

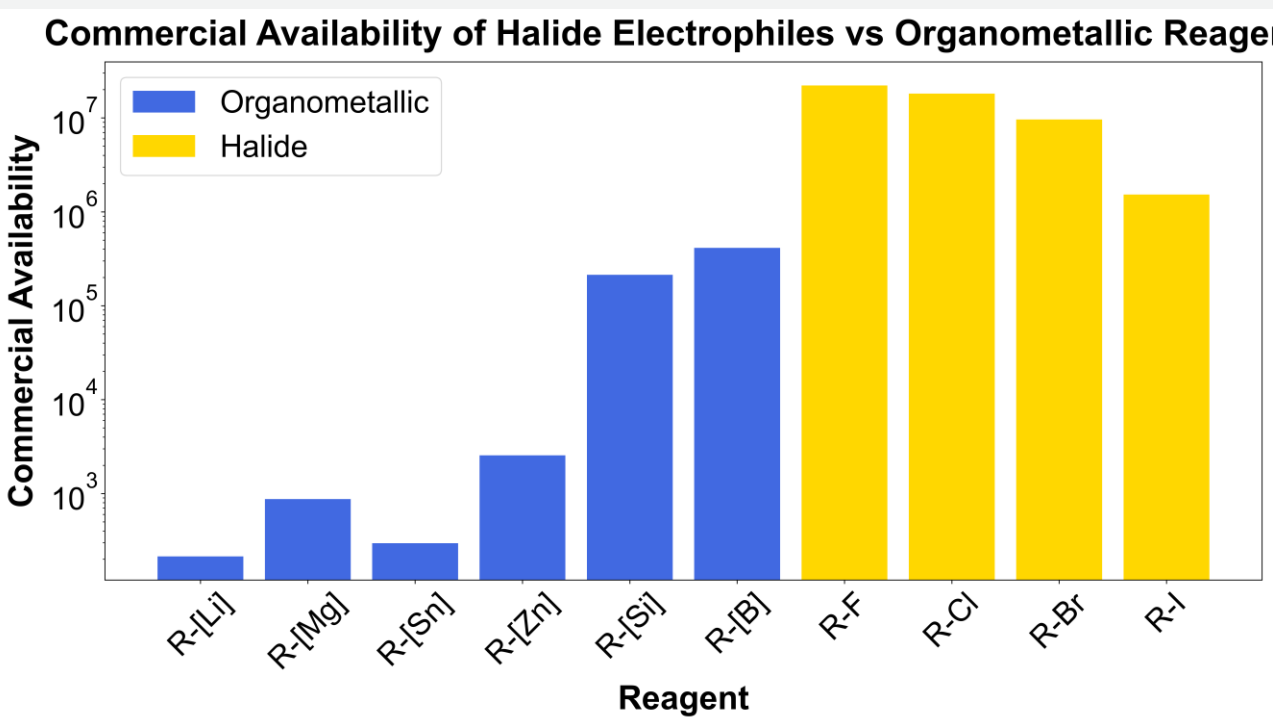
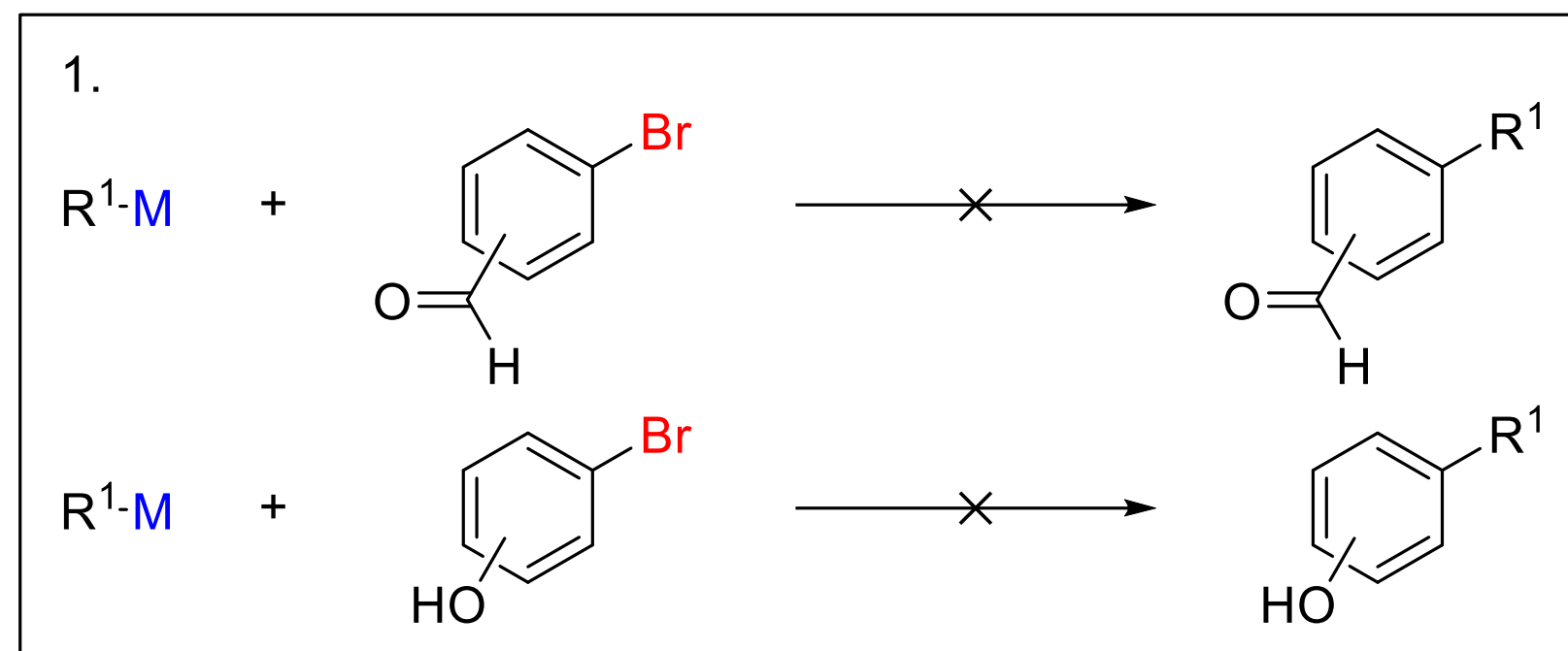
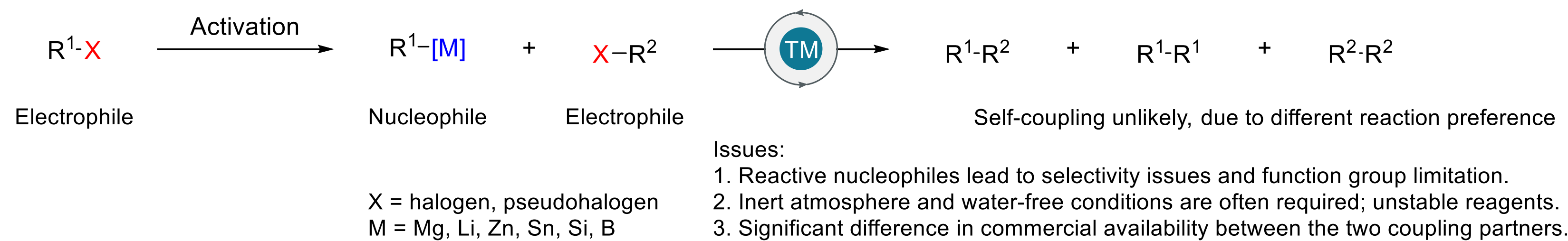
Screening of a Ni-Catalyzed Cross-Electrophile Coupling of Aryl Halides with Alkyl Halides

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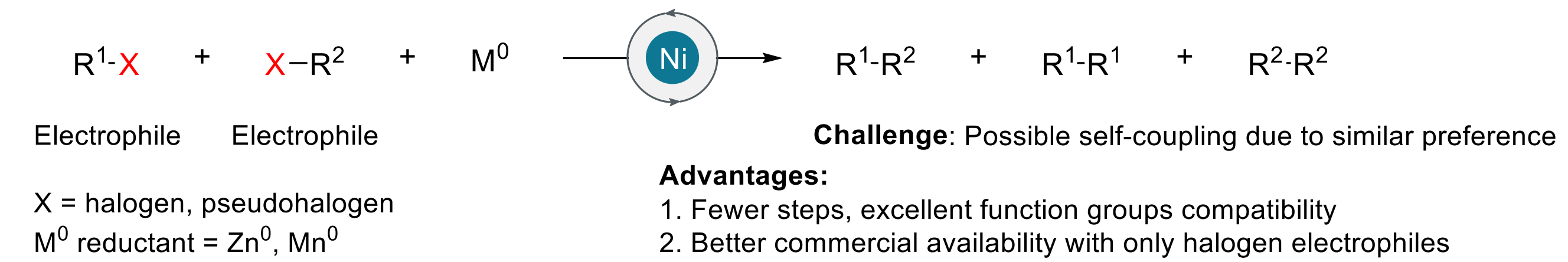
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Introduction

Conventional cross-coupling reactions

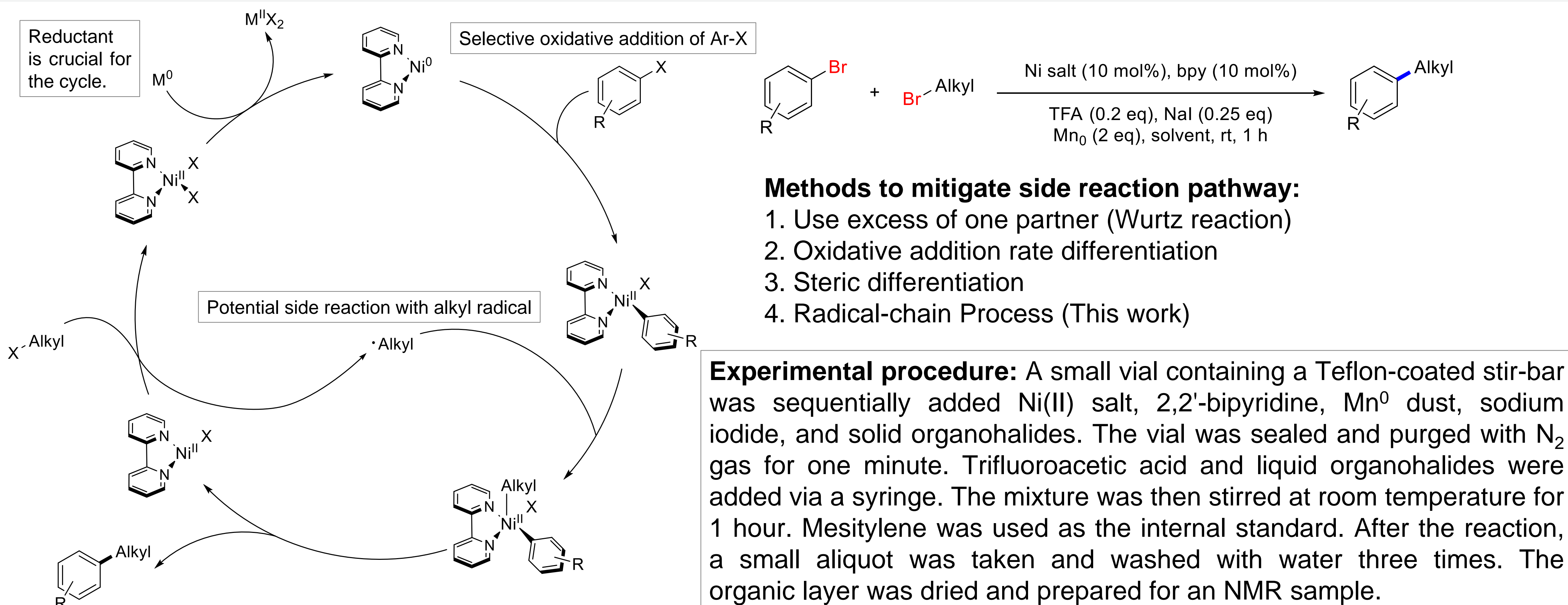


Cross-electrophile coupling (XEC) reactions



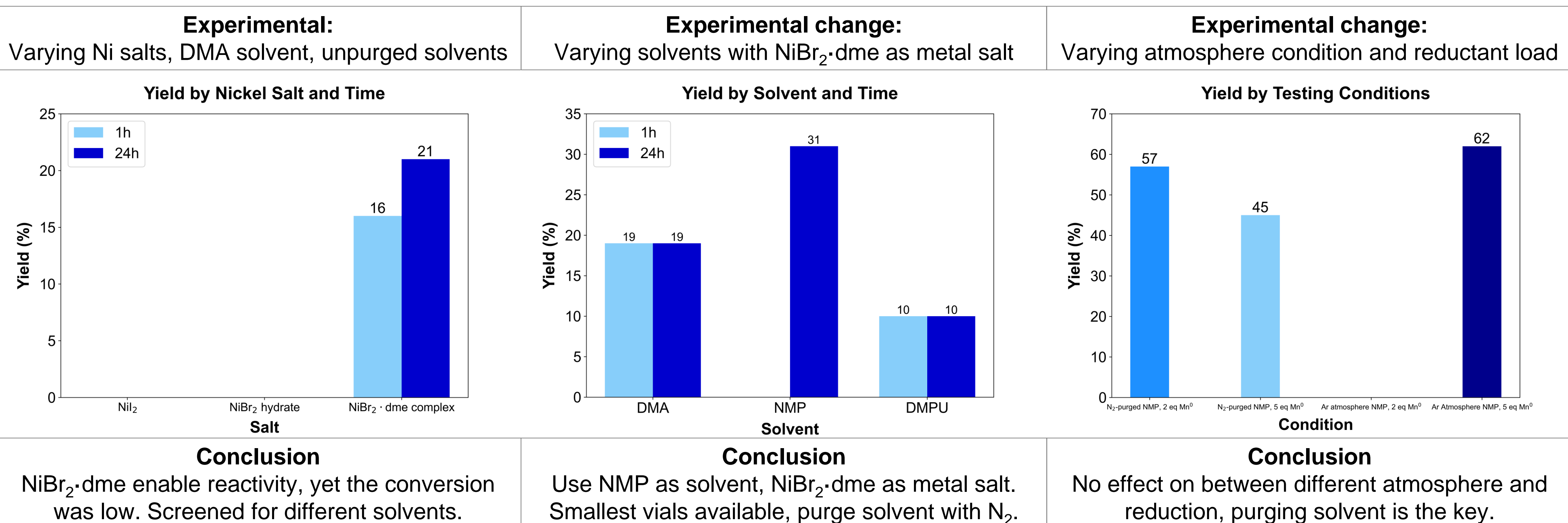
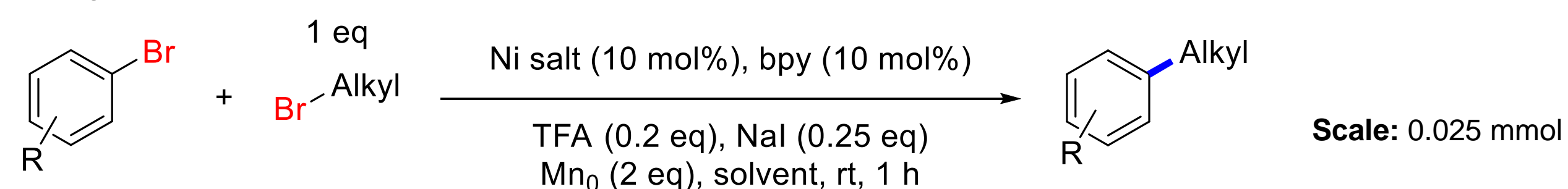
This project: Assess how reaction parameters affect on yield and side reaction pathways

Mechanism & Experimental Procedure



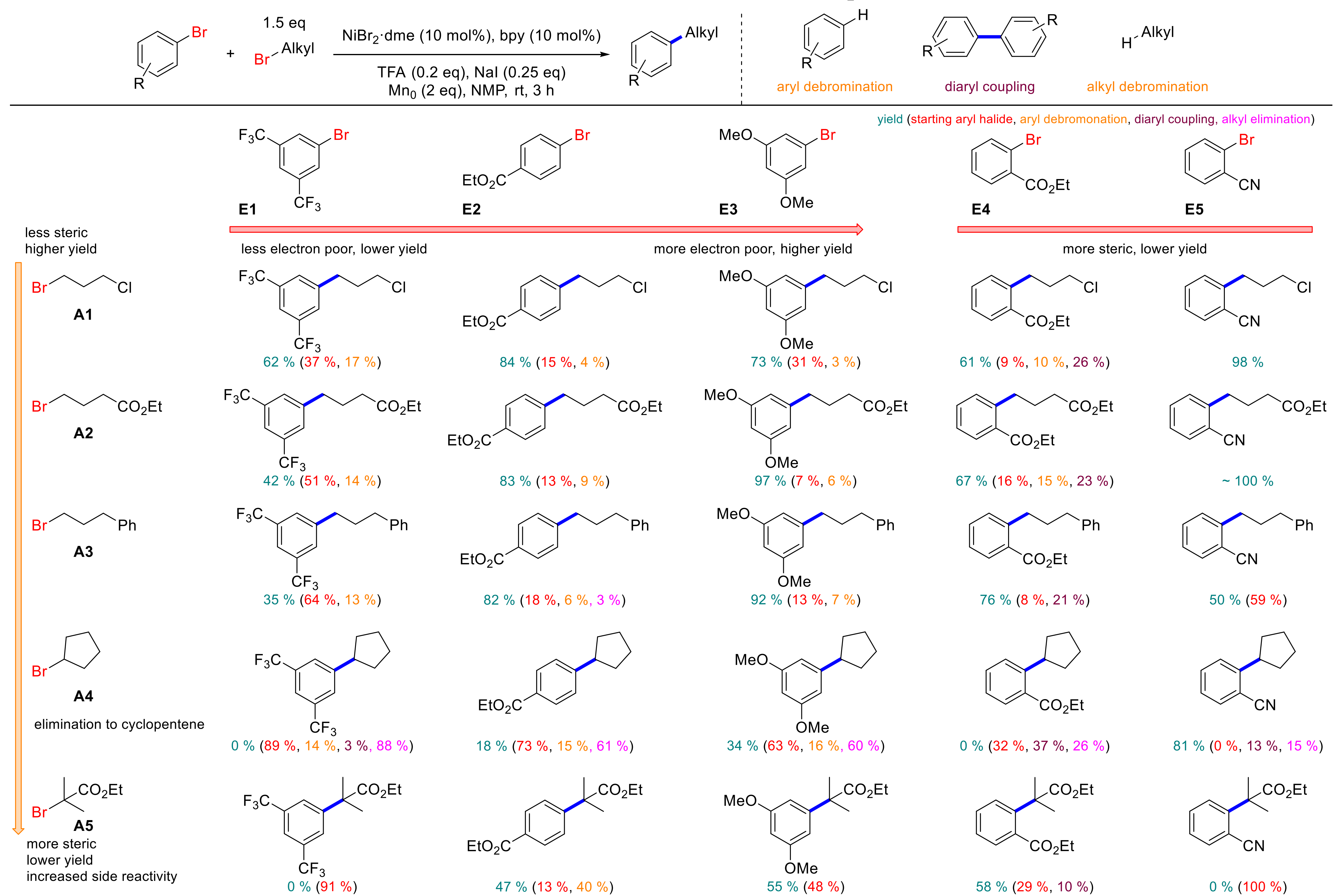
Solvent Identity & Metal Salts Solubility & Atmosphere Condition on Reactivity

No reactivity following the benchtop procedure in literature, screened for the suitable reaction conditions

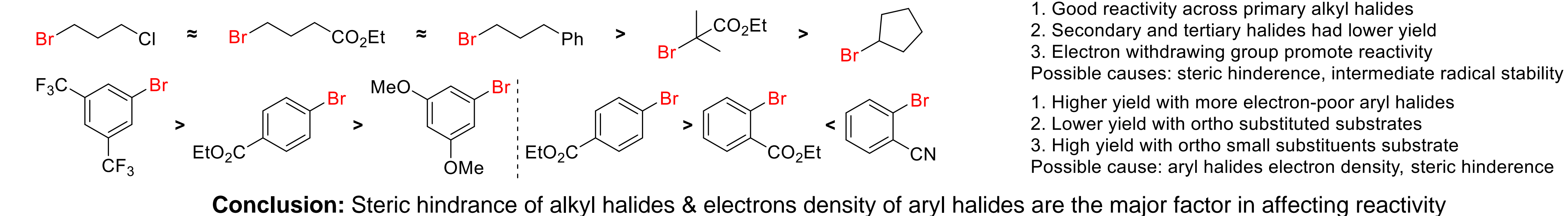


Results: Substrate stereoelectronic effect on reactivity

Hypothesis: more electron-poor & less sterically hindered substrates promote reactivity
Experimental improvement: 1.5 equivalent alkyl bromide, N_2 purged solvent, smaller vial

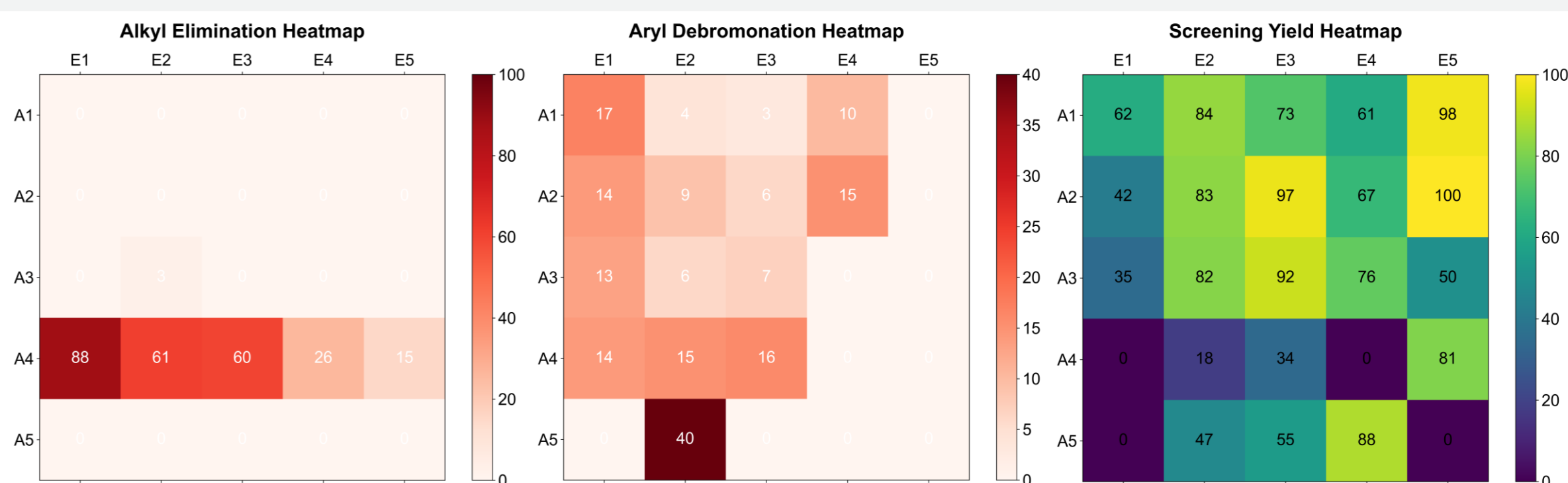


Substrate reactivity



Summary & Conclusions

This study underscores the critical role of metal solubility and solvent preparation in cross-electrophile coupling reactions between aryl halides with alkyl halides, with NMP solvent and N_2 -purged conditions significantly increased yields. Less sterically hindered primary alkyl halides and electron-poor aryl halides were the more reactive. Steric hindered second and tertiary alkyl substrates also exhibited reactivity albeit with lower yield. These data can provide helpful information regarding substrate selection in future synthesis using this reaction.



Literature cited & Acknowledgement

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