



Fig. 10. Regioselective hydroxylation by UPO. Regioselective conversion of vitamin D₃ (**1**) into 25-hydroxyvitamin D₃ (**2**) by *Coprinopsis cinerea* UPO (**A**) was shown by GC-MS profiles of reactions (**B**, black line) compared with controls (**B**, red line), and explained by PELE simulations revealing an optimal minimum for oxygen transfer from heme compound-I to substrate C₂₅ after its diffusion at the heme access channel (**C**). Double peaks in **B** are pyroisomers formed during GC-MS analysis. Substrate and cofactor in **C** are shown as CPK-colored sticks, while relevant amino acid residues are shown as CPK spheres (part of the solvent access surface is also shown). Adapted from Lucas et al. (2016).