Synthesis and Theoretical Calculations of Tetrahydropyranochromene Framework

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Tetrahydropyranochromene is a common framework for several polyphenolic natural products including calyxins and epicalyxins I and J \cite{1-3} that are biologically active compounds isolated from dry seeds of \textit{Alpinia blepharocalyx}. Herein, we have synthesized a model having tetrahydropyranochromene unit (shown bold) along with two phenyl groups at C-7 and C-7' to address the stereochemistries at these positions. We have also performed theoretical calculations at different levels on our model system. Our experimental result shows a strong preference for the formation of a syn isomer and our theoretical calculations suggest that syn preference is attributed to a favorable \(\pi-\pi\) stacking interaction between the aromatic rings at C-7 and C-7'.

Reference: