

Supporting Information

Article

Zinc Binding to NAP-Type Neuroprotective Peptides: Nuclear Magnetic Resonance Studies and Molecular Modeling

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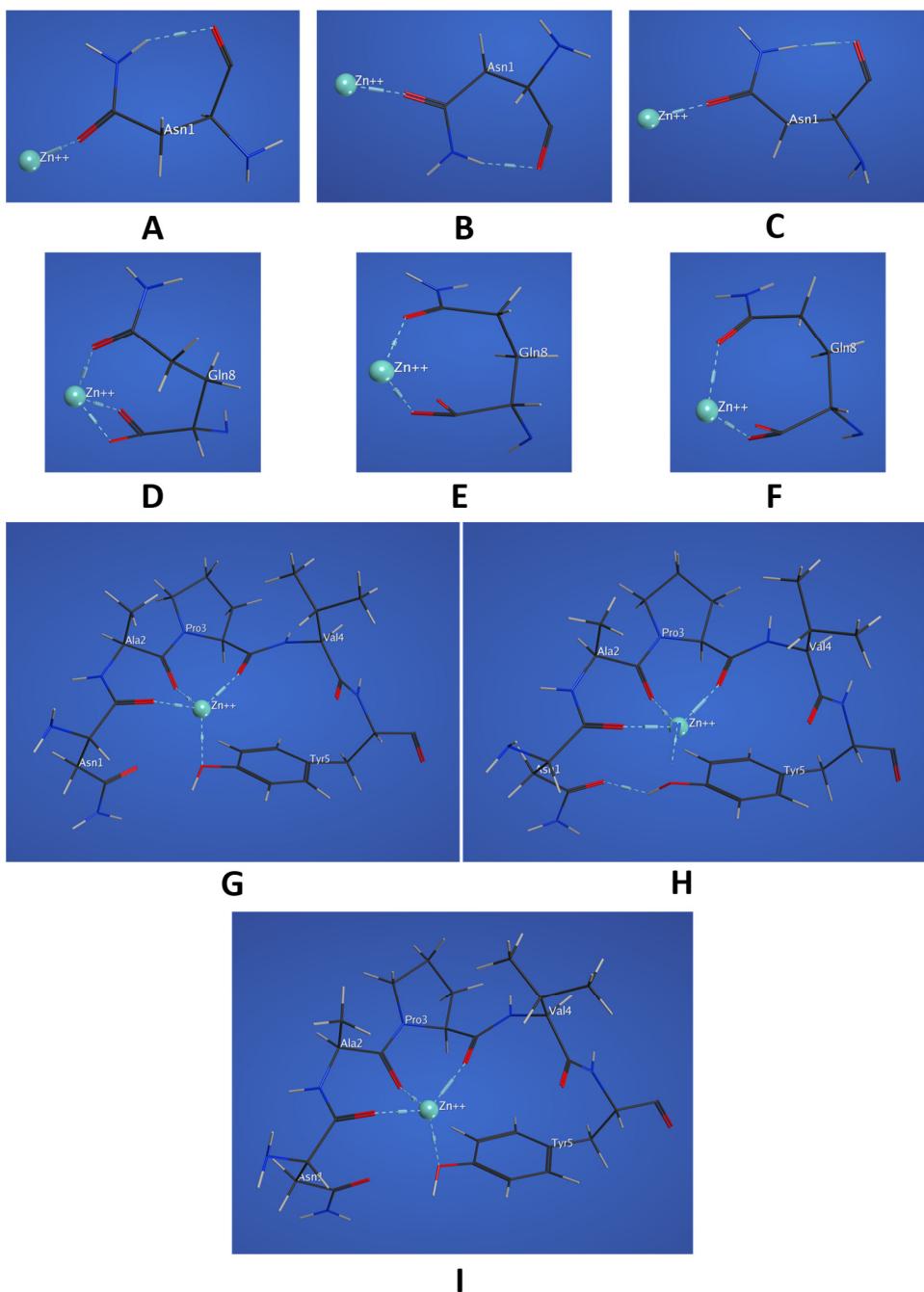


Figure S1. The structures at 310.15 K following molecular dynamics using 3 algorithms: (A) NAP-Zn²⁺-Asn¹ with NPA, (B) NAP-Zn²⁺-Asn¹ with NHA, (C) NAP-Zn²⁺-Asn¹ with BER, (D) NAP-Zn²⁺-Gln⁸ with NPA, (E) NAP-Zn²⁺-Gln⁸ with NHA, (F) NAP-Zn²⁺-Gln⁸ with BER, (G) NAPY-Zn²⁺ with NPA, (H) NAPY-Zn²⁺ with NHA and (G) NAPY-Zn²⁺ with BER.

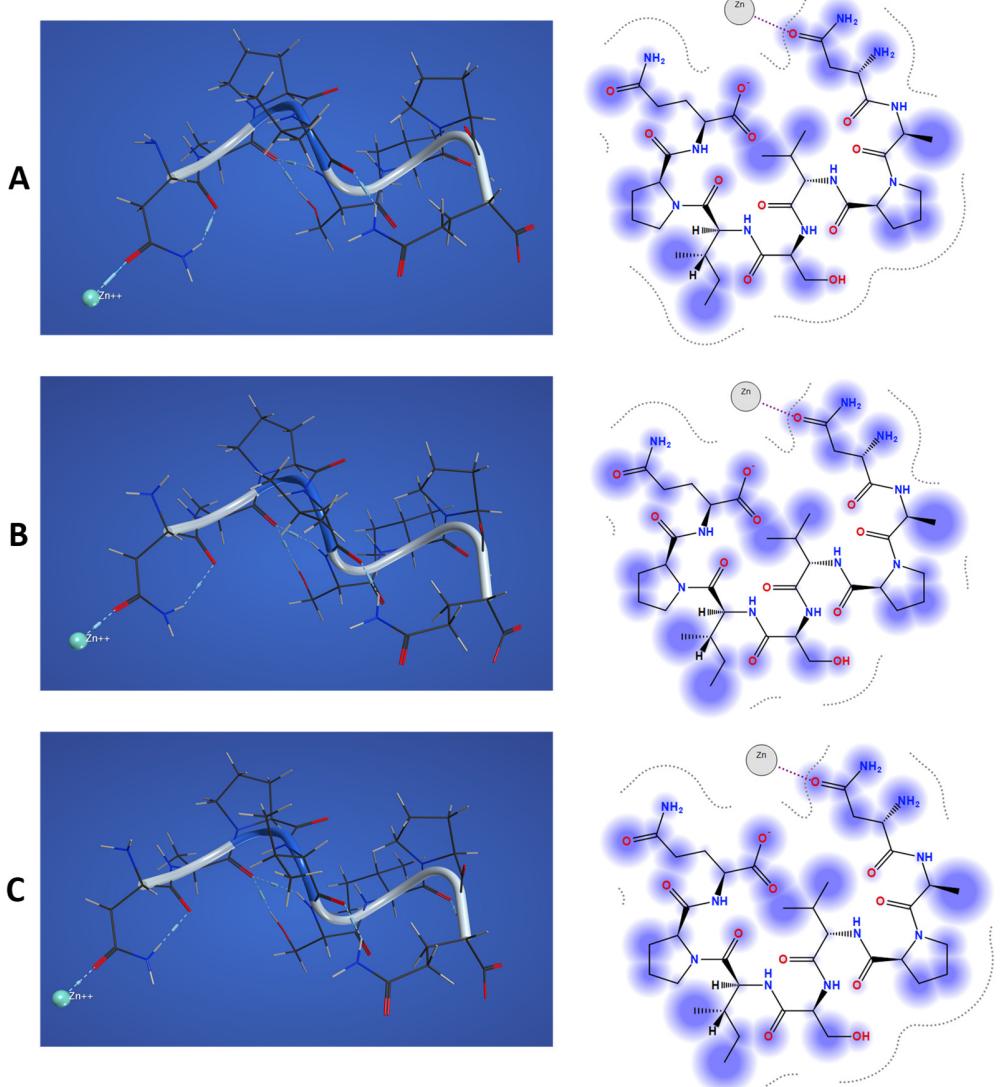


Figure S2. Molecular dynamics of NAP- Zn^{2+} -Asn¹ complex, at (A) Flexible Alignment condition, (B) 298.15 K and (C) 310.15 K using NPA/NHA/BER algorithm.

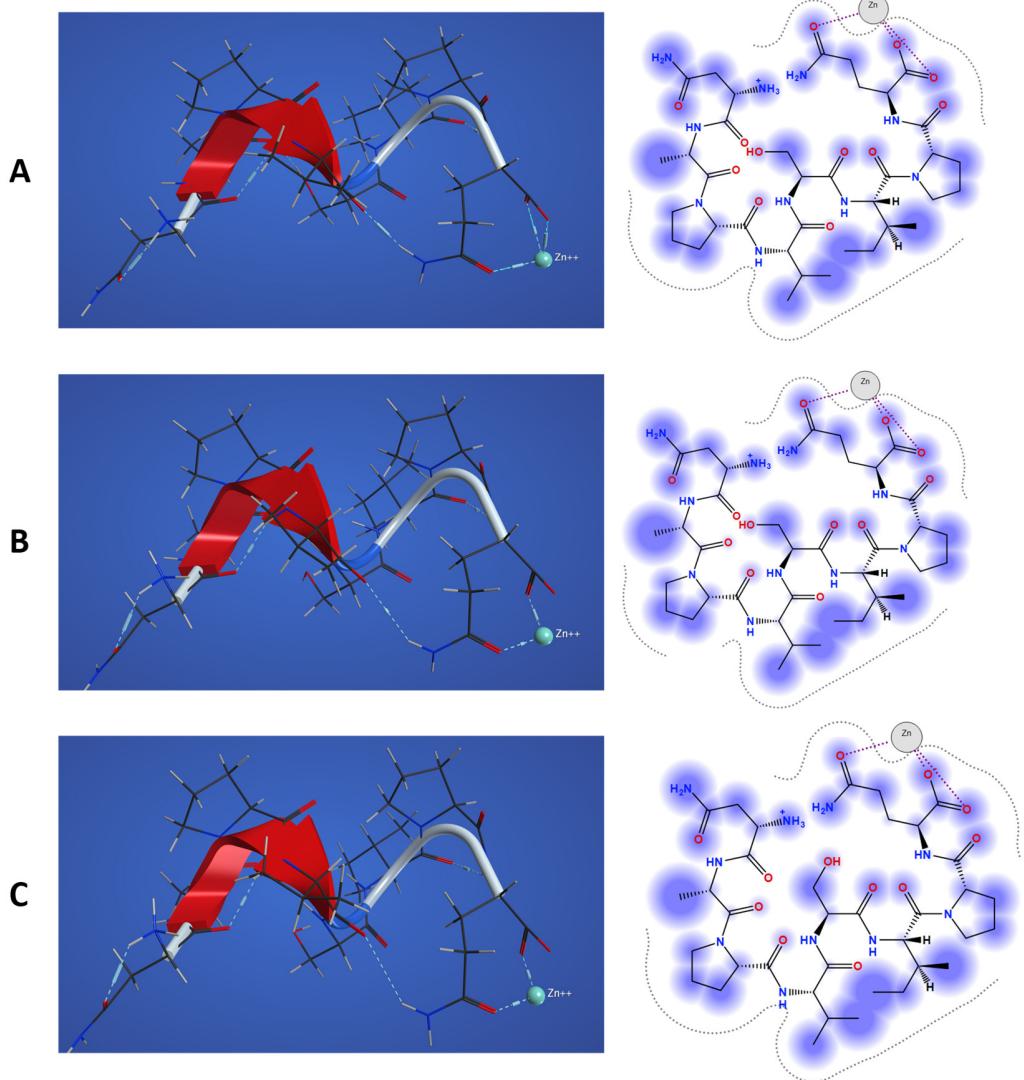


Figure S3. Molecular dynamics of NAP-Zn²⁺-Gln⁸ complex, at (A) Flexible Alignment condition, (B) 298.15 K and (C) 310.15 K using NPA/NHA/BER algorithm.

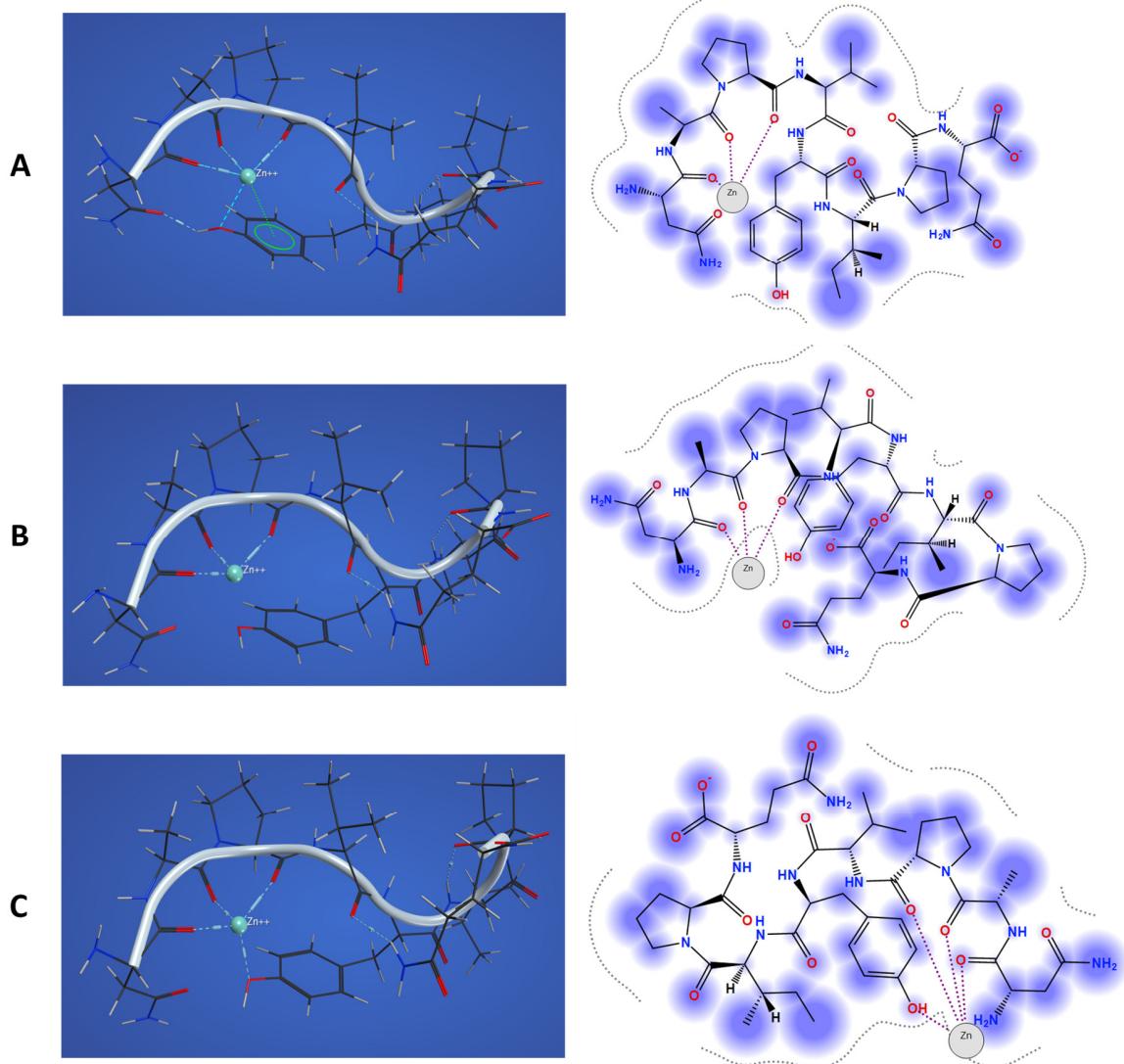


Figure S4. Molecular dynamics of NAPY-Zn²⁺ complex, at (A) Flexible Alignment condition, (B) 298.15 K and (C) 310.15 K using NPA/NHA/BER algorithm.

Table S1. The molecular parameters of NAP/NAPY-Zn²⁺ complex according to the MD simulation with NPA, NHA and BER algorithms.

Complex	Receptor	Interaction type	Distance (Å) NPA/NHA/BER	Energy (kcal/mol) NPA/NHA/BER
NAP-Zn ²⁺ Asn ¹ (0)	O ^{sp2}	Metal	1.97	-4.7
NAP-Zn ²⁺ Asn ¹ (298.15K)	O ^{sp2}	Metal	1.72 1.74 1.68	-4.0 -4.6 -4.4
NAP-Zn ²⁺ Asn ¹ (310.15K)	O ^{sp2}	Metal	1.76 1.76 1.71	-4.2 -4.2 -4.7
NAP-Zn ²⁺ Gln ⁸ (0)	O ^{sp2} (acid)	Metal	2.41	-1.9
	O ^{sp3} (acid)	Metal	1.85	-4.2
	O ^{sp2}	Metal	2.06	-2.9
	O ^{sp2} (acid)	Ionic	2.41	-9.9
	O ^{sp3} (acid)	Ionic	1.85	-19.4
NAP-Zn ²⁺ Gln ⁸ (298.15K)	O ^{sp2} (acid)	Metal	1.76 1.74 1.75	-3.1 -3.3 -3.6
	O ^{sp3} (acid)	Metal	1.69 1.69 1.68	-3.1 -3.1 -3.5
	O ^{sp2}	Metal	1.82 1.74 1.78	-2.7 -2.8 -2.3
	O ^{sp2} (acid)	Ionic	1.76 1.74 1.75	-21.6 -22.0 -21.6
	O ^{sp3} (acid)	Ionic	1.69 1.69 1.68	-21.4 -23.2 -21.5
	O ^{sp2} (acid)	Metal	1.73 1.76 1.76	-3.8 -3.6 -3.5
	O ^{sp3} (acid)	Metal	1.74 1.69 1.67	-3.6 -3.4 -3.6
	O ^{sp2}	Metal	1.76 1.76 1.84	-3.0 -2.5 -2.7
	O ^{sp2} (acid)	Ionic	1.73 1.76 1.76	-22.3 -21.5 -21.5
	O ^{sp3} (acid)	Ionic	1.74 1.69 1.67	-22.0 -23.2 -24.0
NAP-Zn ²⁺ Gln ⁸ (310.15K)	O ^{sp2} (acid)	Metal	1.73 1.76 1.76	-3.8 -3.6 -3.5
	O ^{sp3} (acid)	Metal	1.74 1.69 1.67	-3.6 -3.4 -3.6
	O ^{sp2}	Metal	1.76 1.76 1.84	-3.0 -2.5 -2.7
	O ^{sp2} (acid)	Ionic	1.73 1.76 1.76	-22.3 -21.5 -21.5
	O ^{sp3} (acid)	Ionic	1.74 1.69 1.67	-22.0 -23.2 -24.0

NAPY-Zn ²⁺ (0)	O ^{sp2} (Asn ¹)	Metal	2.11	-2.8
	O ^{sp2} (Ala ²)	Metal	2.12	-1.7
	O ^{sp2} (Pro ³)	Metal	2.13	-3.1
NAPY-Zn ²⁺ (298.15K)	O ^{sp2} (Asn ¹)	Metal	1.84	-2.4
			1.82	-2.5
			1.80	-2.6
	O ^{sp2} (Ala ²)	Metal	1.83	-1.8
			1.82	-1.5
			1.90	-1.6
	O ^{sp2} (Pro ³)	Metal	1.90	-3.8
			1.83	-3.5
			1.86	-3.6
NAPY-Zn ²⁺ (310.15K)	O ^{sp2} (Asn ¹)	Metal	1.89	-2.6
			1.95	-2.6
			1.90	-2.4
	O ^{sp2} (Ala ²)	Metal	1.79	-1.8
			1.81	-1.8
			1.84	-1.6
	O ^{sp2} (Pro ³)	Metal	1.82	-3.5
			1.88	-3.7
			1.90	-3.6

where: NPA (Nosé-Poincaré-Andersen), NHA (Nosé-Hoover-Andersen), BER (Berendsen equations) and acid – the carboxyl group of glutamine.