

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S0	SUSDAT	Merged NORMAN Suspect List: SusDat	Interactive Data table SusDat with Haz and Expo scores as XLSX , CSV (18/01/2022) MetFrag CSV (03/03/2020) CompTox SUSDAT List	SusDat InChIKeys: All, MS-ready (18/01/2022)	A merged list of >111,000 structures from SLE suspect lists. See interactive version . Compiled by Reza Aalizadeh, Nikiforos Alygizakis and Lubos Cirka, University of Athens/EI, including RTI and toxicity values, with Hazard and Exposure values provided by Stellan Fischer, KEMI, documented here . DOI: 10.5281/zenodo.2664077
S1	MASSBANK	NORMAN Compounds in MassBank	CSV , XLSX with Fragments (3/10/2017). CompTox MassBank EU Reference List , MassBank EU Special Cases , Fragment Download	MassBankEUInChIKeys (17/06/2019)	www.massbank.eu Stravs <i>et al.</i> 2013. DOI: 10.1002/jms.3131 DOI: 10.5281/zenodo.2621390
S2	STOFFIDENT	HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances	STOFF-IDENT as XLSX , CSV (18/06/2019) CompTox STOFF-IDENT List	STOFF-IDENT InChIKeys (6/09/2017)	The database enables the search for exact masses from target or unknown lists and the automatic use of a Retention Time Index. See: https://water.for-ident.org/#!home . DOI: 10.5281/zenodo.2621451
S3	NORMANCT15	NORMAN Collaborative Trial Targets and Suspects	LC-MS: CSV , XLSX (3/10/2017) GC-MS: CSV , XLSX (3/10/2017) CompTox NORMANCT15 List	LC-MS InChIKeys (31/10/2016) GC-MS InChIKeys (31/10/2016)	Schymanski <i>et al.</i> 2015. DOI: 10.1007/s00216-015-8681-7 DOI: 10.5281/zenodo.2621478
S4	UJIBADE	University of Jaume I	Bade <i>et al</i> CSV , XLSX (3/10/2017) CompTox UJIBADE List	Bade et al InChIKeys (28/11/2015)	Bade <i>et al</i> 2015, Sci. Tot. Environ. 538: 934-941. DOI: 10.1016/j.scitotenv.2015.08.078 DOI: 10.5281/zenodo.2621916
S5	KWRSJERPS	KWR Drinking Water Suspect List	KWR Suspects CSV , XLSX (3/10/2017) CompTox KWRSJERPS List	KWR InChIKeys (15/03/2016)	Sjerps <i>et al.</i> 2016 Water Research 93: 254-264. DOI: 10.1016/j.watres.2016.02.034 DOI: 10.5281/zenodo.2621941
S6	ITNANTIBIOTIC	Antibiotic List: ITN MSCA ANSWER	Antibiotic CSV , XLSX (3/10/2017) Antibiotics Step 1 CYP Metabolites CSV , XLSX (02/05/2022) CompTox ITN ANTIBIOTIC List	Antibiotic InChIKeys (16/06/2016) Step 1 CYP Metabolites InChIKeys (02/05/2022)	A list of antibiotics compiled by Nikiforos Alygizakis (EI/Uni Athens). See e.g. Paulus <i>et al</i> 2019 DOI: 10.1016/j.ijheh.2019.01.004 Suspect list of human phase-I antibiotic metabolites, created with BioTransformer (v3.0.0) provided by Tim Jonkers (VU, NL). Jonkers <i>et al</i> (in prep.) DOI: 10.5281/zenodo.2621956

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S7	EAWAGSURF	Eawag Surfactants Suspect List	Suspect formulas: CSV , XLSX Plus representative structures: CSV , XLSX (21/11/2020) CompTox EAWAGSURF List	EAWAGSURF Representative InChIKeys (21/11/2020)	Schymanski <i>et al.</i> 2014. DOI: 10.1021/es4044374 DOI: 10.5281/zenodo.2621971
S8	ATHENSSUS	University of Athens Surfactants and Suspects List	Gago Ferrero <i>et al</i> CSV , XLSX (3/10/2017) CompTox ATHENSSUS List	UniAthens InChIKeys (28/01/2016)	Gago-Ferrero <i>et al.</i> 2015. DOI: 10.1021/acs.est.5b03454 DOI: 10.5281/zenodo.2621979
S9	PFASTRIER	PFAS Suspect List: fluorinated substances	CSV (MassHunter format; 26/11/2015), XLSX (several sheets; 26/11/2015) Merged CSV (14/11/2019) CompTox PFAS TRIER List	PFAS InChIKeys (26/11/2015)	Kindly supplied by Xenia Trier, David Lunderberg and colleagues. Reference information contained in files. DOI: 10.5281/zenodo.2621988
S10	SWISSPHARMA	Pharmaceutical List with Consumption Data	Swiss Pharma CSV , XLSX (3/10/2017) CompTox SWISSPHARMA List	Pharma MS-ready InChIKeys (02/05/2017)	Table S2 from Singer <i>et al.</i> 2016. DOI: 10.1021/acs.est.5b03332 DOI: 10.5281/zenodo.2623484
S11	SWISSPEST	Swiss Insecticides, Fungicides and TPs	Swiss Pesticides CSV , XLSX (3/10/2017) CompTox SWISSPEST List	Pesticide MS-ready InChIKeys (08/05/2017)	Table S1 from Moschet <i>et al.</i> 2013. DOI: 10.1021/ac4021598 DOI: 10.5281/zenodo.2623740
S12	NORMANEWS	NormaNEWS for Retrospective Screening of New Emerging Contaminants	NormaNEWS CSV , XLSX (3/10/2017) CompTox NORMANEWS List	NormaNEWS InChIKeys (8/05/2017)	NormaNEWS list provided by Nikiforos Alygizakis, Saer Samanipour and Kevin Thomas. See Alygizakis <i>et al</i> 2018 DOI: 10.1021/acs.est.8b00365 DOI: 10.5281/zenodo.2623815
S13	EUCOSMETICS	Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)	Merged Cosmetics CSV (4/05/2017) CompTox EU Cosmetics List	Merged Cosmetics InChIKeys (4/05/2017)	The scientific committee on cosmetic products and non-food products Intended for consumers - SCCNFP/0389/00 Final and Commission Decision 2006/257/EC amending the Decision 96/335/EC. Provided by Peter von der Ohe, UBA, curated by Reza Aalizadeh, University of Athens. DOI: 10.5281/zenodo.2624118

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S14	KEMIPFAS	PFAS Highly Fluorinated Substances List: KEMI	KEMI PFAS Full List XLSX , CSV (1/02/2017) KEMI PFAS Structures XLSX , CSV (3/07/2017) CompTox KEMI PFAS List	KEMI PFAS InChIKeys (25/07/2017)	Appendix 2 from Swedish Chemicals Agency KEMI Report 7/15 . Provided by Stellan Fischer, KEMI. Registration and mapping to CompTox Dashboard by Antony Williams, US EPA. DOI: 10.5281/zenodo.2621524
S15	NORMANPRI	NORMAN Priority List	NORMAN Priority CSV (13/7/2017) CompTox NORMAN Priority List	NORMAN Priority InChIKeys (16/05/2017)	Priority substances from NORMAN WG-1 (Prioritisation), provided by Valeria Dulio. DOI: 10.5281/zenodo.2624272
S16	FRENCHLIST	French Monitoring List	French List CSV (8/05/2017) CompTox French Monitoring List	French List Unique InChIKeys (8/05/2017)	Provided by Valeria Dulio, curated by Reza Aalizadeh, University of Athens. DOI: 10.5281/zenodo.2624324
S17	KEMIMARKET	KEMI Market List	KEMI Market List MS-ready (12/05/2017) KEMI Market List XLSX with (12 MB) or without (1MB) structures (29/12/2017), as CSV (06/02/2020) CompTox KEMI Market List	KEMI Market MS-ready InChIKeys (12/05/2017) KEMI Market Full InChIKeys (29/12/2017), updated 21/11/2019)	Provided by Stellan Fischer, KEMI including Hazard and Exposure scores, documented here . Curated by Reza Aalizadeh, University of Athens. DOI: 10.5281/zenodo.2628786
S18	TSCASURF	TSCA Surfactants	Surfactants XLSX , CSV (25/07/2017) TSCA PEG XLSX , CSV (25/07/2017) CompTox TSCA Surfactant List (subset)	Not applicable	Surfactant information compiled from TSCA by James Little while at Eastman Chemical. More information here . DOI: 10.5281/zenodo.2628791
S19	MZCLOUD	mzCloud Compounds	mzCloud Compounds XLSX , CSV (01/04/2019) CompTox mzCloud List	mzCloud InChIKeys (01/04/2019)	List of compounds on the mzCloud mass spectral database, provided by Robert Mistrík, update by Nikiforos Alygizakis. DOI: 10.5281/zenodo.2628860
S20	BISPHENOLS	Bisphenols	Bisphenols CSV , XLS (01/05/2020) CompTox Bisphenols List	Bisphenol InChIKeys (01/05/2020)	Bisphenols available at NILU (Pawel Rostkowski) and from Table 3 of report 5/17 by KEMI (Swedish with English summary). Extended to include exposure scores Jan. 2019 and source information May 2020. DOI: 10.5281/zenodo.2631744

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S21	UATHTARGETS	University of Athens Target List	Target List CSV , XLSX (8/2/2022) CompTox UATHTARGETS List	UoA Targets InChIKeys (8/02/2022)	List of target substances from University of Athens, provided by Nikiforos Alygizakis. For more see Alygizakis <i>et al.</i> 2019, DOI: 10.1016/j.envint.2019.03.060 , DOI: 10.5281/zenodo.2632410
S22	EPACONS	US EPA Consumer Product Suspect List	Original File XLSX (1/03/2018) Merged Suspects XLSX (1/03/2018) Merged Suspects CSV (1/03/2018) CompTox EPACONS List	Merged Consumer Product InChIKeys (1/03/2018)	Suspects in supporting information from Phillips <i>et al.</i> 2018, DOI: 10.1021/acs.est.7b04781 - Suspect Screening Analysis of Chemicals in Consumer Products with GCxGC-TOF/MS matched with NIST. DOI: 10.5281/zenodo.2648758
S23	EIUBASURF	Surfactant Suspect List from EI and UBA	Surfactant List XLSX (19/06/2018) Surfactant List CSV (19/06/2018) CompTox EIUBASURF List	EI UBA Surfactant InChIKeys (19/06/2018)	A compiled list of eco-labeled surfactants from Environmental Institute (EI, SK) and the German Federal Environmental Agency (UBA, DE) assigning chemical structures to UVCB chemicals based on names and prior knowledge. Provided by Nikiforos Alygizakis, EI. DOI: 10.5281/zenodo.2648764
S24	HUMANNEUR OTOX	List of Human Neurotoxins	Human Neurotoxin List XLS , CSV (19/06/2018) CompTox HUMANNEUROTOX List	Human Neurotox InChIKeys (19/06/2018)	A set of chemicals listed as neurotoxicants by Grandjean and Landrigan, DOI: 10.1016/S0140-6736(06)69665-7 . List provided by Emma Schymanski/Antony Williams. DOI: 10.5281/zenodo.2648768
S25	OECDPFAS	List of PFAS from the OECD	OECD PFAS Original List (20/06/2018) OECD PFAS CompTox XLSX , CSV (22/01/2019) OECD PFAS Life Apex XLSX (06/05/2019) CompTox PFASOECD List CompTox PFASOECDNA List	OECD PFAS CompTox InChIKeys (22/01/2019) OECDPFASNA InChIKeys (06/05/2019)	A list of PFAS released by the OECD, provided by Zhanyun Wang. Details in this OECD Monograph . Extensive registration and curation performed by CompTox Dashboard team (see CompTox files). Curated version for Life Apex provided by Nikiforos Alygizakis (EI, UoA). DOI: 10.5281/zenodo.2648775
S26	MYCOTOXINS	List of Mycotoxins from AAFC	Mycotoxins CSV , XLSX (23/01/2019) CompTox MYCOTOXINS List	Mycotoxin InChIKeys (21/06/2018)	A list of mycotoxins and fungal secondary metabolites provided by Justin Renaud and Mark Sumarah (Agriculture and Agri-Food Canada / Government of Canada). DOI: 10.5281/zenodo.2648815

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S27	KWRSJERPS2	Extended Suspect List from Sjerps <i>et al</i> (KWRSJERPS)	Full Suspect List Original File, CSV (21/06/2018) CompTox KWRSJERPS2 List	KWRSJERPS2 InChIKeys (06/05/2019)	Table S4 from Sjerps <i>et al.</i> 2016 Water Research 93: 254-264. DOI: 10.1016/j.watres.2016.02.034 DOI: 10.5281/zenodo.2648817
S28	EUBIOCIDES	Biocides from the NORMAN Priority List	EU Biocide List and data XLSX, CSV (30/07/2018) CompTox EUBIOCIDES List	All EU Biocide (salts and MS-ready) InChIKeys (30/07/2018)	Compounds currently used in the EU as biocides (and partly also as PPP or industrial chemicals) or compounds recently banned as biocides from the 2015 NORMAN priority list, which have been prioritized and assessed for exposure by NORMAN using data from ECHA and other sources. Provided by H. Rüdél, Fraunhofer IME. DOI: 10.5281/zenodo.2648819
S29	PHYTOTOXINS	Toxic Plant Phytotoxin (TPPT) Database	TPPT Original File (27/06/2018) TPPT Phytotoxins CSV, XLSX (20/11/2019) CompTox PHYTOTOXINS List	TPPT InChIKeys (20/11/2019)	A comprehensive toxic plant-phytotoxin (TPPT) database provided by Günthardt <i>et al</i> 2018, DOI: 10.1021/acs.jafc.8b01639 . More information on the Agroscope TPPT website . DOI: 10.5281/zenodo.2652993
S30	PHENANTIOX	A list of Phenolic Antioxidants from KEMI and NILU	Phenantiox CSV, XLSX (23/01/2019) CompTox PHENANTIOX List	Phenantiox InChIKeys (23/01/2019)	A list of possible phenolic antioxidants with exposure scores compiled by Stellan Fischer (KEMI) and Pawel Rostkowski (NILU). Mapped to CompTox information using CAS numbers. DOI: 10.5281/zenodo.2653011
S31	WRTMSD	Wiley Registry of Tandem Mass Spectral Data, MSforID	WRTMSD CSV, XLSX (24/01/2019) CompTox WRTMSD List	WRTMSD InChIKeys (24/01/2019)	The "Wiley Registry of Tandem Mass Spectral Data, MSforID" contains high-quality tandem MSacquired on a QqTOF instrument, developed by Herbert Oberacher (Medical University of Innsbruck, Austria). More information at www.msforid.com DOI: 10.5281/zenodo.2653016
S32	REACH2017	>68,600 REACH Chemicals	REACH2017 XLSX, CSV (06/11/2020) CompTox REACH2017 List	REACH2017 InChIKeys (06/11/2020)	A list of >68,600 REACH chemicals including InChIKeys and spectral information, provided by N. Alygizakis and J. Slobodnik, EI. DOI: 10.5281/zenodo.2653020
S33	SOLUTIONSMLOS	Chemicals used for Modelling in SOLUTIONS	SOLUTIONSMLOS XLSX, CSV (06/11/2020) CompTox SOLUTIONSMLOS List	SOLUTIONSMLOS InChIKeys (06/11/2020)	SOLUTIONSMLOS contains the 6462 chemicals used for modelling in the SOLUTIONS project (www.solutions-project.eu/), provided by Jaroslav Slobodnik (EI). DOI: 10.5281/zenodo.2653022

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S34	EXPOSOMEXPL	Biomarkers from Exposome Explorer	Exposome Explorer Biomarkers Download XLSX (24/01/2019) EXPOSOMEXPL Mapped CSV , XLSX (24/01/2019) CompTox EXPOSOMEXPL List	EXPOSOMEXPL InChIKeys (24/01/2019)	The Exposome-Explorer (http://exposome-explorer.iarc.fr/) is dedicated to biomarkers of exposure to environmental risk factors for diseases (Neveu <i>et al</i> 2017, DOI: 10.1093/nar/gkw980). Provided by Reza Salek and Vanessa Neveu (IARC), mapping files to all discrete chemicals by A. Williams/E. Schymanski. DOI: 10.5281/zenodo.2653031
S35	INDOORCT16	Indoor Environment Substances from 2016 Collaborative Trial	Indoor CT Lists XLSX (14/02/2019) INDOORCT16 Merged CSV , XLSX (14/02/2019) CompTox INDOORCT16 List	INDOORCT16 Merged InChIKeys (14/02/2019)	Lists of GC-MS and LC-MS compounds and DSFP output, plus merged files from the Indoor Dust Collaborative Trial, 2016 provided by Peter Haglund (UMU) and Pawel Rostkowski (NILU). Details in Rostkowski <i>et al.</i> 2019 DOI: 10.1007/s00216-019-01615-6 . DOI: 10.5281/zenodo.2653206
S36	UBAPMT	Potential Persistent, Mobile and Toxic (PMT) substances	UBAPMT as CSV , XLSX (25/04/2022) CompTox UBAPMT List	UBAPMT InChIKeys (25/04/2022)	A list of REACH substances that could fulfil proposed (very) Persistent, (very) Mobile and Toxic (PMT/vPvM) criteria according to UBA , Germany and also currently proposed by the European Commission (EC) for the CLP criteria. Derived from a research project by Norwegian Geotechnical Institute (NGI). Updated version provided by Hans Peter Arp, details in UBA Report 126/2019 and in an upcoming 2022 revised version. Funding was provided by the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety of Germany (FKZ3719654080). DOI: 10.5281/zenodo.2653212
S37	LITMINEDNEURO	Neurotoxicants from literature mining PubMed	LITMINEDNEURO CSV , XLSX (25/01/2019) CompTox LITMINEDNEURO List	LITMINEDNEURO InChIKeys (25/01/2019)	A list of chemicals associated with neurotoxicity compiled through systematic literature mining of PubMed using MeSH terms, compiled by Nancy Baker, Antony Williams (US EPA) and Emma Schymanski (LCSB), details in Schymanski <i>et al</i> (2019) DOI: 10.1039/C9EM00068B . DOI: 10.5281/zenodo.2653214
S38	SOLNSLMCTPS	SOLUTIONS Predicted Transformation Products by LMC	Original File XLSX , CSV (14/02/2019) CompTox SOLNSLMCTPS List	SOLNSLMCTPS InChIKeys (14/02/2019)	Predicted Transformation Products calculated by LMC during the SOLUTIONS project, interactive table available here . DOI: 10.5281/zenodo.2653560

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S39	KEMIWWSUS	Wastewater Suspect List based on Swedish Product Data	Wastewater Suspect List XLSX , CSV (14/11/2019) CompTox KEMIWWSUS List	KEMIWWSUS InChIKeys (12/02/2019)	A prioritized list of 1,123 substances relevant for wastewater based on Swedish product registry data, including scores. Provided by Stellan Fischer, KEMI. DOI: 10.5281/zenodo.2653566
S40	ALGALTOX	Algal toxins list from CompTox	ALGALTOX XLSX , CSV (14/02/2019) CompTox ALGALTOX List	ALGALTOX InChIKeys (14/02/2019)	List of algal toxins (generated during blooms) from the CompTox Chemicals Dashboard. DOI: 10.5281/zenodo.2656710
S41	CCL4	CCL 4 Contaminant Candidate List	CCL4 XLSX , CSV (14/02/2019) CompTox CCL4 List	CCL4 InChIKeys (14/02/2019)	Contaminants that are not (yet) regulated in the USA but are known or anticipated to occur in public water systems; from CompTox. DOI: 10.5281/zenodo.2656716
S42	HDXNOEX	Hydrogen Deuterium Exchange (HDX) Standard Set	HDXNOEX XLSX , CSV (14/02/2019) CompTox HDXNOEX List CompTox HDXEXCH List	HDXNOEX InChIKeys (14/02/2019)	Environmental standard set used to investigate hydrogen deuterium exchange in small molecule HRMS (Ruttkies et al. 2019, DOI: 10.1007/s00216-019-01885-0). HDXEXCH list also contains observed deuterated species. DOI: 10.5281/zenodo.2656724
S43	NEUROTOXINS	Neurotoxicants Collection from Public Resources	NEUROTOXINS XLSX , CSV (14/02/2019) CompTox NEUROTOXINS List	NEUROTOXINS InChIKeys (14/02/2019)	A list of neurotoxicants compiled from public resources, details on CompTox and Schymanski et al. (2019) DOI: 10.1039/C9EM00068B . DOI: 10.5281/zenodo.2656729
S44	STATINS	Statins Collection from Public Resources	STATINS XLSX , CSV (14/02/2019) CompTox STATINS List	STATINS InChIKeys (14/02/2019)	A list of statins (lipid-lowering medications) compiled from public resources, details on CompTox. DOI: 10.5281/zenodo.2656736
S45	SYNTHCANNAB	Synthetic Cannabinoids	SYNTHCANNAB XLSX , CSV (17/06/2019) CompTox SYNTHCANNAB List	SYNTHCANNAB InChIKeys (17/06/2019)	A list of synthetic cannabinoids compounds assembled from public resources, from CompTox. DOI: 10.5281/zenodo.2656740
S46	PFASNTREV19	List of PFAS reported in Non-Target HRMS Studies (Liu et al 2019)	Table 1 from Liu et al as PDF MS-ready form in XLSX (formatted) and CSV (17/04/2019) CompTox PFASNTREV19 List	PFASNTREV19 InChIKeys (17/04/2019)	List compiled in the non-target HRMS PFAS review by Liu et al 2019, DOI: 10.1016/j.trac.2019.02.021 . MS-ready list prepared by Yanna Liu, Lisa D'Agostino, Emma Schymanski and Jon Martin. Note not all entries have structures. DOI: 10.5281/zenodo.2656744

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S47	ECHAPLASTICS	A list from the Plastic Additives Initiative Mapping Exercise by ECHA	Merged ECHA Plastic Additives with Structures XLSX , CSV (06/03/2019) CompTox ECHAPLASTICS List	ECHA Plastic Additives InChIKeys (06/03/2019)	List with several categories released on https://echa.europa.eu/mapping-exercise-plastic-additives-initiative and mapped to structures by CAS and Name by E. Schymanski. DOI: 10.5281/zenodo.2658139
S48 S49	CPPDBLISTA CPPDBLISTB	Database of Chemicals associated with Plastic Packaging (CPPdb)	CPPdb Original File (List A and B) XLSX (06/03/2019) Mapped Files (06/03/2019): Table 2 from Groh et al as XLSX , CSV CPPdb List A XLSX , CSV CPPdb List B XLSX , CSV CompTox CPPDBLISTA List CompTox CPPDBLISTB List	Table 2 Groh et al. InChIKeys CPPdb List A InChIKeys CPPdb List B InChIKeys (all 06/03/2019)	A database of chemicals likely (List A, 903) and possibly (List B, 3353) associated with plastic packaging, with hazard data, from Groh et al 2019 DOI: 10.1016/j.scitotenv.2018.10.015 . Mapped to structures by CAS/Name by K. Groh & E. Schymanski. Latest version (last update Oct 2018): DOI: 10.5281/zenodo.1287773 List A DOI: 10.5281/zenodo.2658143 List B DOI: 10.5281/zenodo.2658152
S50	CCSCOMPEND	The Unified Collision Cross Section (CCS) Compendium	CCS as CSV , XLSX (04/03/2019) CompTox CCSCOMPEND List	CCS InChIKeys (29/03/2019)	>3800 experimental collision cross section values (drift tube MS), provided by Jackie Picache and John McLean, Vanderbilt. Further details available here: https://lab.vanderbilt.edu/mclean-group/collision-cross-section-database/ DOI: 10.5281/zenodo.2658162
S51	WRIGCHRMS	GC-HRMS target list of WRI	WRIGCHRMS XLSX , CSV (04/04/2019) CompTox WRIGCHRMS List	WRIGCHRMS InChIKeys (04/04/2019)	GC-HRMS target list of WRI. The method was established by Agilent. The list was provided by Michal Kirchner (Slovak Water Research Institute, WRI) and curated by Nikiforos Alygizakis (EI/UoA) DOI: 10.5281/zenodo.2658169
S52	THSMOKE	Thirdhand Smoke (THS) Compounds	THSMOKE XLSX , CSV (06/05/2019) CompTox THSMOKE List	THSMOKE InChIKeys (06/05/2019)	Thirdhand Smoke (THS, the tobacco-related gases and particles that become embedded in materials), suspect list compiled by Sonia Torres and Noelia Ramirez (IISPV-URV) and Emma Schymanski (LCSB). DOI: 10.5281/zenodo.2669466
S53	UFZWANATARG	Target Compounds from UFZ WANA	Target List as XLSX , CSV (11/08/2019) CompTox UFZWANATARG List	UFZWANATARG InChIKeys – All , LC , GC (11/08/2019)	List of target compounds (LC and GC) measured at WANA, UFZ (Leipzig, Germany), provided by Tobias Schulze and Martin Krauss. DOI: 10.5281/zenodo.3365549

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S54	EFSAPRI	European Food Safety Authority Priority Substances	EFSAPRI Full List XLSX (10/06/2019) EFSAPRI 212 List XLSX , CSV (18/06/2019) CompTox EFSAPRI List	EFSAPRI 212 InChIKeys (18/06/2019)	List of 212 REACH substances prioritized by Oltmanns <i>et al.</i> , DOI: 10.2903/sp.efsa.2019.EN-1597 , European Food Safety Authority (EFSA). 2,336 compounds were assessed for (i) environmental release, (ii) biodegradation, (iii) bioaccumulation in food/feed and (iv) toxicity, resulting in 212 priority compounds. DOI: 10.5281/zenodo.3248993
S55	ZINC15PHARMA	>8600 Pharmaceuticals from ZINC15	Original file with Fragments as CSV , XLSX (06/11/2020) CompTox ZINC15PHARMA List	ZINC15PHARMA MS-ready InChIKeys (06/11/2020)	A list of >8600 pharmaceuticals retrieved from ZINC15 , curated and provided by Reza Aalizadeh, University of Athens. DOI: 10.5281/zenodo.3247749
S56	UOATARGPHARMA	Target Pharmaceutical/Drug List from University of Athens	Target List CSV , XLSX (18/06/2019) CompTox UOATARGPHARMA List	UOATARGPHARMA InChIKeys (18/06/2019)	LC-MS/MS target list of University of Athens containing illicit drugs and pharmaceuticals. Provided by Nikiforos Alygizakis (EI/UoA) and Nikolaos Thomaidis (UoA). DOI: 10.1021/acs.est.6b02417 , 10.1016/j.scitotenv.2015.09.145 , 10.5281/zenodo.3248837
S57	GREEKPHARMA	Suspect Pharmaceuticals from the National Organization of Medicine, Greece	Suspect List CSV , XLSX (18/06/2019) CompTox GREEKPHARMA List	GREEKPHARMA InChIKeys (18/06/2019)	A pharmaceutical suspect list containing antibiotics, antidepressants, antipsychotics, benzodiazepines, NSAIDs, antilipidemic drugs, antiepileptic drugs, antiulcer drugs, antihypertensive and diuretic drugs, extracted from the National Organization for Medicines of Greece. This is complementary to UOATARGPHARMA. Provided by Katerina Galani (UoA), Nikiforos Alygizakis (EI/UoA) and Nikolaos Thomaidis (UoA). DOI: 10.5281/zenodo.3248883
S58	PSYCHOCANNAB	Synthetic Cannabinoids and Psychoactive Compounds	PSYCHOCANNAB XLSX , CSV (17/06/2019) CompTox PSYCHOCANNAB List	PSYCHOCANNAB InChIKeys (17/06/2019)	A list of synthetic cannabinoids and psychoactive compounds assembled from public resources, from CompTox Chemicals Dashboard. DOI: 10.5281/zenodo.3247723
S59	NPINESCT	Natural Product Insecticides	NPINSECT XLSX , CSV (20/11/2019) CompTox NPINSECT List	NPINSECT InChIKeys (20/11/2019)	A list of 83 naturally occurring insecticides curated and provided by Reza Aalizadeh (University of Athens). DOI: 10.5281/zenodo.3544741

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S60	SWISSPEST19	Swiss Pesticides and Metabolites from Kiefer et al 2019	Original file as XLSX (17/11/2019) SWISSPEST19 as XLSX , CSV (25/04/2020) CompTox SWISSPEST19 List	SWISSPEST19 InChIKeys (17/11/2019)	Swiss pesticides (plant protection products) and metabolites from Kiefer et al 2019 (Eawag), Tables SI-B 1 and 2. DOI: 10.1016/j.watres.2019.114972 , 10.5281/zenodo.3544759
S61	UJICCSLIB	Collision Cross Section (CCS) Library from UJI	UJI CCS Library as XLSX , CSV (21/11/2019) CompTox UJICCSLIB List	UJICCSLIB InChIKeys (21/11/2019)	A list of 970 collision cross section values from 556 compounds (both positive and negative ionization modes, and N2 as a drift gas using TWIMS-QTOF instrument) provided by Celma et al. (2020) DOI: 10.1021/acs.est.0c05713 , 10.5281/zenodo.3549476
S62	NORMANEWS2	NormaNEWS2: Retrospective Screening of New Emerging Contaminants	NormaNEWS2 as XLSX , CSV (03/02/2020) CompTox NORMANEWS2 List	NormaNEWS2 InChIKeys (03/02/2020)	List of suspects provided by many contributors to NormaNEWS2 , collated by Kevin Thomas and colleagues at UQ. DOI: 10.5281/zenodo.3634963
S63	UBADWGW	Substances Detected in Drinking (DW) or Groundwater (GW)	UBADWGW Original File Lists 5-7 as XLSX (04/02/2020) UBADWGW as XLSX , CSV (04/20/2020) CompTox UBADWGW List	UBADWGW InChIKeys (04/20/2020)	A list of REACH registered substances (Lists 5-7) detected in drinking (DW) or groundwater (GW) that do not meet PMT criteria. Derived from a research project by Norwegian Geotechnical Institute (NGI). This couples with S36 UBAPMT (Lists 1-4) in the updated version provided by Hans Peter Arp, details in this technical note (UBA Report 126/2019) . DOI: 10.5281/zenodo.3637629
S64	NATOXAQ	NaToxAq: Natural Toxins and Drinking Water Quality - From Source to Tap	NaToxAq as XLSX , CSV (03/03/2020) CompTox NATOXAQ List	NaToxAq InChIKeys (03/03/2020)	NaToxAq (https://natoxaq.ku.dk) is a European Training Network (ETN) funded by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722493, to produce knowledge about natural toxins in aquatic environments. This is a list of all NaToxAq chemicals registered in MassBank within the project, provided by Tobias Schulze, UFZ. DOI: 10.5281/zenodo.3695174
S65	UATHTARGETS GC	University of Athens GC-APCI-HRMS Target List	UATHTARGETSGC XLSX , CSV (15/04/2020), CompTox UATHTARGETSGC List	UATHTARGETSGC InChIKeys (15/04/2020)	GC-APCI-HRMS target list of University of Athens. Provided by the research group of Prof. Nikolaos Thomaidis (http://trams.chem.uoa.gr/). Dataset DOI: 10.5281/zenodo.3753371

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S66	EAWAGTPS	Parent-Transformation Product Pairs from Eawag	EAWAGTPS XLSX , CSV (15/05/2020) CompTox EAWAGTPS List	EAWAGTPS InChIKeys (15/05/2020)	Parent-Transformation Product Pairs of various micropollutants from Eawag: Swiss Federal Institute for Aquatic Science and Technology (https://www.eawag.ch/en/), described in Schollee et al 2017 DOI: 10.1007/s13361-017-1797-6 . Dataset DOI: 10.5281/zenodo.3754448
S67	TBUTYLPHENOLS	List of tert-butyl phenols from KEMI	TBUTYLPHENOLS XLSX , CSV (01/05/2020) CompTox TBUTYLPHENOLS List	TBUTYLPHENOLS InChIKeys (01/05/2020)	A list of tert-butyl phenols from KEMI (Swedish Chemicals Agency), partner list to BISPENOLS. Includes exposure score. Dataset DOI: 10.5281/zenodo.3779848
S68	HSDBTPS	Transformation Products Extracted from HSDB Content in PubChem	HSDBTPS Structures CSV and Transformations CSV (16/05/2020) CompTox HSDBTPS List	HSDBTPS InChIKeys (28/05/2020)	HSDBTPS is a list of metabolites / transformation products (plus parents) extracted from the "Metabolites/Metabolism" section from HSDB (Hazardous Substance Data Bank) in PubChem (https://pubchem.ncbi.nlm.nih.gov/source/11933). Details in Krier et al. (2022) DOI: 10.1016/j.envint.2021.106885 Dataset DOI: 10.5281/zenodo.3827487
S69	LUXPEST	Pesticide Screening List for Luxembourg	LUXPEST XLSX , CSV (29/07/2021) CompTox LUXPEST List	LUXPEST InChIKeys (28/05/2020)	A pesticide screening list for Luxembourg, compiled from multiple sources by Jessy Krier, described in Krier et al. (2022) DOI: 10.1016/j.envint.2021.106885 Dataset DOI: 10.5281/zenodo.3862688
S70	EISUSGCEIMS	Environmental Institute GC-EI-MS suspect list	EISUSGCEIMS XLSX , CSV (15/06/2020) CompTox EISUSGCEIMS List	EISUSGCEIMS InChIKeys (15/06/2020)	GC-EI-MS suspect list of Environmental Institute. Provided by Peter Oswald, Nikiforos Alygizakis, Martina Oswaldova, Jaroslav Slobodnik. Dataset DOI: 10.5281/zenodo.3894827
S71	CECSCREEN	HBM4EU CECscreen: Screening List for Chemicals of Emerging Concern Plus Metadata and Predicted Phase 1 Metabolites	CECscreen as XLSX , CSV , README (1/7/2020) CECscreen Metabolite DB as XLSX , CSV (1/7/2020) CECscreen CompTox DB as XLSX , CSV (1/7/2020) CECscreen OPERA Predictions as XLSX , CSV , README (1/7/2020)	CECscreen InChIKeys (1/7/2020) CECscreen Metabolite InChIKeys (1/7/2020)	CECscreen is part of the HBM4EU project (coord. UBA) > WP16 "emerging chemicals" (lead INRA, JP Antignac/L Debrauwer) > Task 16.1 (lead IRAS, J Vlanderen / R Vermeulen) > Main contributor (J Meijer) >Involved Partners (M Lamoree, T Hamers, S Hutinet, A, Covaci, C Huber, M Krauss, DI Walker, EL Schymanski). Meijer et al (2021) DOI: 10.1016/j.envint.2021.106511 . Dataset DOI: 10.5281/zenodo.3956586 .

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
			CompTox CECSCREEN List		
S72	NTUPHTW	Pharmaceutically Active Substances Suspect List from National Taiwan University	NTUPHTW as XLSX , CSV (22/7/2020) CompTox NTUPHTW List	NTUPHTW InChIKeys (22/7/2020)	A suspect list based on Agilent PCDLs containing pharmaceutically active substances from the College of Public Health, National Taiwan University, kindly provided by Wen-Ling Chen, details in Chen et al (2021) DOI: 10.1016/j.scitotenv.2020.141519 Dataset DOI: 10.5281/zenodo.3955664 .
S73	METXBIODB	Metabolite Reaction Database from BioTransformer	MetXBioDB substances as CSV (06/11/2020) MetXBioDB Transformations as CSV (06/11/2020) CompTox METXBIODB List	MetXBioDB InChIKeys (06/11/2020)	The Metabolite Reaction Database, MetXBioDB, is a biotransformation database used to improve the knowledge- and machine learning-based systems of BioTransformer (http://biotransformer.ca/) by Djoumbou-Feunang et al (2019), DOI: 10.1186/s13321-018-0324-5 . Dataset DOI: 10.5281/zenodo.4056560
S74	REFTPS	Transformation Products and Reactions from Literature	REFTPS substances as CSV (25/01/2022) REFTPS Transformations as CSV (25/01/2022) CompTox REFTPS List (coming soon)	REFTPS InChIKeys (25/01/2022)	This dataset is for users to contribute transformation products and reactions in the literature to the NORMAN SLE, SusDat and the PubChem Transformations section. Dataset DOI: 10.5281/zenodo.4318838
S75	CYANOMETDB	Comprehensive database of secondary metabolites from cyanobacteria	CyanoMetDB as XLSX , CSV CyanoMetDB References as XLSX , CSV CyanoMetDB MetFrag CSV (19/02/2021) CompTox CYANOMETDB List (19/02/2021)	CyanoMetDB InChIKeys (19/02/2021)	CyanoMetDB is a comprehensive database of secondary metabolites from cyanobacteria manually curated from primary references described in Jones et al (2021), DOI: 10.1016/j.watres.2021.117017 . Dataset DOI: 10.5281/zenodo.4551528
S76	LUXPHARMA	Pharmaceuticals Marketed in Luxembourg	LUXPHARMA as XSLX , CSV (06/03/2021) CompTox LUXPHARMA List	LUXPHARMA InChIKeys (06/03/2021)	Pharmaceuticals marketed in Luxembourg from the CNS , provided by R. Singh et al. (2021) DOI: 10.1021/acsenvironau.1c00008). List downloaded from here . Dataset DOI: 10.5281/zenodo.4587355 .

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S77	FCCDB	Food Contact Chemicals Database v5.0	FCCdb as XSLX , CSV (02/04/2021) CompTox FOODCONTACTSDB List (20/02/2021)	FCCdb InChIKeys (02/04/2021)	FCCdb contains information on intentionally added food contact chemicals as described by Groh <i>et al.</i> (2020) DOI: 10.1016/j.envint.2020.106225 and DOI: 10.5281/zenodo.4296944 , structures added by P. Chirsir (LCSB). Dataset DOI: 10.5281/zenodo.4625495 .
S78	SLUPESTTPS	Pesticides and TPs from SLU, Sweden	SLUPestTPs as XLSX , CSV (14/04/2021) SLUPestTPs Transformations as CSV (14/04/2021) CompTox SLUPESTTPS List	SLUPestTPs InChIKeys (14/04/2021)	Suspect list of pesticides and pesticide transformation products (TPs) from SLU, created based on Sweden's national monitoring program and the pesticide properties database (PPDB) described in Frank Menger <i>et al</i> (2021) DOI: 10.1021/acs.est.1c00466 . Dataset DOI: 10.5281/zenodo.4687924 .
S79	UACCSCEC	Collision Cross Section (CCS) Library from UAntwerp	UACCSCEC as XLSX , CSV (20/04/2021) CompTox UACCSCEC List	UACCSCEC InChIKeys (20/04/2021)	Collision cross section (CCS) values of 311 adducts of 148 contaminants of emerging concern (CECs) and their metabolites measured with drift tube ion mobility high resolution mass spectrometry (positive and negative ionization, N2 drift gas) as described in Belova <i>et al</i> (2021) DOI: 10.1021/acs.analchem.1c00142 . Dataset DOI: 10.5281/zenodo.4704648 .
S80	PFASGLUEGE	Overview of PFAS Uses	Original Files as XLSM ESI-2 , ESI-3 PFAS Substances as XLSX , CSV PFAS Use Information (single sheet) as XLSX , CSV (24/06/2021) CompTox PFASGLUEGE List	PFASGLUEGE InChIKeys (24/06/2021)	An overview of the uses of per- and polyfluoroalkyl substances (PFAS) from Glüge <i>et al</i> (2020) DOI: 10.1039/D0EM00291G . Dataset DOI: 10.5281/zenodo.5029173 .
S81	THSTPS	Thirdhand Smoke Specific Metabolites	THSTPS in XLSX , CSV (02/09/2021) THSTPS Transformations in CSV (02/09/2021) CompTox THSTPS List	THSTPS InChIKeys (02/09/2021)	A list of Thirdhand Smoke (THS) specific metabolites compiled by Carla Merino, Noelia Ramirez and colleagues (IISPV-URV). Dataset DOI: 10.5281/zenodo.5394629
S82	EAWAGPMT	PMT Suspect List from Eawag	EAWAGPMT in XLSX , CSV (10/09/2021) CompTox EAWAGPMT List	EAWAGPMT InChIKeys (10/09/2021)	A PMT suspect screening list containing >1100 entries from Kiefer <i>et al</i> (2021), DOI: 10.1016/j.watres.2021.116994 . Dataset DOI: 10.5281/zenodo.5500131

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S83	CCL5	Contaminant Candidate List CCL 5 (Draft)	CCL5 in XLSX , CSV (23/11/2021) CompTox CCL5 List (coming soon...)	CCL5 InChIKeys (23/11/2021)	The CCL 5 is a (currently draft) list of contaminants that are currently not subject to any proposed or promulgated US primary drinking water regulations, but are known or anticipated to occur in public water systems. Microcystins are listed in S85. From: https://www.epa.gov/ccl/contaminant-candidate-list-5-ccl-5 . Dataset DOI: 10.5281/zenodo.5533801
S84	UFZHSFPMT	PMT Suspect List from UFZ and HSF	UFZHSFPMT in XLSX , CSV (29/09/2021) CompTox UFZHSFPMT List	UFZHSFPMT InChIKeys (29/09/2021)	A suspect screening list of 1310 potentially persistent and mobile chemicals from UFZ and HSF, described in Neuwald, Muschket <i>et al.</i> (2021) DOI: 10.1016/j.watres.2021.117645 & 10.5281/zenodo.5503379 Dataset DOI: 10.5281/zenodo.5535287
S85	MICROCYSTINS	MICROCYSTINS from CyanoMetDB	MICROCYSTINS in XLSX , CSV (10/11/2021) CompTox MICROCYSTINS List (coming soon...)	MICROCYSTINS InChIKeys (10/11/2021)	A list of over 300 microcystins extracted from CyanoMetDB (latest version), mostly of natural origin. Provided by L. Janssen, Eawag. Dataset DOI: 10.5281/zenodo.5665355
S86	TATTOOINK	TATTOOINK as per EU regulation 2020/2081	TATTOOINK in XLSX , CSV (18/11/2021) CompTox TATTOOINK List	TATTOOINK InChIKeys (18/11/2021)	A list of regulated ingredients for tattoo ink and permanent make up, Appendix 13 added to Commission Regulation (EU) 2020/2081 , 14 December 2020 amending Annex XVII of REACH . Dataset DOI: 10.5281/zenodo.5710243
S87	CHLORINETPS	List of chlorination byproducts of 137 CECs and small disinfection byproducts	CHLORINETPS in XLSX , CSV (09/12/2021) CompTox CHLORINETPS List	CHLORINETPS InChIKeys (09/12/2021)	A list of chlorination byproducts of 137 contaminants of emerging concern (CECs) and small molecular weight disinfection byproducts from the CHLORINE_TPs database, described in Postigo <i>et al</i> DOI: 10.1016/j.teac.2021.e00148 . 91% are amenable to LC-ESI-HRMS. Dataset DOI: 10.5281/zenodo.5767356
S88	UBABIOCIDES	List of Prioritized Biocides from UBA	UBABIOCIDES in XLSX , CSV (09/12/2021) CompTox UBABIOCIDES List	UBABIOCIDES InChIKeys (09/12/2021)	A merged list of prioritized biocidal active substances provided by UBA (German Environment Agency) and relevant transformation products, released Sept. 2021 (PDF) and updating UBA Texte 114/2017 . Dataset DOI: 10.5281/zenodo.5767494

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S89	PRORISKPFAAS	List of PFAS Compiled from NORMAN SusDat	PRORISKPFAAS in XLSX , CSV (09/12/2021) CompTox PRORISKPFAAS List	PRORISKPFAAS InChIKeys (09/12/2021)	A compiled list of 4777 PFAS occurring in NORMAN SusDat, created by merging SLE lists S9, S14, S25, S46, and S80 and searching for additional fluorinated content in SusDat. Provided by Kelsey Ng, El (manuscript in prep.). Dataset DOI: 10.5281/zenodo.5769582
S90	ZEROPMBOX1	ZeroPM Box 1 Substances	ZeroPM Box 1 as XLSX , CSV (15/01/2022) CompTox ZEROPMBOX1 List	ZeroPM Box1 InChIKeys (15/01/2022)	This list contains representative PFAS, triazoles and triazines, the "Box 1" substances to kick-off the H2020 project ZeroPM (https://zeropm.eu). Dataset DOI: 10.5281/zenodo.5854251
S91	CECTOYS	Chemicals of Emerging Concern (CECs) in plastic toys	CECTOYS in XLSX , CSV (31/01/2022)	CECTOYS InChIKeys (31/01/2022)	A list of 126 Chemicals of EmergingConcern (CECs) found in plastic toys described in Aurisano et al. The list is categorized into four based on being included in regulatory lists of concern as well as reported hazard index (HI) and child cancer risk (CCR) based criteria. DOI: 10.1016/j.envint.2020.106194 . Dataset DOI: 10.5281/zenodo.5933614
S92	FLUOROPHARMA	List of 340 ATC classified fluoro-pharmaceuticals	FLUOROPHARMA in XLSX , CSV (05/02/2022) CompTox List FLUOROPHARMA (coming soon...)	FLUOROPHARMA InChIKeys (05/02/2022)	A list of 340 fluoro pharmaceuticals classified as per WHO's Anatomical Therapeutic Chemical (ATC) classification based on their medical application, described in Inoue et al DOI: 10.1021/acsomega.0c00830 . Dataset DOI: 10.5281/zenodo.5979647
S93	CECMOUTHIN G	Chemicals of Emerging Concern (CECs) in children's mouthing exposure	CECMOUTHIN G Substances in XLSX , CSV (05/02/2022) CECMOUTHIN G Values in XLSX , CSV (05/02/2022)	CECMOUTHIN G InChIKeys (05/02/2022)	A dataset of 60 Chemicals of Emerging Concern (CECs) and their chemical migration rate into saliva due to mouthing exposure in children studied in Aurisano et al DOI: 10.1038/s41370-021-00354-0 . Dataset DOI: 10.5281/zenodo.5979673
S94	FLUROPEST	List of 423 FRAC/HRAC/IRAC classified fluoro-agrochemicals	FLUROPEST in XLSX , CSV (21/02/2022) CompTox List FLUROPEST (coming soon...)	FLUROPEST InChIKeys (21/02/2022)	A list of 423 Fungicide Resistance Action Committee (FRAC), Herbicide Resistance Action Committee (HRAC) or Insecticide Resistance Action Committee (IRAC) classified fluoro-agrochemicals based on their chemotype and mode of action, described in Ogawa et al DOI: 10.1016/j.isci.2020.101467 . Dataset DOI: 10.5281/zenodo.6201559

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S95	PFASANEXCH	PFAS List from the NORMAN PFAS Analytical Exchange Activity	PFASANEXCH in XLSX , CSV (25/03/2022)	PFASANEXCH InChIKeys (25/03/2022)	A list from the PFAS Analytical Exchange Activity, part of NORMAN Joint Programme of Activities (JPA) 2021 coordinated by UK Environment Agency. This activity aimed to gain an understanding of the current analytical capability of PFAS as Limit of Detection (LOD) in participating international laboratories. Dataset DOI: 10.5281/zenodo.6384309
S96	ECIPFAS	Updatable List to add PFAS Structures to Public Resources from ECI (UniLu)	ECIPFAS in XLSX , CSV (28/03/2022)	ECIPFAS InChIKeys (28/03/2022)	This dataset is for users to contribute PFAS from the literature or other documents to the NORMAN SLE, SusDat and PubChem (to fill database gaps). Dataset DOI: 10.5281/zenodo.6389740
S97	UBABPAALT	List of Bisphenol A Alternatives from UBA	UBABPAALT as XLSX , CSV (01/04/2022)	UBABPAALT InChIKeys (01/04/2022)	A list of Bisphenol A alternatives provided by UBA (German Environment Agency) from UBA Report 123/2019 . Dataset DOI: 10.5281/zenodo.6405325
S98	TIRECHEM	Tire-Related Chemicals in Environment from Literature	TIRECHEM as XLSX , CSV (01/04/2022)	TIRECHEM InChIKeys (01/04/2022)	This list includes tire-related chemicals found in the environment plus analytical data from literature studies and will be expanded as new data is published. Dataset DOI: 10.5281/zenodo.6405358

About NORMAN-SLE (header at <https://www.norman-network.com/nds/SLE/>)

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2015 as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring questions. The NORMAN-SLE documents all individual collections that form a part of the merged collection [NORMAN SusDat](#). The original SLE lists should be consulted to verify SusDat information if necessary (see Source column in SusDat). NORMAN-SLE versions are tracked on [Zenodo](#).

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