Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

"Effect of Zn^{2+} ions on the assembly of amylin oligomers: Insight into the molecular mechanisms"

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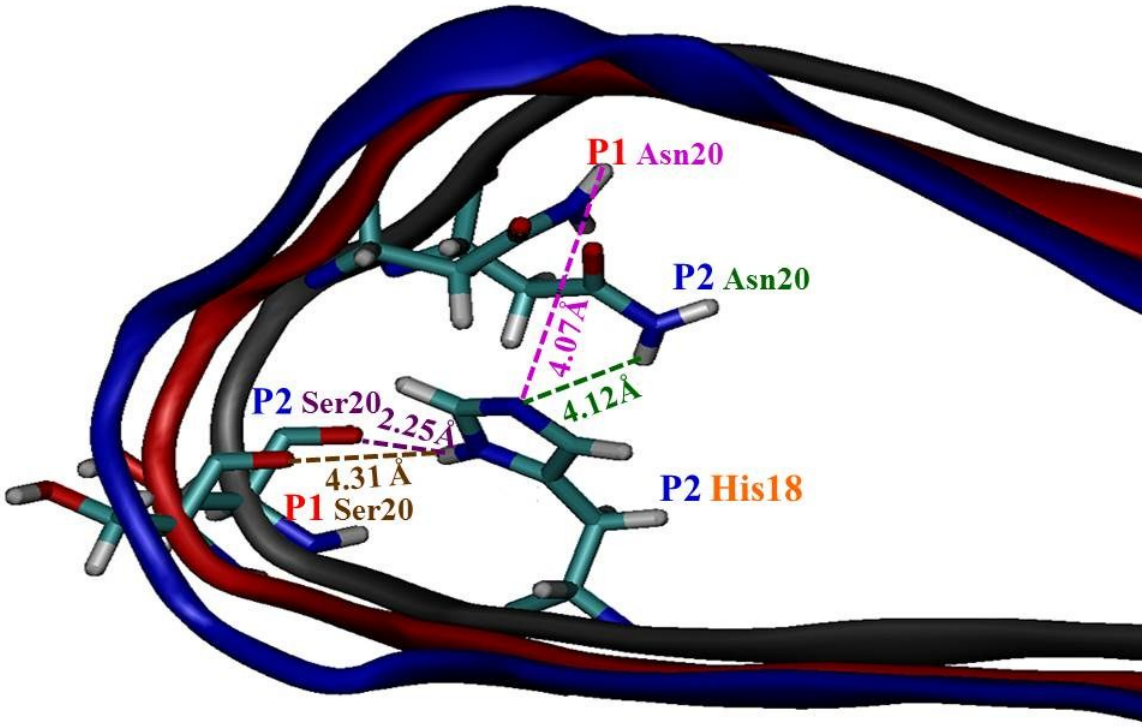

Figure S1: Illustration of the inside the core domain of model Q1 that is based on model A1. The core domain in which the His18 suppose to bind Zn^{2+} ion can not accommodate the Zn^{2+} ion, therefore in the minimization process the Zn^{2+} ions were escaped from the binding site core domain.

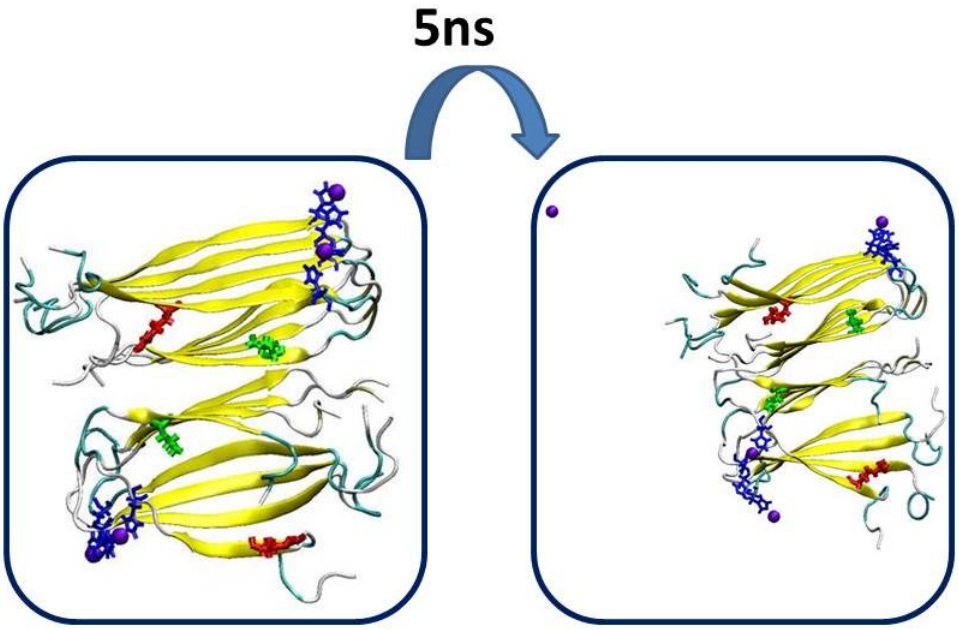

Figure S2: Simulations of model S2 illustrate that Zn^{2+} ions were escaped from the binding site.

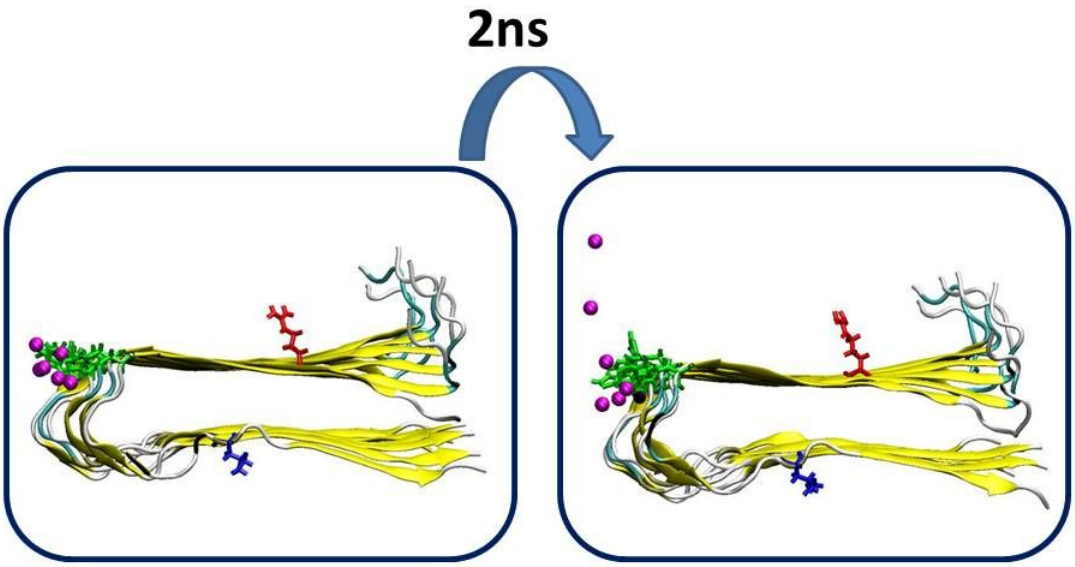

Figure S3: Simulations of model R1 with Zn^{2+}:amylin ratio of 1:1 illustrate that after 2 ns the Zn^{2+} ions were escaped from the binding site.

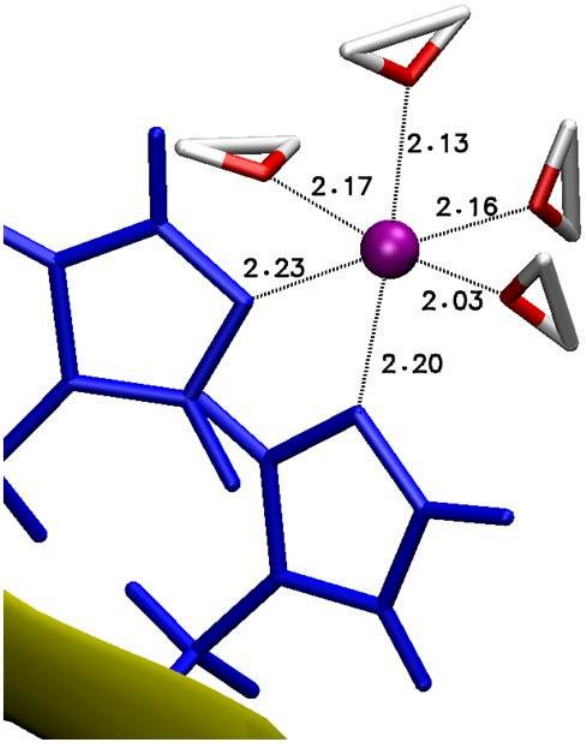

Figure S4: Illustration of one of the binding sites of Zn^{2+} ions in model R1 with the Zn^{2+}:amylin ratio of 1:2. Four water molecules complete the coordination with the Zn^{2+} ion.

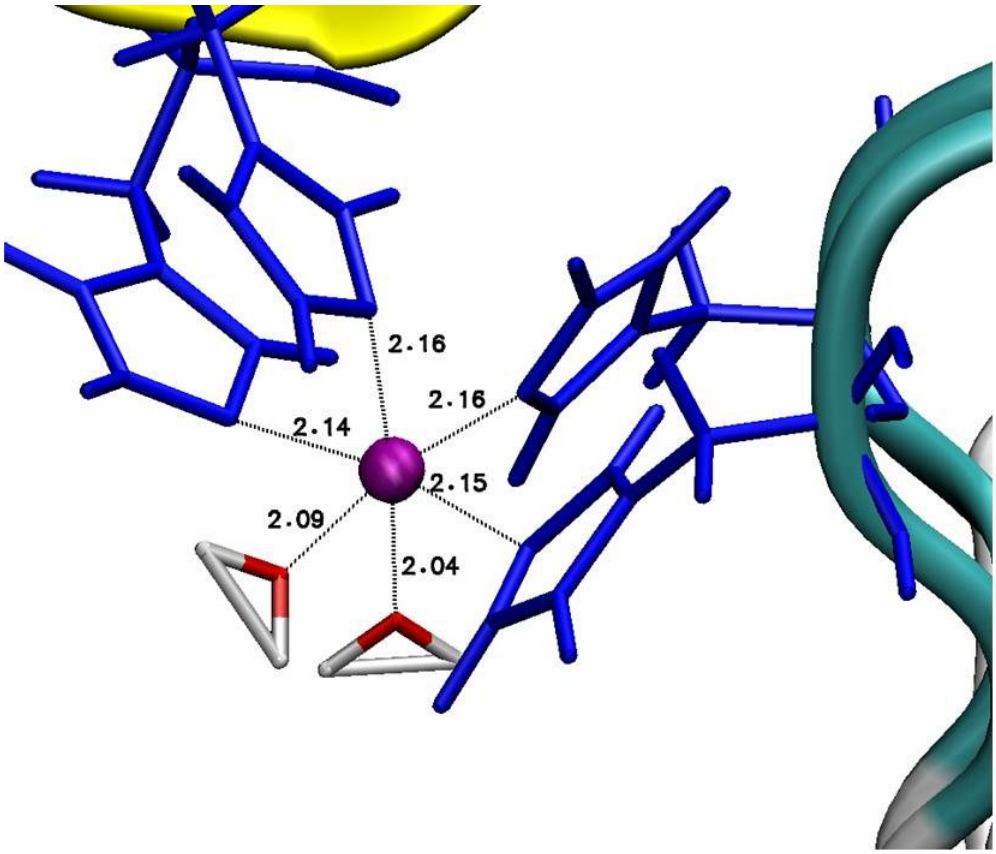

Figure S5: Illustration of one of the binding sites of Zn^{2+} ions in model S3 with the Zn^{2+}:amylin ratio of 1:4. Two water molecules complete the coordination with the Zn^{2+} ion.

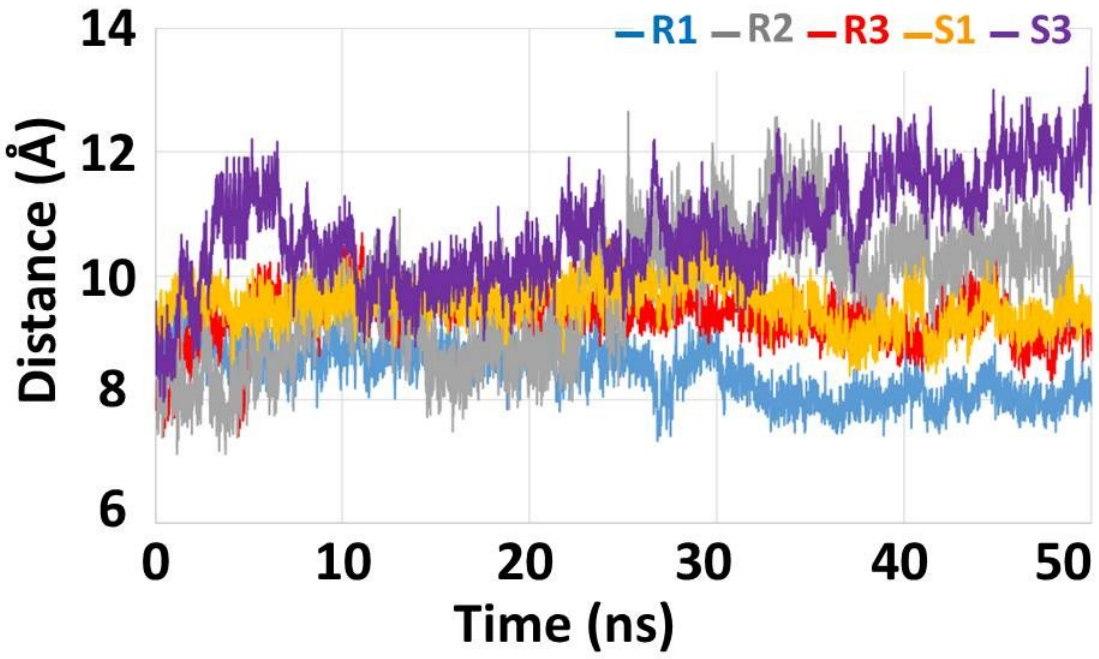

Figure S6: The averaged inter-sheet (Cα backbone-backbone) distances for simulated models of Zn^{2+}-amylin oligomers models R1, R2 and S1 and with Zn^{2+}:amylin ratio of 1:2, and models R3 and S3 with ratio of 1:4.

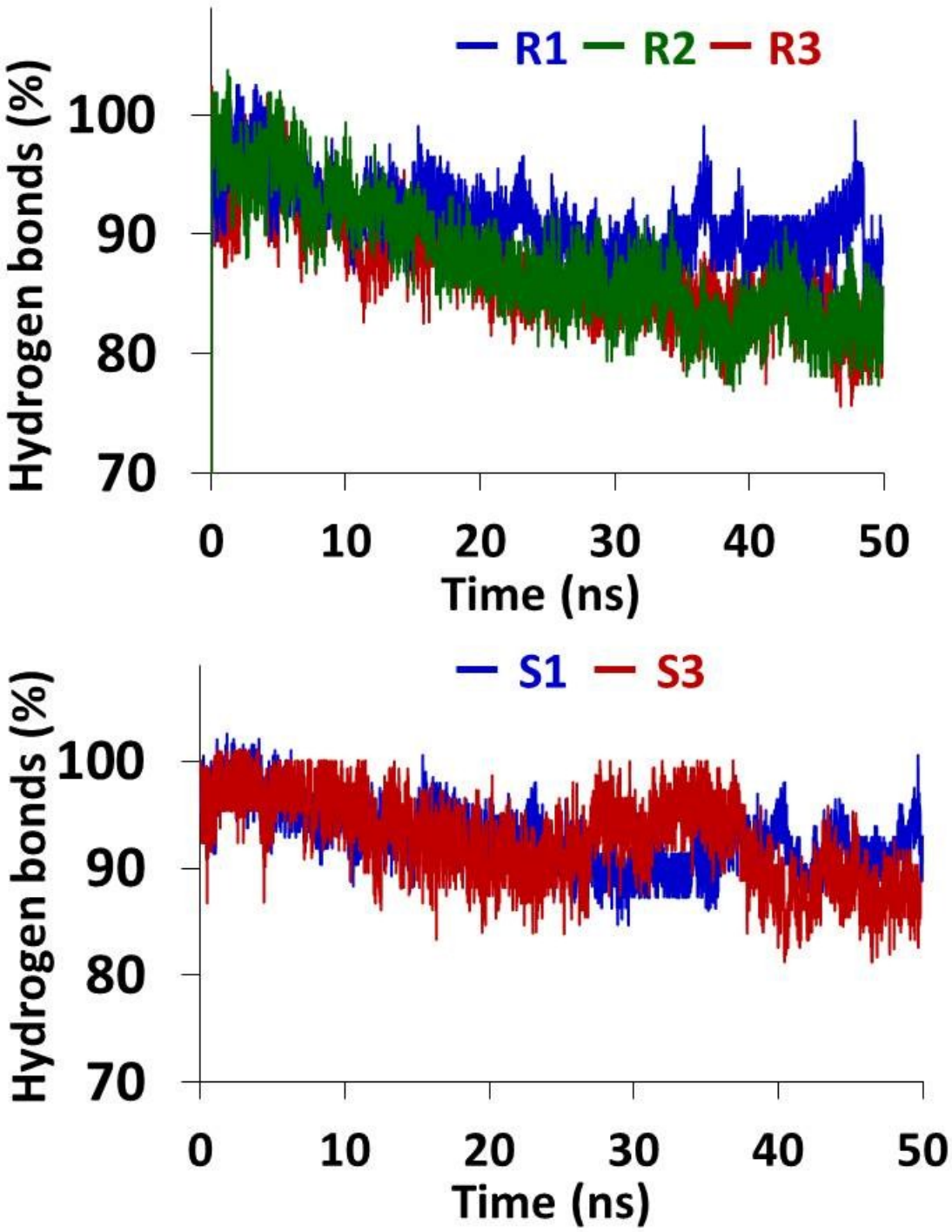

Figure S7: The fraction of the number of hydrogen bonds (in percentage) between all β-strands compare to the number in the initial constructed model, for models of Zn^{2+}-amylin oligomers models R1, R2 and S1 and with Zn^{2+}:amylin ratio of 1:2, and models R3 and S3 with ratio of 1:4.

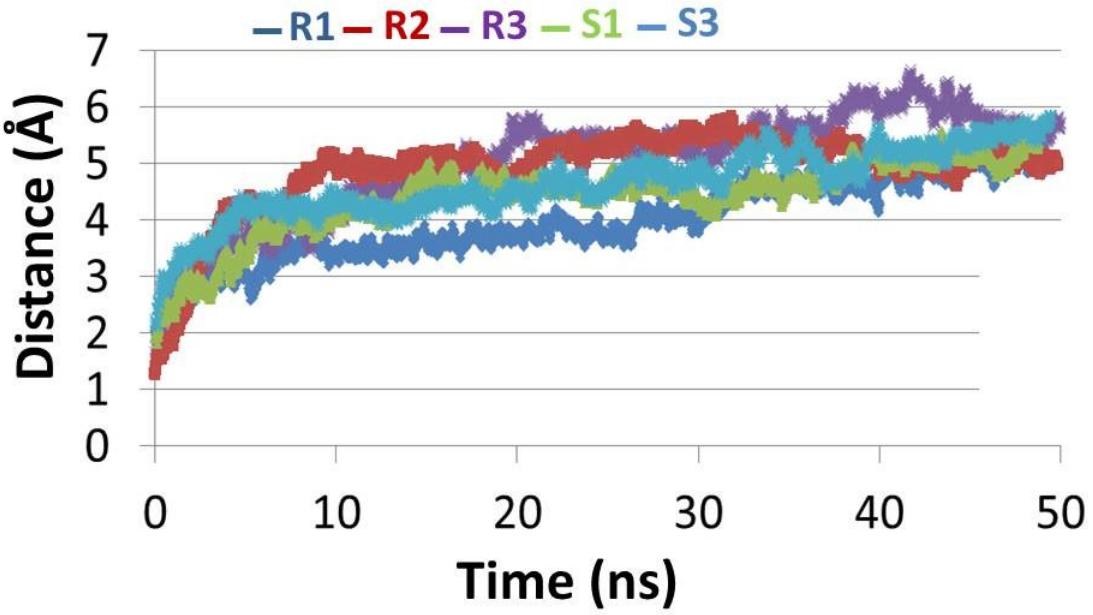

Figure S8: RMSDs of models of Zn^{2+}-amylin oligomers models R1, R2 and S1 and with Zn^{2+}:amylin ratio of 1:2, and models R3 and S3 with ratio of 1:4.

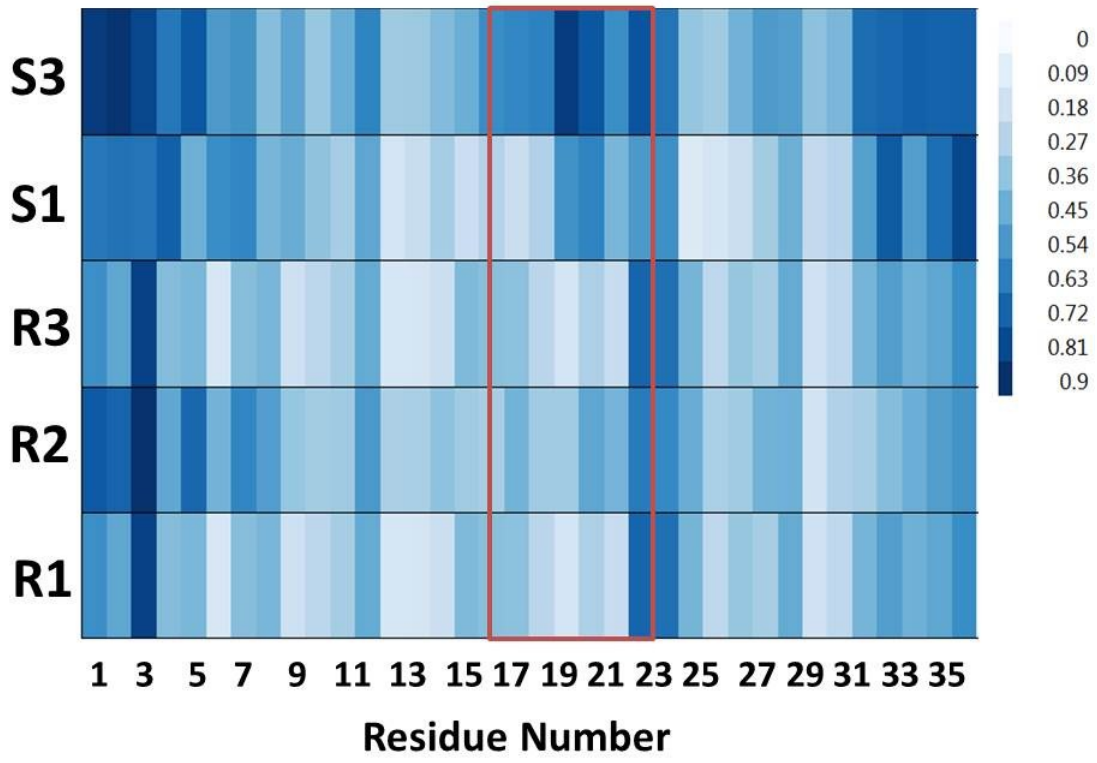

Figure S9: Average number of water molecules around each side-chain Cβ carbon (within 4 Å) for Zn^{2+}-amylin oligomers models R1, R2 and S1 and with Zn^{2+}:amylin ratio of 1:2, and models R3 and S3 with ratio of 1:4.

Table S1: The angles (in degree) His-Zn^{2+}-His, His-Zn^{2+}-Water, Water-Zn^{2+}-Water in the binding site of model R1 (Figure S4).

HIS1	HIS1	HIS2	Water1	Water2	Water3	Water4
HIS1	---------	88.14	84.58	--------	91.52	103.984
HIS2	88.14	--------	91.80	93.71	----------	88.77
Water1	84.58	91.80	---------	87.81	92.29	----------
Water2	---------	93.71	87.813	---------	87.08	83.75
Water3	91.52	---------	92.29	87.08	--------	88.0
Water4	103.984	88.77	---------	83.75	88.0	---------

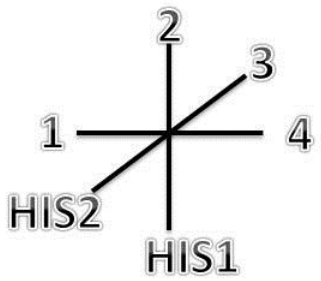

Table S2: The angles (in degree) His-Zn^{2+}-His, His-Zn^{2+}-Water, Water-Zn^{2+}-Water in the binding site of model S3 (Figure S5).

HIS1	HIS1	HIS2	HIS3	HIS4	Water1	Water2
HIS1	----------	91.52	94.963	101.463	----------	88.43
HIS2	91.52	----------	96.113	----------	81.68	88.243
HIS3	94.963	96.113	----------	86.33	94.283	----------
HIS4	101.463	----------	86.33	----------	84.91	88.94
Water1	----------	81.68	94.28	84.91	----------	82.85
Water2	88.43	88.24	----------	88.94	82.85	----------

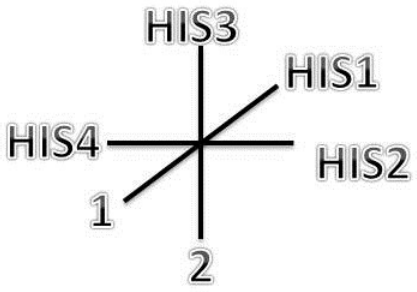

Table S3: The conformational energies (computed using the GBMV calculations) and the standard deviations.

Model	Energy (kcal/mol)	Standard deviation (kcal/mol)
M2	-6908	147
M2d	-6850	146
M5	-6668	151
R1	-9125	155
R2	-9095	165
R3	-7722	159
S1	-8998	217
S3	-7550	146