Supplementary tables with data obtained from models 1-10 clustering as cluster 1-3

Supplementary Table 1. Selected models of the His6: Aβ peptide complex forming the Cluster 1

Cluster 1	Receptor (Aβ peptide)	Ligand (His6)	H-bond	Salt bridges	Binding Energy Δ^{i}G kcal/mol
Model 1	HIS13, **LYS16**, **LEU17**, **PHE20**, **ALA21**, **VAL24**, **GLY25**, **LYS28**, **ILE31**, **LEU34**, **MET35**, GLY38, VAL39, ALA42	**HIS1,** **HIS3,** **HIS4,** **HIS5,** **HIS6**	GLY38:HIS6 ALA42:HIS6	ALA42: HIS6	-6.6
Model 4	**LYS16**, **LEU17**, VAL18, **PHE20**, **ALA21**, GLU22, **VAL24**, **GLY25**, SER26, LYS28, **ILE31**, LEU34, **MET35**	**HIS1,** HIS2, **HIS3,** **HIS4,** **HIS5,** **HIS6**	LEU17:HIS4 ALA21:HIS3	GLU22: HIS1	-4.3
Model 7	**LYS16**, **LEU17**, VAL18, **PHE20**, **ALA21**, GLU22, ASP23, **VAL24**, **GLY25**, **LYS28**, ALA30, **ILE31**, GLY33, **LEU34**, **MET35**	**HIS1,** HIS2, **HIS3,** **HIS4,** **HIS5,** **HIS6**	**ALA21:HIS3**		**-6.8**
Model 8	HIS13, **LYS16**, **LEU17**, VAL18, **PHE20**, **ALA21**, **VAL24**, **GLY25**, LYS28, **ILE31**, **LEU34**, **MET35**, GLY38, VAL39, ALA42	**HIS1,** HIS2, **HIS3,** **HIS4,** **HIS5,** **HIS6**	GLY38:HIS3		-6.6
Selected amino acids constituting the interacting interface	**LYS16,LEU1,PHE20,LA21,VAL24,GLY25,LYS2,ILE31, LEU34,MET35,**	**HIS1,HIS3 HIS4,HIS5 ,HIS6**			**-6.8**

Cluster 2	Receptor (Aβ peptide)	Ligand (His6)	H-bond	Salt bridges	Binding Energy Δ^{i}G kcal/mol
Model 2	ASP1, ALA2, **GLU3**, **HIS6**, **ASP7**, **TYR10**, **HIS14**	**HIS1**, **HIS2**, HIS3, HIS4, HIS5, **HIS6**			-1.4
Model 5	ALA2, **GLU3**, **HIS6**, **ASP7**, **TYR10**, **HIS14**, LEU17	**HIS1**, **HIS2**, HIS3, HIS5, **HIS6**	HIS6: HIS5 HIS6:HIS6 GLY9:HIS1 GLY9:HIS1 TYR10:HIS1		-4.1
Model 9	**GLU3**, PHE4, **HIS6**, **ASP7**, **TYR10**, **HIS14**, GLN15, LEU17, VAL18	**HIS1**, **HIS2**, HIS5, **HIS6**	GLU3:HIS5 HIS6:HIS5 ASP7:HIS6	GLU3:HIS6 GLU11:HIS2	**-4.8**
Model 10	ALA2, **GLU3**, **HIS6**, **ASP7**, **TYR10**, **HIS14**	**HIS1**, **HIS2**, HIS3, HIS4, **HIS6**	ALA2:HIS3 GLU3:HIS2 GLU3:HIS1 ASP7:HIS2 GLY9:HIS6	GLU3:HIS1 ASP7:HIS2	-3.3
Selected amino acids constituting the interacting interface	**GLU3**, **HIS6**, **ASP7**, **TYR10**, **HIS14**	**HIS1**, **HIS2**, **HIS6**			**-4.8**

Supplementary Table 2. Selected models of the His6: Aβ peptide complex forming the Cluster 2

Cluster 3	Receptor (Aβ peptide)	Ligand (His6)			Binding Energy ΔⁱG kcal/mol
Model 3	**GLY9**, TYR10, VAL12, HIS13, HIS14, LEU17, **VAL18**	HIS1, **HIS2**, HIS3, HIS4, HIS5, HIS6	TYR10: HIS6 HIS14:HIS4		-2.6
Model 6	ASP7, SER8, **GLY9**, GLU11, **VAL12**, GLN15, LYS16, PHE19	HIS1, **HIS2**, HIS6	GLN15:HIS3 ASP7:HIS2 GLN15:HIS2	ASP7:HIS2 ASP7:HIS2 GLU11:HIS2 GLU11:HIS2	-1.7
Selected amino acids constituting the interacting interface	**GLY9**, **VAL18**	**HIS1**, **HIS2**, **HIS6**			**-2.6**

Supplementary Table 3. Selected models of the His6: Aβ peptide complex forming the Cluster 3