ABSTRACT

Computational Models of the Transmission of Chirality: The Chemical Evolution of Homochirality, A Biosignature of Life

By Erin Murdoch, Dr. Pauline Schwartz, Dr. Carl Barratt

METHOD & MATERIALS

ABSTRACT

The goal was to learn if conditions could be found that supported the notion that homochirality could evolve from an initial template molecule. Many different models were tested with arbitrary activation energies. The output from Kinetecs was a data sheet, which was produced showing chemical reactions. The graph showing the concentrations of the R and S enantiomers at each temperature is important for understanding the chirality (R) for each individual molecule after the template was used. The output from Kinetecs showed a split in symmetry for the template molecules being used at some point in time on early Earth. [1]

In earlier studies, we showed how one stereoisomer might be favored over the other. In this model, we focused on the R enantiomer and found that with the initial template molecule, the achiral substrate binds to the template and reacts following the initial reaction so it results in a molecule with a structure that favors one of the structures.

The most important finding was that whenever the initial concentrations for the R molecules were greater than the S molecules for all of the stereoisomers, the chemical system favored homochirality for the R forms. Even when the difference between R1 and S1, for example, was as small as 1 X 10^-14 M, breaking symmetry favored the R form throughout the model.

In the present model, only three different sets of Rn and Sn were used. Further investigation would need to be done in order to determine if this would hold true for more molecules, such as the 20 L-amino acids.

RESULTS

The graph shows homochirality in favor of R at 300 K with concentrations R1=25 & S1=25 & S3=0.0 M. Homochirality can be seen in the initial concentrations.

CONCLUSIONS

A possible chemical model of reactions has been developed that shows a system of reactions under specific conditions that suggests that once homochirality broke on early earth, that first amino acid was used as a template for all other amino acids. This is significant because it gives a possible explanation for how despite nature's tendency toward equal concentrations of each chirality, life developed with specifically L–amino acids. [4]

DISCUSSION

REFERENCES

ACKNOWLEDGEMENTS

At the current point in time, there is still no complete understanding of how life formed on early Earth. One mystery is the evolution of homochirality: many biologically important molecules have two stereoisomers: L- and D-. For reasons we do not yet understand, all amino acids, the building blocks of proteins, are L-amino acids. How did this happen?

We designed computational models of chemical systems to understand the transmission of chirality from a molecular template. In the model, we found conditions showing that with an exceedingly small excess of the L- form of precursors, there was a large production of L- molecules; we learned that breaking of chirality specifically requires that the template and reacts following the initial reaction so it results in a molecule with a structure that favors one of the structures.

At the current point in time, there is still no complete understanding of how life formed on early Earth. One mystery is the evolution of homochirality: many biologically important molecules have two stereoisomers: L- and D-. For reasons we do not yet understand, all amino acids, the building blocks of proteins, are L-amino acids. How did this happen?

We designed computational models of chemical systems to understand the transmission of chirality from a molecular template. In the model, we found conditions showing that with an exceedingly small excess of the L- form of precursors, there was a large production of L- molecules; we learned that breaking of chirality specifically requires that the template and reacts following the initial reaction so it results in a molecule with a structure that favors one of the structures.