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Synthesis of 2-amino alcohols from imidazole derivatives: Experimental and *in silico* study

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β-Amino alcohols are promising molecules as synthons and also possess significant biological activity. The synthesis of β-amino alcohols mainly involves reaction of epichlorohydrin with various amines. Most of the reported work ignores the side products formed during the course of the reaction. In an ongoing effort to discover newer imidazole-based compounds, which can act as synthon for the synthesis of β-amino alcohols, a novel series of imidazole based epoxides have been designed and synthesized using a mild, efficient, and metal free approach. Starting from N_1-hydroxy-2,4,5-trisubstituted-imidazoles and epichlorohydrin as precursor compounds, a series of molecules have been obtained which may have higher potential to show biological activity. We have come across two different products which might have significant importance for the derivatization leading to the formation of biologically active molecules. To support the experimental findings, we have also performed Density Functional Theory (DFT) calculations. On the basis of the experimental findings and theoretical calculations we have proposed a possible reaction pathway that can lead to the desired product formation.

Keywords: N_1-Hydroxy-imidazole, Oxiranes, Epichlorohydrin, DFT, β-Amino alcohols