Electronic Supplementary Material (ESI) for Analytical Methods.

ELECTRONIC SUPPLEMENTARY INFORMATION FOR:

RAPID DIRECT ANALYSIS OF RIVER WATER AND MACHINE LEARNING ASSISTED SUSPECT SCREENING OF EMERGING CONTAMINANTS IN PASSIVE SAMPLER EXTRACTS

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S1 – List of analytical standards used for targeted LC-MS/MS analysis

Reference standards for 1,1-Dimethyl-3-phenylurea, 2-(Thiocyanomethylthio)benzothiazole, 2,4,6-Tris(dimethylamino)-1,3,5-triazine, 4-Fluoromethcathinone, 4-Methylethcathinone, 6a-Methylprednisolone, Acetamiprid, Aclonifen, Alprazolam, Ametryn, Amiodarone, Amitriptyline, Amlodipine, Amphetamine, Antipyrine, Aramite, Atorvastatin, Atrazine, Azelnidipinem, Azithromycin, Azoxystrobin, Beclomethasone dipropionate, Benoxacor, Bensulide, Benzatropine, Benzoylecgonine, Betaxolol, Bezafibrate, Bisoprolol, Bupropion, Buspirone, Butocarboximsulfoxide, BZE , Carazolol, Carbamazepine, Carbamazepine epoxide, Carboxine, Carfentrazone-ethyl, CBZ epoxide, Celecoxib, Chloramphenicol, Chlorbufam, Chlorotetracycline, Chlorpromazine, Cilazapril, Citalopram, Clarithromycin, Clodinafop-propargyl, Clofibric Acid, Clopidogrel, Clothianidin, Clotrimazole, Clozapine, Cocaine, Cotinine, Cyclouron, Cycloxydim, Cymoxanil, Cyphenothrin, Diazepam, Diclofenac, Diflubenzuron, Dimethametryn, Dimethomorph, Dimetridazole, Dioxacarb, Diphenhydramine, Disulfoton sulfone, Diuron (DCMU) , Enalapril, Ethirimol, Ethofumesate, Famoxadone, Fenofibrate, Fenoxaprop-ethyl, Flufenoxuron, Fluocinonide, Fluoxetine, Flurbiprofen, Flurochloridone, Flutamide, Flutolanil, Fuberidazole, Gemfibrozil, Haloperidol, Hydrochlorothiazide, Ibuprofen, Imidacloprid, Indomethacin, Isocarbamide, Isradipine, Josamycin, Ketamine, Ketoconazole, Ketoprofen, Ketotifen, Levamisole, Levocabastine, Levonorgestrel, Lidocaine, Lincomycin, Lorazepam, MDMA, Meclizine, Meclofenamic acid, Medroxyprogesterone, Mefenamic Acid, Memantine, Mephedrone, Mephosfolan, Metformin, Methamphetamine, Methcathinone, Methedrone, Methylphenidate, Metoprolol, Miconazole, Morphine, N-Cyclopropyl-1,3,5-triazin-2,4,6-triamine, Nadolol, Naproxen, Nicotine, Nifedipine, Nitenpyram, Nordiazepam, Norethisterone, Norfluoxetine, Nortryptyline, Octachlorodibenzodioxin (OCDD) , Orphenadrine, Oxamyl, Oxazepam, Oxycarboxin, Oxycodone, Oxytetracycline, Paroxetine, Picoxystrobin, Piperophos, Pirenzepine, Pretilachlor, Prodiamine, Prometon, Prometryn, Propamocarb, Propanolol, Propazine, Pymetrozine, Pyracarbolid, Pyraclostrobin, Pyraflufen-ethyl, Pyridaben, Pyriproxyfen, Risperidone, Rizatriptan, Ronidazole, Roxithromycin, Salbutamol, Salicylic Acid, Sertraline, Simazine, Spinosyn A, Spinosyn D, Spiramycin, Sulfadimethoxine, Sulfamerazine, Sulfamethazine, Sulfamethoxazole, Sulfamonomethoxine, Sulfapyridine, Sulfathiazolev, Sulfisoxazole, Tacrine, Tamsulosin, Temazepam, Terbutryn, Terfenadine, Thiacloprid, Thiamethoxam, Thiazopyr, Timolol, Tramadol, Trimethoprim, Valsartan, Venlafaxine, Verapamil, Warfarin and Ziprasidone were sourced from QMX (Essex, UK). Deuterated internal standards for amitriptyline-d3-HCl, amphetamine-d6 , benzoylecgonine-d3, betaxolol-d7-HCl, celecoxib-d7, cetrizine-d4, clarithromycin-d3, clothianidin-d3, cocaine-d3, cotinine-d3, diazepam-d6, fluoxetine-d6, haloperidol-d4, ketamine-d4-HCl, lidocaine-d10-HCl, lorazepam-d4, MDMA-d5, methylone-d3, methylphenidate-d9, metoprolol-d7-HCl, morphine-d3, nicotine-d4, nifedipine-d4, nortriptyline-d3-HCl, oxazepam-d5, risperidone-d4, sertraline-d3, sulfamethazine-d4, temazepam-d5, thiamethoxam-d3, tramadol-13C1, d3, trimethoprim-d3, venlafaxine-d6-HCl and verapamil-d3-HCl were purchased from Sigma Aldrich and QMX (Essex, UK).

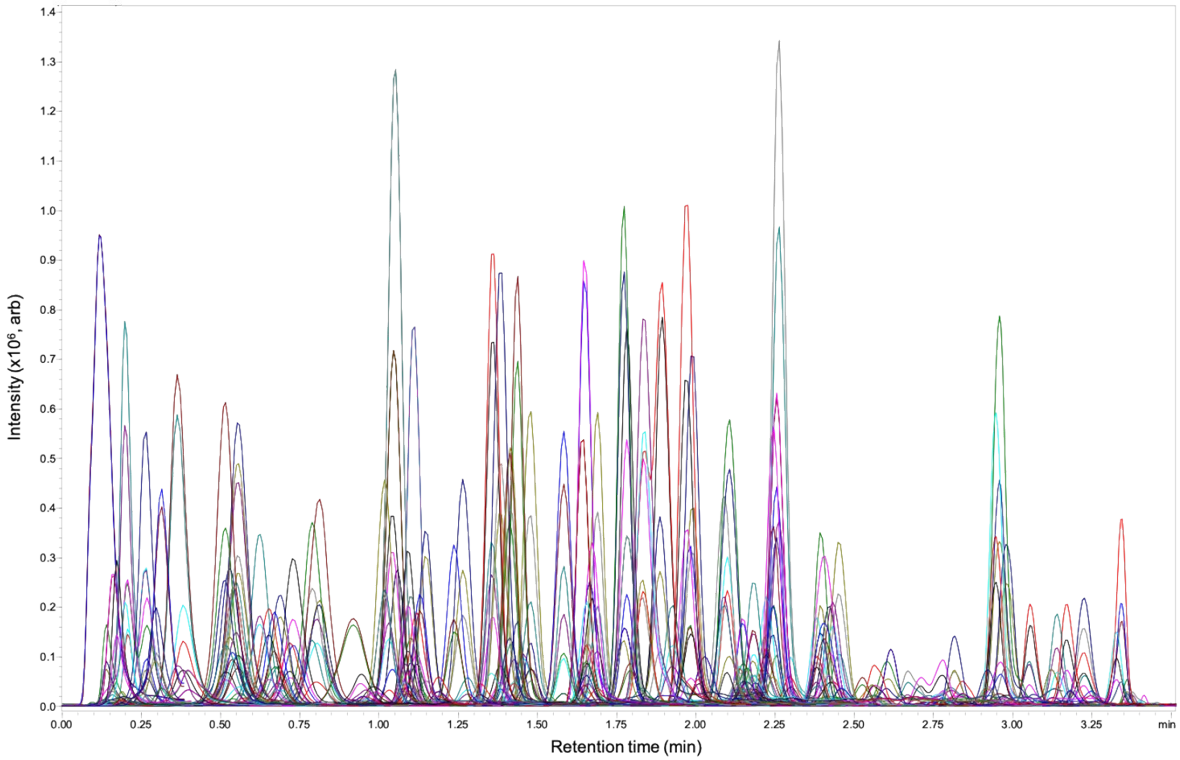

Figure S1 – Elution profile of a 500 ng/L standard mix containing 164 pharmaceuticals, illicit substances, metabolites, pesticides and 34 SIL-IS using the rapid targeted LC-MS/MS method.

Table S1 – MRM scheduling parameters for the rapid targeted LC-MS/MS method[1]

Compounds	Precursor (m/z)	Transition (m/z)	Polarity	Dwell Time (ms)	Collision Energy (V)
2-(Thiocyanomethylthio) benzothiazole	238.7	180.1	+	2	-14
		136.1	+	2	-26
4-Methylethcathinone	192.1	174.2	+	5	-16
		144.1	+	5	-29
Acetamiprid	233	126.1	+	13	-21
Alprazolam	309.1	281.1	+	2	-26
		205.1	+	2	-40
Ametryn	228.1	186.1	+	4	-20
		96.1	+	4	-28
Amiodarone	645.8	58.2	+	20	-49
		100.2	+	20	-30
Amitriptyline	278.2	91.1	+	4	-27
		105.1	+	4	-25
Amitriptyline-d3	281.1	233.2	+	4	-17
		105.2	+	4	-23
Amlodipine	409.1	238.2	+	6	-12
Antipyrine	188.9	77.2	+	5	-40
		56.2	+	5	-32
Atorvastatin	559.1	440.3	+	5	-23
		250.2	+	5	-43
Atrazine	216.1	174.1	+	14	-18
Azelnidipine	583.2	167.2	+	2	-27
		165.2	+	2	-55
Azithromycin	749.6	591.4	+	2	-30
		158.3	+	2	-40
Azoxystrobin	404.2	372.1	+	2	-16
		344.1	+	2	-26
Benoxacor	260	149.2	+	2	-18
		134.1	+	2	-29
Bensulide	398.1	158.1	+	1	-24
		217.9	+	1	-17
Benzatropine	308.1	167.2	+	5	-30
		265.2	+	5	-52
Benzoylecgonine, BZE	290.1	168.2	+	11	-19
Benzoylecgonine, BZE-d3	293.1	171.2	+	11	-20
Betaxolol	308.3	116.2	+	4	-21
		72.2	+	4	-24

Table S1 continues on the next page

Betaxolol-d7	315.2	123.3	+	4	-22
		105.3	+	4	-24
Bezafibrate	360.2	274	-	5	17
		154.1	-	5	29
Bisoprolol	326.2	116.2	+	5	-19
		74.2	+	5	-26
Bupropion	240.1	184.2	+	4	-13
		131.2	+	4	-26
Buspirone	386.1	122.2	+	2	-30
		109.2	+	2	-46
Carazolol	299.1	116.2	+	6	-21
		222.2	+	6	-21
Carbamazepine	237.1	194	+	4	-20
		192.1	+	4	-25
Carboxine	236	143.1	+	13	-15
Carfentrazone-ethyl	412.1	346	+	2	-17
		366	+	2	-19
Carbamazepine epoxide	252.9	180.2	+	4	-29
		236.2	+	4	-12
Celecoxib	382.1	362.1	+	4	-28
		300.2	+	4	-28
Celecoxib-d7	389	369.1	+	2	-29
		289.2	+	2	-37
Chloramphenicol	322.7	152.2	-	5	17
		257	-	5	11
Cilazapril	418	211.2	+	5	-20
		70.2	+	5	-46
Citalopram	325.1	109.2	+	4	-26
		262.2	+	4	-20
Clarithromycin	748.2	158.2	+	2	-34
		290.4	+	2	-20
Clarithromycin-d3	751.2	161.2	+	2	-28
		593.4	+	2	-22
Clozapine	327.2	270.2	+	2	-23
		192.1	+	2	-45
Cocaine	304.2	182.3	+	5	-21
		82.1	+	5	-35
Cocaine-d3	307.1	185.2	+	5	-21
		77.2	+	5	-54
Cyclouron	199.1	72.2	+	3	-25
		89.2	+	3	-14

Table S1 continues on the next page

Cycloxyidim	326.1	280.2	+	5	-14
		180.2	+	5	-22
Cymoxanil	199.2	111.2	+	3	-19
		83	+	3	-27
Diazepam	285.1	154.1	+	2	-28
		193.1	+	2	-29
Diazepam-d6	289.9	198.2	+	2	-33
		154.2	+	2	-27
Diclofenac	296	215.1	+	6	-20
		214	+	6	-40
Diflubenzuron	311	158.1	+	1	-16
		141.1	+	1	-32
Dimethametryn	256.1	186.2	+	2	-22
		68.1	+	2	-44
Diphenhydramine	256	167.1	+	2	-11
		152	+	2	-40
Famoxadone	375.8	196.1	+	6	-21
Fenoxaprop-ethyl	362.1	288.1	+	2	-18
		121.1	+	2	-33
Fenuron	165	72.2	+	5	-22
		46.1	+	5	-14
Flufenoxuron	489.1	158.1	+	2	-21
		141	+	2	-39
Fluocinonide	494.9	337.2	+	6	-19
Fluoxetine	310.2	44.2	+	2	-16
		148.2	+	2	-10
Fluoxetine-d6	316.1	44.2	+	2	-15
		154.3	+	2	-9
Flutamide	275	202	-	2	23
		205	-	2	21
Flutolanil	324.3	242.2	+	2	-26
		262.2	+	2	-19
Fuberidazole	184.9	157.2	+	5	-21
		156.2	+	5	-27
Hydrochlorothiazide	296	269	-	10	19
Imidacloprid	256.1	175.1	+	5	-19
		209.1	+	5	-18
Indomethacin	356.5	312.3	-	14	11
Isocarbamid	186.1	87	+	2	-16
		44.2	+	2	-32

Table S1 continues on the next page

Isradipine	370.2	119	-	2	16
		250	-	2	16
Josamycin	828.5	109.3	+	6	-47
Ketamine	238.1	125	+	5	-26
		207	+	5	-15
Ketamine-d4	242.1	129.2	+	5	-28
		211.3	+	5	-15
Ketoconazole	533	491.1	+	4	-31
		82.2	+	4	-47
Ketotifen	310	96.2	+	10	-24
Levamisole	207.1	180	+	10	-24
		91.1	+	10	-41
Levocabastine	421.4	174.2	+	6	-32
		70.2	+	6	-37
Lidocaine	235	86.1	+	5	-19
		58.1	+	5	-45
Lidocaine-d10	245.2	96.3	+	13	-22
MDMA	194.1	163.1	+	5	-13
		105.1	+	5	-25
MDMA-d5	199.1	165.3	+	5	-14
		107.2	+	5	-25
Meclizine	391.1	201.1	+	1	-20
		165.1	+	1	-55
Medroxyprogesterone	345.1	123.2	+	2	-26
		97.2	+	2	-27
Mefenamic acid	240	196.2	-	12	18
Memantine	180.3	163.3	+	6	-18
		107.3	+	6	-26
Mephedrone	178.3	145.1	+	10	-21
		160.3	+	10	-16
Mephosfolan	270.1	140	+	12	-25
Methamphetamine	150.1	91.1	+	5	-19
		119.1	+	5	-10
Methedrone	194.3	176.2	+	5	-15
		161.1	+	5	-21
Methylphenidate	234.2	84.1	+	6	-20
		56.1	+	6	-45
Methylphenidate-d9	243.3	93.3	+	6	-24
		61.2	+	6	-50

Table S1 continues on the next page

Metoprolol	268.2	116.2	+	5	-21
		159.1	+	5	-22
Metoprolol-d7	275.2	123.2	+	5	-21
		105.2	+	5	-22
Nadolol	310.3	254.2	+	3	-17
		236.2	+	3	-21
Nifedipine	345.2	222.1	-	3	10
		122	-	3	12
Nifedipine-d4	349	222.1	-	3	10
		126.1	-	3	12
Nordiazepam	270.8	140.2	+	2	-28
		208.1	+	2	-28
Nordiazepam-d5	275.9	213.3	+	2	-28
		140.2	+	2	-31
Norethisterone	299.1	109.2	+	2	-26
		231.2	+	2	-20
Nortriptyline	264.2	233.1	+	4	-15
		91.1	+	4	-25
Nortriptyline-d3	267	233.2	+	4	-15
		105.2	+	4	-22
Orphenadrine	270.1	181.2	+	4	-13
		166.1	+	4	-28
Oxamyl	237.1	72.1	+	4	-12
		90.2	+	4	-10
Oxazepam	287.2	241.2	+	5	-24
		269.1	+	5	-15
Oxazepam-d5	292	246.2	+	5	-24
		274.1	+	5	-17
Oxycarboxin	268.1	175	+	5	-14
		147	+	5	-27
Oxycodone	316.2	298.2	+	20	-19
		241.1	+	20	-30
Picoxystrobin	368	145.2	+	1	-22
		205.2	+	1	-10
Piperophos	353.9	171.1	+	2	-22
		255.1	+	2	-14
Pirenzipine	352.1	113.3	+	5	-22
		70.2	+	5	-46
Pretilachlor	312.2	252.1	+	2	-17
		176.1	+	2	-29

Table S1 continues on the next page

Prodiamine	349.2	232	-	2	24
		216	-	2	29
Prometon	226.1	184.2	+	5	-20
		142.2	+	5	-23
Prometryn	242.2	158.1	+	2	-25
		200	+	2	-20
Propanolol	260.1	116.2	+	4	-19
		183.2	+	4	-20
Propazine	230.1	188.2	+	4	-19
		146.1	+	4	-24
Pymetrozine	218.1	105.1	+	6	-21
		79	+	6	-45
Pyracarbolid	218.1	125.1	+	3	-18
		97.1	+	3	-28
Pyraclostrobin	390.1	194.1	+	2	-15
		163.1	+	2	-27
Pyraflufen-ethyl	413	339	+	2	-20
		253.1	+	2	-35
Pyridaben	364.8	147.2	+	3	-25
		309.1	+	3	-14
Risperidone	411.2	191.1	+	10	-31
		69.1	+	10	-50
Risperidone-d4	415.2	195.2	+	10	-30
Rizatriptan	270.1	201.2	+	5	-14
		158.2	+	5	-21
Ronidazole	201	140.2	+	11	-13
Roxithromycin	837.3	679.4	+	4	-22
		158.1	+	4	-34
Sertraline	306.1	159	+	4	-26
		275.1	+	4	-15
Sertraline-d3	309	159.1	+	4	-28
		275.1	+	4	-14
Simazine	202.1	104	+	5	-25
		68.1	+	5	-32
Spinosyn A	732.6	142.1	+	5	-34
		98	+	5	-40
Spinosyn D	746.6	142.1	+	6	-36
		98	+	6	-40
Spiramycin	843.5	174.2	+	10	-36

Table S1 continues on the next page

Sulfadimethoxine	311.1	156	+	10	-20
		92.1	+	10	-32
Sulfamerazine	265.1	92.1	+	3	-34
		156	+	3	-17
Sulfamethazine	278.9	186.1	+	6	-17
		124.2	+	6	-24
Sulfamethazine-d4	282.8	186.2	+	3	-20
		124.2	+	3	-25
Sulfamethoxazole	254.1	156	+	6	-18
		92.2	+	6	-31
Sulfamonomethoxine	281.1	156.1	+	4	-18
		92.2	+	4	-33
Sulfapyridine	250	156	+	4	-17
		92.1	+	4	-32
Sulfathiazole	256	156	+	8	-16
		92.2	+	8	-27
Sulfisoxazole	268	156.1	+	13	-15
		113.2	+	13	-16
Tacrine	199	171.2	+	6	-30
		144.1	+	6	-36
Tamsulosin	409.1	228.1	+	4	-24
		271.2	+	4	-20
Temazepam	301.1	255.1	+	4	-25
		283.2	+	4	-13
Temazepam-d5	306	260.1	+	10	-24
Terbutryn	242.1	186.1	+	2	-20
		158.2	+	2	-24
Terfenadine	472.4	436.3	+	6	-28
		454.3	+	6	-22
Thiacloprid	253.1	126.1	+	4	-22
		90.1	+	4	-38
Thiamethoxam	292	211.1	+	2	-13
		181	+	2	-24
Thiamethoxam-d3	296.6	214.1	+	3	-12
		184.1	+	3	-24
Thiazopyr	397	377.1	+	6	-23
Timolol	317.1	261.1	+	13	-17
Tramadol	264.1	58.2	+	14	-16
Tramadol-13C1, d3	268.3	58.2	+	14	-23

Table S1 continues on the next page

Trimethoprim	291.1	230.1	+	5	-25
		123.2	+	5	-28
Trimethoprim-d3	294.1	230.2	+	5	-25
		123.2	+	5	-26
Valsartan	436.4	291.2	+	5	-18
		235.2	+	5	-17
Venlafaxine	278.2	58.1	+	5	-19
		260.2	+	5	-15
Venlafaxine-d6	284.2	64.2	+	5	-23
		260.2	+	5	-15
Verapamil	455.2	165.2	+	2	-29
		414.4	+	2	-16
Verapamil-d3	458.2	165.2	+	2	-29
		306.3	+	2	-26
Warfarin	309.2	163.1	+	5	-16
		251.1	+	5	-20
Ziprasidone	413.1	194.1	+	2	-30

S2 – List of pesticide standards used to train predictive retention time model

Reference standards for: 2,3,5-Trimethacarb, Acephate, Acetamiprid, Alanycarb, Aldicarb, Amidosulfuron, Aminocarb, Avermectin B1a, Avermectin B1b, Azaconazole, Azamethiphos, Azinphos-ethyl, Azinphos-methyl, Azoxystrobin, Beflubutamid, Benalaxyl, Benzoximate, Bifenazate, Bispyribac, Bitertanol, Boscalid, Bromuconazole, Bupirimate, Buprofezin, Butocarboxim, Carbaryl, Carbendazim, Carbofuran, Carboxin, Carfentrazone-ethyl, Chlorantraniliprole, Chlorfenvinphos, Chloridazon, Chloroxuron, Chlorpyrifos, Chlorpyrifos-methyl, Chlorsulfuron, Chlortoluron, Clethodim, Clofentezin, Clomazone, Coumaphos, Cyazofamid, Cycluron, Cymoxanil, Cyproconazole(I), Cyproconazole(II), Cyprodinil, DEET / Diethyltoluamide, Desmedipham, Diazinon, Dichlorvos, Diethofencarb, Difenconazole(I), Diflubenzuron, Diflufenican, Dimethachlor, Dimethoate, Dimethomorph(E), Dimethomorph(Z), Dimoxystrobin, Diniconazole(I), Dinotefuran, Dioxacarb, Disulfoton, Diuron, Epoxiconazole, Ethidimuron, Ethion, Ethirimol, Ethofumesate, Ethoxyquin, Famoxadone, Fenamidone, Fenamiphos, Fenarimol, Fenbuconazole, Fenhexamid, Fenobucarb, Fenoxycarb, Fenpropidin, Fenpyroximate, Fenuron, Fipronil, Flazasulfuron, Flonicamid, Fluazinam, Flubendiamide, Fludioxonil, Flufenacet, Flufenoxuron, Flumetsulam, Flumioxazin, Fluometuron, Fluopicolid, Fluoxastrobin, Fluquinconazole(I), Flusilazol, Flutriafol, Foramsulfuron, Forchlorfenuron, Fosthiazate, Fuberidazole, Furalaxyl, Furathiocarb, Halofenozide, Halosulfuron-methyl, Hexaconazole(I), Hexaflumuron, Hexythiazox, Hydramethylnon, Imidacloprid, Indoxacarb, Ipconazole(II), Iprovalicarb, Isocarbophos, Isofenphos methyl, Isoprothiolane, Isoxaben, Isoxaflutole, Ivermectin B1a, Kresoxim-methyl, Lenacil, Linuron, Lufenuron, Malaoxon, Malathion, Mandipropamid, Mecarbam, Mepanipyrim, Mesosulfuron-methyl, Metaflumizone, Metalaxyl, Metamitron, Metazachlor, Metconazole(I), Methabenzthiazuron, Methacrifos, Methamidophos, Methidathion, Methiocarb, Methomyl, Methoprotryne, Methoxyfenozide, Metobromuron, Metolachlor, Metrafenone, Metribuzin, Metsulfuron-methyl, Mevinphos, Mexacarbate, Molinate, Monocrotophos, Moxidectin, Myclobutanil, Nicosulfuron, Nitenpyram, Novaluron, Omethoate, Oxadiazon, Oxadixyl, Oxamyl, Oxasulfuron, Paclobutrazol, Penconazole, Pencycuron, Phenmedipham, Phosalone, Phosmet, Phosphamidon, Phoxim, Picolinafen, Picoxystrobin, Pirimicarb, Pirimiphos-methyl, Prochloraz, Profenofos, Promecarb, Prometon, Propamocarb, Propaquizafop, Propetamphos, Propiconazole(II), Propoxur, Propyzamide, Proquinazid, Pymetrozine, Pyracarbolid, Pyraclostrobin, Pyrimethanil, Pyriproxyfen, Quinalphos, Quinmerac, Quinoclamine, Quinoxyfen, Rimsulfuron, Rotenone, Silthiofam, Spinosyn A, Spinosyn D, Spirodiclofen, Spiromesifen, Spirotetramat, Spiroxamine, Sulfentrazone, Tebuconazole(I), Tebufenozide, Tebufenpyrad, Tebuthiuron, Teflubenzuron, Temephos, Tepraloxydim, Terbufos, Tetraconazole, Thiabendazole, Thiacloprid, Thiamethoxam, Thidiazuron, Thifensulfuron-methyl, Thiodicarb, Thiofanox, Tifatol, Tolclofos-methyl, Tolylfluanide, Tralkoxydim, Triadimefon, Triadimenol, Triasulfuron, Triazophos, Tribenuron-methyl, Trichlorfon, Tricyclazole, Trietazine, Trifloxystrobin, Triflumizol, Triflumuron, Triticonazole(II), Vamidothion and Zoxamide were sourced from Agilent Technologies UK Ltd.

S3 – Abiotic river conditions during sampling campaigns

Changes in temperature, salinity, pH, flow rate and fouling have previously been shown to alter significantly the performance of passive sampler devices[3]. During both deployments there were no reported untreated wastewater discharges to the River Thames via CSOs, though in the fortnight preceding the winter deployment there were three discharge events of untreated sewage and diluted storm water on the 7th, 15th and 16th December, 2018[4]. There was no significant evidence of fouling on the passive sampler devices collected after either deployment. Previously, it was shown that dissolved oxygen (DO) and ammonium concentration recovered approximately within 48 h following a CSO event. These conditions were therefore consistent throughout both deployments, but, in general, were both lower in winter (Figure S2). However, despite this, the average pH of the River Thames during both deployments remained relatively constant at 7.9±0.04 and 7.8±0.05 for winter and summer, respectively. In the six months preceding both deployments, the South East region of England, which encompasses the River Thames catchment area, received a total of 386 mm and 289 mm of rainfall (monthly average of 64.4 mm and 48.2 mm)[5] for winter and summer, respectively. Salinity profiles in summer predictably followed tidal flood and ebb cycles, but, likely due to higher rainfall and run-off to the river upstream, was less pronounced in the winter campaign given the higher proportion of freshwater. Flow data measured at the Kingston monitoring station revealed relatively higher and more variable influx of flow from the upper Thames catchment in winter (51 ± 30 m^3/s and 8±1 m^3/s in winter and summer, respectively, (Figure S3)). The water temperature was also markedly different between both deployments (winter=8.4±0.3^oC; summer=20±1.5^oC). Temperature has been shown to affect pharmaceutical-type compounds with up to a two-fold increase in R_s over this range reported previously.[6–8]

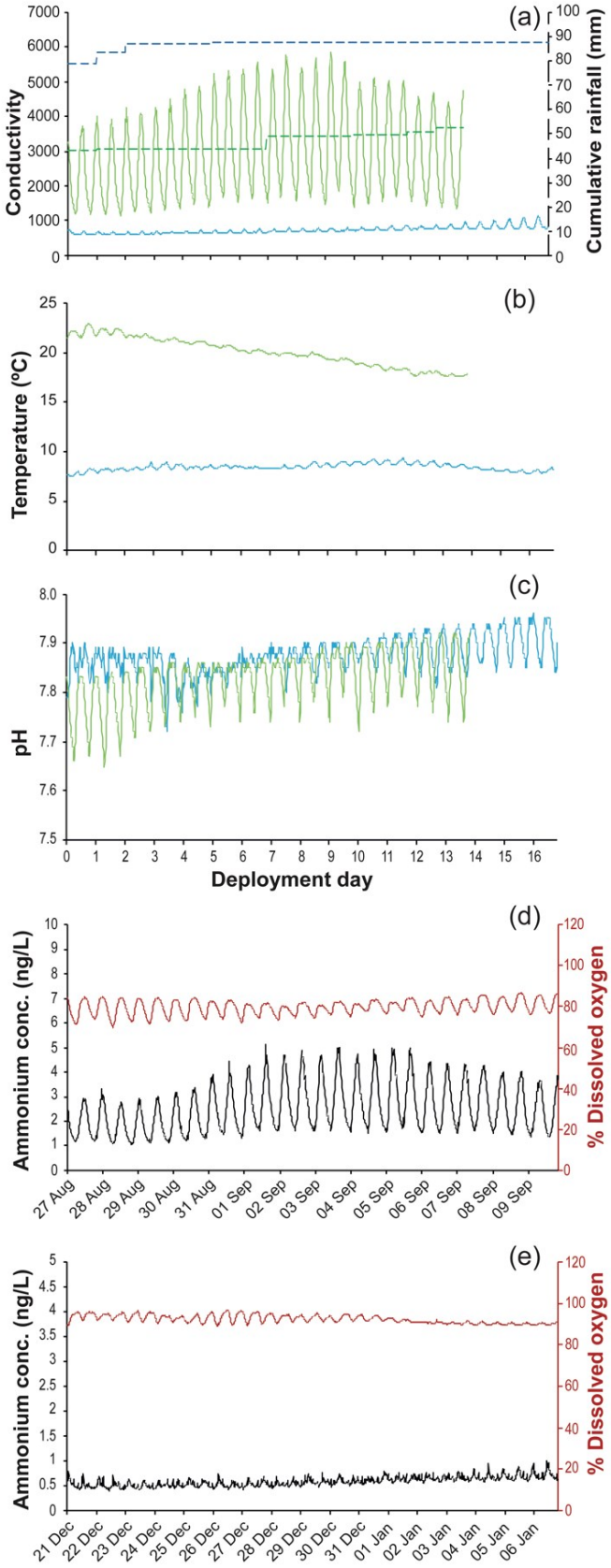

Figure S2 – Continuous monitoring (acquisition frequency=15 min) of abiotic data of the River Thames over the winter (blue) and summer (green) deployments for (a) conductivity with cumulative rainfall data, (b) temperature, (c) pH, and % DO (red) and ammonium concentration (black) for the summer (d) and winter (e) deployments.

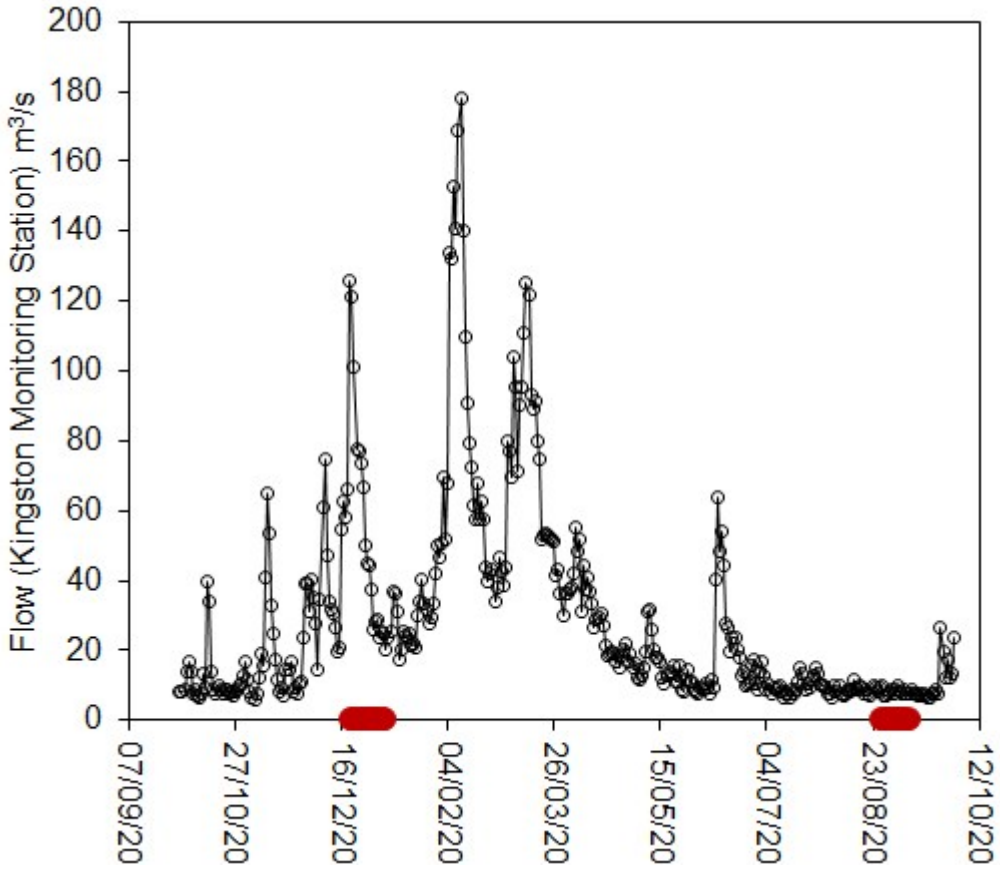

Figure S3 – Flow data for the River Thames measured at the Kingston monitoring station, UK (Data from the UK National River Flow Archive). Flow data represents only the non-tidal region of the Thames to illustrate influx of freshwater to the tidal region under investigation. Red intervals represent the two sampling campaigns, i.e, left: winter; right: summer.

Table S2 – Additional targeted direct injection LC-MS/MS analytical method performance data for precision and accuracy.

Analyte	Matrix Effect (%)[a]	Precision[b]		Accuracy (%)[b]	
	@1000 ng/L	100 ng/L	1000 ng/L	100 ng/L	1000 ng/L
4-Fluoromethacationone	-18	7	8	-1	0
Acetamiprid	6	14	3	-7	-2
Amitriptyline	-35	11	9	3	1
Amphetamine	-14	18	10	0	1
Azoxystrobin	-5	7	6	-3	-1
Benzoylecgonine	1	2	4	-3	0
Bisoprolol	14	3	5	-6	-1
Carbamazepine	12	4	2	-14	-2
Citalopram	26	2	5	-5	-1
Clopidogrel	2	11	4	-8	0
Clozapine	59	10	6	-3	-1
Cocaine	-4	8	5	-4	0
Cyclouron	2	24	6	-7	-1
Diclofenac	2	9	5	-11	-2
Fenuron	-6	5	5	-1	-1
Imidacloprid	12	24	9	-11	-1
Ketamine	4	5	4	-6	0
Lidocaine	1	3	3	-9	-1
MDMA	3	4	6	-3	0
Memantine	9	5	6	-4	0
Methamphetamine	2	3	5	-4	0
Nicotine	-3	6	6	-22	-2
Oxazepam	8	10	5	-8	0
Propamocarb	-2	6	4	2	0
Propanolol	19	8	7	4	7
Pyracarbolid	-8	4	4	0	-1
Salicylic acid	128	7	60	-4	9
Sulfapyridine	3	4	5	-11	-1
Temazepam	2	7	6	-1	0
Terbutryn	0	17	5	-5	-1
Tramadol	0	2	3	-14	-2
Trimethoprim	-4	5	2	-5	0
Venlafaxine	1	2	5	-9	-1

[a] details as per Table 1; [b] represents mean of % inaccuracy and imprecision for *n*=6 replicate river water samples (River Thames, UK) spiked with 100 and 1000 ng/L of all detected analytes (negative values for accuracy represent % underestimates of the expected concentration and vice versa).

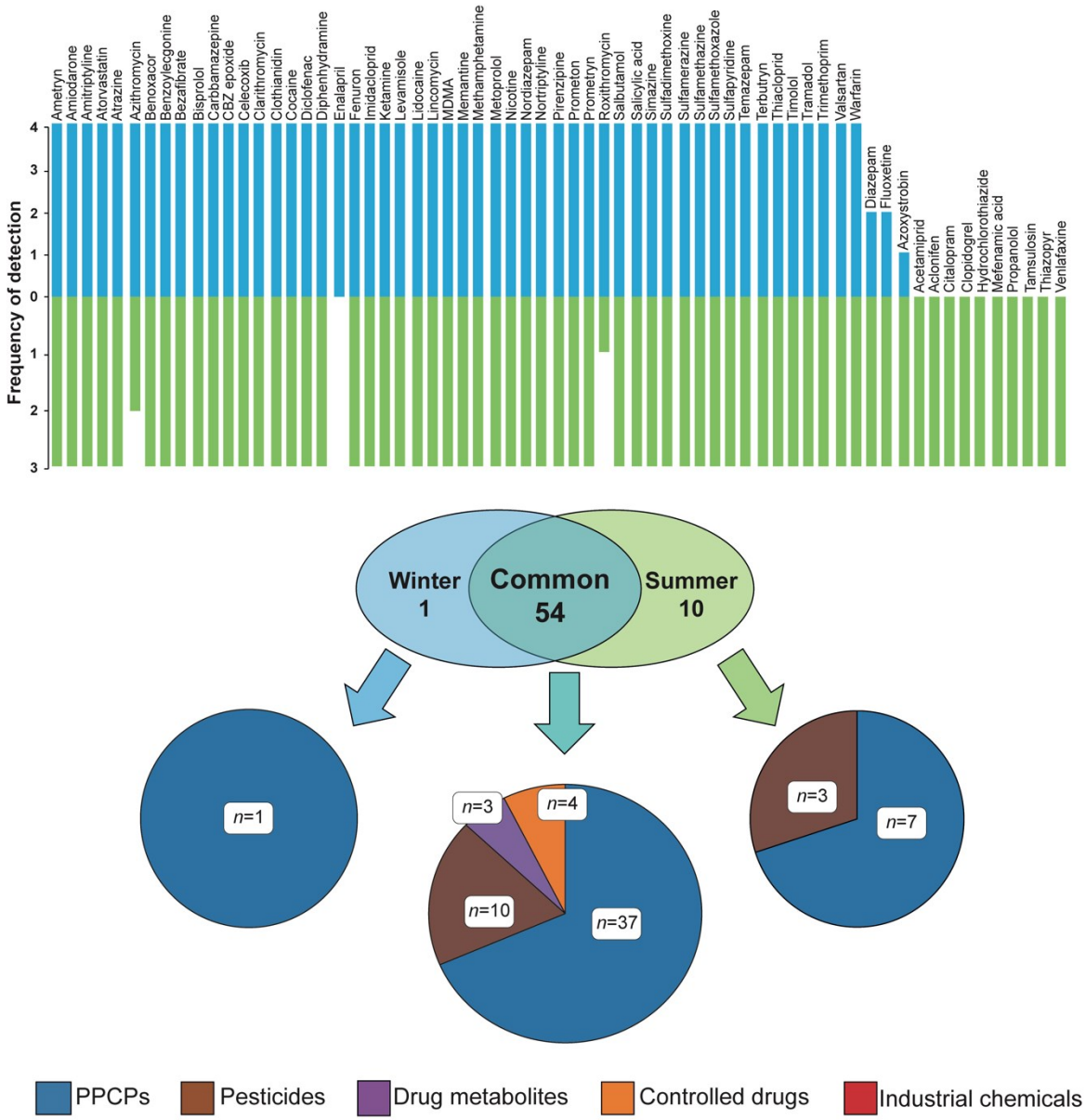

Figure S4 – Top: Frequency of detection of compounds in replicate passive sampler extracts (blue=winter; *n*=4, green=summer; *n*=3 samplers) identified using targeted screening. Bottom: Differences in compound occurrence between campaigns and overall proportion based on chemical classification. *n*=number of unique compounds within each class.

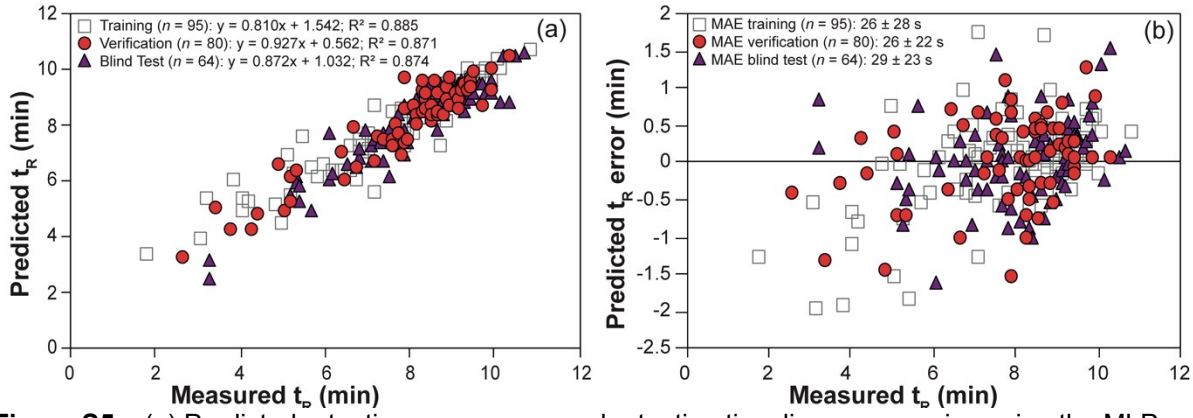

Figure S5 – (a) Predicted retention verse measured retention time linear regression using the MLP prediction model, training set (grey squares, *n*=95), verification set (purple triangles, *n*=80), and blind set (red circles, n=64). (b) Residual error of the predicted retention times.

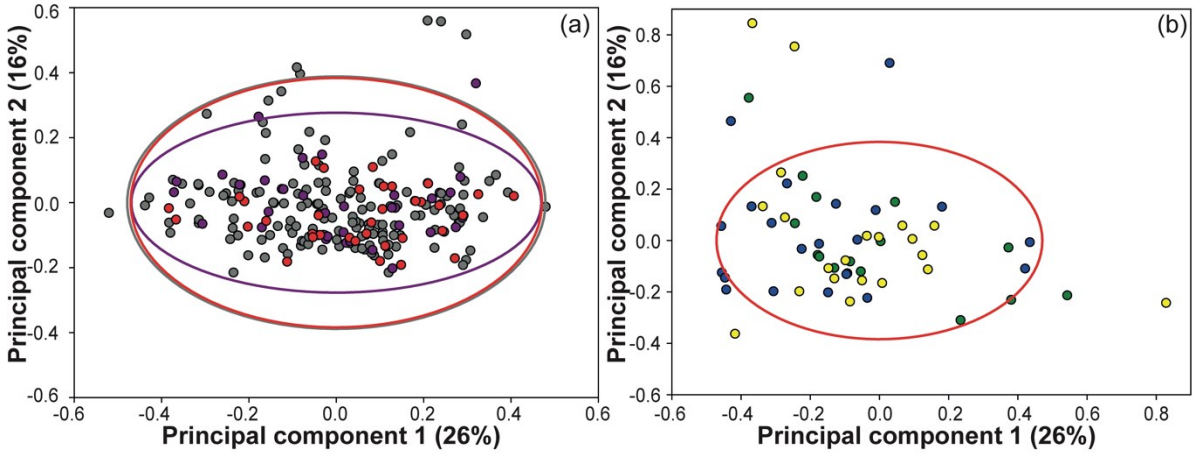

Figure S6 – PCA analysis on the 16 molecular descriptors used to generate the retention time model in order to define the applicability domain of the model and application to the unknown samples from screening. (a) model training (grey), verification (purple) and test (red) cases with a 95% confidence ellipse. (b) model matches from the machine learning assisted suspect screening workflow (blue=winter, green=summer, yellow=common to both) with the test 95% confidence ellipse.

Table S3 – Molecular descriptors used for ANN retention time prediction

Name	SMILES	Ui	Hy	MLOGP	ALOGP	nBnz	nDB	nTB	nR04	nR05	nR06	nR07	nR08	nR09	LogD (pH = 3)	nC	nO
1-Methyleneandrosterone	CC12CCC3C(C1CCC2=O)CCC4C3(C(=C)CC(C4)O)C	1.58	-0.44	3.92	3.50	0	2	0	0	1	3	0	0	1	3.78	20	2
10,11-Dihydroxycarbazepine	C1=CC=C2C(=C1)C(C(C3=CC=CC=C3N2C(=O)N)O)O	3	1.93	1.21	1.19	2	1	0	0	0	2	1	0	0	0.45	15	3
17α-Estradiol (Alfatradiol)	CC12CCC3C(C1CCC2O)CCC4=C3C=CC(=C4)O	2	0.21	3.63	3.81	1	0	0	0	1	3	0	0	1	3.62	18	2
2-Aminobenzimidazole	C1=CC=C2C(=C1)NC(=N2)N	2.58	1.69	1.27	1.14	1	0	0	0	1	1	0	0	1	-1.42	7	0
2-EMC / 2-Ethylmethcathinone	CCC1=CC=CC=C1C(=O)C(C)NC	2.32	-0.31	2.41	2.57	1	1	0	0	0	1	0	0	0	-0.9	12	1
2-Hydroxyethyl salicylate	C1=CC=C(C(=C1)C(=O)OCCO)O	2.32	0.60	1.49	0.88	1	1	0	0	0	1	0	0	0	1.62	9	4
2-Hydroxypropyl salicylate	CC(COC(=O)C1=CC=CC=C1O)O	2.32	0.55	1.79	1.26	1	1	0	0	0	1	0	0	0	1.95	10	4
2-Ketoglutaric acid	C(CC(=O)O)C(=O)C(=O)O	2	0.94	-0.83	-0.67	0	3	0	0	0	0	0	0	0	-1.88	5	5
2-MEC / 2-Methylethcathinone	CCNC(C)C(=O)C1=CC=CC=C1C	2.32	-0.31	2.41	2.47	1	1	0	0	0	1	0	0	0	-0.9	12	1
2-MeO-MA (Methoxyphenamine)	CC(CC1=CC=CC=C1OC)NC	2	-0.28	2.22	2.05	1	0	0	0	0	1	0	0	0	-1.08	11	1
2-Methylbenzophenone (o-Methylbenzophenone)	CC1=CC=CC=C1C(=O)C2=CC=CC=C2	3	-0.91	3.85	3.72	2	1	0	0	0	2	0	0	0	3.38	14	1
2-Naepaine	CCCCCNCCOC(=O)C1=CC=C(C=C1)N	2.32	1.14	2.39	2.33	1	1	0	0	0	1	0	0	0	-0.03	14	2
2-Nitrophenol	C1=CC=C(C(=C1)[N+](=O)[O-])O	2.58	0.03	1.35	1.46	1	2	0	0	0	1	0	0	0	1.81	6	3
2-Phenylbutyric acid	CCC(C1=CC=CC=C1)C(=O)O	2.32	-0.24	2.39	2.39	1	1	0	0	0	1	0	0	0	2.13	10	2
2,3-DMMC / 2,3-Dimethylmethcathinone	CC1=C(C(=CC=C1)C(=O)C(C)NC)C	2.32	-0.31	2.41	2.60	1	1	0	0	0	1	0	0	0	-1.09	12	1
2,3-MDPEA / 2,3-Methylenedioxyphenethylamine	C1OC2=CC=CC(=C2O1)CCN	2	0.59	1.08	1.03	1	0	0	0	1	1	0	0	1	-1.56	9	2
2,4-D / 2,4-Dichlorophenoxyacetic acid	C1=CC(=C(C=C1Cl)Cl)OCC(=O)O	2.32	-0.05	2.35	2.81	1	1	0	0	0	1	0	0	0	2.53	8	3
2,4-Dinitrophenol	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	3	0.10	1.39	0	1.35	1	4	0	0	0	1	0	0	0	1.62	6
2,4-DMMC / 2,4-Dimethylmethcathinone	CC1=CC(=C(C=C1)C(=O)C(C)NC)C	2.32	-0.31	2.41	2.60	1	1	0	0	0	1	0	0	0	-1.08	12	1
2C-E / 2,5-Dimethoxy-4-ethylphenethylamine	CCC1=CC(=C(C=C1OC)CCN)OC	2	0.43	1.94	2.17	1	0	0	0	0	1	0	0	0	-0.74	12	2
2C-H / 2,5-Dimethoxyphenethylamine (Benzeneethanamine)	COC1=CC(=C(C=C1)OC)CCN	2	0.53	1.36	1.22	1	0	0	0	0	1	0	0	0	-1.62	10	2
3-Aminophenol	C1=CC(=CC(=C1)O)N	2	1.88	0.89	0.82	1	0	0	0	0	1	0	0	0	-0.75	6	1
3-EMC / 3-Ethylmethcathinone	CCC1=CC(=CC=C1)C(=O)C(C)NC	2.32	-0.31	2.41	2.57	1	1	0	0	0	1	0	0	0	-0.9	12	1
3-Hydroxylidocaine	CCN(CC)CC(=O)NC1=C(C=CC(=C1C)O)C	2.32	0.37	1.98	2.57	1	1	0	0	0	1	0	0	0	-1.32	14	2

Table S3 continues on the next page

3-MEC / 3-Methylethcathinone	CCNC(C)C(=O)C1=CC=CC(=C1)C	2.32	-0.31	2.41	2.47	1	1	0	0	0	1	0	0	0	-0.91	12	1
3-methyl BP / 3-Methylbuphedrone	CCC(C(=O)C1=CC=CC(=C1)C)NC	2.32	-0.31	2.41	2.64	1	1	0	0	0	1	0	0	0	-0.91	12	1
3-Methyl-2-oxopentanoic acid	CCC(C)C(=O)C(=O)O	1.58	0.00	0.43	1.09	0	2	0	0	0	0	0	0	0	0.13	6	3
3,4-DMMC / 3,4-Dimethylmethcathinone	CC1=C(C=C(C=C1)C(=O)C(C)NC)C	2.32	-0.31	2.41	2.60	1	1	0	0	0	1	0	0	0	-1.09	12	1
3,4-Methylenedioxybenzoic acid (Piperonylic acid)	C1OC2=C(O1)C=C(C=C2)C(=O)O	2.32	-0.08	0.94	1.20	1	1	0	0	1	1	0	0	1	1.69	8	4
4-Aminosalicylic acid	C1=CC(=C(C=C1N)O)C(=O)O	2.32	2.68	0.00	0.42	1	1	0	0	0	1	0	0	0	0.6	7	3
4-Biphenylacetic acid	C1=CC=C(C=C1)C2=CC=C(C=C2)CC(=O)O	3	-0.35	3.25	2.99	2	1	0	0	0	2	0	0	0	3.23	14	2
4-EMC / 4-Ethylmethcathinone	CCC1=CC=C(C=C1)C(=O)C(C)NC	2.32	-0.31	2.41	2.57	1	1	0	0	0	1	0	0	0	-0.9	12	1
4-HO-DBT	CCCCN(CCCC)CCC1=CNC2=C1C(=CC=C2)O	2.58	0.24	3.10	4.91	1	0	0	0	1	1	0	0	1	1.09	18	1
4-Hydroxyphenyl-pyruvic acid	C1=CC(=CC=C1CC(=O)C(=O)O)O	2.58	0.60	0.62	0	0.94	1	2	0	0	0	1	0	0	0	-0.07	9
4-MEC / 4-Methylethcathinone	CCNC(C)C(=O)C1=CC=C(C=C1)C	2.32	-0.31	2.41	2.47	1	1	0	0	0	1	0	0	0	-0.9	12	1
4-Methoxybenzaldehyde (Anisaldehyde)	COC1=CC=C(C=C1)C=O	2.32	-0.77	1.49	1.57	1	1	0	0	0	1	0	0	0	1.71	8	2
4-methyl BP (4-Methylbuphedrone)	CCC(C(=O)C1=CC=C(C=C1)C)NC	2.32	-0.31	2.41	2.64	1	1	0	0	0	1	0	0	0	-0.9	12	1
4-Methyl-2-oxopentanoic acid	CC(C)CC(=O)C(=O)O	1.58	0.00	0.43	0.88	0	2	0	0	0	0	0	0	0	0.13	6	3
4-Nitrophenol	C1=CC(=CC=C1[N+](=O)[O-])O	2.58	0.03	1.35	0	1.46	1	2	0	0	0	1	0	0	0	1.71	6
5-Aminosalicylic acid	C1=CC(=C(C=C1N)C(=O)O)O	2.32	2.68	1.10	0.42	1	1	0	0	0	1	0	0	0	-1.24	7	3
5-EAPB / 5-(2-Ethylaminopropyl)Benzofuran	CCNC(C)CC1=CC2=C(C=C1)OC=C2	2.58	-0.33	2.42	2.72	1	0	0	0	1	1	0	0	1	-0.04	13	1
5-MAPDB	CC(CC1=CC2=C(C=C1)OCC2)NC	2	-0.31	2.11	2.12	1	0	0	0	1	1	0	0	1	-0.77	12	1
5-Methylbenzotriazole	CC1=CC2=NNN=C2C=C1	2.58	-0.07	1.41	1.88	1	0	0	0	1	1	0	0	1	1.74	7	0
8-Hydroxyefavirenz	C1CC1C#CC2(C3=C(C(=CC(=C3)Cl)O)NC(=O)O2)C(F)(F)F	2.81	0.44	2.80	0	4.11	1	1	1	0	0	2	0	0	0	4.25	14
9-Octadecenamide (Oleamide)	CCCCCCCCC=CCCCCCCCC(=O)NCCC1=CC(=C(C=C1)O)O	2.58	0.77	5.53	7.81	1	2	0	0	0	1	0	0	0	7.6	26	3
Aceburic acid	CC(=O)OCCCC(=O)O	1.58	0.03	0.43	0.05	0	2	0	0	0	0	0	0	0	0.45	6	4
Acetochlor OXA (Acetochlor OA)	CCC1=CC=CC(=C1N(COCC)C(=O)C(=O)O)C	2.58	-0.25	2.06	2.54	1	2	0	0	0	1	0	0	0	0.93	14	4
Acetohexamide	CC(=O)C1=CC=C(C=C1)S(=O)(=O)NC(=O)NC2CCCCC2	3	0.39	1.25	2.12	1	4	0	0	0	2	0	0	0	2.27	15	4
Adipic acid	C(CCC(=O)O)CC(=O)O	1.58	0.84	0.43	0	0.50	0	2	0	0	0	0	0	0	0	0.12	6
Alantolactone	CC1CCCC2(C1=CC3C(C2)OC(=O)C3=C)C	2	-0.86	3.45	3.31	0	3	0	0	1	2	0	0	1	3.74	15	2
Allylescaline	COC1=CC(=CC(=C1OCC=C)OC)CCN	2.32	0.41	1.58	1.82	1	1	0	0	0	1	0	0	0	-1.62	13	3

Table S3 continues on the next page

Alprenolol	CC(C)NCC(COC1=CC=CC=C1CC=C)O	2.32	0.32	2.37	2.64	1	1	0	0	0	1	0	0	0	-0.32	15	2
Amisulpride	CCN1CCCC1CNC(=O)C2=CC(=C(C=C2OC)N)S(=O)(=O)CC	2.81	1.04	1.20	1.13	1	3	0	0	1	1	0	0	0	-1.72	17	4
Angelic acid	CC=C(C)C(=O)O	1.58	0.05	0.89	1.32	0	2	0	0	0	0	0	0	0	1.31	5	2
Aniline	C1=CC=C(C=C1)N	2	0.85	1.51	1.08	1	0	0	0	0	1	0	0	0	-0.4	6	0
Apocynin	CC(=O)C1=CC(=C(C=C1)O)OC	2.32	-0.16	1.24	1.29	1	1	0	0	0	1	0	0	0	1.4	9	3
Aspirin (Acetylsalicylic acid)	CC(=O)OC1=CC=CC=C1C(=O)O	2.58	-0.13	1.70	1.20	1	2	0	0	0	1	0	0	0	1.27	9	4
Atenolol	CC(C)NCC(COC1=CC=C(C=C1)CC(=O)N)O	2.32	1.99	0.92	0.67	1	1	0	0	0	1	0	0	0	-2.86	14	3
Atrolactamide	CC(C1=CC=CC=C1)(C(=O)N)O	2.32	1.47	0.84	0.53	1	1	0	0	0	1	0	0	0	0.27	9	2
α-PPP / α-Pyrrolidinopropiophenone	CC(C(=O)C1=CC=CC=C1)N2CCCC2	2.32	-0.85	2.29	2.63	1	1	0	0	1	1	0	0	0	-0.55	13	1
BAM / Dichlorbenzamide	C1=CC(=C(C(=C1)Cl)C(=O)N)Cl	2.32	0.75	2.48	0	2.16	1	1	0	0	0	1	0	0	0	1.28	7
Benhepazone	C1=CC=C(C=C1)CN2C3=CC=CC=CC3=NC2=O	3.17	-0.82	2.46	0	2.42	1	5	0	0	1	1	1	0	0	1.69	15
Benzhydryl cyanide (Methadone intermediate-1)	C1=CC=C(C=C1)C(C#N)C2=CC=CC=C2	3.17	-0.91	3.31	3.24	2	0	1	0	0	2	0	0	0	3.34	14	0
Benzocaine	CCOC(=O)C1=CC=C(C=C1)N	2.32	0.59	1.78	1.29	1	1	0	0	0	1	0	0	0	1.71	9	2
Benzododecinium (Ajatin)	CCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1	2	-0.94	2.55	5.53	1	0	0	0	0	1	0	0	0	2.43	21	0
Benzoic acid	C1=CC=C(C=C1)C(=O)O	2.32	-0.11	1.70	1.43	1	1	0	0	0	1	0	0	0	1.84	7	2
Benzylformate	C1=CC=C(C=C1)CC(=O)[O-]	2.32	-0.77	1.77	0.79	1	1	0	0	0	1	0	0	0	1.51	8	2
Bicalutamide	CC(CS(=O)(=O)C1=CC=C(C=C1)F)(C(=O)NC2=CC(=C(C=C2)C#N)C(F)(F)F)O	3.58	0.36	2.74	0	2.93	2	3	1	0	0	2	0	0	0	2.53	18
Bis(2-ethylhexyl) phthalate (DEHP)	CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC	2.58	-0.85	5.43	0	7.57	1	2	0	0	0	1	0	0	0	7.91	24
Bucolome	CCCCC1C(=O)NC(=O)N(C1=O)C2CCCCC2	2	-0.25	1.57	2.85	0	3	0	0	0	2	0	0	0	2.79	14	3
Bupicomide	CCCCC1=CN=C(C=C1)C(=O)N	2.32	0.53	1.02	1.96	0	1	0	0	0	1	0	0	0	0.7	10	1
Butacarb	CC(C)(C)C1=CC(=CC(=C1)OC(=O)NC)C(C)(C)C	2.32	-0.35	3.43	4.39	1	1	0	0	0	1	0	0	0	4.39	16	2
Butethamate	CCC(C1=CC=CC=C1)C(=O)OCCN(CC)CC	2.32	-0.83	3.16	3.48	1	1	0	0	0	1	0	0	0	0.45	16	2
Butoxycaine	CCCCOC1=CC=C(C=C1)C(=O)OCCN(CC)CC	2.32	-0.80	3.14	3.83	1	1	0	0	0	1	0	0	0	1.11	17	3
Butyl 4-hydroxybenzoate (Butylparaben)	CCCCOC(=O)C1=CC=C(C=C1)O	2.32	-0.24	2.38	2.75	1	1	0	0	0	1	0	0	0	3.18	11	3
Butylacetanilide (Bumadizone artifact)	CCCCN(C1=CC=CC=C1)C(=O)C	2.32	-0.84	2.82	2.49	1	1	0	0	0	1	0	0	0	2.41	12	1
BZP / Benzylpiperazine	C1CN(CCN1)CC2=CC=CC=C2	2	-0.28	1.56	0	1.33	1	0	0	0	0	2	0	0	0	-2.09	11
Caffeic acid	C1=CC(=C(C=C1C=CC(=O)O)O)O	2.58	1.46	0.89	1.37	1	2	0	0	0	1	0	0	0	1.31	9	4
Camphor	CC1(C2CCC1(C(=O)C2)C)C	1	-0.88	2.36	1.94	0	1	0	0	2	1	0	0	0	2.49	10	1

Cantharidin	CC12C3CCC(C1(C(=O)OC2=O)C)O3	1.58	-0.70	1.35	0.72	0	2	0	0	3	1	0	1	1	0.37	10	4
Carbofuran phenol (Carbofuranphenol)	CC1(CC2=C(O1)C(=CC=C2)O)C	2	-0.24	1.81	2.20	1	0	0	0	1	1	0	0	1	2.35	10	2
Carisoprodol	CCCC(C)(COC(=O)N)COC(=O)NC(C)C	1.58	1.25	0.75	0	2.20	0	2	0	0	0	0	0	0	0	1.93	12
Celiprolol	CCN(CC)C(=O)NC1=CC(=C(C=C1)OCC(CNC(C)(C)C)O)C(=O)C	2.58	0.94	1.70	1.60	1	2	0	0	0	1	0	0	0	-1.04	20	4
Cetirizine	C1CN(CCN1CCOCC(=O)O)C(C2=CC=CC=C2)C3=CC=C(C=C3)Cl	3	-0.35	2.58	3.68	2	1	0	0	0	3	0	0	0	-0.28	21	3
Ciclacillin	CC1(C(N2C(S1)C(C2=O)NC(=O)C3(CCCCC3)N)C(=O)O)C	2	1.91	1.07	0.58	0	3	0	1	1	1	1	0	0	-1.68	15	4
Ciramadol	CN(C)C(C1CCCCC1O)C2=CC(=CC=C2)O	2	0.32	2.07	2.62	1	0	0	0	0	2	0	0	0	-0.54	15	2
Citric acid	C(C(=O)O)C(CC(=O)O)(C(=O)O)O	2	2.64	-1.17	-1.40	0	3	0	0	0	0	0	0	0	-2.14	6	7
Clarithromycin-N-oxide	CCC1C(C(C(C(=O)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)[N+](C)(C)[O-])O)(C)OC)C)C)O)(C)O	1.58	1.31	-3.54	0	-0.19	0	2	0	0	0	2	0	0	0	0.13	38
Clobazam (Urbadan)	CN1C(=O)CC(=O)N(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3	3.17	-0.75	2.95	0	2.74	2	2	0	0	0	2	1	0	0	2.29	16
Clofibric acid	CC(C)(C(=O)O)OC1=CC=C(C=C1)Cl	2.32	-0.17	2.38	2.73	1	1	0	0	0	1	0	0	0	2.52	10	3
Codeine-N-oxide	C[N+]1(CCC23C4C1CC5=C2C(=C(C=C5)OC)OC3C(C=C4)O)[O-]	2.32	-0.33	-1.49	-0.61	1	1	0	0	1	4	0	1	3	-1.73	18	4
Coumaric acid	C1=CC(=CC=C1C=CC(=O)O)O	2.58	0.59	1.43	1.63	1	2	0	0	0	1	0	0	0	1.67	9	3
Coumarin	C1=CC=C2C(=C1)C=CC(=O)O2	2.58	-0.79	2.26	1.90	1	2	0	0	0	2	0	0	0	1.85	9	2
Crotamiton	CCN(C1=CC=CC=C1C)C(=O)C=CC	2.58	-0.85	3.01	3.09	1	2	0	0	0	1	0	0	0	2.34	13	1
Crotetamide	CCC(C(=O)N(C)C)N(CC)C(=O)C=CC	2	-0.73	1.41	1.41	0	3	0	0	0	0	0	0	0	0.51	12	2
Cyclexanone	C1CC=C(C1)C2(CCCC2=O)CCN3CCOCC3	1.58	-0.83	2.15	2.19	0	2	0	0	2	1	0	0	0	-1	16	2
Diatrizoate (Amidotrizoic acid)	CC(=O)NC1=C(C(=C(C(=C1I)C(=O)O)I)NC(=O)C)I	2.81	1.30	2.76	0	1.41	1	3	0	0	0	1	0	0	0	0.1	11
Dibutylamine	CCCCNCCCC	0	-0.21	2.27	2.44	0	0	0	0	0	0	0	0	0	-0.54	8	0
Dicamba	COC1=C(C=CC(=C1C(=O)O)Cl)Cl	2.32	-0.05	2.62	0	2.75	1	1	0	0	0	1	0	0	0	2.08	8
Dicyandiamidine (Guanylurea)	C(=NC(=O)N)(N)N	1.58	6.40	-1.71	-1.27	0	2	0	0	0	0	0	0	0	-3.74	2	1
Diethanolamine	C(CO)NCCO	0	2.21	-0.92	0	-1.29	0	0	0	0	0	0	0	0	0	-4.31	4
Dimethyl-4-aminophenol	CN(C)C1=CC=C(C=C1)O	2	-0.16	1.58	1.72	1	0	0	0	0	1	0	0	0	-0.83	8	1
Dinoprop	CC1=C(C(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O)C(C)C	3	-0.08	2.70	3.03	1	4	0	0	0	1	0	0	0	3.3	10	5
Dinoseb (Subitex)	CCC(C)C1=C(C(=CC(=C1)[N+](=O)[O-])[N+](=O)[O-])O	3	-0.08	2.70	3.00	1	4	0	0	0	1	0	0	0	3.29	10	5
Dinoterb	CC(C)(C)C1=C(C(=CC(=C1)[N+](=O)[O-])[N+](=O)[O-])O	3	-0.08	2.70	2.75	1	4	0	0	0	1	0	0	0	3.52	10	5
Disopyramide	CC(C)N(CCC(C1=CC=CC=C1)(C2=CC=CC=N2)C(=O)N)C(C)C	3	0.19	2.47	3.42	1	1	0	0	0	2	0	0	0	-1.17	21	1

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DLTDP / Dilaurylthiodipropionate (Cyanox LTDP)	CCCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCC	1.58	-0.85	7.28	10.66	0	2	0	0	0	0	0	0	0	12.24	30	4
DNOC / 2,4-Dinitro-o-kresol	CC1=CC(=CC(=C1O)[N+](=O)[O-])[N+](=O)[O-]	3	0.04	1.75	0	1.84	1	4	0	0	0	1	0	0	0	2.25	7
Docusate hydrogen	CCCCC(CC)COC(=O)CC(C(=O)OCC(CC)CCCC)S(=O)(=O)O	2.32	-0.29	3.01	5.15	0	4	0	0	0	0	0	0	0	1.69	20	7
Dodemorph	CC1CN(CC(O1)C)C2CCCCCCCCCCC2	0	-0.89	3.72	5.36	0	0	0	0	0	1	0	0	0	2.55	18	1
Dorzolamide	CCNC1CC(S(=O)(=O)C2=C1C=C(S2)S(=O)(=O)N)C	2.91	1.35	-0.03	0	0.27	0	4	0	0	1	1	0	0	1	-3.27	10
Enfenamic acid	C1=CC=C(C=C1)CCNC2=CC=CC=C2C(=O)O	3	0.32	3.20	3.15	2	1	0	0	0	2	0	0	0	3.99	15	2
Erythromycin	CCC1C(C(C(C(=O)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)O)C)O)(C)O	1.58	2.01	-0.14	1.65	0	2	0	0	0	2	0	0	0	-0.66	37	13
Ethenzamide	CCOC1=CC=CC=C1C(=O)N	2.32	0.59	1.38	1.16	1	1	0	0	0	1	0	0	0	1.06	9	2
Ethomoxane	CCCCNCC1COC2=C(O1)C(=CC=C2)OCC	2	-0.30	1.80	2.91	1	0	0	0	0	2	0	0	0	-0.09	15	3
Ethyl 4-hydroxybenzoate (Ethylparaben)	CCOC(=O)C1=CC=C(C=C1)O	2.32	-0.16	1.78	1.77	1	1	0	0	0	1	0	0	0	2.53	9	3
Ethyl 5-methoxysalicylate	CCOC(=O)C1=C(C=CC(=C1)OC)O	2.32	-0.17	2.06	1.75	1	1	0	0	0	1	0	0	0	2.63	10	4
Ethyl phenylacetate	CCOC(=O)CC1=CC=CC=C1	2.32	-0.81	2.39	2.07	1	1	0	0	0	1	0	0	0	2.37	10	2
Eugenol	COC1=C(C=CC(=C1)CC=C)O	2.32	-0.24	2.11	2.55	1	1	0	0	0	1	0	0	0	2.48	10	2
Fenchone	CC1(C2CCC(C2)(C1=O)C)C	1	-0.88	2.36	2.36	0	1	0	0	2	1	0	0	0	2.64	10	1
Fexofenadine	CC(C)(C1=CC=C(C=C1)C(CCCN2CCC(CC2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)O)C(=O)O	3.46	0.67	4.09	5.62	3	1	0	0	0	4	0	0	0	1.88	32	4
Flecainide	C1CCNC(C1)CNC(=O)C2=C(C=CC(=C2)OCC(F)(F)F)OCC(F)(F)F	2.32	0.39	2.51	0	3.57	1	1	0	0	0	2	0	0	0	0.04	17
Flucytosine	C1=NC(=O)NC(=C1F)N	2	2.04	-0.23	-0.62	0	3	0	0	0	1	0	0	0	-2.06	4	1
Formetanate	CNC(=O)OC1=CC=CC(=C1)N=CN(C)C	2.58	-0.17	1.51	1.66	1	2	0	0	0	1	0	0	0	-0.59	11	2
Furegrelate	C1=CC(=CN=C1)CC2=CC3=C(C=C2)OC(=C3)C(=O)O	3.32	-0.30	1.66	2.85	1	1	0	0	1	2	0	0	1	1.26	15	3
Gallic acid	C1=C(C=C(C(=C1O)O)O)C(=O)O	2.32	2.62	0.07	0.63	1	1	0	0	0	1	0	0	0	0.64	7	5
GHB / γ-Hydroxybutyric acid	C(CC(=O)O)CO	1	1.12	-0.25	-0.33	0	1	0	0	0	0	0	0	0	-0.65	4	3
Glutaral	C(CC=O)CC=O	1.58	-0.67	0.08	0.14	0	2	0	0	0	0	0	0	0	0.18	5	2
GVL (γ-Valerolactone)	CC1CCC(=O)O1	1	-0.67	0.60	0.65	0	1	0	0	1	0	0	0	0	-0.16	5	2
Heptaminol	CC(CCCC(C)(C)O)N	0	1.59	1.39	0.87	0	0	0	0	0	0	0	0	0	-2.09	8	1
Heptyl 2-amino-2-phenylacetate	CCCCCCCOC(=O)C(C1=CC=CC=C1)N	2.32	0.32	2.91	3.58	1	1	0	0	0	1	0	0	0	0.96	15	2
Hexachlorophene	C1=C(C(=C(C(=C1Cl)Cl)CC2=C(C(=CC(=C2Cl)Cl)Cl)O)O)Cl	2.81	0.47	4.80	7.26	2	0	0	0	0	2	0	0	0	7.25	13	2
Hexetylamine	CCC(C1CCCCC1)C(=O)OCCN(CC)CC	1	-0.83	3.07	4.15	0	1	0	0	0	1	0	0	0	1.44	16	2

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Homocamfin	CC1=CC(=O)CC(C1)C(C)C	1.58	-0.88	2.25	2.56	0	2	0	0	0	1	0	0	0	2.39	10	1
Hymecromone	CC1=CC(=O)OC2=C1C=CC(=C2)O	2.58	-0.20	2.00	2.08	1	2	0	0	0	2	0	0	0	1.97	10	3
Imazapyr	CC(C)C1(C(=O)NC(=N1)C2=C(C=CC=N2)C(=O)O)C	2.81	0.44	1.22	1.29	0	3	0	0	1	1	0	0	0	-0.21	13	3
Iminostilbene	C1=CC=C2C(=C1)C=CC3=CC=CC=C3N2	3	-0.39	3.31	3.54	2	1	0	0	0	2	1	0	0	3.52	14	0
Indanorex	CCC(C1(CC2=CC=CC=C2C1)O)N	2	1.24	2.24	1.58	1	0	0	0	1	1	0	0	1	-1.26	12	1
Iohexol	CC(=O)N(CC(CO)O)C1=C(C(=C(C(=C1I)C(=O)NCC(CO)O)I)C(=O)NCC(CO)O)I	2.81	5.02	-0.30	0	-1.84	1	3	0	0	0	1	0	0	0	-3.17	19
Iomeprol	CN(C1=C(C(=C(C(=C1I)C(=O)NCC(CO)O)I)C(=O)NCC(CO)O)I)C(=O)CO	2.81	4.27	0.00	-1.25	1	3	0	0	0	1	0	0	0	-2.61	17	8
Iopamidol	CC(C(=O)NC1=C(C(=C(C(=C1I)C(=O)NC(CO)CO)I)C(=O)NC(CO)CO)I)O	2.81	5.18	0.00	-1.08	1	3	0	0	0	1	0	0	0	-2.31	17	8
Irbesartan	CCCCC1=NC2(CCCC2)C(=O)N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NNN=N5	3.52	-0.37	5.11	0	4.93	2	2	0	0	3	2	0	0	0	3.26	25
Irganox 1076	CCCCCCCCCCCCCCCCCCOC(=O)CCC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C	2.32	-0.53	8.28	12.43	1	1	0	0	0	1	0	0	0	13.33	35	3
Isopentedrone	CCCC(=O)C(C1=CC=CC=C1)NC	2.32	-0.31	2.15	2.17	1	1	0	0	0	1	0	0	0	-1.09	12	1
Lamotrigine	C1=CC(=C(C(=C1)Cl)Cl)C2=C(N=C(N=N2)N)N	2.81	2.32	2.79	0	2.43	1	0	0	0	0	2	0	0	0	-0.46	9
Levetiracetam	CCC(C(=O)N)N1CCCC1=O	1.58	0.67	-0.08	-0.20	0	2	0	0	1	0	0	0	0	-0.74	8	2
MCPA methylester	CC1=C(C=CC(=C1)Cl)OCC(=O)OC	2.32	-0.70	2.38	2.88	1	1	0	0	0	1	0	0	0	2.61	10	3
MDPEA (Homopiperonylamine)	C1OC2=C(O1)C=C(C=C2)CCN	2	0.59	1.08	1.03	1	0	0	0	1	1	0	0	1	-1.56	9	2
Meclofenamic acid	CC1=C(C(=C(C=C1)Cl)NC2=CC=CC=C2C(=O)O)Cl	3	0.39	3.99	0	4.80	2	1	0	0	0	2	0	0	0	5.92	14
Meconin (Opianyl)	COC1=C(C2=C(COC2=O)C=C1)OC	2.32	-0.70	1.15	1.41	1	1	0	0	1	1	0	0	1	1.07	10	4
Methyl methacrylate	CC(=C)C(=O)OC	1.58	-0.67	0.89	1.17	0	2	0	0	0	0	0	0	0	1.4	5	2
Methyltestosterone	CC12CCC(=O)C=C1CCC3C2CCC4(C3CCC4(C)O)C	1.58	-0.44	3.92	3.54	0	2	0	0	1	3	0	0	1	3.53	20	2
Methylthiouracil	CC1=CC(=O)NC(=S)N1	2	0.95	0.10	0.40	0	3	0	0	0	1	0	0	0	-0.4	5	1
Metolcarb	CC1=CC(=CC=C1)OC(=O)NC	2.32	-0.16	1.51	2.08	1	1	0	0	0	1	0	0	0	1.73	9	2
Metyridine	COCCC1=CC=CC=N1	2	-0.77	0.65	0.95	0	0	0	0	0	1	0	0	0	-0.58	8	1
Mitragynine (9-methoxy Corynantheidine)	CCC1CN2CCC3=C(C2CC1C(=COC)C(=O)OC)NC4=C3C(=CC=C4)OC	3	-0.37	2.10	3.59	1	2	0	0	1	3	0	0	2	1.01	23	4
Morpholine	C1COCCN1	0	0.16	-0.47	0	-0.53	0	0	0	0	0	1	0	0	0	-3.68	4
Moxisylyt	CC1=CC(=C(C=C1OC(=O)C)C(C)C)OCCN(C)C	2.32	-0.79	2.89	0	3.40	1	1	0	0	0	1	0	0	0	-0.01	16
N-(2-Hydroxyphenyl)piperazine	C1CN(CCN1)C2=CC=CC=C2O	2	0.53	0.97	1.15	1	0	0	0	0	2	0	0	0	-2.91	10	1
N-(4-Tolyl)piperazine	CC1=CC=C(C=C1)N2CCNCC2	2	-0.28	1.83	0	1.90	1	0	0	0	0	2	0	0	0	-2.16	11

Table S3 continues on the next page

N-Acetyl-N-methylamphetamine (N-Acetyl-N-methylamfetamine)	CC(CC1=CC=CC=C1)N(C)C(=O)C	2.32	-0.84	2.55	1.86	1	1	0	0	0	1	0	0	0	2.01	12	1
N-Desmethyltramadol	CNCC1CCCCC1(C2=CC(=CC=C2)OC)O	2	0.32	2.07	2.17	1	0	0	0	0	2	0	0	0	-0.86	15	2
N-ethyl-N-Methylcathinone	CCN(C)C(C)C(=O)C1=CC=CC=C1	2.32	-0.84	2.41	2.52	1	1	0	0	0	1	0	0	0	-0.73	12	1
Nafimidone	C1=CC=C2C=C(C=CC2=C1)C(=O)CN3C=CN=C3	3.32	-0.82	2.46	2.30	2	1	0	0	1	2	0	0	0	0.07	15	1
NEB / N-Ethylbuphedrone	CCC(C(=O)C1=CC=CC=C1)NCC	2.32	-0.31	2.41	2.50	1	1	0	0	0	1	0	0	0	-0.73	12	1
Nicethamide	CCN(CC)C(=O)C1=CN=CC=C1	2.32	-0.75	1.02	0.79	0	1	0	0	0	1	0	0	0	-0.13	10	1
Nicotiniacid propylester	CCCOC(=O)C1=CN=CC=C1	2.32	-0.73	1.12	1.41	0	1	0	0	0	1	0	0	0	1.32	9	2
Nicotinyl alcohol	C1=CC(=CN=C1)CO	2	-0.04	-0.03	0.07	0	0	0	0	0	1	0	0	0	-1.72	6	1
Nitramisole	C1CSC2=NC(CN21)C3=CC(=CC=C3)[N+](=O)[O-]	2.81	-0.63	2.22	2.71	1	3	0	0	2	1	0	1	0	0.03	11	2
O-Desmethylvenlafaxine (Desvenlafaxine)	CN(C)CC(C1=CC=C(C=C1)O)C2(CCCCC2)O	2	0.29	2.32	2.77	1	0	0	0	0	2	0	0	0	-0.46	16	2
O-DT / O-Desmethyltramadol	CN(C)CC1CCCCC1(C2=CC(=CC=C2)O)O	2	0.32	2.07	2.45	1	0	0	0	0	2	0	0	0	-1.01	15	2
o-Toluidine	CC1=CC=CC=C1N	2	0.73	1.86	1.57	1	0	0	0	0	1	0	0	0	0.04	7	0
Octacaine	CCN(CC)C(C)CC(=O)NC1=CC=CC=C1	2.32	-0.31	2.52	2.28	1	1	0	0	0	1	0	0	0	-0.78	14	1
Octodrine	CC(C)CCCC(C)N	0	0.63	2.27	2.22	0	0	0	0	0	0	0	0	0	-0.49	8	0
OD PABA / Octyldimethyl PABA (Padimate O)	CCCCC(CC)COC(=O)C1=CC=C(C=C1)N(C)C	2.32	-0.84	3.94	4.86	1	1	0	0	0	1	0	0	0	5.08	17	2
Oxcarbazepine	C1C2=CC=CC=C2N(C3=CC=CC=C3C1=O)C(=O)N	3.17	0.34	2.19	2.13	2	2	0	0	0	2	1	0	0	1.87	15	2
Oxiniacic acid	C1=CC(=C[N+](=C1)[O-])C(=O)O	2.58	0.03	-1.80	-0.56	0	2	0	0	0	1	0	0	0	-1.01	6	3
Oxprenolol	CC(C)NCC(COC1=CC=CC=C1OCC=C)O	2.32	0.34	1.83	0	2.23	1	1	0	0	0	1	0	0	0	-0.81	15
Oxycodone	CN1CCC23C4C(=O)CCC2(C1CC5=C3C(=C(C=C5)OC)O4)O	2.32	-0.33	1.38	0	1.03	1	1	0	0	1	4	0	1	3	-2.18	18
p-Phenetidine	CCOC1=CC=C(C=C1)N	2	0.65	1.58	1.42	1	0	0	0	0	1	0	0	0	-0.85	8	1
Palmidrol	CCCCCCCCCCCCCCCC(=O)NCCO	1	0.24	4.45	5.43	0	1	0	0	0	0	0	0	0	5.98	18	2
Parapropamol	CCC(=O)NC1=CC=C(C=C1)O	2.32	0.59	1.38	1.35	1	1	0	0	0	1	0	0	0	0.77	9	2
Paroxypropione	CCC(=O)C1=CC=C(C=C1)O	2.32	-0.21	1.81	1.97	1	1	0	0	0	1	0	0	0	1.99	9	2
Pentedrone	CCCC(C(=O)C1=CC=CC=C1)NC	2.32	-0.31	2.41	2.61	1	1	0	0	0	1	0	0	0	-0.73	12	1
PFOA / Perfluorooctanoic acid	C(=O)(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)O	1	0.12	4.17	3.81	0	1	0	0	0	0	0	0	0	3.1	8	2
Phendimetrazine	CC1C(OCCN1C)C2=CC=CC=C2	2	-0.84	1.84	2.00	1	0	0	0	0	2	0	0	0	-1.17	12	1
Phenopyrazone	C1=CC=C(C=C1)C2C(=O)NN(C2=O)C3=CC=CC=C3	3.17	-0.30	2.47	1.84	2	2	0	0	1	2	0	0	0	1.9	15	2

Table S3 continues on the next page

Phenyl acetate	CC(=O)OC1=CC=CC=C1	2.32	-0.77	2.03	1.60	1	1	0	0	0	1	0	0	0	1.64	8	2
Phenylacetic acid	C1=CC=C(C=C1)CC(=O)O	2.32	-0.16	1.77	1.47	1	1	0	0	0	1	0	0	0	1.51	8	2
Phenylacrylic acid (Cinnamic acid)	C1=CC=C(C=C1)C=CC(=O)O	2.58	-0.21	2.00	1.90	1	2	0	0	0	1	0	0	0	2.3	9	2
Phenylalanine	C1=CC=C(C=C1)CC(C(=O)O)N	2.32	1.47	-0.97	0.96	1	1	0	0	0	1	0	0	0	-1.49	9	2
Phenylpyruvic acid	C1=CC=C(C=C1)CC(=O)C(=O)O	2.58	-0.16	1.16	1.21	1	2	0	0	0	1	0	0	0	0.46	9	3
Phenytoin	C1=CC=C(C=C1)C2(C(=O)NC(=O)N2)C3=CC=CC=C3	3.17	0.34	1.79	0	2.11	2	2	0	0	1	2	0	0	0	2.42	15
Pholcodine	CN1CCC23C4C1CC5=C2C(=C(C=C5)OCCN6CCOCC6)OC3C(C=C4)O	2.32	-0.37	1.73	1.46	1	1	0	0	1	5	0	1	3	-3.24	23	4
Pirnabine	CC1CCC2=C(C1)C3=C(C=C(C=C3OC(=O)C)C)OC2(C)C	2.58	-0.85	3.93	4.56	1	2	0	0	0	3	0	0	0	5.58	19	3
Practolol	CC(C)NCC(COC1=CC=C(C=C1)NC(=O)C)O	2.32	1.15	1.19	0.75	1	1	0	0	0	1	0	0	0	-2.27	14	3
Procinolol	CC(C)NCC(COC1=CC=CC=C1C2CC2)O	2	0.32	2.07	2.45	1	0	0	0	0	1	0	0	0	-0.35	15	2
Proguanil	CC(C)N=C(N)N=C(N)NC1=CC=C(C=C1)Cl	2.58	3.12	2.60	2.64	1	2	0	0	0	1	0	0	0	-0.15	11	0
Propetamide	CCCNC(=O)C(C)NC1=CC=C(C=C1)OCC	2.32	0.37	1.98	2.49	1	1	0	0	0	1	0	0	0	0.73	14	2
Propivan	CCCC(C1=CC=CC=C1)C(=O)OCCN(CC)CC	2.32	-0.84	3.41	3.93	1	1	0	0	0	1	0	0	0	0.82	17	2
Propyphenazone	CC1=C(C(=O)N(N1C)C2=CC=CC=C2)C(C)C	2.58	-0.81	3.12	2.77	1	2	0	0	1	1	0	0	0	2.13	14	1
Pulegon	CC1CCC(=C(C)C)C(=O)C1	1.58	-0.88	2.25	2.75	0	2	0	0	0	1	0	0	0	3.12	10	1
Pyruvic acid	CC(=O)C(=O)O	1.58	0.31	-0.81	0	-0.49	0	2	0	0	0	0	0	0	0	-1.39	3
Quatacaine	CCCNC(C)(C)C(=O)NC1=CC=CC=C1C	2.32	0.35	2.52	2.58	1	1	0	0	0	1	0	0	0	-0.77	14	1
Saccharin	C1=CC=C2C(=C1)C(=O)NS2(=O)=O	2.81	0.00	0.17	0.36	1	3	0	0	1	1	0	0	1	-0.62	7	3
Sotalol	CC(C)NCC(C1=CC=C(C=C1)NS(=O)(=O)C)O	2.58	1.25	0.71	0.97	1	2	0	0	0	1	0	0	0	-2.81	12	3
Sphingosine	CCCCCCCCCCCCCC=CC(C(CO)N)O	1	1.78	4.04	4.82	0	1	0	0	0	0	0	0	0	2.37	18	2
Stearamide (Octadecanamide)	CCCCCCCCCCCCCCCCCC(=O)N	1	0.21	5.28	6.68	0	1	0	0	0	0	0	0	0	7.36	18	1
Succinic acid	C(CC(=O)O)C(=O)O	1.58	1.08	-0.35	0	-0.41	0	2	0	0	0	0	0	0	0	-0.48	4
Sucralose	C(C1C(C(C(C(O1)OC2(C(C(C(O2)CCl)O)O)CCl)O)O)Cl)O	0	2.89	-0.91	0	-0.70	0	0	0	0	1	1	0	0	0	-0.17	12
Sulcofuron	C1=CC(=C(C=C1NC(=O)NC2=C(C=CC(=C2Cl)OC3=C(C=C(C=C3)Cl)S(=O)(=O)O)Cl)Cl	3.70	1.00	3.31	5.70	3	3	0	0	0	3	0	0	0	1.84	19	5
Sulfanilamide	C1=CC(=CC=C1N)S(=O)(=O)N	2.58	2.76	-0.11	-0.09	1	2	0	0	0	1	0	0	0	-0.68	6	2
Sulfasalazine	C1=CC=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)N=NC3=CC(=C(C=C3)O)C(=O)O	3.81	1.02	1.97	3.89	2	4	0	0	0	3	0	0	0	2.35	18	5
Sulpiride	CCN1CCCC1CNC(=O)C2=C(C=CC(=C2)S(=O)(=O)N)OC	2.81	1.12	0.44	0.83	1	3	0	0	1	1	0	0	0	-2.25	15	4

Table S3 continues on the next page

Tapentadol	CCC(C1=CC(=CC=C1)O)C(C)CN(C)C	2	-0.35	3.04	0	3.44	1	0	0	0	0	1	0	0	0	-0.46	14
TBP / Tributylphosphate	CCCCOP(=O)(OCCCC)OCCCC	1	-0.69	3.23	0	3.63	0	1	0	0	0	0	0	0	0	3.74	12
TCPP / Tri-(2-chloroisopropyl)phosphate	CC(CCl)OP(=O)(OC(C)CCl)OC(C)CCl	1	-0.52	3.23	2.77	0	1	0	0	0	0	0	0	0	2.31	9	4
Terbutol (Terbucarb)	CC1=CC(=C(C(=C1)C(C)(C)C)OC(=O)NC)C(C)(C)C	2.32	-0.37	3.67	4.88	1	1	0	0	0	1	0	0	0	4.7	17	2
Thiram	CN(C)C(=S)SSC(=S)N(C)C	1.58	-0.48	0.45	3.16	0	2	0	0	0	0	0	0	0	1.94	6	0
Thymotic acid	CC1=C(C(=C(C=C1)C(C)C)O)C(=O)O	2.32	0.48	2.89	2.85	1	1	0	0	0	1	0	0	0	2.11	11	3
Tilorone	CCN(CC)CCOC1=CC2=C(C=C1)C3=C(C2=O)C=C(C=C3)OCCN(CC)CC	3	-0.83	3.33	4.56	2	1	0	0	1	2	0	0	2	0.53	25	3
Tolyltriazole (1-Methylbenzotriazole)	CN1C2=CC=CC=C2N=N1	2.58	-0.67	1.41	1.64	1	0	0	0	1	1	0	0	1	1.3	7	0
Tolytriazole (4-Methylbenzotriazole)	CC1=CC=CC2=NNN=C12	2.58	-0.07	1.41	1.88	1	0	0	0	1	1	0	0	1	1.74	7	0
Topiramate	CC1(OC2COC3(C(C2O1)OC(O3)(C)C)COS(=O)(=O)N)C	1.58	0.53	-0.26	-1.81	0	2	0	0	2	1	0	0	2	2.15	12	8
TPPA / Triphenyl phosphate	C1=CC=C(C=C1)OP(=O)(OC2=CC=CC=C2)OC3=CC=CC=C3	3.46	-0.77	4.79	0	4.94	3	1	0	0	0	3	0	0	0	4.12	18
Tramadol-N-oxide	C[N+](C)(CC1CCCCC1(C2=CC(=CC=C2)OC)O)[O-]	2	-0.32	-1.36	0	0.45	1	0	0	0	0	2	0	0	0	-1.32	16
Trebenzomine	CC1C(CC2=CC=CC=C2O1)N(C)C	2	-0.84	2.11	2.43	1	0	0	0	0	2	0	0	0	-0.69	12	1
Trimetazidine	COC1=C(C(=C(C=C1)CN2CCNCC2)OC)OC	2	-0.25	0.75	1.28	1	0	0	0	0	2	0	0	0	-2.12	14	3
Tutocaine	CC(CN(C)C)C(C)OC(=O)C1=CC=C(C=C1)N	2.32	0.37	2.39	1.97	1	1	0	0	0	1	0	0	0	-0.91	14	2
Tyramine	C1=CC(=CC=C1CCN)O	2	1.59	1.31	0.99	1	0	0	0	0	1	0	0	0	-2.57	8	1
Umbelliferone	C1=CC(=CC2=C1C=CC(=O)O2)O	2.58	-0.16	1.70	1.63	1	2	0	0	0	2	0	0	0	1.59	9	3
Usnic acid	CC1=C(C(=C2C(=C1O)C3(C(=CC(=O)C(C3=O)C(=O)C)O2)C)C(=O)C)O	3.17	0.31	0.57	0.61	1	5	0	0	1	2	0	0	2	2.53	18	7
Valdetamide	CCC(CC)(CC=C)C(=O)N	1.58	0.57	1.86	0	2.15	0	2	0	0	0	0	0	0	0	2.19	9
Zaleplone	CCN(C1=CC=CC(=C1)C2=CC=NC3=C(C=NN23)C#N)C(=O)C	3.58	-0.73	2.27	1.85	1	1	1	0	1	2	0	0	1	1.45	17	1
Zingerone	CC(=O)CCC1=CC(=C(C=C1)O)OC	2.32	-0.24	1.57	1.63	1	1	0	0	0	1	0	0	0	1.1	11	3
β-hydroxybutyric acid	CC(CC(=O)O)O	1	1.12	-0.25	-0.28	0	1	0	0	0	0	0	0	0	-0.76	4	3

Table S4 – The frequency of compounds tentatively identified using Agilent commercial databases in water and passive sampler extracts for winter and summer deployments. Along with the predicted and sample t_R and error.

Analyte	CAS number	Measured m/z (ppm) + isotope match	Qualifier fragment(s)	Winter			Summer			Standard t_R error (min)	Current Schymanski framework level (now all raised to 2(a) with t_R prediction or higher with reference standard confirmation)
				Detection rate	Mean measured t_R in sample (min)	Predicted t_R error (min)	Detection rate	Mean measured t_R in sample (min)	Predicted t_R error (min)		
17α-Estradiol	57-91-0	273.1862 (-4.99)[a]	-	1/4	9.68	0.65	1/3	9.68	0.65	-	4[f]
2,4-Dichlorophenoxyacetic acid (2,4-D)	94-75-7	219.9652 (1.31)[b]	-	4/4	7.33	-0.73	-	-	-	-	4[f]
2,4-Dinitro-o-kresol (DNOC)	534-52-1	198.0235 (-1.17)[b]	180.0177	1/4	7.00	-0.65	-	-	-	-	3[h]
3-Hydroxylidocaine	34604-55-2	251.1762 (-3.27)[a]	86.0964	-	-	-	2/3	5.16	0.31	-	2(a)[g]
4-Hydroxyphenyl-pyruvic acid	156-39-8	179.0349 (0.43)[b]	-	2/4	4.92	-0.41	3/3	4.55	-0.78	-	4[f]
5-Methylbenzotriazole	49636-02-4	132.0568 (-0.42)[b]	103.0427, 104.0506, 102.0349,	-	-	-	2/3	5.83	0.42	-	2(a)[g]
8-Hydroxy-efavirenz	205754-32-1	330.0159 (-2.77)[b]	257.9963, 246.0139, 286.0252, 250.0485	4/4	8.69	-0.56	2/3	8.69	-0.56	-	2(a)[g]
9-Octadecenamide	301-02-0	282.2790 (0.47)[a]	247.242, 97.1012, 83.0855, 135.1168, 265.2526	-	-	-	2/3	11.34	0.76	-	2(a)[g]
Amisulpride	71675-85-9	370.1796 (-2.68)[a]	242.0482, 112.1121	-	-	-	3/3	4.25	-0.28	-	2(a)[g]

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Aniline	62-53-3	138.0561 (-0.59)[c], 92.0504 (2.03)[b]	77.0386	4/4	4.02	0.15	-	-	-	-	3[h]
Atenolol	29122-68-7	267.1708 (-1.89)[a]	190.0863, 225.1234, 145.0648, 208.0968, 178.0863	1/4	3.25	-0.08	-	-	-	-	2(a)[g]
Benhepazone	363-13-3	237.1022 (0.34)[a]	-	3/4	7.24	-0.08	3/3	7.23	-0.09	-	4[f]
Benzhydryl cyanide	86-29-3	194.0972 (-3.89)[a]	-	-	-	-	2/3	7.23	-0.46	-	4[f]
Bicalutamide	90357-06-5	429.0539 (-0.42)[b]	255.0375, 185.0328, 184.0375, 173.0067	1/4	7.81	-0.28	-	-	-	-	2(a)[g]
Bis(2-ethylhexyl) phthalate (DEHP)	117-81-7	413.2666 (-0.83)[d], 391.2850 (-1.72)[a]	149.0233, 167.0339, 71.0855	3/4	11.11	0.30	-	-	-	-	2(a)[g]
Butyl 4-hydroxybenzoate	94-26-8	193.0870 (-1.34)[b], 239.0926 (-0.27)[c]	-	-	-	-	2/3	7.97	-0.50	-	4[f]
Butylacetanilide	91-49-6	192.1382 (0.39)[a], 214.1209 (-3.25)[d]	-	4/4	7.67	0.40	-	-	-	-	4[f]
Celiprolol	56980-93-9	380.2554 (-2.62)[a]	324.1918, 306.1812	-	-	-	2/3	5.77	-0.26	-	2(a)[g]
Clarithromycin-N-oxide	118074-07-0	764.4796 (-0.72)[a]	606.3848	3/4	8.34	0.56	1/3	7.15	-0.63	-	3[h]
Clobazam	22316-47-8	301.0750 (-3.98)[a]	-	1/4	7.89	-0.51	1/3	7.88	-0.51	-	4[f]

Table S4 continues on the next page

Crotamiton	483-63-6	204.1392 (-4.24)[a]	136.1121, 134.0600, 69.0335	1/4	8.19	0.75	1/3	8.19	0.74	-	2(a)[g]
Dibutylamine	111-92-2	130.1593 (-2.22)[a]	-	1/4	4.06	-0.24	2/3	4.04	-0.26	-	4[f]
Dicamba	1918-00-9	218.9632 (-4.75)[b]	174.9723	4/4	7.33	-0.51	-	-	-	-	3[h]
Dinoseb	88-85-7	240.0708 (-1.96)[b]	-	2/4	9.19	0.40	-	-	-	-	4[f]
Disopyramide	671-20-0	340.2383 (-0.90)[a]	239.1179	-	-	-	1/3	5.30	-0.28	-	3[h]
Dilaurylthio-dipropionate (DLTDP)	123-28-4	532.4387 (1.24)[e], 515.4123 (1.18)[a], 537.3938 (1.79)[d]	143.0161, 329.2145, 115.0212, 161.0267, 89.0056	-	-	-	3/3	11.28	-0.12	-	2(a)[g]
Dorzolamide	120279-96-1	325.0358 (-3.90)[a]	198.9875	1/4	2.53	0.48	-	-	-	-	2(a)[g]
Erythromycin	114-07-8	734.4701 (-2.26)[a]	576.3742	1/4	8.68	0.02	1/3	8.69	0.02	-	3[h]
Flecainide	54143-55-4	415.1458 (-1.68)[a]	398.1185, 301.0294, 98.0964	3/4	6.56	-0.59	1/3	6.57	-0.59	-	2(a)[g]
Furegrelate	85666-24-6	271.1080 (-1.00)[e]	210.0913	-	-	-	1/3	6.03	-0.75	-	3[h]
Glutaral	111-30-8	99.0451 (0.10)[b], 145.0508 (-1.42)[c]	55.0542	1/4	3.05	-0.35	-	-	-	-	3[h]
GVL (γ-Valerolactone)	108-29-2	99.0451 (0.10)[b], 145.0508 (-1.42)[c]	-	1/4	3.05	-0.17	-	-	-	-	4[f]
Hexachlorophene	70-30-4	402.8442 (-3.89)[b]	366.8659, 194.9177	-	-	-	1/3	10.27	0.17	-	3[h]

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Hymecromone	90-33-5	178.0588 (-4.58)[a]	103.0542	1/4	7.78	0.60	-	-	-	-	3[h]
Irbesartan	138402-11-6	429.2399 (-0.45)[a]	207.0917, 195.1492, 386.2213	2/4	8.26	-0.14	-	-	-	-	2(a)[g]
Irganox 1076	2082-79-3	548.5039 (-0.38)[e], 553.4590 (0.14)[d], 531.4797 (-4.81)[a]	419.3520, 475.4146, 149.0597, 167.0703, 107.0491,	4/4	12.11	0.83	1/3	12.13	0.85	-	2(a)[g]
MCPA methylester	2436-73-9	213.0323 (0.58)[b]	-	1/4	8.23	0.25	1/3	8.23	0.26	-	4[f]
Methylthiouracil	56-04-2	143.0275 (-1.03)[a]	84.0444	1/4	3.33	-0.39	-	-	-	-	2(a)[g]
Nicotinyl alcohol	100-55-0	110.0604 (-3.27)[a]	92.0495	1/4	1.30	-0.17	-	-	-	-	3[h]
O-Desmethylvenlafaxine	93413-62-8	264.1964 (-2.16)[a], 281.2214 (3.52)[e]	58.0651	4/4	5.21	-0.73	3/3	5.03	-0.92	-	2(a)[g]
Octacaine	13912-77-1	235.1804 (0.52)[a]	-	1/4	4.60	0.07	1/3	4.58	0.05	-	4[f]
Oxprenolol	6452-71-7	266.1756 (-1.83)[a]	248.1645	1/4	4.74	-0.86	-	-	-	-	2(a)[g]
Phenopyrazone	3426-01-5	253.0972 (-0.28)[a]	180.0800, 236.0706, 208.0757	1/4	6.03	-0.12	2/3	6.30	0.15	-	2(a)[g]
Phenytoin	57-41-0	253.0972 (-0.28)[a]	182.0964	1/4	6.03	-0.86	2/3	6.30	-0.59	0.06	1[i]
Pholcodine	509-67-1	399.2281 (-0.62)[a]	381.2173	1/4	1.46	-0.16	-	-	-	-	3[h]

Table S4 continues on the next page

Practolol	6673-35-4	267.1708 (-1.89)[a]	190.0863, 225.1234, 178.0863	1/4	3.25	-0.28	-	-	-	-	2(a)[g]
Proguanil	500-92-5	254.1169 (-0.75)[a], 271.1428 (1.57)[e]	170.0480, 153.0214, 102.1026, 128.0262	-	-	-	1/3	6.72	0.03	-	2(a)[g]
Quatacaine	17692-45-4	235.1804 (0.52)[a]	-	1/4	4.60	-0.63	1/3	4.58	-0.65	-	4[f]
Saccharin	81-07-2	181.9919 (-0.79)[b]	105.9604	2/4	2.87	0.44	-	-	-	-	3[h]
Sotalol	3930-20-9	273.1272 (-1.51)[a]	213.0692, 255.1162, 133.0760, 176.1308, 134.0839	1/4	2.93	0.29	1/3	2.91	0.28	-	2(a)[g]
Sulpiride	15676-16-1	342.1488 (-1.65)[a]	112.1121, 214.0162	2/4	3.11	-0.26	3/3	3.09	-0.27	-	2(a)[g]
Tapentadol	175591-23-8	222.1896 (-4.90)[a]	107.0491	3/4	5.42	-0.29	3/3	5.41	-0.29	-	3[h]
Tributylphosphate (TBP)	126-73-8	268.1766 (-4.55)[a]	98.9842, 80.9736	2/4	9.54	-0.03	-	-	-	-	2(a)[g]
Tri-(2-chloroisopropyl)phosphate (TCPP)	13674-84-5	327.0085 (-1.35)[a]	98.9842, 174.9921, 80.9738	4/4	8.35	-0.33	3/3	8.35	-0.34	-	2(a)[g]
Thymotic acid	548-51-6	193.0872 (-0.74)[b]	-	-	-	-	1/3	7.97	-0.28	-	4[f]
Tolytriazole	29878-31-7	132.0568 (-0.42)[b]	103.0427, 104.0506, 102.0349	-	-	-	2/3	5.83	0.42	-	2(a)[g]
Topiramate	97240-79-4	357.1326 (0.44)[e]	184.0968, 127.0390, 264.0536	-	-	-	2/3	6.22	-0.57	-	2(a)[g]
Trimetazidine	13171-25-0	267.1708 (-1.89)[a]	-	1/4	3.25	0.85	-	-	-	-	4[f]

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Tutocaine	891-33-8	251.1757 (-1.32)[a], 273.1560 (4.96)[d]	-	-	-	-	2/3	5.16	-0.02	-	4[f]

[a] $[M+H]^+$ adduct, [b] $[M-H]^-$ adduct, [c] $[M+HCOO]^-$ adduct, [d] $[M+Na]^+$ adduct, [e] $[M+NH_4]^+$ adduct, [f] 'Unequivocal molecular formula' based on precursor ion + isotope pattern, [g] 'Probable structure' based on precursor ion + unique product ion(s), [h] 'Tentative candidates' based on precursor ion + product ions, [i] 'Confirmed structure' based on matching t_R (within 0.2 min) + precursor ion + at least one product ion

S4 – Additional LC-QTOF-MS method conditions

Additional LC-QTOF-MS analysis was performed using a Dionex Ultimate 3000 UHPLC system (Thermo Fisher Scientific, Bremen, Germany) coupled to a Bruker Maxis Impact II Q-TOF detector (Bruker Daltonics, Bremen, Germany) fitted with an electrospray ionisation source. Separations were performed using a Thermo 100 x 2.1 mm, 2.2 µm Dionex Acclaim RSLC 120 C_{18} analytical column fitted with a 1.7 µm Acquity UPLC BEH C_{18} guard column (Waters, Dublin, Ireland). The LC method comprised of a binary gradient of 5 mM ammonium formate and 0.01% v/v formic acid (MPA) to 10% MeOH, 5 mM ammonium formate and 0.01% formic acid (MPB). The elution profile consists of 1-39% B at 0.2 mL/min from 0.00 to 3.00 min; 39-99.9% B at 0.2-0.4 mL/min from 3.00 to 14.00 min; 99.9% B at 0.4-0.48 mL/min from 14.00 to 16.00 min; 99.9-1% B at 0.48 mL/min from 16.00 to 16.10 min; 1% B at 0.48 mL/min hold from 16.10 to 19.00 min; 1% B at 0.48-0.2 mL/min. The re-equilibration time was 0.50 min at 1% B. The column was held at 30 °C with an injection volume of 20 µL. The MS system was used in broadband collision-induced dissociation (bbCID) mode with a scan range of 30-1,000 Da at a rate of 2 Hz. The bbCID mode provides MS and MS/MS simultaneously while operating at two different collision energies. MS spectra were acquired using an energy of 6 eV and the MS/MS spectra were acquired using 30 eV. The capillary and end plate offset voltages were 2,500 V and 500 V. The nebuliser pressure was 2 bar and the drying gas was set to a rate of 8 L/min with a drying temperature of 200°C. The mass axis was calibrated at the beginning of each acquisition using a 1 mM solution of sodium formate in a 1:1:0.01 (H_2O:IPA:Formic acid v/v/v) delivered via syringe pump. All data was evaluated using the TASQ 1.4 software (Bruker Daltonics).

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