

New hydroquinone monoterpenoid and cembranoid-related metabolites from the soft coral *Sarcophyton tenuispiculatum*

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Compound 1 spectroscopic data

FT-MS

Analysis Info

Analysis Name D:\Data\1\SARCOFR325_000003.d
Method broadband first signal
Sample Name Sarco-fr-3-25
Comment ESI Positive

3/14/2018 3:36:51 PM

Instrument: FT-MS solariX

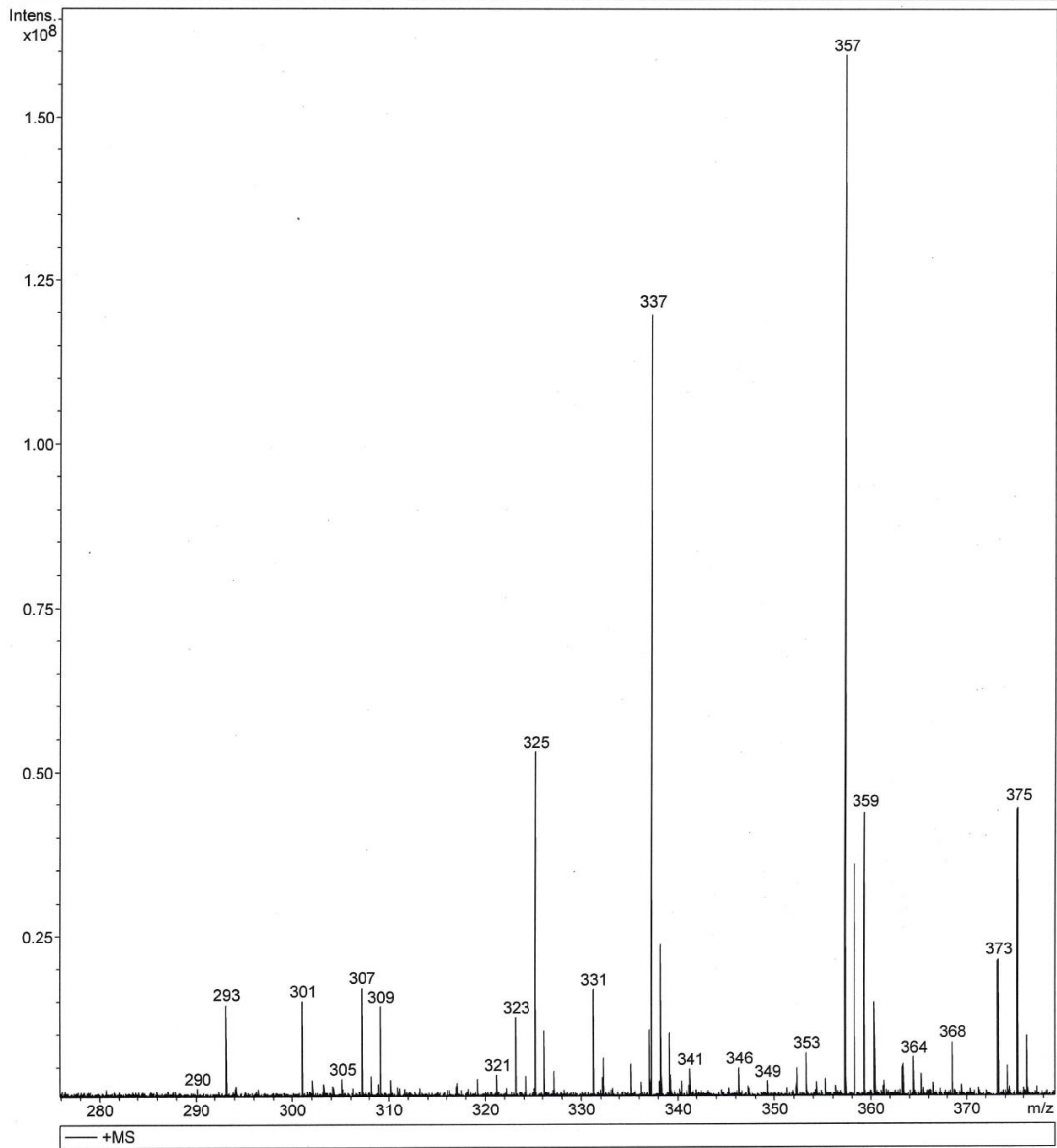


Figure S1: ESIMS spectrum of 1

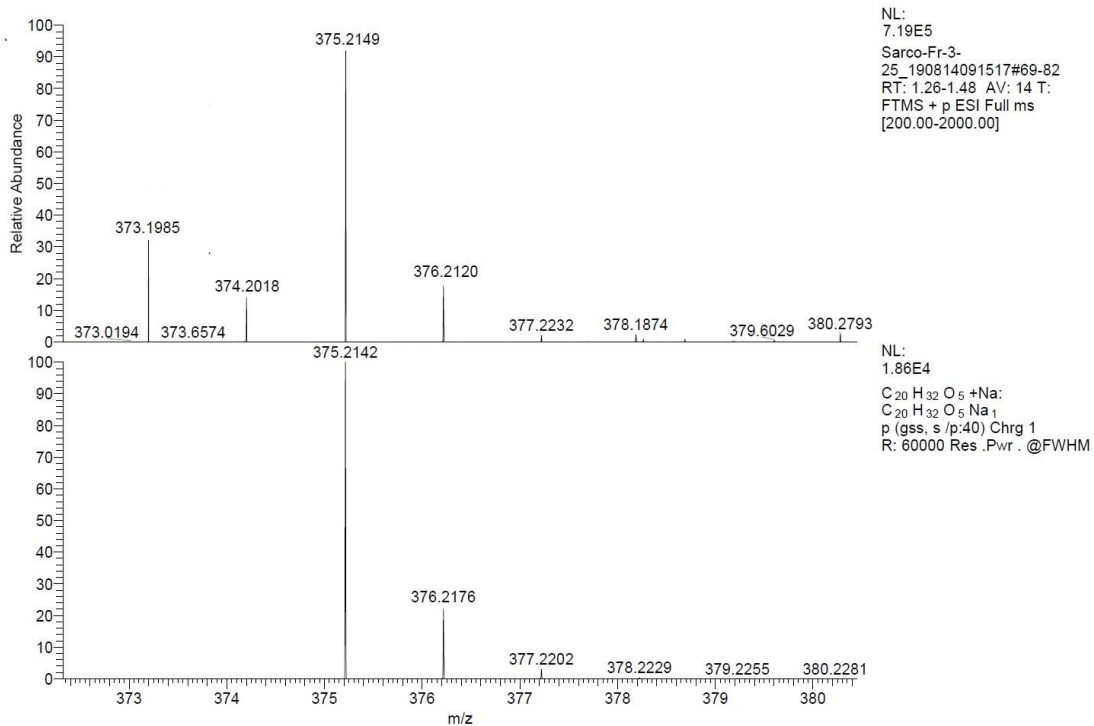


Figure S2: HRESIMS spectrum of 1

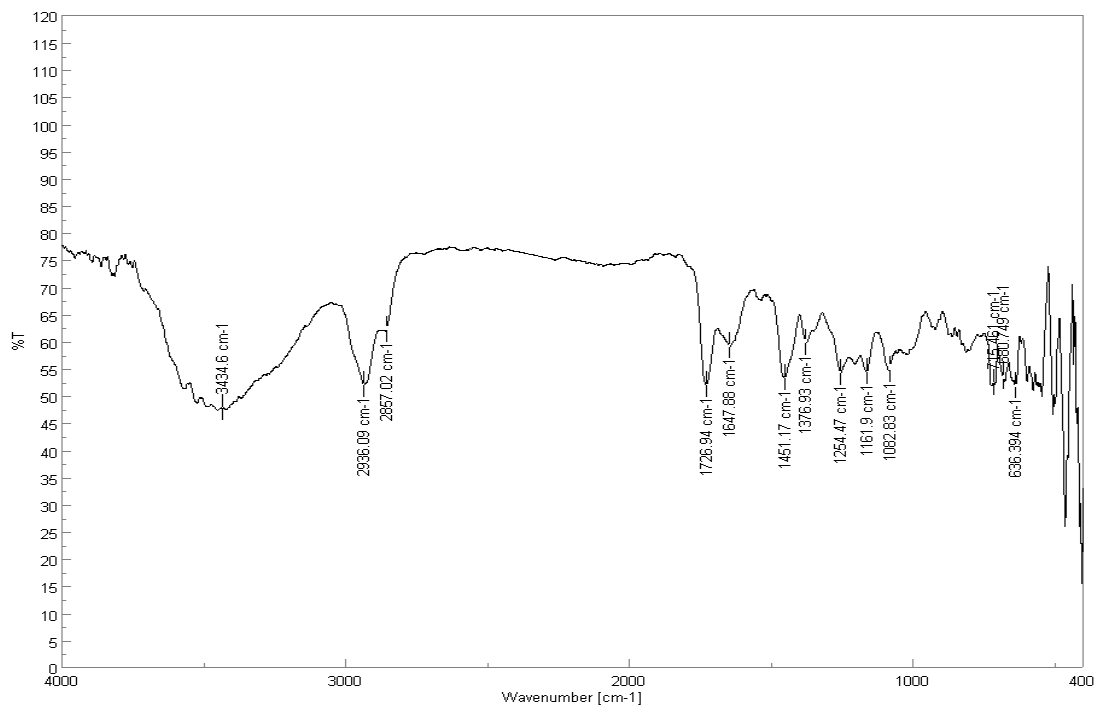


Figure S3: IR spectrum of 1

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 5 2018

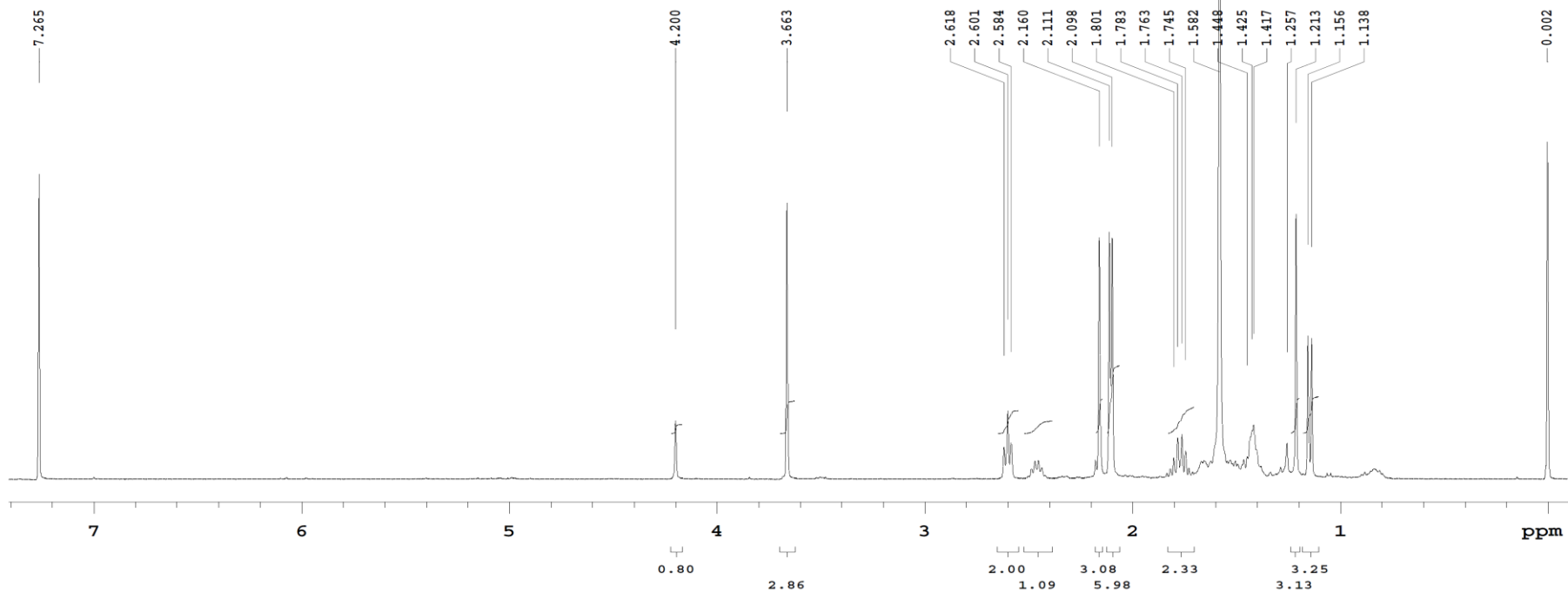
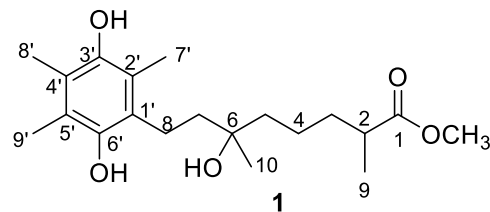


Figure S4: ¹H NMR spectrum of **1** in CDCl₃ at 400 MHz

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 5 2018

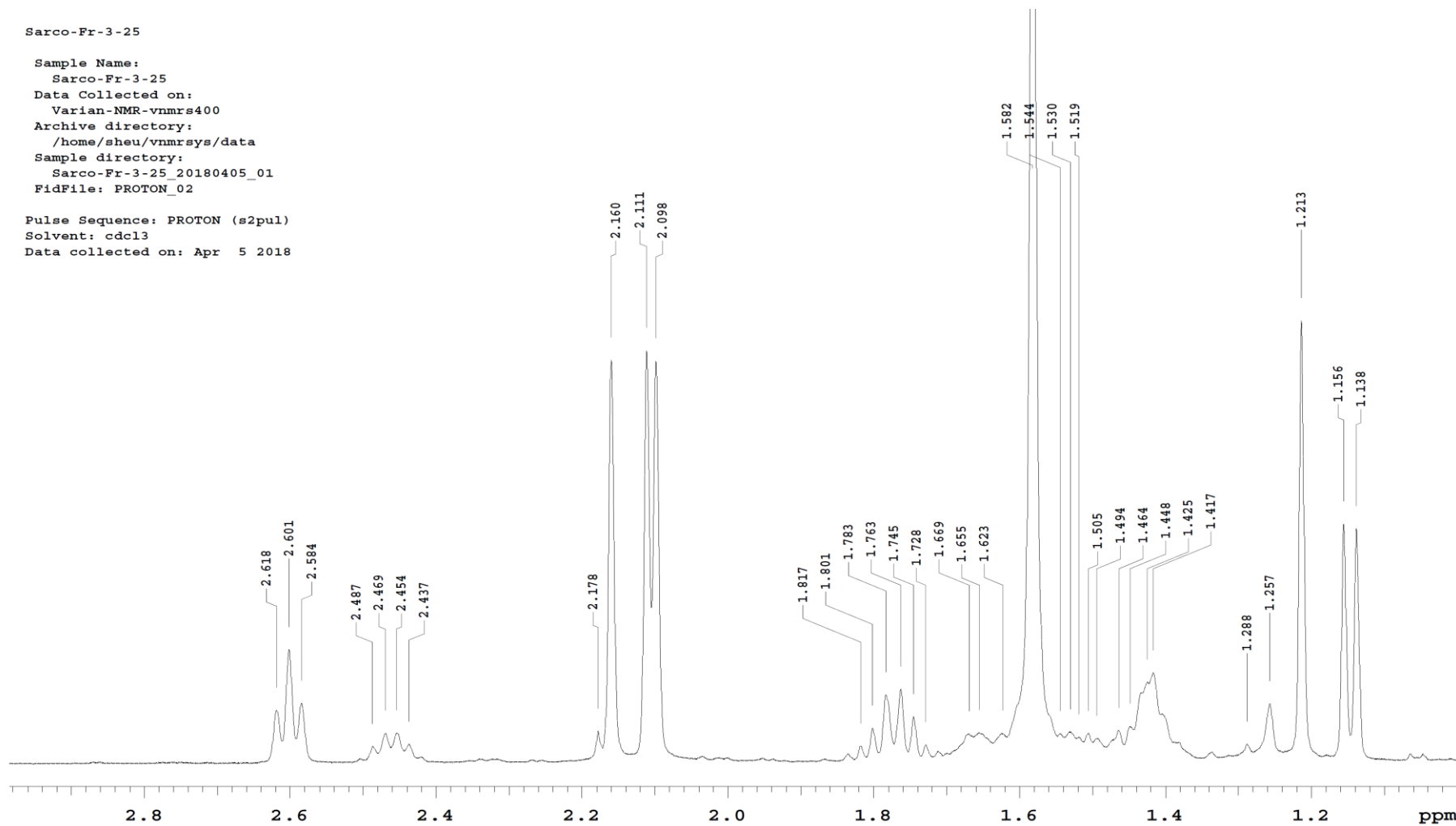


Figure S5: ¹H NMR spectrum (from 1.0 to 3.0 ppm) of 1 in CDCl₃ at 400 MHz

Figure S6: ^{13}C NMR spectrum of **1** in CDCl_3 at 100 MHz

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: DEPT_01

Pulse Sequence: DEPT
Solvent: cdcl3
Data collected on: Apr 6 2018

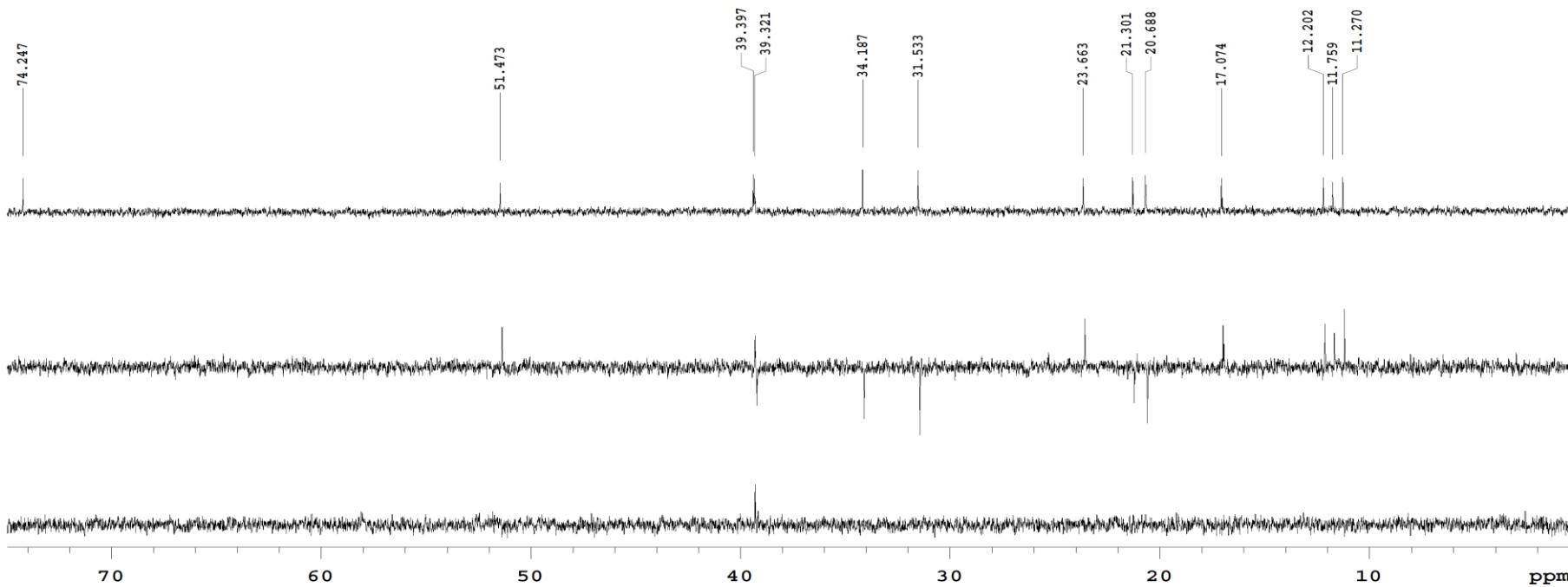


Figure S7: DEPT spectrum of 1

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: HSQCAD_01

Pulse Sequence: HSQCAD
Solvent: cdcl3
Data collected on: Apr 5 2018

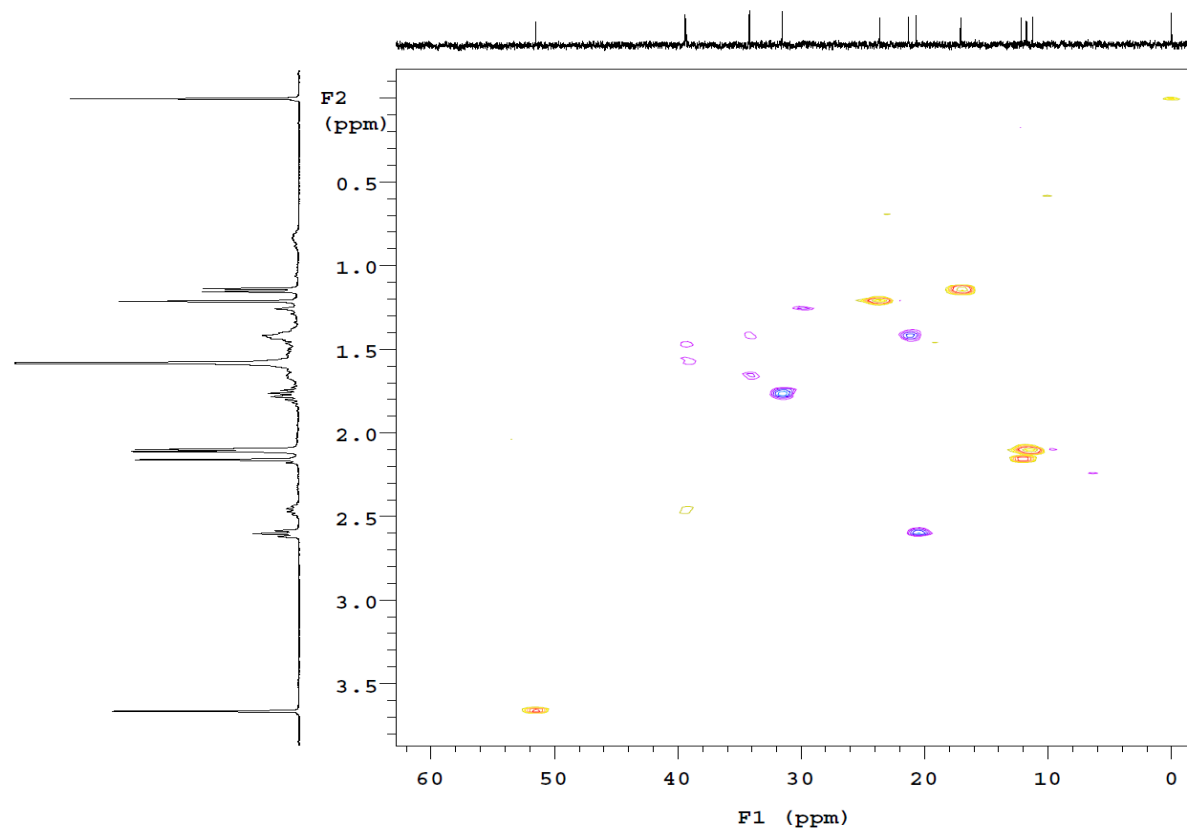


Figure S8: HSQC spectrum of 1

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: gCOSY_01

Pulse Sequence: gCOSY
Solvent: cdcl3
Data collected on: Apr 5 2018

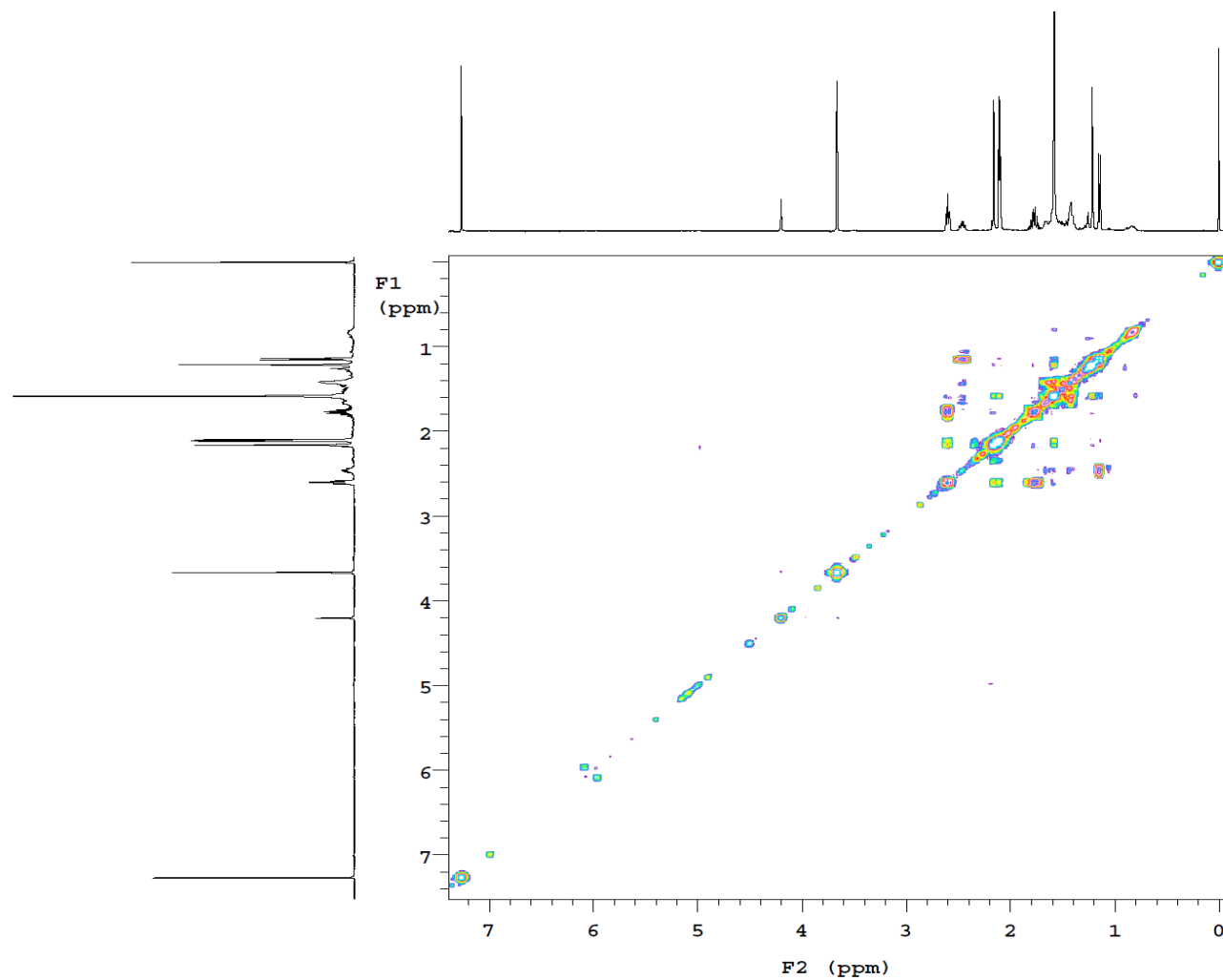


Figure S9: COSY spectrum of 1

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: gHMBCAD_01

Pulse Sequence: gHMBCAD
Solvent: cdcl3
Data collected on: Apr 6 2018

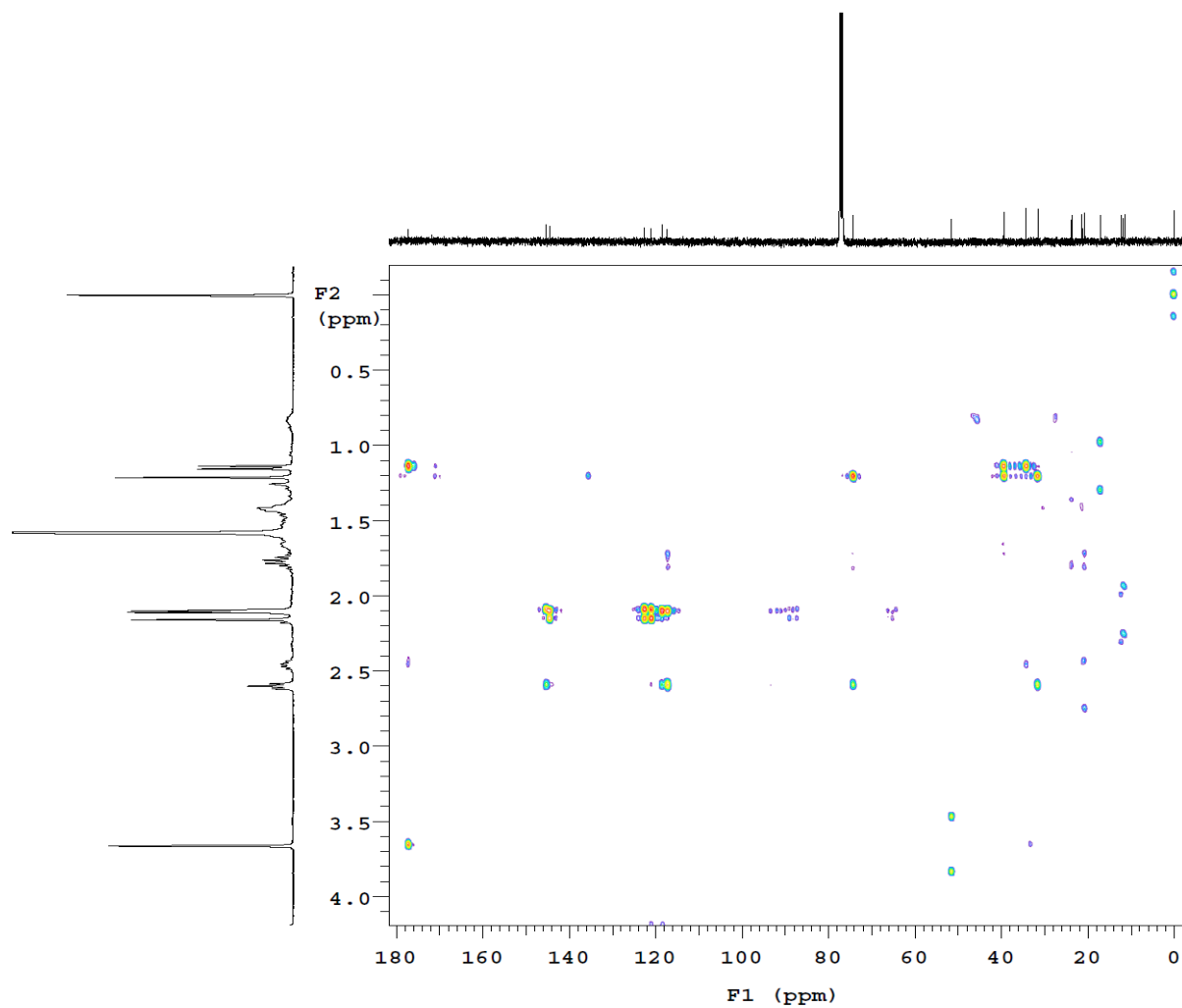


Figure S10: HMBC spectrum of 1

Sarco-Fr-3-25

Sample Name:
Sarco-Fr-3-25
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-3-25_20180405_01
FidFile: NOESY_01

Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Apr 6 2018

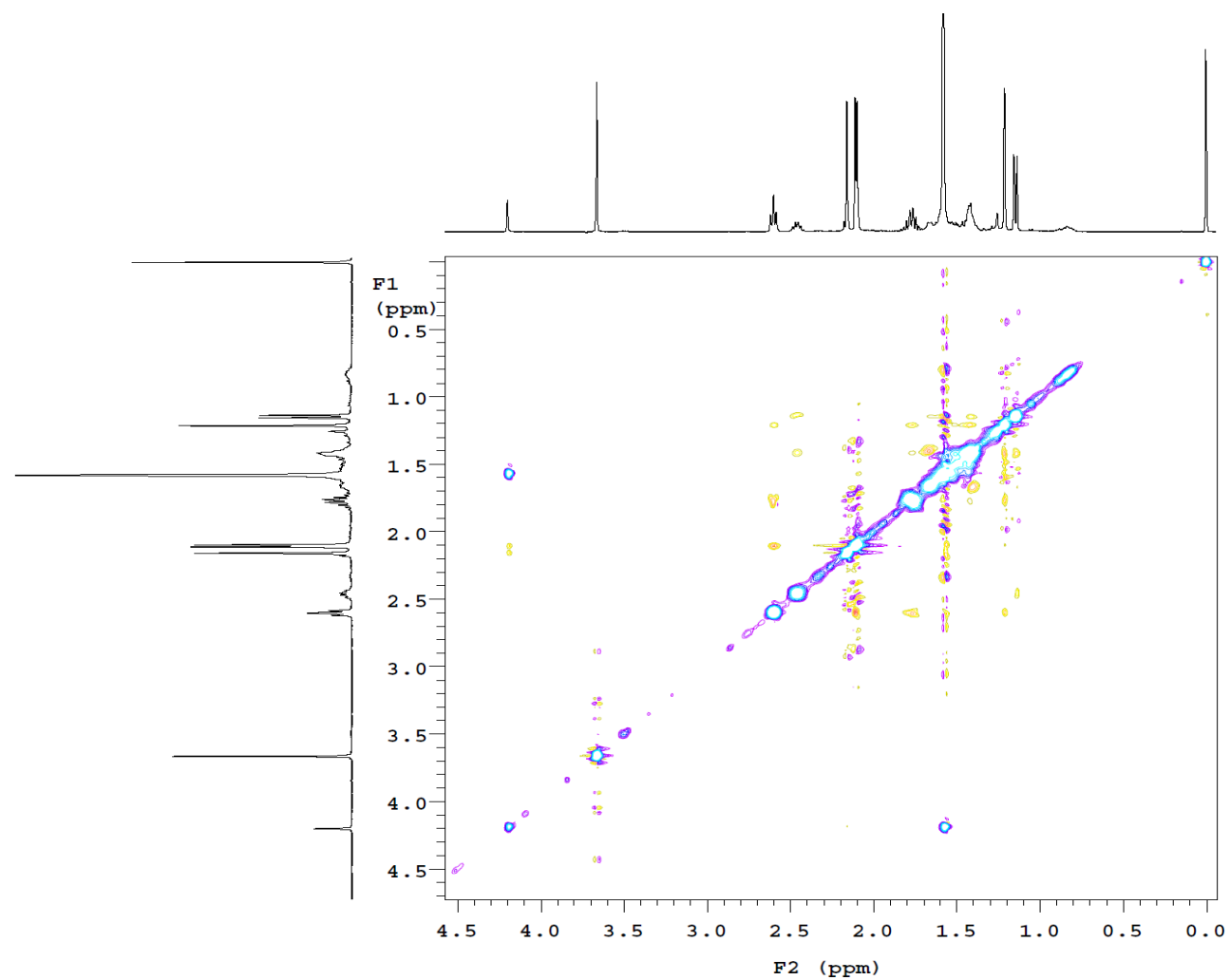


Figure S11: NOESY spectrum of 1

Compound 2 spectroscopic data

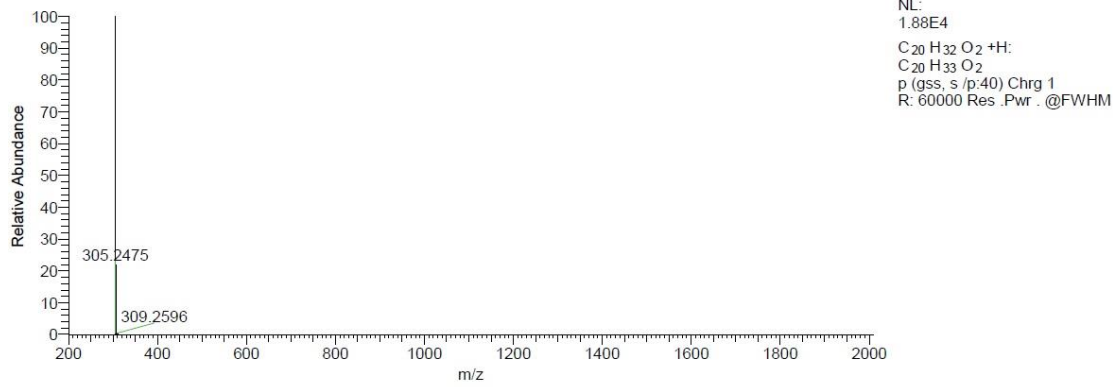


Figure S12: ESIMS spectrum of 2

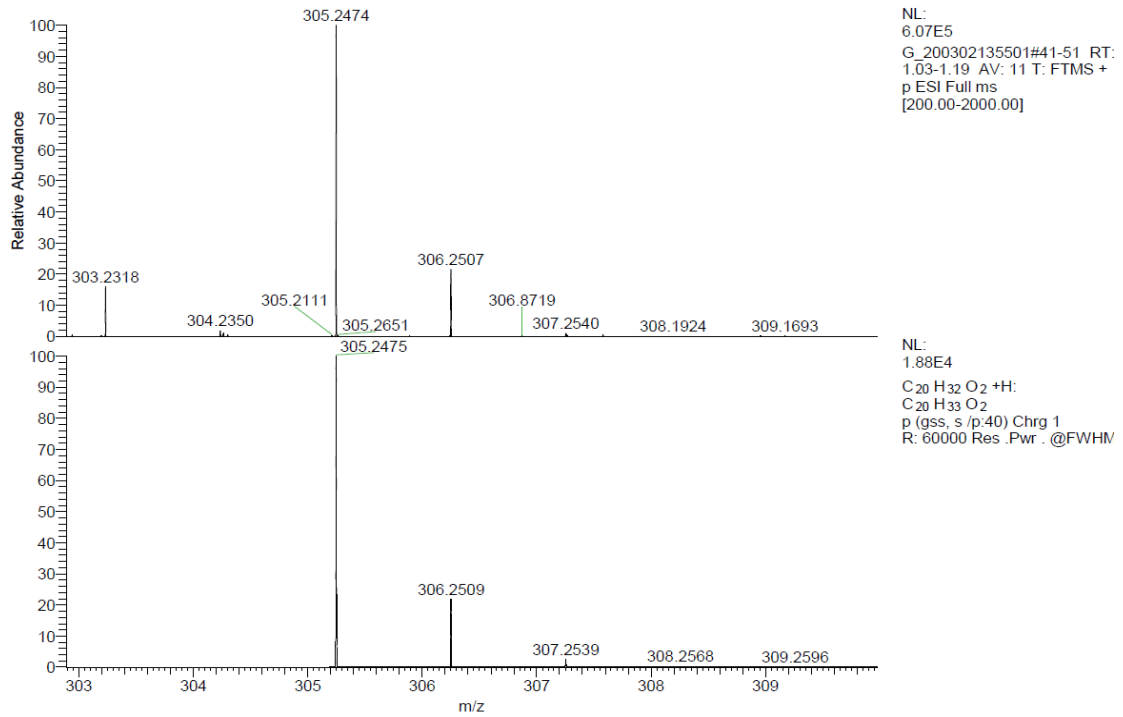


Figure S13: HRESIMS spectrum of 2

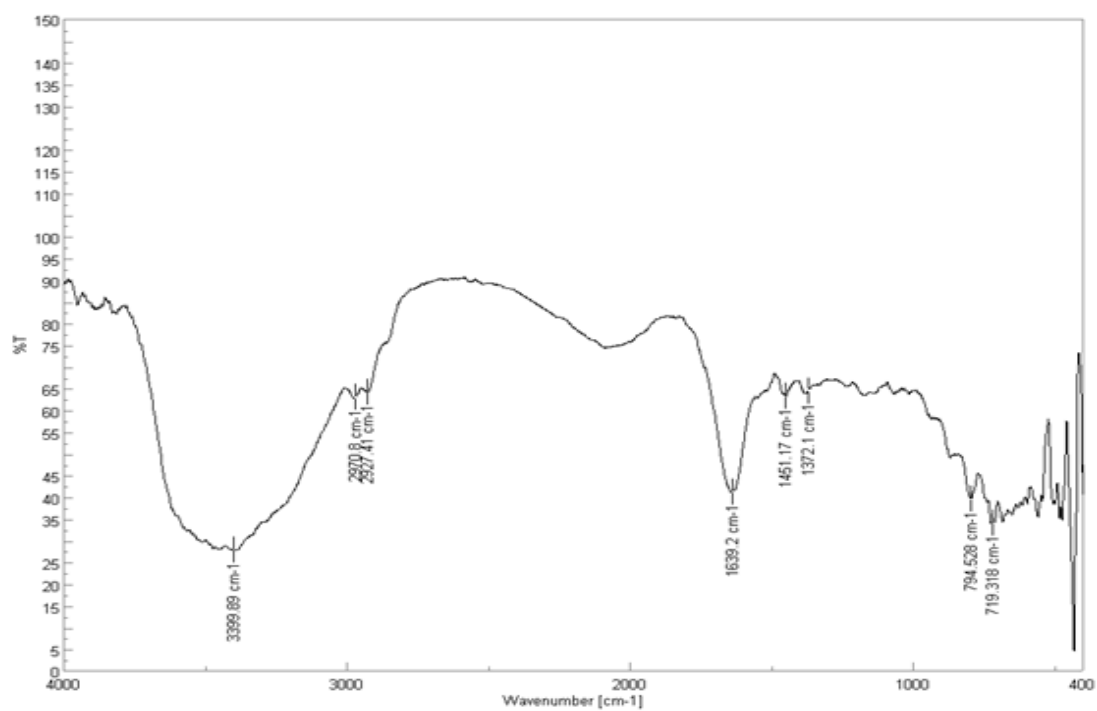


Figure S14: IR spectrum of 2

Sarco-Fr-2-(27-33)-30

Sample Name:

Sarco-Fr-2-27-33-30

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

Sarco-Fr-2-27-33-30_20180311_01

FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 11 2018

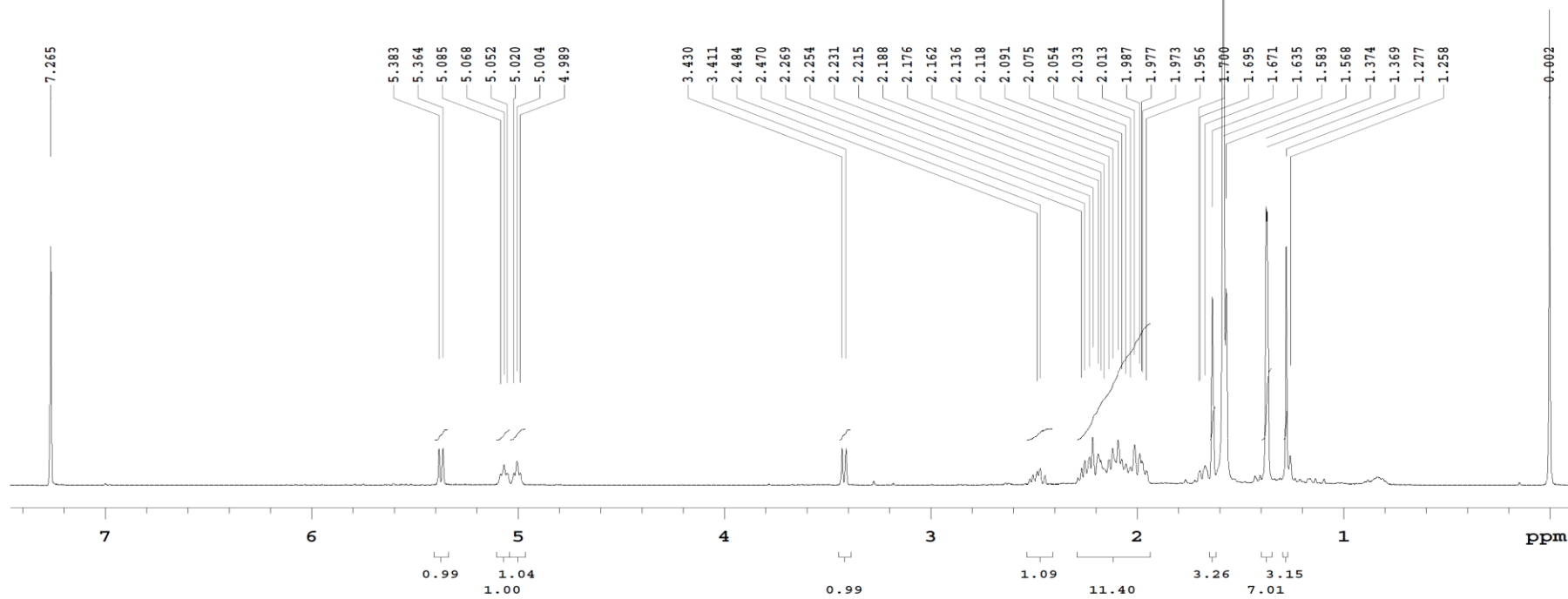
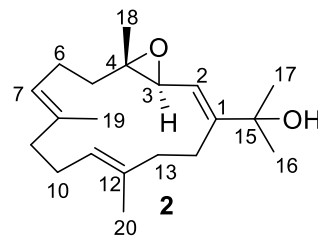


Figure S15: ¹H NMR spectrum of 2 in CDCl₃ at 400 MHz

Sarco-Fr-2- (27-33) -30

Sample Name:

Sarco-Fr-2-_27-33_-30

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

Sarco-Fr-2-_27-33_-30_20180311_01

FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 11 2018

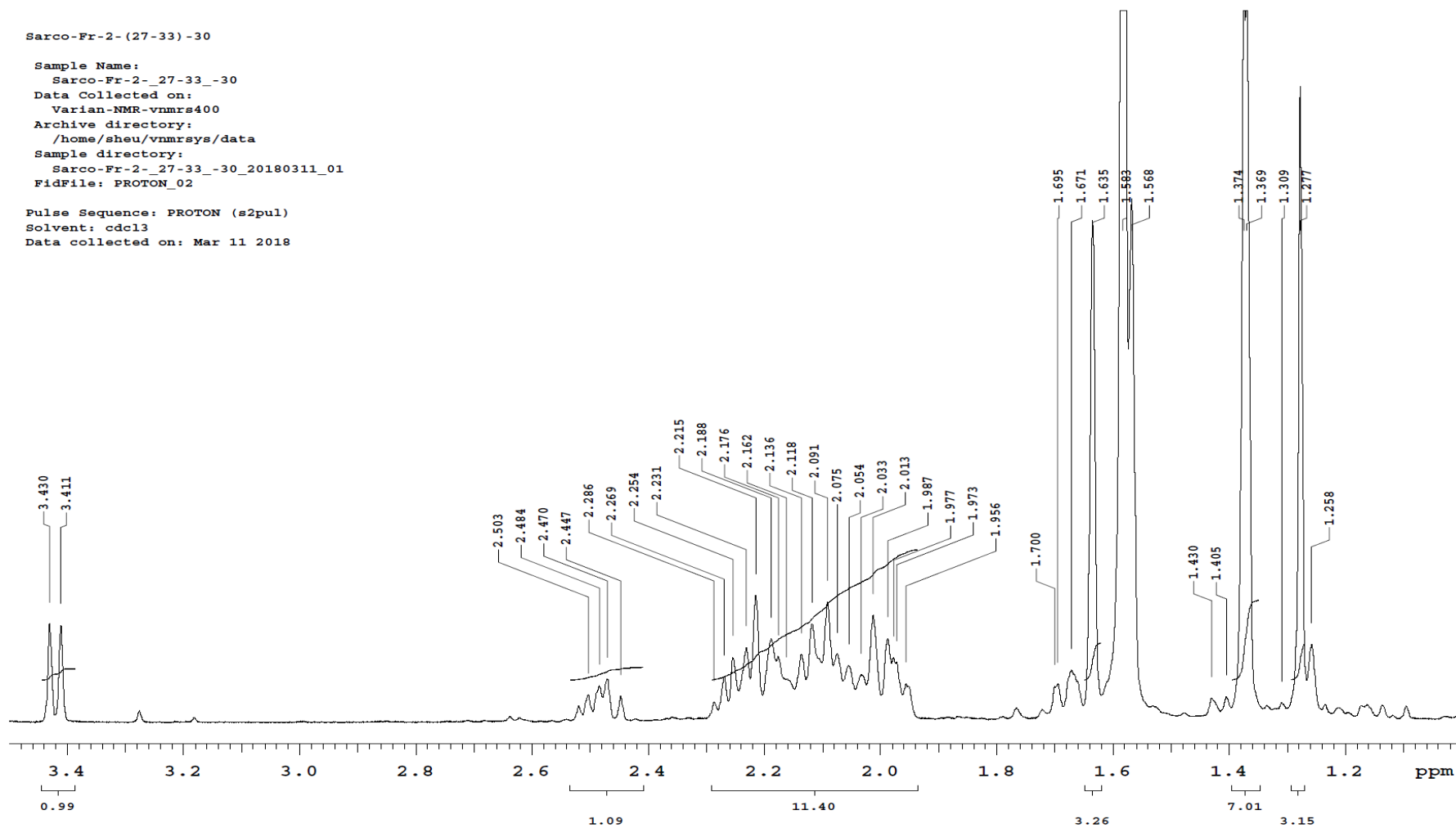


Figure S16: ¹H NMR spectrum (from 1.0 to 3.5 ppm) of 2 in CDCl₃ at 400 MHz

Sarco-Fr-2-(27-33)-30

Sample Name:
Sarco-Fr-2_27-33_30
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2_27-33_30_20180311_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 11 2018

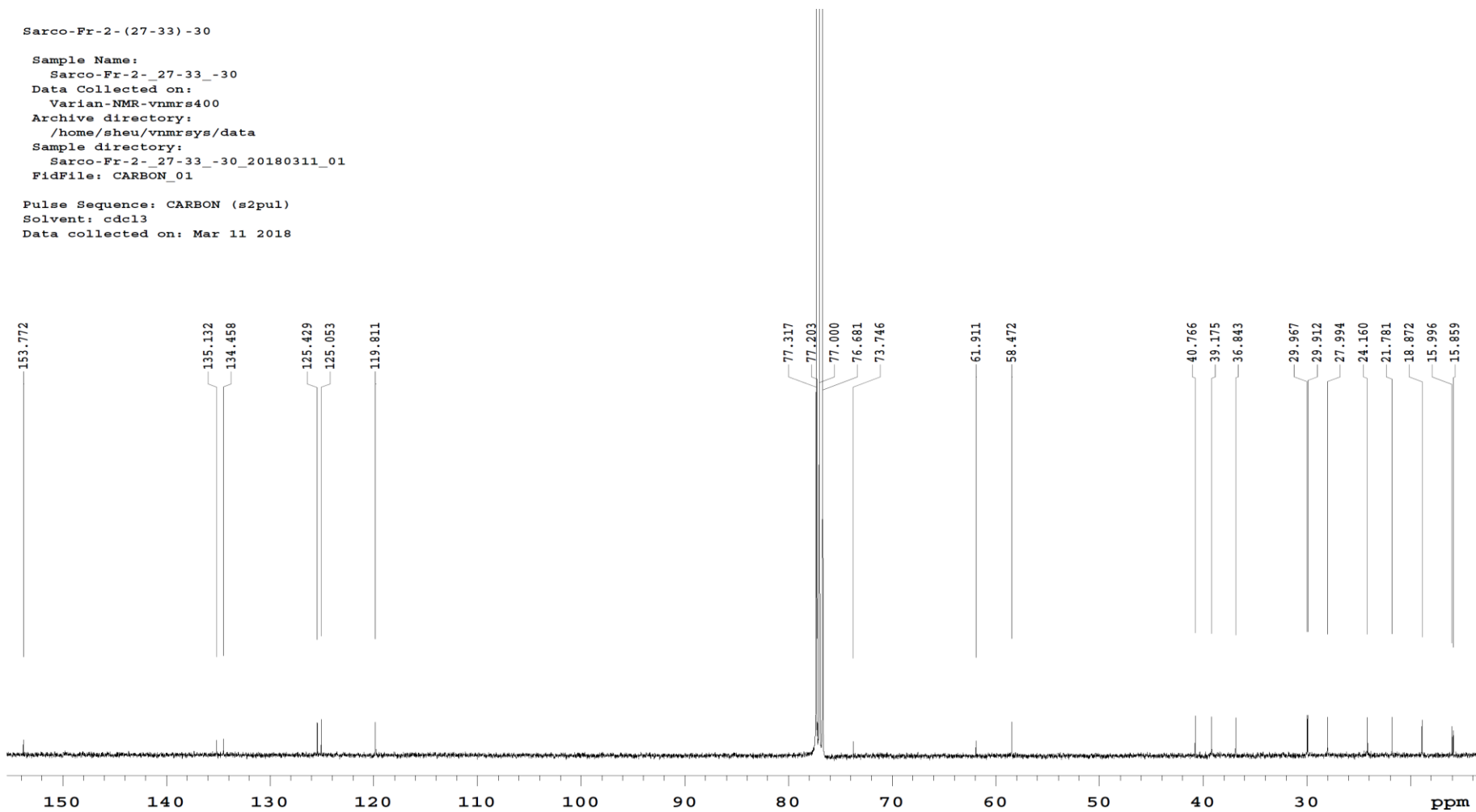


Figure S17: ^{13}C NMR spectrum of **2** in CDCl_3 at 100 MHz

Sarco-Fr-2-(27-33)-30

Sample Name:

Sarco-Fr-2-_27-33_-30

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

Sarco-Fr-2-_27-33_-30_20180311_01

FidFile: DEPT_01

Pulse Sequence: DEPT

Solvent: cdcl3

Data collected on: Mar 11 2018

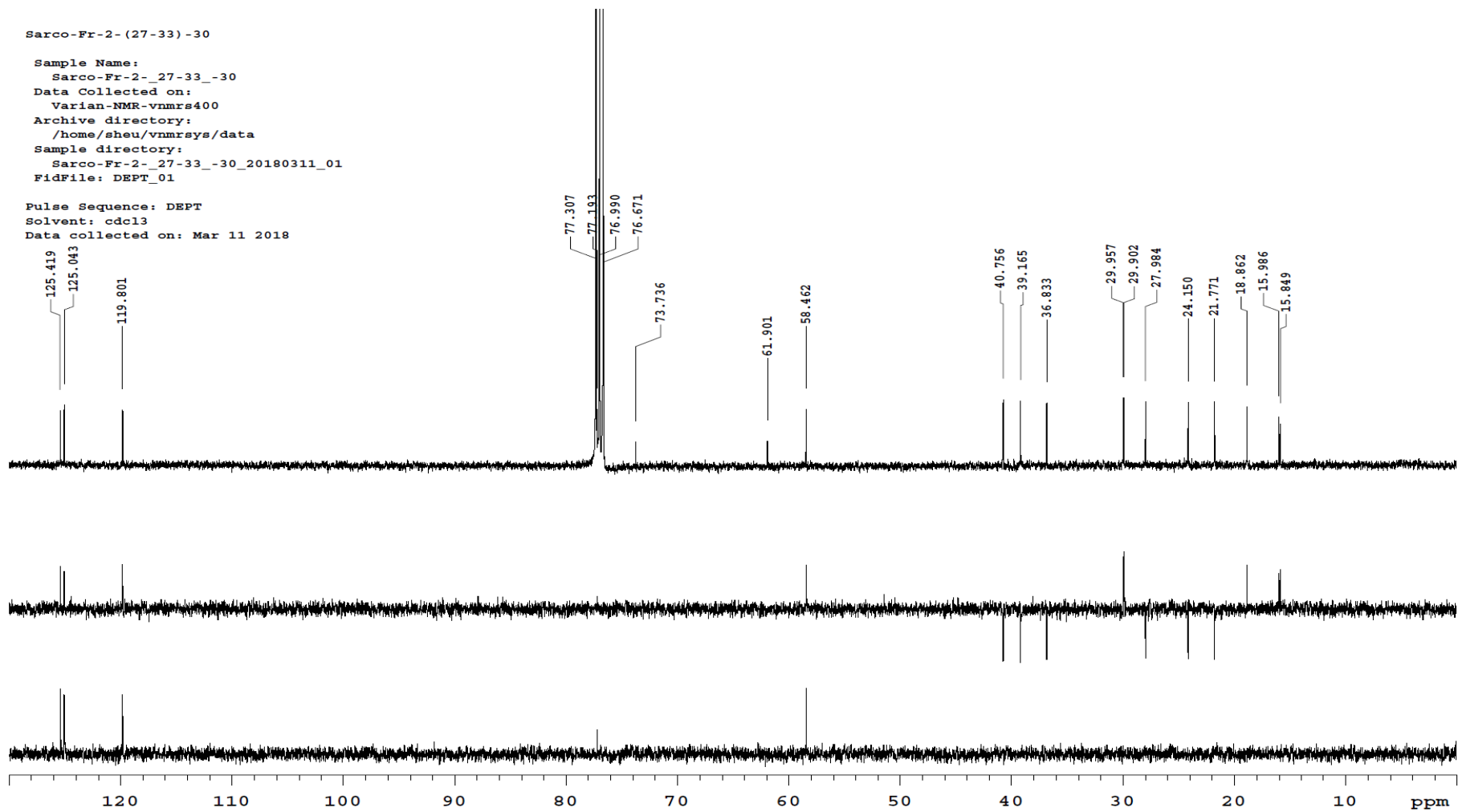


Figure S16: DEPT spectrum of 2

Sarco-Fr-2- (27-33) -30

Sample Name:
Sarco-Fr-2_27-33_-30
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2_27-33_-30_20180311_01
FidFile: HSQCAD_01

Pulse Sequence: HSQCAD
Solvent: cdcl3
Data collected on: Mar 11 2018

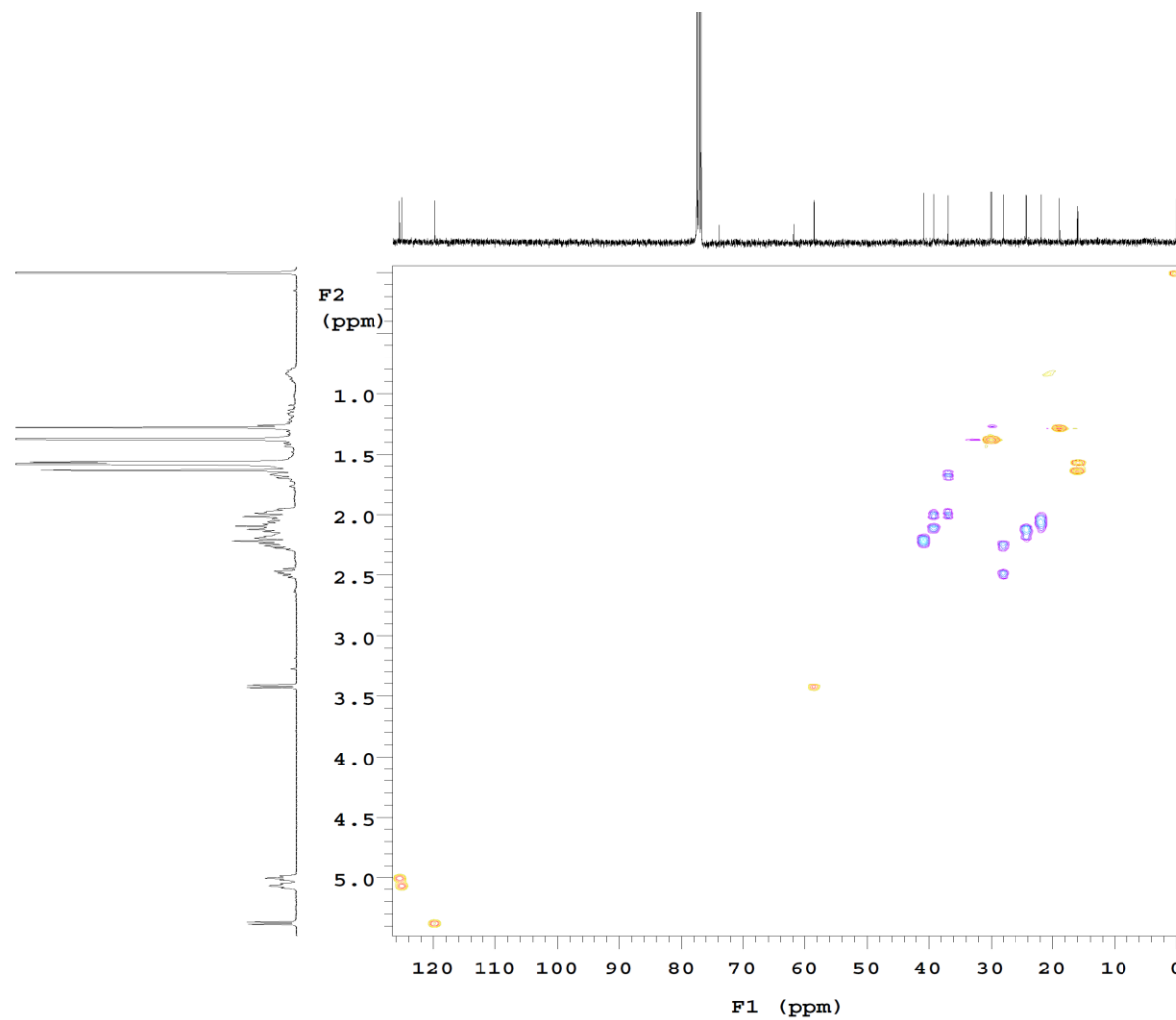


Figure S19: HSQC spectrum of 2

Sarco-Fr-2-(27-33)-30

Sample Name:
Sarco-Fr-2_27-33_30
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2_27-33_30_20180311_01
FidFile: gCOSY_01

Pulse Sequence: gCOSY
Solvent: cdcl3
Data collected on: Mar 12 2018

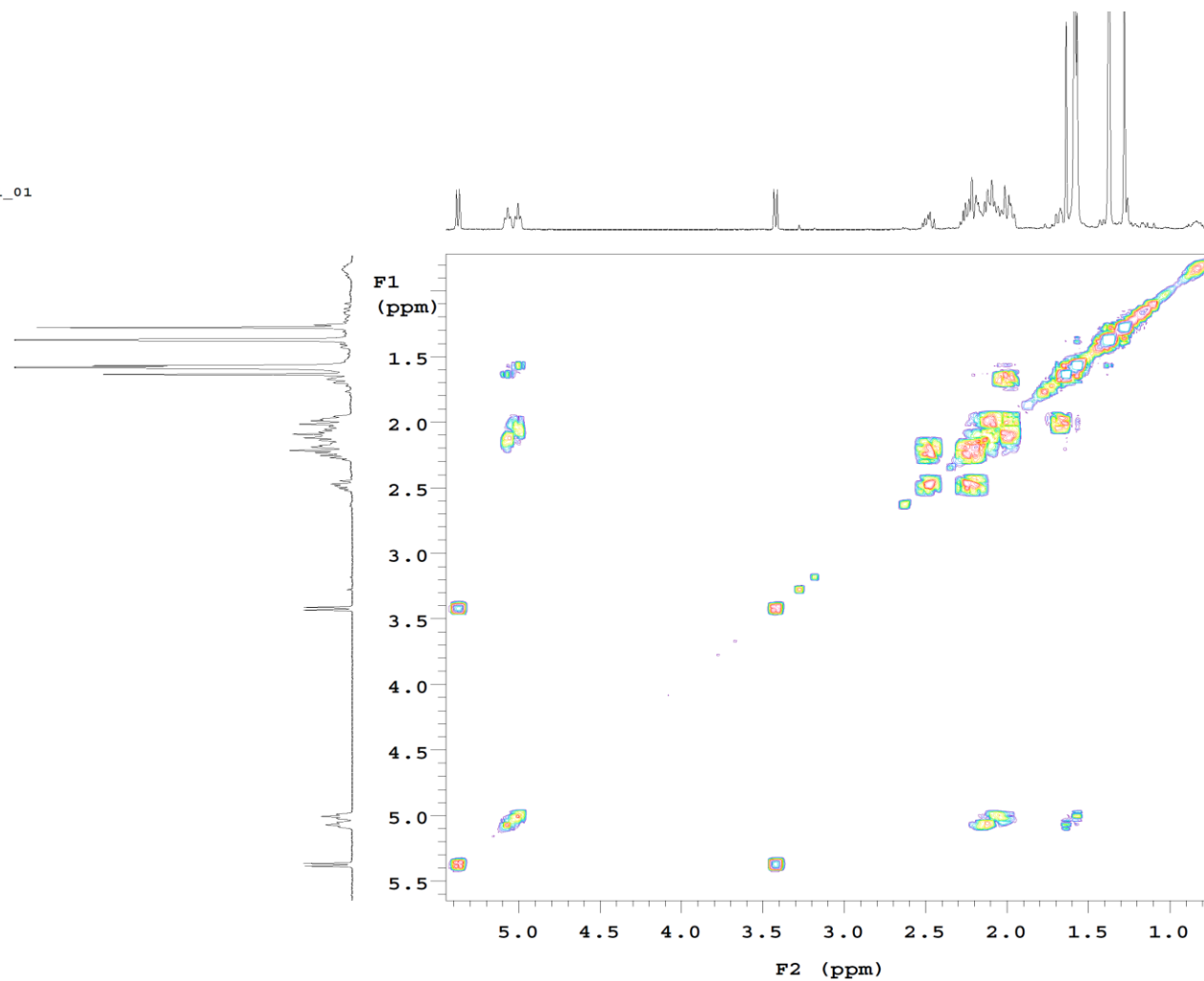


Figure S20: COSY spectrum of 2

Sarco-Fr-2-(27-33)-30

Sample Name:
Sarco-Fr-2-27-33-30
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2-27-33-30_20180311_01
FidFile: gHMBCAD_01

Pulse Sequence: gHMBCAD
Solvent: cdcl3
Data collected on: Mar 12 2018

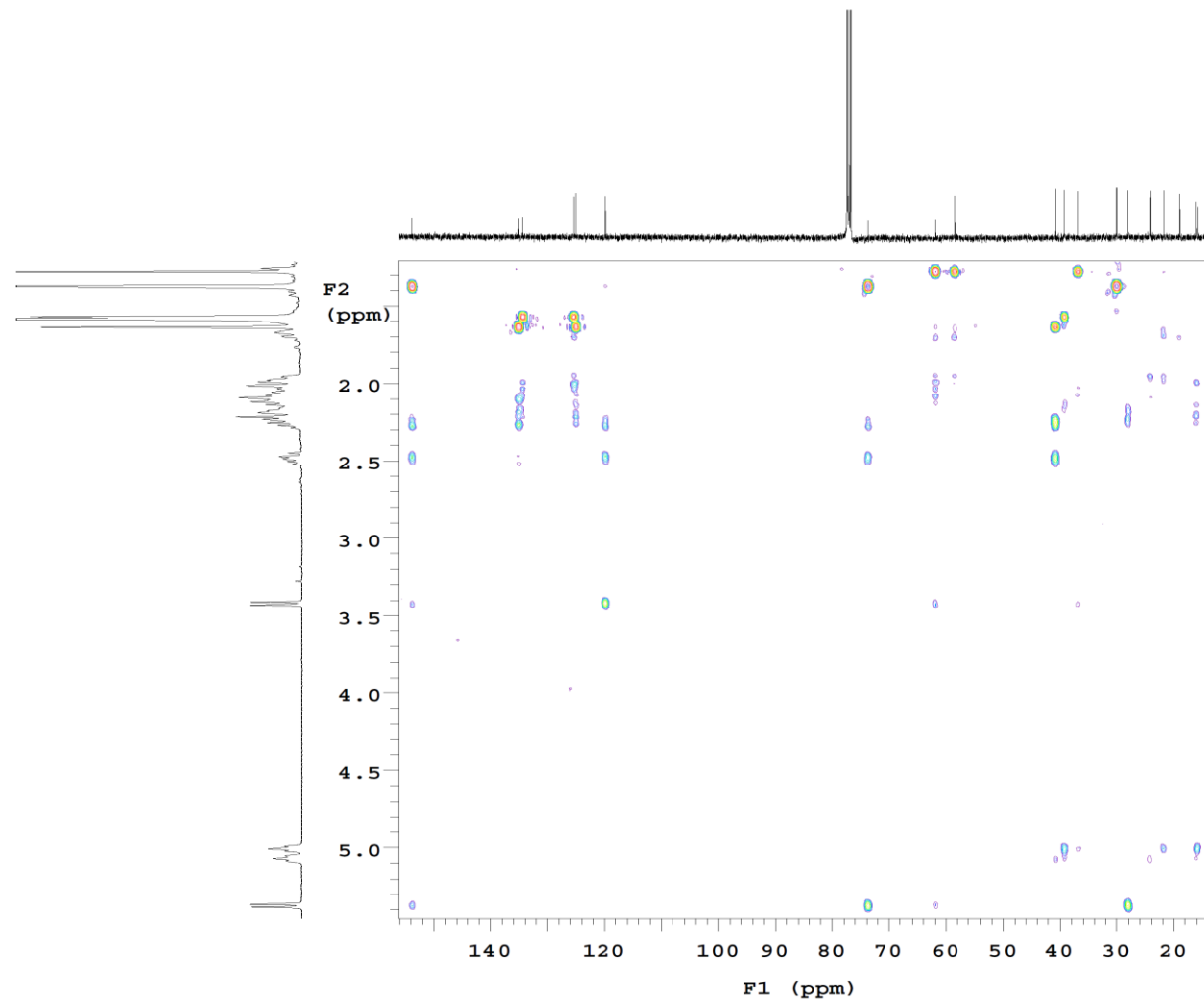


Figure S21: HMBC spectrum of 2

Sarco-Fr-2-(27-33)-30

Sample Name:
Sarco-Fr-2-_27-33_-30
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2-_27-33_-30_20180311_01
FidFile: NOESY_01

Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Mar 12 2018

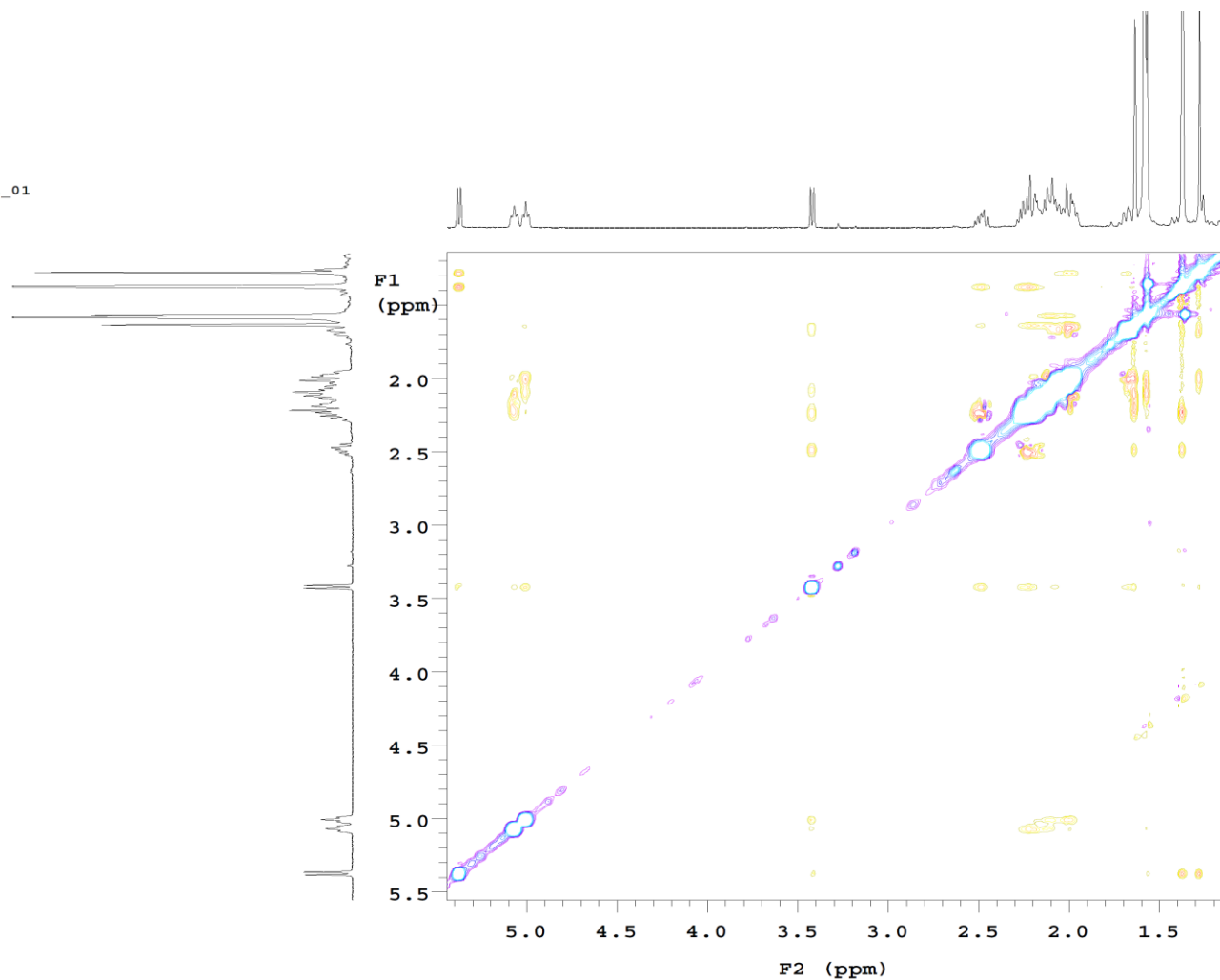


Figure S22: NOESY spectrum of 2

Compound 3 spectroscopic data

FT-MS

Analysis Info

Analysis Name D:\Data\1\SARCOFR24019_000003.d
Method broadband first signal
Sample Name Sarco-fr-2-40-27
Comment ESI Positive

2/27/2018 2:17:51 PM

Instrument: FT-MS solariX

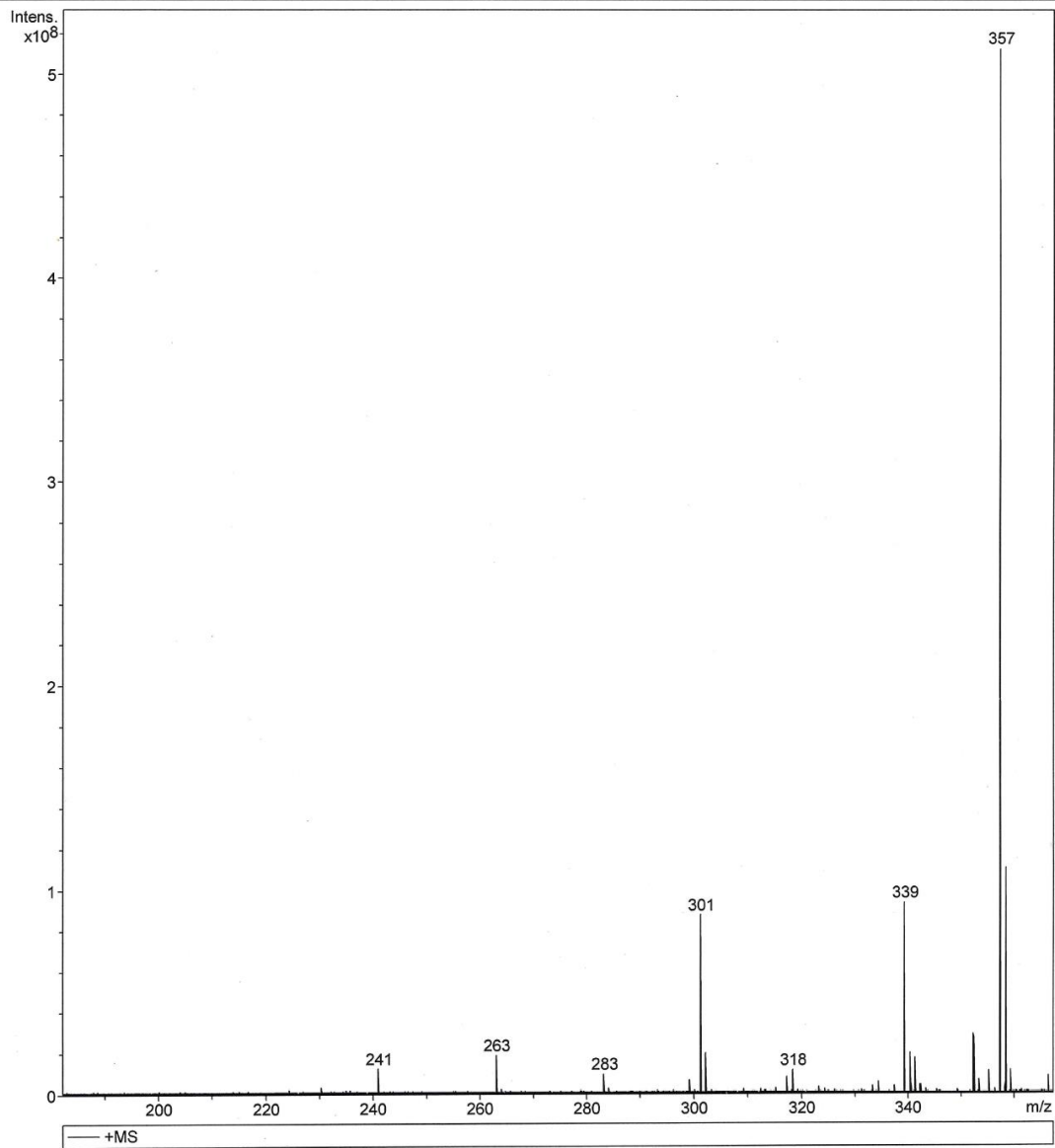


Figure 23: ESIMS spectrum of 3

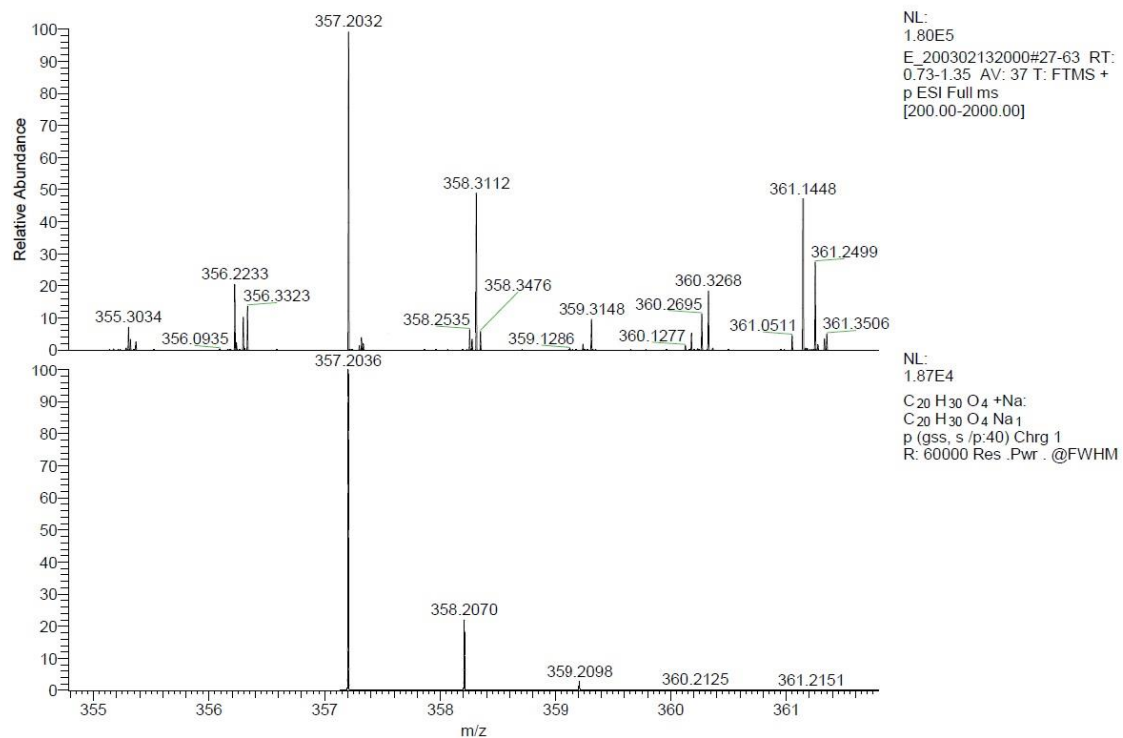


Figure S24: HRESIMS spectrum of 3

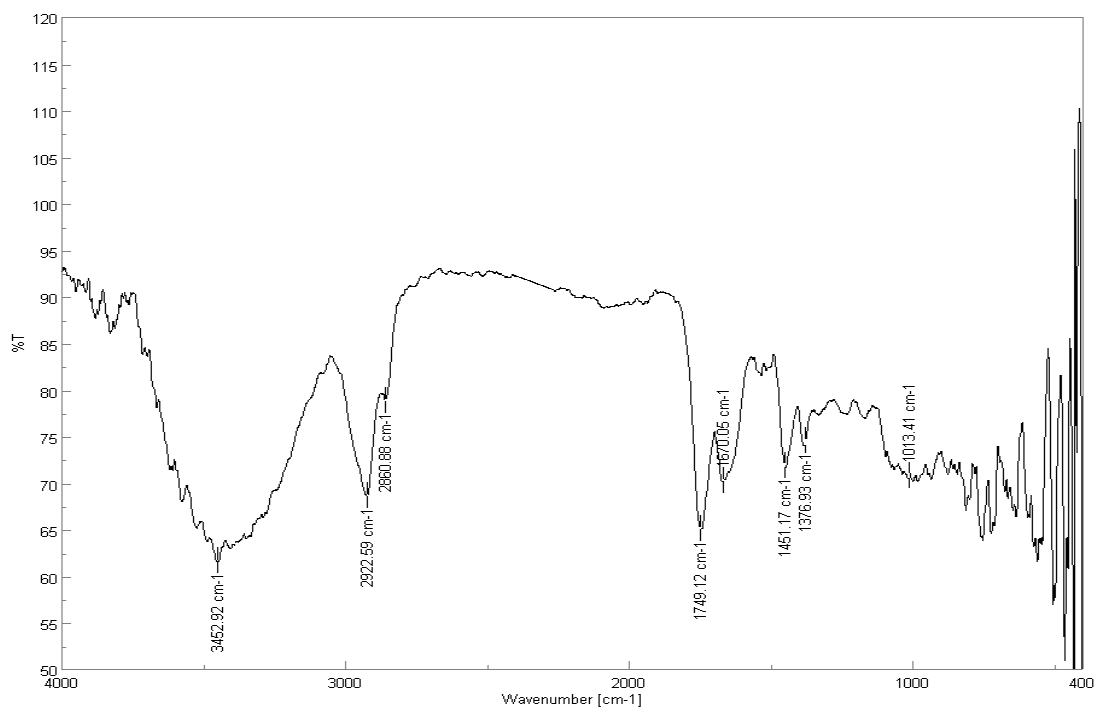


Figure S25: IR spectrum of 3

Sarco-fr-2-40-(17-19)-27

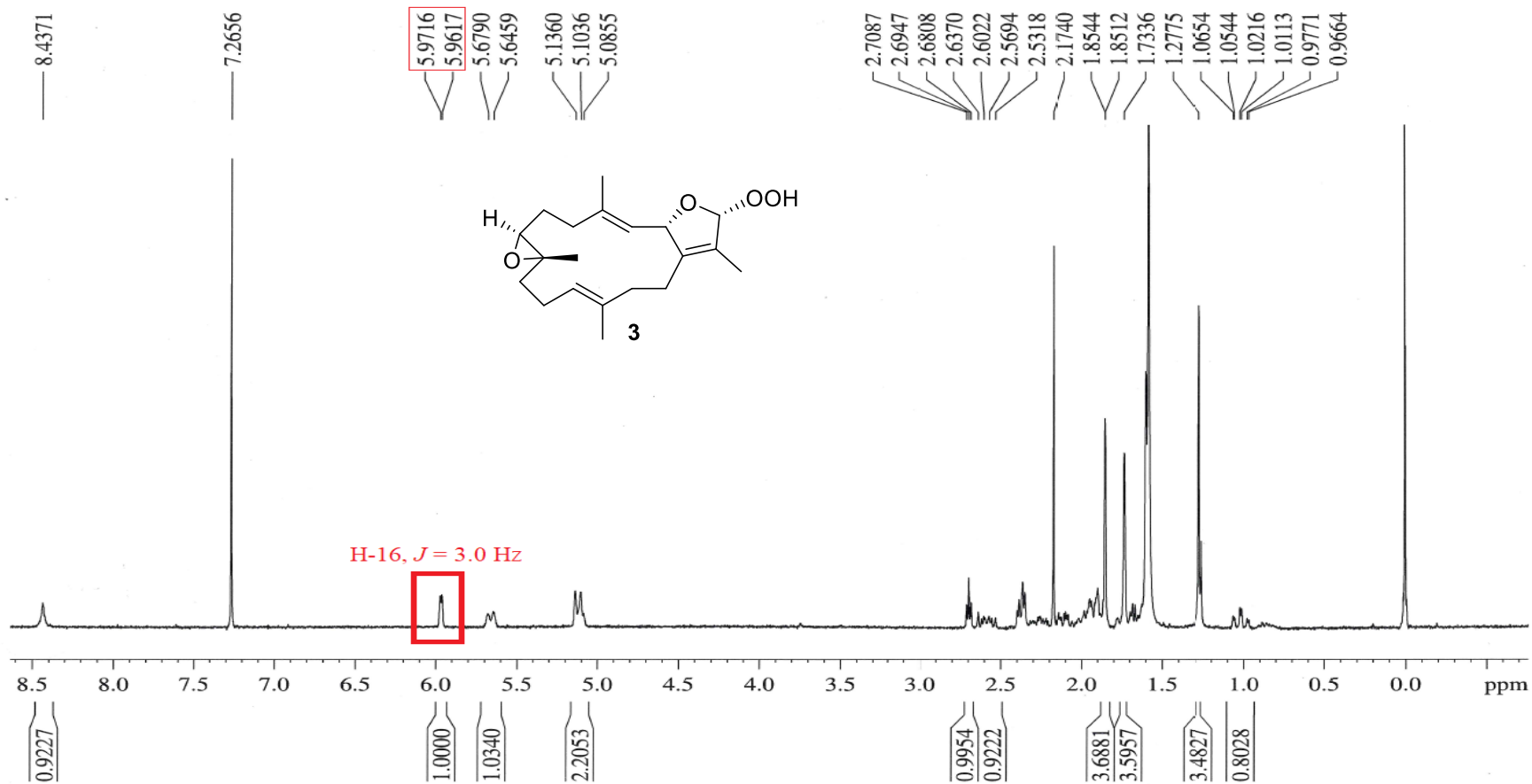


Figure S26: ^1H NMR spectrum of 3 in CDCl_3 at 300 MHz

Sarco-Fr-2-40-17-27

Sample Name:
Sarco-Fr-2-40-17-27
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2-40-17-27_20180401_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 1 2018

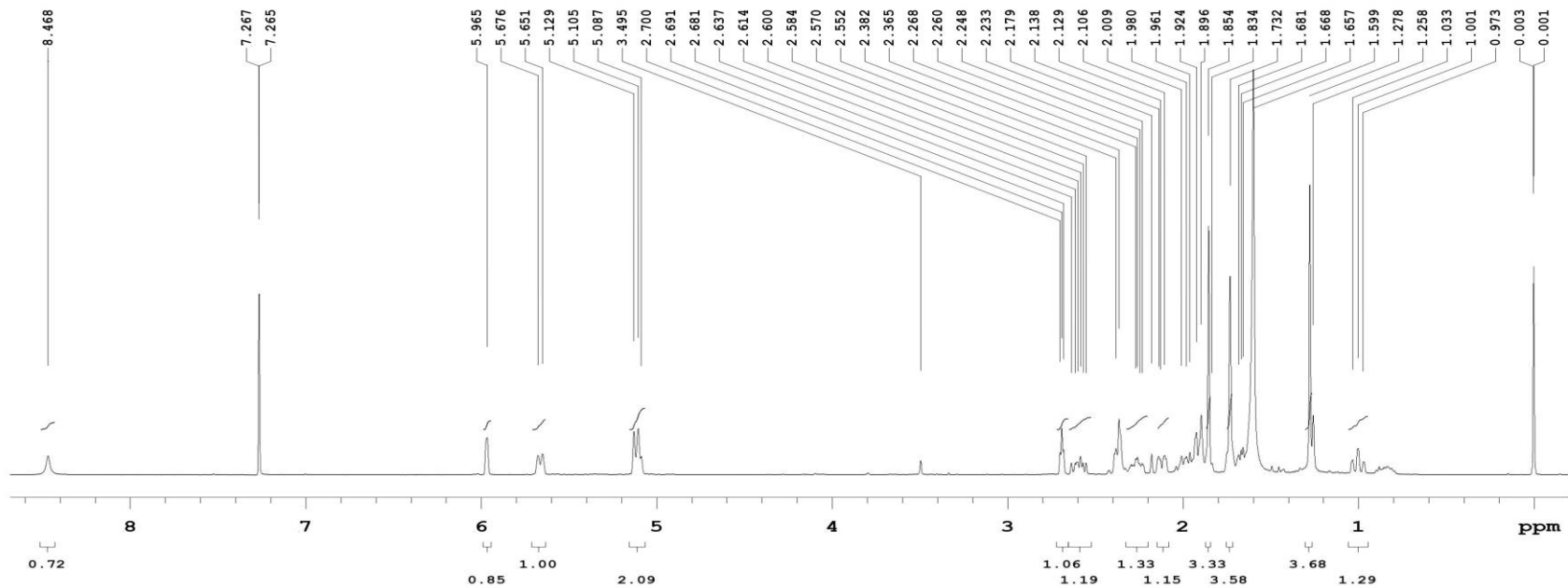


Figure S27: ^1H NMR spectrum of **3** in CDCl_3 at 400 MHz

Sarco-Fr-2-40-17-27

Sample Name:

Sarco-Fr-2-40-17-27

Data Collected on:

Varian-NMR-vmrms400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

Sarco-Fr-2-40-17-27_20180401_01

FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Apr 1 2018

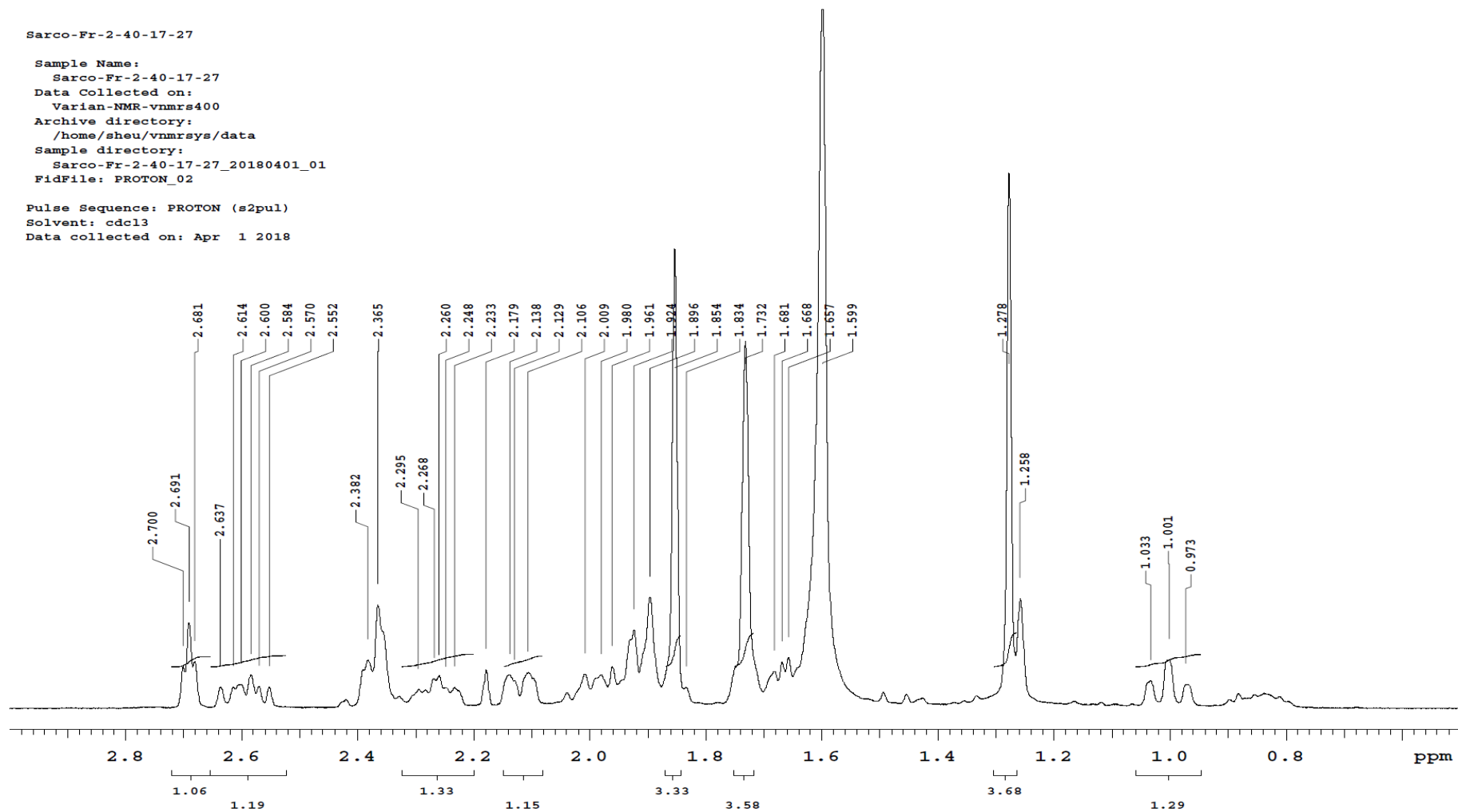


Figure S28: ^1H NMR spectrum (from 0.5 to 3.0 ppm) of **3** in CDCl_3 at 400 MHz

Sarco-Fr-2-40-17-27

Sample Name:
Sarco-Fr-2-40-17-27
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2-40-17-27_20180401_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 1 2018

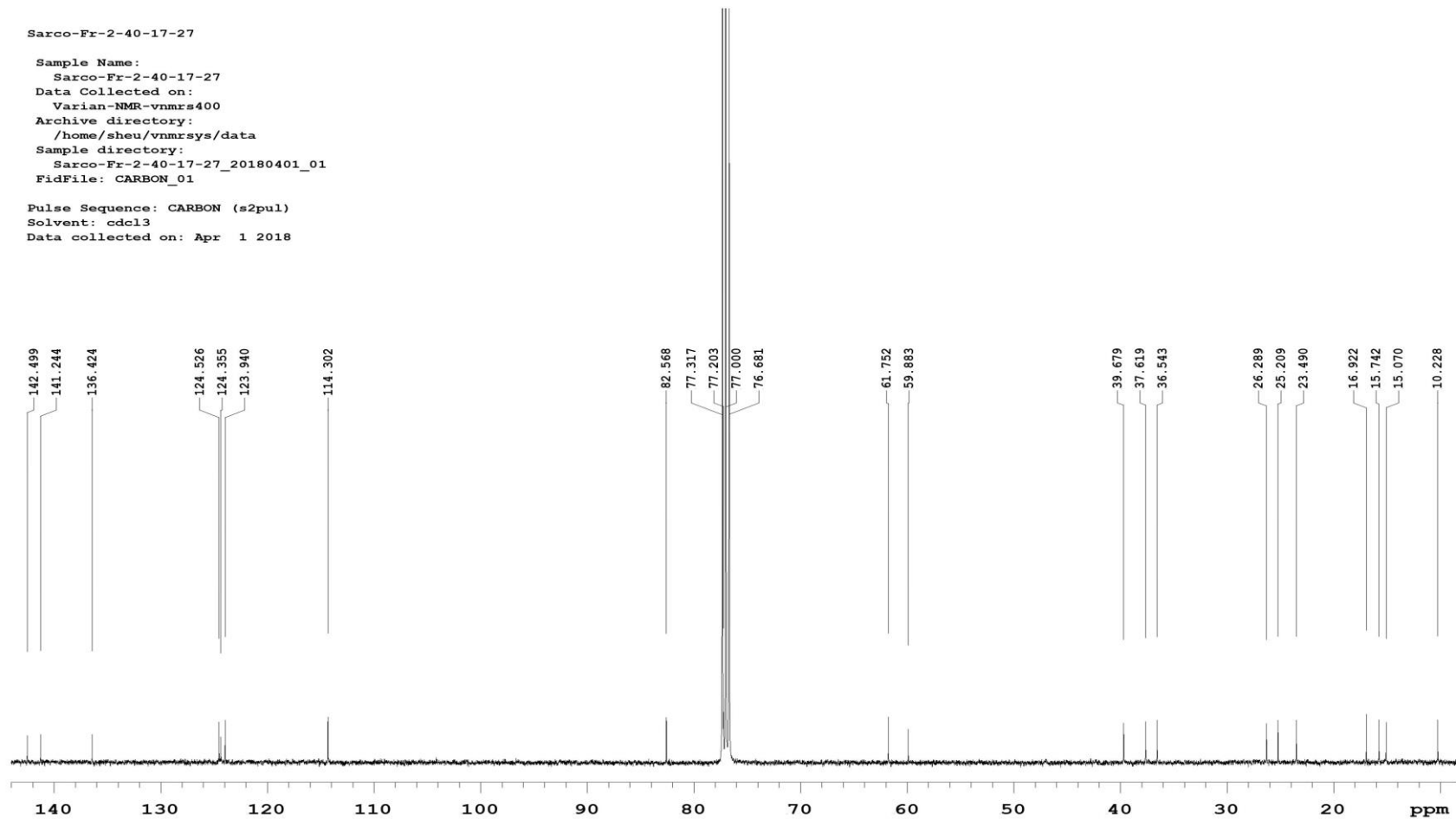


Figure S29: ¹³C NMR spectrum of **3** in CDCl₃ at 100 MHz

Sarco-Fr-2-40-17-27
Sample Name:
Sarco-Fr-2-40-17-27
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2-40-17-27_20180401_01
FidFile: DEPT_01
Pulse Sequence: DEPT
Solvent: cdcl3
Data collected on: Apr 1 2018

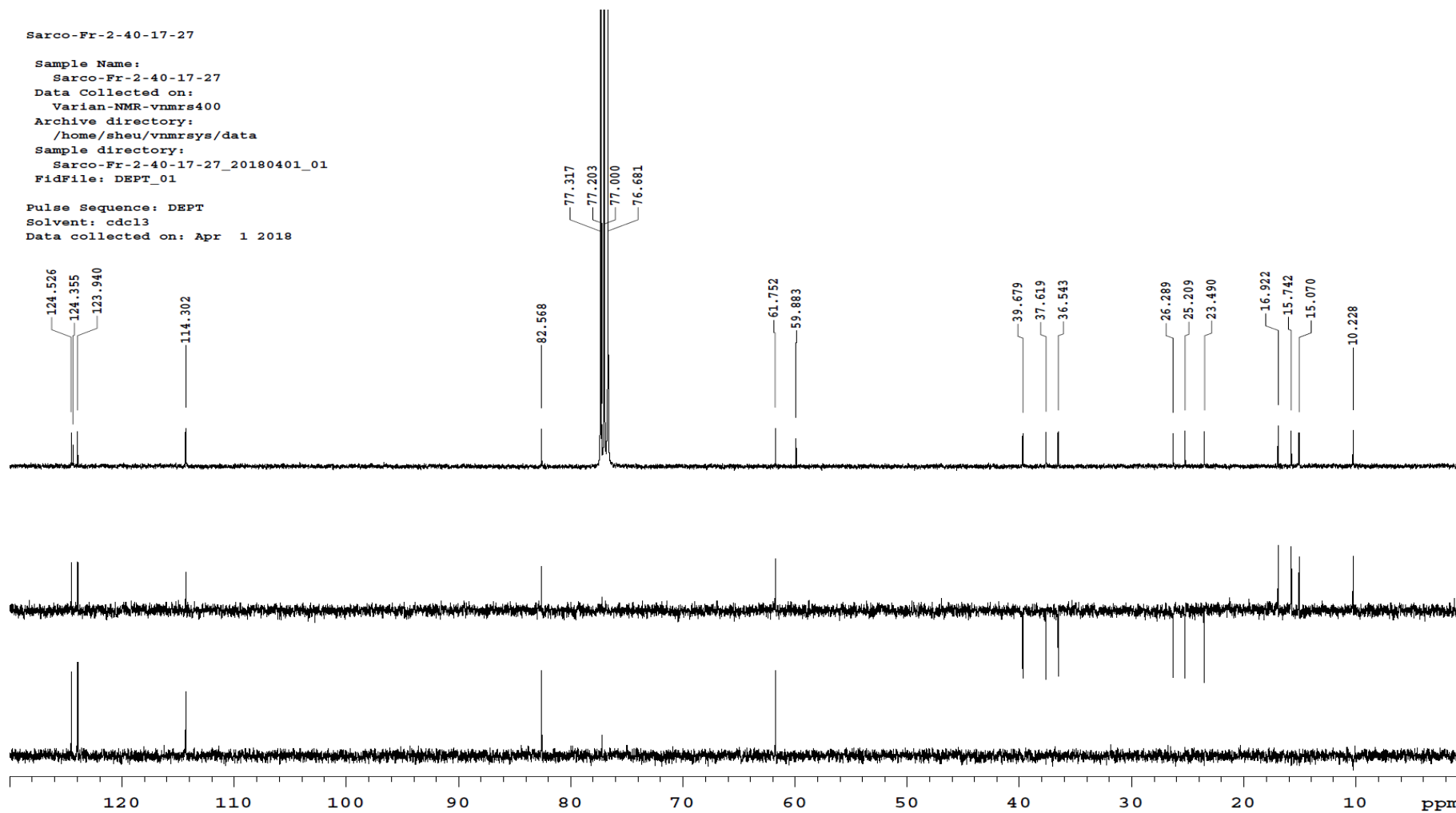


Figure S30: DEPT spectrum of 3

Sarco-Fr-2-40-17-27

Sample Name:
Sarco-Fr-2-40-17-27
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
Sarco-Fr-2-40-17-27_20180401_01
FidFile: HSQCAD_01

Pulse Sequence: HSQCAD
Solvent: cdcl3
Data collected on: Apr 1 2018

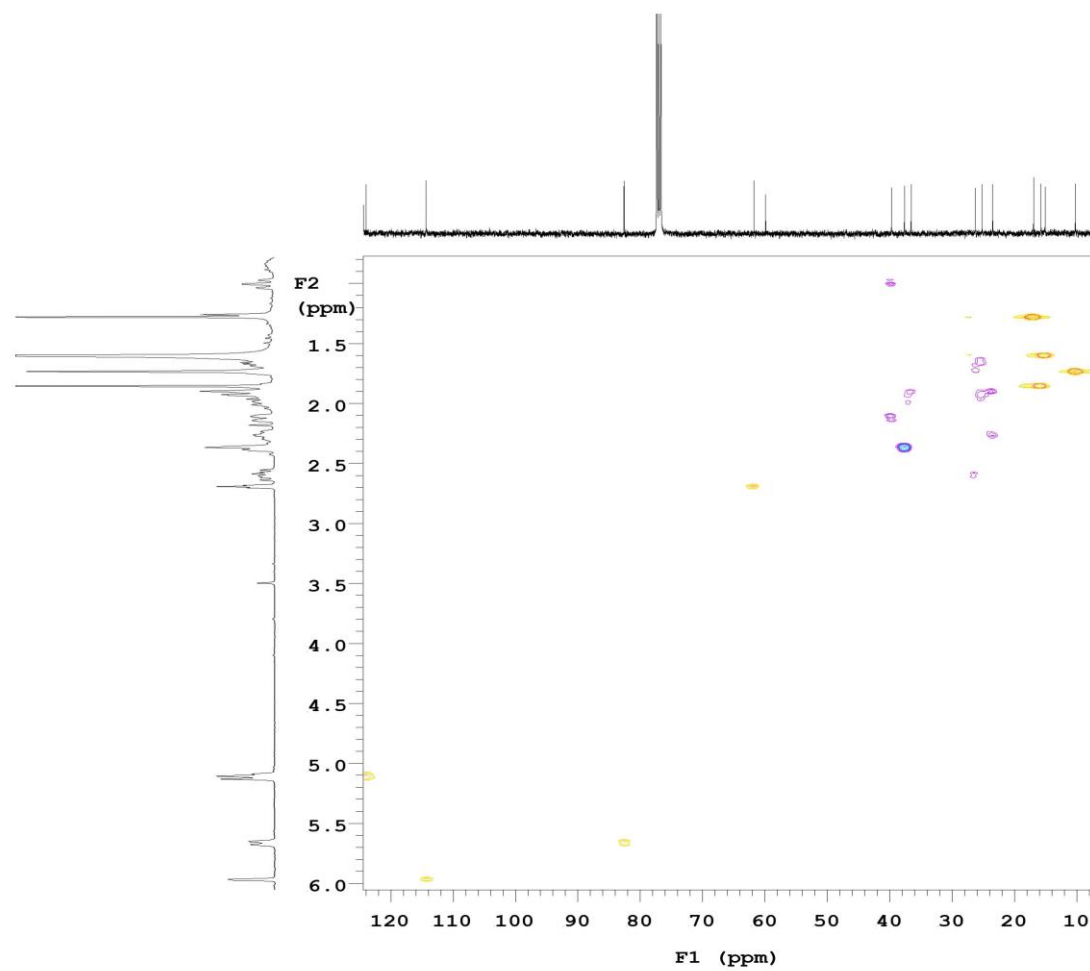


Figure S31: HSQC spectrum of 3

Sarco-Fr-2-40-17-27

Sample Name:

Sarco-Fr-2-40-17-27

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

Sarco-Fr-2-40-17-27_20180401_01

FidFile: gCOSY_01

Pulse Sequence: gCOSY

Solvent: cdcl3

Data collected on: Apr 1 2018

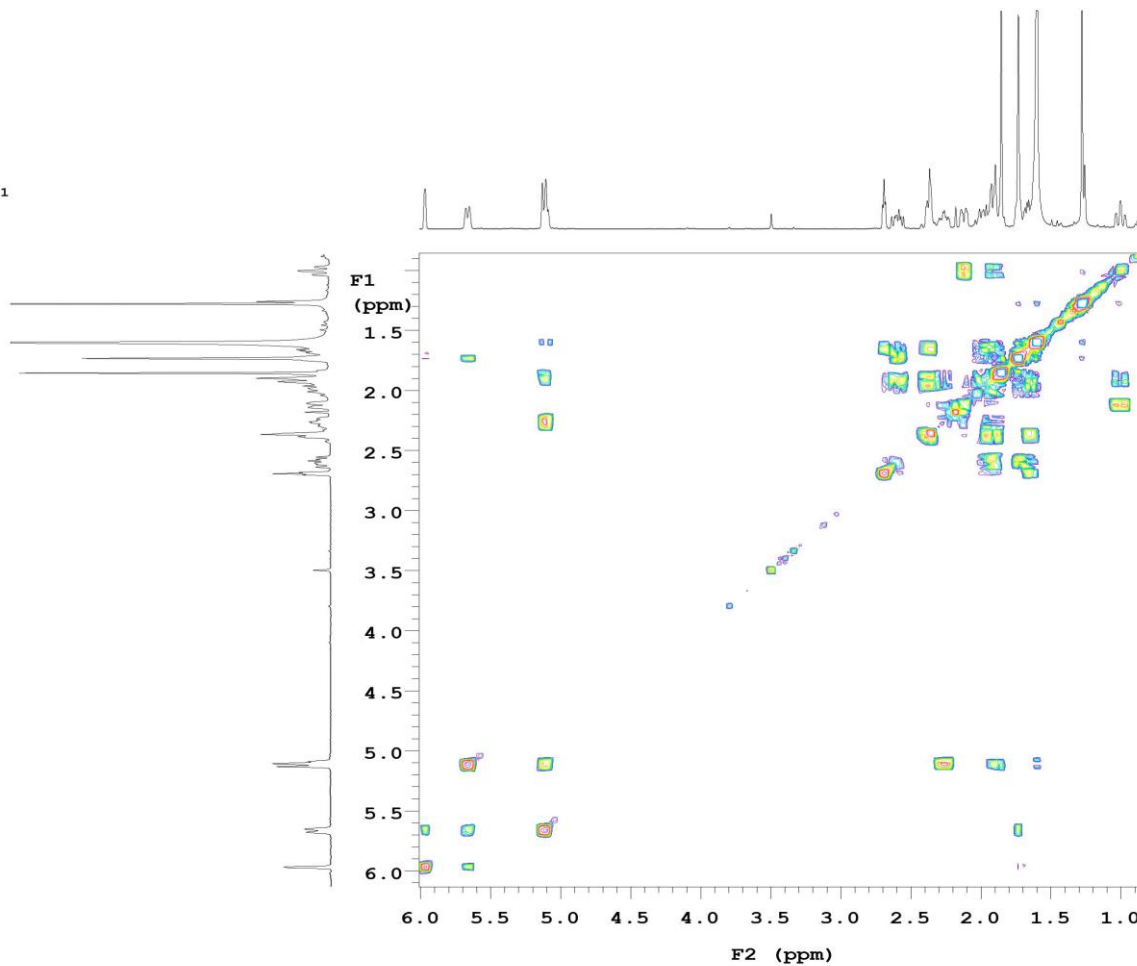


Figure S32: COSY spectrum of 3

Sarco-Fr-2-40-17-27

Sample Name:

Sarco-Fr-2-40-17-27

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

Sarco-Fr-2-40-17-27_20180401_01

FidFile: gHMBCAD_01

Pulse Sequence: gHMBCAD

Solvent: cdcl3

Data collected on: Apr 2 2018

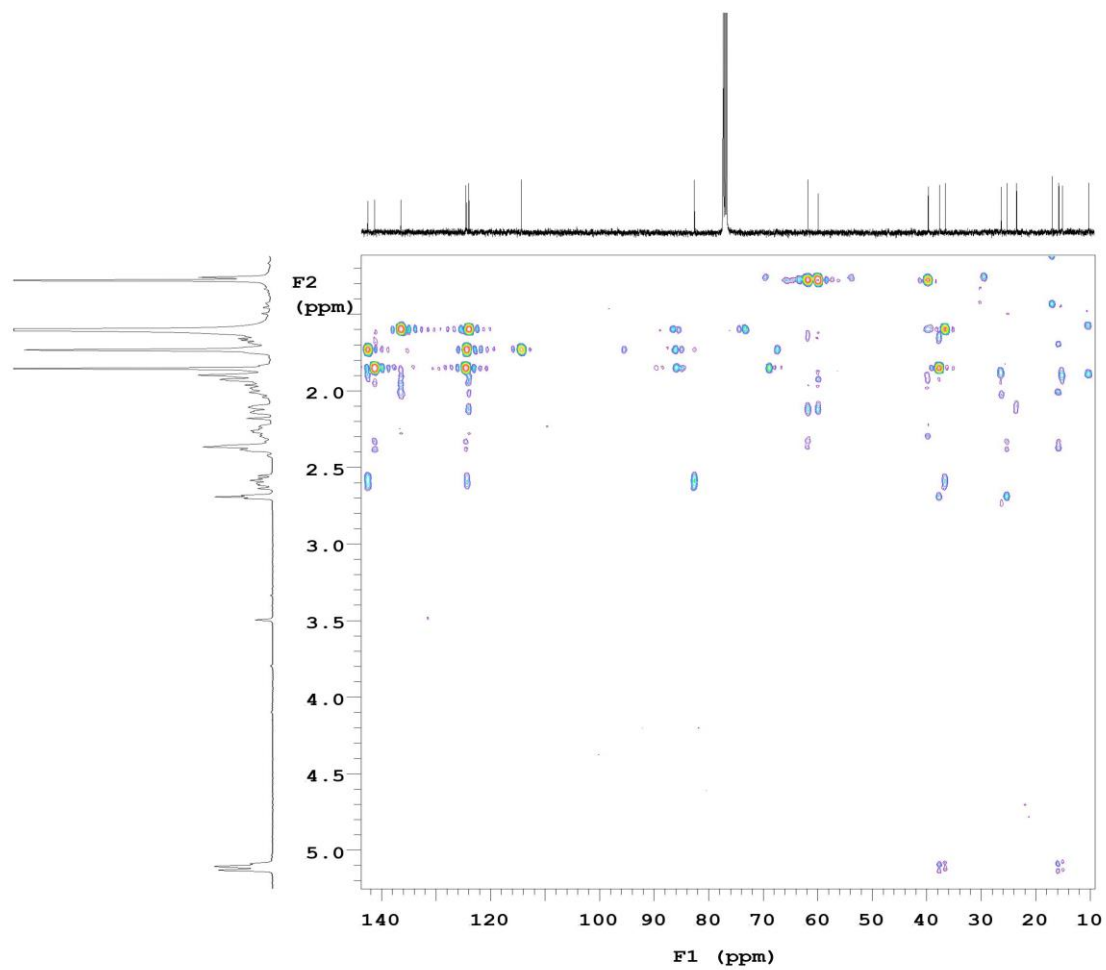


Figure S33: HMBC spectrum of 3

Sarco-Fr-2-40-17-27

Sample Name:

Sarco-Fr-2-40-17-27

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

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Pulse Sequence: NOESY

Solvent: cdcl3

Data collected on: Apr 2 2018

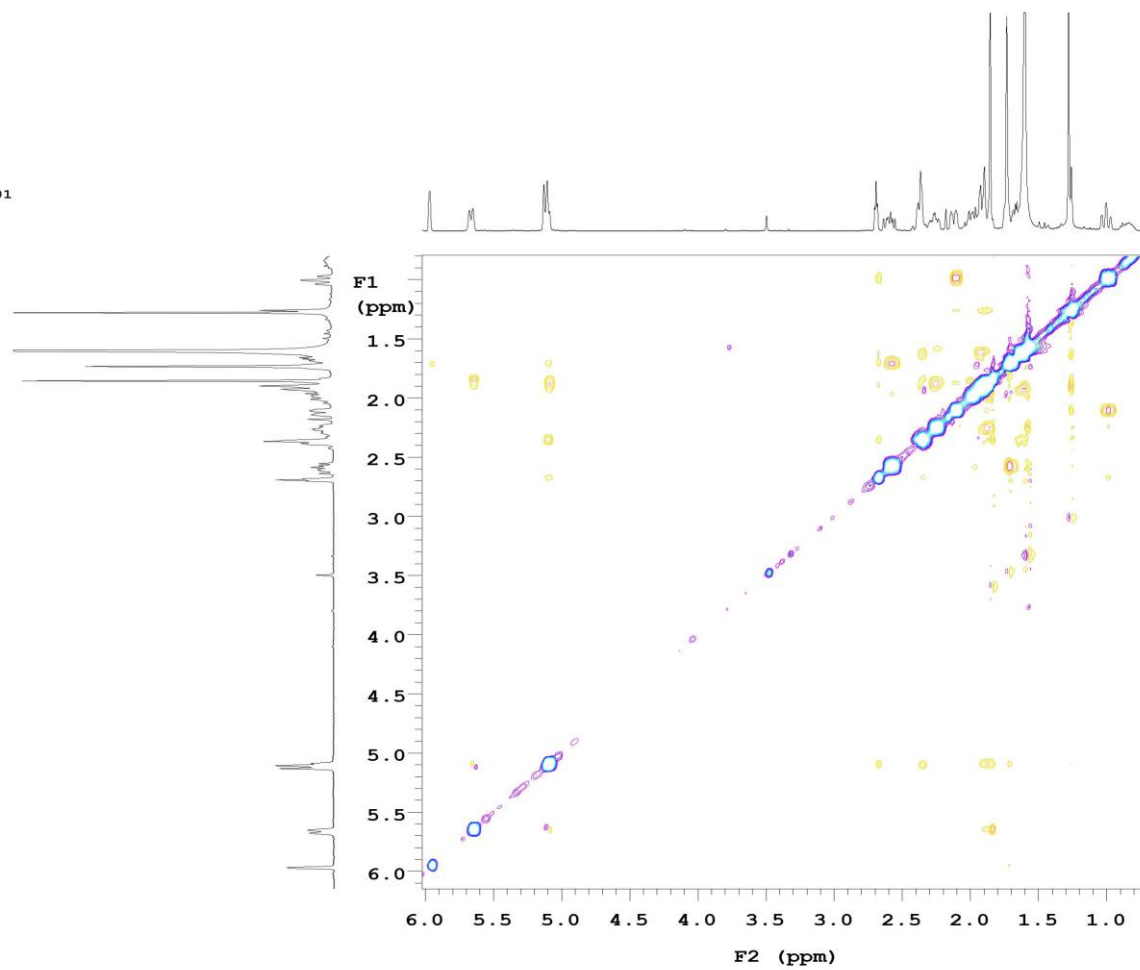


Figure S34: NOESY spectrum of 3

Compound 4 spectroscopic data

FT-MS

Analysis Info

Analysis Name D:\Data\1\F110852_000002.d
Method broadband first signal
Sample Name Sarco-fr-2-42
Comment ESI Positive

3/30/2016 1:51:40 PM

Instrument: FT-MS solarix

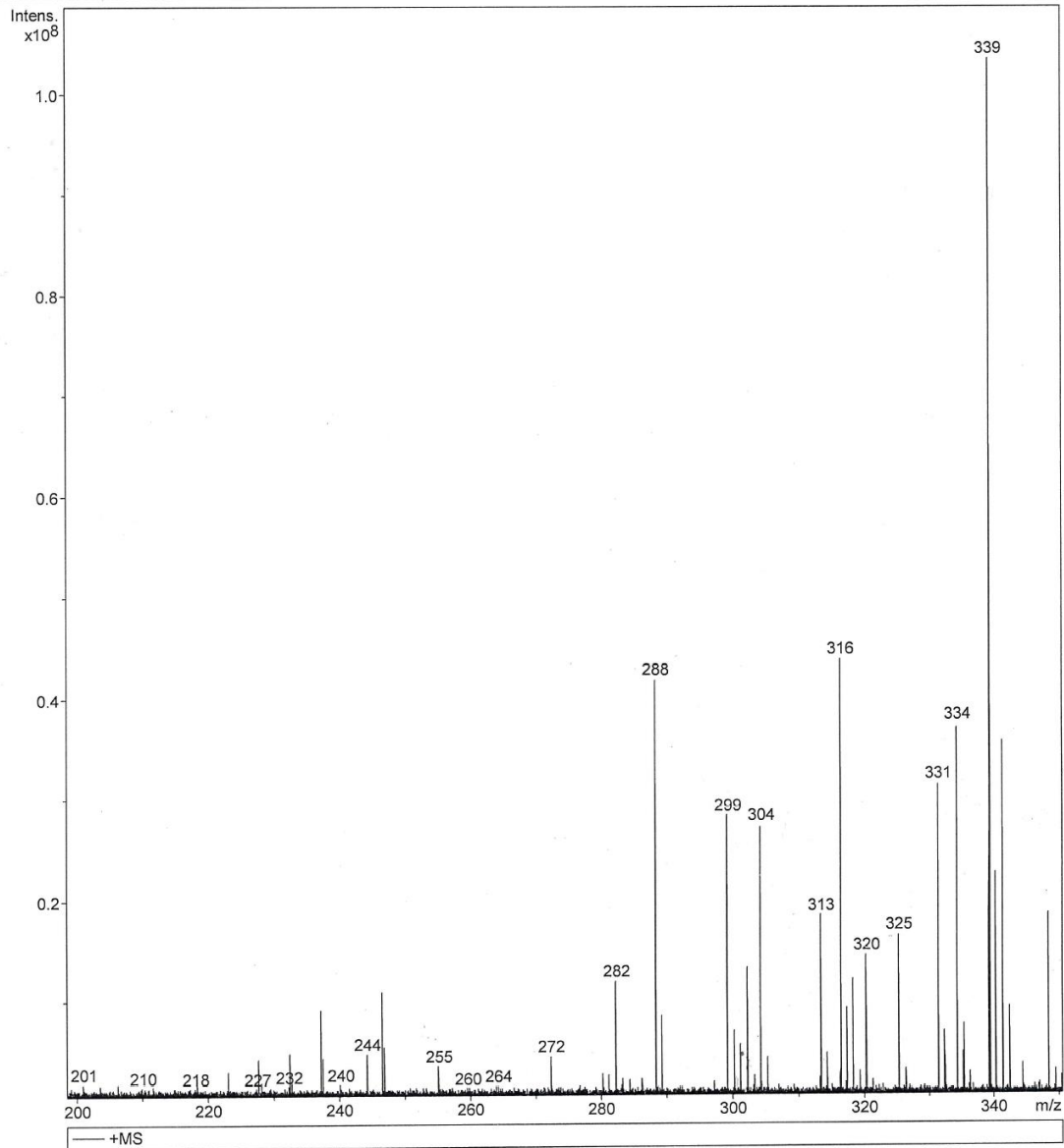


Figure S35: ESIMS spectrum of 4

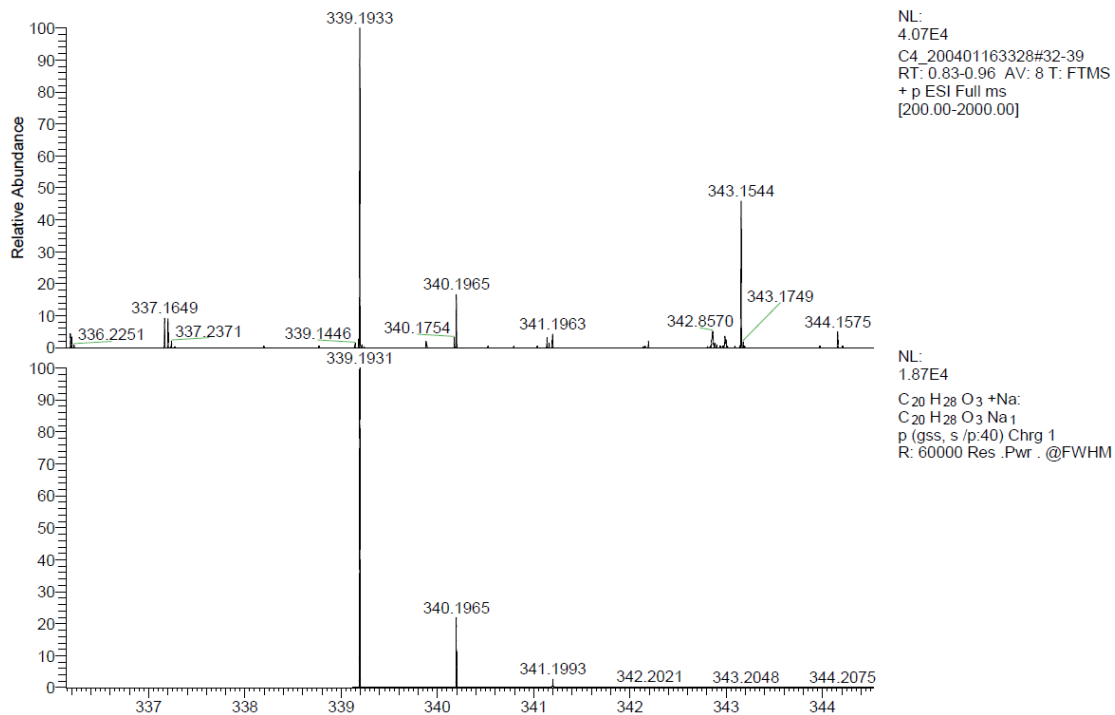


Figure S36: HRESIMS spectrum of 4

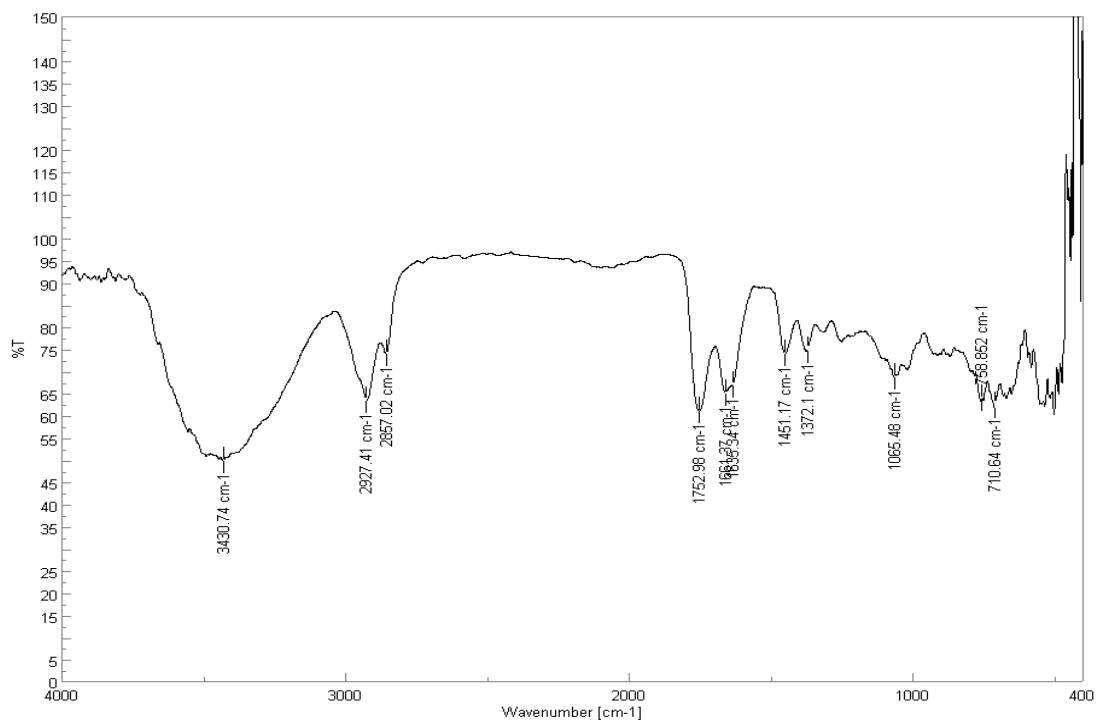


Figure S37: IR spectrum of 4

Sarco-Fr-2-42

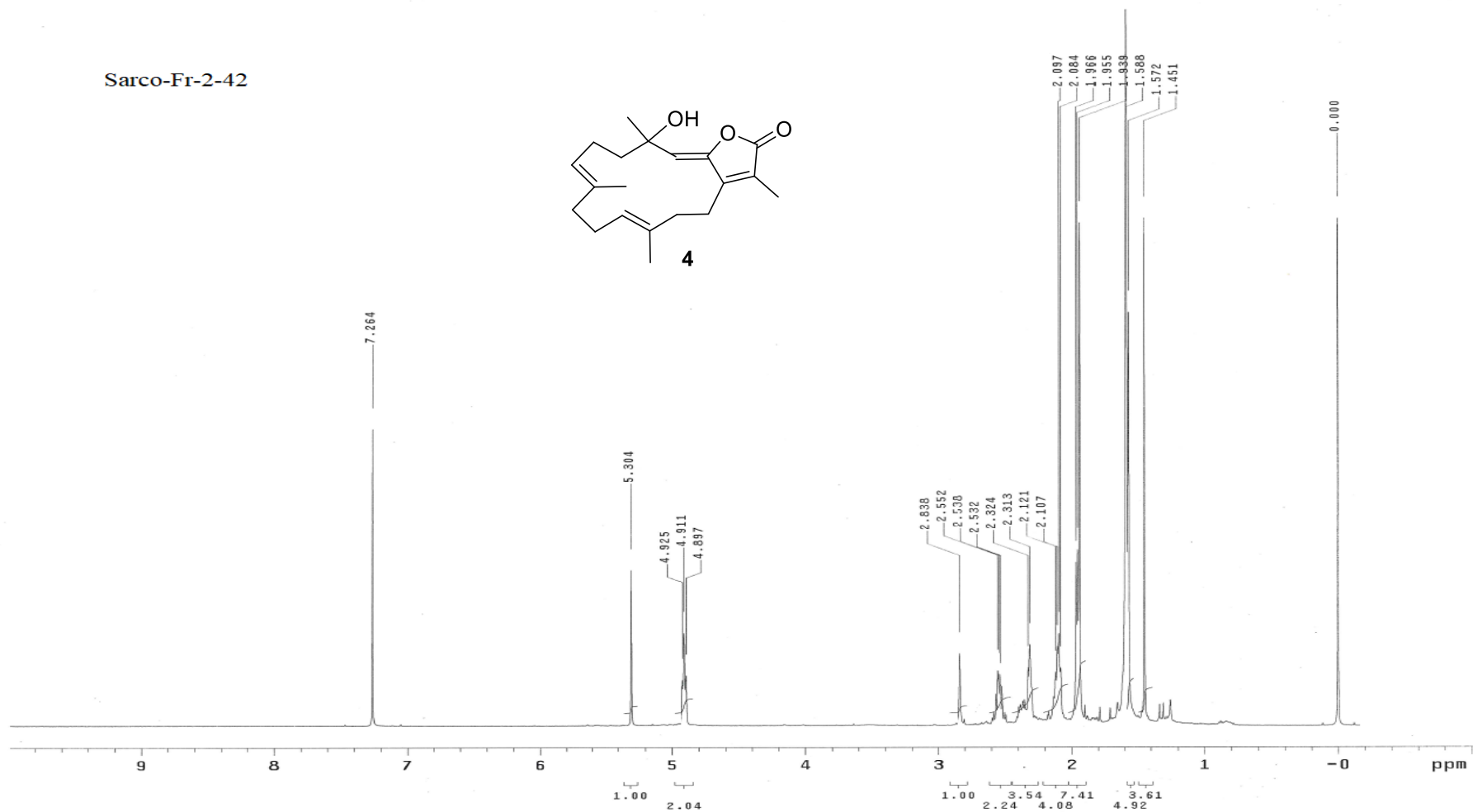
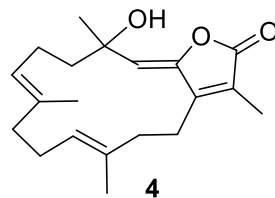


Figure S38: ¹H NMR spectrum of 4 in CDCl₃ at 500 MHz

Sarco-Fr-2-42

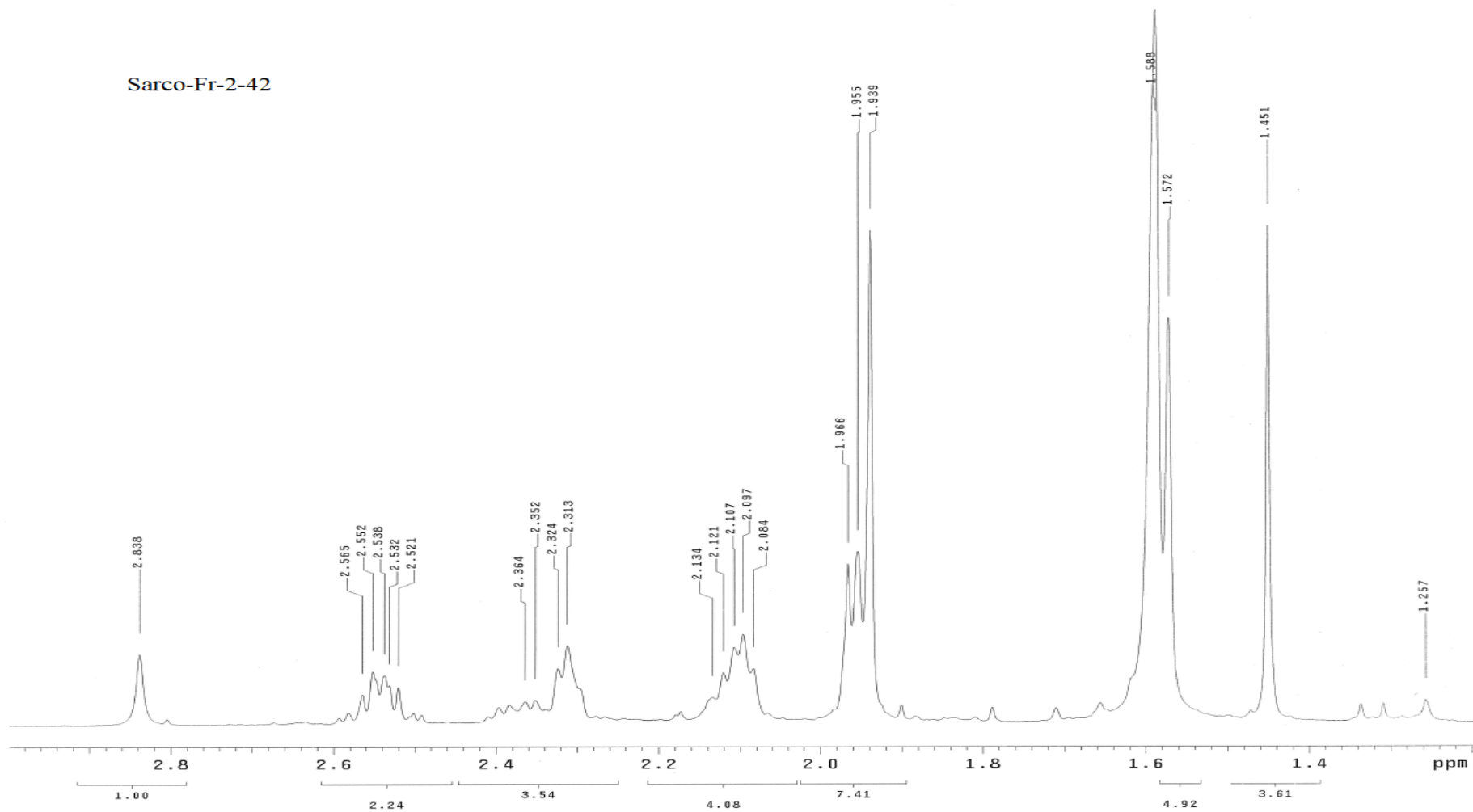


Figure S39: ¹H NMR spectrum (from 1.2 to 3.0 ppm) of **4** in CDCl₃ at 500 MHz

Sarco-Fr-2-42

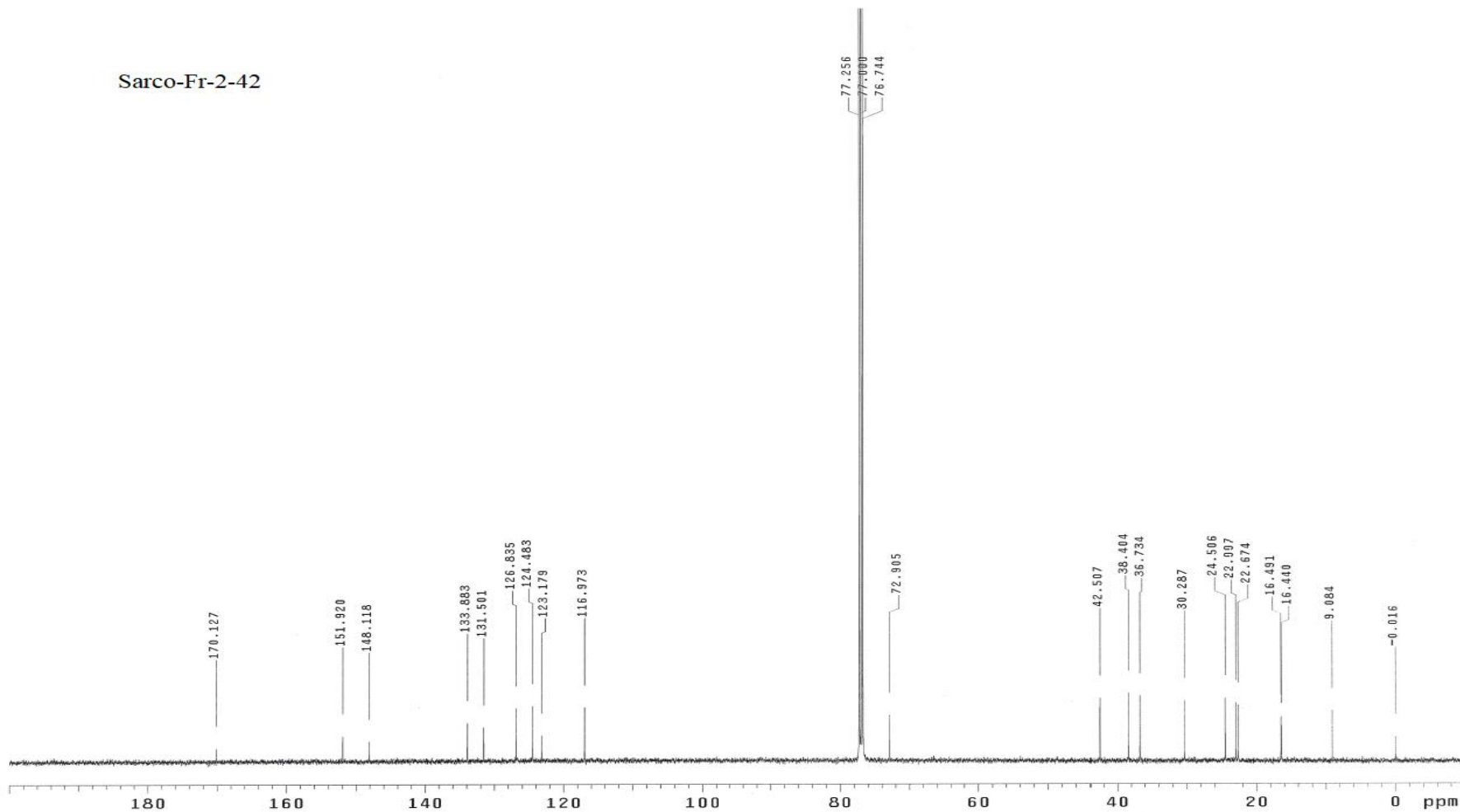


Figure S40: ¹³C NMR spectrum of **4** in CDCl₃ at 125 MHz

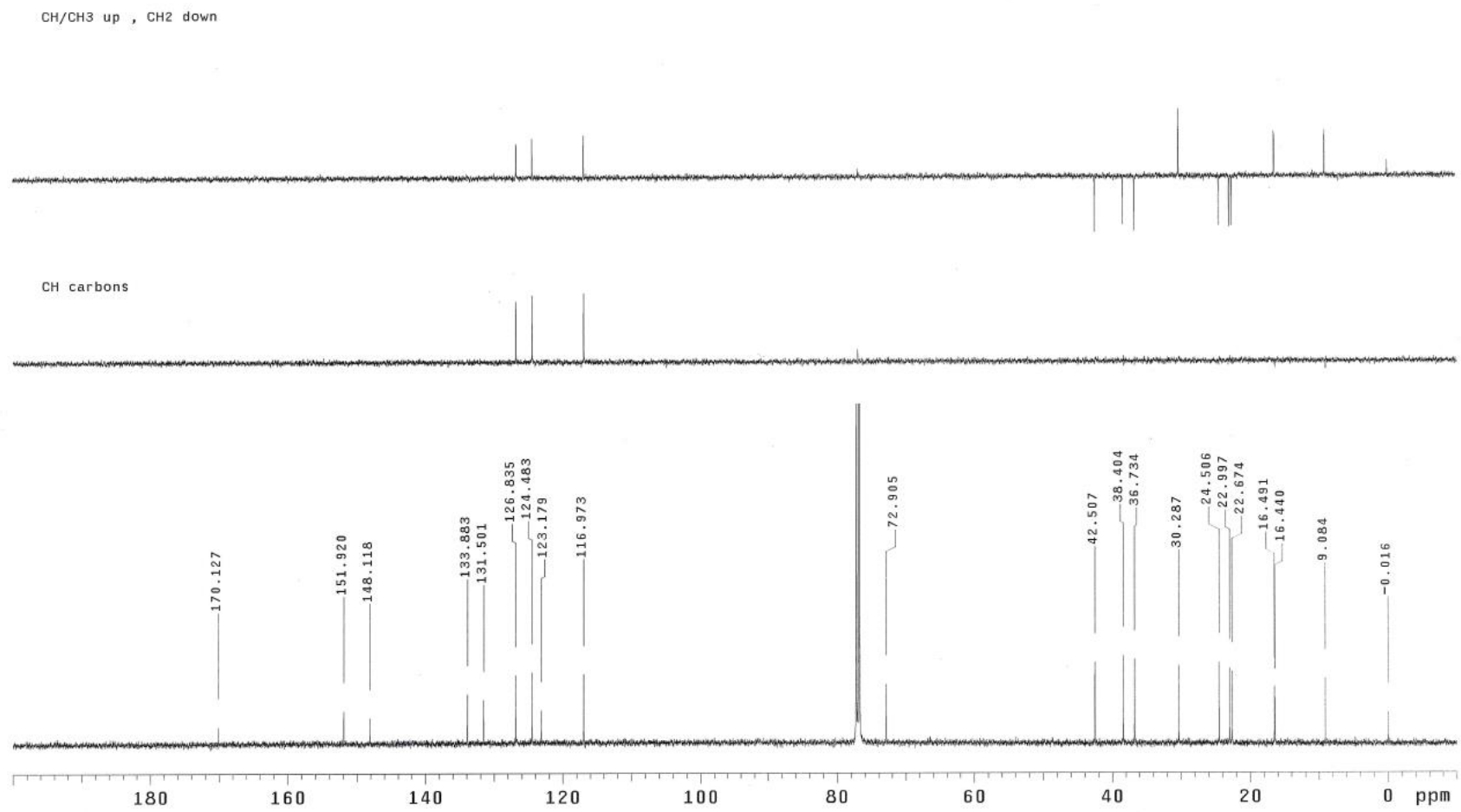


Figure S41: DEPT spectrum of 4

Sarco-Fr-2-42

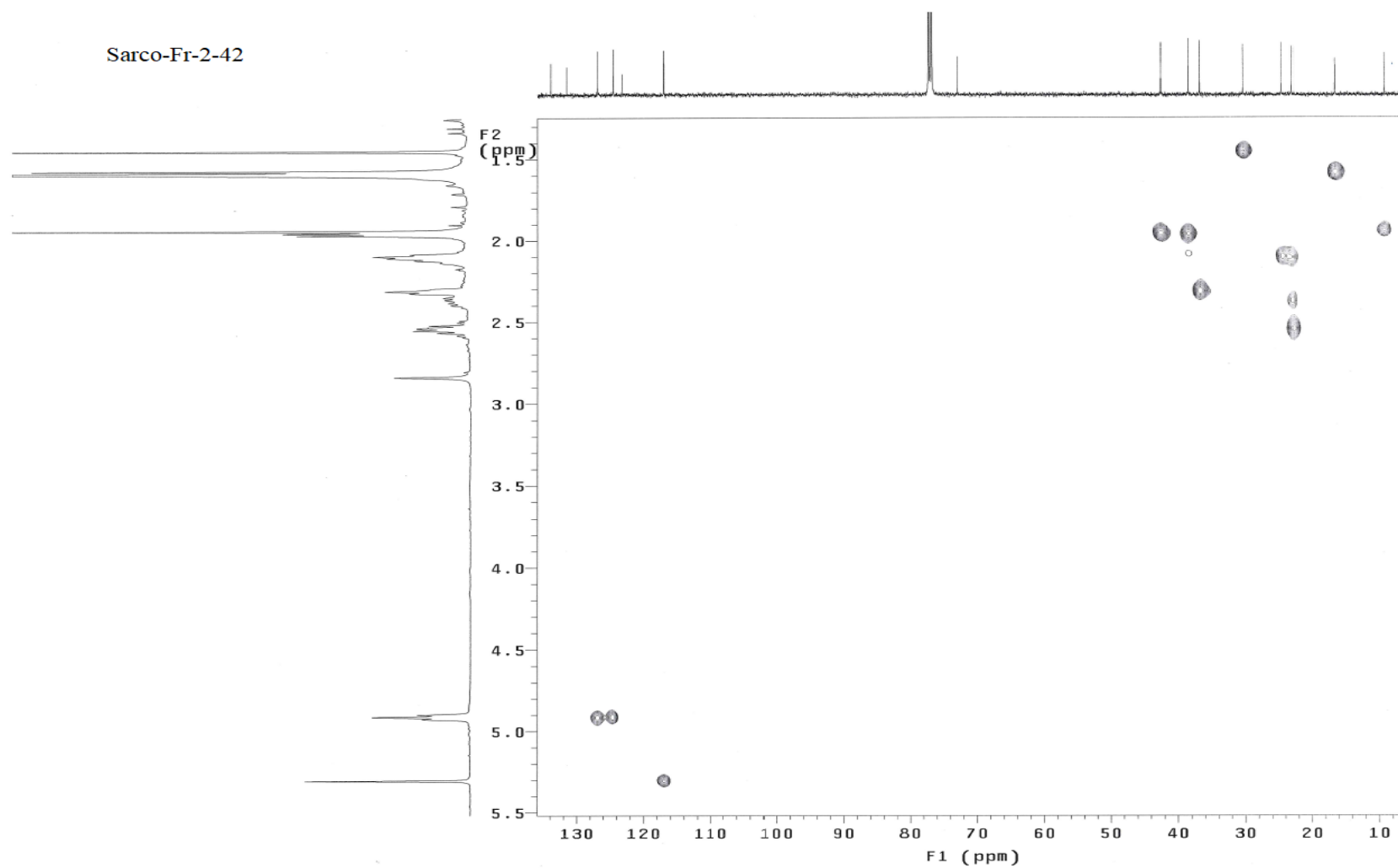


Figure S42: HSQC spectrum of 4

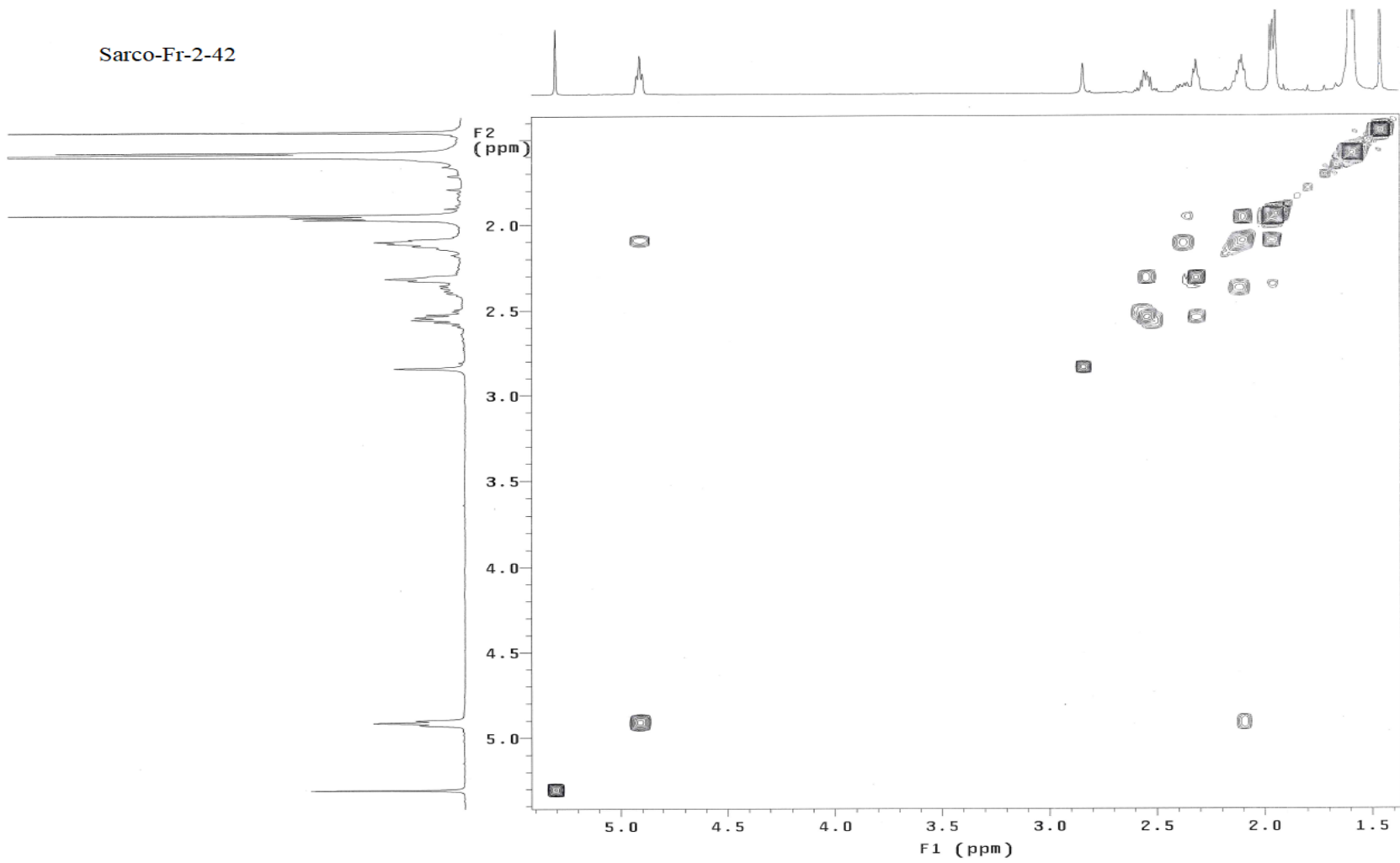


Figure S43: COSY spectrum of 4

Sarco-Fr-2-42

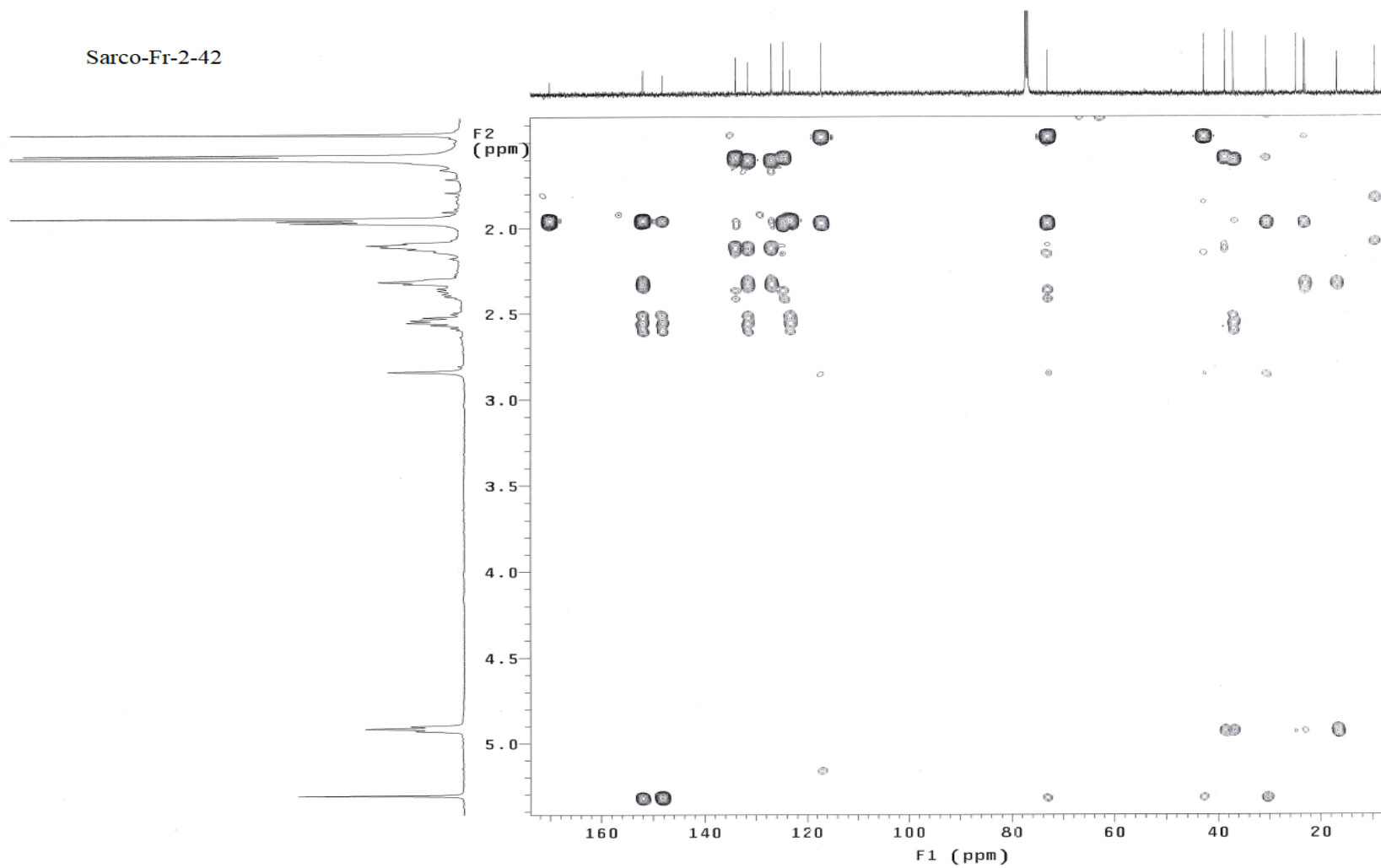


Figure S44: HMBC spectrum of 4

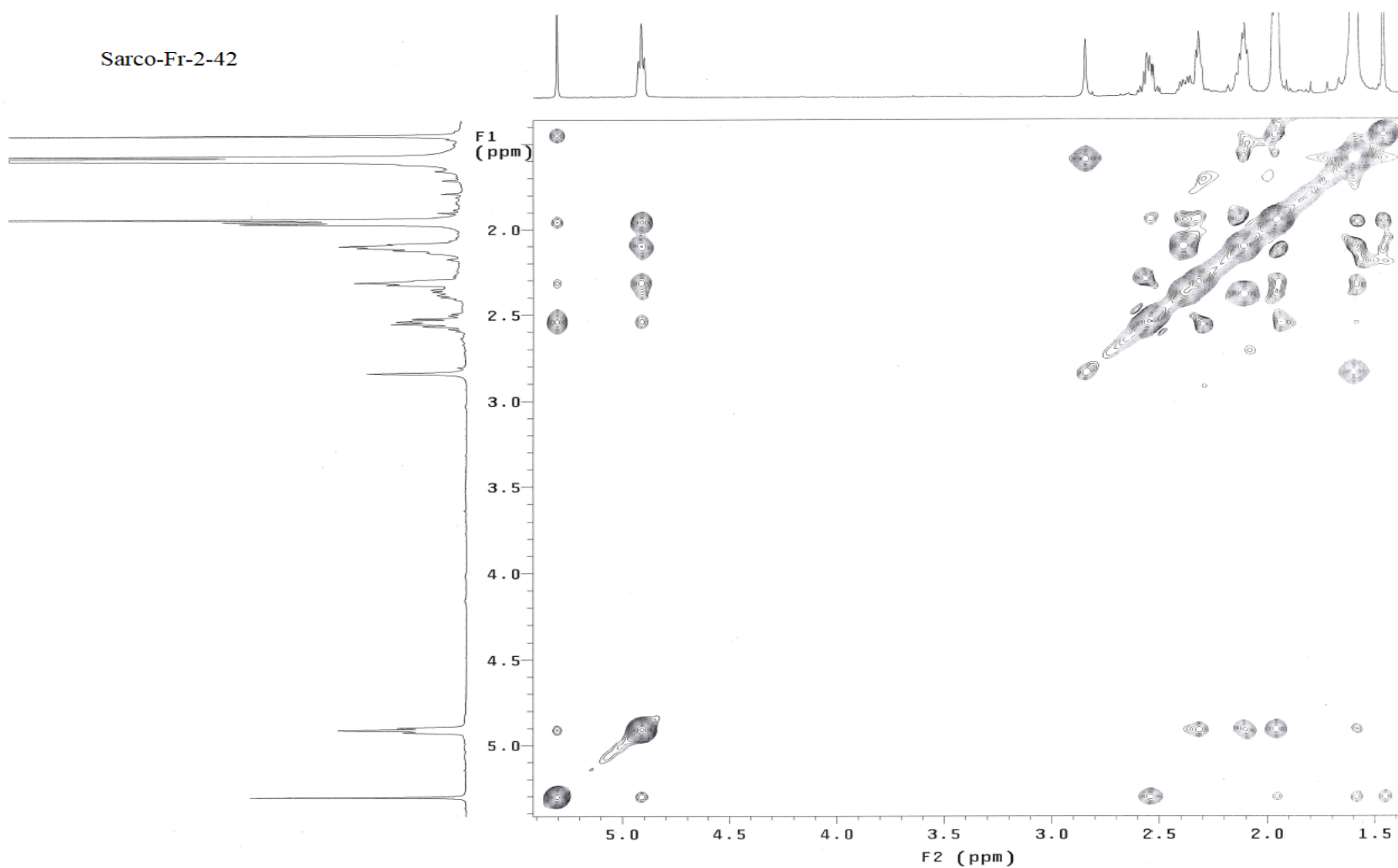


Figure S45: NOESY spectrum of 4