

Suppl. 4: Reactions for typical route selections

The following tables list the reactions utilized in two typical route selection scenarios

(see Section 3.3 and Table 1).

It turns out that most of the synthesis procedures are quite common, which makes our method a useful tool for synthetic chemists.

Reactions Rgroup Enumeration 18x18	Frequency
Imidazole synthesis	23
Fluoro N-arylation	10
Bromo N-arylation	9
SNAr ether synthesis	9
Fluorination	5
Unrecognized	5
Carboxylic ester + amine reaction	3
Friedel-Crafts acylation	2
Bromo Sonogashira coupling	1
Carboxylic acid to acid chloride	1
Ullmann-type biaryl coupling	1
Bromo N-arylation	1
Wurtz-Fittig coupling	1
Carboxylic acid to acid chloride	1
Aldehyde reductive amination	1

Reactions MMP Transformation 5x5	Frequency
Carboxylic acid + amine condensation	24
Methoxy to hydroxy	11
Williamson ether synthesis	8
Mitsunobu aryl ether synthesis	3
Unrecognized	2