

# Package ‘SMAD’

April 11, 2023

**Type** Package

**Title** Statistical Modelling of AP-MS Data (SMAD)

**Version** 1.14.1

**Description** Assigning probability scores to prey proteins captured in affinity purification mass spectrometry (AP-MS) experiments to infer protein-protein interactions. The output would facilitate non-specific background removal as contaminants are commonly found in AP-MS data.

**Depends** R (>= 3.6.0), RcppAlgos

**Imports** magrittr (>= 1.5), dplyr, stats, tidyr, utils, Rcpp (>= 1.0.0)

**LinkingTo** Rcpp

**License** MIT + file LICENSE

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 7.1.0

**Suggests** knitr, rmarkdown, testthat, BiocStyle

**VignetteBuilder** knitr

**biocViews** MassSpectrometry, Proteomics, Software

**git\_url** <https://git.bioconductor.org/packages/SMAD>

**git\_branch** RELEASE\_3\_16

**git\_last\_commit** 59ba03c

**git\_last\_commit\_date** 2022-11-27

**Date/Publication** 2023-04-10

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 CompPASS

*CompPASS*


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## Description

CompPASS Comparative Proteomic Analysis Software Suite (CompPASS) is based on spoke model. This algorithm was developed by Dr. Mathew Sowa for defining the human deubiquitinating enzyme interaction landscape (Sowa, Mathew E., et al., 2009). The implementation of this algorithm was inspired by Dr. Sowa's online tutorial (<http://besra.hms.harvard.edu/ipmsmsdbs/cgi-bin/tutorial.cgi>). The output includes Z-score, S-score, D-score and WD-score. This function also computes entropy and normalized WD-score. The source code for this function was based on the source code. <https://github.com/dnusinow/cRomppass>

## Usage

```
CompPASS(datInput)
```

## Arguments

datInput	A dataframe with column names: idRun, idBait, idPrey, countPrey. Each row represent one unique protein captured in one pull-down experiment
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## Value

A data frame consists of unique bait-prey pairs with Z-score, S-score, D-score and WD-score indicating interacting probabilities.

## Author(s)

Qingzhou Zhang, <zqzneptune@hotmail.com>

## References

- Sowa, Mathew E., et al. "Defining the human deubiquitinating enzyme interaction landscape." Cell 138.2 (2009): 389-403. <https://doi.org/10.1016/j.cell.2009.04.042>
- Huttlin, Edward L., et al. "The BioPlex network: a systematic exploration of the human interactome." Cell 162.2 (2015): 425-440. <https://doi.org/10.1016/j.cell.2015.06.043>
- Huttlin, Edward L., et al. "Architecture of the human interactome defines protein communities and disease networks." Nature 545.7655 (2017): 505. <https://www.nature.com/articles/nature22366>

**Examples**

```
data(TestDatInput)
datScore <- CompPASS(TestDatInput)
head(datScore)
```

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DICE

*DICE*

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**Description**

DICE The Dice coefficient is used to score the interaction affinity between two proteins.

**Usage**

```
DICE(datInput)
```

**Arguments**

`datInput` A dataframe with column names: `idRun`, `idPrey`. Each row represent one unique protein captured in one pull-down experiment.

**Value**

A dataframe consists of pairwise combination of preys identified in the input with DICE scores.

**Author(s)**

Qingzhou Zhang, <qzqneptune@hotmail.com>

**References**

Bing Zhang et al., From pull-down data to protein interaction networks and complexes with biological relevance, *Bioinformatics*, Volume 24, Issue 7, 1 April 2008, Pages 979–986, <https://doi.org/10.1093/bioinformatics/btn036>

**Examples**

```
data(TestDatInput)
datScore <- DICE(TestDatInput)
head(datScore)
```

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Hart

*Hart*

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### Description

Hart Scoring algorithm based on a hypergeometric distribution error model (Hart et al.,2007).

### Usage

```
Hart(datInput)
```

### Arguments

datInput            A dataframe with column names: idRun, idPrey. Each row represent one unique protein captured in one pull-down experiment.

### Value

A dataframe consists of pairwise combination of preys identified in the input with Hart scores indicating interacting probabilities computed from negative log transformed Hypergeometric test P-values.

### Author(s)

Qingzhou Zhang, <zqzneptune@hotmail.com>

### References

Hart, G. Traver, Insuk Lee, and Edward M. Marcotte. 'A high-accuracy consensus map of yeast protein complexes reveals modular nature of gene essentiality.' BMC bioinformatics 8.1 (2007): 236. <https://doi.org/10.1186/1471-2105-8-236>

### Examples

```
data(TestDatInput)
datScore <- Hart(TestDatInput)
head(datScore)
```

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HG	<i>HGScore</i>
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### Description

HGScore Scoring algorithm based on a hypergeometric distribution error model (Hart et al.,2007) with incorporation of NSAF (Zybailov, Boris, et al., 2006) . This algorithm was first introduced to predict the protein complex network of *Drosophila melanogaster* (Guruharsha, K. G., et al., 2011). This scoring algorithm was based on matrix model.

### Usage

```
HG(datInput)
```

### Arguments

datInput	A dataframe with column names: idRun, idPrey, countPrey, lenPrey. Each row represent one unique protein captured in one pull-down experiment.
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### Value

A dataframe consists of pairwise combination of preys identified in the input with HG scores indicating interacting probabilities computed from negative log transformed Hypergeometric test P-values.

### Author(s)

Qingzhou Zhang, <qzqneptune@hotmail.com>

### References

Guruharsha, K. G., et al. 'A protein complex network of *Drosophila melanogaster*.' *Cell* 147.3 (2011): 690-703. <https://doi.org/10.1016/j.cell.2011.08.047>

Hart, G. Traver, Insuk Lee, and Edward M. Marcotte. 'A high-accuracy consensus map of yeast protein complexes reveals modular nature of gene essentiality.' *BMC bioinformatics* 8.1 (2007): 236. <https://doi.org/10.1186/1471-2105-8-236>

Zybailov, Boris, et al. 'Statistical analysis of membrane proteome expression changes in *Saccharomyces cerevisiae*.' *Journal of proteome research* 5.9 (2006): 2339-2347. <https://doi.org/10.1021/pr060161n>

### Examples

```
data(TestDatInput)
datScore <- HG(TestDatInput)
head(datScore)
```

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PE

*PE*

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### Description

PE Incorporated both spoke and matrix model.

### Usage

```
PE(datInput, rBait = 0.37, cntPseudo = 1)
```

### Arguments

<code>datInput</code>	A dataframe with column names: <code>idRun</code> , <code>idBait</code> , <code>idPrey</code> , Each row represent one unique protein captured in one pull-down experiment.
<code>rBait</code>	The value of the 'r' parameter as described in the publication.
<code>cntPseudo</code>	The value of the 'pseudo count' parameter.

### Value

A dataframe consists of protein-protein interactions from both Spoke and Matrix model.

### Author(s)

Qingzhou Zhang, <zqzneptune@hotmail.com>

### References

Collins, Sean R., et al. "Toward a comprehensive atlas of the physical interactome of *Saccharomyces cerevisiae*." *Molecular & Cellular Proteomics* 6.3 (2007): 439-450. <https://doi.org/10.1074/mcp.M600381-MCP200>

### Examples

```
data(TestDatInput)
datScore <- PE(TestDatInput, 0.37, 1)
head(datScore)
```

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TestDatInput	<i>Test data for SMAD</i>
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**Description**

It is a subset of unfiltered BioPlex 2.0 consisting of apoptosis as bait proteins

**Usage**

```
data(TestDatInput)
```

**Format**

A data frame with 5000 rows and 5 variables

**Details**

- idRun A unique identifier for one AP-MS run
- idBait A unique identifier for the bait protein
- idPrey A unique identifier for the prey protein
- countPrey Sepctra/Peptider count for the prey protein
- lenPrey Protein length for the prey protein

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