



Supporting Information

for

Semisynthetic derivatives of massarilactone D with cytotoxic and nematicidal activities

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Copies of NMR, mass, and UV spectra for compounds 2–8

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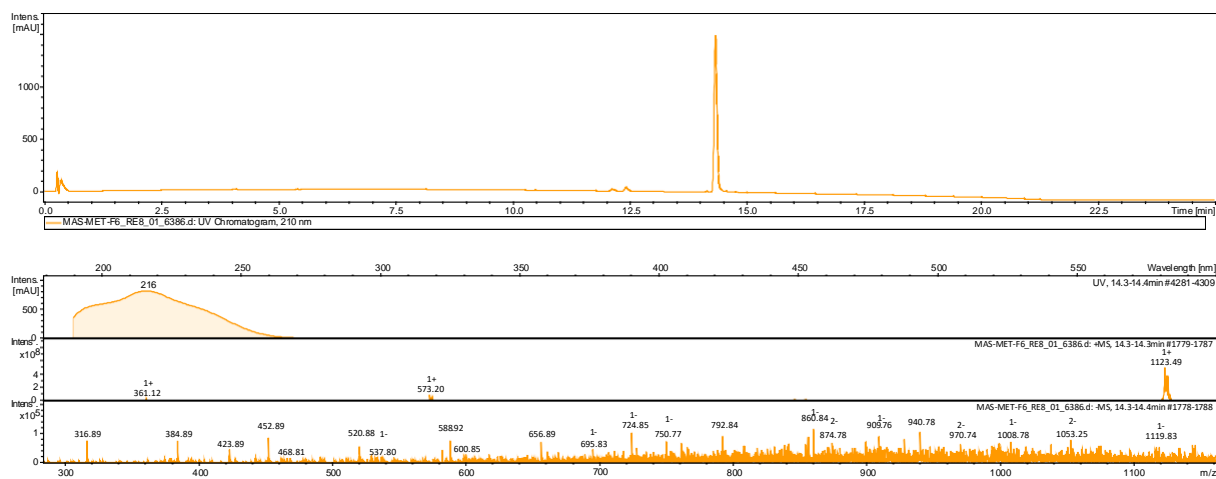


Figure S1: LC-UV-ESIMS spectra of compound **2**



Figure S2: UV-HRESIMS spectra of compound **2**.

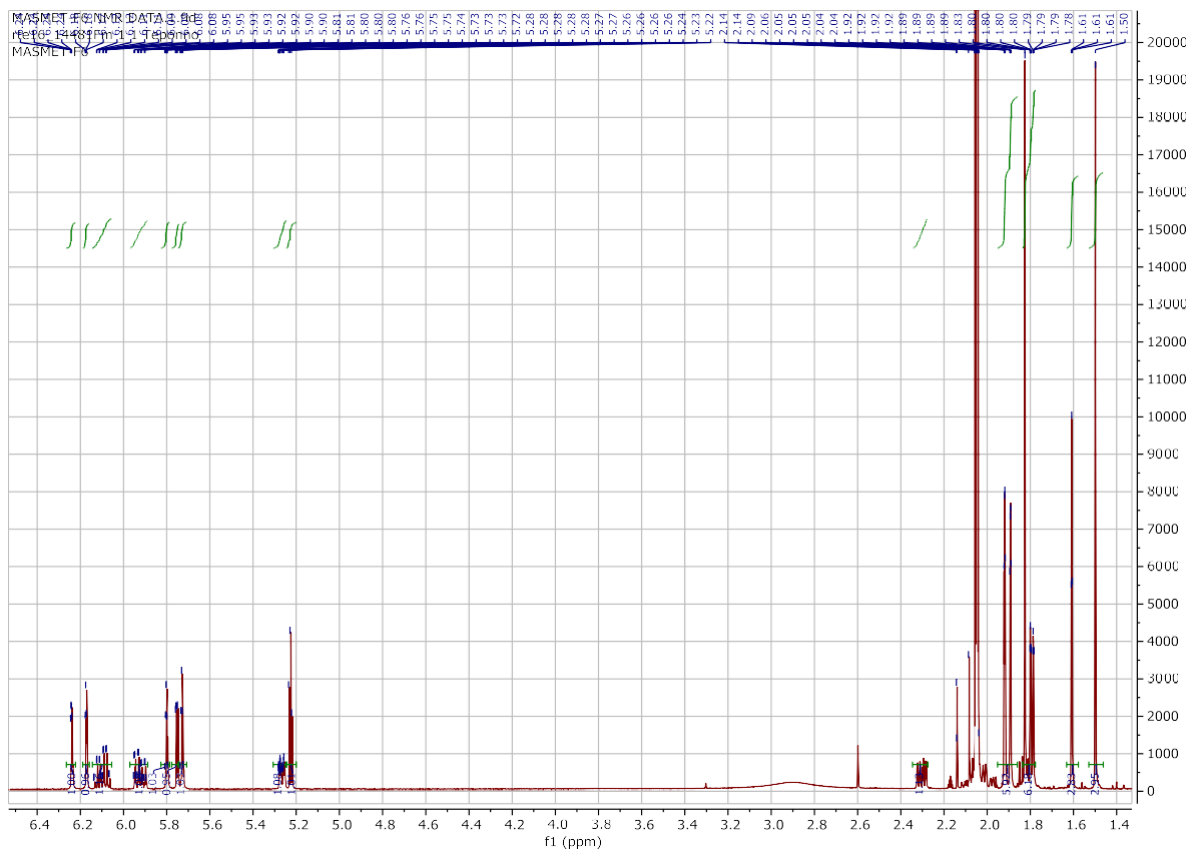


Figure S3: ^1H NMR spectrum of compound **2** in acetone- d_6 at 500 MHz.

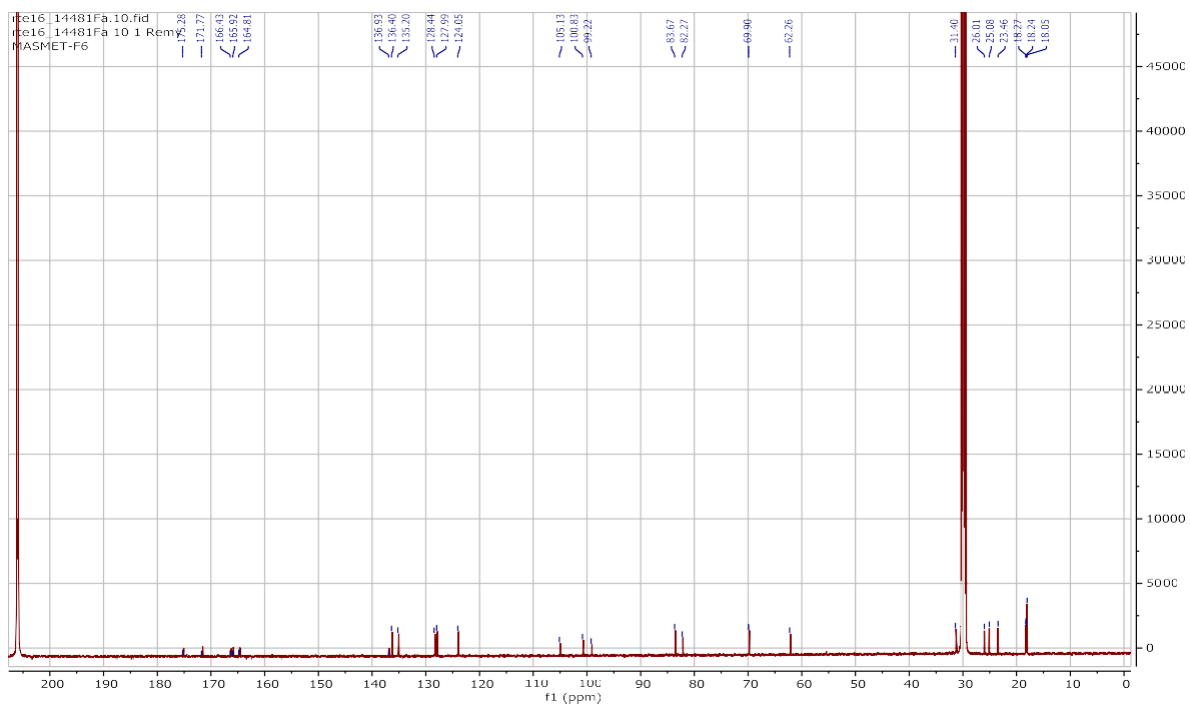


Figure S4: ^{13}C NMR spectrum of compound **2** in acetone- d_6 at 125 MHz.

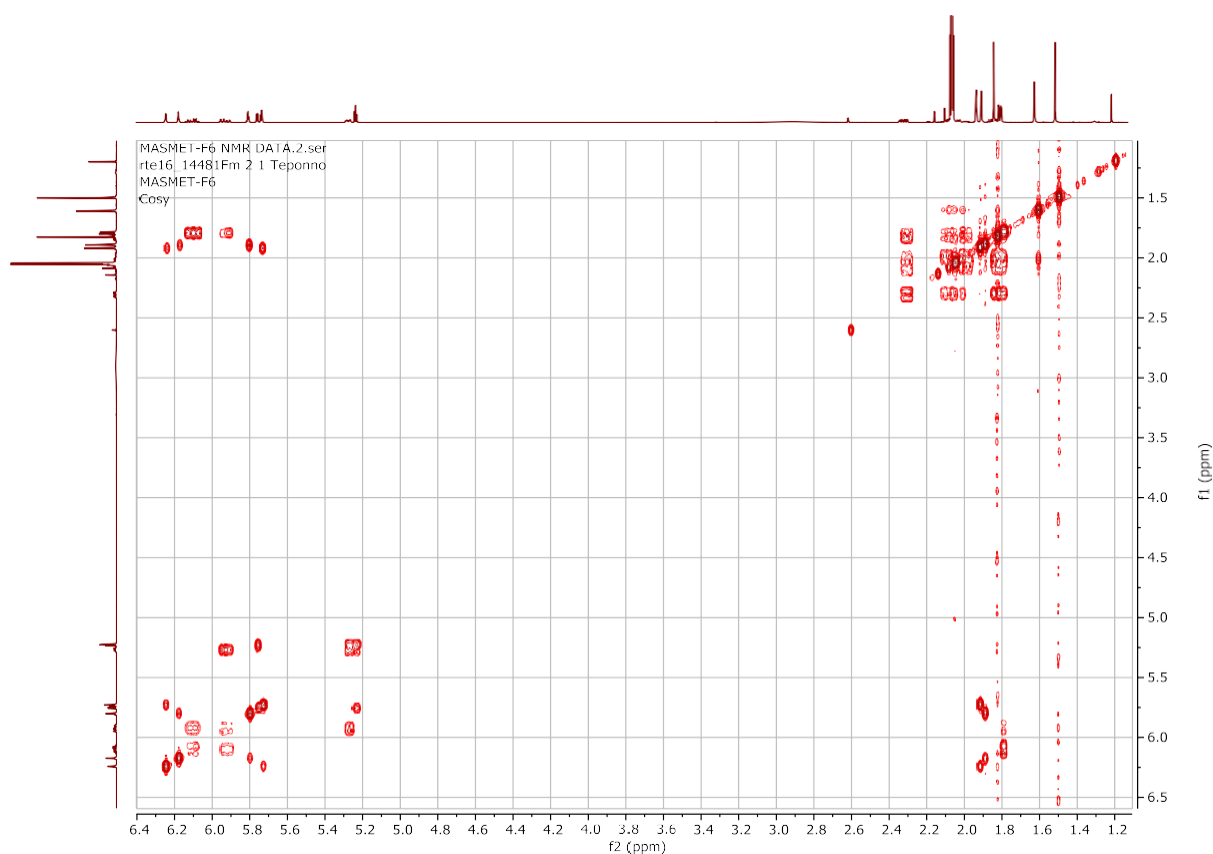


Figure S5: ^1H - ^1H COSY spectrum of compound **2** in acetone- d_6

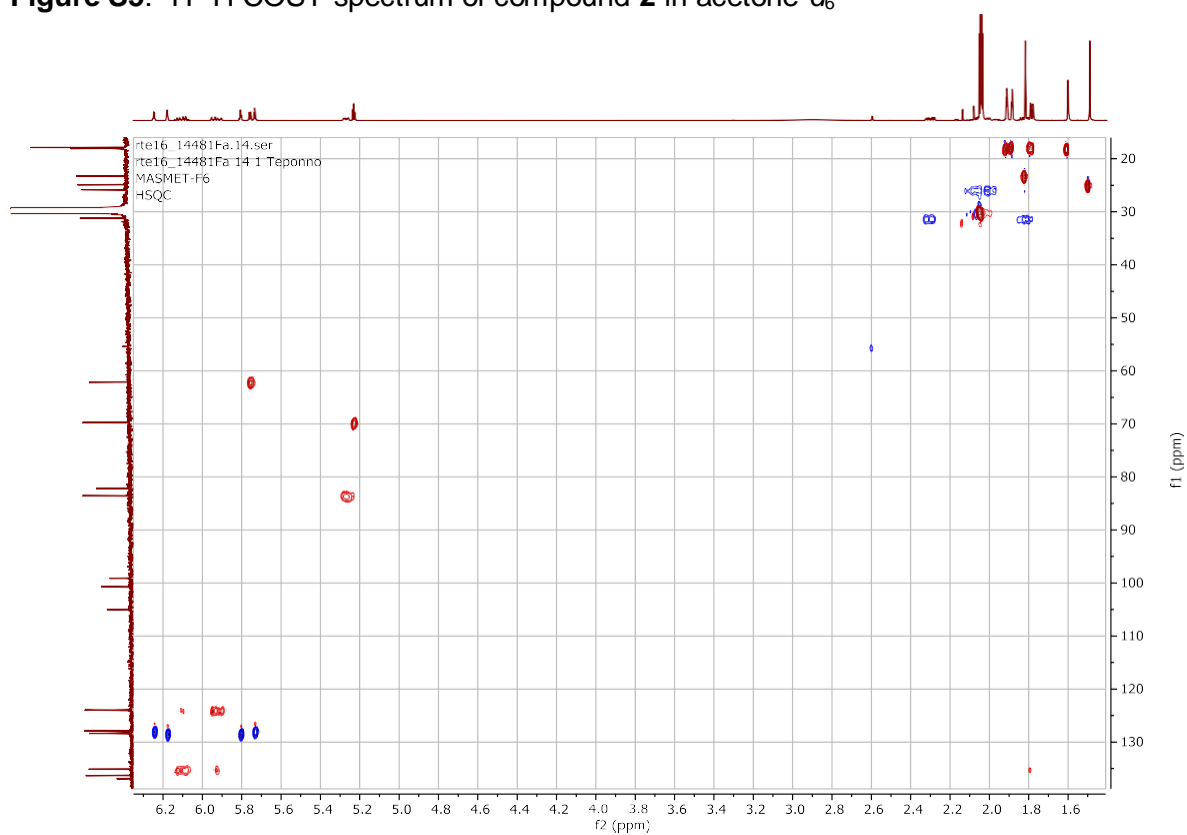


Figure S6: HSQC spectrum of compound **2** in acetone- d_6

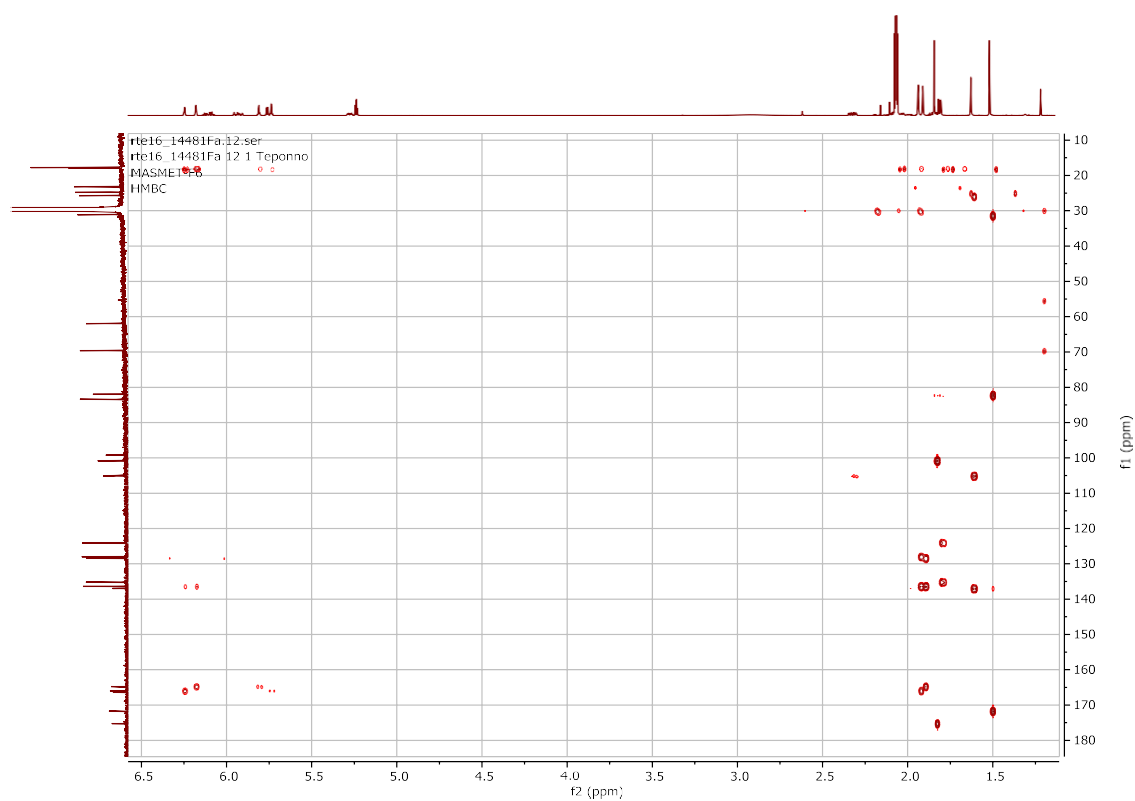


Figure S7: HMBC spectrum of compound **2** in acetone- d_6

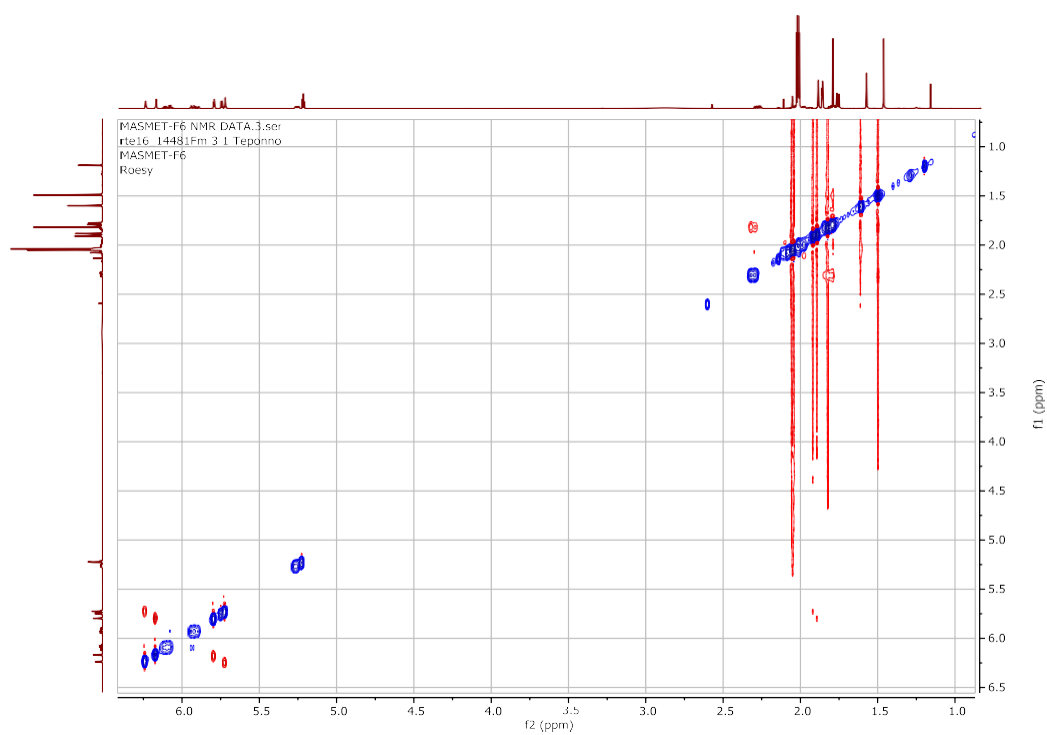


Figure S8: ROESY spectrum of compound **2** in acetone- d_6

Spectrum Peak Pick Report

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Data Set: MAS-MET-F6-0.075 - RawData

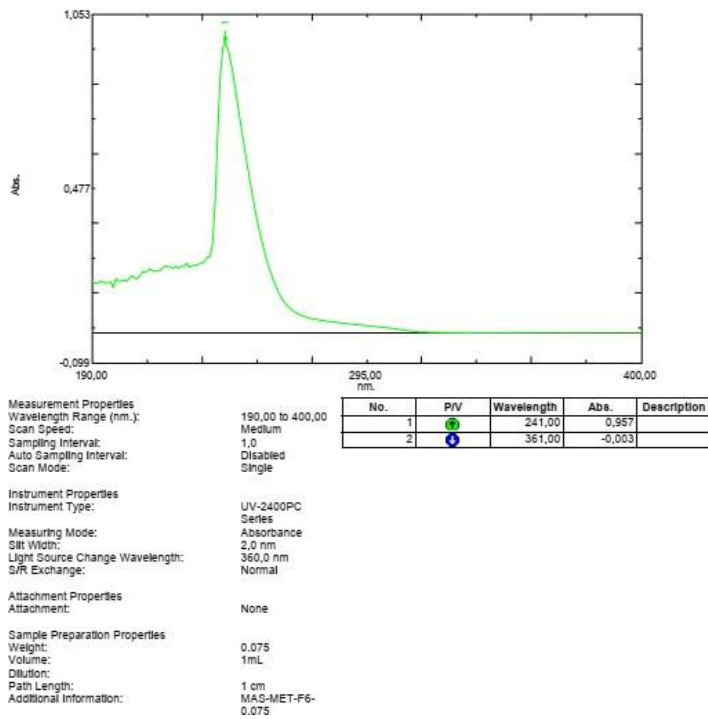


Figure S9: UV spectrum of compound 2

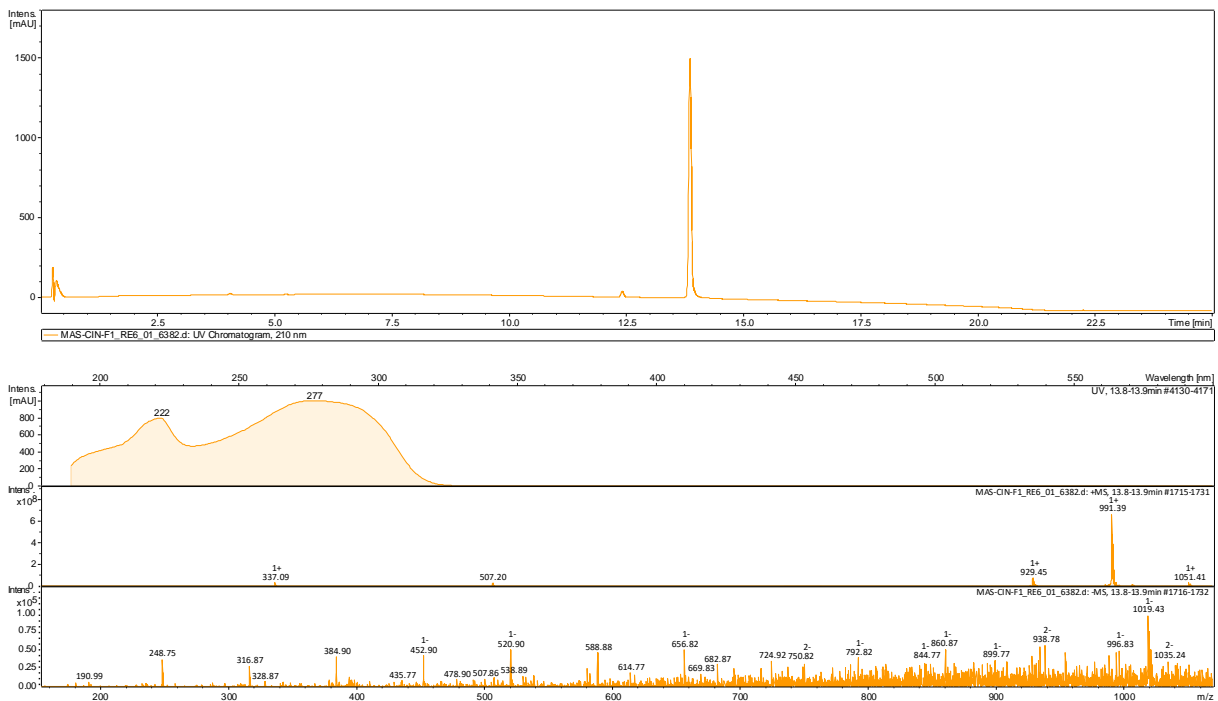


Figure S10: LC-UV-ESIMS spectra of compound 3.

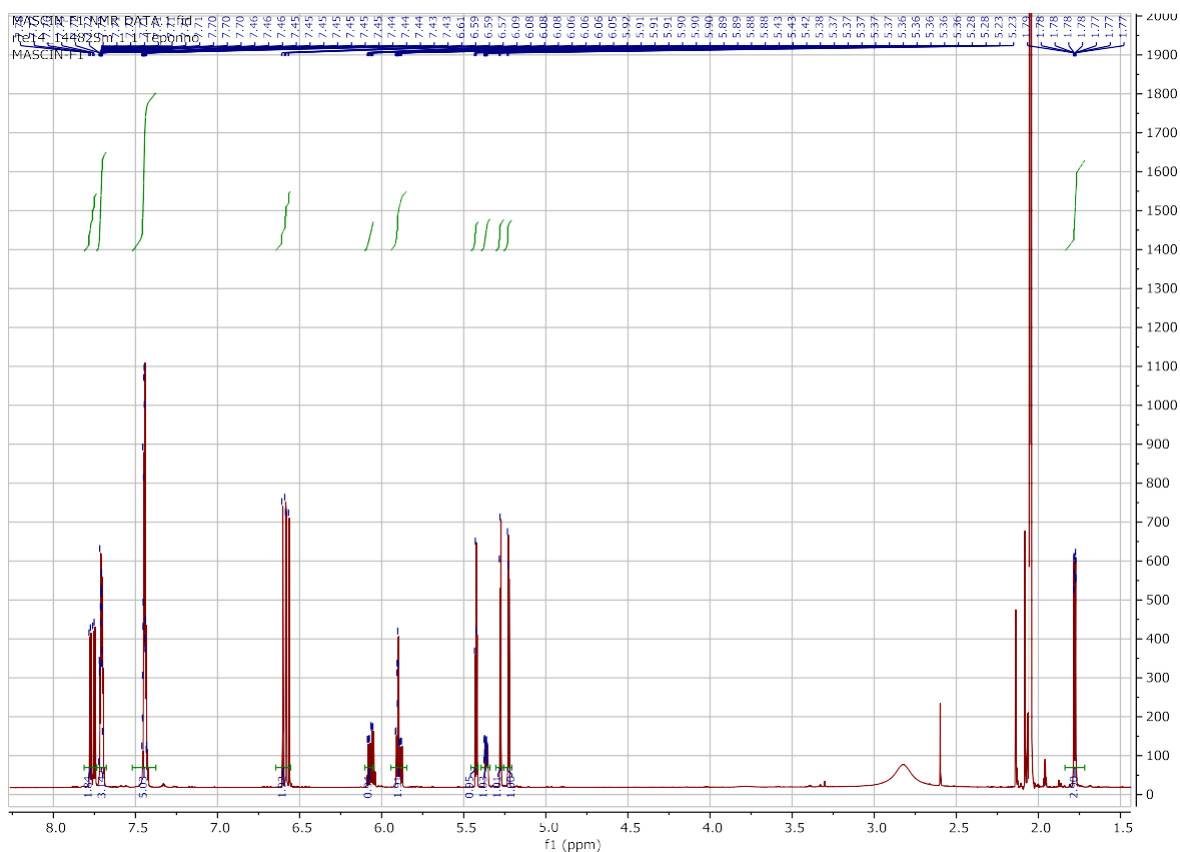


Figure S11: ^1H NMR spectrum of compound **3** in acetone- d_6 at 700 MHz.

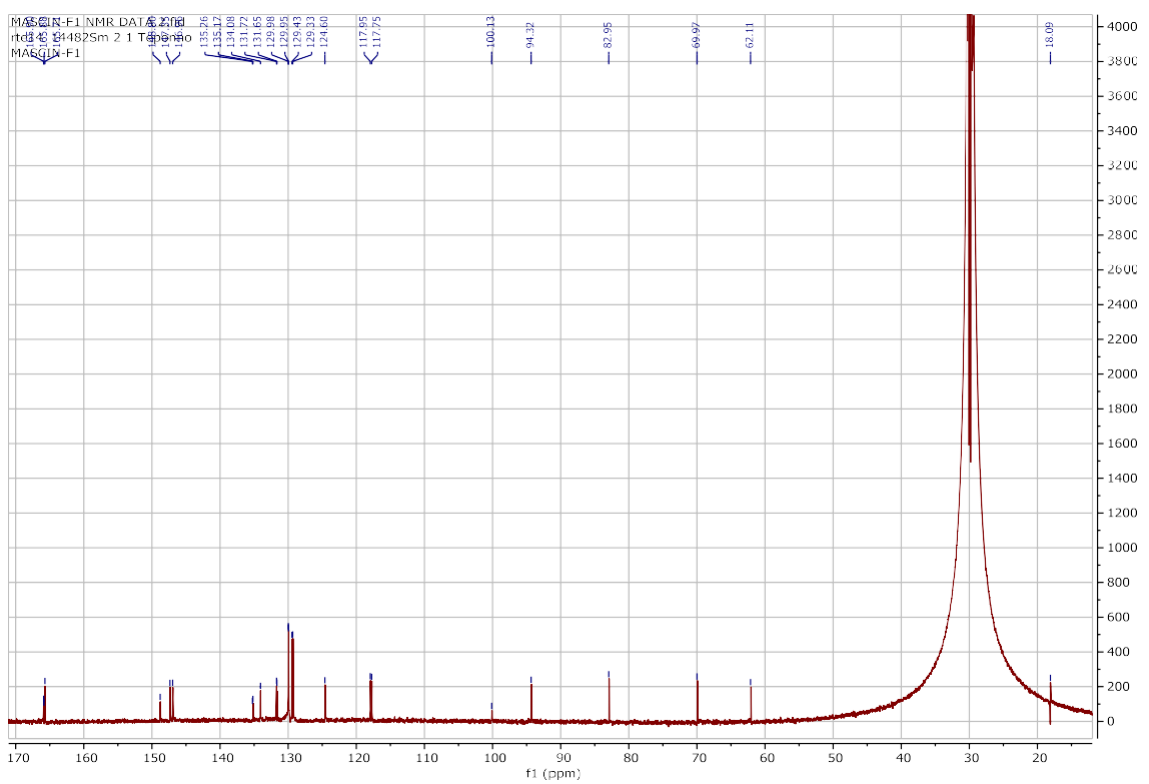


Figure S12: ^{13}C NMR spectrum of compound **3** in acetone- d_6 at 175 MHz.

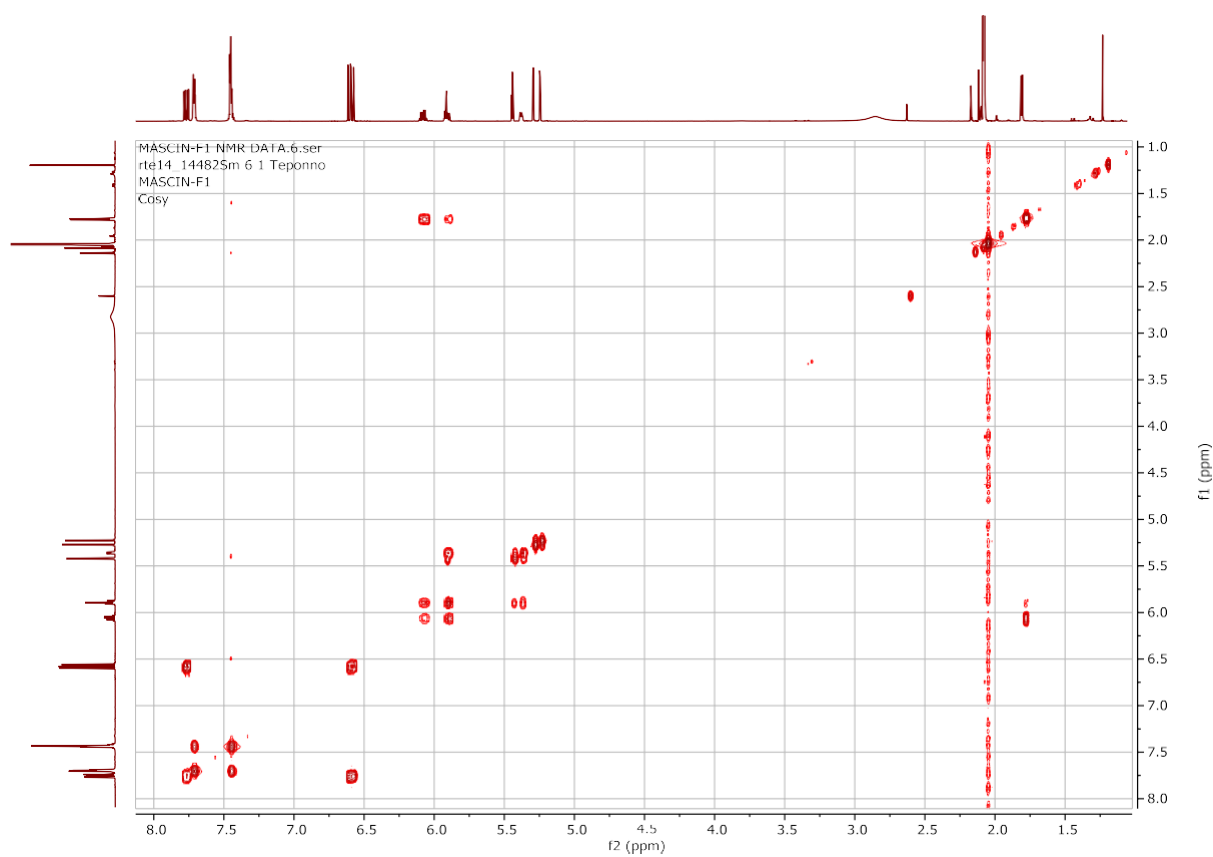


Figure S13: ^1H - ^1H COSY spectrum of compound **3** in acetone- d_6

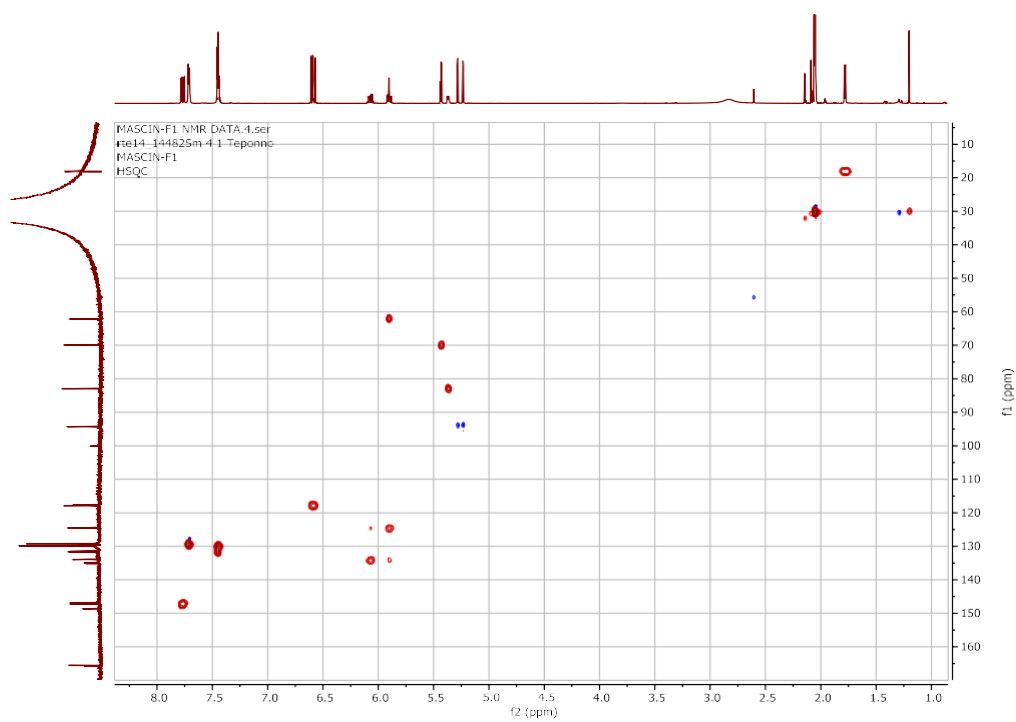


Figure S14: HSQC spectrum of compound **3** in acetone- d_6

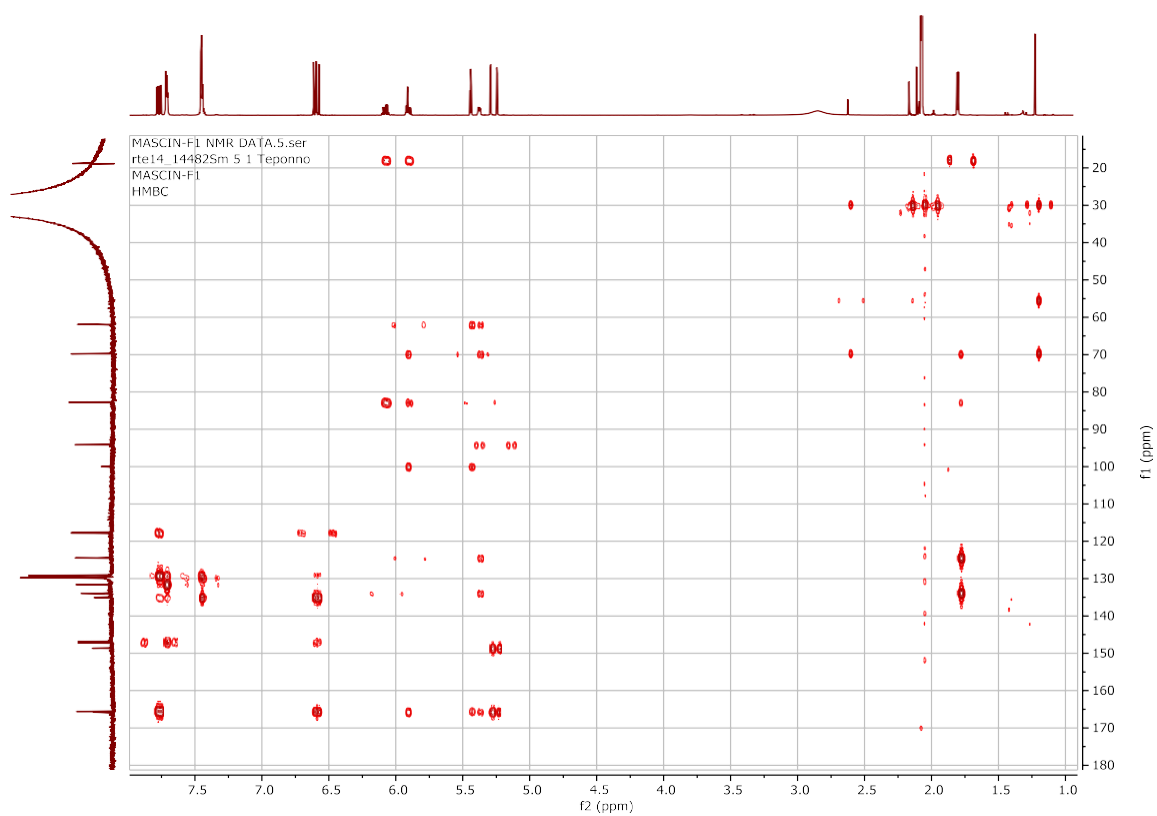


Figure S15: HMBC spectrum of compound 3 in acetone- d_6

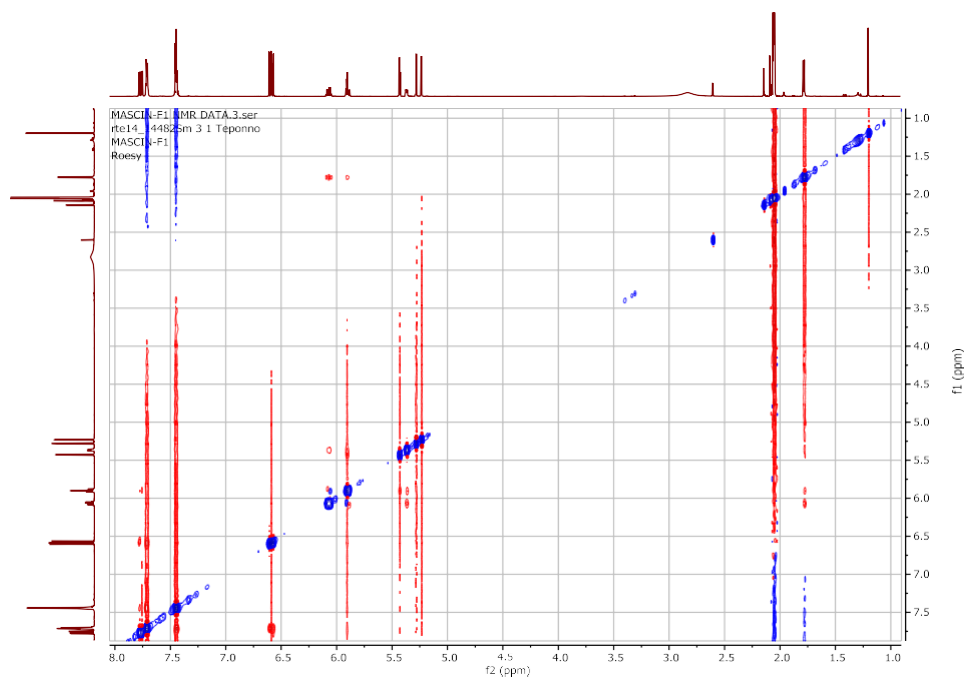


Figure S16: ROESY spectrum of compound 3 in acetone- d_6

Spectrum Peak Pick Report

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Data Set: MAS-CIN-F1-0.01875 - RawData

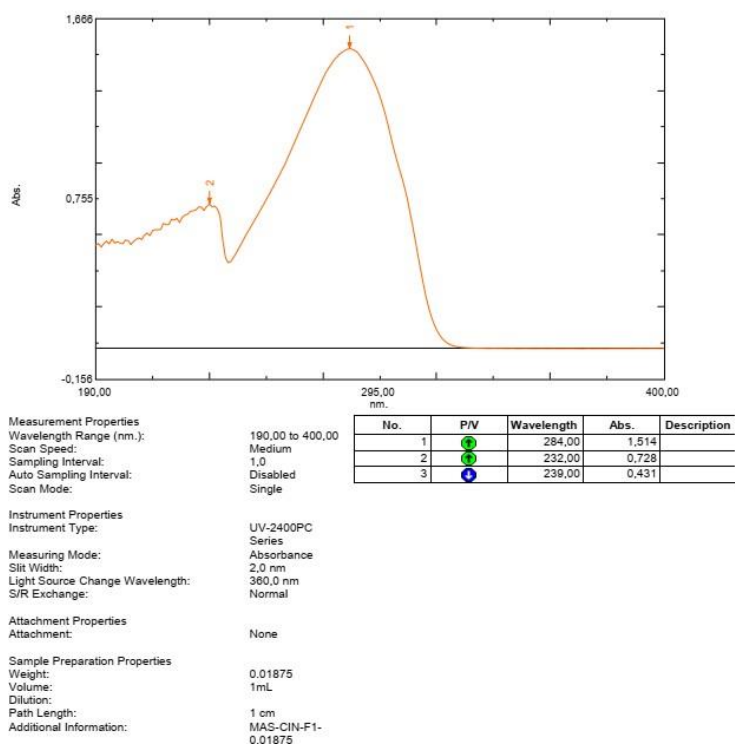


Figure S17: UV spectrum of compound 3

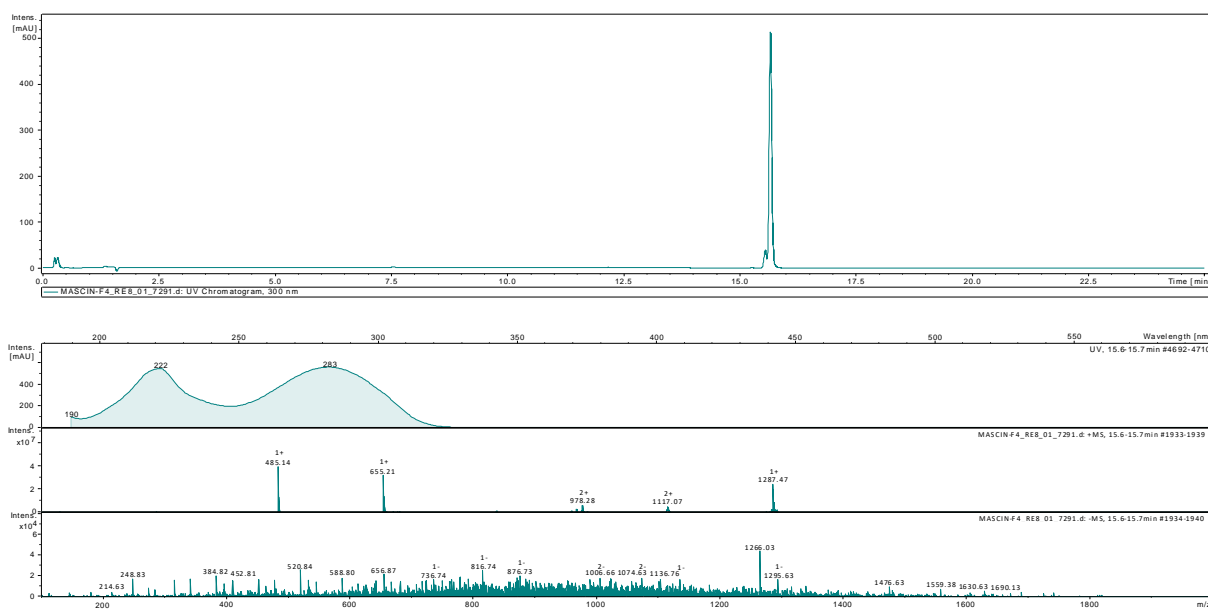
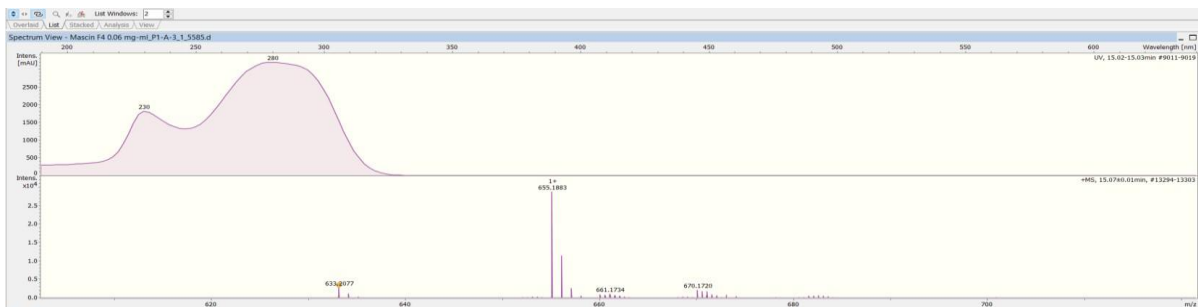


Figure S18: LC-UV-ESIMS spectra of compound 4



SmartFormula Manually

Lower formula:

Upper formula:

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos: Collect adducts

Adducts, neg:

Measured m/z: Tolerance: ppm Charge:

Meas. m/z	#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb [neutral]	e ⁻ Conf	N-Rule	[err]
633.2077	1	C ₃₈ H ₃₃ O ₉	633.2119	4.2	6.6	11.3	23.0	even	ok	
633.2077	4	C ₃₅ H ₂₉ N ₁₀ O ₃	633.2106	2.8	4.5	14.0	29.0	even	ok	
633.2077	6	C ₃₄ H ₂₉ N ₆ O ₇	633.2092	1.5	2.4	18.2	24.0	even	ok	
633.2077	7	C ₃₁ H ₂₁ N ₄ O	633.2079	0.2	0.2	21.9	30.0	even	ok	
633.2077	9	C ₃₃ H ₃₃ H ₂ O ₁₁	633.2079	0.2	0.3	27.2	19.0	even	ok	
633.2077	10	C ₃₀ H ₂₅ H ₁₂ O ₅	633.2065	-1.2	-1.9	29.6	25.0	even	ok	
633.2077	2	C ₃₇ H ₂₇ H ₇ O ₄	633.2119	4.2	6.6	13.5	28.5	odd	ok	
633.2077	3	C ₃₆ H ₃₁ N ₃ O ₈	633.2106	2.8	4.5	13.7	23.5	odd	ok	
633.2077	5	C ₃₃ H ₂₃ H ₃ O ₂	633.2092	1.5	2.4	17.1	29.5	odd	ok	
633.2077	8	C ₃₂ H ₂₇ H ₉ O ₆	633.2079	0.2	0.3	23.7	24.5	odd	ok	
633.2077	11	C ₃₁ H ₃₁ N ₅ O ₁₀	633.2065	-1.2	-1.9	33.1	19.5	odd	ok	
633.2077	12	C ₃₀ H ₃₅ N ₀ D ₁₄	633.2052	-2.5	-4.0	43.6	14.5	odd	ok	

Automatically locate monoisotopic peak: Maximum number of formulas:

Check rings plus double bonds Minimum: Maximum:

Organic compounds Electron configuration:

Filter H/C element ratio Minimum: Maximum:

Estimate carbon number Generate immediately

Figure S19: UV-HRESIMS spectra of compound 4.

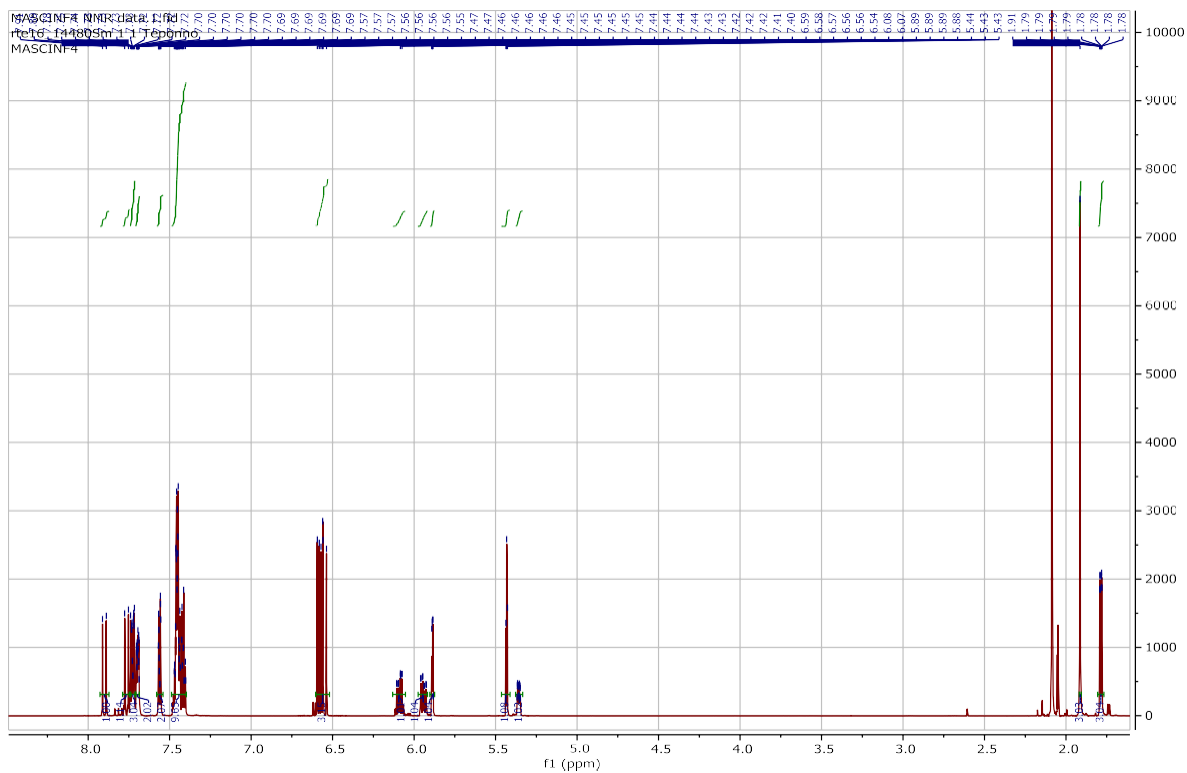


Figure S20: ^1H NMR spectrum of compound **4** in acetone- d_6 at 700 MHz.

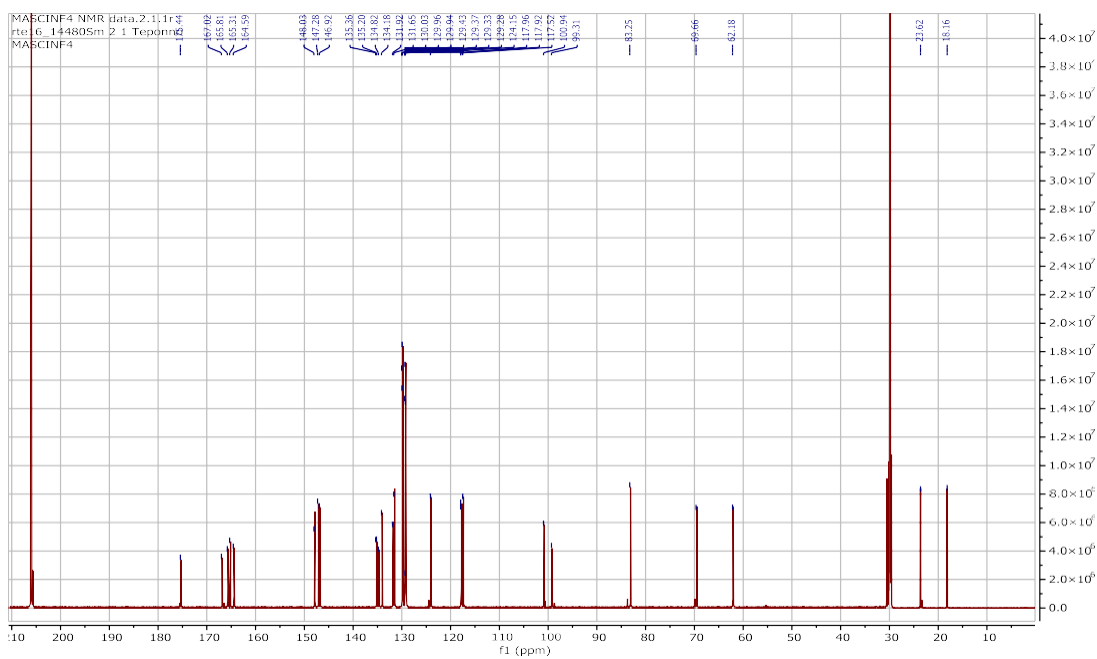


Figure S21: ^{13}C NMR spectrum of compound **4** in acetone- d_6 at 175 MHz.

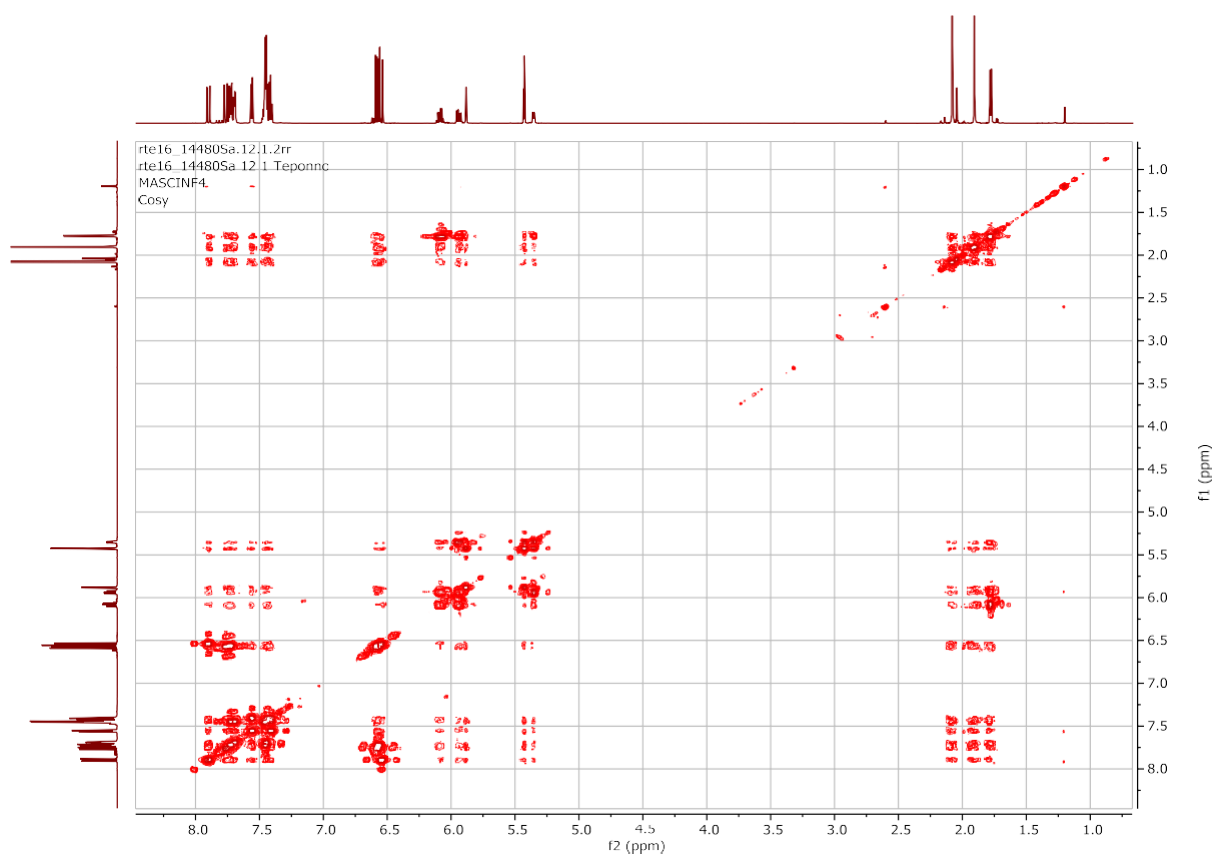


Figure S22: ^1H - ^1H COSY spectrum of compound **4** in acetone- d_6 .

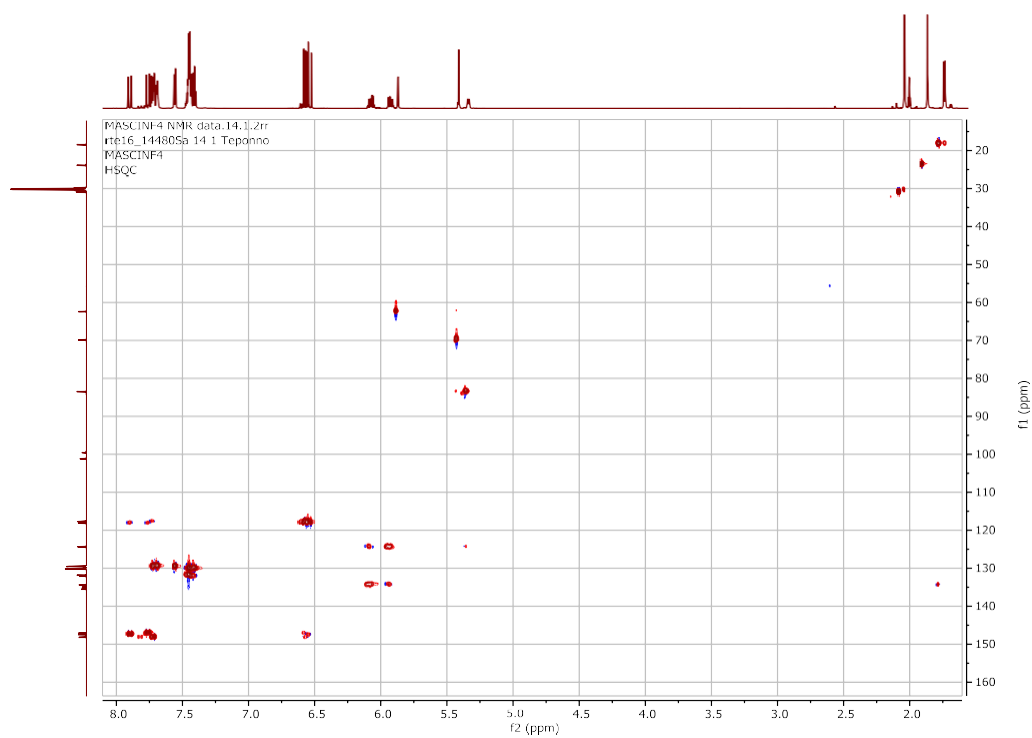


Figure S23: HSQC spectrum of compound **4** in acetone- d_6 .

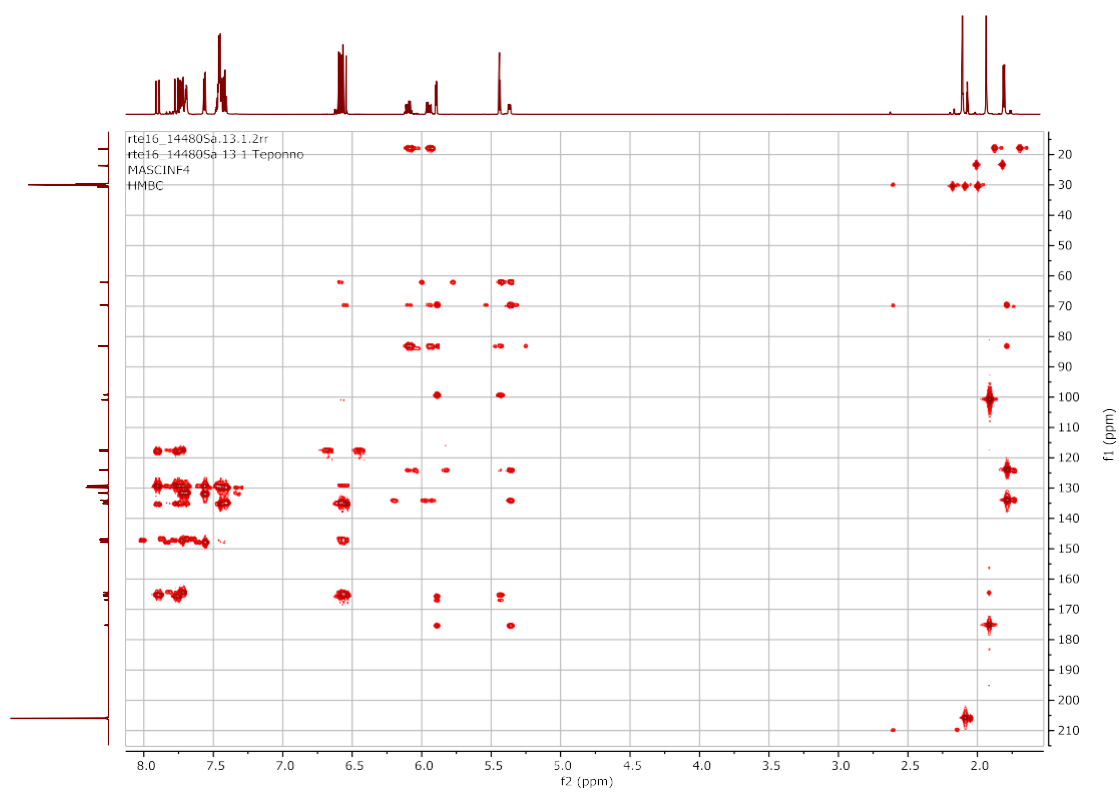


Figure S24: HMBC spectrum of compound **4** in acetone- d_6 .

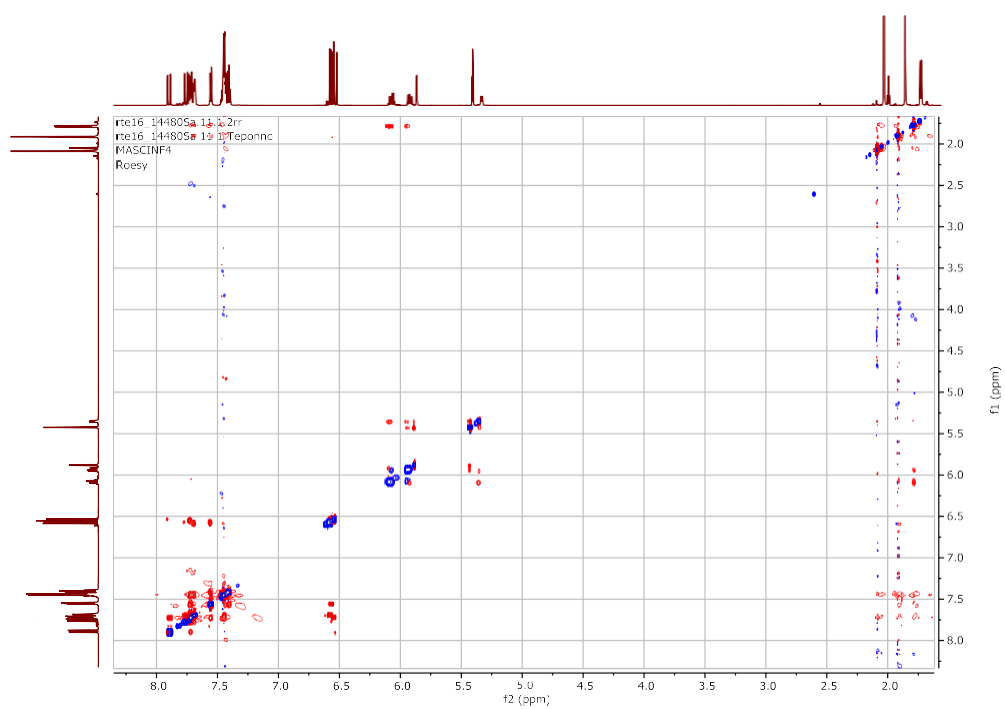


Figure S25: ROESY spectrum of compound **4** in acetone- d_6 .

Spectrum Peak Pick Report

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Data Set: MAS-CIN-F2-0.009375 - RawData

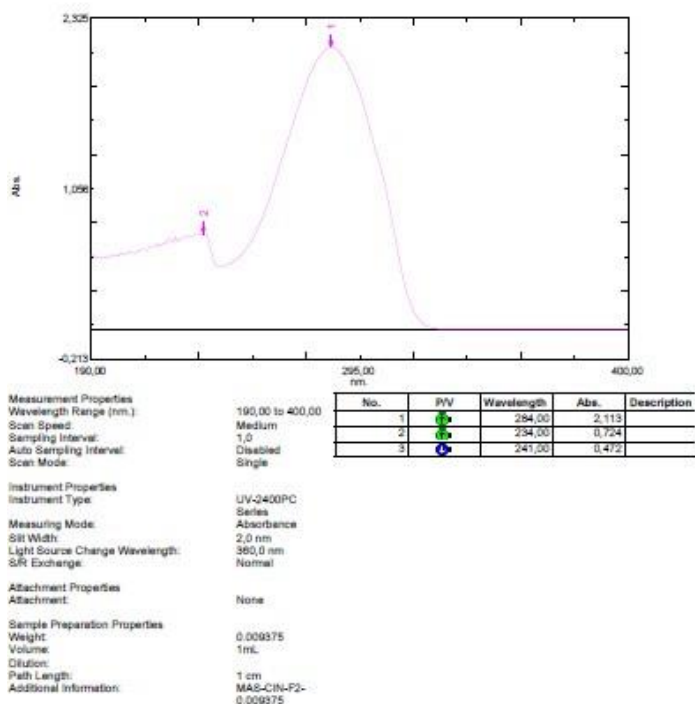


Figure S26: UV spectrum of compound 4 in acetone- d_6 .

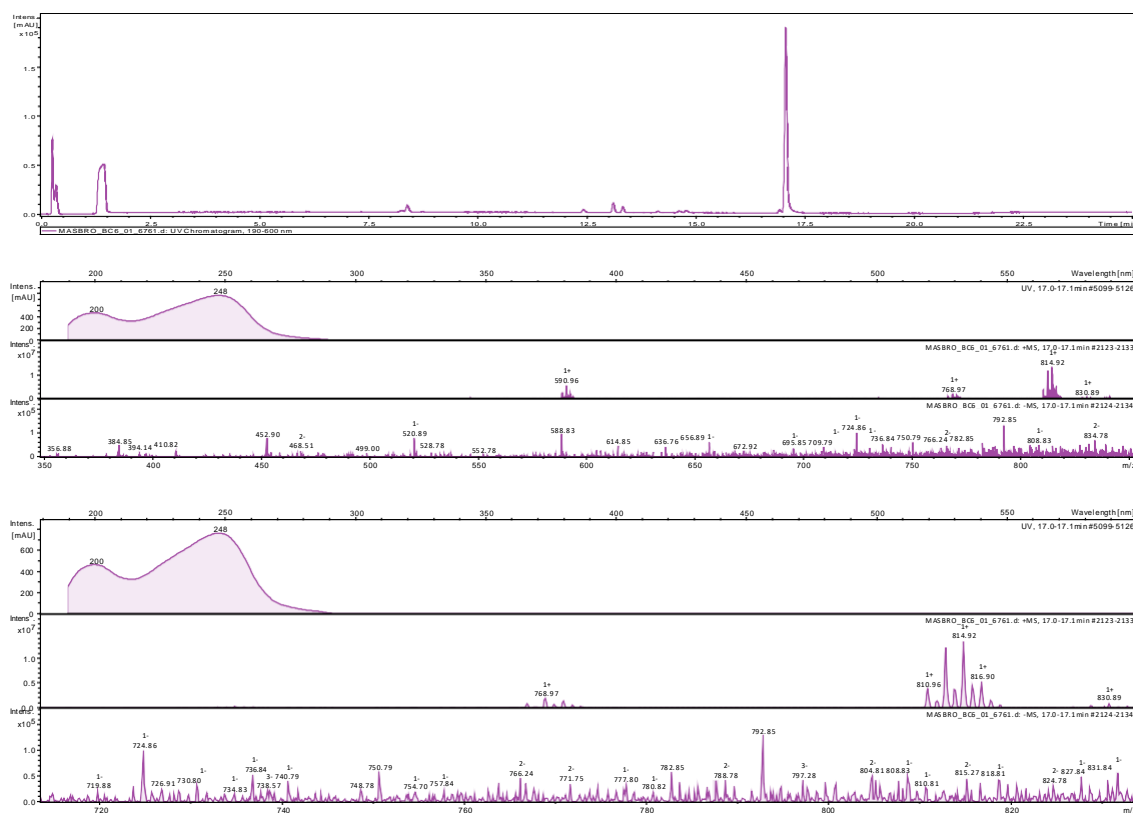


Figure S27: LC-UV-ESIMS spectra of compound 5.

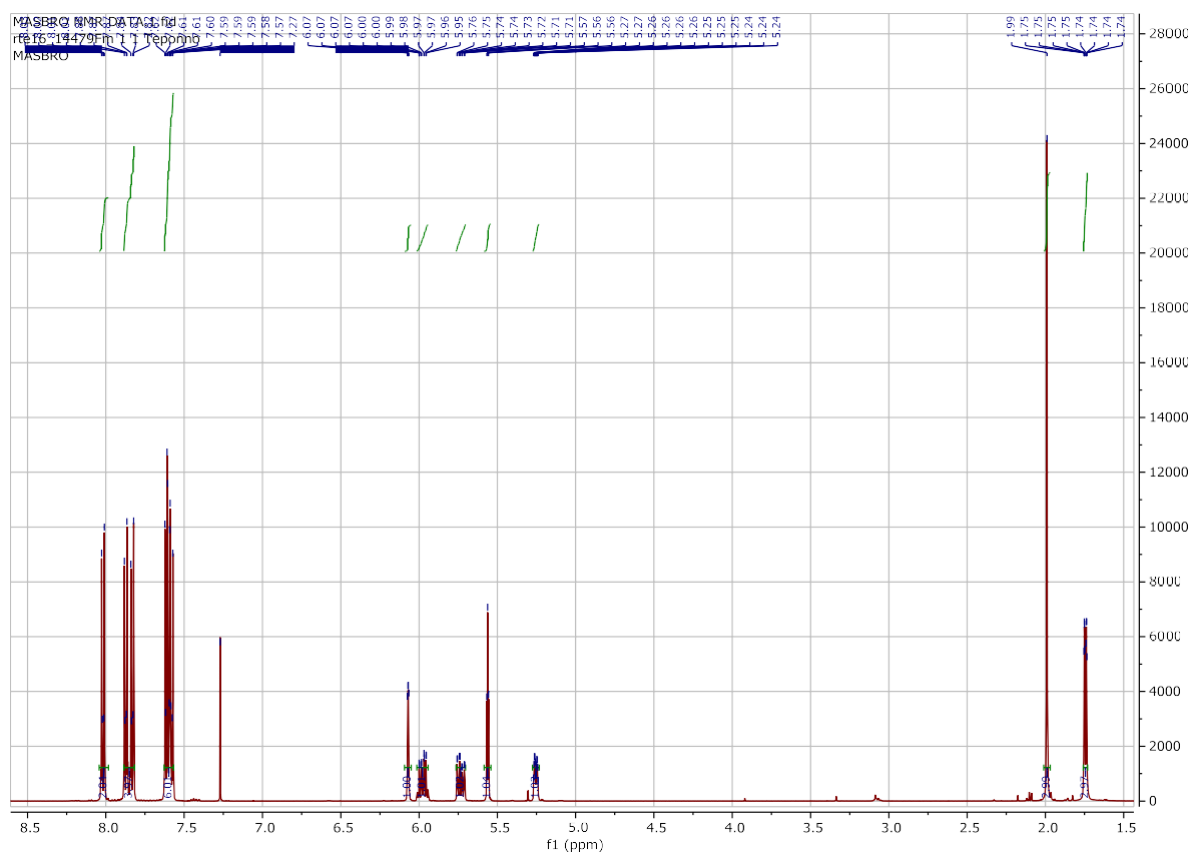


Figure S28: ^1H NMR spectrum of compound **5** in CDCl_3 at 500 MHz.

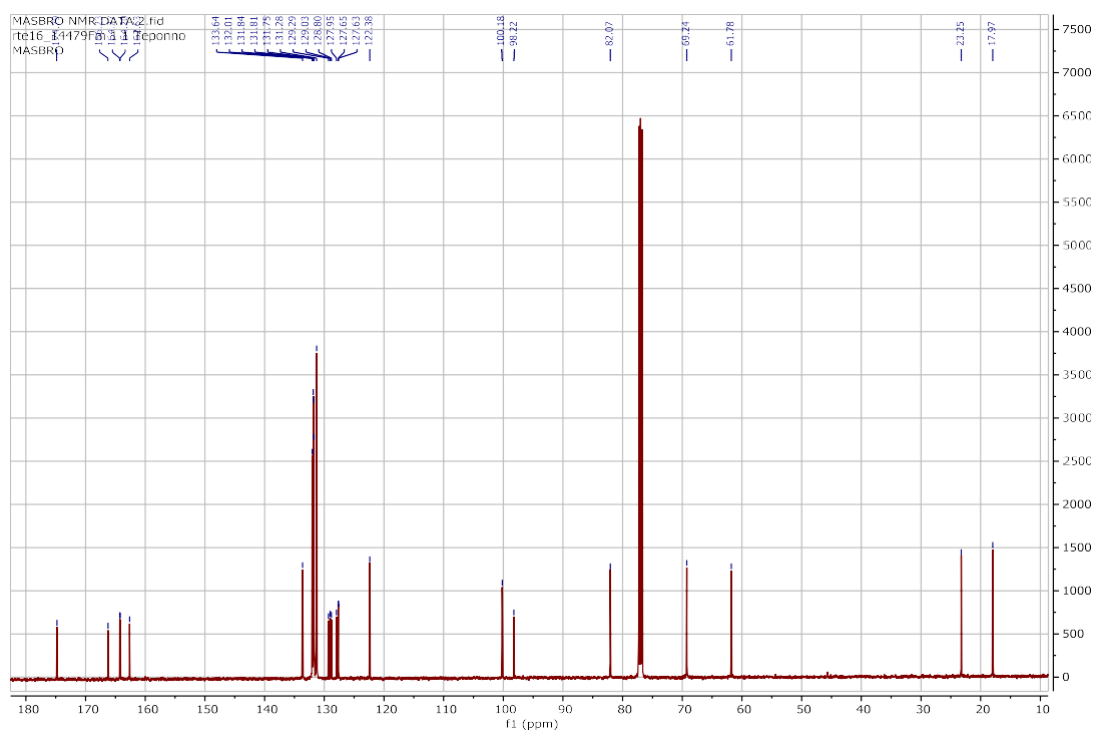


Figure S29: ^{13}C NMR spectrum of compound **5** in CDCl_3 at 125 MHz.

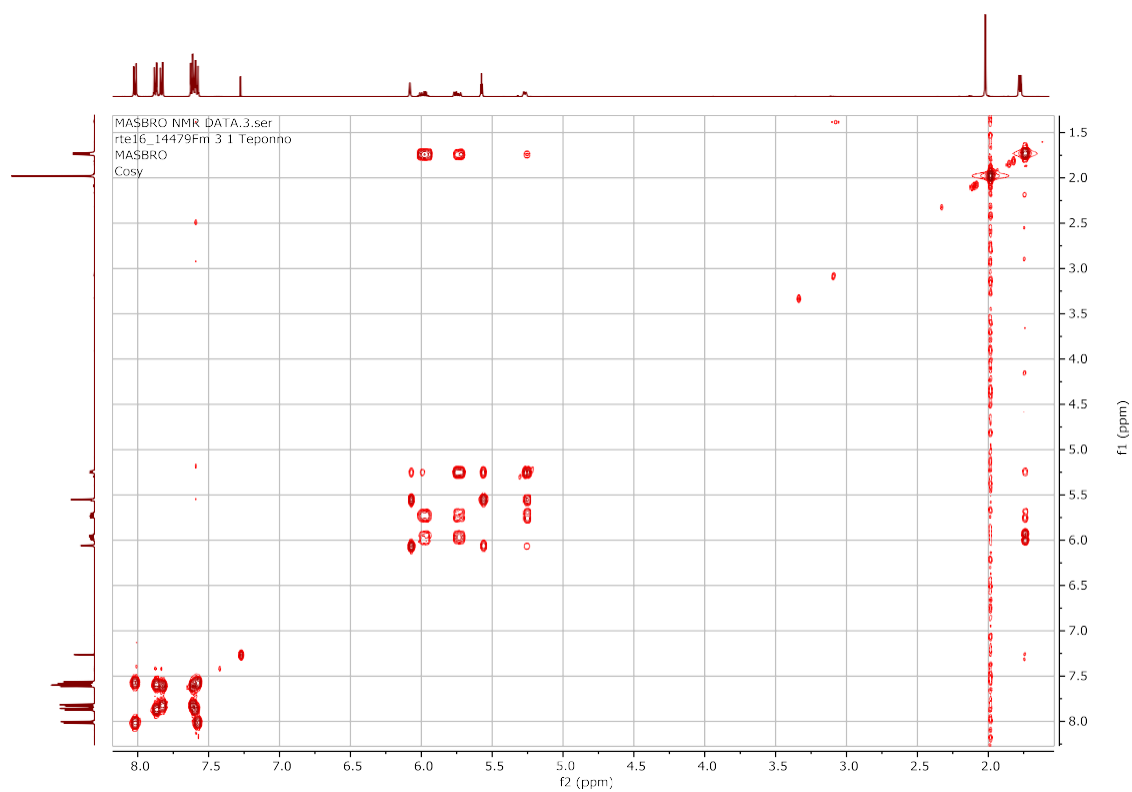


Figure S30: ^1H - ^1H COSY spectrum of compound **5**.

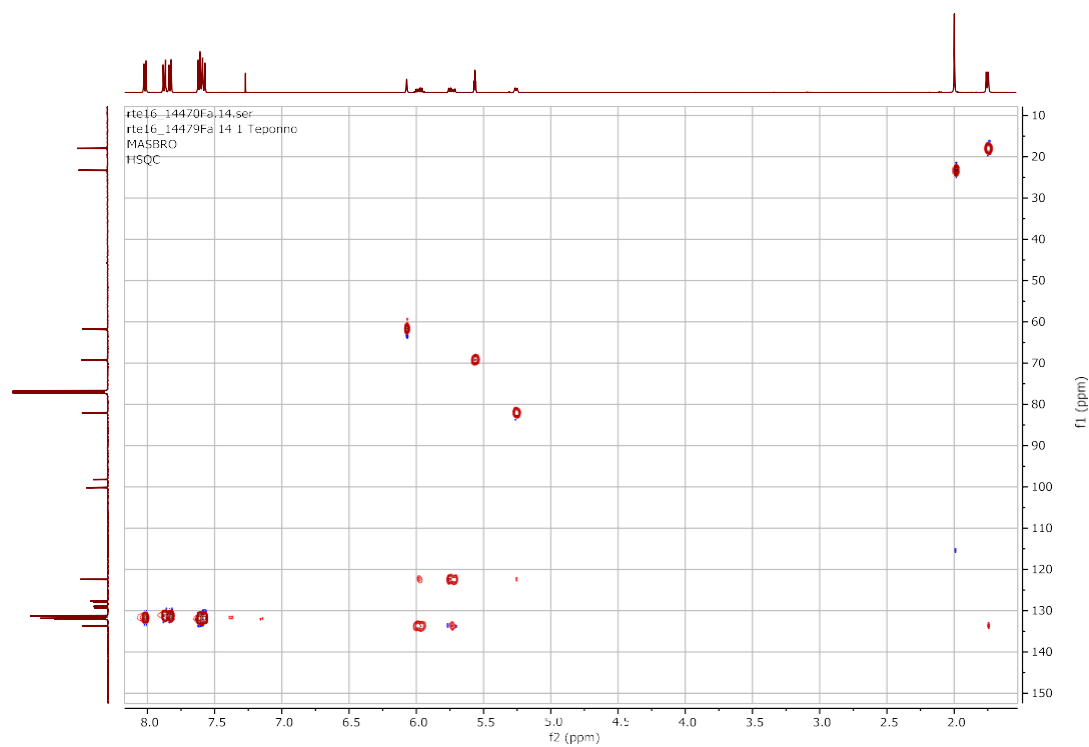


Figure S31: HSQC spectrum of compound **5**.

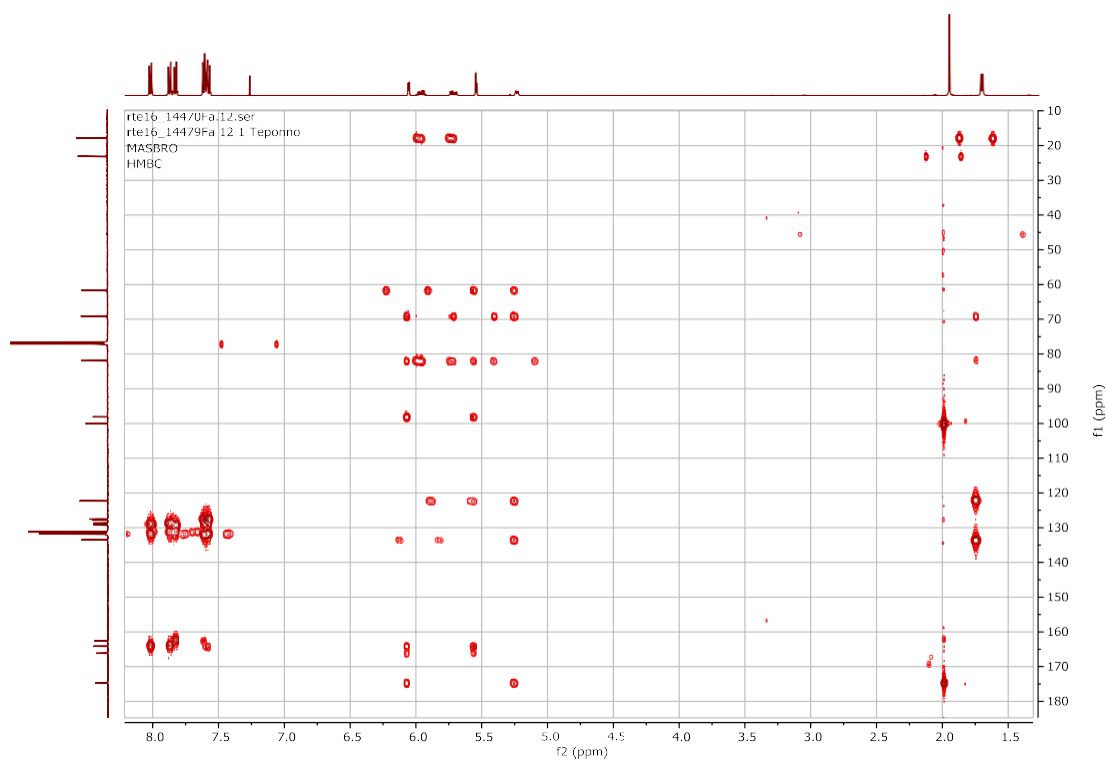


Figure S32: HMBC spectrum of compound 5.

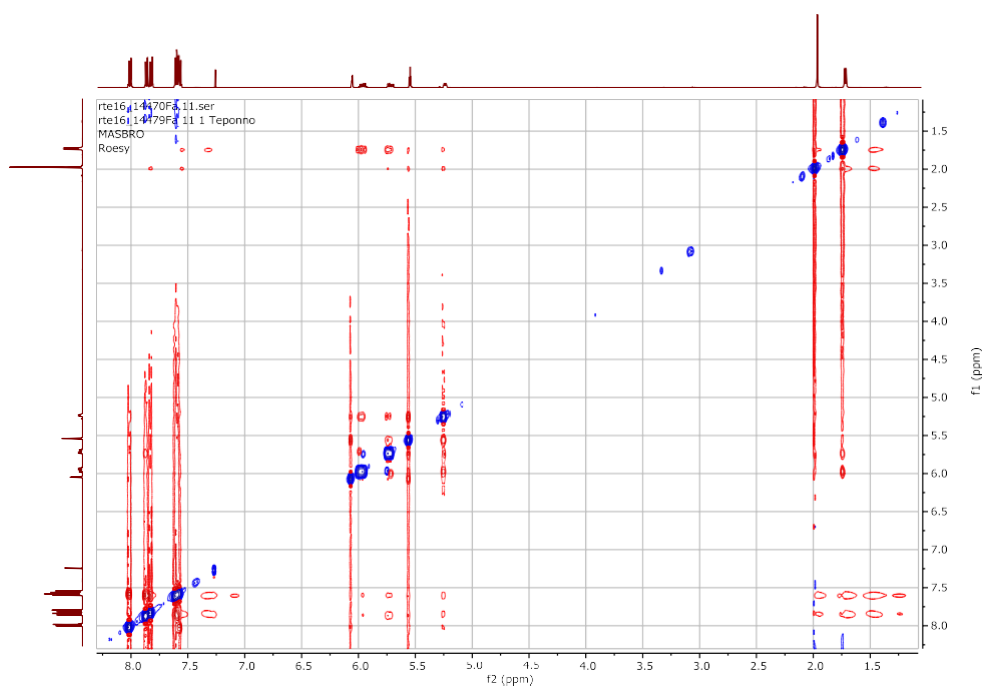


Figure S33: ROESY spectrum of compound 5.

Spectrum Peak Pick Report

20.04.2018 13:09:12

Data Set: MAS-BRO-F6-0.0375 - RawData

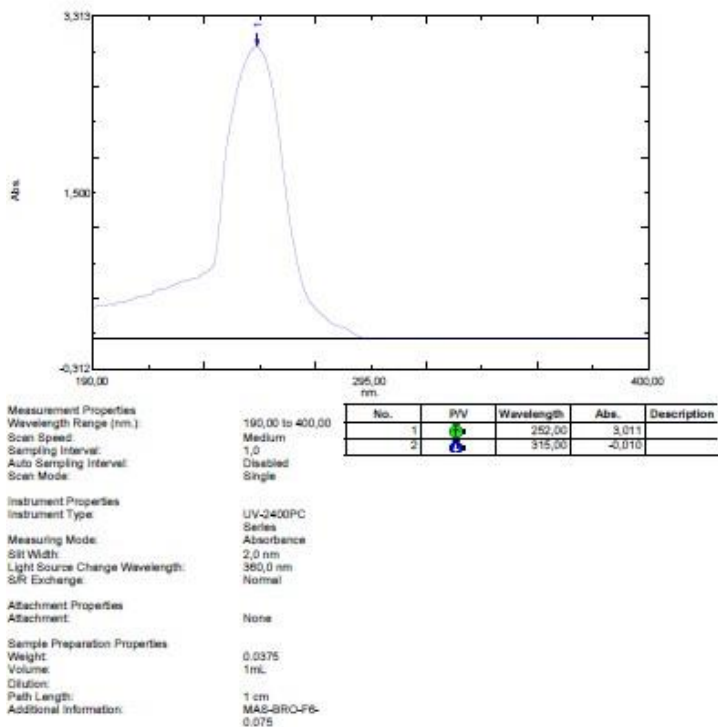


Figure S34: UV spectrum of compound 5.

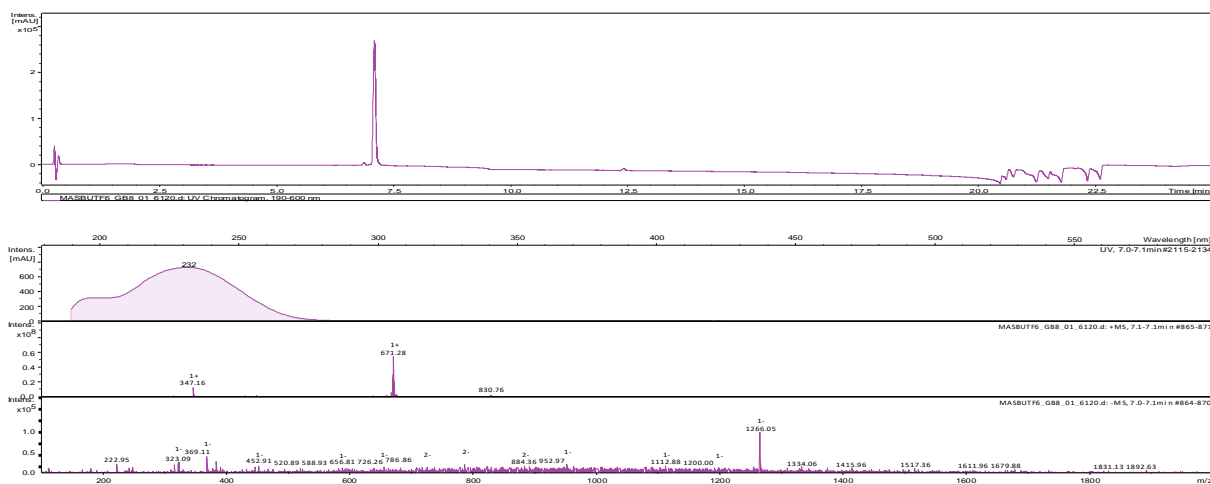


Figure S35: LC-UV-ESIMS spectra of compound 6

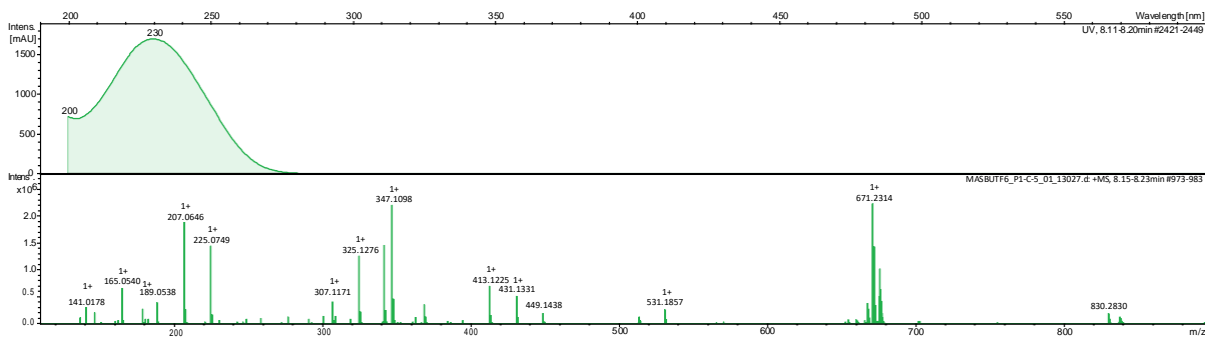


Figure S36: UV-HRESIMS spectra of compound **6**.

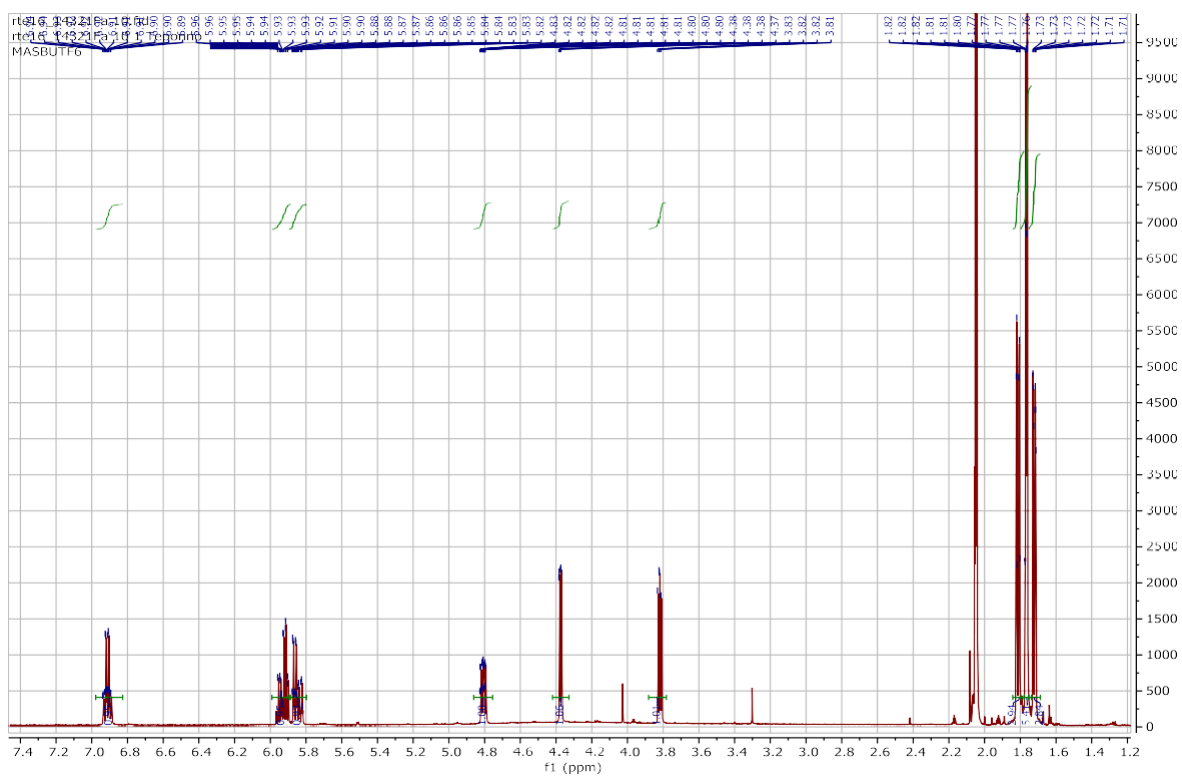


Figure S37: ¹H NMR spectrum of compound **6** in acetone-*d*₆ at 500 MHz.

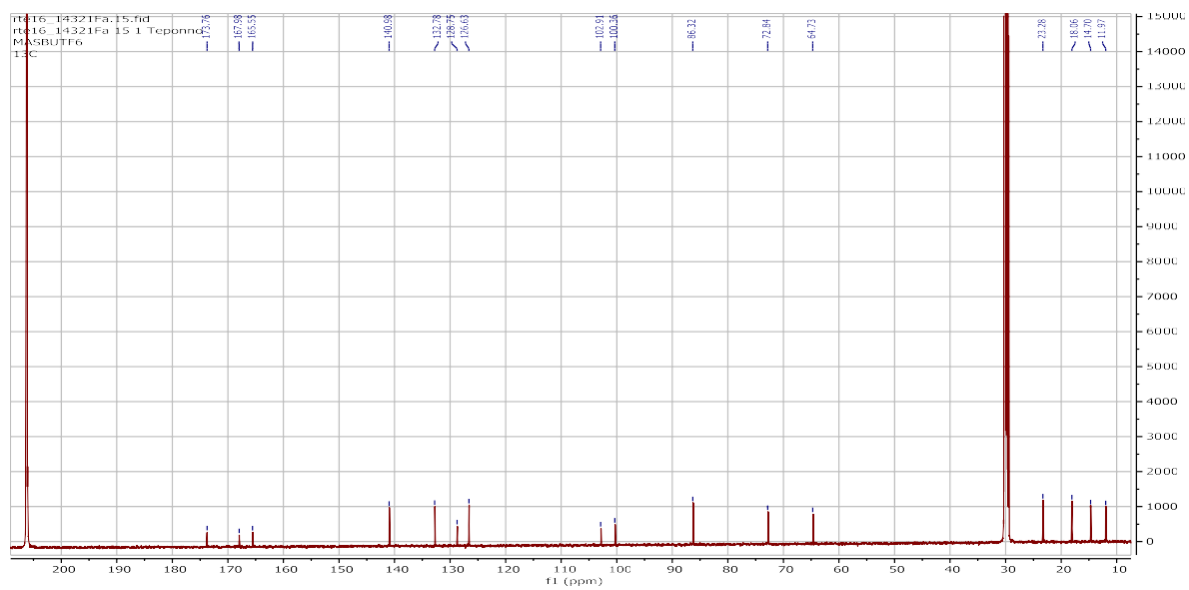


Figure S38: ^{13}C NMR spectrum of compound **6** in acetone- d_6 at 125 MHz.

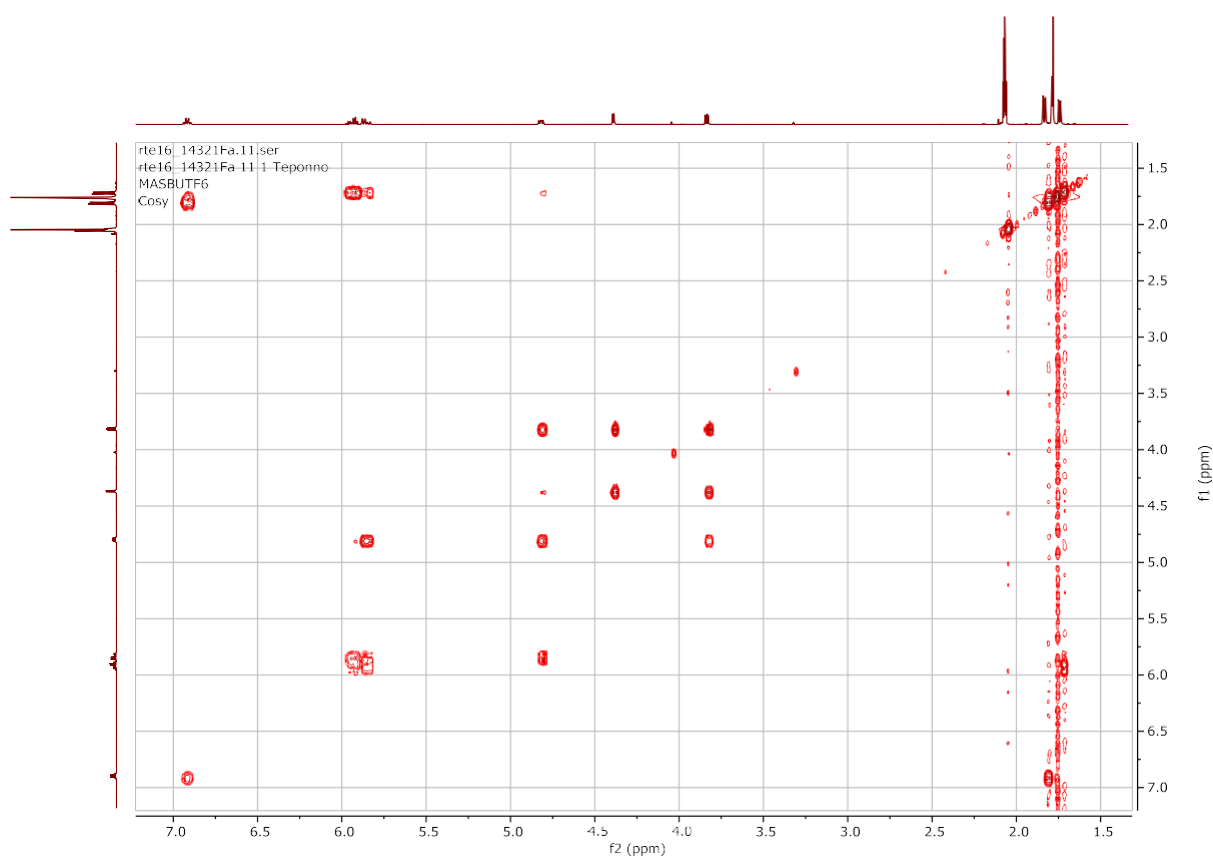


Figure S39: ^1H - ^1H spectrum of compound **6** in acetone- d_6 .

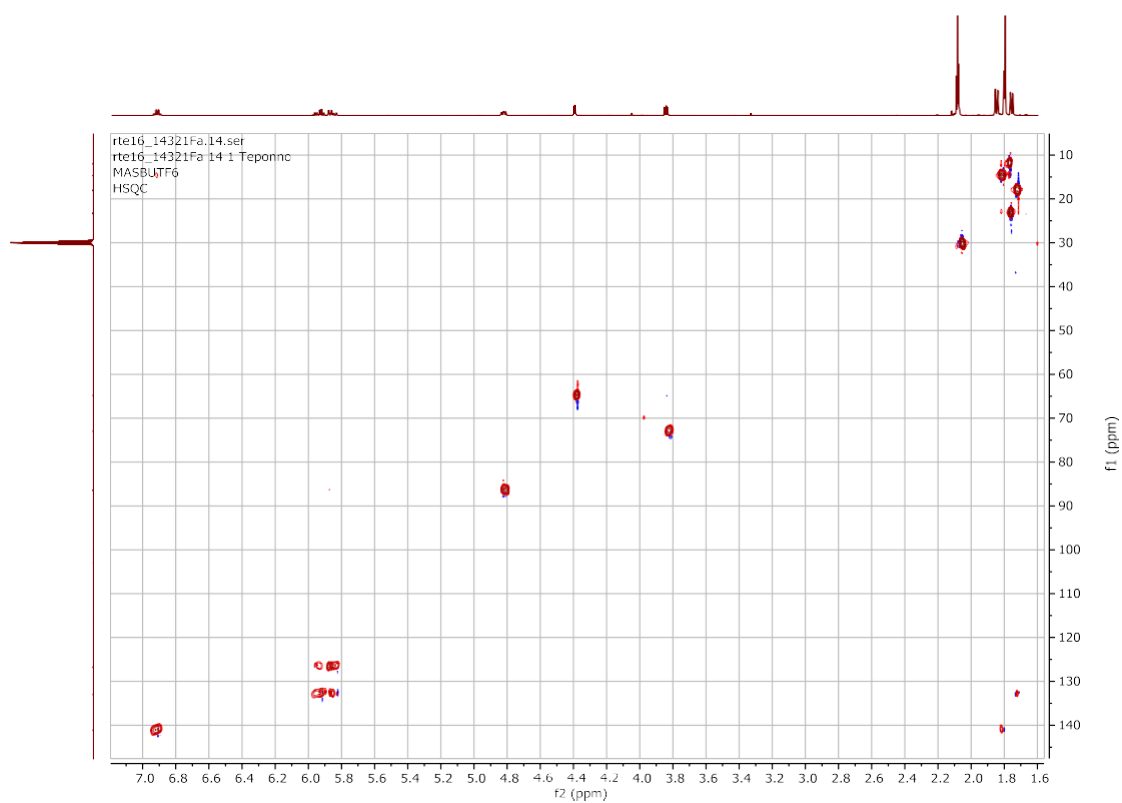


Figure S40: HSQC spectrum of compound **6** in acetone- d_6 .

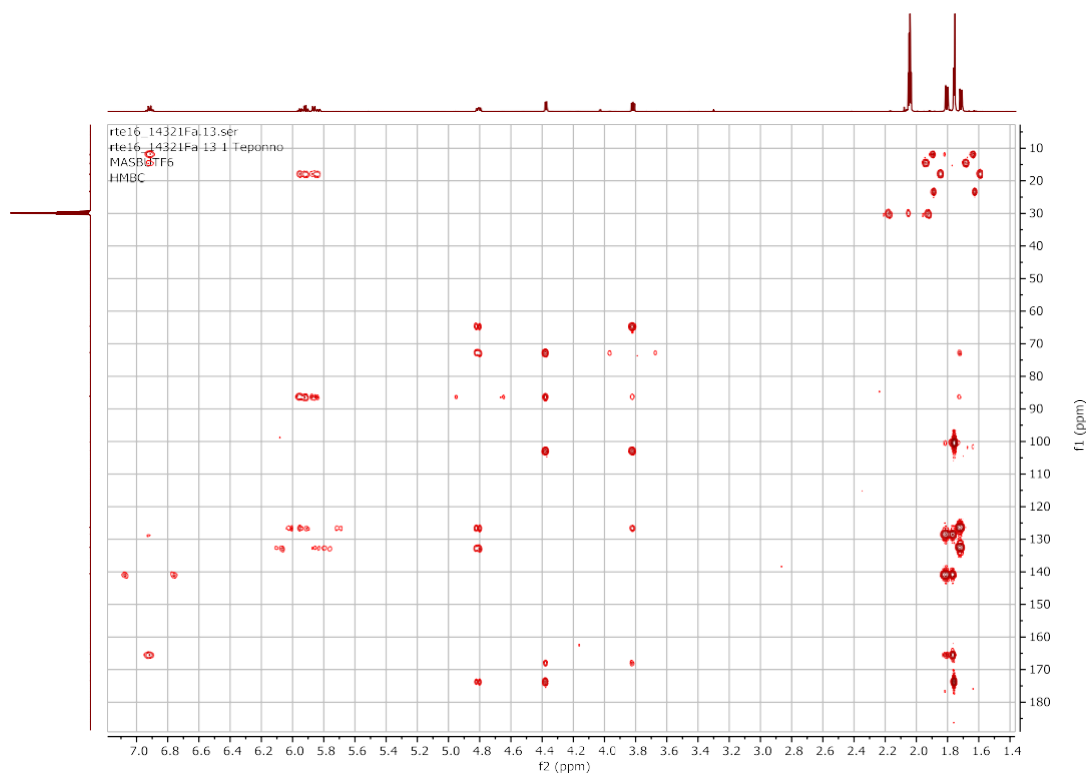


Figure S41: HMBC spectrum of compound **6** in acetone- d_6 .

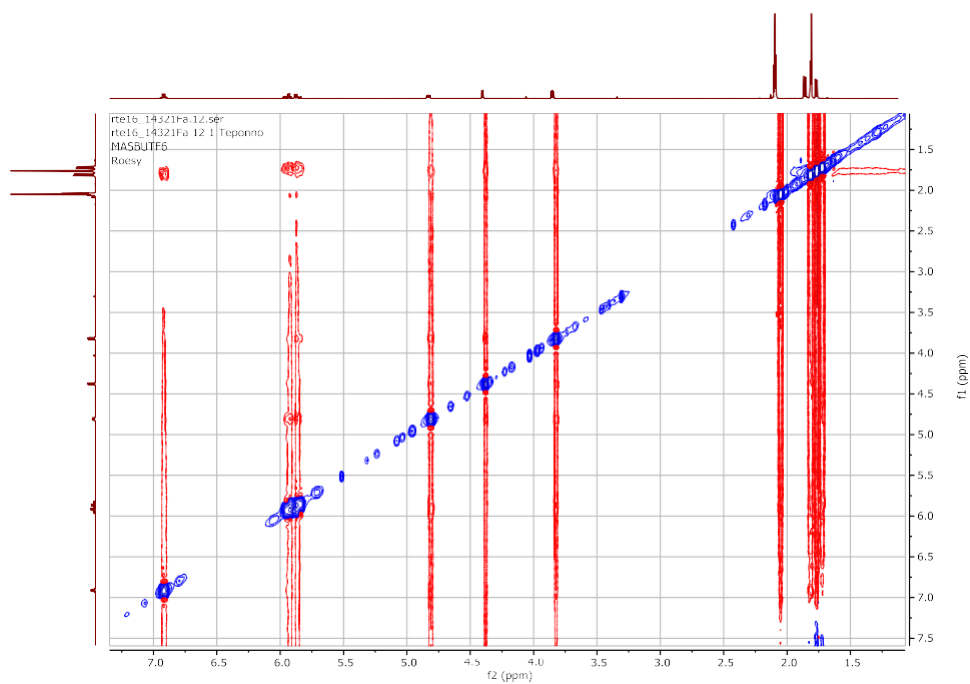
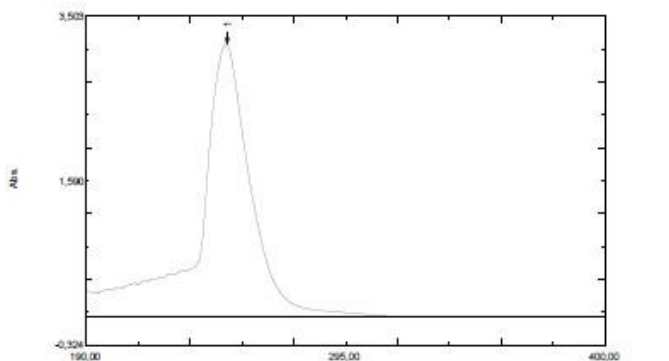


Figure S42: ROESY spectrum of compound 6 in acetone- d_6 .

Spectrum Peak Pick Report

20.04.2018 12:54:06

Data Set: MAS-BUT-F6-0.15 - RawData



Measurement Properties		No.	PPV	Wavelength	Abs.	Description
Wavelength Range (nm):	190,00 to 400,00	1	100	247,00	3,184	
Scan Speed:	Medium					
Sampling Interval:	1,0					
Auto Sampling Interval:	Disabled					
Scan Mode:	Single					
Instrument Properties						
Instrument Type:	UV-2400PC					
Measuring Mode:	Absorbance					
Slit Width:	2,0 nm					
Light Source Change Wavelength:	360,0 nm					
Slit Exchange:	Normal					
Attachment Properties						
Attachment:	None					
Sample Preparation Properties						
Weight:	0,15					
Volume:	1mL					
Dilution:						
Path Length:	1 cm					
Additional Information:	MAS-BUT-F6					

Figure S43: UV spectrum of compound 6.

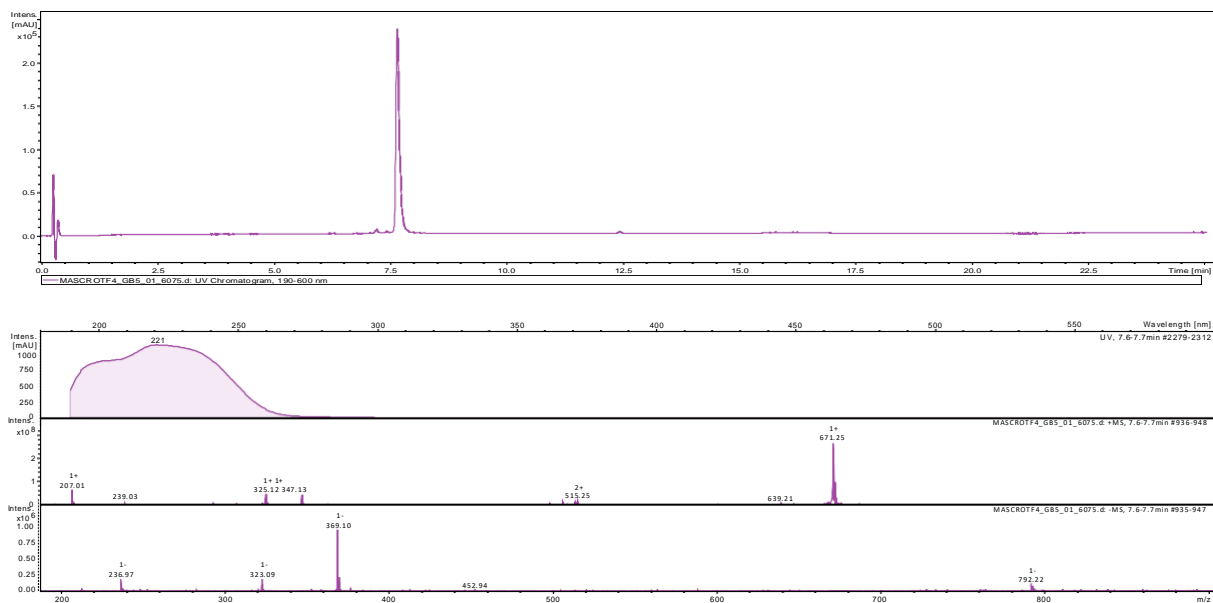


Figure S44: LC-UV ESIMS spectra of compound 7

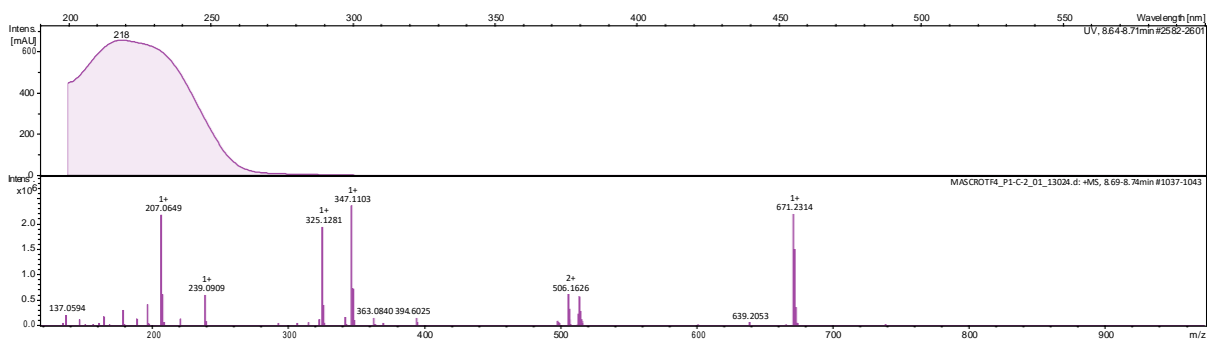


Figure S45: UV-HRESIMS spectrum of compound 7.

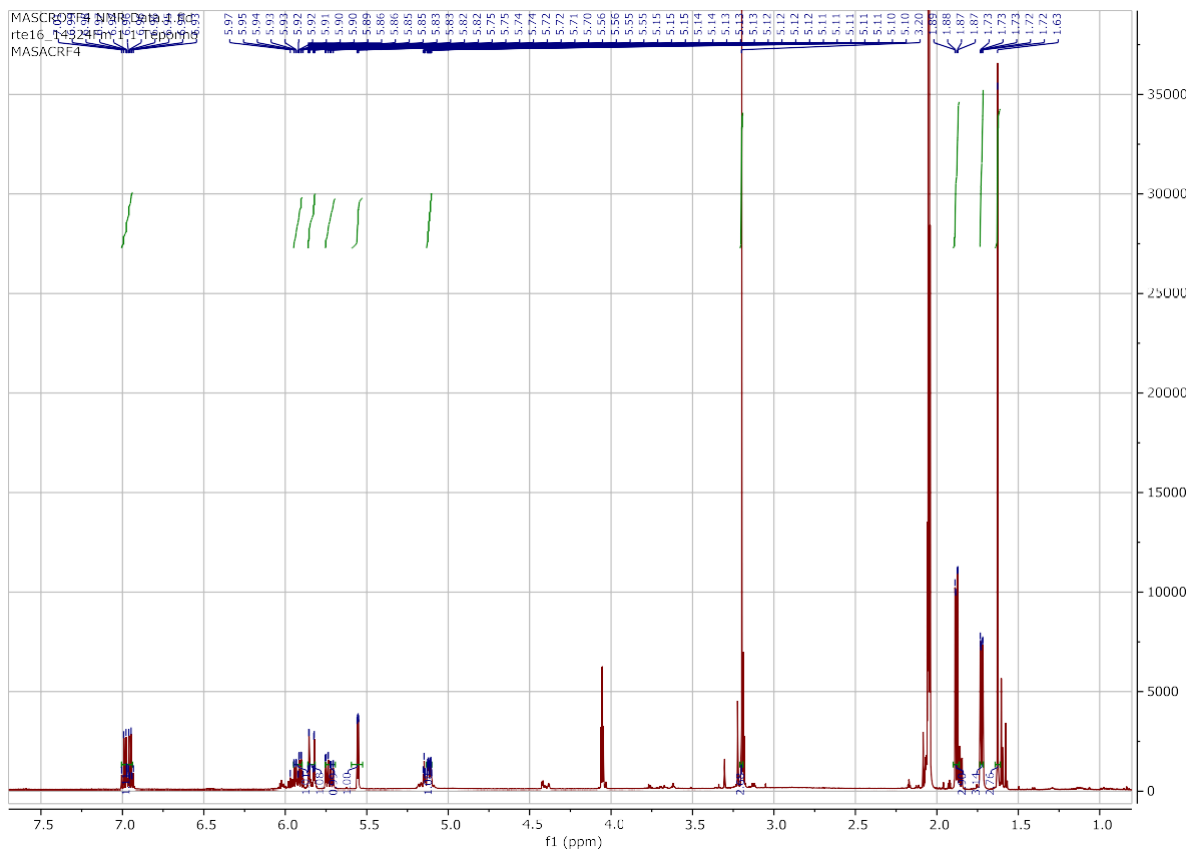


Figure S46: ^1H NMR spectrum of compound **7** in acetone- d_6 at 500 MHz.

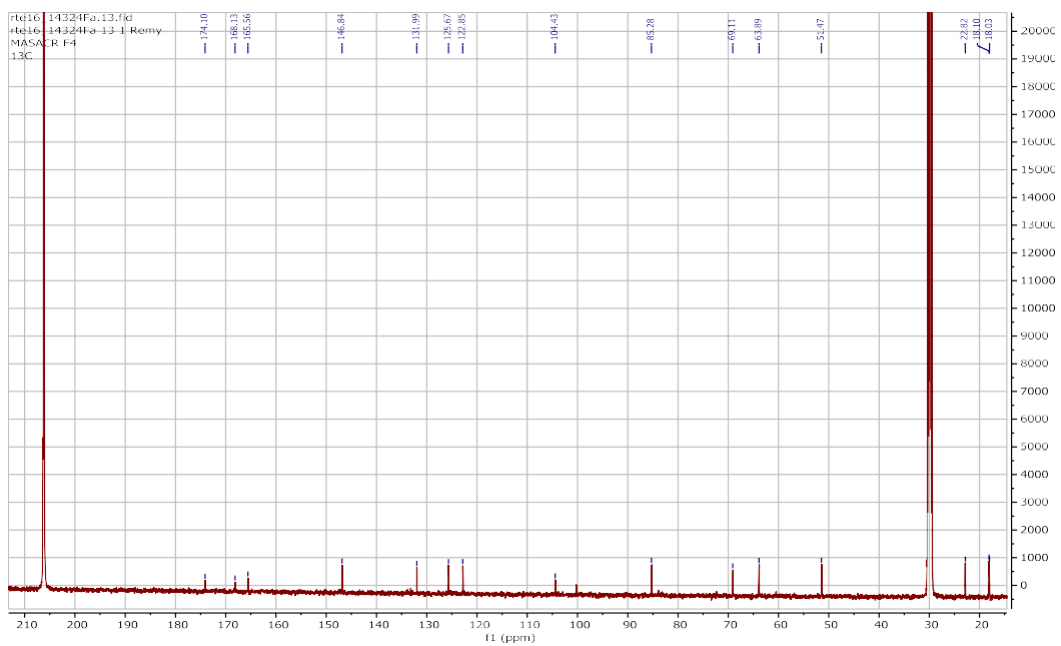


Figure S47: ^{13}C NMR spectrum of compound **7** in acetone- d_6 at 125 MHz.

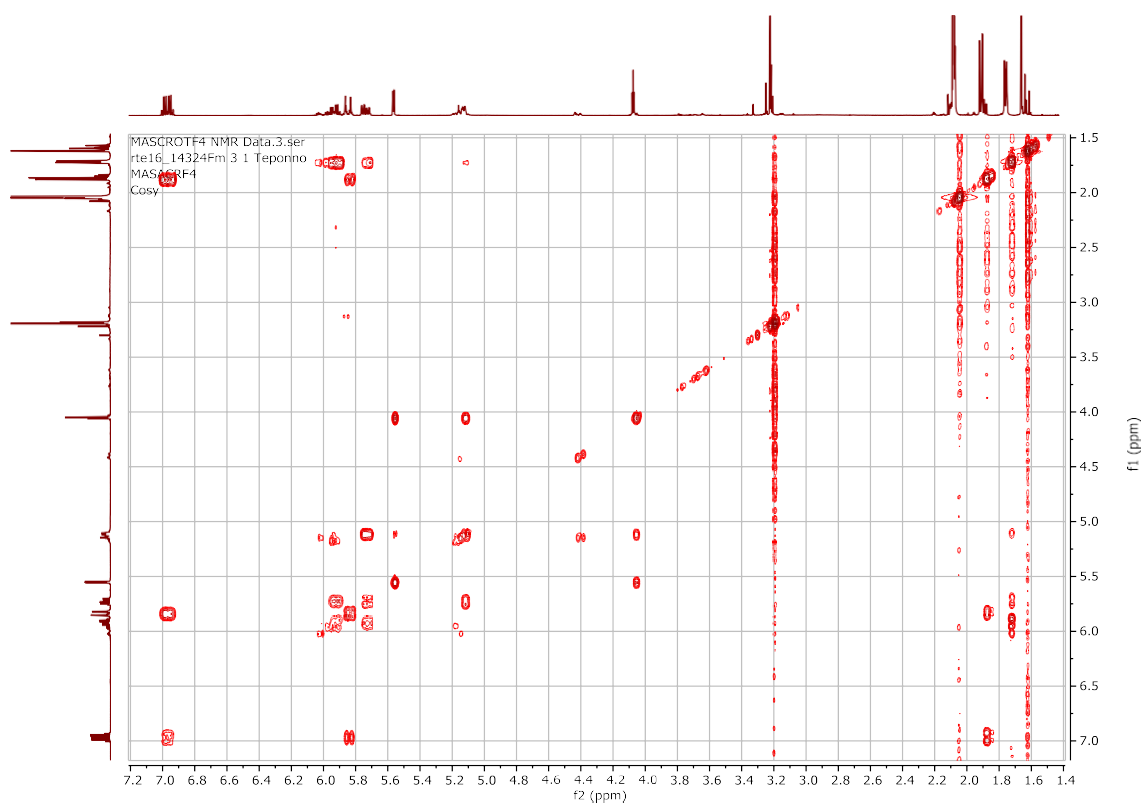


Figure S48: ^1H - ^1H COSY spectrum of compound **7** in acetone- d_6 .

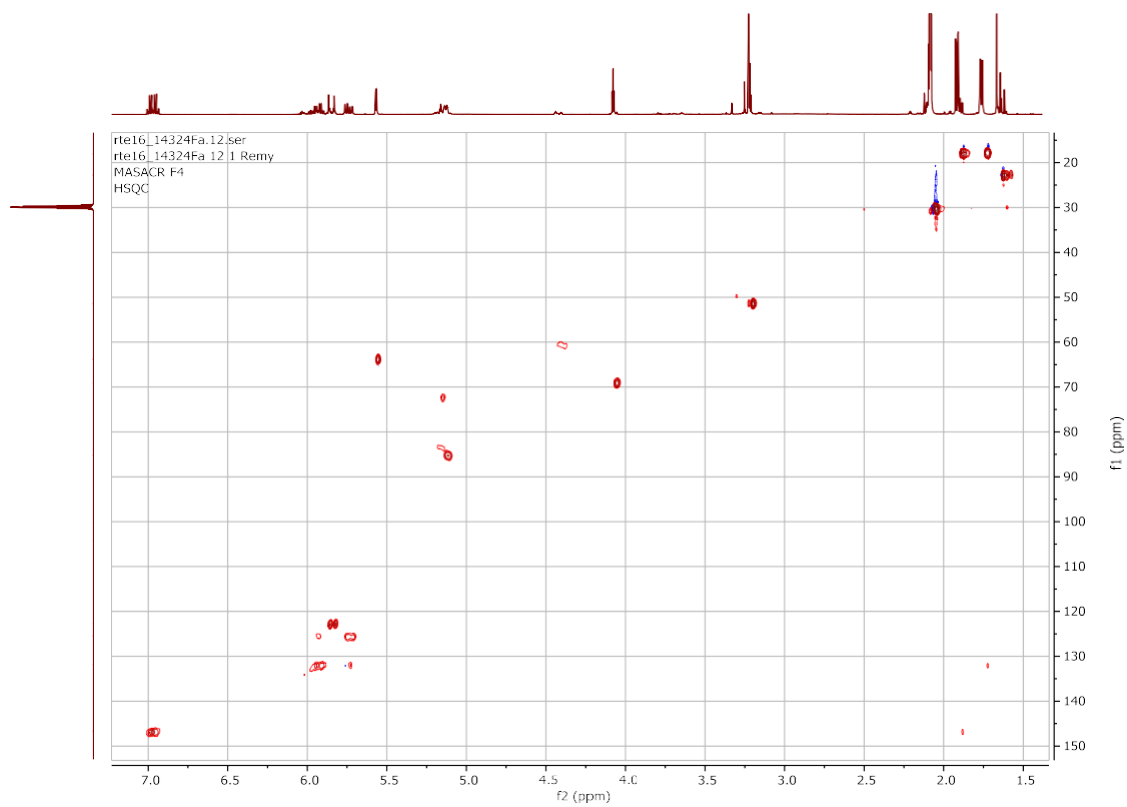


Figure S49: HSQC spectrum of compound **7** in acetone- d_6 .

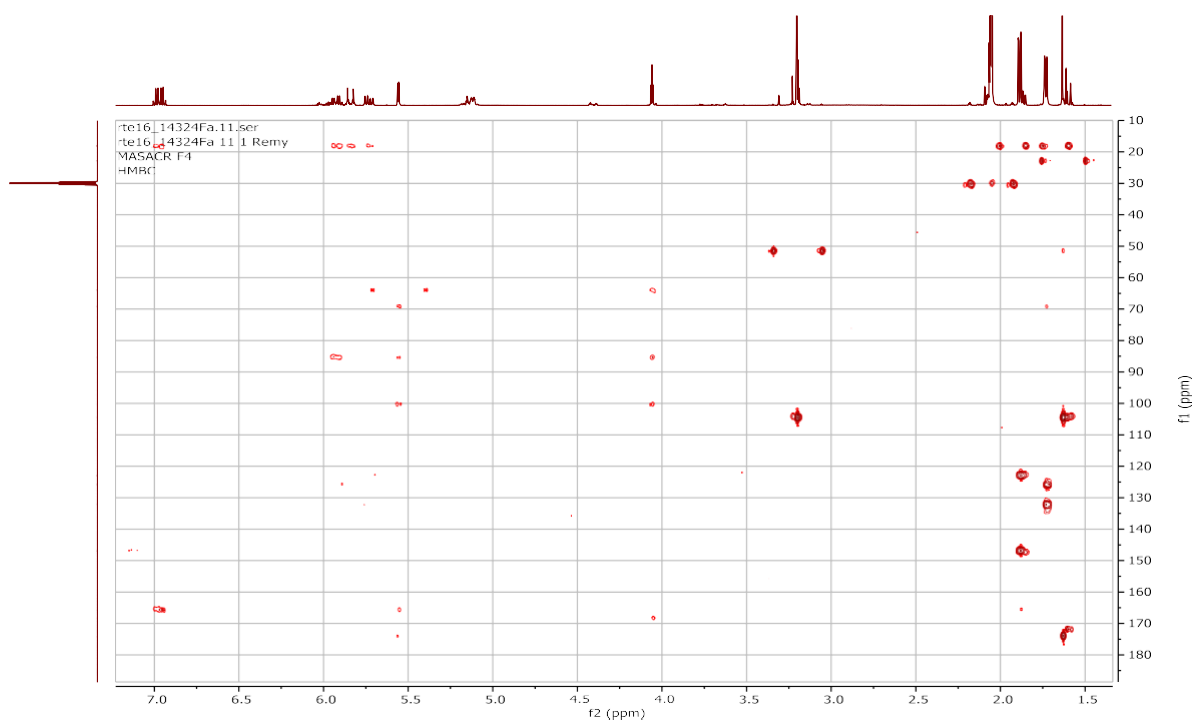


Figure S50: HMBC spectrum of compound **7** in acetone- d_6 .

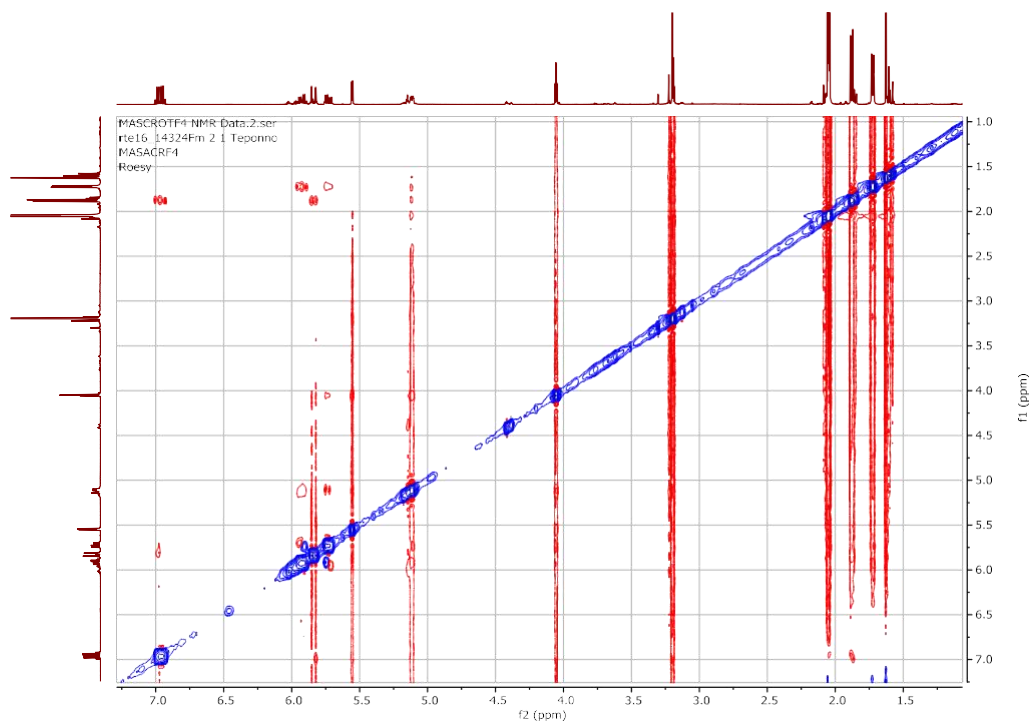


Figure S51: ROESY spectrum of compound **7** in acetone- d_6 .

Spectrum Peak Pick Report

20.04.2018 13:40:51

Data Set: MAS-CROT-F4-0.075 - RawData

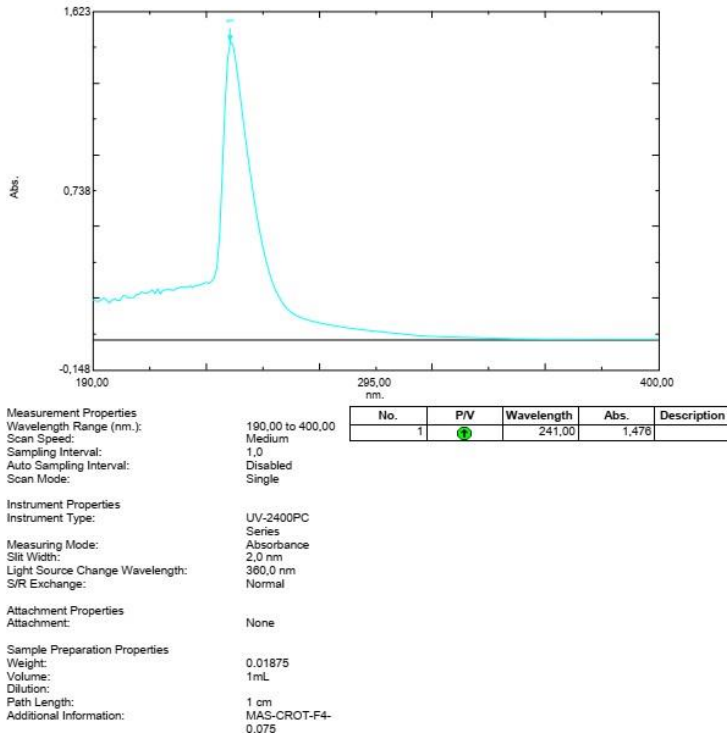


Figure S52: UV spectrum of compound 7.

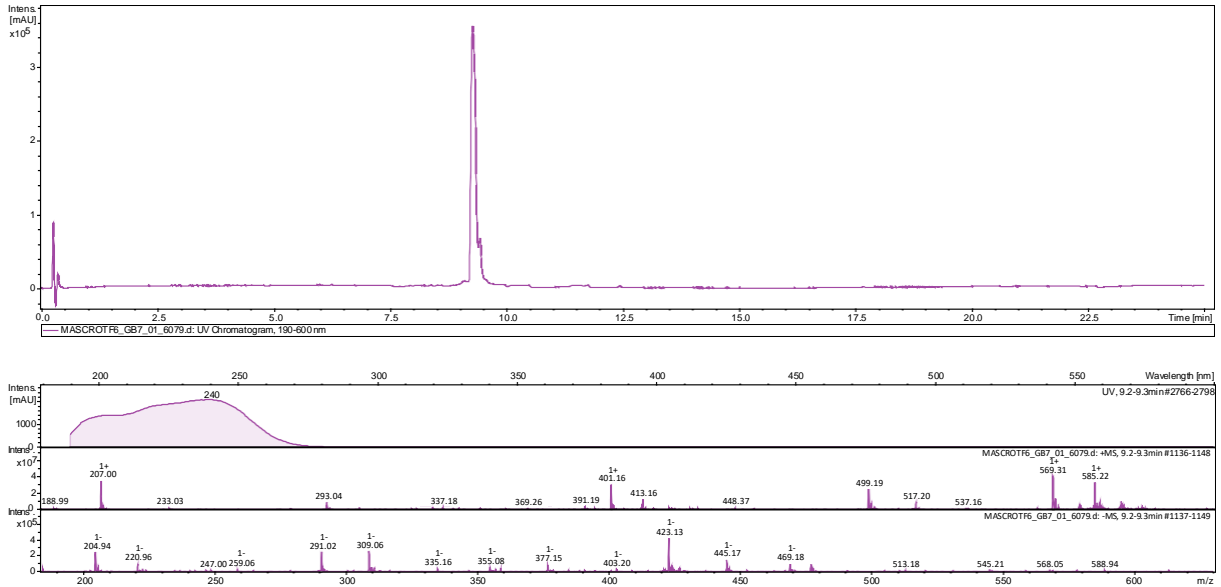


Figure S53: LC-UV-ESIMS spectrum of compound 8.

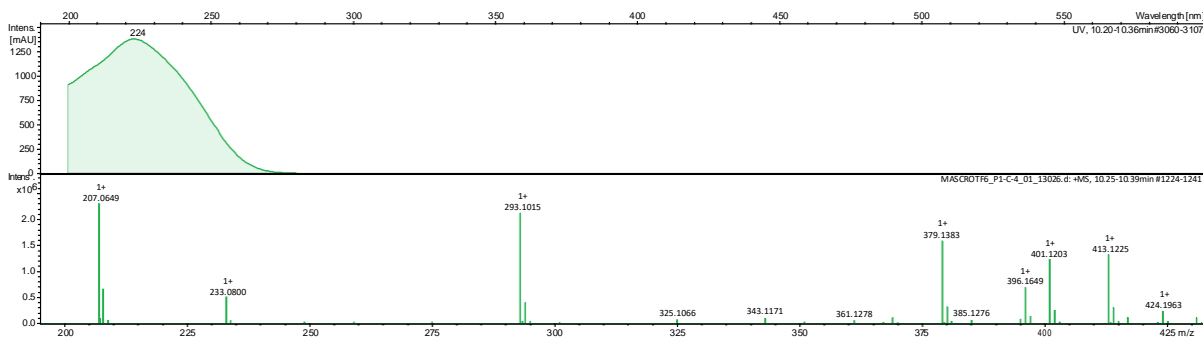


Figure S54: UV-HRESIMS spectrum of compound **8**.

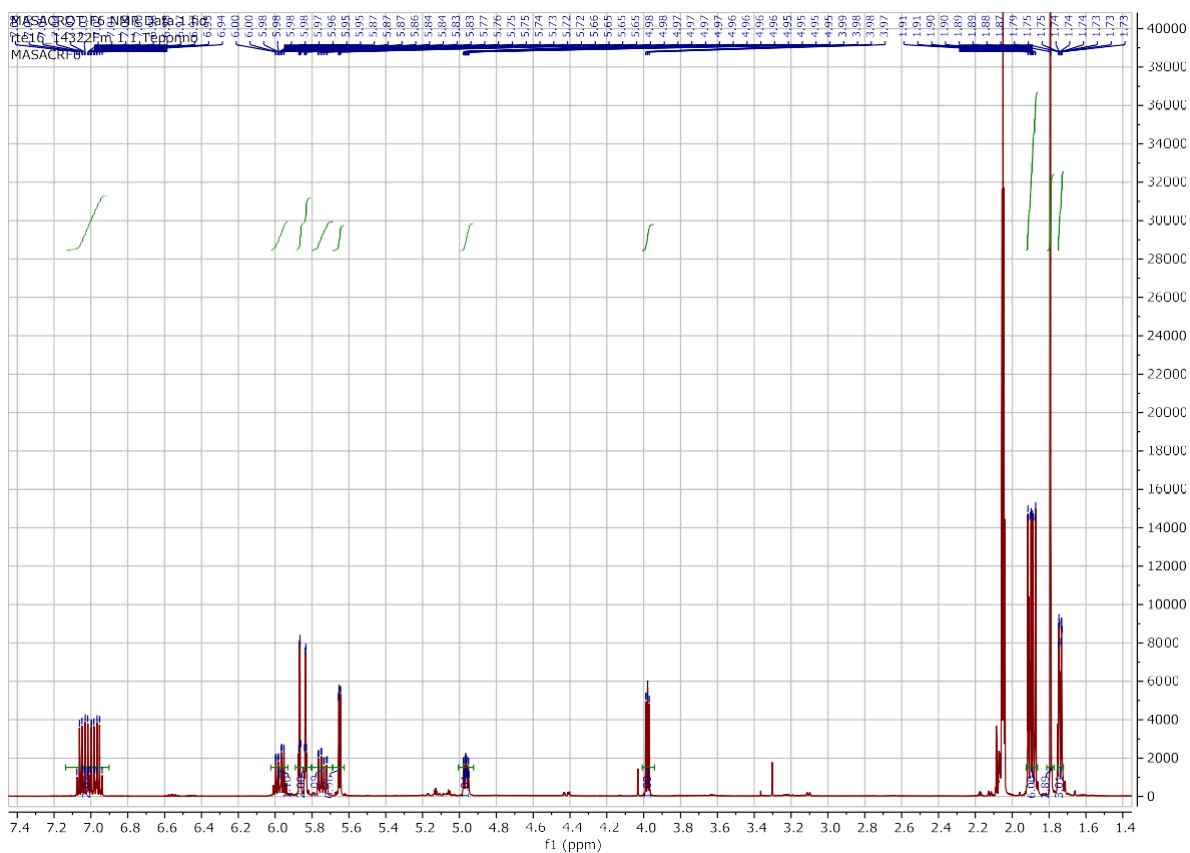


Figure S55: ¹H NMR spectrum of compound **8** in acetone-*d*₆ at 500 MHz.

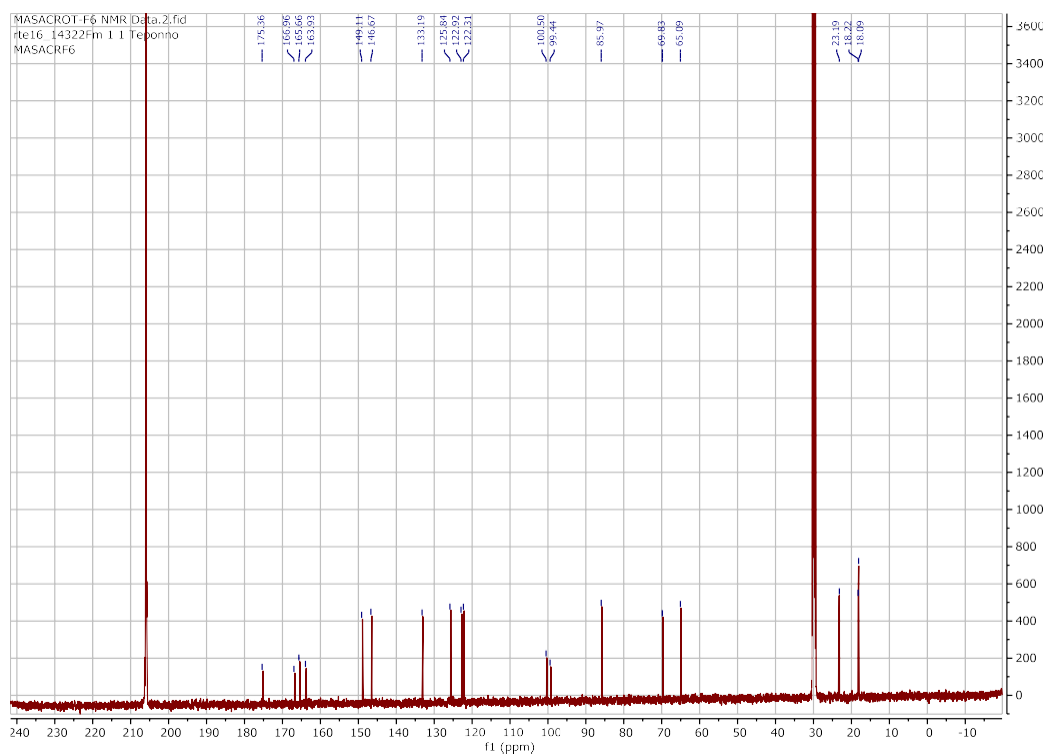


Figure S56: ^{13}C NMR spectrum of compound **8** in acetone- d_6 at 125 MHz.

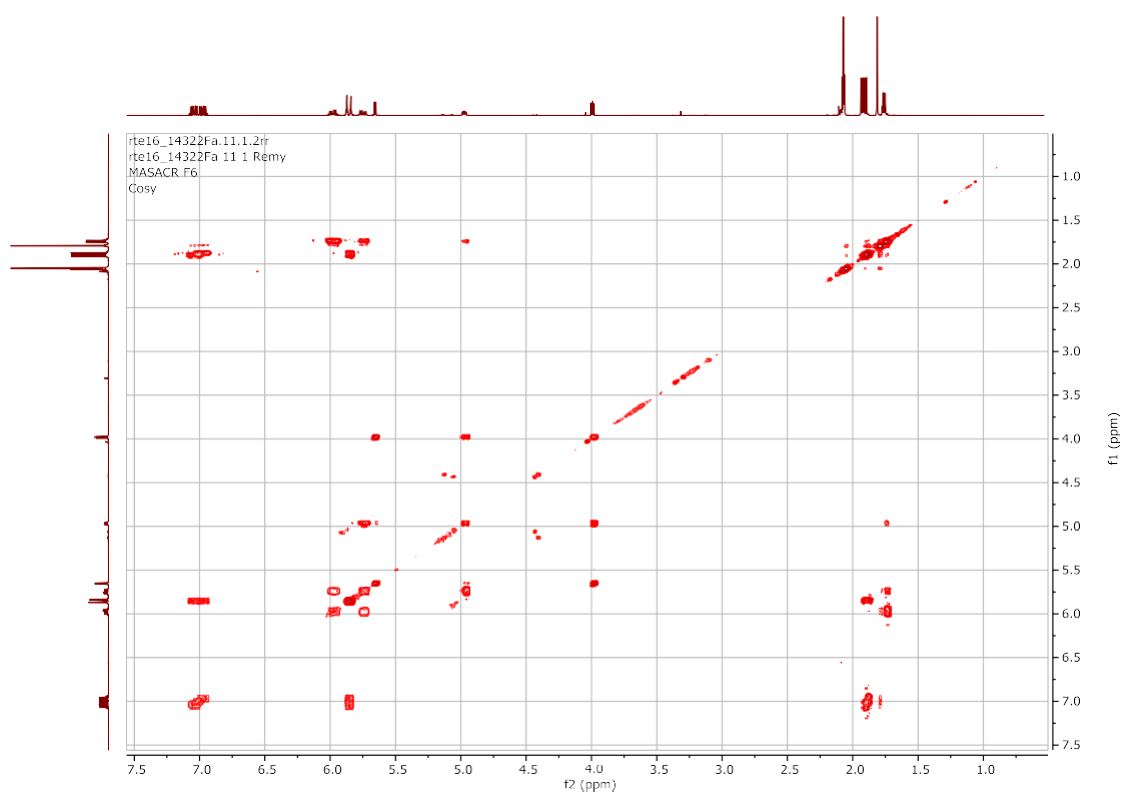


Figure S57: ^1H - ^1H COSY spectrum of compound **8** in acetone- d_6 .

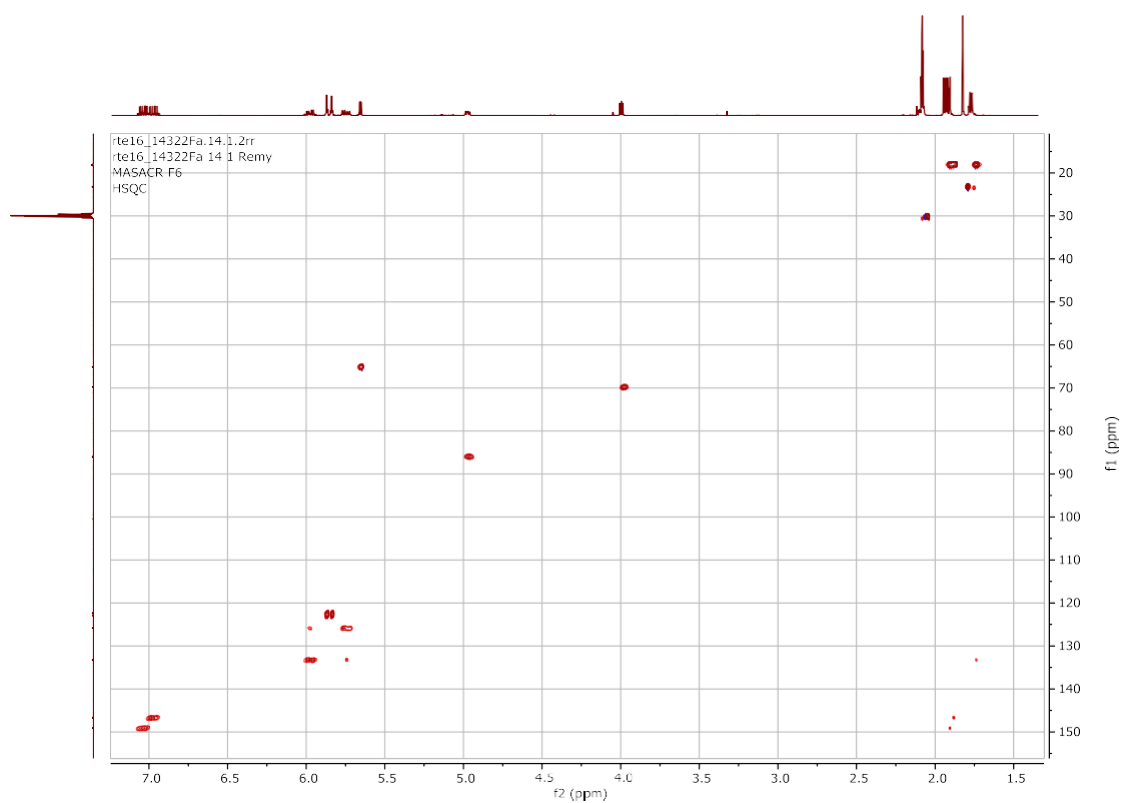


Figure S58: HSQC spectrum of compound **8** in acetone- d_6 .

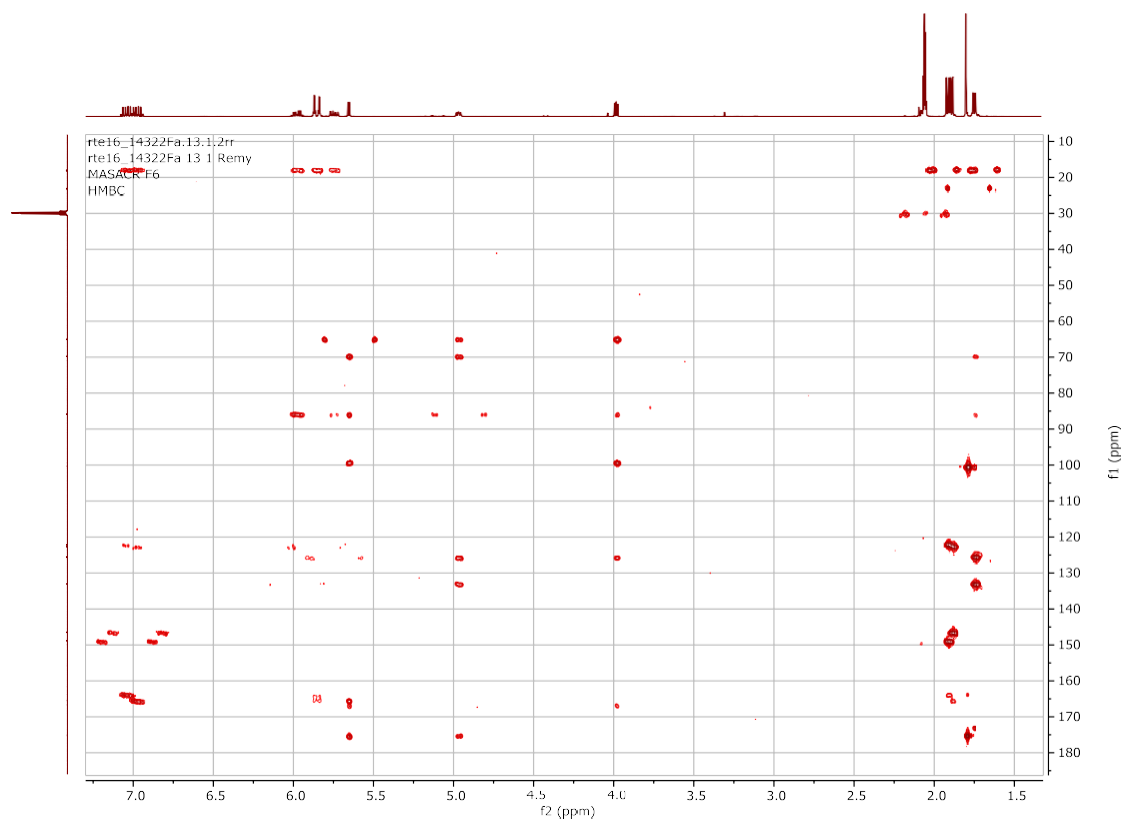


Figure S59: HMBC spectrum of compound **8** in acetone- d_6 .

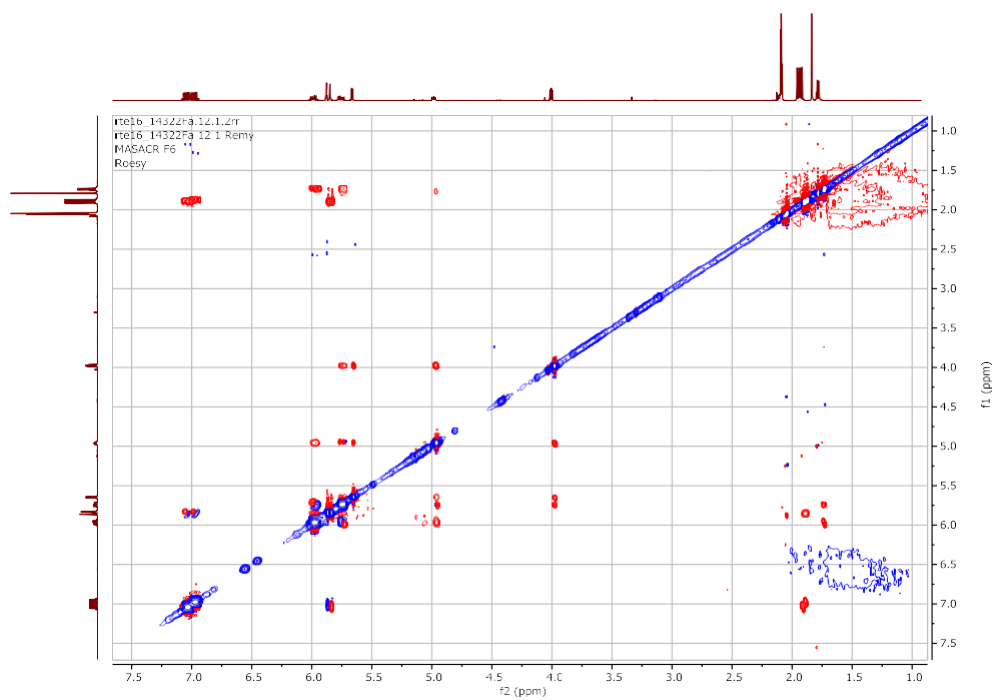
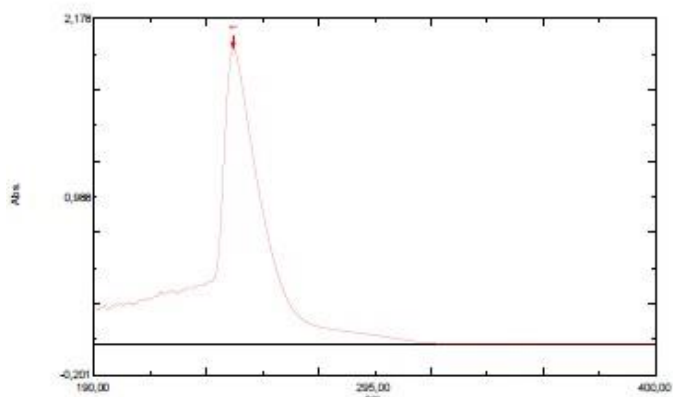


Figure S60: ROESY spectrum of compound **8** in acetone- d_6 .

Spectrum Peak Pick Report

20.04.2018 12:59:29

Data Set: MAS-CROT-F6-0.075 - RawData



Measurement Properties
Wavelength Range (nm):
Scan Speed:
Sampling Interval:
Auto Sampling Interval:
Scan Mode:

190.00 to 400.00
Medium
1.0
Disabled
Single

Instrument Properties

Instrument Type:

UV-2400PC

Measuring Mode:

Series

Measuring Mode:

Absorbance

Slit Width:

2.0 nm

Light Source Change Wavelength:

360.0 nm

S/R Exchange:

Normal

Attachment Properties

Attachment:

None

Sample Preparation Properties

Weight:

0.075

Volume:

1mL

Dilution:

1 cm

Path Length:

MAS-CROT-F6-

Additional Information:

0.075

No.	PVV	Wavelength	Abs.	Description
1	0.0	242.00	1.079	

Figure S61: UV spectrum of compound **8**.

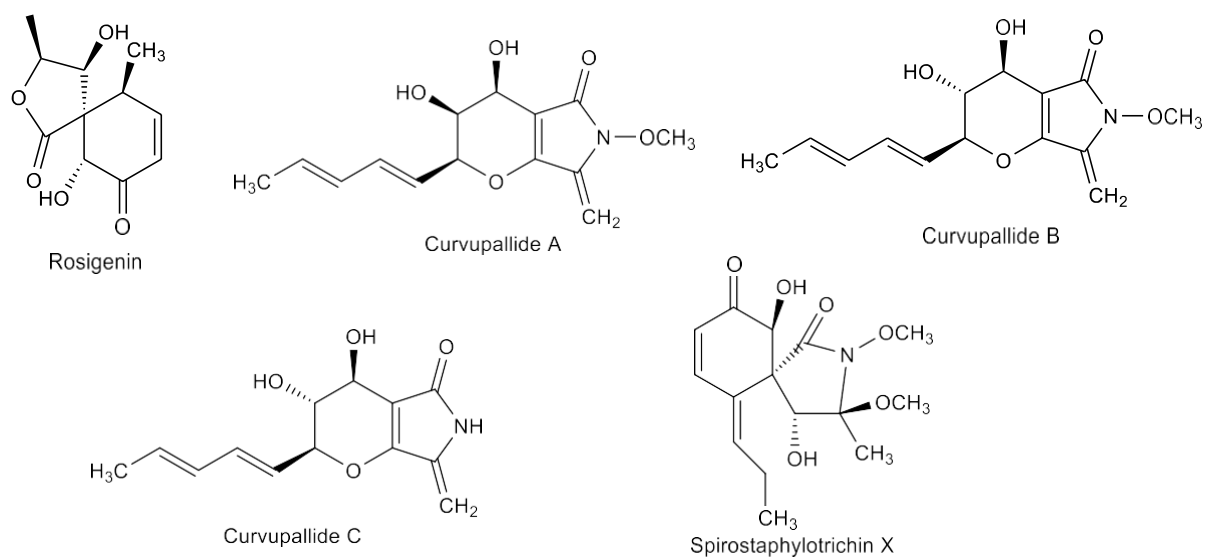


Figure S62: Chemical structures of rosigenin, curvupallides A–C, and spirostaphylotrichin X.