
# Distributed end-to-end drug similarity analytics and visualization workflow

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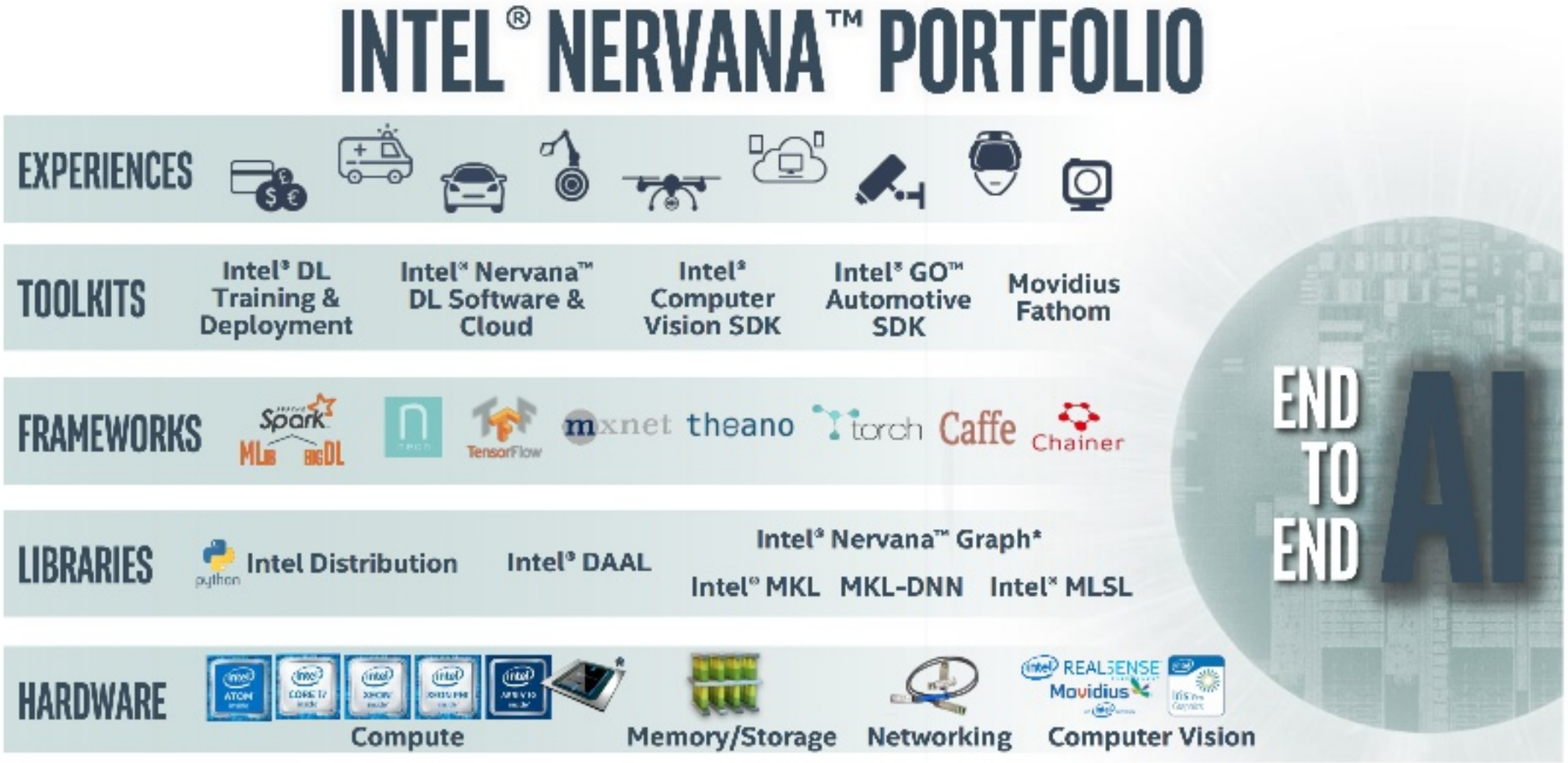
# Who we are?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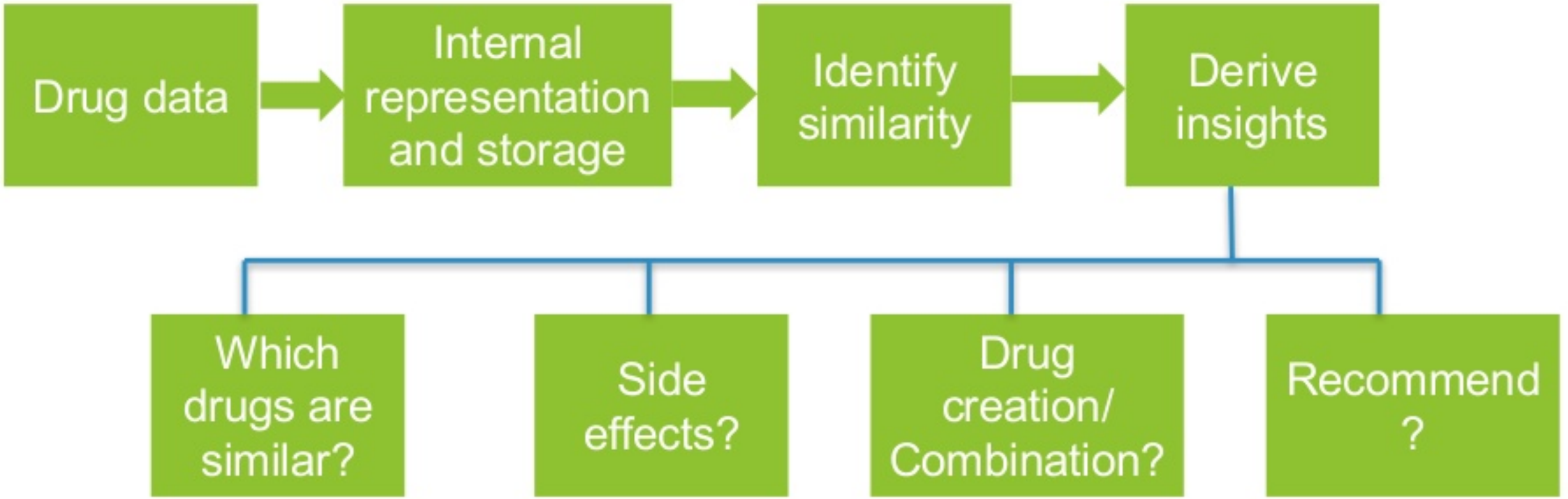
# Agenda

- Chemical Similarity
- Use-case overview
- Drug data & SMILES
- Tanimoto Co-efficient
- Graph Analytics
- Apache Spark
- Spark-tk library
- Superset visualization
- Demo
- Next steps

# Chemical Similarity

- Similarity of chemical elements, molecules or chemical compounds
- Structural or functional
- **Usages:**
  - Predicting properties of chemical compounds
  - Designing chemicals with predefined set of properties
  - Drug design

# Use-case overview



# SMILES

**S**implified **M**olecular **I**nput **L**ine **E**ntry **S**ystem

– Typographical method using printable characters for entering and representing molecules and reactions

| SMILES | Name | SMILES | Name |
|---|---|---|---|
| CC | ethane | [OH3+] | hydronium ion |
| O=C=O | carbon dioxide | [2H]O[2H] | deuterium oxide |
| C#N | hydrogen cyanide | [235U] | uranium-235 |
| CCN(CC)CC | triethylamine | F/C=C/F | E-difluoroethene |
| CC(=O)O | acetic acid | F/C=C\F | Z-difluoroethene |
| C1CCCCC1 | cyclohexane | N[C@@H](C)C(=O)O | L-alanine |
| c1ccccc1 | benzene | N[C@H](C)C(=O)O | D-alanine |

# Drug data

## Raw data format

| id | name | SMILES | chembl_id | chebi_id | DrugBank | PubChem | MeSH_ID | KEGG_drug |
|---|---|---|---|---|---|---|---|---|
| 0 | levodopa | C1=CC(=C(C=C1C[C@@H](C(=O)O)N)O)O | CHEMBL1009 | 15765 | DB01235 | 6047 | D007980 | D00059 |
| 1 | nipecotic acid | C1CC(CNC1)C(=O)O | CHEMBL277498 | 116931 | NA | 4498 | C030278 | NA |
| 2 | betaxolol | CC(C)NCC(COC1=CC=C(C=C1)CCOCC2CC2)O | CHEMBL423 | 3082 | DB00195 | 2369 | D015784 | NA |
| 3 | oxybutynin | CCN(CC)CC#CCOC(=O)C(C1CCCCC1)(C2=CC=CC=C2)O | CHEMBL1231 | 7856 | DB01062 | 4634 | C005419 | D00465 |
| 4 | indapamide | CC1CC2=CC=CC=C2N1NC(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N | CHEMBL406 | 100619 | DB00808 | 3702 | D007190 | D00345 |
| 5 | anabasine | C1CCNC(C1)C2=CN=CC=C2 | CHEMBL280963 | 28986 | NA | 2181 | D000691 | NA |
| 6 | tamoxifen | CC/C(=C(\C1=CC=CC=C1)/C2=CC=C(C=C2)OCCN(C)C)/C3=CC=CC=C3 | CHEMBL83 | 41774 | DB00675 | 2733526 | D013629 | D00966 |
| 7 | eucatropine | CC1CC(CC(N1C)(C)C)OC(=O)C(C2=CC=CC=C2)O | CHEMBL1618660 | NA | NA | 7534 | NA | NA |
| 8 | flucytosine | C1=NC(=O)NC(=C1F)N | CHEMBL1463 | 5100 | DB01099 | 3366 | D005437 | D00323 |
| 9 | terazosin | COC1=C(C=C2C(=C1)C(=NC(=N2)N3CCN(CC3)C(=O)C4CCCO4)N)OC | CHEMBL611 | 9445 | DB01162 | 5401 | C041226 | NA |
| 10 | citiolone | CC(=O)NC1CCSC1=O | CHEMBL2104457 | NA | NA | 14520 | C000486 | NA |
| 11 | nitrofurantoin | C1C(=O)NC(=O)N1/N=C\C2=CC=C(O2)[N+](=O)[O-] | CHEMBL572 | 116592 | DB00698 | 5353830 | D009582 | D00439 |
| 12 | lomustine | C1CCC(CC1)NC(=O)N(CCCl)N=O | CHEMBL514 | 110898 | DB01206 | 3950 | D008130 | D00363 |
| 13 | meptazinol | CCC1(CCCCN(C1)C)C2=CC(=CC=C2)O.Cl | CHEMBL314437 | 239237 | NA | 65483 | D008621 | NA |
| 14 | rilmenidine | C1CC1C(C2CC2)NC3=NCCO3 | CHEMBL289480 | 160422 | NA | 68712 | C032302 | NA |
| 15 | bufexamac | CCCCOC1=CC=C(C=C1)CC(=O)NO | CHEMBL94394 | 253408 | NA | 2466 | D002019 | NA |
| 16 | mebhydrolin | CN1CCC2=C(C1)C3=CC=CC=C3N2CC4=CC=CC=C4 | CHEMBL1625607 | NA | NA | 22530 | C005139 | NA |
| 18 | piperidolate | CCN1CCCC(C1)OC(=O)C(C2=CC=CC=C2)C3=CC=CC=C3.Cl | CHEMBL1474977 | 998861 | NA | 8520 | C010293 | NA |
| 20 | metamizole sodium | CC1=C(C(=O)N(N1C)C2=CC=CC=C2)N(C)CS(=O)(=O)[O-].[Na+] | CHEMBL487894 | 59033 | DB04817 | 522325 | D004177 | NA |
| 21 | sulfamethoxazole | CC1=CC(=NO1)NS(=O)(=O)C2=CC=C(C=C2)N | CHEMBL443 | 9332 | DB01015 | 5329 | D013420 | D00447 |

# Tanimoto Co-efficient

- Range from 0 to 1; 1 being most similar
- Similarity ratio over bitmaps
- Each bit of fixed-size array represents presence or absence of a characteristic

Presented in mathematical terms, if samples *X* and *Y* are bitmaps, $X_i$ is the *i*th bit of *X*, and $\wedge$, $\vee$ are bitwise *and*, *or* operators respectively, then the similarity ratio $T_s$ is

$$T_s(X, Y) = \frac{\sum_i (X_i \wedge Y_i)}{\sum_i (X_i \vee Y_i)}$$

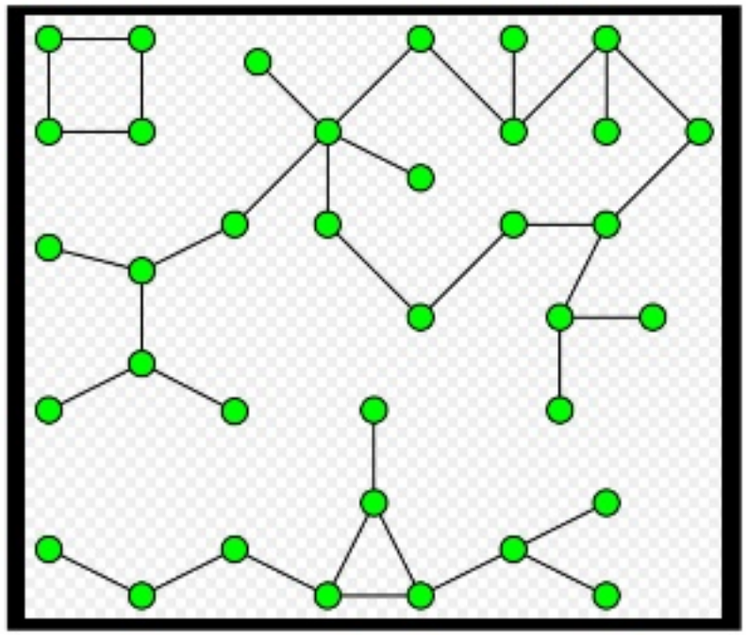
https://en.wikipedia.org/wiki/Jaccard_index#Tanimoto_similarity_and_distance

# Graph Analytics

- Mathematical structures used to model pairwise relations between objects
- Vertices/nodes/points connected by edges/arcs/lines
- Undirected edges: No distinction between the two vertices associated with each edge
- Weighted edges: Each edge has a value/weight associated with it

# Connected components

- Form subgraphs in which any two vertices are connected by edges



Clusters of similar drugs?

https://en.wikipedia.org/wiki/Connected_component_(graph_theory)

# Clustering co-efficient

Numerical metrics for drug graph?

- Measure of the degree to which nodes in a graph tend to cluster together
- **Global** clustering co-efficient – overall indication of the clustering in the network
- **Local** clustering co-efficient – indication of the embeddedness of single nodes

# Label propagation


- Finding communities in data
  - Communities structure: if the nodes of the graph can be easily grouped into densely connected sets of nodes(potentially overlapping)
- **Principle:** Pairs of nodes are more likely to be connected if they are both members of the same community(ies)
- Efficient run time
- Requires no apriori information to run

# Closeness Centrality

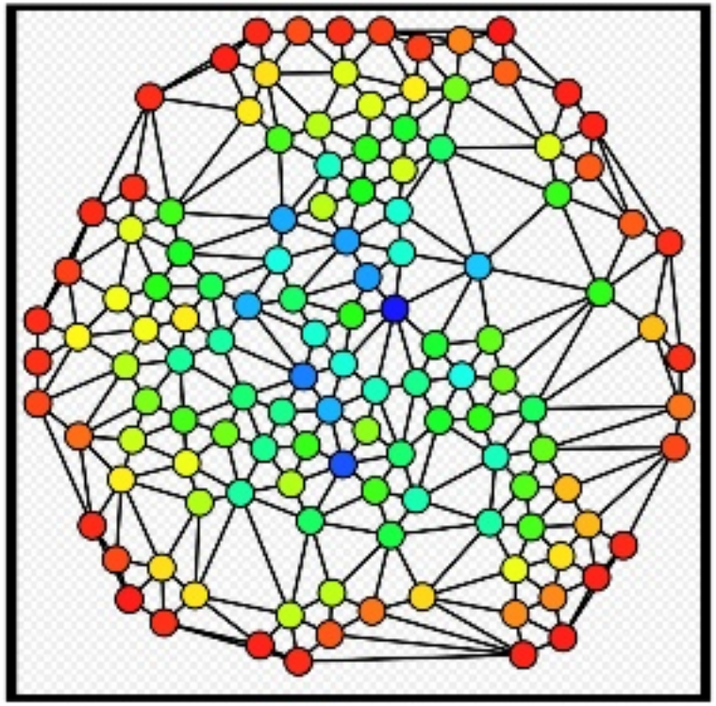
What drugs are most similar to others?

- Average length of the shortest path between the node and all other nodes
- More central a node, the closer it is to all other nodes

# Betweenness centrality

Which drugs stand between each other?

- Quantify the **number of times a node acts as bridge** along the shortest path between two nodes
- Vertices that have a high probability to occur on a randomly chosen shortest path have high betweennness



https://en.wikipedia.org/wiki/Betweenness_centrality

# Degree Centrality


- Identify most important vertices in a graph
- Number of edges incident upon a node
- Immediate risk of a node for catching network flow
- Directed graphs: indegree and outdegree

# Why Spark?

- Spark Core
- Spark SQL
- GraphX
- MIlib
- Spark Streaming

# Spark-tk Introduction

- Open source library enhancing the Spark experience
- APIs for feature engineering, ETL, graph construction, machine learning, scoring
- Abstraction level familiar to data scientists; removes complexity of parallel processing
- Lower level Spark APIs seamlessly exposed
- Easy to build apps plugging in other tools/libraries

https://github.com/trustedanalytics/spark-tk

http://trustedanalytics.github.io/spark-tk/

# Spark-tk components

- **Frames:**
  - Scalable data frame representation
  - More intuitive than low level HDFS file and Spark RDD/DataFrame/DataSet formats; schema inference
  - APIs to manipulate the data frames for feature engineering and exploration, such as joins and aggregations
  - Run user-defined transformations and filters using distributed processing
  - Input to our models
  - Easy to go from Spark-tk Frames to Spark representations

# Spark-tk components

- **Graphs**
  - Scalable graph representation based on Frames for vertices and edges
  - In house distributed algorithms for graph analytics using GraphX
  - Supports importing/exporting to OrientDB's scalable graph databases – visualize, real-time graph querying
  - Store massive graphs

# Spark-tk components

- **Machine Learning & Streaming**
  - Time series analysis
  - Recommender systems
  - Topic Modeling
  - Clustering
  - Classification/Regression
  - Image processing
  - Scikit learn Models
  - Streaming via Scoring engine

# RDKit

- Open source Cheminformatics and Machine Learning Software written in C++ and Python
- SMILES String of a drug → RDKit's Mol object
- Compute Similarity on two Mol objects:

```
DataStructs.FingerprintSimilarity(FingerprintMols.FingerprintMol(mol1),
                                  FingerprintMols.FingerprintMol(mol2))
```

http://www.rdkit.org/

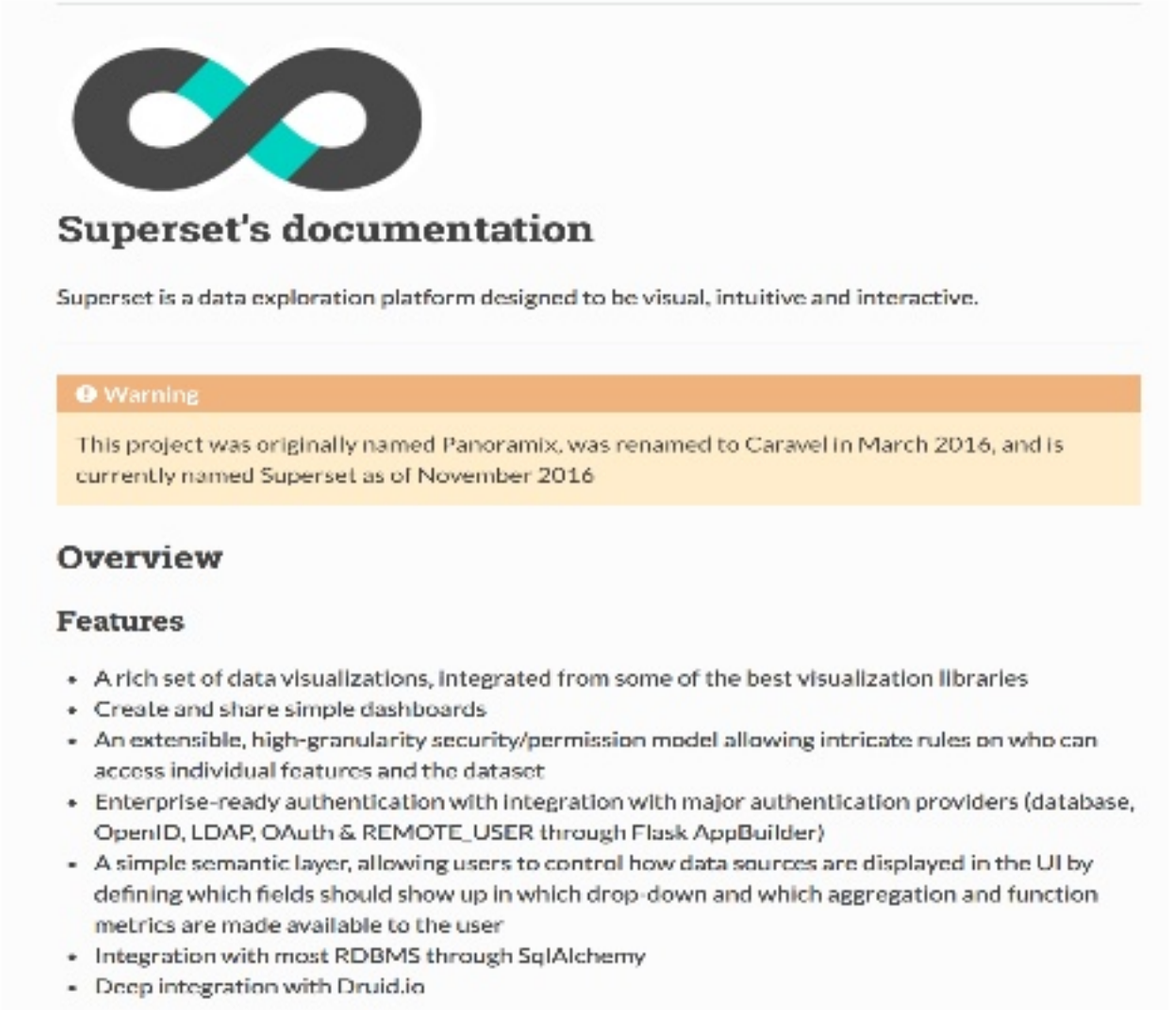
http://www.rdkit.org/docs/api/index.html

# Spark-tk backend

Import/export from:

- CSV
- Hbase
- JDBC
- Hive
- JSON
- Pandas
- OrientDB
- Frame to/from Spark objects

# Visualization with Superset



## Superset's documentation

Superset is a data exploration platform designed to be visual, intuitive and interactive.

**Warning**

This project was originally named Panoramix, was renamed to Caravel in March 2016, and is currently named Superset as of November 2016

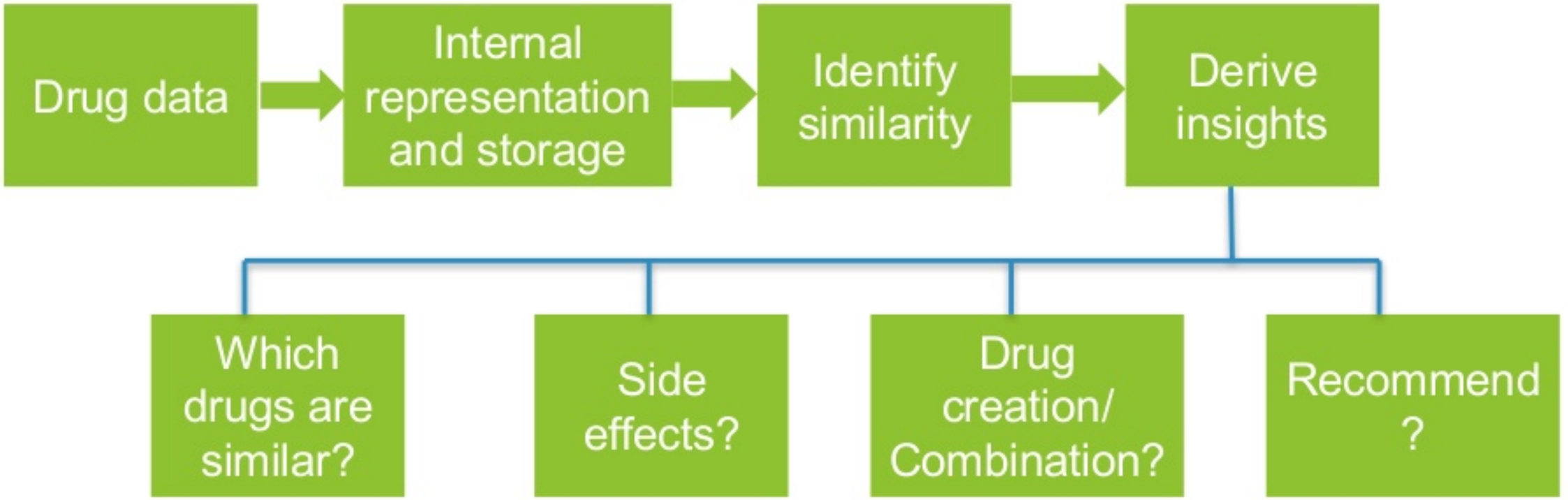
### Overview

#### Features

- A rich set of data visualizations, integrated from some of the best visualization libraries
- Create and share simple dashboards
- An extensible, high-granularity security/permission model allowing intricate rules on who can access individual features and the dataset
- Enterprise-ready authentication with integration with major authentication providers (database, OpenID, LDAP, OAuth & REMOTE_USER through Flask AppBuilder)
- A simple semantic layer, allowing users to control how data sources are displayed in the UI by defining which fields should show up in which drop-down and which aggregation and function metrics are made available to the user
- Integration with most RDBMS through SqlAlchemy
- Deep integration with Druid.io

https://github.com/airbnb/superset; http://airbnb.io/superset/

# Use-case overview



# Demo

# Next steps

- Further investigate Side effects and implications of drug interactions
- Combine with patient Electronic Health Records and train models
- Drug recommendations/suggestions


# Thank You.

https://github.com/trustedanalytics/spark-tk

http://trustedanalytics.github.io/spark-tk/

# Backup – Jupyter Notebook

## Drug Similarity Analytics Demo

This notebook demonstrates the process of importing and cleaning drug data, using rdkit to calculate the tanimoto coefficient to compare each drug, creating a sparktk graph, running degree centrality, and then exporting the data to a table in a postgres database.

We start out by importing the rdkit and sparktk libraries:

In [1]:
```
# rdkit imports for using SMILES index to get molecule fingerprint and tanimoto calculation
from rdkit import Chem
from rdkit import DataStructs
from rdkit.Chem.Fingerprints import FingerprintMols
import sys
sys.path.append('/home/dmsuehir/anaconda2/envs/my-rdkit-env/')

# import sparktk and create a sparktk context, with postgresql paths
import sparktk
submit_args = "--jars /home/dmsuehir/.m2/repository/postgresql/postgresql/8.4-702.jdbc4/postgresql-8.4-702.jdbc4.jar "
\
          "--driver-class-path /home/dmsuehir/.m2/repository/postgresql/postgresql/8.4-702.jdbc4/postgresql-8.4-702.j
dbc4.jar"
spark_conf = '/home/dmsuehir/superset_demo/sparktk.conf'
tc = sparktk.TkContext(pyspark_submit_args=submit_args,extra_conf_file=spark_conf, extra_conf_dict={"spark.dynamicAllo
cation.enabled": "true", "spark.sql.shuffle.partitions": 200})
```

## Import data into frames

We start out with raw data in a `drugs.csv` file, which we will import into a `frame`, using sparktk. The frame `inspect()` method gives a preview of a few columns of data.

In [2]:
```
drugs_csv_path = "hdfs://10.7.151.77/user/atkuser/drugs.csv"
nodes_frame = tc.frame.import_csv(drugs_csv_path, delimiter="\t", header=True)
nodes_frame.schema
```

Out[2]:
```
[('id', int),
 ('name', str),
 ('CAS', str),
 ('chembl_id', str),
 ('chebi_id', str),
 ('DrugBank', str),
 ('PubChem', str),
 ('MeSH_ID', str),
 ('KEGG_drug', str),
 ('SMILES', str),
 ('InChI', str)]
```

SPARK SUMMIT 2017

In [3]:
```
# Drop columns that we don't need and then inspect data
nodes_frame.drop_columns(["CAS", "chembl_id", "chebi_id", "DrugBank", "PubChem", "MeSH_ID", "KEGG_drug", "InChI"])
nodes_frame.inspect()
```

Out[3]:
```
[#]  id  name
=======================
[0]   0  vanoxerine
[1]   1  nipecotic acid
[2]   2  betaxolol
[3]   3  oxybutynin
[4]   4  indapamide
[5]   5  5248896
[6]   6  tamoxifen
[7]   7  halcinonide
[8]   8  flucytosine
[9]   9  terazosin

[#]  SMILES
================================================================================
[0]  C1=CC=C(C=C1)/C(=N/NC2=C(C=C(C=C2)[N+](=O)[O-])[N+](=O)[O-])/CCl
[1]  C1CC(CNC1)C(=O)O
[2]  CC(C)NCC(COC1=CC=C(C=C1)CCOCC2CC2)O
[3]  CCN(CC)CC#CCOC(=O)C(C1CCCCC1)(C2=CC=CC=C2)O
[4]  CC1CC2=CC=CC=C2N1NC(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N
[5]  C1(C(C([N-]C(C1Cl)Cl)C(=O)O)Cl)N.C1(C(=C(C(=C([N-]1)Cl)Cl)N)Cl)C(=O)O.[NH2-].O.O.[Mn].[Mn].[Mn+2]
[6]  CC/C(=C(\C1=CC=CC=C1)/C2=CC=C(C=C2)OCCN(C)C)/C3=CC=CC=C3
[7]  C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@]2([C@H](C[C@]4([C@H]3C[C@@H]5[C@]4(OC(O5)(C)C)C(=O)CCl)C)O)F
[8]  C1=NC(=O)NC(=C1F)N
[9]  COC1=C(C=C2C(=C1)C(=NC(=N2)N3CCN(CC3)C(=O)C4CCCO4)N)OC
```

## Calculating the similarity between drugs

Next, we are going to compare the similarity between drugs by calculating the tanimoto coefficient. First, we will create an frame of edges which will connect one drug to another (representing the two drugs that we will compare). For simplicity, we are importing this data from a file that has already been saved off with the top 20 most similar connections for each drug.

In [4]:
```
edges_csv_path = "hdfs://10.7.151.77/user/atkuser/drug-edges-20.csv"
schema = [("source_id", int), ("dest_id", int)]
edges_frame = tc.frame.import_csv(edges_csv_path, schema=schema, header=True, delimiter="\t")
edges_frame.inspect()
```

Out[4]:

| [#] | source_id | dest_id |
|---|---|---|
| [0] | 190 | 638 |
| [1] | 190 | 1260 |
| [2] | 190 | 100 |
| [3] | 190 | 916 |
| [4] | 190 | 139 |
| [5] | 190 | 228 |
| [6] | 190 | 201 |
| [7] | 190 | 62 |
| [8] | 190 | 935 |
| [9] | 190 | 77 |

In [5]:
```
print "Nodes: {0}".format(nodes_frame.count())
print "Edges: {0}".format(edges_frame.count())
```

```
Nodes: 1278
Edges: 25560
```

Next, we join the `nodes_frame` with the `edges_frame` so that we have one frame with the drug information (drug name and SMILES index) for the source and destination (the two drugs that we are comparing).

In [6]:
```
# join the edges frame with nodes to get the smiles index for the source/target
joined = nodes_frame.join_right(edges_frame, left_on="id", right_on="source_id")
joined = nodes_frame.join_right(joined, left_on="id", right_on="dest_id")
joined.rename_columns({"name_R":"source_name", "SMILES_R":"source_SMILES","name_L":"target_name","SMILES_L":"target_SM
ILES"})
joined.inspect()
```

Out[6]:
```
[#]  target_name  target_SMILES
=================================================================================
[0]  5224221      Cl=CC(=C(C=C1C2=CSC(=N2)C3=CC4=C(C=CC(=C4)Br)OC3=O)Cl)Cl
[1]  5224221      Cl=CC(=C(C=C1C2=CSC(=N2)C3=CC4=C(C=CC(=C4)Br)OC3=O)Cl)Cl
[2]  5224221      Cl=CC(=C(C=C1C2=CSC(=N2)C3=CC4=C(C=CC(=C4)Br)OC3=O)Cl)Cl
[3]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O
[4]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O
[5]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O
[6]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O
[7]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O
[8]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O
[9]  decitabine   Cl[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O

[#]  source_name
=================
[0]  merbromin
[1]  oxaprozin
[2]  nizatidine
[3]  azacitidine
[4]  rilmenidine
[5]  minoxidil
[6]  8-azaguanine
[7]  idoxuridine
[8]  trifluridine
[9]  riboflavin

[#]  source_SMILES
=================================================================================
[0]  Cl=CC=C(C(=Cl)C2=C3C=C(C(=O)C=C3OC4=C(C(=C(C=C24)Br)[O-])[Hg])Br)C(=O)[O-].O.O.O.O.[Na+].[Na+]
[1]  Cl=CC=C(C=Cl)C2=C(OC(=N2)CCC(=O)O)C3=CC=CC=C3
[2]  CN/C(=C\[N+](=O)[O-])/NCCSCC1=CSC(=N1)CN(C)C
[3]  Cl=NC(=NC(=O)N1[C@H]2[C@@H]([C@@H]([C@H](O2)CO)O)O)N
[4]  ClCC1C(C2CC2)NC3=NCCO3
```

Now that we have a frame (called `joined`) that has all the data that we need in order to compare drugs, we are defining a function (`calculate_tanimoto`) that uses the `rdkit` libraries to calculate the tanimoto coefficient from two SMILES strings. We are then adding a new column to the frame using the `calculate_tanimoto()` function. A column with the rounded tanimoto coefficient is also added to the frame, to be used later with generating a histogram.

In [7]:
```
# define function returns the tanimoto coefficient based on the SMILES index for two drugs
def calculate_tanimoto(smiles1, smiles2):
    mol1 = Chem.MolFromSmiles(smiles1)
    mol2 = Chem.MolFromSmiles(smiles2)
    return DataStructs.FingerprintSimilarity(FingerprintMols.FingerprintMol(mol1),FingerprintMols.FingerprintMol(mol2)
)

# add a column with the calculated tanimoto coefficient
joined.add_columns(lambda row: calculate_tanimoto(row.source_SMILES, row.target_SMILES), ("tanimoto", float))
joined.add_columns(lambda row: round(row.tanimoto,1), ("rounded_tanimoto", float))

joined.inspect(20, columns=["source_name", "target_name", "tanimoto", "rounded_tanimoto"])
```

Out[7]:

| [##] | source_name | target_name | tanimoto | rounded_tanimoto |
|---|---|---|---|---|
| [0] | merbromin | 5224221 | 0.442685243825 | 0.4 |
| [1] | oxaprozin | 5224221 | 0.302759134974 | 0.3 |
| [2] | nizatidine | 5224221 | 0.364485981308 | 0.4 |
| [3] | azacitidine | decitabine | 0.833558863329 | 0.8 |
| [4] | rilmenidine | decitabine | 0.405829596413 | 0.4 |
| [5] | minoxidil | decitabine | 0.329758713137 | 0.3 |
| [6] | 8-azaguanine | decitabine | 0.363150867824 | 0.4 |
| [7] | idoxuridine | decitabine | 0.525720164609 | 0.5 |
| [8] | trifluridine | decitabine | 0.504347826087 | 0.5 |
| [9] | riboflavin | decitabine | 0.304016620499 | 0.3 |
| [10] | zalcitabine | decitabine | 0.544589774078 | 0.5 |
| [11] | zidovudine | decitabine | 0.429609445958 | 0.4 |
| [12] | promethazine | prochlorperazine | 0.75415282392 | 0.8 |
| [13] | Prestwick-685 | prochlorperazine | 0.307639836289 | 0.3 |
| [14] | trazodone | prochlorperazine | 0.326105810928 | 0.3 |
| [15] | perphenazine | prochlorperazine | 0.979651162791 | 1.0 |
| [16] | moracizine | prochlorperazine | 0.612798264642 | 0.6 |
| [17] | clozapine | prochlorperazine | 0.304273504274 | 0.3 |
| [18] | diazoxide | prochlorperazine | 0.312984496124 | 0.3 |
| [19] | mesoridazine | prochlorperazine | 0.624309392265 | 0.6 |

## Graph analytics using degree centrality

In order to run graph algorithms using sparktk, we'll need to create a `graph` object using a frame of nodes and a frame of edges. We will use the original `nodes_frame` to create the graph, and then create a new frame of `graph_edges`. The csv being imported to create the `graph_edges` frame has columns for `src`, `dst`, and `tanimoto` and is filtered to only include connections where the tanimoto coefficient is greater than 0.4.

In [8]:
```
edge_schema = [("src", int),("dst", int),("tanimoto",float)]
graph_edges = tc.frame.import_csv("hdfs://10.7.151.77/user/atkuser/drug-edges-gt-4.csv", schema=edge_schema)
graph_edges.inspect()
```

Out[8]:
```
[#]  src   dst  tanimoto
==============================
[0]   631   31  0.494117647059
[1]    32   31       0.47265625
[2]   234   31   0.40782122905
[3]   634   31           0.44
[4]   834   31  0.447058823529
[5]    35   31  0.476767676768
[6]   236   31  0.443264393516
[7]  1036   31  0.446569178853
[8]    37   31   0.41488162345
[9]  1237   31  0.412100456621
```

In [9]:
```
# create graph
graph = tc.graph.create(nodes_frame, graph_edges)

# run degree centrality algorithm, and then sort frame to find drugs with more high tanimoto connections
result = graph.degree_centrality("out")
result.sort("degree_centrality", False)
result.inspect(20, columns=["name", "degree_centrality"])
```

Out[9]:
```
[##]  name                    degree_centrality
============================================
[0]   isometheptene              0.980422866092
[1]   oxamic acid                0.978073610023
[2]   3-nitropropionic acid      0.977290524667
[3]   pentolonium                0.972592012529
[4]   heptaminol                 0.969459671104
[5]   carbachol                  0.960062646829
[6]   mephentermine              0.946750195771
[7]   mevalolactone              0.942051683634
[8]   nipecotic acid             0.939702427565
[9]   paracetamol                0.935003915427
[10]  bemegride                  0.926389976507
```

## Exporting data to postgres and creating tables in superset

In order to visualize the data in superset, we need to export the data to a database. sparktk has methods that make it easy to export to database such as postgres, which is being used in this demo. Once the frame has been exported to postgres, we then use superset's python library to add the table so that the data can be viewed from the superset dashboard.

In [10]:
```
%%capture
import superset
```

In [11]:
```
def create_table(frame, database_name, table_name, table_description=""):
    # export train frame to postgres, and create table in superset
    db_connection_str = "jdbc:postgresql://localhost/{0}?user=*&password=*".format(database_name)
    frame.export_to_jdbc(db_connection_str, table_name)
    sql_table = superset.models.SqlaTable

    tbl = superset.db.session.query(sql_table).filter_by(table_name=table_name).first()

    if not tbl:
        tbl = sql_table(table_name=table_name)

    # copy database info from the existing table - replace this with getting Database
    db = superset.db.session.query(superset.models.Database).filter_by(database_name=database_name).first()

    # set table properties
    tbl.database = db
    tbl.description = table_description
    tbl.is_featured = True

    # merge and commit table
    superset.db.session.merge(tbl)
    superset.db.session.commit()
    tbl.fetch_metadata()
```

In [12]:
```
create_table(joined, database_name="postgres", table_name="drug_graph2")
```

# Backup – Superset Dashboard

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## Drug Graph ★

**DrugFilter**

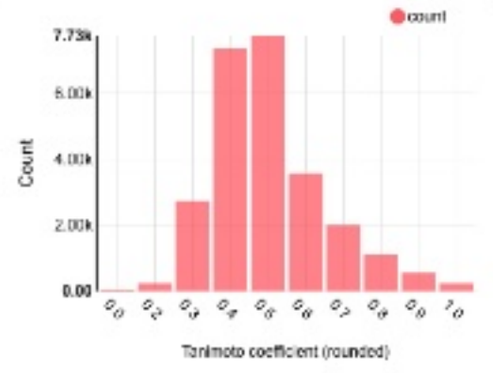
source_name

Select [source_name]

target_name

Select [target_name]

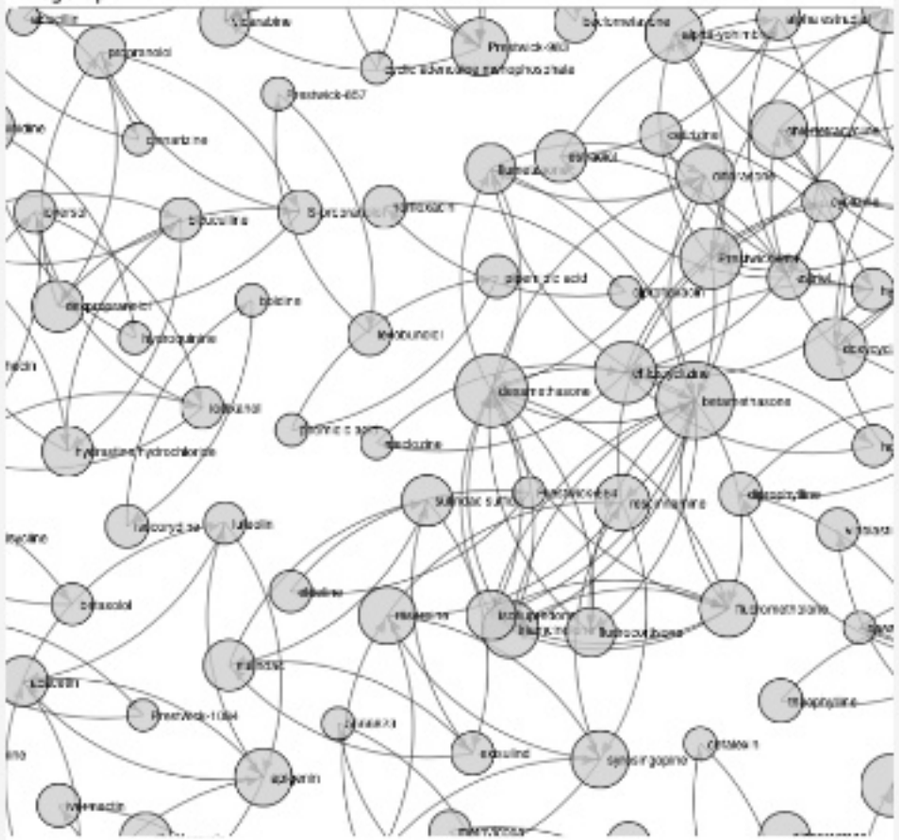
**Tanimoto distribution**




**Drug Connection Count**

| count |
|---|
| 25560 |

**DrugGraph**



**Drug Table**

Show 25 entries

| source_name | target_name | tanimoto |
|---|---|---|
| cinchonine | cinchonidine | 1 |
| alpha estradiol | estradiol | 1 |
| flumetasone | diflorasone | 1 |
| corynanthine | alpha-yohimbine | 1 |
| dexamethasone | betamethasone | 1 |
| (+)-isoprenaline | (-)-isoprenaline | 1 |
| etiocholanolone | epiandrosterone | 1 |
| cinchonidine | cinchonine | 1 |
| dexpropranolol | S-propranolol | 1 |
| androsterone | epiandrosterone | 1 |
| benzylpenicillin | benzathine benzylpenicillin | 1 |
| paromomycin | neomycin | 1 |
| estradiol | alpha estradiol | 1 |
| epivincamine | vincamine | 1 |
| Prestwick-585 | clofazimine | 1 |
| androsterone | etiocholanolone | 1 |
| emetine | cephaeline | 1 |
| propranolol | S-propranolol | 1 |
| propranolol | dexpropranolol | 1 |
| (+/-)-catechin | Prestwick-642 | 1 |
| tretinoin | isotretinoin | 1 |
| Prestwick-557 | levobunolol | 1 |
| (-)-isoprenaline | (+)-isoprenaline | 1 |
| corynanthine | yohimbine | 1 |
| S-propranolol | propranolol | 1 |

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Superset Security Manage Sources Slices Dashboards SQL Lab

# Drug Graph ★

## DrugFilter

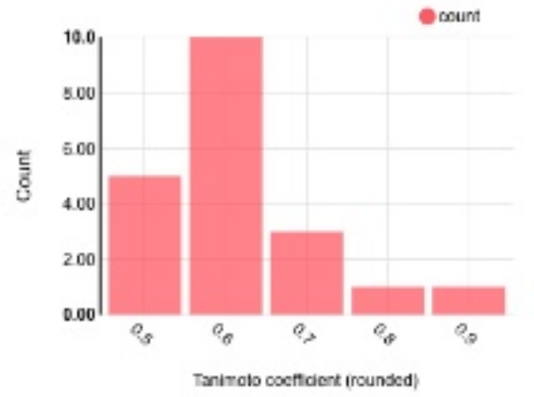
source_name

× levodopa

target_name

Select [target_name]

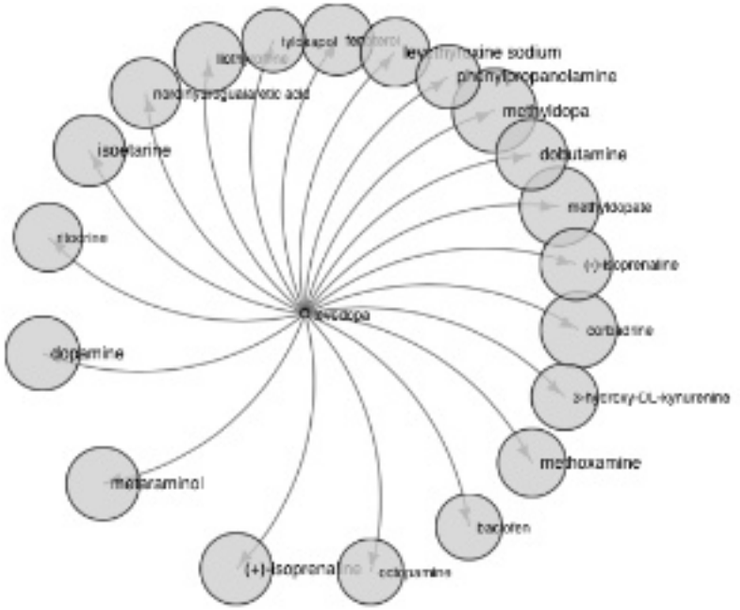
## Tanimoto distribution




## Drug Connection Count

| count |
|---|
| 20 |

## DrugGraph




## Drug Table

Show 25 entries

| source_name | target_name | tanimoto |
|---|---|---|
| levodopa | methyldopa | 0.898181818181818 |
| levodopa | methyldopate | 0.781645569620253 |
| levodopa | corbadrine | 0.72318339100346 |
| levodopa | dopamine | 0.676113360323887 |
| levodopa | metaraminol | 0.653710247349823 |
| levodopa | (-)-isoprenaline | 0.628289473684211 |
| levodopa | (+)-isoprenaline | 0.628289473684211 |
| levodopa | fenoterol | 0.625 |
| levodopa | isoetarine | 0.622093023255814 |
| levodopa | dobutamine | 0.616393442622951 |
| levodopa | nordihydroguaiaretic acid | 0.592982456140351 |
| levodopa | liothyronine | 0.581578947368421 |
| levodopa | levothyroxine sodium | 0.58005249343832 |
| levodopa | ritodrine | 0.565916398713826 |
| levodopa | methoxamine | 0.5625 |
| levodopa | 3-hydroxy-DL-kynurenine | 0.526992287917738 |
| levodopa | baclofen | 0.518633540372671 |
| levodopa | octopamine | 0.512820512820513 |
| levodopa | phenylpropanolamine | 0.49014440433213 |
| levodopa | tyloxapol | 0.466887417218543 |

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