Supporting Information

Quantitative Perspective on Online Flow Reaction Profiling Using a Miniature Mass Spectrometer

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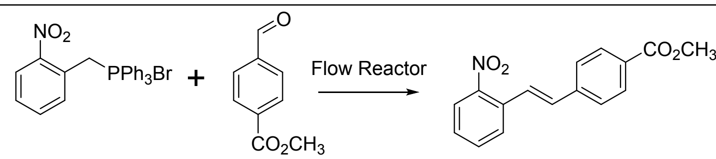
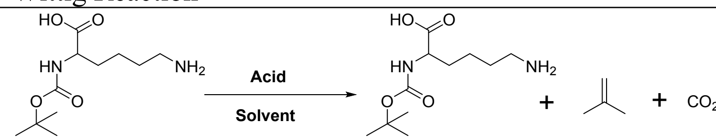
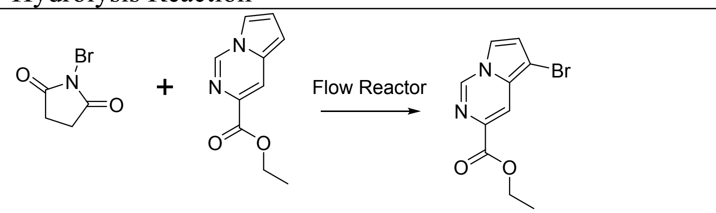
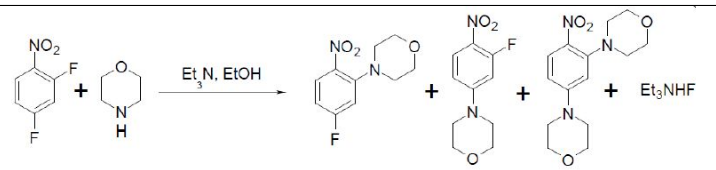
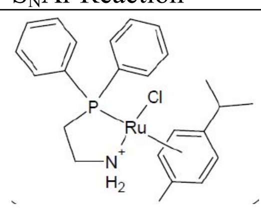
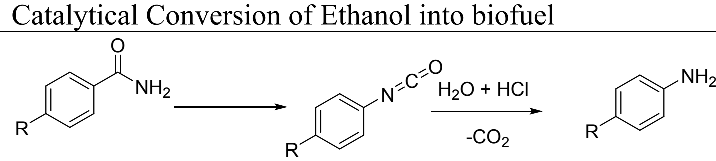
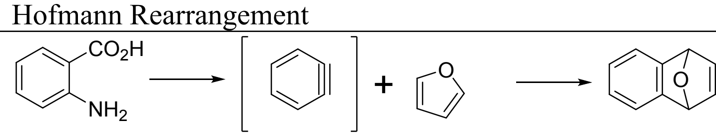
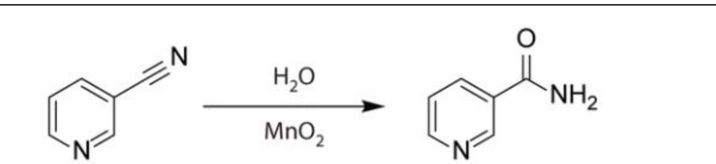
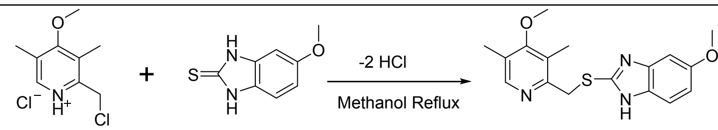
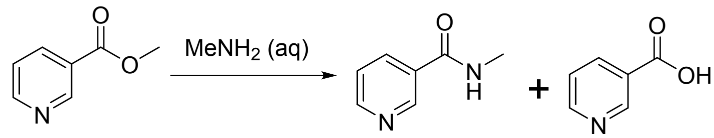
Table S1. Summary of recent literature of mini-MS reaction monitoring showing the substrates, reaction types and profiling methods

Ionization Source	**MS Type**	**Substrates and Reactions**	**Reaction Profiling Method**	**Reference**
Chip-ESI	Mini-MS	 Wittig Reaction	Monitoring SM and Product	[1]
Chip-ESI	Mini-MS	 Hydrolysis Reaction	Monitoring SM and Product	[2]
Chip-ESI	Mini-MS	 Bromination Reaction	Monitoring SM and Product	[3]
Chip-ESI	Mini-MS	 S_NAr Reaction	Monitoring SM and Product	[4]
Chip-ESI	Mini-MS	 Catalytical Conversion of Ethanol into biofuel	Only Monitoring Catalyst	[5]
Chip-ESI	Mini-MS	 Hofmann Rearrangement	Monitoring SM, Intermediate and Product	[6]
Chip-ESI	Mini-MS	 Diels-Alder Reaction	Monitoring SM, Intermediate and Product	[7]
ESI	Mini-MS		Monitoring SM and Product	[8]

		Cyano-hydrolysis		
ESI	Mini-MS	 SN2 Reaction	Monitoring SM and Product	[9]
ESI	Mini-MS	 Ester Hydrolysis	Monitoring SM and Product	[10]

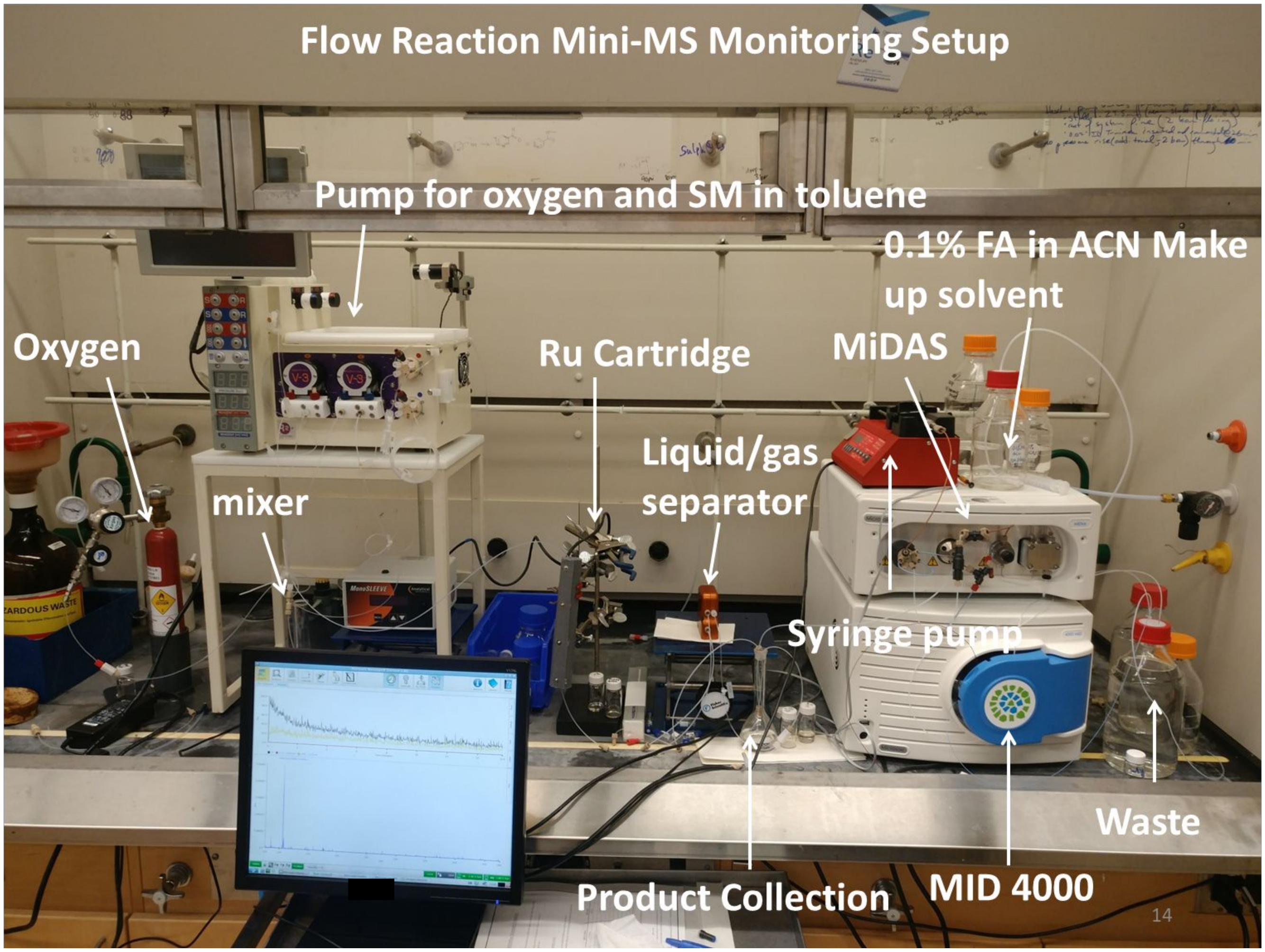


Figure S1. The flow reaction setup with Microsaic miniature MS 4000 MiD and online dilutor MiDAS.

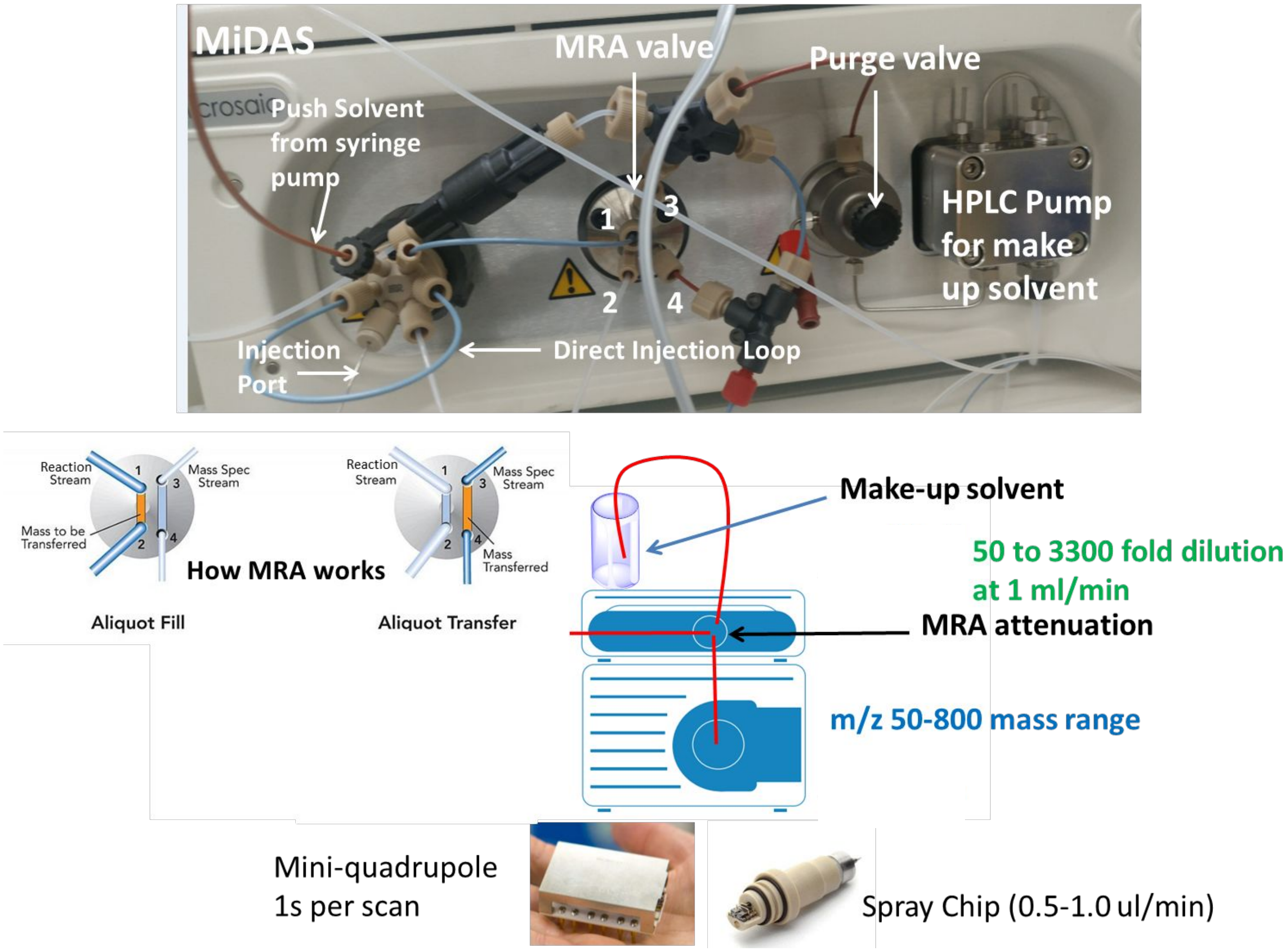


Figure S2. The setup of Microsaic miniature MS 4000 MiD and online dilutor MiDAS.

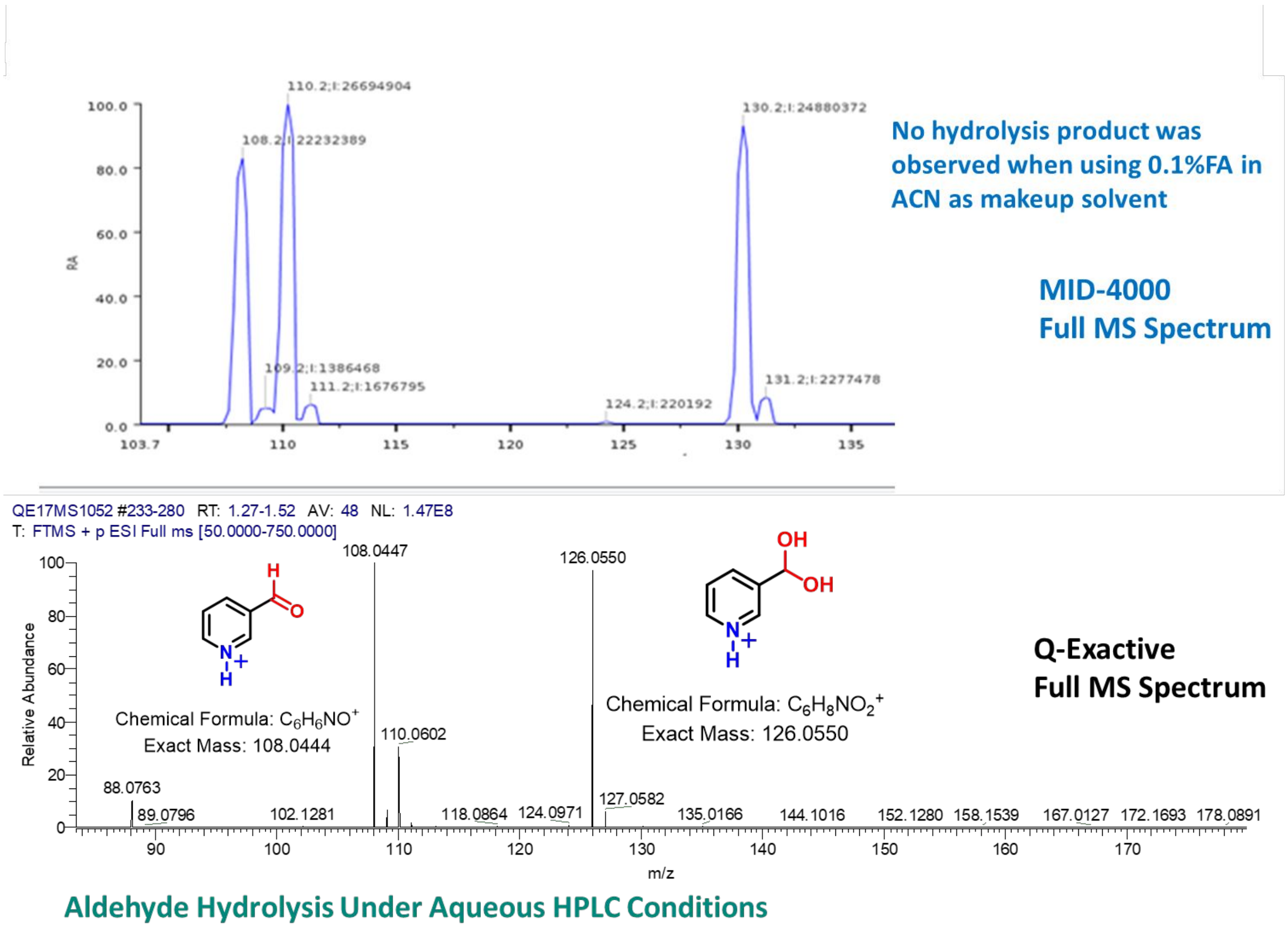


Figure S3. The MS spectrum of aldehyde SM with m/z 108 showed significant on-column hydrolysis product m/z 126 when analyzed with reverse phase LCMS; Whereas no aldehyde hydrate was observed in -4000 MiD when using 0.1% formic acid in 100% ACN as the makeup solvent in MiDAS.

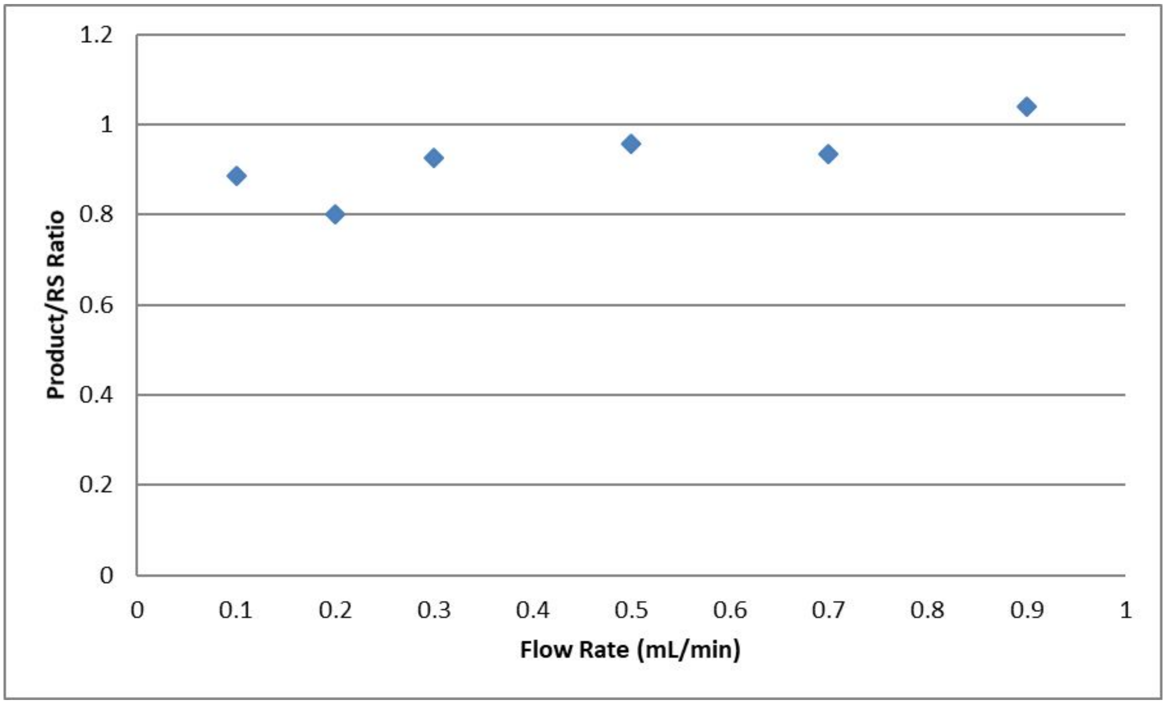


Figure S4. The effect of reaction flow rate on the product/RS ratio was studied in the external RS approach (Figure S4). The solution of product standard (0.2 mol/L in acetonitrile) was introduced directly into the mini-MS module through a syringe pump at varied flow rate from 0.1 to 0.9 mL/min. The attenuation (2000X) and makeup flow rate (1 mL/min) were maintained constant. The results showed that the product/RS ratio changed 25% from 0.8 to 1.0 with the reaction flow rate increased from 0.1 mL/min to 0.9 mL/min. This indicated that the flow rate has some impact on the quantitation result.

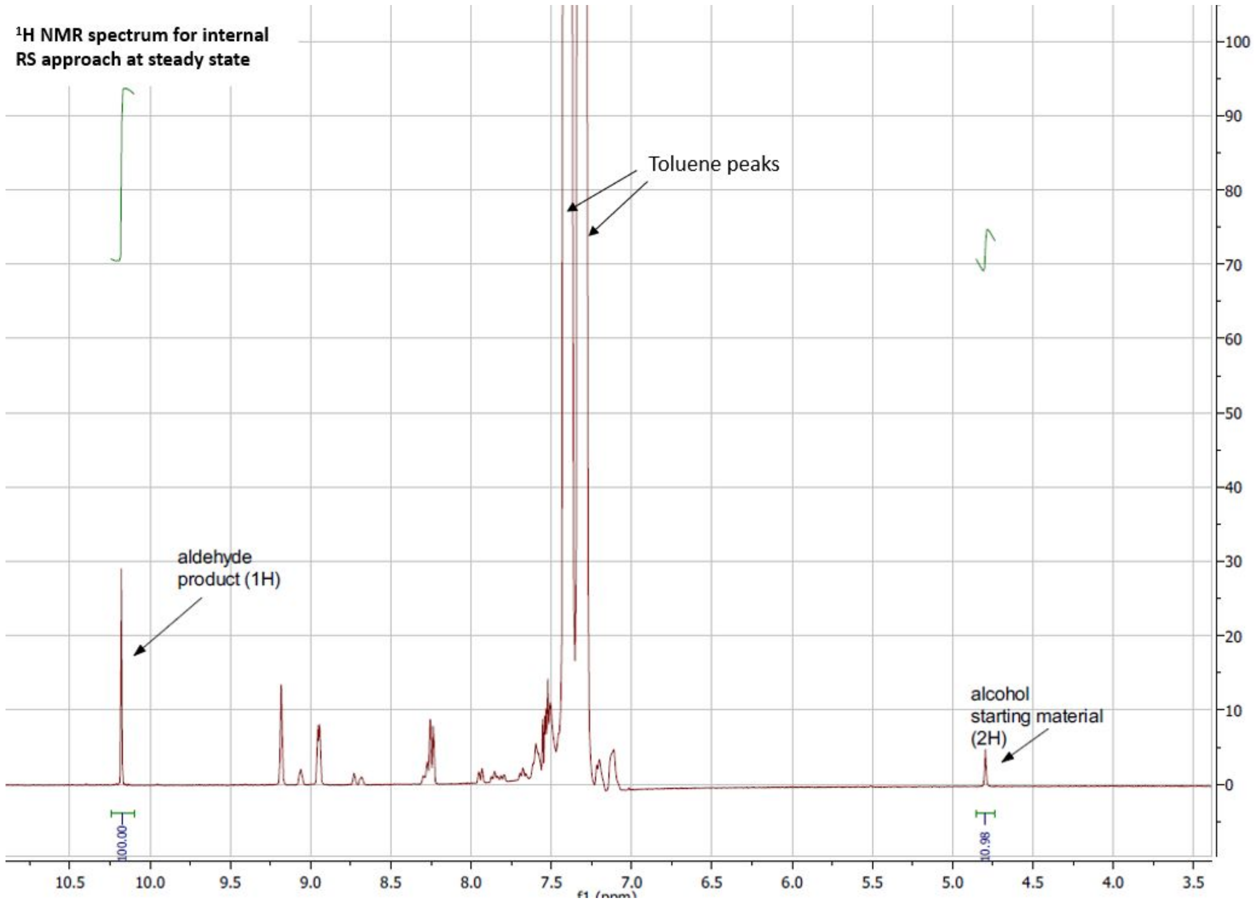


Figure S5. ^{1}H NMR spectrum of reaction stream sampled at steady state for the internal reference standard approach. Peaks corresponding to quinoline reference standard not visible due to peak overlap and low concentrations.

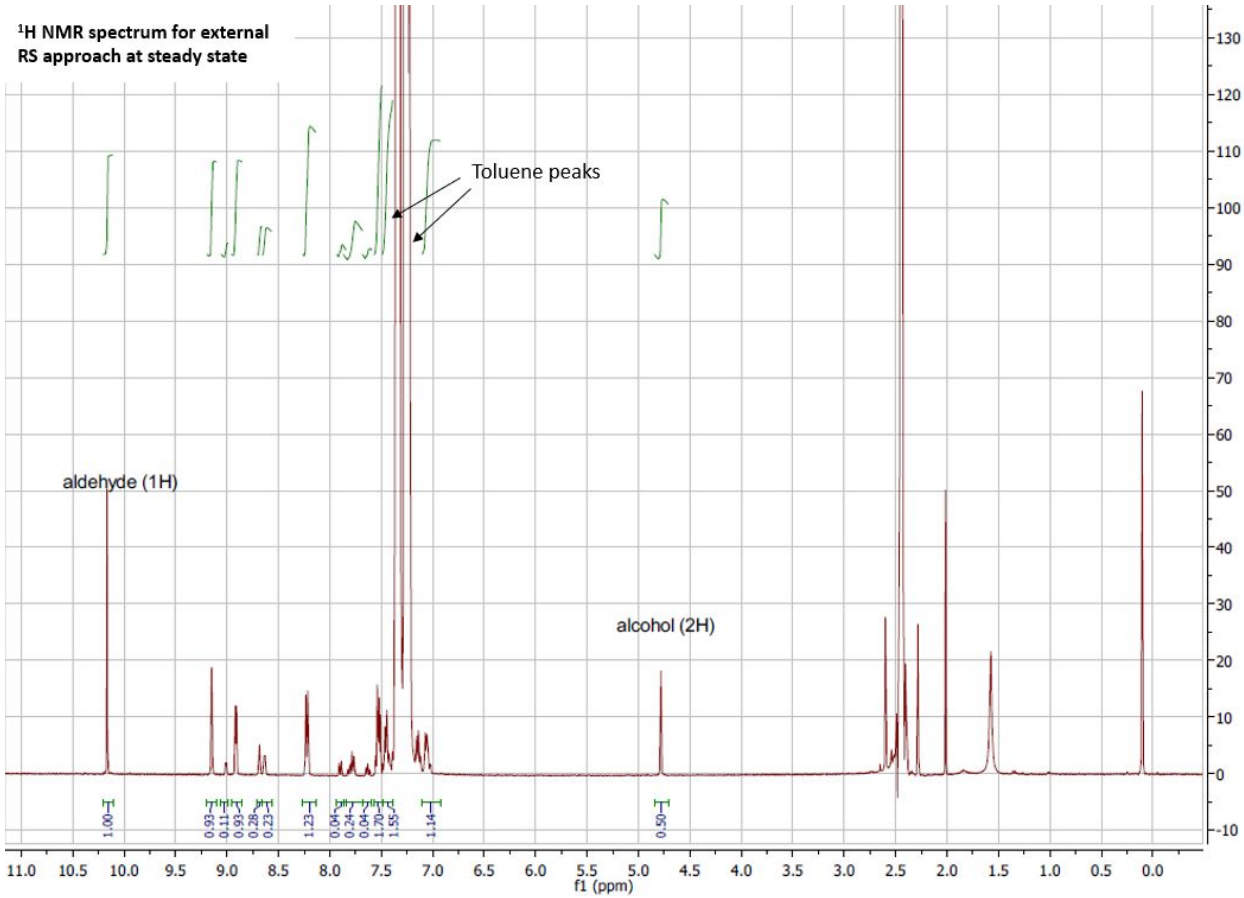


Figure S6. ^{1}H NMR spectrum of reaction stream sampled at steady state for the external reference standard approach.

Supporting Information References:

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