

Report II : Molecular machine learning with conformer ensembles

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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)
```

```
##      speed      dist
##  Min.   : 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.:19.0    3rd Qu.: 56.00
## Max.   :25.0    Max.   :120.00
```

Including Plots

You can also embed plots, for example:



Note that the `echo = FALSE` parameter was added to the code chunk to prevent printing of the R code that generated the plot.