

## Supporting Information

for

### **Trogopterins A–C: Three new neolignans from feces of *Trogopterus xanthipes***

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TXE16-4\_wet1d  
File: xp  
Pulse Sequence: wet1D

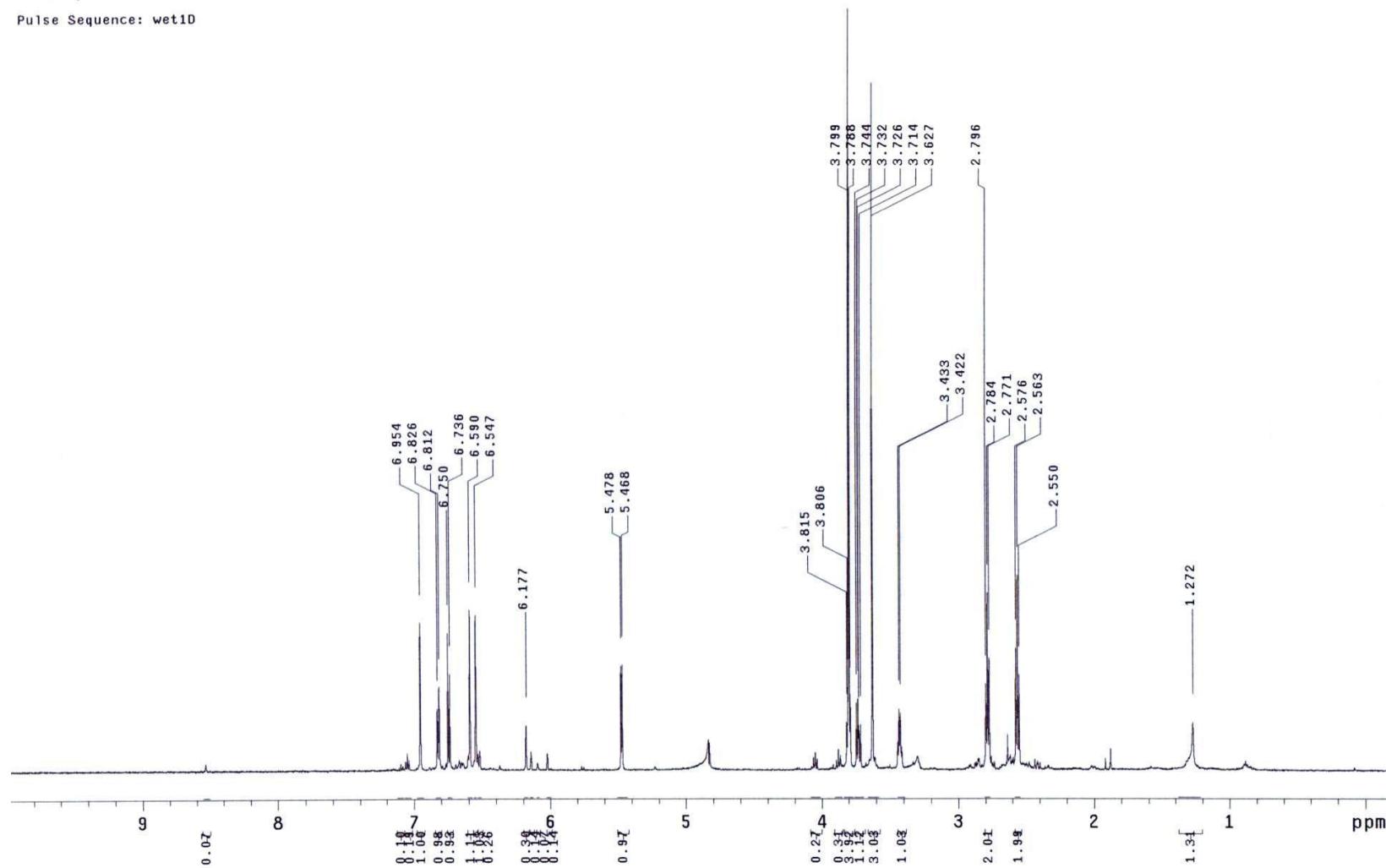


Figure S1:  $^1\text{H}$  NMR spectrum of compound 1 (DMSO- $d_6$ , 300 MHz).

TXE 16-4

File: xp

Pulse Sequence: s2pul

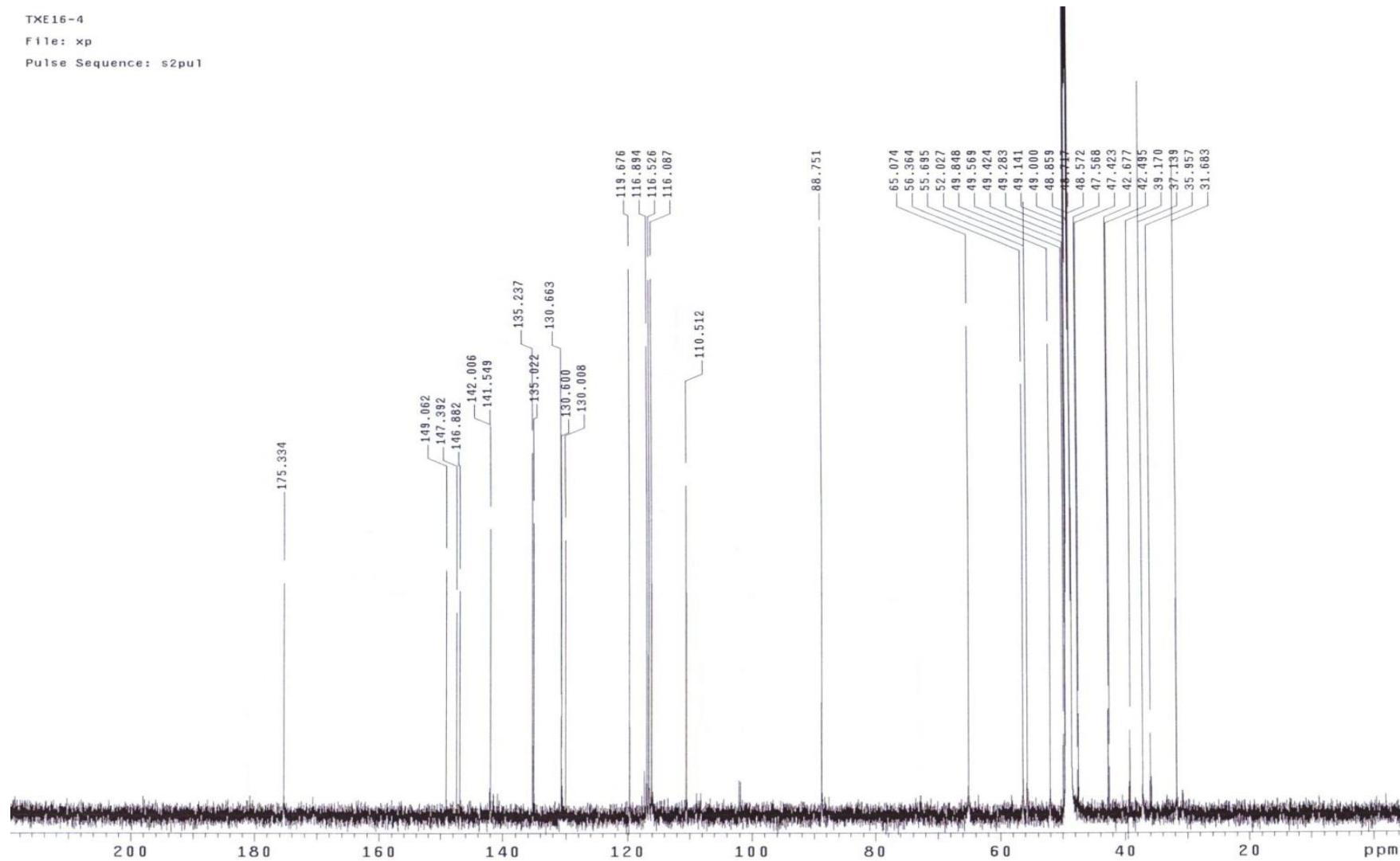


Figure S2:  $^{13}\text{C}$  NMR spectrum of compound 1 (DMSO- $\text{d}_6$ , 75 MHz).

TXE16-4  
File: xp  
Pulse Sequence: gCOSY  
Solvent: cd3od  
Temp. 25.0 C / 298.1 K  
Operator: vnmri  
VNMRs-600 "ynnmr600"  
Relax, delay 1.000 sec  
Acq. time 0.160 sec  
Width 6410.3 Hz  
2D Width 6410.3 Hz  
8 repetitions  
512 increments  
OBSERVE H1, 599.8582915 MHz  
DATA PROCESSING  
Sine bell 0.080 sec  
F1 DATA PROCESSING  
Sine bell 0.160 sec  
FT size 8192 x 8192  
Total time 1 hr, 32 min, 51 sec

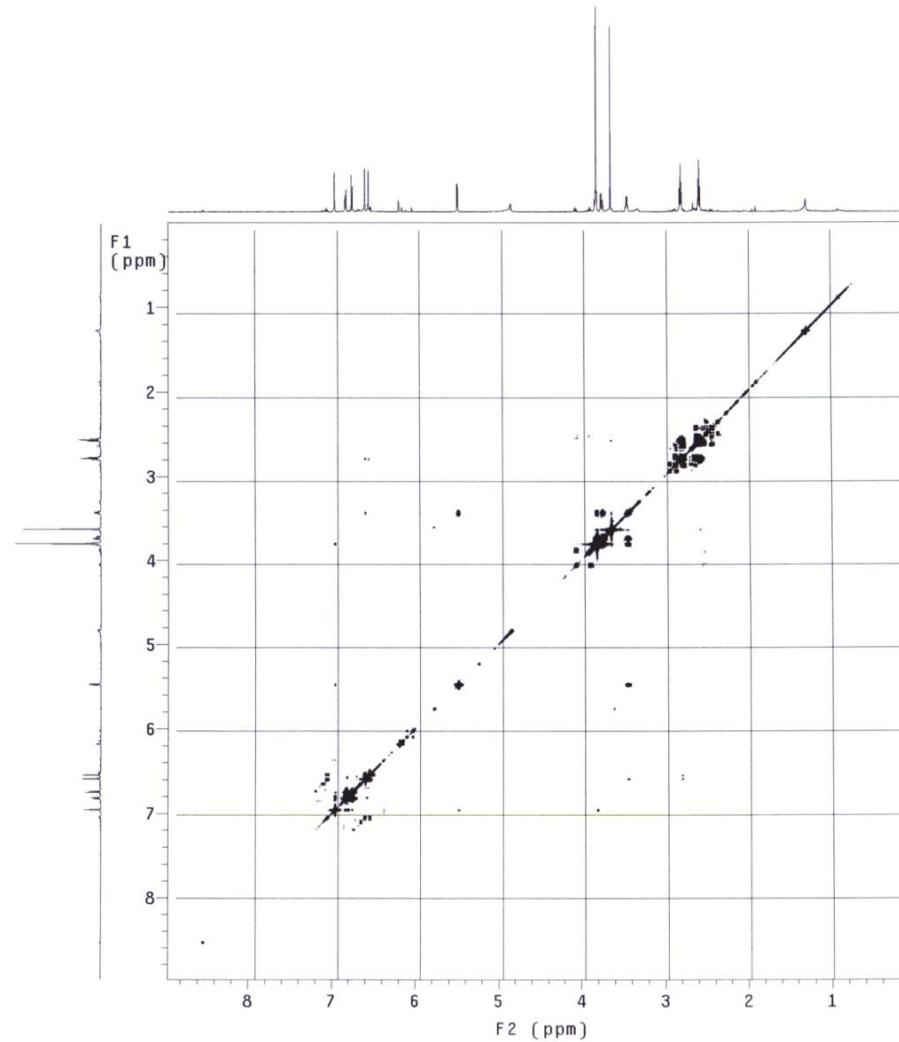


Figure S3:  $^1\text{H}$ , $^1\text{H}$  COSY spectrum of compound 1 (DMSO- $d_6$ , 600 MHz).

TXE16-4  
File: xp  
Pulse Sequence: gHMQC  
Solvent: cd3od  
Temp. 25.0 C / 298.1 K  
operator: vnmri  
VNMRs-600 "ynmrr600"  
Relax. delay 1.000 sec  
Acq. time 0.128 sec  
Width 6410.3 Hz  
2D Width 25641.0 Hz  
16 repetitions  
2 x 512 increments  
OBSERVE H1, 599.8582903 MHz  
DECOUPLE C13, 150.8457980 MHz  
Power 37 dB  
on during acquisition  
off during delay  
w40\_swpg modulated  
DATA PROCESSING  
Gauss apodization 0.059 sec  
F1 DATA PROCESSING  
Gauss apodization 0.018 sec  
FT size 4096 x 4096  
Total time 6 hr, 27 sec

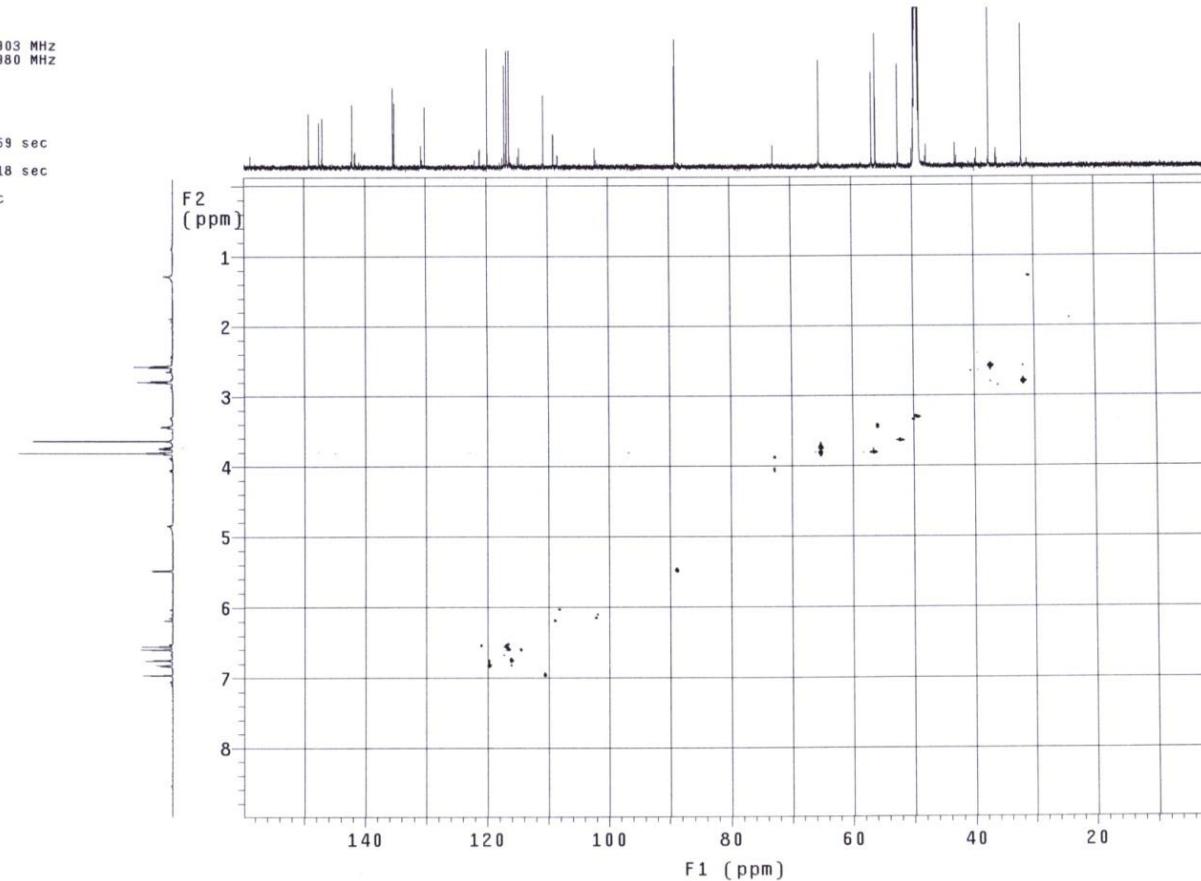


Figure S4: HMQC spectrum of compound 1 (DMSO-*d*<sub>6</sub>, 600 MHz).

TXE16-4

File: xp

Pulse Sequence: gHMBC

Solvent: cd3od

Temp. 25.0 C / 298.1 K

Operator: vnmri1

VNMRs-600 "ynnmr600"

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.128 sec

Width 6410.3 Hz

2D Width 30165.9 Hz

32 repetitions

512 increments

OBSERVE H1, 599.8582933 MHz

DATA PROCESSING

Sine bell 0.064 sec

F1 DATA PROCESSING

Sine bell 0.017 sec

FT size 4096 x 4096

Total time 6 hr, 12 min, 14 sec

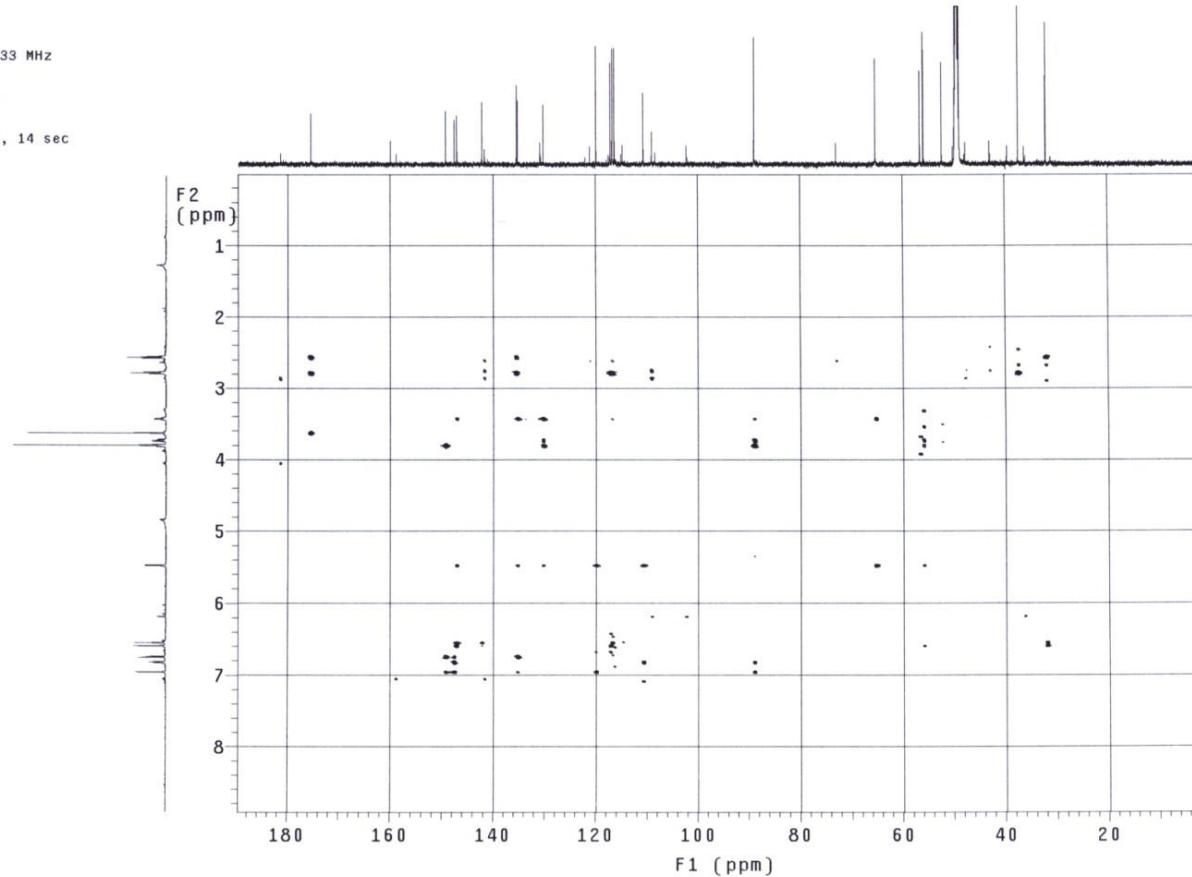


Figure S5: HMBC spectrum of compound 1 (DMSO-*d*<sub>6</sub>, 600 MHz).

TXE16-4  
File: xp  
Pulse Sequence: NOESY  
Solvent: cd3od  
Temp. 25.0 C / 298.1 K  
Operator: vnmr1  
VNMRs-600 "ynmr600"  
Relax. delay 1.000 sec  
Mixing 0.400 sec  
Acq. time 0.160 sec  
Width 6410.3 Hz  
2D Width 6410.3 Hz  
16 repetitions  
2 x 512 increments  
OBSERVE H1, 599.8582914 MHz  
DATA PROCESSING  
Gauss apodization 0.074 sec  
F1 DATA PROCESSING  
Gauss apodization 0.148 sec  
FT size 5192 x 8192  
Total time 7 hr, 45 min, 43 sec

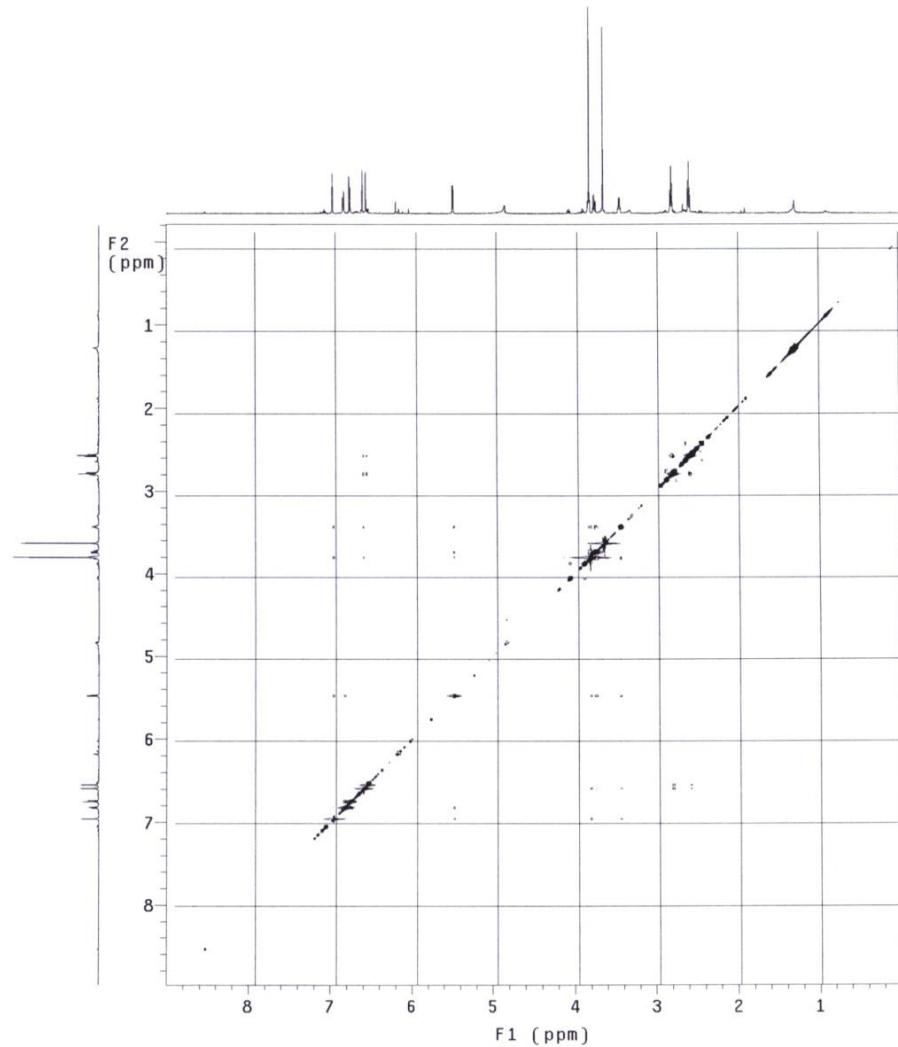


Figure S6: NOESY spectrum of compound 1 (DMSO-*d*<sub>6</sub>, 600 MHz).

File: 10221  
Sample: TXE-1

Date Run: 12-12-2013  
Ionization mode: EI+

Time Run: 11:21:59

Instrument: JEOL JMS600  
Inlet: Direct Probe

R.T.: 1:45.6

Scan: 139-163  
Base: m/z 344; 6.1%FS

TIC: 1084381

Selected Isotopes : $C_{0-50}H_{0-100}O_{0-10}$			Error Limit : 20 ppm	
<u>Measured Mass</u>	<u>% Base</u>	<u>Formula</u>	<u>Calculated Mass</u>	<u>Error</u>
374.1364	39.8%	$C_{27}H_{18}O_2$	374.1307	-15.0
		$C_{20}H_{22}O_7$	374.1365	0.4

Figure S7: HREIMS of compound 1.

TXE 17-3

File: xp

Pulse Sequence: s2pul

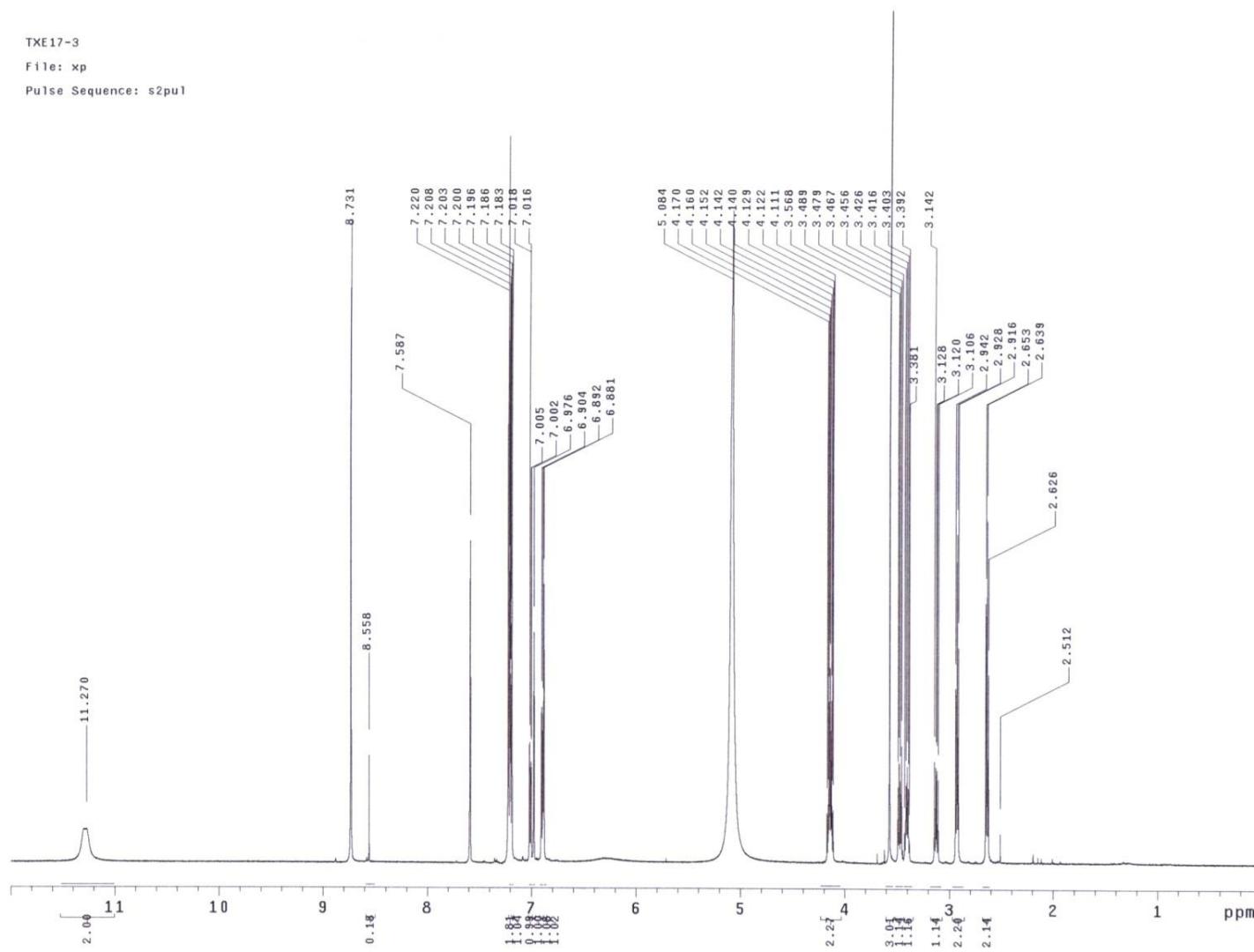
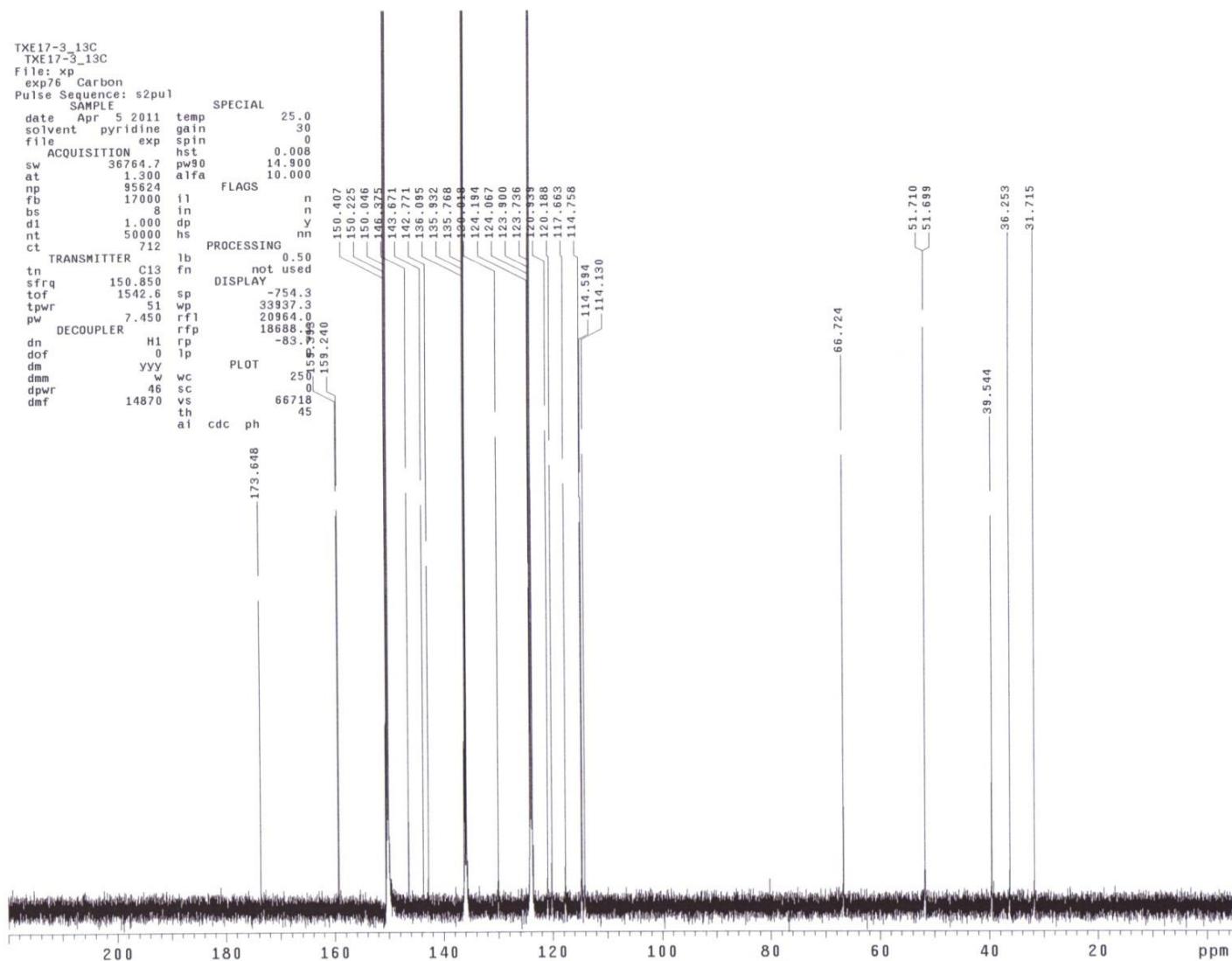


Figure S8:  $^1\text{H}$  NMR spectrum (pyridine- $d_5$ , 600 MHz) of compound 2.

```

TXE17-3_13C
TXE17-3_13C
File: xp
exp76 Carbon
Pulse Sequence: s2pul
  SAMPLE          SPECIAL
  date  Apr 5 2011  temp    25.0
  solvent  pyridine  gain    30
  file    exp      spin    0
  ACQUISITION  hst      0.008
  sw      36764.7  pw90   14.900
  at      1.300    alfa   10.000
  np      95624    FLAGS
  fb      17000    11     in     n
  bs      8        in     y
  d1      1.000    dp      nn
  nt      50000   hs      nn
  ct      712      PROCESSING
  TRANSMITTER 1b      0.50
  tn      C13    fn      not used
  sfrq   150.850  DISPLAY
  tof    1542.6   sp      -754.3
  tpwr   51      wp      33937.3
  pw     7.450    rf1     20964.0
  DECOUPLER rfp     18688.4
  dn      H1      rp      -83.448
  dof     0      lp
  dm      yyy    PLOT
  dmm    250      wc      0
  dpwr   46      sc      0
  dmf    14870   vs      66718
  th      45
  a1      cdc    ph

```



TXE17-3

File: xp

Pulse Sequence: gCOSY

Solvent: pyridine

Temp. 25.0 C / 298.1 K

Operator: vnmr1

VNMRS-600 "ynnmr600"

Relax. delay 1.000 sec

Acc. time 0.139 sec

Width 7352.8 Hz

2D Width 7352.8 Hz

80 repetitions

256 increments

OBSERVE H1 599.8558984 MHz

DATA PROCESSING

Sine bell 0.070 sec

F1 DATA PROCESSING

Sine bell 0.070 sec

FT size 8192 x 8192

Total time 40 min, 22 sec

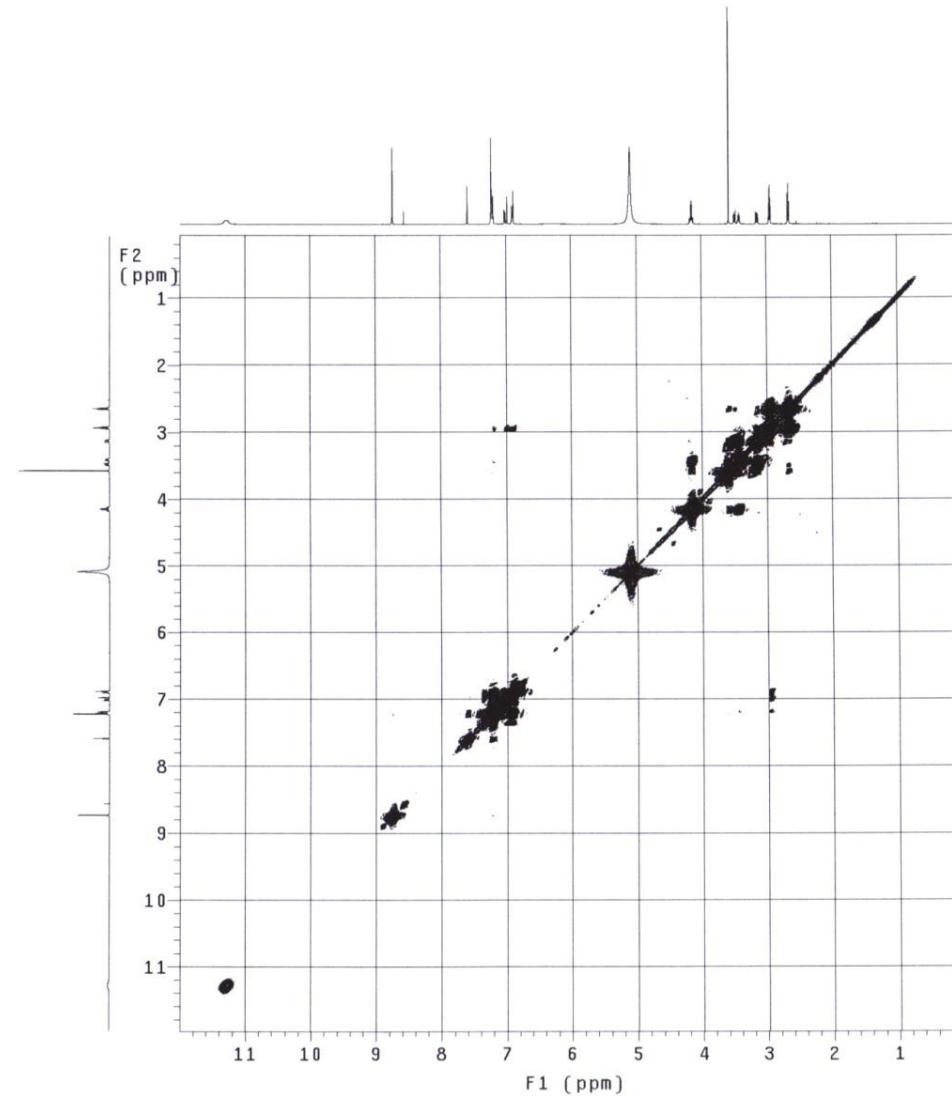


Figure S10:  $^1\text{H}$ , $^1\text{H}$  COSY spectrum (pyridine- $d_5$ , 600 MHz) of compound 2.

TXE17-3\_(2)

File: xp

Pulse Sequence: gHMQC

Solvent: pyridine

Temp. 25.0 C / 298.1 K

Operator: vnmr1

VNMRs-600 "vnmr600"

Relax. delay 1.000 sec

Acq. time 0.128 sec

Width 7440.5 Hz

2D Width 30165.9 Hz

32 repetitions

2 x 512 increments

OBSERVE H1, 599.8550044 MHz

DECOUPLE C13, 150.8474194 MHz

Power 37 dB

on during acquisition

off during delay

W40\_swpfg modulated

DATA PROCESSING

Gauss apodization 0.059 sec

F1 DATA PROCESSING

Gauss apodization 0.024 sec

FT size 8192 x 8192

Total time 10 hr, 43 min, 55 sec

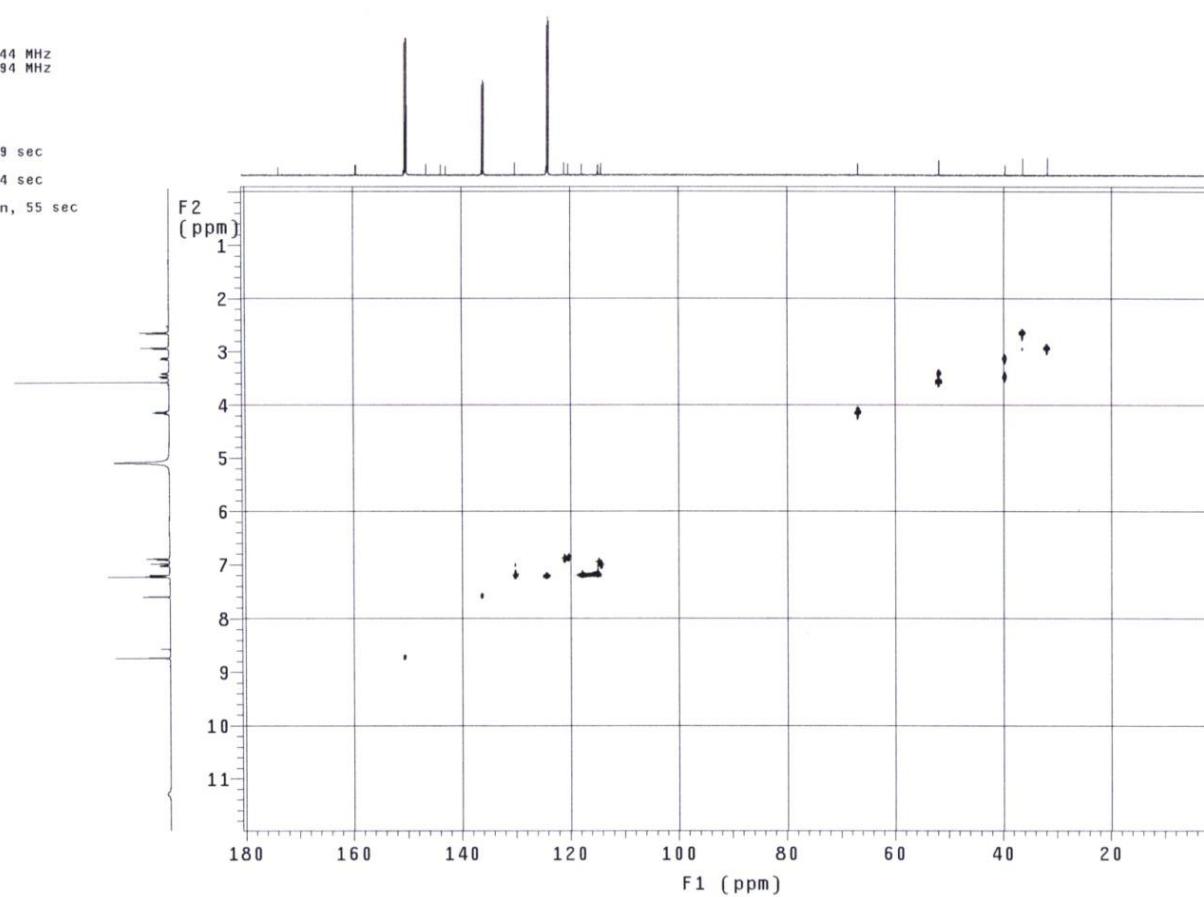


Figure S11: HMQC spectrum (pyridine- $d_5$ , 600 MHz) of compound 2.



File: 10220  
Sample: TXE-2

Date Run: 12-12-2013  
Ionization mode: EI+

Time Run: 09:56:10

Instrument: JEOL JMS600  
Inlet: Direct Probe

R.T.: 2:47.3

Scan: 140  
Base: m/z 330; 8.4%FS

TIC: 684936

Selected Isotopes : $C_{0-50}H_{0-100}O_{0-10}$			Error Limit : 20 ppm	
<u>Measured Mass</u>	<u>% Base</u>	<u>Formula</u>	<u>Calculated Mass</u>	<u>Error</u>
330.1469	100.0%	$C_{26}H_{18}$	330.1409	-18.0
		$C_{19}H_{22}O_5$	330.1467	-0.6
		$C_{12}H_{26}O_{10}$	330.1526	17.0

Figure S13: HREIMS of compound 2.

TXE3233-10-Y-1

File: xp

Pulse Sequence: s2pul

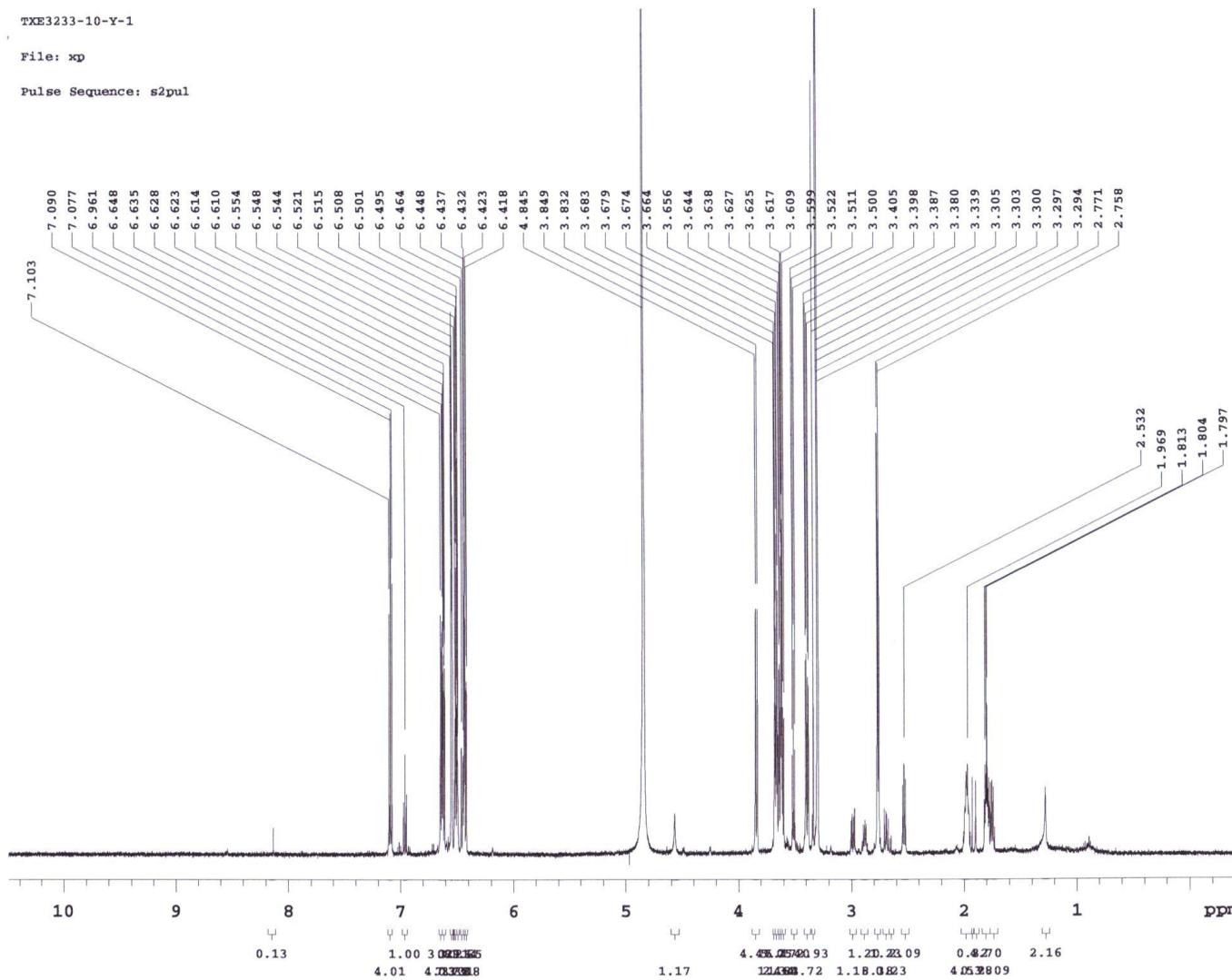


Figure S14:  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 600 MHz) of compound 3.

TXE3233-10-Y-1

File: xp

Pulse Sequence: s2pul

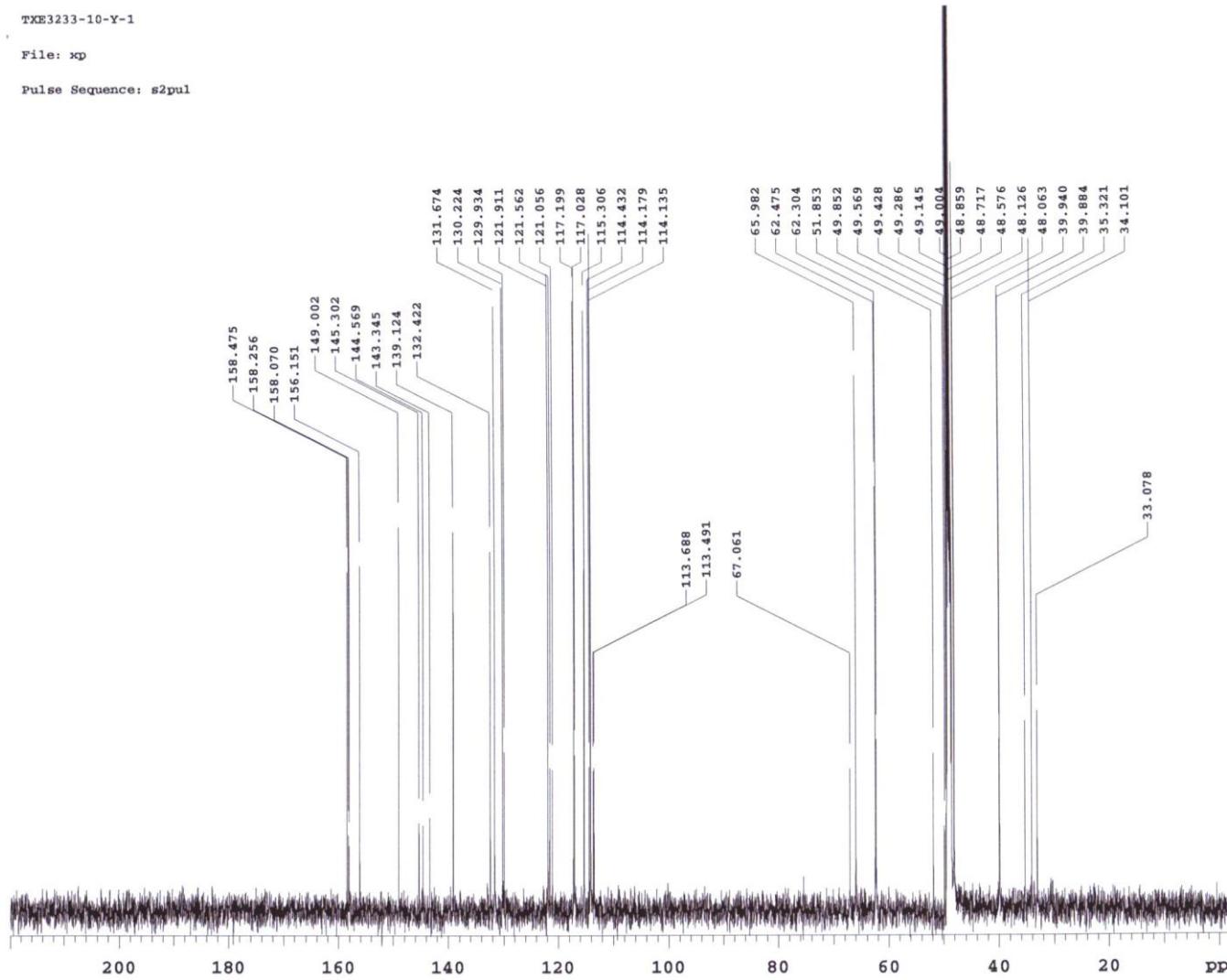


Figure S15:  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 600 MHz) of compound 3.

TXE3233-10-Y-1

File: xp

Pulse Sequence: gCOSY

Solvent: cd3od

Temp. 25.0 C / 298.1 K

Operator: vnmri

VNMRS-600 "ynmnmr600"

Relax. delay 1.000 sec

Acq. time 0.203 sec

Width 5040.3 Hz

2D Width 5040.3 Hz

8 repetitions

512 increments

OBSERVE H1, 599.8582852 MHz

DATA PROCESSING

Sine bell 0.102 sec

F1 DATA PROCESSING

Sine bell 0.203 sec

FT size 8192 x 8192

Total time 1 hr, 36 min, 34 sec

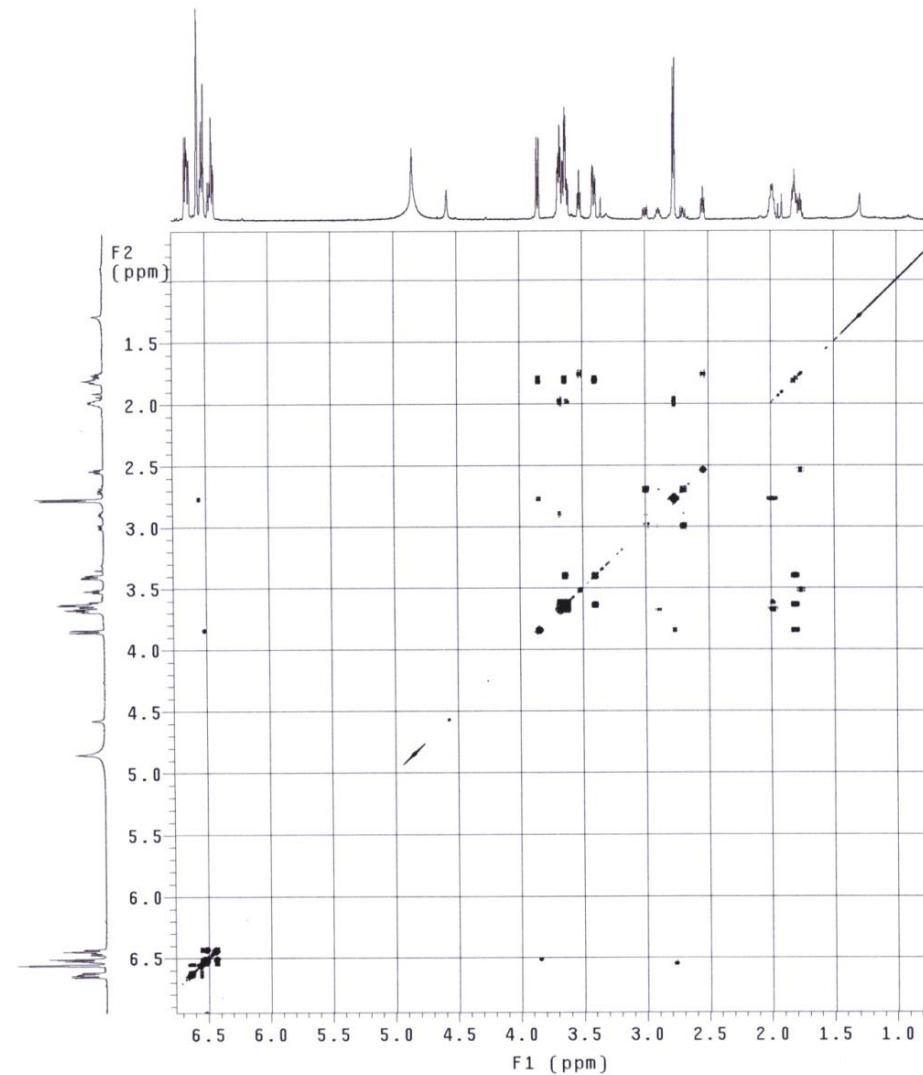


Figure S16:  $^1\text{H}$ , $^1\text{H}$  COSY spectrum (CD<sub>3</sub>OD, 600 MHz) of compound 3.

TXE3233-10-Y-1

File: xp

Pulse Sequence: gHMQC

Solvent: cd3od

Temp. 25.0 C / 298.1 K

Operator: vnmri1

VNMR-600 "ynnmr600"

Relax. delay 1.000 sec

Acq. time 0.128 sec

Width 5319.1 Hz

2D Width 25641.0 Hz

32 repetitions

2 x 264 increments

OBSERVE H1, 593.8582843 MHz

DECOPLE Q13, 150.8457980 MHz

Power 36

on during acquisition

off during delay

W40\_swpfg modulated

DATA PROCESSING

Gauss apodization 0.059 sec

F1 DATA PROCESSING

Gauss apodization 0.009 sec

FT size 2048 x 4096

Total time 5 hr, 21 min, 18 sec

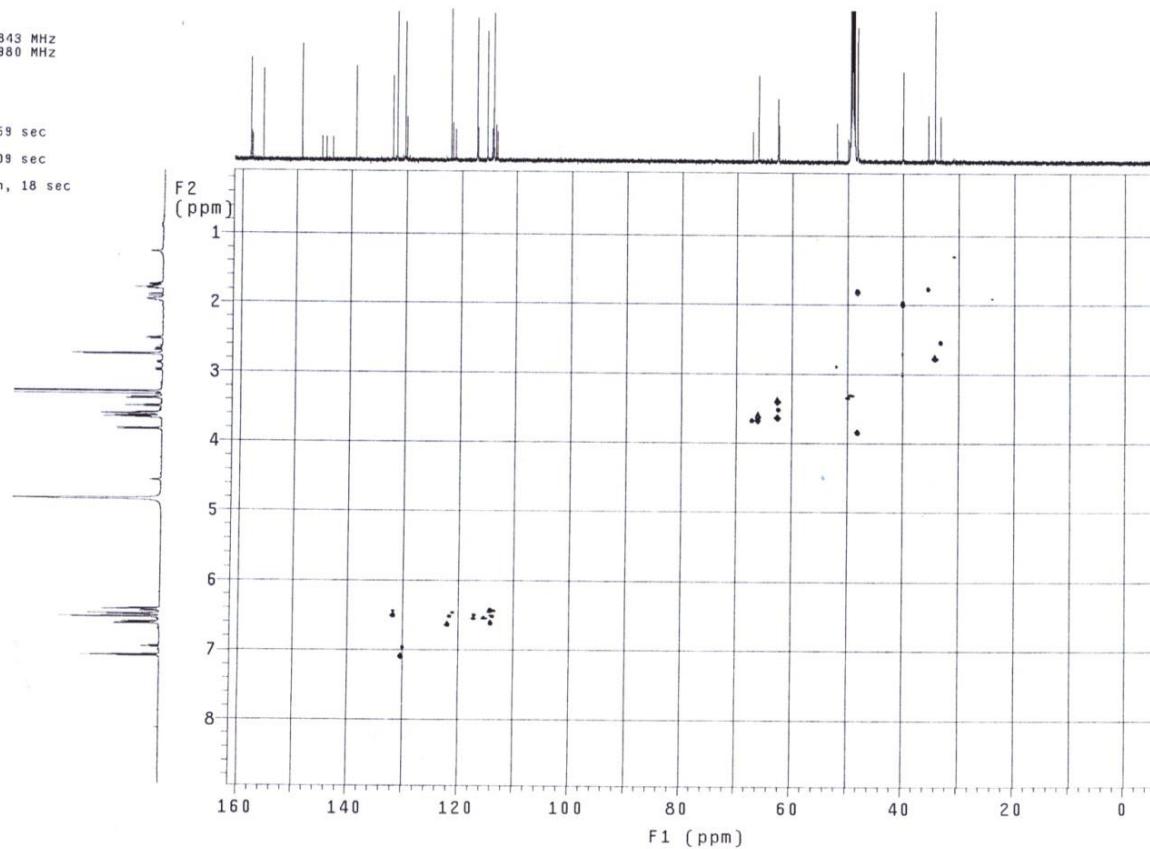


Figure S17: HMQC spectrum (CD<sub>3</sub>OD, 600 MHz) of compound 3.

TXE3233-10-Y-1

File: xp

Pulse Sequence: gHMBC

Solvent: cd3od  
Temp. 25.0 C / 298.1 K  
Operator: vnmri  
VNMRs-600 "vnmmr600"

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.128 sec

Width 5319.1 Hz

2D Width 36199.1 Hz

32 repetitions

512 increments

OBSERVE H1, 599.8582872 MHz

DATA PROCESSING

Sine bell 0.064 sec

F1 DATA PROCESSING

Sine bell 0.014 sec

FT size 2048 x 4096

Total time 5 hr, 34 min, 4 sec

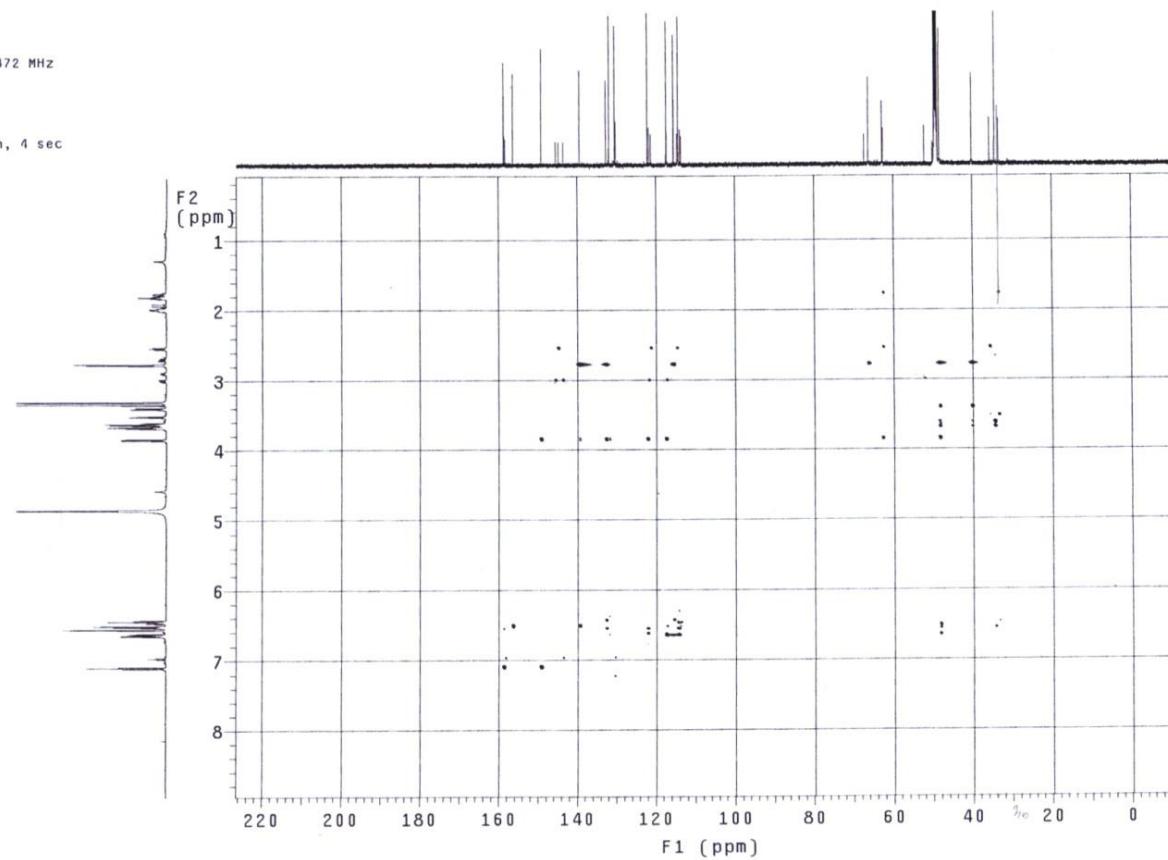


Figure S18: HMBC spectrum (CD<sub>3</sub>OD, 600 MHz) of compound 3.

TXE3233-10-Y-1

File: xp

Pulse Sequence: NOESY

Solvent: CD<sub>3</sub>OD  
Temp. 25.0 C / 298.1 K  
operator: vnmri  
VNMRs-600 "ynnmr600"

Relax. delay 1.000 sec  
mixing 0.700 sec  
Acq. time 0.161 sec  
Width 6345.2 Hz  
2D Width 6345.2 Hz  
16 repetitions  
2 x 512 increments  
OBSERVE H1, 599.8582877 MHz  
DATA PROCESSING  
Gauss apodization 0.075 sec  
F1 DATA PROCESSING 0.074 sec  
Gauss apodization 0.074 sec  
FT size 4096 x 4096  
Total time 8 hr, 30 min, 23 sec

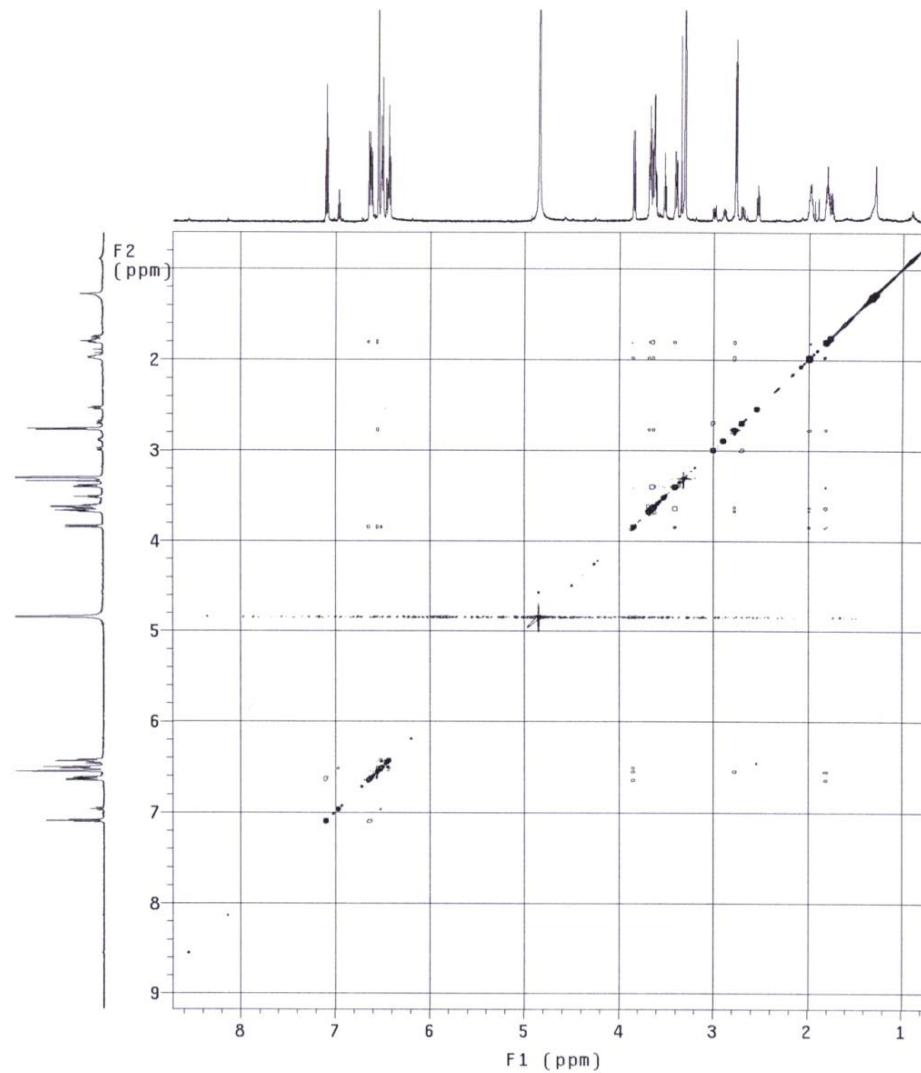


Figure S19: NOESY spectrum (CD<sub>3</sub>OD, 600 MHz) of compound 3.

[ Elemental Composition ]

Data : EI636

Date : 01-Apr-2014 20:03

Page: 1

Sample: TXE 3

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 0.31 min

Scan#: (14,16)

Elements : C 40/0, H 49/0, O 10/0

Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5

Unsaturation (U.S.) : -0.5 - 10.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
300.1360	100.0	-0.7 / -0.2	9.0	C 18 H 20 O 4

[ Theoretical Ion Distribution ]

Molecular Formula : C18 H20 O4

Page: 1

(m/z 300.1362, MW 300.3544, U.S. 9.0)

Base Peak : 300.1362, Averaged MW : 300.3524(a), 300.3532(w)

m/z	INT.
300.1362	100.0000 *****
301.1395	20.1726 *****
302.1422	2.7252 **
303.1448	0.2766
304.1474	0.0226
305.1500	0.0016

Figure S20: HREIMS of compound 3.