Non-Covalent Bonding Interaction of *epi*-Cinchonidine

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As a noncovalent interaction of a chiral scaffold in catalysis, pnicogen bonding of epi-Cinchonidine (epi-CD), a cinchona alkaloid was simulated to consider whether the interaction can have the potential controlling enantiotopic face such like hydrogen bonding. Among five reactive functional groups in epi-CD, stable complex of the hydroxyl group (X-epi-CD1) at the C17 or the quinoline ring (X-epi-CD2) with pnictide family analytes (X = Substituted phosphine (PX) i.e., F, Br, Cl, CF3, CN, HO, NO2 and CH3, and pnictide family analytes i.e., PBr3, BiI3, SbI3, and AsI3) were predicted with intermolecular interaction energies, charge transfer (QMulliken and QNBO), and band gap energies of HOMO-LUMO (Eg) at the B3LYP/6-31G (d, p) level of DFT theory. It was found that dominant site of pnicogen bonding in epi-CD is the quinoline ring (N16 atom) rather than the hydroxyl group (O36 atom). In addition, the UV-vis spectra of the complex was calculated by time-dependent density functional theory (TD-DFT) and compared with experimental measurement at the B3LYP/6-31+G (d, p). Through these calculations, two intermolecular interactions (H-bond vs pnicogen bond) of epi-CD were compared.