

Supporting Information

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A new sesquiterpene from the endophytic fungus *Nigrospora sphaerica* #003

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Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

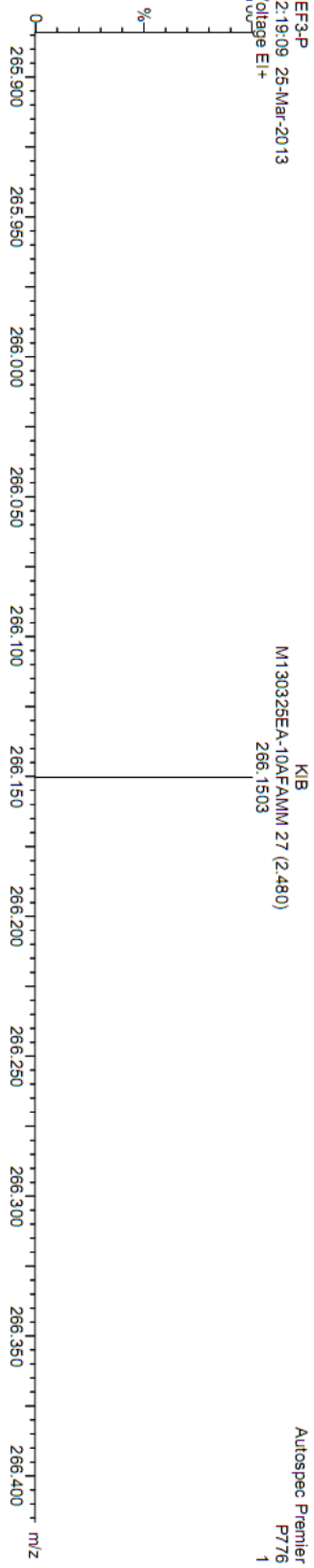
13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 3-5

LEF3-P
12:19:09 25-Mar-2013

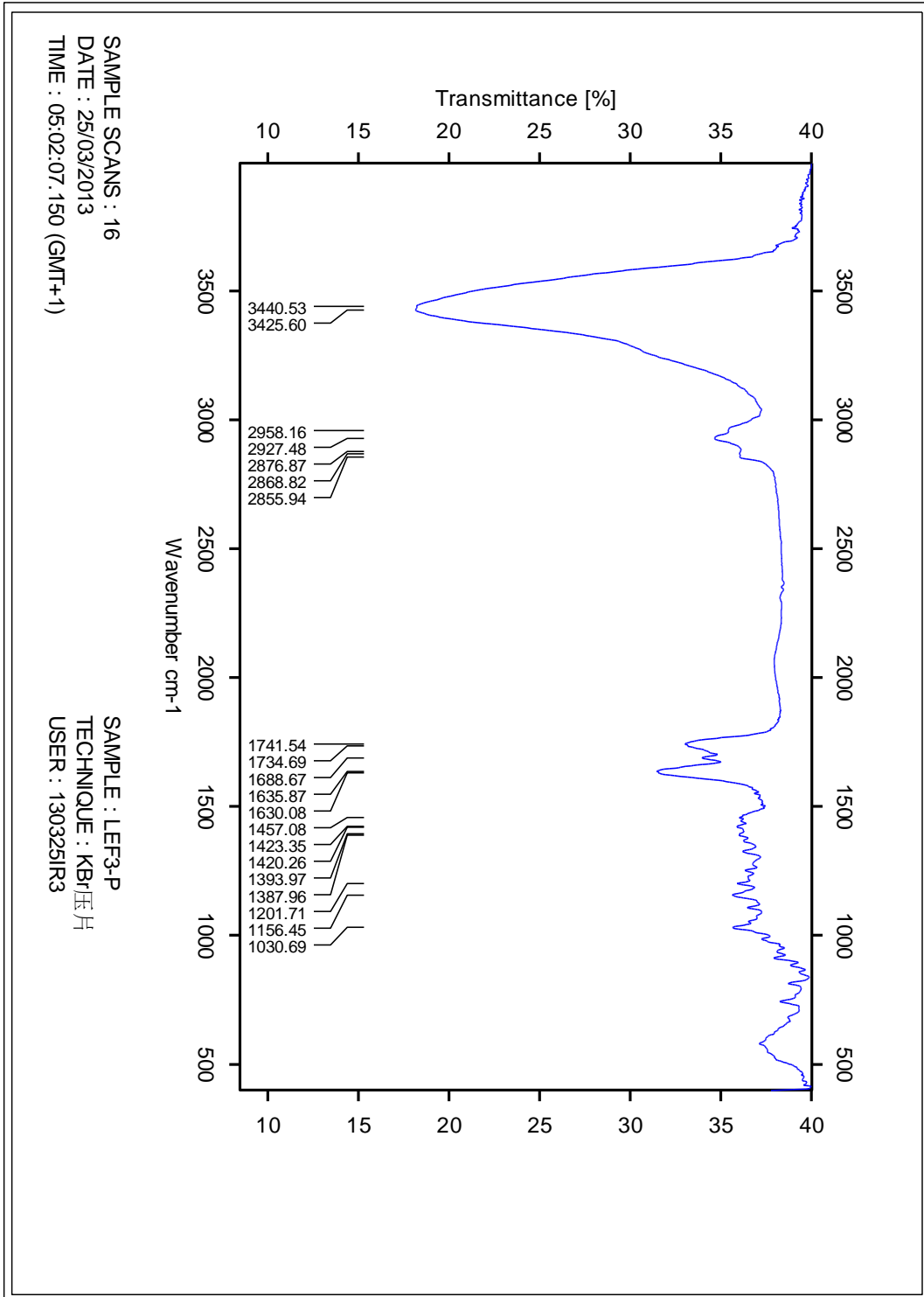
Voltage EI+
100V



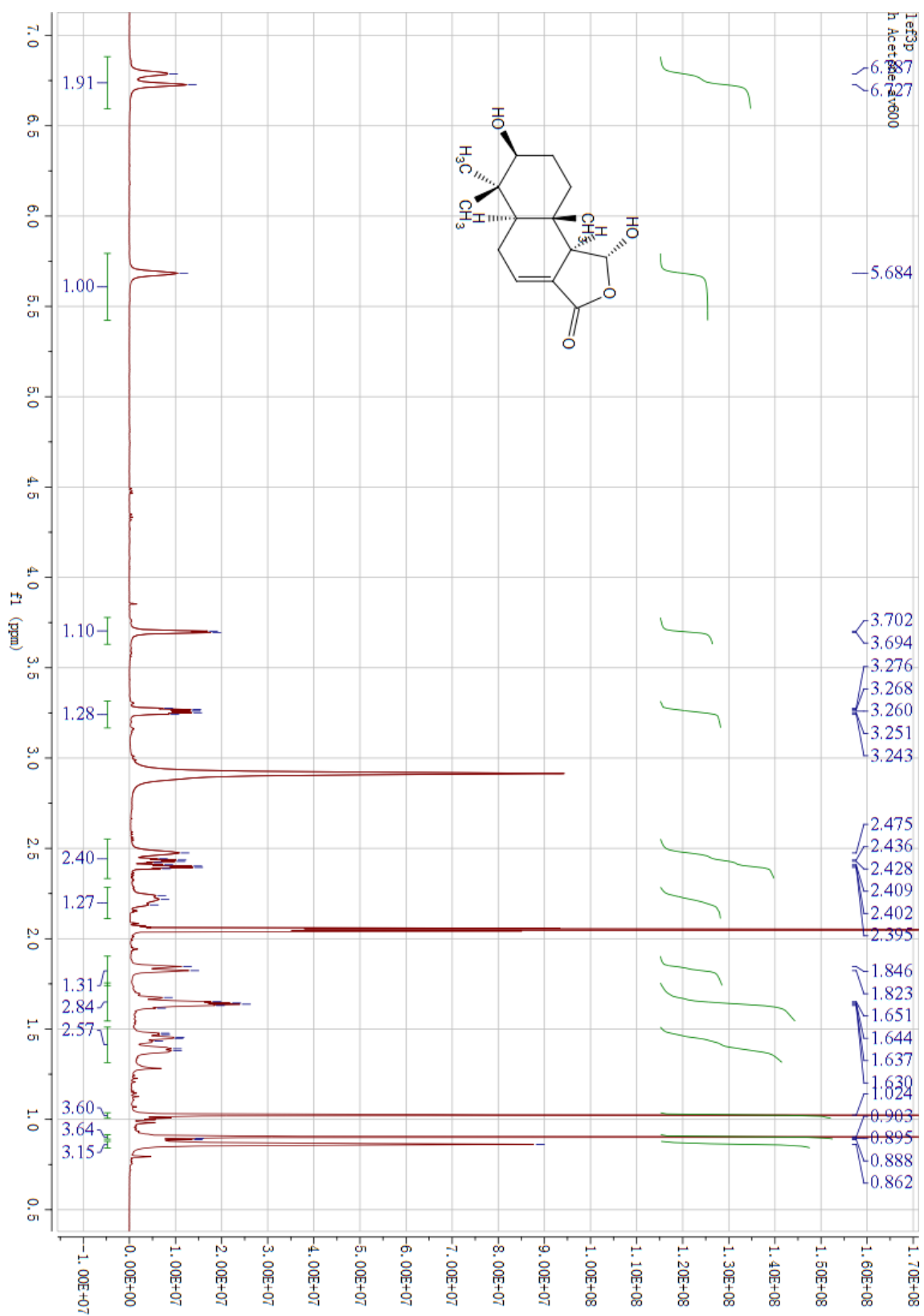
Minimum: -10.0
Maximum: 120.0

Mass	Calc. Mass	MDA	PPM	DBE	I-FIT	Formula
266.1503	266.1518	-1.5	-5.6	5.0	5546026.0	C15 H22 O4

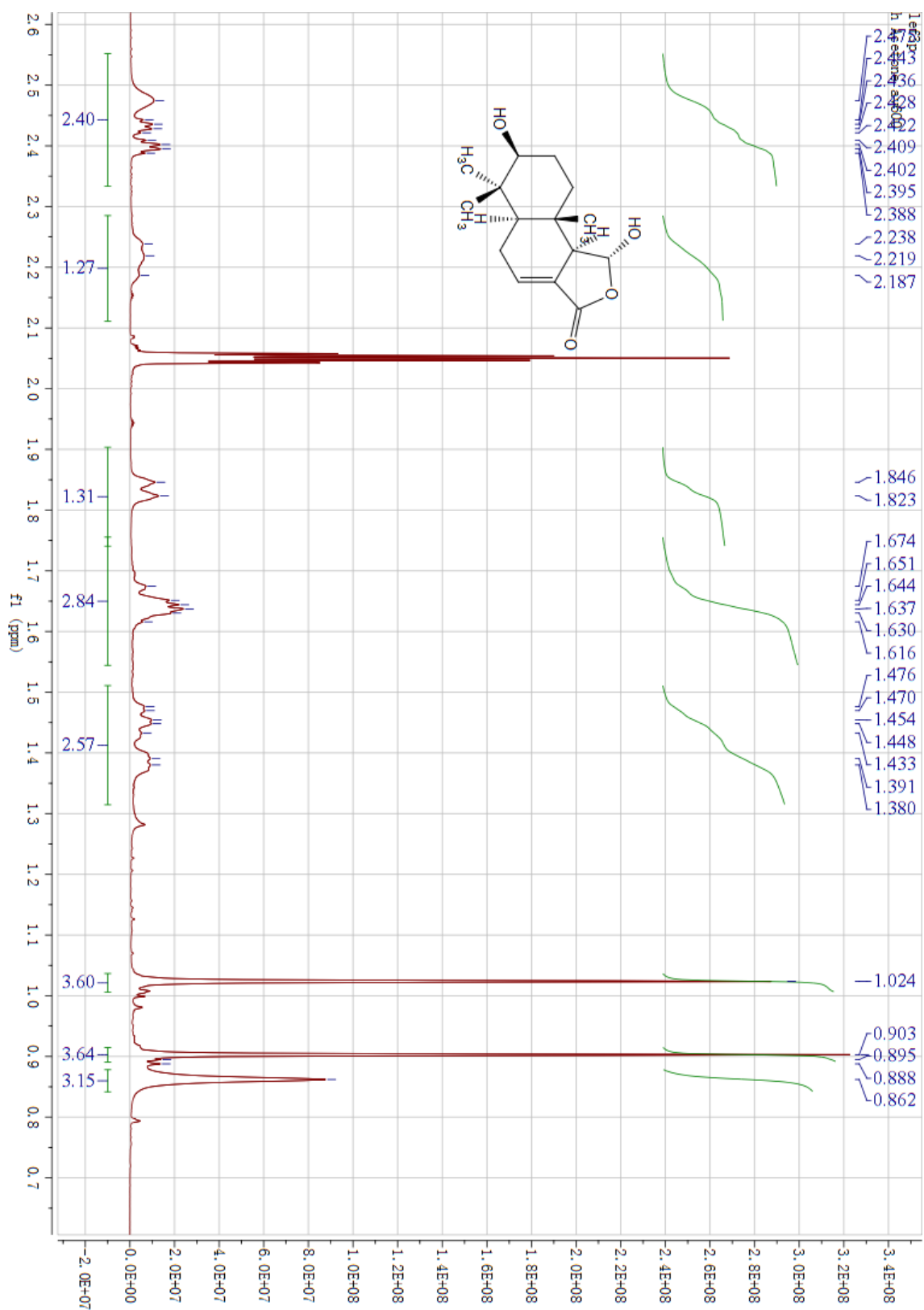
S1: HRESI-MS Spectrum of 3β-OH-dendocarbin A (1)



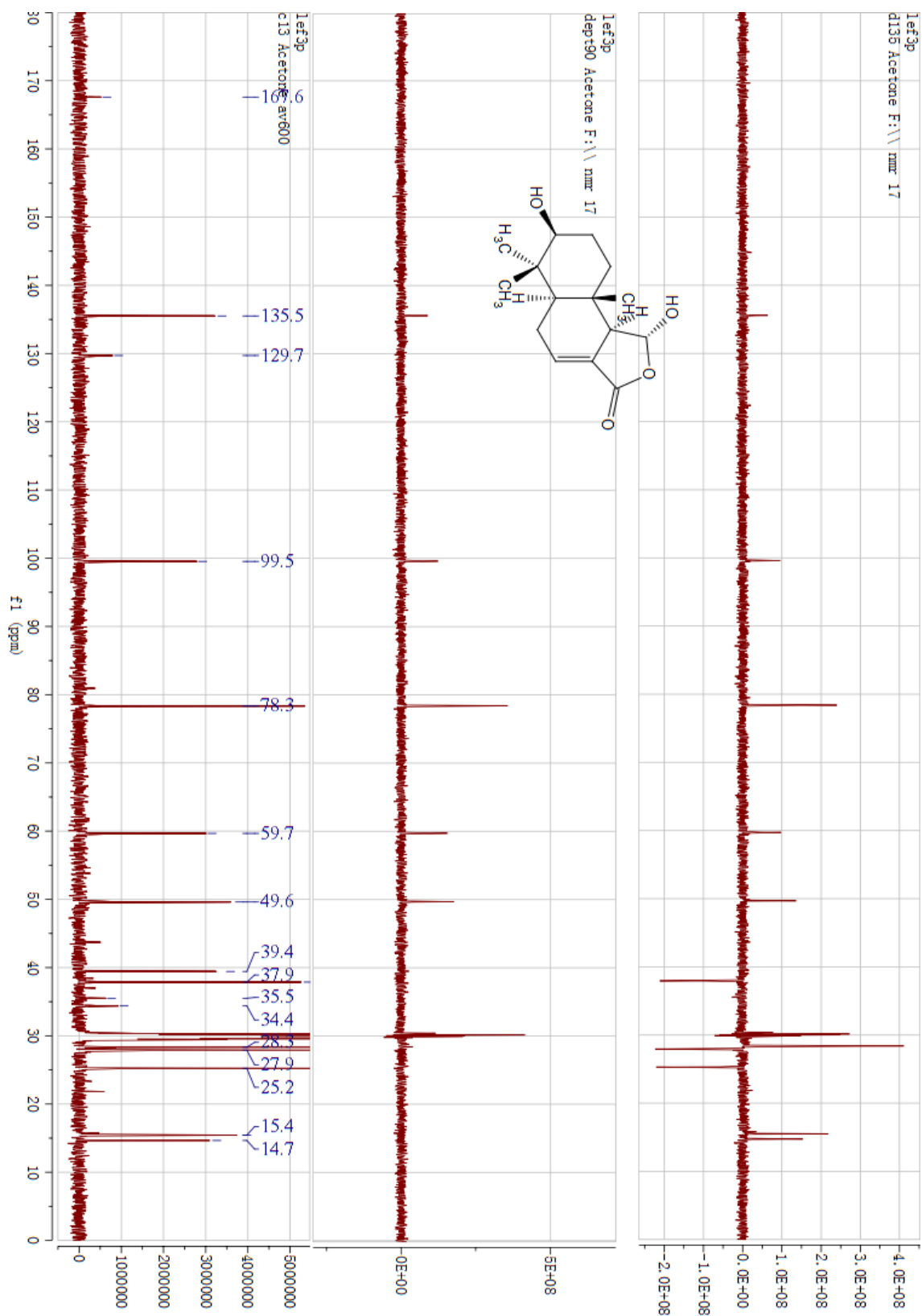
S2: IR Spectrum of 3β-OH-dendocarbin A (1)



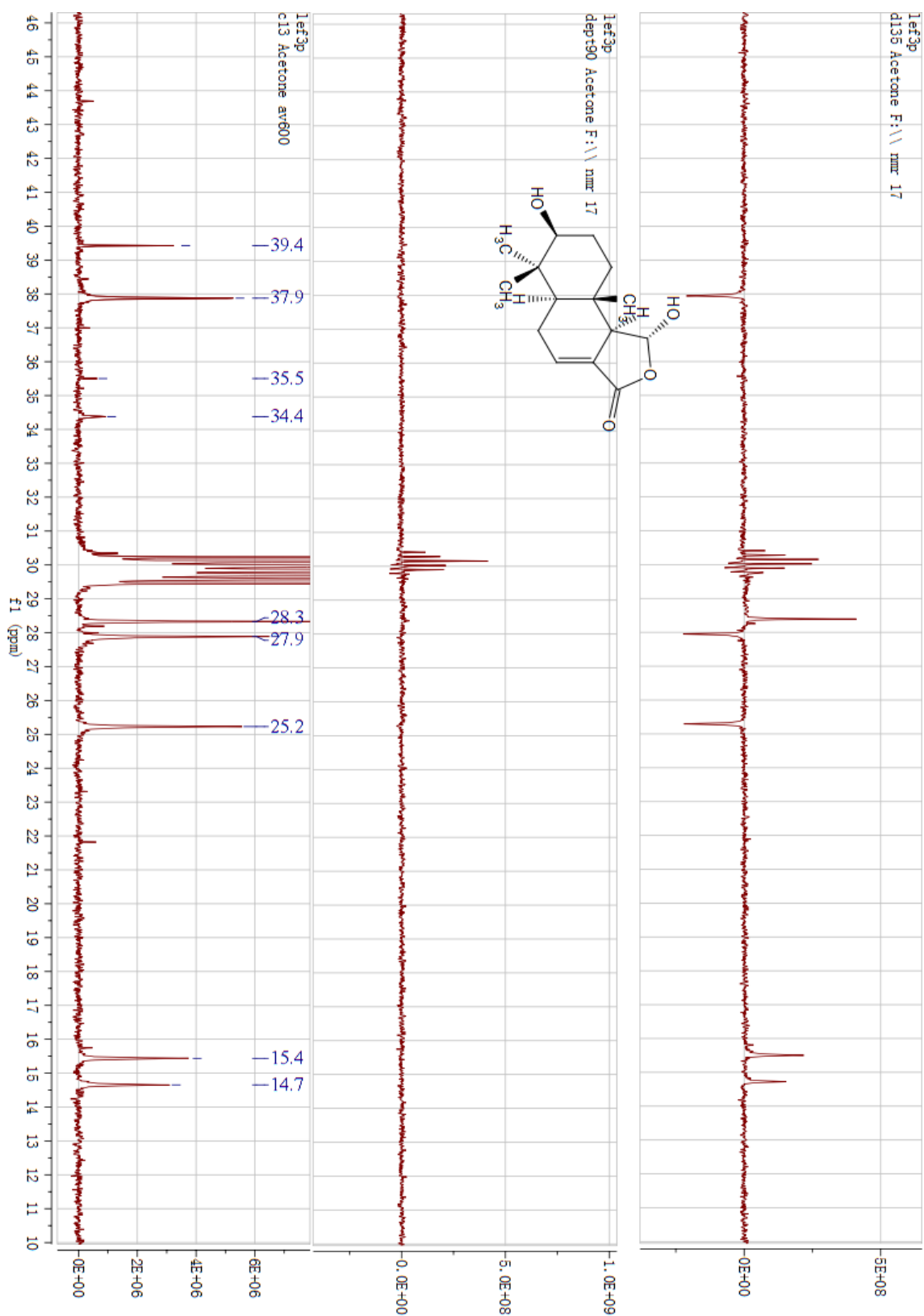
S3: ¹H-NMR (600 MHz, Acetone-*d*₆) Spectrum of 3β-OH-dendocarbin A (**1**)



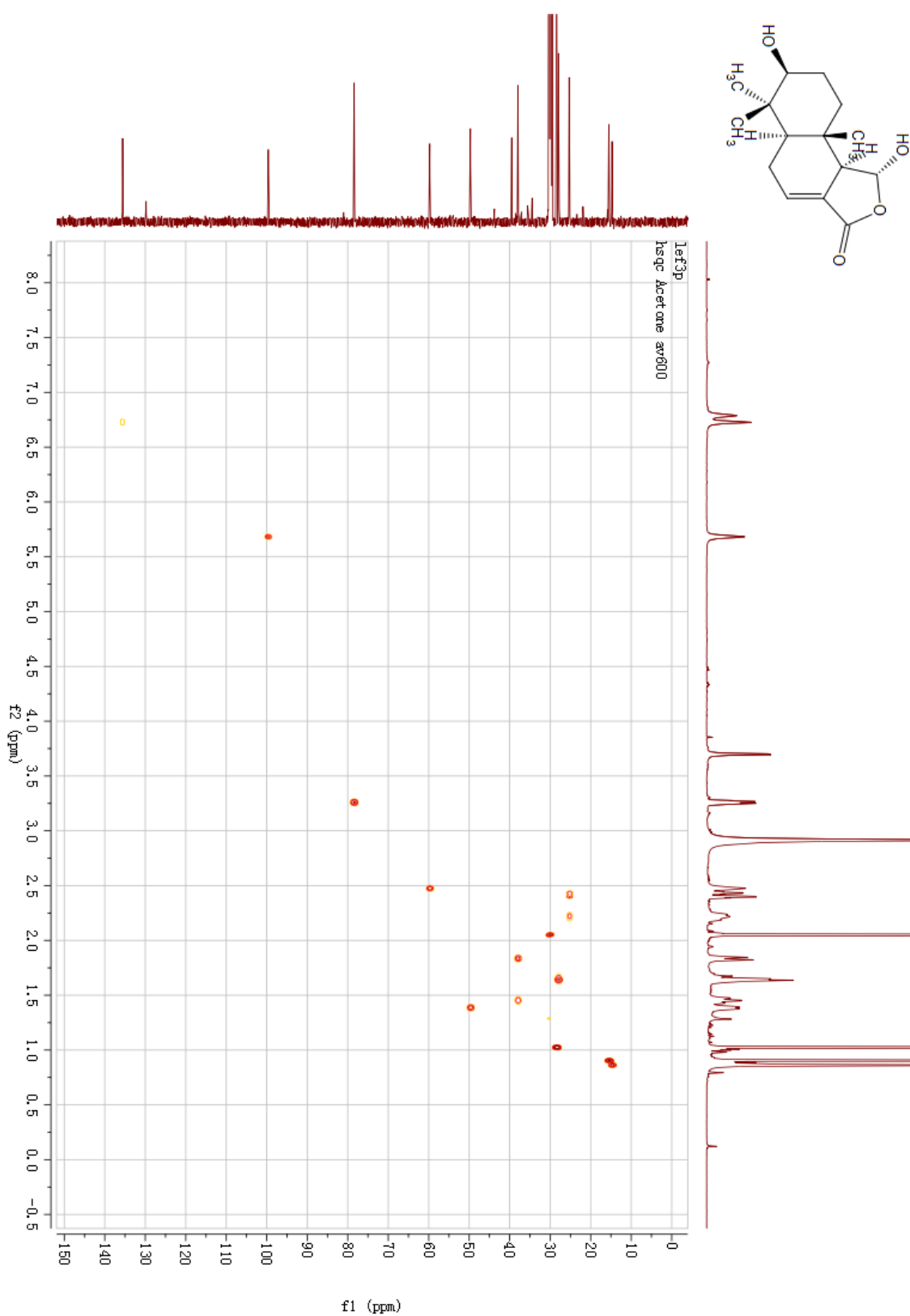
S4: Expansion of the ¹H-NMR Spectrum of 3β-OH-dendocarbin A (1)



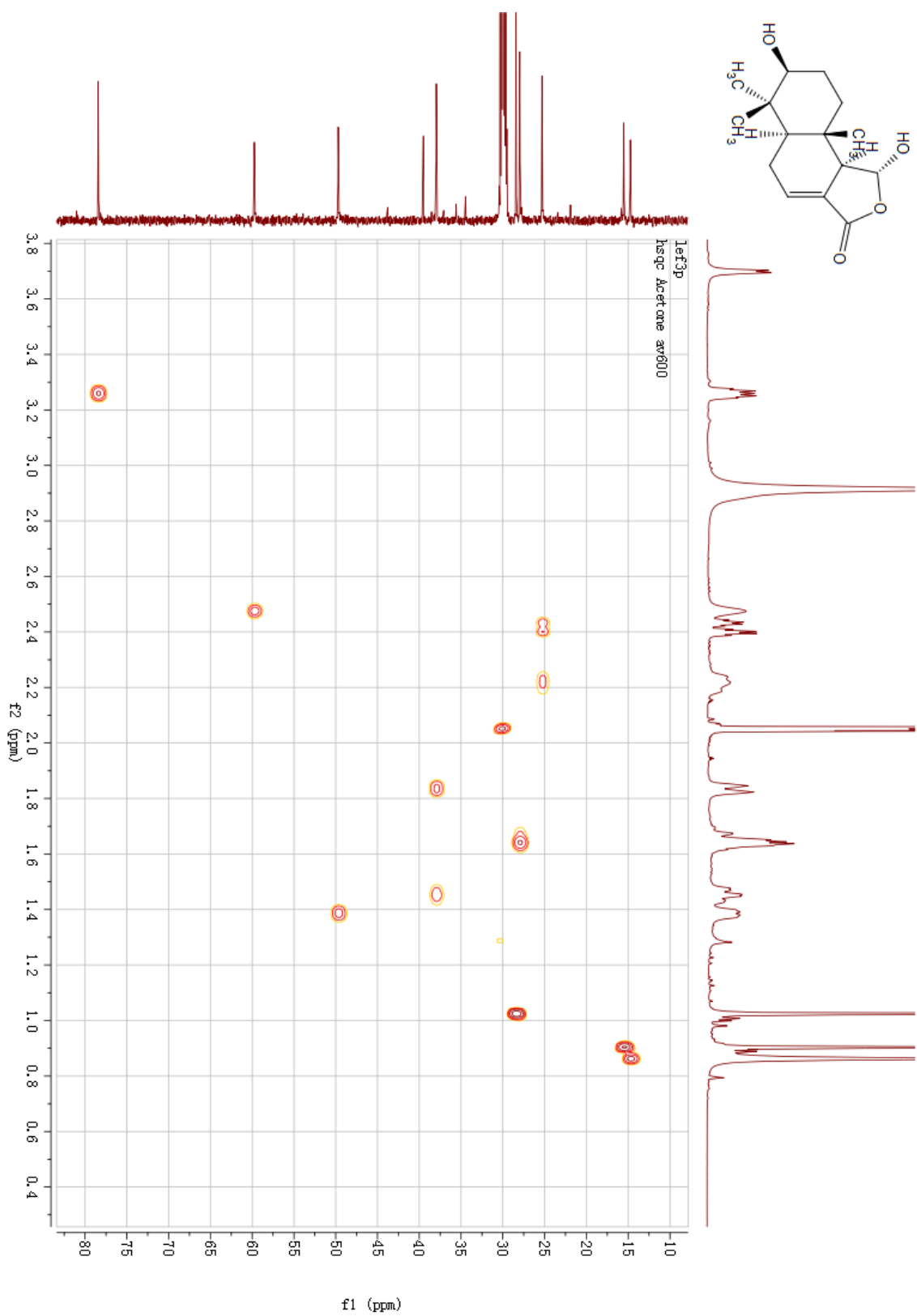
S5: ¹³C and DEPT NMR (150 MHz, Acetone-*d*₆) spectra of 3β-OH-dendocarbin A (1)



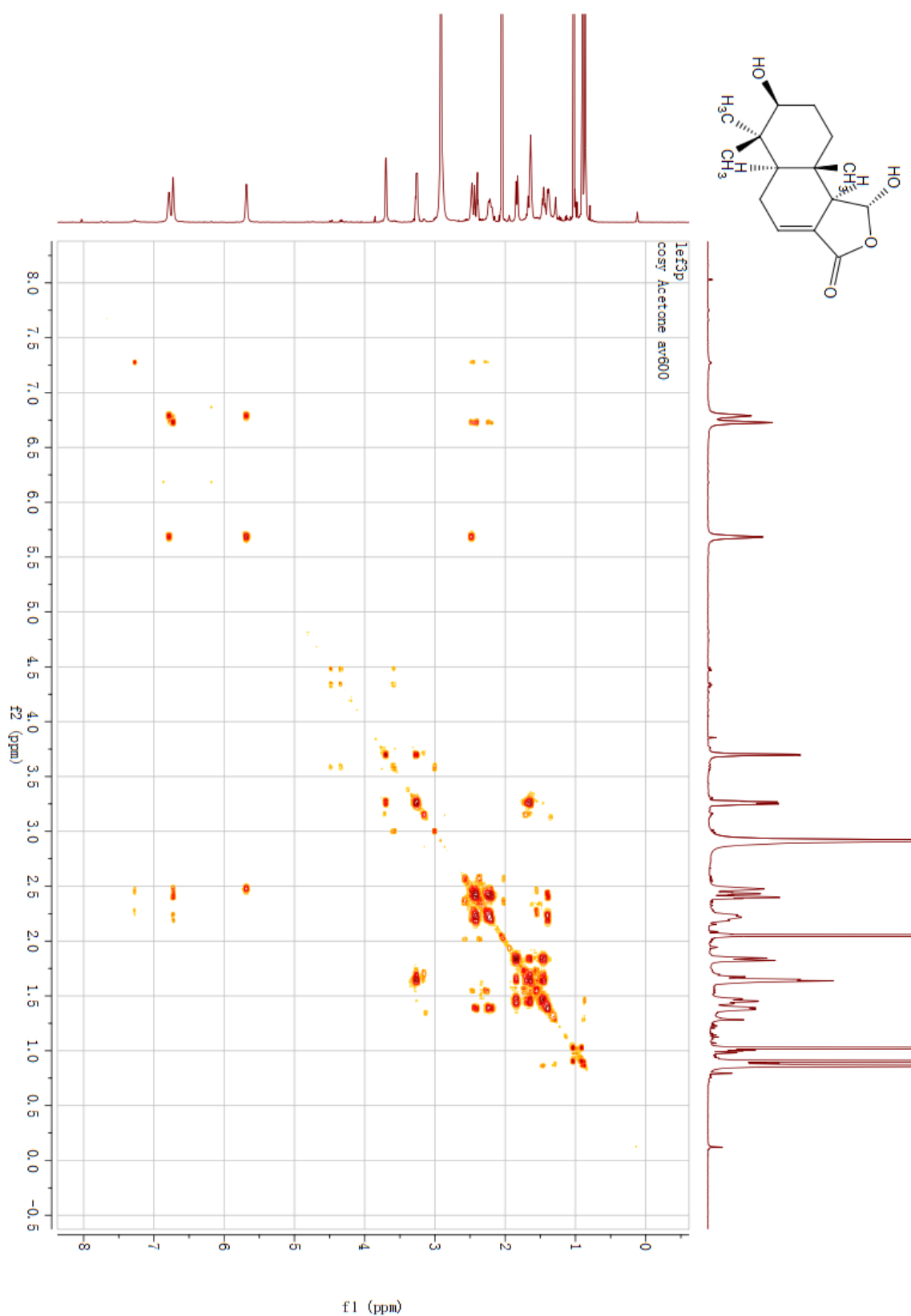
S6: Expansion of the ^{13}C -NMR + DEPT Spectrum of 3β -OH-dendocarbin A (**1**)



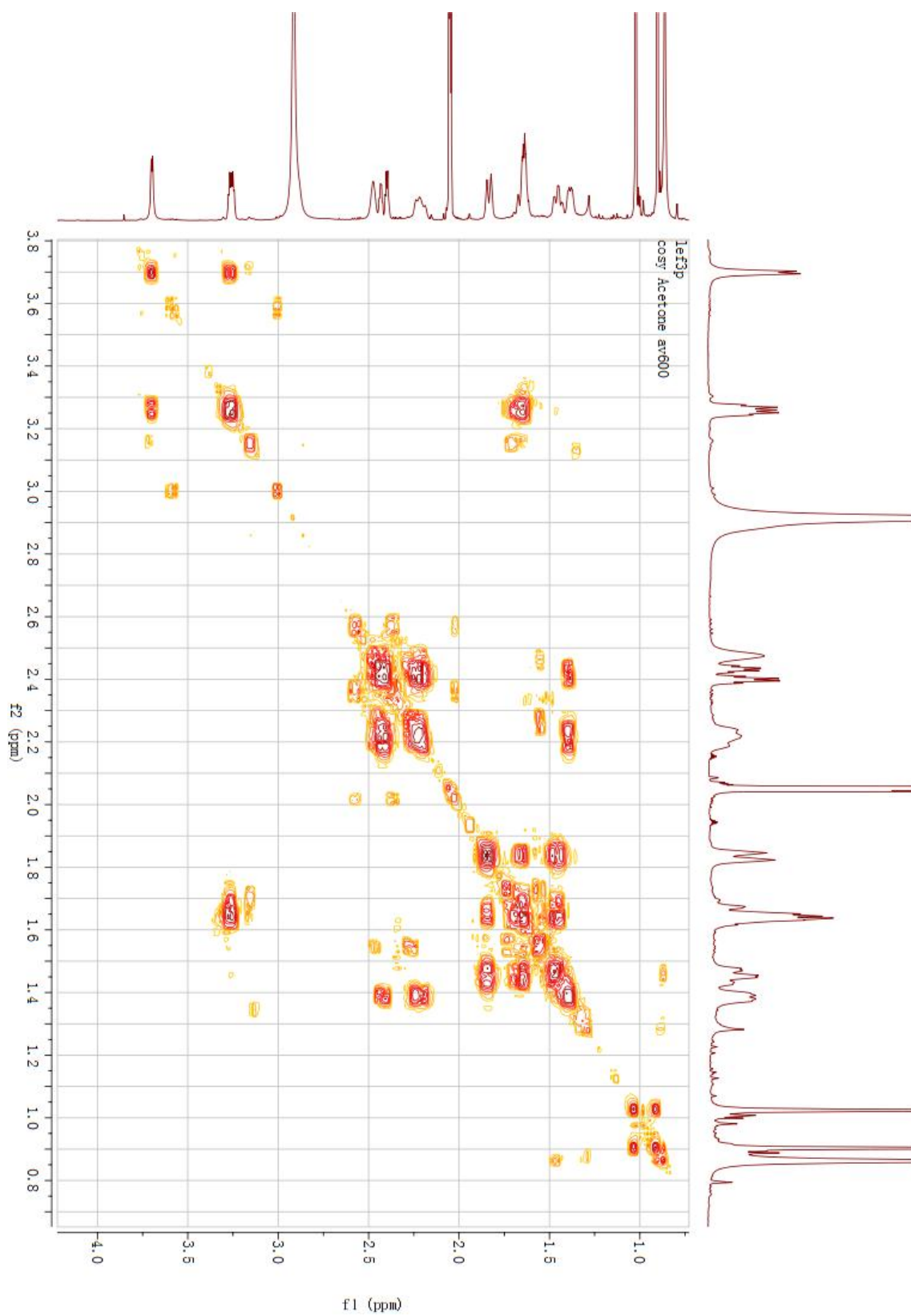
S7: HSQC Spectrum of 3β-OH-dendocarbin A (**1**)



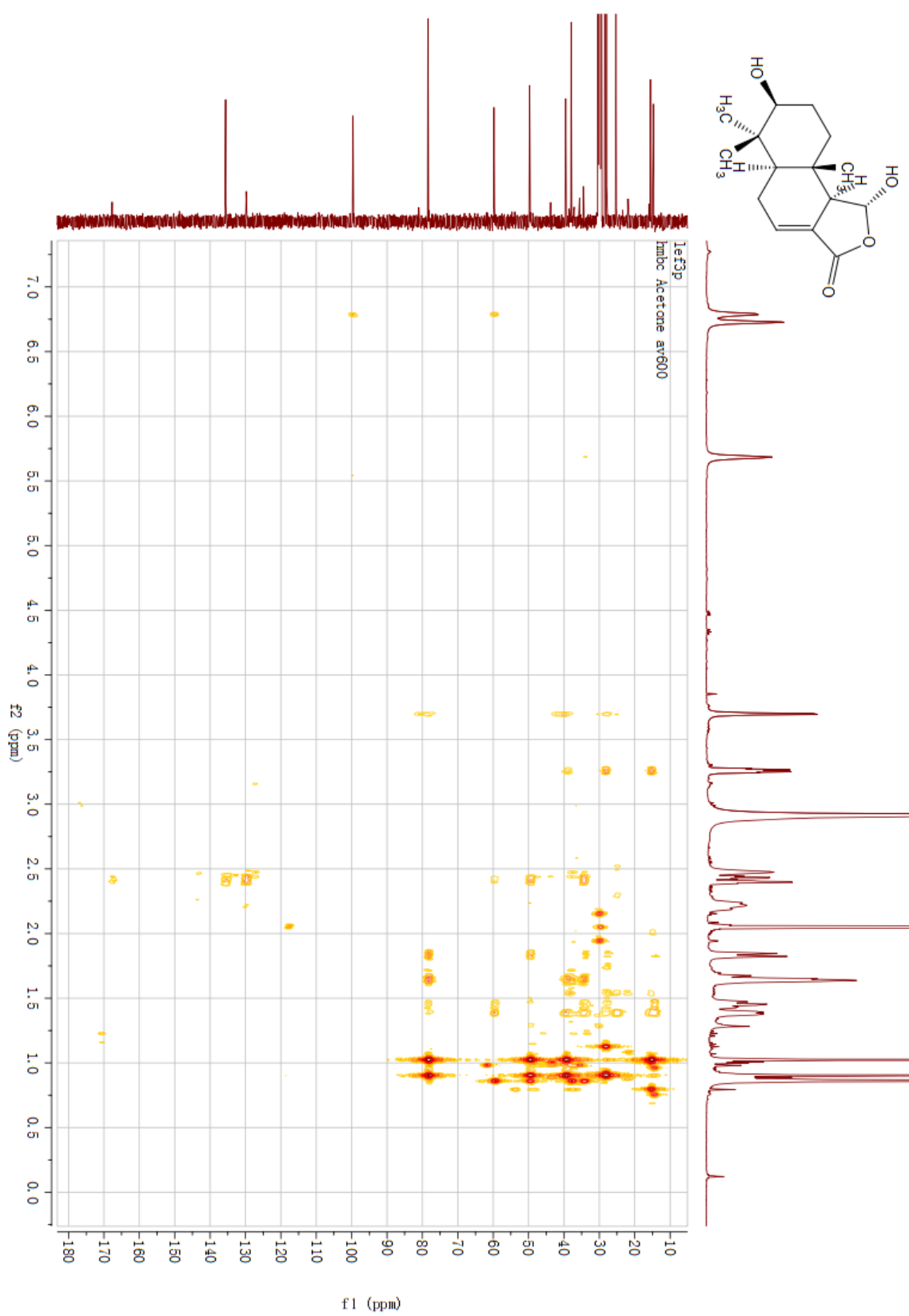
S8: Expansion of the HSQC Spectrum of 3β-OH-dendocarin A (**1**)



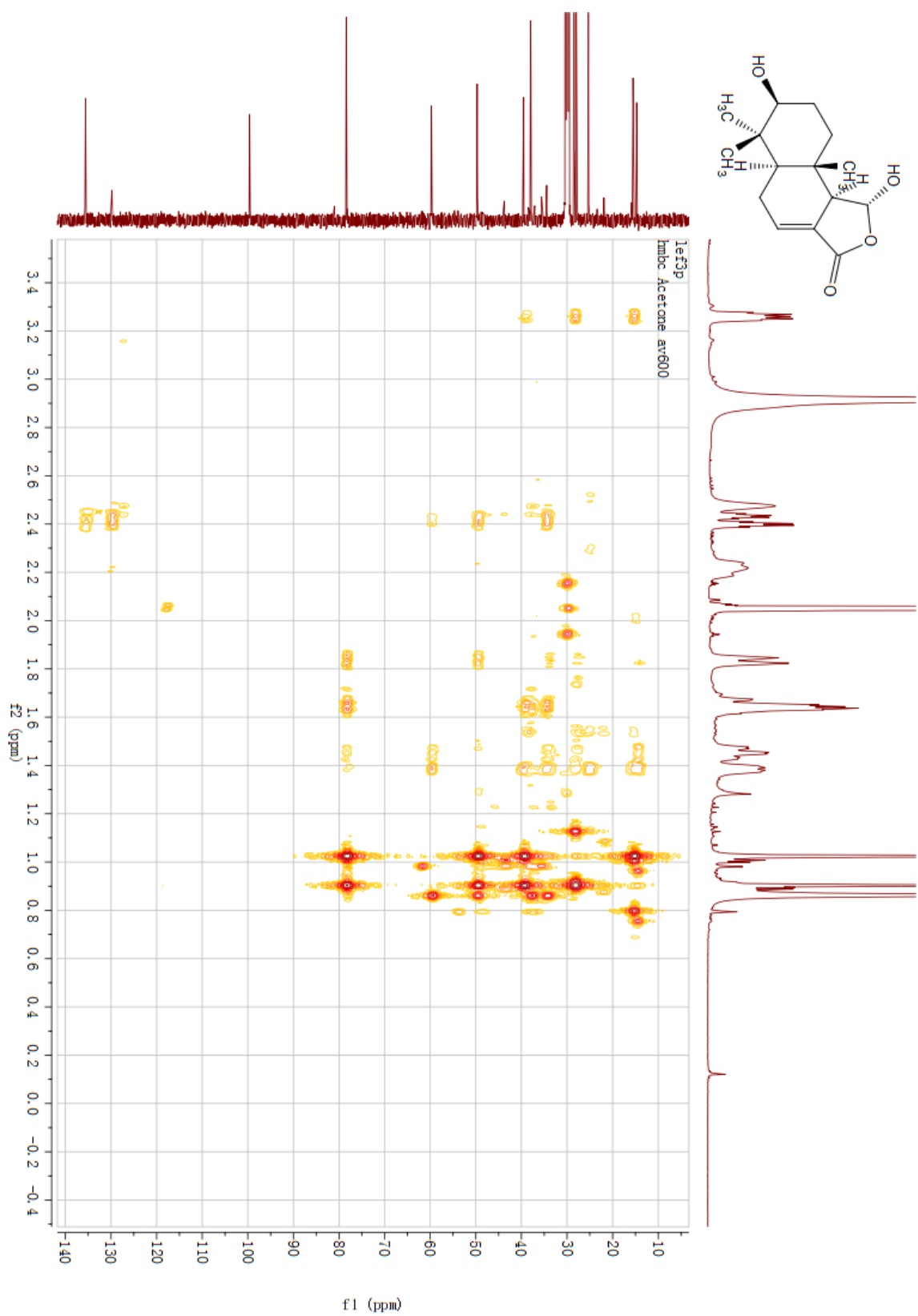
S9: COSY (600 MHz) Spectrum of 3β-OH-dendocarin A (**1**)



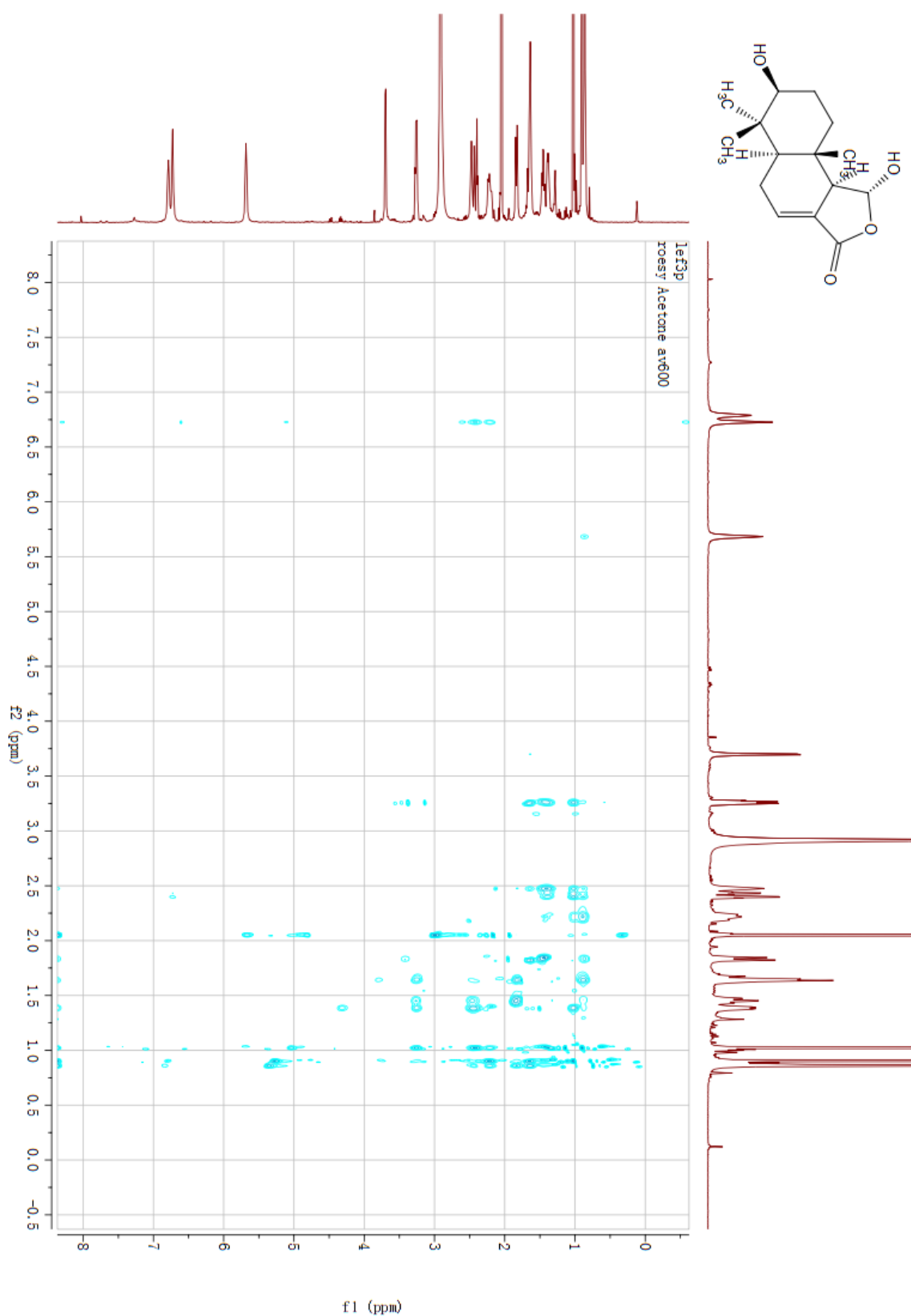
S10: Expansion of COSY (600 MHz) Spectrum of 3 β -OH-dendocarbin A (**1**)



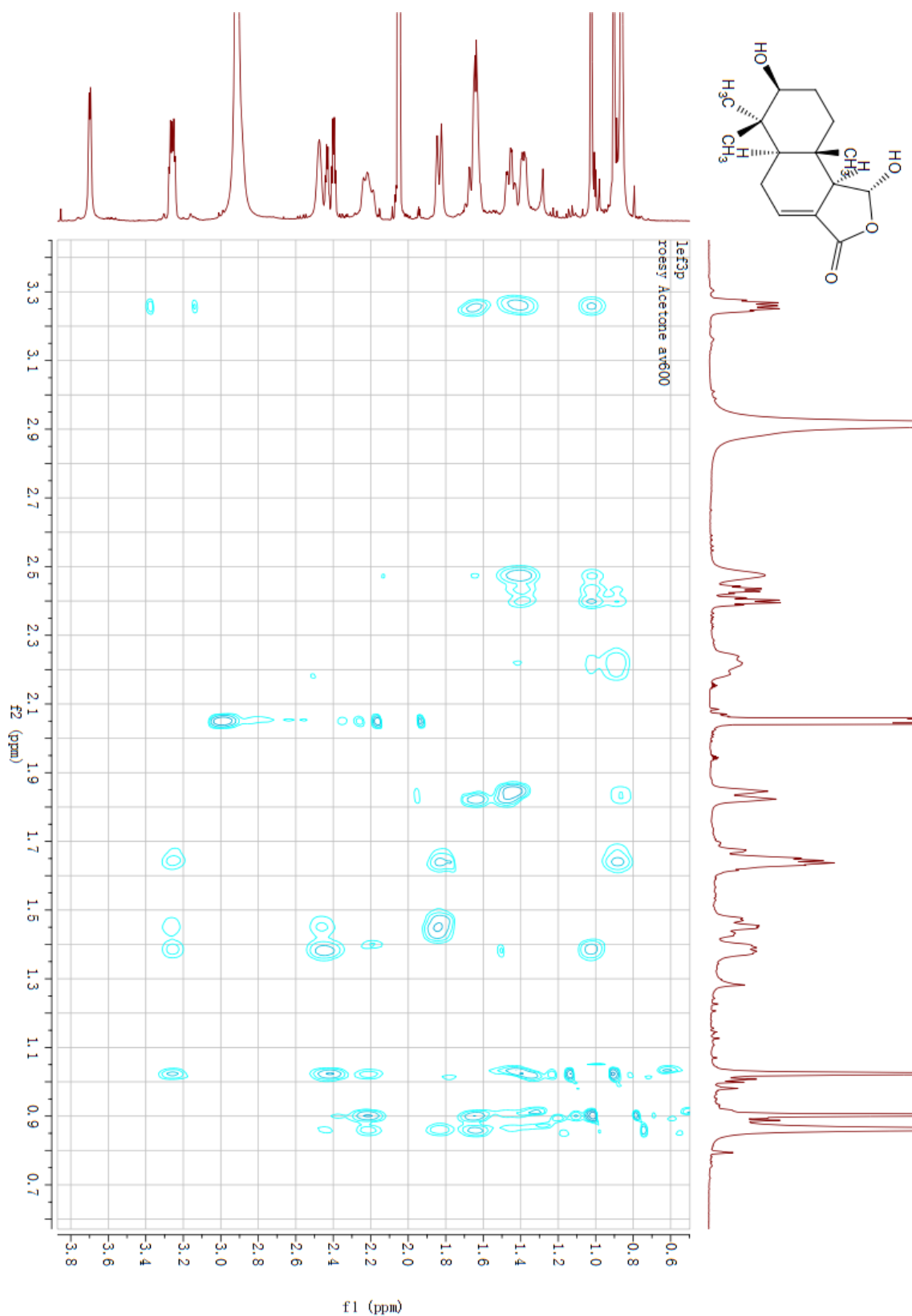
S11: HMBC Spectrum of 3β-OH-dendocarin A (**1**)



S12: Expansion of HMBC Spectrum of 3β-OH-dendocarin A (1)



S13: ROESY spectrum of 3β-OH-dendocarbin A (1)



S14: Expansion of ROESY spectrum of 3β-OH-dendocarin A (**1**)