Quantum and Molecular Analysis of MDPV Analogs

Naveen Chandra Kotha and Dr. Carol Parish

COUNTS Program, Department of Chemistry, University of Richmond

John Randolph Tucker High School

Richmond, VA 23173

The compound Methylenedioxypyrovalerone (MDPV) ($C_{16}H_{21}NO_3$ - 275.343 g/mol) is a psychoactive drug - a chemical substance that affects brain function and the central nervous system - that shows signs of stimulant properties, which enhance mental or physical functions in most cases of use. MDPV achieves these effects by acting as a norepinephrine-dopamine reuptake inhibitor (NDRI). MDPV has not been approved by the Food and Drug Administration (FDA) for medical use due to its strength and tendency to become addictive. This drug has been found to be four times as potent as methylphenidate, a drug previously used to treat ADHD. As a stimulant, MDPV has been recorded to produce effects similar to those of cocaine, methylphenidate, and the amphetamines. The primary psychological effects of MDPV usually last for approximately 3 to 4 hours, while residual effects, such as hypertension, usually last for approximately 6 to 8 hours. Higher doses of MDPV have been known to cause prolonged, intense panic attacks, psychotic behavior due to sleep deprivation, and even death. The focus of this computational research was to model the structures of the MDPV analog molecules, calculate their theoretical quantum and molecular characteristics, and compare them to experimentally gathered data to find any existing correlations. These correlations will then be used in a study to better understand the mechanisms through which molecules of MDPV and its analogs bind to dopamine-transporting proteins and hinder the reuptake of dopamine in the system.