

Fatty Acid Conjugates of Toluidine Blue O as Amphiphilic Photosensitizers: Synthesis, Solubility, Photophysics and Photochemical Properties(dagger)

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[Ver número de ResearchID y ORCID de Web of Science](#)

PHOTOCHEMISTRY AND PHOTOBIOLOGY

DOI: 10.1111/php.13304



Acceso anticipado: JUL 2020

Tipo de documento: Article; Early Access

[Ver impacto de la revista](#)

Abstract

Toluidine blue O (TBO) is a water-soluble photosensitizer that has been used in photodynamic antimicrobial and anticancer treatments, but suffers from limited solubility in hydrophobic media. In an effort to incrementally increase TBO's hydrophobicity, we describe the synthesis of hexanoic (TBOC6) and myristic (TBOC14) fatty acid derivatives of TBO formed in low to moderate percent yields by condensation with the free amine site. Covalently linking 6 and 14 carbon chains led to modifications of not only TBO's solubility, but also its photophysical and photochemical properties. TBOC6 and TBOC14 derivatives were more soluble in organic solvents and showed hypsochromic shifts in their absorption and emission bands. The solubility in phosphate buffer solution was low for both TBOC6 and TBOC14, but unexpectedly slightly greater in the latter. Both TBOC6 and TBOC14 showed decreased triplet excited-state lifetimes and singlet oxygen quantum yields in acetonitrile, which was attributed to heightened aggregation of these conjugates particularly at high concentrations due to the hydrophobic "tails." While in diluted aqueous buffer solution, indirect measurements showed similar efficiency in singlet oxygen generation for TBOC14 compared to TBO. This work demonstrates a facile synthesis of fatty acid TBO derivatives leading to amphiphilic compounds with a delocalized cationic "head" group and hydrophobic "tails" for potential to accumulate into biological membranes or membrane/aqueous interfaces in PDT applications.

Palabras clave

KeyWords Plus: [SET MODEL CHEMISTRY](#); [PHOTODYNAMIC THERAPY](#); [IN-VITRO](#); [TOTAL ENERGIES](#); [CATIONIC DYES](#); [CANCER](#); [MOLECULES](#); [2-ANTHRACENECARBOXYLATE](#); [PHOTOCYCLODIMERIZATION](#); [DERIVATIVES](#)

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Financiación

Entidad financiadora Mostrar más información	Número de concesión
CONICYT through their FONDECYT research program	1160443
CONICYT/FONDEQUIP/UHPLC-MS/MS	EQM 120065
ANID FONDECYT/POSTDOCTORADO	3200403
National Science Foundation (NSF)	CHE-1856765
CONICYT/FONDEQUIP/Laser Flash Photolysis	EQM160099
	CONICYT-PCHA/Doctorado Nacional/2015-21150894

[Ver texto de financiación](#)

Editorial

WILEY, 111 RIVER ST, HOBOKEN 07030-5774, NJ USA

Información de la revista

- **Impact Factor:** [Journal Citation Reports](#)

Categorías / Clasificación

Áreas de investigación:Biochemistry & Molecular Biology; Biophysics

Categorías de Web of Science:Biochemistry & Molecular Biology; Biophysics

Información del documento

Idioma:English

Número de acceso: WOS:000551168600001

ID de PubMed: 32619275

ISSN: 0031-8655

eISSN: 1751-1097