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SUPPLEMENT

applied *in silico* using the OECD's QSAR toolbox to categorise over 300 compounds from EFSA's database into one of three classes, under the Cramer decision tree. These three classes are reflective of toxicity and identify low (class I), moderate (class II), and high (class III) toxicity. The lognormal cumulative distributions of reference points for compounds were plotted for each of the three classes. The fifth percentile of each cumulative distribution was used to derive a TTC value by applying an uncertainty factor of 100, and factoring in average human weight. EFSA's TTC values were used to compare against the original threshold values for protectiveness. Results showed the threshold value derived for Cramer class III was protective of the original threshold value. However, Cramer class I fell below the original threshold value, while Cramer class II had too few compounds to carry statistical weight. Our analysis shows that the TTC approach is protective for chemicals pertinent to food safety. However, further expansion of the TTC dataset would be beneficial for refining TTC values.

44. Food packaging contaminants: estimating dietary exposure

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The safety of packaging materials is of great concern for food safety as low-molecular-weight substances can migrate from the packaging into the food and can cause harmful effects to human health through dietary exposure. Exposure assessment is one of the essential aspects in the risk assessment process. To estimate the exposure to migrated substances from food-contact materials several methods have been applied. In the European Union, a conservative assumption is adopted, namely a person of 60 kg body weight consumes daily 1 kg of food packed in a cubic container of 6 dm^2. The exposure can also be estimated more realistically by combining the migrated substance concentration in food and the consumption data obtained from consumer surveys. More refined approaches have also been used; as part of the European Project FACET (Flavours, Additives and Food-Contact Materials Exposure Task) a probabilistic modelling tool to estimate the exposure to migrated substances from food-contact materials was designed. This model allows the exposure assessment of migrated substances using information on packaging (use, composition), consumption data, etc.

In the present work, the dietary exposure from cereal-based foods in plastic packaging, to acetyl tributyl citrate (ATBC), a common plasticizer used in the manufacture of packaging materials was determined using a Total Diet Study (TDS) approach and was also estimated using the FACET exposure tool.

The results obtained with the TDS approach agree closely with those estimated with the FACET exposure model. So, for example the mean dietary exposures of ATBC were 1.01 µg/kg bw/day for the group 1–3 years; 2.01 µg/kg bw/day for the group 3–9 years and 1.27 µg/kg bw/day for the group 10–17 years. Those obtained with the FACET tool were 1.5 µg/kg bw/day for the group 1–3 years; 1.52 µg/kg bw/day for the group 3–9 years and 0.9362 µg/kg bw/day for the group 10–17 years. In all cases, mean dietary exposures to ATBC were below the tolerable daily intake (TDI) of 1.0 mg/kg body weight set by the EU for ATBC.

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Key words: exposure assessment, TDS, ATBC, FACET exposure model

45. Metals in Undaria pinnatifida

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There is no doubt that the dietary consumption of algae that has been traditionally consumed in Asia is expanding to Europe. *Undaria pinnatifida* or wakame, belonging to the brown algae, is one of the most widely consumed algae, especially for its beneficial properties. Numerous studies have shown that *U. pinnatifida* has a high capacity for metal absorption, which is of both nutritional and toxicological interest. However, its full metal profile has been little studied.

The objective of this study is to determine the levels of 20 metals (Na, K, Mg, Ca, Fe, Zn, Cu, Cr, B, Ba, Pb, Cd, Al, Sr, Li, Ni, Co, Mn, Mo and V) in 25 *U. pinnatifida* samples from two geographical areas (Asia n = 10; Europe n = 15), using Inductively Coupled Plasma–Optical Emission Spectrometry (ICP–OES) to evaluate the nutritional value and toxicological risk of its metal content based on the recommended consumption of *U. pinnatifida* (5 g dehydrated algae/day) and the Recommended Daily Intake and maximum tolerated intakes.

While samples of *U. pinnatifida* from Asia have the highest concentrations of elements such as Na (28.2 ± 2.71 g/kg dry weight) or Fe (58.8 ± 17.3 mg/kg dw), the samples from the European coastal waters contain the highest levels of Zn (40 ± 32 mg/kg dw). Among the metals of toxicological interest, Al stands out with levels of 31.5 ± 17.3 mg/kg dw in algae from Europe that are higher than those found in samples from Asia (20.0 ± 4.4 mg/kg dw). The