アニオン性置換基を有する水溶性 pH 応答型シアニン色素の開発

(京大院工)○Shuai Shao・ Huiying Mu・三木康嗣・大江浩一 Development of Water-soluble pH-Responsive Cyanine Dyes Containing Anionic Substituents (*Graduate School of Engineering, Kyoto University*) ○Shuai Shao, Huiying Mu, Koji Miki, Kouichi Ohe

A series of water-soluble near-infrared fluorescent probes was prepared based on the indocyanine green (ICG) platform, which are useful through a pH-dependent ring-opening process (Figure 1a). We found that parent probe **CypH0** has the lower pH-responsiveness in pure buffered solutions due to dye-aggregation, which is compared with the case in aqueous solutions after dispersed by TritonX-100 (Figure 1b). [1, 2] The incorporation of various number of anionic sulfonate groups to **CypHs** alleviated dyes' aggregation and improved their pH responsiveness in aqueous solutions, especially for the case of **CypH3** and **CypH4** which containing two or three anionic substituents (Figures 1c and 1d).

Keywords: pH-responsive, cyanine dye, anionic groups, fluorescent probe

我々は、インドシアニングリーン(ICG)の分子構造を基に、開環プロセスによって pH 応答性を示す水溶性近赤外蛍光プローブを合成した(図 1a)。プローブ CypH0 は TritonX-100 の存在下で良い pH 応答性を示したが、TritonX-100 を含まない緩衝液中では色素の凝集が起こり、pH 応答性は低下した(図 1b)[1,2]。一方、CypH0 に異なる数のアニオン性スルホナト基を導入することで、色素の凝集が緩和された。特に、2 つまたは 3 つのアニオン性置換基を有する CypH3 と CypH4 が水溶液中でも良い pH 応答性を示した(図 1c, 1d)。

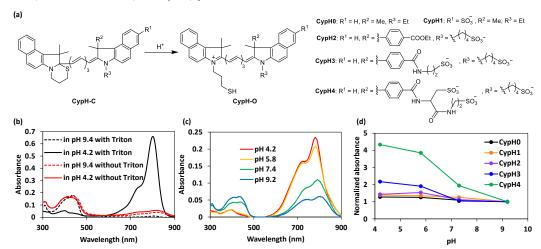


Figure 1. (a) Transformation of **CypHs** from their close-ring forms to open-ring forms. (b) Absorption spectra of **CypH0** in aqueous solutions with/without Triton X-100. (c) pH-Dependent absorption spectra of **CypH4** in buffered aqueous solutions at different pH without Triton X-100. (d) Comparison of **CypHs** with normalized absorption maximum assigned to non-aggregated dye form.

[1] K. Miki, K. Kojima, K. Oride, H. Harada, A. Morinibu, K. Ohe, *Chem. Commun.* **2017**, *53*, 7792–7795.

[2] H. Mu, K. Miki, H. Harada, K. Tanaka, K. Nogita, K. Ohe, ACS Sens. 2021, 6, 123–129.