

Supporting information

Synthesis, Basicity, Structural Characterization and Biochemical Properties of Two [(3-Hydroxy-4-pyron-2-yl)methyl]amine Derivatives Showing Anti-neoplastic Features.

Stefano Amatori, Gianluca Ambrosi, Mirco Fanelli,^{*} Mauro Formica, Vieri Fusi,^{*} Luca Giorgi Eleonora Macedi, Mauro Micheloni, Paola Paoli,^{*} Roberto Pontellini and Patrizia Rossi

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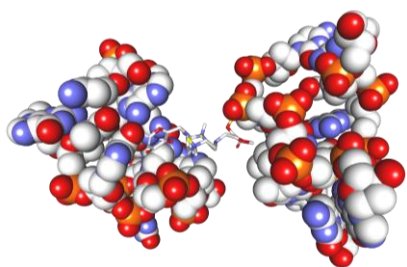
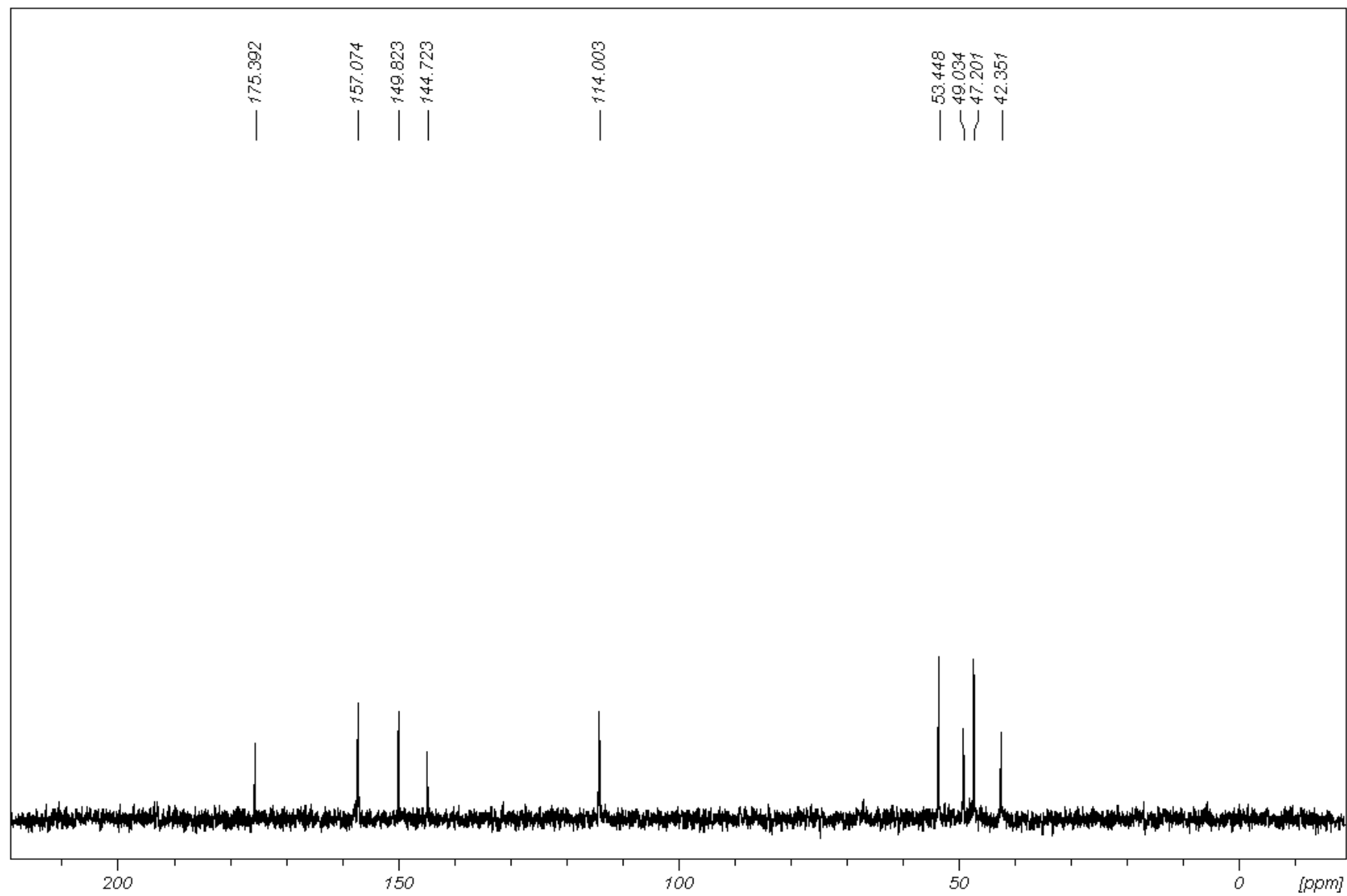
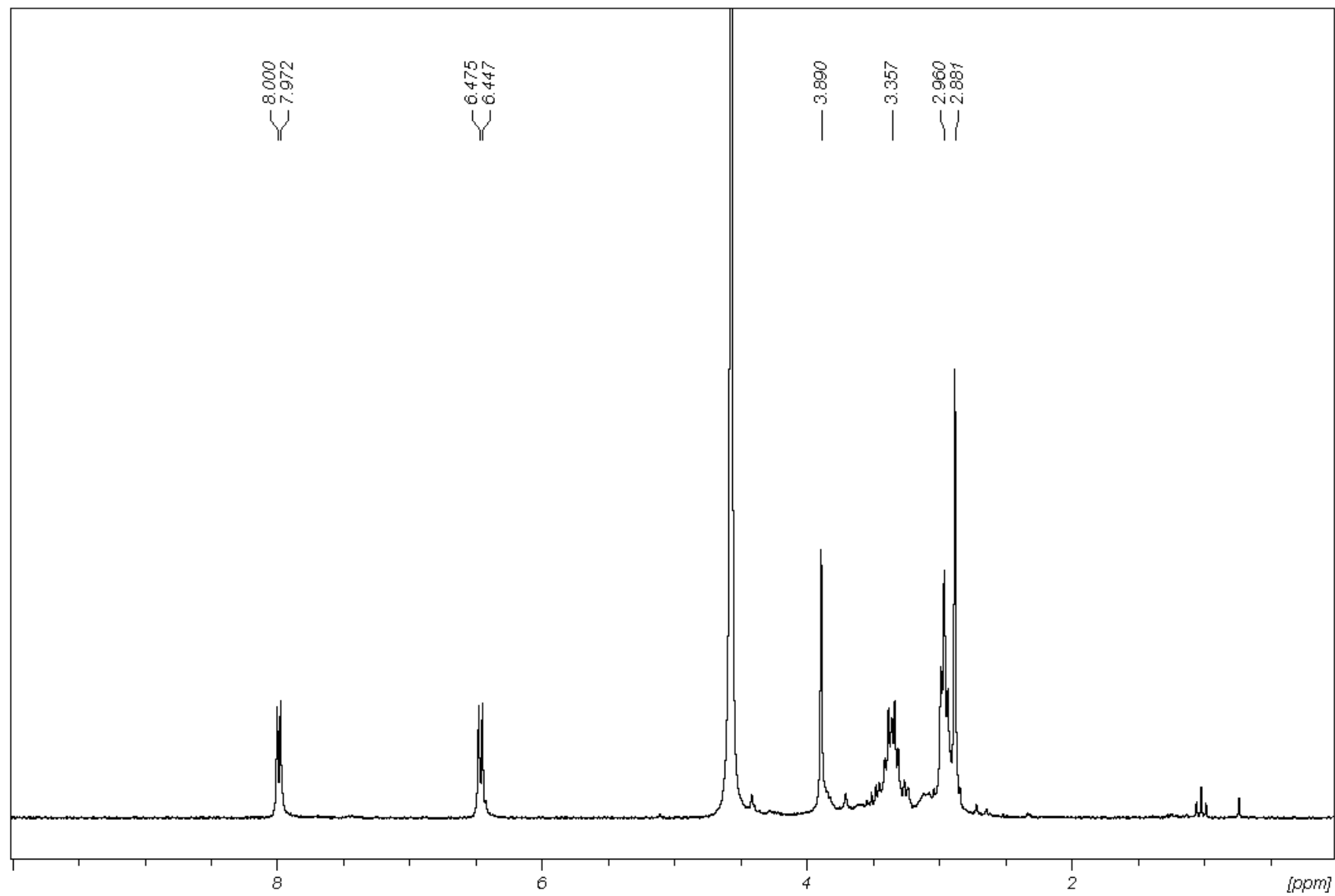


Table S1. Crystallographic data and refinement parameters for compounds **6** and **7**

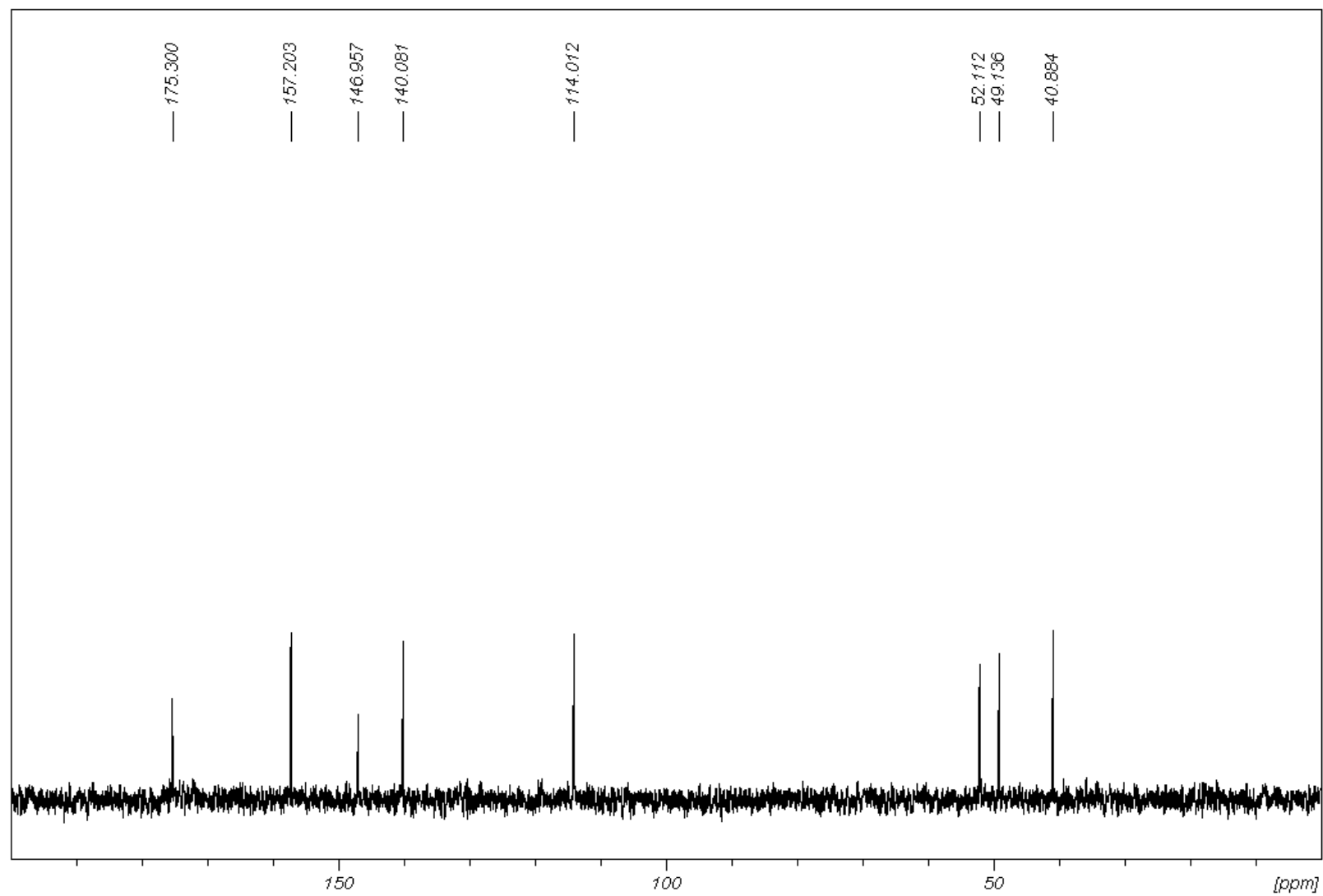
	6	7
formula	[H ₂ Malten](ClO ₄) ₂ ·2(H ₂ O)	[H ₂ Maltonis](ClO ₄) ₂
MW	573.28	647.42
T (K)	120	150
λ (Å)	0.71069	0.71069
Crystal system, space group	Triclinic, P-1	Monoclinic, P2 ₁ /n
Unit cell dimensions (Å, °)	a = 7.871(2), α = 72.08(3) b = 8.087(3), β = 67.16(3) c = 10.307(4), γ = 76.62(2)	a = 12.0642(6) b = 12.2497(8), β = 94.866(5) c = 18.740(1)
Volume (Å ³)	570.6(3)	2759.5(3)
Z, D _c (mg/cm ³)	1, 1.668	4, 1.558
μ (mm ⁻¹)	0.371	0.313
F(000)	298	1352
Crystal size (mm)	0.5x0.3x0.2	0.4x0.4x0.3
2 θ range (°)	8 - 56	8 - 56
Reflections collected /unique	5450 / 2488	16896 / 6007
Data / parameters	2488 / 215	6007 / 515
Final R indices [I>2 σ (I)]	R1 = 0.0627, wR2 = 0.1673	R1 = 0.0380, wR2 = 0.0742
R indices (all data)	R1 = 0.0868, wR2 = 0.1893	R1 = 0.0820, wR2 = 0.0857
GOF's	1.032	0.907



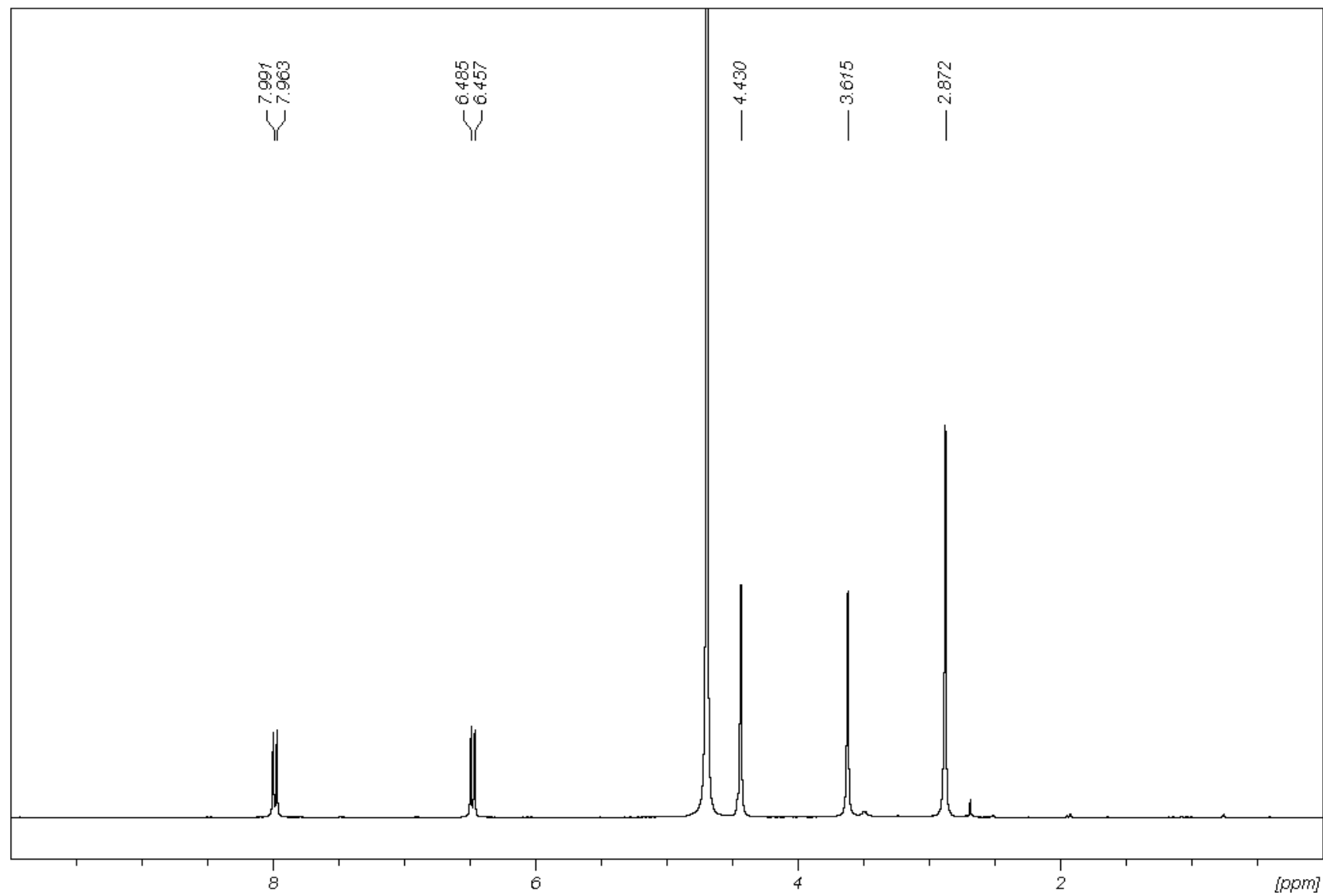
^{13}C NMR spectrum of Maltonis (D_2O pH = 2, 25 °C)



^1H NMR spectrum of Maltonis (D_2O pH = 2, 25 °C)



^{13}C NMR spectrum of Malten (D_2O pH = 2, 25 °C)



^1H NMR spectrum of Malten (D_2O pH = 2, 25 °C)