# Report III : Torsional Geometric Generation of Molecular 3D Conformer Ensembles (GEOMOL)

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#### R Markdown

This is an R Markdown document. Markdown is a simple formatting syntax for authoring HTML, PDF, and MS Word documents. For more details on using R Markdown see http://rmarkdown.rstudio.com.

When you click the **Knit** button a document will be generated that includes both content as well as the output of any embedded R code chunks within the document. You can embed an R code chunk like this:

#### summary(cars)

```
##
                         dist
        speed
##
           : 4.0
                    Min.
                           : 2.00
    1st Qu.:12.0
                    1st Qu.: 26.00
##
##
    Median:15.0
                    Median: 36.00
    Mean
           :15.4
                    Mean
                           : 42.98
                    3rd Qu.: 56.00
    3rd Qu.:19.0
    Max.
           :25.0
                    Max.
                           :120.00
```

## **Including Plots**

You can also embed plots, for example:



Note that the  $\mbox{echo}$  = FALSE parameter was added to the code chunk to prevent printing of the R code that generated the plot.