In Vitro Approach to Grouping of Complex Substances and UVCBs: A Case Study of Olefin Streams

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ABSTRACT

Complex substances can pose a major challenge for registration and health assessments because of the unknown or variable composition. Complex mixture products and biological UVCBs (variants) of these products. Regulatory submissions of UVCB substances under the high production volume program in the US and Europe include grouping and read-across methods to fit data gaps. However, general concerns were raised about the provision of grouping being based on broad categories, parameters that the manufacturing process can change, and the variability in compositions based on the source of crude oil or natural gas and manufacturing process variables. Previously, we showed that a simple bioactivity profile of Dictyostelium discoideum can be used to discern grouping of three classes through “biological read-across”. This project aimed to apply a “biological read-across” principle to grouping complex substances in a case study of two parallel stream categories for human health and ecotoxicity, and microbial and odour/corrosion issues. A suite of human and plant stem cell–derived assay systems was used to characterize a total of 45 substances. Hierarchical clustering was used to cluster groups of substances and to determine the OTU mapping. Priority list (ToxPi) approach to determine similarity in bioactivity and to establish groups of the screened substances and supporting chemicals. Equipped with a contact with the Human Health and Ecotoxicity Chemistry Task Force, we used a scheme to group the substances into the American Chemistry Council’s Definition Panel and the Members of the Lower Olefins and Aromatics REACH Consortium.

RESULTS

Hierarchical clustering was used to cluster groups of substances and to determine the OTU mapping. Priority list (ToxPi) approach to determine similarity in bioactivity and to establish groups of the screened substances and supporting chemicals. Equipped with a contact with the Human Health and Ecotoxicity Chemistry Task Force, we used a scheme to group the substances into the American Chemistry Council’s Definition Panel and the Members of the Lower Olefins and Aromatics REACH Consortium.

Olefin ID: Neat Substance: ToxPi’s of the Bioactivity (extracts):

OBJECTIVES

To establish a “biological read-across” method to group complex substances in a case study. This project aimed to apply a “biological read-across” principle to grouping complex substances in a case study of olefin stream categories for human health and ecotoxicity, and microbial and odour/corrosion issues. A suite of human and plant stem cell–derived assay systems was used to characterize a total of 45 substances. Hierarchical clustering was used to cluster groups of substances and to determine the OTU mapping. Priority list (ToxPi) approach to determine similarity in bioactivity and to establish groups of the screened substances and supporting chemicals. Equipped with a contact with the Human Health and Ecotoxicity Chemistry Task Force, we used a scheme to group the substances into the American Chemistry Council’s Definition Panel and the Members of the Lower Olefins and Aromatics REACH Consortium.

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CONCLUSIONS

Grouping based on bioactivity is evident within the lower UVCB category, though it is much less evident in the Lower Benzene Naphthas category.

Future work: These chemical substances provided additional understanding of the underlying complexity and variability among complex between different and within the same manufacture streams.

FUTURE WORK

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