



Development of new molecular descriptors and their application to the virtual chemical screening and pharmacological profiling of large chemical libraries

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Objectives

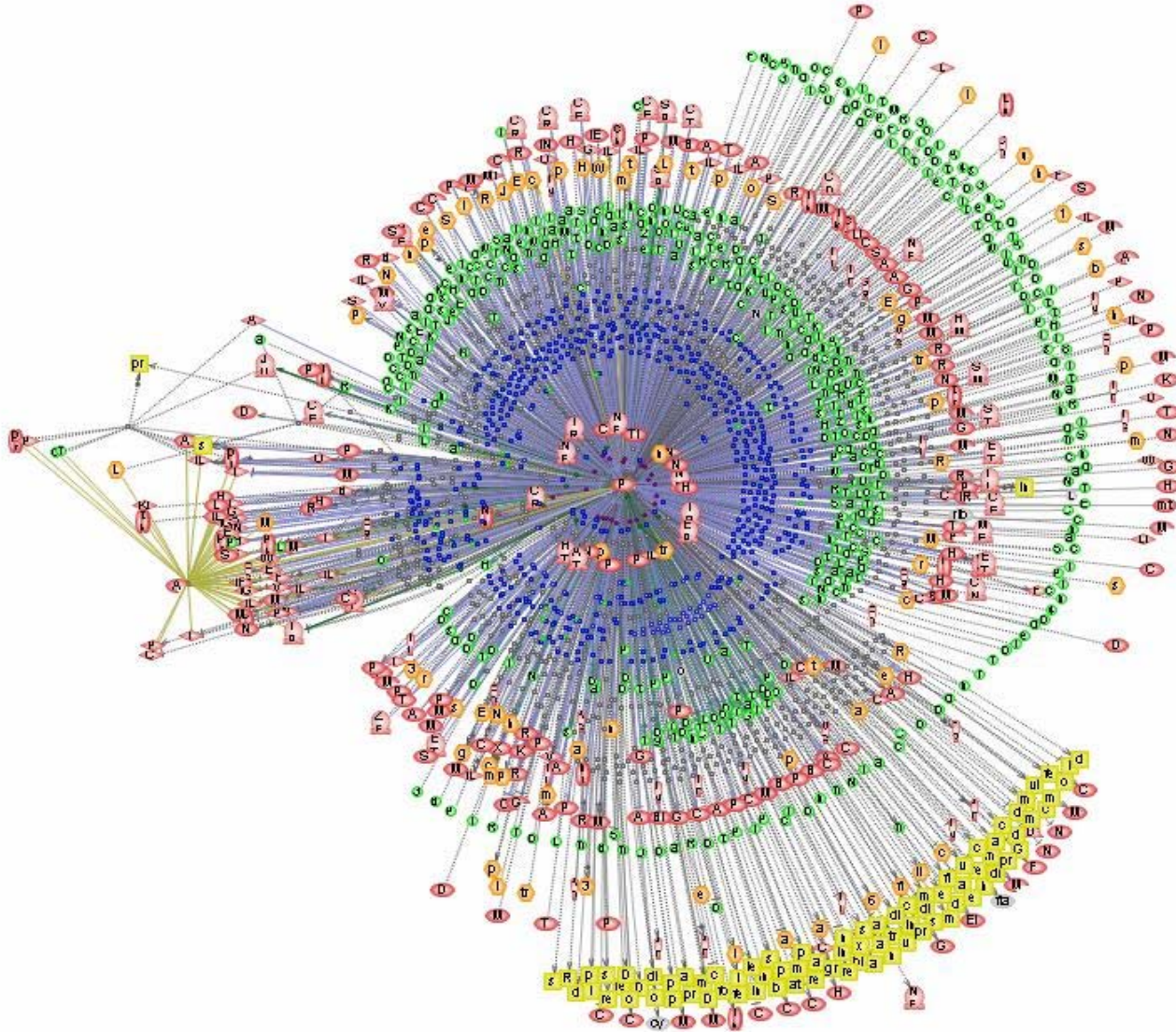
> *In silico* pharmacology

Predict likeliness of interaction between a small molecule and a given target

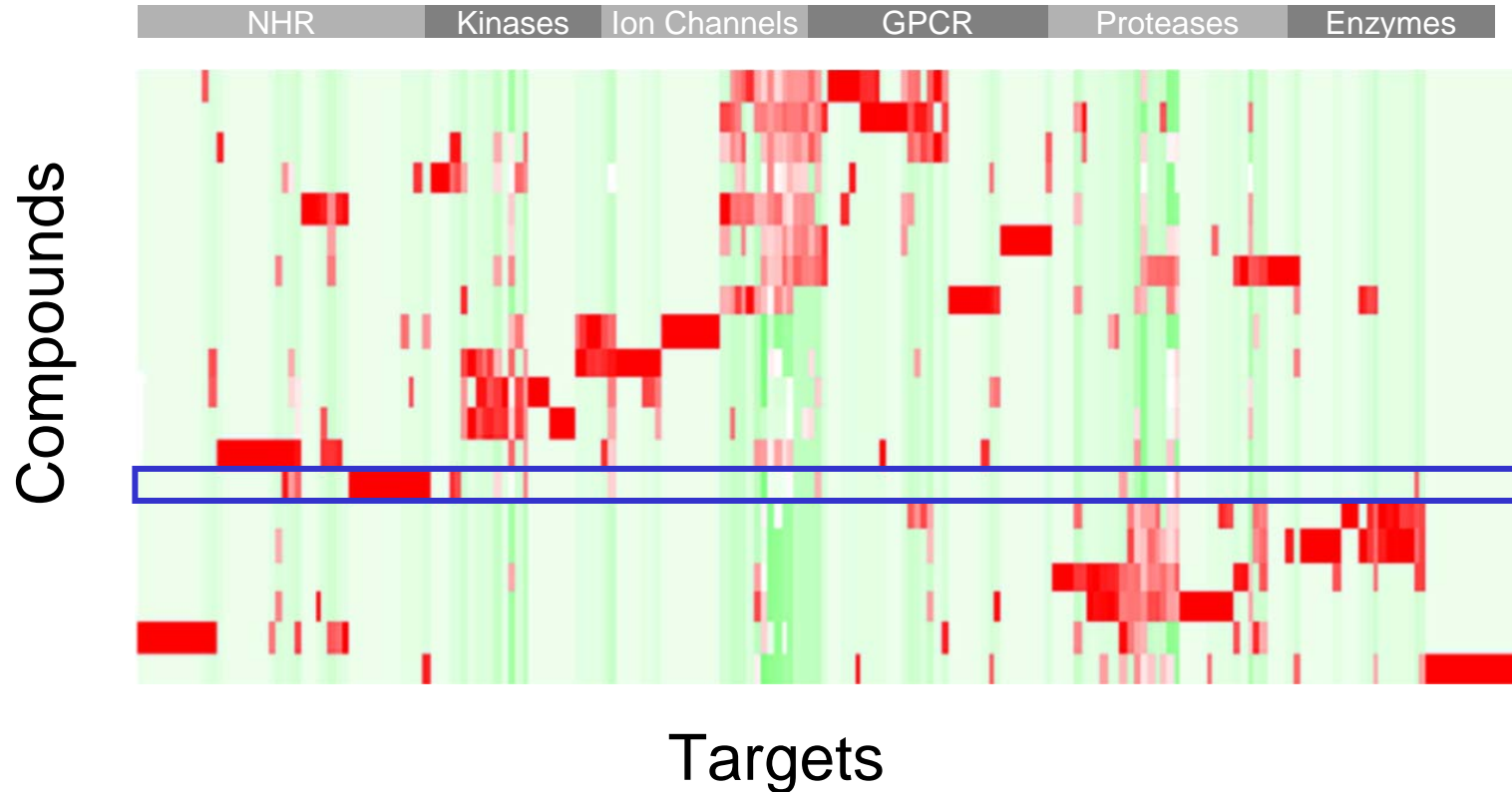
Introduction: Traditional Drug Discovery

Compound	IC50 COX-2 (nM)	IC50 COX-1 (nM)
CN000001	30	500
CN000002	500	1000
CN000003	450	3000
CN000004	2	6000
CN000005	1	4700
CN000006	60	120
CN000007	1000	300
CN000008	30	4400
CN000009	26	2200
CN000010	50	300
CN000011	40	460
CN000012	30	20
CN000013	1200	100
CN000014	380	4470
CN000015	400	370
CN000016	36	1680
CN000017	22	462
CN000018	10	470
CN000019	1	250
CN000020	0,5	1300
CN000021	7	1500
CN000022	10	1600

Introduction: The Real World of the Target



Introduction: Necessary Drug Discovery



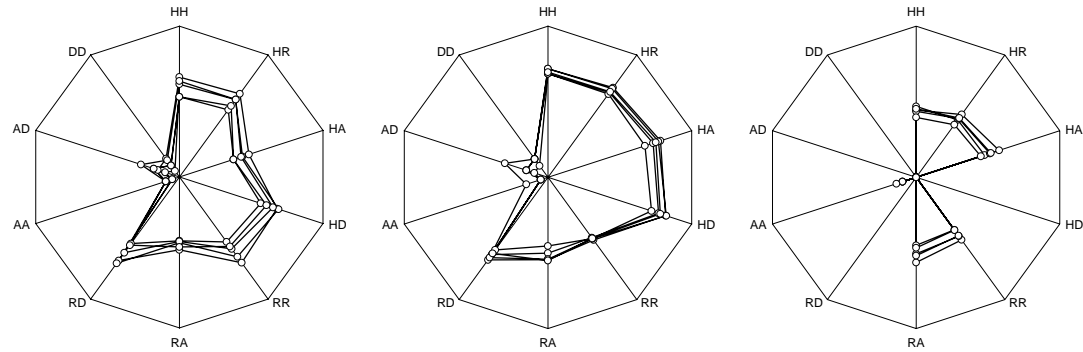
However... we cannot synthesise and test everything

Methods

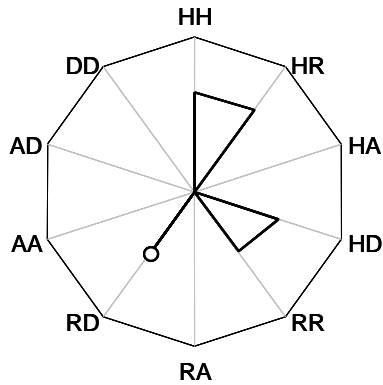
- > Develop a set of topological molecular descriptors
- > Use them to perform virtual screening and virtual profiling

Ligand-based Approach to Chemogenomic Profiling

Targets (Ligand-based Description)



Molecules



-
-
-

1.7

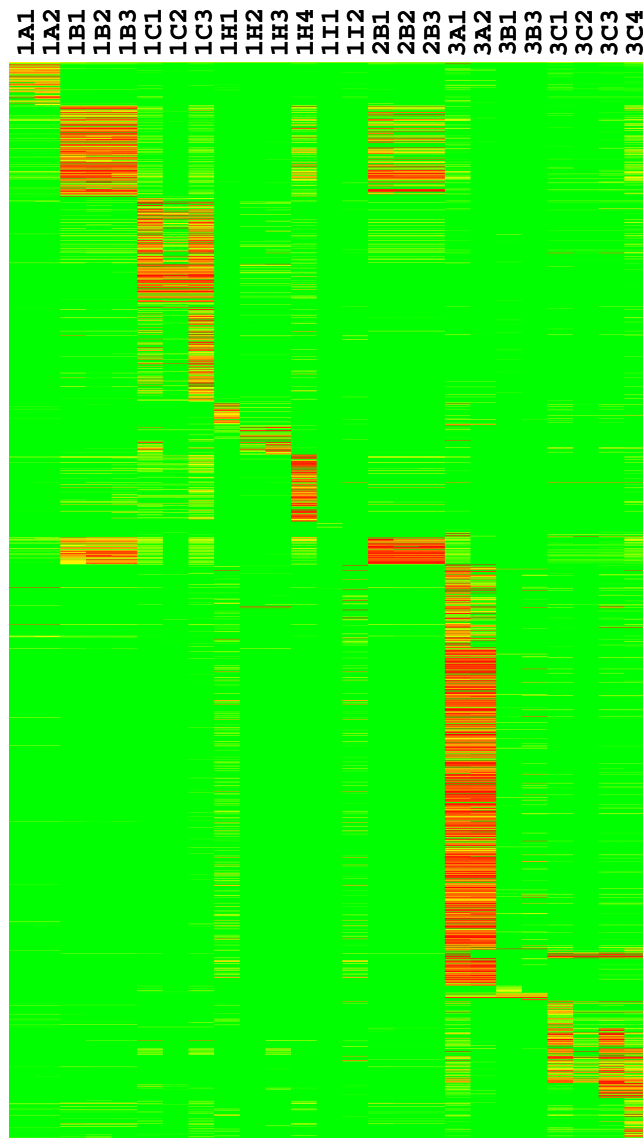
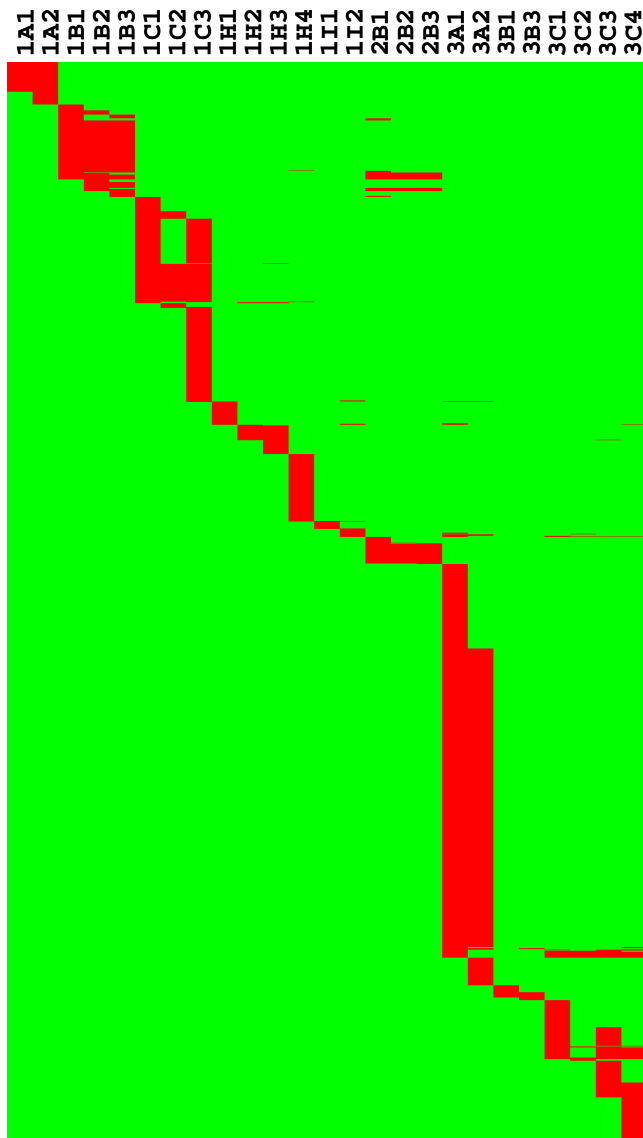
2.6

1.2

Minimum SHED Euclidean Distance
(closest annotated compound to molecule)

Ligand-based Profiling: Development

2033 annotated compounds





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