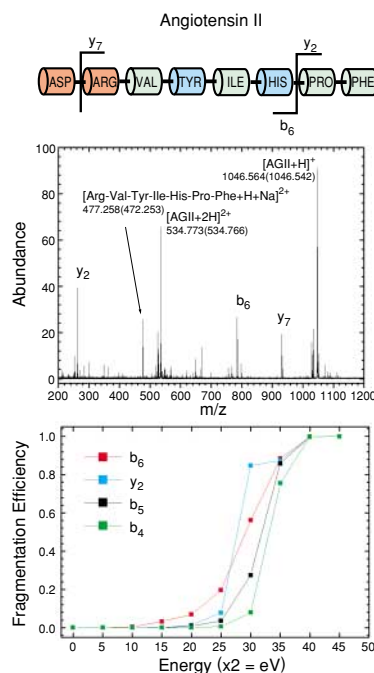


Fragmentation Studies for Peptides Using Mass Spectrometry: Experiment and Simulation

Kazuhiko FUKUI
 Computational Biology
 Research Center
 e-mail:
 k-fukui@aist.go.jp
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In recent years there has been significant interest in fragmentation analysis of peptides and proteins using mass spectrometry (MS) combined with infrared multiphoton dissociation (IRMPD) and collision induced dissociation (CID) technique. We investigate the cleavage of polypeptides induced at the backbone amine bonds by using the CO₂ laser peptide cleavage IRMPD technique. MS experiments are performed in electrospray ionization fourier-transform ion cyclotron resonance (FTICR) MS, and the results are compared with those of CID experiment. In addition, we theoretically model the fragmentation of the peptides under vacuum conditions using molecular dynamics. The dissociation energy and proton affinity for the peptide bonds (C'-N bond) are also obtained using *ab initio* calculations.

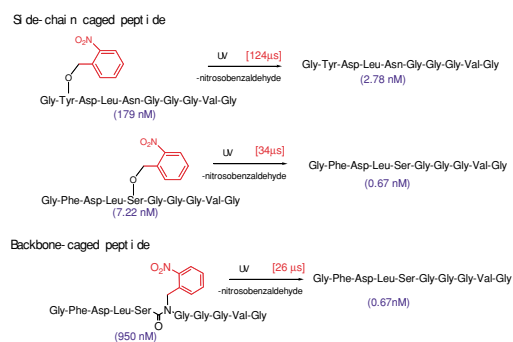


ESI-FTICR Spectrum and product efficiency curves obtained from CID experiment

Caged Peptide: Imprisonment of Biologically Active Peptides in a Photocleavable “Cage”

Yoshiro TATSU
 Special Division for Human
 Life Technology
 e-mail:
 y-tatsu@aist.go.jp
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Caged peptides, whose activities are masked by the introduction of photocleavable groups, have recently been recognized as a useful tool to elucidate various biological phenomena with a high spatial and temporal resolution, even in living cells. AIST has developed two types of caged peptides; side-chain caged peptides and backbone-caged peptides. The technique was applied to sperm activating peptide (speract). The backbone-caged speract showed superior features to those of the side-chain caged speract: greater caging ability and faster photolysis rate. The caging strategy described can be used as a general procedure to cage any biologically active peptide.



Caged sperm activating peptides. Nitrobenzyl groups shown in red are photo-cleaved and intact peptides are produced by UV-irradiation. The value under each peptide is the IC₅₀, and the value above each arrow is the half-life of the intermediate during photolysis.