

**Ultrasound-Accelerated, Concise & Highly Efficient synthesis of 2-Oxazoline derivatives using Heterogenous Calcium Ferrite Nanoparticles and their DFT Studies**

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### Material & Methods

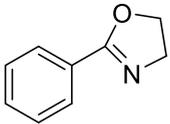
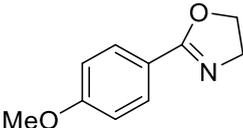
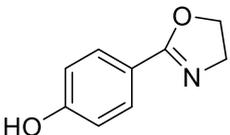
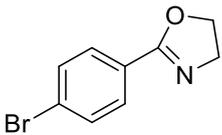
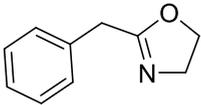
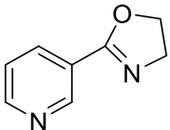
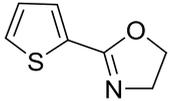
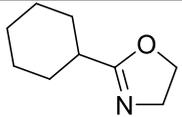
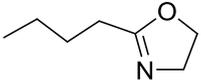
The required chemicals for the synthesis of calcium ferrite nanoparticles were of analytical grade. Calcium Nitrate [Ca (NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O], Ferric Nitrate [Fe (NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O], and Sodium Hydroxide [NaOH] were purchased from SD fine chemicals, India and were used without any further purifications. The used double distilled water was prepared in the laboratory. In addition, a hot plate with magnetic stirrer, small magnetic stirring bar, beaker, oven and a furnace were used for the synthesis of required nano materials. All purchased chemicals were used as received. All melting points are uncorrected.

All the reactions were performed in an oven-dried Schlenk flask. Column chromatography was performed using silica gel (mesh 100-200). TLC analysis was performed on commercially prepared 60 F254 silica gel plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I<sub>2</sub> chamber. The <sup>1</sup>H NMR spectra were recorded in CDCl<sub>3</sub> on a Jeol JNM-ECX400P at 400 MHz. Chemical shifts for carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, br s = broad singlet), coupling constants in Hertz, and integration.

The synthesized CaFe<sub>2</sub>O<sub>4</sub> nanoparticles were characterized by X-ray diffraction (XRD) [JNU, New Delhi], Transmission Electron Microscopy (TEM) [IARI, New Delhi], FT-IR and N<sub>2</sub> adsorption–desorption isotherm analysis (BET Analysis) [University of Delhi, New Delhi].

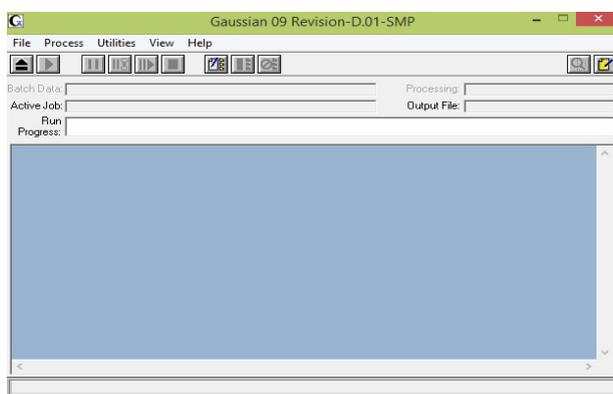
X-ray diffraction (PXRD) pattern was collected using a high resolution X'Pert PAN analytical diffractometer equipped with a Xe proportional detector employing Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ). It was recorded with a scan rate of 4.0 s per step and step size of 0.04° at 25 °C over the 2 $\theta$  range of 10-80°. The TEM images were carried out using an FEI Technai G2 20 electron microscope operating at 200 kV and also calculated the surface area of the nanoparticles using BET analysis.

**Nomenclature & Structure of compounds:**

S. No	Entry	Structure	General Name	IUPAC Name
1	3a		2-Phenyl oxazoline	2-phenyl-4,5-dihydrooxazole
2	3b		2-(4- Methoxyphenyl) oxazoline	2-(4-methoxyphenyl)-4,5-dihydrooxazole
3	3c		2-(4- Hydroxyphenyl) oxazoline	4-(4,5-dihydrooxazol-2-yl) phenol
4	3d		2-(4-Bromophenyl) oxazoline	2-(4-bromophenyl)-4,5-dihydrooxazole
5	3e		2- Benzyl oxazoline	2-benzyl-4,5-dihydrooxazole
6	3f		2-(3-Pyridyl)-2-oxazoline	2-(pyridin-3-yl)-4,5-dihydrooxazole
7	3g		2-(2-Thienyl)-2- oxazoline	2-(thiophen-2-yl)-4,5-dihydrooxazole
8	3h		2-(cyclohexyl)-2-oxazoline	2-cyclohexyl-4,5-dihydrooxazole
9	3i		2-(n-Butyl)-2-oxazoline	2-butyl-4,5-dihydrooxazole
10	3j		2-Methyl-2-oxazoline	2-methyl-4,5-dihydrooxazole

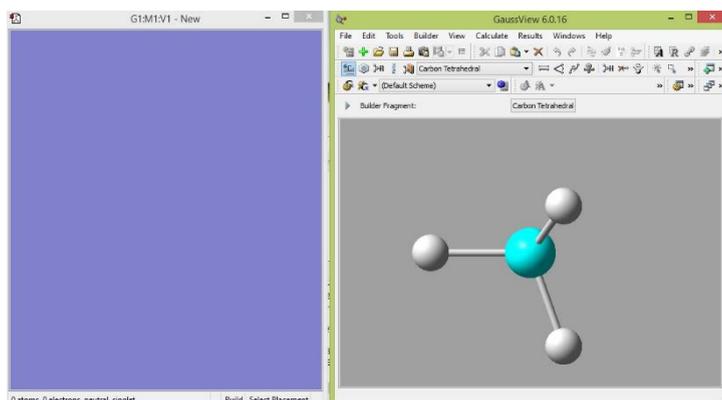
## Computational Studies:

In the present study, Quantum chemical calculations were used initially to optimize the geometry of all the molecules using Density Functional Theory (DFT), (B3LYP) method and 6-311++G (d,p) basis set with the aid of Gaussian 09 program package and Gauss View – 6.0. In 1970, *John Pople et al* at Carnegie- Mellon University released one of the most useful software called Gaussian for quantum mechanical calculations provide the information about various molecular properties of chemical molecules using fundamental laws of quantum mechanics. Now a days, the available updated version of gaussian software program is Gaussian 09 which is extensively used by chemists, chemical engineers, physicists and biochemists across the world. The graphical Interface of the Gaussian 09 is shown in Figure 1.



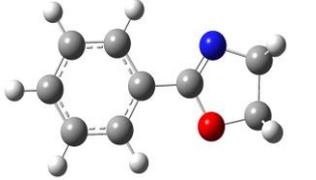
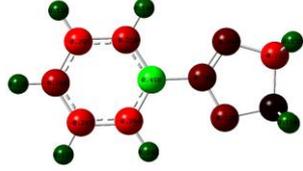
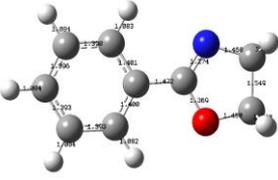
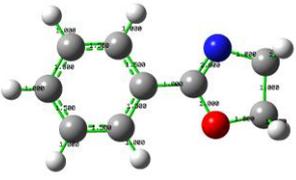
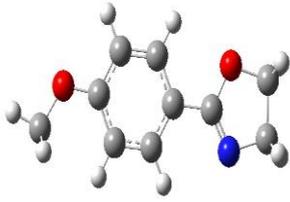
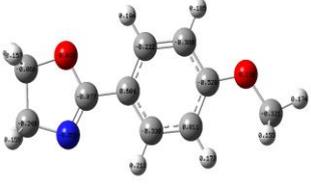
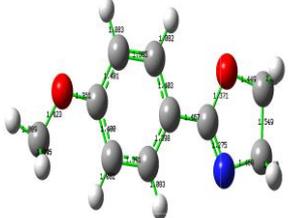
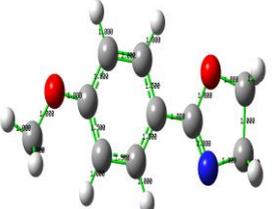
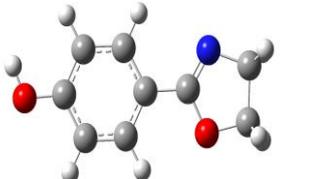
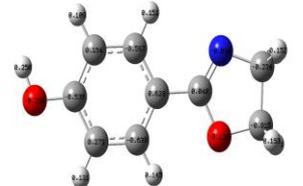
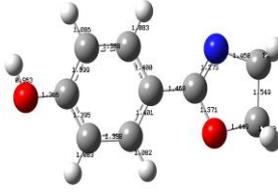
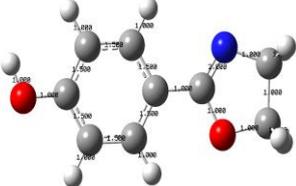
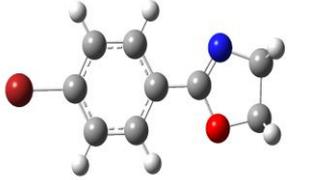
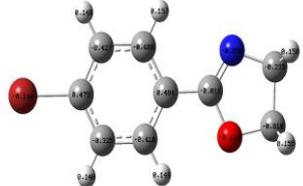
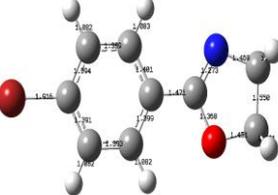
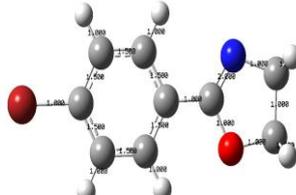
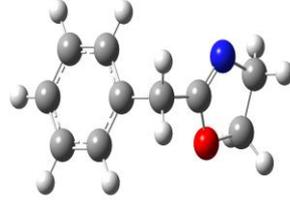
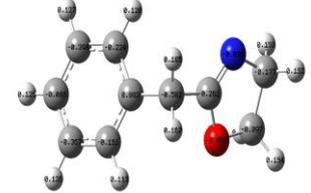
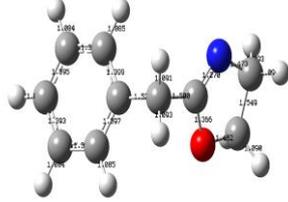
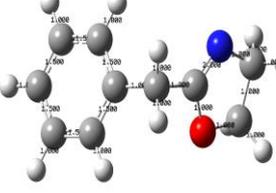
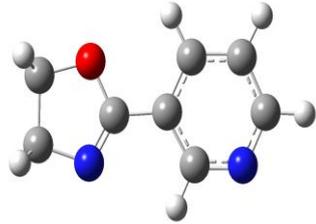
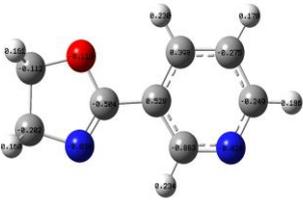
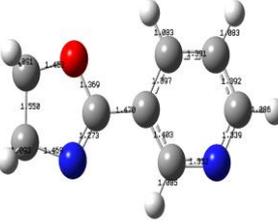
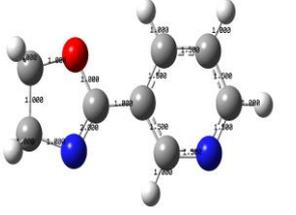
**Figure 1: Graphical Interface of the Gaussian 09**

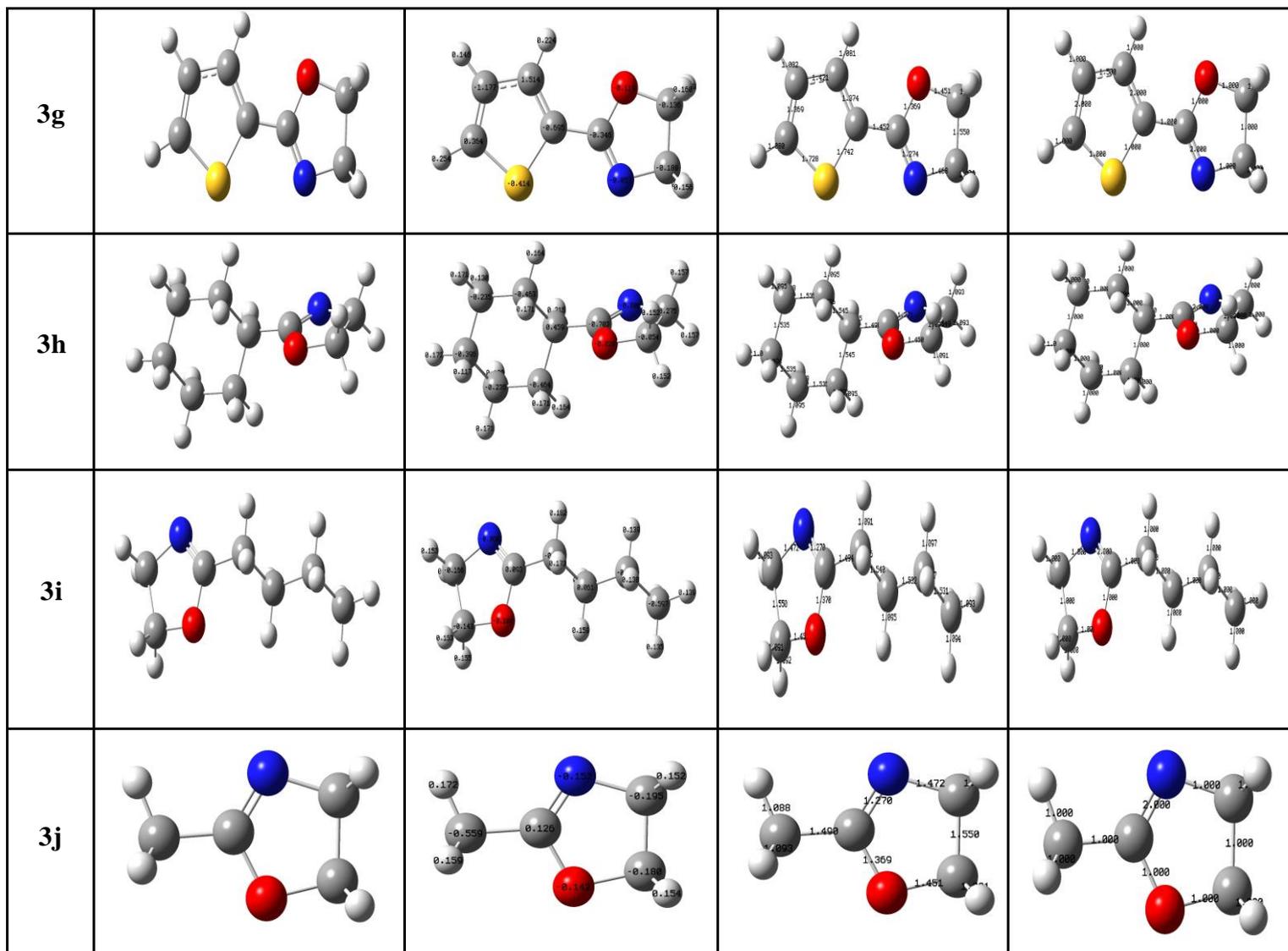
Gauss-View is widely used visualization and modeling software of Gaussian developed by Semichem Inc., but distributed with Gaussian. The available updated version of Gauss - View software program is Gauss - View 6 which creates the input files for Gaussian calculations and also renders the output. The graphical interface of Gauss-View 6.0 is shown in Figure 2.



**Figure 2. Graphical interface of Gauss-View 6.0**

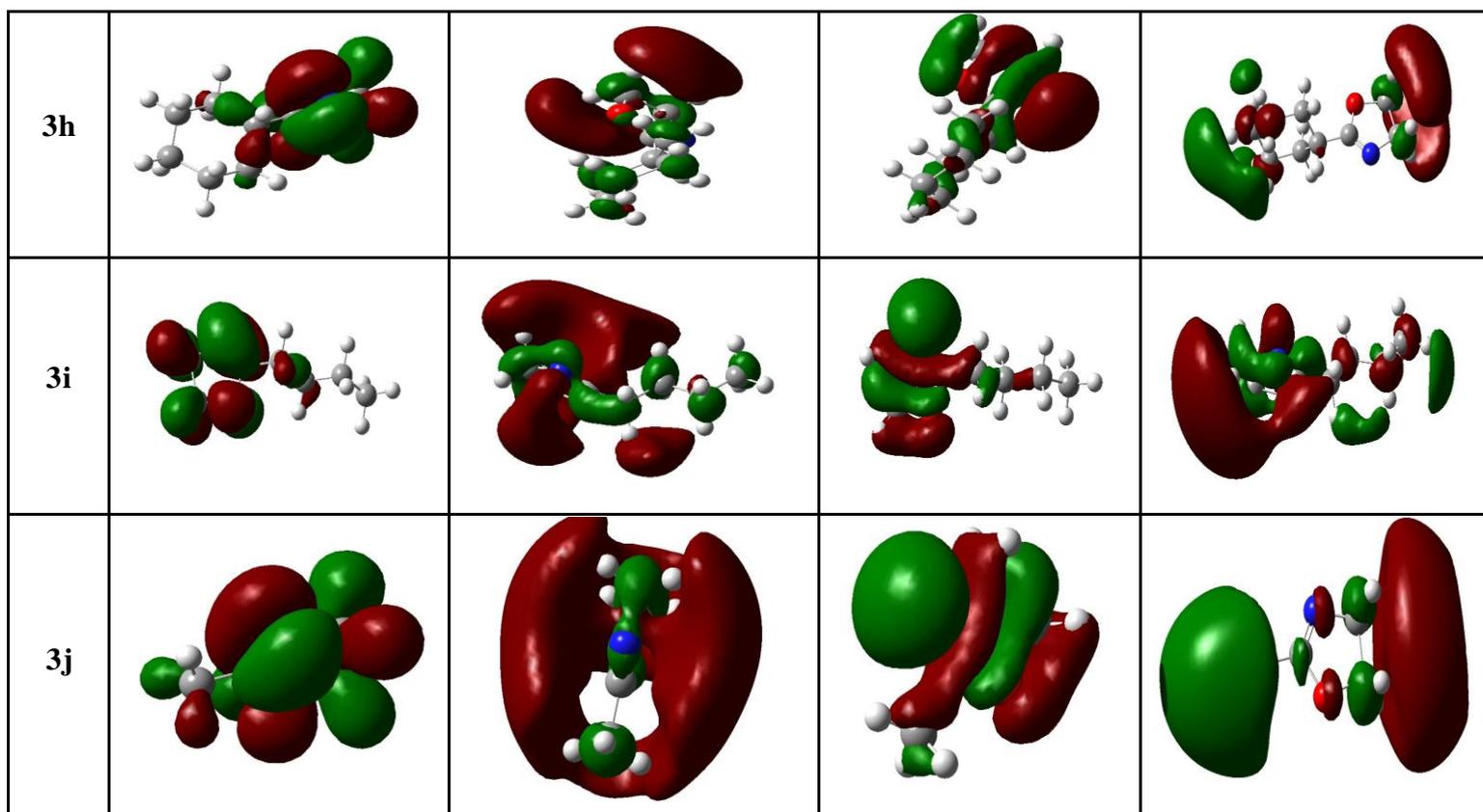
# Molecular Geometry:

Entry	Optimized Geometry	Mulliken Charges	Bond Lengths	Bond Orders
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3b				
3c				
3d				
3e				
3f				

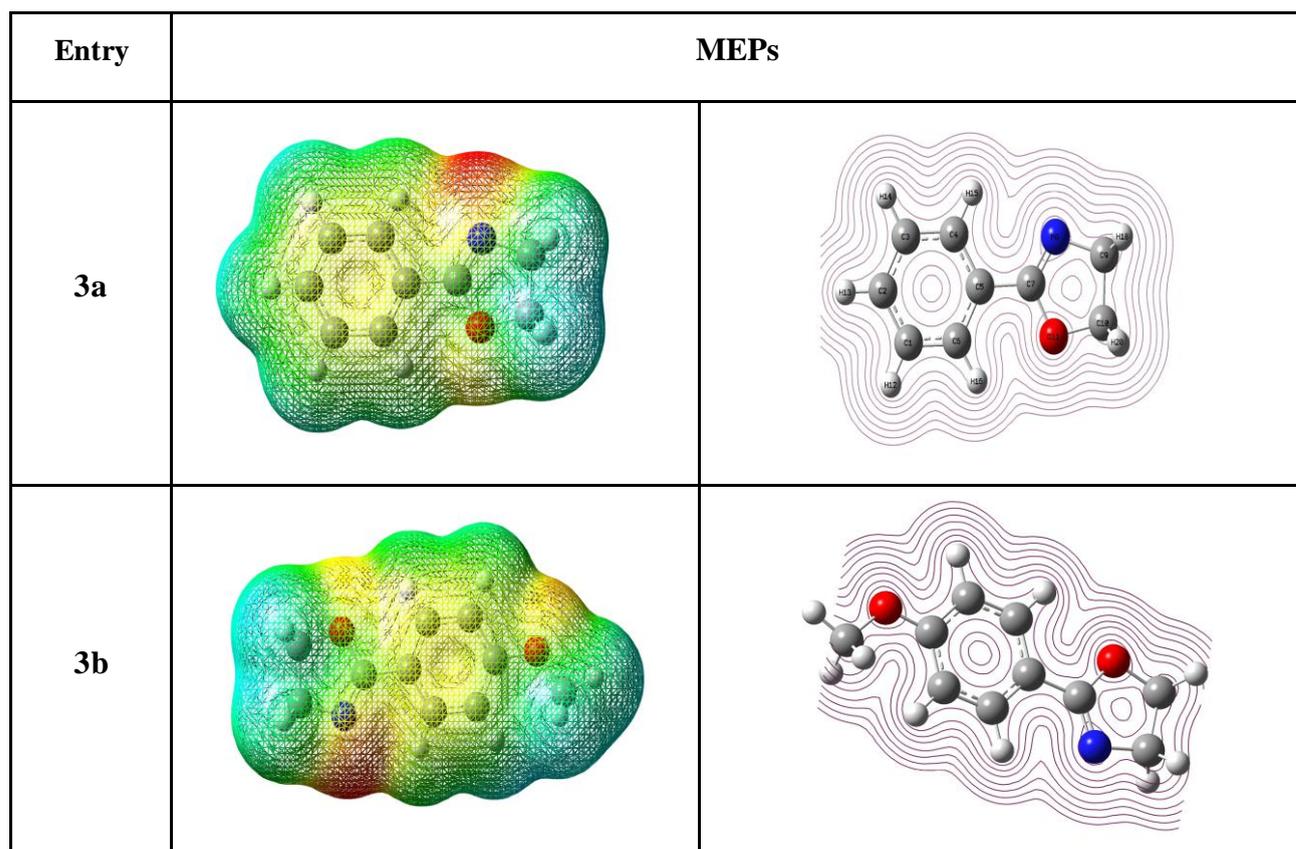


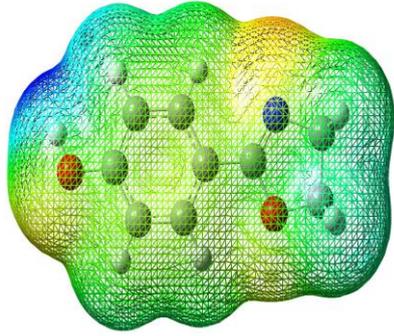
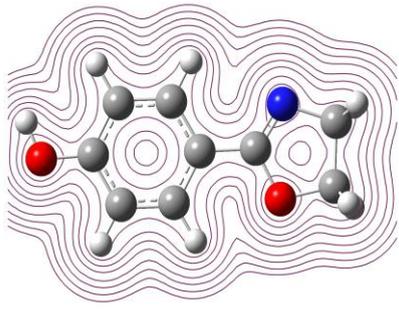
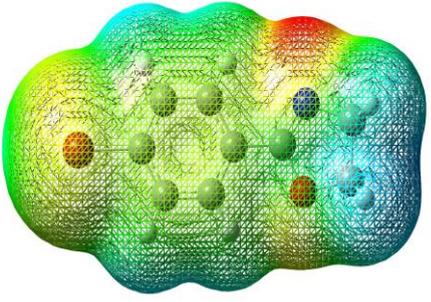
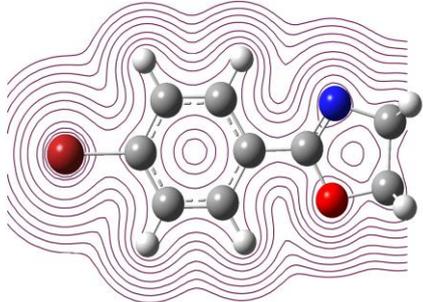
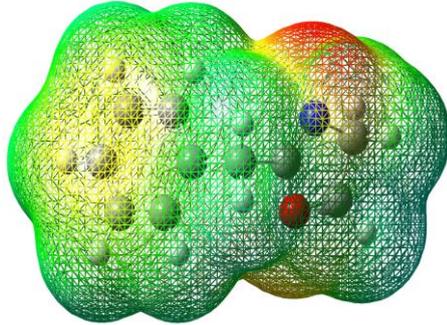
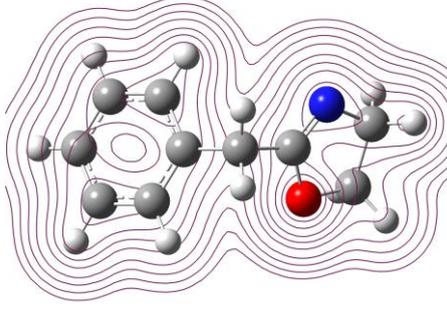
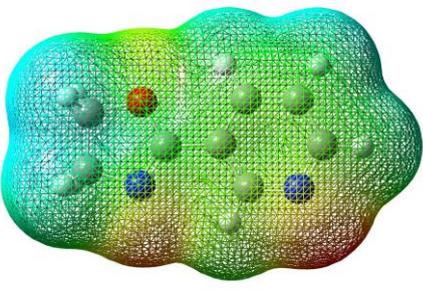
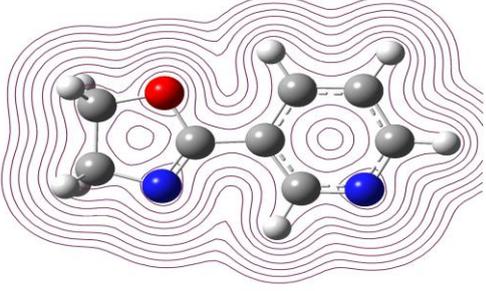
# Frontier Molecular Orbitals

Entry	HOMO	LUMO	HOMO-1	LUMO+1
3a				
3b				
3c				
3d				
3e				
3f				
3g				



### Molecular Electrostatic Potential Map



3c		
3d		
3e		
3f		
3g	