

QUANTUM CHEMICAL CALCULATIONS FOR STRUCTURAL GEOMETRIES AND BONDING THERMODYNAMICS OF HISTAMINE AND TARGETTED CATECHOLAMINES. Jewel Harper, Morgan Bernard, Insu F. Hahn, Dept. of Biology and Dept. of Chemistry & Biochemistry, Hampton University. Histamine and catecholamines such as dopamine, norepinephrine, and gamma-aminobutyric acid are critical neurotransmitters involved in physiological stress responses and neural signaling. These biosynthesized neurotransmitters are derived from amino acids, oxidations and lack alpha-carboxylates. These compounds are produced by both mast cell in tissues, nerve tissues or the adrenal glands located above the kidneys and are excreted through urine. During stress, these compounds are secreted as catabolic hormones that catalyze a range of metabolic processes, including an increase in lactic and ketoacid production. In this computational study, the proven semi-empirical quantum chemical computational methods were used to understand the snapshot of structural geometries and comparative thermochemical bonding properties (i.e., stability and reactivity) during their biosynthetic pathways of catecholamines and histamine. Computed heat of formation values indicate that most catecholamines are more stabilized in aqueous solution compared to the gas phase. The results suggest that histamine formation is the most thermodynamically favorable among the tested molecules, whereas dopamine formation is comparatively less favorable under the modeled conditions. The calculated stability order was determined to be: Histamine > Norepinephrine > GABA > Dopamine. These research outcomes could contribute to a correct and precise understanding of molecular-level biochemical pathways of histamine and catecholamines. By integrating structural modeling with quantitative energetic analysis, this study offers a comparative perspective that strengthens mechanistic understanding of these stress-related biomolecules. Future studies aim to obtain high-level ab initio quantum chemical properties of those neurotransmitters. (Supported by: DOEd, R. McNair Program, Hampton Univ.). Author contact: Insu F. Hahn, [insu.hahn@hamptonu.edu](mailto:insu.hahn@hamptonu.edu)