R documentation

of 'trainChemPC.Rd'

December 1, 2013

---

trainChemPC *trainChemPC*

Description

This function performs learning step of GP and EI.

Usage

```
trainChemPC( trainData, targetVector)
```

Arguments

trainData	trainData specifies a data frame including an array of a training data with dimension of n*m. This data is used in to find a hyperlog vector.
targetVector	targetVector is a one dimensional array with n rows which is equal to number of rows in trainData.

Details

This function performs training step of GP or EI by finding a loghyper using gpr package. A loghyper can be used to predict potent compounds.

Value

It returns a vector that holds a calculated loghyper.

Author(s)

Mohsen Ahmadi

References

1. Predicting Potent Compounds via Model-Based Global Optimization, Journal of Chemical Information and Modeling, 2013, 53 (3), pp 553-559, M Ahmadi, M Vogt, P Iyer, J Bajorath, H Froehlich. 2. Software MOE is used to calculate the numerical descriptors in data sets. Ref: http://www.chemcomp.com/MOE-Molecular_Operating_Environment.htm 3. ChEMBL was the source of the compound data and potency annotations in data sets. Ref: https://www.ebi.ac.uk/chembl/

Examples

```
library(gpr)
library(SimuChemPC)
a = as.data.frame(array(1:10, dim=c(2,5)))
b = array(1:2)
myloghyper = trainChemPC( a, b)
```

Index