

Electronic Supplementary Information

Design of Carboxylate-Based Ionic Liquids (ILs) Containing OH and CF₃ groups; Influence of Intramolecular Hydrogen Bond and Inductive Effect on Binding Energy between Cation and Anion of ILs, A DFT study

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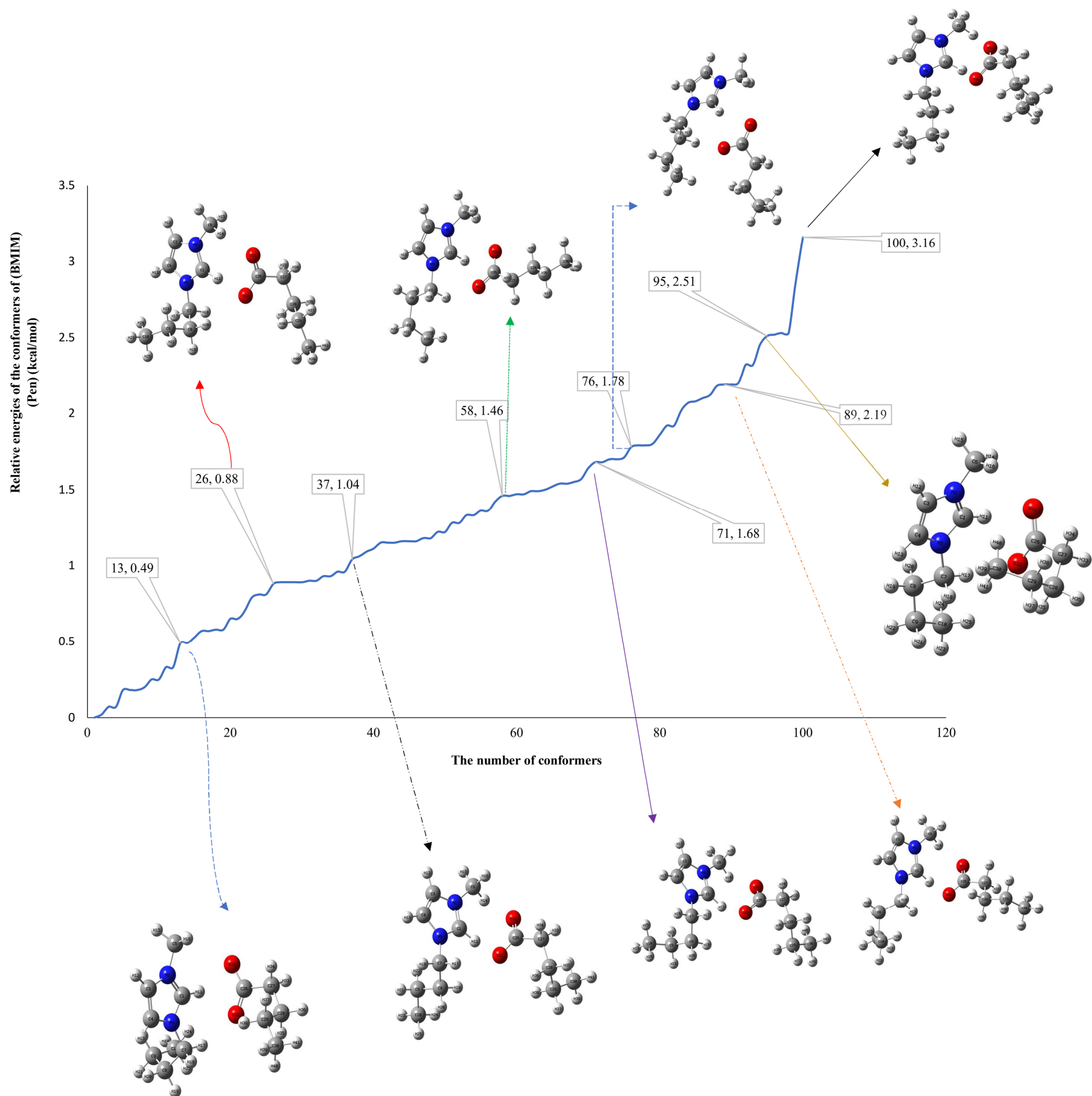


Figure S1. Relative energies of the conformers of (BMIM) (Pen) with respect to the most stable conformer

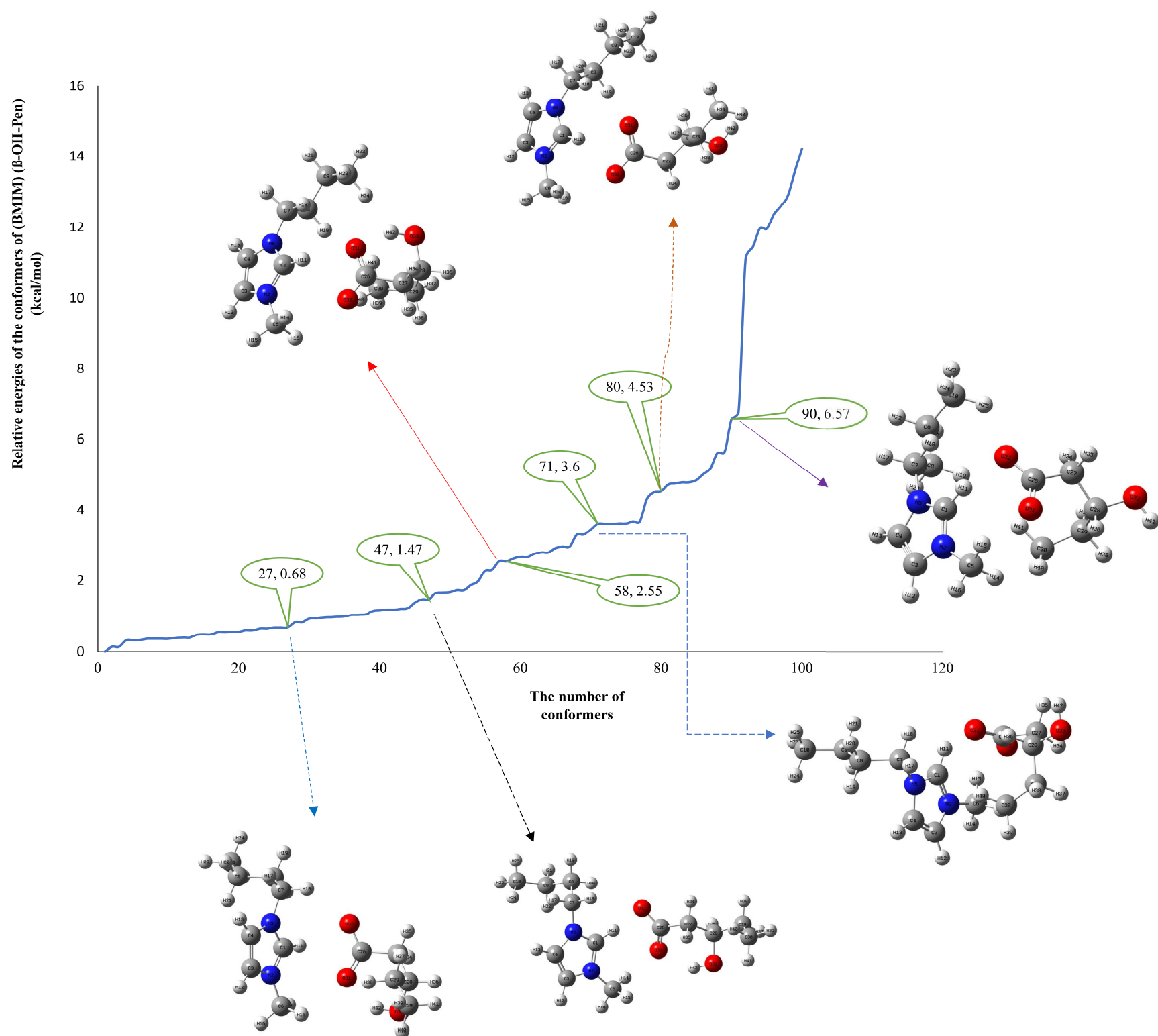


Figure S2. Relative energies of the conformers of (BMIM) (β -OH-Pen) with respect to the most stable conformer

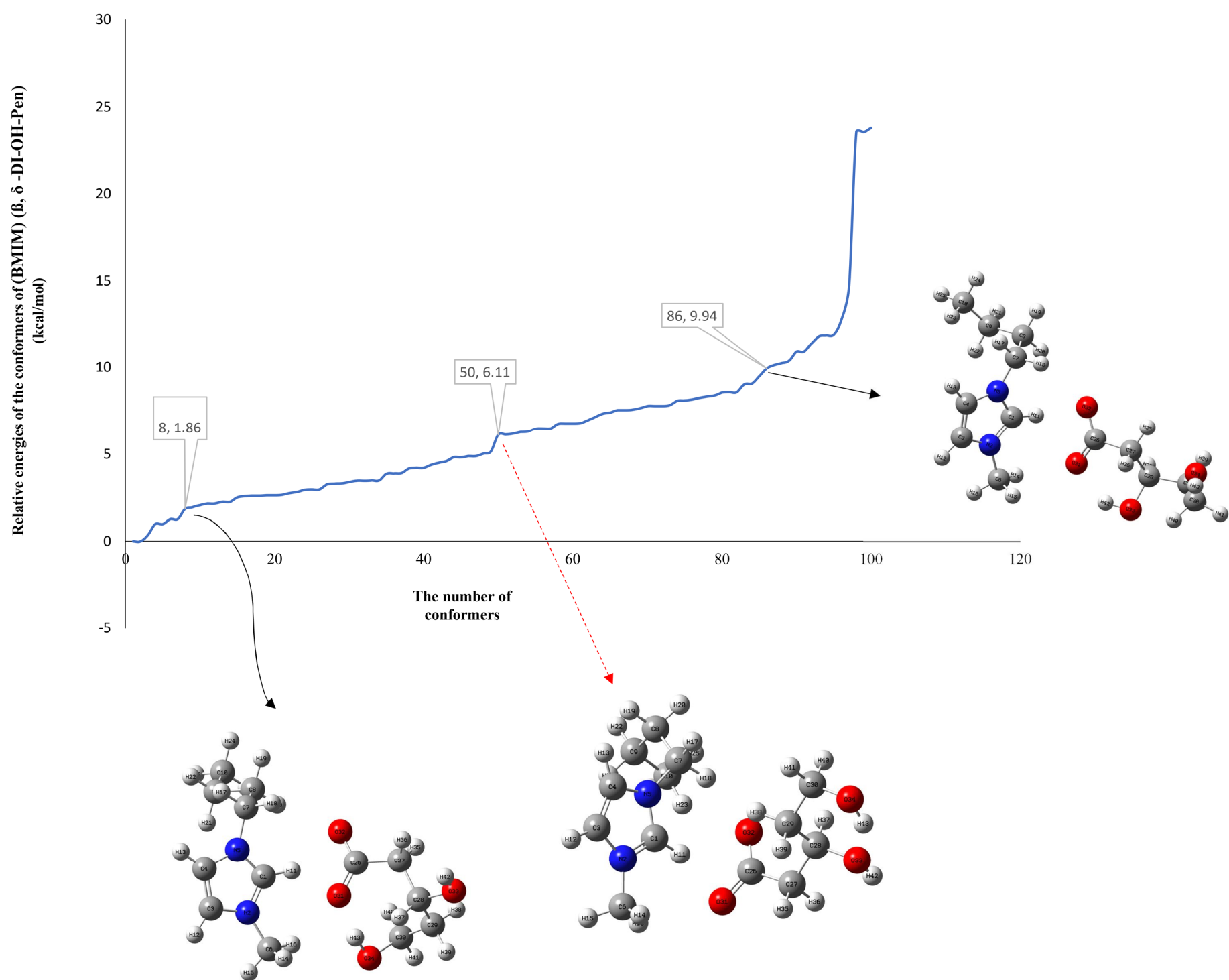


Figure S3. Relative energies of the conformers of (BMIM) (β, δ -DI-OH-Pen) with respect to the most stable conformer

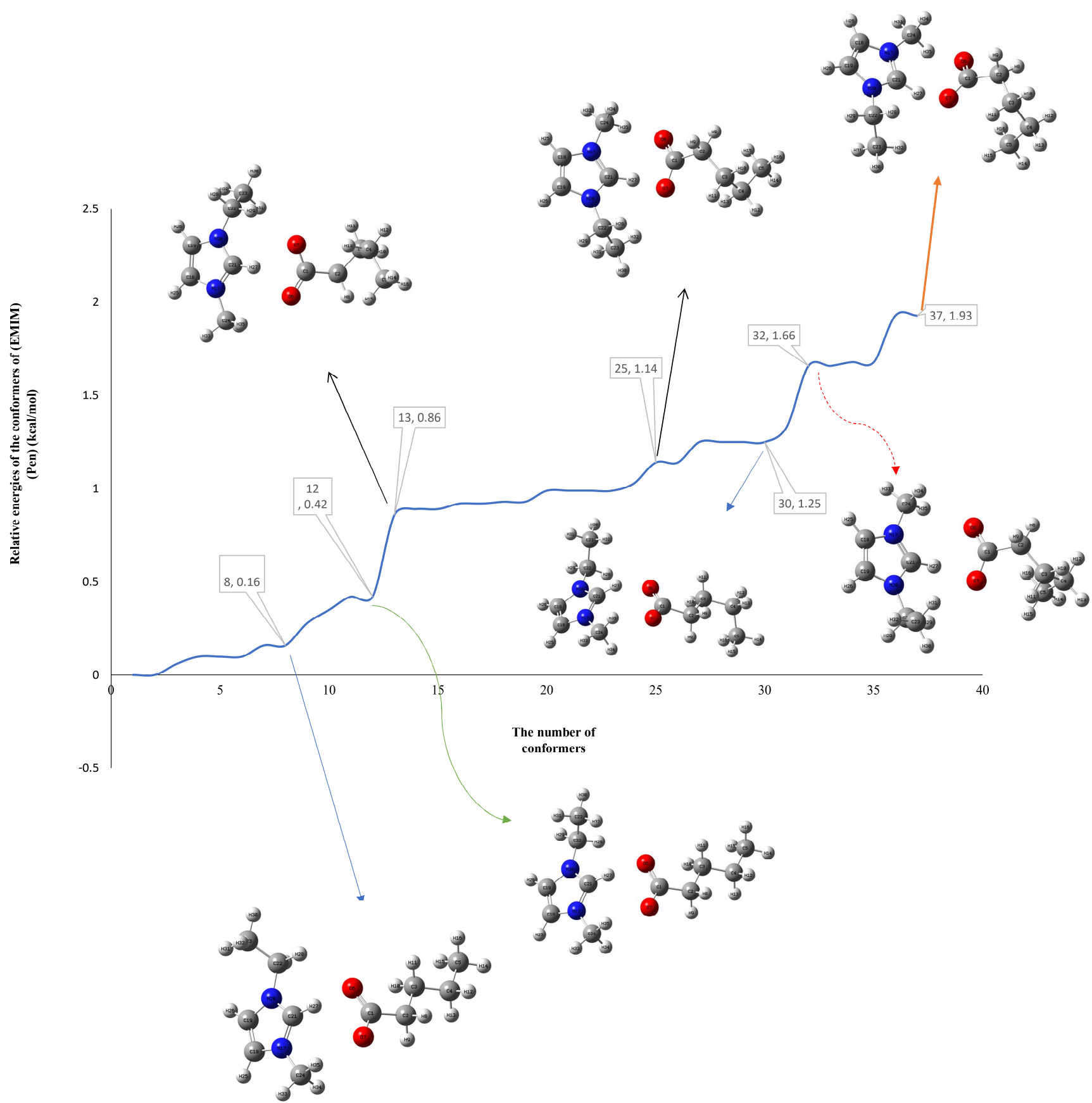


Figure S4. Relative energies of the conformers of (EMIM) (Pen) with respect to the most stable conformer.

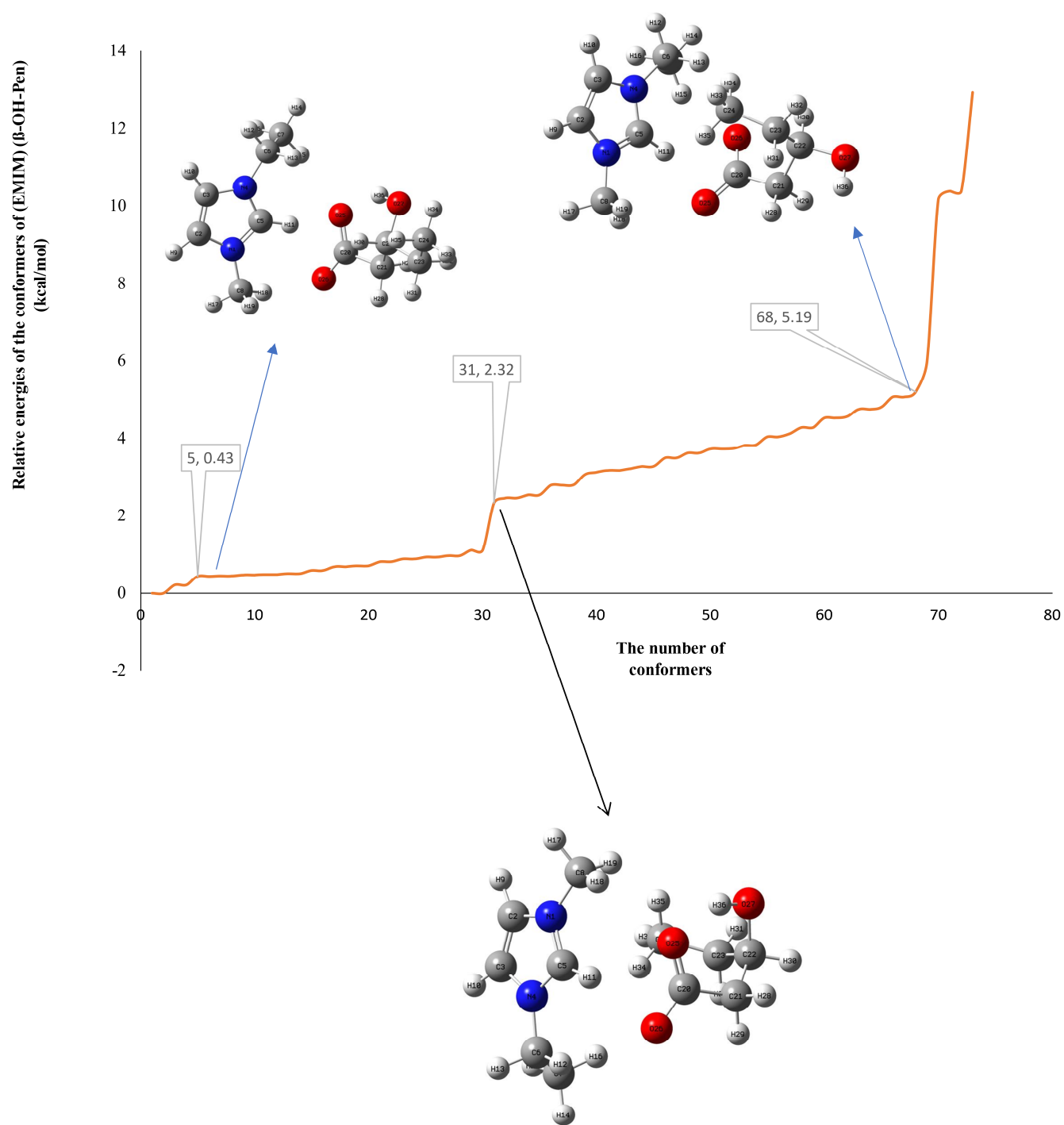


Figure S5. Relative energies of the conformers of (EMIM) (β -OH-Pen) with respect to the most stable conformer

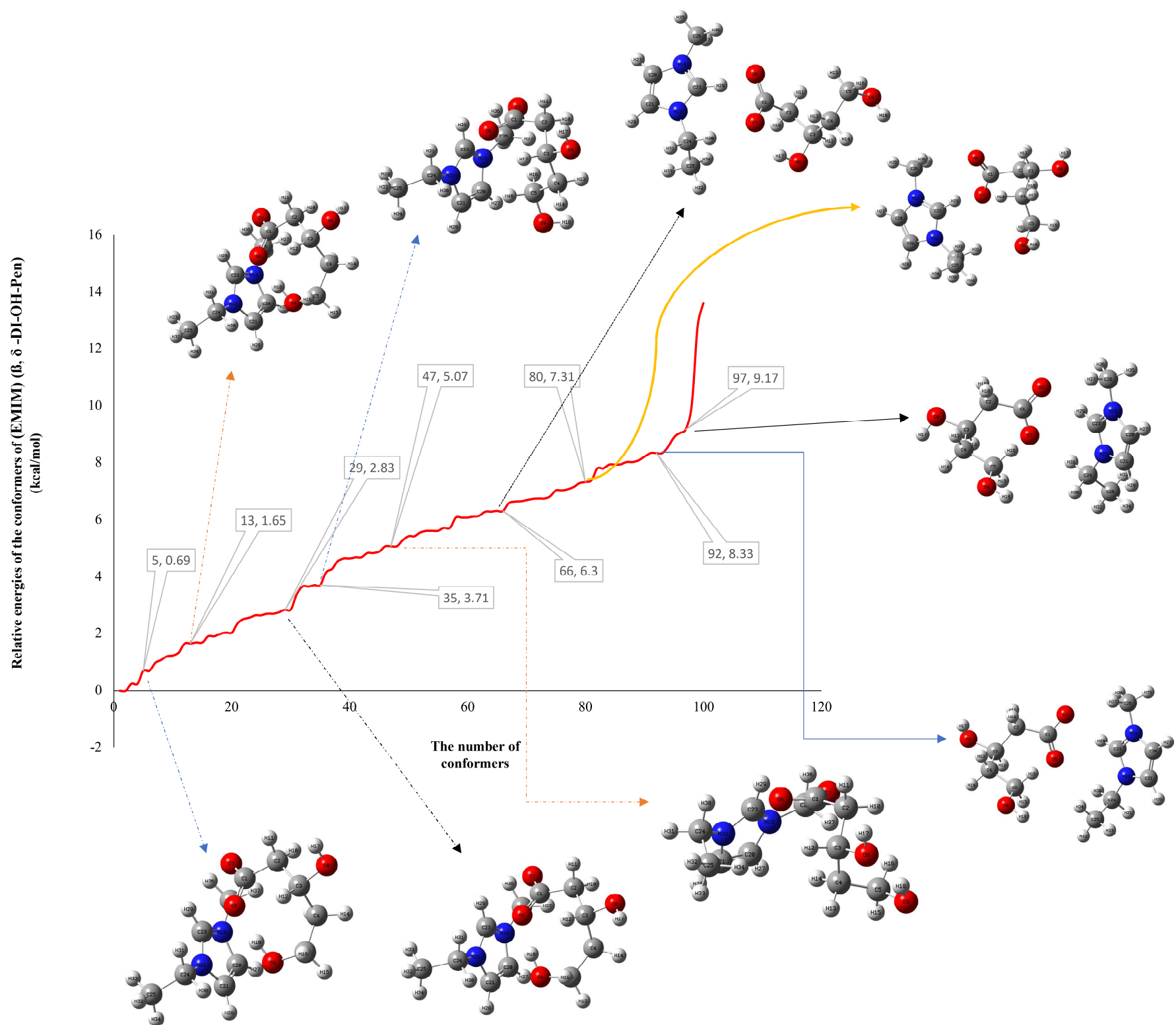


Figure S6. Relative energies of the conformers of (EMIM) (β , δ -DI-OH-Pen) with respect to the most stable conformer