

Halogen-enriched fragment libraries as chemical probes for halogen bonding.

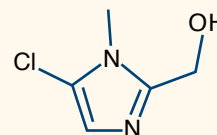
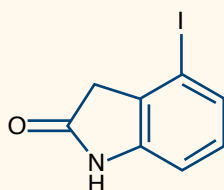
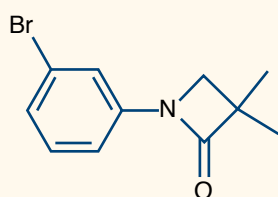
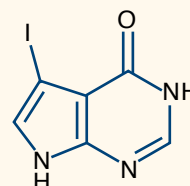
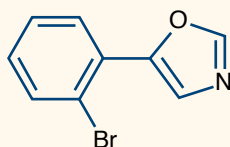
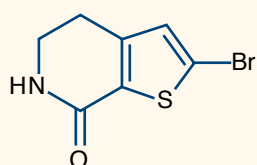
Halogen bonds have recently gained attention in life sciences and drug discovery. However, it can be difficult to harness their full potential, when newly introducing them into an established hit or lead structure by molecular design. A possible solution to overcome this problem is the use of halogen-enriched fragment libraries (HEFLibs), which consist of chemical probes that provide the opportunity to identify halogen bonds as one of the main features of the binding mode [1].

- Halogen-enriched fragment libraries (HEFLibs) are collections of small molecules sharing the advantages of regular fragments as chemical probes.
- HEFLibs enhance the probability to identify favourable halogen bonds in a protein binding site early in a fragment-based drug discovery campaign.
- HEFLibs help to probe protein binding sites for atypical recognition motifs and halophilic environments.
- HEFLibs provide intrinsic advantages for crystallography.
- HEFLibs offer the opportunity to use the aromatic halides as synthetic handles in organometallic crosscoupling reactions during fragment evolution.

BIONET HEFLib

A BIONET HEFLib has been constructed employing Rule of Three and industry standard substructure filtering including PAINS analysis. All Fragments are soluble in DMSO at 100mM and have a cLogS value greater than -4.

Examples of BIONET Halogen Enriched Fragments



[1] Frontiers in Chemistry | www.frontiersin.org 1 February 2019 | Volume 7 | Article 9

BIONET Halogen Enriched Fragments are available custom-weighted
in milligram or micromolar quantities as dry
powders or DMSO solutions.

BIONET
Fragment Libraries

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