ChIP Incompatibility Filters

Filter Name	Type	Description
>1 acyl halide and related	SMARTS	includes carboxylic acid halides and derivatives like chloroformates, carbamoyl-, imidoyl halides, etc.
>1 aldehyde	SMARTS	R no heteroatom no isocyanate, ketene, etc.
>1 alkyl bromide / iodide	SMARTS	no acyl halide or related or vinyl halide
>1 amine aromatic primary	SMARTS	aromatic carbon bound to N, N not charged
>1 amines (aromatic/aliphatic, primary or secondary)	SMARTS	no amide, enamine, etc., no heteroatom bound to N, N not charged
>1 amines nucleophilic (aliphatic primary or secondary)	SMARTS	no amide, enamine, etc, no heteroatom bound to N, no aromatic carbon bound to N, N not charged
>1 aryl bromide / iodide	SMARTS	any aryl bromide / iodide
>1 aryl halide	SMARTS	any aryl halide
>1 boronic acid derivative	SMARTS	any boronic acid derivative, aromatic or aliphatic
>1 carbonyl acid	SMARTS	any carboxylic or carbamic acid, etc.
>1 carboxylic acid anhydrides	SMARTS	carbon must be bound to carbonyl
>1 carboxylic acid ester	SMARTS	no heteroatom bound to carbonyl or oxygen, no acid, no anydride, etc
>1 isocyanate / isothiocyanate	SMARTS	no restrictions to nitrogen substituents
>1 ketone or aldehyde	SMARTS	R no heteroatom, no isocyanate, ketene, etc.
>1 NH any	SMARTS	R can be anything
>1 thioamide and related (any)	SMARTS	any substitution
>1 thiol and related (nucleophic)	SMARTS	any SH or negative S
>2 NH any	SMARTS	R can be anything
acidic compounds I	combination	sulfonyl acids and carboxylic acids
acyl anhydrides and derivatives	SMARTS	anhydrides, bicarbonates, thio and imino derivatives, etc.
acyl halide and related	SMARTS	includes carboxylic acid halides and derivatives like chloroformates, carbamoyl-, imidoyl halides, etc.
acylators I	combination	acyl anhydrides, acyl halides, isocyanates/isothiocysnates, sulfonyl halides
alcohol aliphatic (prim, sec, tert)	MOL	any aliphatic prim, sec, or tert alcohol except methanol
alcohol aliphatic primary	MOL	as drawn

alcohol aliphatic secondary	MOL	as drawn
alcohol aliphatic	SMARTS	no carboxylic acid, enole, etc, no heteroatom bound to oxygen, no aromatic alcohol, no hydrates
alcohol aliphatic tertiary	MOL	as drawn
alcohol and related (any)	SMARTS	aromatic/aliphatic no carboxylic acid, etc., includes hydroxylamines and -amides, hydrates, etc., no other atom than C,N bound to O
alcohol aromatic	SMARTS	any aromatic alcohol
aldehyde	SMARTS	R no heteroatom no isocyanate, ketene, etc.
alkyl bromide / iodide prim.	SMARTS	
alkyl bromide / iodide	SMARTS	no acyl or vinyl halide or related
alkyl di- or tri- bromide/iodide	SMARTS	no acyl or vinyl or related
alkylators I	combination	alkyl bromides/iodides/sulfonates
alpha halo ketone / aldehyde	SMARTS	
amidine derivative unsubst. (any)	SMARTS	guanidine, amidine, isourea, isothiourea, etc.; R can be anything
amine aliphatic (primary or secondary)	SMARTS	no amide, enamine, etc, no hereroatom bound to N, no aromatic carbon bound to N, N not charged
amine aliphatic mono	MOL	
amine aliphatic primary (branched0-2)	MOL	
amine aliphatic primary branched0	MOL	
amine aliphatic primary branched1	MOL	
amine aliphatic primary branched2	MOL	
amine aliphatic primary	SMARTS	no aminde, enamine, etc, no heteroatom bound to N, no aromatic carbon bound to N, N not charged
amine aliphatic secondary (not primary)	SMARTS	no amide, enamine, etc, no heteroatom bound to N, no aromatic carbon bound to N, N not charged
amine aliphatic secondary branched00	MOL	
amine aliphatic secondary branched01	MOL	
amine aliphatic secondary branched11	MOL	
amine aliphatic secondary branched12	MOL	
amine aliphatic secondary branched22	MOL	

amine aromatic primary or secondary	SMARTS	aromatic carbon bound to N, no amide, no enamine, etc. no heteroatom bound to N, N not charged
amine aromatic primary	SMARTS	aromatic carbon bound to N, N not charged
amine aromatic secondary (not primary)	SMARTS	aromatic carbon bound to N, no amide, no enamine, etc. no heteroatom bound to N, N not charged
amine aromatic/aliphatic primary or secondary	SMARTS	no amide, no enamine, etc, no heteroatom bound to N, N not charged
amino 2-arylamide (chain)	SMARTS	any 2-amino arylamide not in a ring
amino 2-arylamine	SMARTS	any 1,2-diamino-aryl
aminoaryl amide/urea	SMARTS	any 2-aminoaryl-(NH)-amide, thioamide, urea, thiourea, etc.; not amido aryl amide
aniline	MOL	as drawn
aryl boronic acid (5 or 6-ring)	SMARTS	any 5- or 6-ring aryl boronic acid
aryl bromide / iodide (mono , 6-ring)	SMARTS	any 6-ring-aryl mono-bromide / iodide
aryl bromide / iodide (mono, 5-ring)	SMARTS	any 5-ring aryl mono-bromide / iodide
aryl bromide / iodide	SMARTS	any aryl bromide / iodide
aryl halide activated (I)	SMARTS	pyridyl, pyrimidyl, triazyl, halide, etc.
aryl halide activated (II)	SMARTS	pyridyl, pyimidyl, triazyl, halide or o-/ p-nitro aryl fluoride/chloride
aryl halide	SMARTS	any aryl halide
aryl mono bromide/iodide (5 or 6-ring)	SMARTS	any 5- or 6-ring aryl mono-bromide / iodide
aryl nitro (any)	SMARTS	any aryl nitro
aryl o- or p-nitro fluoride/chloride	SMARTS	
aryl o-,p-di-nitro fluoride/chloride	SMARTS	any substitution
aryl o-nitro fluoride/chloride	SMARTS	any substitution
aryl p-nitro fluoride/chloride	SMARTS	any substitution
boronic acid derivative	SMARTS	any boronic acid derivative, aromatic or aliphatic
bromo/iodo ketone/aldehyde (alpha)	SMARTS	
carbamic acid	MOL	as drawn
carbamic acid	SMARTS	no restrictions to N substituents
carbonyl chloride	SMARTS	acid chloride, chloroformate, chloroformamidine (aliphatic, aromatic)
carboxylic acid	MOL	as drawn
carboxylic acid anhydride	SMARTS	carbon must be bound to carbonyl
carboxylic acid bromide	MOL	as drawn
carboxylic acid chloride	MOL	as drawn

carboxylic acid chloride	SMARTS	no chloroformate or chloroformamidine, etc.
carboxylic acid ester	SMARTS	no heteroatom bound to carbonyl or oxygen, no acid, no anydride, etc
carboxylic acid fluoride	MOL	as drawn
carboxylic acid halide	combination	any carboxylic acid halide
carboxylic acid iodide	MOL	as drawn
carboxylic acid methyl ester	SMARTS	no heteroatom bound to carbonyl
carboxylic acid	SMARTS	no carbamic acid, etc.
elements all	SMARTS	any element (aromatic or aliphatic, any isotope)
elements except H,B,C,N,O,F,Si,P,S,Cl,Br,I	SMARTS	includes aromatic, aliphatic, isotopes
elements except H,B,C,N,O,F,Si,P,S,Cl,Br,I (includes X)	SMARTS	not any of these elements (arom, aliph, isotopes)
elements except H,C,N,O,F,S,Cl,Br,I (includes X)	SMARTS	not any of these elements (arom, aliph, isotopes)
elements except H,Li,B,C,N,O,F,Na,Mg,Si,P,S,Cl,Br,K, Ca,I,Cs (includes X)	SMARTS	not any of these elements (arom, aliph, isotopes)
elements H,C,N,O,F,P,S,Cl,Br,I	SMARTS	must be one of the elements above (aromatic or aliphatic or any isotope)
elements non-standard (stable) isoptopes of H,C,N,O,F,S,Cl,Br,I	SMARTS	all stable non-standard isotopes of the elements above (arom, aliph)
elements non-standard (stable) isoptopes of H,C,N,O,F,Si,P,S,Cl,Br,I	SMARTS	all stable non-standard isotopes of the elements above (arom, aliph)
hydrazine nucleophilic aliphatic/aromatic	SMARTS	no hydrazides and derivatives
hydrogen halides (HCl, HBr, HI)	SMARTS	hydrogen halide
hydroxamic acid	MOL	as drawn
hydroxamic acid	SMARTS	no heteroatom bound to carbonyl
hydroxyaryl amide/urea	SMARTS	any 2-hydroxyaryl-(NH)-amide, thioamide, urea, thiourea, etc.
isocyanates / isothiocyanates and derivatives	SMARTS	R can be anything
isocyanates aromatic	SMARTS	aromatic carbon bound to nitrogen
isocyanates	SMARTS	no hetereoatom bound to nitrogen
isothiocyanates	SMARTS	no hetereoatom bound to nitrogen
ketone or aldehyde	SMARTS	R no heteroatom no isocyanate, ketene, etc.
ketone	SMARTS	no aldehyde, R no heteroatom, no isocyanate, ketene, etc.

mercapto 2-arylamine	SMARTS	any 2-mercapto-arylamine (NH)
mercaptoaryl amide/urea	SMARTS	any 2-mercaptoaryl-(NH)-amide, thioamide, urea, thiourea, etc.
NH any	SMARTS	R can be anything
nitro aliphatic (any)	SMARTS	nitro bound to any aliphatic element
nitrophenyl carbamate	MOL	p-nitrophenyl carbamate
nucleophiles basic I	combination	nitrogen and thio nucleophiles (aliphatic amines, hydrazines, guanidines, thiol-derivatives)
OH any	SMARTS	R can be anything
pyridine chloride-2	SMARTS	any substitution
pyridinone derivative	SMARTS	any 1H-pyridin-2-one derivative, no pyridine-2,6-dione, etc.
pyrimidine chloride-2	SMARTS	
pyrimidine chloride-4	SMARTS	
pyrimidinedione derivative	SMARTS	any 1H-pyrimidine-2,4-dione derivative, no triazinanetrione or pyrimidinetrione
sulfonic acid	MOL	as drawn
sulfonic acid aromatic phenyl	MOL	as drawn
sulfonic acid chloride	SMARTS	R must be carbon
sulfonic acid	SMARTS	R must be carbon
sulfonyl acid (any)	SMARTS	sulfonic acid, sulfinic acid, etc.
sulfonyl alkyl ester, anydride, sulfate, etc.	SMARTS	any substitution allowed
sulfonyl halide (any)	SMARTS	sunfonic acid halide, sulfinyl halide, etc.
thioamide and related (any)	SMARTS	any substitution
thioamide N-unsubst.	SMARTS	R must be carbon
thiol aliphatic primary	MOL	as drawn
thiol and related (nucleophic)	SMARTS	any SH or negative S
thiourea N-unsubst.	SMARTS	any aromatic or aliphatic N-unsubstituted thiourea
triazine chloride	SMARTS	
ureido aryl 2-(methyl carboxylate) (chain)	SMARTS	any 2-ureido aryl methyl carboxylate not in a ring
ureido aryl 2-carboxylic acid (chain)	SMARTS	any 2-ureido aryl carboxylic acid not in a ring