【Grant-in-Aid for Scientific Research (S)】
Biological Sciences (Medicine, dentistry, and pharmacy I)

Title of Project : Towards Next-Generation Aromatic Chemistry: Development of Synthetic Methods, Theory and Novel Functionalities

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Research Area : Organic Synthesis, Elements Chemistry, Theoretical Chemistry
Keywords : Aromaticity, Molecular Transformation, Material Science, Spectroscopy

【Purpose and Background of the Research】

Sophisticated aromatic compounds that interact with light are required for various advanced technologies, including storage media, organic semiconductors, laser printers, photodynamic therapy of cancer, nonlinear optics, deodorants, and molecular imaging. This project aims to develop new synthetic methods, to extend theoretical principles, and to obtain aromatic molecules with unique functionalities suitable for next-generation technological applications.

【Research Methods】

Interdisciplinary research from various viewpoints, including organic chemistry, physical chemistry, and theoretical chemistry, is needed to develop novel functionalized aromatic molecules for many future applications. We intend to focus on the following four areas:

① Development of breakthrough synthetic processes to construct aromatic rings and to provide new tools for chemo-, regio- and stereo-selective introduction of various functional groups into aromatic molecules
② Systematically extending our understanding of the principles of aromaticity (theoretical investigation of the origin of homo-, Mobius-, anti-, and non-aromaticities)
③ Construction of novel metal-containing (organic-inorganic hybrid-type) aromatic compounds, aiming at the emergence of new features that have not been observed in usual organic aromatics
④ Creation of stable near-infrared light-emitting aromatic molecules having a low HOMO level, with potential applications for organic solar cells, photodynamic therapy of cancer, and near-infrared imaging

【Expected Research Achievements and Scientific Significance】

A potential application for the unusual light-capturing ability of next-generation aromatic compounds could be in tandem solar cells. Such compounds could also be useful for cancer treatment by photodynamic therapy with light-absorbing compounds. By specifically illuminating the tumor, only cancerous cells are heated and consequently killed. As infrared light penetrates well through human tissue, photodynamic compounds that absorb strongly in this wavelength region are particularly desirable for this purpose.

【Publications Relevant to the Project】

1. A. Muranaka, S. Yasuike, C-Y. Liu, J. Kurita, N. Kakusawa, T. Tsuchiya, M. Okuda, N. Kobayashi, Y. Matsumoto, K. Yoshida, D. Hashizume, M. Uchiyama, “Effect of Periodic Replacement of the Heteroatom on the Spectroscopic Properties of Indole and Benzofuran Derivatives”, *J. Phys. Chem. A*, **2009**, *113*, 464-473.
2. A. Muranaka, M. Yonehara, M. Uchiyama, “Azulenocyanine: A New Family of Phthalocyanines with Intense Near-IR Absorption”, *J. Am. Chem. Soc.,* **2010**, *132,* 7844-7845.
3. Y. Yamamoto, Y. Hirata, M. Kodama, T. Yamaguchi, S. Matsukawa, K-Y Akiba, D. Hashizume, F. Iwasaki, A. Muranaka, M. Uchiyama, P. Chen, K. Kadish, N. Kobayashi, “Synthesis, Reactions, and Electronic Properties of 16 π-electron Octaisobutyltetraphenylporphyrin (OiBTPP)”, *J. Am. Chem. Soc.,* **2010**, *132,* 12627-12638.

【Term of Project】

FY2012-2016

【Budget Allocation】

167,800 Thousand Yen

【Homepage Address and Other Contact Information】

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