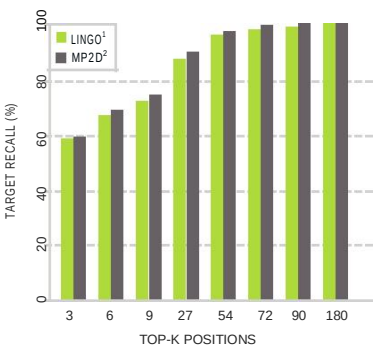
# PYTHIA

## Discovering your pharmacology profiles

Pythia predicts both therapeutic targets and off-targets for molecules. Medical indications are also suggested.
3,150 targets and 90 disease areas are considered

## Targets and Indications

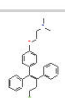
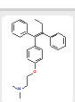
Pythia ranks targets.
In the first 3 target positions, Pythia detects 55% of the targets of a molecule.
Pythia predicts medical indications.
In 50% of the cases, the right indication is predicted in the first two positions.



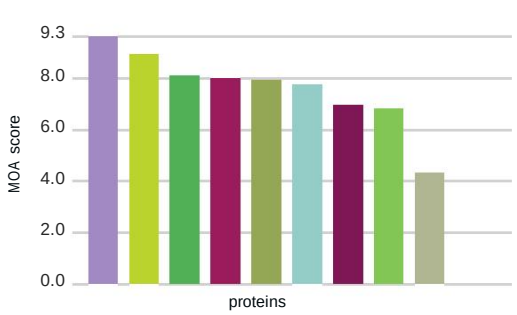

### ADVANTATGES

Evaluate mixtures.
Extendable to more targets.

### EXAMPLE OF PYTHIA RUN

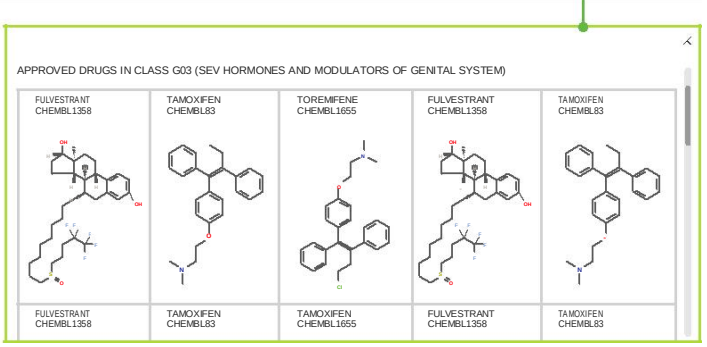
| Target | Associated gene | Organism | MoA Score | Structure | Molecule | Similarity | Activity | Source |
|---|---|---|---|---|---|---|---|---|
| Estrogen receptor beta | ESTRB , NR3A2, ESR2 | Homo sapiens | 9.29 |  | CHEMBL83 | 1.0000 | pKi=9.29 | ACS Med Clem Dell., 2012 3.3, 207,210 |
| Anti estrpgen binding site (AEBS) | EBP, D7SR, DHCR7 | Homo sapiens | 9.00 |  | CHEMBL83 | 1.0000 | pkd=9.00 | J. Med. Chem., 2003, 46, 6, 883, 908 |

### PYTHIA INDICATIONS

| MoA profile | ATC code | TI score | Indications |
|---|---|---|---|
|  | L02BA | 1 | L1 ANTINEOPLASTIC IMMUNOMODULATING AGENTS<br>L2 ENDOCRINE THERAPY<br>L3 HORMONE ANTAGONISTS AND RELATED AGENTS<br>L4 Anti-estrogens |



Calculated on the basis of the whole target profile




### EXPERIMENTAL VALIDATION

Pythia was used for a molecule active in cancer. Two top-ranked targets were chosen for experimental testing.
Both showed to interact with the molecule in the high nanomolar - low micromolar range.


1 Vidal D et al (2005) J Chem Inf Model, 45, 386-393.
2 Bender A et al (2004) J Chem Inf Comput Sci, 44, 1708-1718.
3 Gaulton A et al (2011) Nucleic Acids Res, 40, 1100-1107.