

## ESI: Fundamental reaction pathway and free energy profile for proteasome inhibition by syringolin A (SylA)

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**Running title:** Reaction pathway for proteasome inhibition by SylA

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Table S1. Absolute QM/MM energies (in Hartree) calculated at the QM/MM (B3LYP/6-31++G\*\*):AMBER) level (single-point energy calculations) using the geometries optimized at the QM/MM(B3LYP/6-31G\*):AMBER) level.

State	Energy
ER	-1864.49293844
TS1	-1864.47264264
INT1	-1864.50238344
TS2	-1864.47969914
INT2	-1864.48317333
TS3	-1864.48255882
EP	-1864.52221434