

Notat vedrørende kemisk analyse af miljøfarlige forurenende stoffer i slam fra renseanlæg

Miljøstyrelsen fik ultimo 2021 udført analyser af slam fra fem spildevandsanlæg. Opgaven var opdelt i fire delopgaver med analyse for; 1) lægemidler, 2) biocider og andre stoffer, 3) PFAS og 4) non-targeted analyse. Eurofins udførte delopgaver 1-3 og Aarhus Universitet udførte delopgave 4. De fem spildevandsanlæg var Bjergmarken (Roskilde), Egå (Aarhus), Ejby Mølle (Odense), Herning og Måløv.

Delopgaver 1-3 (måltrettet analyser)

- I alt er der analyseret for 454 lægemidler, biocider, PFAS og andre stoffer i delopgave 1-3.
- Der blev fundet og bestemt koncentrationer for 53 forskellige stoffer (**Tabel 1**).
- Der blev målt for yderligere 401 stoffer der ikke blev fundet (**Tabel A1**).
- Der er brugt forskellige prøveforberedelses- og analysemetoder, som væskevæske og fastfase ekstraktion og gas og væske kromatografi koblet med massespektrometri.
- Delprøver for 6PPD-quinone blev analyseret ved Eurofins i Sacramento, USA. Forsendelsespapirer viser at prøverne var ikke opbevaret på køl/frost under transport.
- Det er ikke muligt at vurdere analysekvaliteten, såsom genfindning, da der ikke er oplysninger om de anvendte surrogat standarder (interne standarder), på nær i et enkelt tilfælde (6PPD-quinone).
- Eurofins har interne kvalitetskontrol parametre og kriterier på surrogat standarder, men kan ikke oplyses til dette notat arbejde (personlig komm. med Eurofins, Lea Mejdahl Lind).
- Partikelbundet MFS vil sandsynligvis kun delvist eller ikke bliver ekstraheret med de anvendte metoder.
- Tørstof af slam var i gennemsnit 23.5% (interval: 18.6-30.4%)
- Rapporteret detektionsgrænser for de 454 stoffer er i mellem 0.001 til 0.5 mg/kg tørstof.
- Den ekspanderede relative måleusikkerhed er typisk højere end 49%.
- Størstedelen af stofferne er rapporteret 'detekteret' men med koncentrationer typisk angivet som 'mindre end' to gange detektionsgrænsen, f.eks. Cyfluthrin-beta <0.020 mg/kg.
- MFS der er opgivet med 'mindre end' ('<') koncentrationer betragtes som "ikke detekteret" (personlig komm. med Eurofins, Lea Mejdahl Lind) og er ikke medtaget i dette notat.
- Derudover er der analyseret to vandfraktioner. Brug af vandige koncentrationer er (sandsynligvis) ikke retvisende for MFS koncentrationer i slam. De to vandige prøver er ikke taget med i dette notat.

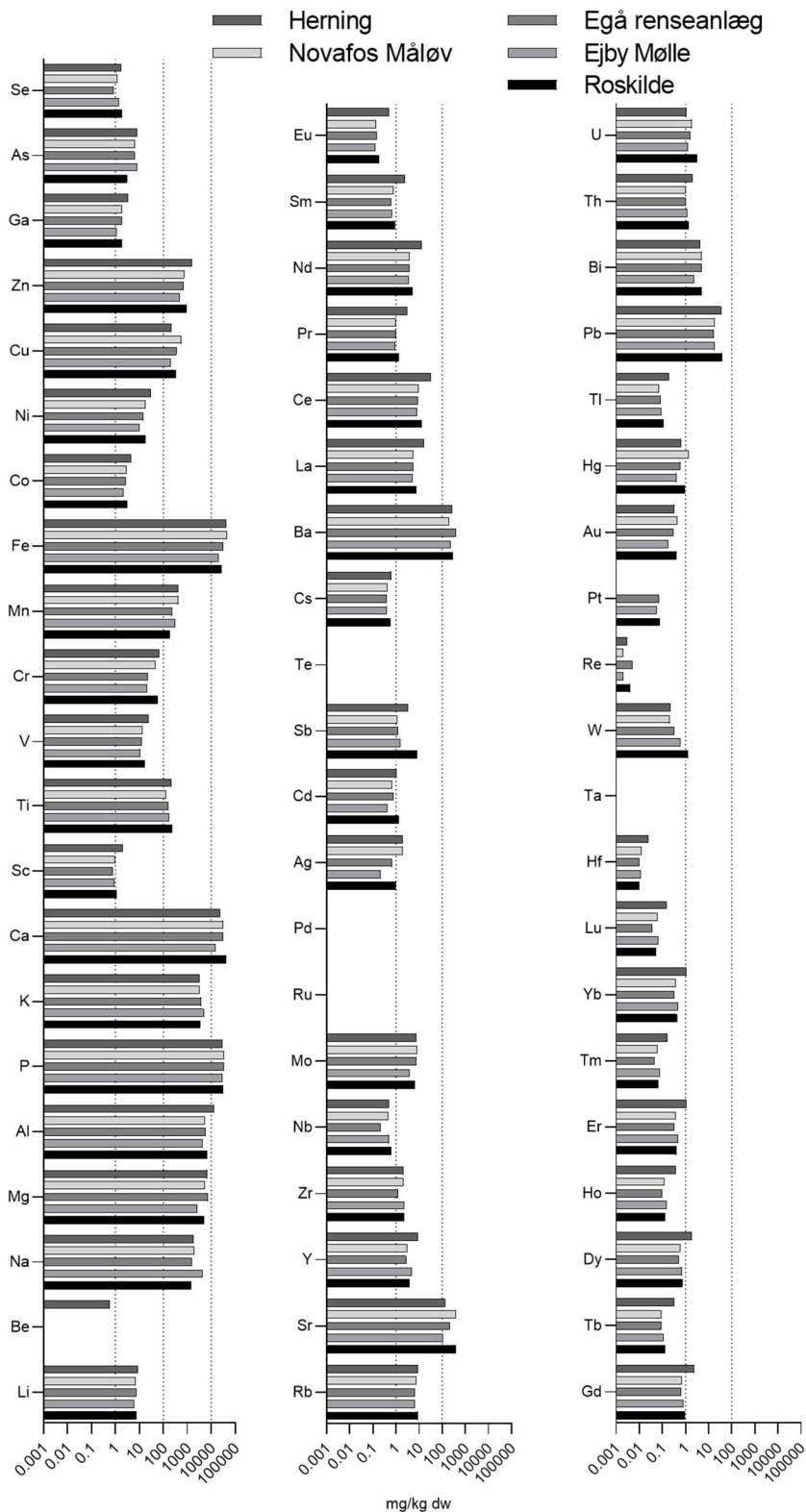
Delopgave 4 (non-targeted analyse)

- Slamprøverne blev ekstraheret med state-of-the-art metoder (pressurized liquid extraction) der anses for at ekstrahere en større andel af MFS i sammenligning med metoderne anvendt i delopgaverne 1-3.
- Fem forskellige høj-opløsningsmassespektrometri platforme blev anvendt til analyserne.
- Koncentrationer af 61 uorganiske elementer blev bestemt med ICP-MS (**Fig 1**).
- Ca. 20,000 organiske stoffer blev detekteret med NTA.
- 41 stoffer identificeret (identifikationsniveau 1) med detektionsfrekvens og estimeret koncentrationer (**Tabel 2**).
- Tentative stofnavne på 1,751 stoffer for identifikationsniveau 2 og 7,091 stoffer for identifikationsniveau 3, og yderligere 15,471 stoffer kombineret på niveau 4 og 5.
- Af de 1,751 stoffer på identifikationsniveau 2 er de 695 stoffer bestemt med LC platforme (og angivet i **Tabel A2**)
- Det var muligt at finde 26 MFS (angivet i stoflister fra delopgave 1-3) i NTA datasættet (**Tabel 3**).
- Der arbejdes forsat (retrospektivt) med at identificere flere stoffer i NTA datasættet.
- Isotopmærket surrogat standarder (interne standarder) blev tilsat prøverne før ekstraktion (32 surrogat standarder for GC workflow og 15 til LC workflow).
- Gennemsnitlig genfinding for surrogat standarder var 39% og 84% for hhv. GC og LC workflow.

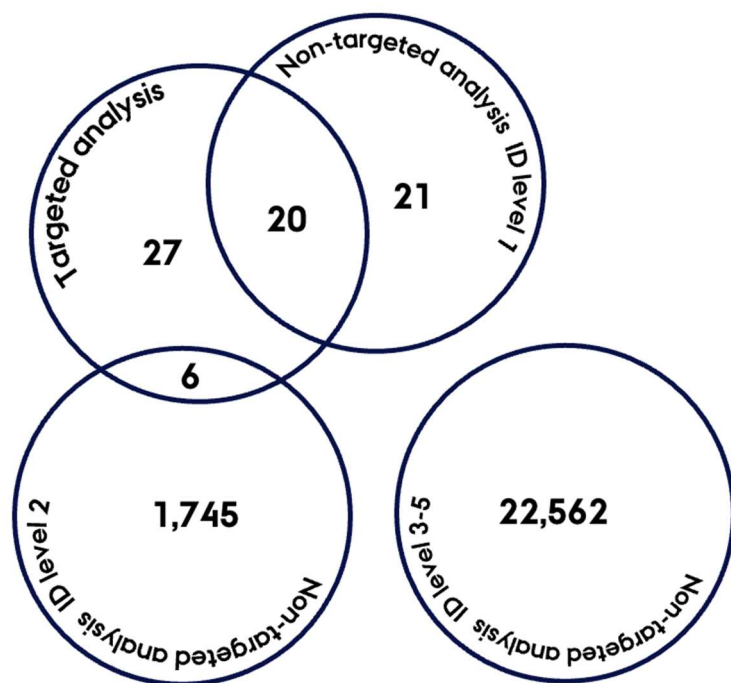
Sammenligning af målrettet og ikke-målrettet analyse

- Målrettede analyser detekterer 53 MFS. Af disse 53 MFS bliver de 26 stoffer også er fundet ved NTA (**Figur 2**).
- NTA detekterer yderligere 11 MFS der måles for ved målrettet analyser, men de målrettede analyser finder dem ikke.
- NTA detekterer yderligere 20,000 stoffer.
- Multivariable dataanalyse (PCA) viser at nogle rensningsanlæg har ensartet kemisk fingeraftryk, mens andre er meget forskellige (**Figur 3**).

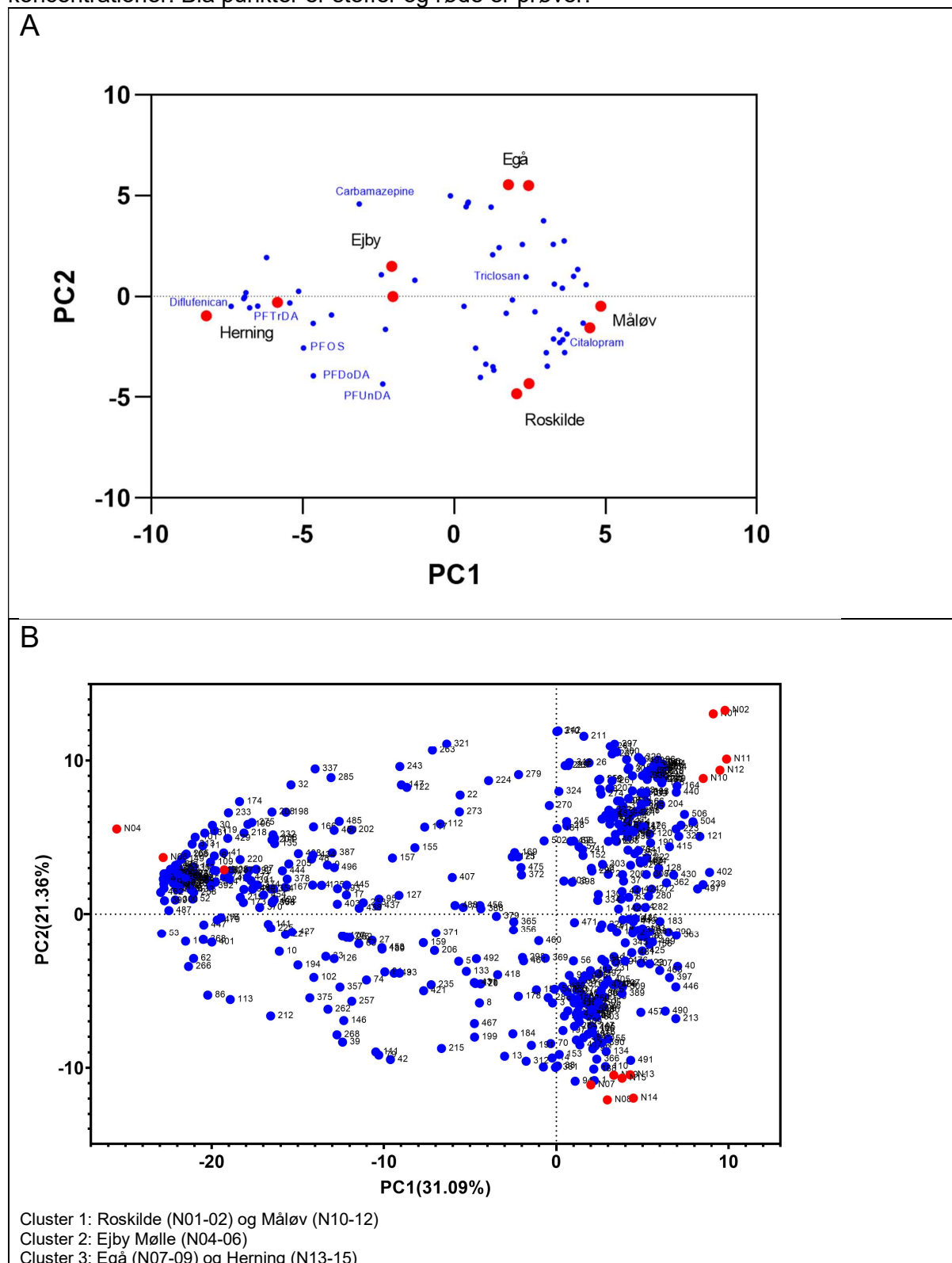
Figur 1. Uorganiske elementer (61) bestemt ved ICP-MS (mg/kg ts).



Figur 2. Fundne stoffer med målrettet og ikke målrettet metoder. Bemærk identifikationsniveau 2 er for LC-baseret stoffer (695, heraf 6 delt med målrettet analyse) og 1056 er GC-baseret stoffer. NTA-bestemte stoffer på identifikationsniveau 3-5 (22,562 stoffer) kan indeholde de 27 stoffer der er bestemt med målrettet analyse.



Figur 3. A) PCA biplot for de bestemte 53 stoffer med målrettet analyse og de fem rensningsanlæg. B) Tilsvarende PCA biplot for NTA af 509 stoffer som der kunne estimeres koncentrationer. Blå punkter er stoffer og røde er prøver.



Tabel 1. Detekterede (53) stoffer og koncentrationer i slam for delopgaver 1-3 med målrettet analyser. Koncentration angivet som gennemsnit af duplikat analyse med relativ standardafvigelse (%). Ikke detekteret (ingen værdi).

#	mg/kg tørstof	Type	Roskilde		Aarhus		Odense		Herning		Måløv	
			'Bjergmarken'		'Egå'		'Ejby Mølle'					
1	6PPD-quinone	I	0.0013	0%	0.0003	20%	0.0030	7%	0.0033		0.0020	4%
2	6:2 FTS (Fluortelomersulfonat)	I					0.0004				0.0003	
3	PFDA (Perfluordekansyre)	I	0.0039	4%	0.0017	8%	0.0021	0%	0.0020	11%	0.0048	12%
4	PFDoDA (Perfluordodekansyre)	I	0.0015	9%	0.0007	9%	0.0014	5%	0.0017	4%	0.0011	14%
5	PFHpS (Perfluorheptansulfonsyre)	I	0.0028	39%								
6	PFHxA (Perfluorhexansyre)	I	0.0005	10%	0.0003		0.0003				0.0003	12%
7	PFNA (Perfluorononansyre)	I	0.0006	19%	0.0003		0.0003				0.0007	4%
8	PFOA (Perfluoroktansyre)	I	0.0006	11%	0.0004	4%	0.0004	17%	0.0003	9%	0.0008	1%
9	PFOS (Perfluoroktansulfonsyre)	I	0.0079	0%	0.0042	17%	0.0038	15%	0.010	10%	0.0041	5%
10	PFOSA (Perfluoroktansulfonamid)	I	0.0010	7%	0.0007	14%	0.0007	10%	0.0014	5%	0.0018	8%
11	PFTTrDA (Perfluortridekansyre)	I					0.0007		0.0004	11%		
12	PFUnDA (Perfluorundekansyre)	I	0.0011	22%	0.0005	11%	0.001	0%	0.00099	1%	0.0008	29%
13	Triclosan	PCP	0.12	0%	0.14	5%	0.09	0%	0.16		0.11	0%
14	Diflufenican	P	0.030	0%	0.020	0%	0.045	16%	0.13	11%		
15	Propiconazol (sum of isomers)	P							0.055	13%	0.030	0%
16	Prosulfocarb	P	0.095	7%	0.055	13%	0.085	8%	1.25	6%		
17	Terbutryn	P							0.054	13%		
18	DDD, o,p'-	PM	0.26	58%	0.011		0.035	2%				
19	Piperonyl butoxid (PBO)	PS					0.02		0.032	7%		
20	Permethrin, -cis	LP	0.13	6%	0.28	8%	0.19	4%	0.92		0.15	5%
21	Permethrin, -trans	LP	0.093	26%	0.24	9%	0.24	3%	1.60	0%	0.087	16%
22	Permetrin	LP	0.11	7%	0.27	5%	0.22	10%	1.25	6%	0.12	0%
23	Acetylsalicylsyre (Asprin)	L			0.24	6%	0.57	19%	0.45	50%		
24	Amiodaron	L	0.058	5%	0.21	0%	0.16	14%	0.035		0.17	4%
25	Amisulprid	L	0.16	5%	0.10	8%	0.079	2%	0.17	4%	0.027	0%
26	Amitriptylin	L	0.13	11%	0.17	4%	0.069	11%	0.076	82%	0.19	19%
27	Azithromycin	L			0.14	5%					0.16	9%
28	Carbamazepin	L			0.057	0%	0.03	14%	0.047	12%	0.024	3%
29	Carvedilol	L	0.098	2%	0.12	0%	0.11	17%	0.033		0.13	33%
30	Cetirizin	L	0.18	8%	0.13	6%	0.10	1%	0.066	74%	0.14	16%
31	Ciprofloxacin	L	2.00	28%	2.55	47%	1.65	4%	1.45	5%	3.30	26%
32	Citalopram	L	0.27	0%	0.21	3%	0.11	0%	0.15	73%	0.27	3%
33	Clotrimazol	L	0.41	5%	0.46	5%	0.3	5%	0.29	7%	0.53	1%
34	Diclofenac	L	0.063	6%	0.044	5%	0.024	3%	0.027	3%	0.049	4%
35	Doxicyklin	L	0.30	9%	0.20	0%					0.32	13%
36	Fexofenadin	L	1.30	11%	0.69	31%	0.59	10%	0.95	8%	0.96	21%
37	Fluoxetin	L	0.045	14%								
38	Ketoconazol	L	1.20	0%	1.20	0%	0.99	16%	0.84	17%	1.20	24%
39	Koffein	L					0.047					
40	Lamotrigin	L	0.34	8%	0.53	28%	0.17	30%	0.32	2%	0.31	14%
41	Losartan	L	0.43	3%	0.45	5%	0.25	3%	0.41	12%	0.44	8%
42	Metoprolol	L	0.062	0%	0.12	0%	0.094	10%	0.032	13%	0.13	6%
43	Mianserin	L									0.028	18%
44	Miconazol	L	0.28	3%	0.36	2%	0.27	16%	0.31	55%	0.34	2%
45	Ofloxacin	L			0.24	3%						
46	Propanolol	L	0.053	4%	0.028	0%	0.031	14%	0.05		0.071	13%
47	Sertralin og norsertralin	L	1.65	4%	2.10	0%	1.40	10%	1.28	58%	1.45	24%
48	Tetracycline + epi-tetracycline	L	0.36	8%	0.44	18%	0.25	0%	0.69	20%	0.34	4%
49	Tramadol	L			0.090	0%	0.026	5%	0.037	29%	0.025	6%
50	Valsartan	L									0.021	
51	Venlafaxin	L			0.054	3%	0.035	6%				
52	Østron	LM			0.18	4%	0.077		0.076	12%	0.080	12%
53	Progesteron	LM	0.027	0%	0.28	3%	0.034	2%	0.059	12%		

Type: I, industriel; PCP, personal care product; P, pesticid/biocid; PM, pesticid metabolit; PS, pesticid formuleringssynergist; LP, lægemiddel/pesticid; L, lægemiddel; LM, lægemiddel/endogen metabolit.

Tabel 2. Bekræftet (41) stoffer fundet med NTA (på identifikationsniveau 1) og estimeret minimum og maksimum slam koncentrationer.

#	Stof	C _{min} (mg/kg)	C _{max} (mg/kg)	D _f (%)
1	1H-Benzotriazole	0.057	3.28	100
2	2,6-Dichlorophenol	n.c.	n.c.	40
3	4-Methyl-1H-benzotriazole	0.20	0.61	100
4	5-Methyl-1H-benzotriazole	0.031	1.58	100
5	Aspartame	0.090	0.69	60
6	Azithromycin	0.011	2.81	40
7	Bisphenol S	25	116	60
8	Caffeine	0.103	9.08	40
9	Carbamazepine	n.c.	n.c.	100
10	Cetirizine	0.016	0.052	80
11	Citalopram	0.11	1.12	80
12	Clomazone	n.c.	n.c.	40
13	Cotinine	n.c.	n.c.	60
14	Daidzein	0.019	2.96	80
15	Dimethyl phthalate	0.19	0.96	80
16	Ethylparaben	0.29	0.95	100
17	Fexofenadine	0.017	0.19	100
18	Furosemide	0.031	0.085	100
19	Genistein	0.042	0.070	20
20	Lamotrigine	n.c.	n.c.	80
21	Losartan	0.069	0.50	100
22	Methylparaben	0.29	0.95	100
23	Metoprolol	0.082	1.02	80
24	Miconazole	n.c.	n.c.	60
25	Nicotine	0.10	0.81	60
26	Propranolol	0.019	0.45	80
27	Prosulfocarb	0.081	0.31	60
28	Salicylic acid	0.099	4.05	100
29	Sertraline	0.009	0.36	100
30	Terbutryn	0.073	0.65	60
31	Tributyl phosphate	0.093	0.34	100
32	Triisobutyl phosphate	n.c.	n.c.	100
33	Tris(2-butoxyethyl) phosphate	0.13	0.75	40
34	Vanillin	0.64	17.4	100
35	Venlafaxine	0.004	0.60	100
36	Diclofenac	0.004	0.070	100
37	Ibuprofen	0.015	0.090	80
38	Perfluorodecanoic acid (PFDA)	0.002	0.011	100
39	Perfluorooctanesulfonic acid (PFOS)	0.003	0.053	100
40	Perfluorononanoic acid (PFNA)	0.001	0.002	60
41	Perfluorooctanesulfonamide (PFOSA)	0.001	0.003	40

n.c., ikke muligt at bestemme koncentration; D_f (%), detektionsfrekvens.

Tabel 3. Detekteret (26) MFS i NTA datasæt vha stoffliste søgning angivet i delopgave 1-3.

Stof	ID	Stof	ID	Stof	ID
beta-Estradiol	2	Propranolol	1	Pyrethrin	2
(+)-Estrone	3	Tramadol	3	6PPD	2
Azithromycin	1	Carbamazepine	1	6PPD-Quinone	2
Citalopram	1	Telmisartan	2	Perfluorononanoic acid (PFNA)	1
Clarithromycin	2	Metoprolol	1	Perfluorodecanoic acid (PFDA)	1
Diclofenac	1	Sertraline	1	Perfluorododecanoic acid (PFDoA)	3
(-)-Erythromycin	2	Trimethoprim	3	Perfluorooctanesulfonic acid (PFOS)	1
Ibuprofen	2	Venlafaxine	1	Perfluorooctanesulfonamide (PFOSA)	1
2-hydroxyibuprofen	1	DDAC*	2		

*ID, identifikationsniveau; *, Didecyltrimethylammonium (bemærk at dioctyltrimethylammonium og dodecyltrimethylammonium er også fundet vha. NTA).*

Appendix

Tabel A1. Stoffer (401) der blev målt for med målrettet analyser, men ikke fundet i slam for delopgaver 1-3.

2-(4-chlorophenoxy)propionsyre	Boscalid	DDM	Fenofibric syre
2,4-D	Bromacil	DDT, o,p'-	Fenoxaprop-P-ethyl
2,4-dichlorphenol	Bromocriptin	DDT, p,p'-	Fenpyrazamin
2,4-methoxychlor	Bromoxynil	DEET (Diethyltoluamid)	Fenvalerat
2,4,5-T	Budesonid	Deltamethrin	Flamprop-isopropyl
4-Acetamidoantipyrin	Buprofezin	Desmedipham	Flonicamid
4-chlor-2-methylphenol	Buspiron	Diatrizoat (Amidotrizoat)	Florasulam
4-chlor-3-methylphenol	Candesartan	Dicamba	Florfenicol
4-Demethyltrimethoprim	Captafol	Dichlobenil	Fluazifop-P-butyl
4-Formylaminoantipyrin (Formyl-AAP)	Carbofuran	Dichlofluanid	Fluazinam
4,4'-Diaminodiphenylsulfon (DDS)	Carfentrazone-ethyl	Dichloroctylisothiazolinon	Flubendazol
4,4'-DDMU	Carprofen	Dichlorprop + Dichlorprop-P	Flucloxacillin
5-methylbenzotriazol	Chinomethionat	Dichlorvos	Fluconazol
Acetamidiprid	Chlorbensid	Dicofol	Flucythrinat
Acetanilid	Chlordan, alpha- (cis)	Dieldrin	Fludioxonil
Acetylsulfamethoxazol	Chlordan, gamma- (trans)	Difenoconazol	Fluopicolid
Aclonifen	Chlordecon	Diflubenzuron	Fluopyram
Acrinathrin	Chlorfenson	Dimethoat	Fluroxypyr
Alachlor	Chlorfenvinphos	Dimethomorph	Flutamid
Aldrin	Chloridazon	Dimetridazol	Fluticason Propionat
Allethrin	Chloridazon, desphenyl-	Dinoseb	Flutolanil
Amidosulfuron	Chloridazon, methyl-desphenyl-	Dinoterb	Fluvastatin
Amilorid	Chlormephos	Diuron	Fluvoxamin
Aminopyralid	Chloroneb	Doxorubicin	Fluxapyroxad
Amisulbrom	Chloropropylate	Emamektin B1A Benzoat	Foramsulfuron
Amoxicillin	Chloroxuron	Emamektin B1B Benzoat	Fuberidazol
Ampicillin	Chlorpropham	Enalapril	Furathiocarb
Antraquinone	Chlorpyrifos	Endosulfan (sum)	Furosemid
Atenolol	Chlorsulfuron	Endosulfan-sulfat	Gabapentin
Atrazin	Chlorthalonil	Endosulfan, alpha-	Gemfibrozil
Atrazin, desethyl-	Clarithromycin	Endosulfan, beta-	Glibenclamid
Atrazin, desethyl-desisopropyl-	Clenbuterol	Endrin	Halauxifen-methyl
Atrazin, desisopropyl-	Clindamycin	Endrin keton	HCH, alfa-
Azathioprin	Clofibrinsyre	Endrin-aldehyd	HCH, beta-
Azinphos-methyl	Clopyralid	Enrofloxacin	HCH, delta-
Azoxystrobin	Clothianidin	Entacapon	HCH, gamma- (Lindan)
BAM (2,6-dichlorbenzamid)	Cloxacillin	Epoconazol	Heptachlor
Beclomethason	Cyanazine	Eprosartan	Heptachlorepoxyd, cis-
Bendroflumethiazid	Cyazofamid	Erythromycin	Heptachlorepoxyd, trans-
Bentazon	Cyclophosphamid	Esfenvalerat	Hexachlorbenzen (HCB)
Benzathin benzylpenicillin G	Cyfluthrin	Estradiol (17β-Estradiol)	Hexachlorbutadien
Benzotriazol	Cyfluthrin-beta	Ethinyl-Estradiol	Hexazinon
Benzovindiflupyr	Cyhalothrin, lambda-(incl. Cyhalothrin, gamma-)	Ethofumesat	Hexythiazox
Bezafibrat	Cymoxanil	Ethofumesat-2-keto	Hydrochlorothiazid
BHC (Benzahex)	Cypermethrin	Famoxadon	Hydrocortison
Bifenazat	Cypermethrin, alpha-	Febantel	Hymexazol
Bifenox	Cyproconazole	Felodipin	Ibuprofen
Biphenthrin	Cyprodinil	Fenamidon	Ifosfamid
Bisoprolol (β-Adrenergics)	Dalapon	Fenbendazol	Imidacloprid
Bitertanol	DDD, p,p'-	Fenhexamid	Indoxacarb (sum, R+S isomers)
Bixafen	DDE, o,p-	Fenitrothion	Iodosulfuron-methyl-natrium

Tabel A1 forsat.

Iopamidol	Napropamide	Pivmecillinam	Tamoxifen
Iopromid	Naproxen	Praziquantel	tau-Fluvalinat
Ipratropium	Nebivolol	Primidon	Tebuconazol
Iprodion	Nelfinavir	Primisulfuron methyl	Tecnazen
Irbesartan	Nicosulfuron	Prochloraz	Teflubenzuron
Irgarol	Nitenpyram	Prometryn	Tefluthrin
Isodrin	Nonachlor-cis	Propachlor	Tepraloxymid
Isoproturon	Nonachlor, trans-	Propafenon	Terbacil
Isoxaben	Norethisteron	Propaquizafop	Terbutalin
Ivermectin	Norfloxacin	Propazin	Terbutylazin
Ketoprofen	Omethoat	Propoxycarbazon	Terbutylazin, desethyl-
Kresoxim-methyl	Østriol	Propyphenazon	Testosteron
Kvinmerac	Oxadiazon	Propyzamide	Tetradifon
Lenacil	Oxcarbazepin	Proquinazid	Tetramethrin
Levonorgestrel	Oxolinsyre	Pymetrozin	Thiaclopid
Lidocain	Oxychloridan	Pyraclostrobin	Thiamethoxam
Linuron	Oxymetazolin	Pyrantel	Thiencarbazon-methyl
Loratadin	Oxytetracyklin	Pyrethrin I	Thifensulfuron methyl
Malathion	p,p'-DDE	Pyridat	Tiamulin
Mandipropamid (any ratio of constituent isomers)	Paclotbutrazol	Pyrimethanil	Tolclofos-methyl
MCPA	Paracetamol	Pyriofenon	Tolyfluamid
MCPB	Parathion-ethyl	Pyroxsulam	Toremifen
Mebendazol	Parathion-methyl	Quinoclamid	Tralkoxydim
Mecoprop + Mecoprop-P	Paroxetin	Quinoxyfen	Transfluthrin
Mepanipyrim	Penconazol (sum of constituent isomers)	Quintozen	Triadimefon
Mesosulfuron methyl	Pendimethalin	Quizalofop-P-ethyl	Triadimenol
Metaflumizon (sum af E- og Z- isomerer)	Penflufen	Raloxifen	Triallat
Metalaxyl	Penicillin G (benzylpenicillin)	Ramipril	Triasulfuron
Metamitron	Pentachloranisol	Rimsulfuron	Trichlorfon
Metamitron-desamino	Pentachlorbenzen	Rosuvastatin	Triclocarban
Metazachlor	Pentoxifyllin	Roxithromycin	Triclosan-Methyl
Metconazol	Perthane	S-Metolachlor	Trifloxystrobin
Methabenzthiazuron	PFBA (Perfluorbutansyre)	Salbutamol	Trifluralin
Methiocarb	PFBS (Perfluorbutansulfonsyre)	Salmeterol	Triflusulfuron-methyl
Methotrexat	PFDoDS (Perfluordodekansulfonsyre)	Sedaxan	Trimethoprim
Methoxychlor-olefin, p,p'	PFDS (Perflordekane-sulfonsyre)	Simazin	Trinexapac-ethyl
Methoxychlor, p,p'	PFHpA (Perfluorheptansyre)	Simvastatin	Triticonazole
Methylprednisolon	PFHxS (Perfluorhexansulfonsyre)	Sotalol	Tritosulfuron
Metoxuron	PFNS (Perfluoronansulfonsyre)	Spinosad (total)	Tylosin
Metribuzin	PFPeA (Perfluorpentansyre)	Spirodiclofen	Verapamil
Metribuzin-desamino	PFPeS (Perfluorpentansulfonsyre)	Spirotetramat	Vinclozolin
Metribuzin-desaminodiketo	PFTTrDS (Perfluortridekane-sulfonsyre)	Sulfadiazin	Warfarin
Metribuzin-diketo	PFUnDS (Perfluorundekane-sulfonsyre)	Sulfadimidin (Sulfamethazin)	Xylometazolin
Metronidazol	Phenazon	Sulfadoxin	Zoxamid
Metsulfuron methyl	Phenmedipham	Sulfaguanidin	
Mevinphos	Phenothrin	Sulfamerazin	
Mirex	Picloram	Sulfamethizol	
Mometasonfuroat	Picoxystrobin	Sulfamethoxazol	
Moxifloxacin	Pinoxaden	Sulfathiazol	
N-(2,6-dimethylphenyl)-N-(methoxyacetyl)alanin	Piperacillin	Sulfosulfuron	
N-Demethylerythromycin A	Pirimicarb	Sulfotep	

Tabel A2. Stoffer (695) fundet ved NTA LC platforme og identificeret til niveau 2.

(-)-Caryophyllene oxide	1-(3,4-dimethoxyphenyl)ethan-1-one oxime
(-)-Erythromycin	1-(4-hydroxyphenyl)propane-1,2-diol
(+/-)-C75	1-(4-hydroxyphenyl)propane-1,2-diol_02
(+/-)-Gingerol	1-(4-methoxyphenyl)propane-1,2-diol
(+/-)11(12)-DIHET	1-(4-methoxyphenyl)propane-1,2-diol_02
(+/-)12(13)-DIHOME	1-(Carboxymethyl)cyclohexanecarboxylic acid
(+/-)12(13)-DIHOME_02	1-(Carboxymethyl)cyclohexanecarboxylic acid_02
(+/-)12(13)-DIHOME_03	1-[(2,5,5,8a-tetramethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl)methyl]-4-(hydroxymethyl)-7-oxabicyclo[4.1.0]hept-3-ene-2,5-diol
(+/-)12(13)-DIHOME_04	1-Methyl-1H-benzotriazole
(+/-)19(20)-DiHDPA	1-Phenyl-1H-pyrazole
(+/-)5(6)-EET Ethanolamide	1-Tetradecylamine
(+/-)5(6)-EET Ethanolamide_02	1,2-Benzisothiazolin-3-one
(+/-)9-HpODE	1,2-dihydroxyheptadec-16-yn-4-yl acetate
(+/-)9(10)-EpOME	1,2,3,4-Tetramethyl-1,3-cyclopentadiene
(+/-)9(10)-EpOME_02	1,3-Dimethylpiperidine-2,4-dione
(±)12(13)-DIHOME	1,3,7-Trimethyluric acid
(±)19(20)-DiHDPA	1,4a-dimethyl-9-oxo-7-(propan-2-yl)-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylic acid
(±)9-HpODE	1,5-Isoquinolinediol
(±)9-HpODE_02	1,5-Isoquinolinediol_02
(±)9-HpODE_03	1,5-Isoquinolinediol_03
(11E,15Z)-9,10,13-trihydroxyoctadeca-11,15-dienoic acid	10-HDA
(12Z)-9,10,11-trihydroxyoctadec-12-enoic acid	10-HDA_02
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	10-HDA_03
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid_02	10-hexyl-11,12-dioxatricyclo[7.2.1.01,6]dodecane-2,5-diol
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid_03	10-hydroxycapric acid
(1R,2R,6R,9R)-2,11,11-trimethyl-3-oxotricyclo[4.3.2.0Åa,â µ]undecane-9-carboxylic acid	10-hydroxycapric acid_02
(1R,2S,3R,4R)-3-[(Cyclopentylmethyl)amino]-4-phenyl-1,2-cyclopentanediol	10-hydroxycapric acid_03
(1R,4aS)-7-(2-Hydroxypropan-2-yl)-1,4a-dimethyl-9-oxo-3,4,10,10a-tetrahydro-2H-phenanthrene-1-carboxylic acid	10-Hydroxycarbazepine
(2'R,3R,4'R,4a'R,5S,8a'S)-5-(3-Furyl)-4'-hydroxy-4a',5'-bis(hydroxymethyl)-2'-methyl-3',4,4',4a',5',7',8',8a'-octahydro-2'H-spiro[furan-3,1'-naphthalen]-2-one	10-Hydroxydecanoate
(2E,4E,9Z)-1-(piperidin-1-yl)hexadeca-2,4,9-trien-1-one	10-Hydroxydecanoate_02
(2E,4E)-3,5,7-Trimethyl-2,4-octadienedioic acid	10-Nitrolinoleate
(2R,3R,4S,5S,6R)-2-[[[(2E)-4-ethenyl-2,5-dimethylhexa-2,5-dien-1-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	10-Propoxydecanoic acid
(2R,5R,6R)-3-[(1E,3E)-hepta-1,3-dien-1-yl]-5,6-dihydroxy-2-(hydroxymethyl)cyclohexan-1-one	10-Propoxydecanoic acid_02
(3E)-1-[5-[(1E)-1,3-Butadien-1-yl]-4-hydroxytetrahydro-3-furanyl]-3-pentene-1,2-diol	10,20-dihydroxy-6,10,23-trimethyl-4-azahexacyclo[12.11.0.02,11.04,9.015,24.018,23]pentacosan-17-one
(3S,4aR,5R,6R)-3,6-dihydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one	11-Oxoetiocolanolone
(3S,4aR,5R,6R)-3,6-dihydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one_02	12-hydroxy-13-(hydroxymethyl)-3,5,7-trimethyltetradeca-2,4-dienedioic acid
(3S,4R)-3-(1-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one	12-Hydroxydodecanoic acid
(3S,4R)-3-(1-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one_02	12-Hydroxydodecanoic acid_02
(5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid	12-Hydroxydodecanoic acid_03
(5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid_02	12-Hydroxydodecanoic acid_04
(5Z)-3-Hydroxy-5-dodecenoic acid	12-Oxo phytodienoic acid
(9-hydroxy-8,8-dimethyl-2-oxo-9,10-dihydropyrano[2,3-f]chromen-10-yl) 2-methylbut-2-enoate	12-Oxo phytodienoic acid_02
(R)-3-Hydroxy myristic acid	13,14-dihydro-15-keto-tetranor Prostaglandin F1?
(R)-3-Hydroxy myristic acid_02	13(S)-HOTrE
(R)-3-Hydroxy myristic acid_03	13(S)-HOTrE_02
[3-((3-((Cyclopropylmethyl)amino)-3-oxetanyl)methyl)-1,2-oxazol-5-yl]methanol	13(S)-HOTrE_03
[3-((3-((4-(Hydroxymethyl)cyclohexyl)amino)-3-oxetanyl)methyl)-1,2-oxazol-5-yl]methanol	15-Deoxy-Δ12,14-prostaglandin A1
1-(2-Furylmethyl)-5-oxopyrrolidine-3-carboxylic acid	15-Deoxy-Δ12,14-prostaglandin A1_02
1-(2-Morpholinophenyl)dihydro-1H-pyrrole-2,5-dione	15,16-dihydroxyoctadeca-10,13-dienoic acid
1-(2,4-dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)propan-1-one	16-Heptadecyne-1,2,4-triol
(-)-Caryophyllene oxide	1-(3,4-dimethoxyphenyl)ethan-1-one oxime

Tabel A2 fortsat.

16-Hydroxyhexadecanoic acid_02	2-methyl-2,3,4,5-tetrahydro-1,5-benzoxazepin-4-one
16,16-Dimethyl prostaglandin A1	2-Methyl-5-propionylfuran
16,16-Dimethyl prostaglandin A1_02	2-Methylbutyl beta-D-glucopyranoside
16,16-Dimethyl prostaglandin A1_03	2-Naphthylamine
17 α -Methyl-androstan-3-hydroxyimine-17 β -ol	2-Octenedioic acid
19-Nortestosterone	2-Octenedioic acid_02
19-Nortestosterone_02	2-Oxindole
1a,1b-Dihomo prostaglandin F2 α	2-piperidinobenzoic acid
1H-indene-3-carboxamide	2-Quinolinecarboxylate
2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid	2,2-Dimethyl-N-[(2R,4S,5R)-5-{2-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl}-1-azabicyclo[2.2.2]oct-2-yl]methyl]propanamide
2-(2-hydroxyphenyl)-3,4-dihydroquinazolin-4-one	2,2,6,6-Tetramethyl-4-piperidinol
2-(2,5-Dimethyl-1H-pyrrol-1-yl)isoindoline-1,3-dione	2,3-Dihydroxypropyl 9-hydroxynonanoate
2-(6-Hydroxyhexyl)-3-methylenesuccinic acid	2,3-Dihydroxypropyl 9-hydroxynonanoate_02
2-(6-Hydroxyhexyl)-3-methylenesuccinic acid_02	2,3-dinor Prostaglandin E1
2-(7-hydroxy-6-methyloctyl)-2H-furan-5-one	2,3-Dinor-8-epi-prostaglandin F2 α
2-(7-hydroxy-6-methyloctyl)-2H-furan-5-one_02	2,3,5,6-Tetramethylpyrazine
2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid	2,4-Diaminoanisole
2-(Cyclohexylmethylidene)-1,2,3,4-tetrahydronaphthalen-1-one	2,4-Quinolinediol
2-[(1S)-1-Hydroxyethyl]-4(1H)-quinazolinone	2,4,5-Trimethylaniline
2-[5-(2-hydroxypropyl)oxolan-2-yl]propanoic acid	2,6-Di-tert-butyl-1,4-benzoquinone
2-Amino-3-methoxybenzoic acid	2'-Deoxyadenosine
2-Arachidonoyl glycerol	2'-Deoxyguanosine
2-Arachidonoyl glycerol_02	2'-Deoxyinosine
2-Chlorobenzoic acid	2'-O-Methylguanosine
2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine (EDDP)	2',4'-Dihydroxyacetophenone
2-Furyl(5-hydroxy-1-benzofuran-3-yl)methanone	3-(1-hydroxyethyl)-2,3,6,7,8,8a-hexahydropyrrolo[1,2-a]pyrazine-1,4-dione
2-Hexyl-3-methylenesuccinic acid	3-(1-Hydroxyhexyl)-4-(hydroxymethyl)dihydro-2(3H)-furanone
2-hexylpentanedioic acid	3-(2-Hydroxy-4-methoxy-phenyl)-acrylic acid
2-hexylpentanedioic acid	3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-chromen-7-ol
2-Hydroxy-4-(4-hydroxyphenyl)butanoic acid	3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid
2-Hydroxybenzothiazole	3-(2-Hydroxyethyl)indole
2-Hydroxycinnamic acid	3-(2-methyl-3-oxo-2,5,6,7,8,8a-hexahydro-1H-naphthalen-1-yl)propanoic acid
2-Hydroxyibuprofen	3-(3,4-dimethoxyphenyl)prop-2-en-1-ol
2-hydroxyiminoindane-1,3-dione	3-(4-hydroxy-3-methoxyphenyl)propanoic acid
2-Hydroxyisovaleric acid	3-(4-hydroxy-3-methoxyphenyl)propanoic acid_02
2-Hydroxyisovaleric acid_02	3-(4,5-diphenyl-1,3-oxazol-2-yl)propanoic acid
2-Hydroxyisovaleric acid_03	3-(5,6-dihydroxyheptyl)-4-methyl-2H-furan-5-one
2-Hydroxyisovaleric acid_04	3-(5,6-dihydroxyheptyl)-4-methyl-2H-furan-5-one_02
2-Hydroxyisovaleric acid_05	3-(propan-2-yl)-octahydropyrrolo[1,2-a]pyrazine-1,4-dione
2-Hydroxymyristic acid	3-(propan-2-yl)-octahydropyrrolo[1,2-a]pyrazine-1,4-dione_02
2-Hydroxymyristic acid_02	3-Acetyl-2,5-dimethylfuran
2-Hydroxymyristic acid_03	3-Amino-3-(4-hydroxyphenyl)propanoic acid
2-Hydroxyphenylacetic acid	3-butan-2-yl-2,3,6,7,8,8a-hexahydropyrrolo[1,2-a]pyrazine-1,4-dione
2-Hydroxyquinoline	3-Chloroamphetamine
2-Hydroxyquinoline_02	3-Ethyl-4-hydroxy-1-phenyl-1,2-dihydroquinolin-2-one
2-Isobutyl-3-methoxypyrazine	3-hepta-1,3-dienylpentanedioic acid
2-Methoxy-5-methylaniline	3-heptyl-3,6-dihydro-1H-furo[3,4-c]furan-4-one
2-Methoxyestrone	3-Hydroxy caprylic acid
2-methyl-1,2-dihydrophthalazin-1-one	3-Hydroxy-3-methylbutanoic acid
2-methyl-1,2-dihydrophthalazin-1-one_02	3-Hydroxy-4-(2-hydroxy-6-methyl-2-heptanyl)benzoic acid
16-Hydroxyhexadecanoic acid_02	2-methyl-2,3,4,5-tetrahydro-1,5-benzoxazepin-4-one

Tabel A2 fortsat.

3-hydroxy-7-methoxy-3H-2-benzofuran-1-one	4-Dimethylaminocinnamaldehyde
3-Hydroxybutyric acid	4-Dodecylbenzenesulfonic acid
3-Hydroxybutyric acid_02	4-Dodecylbenzenesulfonic acid_02
3-Hydroxybutyric acid_03	4-Ethylbenzaldehyde
3-Hydroxybutyric acid_04	4-hydroxy-3-(7-hydroxy-3,7-dimethyl-4-oxooct-5-enyl)-5-(3-methylbut-2-enyl)benzoic acid
3-Hydroxydecanedioic acid	4-Hydroxybenzaldehyde
3-Hydroxydecanoic acid	4-Hydroxybenzaldehyde_02
3-hydroxydodec-5-enoic acid	4-Hydroxyephedrine
3-hydroxydodec-5-enoic acid_02	4-Hydroxyindole
3-hydroxydodec-5-enoic acid_03	4-Hydroxyphenylacetic acid
3-Hydroxymandelic acid	4-Hydroxyphenylacetic acid_02
3-hydroxyoctanoic acid	4-Hydroxypropranolol
3-hydroxyoctanoic acid	4-Indocarbalddehyde
3-hydroxyoctanoic acid_02	4-Methoxybenzaldehyde
3-hydroxyoctanoic acid_03	4-Methoxycinnamaldehyde
3-Hydroxypyridine	4-methyl-2-oxo-1,2-dihydroquinoline-3-carbonitrile
3-hydroxyquinclidine-3-carbonitrile hydrochloride	4-methyl-2,3-dihydro-1H-pyrrolo[3,4-c]quinoline-1,3-dione
3-Methoxyphenylacetic acid	4-methyl-5-oxo-2-pentyl-2,5-dihydrofuran-3-carboxylic acid
3-Methyl-2-Oxindole	4-Methyl-5-thiazoleethanol
3-Methyl-2-quinoxalinol	4-methylpyridine-3-sulfonic acid
3-Methyl-5-(5,5,8a-trimethyl-2-methylene-7-oxodecahydro-1-naphthalenyl)pentyl acetate	4-oxododecanedioic acid
3-Methyl- α -pyrrolidinobutiophenone	4-oxododecanedioic acid_02
3-Methylene-4-[(2E)-3-methyl-4-(4-methyl-5-oxotetrahydro-2-furanyl)-2-buten-1-yl]dihydro-2(3H)-furanone	4-oxododecanedioic acid_03
3-propan-2-yl-2,3,6,7,8,8a-hexahydropyrrolo[1,2-a]pyrazine-1,4-dione	4-Phenylbutyric acid
3,14-dihydro-15-keto-tetranor Prostaglandin E2	4-Pyridoxate
3,4-Dihydroxybenzoate	4,4-dimethyl-1-(3-nitrophenyl)-2-(1H-1,2,4-triazol-1-yl)pent-1-en-3-one
3,4-Dimethylbenzoic acid	4,5-Dicaffeoylquinic acid
3,4-Dimethylbenzoic acid_02	4,6-Dimethyl-2(1H)-pyrimidinone
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	4,7-dimethylpyrazolo[5,1-c][1,2,4]triazine-3-carbonitrile
3,5-Dimethyl-1-phenylpyrazole	4,8-Dihydroxy-6-methoxy-3-methyl-3,4-dihydro-1H-isochromen-1-one
3,8,9-trihydroxy-10-propyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	4',7-Dihydroxyflavanone
3',4'-Dimethoxyacetophenone	5-(1-Hydroxybutyl)-4-methoxy-6-methyl-2H-pyran-2-one
3',4'-Dimethoxyacetophenone_02	5-(1,2,4a,5-tetramethyl-7-oxo-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl)-3-methylpentanoic acid
3',5'-Dimethoxy-4'-hydroxyacetophenone	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one
3a-hydroxy-3-(hydroxymethyl)-1,1,3,5-tetramethyl-octahydro-1H-indene-4-carboxylic acid	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one_02
4-(1H-imidazol-1-yl)benzoic acid	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one_03
4-(2-methyl-6-oxopyran-3-yl)butanoic acid	5-(hydroxymethyl)-2-(2-hydroxy-6-methylheptan-2-yl)phenol
4-(2,3-dihydroxy-3-methylbutoxy)-7H-furo[3,2-g]chromen-7-one	5-(hydroxymethyl)-3-(1-hydroxy-4-methylhexyl)oxolan-2-one
4-(4-hydroxy-3,5-dimethylphenyl)-2-methylphthalazin-1(2H)-one	5-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]-2-methylcyclohex-5-ene-1,2,4-triol
4-(5,6-Dihydroxyheptyl)-3-methyl-2(5H)-furanone	5-[(2Z,8Z)-2,8-Pentadecadien-1-yl]-1,3-benzenediol
4-(Diethylamino)salicylaldehyde	5-butyl-6-(hydroxymethyl)-4-methoxypyran-2-one
4-(Dimethylamino)benzophenone	5-Chlorosalicylic acid
4-(hydroxymethyl)-3-(1-hydroxy-5-methylhexyl)oxolan-2-one	5-Ethylcyclohexane-1,3-dione
4-(hydroxymethyl)-3-(1-hydroxy-5-methylhexyl)oxolan-2-one_02	5-Hydroxyindole-3-acetic acid
4-(hydroxymethyl)-3-(1-hydroxy-5-methylhexyl)oxolan-2-one_03	5-Hydroxyindole-3-acetic acid_02
4-[3-(4-phenoxyphenyl)-1H-pyrazol-5-yl]morpholine	5-Hydroxytryptophan
4-Acetamidobenzaldehyde	5-Methoxyindole
4-Acetamidobenzoic acid	5-Methyl-2-(4-methylphenyl)-2,4-dihydro-3H-pyrazol-3-one
4-Chlorophenylacetic acid	5,6-dimethyl-4-oxo-4H-pyran-2-carboxylic acid
4-Cyanoindole	5,6-Dimethylbenzimidazole
3-hydroxy-7-methoxy-3H-2-benzofuran-1-one	4-Dimethylaminocinnamaldehyde

Tabel A2 fortsat.

5,6,7-Trimethoxy-2H-chromen-2-one	Adipate
5,6,7,8-Tetrahydro-2-naphthol	Adipic acid
5,7-Dihydroxy-11-oxotetranorprostanic acid	Aflatoxin G2
5,7-Dihydroxy-4-methylcoumarin	Ageratriol
5,8-dihydroxy-10-methyl-5,8,9,10-tetrahydro-2H-oxecin-2-one	Ageratriol_02
5,8-dihydroxy-10-methyl-5,8,9,10-tetrahydro-2H-oxecin-2-one_02	Aleuritic acid
5'-S-Methyl-5'-thioadenosine	Alfuzosin
5(Z),8(Z),11(Z)-Eicosatrienoic acid methyl ester	alpha-Linolenic acid
5(Z),8(Z),11(Z)-Eicosatrienoic acid methyl ester_02	Alprenolol
5 α -Dihydrotestosterone	Amisulpride
6-(3,4-dihydroxypent-1-enyl)pyran-2-one	Anandamide (AEA)
6-(3,4-dihydroxypent-1-enyl)pyran-2-one_02	Anandamide (AEA)_02
6-(hydroxymethyl)pyridin-3-ol	Anthranilic acid
6-Carboxyhexanoate	Apocynin
6-Carboxyhexanoate_02	Apocynin_02
6-Heptyl-4,6-dihydro-1H,3H-furo[3,4-c]furan-1-one	Arachidonoyl serinol
6-hydroxyoctadec-4-enoic acid	Artemisinin
6-Methoxyquinoline	Astragaline
6-Methoxyquinoline_02	Avocadyne 1-acetate
6-Methyl-2-pyridinemethanol	Azelaic acid
6-methyl-5-nitroquinoline	Azelaic acid_02
6-Pentyl-2H-pyran-2-one	Azelaic acid_03
6-Quinolinecarboxylic acid	Azelate
6,7-dihydro-5H-dibenzo[d,f][1,3]diazepin-6-one	Benzamide
6PPD-Quinone (2-((4-Methylpentan-2-yl)amino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione)	Benzoic acid
6 β -Naloxol	Benzophenone
7-(2-aminophenyl)heptanoic acid	Benzophenone-1 (BP-1)
7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylic acid	Benzothiazole
7-Ketochenodeoxycholate	Benzothiazole_02
7-Ketochenodeoxycholate_02	Benzydamine
7-Ketodeoxycholic acid	beta-Estradiol
7,8-Dihydroxy-4-methylcoumarin	Beta-Glycerophosphate
7(S),17(S)-Dihydroxy-8(E),10(Z),13(Z),15(E),19(Z)-docosapentaenoic acid	Bicalutamide
8-{3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl}octanoic acid	Biotin
8-hydroxy-8-(3-octyloxiran-2-yl)octanoic acid	Bis(2-ethylhexyl) amine
8-Hydroxyquinoline	Bis(2-ethylhexyl) amine_02
8-iso Prostaglandin F1?	Butyl benzoate
9-(Methoxycarbonyl)-9-decenoic acid	Caffeate
9-methoxy-9-oxononanoic acid	Caffeic acid
9-methoxy-9-oxononanoic acid_02	Caffeic acid_02
9-Oxo-10(E),12(E)-octadecadienoic acid	Cannabidiolic acid
9-Oxo-10(E),12(E)-octadecadienoic acid_02	Cannabigerolic acid
9-Oxo-ODE	Caprolactam
9-Oxo-ODE_02	Caprolactam_02
9-Oxo-ODE_03	Caproleic acid
9S,13R-12-Oxophytodienoic acid	Caproleic acid_02
Acetophenone	Caprylic acid
Acetophenone_02	Carvedilol
Adenine	CB-52
Adenosine	Cetrimonium
5,6,7-Trimethoxy-2H-chromen-2-one	Adipate

Tabel A2 fortsat.

Chenodeoxycholic Acid	Dodecyltrimethylammonium
Chlorogenic acid	Dodecyltrimethylammonium_02
Chlorprothixene	Edaravone
Choline	Edaravone_02
Choline_02	Eicosapentaenoic acid ethyl ester
Ciprofloxacin	Eicosapentaenoic acid methyl ester
Ciprostene	Equol
cis-12-Octadecenoic acid methyl ester	Eriodictyol
cis-5-Dodecenoate	Erucamide
cis-5-Dodecenoate_02	Ferulate
Citramalate	Fingolimod
Clarithromycin	Flavin mononucleotide (FMN)
Climbazole	FLK
Clopidogrel carboxylic acid	FLK_02
Clotrimazole	FNK
Clozapine	Formononetin
Codeine	FPH
Corchorifatty acid F	Galangin
Corchorifatty acid F_02	Galaxolidone
Cyclo(leucylprolyl)	GLK
Cyclo(phenylalanyl-prolyl)	Glutaric acid
Cyclohexanecarboxylic acid	Glycitein
Cyclohexylamine	Glycochenodeoxycholate
D-(+)-Tryptophan	Glycochenodeoxycholic acid
Decanamide	Glycocholate
Dehydroepiandrosterone (DHEA)	Glycocholic acid
Dehydrolithocholic acid	Glycoursodeoxycholic acid
Deoxycholate	Gramine
Deoxyguanosine monophosphate	Guanine
Detomidine	Guanosine
Dibenzylamine	Heptanoic acid
Didecyltrimethylammonium	Heptanophenone
Diethyleneglycol dibenzoate	Hesperetin
Dihydroaspyrone	Hesperidin
Diisobutyl adipate	Hexadecanamide
Dimethyl sebacate	Hexadecanedioic acid
Dimethyl terephthalate	Hexadecanedioic acid_02
Dioctyltrimethylammonium chloride	Hexadecanedioic acid_03
Diphenhydramine	Homo-anatoxin
Dipropylene glycol dimethyl ether	Hydrocinnamic acid
DL-Arginine	Hyodeoxycholic acid
DL-Hydroxycitronellal	ILK
DL-Tryptophan	Indole
DL- α -Methoxyphenylacetic acid	Indole-3-acetic acid
DL- β -Leucine	Indole-3-acrylic acid
Docosahexaenoic acid	Indole-3-aldehyde
Docosahexaenoic acid ethyl ester	Indole-3-aldehyde_02
Docosahexaenoic acid_02	Indole-3-butyric acid
Dodecyl sulfate	Indole-3-carboxylic acid
Dodecylamine	Indole-3-carboxylic acid_02
Chenodeoxycholic Acid	Dodecyltrimethylammonium

Tabel A2 fortsat.

Indole-3-carboxylic acid_03	Methyl picolinate
Indole-3-Methyl Acetate	Methyl-2-aminobenzoate
indoline-2-carboxylic acid	Methylmalonic acid
IPK	Mirtazapine
Isoferulic acid	MLK
Isoleucine	MLK_02
Isophorone	Mono(2-ethylhexyl) phthalate (MEHP)
Isophthalic acid	Mono(2-ethylhexyl) phthalate (MEHP)_02
Isorhapontigenin	Monobutyl phthalate
Jasmone	Monolaurin
Jasmone_02	Myristoleic acid
Jasmonic acid	Myristyl sulfate
Jasmonic acid_02	Myristyl sulfate_02
Ketoconazole	Myristyl sulfate_03
Ketoleucine	N-(1-hydroxy-3-methylpentan-2-yl)-2-methylhexa-2,4-dienamide
Ketoleucine_02	N-(1-hydroxy-3-phenylpropan-2-yl)acetamide
Kynurenic acid	N-(1-hydroxy-3-phenylpropan-2-yl)acetamide_02
Kynurenic acid_02	N-(2,4-Dimethylphenyl)formamide
L-Glutamic acid	N-(4-oxopentyl)acetamide
L-Kynurenine	N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl}acetamide
L-Norleucine	N-Desmethyltramadol
L-Phenylalanine	N-Ethylbuphedrone
L-Phenylalanine_02	N-Feruloyloctopamine
L-Tyrosine	N-Methyl-2-pyrrolidone
L-Tyrosine methyl ester	N-Methyldioctylamine
Lauric acid	N-Octyl-2-pyrrolidone
Lauroctam	N,N'-Dicyclohexylurea
Limonene-1-OOH	N6-Me-dA
Limonene-2-OOH	N6-Methyladenine
Linalool-6-OOH	Naringenin
Linalool-7-OOH	Neochlorogenic acid
Lithocholic acid	Nicotinamide
LLK	Nitrobenzene
LLK_02	Norsertaline
Lumichrome	Nortriptyline
Mandelate	O-Desmethyl-cis-tramadol
Maprotiline	O-Desmethyltramadol
Mebendazole	O-Desmethylvenlafaxine
Mebendazole amine	octadec-9-ynoic acid
Medroxyprogesterone	Octadecanamine
Meperidine	Octyl hydrogen phthalate
Methanandamide	OPEO
Methasterone	Oxazepam
methyl 2,4-dihydroxy-3,6-dimethylbenzoate	Oxepanone
Methyl 3-hydroxythieno[2,3-b]pyridine-2-carboxylate	Oxepanone_02
Methyl cinnamate	Oxoglutarate
Methyl dihydrojasmonate	p-Coumaric acid
Methyl dihydrojasmonate_02	p-Coumaric acid_02
Methyl isonicotinate	Palmitoleic acid
Methyl palmitate	Palmitoyl ethanolamide
Indole-3-carboxylic acid_03	Methyl picolinate

Tabel A2 fortsat.

Palmitoyl ethanolamide_02	Stearidonic acid_02
Paraxanthine	Stearoyl ethanolamide
PEG Monolaurate n5	Suberic acid
PEG Monolaurate n6	Sulcatol
PEG n15	Sulcatol_02
PEG n16	Sulfapyridine
PEG n7	Syringic acid
PEG n8	Syringic acid-02
Perillartine	Tauroursodeoxycholic acid
Pestalotin	Telmisartan
Phenazone	Tenuazonic acid
Phenethylamine	Terbinafine
Phenylethanolamine	Testosterone propionate
Phenylglyoxylic acid	Tetradecanedioic acid
Phenylpyruvic acid	Tetrahydrocortisone
Piperine	Tetramethylpyrazine
Piperonylonitrile	Tetranor-12R-HETE
Piperonylonitrile_02	Texanol
PPG n10	Texanol_02
PPG n4	Texanol_03
PPG n6	Thymidine
PPG n7	Thymine
PPG n8	Tiglic acid
PPG n9	Tolycaine
Progesterone	Tomatidine
Prostaglandin A1 ethyl ester	trans-3-Hydroxycotinine
Prostaglandin A2	trans-Cinnamic acid
Protectin D1	trans-Δ ² -11-Methyl-dodecenoic acid
Pyrethrin	Traumatic acid
Quercetin-3β-D-glucoside	Traumatic acid_02
Quetiapine	Trilostane
Quinazoline-2,4-diol	Triphenylphosphine oxide
R-Palmitoyl-(2-methyl) ethanolamide	Tropine
Raltegravir	Tryptamine
Rexamino	Tyrosylalanine
Riboflavin	Undecanoic acid
Ricinine	Ursocholic acid
RLK	Valeric acid
S-Cathinone	Valpromide
Sedanolide	Vanillic acid
Sedanolide_02	VLK
Senkyunolide H	Xanthohumol
Senkyunolide H_02	Xanthurenic acid
Sildenafil	YLK
Sinapinic acid	YNK
Solanidine	
Sorbic acid	
Sorbic acid_02	
Stearamide	
Stearidonic acid	
Palmitoyl ethanolamide_02	