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High-throughput virtual screening of chalcone compounds against diverse targets-development and use of a specific chalcone virtual library

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The chalcone family of compounds are well-known for their different therapeutic properties including anti-inflammatory, anti-microbial or anti-cancer activities, although the mechanism in many cases is not well understood. The generation of a virtual library mimicking the aldol condensation was effected with a view to expansion with aliphatic side chains as a result of alkyl halide reactivity. This virtual library was based on a very specific set of criteria with respect to substituents and with availability of the starting materials (substituted acetophenones and benzaldehyde derivatives) from suppliers for actual experimental work. The resulting 8063 compounds in the library were subjected to semiempirical AM1 geometry optimizations with the use of Gaussian 09, prior to virtual screening (docking using Autodock Vina) against 17 targets including HIV-1 integrase, MRSA pyruvate kinase, HSP09, COX-1, COX-2, ALR2, MAOA and AMOB, acetyl choline esterase A and B and PLA2 (including more than one enzymatic structure where conformers are available). The choice of targets related to the existence in the literature of similar compounds to those in this library having experimental activities against these targets. Lead compounds have been identified, and molecular dynamics has provided information about the strength of binding in several cases.

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