130 - Effect of the (n +1) residue on peptide deamidation

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Deamidation occurs spontaneously in peptides and proteins [1]. Many reports show that deamidation has a substantial effect on protein structure, function and stability. An experimental study on pentapeptides [2] shows that Asn deamidation rates are directly related to primary structure near Asn, with a prominent effect from the carboxyl-side (Yyy). We explore the correlation between experimental deamidation rates and primary structure for two pentapeptides (Yyy=Gly, Ile), to identify the factors causing this dependence. A pentapeptide in a water box is subject to Replica-Exchange Molecular Dynamics (REMD) calculations performed with GROMACS 4 software. Furthermore, a succinimide-mediated reaction [3] is investigated with QM/MM calculations utilizing the CP2K code using Nudged-Elastic-Band (NEB) calculations.[p] [p] [p][1] Robinson, NE, Robinson, AB *Proc. Natl. Acad. Sci. USA* **2001** , 98, 944.[p][2] Robinson, NE *J. Peptide Res.* **2004** , 63, 426.[p][3] Catak, S., Monard, G., Aviyente, V., Ruiz-López, MF *J. Phys. Chem. A* **2009** , 113, 1111.

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