

蛍光性核酸の開発と応用

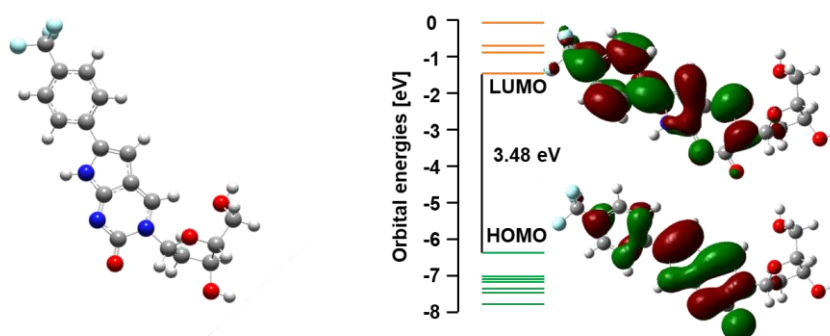
Development and application of fluorescent nucleoside

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研究成果概要

In the present study, we utilized the supercomputer system in Chemistry Research Institute, Kyoto University to perform DFT calculation for developing new fluorescent nucleoside. We mainly operated Guassian 16W software pack for the DFT and TD-DFT calculation in very high convergence level ( $1.0 \times 10^{-6}$ ) supported by supercomputer system (**Figure 1**). Due the importance of the fluorescence small molecules applying for in vivo imaging and detection, numerous fluorescent dyes and molecules have been designed and synthesized. Among them, the utility of fluorescent nucleosides is amplified when incorporated sequence-specifically into programmable DNA/RNA oligonucleotides. Because of their stable orientations, and minimal disturbance of native DNA folding and interactions, emissive isomorphous nucleoside analogues are versatile tools for the accurate analysis of DNA structural heterogeneity. We report on a bifunctional trifluoromethylphenylpyrrolocytidine derivative (FPdC) that displays an unprecedented quantum yield and highly sensitive  $^{19}\text{F}$  NMR signal. This is the first report of a cytosine-based dual-purpose probe that can be used for both fluorescence and  $^{19}\text{F}$  NMR spectroscopy. The synthesis and characterization of FPdC and FPdC-containing DNA are described.



**Figure 1.** DFT calculation results of newly developed fluorescent nucleoside

発表論文(謝辞なし)

“Synthesis and Application of  $^{19}\text{F}$ -labeled Fluorescent Nucleoside as a Dual-mode Probe for I-motif DNAs”, *RSC Chem. Biol.* under revision.