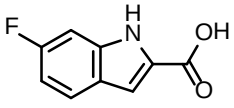
Essential Fragment Library

- **320 compounds**
- **Elaborated tool for initial screen**

Small fragment subset of 320 compounds designed in collaboration with research group at University of Cambridge for primary screen of *novel or difficult targets*.

- *Increased hit probability* – the structures are based on frequently reported fragment hits and scaffolds derived from experimentally determined structures of protein-ligand complexes (extracted from PDB ligand database).
- *Suitable for different screening assays* such as fluorescence polarization anisotropy, SPR, ligand-based NMR, thermal shift etc.
- *Experimentally assured solubility* at 1 mM, 2mM concentrations in PBS buffer and at 200mM in DMSO solution.
- *Experimentally confirmed chemical stability* in aqueous buffer solution (pH 6.5–7.5) at 30 °C for 24 h (LCMS method)

Molecular properties	Design	Filters
MW 110 - 250	Manual selection: indoles 20%, quinolines 18%, qunazolines 5%, morpholines 20%, pyrimidines 15%; carboxylic acids preferred; fragments reported in PDB, CREDO, iPPI-DB	Reactive groups Toxicophores Groups with fluorescence interference at 488/520 nm Groups with affinity to CMD-coated surface
ClogP -2.5 - 2.5		
HBA 0 - 5		
HBD 0 - 3		
TPSA ≤ 75 Å^2		



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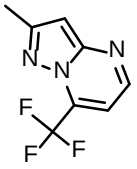

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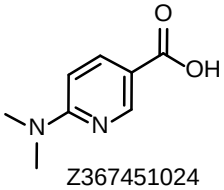

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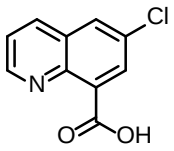

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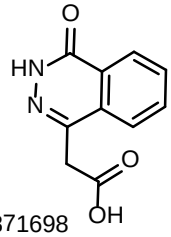

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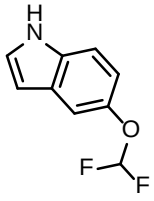

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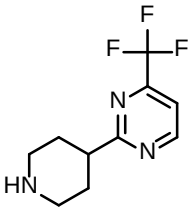

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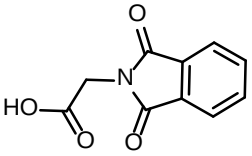

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