CASE STUDY

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 CO_2 emissions compared to the original route. The transfer to the manufacturing plant proceeded 'right first time'.




The team: Dr Guy Brenchley, Dr Jo Sampson, Dr Dan Richards & Dr Monica Trues-Suarez

Old Process	New Process
Br_2 in 33% HBr/AcOH	NBS in iPrOAc
Solvent Swap to PhMe	No Solvent Swap
Two crystallisations required for purification	Crystallisation from reaction solvent
Variable yields and material colour	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 CO_2 look like?

659 tonnes **CO_2 saved***

This equals...

140
cars driven for 1 year

or

84 Million
Smartphones charged

*per 10 tonnes of key intermediate

Find out more: catsci.com