

QM/MM Study of the Catalytic Mechanism of Nicotinamidase

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Table S1 The values of d1, d2, d3 and d4 in the optimized structure of all species involved in the reaction.

d1: distance between H1 atom of K122 and oxygen atom of D8 carboxyl group;

d2: distance between H2 atom of K122 and sulfur atom of C167 sulfhydryl group;

d3: distance between hydrogen atom of A163 amide backbone and carboxyl oxygen atom of substrate;

d4: distance between hydrogen atom of C167 amide backbone and carboxyl oxygen atom of substrate;

	d1 (Å)	d2 (Å)	d3 (Å)	d4 (Å)
R	1.68	2.77	1.80	3.31
TS1	2.29	2.52	1.88	2.79
IM1	2.27	2.05	1.97	3.64
TS2-1	1.64	2.44	1.76	2.34
TS2-2	1.94	2.37	1.98	3.80
IM2-1	2.03	2.78	1.75	2.13
IM2-2	1.85	2.61	3.18	5.34
TS3-1	1.91	2.59	1.75	2.20
TS3-2	1.81	2.42	1.77	2.93
IM3	1.73	2.65	1.76	2.18
TS4	1.68	2.70	1.81	2.20
IM4	1.59	2.82	2.03	2.14
IM5	1.71	3.31	2.02	2.14
TS5	1.94	3.34	1.78	2.35
IM6	2.27	3.15	1.77	2.27
TS6	2.49	2.77	1.78	2.40
IM7	2.83	2.37	1.81	2.86
TS7	2.47	2.44	1.79	2.70
P	1.33	3.30	1.74	2.85

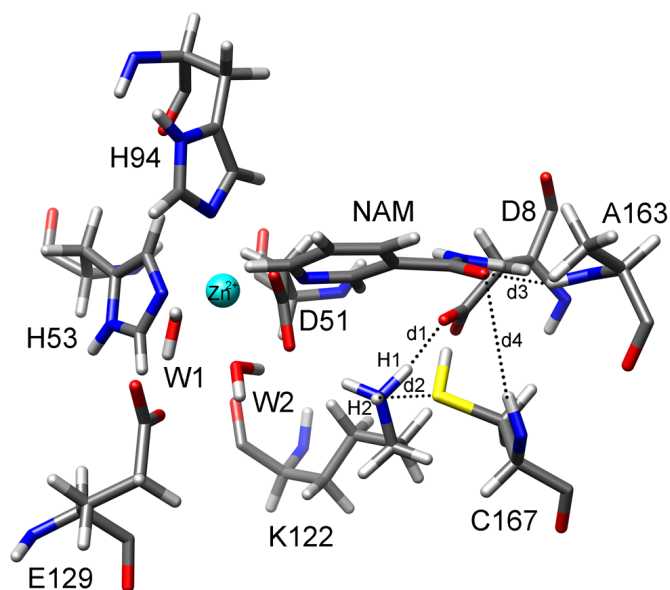


Figure S1 Time dependences of RMSDs (ns) from 5ns MD simulations in (a) deamination process and (b) hydrolysis process.

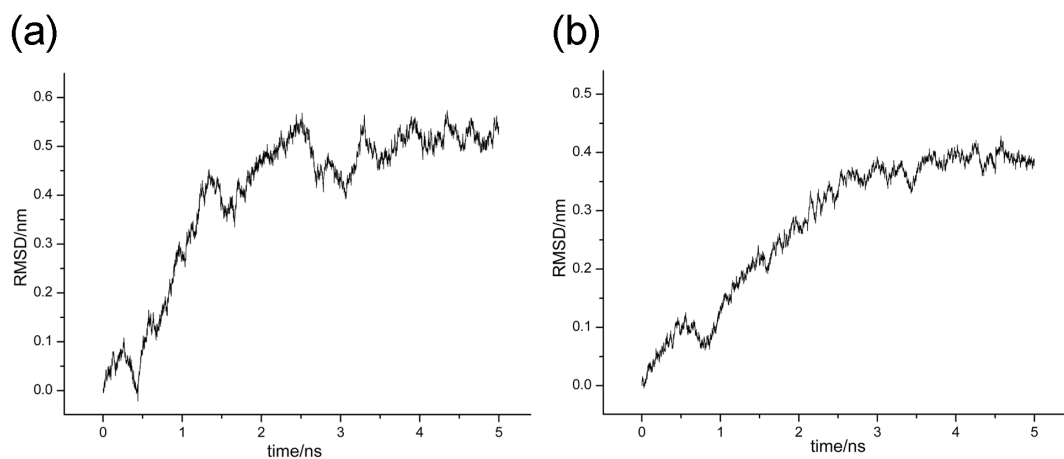


Figure S2 B3LYP/6-31G(d,p)//CHARMM22 energy profile along the reaction coordinate in HL-p3.

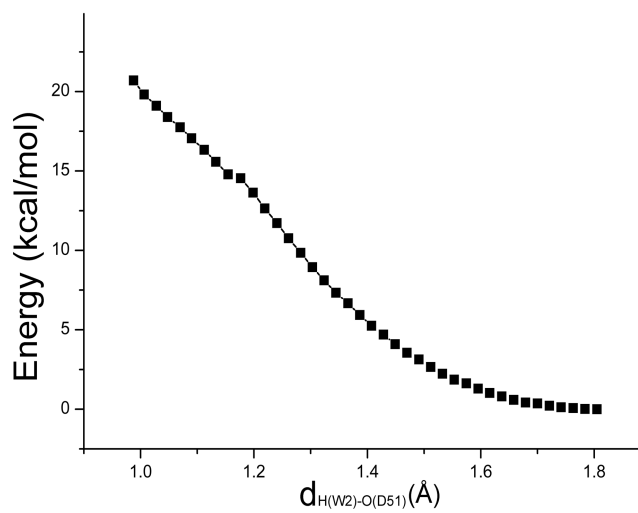


Figure S3 The distances between Zn^{2+} and the ligated atoms of Zn-coordinated molecules (a), the ESP charges of Zn-binding site without NAM (b), and the ESP charges of Zn^{2+} and Zn-coordinated residues and water (c) of species in DA-p2 for deamination process and HL-p1 for hydrolysis process.

