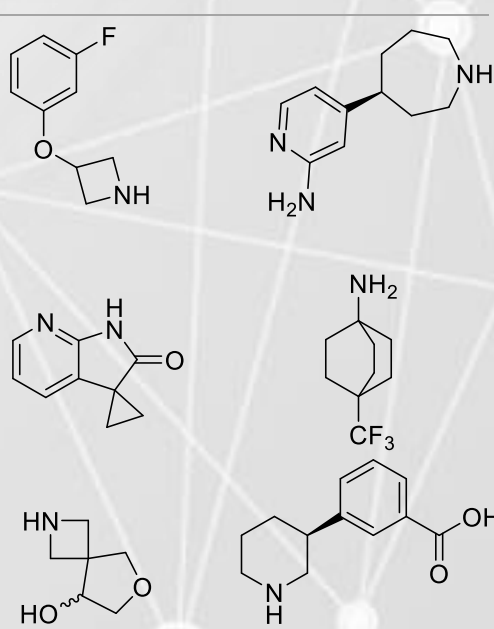


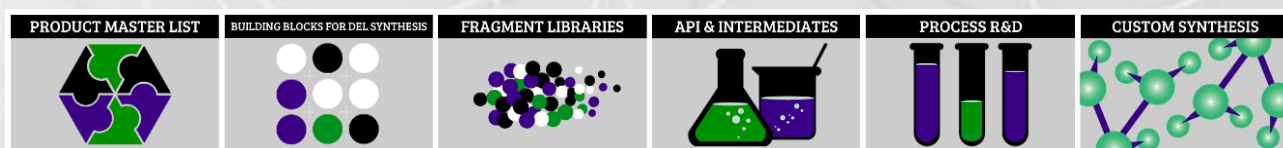
Molecules of the Month Fragment Library

LCC have designed a 3D-rich fragment library based on sp^3 -rich heterocyclic cores. The library contains over 4000 Ro3 compliant compounds and its high sp^3 fraction (0.23-1.00; average 0.52) and diversity maximise the coverage of chemical space. Each compound has no more than one chiral centre and at least one growth-vector for hit expansion. The cyclic structure of the fragment cores ensures a low number of rotatable bonds and the predicted solubility (cLogS) is in accordance with other specialised libraries.

Molecular properties and filters applied are summarised in the table below.

Molecular property	Library range; Library average	Example Fragments
MW	≤ 300; 184	
Heavy atom count	5-17; 13.1	
cLogP	≤ 3	
cLogS	≥ -3.5	
HBD	≤ 3	
HBA	≤ 3	
RotB	≤ 3	
TPSA	0-69.11; 33.28	
Fsp ³	0.23-1.00; 0.52	
Chiral centres	≤ 1	

Should you require any further information regarding the any of our products do not hesitate to get in touch with us. Alternatively, if you would like to explore our complete range of products and services, please use the enquiry button at the top of our webpage to get in touch.



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