Supporting Information

Unravelling the intramolecular cyclization mechanism of oxidized tryptophan in aqueous solution as a function of pH

Jefferson Méndez-Hurtado\textsuperscript{a}, Ramón López\textsuperscript{a}, M. Isabel Menéndez\textsuperscript{a*}, Manuel F. Ruiz-López\textsuperscript{b*}

\textsuperscript{a}Departamento de Química Física y Analítica. Universidad de Oviedo. C/ Julián Clavería 8, 33006 Oviedo, Spain. E-mail: isabel@uniovi.es. Fax: +34-985103125

\textsuperscript{b}Theoretical Chemistry and Biochemistry group, SRSMC, Nancy-University. CNRS, BP 239, 54506 Vandoeuvre-lès-Nancy Cedex, France. E-mail: Manuel.Ruiz@univ-lorraine.fr. Fax: +33-383684371

Figure S1. Page 2

Figure S2. Page 3
Figure S1. Gibbs energy profiles for the initial proton transfer from the ammonium to the carboxylate group, and conformational rearrangements to arrive at the neutral Trp-OOH conformer ready to undergo cyclization along the C-route considering zero and two explicit water molecules.
Figure S2. Gibbs energy profiles for the routes from N2 to Zc-amino considering zero and two explicit water molecules