

Supplementary Data for HB7543

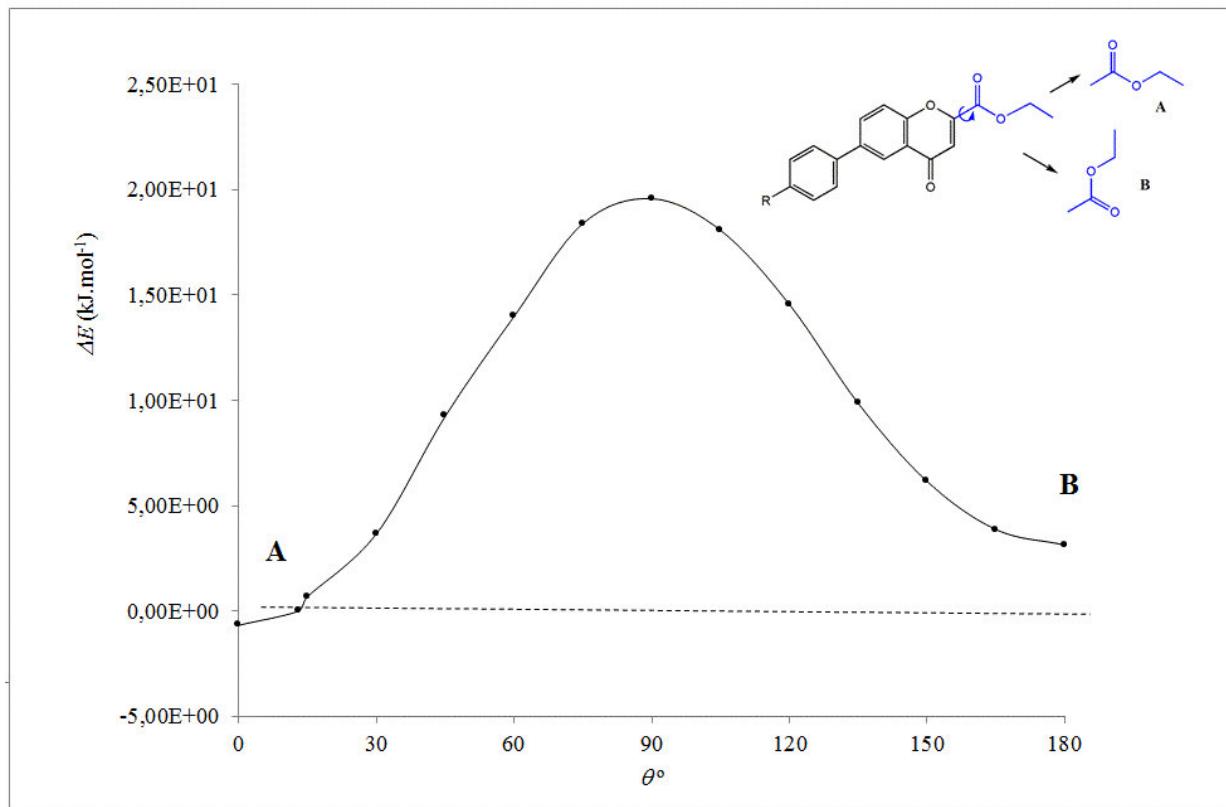


Figure 10 (supplementary): calculated gas-phase energies for the possible conformations for the studied compounds related to a hemisphere rotation of the ester group with respect to the chromone residue. Those lie between the boundary conformation A where the carbonyl groups are *trans*-related and conformation B where they are *cis*-related.

Gas-phase *ab initio* single point calculations for compound (**2**) for geometries between conformations A and B were carried out at the B3LYP/6-311+G(d) level of theory and are referred to the single point energy of compound (**2**) with the geometry obtained by X-ray analysis, $\theta = 13^\circ$. The B3LYP model combines the hybrid exchange functional of Becke (1997) with the gradient-correlation functional of Lee *et al.* (1988) and the split-valence polarized 6-311+G(d, p) basis set (Hehre *et al.*, 1988), level of theory as implemented in Gaussian 03 (Frisch *et al.*, 2004).

References

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