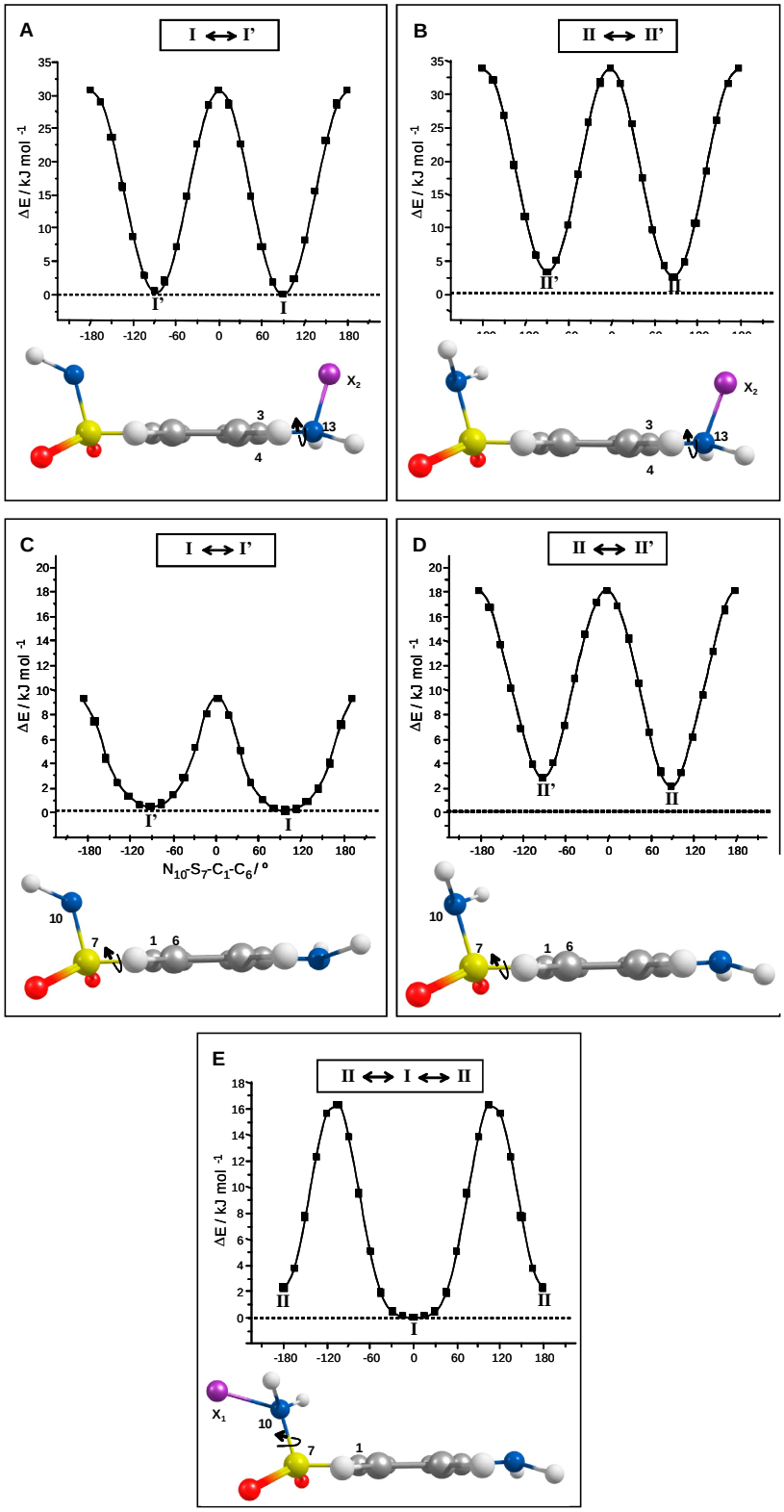

Figure S2. A-D: DFT(B3LYP)/6-311++G(d,p) calculated potential energy profiles corresponding to the torsional interconversion pathways relating the pairs of conformers of SA which differ by the relative orientation of the aniline NH_2 group (I,I' and II, II'): A, B, rotation about the N_{13}–C_4 bond; C, D, rotation about the S_7–C_1 bond; E: DFT(B3LYP)/6-311++G(d,p) calculated potential energy profile corresponding to the torsional interconversion pathway between conformers I and II: rotation about the N_{10}–S_7 bond. X_1 and X_2 are dummy atoms used to define the torsional coordinates about the S_7–C_1 and N_{13}–C_4 bond, respectively. The zero in the energy scales corresponds always to the energy of the most stable conformer I.