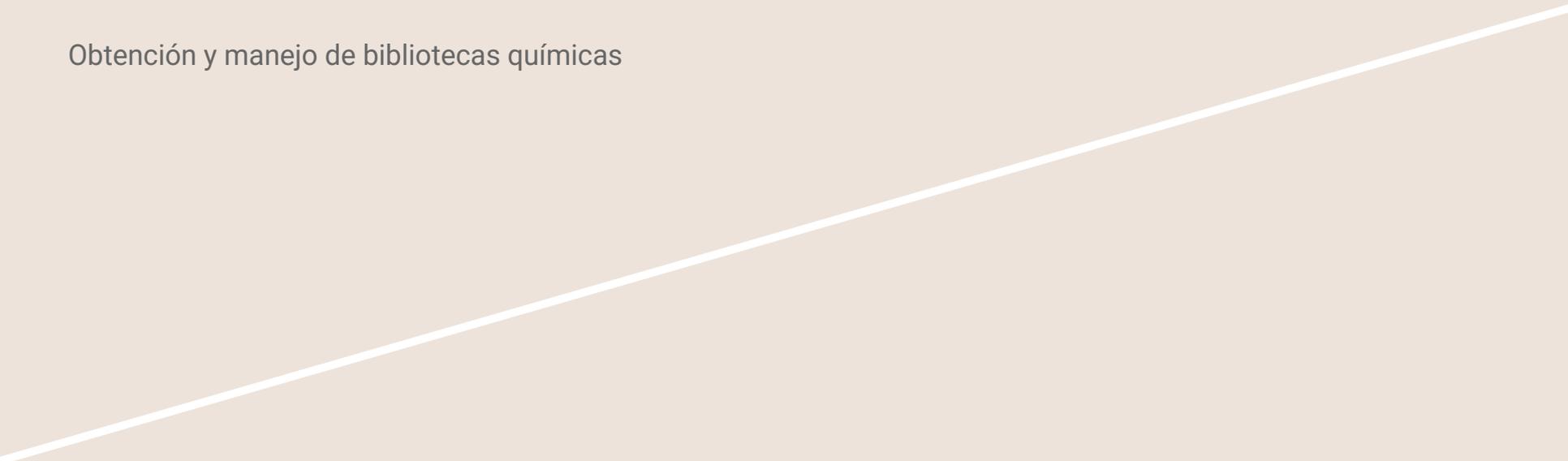


TP2

Obtención y manejo de bibliotecas químicas



Objetivos

- 1) Obtener sets de datos de compuestos químicos
 - 2) Aprender a trabajar con tablas de compuestos
 - 3) Realizar limpieza y normalización de datos químicos
- 

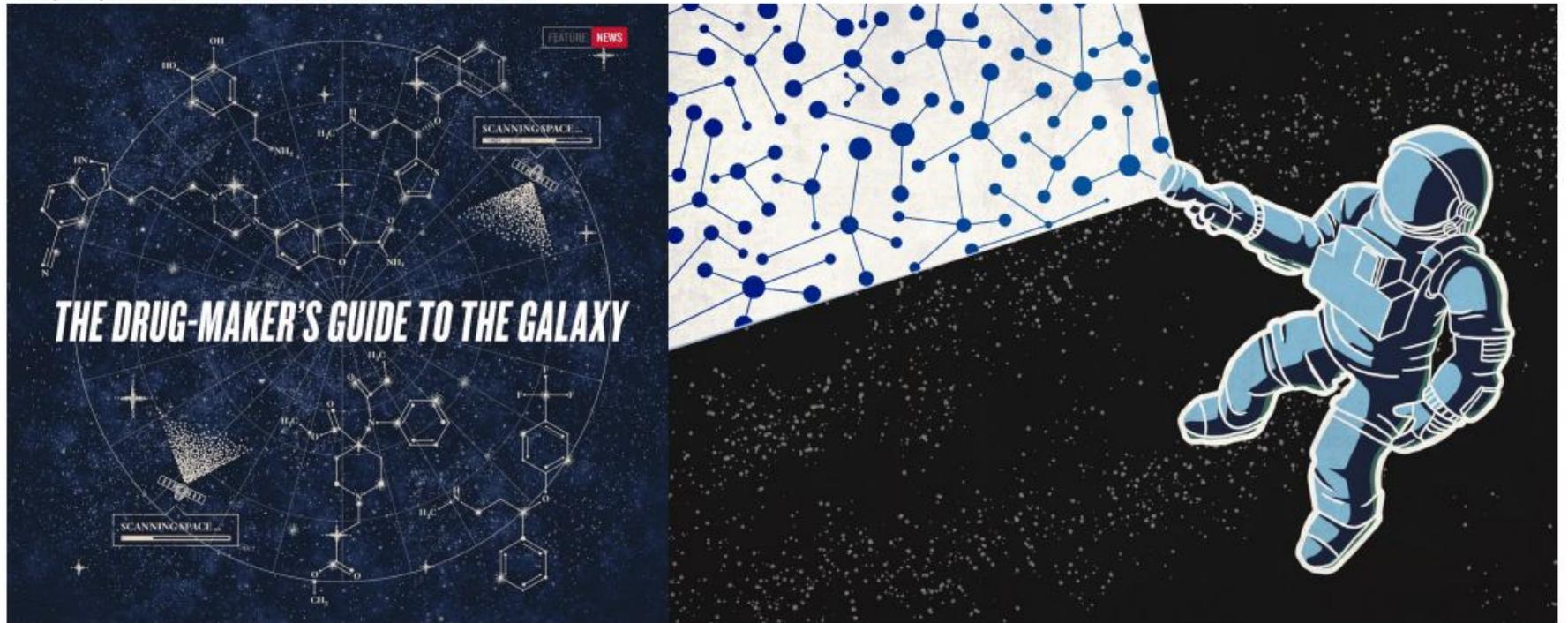
Organización de la clase

9:00 a 9:30	Introducción al TP
9:30 a 10:30	Trabajo en la guía de ejercicios (Parte 1: Obtención de datos)
10:30 a 11:00	Recreo
11:00 a 12:00	Trabajo en la guía de ejercicios (Parte 2: Análisis de conjuntos de datos)
12:00 a 13:00	Lectura de paper y puesta en común

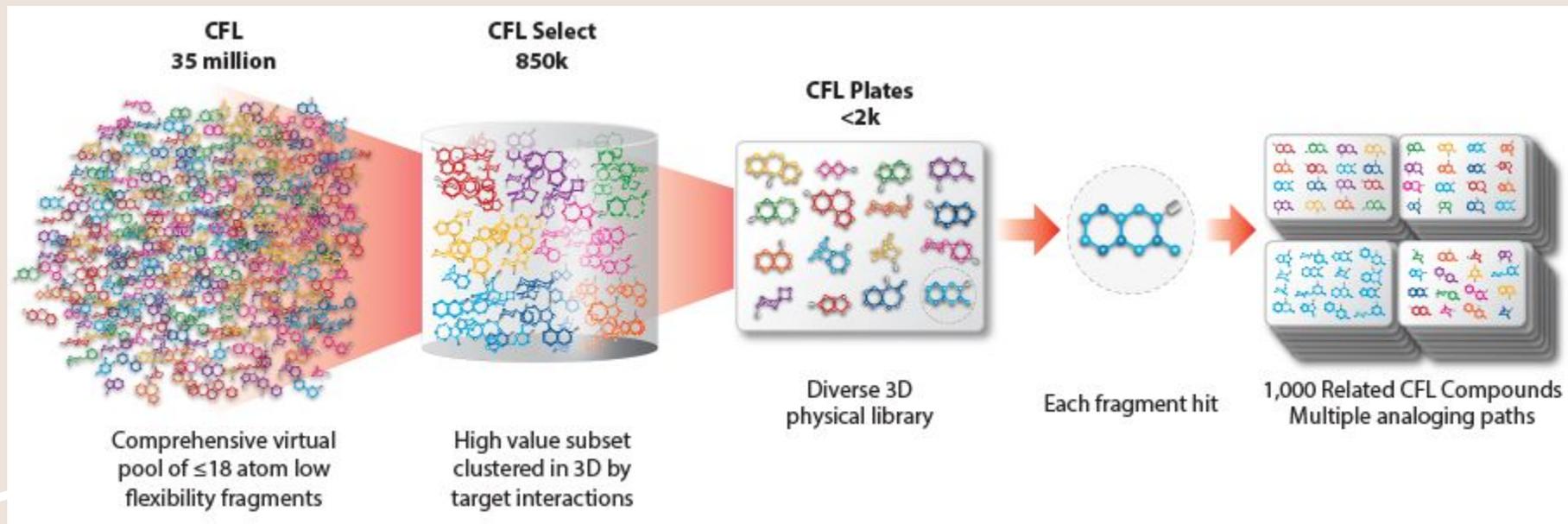
Espacio Químico

Mullard A. The drug-maker's guide to the galaxy. *Nature*. 2017
549(7673):445-447. doi: 10.1038/549445a. PMID: 28959982.

<https://extrapolations.com/what-is-chemical-space/>

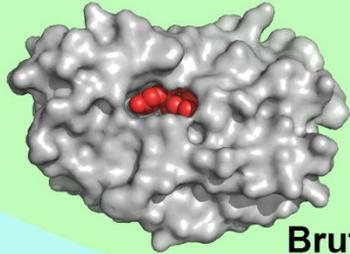


Espacio Químico

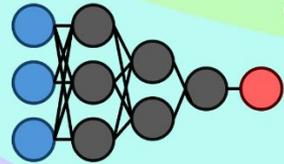


Construcción de librerías químicas

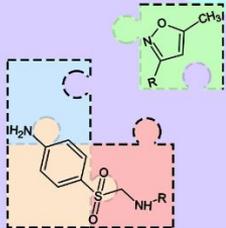
Billion-sized libraries



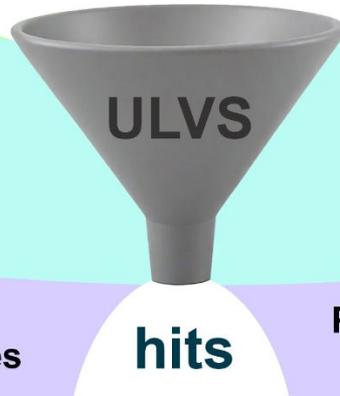
Brute-force docking



ML-based approaches

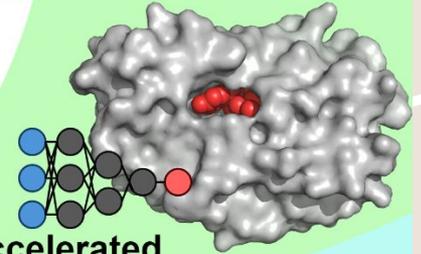


Reaction and building block-based approaches

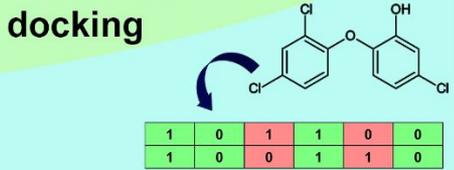


ULVS

hits

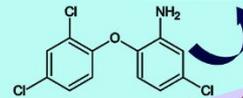


ML-accelerated docking

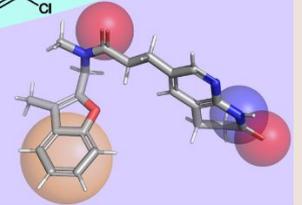


Similarity search

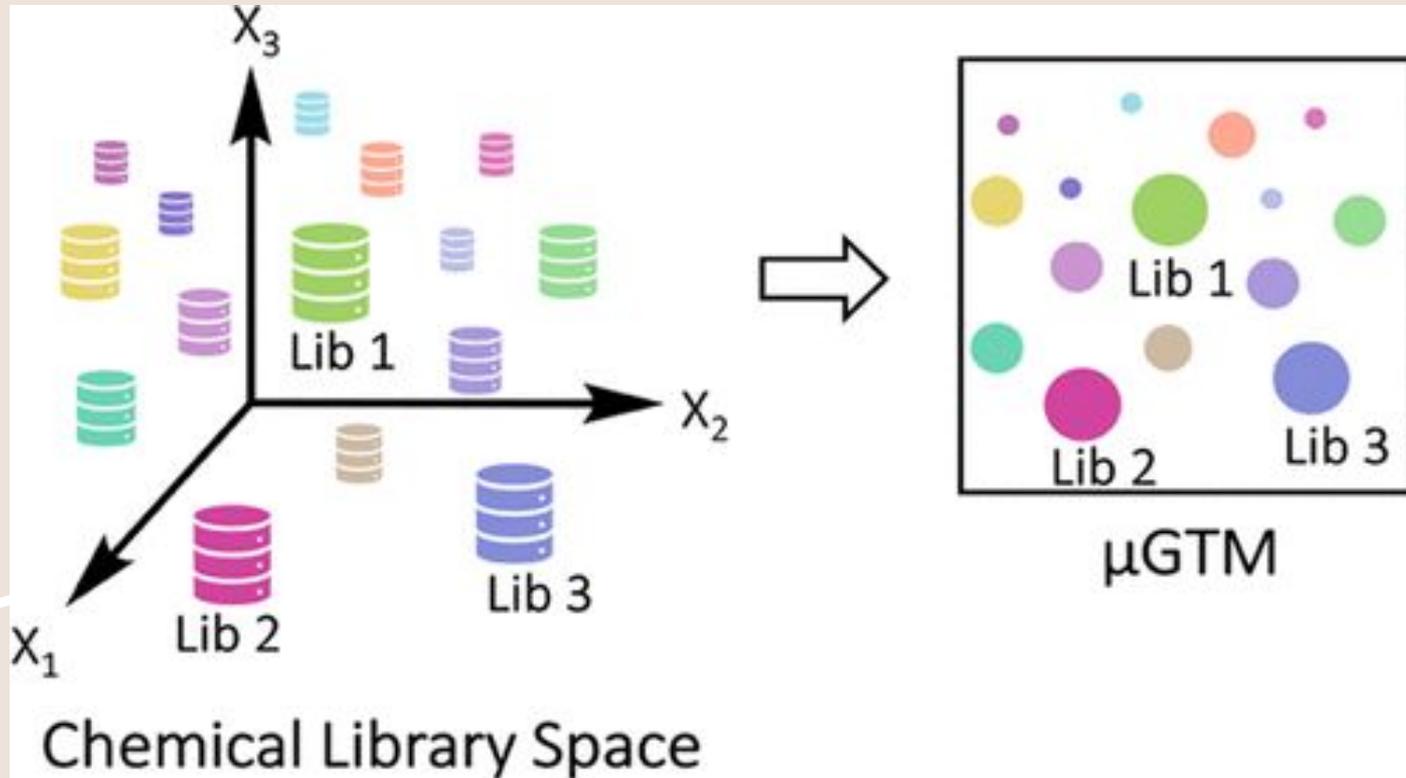
1	0	1	1	0	0
1	0	0	1	1	0



Pharmacophore search



Construcción de librerías químicas



Base de Datos

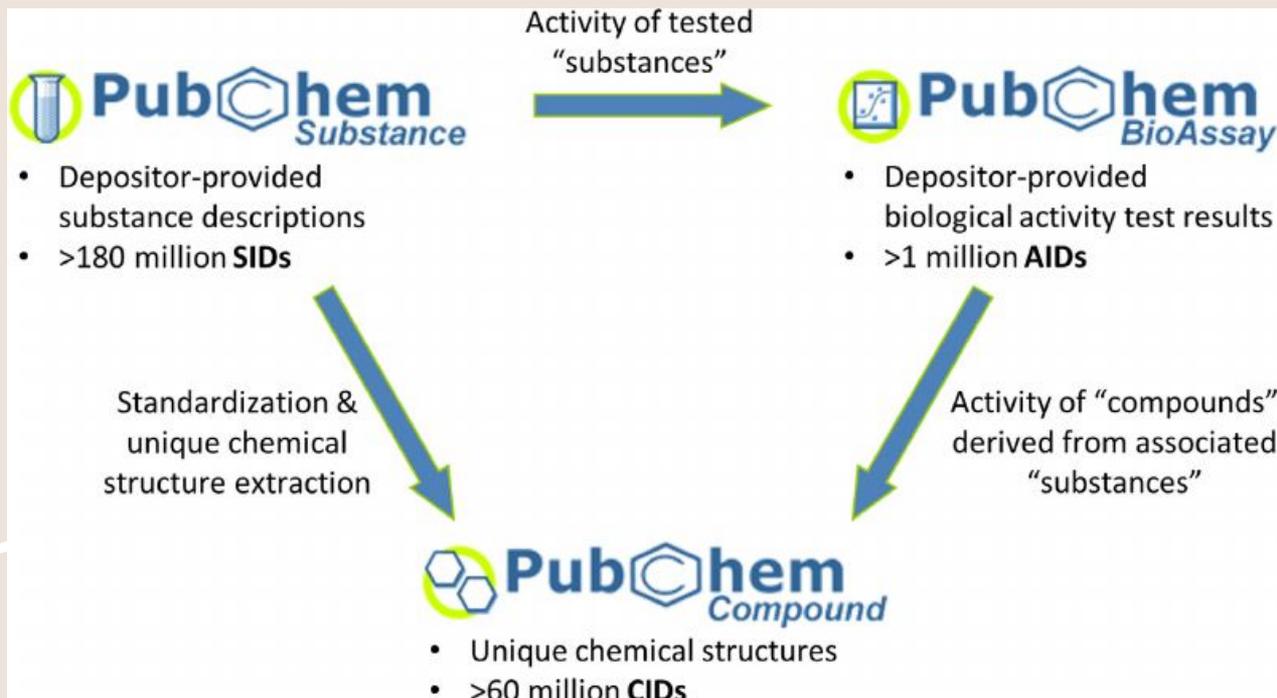
Pub  hem

Vs

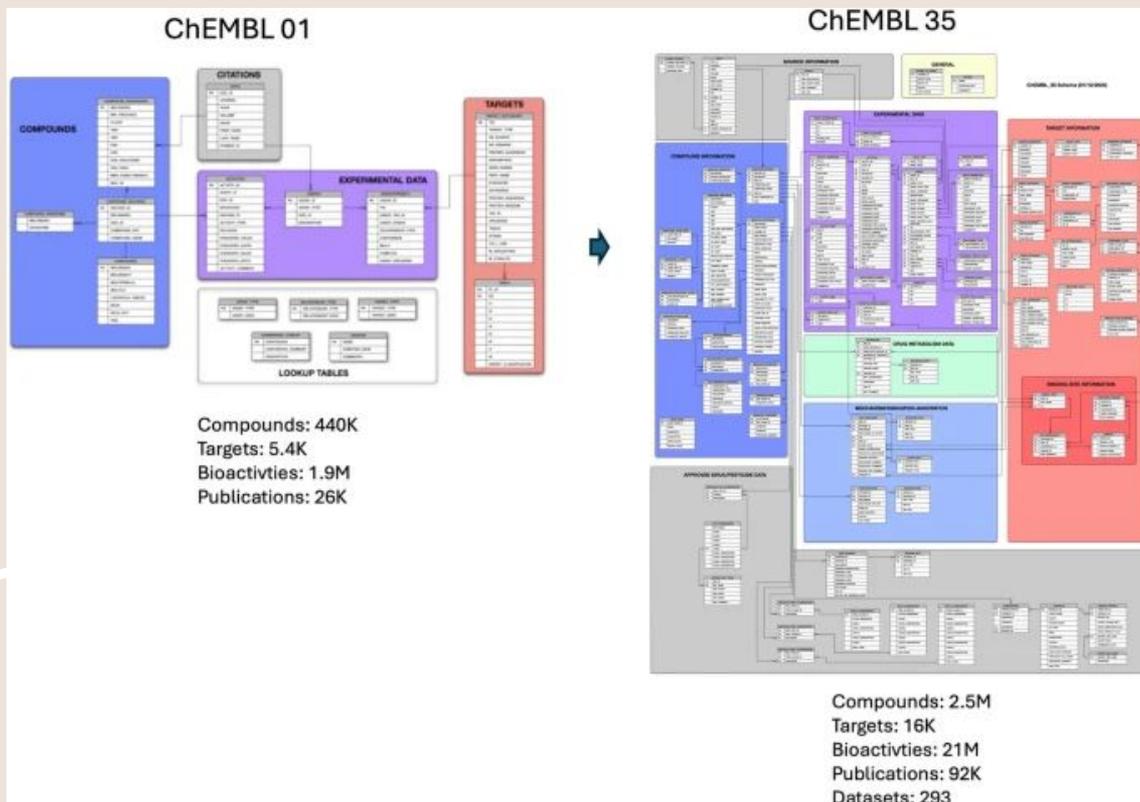
 ChEMBL

Base de Datos

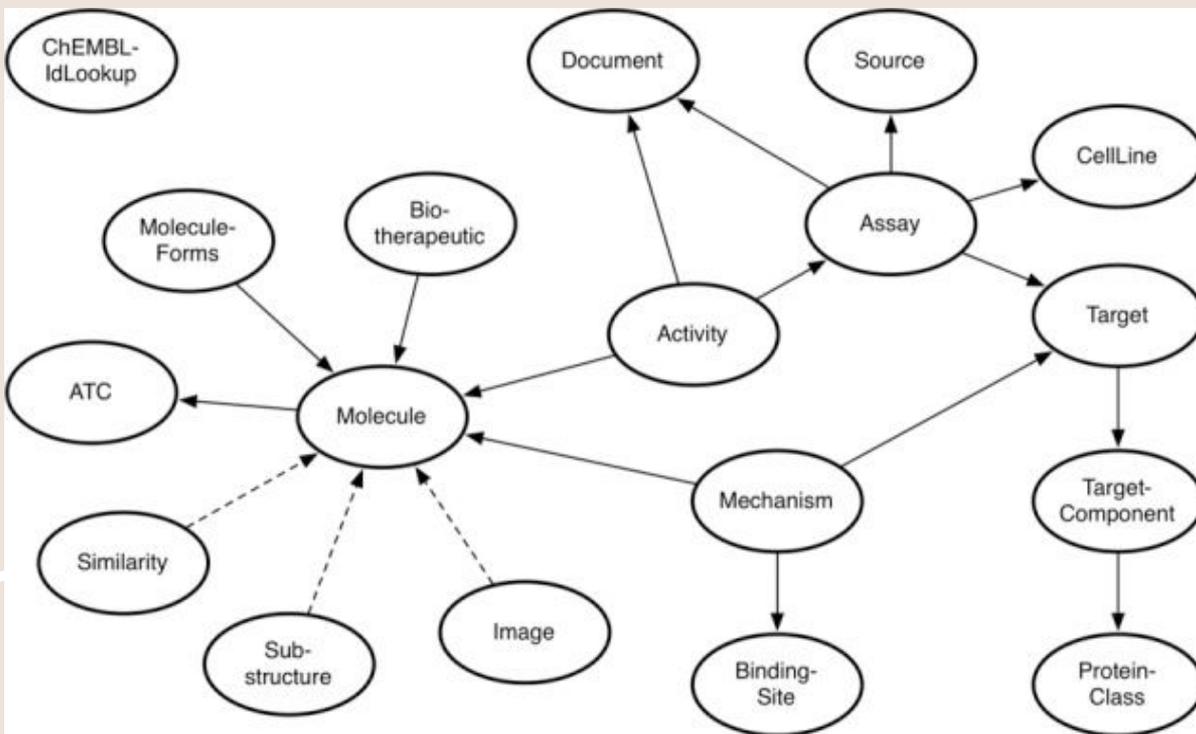
PubChem



Base de Datos



Base de Datos



<https://pmc.ncbi.nlm.nih.gov/articles/PMC4489243/>

Limpieza de datos!

Para todo trabajo bioinformático es fundamental el tratamiento de los datos para descartar valores nulos y repetidos.



Cierre



pubs.acs.org/acschemicalbiology

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Open Access



Article

Enhancing the Small-Scale Screenable Biological Space beyond Known Chemogenomics Libraries with Gray Chemical Matter—Compounds with Novel Mechanisms from High-Throughput Screening Profiles

Jason R. Thomas,^{*,∇} Claude Shelton, IV, Jason Murphy, Scott Brittain, Mark-Anthony Bray, Peter Aspesi, John Concannon, Frederick J. King, Robert J. Ihry, Daniel J. Ho, Martin Henault, Andrea Hadjikyriacou, Marilisa Neri, Frederic D. Sigoillot, Helen T. Pham, Matthew Shum, Louise Barys, Michael D. Jones, Eric J. Martin, Anke Blechschmidt, Sébastien Rieffel, Thomas J. Troxler, Felipa A. Mapa, Jeremy L. Jenkins, Rishi K. Jain, Peter S. Kutchukian, Markus Schirle, and Steffen Renner^{*,∇}



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<https://pubs.acs.org/doi/10.1021/acschembio.3c00737?ref=PDF>

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Novartis / GreyChemicalMatter

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GreyChemicalMatter Public

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main 1 Branch 0 Tags

Go to file Add file Code

Renner, Steffen refined README 4276375 · 2 years ago 3 Commits

create_gcm	initial commit	2 years ago
gcm_tables	initial commit	2 years ago
.gitignore	Initial commit	2 years ago
LICENSE	Initial commit	2 years ago
README.md	refined README	2 years ago

About

A pipeline to identify bioactive small molecules with likely novel modes of actions and dynamic SAR from historic cell-HTS profiles, with an example application and hitlist from PubChem data

- Readme
- MIT license
- Activity
- Custom properties

<https://github.com/Novartis/GreyChemicalMatter>

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