

Package ‘omd’

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Type Package

Title filter the molecular descriptors for QSAR

Version 1.0

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Description This package including two useful function, which can be used for filter the molecular descriptors matrix for QSAR.

License GPL (>= 2)

LazyLoad yes

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omd-package *filter and optimize the molecular descriptors for QSAR*

Description

This package including two useful function, which can be used for filter the molecular descriptors matrix for QSAR.

Details

Package: omd
Type: Package
Version: 1.0
Date: 2009-09-16
License: GPL (>= 2)
LazyLoad: yes

omd including two functions, fcons and fcor, which can delete constant and high correlated molecular descriptors, respectively.

Author(s)

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References

Ma B, Chen HH, He Y, Xu JM 2009 Quantitative structure-activity relationship (QSAR) models based on molecular structure and effect sizes of polycyclic aromatic hydrocarbons (PAHs) dissipation in rhizosphere. Environmental Pollution (Submitted).

fcons *filter the constant molecular descriptors*

Description

this function can filter the constant molecular descriptors in data matrix.

Usage

```
fcons(indices,k)
```

Arguments

indices a matrix contain a range of molecular descriptors
k a number define what is constant molecular descriptors

Details

The constant molecular descriptors depend on the number of values for one molecular descriptors, we can define it as one, two, three or even more. This depends on the condition of matrix and the aim of the study.

Value

the returned value is a matrix excluding the defined constant molecular descriptors

Author(s)

Ma B

fhcor *filter molecular descriptors with high correlation coefficient*

Description

this function can filter the molecular descriptors with high correlation coefficient in data matrix.

Usage

```
fhcor(indices,k)
```

Arguments

indices a matrix contain a range of molecular descriptors
k a number define high correlation between molecular descriptors

Details

The correlation coefficient between molecular descriptors is generally 0.95, but we also set as 0.99 or 0.9, depended on the aim and condition of study.

Value

the returned value is a matrix excluding the defined high correlation coefficient molecular descriptors

Author(s)

Ma B

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