

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

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5-Fluorouracil (5-FU) is a popular anticancer drug chiefly used by chemotherapy patients. This drug(compound) is known to undergo certain structural changes when the environment it is exposed to changes(ei. Temperature, acidic conditions, basic conditions; types of light exposure , etc.). The resulting modified states this drug may assume is believed to influence the adverse reactions that patients may experience as well as the toxicity risks after these drugs are situated in the environment(lakes, rivers, ponds, soil; air). This study took the 6 most assumed to be structural forms of 5-FU and modeled each(theoretical or simulated representations) in order to do various analytical predictions on each then compare with real in lab analytical investigations. Comparing predictions with actual enabled a deduction of what structural form 5-FU may mainly exist as within aqueous solutions while also establishing systematic approaches for distinguishing amongst similar structures.

Afterwards, four applicable sets of simulated environmental conditions were applied towards 5-FU in order to see the effects each may have with respect to 5-FU degrading. Thermal/Saline(High temperatures combined with aqueous salty conditions) and Photolytic/Alkali(UV light combined with basic aqueous conditions) 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. This study also showed the importance in considering the unpredictable effects that combined conditions may have on a drug's degradation process. Finally, an effort was made to try and identify what the drug degraded to but was limited in doing so due to the lack of accessibility to all applicable standards for the compounds(many of which toxic) that 5-FU may degrade to; regardless, this study's statement was made.