

Novel Bromination Process slashes PMI



The challenge

CatSci was tasked with designing a new bromination method for a key reaction intermediate. Use of bromine rendered the previous process unsuitable for a larger campaign and would require expensive and time-consuming alterations to the plant.



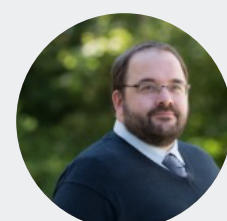
How?

Leveraging its collective expertise in route design, the CatSci team spotted an opportunity to utilise a little-used amide functionalisation method. This method would simultaneously activate the substrate towards bromination and offer in situ protection of a functionality that could otherwise competitively react.



The achievement

A novel, two-step route to the desired compound was first developed using NBS as the brominating agent. Process development telescoped this into a one-pot procedure. In addition to avoiding use of bromine, the new route also afforded the product in higher yields and was more environmentally sustainable, delivering an impressive 45% drop in CO₂ emissions compared to the original route. The transfer to the manufacturing plant proceeded 'right first time'.



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Old Process

Br₂ in 33% HBr/AcOH

Solvent Swap to PhMe

Two crystallisations
required for purification

Variable yields and
material colour



New Process

NBS in iPrOAc

No Solvent Swap

Crystallisation from
reaction solvent

Higher yields and
consistent purity

Facts and Figures

PMI
52% lower



Water Waste
52% less



Solvent Waste
23% less



What does a 45% reduction in CO₂ look like?

659 tonnes CO₂ saved*

This equals...

140
cars driven for 1 year



or

84 Million
Smartphones charged



*per 10 tonnes of key intermediate

