

ChIP Introspective Filters

Filter Name	Type	Description
aldehyde	SMARTS	R no heteroatom no isocyanate, ketene, etc.
amine aliphatic (primary or secondary)	SMARTS	
amine aliphatic primary	SMARTS	
amine aliphatic secondary (not primary)	SMARTS	
amine aromatic primary	SMARTS	
amine aromatic primary or secondary	SMARTS	
amine aromatic secondary (not primary)	SMARTS	
amine aromatic/aliphatic primary or secondary	SMARTS	
aryl amide 2-amino (chain)	SMARTS	amide nitrogen of any 2-amino aryl amide not in a ring
aryl boronic acid	SMARTS	any aryl boronic acid
aryl bromide / iodide	SMARTS	any aryl bromide / iodide
aryl nitro (any)	SMARTS	any aryl nitro
carbonyl chloride	SMARTS	carbonyl C of acid chloride, chloroformate, chloroformamide (aliphatic, aromatic)
carboxylic acid	SMARTS	any carboxylic acid, R must be carbon
carboxylic acid chloride	SMARTS	no chloroformate or chloroformamide, etc.
carboxylic acid methyl ester	SMARTS	no heteroatom bound to carbonyl
ketone	SMARTS	no aldehyde, R no heteroatom, no isocyanate, ketene, etc.
ketone or aldehyde	SMARTS	R no heteroatom, no isocyanate, ketene, etc
ureido aryl 2-(methyl carboxylate) (chain)	SMARTS	urea nitrogen of any 2-ureido aryl methyl carboxylate not in a ring
ureido aryl 2-carboxylic acid (chain)	SMARTS	urea nitrogen of any 2-ureido aryl carboxylic acid not in a ring