

## **Get MACCS Keys**

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### **Notes:**

1. This Jython script works in Sarchitect Designer version 2.2
2. Learn about Sarchitect Designer – <http://www.strandls.com/sarchitect/index.html>
3. Get Sarchitect – <http://www.strandls.com/sarchitect/freetrial.php>

*The actual script follows this discussion on page 2. It is also accessible directly from the webpage in .py format.*

### **Discussion:**

The script displays 166 MACCS Keys for the given compounds in a 166 columns table view. Such information may be helpful in say, running clustering or similarity analysis based on the MACCS keys.

Input:

- i) 'Molecule'/'Structure'/'Optimized Structures' column
- ii) 'Identifier' column

(Change the column names in the script, at lines#24 & #25, if your input columns are differently named).

Output:

MACCS keys displayed in a (total\_rows \* 166\_column) table view. Presently, one needs to export this table either back to the spreadsheet (as appended columns) or externally as a text file & open it again in sarchitect designer 2.2 to run further analysis.

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### **Cite this as:**

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##
##
## sarchitect designer 2.2 script to get MACCS Keys (length 166) in individual columns
##
## INPUT: 'Molecule'/Structure'/Optimized Structures' column;
##      this would be used by backend to compute MACCS Keys (166 bit-length)
##
##      'Identifier' column for some formatted table-view
##
##
## OUTPUT: MACCS Keys in a (total_rows X 166_column) table view.
##
##
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##
##

from script.omega import createComponent, showDialog
from javax.swing import *

dataset = script.project.getActiveDataset()

strCol = dataset.getColumn('Structure') ## change this according to your data
id_col = dataset.getColumn('Identifier') ## change this according to your data

result = script.algorithm.ComputeMACCSKey(structure=strCol).execute(displayResult=0)
keys = result['maccskeymatrix']
#print keys[0]

rows = [ ]
for colldx in range(len(keys[0])):
    col = [ ]
    for rowldx in range(len(keys)):
        val = keys[rowldx][colldx]
        col.append(val)
    #print col
    new_col = script.dataset.createIntColumn("Key" + str([colldx+1]), col)
    rows.append(new_col)

## end of for loop

## create dataset, launch view
tmpset = script.dataset.createDataset("Keys", [id_col])
for i in range(len(rows)):
    tmpset.addColumn(rows[i])

view = script.view.Table(dataset=tmpset,rowHeight=20)
view.__state__['enableExportColumns'] = 1
view.show()

## report completion
```

```
parent=script.tool.getTool().getFrame()
mesg = "Done With Script Execution."
JOptionPane.showMessageDialog(parent,mesg,"STATUS!",JOptionPane.INFORMATION_MESS
AGE)
```

```
##
## END
##
```

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