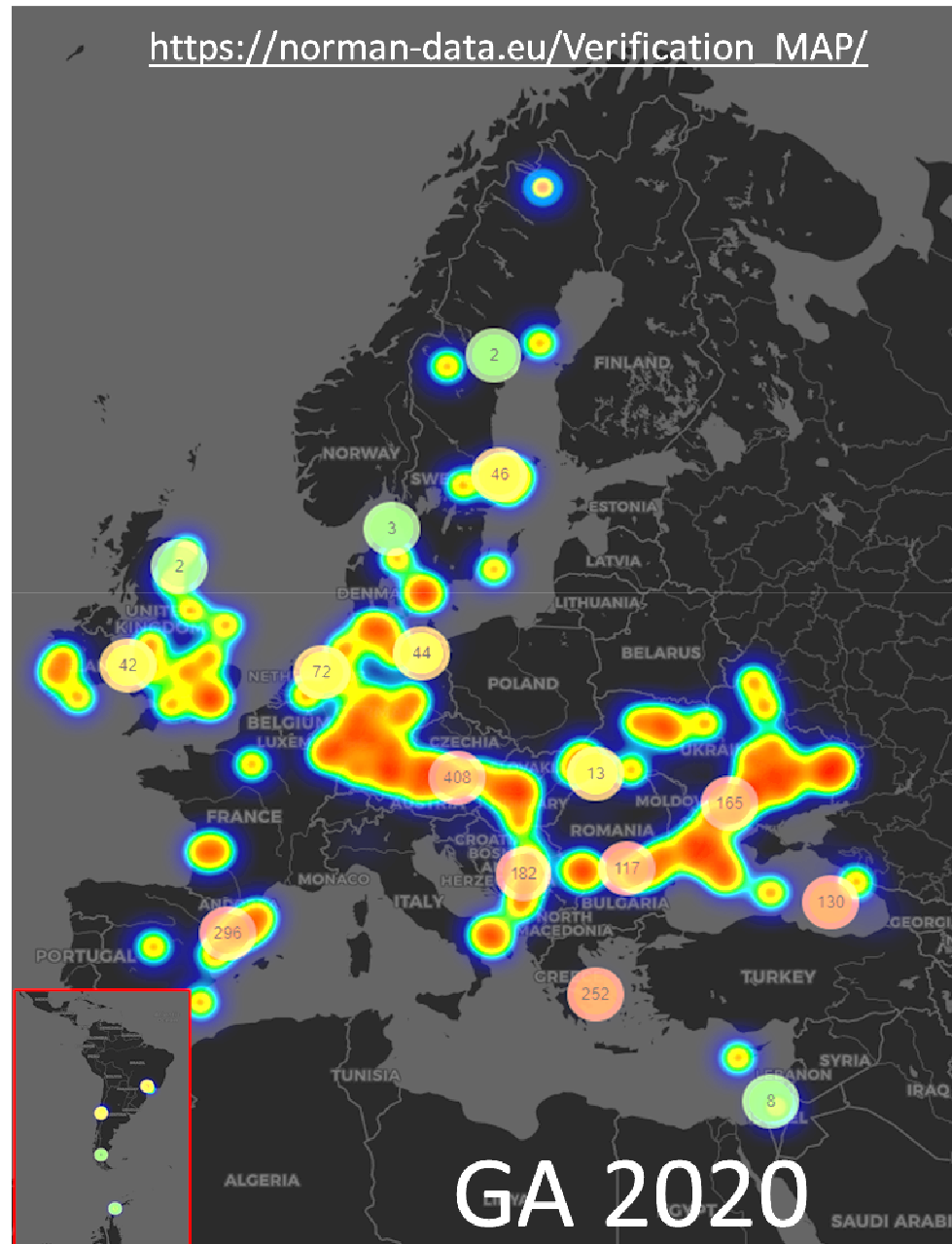# Prototype to store wide-scope suspect screening results

Nikiforos Alygizakis

NORMAN GA meeting
2nd December 2020
Virtual meeting

NORMAN DSFP

https://norman-data.eu/Verification_MAP/

GA 2020

Output of massive suspect screening exercises

Compound information

NORMAN ID	Compounds	Formula	CAS_RN	SMILES	InChI	InChIKey
NS00032465	4-(4-Methoxyphenyl)butan-1-ol	C11H16O2	CAS_RN: 52244-70-9	Lccc(CCCCC	-10(6-8-11	TLNO-UHF
NS00010583	9,10-Dihydroxystearic acid	C18H36O4	CAS_RN: 120-87-6	C(CCCCCC(	4-11-8-6-9	FMSP-UH
NS00035021	Octanoic anhydride	C16H30O3	CAS_RN: 623-66-5	(=O)OC(=C	15(17)19-1	RZODZ-UHI
NS00011498	Nonanedioic acid	C9H16O4	CAS_RN: 123-99-9	)CCCCCCCC	2-1-3-5-7-9	GNYIS-UHF

Ecotoxicological information

PNECfw ug l	PNECmarine ug l	PNECsed ugkg dw	PNECbio ugkg ww	Scientific name|Endpoint|Duration|Effect	AF	PNEC type	Uncertainty P-PNEC
9.81	0.98	56.7	306	Daphnia magna||LC50|48 h|mortality	1000	P-PNEC pred	Covered by Model
0.33	0.033	0.53	608	Selenastrum capricornutum||EC50|72 h|immobilisation	1000	P-PNEC pred	Experimental proof is needed
0.32	0.032	36.4	136	Selenastrum capricornutum||EC50|72 h|immobilisation	1000	P-PNEC pred	Covered by Model
68.6	6.86	862	136	Daphnia magna||LC50|48 h|mortality	1000	P-PNEC pred	Covered by Model

Identification information

MassErrorScore	RTI score	IsotopicFitScore	PlausibilityScore	SpectralSimilarity	NumFragments	PredictedFragments	group
0.91	0.89	0.61	0.9752	0.7752	17	TRUE	P803_17
0.88	0.76				13	TRUE	N4099_1
0.79	0.61	0.57	0.35	0.37	14	TRUE	P3441_1
0.97	0.92				5	FALSE	N9187_3

Semiquantitative information

est_Budz	ein_Pass	ampling Site 3	ampling Site 8	Kalinkov	_Noviz	Vratsa	urgiu_Gi		Pancevo_rm Kilia ar		i_U lesti_Gala	ilistra_Silis
18.3	3.1	6.0	7.2	0.0	1.0	0.1	0.1	1.4	1.0	.0	0.9	1.1
29.2		58.8	70.8	2.0	3.0	3.0	7.0		1.6	1.1		
132.0	191.0	77.0	43.1	24.0	55.0	28.0	79.0		64.0	92.7		72.8
411.6		637.6	517.1	27.0	33.0	48.0	55.0		7.0	5.6	6.0	5.4

Prioritization indicators

FoA Sed	FoA Biota	FoA GW	FoA EWW	FoA SW	FoE Sed	FoE Biota	FoE GW	FoE EWW	FoE SW	EoE Sed	EoE Biota	EoE GW	EoE EWW	EoE SW	ExposureScore_Water_KEMI	HazScore_EcoChronic_KEMI
100	100	71	73	100	0	0	0	0	0	0	0	0	0	0	0.09	0.12
75	100	100	100	51	75	0	11	100	31	1	0	6	66	5	0.11	0.02
100	100	100	82	41	100	7	8	82	9	4	2	2	28	3	0.13	0.02
50	100	100	100	73	0	0	14	0	0	0	0	2	0	0	0.51	0.01

JDS4
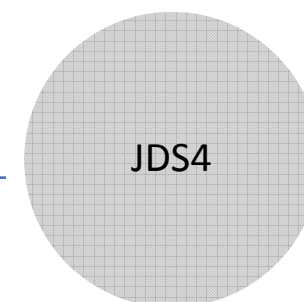
X ... (65k rows)

EMPODAT SUSPECTS
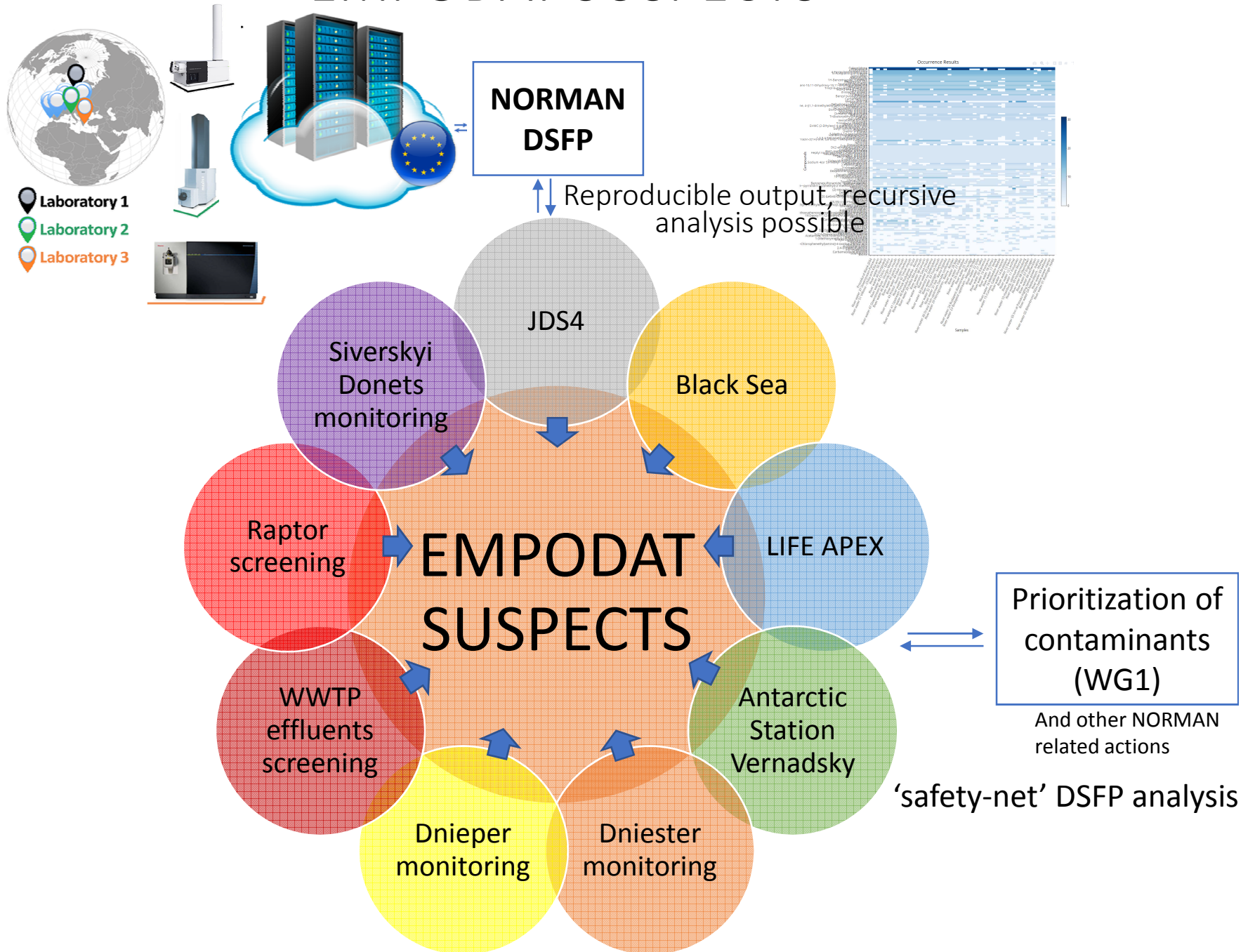
Thank you for the attention!