antioxidants

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Supplementary material

Article

Exploring the Anti-Inflammatory and Antioxidant Potential, Metabolite Composition and Inorganic Profile of *Cistus monspeliensis* L. Aerial Parts and Roots

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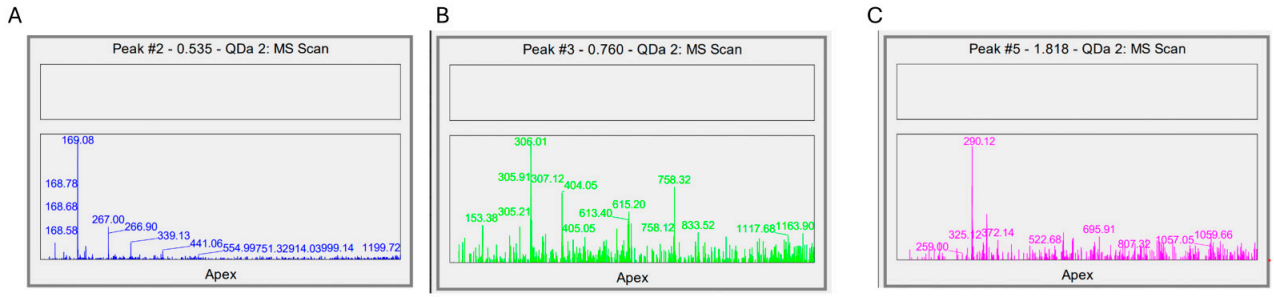

Figure S1. UHPLC-MS analysis of R. Mass spectra in negative ion mode -QDa 2- A) Mass spectrum at retention time 0.535 min interpreted as gallic acid (exact mass 170.12 Da) which gave m/z value 169.08 [M-H]. **B)** Mass spectrum at retention time 0.760 min interpreted as gallocatechin or epigallocatechin (exact mass 306.267 Da) which gave m/z value 306.01 [$M^{\cdot+}$].**C)** Mass spectrum at retention time 1.818 min interpreted as catechin or epicatechin (exact mass 290.26 Da) which gave m/z value 290.12 [$M^{\cdot+}$].

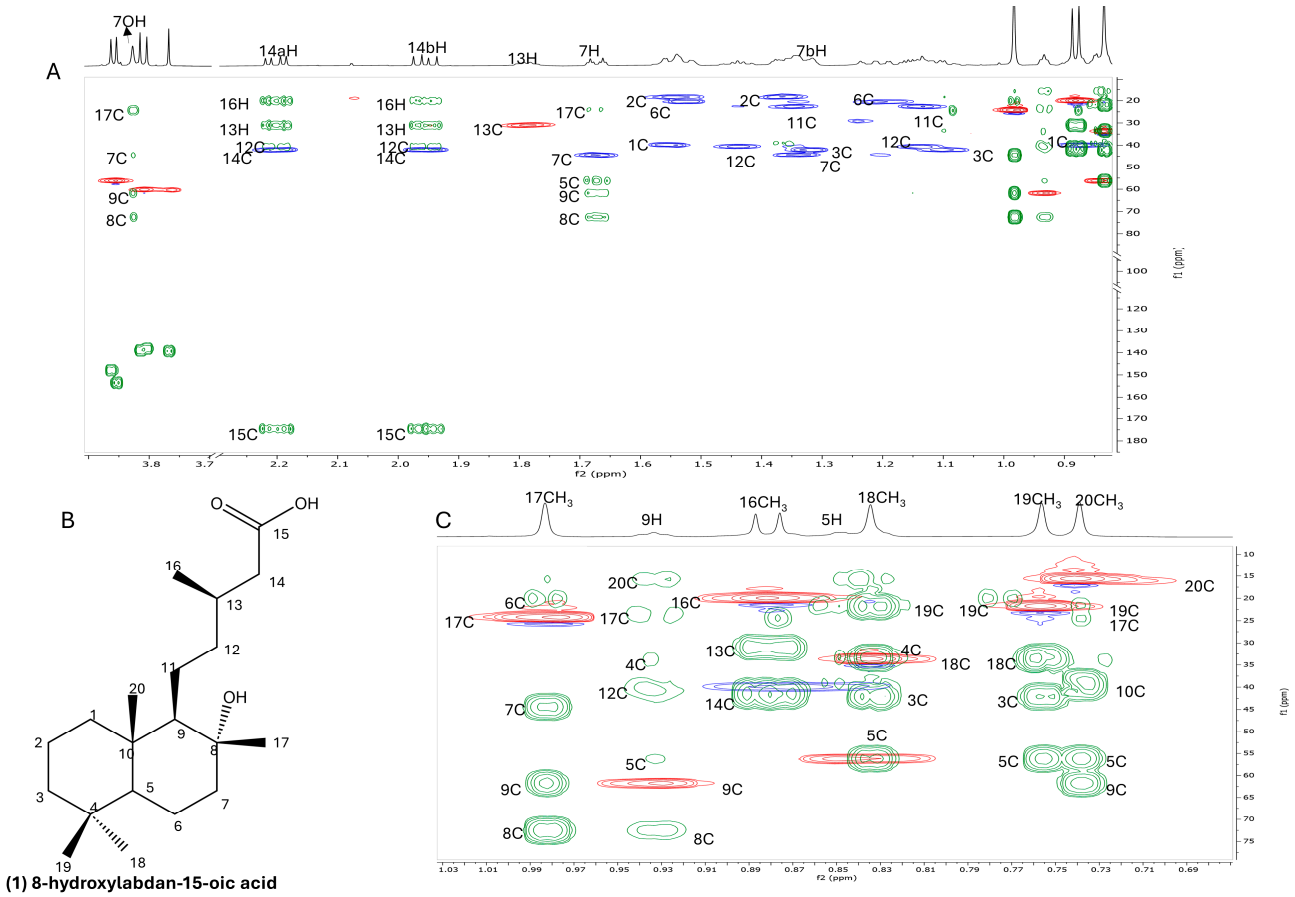

Figure S2. NMR-based structural elucidation of 8-hydroxylabdan-15-oic acid A) Superimposed HSQC and HMBC spectra of APCl subfraction 8 from which the compound was characterized (green dots = HMBC correlations; bule and red = HSQC correlations). **B)** Structure of the compound **C)** Spectral range between δ 0.60 - 1.03 highlighting the signals of the methyl groups.

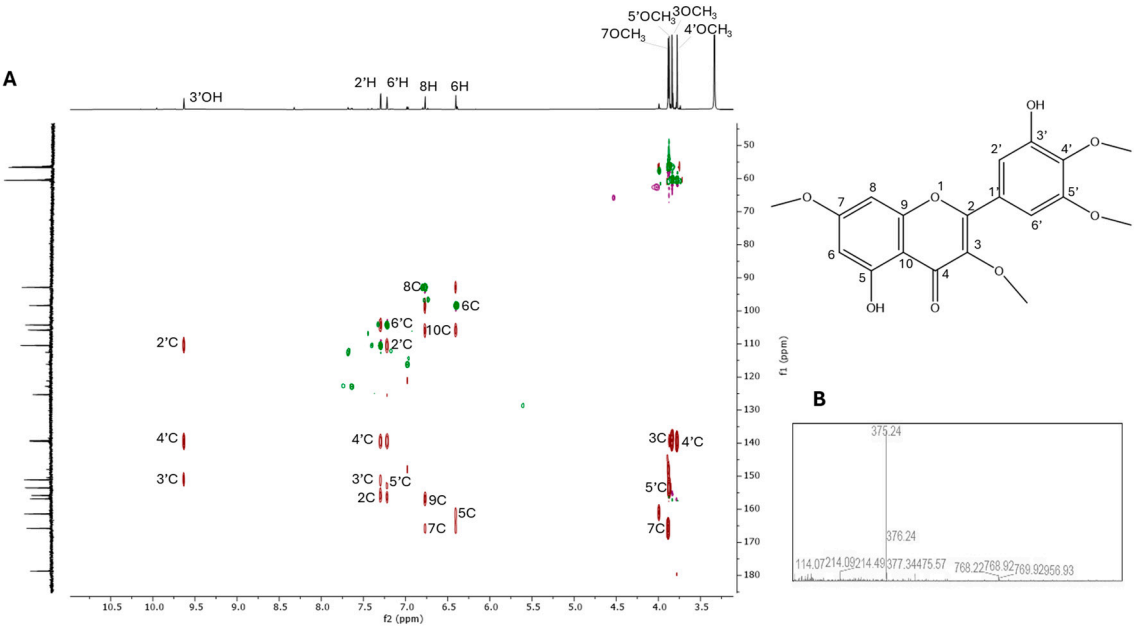

Figure S3. Structural elucidation of myricetin 3,7,4′,5′-tetramethyl ether. A) Superimposed HSQC (green dots) and HMBC (red dots) spectra in deuterated DMSO of APEt subfraction 1 from which the compound was characterized. **B)** Mass spectra in QDa 1 of the same subfraction showing m/z 375.24 interpreted as $[M+H]^+$ (exact mass of myricetin 3,7,4′,5′-tetramethyl ether 374.10 Da).

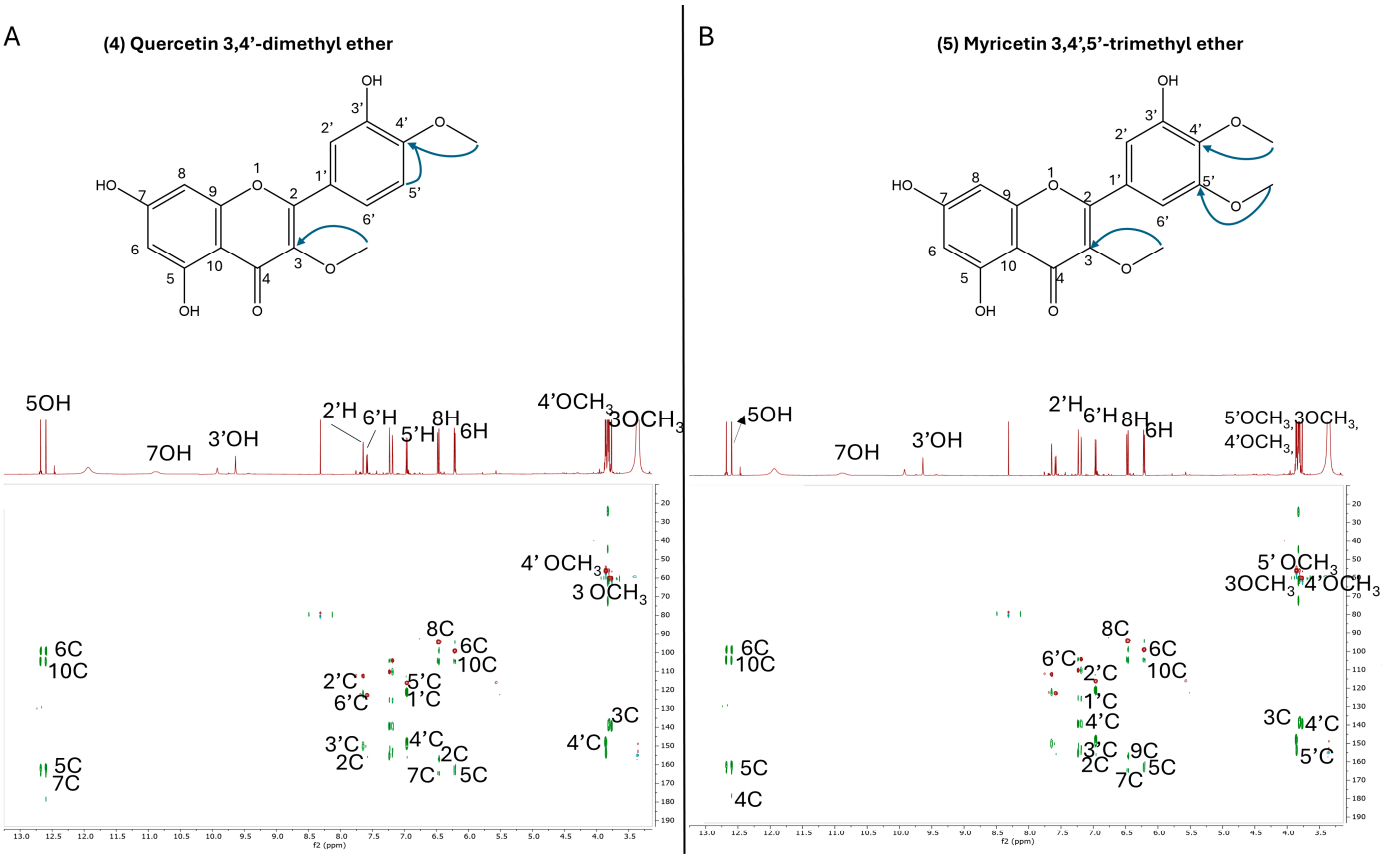

Figure S4. Structural elucidation of quercetin 3,4′-dimethyl ether (A) and myricetin 3,4′,5′-trimethyl ether (B). Superimposed HSQC and HMBC spectra of APCl subfraction 8 from which the two compounds were characterized (**A** and **B** bottom). The blue arrows indicate the HMBC correlations which were crucial to determine the position of methoxyl groups on the molecules.

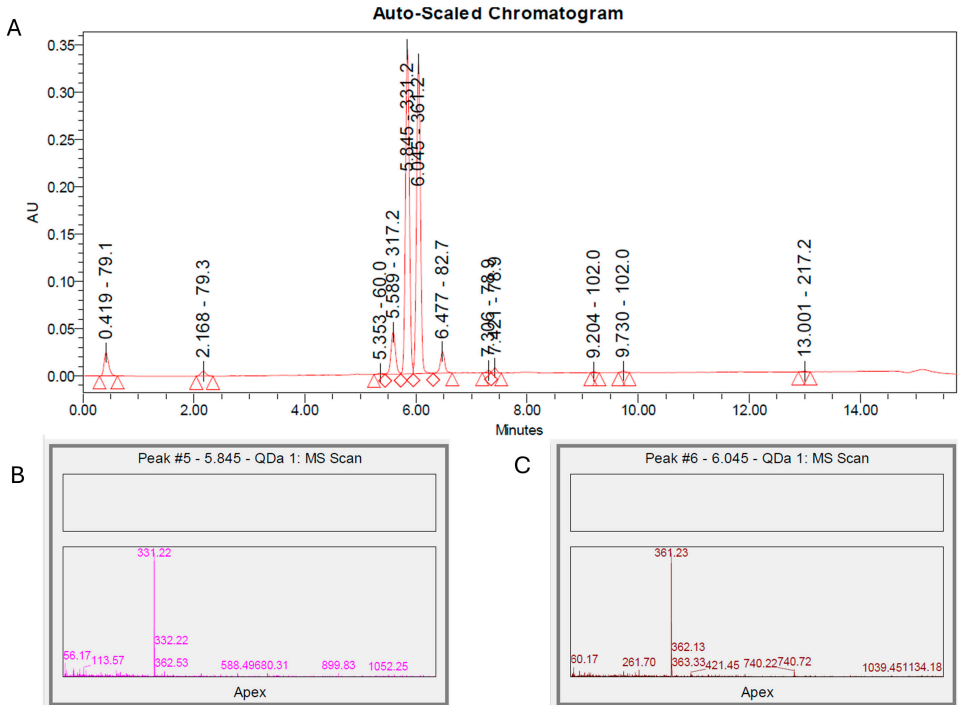

Figure S5. UHPLC-MS analysis of APCl subfraction 8 A) Chromatogram at 260 nm **B)** Mass spectra of peak at RT 5.84 min showing m/z 331.22 interpreted as $[M+H]^+$ (exact mass of quercetin 3,4′-dimethyl ether = 330.0740 Da) **C)** Mass spectra of peak at RT 6.045 min showing m/z 361.23 interpreted as $[M+H]^+$ (exact mass of myricetin 3,4′,5′-trimethyl ether = 360.0845 Da).

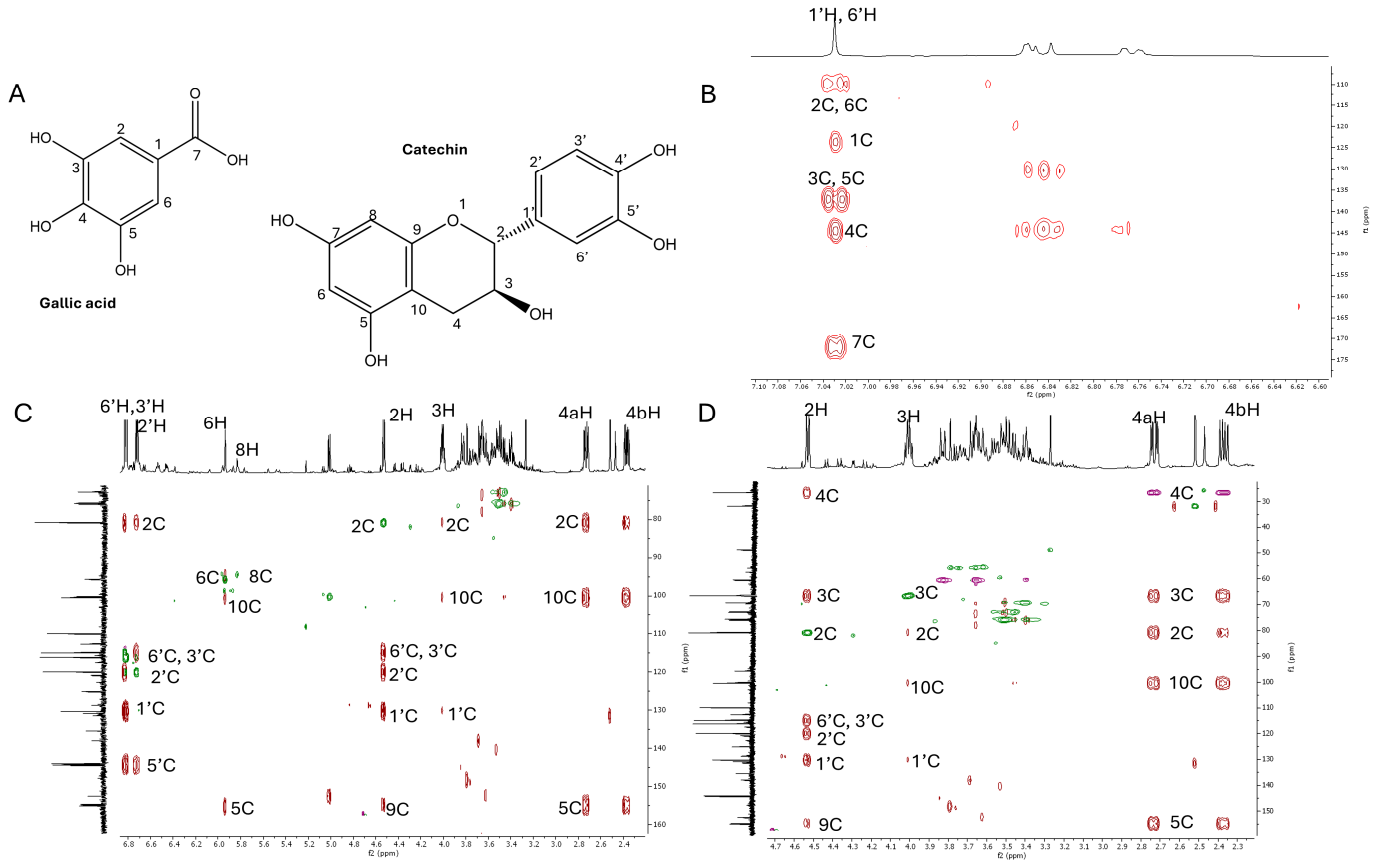

Figure S6. NMR-based structural elucidation of gallic acid and catechin. A) Structures of the two molecules of interest, **B)** HMBC spectrum of subfraction 14 of APEt showing the heteronuclear correlations in gallic acid molecule. **C)** and **D)** superimposed HSQC and HMBC spectra of APEt subfraction 15 from which catechin was characterized.

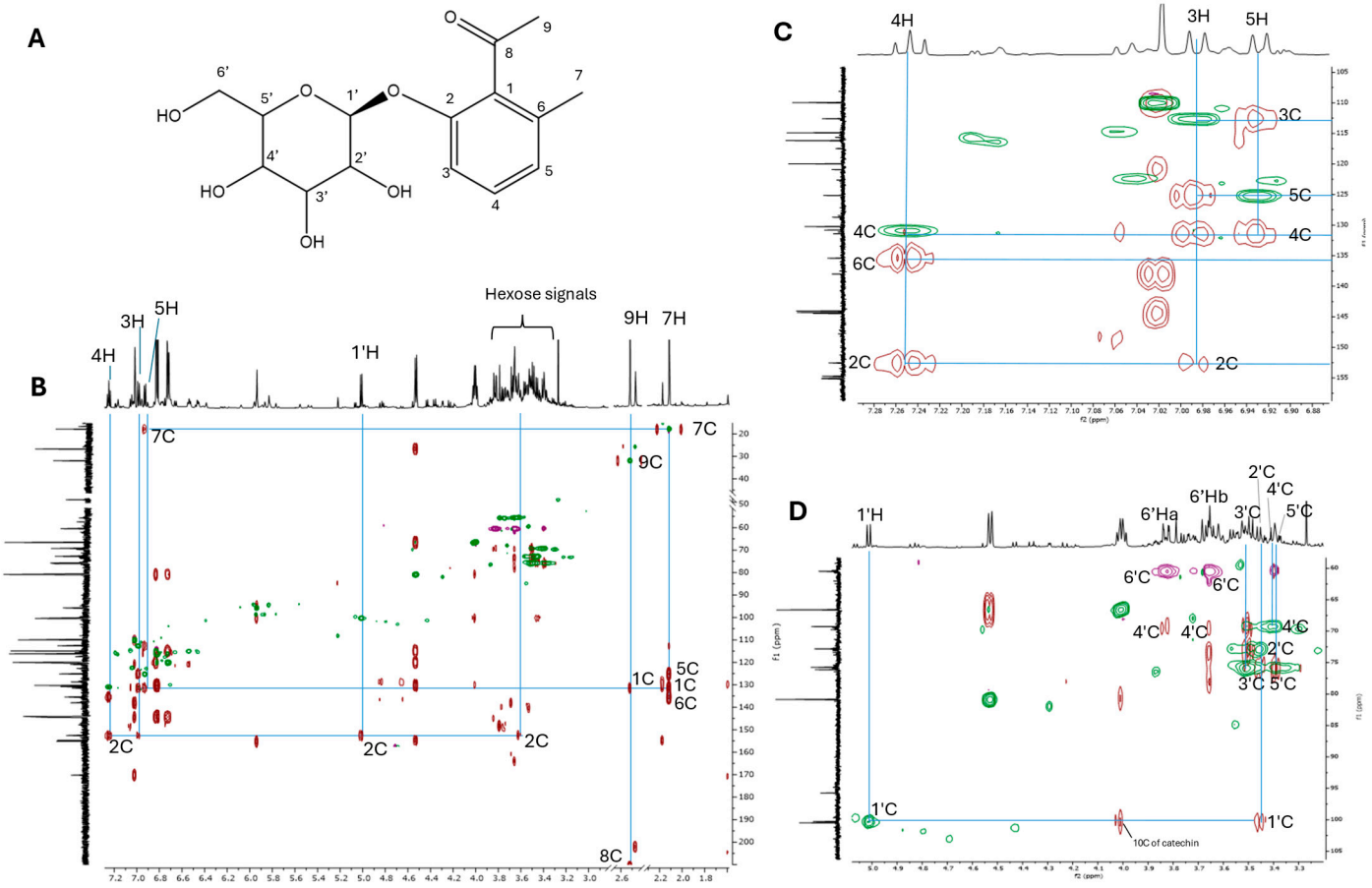

Figure S7. NMR-based structural elucidation of 1-(2-hydroxy-6-methylphenyl)ethanone 2-O-β-hexoside. A) Molecular structure **B)** Superimposed HSQC and HMBC spectra of APEt subfraction 15 from which the compound was characterized. The extended regions **C)** and **D)** show the correlations between aromatic protons and glycosidic protons, respectively.

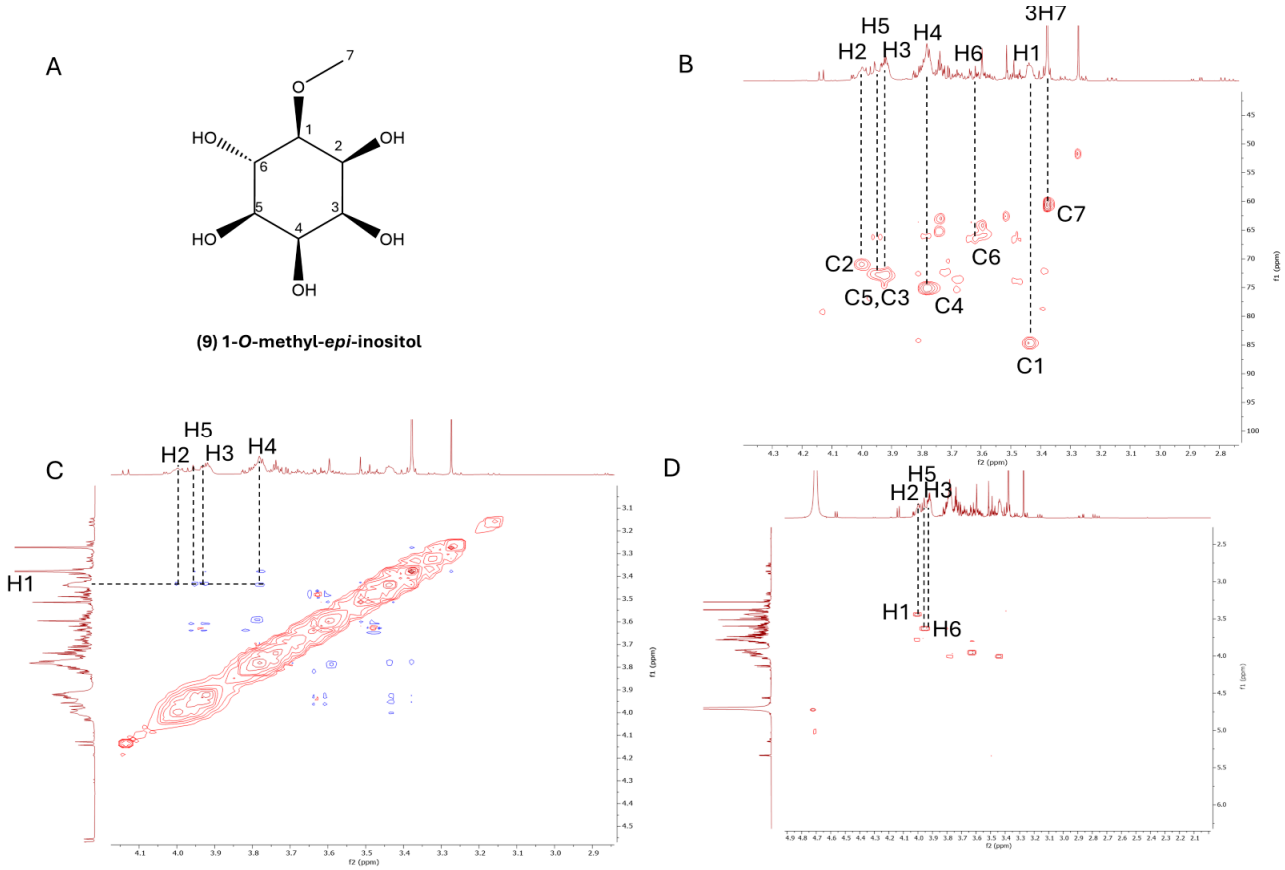

Figure S8. NMR-based structural elucidation of 1-*O*-methyl-*epi*-inositol in D_2O A) Molecular structure, **B)** HMBC spectrum of RW subfraction 20 from which the compound was characterized, **C)** 2D-NOESY, **D)** COSY (the diagonal was suppressed)