MOLECULAR SCAFFOLD DEVELOPMENT OF TERTIARY AMINE CHALCONES FOR INHIBITION OF LYCOPENE CYCLASE IN FRUIT

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Lycopene, a known anti-oxidant, is transformed into β-carotene and other carotenoids by a class of enzymes referred to as lycopene cyclases. Developing potential inhibitors of lycopene cyclases could yield further understanding of the structural and functional properties of these enzymes and eventually serve to manipulate lycopene levels in fruits and vegetables. Previously reported aryl tertiary amine-containing compounds, when protonated at physiological pH, act as transition-state inhibitors of these cyclizing enzymes. Our proposed scaffold yields a series of substituted chalcones containing the core structure of the known inhibitor *N,N*-diethyl-*N*-[2-(4-methylphenoxy)ethyl]amine (MPTA). However, the initial scaffold design involved the aldol condensation of a deactivated aldehyde and ketone under relatively harsh conditions. Though various methods exist for this specific transformation, we developed a novel, safe, cost-effective application of the aldol condensation using a domestic microwave and potassium carbonate with iodine impregnated alumina. Reaction conditions including catalyst, base, and microwave intensity were optimized. Herein, we report the molecular scaffold development and synthesis of several tertiary amine chalcones with the potential for activity against lycopene cyclases in fruits and vegetables.

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