Exclusion criteria of the Maybridge Screening Collection database

The following chemical moieties have been excluded from our database to produce a set of chemical structures that will have the maximum diversity and "drug-like" properties. Removal of these moieties will minimise the number of potential 'false leads'. This should result in a better percentage of genuine leads for optimisation and eliminate the time and monies expended on following unsuitable hits. The excluded chemical moieties have been carefully selected from data and other information sources by Maybridge since the early 1990s, when HTS came to the forefront of lead identification. Using this data and Maybridge's own experience of over 40 years, this database will be the ideal candidate for use in HTS programs.

Excluded chemical moieties:

Following is a comprehensive listing of these and a brief explanation of why they have been excluded.

Chemical moiety	Reasoning
Acyl Halides	Covalent bonding
Sulphonyl Halides	Covalent bonding
Alkyl Halides	Covalent bonding
Isocyanates	Covalent bonding
Isothiocyanates	Covalent bonding
Activated Halides *	Covalent bonding
Anhydrides	Covalent bonding
Aldehydes (incl aminoformyl moieties)	Covalent bonding
Hydrazines	Covalent bonding
Azides	Toxicity
Diazonium salts	Toxicity
Quaternary salts (including N-Oxides)	Toxicity
Nitrosos	Toxicity
Aziridines **	Toxicity/Covalent bonding
Epoxides	Covalent bonding
Thiols***	Toxicity/Covalent bonding
Disulphides	Toxicity/Covalent bonding
Picrates	Toxicity
Perchlorates (Periodates)	Toxicity
Simple Anilines and Phenols	Toxicity
1,2-Dicarbonyls****	Toxicity
Vinyl Ketones (Michael Acceptors)#	Covalent bonding
Nitro groups (max. of 2)	Toxicity/Solubility
Halo atoms (max. of 5)##	Toxicity
Metals###	Toxicity
Simple molecules	Simple
MW <150	Simple

*compounds classified as activated halides consist of the 4 following moieties:

- halide with a NO2 ortho to the halide e.g. 2-Chloronitrobenzene
- halide with a NO2 para to the halide e.g. 4-Chloronitrobenzene

- halide with a hetero ring N ortho to the halide e.g. 2-Chloropyridine

- halide with a hetero ring N para to the halide e.g. 4-Chloropyridine (where N activation may be of some significance in some screening programmes).

**aziridines which have a free NH moiety on the aziridine ring.

***thiols where the thiol moiety cannot exist as the thione i.e. benzene thiol excluded, but 1,2,4-Triazole-3-thione included.

****chain dicarbonyls are excluded, ring dicarbonyls are included i.e. glyoxalates excluded, ring substituted isatin moieties included.

#Vinyl ketones moieties have been excluded where the vinyl ketone is directly attached to a ring system and the other end of the moiety has not been substituted. i.e. Cinnamic acid, simple ester, amide nitrile etc would be excluded. Where a cinnamoyl chloride has been reacted with a R-NH2, these would be included. Compounds of type Ring-COCH=CH-Ring (Chalcones) are excluded. For further information on this exclusion criteria please contact Maybridge.

##Halo atoms maximum 5. When calculating this, exclusion salts are not included and a trifluoromethyl group is taken as only 1 halo. All Trichlorovinyl moieties have been excluded.

###Metals, Sodium and Potassium salts of acids are included.

Compounds excluded from the Maybridge Screening Collection for any of the above reasons are still held at Maybridge. Customers requiring a database of these can request it from Maybridge.