Effects by pH on the peptide-binding site of two aspartic acid molecules

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Proteins, which have important roles as enzymes in many biological reactions, are consisted of 20 kinds of L-\textalpha{}-amino acids. These amino acids are connected with peptide bonds that combine N in \textalpha{}-amino group to C in \textalpha{}-carboxyl group. There are several proteinogenic amino acids containing two carboxyl groups or two amino groups. Even these amino acids, natural peptide bond found in proteins connects the \textalpha{}-amino group to the \textalpha{}-carboxyl group. The regioselective peptide binding might have been formed in early stage of chemical evolution because reactive side chain of these amino acids are important for basic functions of proteins. In such case, geological setting or geological events must lead the regioselective peptide bound. In this study, we tried to constrain geological setting for regioselectivity using aspartic acid (Asp) as a model amino acid. Asp has \textalpha{}- and \beta{}-carboxyl group that have slightly different pKa. To evaluate favorable geological settings for peptide formation with \textalpha{}-carboxyl carbon, we investigated the effects by different pH at high temperature and high pressure simulating difference in pH of pore water in deep-sea sediments. Asp solutions with pH ranging from 1.5 to 12.1 were heated and compressed for 1 – 8 days at 100 °C and 100 MPa. After incubation, the products were analyzed by liquid chromatography mass spectrometry. We also investigated the effects by pH on decomposition rate of Asp to evaluated suitable pH conditions for \textalpha{}-peptide formation. The decomposition rates of Asp were greater in higher pH and the peptides formed were different with varying pH. These results suggest that environments suitable for \textalpha{}-peptide formation were limited by pH.

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