Application of digital-archiving of HRMS chromatograms by Digital Sample Freezing Platform

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Meeting with ICPDR

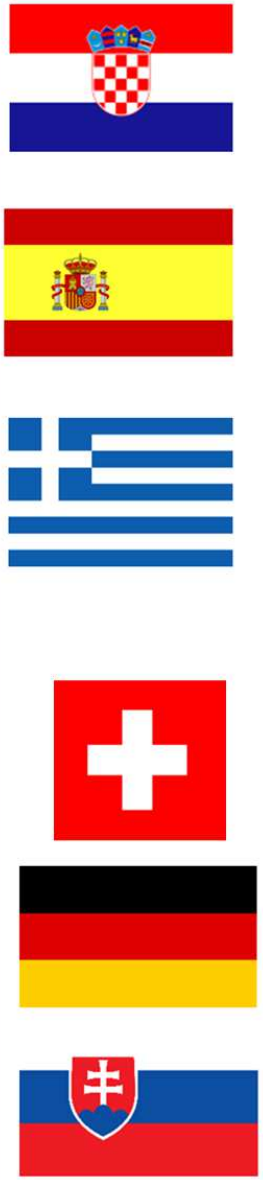
France, 07 Sept 2018

Contents

- Introduction
- Background Information
- Description of NTS DCT
- How to upload chromatograms to DSFP
- Description of DSFP (Single search & Batch-mode module)
- Applications
- Conclusions

Introduction

Environmental Samples (e.g. Wastewater from WWTPs, Danube River samples)



Digital Freezing of Samples

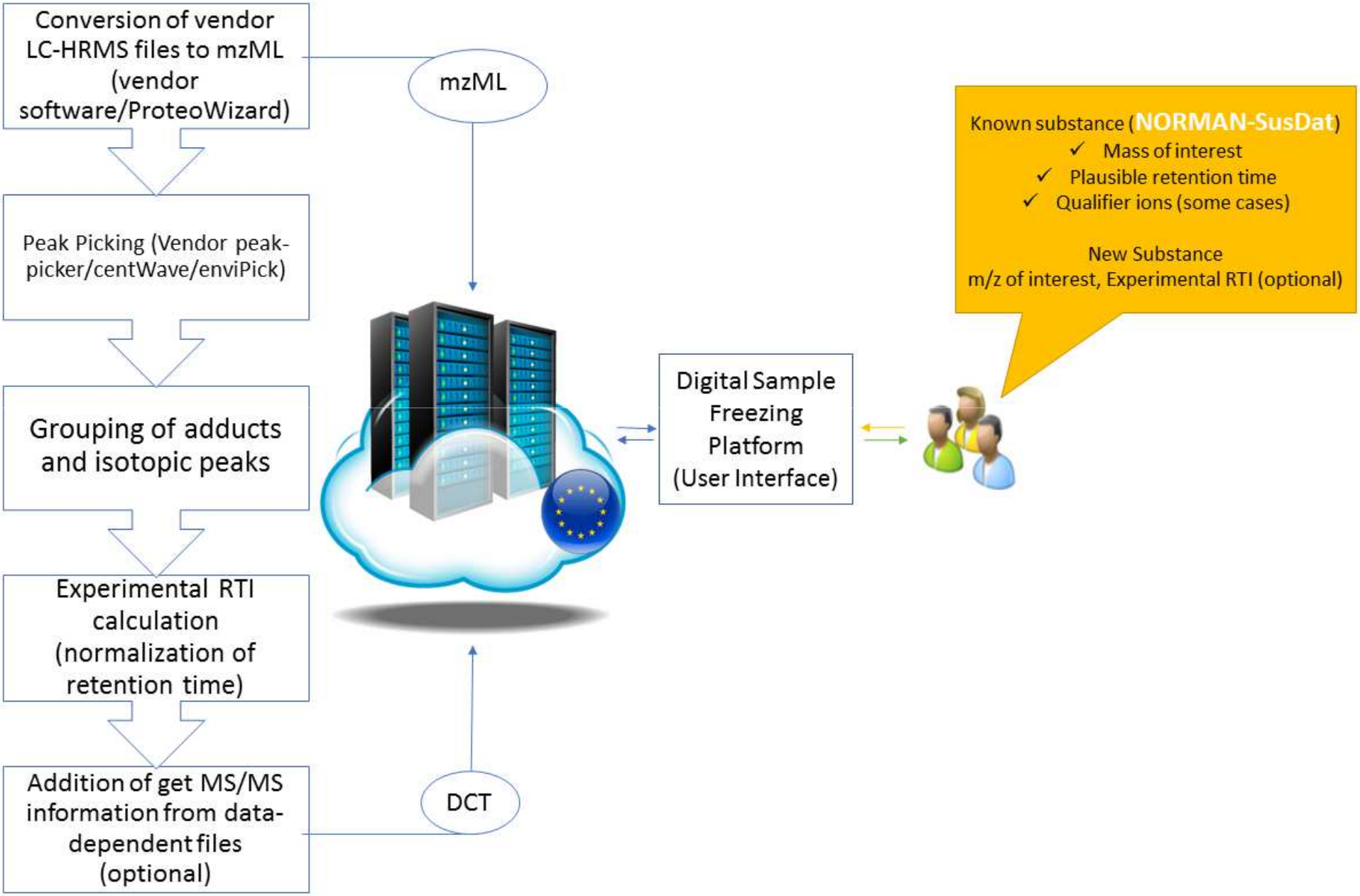
Design of platform accessible to everyone (Go-back-in-time capabilities)

normanEWS

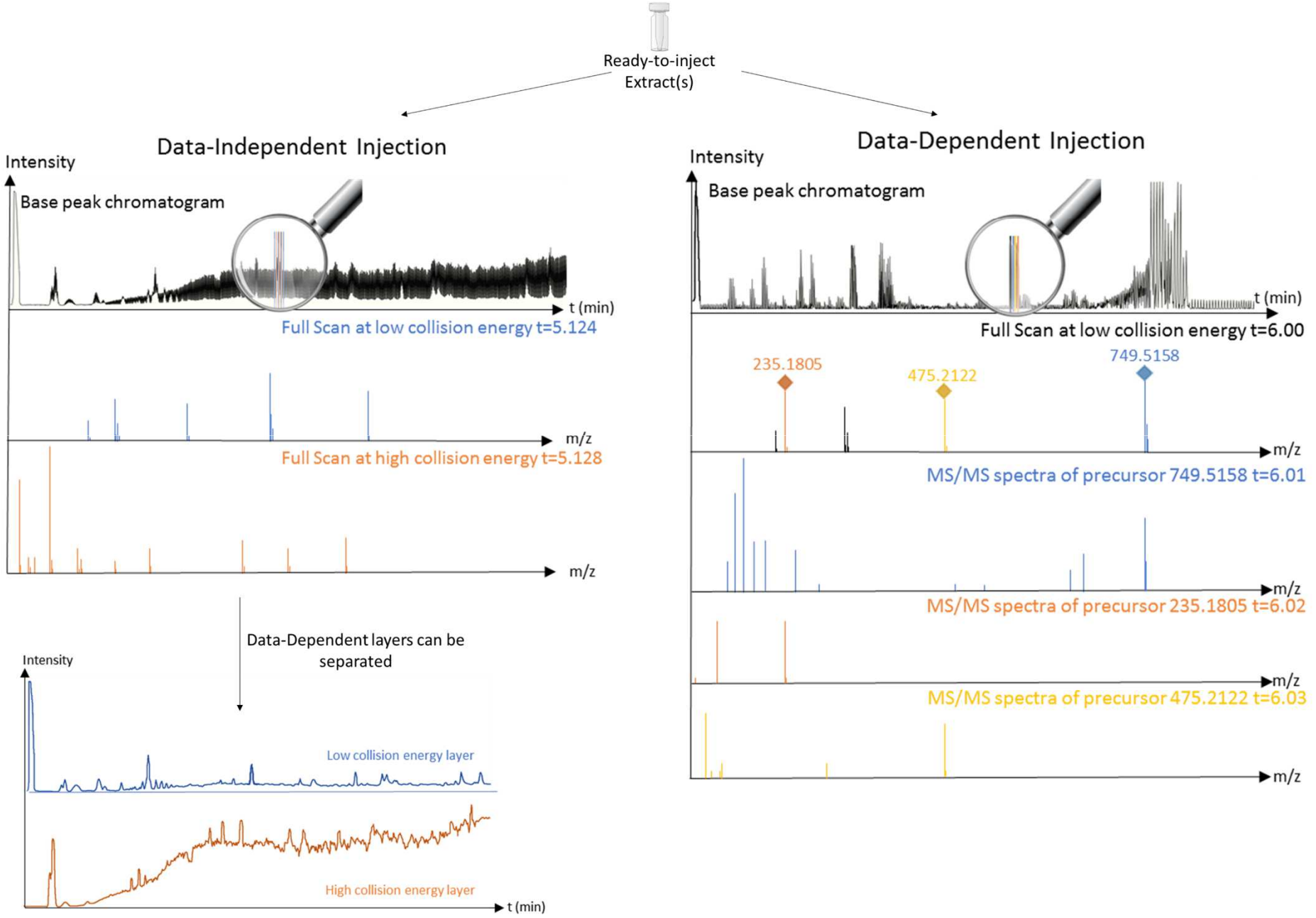
Small scale testing of digital freezing

Alygizakis et al., ES&T, 2018

Introduction



Background Information



Background Information

Full scan Positive

Full scan Negative

Data Independent Positive

Data Independent Negative

Data-Dependent 5 precursors Positive

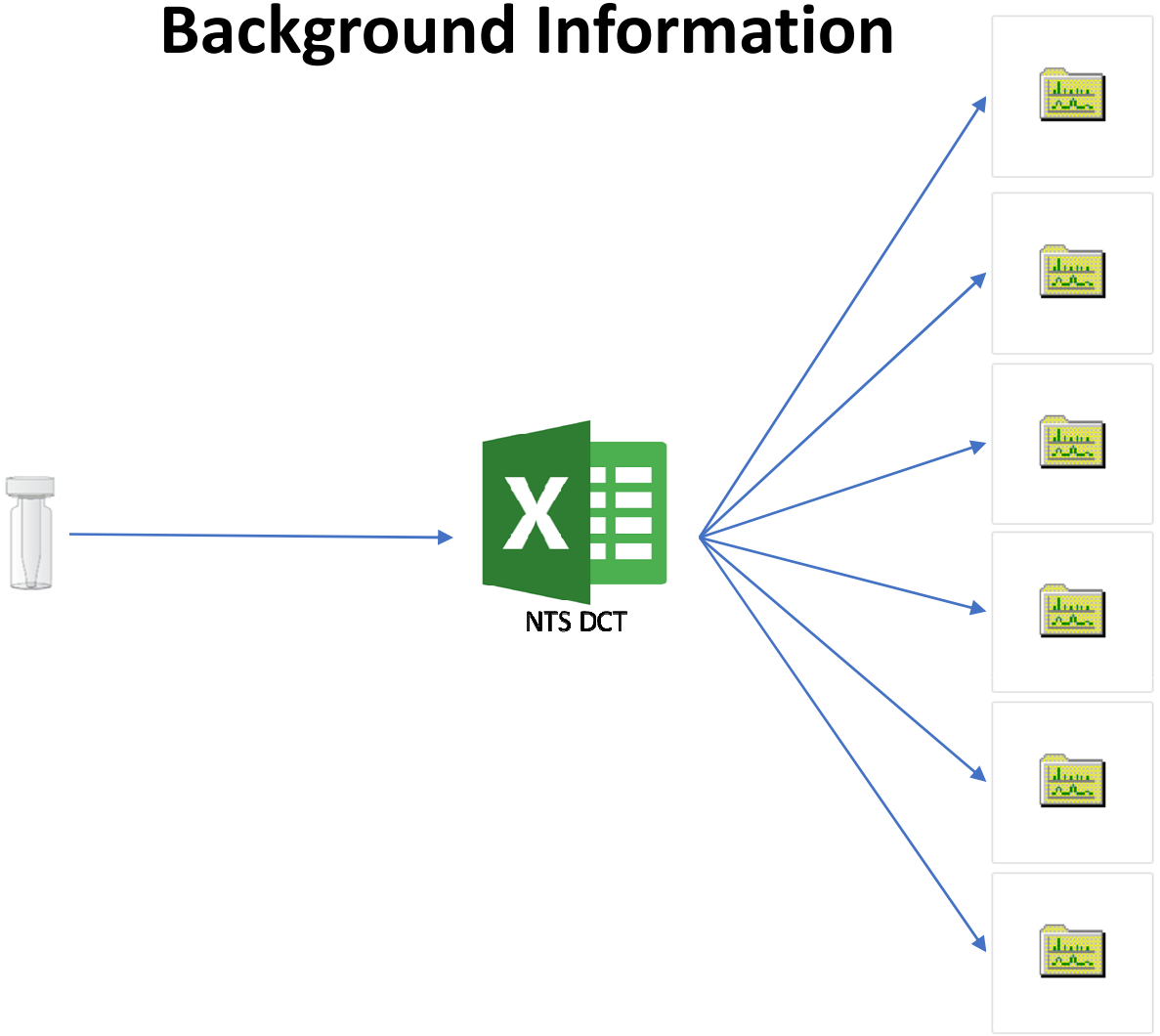
Data-Dependent 5 precursors Negative

NTS DCT

Size: Few GB-hundreds MB

Size: Few MB

Background Information



1 environmental sample → 1 Excel-based DCT → Multiple chromatograms

Description of NTS DCT

Description of NTS DCT

NTS DCT

Who is contributing the sample?

ORGANISATION DETAILS		
Organisation	Name:	Environmental Institute
	City:	Koš
	Country:	Slovakia
Laboratory performing the analysis	Name:	Environmental Institute
	City:	Koš
	Country:	Slovakia
Contact person	Family name:	Slobodnik
	First name(s):	Jaroslav
	E-mail:	slobodnik@ei.sk
	Phone:	00421915799688

For Retention time prediction

Positive Ionization

Substance name	CAS number	SMILES	Mol. Formula	$[M+H]^+$	Retention time (min)
Guanylurea	141-83-3	C(=NC(=O)N)(N)N	C2H6N4O	103.0614	1.344
Amitrol	61-82-5	Nc1nnc[nH]1	C2H4N4	85.0509	1.411
Histamine	51-45-6	c1c([nH]cn1)CCN	C5H9N3	112.0869	1.694
Chlormequat*	999-81-5	C[N+](C)(C)CCCl	C5H13ClN	122.0731	#N/A
Methamidophos	10265-92-6	COP(=O)(N)SC	C2H8NO2PS	142.0086	2.694
Vancomycin*	1404-90-6	[C(=O)N[C@H]5C(=O)N[C@@H]7c8ccc(c(c8	C66H75Cl2N9O24	724.7224	3.178
Cefoperazone	62893-19-0	2NC(=O)[C@H](c3ccc(O)cc3)NC(=O)N4C(=O	C25H27N9O8S2	646.1497	4.378
Trichlorfon (Dylox)	52-68-6	COP(=O)(C(C(Cl)(Cl)Cl)O)OC	C4H8Cl3O4P	256.9299	5.212
Butocarboxim	34681-10-2	CC(C(=NOC(=O)NC)C)SC	C7H14N2O2S	191.0849	6.062
Dichlorvos	62-73-7	COP(=O)(OC)OC=C(Cl)Cl	C4H7Cl2O4P	220.9532	7.012
Tylosin	1401-69-0	[C@H]([C@@H]([C@H](O2)C)O[C@H]3C[C	C46H77NO17	916.5264	7.829
TCMTB	21564-17-0	c1ccc2c(c1)nc(s2)SCSC#N	C9H6N2S3	238.9766	9.312
Rifaximin	80621-81-4	C/[C@@H]([C@H]([C@H]([C@@H]([C@@H	C43H51N3O11	786.3596	9.995
Spinosad A (Spinosyn A)	131929-60-7	@H]3[C@@H]2CC(=O)O1)O[C@H]5[C@@H	C41H65NO10	732.4681	11.379
Emamectin B1a	121124-29-6	H]5[C@@]4([C@@H](C=C([C@H]5O)C)C(=(	C49H75NO13	886.5311	12.429
Avermectin B1a***	71751-41-2	@H]5[C@@]4([C@@H](C=C([C@H]5O)C)C(	C48H72O14	890.5260	13.762
Nigericin	28380-24-7	@@H](C[C@@](O3)(C)[C@H]4CC[C@@](	C40H68O11	725.4834	13.845
Ivermectin B1a****	70288-86-7	@H]5[C@@]4([C@@H](C=C([C@H]5O)C)C(=	C48H74O14	892.5417	14.562

RTI mixture

Sample meta-data

Sample indentification	COUNTRY		SAMPLING SITE / STATION														DATA SOURCE				
	Name of country	Name of other country	Station name and codes				Longitude					Latitude					Precision of coordinates	Type of data source	Type of monitoring		Title of project
			Name	National code	Relevant EC code - WISE	Relevant EC code - Other	East / West	°	`	``	Decimal	North / South	°	`	``	Decimal				Other	
wastewater Stuttgart Muhlhausen	Germany		wastewater Stuttgart Mul	DEU			E	9	13	28.3296	ast/West	N	48	50	35.772	rth/Sout	Average (range 10-100 m)	Surveys	Investigative		ITN ANSWER
x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

Instrumental method meta-data

												Mass spectrometer		
Serial No.	Method name (TARGET 1/2/... – substance information; SUSPECT 1/2/...; NON-TARGET 1/2/...; UNKNOWN 1/2...)	Instrument manufacturer	Model type and number	Analytical column	Column dimensions [mm; mm; µm]	Solvent used for sample reconstitution	Injection volume	Column temperature	Composition of the mobile phase	Mobile phase gradient programme	Mobile phase flow rate [mL/min]	Scan range from - to [m/z]	SIM	SRM
					Length; I.D.; particle size		[µl]	[°C]					m/z	m/z
EXAMPLE	EXAMPLE		EXAMPLE		EXAMPLE		EXAMPLE		EXAMPLE		EXAMPLE			EXAMPLE
LC000	TARGET1_Acesulfame	Thermo Fisher Scienti	LTQ Orbitrap XL	Waters Xbridge (	50; 2.1; 3.5	Methanol/Water 10/90	20	30	A=water+0.1%	0 %B(0);100% over 17m	0.2	100-1000		
YOUR DATA		YOUR DATA		YOUR DATA		YOUR DATA		YOUR DATA		YOUR DATA				YOUR DATA
LC001	All_Ions_MS_positive.m	Agilent	Q-TOF 6550 iFunne	Eclipse PLUS C18	100;2.1;1.8	Methanol/Water 10/90	50	50	mmonium acet	0);100% over 17min;100	0.4	50-1000		

Description of NTS DCT

Sample mass spectral information (MS1 information)

Sample identification (link to the raw data file name)	Retention time in the 1st column [min]	Retention time in the 2nd column [sec]	Mass of ion [m/z] (peak or component)	Intensity of the ion	Intensity of the ion in the blank	Ion type	Other	MS/MS available	Category	Proposed identification (name of the substance or n.i. for not identified)	Molecular formula	Exact. Mass
	EXAMPLE		EXAMPLE		EXAMPLE				EXAMPLE		EXAMPLE	
ElbeSW01	4.64		216.1012	1666665	0	M+		Yes	Target	atrazine	C8H14Cl1N5	
DanubeSED01	16.64		243	14222	0	Other	Base	No	Unknown	n.i.	n/a	
YOUR DATA			YOUR DATA		YOUR DATA				YOUR DATA		YOUR DATA	

Identifier: SMILES	CAS No.	Estimated concentration [ug/l]	Level of confirmation of identification	Component information	Fragment masses of detected compounds	Retention Time index LC-MS (UoA approach)	Date of sampling (DD/MM/YYYY)	Date of analysis (DD/MM/YYYY)	Serial No. in Method LC-MS(MS) or GC-MS(MS) worksheet
EXAMPLE		EXAMPLE	EXAMPLE			EXAMPLE			EXAMPLE
c1(nc(nc(n1)Cl)NCC)NC(C)C	1912-24-9	0.25	reference standard, ratio of MS/MS				12/12/2013	12/13/2013	LC001, LC002, GC001
n/a	n/a	0.15	characteristic pattern at ion 243 shows presence of chlorine atom	245.0322 25.3, 258.3405 32.5, 260.0665 60.0		1954.19	12/12/2013	12/13/2013	GC001
YOUR DATA		YOUR DATA		YOUR DATA			YOUR DATA		YOUR DAT

LC-MS - files attached				GC-MS - files attached
Raw chromatogram; Positive/Negative mode; MS-MS... (Organization abbreviation_Ionization mode [POS/NEG]_Collision Energy in eV or %_ Instrument_ Matrix_Sampling Site_Country_Date of Sampling [DD.MM.YYYY]_ Project abbreviation_Unique Sample ID.mzML)				Raw chromatogram; EI/PCI/NCI; MS/MS... (mzML) (Organization abbreviation_Ionization mode [POS/NEG]_Collision Energy in eV or %_ Instrument_ Matrix_Sampling Site_Country_Date of Sampling [DD.MM.YYYY]_ Project abbreviation_Unique Sample ID.mzML)
No. of peaks	Intensity cut-off value	Data analysis report (mzML)	Data aquisition	
10,021	0	UFZ_POS_4eV_LC-ESI-Orbitrap-MS_Elbe_Leipzig_Germany_NoProject_01.01.2014.mzML	Auto MS/MS 5 the most abundant precursors per scan	
			MRM	EI_POS_70eV_GC-EI-MS_Danube_Bratislava_Slovakia_JDS3_01.02.2014.mzML

Description of NTS DCT

NTS DCT

Sample mass spectral information (MS/MS information)

Mass of ion [m/z]	Retention time [min]	Intensity of the ion	File
88.11185	0.319	6116	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
74.09629	0.319	15452	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
270.97746	0.319	5356	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
216.99223	0.802	2948	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
157.01292	0.869	1896	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
193.12252	0.886	1736	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
128.06199	0.369	1500	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML
129.01806	0.936	3512	EI_POS_25_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.mzML

Spiked compounds information (SemiQuantification)

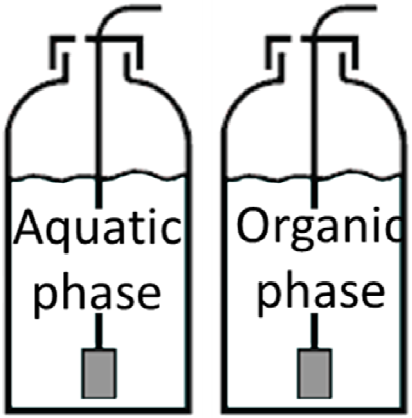
Spiked Compound Name	SMILES	Concentation level units	Response expression [Peak Area or Maximum Intensity]	Concentation level 1	Response at concentration level 1	Concentation level 2	Response at concentration level 2	Concentation level 3	Response at concentration level 3	Concentation level 4	Response at concentration level 4
Example							Example				
Clarithromycin	)C)O[C@H]2C[C@(	ng/L	Peak Area	12.5	12526	25.0	27536	50.0	55456	75.0	78985
Ciprofloxacin	CCNCC3)n(cc(c2=C	ng/L	Peak Area	18	2562	45	12365	150	102568	NA	NA
YOUR DATA							YOUR DATA				

How to upload chromatograms to DSFP

How to upload chromatograms to DSFP

Ready-to-inject Extract(s)

RTI mixture

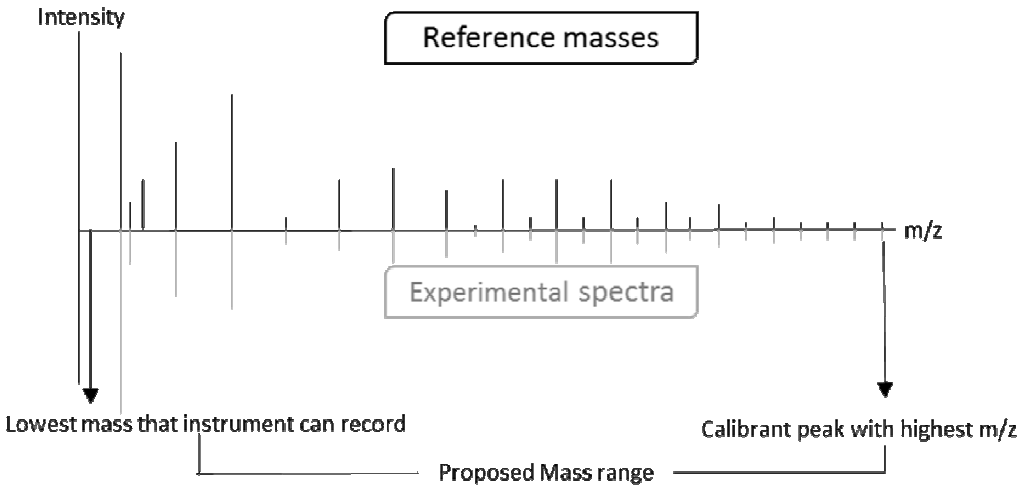


Mobile Phases

RP column

Clean ion source

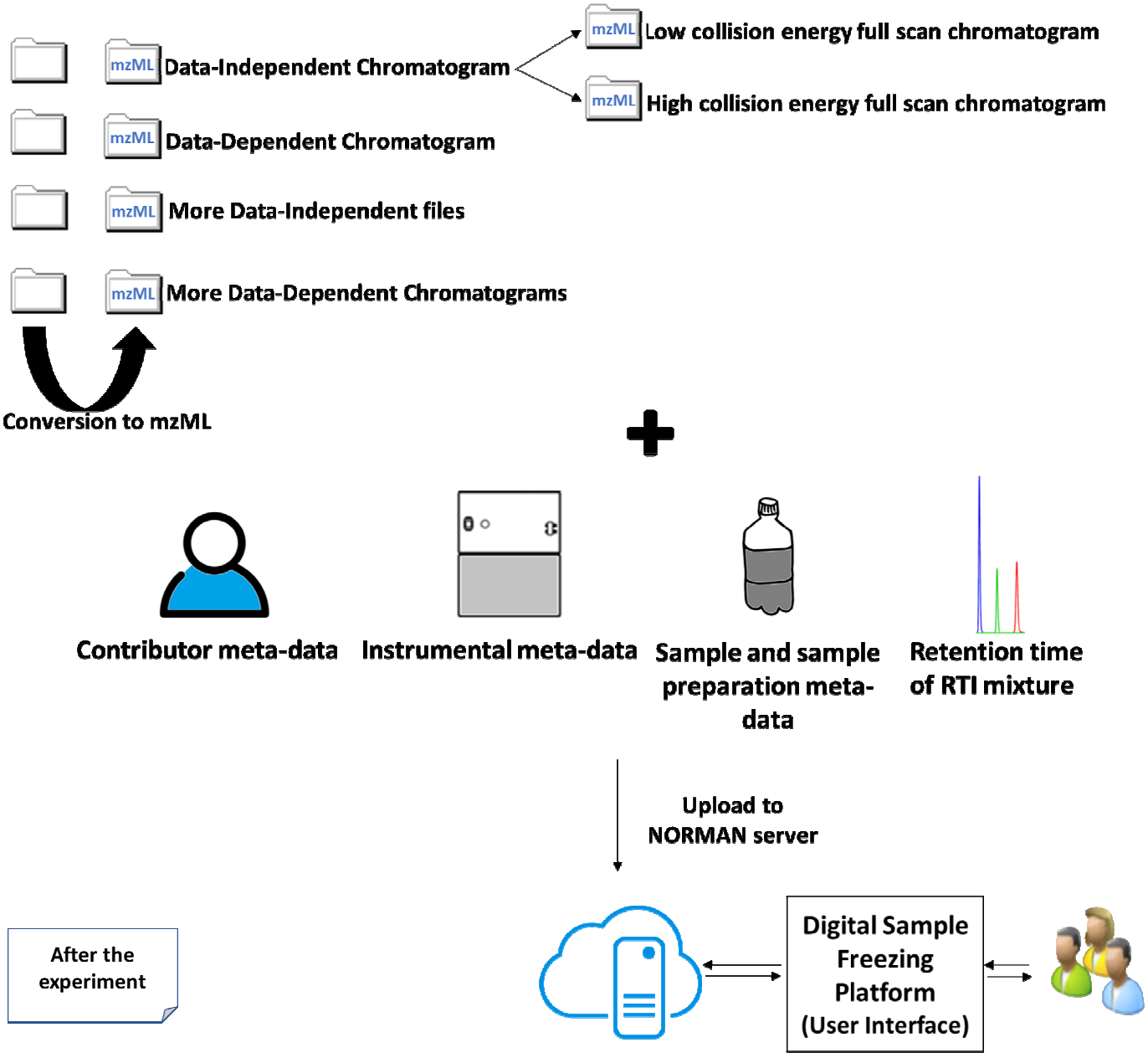
External Calibration of HRMS



Well-calibrated instrument for whole mass range

a.Before the experiment

How to upload chromatograms to DSFP



NORMAN Digital Sample Freezing Platform | Main Page | Batch mode | Contribute | More

Basic-Information | Sample-MetaData | Instrumental-MetaData | RTI_Calibration | Upload-Files

Who is contributing

All fields are compulsory

Institute Name

Organization City

City X

Organization Country

Country X

Laboratory performing the analysis

Laboratory of X

City of the laboratory performing the analysis

City X

Country of the laboratory performing the analysis

Country X

Contact person family name

Surname

Contact person first name

Name

NORMAN Digital Sample Freezing Platform | Main Page | Batch mode | Contribute | More

Basic-Information | Sample-MetaData | Instrumental-MetaData | RTI_Calibration | Upload-Files

Who is contributing

All fields are compulsory

Institute Name

EI - Environmental Institute

Organization City

Kos

Organization Country

Slovakia

Laboratory performing the analysis

Environmental Institute

City of the laboratory performing the analysis

Kos

Country of the laboratory performing the analysis

Slovakia

Contact person family name

Slobodnik

Contact person first name

Jaroslav

What is contributing

All fields are compulsory

Instrument

LC-ESI-QTOF

Short name describing the sample

Danube JDS53

Title of Project (Acronym)

Joint Danube Survey 3

Country from which the sample was taken

Romania

City from which the sample was taken

Tulcea

Sampling Date in dd-mm-yyyy

08-03-2016

Analysis Date in dd-mm-yyyy

28-04-2016

How many times has the sample been preconcentrated (Preconcentration factor)

40000

Unique identifier

R042816

Proceed to step 2/5

NORMAN Digital Sample Freezing Platform | Main Page | Batch mode | Contribute | More

Basic-Information | Sample-MetaData | Instrumental-MetaData | RTI_Calibration | Upload-Files

General Sample Information

Longitude in Decimal (Compulsory)

28.8242

Latitude in Decimal (Compulsory)

45.1935434

Precision of coordinates (Compulsory)

Average (range 10-100 m)

Type of data source

Surveys

Type of monitoring

Investigative

If sample was taken from border among 2 countries, which is the 2nd country

Specify any remarks or important extra information regarding the samples

Type of matrix (Compulsory)

Choose matrix from the list

Type of matrix (Compulsory)

Municipal

Fraction (Compulsory)

Dissolved fraction

Type of waste water (Compulsory)

Waste water - Municipal

Proxy pressures

Name of river basin

Specify

Additional Information

pH

7.5

Temperature [°C]

19.4

Dissolved organic carbon [mg/l]

35

Capacity by population equivalent (Compulsory)

5200000

Daily flow [m3/day] (Compulsory)

703586

Type of treatment plant (Compulsory)

6'. Pretreatment + primary sedimentation tank+ activated sludge including SBR (C ± N + P)

Type of tertiary treatment (Compulsory)

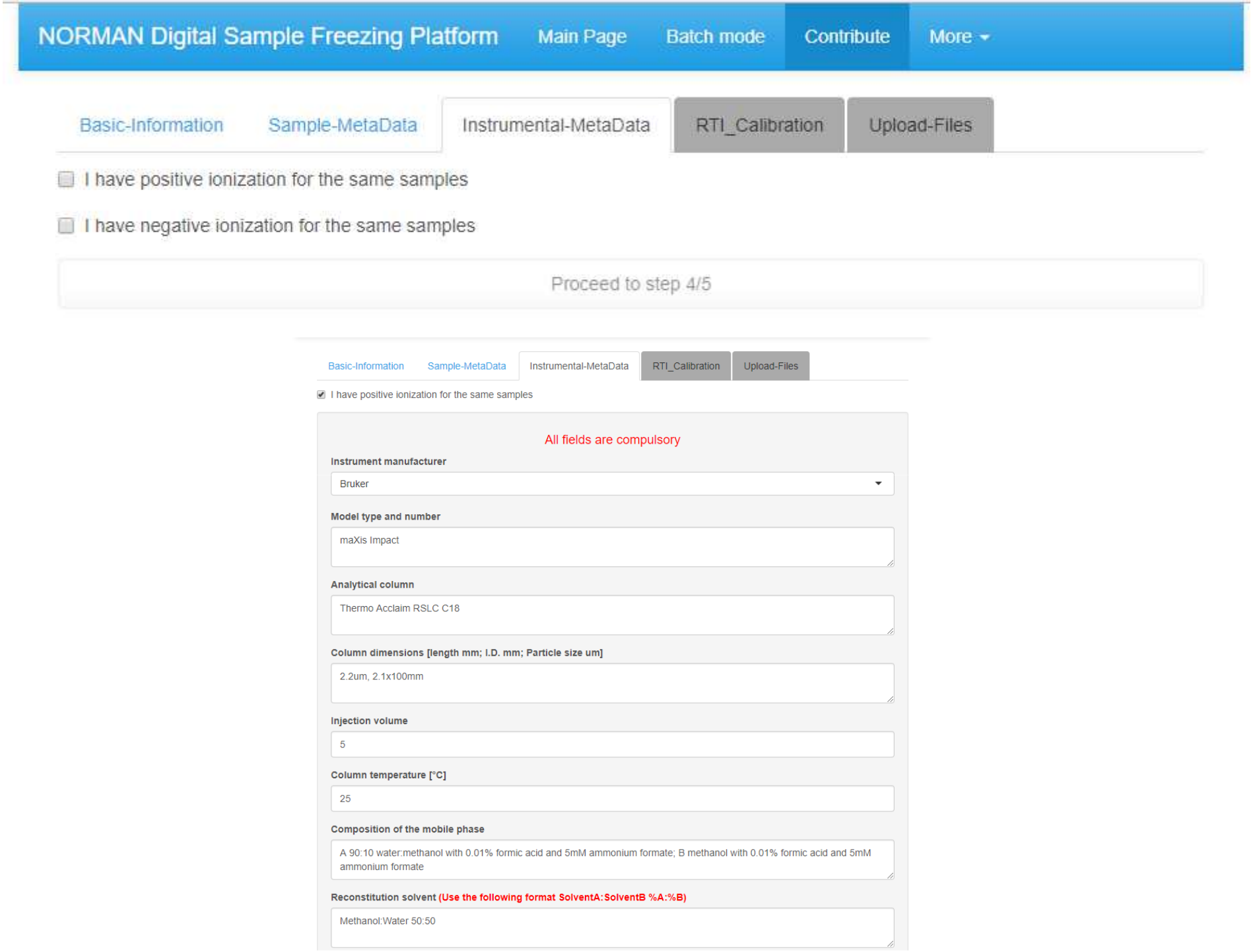
F. Tertiary membrane + reverse osmosis+ chorination

MES:Dry matter content [mg/l]

SRT [day]

Volume of the reactor [m3]

Proceed to step 3/5


NORMAN Digital Sample Freezing Platform
Main Page
Batch mode
Contribute
More
Basic-Information
Sample-MetaData
Instrumental-MetaData
RTI_Calibration
Upload-Files
I have positive ionization for the same samples
I have negative ionization for the same samples
Proceed to step 4/5
Basic-Information
Sample-MetaData
Instrumental-MetaData
RTI_Calibration
Upload-Files
I have positive ionization for the same samples
All fields are compulsory
Instrument manufacturer
Bruker
Model type and number
maXis Impact
Analytical column
Thermo Acclaim RSLC C18
Column dimensions [length mm; I.D. mm; Particle size um]
2.2um, 2.1x100mm
Injection volume
5
Column temperature [°C]
25
Composition of the mobile phase
A 90:10 water:methanol with 0.01% formic acid and 5mM ammonium formate; B methanol with 0.01% formic acid and 5mM ammonium formate
Reconstitution solvent (Use the following format SolventA:SolventB %A:%B)
Methanol:Water 50:50

NORMAN Digital Sample Freezing Platform | Main Page | Batch mode | Contribute | More

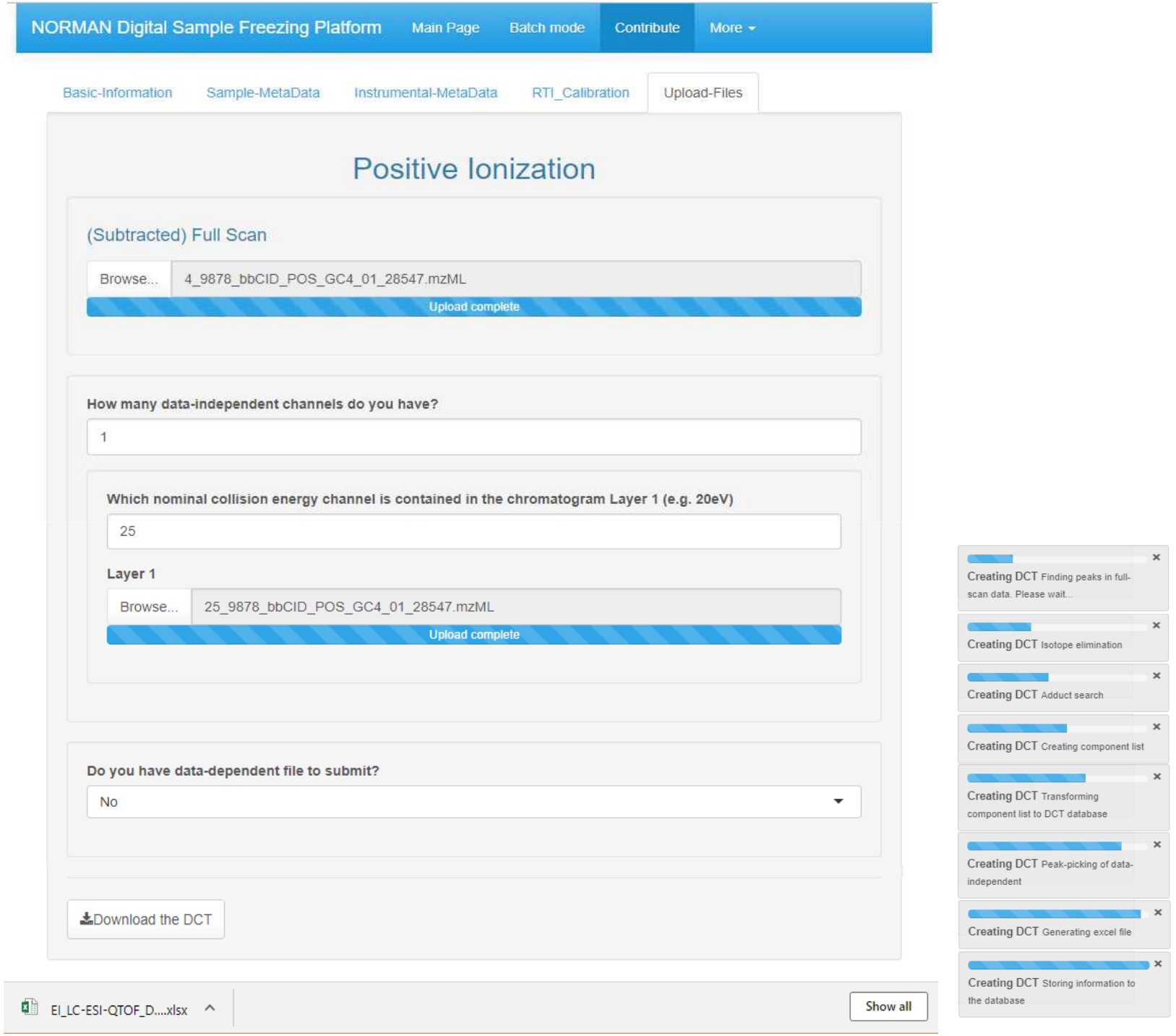
Basic-Information | Sample-MetaData | Instrumental-MetaData | RTI_Calibration | Upload-Files

☐ I have not injected these these calibrants OR I am using GC-HRMS

You have to input the RT of the calibrants. Let the cells empty for compounds without RT.

	Name	RT	CAS	Formula	Ion
1	Guanylurea	1.325	141-83-3	C2H6N4O	103.0614
2	Amitrol	1.392	61-82-5	C2H4N4	85.0509
3	Histamine	1.642	51-45-6	C5H9N3	112.0869
4	Chlormequat	1.875	999-81-5	C5H13ClN	122.0731
5	Methamidophos	2.625	10265-92-6	C2H8NO2PS	142.0086
6	Vancomycin	3.192	1404-90-6	C66H75Cl2N9O24	724.7224
7	Cefoperazone	4.342	62893-19-0	C25H27N9O8S2	646.1497
8	Trichlorfon (Dylox)	5.142	52-68-6	C4H8Cl3O4P	256.9299
9	Butocarboxim	5.992	34681-10-2	C7H14N2O2S	191.0849
10	Dichlorvos	6.908	62-73-7	C4H7Cl2O4P	220.9532
11	Tylosin	7.975	1401-69-0	C46H77NO17	916.5264
12	TCMTB	9.208	21564-17-0	C9H6N2S3	238.9766
13	Rifaximin	10.025	80621-81-4	C43H51N3O11	786.3596
14	Spinosad A (Spinosyn A)	11.525	131929-60-7	C41H65NO10	732.4681
15	Emamectin B1a	12.475	121124-29-6	C49H75NO13	886.5311
16	Avermectin B1a (Abamectin)	13.674	71751-41-2	C48H72O14	890.5260
17	Nigericin	13.908	28380-24-7	C40H68O11	725.4834
18	Ivermectin B1a	14.458	70288-86-7	C48H74O14	892.5436

Proceed to step 5/5


NORMAN Digital Sample Freezing Platform
Main Page
Batch mode
Contribute
More
Basic-Information
Sample-MetaData
Instrumental-MetaData
RTI_Calibration
Upload-Files
Positive Ionization
(Subtracted) Full Scan
Browse...
4_9878_bbCID_POS_GC4_01_28547.mzML
Upload complete
How many data-independent channels do you have?
1
Which nominal collision energy channel is contained in the chromatogram Layer 1 (e.g. 20eV)
25
Layer 1
Browse...
25_9878_bbCID_POS_GC4_01_28547.mzML
Upload complete
Do you have data-dependent file to submit?
No
Download the DCT
EI_LC-ESI-QTOF_D....xlsx
Show all
Creating DCT Finding peaks in full-scan data. Please wait...
Creating DCT Isotope elimination
Creating DCT Adduct search
Creating DCT Creating component list
Creating DCT Transforming component list to DCT database
Creating DCT Peak-picking of data-independent
Creating DCT Generating excel file
Creating DCT Storing information to the database

Description of DSFP (Single search & Batch-mode module)

NORMAN Digital Sample Freezing Platform | Main Page | Batch mode | Contribute

Substance name or CAS or StdInChIKey

Compound

OR

Precursor m/z

254.059389

Mass error in Da (Switch to ppm)

0.003 — 0.05

0.0,005 0.005 0.01 0.015 0.02 0.025 0.03 0.035 0.04 0.045 0.05

RTI Tolerance (%)

0 — 20 — 100

0 10 20 30 40 50 60 70 80 90 100

Submit Job

Contributed Samples | Results | Chromatograms | Interactive Map | Help

Show 10 entries

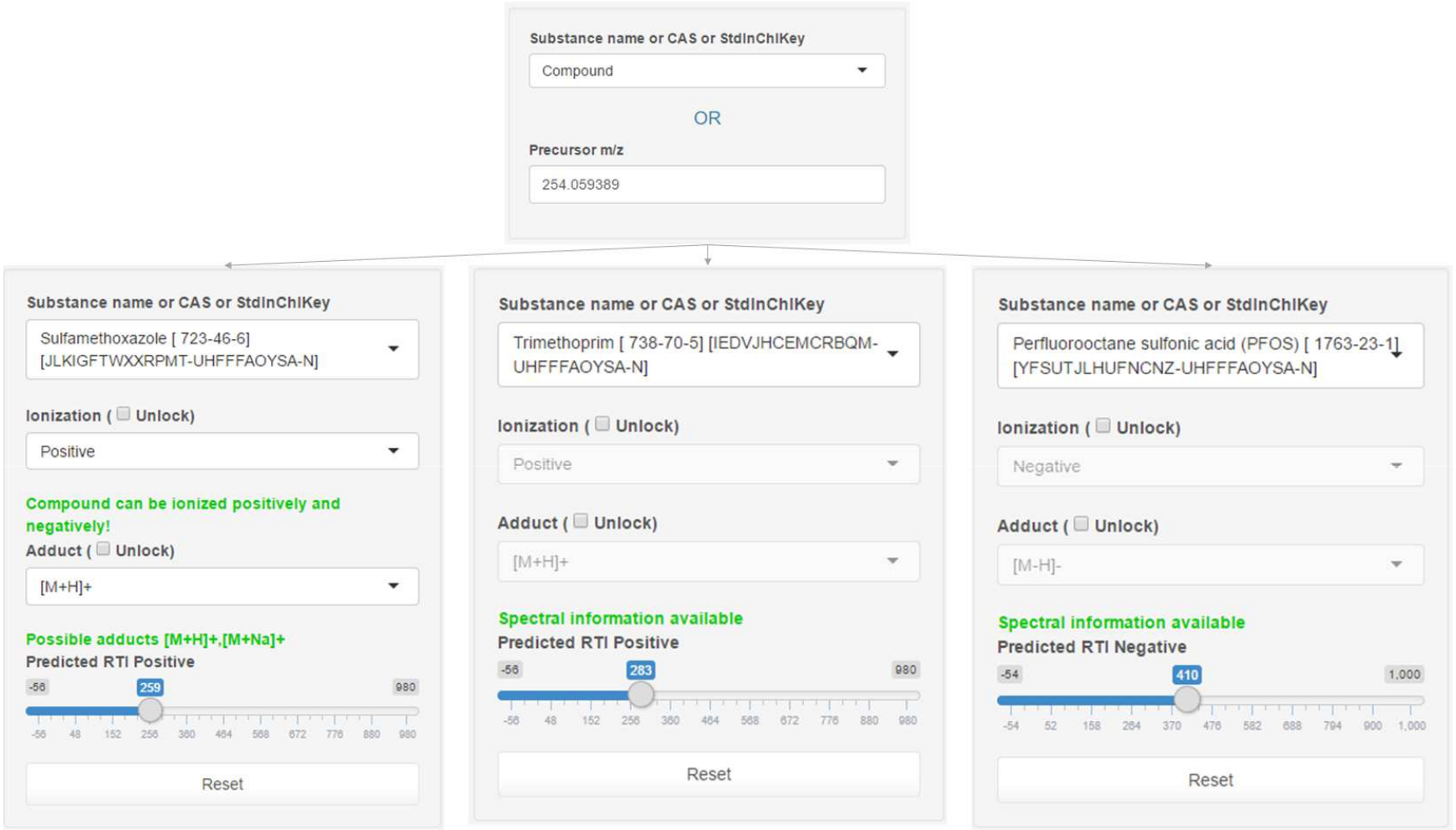
Search:

	Select per page	Country	Matrix	Project
	All	All	All	All
391 ⊕	UJI_LC-ESI-QTOF_Dust UJI_Toronto_Canada_23.08.2016_NORMAN-CT2015_C092016.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
389 ⊕	UoA_LC-ESI-QTOF_Blank for Dust UoA_Toronto_Canada_23.08.2016_NORMAN-CT2015_15522.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
387 ⊕	UoA_LC-ESI-QTOF_Dust UoA_Toronto_Canada_23.08.2016_NORMAN-CT2015_15523.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
385 ⊕	NILU_LC-ESI-QTOF_Dust NILU_Toronto_Canada_23.08.2016_NORMAN-CT2015_C111216.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
383 ⊕	IVL_LC-ESI-QFT_Blank for Dust IVL_Toronto_Canada_23.08.2016_NORMAN-CT2015_C091416.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
381 ⊕	IVL_LC-ESI-QFT_Dust IVL_Toronto_Canada_23.08.2016_NORMAN-CT2015_C091416.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
379 ⊕	ACES_LC-ESI-QFT_Blank for Dust ACES_Toronto_Canada_23.08.2016_NORMAN-CT2015_C090516.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
377 ⊕	ACES_LC-ESI-QFT_Dust ACES_Toronto_Canada_23.08.2016_NORMAN-CT2015_C090516.xlsx	Canada	Air-Indoor	NORMAN DUST CT 2015
375 ⊕	EI_LC-ESI-QTOF_Procedural Blank for Effluent wastewater Nicosia_Nicosia_Cyprus_04.12.2017_ITN ANSWER_26099.xlsx	Cyprus	Water-Waste water-Municipal	ITN ANSWER
373 ⊕	EI_LC-ESI-QTOF_Effluent wastewater Nicosia 4th week_Nicosia_Cyprus_04.12.2017_ITN ANSWER_26107.xlsx	Cyprus	Water-Waste water-Municipal	ITN ANSWER

Showing 1 to 10 of 231 entries

Previous 1 2 3 4 5 … 24

Compound selection



Compounds with prior-knowledge on spectral behavior:

- ✓ Ionization pre-selection
- ✓ Adduct pre-selection
- ✓ Qualifier fragments in evaluation of chromatograms module

Contributed Samples | Results | Chromatograms | Interactive Map | Help

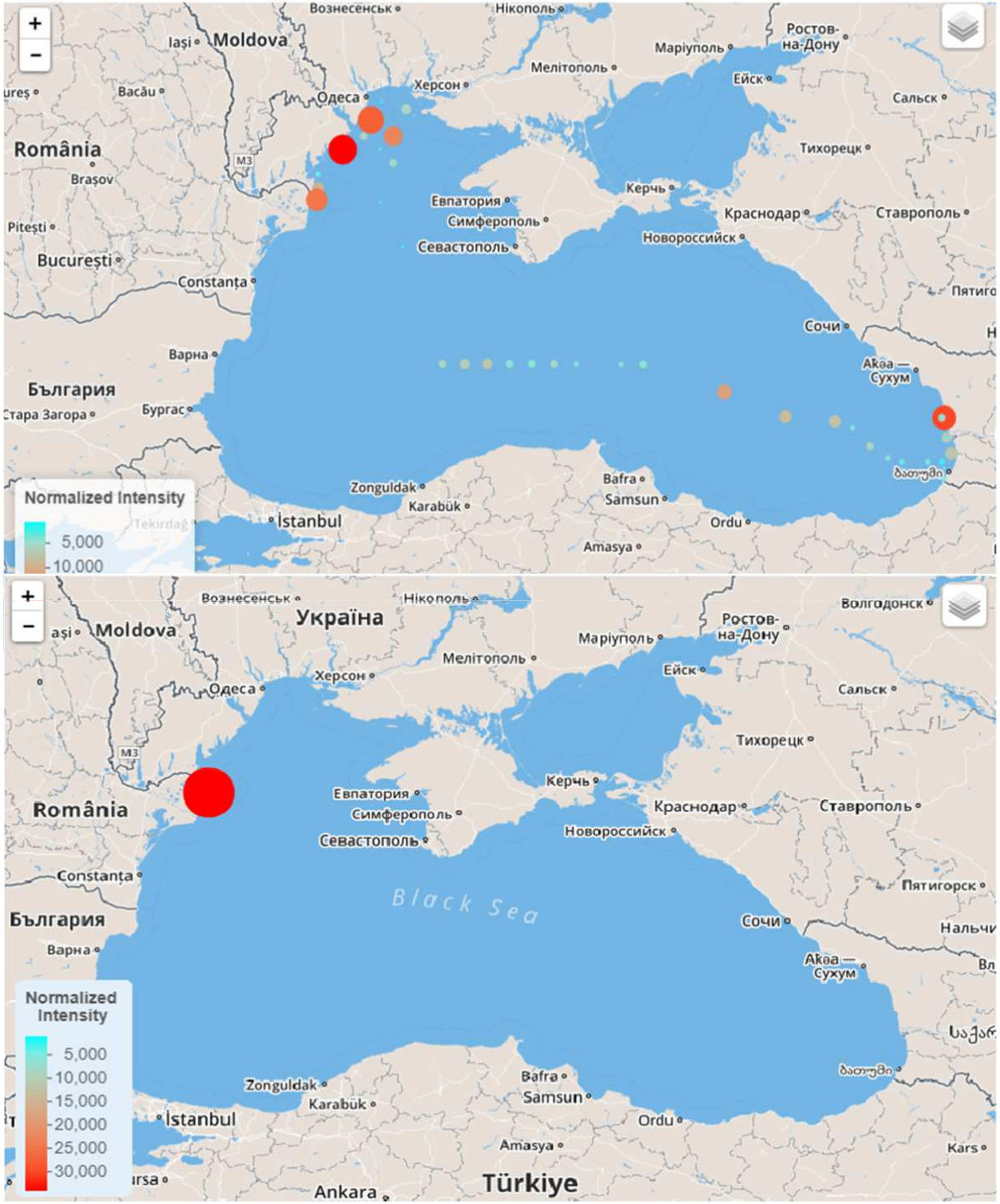
ow 10 entries

Search:

	Select per page	Country	Matrix	Project
	All	Austria Bulgaria Canada Croatia Cyprus Czech Republic Georgia	Air-Indoor Biota-Teritorial (marine) water Sediment-Territorial (marine) water Water-Surface water-River water Water-Surface water-Territorial (marine) water Water-Waste water- Municipal and Industrial	EMBLAS-II (Survey 2016) EMBLAS-II (Survey 2017) ITN ANSWER Joint Danube Survey 3 NORMAN DUST CT 2015 SOLUTIONS & ITN ANSWER
162 ⊕	UoA_LC-ESI-QTOF_Seawater GE01_Black Sea_Georgia_28.05.2016_EMBLAS II_17831.xlsx	Georgia	Water-Surface water-Territorial (marine) water	EMBLAS-II (Survey 2016)
161 ⊕	UoA_LC-ESI-QTOF_Seawater GE02_Black Sea_Georgia_28.05.2016_EMBLAS II_17832.xlsx	Georgia	Water-Surface water-Territorial (marine) water	EMBLAS-II (Survey 2016)
160 ⊕	UoA_LC-ESI-QTOF_Seawater GE03_Black Sea_Georgia_31.05.2016_EMBLAS II_17833.xlsx	Georgia	Water-Surface water-Territorial (marine) water	EMBLAS-II (Survey 2016)
159 ⊕	UoA_LC-ESI-QTOF_Seawater GE04_Black Sea_Georgia_31.05.2016_EMBLAS II_17834.xlsx	Georgia	Water-Surface water-Territorial (marine) water	EMBLAS-II (Survey 2016)
158 ⊕	UoA_LC-ESI-QTOF_Seawater GE05_Black Sea_Georgia_28.05.2016_EMBLAS II_17835.xlsx	Georgia	Water-Surface water-Territorial (marine) water	EMBLAS-II (Survey 2016)
157 ⊕	UoA_LC-ESI-QTOF_Seawater GE07_Black Sea_Georgia_30.05.2016_EMBLAS II_17836.xlsx	Georgia	Water-Surface water-Territorial (marine) water	EMBLAS-II (Survey 2016)

Column visibility | Copy | CSV | Excel | Print | Show 100 entries | Search:

Select per page	Retention time [min]	Mass of ion [m/z]	Intensity	MS/MS available	Proposed substance	Level of confirmation of identification	RTI	Qualifier Ions [mz/RT (min)/Intensity]
All					/	All		All
UoA_LC-ESI-QTOF_Sediment GE01_Black Sea_Georgia_28.05.2016_EMBLAS II_18223	7.55	505.2094	1820	No	Chlorhexidine	Exact mass Plausible RT and 9 fragments	477	336.1703/7.61/4396 201.1820/7.59/2120 184.1550/7.61/4928 178.0166/7.61/476 170.0473/7.61/11056 159.1599/7.61/904 153.0210/7.61/9428 128.0263/7.61/3340 125.1077/7.61/7920
UoA_LC-ESI-QTOF_Sediment GE02_Black Sea_Georgia_28.05.2016_EMBLAS II_18224	7.55	505.2103	2640	No	Chlorhexidine	Exact mass Plausible RT and 12 fragments	477.1	353.1967/7.61/4620 336.1696/7.61/4092 195.0425/7.61/1180 184.1547/7.61/3728 178.0160/7.58/580 170.0469/7.60/11888 167.1275/7.63/1308 159.1593/7.63/852 153.0206/7.60/8336 128.0260/7.61/2868 125.1073/7.60/7600 100.1124/7.63/3820
UoA_LC-ESI-QTOF_Sediment GE08_Black Sea_Georgia_30.05.2016_EMBLAS II_18226	7.47	505.2108	3544	No	Chlorhexidine	Exact mass Plausible RT and 13 fragments	470.7	488.1832/7.46/1416 353.1956/7.46/4008 336.1695/7.48/5000 201.1816/7.46/1812 195.0427/7.48/1596 184.1550/7.46/5448 178.0157/7.46/512 170.0472/7.46/17060 167.1283/7.46/2612 159.1596/7.48/1020 153.0208/7.48/10072 128.0266/7.48/3480 125.1077/7.46/8036



DEET detected in many seawater samples from the Black Sea

Example of point and widespread detection

Monensine detected only at 1 sampling station

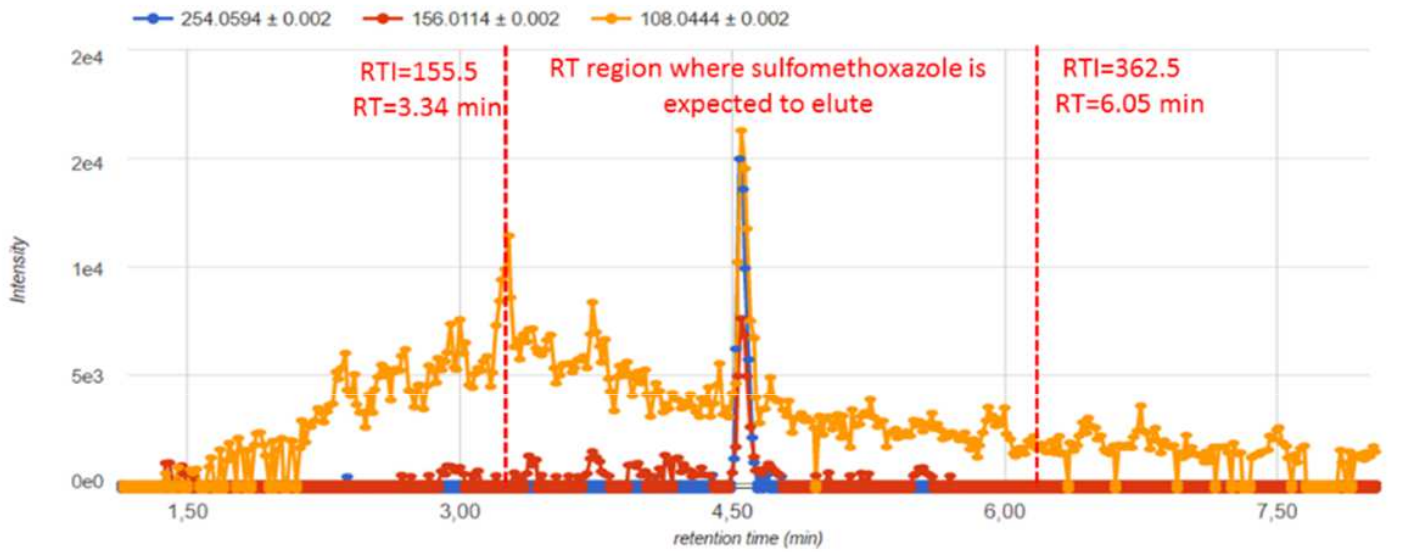
Select Chromatogram

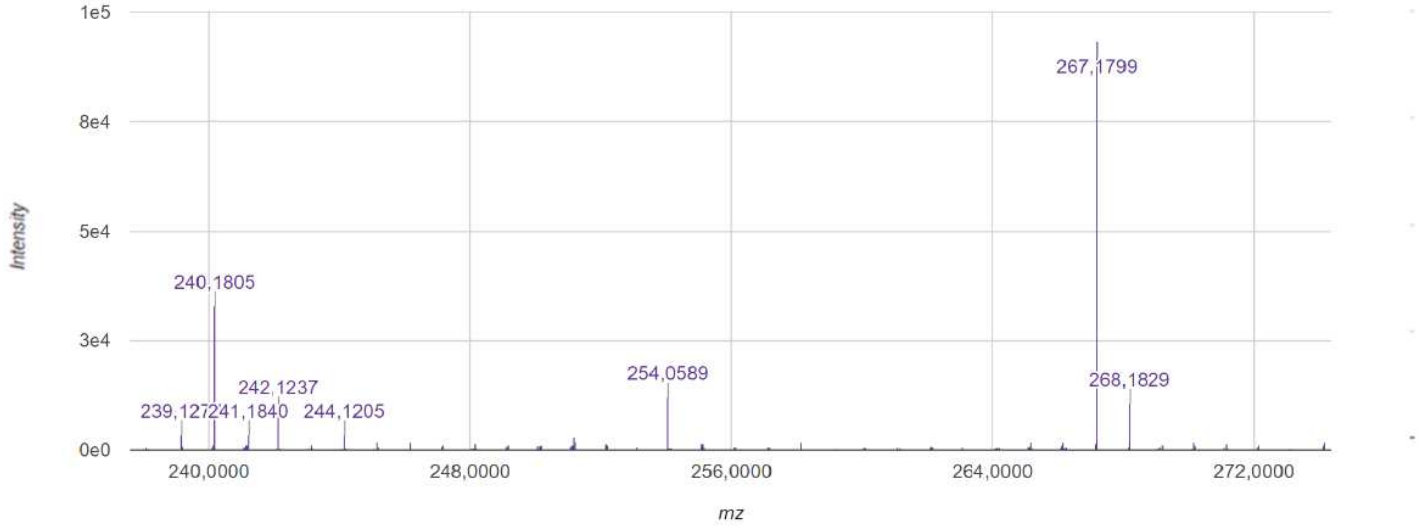
UoA_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.xlsx

Interactive table

	mz	accuracy_mDa	chromatogram	show
1	254.0594	0.0020	UoA_POS_4eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML	☑
2	156.0114	0.0020	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML	☑
3	108.0444	0.0020	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML	☑
4	92.0495	0.0020	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML	☑

Submit (Press the button everytime changes are done to the table above)





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Step 1: Select compounds that you want to screen

You selected 0 compound.

Compound lists from Suspect list exchange

Nothing selected

Select/Deselect current page

Show 10 **entries** **Search:**

	Name	Formula	CAS number	InChIKey	ChemSpiderID
	All	All	All	All	All
1	Sulfaclozine	C10H9Cl1N4O2S1	CAS_RN: 102-65-8	QKLPUVXBJHRFQZ-UHFFFAOYSA-N	60252
2	Sulfachlorpyridazine	C10H9Cl1N4O2S1	CAS_RN: 80-32-0	XOXHILFPRYWFOD-UHFFFAOYSA-N	6382
3	Sulfaguanidine	C7H10N4O2S1	CAS_RN: 57-67-0	BRBKOPJOKNSWSG-UHFFFAOYSA-N	5133
4	Sulfamerazine	C11H12N4O2S1	CAS_RN: 127-79-7	QPPBRPIAZZHUNT-UHFFFAOYSA-N	5134
5	Sulfamethizole	C9H10N4O2S2	CAS_RN: 144-82-1	VACCAVUAMIDAGB-UHFFFAOYSA-N	5137
6	Sulfamoxole	C11H13N3O3S1	CAS_RN: 729-99-7	CYFLXLSBHQBMFT-UHFFFAOYSA-N	12361
7	Sulfanilamide	C6H8N2O2S1	CAS_RN: 1337-39-9	FDDDEECHVMSUSB-UHFFFAOYSA-N	5142
8	Cefoperazone	C25H27N9O8S2	CAS_RN: 62893-19-0	GCFBRXLSHGKWDP-WJONJSRFSA-N	5408849
9	Tiamulin	C28H47N1O4S1	CAS_RN: 55297-95-5	UURAUHCOJAIIRQ-QGLSALSOSA-N	571196
10	Albendazole Sulfoxide	C12H15N3O3S1	CAS_RN: 54029-12-8	VXTGHWHFYNYFFV-UHFFFAOYSA-N	75767

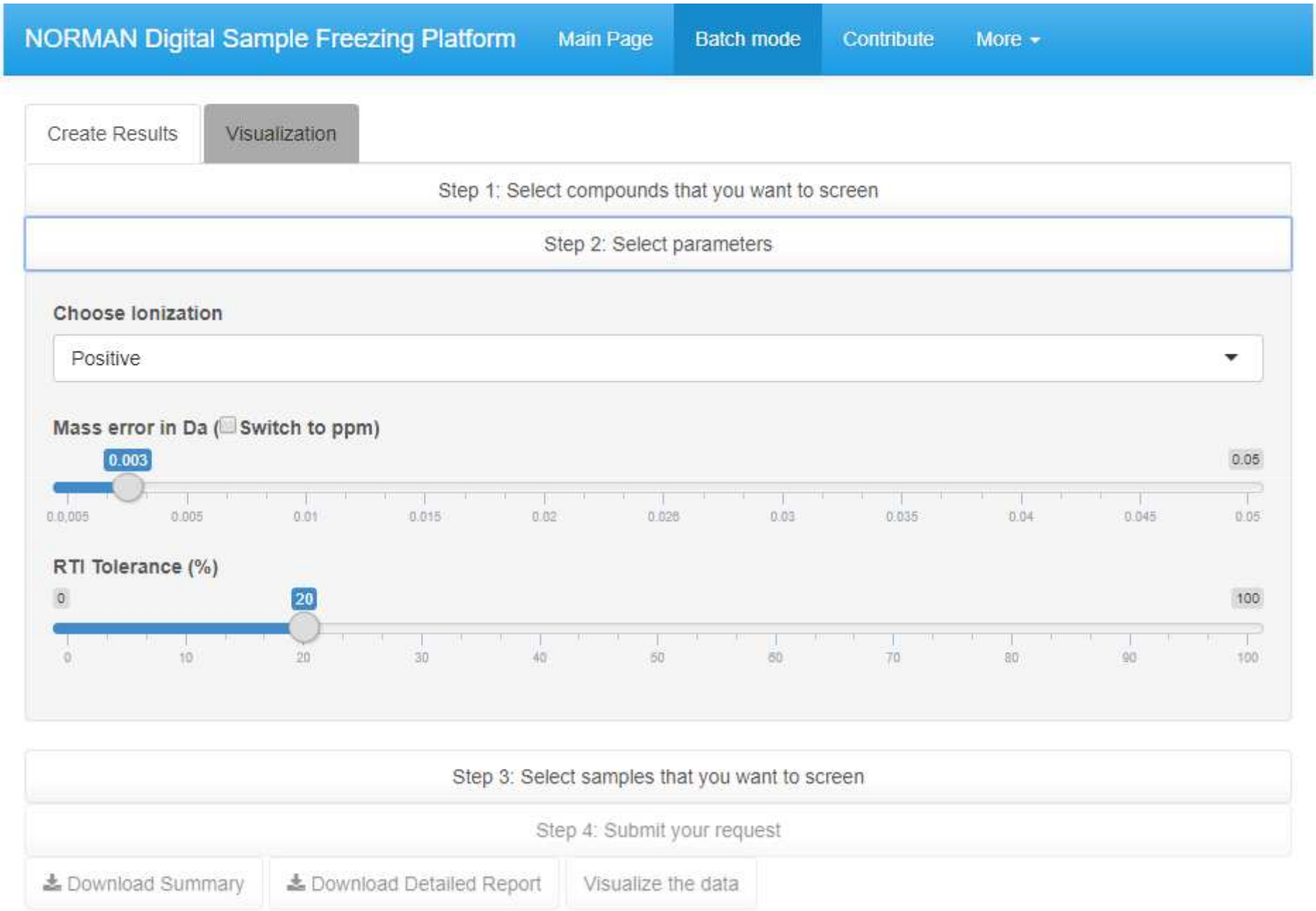
Showing 1 to 10 of 40,053 entries

Previous 1 2 3 4 5 … 4006 Next

Step 2: Select parameters

Step 3: Select samples that you want to screen

Step 4: Submit your request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Step 2: Select parameters
Choose Ionization
Positive
Mass error in Da (Switch to ppm)
0.003
0.05
0.0,005
0.005
0.01
0.015
0.02
0.026
0.03
0.035
0.04
0.045
0.05
RTI Tolerance (%)
0
20
100
0
10
20
30
40
50
60
70
80
90
100
Step 3: Select samples that you want to screen
Step 4: Submit your request
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Step 1: Select compounds that you want to screen

Step 2: Select parameters

Step 3: Select samples that you want to screen

Show 10 entries

Search:

		Select per page	Country	Matrix	Project
		All	All	All	All
545	⊕	EI_LC-ESI-QTOF_Danube JDS53_Tulcea_Romania_08.03.2016_Joint Danube Survey 3_R042816.xlsx	Romania	Water-Waste water-Municipal	Joint Danube Survey 3
543	⊕	EI_LC-ESI-QTOF_Effluent wastewater Stuttgart Muhlhausen_Stuttgart_Germany_03.05.2018_ITN ANSWER_28543.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
541	⊕	EI_LC-ESI-QTOF_Procedural Blank wastewater from Germany_Gottingen_Germany_03.05.2018_ITN ANSWER_28513.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
539	⊕	EI_LC-ESI-QTOF_Effluent wastewater Bondorf Hailfingen_Herrenberg_Germany_03.05.2018_ITN ANSWER_28545.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
535	⊕	EI_LC-ESI-QTOF_Effluent wastewater Eutin_Neustadt_Germany_03.05.2018_ITN ANSWER_28541.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
533	⊕	EI_LC-ESI-QTOF_Effluent wastewater Wevelinghofen_Grevenbroich_Germany_03.05.2018_ITN ANSWER_28539.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
531	⊕	EI_LC-ESI-QTOF_Effluent wastewater Lauterhofen dry weather_Amberg_Germany_03.05.2018_ITN ANSWER_28537.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
529	⊕	EI_LC-ESI-QTOF_Effluent wastewater Schonerlinde_Berlin_Germany_03.05.2018_ITN ANSWER_28535.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
527	⊕	EI_LC-ESI-QTOF_Effluent wastewater Karlstadt_Wurzburg_Germany_03.05.2018_ITN ANSWER_28533.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER
525	⊕	EI_LC-ESI-QTOF_Effluent wastewater Hattingen_Hattingen_Germany_03.05.2018_ITN ANSWER_28531.xlsx	Germany	Water-Waste water-Municipal	ITN ANSWER

Showing 1 to 10 of 307 entries

Previous 1 2 3 4 5 … 31 Next

Step 4: Submit your request

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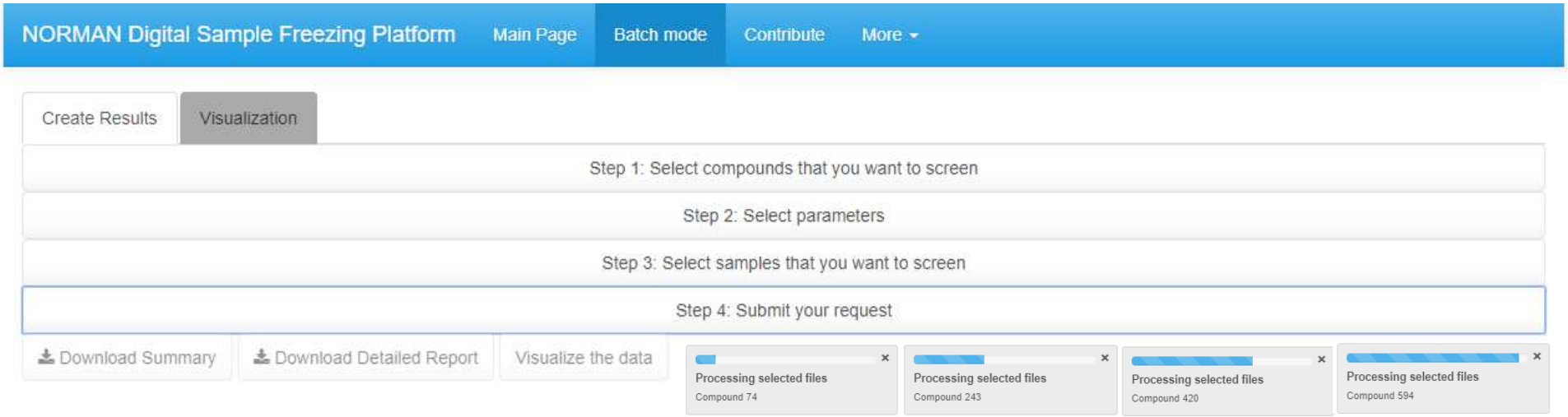
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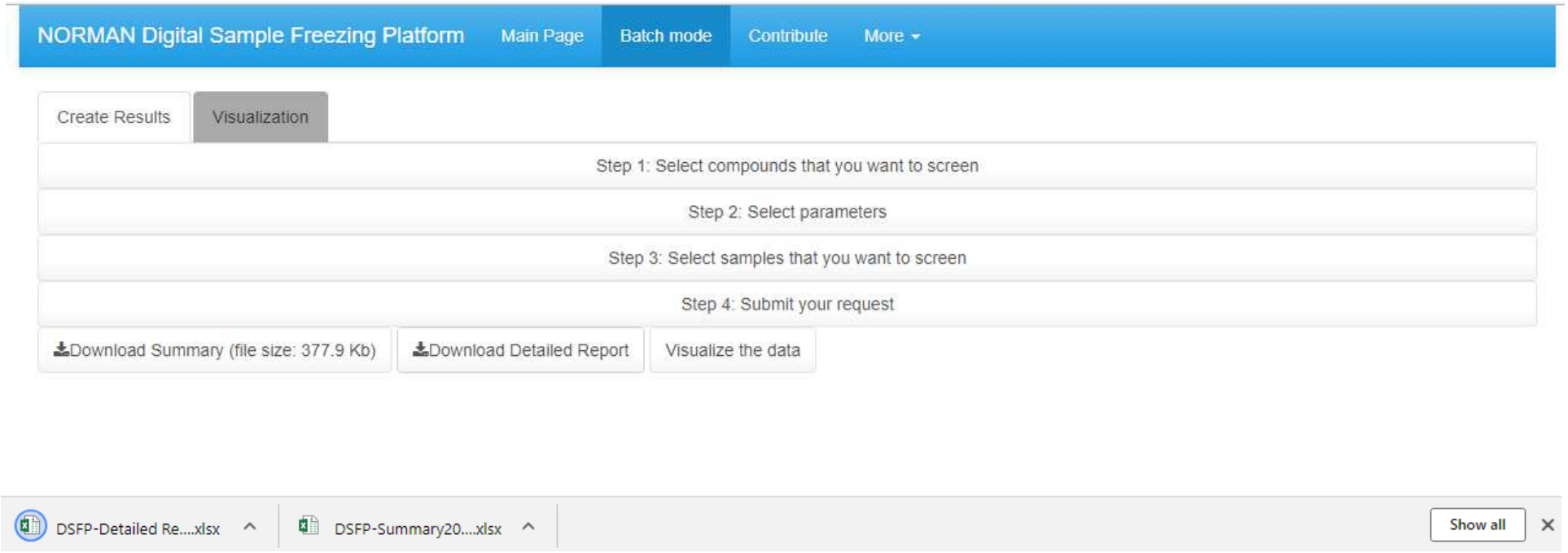
Processing selected files
Compound 74
Processing selected files
Compound 243
Processing selected files
Compound 420
Processing selected files
Compound 594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More
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Visualization
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DSFP-Summary20....xlsx
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Selection of data

Compounds with:

>1 fragments

Compounds with spectral information from libraries (No predicted MS/MS fragments)

Yes

Apply changes

Appearance

Height

330

Width

300

Size Letters Y

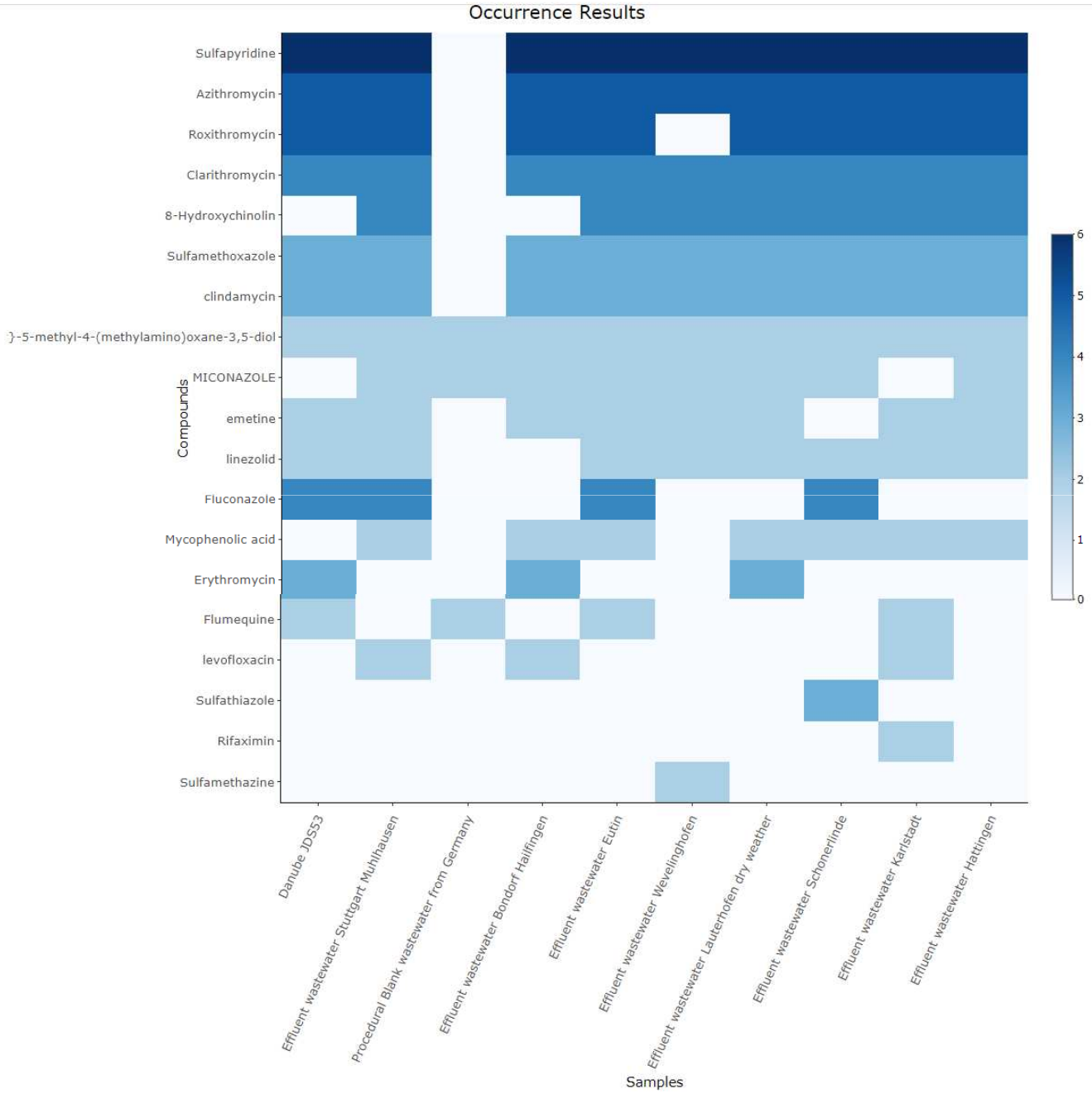
10

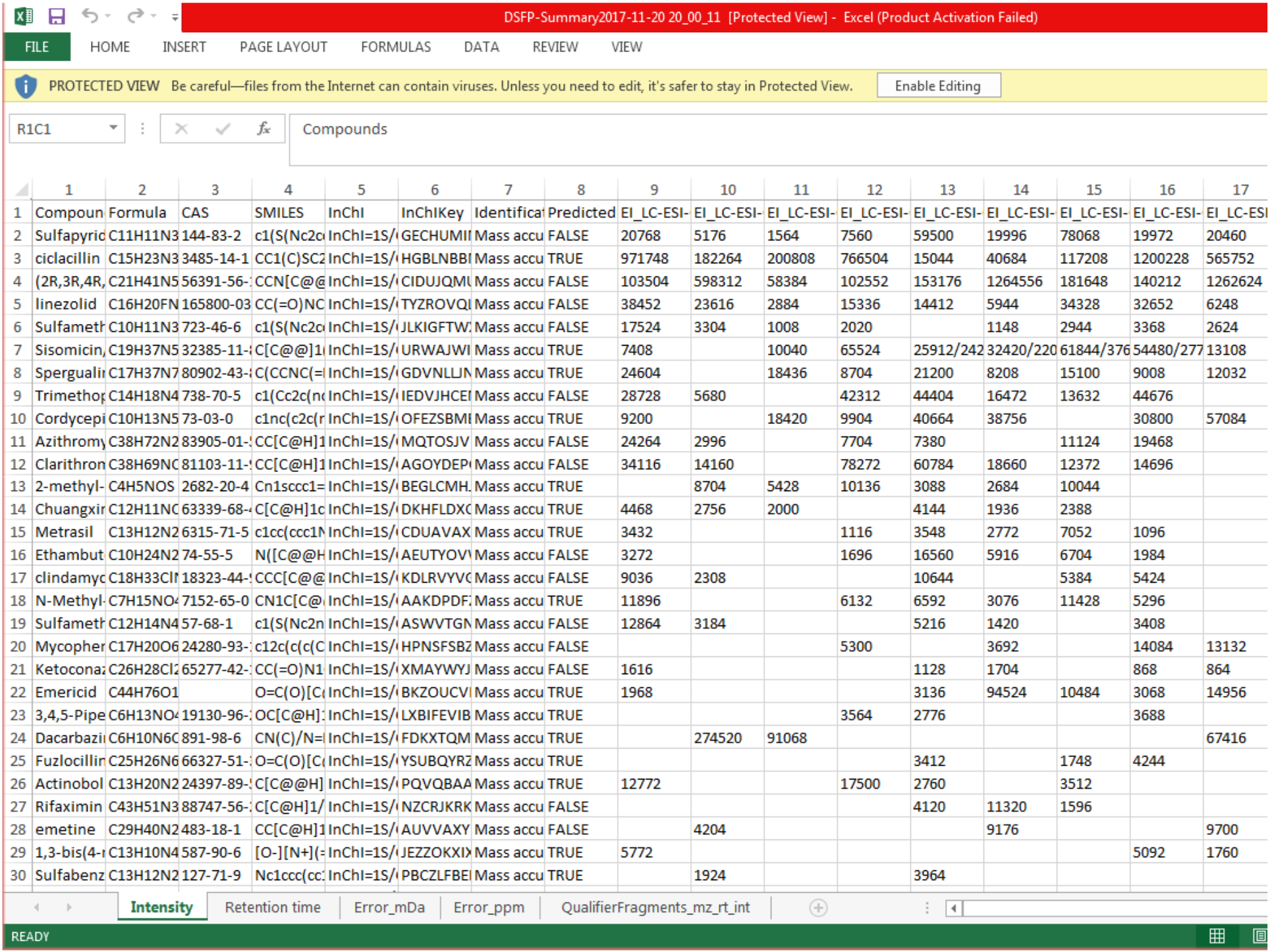
Size Letters X

10

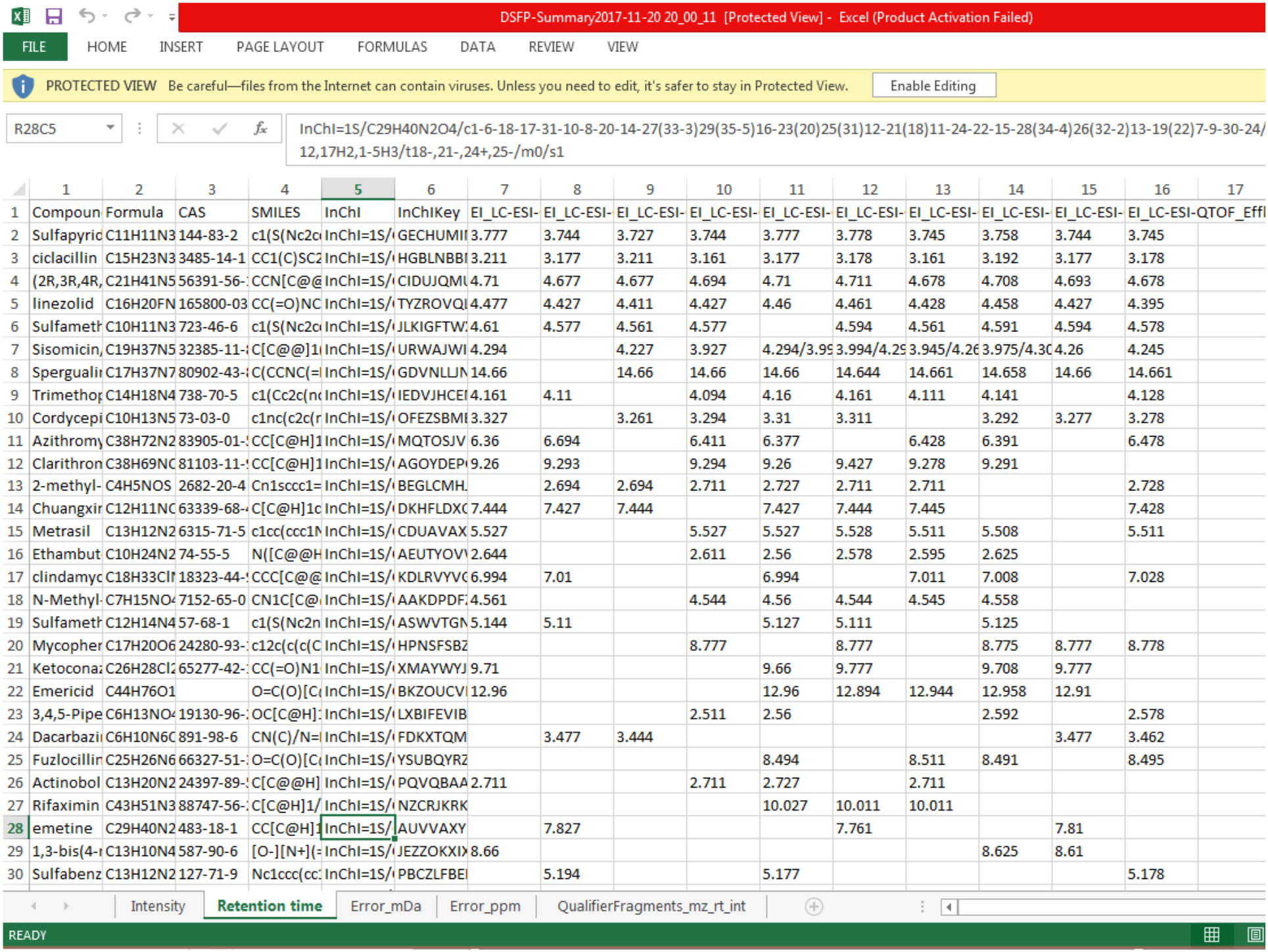
Rotation of labels on x-axis

65

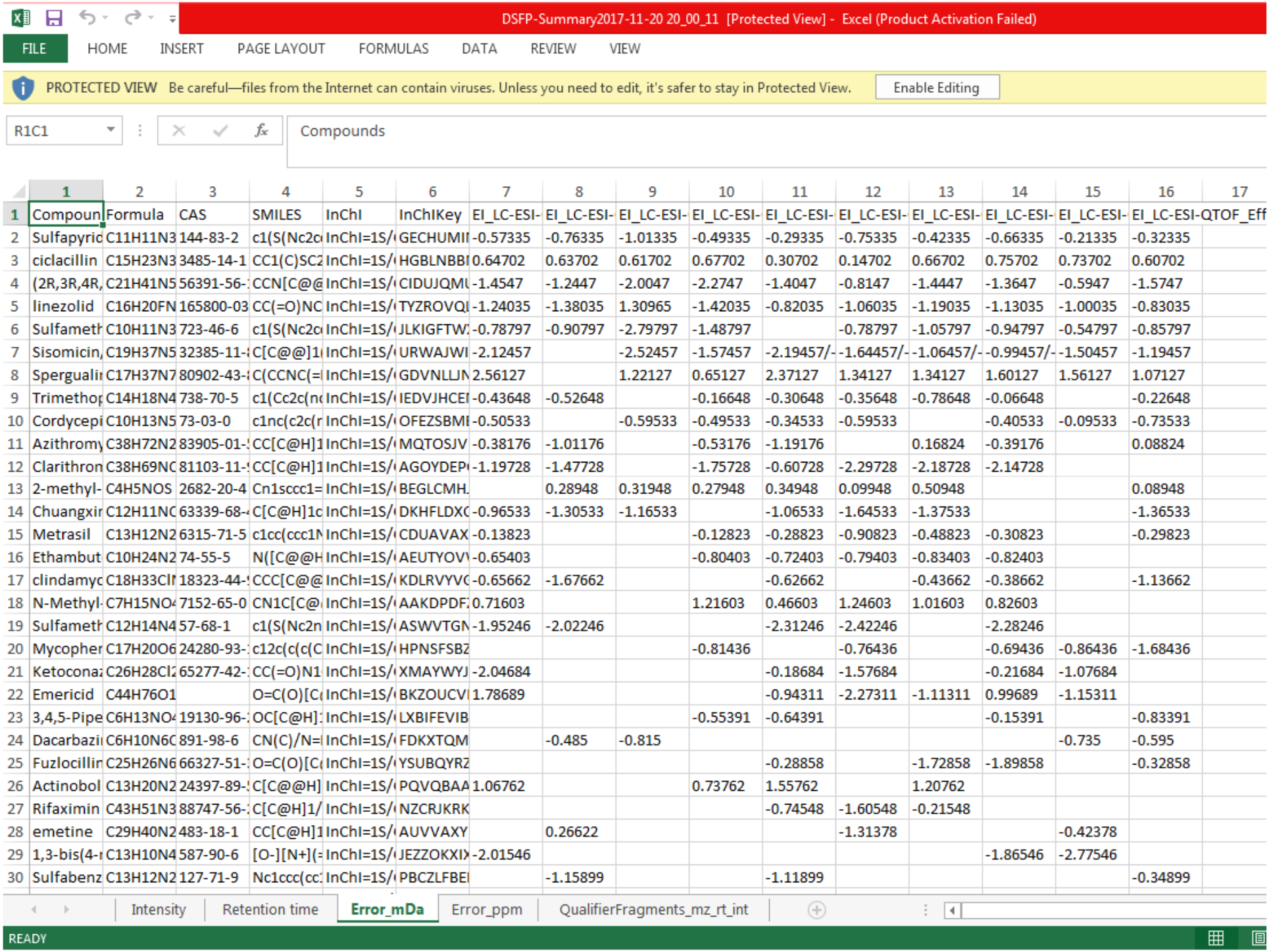




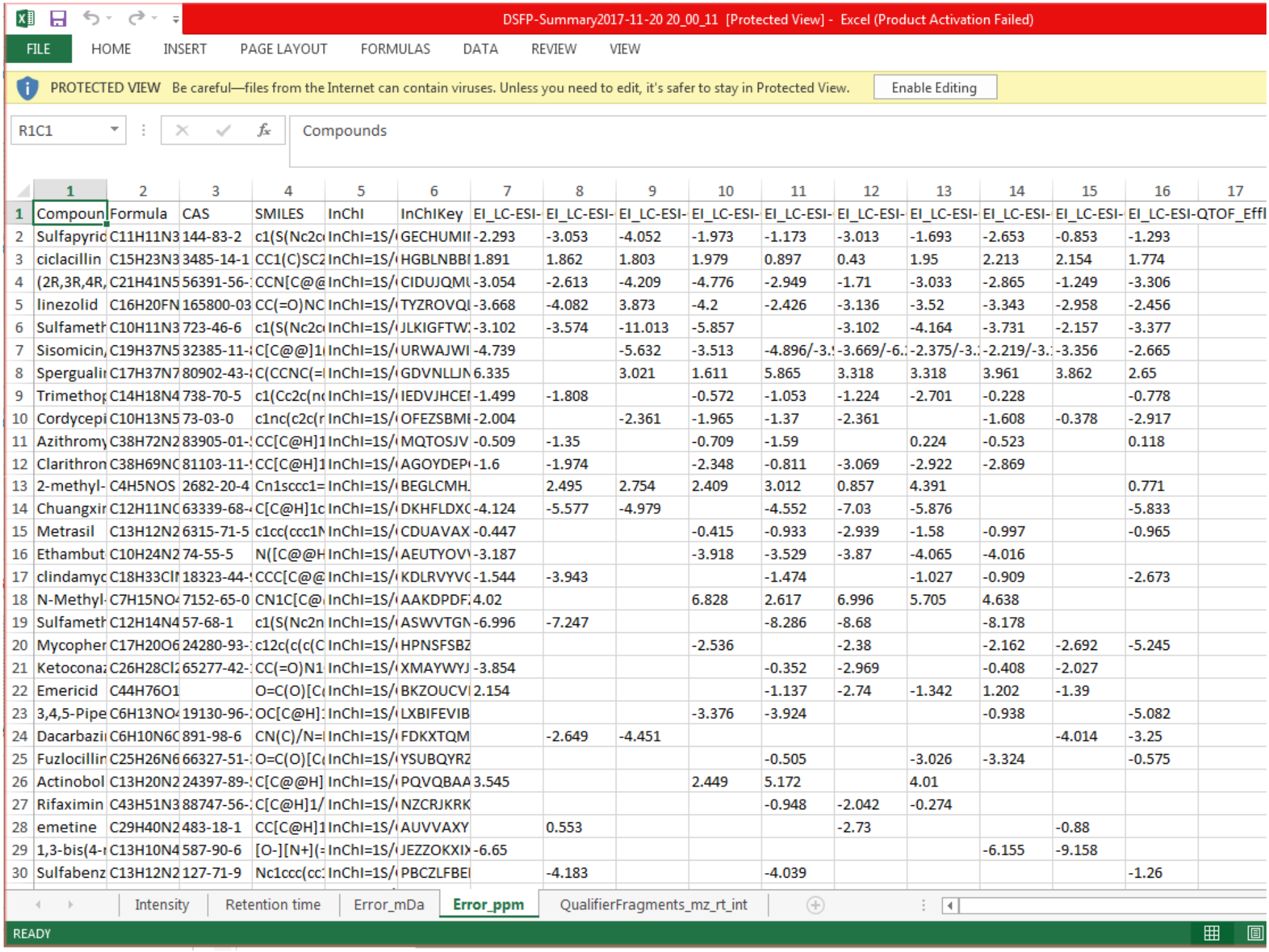
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	Compoun	Formula	CAS	SMILES	InChI	InChIKey	Identificat	Predicted	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI
2	Sulfapyric	C11H11N3	144-83-2	c1(S(Nc2c	InChI=1S/(	GECHUMIF	Mass accu	FALSE	20768	5176	1564	7560	59500	19996	78068	19972	20460
3	ciclacillin	C15H23N3	3485-14-1	CC1(C)SC2	InChI=1S/(	HGBLNBBI	Mass accu	TRUE	971748	182264	200808	766504	15044	40684	117208	1200228	565752
4	(2R,3R,4R,	C21H41N5	56391-56-	CCN[C@@	InChI=1S/(	CIDUJQMU	Mass accu	FALSE	103504	598312	58384	102552	153176	1264556	181648	140212	1262624
5	linezolid	C16H20FN	165800-03	CC(=O)NC	InChI=1S/(	TYZROVQI	Mass accu	FALSE	38452	23616	2884	15336	14412	5944	34328	32652	6248
6	Sulfameth	C10H11N3	723-46-6	c1(S(Nc2c	InChI=1S/(	JLKIGFTW	Mass accu	FALSE	17524	3304	1008	2020		1148	2944	3368	2624
7	Sisomicin,	C19H37N5	32385-11-	C[C@@]1(	InChI=1S/(	URWAJWI	Mass accu	TRUE	7408		10040	65524	25912/242	32420/220	61844/376	54480/277	13108
8	Sperguali	C17H37N7	80902-43-	C(CCNC(=	InChI=1S/(	GDVNLLJN	Mass accu	TRUE	24604		18436	8704	21200	8208	15100	9008	12032
9	Trimethop	C14H18N4	738-70-5	c1(Cc2c(nc	InChI=1S/(	IEDVJHCE	Mass accu	FALSE	28728	5680		42312	44404	16472	13632	44676	
10	Cordycepi	C10H13N5	73-03-0	c1nc(c2c(n	InChI=1S/(	OFEZSBMI	Mass accu	TRUE	9200		18420	9904	40664	38756		30800	57084
11	Azithromy	C38H72N2	83905-01-	CC[C@H]1	InChI=1S/(	MQTOSJV	Mass accu	FALSE	24264	2996		7704	7380		11124	19468	
12	Clarithron	C38H69NC	81103-11-	CC[C@H]1	InChI=1S/(	AGOYDEP	Mass accu	FALSE	34116	14160		78272	60784	18660	12372	14696	
13	2-methyl-	C4H5NOS	2682-20-4	Cn1sccc1=	InChI=1S/(	BEGLCMH.	Mass accu	TRUE		8704	5428	10136	3088	2684	10044		
14	Chuangxir	C12H11NC	63339-68-	C[C@H]1c	InChI=1S/(	DKHFLDXC	Mass accu	TRUE	4468	2756	2000		4144	1936	2388		
15	Metrasil	C13H12N2	6315-71-5	c1cc(ccc1N	InChI=1S/(	CDUAVAX	Mass accu	TRUE	3432			1116	3548	2772	7052	1096	
16	Ethambut	C10H24N2	74-55-5	N([C@@H	InChI=1S/(	AEUTYOV	Mass accu	FALSE	3272			1696	16560	5916	6704	1984	
17	clindamyc	C18H33ClN	18323-44-	CCC[C@@	InChI=1S/(	KDLRVYVC	Mass accu	FALSE	9036	2308			10644		5384	5424	
18	N-Methyl-	C7H15NO4	7152-65-0	CN1C[C@(	InChI=1S/(	AAKDPDF	Mass accu	TRUE	11896			6132	6592	3076	11428	5296	
19	Sulfameth	C12H14N4	57-68-1	c1(S(Nc2n	InChI=1S/(	ASWVTGN	Mass accu	FALSE	12864	3184			5216	1420		3408	
20	Mycopher	C17H20O6	24280-93-	c12c(c(c(C	InChI=1S/(	HPNSFSBZ	Mass accu	FALSE				5300		3692		14084	13132
21	Ketoconaz	C26H28Cl2	65277-42-	CC(=O)N1	InChI=1S/(	XMAYWYJ	Mass accu	FALSE	1616				1128	1704		868	864
22	Emericid	C44H76O1		O=C(O)[C(	InChI=1S/(	BKZOUCVI	Mass accu	TRUE	1968				3136	94524	10484	3068	14956
23	3,4,5-Pipe	C6H13NO4	19130-96-	OC[C@H]1	InChI=1S/(	LXBIFEVIB	Mass accu	TRUE				3564	2776			3688	
24	Dacarbazi	C6H10N6C	891-98-6	CN(C)/N=(	InChI=1S/(	FDKXTQM	Mass accu	TRUE		274520	91068						67416
25	Fuzlocillin	C25H26N6	66327-51-	O=C(O)[C(	InChI=1S/(	YSUBQYRZ	Mass accu	TRUE					3412		1748	4244	
26	Actinobol	C13H20N2	24397-89-	C[C@@H]	InChI=1S/(	PQVQBAA	Mass accu	TRUE	12772			17500	2760		3512		
27	Rifaximin	C43H51N3	88747-56-	C[C@H]1/	InChI=1S/(	NZCRJKRK	Mass accu	FALSE					4120	11320	1596		
28	emetine	C29H40N2	483-18-1	CC[C@H]1	InChI=1S/(	AUVVAXY	Mass accu	FALSE		4204				9176			9700
29	1,3-bis(4-r	C13H10N4	587-90-6	[O-][N+](=	InChI=1S/(	JEZZOKXI	Mass accu	TRUE	5772							5092	1760
30	Sulfabenz	C13H12N2	127-71-9	Nc1ccc(cc1	InChI=1S/(	PBCZLFBE	Mass accu	TRUE		1924			3964				



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	Compoun	Formula	CAS	SMILES	InChI	InChIKey	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-QTOF_Effl	
2	Sulfapyrid	C11H11N3	144-83-2	c1(S(Nc2c	InChI=1S/(	GECHUMII	3.777	3.744	3.727	3.744	3.777	3.778	3.745	3.758	3.744	3.745	
3	ciclacillin	C15H23N3	3485-14-1	CC1(C)SC2	InChI=1S/(	HGBLNBBI	3.211	3.177	3.211	3.161	3.177	3.178	3.161	3.192	3.177	3.178	
4	(2R,3R,4R,	C21H41N5	56391-56-	CCN[C@@	InChI=1S/(	CIDUJQMU	4.71	4.677	4.677	4.694	4.71	4.711	4.678	4.708	4.693	4.678	
5	linezolid	C16H20FN	165800-03	CC(=O)NC	InChI=1S/(	TYZROVQL	4.477	4.427	4.411	4.427	4.46	4.461	4.428	4.458	4.427	4.395	
6	Sulfameth	C10H11N3	723-46-6	c1(S(Nc2c	InChI=1S/(	JLKIGFTW	4.61	4.577	4.561	4.577		4.594	4.561	4.591	4.594	4.578	
7	Sisomicin,	C19H37N5	32385-11-5	C[C@@]1(	InChI=1S/(	URWAJWI	4.294		4.227	3.927	4.294/3.95	3.994/4.25	3.945/4.26	3.975/4.30	4.26	4.245	
8	Sperguali	C17H37N7	80902-43-8	C(CCNC(=	InChI=1S/(	GDVNLLJN	14.66		14.66	14.66	14.66	14.644	14.661	14.658	14.66	14.661	
9	Trimethop	C14H18N4	738-70-5	c1(Cc2c(nc	InChI=1S/(	IEDVJHCEI	4.161	4.11		4.094	4.16	4.161	4.111	4.141		4.128	
10	Cordycepi	C10H13N5	73-03-0	c1nc(c2c(r	InChI=1S/(	OFEZSBMI	3.327		3.261	3.294	3.31	3.311		3.292	3.277	3.278	
11	Azithromy	C38H72N2	83905-01-5	CC[C@H]1	InChI=1S/(	MQTOSJV	6.36	6.694		6.411	6.377		6.428	6.391		6.478	
12	Clarithron	C38H69NC	81103-11-9	CC[C@H]1	InChI=1S/(	AGOYDEP	9.26	9.293		9.294	9.26	9.427	9.278	9.291			
13	2-methyl-	C4H5NOS	2682-20-4	Cn1sccc1=	InChI=1S/(	BEGLCMH.		2.694	2.694	2.711	2.727	2.711	2.711			2.728	
14	Chuangxir	C12H11NC	63339-68-4	C[C@H]1c	InChI=1S/(	DKHFLDXC	7.444	7.427	7.444		7.427	7.444	7.445			7.428	
15	Metrasil	C13H12N2	6315-71-5	c1cc(ccc1N	InChI=1S/(	CDUAVAX	5.527			5.527	5.527	5.528	5.511	5.508		5.511	
16	Ethambut	C10H24N2	74-55-5	N([C@@H	InChI=1S/(	AEUTYOV	2.644			2.611	2.56	2.578	2.595	2.625			
17	clindamyc	C18H33ClN	18323-44-9	CCC[C@@	InChI=1S/(	KDLRVYVC	6.994	7.01			6.994		7.011	7.008		7.028	
18	N-Methyl-	C7H15NO4	7152-65-0	CN1C[C@(	InChI=1S/(	AAKDPDF	4.561			4.544	4.56	4.544	4.545	4.558			
19	Sulfameth	C12H14N4	57-68-1	c1(S(Nc2n	InChI=1S/(	ASWVTGN	5.144	5.11			5.127	5.111		5.125			
20	Mycopher	C17H20O6	24280-93-1	c12c(c(c(C	InChI=1S/(	HPNSFSBZ				8.777		8.777		8.775	8.777	8.778	
21	Ketoconaz	C26H28Cl2	65277-42-1	CC(=O)N1	InChI=1S/(	XMAYWYJ	9.71				9.66	9.777		9.708	9.777		
22	Emericid	C44H76O1		O=C(O)[C(	InChI=1S/(	BKZOUCV	12.96				12.96	12.894	12.944	12.958	12.91		
23	3,4,5-Pipe	C6H13NO4	19130-96-3	OC[C@H]1	InChI=1S/(	LXBIFEVIB				2.511	2.56			2.592		2.578	
24	Dacarbazi	C6H10N6O	891-98-6	CN(C)/N=(	InChI=1S/(	FDKXTQM		3.477	3.444						3.477	3.462	
25	Fuzlocillin	C25H26N6	66327-51-1	O=C(O)[C(	InChI=1S/(	YSUBQYRZ					8.494		8.511	8.491		8.495	
26	Actinobol	C13H20N2	24397-89-5	C[C@@H]	InChI=1S/(	PQVQBAA	2.711			2.711	2.727		2.711				
27	Rifaximin	C43H51N3	88747-56-3	C[C@H]1/	InChI=1S/(	NZCRJKRK					10.027	10.011	10.011				
28	emetine	C29H40N2	483-18-1	CC[C@H]1	InChI=1S/(	AUVVAXY		7.827				7.761			7.81		
29	1,3-bis(4-r	C13H10N4	587-90-6	[O-][N+](=	InChI=1S/(	JEZZOKXI	8.66							8.625	8.61		
30	Sulfabenz	C13H12N2	127-71-9	Nc1ccc(cc1	InChI=1S/(	PBCZLFBE		5.194			5.177					5.178	



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	Compoun	Formula	CAS	SMILES	InChI	InChIKey	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	QTOF_Eff
2	Sulfapyrid	C11H11N3	144-83-2	c1(S(Nc2c	InChI=1S/(	GECHUMII	-0.57335	-0.76335	-1.01335	-0.49335	-0.29335	-0.75335	-0.42335	-0.66335	-0.21335	-0.32335	
3	ciclacillin	C15H23N3	3485-14-1	CC1(C)SC2	InChI=1S/(	HGBLNBBI	0.64702	0.63702	0.61702	0.67702	0.30702	0.14702	0.66702	0.75702	0.73702	0.60702	
4	(2R,3R,4R,	C21H41N5	56391-56-	CCN[C@@	InChI=1S/(	CIDUJQMU	-1.4547	-1.2447	-2.0047	-2.2747	-1.4047	-0.8147	-1.4447	-1.3647	-0.5947	-1.5747	
5	linezolid	C16H20FN	165800-03	CC(=O)NC	InChI=1S/(	TYZROVQI	-1.24035	-1.38035	1.30965	-1.42035	-0.82035	-1.06035	-1.19035	-1.13035	-1.00035	-0.83035	
6	Sulfameth	C10H11N3	723-46-6	c1(S(Nc2c	InChI=1S/(	JLKIGFTW	-0.78797	-0.90797	-2.79797	-1.48797		-0.78797	-1.05797	-0.94797	-0.54797	-0.85797	
7	Sisomicin,	C19H37N5	32385-11-	C[C@@]1(	InChI=1S/(	URWAJWI	-2.12457		-2.52457	-1.57457	-2.19457/-	-1.64457/-	-1.06457/-	-0.99457/-	-1.50457	-1.19457	
8	Sperguali	C17H37N7	80902-43-	C(CCNC(=	InChI=1S/(	GDVNLLJN	2.56127		1.22127	0.65127	2.37127	1.34127	1.34127	1.60127	1.56127	1.07127	
9	Trimethop	C14H18N4	738-70-5	c1(Cc2c(nc	InChI=1S/(	IEDVJHCE	-0.43648	-0.52648		-0.16648	-0.30648	-0.35648	-0.78648	-0.06648		-0.22648	
10	Cordycepi	C10H13N5	73-03-0	c1nc(c2c(r	InChI=1S/(	OFEZSBMI	-0.50533		-0.59533	-0.49533	-0.34533	-0.59533		-0.40533	-0.09533	-0.73533	
11	Azithromy	C38H72N2	83905-01-	CC[C@H]1	InChI=1S/(	MQTOSJV	-0.38176	-1.01176		-0.53176	-1.19176		0.16824	-0.39176		0.08824	
12	Clarithron	C38H69NC	81103-11-	CC[C@H]1	InChI=1S/(	AGOYDEP	-1.19728	-1.47728		-1.75728	-0.60728	-2.29728	-2.18728	-2.14728			
13	2-methyl-	C4H5NOS	2682-20-4	Cn1sccc1=	InChI=1S/(	BEGLCMH.		0.28948	0.31948	0.27948	0.34948	0.09948	0.50948			0.08948	
14	Chuangxir	C12H11NC	63339-68-	C[C@H]1c	InChI=1S/(	DKHFLDXC	-0.96533	-1.30533	-1.16533		-1.06533	-1.64533	-1.37533			-1.36533	
15	Metrasil	C13H12N2	6315-71-5	c1cc(ccc1N	InChI=1S/(	CDUAVAX	-0.13823			-0.12823	-0.28823	-0.90823	-0.48823	-0.30823		-0.29823	
16	Ethambut	C10H24N2	74-55-5	N([C@@H	InChI=1S/(	AEUTYOV	-0.65403			-0.80403	-0.72403	-0.79403	-0.83403	-0.82403			
17	clindamyc	C18H33ClI	18323-44-	CCC[C@@	InChI=1S/(	KDLRVYVC	-0.65662	-1.67662			-0.62662		-0.43662	-0.38662		-1.13662	
18	N-Methyl-	C7H15NO4	7152-65-0	CN1C[C@	InChI=1S/(	AAKDPDF	0.71603			1.21603	0.46603	1.24603	1.01603	0.82603			
19	Sulfameth	C12H14N4	57-68-1	c1(S(Nc2n	InChI=1S/(	ASWVTGN	-1.95246	-2.02246			-2.31246	-2.42246		-2.28246			
20	Mycopher	C17H20O6	24280-93-	c12c(c(c(C	InChI=1S/(	HPNSFSBZ				-0.81436		-0.76436		-0.69436	-0.86436	-1.68436	
21	Ketoconaz	C26H28Cl2	65277-42-	CC(=O)N1	InChI=1S/(	XMAYWYJ	-2.04684				-0.18684	-1.57684		-0.21684	-1.07684		
22	Emericid	C44H76O1		O=C(O)[C@	InChI=1S/(	BKZOUCVI	1.78689				-0.94311	-2.27311	-1.11311	0.99689	-1.15311		
23	3,4,5-Pipe	C6H13NO4	19130-96-	OC[C@H]1	InChI=1S/(	LXBIFEVIB				-0.55391	-0.64391			-0.15391		-0.83391	
24	Dacarbazi	C6H10N6C	891-98-6	CN(C)/N=N	InChI=1S/(	FDKXTQM		-0.485	-0.815						-0.735	-0.595	
25	Fuzlocillin	C25H26N6	66327-51-	O=C(O)[C@	InChI=1S/(	YSUBQYRZ					-0.28858		-1.72858	-1.89858		-0.32858	
26	Actinobol	C13H20N2	24397-89-	C[C@@H]	InChI=1S/(	PQVQBAA	1.06762			0.73762	1.55762		1.20762				
27	Rifaximin	C43H51N3	88747-56-	C[C@H]1/	InChI=1S/(	NZCRJKRK					-0.74548	-1.60548	-0.21548				
28	emetine	C29H40N2	483-18-1	CC[C@H]1	InChI=1S/(	AUVVAXY		0.26622				-1.31378			-0.42378		
29	1,3-bis(4-(	C13H10N4	587-90-6	[O-][N+](=	InChI=1S/(	JEZZOKXI	-2.01546							-1.86546	-2.77546		
30	Sulfabenz	C13H12N2	127-71-9	Nc1ccc(cc	InChI=1S/(	PBCZLFBE		-1.15899			-1.11899					-0.34899	


DSFP-Summary2017-11-20 20_00_11 [Protected View] - Excel (Product Activation Failed)

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW

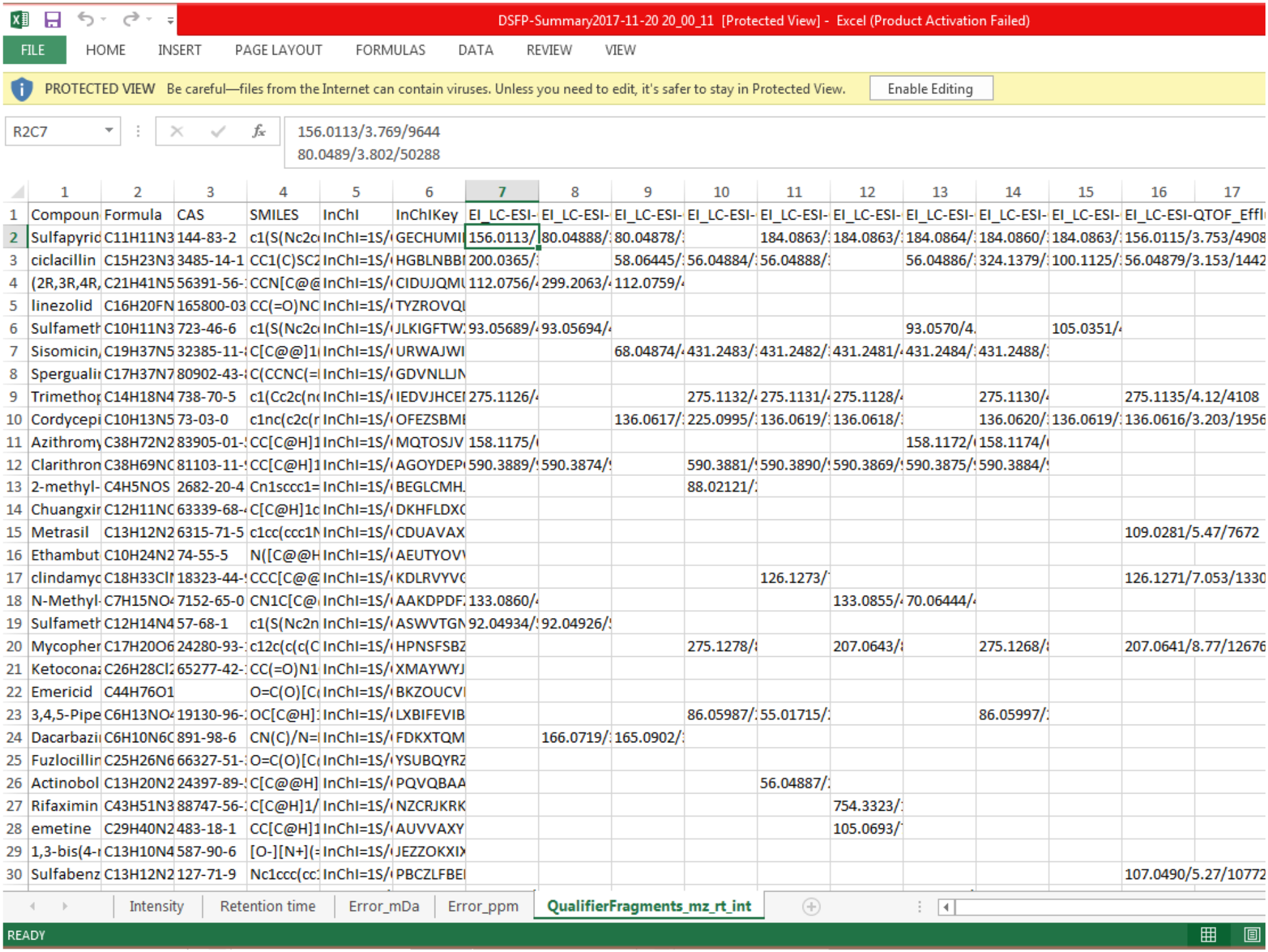
PROTECTED VIEW Be careful—files from the Internet can contain viruses. Unless you need to edit, it's safer to stay in Protected View. Enable Editing

R1C1 Compounds

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	Compoun	Formula	CAS	SMILES	InChI	InChIKey	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-	EI_LC-ESI-QTOF_Effl	
2	Sulfapyric	C11H11N3	144-83-2	c1(S(Nc2c	InChI=1S/(	GECHUMII	-2.293	-3.053	-4.052	-1.973	-1.173	-3.013	-1.693	-2.653	-0.853	-1.293	
3	ciclacillin	C15H23N3	3485-14-1	CC1(C)SC2	InChI=1S/(	HGBLNBBI	1.891	1.862	1.803	1.979	0.897	0.43	1.95	2.213	2.154	1.774	
4	(2R,3R,4R,	C21H41N5	56391-56-	CCN[C@@	InChI=1S/(	CIDUJQMU	-3.054	-2.613	-4.209	-4.776	-2.949	-1.71	-3.033	-2.865	-1.249	-3.306	
5	linezolid	C16H20FN	165800-03	CC(=O)NC	InChI=1S/(	TYZROVQI	-3.668	-4.082	3.873	-4.2	-2.426	-3.136	-3.52	-3.343	-2.958	-2.456	
6	Sulfameth	C10H11N3	723-46-6	c1(S(Nc2c	InChI=1S/(	JLKIGFTW	-3.102	-3.574	-11.013	-5.857		-3.102	-4.164	-3.731	-2.157	-3.377	
7	Sisomicin,	C19H37N5	32385-11-	C[C@@]1(	InChI=1S/(	URWAJWI	-4.739		-5.632	-3.513	-4.896/-3.	-3.669/-6.	-2.375/-3.	-2.219/-3.	-3.356	-2.665	
8	Sperguali	C17H37N7	80902-43-	C(CCNC(=	InChI=1S/(	GDVNLLJN	6.335		3.021	1.611	5.865	3.318	3.318	3.961	3.862	2.65	
9	Trimethop	C14H18N4	738-70-5	c1(Cc2c(nc	InChI=1S/(	IEDVJHCE	-1.499	-1.808		-0.572	-1.053	-1.224	-2.701	-0.228		-0.778	
10	Cordycepi	C10H13N5	73-03-0	c1nc(c2c(r	InChI=1S/(	OFEZSBMI	-2.004		-2.361	-1.965	-1.37	-2.361		-1.608	-0.378	-2.917	
11	Azithromy	C38H72N2	83905-01-	CC[C@H]1	InChI=1S/(	MQTOSJV	-0.509	-1.35		-0.709	-1.59		0.224	-0.523		0.118	
12	Clarithron	C38H69NC	81103-11-	CC[C@H]1	InChI=1S/(	AGOYDEP	-1.6	-1.974		-2.348	-0.811	-3.069	-2.922	-2.869			
13	2-methyl-	C4H5NOS	2682-20-4	Cn1sccc1=	InChI=1S/(	BEGLCMH.		2.495	2.754	2.409	3.012	0.857	4.391			0.771	
14	Chuangxir	C12H11NC	63339-68-	C[C@H]1c	InChI=1S/(	DKHFLDXC	-4.124	-5.577	-4.979		-4.552	-7.03	-5.876			-5.833	
15	Metrasil	C13H12N2	6315-71-5	c1cc(ccc1N	InChI=1S/(	CDUAVAX	-0.447			-0.415	-0.933	-2.939	-1.58	-0.997		-0.965	
16	Ethambut	C10H24N2	74-55-5	N([C@@H	InChI=1S/(	AEUTYOV	-3.187			-3.918	-3.529	-3.87	-4.065	-4.016			
17	clindamyc	C18H33ClN	18323-44-	CCC[C@@	InChI=1S/(	KDLRVYVC	-1.544	-3.943			-1.474		-1.027	-0.909		-2.673	
18	N-Methyl-	C7H15NO4	7152-65-0	CN1C[C@(	InChI=1S/(	AAKDPDF	4.02			6.828	2.617	6.996	5.705	4.638			
19	Sulfameth	C12H14N4	57-68-1	c1(S(Nc2n	InChI=1S/(	ASWVTGN	-6.996	-7.247			-8.286	-8.68		-8.178			
20	Mycopher	C17H20O6	24280-93-	c12c(c(c(C	InChI=1S/(	HPNSFSBZ				-2.536		-2.38		-2.162	-2.692	-5.245	
21	Ketoconaz	C26H28Cl2	65277-42-	CC(=O)N1	InChI=1S/(	XMAYWYJ	-3.854				-0.352	-2.969		-0.408	-2.027		
22	Emericid	C44H76O1		O=C(O)[C(	InChI=1S/(	BKZOUCVI	2.154				-1.137	-2.74	-1.342	1.202	-1.39		
23	3,4,5-Pipe	C6H13NO4	19130-96-	OC[C@H]1	InChI=1S/(	LXBIFEVIB				-3.376	-3.924			-0.938		-5.082	
24	Dacarbazi	C6H10N6C	891-98-6	CN(C)/N=(	InChI=1S/(	FDKXTQM		-2.649	-4.451						-4.014	-3.25	
25	Fuzlocillin	C25H26N6	66327-51-	O=C(O)[C(	InChI=1S/(	YSUBQYRZ					-0.505		-3.026	-3.324		-0.575	
26	Actinobol	C13H20N2	24397-89-	C[C@@H]	InChI=1S/(	PQVQBAA	3.545			2.449	5.172		4.01				
27	Rifaximin	C43H51N3	88747-56-	C[C@H]1/	InChI=1S/(	NZCRJKRK					-0.948	-2.042	-0.274				
28	emetine	C29H40N2	483-18-1	CC[C@H]1	InChI=1S/(	AUVVAXY		0.553				-2.73			-0.88		
29	1,3-bis(4-r	C13H10N4	587-90-6	[O-][N+](=	InChI=1S/(	JEZZOKXI	-6.65							-6.155	-9.158		
30	Sulfabenz	C13H12N2	127-71-9	Nc1ccc(cc1	InChI=1S/(	PBCZLFBE		-4.183			-4.039					-1.26	

Intensity | Retention time | Error_mDa | Error_ppm | QualifierFragments_mz_rt_int

READY


DSFP-Summary2017-11-20 20_00_11 [Protected View] - Excel (Product Activation Failed)
FILE
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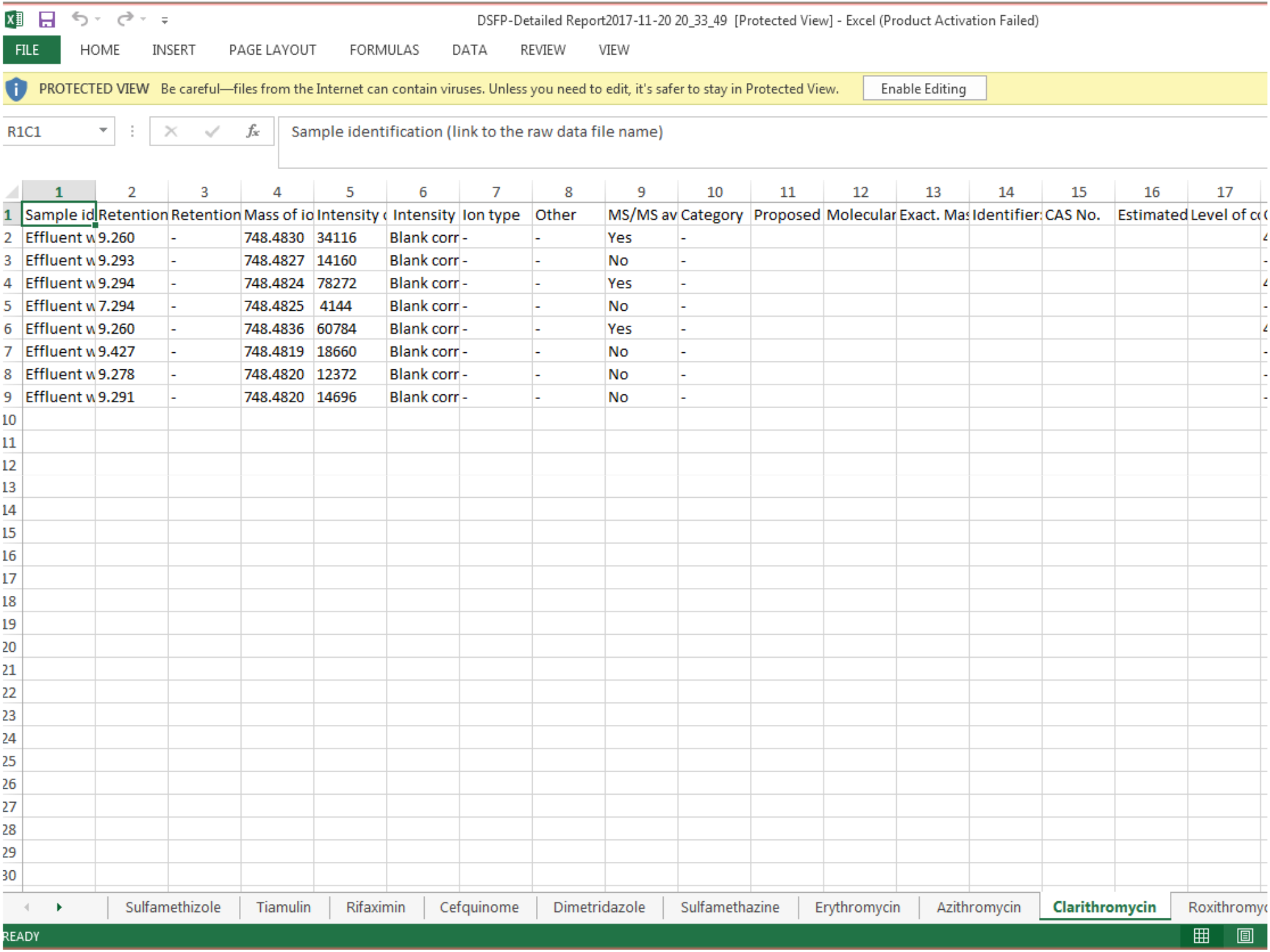
PAGE LAYOUT
FORMULAS
DATA
REVIEW
VIEW
PROTECTED VIEW Be careful—files from the Internet can contain viruses. Unless you need to edit, it's safer to stay in Protected View.
Enable Editing
R2C7
156.0113/3.769/9644
80.0489/3.802/50288
Intensity
Retention time
Error_mDa
Error_ppm
QualifierFragments_mz_rt_int
READY


DSFP-Detailed Report2017-11-20 20_33_49 [Protected View] - Excel (Product Activation Failed)

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R1C1 Sample identification (link to the raw data file name)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	Sample id	Retention	Retention	Mass of io	Intensity	Intensity	Ion type	Other	MS/MS av	Category	Proposed	Molecular	Exact. Mas	Identifier:	CAS No.	Estimated	Level of c
2	Effluent w	9.260	-	748.4830	34116	Blank corr	-	-	Yes	-							
3	Effluent w	9.293	-	748.4827	14160	Blank corr	-	-	No	-							
4	Effluent w	9.294	-	748.4824	78272	Blank corr	-	-	Yes	-							
5	Effluent w	7.294	-	748.4825	4144	Blank corr	-	-	No	-							
6	Effluent w	9.260	-	748.4836	60784	Blank corr	-	-	Yes	-							
7	Effluent w	9.427	-	748.4819	18660	Blank corr	-	-	No	-							
8	Effluent w	9.278	-	748.4820	12372	Blank corr	-	-	No	-							
9	Effluent w	9.291	-	748.4820	14696	Blank corr	-	-	No	-							
10																	
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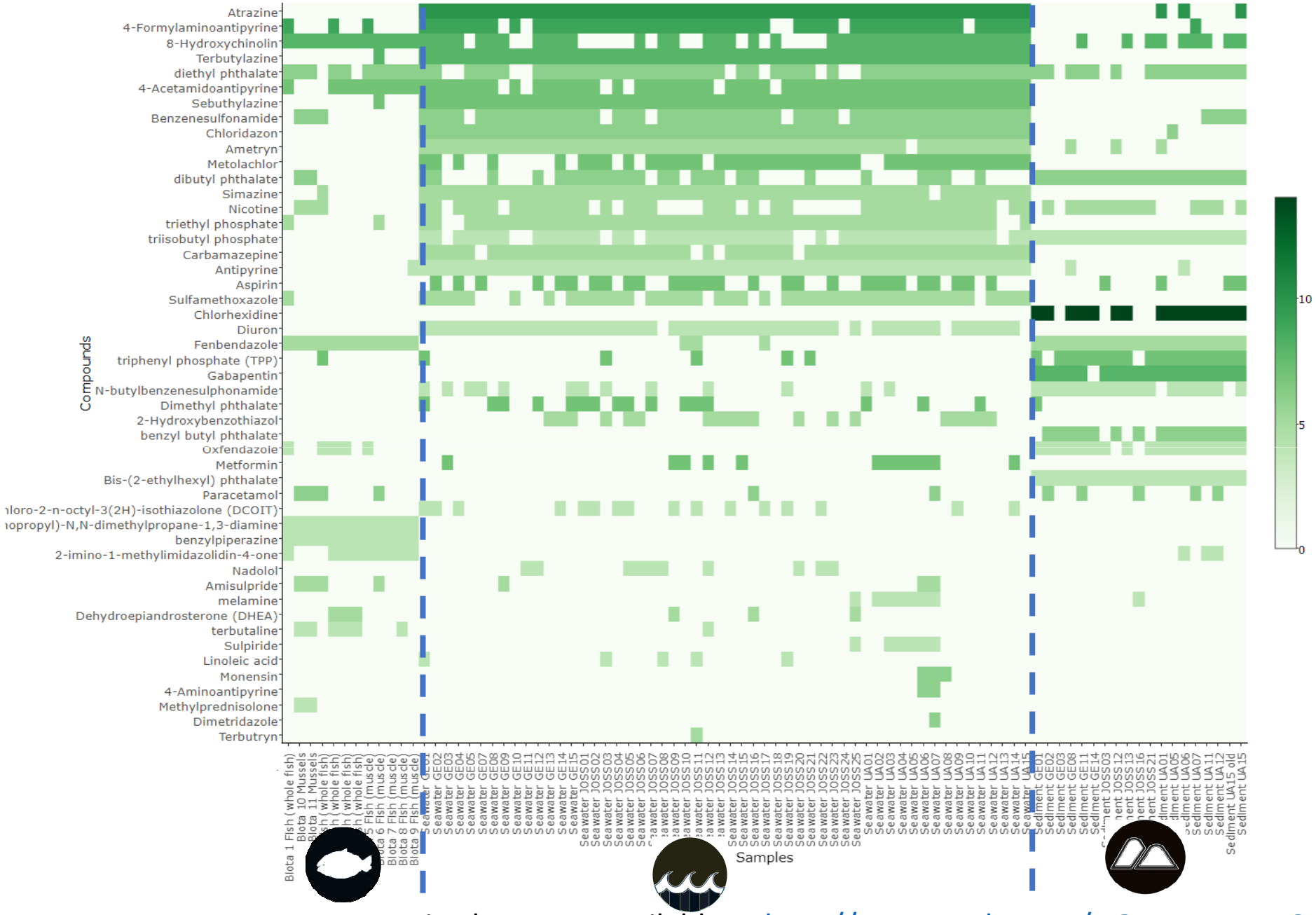
Sulfamethizole | Tiamulin | Rifaximin | Cefquinome | Dimetridazole | Sulfamethazine | Erythromycin | Azithromycin | **Clarithromycin** | Roxithromyc

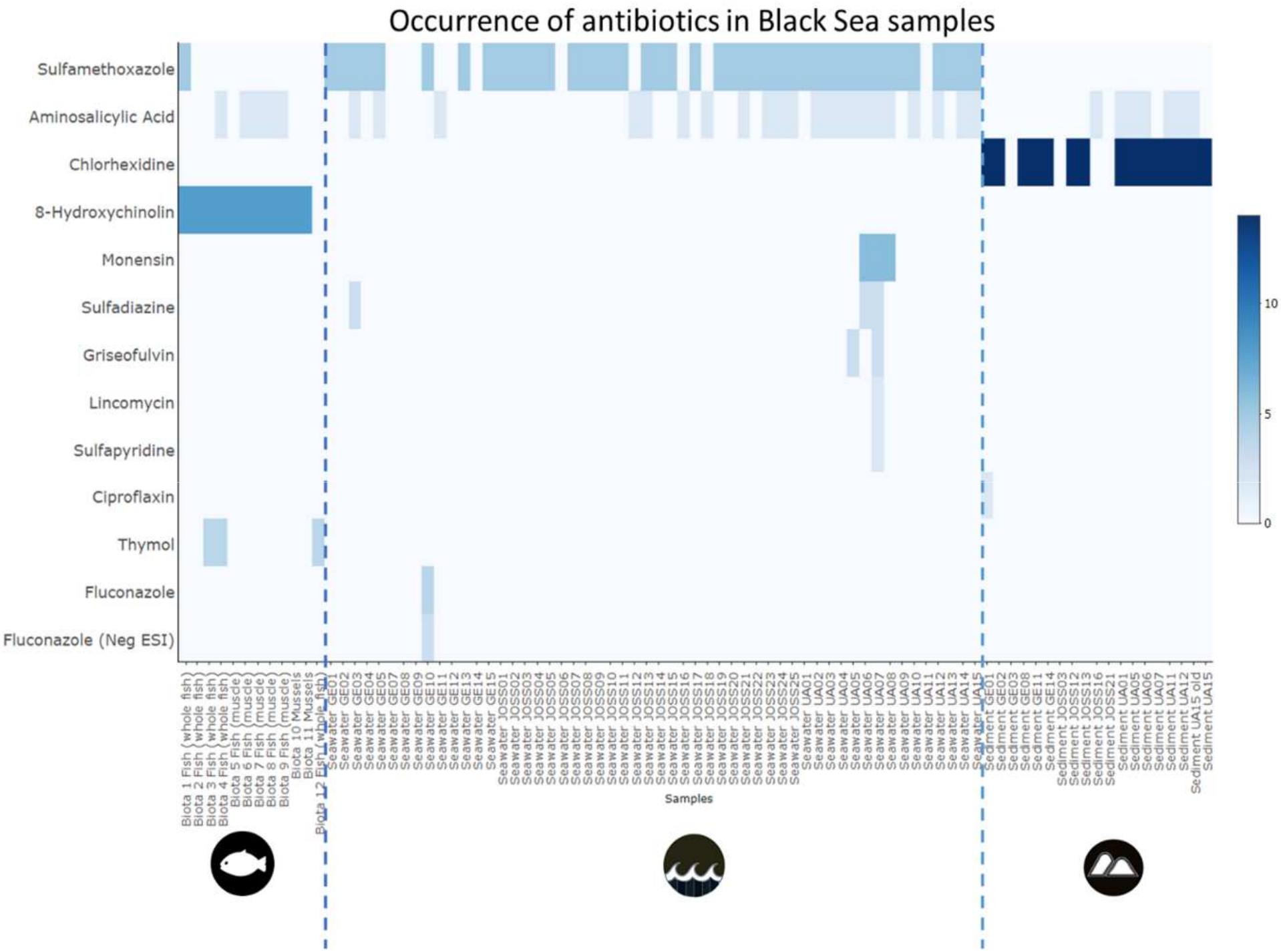
READY

Applications

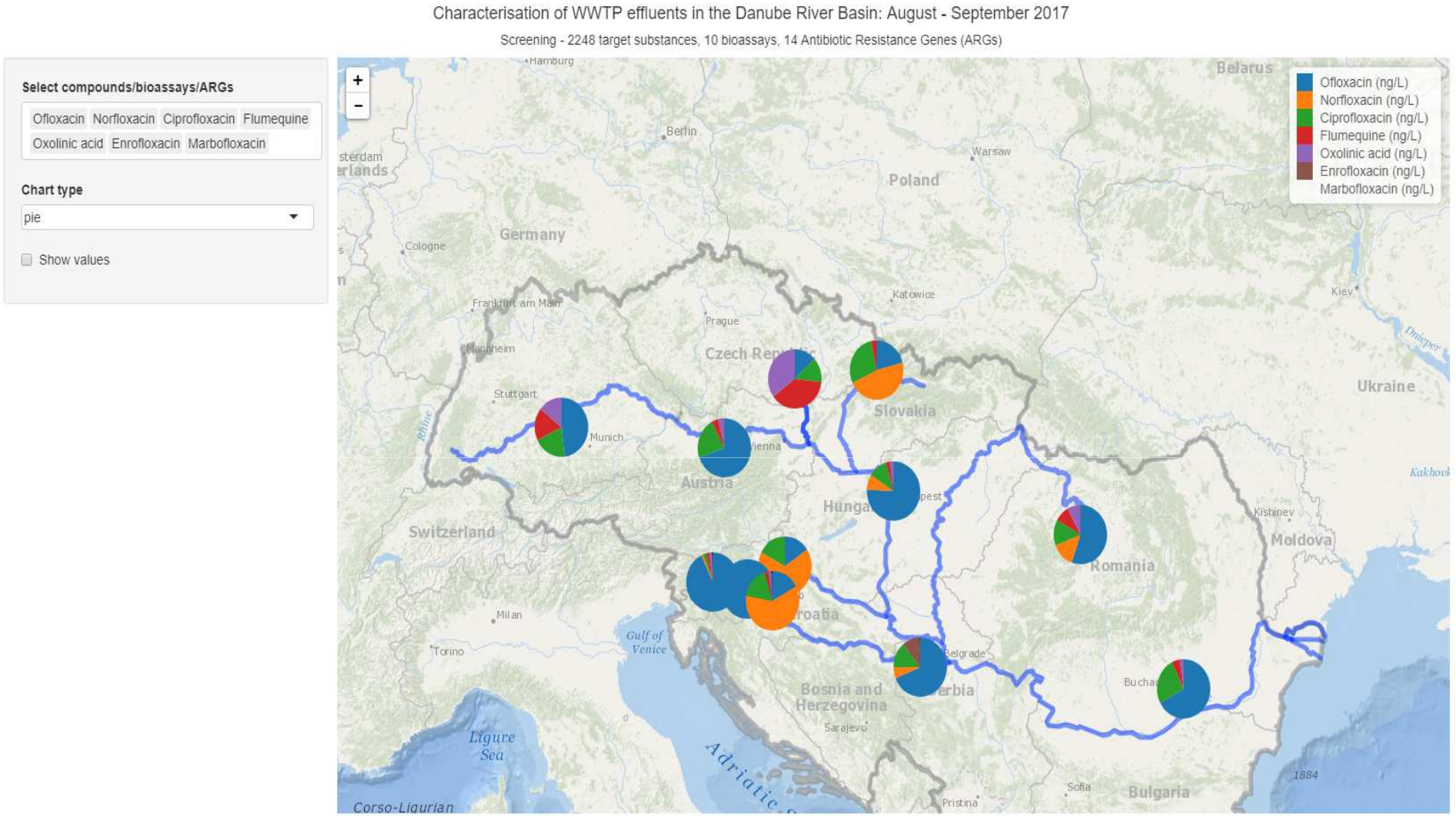
Screening of REACH compounds in samples from Black Sea



Interactive heatmap available at http://norman-data.eu/NORMAN-REACH


Occurrence of antibiotics in Black Sea samples
Sulfamethoxazole
Aminosalicylic Acid
Chlorhexidine
8-Hydroxychinolin
Monensin
Sulfadiazine
Griseofulvin
Lincomycin
Sulfapyridine
Ciproflaxin
Thymol
Fluconazole
Fluconazole (Neg ESI)
10
5
0
Biota 1 Fish (whole fish)
Biota 2 Fish (whole fish)
Biota 3 Fish (whole fish)
Biota 4 Fish (whole fish)
Biota 5 Fish (muscle)
Biota 6 Fish (muscle)
Biota 7 Fish (muscle)
Biota 8 Fish (muscle)
Biota 9 Fish (muscle)
Biota 10 Mussels
Biota 11 Mussels
Biota 12 Fish (whole fish)
Seawater GE01
Seawater GE02
Seawater GE03
Seawater GE04
Seawater GE05
Seawater GE07
Seawater GE08
Seawater GE09
Seawater GE10
Seawater GE11
Seawater GE12
Seawater GE13
Seawater GE14
Seawater GE15
Seawater JOSS01
Seawater JOSS02
Seawater JOSS03
Seawater JOSS04
Seawater JOSS05
Seawater JOSS06
Seawater JOSS07
Seawater JOSS08
Seawater JOSS09
Seawater JOSS10
Seawater JOSS11
Seawater JOSS12
Seawater JOSS13
Seawater JOSS14
Seawater JOSS15
Seawater JOSS16
Seawater JOSS17
Seawater JOSS18
Seawater JOSS19
Seawater JOSS20
Seawater JOSS21
Seawater JOSS22
Seawater JOSS23
Seawater JOSS24
Seawater JOSS25
Seawater UA01
Seawater UA02
Seawater UA03
Seawater UA04
Seawater UA05
Seawater UA06
Seawater UA07
Seawater UA08
Seawater UA09
Seawater UA10
Seawater UA11
Seawater UA12
Seawater UA13
Seawater UA14
Seawater UA15
Sediment GE01
Sediment GE02
Sediment GE03
Sediment GE08
Sediment GE11
Sediment GE14
Sediment JOSS03
Sediment JOSS12
Sediment JOSS13
Sediment JOSS16
Sediment JOSS21
Sediment UA01
Sediment UA05
Sediment UA06
Sediment UA07
Sediment UA11
Sediment UA12
Sediment UA15 old
Sediment UA15
Samples

Screening of compounds in effluent wastewater from Danube river basin



Interactive map available at http://norman-data.eu/EWW_DANUBE

Conclusions-Benefits of DSFP

- Better data management achieved by digital archiving of the HRMS chromatograms
- Fast and reliable screening of many samples for thousands emerging substances
- Update of your suspect list with new environmentally-relevant contaminants (SusDat)
- Continuous update of the fragment list of the compounds in the suspect list
- Receive enhancements in DSFP (time-series analysis, isotopic fit score, semi-quantification of detected suspects, better data analysis and visualization features)

Thanks for your attention!