

## THEORETICAL MODEL OF PHYSISORPTION EFFECT OF CO ON CONIINE AND FURANOCOUMARINS FOR AIR PURIFICATION

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For the first time in the present work, the adsorption properties of the Coniine and Furanocoumarins at the non-bonded interaction with CO was investigated by density functional theory (DFT/B3LYP/MidiX, DFT/M062X/6-311+G\* levels of theory) in the solvent water.

**Keywords:** physisorption, DFT method, Coniine, Furanocoumarins, Air Purification.

For the first time in the present study, the non-bonded interaction of the Coniine and Furanocoumarins with carbon monoxide (CO) was investigated by density functional theory (DFT/B3LYP/MidiX, DFT/M062X/6-311+G\*) in the gas phase and solvent water. The adsorption of the CO over C<sub>8</sub>H<sub>17</sub>N was affected on the electronic properties such as E<sub>HOMO</sub>, E<sub>LUMO</sub>, the energy gap between LUMO and HOMO, global hardness. Furthermore, chemical shift tensors and natural charge of the C<sub>8</sub>H<sub>17</sub>N and complex C<sub>8</sub>H<sub>17</sub>N/CO were determined and discussed [1]. According to the natural bond orbital (NBO) results, the molecule C<sub>8</sub>H<sub>17</sub>N and CO play as both electron donor and acceptor at the complex C<sub>8</sub>H<sub>17</sub>N/CO in the gas phase and solvent water. On the other hand, the charge transfer is occurred between the bonding, antibonding or nonbonding orbitals in two molecules C<sub>8</sub>H<sub>17</sub>N and CO. We have also investigated the charge distribution for the complex C<sub>8</sub>H<sub>17</sub>N/CO by molecular electrostatic potential (MEP) calculations using the M062X/6-311+G\* level of theory. The electronic spectra of the C<sub>8</sub>H<sub>17</sub>N and complex C<sub>8</sub>H<sub>17</sub>N/CO were calculated by time dependent DFT (TD-DFT) for investigation of the maximum wavelength value of the C<sub>8</sub>H<sub>17</sub>N before and after the non-bonded interaction with the CO in the gas phase and solvent water. Therefore, C<sub>8</sub>H<sub>17</sub>N can be used as strong absorbers for air purification and reduce environmental pollution [2].

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## EFFECTIVENESS OF PRENATAL DIAGNOSTICS OF CONGENITAL DEVELOPMENT DISORDERS IN THE REPUBLIC OF BELARUS ACCORDING TO THE DATA OF THE BELARUSIAN REGISTER

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**Keywords:** congenital malformations, the effectiveness of prenatal diagnosis.

Congenital malformations (CHD) in recent decades have occupied a major place in the world among the causes of stillbirth, infant and child morbidity, disability, and mortality.