Intro

- In AstraZeneca since 2022
- Member of MolecularAI (Ola Engkvist)
- Project & team lead: QuantiumAI, Chemistry HTE & automation

Drug Discovery:
Computational Chemistry

Drug Discovery:
Medicinal Chemistry

Organic Synthesis &
Flow Chemistry

Physical Organic &
Quantum Chemistry

Machine Learning &
programming

Experimental chemistry

Organic Synthesis & Flow Chemistry

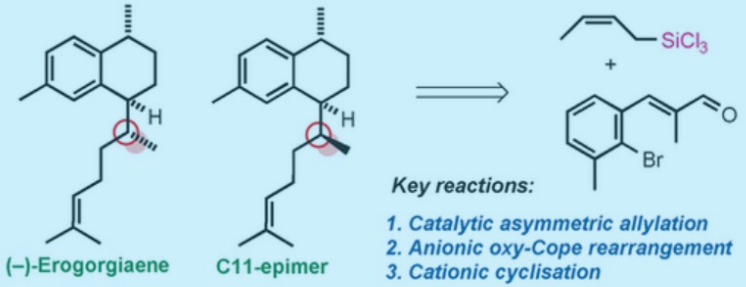
- Multi-step organic synthesis
- Air- and moisture sensitive methods
- Flow chemistry method development
- Electrochemistry, photochemistry & microwave assisted synthesis

UNIVERSITY of GLASGOW

UNIVERSITY OF OXFORD

Loughborough University

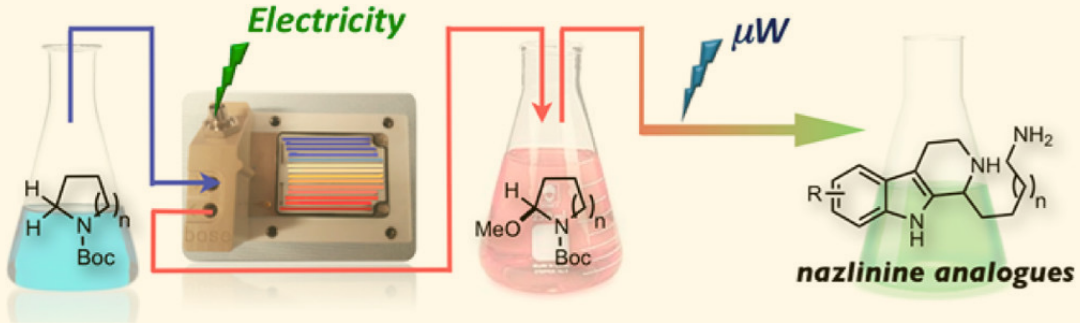
UNIVERSITY OF CAMBRIDGE



Abstract

A short, nine-step, highly enantioselective synthesis of (−)-erogorgiaene and its C-11 epimer is reported. The key stereochemistry controlling steps involve catalytic asymmetric crotylation, anionic oxy-Cope rearrangement and cationic cyclisation. (−)-Erogorgiaene exhibited promising antitubercular activity against multidrug-resistant strains of *Mycobacterium tuberculosis*.

doi.org/10.1002/chem.201602440

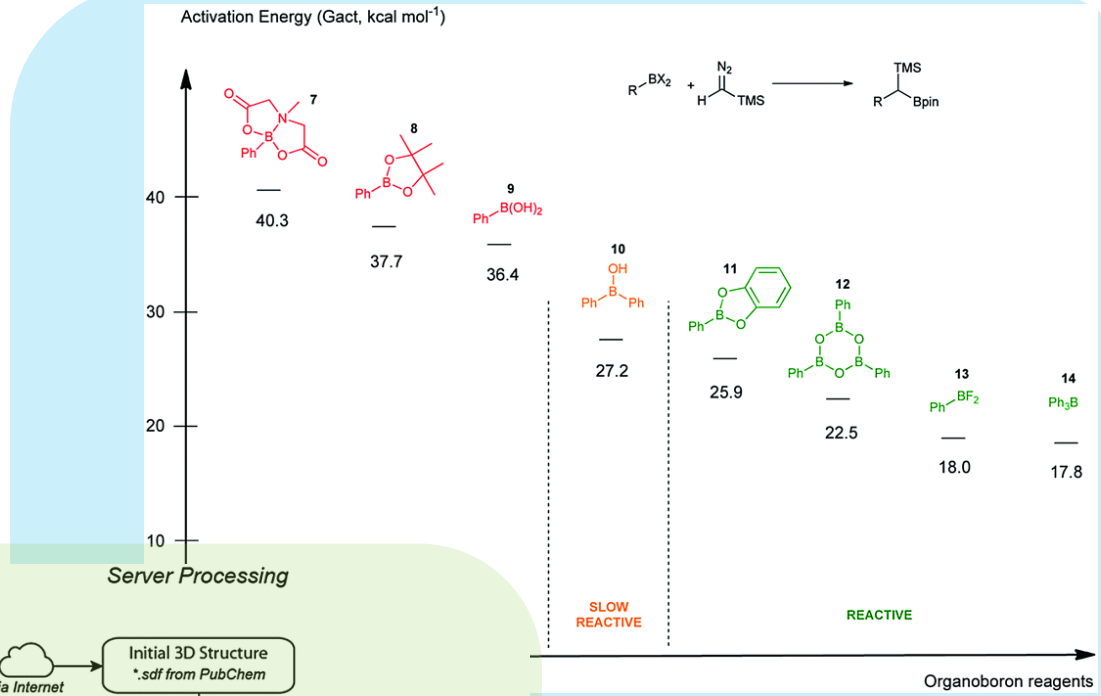


doi.org/10.1021/ol502201d

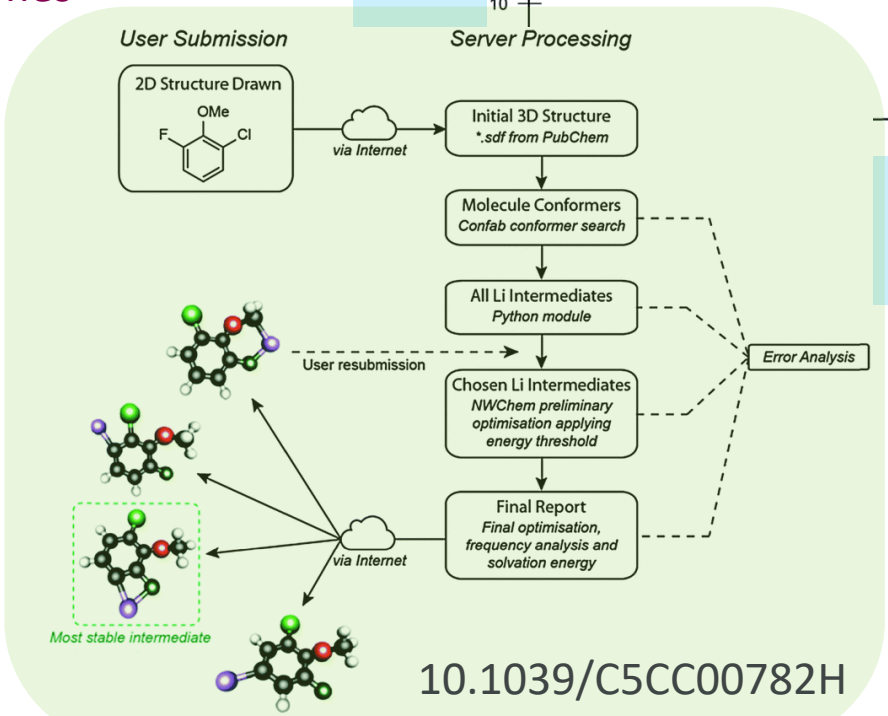
Computational chemistry

Physical Organic & Quantum Chemistry

- DFT studies to propose new reagents and catalytic systems in flow chemistry
- DFT studies to underpin reaction mechanisms in organocatalysis
- Automated system to predict reaction outcomes at the DFT level



DOI: 10.1039/C7SC02264F



10.1039/C5CC00782H

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Pharmaceutical industry

Drug Discovery: Computational Chemistry

- Chemoinformatics & QSAR project support
- 3D modelling project support, including docking & MD
- SAR analysis and ligand-target interactions mapping using FMO method
- Co-developer of the ML workflows for the CADD

Drug Discovery: Medicinal Chemistry

- MedChem project development
- Development of heterocyclic synthesis methods for the array chemistry
- SME in flow chemistry methods integration in industrial settings

AIChemist projects

DC3. Predicting Side Reactions Using a Combined Metadynamics-xTB and ML Approach

Academic supervisor: prof Jan Jensen (University of Copenhagen)
AIChemist PhD fellow*: Karoline Schjelde

DC4. Prediction of optimal reaction conditions using Artificial Intelligence tools

Academic supervisor: prof Alexandre Varnek (University of Strasbourg)
AIChemist PhD fellow: TBD

DC5. Multi-task Neural Network reactivity prediction using in-silico simulations and synthesis experimental data

Academic supervisor: prof Mike Preuss (University of Leiden)
AIChemist PhD fellow: Bob van Schendel