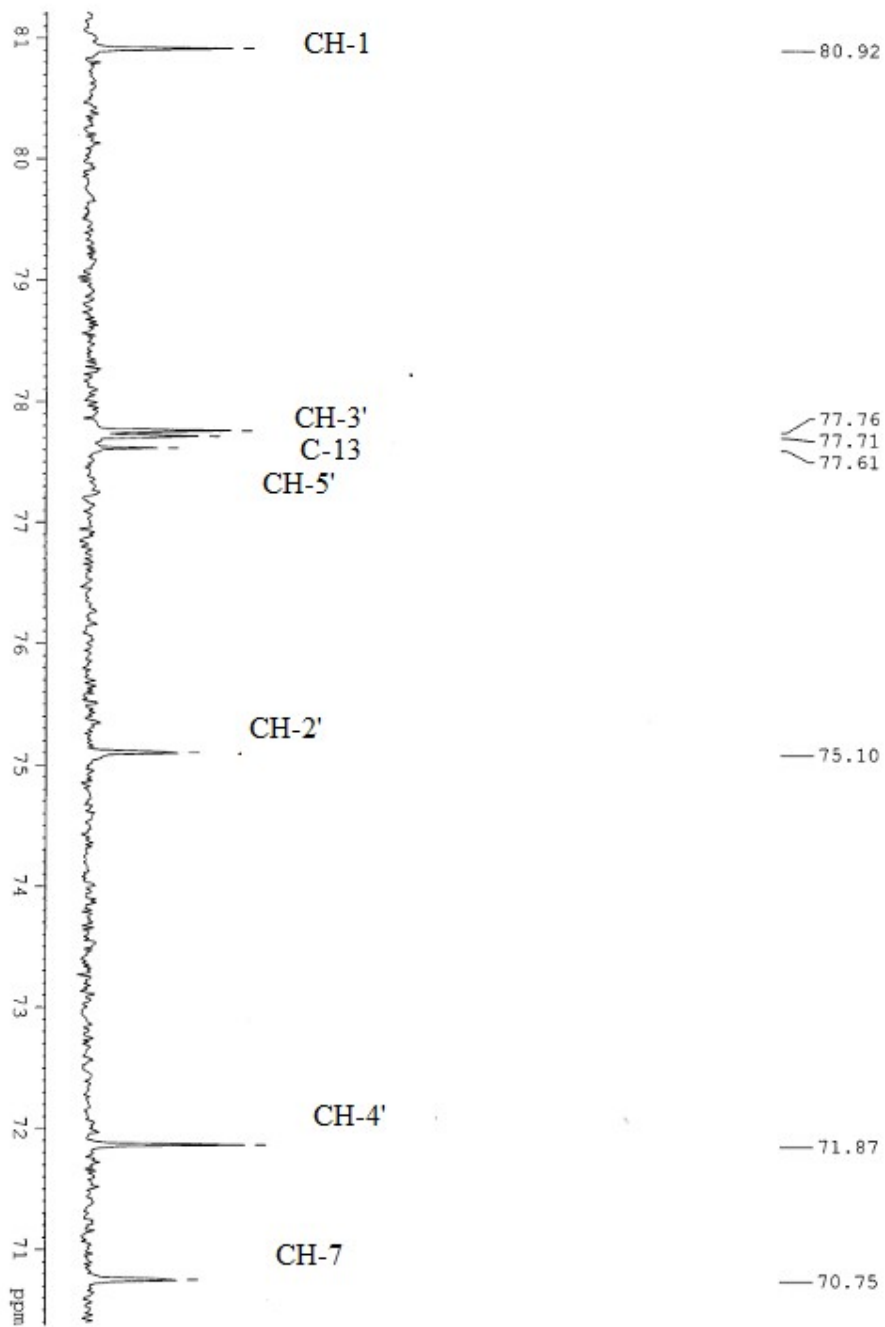
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 SFO1: 150.9453107 MHz

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 NUC2: 1H
 P2: 65.00 usec
 PL2: 3.30 dB
 PL12: 22.06 dB
 PL13: 27.00 dB
 PL2W: 9.16420078 MHz
 PL1W: 0.12182353 MHz
 PL1SW: 0.03909280 MHz
 SFO2: 600.2336014 MHz
 SI: 15384
 SE: 150.9277901 MHz
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S7: ¹³C-NMR, BB (150 MHz, CD₃OD) Spectrum of Compound 1 (rugosodon)

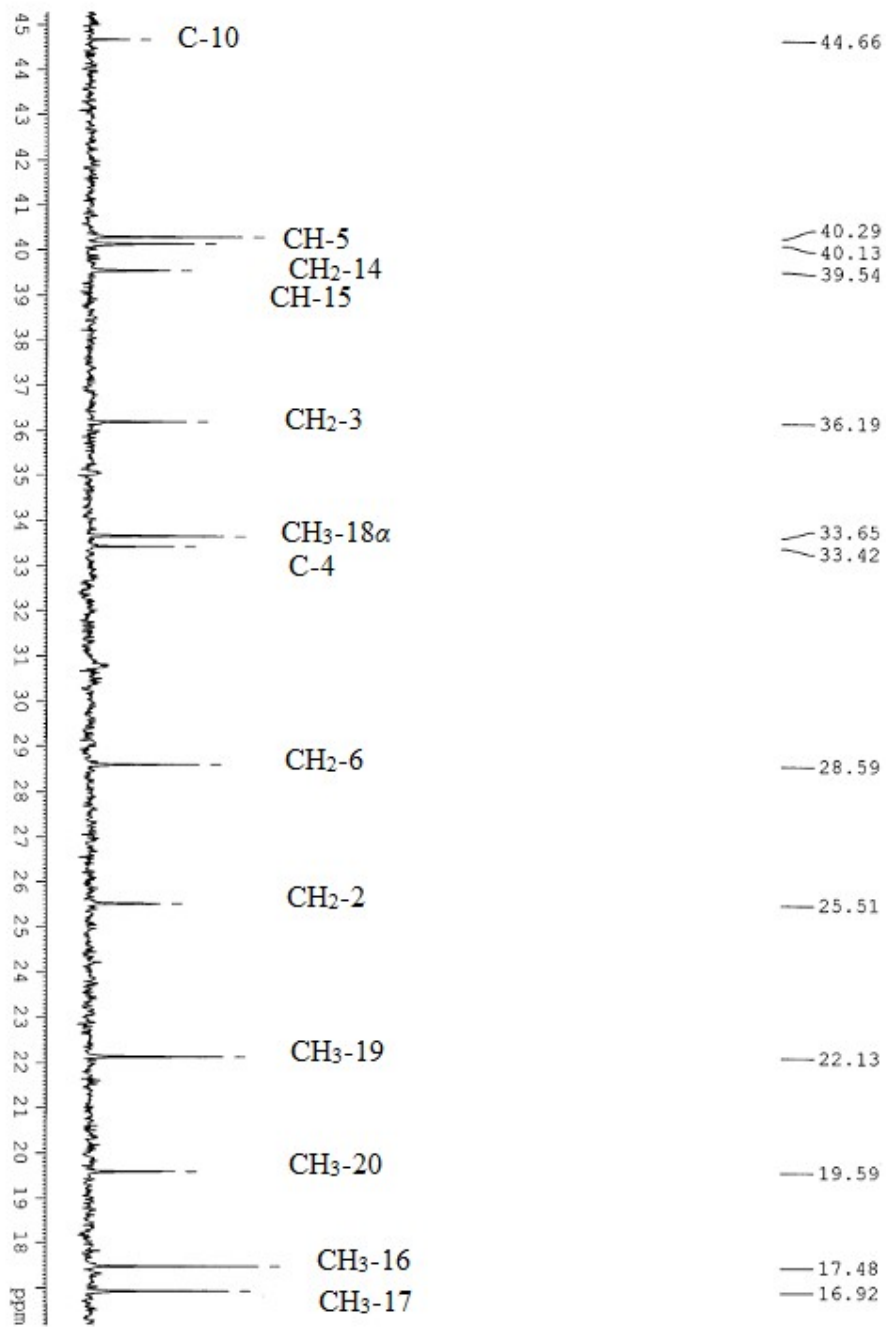


S8: Expansion of the ^{13}C -NMR, BB of Compound 1 (rugosodon)

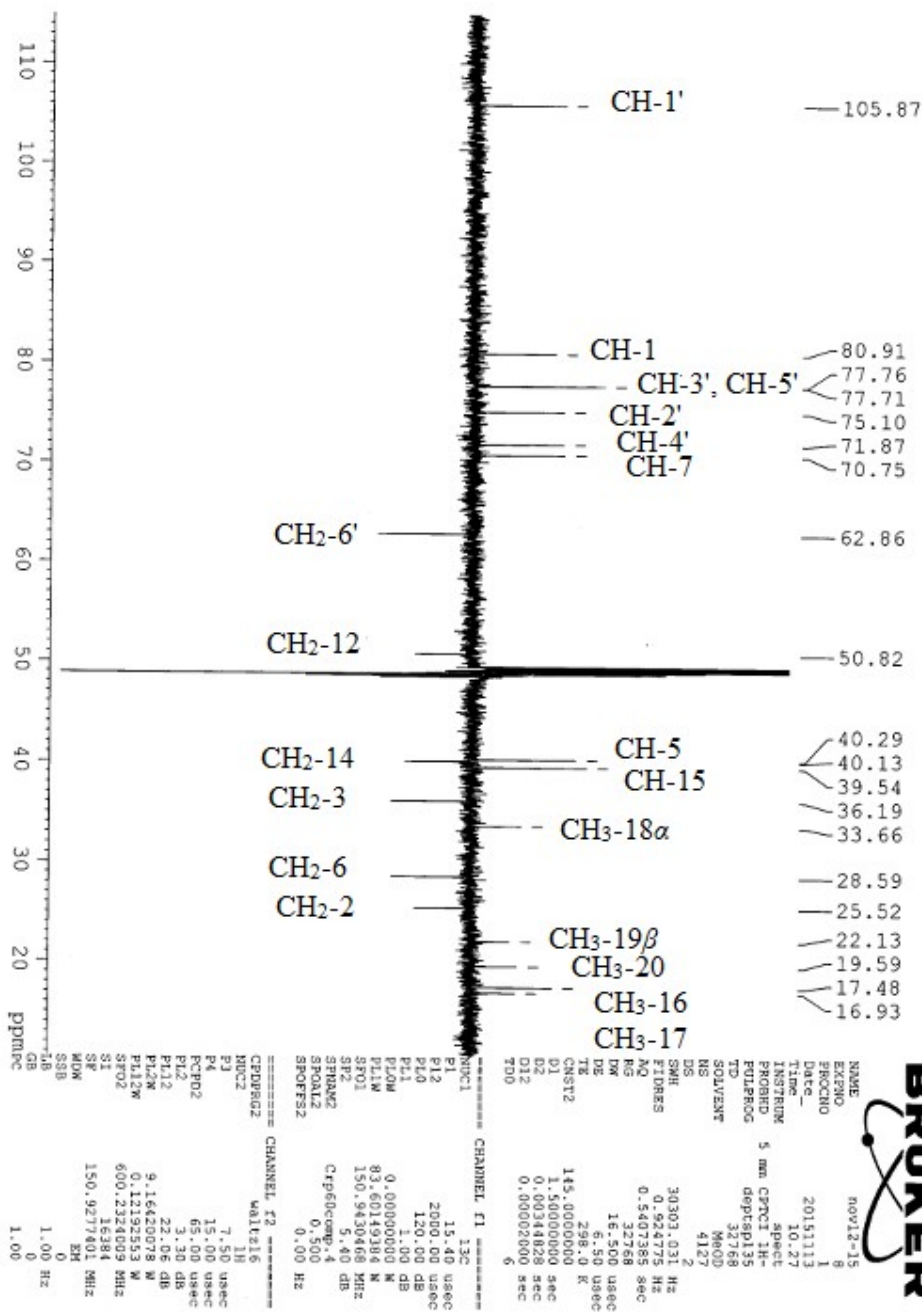


ARIFULLAH/DR. BINN/ARF-15M/CD30D
BB

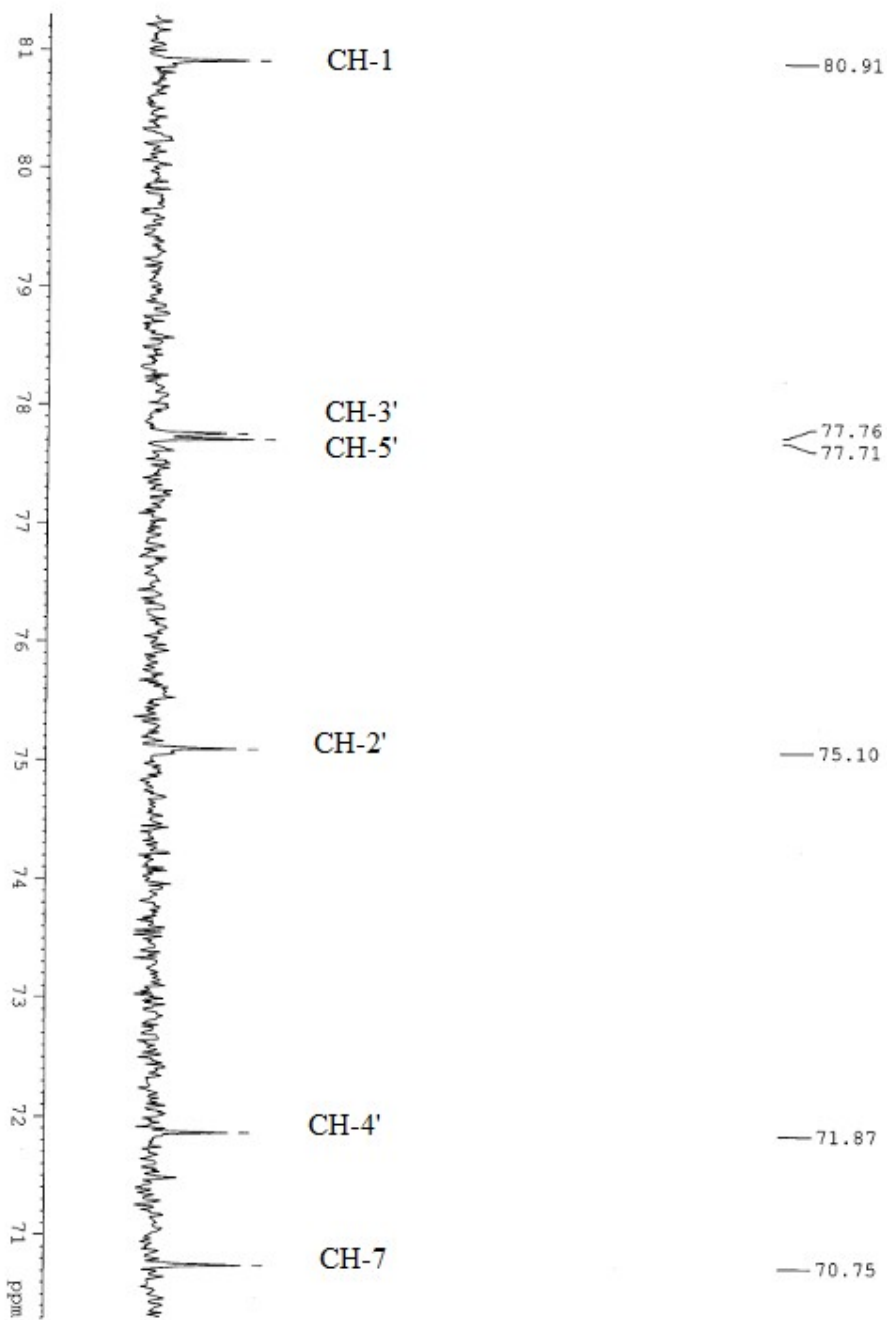
S9: Expansion of the ¹³C-NMR, BB of Compound 1 (rugosodon)



S10: Expansion of the ¹³C-NMR, BB of Compound **1** (rugosodon)

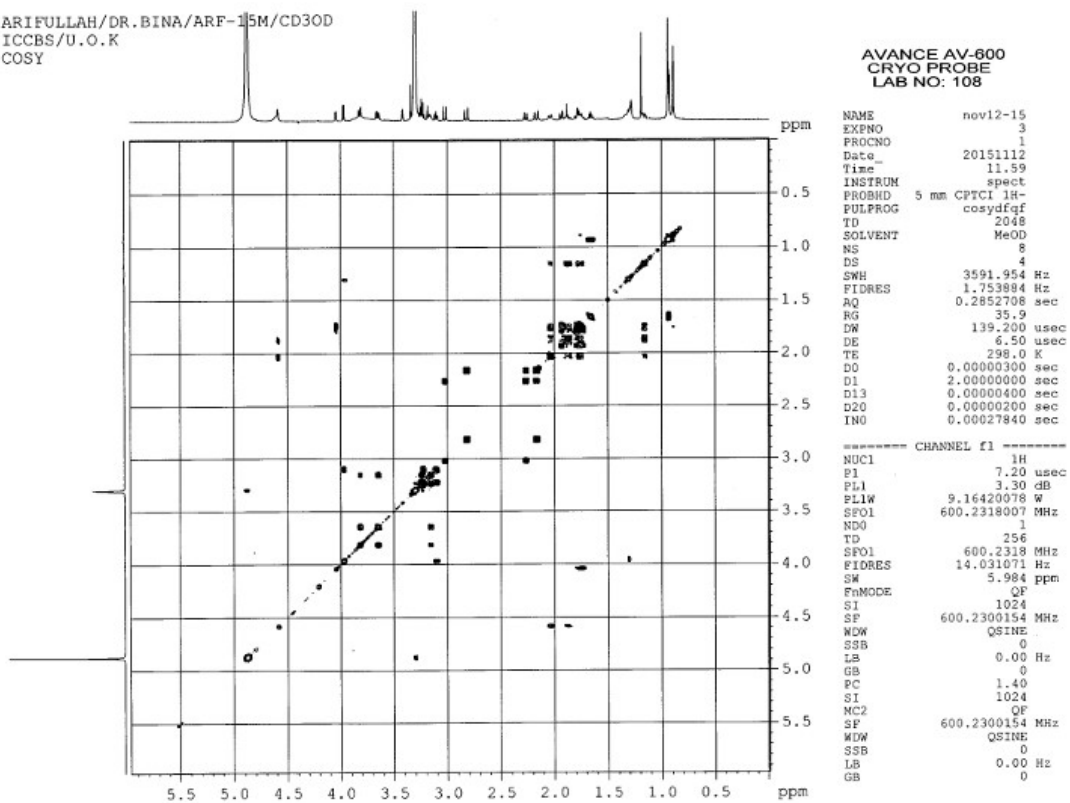


S11: ¹³C-NMR, DEPT-135 (150 MHz, CD₃OD) of Compound 1 (ruginosodon)

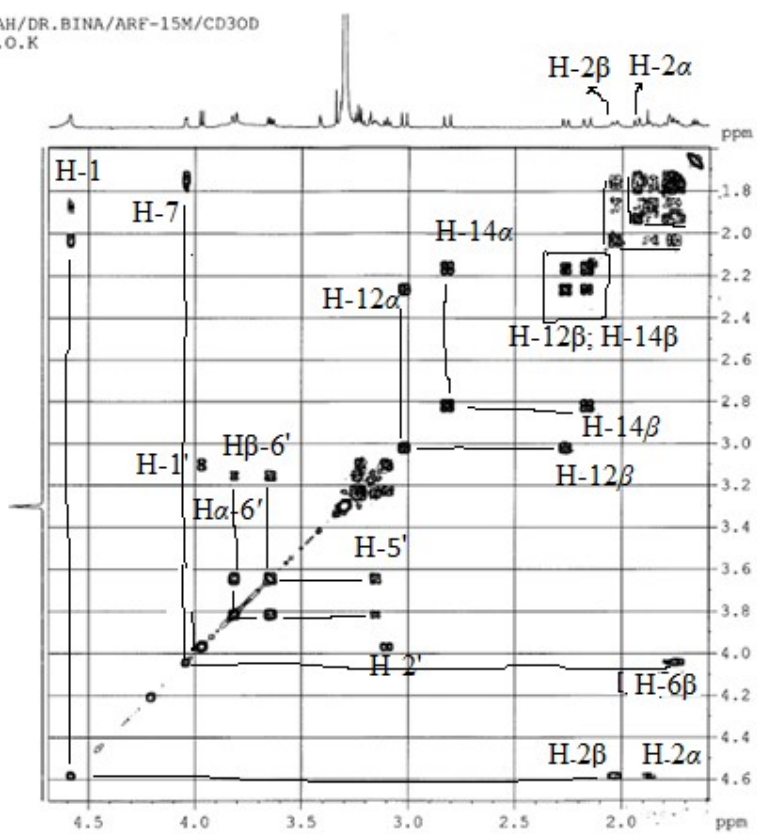


S12: Expansion of the ^{13}C -NMR, DEPT 90 of Compound **1** (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD3OD
ICCBS/U.O.K
COSY

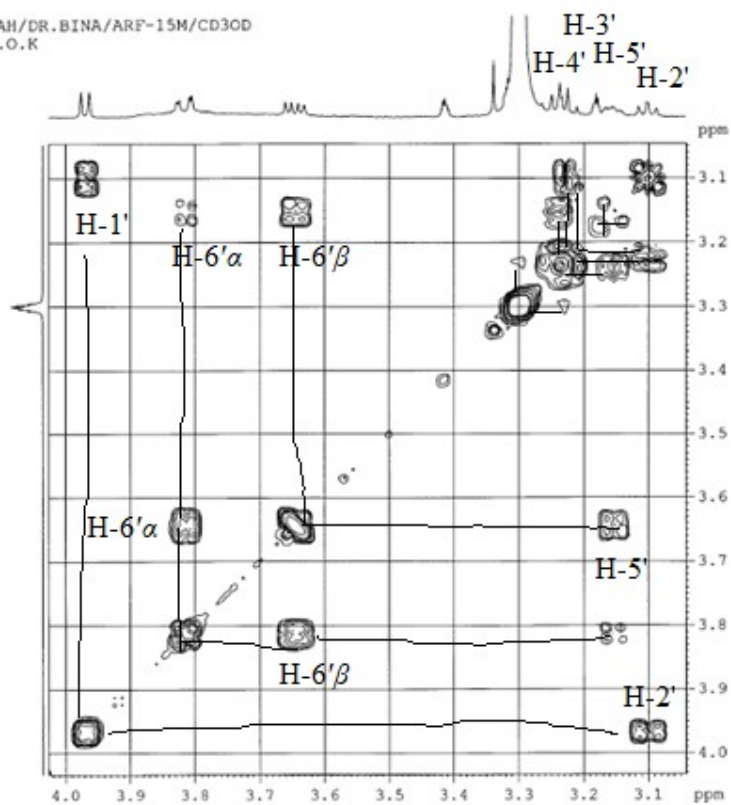


S13: COSY (600 MHz) Spectrum of Compound 1 (rugosodon)



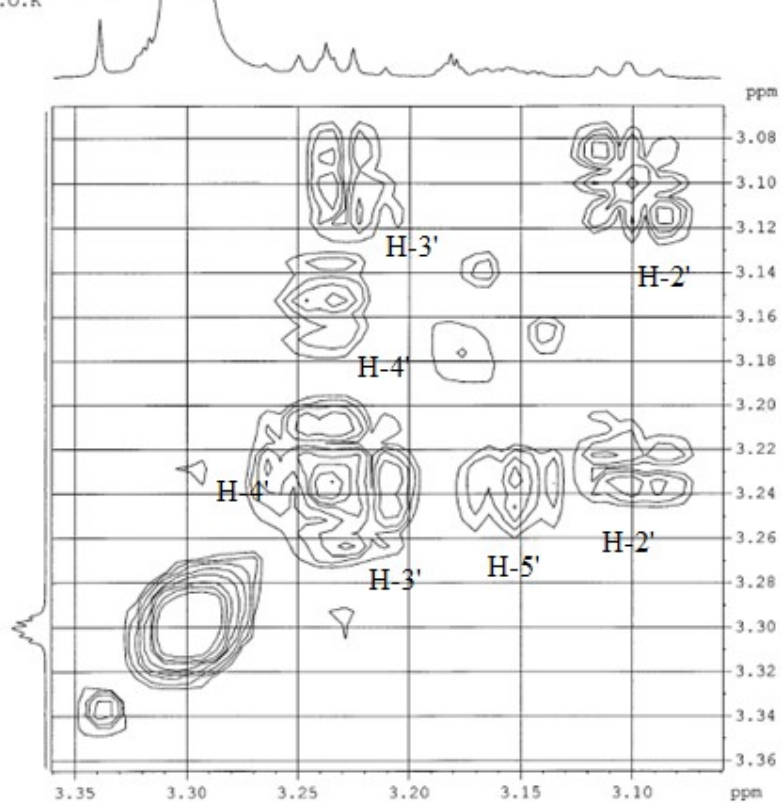
S14: Expansion of the COSY Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR.BINA/ARF-15M/CD3OD
ICCBS/U.O.K
COSY



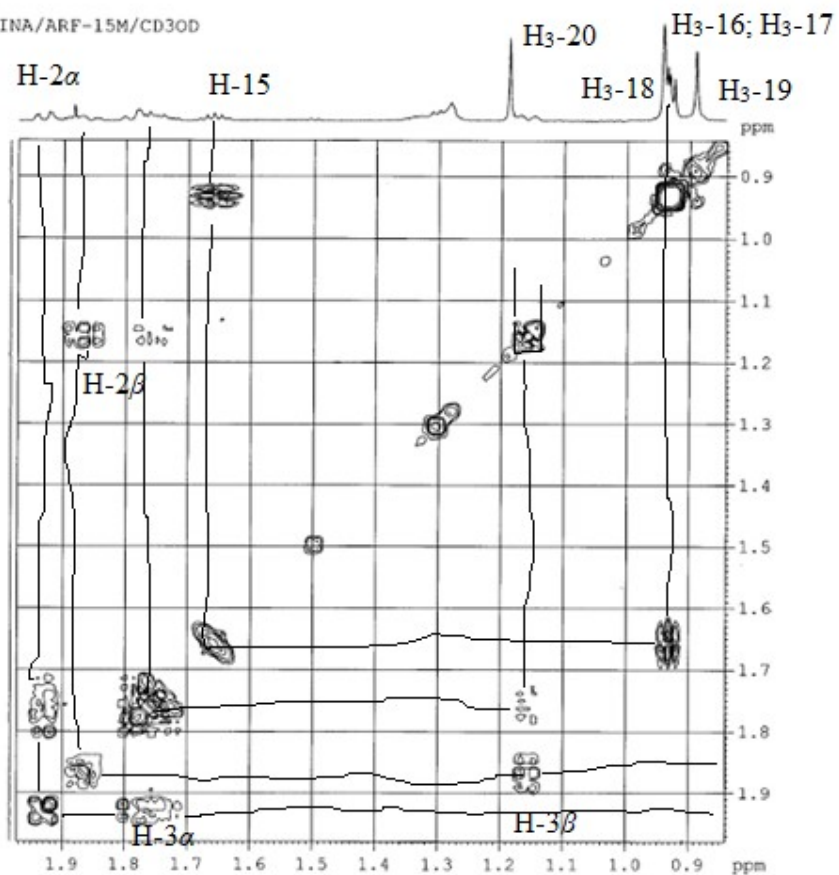
S15: Expansion of the COSY Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD30D
ICCBS/U.O.K
COSY



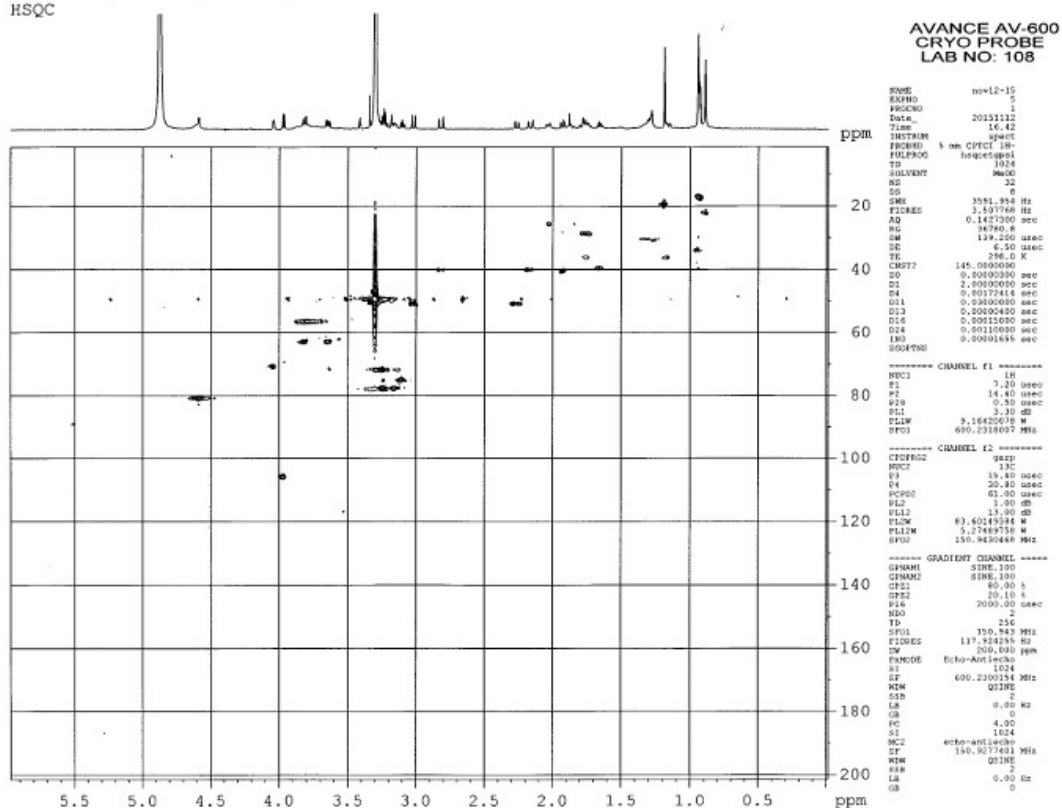
S16: Expansion of the COSY Spectrum of Compound **1** (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD3OD
ICCBS/U.O.K
COSY

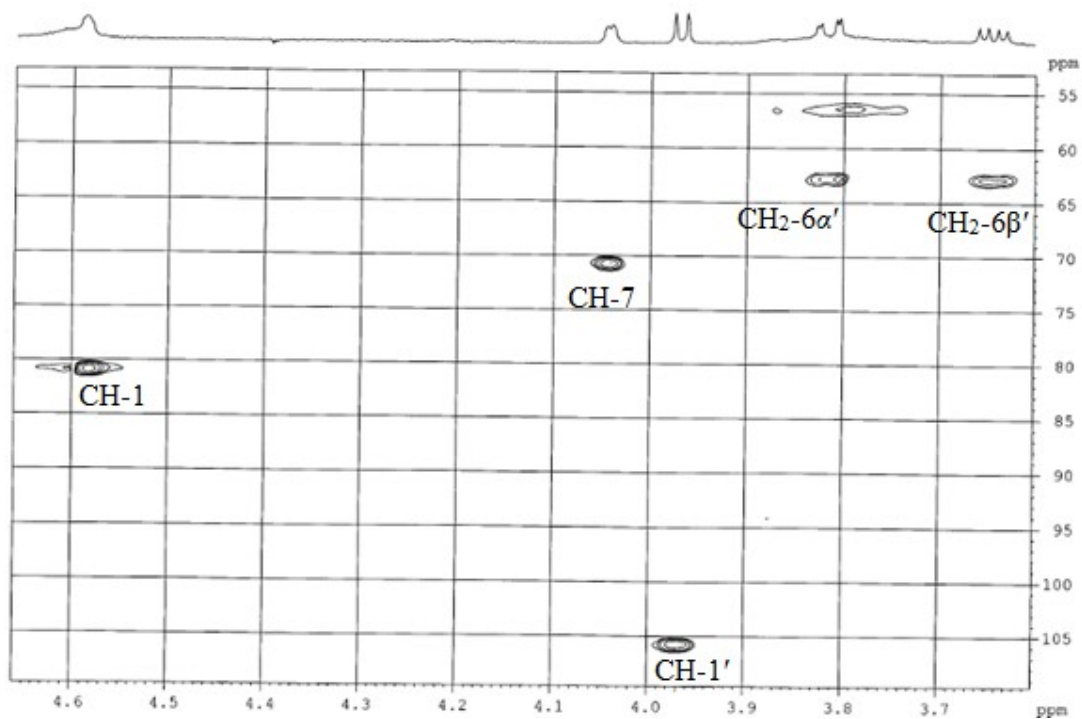


S17: Expansion of the COSY Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD3OD
HSQC

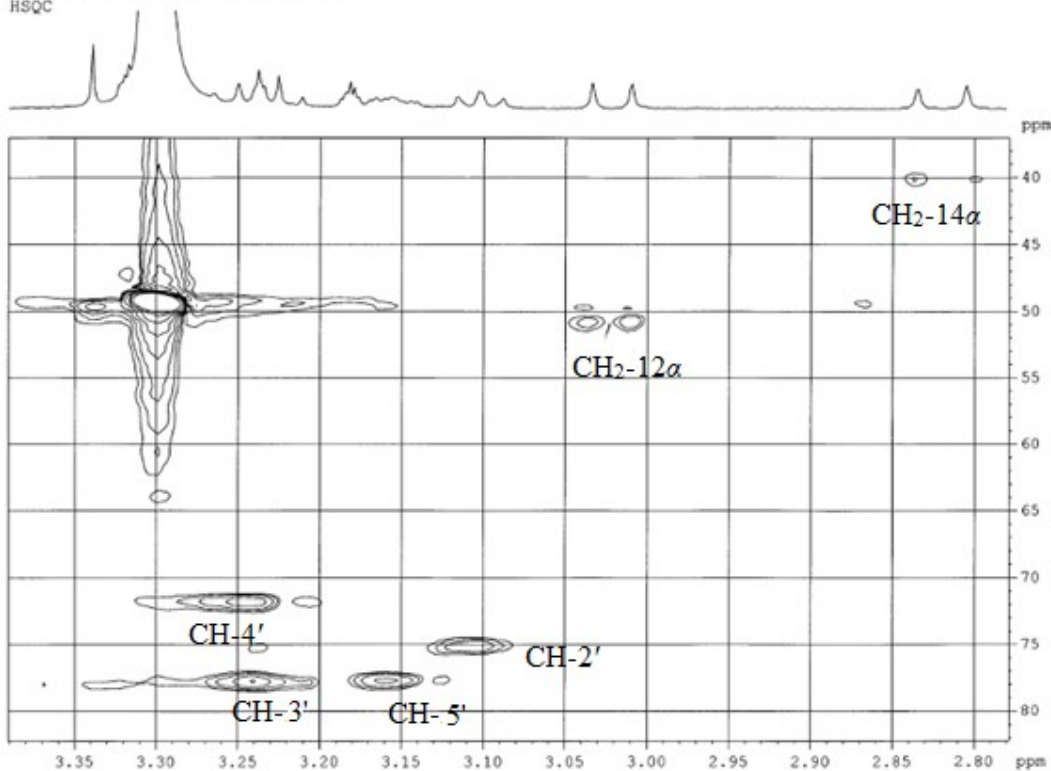


S18: HSQC (600 MHz) Spectrum of Compound 1 (rugosodon)



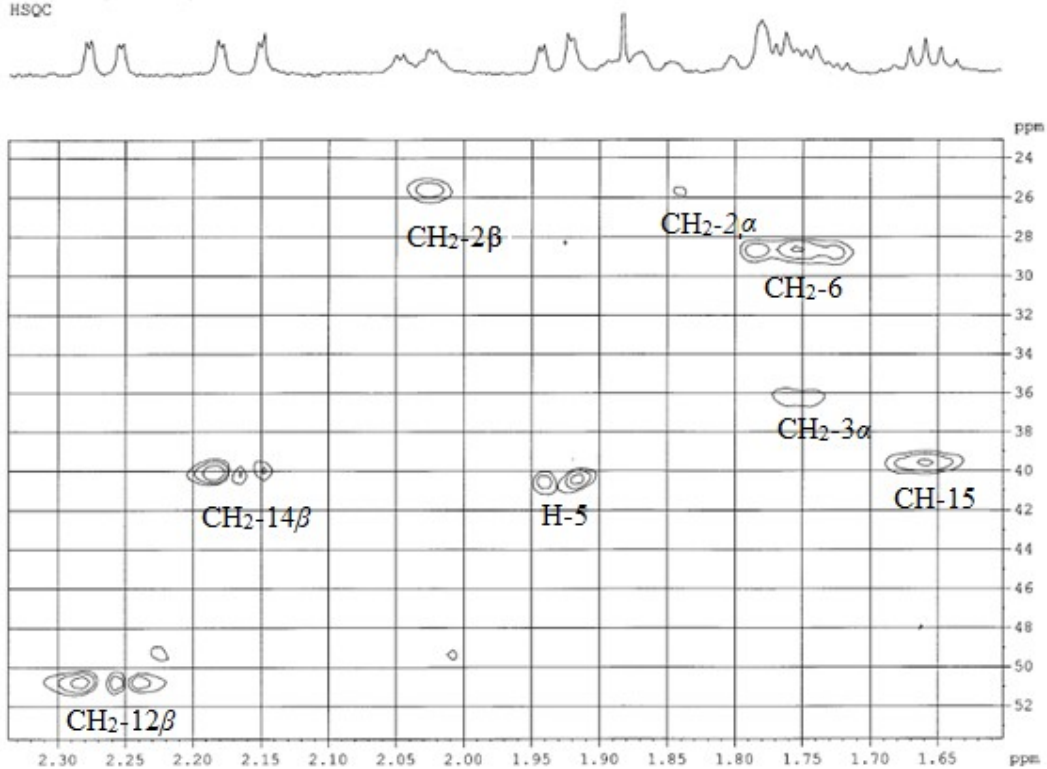
S19: Expansion of the HSQC Spectrum of Compound **1** (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD3OD
HSQC



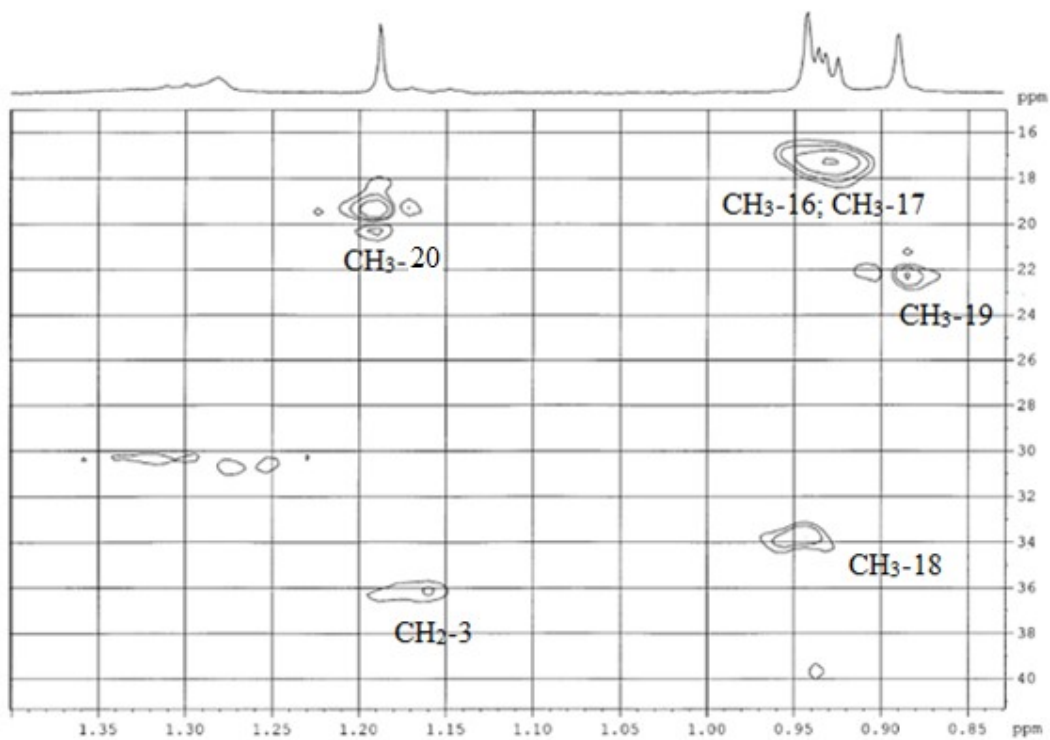
S20: Expansion of the HSQC Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD30D
HSQC



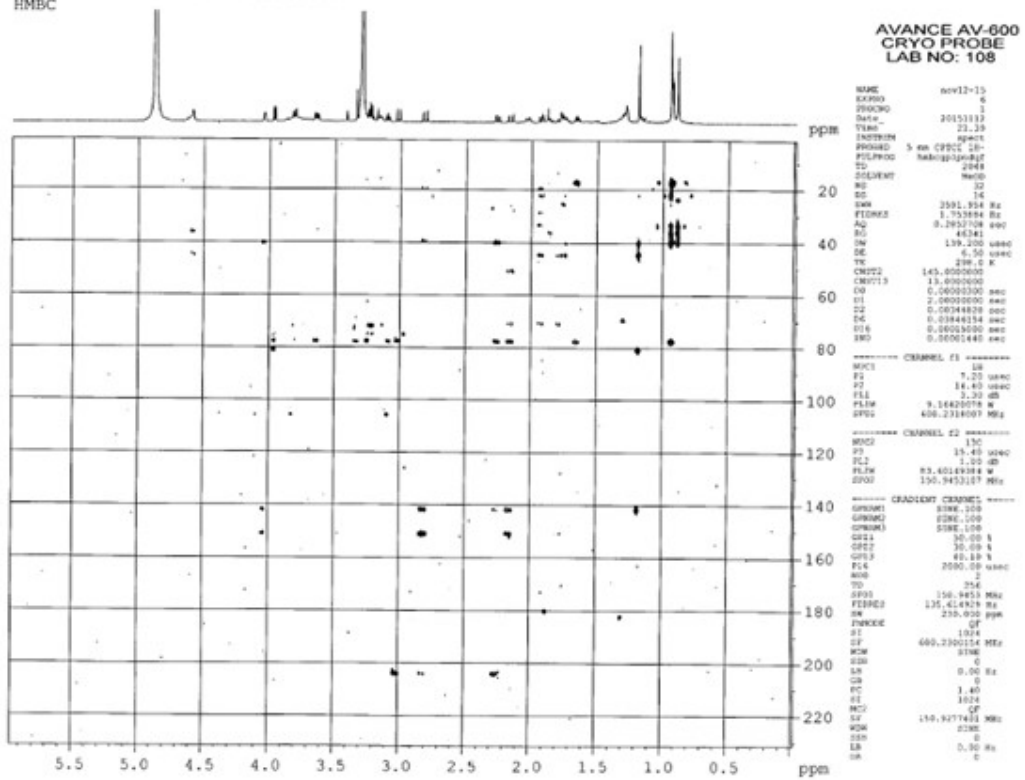
S21: Expansion of the HSQC Spectrum of Compound **1** (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD300
HSQC



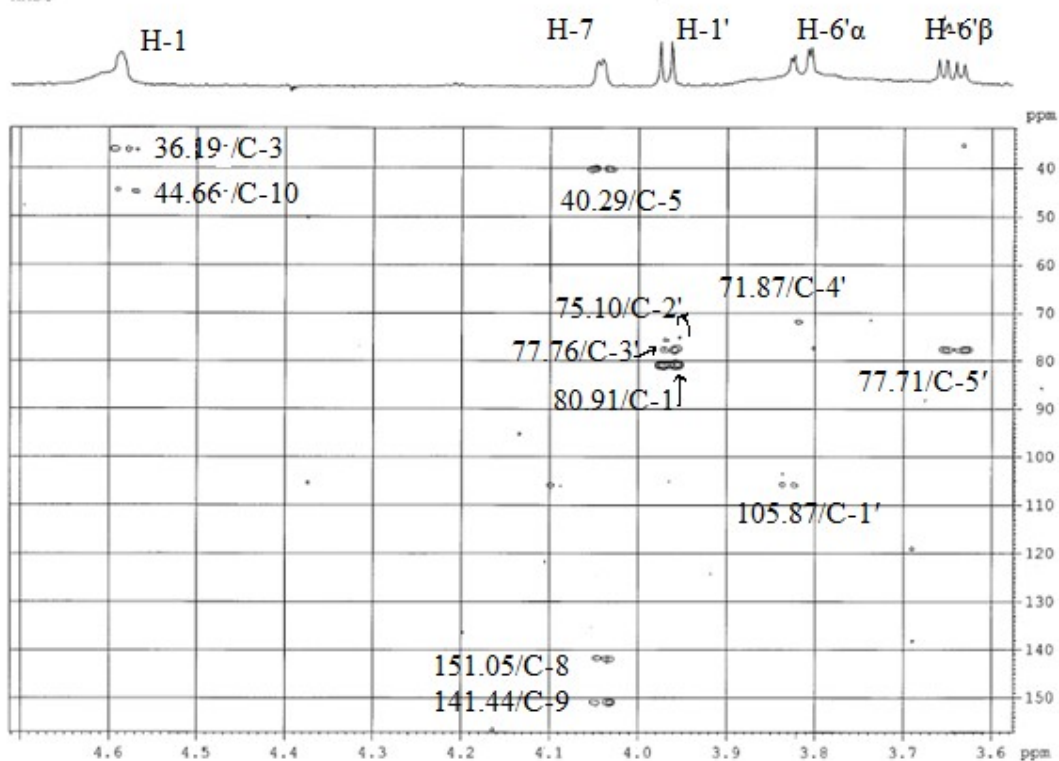
S22: Expansion of the HSQC Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR. BINA/ARF-15M/CD3OD
HMBC



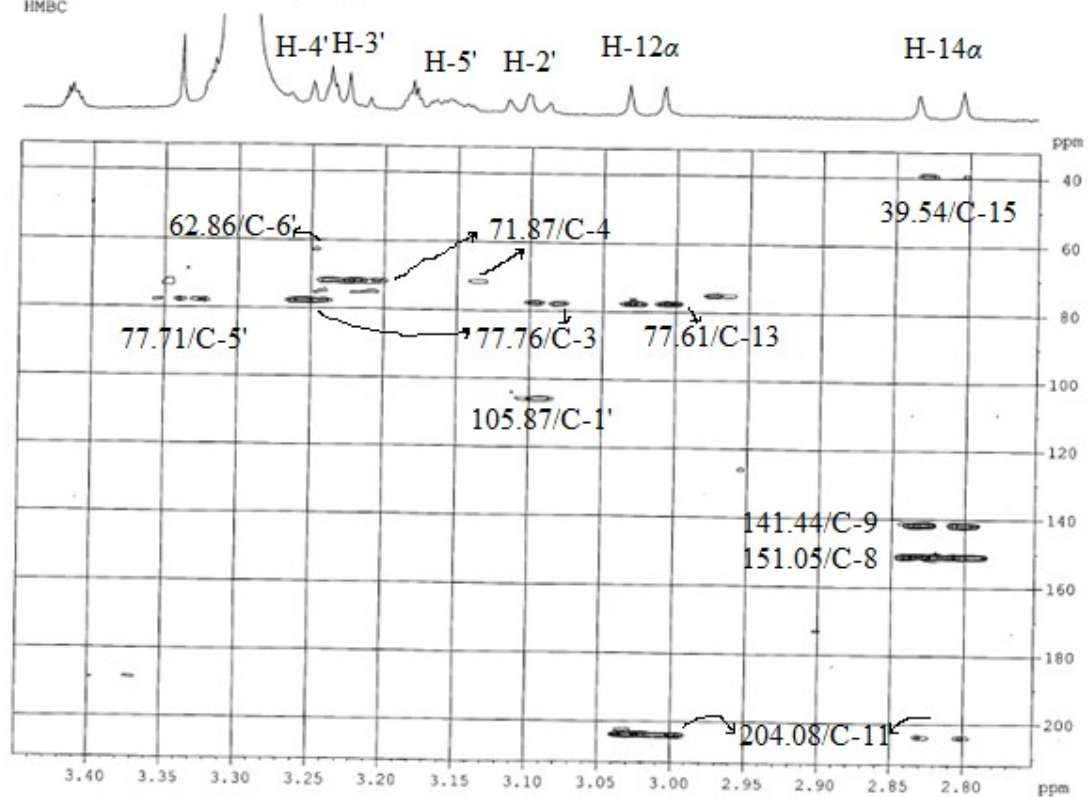
S23: HMBC (600 MHz) Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR.BINA/ARF-15M/CD3OD
HMBC

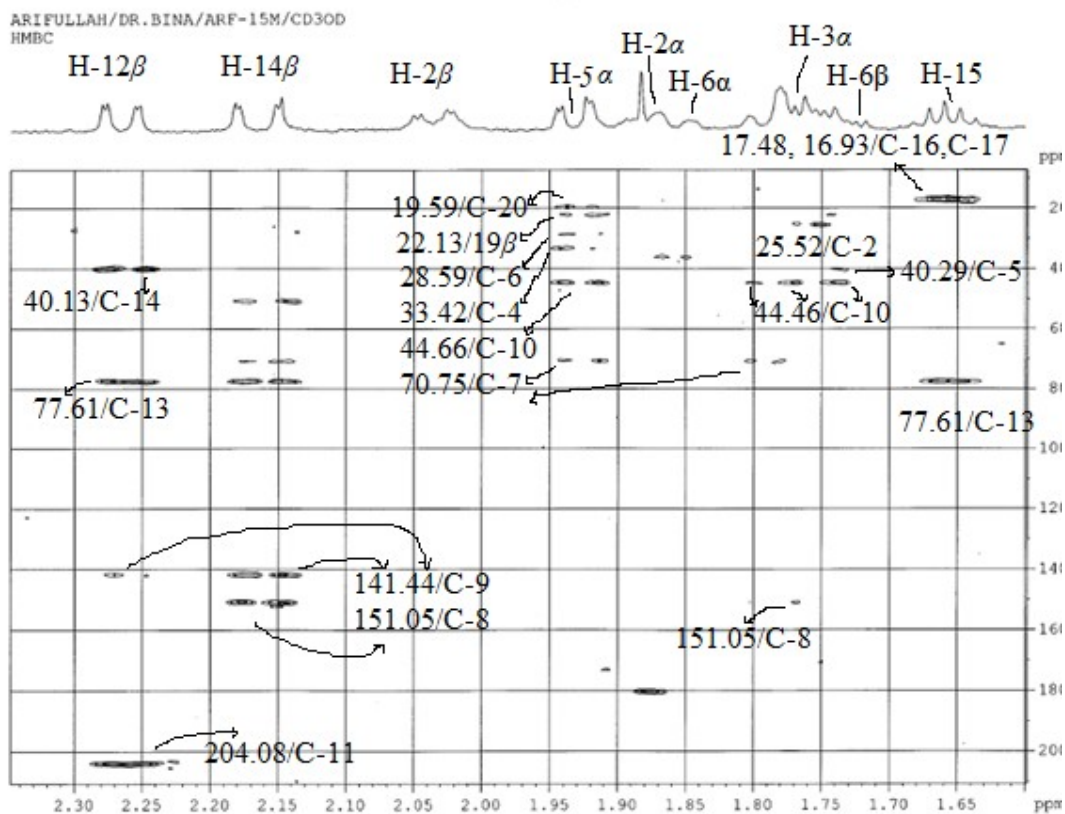


S24: Expansion of the HMBC Spectrum of Compound 1 (rugosodon)

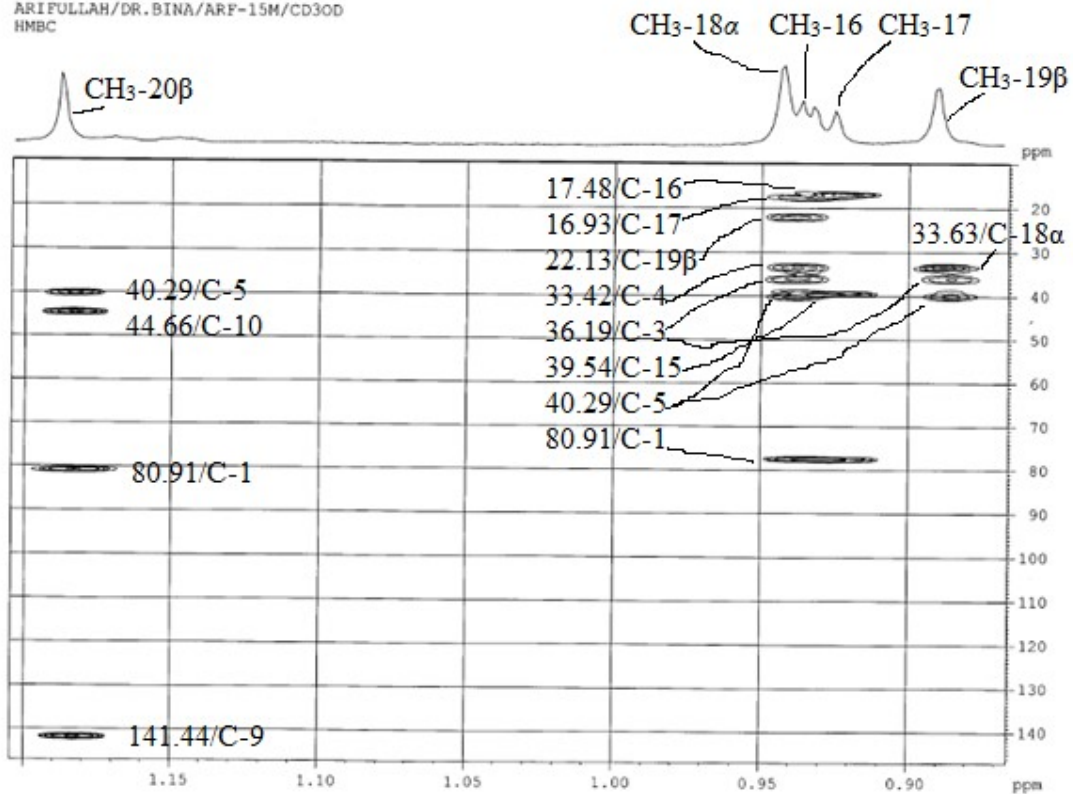
ARIFULLAH/DR.BINA/ARF-15M/CD3OD
HMBC



S25: Expansion of the HMBC Spectrum of Compound 1 (rugosodon)

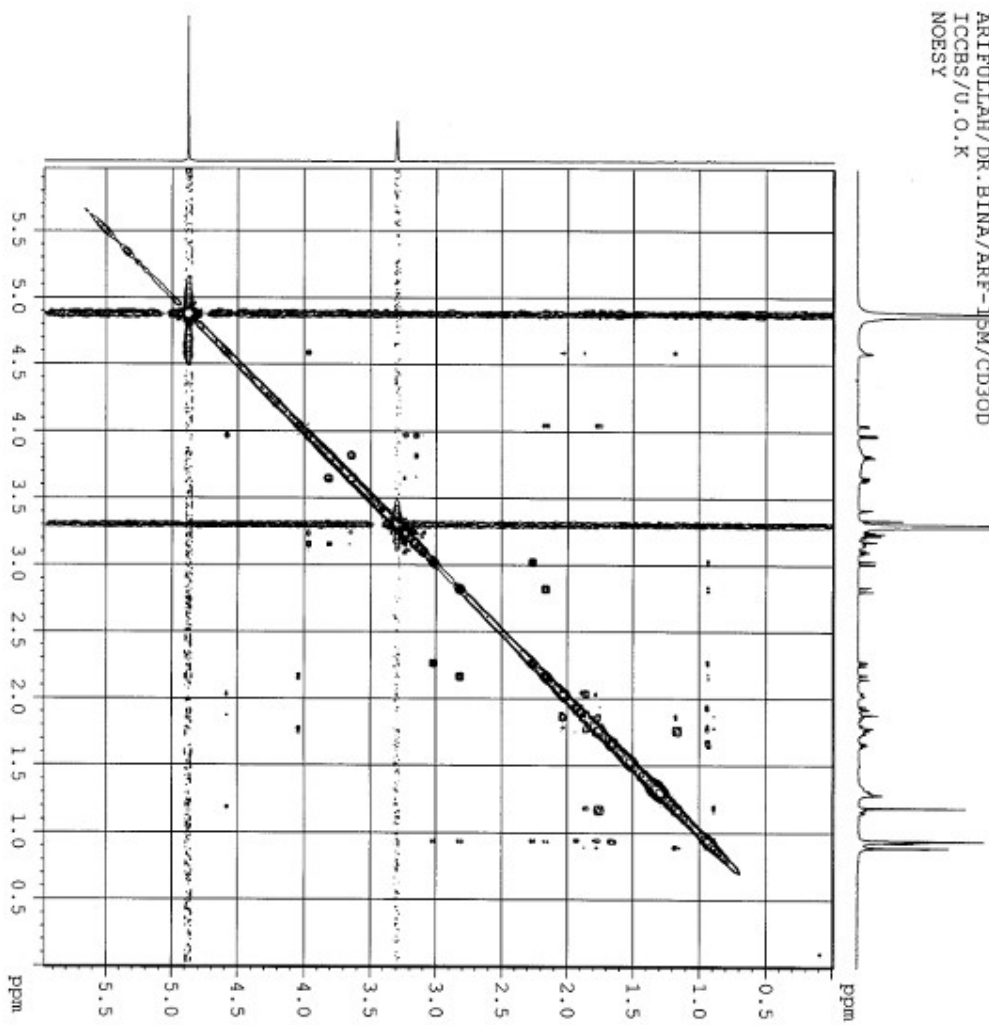


S26: Expansion of the HMBC Spectrum of Compound **1** (rugosodon)



S27: Expansion of the HMBC Spectrum of Compound 1 (rugosodon)

ARIFULLAH/DR. BINIA/ARF-15M/CD3OD
 ICCBS/U.O.K
 NOESY



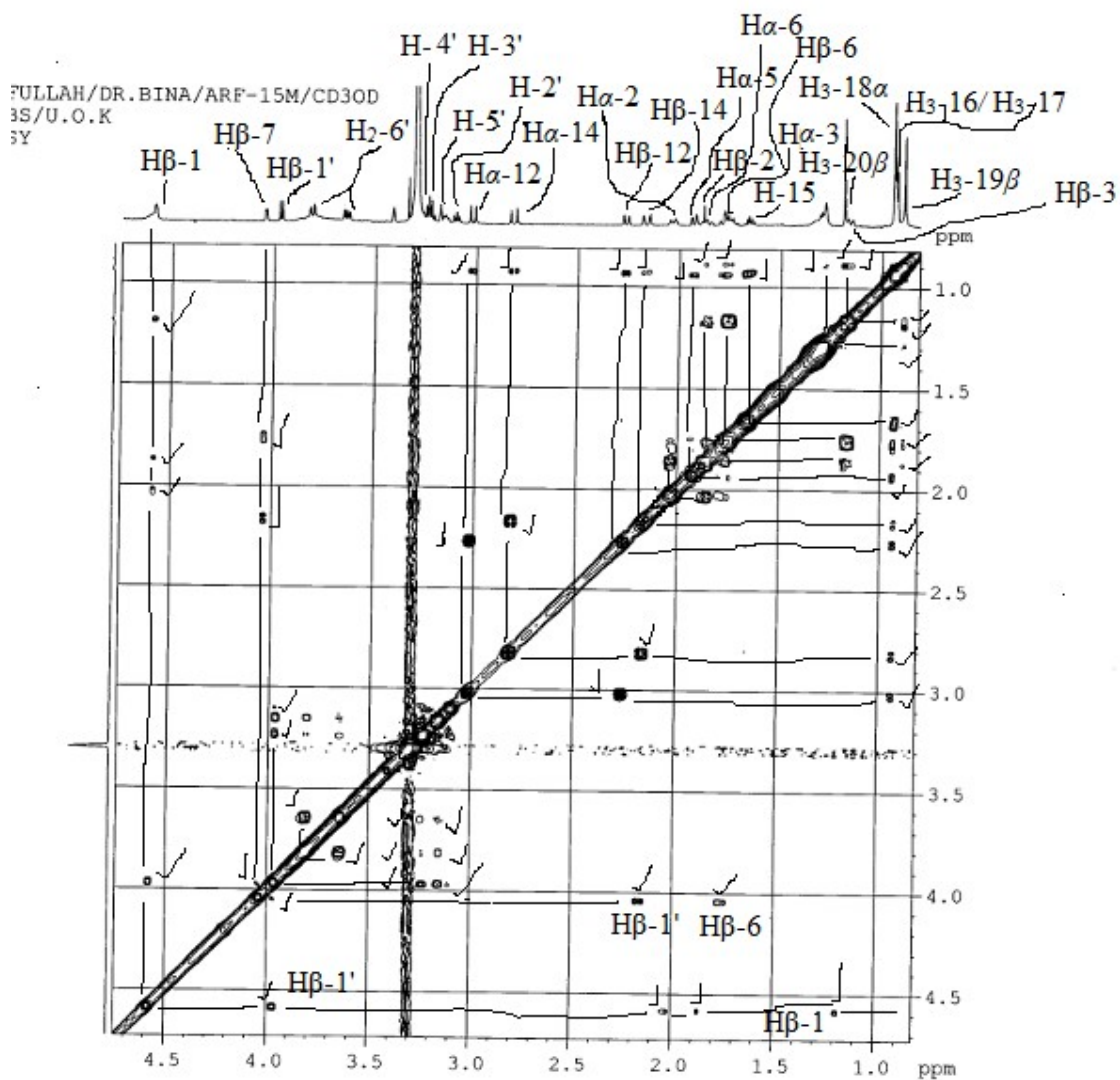
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 LAB NO: 108

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TD            1024
SOLVENT       MeOD
NS            16
DS            4
SWH           3591.954 Hz
FIDRES       0.1427300 sec
AQ           0.1427300 sec
RG           64
OR           139.200 usec
DE           6.50 usec
TE           298.0 K
D0           0.00012978 sec
D1           2.00000000 sec
D16          0.00015000 sec
RG           0.00027840 sec
IN0          0.00027840 sec

===== CHANNEL f1 =====
NUC1          1H
P1           7.40 usec
PL1          14.00 dB
SFO1         600.2300154 MHz
===== GRADIENT CHANNEL =====
GPRAM1       SINE,100
GPRAM2       SINE,100
GPR1         40.00 %
GPR2         -40.00 %
P16          2000.00 usec
NUC          1
TD           256
PROG         600-230
SFORES       14.0310154 MHz
SM           5.984 Ppm
FWDORDE      STARGZ-TPEI
SI           1024
SF           600.2300154 MHz
WDW          GSIINE
SSB          2
LB           0.00 Hz
GB           0
  
```

S28: NOESY (600 MHz) Spectrum of Compound 1 (rugosodon)



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