Supplementary Materials

Mn(II) complexes of enlarged scorpiand-type azamacrocycles as mimetics of MnSOD enzyme

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[1] Molecular Science Institute, Universidad de Valencia, C/catedrático José Beltrán no. 2, 46980 Paterna, Valencia, Spain.; teresa.albelda@uv.es (M.T.A.); salvador.blasco@uv.es (S.B.); enrique.garcia-es@uv.es (E.G.E.)

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Table of contents

Table S1. Characterization data (^{1}H and ^{13}C NMR and Elemental Analysis) of **L1-3**

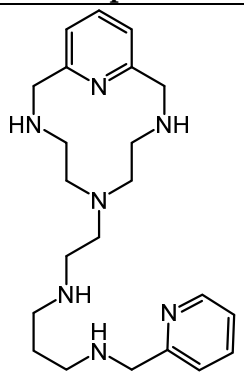
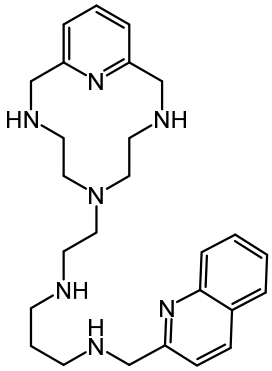
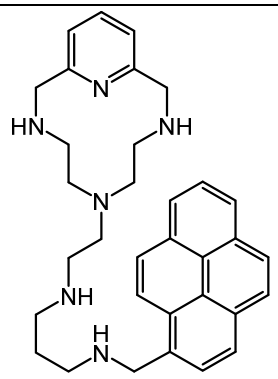
Compound	Characterization data
 **L1**	**^{1}H NMR (D_2O, 300 MHz)**: δ_H 8.83 (d, J=6 Hz, 1H), 8.51 (t, J=8 Hz, 1H), 8.03 (d, J=8 Hz, 1H), 8.00 (m, 2H), 7.49 (d, J=8 Hz, 2H), 4.69 (s, 2H), 4.68 (s, 4H), 3.34 (m, 10H), 3.10 (t, J=8 Hz, 2H), 2.98 (m, 4H), 2.28 (m, 2H). **^{13}C NMR (D_2O, 75.43 MHz)**: δ_C 149.2, 146.4, 145.5, 140.1, 127.5, 127.4, 122.6, 51.3, 50.8, 49.9, 48.9, 46.3, 45.3, 45.2, 44.0, 23.1. **Anal. Calc.** for $C_{22}H_{35}N_7 \cdot 5HCl \cdot 2H_2O$: C, 42.9; H, 7.2; N, 15.9. Exp.: C, 42.4; H, 7.5; N, 15.4.
 **L2**	**^{1}H NMR (D_2O, 300 MHz)**: δ_H 8.41 (d, J = 8Hz, 1H), 7.97 (d, J = 9 Hz, 1H), 7.92 (d, J = 9 Hz, 1H), 7.82 (t, J = 8, 1H), 7.77 (t, J = 8, 1H), 7.59 (t, J = 8, 1H), 7.50 (d, J = 8, 1H), 7.32 (d, J = 8 Hz, 2H), 4.52 (s, 2H), 4.49 (s, 4H), 3.16 (m, 10H), 2.93 (t, J = 8 Hz, 2H), 2.78 (m, 4H), 2.12 (m, 2H). **^{13}C NMR (D_2O, 75.43 MHz)**: δ_C 149.13, 148.85, 143.36, 142.84, 139.76, 133.39, 129.14, 128.71, 128.33, 124.41, 122.16, 121.03, 66.55, 50.86, 50.43, 49.66, 49.49, 45.87, 44.95, 43.55, 22.75. **Anal. Calc.** for $C_{26}H_{37}N_7 \cdot 5HCl$: C, 49.7; H, 6.7; N, 15.6. Exp.: C, 51.3; H, 7.5; N, 15.3.
 **L3**	**^{1}H NMR (D_2O, 300 MHz)**: δ_H 7.98 (t, J = 8 Hz, 2H), 7.80 (m, 5H), 7.61 (m, J = 9 Hz, 3H), 7.31 (d, J = 8 Hz, 2H), 4.49 (s, 2H), 4.45 (s, 4H), 3.05 (m, 10H), 2.85 (m, 2H), 2.61 (t, J = 5 Hz, 4H), 1.97 (m, 2H). **^{13}C NMR (D_2O, 75.43 MHz)**: δ_C 149.1, 140.1, 131.8, 130.8, 130.1, 128.8, 128.7, 128.6, 128.4, 127.3, 126.7, 126.2, 126.1, 125.0, 123.6, 123.3, 122.4, 121.48, 51.0, 50.5, 49.8, 46.1, 44.4, 43.5, 23.0. **Anal. Calc.** for $C_{33}H_{40}N_6 \cdot 4HCl \cdot 3H_2O$: C, 55.0; H, 7.0; N, 11.7. Exp.: C, 54.9; H, 6.9; N, 11.8.

Figure S1. Molar distribution diagrams of the different protonated species.