

SubStructure Analysis for CGAS Project

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Loading the required packages

```
library("ChemmineR")  
library("fmcsR")  
library("ape")
```

```
## Warning: package 'ape' was built under R version 4.0.3
```

Setting up the working directory

```
setwd("D:/Google Drive/PhD/Courses/Semester 2/CGS/Project")
```

Loading the sdf file - the sdf file was generated using openbabel gui from the SMILES of the molecules

```
AI <- read.SDFset("Actives_Inactives.sdf")
```

Calculating the pairwise similarity matrix for all the molecules

```
d1 <- data.frame(sapply(cid(AI), function(x) fmcsBatch(AI[x], AI, au=0, bu=0, matching.mode="aromatic")
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 6  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 4  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 6  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 2  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 1  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 3  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
## Warning in fmcsBatch(AI[x], AI, au = 0, bu = 0, matching.mode = "aromatic"): 3  
## comparisons exeeded the timeout of 60000ms and did not complete
```

```
head(d1)
```

```
##      CMP1      CMP2      CMP3      CMP4      CMP5      CMP6 CMP7      CMP8
## CMP1  1.0 0.6000000 0.6000000 0.8000000 0.6000000 0.6000000 0.75 0.6000000
## CMP2  0.6 1.0000000 0.6363636 0.5714286 1.0000000 1.0000000 1.00 0.4000000
## CMP3  0.6 0.6363636 1.0000000 0.8571429 0.7777778 0.7000000 1.00 0.6000000
## CMP4  0.8 0.5714286 0.8571429 1.0000000 0.4285714 0.5714286 1.00 0.8571429
## CMP5  0.6 1.0000000 0.7777778 0.4285714 1.0000000 1.0000000 0.75 0.3333333
## CMP6  0.6 1.0000000 0.7000000 0.5714286 1.0000000 1.0000000 1.00 0.4000000
##      CMP9      CMP10      CMP11      CMP12      CMP13      CMP14      CMP15
## CMP1 0.8000000 0.6000000 0.8000000 0.2000000 0.6000000 0.4000000 0.6000000
## CMP2 0.6666667 1.0000000 0.5000000 0.5454545 0.7272727 0.8750000 0.9000000
## CMP3 0.8333333 0.7777778 0.5000000 0.5454545 0.7272727 0.8750000 0.7000000
## CMP4 0.8333333 0.5714286 0.5714286 0.2857143 0.4285714 0.2857143 0.5714286
## CMP5 0.5000000 0.8888889 0.3750000 0.6666667 0.7777778 0.8750000 0.8888889
## CMP6 0.6666667 1.0000000 0.5000000 0.6000000 0.8000000 0.8750000 0.9000000
##      CMP16      CMP17      CMP18      CMP19      CMP20      CMP21      CMP22
## CMP1 0.4000000 0.6000000 0.6000000 0.4000000 0.6000000 0.8000000 0.6000000
## CMP2 1.0000000 0.4000000 0.3333333 0.8888889 0.4444444 0.6666667 0.6363636
## CMP3 0.8750000 0.6000000 0.5555556 0.6666667 0.6666667 0.8333333 0.9090909
## CMP4 0.2857143 0.8571429 0.7142857 0.2857143 0.8571429 0.8333333 0.8571429
## CMP5 0.8750000 0.3333333 0.2222222 0.7777778 0.3333333 0.5000000 0.7777778
## CMP6 0.8750000 0.4000000 0.3333333 0.7777778 0.4444444 0.6666667 0.7000000
##      CMP23 CMP24 CMP25 CMP26      CMP27      CMP28      CMP29      CMP30
## CMP1 0.6000000 0.25 0.8 0.5 0.6000000 0.2000000 0.6000000 0.6000000
## CMP2 0.5000000 0.25 0.8 0.5 0.5454545 0.6000000 0.6666667 0.3636364
## CMP3 0.6666667 0.25 0.8 0.5 0.6363636 0.6000000 0.6666667 0.5454545
## CMP4 0.6666667 0.25 0.8 0.5 0.7142857 0.1428571 0.6666667 0.8571429
## CMP5 0.5000000 0.25 0.6 0.5 0.6666667 0.6666667 0.5000000 0.3333333
## CMP6 0.5000000 0.25 0.8 0.5 0.6000000 0.6000000 0.6666667 0.4000000
##      CMP31      CMP32 CMP33 CMP34      CMP35      CMP36      CMP37      CMP38
## CMP1 0.4000000 0.6000000 0.2 0.6 0.2000000 0.6000000 0.8000000 0.6000000
## CMP2 1.0000000 0.7000000 0.2 0.8 0.8333333 0.6666667 0.1818182 0.5000000
## CMP3 0.8571429 0.8000000 0.2 1.0 0.8333333 0.8333333 0.3636364 0.7500000
## CMP4 0.2857143 0.7142857 0.2 1.0 0.1666667 0.8333333 0.7142857 0.8571429
## CMP5 1.0000000 0.7777778 0.2 0.6 0.8333333 0.5000000 0.2222222 0.3750000
## CMP6 1.0000000 0.7000000 0.2 0.8 0.8333333 0.6666667 0.2000000 0.5000000
##      CMP39      CMP40      CMP41      CMP42      CMP43      CMP44      CMP45
## CMP1 0.6000000 0.4000000 0.8000000 0.6000000 0.8000000 0.6000000 0.6000000
## CMP2 0.3636364 1.0000000 0.2727273 0.9090909 0.3636364 1.0000000 0.7000000
## CMP3 0.3636364 1.0000000 0.4545455 0.6363636 0.4545455 0.6363636 0.7000000
## CMP4 0.5714286 0.2857143 0.7142857 0.5714286 0.7142857 0.5714286 0.4285714
## CMP5 0.4444444 1.0000000 0.3333333 1.0000000 0.3333333 1.0000000 0.7777778
## CMP6 0.4000000 1.0000000 0.3000000 1.0000000 0.4000000 1.0000000 0.7000000
##      CMP46      CMP47      CMP48      CMP49      CMP50      CMP51      CMP52
## CMP1 1.0000000 0.8000000 0.4000000 0.6000000 0.6000000 0.6000000 0.6000000
## CMP2 0.6363636 0.2727273 1.0000000 0.3636364 0.8181818 0.7272727 0.8181818
## CMP3 0.7272727 0.4545455 0.8750000 0.5454545 0.6363636 0.7272727 0.7272727
## CMP4 0.7142857 0.7142857 0.2857143 0.8571429 0.7142857 0.4285714 0.4285714
## CMP5 0.7777778 0.3333333 1.0000000 0.3333333 0.8888889 0.7777778 0.8888889
## CMP6 0.7000000 0.3000000 1.0000000 0.4000000 0.9000000 0.8000000 0.8000000
##      CMP53      CMP54      CMP55      CMP56      CMP57      CMP58      CMP59
## CMP1 0.6000000 0.8000000 0.6000000 0.4000000 0.6000000 0.6000000 0.6000000
```

```

## CMP2 0.6363636 0.3636364 0.3636364 0.6363636 0.8181818 0.8181818 0.8181818
## CMP3 0.6363636 0.4545455 0.5454545 0.5454545 0.6363636 0.7272727 0.7272727
## CMP4 0.4285714 0.7142857 0.8571429 0.2857143 0.5714286 0.4285714 0.4285714
## CMP5 0.7777778 0.3333333 0.3333333 0.7777778 0.8888889 0.8888889 0.8888889
## CMP6 0.7000000 0.4000000 0.4000000 0.7000000 0.9000000 0.8000000 0.8000000
##      CMP60      CMP61      CMP62      CMP63      CMP64      CMP65      CMP66
## CMP1 0.6000000 0.6000000 0.4000000 0.8000000 0.8000000 0.8000000 1.0000000
## CMP2 0.8181818 0.8181818 0.2727273 0.8000000 0.2727273 0.5714286 0.7272727
## CMP3 0.9090909 0.7272727 0.2727273 0.8000000 0.4545455 0.7142857 0.9090909
## CMP4 0.7142857 0.4285714 0.2857143 0.5714286 0.7142857 0.7142857 0.7142857
## CMP5 0.8888889 0.8888889 0.3333333 0.8888889 0.3333333 0.4285714 0.8888889
## CMP6 0.9000000 0.8000000 0.3000000 0.8000000 0.3000000 0.5714286 0.8000000
##      CMP67      CMP68      CMP69      CMP70      CMP71      CMP72      CMP73
## CMP1 0.8000000 0.8000000 0.6000000 0.8000000 0.8000000 0.8000000 1.0000000
## CMP2 0.4000000 0.4000000 0.3333333 0.2727273 0.7272727 0.8181818 0.2727273
## CMP3 0.6000000 0.6000000 0.3333333 0.4545455 1.0000000 0.9090909 0.4545455
## CMP4 0.8571429 0.8571429 0.5000000 0.7142857 0.8571429 0.7142857 0.7142857
## CMP5 0.3333333 0.3333333 0.3333333 0.3333333 0.8888889 0.8888889 0.3333333
## CMP6 0.4000000 0.4000000 0.3333333 0.3000000 0.8000000 0.9000000 0.3000000
##      CMP74      CMP75      CMP76 CMP77      CMP78      CMP79      CMP80
## CMP1 0.8000000 0.8000000 0.6000000 0.2 0.8000000 0.8000000 0.8000000
## CMP2 0.2727273 0.8181818 0.4285714 0.2 0.2727273 0.3636364 0.3636364
## CMP3 0.4545455 0.8181818 0.7142857 0.2 0.4545455 0.6363636 0.5454545
## CMP4 0.7142857 0.7142857 0.7142857 0.2 0.7142857 0.8571429 0.8571429
## CMP5 0.3333333 0.8888889 0.2857143 0.2 0.3333333 0.3333333 0.3333333
## CMP6 0.3000000 0.8000000 0.4285714 0.2 0.3000000 0.4000000 0.4000000
##      CMP81      CMP82      CMP83      CMP84      CMP85      CMP86      CMP87
## CMP1 0.8000000 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000
## CMP2 0.2727273 0.6666667 0.8181818 0.7500000 0.7000000 0.7272727 0.7272727
## CMP3 0.4545455 0.8333333 0.6363636 0.7500000 0.8000000 0.7272727 0.7272727
## CMP4 0.7142857 0.8333333 0.5714286 0.4285714 0.4285714 0.4285714 0.4285714
## CMP5 0.3333333 0.5000000 0.8888889 0.6250000 0.7777778 0.7777778 0.7777778
## CMP6 0.3000000 0.6666667 0.9000000 0.7500000 0.7000000 0.8000000 0.7000000
##      CMP88      CMP89      CMP90      CMP91      CMP92      CMP93      CMP94
## CMP1 0.4000000 0.4000000 0.4000000 0.6000000 0.6000000 0.6000000 0.2000000
## CMP2 0.8888889 0.6363636 0.6363636 0.8181818 0.8181818 1.0000000 0.6666667
## CMP3 0.7777778 0.6363636 0.6363636 0.7272727 0.6363636 0.6363636 0.6666667
## CMP4 0.4285714 0.2857143 0.2857143 0.4285714 0.5714286 0.5714286 0.1428571
## CMP5 0.7777778 0.7777778 0.7777778 0.8888889 0.8888889 1.0000000 0.6666667
## CMP6 0.8888889 0.7000000 0.7000000 0.8000000 0.9000000 1.0000000 0.6666667
##      CMP95      CMP96      CMP97      CMP98      CMP99      CMP100      CMP101
## CMP1 0.4000000 0.6000000 0.6000000 0.4000000 0.4000000 0.6000000 0.6000000
## CMP2 0.8750000 0.4285714 0.8571429 0.8571429 0.8571429 0.7272727 0.8888889
## CMP3 0.8750000 0.7142857 0.7142857 0.7142857 0.7142857 0.7272727 0.8888889
## CMP4 0.2857143 0.7142857 0.4285714 0.4285714 0.4285714 0.4285714 0.4285714
## CMP5 0.8750000 0.2857143 0.8571429 0.7142857 0.7142857 0.8888889 0.7777778
## CMP6 0.8750000 0.4285714 0.8571429 0.8571429 0.8571429 0.8000000 0.8888889
##      CMP102      CMP103      CMP104      CMP105      CMP106      CMP107      CMP108
## CMP1 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000
## CMP2 0.9090909 0.7000000 0.8000000 0.9000000 0.8181818 0.9090909 0.7000000
## CMP3 0.6363636 0.8000000 0.8000000 0.8000000 0.7272727 0.6363636 1.0000000
## CMP4 0.5714286 0.4285714 0.4285714 0.4285714 0.4285714 0.5714286 0.7142857
## CMP5 1.0000000 0.7777778 0.8888889 0.8888889 0.8888889 1.0000000 0.7777778
## CMP6 1.0000000 0.7000000 0.8000000 0.9000000 0.9000000 1.0000000 0.7000000

```

##	CMP109	CMP110	CMP111	CMP112	CMP113	CMP114	CMP115
##	CMP1	0.8000000	0.8000000	0.8000000	0.8000000	0.4000000	0.50 0.8000000
##	CMP2	0.3636364	0.3636364	0.4444444	0.3750000	0.8750000	0.75 0.2727273
##	CMP3	0.4545455	0.4545455	0.5555556	0.6250000	0.8750000	0.75 0.4545455
##	CMP4	0.7142857	0.7142857	0.7142857	0.7142857	0.2857143	0.75 0.7142857
##	CMP5	0.3333333	0.3333333	0.3333333	0.2500000	0.8750000	0.50 0.3333333
##	CMP6	0.4000000	0.4000000	0.4444444	0.3750000	0.8750000	0.75 0.3000000
##	CMP116	CMP117	CMP118	CMP119	CMP120	CMP121	CMP122
##	CMP1	0.8000000	0.4000000	0.6000000	0.6000000	0.6000000	0.6000000 0.6000000
##	CMP2	0.5714286	0.8750000	0.4285714	0.3750000	0.5000000	0.3333333 0.4444444
##	CMP3	0.7142857	0.8750000	0.7142857	0.6250000	0.8333333	0.5555556 0.6666667
##	CMP4	0.7142857	0.2857143	0.7142857	0.7142857	0.8333333	0.7142857 0.8571429
##	CMP5	0.4285714	0.8750000	0.2857143	0.2500000	0.3333333	0.2222222 0.3333333
##	CMP6	0.5714286	0.8750000	0.4285714	0.3750000	0.5000000	0.3333333 0.4444444
##	CMP123	CMP124	CMP125	CMP126	CMP127	CMP128	CMP129
##	CMP1	0.6000000	0.6000000	0.6000000	0.6000000	0.6000000	0.6000000 0.6000000
##	CMP2	0.2857143	0.3750000	0.3636364	0.3636364	0.3636364	0.8181818 0.8000000
##	CMP3	0.5714286	0.6250000	0.5454545	0.5454545	0.5454545	0.6363636 0.8000000
##	CMP4	0.5714286	0.7142857	0.8571429	0.8571429	0.8571429	0.5714286 0.4285714
##	CMP5	0.2857143	0.2500000	0.3333333	0.3333333	0.3333333	0.8888889 0.7777778
##	CMP6	0.2857143	0.3750000	0.4000000	0.4000000	0.4000000	0.9000000 0.8000000
##	CMP130	CMP131	CMP132	CMP133	CMP134	CMP135	CMP136
##	CMP1	0.4000000	0.6000000	0.6000000	0.4000000	0.6000000	0.6000000 0.6000000
##	CMP2	0.9090909	0.5000000	1.0000000	0.8000000	0.7272727	0.2727273 0.6666667
##	CMP3	0.6363636	0.8333333	0.6363636	0.7000000	0.7272727	0.4545455 0.6666667
##	CMP4	0.4285714	0.8333333	0.5714286	0.4285714	0.4285714	0.7142857 0.6666667
##	CMP5	0.8888889	0.3333333	1.0000000	0.7777778	0.8888889	0.3333333 0.5000000
##	CMP6	0.9000000	0.5000000	1.0000000	0.8000000	0.8000000	0.3000000 0.6666667
##	CMP137	CMP138	CMP139	CMP140	CMP141	CMP142	CMP143
##	CMP1	0.6000000	0.8000000	0.6000000	0.8000000	0.2 0.6000000	0.6000000
##	CMP2	0.5000000	0.5454545	0.3636364	0.5454545	0.4 0.8181818	0.7777778
##	CMP3	0.7500000	0.7272727	0.4545455	0.9090909	0.4 0.7272727	0.8888889
##	CMP4	0.8571429	0.8571429	0.7142857	0.8571429	0.2 0.4285714	0.5714286
##	CMP5	0.3750000	0.6666667	0.3333333	0.6666667	0.4 0.8888889	0.7777778
##	CMP6	0.5000000	0.6000000	0.4000000	0.6000000	0.4 0.8000000	0.7777778
##	CMP144	CMP145	CMP146	CMP147	CMP148	CMP149	CMP150
##	CMP1	0.4000000	0.4000000	0.6000000	0.4000000	0.8000000	0.4000000 0.6000000
##	CMP2	0.6363636	0.6363636	0.5000000	0.9000000	0.2857143	0.2857143 0.4444444
##	CMP3	0.6363636	0.5454545	0.8333333	0.7000000	0.5714286	0.2857143 0.5555556
##	CMP4	0.2857143	0.2857143	0.8333333	0.4285714	0.7142857	0.2857143 0.7142857
##	CMP5	0.7777778	0.7777778	0.3333333	0.7777778	0.2857143	0.2857143 0.3333333
##	CMP6	0.7000000	0.7000000	0.5000000	0.8000000	0.2857143	0.2857143 0.4444444
##	CMP151	CMP152	CMP153	CMP154	CMP155	CMP156	CMP157
##	CMP1	0.8000000	0.6000000	0.6000000	1.0000000	0.6000000	0.8000000 0.8000000
##	CMP2	0.5000000	0.7000000	0.3636364	0.3636364	0.2727273	0.5000000 0.3636364
##	CMP3	0.8333333	0.6000000	0.5454545	0.5454545	0.4545455	0.6250000 0.4545455
##	CMP4	0.8333333	0.4285714	0.8571429	0.8571429	0.7142857	0.7142857 0.7142857
##	CMP5	0.3333333	0.7777778	0.3333333	0.3333333	0.2222222	0.3750000 0.3333333
##	CMP6	0.5000000	0.7000000	0.4000000	0.4000000	0.3000000	0.5000000 0.4000000
##	CMP158	CMP159	CMP160	CMP161	CMP162	CMP163	CMP164
##	CMP1	0.2000000	0.6000000	0.6000000	0.8000000	0.8000000	0.4000000 0.8000000
##	CMP2	0.5454545	0.3636364	0.5000000	0.3636364	0.8181818	0.2500000 0.2727273
##	CMP3	0.5454545	0.5454545	0.8333333	0.5454545	0.9090909	0.2500000 0.4545455
##	CMP4	0.1428571	0.8571429	0.8333333	0.8571429	0.7142857	0.2857143 0.7142857

```

## CMP5 0.6666667 0.3333333 0.3333333 0.3333333 0.8888889 0.2500000 0.3333333
## CMP6 0.6000000 0.4000000 0.5000000 0.4000000 0.8000000 0.2500000 0.3000000
##      CMP165      CMP166      CMP167      CMP168      CMP169      CMP170      CMP171
## CMP1 0.8000000 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000 0.6000000
## CMP2 0.3636364 0.6363636 0.7272727 0.8181818 0.7272727 0.8888889 0.7272727
## CMP3 0.4545455 0.5454545 0.9090909 0.9090909 0.8181818 0.8888889 0.7272727
## CMP4 0.7142857 0.5714286 0.7142857 0.7142857 0.5714286 0.4285714 0.4285714
## CMP5 0.3333333 0.7777778 0.8888889 0.8888889 0.8888889 0.8888889 0.8888889
## CMP6 0.4000000 0.7000000 0.8000000 0.8000000 0.8000000 0.8888889 0.8000000
##      CMP172      CMP173      CMP174      CMP175      CMP176      CMP177      CMP178
## CMP1 0.8000000 0.8000000 0.8000000 0.8000000 0.8000000 0.8000000 0.6000000
## CMP2 0.4000000 0.8181818 0.6666667 0.2727273 1.0000000 0.2727273 0.8181818
## CMP3 0.6000000 0.8181818 0.8333333 0.4545455 0.8181818 0.4545455 0.7272727
## CMP4 1.0000000 0.7142857 0.8333333 0.7142857 0.7142857 0.7142857 0.4285714
## CMP5 0.3333333 0.8888889 0.5000000 0.3333333 1.0000000 0.3333333 0.8888889
## CMP6 0.4000000 0.9000000 0.6666667 0.3000000 1.0000000 0.3000000 0.9000000
##      CMP179      CMP180      CMP181      CMP182      CMP183      CMP184      CMP185
## CMP1 0.6000000 0.8000000 0.4000000 0.8000000 0.8000000 0.8000000 0.8000000
## CMP2 0.8000000 0.2500000 0.8181818 0.5714286 0.6666667 0.3636364 0.7272727
## CMP3 0.8000000 0.5000000 0.6363636 0.7142857 0.8333333 0.6363636 1.0000000
## CMP4 0.4285714 0.7142857 0.4285714 0.7142857 0.8333333 0.8571429 0.8571429
## CMP5 0.8888889 0.2500000 0.8888889 0.4285714 0.5000000 0.3333333 0.8888889
## CMP6 0.8000000 0.2500000 0.9000000 0.5714286 0.6666667 0.4000000 0.8000000
##      CMP186      CMP187      CMP188      CMP189      CMP190      CMP191      CMP192
## CMP1 0.8000000 0.8000000 0.8000000 0.8000000 0.8000000 0.6 0.8000000
## CMP2 0.6363636 0.9090909 0.9090909 0.9090909 0.2222222 0.6 0.4444444
## CMP3 1.0000000 0.8181818 0.8181818 0.8181818 0.4444444 0.6 0.6666667
## CMP4 0.8571429 0.7142857 0.7142857 0.7142857 0.7142857 0.6 0.8571429
## CMP5 0.7777778 1.0000000 1.0000000 0.8888889 0.2222222 0.6 0.3333333
## CMP6 0.7000000 0.9000000 0.9000000 0.9000000 0.2222222 0.6 0.4444444
##      CMP193      CMP194      CMP195      CMP196      CMP197      CMP198      CMP199
## CMP1 0.8000000 0.8000000 0.6000000 0.6000000 0.8000000 0.8000000 0.8000000
## CMP2 0.4444444 0.5454545 0.7272727 0.2727273 0.6666667 1.0000000 0.7272727
## CMP3 0.6666667 0.7272727 0.8181818 0.4545455 0.8333333 0.8181818 0.6363636
## CMP4 0.8571429 0.5714286 0.7142857 0.7142857 0.8333333 0.7142857 0.7142857
## CMP5 0.3333333 0.6666667 0.8888889 0.2222222 0.5000000 1.0000000 0.8888889
## CMP6 0.4444444 0.6000000 0.8000000 0.3000000 0.6666667 1.0000000 0.8000000
##      CMP200      CMP201      CMP202      CMP203      CMP204      CMP205      CMP206
## CMP1 0.8000000 0.8000000 0.8000000 0.8000000 0.6000000 0.8000000 0.8000000
## CMP2 0.5000000 0.4000000 0.6363636 0.2727273 0.2727273 0.1818182 0.2727273
## CMP3 0.7500000 0.6000000 0.5454545 0.4545455 0.4545455 0.3636364 0.4545455
## CMP4 0.8571429 0.8571429 0.7142857 0.7142857 0.7142857 0.7142857 0.7142857
## CMP5 0.3750000 0.3333333 0.7777778 0.3333333 0.2222222 0.2222222 0.3333333
## CMP6 0.5000000 0.4000000 0.7000000 0.3000000 0.3000000 0.2000000 0.3000000
##      CMP207      CMP208      CMP209      CMP210      CMP211      CMP212      CMP213
## CMP1 0.8000000 0.6000000 0.8000000 0.4000000 1.0000000 0.8000000 0.8000000
## CMP2 0.5454545 0.6666667 0.8181818 0.8181818 0.9090909 0.8181818 0.2727273
## CMP3 0.7272727 0.5555556 0.9090909 0.6363636 0.8181818 0.9090909 0.4545455
## CMP4 0.8571429 0.4285714 0.7142857 0.2857143 0.5714286 0.7142857 0.7142857
## CMP5 0.6666667 0.6666667 0.8888889 0.8888889 1.0000000 1.0000000 0.3333333
## CMP6 0.6000000 0.6666667 0.9000000 0.8000000 0.9000000 0.9000000 0.3000000
##      CMP214      CMP215      CMP216      CMP217      CMP218      CMP219      CMP220
## CMP1 0.8000000 0.8000000 0.8000000 0.6000000 0.8000000 0.8000000 0.8000000
## CMP2 0.2727273 0.7272727 0.4444444 0.2000000 0.6363636 0.3636364 0.2727273

```

```

## CMP3 0.4545455 0.6363636 0.6666667 0.4000000 0.8181818 0.5454545 0.4545455
## CMP4 0.7142857 0.7142857 0.8571429 0.5714286 0.7142857 0.8571429 0.7142857
## CMP5 0.3333333 0.8888889 0.3333333 0.2222222 0.7777778 0.3333333 0.3333333
## CMP6 0.3000000 0.8000000 0.4444444 0.2000000 0.7000000 0.4000000 0.3000000
##      CMP221      CMP222      CMP223      CMP224      CMP225      CMP226      CMP227
## CMP1 0.6000000 0.6000000 0.6000000 0.4000000 0.6000000 0.8000000 0.8000000
## CMP2 0.6363636 0.5000000 0.2727273 0.7272727 0.3636364 0.8181818 0.8181818
## CMP3 0.6363636 0.5000000 0.3636364 0.6363636 0.5454545 0.9090909 0.9090909
## CMP4 0.5714286 0.5714286 0.5714286 0.2857143 0.8571429 0.7142857 0.7142857
## CMP5 0.7777778 0.3750000 0.3333333 0.8888889 0.3333333 1.0000000 1.0000000
## CMP6 0.7000000 0.5000000 0.3000000 0.8000000 0.4000000 0.9000000 0.9000000
##      CMP228      CMP229      CMP230      CMP231      CMP232      CMP233      CMP234
## CMP1 0.6 0.4000000 0.6000000 0.6000000 0.6000000 0.4000000 0.6000000
## CMP2 0.8 0.8181818 0.3636364 0.3636364 0.7272727 0.7272727 0.2727273
## CMP3 0.8 0.6363636 0.3636364 0.5454545 0.6363636 0.6363636 0.3636364
## CMP4 0.8 0.2857143 0.5714286 0.8571429 0.5714286 0.2857143 0.5714286
## CMP5 0.6 0.8888889 0.3333333 0.3333333 0.8888889 0.8888889 0.3333333
## CMP6 0.8 0.8000000 0.4000000 0.4000000 0.8000000 0.8000000 0.3000000
##      CMP235      CMP236      CMP237      CMP238      CMP239      CMP240      CMP241
## CMP1 0.6000000 0.6000000 0.6000000 0.8000000 0.6000000 0.4000000 0.6000000
## CMP2 0.6363636 0.6363636 0.2727273 0.8181818 0.8181818 0.6363636 0.5454545
## CMP3 0.6363636 0.6363636 0.3636364 0.6363636 0.7272727 0.6363636 0.5454545
## CMP4 0.5714286 0.4285714 0.5714286 0.7142857 0.4285714 0.4285714 0.5714286
## CMP5 0.7777778 0.7777778 0.2222222 0.8888889 0.8888889 0.7777778 0.6666667
## CMP6 0.7000000 0.7000000 0.3000000 0.8000000 0.9000000 0.7000000 0.6000000
##      CMP242      CMP243      CMP244      CMP245      CMP246      CMP247      CMP248
## CMP1 0.6000000 0.6000000 0.6000000 0.8000000 0.8000000 0.6000000 0.8000000
## CMP2 0.3636364 0.2727273 0.5000000 0.3636364 0.2727273 0.2727273 0.8181818
## CMP3 0.5454545 0.3636364 0.5000000 0.5454545 0.4545455 0.4545455 0.6363636
## CMP4 0.8571429 0.5714286 0.4285714 0.8571429 0.7142857 0.7142857 0.7142857
## CMP5 0.3333333 0.3333333 0.5555556 0.3333333 0.3333333 0.2222222 0.8888889
## CMP6 0.4000000 0.3000000 0.5000000 0.4000000 0.3000000 0.3000000 0.8000000
##      CMP249      CMP250      CMP251      CMP252      CMP253      CMP254      CMP255
## CMP1 0.6000000 0.6000000 0.8000000 0.8000000 1.0000000 0.8000000 0.6000000
## CMP2 0.3636364 0.3636364 0.2727273 0.2727273 0.7272727 0.6363636 0.7272727
## CMP3 0.3636364 0.3636364 0.4545455 0.4545455 0.7272727 0.8181818 0.6363636
## CMP4 0.5714286 0.5714286 0.7142857 0.7142857 0.7142857 0.5714286 0.5714286
## CMP5 0.3333333 0.3333333 0.3333333 0.3333333 0.8888889 0.7777778 0.8888889
## CMP6 0.4000000 0.4000000 0.3000000 0.3000000 0.8000000 0.7000000 0.8000000
##      CMP256      CMP257      CMP258      CMP259      CMP260      CMP261      CMP262
## CMP1 0.8000000 0.4000000 0.4000000 0.4000000 0.6000000 0.8000000 0.4000000
## CMP2 0.8181818 0.8181818 0.7272727 0.8181818 0.3636364 0.2727273 0.8181818
## CMP3 0.9090909 0.6363636 0.6363636 0.6363636 0.5454545 0.4545455 0.6363636
## CMP4 0.7142857 0.2857143 0.2857143 0.2857143 0.8571429 0.7142857 0.2857143
## CMP5 0.8888889 0.8888889 0.8888889 0.8888889 0.3333333 0.3333333 0.8888889
## CMP6 0.8000000 0.8000000 0.8000000 0.8000000 0.4000000 0.3000000 0.8000000
##      CMP263      CMP264      CMP265      CMP266      CMP267      CMP268      CMP269
## CMP1 0.8000000 0.4000000 0.4000000 0.6000000 0.8000000 0.4000000 0.8000000
## CMP2 0.8181818 0.7272727 0.7272727 0.8181818 0.7272727 0.5454545 0.8181818
## CMP3 0.6363636 0.6363636 0.6363636 0.7272727 0.6363636 0.5454545 0.7272727
## CMP4 0.7142857 0.2857143 0.2857143 0.4285714 0.7142857 0.2857143 0.8571429
## CMP5 0.8888889 0.8888889 0.8888889 0.8888889 0.8888889 0.6666667 0.8888889
## CMP6 0.8000000 0.8000000 0.8000000 0.9000000 0.8000000 0.6000000 0.8000000
##      CMP270      CMP271      CMP272      CMP273      CMP274      CMP275      CMP276

```

```
## CMP1 0.4000000 0.4000000 0.4000000 0.4000000 0.4000000 0.4000000 0.4000000
## CMP2 0.6363636 0.7272727 0.8181818 0.7272727 0.8181818 0.7272727 0.8181818
## CMP3 0.6363636 0.6363636 0.6363636 0.6363636 0.6363636 0.6363636 0.6363636
## CMP4 0.2857143 0.2857143 0.2857143 0.2857143 0.2857143 0.2857143 0.2857143
## CMP5 0.7777778 0.8888889 0.8888889 0.8888889 0.8888889 0.8888889 0.8888889
## CMP6 0.7000000 0.8000000 0.8000000 0.8000000 0.8000000 0.8000000 0.8000000
##      CMP277      CMP278      CMP279      CMP280      CMP281      CMP282      CMP283
## CMP1 0.4000000 0.4000000 0.4000000 0.4000000 0.4000000 0.6000000 0.6000000
## CMP2 0.7272727 0.8181818 0.6363636 0.7272727 0.7272727 0.2727273 0.3636364
## CMP3 0.6363636 0.6363636 0.5454545 0.6363636 0.6363636 0.3636364 0.5454545
## CMP4 0.2857143 0.2857143 0.2857143 0.2857143 0.2857143 0.5714286 0.8571429
## CMP5 0.8888889 0.8888889 0.7777778 0.8888889 0.8888889 0.2222222 0.3333333
## CMP6 0.8000000 0.8000000 0.7000000 0.8000000 0.8000000 0.3000000 0.4000000
##      CMP284      CMP285      CMP286      CMP287      CMP288      CMP289      CMP290
## CMP1 0.6000000 0.6000000 0.6000000 0.8000000 0.8000000 0.6000000 0.6000000
## CMP2 0.3000000 0.2727273 0.7000000 0.3636364 0.2727273 0.2727273 0.2727273
## CMP3 0.4000000 0.4545455 0.7000000 0.4545455 0.4545455 0.3636364 0.4545455
## CMP4 0.5714286 0.7142857 0.4285714 0.7142857 0.7142857 0.5714286 0.7142857
## CMP5 0.2222222 0.3333333 0.7777778 0.3333333 0.3333333 0.3333333 0.2222222
## CMP6 0.3000000 0.3000000 0.7000000 0.4000000 0.3000000 0.3000000 0.3000000
##      CMP291      CMP292      CMP293      CMP294      CMP295      CMP296      CMP297
## CMP1 0.8000000 0.6000000 0.8000000 0.8000000 0.8000000 0.8000000 0.8000000
## CMP2 0.2727273 0.1818182 0.3636364 0.8181818 1.0000000 0.3636364 0.3636364
## CMP3 0.4545455 0.3636364 0.5454545 0.9090909 0.6363636 0.5454545 0.4545455
## CMP4 0.7142857 0.5714286 0.8571429 0.7142857 0.7142857 0.8571429 0.7142857
## CMP5 0.3333333 0.2222222 0.3333333 0.8888889 1.0000000 0.3333333 0.3333333
## CMP6 0.3000000 0.2000000 0.4000000 0.9000000 1.0000000 0.4000000 0.4000000
```

Saving th csv file

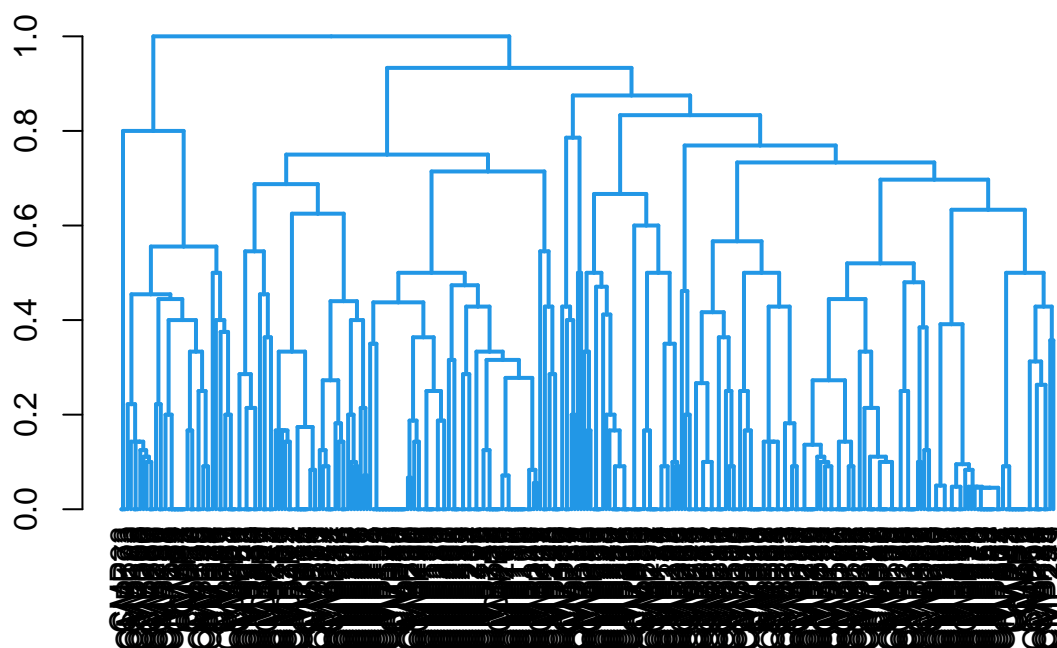
```
write.csv(d1, file = "Similarity_Matrix_Actives_Inactives.csv")
```

Performing heirachial clustering on the above generated matrix

```
hc1 <- hclust(as.dist(1-d1), method = "complete")
```

Plotting dendrogram after heirarchial clustering

```
plot(as.dendrogram(hc1), edgePar = list(col = 4, lwd = 2, horiz = TRUE))
```



We want circular dendrogram with the names of the molecules as well as the colors for their respective groups i.e. Active or Inactive. Therefore, we save the following tree as .newick file which will then be used to create a dendrogram using iTOL, an open source online tool to render phylogeny

```
my_tree1 <- as.phylo(hc1)
write.tree(phy = my_tree1, file="Tree_Actives_Inactives.newick")
```