Supplementary data for

Dehydrochlorination mechanism of γ-hexachlorocyclohexane degraded by dehydrochlorinase LinA from Sphingomonas paucimobilis UT26

Xiaowen Tang, Ruiming Zhang, Qingzhu Zhang*, Wenxing Wang

Environment Research Institute, Shandong University,
Jinan 250100, P. R. China

Keywords
γ-Hexachlorocyclohexane, Dehydrochlorinase LinA, Degradation, Quantum mechanics/molecular mechanics, Boltzmann-weighted average,

*Corresponding authors. E-mail: zqz@sdu.edu.cn,
Fax: 86-531-8836 1990
Twenty pages

Contains additional details on the methods, three Figures, and the coordinates of the docked structures, MD snapshots, QM-optimized structures and QM/MM-optimized structures.

**Figure S1.** Root-mean-square deviations (RMSD) of the backbone for molecular dynamic simulation of $\gamma$-HCH reaction system (A) and $\gamma$-PCCH-1 reaction system (B). Key distance variations along the molecular dynamic simulation of $\gamma$-HCH reaction system (C) and $\gamma$-PCCH-1 reaction system (D).

**Figure S2.** The three dimensional structures of the docked structure, the MD snapshot, and the QM/MM-optimised structure in the $\gamma$-HCH reaction system. The key residues are shown in ball and stick representation. The values exhibited in MD snapshot and QM/MM-optimised structure are the average distance in the molecular dynamic simulation and the five pathways QM/MM optimizations. The unit of distance is in Å.

**Figure S3.** The three dimensional structures of the docked structure, the MD snapshot, and the QM/MM-optimised structure in the $\gamma$-PCCH-1 reaction system. The key residues are shown in ball and stick representation. The values exhibited in MD snapshot and QM/MM-optimised structure are the average distance in the molecular dynamic simulation and the five pathways QM/MM optimizations. The unit of distance is in Å.
Additional details on the methods

The protonation states of ionizable residues were determined on the basis of the pKa values obtained via the PROPKA procedure and were manually verified through visual inspection, especially for the residues around the active site. The pH value used (pH=8.3) during pKa calculation is same as experimentally used pH value in determining the $k_{cat}$ ($I$). The protonation states of the ionizable residues (Glu, Asp, Arg, Cys, Lys, and His residues) are all set in the standard state. For three histidine residues of enzyme LinA, the protonation states are listed as follows: Hsd69, Hsd73, and Hsd143. This was carefully determined based on the manual visual inspection and the results given by MolProbity software (http://molprobity.biochem.duke.edu), especially for the active site residue Hsd73. The MolProbity software is also used to check the flipped residues, finding that Gln28 and Asn77 are flipped. Note that we follow the nomenclature in CHARMM and the CHARMM22 force field is used for the simulation. Important CHARMM simulation parameters are listed as follows (for explanation of the nomenclatures, see http://www.charmm.org/documentation/c34b1/dynamc.html):

The relevant codes for cutoff: “update group noextend fswitch cdie vdw vswitched eps 1.0 cutnb 14.0 ctofnb 13.0 ctonnb 12.0 vgroup WMIN 1.2 inbf 25”; time step for dynamics in picoseconds: timestp 0.001; the frequency for checking whether an atom is in the Langevin region: ilbfrq 50; a Gaussian distribution of velocities: iasvel 1; simulation temperature: 298.15 K.

Optimization parameters for QM/MM calculations are listed as follows
(most are set in default; for explanation of the nomenclatures, see http://yfaat.ch.huji.ac.il/chemshell-31/manual/hdlcopt.html):

Optimization parameters for reactants, intermediates, and products:
Memory=100; mode=1; contyp=0; reghdl=60; cfact=0.5; recalc=0; toler=0.00045; printl=0; maxfun=100000; update_procedure=hdlcoupdate; theory=hybrid.

Optimization parameters for transition states: Memory=100; contyp=0; ctfirst=1; reghdl=200; cfact=1; maxfun=100000; toler=0.00045; mode=1; lockon=0; update_procedure=hdlcoupdate; theory=hybrid.

In our QM/MM calculations, each residue of the protein, each water molecule, and substrates (γ-HCH and γ-PCCH-1) are defined as HDLC residues. The transition state structure was determined by scanning the potential energy profile from the reactant to the product, reaction coordinates were defined as “d(C2-Cl2)-d(Nε-H1)” for γ-HCH reaction system and “d(C5-Cl5)-d(Nε-H4)” for γ-PCCH-1 reaction system.

For microiterative TS optimisations, all the QM atoms are considered in the inner region.

References:

Figure S1
Figure S2
Figure S3
Docked structure (His73 and γ-HCH)

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