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Explorations into isomeric peptides of opposite directionalities by tandem mass spectrometry

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Only one and not the other, 'retro' direction that every protein sequence takes is a curious evolutionary question for both biology and mass spectrometric analysis of proteomes. Further impetus on retro sequences came from bioinformatic analysis of proteins revealing the presence of unique inverted peptide sequence pairs of lengths 5-12 and 18 amino acid residues accommodated in natural proteins [Sridhar&Guruprasad 2014]. Consequently we decided to address this question by MS/MS using ribonuclease A derived S peptide: K1ETAAAKFERQHMDSS16 vs Retro S (RS) peptide: S1SDMHQREFKAAATEK16 as models. Collision induced dissociation was carried out within linear trap quadrupole at different collision energies (CEs), on $[M^+2H]2^+$ precursor ions (m/z 918.44) produced by electrospray ionization of the two peptides and product ion analysis was by orbitrap. Degree of fragmentation of each of the fifteen peptide bonds of peptide molecular ions was determined by estimating relative abundance of b- and y- ions, with reference to precursor ions, at every CE. The greater fragility of RS peptide than S peptide was evident from determinations of minimum CE, at which, the precursor ion population is 50% (CE50) or 0% of the initial populations (CE*). The values of CE50 and (CE*) were 23.6(30) and 22.6(28) for S and RS peptides, respectively. In view of the conformational propensity of S peptide to be more structured than RS peptide [Pal-Bhowmick et al. 2007), our data suggest that solution structures of these peptides may be preserved also in gas phase. This augurs well for application of high-resolution CID to probe conformational properties of peptides in gas phase.

Biography

Dinkar Sahal's laboratory epitomizes a vibrant atmosphere for both design and discovery of novel antibiotic peptides and antimalarial drugs. The foundations for understanding the mechanisms of action and discovery of the origins of potency, synergy among antibiotics and broad spectrum of action of antibiotic peptides has been laid in his laboratory. Likewise discovery of novel drugs against drug resistant malaria is a major passion of his laboratory. He has published more than 75 papers in reputed journals and has been serving as a Reviewer and an Editorial Board Member of different journals.

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