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The new Safirinium P and Q derivatives for improved detection by mass spectrometry

Safirinium P are the fluorescent derivtives of 2,2-dialkyl-5,7-dimethyl-2,3-dihydro-[1,2,4]triazolo[4,3-a]pyridin-2-ium chlorides and Safirinium Q of their quinoline analogues, discovered by Sączewski et al. Thanks to the presence of quarternary ammonium salt, they may find an application in ionization tagging in mass spectrometry. We incorporated the Safinium systems in various peptides and ubiquitin hydrolisate and examined their applicability in signals enhancing. Furthermore we synthesized a new analogue of Safirinium Q containing the proline residue (SafQPro). We performed the structure optimization by DFT method to examine the presence of hydrogen bonding. According to its 3-dimensional structure, it could form one or two intramolecular or intermolecular hydrogen bonds and it is potentially possible to form the four stereoisomers: R,R R,S S,R S,S.

The results prooved the signal enhancing in mass spectrometry of peptides tagged by Safirinium systems and the dimensional structure of SafQPro was discovered.

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