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THE PEOPLE



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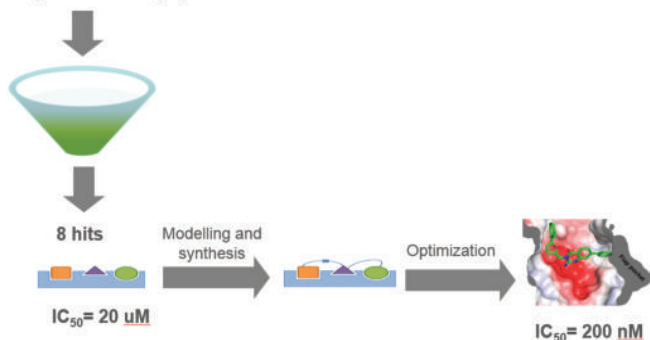


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THE PROJECTS

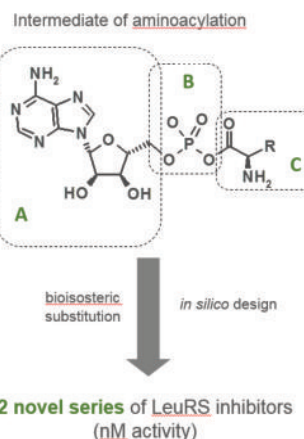
Fragment based discovery of Plm inhibitors as anti-malarials

1000 fragment screening by NMR



J. Med. Chem. 2016, 59, 374

Rational design of LeuRS inhibitors as anti-bacterials



WO2015063544

THE EQUIPMENT

- ✓ up to 100 FTE for synthetic chemistry
- ✓ up to 2000 m² fully equipped lab space for organic synthesis work
- ✓ 300 MHz, 400 Mz, 600 MHz, and 800 MHz NMR systems
- ✓ q-ToF HRMS system coupled to LC
- ✓ FT-IR spectrometer with IR spectra library
- ✓ powder and single crystal X-ray spectrometers
- ✓ GC-based microanalysis system
- ✓ preparative flash and HPLC chromatography with UV, ELSD, and MS detectors
- ✓ analytical HPLC with UV, fluorescence, light scattering MS detectors
- ✓ analytical GC with FID and GC detectors
- ✓ vacuum centrifuges and sample evaporation systems
- ✓ parallel synthesis carousel stations, microwave synthesizer and flow systems
- ✓ Isothermal Titration Calorimeter
- ✓ Surface Plasmon Resonance spectrometer

THE OUTPUT

1. Charlton *et al.* ACS Med. Chem. Lett. 2018, 9, 84
2. Zalubovskis *et al.* J. Enzyme Inhib. Med. Chem. 2018, 33, 147
3. Bobileva *et al.* Bioorg. Med. Chem. 2017, 25, 4314
4. Aleksis *et al.* Biochimie 2017, 140, 176
5. Rasina *et al.* J. Med. Chem. 2016, 59, 374.

Networks: IMI NDBB ENABLE; H2020-MSCA-ITN: INTEGRATE, CARTNET, IT-DED³; H2020-MSCA-RISE: PELICO; H2020-SC-1-HCO: Alliance4Life; H2020-PHC: BATCURE
Research collaboration: EU 116; US 15; Africa 4; Middle East 2; Asia Pacific 11
Industrial partners from EU, US, China: 14
Patents: 16 PCT applications in last 5 years

THE MEDCHEM

Preclinical drug discovery

- ✓ synthetic hit-to-lead and lead-to-CD programs
- ✓ in silico modelling, structural biology research
- ✓ identification of new drug targets
- ✓ biophysical & biochemical screening
- ✓ bioanalytical assays
- ✓ development of *in vitro*, *ex vivo*, *in vivo* activity testing systems
- ✓ *in vivo* studies of toxicity and ADME

Strategies applied for the lead identification

- ✓ fragment based lead discovery
- ✓ synthesis of HTS screening hit analogue series
- ✓ synthesis of focused compound libraries
- ✓ synthesis of natural product analogues
- ✓ rational or mechanism based drug development

THE FUTURE

- ✓ Expanding the natural product based drug discovery
- ✓ Implementation of biological synthesis
- ✓ Development of targeted drug delivery systems