SUPPLEMENTARY MATERIAL

Chemical constituent from the roots of *Solanum melongena* L.

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ABSTRACT

Three new compounds (**1-3**), were isolated from the ethanol extract of the roots of *Solanum melongena* L., together with twenty-seven knowns (**4-30**). On basis of their 1D and 2D NMR data, the chemical structures of islated compounds were elucidated combined with HR-MS and the relative values in literatures. In addition, the isolations were evaluated for the potential anti-inflammatory activity, by virtue of RAW 264.7 cells model induced by lipopolysaccharide (LPS)in vitro inhibitory activities on nitric oxide (NO) production. Compounds **12** and **21** showed moderate inhibition of NO production with IC_{50} values of 32.8 and 20.2 μM, respectively.

Keywords: *Solanum*, lignanamides, natural products, anti-inflammatory activity

Legends

Figure. S1: ^{1}H-NMR spectrum of compound **1**

Figure. S2: ^{13}C NMR spectrum of compound **1**

Figure. S3: DEPT-135 spectrum of compound **1**

Figure. S4: HSQC spectrum of compound **1**

Figure. S5: ^{1}H-^{1}H COSY spectrum of compound **1**

Figure. S6: HMBC spectrum of compound **1**

Figure. S7: HR-ESI-MS spectrum of compound **1**

Figure. S8: ^{1}H-NMR spectrum of compound **2**

Figure. S9: ^{13}C NMR spectrum of compound **2**

Figure. S10: HR-ESI-MS spectrum of compound **2**

Figure. S11: ^{1}H-NMR spectrum of compound **3**

Figure. S12: ^{13}C NMR spectrum of compound **3**

Figure. S13: DEPT-135 spectrum of compound **3**

Figure. S14: HSQC spectrum of compound **3**

Figure. S15: ^{1}H-^{1}H COSY spectrum of compound **3**

Figure. S16: HMBC spectrum of compound **3**

Figure. S17: NOESY spectrum of compound **3**

Figure. S18: HR-ESI-MS spectrum of compound **3**

Figure. S19: Key HMBC and ^{1}H-^{1}H COSY correlations of compounds **1-3**

Figure. S20: Chemical structures of compounds **4-30**

Table. S1 ^{13}C-NMR (100 MHz) data of compounds **4-20**

Table. S2 ^{13}C-NMR (100 MHz) data of compounds **21-30**

Table. S3 Inhibitory effects of compounds **1-30** on NO production by LPS-induced RAW264.7 cells

Figure. S1: ^{1}H-NMR Spectrum of Compound **1**

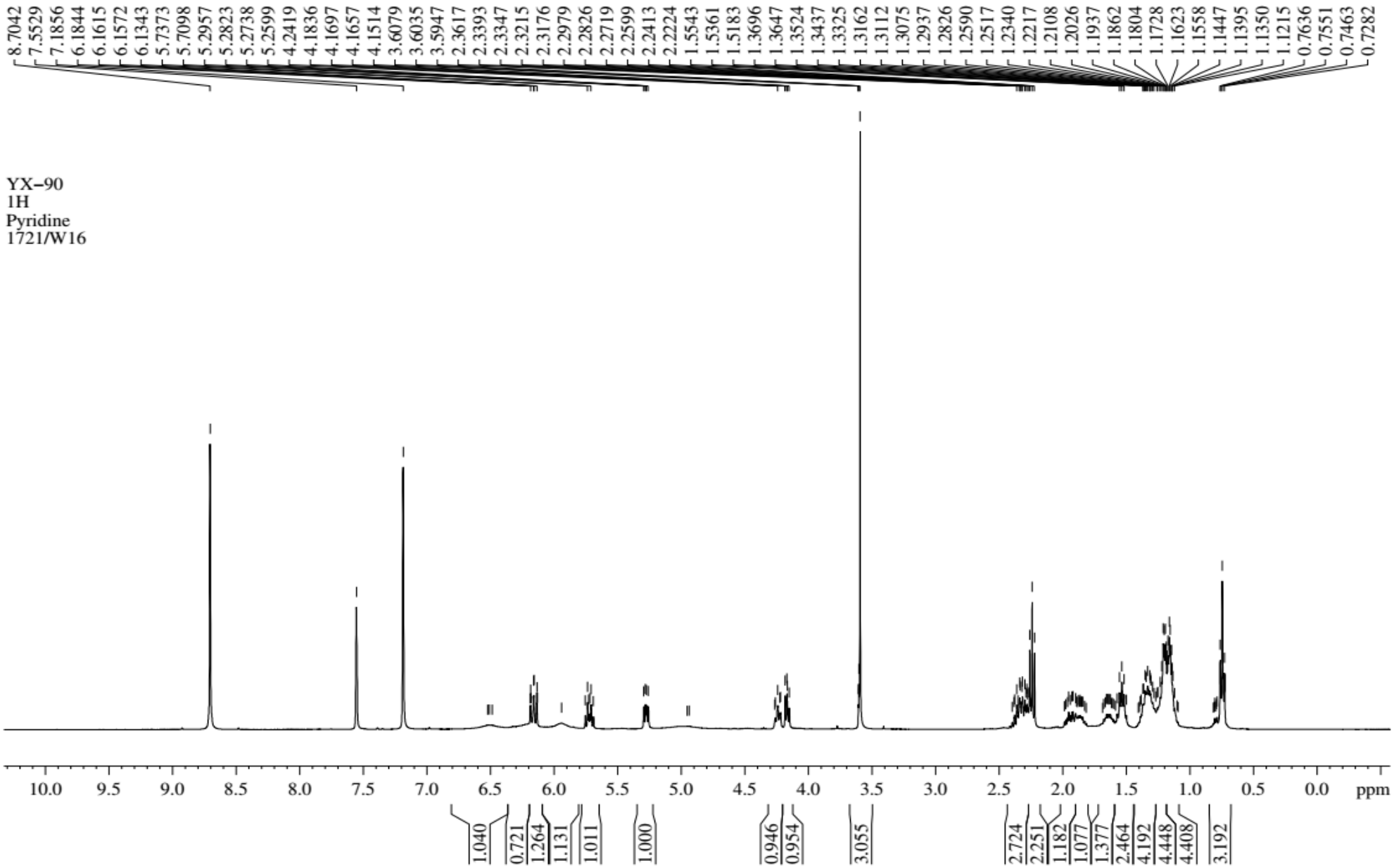


Figure. S2: ^{13}C NMR spectrum of Compound **1**

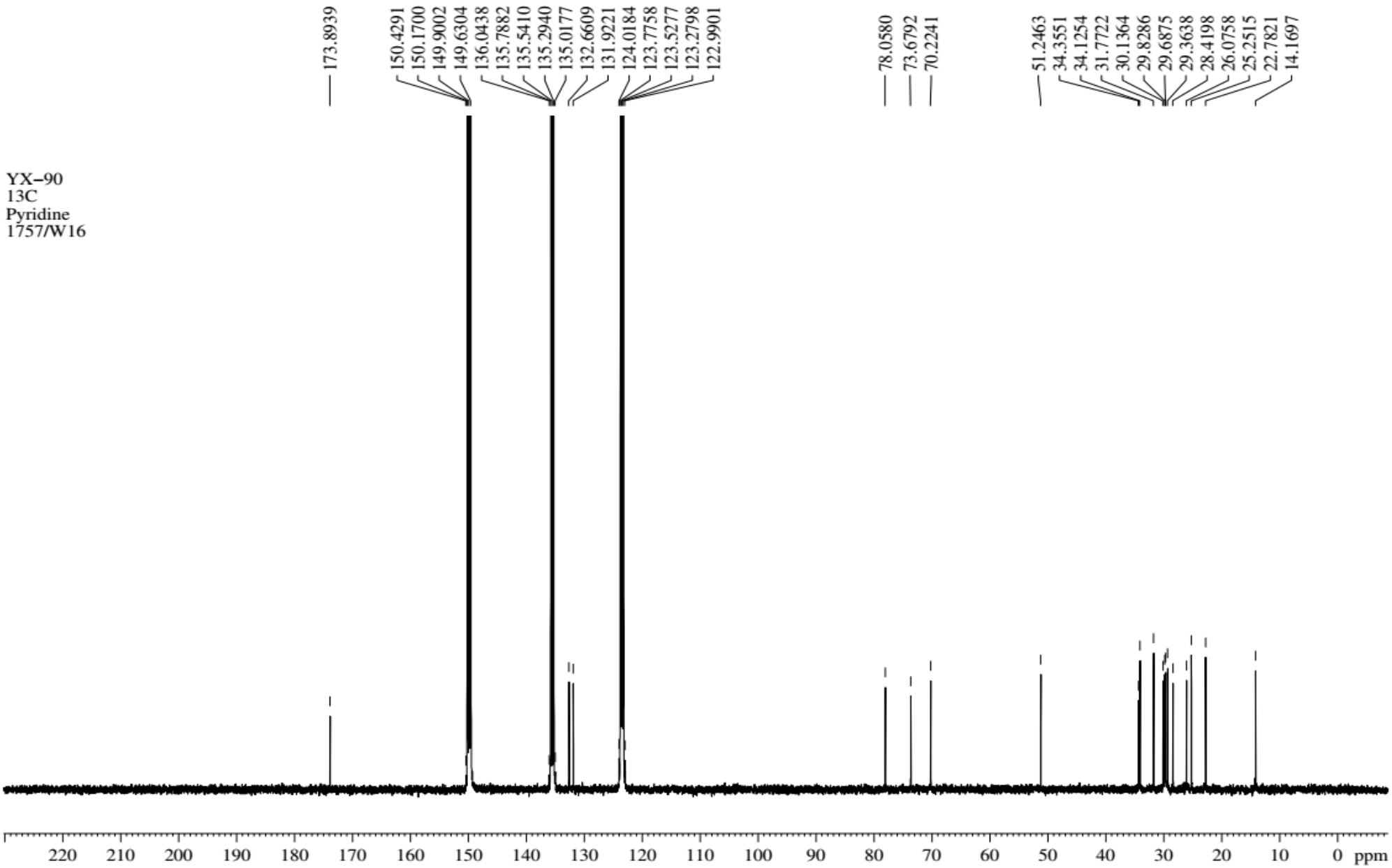


Figure. S3: DEPT-135 spectrum of Compound **1**

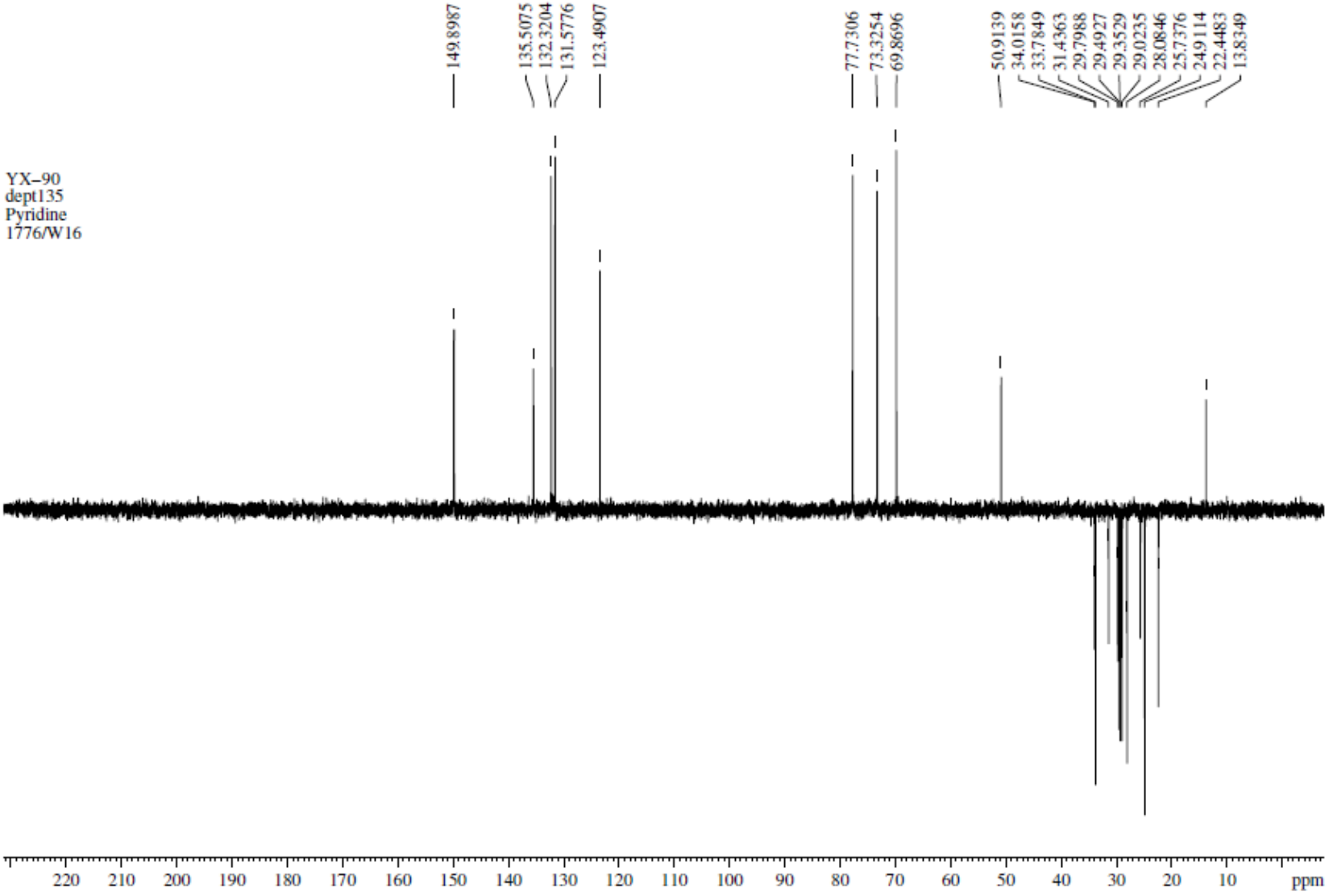


Figure. S4: HSQC spectrum of Compound **1**

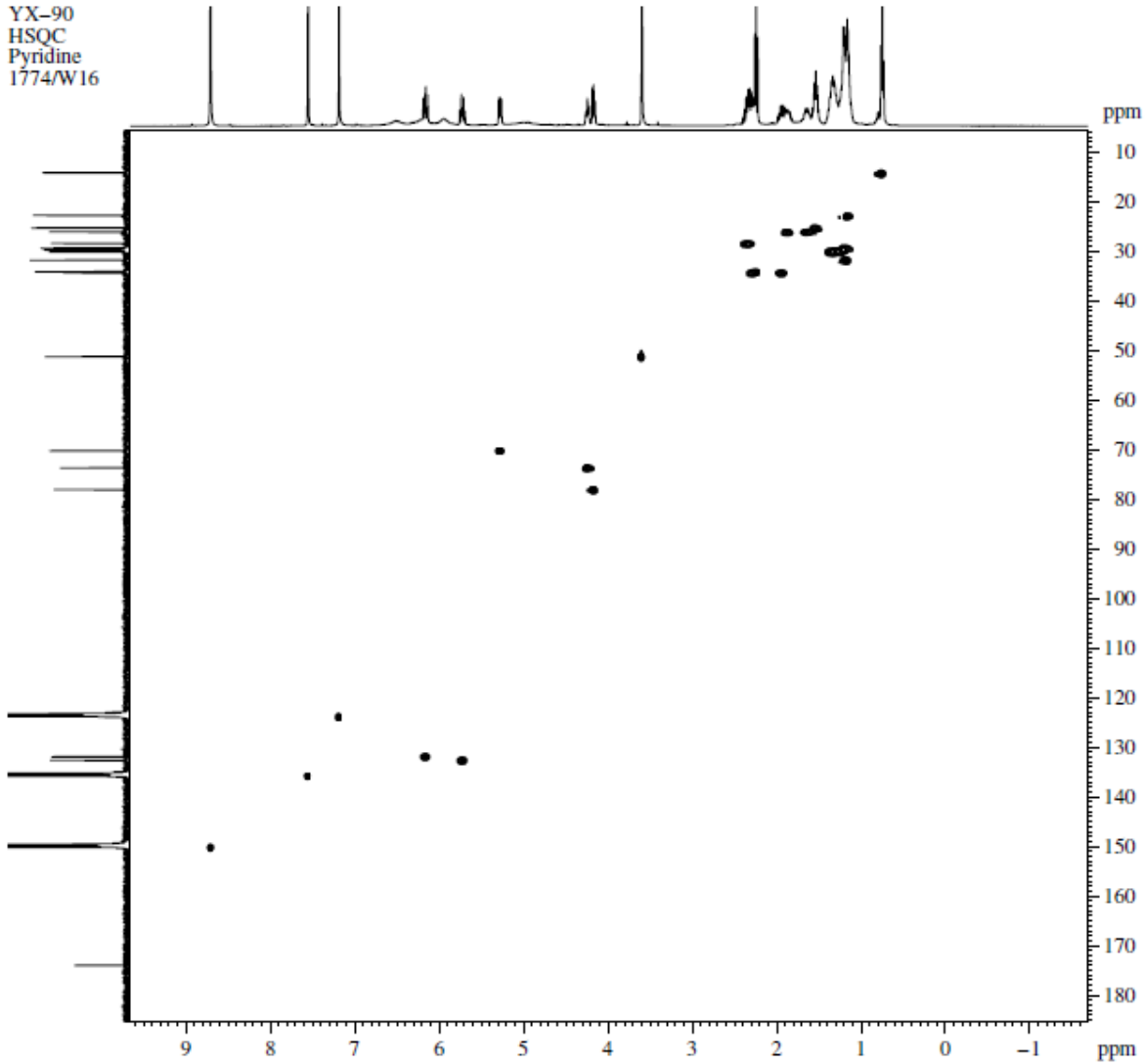


Figure. S5: ^{1}H-^{1}H COSY spectrum of Compound **1**

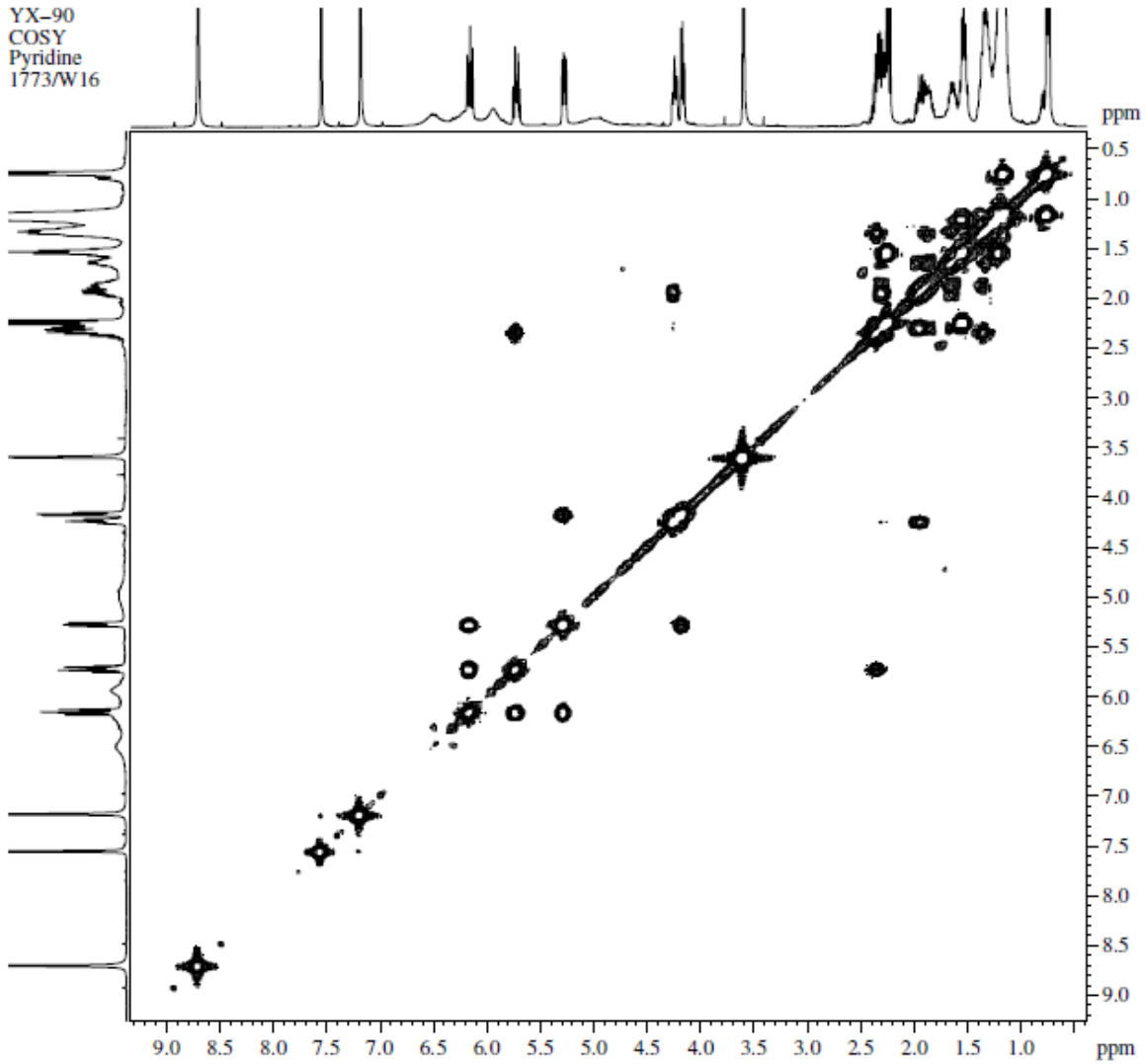


Figure. S6: HMBC spectrum of Compound **1**

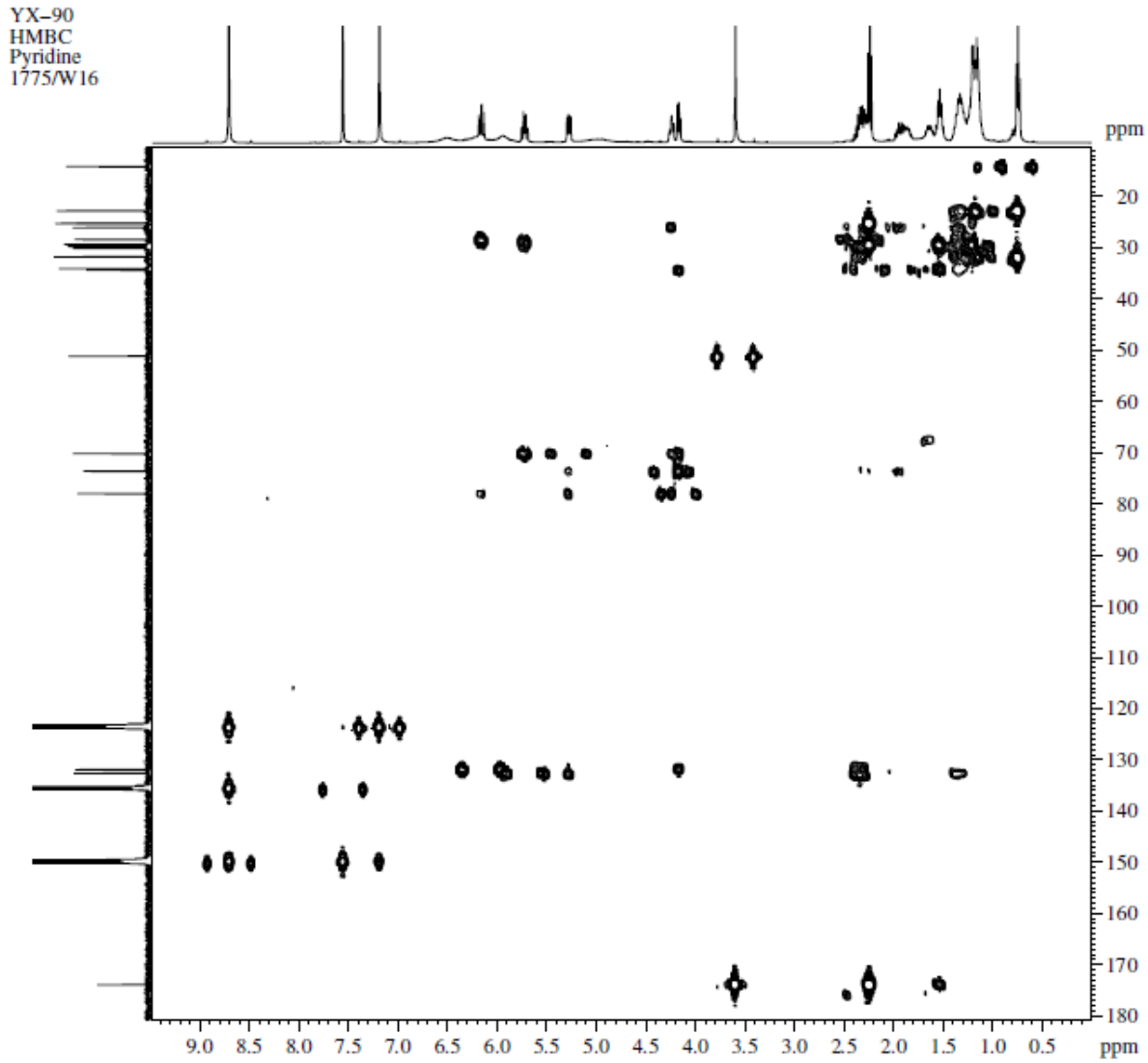


Figure. S7: HR-ESI-MS spectrum of Compound **1**

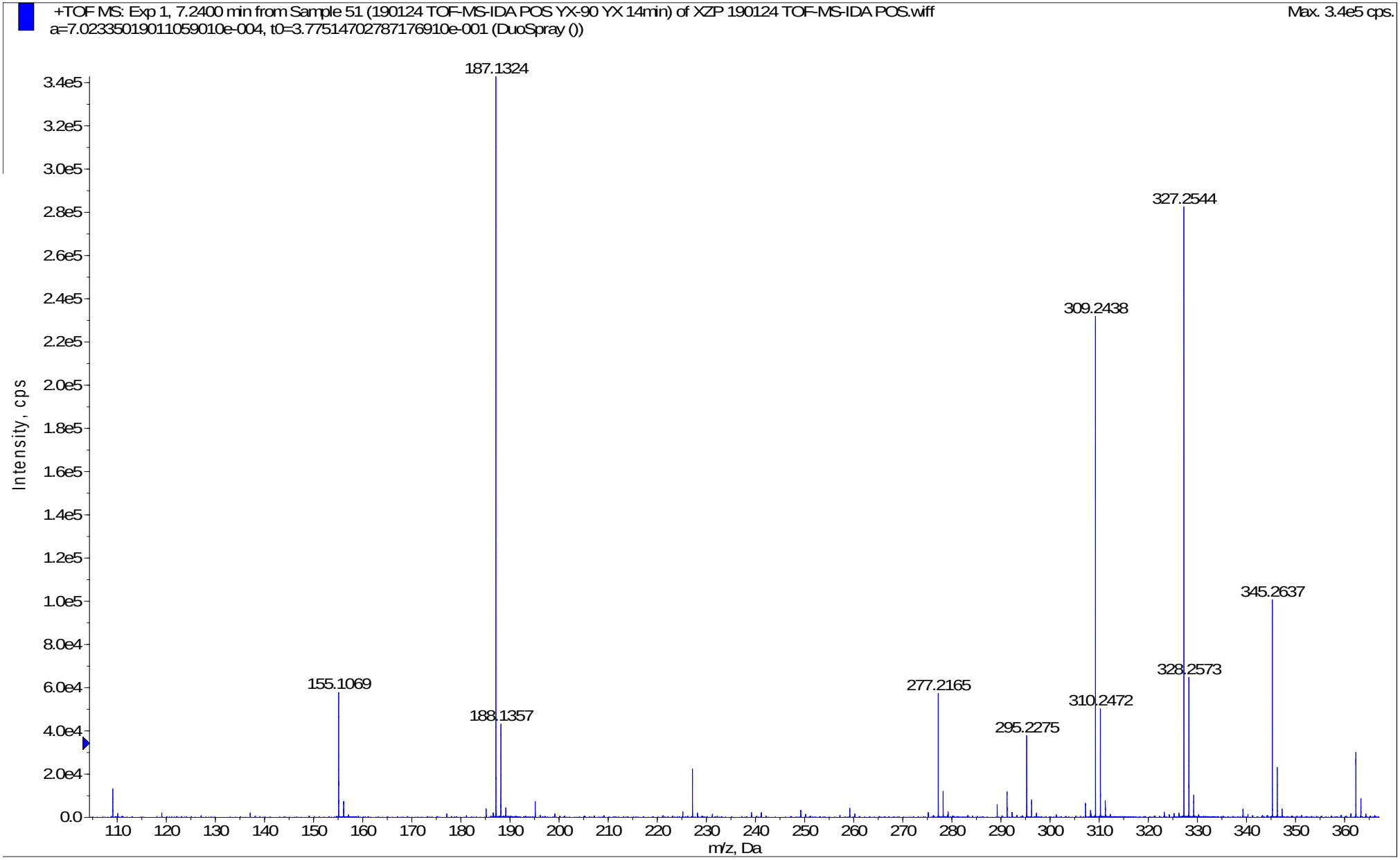


Figure. S8: ^{1}H-NMR Spectrum of Compound **2**

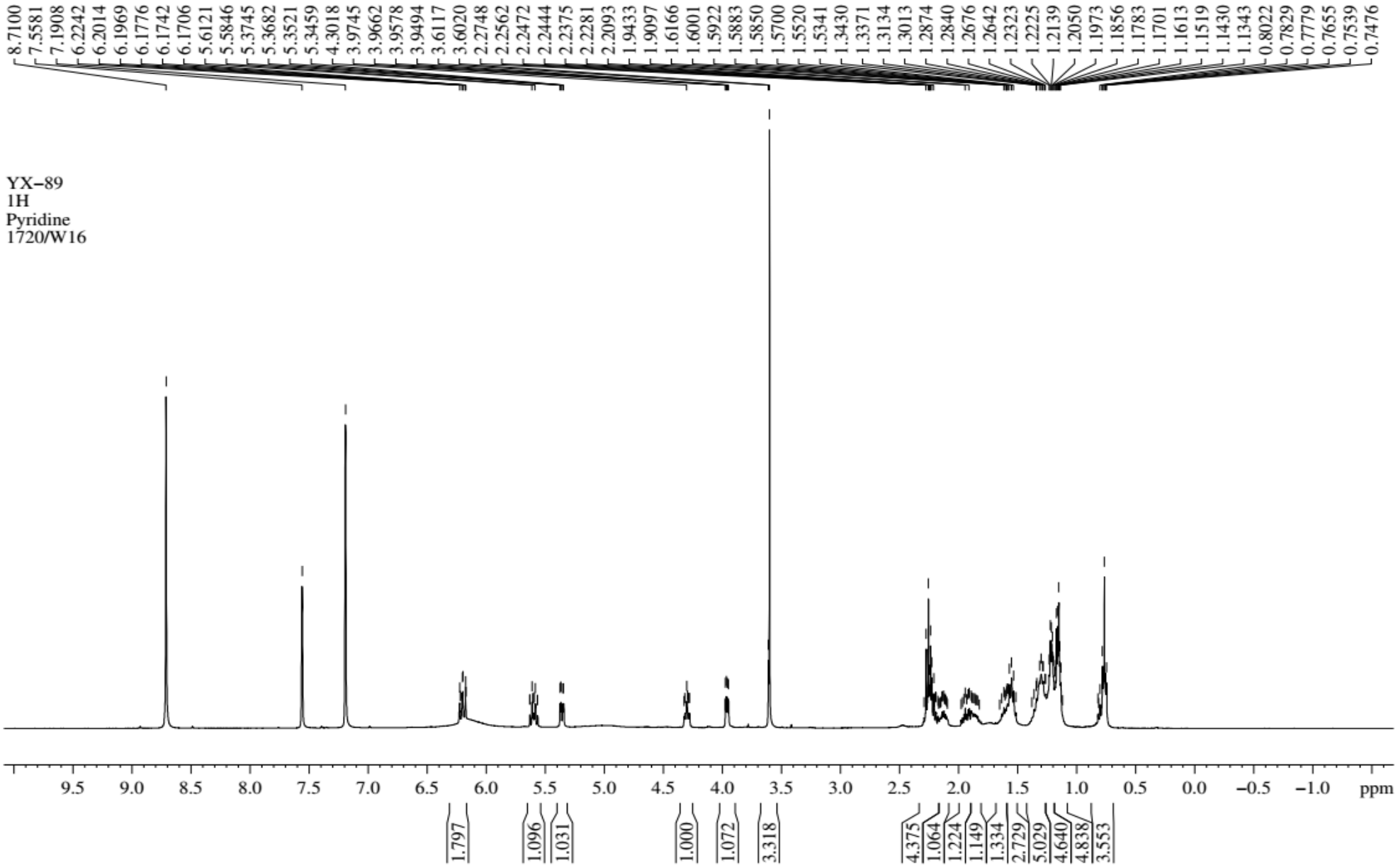


Figure. S9: ^{13}C NMR spectrum of Compound **2**

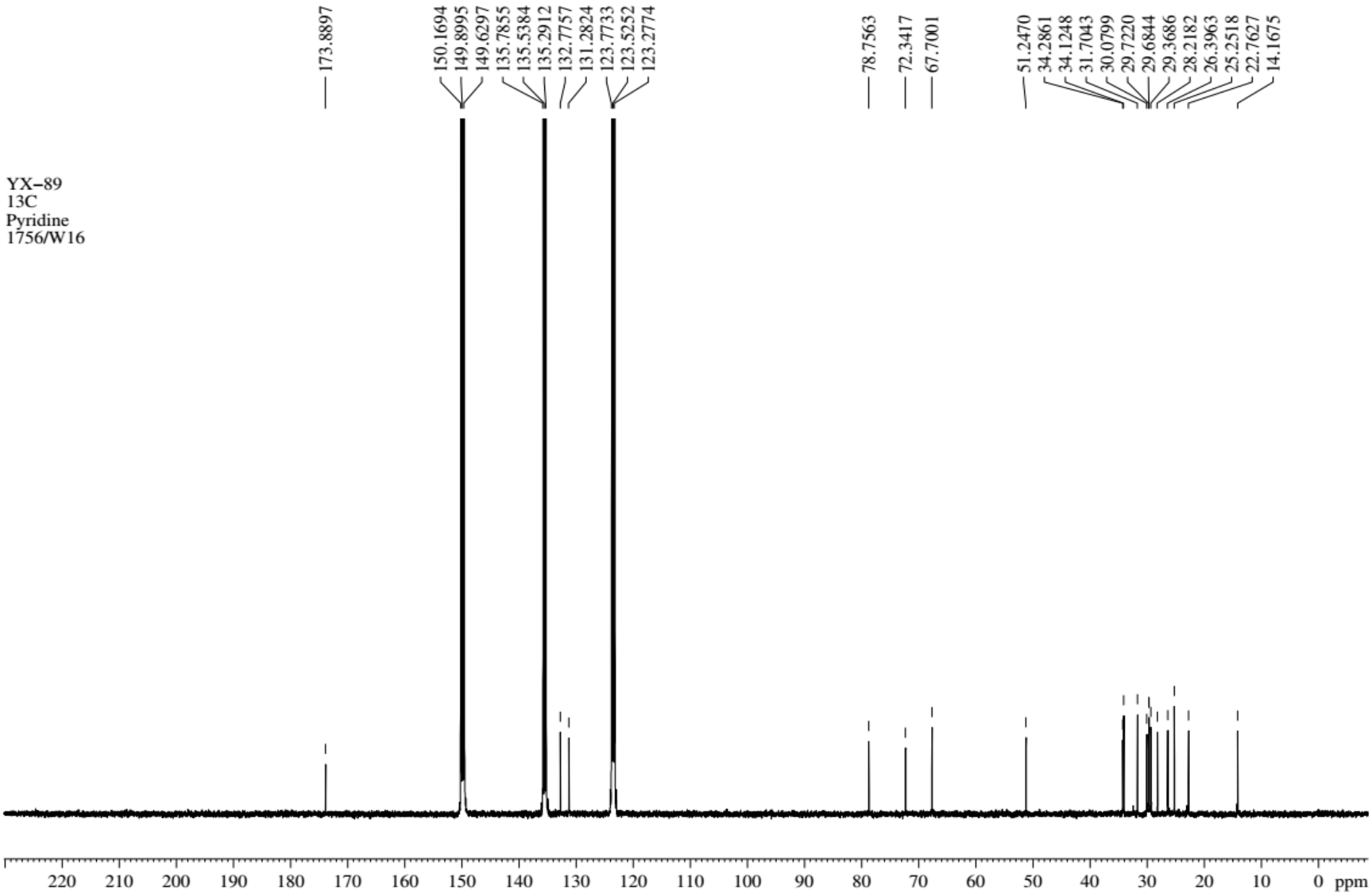


Figure. S10: HR-ESI-MS spectrum of Compound **2**

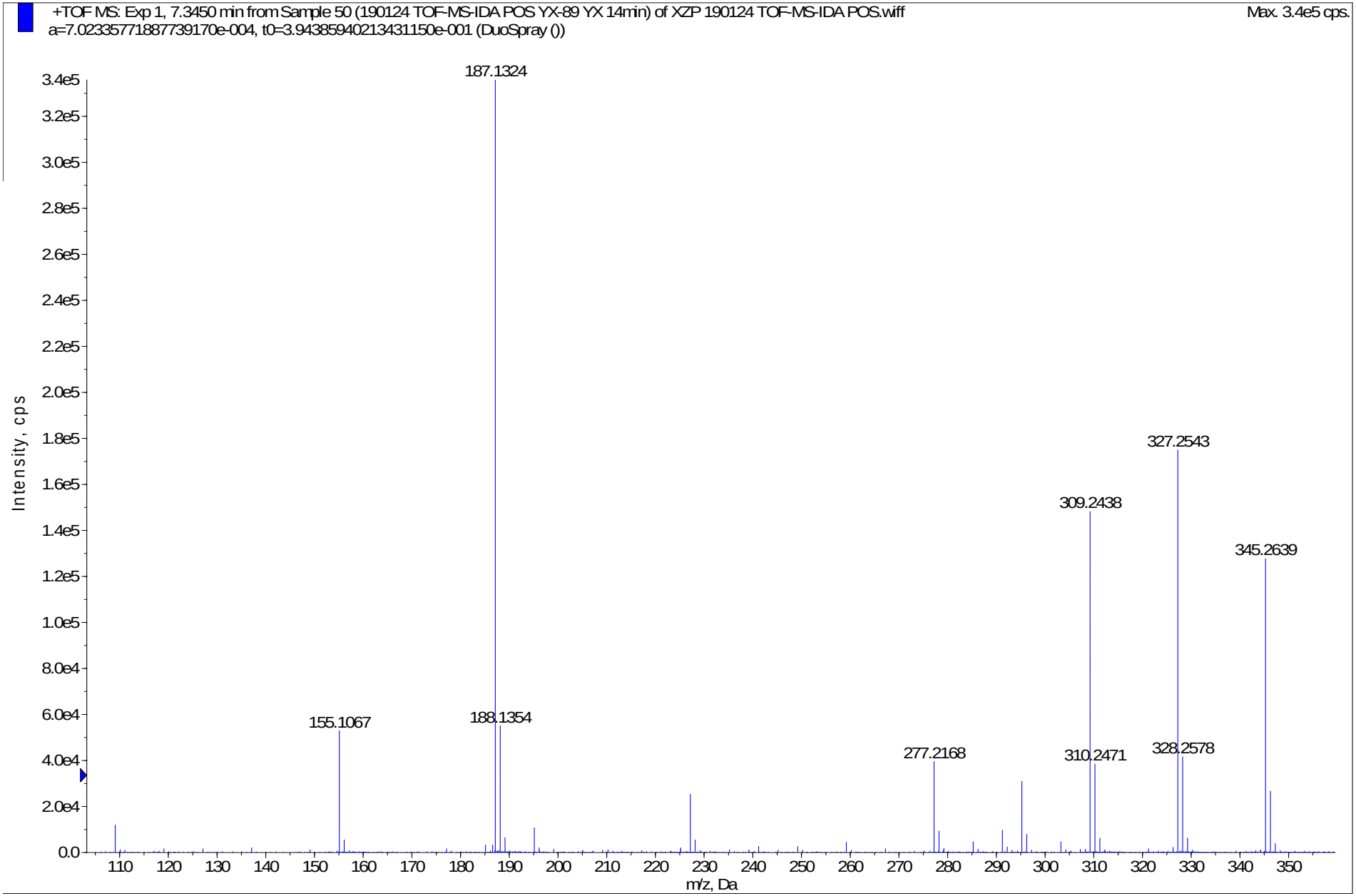


Figure. S11: ^{1}H-NMR Spectrum of Compound **3**

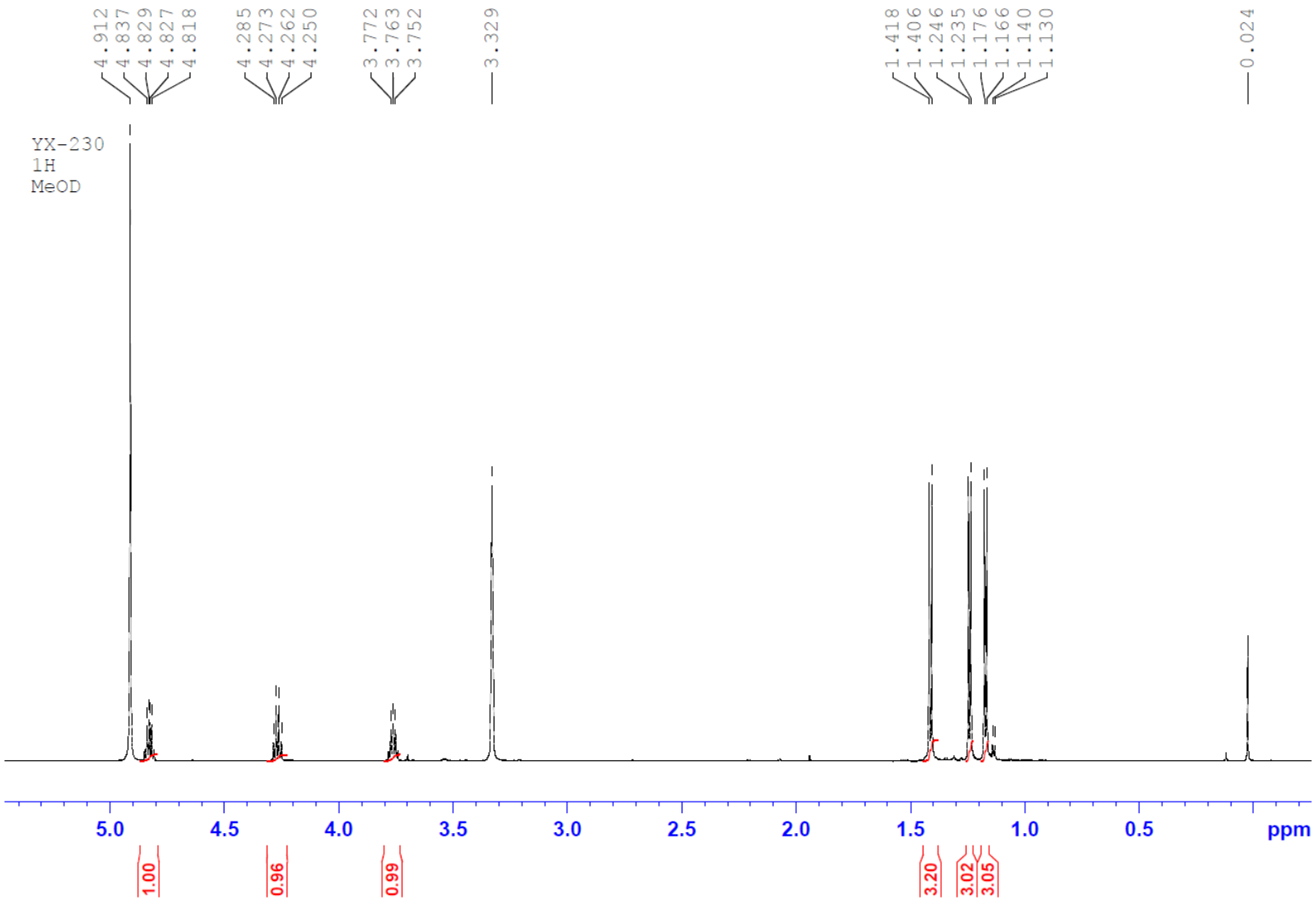


Figure. S12: ^{13}C NMR spectrum of Compound **3**

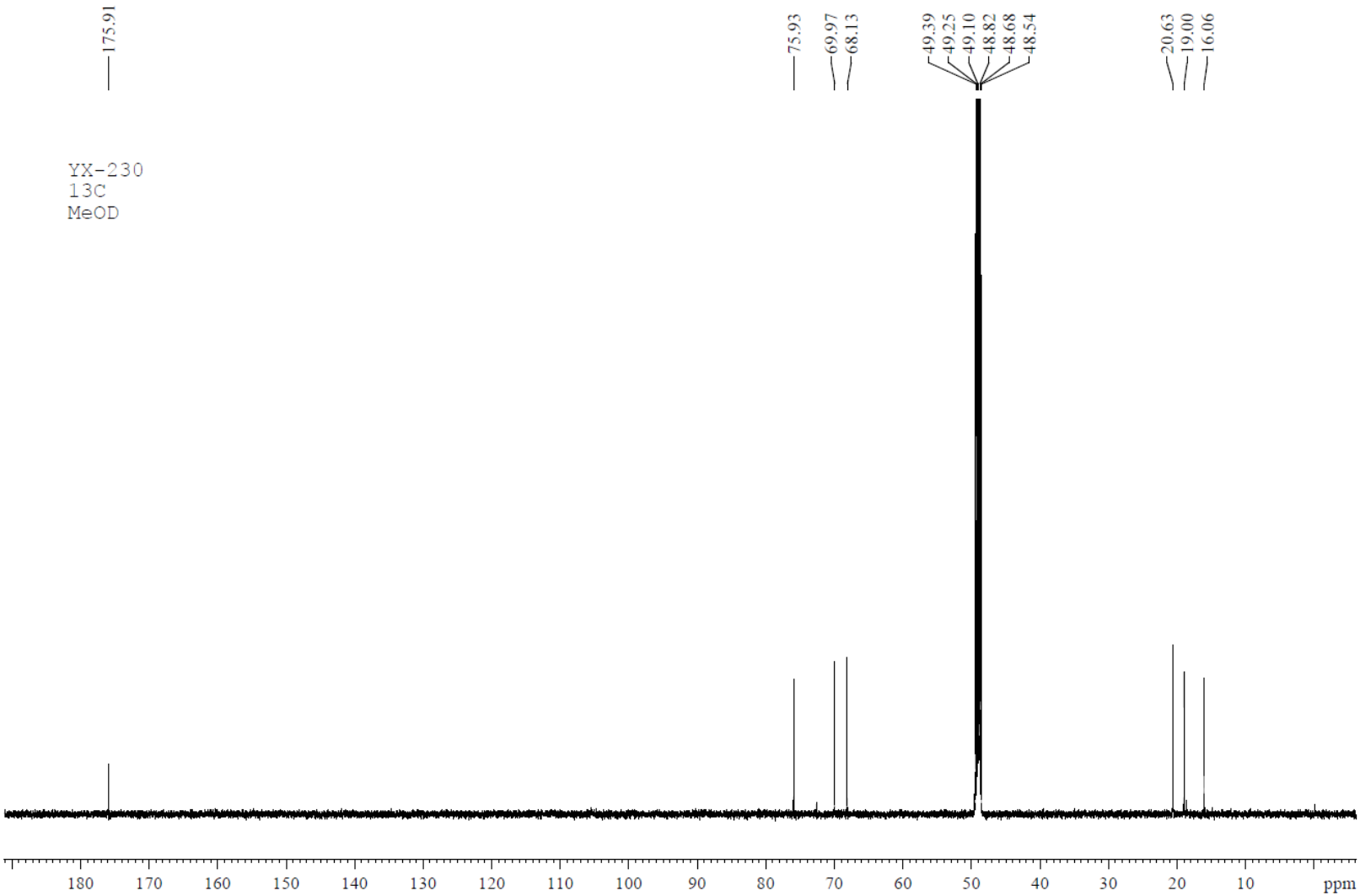


Figure. S13: DEPT-135 spectrum of Compound **3**

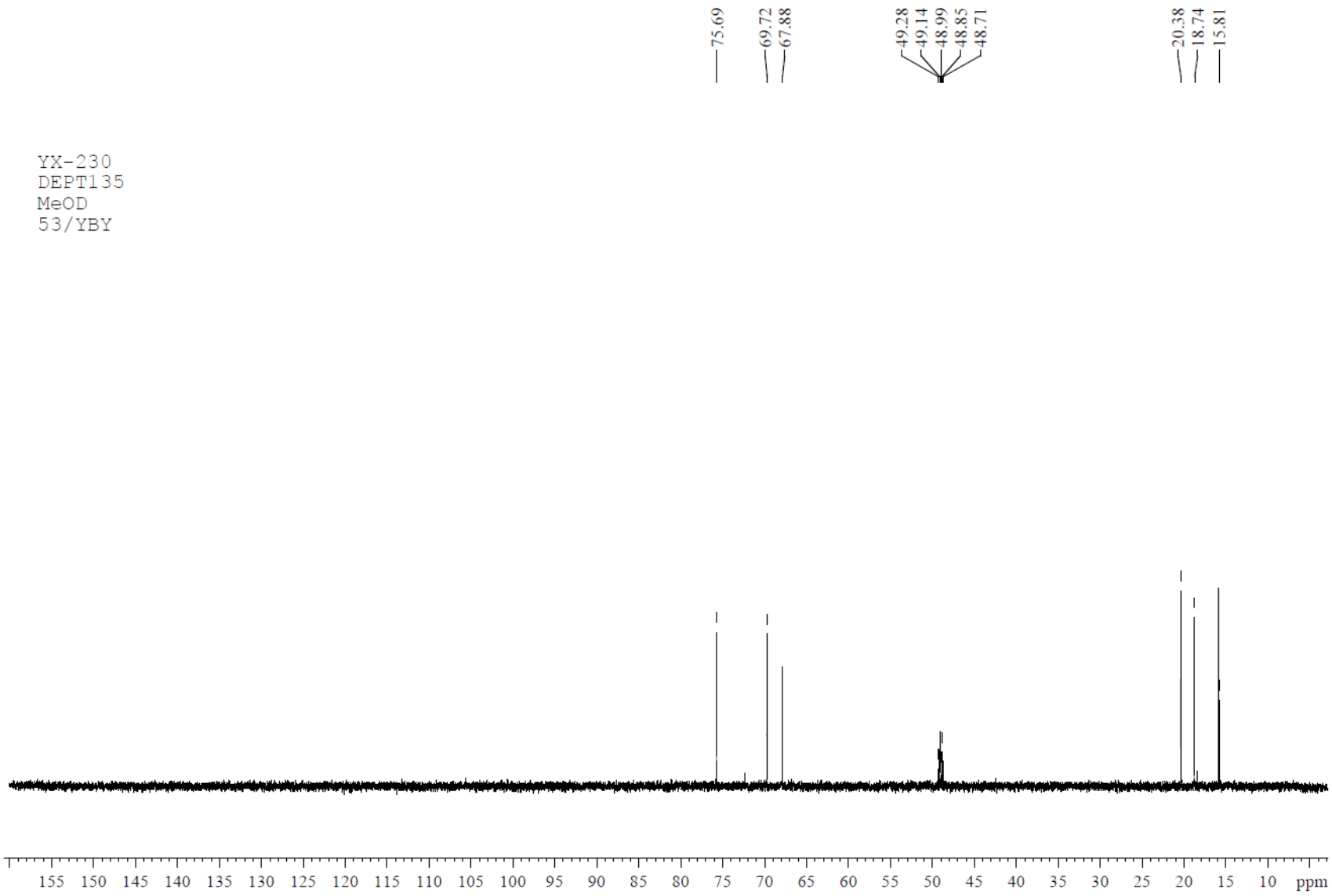
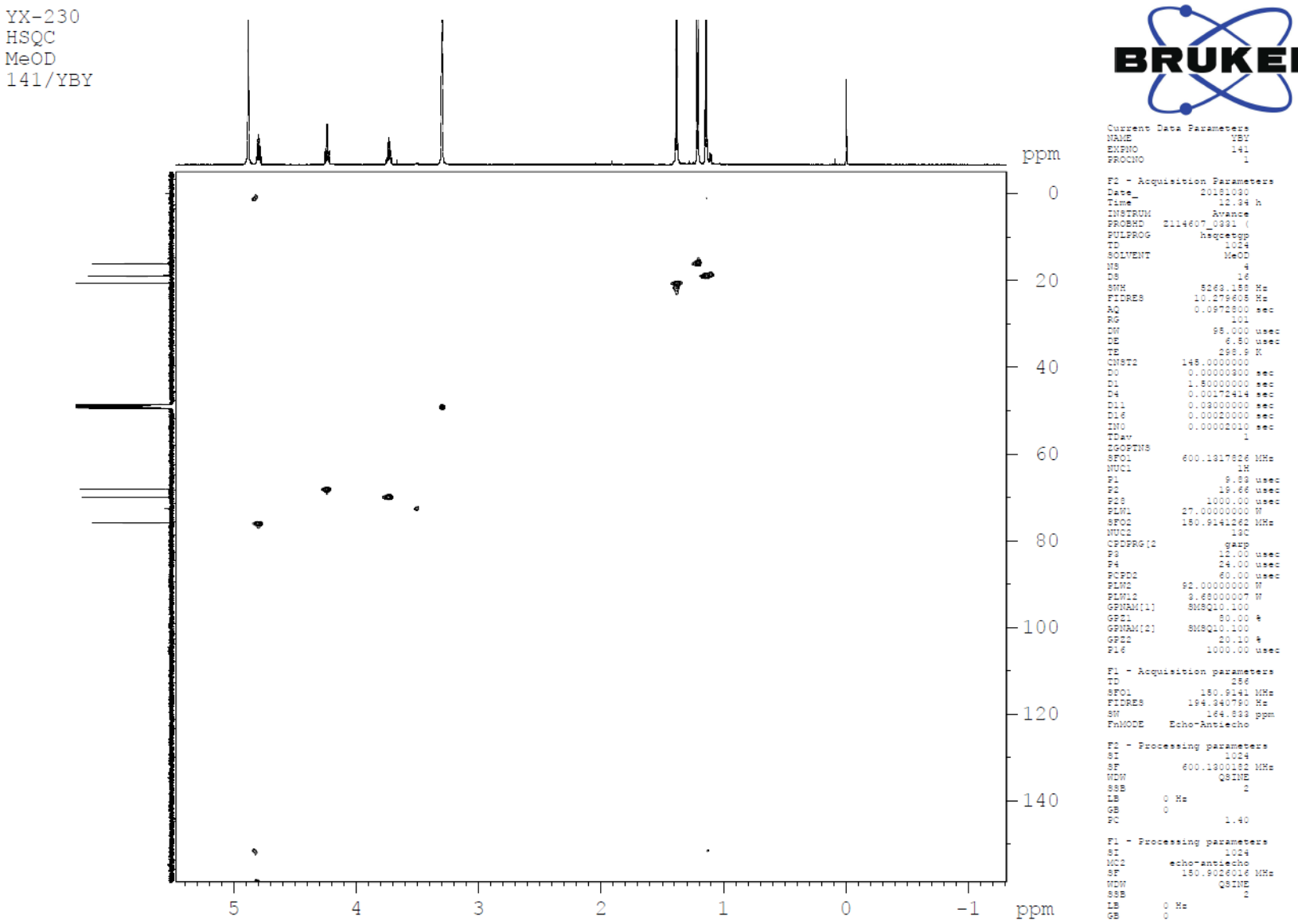


Figure. S14: HSQC spectrum of Compound **3**

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PROCNO                 1

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PULPROG         hsqcetgp
TD                 1024
SOLVENT            MeOD
NS                    4
DS                   16
SWH              5263.158 Hz
FIDRES        10.279605 Hz
AQ            0.0972800 sec
RG                  101
DW               95.000 usec
DE                 6.50 usec
TE               298.9 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
IN0           0.00002010 sec
TD0                   1
ZGOPTNS
SFO1         600.1317826 MHz
NUC1                 1H
P1                 9.83 usec
P2                19.66 usec
P28             1000.00 usec
PLW1         27.00000000 W
SFO2         150.9141262 MHz
NUC2                13C
CPDPRG[2            garp
P3                12.00 usec
P4                24.00 usec
PCPD2             60.00 usec
PLW2         92.00000000 W
PLW12         3.65000007 W
GPNAM[1]      SMSQ10.100
GPZ1               80.00 %
GPNAM[2]      SMSQ10.100
GPZ2               20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  256
SFO1            150.9141 MHz
FIDRES       194.940790 Hz
SW              164.833 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
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SF           600.1300162 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
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SF           150.9026016 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
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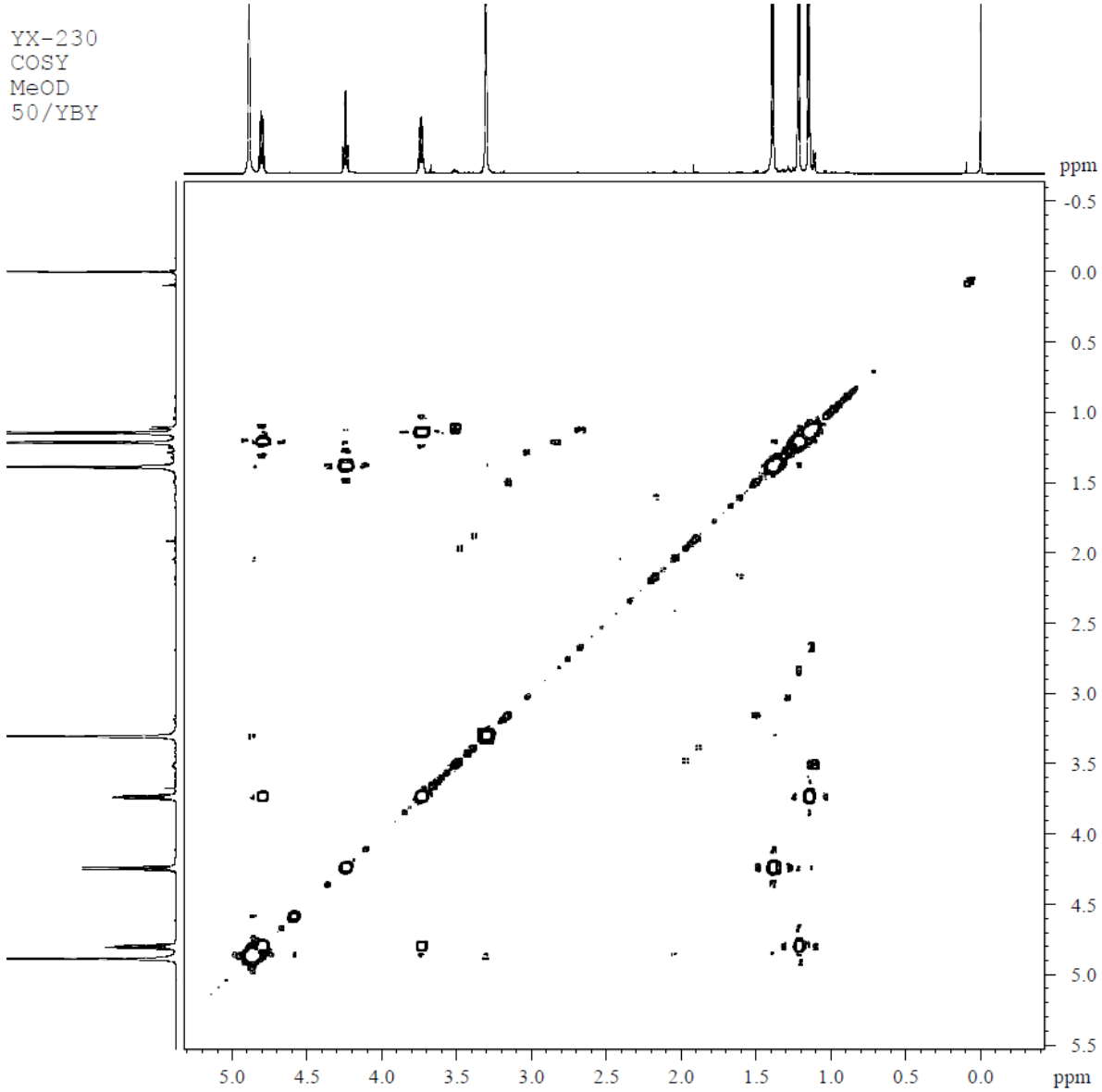
Figure. S15: ^{1}H-^{1}H COSY spectrum of Compound **3**

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EXPNO                  50
PROCNO                  1

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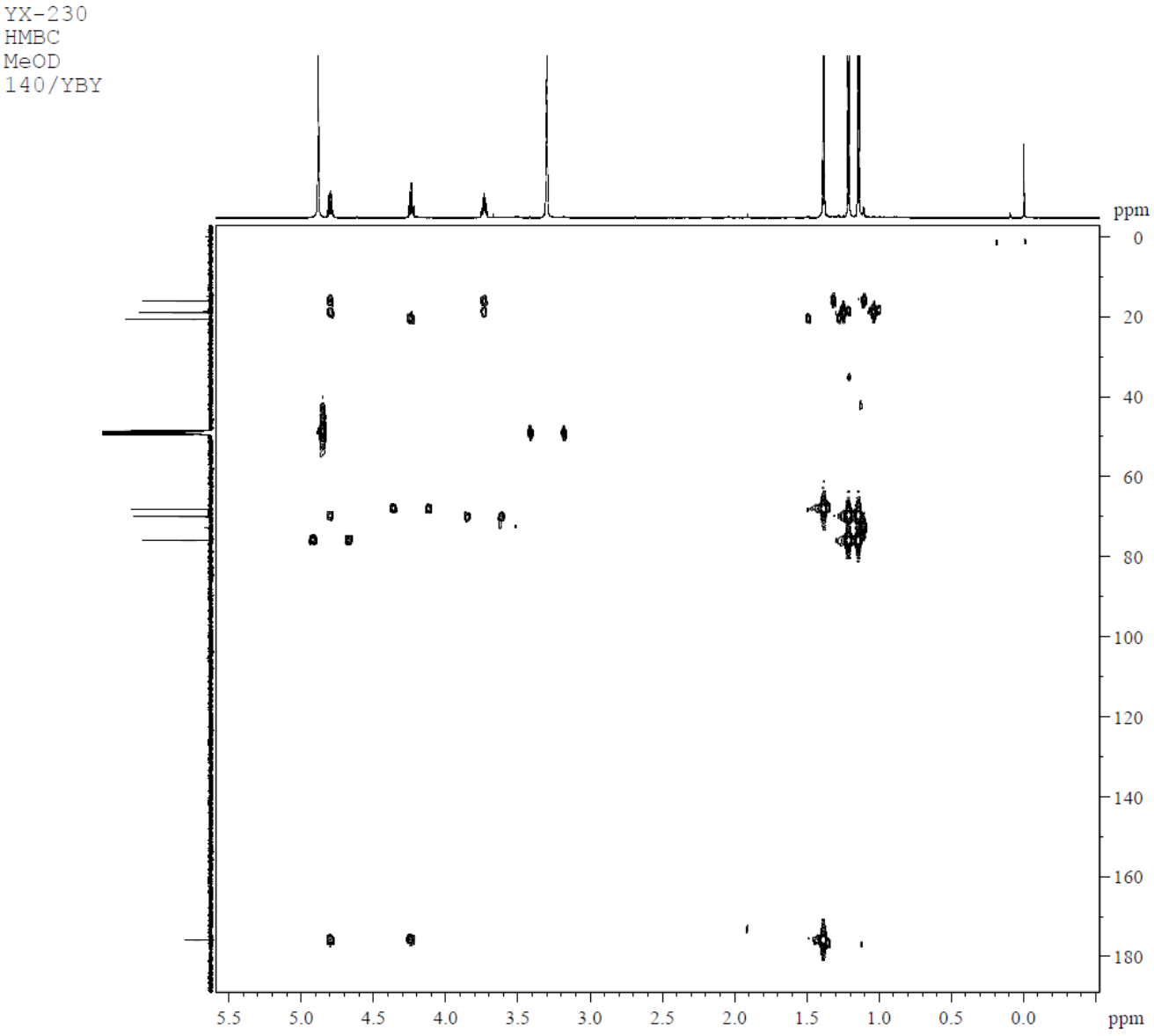
PULPROG       cosygpppqf
TD                   2048
SOLVENT             MeOD
NS                      6
DS                     16
SWH             3703.704 Hz
FIDRES          3.616898 Hz
AQ              0.2764800 sec
RG                    101
DW                135.000 usec
DE                   6.50 usec
TE                  296.8 K
D0             0.00000300 sec
D1             1.93651104 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00027000 sec
TDav                    1
SFO1          600.1314866 MHz
NUC1                   1H
P0                   9.03 usec
P1                   9.03 usec
P17               2500.00 usec
PLW1          27.00000000 W
PLW10          4.17439985 W
GPNAM[1]       SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            600.1315 MHz
FIDRES          57.870369 Hz
SW                  6.171 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF            600.1300102 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                    QF
SF            600.1300102 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
```

Figure. S16: HMBC spectrum of Compound **3**

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EXPNO                140
PROCNO                 1

F2 - Acquisition Parameters
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PULPROG      hmbctgpndqf
TD                  2048
SOLVENT             MeOD
NS                     8
DS                    16
SWH             5263.158 Hz
FIDRES          5.139802 Hz
AQ            0.1945600 sec
RG                   101
DW                95.000 usec
DE                 6.50 usec
TE                298.6 K
CNST13         8.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00001510 sec
TDav                   1
SFO1         600.1317826 MHz
NUC1                  1H
P1                  9.83 usec
P2                 19.66 usec
PLW1         27.00000000 W
SFO2         150.9178988 MHz
NUC2                 13C
P3                 12.00 usec
PLW2         92.00000000 W
GPNAM[1]      SMSQ10.100
GPZ1                50.00 %
GPNAM[2]      SMSQ10.100
GPZ2                30.00 %
GPNAM[3]      SMSQ10.100
GPZ3                40.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1            150.9178 MHz
FIDRES       517.384084 Hz
SW              219.403 ppm
FnMODE                QF

F2 - Processing parameters
SI                  2048
SF          600.1300182 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF          150.9026016 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
```
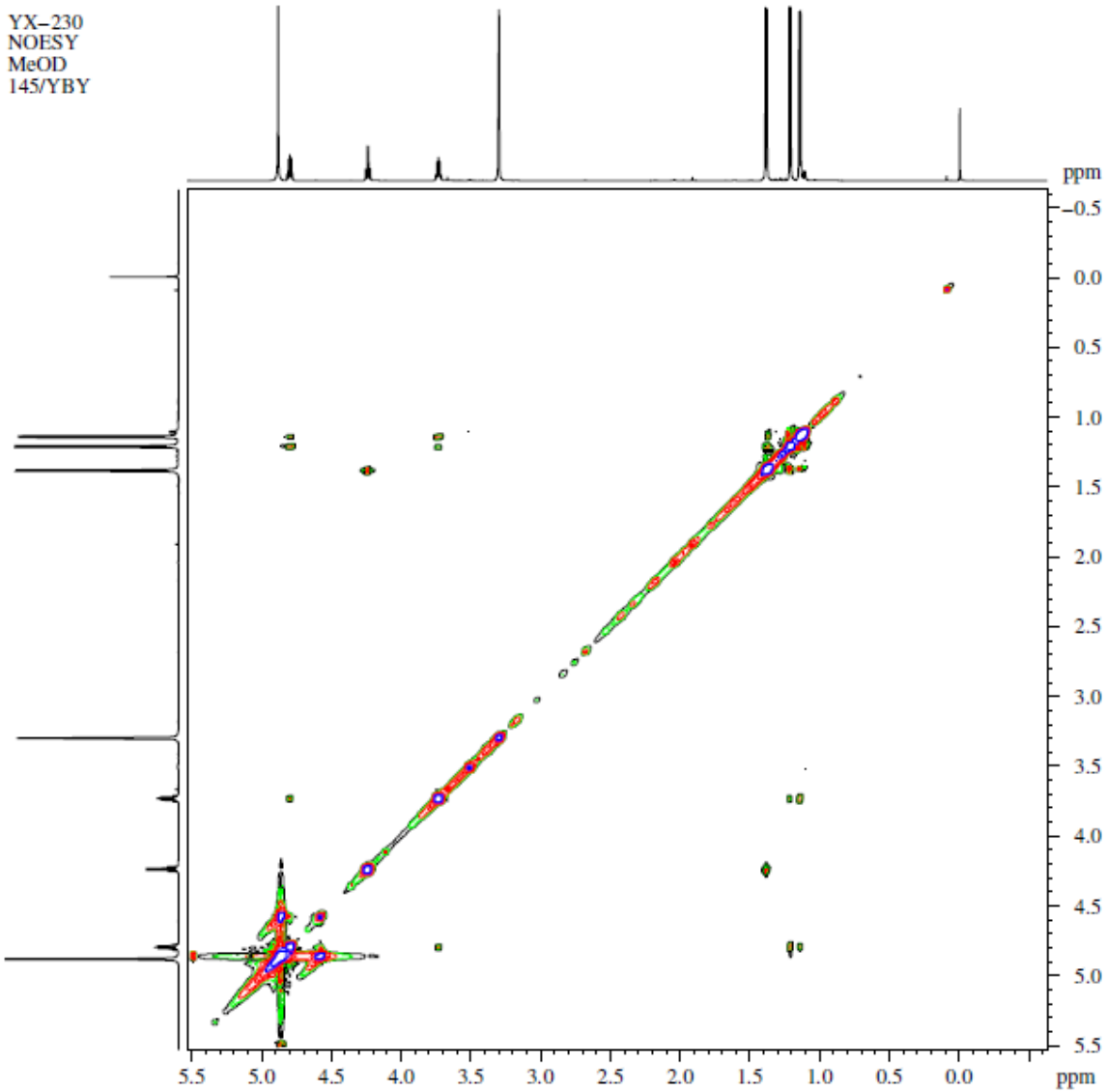

Figure. S17: NOESY spectrum of Compound **3**

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PULPROG     noesygpphpp
TD                 1024
SOLVENT            MeOD
NS                   32
DS                   32
SWH            3703.704 Hz
FIDRES         7.233796 Hz
AQ            0.1382900 sec
RG                  101
DW              135.000 usec
DE                10.62 usec
TE                297.7 K
D0            0.00012248 sec
D1            1.98566401 sec
D8            0.69999999 sec
D11           0.03000000 sec
D12           0.00002000 sec
D16           0.00020000 sec
IN0           0.00027000 sec
ND0                    1
TD                   256
SFO1           600.1315 MHz
FIDRES        14.467592 Hz
SW                6.171 ppm
FnMODE      States-TPPI
SI                 1024
SF          600.1300182 MHz
WDW               QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
PC                 1.00
SI                 1024
MC2         States-TPPI
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WDW               QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
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Figure. S18: HR-ESI-MS spectrum of Compound **3**

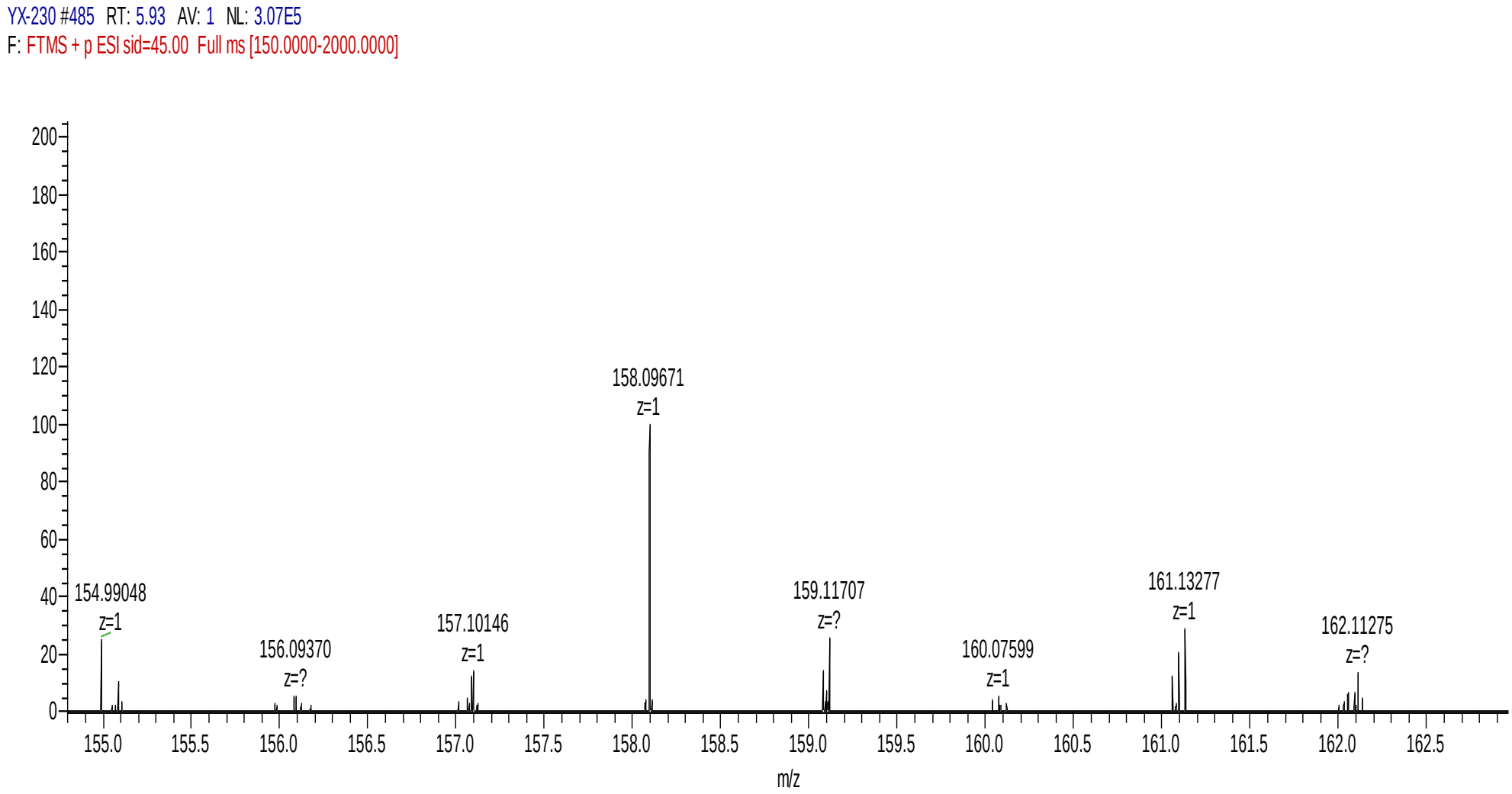

Figure. S19: Key HMBC and ^{1}H-^{1}H COSY correlations of compounds **1-3**

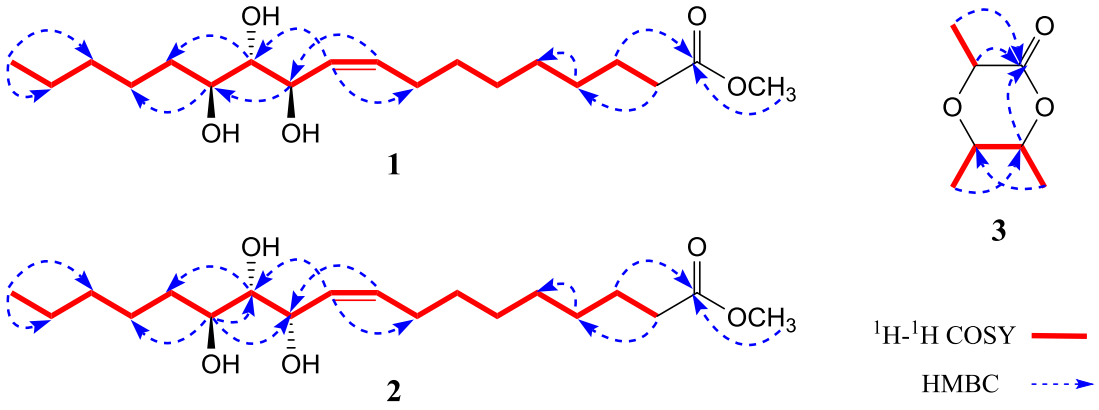

Figure. S20: Chemical structures of compounds **4-30**

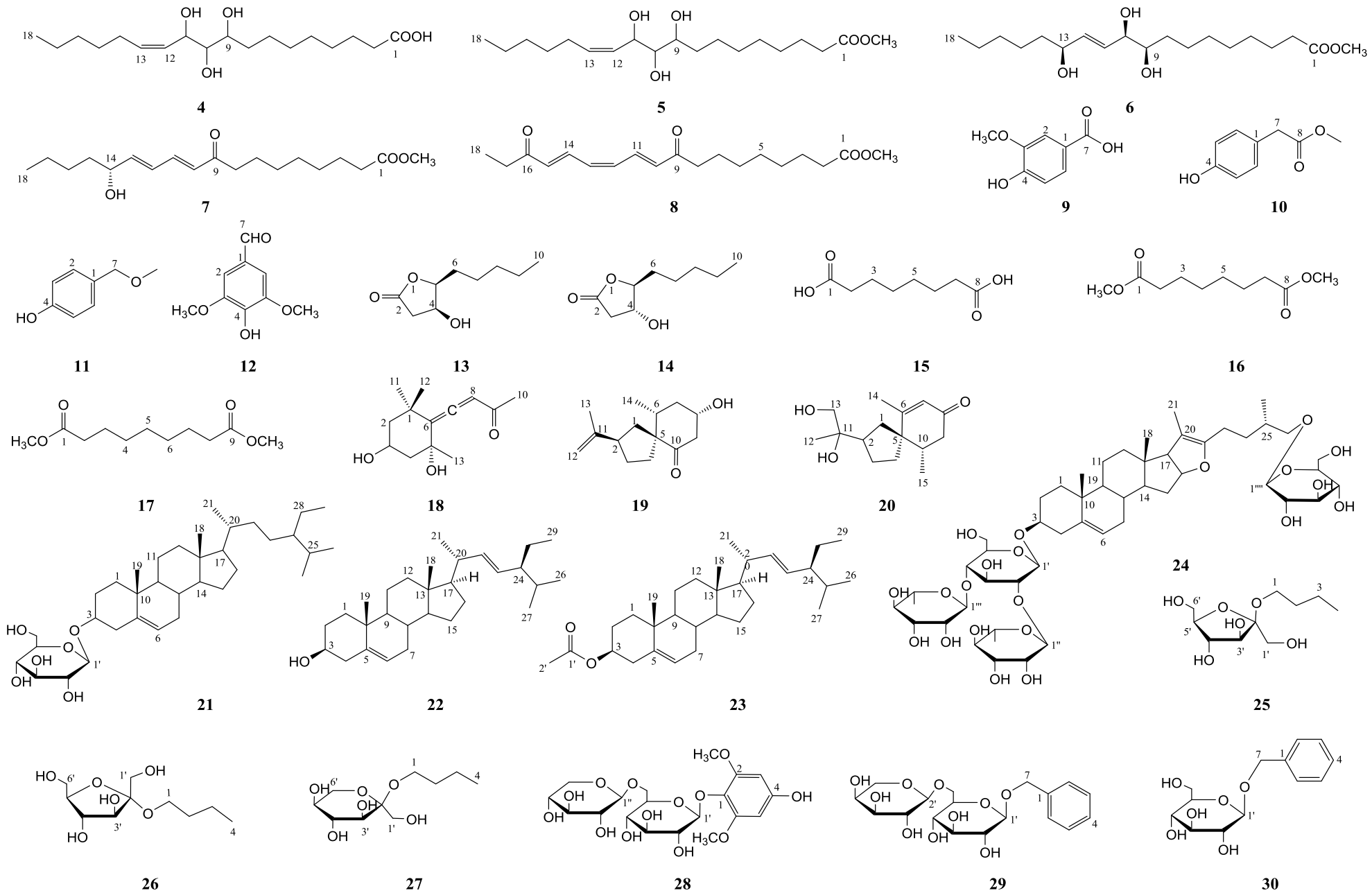

Table. S1 ^{13}C-NMR (100 MHz) data of **4-20** ([a] Measured in CD_3OD [b] Measured in C_5D_5N [c] Measured in $CDCl_3$)

NO.	4[a]	5[a]	6[a]	7[a]	8[a]	9[a]	10[a]	11[a]	12[a]	13[a]	14[a]	15[a]	16[a]	17[a]	18[a]	19[a]	20[a]
1	177.8	176.0	175.6	176.0	176.0	123.1	126.3	130.0	129.2			177.9	176.0	176.0	37.0	36.0	37.8
2	35.0	34.8	34.8	38.0	34.8	113.8	131.3	130.8	108.2	178.9	178.1	35.0	34.7	34.8	50.0	48.4	46.8
3	26.1	26.0	26.0	27.7	25.9	152.7	116.3	116.1	149.6	40.4	38.1	29.9	30.0	30.2	64.4	32.1	28.2
4	30.2	30.2	30.2	30.0	30.0[*]	148.7	157.6	158.3	143.8	69.6	72.2	26.0	25.9	30.1	49.8	31.4	35.1
5	30.4	30.4	30.4	30.1	30.1[*]	115.8	116.3	116.1	149.6	87.1	89.9	26.0	25.9	26.0	72.4	60.1	51.1
6	30.5	30.5	30.6	30.1	30.1[*]	125.3	131.3	130.8	108.2	32.9	33.9	29.9	30.0	30.1	120.0	37.7	171.0
7	26.3	26.4	26.5	25.5	25.3	170.0	40.9	75.5	192.9	26.3	26.2	35.0	34.7	30.2	211.5	40.7	125.8
8	34.1	34.1	33.8	41.1	41.4		174.6			29.4	32.6	177.9	176.0	34.8	101.1	69.4	202.1
9	73.7	73.7	75.3	203.7	203.1					23.6	23.5			176.0	200.8	48.2	43.7
10	78.2	78.2	75.4	130.3	133.2[#]					14.3	14.3				26.5	213.1	39.9
11	69.8	69.9	136.5	144.3	142.6[ϕ]										29.3	148.9	74.4
12	129.5	129.6	130.9	128.8	139.8[Δ]										32.3	109.3	22.5
13	135.0	135.0	73.2	148.5	140.0[Δ]										30.8	21.1	70.1
14	28.9	28.9	38.4	72.6	142.4[ϕ]											16.4	21.3
15	30.7	30.7	26.2	37.8	133.4[#]												16.1
16	32.7	32.7	33.5	28.7	203.4												
17	23.6	23.6	23.7	23.7	34.6												
18	14.4	14.4	14.5	14.4	8.3												
OCH_3		51.9	51.9	52.0	51.9	56.3	52.4	57.8	56.8				51.9	52.0			
OCH_3									56.8				51.9	52.0			

[*, #, ϕ, Δ]: exchangeable

Table. S2 ^{13}C-NMR (100 MHz) data of **21-30** ([a] Measured in CD_3OD [b] Measured in C_5D_5N [c] Measured in $CDCl_3$)

NO.	21[b]	22[b]	23[c]	24[c]	25[a]	26[a]	27[a]	28[a]	29[a]	30[a]
1	38.0	37.5	37.2	38.2	62.2	61.6	61.6	129.4	139.1	139.0
2	30.6	30.2	31.9	34.8	33.5	33.3	33.3	154.8	129.2	129.2
3	78.5	78.5	71.8	73.7	20.4	20.4	20.5	94.5	129.3	129.3
4	39.4	39.3	42.3	45.9	14.4	14.2	14.3	155.9	128.7	128.7
5	141.2	140.9	140.7	139.8				94.5	129.3	129.3
6	122.2	121.9	121.7	122.7				154.8	129.2	129.2
7	32.9	32.2	31.6	32.0					71.9	71.8
8	31.9	32.1	31.9	32.0						
9	50.8	50.3	50.1	50.1						
10	37.5	36.9	36.5	37.1						
11	21.7	21.3	21.1	21.1						
12	40.1	39.9	39.7	39.8						
13	43.9	42.5	42.2	42.4						
14	55.4	56.8	55.9	56.8						
15	35.0	24.5	24.2	25.2						
16	84.9	28.5	28.9	29.2						
17	65.0	56.2	56.8	56.1						
18	14.6	21.2	12.0	12.0						
19	19.9	20.0	19.4	19.4						
20	104.0	36.4	40.4	36.7						
21	12.3	19.4	21.2	21.2						
22	152.8	34.2	138.3	138.4						
23	34.0	26.4	129.3	129.3						
24	24.2	46.0	51.2	51.3						
25	31.9	29.5	31.9	29.8						
26	75.4	19.0	19.0	21.3						
27	17.8	19.2	21.1	23.1						
28		23.4	25.4	27.9						
29		12.0	12.2	11.9						

NO.	21[b]	22[b]	24[c]	25[a]	26[a]	27[a]	28[a]	29[a]	30[a]
1'	100.7	102.6	173.4	61.9	61.9	63.4	105.9	103.4	103.3
2'	79.0	75.3	22.8	105.2	108.7	101.6	74.8	75.1	75.1
3'	77.4	78.6		78.4	83.2	70.5	77.4	78.0	78.1
4'	78.4	71.7		77.3	78.5	71.5	71.2	71.7	71.7
5'	78.2	78.1		83.3	83.8	71.1	77.4	77.0	78.0
6'	61.7	62.8		65.0	62.7	65.1	69.2	69.5	62.8
1''	102.5						105.1	105.2	
2''	73.0						75.5	72.4	
3''	73.2						77.7	74.2	
4''	74.4						71.2	69.5	
5''	70.0						66.7	66.7	
6''	19.1								
1'''	103.4								
2'''	73.0								
3'''	73.3								
4'''	74.6								
5'''	70.9								
6'''	19.0								
1''''	105.4								
2''''	75.7								
3''''	78.7								
4''''	72.2								
5''''	79.1								
6''''	63.3								
OCH_3							56.7		

Table S3. Inhibitory Effects of Compounds **1-30** on NO Production by LPS-induced RAW264.7 cells

Compound	IC_{50} (mean ± SD, μM)	Compound	IC_{50} (mean ± SD, μM)
Indomethacina[a]	39.6±2.2	**16**	>80
1	>80	**17**	>80
2	>80	**18**	-
3	-	**19**	>80
4	>80	**20**	60.0±4.1
5	>80	**21**	20.2±2.2
6	>80	**22**	>80
7	>80	**23**	>80
8	>80	**24**	>80
9	45.7±2.8	**25**	>80
10	>80	**26**	>80
11	>80	**27**	>80
12	32.8±2.7	**28**	56.7±3.1
13	-	**29**	>80
14	-	**30**	>80
15	>80		

[a] Positive control