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).