Public Abstract

First Name:Eddie

Middle Name:LaReece

Last Name:Pittman

Adviser's First Name:Renee

Adviser's Last Name:JiJi

Co-Adviser's First Name:Chung-ho

Co-Adviser's Last Name:Lin

Graduation Term:SP 2015

Department:Chemistry

Degree:PhD

Title:Spectroscopic Distinguishability, Forced Degradation Kinetics and LC-MS/MS degradation product characterizations involving 5-Fluorouracil and similar or affiliated compounds in relation to Environmental Concerns

ACADEMIC ABSTRACT

5-Fluorouracil (5-FU) is a commonly used antiviral and anticancer drug. 5-FU is believed to exist in various tautomeric forms, which are believed to contribute to 5-FU's cytotoxicity. In order to understand the activity of 5-FU in biological and environmental settings, a combined theoretical and experimental approach was used to determine the predominant tautomer in aqueous environments. Spectral characterization of 5-FU will enable development of improved analytical methods for 5-FU. The structures of the 6 most relevant tautomers of 5-FU were optimized using DFT (B3LYP/6-311++G(d, p)) and their respective UV absorption, IR, Raman and NMR spectra calculated. The UV resonance Raman spectrum of 5-FU is also reported. The C=O (1711(cm-1)), C=C (1673(cm-1)) and C-N (1463(cm-1)) and N-H (1510(cm-1)) stretching frequencies are strongly enhanced in the deep UV resonance Raman spectrum of 5-FU. Comparison of the theoretical spectra with measured UV absorption, IR, UV Raman and NMR indicate that the 5-FU keto tautomer is the predominant species in aqueous environments.

Four applicable set of environmental conditions were applied towards 5-FU which all produced results that can be used to help further the overall agenda. Thermal/Saline and Photolytic/Alkali both completely degraded 5-FU but Thermal/Saline did it quicker. While the Thermal/Alkali caused some degradation over the course of a week, Thermal/Acidic didn't come close to matching over the same period of time. Synergism was demonstrated and definitely raises even more concerns regarding the realistic adverse potential these sort of compounds may have once they make their way into the environment; thus, this study's statement was made.