Introduction to CellMiner

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Topics to be Covered

- Introduction to CellMiner
- Introduction to rcellminer

What is CellMiner?

- Website:
  - http://discover.nci.nih.gov/cellminer
- Retrieval and integration for NCI-60 datasets: molecular and pharmacological
- NCI-60
  - 60 human cancer cell lines from 9 tissues of origin: breast, central nervous system, colon, leukemia, melanoma, non-small cell lung, ovarian, prostate, and renal
  - Used by the Developmental Therapeutics Program of the National Cancer Institute to screen over 100,000 chemical compounds and natural products
- A subset of ~21,000 drugs is provided by CellMiner
- Drug activity levels expressed as 50% growth-inhibitory levels (GI50) were determined at 48 hours using the sulforhodamine B (SRB) assay
  - Determines cell density based on the measurement of total cellular protein

What is rcellminer?

- Website and Tutorial (Vignette):
  - https://www.bioconductor.org/packages/release/bioc/html/rcellminer.html
- Publication:
  - http://www.ncbi.nlm.nih.gov/pubmed/26635141
- Provides programmatic access to CellMiner NCI-60 data
- Data Types
  - Gene and protein expression, copy number, whole exome mutations, etc
  - Activity data for ~21K compounds and information on their structure, mechanism of action, and repeat screens
- Easy visualization of compound structures, activity patterns, and molecular feature profiles
- Embedded R Shiny applications allow interactive data exploration

Pattern Comparison using rcellminer

```r
library(rcellminer)

# Get drug and expression data
drugAct <- exprs(getAct(rcellminerData::drugData))
expData <- getAllFeatureData(rcellminerData::molData)[["exp"]]

# Create pattern of interest
patternOfInterest <- expData["SLFN11", ]

# Run pattern comparison to get correlated drugs and other gene expressions
r1 <- patternComparison(patternOfInterest, drugAct)
r2 <- patternComparison(patternOfInterest, expData)

head(r1, 3)
```

```
             COR         PVAL
639174 0.8343842 1.227589e-16
681636 0.7967239 1.243962e-13
34462  0.7950691 3.302182e-14
```

```r
head(r2, 3)
```

```
               COR         PVAL
SLFN11   1.0000000 0.000000e+00
BCAT1    0.5847423 9.298535e-07
CCDC181  0.5766713 1.419268e-06
```

Embedded Shiny Applications

- Simplified web applications to do common data exploration tasks
  - Compare any two molecular and drug profiles
  - Find related structures
  - View information on repeat screening for drug compounds

Getting Help

- CellMiner
  - webadmin@discover.nci.nih.gov
- rcellminer
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