

Summary of Oral Available Small Molecule IL-6 Inhibitor Project



in silico screening by INTENDD®
for 1st hit



in silico screening by INTENDD®
for 2nd hit



Medicinal chemists
and AI-guided INTENDD®
for hit to lead generation

10 million purchase
compounds

1st hit

K_D: 35 μM Mw: 370
clogP: 4.39 -8.4 kcal/mol

2nd hit

D002: K_D = 0.32 μM
D003: K_D = 0.28 μM
D005: K_D = 9.50 μM
D006: K_D = 1.50 μM (most druglike compound)

Synthesis 86 compounds including AI high scored 54 compounds.....

- Double digits nM K_D value 26 compounds including 14.7 nM and 10.6 nM (racemate 21.1 nM) compounds
- Triple digits K_D value 28 compounds
- 96% of AI good prediction rate to high affinity class
- K_D improving 2380 or 3317 folds from 1st hit
- **Creating lead optimized compounds including more bulky for improving receptor binding inhibition for next stage rapidly**