【Grant-in-Aid for Scientific Research (S)】

Broad Section E

Title of Project： Development of DYASIN: Novel Approach to Enantioenriched Chiral Molecules

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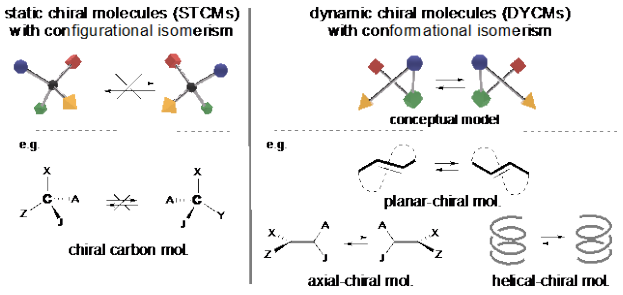
Keyword：dynamic asymmetric induction, optically active, dynamic chiral molecule, static chiral molecule, outer chiral source

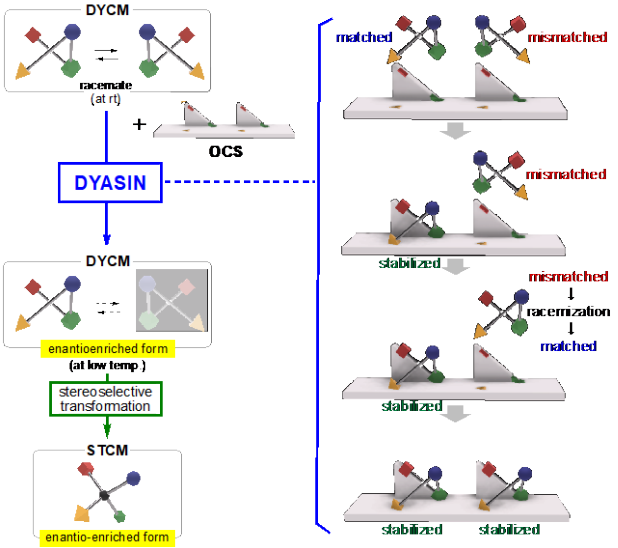
【Purpose and Background of the Research】

In modern organic chemistry, chemists have put forth considerable efforts in order to obtain the desired enantiomers selectively. Chiral molecules with configurational isomerism of an asymmetric carbon represent a principal motif in this field. In general, the chirality of an asymmetric carbon is thermally stable, and hence it can be called "static chirality". Developed approaches towards enantioenriched static chiral molecules (STCMs) are generally classified by i) the separation of enantiomers from racemates, also known as "optical resolution" or ii) the synthesis of chiral molecules with stereoselective bond formation, so called "asymmetric synthesis". On the other hand, it is well known that molecular chirality can also be caused by conformational isomerism and many examples are dynamic, i.e., conversion of enantiomers via bond rotation, in sharp contrast to STCM. This dynamic chirality often causes difficulties in handling the enantioenriched forms of molecules due to stereochemical instability. Meanwhile, dynamic chiral molecules (DYCMs) have a potential advantage in that the enantioenriched forms can be prepared in a very different way from STCM.



【Research Methods】

In this regard, we envisioned that if the chirality was adequately dynamic at ambient temperature, DYCMs could be influenced by an enantioenriched outer chiral source (OCS), and the effect would not be the same between enantiomers; thus, racemic DYCMs could be converted into their enantioenriched forms via thermodynamically controlled isomerization. If the bias towards one enantiomer was sufficiently high, the process would be practically useful. This process is hereafter referred to as "dynamic asymmetric induction (DYASIN)" where DYCMs and an OCS are presented in a conceptual rendering. Although the resulting enantioenriched DYCM is stereochemically labile, it can be isolated without racemization from the system by quick separation at appropriately low temperatures, and would be converted into stereochemically more stable molecules, i.e., STCM or semi-STCM, via proper transformations.



DYASIN would be the efficient technology for the preparation of enantioenriched chiral molecules and open new avenues in the chemistry of chiral molecules.

【Publications Relevant to the Project】

・ Preparation of Enantioenriched Chiral Organic Molecules by Dynamic Asymmetric Induction from Outer Chiral Source. Igawa, K.; Kawasaki, Y.; Ano, Y.; Kashiwagi, T.; Ogawa, K.; Hayashi, J.; Morita, R. Yoshioka, Y.; Uehara, K.; Tomooka, K. *Chem. Lett.* **2019**, *48*, 726-729.

【Term of Project】

FY2020-2024

【Budget Allocation】

152,800 Thousand Yen

【Homepage Address and Other Contact Information】

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