Supplementary Information for

A Family of dioxo-Molybdenum (VI) Complexes of N_2X Heteroscorpionate Ligands of Relevance to Molybdoenzymes

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Table S1. Selected Bond Lengths (Å) and Angles (°) for L1OMoO_2Cl

Mo-O2	1.710(6)
Mo-O2A	1.710(6)
Mo-Cl	2.373(3)
Mo-N2	2.373(8)
Mo-N2A	2.373(8)
Mo-O1	1.898(9)
O2-Mo-O2A	101.9(5)
O2-Mo-N2	91.2(3)
O2-Mo-N2A	166.8(3)
O2-Mo-Cl	94.5(2)
O2-Mo-O1	99.2(2)
O2A-Mo-N2	91.2(3)
O2A-Mo-N2A	166.8(3)
O2A-Mo-Cl	94.5(2)
O2A-Mo-O1	99.2(2)
N2-Mo-N2A	75.7(4)
N2-Mo-Cl	82.6(2)
N2-Mo-O1	80.2(3)
N2A-Mo-Cl	82.6(2)
N2A-Mo-O1	80.2(3)
Cl-Mo-O1	158.1(2)

Table S2. Selected Bond Lengths (Å) and Angles (°) for L3SMoO$_2$Cl

Mo-O1	1.694(6)
Mo-O2	1.694(6)
Mo-Cl	2.384(4)
Mo-N1	2.346(7)
Mo-N2	2.346(7)
Mo-S	2.421(4)
O1-Mo-O1A	103.9(5)
O1-Mo-N1	166.6(3)
O1-Mo-N2	89.5(3)
O1-Mo-Cl	97.7(3)
O1-Mo-S	95.9(3)
O1A-Mo-N1	89.5(3)
O1A-Mo-N1A	166.6(3)
O1A-Mo-Cl	97.7(3)
O1A-Mo-S	95.9(3)
N1-Mo-N1A	77.1(3)
N1-Mo-Cl	81.3(2)
N1-Mo-S	81.5(2)
N1A-Mo-Cl	81.3(2)
N1A-Mo-S	81.5(2)
Cl-Mo-S	157.8(1)

Table S3. Selected Bond Lengths (Å) and Angles (°) for L4OMoO$_2$Cl

Mo-O4	1.754(8)
Mo-O3	1.769(7)
Mo-Cl	2.233(4)
Mo-N1	2.212(9)
Mo-N3	2.323(9)
Mo-O1	2.130(7)
O4-Mo-O3	103.3(3)
O4-Mo-N1	94.4(4)
O4-Mo-N3	167.7(4)
O4-Mo-Cl	96.0(3)
O4-Mo-O1	92.9(3)
O3-Mo-N1	89.6(3)
O3-Mo-N3	85.8(3)
O3-Mo-Cl	100.8(3)
O3-Mo-O1	160.3(3)
N1-Mo-N3	77.1(3)
N1-Mo-Cl	163.2(2)
N1-Mo-O1	77.9(3)
N3-Mo-Cl	90.4(2)
N3-Mo-O1	76.7(3)
Cl-Mo-O1	88.4(2)

Table S4. Selected Bond Lengths (Å) and Angles (°) for L5OMoO$_2$Cl

Mo-O1	1.697(4)
Mo-O2	1.696(4)
Mo-Cl	2.395(2)
Mo-N2	2.374(5)
Mo-N4	2.354(5)
Mo-O3	1.911(4)
O1-Mo-O2	104.8(2)
O1-Mo-N2	89.2(2)
O1-Mo-N4	164.5(2)
O1-Mo-Cl	94.1(2)
O1-Mo-O3	99.5(2)
O2-Mo-N2	165.8(2)
O2-Mo-N4	90.4(2)
O2-Mo-Cl	94.4(2)
O2-Mo-O3	100.9(2)
N2-Mo-N4	75.5(2)
N2-Mo-Cl	82.3(1)
N2-Mo-O3	78.4(2)
N4-Mo-Cl	81.6(1)
N4-Mo-O3	80.1(2)
Cl-Mo-O3	156.1(1)