

Agnostic Use of Automation to Accelerate Drug Discovery: An introduction to the J&J Chemical Capabilities team in Toledo (Spain)

Javier Mazuela, Irini Abdiaj, Lourdes Linares, Jose Enrique Gomez; Anxo Rey Blanco; Brenda Pijper; Santiago Cañellas; Jesus Alcazar

*Janssen-Cilag, S.A. Rio Jarama 75, 45007 Toledo, Spain

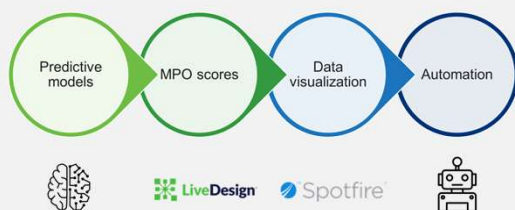
OBJECTIVES AND CAPABILITIES



- Drive innovation and accelerate DMTA: **Automation**
- Fast-acting & efficient library **design & execution** team
- Synthetic **methodology agnostic**
- Enable **new methodologies** to access broader chemical space
- Promote **enabling technologies** across departments
- Provide **alternative solutions** to chemistry challenges

APPROACH

Library Desing



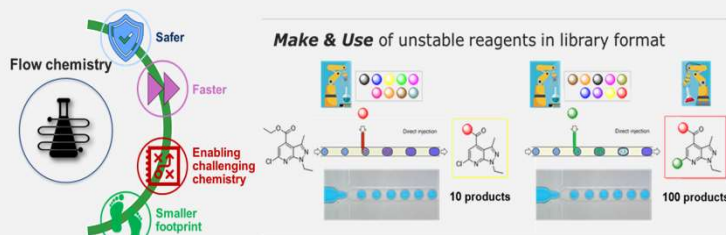
Modular Approach: Play&Go End-to-end synthesis



Sample preparation Reaction execution Work-up Analysis HTP Post-purification



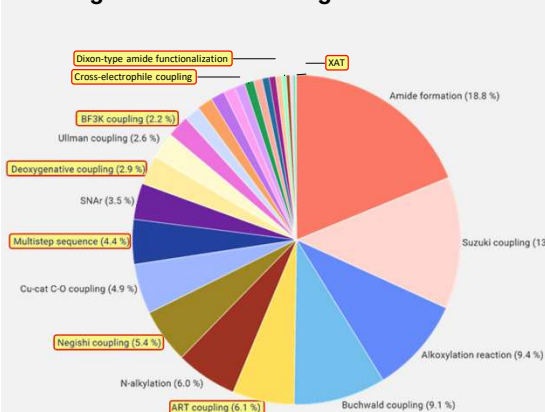
Flow Chemistry



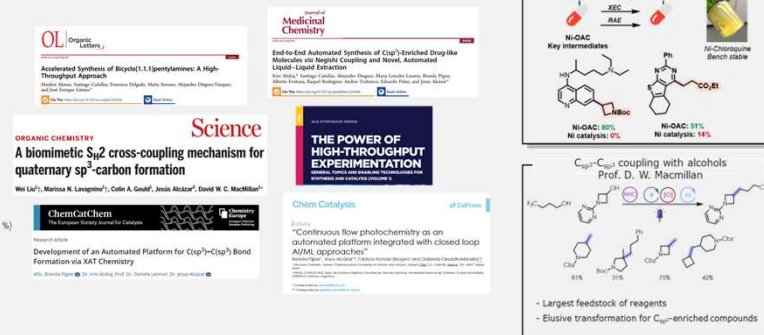
- Amide coupling
- Reductive amination
- Sulfonamide synthesis
- Azide formation and Cu-AAC
- S_NAr
- N-alkylation
- Ni-cat methoxy functionalization
- Photoredox ART coupling

OUTCOME

Enabling modern methodologies



Innovation & Collaborations



Project's impact (yearly)

2-5 impact in NME delivery
In vivo tool compounds identified
Opened new chemical space
Accelerated go/no-go decision

20-30 reaction types in 2023
5 from internal research
>20 projects supported