

Poster Presentation

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Structure Determination of C₂₃H₁₉N₄OBr from Synchrotron Data

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A significant part of medicine is based on the discovery and development of drugs. It is very important to know the crystal structure of pharmaceutical compounds for fundamental understanding of structure, physical and chemical properties. Many of these materials are available only as powders. So any structural information must be obtained from powder diffraction. I am going to present following the stages while solving the structure of C₂₃H₁₉N₄OBr, 2-[3-phenyl-4(m-bromophenyl)-2-pyrazolin-1-yl]-3-methyl-4(3H)-quinazolinone, from 2-pyrazolines derivatives. The compounds are known to display various biological properties such as fungicidal insecticidal, anti bacterial, anti viral activities, pharmacological properties such as antiinflammatory agents and have industrial properties(1). The powder diffraction data was collected with Debye Scherrer camera at the BL01C2 beamline at room temperature in National Synchrotron Radiation Research Center(NSRRC), Taiwan. X-ray of wavelength was 1.0333Å. This compound crystallizes in orthorhombic system space group P bca, Z=8, unit cell parameters of a=25.83(1)Å, b=15.55(5)Å, c=10.63(3)Å, and V=4266.0(10)Å³. Reliability factors were reached Rwp=0.075, Rp=0.053, RB=0.086 ve S=1.31 after Rietveld refinement.

Keywords: structure determination, synchrotron x-ray powder diffraction, drug design