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ABSTRACT BOOK

STRUCTURAL OPTIMIZATION, IN VITRO CHARACTERIZATION AND IN SILICO PHARMACOPHORE MODELING OF A NEW ANTIPLASMODIAL CHEMOTYPE

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Malaria is the most common parasitic disease worldwide, and the third deadliest infection after HIV and tuberculosis. Due to the risk of diffusion of artemisinin resistance in Africa, new drugs for ensuring efficacious antimalarial treatment are urgently needed. In one of our previous communications, we reported the discovery of a new 4,4'-oxybisbenzoic acid-based chemotype with promising antimalarial activity against both CQ-sensitive and CQ-resistant *P. falciparum* (Pf) strains.[1] Here, we present our exploration of the structural requirements for the inhibition of Pf growth by this new chemotype through a detailed SAR investigation focused, also, on the improvement of its drug-likeness parameters. Our investigation led to the identification of the potent antiplasmodial compound, DC18.
An *in silico* analysis was run to build a pharmacophore model for this new, still target-less, antiplasmodial chemotype.

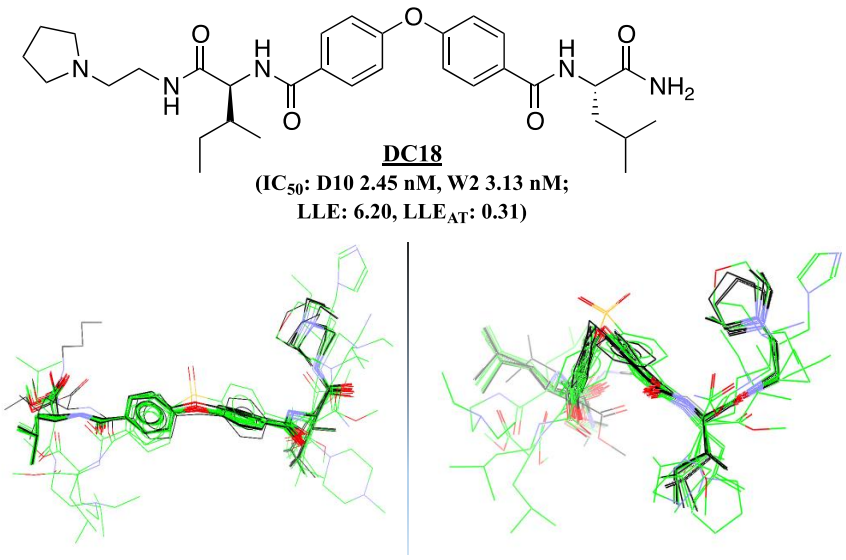

Figure 1. Structure of DC18 (up) and its ligand overlay-based pharmacophore modeling (down).

References

1. Pancotti, A.; Parapini, S.; Dell'Agli, M.; Gambini, L.; Galli, C.; Sangiovanni, E.; Basilico, N.; Bosisio, E.; Taramelli, D.; Romeo, S. *Med. Chem. Commun.* **2015**, *6*, 1173-1177.