MS41-P03 | AMINE-IMINE PROTON TAUTOMERISM IN ISOMERIC 2-PHENYLAMINO-1,3-THIAZOL-4(5H)- AND 4-PHENYLAMINO-1,3-THIAZOL-2(5H)-ONE DERIVATIVES

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Newly synthesized derivatives of 2-phenylamino-5-dimethylaminomethylidene-1,3-thiazole-4(5*H*)-one and 4-phenylamino-5-dimethylaminomethylidene-1,3-thiazolin-2(5*H*)-one, with the potential to form tautomeric equilibria, have been studied by single-crystal X-ray diffraction, in order to determine the tautomeric form induced by -CF_3 substitution at the *para* position of the phenyl ring.

Location of the amidine hydrogen atom, carried out using difference electron density maps, unambiguously revealed the prevalence of the amino tautomeric form, with the H atom placed outside the thiazolinone cycle. This observation is corroborated by the presence of an intermolecular N–H···O hydrogen bond, with the exocyclic nitrogen atom as the donor and the carbonyl O atom as the acceptor. The thiazolinone and phenyl rings are nearly coplanar, facilitating a non-classical intramolecular C–H···N hydrogen bond between the phenyl ring H atom at the *ortho* position and the thiazolinone N atom, which further stabilizes the amino tautomeric form.

In addition, the conformational isomerism of the title molecules will be discussed in the context of biological activity of heterocyclic compounds and as an important factor influencing intermolecular interactions and crystal packing.

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