



Fig. 16. Polyaniline production with a laccase double mutant (DM). **A.** Formula of conductive polyaniline. **B.** Two mutations predicted by PELE simulations enabled efficient electron transfer (estimated by QM/MM calculations) from docked aniline (CPK-colored spheres) to laccase copper-1 (cyan spheres) in DM (right) compared with parental laccase (left). **C.** Experimental demonstration of faster polyaniline production (left) and darker color (right) by DM compared with parental laccase. Adapted from Santiago et al. (2016).