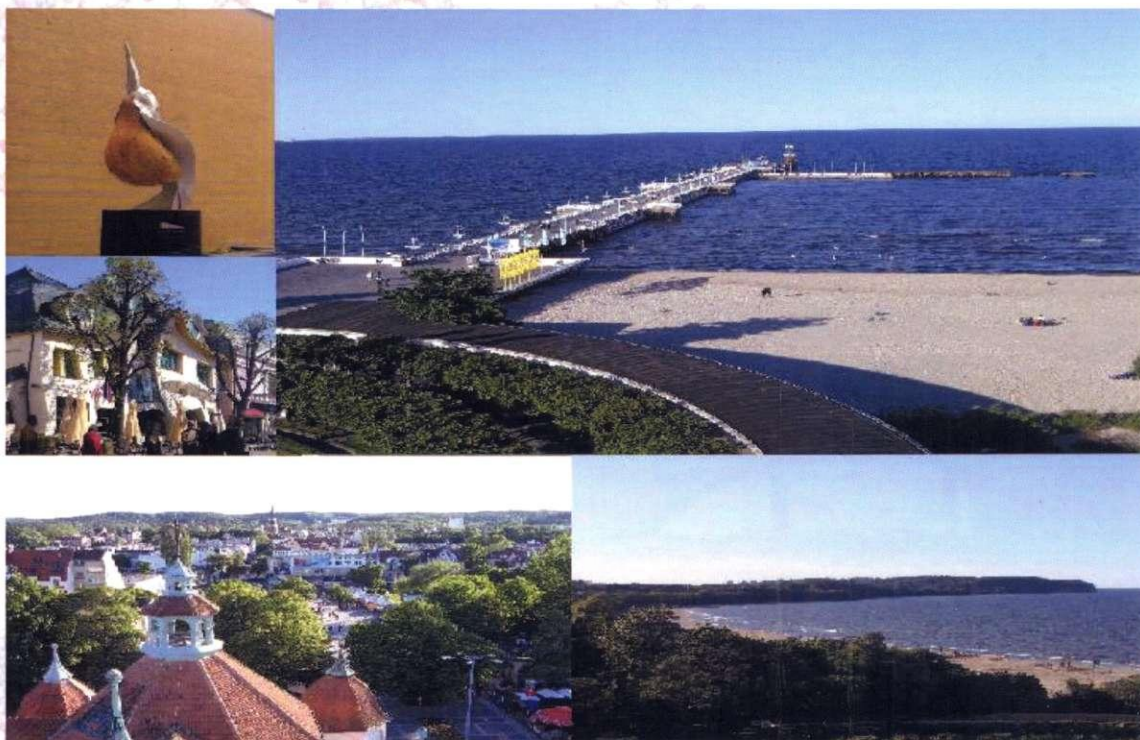


**Radiation Damage in Biomolecular
Systems: *Nanoscale Insights into
Ion-Beam Cancer Therapy***

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BOOK OF ABSTRACTS

Interaction of energetic photons with bare and nanosolvated biopolymers isolated in the gas phase

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Gas phase VUV and X-ray single-photon photoionization spectroscopy of electrospray-produced protonated bare and nanosolvated biopolymers has been performed by means of coupling a linear quadrupole ion trap with a synchrotron beamline (Fig. 1) [1]. Our results demonstrated a strong correlation between the ionization energy of a protein and both its charge state and structure [2]. Also, we have reported the first inner-shell spectroscopy of gaseous protein ions, showing a striking apparent stability of the large photoions arising from direct photoionization or Auger processes [3]. Finally, our most recent measurements in the VUV domain showed that although the nanosolvation of a protonated peptide dimer with only 3 water molecules has a limited impact on the three dimensional structure of this fragile complex, it increases dramatically its stability and prevents apparent photo-fragmentation. The latter experimental results have been confirmed theoretically by using molecular dynamics and density functional theory.

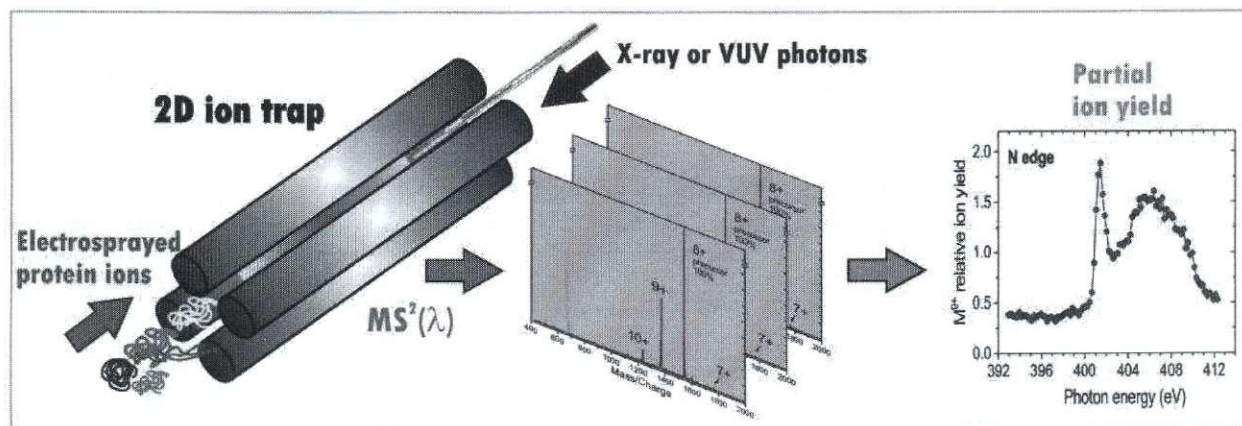


Figure 1: Schematic drawing of the experimental method.

Acknowledgments: Support by ANR-08-BLAN-0065 (France), "PavleSavic" bilateral project, MESTD RS (#171020, #171033) and COST MP1002. Data obtained at the SOLEIL synchrotron (Proposals 20100847,20110324, 20110694,20120117).

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VUV photodissociation of bare and nanosolvated protonated nucleotide isolated in the gas phase

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We have studied the photo-induced fragmentation of bare and nanosolvated protonated adenosine 5-monophosphate (AMP) as a function of VUV photon energy. The experiment was performed by coupling a linear ion trap with a VUV synchrotron beam [1]. The theoretical modeling was done by using molecular dynamics and DFT theoretical methods. The obtained results can help comprehending the protecting role of nanosolvation and the most probable structural arrangements of solvated species and their properties.

Figure 1a shows the tandem mass spectrum (MS²) recorded upon photo-irradiation of protonated AMP at the photon energy 7.5 eV. The interaction of photons with the trapped AMP ions induces a cleavage of the N-glycosidic bond between sugar and adenine, leading to dissociation of the nucleotide and production of the ionic fragment at m/z 136 (protonated adenine). However, the nanosolvation of the protonated AMP nucleotide with only three water molecules efficiently quenches the photo-fragmentation (Figure 1b) that lead to a protonated base.

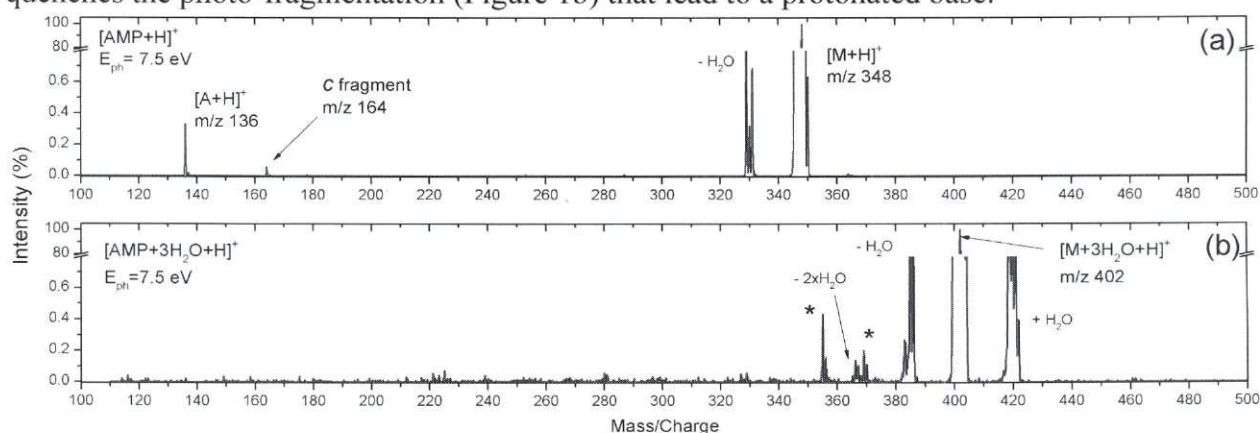


Figure 1: Tandem ESI/photoionization mass spectra of bare (a) and hydrated (b) AMP.

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