RapidTox Human Health Assessment Workflow Report

Perfluorooctanesulfonic acid (DTXSID: DTXSID3031864 | CASRN: 1763-23-1)

Session Report ID: 4028e082860e7f6d018626c73c190000

Click here to download the landscape report

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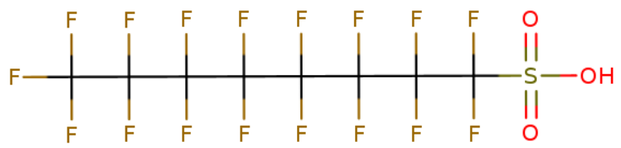

BACKGROUND

The RapidTox “Human Health Assessment” workflow is designed to surface and deliver Human Health Assessment relevant to the evaluation of chemicals, where and when available, such as:

- empirical or predicted physicochemical properties,
- environmental fate and transport parameters,
- in vivo human epidemiological and/or experimental animal hazard and dose-response data (e.g., existent cancer and non-cancer human health toxicity values; existent candidate points-of-departure),
- surrogate POD(s) from analogue chemical(s) via structure-activity/read-across, and
- in vitro bioactivity-based data converted and contextualized for application to human health assessment.

A RapidTox workflow session report is representative of user-specific selections and may or may not represent the totality of information available for a given chemical at the time the session was run. Each completed workflow session, for a given chemical, results in both a user specific session report and a total data landscape report that entails the totality of relevant a priori existent empirical or predicted data across the workflow modules, for user convenience and historical reporting purposes.

The primary objective of the RapidTox Human Health Assessment workflow, and resultant session report, is to provide an expedient path to chemical-specific information that informs human health hazard identification and dose-response assessment associated with chronic and/or subchronic exposure durations. For quantitative dose-response assessment, this session report may contain a combination of existent human health toxicity values and/or points-of-departure (PODs), based on extent assessments or reports from sources such as EPA’s IRIS or

A RapidTox session report, or the corresponding total data landscape report, is not intended to be a comprehensive treatise on the chemical or toxicological nature of this substance. Rather the information surfaced and selected by the user contained in a session report is intended to either directly support decision-making under the purview of the user, or, serve as a seminal starting point for development of a more involved health assessment product.

QUALITY ASSURANCE

This RapidTox workflow environment is a compilation of information harvested from many sites, databases and sources, including U.S. Federal and state agencies and institutions and international bodies, which can save the user time by providing information in one location. The data are not reviewed by U.S. EPA – the user must apply judgment in use of the information. You should consult the original scientific assessment, report, published paper or data source, if possible, to ensure an understanding of the context of the data contained in the workflow. The views and opinions of the developers of the workflow expressed herein do not necessarily state or reflect those of the U.S. EPA and shall not be used for advertising or product endorsement purposes.

DISCLAIMERS

The RapidTox Human Health Assessment session report provides toxicity values (e.g., existent cancer and non-cancer tox values and/or PODs), brief tabular level information about the effects of the chemical, opportunities to identify analogue chemical(s) and associated surrogate toxicity data and leverage available bioactivity data to identify corresponding administered dose equivalent-based PODs, when and where data are available. The evidence on which a user-selected value is based, including the strengths and limitations is not provided in the session report. All users are advised to review the information provided in this workflow session report to ensure that the value(s) selected is/are appropriate for the types of exposures and circumstances in question and the screening-level decisions that would be supported by the report. U.S. EPA Programs, Regions or States who choose to use values selected in a RapidTox Human Health Assessment workflow session are advised that EPA/ORD resources will not generally be used to respond to challenges, if any, of quantitative values assembled, derived, and/or applied by a user. This session report has not been reviewed in accordance with U.S. EPA policy or approved for publication; meeting such objectives is the sole responsibility of the user. Mention of trade names or commercial products in the workflow user interface or in a corresponding session report does not constitute endorsement or recommendation for use.

QUESTIONS REGARDING RAPIDTOX HUMAN HEALTH ASSESSMENT REPORT

Questions regarding the content of this RapidTox Human Health Assessment workflow session report should be directed to the point of contact for RapidTox Jason Lambert

COMMONLY USED ABBREVIATIONS AND ACRONYMS

a2u-g alpha 2u-globulin
ACGIH American Conference of Governmental Industrial Hygienists
AIC Akaike's information criterion
ALD approximate lethal dosage
ALT alanine aminotransferase
AR androgen receptor
AST aspartate aminotransferase
atm atmosphere
ATSDR Agency for Toxic Substances and Disease Registry
BMD benchmark dose
BMDL benchmark dose lower confidence limit
BMDS Benchmark Dose Software
BMR benchmark response
BUN blood urea nitrogen
BW body weight
CA chromosomal aberration
CAS Chemical Abstracts Service
CASRN Chemical Abstracts Service registry number
CBI covalent binding index
CHO Chinese hamster ovary (cell line cells)
CL confidence limit
CNS central nervous system
CPHEA Center for Public Health and Environmental Assessment
CPN chronic progressive nephropathy
CYP450 cytochrome P450
DAF dosimetric adjustment factor
DEN diethylnitrosamine
DMSO dimethylsulfoxide
DNA deoxyribonucleic acid
EPA Environmental Protection Agency
ER estrogen receptor
FDA Food and Drug Administration
FEV1 forced expiratory volume of 1 second
GD gestation day
GDH glutamate dehydrogenase
GGT -glutamyl transferase
GSH glutathione
GST glutathione-S-transferase
Hb/g-A animal blood-gas partition coefficient
Hb/g-H human blood-gas partition coefficient
HEC human equivalent concentration
HED human equivalent dose
i.p. intraperitoneal
IRIS Integrated Risk Information System
IVF in vitro fertilization
LC50 median lethal concentration
LD50 median lethal dose
LOAEL lowest-observed-adverse-effect level
MN micronuclei
MNPCE micronucleated polychromatic erythrocyte
MOA mode of action
MTD maximum tolerated dose
NAG N-acetyl--D-glucosaminidase
NCI National Cancer Institute
NOAEL no-observed-adverse-effect level
NTP National Toxicology Program
NZW New Zealand White (rabbit breed)
OCT ornithine carbamoyl transferase
ORD Office of Research and Development
PBPK physiologically based pharmacokinetic
PCNA proliferating cell nuclear antigen
PND postnatal day
POD point of departure
PODADJ duration-adjusted POD
QSAR quantitative structure-activity relationship
RBC red blood cell
RDS replicative DNA synthesis
RfC inhalation reference concentration
RfD oral reference dose
RGDR regional gas dose ratio
RNA ribonucleic acid
SAR structure-activity relationship
SCE sister chromatid exchange
SD standard deviation
SDH sorbitol dehydrogenase
SE standard error
SGOT serum glutamic oxaloacetic transaminase, also known as AST
SGPT serum glutamic pyruvic transaminase, also known as ALT
SSD systemic scleroderma
TCA trichloroacetic acid
TCE trichloroethylene
TWA time-weighted average
UF uncertainty factor
UFA interspecies uncertainty factor
UFC composite uncertainty factor
UFD database uncertainty factor
UFH intraspecies uncertainty factor
UFL LOAEL-to-NOAEL uncertainty factor
UFS subchronic-to-chronic uncertainty factor
U.S. United States of America
WBC white blood cell

Perfluorooctanesulfonic acid (DTXSID: DTXSID3031864 | CASRN: 1763-23-1)

Physchem Data

Property	Exper Avg	Pred Avg	Exper Median	Pred Median	Exper Range	Pred Range	Unit
Boiling Point	169	231	148	229	133 to 249	219 to 244	°C
Density	-	1.84	-	1.84	-	1.84 to 1.85	g/cm^3
Henry's Law	-	1.80e-11	-	1.80e-11	-	1.80e-11	atm-m3/mole
LogKoa: Octanol-Air	-	4.75	-	4.75	-	4.75	-
LogKow: Octanol-Water	5.61	5.77	5.50	5.94	4.30 to 7.03	4.18 to 7.03	-
Melting Point	-	84.1	-	51.9	-	15.2 to 185	°C
Vapor Pressure	2.48e-06	2.48e-06	2.48e-06	2.48e-06	2.48e-06	2.48e-06	mmHg
Water Solubility	1.14e-03	1.56e-03	1.14e-03	4.11e-04	1.14e-03	6.25e-09 to 5.40e-03	mol/L

Env/Fate Data

Property	Exper Avg	Pred Avg	Exper Median	Pred Median	Exper Range	Pred Range	Unit
Biodeg. Half-Life	-	4.92	-	4.92	-	4.92	days
Soil Adsorp. Coeff. (Koc)	-	1.46e+03	-	1.46e+03	-	354 to 2.56e+03	L/kg

No In Vivo Toxicity Values Located

No In Vivo Toxicity POD Values Located

Analogue Selection Data

Selected Analogue	Dtxsid	Structural Similarity	Surrogate POD Type	Value	Units	Study Type	Justification	POD source
Potassium perfluorobutanesulfonate	DTXSID3037707	0.98	NOAEL	200	mg/kg-day	subchronic	RAPIDTOX-1382 RAPIDTOX-1382 RAPIDTOX-1382	ECHA

ToxCast Model Data

Model	Receptor	Agonist	Antagonist	Binding
CERAPP Potency Level (Consensus)	Estrogen	0	0	0

ToxCast Model Data

Model	Receptor	Agonist	Antagonist	Binding
CERAPP Potency Level (From Literature)	Estrogen	Inactive	Inactive	Inactive
COMPARA (Consensus)	Androgen	0	0	0

BER Data

Pod Drop down	Exposure Value	Exposure Units	BER	BER Type
3.71e-04	1.38e-04	mg/kg/day	2.68	BER
3.71e-04	2.06e-06	mg/kg/day	1.14e+03	BER Median

No In Vivo Toxicity POD Values Located

POD Summary: Analogue

POD Summary: Analogue

Preferred Name	Type	Value	Units	Exposure Route	Species	Critical Effect	Study Type	Source	Justification
Potassium perfluorobutanesulfonate	NOAEL	200	mg/kg-day	oral	Rat	kidney: histopathology: non-neoplastic	subchronic	ECHA	RAPIDTOX-1382 RAPIDTOX-1382 RAPIDTOX-1382

POD Summary: Bioactivity

Pod Drop down	Exposure Value	Exposure Units	BER	BER Type
3.71e-04	1.38e-04	mg/kg/day	2.68	BER
3.71e-04	2.06e-06	mg/kg/day	1.14e+03	BER Median

No Uncertainty Data