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## N°942 / TOPIC(s) : Alternative solvents / Industrial chemistry

Technology and Green Chemistry in the Pharmaceutical Industry

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# PURPOSE OF THE ABSTRACT

## INTRODUCTION

Technologies, such as synthetic biochemistry, photochemistry, flow chemistry, electrochemistry and catalysis are recognised as having great potential to minimise the environmental impact of routes to complex molecules, such as those made by the pharmaceutical industry. Case studies will explore some of the advantages and current limitations of these techniques.

#### RESULTS AND DISCUSSION

In one case study, aminocarbonylation permits replacement of a 3-step conversion of an aryl halide, to an ester, to an acid, to an amide, with a single step. Such an approach facilitates a shorter, higher yielding, more efficient syntheses. In another case study, synthetic biochemistry is able to facilitate transformations which otherwise would have taken multiple steps.

#### CONCLUSION

The power of these approaches is only realised by the appropriate use of technology and data handling which facilitates high throughput screening of conditions.

#### ACKNOWLEDGEMENTS

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## **FIGURES**



						Conve	ersion						
	1	2	3	4	5	6	7	8	9	10	11	12	
.[		28.6	82.3	24.3	53.0		-	-	-	-	10.4	22.8	
	37.4	-	37.9	48.1	39.9	8.2	-	-	-	14.1	-	20.8	
:	35.0	42.3	95.0	23.3		20.3		71.1	45.9		-	45.4	
١		34.1	55.8	11.9	-	67.4		18.0		-	-	13.9	
	-	-	-	-	0.0	0.0	45.9	45.8	37.7	43.1	44.2	42.0	
		51.3	39.1	61.7	16.6	-	-	-	-	-	-	41.2	
	-	60.1	40.7	39.9	-	21.4	-	22.0		0.0		54.8	
۰.													
	8.2	36.3		20.0			-	14.3	27.4			30.9	
	8.2	36.3		20.0	-	e	- e	14.3	27.4			30.9	
	8.2	36.3 2	-	20.0	- 5	6	e 7	8	9	10	11	30.9	
	8.2 1	36.3 2 99.9	- 3 99.9	20.0 4 99.9	- 5 99.9	- 6 -	e 7 -	8	9	10	11 99.9	30.9 12 99.9	
	8.2 1 99.9	36.3 2 99.9 -	- 3 99.9 99.9	20.0 4 99.9 99.9	- 5 99.9 99.9	- 6 - 99.9	e 7	8 - -	9	10 99.9	- 11 99.9 -	30.9 12 99.9 99.9	
	8.2 1 - 99.9 99.9	36.3 2 99.9 99.9	3 99.9 99.9 99.9	20.0 4 99.9 99.9 99.9	- 5 99.9 99.9 -	- 6 - 99.9 99.9	e 7 -	14.3 8 - - 99.9	9 - - 99.9	10 - - 	- 11 99.9	30.9 12 99.9 99.9 99.9	
	8.2 1 99.9	36.3 2 99.9 99.9 99.9	- 3 99.9 99.9 99.9 99.9 99.9	4 99.9 99.9 99.9 99.9 99.9	5 99.9 99.9	6 - 99.9 99.9 99.9	- 7 - -	8 - - 99.9 99.9	9 - - 99.9 -	10	11 99.9	30.9 12 99.9 99.9 99.9 99.9 99.9	
	8.2 1 - 99.3 99.9 -	2 99.9 99.9 99.9	- 99.9 99.9 99.9 99.9 99.9	20.0 4 99.9 99.9 99.9 99.9	- 5 99.9 99.9 - -	- 6 93.9 99.9 99.9	e 7	14.3 8 -	9 - - 99.9 99.9	10 99.9	11 99.9	30.9 12 99.9 99.9 99.9 99.9 99.9	
	8.2 1	2 99.9 99.9 99.9 99.9	- 3 99.9 99.9 99.9 99.9 99.9 - 99.9	20.0 4 99.9 99.9 99.9 99.9 99.9	5 99.9 92.3	- 6 - 99.9 99.9 - -	e 7 - - - - - - - - - - - - - - - - - -	8 - - 99.9 99.9 - 99.3 - -	9 - - 99.9 99.9	10 99.9 99.9	11 99.9	30.9 12 99.9 99.9 99.9 99.9 99.9 99.9 99.9	
	8.2 1	36.3 2 99.9 99.9 99.9 99.9 99.9 99.9	- 3 99.9 93.3 99.9 99.9 - 99.9 - 99.9 99.9	20.0 4 99.9 99.9 99.9 99.9 - 99.9 - 99.9 99.9	5 99.9 97.9	- 6 - 99.9 99.9 - - - 99.9	C 7 </td <td>14.3 8 - 99.9 99.9 -99.3 - 99.9</td> <td>9 - - 99.9 99.9</td> <td>10 </td> <td>11 99.9</td> <td>30.9 12 99.9 99.9 99.9 99.9 99.9 99.9 99.9</td> <td></td>	14.3 8 - 99.9 99.9 -99.3 - 99.9	9 - - 99.9 99.9	10 	11 99.9	30.9 12 99.9 99.9 99.9 99.9 99.9 99.9 99.9	

# FIGURE 1

## Figure 1.

3-D plot of yield against two variables, temperature and amount of catalyst for a sample aminocarbonylation

### FIGURE 2 Figure 2.

Sample output of yield and e.e. from a ketoreductase screen

# **KEYWORDS**

Design of Experiments, | Catalysis | Amincarbonylation

# BIBLIOGRAPHY