

SUPPLEMENTARY DATA

Centaurea microcarpa Coss. & Dur (Asteraceae) extracts: New cyanogenic glucoside and other constituents

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Abstract

The phytochemical investigation of both chloroform and ethyl acetate extracts of *Centaurea microcarpa* Coss. & Dur. led to the isolation of a new cyanogenic glucoside 6'-methacrylate prunasin (**3**) together with seven known compounds: hydroxy-11 β ,13-dihydro onopordaldehyde (**1**), β -sitosterol (**2**), daucosterol (**4**), nepetin (**5**), prunasin (**6**), astragalin (**7**) and 7-*O*- β -D-glucopyranosyl centaureidin (**8**). Their structures were established by spectral analysis, mainly UV, IR, ESI-MS, 1D & 2D-NMR experiments (COSY, HSQC, HMBC and ROESY).

Keywords: *Centaurea microcarpa*, eudesmanolide, cyanogenic glucoside, sterol, flavonoids.

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Figure S11. Representative ROESY correlations for **3**

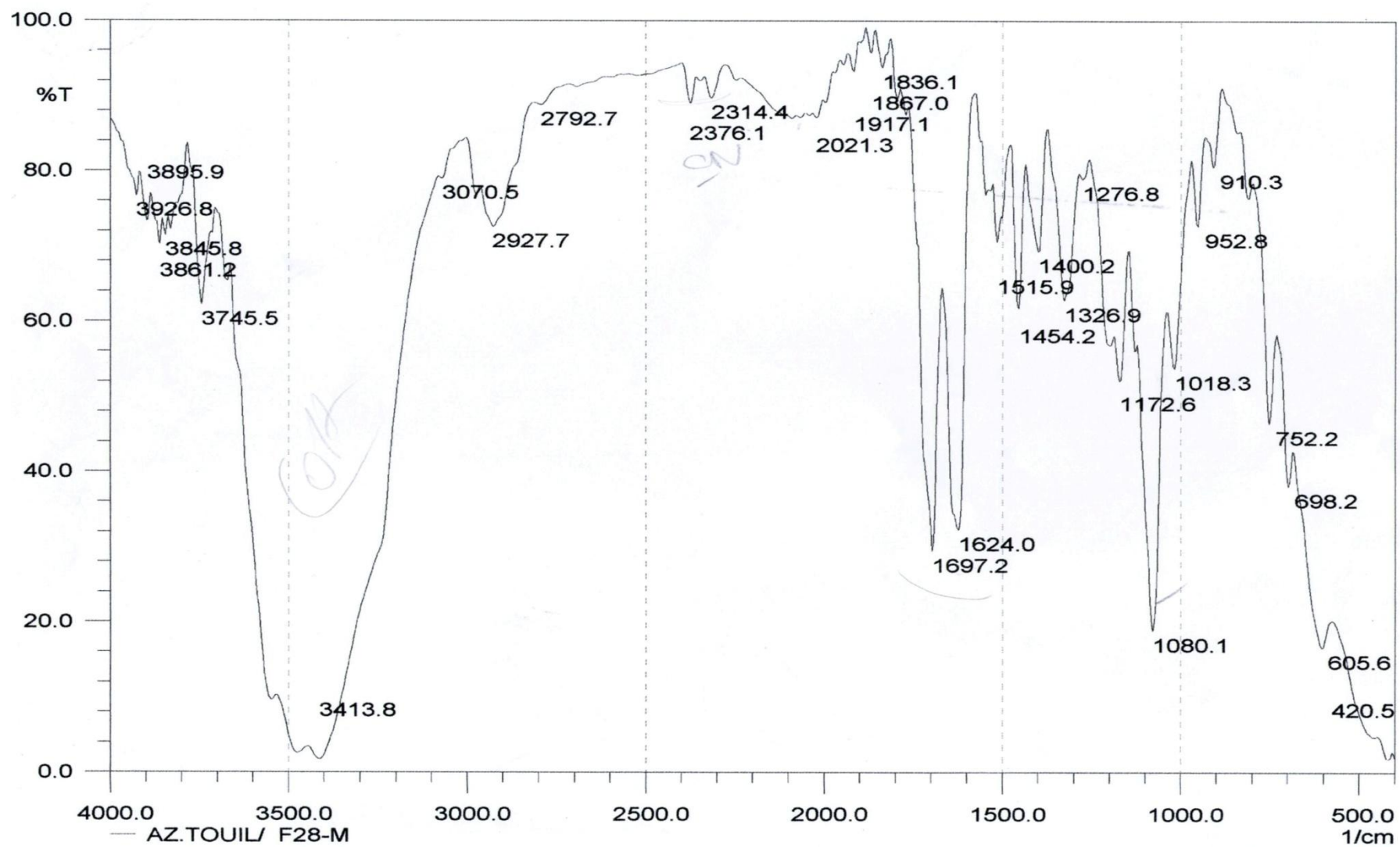


Figure S1. IR spectrum of compound 3

Elemental Composition Report

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Multiple Mass Analysis: 7 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1802 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)

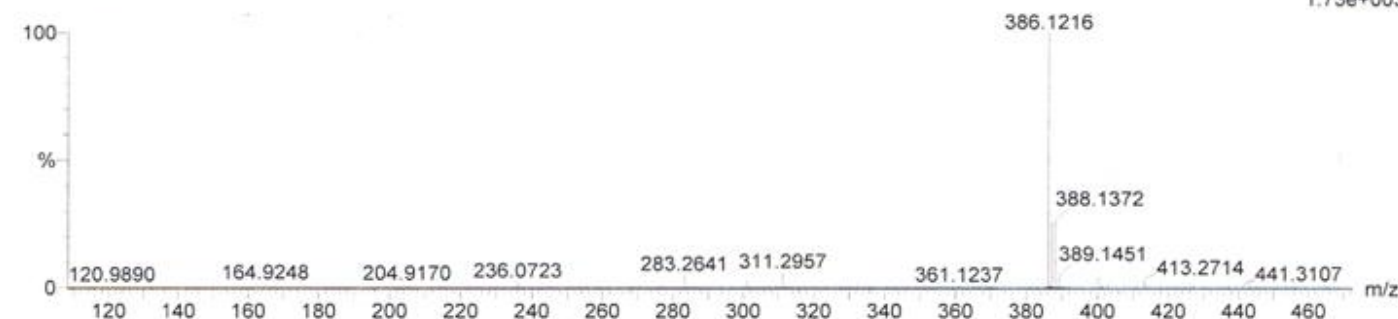
Elements Used:

C: 0-90 H: 0-120 N: 0-1 O: 0-25 Na: 0-1

Francisco Leon (FBJ)

13 (0.466)

2: TOF MS ES+
1.73e+003



Minimum:	4.00				0.0		
Maximum:	100.00		100.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
400.1425	4.46	---					
389.1451	4.63	389.1448	0.3	0.8	5.5	0.2	C17 H25 O10
388.1372	26.51	388.1372	0.0	0.0	7.5	1.3	C18 H23 N O7 Na
387.1253	25.73	387.1267	-1.4	-3.6	3.5	178.4	C15 H24 O10 Na
386.1216	100.00	386.1216	0.0	0.0	8.5	177.4	C18 H21 N O7 Na
311.2957	5.92	311.2950	0.7	2.2	1.5	3.0	C20 H39 O2
283.2641	4.93	283.2637	0.4	1.4	1.5	2.0	C18 H35 O2

Figure S2. HRESI-MS spectrum of compound 3

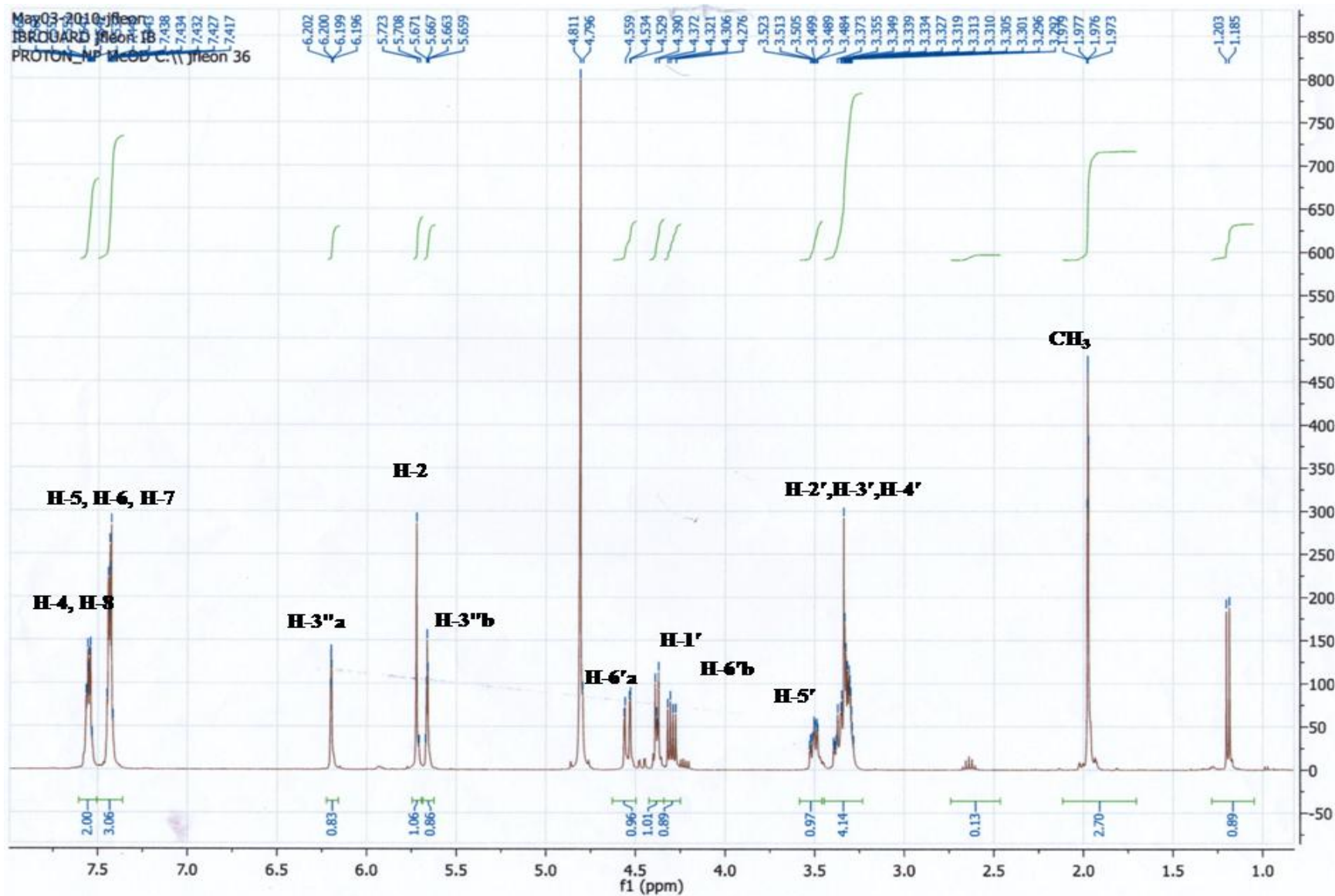


Figure S3. ¹H NMR of compound 3 in CD₃OD at 400 MHz

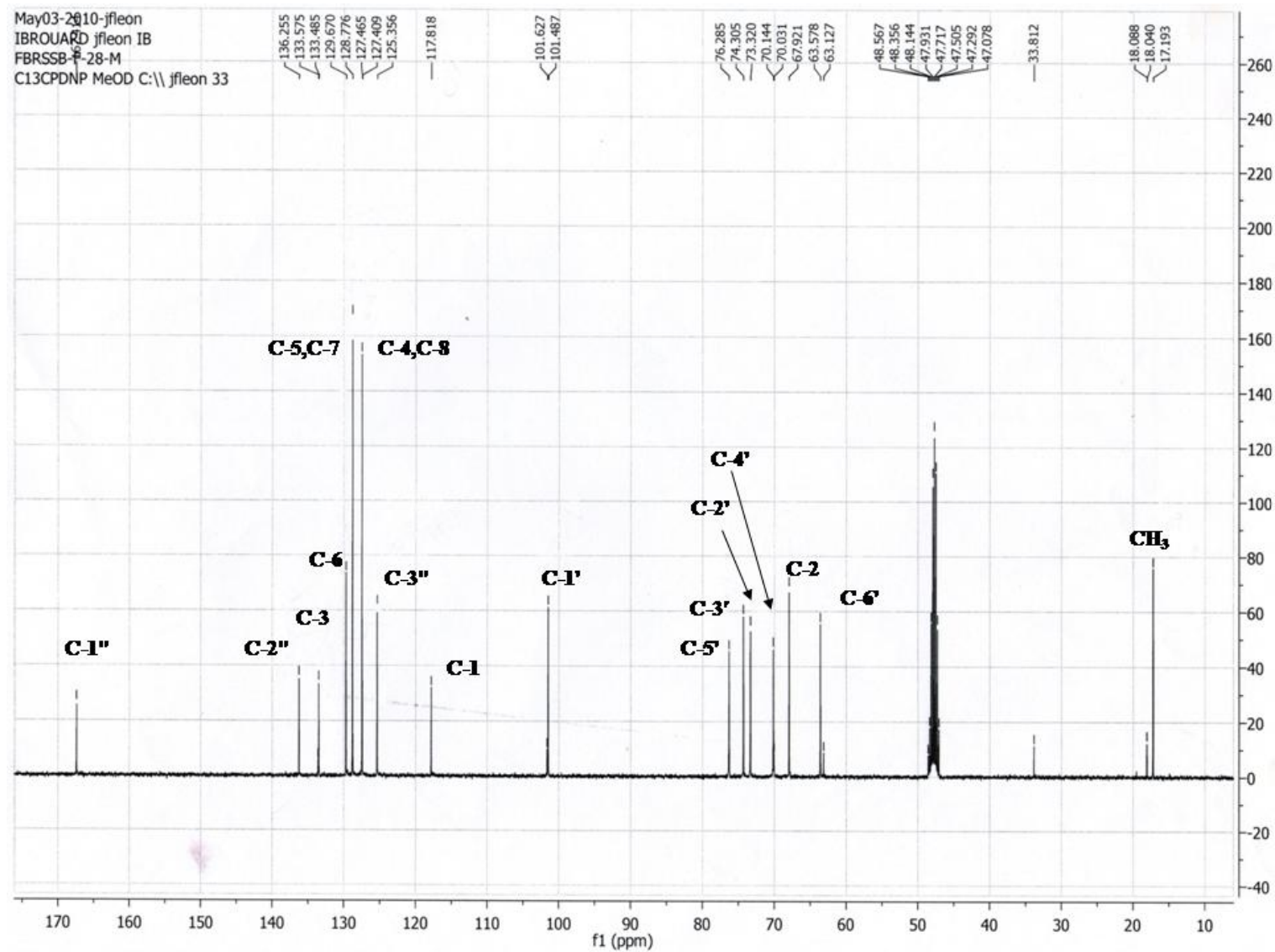


Figure S4. ^{13}C NMR of compound 3 in CD_3OD at 100 MHz

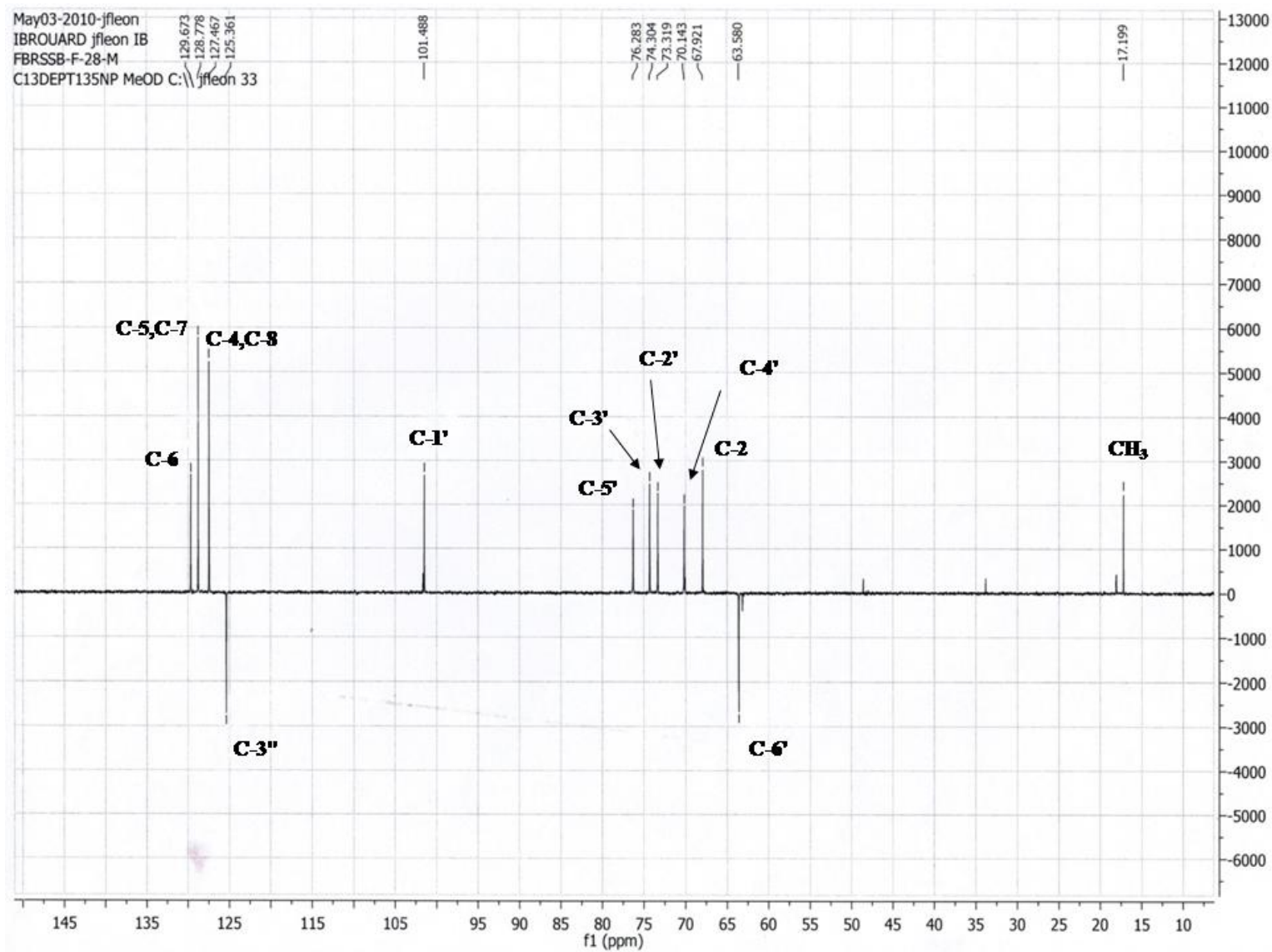


Figure S5.DEPT 135 of compound 3 in CD₃OD at 100 MHz

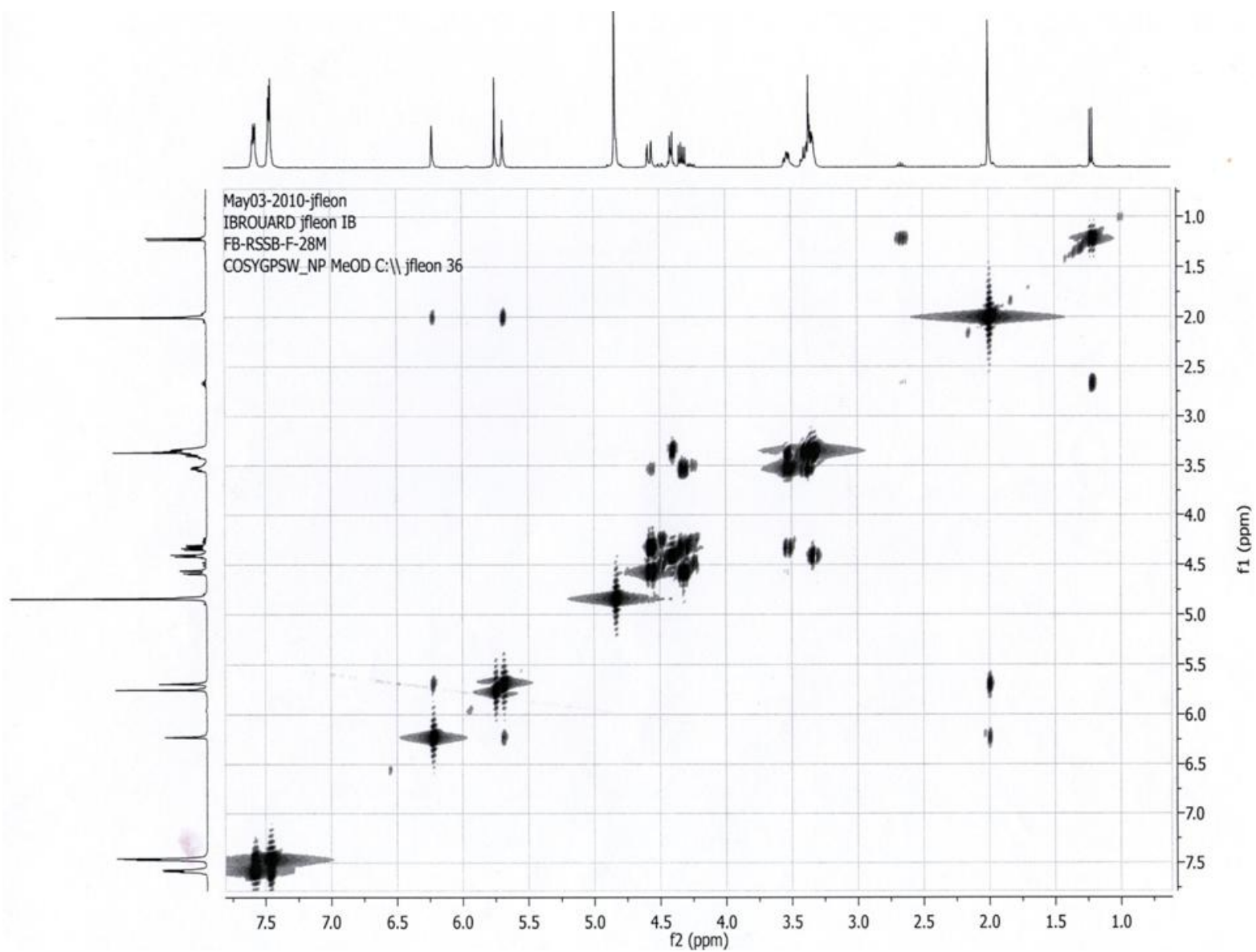


Figure S6. COSY of compound **3** in CD₃OD at 400 MHz

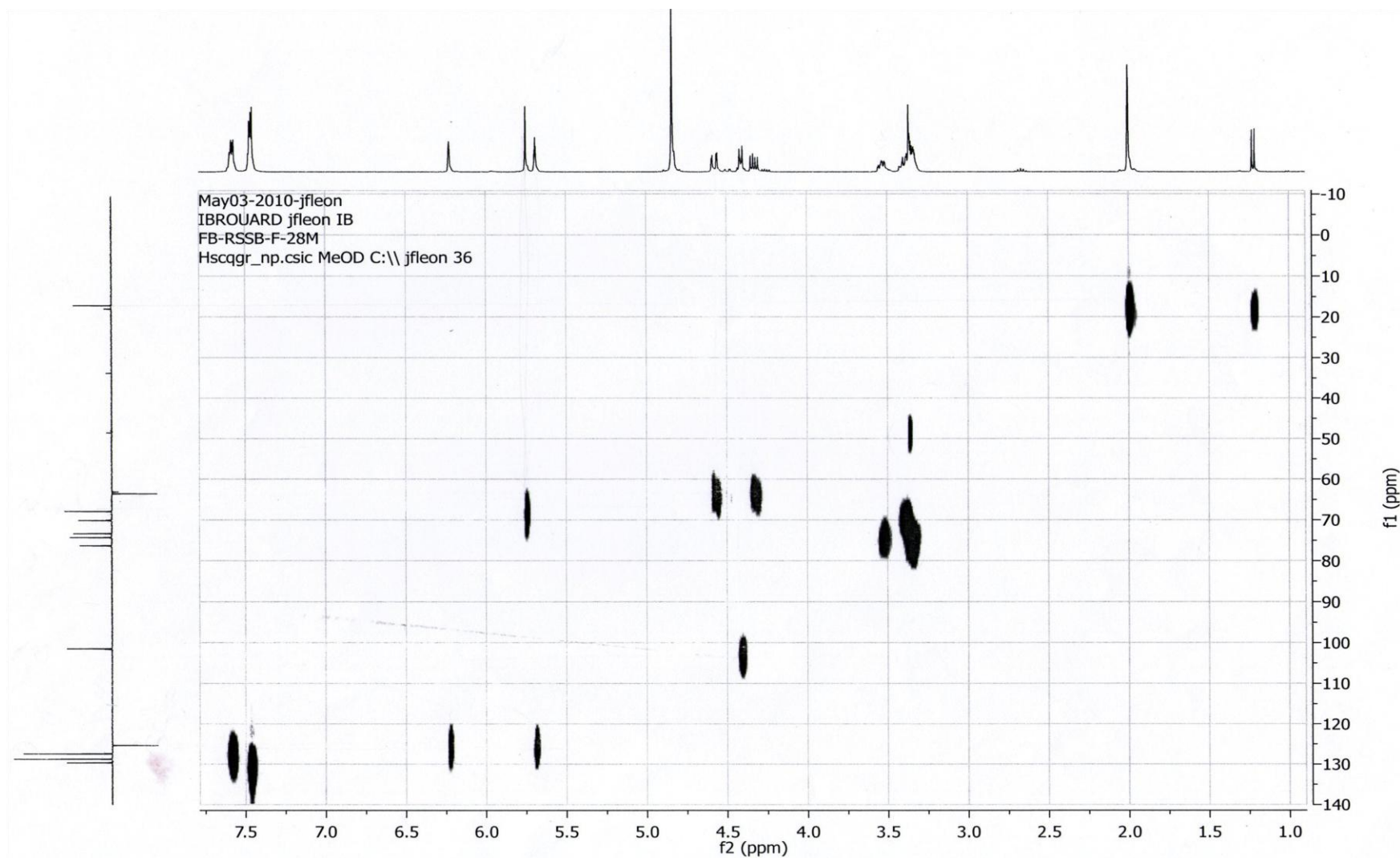


Figure S7. HSQC of compound **3** in CD₃OD at 400 MHz

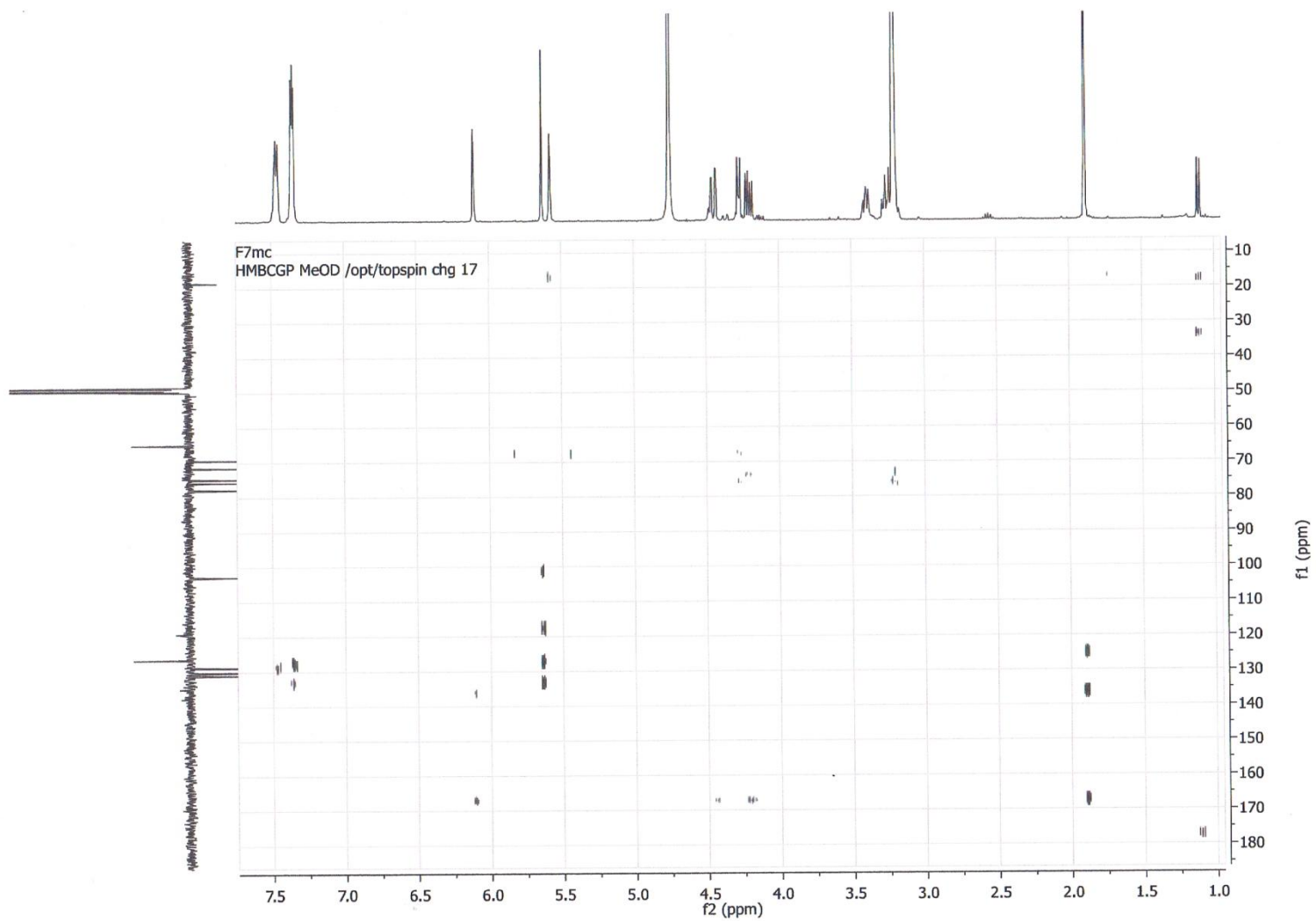


Figure S8. HMBC of compound **3** in CD₃OD at 400 MHz

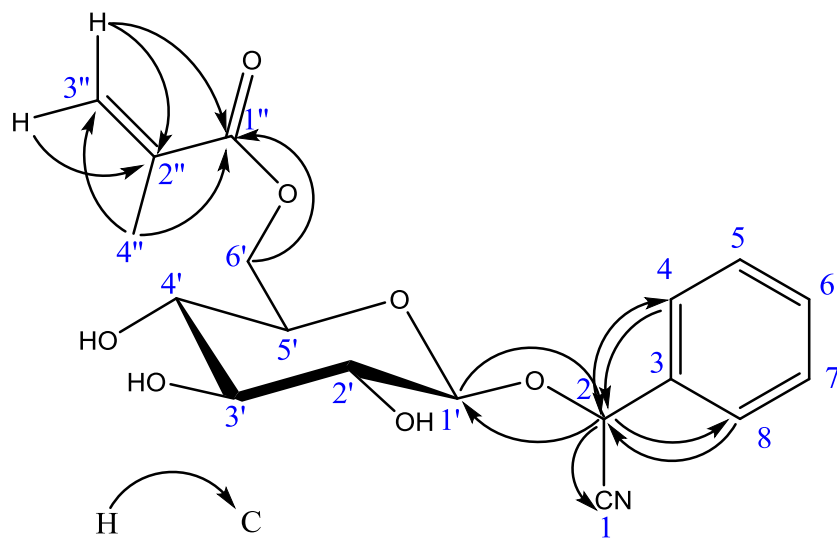


Figure S9. Representative HMBC correlations for **3**

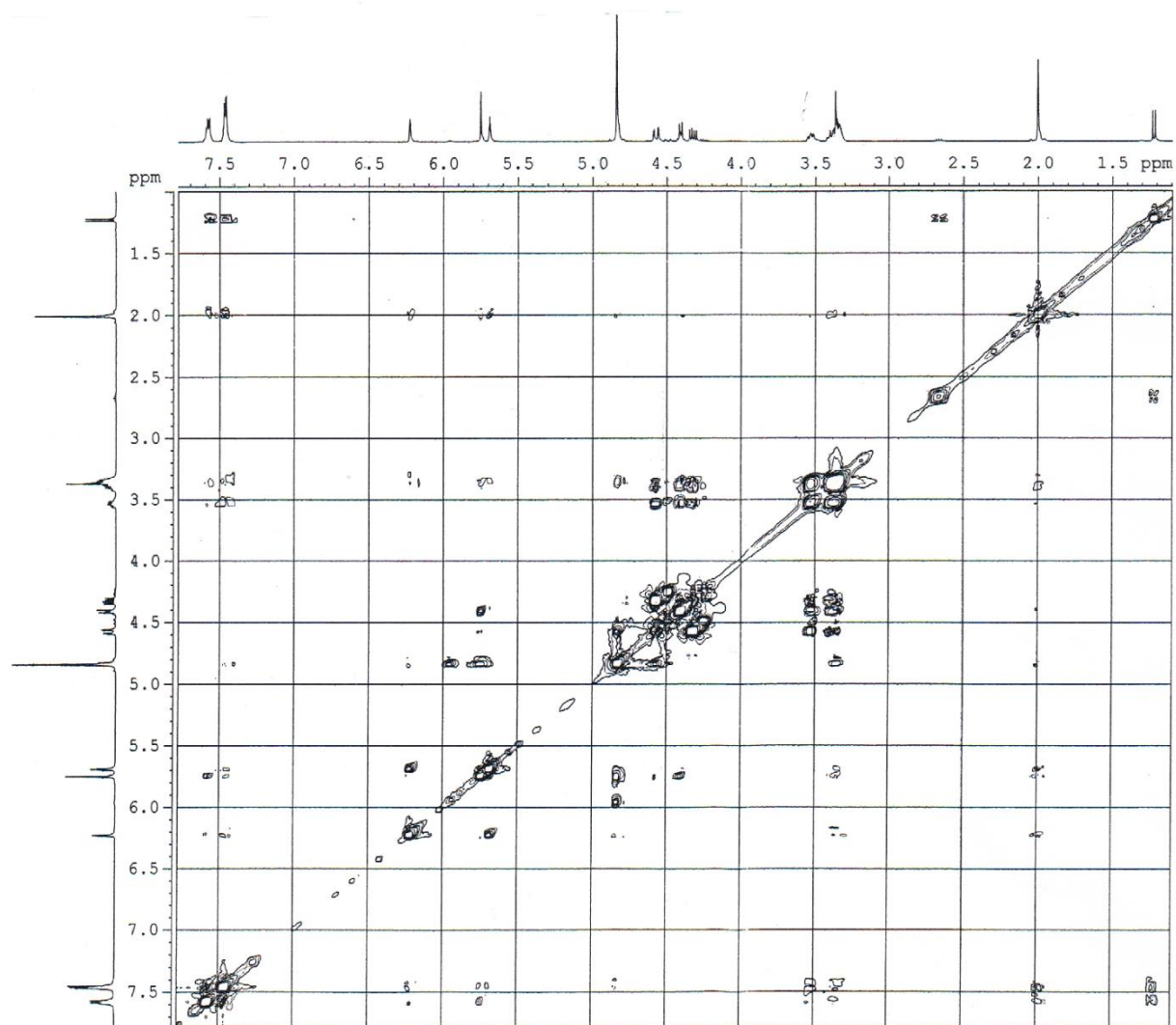


Figure S10. ROESY of compound **3** in CD₃OD at 400MHz

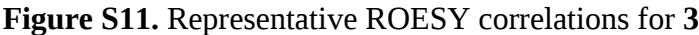


Figure S11. Representative ROESY correlations for **3**