Identification, Curation, and Prioritization of Food-Use Chemicals In ToxCast

M Krishan1, TD Trautman2, DF Kapraun3, LA Fix4, and AL Karmaus5

1ILSI NA, Washington, DC, USA; 2Retired, General Mills, Minneapolis, MN, USA; 3EPA/ORD/NCCT, RTP, NC, USA; 4Unilever, Englewood Cliffs, NJ, USA; 5ILS, RTP, NC, USA

EVALUATION OF FOOD-USE CHEMICALS IN TOXCAST

EVALUATION OF FOOD-USE CHEMICALS IN TOXCAST

ABSTRACT

Evaluating the thousands of chemicals that are directly added to or come in contact with food poses a great challenge due to the time, cost, and sheer volume of data necessary to conduct comprehensive toxicological testing. This study compiled a list of food-use chemicals in the United States (US) and demonstrated approaches amenable to the evaluation of this large and diverse chemical inventory. By applying a cytotoxicity filtering approach wherein only assay endpoints with an AC50 below the cytotoxicity center are considered, the average number of active endpoints per chemical was reduced to an average of ~5 assay endpoints. The compilation and analysis of ToxCast food-use chemicals is critical for the development of risk management strategies.

INTRODUCTION AND SPECIFIC AIMS

A large diversity of chemicals can end up in food. These chemicals come from a variety of sources including direct addition to food, food contact from packaging or handling, and residues from food production. The mechanistic understanding and regulation of such food-relevant chemicals is starkly insufficient. In the United States, 1530 food-use chemicals are listed in use; however, many chemicals lack critical information (refined: 8659 total chemicals). This study compiled a list of food-use chemicals and analyzed their properties.

COMPILATION OF A FOOD-USE CHEMICAL INVENTORY

The ToxCast food-use chemical inventory was evaluated to determine the number of assay endpoints per chemical in each category was summarized in Table 1. For both indirect additives and direct additives, the average number of active endpoints per chemical was reduced from the total number of assay endpoints per chemical. The number of assay endpoints per chemical for both indirect and direct additives was reduced to an average of ~5 assay endpoints. The compilation and analysis of ToxCast food-use chemicals is critical for the development of risk management strategies.

SUMMARY

This work represents the first comprehensive evaluation of food-relevant chemicals in the ToxCast inventory. To accomplish this task, we compiled a list of food-use chemicals identified as 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. This inventory was mined for chemicals, identifying 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. For chemicals appearing in multiple resources, duplicates were removed and preference was given to classification as a direct food additive > food contact substance > pesticide. Of this food-relevant chemical inventory, 1530 were in ToxCast revealed that only 10% of direct additives elicited cytotoxicity, while 24% of indirect additives and 41% of pesticides/residues were cytotoxic. To address the need to prioritize chemical mixtures, we used frequent itemset mining (FIM) to identify which individual chemicals were re-categorized based on exposure likelihood and sheer volume of data necessary to thoroughly conduct comprehensive toxicological testing. This study compiled a list of food-use chemicals and analyzed their properties.

Table 1: Mixture with the Highest Frequency in the Food Contact Substance (FCS) Notices Inventory

Summary

This poster does not reflect EPA policy. Agnes Karmaus

This work represents the first comprehensive evaluation of food-relevant chemicals in the ToxCast inventory. To accomplish this task, we compiled a list of food-use chemicals identified as 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. This inventory was mined for chemicals, identifying 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. For chemicals appearing in multiple resources, duplicates were removed and preference was given to classification as a direct food additive > food contact substance > pesticide. Of this food-relevant chemical inventory, 1530 were in ToxCast revealed that only 10% of direct additives elicited cytotoxicity, while 24% of indirect additives and 41% of pesticides/residues were cytotoxic. To address the need to prioritize chemical mixtures, we used frequent itemset mining (FIM) to identify which individual chemicals were re-categorized based on exposure likelihood and sheer volume of data necessary to thoroughly conduct comprehensive toxicological testing. This study compiled a list of food-use chemicals and analyzed their properties.

Table 1: Mixture with the Highest Frequency in the Food Contact Substance (FCS) Notices Inventory

Summary

This poster does not reflect EPA policy. Agnes Karmaus

This work represents the first comprehensive evaluation of food-relevant chemicals in the ToxCast inventory. To accomplish this task, we compiled a list of food-use chemicals identified as 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. This inventory was mined for chemicals, identifying 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. For chemicals appearing in multiple resources, duplicates were removed and preference was given to classification as a direct food additive > food contact substance > pesticide. Of this food-relevant chemical inventory, 1530 were in ToxCast revealed that only 10% of direct additives elicited cytotoxicity, while 24% of indirect additives and 41% of pesticides/residues were cytotoxic. To address the need to prioritize chemical mixtures, we used frequent itemset mining (FIM) to identify which individual chemicals were re-categorized based on exposure likelihood and sheer volume of data necessary to thoroughly conduct comprehensive toxicological testing. This study compiled a list of food-use chemicals and analyzed their properties.

Table 1: Mixture with the Highest Frequency in the Food Contact Substance (FCS) Notices Inventory

Summary

This poster does not reflect EPA policy. Agnes Karmaus

This work represents the first comprehensive evaluation of food-relevant chemicals in the ToxCast inventory. To accomplish this task, we compiled a list of food-use chemicals identified as 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. This inventory was mined for chemicals, identifying 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. For chemicals appearing in multiple resources, duplicates were removed and preference was given to classification as a direct food additive > food contact substance > pesticide. Of this food-relevant chemical inventory, 1530 were in ToxCast revealed that only 10% of direct additives elicited cytotoxicity, while 24% of indirect additives and 41% of pesticides/residues were cytotoxic. To address the need to prioritize chemical mixtures, we used frequent itemset mining (FIM) to identify which individual chemicals were re-categorized based on exposure likelihood and sheer volume of data necessary to thoroughly conduct comprehensive toxicological testing. This study compiled a list of food-use chemicals and analyzed their properties.

Table 1: Mixture with the Highest Frequency in the Food Contact Substance (FCS) Notices Inventory

Summary

This poster does not reflect EPA policy. Agnes Karmaus

This work represents the first comprehensive evaluation of food-relevant chemicals in the ToxCast inventory. To accomplish this task, we compiled a list of food-use chemicals identified as 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. This inventory was mined for chemicals, identifying 8659 unique chemicals, which were grouped into three putative categories: (1) direct food additives, (2) food contact substances, and (3) pesticides. For chemicals appearing in multiple resources, duplicates were removed and preference was given to classification as a direct food additive > food contact substance > pesticide. Of this food-relevant chemical inventory, 1530 were in ToxCast revealed that only 10% of direct additives elicited cytotoxicity, while 24% of indirect additives and 41% of pesticides/residues were cytotoxic. To address the need to prioritize chemical mixtures, we used frequent itemset mining (FIM) to identify which individual chemicals were re-categorized based on exposure likelihood and sheer volume of data necessary to thoroughly conduct comprehensive toxicological testing. This study compiled a list of food-use chemicals and analyzed their properties.