UTILIZATION OF PREDICTIVE TOXICOLOGY SOFTWARE AND SIMILAR TOOLS FOR HEALTH RISK ASSESSMENT OF CHEMICALS AND POLYMERS

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The Canadian New Substances Regulatory Program carries out the assessment of environmental and health risks of chemicals and polymers that notifiers intend to import or manufacture in Canada and that do not already exist on the Canadian Domestic Substances List. A variety of physical, chemical and biological test data is provided by the notifiers, however, despite this, at times 'data-gaps' remain. An attempt to bridge this hiatus is carried out by Health Canada evaluators with the aim of conducting as complete an evaluation of the toxicity and exposure profiles of these substances, as is possible and feasible.

Some of the tools that we at Health Canada employ are based on SAR/QSAR relationships, and include, in-house databases structured around commercially available chemical database systems, and predictive toxicity software that utilize SAR/QSAR paradigms, etc. A separate suite of software is also utilized for estimating physical/chemical parameters and exposure scenarios by our chemists.

In our experience, these tools have been found to be useful in providing some of the missing or unavailable information that is necessary for our risk assessments. These tools also serve well in examining the validity of utilizing related informtion-rich chemical substances as analogs or surrogates for providing 'read across' information in selected cases. Such validation typically includes not only the comparison of the structure-based physical, chemical and toxicity profiles but also of justifiable similarities between the metabolic fates of the substances under examination.

Some of these considerations will be elaborated through suitable illustrations and some of the desirable strengths and features in these categories of software shall be discussed, from the perspectives of a regulatory user of these tools.