Activities of the NORMAN network: sharing knowledge and harmonization of practices for a more effective application of NTS techniques in environmental monitoring

Nikiforos Alygizakis

APRONA – Technical seminar on cross-border non-targeted analysis
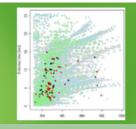
26th April 2022
Virtual meeting

Contents

- NORMAN Association

- Suspect List Exchange (SLE)

- Substance Database (SusDat)

- Factsheets and Ecotoxicology database for the collection of prioritization-relevant information

- Digital Sample Freezing Platform (DSFP) – current status and upcoming integrations

NORMAN

Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

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WELCOME TO THE NORMAN NETWORK

The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. It specifically seeks both to promote and to benefit from the synergies between research teams from different countries in the field of emerging substances.

Who should be part of the network?

All interested stakeholders dealing with emerging substances – whether in studying their occurrence and effects or risk assessment and risk management:

» Competent authorities / Reference laboratories: i.e. institutes and organisations designated by the competent authorities at the national level to offer technical and scientific support in specific fields related to environmental protection.
» Research centres and academia.
» Industry stakeholders.
» Government institutions and standardisation bodies.

Are you involved in research on the occurrence and environmental effects of emerging substances? Or are you concerned with the assessment and management of the risks associated with them? If so, you are a potential stakeholder in the NORMAN network.

If you are interested in this initiative, which has attracted a membership of more than 80 leading laboratories and authorities across Europe, North America and Asia, please contact:

Ms.Valeria DULIO,
Executive Secretary of the NORMAN network
INERIS, Direction Scientifique
Rue Jacques Taffanel – Parc Technologique ALATA
F-60550 Verneuil-en-Halatte,
E-mail address: **valeria.dulio@ineris.fr**

Read more

Highlights

Inter-lab 2021 NORMAN network PFAS Analytical Exchange report now published

Technical Proposal for Effect-Based Monitoring and Assessment under the Water Framework Directive now published

Voice your **support for a global science-policy body on chemicals and waste**

OSPAR Commission is now on board as **Associate member of the NORMAN network**

NORMAN and PARC partnership: let's cooperate!

NORMAN and SCORE contribute to international efforts to tackle the Covid19 pandemic

NORMAN & Water Europe Position Paper "CECs in Urban Wastewater" – Recommendations for UWWT Directive review

Non-target screening can support regulatory environmental monitoring and chemicals management

NORMAN contributes to **recommendations for estrogens monitoring in the aquatic environment**

The **Norman Early Warning System (NormaNEWS)**: a new retrospective analysis exchange platform for laboratories active in non-target screening
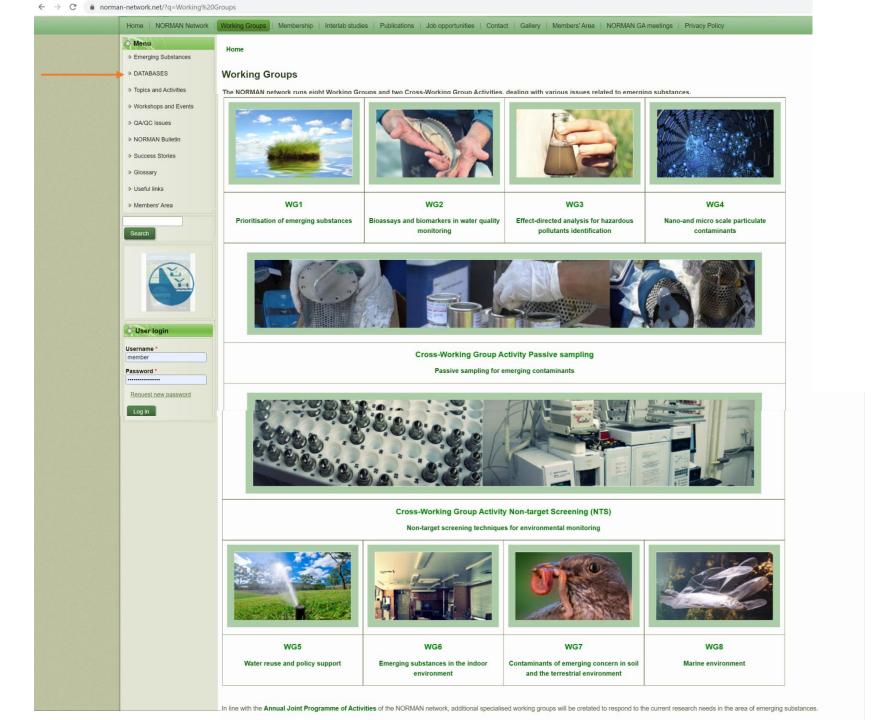
ARCHIVE

Upcoming Events

- Upcoming Events will be announced soon.

Recent Events

- **NORMAN 13th General Assembly meeting** - 1-2 December 2021 (virtual)
- **WG 4 Microplastics meeting** (virtual) - 10 November 2021

Environmental Sciences Europe

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member

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Home

Working Groups

The NORMAN network runs eight Working Groups and two Cross-Working Group Activities, dealing with various issues related to emerging substances.

WG1

Prioritisation of emerging substances

WG2

Bioassays and biomarkers in water quality monitoring

WG3

Effect-directed analysis for hazardous pollutants identification

WG4

Nano-and micro scale particulate contaminants

Cross-Working Group Activity Passive sampling

Passive sampling for emerging contaminants

Cross-Working Group Activity Non-target Screening (NTS)

Non-target screening techniques for environmental monitoring

WG5

Water reuse and policy support

WG6

Emerging substances in the indoor environment

WG7

Contaminants of emerging concern in soil and the terrestrial environment

WG8

Marine environment

In line with the **Annual Joint Programme of Activities** of the NORMAN network, additional specialised working groups will be created to respond to the current research needs in the area of emerging substances.

NORMAN Database System

NORMAN organises the development and maintenance of various web-based databases for the collection & evaluation of data / information on emerging substances in the environment

SEARCH All Databases

Searching for individual substance or group(s) of substances in all databases

Note: Click on a link below to go to an individual database home page

SARS-CoV-2 in sewage

A database with the latest information on SARS-CoV-2 in sewage across Europe and internationally; including a common protocol for sample collection, storage, extraction, analysis and data sharing to support the development of an international comparable data set.

Substance Database

A merged list of NORMAN substances; Central Database to access various lists of substances for suspect screening and prioritisation

Chemical Occurrence Data

A database of geo-referenced monitoring data on emerging substances

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A platform for systematic collection and evaluation of ecotoxicity studies for harmonised derivation of environmental quality standards

Suspect List Exchange

Central Database to access various lists of substances for suspect screening and prioritisation

Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices

MassBank Europe

A database of mass spectra of emerging substances to support identification of unknown substances

Digital Sample Freezing Platform

A database of mass chromatograms obtained by LC-HR-MS for retrospective screening of environmental samples

Indoor Environment

A database of data in indoor environment matrices

Passive Sampling

A database of data obtained with passive samplers

Substance Factsheets

A summary information on individual substances from all NORMAN Database System modules

Prioritisation

Results of prioritisation of NORMAN substances using the NORMAN Prioritisation Framework

Bioassays Monitoring Data

A database of data obtained by analysis of environmental samples with bioassayss

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NORMAN SUBSTANCE DATABASE

NORMAN Suspect List Exchange – NORMAN 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.

Comments and contributions are welcome - please email us at suspects@normandata.eu.

Please refer to our documentation pages for: citation instructions, credits, updates, license details, SDFs and other useful tips!

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 (06/11/2020) MetFrag CSV (03/03/2020) CompTox SUSDAT List	SusDat InChIKeys: All, MS-ready (18/06/2020)	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. *Work in progress ... please report any issues!* DOI: 10.5281/zenodo.2664077
S1	MASSBANK	**NORMAN Compounds in MassBank**	CSV, XLSX with Fragments (3/10/2017) CompTox MassBank EU Reference List CompTox MassBank EU Special Cases CompTox Fragment Download	MassBankEUInChIKeys (17/06/2019)	www.massbank.eu Stravs *et al.* 2013. DOI: 10.1002/jms.3131 DOI: 10.5281/zenodo.2621390

• • •

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

Harmonized format for SLE

Name	SMILES	onoisotopic_ma	Formula	InChI	InChIKey	CAS	PubChemCID	ChemSpiderID	DTXSID
Amikacin	)@H]([C@H]([C@@H]	585.28574	C22H43N5O13	32)11(26)12(30)10(5	HBTVXHDL-RMDFU\	37517-28-5	37768	34635	DTXSID3022586
Apramycin	]([C@@H]([C@H]3O)(	539.28026	C21H41N5O11	5-17-6(23)2-5(22)12(	QTQHRASN-XQENGI	37321-09-8	3081545	2339128	DTXSID5045465
1-Deoxymannojirimycin	)H]([C@@H]([C@H]()	163.08446	C6H13NO4	10)6(11)4(9)1-7-3/h	VIBLOUGU-KVTDHH(	90254-10-7	72258	65214	-
1-Deoxynojirimycin	@H]([C@@H]([C@H](	163.08446	C6H13NO4	10)6(11)4(9)1-7-3/h	VIBLOUGU-JGWLITM	70956-02-4	29435	27360	DTXSID70172647
G 418/Geneticin	C[C@H]([C@@H]([C@	496.27444	C20H40N4O10	3(29)17(24-3)20(2,3(	JRSDMWLG-DJWUNF	49863-47-0	123865	110402	DTXSID10198129
Gentamicin	)H](C[C@@H]([C@H]	463.30060	C20H41N5O7	18-10(21)5-4-9(30-1{	MICFMACRA-XHEDQ\	52093-21-7	3037206	2301017	-
Hygromycin B	]([C@H]([C@H](O2)C(	527.23264	C20H37N3O13	)13(30)12(29)14(34-2	XAQVGOGFE-KPBUC\	31282-04-9	35766	32900	-
Kanamycin	([C@@H]([C@H](O2)(	484.23806	C18H36N4O11	7-11(26)8(22)9(24)7(	DSQTJFQJX-NOAMYH	59-01-8	6032	5810	DTXSID3023184
N-Methyl-1-deoxynojirimycin	([C@H]([C@@H]([C@	177.10011	C7H15NO4	2)6(11)4(8)3-9/h4-7:	DFZMNYDLR-XZBKPI	7152-65-0	92381	83403	-
Neomycin	)O)O)N)O[C@H]3[C@	614.31229	C23H46N6O13	)41-22-11(29)16(35)	TALBVVCIT-VCIWKG	119-04-0	8378	8075	DTXSID2023359
Netilmicin	2[C@@H]([C@H]([C@	475.30060	C21H41N5O7	5(28)18(25-3)21(2,2{	MULVCIBT-MQDUPKI	56391-56-1	441306	20152952	-
Paromomycin	)O)O)N)O[C@H]3[C@	615.29630	C23H45N5O14	)40-22-11(28)16(35)(	PSAJZTQNH-LSWIJE(	7542-37-2	165580	145115	DTXSID8023424
Ribostamycin	C@H]([C@@H]([C@H	454.22749	C17H34N4O10	1-17-13(27)11(25)7(3	URZWSPSBC-VVPCIN	25546-65-0	33042	30581	-
Sisomicin/Sisomycin	@@H](C[C@@H]([C@	447.26930	C19H37N5O7	30-17-9(21)4-3-8(6-2	IWIAIPFPJE-YFMIWBI	32385-11-8	36119	33222	-
Spectinomycin	@H]3[C@H]([C@@H]	332.15835	C14H24N2O7	.8)8(16-3)11(12)23-1	IHTNXNPBV-WXKVU\	1695-77-8	15541	14785	DTXSID9023592
Streptomycin	H]([C@H]2O)O)NC(=N	581.26567	C21H39N7O12	7-19(22)23)12(33)14(	PVAKXKNQ-HZYVHM,	57-92-1	19649	18508	DTXSID4023597
Streptozocin	H]([C@@H]([C@H](O	265.09100	C8H15N3O7	13)3(2-12)18-7(4)15,	PLLKMAKR-GKHCUFF	18883-66-4	29327	27273	DTXSID2021282
Tobramycin	C@H]([C@@H]([C@H	467.25913	C18H37N5O9	27)11(23)12(26)10(4-	XFDBBNBW-PBSUHM	32986-56-4	36294	33377	DTXSID8023680
Tunicamycin	]([C@H]([C@@H](O2)	816.40043	C37H60N4O16	3)41-15-14-24(46)40-	NZVFGCAF-WPTOCQ	-	16220051	17347361	-
Neamine	)O[C@@H]2[C@@H](	322.18523	C12H26N4O6	)1-3(14)7(17)10(11):	PQNSDJLI-HKEUSBC\	1404-04-2	72392	65325	DTXSID7023358
Gentamicin C1a	@H](C[C@@H]([C@H	449.28495	C19H39N5O7	30-17-9(21)4-3-8(6-2	TMJINRLTH-BOZYPMI	1405-41-0	72396	65329	DTXSID4023092
Kanamycin B	]([C@@H]([C@H](O2	483.25404	C18H37N5O10	.3(28)8(22)10(25)7(3	VUUNMCJE-FQSMHN	4696-76-8	439318	388449	DTXSID8023185
Gramicidin S	)N[C@@H](C(=O)N3C(	1140.70594	C60H92N12O10	18-26-48(72)56(78)6{	JGZBVDSGL-XNNAEK(	113-73-5	73357	66085	DTXSID6046008
Dibekacin	C@@H]([C@H]2O)O[(	451.26421	C18H37N5O8	26)11(23)12(25)10(5-	DBDPYCEO-XVZSLQN	34493-98-6	470999	413666	DTXSID2022915
Dihydrostreptomycin	H]([C@H]2O)O)NC(=N	583.28132	C21H41N7O12	7-19(22)23)12(33)14(	WOLISCLQ-HZYVHM,	128-46-1	439369	388489	DTXSID0022937
Lividomycin A	@H]([C@H](O3)CO)O[	761.35421	C29H55N5O18	)1-8(32)22(25)49-26-	AUGBTYDFR-SWMBIF	112-22-1	72394	65327	DTXSID8023218
Kanamycin C	]([C@@H]([C@H](O2	484.23806	C18H36N4O11	(22)12(27)11(26)7(3-	YJKESFZMB-FQSMHN	2280-32-2	439582	388665	DTXSID3023186
Astromicin	H]2[C@H]([C@@H]([C	405.25873	C17H35N5O6	(15)25)22(2)10(23)6-	MYXGFNAEJ-APGVDK	55779-06-1	5284517	4447577	DTXSID2022624
Gentamicin C1	([C@@H]([C@H]2O)(	477.31625	C21H43N5O7	(28)18(26-4)21(2,29)	DELHUEMR-URQXQF	1403-66-3	441305	390067	-

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NORMAN SUSPECT LIST EXCHANGE

NORMAN Substance Database – NORMAN SusDat

Search

About NORMAN SusDat:

NORMAN SusDat is a "living database" compiling information provided by NORMAN network members and external contributors via the NORMAN Suspect List Exchange (NORMAN-SLE). NORMAN SusDat merges the many chemical lists on the SLE into a common format and includes all data suitable for screening purposes, along with selected identifiers and predicted values as a service for NORMAN members and beyond. SusDat is undergoing constant development and improvement to expand the coverage, together with contributors and cheminformatics experts. The original lists on the NORMAN-SLE should be consulted to verify chemical information if necessary (see Source column). Comments and contributions are welcome - please email us at suspects@normandata.eu.

[Search] [Show All Substances]

Search criteria – Use Category

- ☐ Biocides (BIOCID)
- ☐ Drinking water chemicals (DW)
- ☐ Drugs of abuse (DOA)
- ☐ Flame retardants (FRET)
- ☐ Food additives (FOODA)
- ☐ Food contact chemicals (FOODC)
- ☐ Human metabolites (HUME)
- ☐ Human neurotoxins (HUTOX)
- ☐ Indoor environment substances (INDOOR)
- ☐ Industrial chemicals (IND)
- ☐ Metals and their compounds (MET)
- ☐ Natural toxins (NATOX)
- ☐ Per- and polyfluoroalkyl substances (PFAS)
- ☐ Persistent, mobile and toxic substances (PMT)

Search criteria – Individual substance(s)

Enter a part of the 'SusDat ID' or 'Substance Name' or 'CAS No' or 'StdInChIKey' -

Search criteria – Batch search

- ☐ S1/MASSBANK NORMAN Compounds in MassBank
- ☐ S2/STOFFIDENT HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances
- ☐ S3/NORMANCT15 NORMAN Collaborative Trial Targets and Suspects
- ☐ S4/UJIBADE University of Jaume I
- ☐ S5/KWRSJERPS KWR Drinking Water Suspect List
- ☐ S6/ITNANTIBIOTIC Antibiotic List: ITN MSCA ANSWER
- ☐ S7/EAWAGSURF Eawag Surfactants Suspect List
- ☐ S8/ATHENSSUS University of Athens Surfactants and Suspects List
- ☐ S9/PFASTRIER PFAS Suspect List: fluorinated substances
- ☐ S10/SWISSPHARMA Pharmaceutical List with Consumption Data
- ☐ S11/SWISSPEST Swiss Insecticides, Fungicides and TPs
- ☐ S12/NORMANEWS NormaNEWS for Retrospective Screening of New Emerging Contaminants
- ☐ S13/EUCOSMETICS Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)

NORMAN WEBSITE | NORMAN DATABASE SYSTEM | HOME | LOGIN

NORMAN SUSPECT LIST EXCHANGE

Source
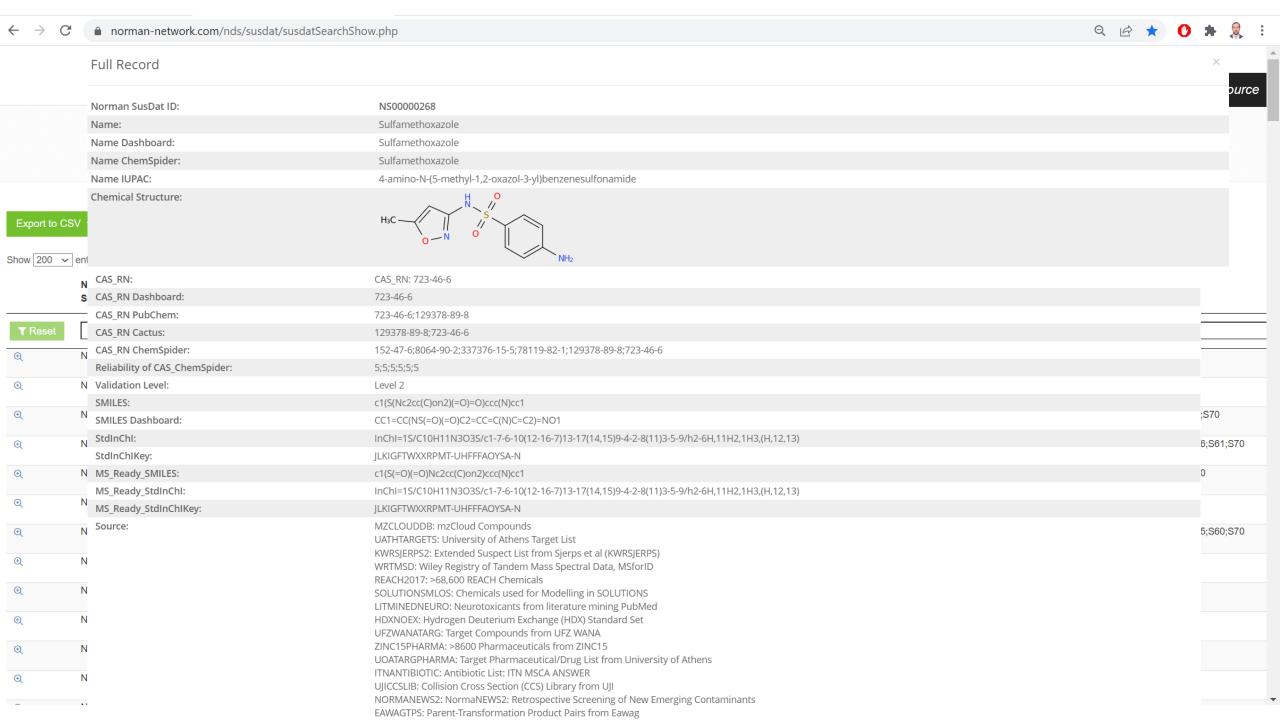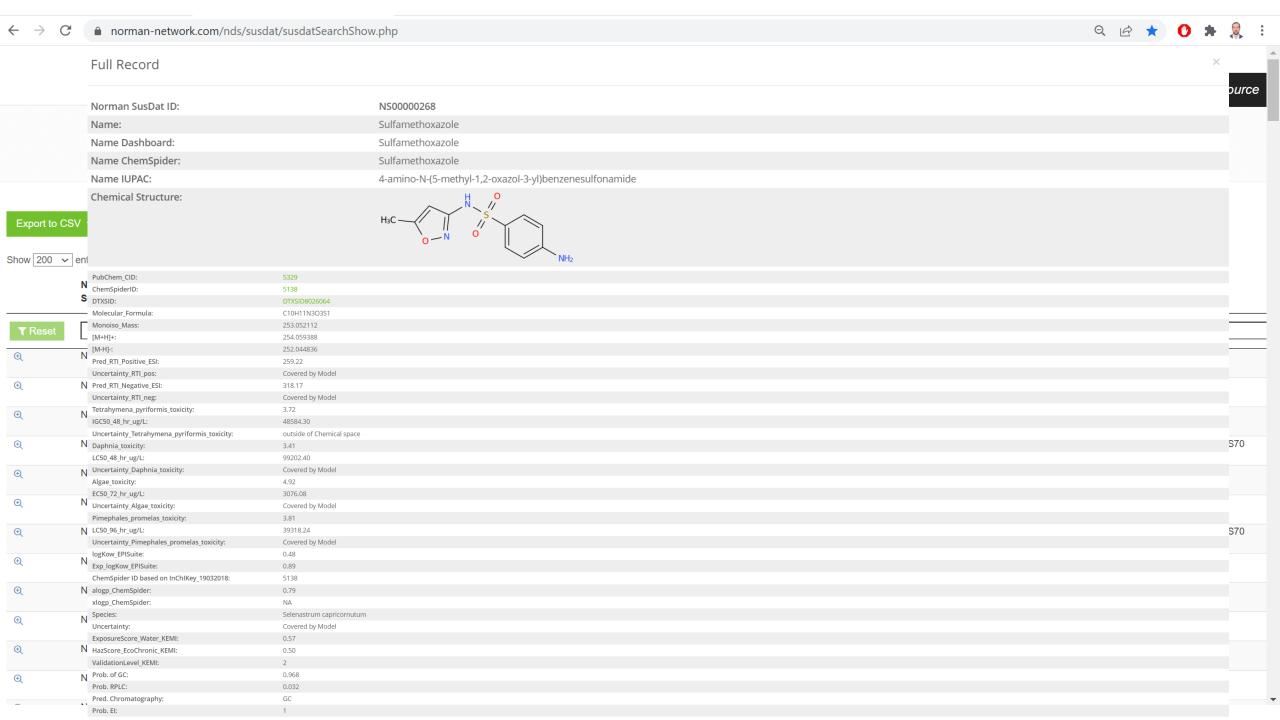
NORMAN Substance Database – NORMAN SusDat

Search / Results

Export to CSV ⌄
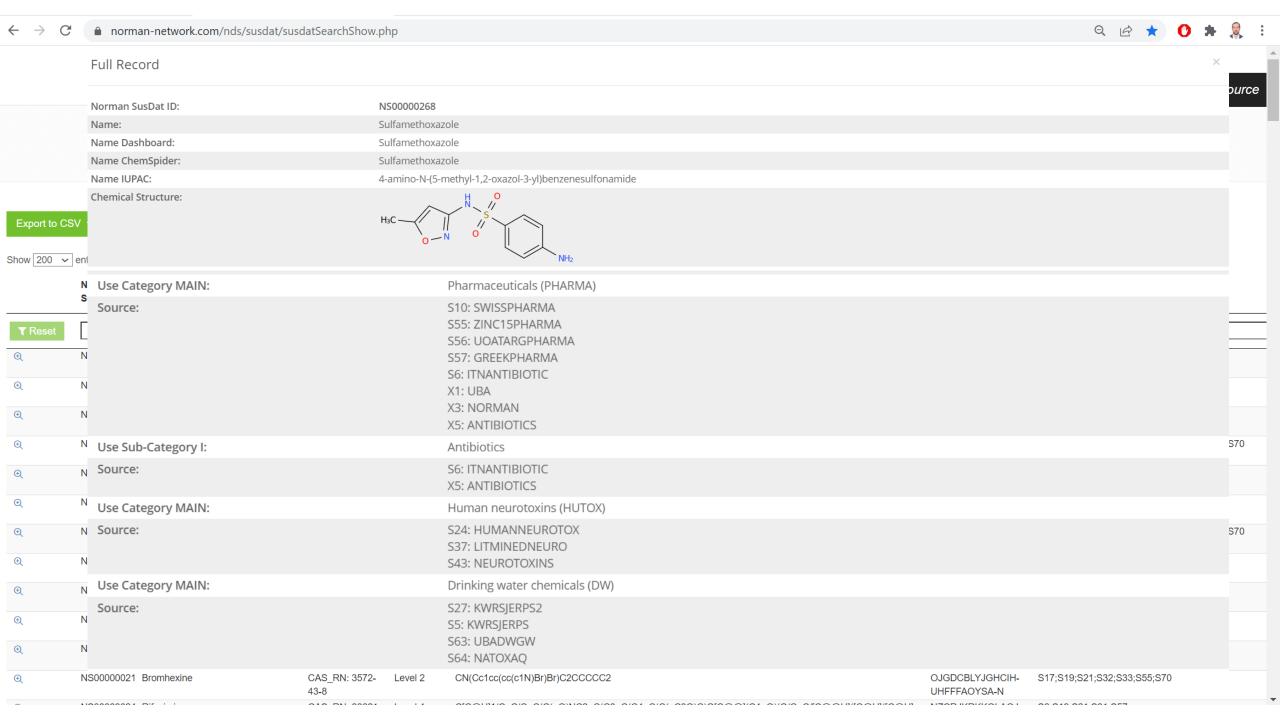
Show 200 ⌄ entries

	Norman SusDat ID	Name	CAS_RN	Validation Level	SMILES	StdInChIKey	Source
⊕	NS00000001	Sulfaclozine	CAS_RN: 102-65-8	Level 4	c1cc(ccc1N)S(=O)(=O)Nc2cncc(n2)Cl	QKLPUVXBJHRFQZ-UHFFFAOYSA-N	S1;S2;S6;S17;S21;S32;S33;S56
⊕	NS00000002	Sulfachloropyridazine	CAS_RN: 80-32-0	Level 2	c1cc(ccc1N)S(=O)(=O)Nc2ccc(nn2)Cl	XOXHILFPRYWFOD-UHFFFAOYSA-N	S1;S2;S6;S17;S19;S21;S31;S32;S56
⊕	NS00000003	Sulfaguanidine	CAS_RN: 57-67-0	Level 2	c1cc(ccc1N)S(=O)(=O)NC(=N)N	BRBKOPJOKNSWSG-UHFFFAOYSA-N	S1;S6;S19;S21;S31;S32;S33;S50;S56;S70
⊕	NS00000004	Sulfamerazine	CAS_RN: 127-79-7	Level 2	Cc1ccnc(n1)NS(=O)(=O)c2ccc(cc2)N	QPPBRPIAZZHUNT-UHFFFAOYSA-N	S6;S19;S21;S31;S32;S33;S53;S55;S56;S61;S70
⊕	NS00000005	Sulfamethizole	CAS_RN: 144-82-1	Level 2	Cc1nnc(s1)NS(=O)(=O)c2ccc(cc2)N	VACCAVUAMIDAGB-UHFFFAOYSA-N	S6;S19;S21;S31;S32;S33;S55;S56;S70
⊕	NS00000006	Sulfamoxole	CAS_RN: 729-99-7	Level 2	Cc1c(oc(n1)NS(=O)(=O)c2ccc(cc2)N)C	CYFLXLSBHQBMFT-UHFFFAOYSA-N	S6;S19;S21;S31;S32;S33;S55;S56
⊕	NS00000007	Sulfanilamide	CAS_RN: 63-74-1	Level 4	c1cc(ccc1N)S(=O)(=O)N	FDDDEECHVMSUSB-UHFFFAOYSA-N	S6;S19;S21;S31;S32;S33;S38;S50;S55;S60;S70
⊕	NS00000009	Tiamulin	CAS_RN: 55297-95-5	Level 2	CCN(CC)CCSCC(=O)O[C@@H]1C[C@@]([C@H]([C@@H]([C@@]23CC[C@H]([C@@]1([C@@H]2C(=O)CC3)C)C)C)O)(C)C=C	UURAUHCOJAIIRQ-QGLSALSOSA-N	S6;S21;S56;S61
⊕	NS00000010	Albendazole oxide	CAS_RN: 54029-12-8	Level 2	CCCS(=O)c1ccc2c(c1)nc([nH]2)NC(=O)OC	VXTGHWHFYNYFFV-UHFFFAOYSA-N	S1;S19;S55
⊕	NS00000016	Mabuterol	CAS_RN: 56341-08-3	Level 2	CC(C)(C)NCC(c1cc(c(c(c1)Cl)N)C(F)(F)F)O	JSJCTEKTBOKRST-UHFFFAOYSA-N	S6;S19;S21;S61

Showing 1 to 200 of 109,567 entries

Previous 1 2 3 4 5 … 548 Next

Full Record

Norman SusDat ID:	NS00000268
Name:	Sulfamethoxazole
Name Dashboard:	Sulfamethoxazole
Name ChemSpider:	Sulfamethoxazole
Name IUPAC:	4-amino-N-(5-methyl-1,2-oxazol-3-yl)benzenesulfonamide
Chemical Structure:	

Export to CSV

Show 200 ent

CAS_RN:	CAS_RN: 723-46-6
CAS_RN Dashboard:	723-46-6
CAS_RN PubChem:	723-46-6;129378-89-8
CAS_RN Cactus:	129378-89-8;723-46-6
CAS_RN ChemSpider:	152-47-6;8064-90-2;337376-15-5;78119-82-1;129378-89-8;723-46-6
Reliability of CAS_ChemSpider:	5;5;5;5;5;5
Validation Level:	Level 2
SMILES:	c1(S(Nc2cc(C)on2)(=O)=O)ccc(N)cc1
SMILES Dashboard:	CC1=CC(NS(=O)(=O)C2=CC=C(N)C=C2)=NO1
StdInChI:	InChI=1S/C10H11N3O3S/c1-7-6-10(12-16-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2,1H3,(H,12,13)
StdInChIKey:	JLKIGFTWXXRPMT-UHFFFAOYSA-N
MS_Ready_SMILES:	c1(S(=O)(=O)Nc2cc(C)on2)ccc(N)cc1
MS_Ready_StdInChI:	InChI=1S/C10H11N3O3S/c1-7-6-10(12-16-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2,1H3,(H,12,13)
MS_Ready_StdInChIKey:	JLKIGFTWXXRPMT-UHFFFAOYSA-N
Source:	MZCLOUDDB: mzCloud Compounds
	UATHTARGETS: University of Athens Target List
	KWRSJERPS2: Extended Suspect List from Sjerps et al (KWRSJERPS)
	WRTMSD: Wiley Registry of Tandem Mass Spectral Data, MSforID
	REACH2017: >68,600 REACH Chemicals
	SOLUTIONSMLOS: Chemicals used for Modelling in SOLUTIONS
	LITMINEDNEURO: Neurotoxicants from literature mining PubMed
	HDXNOEX: Hydrogen Deuterium Exchange (HDX) Standard Set
	UFZWANATARG: Target Compounds from UFZ WANA
	ZINC15PHARMA: >8600 Pharmaceuticals from ZINC15
	UOATARGPHARMA: Target Pharmaceutical/Drug List from University of Athens
	ITNANTIBIOTIC: Antibiotic List: ITN MSCA ANSWER
	UJICCSLIB: Collision Cross Section (CCS) Library from UJI
	NORMANEWS2: NormaNEWS2: Retrospective Screening of New Emerging Contaminants
	EAWAGTPS: Parent-Transformation Product Pairs from Eawag

Full Record

Norman SusDat ID:	NS00000268
Name:	Sulfamethoxazole
Name Dashboard:	Sulfamethoxazole
Name ChemSpider:	Sulfamethoxazole
Name IUPAC:	4-amino-N-(5-methyl-1,2-oxazol-3-yl)benzenesulfonamide

Chemical Structure:

Export to CSV

Show 200 ent

Reset

PubChem_CID:	5329
ChemSpiderID:	5138
DTXSID:	DTXSID8026064
Molecular_Formula:	C10H11N3O3S1
Monoiso_Mass:	253.052112
[M+H]+:	254.059388
[M-H]-:	252.044836
Pred_RTI_Positive_ESI:	259.22
Uncertainty_RTI_pos:	Covered by Model
Pred_RTI_Negative_ESI:	318.17
Uncertainty_RTI_neg:	Covered by Model
Tetrahymena_pyriformis_toxicity:	3.72
IGC50_48_hr_ug/L:	48584.30
Uncertainty_Tetrahymena_pyriformis_toxicity:	outside of Chemical space
Daphnia_toxicity:	3.41
LC50_48_hr_ug/L:	99202.40
Uncertainty_Daphnia_toxicity:	Covered by Model
Algae_toxicity:	4.92
EC50_72_hr_ug/L:	3076.08
Uncertainty_Algae_toxicity:	Covered by Model
Pimephales_promelas_toxicity:	3.81
LC50_96_hr_ug/L:	39318.24
Uncertainty_Pimephales_promelas_toxicity:	Covered by Model
logKow_EPISuite:	0.48
Exp_logKow_EPISuite:	0.89
ChemSpider ID based on InChIKey_19032018:	5138
alogp_ChemSpider:	0.79
xlogp_ChemSpider:	NA
Species:	Selenastrum capricornutum
Uncertainty:	Covered by Model
ExposureScore_Water_KEMI:	0.57
HazScore_EcoChronic_KEMI:	0.50
ValidationLevel_KEMI:	2
Prob. of GC:	0.968
Prob. RPLC:	0.032
Pred. Chromatography:	GC
Prob. EI:	1

Full Record

ource

Norman SusDat ID:	NS00000268
Name:	Sulfamethoxazole
Name Dashboard:	Sulfamethoxazole
Name ChemSpider:	Sulfamethoxazole
Name IUPAC:	4-amino-N-(5-methyl-1,2-oxazol-3-yl)benzenesulfonamide
Chemical Structure:	

Export to CSV

Show 200 ent

Reset

Use Category MAIN:	Pharmaceuticals (PHARMA)
Source:	S10: SWISSPHARMA
	S55: ZINC15PHARMA
	S56: UOATARGPHARMA
	S57: GREEKPHARMA
	S6: ITNANTIBIOTIC
	X1: UBA
	X3: NORMAN
	X5: ANTIBIOTICS
Use Sub-Category I:	Antibiotics
Source:	S6: ITNANTIBIOTIC
	X5: ANTIBIOTICS
Use Category MAIN:	Human neurotoxins (HUTOX)
Source:	S24: HUMANNEUROTOX
	S37: LITMINEDNEURO
	S43: NEUROTOXINS
Use Category MAIN:	Drinking water chemicals (DW)
Source:	S27: KWRSJERPS2
	S5: KWRSJERPS
	S63: UBADWGW
	S64: NATOXAQ

NS00000021	Bromhexine	CAS_RN: 3572-43-8	Level 2	CN(Cc1cc(cc(c1N)Br)Br)C2CCCCC2	OJGDCBLYJGHCIH-UHFFFAOYSA-N	S17;S19;S21;S32;S33;S55;S70

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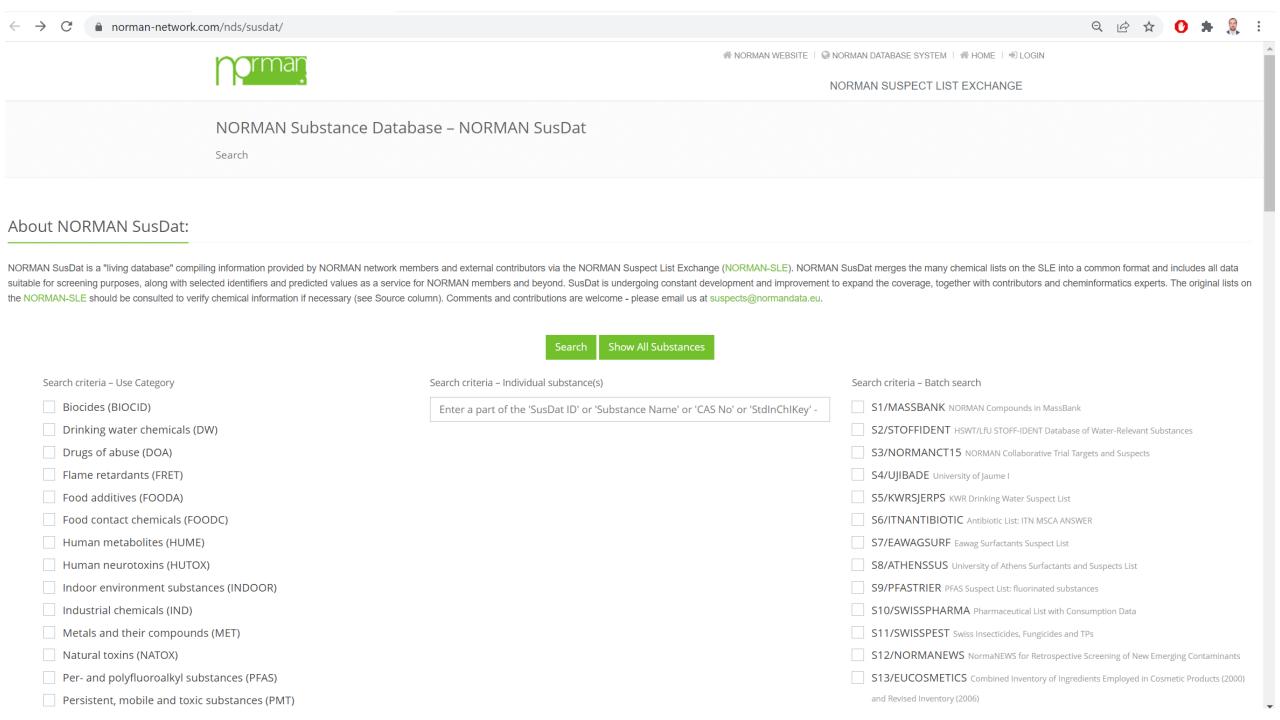## Prioritisation

Results of prioritisation of NORMAN substances using the NORMAN Prioritisation Framework

Bioassays Monitoring Data

A database of data obtained by analysis of environmental samples with bioassayss

SEARCH SUBSTANCE

NORM

Factsheets for: **Sulfamethoxazole**

Search cr

sulfam

Show

⊙ 4-Ni

⊙ 5-Hy

⊙ Azos

⊙ Des

⊙ Isos

⊙ N(1)

⊙ N-Ac

⊙ N4-a

⊙ N4-

⊙ o-ch

⊙ Sulf

⊙ Sulf

⊙ Sulf

⊙ Trim

⌄ CHEMICAL IDENTITY
⌄ MAJOR USES
⌄ EXISTING EVALUATIONS AND REGULATORY INFORMATION
⌄ PROPERTIES
⌄ ENVIRONMENTAL OCCURENCE (all data)
⌄ ENVIRONMENTAL OCCURENCE (detailed information)
⌄ (ECO)TOXICITY
⌄ PBT/vPvB & PMT/vMT (NORMAN)
⌄ CMR & ED (NORMAN)
⌄ POTENTIAL RISK OF EXCEEDANCE OF LOWEST PNEC
⌄ CONCLUSIONS AND RECOMMENDATIONS
⌄ BIBLIOGRAPHY, SOURCES AND SUPPORTIVE INFORMATION

⌃ ENVIRONMENTAL OCCURENCE (all data)

Occurrence data (NORMAN – all data)

Surface water (relevant matrix)	No. of Countries	No. of Countries with Analysis > LOQ	No. of Stations	No. of Stations with Analysis > LOQ	No. of Analysis	Frequency of Quantification
Value	20	18	743	511	3367	62.46 %
Score[1]	n.a.	1	n.a.	0.5	n.a.	0.62

Occurrence data (NORMAN – recent data[2])

Surface water (relevant matrix)	No. of Countries	No. of Countries with Analysis > LOQ	No. of Stations	No. of Stations with Analysis > LOQ	No. of Analysis	Frequency of Quantification
Value	6	5	84	28	98	28.57 %
Score[1]	n.a.	0.5	n.a.	0.2	n.a.	0.29

SELECT * FROM environmental_occurence_all_data_loq LEFT JOIN empodat.data_matrice ON tab_matrix = matrice_id WHERE sus_id = '268' AND tab_matrix < 9 ORDER BY tab_matrix

LOQ_{min}, Median, Max and MEC_{95} (NORMAN – all data[1])

Matrix	LOQ_{min} [µg/L]	Median concentration [µg/L]	Max concentration [µg/L]	MEC_{95} [µg/L] (all data)	MEC_{95} [µg/L] (recent data)

[1] According to the NORMAN Prioritisation Methodology (Dulio & von der Ohe 2013)

[2] Occurrence data from 2017 – 2022

MEC_{95} is the 95th percentile of the measured Maximum Environmental Concentrations at one site

ENVIRONMENTAL OCCURENCE (detailed information)

Per Country

Show 10 entries   Search:

Country	No. of stations	No. of analyses	2002	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019
Antarctica	1	4																4	
Austria	22	169					16						74	52			4		23
Belgium	1	50						14	10	26									
Bulgaria	31	156					28						55	34					39
Croatia	23	125					10						58	33			8		16
Czech Republic	14	25					4										4	4	13
France	346	5901				54					3830	746	236	224	374	326	110		1
Georgia	39	103														62	21		20
Germany	241	3076			38	146	108			272	456	720	1212	44	14	1	5	26	34
Greece	2	2																	2

Showing 1 to 10 of 26 entries   Previous **1** 2 3 Next

Per Matrix

Show 10 entries   Search:

Matrix	Total no. of analyses	No. of analyses above LoQ	Max	Median	Unit	Lowest PNEC	EQS
	20				µg/kg wet weight	5.95	
Biota - Coastal water	49				µg/kg wet weight	5.95	
Biota - Lake water	13				µg/kg wet weight	5.95	
Biota - River water	29	9	29	6	µg/kg wet weight	5.95	
Biota - Terrestrial	12				µg/kg wet weight	5.95	
Biota - Territorial (marine) water	23	1	34.445	34.445	µg/kg wet weight	5.95	
Biota - Transitional water	1				µg/kg wet weight	5.95	
Ground water	1975	40	0.043	0.005	µg/l	0.6	
Sediments - Lake water	19				µg/kg dry weight	3.67	
Sediments - River water	16				µg/kg dry weight	3.67	

Showing 1 to 10 of 22 entries   Previous **1** 2 3 Next

⯅ (ECO)TOXICITY

Lowest PNEC fresh water (µg/L)	0.6
Experimental / predicted	n.r.
Species	*n.r.*
AF	0
Endpoint	
Reference	PNEC-ID-0257944
Lowest PNEC marine water (µg/L)	0.06
Lowest PNEC sediment (µg/kg dw)	3.67
Lowest PNEC biota (µg/kg ww)	5.95

⯅ PBT/vPvB & PMT/vMT (NORMAN)

P criterion	P score	B criterion	B score	M criterion	M score	T criterion	T score	PBT evaluation	vPvB evaluation	PBT / vPvB score	PMT evaluation	vPvM evaluation	vMT evaluation	PMT / vPvM / vMT Score	PB Score	PBMT score	Source
not available	0	not B	0	vM	1	potentially T	0.5	not available	not available	0	not PMT	not vPvM	not vMT	0		0.38	Norman
	1.00		0.00	vM	1		0			0					0	0.50	Janus

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norman

SEARCH ECOTOX DATA   SEARCH QUALITY TARGET   LOWEST PNECS   DCT DOWNLOAD

NORMAN Ecotoxicology Database — Lowest PNECs

The Lowest PNECs shown in the table below for different matrices are used primarily for prioritisation purposes. Experimental and predicted Lowest PNECs, which were voted by NORMAN ecotoxicology experts are addressed as 'verified'.

Most of the Lowest PNECs were derived for freshwater. Unless there is an experimental value for other matrices, the following calculations were used for derivation of the Lowest PNECs in:

- **Marine water** – Lowest PNECfw/10
- **Sediments** – Lowest PNECfw*2.6*(0.615+0.019*Koc)
- **Biota** – PNECfw*BCF
- **Marine biota** – PNECfw*BCF/10
- **Biota - molluscs** – PNECfw*BCF/4
- **Marine biota - molluscs** – PNECfw*BCF/10/4

⬇ Export to CSV

◉ Show all Lowest PNECs – predicted by QSAR and experimentally-based values

◯ Show all Lowest PNECs verified by NORMAN

Show [200 ▾] entries   Search: [   ]

Norman SusDat ID	Substance	CAS No.	Lowest PNECfw [µg//l]	Lowest PNECmarine [µg//l]	Lowest PNECsed_fw [µg//kg dw]	Lowest PNECsed_marine [µg//kg dw]	Lowest PNECbio_fw [µg//kg ww]	Lowest PNECbio_marine [µg//kg ww]
NS00026758	((((4-Methylphenyl)sulphonyl)oxy)imino)malononitrile	CAS_RN: 20893-01-0	6.96	0.7	17.9	1.79	30.6	3.06
NS00020523	(((2-((2-((2-Aminoethyl)amino)ethyl)amino)ethyl)amino)methyl)phenol	CAS_RN: 51818-54-3	11.3	1.13	185	18.5	9.59	0.96
NS00036082	(((2-Chloroethyl)sulphonyl)methyl)benzene	CAS_RN: 66998-67-2	9.71	0.97	51.3	5.13	246	24.6
NS00038505	(((9-Oxo-9H-thioxanthen-2-yl)methyl)thio)acetic acid	CAS_RN: 84434-06-0	1.63	0.16	49.6	4.96	4.97	0.5
NS00033073	(((Diethylamino)thioxomethyl)thio)acetic acid	CAS_RN: 5439-93-0	14.1	1.41	123	12.3	36.2	3.62
NS00011060	(((Perfluorodecyl)ethylsulphonyl)methylamino)ethyl acrylate	CAS_RN: 72276-05-2	0.051	0.0051	396	39.6	10.2	1.02
NS00029859	(((Phenylmethoxy)methoxy)methoxy)methanol	CAS_RN: 35445-71-7	127	12.7	337	33.7	516	51.6

Showing 1 to 200 of 64,478 entries

Previous   1   2   3   4   5   …   323   Next

NORMAN Database System [R] Customized Statistics

Substances (list of NORMAN SUSDAT IDs separated by a comma)

Substance	Country	>= X countries with analysis
All	All	4

Matrix	From year	To year	>= X sites with analysis
All	2017	2022	100

Fractions	Waste water	>= X sites with conc > LoQ
All	All	50

River Basin / Sea region	Dilution factor waste water *	>= X sites with LOQmin < lowest PNEC
All	5	100

Source (list of data files)	Ground water PNECs
All	Same as freshwater

Run

Marine biota PNECs

PNECbio_marine

* IF matrix All OR Waste water THEN conversion from c_{ww} to c_{fw}

List of indicators and cut-off values applied for the allocation of the candidate substances to action categories 1 to 6 (PDF format)

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DSFP Digital Sample Freezing Platform

Home   Contributors   About

Welcome to DSFP

DSFP was created to host liquid chromatography-high resolution-mass spectrometry (LC-HRMS) and gas chromatography-high resolution-mass spectrometry (GC-HRMS) data.

[   ] **Go**

Welcome to the Digital Sample Freezing Platform (DSFP)! The DSFP hosts liquid chromatography-high resolution-mass spectrometry (LC-HRMS) and gas chromatography-high resolution-mass spectrometry (GC-HRMS) data from various contributing organisations. The DSFP enables retrospective suspect screening of chemicals making use of the NORMAN Database System. It seeks to foster and benefit from the synergies between research teams across the globe. Researchers and research groups interested in the study of chemicals in the environment, food, and human biomonitoring are welcome to contribute and employ their digitally frozen data on DSFP!

👤 User area

3
Collections

25
Samples

58
Files

Latest Collections

LIFE APEX

This is the LIFE APEX tier 1 collection.

JDS4

This collection includes the Joint Danube Survey 4 samples.

another test

ewtw

NORMAN Database System

SEARCH All Databases
Suspect List Exchange
NORMAN Substance Database
Chemical Occurrence Data
Bioassays Monitoring Data
Antibiotic Resistance Bacteria/Genes
NORMAN Massbank

Contact Us

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Email: norman@ei.sk
Url: https://www.norman-network.com/
Url: https://www.norman-network.net/
Url: https://www.normandata.eu/

Log in

Username *

nalygizakis

Enter your DSFP username.

Password *

••••••

Enter the password that accompanies your username.

Log in

Create new account

Forgot your password?

dev.norman-data.eu/user/register

DSFP

Create new account

Email address *

A valid email address. All emails from the system will be sent to this address. The email address is not made public and will only be used if you wish to receive a new password or wish to receive certain news or notifications by email.

Username *

Several special characters are allowed, including space, period (.), hyphen (-), apostrophe ('), underscore (_), and the @ sign.

∨ Picture

∧ Contributor profile

First name

Last name

Affiliation

- None -

Phone

Create new account   Cancel

Back to site

My contributions

Overview   Account settings   Contributor profile

1 labs

more

1 instruments

more

2 collections

more

57 files

more

Welcome to the contributor's area! In this page, you can complete your profile and associate it with an organization. Afterwards, you can add one or more laboratories in your organization. Each laboratory can have one or more analytical instruments with one or more instrumental setups. This procedure is done once and can be referenced later during the contribution process.

Adding at least one laboratory and one instrument with one setup will allow you to upload collections. A collection is a group of samples that were collected during a monitoring campaign or during a project. The collection contains samples for which you will be required to provide the respective mzML files.

You will find additional information and guidance on the top of every page.

DSFP

My Labs

Your organization may have one or
the button "Add". The fields that yo

- The name, the logo and a short
- The full address of the laborat
- The contact name and email of t

+ Add a lab

ID	Lab Title
295	Trace Analysis Mass Spectrometr

Back to site

Create Lab

Lab name *

Short description

| B | I | ⎘ | ⎘ | ☰ | ☰ | ❝ | 🖼 | Format ▾ | ⬛ Source |

About text formats

⌄ Address

Contact name

Contact e-mail

⌄ Logo

Delete
delete

Edit
edit

Cancel   **Save**

dev.norman-data.eu/user/instruments

My Instruments

Your laboratory may be equipped wit[...]
may add them by pressing the butto[...]
to fill in are:

- An instrument alias and the instru[...]
- A short description of the instrum[...]
- The manufacturer and the model [...]

Afterwards, you need to add one or n[...]
specify:

- The chromatographic separation [...]
  column model, column characteri[...]
- The detection settings (m/z scan [...]
  parameters)
- The retention time of LC or GC ca[...]
  this information will harmonize th[...]
- Spiked compounds in case a stan[...]
  information is useful for semi-qua[...]

+ Add an instrument

Create Instrument   ✕

Instrument alias *

Short description

| B | *I* | link | unlink | ≣ | ≣ | " | 🖬 | Format ▾ | | Source |

About text formats

Manufacturer

- None -   ▾

Model

- None -   ▾

Belongs to (Lab) *

Instrument type *

- Select -   ▾

Cancel   **Save**

ID	Instrument alias		nstrument Setups	Delete	Edit
297	Bruker maXis QTOF		setups	delete	edit

My Instruments | DSFP

dev.norman-data.eu/user/instruments

DSFP

My Instruments

Your laboratory may be equ
may add them by pressing
to fill in are:

- An instrument alias and
- A short description of th
- The manufacturer and t

Afterwards, you need to ad
specify:

- The chromatographic se
  column model, column
- The detection settings (
  parameters)
- The retention time of LC
  this information will har
- Spiked compounds in ca
  information is useful for

+ Add an instrument

Instrument Setups for Bruker maXis QTOF ✕

+ Add a setup

Setup alias	Ionization type	Updated	Submitted by	Edit	Delete	Duplicate
Setup #1 (completed)	positive	Mon, 01/24/2022 - 16:59	admin	edit	delete	duplicate
Another example of a setup (completed)	negative	Mon, 01/24/2022 - 17:02	admin	edit	delete	duplicate
LC Positive maXis QTOF (completed)	positive	Mon, 01/24/2022 - 19:02	nalygizakis	edit	delete	duplicate
Negative maXis QTOF (draft)		Mon, 01/24/2022 - 19:00	nalygizakis	edit	delete	duplicate
Setup #3 (draft)	positive	Mon, 01/24/2022 - 21:26	admin	edit	delete	duplicate
Setup test #2.1 (completed)	positive	Thu, 02/03/2022 - 17:40	API publisher	edit	delete	duplicate
Setup test #2.2 (draft)	positive	Thu, 02/03/2022 - 17:42	API publisher	edit	delete	duplicate

ID	Instrument alias	Title	Lab	Instrument Setups	Delete	Edit
297	Bruker maXis QTOF	Bruker maXis QTOF	Trace Analysis Mass Spectrometry (TrAMS)	7 setups	delete	edit

Bruker maXis QTOF: Instrument setup

View   Results

(1) **Setup information**   (2) Separation settings   (3) Detection settings   (4) Ionization-specific settings   (5) Spiked compounds   (6) Complete

Setup alias

Instrument

Bruker maXis QTOF ⌄

0%

Remarks

Instrument type

LC-ESI-QTOF

Ionization type

- None - ⌄

Save Draft   **Next >**   **Cancel**

Bruker maXis QTOF: Instrument setup

1 Setup information ——— **2** Separation settings ——— **3** Detection settings ——— **4** Ionization-specific settings ——— **5** Spiked compounds ——— **6** Complete

Column Model

🔍

Column Manufacturer

🔍

Reconstitution solvent (solvent in the vial)

🔍

Solvents

⊕ ⊖

Mobile phase

	Time	Solvent A	Solvent B	Solvent C	Solvent D	Flow	Total
1							
2							
3							
4							
5							

Column characteristics

Length of column

Length of column in mm

Internal diamater

Internal diameter in mm

Particle size

Particle size in μm

Injection volume

Value in μL

Temperature

Value in C

20%

Save Draft | < Previous | Next > | Cancel

dev.norman-data.eu/form/instrument-setup?source_entity_type=node&source_entity_id=297&destination=/user/instruments&page=3

Bruker maXis QTOF: Instrument setup

1 — Setup information
2 — Separation settings
3 — Detection settings
4 — Ionization-specific settings
5 — Spiked compounds
6 — Complete

Scan range

From

50

To

1000

Ionization parameters

Collision energy

Ionization (ESI/APCI/APPI)

- None -

Different methods of mass fragmentation

○ CID
○ ECD
○ EDD
○ HCD
○ NETD
○ Other
○ SID

Peak-picking parameters

ppm tolerance

Peakwidth Min

Peakwidth Max

Minimum number of scans

Minimum intensity

Componentization parameters

Expression of mass accuracy

- None - ⌄

Electronic noise cutoff

Accuracy full scan (MS)

40%

Save Draft   < Previous   Next >   Cancel

Bruker maXis QTOF: Instrument setup

RTI Calibrants

60%

	Name	RT	CAS	Formula	Ion
1	Guanylurea	1.33	141-83-3	C2H6N4O	103.06
2	Amitrol	1.39	61-82-5	C2H4N4	85.05
3	Histamine	1.64	51-45-6	C5H9N3	112.09
4	Chlormequat	1.88	999-81-5	C5H13ClN	122.07
5	Methamidophos	2.63	10265-92-6	C2H8NO2PS	142.01
6	Vancomycin	3.19	1404-90-6	C66H75Cl2N9O24	724.72
7	Cefoperazone	4.34	62893-19-0	C25H27N9O8S2	646.15
8	Trichlorfon (Dylox)	5.14	52-68-6	C4H8Cl3O4P	256.93
9	Butocarboxim	5.99	34681-10-2	C7H14N2O2S	191.08
10	Dichlorvos	6.91	62-73-7	C4H7Cl2O4P	220.95
11	Tylosin	7.98	1401-69-0	C46H77NO17	916.53
12	TCMTB	9.21	21564-17-0	C9H6N2S3	238.98
13	Rifaximin	10.03	80621-81-4	C43H51N3O11	786.36
14	Spinosad A (Spinosyn A)	11.53	131929-60-7	C41H65NO10	732.47
15	Emamectin B1a	12.48	121124-29-6	C49H75NO13	886.53
16	Avermectin B1a (Abamectin)	13.67	71751-41-2	C48H72O14	890.53
17	Nigericin	13.91	28380-24-7	C40H68O11	725.48
18	Ivermectin B1a	14.46	70288-86-7	C48H74O14	892.54

Save Draft   < Previous   Next >   Cancel

DSFP

Bruker maXis QTOF: Instrument s... ✕ +

← → C 🔒 dev.norman-data.eu/form/instrument-setup?source_entity_type=node&source_entity_id=297&destination=/user/instruments&page=5

Bruker maXis QTOF: Instrument setup

```
  (1)              (2)               (3)                (4)              (5)              (6)
Setup         Separation         Detection       Ionization-specific   Spiked         Complete
information    settings           settings        settings              compounds
```

Spiked compounds

80%

	Spiked Compound Name	SMILES ↑	Conc units	Response expression	Conc 1	Response 1	Conc 2	Response 2	Conc 3	Response 3	Conc 4	Response 4	Conc 5	Response 5	Conc 6	Respo
1	Benzotriazole (BTR)	c1ccc2c(c1)[nH]nn2	ug/L	Peak Area	25	94301.000	50	177107.000	75	265660.000	100	459322.000	150	530860.000	300	1174
2	Benzothiazole-2-Amino	c1ccc2c(c1)nc(s2)N	ug/L	Peak Area	25	276787.000	50	499565.000	75	749348.000	100	1207429.000	150	1438679.000	300	3081
3	Benzotriazole-5-Me	Cc1ccc2c(c1)[nH]nn2	ug/L	Peak Area	25	116767.000	50	218648.000	75		100	528229.000	150	641686.000	300	1324
4	Benzotriazole-5,6-di-Me	Cc1ccc2c(c1)[nH]nn2	ug/L	Peak Area	25	85291.000	50	159265.000	75		100	388938.000	150	456477.000	300	970
5	Benzotriazole-1-Methyl	Cn1c2ccccc2nn1	ug/L	Peak Area	25	138969.000	50	268138.000	75		100	702812.000	150	913133.000	300	1751

Save Draft   < Previous   Submit   Cancel

dev.norman-data.eu/user/collections

DSFP

Home > User area

Back to site

My collections

A collection is a group of samples gathered during a sampling campaign or during a project. You are requested to provide:

- A title and a short description for the collection,
- The desired access level of the dataset,
- The location and date of the collected samples,
- The mzML data.

+ Add a collection

ID	Title	Status	Samples	Edit	Delete
348	JDS4	Published	0 samples	edit	delete
333	LIFE APEX	Published	20 samples	edit	

Home > Node > Add Content > Data

← Back to site

Create Collection

[Save]

Metadata *   Resources

Title *
Short and concise title of the project (e.g. JDS4, ANSWER, SOLUTIONS)

Description *
Description with sufficient detail to enable a user to quickly understand whether the contribution is of interest.

Public Access Level *
This refers to how the data can be accessed.

public ▾

Frequency
Frequency with which dataset is updated on the DSFP online platform. Defaults to one year.

Annual ▾

Release Date

mm/dd/yyyy   --:--:-- -- 🕐

Date of formal issuance.

Last Update *

mm/dd/yyyy   --:--:-- -- 🕐

Most recent date on which the dataset was changed, updated or modified.

License
The license dataset or API is published with. See Open Licenses for more information.

- None - ▾

Relevant Location
If your dataset has a spatial component, please provide location such as place name or latitude/longitude pairs.

Temporal Information

Start date
mm/dd/yyyy 📅   --:--:-- -- 🕐

End date
mm/dd/yyyy 📅   --:--:-- -- 🕐

The start and end dates for which the dataset is applicable.

∨ Organization

∨ Contact details

Matrix

Matrix

- None -

The matrix of the collected data. This will be auto-populated with the matrices reported in your submitted samples.

Keywords

Tag *

- Select -

Supporting materials

○ Upload Data File   ○ Link to Data File

[Add one more]

Supporting materials such as technical information about the instruments, relevant publications etc.

DSFP

Home > User area

My collections

A collection is a group of samp
project. You are requested to pr

- A title and a short descriptic
- The desired access level of t
- The location and date of the
- The mzML data.

+ Add a collection

ID	Title		Delete
348	JDS4		delete
333	LIFE APEX		

Samples   ✕

Back to site

+ Add a sample

Short name for contribution	Cities	Country	Matrix	Instrument setup used	Edit	Delete	Duplicate
LIFE APEX 01 Bream muscle from Danube Jochenstein	• Jochenstein		Environmental monitoring (Biota)	Bruker maXis QTOF: Submission #10	edit	delete	duplicate
LIFE APEX 02 Bream muscle from Elbe	• Wittenberge	Germany	Environmental monitoring (Biota)	Bruker maXis QTOF: Submission #10	edit	delete	duplicate
LIFE APEX 03 Bream muscle from Rhine Bimmen	• Emmerich	Germany	Environmental monitoring (Biota)	Bruker maXis QTOF: Submission #10	edit	delete	duplicate
LIFE APEX 04 Bream muscle from Belauer See	• Neumunster	Germany	Environmental monitoring (Biota)	Bruker maXis QTOF: Submission #10	edit	delete	duplicate
LIFE APEX 05 Bream muscle from Saar Gudingen	• Saarbrucken	Germany	Environmental monitoring (Biota)	Bruker maXis QTOF: Submission #10	edit	delete	duplicate

DSFP

LIFE APEX: Sample

```
  1 ———————————— 2 ———————————— 3 ———————————— 4
Metadata          Matrix           Files          Complete
```

0%

Metadata

Collection

LIFE APEX   ⌄

Sample type

- None -   ⌄

Short name for contribution

Sampling date

mm/dd/yyyy 📅   --:-- -- 🕐

Analysis date

mm/dd/yyyy 📅   --:-- -- 🕐

Instrument setup used

| Bruker maXis QTOF - Setup #1 | Bruker maXis QTOF - Another example of a setup | Bruker maXis QTOF - LC Positive maXis QTOF |

| Bruker maXis QTOF - Setup test #2.1 |

Monitoring scale

| 0 | 1 | 2 | 3 |

Admin level of the area monitored (0 = country/region/sovereignty, 1=province/state/dependency, 2 = county/commune/municipality, 3=city/town/village/settlement)

Latitude

37.9736144

Longitude

23.775171

⬤ Locate on map

[Save Draft] [Next >] [Cancel]

LIFE APEX: Sample

33%

Matrix

Environmental monitoring	Human biomonitoring	Foodomics

| Surface water | Groundwater | Wastewater | Biota | Sediment | Sludge | Soil | SPM | Indoor Air | Ambient Air | Workplace Air | Emission Air |

Groundwater fraction

- None -

River basin name

Proxy pressures

- None -

Type of sampling depth

- None -

Depth (m)

pH

Temperature (°C)

Dissolved organic carbon (mg/L)

Save Draft   < Previous   Next >   Cancel

LIFE APEX: Sample

①————————②————————③————————④
Metadata   Matrix   **Files**   Complete

67%

Sample Files

⌃ Full scan

File upload

Drop files here to upload them

or

[Select files]

One file only.
1 GB limit.
Allowed types: mzml.

⌃ Data-dependent

File upload

Drop files here to upload them

or

[Select files]

One file only.
1 GB limit.
Allowed types: mzml.

⌃ Data-independent

◯ I have files per collision channel

File upload

Drop files here to upload them

or

[Select files]

One file only.
1 GB limit.
Allowed types: mzml.

[Save Draft] [< Previous] [Submit] [Cancel]

Digital Sample Freezing Platform

Home   Contributors   About

Welcome to DSFP

DSFP was created to host liquid chromatography-high resolution-mass spectrometry (LC-HRMS) and gas chromatography-high resolution-mass spectrometry (GC-HRMS) data.

[   ]   **Go**

Welcome to the Digital Sample Freezing Platform (DSFP)! The DSFP hosts liquid chromatography-high resolution-mass spectrometry (LC-HRMS) and gas chromatography-high resolution-mass spectrometry (GC-HRMS) data from various contributing organisations. The DSFP enables retrospective suspect screening of chemicals making use of the NORMAN Database System. It seeks to foster and benefit from the synergies between research teams across the globe. Researchers and research groups interested in the study of chemicals in the environment, food, and human biomonitoring are welcome to contribute and employ their digitally frozen data on DSFP!

   👤 User area

🔍 **LIFE APEX DSFP Demo - Google Search**

google.com/search?q=LIFE+APEX+DSFP&rlz=1C1CHBD_enGR948GR948&sxsrf=APq-WBt98NAFpTCl-ccbKSGcguM7j3CDZA%3A16509207365

Google   LIFE APEX DSFP ✕ 🎤 🔍

🔍 All   🖼 Images   📍 Maps   ◎ Shopping   ▶ Videos   ⋮ More   Tools

About 15,200 results (0.47 seconds)

https://dev.norman-data.eu › dataset ⋮

LIFE APEX - Dataset - DSFP Demo

7 days ago — **DSFP** was created to host liquid chromatography-high resolution-mass spectrometry (LC-HRMS) and ... This is the **LIFE APEX** tier 1 collection.

People also search for		✕
norm database	ecotox database	
empodat	norman sle	
norman susdat	massbank	

Antibiotic Resistance Bacteria/Genes
NORMAN Massbank

Near future plans – Integration of search mode

Near future plans – Upload of existing samples

Sept 2021

https://norman-data.eu/Verification_MAP

Near future plans – Upload of existing samples

Antarctica
CONnECT
UBA-HELCOM
LIFE APEX
Dnieper
DIANYA wastewater
White-tailed sea eagle
Ferrets
Black-tailed godwit
Raptor eggs
Peregrine falcon

https://norman-data.eu/Verification_MAP

Near future plans – Integration of suspect screening prioritization

Near future plans – Integration of suspect screening prioritization

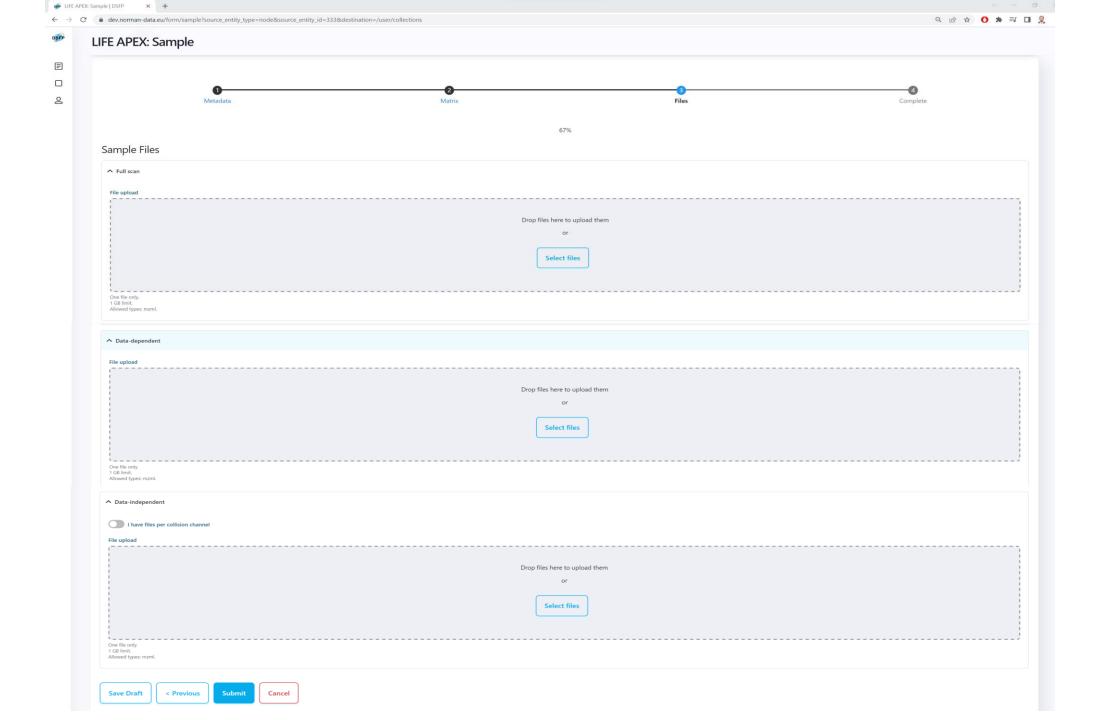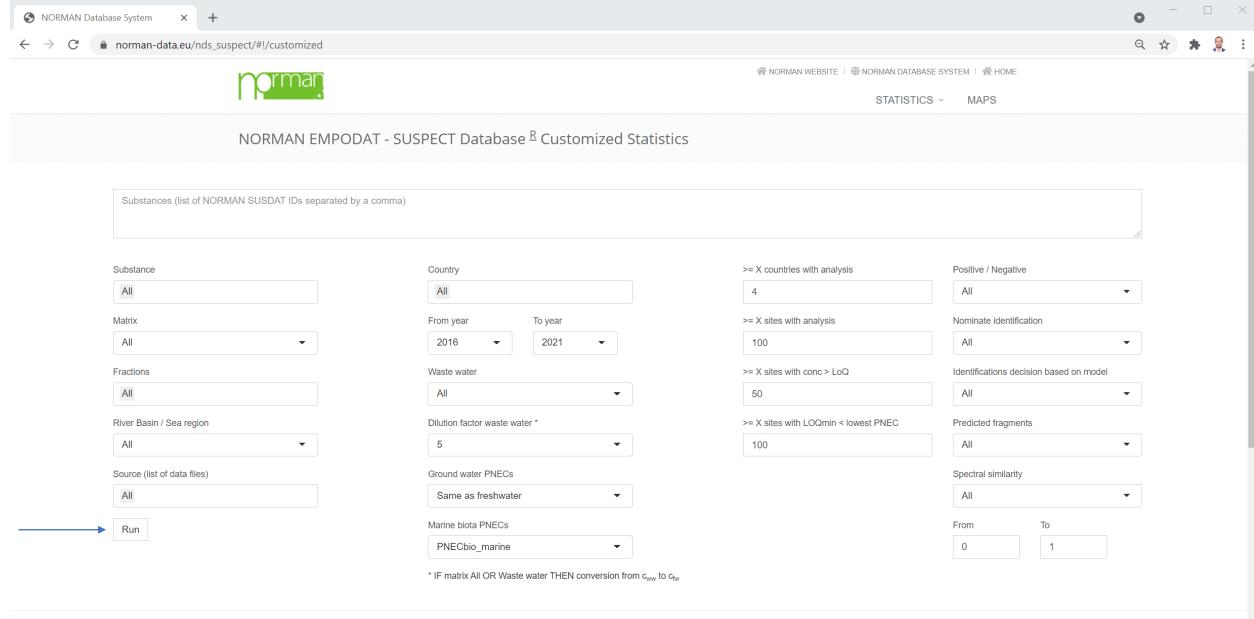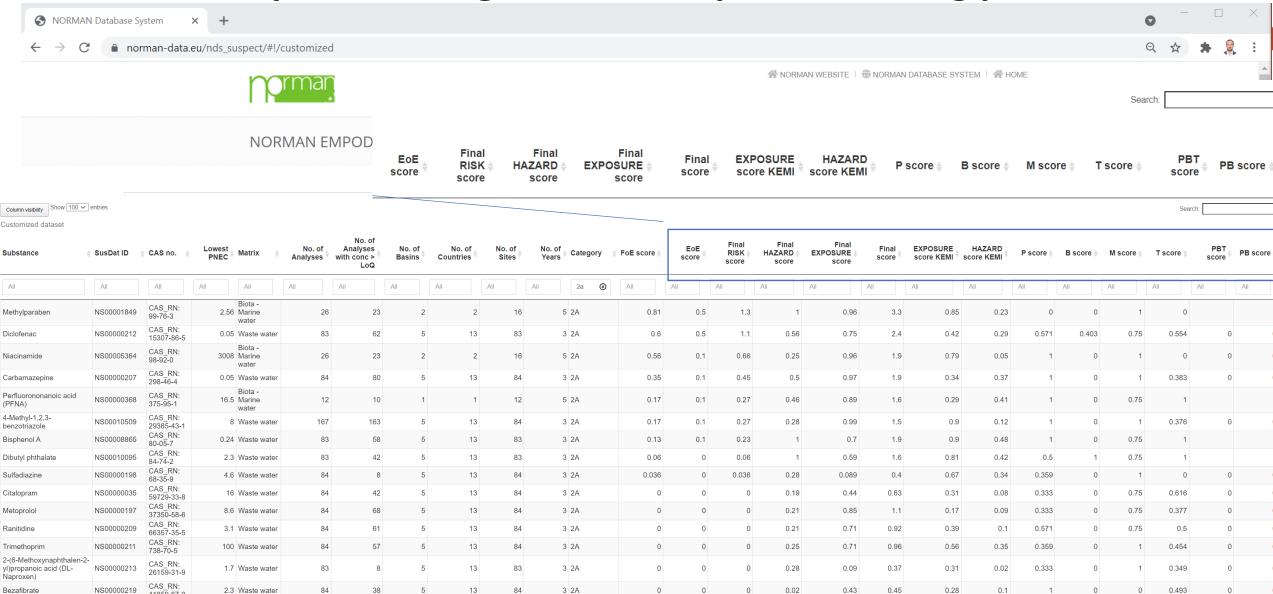| Substance	SusDat ID	CAS no.	Lowest PNEC	Matrix	No. of Analyses	No. of Analyses with conc > LoQ	No. of Basins	No. of Countries	No. of Sites	No. of Years	Category	FoE score	EoE score	Final RISK score	Final HAZARD score	Final EXPOSURE score	Final score	EXPOSURE score KEMI	HAZARD score KEMI	P score	B score	M score	T score	PBT score	PB score
Methylparaben	NS00001849	CAS_RN: 99-76-3	2.56	Biota - Marine water	26	23	2	2	16	5	2A	0.81	0.5	1.3	1	0.96	3.3	0.85	0.23	0		1	0		
Diclofenac	NS00000212	CAS_RN: 15307-86-5	0.05	Waste water	83	62	5	13	83	3	2A	0.6	0.5	1.1	0.56	0.75	2.4	0.42	0.29	0.571	0.403	0.75	0.554	0	
Niacinamide	NS00005364	CAS_RN: 98-92-0	3008	Biota - Marine water	26	23	2	2	16	5	2A	0.56	0.1	0.66	0.25	0.96	1.9	0.79	0.05	1		1	0	0	
Carbamazepine	NS00000207	CAS_RN: 298-46-4	0.05	Waste water	84	80	5	13	84	3	2A	0.35	0.1	0.45	0.5	0.97	1.9	0.34	0.37	1		1	0.383	0	
Perfluorononanoic acid (PFNA)	NS00000368	CAS_RN: 375-95-1	16.5	Biota - Marine water	12	10	1	2	12	5	2A	0.17	0.1	0.27	0.46	0.89	1.6	0.29	0.41		0.75		1		
4-Methyl-1,2,3-benzotriazole	NS00010509	CAS_RN: 29385-43-1	8	Waste water	167	163	5	13	84	3	2A	0.17	0.1	0.27	0.28	0.99	1.5	0.9	0.12	1		1	0.376	0	
Bisphenol A	NS00008865	CAS_RN: 80-05-7	0.24	Waste water	83	58	5	13	83	3	2A	0.13	0.1	0.23	1	0.7	1.9	0.9	0.48	1		0.75		0	
Dibutyl phthalate	NS00010095	CAS_RN: 84-74-2	2.3	Waste water	83	42	5	13	83	3	2A	0.06	0	0.06	1	0.59	1.6	0.81	0.42	0.5	1	0.75		1	
Sulfadiazine	NS00000198	CAS_RN: 68-35-9	4.6	Waste water	84	8	5	13	84	3	2A	0.036	0	0.036	0.28	0.089	0.4	0.67	0.34	0.359		1	0	0	
Citalopram	NS00000035	CAS_RN: 59729-33-8	16	Waste water	84	42	5	13	84	3	2A	0	0	0.19	0.44	0.63	0.31	0.08	0.333		0.75	0.616	0		
Metoprolol	NS00000197	CAS_RN: 37350-58-6	8.6	Waste water	84	68	5	13	84	3	2A	0	0	0.21	0.85	1.1	0.17	0.09	0.333		0.75	0.377	0		
Ranitidine	NS00000209	CAS_RN: 66357-35-5	3.1	Waste water	84	61	5	13	84	3	2A	0	0	0.21	0.71	0.92	0.39	0.1	0.571		0.75	0.5	0		
Trimethoprim	NS00000211	CAS_RN: 738-70-5	100	Waste water	84	57	5	13	84	3	2A	0	0	0.25	0.71	0.96	0.56	0.35	0.359		1	0.454	0		
2-(6-Methoxynaphthalen-2-yl)propanoic acid (DL-Naproxen)	NS00000213	CAS_RN: 26159-31-9	1.7	Waste water	83	8	5	13	83	3	2A	0	0	0.28	0.09	0.37	0.31	0.02	0.333		1	0.349	0		
Bezafibrate	NS00000219	CAS_RN: 41859-67-0	2.3	Waste water	84	38	5	13	84	3	2A	0	0	0.02	0.43	0.45	0.28	0.1	1		0	0.493	0		

List of indicators and cut-off values applied for the allocation of the candidate substances to action categories 1 to 6 (PDF format)
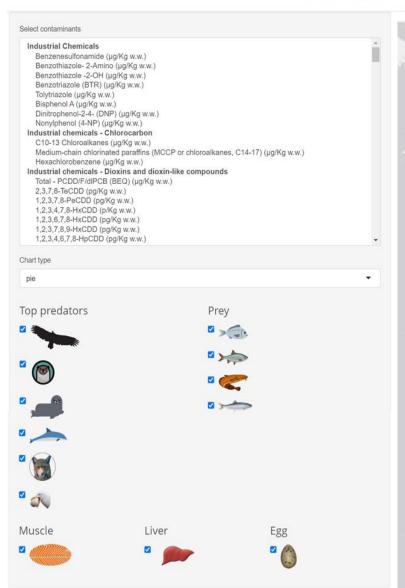
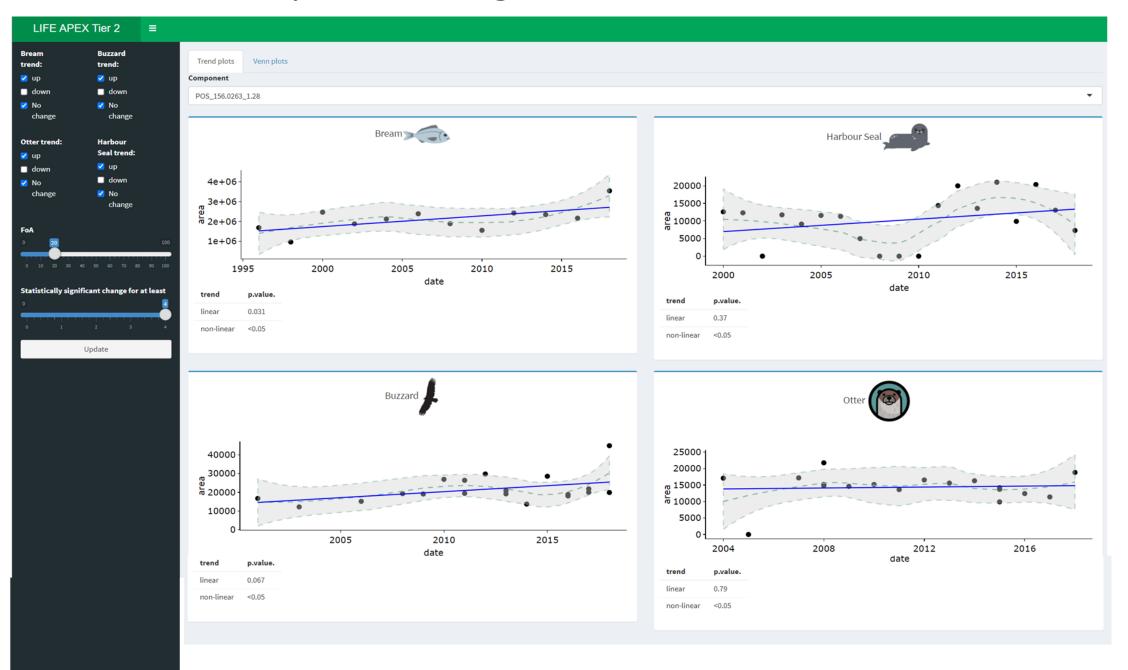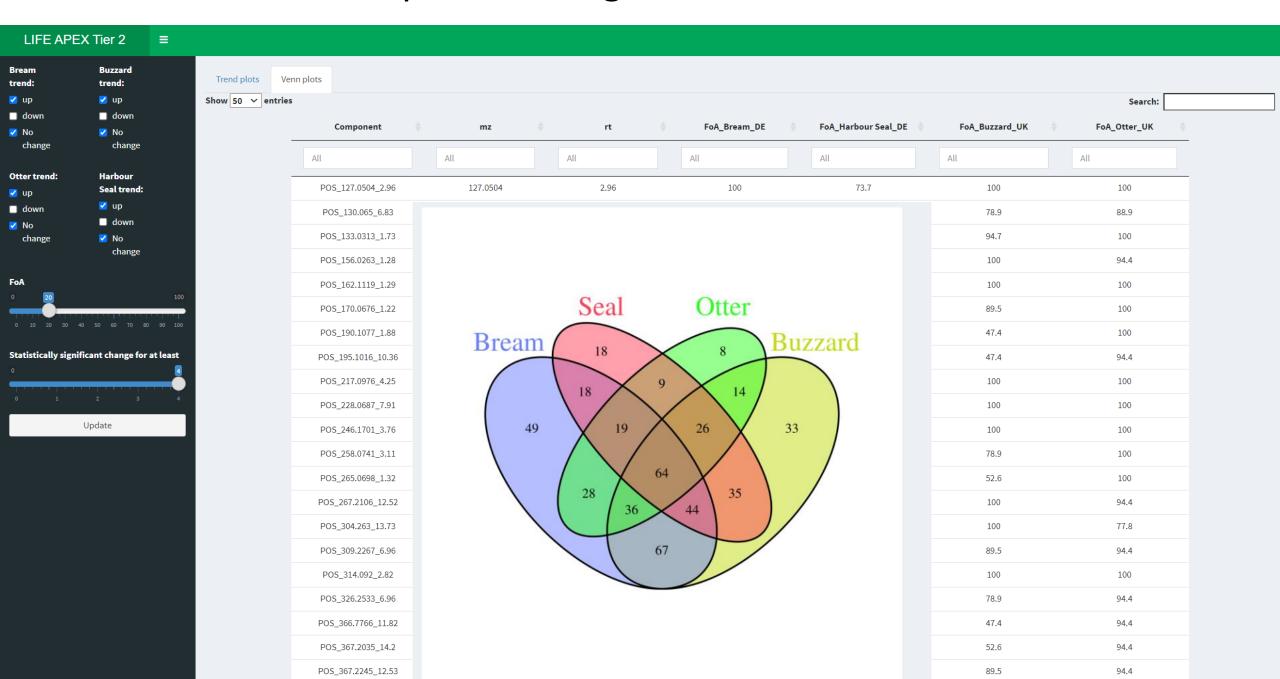# Near future plans – Integration of visualization tools

LIFE APEX samples (198) – Results of target analyses (116 substances) and wide-scope target screening (2,316 substances) of chemical contaminants in top predators and their prey (in µg/Kg w.w. unless otherwise stated)

Shown only concentrations above LOQ

Select contaminants

Industrial Chemicals
Benzenesulfonamide (µg/Kg w.w.)
Benzothiazole- 2-Amino (µg/Kg w.w.)
Benzothiazole -2-OH (µg/Kg w.w.)
Benzotriazole (BTR) (µg/Kg w.w.)
Tolytriazole (µg/Kg w.w.)
Bisphenol A (µg/Kg w.w.)
Dinitrophenol-2-4- (DNP) (µg/Kg w.w.)
Nonylphenol (4-NP) (µg/Kg w.w.)
Industrial chemicals - Chlorocarbon
C10-13 Chloroalkanes (µg/Kg w.w.)
Medium-chain chlorinated paraffins (MCCP or chloroalkanes, C14-17) (µg/Kg w.w.)
Hexachlorobenzene (µg/Kg w.w.)
Industrial chemicals - Dioxins and dioxin-like compounds
Total - PCDD/F/dlPCB (BEQ) (µg/Kg w.w.)
2,3,7,8-TeCDD (pg/Kg w.w.)
1,2,3,7,8-PeCDD (pg/Kg w.w.)
1,2,3,4,7,8-HxCDD (p/Kg w.w.)
1,2,3,6,7,8-HxCDD (pg/Kg w.w.)
1,2,3,7,8,9-HxCDD (pg/Kg w.w.)
1,2,3,4,6,7,8-HpCDD (pg/Kg w.w.)

Chart type

pie

Top predators

Prey

Muscle

Liver

Egg

1996-02

Near future plans – Integration of visualization tools

Near future plans – Integration of visualization tools

LIFE APEX Tier 2 ☰

Bream trend:
- ☑ up
- ☐ down
- ☑ No change

Buzzard trend:
- ☑ up
- ☐ down
- ☑ No change

Otter trend:
- ☑ up
- ☐ down
- ☑ No change

Harbour Seal trend:
- ☑ up
- ☐ down
- ☑ No change

FoA
0 — 20 — 100
0 10 20 30 40 50 60 70 80 90 100

Statistically significant change for at least
0 — 4
0 1 2 3 4

Update

Trend plots | Venn plots

Show 50 entries   Search: [   ]

Component	mz	rt	FoA_Bream_DE	FoA_Harbour Seal_DE	FoA_Buzzard_UK	FoA_Otter_UK
All	All	All	All	All	All	All
POS_127.0504_2.96	127.0504	2.96	100	73.7	100	100
POS_130.065_6.83					78.9	88.9
POS_133.0313_1.73					94.7	100
POS_156.0263_1.28					100	94.4
POS_162.1119_1.29					100	100
POS_170.0676_1.22					89.5	100
POS_190.1077_1.88					47.4	100
POS_195.1016_10.36					47.4	94.4
POS_217.0976_4.25					100	100
POS_228.0687_7.91					100	100
POS_246.1701_3.76					100	100
POS_258.0741_3.11					78.9	100
POS_265.0698_1.32					52.6	100
POS_267.2106_12.52					100	94.4
POS_304.263_13.73					100	77.8
POS_309.2267_6.96					89.5	94.4
POS_314.092_2.82					100	100
POS_326.2533_6.96					78.9	94.4
POS_366.7766_11.82					47.4	94.4
POS_367.2035_14.2					52.6	94.4
POS_367.2245_12.53					89.5	94.4

Venn diagram:
Bream, Seal, Otter, Buzzard
18, 8, 9, 14, 18, 19, 26, 33, 49, 28, 64, 35, 36, 44, 67

Near future plans – Integration of visualization tools

Why to use NDS and DSFP

- Keeps your HRMS data well-organized

- Helps to comply with FAIR rules, which is mandatory for EU projects

- Helps to gain useful insights from automated visualization and statistical tools

- Make the data available to the scientific community and stimulates cooperation among researchers

- Enables wide-scope suspect screening with possibility to perform retrospective screening

- Gain visibility within DSFP (contributors area), in Google (results are indexed) and in academia (each collection will receive DOI in the future)

- Support the effort to collect a critical amount of data which is needed in regulatory frameworks

- DSFP to act as a safety-net and early warning system for chemicals in Europe and beyond (connection with PARC)

- Create your own DSFP account today (**dev.norman-data.eu**)!

Thank you for your attention!

Nikiforos Alygizakis

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@nikiforosgr

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