Indian Journal of Heterocyclic Chemistry
Vol. 36 - Number 02 (Apr-Jun 2026) 269-275
https://connectjournals.com/01951.2026.36.269
https://doi.org/10.59467/IJHC.2026.36.269

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Molecular modeling studies on novel xanthone derivatives targeting multiple diseases

Darakhshan Parveen[1]*, Amrita Parle[1], Mandeep Kumar Gupta[2], Rajnish Srivastava[3], Krishna Varshney[4] and Sudhansu Ranjan Swain[5]

[1]Department of Pharmaceutical Chemistry, Delhi Pharmaceutical Sciences and Research University, New Delhi, India
[2]Department of Pharmaceutical Chemistry, Amity Institute of Pharmacy, Amity University, Lucknow, Uttar Pradesh, India
[3]Department of Pharmacology, Chitkara University School of Pharmacy, Chitkara University, Baddi, Himachal Pradesh, India
[4]Department of Pharmacology, Institute of Pharmaceutical Research, GLA University, Mathura, Uttar Pradesh, India
[5]Department of Pharmacognosy, Moradabad Educational Trust Group of Institutions Faculty of Pharmacy, Moradabad, Uttar Pradesh, India

ABSTRACT Post-COVID-19, people are suffering from multiple diseases at the same time. Therefore, a medication/ molecule is needed that targets multiple diseases, and xanthone is one such moiety. Xanthone is a basic active compound having a tricyclic planar bone and a pyran ring. The fused pyran ring carries a phenyl ring on each side. In the present study, this moiety was exploited to ensure its diverse pharmacological activities. Hence, in the future, it can be a savior of mankind as it can be used to treat patients with multiple diseases. *In silico* studies were performed on thirty designed novel 3-aminoalkoxy derivatives of xanthone. Molecular docking was carried out on the test ligands with receptors, peroxisome proliferator-activated receptor gamma (PPAR-Y), cyclooxygenase-2 (COX-2), plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS), and xanthine oxidoreductase, respectively. Among all the designed ligands, LIG14 showed the best docking score of −12.86, −10.1, and −9.9 kcal/mol against receptors, PPAR-Y. COX-2, and PfDHFR-TS, respectively, for antidiabetic, analgesic, and anti-malarial activity. Furthermore, other designed ligands than LIG14 also showed appreciable activity. The interactions observed in molecular docking were preserved during the molecular dynamic simulation. Finally, it was concluded that as all our designed ligands showed significant binding potential and also LIG14 possessed to be highly active against three different receptors, further *in vitro* and *in vivo* studies should be conducted so that it can be used to treat patients with multiple diseases.

KEY WORDS Xanthone, Molecular docking, Molecular dynamics, Peroxisome proliferator-activated receptor gamma, Cyclooxygenase-2, Xanthine oxidoreductase, Plasmodium falciparum dihydrofolate reductase-thymidylate synthase.

How to cite this article: Parveen, D., Parle, A., Gupta, M.K., Srivastava, R., Varshney, K. and Swain, S.R. Molecular modelling studies on novel xanthone derivatives targeting multiple diseases, *Indian J. Heterocycl. Chem.*, **2026**, *36*, 269–275. *https://doi.org/10.59467/IJHC.2026.36.269*