

A small azide-modified thiazole-based reporter molecule for fluorescence and mass spectrometric detection.

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Abstract

Molecular probes are widely used tools in chemical biology that allow tracing of bioactive metabolites and selective labeling of proteins and other biomacromolecules. A common structural motif for such probes consists of a reporter that can be attached by copper(I)-catalyzed 1,2,3-triazole formation between terminal alkynes and azides to a reactive headgroup. Here we introduce the synthesis and application of the new thiazole-based, azide-tagged reporter 4-(3-azidopropoxy)-5-(4-bromophenyl)-2-(pyridin-2-yl)thiazole for fluorescence, UV and mass spectrometry (MS) detection. This small fluorescent reporter bears a bromine functionalization facilitating the automated data mining of electrospray ionization MS runs by monitoring for its characteristic isotope signature. We demonstrate the universal utility of the reporter for the detection of an alkyne-modified small molecule by LC-MS and for the visualization of a model protein by in-gel fluorescence. The novel probe advantageously compares with commercially available azide-modified fluorophores and a brominated one. The ease of synthesis, small size, stability, and the universal detection possibilities make it an ideal reporter for activity-based protein profiling and functional metabolic profiling.

Identifier

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