Chemistry of firefly bioluminescence
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Firefly bioluminescence\(^1\) is produced by chemical reactions (luciferin-luciferase reaction) in the bodies of insects. Firefly bioluminescence finds many applications including in research in the life sciences, reporter assays, bioluminescence in vivo imaging.

Research on oncology and regenerative medicine requires NIR (near infrared ray) probes. Although Amino luciferin (ca. 610 nm) and Tripluc\(^\circ\) (ca. 630 nm) are commercially available, they do not cover the optical window\(^2\) region of 650-1000 nm: NIR.

In an innovative approach, we synthesized Aka Lumine\(^\circ\)\(^3\) and TokeOni\(^4\) having \(\lambda_{\text{max}}\) 675nm by analyzing data on structure and activity relationships\(^5\).

Whereas AkaLumine is the only commercially available luminescence probe with an optical window region, it has low water solubility (0.2 mg/ml). So the AkaLumine\(^8\) requires improvement. To resolve the problem of water solubility we succeeded in synthesizing next generation in vivo bioluminescence probe “TokeOni” with improved water solubility of 100 to 200 folds compared with AkaLumine\(^\circ\).

Furthermore, we observed a 10 fold higher luminescence than the AkaLumine during vivo imaging on mice\(^6\). Although “TokeOni” is an excellent material, it has strong acidity (pH = 2), that causes problems in some animal experiment research. So we synthesized a new material “SeMpai” that has NIR activity under neutral buffer conditions. “SeMpai” will put on the international market soon.

Reference
2) Ralph Weissleder, “A clearer vision for in vivo imaging”, nature biotechnology 19, 316 (2001)
3) Wako Pure Chemical Industries, Ltd. (http://www.wako-chem.co.jp/siyaku/product/life/AkaLumine/)