

Chemogenomics View of Pain Drug Discovery

Miguel Angel Dávila Jaramillo. M.D

*Chemogenomics Laboratory
Research Group on Biomedical Informatics
Institut Municipal d'Investigació Mèdica
Universitat Pompeu Fabra
Parc de Recerca Biomèdica de Barcelona*

Objectives

- ❑ **Collecting, organising, storing, integrating and exploiting the target and chemical space relevant to pain drug discovery that been covered to date.**

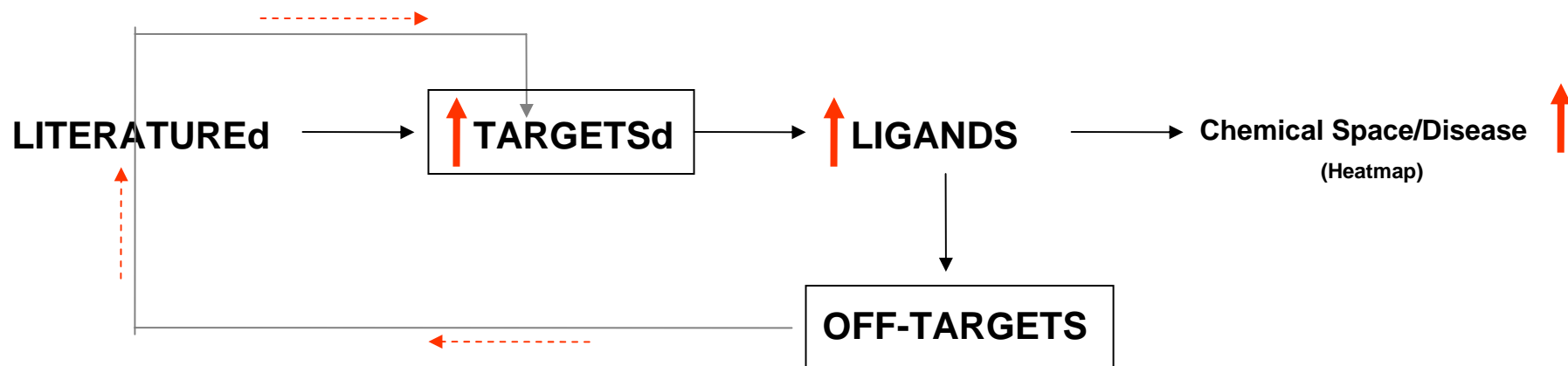
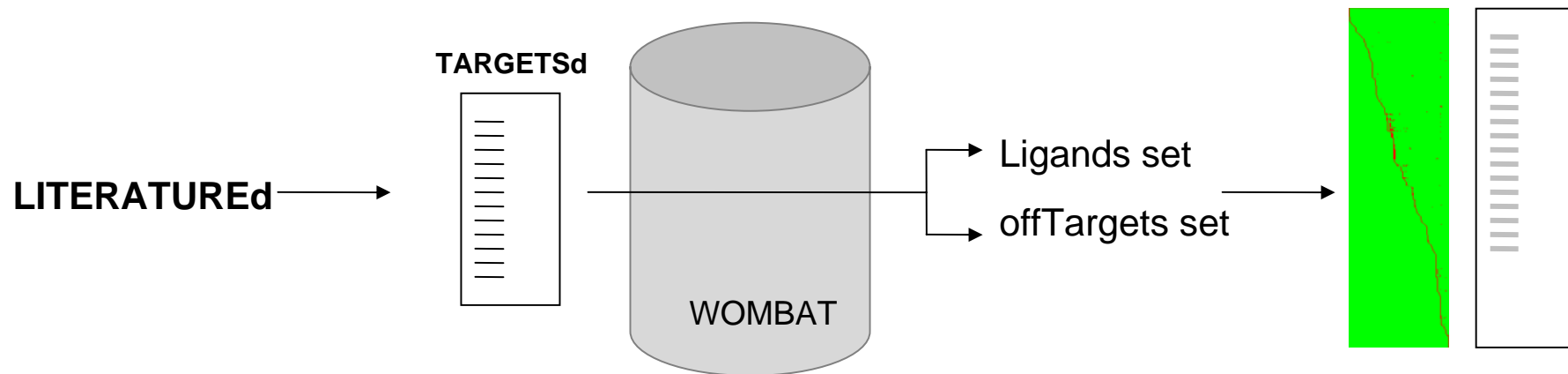
Justification

- Compilation, classification and integration of the chemogenomics to improve efficiency and a knowledge-based strategy can provide a wider perspective to modern pain treatments and make future drug discovery efforts more efficient**

Research Questions

- The multitude of potential drugs targets emerging from genome sequencing demands new approaches to drug discovery**
- The gaps in the compound-activity matrix reflex serious difficulties in data mining and reduce practical utilities of the biological tested compounds**

Methodology



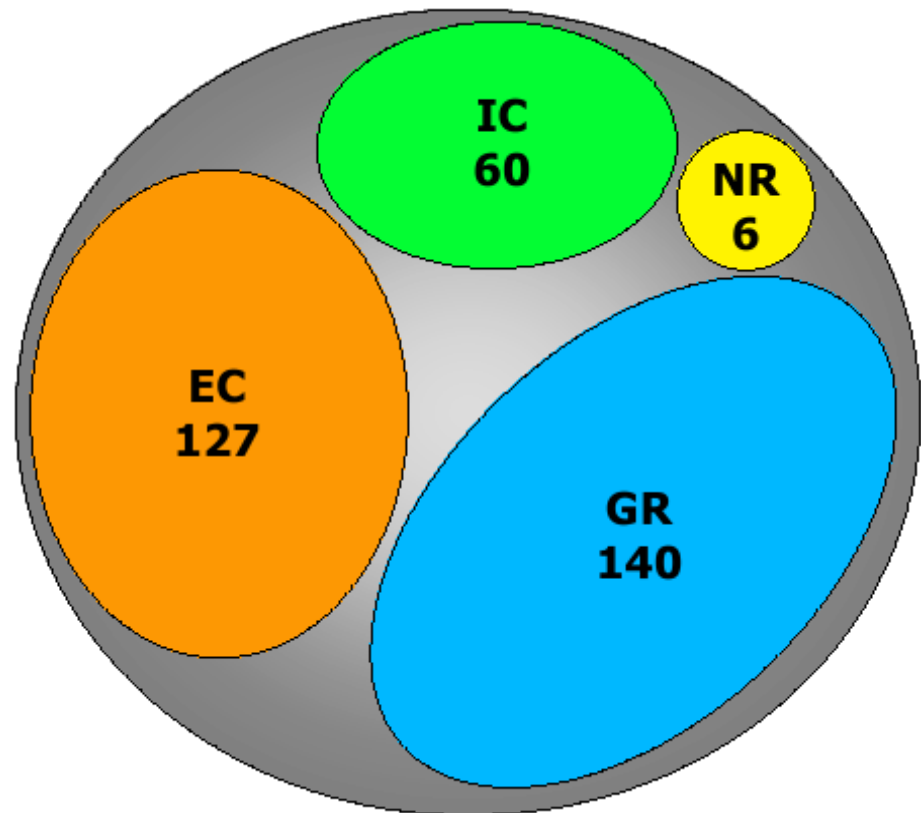
Results and Discussion

PubMed and Science Direct search

153 Journals

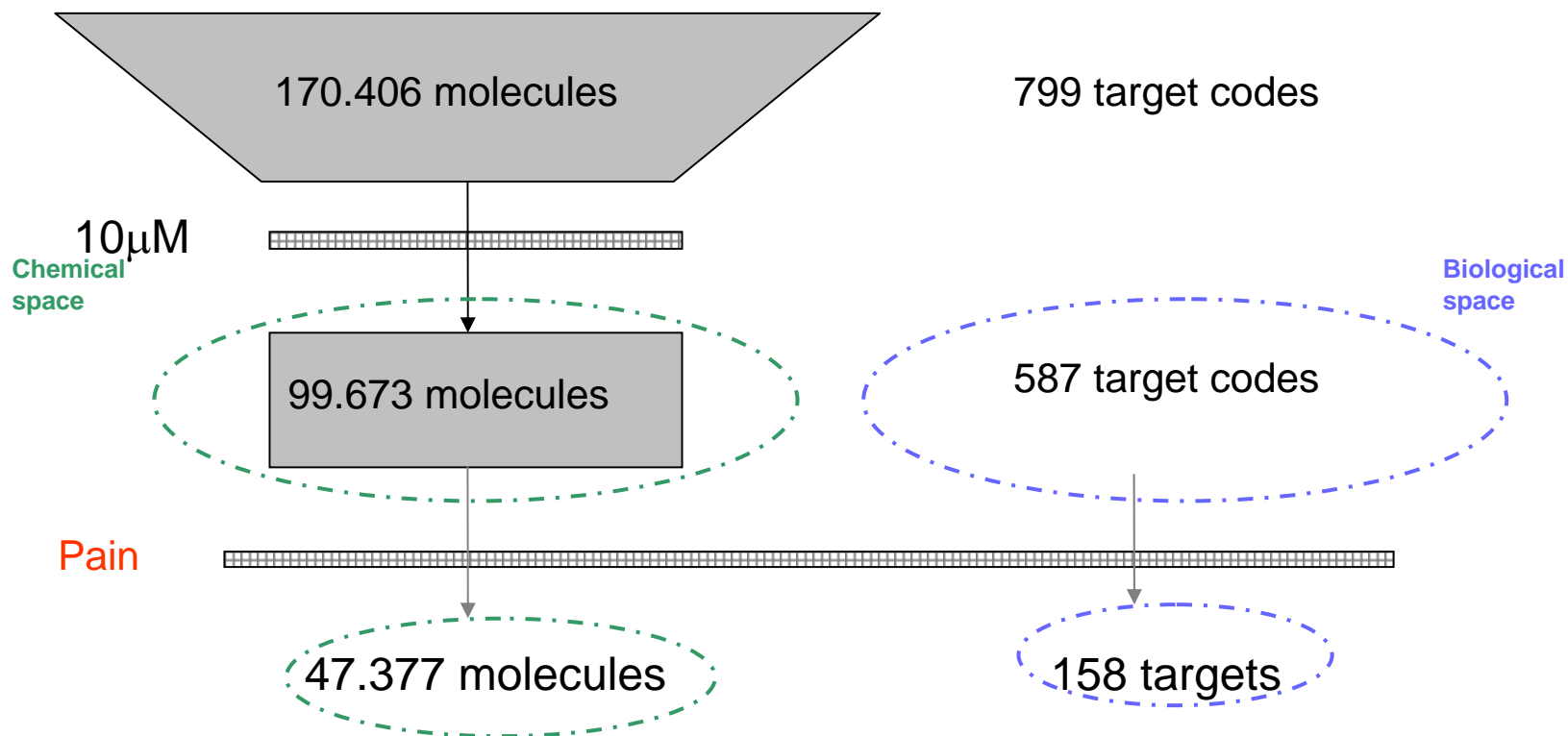
802 Publications

Target Space for Pain



Results and Discussion

Chemical Space for Pain

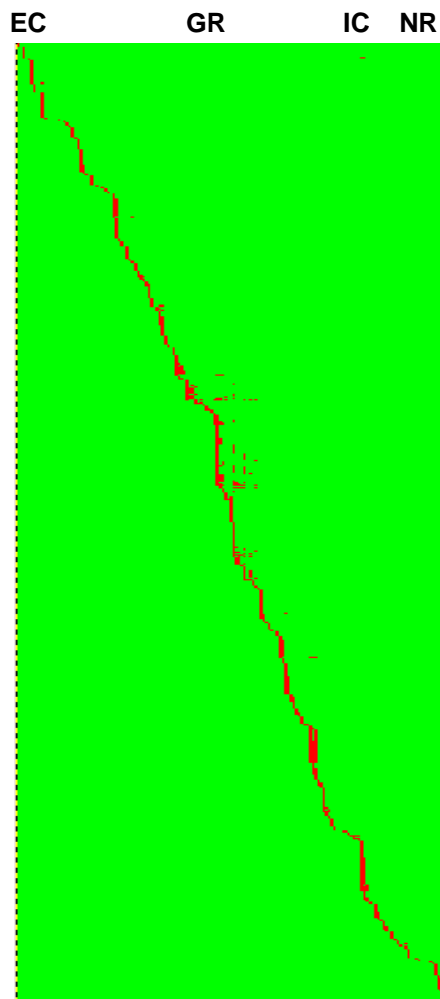


Results and Discussion

Protein family	N° Ligands
EC	15.469
GR	29.442
IC	730
NR	1.816

47.377 molecules

Computation requirements
≈ 3 Gb mem



158 Targets



185 Off-targets

Future Research Plan

- Fill the gaps of pharmacological matrices.**
- Construct structure database for pain targets and off-targets.**
- Identification of novel chemical entities for pain targets.**