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A Study of Adamantane Based Ester: Synthesis, Crystallographic Insight and Against Acetylcholinesterase Activity

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Adamantyl-based compounds are commercially important in the treatments for neurological and type-2 diabetes diseases, beside their anti-viral abilities. Their values in drug design are chronicled as multi-dimensional. In this study, a series of 2-(adamantan-1-yl)-2-oxoethyl benzoates, **2**(**a**-**q**), and 2-(adamantan-1-yl)-2-oxoethyl 2-pyridinecarboxylate, **2r,** were synthesized by reacting 1-adamantyl bromomethyl ketone with various carboxylic acids using potassium carbonate in dimethylformamide medium at ambient temperature. Three-dimensional structures studied using X-ray diffraction analysis suggests that adamantyl moiety can be served as an efficient building block to synthesize 2-oxopropyl benzoate derivatives with *synclinal* conformation and looser-packed crystal packing system. The activities of the synthesized compounds toward the enzyme AChE were determined by using Ellman's colorimetric method and were compared in terms of their molecular structures. Inhibitory activity increased as the compound possess electron donating substituents at the *–meta* position, while the most significant AChE inhibitor with an IC_{50} value of 28.33 ± 2.89 µg/mL is compound **2e** with dichloro substituents at *–orto* and *–para* position. Through molecular docking simulations, the most potent derivative (compound **2e**) inhibited the AChE enzyme is through binding to the peripheral anionic site (PAS) and not to its acylation site (A site).