



Supporting Information

for

Bipolenins K–N: New sesquiterpenoids from the fungal plant pathogen *Bipolaris sorokiniana*

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NMR, IR and MS spectra of compounds 1–4

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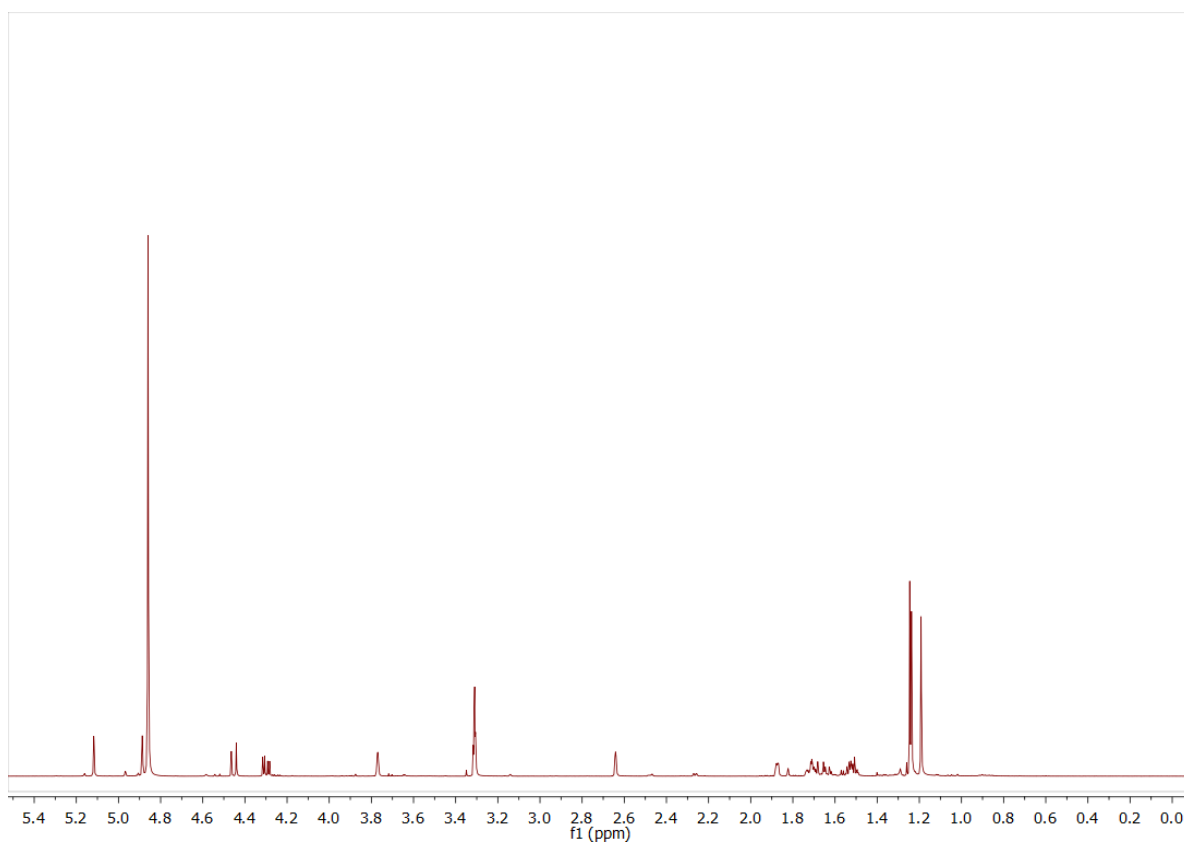


Figure S1: ¹H NMR spectrum (500 MHz) of **1** in CD₃OD

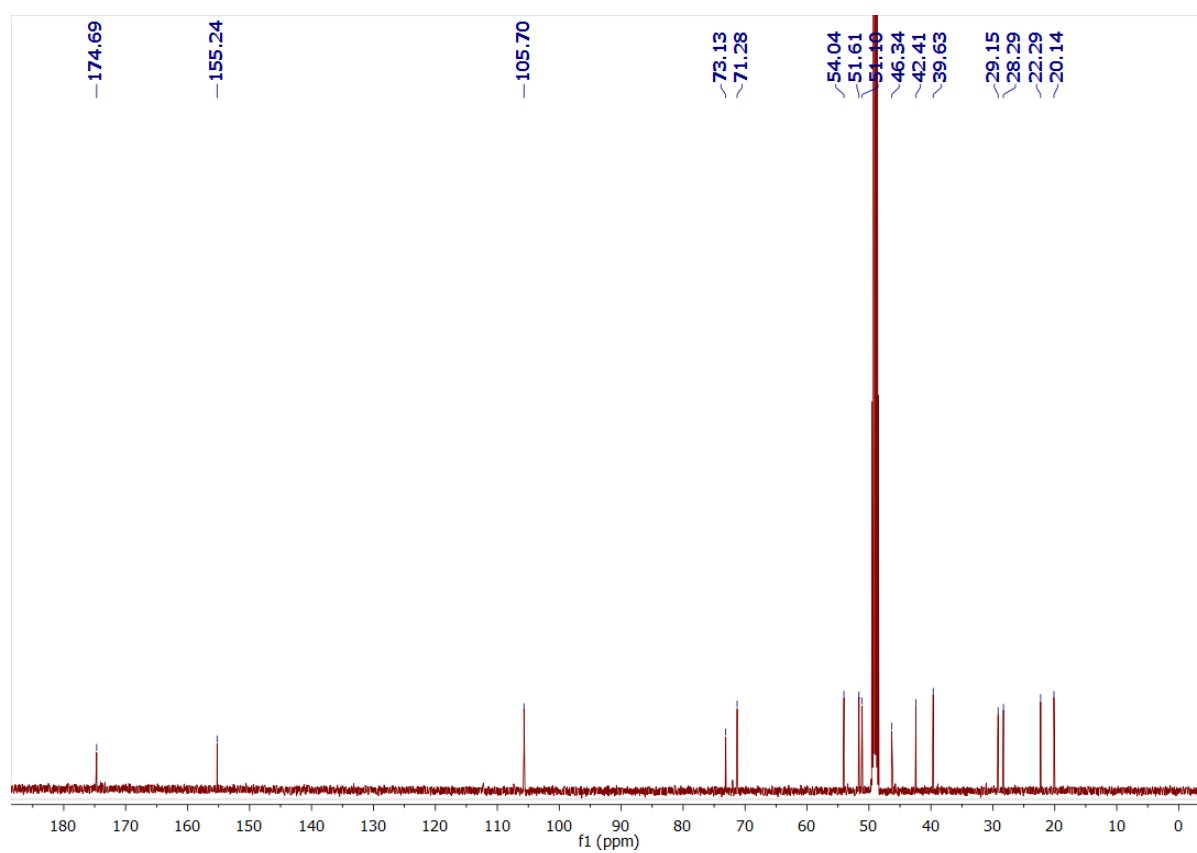


Figure S2: ¹³C NMR spectrum (125 MHz) of **1** in CD₃OD

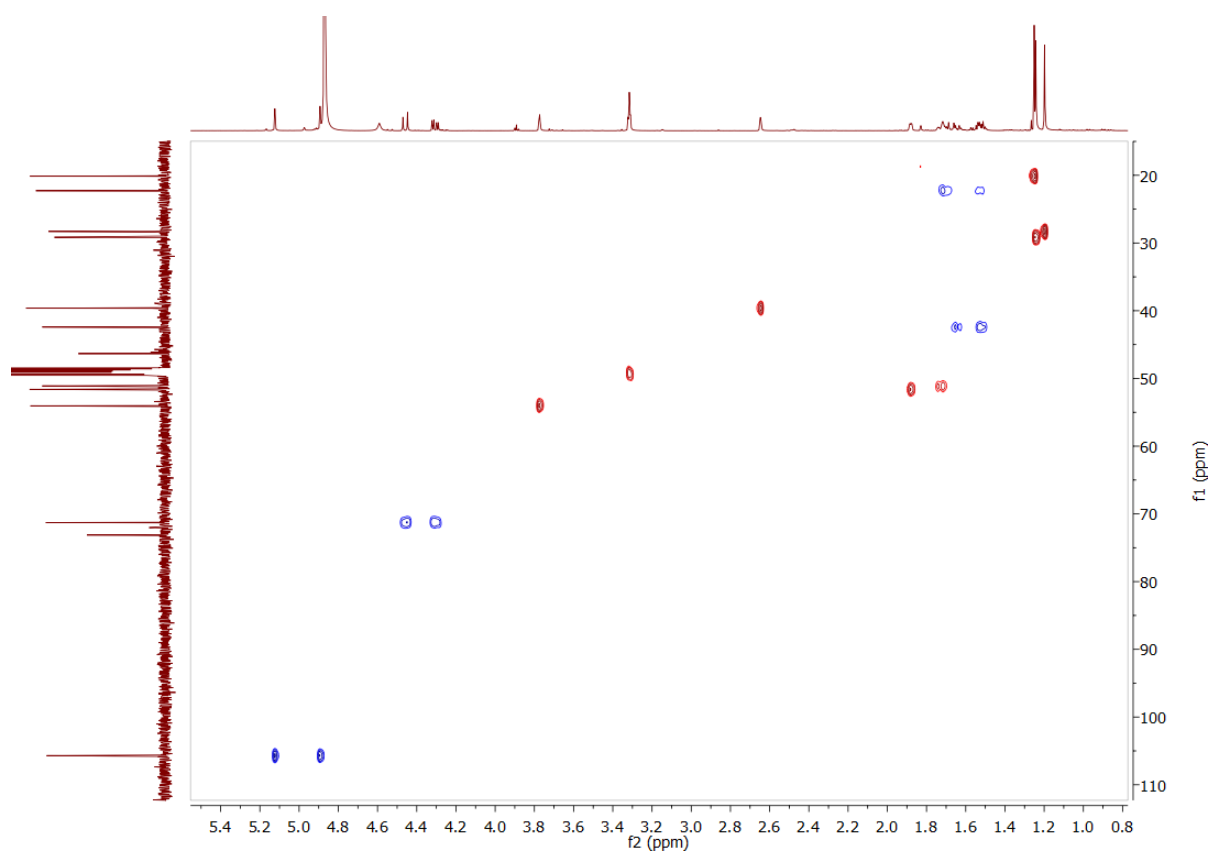


Figure S3: HSQC spectrum (500 MHz) of **1** in CD₃OD

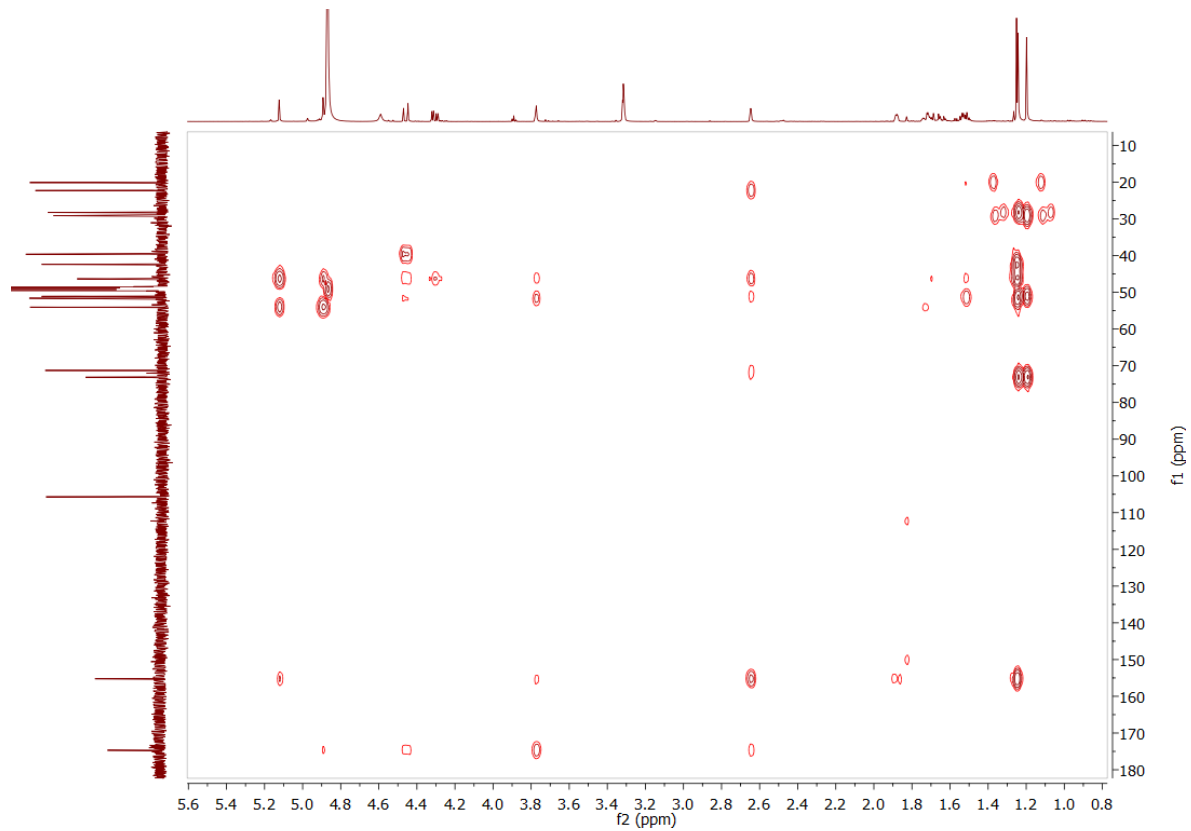


Figure S4: HMBC spectrum (500 MHz) of **1** in CD₃OD

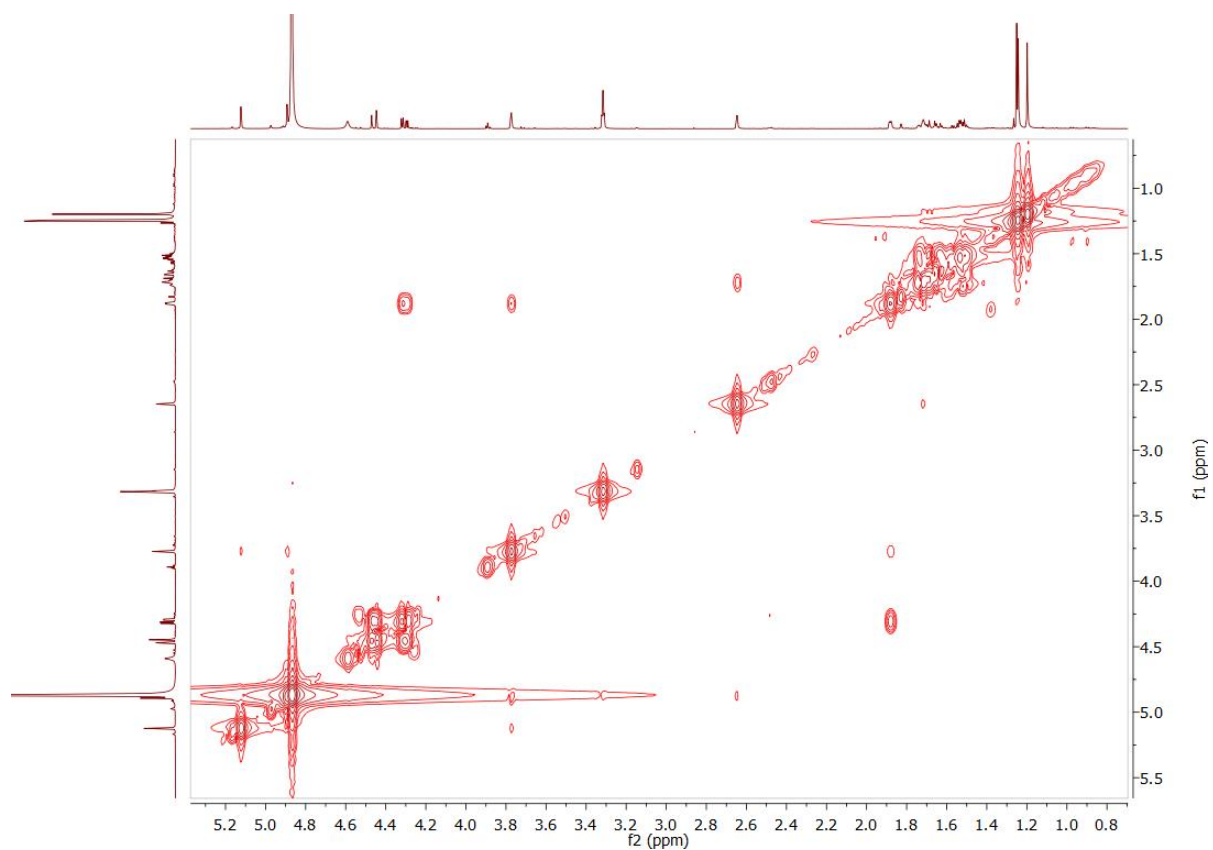


Figure S5: ^1H - ^1H COSY spectrum (500 MHz) of **1** in CD_3OD

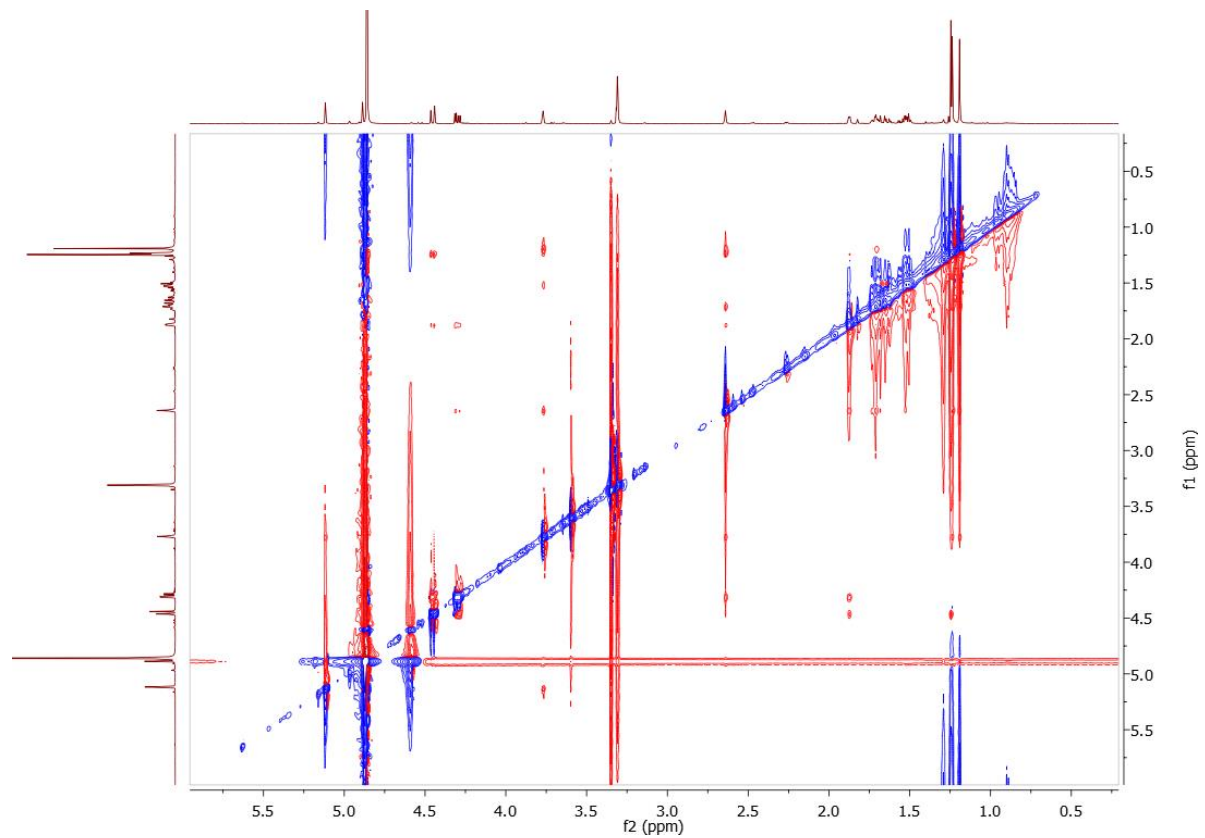


Figure S6: NOESY spectrum (500 MHz) of **1** in CD_3OD

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

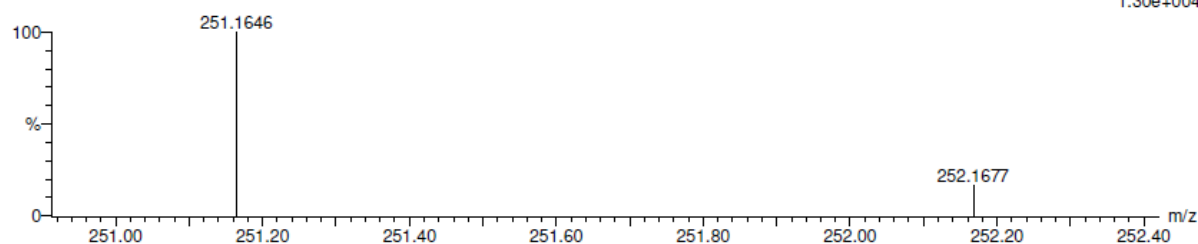
C: 0-20 H: 0-30 O: 0-5 Na: 0-1

ESI+BF12-1729-Jan-2019ESI+BF12-17

ESI+BF12-17

BF12-17+ESI 82 (1.799)

1: TOF MS ES+
1.30e+004



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
251.1646	251.1647	-0.1	-0.4	4.5	24.9	0.1	C15 H23 O3
	251.1623	2.3	9.2	1.5	26.8	2.0	C13 H24 O3 Na

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

32 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

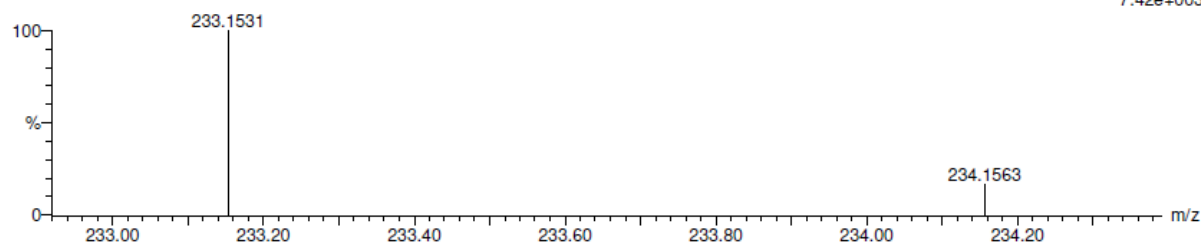
C: 0-20 H: 0-30 O: 0-5 Na: 0-1

ESI+BF12-1729-Jan-2019ESI+BF12-17

ESI+BF12-17

BF12-17+ESI 82 (1.799)

1: TOF MS ES+
7.42e+003



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
233.1531	233.1517	1.4	6.0	2.5	23.4	0.6	C13 H22 O2 Na
	233.1542	-1.1	-4.7	5.5	23.5	0.8	C15 H21 O2

Figure S7: HRESIMS spectrum of 1

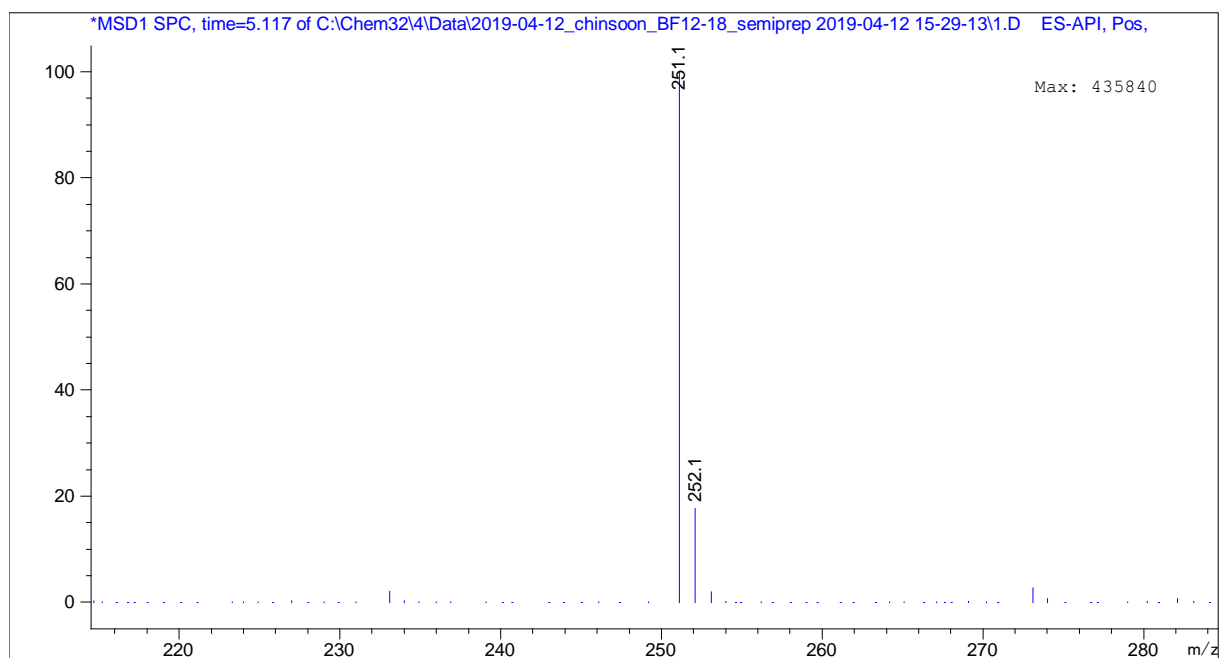


Figure S8: ESIMS spectrum of **1**

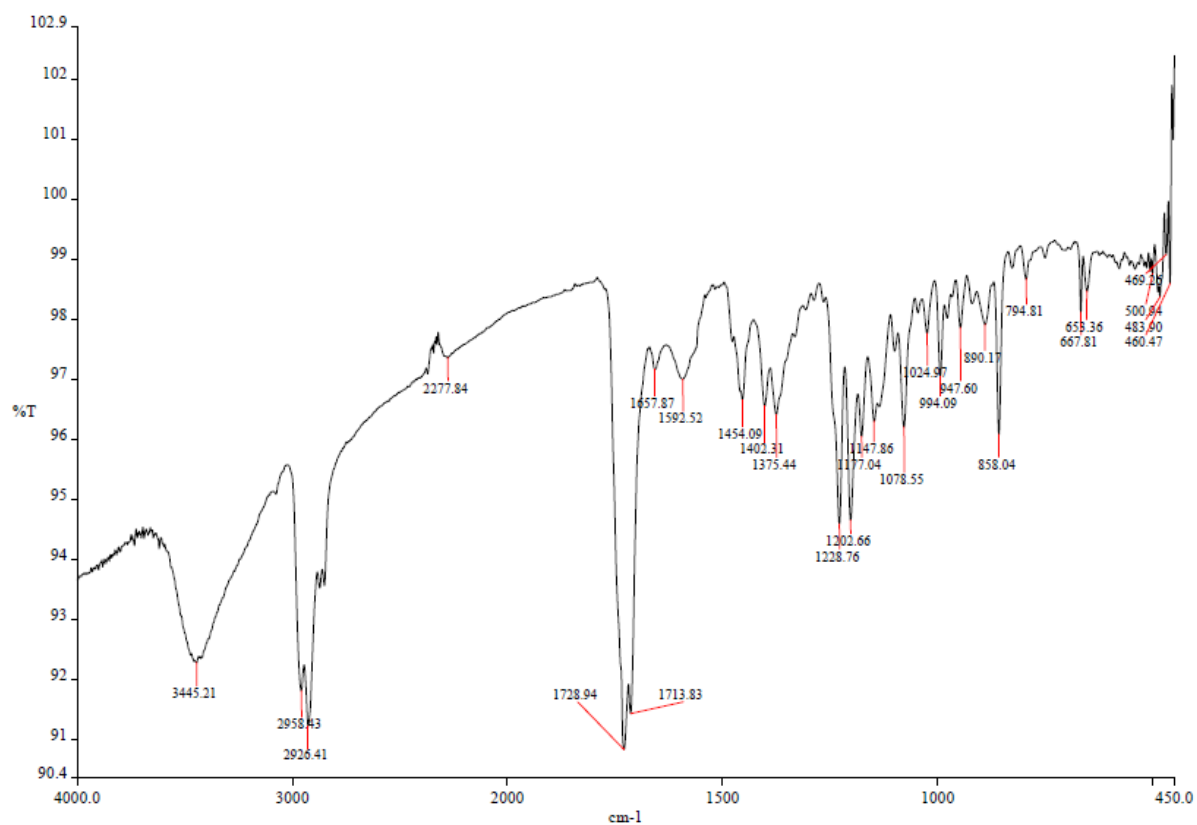


Figure S9: IR spectrum of **1**

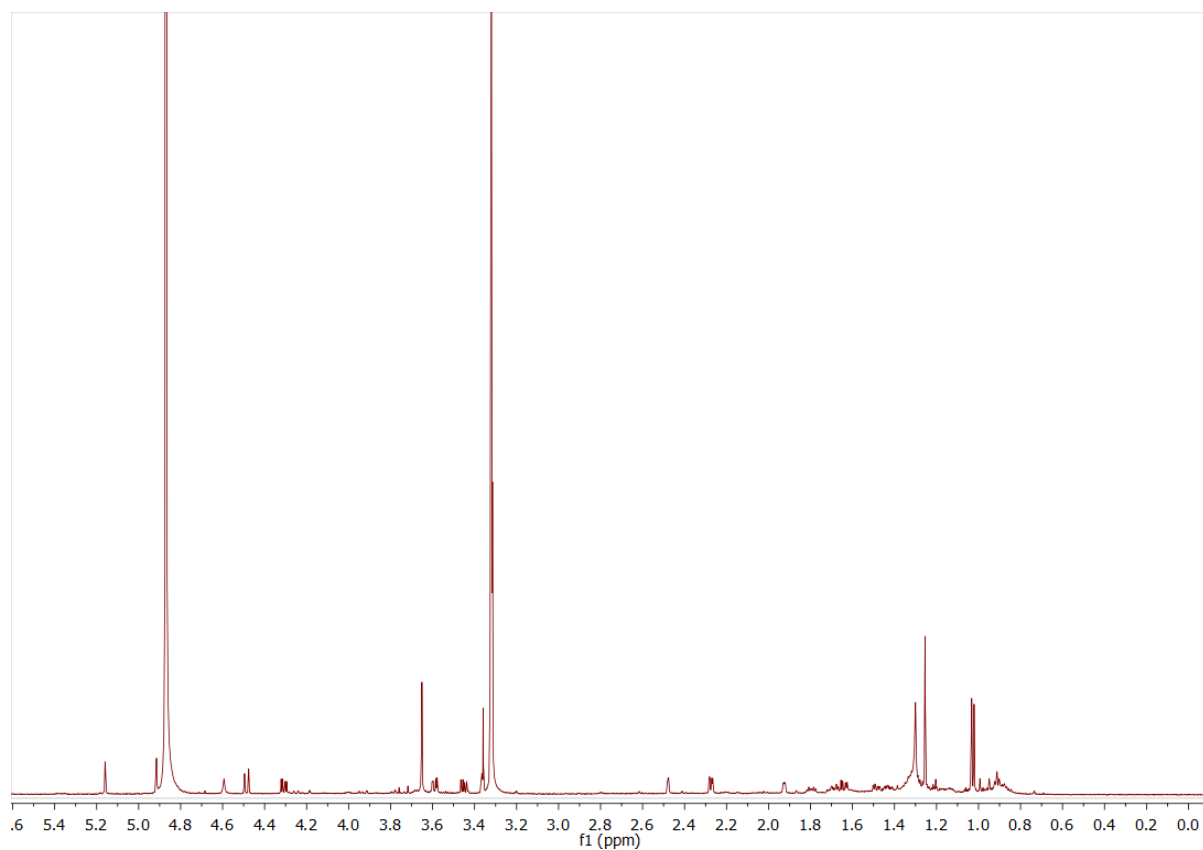


Figure S10: ^1H NMR spectrum (600 MHz) of **2** in CD_3OD

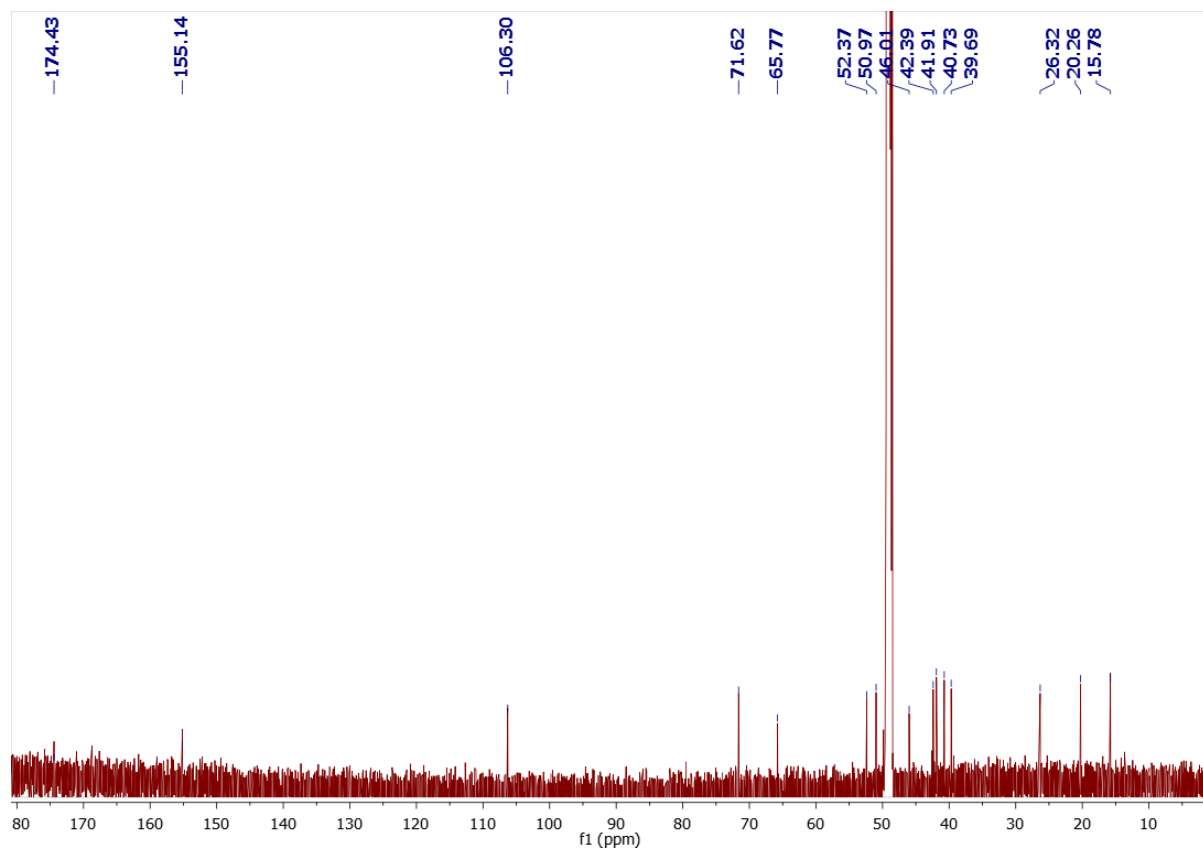


Figure S11: ^{13}C NMR spectrum (150 MHz) of **2** in CD_3OD

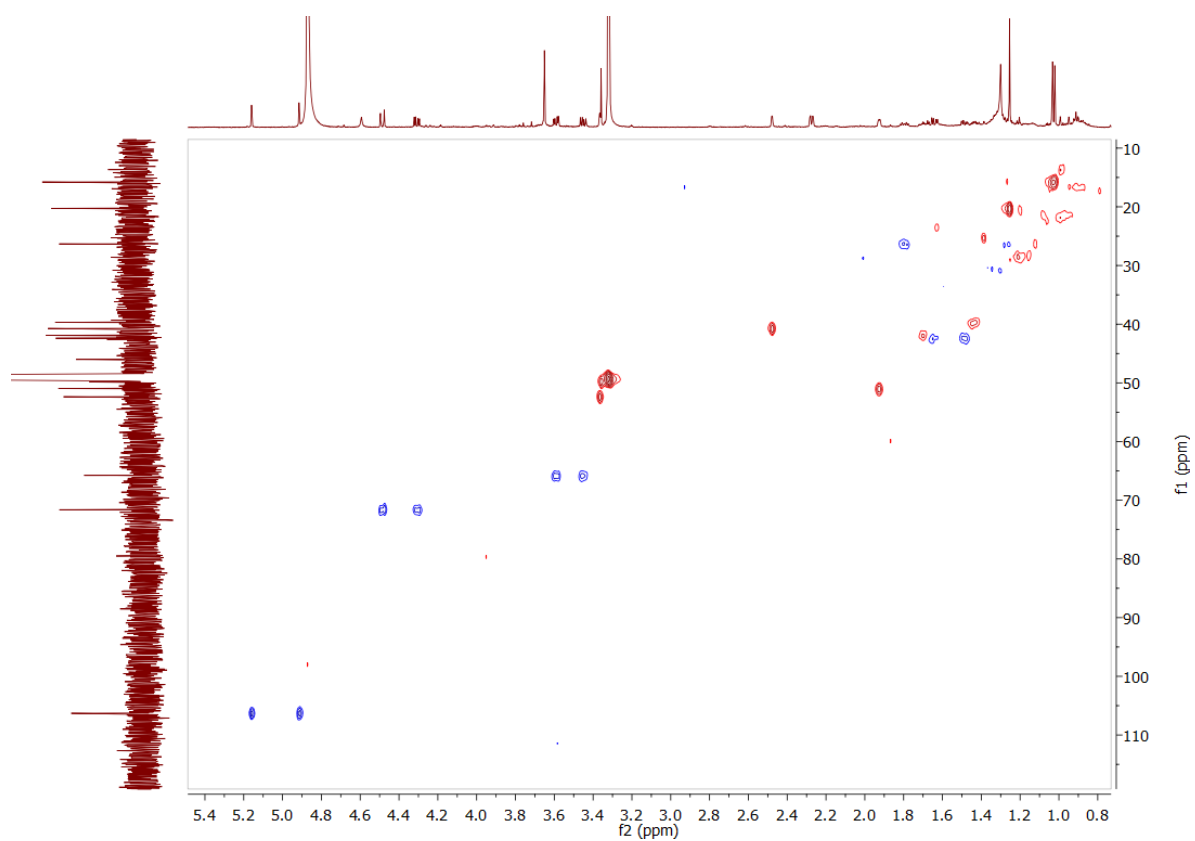


Figure S12: HSQC spectrum (600 MHz) of **2** in CD₃OD

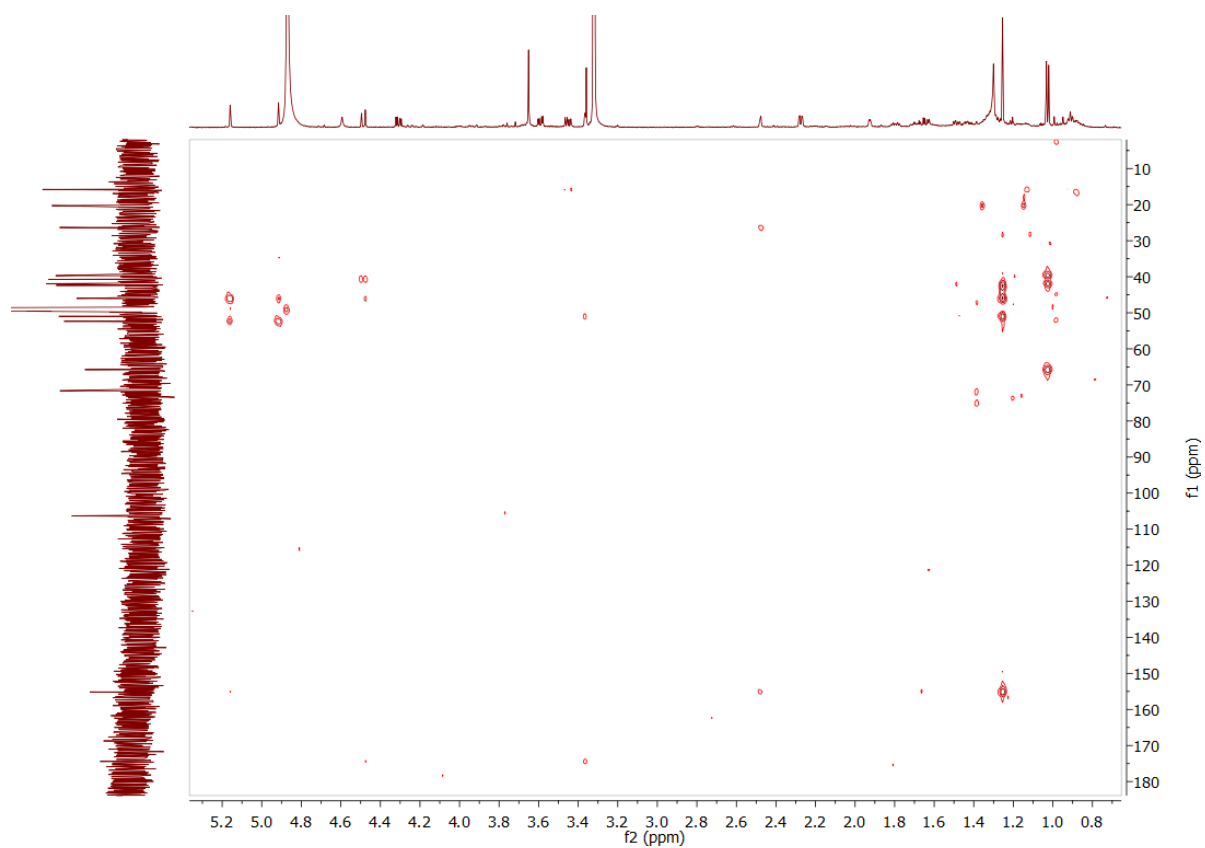


Figure S13: HMBC spectrum (600 MHz) of **2** in CD₃OD

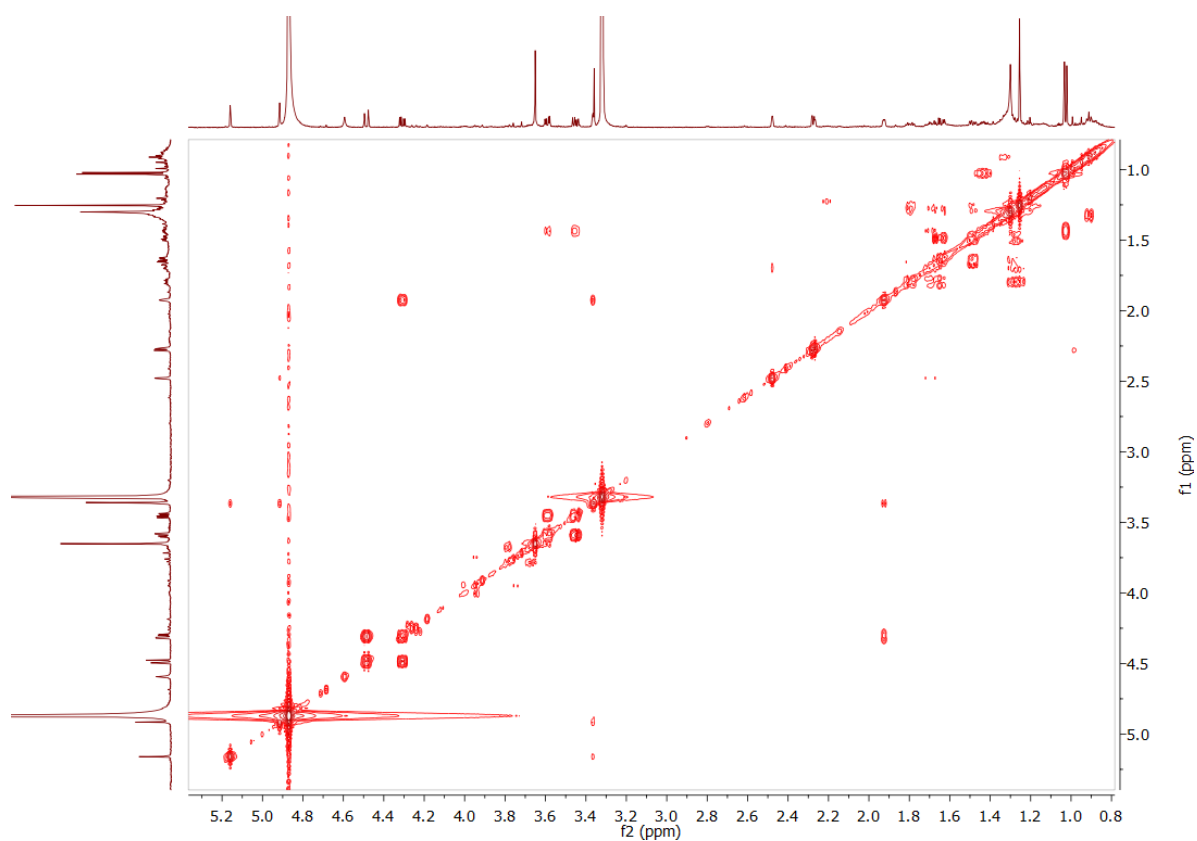


Figure S14: ^1H - ^1H COSY spectrum (600 MHz) of **2** in CD_3OD

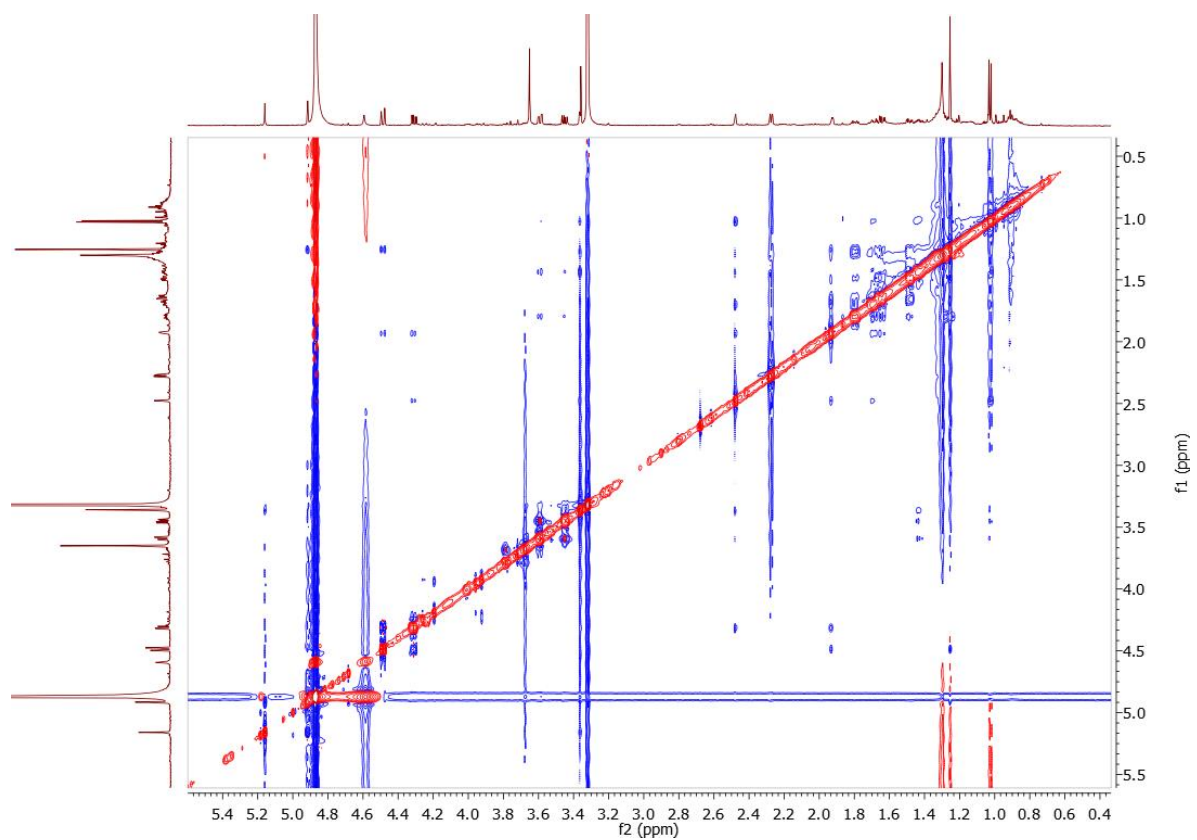


Figure S15: NOESY spectrum (600 MHz) of **2** in CD_3OD

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

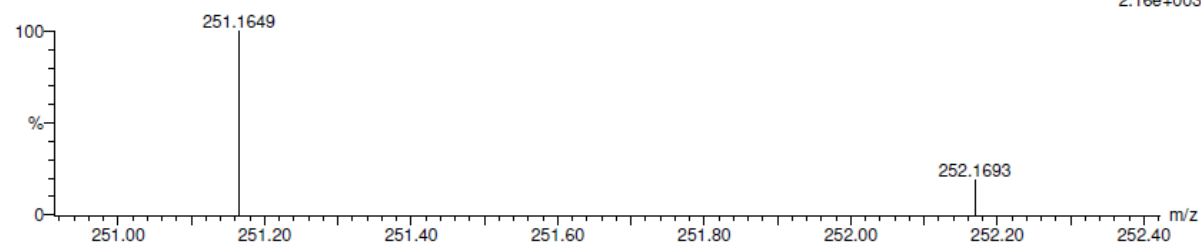
C: 0-50 H: 0-50 O: 0-10

BF12-1415-Apr-2019BF12-14

BF12-14

BF12-14 9 (0.195)

1: TOF MS ES+
2.16e+003



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
251.1649	251.1647	0.2	0.8	4.5	19.6	0.0	C15 H23 O3

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

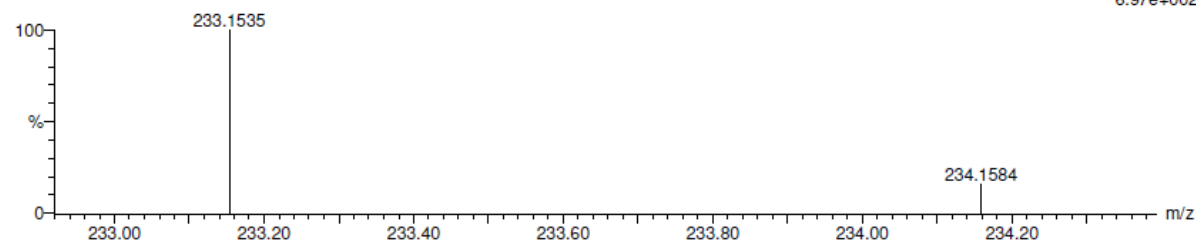
C: 0-50 H: 0-50 O: 0-10

BF12-1415-Apr-2019BF12-14

BF12-14

BF12-14 9 (0.195)

1: TOF MS ES+
6.97e+002



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
233.1535	233.1542	-0.7	-3.0	5.5	14.8	0.0	C15 H21 O2

Figure S16: HRESIMS spectrum of **2**

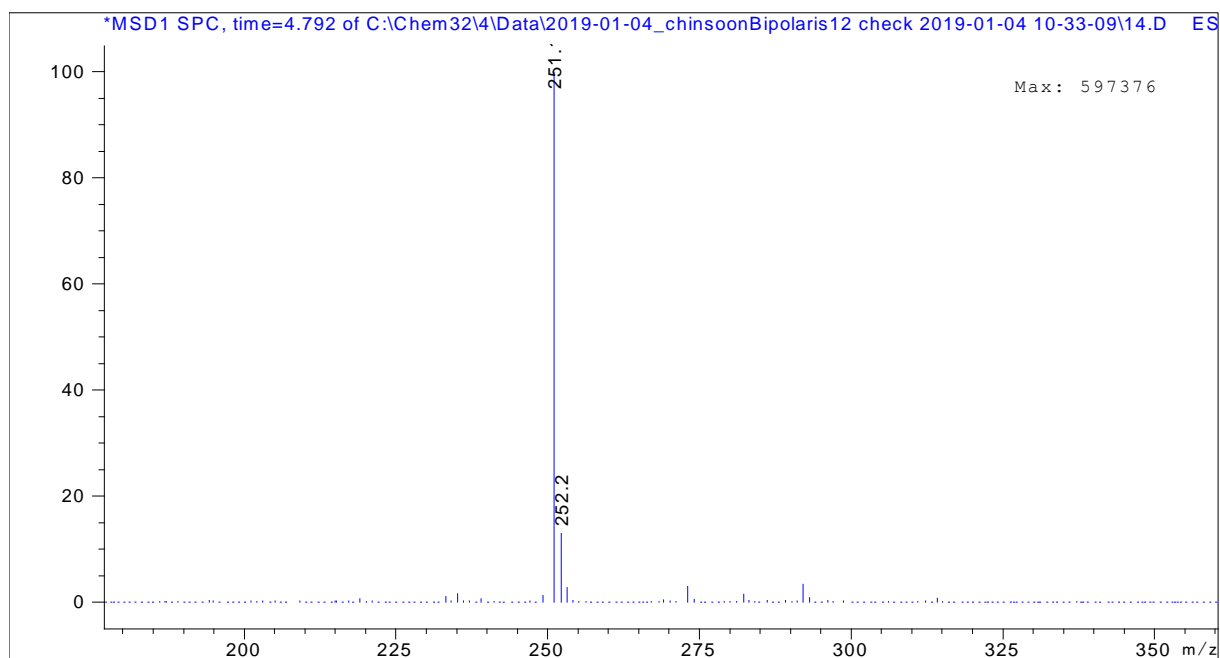


Figure S17: ESIMS spectrum of **2**

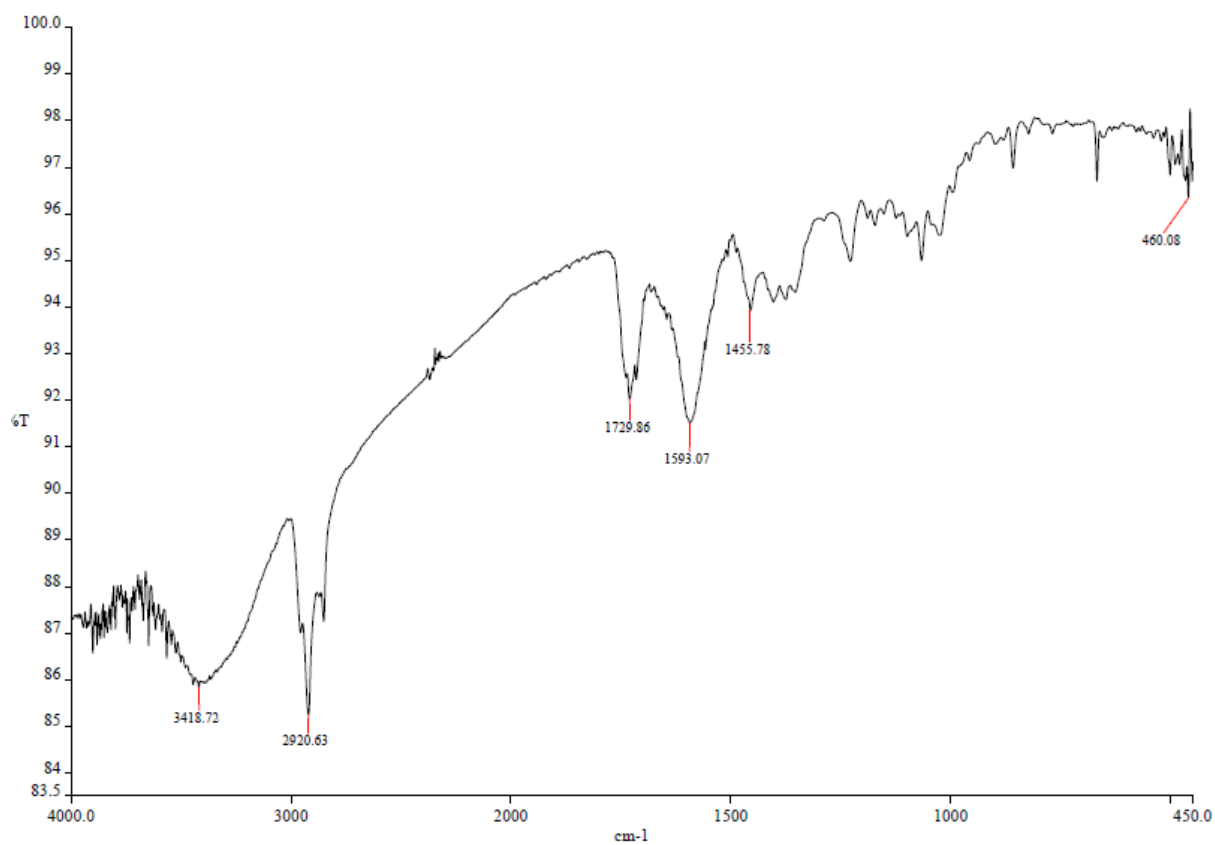


Figure S18: IR spectrum of **2**

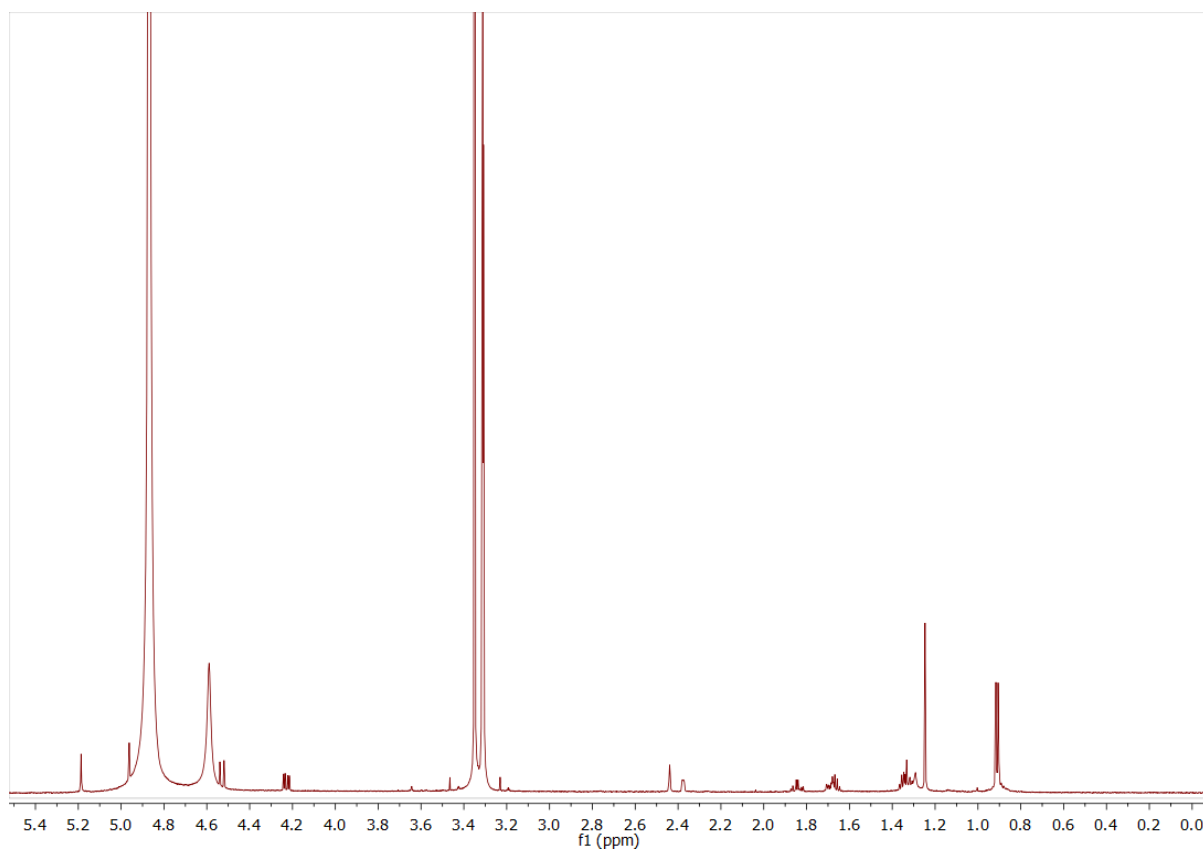


Figure S19: ¹H NMR spectrum (600 MHz) of **3** in CD₃OD

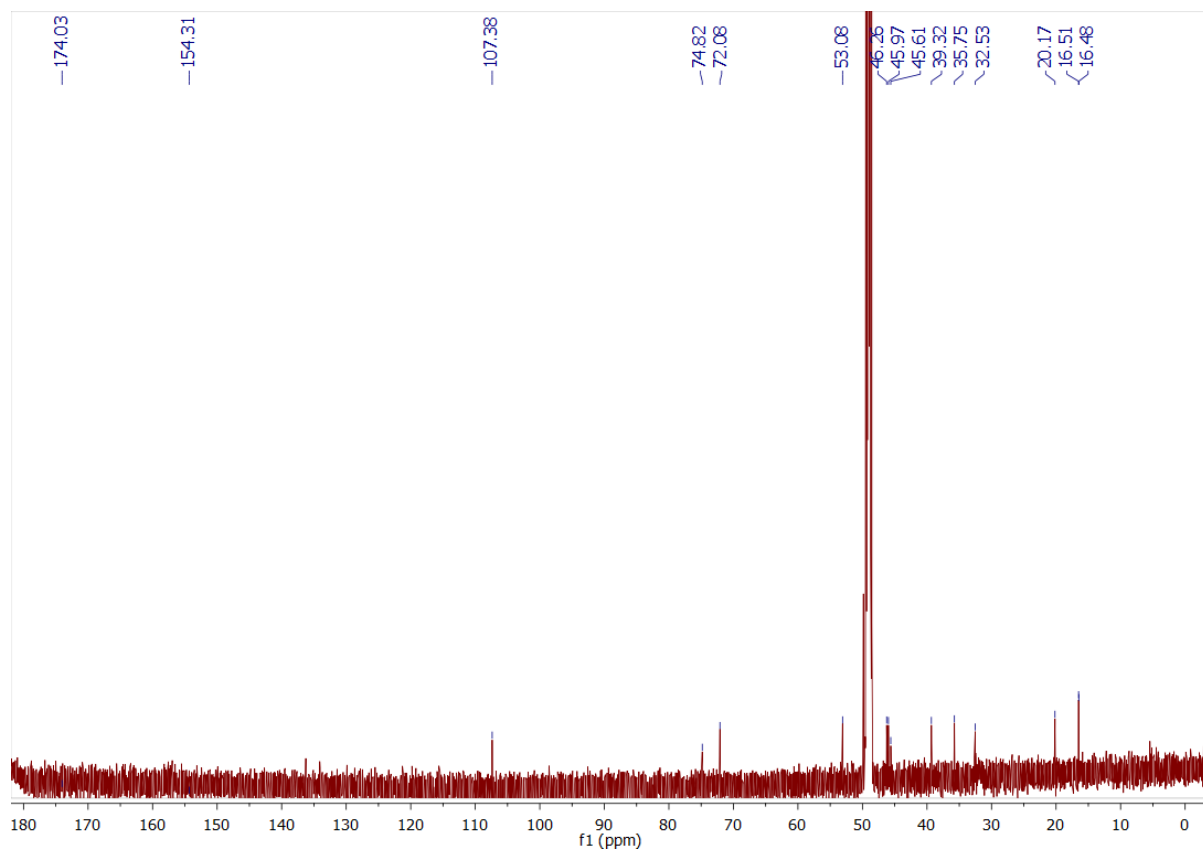


Figure S20: ¹³C NMR spectrum (150 MHz) of **3** in CD₃OD

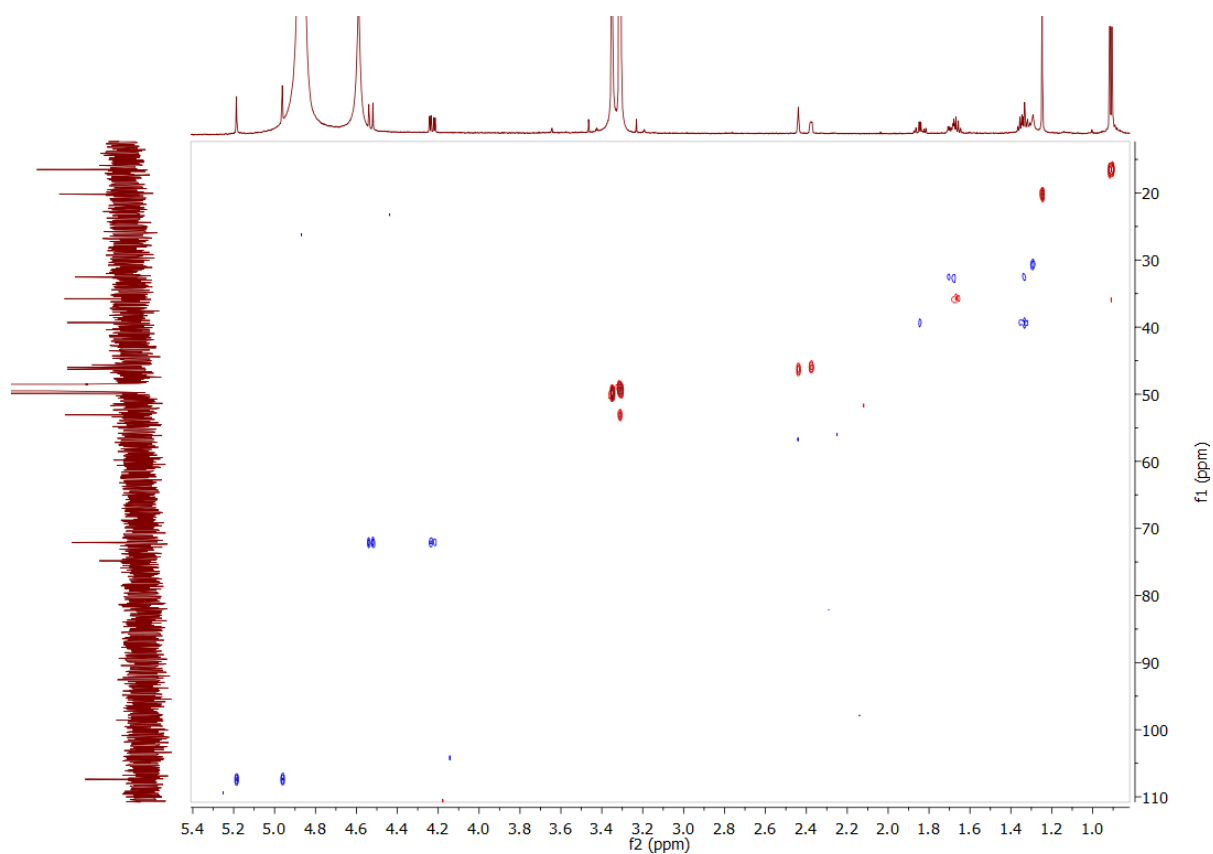


Figure S21: HSQC spectrum (600 MHz) of **3** in CD₃OD

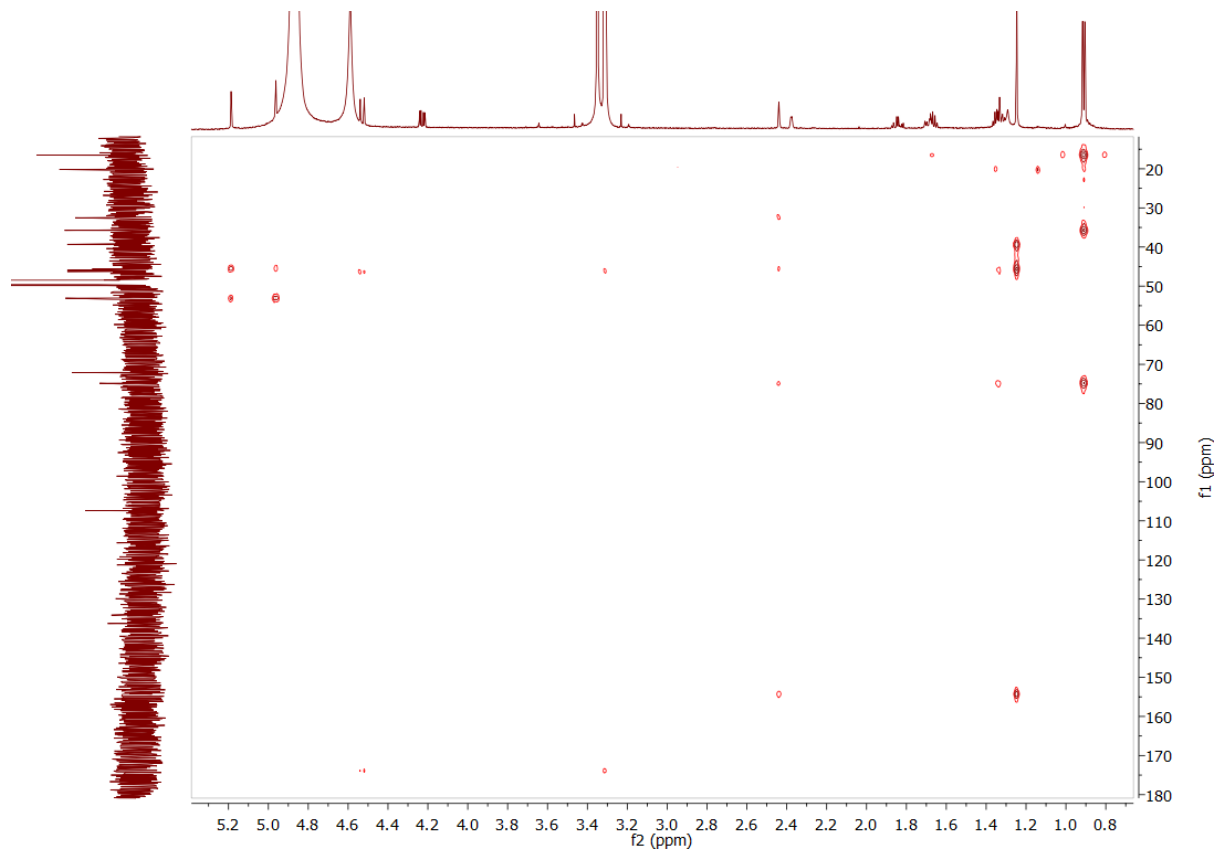


Figure S22: HMBC spectrum (600 MHz) of **3** in CD₃OD

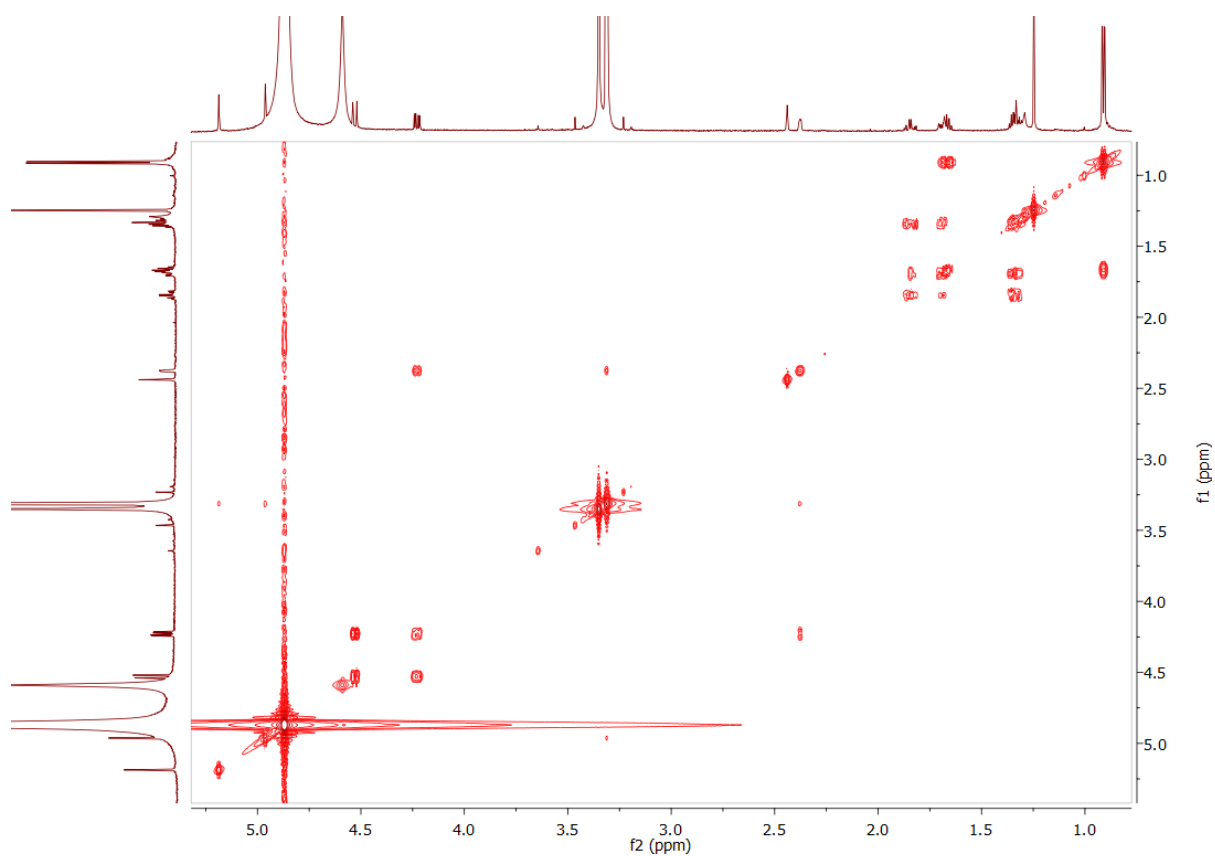


Figure S23: ^1H - ^1H COSY spectrum (600 MHz) of **3** in CD_3OD

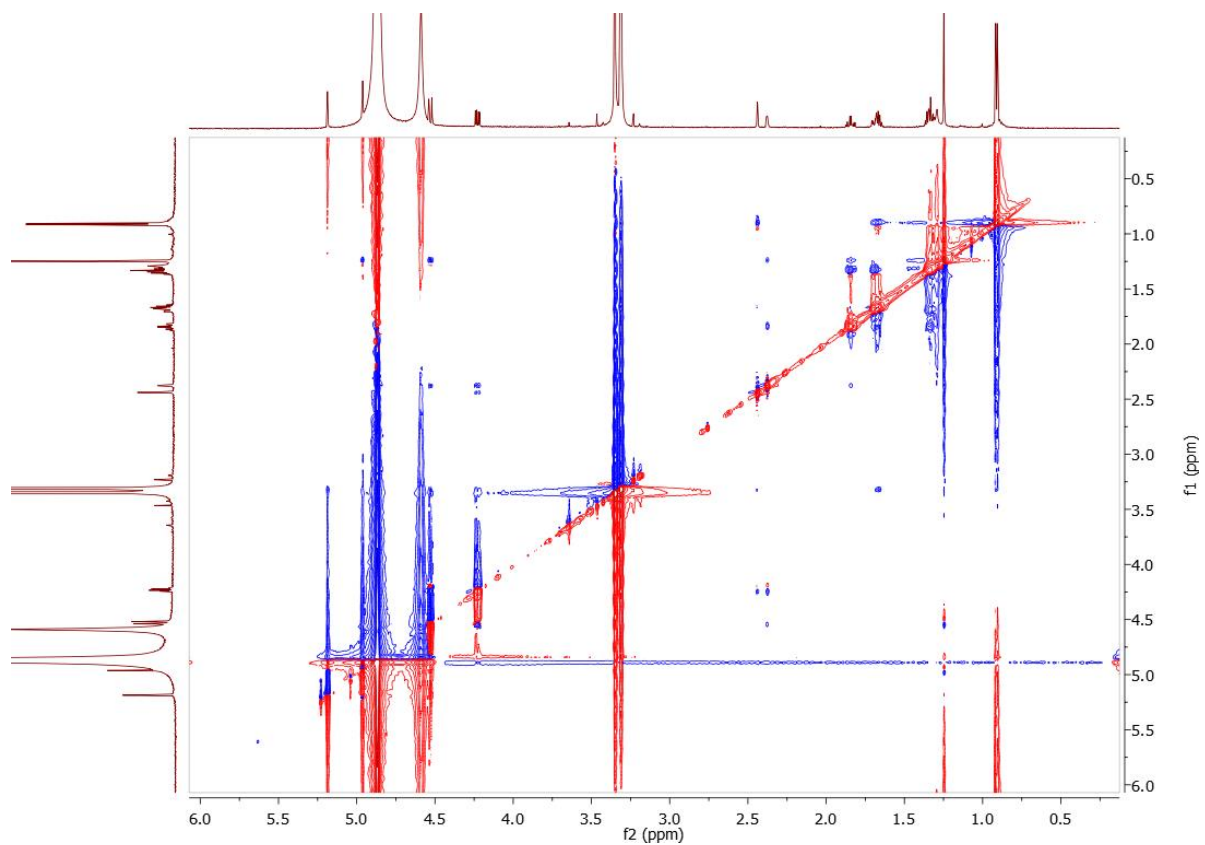


Figure S24: NOESY spectrum (600 MHz) of **3** in CD_3OD

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

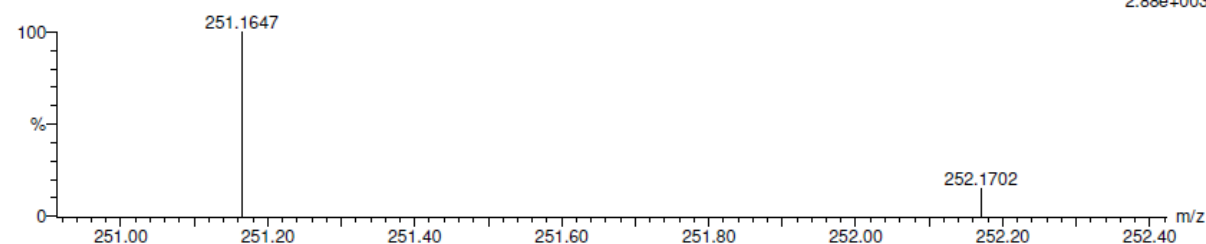
C: 0-50 H: 0-50 O: 0-10

BF12-8-215-Apr-2019BF12-8-2

BF12-8-2

BF12-8-2 9 (0.195)

1: TOF MS ES+
2.88e+003



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
251.1647	251.1647	0.0	0.0	4.5	22.2	0.0	C15 H23 O3

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

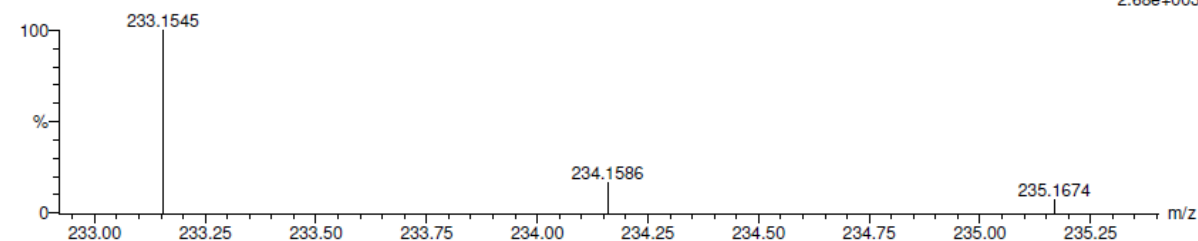
C: 0-50 H: 0-50 O: 0-10

BF12-8-215-Apr-2019BF12-8-2

BF12-8-2

BF12-8-2 10 (0.212)

1: TOF MS ES+
2.68e+003



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
233.1545	233.1542	0.3	1.3	5.5	16.9	0.0	C15 H21 O2

Figure S25: HRESIMS spectrum of 3

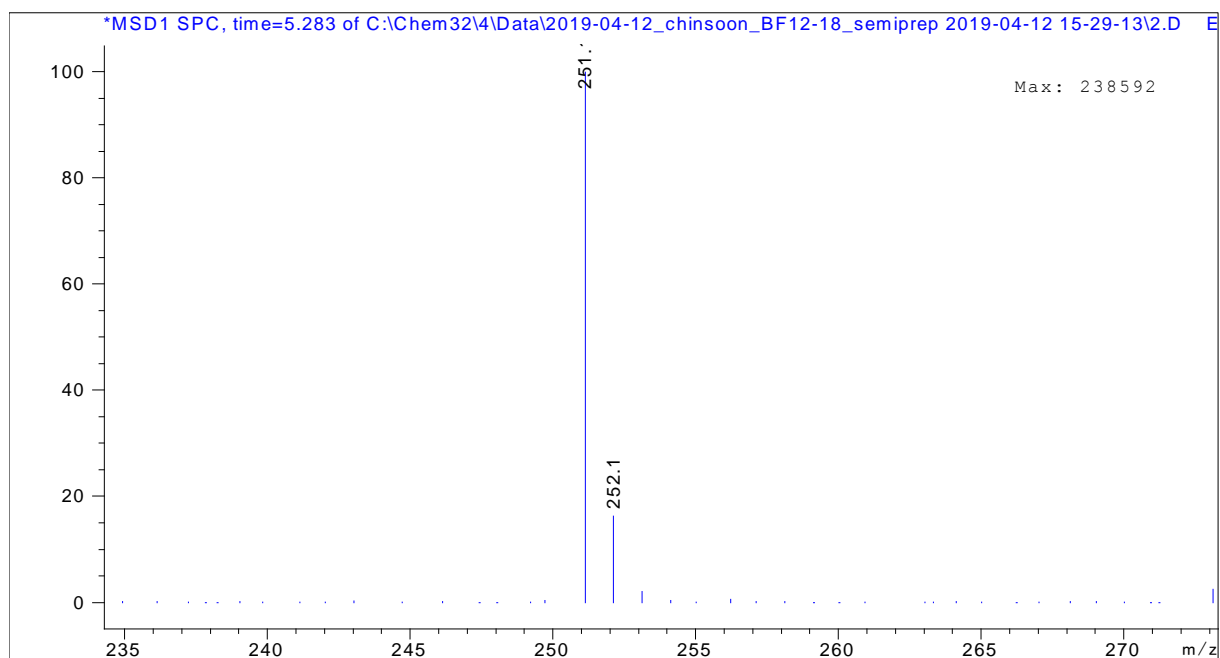


Figure S26: ESIMS spectrum of **3**

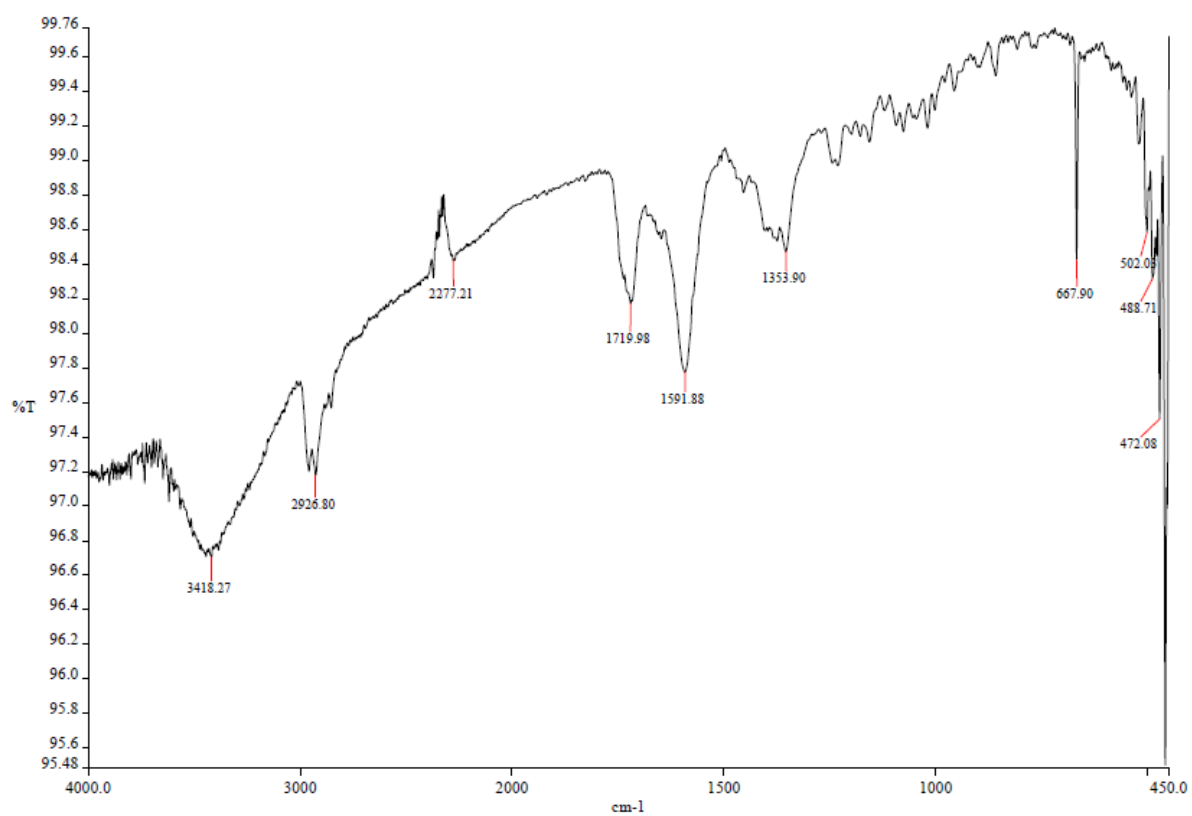


Figure S27: IR spectrum of **3**

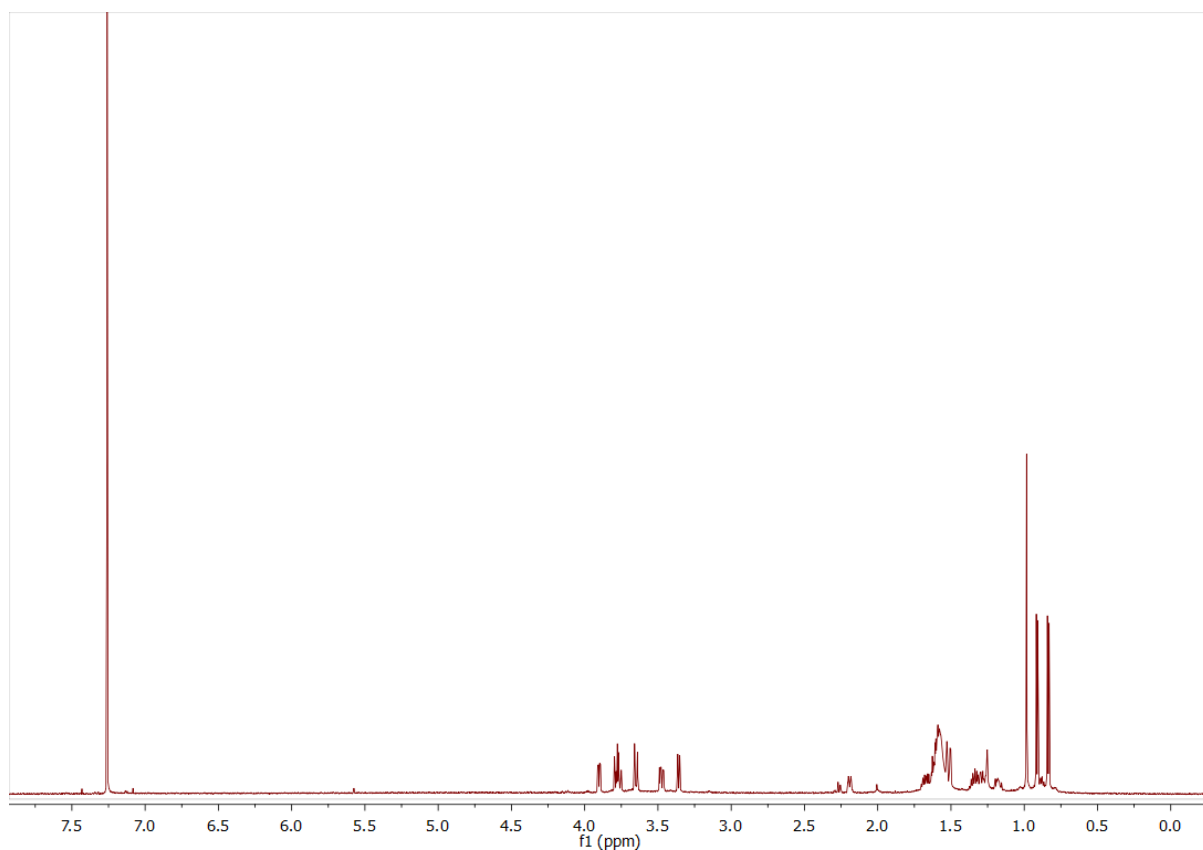


Figure S28: ^1H NMR spectrum (600 MHz) of **4** in CDCl_3

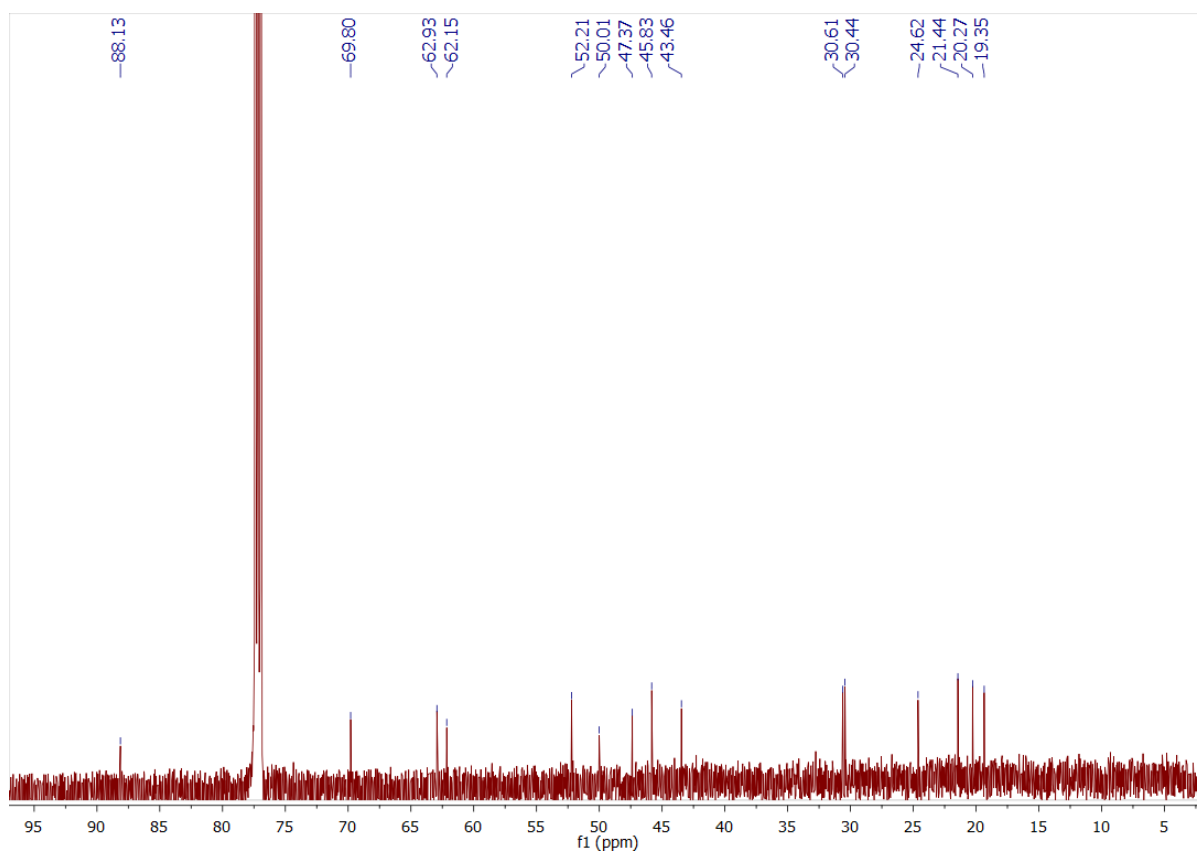


Figure S29: ^{13}C NMR spectrum (150 MHz) of **4** in CDCl_3

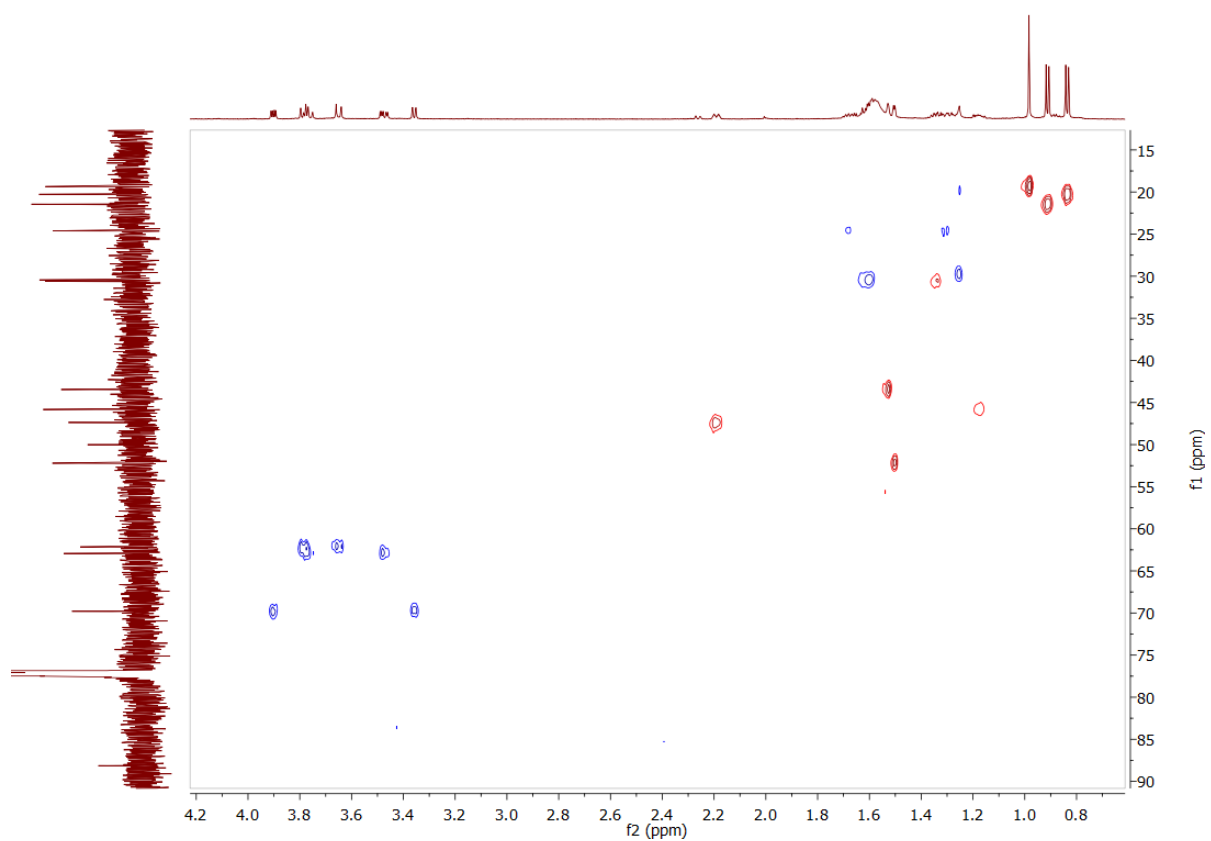


Figure S30: HSQC spectrum (600 MHz) of **4** in CDCl_3

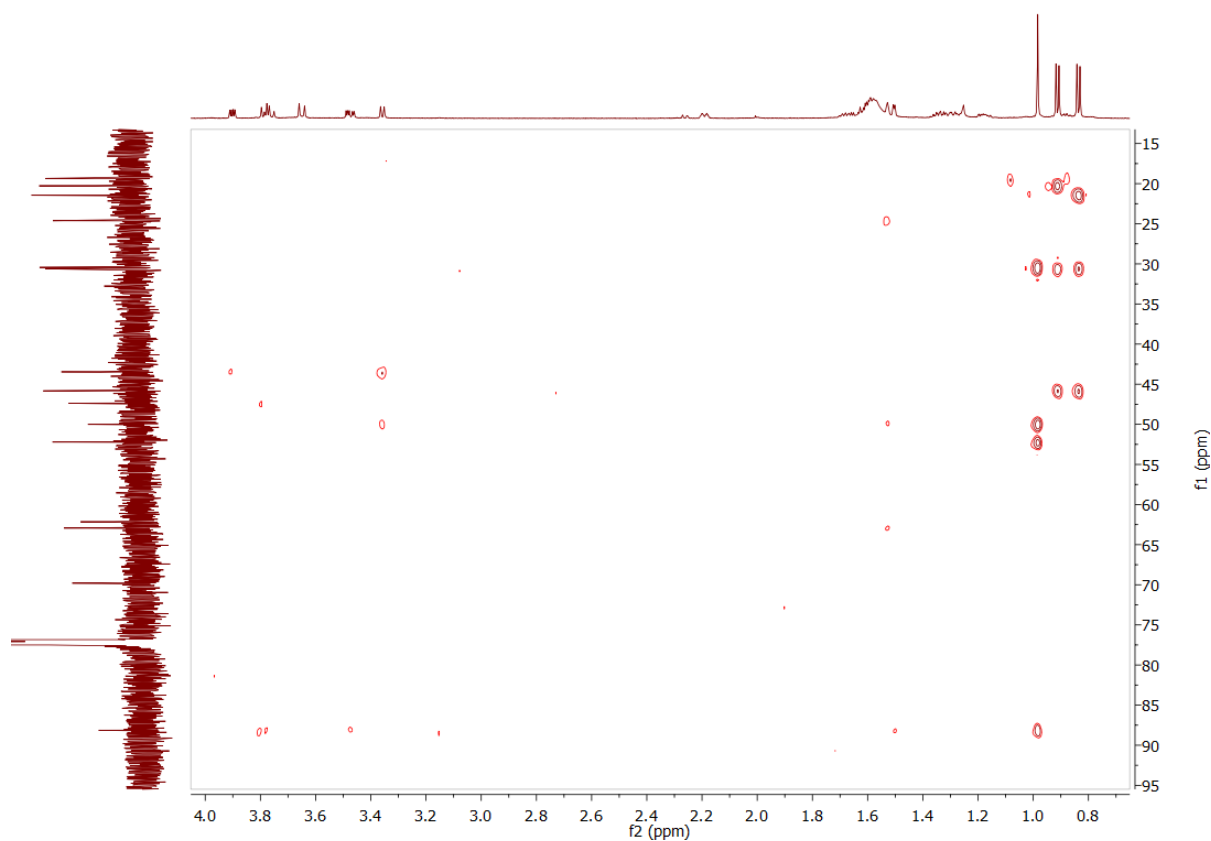


Figure S31: HMBC spectrum (600 MHz) of **4** in CDCl_3

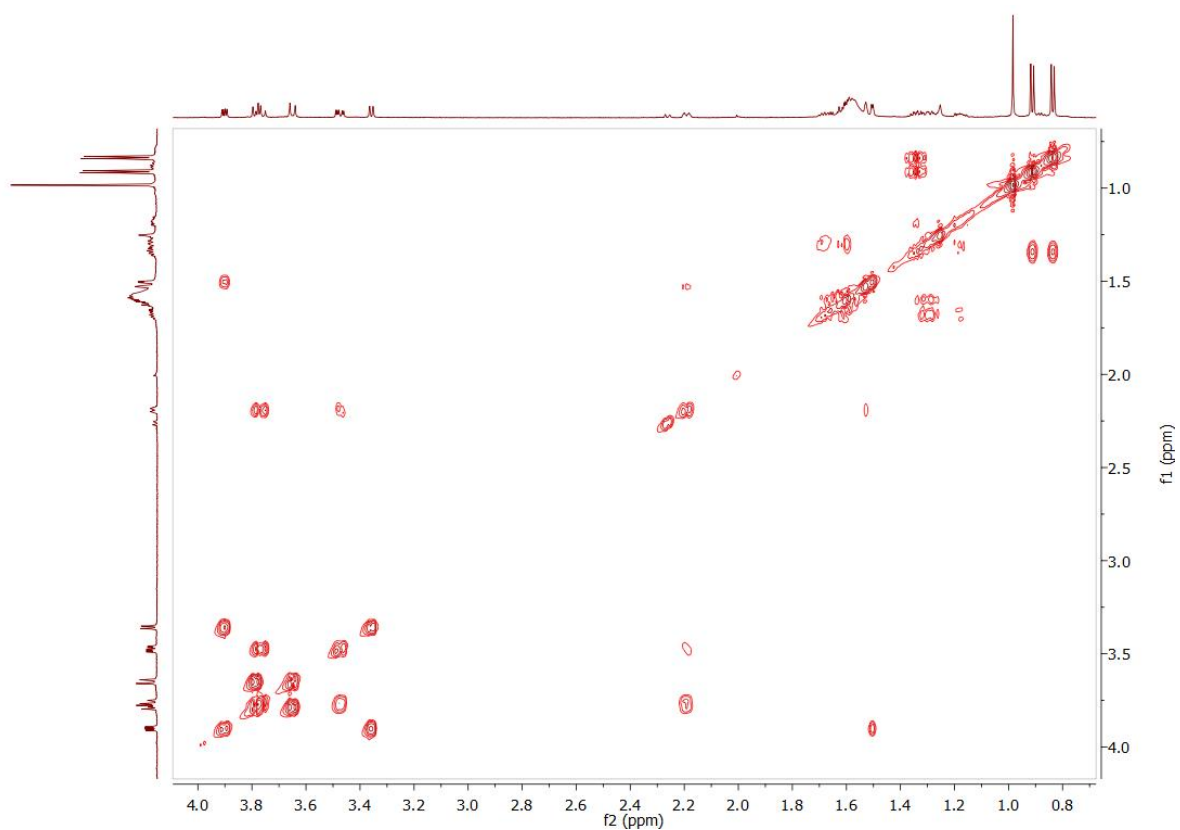


Figure S32: ^1H - ^1H COSY spectrum (600 MHz) of **4** in CDCl_3

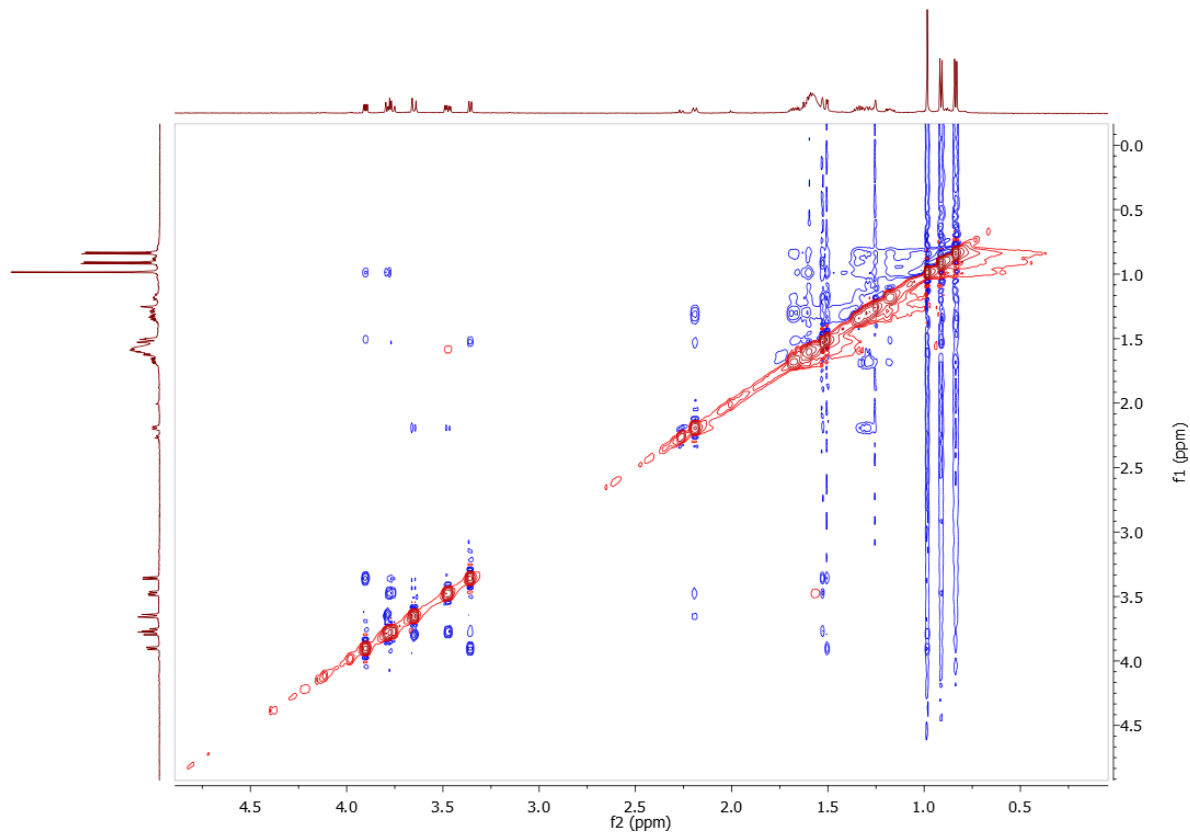


Figure S33: NOESY spectrum (600 MHz) of **4** in CDCl_3

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

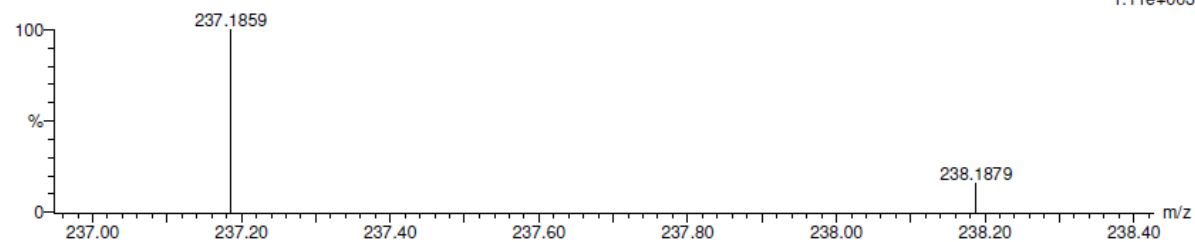
C: 0-50 H: 0-50 O: 0-10

BF14-1-103-May-2019BF14-1-1

BF14-1-1

BF14-1-1_4 10 (0.212)

1: TOF MS ES+
1.11e+003



Minimum:				-1.5				
Maximum:	5.0	10.0		50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
237.1859	237.1855	0.4	1.7	3.5	16.7	0.0	C15	H25 O2

Figure S34: HRESIMS spectrum of **4**

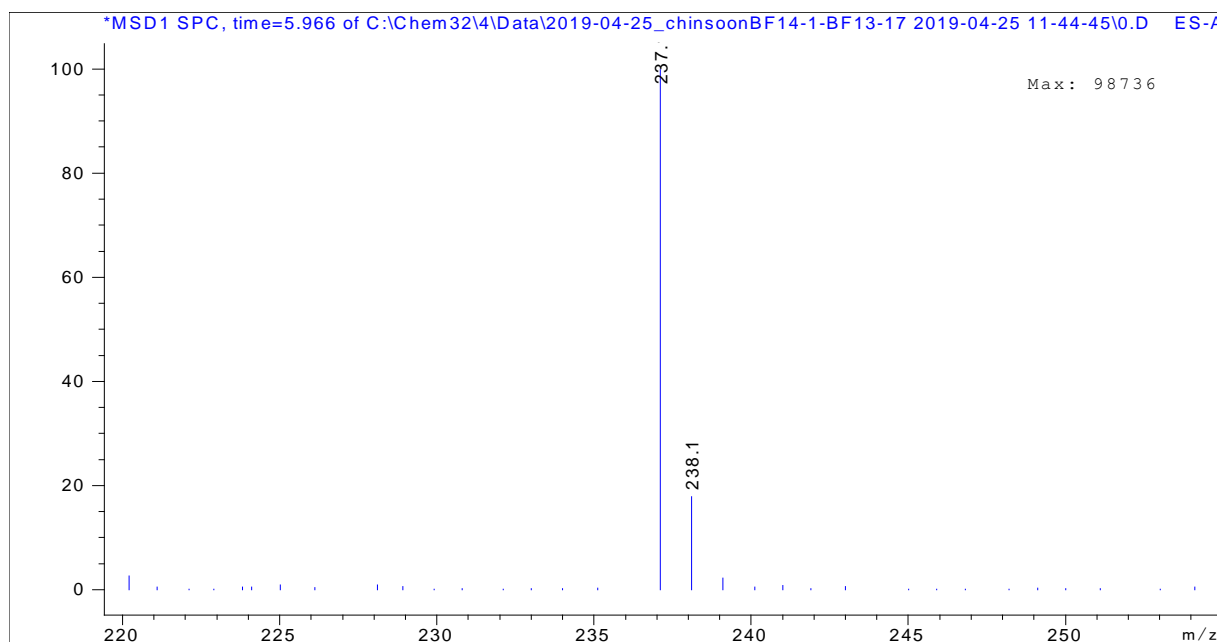


Figure S35: ESIMS spectrum of **4**

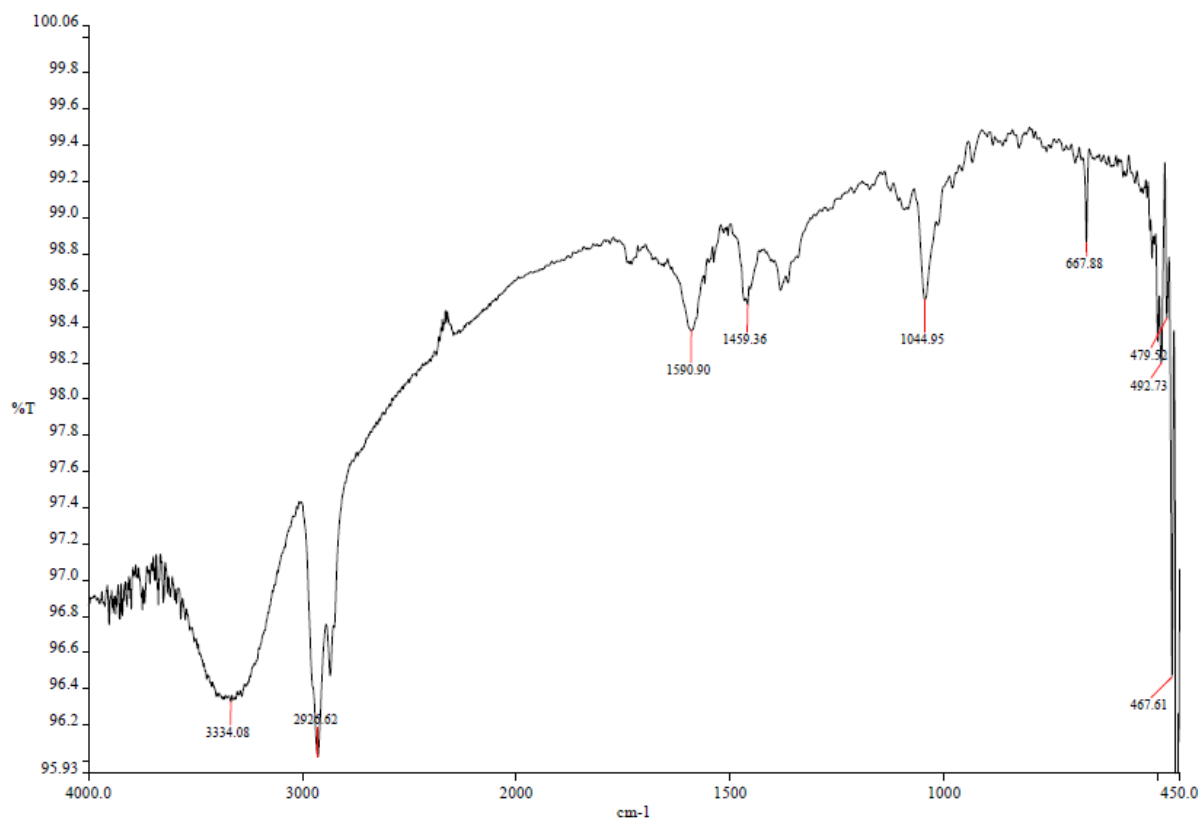


Figure S36: IR spectrum of **4**

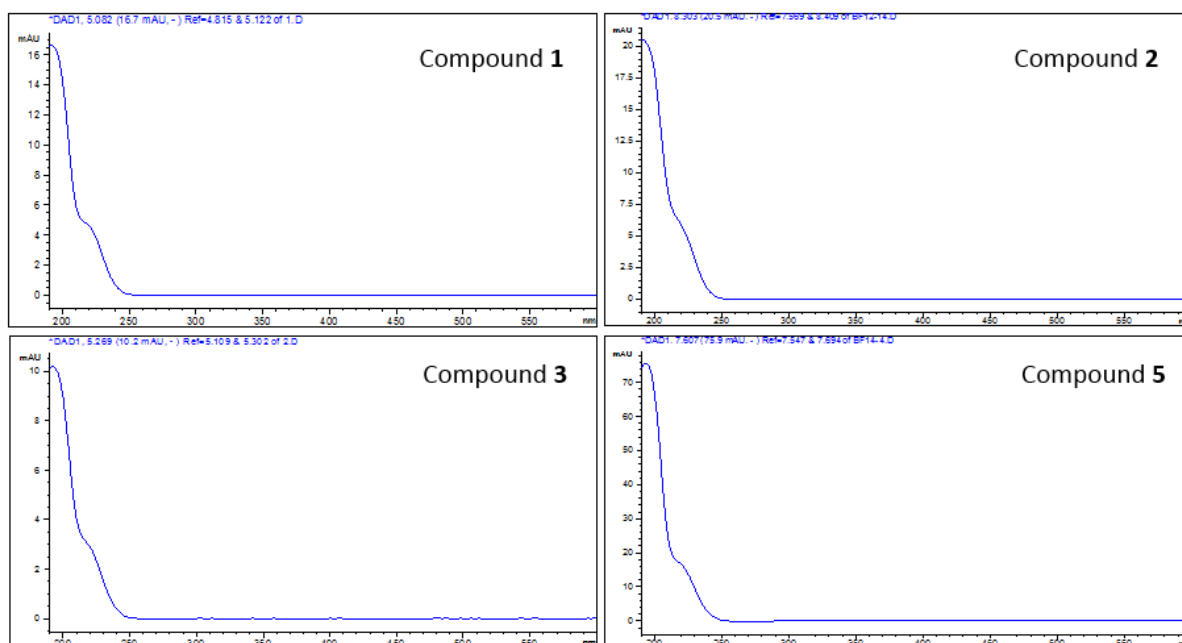


Figure S37: UV-vis spectrum of **1–3** and **5**

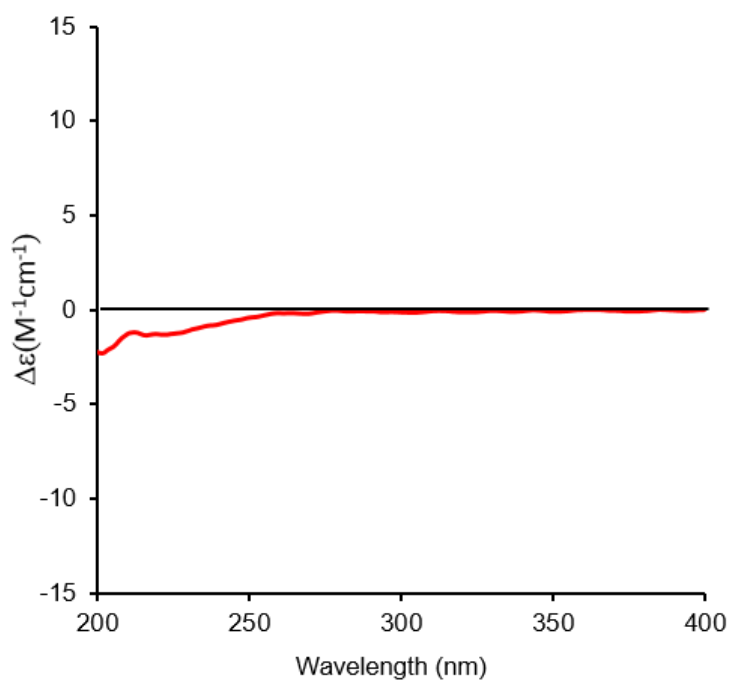


Figure S38: ECD spectrum of **4**

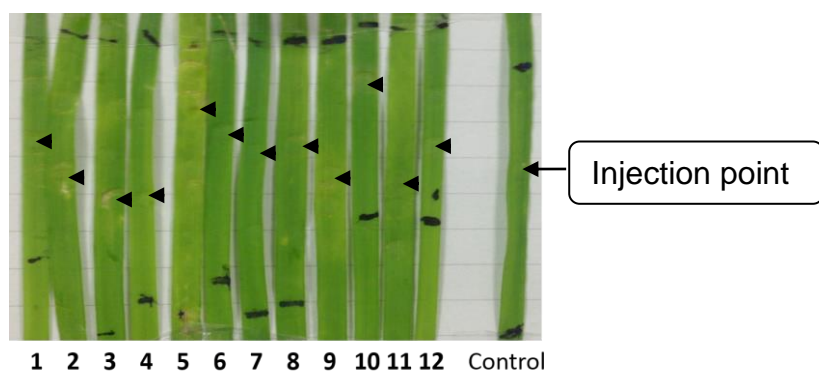


Figure S39: Phytotoxic activity of **1–12** against wheat leaves at 200 ppm

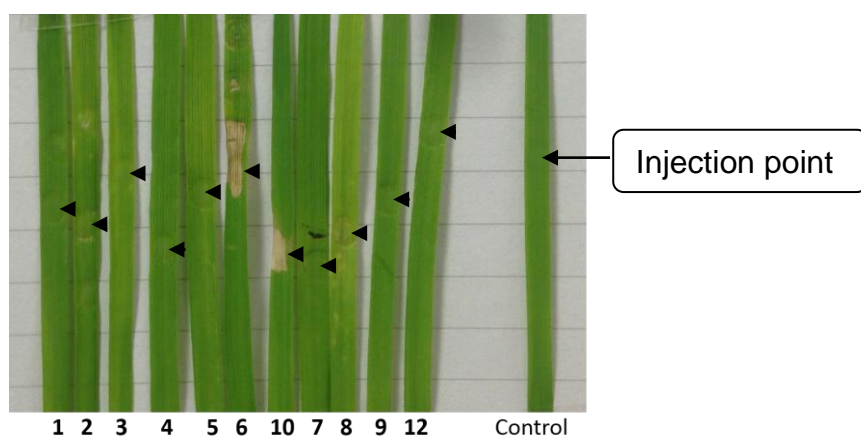


Figure S40: Phytotoxic activity of **1–10** and **12** against wheat leaves at 500 ppm

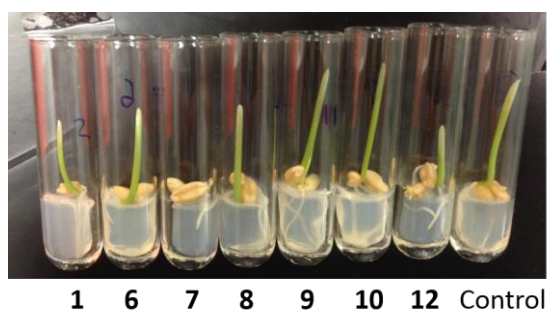


Figure S41: Phytotoxic activity of **1**, **6–10** and **12** against wheat germination at 100 ppm on day 5

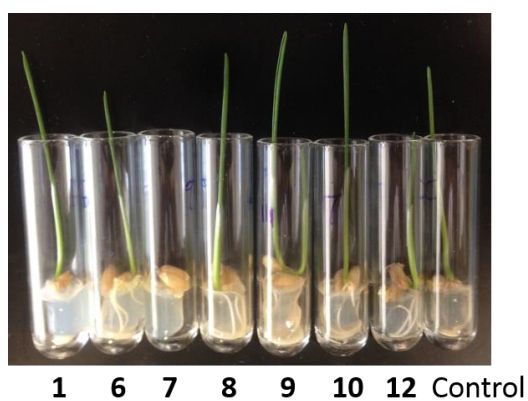


Figure S42: Phytotoxic activity of **1**, **6–10** and **12** against wheat germination at 100 ppm on day 7