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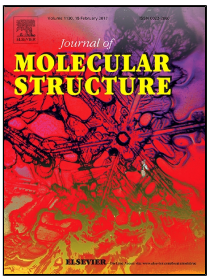

Vibrational Spectroscopic, Molecular Docking and Quantum Chemical Studies on 6-aminonicotinamide

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Highlights

- ✓ Conformational analysis was carried out for the 6-aminonicotinamide (ANA) molecule.
- ✓ The observed vibrational frequencies were assigned and compared with the calculated frequencies.
- ✓ UV-Vis spectra were simulated and compared with the experimentally observed spectrum.
- ✓ Inhibitory nature against Alzheimer's disease was predicted by molecular docking.
- ✓ Fukui function calculation and FMOs analysis predicted the molecular reactivity.