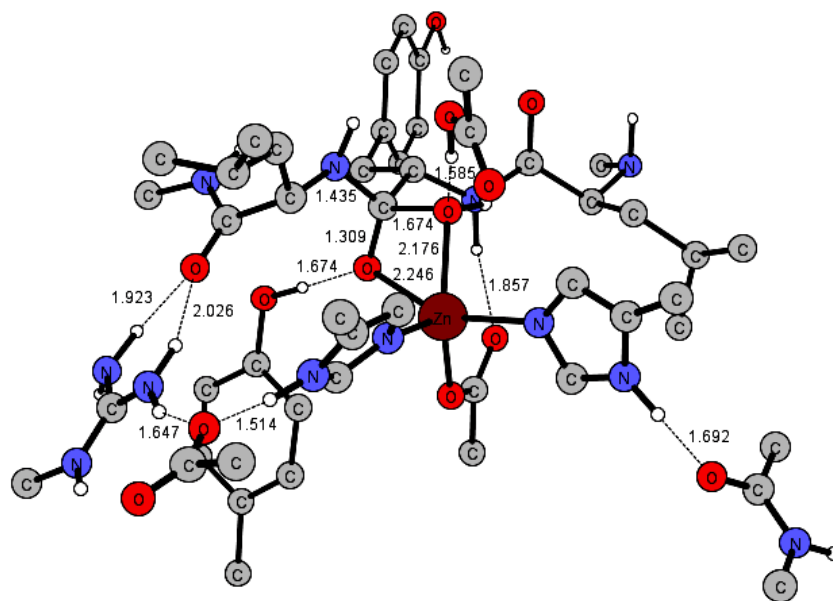
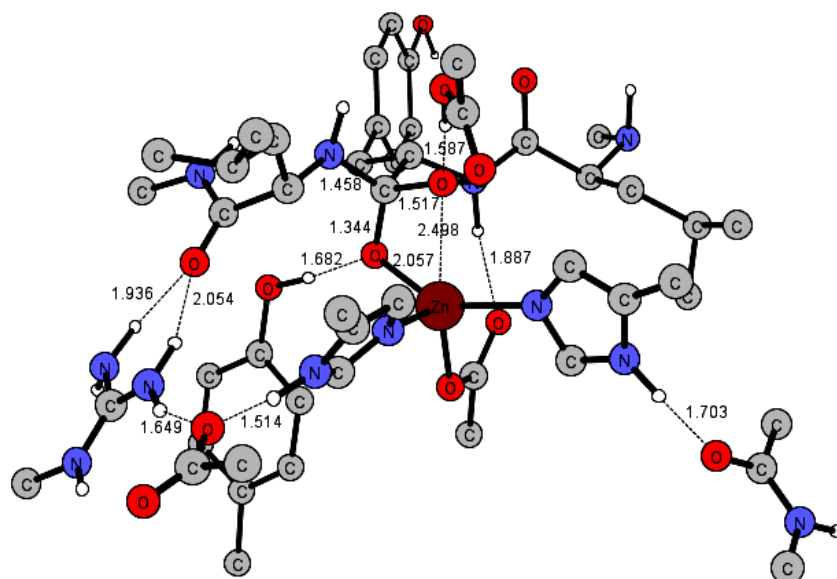


Figure S1: Optimized structure of the enzyme-CH₃NH-Leu-Tyr-Leu-CONHCH₃ substrate complex. Only the most significant hydrogen atoms are reported. Stars indicate the atoms kept fixed to their crystallographic positions during optimizations. Atoms directly involved in the catalytic reaction are numbered in orange (in the other figures this numeration is not reported but it the same). Distances are in Å.

TS1



INT1



TS2

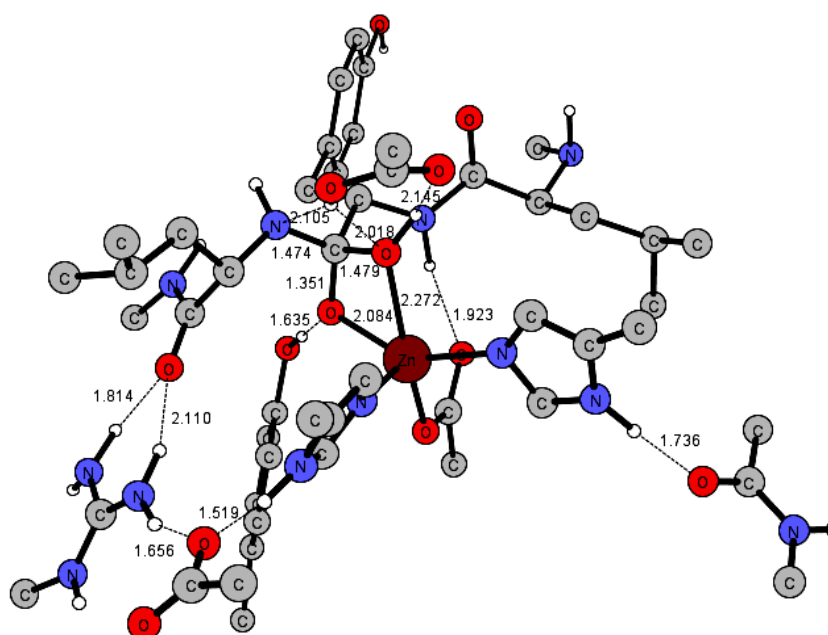
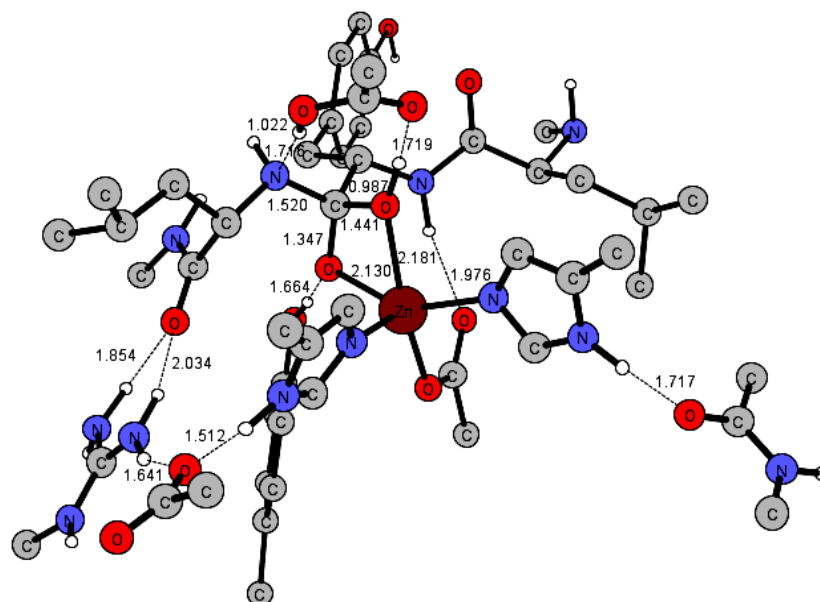
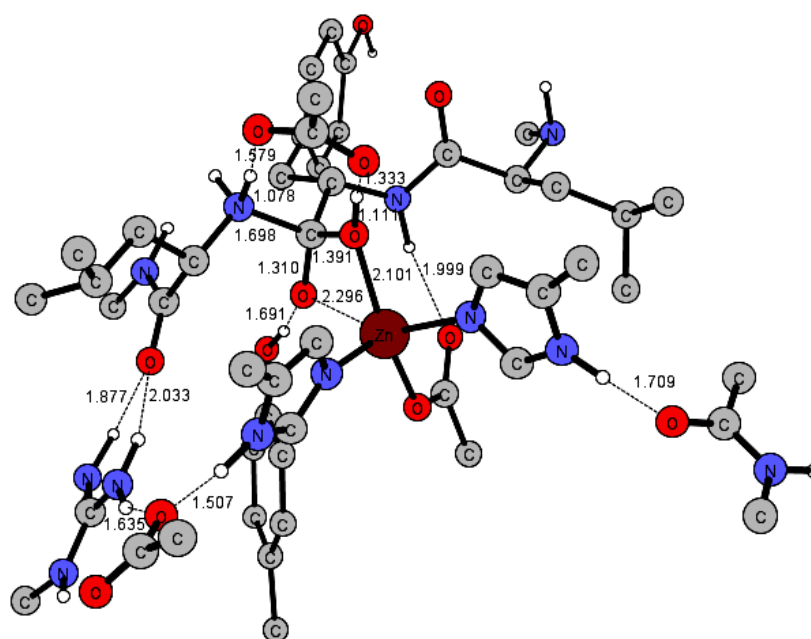


Figure S2: Stationary points (TS1, INT1 and TS2) on the IDE energetic profile.

INT2



TS3



PROD

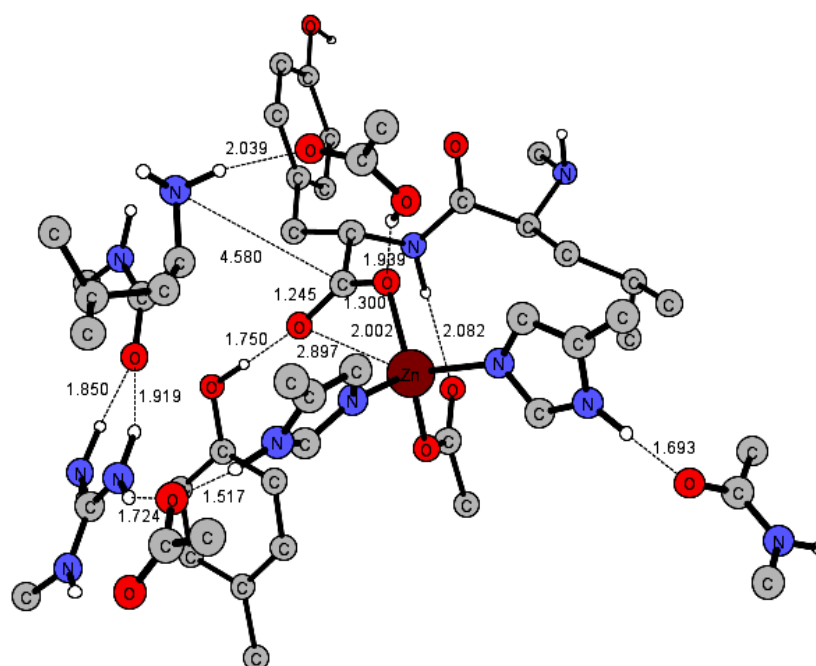


Figure S3: Stationary points (INT2, TS3 and PROD) on the IDE energetic profile