

アルキニル結合型 BODIPY 誘導体が示す疎水性相互作用を利用したオリゴ糖の定量的検出

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Quantitative detection of oligosaccharides utilizing hydrophobic interactions of alkynyl-linked BODIPY derivatives

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Oligosaccharides are among the most challenging biomolecules to analyze due to their structural diversity and conformational flexibility. We developed a new class of saccharide-sensing fluorescent probes, BoliFluor, derived from the hydrophobic dye BODIPY, in which saccharide-recognition groups were introduced via click chemistry. BoliFluor **2**, bearing a phenyl substituent, showed an excellent linear fluorescence response (0.10–1.5 mM) toward cyclic and linear maltooligosaccharides with six to eight glucose units, whereas BoliFluor **1**, containing a heptyl group, exhibited no response to linear maltooligosaccharides.

In this research, further investigation into side-chain effects revealed that alkynyl, alkenyl, and alkyl substituents of comparable hydrophobicity exhibited opposite behaviors in aqueous media—either promoting or suppressing dimerization. The alkynyl group, in particular suppressed dimerization effectively, in contrast to the alkenyl and alkyl analogues. These findings suggest that noncovalent interactions among hydrocarbon chains are strongly influenced by hydration structures, and that rational modulation of these effects enables precise control over hydrophobic interaction-driven aggregation. This principle provides a versatile foundation for designing high-performance fluorescent probes capable of dynamic and selective saccharide recognition.

Keywords: BODIPY; fluorescent probe; alkyne

多種多様な構造をもつオリゴ糖は定量分析が一般に難しい。我々は、疎水性蛍光色素 BODIPY を基盤に、糖鎖親和性官能基をクリック反応で導入した新規蛍光プローブ BoliFluor を開発した。BoliFluor **2** は環状および直鎖マルトオリゴ糖に対し 0.10–1.5 mM で優れた直線的蛍光応答を示したが、BoliFluor **1** は直鎖マルトオリゴ糖に反応しなかった。本研究では、側鎖の構造を変化させた検討により、同等の疎水性をもつアルキン・アルケン・アルカン側鎖が水中で相反する二量体化挙動を示すことを見出した。特にアルキニル基は水溶液中の二量体化を抑制する特異な効果を示した。これらの知見は、非共有結合相互作用の精密制御に基づく分子設計指針を提示し、疎水性相互作用を駆動力とする高感度糖鎖認識プローブの新たな展開を可能にした。