Supplementary Materials

Characterization of Na/K-ATPase interaction with selected Au(III) and Pt(II)complexes: experimental and theoretical approach

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SM.1 Analysis of accessible surface of residues in selected inhibitory sites of Na/K-ATPase

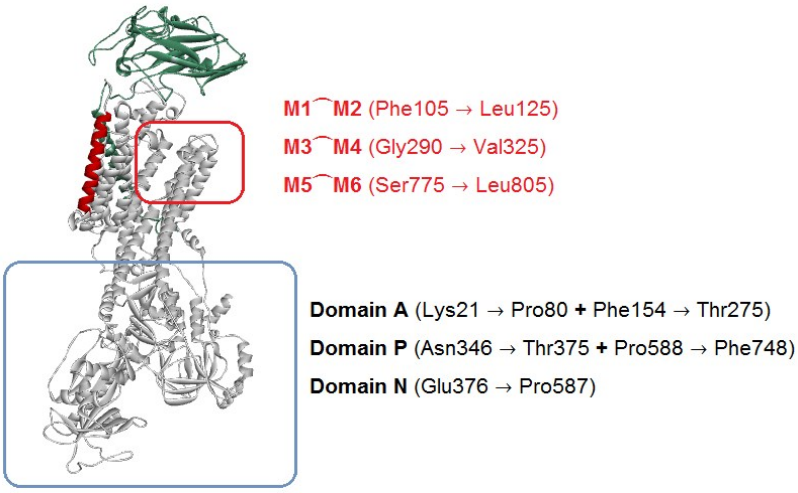

Fig. S1. Localization and sequences of SASA analyzed amino acids residues.

SM.2 Docking studies

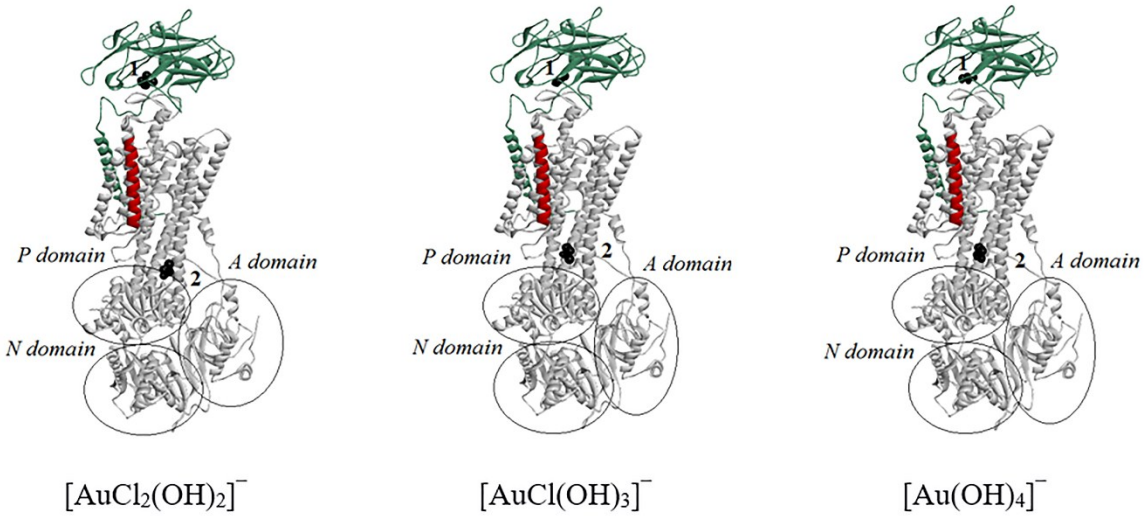

Fig. S2. Binding sites in E1 conformation of Na/K-ATPase for $[AuCl_4]^-$ hydrolyzed species.

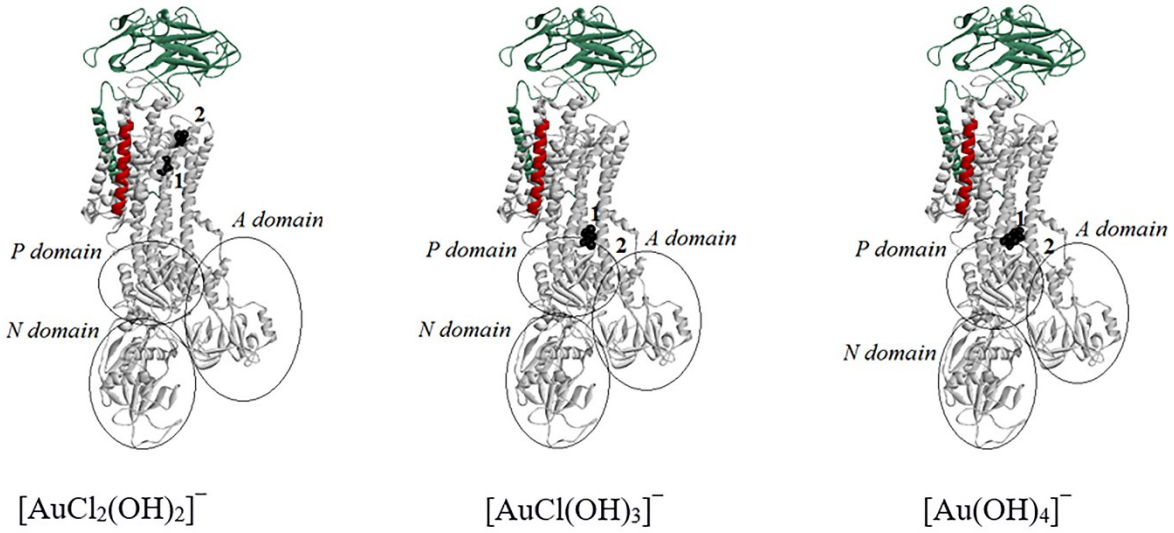

Fig. S3. Binding sites in E2P conformation of Na/K-ATPase for $[AuCl_4]^-$ hydrolyzed species.

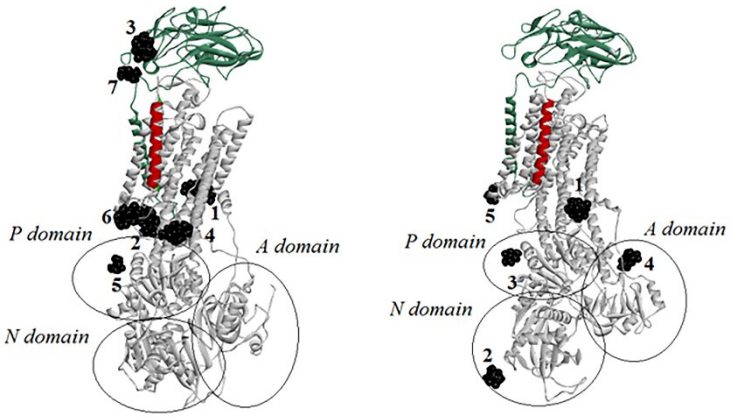

Fig. S4. Binding sites in E1 and E2P conformation of Na/K-ATPase for $[PtClOH(dmso)_2]$ complexes.

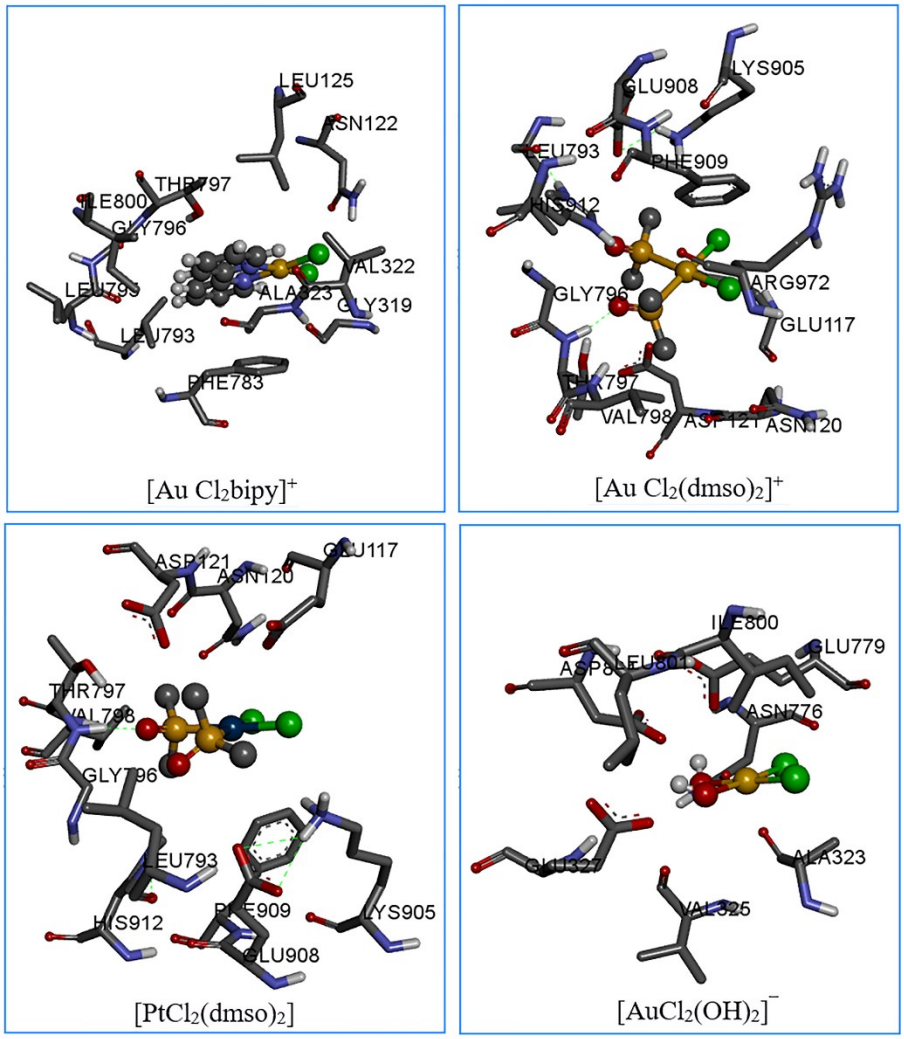

Fig. S5. Amino acid environment of complexes bound in the ion channel of Na/K-ATPase with E2P conformation.

Table S1. Nature of amino acid from environment of complexes bonded in the ion channel of Na/K-ATPase with E2P conformation.

Metal Complex	Number of amino-acid residues			
	Nonpolar	Polar	Positive	Negative
$[AuCl_2bipy]^+$	9	2	0	0
$[AuCl_2(dmso)_2]^+$	5	3	1	3
$[PtCl_2(dmso)_2]$	5	2	0	3
$[AuCl_2(OH)_2]^-$	3	1	0	3

SM.3 Binding sites of hydrolyzed Au(III) and Pt(II) species

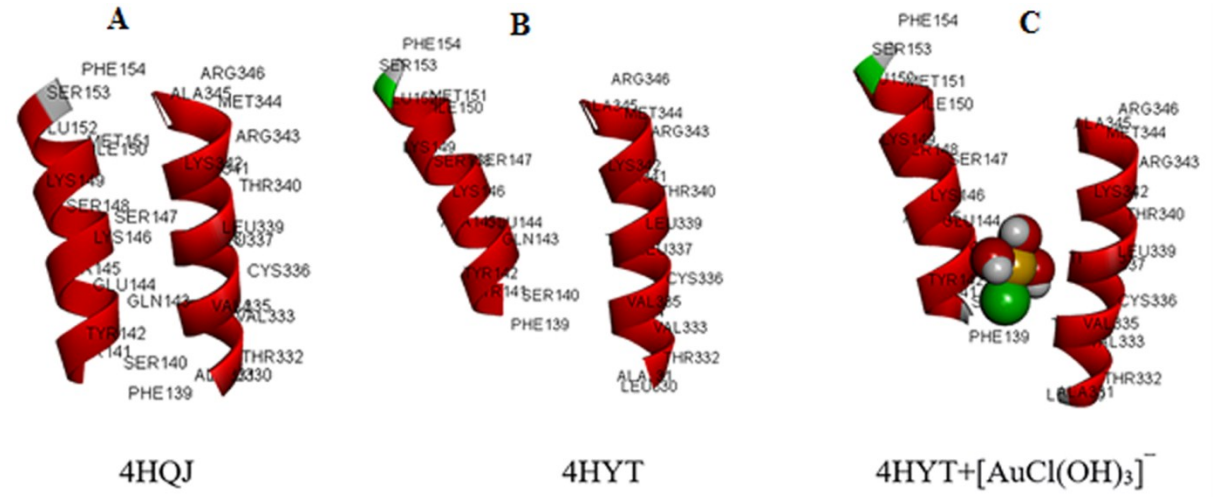

Fig. S6. Selected sequences of M2 and M4 helices in (A) E1 (4HQJ) and (B) E2P (4HYT) and (C) the system 4HYT+$[AuCl(OH)_3]^-$.

This figure illustrates the selected sequences of M2 and M4 helices with amino acid residues favourable for binding Au(III) hydrolyzed species, using the system 4HYT+ $[AuCl(OH)_3]^-$ as an example. The equilibrium between E1 and E2P conformations leads to "shearing" of these helices, as well as their moving away. Binding of the complex ions between M2 and M4 helices in both enzyme conformations affects on their equilibrium disabling this shearing and moving, thus inhibiting the enzyme activity.