# Supporting Information

for

# Inherent atomic mobility changes in carbocation intermediates during the sesterterpene cyclization cascade

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# How to use in house software to calculate inherent atomic mobility

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**How to use in house software to calculate inherent atomic mobility**

1. **The preparation of input file.**
   In this study, all IRC calculations were carried out using GRRM11. The GRRM's log files need to be converted to appropriate format as shown in S1.log and S2.log.

2. **Calculation of inherent atomic mobility.**
   Please compile S3.cpp as following.

   *g++ S3.cpp −o S3*

   Then, execute S3 as following.
   *./S3 [inputfile]*
   This software generates two csv files; *output_all.csv* and *output_carbon.csv*.

3. **Analysis**
   Open the *output_carbon.csv* and make heat map using Microsoft Excel.