compounds selection

SDF of a sublibrary

visualization of selected structures

SDF of a library

cmp.parse

descriptor database
db$descdb[[i]]

cmp.duplicated

duplication array
cmp.parse1
db.explain
descriptor description

cmp.search

SDF of a compound

cmp.similarity

similar compounds

cluster size statistics

cluster sizestat

cluster visualization

cluster

clusters

cmp.cluster

comparison

searching

similar value

cmp.search

SDF of a sublibrary

cmp.duplicated