

## **Description of Additional Supplementary Files**

File Name: Supplementary Dataset 1

Description: The force field parameters for p-nitrophenyl benzoate.

File Name: Supplementary Dataset 2

Description: The coordinates of QM/MM stationary points of QW10 and QW4 mutants.

File Name: Supplementary Dataset 3

Description: the PDB file of the docked structures and the equilibrated MD structures of WT.

File Name: Supplementary Dataset 4

Description: the PDB file of the docked structures and the equilibrated MD structures of QW2.

File Name: Supplementary Dataset 5

Description: the PDB file of the docked structures and the equilibrated MD structures of QW10.

File Name: Supplementary Dataset 6

Description: the PDB file of the docked structures and the equilibrated MD structures of QW4.