Supporting Information.

Mechanistic explanation of the weak carbonic anhydrase's esterase activity

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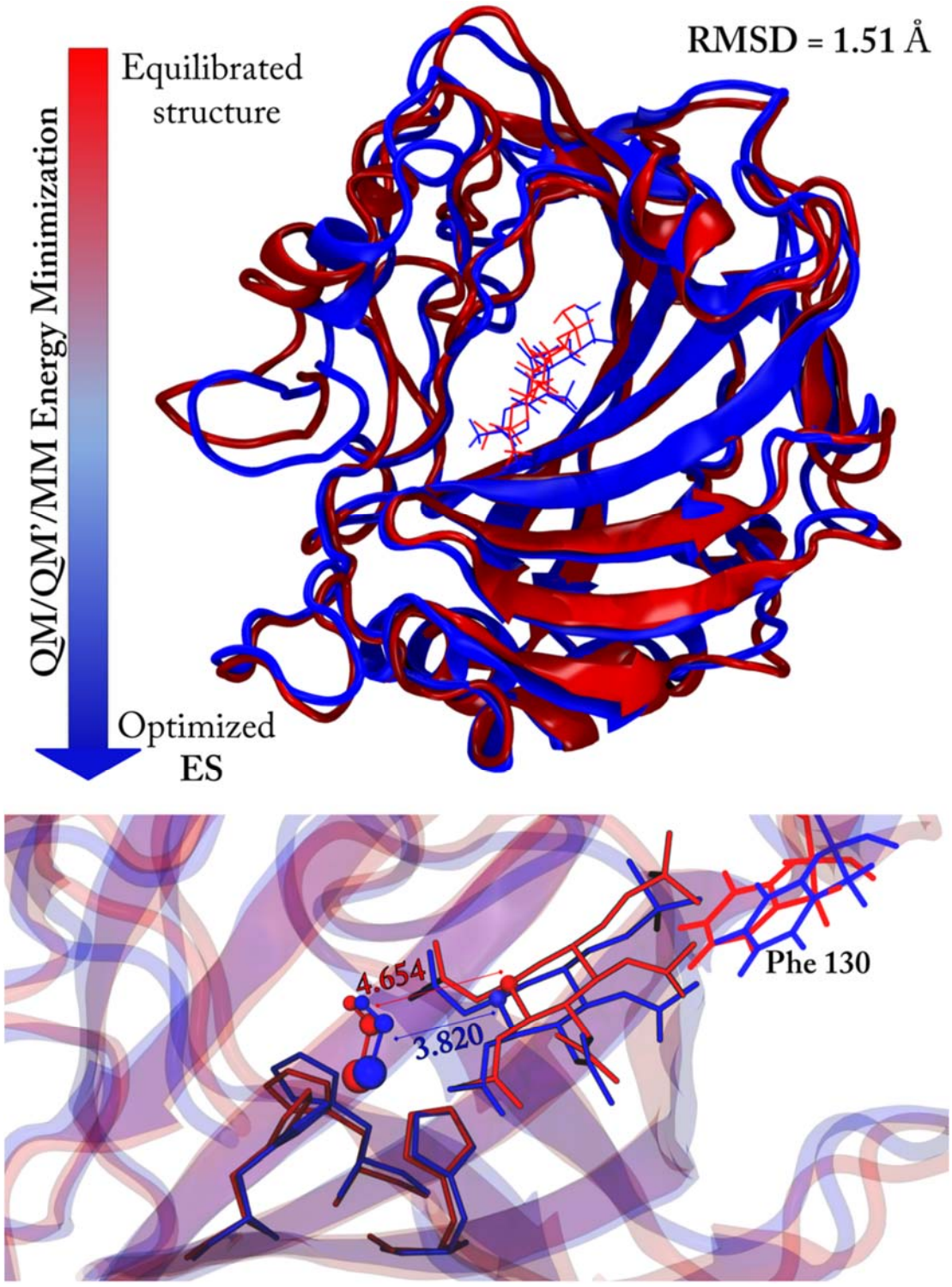

Figure S1 Calculated RMSD of the protein backbone in the optimized geometry respect to the initial conformation. The RED color is associated to the starting geometry while the BLU one is related to the optimized ES.

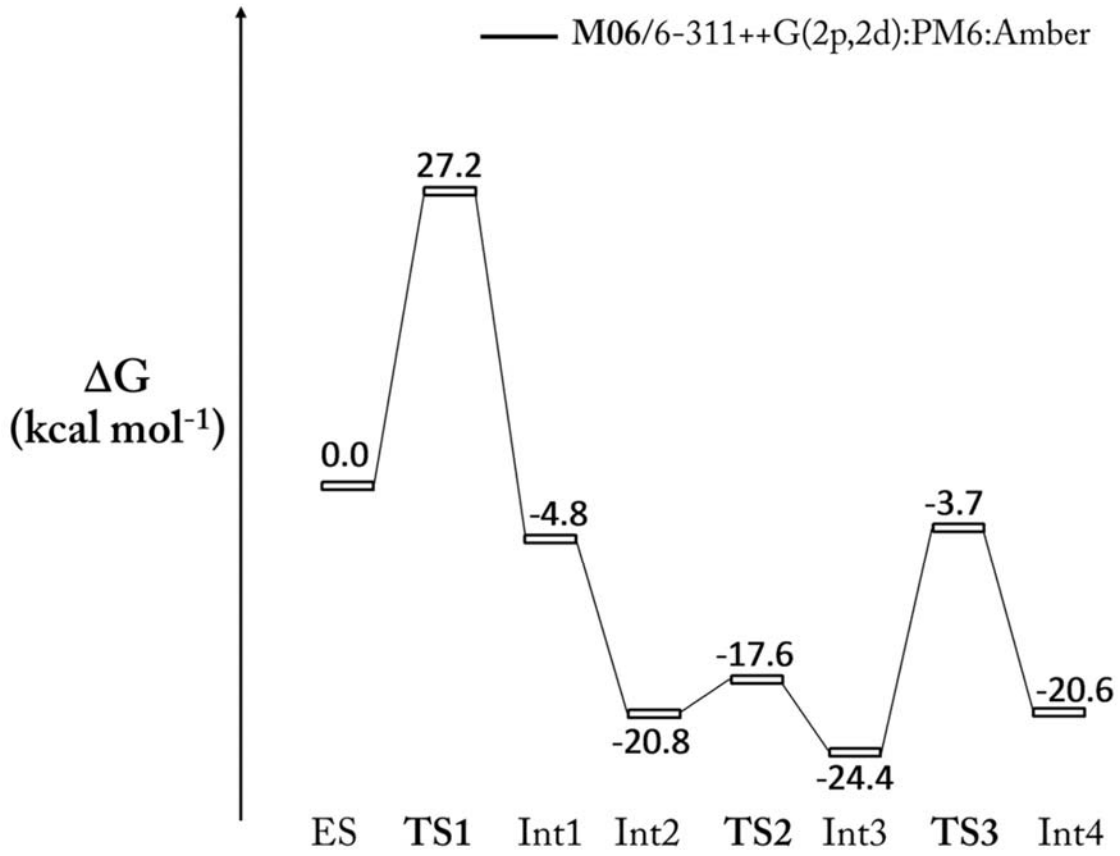

Figure S2 M06 free energies related to the investigated mechanism.

Table S1. Electronic energies comparison at DFT/6-311++G(2d,2p):PM6:AMBER level of theory with B3LYP, B3LYP-D3 and M06 functionals.

	B3LYP ΔE (kcal·mol^{-1})	B3LYP-D3 ΔE (kcal·mol^{-1})	M06 ΔE (kcal·mol^{-1})
ES	0.0	0.0	0.0
TS1	20.7	14.3	15.6
Int1	-38.5	-38.6	-18.3
Int2	-36.5	-38.4	-32.7
TS2	-29.6	-34.7	-28.9
Int3	-39.4	-38.7	-36.8
TS3	-16.5	-22.7	-17.1
Int4	-36.0	-38.9	-32.8