Supporting Information

Zn^{2+} Effect on Structure and Residual Hydrophobicity of Amyloid β-peptide Monomers

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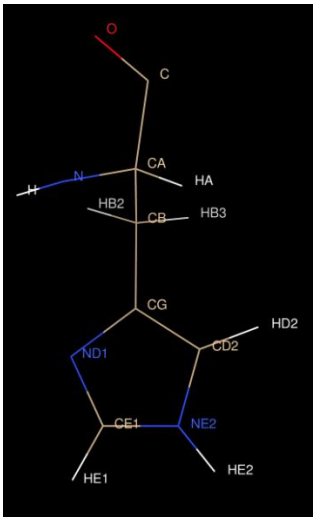
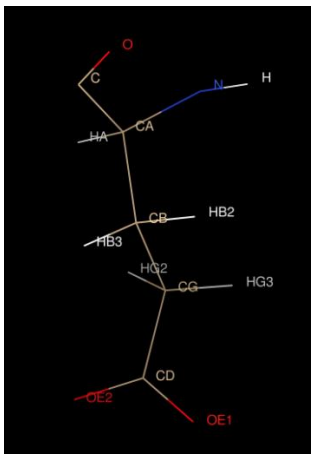
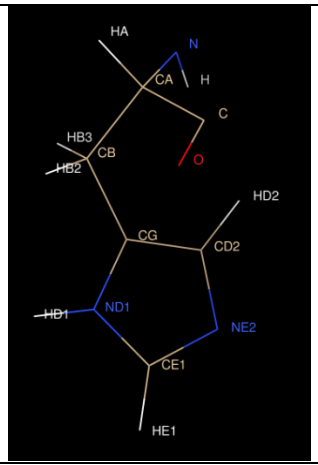
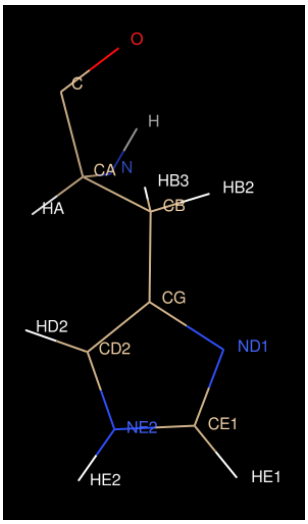
Table S1. Partial charges for coordinated residues.

Residue	Atom name[a]	Atom type	Charge	Structure
HE1 (H6)	N	N	-0.415700	
	H	H	0.271900	
	CA	CT	-0.058100	
	HA	H1	0.136000	
	CB	CT	0.058300	
	HB2	HC	0.114570	
	HB3	HC	0.114570	
	CG	CC	-0.043310	
	ND1	NX	-0.198910	
	CE1	CR	-0.009780	
	HE1	H5	0.134920	
	NE2	NA	-0.189620	
	HE2	H	0.349190	
	CD2	CW	-0.133570	
	HD2	H4	0.190530	
	C	C	0.597300	
	O	O	-0.567900	
GL1 (E11)	N	N	-0.516300	
	H	H	0.293600	
	CA	CT	0.039700	
	HA	H1	0.110500	
	CB	CT	0.581620	
	HB2	HC	-0.134240	
	HB3	HC	-0.134240	
	CG	CT	-0.700390	
	HG2	HC	0.197050	
	HG3	HC	0.197050	
	CD	C	0.774140	
	OE1	OX	-0.670180	
	OE2	OX	-0.570840	
	C	C	0.536600	
	O	O	-0.581900	
HD1 (H13)	N	N	-0.415700	
	H	H	0.271900	
	CA	CT	0.018800	
	HA	H1	0.088100	
	CB	CT	-0.051150	
	HB2	HC	0.065360	
	HB3	HC	0.065360	
	CG	CC	0.259530	
	ND1	NA	-0.454930	
	HD1	H	0.385450	
	CE1	CR	0.088640	
	HE1	H5	0.202510	

	NE2	NY	-0.117300	
	CD2	CV	-0.280100	
	HD2	H4	0.154080	
	C	C	0.597300	
	O	O	-0.567900	
HE2 (H14)	N	N	-0.415700	
	H	H	0.271900	
	CA	CT	-0.058100	
	HA	H1	0.136000	
	CB	CT	0.058300	
	HB2	HC	0.114570	
	HB3	HC	0.114570	
	CG	CC	-0.043310	
	ND1	NX	-0.198910	
	CE1	CR	-0.009780	
	HE1	H5	0.134920	
	NE2	NA	-0.189620	
	HE2	H	0.349190	
	CD2	CW	-0.133570	
	HD2	H4	0.190530	
	C	C	0.597300	
	O	O	-0.567900	
ZN1 (Zn)	ZN	ZN	0.567120	/

[a] refer to structure

Table S2. Bond parameters for the active site.

	Force constant (kcal/mol·Å ^{2})	Bond length (Å)
CB-NX	414.00	1.391
CK-NX	529.00	1.304
CC-NX	410.00	1.394
CR-NX	488.00	1.335
CV-NX	410.00	1.394
CB-NY	414.00	1.391
CK-NY	529.00	1.304
CC-NY	410.00	1.394
CR-NY	488.00	1.335
CV-NY	410.00	1.394
C -OX	656.00	1.250
ZN-NX	64.03	2.047
ZN-OX	42.30	2.206
ZN-NY	70.96	2.030

Table S3. Angle parameters for the active site.

	Force constant (kcal/mol·rad^2)	Bond angle (degrees)
C -CB-NX	70.000	130.000
CA-CB-NX	70.000	132.400
CB-CB-NX	70.000	110.400
H5-CK-NX	50.000	123.050
N*-CK-NX	70.000	113.900
CT-CC-NX	70.000	120.000
CW-CC-NX	70.000	120.000
H5-CR-NX	50.000	120.000
NA-CR-NX	70.000	120.000
CC-CV-NX	70.000	120.000
H4-CV-NX	50.000	120.000
CB-NX-CK	70.000	103.800
CC-NX-CR	70.000	117.000
CR-NX-CV	70.000	117.000
C -CB-NY	70.000	130.000
CA-CB-NY	70.000	132.400
CB-CB-NY	70.000	110.400
H5-CK-NY	50.000	123.050
N*-CK-NY	70.000	113.900
CT-CC-NY	70.000	120.000
CW-CC-NY	70.000	120.000
H5-CR-NY	50.000	120.000
NA-CR-NY	70.000	120.000
CC-CV-NY	70.000	120.000
H4-CV-NY	50.000	120.000
CB-NY-CK	70.000	103.800
CC-NY-CR	70.000	117.000
CR-NY-CV	70.000	117.000
CT-C -OX	70.000	117.000
OX-C -OX	80.000	126.000
NY-ZN-NX	24.293	104.969
C -OX-ZN	87.595	90.001
CR-NX-ZN	45.668	126.813
CC-NX-ZN	47.595	125.495
CV-NY-ZN	41.525	128.619
OX-ZN-OX	67.656	58.896
OX-ZN-NY	36.259	103.243
OX-ZN-NX	37.639	117.686
NX-ZN-NX	25.616	103.459
CR-NY-ZN	40.495	124.609

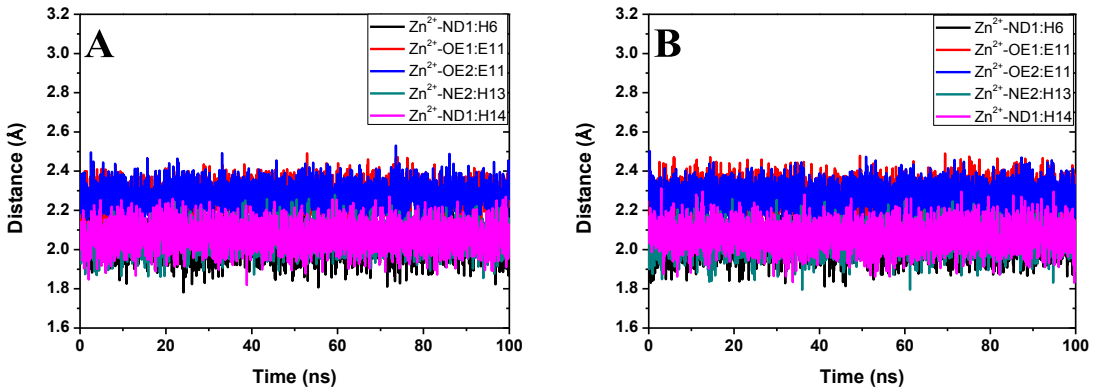


Figure S1. Distances between Zn^{2+} and coordinated atoms of Aβ peptides. (A) Zn^{2+}-Aβ40 and (B) Zn^{2+}-Aβ42.

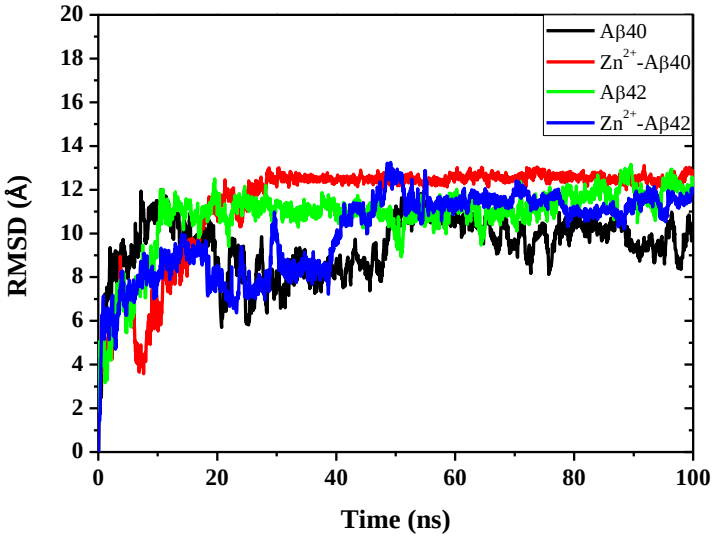


Figure S2. Backbone Root-Mean-Square Deviation of Aβ40, Zn^{2+}-Aβ40, Aβ42, and Zn^{2+}-Aβ42, respectively.

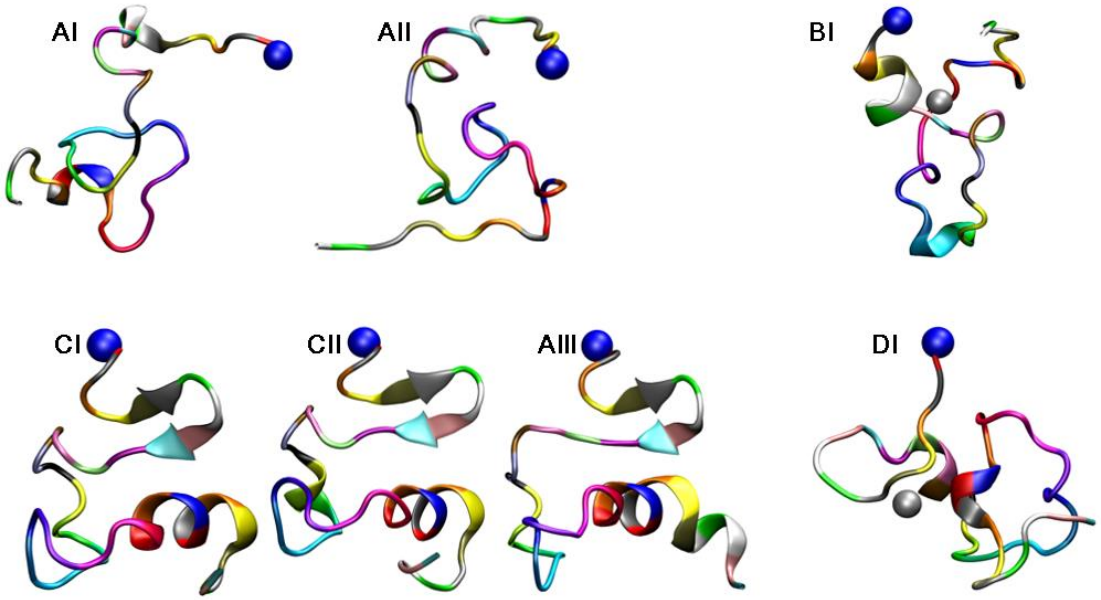


Figure S3. Basin structures of Aβ40, Zn^{2+}-Aβ40, Aβ42, and Zn^{2+}-Aβ42 in free energy landscapes. The first N in blue and Zn^{2+} in gray.