THEORETICAL STUDIES OF 1,2,4-TRIAZOLES

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Computational chemistry is the atomic and molecular modeling of chemistry in computer environment by using theoretical chemistry methods derived from physics principles such as quantum mechanics, molecular mechanics and molecular dynamics. Scientists need to calculate very cheaply and quickly by computers without the need for physical experiments that can be achieved by working in laboratories. Physicists and chemists have preliminary information about the structure of drugs before synthesis by making calculations on the computer and enable them to determine the desired properties in the drug. Molecule Modeling software provides convenience to those dealing with chemistry. With these programs, molecules can be observed from different angles by rotating them on the computer screen, their isomers and geometric structures can be understood, their energies can be calculated, UV, IR, NMR spectra can be drawn, and even MO diagrams can be accessed (Beytur et al., 2019; Beytur & Avinca, 2021; Gumus & Turker, 2012; Lienard et al., 2015; Rai et al., 2008; Sertçelik, 2021). In addition to experimental methods, computational chemistry methods are also used in the determination of corrosion inhibitors. The activity of an inhibitor, several quantum chemical parameters, can be calculated theoretically without the need for experimentation. The quantum chemical parameters generally used in theoretical studies on corrosion are atomic charges and molecular orbital energies (Karelson et al., 1996; Li et al., 2011).

DFT and HF methods used in theoretical calculations have been widely used in many references in recent years (Karunakaran & Balachandran, 2012; Suvitha et al., 2014). The functional density theory (DFT) method can calculate the physicochemical properties of the investigated molecules at the microscopic level with great precision and low processing cost (Marinho et

al., 2021; Raviprabha & Ramesh S. Bhat, 2019). Density Functional Theory (DFT) can be used to achieve geometric optimization of organic molecule. In addition, infrared (IR) spectra can be simulated and Frontier Molecular Orbitals (FMO) created for electronic characterization and for quantum chemical computations to determine the properties of the molecule as a nucleophile or electrophile parameters (Braga et al., 2016; Kotan et al., 2020; Uğurlu & Beytur, 2020). Ethyl-2-(4-amino-5-oxo-3-(thiophen-2-yl-methyl)-4,5-dihydro-1,2,4-triazol-1-yl) acetate compound was optimized using DFT/ 6–311++G(d,p) basis set and the B3LYP method. Structural parameters of the compound were calculated from the optimized molecular shape. The molecular structure of the related compound was determined by X-ray analysis and compared with experimental data. Theoretical vibration frequencies and NMR chemical shift values were obtained theoretically with the same method and basis set. In addition, molecular electrostatic potential (MEP) map and Mulliken atomic charges were calculated. Structural and spectral data obtained from the theoretical study were compared with the experimental data. Structural parameters and method and basic function selection were found to be appropriate (Çelik & Ünver, 2022).

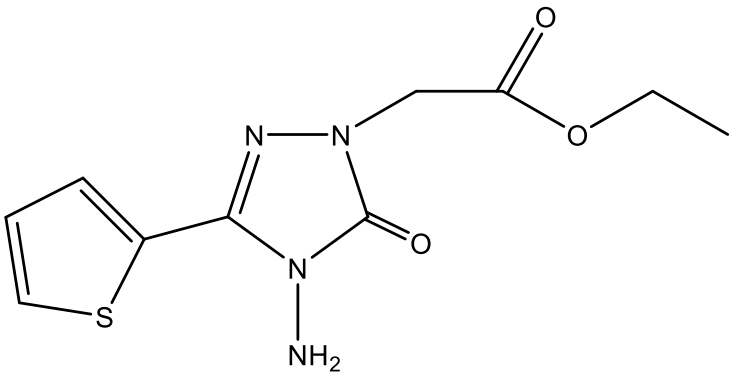

Figure 1. Structure of ethyl-2-(4-amino-5-oxo-3-(thiophen-2-yl-methyl)-4,5-dihydro-1,2,4-triazol-1-yl) acetate compound (Çelik & Ünver, 2022)

4-((4-Ethyl-5-(thiophen-2-yl)-4H-1,2,4-triazol-3-yl)thiomethyl)-7,8-dimethyl-2H-chromen-2-one synthesized by condensation 4-ethyl-5-(thiophen-2-yl)-4H-1,2,4-triazol-3-thiol and 4-(chloromethyl)-7,8-dimethyl-2H-chromen-2-one with medium acetone. The molecular shape was experimentally characterized using FT-IR, ^{1}H- and ^{13}C NMR spectroscopy. The Gaussian 09 program at the B3LYP/cc-pVDZ level of the DFT theory was used to generate the optimized structure of the compound, IR vibrational frequencies, ^{1}H- and ^{13}C NMR chemical shifts, Mulliken atomic charges and HOMO-LUMO energies. Obtained theoretical FT-IR, ^{1}H- and ^{13}C

NMR spectroscopy results were compared with experimental data. Theoretical and experimental results were found to be compatible. The proposed molecular structure is supported by both theoretical and experimental evidence. Dipole moment, hardness, softness, electronegativity, electrophilicity index, nucleophilicity index and chemical potential as electronic structural parameters for the prepared compound were calculated. In addition, the ratio of electrons transferred was calculated to determine the interaction between the iron surface and organic molecules (Parlak et al., 2022).

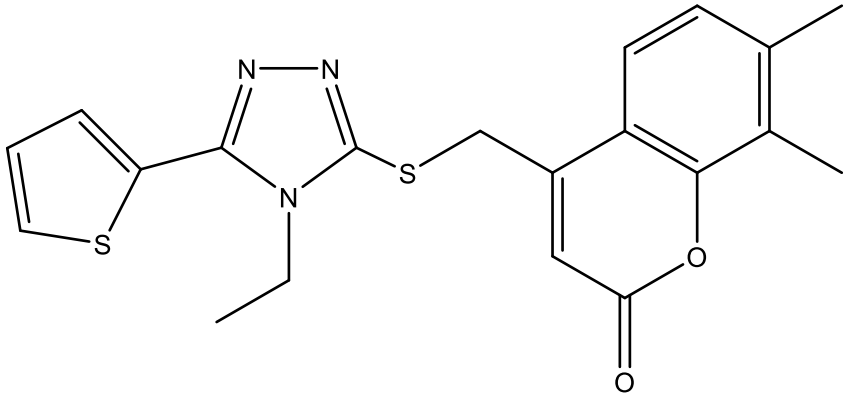

Figure 2. Structure of 4-((4-ethyl-5-(thiophen-2-yl)-4H-1,2,4-triazol-3-yl)thiomethyl)-7,8-dimethyl-2H-chromen-2-one (Parlak et al., 2022)

The N-Aroyl-1,2,4-triazoles TACl and TAM were regioselectively obtained in excellent yields through an efficient N-acylation reaction of 3-amino-5-methylsulfanyl-1H-1,2,4-triazole with aroyl chlorides. The structures of N-aroyl-1,2,4-triazoles were investigated by single-crystal X-ray diffraction and it was observed that their crystal structures were characterized by dimer formation via N–H N bonds. The supramolecular assembly depends on the type of linkages between the dimers and these vary markedly with para-substituted groups on the aroyl group. The ionization potential, electron affinity, electronegativity, electrophilicity index, hardness and chemical potential properties, which were calculated directly with the HOMO and LUMO energies, were determined. In addition, molecular electrostatic potential maps of both molecules showing a negative region on the N2 atom instead of the exocyclic amino group of the 1,2,4-triazole ring were calculated. Vibratory spectral analysis was performed for the N-aroyl-1,2,4-triazoles TAM and TACl using infrared spectroscopy in the range of 400-4000cm^{-1}. The fundamental vibrational frequencies and the intensity of the vibrational bands were evaluated using the density functional theory (DFT) basis set with the standard B3LYP/6–31G(d,p)

method, and a very good agreement was found between the observed and calculated frequencies (Moreno-Fuquen et al., 2021).

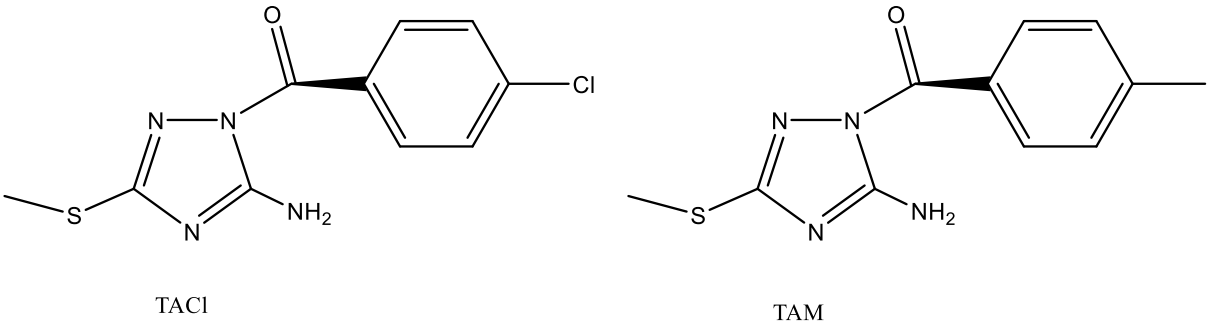

Figure 3. Structure of the N-Aroyl-1,2,4-triazoles TACl and TAM (Moreno-Fuquen et al., 2021)

An enantiomerically pure triazole derivative, (+)-(R)-5-[1-(benzenesulfonamido)-2-phenylethyl]-4-phenethyl-2,4-dihydro-3H-1,2,4-triazole-3 -thion was successfully synthesized in high yield and characterized by spectroscopic techniques (FT-IR and UV-Vis) and single crystal X-ray diffraction analysis. Hirshfeld surface (HS) analysis revealed the nature of intermolecular contacts, fingerprint plots and molecular surface contours. DFT calculations were performed on an isolated molecule in the gas phase using the B3LYP/6–31G(d,p) basis set. The DFT results of the related molecule for the geometric parameters were found to be compatible with the X-ray data. The stability of the molecule resulting from hyperconjugative interactions, charge delocalization was analyzed using natural bond orbital analysis (NBO), and nonlinear optical properties were investigated in the the study (Başaran et al., 2022).

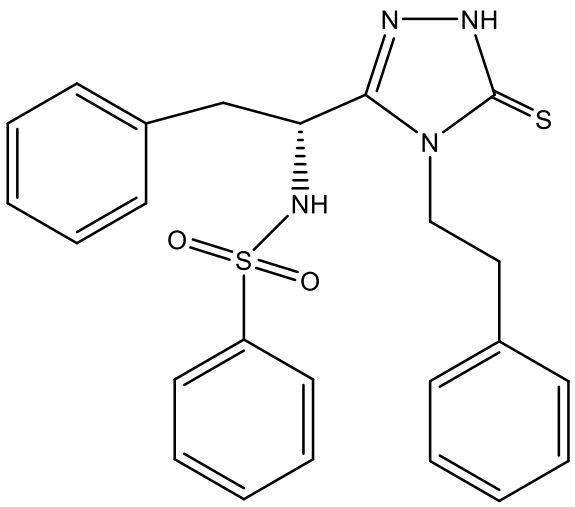

Figure 4. Structure of (+)-(R)-5-[1-(benzenesulfonamido)-2-phenylethyl]-4-phenethyl-2,4-dihydro-3H-1,2,4-triazole-3-thion (Başaran et al., 2022)

{Bis-4-[(3-alkyl-5-oxo-1H-1,2,4-triazol-4(5H)-yl)-imino-methyl]-phenyl} [1,10-biphenyl]-4,40-disulfonates were synthesized by reaction of 3-alkyl-4-amino-4,5-dihydro-1H-1,2,4-triazol-5-ones (T) and bis-(4-formylphenyl) [1,10-biphenyl]-4,40-disulfonate. The structures of these compounds were determined by IR and NMR spectral methods. Corrosion inhibitory activities of related compounds were investigated using quantum mechanical methods. Parameters such as the energy of highest occupied molecular orbital, the energy of the lowest unoccupied molecular orbital, the energy gap and the dipole moment, which are related to the corrosion efficiency of organic compounds with molecular geometry, and especially the electronic properties examined, were determined using the density function theory method. Using these calculation results, properties such as hardness, softness, electronegativity values were calculated. In addition, quantum chemical parameters such as the fraction of electrons transferred between the iron surface and 4,5-dihydro-1H-1,2,4-triazol-5-one derivative compounds were also Calculated (Beytur et al., 2019).

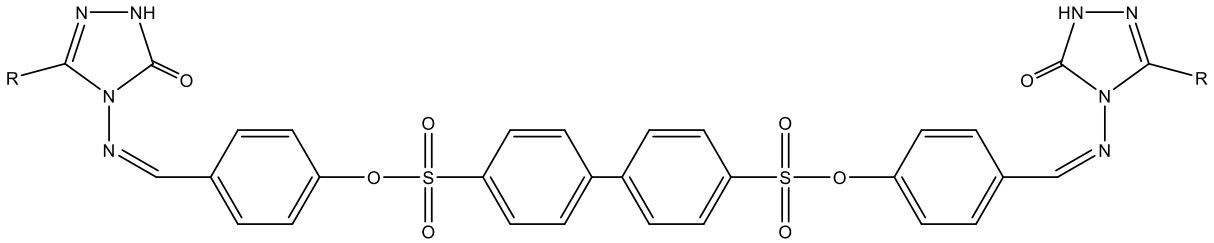

Figure 5. Structure of {Bis-4-[(3-alkyl-5-oxo-1H-1,2,4-triazol-4(5H)-yl)-imino-methyl]-phenyl} [1,10-biphenyl]-4,40-disulfonates (Beytur et al., 2019)

3-Subtitued-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one compounds were synthesized by the reaction 4-amino-(3-substıtued)-4,5-dihydro-1*H*-1,2,4-triazole-5-ones and 3-methylthiophene-2-carbaldehyde. The spectroscopic, electronic, geometric, nonlinear optical properties of titled molecules have been simulated. UV-visible absorption spectra data were calculated by using TD-DFT method in ethanol. Calculation of FT-IR frequencies was performed for the related compounds. The frequencies recorded with the DFT/B3LYP and DFT/B3PW91 methods were compared with the experimental values and it was determined that the B3LYP values were closest to the experimental values. From the optimized structure, ^{13}C-NMR and ^{1}H-NMR chemical shift values were calculated according to the GIAO method using the Gaussian 09W program package in a DMSO solvent environment. It has been seen that the results obtained are compatible with the experimental data. Finally, electronic properties of synthesized molecules such as ionization potential, electron affinity, energy gap, electronegativity, molecular hardness, molecular softness, electrophilic index, nucleophilic index and chemical potential were calculated from HOMO and LUMO energies using DFT/B3LYP and DFT/B3PW91 methods (Beytur & Avinca, 2021).

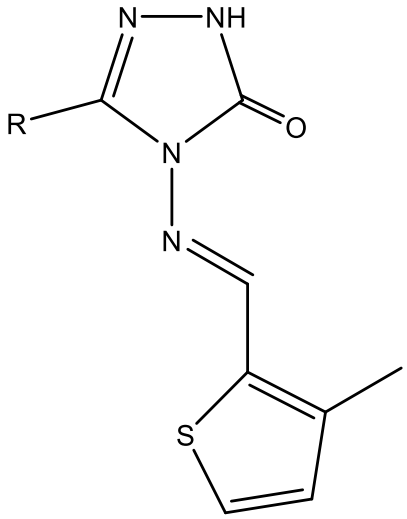

Figure 6. Structure of 3-Subtitued-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one compounds (Beytur & Avinca, 2021)

Corrosion inhibition of mild steel by 3,5-bis(n-pyridyl)-4-amino-1,2,4-triazoles in molar perchloric acid was investigated by gravimetric and electrochemical impedance spectroscopy techniques at 30 °C. 2-PAT, 3-PAT and 4-PAT were obtained with 65%, 95% and 92% protection efficiencies, respectively. It has been determined that the inhibitory properties of n-PAT change with concentration. A significant correlation between inhibition efficiency and

quantum chemical parameters was obtained using the quasi-experimental quantitative structure-activity relationships (QSAR) approach (Lebrini et al., 2008).

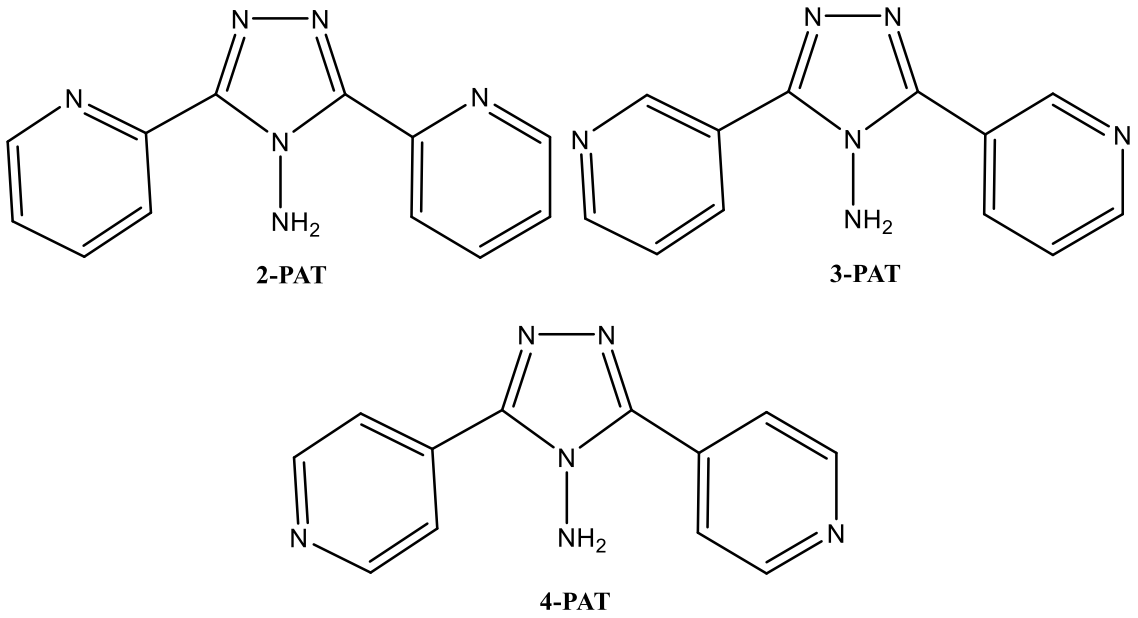

Figure 7. Structure of 3,5-bis(n-pyridyl)-4-amino-1,2,4-triazoles (Lebrini et al., 2008)

The inhibitory effect of 3-amino-1,2,4-triazole-5-thiol (3ATA5T) in 0.5 M HCl on carbon steel (CS) was investigated by electrochemical impedance spectroscopy. The compound of interest was investigated by potentiodynamic measurements at various concentrations and temperatures. According to the obtained results, it was determined that there is a harmony between the experimental and quantum computing parameters. Potential zero charge results determined that the CS surface was positively charged in the presence of 3ATA5T. Quantum chemical calculations showed that the potential zero charge measurements were in agreement with the experimental values (Mert et al., 2011).

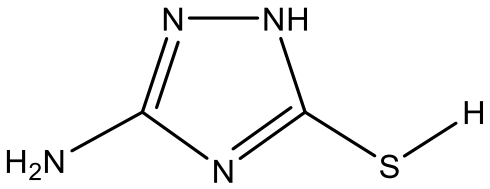

Figure 8. Structure of 3-amino-1,2,4-triazole-5-thiol (3ATA5T) (Mert et al., 2011)

The 5-propyl-4-amino-1,2,4-triazol-3-thion required for the study was obtained experimentally. The structure of the synthesized compound was characterized by spectroscopic (FT-IR and ^{1}H NMR) and structural (single crystal X-ray diffraction) techniques. Geometric parameters of the studied molecule were calculated by HF and DFT (B3LYP) method and analyzed with experimental data. The results showed that the calculated geometric parameters obtained by B3LYP/6-311G+(d,p) method had a better agreement with the experimental data than HF method. FT-IR and 1H NMR spectrum data were analyzed experimentally and theoretically. The theoretically calculated results were compared with the experimental data and found to be compatible with the FT-IR and ^{1}H NMR spectra. The energy gap value between HOMO and LUMO was calculated and the data obtained predicts that charge transfer from the benzene ring to the triazole ring can occur. NBO values were calculated from the optimized structure of the 5-propyl-4-amino-1,2,4-triazol-3-thion molecule using density functional theory (Jin et al., 2014).

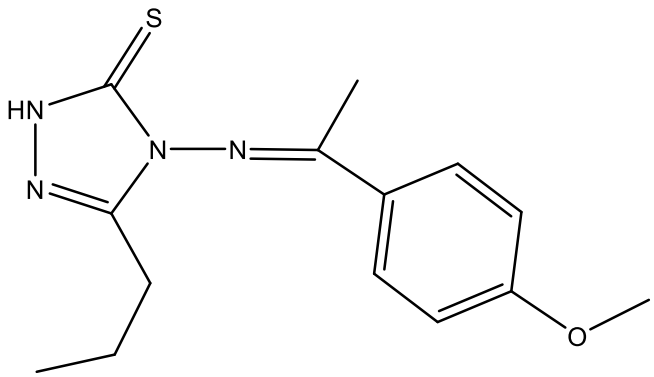

Figure 9. Structure of The 5-propyl-4-amino-1,2,4-triazol-3-thion (Jin et al., 2014)

The electronic structure, molecular properties and vibrational spectra of the 3-(adamantan-1-yl)-4-(4-chlorophenyl)-1H-1,2,4-triazole-5(4H)-thion compound, a new derivative of 1,2,4-triazol-5(4H)-thion were investigated by density functional theory. The hydrogen bonded dimer of the related compound was studied theoretically with the 6-311++G(d,p) diffused and polarized basis set using B3LYP, M06-2X and X3LYP methods. Intermolecular hydrogen bonding was determined using NBO analysis of the studied compound. The experimental FT-IR and FT-Raman spectra of the investigated compound were found to be compatible with the spectral data obtained by the DFT/B3LYP method. The dipole moment, molecular electrostatic potential surface and nonlinear optical properties such as and polarizability, first order static hyperpolarizability of the compound were calculated. The UV-Vis spectrum of the cap

molecule was calculated theoretically. The TD-DFT method was used to calculate the six lowest excited states and their excitation energies (Al-Tamimi, 2016).

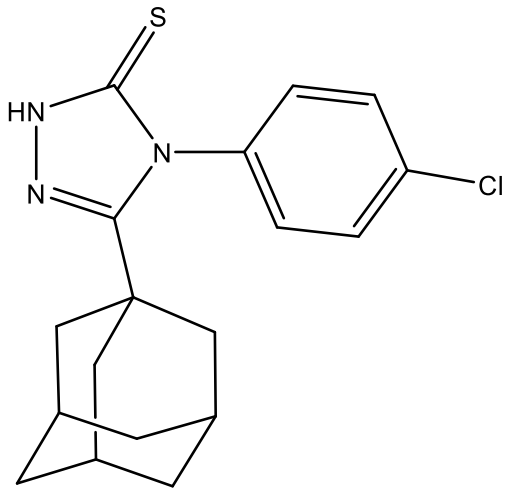

Figure 10. Structure of 3-(adamantan-1-yl)-4-(4-chlorophenyl)-1H-1,2,4-triazole-5(4H)-thion compound (Al-Tamimi, 2016)

4-allyl-5-pyridin-4-yl-2,4-dihydro-3H-1,2,4-triazol-3-thione was synthesized and its structure was investigated by IR-NMR spectroscopy and single-crystal X-ray diffraction. Molecular geometry obtained from X-ray experiment, vibration frequencies, 1H and 13C chemical shift values using gauge including atomic orbital (GIAO) of the compound were calculated using Hartree-Fock (HF) and density functional method (DFT/B3LYP). To determine the conformational conformity, the molecular energy profile of the studied compound was obtained by HF/6−31G(d) and (DFT/B3LYP) calculations. Additionally, frontier molecular orbitals (FMO), molecular electrostatic potential (MEP) and thermodynamic parameters were obtained by HF and DFT functional methods (Cansız et al., 2012).

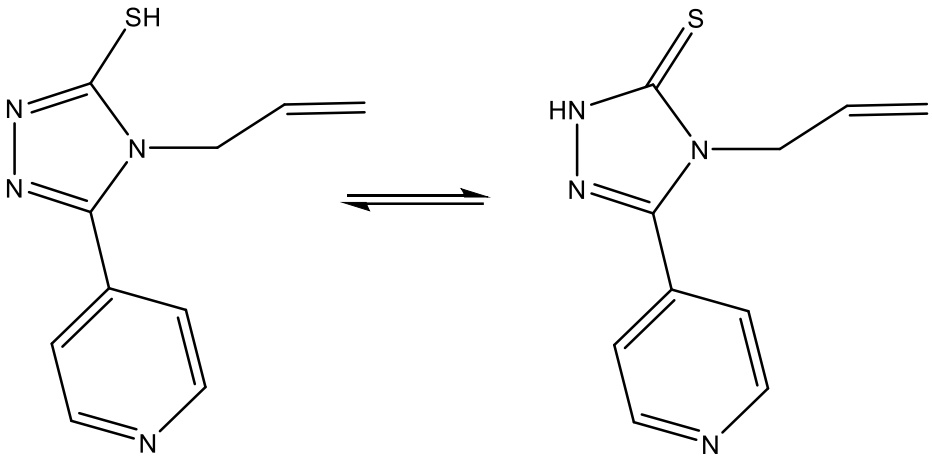

Figure 11. Structure of 4-allyl-5-pyridin-4-yl-2,4-dihydro-3H-1,2,4-triazol-3-thione (Cansız et al., 2012)

4-(4-Methoxyphenethyl)-3,5-dimethyl-4H-1,2,4-triazole was obtained from the reaction of 2-(4-methoxyphenyl)ethanamine with ethyl N'-acetylacetohydrazonate. The structure of the synthesized compound was characterized by IR, 1H/13C NMR, mass spectrometry, elemental analysis, analysis of X-ray crystallography and theoretical methods. The molecular geometry and vibrational frequencies of the relevant compound in the ground state were determined using the density functional method (B3LYP) with the 6-31G(d) basis set. The obtained data proved that the optimized geometry can reproduce the crystal structure well and that the theoretical vibration frequencies are in good agreement with the experimental values. The predicted nonlinear optical properties of the corresponding compound were determined and it was observed that urea was greater in value. The molecular electrostatic potentials and frontier molecular orbitals values of the compound were performed at the B3LYP/6-31G(d) theory level of DFT calculations (Düğdü et al., 2013).

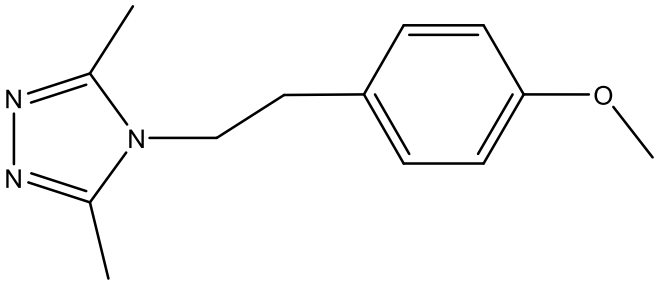

Figure 12. Structure of 4-(4-Methoxyphenethyl)-3,5-dimethyl-4H-1,2,4-triazole (Düğdü et al., 2013)

Experimental and theoretical vibrational frequencies of a newly synthesized 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thion molecule, a potential anti-inflammatory agent, were determined. Experimental Laser-Raman (4000-100 cm^{-1}) and FT-IR spectra (4000-400 cm^{-1}) of the molecule in the solid phase were obtained. The theoretical vibration frequencies and geometric parameters such as bond lengths, bond angles and dihedral angles of the optimized molecule were determined by density functional theory method (DFT/B3LYP). Types and evaluations of vibration frequencies were made with potential energy distribution (PED) analysis using VEDA 4 program. At the same time, the highest occupied molecular orbital (HOMO) energy, lowest unoccupied molecular orbital (LUMO) energy and other related molecular energy values of the 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thion molecule were calculated with the same theoretical calculations (Sert et al., 2014).

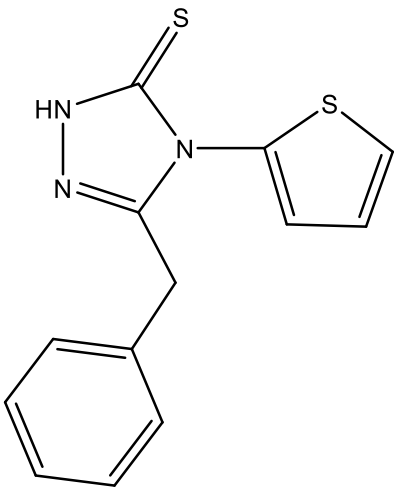

Figure 13. Structure of 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thion molecule (Sert et al., 2014)

Optimization study was carried out for the synthesis of 1,2,4-triazole-Schiff base derivatives. The reaction was carried out for a certain time in a microwave reactor using solvents such as ethanol, methanol or THF. By monomode microwave reactor in water, parameters such as temperature, time and solvent were changed to ensure that the reaction efficiency was at a high rate. The structures of the synthesized 1,2,4-triazole-Schiff base derivatives were characterized by FT-IR, NMR and MS. To determine the molecular geometry, electronic properties and chemical reactivity of the synthesized compounds were theoretically made DFT (density functional theory) and AIM (atoms in molecules) studies (Mermer & Boulebd, 2023).

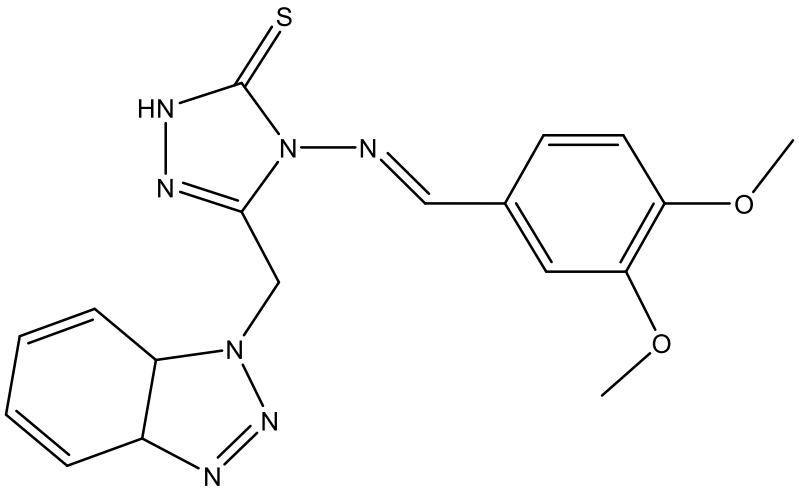

Figure 14. Structure of 1,2,4-triazole-Schiff base derivative (Mermer & Boulebd, 2023).

Various tautomers of 3-amino-1,2,4-triazole were calculated by FT-IR and FT-Raman spectrometry combined with quantum chemical theoretical calculation using PCM solvent model and normal mode analysis. Significant wavelength difference and Raman density patterns in solids and different solvents were obtained. Utilizing these data, NNH···N≤ on the five-membered N-heterocyclic ring is induced by hydrogen bond perturbation through hydrogen bonds. Thanks to the ground state proton transfer reaction mechanism in the five-membered N-heterocyclic ring, it was determined that there is intermolecular hydrogen bonding between the 3AT and protonic solvent molecules (Meng et al., 2018).

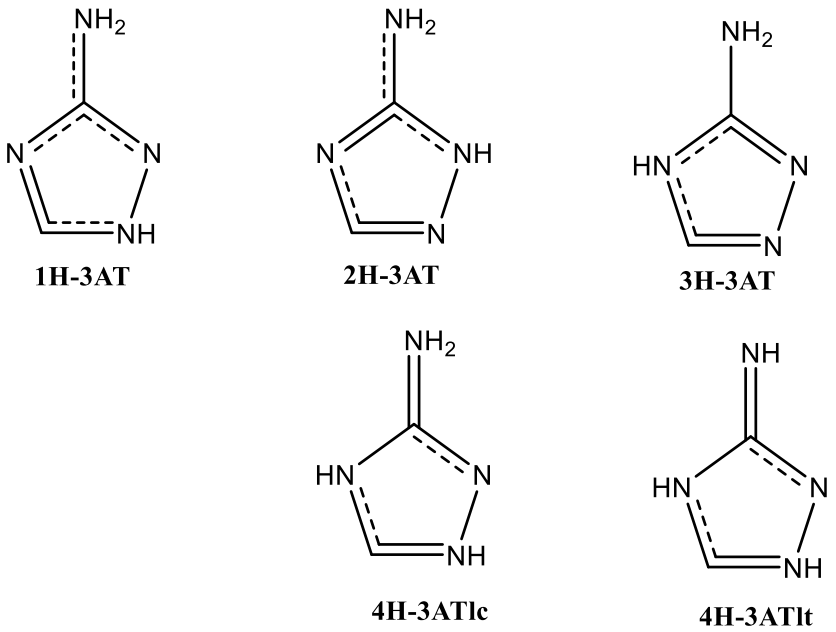

Figure 15. Various tautomers of 3-amino-1,2,4-triazole (Meng et al., 2018)

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