

# In silico Design of Two-photon Fluorescent Probes for Detecting Nitric Oxide

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## Abstract

Nitric oxide (NO) is a ubiquitous signaling molecule in a variety of physiological and pathological process in living organisms. A two-photon probe, i.e., 2-acetyl-6-dialkylaminonaphthalene as the reporter and an o-diaminobenzene as the reaction site for NO, linked by prolinamide (ANO1), has been synthesized. Based on the experimental study, five other two-photon probes have been designed by substituting the naphthalene fluorophore in ANO1 with the luciferin analogue (ANO2), pyrene (substitution at 1,6-position, ANO3, and 2,7-position, ANO3'), fluorene (ANO4), and boron-dipyrromethene (ANO5) units. DFT/TDDFT studies have been conducted on both experimental two-photon probe ANO1 and designed ANOn (n=2–5). Our results indicated that for designed probes, both absorption and emission spectra show red shifts compared with ANO1. The one- and two-photon absorption band positions as well as the emission wavelength do have no significant change for each probe before and after reaction with NO. However, the fluorescence intensities are enhanced after reaction with NO. ANO3 and ANO4 have large two-photon absorption cross sections. Furthermore, analysis of molecular orbitals is exhibited to interpret the photoinduced electron transfer mechanism between the donor and acceptor.

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