

Supporting Information

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New Ergostane-type Steroid Produced by an Endophytic Fungus *Fusarium phaseoli* Isolated from *Chisocheton macrophyllus* (Meliaceae)

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Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

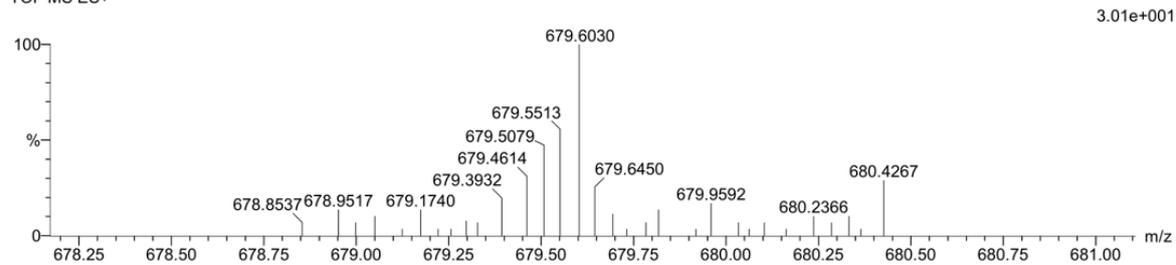
223 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

F1 1 139 (2.380) Cm (136:150)

TOF MS ES+



Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
679.6030	679.6029	0.1	0.1	7.5	56.7	0.0	C46 H79 O3

Figure S1: HRTOF-MS spectrum of 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

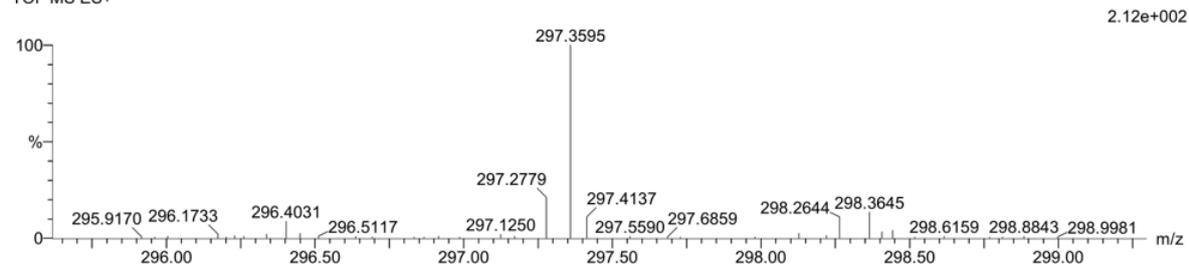
96 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

F1 OLEIC 69 (1.190) Cm (67:69)

TOF MS ES+



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
297.2779	297.2770	0.9	3.0	-1.5	68.5	0.7	C17 H38 O2 Na
	297.2794	-1.5	-5.0	1.5	68.6	0.7	C19 H37 O2

Figure S2: HRTOF-MS spectrum of methyl oleate

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

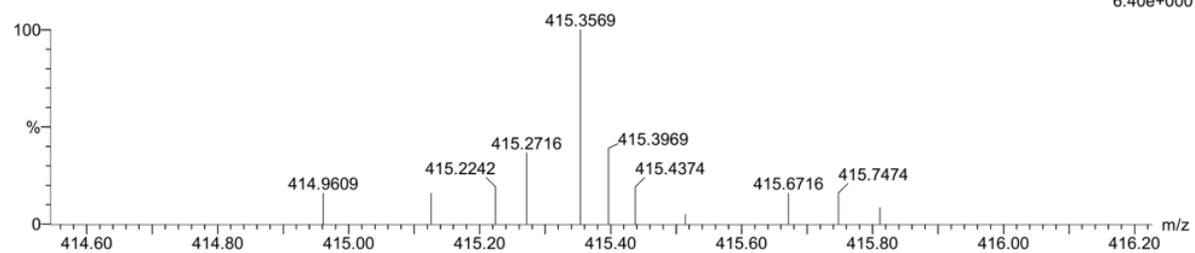
178 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

F1 1 99 (1.700) Cm (99:101)

TOF MS ES+



Minimum:

Maximum:

Minimum:				-1.5
Maximum:	5.0	10.0		50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
415.3569	415.3552	-1.3	-3.1	2.5	23.5	0.6	C26 H48 O2 Na
	415.3576	-3.7	-8.9	5.5	23.6	0.7	C28 H47 O2

Figure S3: HRTOF-MS spectrum of steroid moiety of **1**

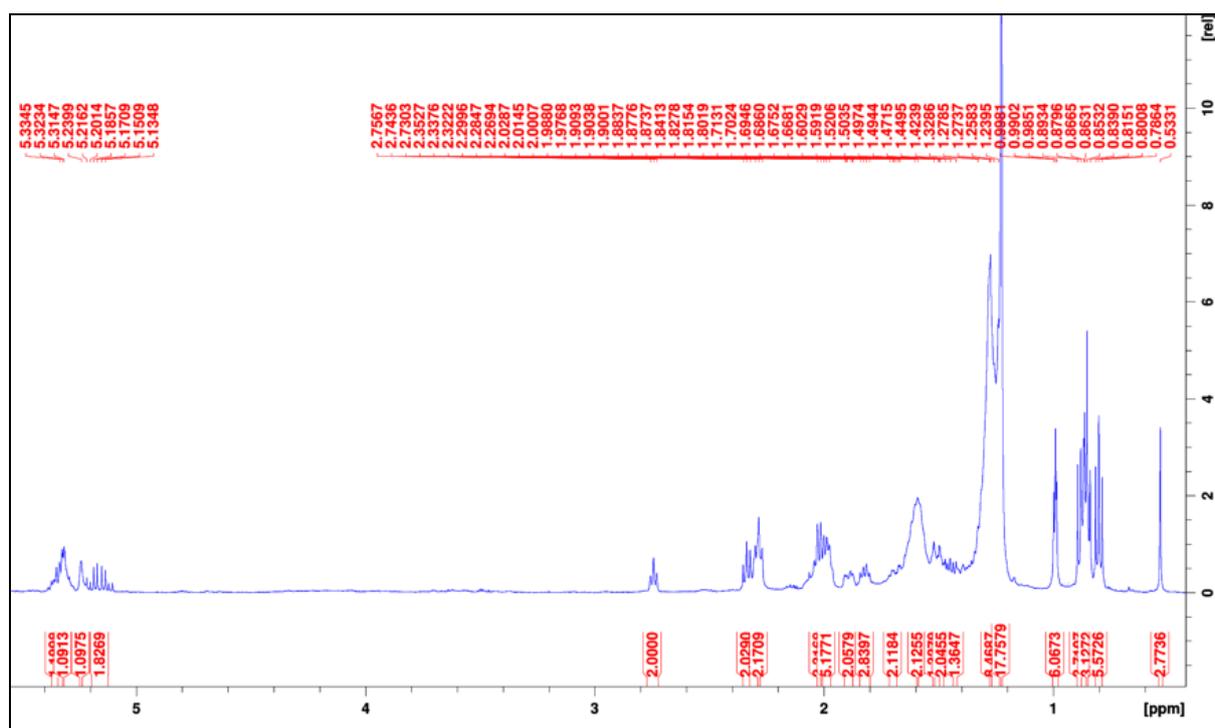


Figure S4: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of **1**

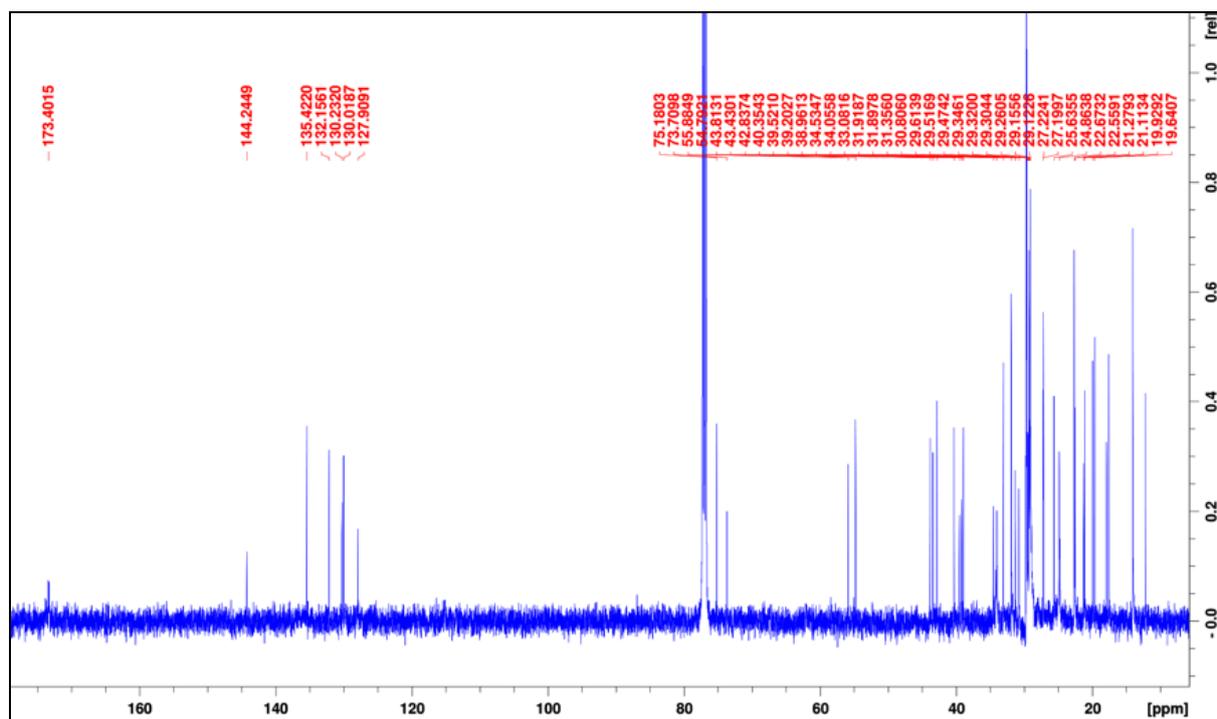


Figure S5: ^{13}C -NMR (125 MHz, CDCl_3) spectrum of **1**

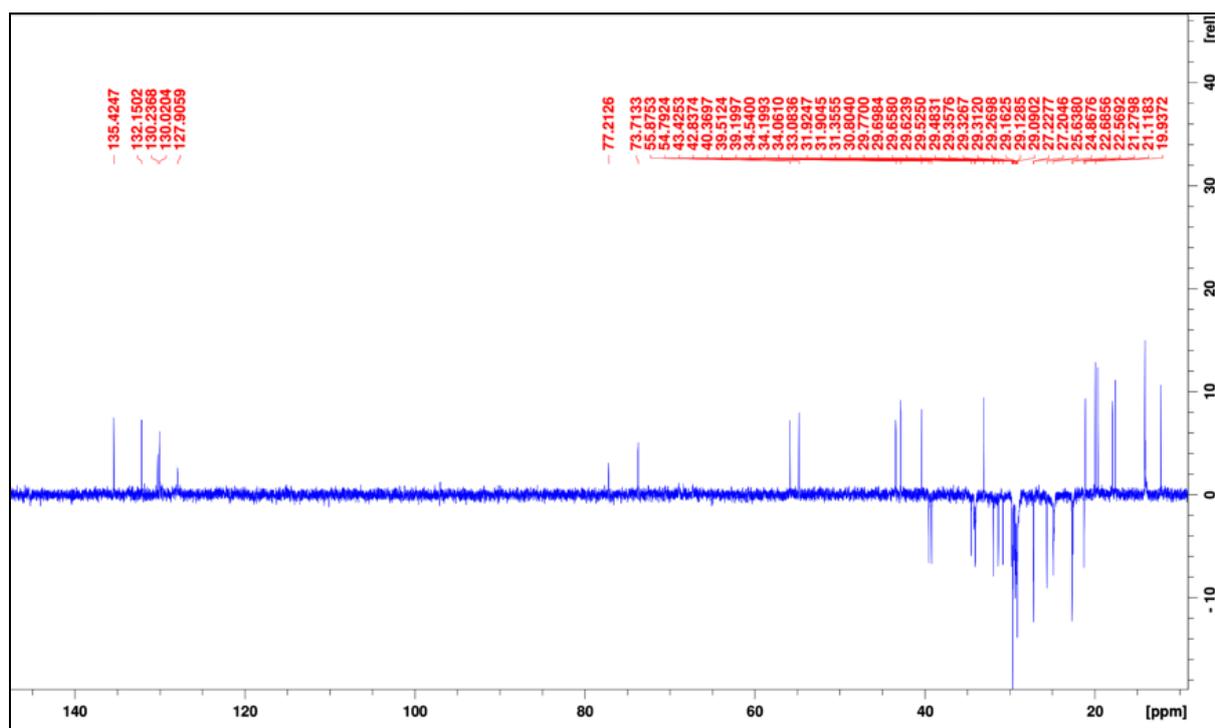


Figure S6: DEPT135 (125 MHz, CDCl₃) spectrum of **1**

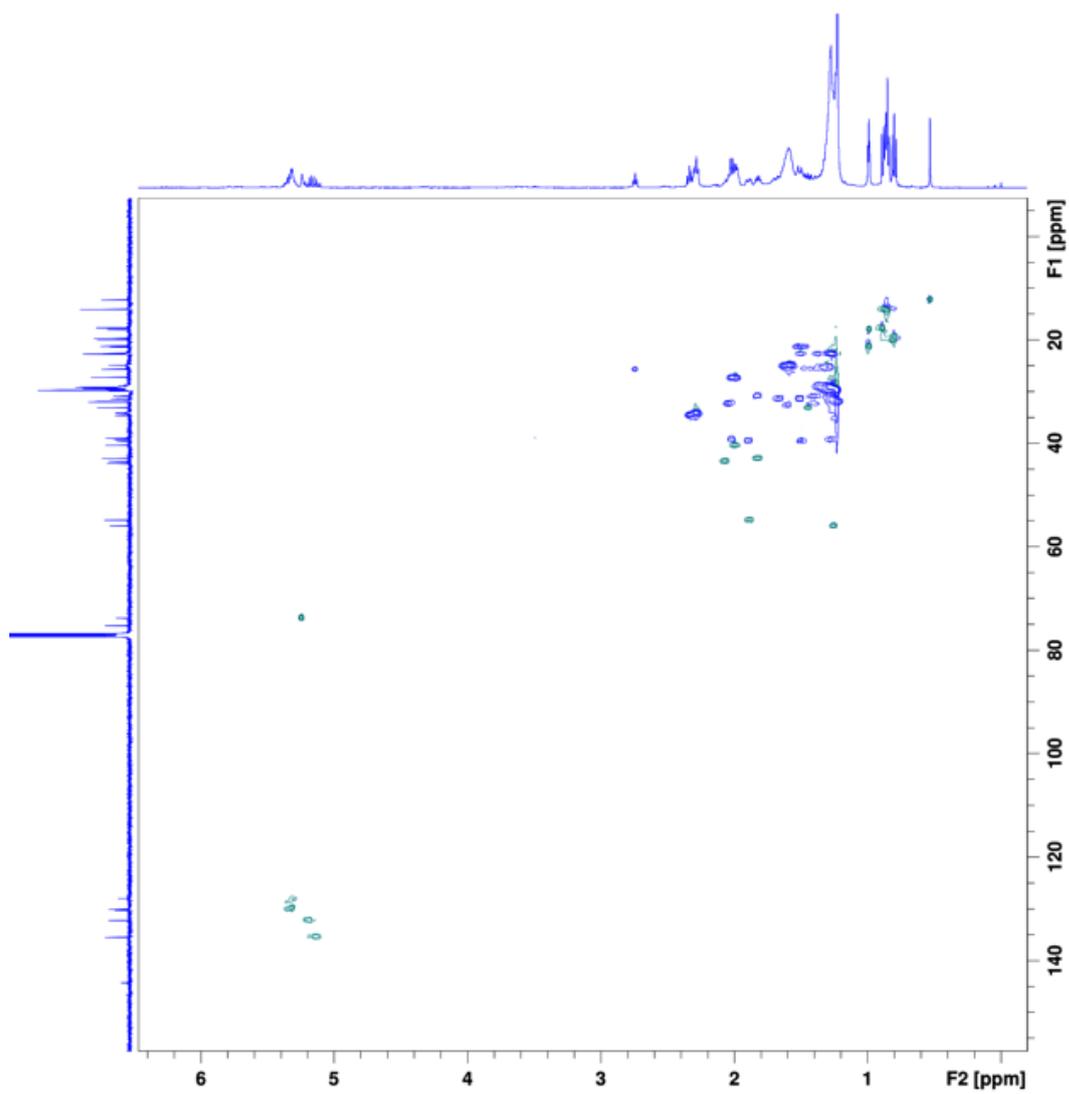


Figure S7: HSQC spectrum of **1**

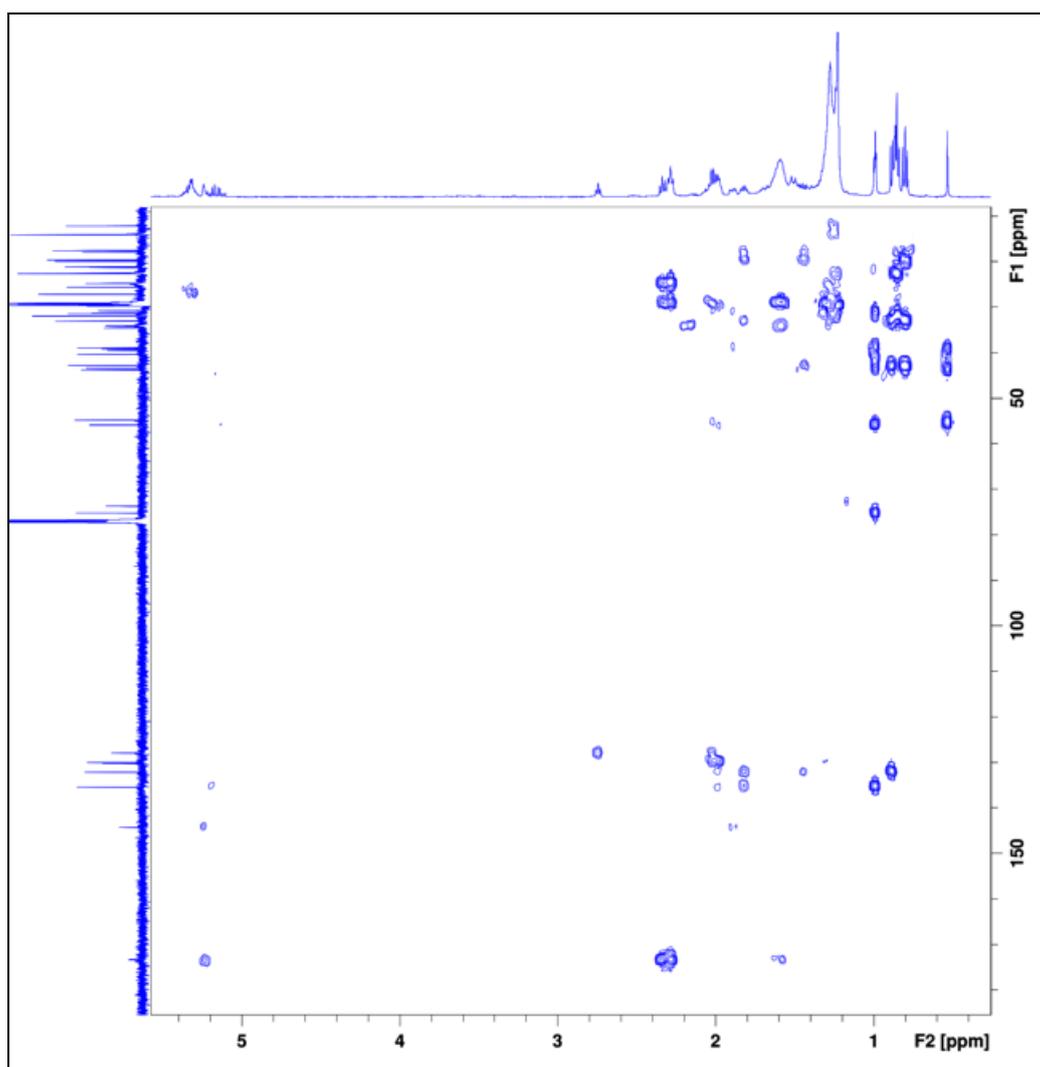


Figure S8: HMBC spectrum of **1**

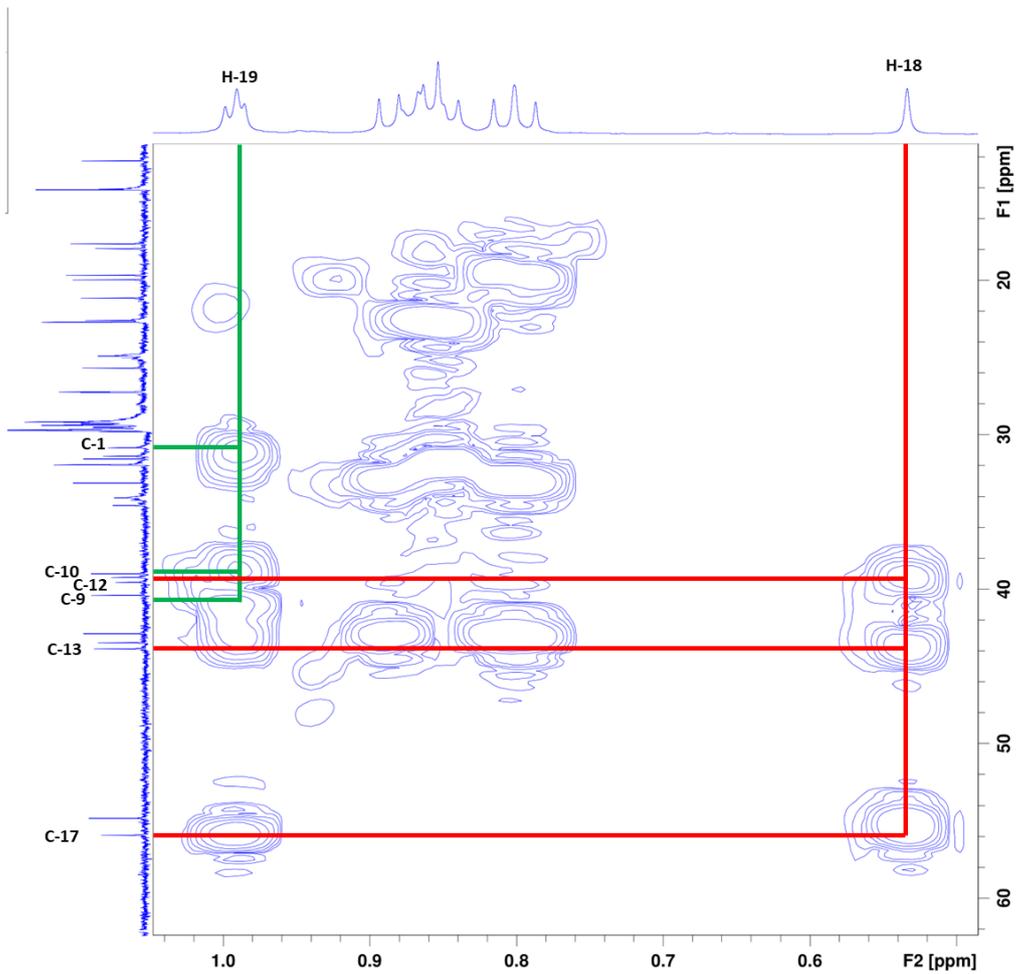


Figure S9: HMBC spectrum of **1** (From $\delta_c 60$ ppm to $\delta_c 10$ ppm)

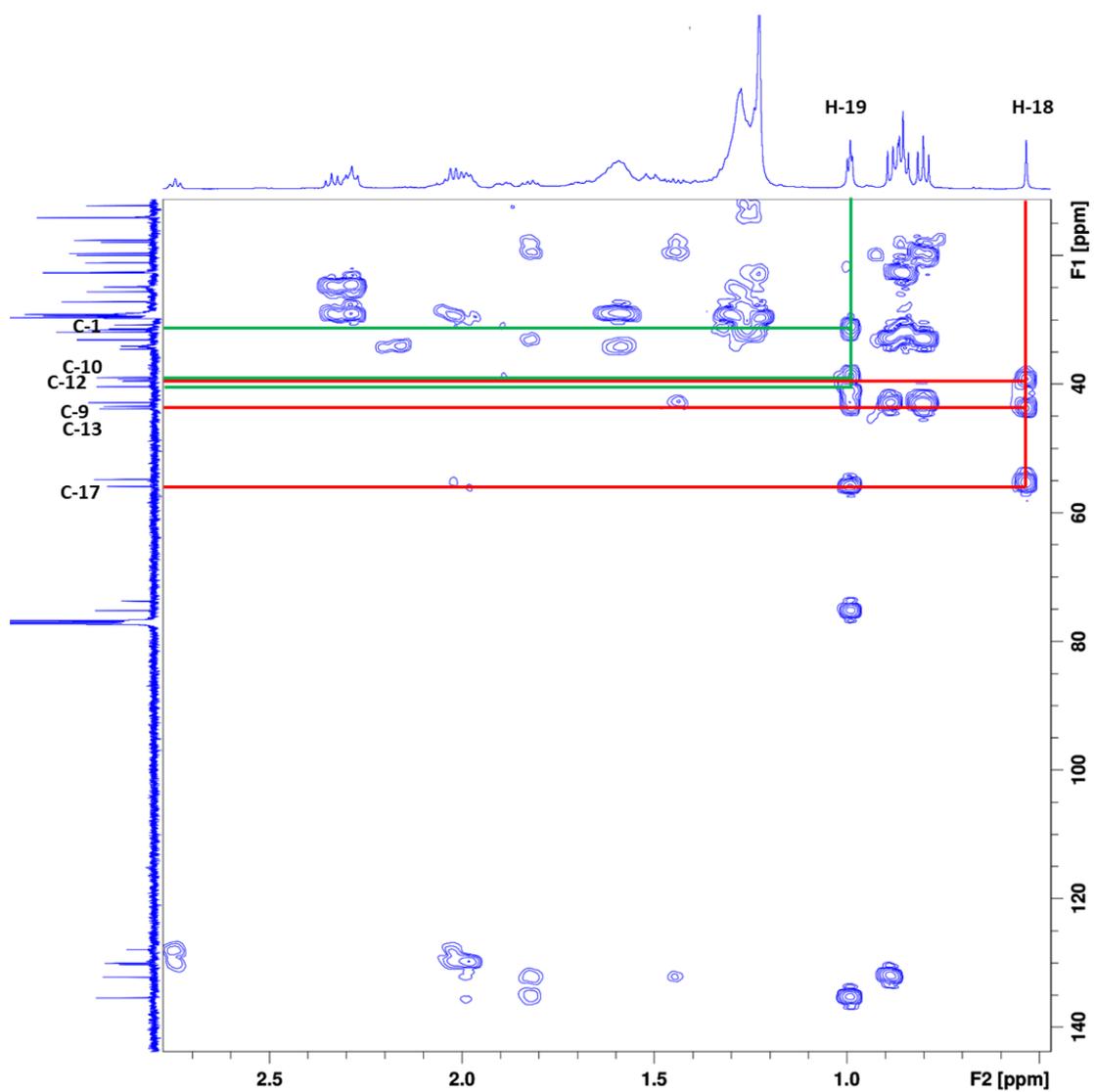


Figure S10: HMBC spectrum of **1** (From δ_C 140 ppm to δ_C 30 ppm)

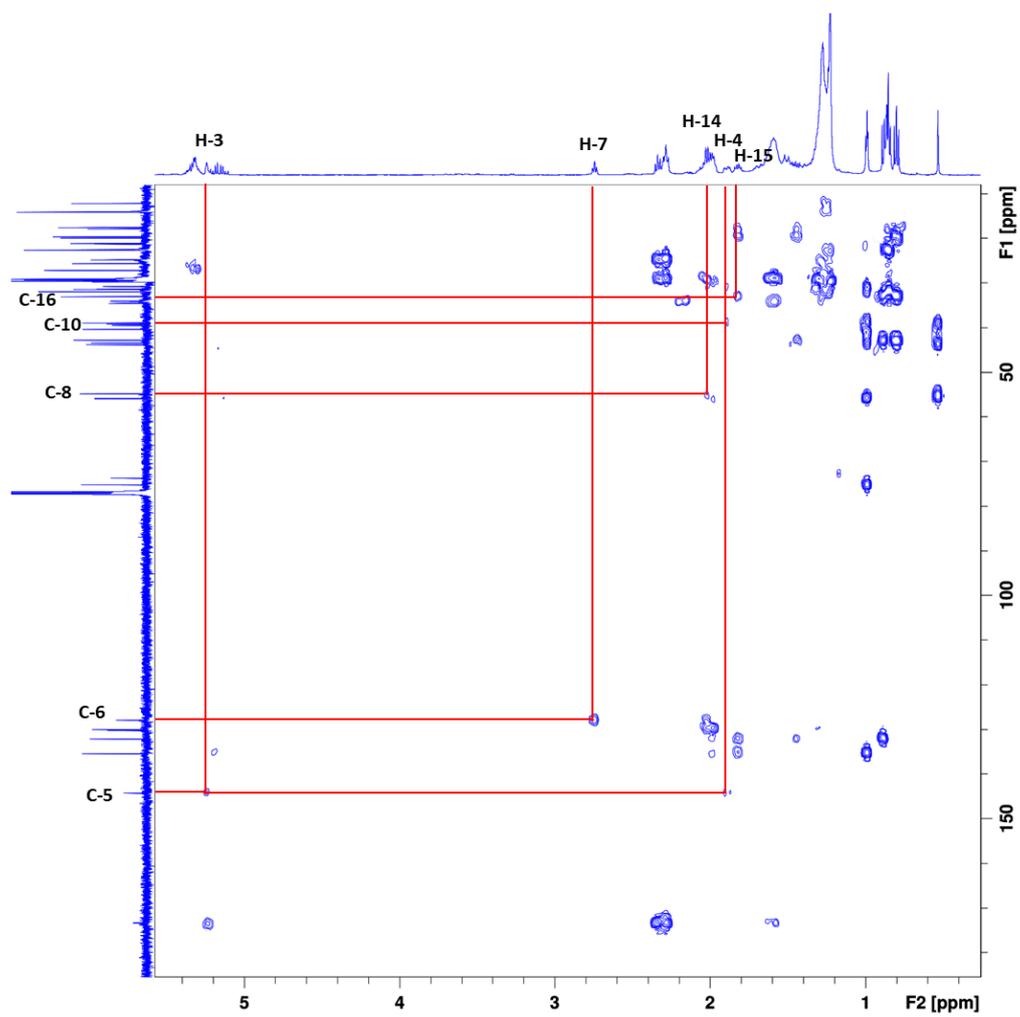


Figure S11: HMBC spectrum of **1** (From δ_c 140 ppm to δ_c 30 ppm)

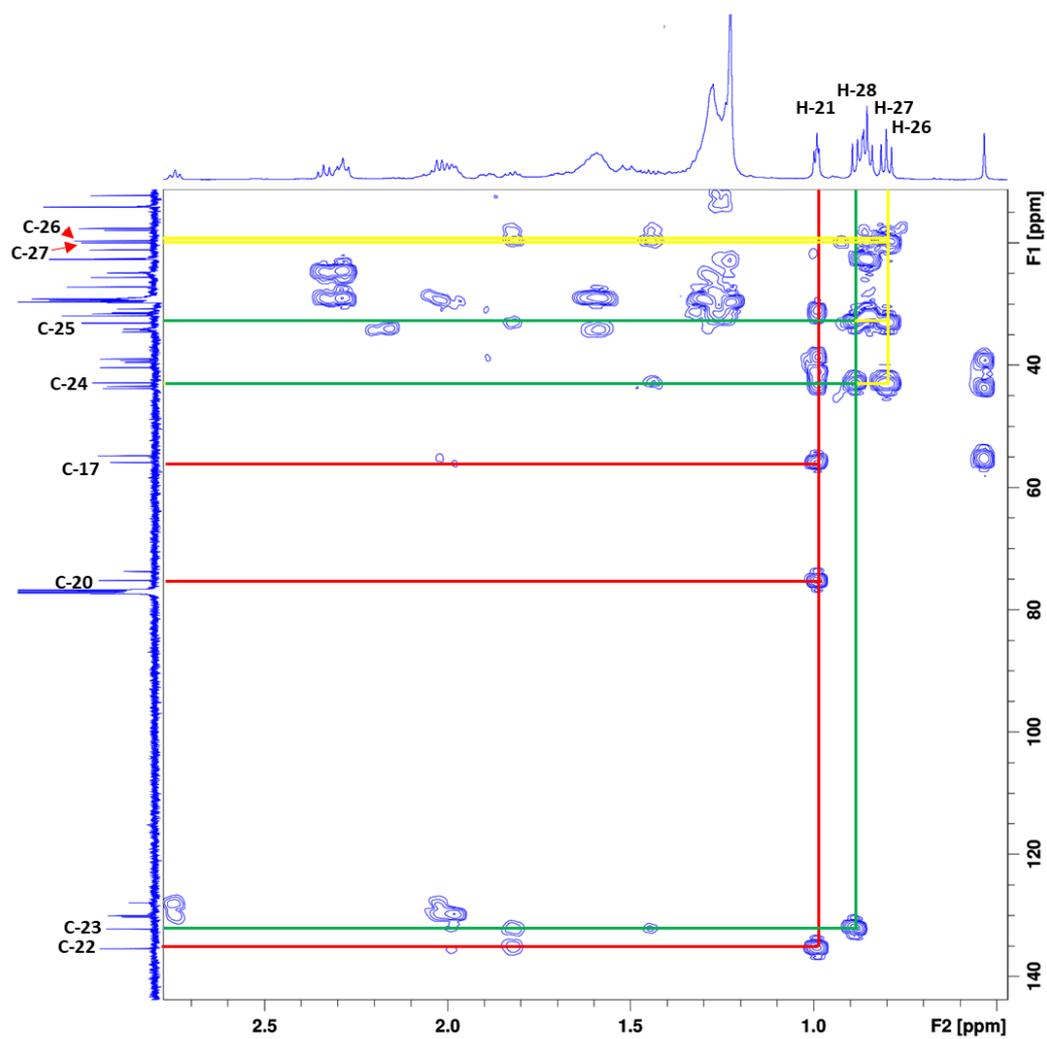


Figure S12: HMBC spectrum of **1** (From δ_c 140 ppm to δ_c 30 ppm)

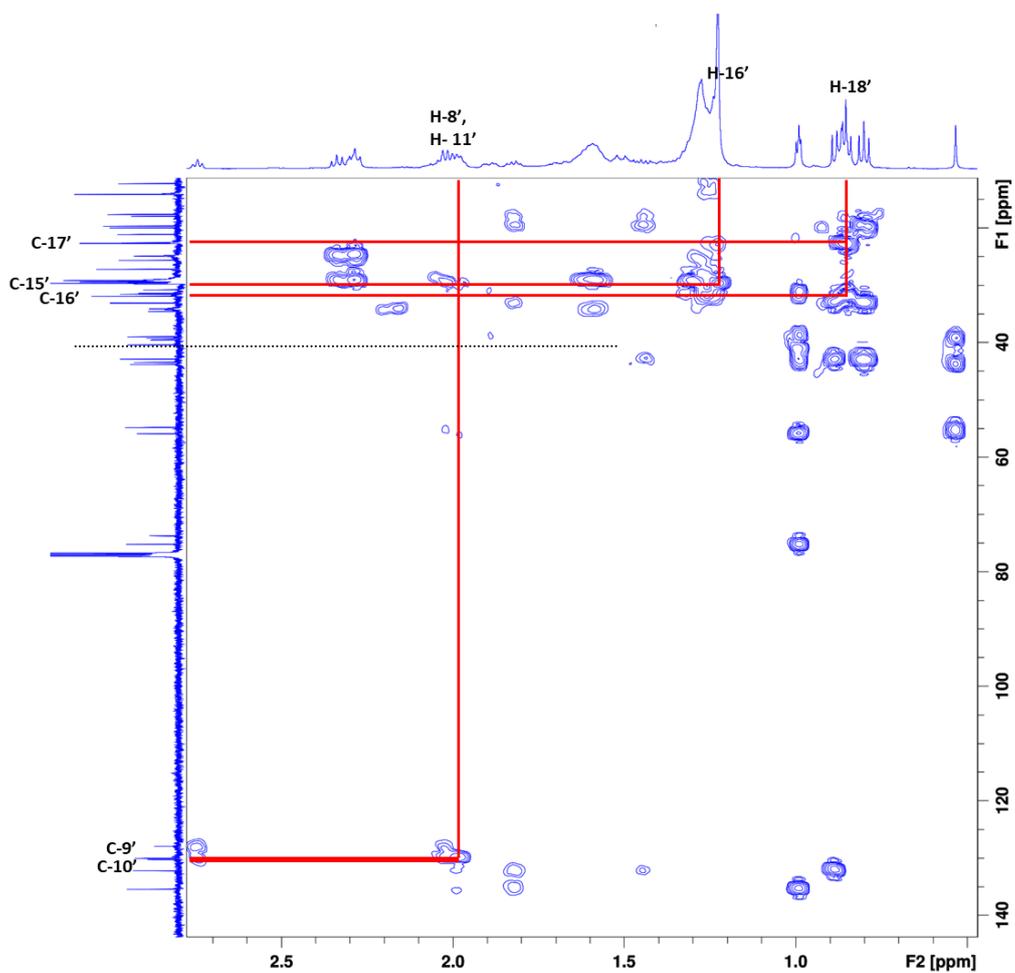


Figure S13: HMBC spectrum of **1** (From δ_C 140 ppm to δ_C 20 ppm)

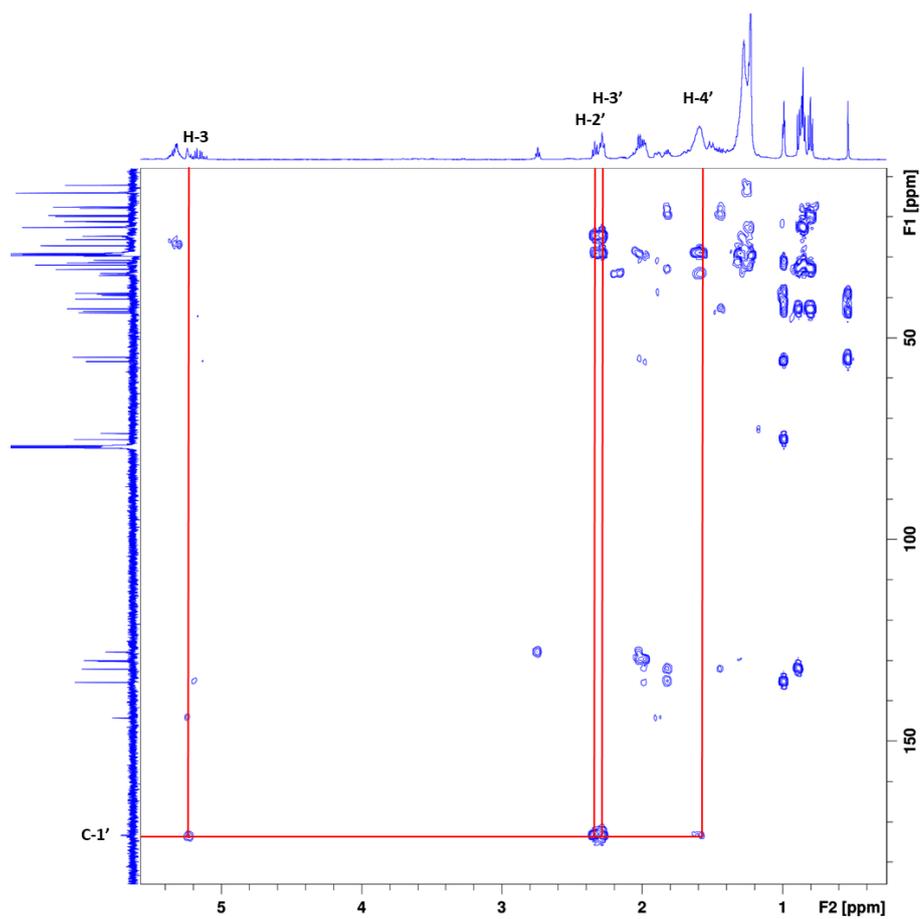


Figure S14: HMBC spectrum of **1** (From δ_C 170 ppm to δ_C 20 ppm)

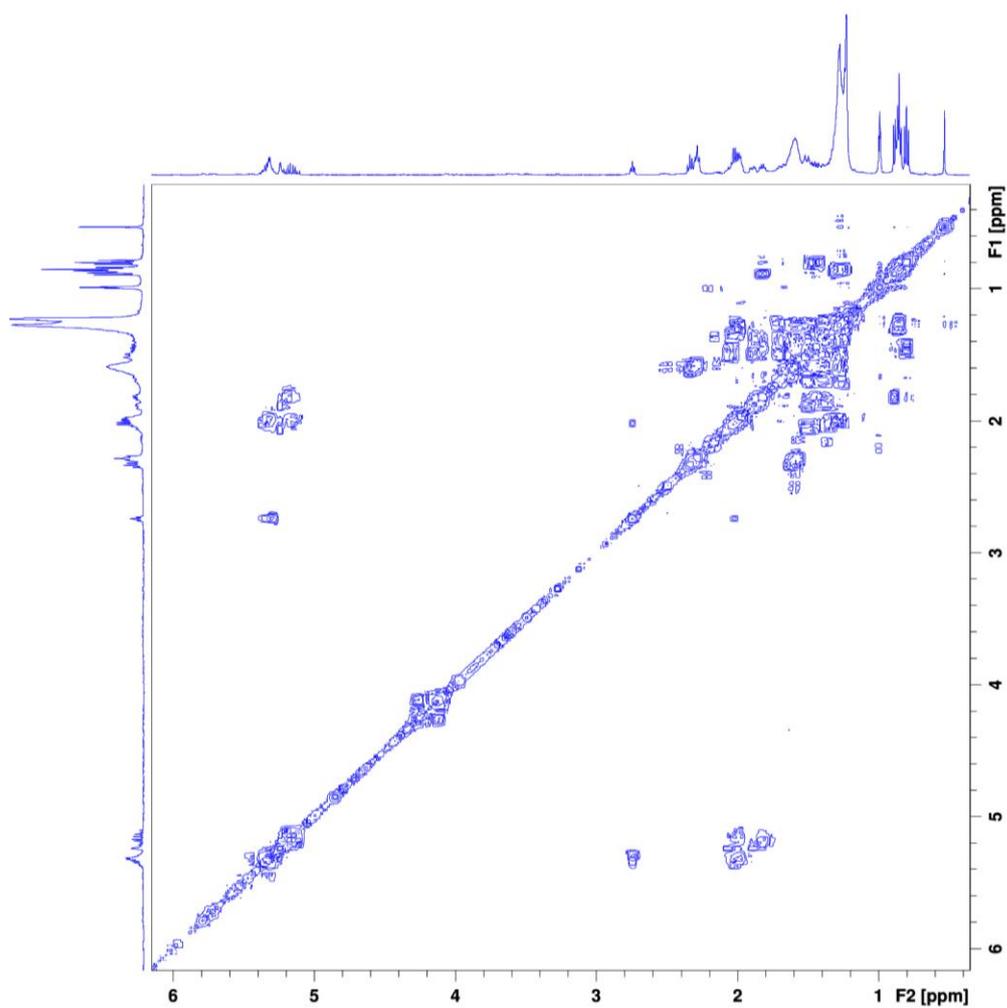


Figure S15: ^1H - ^1H COSY spectrum of **1**

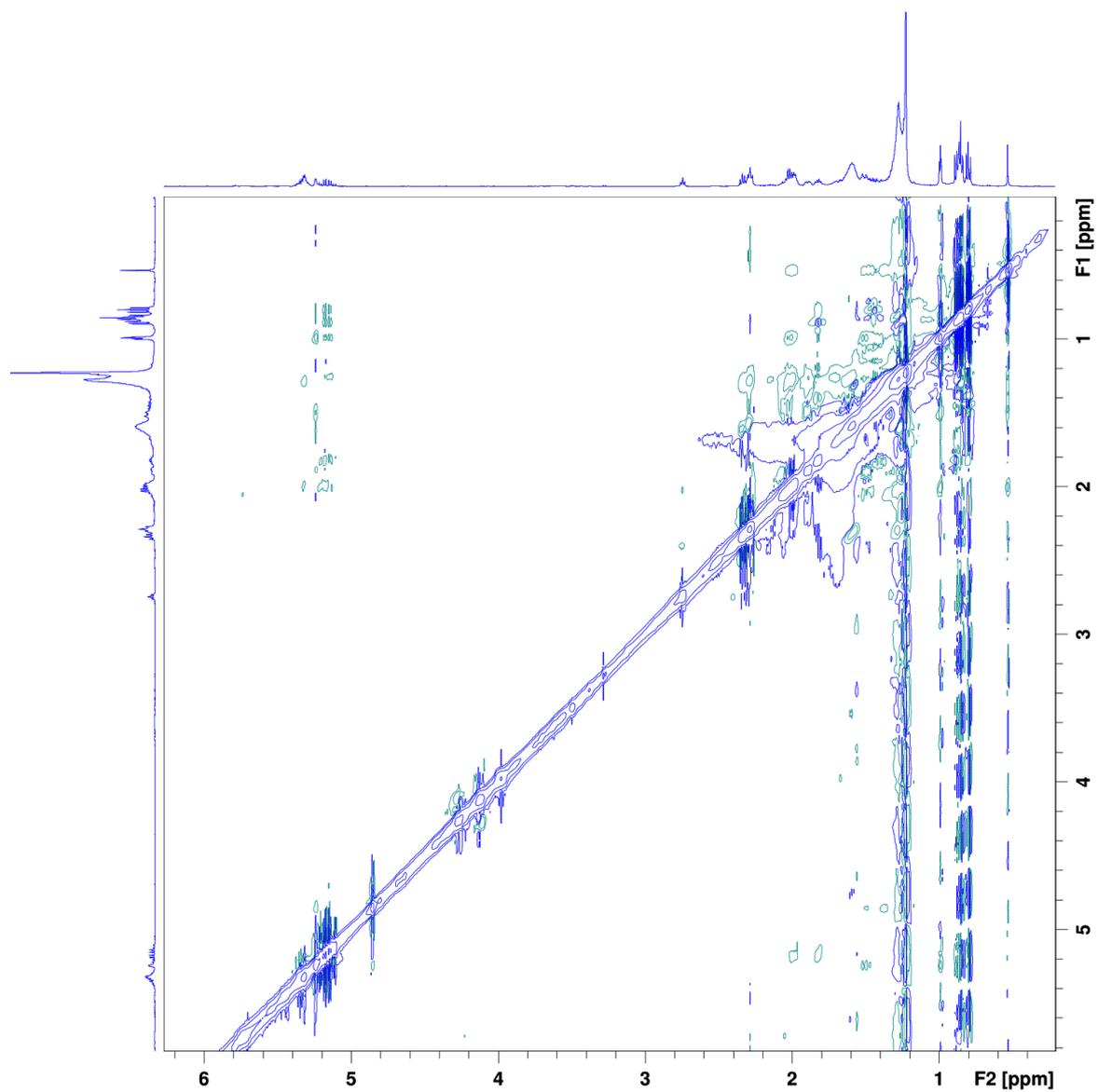


Figure S16: NOESY spectrum of **1**