**A Quest for novel *Pf*-DHFR inhibitors from xanthones of natural origin using contact based ligand virtual screening**

Neglected tropical diseases such as malaria are still an unconquered territory for human exploits in the field of medicinal chemistry. In Malaria, this is primarily ascribed to limited chemotherapies mainly relying on a very few scaffolds or their allied structures such as quinolines, anti-folates and some cyclic endoperoxides. Hence, there is a need for the development of new chemo types as prospective anti-malarials.

Keeping the above in mind, a small yet diverse xanthone library was build and computationally docked against wild type *Pf*-DHFR-TS by Molegro Virtual Docker. For analysis of results an integrated approach based on Re-ranking, Scaling (based on heavy atom counts), Clustering and Visual inspection was implemented. Three compounds **X5**, **X113A** and **X164B** have shown contact footprints similar to the known actives with good scores.

**References**

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