

# HTE-Enabled Suzuki Optimisation for Cost Reduction



## The Challenge

- CatSci was tasked with the optimisation of a current Suzuki cross-coupling, to reduce costs as far as possible whilst maintaining conversion and purity
- The new conditions needed to be demonstrated on a multi-gram scale within 8 weeks from initiation of the project



## How?

- By utilising CatSci's high-throughput department, including solid handling robots and high-throughput data analysis, an expansive chemical space surrounding the current Suzuki conditions were investigated
- Catalysts, ligands, solvents and temperatures screened



## The Achievement

- A reduction from 5 mol% to 0.1 mol% Pd loading was achieved. The ligand loading was also reduced from 10 mol% to 0.2 mol%
- A ligand which was a third of the current ligand cost was identified
- Ultimately, the reaction was shown to be viable on a 20 g scale at 0.05 mol% Pd, in a jacketed vessel



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## Key Results

- **60% overall cost savings**
- 124 experiments conducted over 12 hours of chemists' time
- 172 data points collected
- 100-fold reduction in catalyst and ligand loading
- Swap to a 3-fold cheaper ligand
- Efficient exploration of the chemical space
- Process transferred to manufacturer for implementation on kilogram scale

## HTE Equipment



Labman Multidose  
Solid handler



EuroBio Scorpion  
Liquid handler



Waters ACQUITY  
UPLC I-Class  
High throughput LC  
analysis