Structure Determination from Powder Data of two Sub-peptides of Leu-enkephalin

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The crystal structures of two tripeptides, sub-peptides of leu-enkephalin which belongs to the opiate family of neuropeptides, have been solved from high resolution powder diffraction data using synchrotron radiation. Glycine-phenylalanine-leucine, $C_{13}N_3O_4H_{21}$, is monoclinic, space group $P2_1$, with a = 20.0024(8) Å, b = 4.8738(1) Å, c = 10.2778(2) Å, ß = 103.940(1)°, Z = 2, at room temperature. Glycine-glycine-phenylalanine, $C_{17}N_3O_4H_{24}{\cdot}2H_2O$, recrystalised from water is orthorhombic, space group $P2_12_12_1$, with a = 30.3902(2) Å, b = 10.25972(8) Å, c =4.83972(4) Å, Z = 4. The structures were solved via global optimization, programs TOPAS and FOX, and the use of maximum entropy maps.

Keywords: powder crystallography, peptides, synchrotron x-ray diffraction