High-Performance Liquid Chromatography/Electrospray Ionization–Mass Spectrometry Analysis of Agricultural and Human Health Pharmaceuticals in Surface and Ground Water

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A method is being developed to identify and quantify agricultural and human health pharmaceuticals isolated from surface and ground water. This is an emerging water-quality issue because of the potential for deleterious sublethal effects of pharmaceuticals in water on humans, other animals, and the ecosystems they live in.

Nineteen pharmaceuticals were selected on the basis of predicted environmental loadings calculated from prescriptions and dosages and on the metabolic pathway of the parent pharmaceuticals in mammalian systems. The classes included analgesics, anti-inflammatories, antihypertensives, antianginals, antidepressants, antihyperlipidemics, antibiotics, antiulcerants, and anticoagulants. The pharmaceuticals were isolated from 1-liter water samples using resin-based solid-phase extraction. Extracts were analyzed by high-performance liquid chromatography using a 2-millimeter (mm) x 150-mm column containing a 3 micrometer particle size C-18 reversed phase. All 19 compounds were separated in less than 40 minutes by using a formate-modified, water-acetonitrile gradient. Electrospray ionization–mass spectrometry was used for qualitative identification and quantitation. Fragmentation conditions in the electrospray source were controlled so that three characteristic positive ions were produced for each compound. Selected-ion monitoring was used to maximize sensitivity.

Initial tests indicate that the 19 pharmaceuticals can be detected at individual concentrations as low as 50 to 100 nanograms per liter. Water samples being characterized by this method were collected nationwide from sites where the impact of pharmaceuticals was likely to be high, including sites downstream from wastewater treatment-plant discharge and confined agricultural feeding operations.

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