



Supporting Information

for

Mechanistic insights into hydroxy(tosyloxy)iodobenzene-mediated ditosyloxylation of chalcones: a DFT study

Jai Parkash, Sangeeta Saini, Vaishali Saini, Omkar Bains and Raj Kamal

Beilstein J. Org. Chem. **2025**, 21, 2703–2715. doi:10.3762/bjoc.21.208

Free energy of intermediates and structures corresponding to various intermediates shown in free energy profiles

Table S1: Free energy of intermediates involved in ditosyloxylation reaction of chalcones.

Reactive Intermediates	Total Gibbs free energy (a.u.)
Int2 + [PhIOH] ⁺ + [OTs] ⁻	-3555.421206
Int3 + [PhIOH] ⁺ + [OTs] ⁻ + OH ⁻	-3555.372379
Int3 + PhIO + H ₂ O + OTs ⁻	-3555.452820

The lowering in Gibbs free energy from **Int2** to **Int3** only happens if the hydroxy group of **Int2** interacts with second molecule of dissociated HTIB to form PhIO and H₂O.

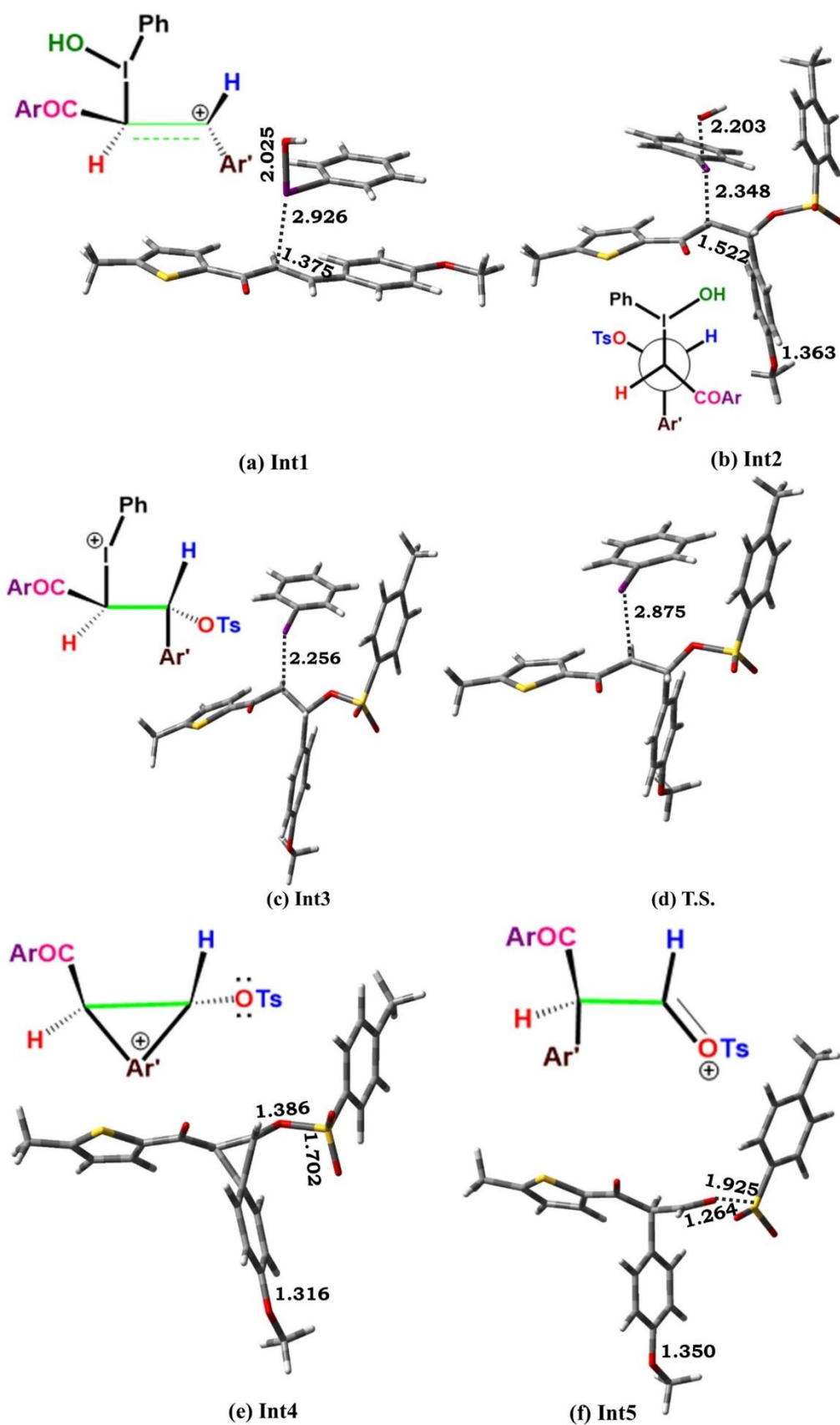


Figure S1: Structures corresponding to various intermediates listed in Table 1 for the reaction of a chalcone with X = -OCH₃.

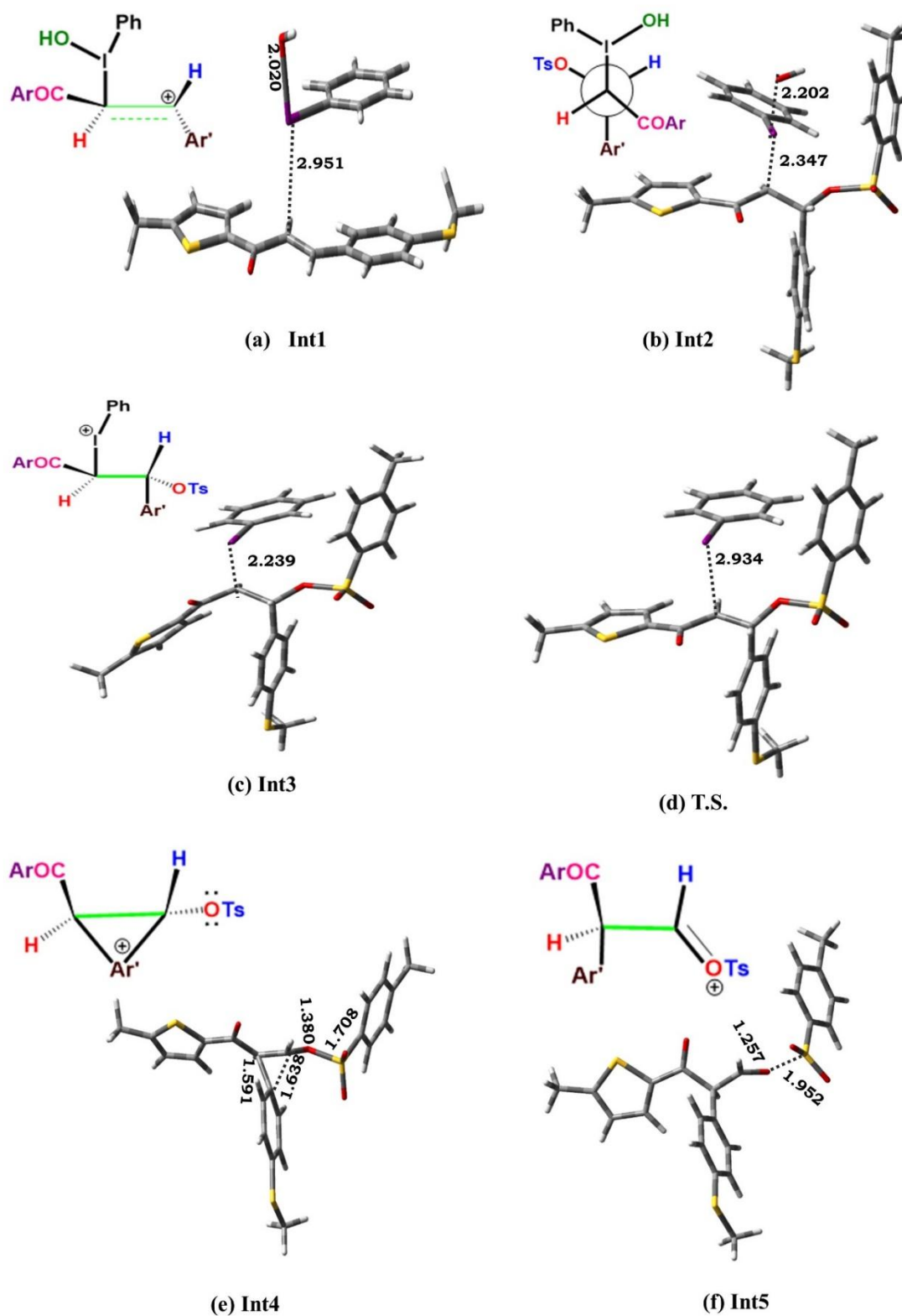


Figure S2: Structures corresponding to various intermediates shown in free energy profile presented in **Figure 1** for X = -SCH₃ leading to formation of β,β -ditosyloxy ketone.

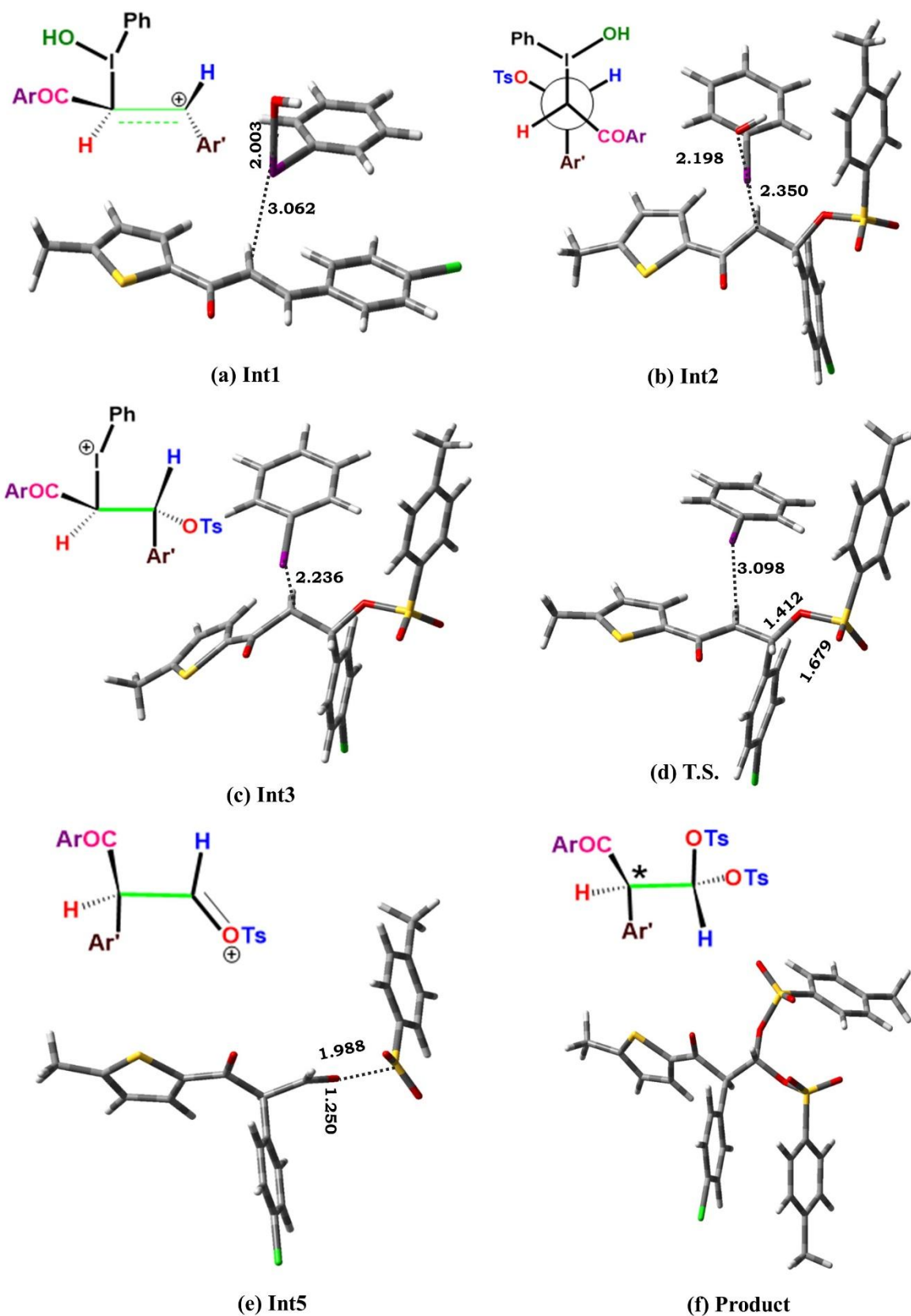


Figure S3: Structures corresponding to various intermediates shown in free energy profile presented in **Figure 2** for X = -Cl leading to formation of β,β -ditosyloxy ketone.

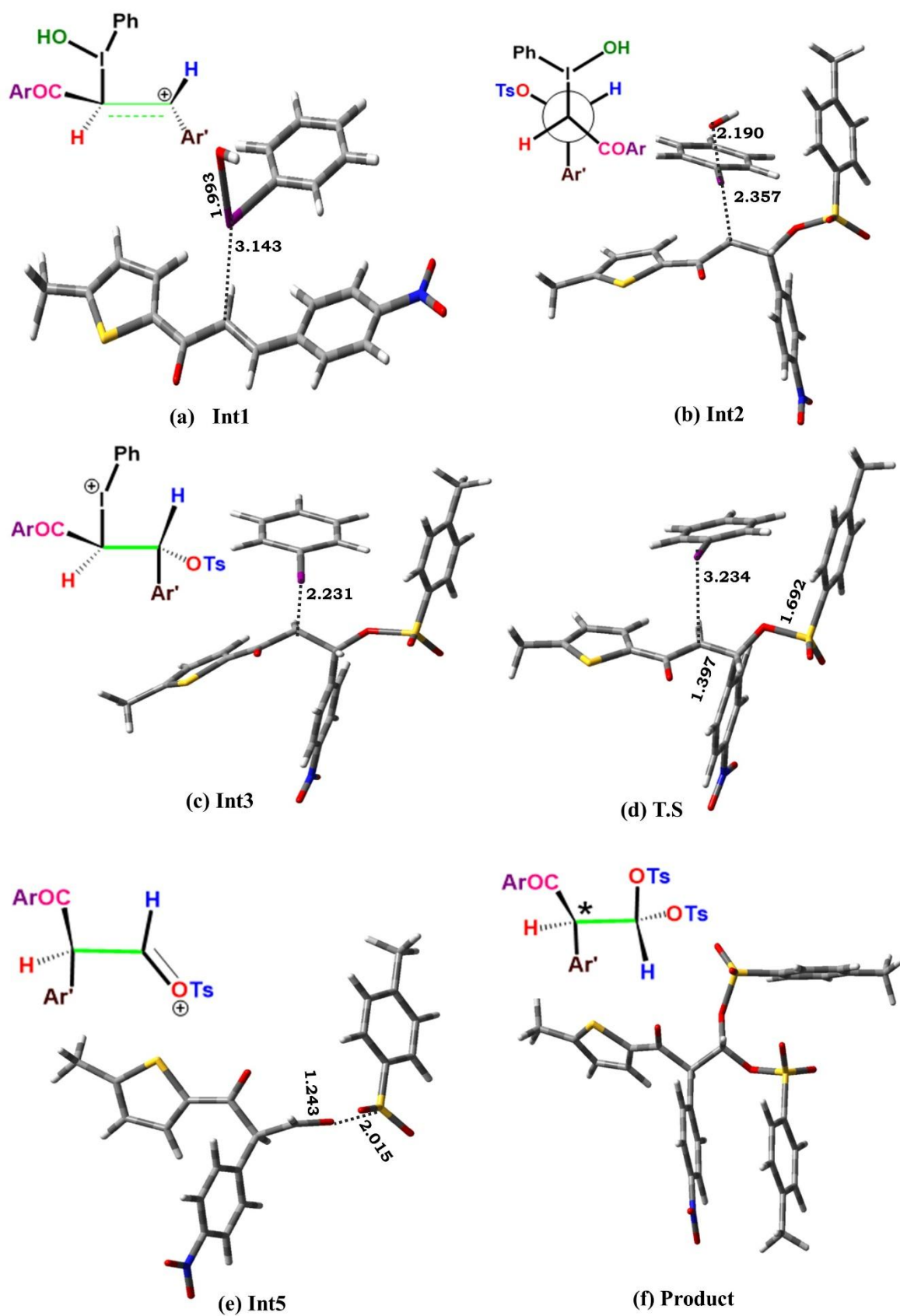


Figure S4: Structures corresponding to various intermediates shown in free energy profile presented in **Figure 3** for X = -NO₂ leading to formation of β,β -ditosyloxy ketone.

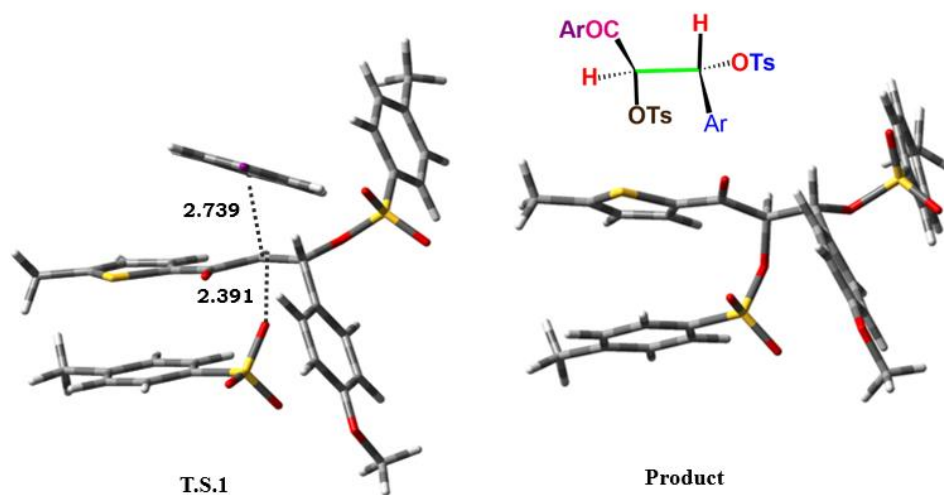


Figure S5: Optimized structure of transition state and product corresponding to free energy profile presented in **Figure 4** for X = -OCH₃. Product is α,β-ditosyloxy ketone. Important bond lengths are reported in Å.

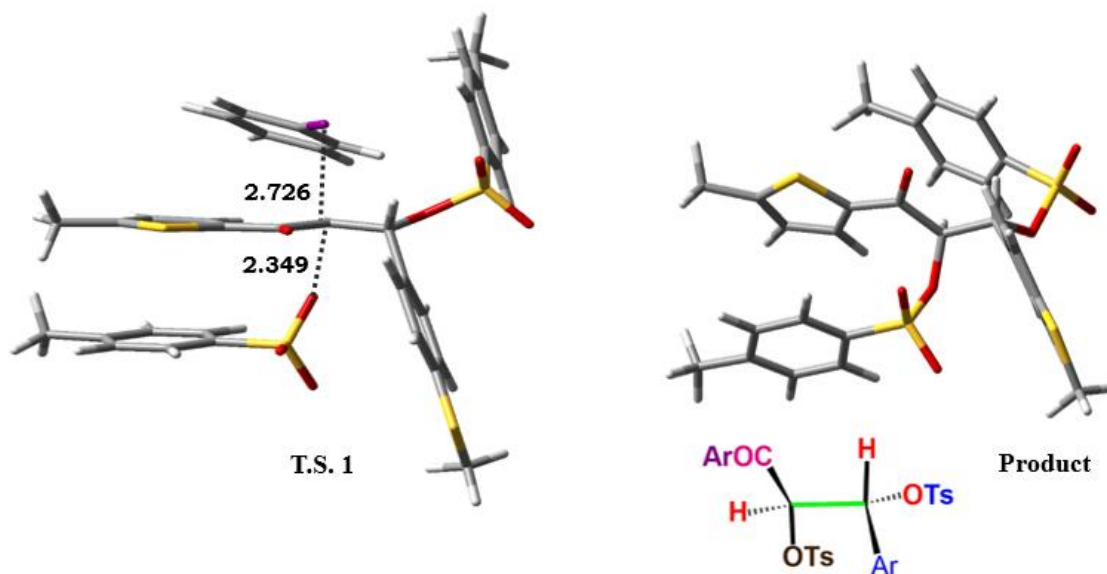


Figure S6: Optimized structure of transition state and product corresponding to free energy profile presented in **Figure 5** for X = -SCH₃. Product is α,β-ditosyloxy ketone. Important bond lengths are reported in Å.

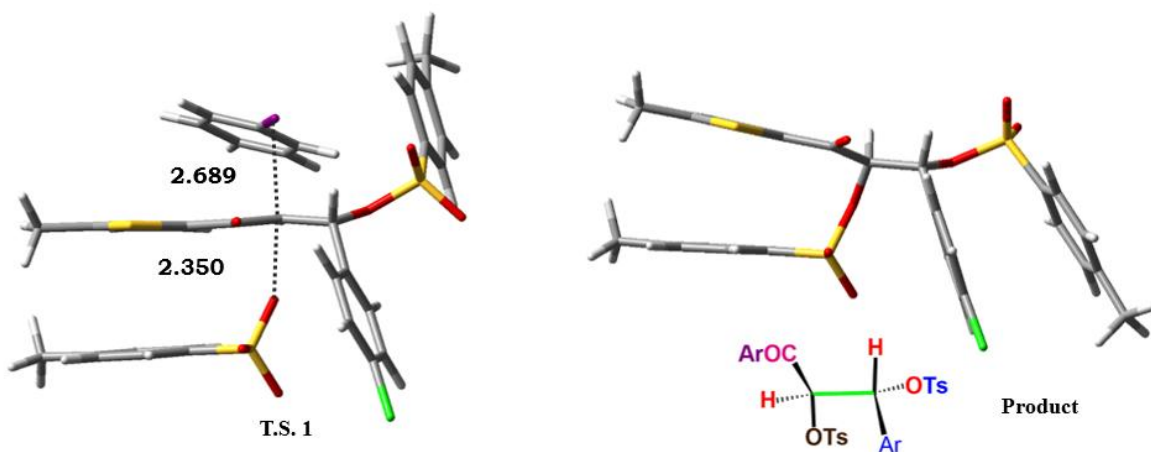


Figure S7: Optimized structure of transition state and product corresponding to free energy profile presented in **Figure 6** for X = -Cl. Product is α,β -ditosyloxy ketone. Important bond lengths are reported in Å.

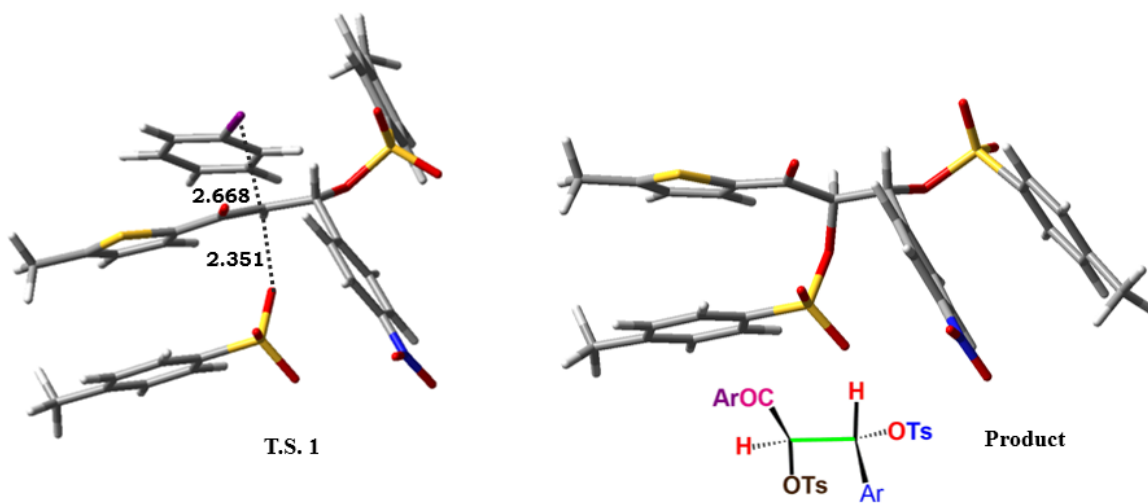


Figure S8: Optimized structure of transition state and product corresponding to free energy profile presented in **Figure 7** for X = -NO₂. Product is α,β -ditosyloxy ketone. Important bond lengths are reported in Å.