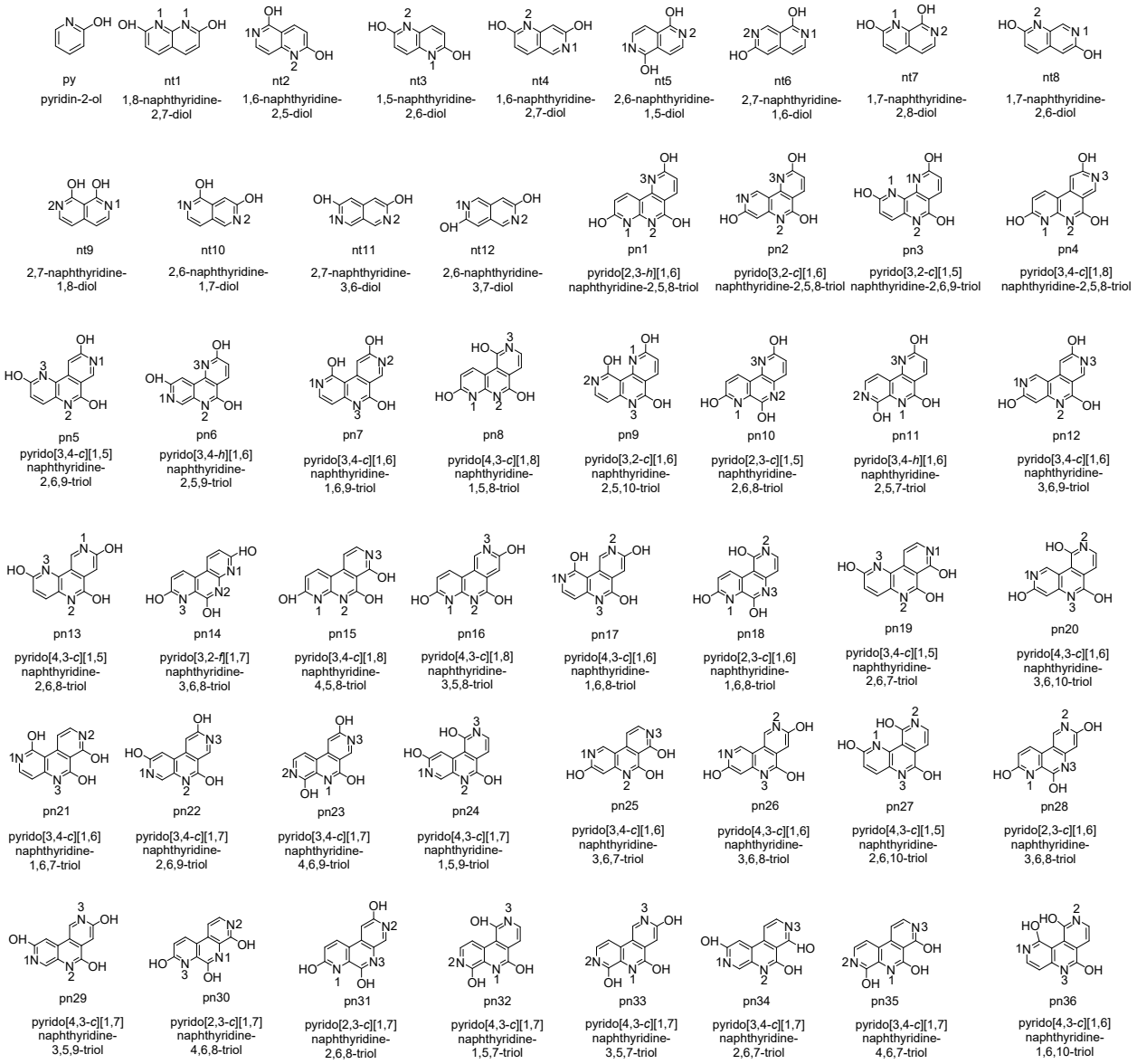

Figure S1. Chemical structures with IUPAC names of hydroxy pyridine (py), 12 dihydroxy naphthyridines (nt), and 36 trihydroxy pyridonaphthyridines (pn).

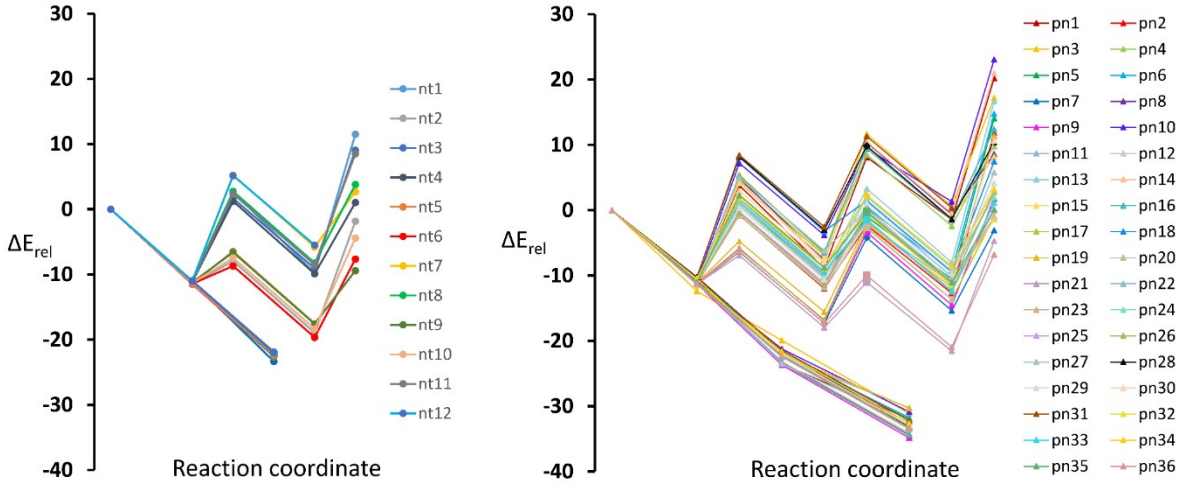

Figure S2. Relative adsorption energy of the CO_2 complexes of nt and pn molecules. All values in kcal/mol.

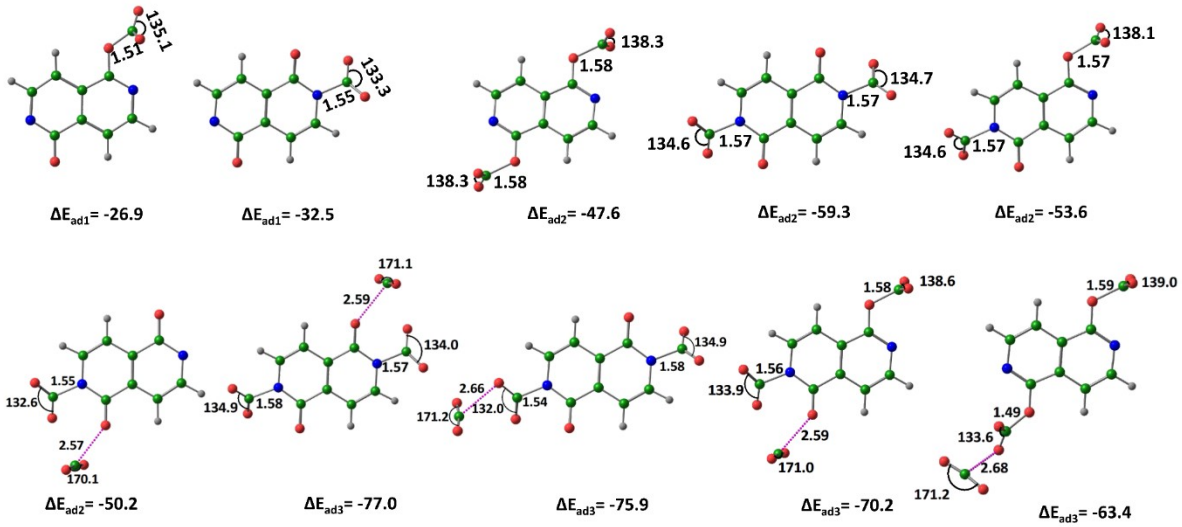

Figure S3. Optimized structures of the CO_2–adsorbed $nt5^{2-}$ at all the possible positions along with its interaction energy in kcal/mol at M06-2X/6-311++G(d,p) level of theory. Distances in Å and angles in degrees.

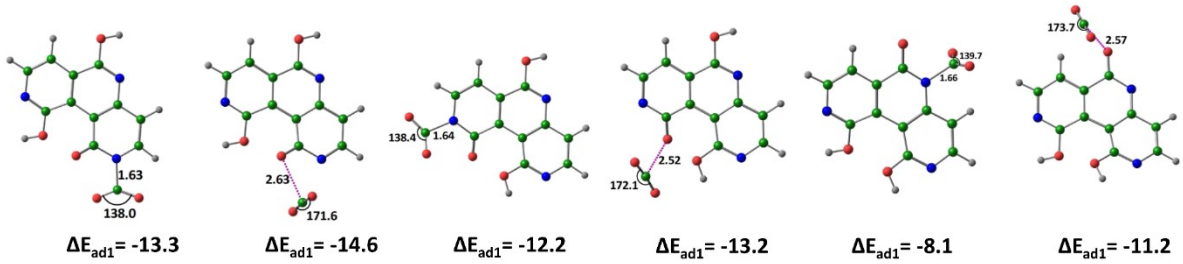

Figure S4. Optimized structures of the CO_2–adsorbed $pn36^{-}$ at all the possible positions along with its interaction energy in kcal/mol at M06-2X/6-311++G(d,p) level of theory. Distances in Å and angles in degrees.

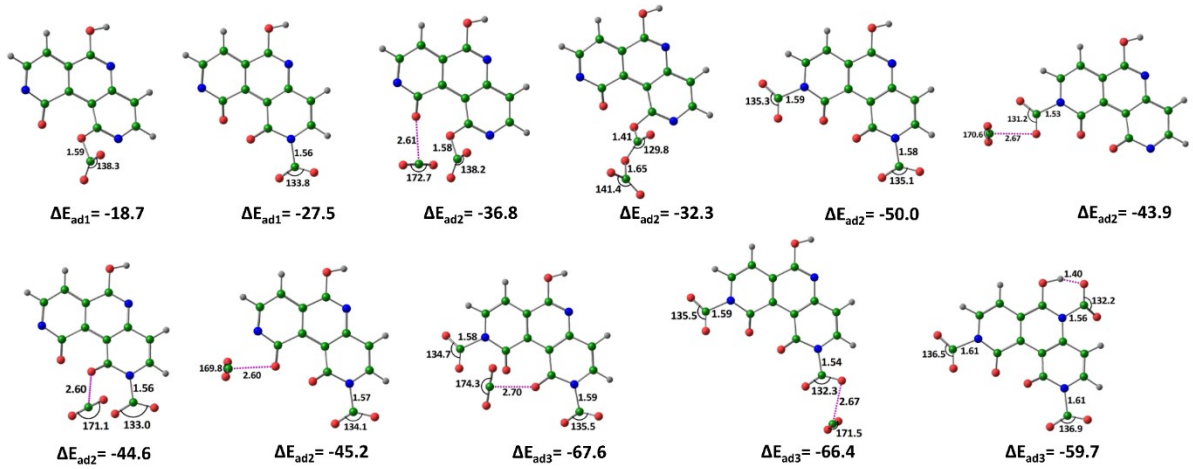

Figure S5. Optimized structures of the CO_2–adsorbed $pn36^{2-}$ at the all the possible positions along with its interaction energy in kcal/mol at M06-2X/6-311++G(d,p) level of theory. Distances in Å and angles in degrees.