# New Biscembranoids Sardigitolides A–D and Known Cembranoid-Related Compounds from *Sarcophyton digitatum*: Isolation, Structure Elucidation, and Bioactivities

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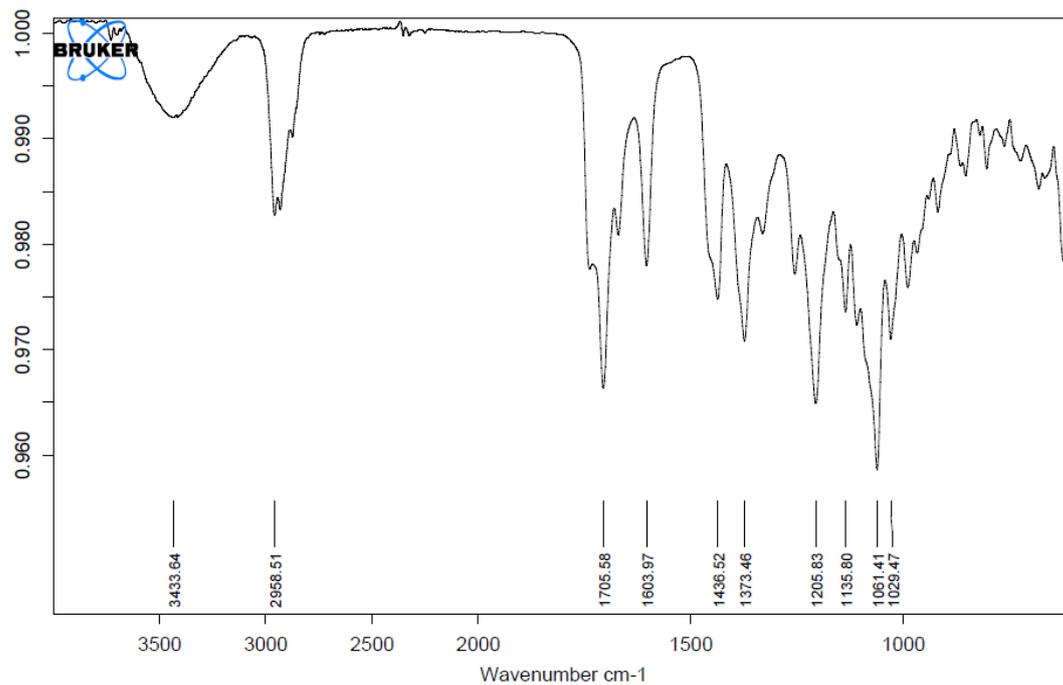
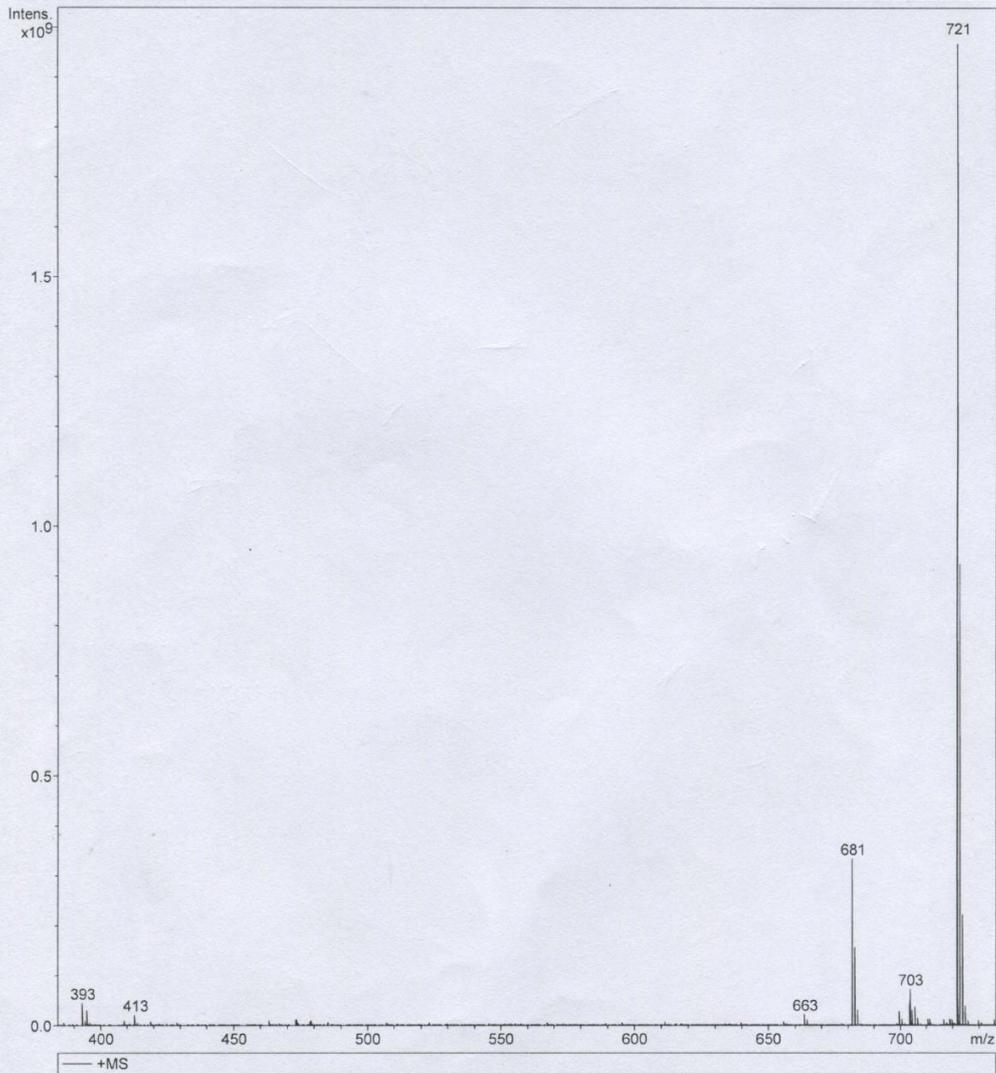Figure S1: IR spectrum of **1**

# FT-MS

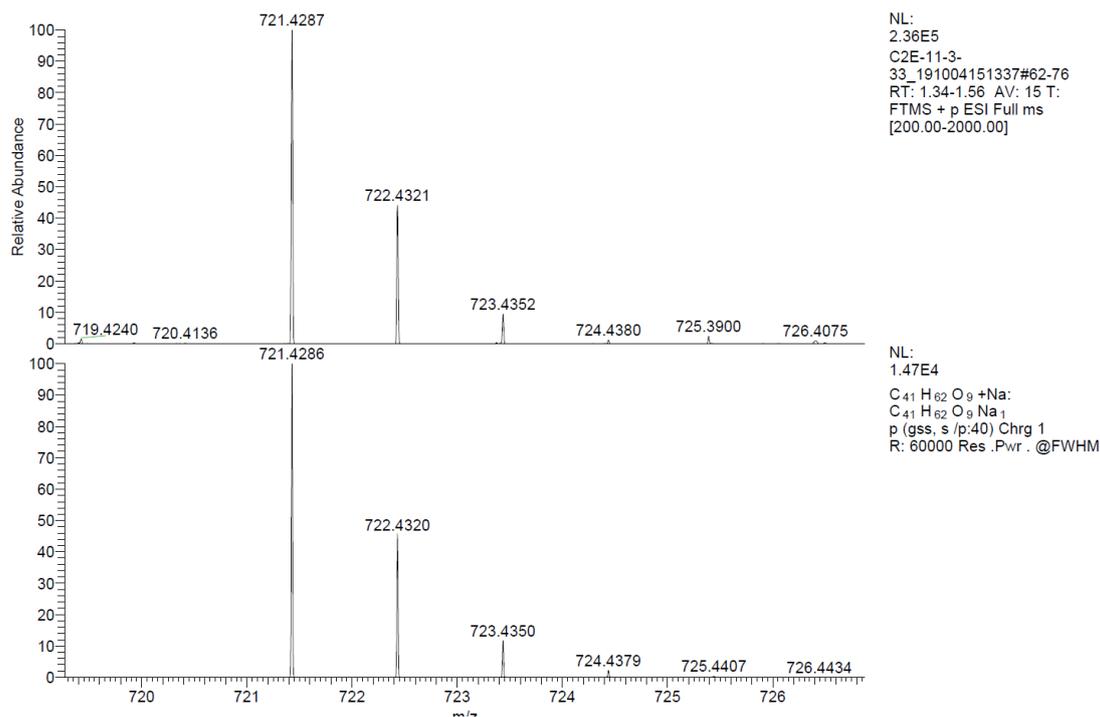Figure S2: ESIMS spectrum of **1**
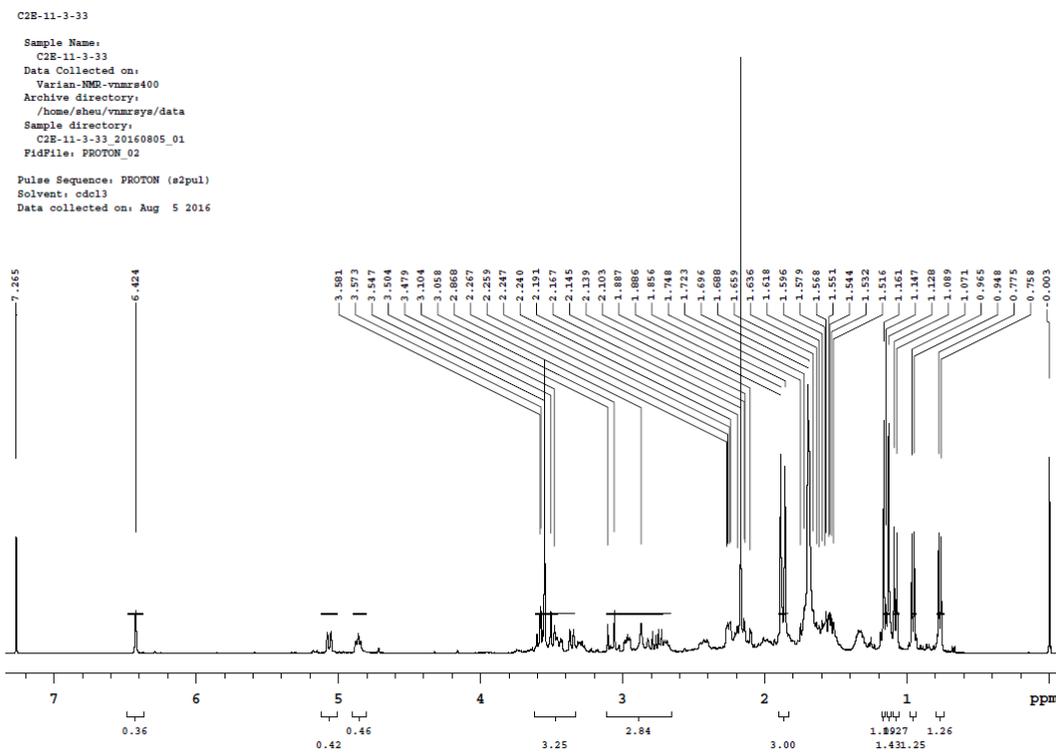
Figure S3: HRESIMS spectrum of **1**



Figure S4: $^1$H NMR spectrum of **1** in CDCl$_3$ at 400 MHz

C2E-11-3-33

Sample Name:
  C2E-11-3-33
Data Collected on:
  Varian-NMR-vnmrs400
Archive directory:
  /home/sheu/vnmrsys/data
Sample directory:
  C2E-11-3-33_20160805_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
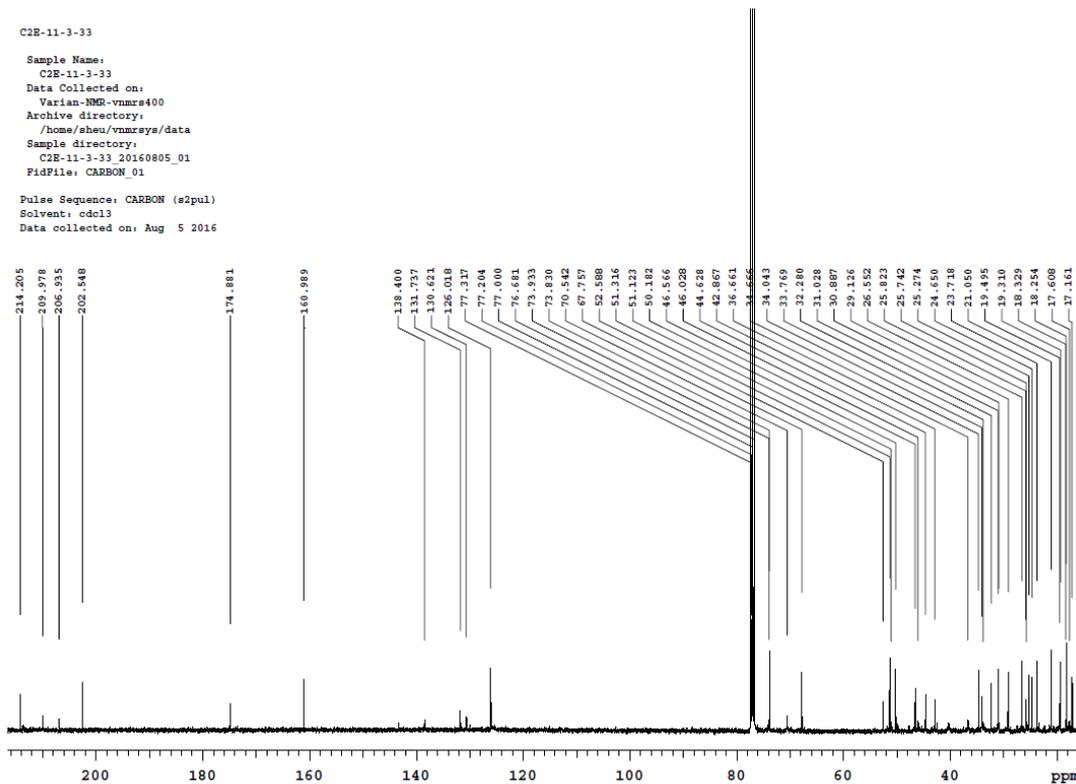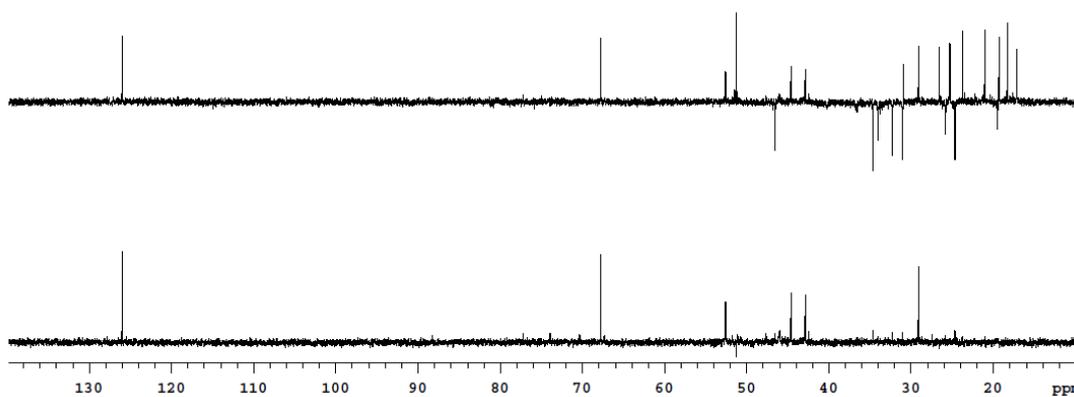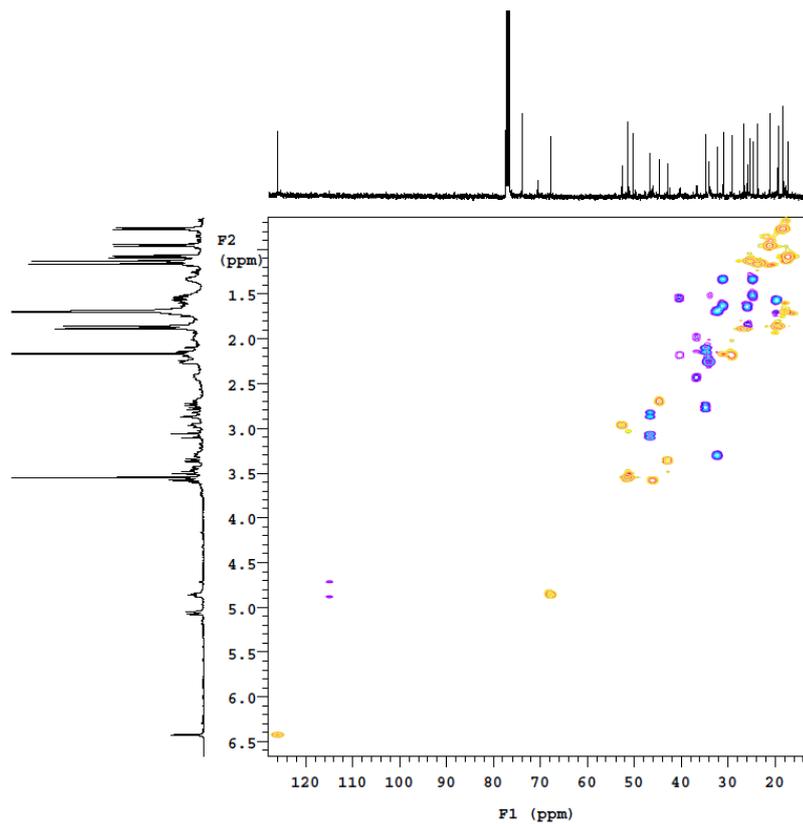Solvent: cdcl3
Data collected on: Aug  5 2016

Figure S5: $^{13}$C NMR spectrum of **1** in CDCl$_3$ at 100 MHz

C2E-11-3-33

Sample Name:
  C2E-11-3-33
Data Collected on:
  Varian-NMR-vnmrs400
Archive directory:
  /home/sheu/vnmrsys/data
Sample directory:
  C2E-11-3-33_20160805_01
FidFile: DEPT_01

Pulse Sequence: DEPT
Solvent: cdcl3
Data collected on: Aug  6 2016

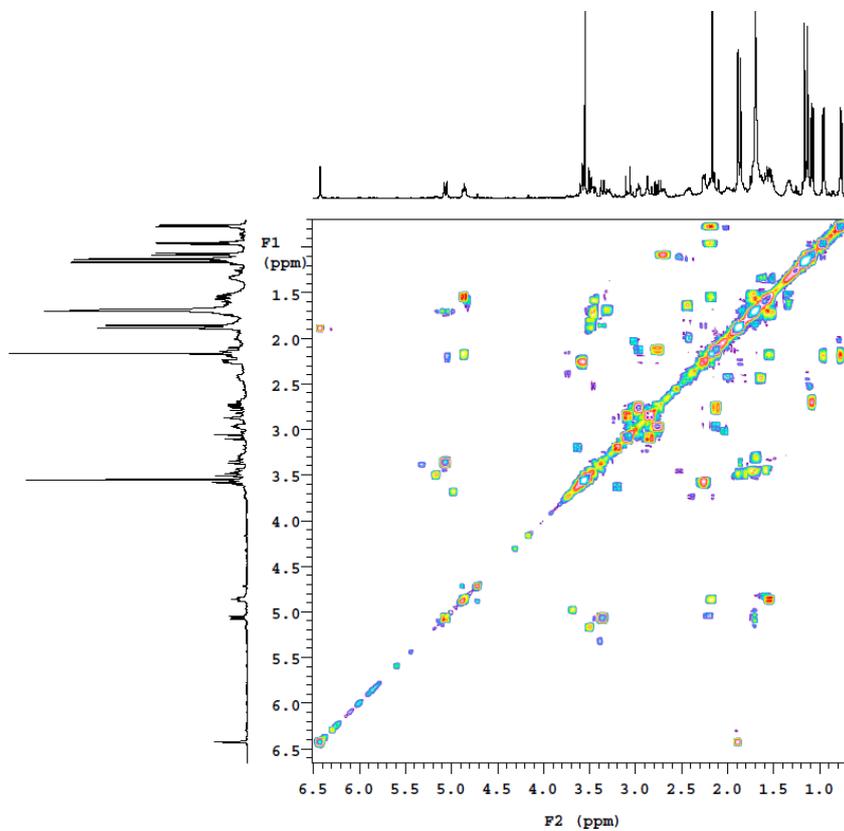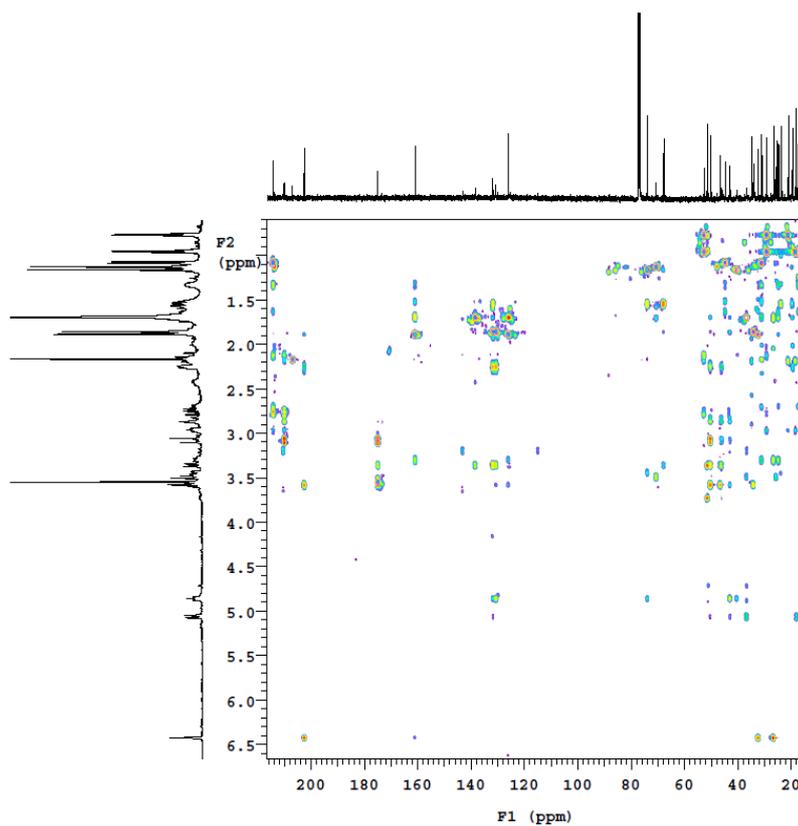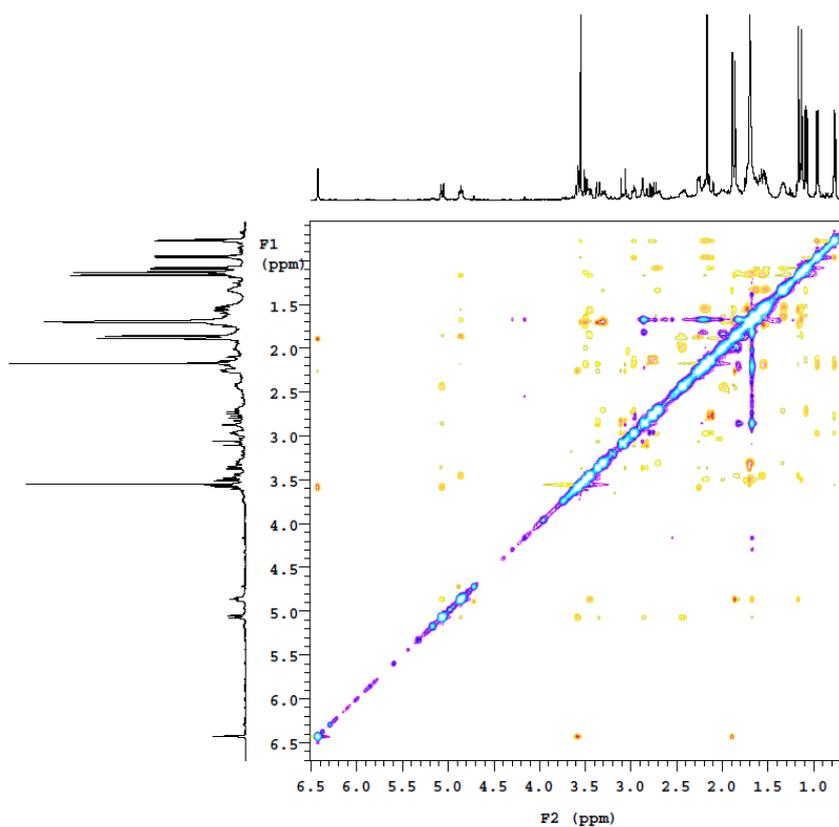Figure S6: DEPT spectrum of **1**

C2E-11-3-33

Sample Name:
   C2E-11-3-33
Data Collected on:
   Varian-NMR-vnmrs400
Archive directory:
   /home/sheu/vnmrsys/data
Sample directory:
   C2E-11-3-33_20160805_01
FidFile: HSQCAD_01

Pulse Sequence: HSQCAD
Solvent: cdcl3
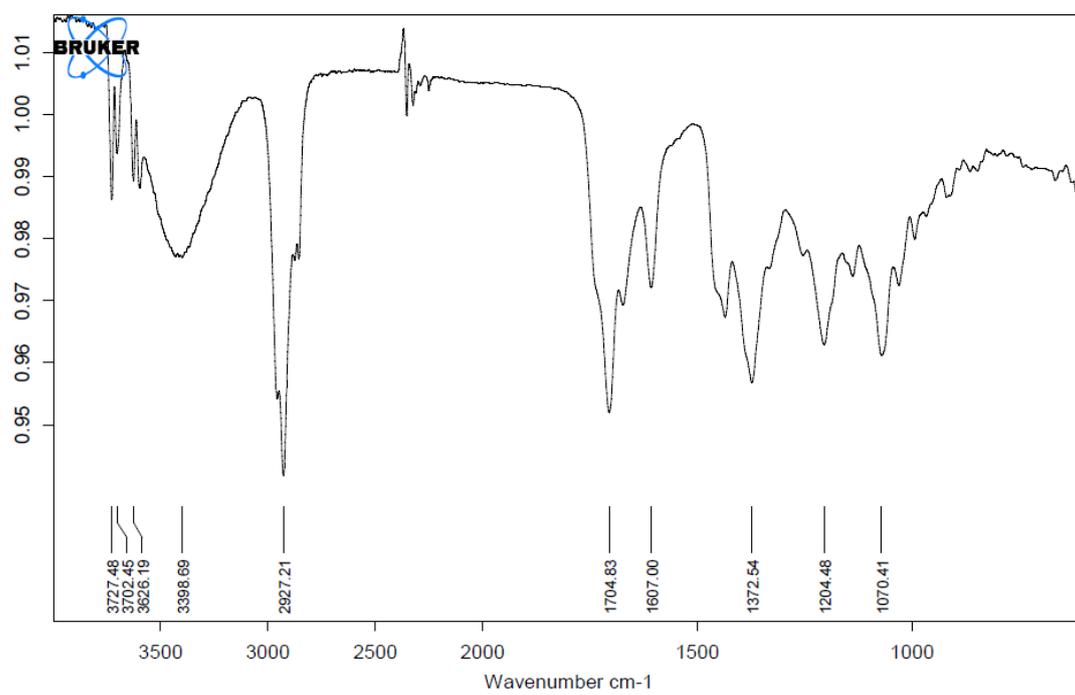Data collected on: Aug  6 2016

Figure S7: HSQC spectrum of **1**

C2E-11-3-33

Sample Name:
   C2E-11-3-33
Data Collected on:
   Varian-NMR-vnmrs400
Archive directory:
   /home/sheu/vnmrsys/data
Sample directory:
   C2E-11-3-33_20160805_01
FidFile: gCOSY_01

Pulse Sequence: gCOSY
Solvent: cdcl3
Data collected on: Aug  6 2016

Figure S8: COSY spectrum of **1**

Figure S9: HMBC spectrum of **1**

Figure S10: NOESY spectrum of **1**
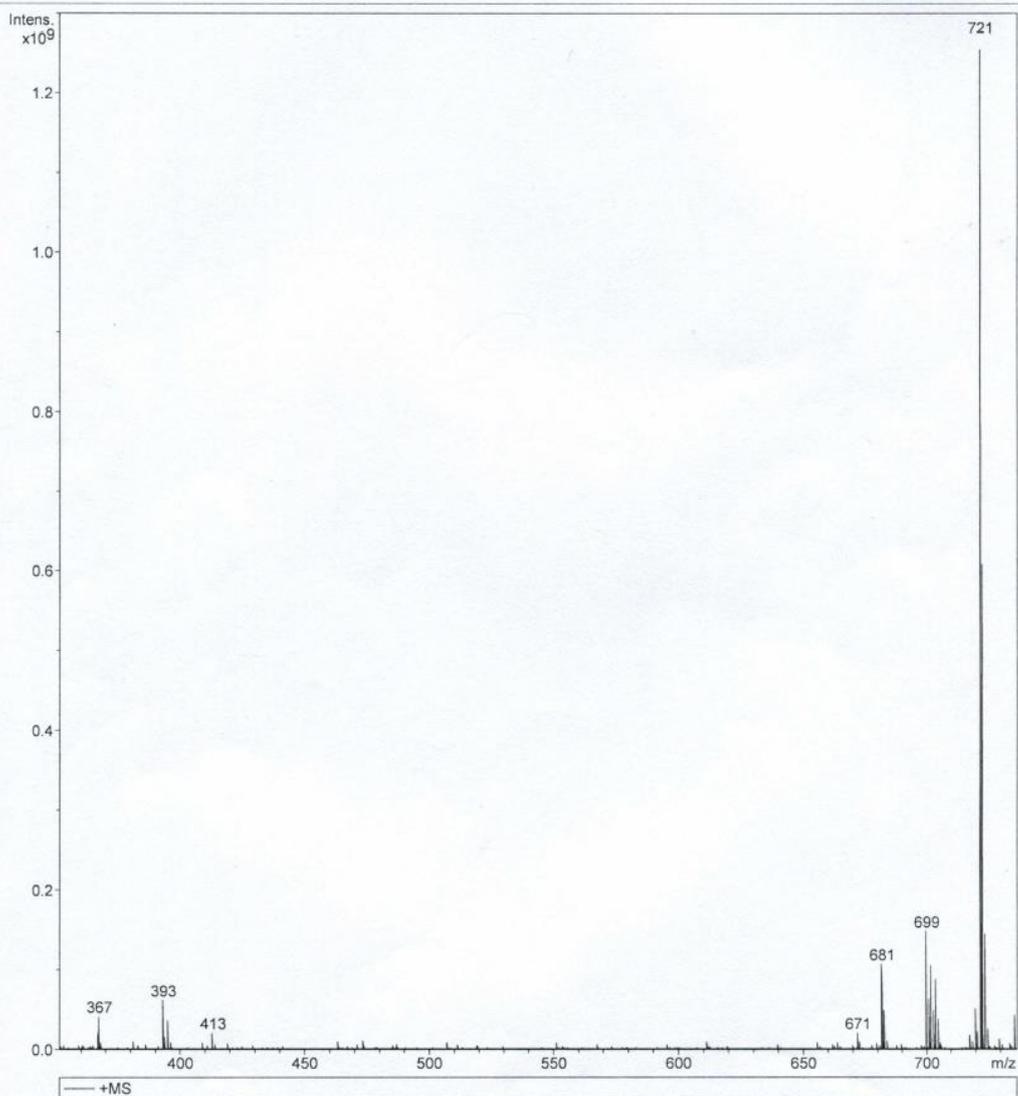
Figure S11: IR spectrum of **2**

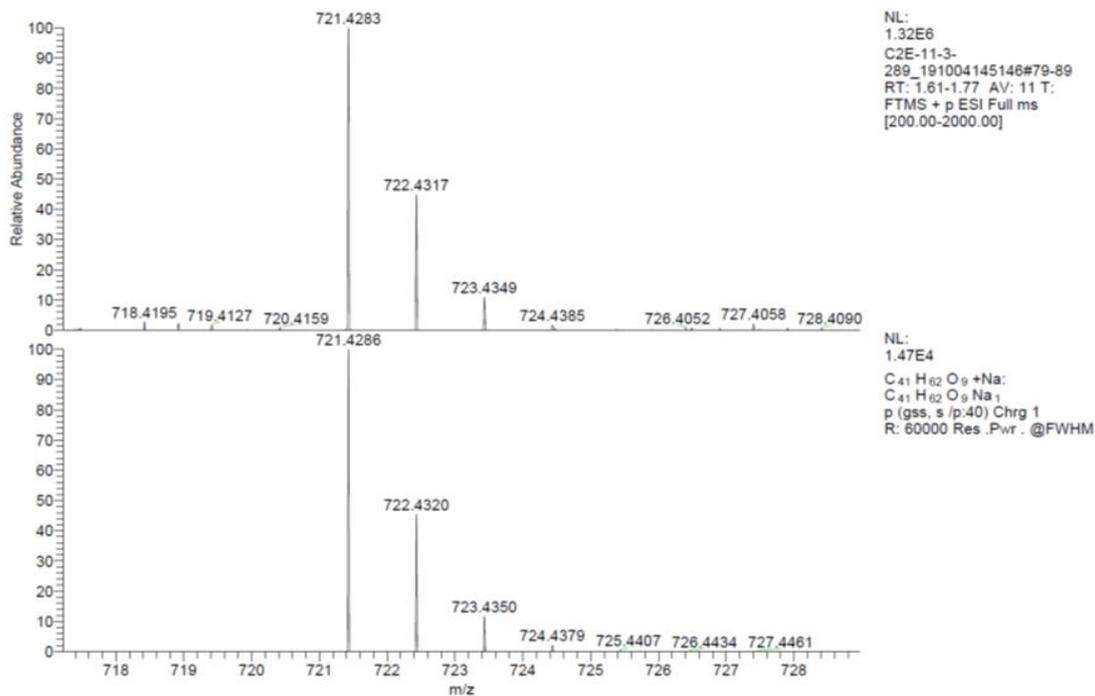Figure 12: ESIMS spectrum of **2**

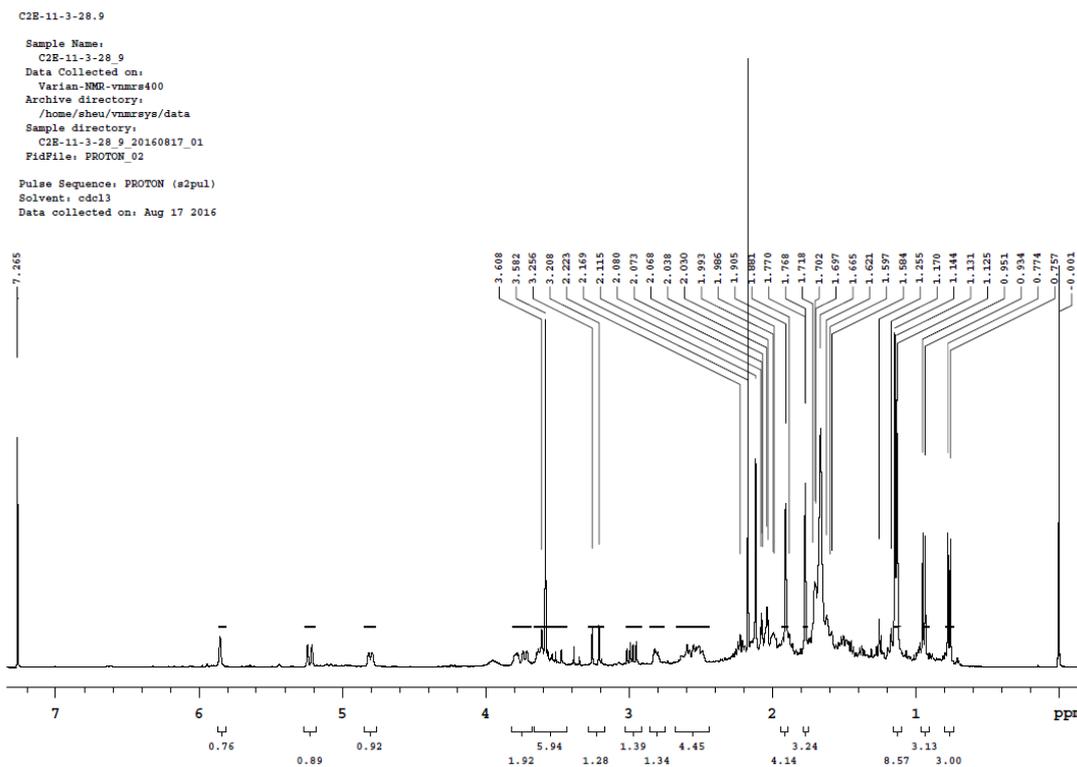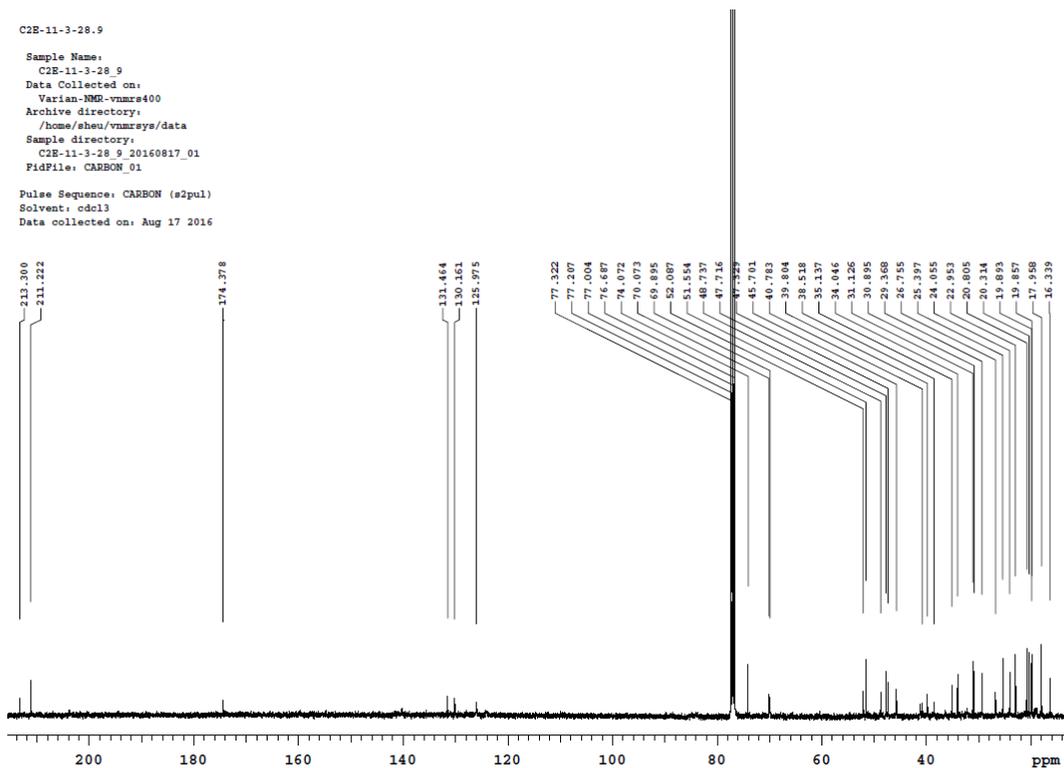Figure S13: HRESIMS spectrum of **2**
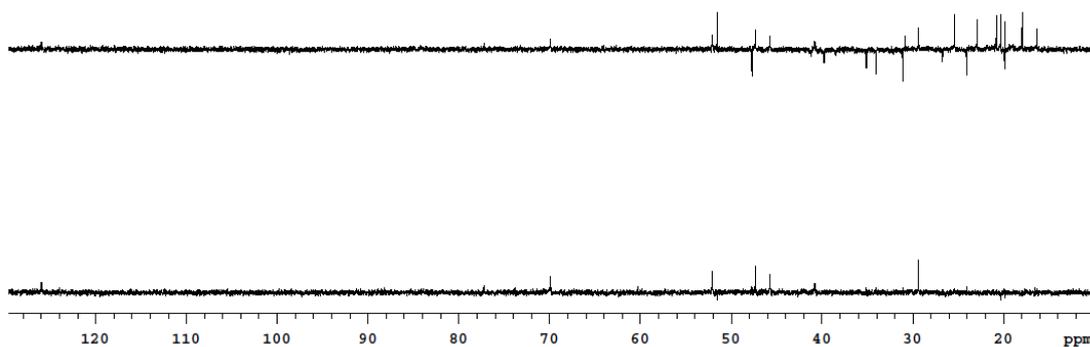


Figure S14: $^{1}$H NMR spectrum of **2** in CDCl$_3$ at 400 MHz

C2E-11-3-28.9

Sample Name:
  C2E-11-3-28_9
Data Collected on:
  Varian-NMR-vnmrs400
Archive directory:
  /home/sheu/vnmrsys/data
Sample directory:
  C2E-11-3-28_9_20160817_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
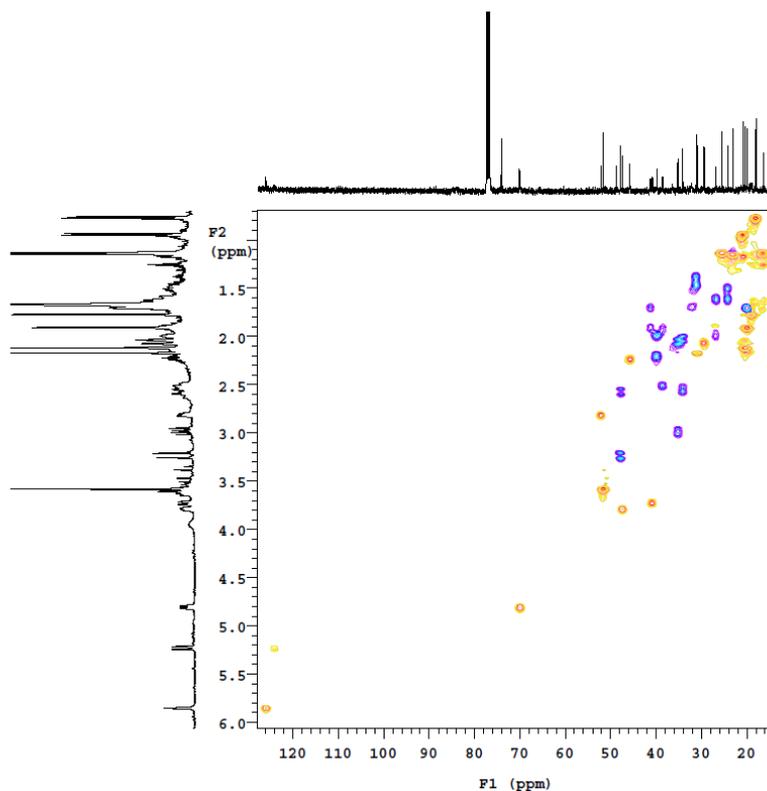Solvent: cdcl3
Data collected on: Aug 17 2016

Figure S15: $^{13}$C NMR spectrum of **2** in CDCl$_3$ at 100 MHz

C2E-11-3-28.9

Sample Name:
  C2E-11-3-28_9
Data Collected on:
  Varian-NMR-vnmrs400
Archive directory:
  /home/sheu/vnmrsys/data
Sample directory:
  C2E-11-3-28_9_20160817_01
FidFile: DEPT_01

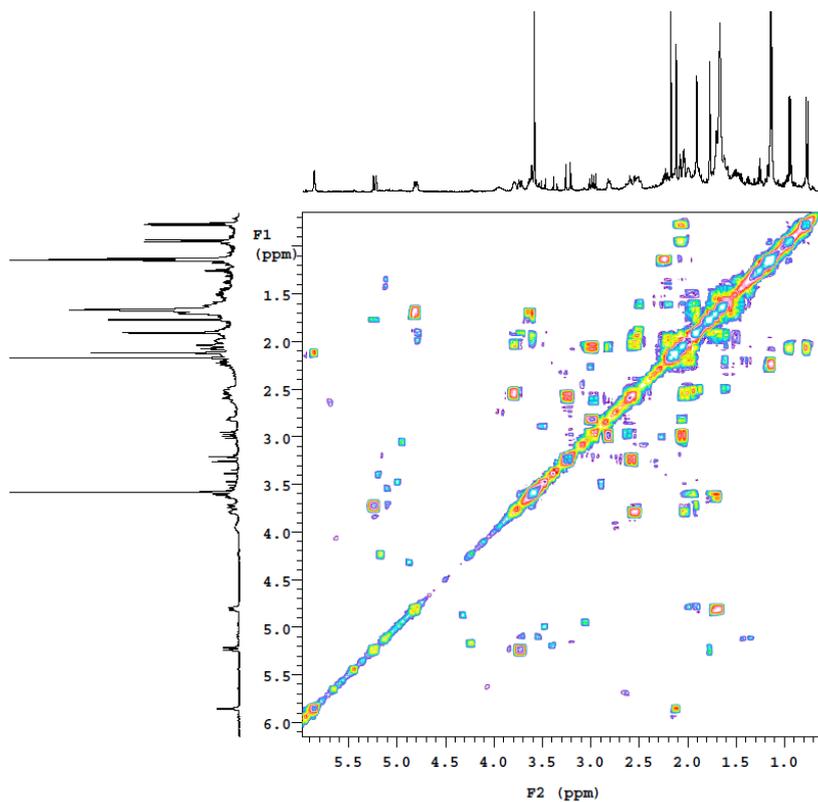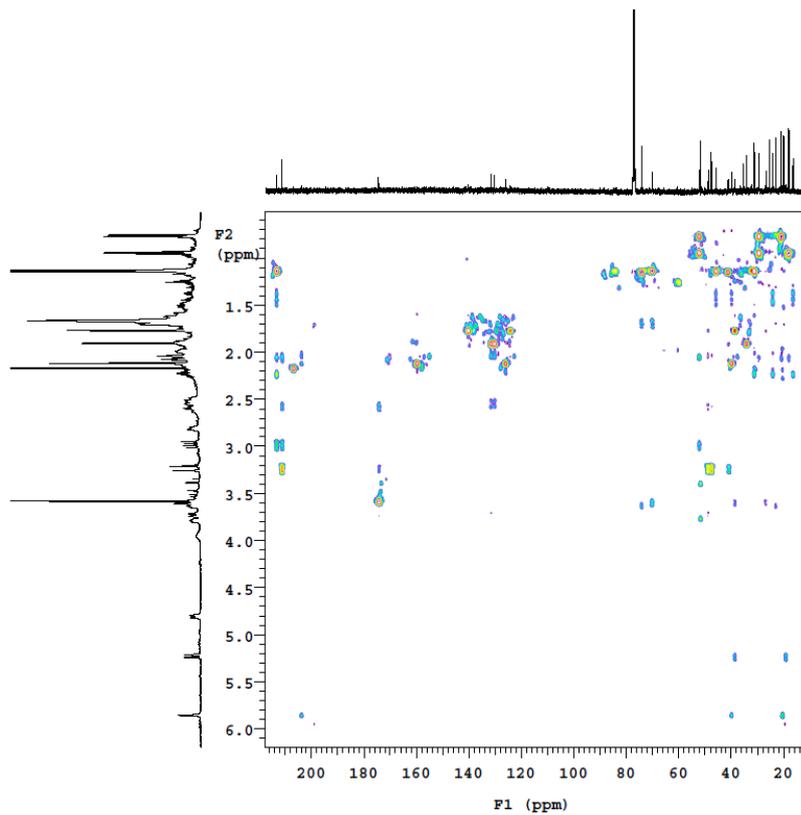Pulse Sequence: DEPT
Solvent: cdcl3
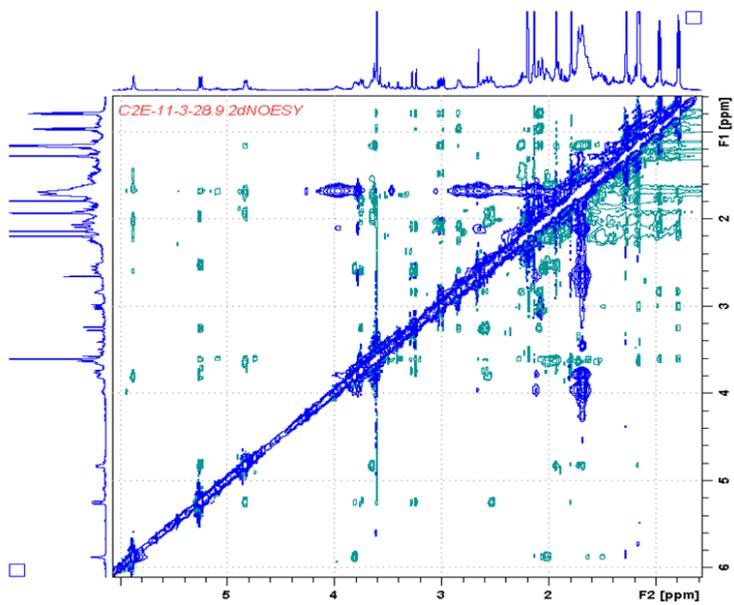Data collected on: Aug 18 2016

Figure S16: DEPT spectrum of **2**

Figure S17: HSQC spectrum of **2**

Figure S18: COSY spectrum of **2**

Figure S19: HMBC spectrum of **2**



Figure S20: NOESY spectrum of **2**
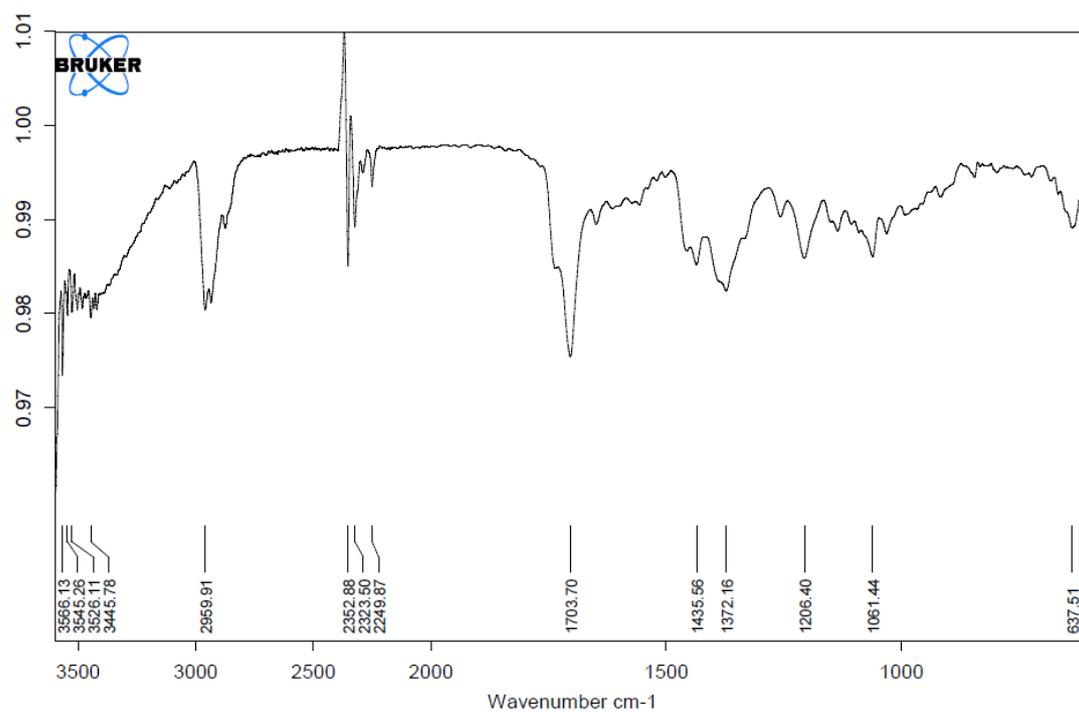
Figure S21: IR spectrum of **3**

**Analysis Info**

| | | |
|---|---|---|
| Analysis Name | D:\Data\a1\C2E11332_000004.d | 8/23/2016 3:46:53 PM |
| Method | broadband first signal | |
| Sample Name | C2E-11-3-32 | Instrument: FT-MS solariX |
| Comment | ESI Positive | |
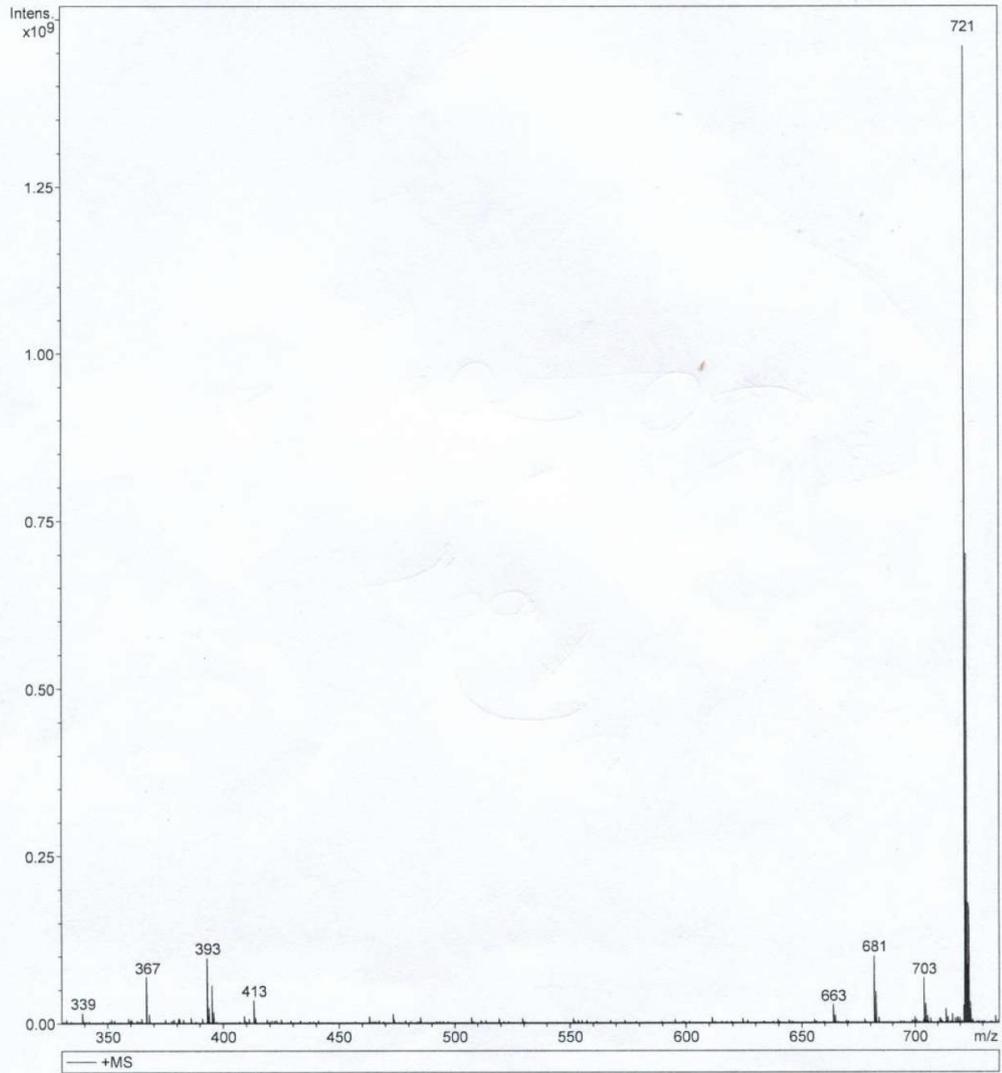


Figure 22: ESIMS spectrum of **3**
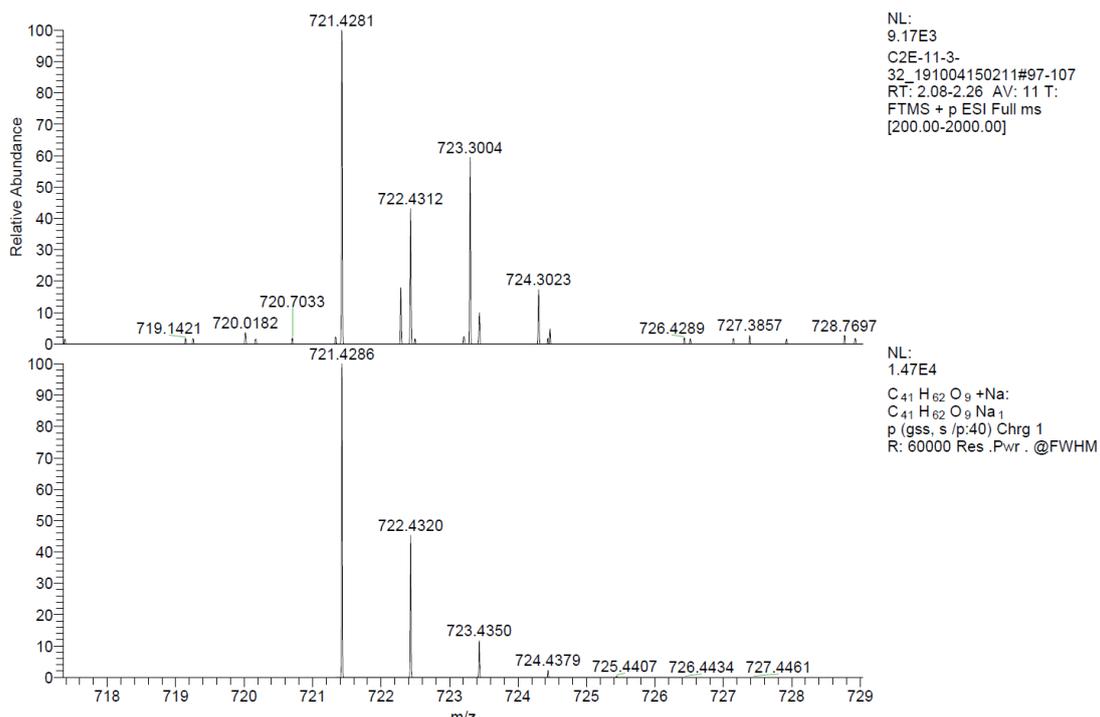
Figure S23: HRESIMS spectrum of **3**

C2E-11-3-32

Sample Name:
C2E-11-3-32
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
C2E-11-3-32_20160810_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 10 2016
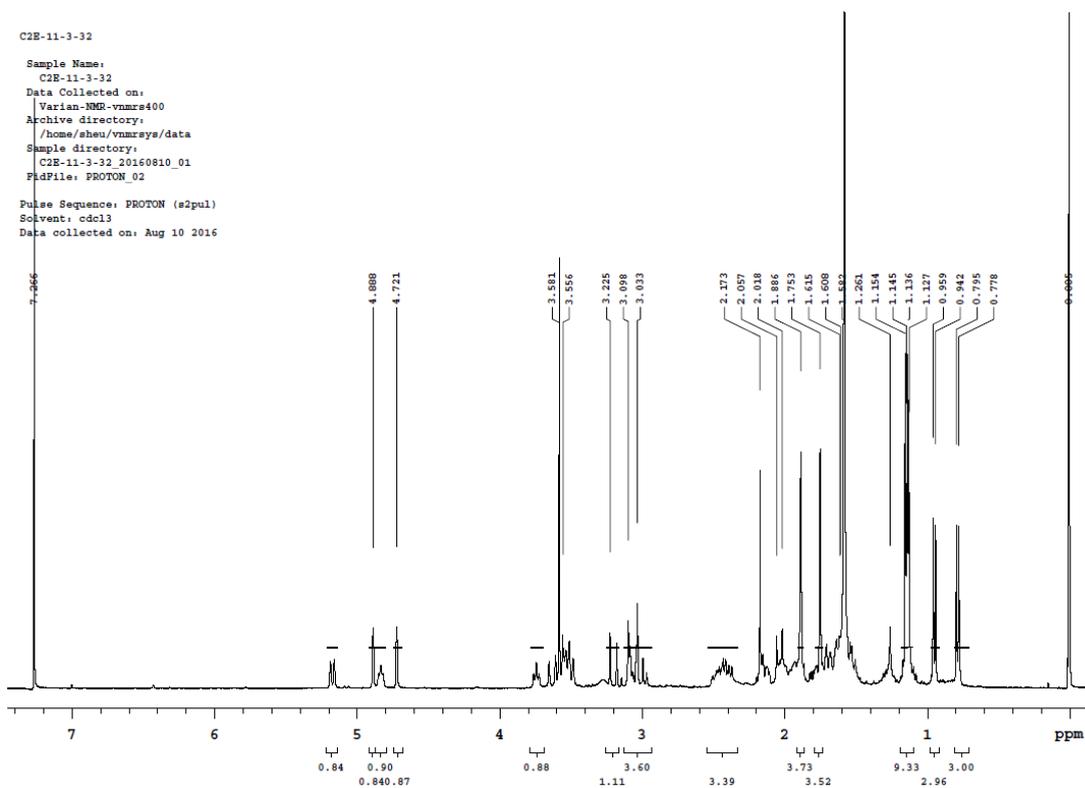
Figure S24: $^1$H NMR spectrum of **3** in CDCl$_3$ at 400 MHz

C2E-11-3-32

  Sample Name:
    C2E-11-3-32
  Data Collected on:
    Varian-NMR-vnmrs400
  Archive directory:
    /home/sheu/vnmrsys/data
  Sample directory:
    C2E-11-3-32_20160810_01
  FidFile: CARBON_01

  Pulse Sequence: CARBON (s2pul)
  Solvent: cdcl3
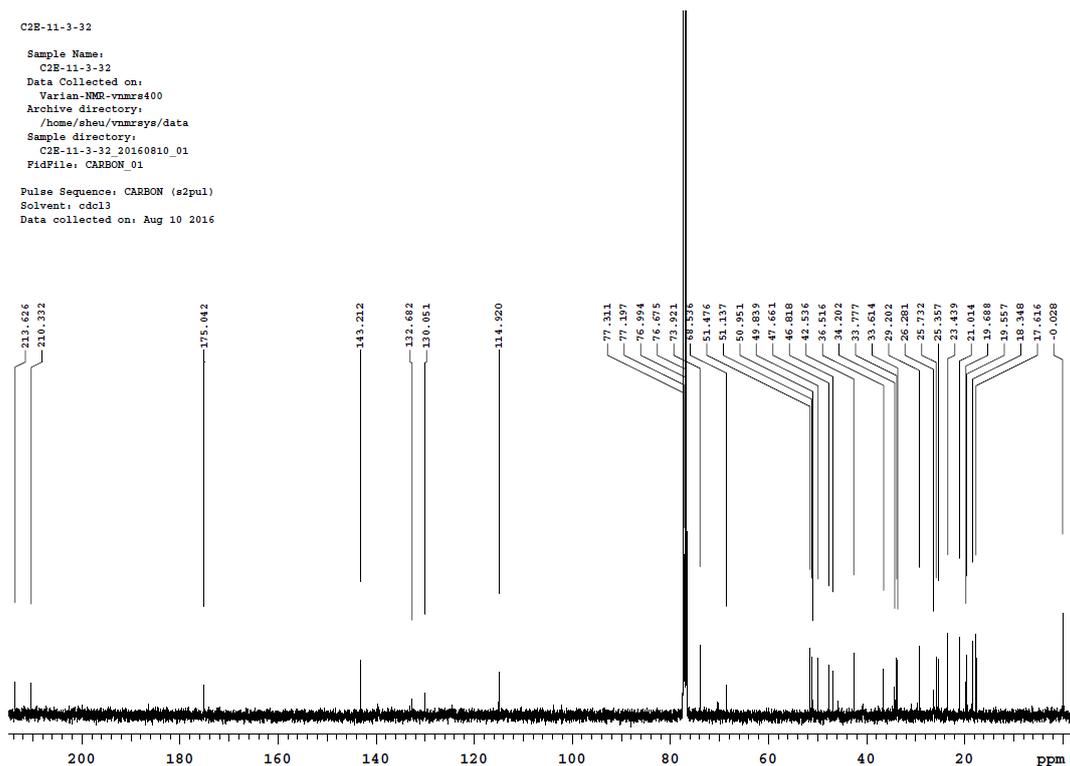  Data collected on: Aug 10 2016

213.626
210.332
175.042
143.212
132.682
130.051
114.920
77.311
77.197
76.994
76.675
73.921
68.536
51.476
51.137
50.951
49.839
47.661
46.818
42.536
36.516
34.202
33.777
33.614
29.202
26.281
25.732
25.357
23.439
21.014
19.688
19.557
18.348
17.616
-0.028

Figure S25: $^{13}$C NMR spectrum of **3** in CDCl$_3$ at 100 MHz

C2E-11-3-32

  Sample Name:
    C2E-11-3-32
  Data Collected on:
    Varian-NMR-vnmrs400
  Archive directory:
    /home/sheu/vnmrsys/data
  Sample directory:
    C2E-11-3-32_20160810_01
  FidFile: DEPT_01

  Pulse Sequence: DEPT
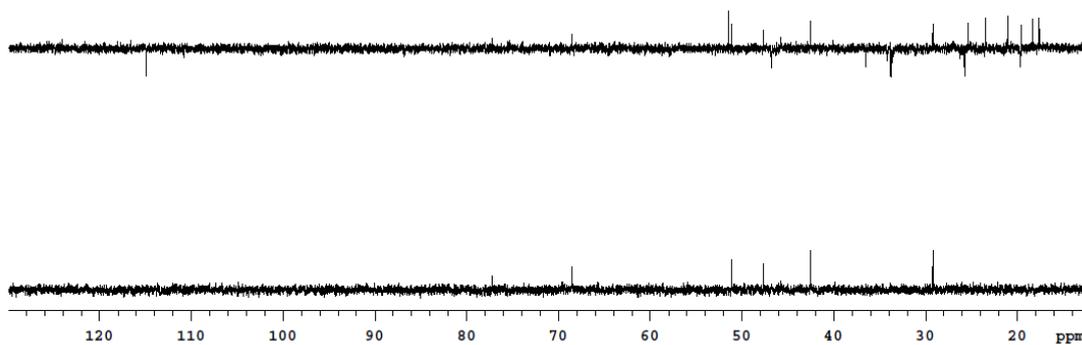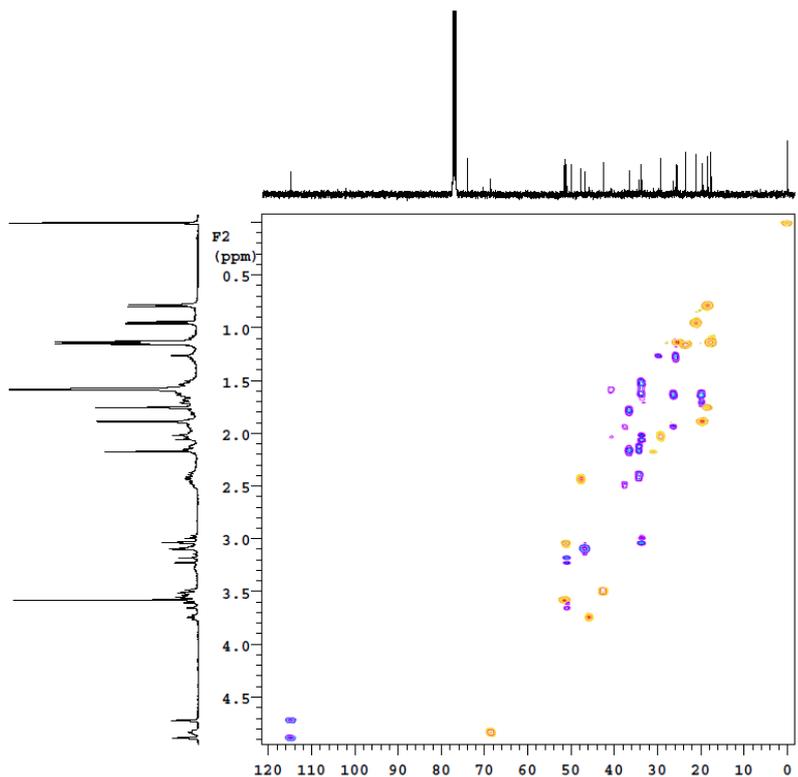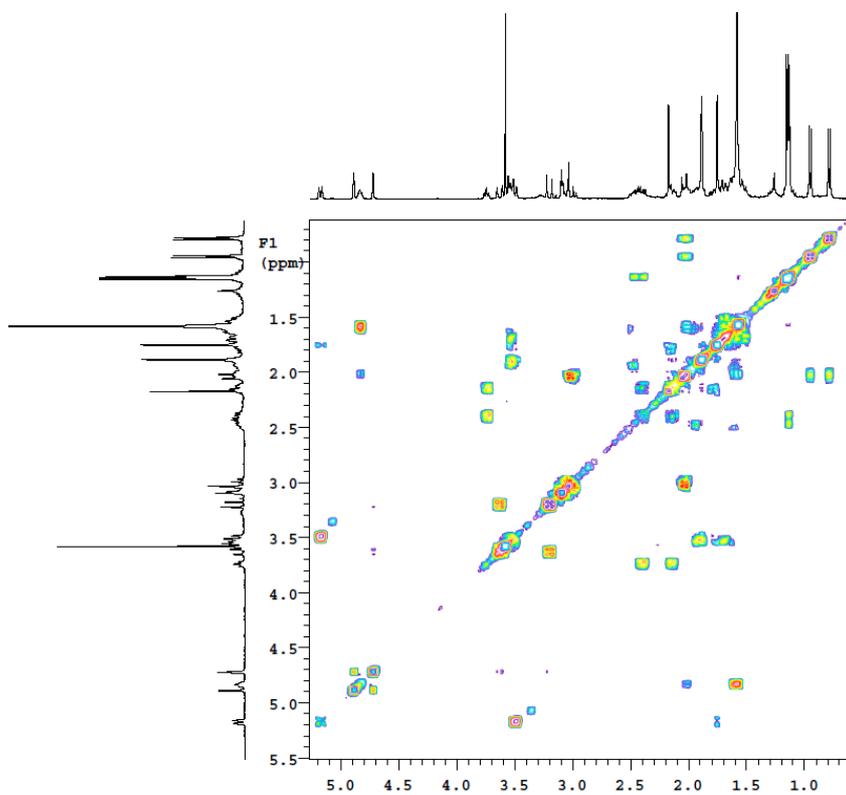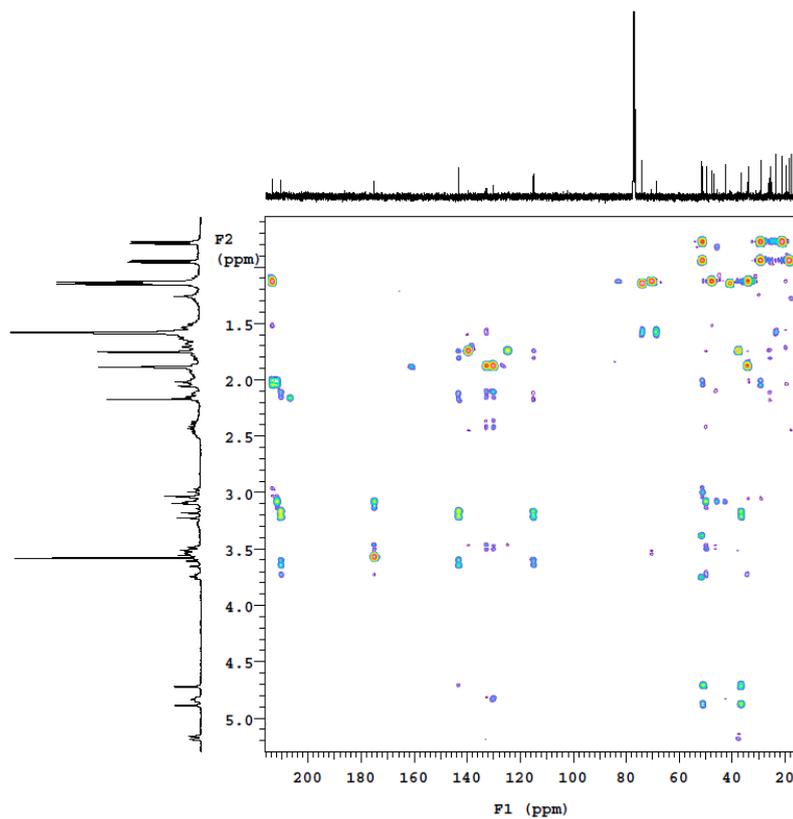  Solvent: cdcl3
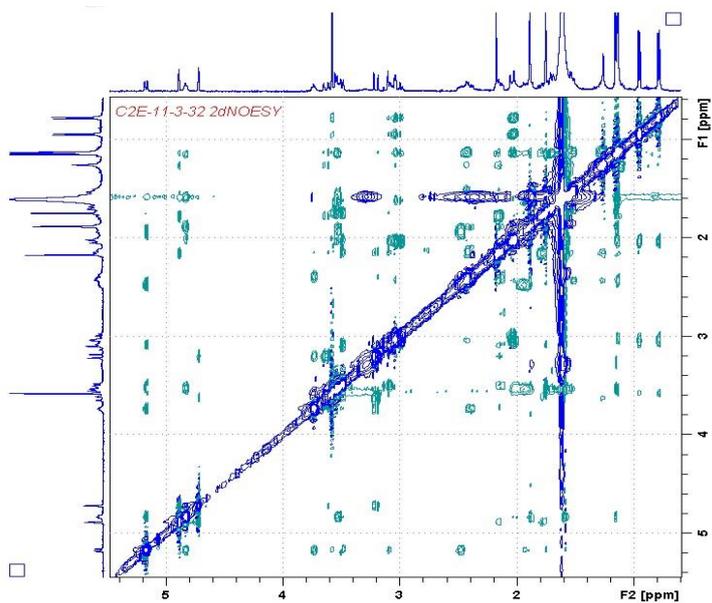  Data collected on: Aug 11 2016

Figure S26: DEPT spectrum of **3**

Figure S27: HSQC spectrum of **3**

Figure S28: COSY spectrum of **3**

Figure S29: HMBC spectrum of **3**



Figure S30: NOESY spectrum of **3**
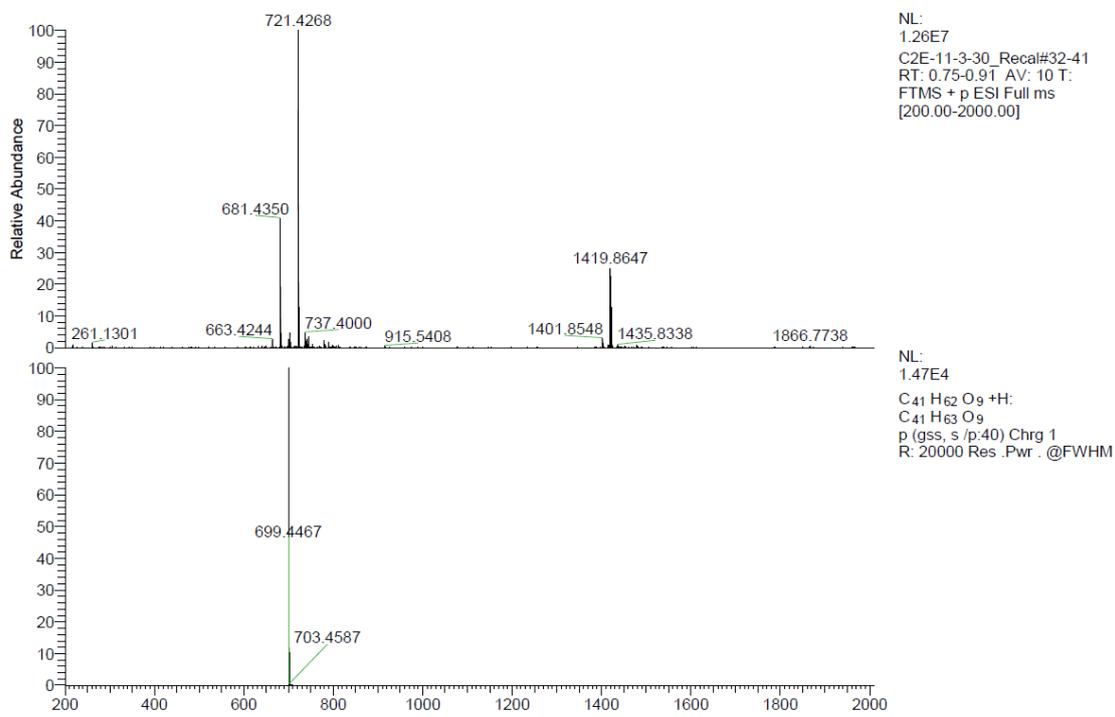
Figure S31: IR spectrum of **4**

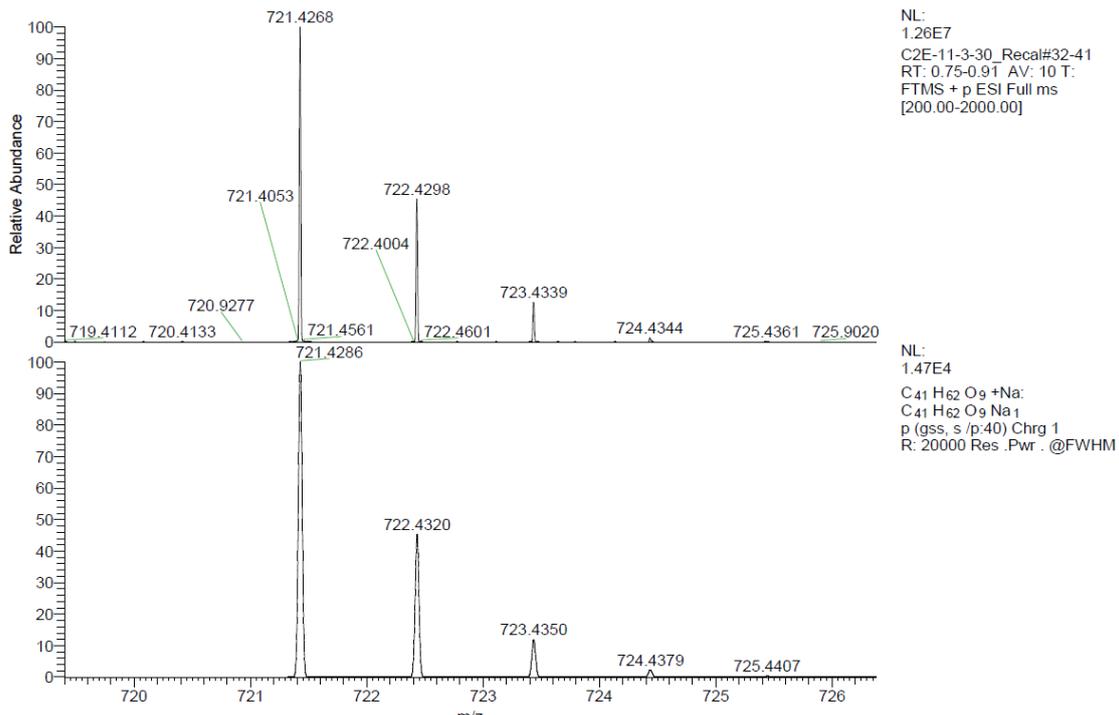Figure S32: ESIMS spectrum of **4**
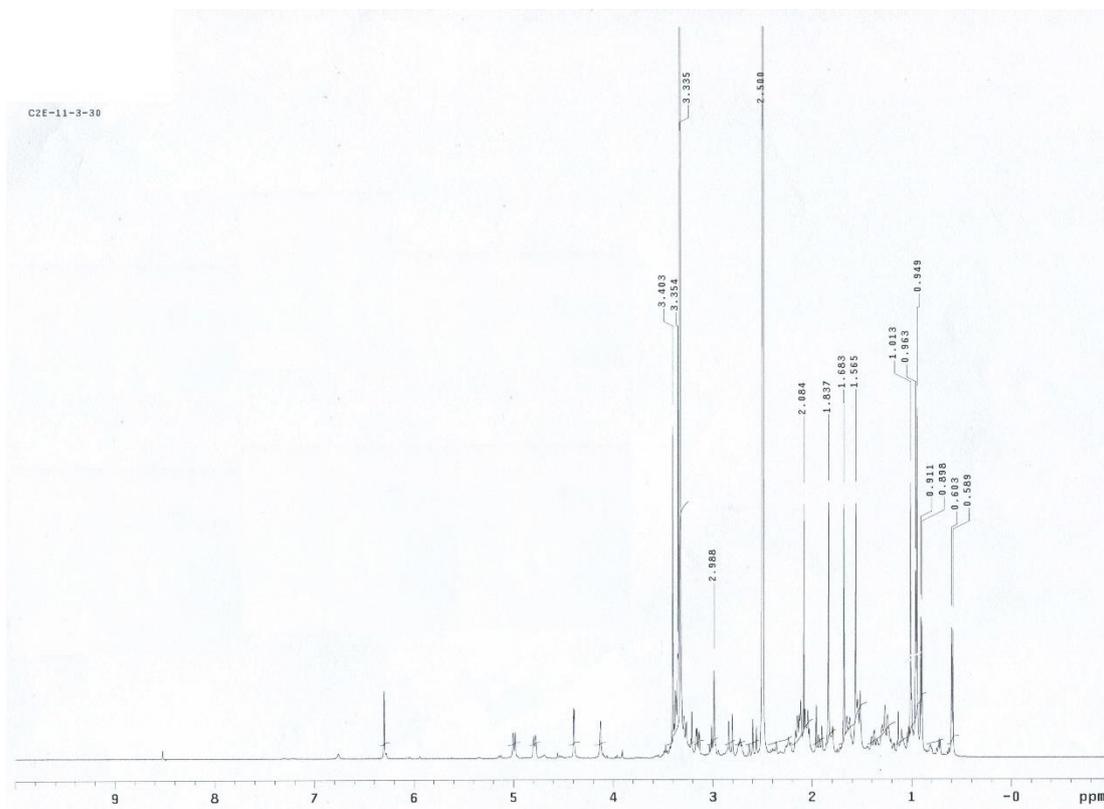
Figure S33: HRESIMS spectrum of **4**,



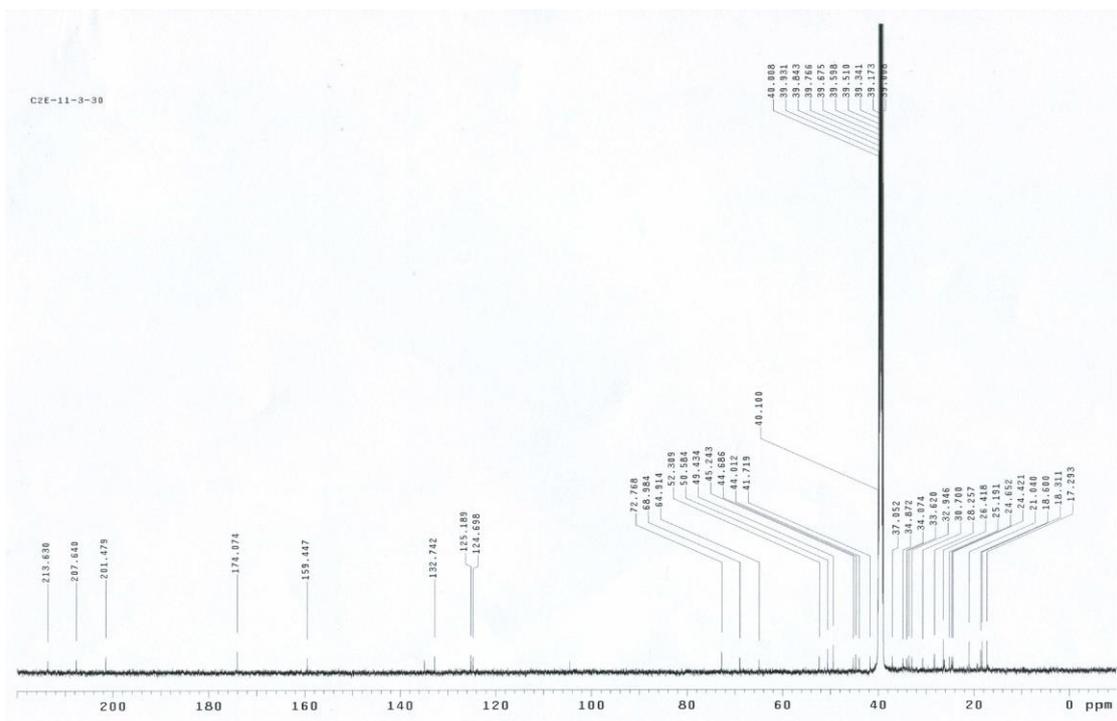Figure S34: $^1$H NMR spectrum of **4** in DMSO-$d_6$ at 500 MHz

Figure S35: $^{13}$C NMR spectrum of **4** in DMSO-$d_6$ at 125 MHz
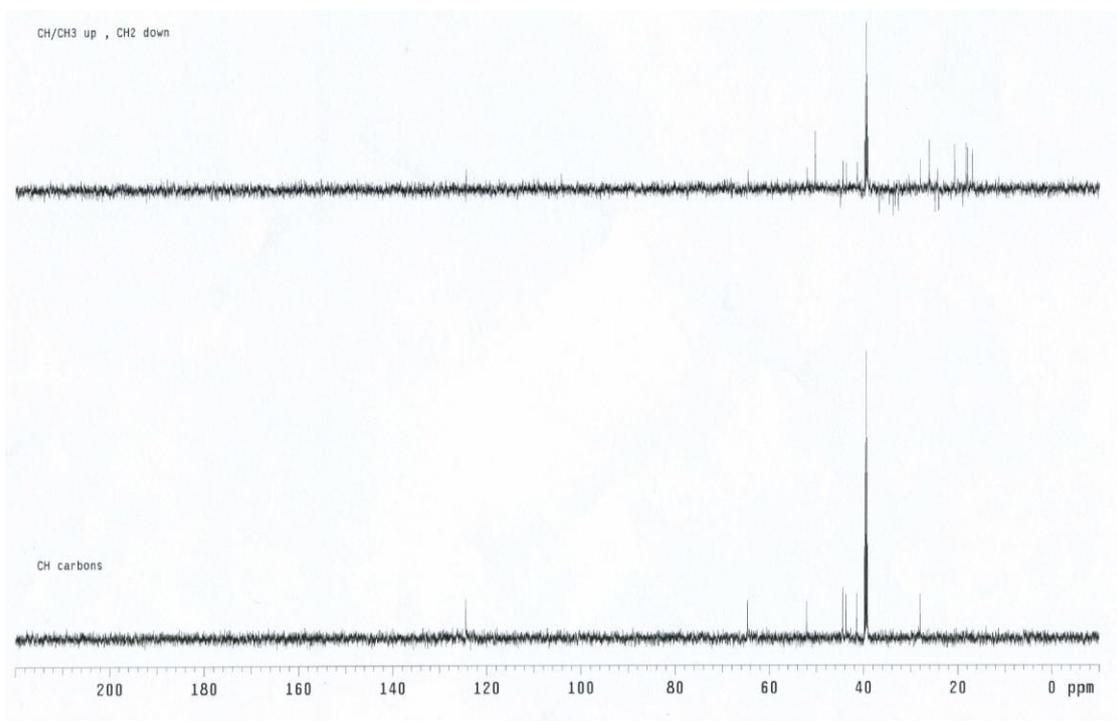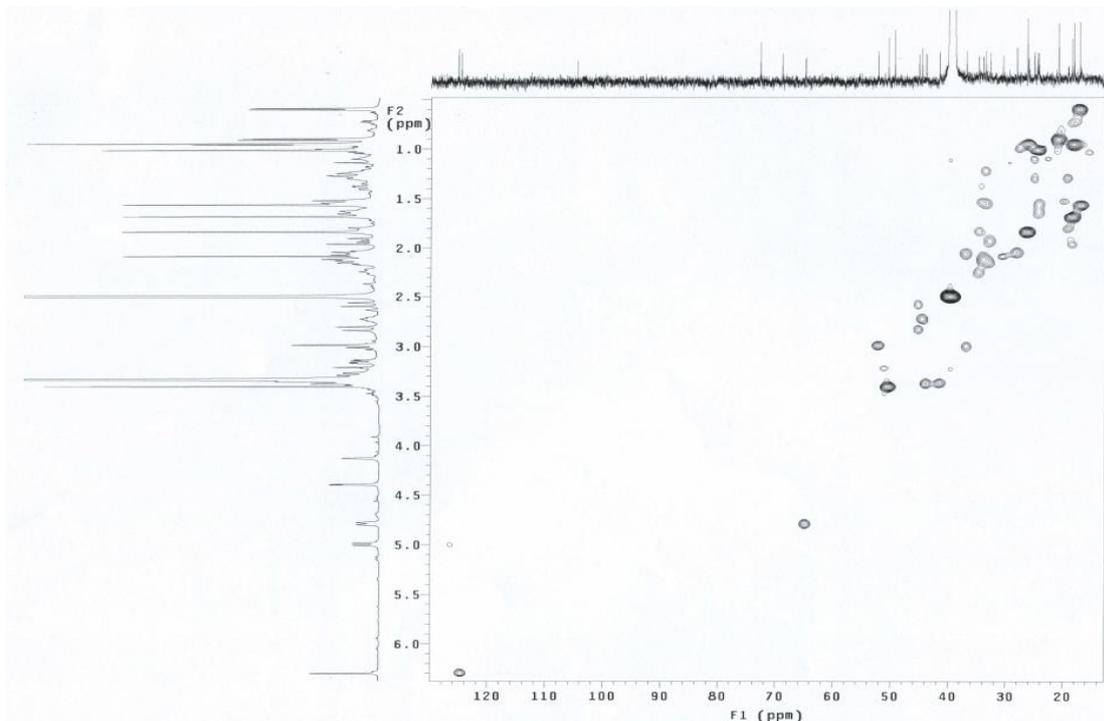


Figure S36: DEPT spectrum of **4**

Figure S37: HSQC spectrum of **4**



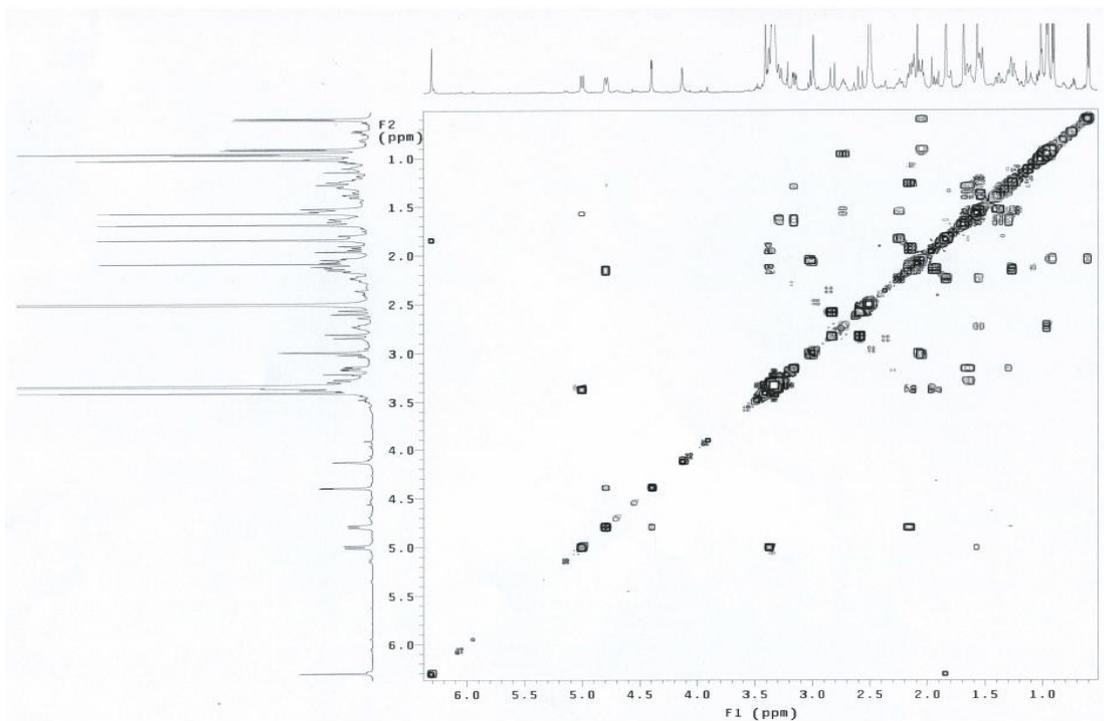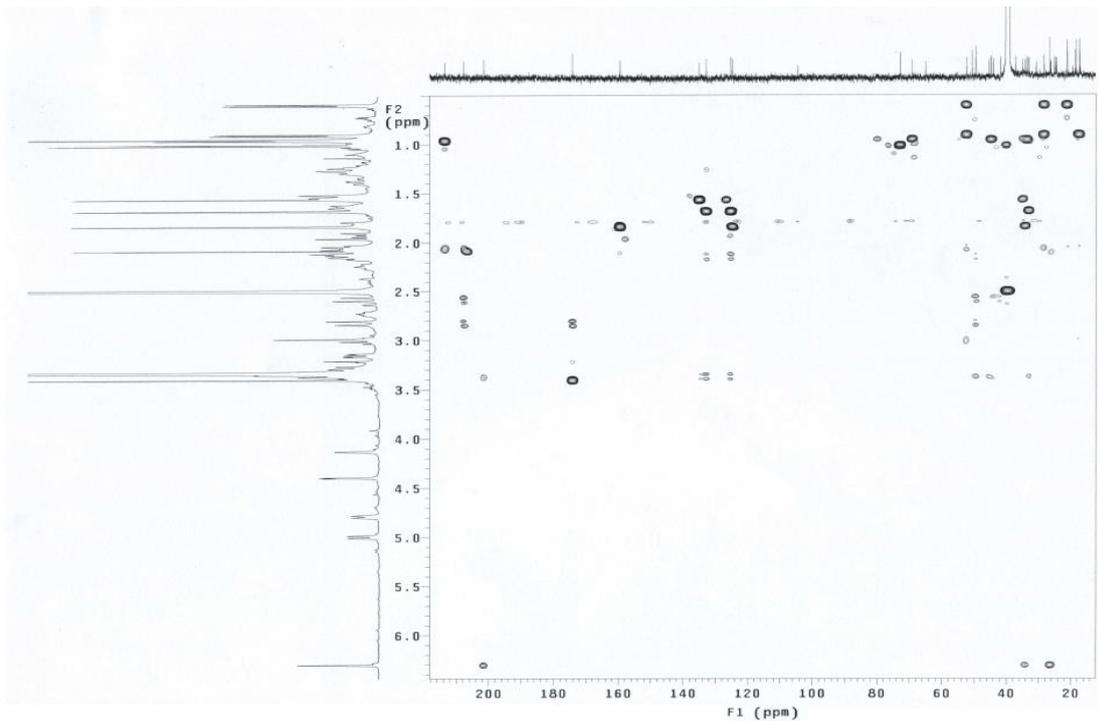Figure S38: COSY spectrum of **4**

Figure S39: HMBC spectrum of **4**

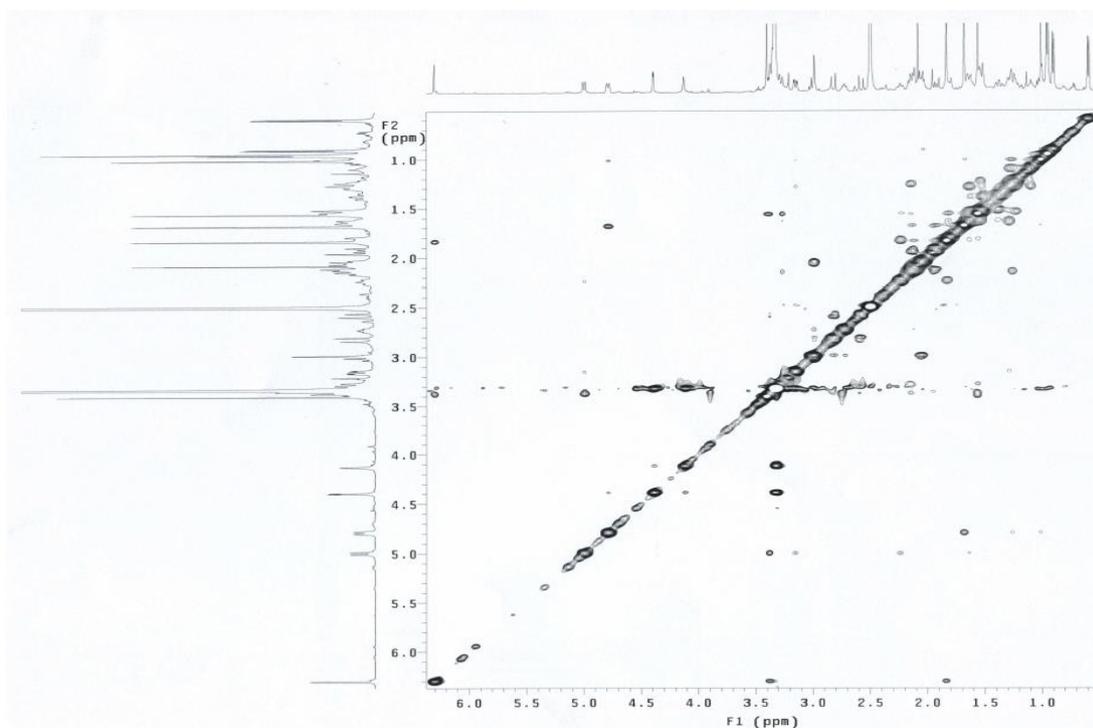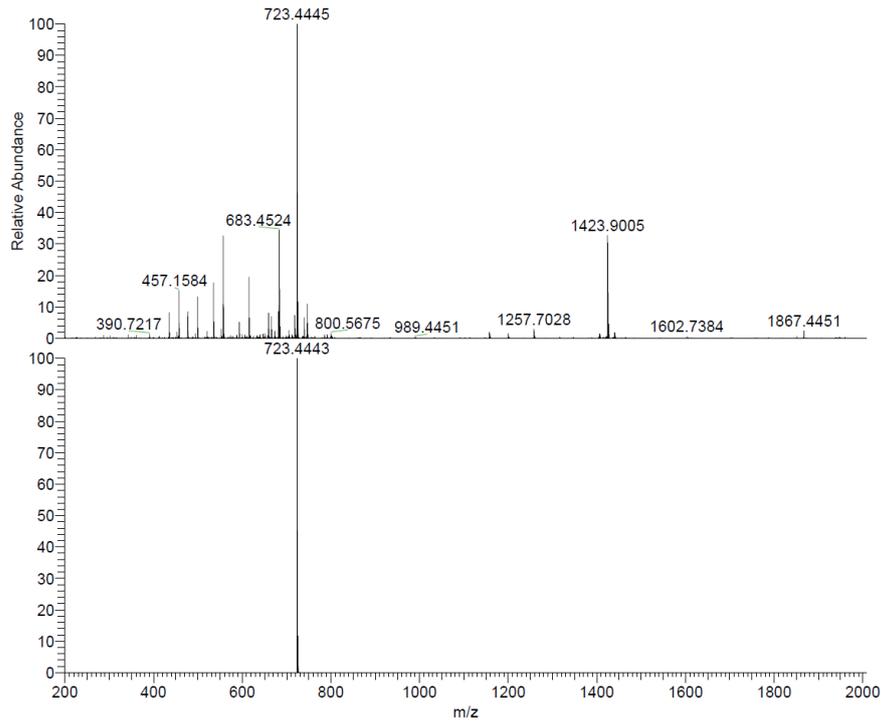

Figure S40: NOESY spectrum of **4**

NL:
1.84E6
C2E-11-4-46_191004152501#104-113
RT: 2.19-2.35 AV: 10 T:
FTMS + p ESI Full ms
[200.00-2000.00]

723.4445

683.4524

457.1584

1423.9005

390.7217    800.5675    989.4451    1257.7028    1602.7384    1867.4451

723.4443

NL:
1.47E4

$C_{41}H_{64}O_9$ +Na:
$C_{41}H_{64}O_9Na_1$
p (gss, s /p:40) Chrg 1
R: 60000 Res .Pwr . @FWHM

Z:\2L13\FC\C2E-11-4-46_191004152501        10/04/19 15:25:01
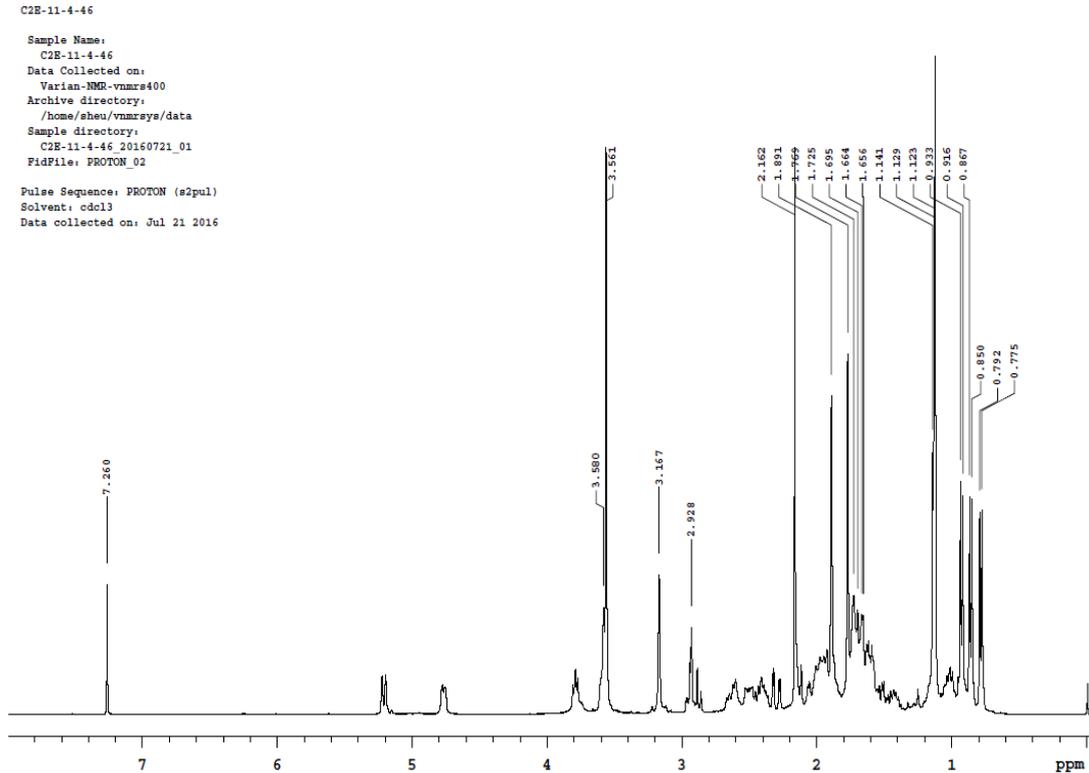
Figure S41: ESIMS spectrum of **5**
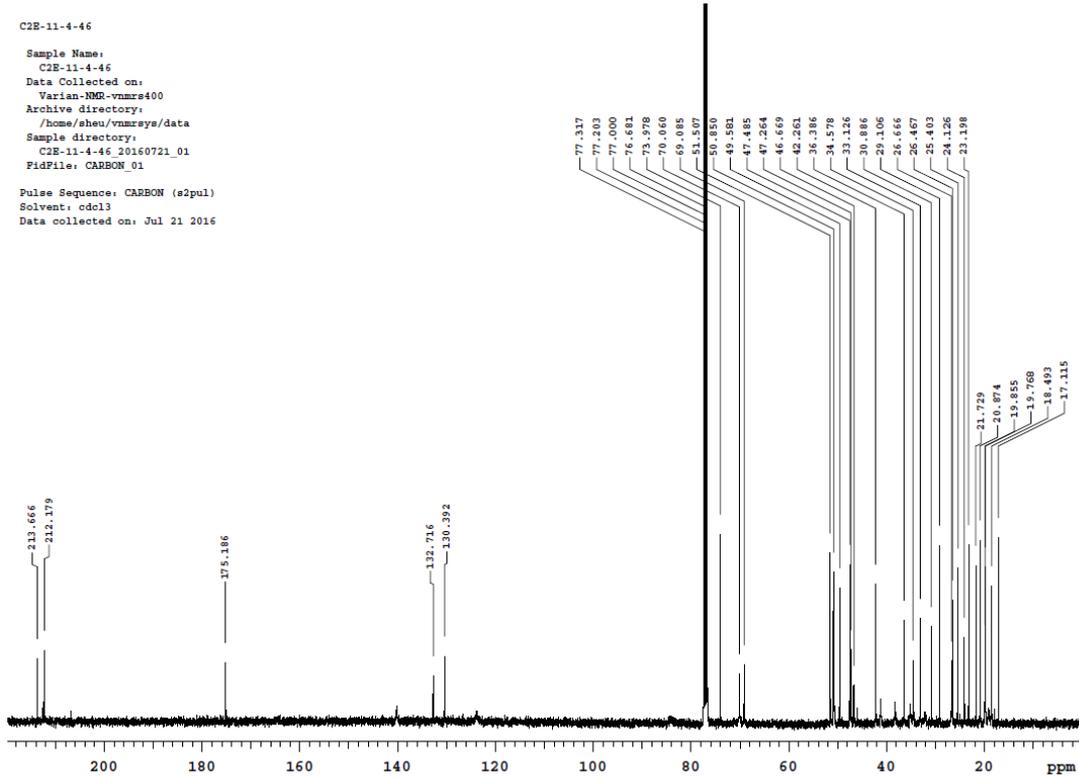


Figure S42: $^1$H NMR spectrum of **5** in CDCl$_3$ at 400 MHz

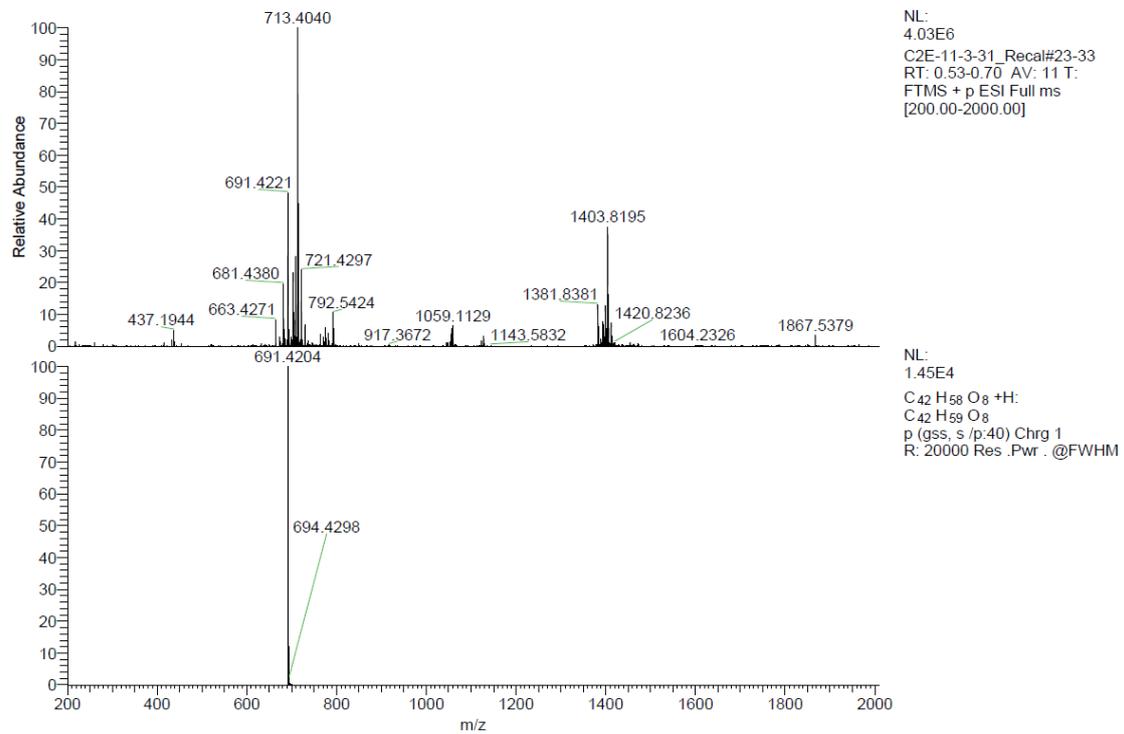Figure S43: $^{13}$C NMR spectrum of **5** in CDCl$_3$ at 100 MHz
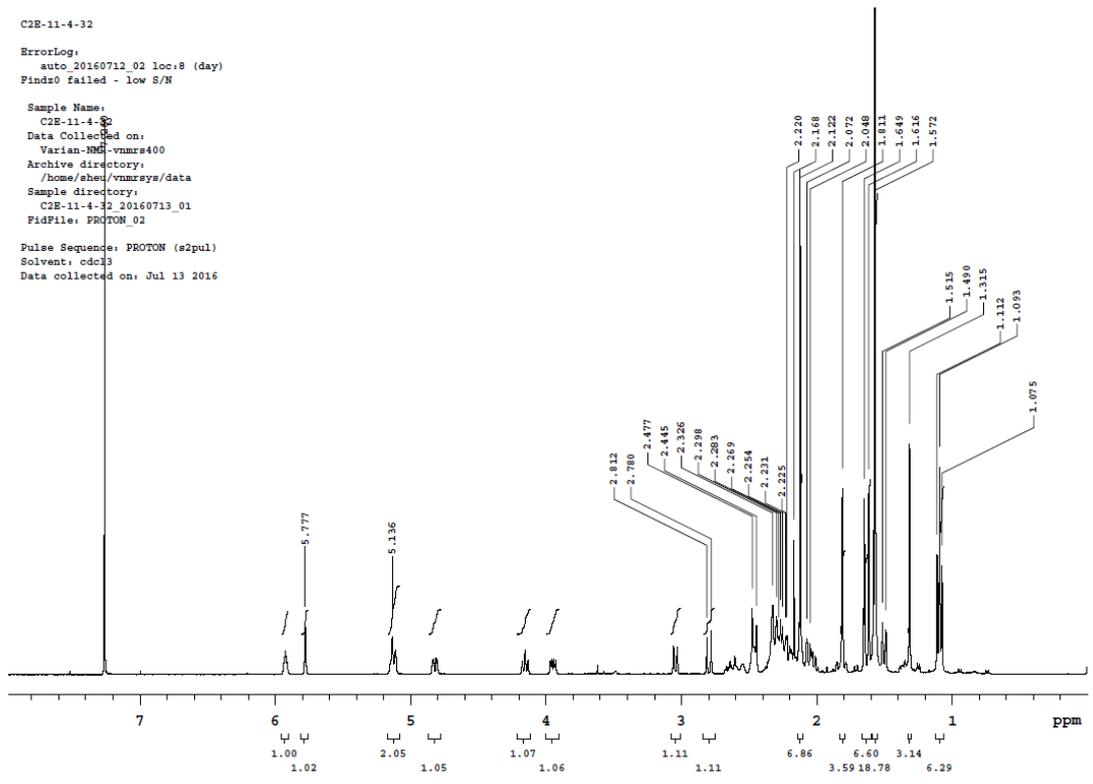


Figure S44: ESIMS spectrum of **6**

C2E-11-4-32

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Findz0 failed - low S/N

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 Data Collected on:
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 Archive directory:
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 Sample directory:
   C2E-11-4-32_20160713_01
 FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 13 2016

Figure S45: $^1$H NMR spectrum of **6** in CDCl$_3$ at 400 MHz

C2E-11-4-32

ErrorLog:
    auto_20160712_02 loc:8 (day)
Findz0 failed - low S/N

 Sample Name:
   C2E-11-4-32
 Data Collected on:
   Varian-NMR-vnmrs400
 Archive directory:
   /home/sheu/vnmrsys/data
 Sample directory:
   C2E-11-4-32_20160713_01
 FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 13 2016

Figure S46: $^{13}$C NMR spectrum of **6** in CDCl$_3$ at 100 MHz
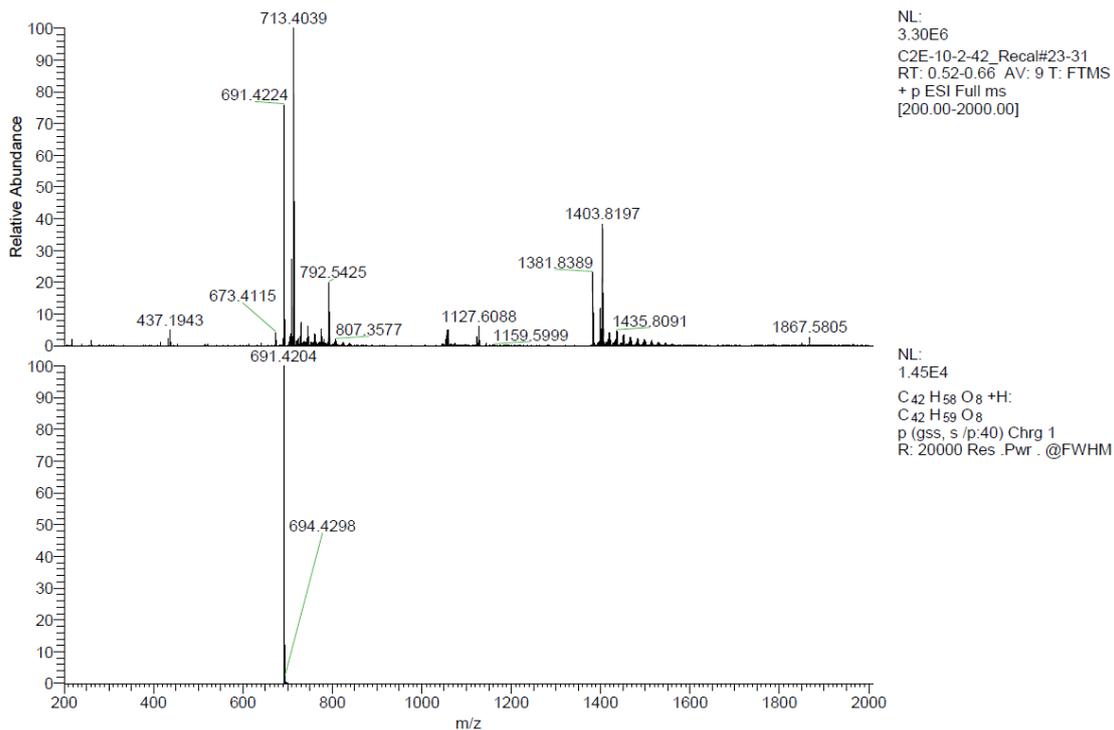
Figure S47: ESIMS spectrum of **7**
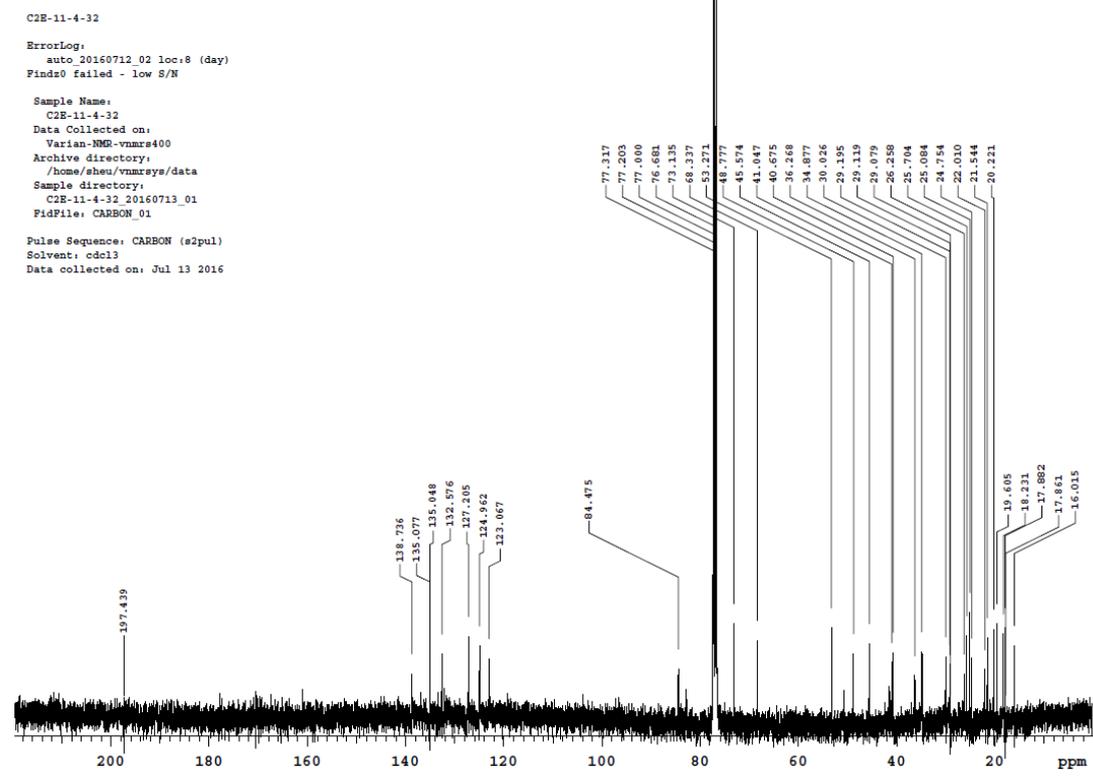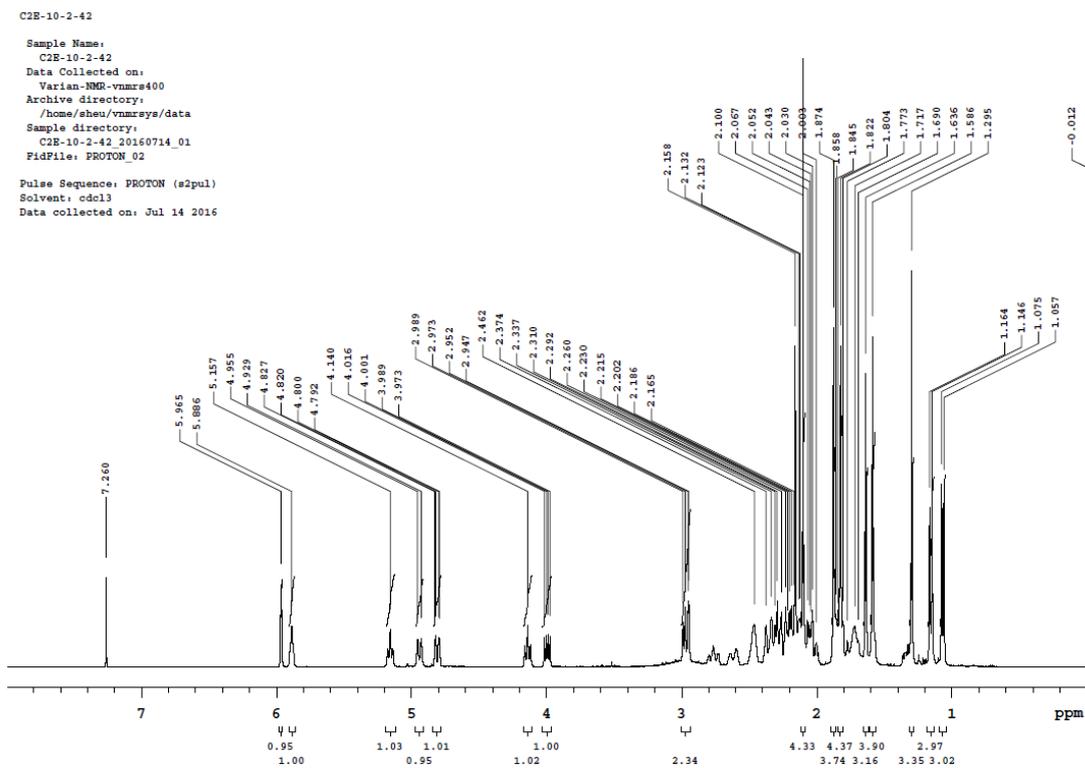


Figure S48: $^1$H NMR spectrum of **7** in CDCl$_3$ at 400 MHz

Figure S49: $^{13}$C NMR spectrum of **7** in CDCl$_3$ at 100 MHz
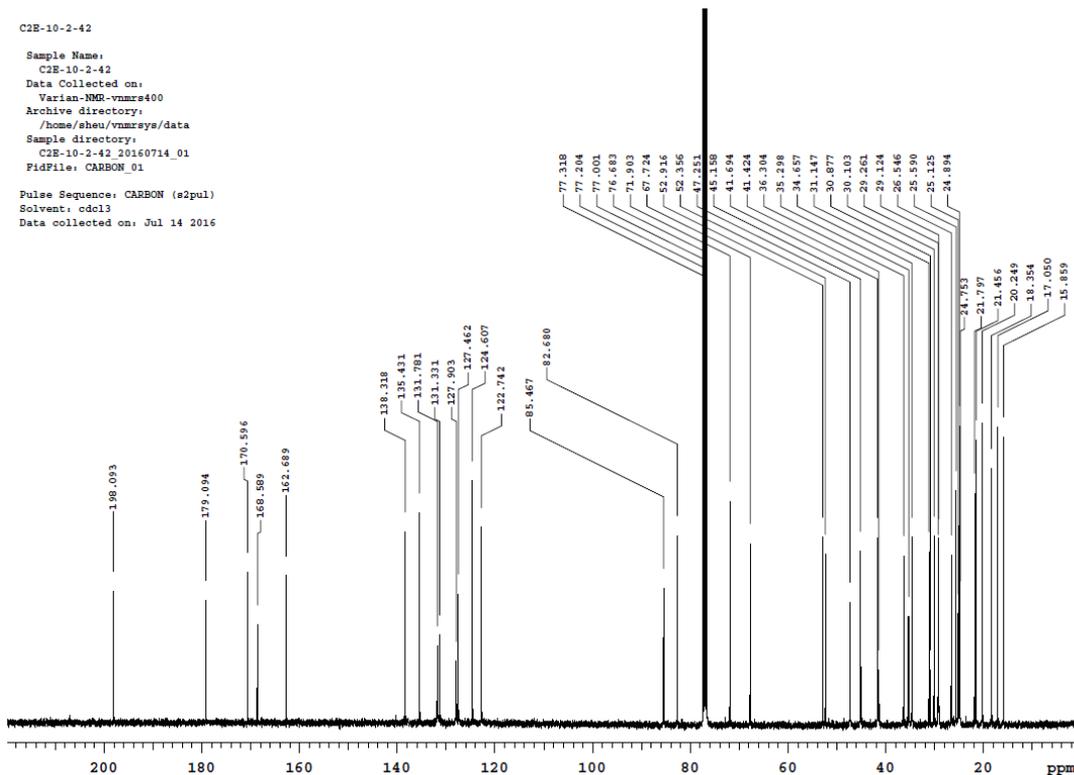
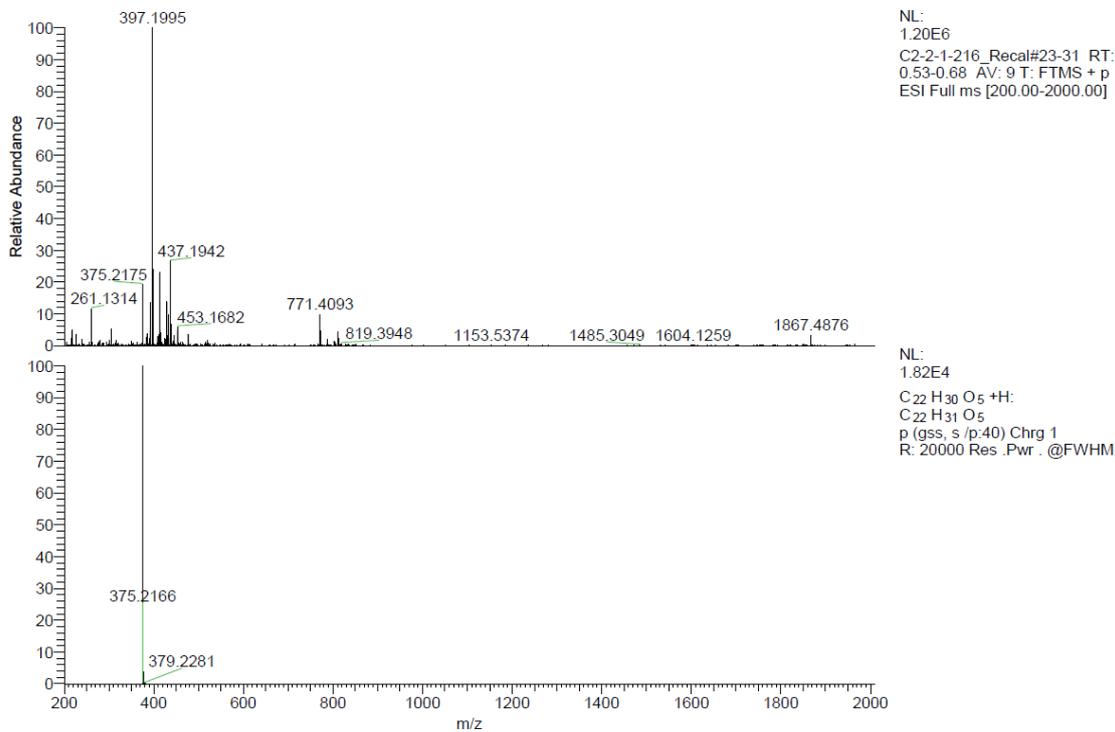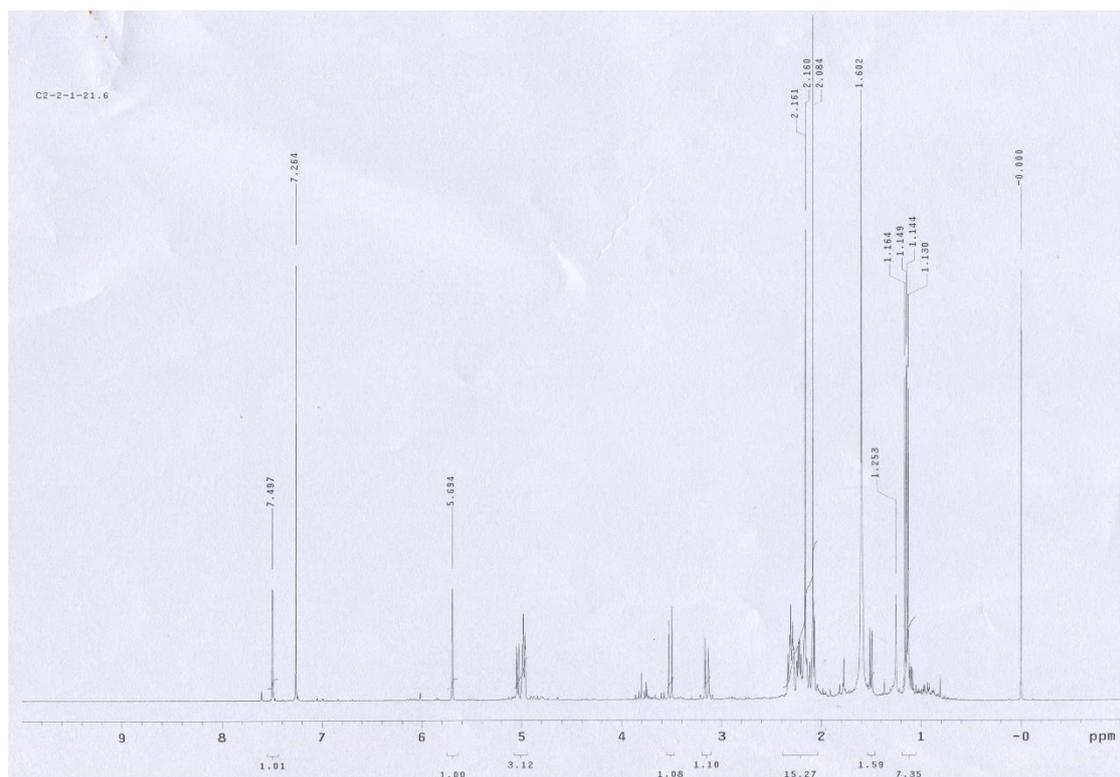Figure S50: ESIMS spectrum of **8**
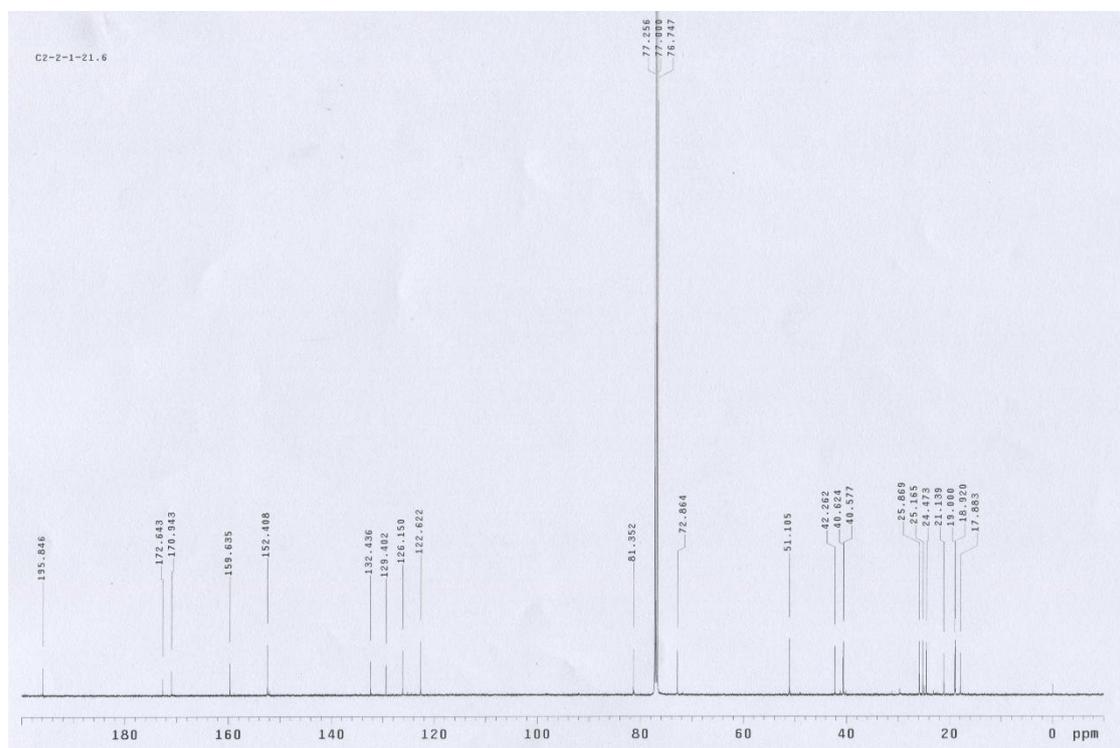
Figure S51: $^1$H NMR spectrum of **8** in CDCl$_3$ at 500 MHz



Figure S52: $^{13}$C NMR spectrum of **8** in CDCl$_3$ at 125 MHz