

Photochemical Transformations of Peptides Containing the *N*-(2-Selenoethyl)glycine Moiety

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Streszczenie

The diselenide bond has attracted considerable attention due to its ability to undergo the metathesis reaction in response to visible light. In our previous study, we demonstrated visible-light-induced diselenide metathesis of selenocysteine-containing linear peptides, allowing for the convenient generation of peptide libraries. Here, we investigated the transformation of linear and cyclic peptides containing the *N*-(2-selenoethyl)glycine moiety. The linear peptides were highly susceptible to the metathesis reaction, whereas the cyclic systems gave only limited conversion yields of the metathesis product. In both cases, side reactions leading to the formation of mono-, di-, and polyselenides were observed upon prolonged irradiation. To confirm the radical mechanism of the reaction, the radical initiator 2,2'-azobis[2-(2-imidazolin-2-yl)propane] dihydrochloride (VA-044) was tested, and it was found to induce diselenide metathesis without photochemical activation. The data were interpreted in the light of quantum-chemical simulations based on density functional theory (DFT). The simulations were performed at the B3LYP-D3BJ/def2-TZVP level of theory using a continuum solvation model (IEF-PCM) and methanol as a solvent.

Słowa kluczowe

Irradiation, Metathesis, Noncovalent interactions, Peptides and proteins, Solvents

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