

Rchemcpp - Kernels for molecules

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1 Introduction

The Rchemcpp package is part of the CRAN project. The functionality of Chemcpp (<http://chemcpp.sourceforge.net/html/index.html>) is provided in R, that is the computation of similarities between molecules by kernel functions. The following kernels are implemented:

- the marginalized graph kernel between labeled graphs (Kashima *et al.* 2004).
- extensions of the marginalized kernel (Mahé *et al.* 2004).
- Tanimoto kernels (Ralaivola *et al.* 2005).
- graph kernels based on tree patterns (Mahé and Vert 2009).
- kernels based on pharmacophores for 3D structure of molecules (Mahé *et al.* 2006).

2 Getting started and quick start

To load the package, enter the following in your R session:

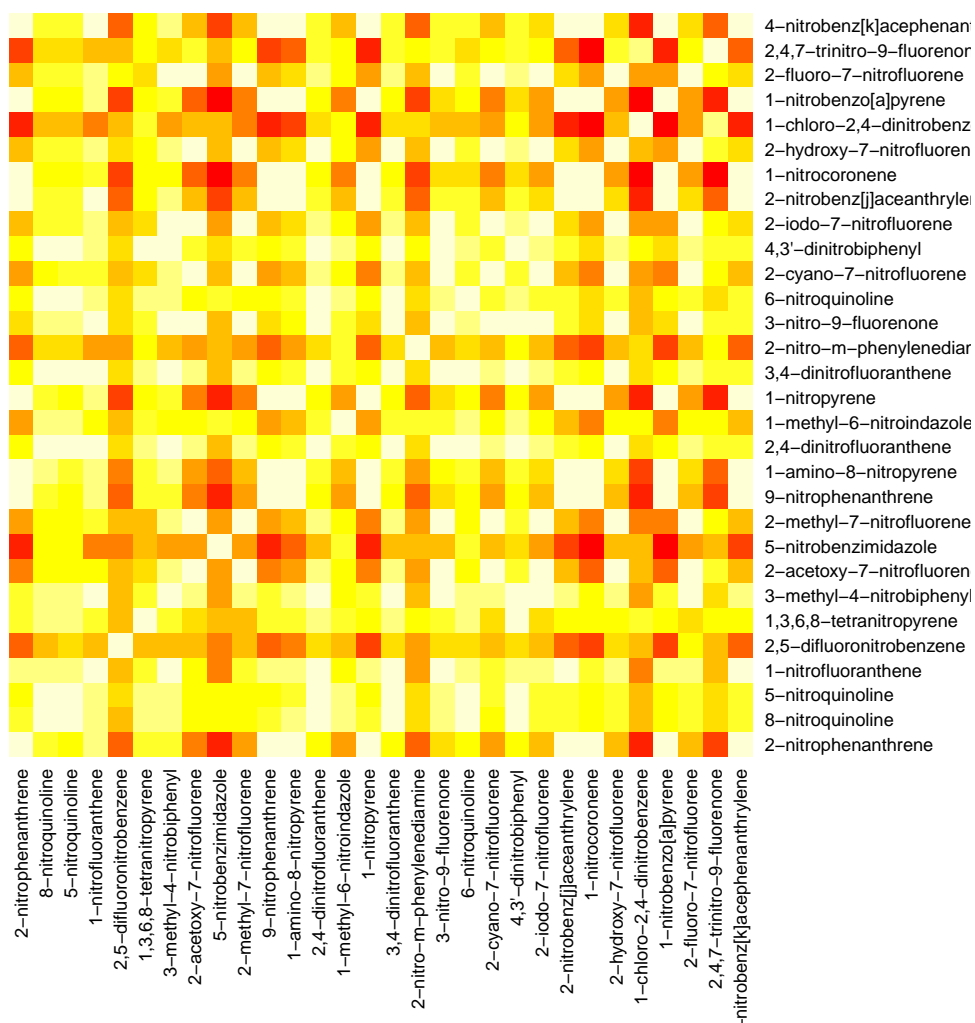
```
> library(Rchemcpp)
```

We enter the filename of and SDF file to the function `sd2gram`. This function computes the similarity of the molecules with the marginalized kernel (Kashima *et al.* 2004) approach.

```
> sdfolder <- system.file("sample_data", package="Rchemcpp")
> sdf <- list.files(sdfolder, full.names=TRUE, pattern="small")
> K <- sd2gram(sdf, returnNormalized=TRUE)
```

The similarity values are now stored in K. We visualize this matrix as a heatmap.

```
> heatmap(K, Rowv=NA, Colv=NA, scale="none")
```

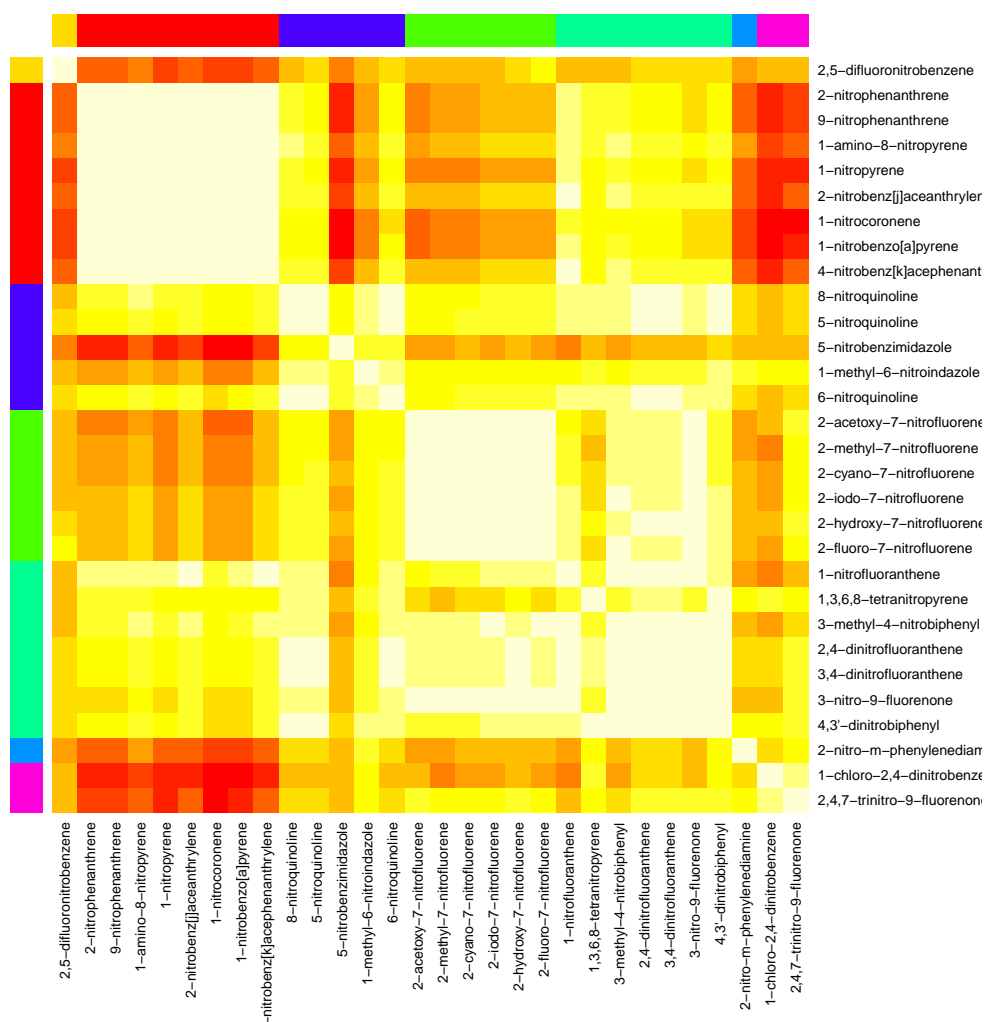


3 Molecular similarity for clustering

Based on the similarity measure we can run clustering algorithms on the data in order to find groups among the molecules. We use Affinity Propagation Clustering (Frey and Dueck 2007) as implemented by Bodenhofer *et al.* (2011) for this task, because the cluster centers are real molecules.

```
> library(apcluster)
> r <- apcluster(K)

> plot(r,K)
```



References

Bodenhofer, U., Kothmeier, A., and Hochreiter, S. (2011). APCluster: an R package for affinity propagation clustering. *Bioinformatics*, **27**, 2463–2464.

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