Oxaaza Cyclophanes in the Recognition of Nucleotides. The Role of oxygen and electron-rich Aromatic Rings

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Electronic Supplementary Information (ESI) available: NMR titrations, distribution diagrams, suggested protonation sequences, calculated minimum energy structures for the ligands and their complexes.
S1. Distribution diagrams for the protonation of the receptors prepared in this work.
S2. Variation of $^1$H NMR signals upon protonation for receptor Re33.
S3. Variation of $^1$H NMR signals upon protonation for receptor Re222.

S4. Variation of $^1$H NMR signals upon protonation for receptor Re343.
S5. Distribution diagrams for the interaction of the receptors prepared in this work with ATP.

S6. Distribution diagrams for the interaction of the receptors prepared in this work with ADP.
S7. Distribution diagram for the interaction of Re343 with AMP.

S8. Variation of the aromatic $^1$H NMR Hb signal of ATP upon interaction with the receptors prepared in this work (red: free ATP).
S9. Comparison of the variation of the aromatic $^1$H NMR Hb signal of ATP upon interaction with the receptors prepared in this work.

S10. Variation of the Pγ signal of ATP upon interaction with the receptors prepared in this work (red: free ATP).
S11. Minimum energy structure calculated for $\text{H}_3\text{Re}^{3+}\text{HATP}^{3-}$

S12. Minimum energy structure calculated for $\text{H}_3\text{Re}^{3+}\text{HATP}^{3-}$

S13. Minimum energy structure calculated for $\text{H}_3\text{Re}^{3+}\text{HADP}^{2-}$
S14. Minimum energy structure calculated for $\text{H}_2\text{Re}^{3+}\text{AMP}^{2-}$