Supplementary Material for Organic & Biomolecular Chemistry

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

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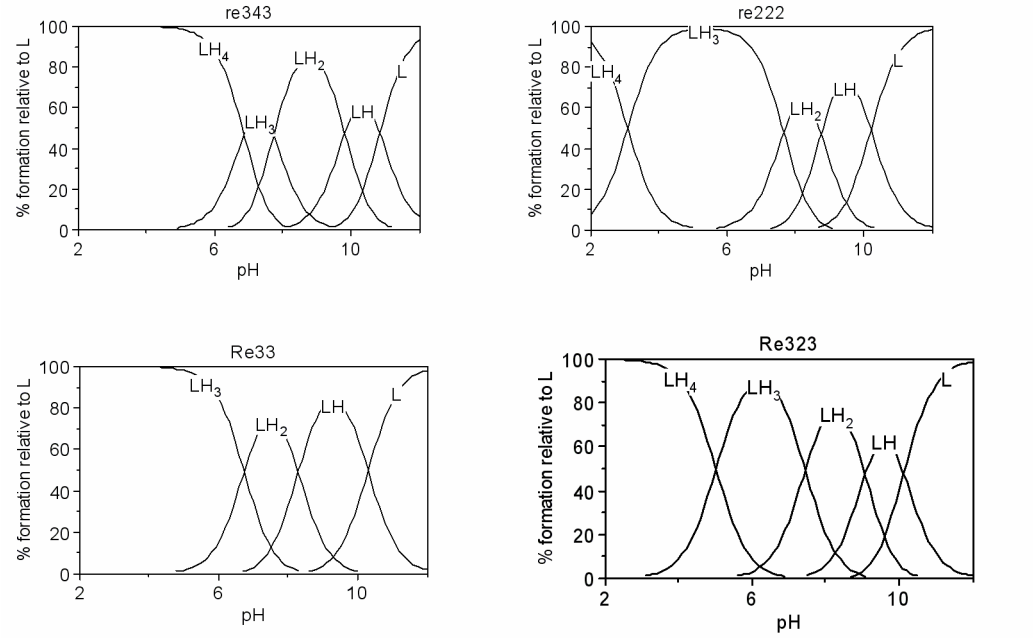
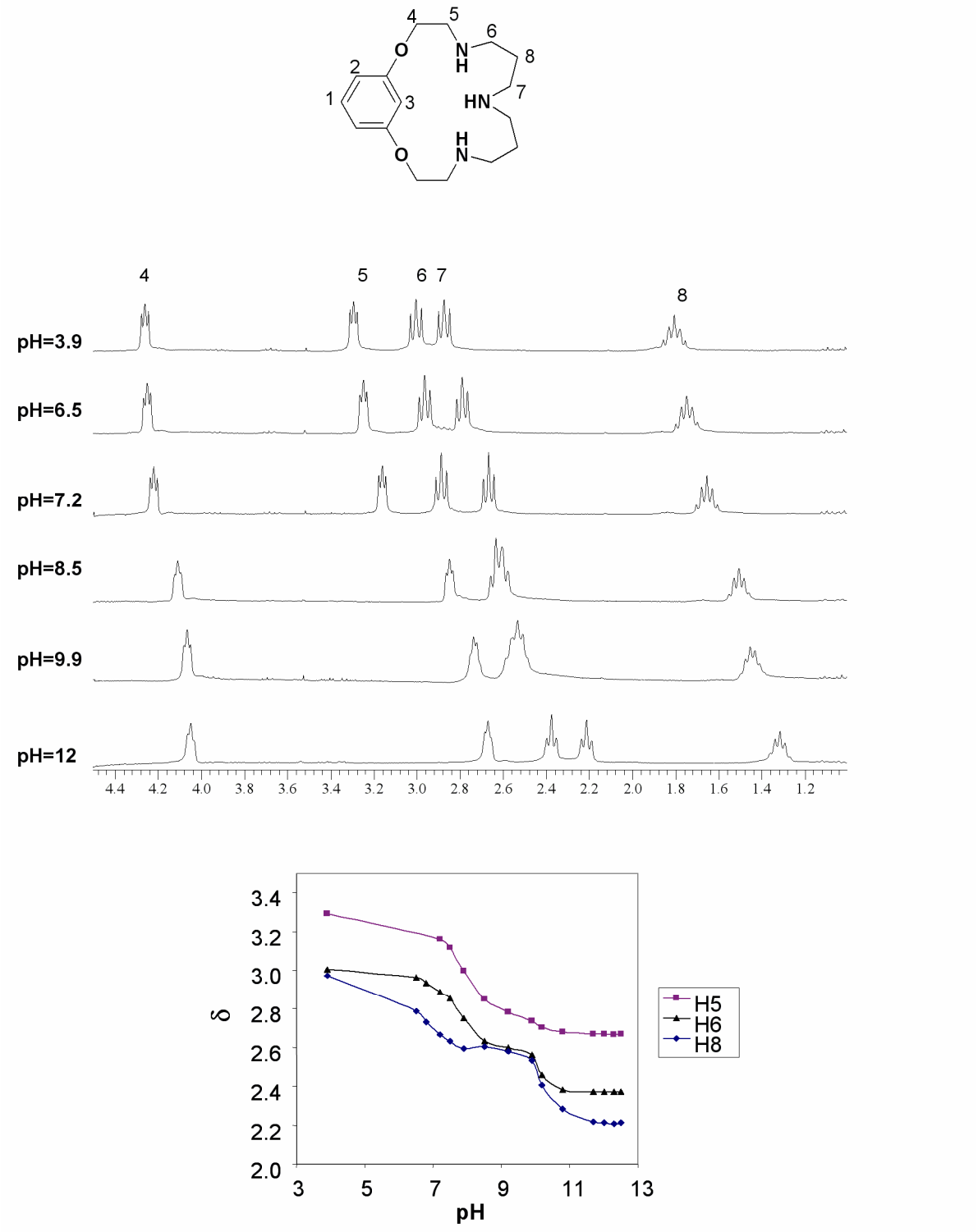
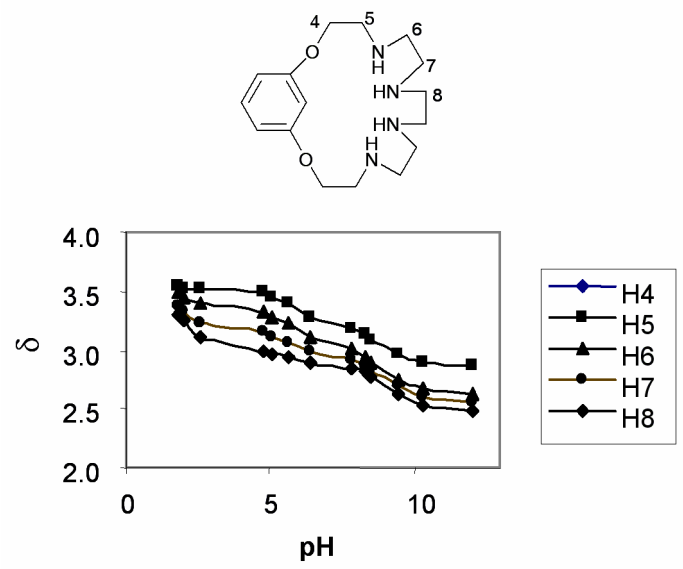
Electronic Supplementary Information (ESI) available: NMR titrations, distribution diagrams, suggested protonation sequences, calculated minimum energy structures for the ligands and their complexes.



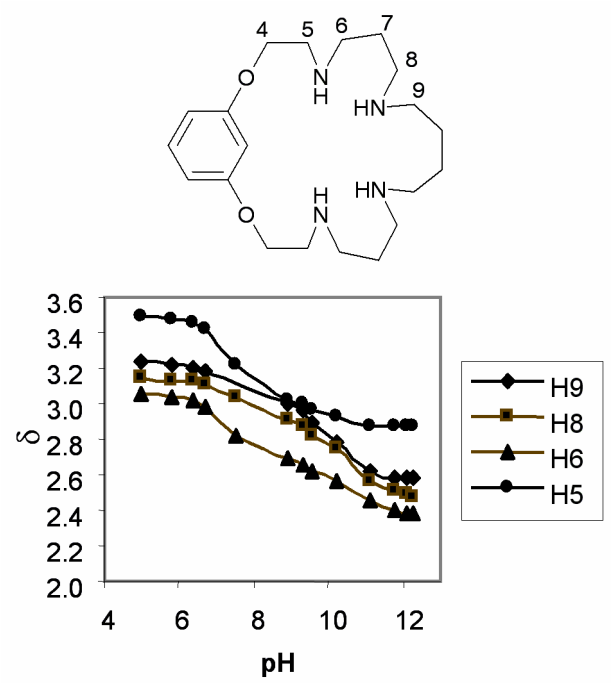
S1. Distribution diagrams for the protonation of the receptors prepared in this work.



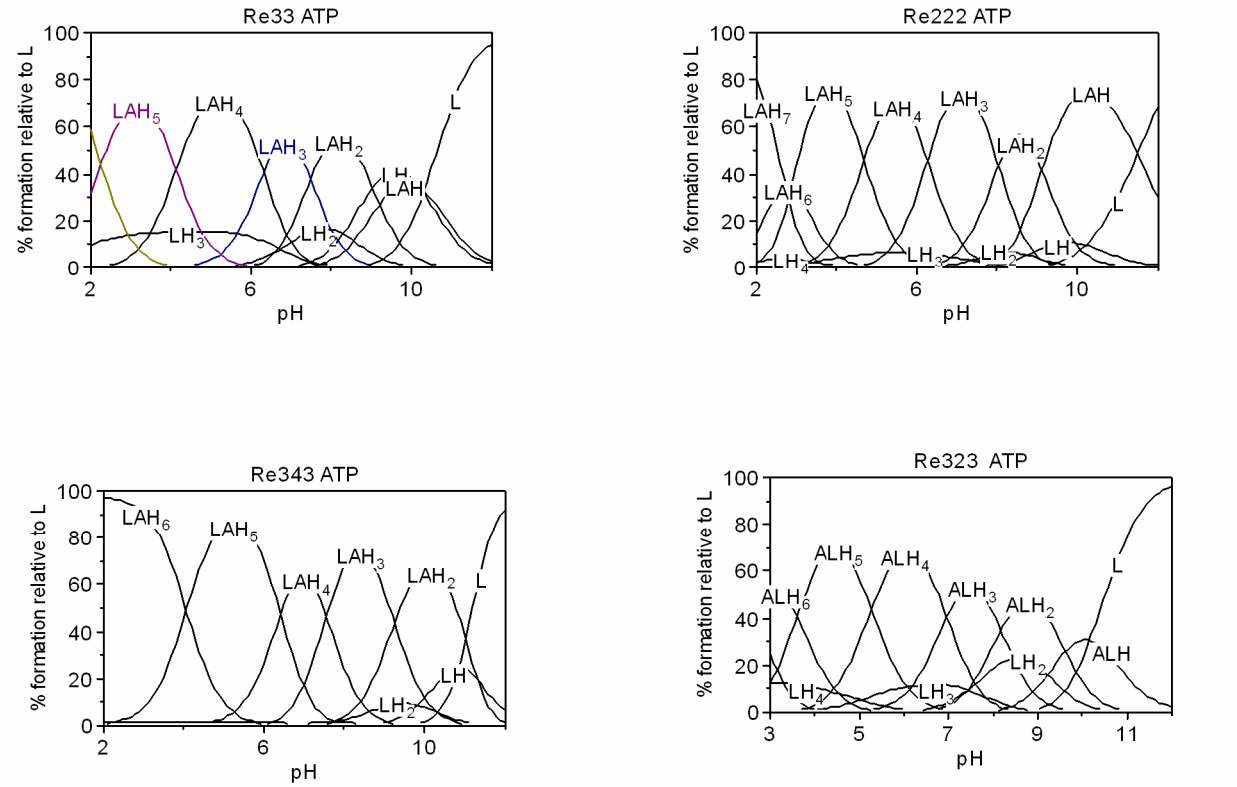
S2. Variation of ^{1}H NMR signals upon protonation for receptor **Re33**.



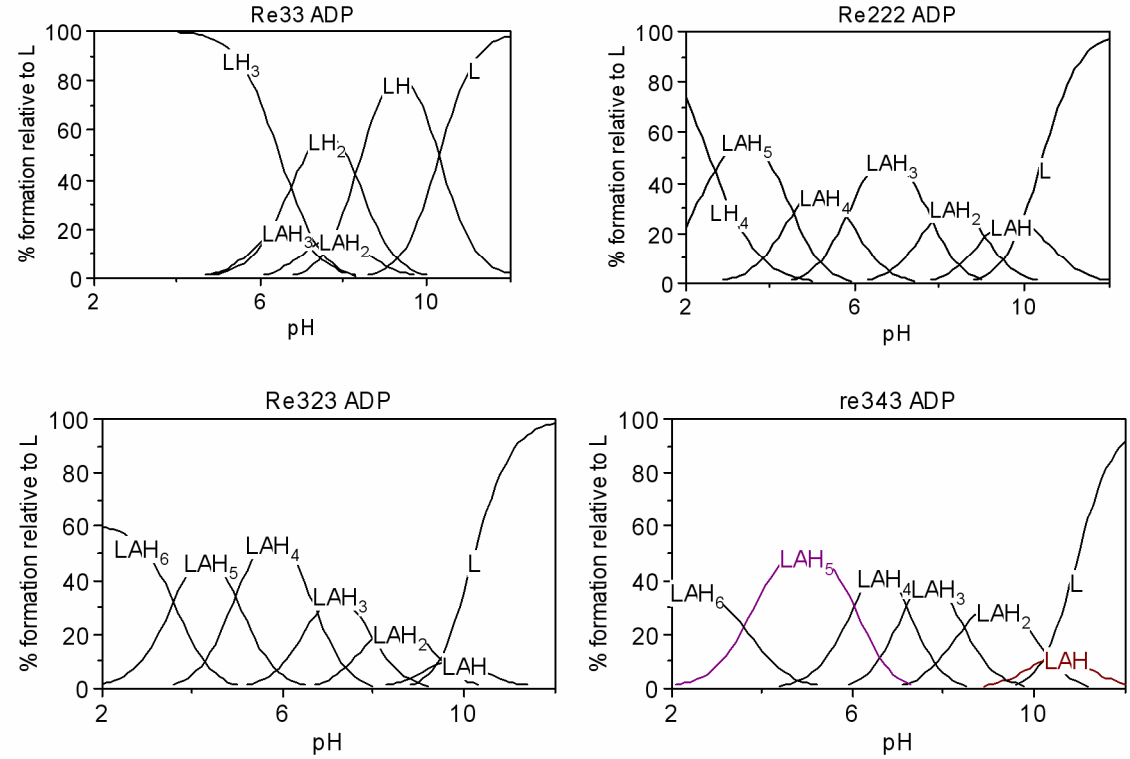
S3. Variation of ^{1}H NMR signals upon protonation for receptor **Re222**.



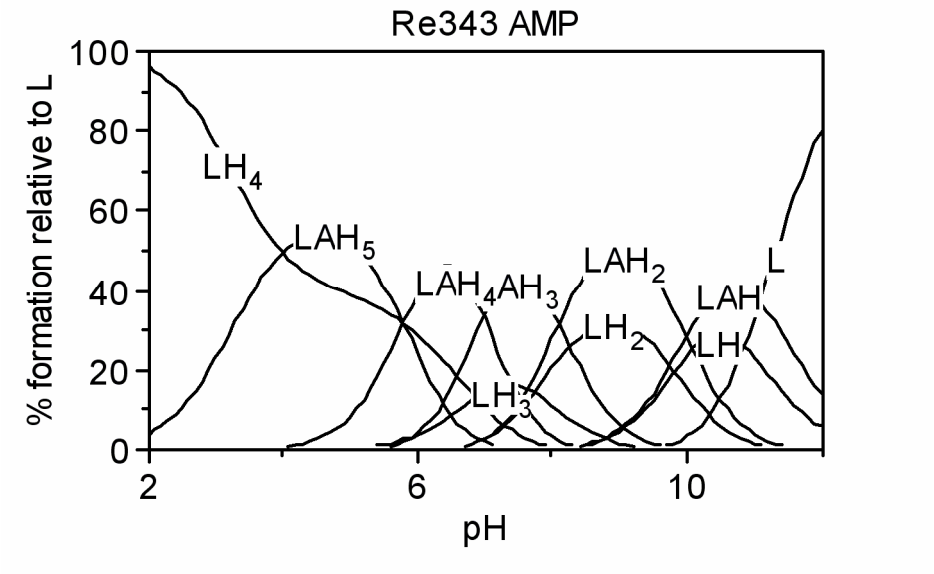
S4. Variation of ^{1}H NMR signals upon protonation for receptor **Re343**.



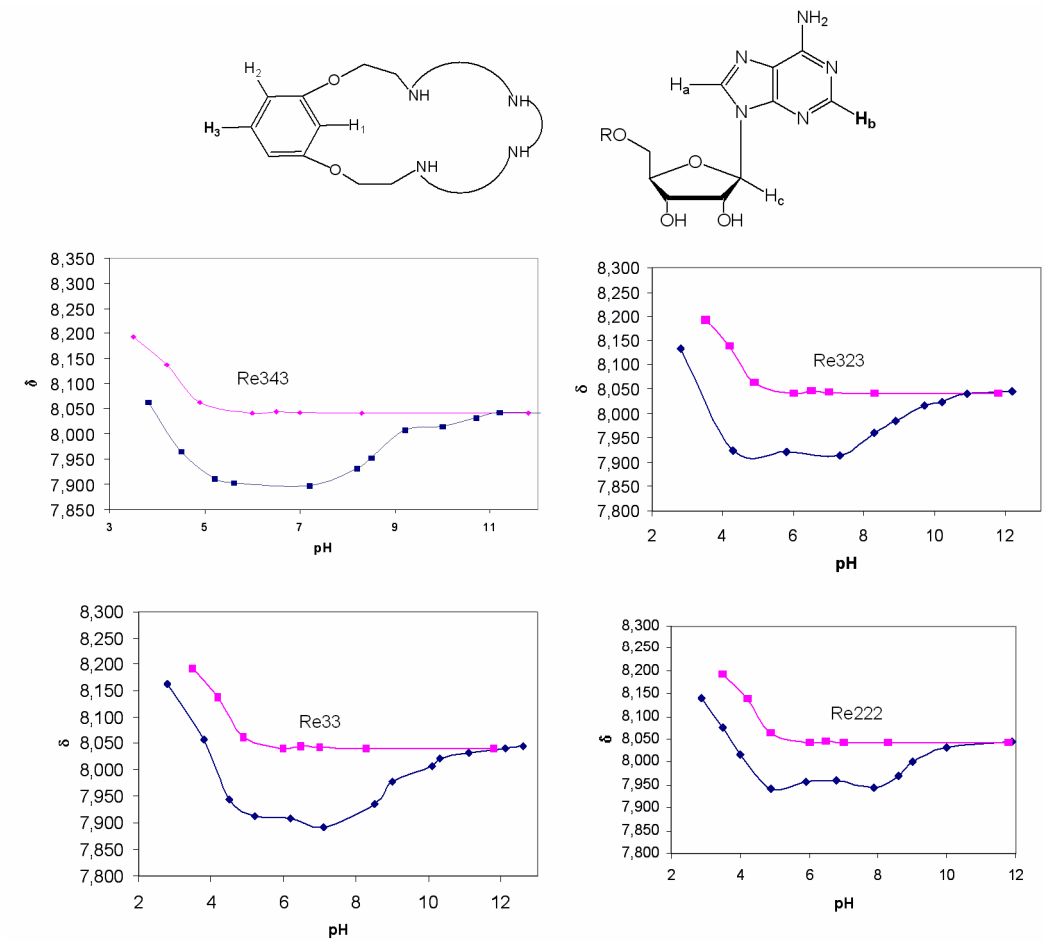
S5. Distribution diagrams for the interaction of the receptors prepared in this work with **ATP**.



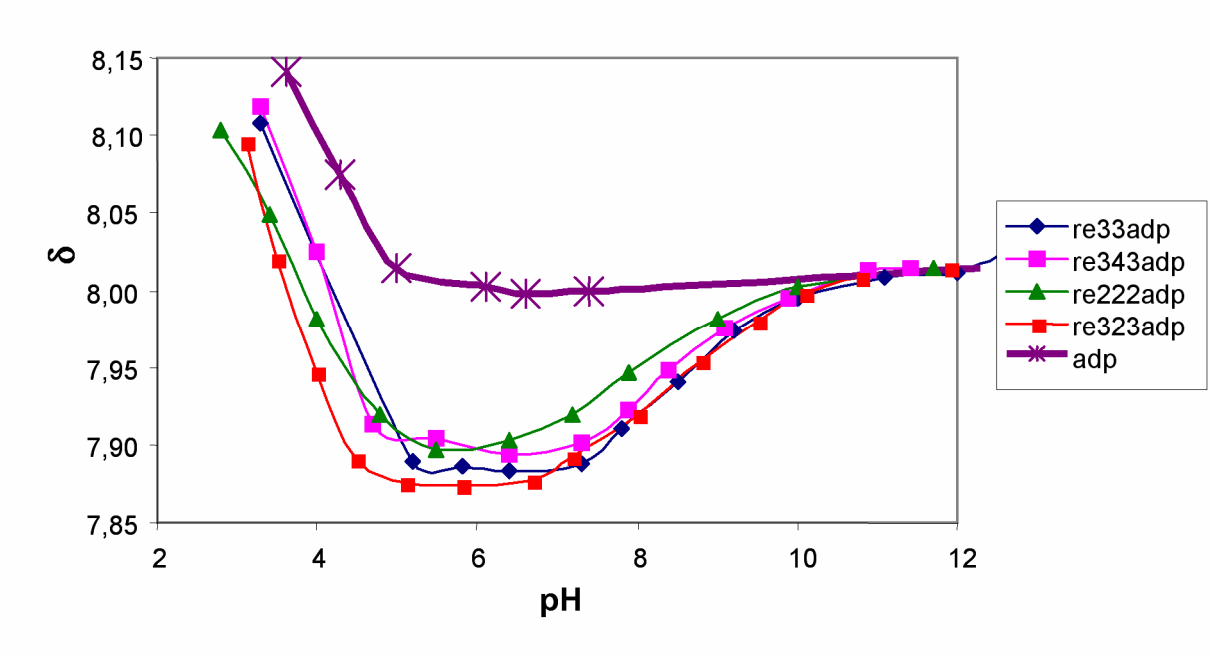
S6. Distribution diagrams for the interaction of the receptors prepared in this work. with **ADP**.



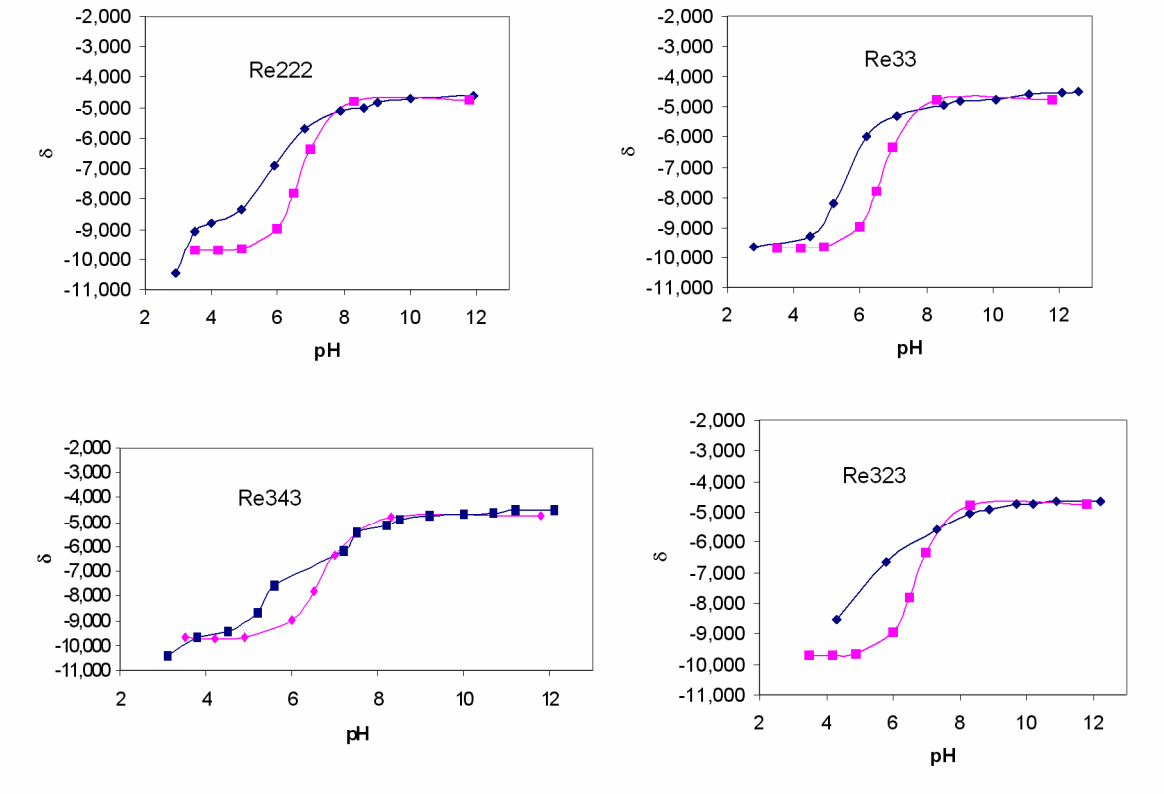
S7. Distribution diagram for the interaction of **Re343** with **AMP**.



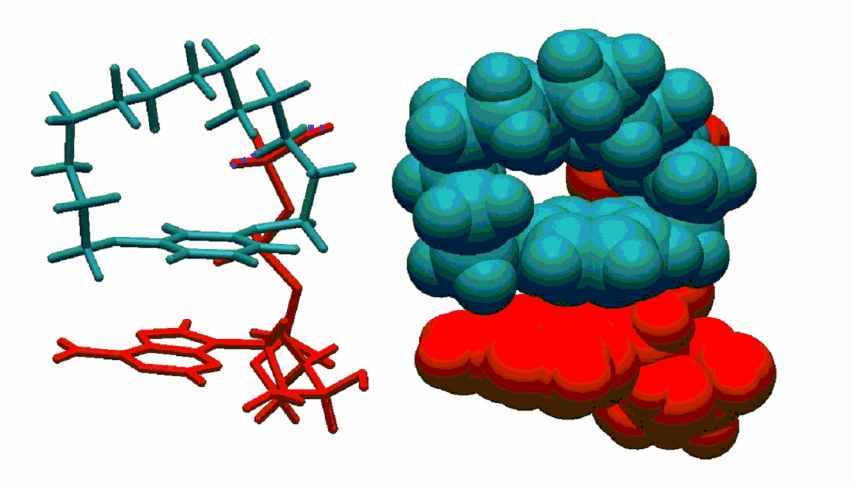
S8. Variation of the aromatic ^{1}H NMR Hb signal of **ATP** upon interaction with the receptors prepared in this work (red: free **ATP**).



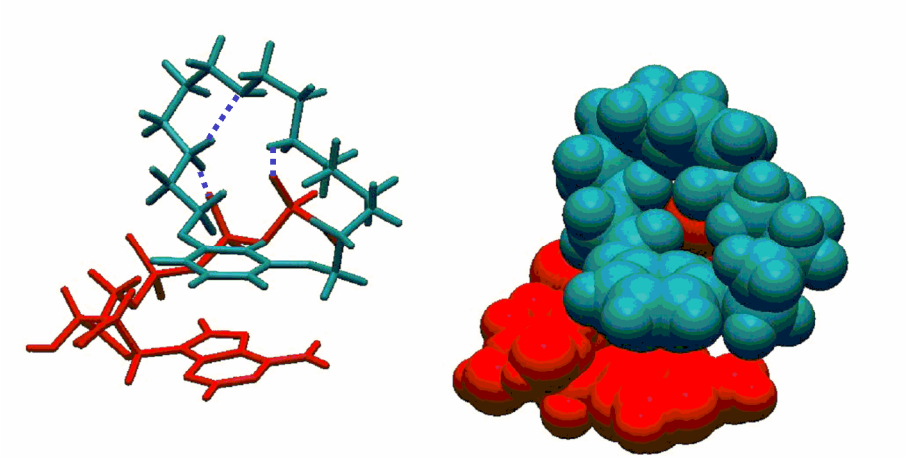
S9. Comparison of the variation of the aromatic ^{1}H NMR Hb signal of **ATP** upon interaction with the receptors prepared in this work.



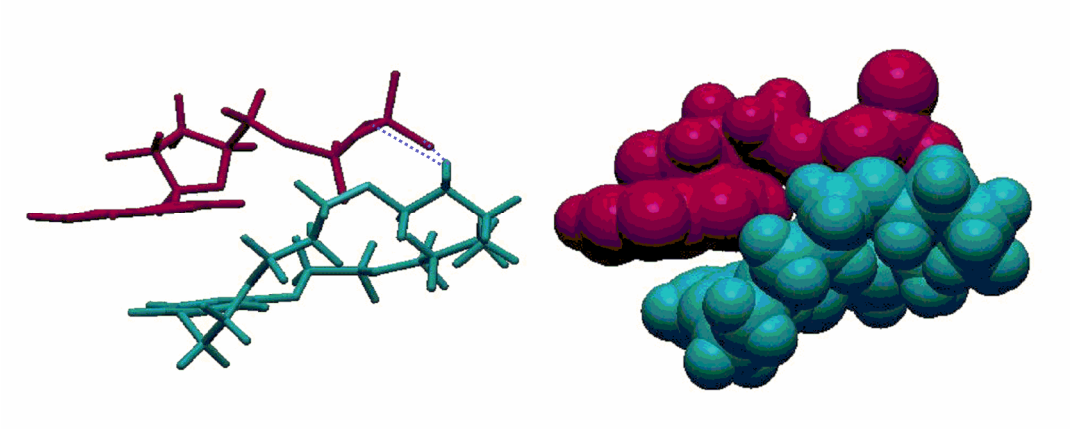
S10. Variation of the Pγ signal of **ATP** upon interaction with the receptors prepared in this work (red: free **ATP**).



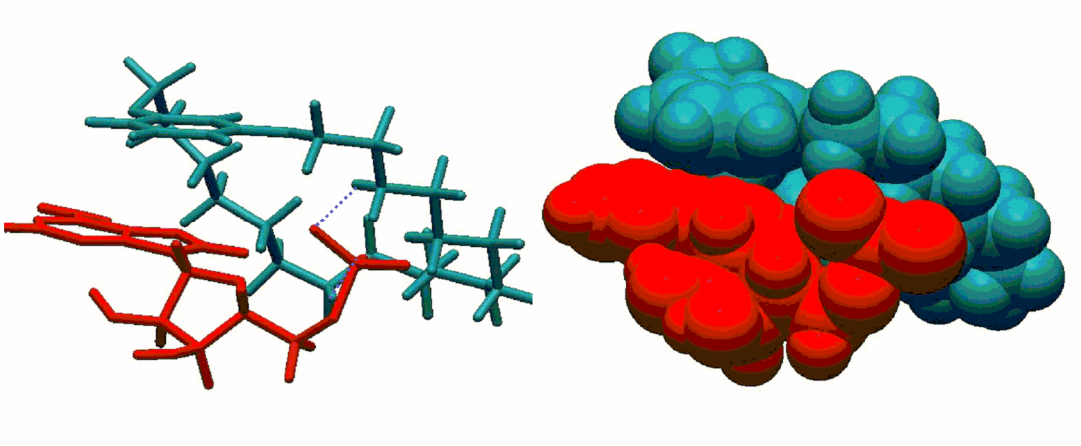
S11. Minimum energy structure calculated for $\mathbf{H_3Re33^{3+}\text{-}HATP^{3-}}$



S12. Minimum energy structure calculated for $\mathbf{H_3Re323^{3+}\text{-}HATP^{3-}}$



S13. Minimum energy structure calculated for $\mathbf{H_3Re343^{3+}\text{-}HADP^{2-}}$



S14. Minimum energy structure calculated for **H_3Re343^{3+}-AMP^{2-}**