Supporting Information

Oxygen K-shell spectroscopy of isolated progressively solvated peptide

Aleksandar R. Milosavljević,*[a] Kari Jänkälä,[b] Miloš Lj. Ranković,[c,d] Francis Canon,[e] John Bozek,[a] Christophe Nicolas[a] and Alexandre Giuliani *[a,f]

[a]*SOLEIL, l'Orme des Merisiers, St Aubin, BP48, 91192 Gif sur Yvette Cedex, France.*

[b]*Nano and Molecular Systems Research Unit, University of Oulu, P.O. Box 3000, 90014 Oulu, Finland*

[c]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia.*

[d]*Present address: Institute of Physical Chemistry J. Heyrovsky, CAS, Dolejškova 3, 18223 Prague 8, Czech Republic*.

[e]*INRA, UMR1324 Centre des Sciences du Goût et de l'Alimentation, F-21000 Dijon, France.*

[f]*INRA, UAR1008, CEPIA, Rue de la Géraudière, BP 71627, 44316 Nantes, France.*

* A.R.M. (***milosavljevic@synchrotron-soleil.fr***) and A.G. (***alexandre.giuliani@synchrotron-soleil.fr***)

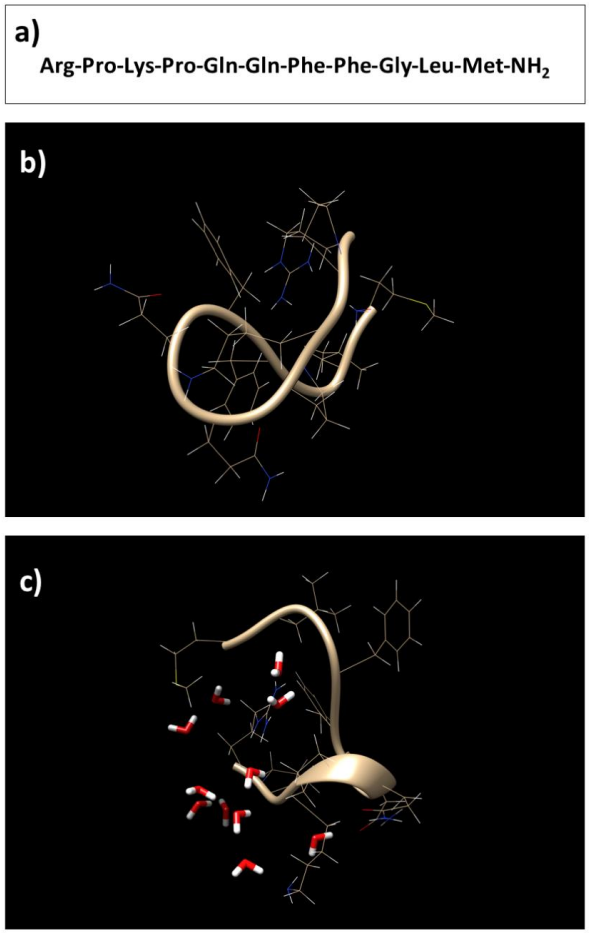

Fig.SI.1 *a) Sequence of Substance P. Example structures from molecular dynamics of b) bare Substance P doubly protonated ion and c) Substance P doubly protonated ion with 11 water molecules.*

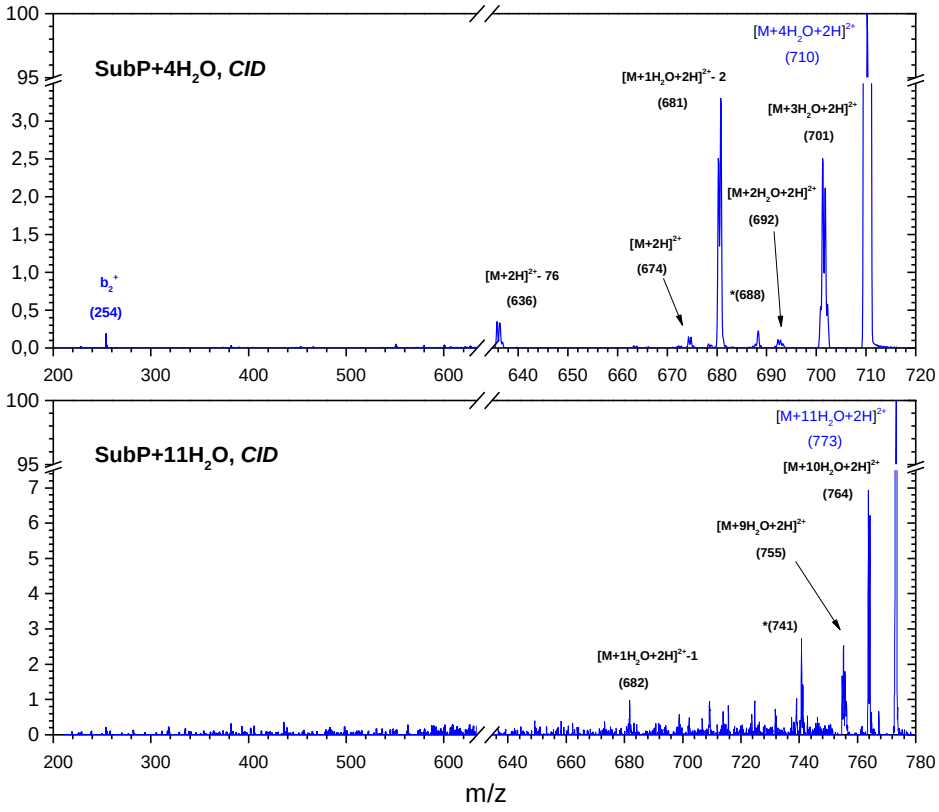

Fig.SI.2 *Collision induced dissociation (CID) of substance P hydrated by 4 water molecules (top) and 11 water molecules (bottom panel).*

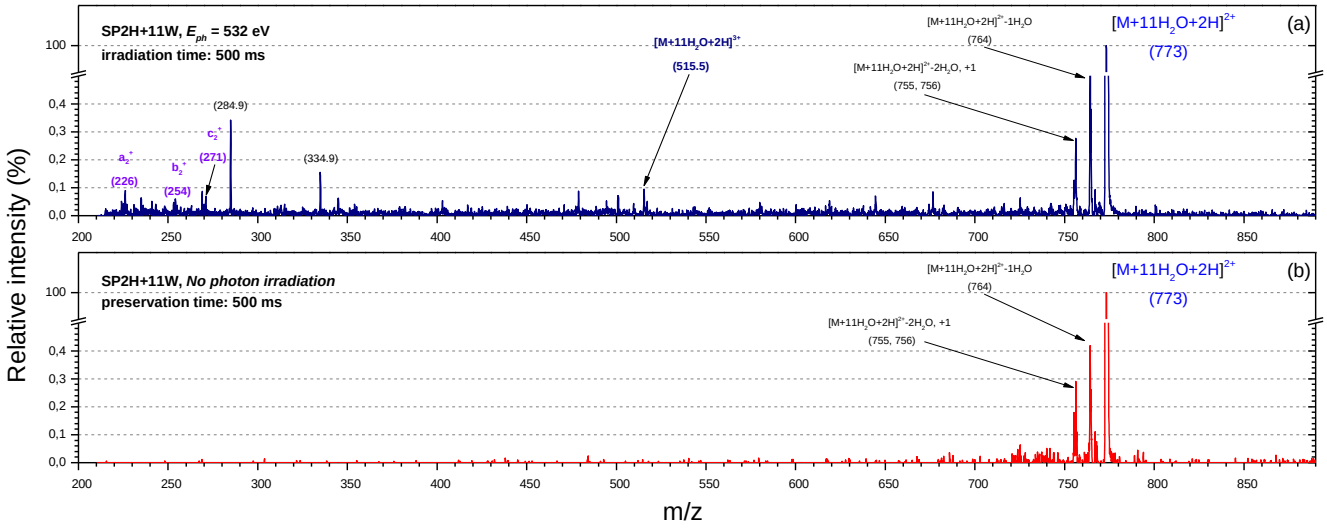

Fig.SI.3 *Top panel: tandem mass spectrum of the Substance with 11 water molecules irradiated at 532 eV for 500 ms, showing the backbone fragments. Bottom panel: mass spectrum of the same precursor ion stored in the same conditions but without photon irradiation. The two water loss peaks are spontaneous evaporation and not triggered by photon absorption.*

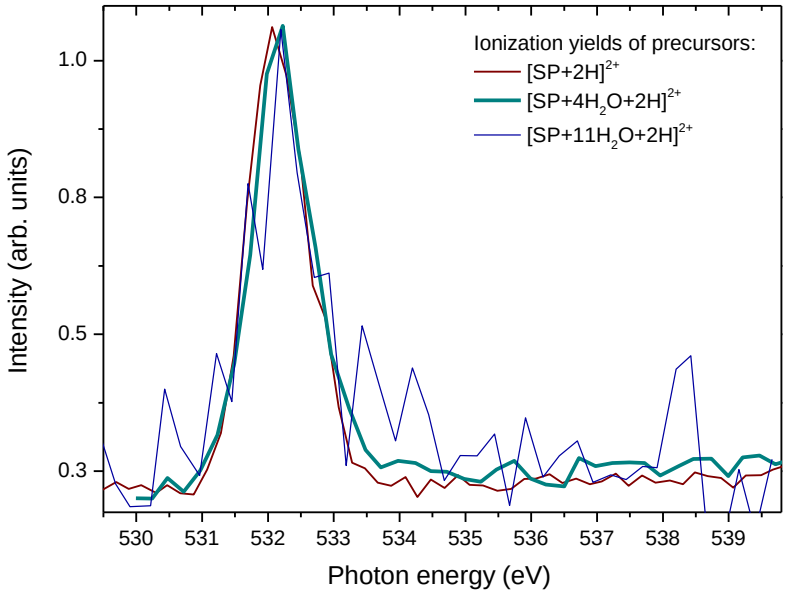

Fig.SI.4 *Ion yields for the triply charged radical cations $[SP+2H]^{3+}$ (brown, m/z 449.6), $[SP+2H+4H_2O]^{3+}$ (green, m/z 473.2) and $[SP+2H+11H_2O]^{3+}$ (blue, m/z 515.5), produced by ionization of the corresponding bare and hydrated doubly charged precursors.*

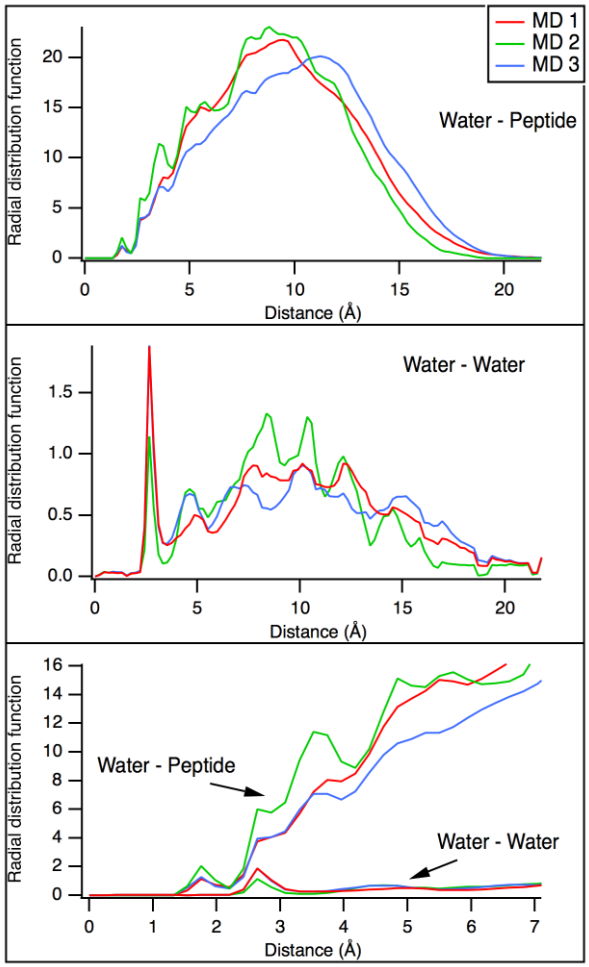

Fig.SI.5 *Calculated radial distribution function for the water peptide distance (top panel), water-water (middle panel) for three molecular dynamic simulations (red, green and blue curves). Bottom panel compares both RDF in the 0-7 Å.*