Structures of Manganese-Mefenamic Acid Complexes Determine Their High Lipoxygenase Inhibitory Activity

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Supplementary data:

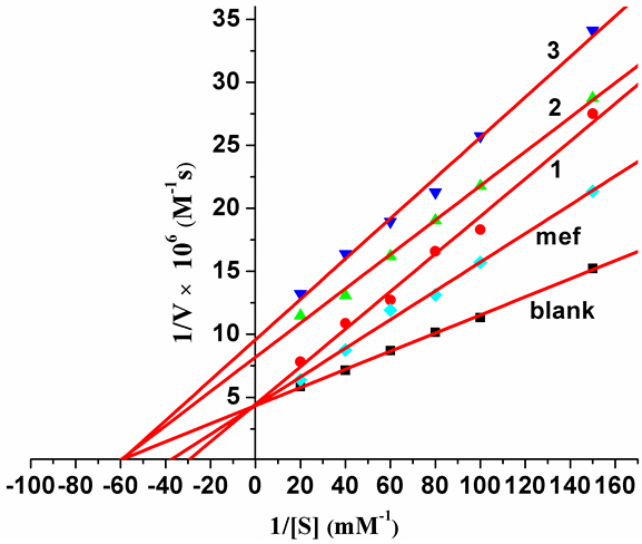

Figure S1. Lineweaver-Burk plots of the inhibition of LOX-1 by the complex **1-3** in H_3BO_3-NaOH buffer (0.1 M, pH 9.0). The reaction was initiated by adding 1×10^{-9} M of LOX-1 to the reaction mixture in the absence or presence of 1×10^{-5} M of the complex.

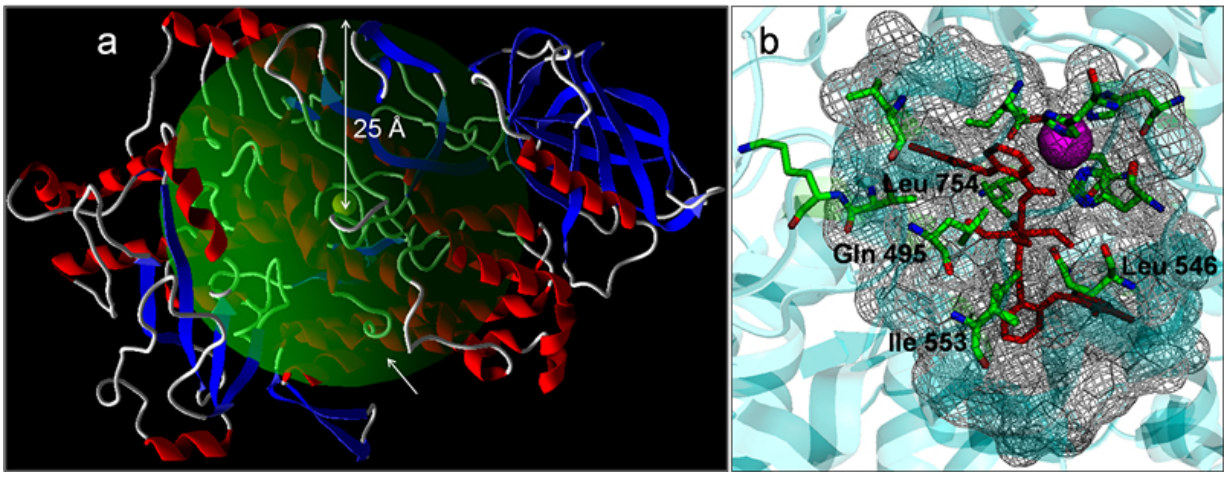

Figure S2. a) The docking area in this work. b) The spatial environment of the complex **1** (red molecule) inside the cavity II_a (gray net area) of LOX-1. Residues Gln495, Leu546, Ile553, and Leu754 surround the four coordinated methanol molecules of the complex **1**.

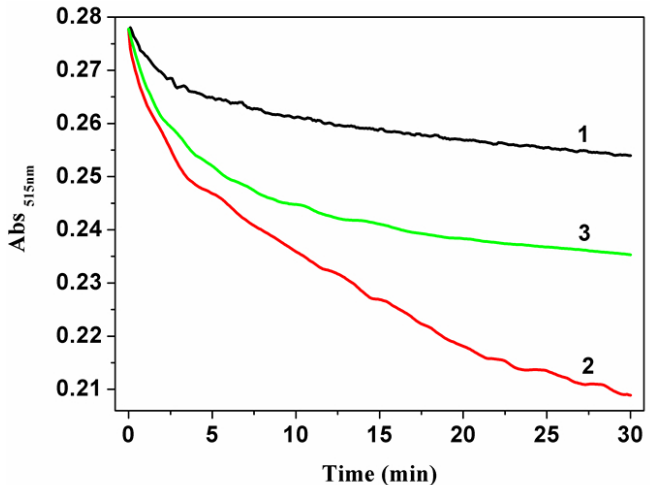

Figure S3. DPPH radical scavenging by the complexes **1-3** in methanol solution containing 1.5% DMF monitored at 515 nm as a function of reaction time at room temperature. [complex] = 0.1 mM, [DPPH] = 0.03 mM.

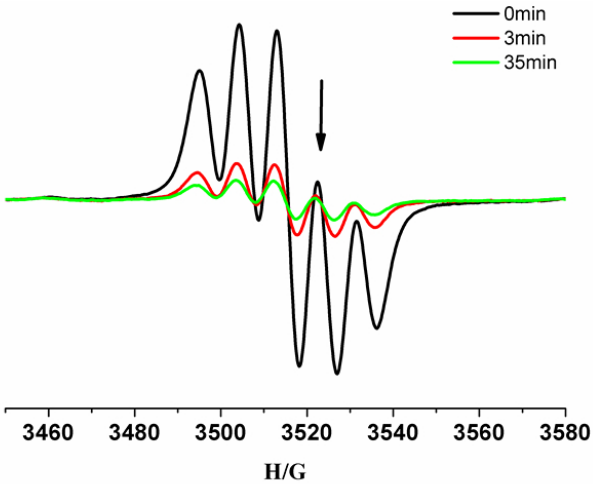

Figure S4. EPR signal intensity of the DPPH in the presence of complex **2** as function of incubation time. Conditions: [complex **2**] = 50 μM in CH_3OH, [DPPH] = 0.3 mM. EPR conditions: microwave frequency, 9.454 GHz; microwave power, 2 mW; modulation frequency, 100 KHz; modulation amplitude, 3 G; T = 303 K.

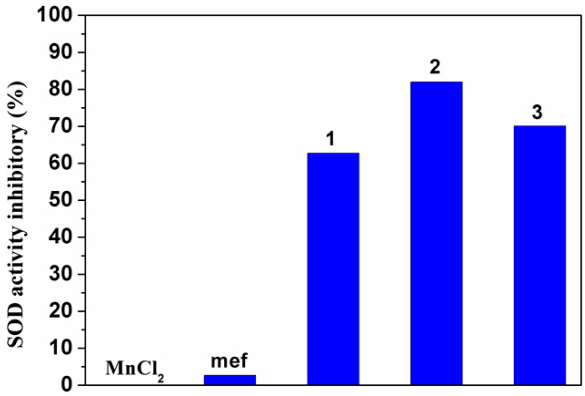

Figure S5. SOD inhibitory activity of the complexes **1-3,** $MnCl_2$, and mefenamic acid. The concentration of the complexes is 1×10^{-5} M.

Table S1 Selected IR data (in cm^{-1}) for the complexes **1-3**.

Complexes	**1**	**2**	**3**
v(O-H)	-	3469	3446
v(N-H)	3314	3306	3299
v_{asym}(C=O)	1613	1609	1612
v_{sym}(C=O)	1391	1385	1387
v(C-H)	748	745	841, 723