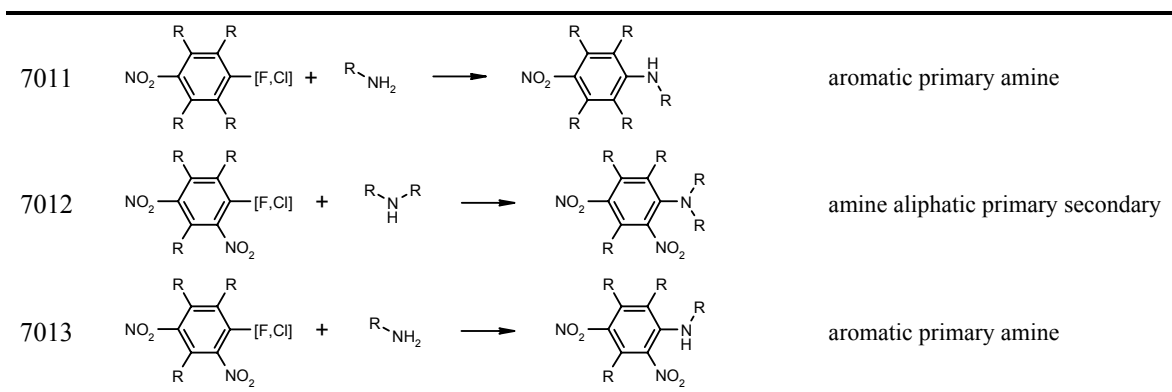
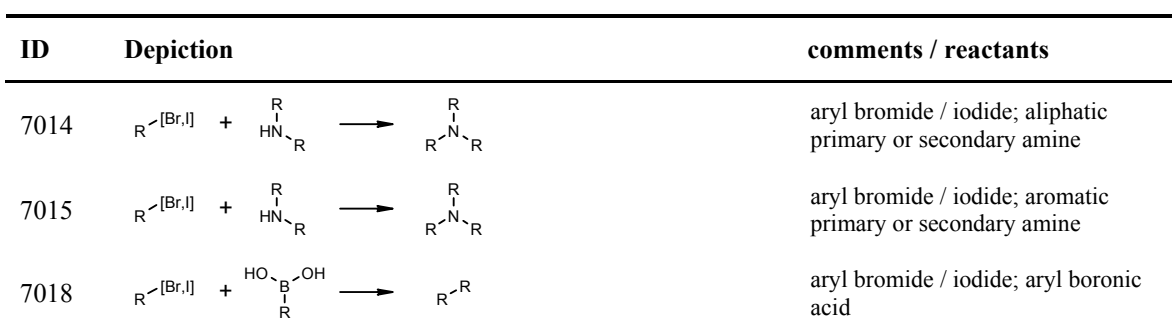


## Subset 1: Nucleophilic Aromatic Substitution Reactions

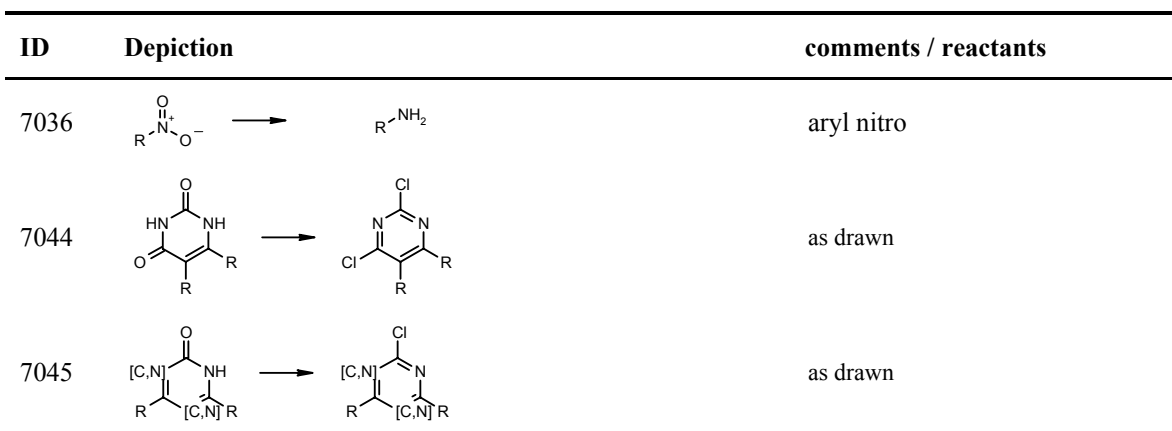
ID	Depiction	comments / reactants
7000		aliphatic primary or secondary amine
7001		aromatic primary amine
7002		aliphatic primary and secondary amine
7003		aromatic primary amine
7004		2-chloropyrimidine, but not 4-chloropyrimidine aliphatic primary or secondary amine
7005		2-chloropyrimidine, but not 4-chloropyrimidine primary aromatic amine
7006		aliphatic primary or secondary amine
7007		aromatic primary amine
7008		aliphatic primary or secondary amine
7009		aromatic primary amine
7010		amine aliphatic primary or secondary



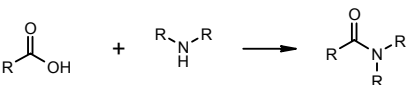
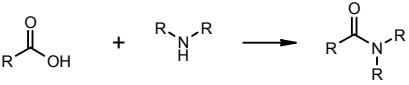
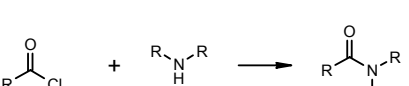

### Subset 2: Pd-Catalyzed Aromatic Substitutions



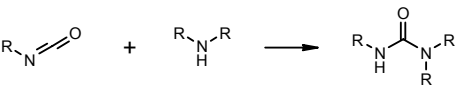
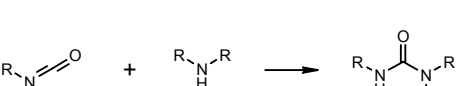
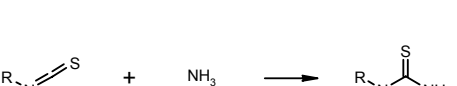


### Subset 3: Functional Group Transformations

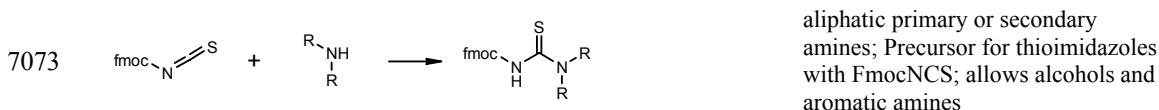


#### Subset 4: Amine Acylation Reactions (Amides / Carbamates)

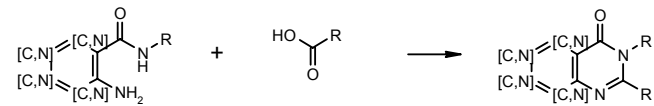
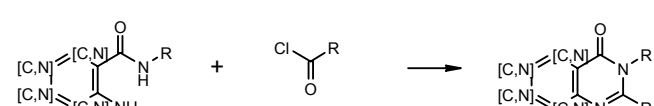
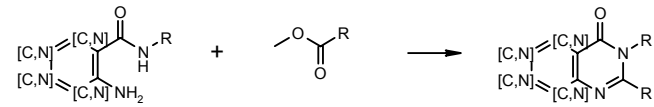
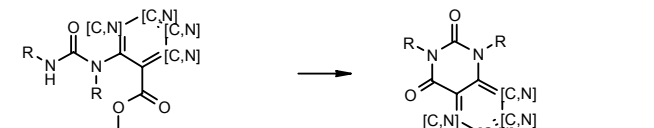
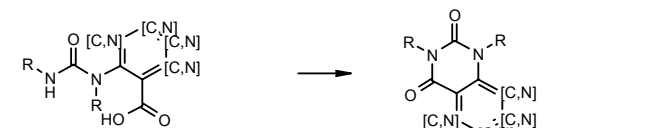
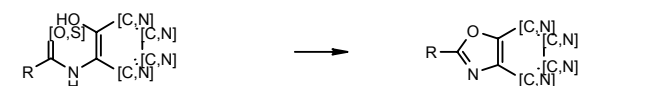
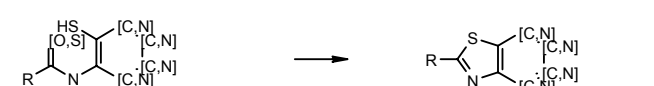
ID	Depiction	comments / reactants
7046		carboxylic acids; aliphatic amines; alcohols and aromatic amines allowed, allows activated aryl halides, no alkylators
7047		carboxylic acids; aromatic amines; not compatible with alcohols and related, no alkylators, allows activated aryl halides
7048		carboxylic acid chlorides, chloroformates, chloroformamidines; aliphatic amines; not compatible with alcohols or aromatic amines, no alkylators, allows activated aryl halides
7049		carboxylic acid chlorides, chloroformates, chloroformamidines; aromatic amines; not compatible with alcohols and related, no alkylators, allows activated aryl halides

#### Subset 5: Amine Acylation Reactions (Ureas / Thioureas)

ID	Depiction	comments / reactants
7062		aliphatic amines; aromatic amines alcohols allowed; activated aryl halides allowed; not compatible with alkylators, other nucleophiles, other acylators, acidic compounds
7063		aromatic amines; alcohols allowed; activated aryl halides allowed; not compatible with alkylators, nucleophiles, other acylators, acidic compounds
7064		ammonia precursors for thioimidazoles; aryl amines and alcohols allowed, no alkylators, other acylators, nucleophiles, acids
7065		primary aryl amine; precursor for 2-amino-benzthioimidazole or 2-amino-benzimidazole, or related aryls; secondary aryl amines and alcohols allowed, no alkylators, other acylators, no acids, no nucleophiles
7072		aryl primary or secondary amines; Precursor for thioimidazoles with FmocNCS



### Subset 6: Formation of Diverse Heterocyclic Systems

ID	Depiction	comments / reactants
7037		any 2-amino arylamide not in a ring; any carboxylic acid; excludes acylators, alkylators, nucleophiles, other acids, activated aryl halides, aryl bromides/iodides
7038		any 2-amino arylamide not in a ring; carboxylic acid chloride, no chloroformate, carbamoyl chloride, etc.; excludes other acylators, alkylators, nucleophiles, acids, activated aryl halides, aryl bromides/iodides
7039		any 2-amino arylamide not in a ring; carboxylic acid methyl ester, does not allow any other ester, which is too restrictive; no differentiation between different ester reactivity; excludes acylators, alkylators, nucleophiles, acids, activated aryl halides, aryl bromides/iodides
7040		any 2-ureido aryl methyl carboxylate not in a ring; excludes, acylators, alkylators, acids, nucleophiles, activated aryl halides, aryl bromides/iodides
7041		any 2-ureido aryl carboxylic acid not in a ring; excludes, acylators, alkylators, acids, nucleophiles, activated aryl halides, aryl bromides/iodides
7066		any 2-hydroxyaryl-(NH)-amide, thioamide, urea, thiourea, etc.; excludes, acylators, alkylators, acids, nucleophiles, activated aryl halides, aryl bromides/iodides
7067		any 2-mercaptoaryl-(NH)-amide, thioamide, urea, thiourea, etc.; excludes, acylators, alkylators, acids, nucleophiles, activated aryl halides, aryl bromides/iodides

7068		any 2-aminoaryl-(NH)-amide, thioamide, urea, thiourea, etc.; not amido aryl amide; excludes, acylators, alkylators, acids, nucleophiles, activated aryl halides, aryl bromide/iodide
7069		1,2-diamino aryl (amino-2-arylamine); carboxylic acid methyl ester, does not allow any other ester, which is too restrictive; no differentiation between different ester reactivity; exclude, nucleophiles, acids, acylators, alkylators, activated aryl halides, aryl bromide/iodide, aldehydes, other esters
7070		1,2-diamino aryl; aldehyde; exclude, nucleophiles, acids, acylators, alkylators, activated aryl halides, aryl bromide/iodide
7071		2-mercapto arylamine; aldehyde; exclude, nucleophiles, acids, acylators, alkylators, activated aryl halides, aryl bromide/iodide, aldehydes

### Subset 7: Formation of Thioimidazoles

ID	Depiction	comments / reactants
7060		thioamide unsubstituted; not compatible with ketones or aldehydes, alkyl bromides / iodides, sulfonyl esters, etc., acidic compounds, nucleophilic compounds
7061		unsubstituted thiourea; not compatible with ketones or aldehydes, alkyl bromides / iodides, sulfonyl esters, etc., acidic compounds, nucleophilic compounds

### Subset 8: Standard Deprotection Steps

ID	Depiction	comments / reactants
7079		Fmoc deprotection, any Fmoc amine or amide aliphatic or aromatic

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7080		→		any boc amine or amide aliphatic or aromatic
7081		→		t-Bu ether, no acid or carbamate
7082		→		t-Bu ester, not carbamate, etc, R must be carbon
7083		→		any trityl ether/ester, thioether/ester derivative
7084		→		any trityl amine / amide aromatic/aliphatic derivative

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