

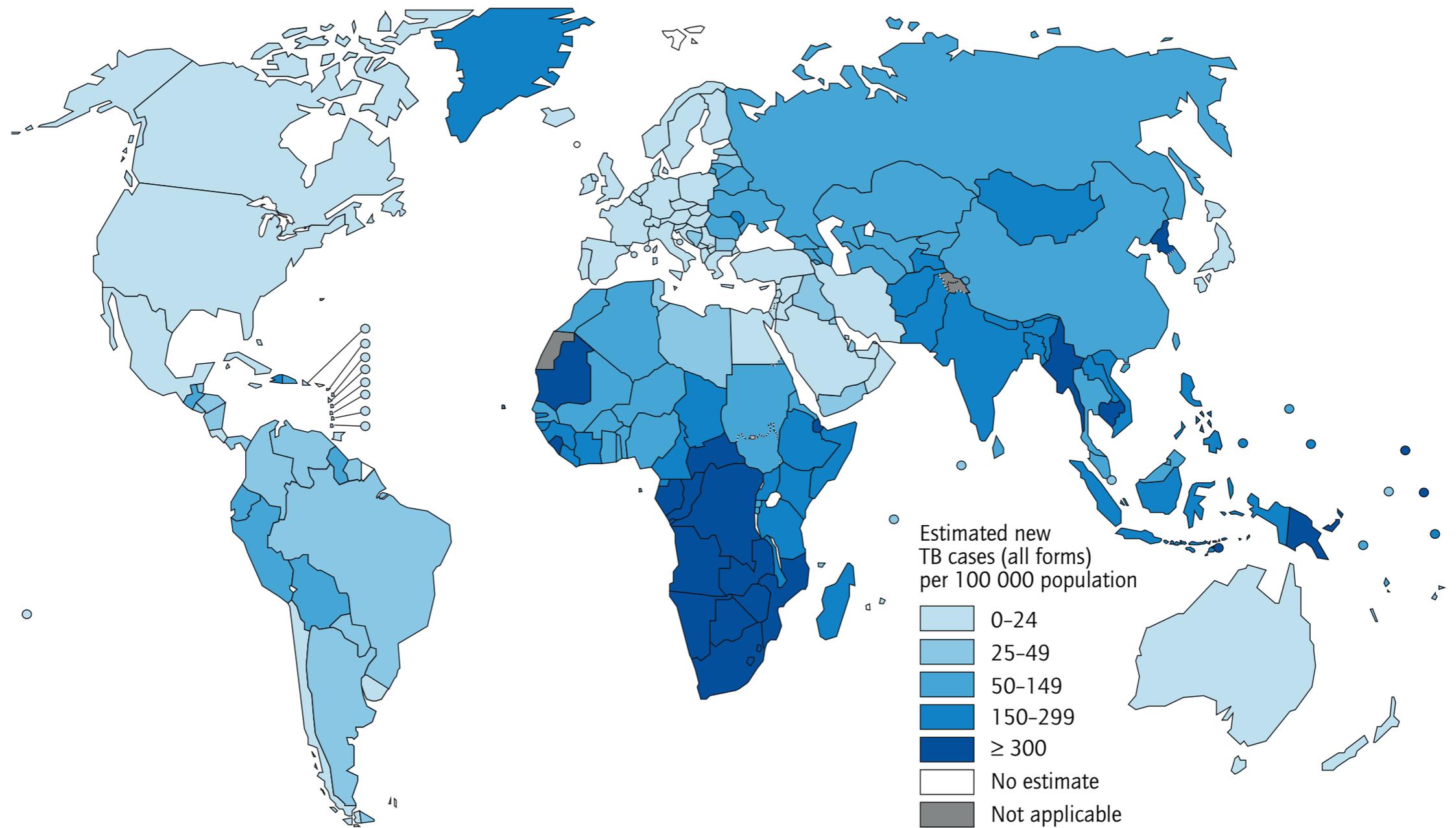
**Target Prediction for an Open
Access Set of Compounds
Active against
*Mycobacterium tuberculosis***

Francisco Martínez-Jiménez
XII Jornadas de Bioinformática, Sevilla

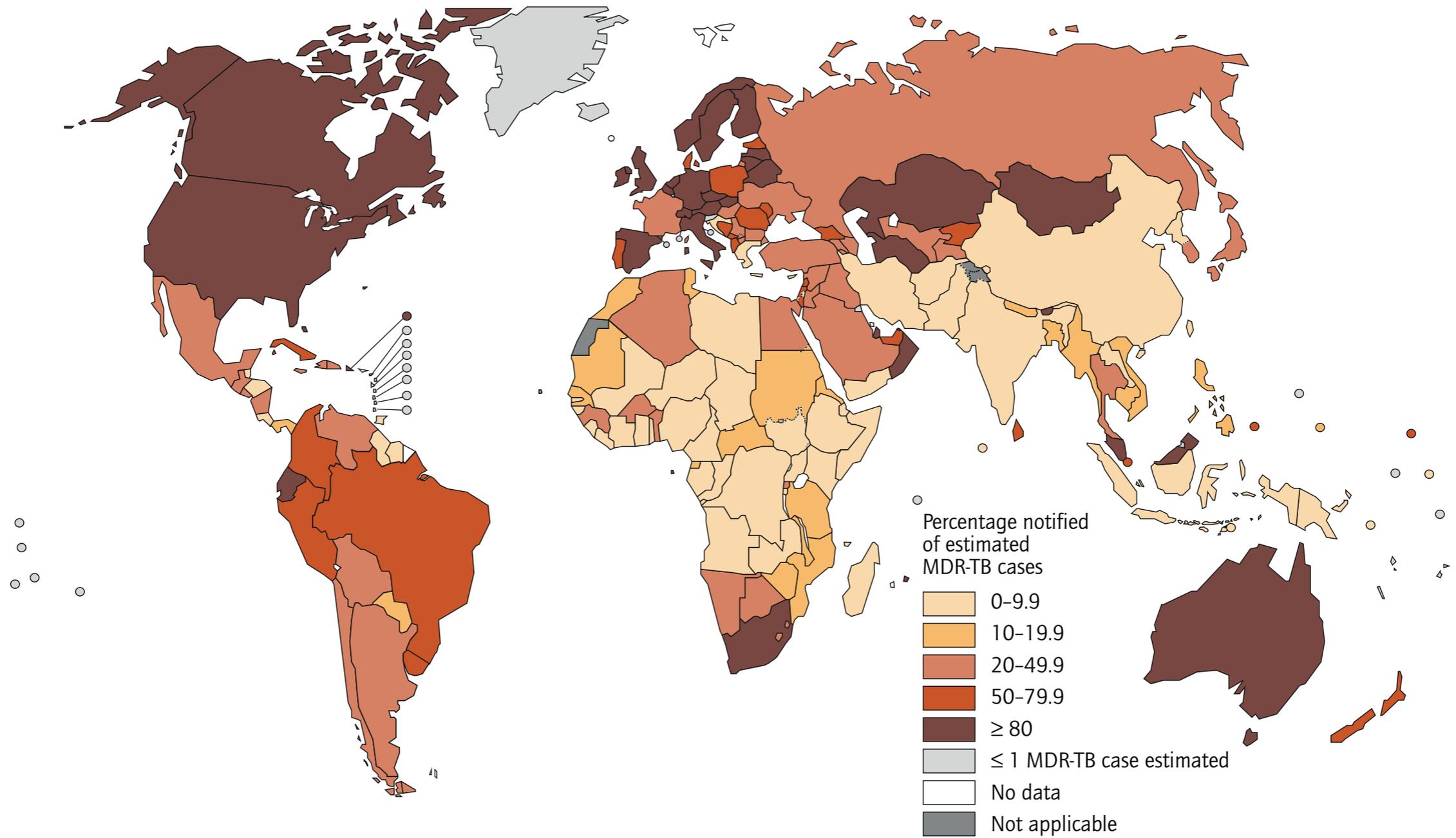
One third of the world's population is infected with Mycobacterium tuberculosis, the causative agent of tuberculosis.

WHOTuber2012. Global Tuberculosis Report 2012.

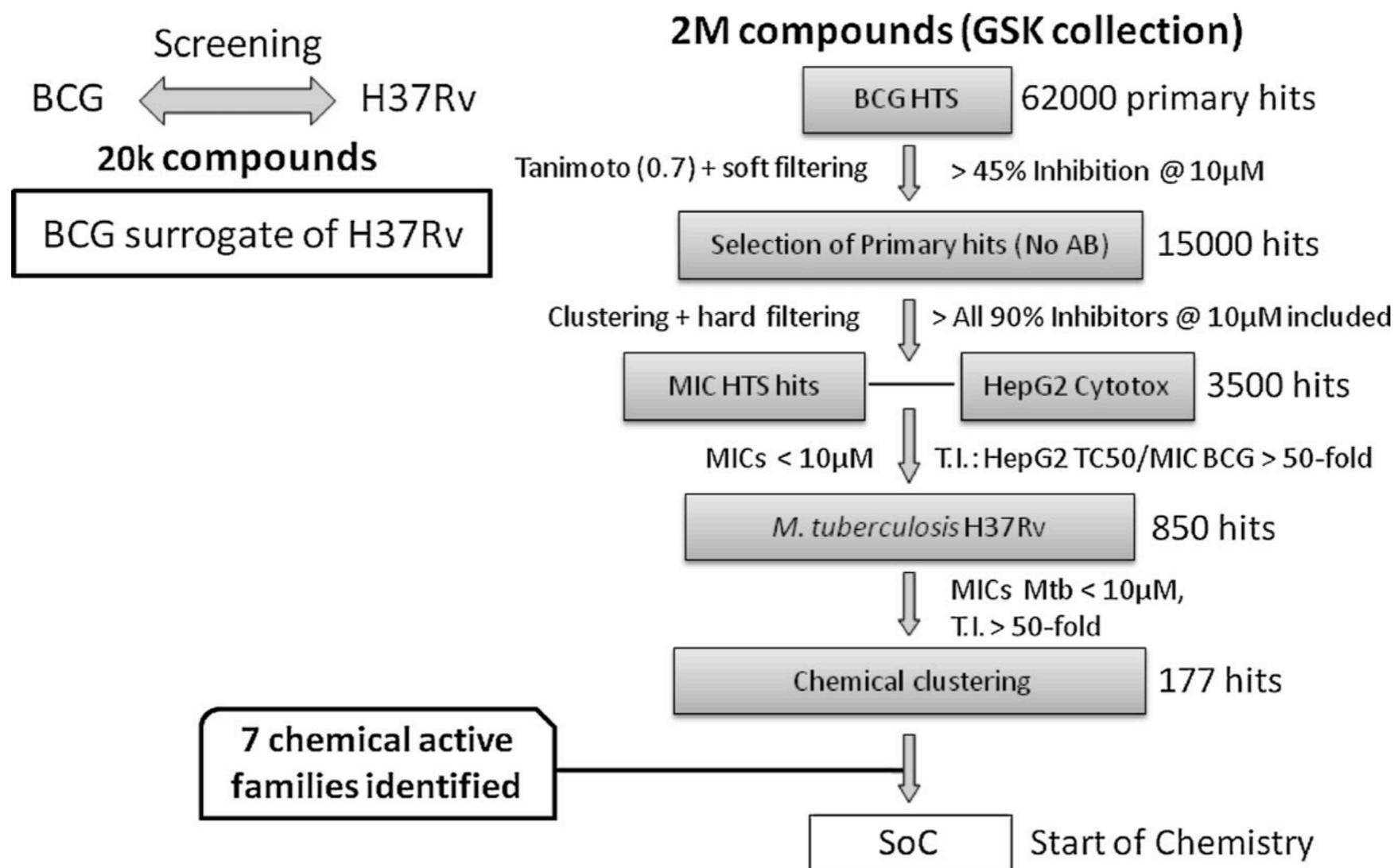
Tuberculosis incidence...



MultiDrugResistant-TB

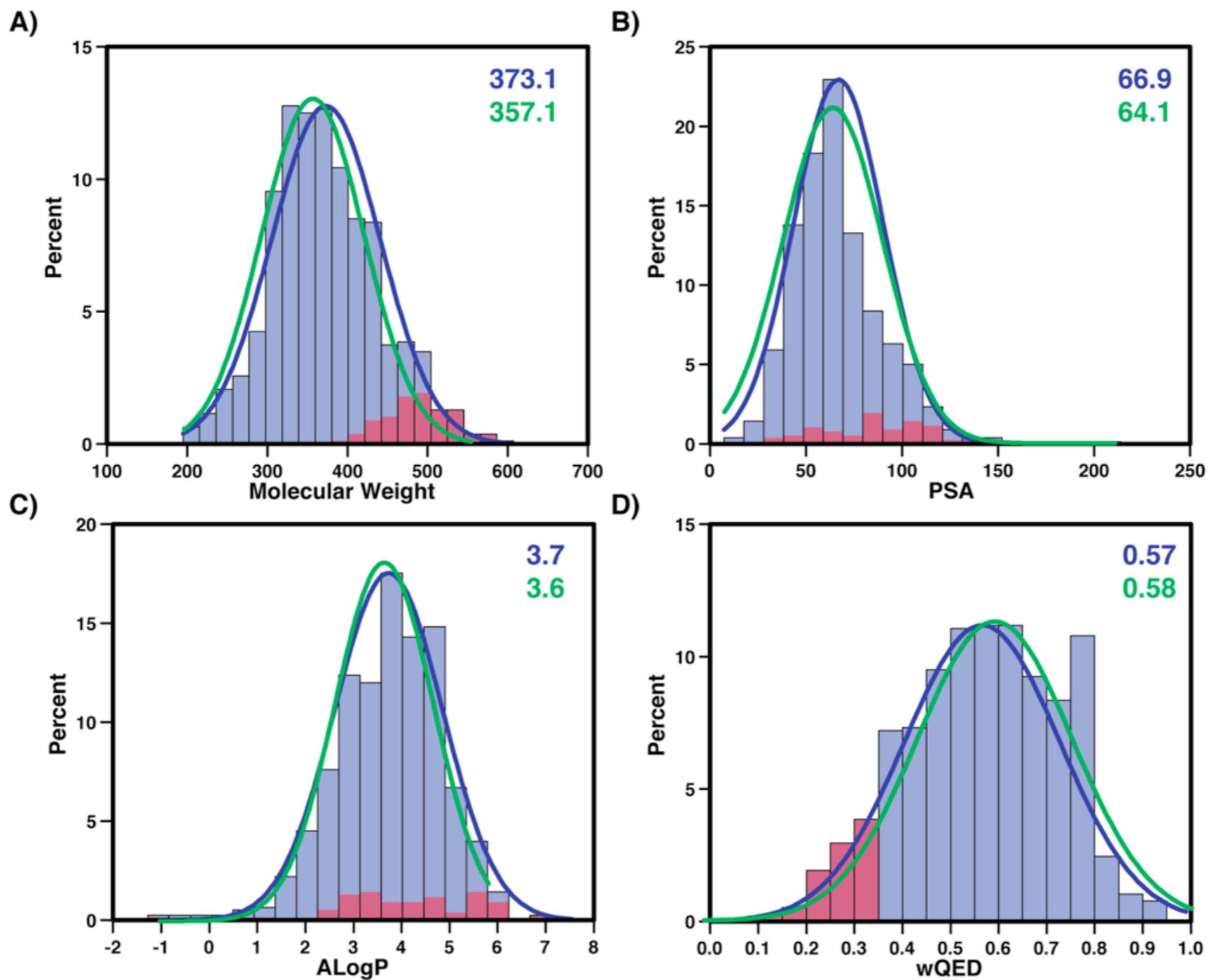


Phenotypic screening against *Mycobacterium tuberculosis*

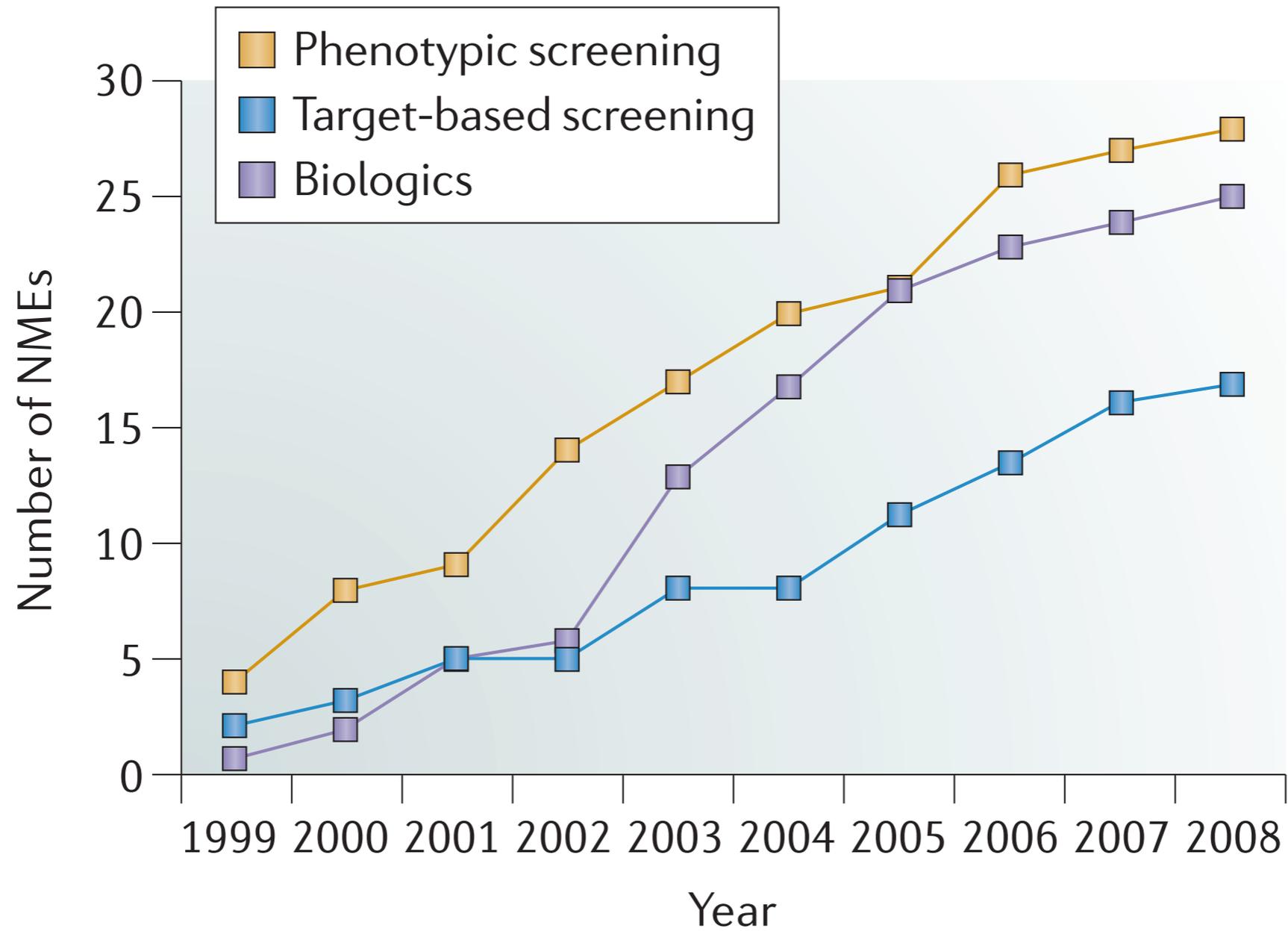


Ballell, L. et al (2013). Fueling open-source drug discovery: 177 small-molecule leads against tuberculosis. *ChemMedChem*.

776 compounds chemical features

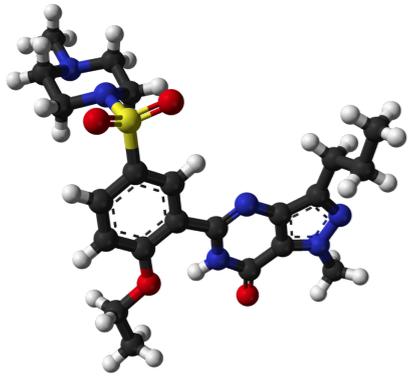


Phenotypic screenings



Swinney, D.C. & Anthony, J. How were new medicines discovered? *Nat. Rev. Drug Discov*

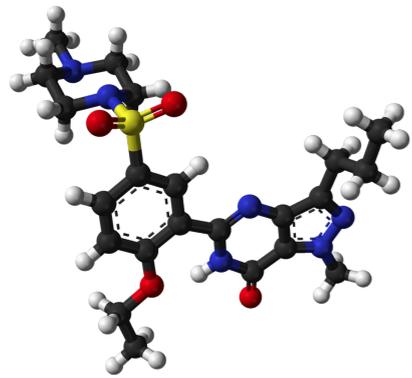
Finding out the mode of action...



Phenotype

Finding out the mode of action...

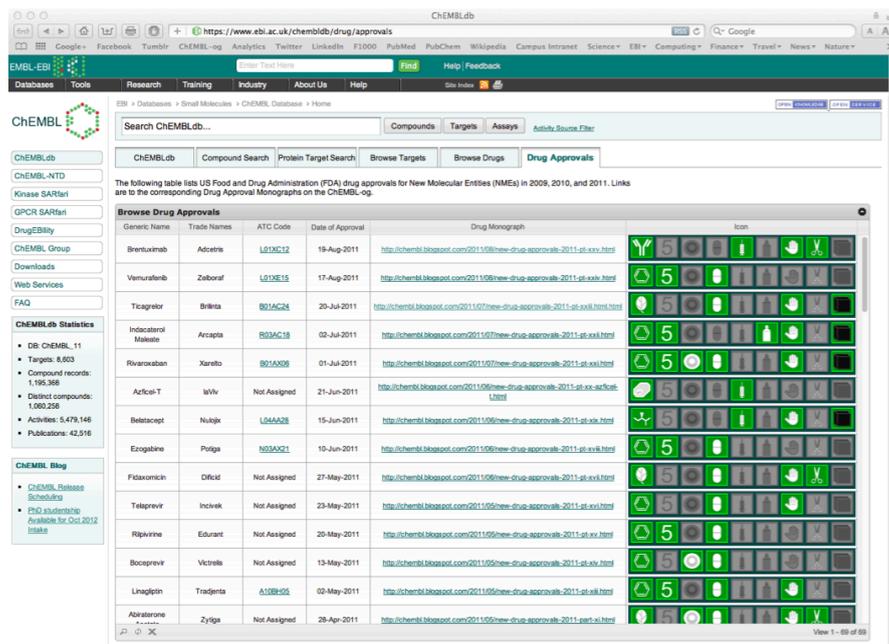
?



Phenotype

Methods

2D-Chemogenomics Approach



The screenshot shows the ChEMBL website interface. At the top, there is a search bar and navigation tabs for 'Compounds', 'Targets', 'Assays', and 'Drug Approvals'. Below the search bar, a table titled 'Browse Drug Approvals' is displayed. The table has columns for 'Generic Name', 'Trade Names', 'ATC Code', 'Date of Approval', and 'Drug Monograph'. The table lists various drugs such as Brentuximab, Venurafenib, Ticagrelor, Indacaterol, Rivaroxaban, Aflibercept, Ezogabine, Fitaxomacin, Telaprevir, Ripivrinne, Boceprevir, Linagliptin, and Abiraterone.

| Generic Name | Trade Names | ATC Code | Date of Approval | Drug Monograph |
|---------------------|-------------|--------------|------------------|---|
| Brentuximab | Adcetris | L01XC12 | 19-Aug-2011 | http://chembl.blogspot.com/2011/08/new-drug-approvals-2011-pt-xxviii.html |
| Venurafenib | Zelboraf | L01XE15 | 17-Aug-2011 | http://chembl.blogspot.com/2011/08/new-drug-approvals-2011-pt-xxviii.html |
| Ticagrelor | Brilinta | B01AC26 | 20-Jul-2011 | http://chembl.blogspot.com/2011/07/new-drug-approvals-2011-pt-xxvii.html |
| Indacaterol Maleate | Arcapta | R03AC19 | 02-Jul-2011 | http://chembl.blogspot.com/2011/07/new-drug-approvals-2011-pt-xxvii.html |
| Rivaroxaban | Xarelto | B01AX09 | 01-Jul-2011 | http://chembl.blogspot.com/2011/07/new-drug-approvals-2011-pt-xxvii.html |
| Aflibercept | IVLu | Not Assigned | 21-Jun-2011 | http://chembl.blogspot.com/2011/06/new-drug-approvals-2011-pt-xxviii.html |
| Belatacept | Nuligx | L04AA08 | 15-Jun-2011 | http://chembl.blogspot.com/2011/06/new-drug-approvals-2011-pt-xxviii.html |
| Ezogabine | Profta | N03AX21 | 10-Jun-2011 | http://chembl.blogspot.com/2011/06/new-drug-approvals-2011-pt-xxviii.html |
| Fitaxomacin | Difival | Not Assigned | 27-May-2011 | http://chembl.blogspot.com/2011/05/new-drug-approvals-2011-pt-xxviii.html |
| Telaprevir | Incevik | Not Assigned | 23-May-2011 | http://chembl.blogspot.com/2011/05/new-drug-approvals-2011-pt-xxviii.html |
| Ripivrinne | Edurant | Not Assigned | 20-May-2011 | http://chembl.blogspot.com/2011/05/new-drug-approvals-2011-pt-xxviii.html |
| Boceprevir | Victrelis | Not Assigned | 13-May-2011 | http://chembl.blogspot.com/2011/05/new-drug-approvals-2011-pt-xxviii.html |
| Linagliptin | Tradjenta | A10BA05 | 02-May-2011 | http://chembl.blogspot.com/2011/05/new-drug-approvals-2011-pt-xxviii.html |
| Abiraterone | Zytiga | Not Assigned | 28-Apr-2011 | http://chembl.blogspot.com/2011/04/new-drug-approvals-2011-pt-xxviii.html |



George Papadatos

John P. Overington

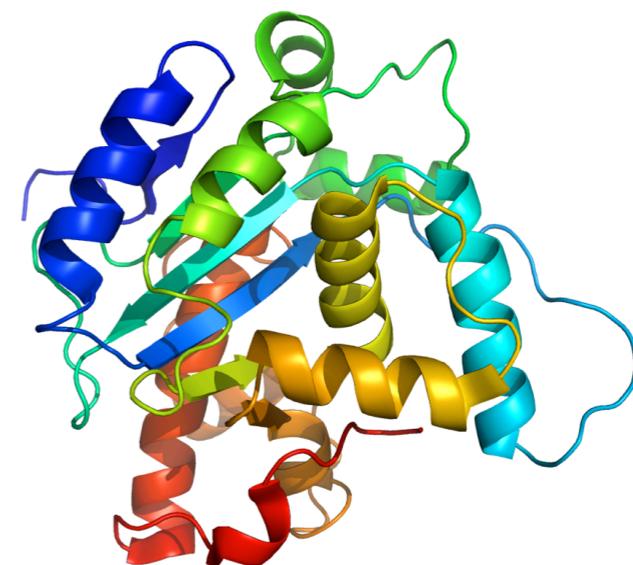
Historical Approach



Vinod Kumar

James Brown

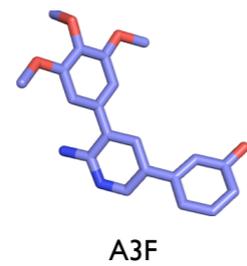
3D-Structural Approach



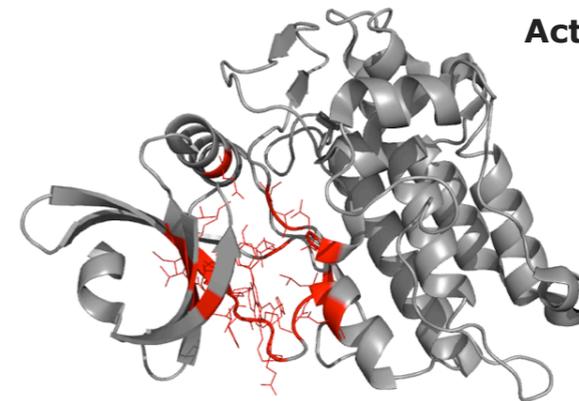
Francisco Martínez-Jiménez

Marc A. Martí-Renom

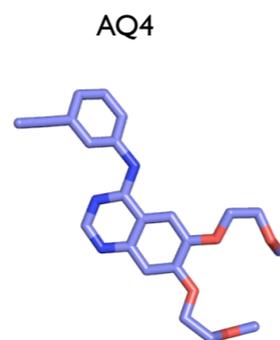
Similar binding-sites tend to bind similar ligands



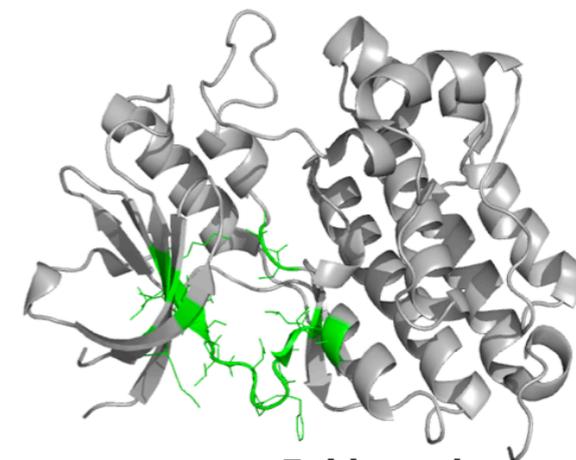
co-crystallized



Similar binding-sites

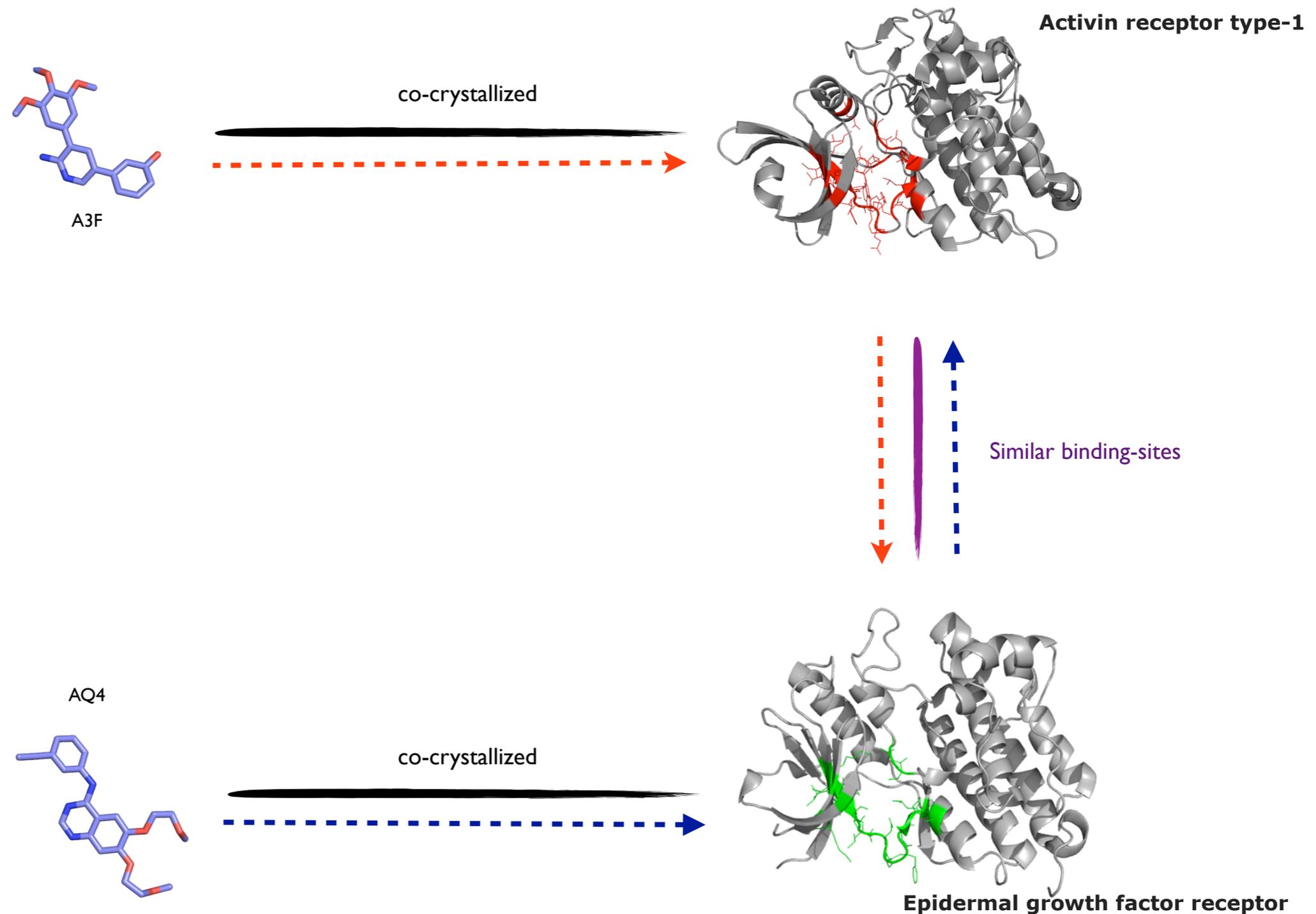


co-crystallized

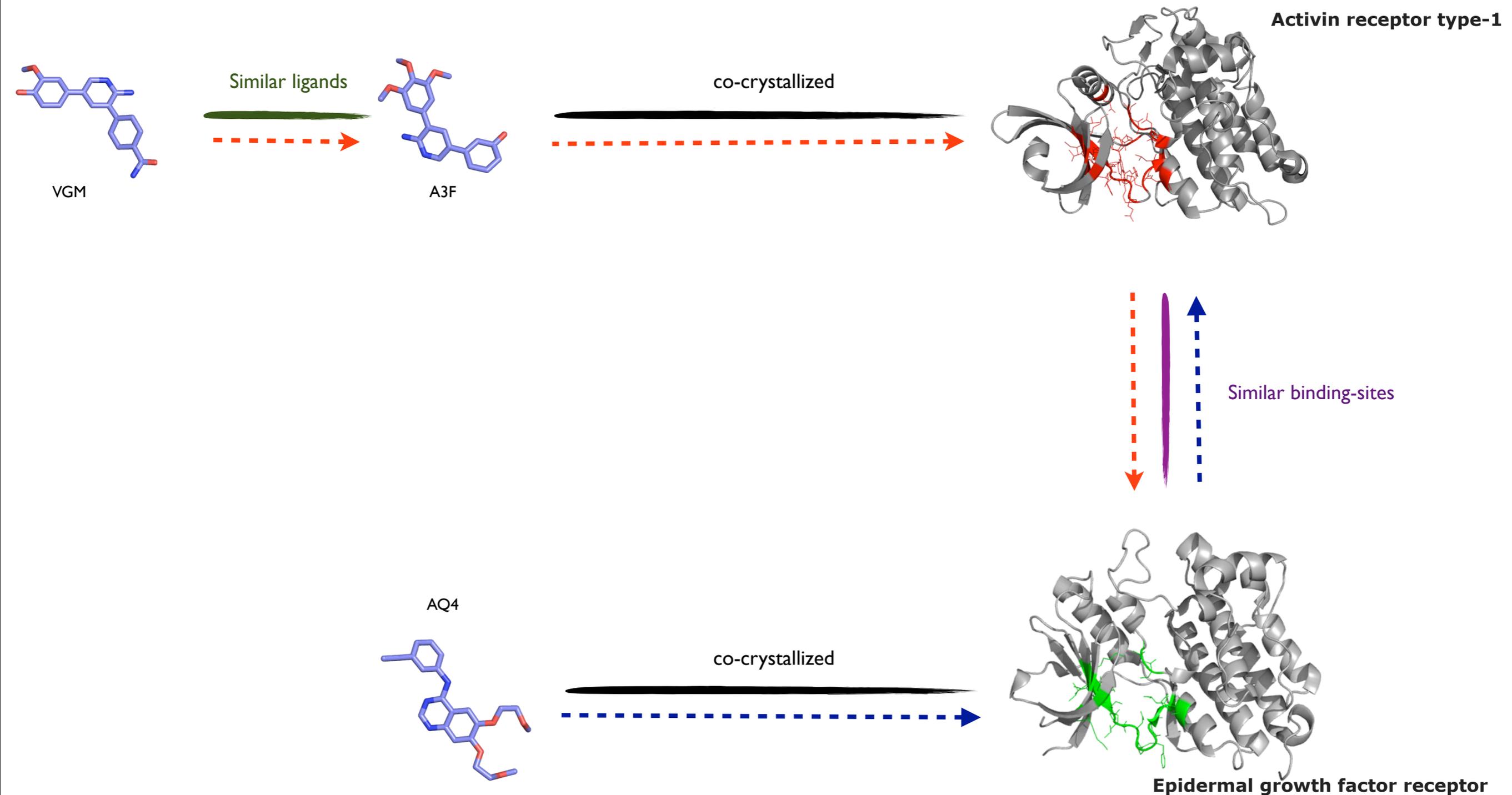


Epidermal growth factor receptor

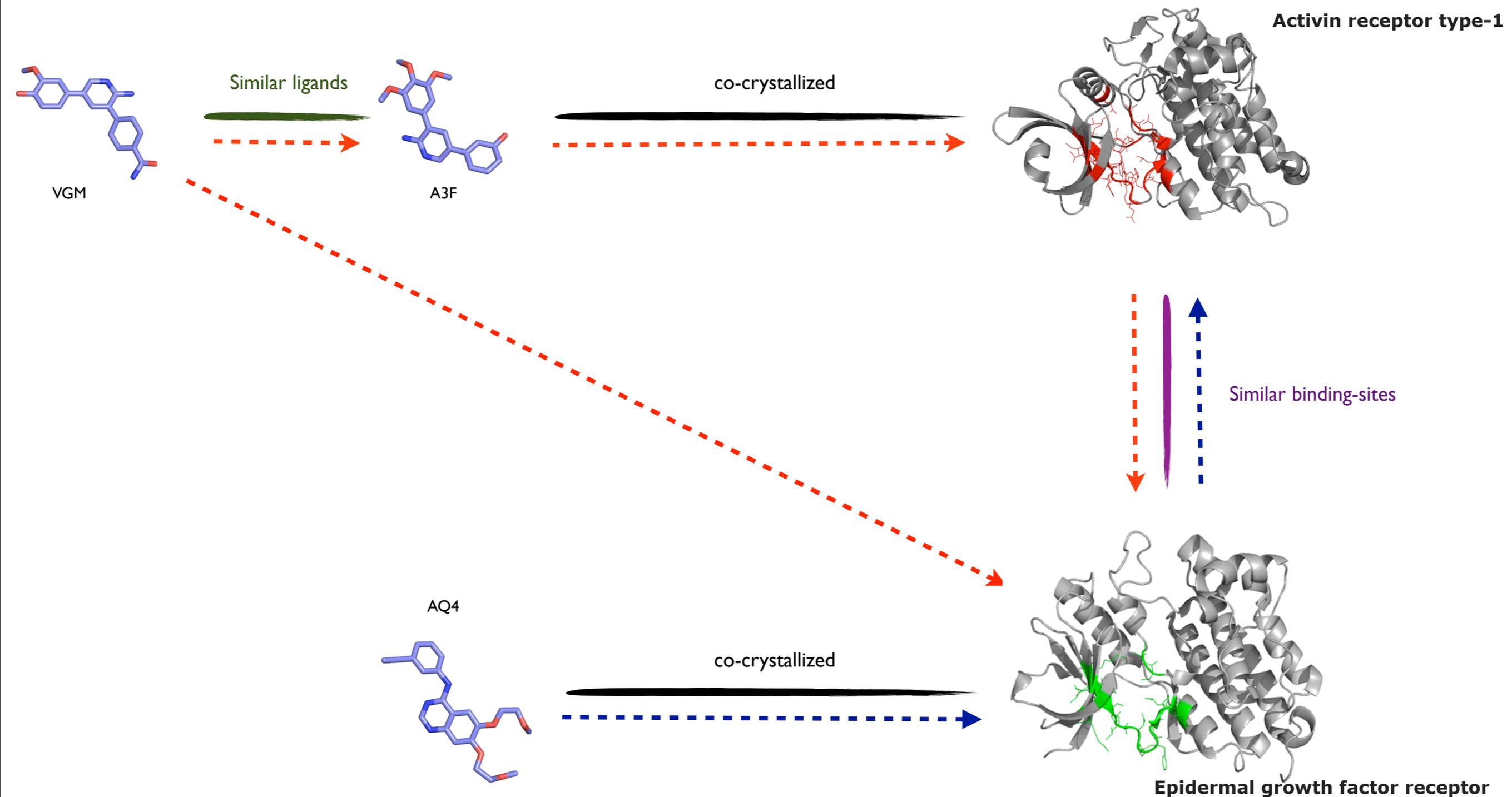
Similar binding-sites tend to bind similar ligands



Similar binding-sites tend to bind similar ligands

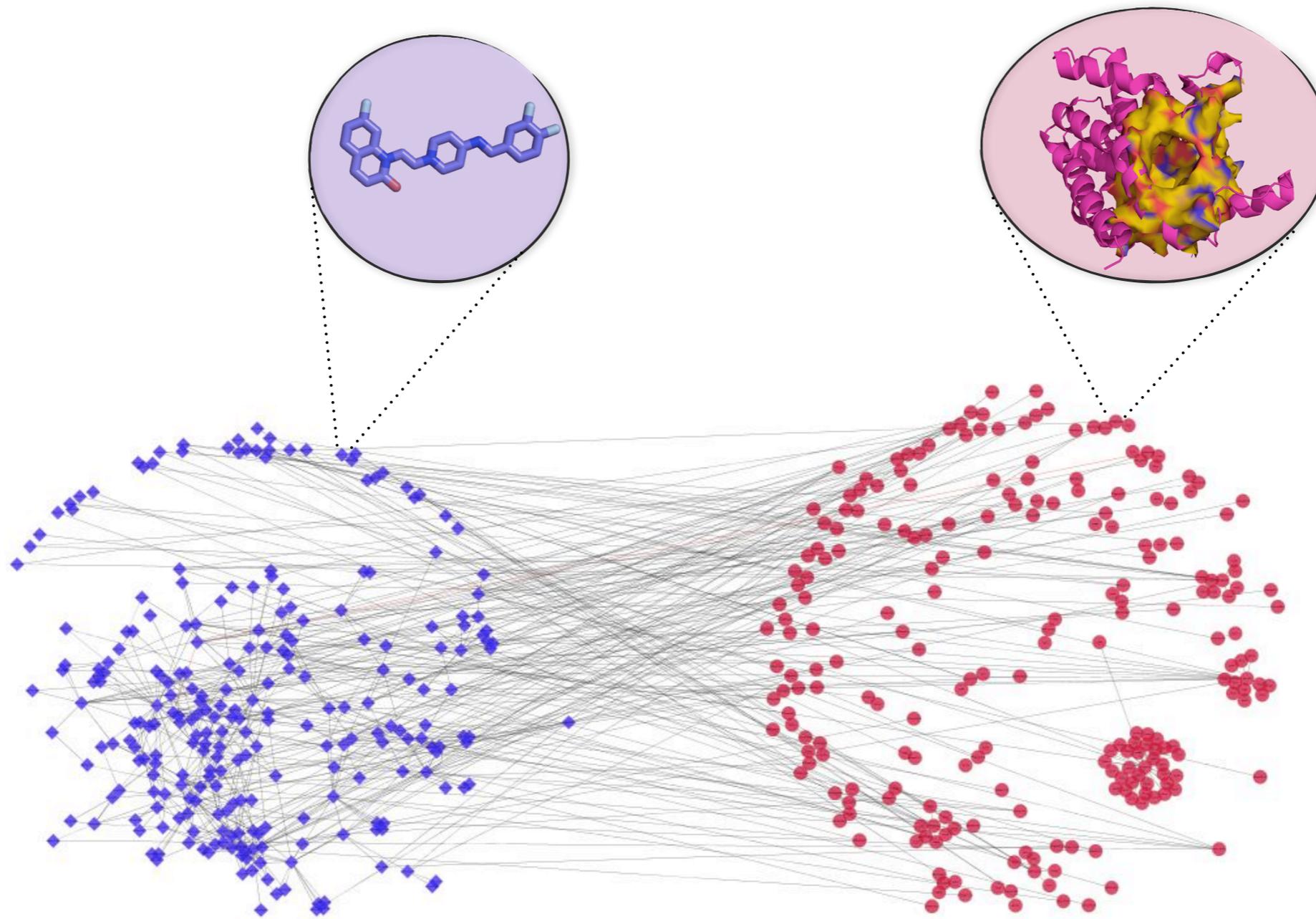


Similar binding-sites tend to bind similar ligands



Network-based Method

nAnnolyze



Applying the method, modeling genomes...

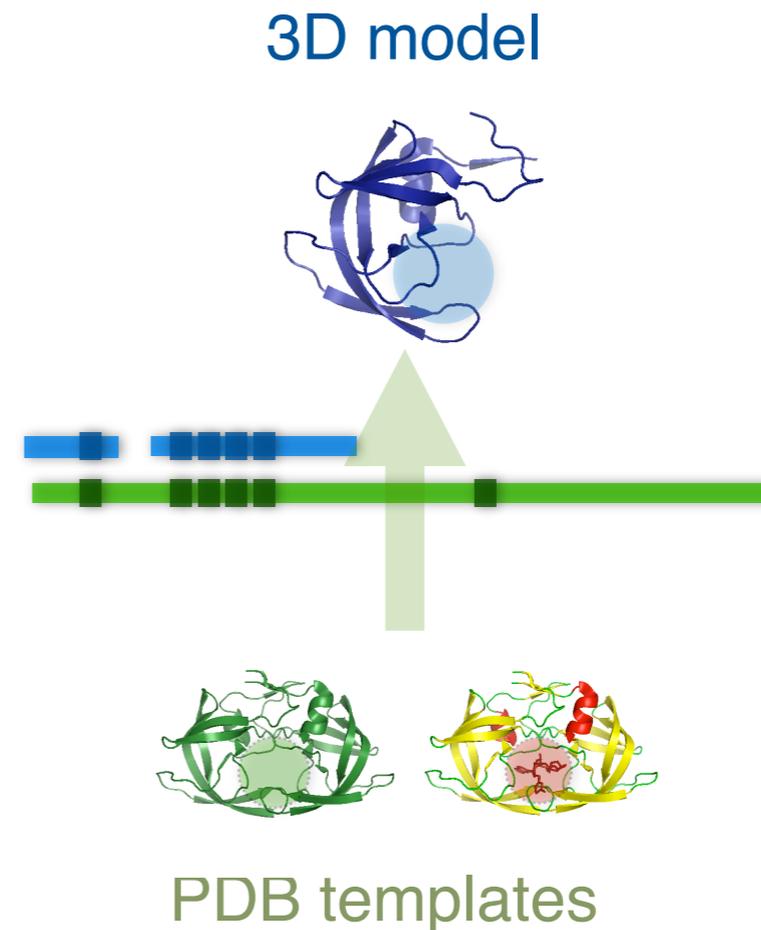
1. Modeling



Ursula Pieper

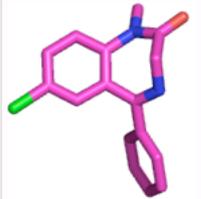
Andrej Sali

2. Binding-site inheritance

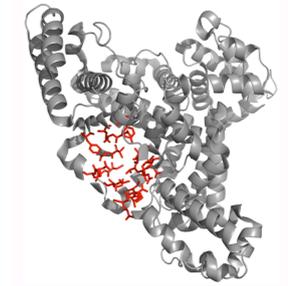
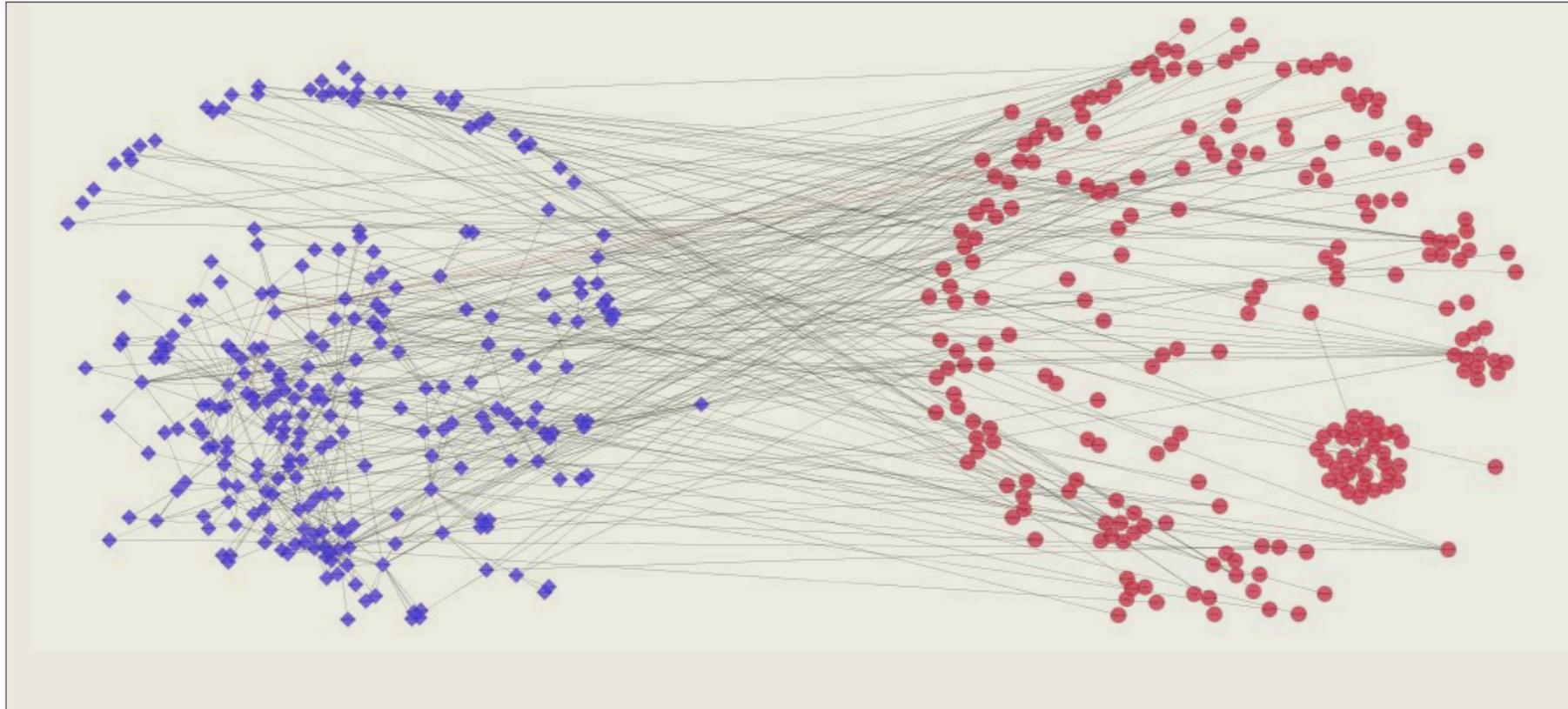


| | Bacterial proteomes |
|-------------------------|--------------------------|
| 3D reliable models | 5,008 no overlapping |
| Different Proteins | 5,008 different proteins |
| Inherited binding-sites | 30,000 |

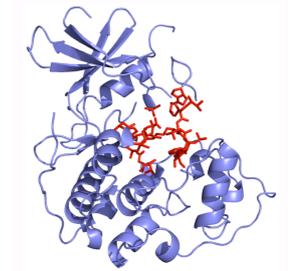
Looking for targets...



GSK
Drug



t1



t2

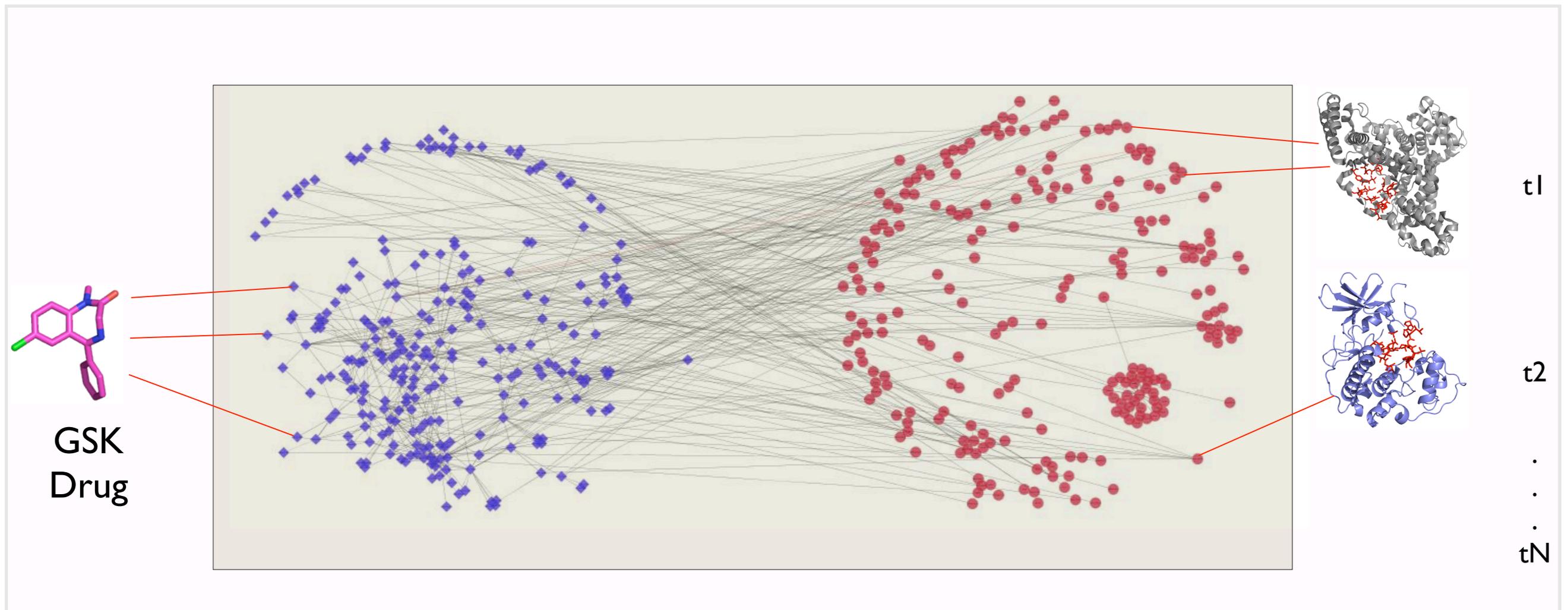
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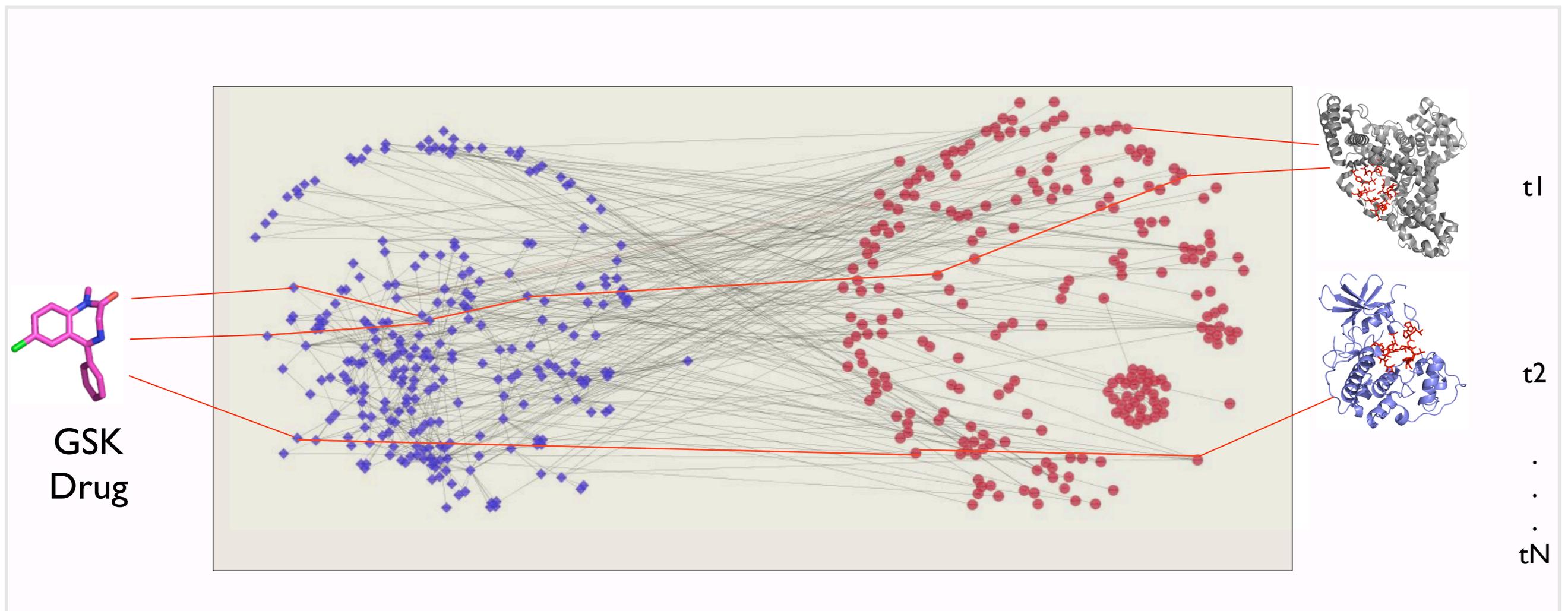
·

tN

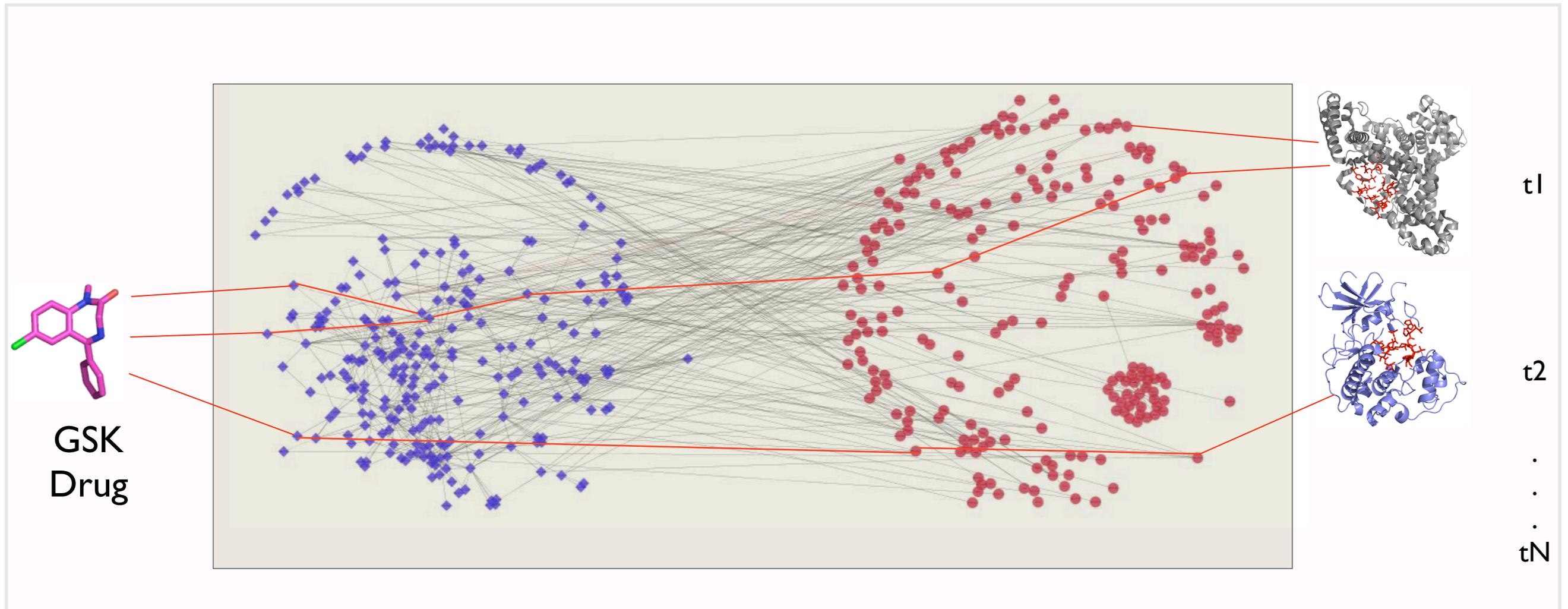
Looking for targets...



Looking for targets...



Looking for targets...

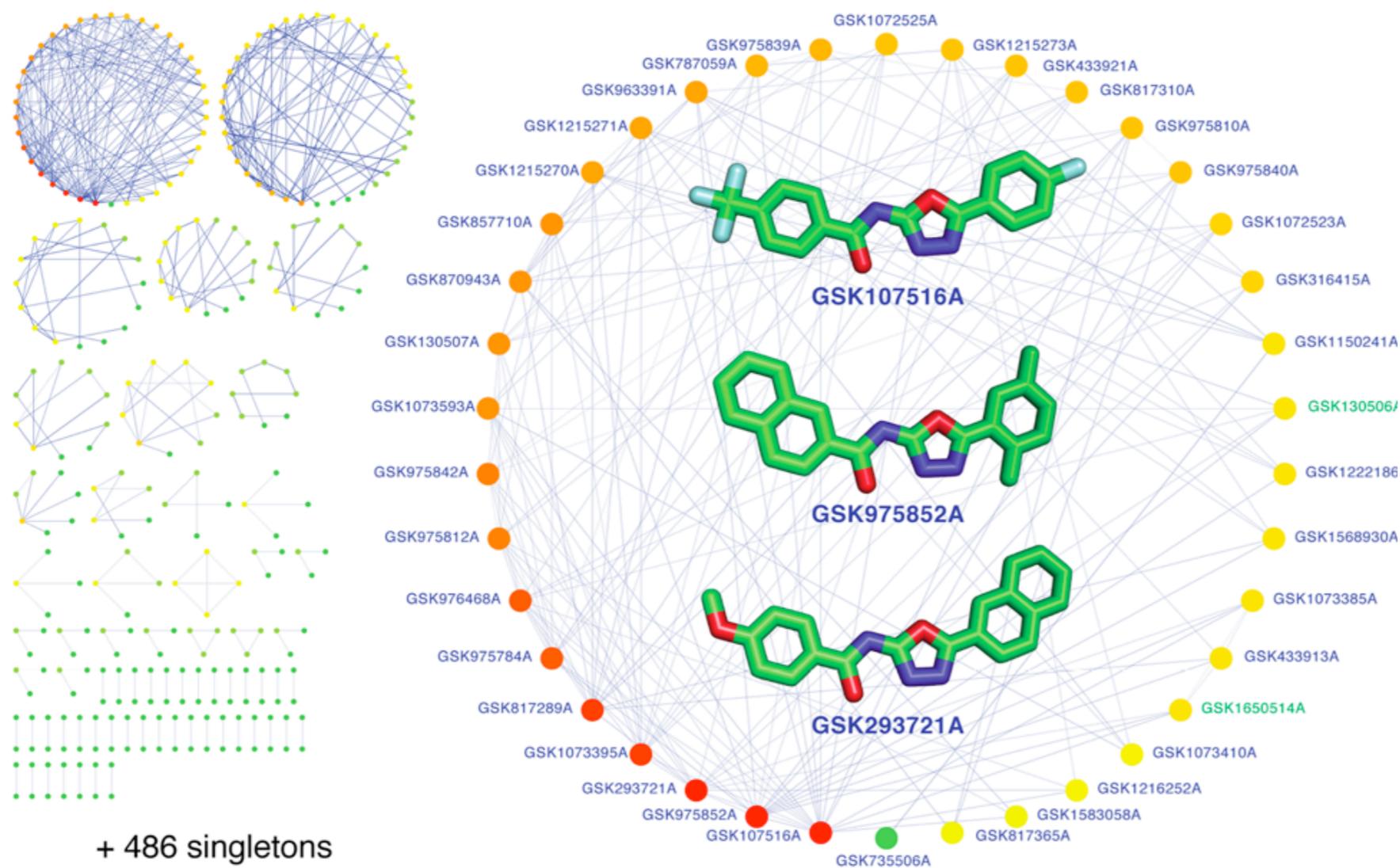


| Ligand | Target | Distance | Global Z-score | Local Z-score |
|--------|-------------|----------|----------------|---------------|
| GSKI | pknB Kinase | 1.3 | -1.6 | -2.5 |
| GSKI | mapB | 2.5 | 2.3 | 1.02 |
| GSKI | sahH | 1.9 | -1.6 | -3.16 |
| GSKI | Mmpl3 | 2.6 | 2.42 | 2.97 |

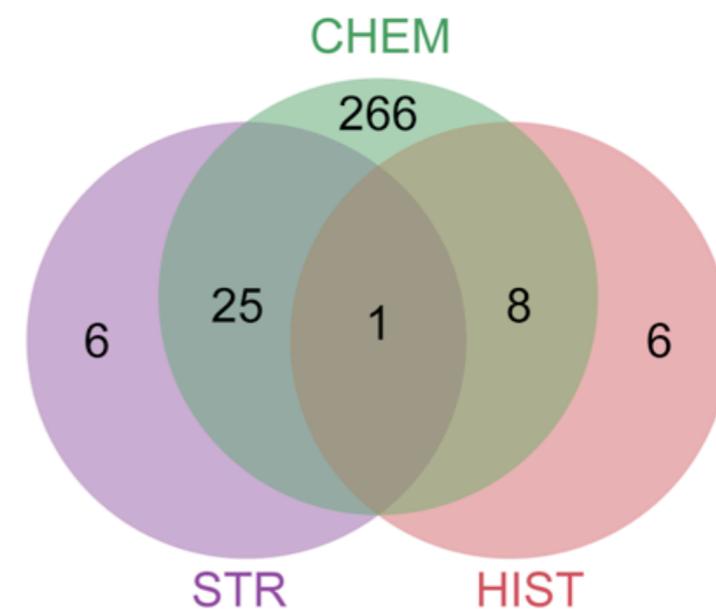
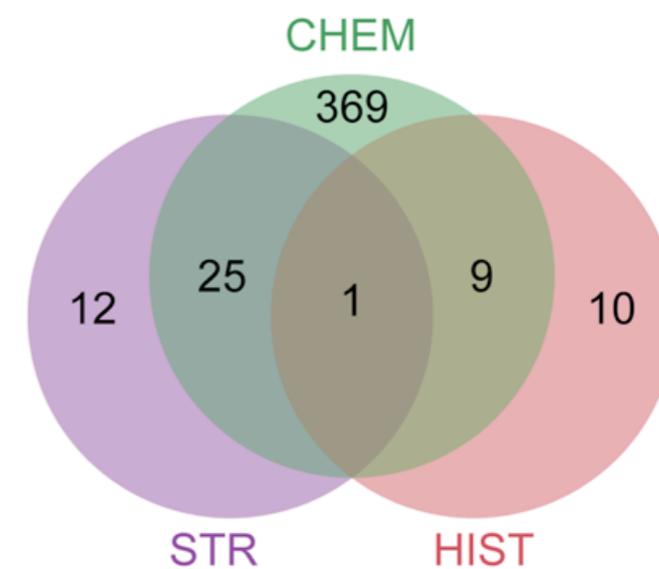
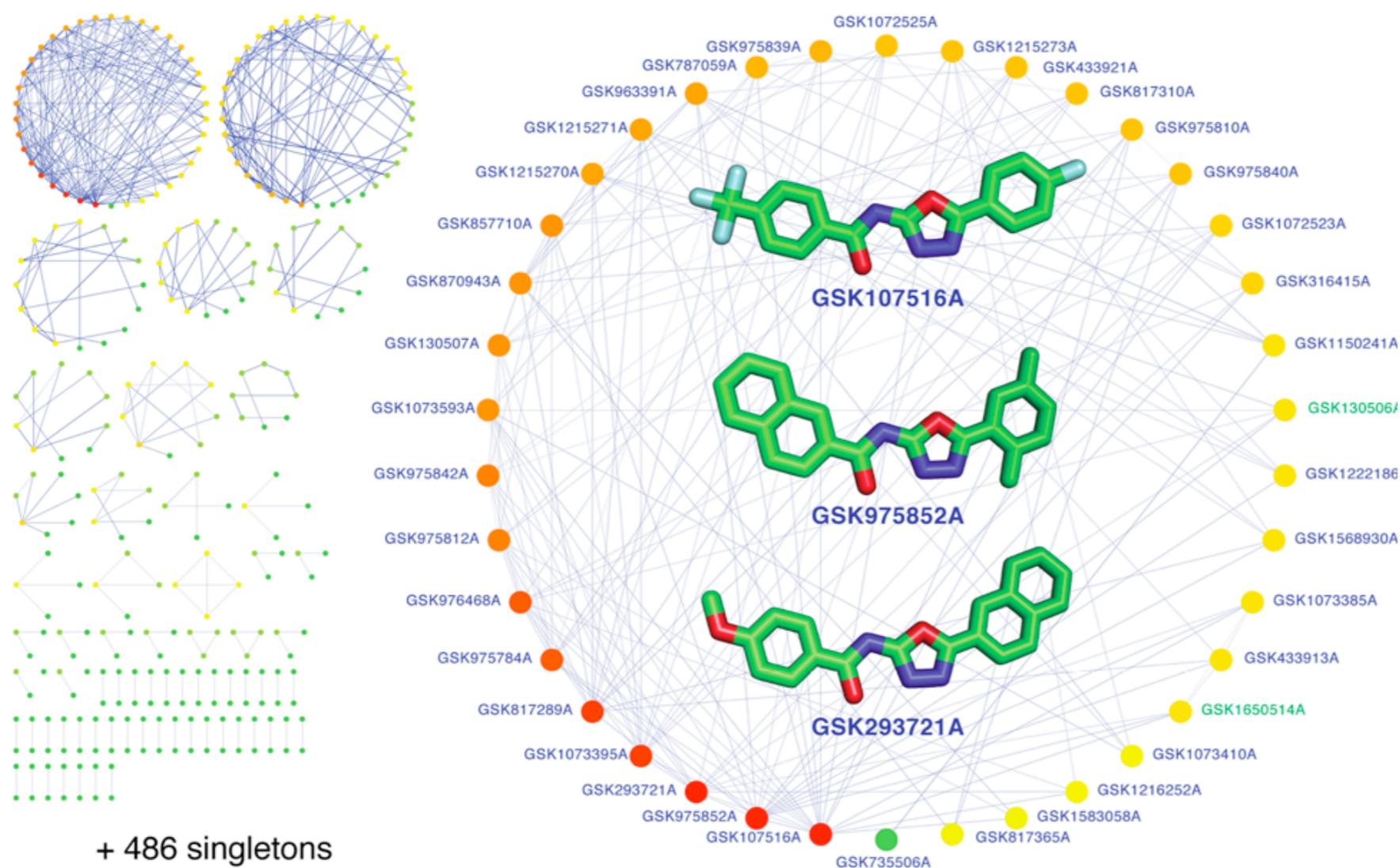
Statistical assessment of predicted links between compounds and targets

- We merged all the predictions from the 3 methods.
- Significance of links using **groups of similar compounds** and the **targets KEGG pathways**.
- LogOdds. Odds of an observation given its probability.
- p-value using Fisher's exact test for 2x2 contingency table comparing two groups of annotations.

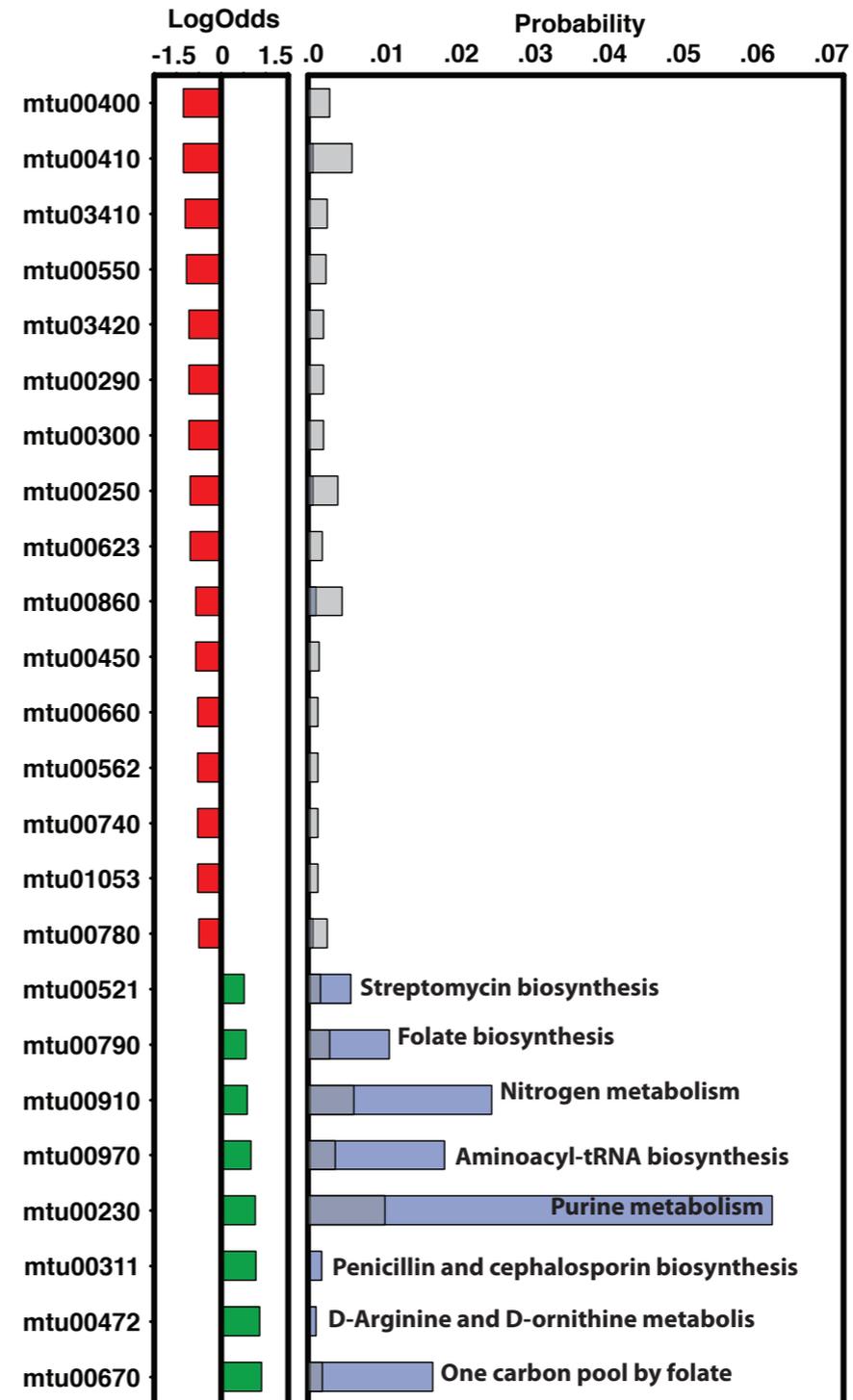
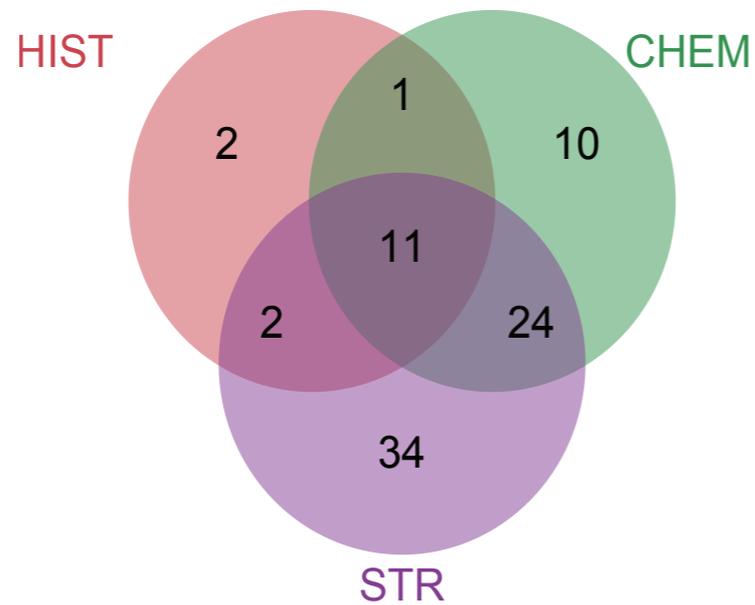
Compound dataset diversity



Compound dataset diversity



Targeting essential aminoacids metabolism pathways



Significant drug-protein pairs

MoA Prediction against TB

Table 2. Significant links between GSK compound families and KEGG pathways.

| GSK Family | Compound | Target | Pathways | |
|------------|--|--|--|---|
| 1 | GSK975784A | Rv2182c | Glycerolipid metabolism (mtu00561) | |
| | | | Glycerophospholipid metabolism (mtu00564) | |
| | | Rv2483c | No Pathway | |
| | GSK975810A | Rv2182c | Glycerolipid metabolism (mtu00561) | |
| | | | Glycerophospholipid metabolism (mtu00564) | |
| | | Rv2483c | No Pathway | |
| | GSK975839A | Rv2182c | Glycerolipid metabolism (mtu00561) | |
| | | | Glycerophospholipid metabolism (mtu00564) | |
| | | | Rv2483c | No Pathway |
| | | Rv2299c | No Pathway | |
| | GSK975840A | Rv2182c | Glycerolipid metabolism (mtu00561) | |
| | | | Glycerophospholipid metabolism (mtu00564) | |
| | | Rv2483c | No Pathway | |
| GSK975842A | Rv2182c | Glycerolipid metabolism (mtu00561) | | |
| | | Glycerophospholipid metabolism (mtu00564) | | |
| | | Rv2483c | No Pathway | |
| | | Rv2045c | No Pathway | |
| | | Rv2139 | Pyrimidine metabolism (mtu00240) | |
| | | Rv2299c | No Pathway | |
| | Rv2483c | No Pathway | | |
| 3 | GSK547481A | Rv0194 | ABC transporters (mtu02010) | |
| | | GSK547490A | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547491A | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547499A | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547500A | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547511A | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547512A | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547527A | Rv1640c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | | Rv3598c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | | Rv0194 | ABC transporters (mtu02010) |
| | | GSK547528A | Rv1640c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | | Rv3598c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| Rv0194 | ABC transporters (mtu02010) | | | |
| GSK547543A | Rv0194 | ABC transporters (mtu02010) | | |
| 7 | GSK1829727A | Rv0053 | Ribosome (mtu03010) | |
| | | Rv0379 | No Pathway | |
| | | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) | |
| | | | Galactose metabolism (mtu00052) | |
| | | | Starch and sucrose metabolism (mtu00500) | |
| | Amino sugar & nucl. sugar metab. (mtu00520) | | | |
| | Streptomycin biosynthesis (mtu00521) | | | |

Table 2. Cont.

| GSK Family | Compound | Target | Pathways | |
|-------------|--|--|--|---------------------------------------|
| | GSK1829729A | Rv3855 | No Pathway | |
| | | Rv0053 | Ribosome (mtu03010) | |
| | | Rv0379 | No Pathway | |
| | | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) | |
| | | | Galactose metabolism (mtu00052) | |
| | | | Starch and sucrose metabolism (mtu00500) | |
| | | | Amino sugar & nucl. sugar metab. (mtu00520) | |
| | | | Streptomycin biosynthesis (mtu00521) | |
| | | GSK1829816A | Rv0053 | Ribosome (mtu03010) |
| | | | | No Pathway |
| | | | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) |
| | | | Rv0379 | No Pathway |
| | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) | | |
| | | Galactose metabolism (mtu00052) | | |
| | | Starch and sucrose metabolism (mtu00500) | | |
| | | Amino sugar & nucl. sugar metab. (mtu00520) | | |
| | | Streptomycin biosynthesis (mtu00521) | | |
| GSK479031A | Rv0053 | Ribosome (mtu03010) | | |
| | | NoPathway (mtu00000) | | |
| | Rv0379 | No Pathway | | |
| | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) | | |
| | | Galactose metabolism (mtu00052) | | |
| | | Starch and sucrose metabolism (mtu00500) | | |
| | Amino sugar & nucl. sugar metab. (mtu00520) | | | |
| | Streptomycin biosynthesis (mtu00521) | | | |
| GSK957094A | Rv3170 | Gly, Ser and Thr metabolism (mtu00260) | | |
| | | Arginine and proline metabolism (mtu00330) | | |
| | | Histidine metabolism (mtu00340) | | |
| | | Tyrosine metabolism (mtu00350) | | |
| | | Phenylalanine metabolism (mtu00360) | | |
| | | Tryptophan metabolism (mtu00380) | | |
| | | Rv0053 | Ribosome (mtu03010) | |
| | | Rv0379 | No Pathway | |
| | | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) | |
| | | | Galactose metabolism (mtu00052) | |
| | | | Starch and sucrose metabolism (mtu00500) | |
| | | | Amino sugar & nucl. sugar metab. (mtu00520) | |
| | Streptomycin biosynthesis (mtu00521) | | | |
| 9 | GSK1188379A | Rv0194 | ABC transporters (mtu02010) | |
| | | GSK1188380A | Rv0194 | ABC transporters (mtu02010) |
| 16 | GSK1825940A | Rv0194 | ABC transporters (mtu02010) | |
| | | GSK1825944A | Rv0194 | ABC transporters (mtu02010) |
| 35 | BRL-101435A | Rv1649 | Aminoacyl-tRNA biosynthesis (mtu00970) | |
| | | Rv2763c | One carbon pool by folate (mtu00670) | |
| | | | Folate biosynthesis (mtu00790) | |
| | | | One carbon pool by folate (mtu00670) | |
| | | Rv2764c | Pyrimidine metabolism (mtu00240) | |
| | | Rv2763c | One carbon pool by folate (mtu00670) | |
| BRL-51093AM | Rv2763c | Folate biosynthesis (mtu00790) | | |
| | Rv2764c | One carbon pool by folate (mtu00670) | | |

Significant drug-protein pairs

MoA Prediction against TB

Table 2. Significant links between GSK compound families and KEGG pathways.

| GSK Family | Compound | Target | Pathways |
|------------|------------|---------|---|
| 1 | GSK975784A | Rv2182c | Glycerolipid metabolism (mtu00561) Glycerophospholipid metabolism (mtu00564) |
| | | Rv2483c | No Pathway |

Table 2. Cont.

| GSK Family | Compound | Target | Pathways |
|------------|-------------|--------|---------------------|
| | GSK1829729A | Rv3855 | No Pathway |
| | | Rv0053 | Ribosome (mtu03010) |
| | | Rv0379 | No Pathway |

| GSK Family | Compound | Target | Pathways |
|------------|-------------|---------|---|
| | | | Pyrimidine metabolism (mtu00240) |
| 173 | GSK1402290A | Rv1640c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | Rv3598c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | Rv3834c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | Rv3105c | No Pathway |
| | | Rv3135 | No Pathway |
| 334 | GSK270671A | Rv1284 | Nitrogen metabolism (mtu00910) |
| | | Rv3588c | Nitrogen metabolism (mtu00910) |
| | | Rv3273 | Nitrogen metabolism (mtu00910) |
| | | Rv1707 | No Pathway |

| | | | |
|---|-------------|---|--|
| | Rv3598c | Aminoacyl-tRNA biosynthesis (mtu00970) | |
| | Rv0194 | ABC transporters (mtu02010) | |
| | GSK547528A | Rv1640c | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | Rv3598c | Aminoacyl-tRNA biosynthesis (mtu00970) | |
| | Rv0194 | ABC transporters (mtu02010) | |
| | GSK547543A | Rv0194 | ABC transporters (mtu02010) |
| 7 | GSK1829727A | Rv0053 | Ribosome (mtu03010) |
| | | Rv0379 | No Pathway |
| | | Rv0650 | Glycolysis/Gluconeogenesis (mtu00010) |
| | | | Galactose metabolism (mtu00052) |
| | | | Starch and sucrose metabolism (mtu00500) |
| | | | Amino sugar & nucl. sugar metab. (mtu00520) |
| | | | Streptomycin biosynthesis (mtu00521) |

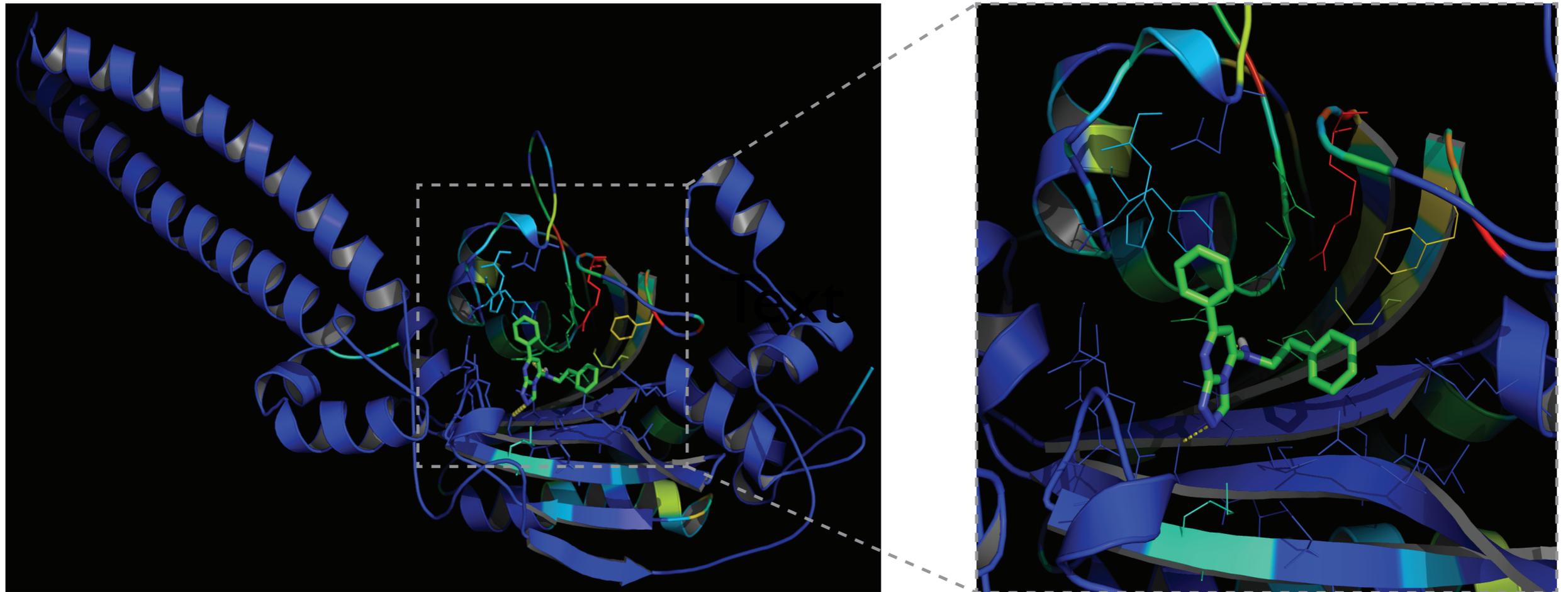
| | | | |
|----|-------------|---------|---|
| | | | Streptomycin biosynthesis (mtu00521) |
| 9 | GSK1188379A | Rv0194 | ABC transporters (mtu02010) |
| | GSK1188380A | Rv0194 | ABC transporters (mtu02010) |
| 16 | GSK1825940A | Rv0194 | ABC transporters (mtu02010) |
| | GSK1825944A | Rv0194 | ABC transporters (mtu02010) |
| 35 | BRL-101435A | Rv1649 | Aminoacyl-tRNA biosynthesis (mtu00970) |
| | | Rv2763c | One carbon pool by folate (mtu00670) |
| | | | Folate biosynthesis (mtu00790) |
| | | | One carbon pool by folate (mtu00670) |
| | | Rv2764c | Pyrimidine metabolism (mtu00240) |
| | BRL-51093AM | Rv2763c | One carbon pool by folate (mtu00670) |
| | | Rv2764c | Folate biosynthesis (mtu00790) |
| | | | One carbon pool by folate (mtu00670) |

GSK1402290A attacking *Aminoacyl-tRNA biosynthesis* pathway

lysyl-tRNA synthetase 2

lysS1 Lysine-tRNA ligase

SERYL-tRNA synthetase SerS



nAnalyze predicted binding-site + Autodock Vina

Experimental validation

a. MapB

b. SahH

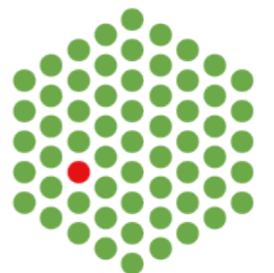
c. AofH

d. EphA

e. SerS?

Stacey Southall

EMBL

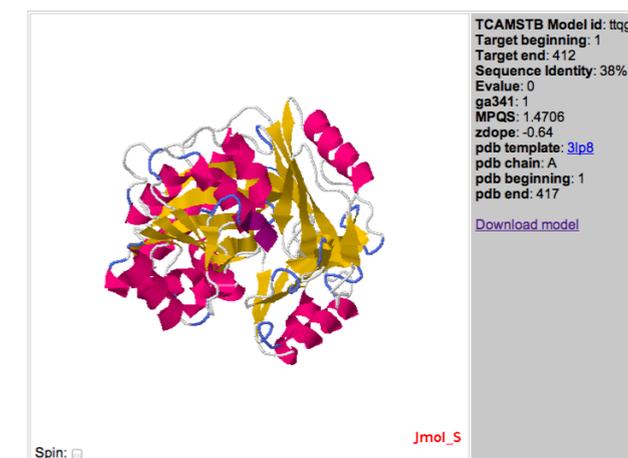
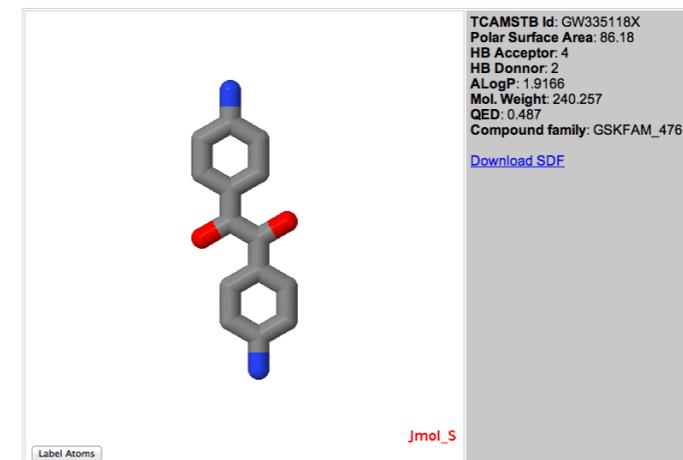


Open Access Drug Discovery

<http://sgt.cnag.cat/TDI/TCAMSTB/>

[Go back to search](#)

| Method | GSK Id | UniProt | Target | 3D | In vitro essential | In vivo essential | Gene names | Gene description | Pathway | Pathway description |
|--------|---------------------------|------------------------|-------------------------|-----------------------|--------------------|-------------------|-------------------------------------|--|--------------------------|---|
| CHEM | GW335118X | P65893 | Rv0772 | Itag | 0.05 | Non Essential | purD Rv0772 MT0796 MTCY369.17 | Phosphoribosylamine-glycine ligase (EC 6.3.4.13) (GARS) (Glycinamide ribonucleotide synthetase) | mbu02230 | Purine metabolism |
| CHEM | GW335118X | P65893 | Rv0772 | Itag | 0.05 | Non Essential | purD Rv0772 MT0796 MTCY369.17 | Phosphoribosylamine-glycine ligase (EC 6.3.4.13) (GARS) (Glycinamide ribonucleotide synthetase) | mbu01100 | Metabolic pathways |
| CHEM | GW335118X | P65893 | Rv0772 | Itag | 0.05 | Non Essential | purD Rv0772 MT0796 MTCY369.17 | Phosphoribosylamine-glycine ligase (EC 6.3.4.13) (GARS) (Glycinamide ribonucleotide synthetase) | mbu01110 | Biosynthesis of secondary metabolites |
| CHEM | GW335118X | Q53823 | Rv0809 | Iuon | Non Essential | Non Essential | purM MT0830 Rv0809 | Phosphoribosylformylglycinamide cyclo-ligase (EC 6.3.3.1) | mbu02230 | Purine metabolism |
| CHEM | GW335118X | Q53823 | Rv0809 | Iuon | Non Essential | Non Essential | purM MT0830 Rv0809 | Phosphoribosylformylglycinamide cyclo-ligase (EC 6.3.3.1) | mbu01100 | Metabolic pathways |
| CHEM | GW335118X | Q53823 | Rv0809 | Iuon | Non Essential | Non Essential | purM MT0830 Rv0809 | Phosphoribosylformylglycinamide cyclo-ligase (EC 6.3.3.1) | mbu01110 | Biosynthesis of secondary metabolites |
| CHEM | GW335118X | Q53488 | Rv2045c | Itrbc | Non Essential | Non Essential | lpT Rv2045c | Probable carboxylesterase LipT (EC 3.1.1.-) | NIA | No Pathway |
| CHEM | GW335118X | P0A546 | Rv2763c | Itra | Non Essential | Non Essential | folA dfrA Rv2763c MT2833 MTV002.28c | Dihydrofolate reductase (EC 1.5.1.3) | mbu00670 | One carbon pool by folate |
| CHEM | GW335118X | P0A546 | Rv2763c | Itra | Non Essential | Non Essential | folA dfrA Rv2763c MT2833 MTV002.28c | Dihydrofolate reductase (EC 1.5.1.3) | mbu00790 | Folate biosynthesis |
| CHEM | GW335118X | P0A546 | Rv2763c | Itra | Non Essential | Non Essential | folA dfrA Rv2763c MT2833 MTV002.28c | Dihydrofolate reductase (EC 1.5.1.3) | mbu01100 | Metabolic pathways |
| CHEM | GW335118X | Q53573 | Rv3588c | Iold | Non Essential | 0.36 | cytT Rv3588c MT3694 | Carbonic anhydrase (EC 4.2.1.1) (Carbonate dehydratase) | mbu00910 | Nitrogen metabolism |
| STR | GW335118X | P63627 | Rv1538c | Itrsa | Non Essential | Non Essential | ansA Rv1538c MT1590 MTCY48.27 | Probable L-asparaginase (L-ASNase) (EC 3.5.1.1) (L-asparagine amidohydrolase) | mbu00250 | Alanine, aspartate and glutamate metabolism |
| STR | GW335118X | P63627 | Rv1538c | Itrsa | Non Essential | Non Essential | ansA Rv1538c MT1590 MTCY48.27 | Probable L-asparaginase (L-ASNase) (EC 3.5.1.1) (L-asparagine amidohydrolase) | mbu00460 | Cyanoamino acid metabolism |
| STR | GW335118X | P63627 | Rv1538c | Itrsa | Non Essential | Non Essential | ansA Rv1538c MT1590 MTCY48.27 | Probable L-asparaginase (L-ASNase) (EC 3.5.1.1) (L-asparagine amidohydrolase) | mbu00910 | Nitrogen metabolism |
| STR | GW335118X | P63627 | Rv1538c | Itrsa | Non Essential | Non Essential | ansA Rv1538c MT1590 MTCY48.27 | Probable L-asparaginase (L-ASNase) (EC 3.5.1.1) (L-asparagine amidohydrolase) | mbu01100 | Metabolic pathways |
| STR | GW335118X | P63627 | Rv1538c | Itrsa | Non Essential | Non Essential | ansA Rv1538c MT1590 MTCY48.27 | Probable L-asparaginase (L-ASNase) (EC 3.5.1.1) (L-asparagine amidohydrolase) | mbu01110 | Biosynthesis of secondary metabolites |
| STR | GW335118X | P63562 | Rv1652 | Itrif | 0.05 | Non Essential | argC Rv1652 MT1690 MTCY06H11.17 | N-acetyl-gamma-glutamyl-phosphate reductase (AGPR) (EC 1.2.1.38) (N-acetyl-glutamate semialdehyde dehydrogenase) (NAGSA dehydrogenase) | mbu00330 | Arginine and proline metabolism |
| STR | GW335118X | P63562 | Rv1652 | Itrif | 0.05 | Non Essential | argC Rv1652 MT1690 MTCY06H11.17 | N-acetyl-gamma-glutamyl-phosphate reductase (AGPR) (EC 1.2.1.38) (N-acetyl-glutamate semialdehyde dehydrogenase) (NAGSA dehydrogenase) | mbu01100 | Metabolic pathways |
| STR | GW335118X | P63562 | Rv1652 | Itrif | 0.05 | Non Essential | argC Rv1652 MT1690 MTCY06H11.17 | N-acetyl-gamma-glutamyl-phosphate reductase (AGPR) (EC 1.2.1.38) (N-acetyl-glutamate semialdehyde dehydrogenase) (NAGSA dehydrogenase) | mbu01110 | Biosynthesis of secondary metabolites |
| STR | GW335118X | P63562 | Rv1652 | Itrif | 0.05 | Non Essential | argC Rv1652 MT1690 MTCY06H11.17 | N-acetyl-gamma-glutamyl-phosphate reductase (AGPR) (EC 1.2.1.38) (N-acetyl-glutamate semialdehyde dehydrogenase) (NAGSA dehydrogenase) | mbu01210 | 2-Oxocarboxylic acid metabolism |
| STR | GW335118X | Q53321 | Rv3171c | Itrse | Non Essential | Non Essential | hpx Rv3171c | POSSIBLE NON-HEME HALOPEROXIDASE HPX (EC 1.11.1.-) | NIA | No Pathway |



Introduce your query molecule

ID of the molecule
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SMILE
 e.g: CC(C(O)=O)C1=CC(F)=C(C=C1)C1=CC=CC=C1

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Visualize:
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 All Go terms and Pathways

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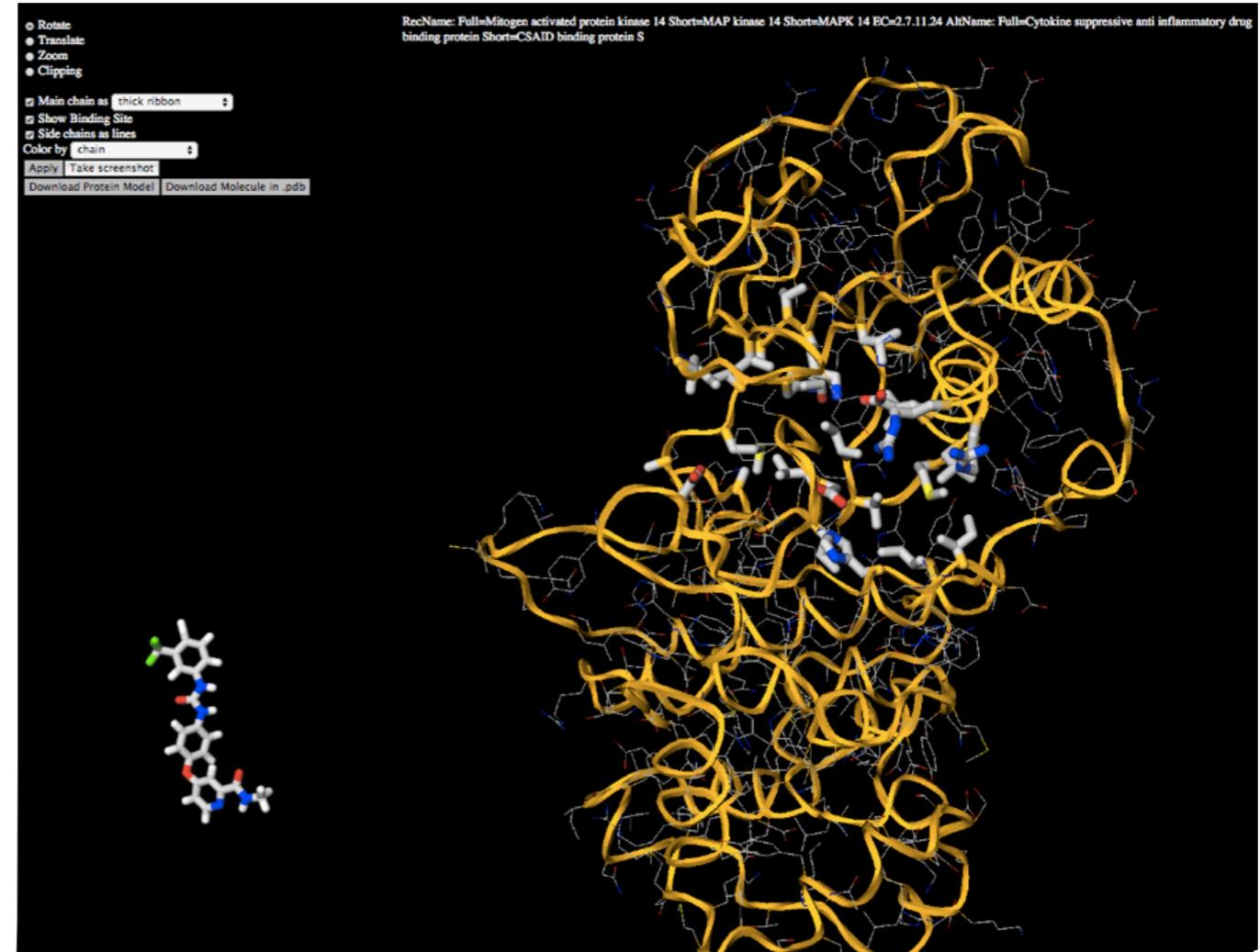
Statistics for Compound

GO terms

Pathways

Best Worst

| Molecule ID | External ID | Target UP | Score | Z-Score-local | Z-Score-global | Description | Binding-Site residues | Visualize... |
|-------------|-------------|------------------------|-------|---------------|----------------|--|---------------------------------------|--------------|
| DB00398 | NP_620581 | Q13083 | 0.99 | -3.23 | -3.30 | RecName: Full=Mitogen-activated protein kinase 14;Short=MAP kinase 14;Short=MAPK 14;EC=2.7.11.24;AltName: Full=Cytokine suppressive anti-inflammatory drug-binding protein;Short=CSAID-binding protein;S | [:A and (30;38;51;52;53;67;70;71;74; | |
| DB00398 | NP_05581 | Q51027 | 0.98 | -4.14 | -3.24 | RecName: Full=Cyclin-dependent kinase 19;EC=2.7.11.22;AltName: Full=CDC2-related protein kinase 6;AltName: Full=Cell division cycle 2-like protein kinase 6;ARName: Full=Cell division protein kinase 1 | [:A and (35;50;51;52;66;69;70;73;78; | |
| DB00398 | NP_00121 | G1T955 | 0.97 | -4.39 | -3.14 | SubName: Full=Uncharacterized protein; | [:A and (27;28;32;35;50;51;52;66;69; | |
| DB00398 | GENSCAN | | 0.96 | -3.21 | -3.06 | | [:A and (924;925;932;950;952;969;97 | |
| DB00398 | NP_00131 | L7B5N2 | 0.94 | -2.91 | -2.95 | SubName: Full=Mitogen-activated protein kinase 14;SubName: Full=Mitogen-activated protein kinase 14 isoform CRA_e; | [:A and (30;35;38;51;70;74;83;84;85; | |



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