



Development of organic molecules with bright circularly polarized luminescence based on cyclodextrins

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Abstract

Circularly polarized luminescence (CPL) is a phenomenon in which the intensity of left- and right-handed rotational luminescence differs during the electronic transition from the excited state to the ground state in a material with a chiral structure. CPL is expected to be applied to optical communication technology to ensure security and biosensors to detect chirality. In this research, we aim at "development of high-brightness CPL organic molecules" and "CPL biosensing" using them, based on our original molecular design strategy.

Background & Results

When CPL is applied to biosensing and imaging, it is desirable to use small organic molecules. However, small molecule-derived CPL is difficult because of its low luminescence quantum yield and CPL anisotropy, as well as the need to properly design its molecular recognition ability. To solve this problem, we designed and synthesized a molecule (Pyrene-cyclodextrin (PCD)), which composed of a chiral cyclic oligosaccharide modified with multiple pyrene dyes, based on our original molecular design strategy. We hypothesized that the multiple pyrene units on the cyclodextrin (CyD) scaffold would form excimer in a restricted space, resulting in a CPL that exhibits high quantum yield and anisotropy due to steric hindrance and cumulative interactions. In addition, PCD is expected to exhibit good focusing properties due to the presence of multiple pyrene units.

PCD can be easily synthesized in a single step from commercially available starting materials and was found to exhibit a high molecular absorption coefficient ($1.0 \times 10^5 \text{ M}^{-1}\text{cm}^{-1}$), polarized luminescence with a good asymmetry factor (1.2×10^{-2}), and a quantum yield (0.39). The CPL brightness of PCD reached $340 \text{ M}^{-1}\text{cm}^{-1}$, which is very high among the organic molecules with CPL activity reported so far and is one of the highest in the world. These results are pioneering achievements that clearly demonstrate the potential of small organic molecules for CPL biosensing.

Significance of the research and Future perspective

CPL is expected to be utilized in a wide range of areas, including next-generation three-dimensional displays, information and communication technology, biosensors, advanced security printing, plant growth promotion, and medical diagnostic applications. Therefore, CPL materials are being actively researched worldwide, but their development into bio-applications is completely unexplored. The realization of the goals of this research plan, namely, "creation of highly brilliant circularly polarizable organic molecules" and "biosensing," is extremely pioneering research that will serve as a milestone toward the development of next-generation diagnostic and imaging technologies. In addition to these CPL applications, this research is also a world-leading study that contributes

to the development of basic research by deepening the science of "excited state chemistry."

Cyclodextrin-type CPL molecule

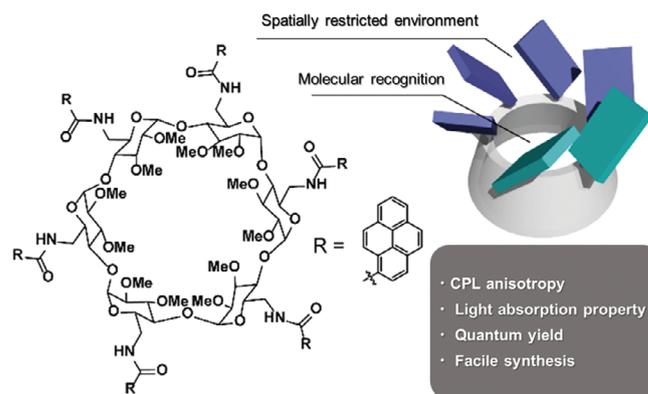


Figure 1. Chemical structure and schematic representation of PCD.

Biomolecule-recognizable CPL molecule

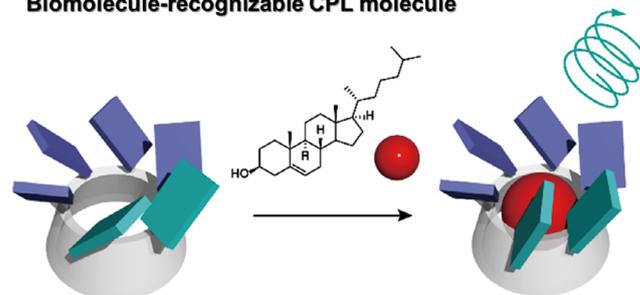
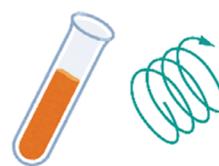


Figure 2. CPL sensing of a biomolecule (cholesterol) by PCD.

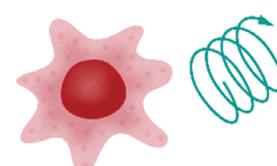
In blood



CPL biosensing

Early diagnosis

In cell



CPL bioimaging

Understanding life phenomena

Figure 3. CPL biological applications for diagnosis and elucidation of life phenomena.

Patent Japanese Patent Application No. 2019-56572**Treatise** Shigemitsu, Hajime; Kawakami, Kosei; Kida, Toshiyuki et al. Cyclodextrins with Multiple Pyrenyl Groups: An Approach to Organic Molecules Exhibiting Bright Excimer Circularly Polarized Luminescence. *Angew. Chem. Int. Ed.* 2022, 61(8), e202114700, doi: 10.1002/anie.202114700**URL****Keyword** cyclodextrin, circularly polarized luminescence, molecular recognition