About section of a profiler
Name of the profiler
Oncologic Primary Classification
Developer; Donator; date; version
Developer: Laboratory of Mathematical Chemistry (LMC), Bourgas, Bulgaria; United States Environmental Protection Agency (EPA) ***Donator:*** Laboratory of Mathematical Chemistry (LMC), Bourgas, Bulgaria; United States Environmental Protection Agency (EPA) ***Version*:** 4.0 December 2016
Relevance/Applicability to endpoint(s)
The OncoLogic Primary Classifier consists of molecular definitions developed by LMC and OECD to mimic the structural criteria of chemical classes of potential carcinogens covered by the U.S. Environmental Protection Agency's OncoLogic™ Cancer Expert System for Predicting the Carcinogenicity Potential. In the QSAR Toolbox, the OncoLogic Primary Classifier is used solely for the purpose of categorization based on the definition of an OncoLogic™ class. The profiler is introduced for categorization purpose and not for predicting carcinogenicity. "Major highlights of SAR features and mechanistic understanding" proposed by EPA have been added to each specific chemical class.
Relevance/Applicability to particular chemical classes
This profiler is applicable to those organic chemicals that have presence of at least one of the 48 alerts specified within the profiler. The presence of an alert is not bounded with parametric ranges; it is based on structural boundaries only. The absence of a structural alert should not be taken as an absence of toxicity.
Approach used to develop the profiler - Concise but informative description of:
a) The aim of the profiler is to investigate presence of alerts within target molecules responsible for the carcinogenic potential of the chemicals.
b) There were no training set chemicals used for the development of the profiler.
c) The Onclogic Primary Classification profiler was developed base on the structural rules implemented in the OncoLogic™ Expert System. The rules implemented in the Expert System were developed jointly by cancer experts and system development experts based on cancer studies and scientific publications.
Summary description of profiles/alerts within the profiler

Profile/structural alert	Phys-chem parameter
Acrylamide Reactive Functional Groups	No parameter
Acrylate Reactive Functional Groups	No parameter
Acyl and Benzoyl Type Compounds	No parameter
Aflatoxin Type Compounds	No parameter
Aldehyde Type Compounds	No parameter

Aliphatic Azo and Azoxy Type Compounds	No parameter
Alkanesulfonoxy Ester Type Compounds	No parameter
Alkyl Sulfate Type Compounds	No parameter
Alpha- and beta-Haloether Reactive Functional Groups	No parameter
Alpha-Haloalkylamine Reactive Functional Groups	No parameter
Alpha-Halothioether Reactive Functional Groups	No parameter
Anhydride Type Compounds	No parameter
Aromatic Amine Type Compounds	No parameter
Arylazo Type Compounds	No parameter
Aryldiazonium Salts	No parameter
Carbamate Type Compounds	No parameter
Carbamyl Halide Type Compounds	No parameter
C-Nitroso and Oxime Type Compounds	No parameter
Coumarine and Furocoumarin Type Compounds	No parameter
Dicarbonyl Type Compounds	No parameter
Epoxide Reactive Functional Groups	No parameter
Ethyleneimine (Aziridine) Reactive Functional Groups	No parameter
Halogenated Aromatic Hydrocarbon Type Compounds	No parameter
Halogenated Cycloalkane Type Compounds	No parameter
Halogenated Linear Aliphatic Hydrocarbone Type Compounds	No parameter
Halogenated Nitroaromatic Type Compounds	No parameter
Hydrazo Type Compounds	No parameter
Lactone Type Reactive Functional Groups	No parameter
Nitroalkane and Nitroalkene Type Compounds	No parameter
Nitrogen Mustards Reactive Functional Groups	No parameter
Nitrosamide Type Compounds	No parameter

Nitrosamine Type Compounds	No parameter
Organophosphorus Type Compounds	No parameter
ortho-Haloganated Heterocyclic Type Compounds	No parameter
Peroxide Type Compounds	No parameter
Phenol Type Compounds	No parameter
Phosgene Type Compounds	No parameter
Polycyclic Aromatic Hydrocarbons - Heterocyclic	No parameter
Polycyclic Aromatic Hydrocarbons - Homocyclic	No parameter
Reactive Ketone Reactive Functional Groups	No parameter
Reactive Sulfone Reactive Functional Groups	No parameter
Silicone and Siloxane Type Compounds	No parameter
Sulfur Mustard Reactive Functional Groups	No parameter
Sultone Reactive Functional Groups	No parameter
Thiocarbamate Type Compounds	No parameter
Thiocarbonyl Type Compounds	No parameter
Triazene Type Compounds	No parameter
Urea Type Compounds	No parameter
Counter category: Not classified	
Similar to other profilers	
The profiler is similar to the ***"Carcinogenicity (genotox and nongenotox) alerts by ISS"*** profiler. The purpose of both profiles is to identify organic chemicals having carcinogenic potential. They both belong to the Endpoint specific type profilers. Based on specific character of the profiler Oncologic Primary Classification could be used for primary categorization as well as for subcategorization purposes.	
Short description of update version	
SMARTS language for describing molecular patterns, i.e. structural boundaries, structural alerts has been implemented in OECD QSAR Toolbox 4.0. As a result ***Oncologic Primary Classification*** has been rewritten but without modifying the knowledge and/or the logic they are based on. Only small distinctions are expected in the profiling results between Toolbox v.3.4 and v 4.0 due to different interpretation of the molecular structures, e.g. for heterocyclic/heteroaromatic compounds.	
Disclaimer	
The designation of an OncoLogic™ class for a chemical per se does not necessarily convey	

any prediction of carcinogenicity potential. For assessing the carcinogenicity potential of the chemical, the users are encouraged to download and run the U.S. EPA's OncoLogic™ model as a stand alone program. OncoLogic™ is a desktop computer program that uses expert rules to evaluates the likelihood that a chemical may cause cancer by evaluating molecular characteristics of the chemical including: structure (reactive functional group and subunits present), physical/chemical properties (stability, solubility, etc.), biological and mechanistic information, as well as possible routes of exposure. OncoLogic™ has been peer reviewed, runs on a Windows® PC, and is being released by EPA at no cost, to be available to any researcher or organization wishing to evaluate cancer potential of chemicals. The OncoLogic 8.0 program can be downloaded from the U.S. EPA website at: https://www.epa.gov/tsca-screening-tools/oncologictm-computer-system-evaluate-carcinogenic-potential-chemicals .

The structural boundaries used to define the chemical classes (e.g. "Alcohol" – chemical class from "Organic functional group" profiler) or alerting groups responsible for the binding with biological macromolecules (e.g. "Aldehydes" – structural alert for protein binding), represent structural functionalities in the molecule which could be used for building chemical categories for subsequent data gap filling. They are not recommended to be used directly for prediction purposes (as SARs).