Supplementary Material for

Computational Evidence for the Degradation Mechanism of Haloalkane Dehalogenase LinB and Mutants of Leu248 to 1-Chlorobutane

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 Table S1. Energy barrier spreads and Boltzmann weighted average barriers calculated

 at B3LYP/cc-pVTZ//CHARMM36 level for the hydrolytic process in s-w-LinB_{Hsd107}

 system.

Systems	<u>s-w-LinB_{Hsd107} model</u>	<u>s-w-LinB_{Hsd107} model</u>
Hydrolysis	Barrier/	Barrier/
Process	(kcal mol ⁻¹)	(kcal mol ⁻¹)
Snapshots/ns	First step	Second step
13	8.7	5.4
13.5	13.4	8.7
14	12.0	8.1
14.5	13.3	11.1
15	14.9	13.9
$\Delta E_{bwa}(kcal mol^{-1})$	9.6	6.4

Figure Captions

Fig. S1. Root-mean-square deviations (RMSD) of the backbone for molecular dynamic simulation of LinB-Hsd107 model (A), LinB-Hse107 model (B), m-LinB_{L248A} model (C), m-LinB_{L248F} model (D).

Fig. S2. Variations of key internuclear distances (H^{α} -Cl¹, H^{β} -Cl¹ and C¹-N^{β}) involved in the productive arrangement of substrate during the molecular dynamics simulation of LinB-Hsd107 model (A), LinB-Hse107 model (B), m-LinB_{L248A} model (C), m-LinB_{L248F} model (D).

Fig. S3. Potential energy profiles for the whole degradation of CB with five conformations calculated at the B3LYP/cc-pVTZ//CHARMM36 level in wild enzyme. The Boltzmann weighted average barriers in every step were also displayed in braces.

Fig. S4. Liner relationship between degradation activity and side chain size by using MLA and MLF model.

Fig. S5. Spatial locations of transition states and products for w-LinB_{Hsd107} model, w-LinB_{Hse107} model, m-LinB_{L248A} model and m-LinB_{L248F} model. The unit of bond distances are in Å.

Fig. S6. Potential energy profiles for the whole degradation of CB with five conformations calculated at the B3LYP/cc-pVTZ//CHARMM36 level in the m- $LinB_{L248F}$ system. The Boltzmann weighted average barriers in every step were also displayed in braces.



Fig. S1



Fig. S2



Reaction Coordinate

Fig. S3



Certain regularity for degradation of 1-CB

Fig. S4



















Fig. S5



Fig. S6