Poster Presentations

[MS24-P38] Experimental and theoretical studies on a novel of a [3,2-α]pyrimidine derivate
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The title molecule, (C_{30}H_{34}N_{2}O_{2}S_{1}), was synthesized and characterized by single-cryystal X-ray diffraction. The compound crystallizes in the triclinic space group P21/c. In addition, the molecular geometry, vibrational frequencies and frontier molecular orbitals analysis of the title compound in the ground state have been calculated by using the HF/6-31G(d) and B3LYP/6-31G(d) methods. Molecular electrostatic potential of the compound was also performed by the theoretical method.

**Keywords:** X-ray, ab-initio calculations.