

Supporting Information

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A New Phenylpropanoid from the Roots of *Solanum melongena* L. and Evaluation of Anti-inflammatory Activity

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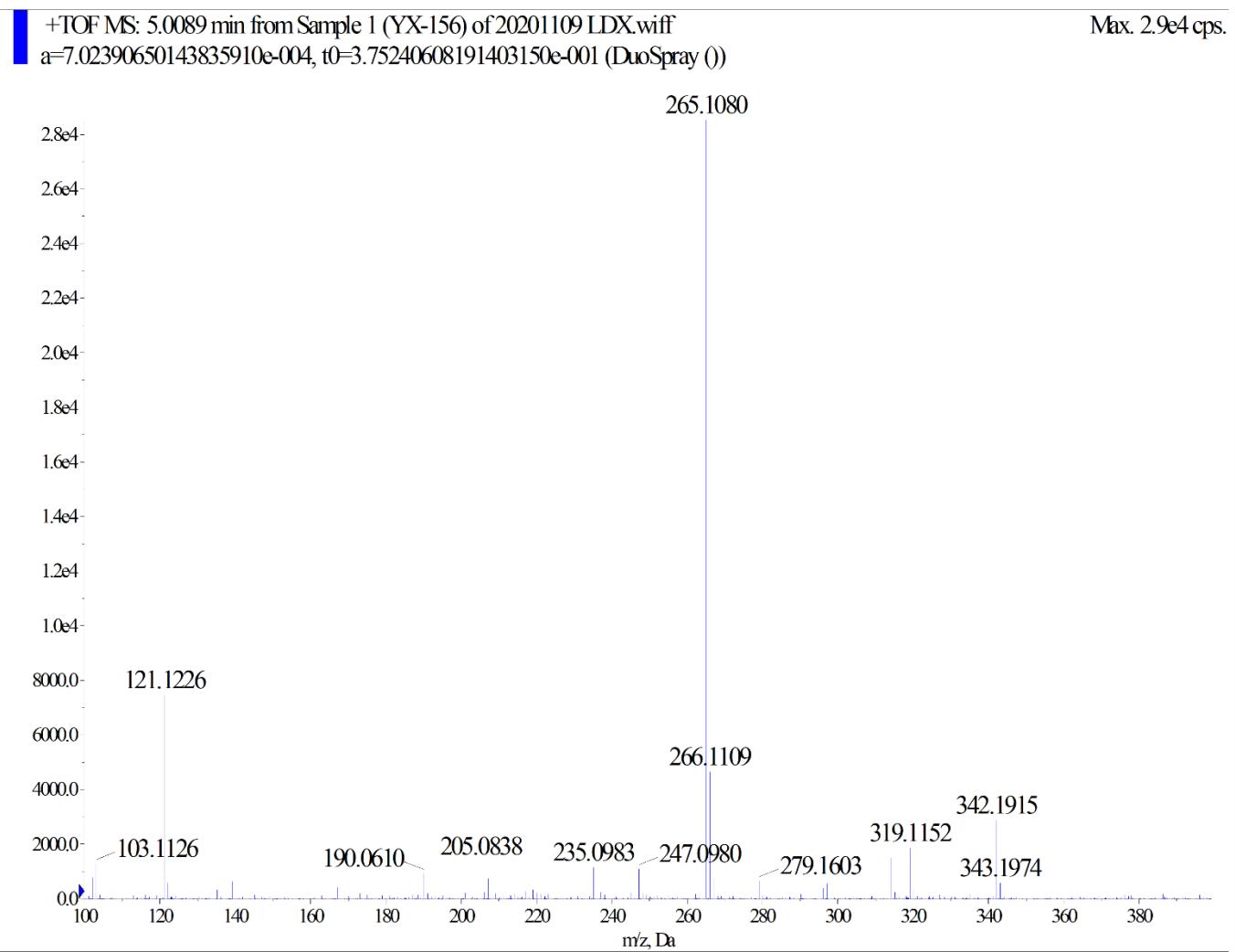


Figure S1: HR-ESI-MS Spectrum of **1** (melongenapanoid A)

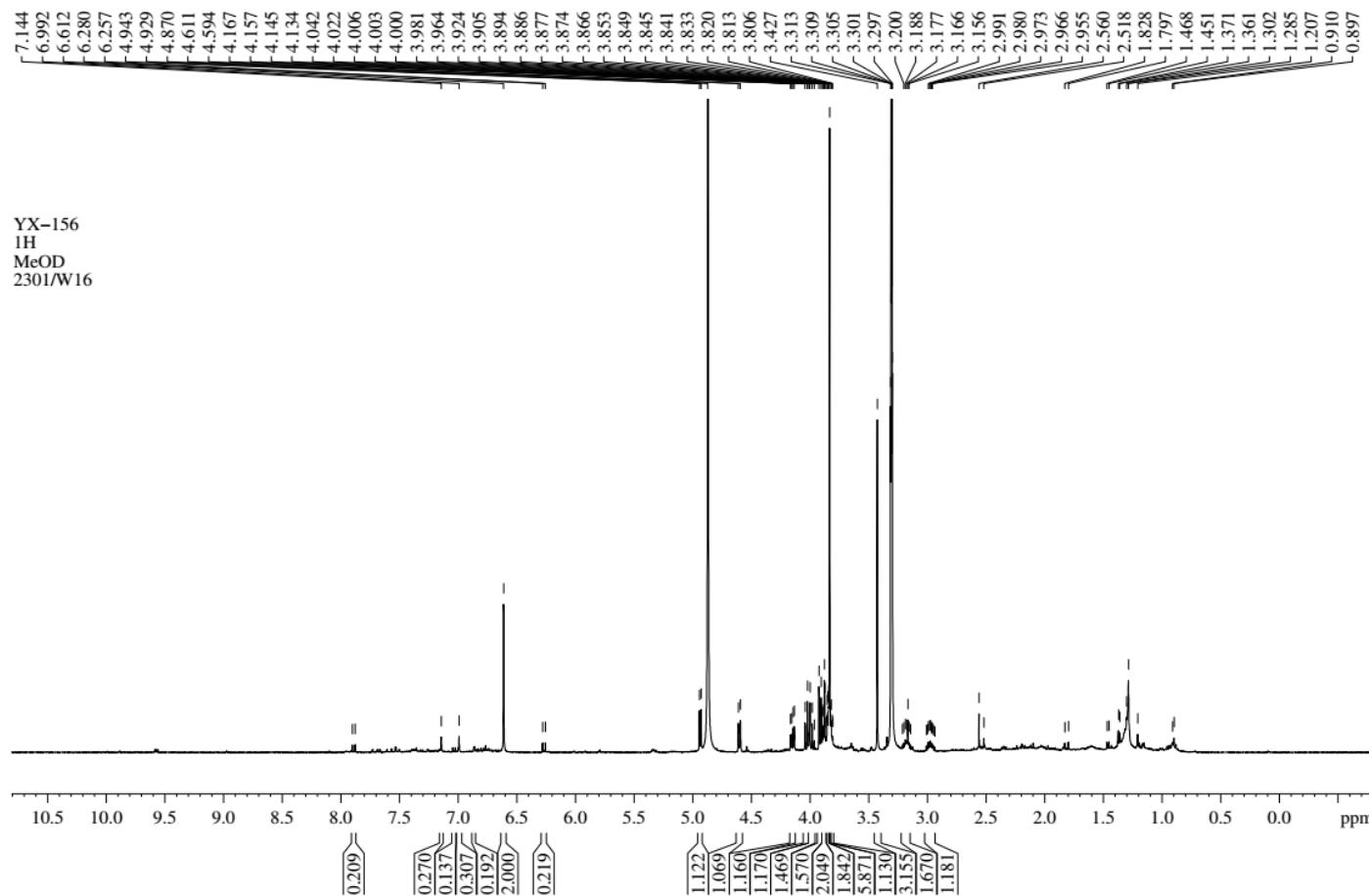


Figure S2: ^1H -NMR (400 MHz, CD_3OD) Spectrum of **1** (melongenapanoid A)

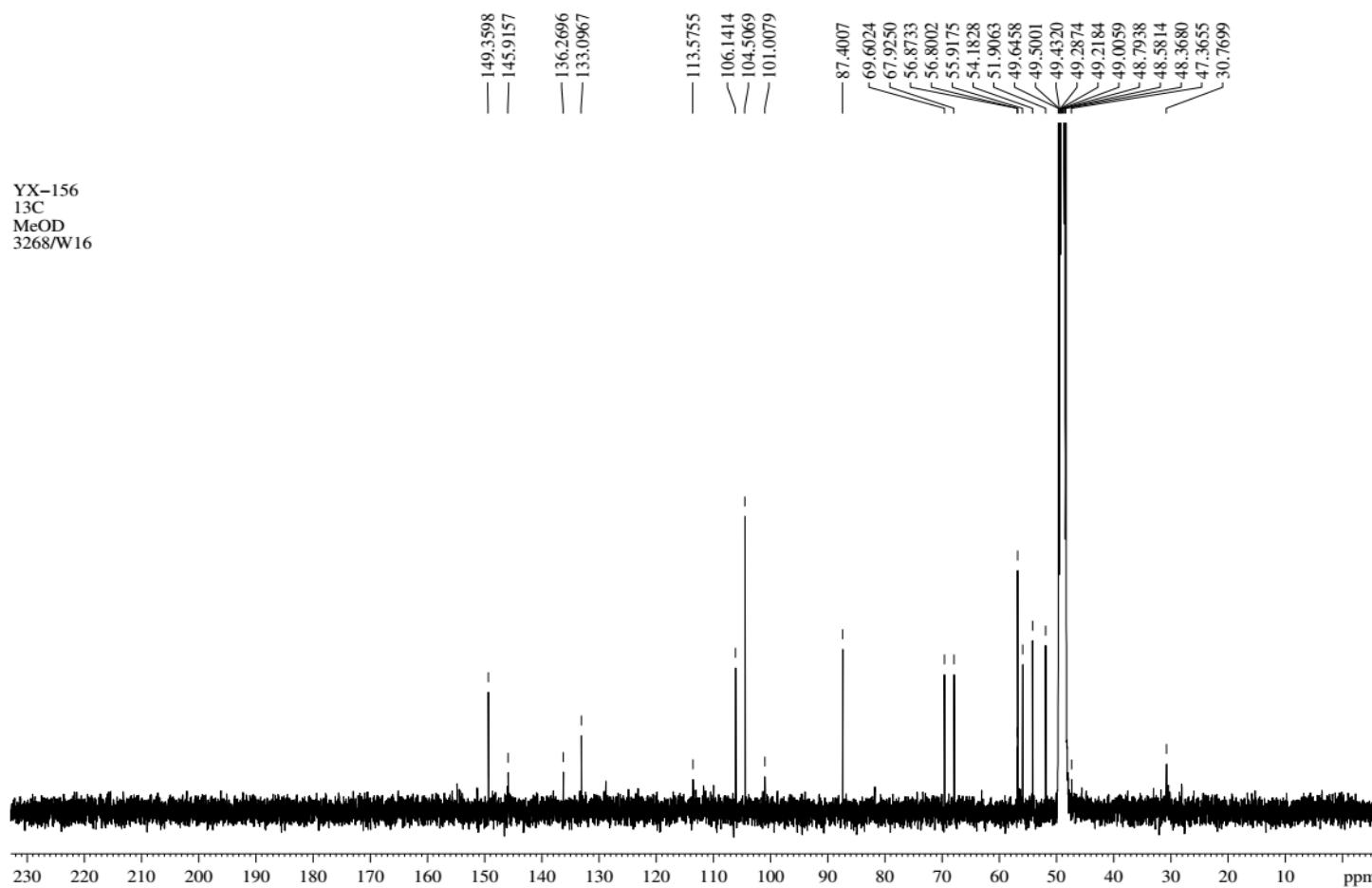


Figure S3: ¹³C-NMR (100 MHz, CD₃OD) Spectrum of **1** (melongenapanoid A)

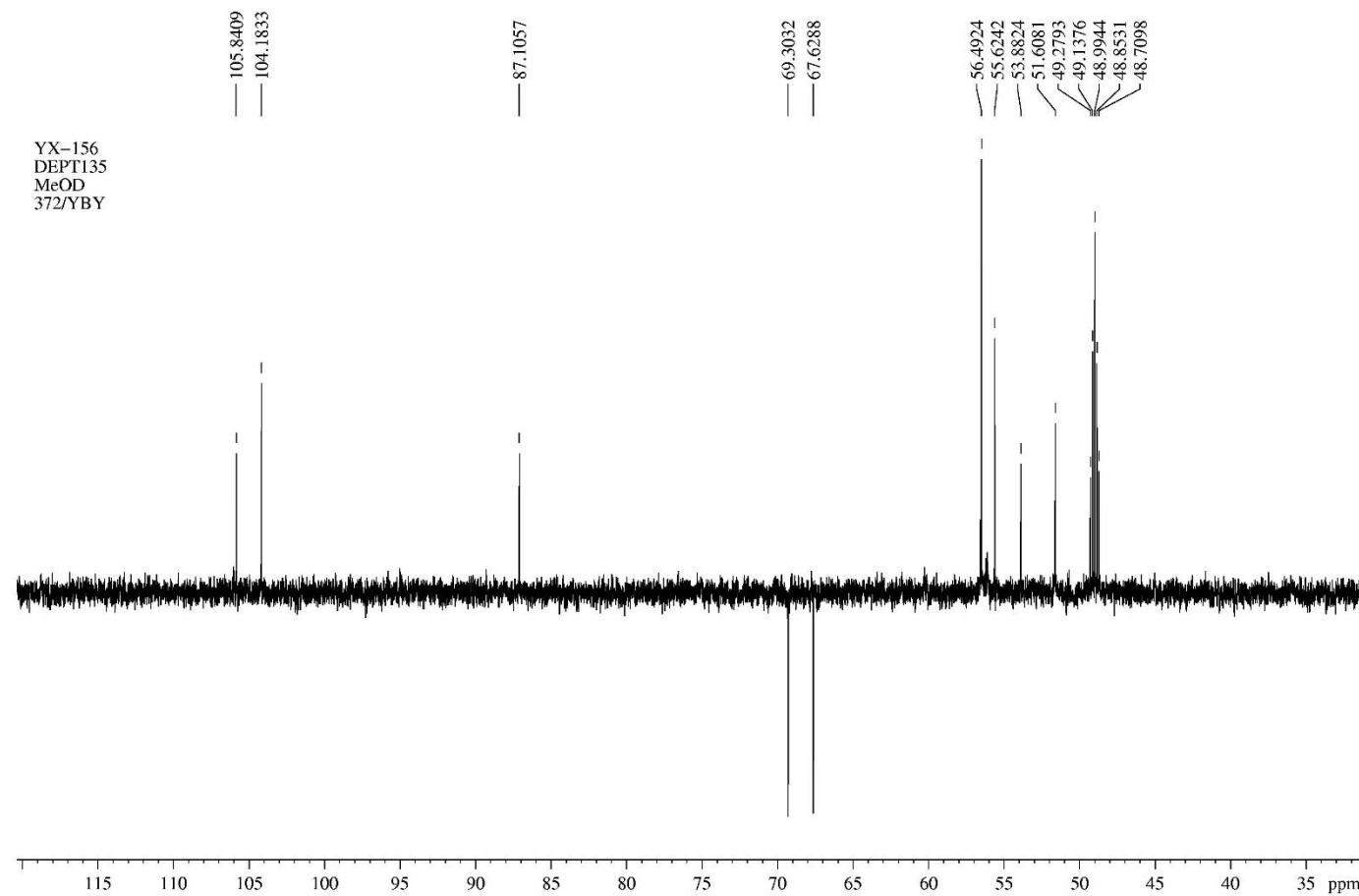


Figure S4: DEPT135 (100 MHz, CD₃OD) Spectrum of **1** (melongenapanoid A)

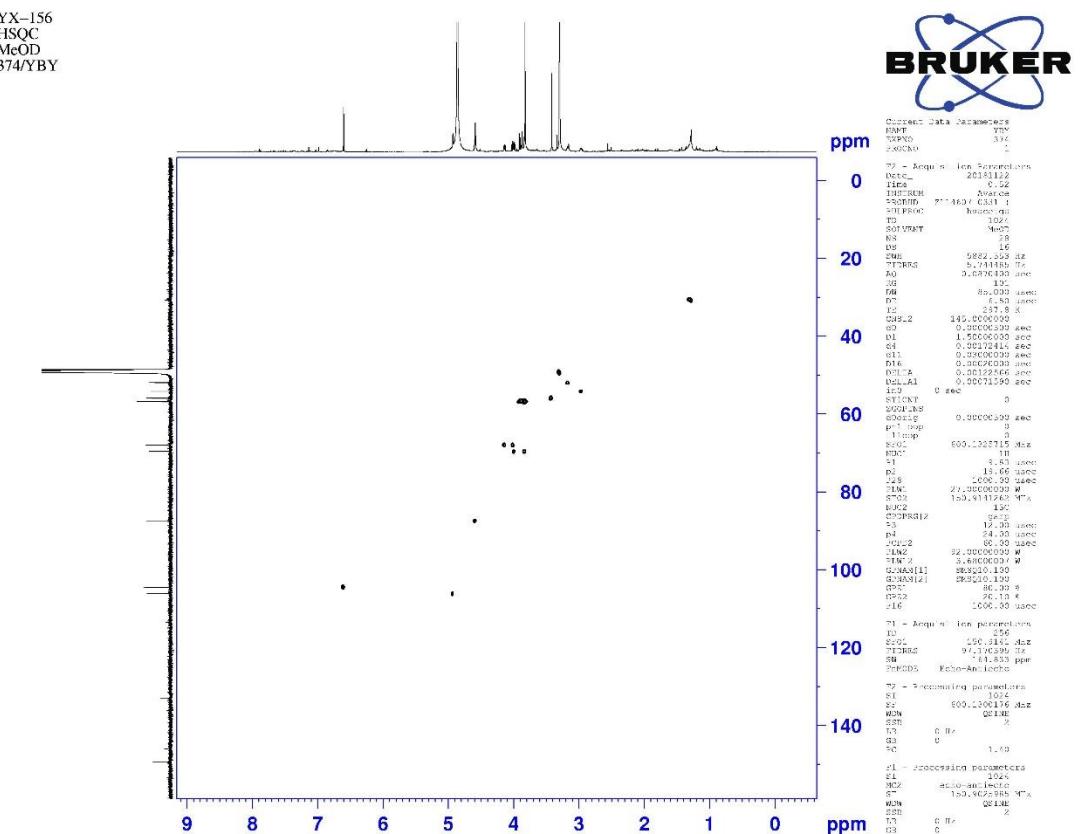


Figure S5: HSQC Spectrum of **1** (melongenapanoid A)

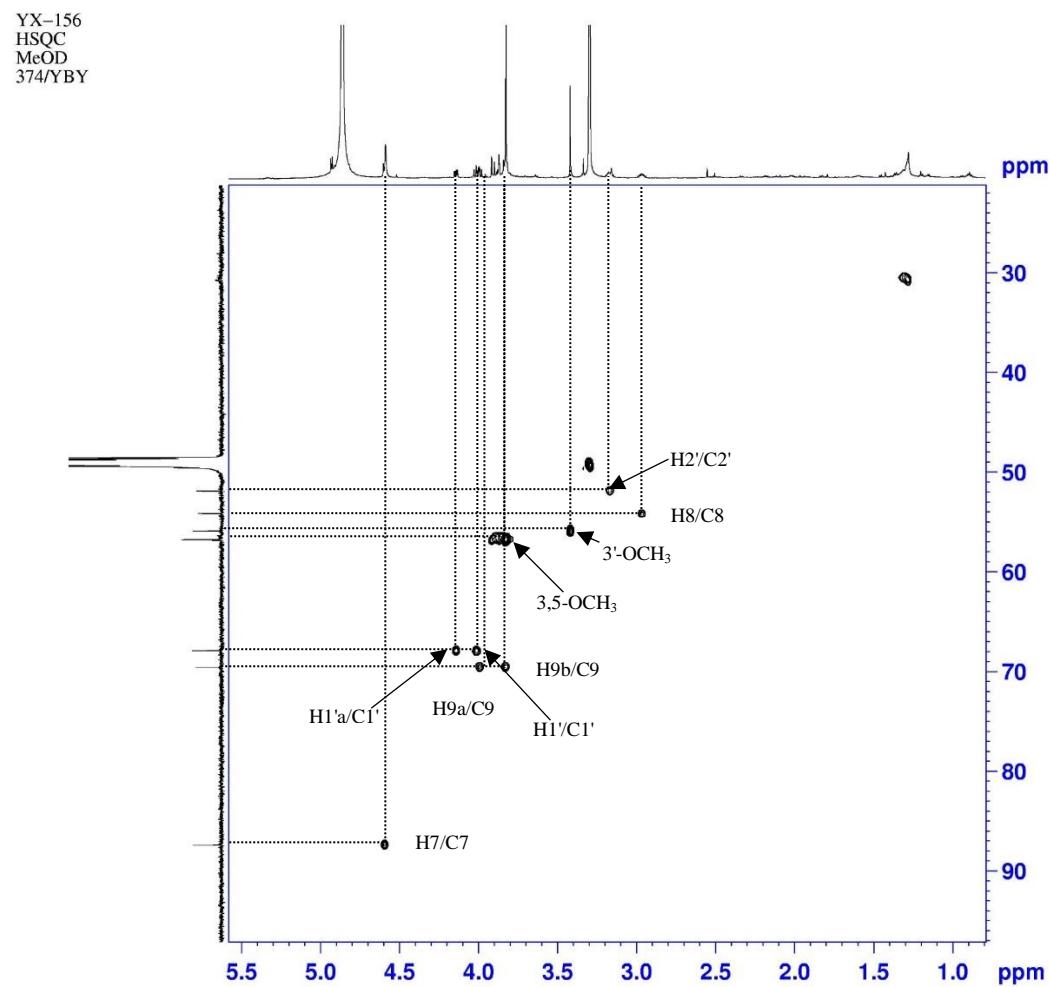


Figure S6: HSQC Spectrum of **1** (melongenapanoid A) (From δ_{C} 30 ppm to δ_{C} 90 ppm)

YX-156
HSQC
MeOD
374/YBY



Current Data Parameters
NAME YBY
EXPNO 374
PROCNO 1

F2 - Acquisition Parameters
D1 2 20181200
TD 65536 0.52
INSTRUM Avance
PROBHD Z114607_0331 (PULPROG hsqc90P
TD 1024
SW1 6.30
SOLVENT MeOD
NS 28
DS 1
SWH 5882.353 Hz
FIDRES 5.745485 Hz
AQ 0.083940 sec
RG 60
DW 85.000 usec
DE 6.50 usec
TE 297.0 K
CNS12 145.000000 sec
d0 0.00000300 sec
D1 1.50000000 sec
d4 0.017214 sec
d11 0.000000 sec
d16 0.00020000 sec
DETA 0.00122566 sec
DETAII 0.00071590 sec
inc 0 sec
SLWME 0
PR1 0.000000 sec
d1orig 0.00000300 sec
p1loop 0
t1loop 0
SF01 600.1325712 MHz
NUCL 1H
P1 3.83 usec
P2 3.66 usec
P2R 1000.0 usec
PLM1 27.0000000 W
SF02 150.9141262 MHz
NUCL 13C
CQ1 0.000000 sec
P3 17.00 usec
P5 24.00 usec
P7 40.00 usec
PLM2 92.0000000 W
PLM3 3.6800000 W
GNDAM[1] 39821.100
GNDAM[2] 39821.000
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SW1 150.90985 MHz
FIDRES 37.170335 Hz
SW 164.833 ppm
PRMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1309176 MHz
WM QSTME
SSB 2
LB 0 Hz
GS 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9025985 MHz
WM QSTME
SSB 2
LB 0 Hz
GS 0

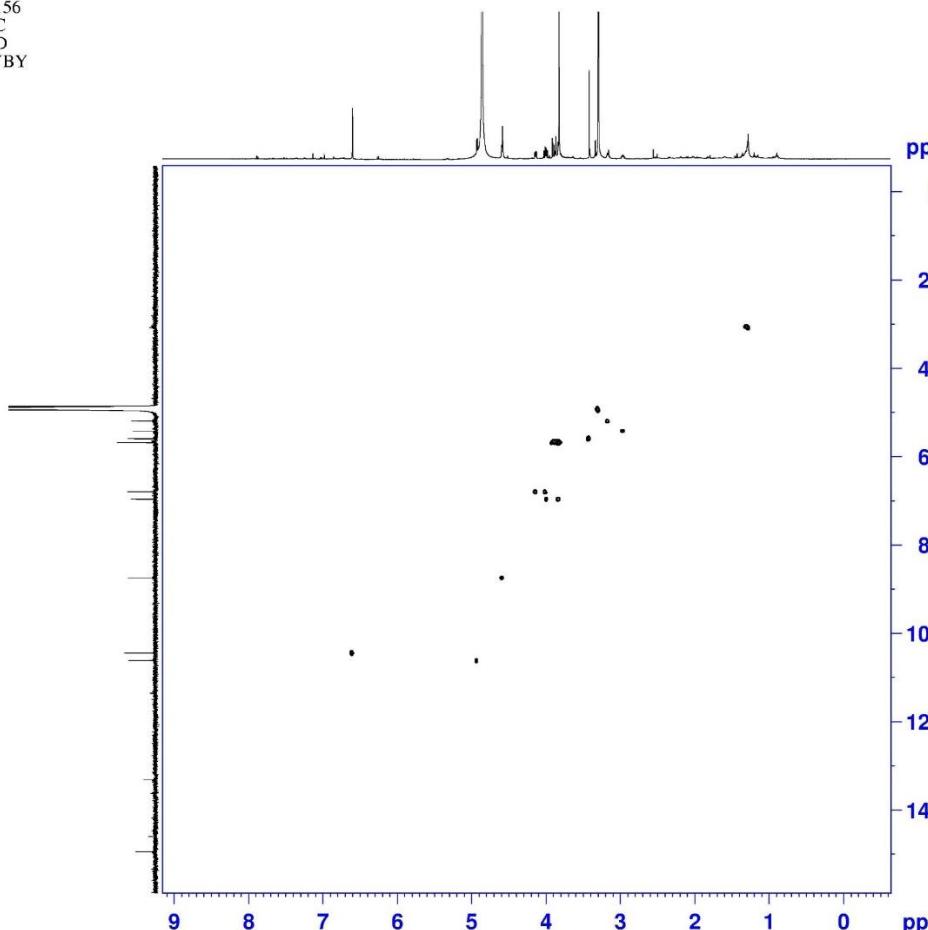


Figure S7: HMBC Spectrum of **1** (melongenapanoid A)

YX-156
HMBC
MeOD
375/YBY

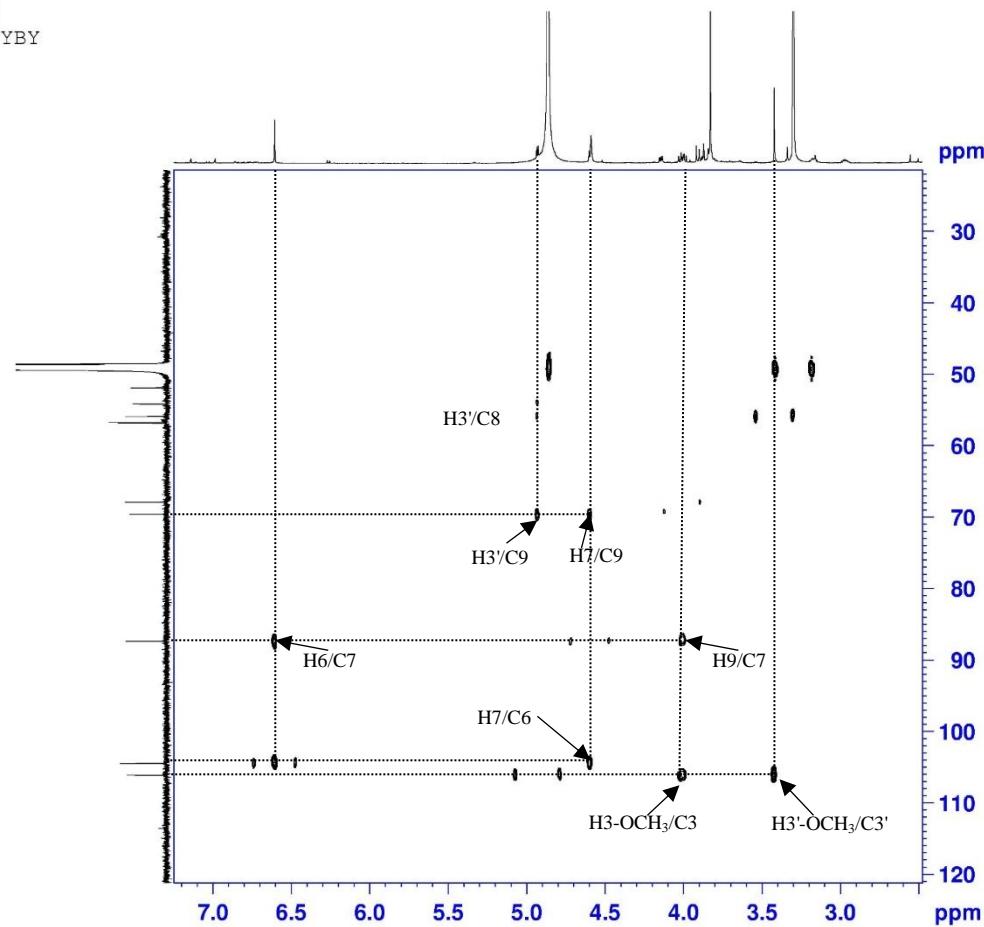


Figure S8: HMBC Spectrum of **1** (melongenapanoid A) (From δ_c 30 ppm to δ_c 120 ppm)

YX-156
COSY
MeOD
373/YBY



Current Data Parameters
NAME YBY
EXPNO 373
PROCNO 1

F2 - Acquisition Parameters
Date_ 2018121
Time 22:40
INSTRUM Avance
PROBHD Z114607_0331 ('
PULPROG cosypprf
TD 2048
SOLVENT MeOD
NS 2
DS 16
SWH 4424.779 Hz
ETDRES 2.160537 Hz
AQ 0.2314240 sec
RG 64
DW 113.000 usec
DE 6.0 usec
TE 297.5 K
d0 0.00000300 sec
D1 1.30169597 sec
d11 0.030000300 sec
d12 0.00002000 sec
d13 0.00000400 sec
D15 0.00002000 sec
in0 0 sec
ST1CNT 0
d0erig 0.00000300 sec
philoop 0
tiloop 0
SP01 600.132339 MHz
NUC1 1H
P0 9.83 usec
P1 9.83 usec
P17 2500.00 usec
PLW1 27.00000000 W
PLW10 4.17439985 W
GEMNAM[1] SWSQ16.130
GR12 1.00 *
E10 1000.00 usec

1
2
3
4
5
6
7

F1 - Acquisition parameters
TD 128
SP01 600.1323 MHz
P1DRES 34.568584 Hz
SW 7.379 ppm
PmMode QF

F2 - Processing parameters
ST 1024
SF 600.1380173 MHz
W0 0 Hz
SSB 0
LB 0 Hz
GS 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 0 QF
SF 600.1380173 MHz
W0 0 Hz
SSB 0
LB 0 Hz
GS 0

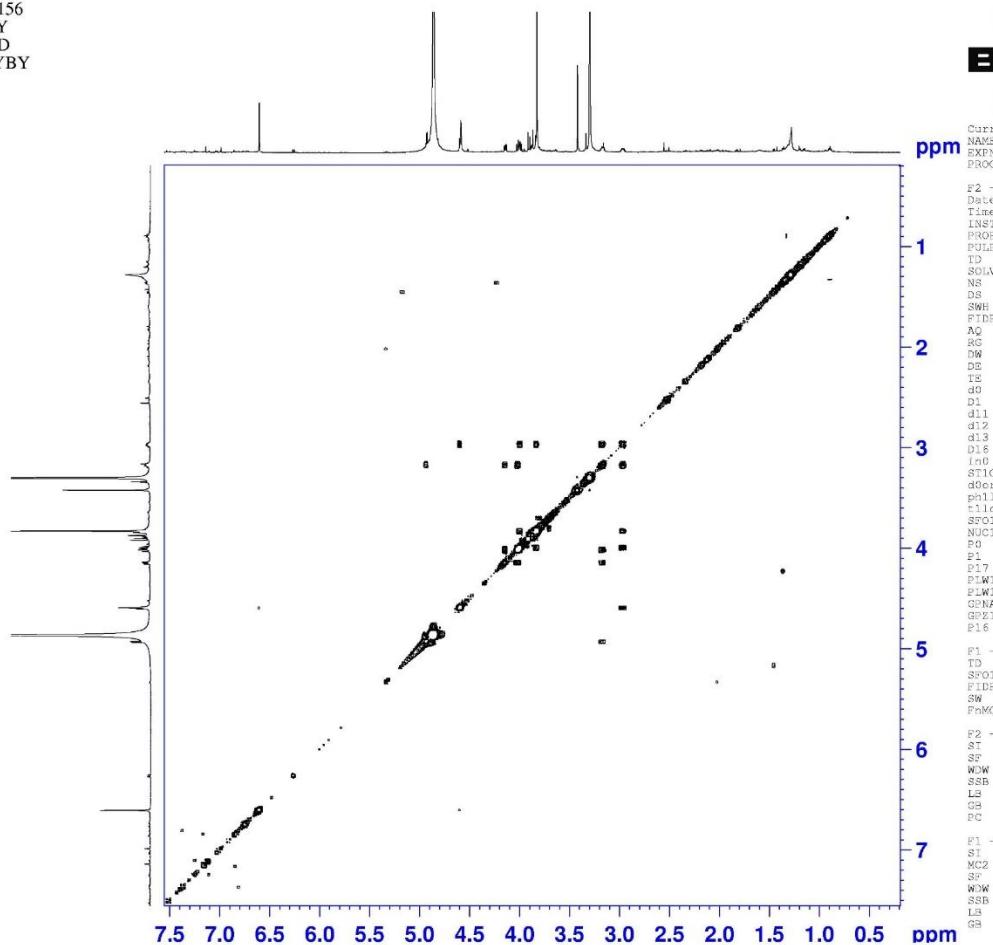


Figure S9: ^1H - ^1H COSY Spectrum of **1** (melongenapanoid A)

Title/Orig YX-156

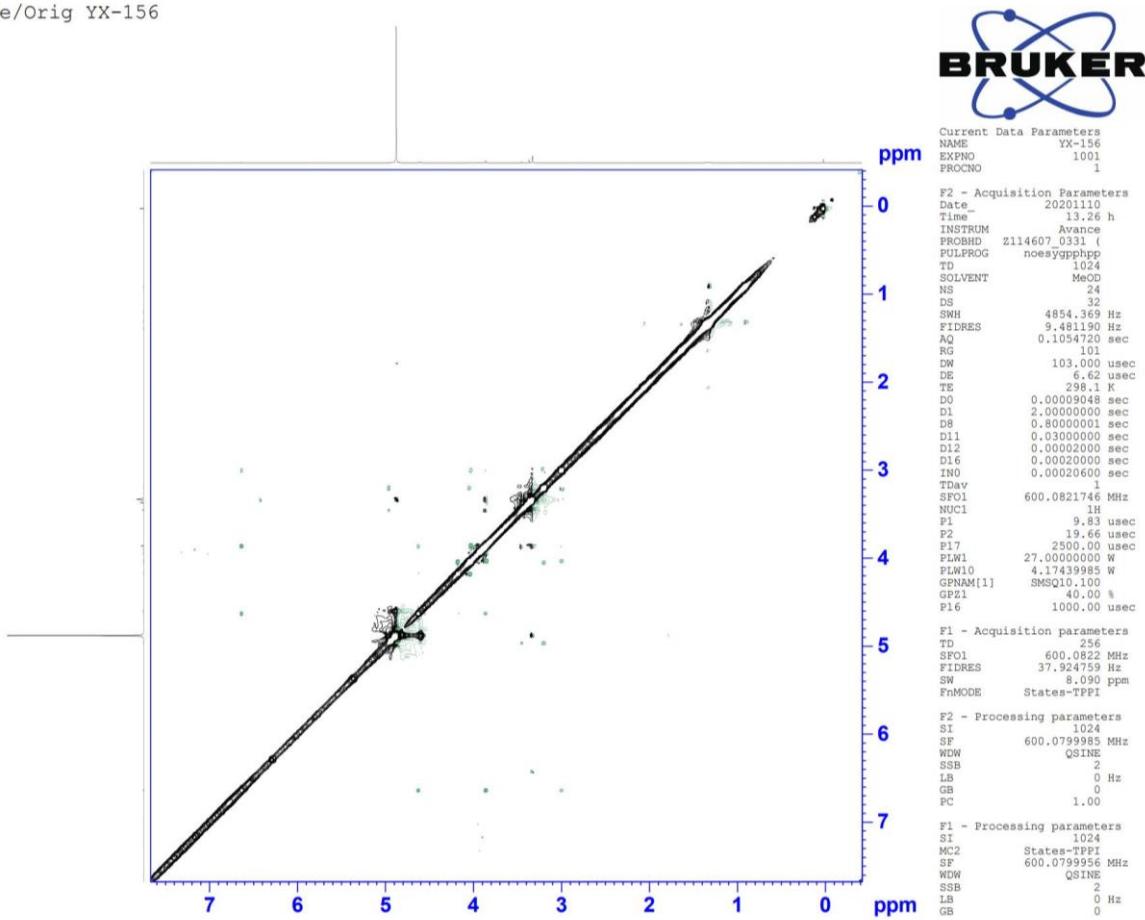


Figure S10: NOESY Spectrum of compound **1** (melongenapanoid A)

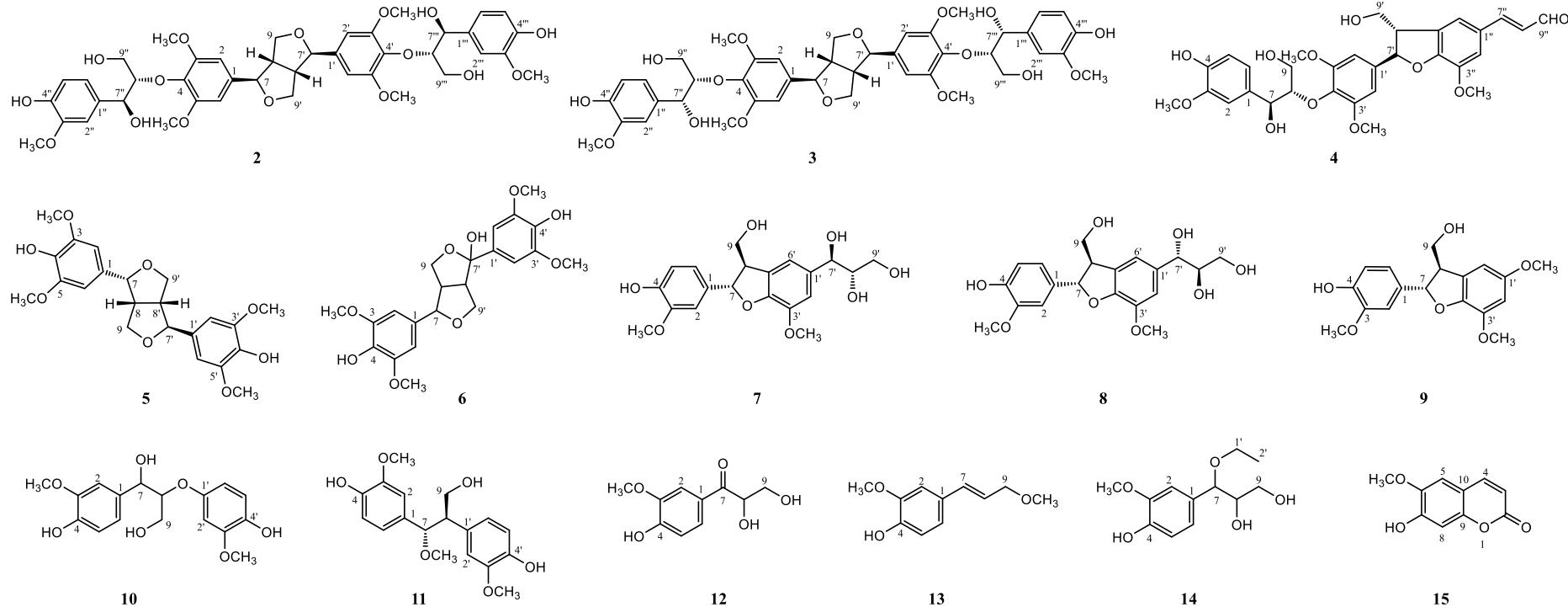


Figure S11: Chemical structures of compounds 2-15

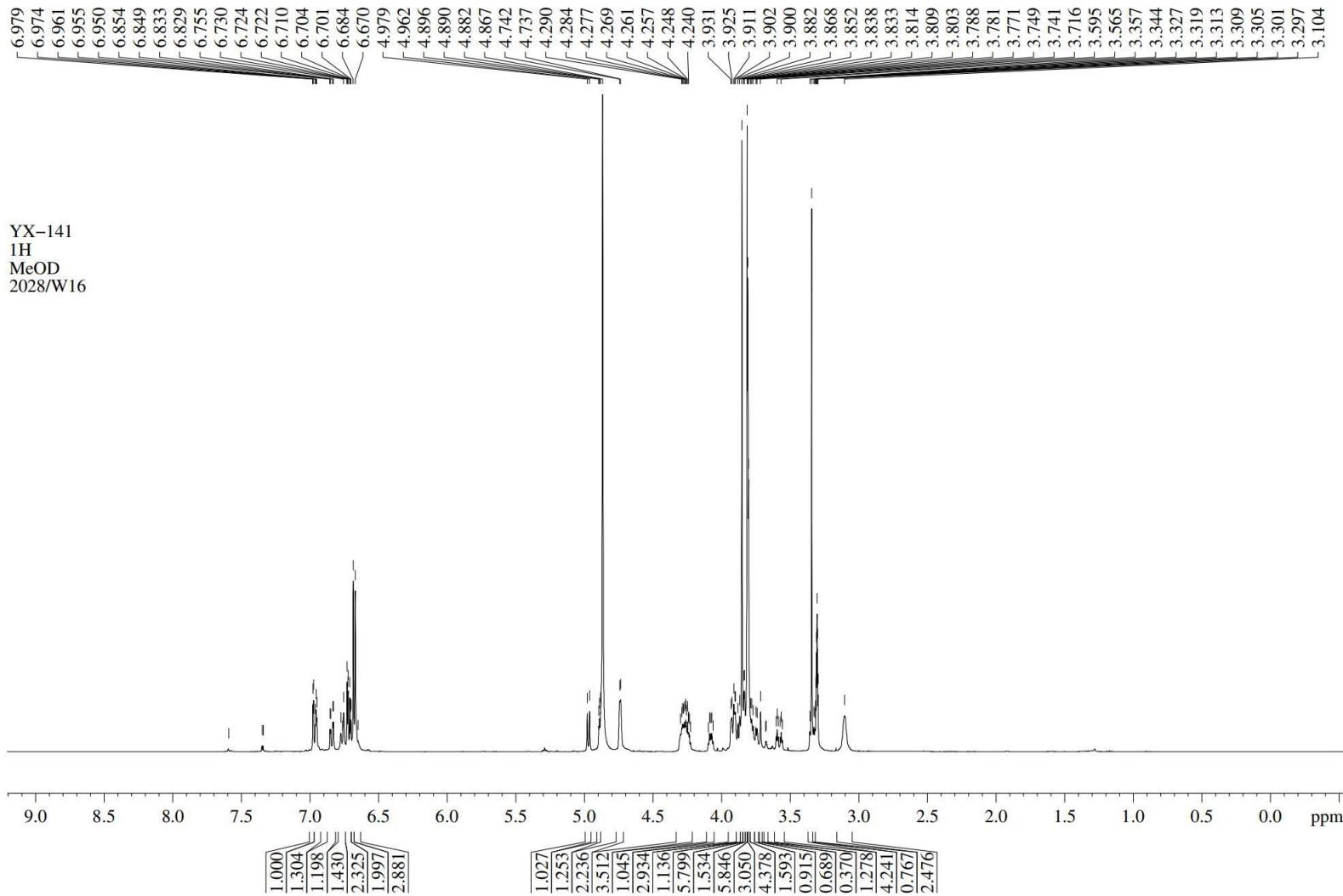


Figure S12: ¹H-NMR (400 MHz, CD₃OD) Spectrum of compound 3

Table S1. ^{13}C -NMR data of **2-15** (100 MHz, CD_3OD)

NO.	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	139.1	138.9	133.7	130.6	133.0	134.7	134.7	132.7	133.8	132.7	128.1	130.3	132.2	
2	104.2	104.2	111.6	104.6	104.6	110.6	110.5	112.4	111.8	115.7	112.4	110.6	111.8	164.1
3	154.3	154.5	148.7	149.4	149.3	149.1	149.1	148.5	148.9	148.5	149.2	149.1	149.1	112.6
4	136.1	136.6	147.1	135.6	136.3	147.6	147.6	146.9	147.2	146.8	153.8	147.8	147.4	146.1
5	154.3	154.5	115.8	149.4	149.3	116.1	116.1	115.4	115.9	114.3	116.0	116.2	116.0	109.9
6	104.2	104.2	120.8	104.6	104.6	120.0	119.7	121.5	120.9	122.6	125.1	121.1	121.4	147.1
7	87.3	87.2	74.4	83.6	89.5	89.1	89.2	87.2	74.4	87.4	199.5	134.4	83.6	152.9
8	55.7	55.7	88.7	51.2	54.4	55.4	55.4	56.3	89.1	57.0	75.5	123.7	77.1	104.0
9	73.0	73.1	61.8	70.7	70.6	64.9	64.8	64.8	61.8	65.0	66.3	74.4	63.9	151.4
10														112.5
1'	139.1	138.9	137.0	133.2	129.6	137.0	136.9	148.7	142.4	132.6				65.2
2'	104.2	104.2	103.9	104.1	105.4	112.6	112.7	107.8	101.7	115.5				15.6
3'	154.3	154.5	154.4	149.2	149.1	145.3	145.3	148.7	154.8	148.3				
4'	136.1	136.6	139.0	136.3	136.7	148.9	148.9	135.1	152.9	146.0				
5'	154.3	154.5	154.4	149.2	149.1	129.8	129.8	131.8	107.9	112.3				
6'	104.2	104.2	103.9	104.1	105.4	116.6	116.6	107.8	122.0	121.6				
7'	87.3	87.2	89.6	89.5	111.8	75.4	75.4							
8'	55.7	55.7	55.0	55.7	58.0	77.6	77.6							
9'	73.0	73.1	64.6	72.1	71.4	64.3	64.3							
1''	133.8	133.4	129.9											
2''	111.6	111.4	114.3											
3''	148.7	148.6	146.1											
4''	147.1	146.9	152.8											
5''	115.8	115.6	130.9											
6''	120.8	120.7	120.0											
7''	74.0	74.0	155.9											
8''	87.3	88.8	127.3											
9''	61.8	61.7	196.1											
1'''	133.8	133.4												
2'''	111.6	111.4												
3'''	148.7	148.6												
4'''	147.1	146.9												
5'''	115.8	115.6												
6'''	120.8	120.7												
7'''	74.0	74.0												
8'''	87.3	88.8												