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Electronic supplementary information

(Very) polar organic compounds in the Danube river basin: Non-target screening workflow and prioritization strategy for extracting highly confident features

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Content:

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Table S1: Targeted analysis of the multicomponent standard: 100 reference compounds were measured in triplicates. The variation of parameter values is indicated by the standard deviation (SD) or the relative standard deviation (RSD). The maximum RT difference (ΔRT) of 1.60 min was found for histamine and this value was set for the RT tolerance of the non-targeted feature extraction method.

Compound name	**InChiKey**	**Log D (pH 7)**	**Mean RT [min]**	**SD RT [min]**	**RSD RT [%]**	**ΔRT (min)**
1-(3-carboxypropyl)-3,7-dimethyl-xanthin	WKASGTGXOGALBG-UHFFFAOYSA-N	-3.6	7.91	0.10	1.29	0.20
1,2,2,6,6-Pentamethyl-4-piperidinol	NWHNXXMYEICZAT-UHFFFAOYSA-N	-2.1	11.82	0.14	1.22	0.28
1,2-Dimethylimidazole	GIWQSPITLQVMSG-UHFFFAOYSA-N	-0.3	9.37	0.16	1.65	0.31
1,3-Dimethyl-2-imidazolidinone	CYSGHNMQYZDMIA-UHFFFAOYSA-N	-0.6	6.02	0.04	0.70	0.08
1-[N,N-Bis(2-hydroxyethyl)amino]-2-propanol	ZFECCYLNALETDE-UHFFFAOYSA-N	-3.2	9.47	0.08	0.86	0.16
1-Methylimidazole	MCTWTZJPVLRJOU-UHFFFAOYSA-N	-0.1	8.56	0.09	1.01	0.16
2-(Butylamino)ethanol	LJDSTRZHPWMDPG-UHFFFAOYSA-N	-2.4	11.55	0.08	0.72	0.15
2,2,6,6-Tetramethyl-4-piperidinol	VDVUCLWJZJHFAV-UHFFFAOYSA-N	-2.3	11.67	0.13	1.14	0.27
2,2,6,6-tetramethyl-4-piperidone	JWUXJYZVKZKLTJ-UHFFFAOYSA-N	-0.3	6.50	0.04	0.69	0.09
2,4-Diamino-6-(hydroxymethyl)pteridine	CYNARAWTVHQHDI-UHFFFAOYSA-N	-1.4	7.74	0.06	0.78	0.12
2,6-Dimethylmorpholine	HNVIQLPOGUDBSU-UHFFFAOYSA-N	-1.3	10.81	0.11	0.99	0.19
2-Aminopyridine	ICSNLGPSRYBMBD-UHFFFAOYSA-N	0.3	6.40	0.00	0.07	0.01
2-Butyne-1,4-diol	DLDJFQGPPSQZKI-UHFFFAOYSA-N	-0.7	11.67	0.12	1.04	0.24
2-Methylimidazole	LXBGSDVWAMZHDD-UHFFFAOYSA-N	-0.6	10.09	0.38	3.77	0.71
2-Phenyl-5-benzimidazole	UVCJGUGAGLDPAA-UHFFFAOYSA-N	0.1	6.96	0.07	1.04	0.13
2-Pyrrolinone	HNJBEVLQSNELDL-UHFFFAOYSA-N	-0.6	6.27	0.10	1.63	0.18
3,4-Diaminobenzoic acid	HEMGYNNCNNODNX-UHFFFAOYSA-N	-1.6	6.49	0.02	0.27	0.03
3-Aminobenzoic acid	XFDUHJPVQKIXHO-UHFFFAOYSA-N	-1.4	8.12	0.13	1.62	0.26
3-Dimethylaminopropiononitrile	MTPJEFOSTIKRSS-UHFFFAOYSA-N	-0.3	6.45	0.04	0.57	0.07
3-Pyridinemethanol	MVQVNTPHUGQQHK-UHFFFAOYSA-N	0.0	6.40	0.02	0.24	0.03
4-(2-Hydroxyethyl)morpholine	KKFDCBRMNNSAAW-UHFFFAOYSA-N	-1.1	7.01	0.04	0.54	0.07
4-Formylmorpholine	LCEDQNDDFOCWGG-UHFFFAOYSA-N	-0.9	6.01	0.02	0.33	0.04
4-Methylimidazole	XLSZMDLNRCVEIJ-UHFFFAOYSA-N	-0.3	9.21	0.20	2.21	0.39
4-Methylmorpholine	SJRJJKPEHAURKC-UHFFFAOYSA-N	-0.7	8.31	0.02	0.23	0.03
4-Pyrimidinol	DNCYBUMDUBHIJZ-UHFFFAOYSA-N	-0.6	6.85	0.14	2.11	0.29

6-Amino-1,3-dimethyl-5-(formylamino)uracil	ZNDGAXCBZGSJGU-UHFFFAOYSA-N	-2.0	6.92	0.05	0.70	0.09
Acamprosate	AFCGFAGUEYAMAO-UHFFFAOYSA-N	-4.1	7.30	0.07	0.98	0.14
Acetaminophen	RZVAJINKPMORJF-UHFFFAOYSA-N	0.9	6.39	0.12	1.82	0.21
Acetylcholine	OIPILFWXSMYKGL-UHFFFAOYSA-N	-4.2	11.66	0.08	0.72	0.15
Acetyllysine	DTERQYGMUDWYAZ-UHFFFAOYSA-N	-3.2	13.04	0.30	2.26	0.58
Adenine	GFFGJBXGBJISGV-UHFFFAOYSA-N	-0.6	7.75	0.06	0.78	0.12
Adenosine	OIRDTQYFTABQOQ-UHFFFAOYSA-N	-2.1	7.71	0.02	0.26	0.04
Allantoin	POJWUDADGALRAB-UHFFFAOYSA-N	-2.4	10.46	0.03	0.32	0.06
Arecoline	HJJPJSXJAXAIPN-UHFFFAOYSA-N	-0.6	6.85	0.02	0.28	0.04
Asulam	VGPYEHKOIGNJKV-UHFFFAOYSA-N	-0.6	6.10	0.07	1.16	0.12
Atenolol	METKIMKYRPQLGS-UHFFFAOYSA-N	-2.1	11.38	0.05	0.47	0.11
Betaine	KWIUHFFTVRNATP-UHFFFAOYSA-O	-3.7	14.94	0.44	2.96	0.77
Bisoprolol-M3	WONQRVASZHJNFS-UHFFFAOYSA-N	-1.2	12.54	0.02	0.18	0.04
Caffeine	RYYVLZVUVIJVGH-UHFFFAOYSA-N	-0.6	6.05	0.01	0.18	0.02
Candesartan	HTQMVQVXFRQIKW-UHFFFAOYSA-N	-0.1	7.18	0.10	1.33	0.18
Chlorsulfuron	VJYIFXVZLXQVHO-UHFFFAOYSA-N	1.6	5.92	0.08	1.28	0.14
Cimetidine	AQIXAKUUQRKLND-UHFFFAOYSA-N	-0.3	7.24	0.07	0.92	0.13
Ciprofloxacin	MYSWGUAQZAJSOK-UHFFFAOYSA-N	-0.8	6.98	0.04	0.53	0.07
Cytosine	OPTASPLRGRRNAP-UHFFFAOYSA-N	-1.2	9.24	0.19	2.04	0.35
Dacarbazine	OMJKFYKNWZZKTK-UXBLZVDNSA-N	-1.7	7.80	0.21	2.75	0.38
Dicyandiamide	QGBSISYHAICWAH-UHFFFAOYSA-N	-1.0	6.63	0.02	0.31	0.04
Diisopropylamine	UAOMVDZJSHZZME-UHFFFAOYSA-N	-1.8	10.94	0.09	0.85	0.17
Dimethylsulfoxide	IAZDPXIOMUYVGZ-UHFFFAOYSA-N	-1.4	6.05	0.01	0.13	0.02
Dipropylamine	WEHWNAOGRSTTBQ-UHFFFAOYSA-N	-1.6	10.58	0.07	0.71	0.15
Ectoine	WQXNXVUDBPYKBA-UHFFFAOYSA-N	-2.5	12.74	0.02	0.13	0.03
Etilefrine	SQVIAVUSQAWMKL-UHFFFAOYSA-N	-1.4	11.38	0.06	0.57	0.13
Famotidine	XUFQPHANEAPEMJ-UHFFFAOYSA-N	-3.0	7.30	0.06	0.83	0.11
Gabapentin	UGJMXCAKCUNAIE-UHFFFAOYSA-N	-1.3	9.98	0.02	0.18	0.03
Gamma-aminobutyric acid	BTCSSZJGUNDROE-UHFFFAOYSA-N	-2.9	13.75	0.04	0.26	0.07

Glycine ethyl ester	NTNZTEQNFHNYBC-UHFFFAOYSA-N	-1.0	6.69	0.04	0.54	0.07
Guanylurea	SQSPRWMERUQXNE-UHFFFAOYSA-N	-2.1	14.51	0.20	1.35	0.36
Histamine	NTYJJOPFIAHURM-UHFFFAOYSA-N	-3.9	15.01	0.80	5.36	1.60
Isopentylamine	BMFVGAAISNGQNM-UHFFFAOYSA-N	-1.8	10.92	0.07	0.66	0.14
L-Alanine	QNAYBMKLOCPYGJ-UHFFFAOYSA-N	-2.8	13.23	0.08	0.60	0.16
Lenalidomid	GOTYRUGSSMKFNF-UHFFFAOYSA-N	-0.7	13.35	0.09	0.66	0.16
Leucine	ROHFNLRQFUQHCH-UHFFFAOYSA-N	-1.6	11.07	0.07	0.64	0.14
Lisinopril	RLAWWYSOJDYHDC-BZSNNMDCSA-N	-3.1	13.07	0.03	0.23	0.05
L-Isoleucine	AGPKZVBTJJNPAG-WHFBIAKZSA-N	-1.5	11.31	0.06	0.55	0.13
L-Phenylalanine	COLNVLDHVKWLRT-UHFFFAOYSA-N	-1.2	10.98	0.08	0.76	0.14
L-Proline	ONIBWKKTOPOVIA-UHFFFAOYSA-N	-2.6	12.50	0.04	0.34	0.08
L-Threonine	AYFVYJQAPQTCCC-GBXIJSLDSA-N	-3.5	11.38	0.10	0.86	0.18
L-Tyrosine	OUYCCCASQSFEME-QMMMGPOBSA-N	-1.5	12.26	0.03	0.28	0.07
Melamine	JDSHMPZPIAZGSV-UHFFFAOYSA-N	-2.0	9.51	0.20	2.05	0.39
Metformin	XZWYZXLIPXDOLR-UHFFFAOYSA-N	-3.7	15.04	0.76	5.04	1.45
Methacrylic acid	CERQOIWHTDAKMF-UHFFFAOYSA-N	-1.2	13.76	0.04	0.30	0.08
Methylisothiazolinone	BEGLCMHJXHIJLR-UHFFFAOYSA-N	0.2	6.07	0.01	0.15	0.02
Metoprolol acid	PUQIRTNPJRFRCZ-UHFFFAOYSA-N	-1.0	12.48	0.01	0.10	0.02
Miglitol	IBAQFPQHRJAVAV-ULAWRXDQSA-N	-3.9	11.58	0.03	0.29	0.06
Moroxydine	KJHOZAZQWVKILO-UHFFFAOYSA-N	-5.4	13.89	0.73	5.23	1.45
N-(Hydroxymethyl)nicotinamide	JRFKIOFLCXKVOT-UHFFFAOYSA-N	-0.8	6.49	0.02	0.27	0.03
N,N'-Ethylenebisacetamide	WNYIBZHOMJZDKN-UHFFFAOYSA-N	-1.8	6.23	0.03	0.56	0.07
N,N'-Trimethyleneurea	NQPJDJVGBDHCAD-UHFFFAOYSA-N	-1.0	6.70	0.03	0.40	0.05
N-[3-(dimethylamino)propyl]methacrylamide	GDFCSMCGLZFNFY-UHFFFAOYSA-N	-1.9	12.21	0.31	2.58	0.62
N-Hydroxyethyl acrylamide	CNCOEDDPFOAUMB-UHFFFAOYSA-N	-0.6	6.21	0.01	0.21	0.02
N-Methylurea	XGEGHDBEHXKFPX-UHFFFAOYSA-N	-1.1	6.24	0.02	0.35	0.04
Norphenylephrine	LRCXRAABFLIVAI-UHFFFAOYSA-N	-1.9	14.32	0.34	2.39	0.63
Omethoate	PZXOQEXFMJCDPG-UHFFFAOYSA-N	-0.6	6.01	0.04	0.63	0.07
Oxaceprol	BAPRUDZDYCKSOQ-WDSKDSINSA-N	-4.7	11.93	0.07	0.55	0.12

Panthenol	SNPLKNRPJHDVJA-ZETCQYMHSA-N	-1.7	6.62	0.03	0.47	0.06
Piracetam	GMZVRMREEHBGGF-UHFFFAOYSA-N	-1.7	6.36	0.05	0.73	0.08
Pregabalin	AYXYPKUFHZROOJ-ZETCQYMHSA-N	-1.4	10.33	0.13	1.30	0.25
Pyridoxine	LXNHXLLTXMVWPM-UHFFFAOYSA-N	-1.0	6.72	0.11	1.58	0.21
Riboflavin	AUNGANRZJHBGPY-UHFFFAOYSA-N	-1.2	7.77	0.06	0.77	0.12
Ritalinic acid	INGSNVSERUZOAK-UHFFFAOYSA-N	-0.4	8.58	0.02	0.18	0.03
Sarcosine	FSYKKLYZXJSNPZ-UHFFFAOYSA-N	-3.2	13.04	0.07	0.57	0.15
Sotalol	ZBMZVLHSJCTVON-UHFFFAOYSA-N	-2.5	10.70	0.13	1.17	0.25
Taurine	XOAAWQZATWQOTB-UHFFFAOYSA-N	-2.6	12.79	0.20	1.53	0.34
Tetraethylene glycol	UWHCKJMYHZGTIT-UHFFFAOYSA-N	-1.4	6.26	0.04	0.56	0.07
Tetraethylene glycol dimethylether	ZUHZGEOKBKGPSW-UHFFFAOYSA-N	-0.1	6.19	0.07	1.19	0.13
Triethanolamine	GSEJCLTVZPLZKY-UHFFFAOYSA-N	-3.3	11.57	0.13	1.15	0.26
Triethylene glycol monomethyl ether	JLGLQAWTXXGVEM-UHFFFAOYSA-N	-0.7	6.03	0.01	0.13	0.01
Triisopropanolamine	SLINHMUFWFWBMU-UHFFFAOYSA-N	-2.9	6.82	0.06	0.88	0.12
Tyramine	DZGWFCGJZKJUFP-UHFFFAOYSA-N	-1.5	11.82	0.16	1.34	0.31
Vidarabine	OIRDTQYFTABQOQ-UHTZMRCNSA-N	-2.1	8.48	0.08	0.95	0.16
Vigabatrin	PJDFLNIOAUIZSL-UHFFFAOYSA-N	-2.1	12.91	0.20	1.52	0.35

Table S2: Targeted analysis to optimize the feature extraction method: 34 reference compounds were measured at two concentration levels, three times in each case (n = 6). The variation of parameter values is indicated by the standard deviation (SD) or the relative standard deviation (RSD). Peak width was expressed by the full width at half maximum (FWHM).

Compound name	InChiKey	log D (pH 7)	Mean m/z [Da]	RSD m/z [ppm]	Mass error [ppm]	ΔMass [Da]	Mean RT [min]	SD RT [min]	RSD RT [%]	Δ RT [min]	Mean peak height [cps/Da]	SD peak height [cps/Da]	Mean peak duration time [min]	SD peak duration time [min]	Mean FWHM [min]	SD FWHM [min]
1,1'-Iminodipropan-2-ol	LVTYICIALWPMFW-UHFFFAOYSA-N	-3.2	134.1199	1.5	17.2	0.0005	14.70	0.06	0.4	0.19	583	529	1.45	0.46	0.52	0.06
1,2,2,6,6-Pentamethyl-4-piperidinol	NWHNXXMYEICZAT-UHFFFAOYSA-N	-2.1	172.1720	2.8	13.8	0.0013	11.77	0.03	0.2	0.08	1065	923	2.32	0.80	0.24	0.04
1-[N,N-Bis(2-hydroxyethyl)amino]-2-propanol	ZFECCYLNALETDE-UHFFFAOYSA-N	-3.2	164.1312	3.1	19.0	0.0013	9.93	0.05	0.5	0.14	3075	2525	2.03	0.47	0.61	0.15
2,2,6,6-Tetramethyl-4-piperidinol	VDVUCLWJZJHFAV-UHFFFAOYSA-N	-2.3	158.1566	1.3	17.1	0.0005	11.57	0.02	0.2	0.05	869	684	0.84	0.30	0.18	0.02
2,4-Diamino-6-hydroxymethylpteridine	CYNARAWTVHQHDI-UHFFFAOYSA-N	-1.4	193.0844	2.0	5.8	0.0006	9.03	0.02	0.2	0.06	871	741	1.29	0.48	0.43	0.10
2-Butylaminoethanol	LJDSTRZHPWMDPG-UHFFFAOYSA-N	-2.4	118.1246	1.8	16.9	0.0009	11.66	0.02	0.2	0.05	956	831	0.64	0.17	0.17	0.03
4-(2-Hydroxyethyl)morpholine	KKFDCBRMNNSAAW-UHFFFAOYSA-N	-1.1	132.1020	0.6	1.0	0.0002	7.81	0.02	0.3	0.05	573	461	1.42	0.52	0.23	0.04
Acetyllysine	DTERQYGMUDWYAZ-UHFFFAOYSA-N	-3.2	189.1232	4.6	-0.9	0.0025	13.08	0.05	0.4	0.15	1792	1459	1.54	0.40	0.37	0.04
Adenine	GFFGJBXGBJISGV-UHFFFAOYSA-N	-0.6	136.0641	2.1	17.1	0.0009	9.01	0.08	0.9	0.20	171	113	0.86	0.28	0.25	0.12
Adenosine	OIRDTQYFTABQOQ-UHFFFAOYSA-N	-2.1	268.1084	0.4	16.1	0.0003	9.04	0.05	0.5	0.13	9339	8182	1.72	0.31	0.44	0.02
Atenolol	METKIMKYRPQLGS-UHFFFAOYSA-N	-2.1	267.1746	1.3	15.9	0.0010	13.87	0.09	0.7	0.24	4156	3705	2.73	0.64	0.87	0.05
Bisoprolol-M3	WONQRVASZHJNFS-UHFFFAOYSA-N	-1.2	254.1427	1.4	15.6	0.0009	12.46	0.01	0.1	0.02	11724	10540	0.88	0.32	0.19	0.03
Creatinine	DDRJAANPRJIHGJ-UHFFFAOYSA-N	-1.5	114.0681	6.9	16.7	0.0021	13.09	0.02	0.2	0.06	626	545	2.06	0.51	0.47	0.17
Ectoine	WQXNXVUDBPYKBA-UHFFFAOYSA-N	-2.5	143.0839	3.7	16.8	0.0013	12.65	0.02	0.1	0.05	2177	1889	0.84	0.21	0.18	0.04

Glutathion	RWSXRVCMGQZWBV-UHFFFAOYSA-N	0.0	308.0919	2.1	2.7	0.0017	12.59	0.03	0.2	0.09	297	224	0.24	0.06	0.10	0.05
Guanylurea	SQSPRWMERUQXNE-UHFFFAOYSA-N	-2.1	103.0618	1.0	3.3	0.0003	14.32	0.01	0.1	0.04	271	154	0.66	0.16	0.23	0.04
Hydroxyproline	PMMYEEVYMWASQN-DMTCNVIQSA-N	-3.7	132.0676	2.9	15.9	0.0011	13.49	0.03	0.2	0.07	531	514	0.67	0.36	0.17	0.03
L-Citrulline	RHGKLRLOHDJJDR-UHFFFAOYSA-N	-3.9	176.1004	4.1	-14.5	0.0020	13.88	0.03	0.2	0.07	854	698	1.20	0.52	0.28	0.16
Glutamate	WHUUTDBJXJRKMK-VKHMYHEASA-N	-5.9	148.0604	3.2	-0.6	0.0013	12.64	0.02	0.2	0.06	241	119	0.71	0.10	0.40	0.36
L-Glutamic acid	WHUUTDBJXJRKMK-UHFFFAOYSA-N	-5.9	148.0630	5.3	1.6	0.0022	12.57	0.02	0.2	0.06	320	192	0.53	0.23	0.19	0.04
Lisinopril	RLAWWYSOJDYHDC-BZSNNMDCSA-N	-3.1	406.2332	2.0	-1.2	0.0018	13.50	0.02	0.2	0.07	662	566	1.55	1.20	0.43	0.21
L-Proline	ONIBWKKTOPOVIA-UHFFFAOYSA-N	-2.6	116.0731	2.5	21.3	0.0009	12.51	0.09	0.7	0.25	336	281	0.89	0.62	0.20	0.12
L-Tyrosine	OUYCCCASQSFEME-QMMMGPOBSA-N	-1.5	182.0827	3.9	8.2	0.0020	12.52	0.05	0.4	0.13	258	162	0.54	0.25	0.20	0.08
Methyl-3-aminocrotonate	XKORCTIIRYKLLG-ONEGZZNKSA-N	-0.2	116.0720	4.7	12.1	0.0014	12.53	0.04	0.3	0.11	166	118	0.73	0.17	0.28	0.08
Metoprolol acid	PUQIRTNPJRFRCZ-UHFFFAOYSA-N	-1.0	268.1547	2.3	1.3	0.0017	12.41	0.01	0.1	0.03	8854	7699	0.95	0.38	0.16	0.01
Miglitol	IBAQFPQHRJAVAV-ULAWRXDQSA-N	-3.9	208.1209	3.5	14.2	0.0020	11.43	0.03	0.3	0.09	589	491	0.77	0.32	0.22	0.03
Moroxydine	KJHOZAZQWVKILO-UHFFFAOYSA-N	-5.4	172.1194	1.2	0.5	0.0006	13.61	0.02	0.1	0.05	1235	1108	3.12	1.14	0.79	0.21
N-Acetylethanolamine	PVCJKHHOXFKFRP-UHFFFAOYSA-N	-1.5	104.0708	2.2	2.2	0.0007	13.77	0.01	0.1	0.04	166	121	0.93	0.37	0.15	0.07
Panthenol	SNPLKNRPJHDVJA-UHFFFAOYSA-N	-1.7	206.1392	1.9	2.5	0.0009	8.35	0.02	0.3	0.06	496	413	1.30	0.42	0.42	0.08
Pyridoxine	LXNHXLLTXMVWPM-UHFFFAOYSA-N	-1.0	170.0844	5.4	19.0	0.0025	7.60	0.01	0.1	0.03	3292	2548	1.19	0.53	0.29	0.07
Sotalol	ZBMZVLHSJCTVON-UHFFFAOYSA-N	-2.5	273.1324	3.3	20.8	0.0025	14.91	0.08	0.5	0.23	4081	3476	2.26	0.40	1.08	0.26

Tranexamic acid	GYDJEQRTZSCIOI-UHFFFAOYSA-N	-1.5	158.1204	3.2	17.9	0.0015	13.95	0.02	0.1	0.04	1581	1364	0.67	0.33	0.14	0.01
Triethylene glycol monomethyl ether[1]	JLGLQAWTXXGVEM-UHFFFAOYSA-N	-0.7	165.1153	3.8	19.1	0.0017	9.55	0.29	3.0	0.61	666	181	1.82	0.43	0.60	0.14
Triisopropanolamine	SLINHMUFWFWBMU-UHFFFAOYSA-N	-2.9	192.1629	4.2	18.3	0.0022	8.64	0.02	0.2	0.04	2743	2250	2.85	0.83	0.76	0.16
Vidarabine	OIRDTQYFTABQOQ-UHTZMRCNSA-N	-2.1	268.1050	2.5	3.6	0.0017	9.79	0.06	0.6	0.14	1949	1667	1.58	0.62	0.43	0.03

Table S3: Detailed descriptions of the 51 samples taken from the Danube river and several of its tributaries are shown below. Geographical coordinates are presented in decimal degrees and the river kilometer of either the Danube or the respective tributary river is given.

Sample number	Location/Country	River	Latitude	Longitude	River kilometer	Sampling date	Comment
1	Böfinger Halde/DE	Danube	48.42405	10.02688	2581	06/29/2019	
2	Bittenbrunn/DE	Danube	48.73599	11.15507	2479	06/29/2019	700 m downstream power station
3	Kelheim/DE	Danube	48.91648	11.86462	2415	06/30/2019	Upstream gauging station
4	Niederalteich/DE	Danube	48.77453	13.00914	2276	06/30/2019	
5	Passau/DE	Inn	48.55678	13.43575	4	07/01/2019	Downstream power station
6	Jochenstein Hinding/AT	Danube	48.58452	13.52854	2218	07/01/2019	
7	Enghagen/AT	Danube	48.24042	14.51204	2113	07/02/2019	
8	Oberloiben/AT	Danube	48.38832	15.52271	2008	07/02/2019	
9	Klosterneuburg/AT	Danube	48.33012	16.32987	1942	07/03/2019	
10	Hainburg/AT	Danube	48.16390	16.99168	1879	07/03/2019	Upstream Morava
11	Pohansko/CZ	Morava, Dyje	48.72349	16.88528	17	07/04/2019	
12	Lanzhot/CZ	Morava	48.68721	16.98931	79	07/04/2019	
13	Devín/SK	Morava	48.18768	16.97596	1	07/05/2019	
14	Bratislava/SK	Danube	48.14232	17.06576	1969	07/05/2019	
15	Čunovo, Gabcikovo resevoir/SK	Danube	48.04025	17.23058	1855	07/03/2019	
16	Medvedov, Medve/SK, HU	Danube	47.78952	17.65977	1806	07/03/2019	
17	Vének/HU	Moson Danube arm	47.73617	17.78158	0	07/04/2019	
18	Gönyű/HU	Danube	47.74265	17.84397	1790	07/04/2019	
19	Komárno/SK	Vah	47.76091	18.14233	3	07/04/2019	
20	Kamenica/SK	Hron	47.82608	18.72334	2	07/05/2019	
21	Salka/SK	Ipeľ	47.88596	18.76256	12	07/05/2019	
22	Szop/HU, SK	Danube	47.81340	18.86323	1707	07/06/2019	
23	Megyeri Bridge/HU	Danube	47.61603	19.10177	1660	07/06/2019	Budapest upstream
24	M0 bridge/HU	Danube	47.38830	19.00408	1630	07/07/2019	Budapest downstream
25	Tass/HU	Ráckevei-Soroksári	47.03398	18.97820	59	07/07/2019	
26	Dunafoldvar/HU	Danube	46.81707	18.92632	1560	07/08/2019	

27	Paks/HU	Danube	46.63373	18.88042	1532	07/08/2019	
28	Baja/HU	Danube	46.20053	18.92350	1481	07/09/2019	
29	Hercegszanto, Batina, Bezdan/HU, HR, RS	Danube	45.91455	18.80593	1434	07/09/2019	
30	Drava/HR	Drava	45.55224	18.86460	5	07/10/2019	5 km upstream Danube confluence
31	Ilok, Backa Palanka/HR, RS	Danube	45.23158	19.36060	1300	07/09/2019	
32	Tiszasziget, Martonoš/HU, RS	Tisza	46.18552	20.10467	163	07/10/2019	
33	Tisza mouth	Tisza	45.14700	20.28087	1	07/09/2019	
34	Jesenice na Dolenjskem/SI	Sava	45.86092	15.69200	729	07/08/2019	
35	Jamena/RS, BA	Sava	44.87828	19.08364	205	07/08/2019	
36	Sava mouth/RS	Sava	44.79300	20.39607	7	07/07/2019	
37	Pancevo/RS	Danube	44.81447	20.64443	1151	07/07/2019	
38	Varvarin/RS	Velika Morava	43.74000	21.38000	154	07/06/2019	
39	Velika Morava mouth/RS	Velika Morava	44.70927	21.03570	1	07/06/2019	
40	Banatska Palanka, Bazias/RS, RO	Danube	44.80510	21.38380	1073	07/05/2019	
41	Radujevac, Gruia/RS, RO	Danube	44.26092	22.68498	847	07/05/2019	
42	Timok mouth/RS, BG	Timok	44.21492	22.67215	0	07/04/2019	
43	Pristol, Novo Selo Harbour/ RO, BG	Danube	44.17230	22.78217	837	07/04/2019	
44	Iskar mouth/ BG	Iskar	43.72990	24.44382	0	07/03/2019	
45	Jantra mouth/ BG	Jantra	43.63748	25.56987	1	07/03/2019	
46	Russenski Lom mouth/ BG	Russenski Lom	43.83482	25.93092	0	07/02/2019	
47	Ruse, Giurgiu/ BG, RO	Danube	43.91083	26.06696	488	07/02/2019	
48	Chiciu, Silistra/ RO, BG	Danube	44.13693	27.05112	375	07/01/2019	
49	Giurgiulesti/ MD, RO	Prut	45.47187	28.19673	1	06/30/2019	
50	Reni/ RO, UA	Danube	45.45630	28.26013	132	06/29/2019	
51	Vilkova/ RO, UA	Danube	45.39455	29.58140	18	06/29/2019	

Table S4: The exact parameter settings of the feature extraction method executed with MZmine 2 software are shown. The RT and mass tolerances, the signal intensity threshold as well as the parameters for wavelet scaling (peak duration range and RT wavelet range) were set based on the target analysis of two synthetic samples (Table S2). When setting these parameters, absolute minima and/or maxima of all compounds and injections were favored over mean values across the six technical replicates (given in brackets) in order to reduce the number of false negative features.

Processing module	**Description**	**Parameter**	**Setting**	**Comment**
Mass detection	Generates a list of ions for each scan	Algorithm	Centroid	Only algorithm available for centroided data
		RT range	5 min – 15 min	Corresponds to the HILIC elution window
		MS levels	1+2	Scan as well as fragmentation experiments were included
		Polarity	+	MS data was acquired in positive ionization mode
		Spectrum type	Centroided	The raw data was centroided during conversion to mzML file format
		Noise level	1.0 cps Da^{-1}, 0.0 cps Da^{-1}	Corresponds to MS level 1 and 2, respectively
ADAP chromatogram builder	Constructs EICs using the ADAP algorithms[1]	Minimum group size in number of scans	5	Corresponds to the expected scan span of a chromatographic peak
		Group intensity threshold	10 cps Da^{-1}	Data points below this threshold were excluded from EIC building
		Minimum highest intensity	49 (166) cps Da^{-1}	Derived from targeted analysis of the synthetic samples (minimum peak height, Table S2)
		m/z tolerance	0.0026 (0.0014) Da	Derived from targeted analysis of the synthetic samples (maximum mass difference)
Smoothing	Applies Savitzky-Golay smoothing to EICs	Filter width	17	Number of data points necessary to smooth HILIC peaks with a FWHM up to 1.08 ± 0.26 min (n = 6)
Chromatogram deconvolution	Separates each chromatogram into	Algorithm	Wavelets (ADAP)	ADAP algorithms reduce the risk of false positives without compromising sensitivity[1]

	individual peaks	S/N threshold	10	Reduces risk of deconvoluting noise
		Minimum feature height	45 (160) cps Da^{-1}	Derived from targeted analysis of the synthetic samples considering smoothing effects
		Coefficient/area threshold	30	Filters out low-quality peaks by maintaining a recovery > 50% of target compounds at a lower concentration level
		Peak duration range	0.13 (0.23) min – 4.40 (3.13) min	Derived from target data of synthetic samples (peak duration time) and iteratively adjusted to increase recovery rates
		RT wavelet range	0.03 (0.10) min – 1.58 (1.09) min	Estimated from target data of synthetic samples (FWHM) and iteratively adjusted to increase recovery rates
		m/z center calculation	Median	
Join aligner	Aligns detected peaks across replicate samples	m/z tolerance	0.0026 (0.0014) Da	
		Weight for m/z	1	
		RT tolerance	1.60 (0.20) min	Derived from target data of the multicomponent standard (maximum RT difference, Table S1)
		Weight for RT	1	
Isotopic peaks grouper	Recognizes isotopic patterns within defined RT and mass ranges and removes all peaks except the highest isotope	m/z tolerance	0.0026 (0.0014) Da	
		RT tolerance	1.60 (0.20) min	
		Maximum charge	1	Predominantly expected for small molecules
		Representative isotope	Lowest m/z	
Adduct search	Recognizes adduct peaks within defined RT and mass range	RT tolerance	1.60 (0.20) min	
		Adduct m/z differences	21.9825 Da, 37.9559 Da,	Correspond to sodium, potassium and ammonium adducts

			17.0265 Da	
		m/z tolerance	0.0026 (0.0014) Da	
		Maximum relative adduct peak height	100%	Full peak height of the adduct was accepted relative to the main peak
Feature list rows filter	Removes features from aligned list based on specified criteria	Maximum peaks in a row	3	Used to filter out peaks found in less than three replicates

[1] O. D. Myers, S. J. Sumner, S. Li, S. Barnes and X. Du, Anal. Chem., 2017, 89, 8696–8703.

Table S5: Target compounds which were identified as false negative features at the end point of the feature extraction workflow are listed below. The standard compounds were contained in two synthetic samples, one at a lower concentration level (c1) and the other one at a higher concentration level (c2) (Table S2). The targets were tracked throughout the steps of the workflow and the points of losses were identified. Green boxes indicate the chromatographic peak or feature corresponding to the target was found, red boxes mean it was not found.

C1	Chromatogram building (1)	Chromatogram building (2)	Chromatogram building (3)	Smoothing (1)	Smoothing (2)	Smoothing (3)	Chromatogram deconvolution (1)	Chromatogram deconvolution (2)	Chromatogram deconvolution (3)	Alignment	Replicate filter	Isotope removal	Adduct removal	
2,2,6,6-Tetramethyl-4-piperidinol														
Creatinine														
Glutathion														
L-Citrulline														
L-Glutamic acid														
Lisinopril														
L-Proline														
L-Tyrosine														
Methyl 3-aminocrotonate														
Miglitol														
N-Acetylethanolamine														
Sotalol														
Vidarabine														

C2														
1,2,2,6,6-Pentamethyl-4-piperidinol														
Glutathion														
Lisinopril														

Table S6: The features of category B defined by their accurate masses and RTs are listed below with the respective candidates suggested by the STOFF-IDENT database. Source indications were taken from the PubChem database[1]. "*" symbolizes that ecotoxicological values are available on the PubChem database and "AT" indicates acute toxicity as specified by the Globally Harmonized System of Classification and Labeling of Chemicals. The candidate substances were searched by their InChiKeys in the MassBank database[2]. The criteria to consider an entry comparable to the observed data were: The MS2 spectra had to be recorded on a LC-ESI-QTOF instrument in positive ionization mode at a collision energy of 20 – 60 eV or ramps which touched that interval.

ID	**Mean mass [Da]**	**Mean RT [min]**	Sample number(s) with (amount n)	**Name**	**InChiKey**	**Elemental formula**	**Monoisotopic mass**	**Log D (pH 7)**	**Source**	**MassBank entry**
1	95.0479 ± 0.0000	10.00 ± 0.00	35, 40 (2)	2-aminopyrimidine	LJXQPZWIHJMPQQ-UHFFFAOYSA-N	C4H5N3	95.0483	-0.1	Ambiguous	No
2	97.9673 ± 0.0001	7.84 ± 0.15	1, 2, 3, 8, 24, 44 (6)	Sulfuric acid	QAOWNCQODCNURD-UHFFFAOYSA-N	H2O4S	97.9674	-5.6	*Industry use (i.e. pigments), consumer use (i.e. air care products)	No
3	99.0681	9.02	32 (1)	1-methyl-2-pyrrolidone	SECXISVLQFMRJM-UHFFFAOYSA-N	C5H9NO	99.0684	-0.4	*Industry use (i.e. solvents), consumer use (i.e. cleaning and furnishing care products)	Yes
4	100.1002 ± 0.0004	11.75 ± 0.02	39, 43, 47 (3)	1-methylpiperazine	PVOAHINGSUIXLS-UHFFFAOYSA-N	C5H12N2	100.1	-2.8	AT Industry use (intermediates)	No
5	100.0997 ± 0.0001	14.79 ± 0.09	1, 2, 3, 4, 5, 6, 7, 8, 9, 10 (10)							
6	113.0584	12.71	7 (1)	2-imino-1-methylimidazolidin-4-one	DDRJAANPRJIHGJ-UHFFFAOYSA-N	C4H7N3O	113.0589	-1.5	Pharmaceutical related, human metabolite	Yes
7	122.0733	8.62	16 (1)	Chlormequat	JUZXDNPBRPUIOR-UHFFFAOYSA-N	C5H13ClN	122.0731	-3.3	*Pesticide	No
8	122.0727 ± 0.0001	12.50 ± 0.06	15, 17, 19, 31, 33, 37, 43, 46, 48, 49, 50, 51 (12)							
9	126.0649 ± 0.0001	12.29 ± 0.05	47, 48, 49, 50 (4)	Melamine	JDSHMPZPIAZGSV-UHFFFAOYSA-N	C3H6N6	126.0654	-2.0	*Industry use (i.e. flame retardants), consumer use (i.e. adhesives)	Yes
10	127.0489 ± 0.0001	13.74 ± 0.08	43, 44, 46, 47, 48, 49, 50 (7)	Cyanurodiamide (=Atrazin-desethyl-desisopropyl-2-hydroxy)	MASBWURJQFFLOO-UHFFFAOYSA-N	C3H5N5O	127.0494	-1.7	Hair conditioner, toys	No
11	128.0582	13.38	35 (1)	5,5-dimethylhydantoin	YIROYDNZEPTFOL-UHFFFAOYSA-N	C5H8N2O2	128.0586	-0.5	*Industry use (i.e. intermediates),	No

									consumer use	
12	128.1310 ± 0.0003	11.14 ± 0.05	41, 46, 47, 49 (4)	1-ethylpyrrolidin-2-ylmethylamine	UNRBEYYLYRXYCG-UHFFFAOYSA-N	C7H16N2	128.1313	-3.2	Pharmaceutical related	No
13	129.1261 ± 0.0001	11.22 ± 0.03	42, 44, 46, 47, 48, 49, 50 (7)	2-piperazin-1-ylethylamine	IMUDHTPIFIBORV-UHFFFAOYSA-N	C6H15N3	129.1266	-5.6	*Industry use (i.e. adhesives), consumer use (i.e. paper products)	Yes
14	132.0781	12.39	49 (1)	2,2-dimethyl-1,3-dioxolan-4-ylmethanol	RNVYQYLELCKWAN-UHFFFAOYSA-N	C6H12O3	132.0786	-0.1	Industry use (i.e. solvents)	No
15	134.0585	9.84	1 (1)	2,2-bis(hydroxymethyl)propionic acid	PTBDIHRZYDMNKB-UHFFFAOYSA-N	C5H10O4	134.0579	-3.8	Industry use (i.e. lubricants), consumer use (i.e. adhesives)	No
16	134.0593 ± 0.0000	10.09 ± 0.00	35, 40 (2)	Nitrilotriacetonitrile	LJAIDEYQVIJERM-UHFFFAOYSA-N	C6H6N4	134.0592	-1.2	[AT] Industry use (ion exchange agents)	No
17	134.0593 ± 0.0000	12.44 ± 0.00	35, 40 (2)							
18	135.0542	13.87	7 (1)	Adenine	GFFGJBXGBJISGV-UHFFFAOYSA-N	C5H5N5	135.0545	-0.6	[AT] Dietary supplement, human metabolite	Yes
19	137.0585 ± 0.0001	9.81 ± 0.03	1, 2, 3, 19 (4)	Isoniazid	QRXWMOHMRWLFEY-UHFFFAOYSA-N	C6H7N3O	137.0589	-0.7	Pharmaceutical	No
20	138.0790	9.78	1 (1)	4-amino-2-(aminomethyl)phenol	PZKNKZNLQYKXFV-UHFFFAOYSA-N	C7H10N2O	138.0793	-2.7	Prohibited/ restricted hair dye	No
21	140.0835 ± 0.0001	8.71 ± 0.16	10, 16, 30, 33, 46 (5)	Octalynol	BQDKCWCMDBMLEH-UHFFFAOYSA-N	C8H12O2	140.0837	-0.4	Fatty acyls	No
22	141.0784	8.76	20 (1)	4-(1-oxo-2-propenyl)-morpholine	XLPJNCYCZORXHG-UHFFFAOYSA-N	C7H11NO2	141.079	-0.1	Industry use (paint and coating additives)	No
23	141.1150	8.13	20 (1)	4-(diethylamino)-2-butyn-1-ol	ACGZBRWTWOZSFU-UHFFFAOYSA-N	C8H15NO	141.1154	-0.8	Pharmaceutical related	No
24	143.9740	5.95	20 (1)	Ethephon	UDPGUMQDCGORJQ-UHFFFAOYSA-N	C2H6ClO3P	143.9743	-2.9	[AT] *Pesticide	No
25	146.1049	14.95	41 (1)	Lysine	KDXKERNSBIXSRK-UHFFFAOYSA-N	C6H14N2O2	146.1055	-5.3	Flavoring agent	Yes
26	148.0746 ± 0.0000	10.05 ± 0.00	35, 40 (2)	Propanenitrile, 2-[bis(cyanomethyl)amino]-	FIIUFZGDWANGEJ-UHFFFAOYSA-N	C7H8N4	148.0749	-0.6	[AT] Ambiguous	No
27	151.0744 ± 0.0003	9.76 ± 0.06	16, 17, 19, 38, 46, 49, 50 (7)	2,3-Diaminobenzamide	NAWJZCSEYBQUGY-UHFFFAOYSA-N	C7H9N3O	151.0746	-0.2	Ambiguous	No

28	152.0833 ± 0.0003	8.64 ± 0.06	2, 14, 25, 29, 30, 47 (6)	(3-chloro-2-hydroxypropyl)trimethylammonium	XIUCEANTZSXBQQ-UHFFFAOYSA-N	C6H15ClNO	152.0837	-3.9	Ambiguous	No
29	152.0835 ± 0.0004	12.59 ± 0.07	26, 36, 42, 46 (4)							
30	152.1307 ± 0.0002	11.19 ± 0.04	41, 42, 43, 44, 46, 47, 48, 49, 50 (9)	1,8-diazabicyclo[5.4.0]undec-7-ene	GQHTUMJGOHRCHB-UHFFFAOYSA-N	C9H16N2	152.1313	-1.6	[AT] Industry use (intermediates, process regulators)	No
31	157.1462 ± 0.0004	11.76 ± 0.02	7, 24, 30, 41, 43, 47, 48, 49, 50, 51 (10)	2,2,6,6-tetramethylpiperidin-4-ol	VDVUCLWJZJHFAV-UHFFFAOYSA-N	C9H19NO	157.1467	-2.3	Industry use (intermediates)	No
32	159.0535 ± 0.0004	12.41 ± 0.02	3, 32 (2)	Methyl 2-hydroxy-2-(1-oxo-2-propenylamino)acetate	YJOJMHVTEACTIC-UHFFFAOYSA-N	C6H9NO4	159.0532	-0.7	Ambiguous	No
33	163.9898 ± 0.0004	10.71 ± 0.07	41, 42, 43, 44, 45, 46, 47, 49 (8)	Pentafluoropropionic acid	LRMSQVBRUNSOJL-UHFFFAOYSA-N	C3HF5O2	163.9897	-1.9	Ambiguous	No
34	164.1044	8.85	7 (1)	2-(2-(2-methoxyethoxy)ethoxy)ethanol	JLGLQAWTXXGVEM-UHFFFAOYSA-N	C7H16O4	164.1049	-0.7	*Industry use (i.e. functional fluids), consumer use (i.e. automotive care products)	No
35	166.0849	7.68	42 (1)	Oxybispropanediol	GPLRAVKSCUXZTP-UHFFFAOYSA-N	C6H14O5	166.0841	-2.5	Industry use (viscosity adjustors)	No
36	169.0851 ± 0.0001	14.93 ± 0.03	48, 49, 50 (3)	1-Methyl-L-Histidin	BRMWTNUJHUMWMS-UHFFFAOYSA-N	C7H11N3O2	169.0851	-3.1	Ambiguous	No
37	169.0854	8.70	25 (1)							
38	169.1100	5.95	46 (1)	Aceclidine	WRJPSSPFHGNBMG-UHFFFAOYSA-N	C9H15NO2	169.1103	-1.9	Pharmaceutical	No
39	169.1100 ± 0.0003	8.43 ± 0.31	8, 20, 29, 36, 44 (5)							
40	169.1098	12.54	18 (1)							
41	171.1253	8.61	7 (1)	1-(aminomethyl)cyclohexaneacetic acid	UGJMXCAKCUNAIE-UHFFFAOYSA-N	C9H17NO2	171.1259	-1.3	Pharmaceutical	Yes
42	175.0632 ± 0.0003	8.59 ± 0.05	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 36, 37, 38, 39, 41, 43, 44, 46, 47, 48,	m-(1-cyanoethyl)benzoic acid	IRYIYPWRXROPSX-UHFFFAOYSA-N	C10H9NO2	175.0633	-1.0	Ambiguous	No

			49, 50, 51 (45)							
43	177.0643	12.62	38 (1)	2-hydroxyethyliminodi(acetic acid)	JYXGIOKAKDAARW-UHFFFAOYSA-N	C6H11NO5	177.0637	-7.6	Adhesive, pesticide	No
44	180.0785 ± 0.0005	8.73	13 (1)	3-(4-Methoxyphenyl)propanoic acid	FIUFLISGGHNPSM-UHFFFAOYSA-N	C10H12O3	180.0786	-0.7	Ambiguous	No
45	182.0215 ± 0.0005	7.65 ± 0.27	5, 9, 10, 24, 26, 30, 33 (7)	Monoperoxyphthalato(2-)	GLVYLTSKTCWWJR-UHFFFAOYSA-N	C8H6O5	182.0215	-2.1	Ambiguous	No
46	182.0923	8.62	25 (1)	Dacarbazine	OMJKFYKNWZZKTK-UXBLZVDNSA-N	C6H10N6O	182.0916	-1.7	Ambiguous	No
47	185.1047 ± 0.0002	12.51 ± 0.06	5, 8, 18, 20 (4)	Ecgonine	PHMBVCPLDPDESM-FKSUSPILSA-N	C9H15NO3	185.1052	-3.1	Narcotic	No
48	186.1365 ± 0.0001	12.59 ± 0.05	5, 8, 18, 20, 29 (5)	N,N'-methylenebismorpholine	MIFZZKZNMWTHJK-UHFFFAOYSA-N	C9H18N2O2	186.1368	-0.1	Pesticide, disinfectant, lubricant, …	No
49	187.1202 ±0.0004	8.17 ± 0.04	20, 29 (2)	(3R)-3-(2-amino-2-oxoethyl)-5-methylhexanoic acid	NPDKTSLVWGFPQG-UHFFFAOYSA-N	C9H17NO3	187.1208	-1.5	Ambiguous	No
50	188.1156 ± 0.0004	13.75 ± 0.06	3, 8 (2)	Acetyllysine	DTERQYGMUDWYAZ-UHFFFAOYSA-N	C8H16N2O3	188.1161	-3.2	Ambiguous	No
51	191.1163	12.92	32 (1)	1-o-tolylbiguanide	SQZCAOHYQSOZCE-UHFFFAOYSA-N	C9H13N5	191.1171	-1.3	Industry use (paints and coatings), consumer use (paints and coatings)	No
52	191.1517 ± 0.0001	13.46 ± 0.07	41, 42, 44 (3)	1,1',1''-nitrilotripropan-2-ol	SLINHMUFWFWBMU-UHFFFAOYSA-N	C9H21NO3	191.1521	-2.9	Industry use (i.e. solvents), consumer use (building materials)	No
53	192.0751	12.59	31 (1)	(2,4-Diaminopteridin-6-yl)methanol	CYNARAWTVHQHDI-UHFFFAOYSA-N	C7H8N6O	192.076	-1.4	Ambiguous	No
54	194.0692 ± 0.0002	13.40 ± 0.01	4, 8, 20 (3)	3-Acetamido-5-aminobenzoic acid	SETVYNZSWPLKAO-UHFFFAOYSA-N	C9H10N2O3	194.0691	-2.3	Ambiguous	No
55	194.1152 ± 0.0001	8.65 ± 0.54	7, 50 (2)	3,6,9-trioxaundecane-1,11-diol	UWHCKJMYHZGTIT-UHFFFAOYSA-N	C8H18O5	194.1154	-1.4	Industry use (i.e. solvents), consumer use (i.e. lubricant)	No
56	199.9895 ± 0.0001	7.67 ± 0.34	47, 48 (2)	4-Thiazoleacetic acid, 2-(formylamino)-a-oxo-	JPJMIBGVCGNFQD-UHFFFAOYSA-N	C6H4N2O4S	199.9892	-3.1	Pharmaceutical related	No
57	201.1728 ± 0.0002	10.14 ± 0 .04	1, 2, 3, 4, 5, 6, 7, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 29, 30, 32, 33, 34, 35, 36,	4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	STEYNUVPFMIUOY-UHFFFAOYSA-N	C11H23NO2	201.1729	-2.6	Ambiguous	Yes

			37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51 (47)							
58	201.1729 ± 0.0003	12.95 ± 0.17	8, 9, 28, 31 (4)							
59	205.0587 ± 0.0004	12.46 ± 0.03	14, 16, 17, 18, 19, 22, 24, 25, 27, 29, 38, 39, 41, 43, 44, 45, 47, 48, 50, 51 (20)	N,N-Bis(carboxymethyl)alanine	CIEZZGWIJBXOTE-UHFFFAOYSA-N	C7H11NO6	205.0586	-9.9	Industry use (i.e. ion exchange agents), consumer use (i.e. laundry and dishwashing products)	No
60	209.0719 ± 0.0002	12.53 ± 0.07	2, 4, 11, 13, 20, 21, 22, 23, 25, 33, 37, 38, 42, 43, 49, 50 (16)	3-morpholin-4-ylpropane-1-sulfonic acid	DVLFYONBTKHTER-UHFFFAOYSA-N	C7H15NO4S	209.0722	-2.7	Industry use (laboratory chemicals, intermediates)	No
61	210.0018 ± 0.0000	11.86 ± 0.00	35, 40 (2)	Dimethipin	PHVNLLCAQHGNKU-UHFFFAOYSA-N	C6H10O4S2	210.0021	-1.5	*Pesticide	No
62	217.1312 ± 0.0003	8.65 ± 0.07	8, 20, 29 (3)	N-[(tert-butoxy)carbonyl]-L-valine	SZXBQTSZISFIAO-UHFFFAOYSA-N	C10H19NO4	217.1314	-1.0	Ambiguous	No
63	217.1304	13.12	21 (1)							
64	219.1470 ± 0.0003	13.41 ± 0.04	7, 21, 22, 25, 27, 30, 32, 36, 37, 41, 42, 43, 44, 47, 48, 49, 50, 51 (18)	Miglustat	UQRORFVVSGFNRO-UTINFBMNSA-N	C10H21NO4	219.1471	-2.7	Pharmaceutical	No
65	221.1420	13.41	31 (1)	3,4-methylenedioxypropylamphetamine	LBXMQBTXOLBCCA-UHFFFAOYSA-N	C13H19NO2	221.1416	-0.3	[AT] Ambiguous	No
66	226.1065	14.95	41 (1)	Nimorazole	MDJFHRLTPRPZLY-UHFFFAOYSA-N	C9H14N4O3	226.1066	-0.1	Pharmaceutical	No
67	233.1621	13.15	21 (1)	Panthenyl ethyl ether	MRAMPOPITCOOIN-UHFFFAOYSA-N	C11H23NO4	233.1627	-0.7	Hair conditioner	No
68	236.1038	7.89	6 (1)	2-Carboxy-Ibuprofen	DIVLBIVDYADZPL-UHFFFAOYSA-N	C13H16O4	236.1049	-2.4	Ambiguous	No
69	240.1222	14.95	42 (1)	(S)-4-amino-5-[(2-(1H-imidazol-4-yl)ethyl)amino]-5-oxopentanoic acid	FLEVPMVPMJVEDN-QMMMGPOBSA-N	C10H16N4O3	240.1222	-3.9	Hair conditioner	No
70	244.9996 ± 0.0008	7.83 ± 0.27	3, 36, 44, 45, 50 (5)	Benzoic acid, 4-(methylsulfonyl)-2-nitro-	QNOUABMNRMROSL-UHFFFAOYSA-N	C8H7NO6S	244.9994	-3.1	Pesticide transformation product	No
71	244.9992 ± 0.0007	9.31 ± 0.03	8, 10, 20, 33, 34 (5)							
72	257.1024	13.80	2 (1)	Benserazide	BNQDCRGUHNALGH-UHFFFAOYSA-N	C10H15N3O5	257.1012	-2.6	Pharmaceutical	No

73	267.0963	8.63	2 (1)	Vidarabine	OIRDTQYFTABQOQ-UHTZMRCNSA-N	C10H13N5O4	267.0968	-2.1	Discontinued pharmaceutical	No
74	270.1063	9.88	23 (1)	Tolonium	KZEUBCUXBNEMSQ-UHFFFAOYSA-O	C15H16N3S	270.1059	-1.0	Ambiguous	No
75	287.0789 ± 0.0003	13.30 ± 0.67	32, 33 (2)	Tenofovir	SGOIRFVFHAKUTI-UHFFFAOYSA-N	C9H14N5O4P	287.0783	-3.5	Pharmaceutical	No
76	306.0013	10.92	39 (1)	2,2'-dithiodi(benzoic acid)	LBEMXJWGHIEXRA-UHFFFAOYSA-N	C14H10O4S2	306.0021	-2.8	Ambiguous	No
77	355.8745 ± 0.0004	5.90 ± 0.04	13, 17 (2)	2,5-dichloro-4,6-dicyano-benzene-1,3-disulfonic acid	KRIHZDRHCUOOQO-UHFFFAOYSA-N	C8H2Cl2N2O6S2	355.8731	-3.5	Pesticide transformation product	No

[1] Compound database PubChem of the National Center for Biotechnology Information, https://pubchem.ncbi.nlm.nih.gov/, (accessed 9 December 2020).
[2] European MassBank mass spectral database of the NORMAN network, https://massbank.eu/MassBank/, (accessed: 1 February 2021).