

Amigo helps Pharma company quickly identify and clean kill an unsuitable route

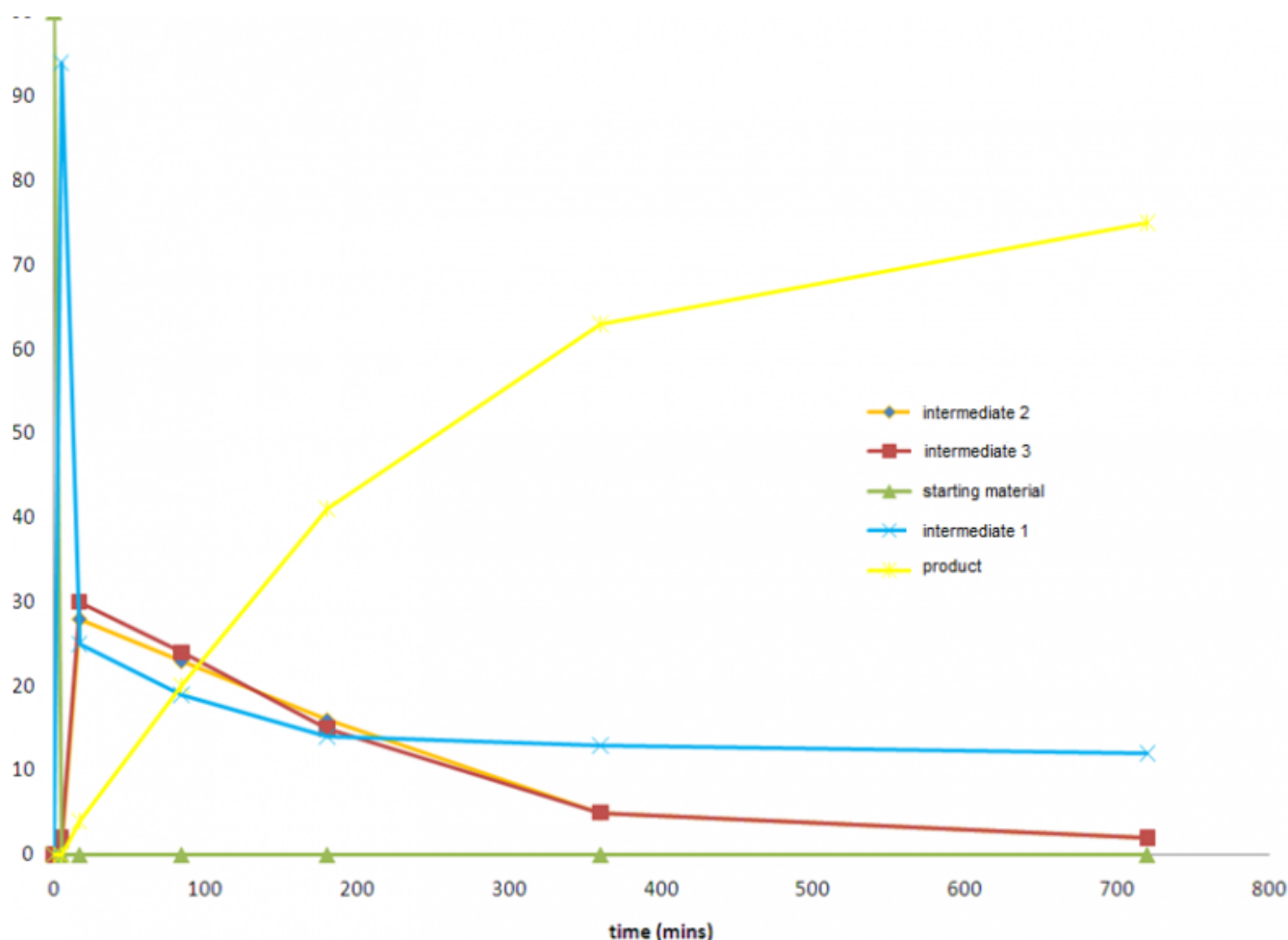
Introduction

A large pharmaceutical company had been investigating a challenging multi-component aldol reaction. The aldol reaction was being evaluated in combination with several other options to assemble richly decorated pharmaceutical intermediate. the group chose to introduce Amigo to the project to obtain better mechanistic understanding. Specifically, Amigo's "Increasing Interval" sampling mode was employed. Here, Amigo automatically doubles the sampling interval throughout the defined reaction time, thus concentrating sampling effort early on.

Study details

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Data from Amigo sampling



Conclusions

- The sample taken at 5mins shows the rapid conversion to the blue intermediate which rapidly converts into the orange and the red intermediate.
- The red intermediate was shown to be non-productive giving incorrect stereochemistry

Highlights

- The group immediately killed the route so efforts could be applied to more promising route candidates.
- Manual sampling of a reaction of greater than 12 hours duration would rarely include a sampling point at 5 mins. Accordingly, the manual experiment did not uncover this fundamental problem thus wasting precious PRD time.