Medicinal Chemistry

Medicinal chemistry relates to the design, synthesis and pharmacological evaluation of compounds leading to the identification of NCEs (New Chemical Entities) that can be developed as medicine for the prevention, treatment or cure of human and animal diseases. At DRILS we are focusing on discovery / identification of NCEs in the area of tuberculosis, obesity, psoriasis, inflammation and cancer. The MOA of some of these NCEs involve interactions with novel pharmacological targets.

Development of new chemical entities in various therapeutic areas such as tuberculosis, inflammation, obesity, psoriasis and cancer.

Prof Manojit Pal's research interests include the development of new chemical entities under the new drug discovery programme in various therapeutic areas namely tuberculosis, inflammation, obesity, psoriasis and cancer. His research group contributed in identification of a small molecule as inhibitor of chorismate mutase that showed proof of concept (POC) in animals (for which patent has been granted in India) and could be effective against tuberculosis (WO 2020/240272 A1). The molecule was found to be effective against MDR-Mtb ATCC 35825 as well as *Staphylococcus aureus*. His group also identified a selective $5HT_{2C}$ agonist (PAAM) towards the potential management of obesity (WO/2021/028935). In another project his group identified a lead molecule as a selective inhibitor of 12R-LOX with anti-psoriatic effects in animal (WO 2020/255156 A1) for which the patent has been granted in India.

His group is also involved in the identification of selective and potent inhibitors of PDE4 for the potential treatment of inflammatory diseases. Previously (1995-98), his team was involved in the development of process and impurity profile for macrolide antibiotics such as Roxithromycin, *Clarithromycin* etc. and the drug sildenafil that was commercialized by Alembic Chem and Sum Pharma, respectively. The other major areas of his focus include transition metal / non-metal catalyzed reactions, sonochemical approaches, green chemistry, heterocycle synthesis etc. (see: Research.com: https://research.com/u/manojit-pal).

Research focus of my group

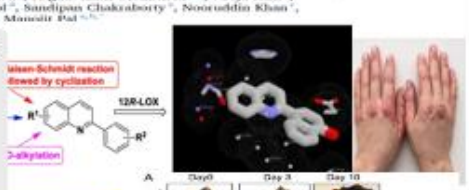
Bioorganic Chemistry

Design, synthesis and evaluation of 2-aryl quinoline derivatives against 12*R*-lipoxygenase (12*R*-LOX): Discovery of first inhibitor of 12*R*-LOX

Harshavardhan Bhuktar, Sharda Shukla, Kumar Reddy Kakularam, Srikanth Battu, Manupati Srikanth, Susmita Srivastava, Raghavender Medishetti, Pooja Rana, P.C. Jagadish, Mahaboobkhan Rasool, Sanelipan Chakraborty, Nooruddin Khan, Palla Reddanna, Srinivas Oruganti, Manojit Pal

Design / synthesis of NCEs in the following areas

Obesity
Inflammation
Tuberculosis
Cancer



DRUG DISCOVERY TODAY

Quinolines: a new hope against inflammation

Soumita Mukherjee and Manojit Pal

Bioorganic Chemistry

Med Chem

$5HT_{2C}$,
12R-LOX, PDE-4
Chorismate mutase
Sirtuins

Organic Synthesis

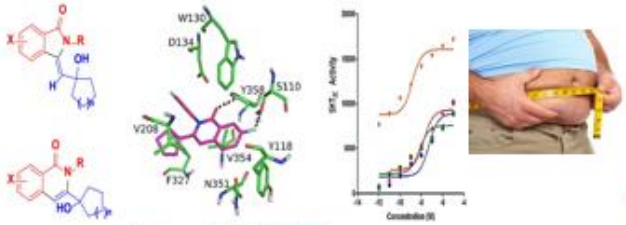
Metal catalysis
Cascade reactions
Coupling-cyclization
MCR

DRLS Lead compound

Baicalein

Sonochemical synthesis and biological evaluation of isoquinolin-1(2*H*)-one/isoindolin-1-one derivatives: Discovery of a positive ago-allosteric modulator (PAAM) of $5HT_{2C}R$

Jetta Sandeep Kumar, Rapaka Naimisha, B. Thirupaiah, Gangireddy Sujeevan Reddy, Navneet Bung, Arijit Roy, Gopalakrishnan Bulusu, Ankita Mishra, Prem N. Yadav, Parimal Misra, Manojit Pal



- First example of PAAM of $5HT_{2C}R$
- Potent activity and selectivity
- Acceptable PK and decreased food intake

Bioorganic Chemistry

Wang resin catalysed sonochemical synthesis of pyrazolo[4,3-*d*] pyrimidinones and 2,3-dihydroquinazolin-4(1*H*)-ones: Identification of chorismate mutase inhibitors having effects on *Mycobacterium tuberculosis* cell viability

Sharda Shukla, R. Nishanth Rao, Harshavardhan Bhuktar, Rebecca Kristina Edwin, Trinath Jannna, Raghavender Medishetti, Shamistha Banerjee, Vasudasaj Bhat Giliyaru, Gautham G. Shenoy, Srinivas Oruganti, Parimal Misra, Manojit Pal