

A bioassay Object

assay identifier (aid)

data source

assay type

target species

scoring method

target(s)

target category

compound activity scores

Compound	Activity	Raw Score
Compound 1	0	56
Compound 2	2	99
...

B bioassayDB SQL Database

activity table

Compound	Activity	Raw Score	Assay
Compound 1	0	56	100
Compound 2	2	99	100
...

assay details table

assay targets table

target protein domains

target protein identifier map

assay data sources



User Supplied Data

Public Domain Data

C bioassaySet Object

compound vs assay activity
sparse matrix

compounds

1	2	...
...	2	1
...	1

assays

all other data from
bioassay child objects

getBioassaySetByCids()
getAssays()

Active or Selective
Targets and Compounds

D Compound-Target Matrix

compound vs target activity
sparse matrix

compounds

1	2
...	...	2	...	1
...	1	...	1	...

targets

perTargetMatrix()

Bioactivity Fingerprints