

## Accepted Manuscript

Theoretical possibility of the chiral recognition of amino acids by a peptide nanoring

Jo Takeuchi, Kyozauro Takeda

PII: S2210-271X(17)30388-2  
DOI: <http://dx.doi.org/10.1016/j.comptc.2017.08.033>  
Reference: COMPTC 2614

To appear in: *Computational & Theoretical Chemistry*

Received Date: 28 May 2017  
Revised Date: 27 August 2017  
Accepted Date: 30 August 2017

Please cite this article as: J. Takeuchi, K. Takeda, Theoretical possibility of the chiral recognition of amino acids by a peptide nanoring, *Computational & Theoretical Chemistry* (2017), doi: <http://dx.doi.org/10.1016/j.comptc.2017.08.033>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# Theoretical possibility of the chiral recognition of amino acids by a peptide nanoring

Jo Takeuchi\*

*Department of Human Science, Takachiho University, Suginami, Tokyo 168-8508, Japan*

Kyozaburo Takeda

*Department of Electrical Engineering and Bioscience, School of Advanced Science and Engineering, Waseda University, Shinjuku, Tokyo 169-8555, Japan*

---

## Abstract

By changing the constituent amino acid residues, peptide nanorings (PNRs) are expected to be applicable to molecular separation technology. In this paper, chiral recognition of guest amino acids by a host PNR is studied using *ab initio* calculations. We designed a theoretical host PNR consisting of four glycine and two D-asparagine residues that would work as a chiral selector even if the guest amino acid is protonated or deprotonated. We then considered the energy stability of the PNR complexes with the D and L bodies of guest amino acids. The PNR showed enhanced properties that could allow for chiral recognition of guest amino acids with polar and dissociable side chains at any solvent pH.

*Keywords:* peptide nanoring, chiral recognition, amino acid, host–guest interaction

---

## 1. Introduction

A peptide nanoring (PNR) is a cyclic polypeptide in which the D and L bodies of amino acid residues are alternately arranged (Fig. 1(a)). One can easily modify the ring size and chemical characteristics of PNRs by changing the number and kind of the constituent amino acid residues. Ghadiri *et al.* archived

---

\*Corresponding author

*Email address:* takeuchi-j@takachiho.ac.jp ( Jo Takeuchi\* )

Download English Version:

<https://daneshyari.com/en/article/5392355>

Download Persian Version:

<https://daneshyari.com/article/5392355>

[Daneshyari.com](https://daneshyari.com)