

Supplementary Information

Angelocunhol: New Erythroxyane Diterpene and Other Compounds from *Simira sampaioana* (Rubiaceae)

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Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

127 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-100 H: 0-1000 O: 0-200 Na: 0-1

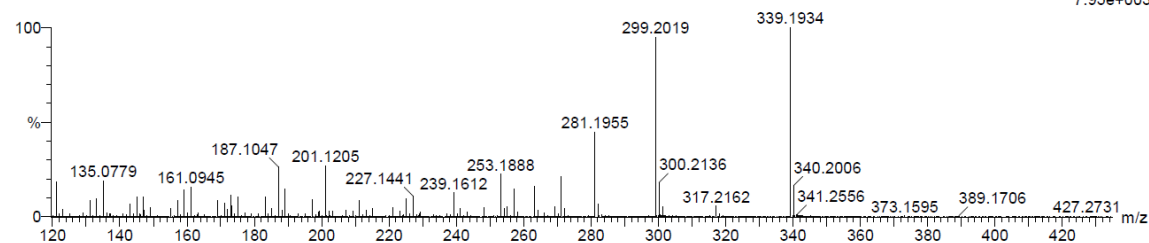
YAA 171

1: TOF MS ES+

02-Sep-2015 22:30:32

SV-24_pos_Drbraz_Kirley 1138 (10.242)

7.95e+003



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
339.1934	339.1936	-0.2	-0.6	6.5	81.7	0.0	C20 H28 O3 Na

Figure S1. HR-ESI-MS spectrum of compound 1.

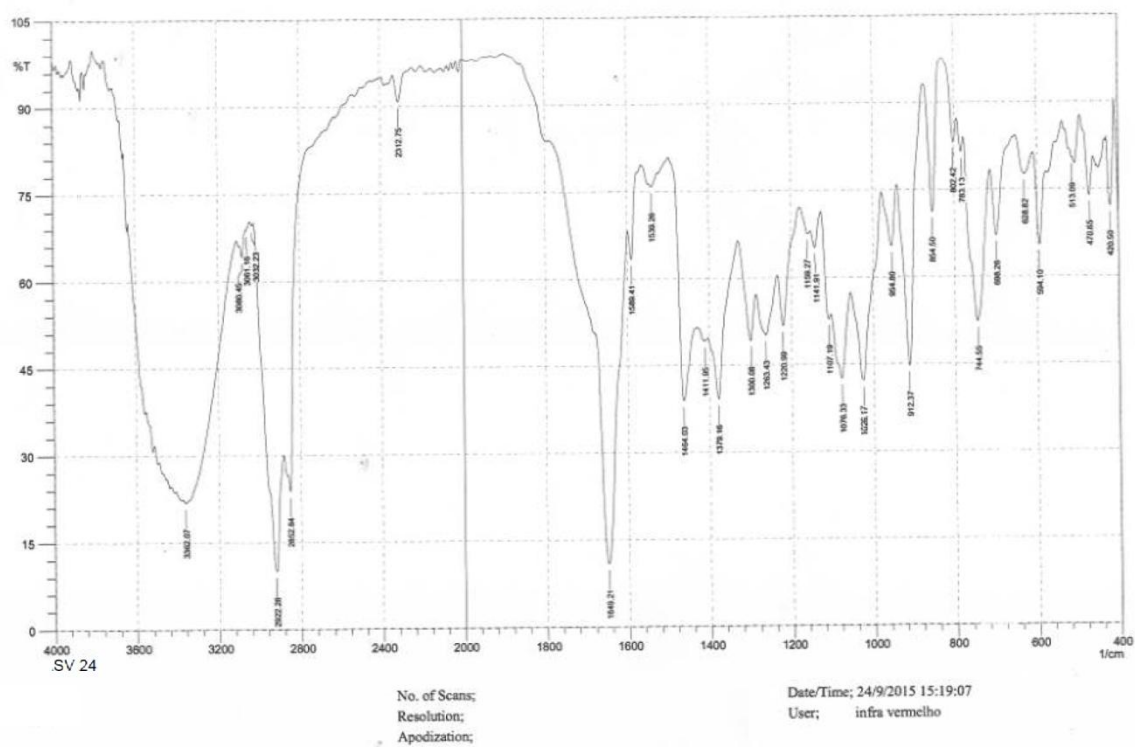


Figure S2. FTIR (KBr) spectrum of compound **1**.

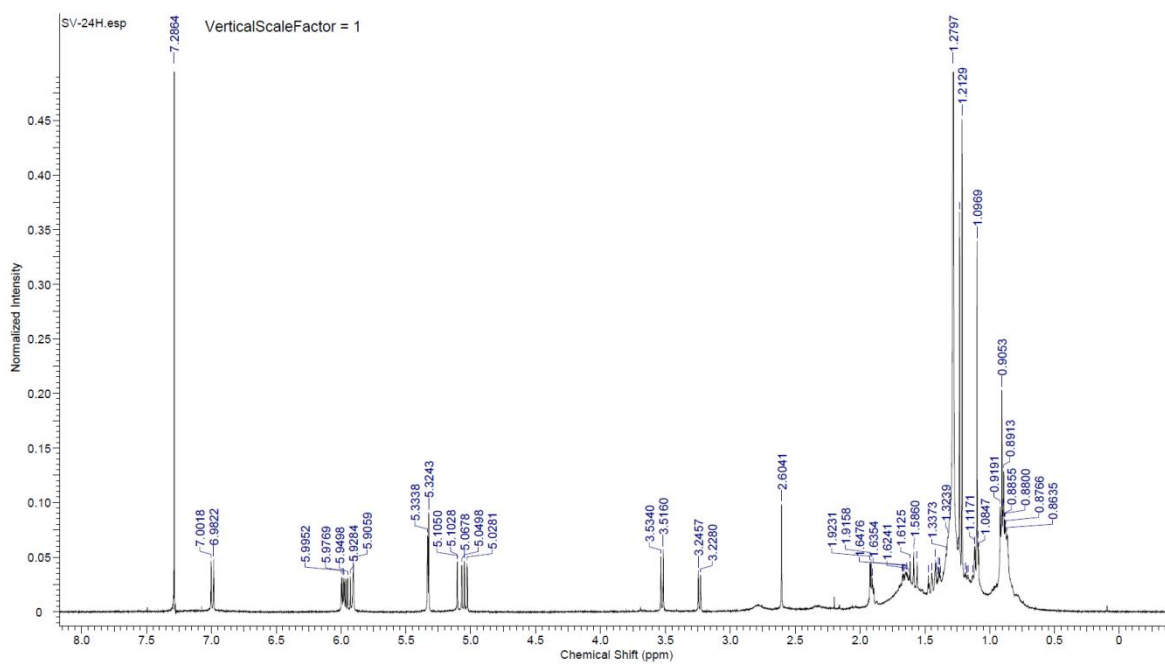


Figure S3. ^1H NMR spectrum (500 MHz, CDCl_3) of compound **1**.

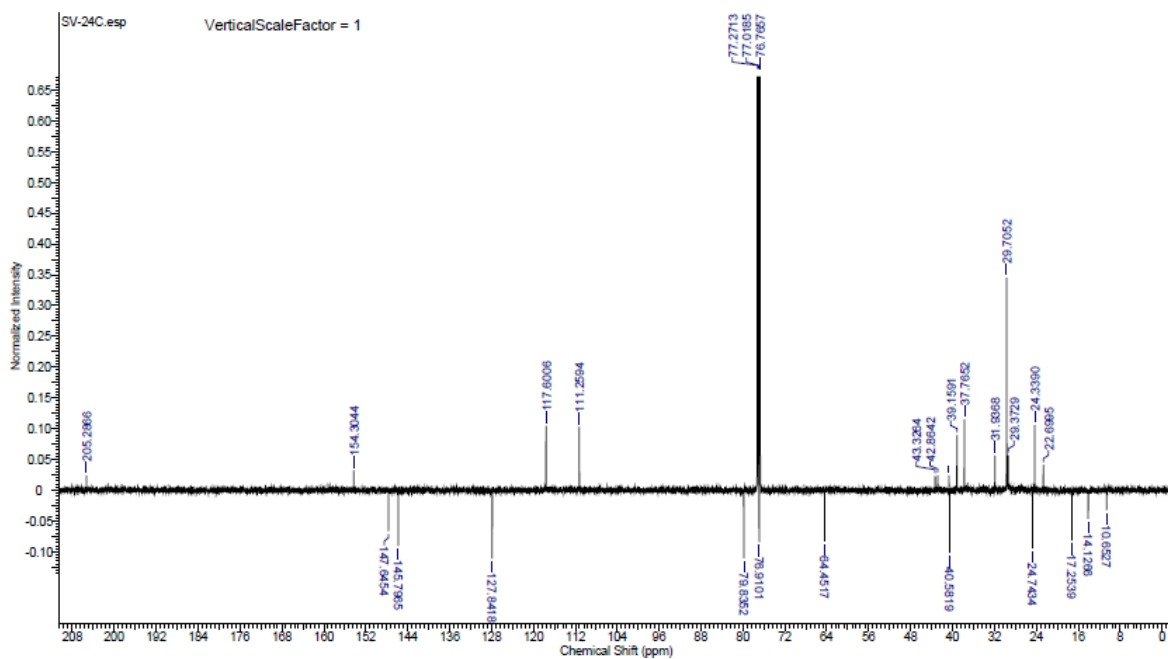


Figure S4. DEPTQ- ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound **1**.

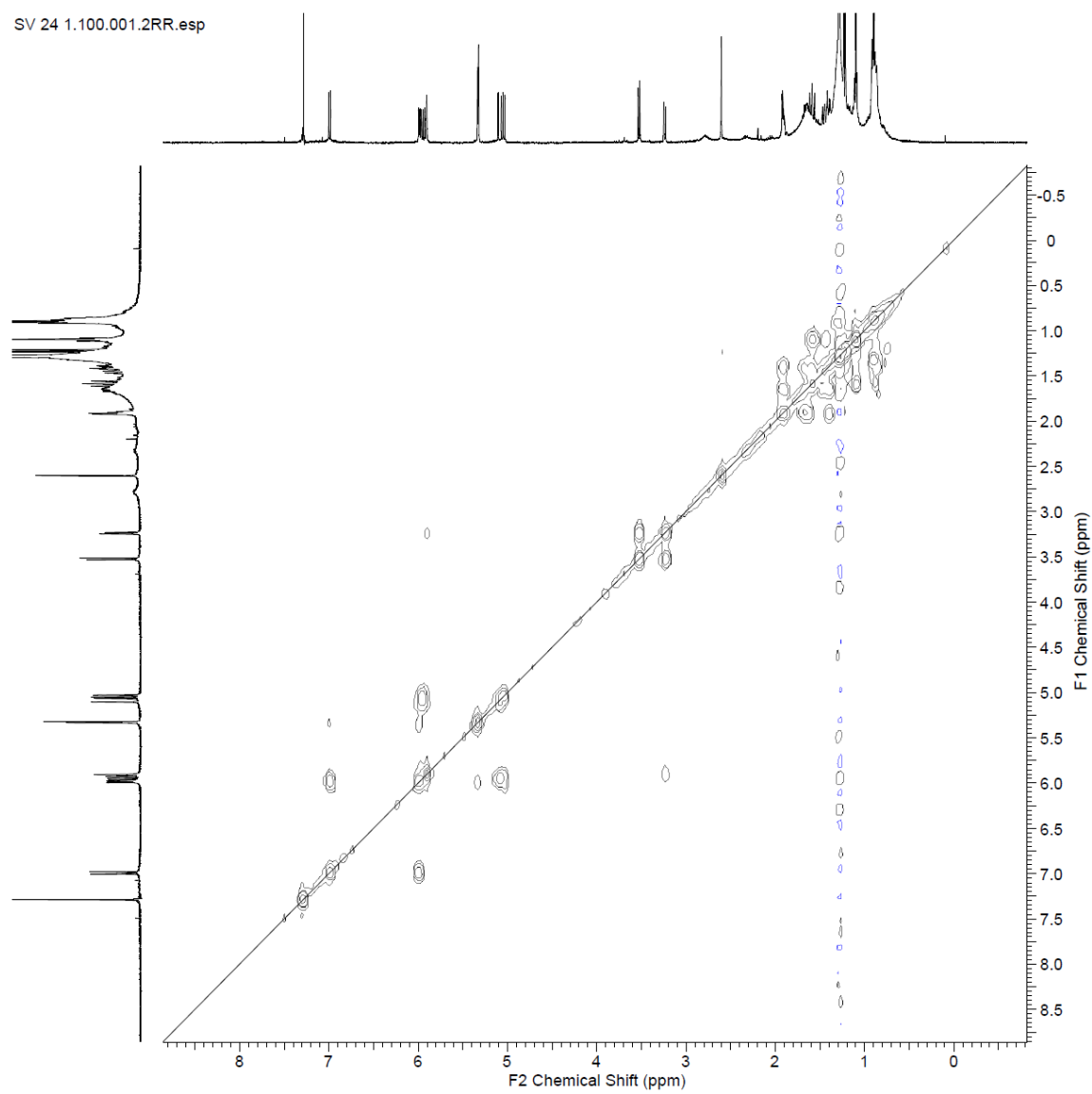


Figure S5. ^1H - ^1H -COSY spectrum of compound **1**.

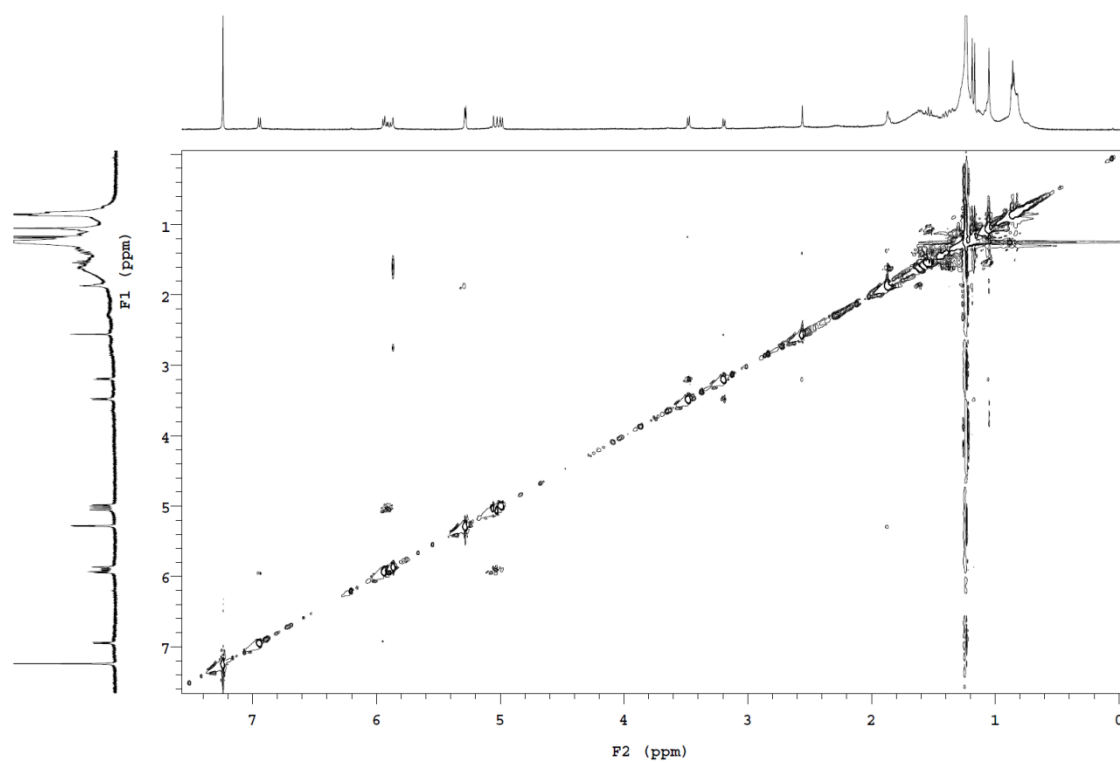


Figure S6. ^1H - ^1H -NOESY spectrum of compound **1**.

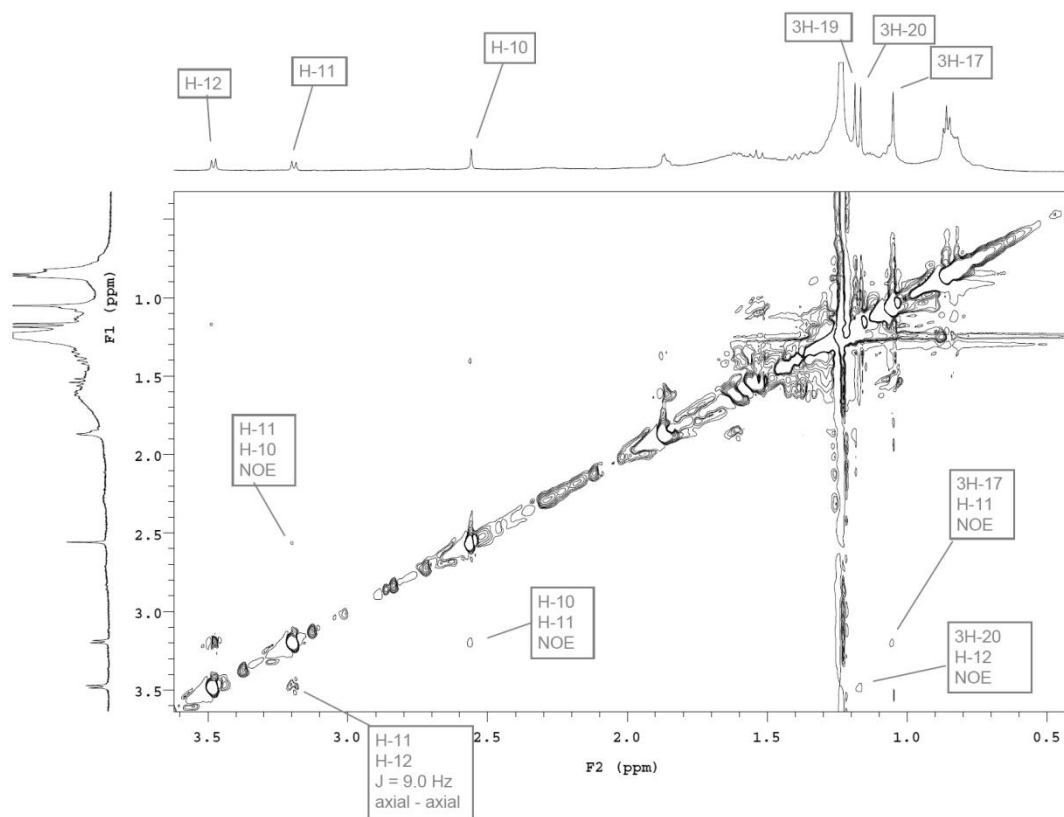


Figure S7. Enlargement ^1H - ^1H -NOESY spectrum of compound **1**.

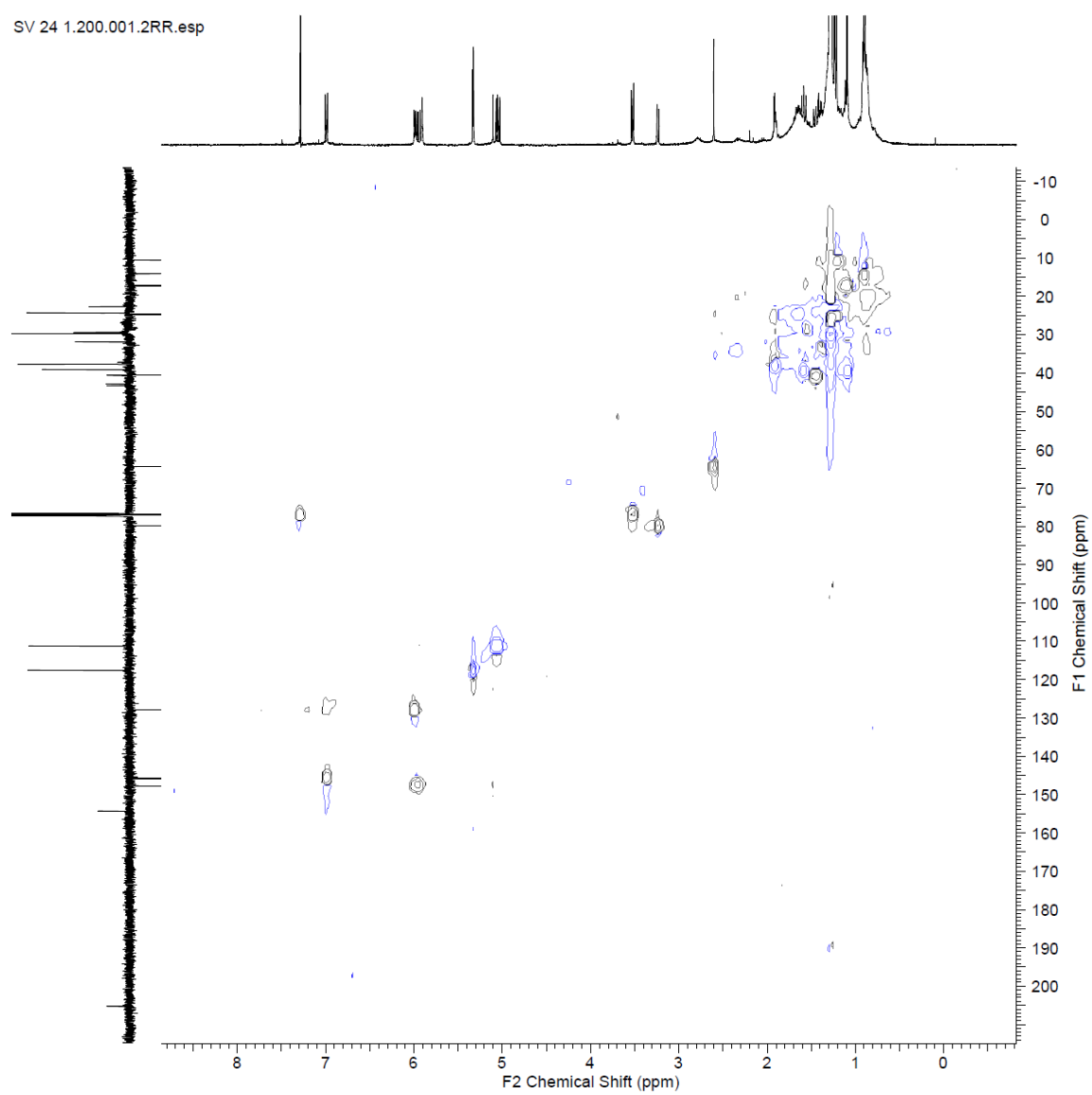


Figure S8. HSQC spectrum of compound **1**.

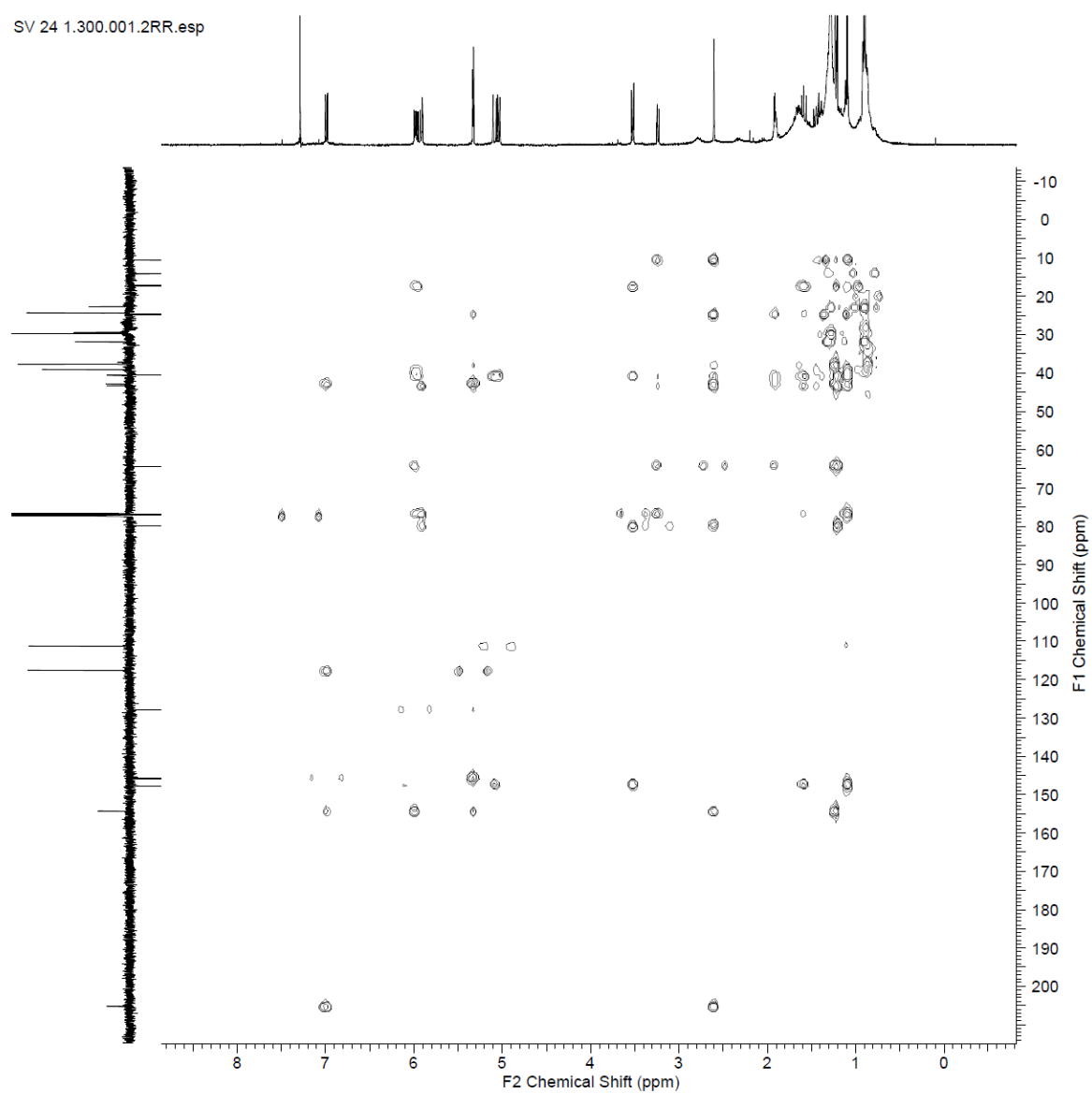


Figure S9. HMBC spectrum of compound **1**.