Supporting information

Novel Chiral (Salen)Mn(III) Complexes Containing a Calix[4]arene Unit in 1,3-alternate conformation as Catalysts for Enantioselective Epoxidation Reactions of (Z)-Aryl Alkenes

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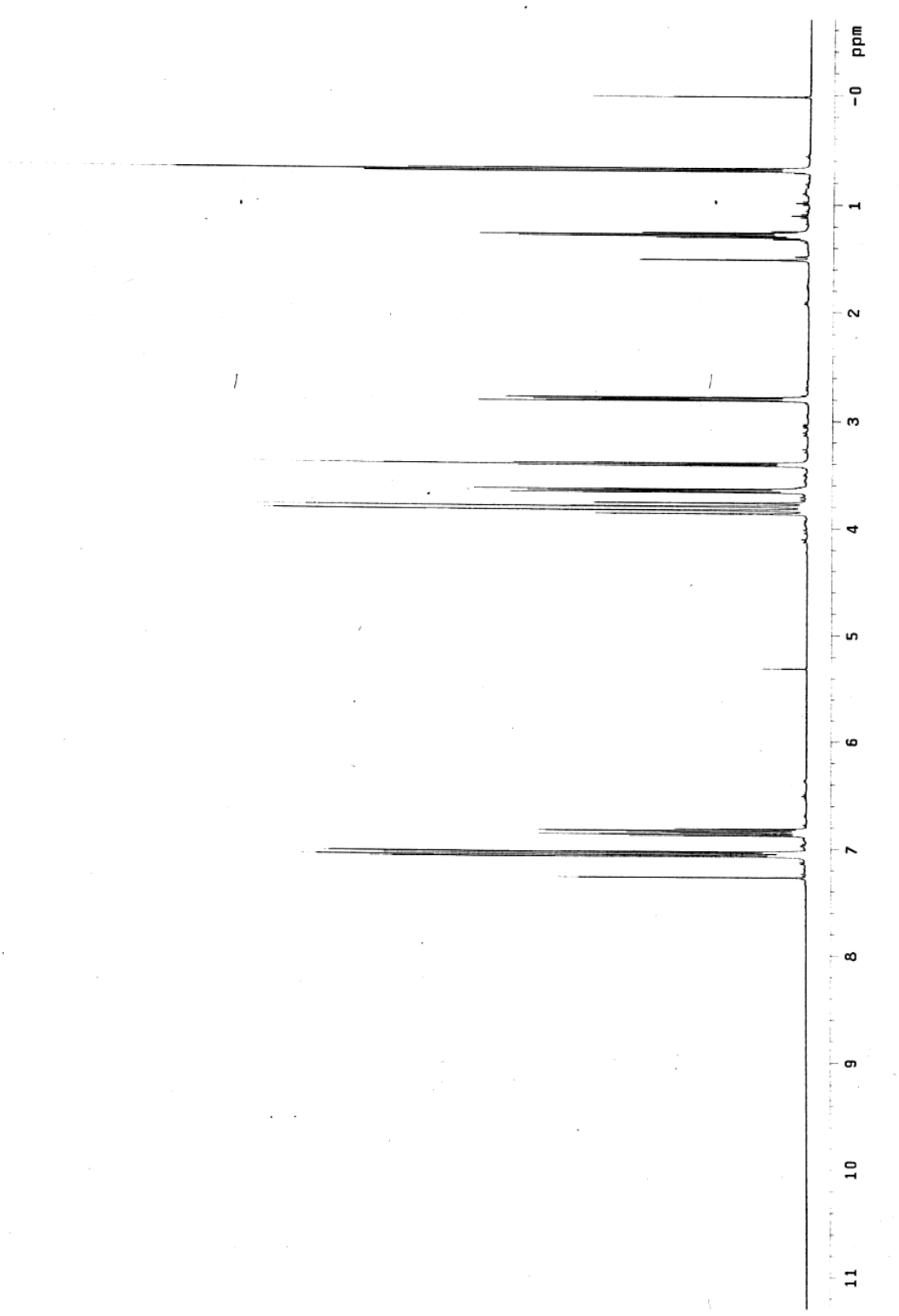

Figure S1. ^{1}H-NMR spectrum of dibromo derivative **6a**

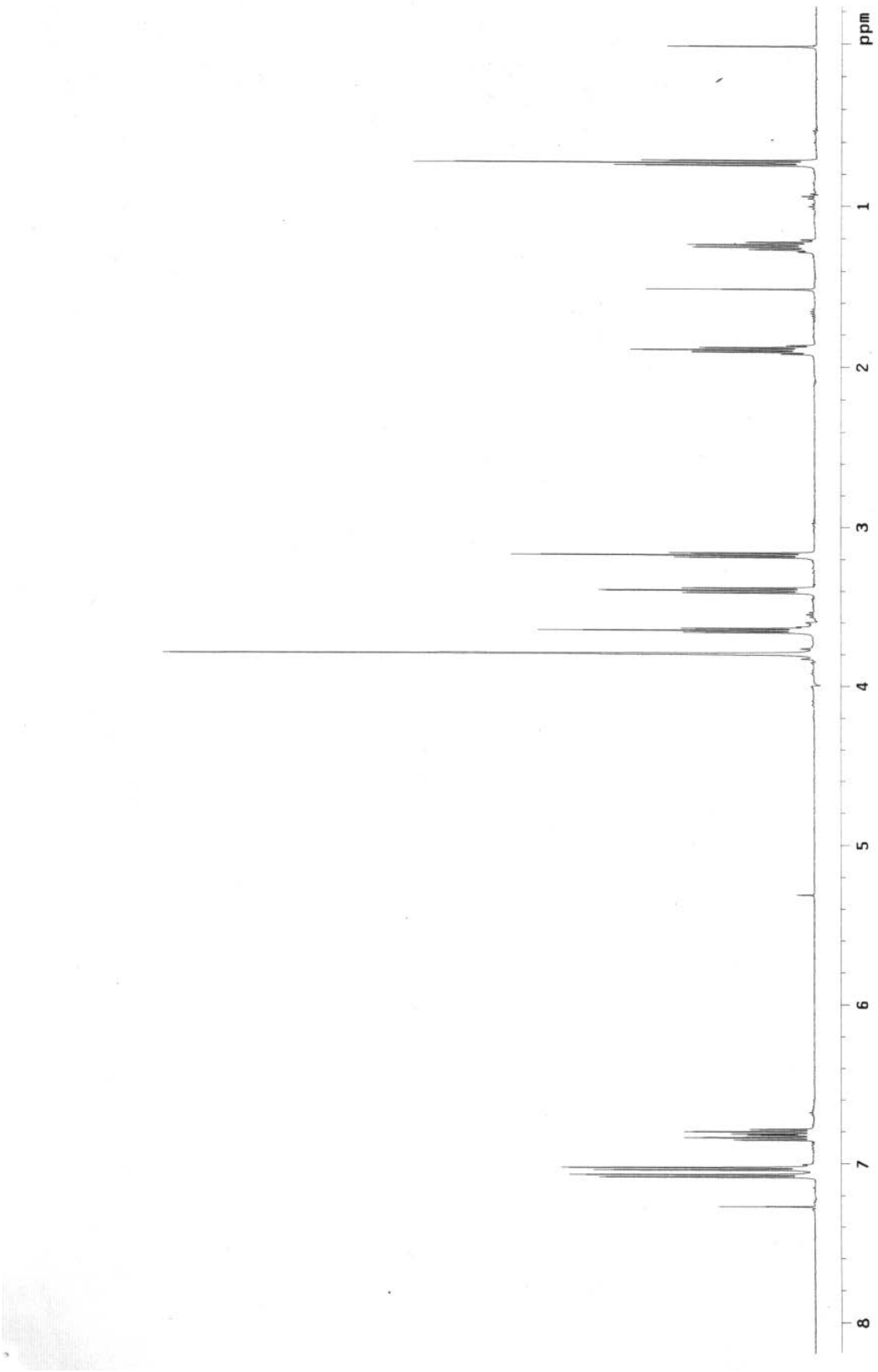

Figure S2. ^{1}H-NMR spectrum of dibromo derivative **6b**

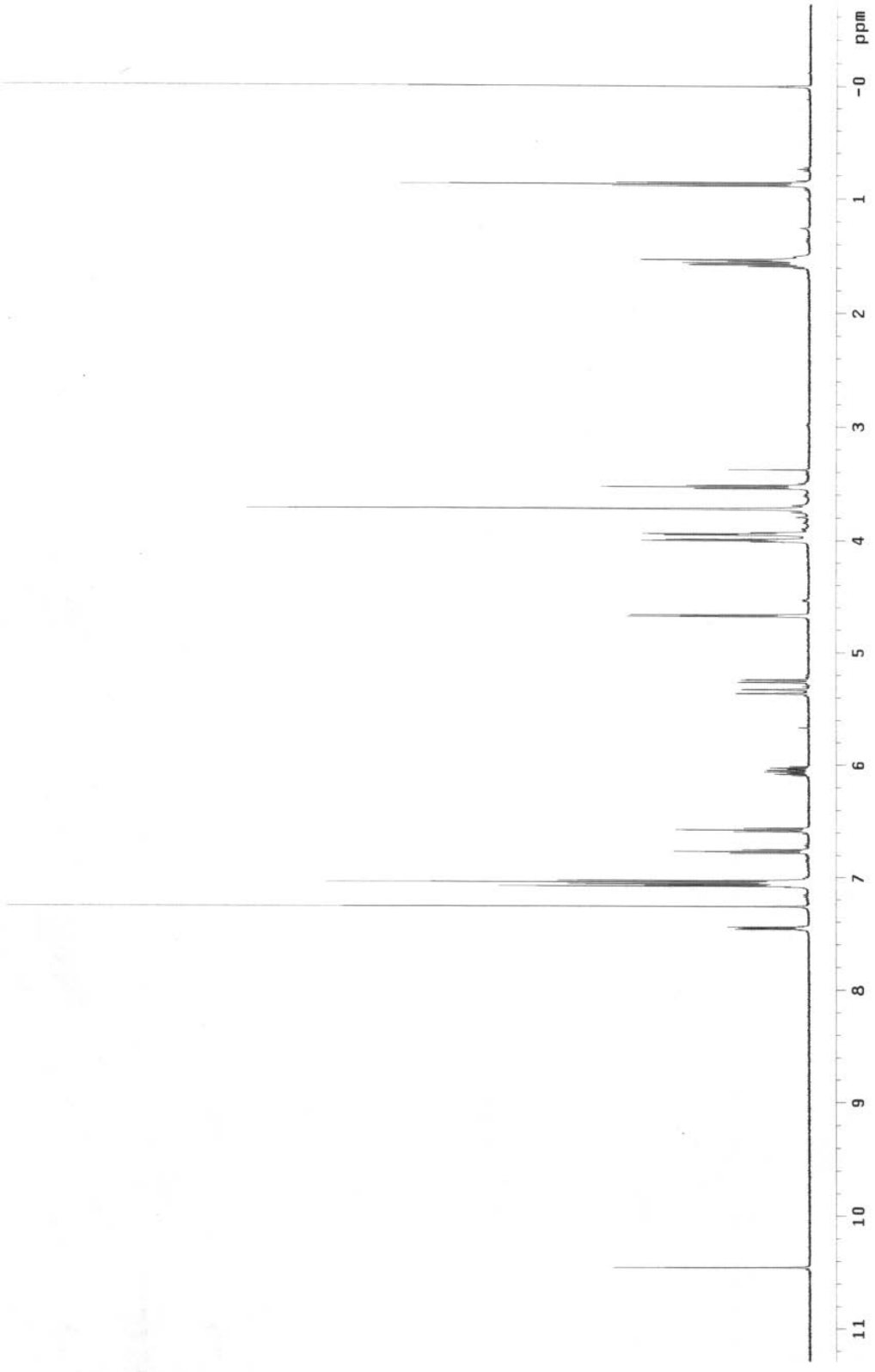

Figure S3. ^{1}H-NMR spectrum of protected aldehyde **7a**

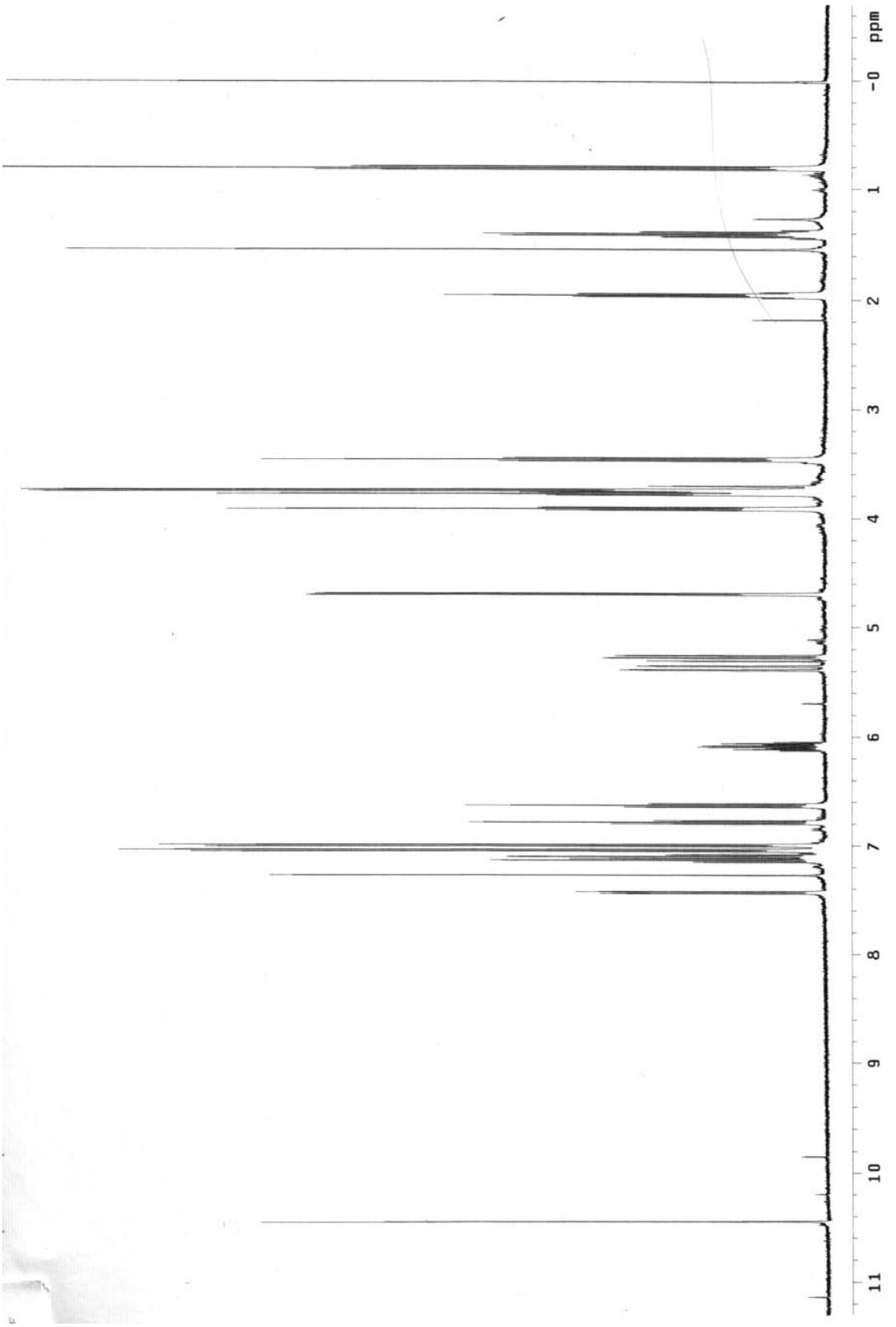

Figure S4. ^{1}H-NMR spectrum of protected aldehyde **7b**

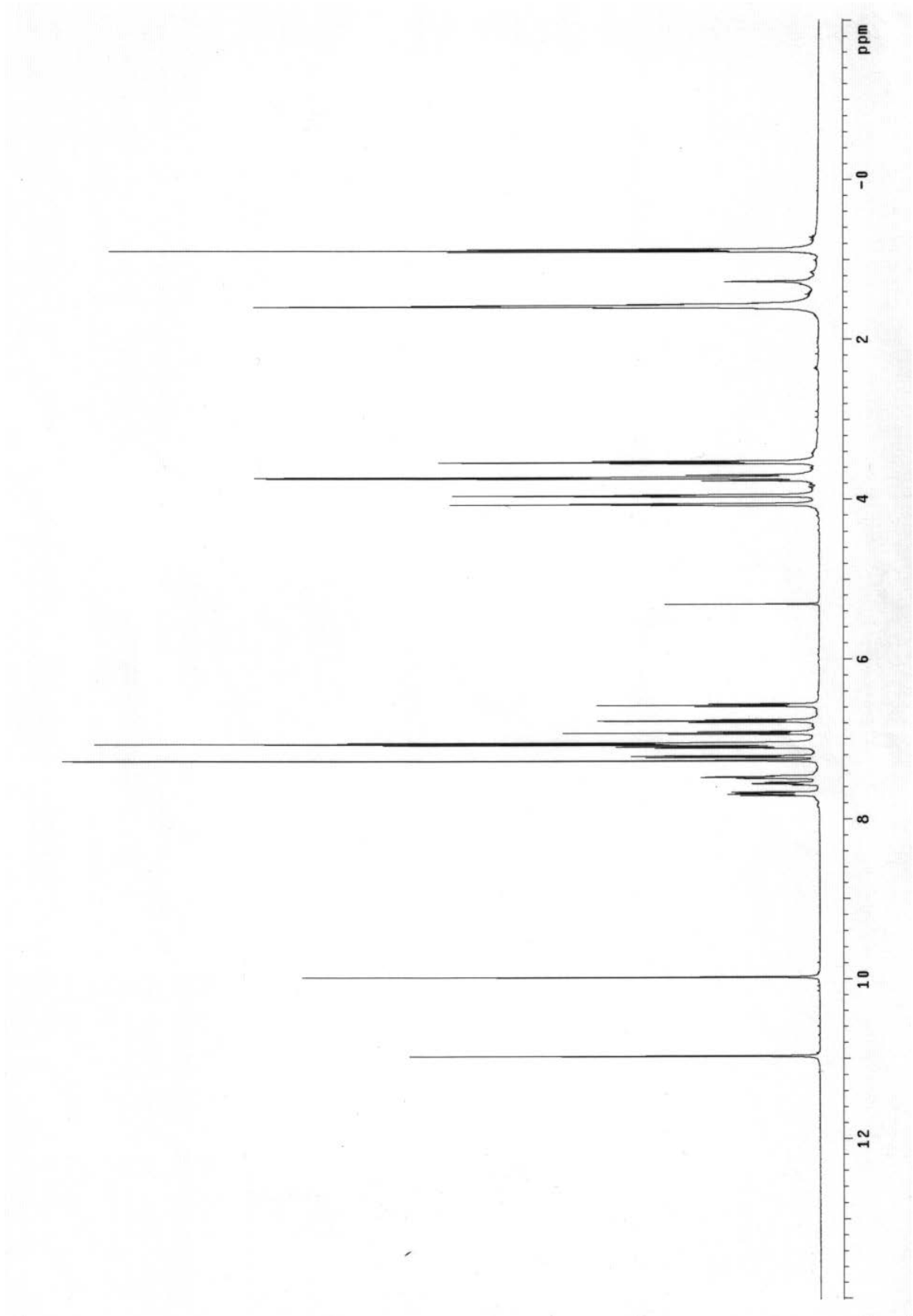

Figure S5. ^{1}H-NMR spectrum of aldehyde **8a**

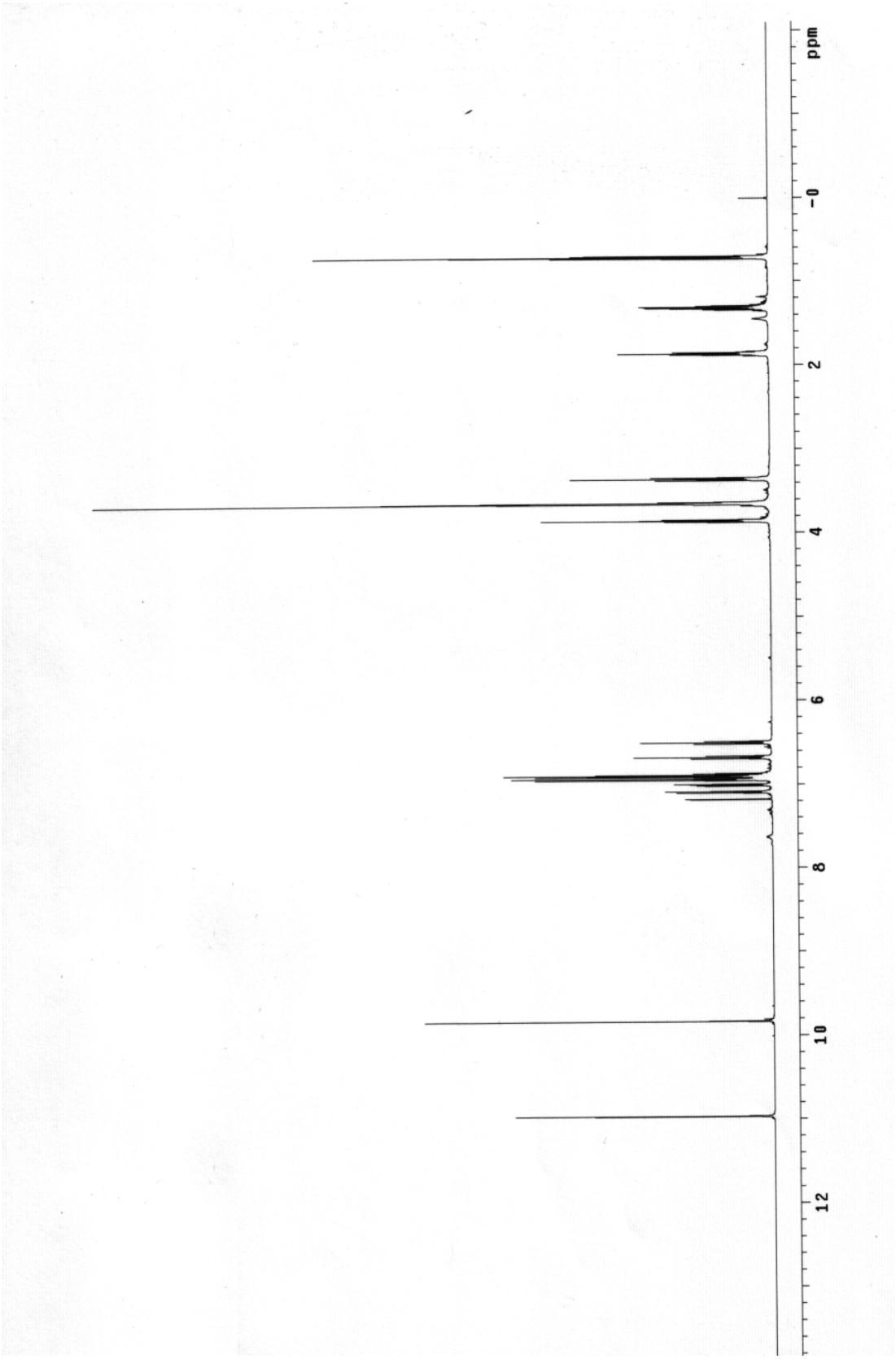

Figure S6. ^{1}H-NMR spectrum of aldehyde **8b**

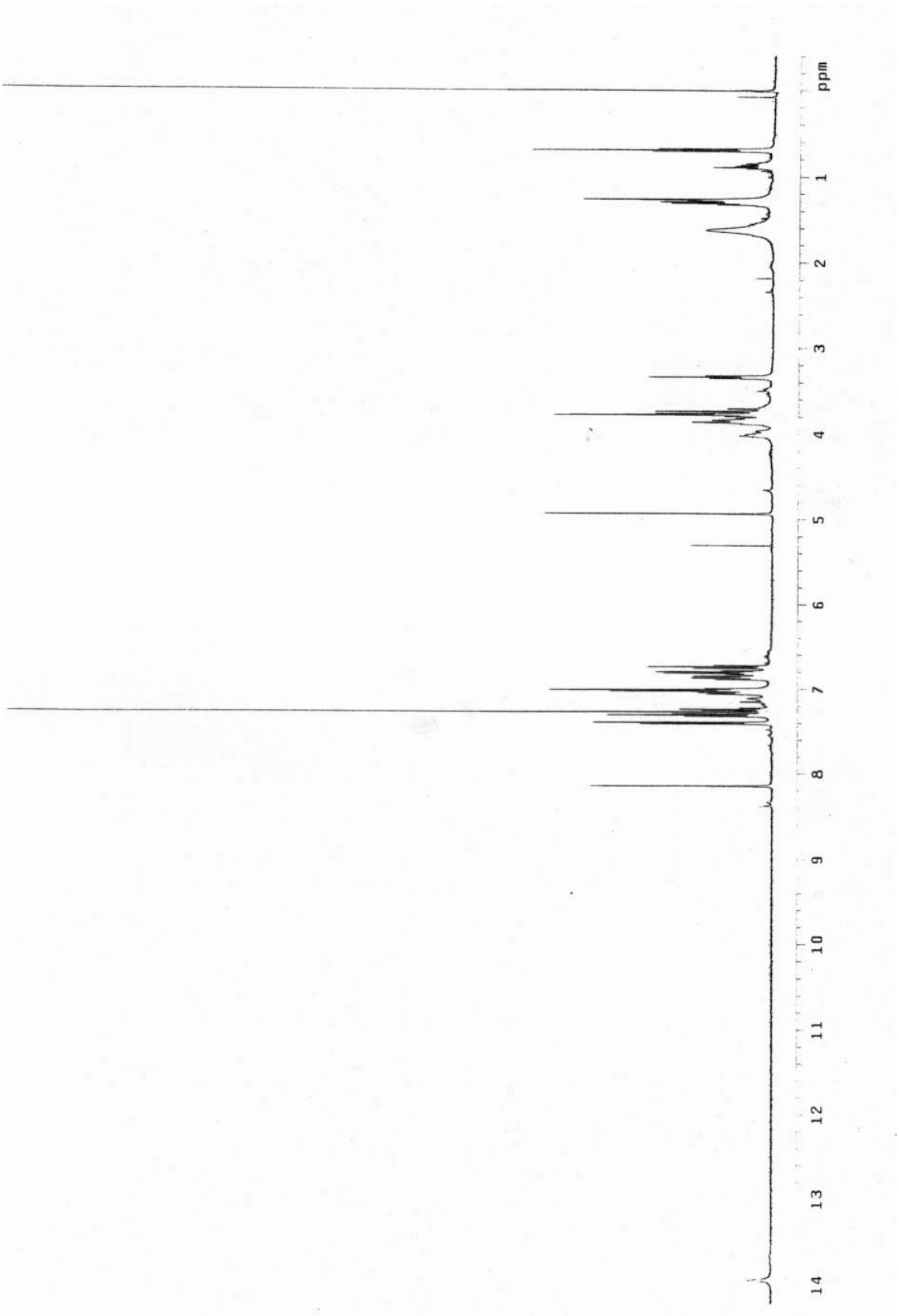

Figure S7. ^{1}H-NMR spectrum of calix[4]arene-salen **1a**

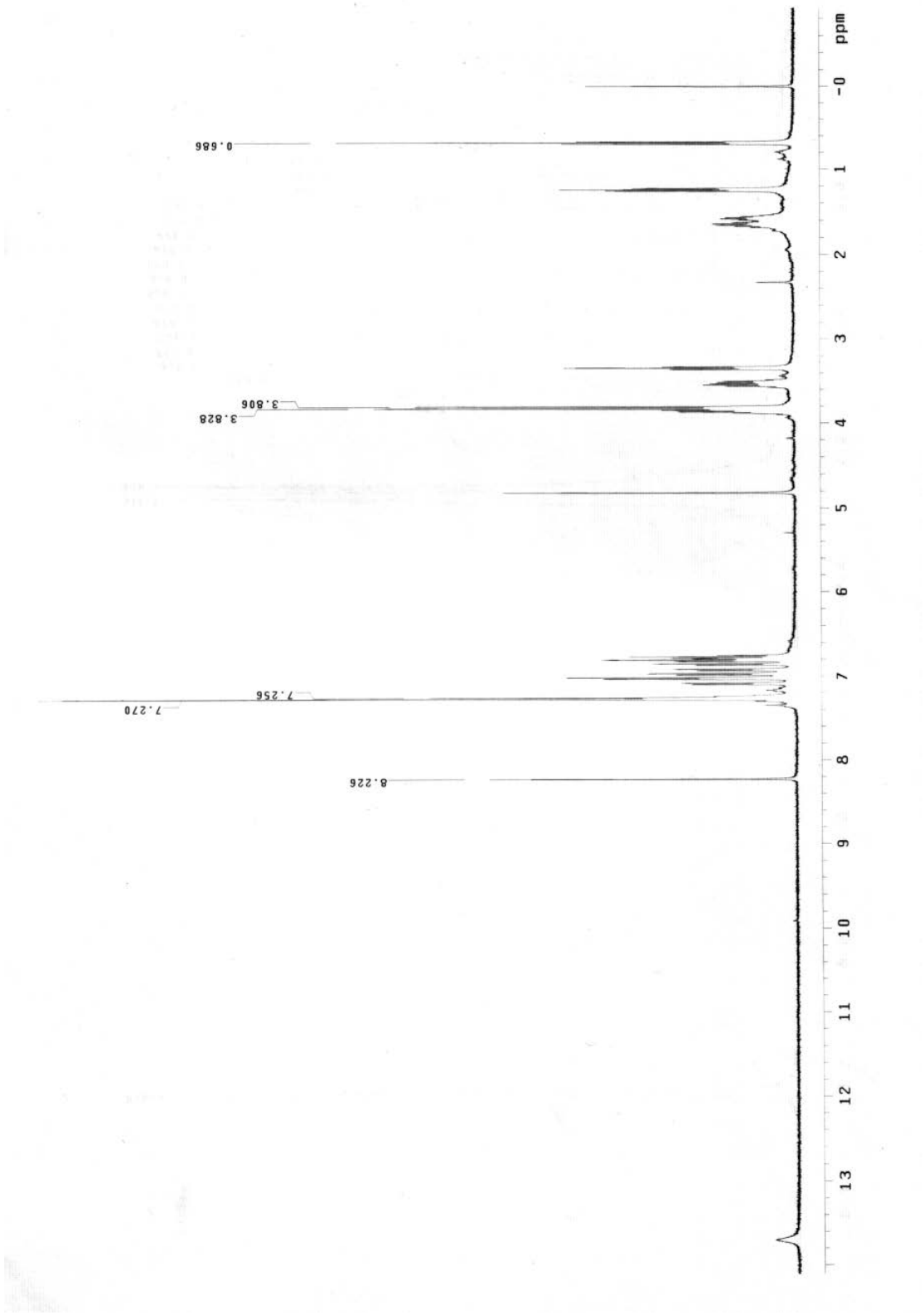

Figure S8. ^{1}H-NMR spectrum of calix[4]arene-salen **1b**

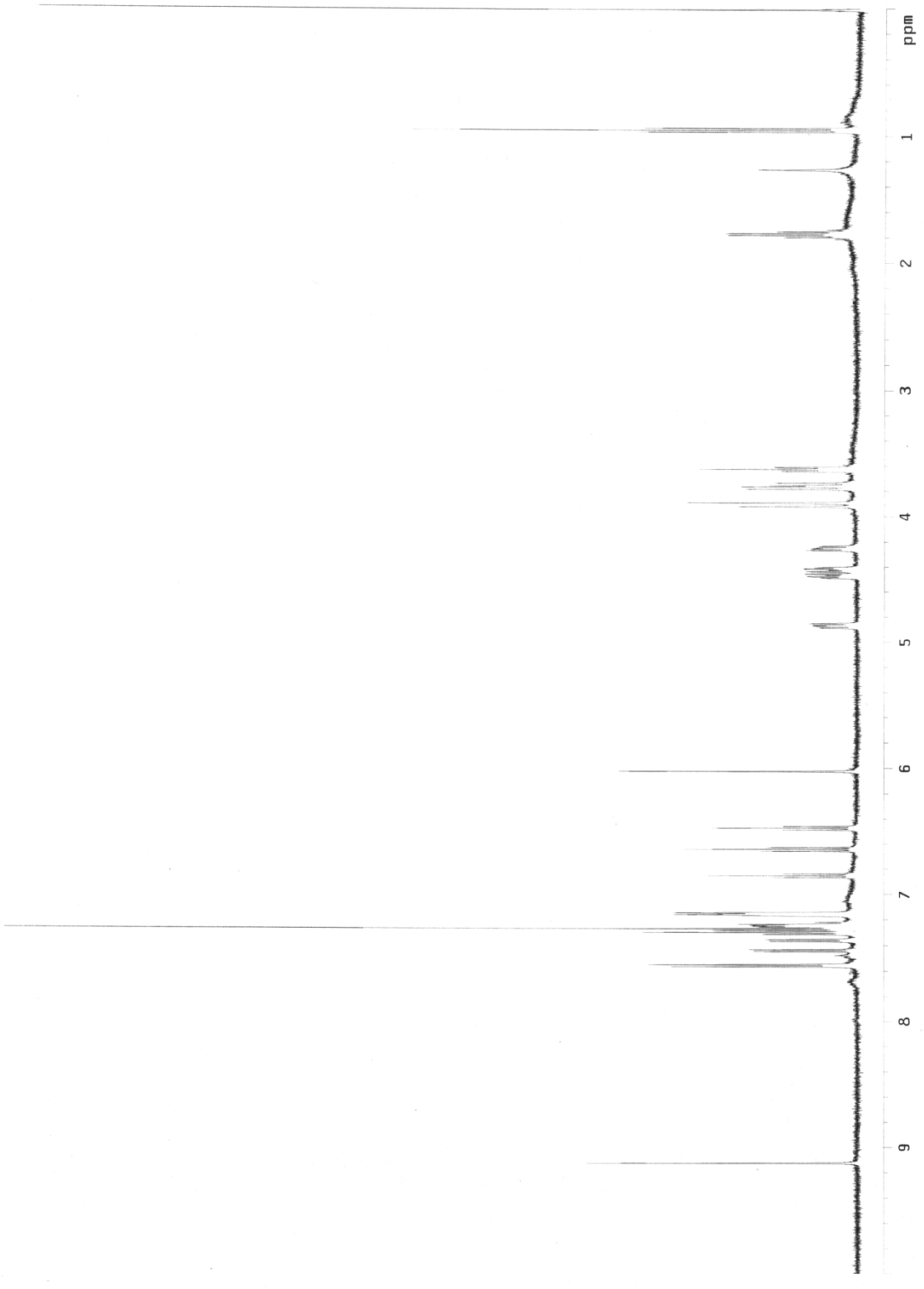

Figure S9. ^{1}H-NMR spectrum of UO_2-calix[4]arene-salen **2a**

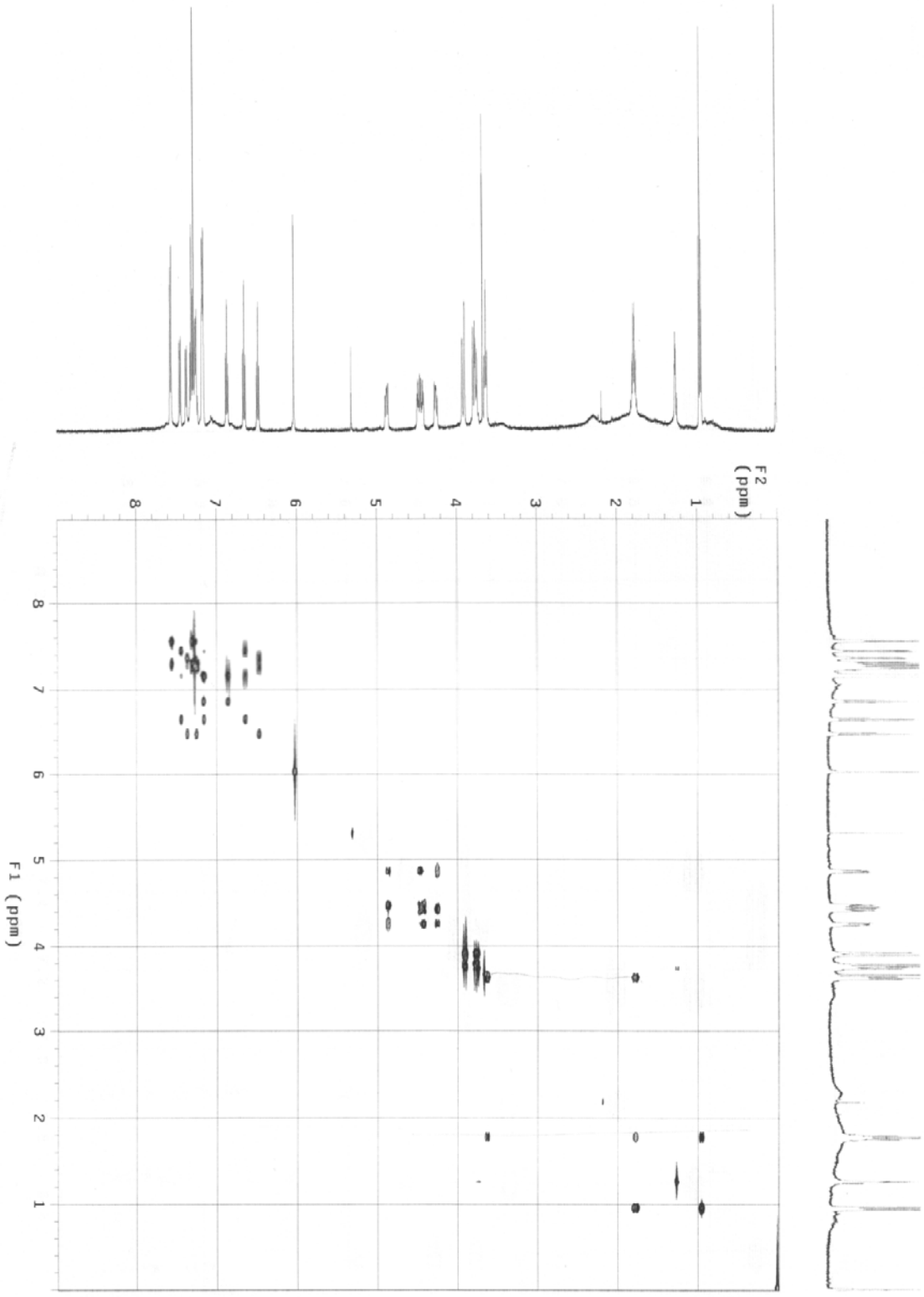

Figure S10. 2D-COSY spectrum of UO_2-calix[4]arene-salen **2a**

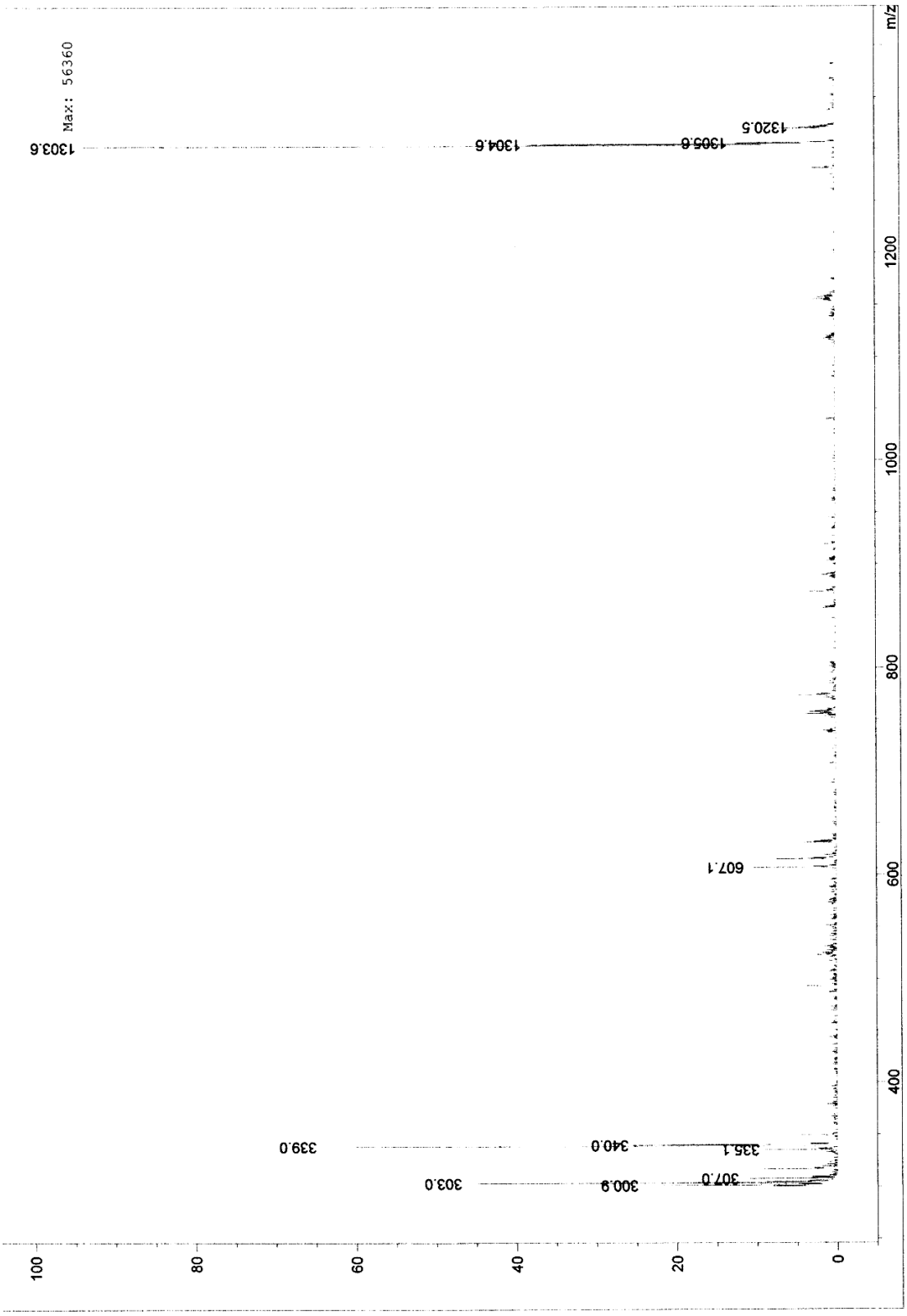

Figure S11. ESI-MS spectrum of UO_2-calix[4]arene-salen **2a**

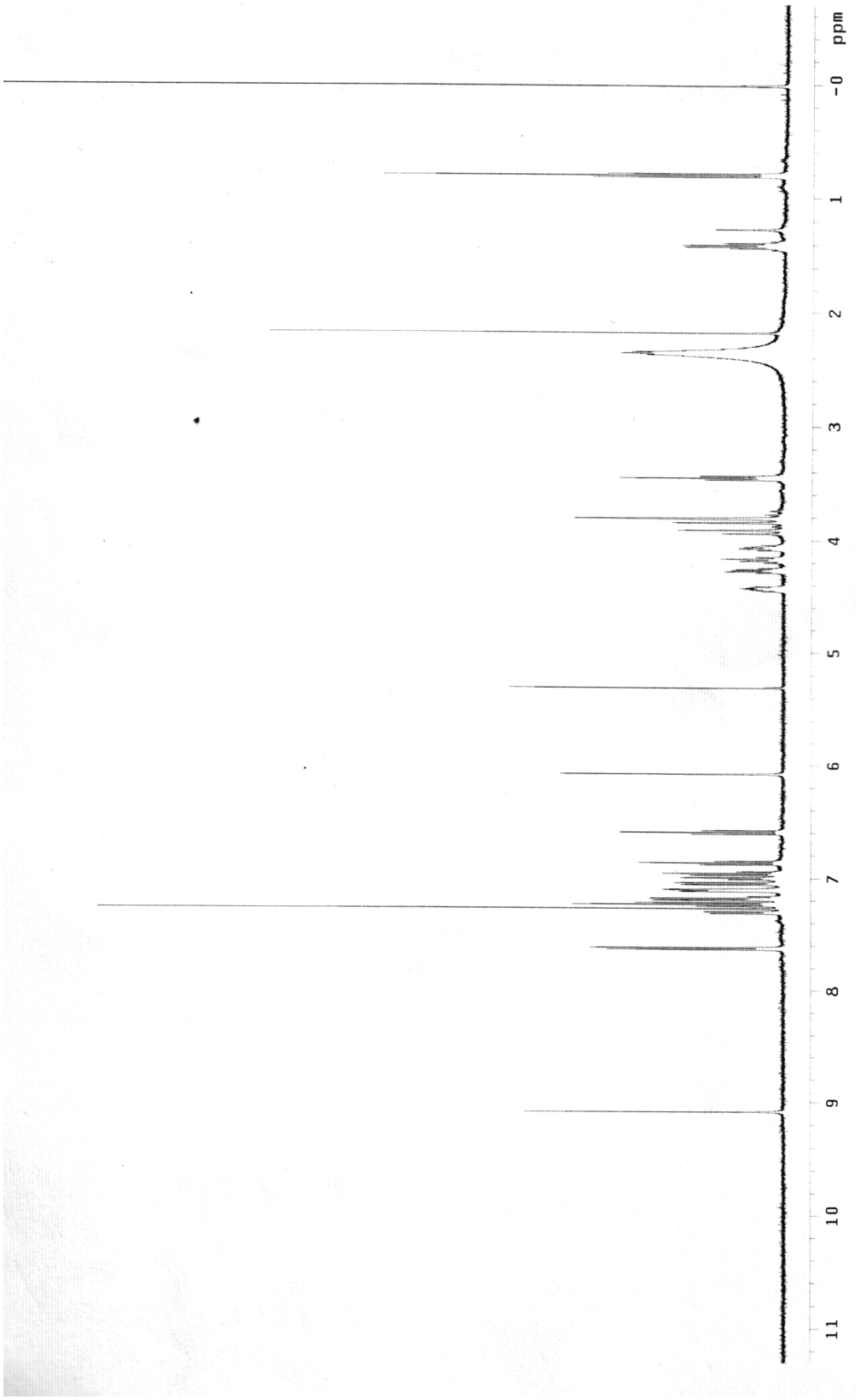

Figure S12. ^{1}H-NMR spectrum of UO_2-calix[4]arene-salen **2b**

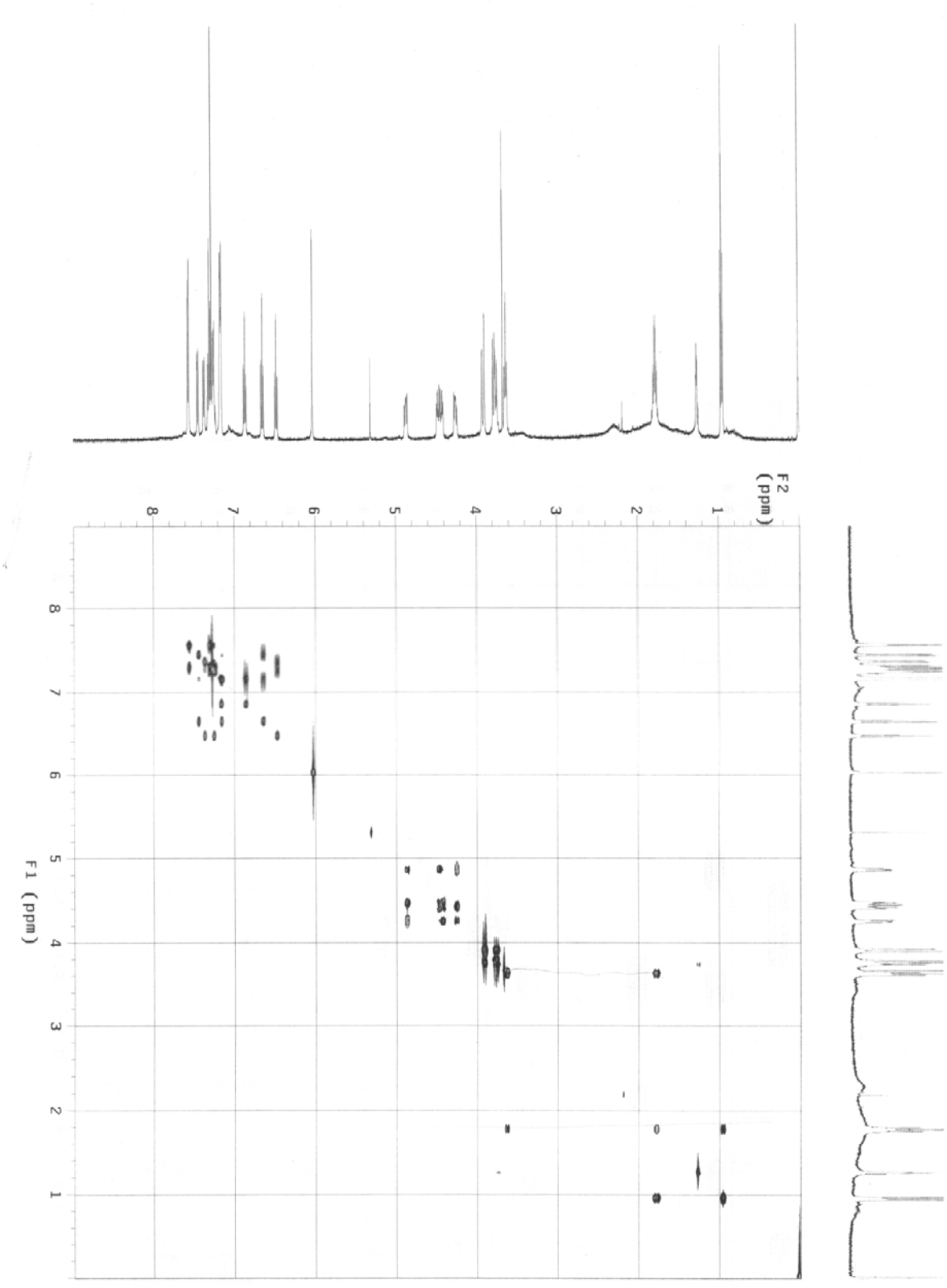

Figure S13. 2D-COSY spectrum of UO_2-calix[4]arene-salen **2b**

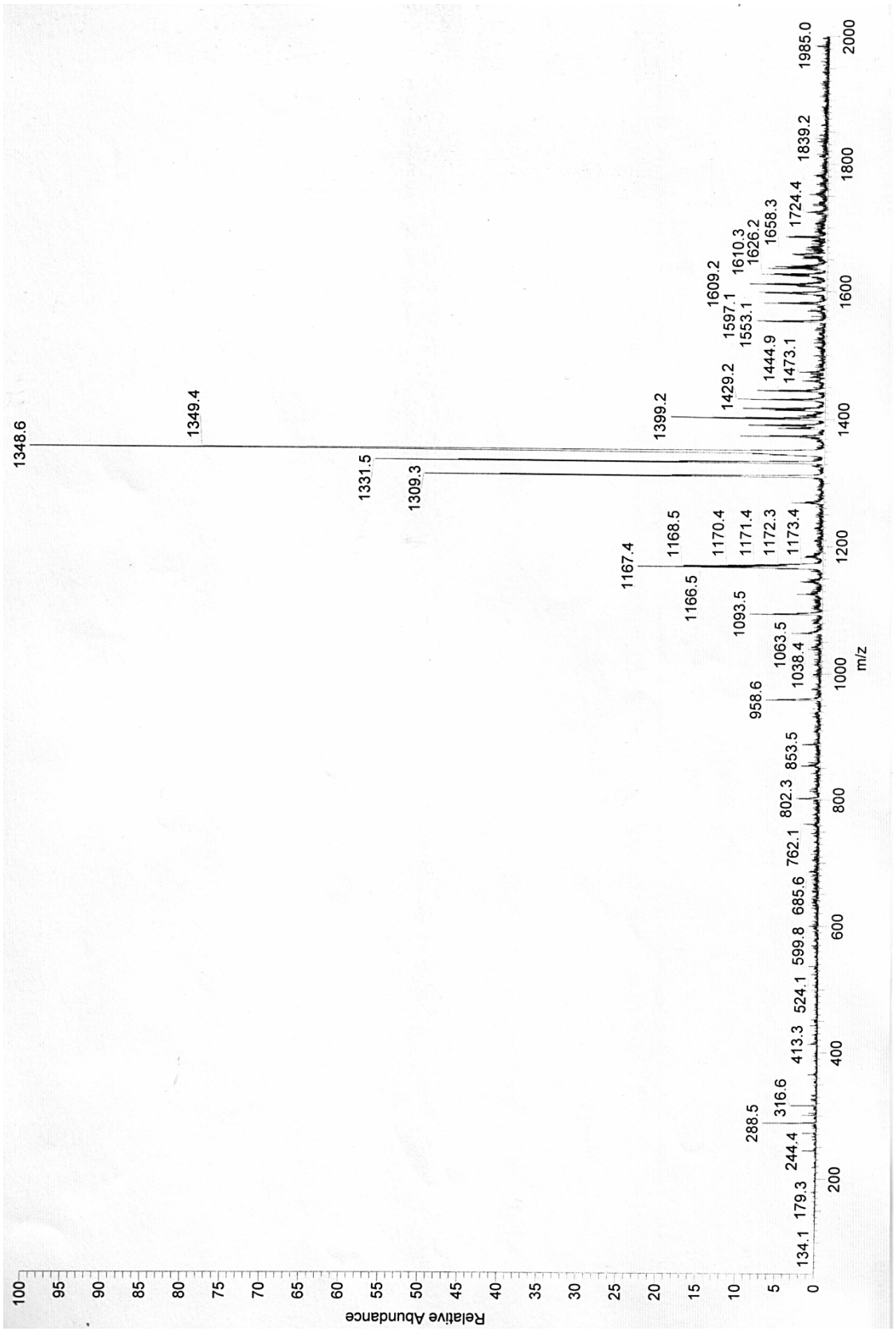

Figure S14. ESI-MS spectrum of UO_2-calix[4]arene-salen **2b**

Figure S15. Variable temperature ^{1}H NMR spectra of UO_2-calix[4]arene-salen **2a**

Figure S16. Variable temperature ^{1}H NMR spectra of UO_2-calix[4]arene-salen **2b**

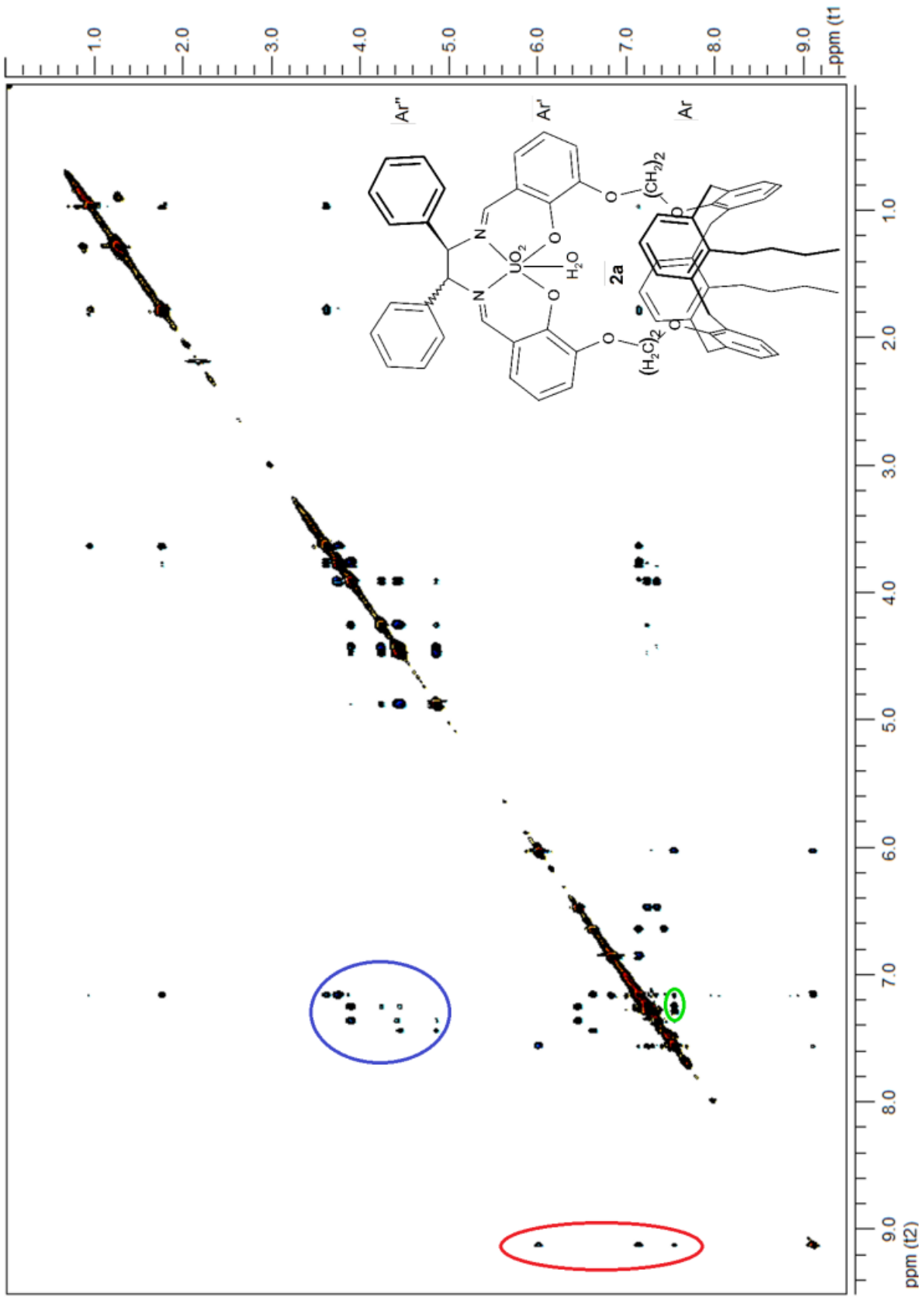

Figure S17. T-ROESY map of UO_2-calix[4]arene-salen **2a**

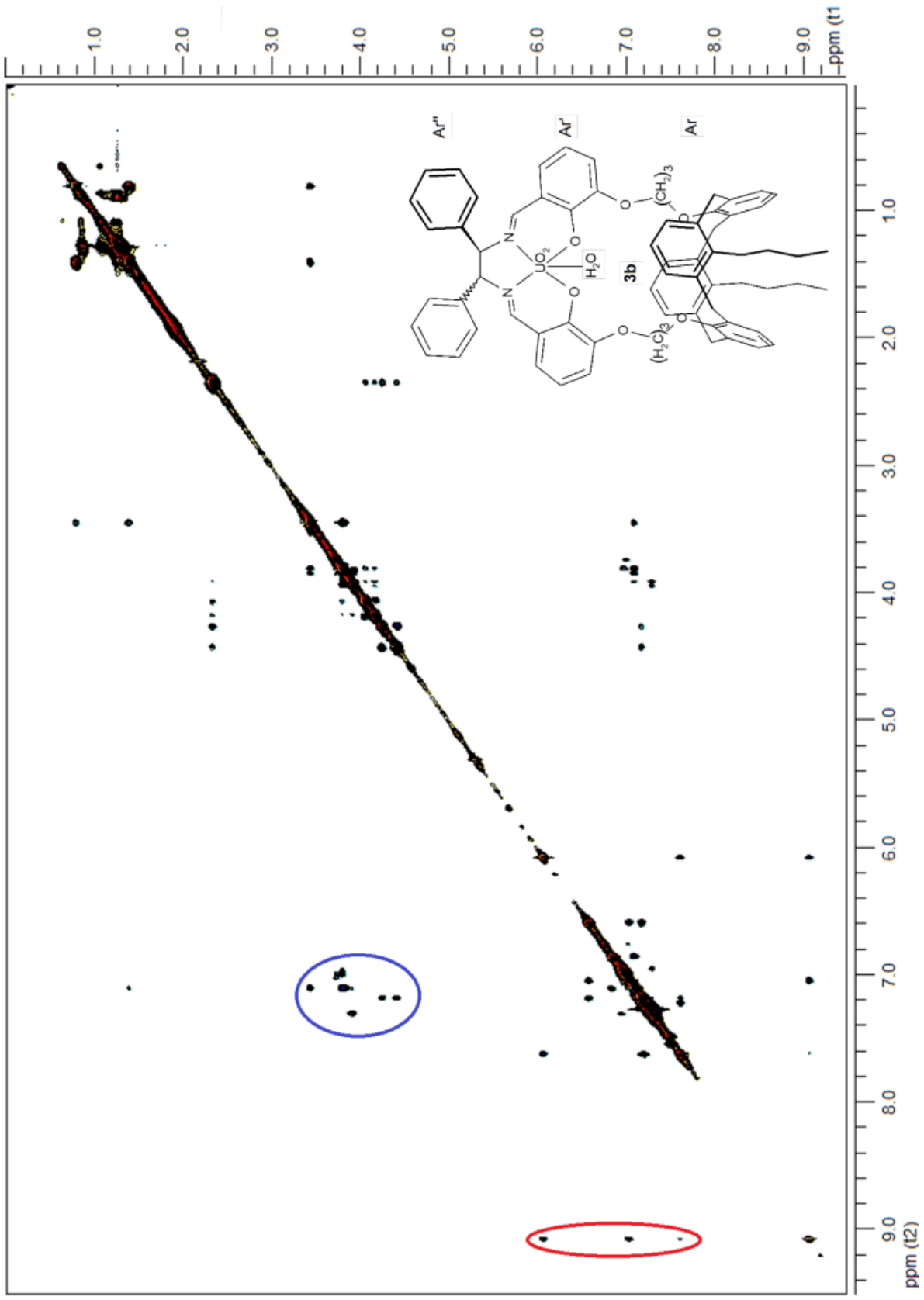

Figure S18. T-ROESY map of UO_2-calix[4]arene-salen **2b**

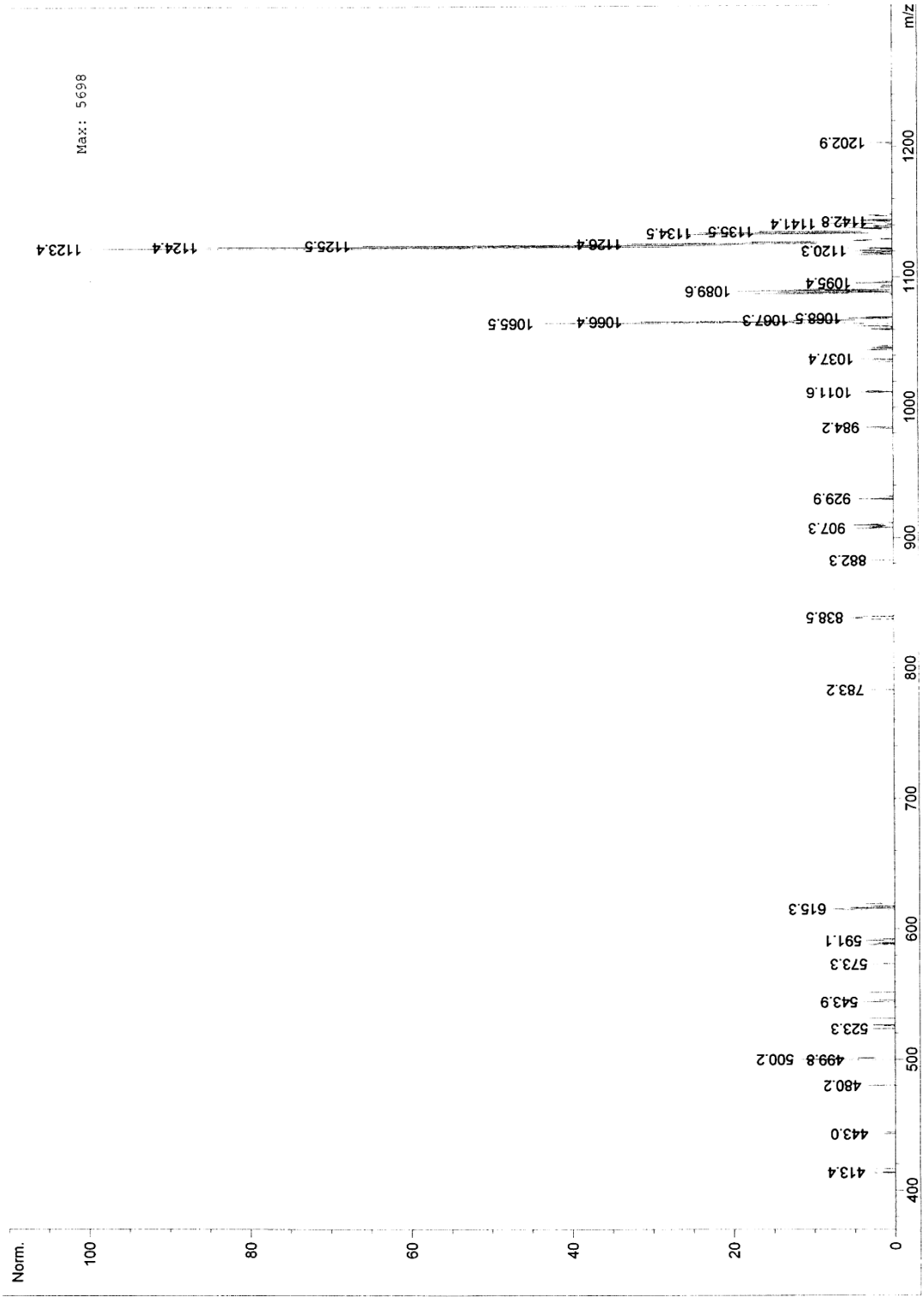

Figure S19. ESI-MS spectrum of Mn-calix[4]arene-salen **3a**

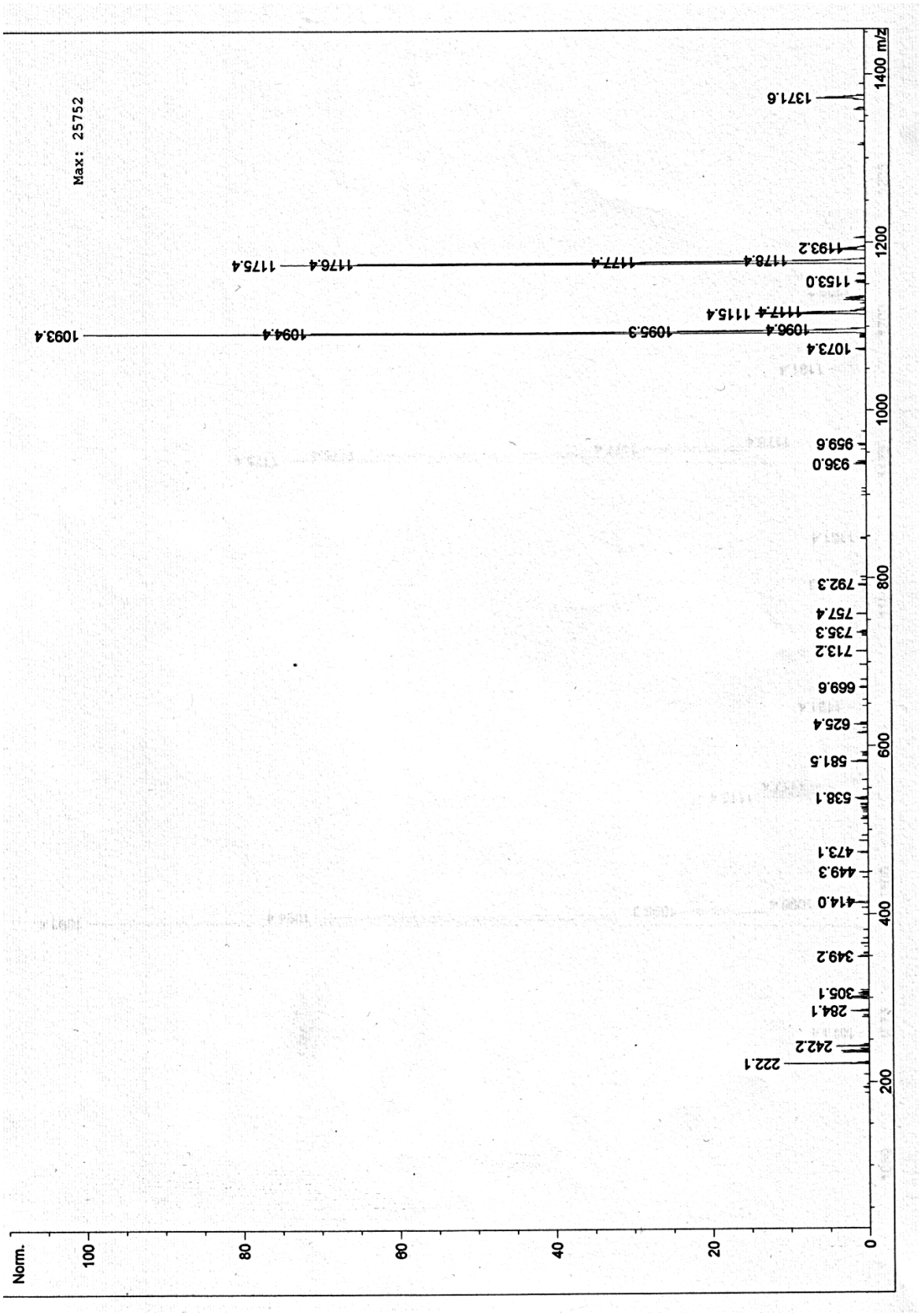

Figure S20. ESI-MS spectrum of Mn-calix[4]arene-salen **3b**

Table S1. Crystal data and structure refinement for UO_2-calix[4]arene-salen **2a**.

Formula	$C_{66}H_{64}N_2O_{11}U$, 2 CH_3CN
T (K)	100(2)
λ (Å)	0.70000
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions (°, Å)	a = 10.36(1), α = 90
	b = 16.91(1), β = 103.68(2)
	c = 17.93(1), γ = 90
V (Å)^3	3052(4)
Z	2
ρ_{calc} (g/mm^3)	1.503
μ (mm^{-1})	2.504
F(000)	1396
ϑ range for data collection (°)	1.65 - 28.10
Reflections collected	10632
Independent reflections	10632 [R(int) = 0.0000]
Data / restraints / parameters	10632 / 52 / 785
GooF	0.994
R_1 [I>2σ(I)], wR_2 [I>2σ(I)]	0.0565, 0.1423
R_1 (all data), wR_2 (all data)	0.0668, 0.1466

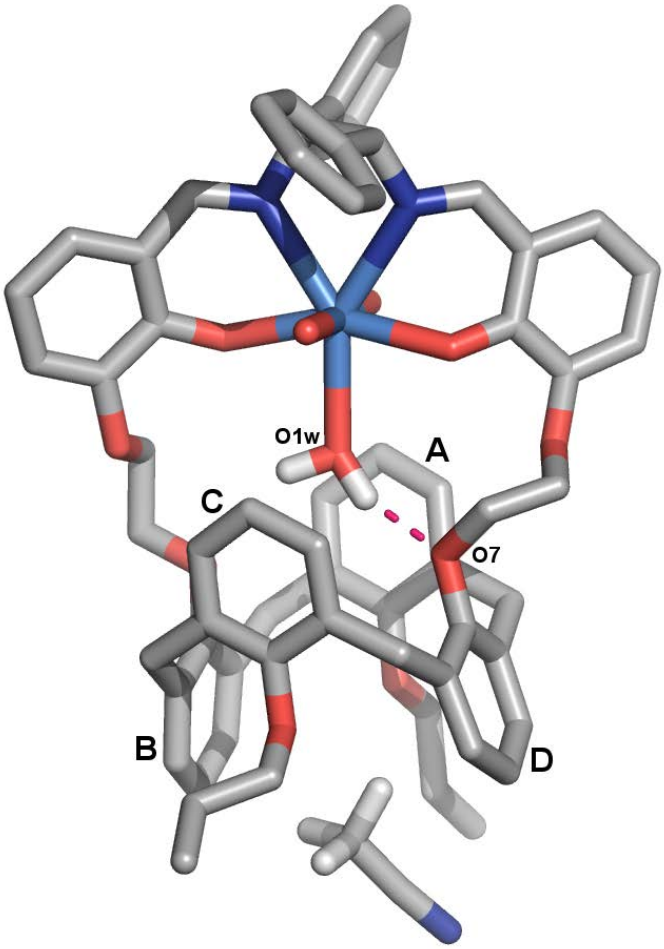

Figure S21. Scheme of the hydrogen bonding involving the water molecule coordinated to uranium center and the calix[4]arene scaffold of UO_2-calix[4]arene-salen **2a**.