ANALYSIS OF CHEMICAL FINGERPRINTS IN COMPLEX HAITIAN WATER MIXTURES

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The degree of environmental pollution in developing countries is limited despite the acknowledged association between chemical exposure and adverse health outcomes. A challenge of resource poor environments is the lack of knowledge about chemical "soups" that are present in diverse water systems. Therefore, researchers have limited knowledge of which chemicals are of concern. Given the presence of potentially thousands of chemicals in aquatic reservoirs, identifying components of chemical 'soups' as a means to better understand exposure and health impacts is warranted. To address this we are employing 'non-targeted' high-resolution mass spectrometry (MS) followed by a custom annotation pipeline to generate chemical fingerprints in collected water samples, and determine, whether toxicity data are (or not) readily available for these chemicals. As a case study, water samples were collected in Gressier, Haiti from 4 wells and 9 surface waters and then subjected to MS identifying over 170 chemicals. Initial categorization analysis shows the greatest number of compounds identified represented in pharmaceuticals (12%), pesticides (13%), and natural products (17%). Overall, surface water samples showed greater chemical contamination compared to well samples. Chemicals such as Diethyl phthalate were detected in only lower portions of the Momance River but absent in the upper regions, suggesting human input at varied locations. These results showcase the utility of non-target chemistry to identify chemical fingerprints in complex water samples where limited background information is available. Our identified chemicals were then compared to an EPA database called Toxcast where biological activity data for over 10,000 chemicals and their ac50's for over 1400 different assays is housed. Our findings showed that of the 173 chemicals identified by MS, 52% had no representation in Toxcast. Future goals are to develop a multi-plex assay that can detect common contaminants that are found in developing countries for which limited toxicity data are available.

PRESENTER BIO: Nima Madani is a 3rd year One Health PhD student in the Department of Environmental and Global Health. He is currently working on an interdisciplinary project that merges computational and molecular toxicology approaches to develop better surveillance tools of micropollutants in understudied water systems.