

Coumarinolignoid and Indole Alkaloids from the Roots of the Hybrid Plant *Citrus x paradisi* Macfad. (Rutaceae)

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Abstract: Phytochemical investigation of the roots of *Citrus x paradisi* Macfad. (Rutaceae) led to the isolation of two new compounds, namely 1-formyl-5-hydroxy-*N*-methylindolin-1-ium (1) and decyloxycleomiscosin D (2), along with ten known compounds 1,1-dimethylpyrrolidin-1-ium-2-carboxylate (3), furan-2,3-diol (4), 5-methoxyseselin (5), umbelliferone (6), scopoletin (7), citracridone I (8), citracridone II (9), citracridone III (10), limonin (11) and lupeol (12). Structures were determined by comprehensive spectroscopic analysis of 1D and 2D NMR and EI- and ESI-MS as well as comparison with published data. Notably, compounds 3 and 4 are reported here from the genus *Citrus* for the first time. In addition, the MeOH extract of the roots and compounds 1 - 7 were screened against the human adenocarcinoma alveolar basal epithelial cell line A549 and the Caucasian prostate adenocarcinoma cell line PC3 using the MTT assay. While the extract showed significant activity with IC₅₀ values of 35.2 and 38.1 µg/mL, respectively, compounds 1 - 7 gave weak activity with IC₅₀ values of 99.2 to 250.2 µM and 99.5 to 192.7 µM, respectively.

Keywords: *Citrus x paradisi*; coumarinolignoid; indole alkaloids; chemotaxonomy; cytotoxicity

COMPOUND 1

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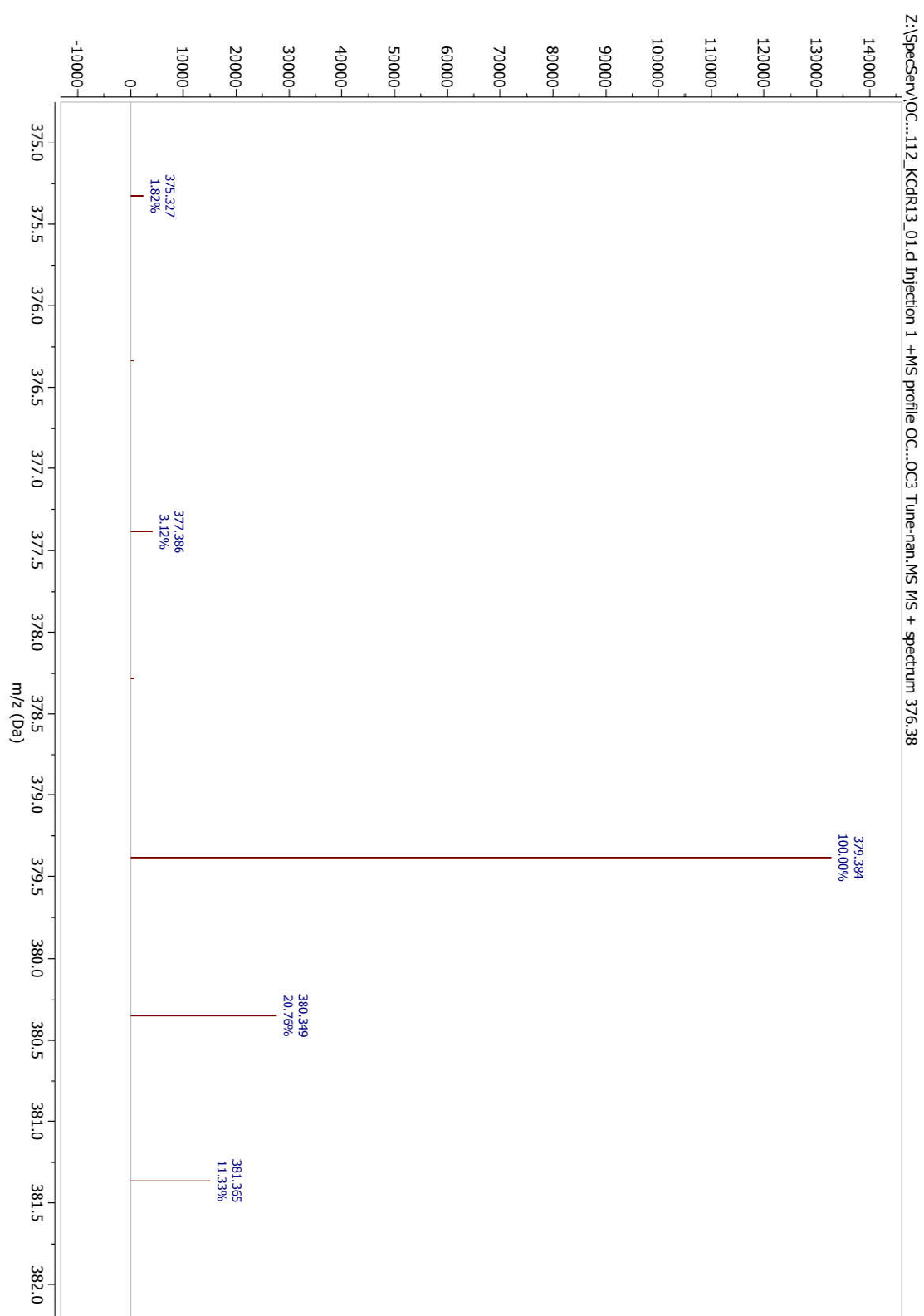
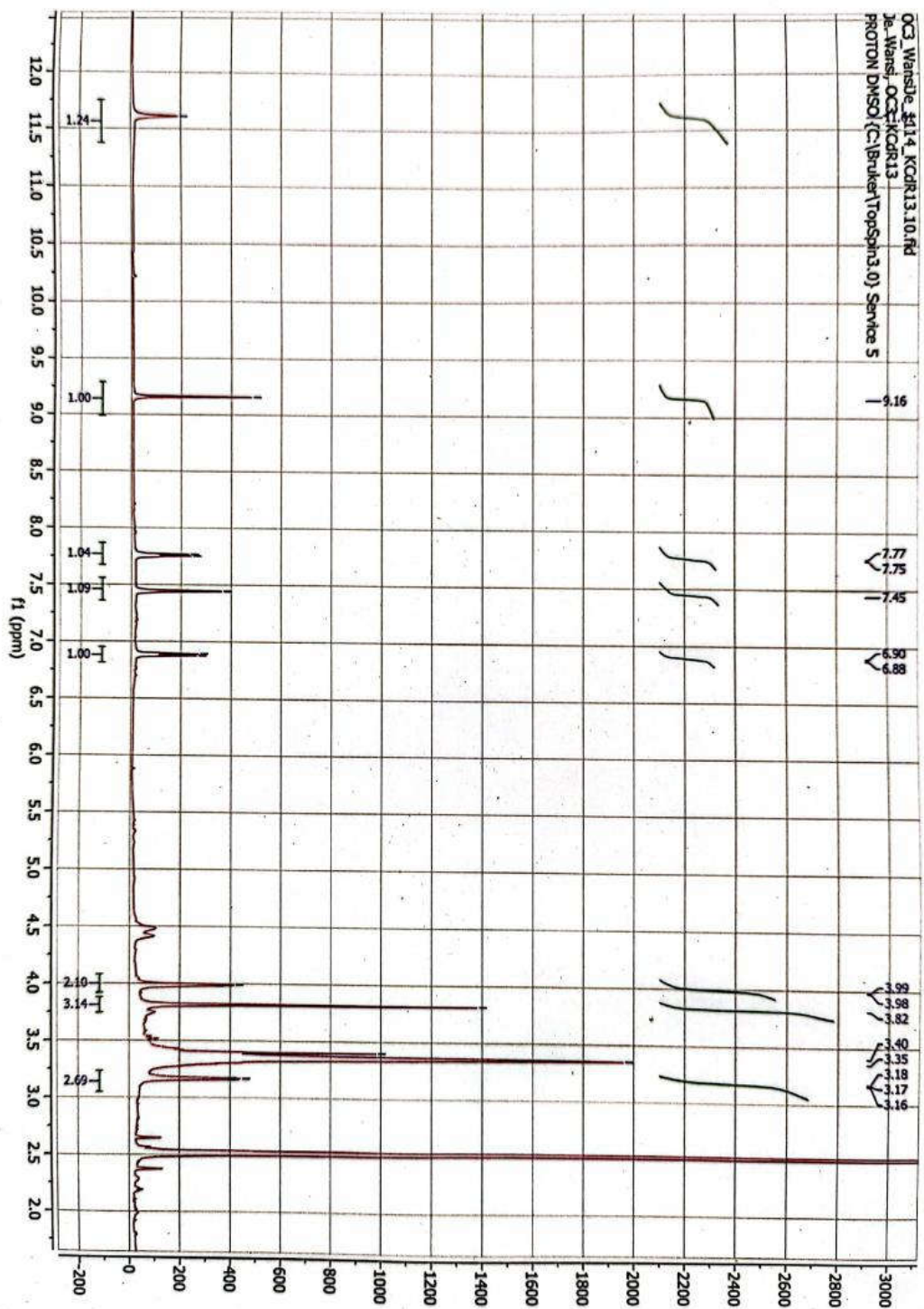


Figure S1: ESIMS of 1



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Figure S2: ^1H NMR of 1

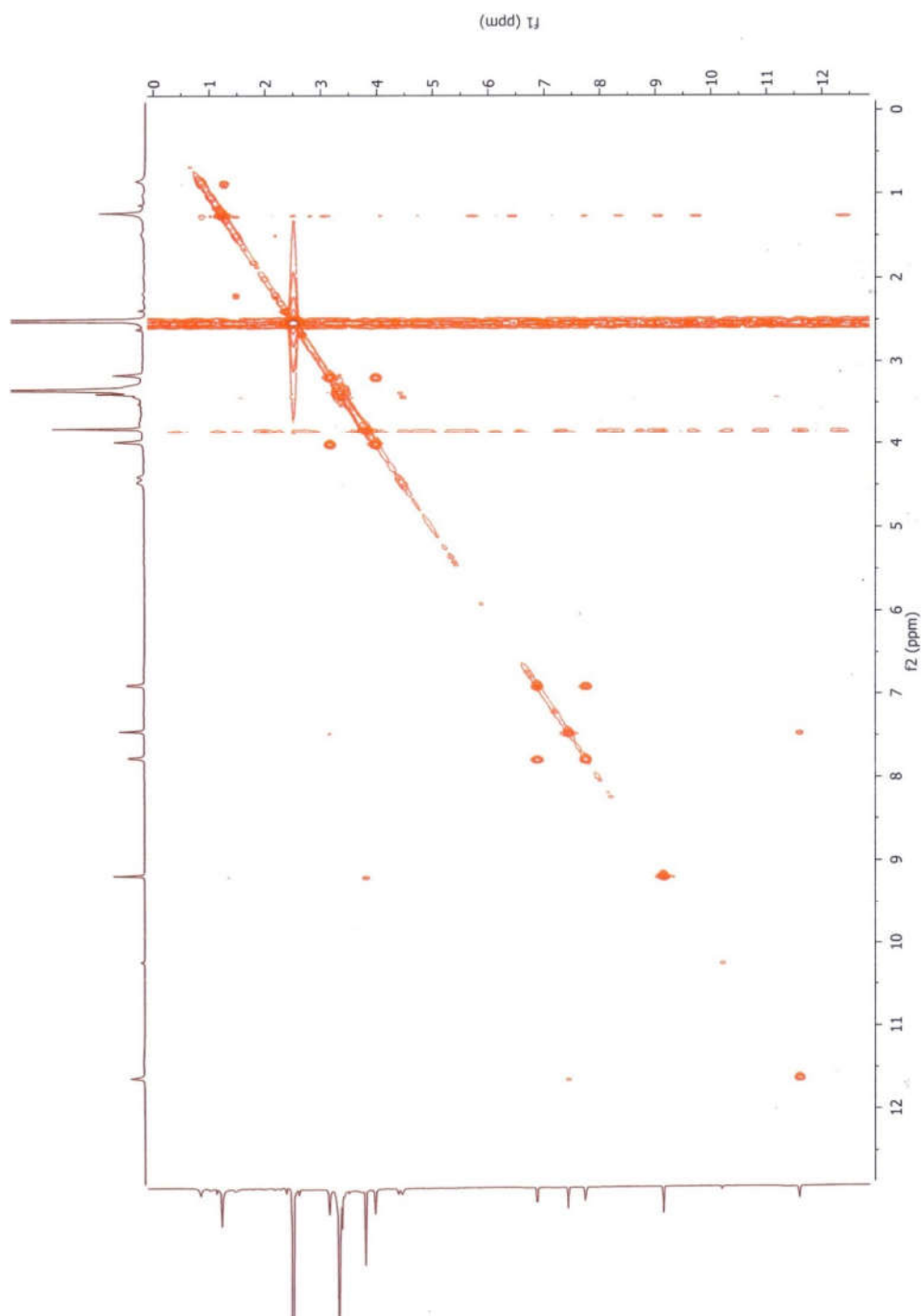


Figure S3: COSY of 1

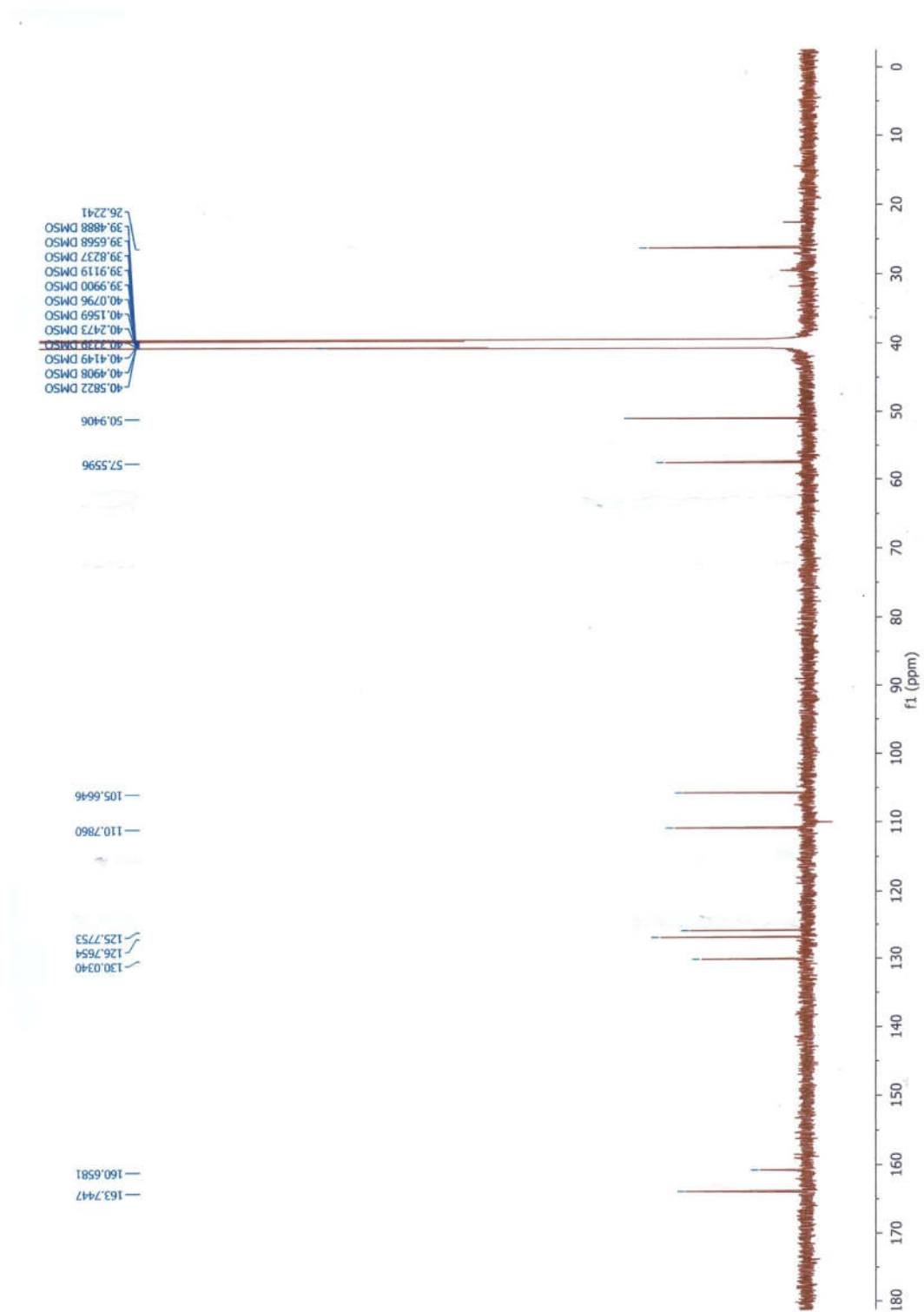


Figure S4: ¹³C-NMR of 1

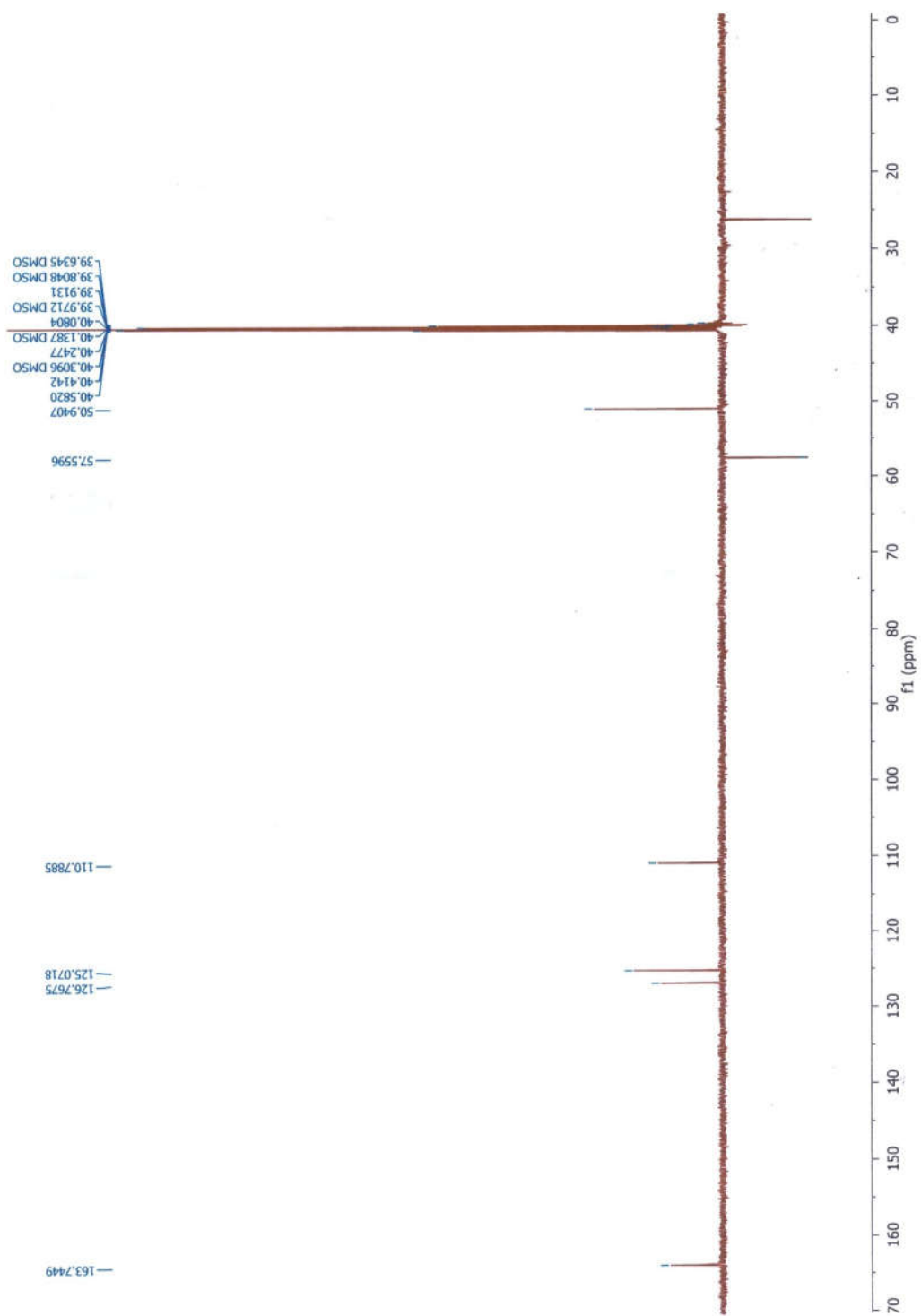


Figure S5: DEPT of 1

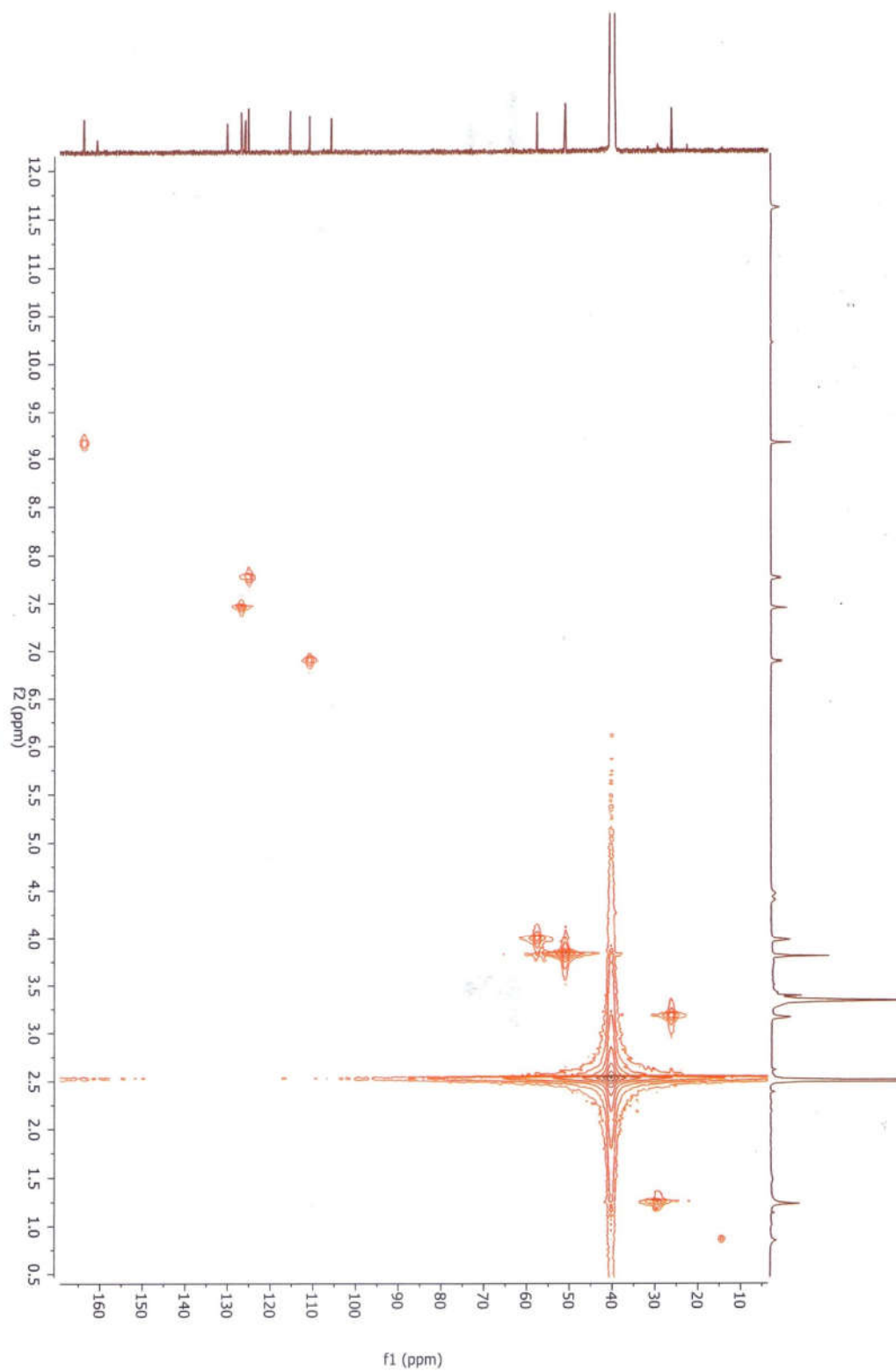


Figure S6: HSQC of 1

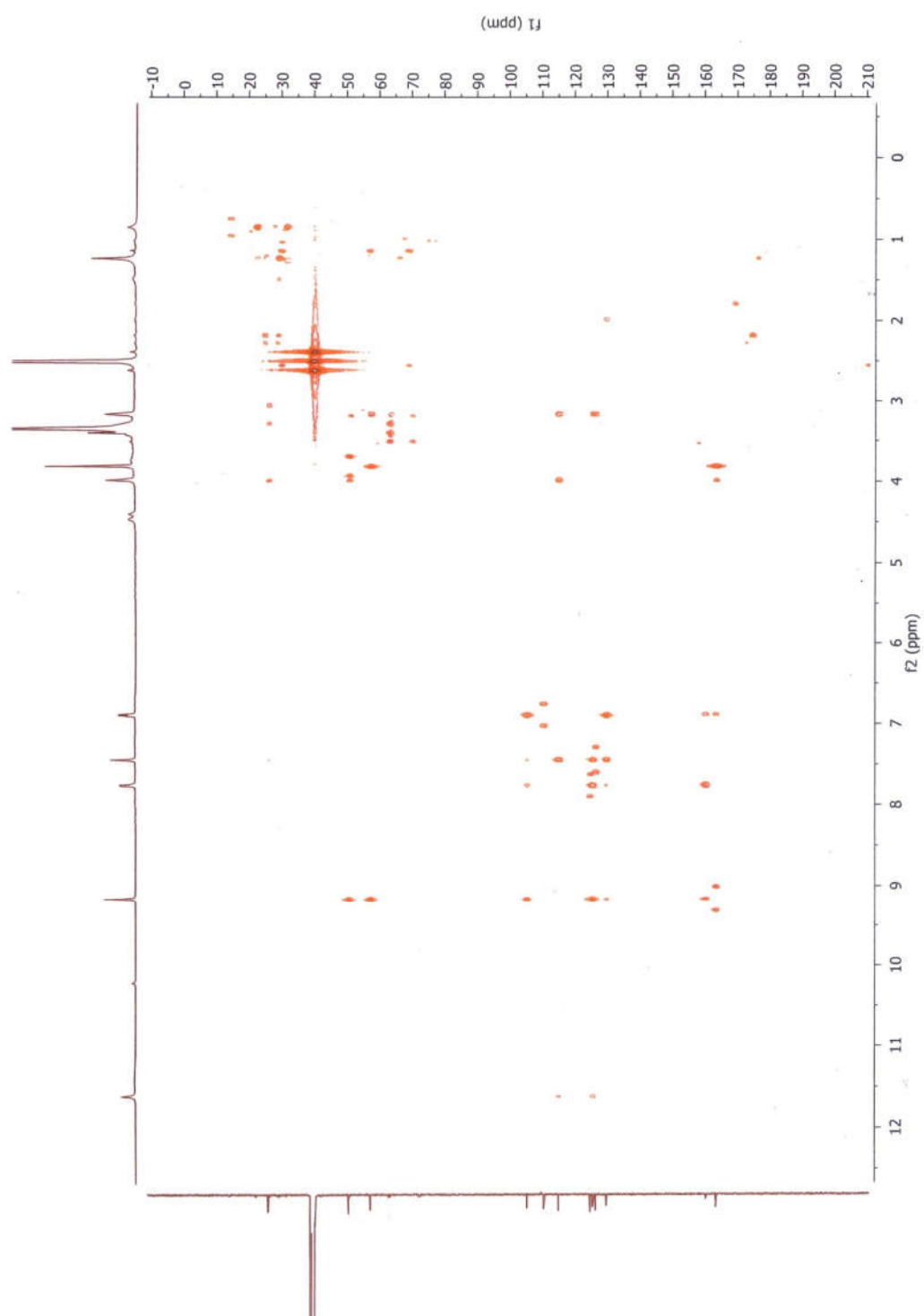


Figure S7: HMBC of 1

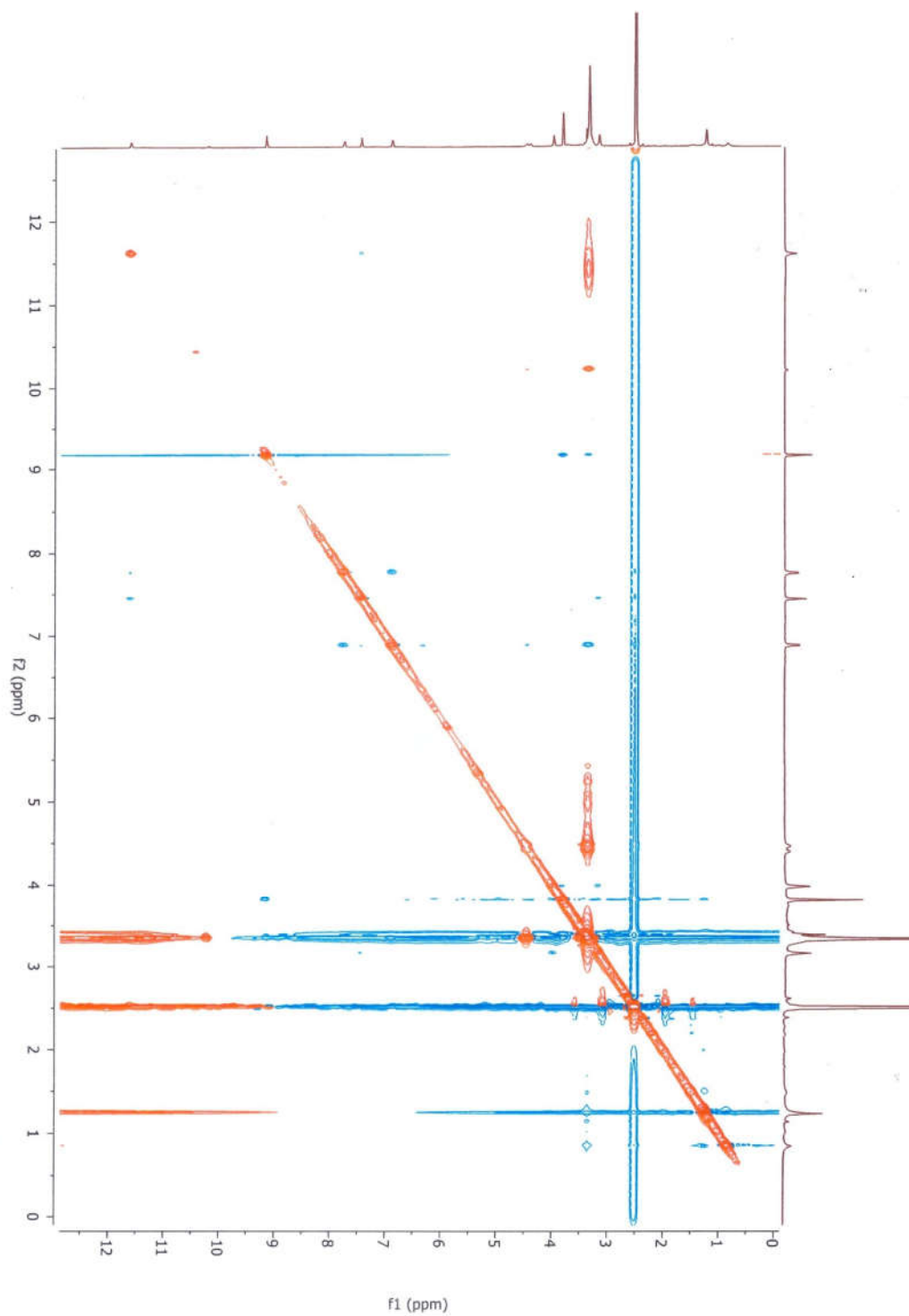
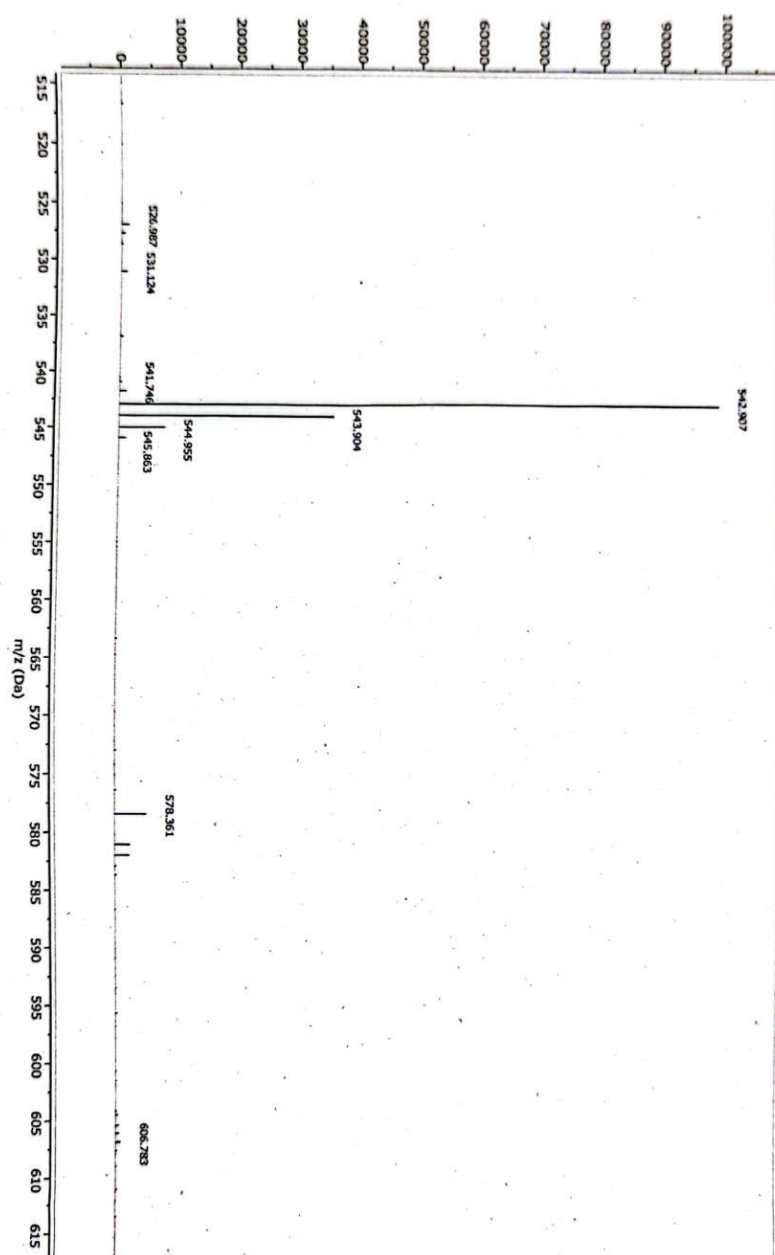


Figure S8: NOESY of 1

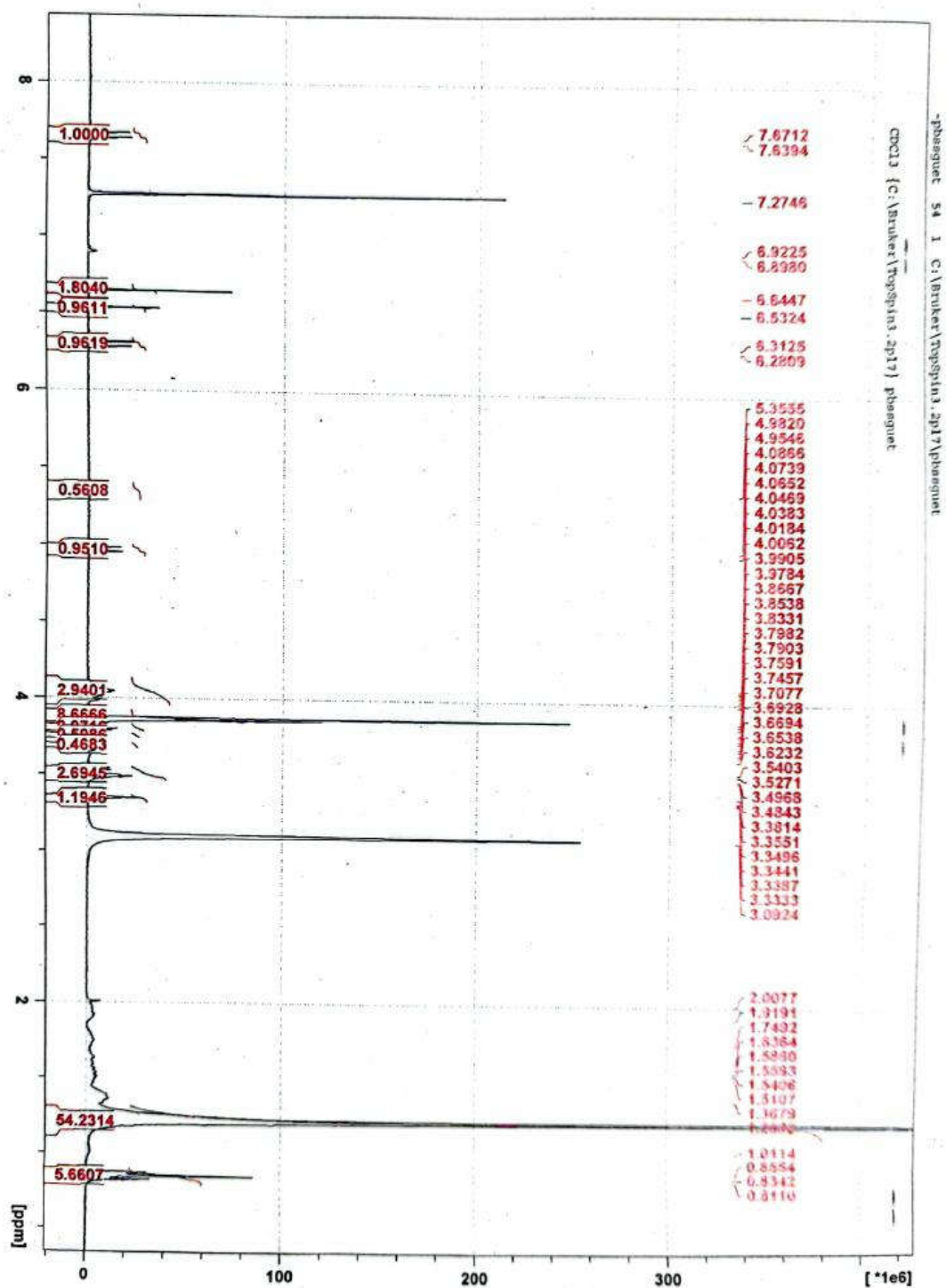
COMPOUND 2

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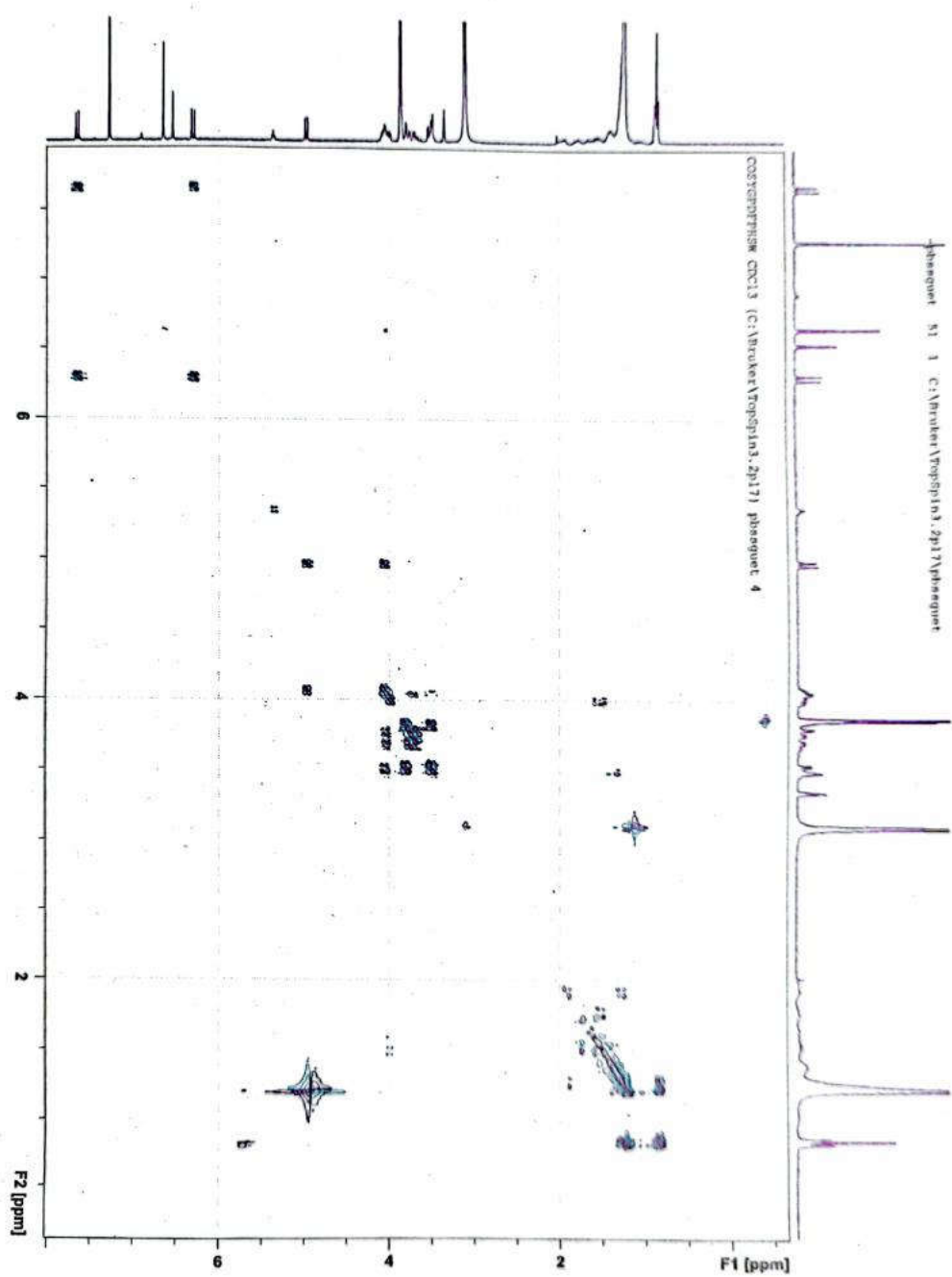
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Figure S9: ESIMS of 2



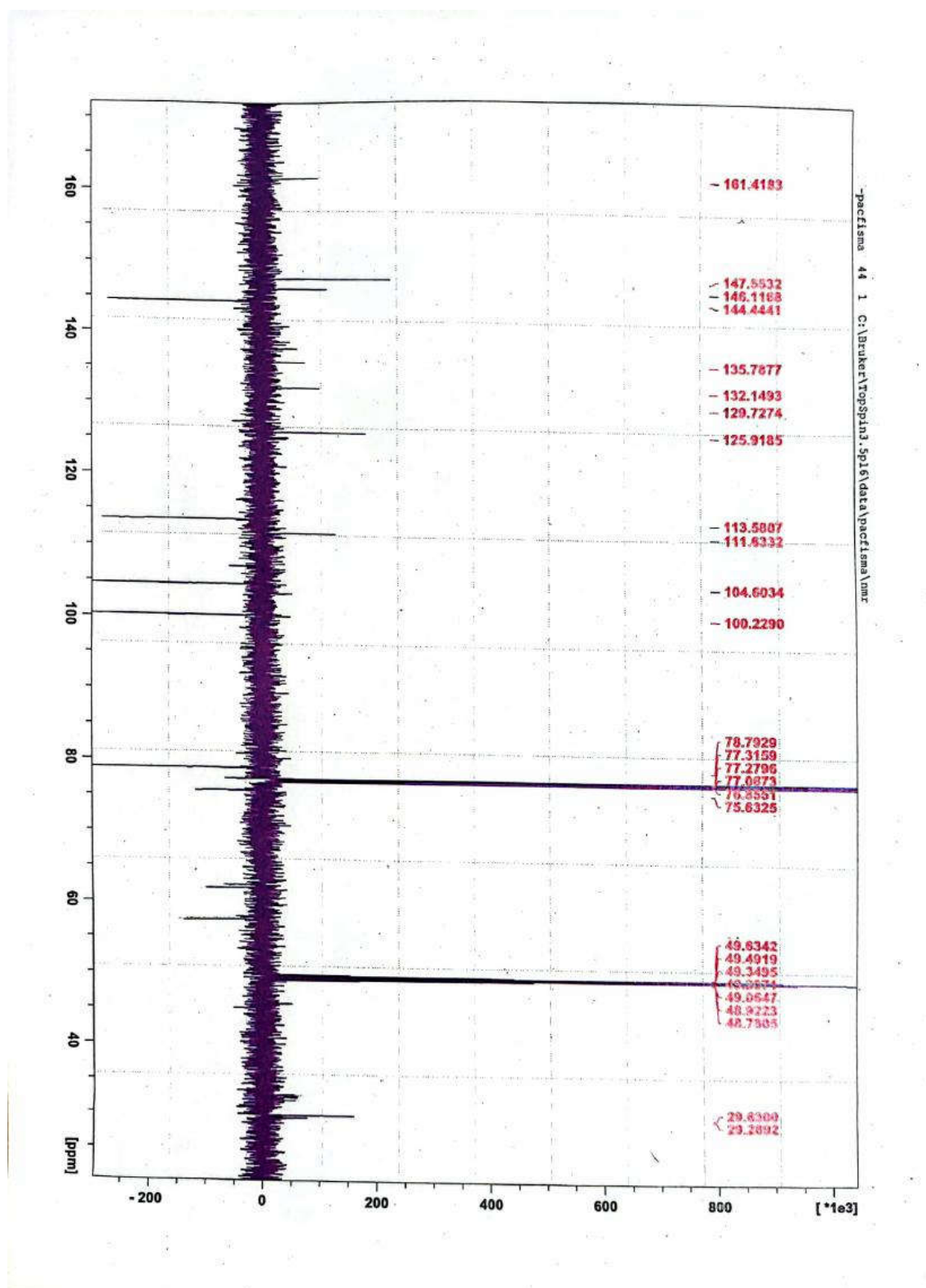
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Figure S10: ^1H NMR of 2



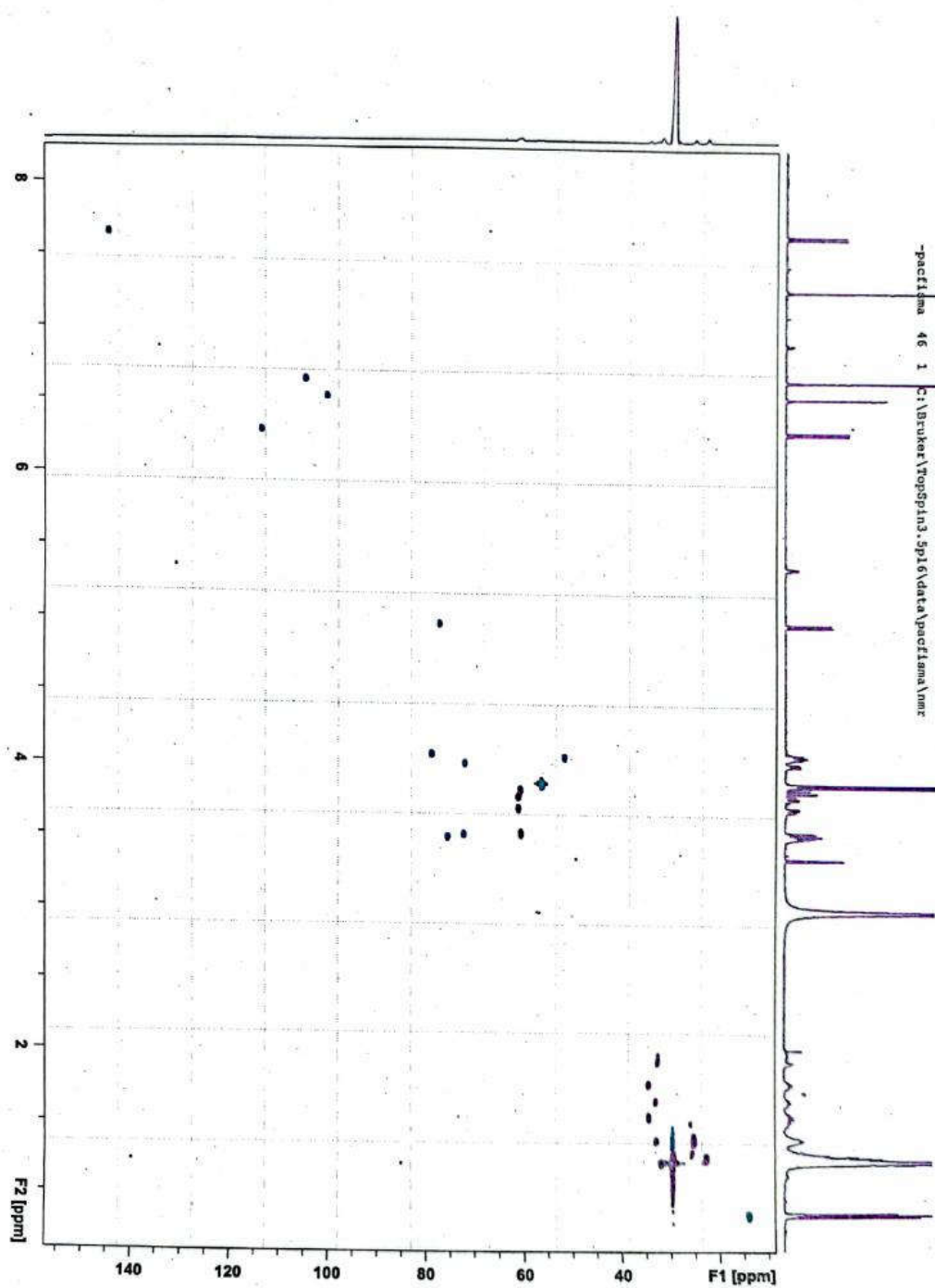
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Figure S11: COSY of 2



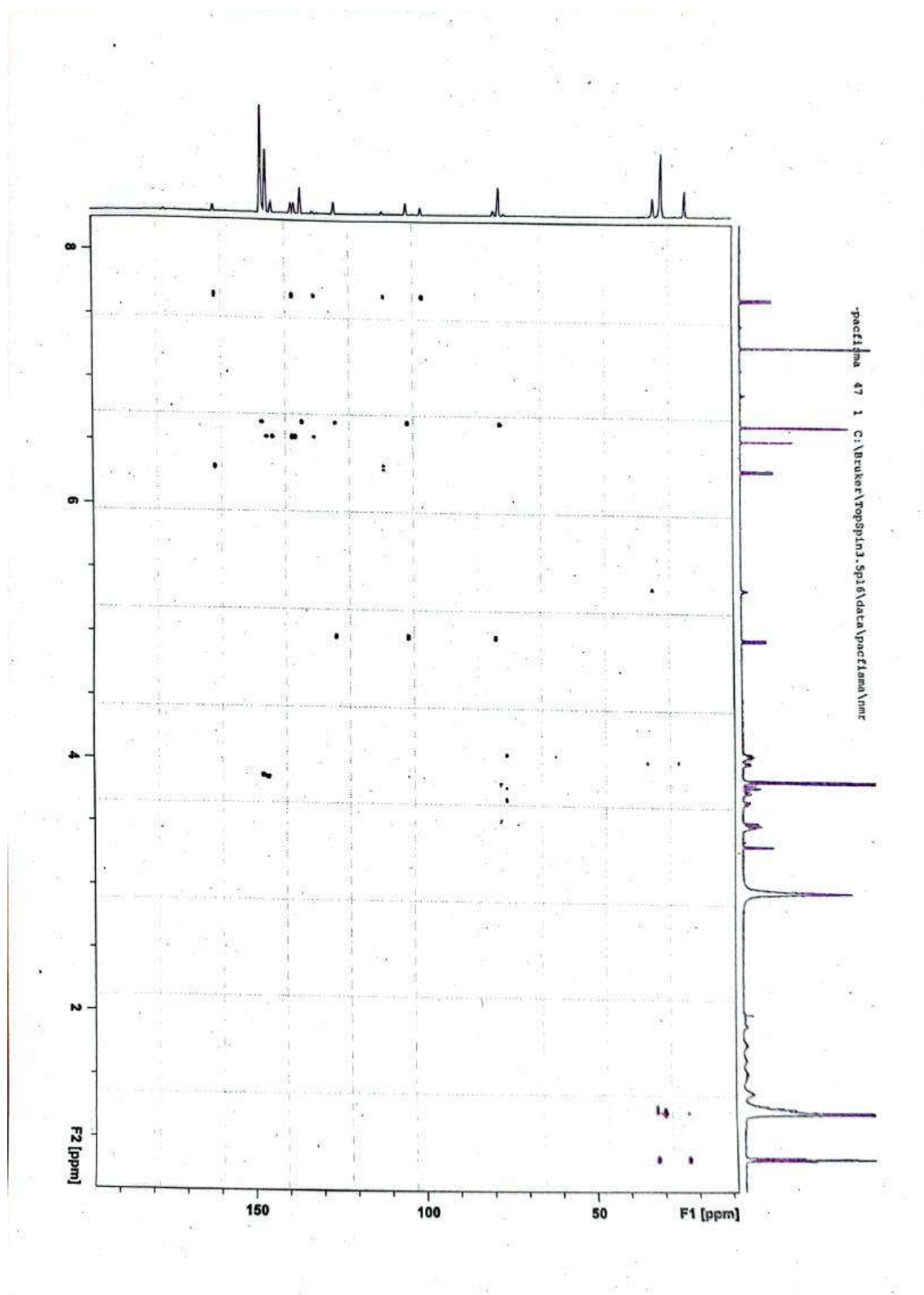
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Figure S13: ^{13}C (J.mod) of 2



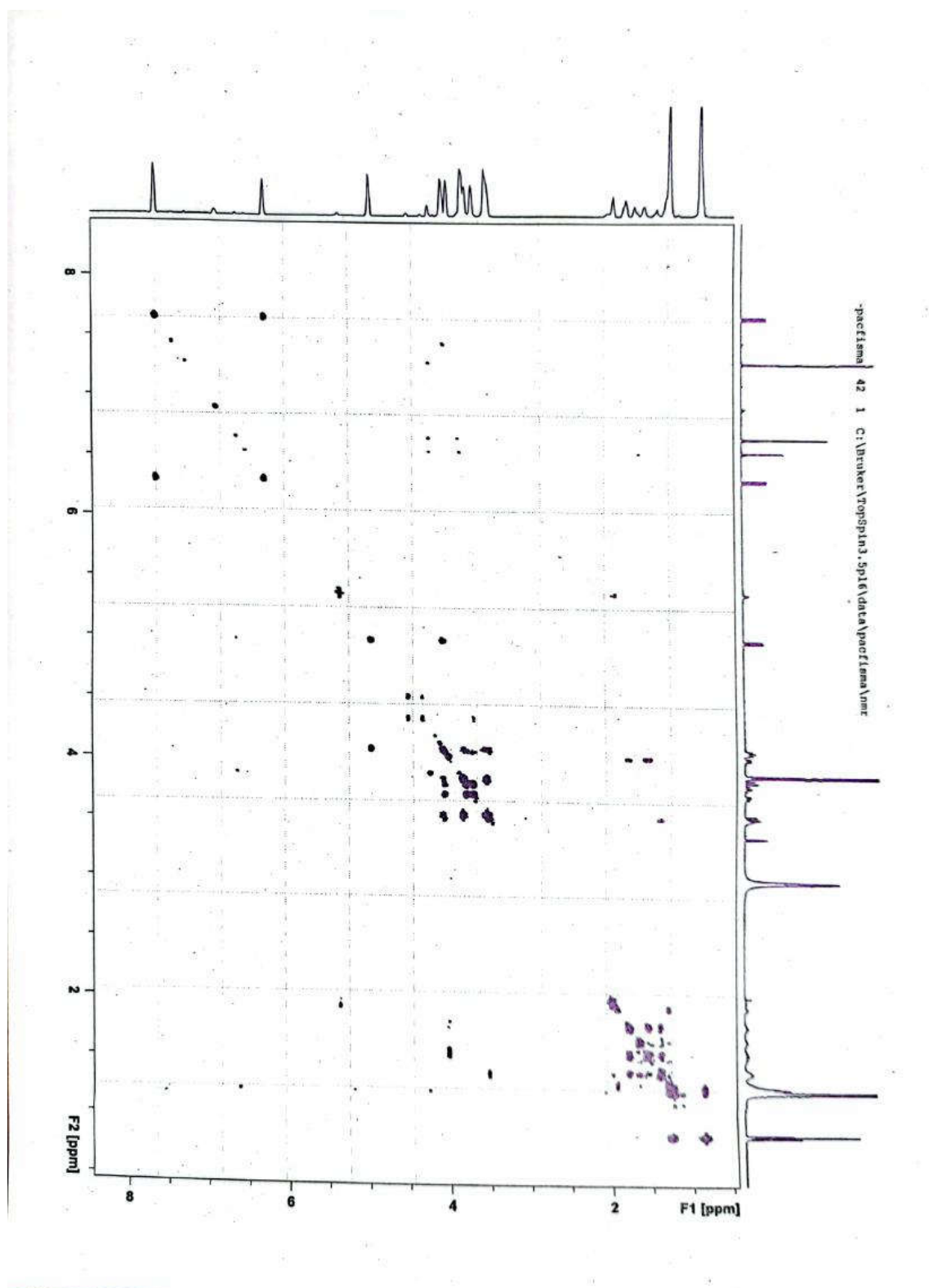
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Figure S15: HSQC of 2



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Figure S15: HMBC of 2



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Figure S16: NOESY of 2

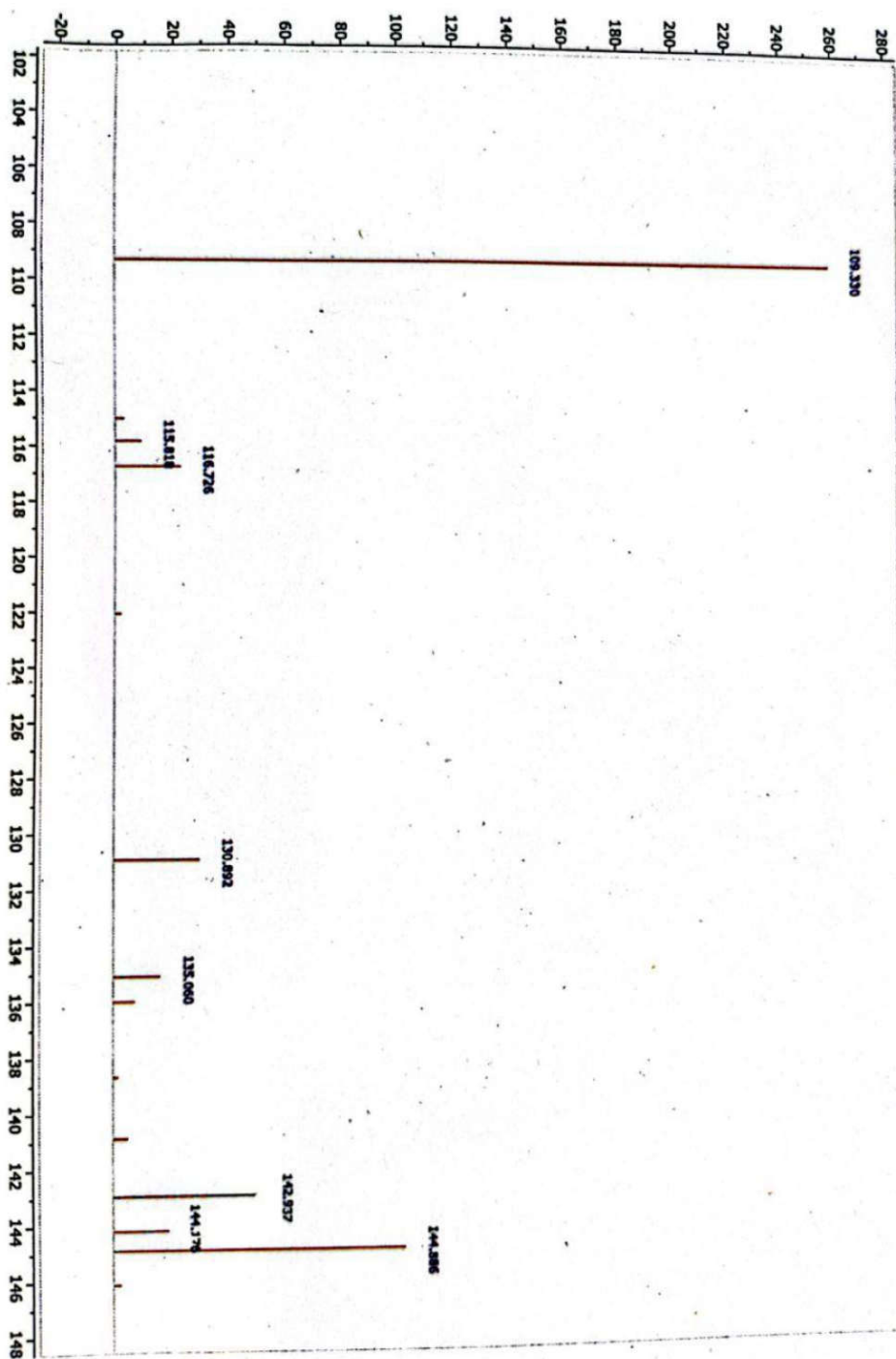


Figure S17: EIMS of nonanol

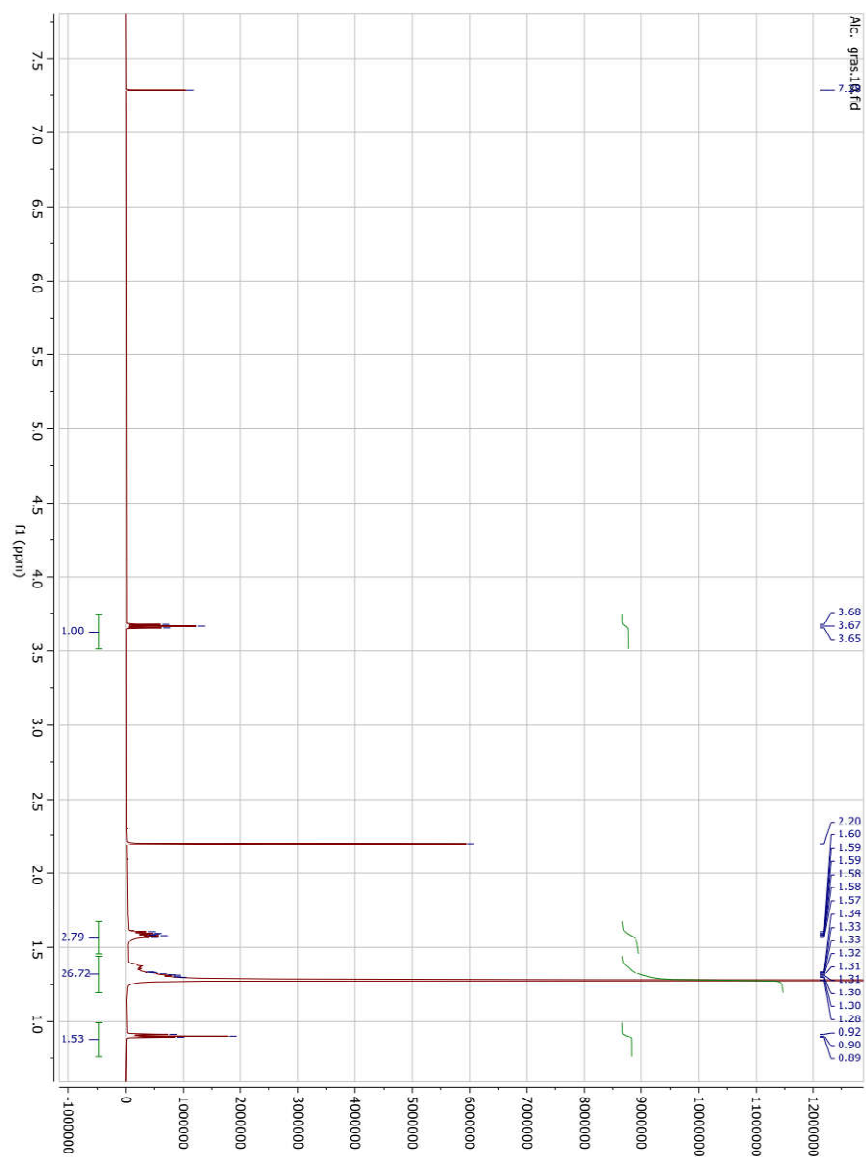


Figure S18: ^1H NMR of nonanol