Quantum Mechanical/Molecular Mechanical Study of Catalytic Mechanism and Role of Key Residues in Methylation Reactions Catalyzed by Dimethylxanthine Methyltransferase in Caffeine Biosynthesis

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Supporting Information

Figure S1, S2 and S3. This material is available free of charge via the Internet at http://pubs.acs.org.

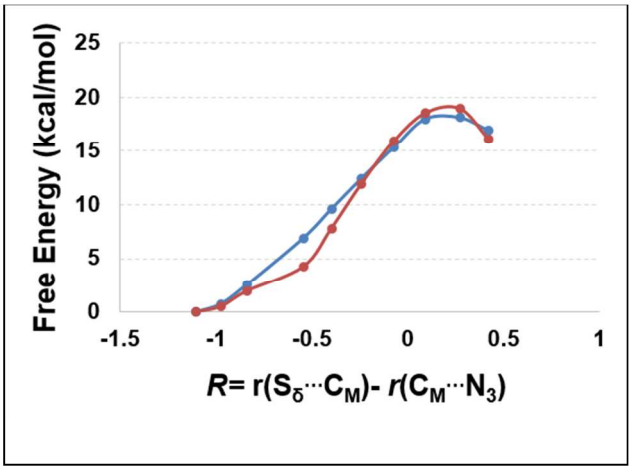

Figure S1. The potential energy curve calculated by the self-consistent charge density functional tight-binding method(SCC-DFTB, in blue) and the single-point energy curve calculated by *ab initio* MP2/6–31G** method(in red) applied in a small model.

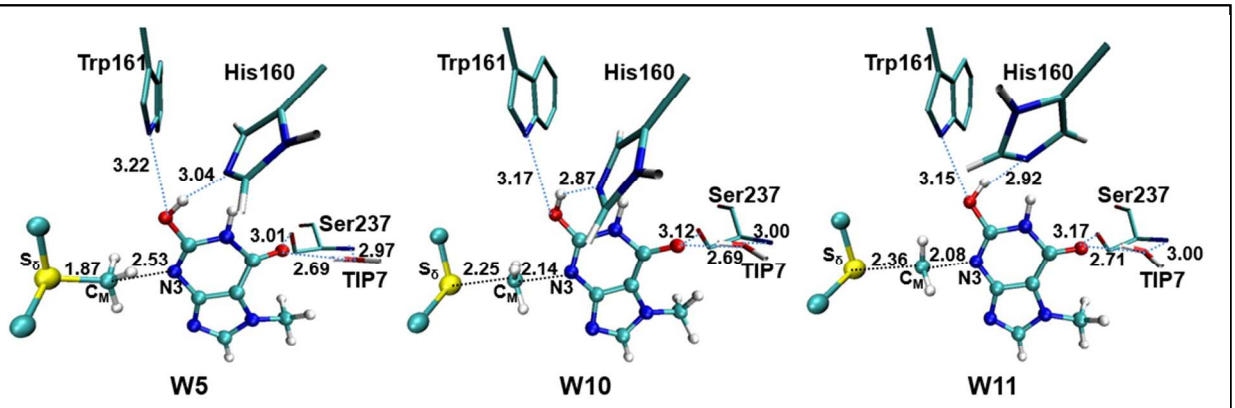

Figure S2. The average active-site structures during the free energy simulation of N3 methylation (7mX->Tb) with the O−H covalent bond on 7mX fixed. The average structures in Window 5(W5, before reaching TS), Window 10(W10, near TS) and Window 11(W11, passed near TS) of N3 methylation are shown.

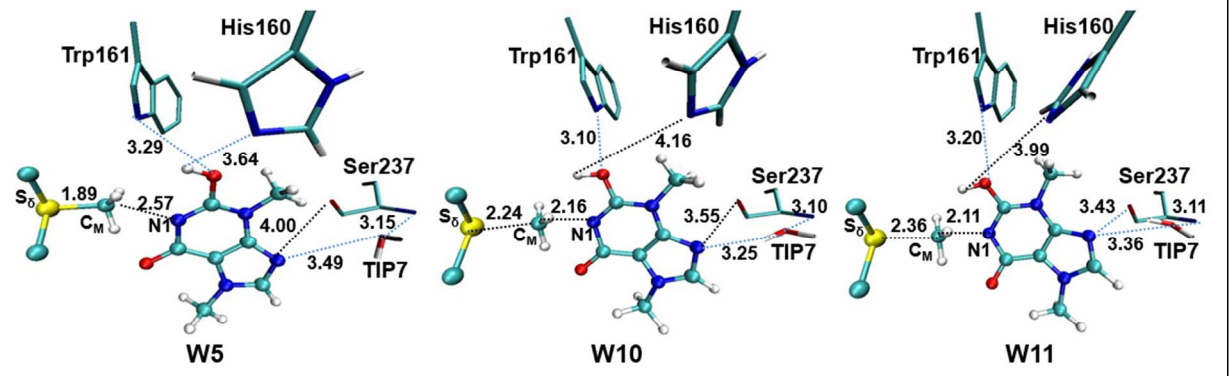

Figure S3. The dynamics of active site during the free energy simulation of N1 methylation (Tb->Cf) with the O−H covalent bond on Tb fixed. The average structures in window 5(W5, before the transition state (TS)), window 10(W10, approaching near TS), window 11(W11, passed near TS) of N1 methylation are shown.