

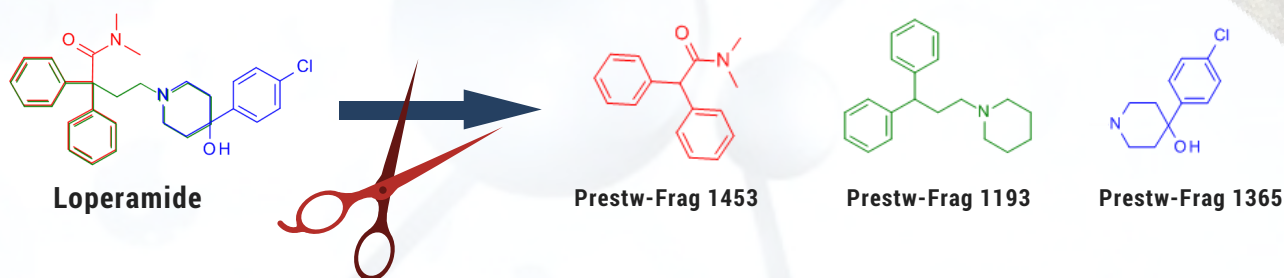
# PRESTWICK DRUG-FRAGMENT LIBRARY

*Accelerate your lead discovery - Innovation in FBDD*



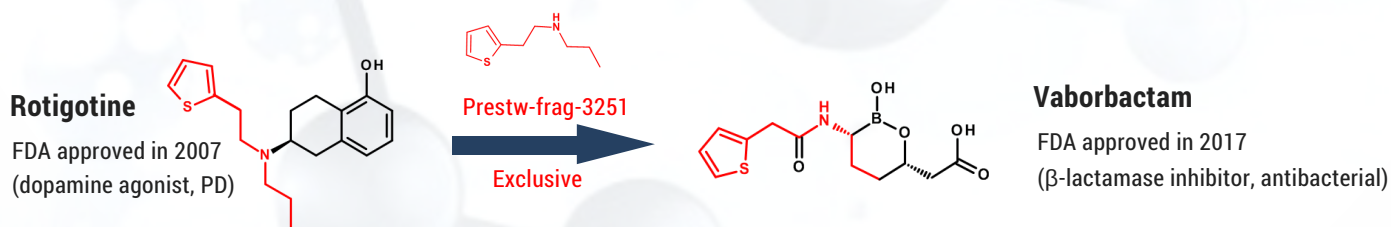
- A unique set of 1464 fragments designed by manual smart fragmentation from approved drugs (FDA, EMA...) up to year 2016
- Two subsets: Ro3 compliant (808 fragments) and Beyond Ro3 (656 fragments)
- Expansion from drug fragment-hits allows the synthesis of molecules with appropriate ADMET properties

## • EXAMPLE OF DRUG FRAGMENTATION

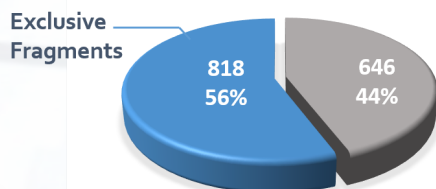


## • ADVANTAGES OF THE PRESTWICK FRAGMENT LIBRARY

- Prestwick fragments match 85% of 2017 FDA-approved drugs



- Prestwick exclusivity



818 (56%) of fragments are unique and can not be found in conventional fragment libraries

## HOW PROVIDED?

- Core set 480 cpds (DMSO solution up to 100mM) ready for screening
- Undissolved (from 10 mg) available for cherry-picking

## Physico-chemical properties

### Ro3 compliant subset

808 fragments

Parameter	Range	Average value
MW	80 - 288	171
clogP	-1.6 - 3.0	1.5
HBD	0 - 3	1.1
HBA	0 - 3	2.1
Rot. bond	0 - 3	1.5
TPSA	3 - 104	42
Heavy atoms	6 - 21	12

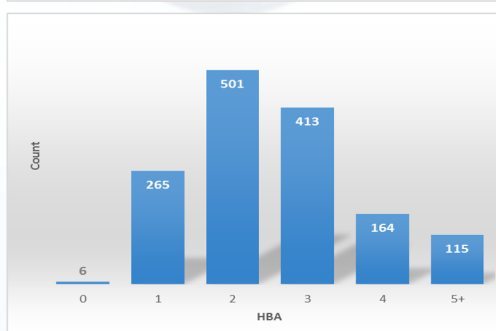
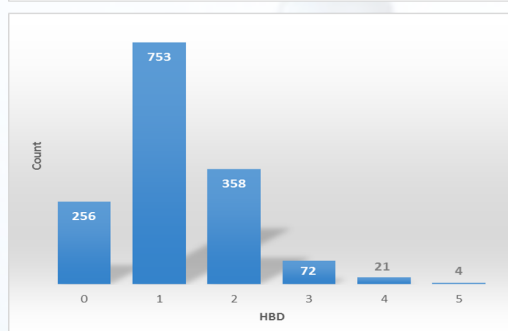
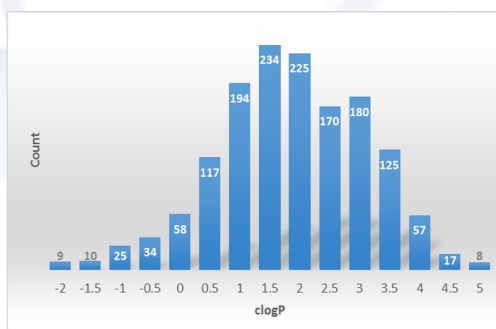
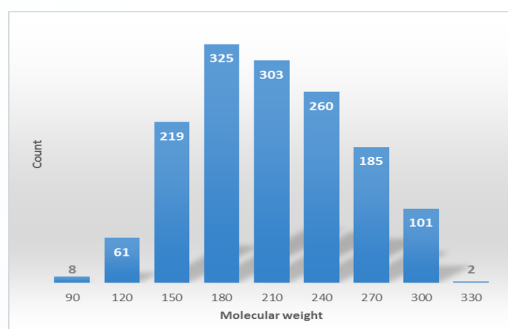
### Beyond Ro3 subset

656 fragments

(75% of fragments comply with 4 of the 5 Ro3 criteria)

Parameter	Range	Average value
MW	101 - 301	223
clogP	-3.1 - 5.0	1.8
HBD	0 - 5	1.3
HBA	0 - 9	3.2
Rot. bond	0 - 9	3.3
TPSA	0 - 144	53
Heavy atoms	6 - 22	16

### Entire library (1464 fragments)



Contact us!



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