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Discriminate between Antibacterial and Non–Antibacterial Drugs Artificial Neutral Networks of a Multilayer Perceptron (MLP) Type Using a Set of Topological Descriptors

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A number of heavy metal toxicity and diseases models have been developed using methods of artificial neutral networks, k–nearest neighbors, linear discriminative analysis, multiple linear regression and have also been compared for their ability to recognize ten types of heavy metal toxicity and diseases that include conventional drugs, inactive drugs likes, antimicrobial substituents and bacterial and human metabolites. A set of topological descriptors has been used to discriminate between antibacterial and non–antibacterial drugs artificial neutral networks of a Multilayer Perceptron (MLP) type. The comparison of the performance by ninety eight computational approaches demonstrated that the neutral nets result in generally more accurate predictions, followed closely by k–nearest neighbor's methods. It is anticipated that the study may bring additional insight into heavy metal toxicity and diseases for conventional drugs, inactive chemicals and metabolic substances and may help in rationalizing design and discovery of novel antimicrobials and human therapeutics with improved, metabolite like properties.

On the other hand, heavy metal toxicity and diseases represent class of natural compounds which Carbene (CH_2), Silylene (SiH_2), Germylene (GeH_2), Tin Dihydride (SnH_2), Lead (II) Hydride and Plumbous Hydride (PbH_2) are some of them. Highly reactive intermediates, Carbene (CH_2), Silylene (SiH_2), Germylene (GeH_2), Tin Dihydride (SnH_2), Lead (II) Hydride and Plumbous Hydride (PbH_2) have attracted much attention in organic, inorganic and physical chemistry [1-14]. Full geometry optimizations are carried out on singlet and triplet states of alkyl substituted Acylic Carbene (CH_2), Acylic Silylene (SiH_2), Acylic Germylene (GeH_2), Acylic Tin Dihydride (SnH_2), Acylic Lead (II) Hydride and Plumbous Hydride (PbH2) by HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP methods using 31G, 6–31G*, 6–31+G*, 6–31G(3df, 3pd), 6–311G, 6–311G* and 6–311+G* basis sets of the Gaussian 09. It should be noted that for methylene (CH_2) and ethylidene (CH_3CH), the triplet state is ground state while for propylidene (CH_3CH_2CH) and other larger substituted Acylic Carbenes (CH_2), the singlet state is ground state. In contrast to Carbene (CH_2), Germylene (GeH_2), Lead (II) Hydride and Plumbous Hydride (PbH_2), the singlet state of Silylene (SiH_2) and Tin Dihydride (SnH_2) is ground state. Also, similar to Carbene (CH_2), Germylene (GeH_2), Lead (II) Hydride and Plumbous Hydride (PbH_2), stability of singlet state is increased with substituting of alkyl groups on Silylene (SiH_2) and Tin Dihydride (SnH_2) centers. By comparing Natural Bond Orbital (NBO) charges on Silylene (SiH_2) and Tin Dihydride (SnH_2) centers and other larger substituted Acylic Silylene (SiH_2) and Acylic Tin Dihydride (SnH_2), the role of methyl group is electron withdrawing respect to or more than Hydrogen (H) atom. Higher electronegativity of methyl group leads to stabilize the singlet respect to triplet state as well as decreasing the singlet–triplet splitting energies. Furthermore, these compounds have anti–spasmodic, anti–inflammatory and sedative effects. In our last study, purification of Carbene (CH_2), Silylene (SiH_2), Germylene (GeH_2), Tin Dihydride (SnH_2), Lead (II) Hydride and Plumbous Hydride (PbH_2) from some chemical compounds was performed. In this editorial, a quantum calculation of Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR–FTIR), HR Mass, UV–Vis, FT–Raman, ^{1}HNMR and ^{13}CNMR spectra was done and also chemical and physical properties of Carbene (CH_2), Silylene (SiH_2), Germylene (GeH_2), Tin Dihydride (SnH_2), Lead (II) Hydride and Plumbous Hydride (PbH_2) was checked. All of the reported calculations in this work were performed by the Gaussian 09. These calculations were employed by HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP methods using 31G, 6–31G*, 6–31+G*, 6–31G(3df, 3pd), 6–311G, 6–311G* and 6–311+G* basis sets of the Gaussian 09. Results indicated that Carbene (CH_2), Silylene (SiH_2), Germylene (GeH_2), Tin Dihydride (SnH_2), Lead (II) Hydride

and Plumbous Hydride (PbH_2) have antioxidant effects and calculations of Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR–FTIR), HR Mass, UV–Vis, FT–Raman, ^{1}HNMR and ^{13}CNMR spectra in B3LYP level and 6–311G* basis set, one better than the other ways and results are more close to experimental spectra.

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