

**Computational Modeling of Mg²⁺ Binding in the Active Site of
Protein Farnesyltransferase**

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Figure S1

Comparison of FPP³⁻ orientation found in WT2 MD simulation and from previous FTase/FPP³⁻ (without Mg²⁺) MD simulation.

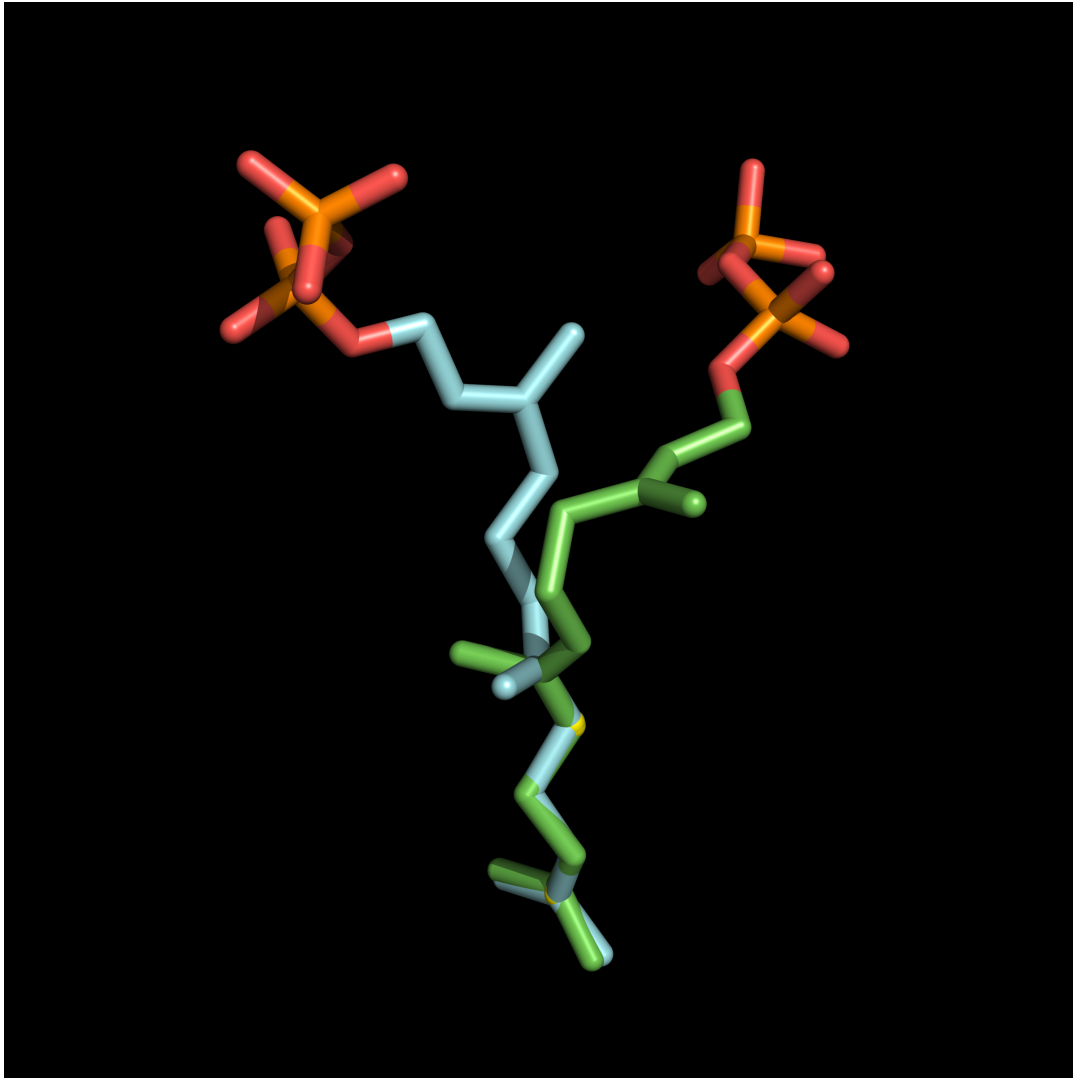


Figure S2

Distribution map of d_{RC} from WT2 MD simulations, in support to an intermediate state existing at $\sim 5\text{\AA}$.

