Table S1. Literature summary of lifestyle biomarkers.

Class/ *Family*	Parent Compound/*Metabolite*	Acronym	Excretion rate (%)	References	Stability in urine	Stability in WW	Detected in IWW	References
Illicit drugs	**Cocaine**		7.5	(Lai et al., 2011)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	Generally low at 2-31°C over 1-3days, high at -20°C for 3 weeks. At pH 2, stable at 2°C and 20°C over 3 days and -	✓	(EMCDDA, 2016)
	Benzoylecgonine		29	(Castiglioni et al., 2013)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	High stability at neutral and low pH from -20°C to 31°C	✓	(McCall et al., 2016; Tang et al., 2014)
	Amphetamine	(R,S)-AMP	36.3	(Gracia-Lor et al., 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	Most studies found <10% transformation at 4 °C and 20°C up to 24 h; one study measured increase of 26-73% at 2°C	✓	(McCall et al., 2016; Tang et al., 2014)
	para-hydroxyamphetamine	(R,S)-pOH-AMP	3	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
	Benzoic acid	(R,S)-benzoic acid	23.7	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
	Hippuric acid	(R,S)-hippuric acid	16.3	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
	1-phenylpropan-2-one	(R,S)-1-phenylpropan-2-one	3.4	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
	Norephedrine	(R,S)-norephedrine	2.4	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
	para-hydroxynoephedrine	(R,S)-pOH-norephedrine	0.4	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
	Methamphetamine	(R,S)-METH	22.7	(Gracia-Lor et al., 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	Stable for up to 24h at 4°C and 20°C	✓	(EMCDDA, 2016; McCall et al., 2016; Tang et al., 2014)
		S(+)-METH	40.9	(Gracia-Lor et al., 2016)				
	Amphetamine	(R,S)-AMP	2.7	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
		S(+)-AMP	9.9	(Gracia-Lor et al., 2016)				
	para hydroxymethamphetamine	(R,S)-pOH-METH	15	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
		S(+)-pOH-METH	10.7	(Gracia-Lor et al., 2016)				
	para hydroxyamphetamine	(R,S)-pOH-AMP	1.1	(Gracia-Lor et al., 2016)				(McCall et al., 2016)
		S(+)-pOH-AMP	0.3	(Gracia-Lor et al., 2016)				
	MDMA		22.5	(Gracia-Lor et al., 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	Stable for up to 24h at 4°C and 20°C	✓	
	MDA		1.8	(Gracia-Lor et al., 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	Stable for up to 24h at 4°C and 20°C	✓	(EMCDDA, 2016; McCall et al., 2016; Tang et al., 2014)
	HMMA		18.2	(Gracia-Lor et al., 2016)			✓	(Castrignanò et al., 2016; McCall et al., 2016)
	HMA		1.2	(Gracia-Lor et al., 2016)			✓	(Castrignanò et al., 2016)
	HHMA		19	(Burgard et al., 2014)				
	THC		0.006	(Castiglioni and Gracia-Lor, 2016)		In spiked unfiltered WW stored at -20 °C: 50% degradation over 7 days and >90% after 123 days	✓	(McCall et al., 2016)
	THC-COOH		0.5	(Castiglioni and Gracia-Lor, 2016)	stable 1 day at room temperature and for 14 days when stored at 2-8°C	in WW at 4 °C and 20 °C over 72 h; high on SPE cartridges over three weeks at -20 °C; high at -20 °C over 3, 7, 17, 27,	✓	(McCall et al., 2016; Tang et al., 2014)
	11-OH-THC		5	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2–8°C	<20% transformation at pH 7.4, pH 2, 10 °C and 20 °C in unfiltered WW	✓	(McCall et al., 2016; Tang et al., 2014)
	Heroin		3.0-50.0	(Burgard et al., 2014)	Stable 1 day at room temperature and for 14 days when stored at 2–8°C	Low stability between -20°C and 19°C	✓	(Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	6-Acetylmorphine		1.3	stiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2–8ºC	Low at 20°C, high at -20°C for up to 27 days	✓	(Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	Morphine		42	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	High stability at 4 °C in unfiltered WW over 24 h; <20% degradation at -20 °C over 3, 7, 17, 27 days	✓	(Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	Codeine		70	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	High: In filtered/unfilteredWW <20% transformation over 24 h at 4 °C, 19°C and room temperature; <10%	✓	(Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	MDEA		19	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2–8◦C	Stable for up to 24h at 4°C and 20°C	✓	(Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	Methadone		27.5	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	20% difference at room temperature and 4 °C; may be prone to sorption; >40% degradation at -20 °C over 123	✓	Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	EDDP		13-30.9	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	Less than 15% difference after 24 h; may be prone to sorption; ca. 40% degradation at 20ºC over 3, 7 and 123	✓	Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	Ketamine		30	(Castiglioni and Gracia-Lor, 2016)	stable 1 day at room temperature and for 14 days when stored at 2–8◦C.	High: at 4°C and room temperature at WWpH and acidified to pH 4 and in milliQ water at 4 °C and room	✓	Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
	Norketamine		1.6	(Castiglioni and Gracia-Lor, 2016)	Stable 1 day at room temperature and for 14 days when stored at 2-8°C	At 4°C and room temperature at WWpH and acidified to pH 4	✓	Castrignanò et al., 2016; McCall et al., 2016; Tang et al., 2014)
Alcohol	**Ethanol**	EtOH		(Wurst et al., 2006)				(Helander and Beck, 2005)
	Ethyl glucuronide	EtG	0.02	(Rodríguez-Álvarez et al., 2015)		Degradation over the 18-hour incubation period and only 50% of the initial compound was present in the final	✓	(Reid et al., 2011)
	Ethyl sulfate	EtS	0.012	(Rodríguez-Álvarez et al., 2015)		Little or no degradation in sewage effluent over a period of 18 hours	✓	(Reid et al., 2011)
Tobacco	**Nicotine**		13	(Castiglioni et al., 2015)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Castiglioni et al., 2015; Senta et al., 2015a)
	Cotinine		30	(Castiglioni et al., 2015)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Castiglioni et al., 2015; Senta et al., 2015a)
	trans-3'-hydroxycotinine		44	(Castiglioni et al., 2015)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Castiglioni et al., 2015; Senta et al., 2015a)

Caffeine	**Caffeine (1,3,7-trimethylxanthine)**	137X	1.2	(Garattini, 1993)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Senta et al., 2015a)
	Paraxanthine (1,7-dimethylxanthine)	17X	6	(Garattini, 1993)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Senta et al., 2015a)
	1-methylxanthine	1X	18	(Garattini, 1993)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Senta et al., 2015a)
	7-methylxanthine	7X	7	(Garattini, 1993)		Stable during 24 h storage at 4 ºC and 20°C	✓	(Senta et al., 2015a)
	1-methyluric acid	1U	25	(Garattini, 1993)				
	1,7-dimethyluric acid	17U	6	(Garattini, 1993)				
	Theophylline (1,3-dimethylxanthine)	13X	1	(Garattini, 1993)				
	Theobromine (3,7-dimethylxanthine)	37X	2	(Garattini, 1993)				
	1,3-dimethyluric acid	13U	2.5	(Garattini, 1993)				
	3,7-dimethyluric acid	37U	0.8	(Garattini, 1993)				
	3-methylxanthine	3X	3	(Garattini, 1993)				
	5-acetylamino-6-formylamino-3-methyluracil	AFMU	15	(Garattini, 1993)	Unstable in urine			
NPS/*Synthetic cannabinoids*	**JWH-018**							
	JWH-018 hydrox at N-alkyl chain					Stable ar room temperature for 24 hours	✓	(Grigoryev et al., 2011; Hutter et al., 2013, 2012; Reid et al., 2014; Wohlfarth et al., 2013)
	JWH-018 hydrox. at indole group							(Grigoryev et al., 2011; Hutter et al., 2013, 2012; Wohlfarth et al., 2013)
	JWH-018 carbox. at N-alkyl chain					Stable ar room temperature for 24 hours		(Grigoryev et al., 2011; Hutter et al., 2013, 2012; Reid et al., 2014; Wohlfarth et al., 2013)
	JWH-018 hydrox. at naphthyl							(Grigoryev et al., 2011)
	JWH-073							
	JWH-073 hydrox. at N-alkyl chain					Unstable at room temperature for 24 hours		(Grigoryev et al., 2011; Hutter et al., 2012; Reid et al., 2014; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-073 hydrox. at indole group							(Hutter et al., 2012)
	JWH-073 carbox. at N-alkyl chain					Stable ar room temperature for 24 hours		(Hutter et al., 2012; Reid et al., 2014; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-081							
	JWH-081 hydrox. at N-alkyl chain							(Hutter et al., 2012; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-081 hydrox. at indole group							(Hutter et al., 2012; Sundström et al., 2013)
	JWH-081 hydrox. at naphthyl group							(Hutter et al., 2012)
	JWH-122						✓	(Borova et al., 2015)
	JWH-122 hydrox. at N-alkyl chain					Unstable at room temperature for 24 hours		(Hutter et al., 2012; Jang et al., 2014; Reid et al., 2014; Sundström et al., 2013)
	JWH-122 hydrox. at indole group							(Hutter et al., 2012; Sundström et al., 2013)
	JWH-122 hydrox. at naphthyl group							(Hutter et al., 2012)
	MAM-2201 carbox. at N-alkyl chain							(Jang et al., 2014)
	JWH-210						✓	(Borova et al., 2015)
	JWH-210 hydrox. at N-alkyl chain							(Hutter et al., 2012; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-210 hydrox. at indole group							(Hutter et al., 2012; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-210 hydrox. at naphthyl group							(Hutter et al., 2012)
	JWH-210 carbox. at N-alkyl chain							(Jang et al., 2014)
	JWH-250							
	JWH-250 hydrox. at N-alkyl chain							(Hutter et al., 2012; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-250 hydrox. at indole group							(Hutter et al., 2012; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-250 hydrox. at phenyl group							(Hutter et al., 2012)
	JWH-250 carbox. at N-alkyl chain							(Sundström et al., 2013; Wohlfarth et al., 2013)
	RCS-4							
	RCS-4 hydrox. at N-alkyl chain							(Hutter et al., 2012; Wohlfarth et al., 2013)
	RCS-4 hydrox. at indole group							(Hutter et al., 2012; Wohlfarth et al., 2013)
	RCS-4 hydrox. at methoxyphenyl group							(Hutter et al., 2012; Wohlfarth et al., 2013)
	RCS-4 carbox. at N-alkyl chain							(Wohlfarth et al., 2013)

	AM-2201							
	AM2201 hydrox. at N-alkyl chain					Unstable at room temperature for 24 hours		(Hutter et al., 2013; Reid et al., 2014; Sundström et al., 2013; Wohlfarth et al., 2013)
	AM2201 hydrox. at indole group							(Hutter et al., 2013; Sundström et al., 2013; Wohlfarth et al., 2013)
	JWH-073 hydrox. at N-alkyl chain							(Hutter et al., 2013)
	JWH-073 carbox. at N-alkyl chain							(Hutter et al., 2013)
	MAM-2201							
	JWH-122 hydrox. at N-alkyl chain							(Jang et al., 2014)
	MAM-2201 hydrox. at N-alkyl chain							(Jang et al., 2014)
	MAM-2201 carbox. at N-alkyl chain							(Jang et al., 2014)
NPS/*Synthetic cathinones*	**Methylone**					High stability (91± 8 %)at 4°C for 7days; medium stability at -20°C (71± 8 %)	✓	(Kinyua et al., 2015; Thai et al., 2016)
	Flephedrone					High stability (88 ± 2 %) at 4°C for 7days; low stability at -20°C (48± 14 %)		(Senta et al., 2015b)
	Methedrone					High stability (94± 5 %)at 4°C for 7days; medium stability at -20°C (85± 13 %)		(Senta et al., 2015b)
	mephedrone					high stability (83±2 %) at 4°C for 7days; low stability at -20°C (57± 13 %)		(Senta et al., 2015b)
	Butylone					High stability (107±13 %) at 4°C for 7days; high stability at -20°C (104± 31 %)		(Senta et al., 2015b)
	4-Methylethcathinone	4-MEC				High stability (84±2 %) at 4°C for 7days; low stability at -20°C (60± 16 %)		(Senta et al., 2015b)
	4-Ethylmethcathinone					Medium stability (80±3 %) at 4°C for 7days; low stability at -20°C (58± 15 %)		(Senta et al., 2015b)
	MDPV					High stability (93±8 %) at 4°C for 7days; medium stability at -20°C (79± 10 %)		(Senta et al., 2015b)
NPS/*Phenethylamines*	**PMMA**						✓	(Kinyua et al., 2015)
	PMA						✓	(Kinyua et al., 2015; Tscharke et al., 2016)
	4- fluoroamphetamine	4-FA				Medium stability (84±11 %)at 4°C for 7days; high stability at -20°C (127± 3 %)		(Senta et al., 2015b)
	4-Ethylthio-2,5-dimethoxyphenethylamine	2C-T-2				Medium stability (80±10 %)at 4°C for 7days; low stability at -20°C (56± 6 %)		(Senta et al., 2015b)
	4-Iodo-2,5-dimethoxyphenethylamine	2C-I				Medium stability (64±12 %)at 4°C for 7days; low stability at -20°C (57± 2 %)		(Senta et al., 2015b)
	4-Propylthio-2,5-dimethoxyphenethylamine	2C-T-7				Medium stability (74±10 %)at 4°C for 7days; low stability at -20°C (51± 0.2 %)		(Senta et al., 2015b)
NPS/*Piperazines*	**BZP**						✓	(Baker and Kasprzyk-Hordern, 2011; Chen et al., 2013; Tscharke et al., 2016)
	TFMPP						✓	(Baker and Kasprzyk-Hordern, 2011; Chen et al., 2013; Tscharke et al., 2016)
NPS/*Arylcycloalkylamines*	**Methoxetamine**						✓	(Baz-Lomba et al., 2016; Kinyua et al., 2015)
NPS/*Synthetic tryptamines*	**5-Methoxy-N,N-diisopropyltryptamine**	5-MeO-DIPT						(Kamata et al., 2006; Narimatsu et al., 2008)
	5-hydroxy-N,N-diisopropyltryptamine	5-OH-DIPT						(Kamata et al., 2006; Narimatsu et al., 2008)
	6-hydroxy-5-methoxy-N,N-diisopropyltrypta	6-OH- 5-MeO-DIPT						(Kamata et al., 2006; Narimatsu et al., 2008)
	5-methoxy-N-isopropyl- tryptamine	5-MeO-NIPT						(Kamata et al., 2006; Narimatsu et al., 2008)
	N,N-Diallyltryptamine	DALT						(Michely et al., 2015)
	5-methoxy- DALT	5-MeO-DALT						(Michely et al., 2015)
NPS/ *Designer benzodiazepines*	**Clonazolam**							(Huppertz et al., 2015)
	Deschloroetizolam							(Huppertz et al., 2015)
	Meclonazepam							(Huppertz et al., 2015)
	Flubromazolam							(Huppertz et al., 2015; Moosmann et al., 2013)
	OH-Flubromazepam							(Huppertz et al., 2015; Moosmann et al., 2013)
	Debrominated flubromazepa							(Huppertz et al., 2015; Moosmann et al., 2013)
	Debrominated-OH- flubromazepam							(Huppertz et al., 2015; Moosmann et al., 2013)

References

Baker, D.R., Kasprzyk-Hordern, B., 2011. Critical evaluation of methodology commonly used in sample collection, storage and preparation for the analysis of pharmaceuticals and illicit drugs in surface water and wastewater by solid phase extraction and liquid chromatography-mass spectrometry. J. Chromatogr. A 1218, 8036–8059. doi:10.1016/j.chroma.2011.09.012

Baz-Lomba, J.A., Reid, M.J., Thomas, K. V., 2016. Target and suspect screening of psychoactive substances in sewage-based samples by UHPLC-QTOF. Anal. Chim. Acta 914, 81–90.

Borova, V.L., Gago-Ferrero, P., Pistos, C., Thomaidis, N.S., 2015. Multi-residue determination of 10 selected new psychoactive substances in wastewater samples by liquid chromatography–tandem mass spectrometry. Talanta 144, 592–603. doi:10.1016/j.talanta.2015.06.080

Burgard, D. a., Banta-Green, C., Field, J. a., 2014. Working upstream: How far can you go with sewage-based drug epidemiology? Environ. Sci. Technol. 48, 1362–1368. doi:10.1021/es4044648

Castiglioni, S., Bijlsma, L., Covaci, A., Emke, E., Hernández, F., Reid, M., Ort, C., Thomas, K. V., Van Nuijs, A.L.N., De Voogt, P., Zuccato, E., 2013. Evaluation of uncertainties associated with the determination of community drug use through the measurement of sewage drug biomarkers. Environ. Sci. Technol. 47, 1452–1460. doi:10.1021/es302722f

Castiglioni, S., Gracia-Lor, E., 2016. Chapter 2. Target drugs residues in wastewater., in: Assessing Illicit Drugs in Wastewater. European Monitoring Centre for Drugs and Drug Addiction, EMCDDA. doi:10.2810/017397

Castiglioni, S., Senta, I., Borsotti, A., Davoli, E., Zuccato, E., 2015. A novel approach for monitoring tobacco use in local communities by wastewater analysis. Tob. Control 24, 38–42. doi:10.1136/tobaccocontrol-2014-051553

Castrignanò, E., Lubben, A., Kasprzyk-Hordern, B., 2016. Enantiomeric profiling of chiral drug biomarkers in wastewater with the usage of chiral liquid chromatography coupled with tandem mass spectrometry. J. Chromatogr. A 1438, 84–99. doi:10.1016/j.chroma.2016.02.015

Chen, C., Kostakis, C., Irvine, R.J., White, J.M., 2013. Increases in use of novel synthetic stimulant are not directly linked to decreased use of 3,4-methylenedioxy-N-methylamphetamine (MDMA). Forensic Sci. Int. 231, 278–283. doi:10.1016/j.forsciint.2013.06.007

EMCDDA, 2016. Wastewater analysis and drugs: a European multi-city study 1–5. doi:http://www.emcdda.europa.eu/topics/pods/waste-water-analysis

Garattini, S., 1993. Caffeine, Coffee and Health. Raven Press, New York.

Gracia-Lor, E., Zuccato, E., Castiglioni, S., 2016. Refining correction factors for back-calculation of illicit drug use. Sci. Total Environ. 573, 1648-1649 . doi:10.1016/j.scitotenv.2016.09.179

Grigoryev, A., Savchuk, S., Melnik, A., Moskaleva, N., Dzhurko, J., Ershov, M., Nosyrev, A., Vedenin, A., Izotov, B., Zabirova, I., Rozhanets, V., 2011. Chromatography-mass spectrometry studies on the metabolism of synthetic cannabinoids JWH-018 and JWH-073, psychoactive components of smoking mixtures. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 879, 1126–1136. doi:10.1016/j.jchromb.2011.03.034

Helander, A., Beck, O., 2005. Ethyl sulfate: a metabolite of ethanol in humans and a potential biomarker of acute alcohol intake. J. Anal. Toxicol. 29, 270–274.

Huppertz, L.M., Bisel, P., Westphal, F., Franz, F., Auwarter, V., Moosmann, B., 2015. Characterization of the four designer benzodiazepines clonazolam, deschloroetizolam, flubromazolam, and meclonazepam, and identification of their in vitro metabolites. Forensic Toxicol. 33, 388–395. doi:10.1007/s11419-015-0277-6

Hutter, M., Broecker, S., Kneisel, S., Auwärter, V., 2012. Identification of the major urinary metabolites in man of seven synthetic cannabinoids of the aminoalkylindole type present as adulterants in “herbal mixtures” using LC-MS/MS techniques. J. Mass Spectrom. 47, 54–65. doi:10.1002/jms.2026

Hutter, M., Moosmann, B., Kneisel, S., Auwärter, V., 2013. Characteristics of the designer drug and synthetic cannabinoid receptor agonist AM-2201 regarding its chemistry and metabolism. J. Mass Spectrom. 48, 885–894. doi:10.1002/jms.3229

Jang, M., Shin, I., Yang, W., Chang, H., Yoo, H.H., Lee, J., Kim, E., 2014. Determination of major metabolites of MAM-2201 and JWH-122 in in vitro and in vivo studies to distinguish their intake. Forensic Sci. Int. 244, 85–91. doi:10.1016/j.forsciint.2014.08.008

Kamata, T., Katagi, M., Kamata, H.T.., Miki, A., Shima, N., Zaitsu, K., Nishikawa, M., Tanaka, H., Honda, K., Tsuchihashi, H., 2006. Metabolism of the psychotomimetic tryptamine derivative 5-methoxy-N,N-diisopropyltrytamine in humans: identificafion and quantification of its urinary metabolites. Drug Metab. Dispos. 34, 281–28. doi:10.1124/dmd.105.005835.United

Kinyua, J., Covaci, A., Maho, W., McCall, A.-K., Neels, H., van Nuijs, A.L.N., 2015. Sewage-based epidemiology in monitoring the use of new psychoactive substances: Validation and application of an analytical method using LC-MS/MS. Drug Test. Anal. 7, 812–818. doi:10.1002/dta.1777

Lai, F.Y., Ort, C., Gartner, C., Carter, S., Prichard, J., Kirkbride, P., Bruno, R., Hall, W., Eaglesham, G., Mueller, J.F., 2011. Refining the estimation of illicit drug consumptions from wastewater analysis: Co-analysis of prescription pharmaceuticals and uncertainty assessment. Water Res. 45, 4437–4448. doi:10.1016/j.watres.2011.05.042

McCall, A.-K., Bade, R., Kinyua, J., Lai, F.Y., Thai, P.K., Covaci, A., Bijlsma, L., van Nuijs, A.L.N., Ort, C., 2016. Critical review on the stability of illicit drugs in sewers and wastewater samples. Water Res. 88, 933–947. doi:10.1016/j.watres.2015.10.040

Michely, J.A., Helfer, A.G., Brandt, S.D., Meyer, M.R., Maurer, H.H., 2015. Metabolism of the new psychoactive substances N,N-diallyltryptamine (DALT) and 5-methoxy-DALT and their detectability in urine by GC–MS, LC–MS n , and LC–HR–MS–MS. Anal. Bioanal. Chem. 407, 7831–7842. doi:10.1007/s00216-015-8955-0

Moosmann, B., Huppertz, L.M., Hutter, M., Buchwald, A., Ferlaino, S., Auwärter, V., 2013. Detection and identification of the designer benzodiazepine flubromazepam and preliminary data on its metabolism and pharmacokinetics. J. Mass Spectrom. 48, 1150–1159. doi:10.1002/jms.3279

Narimatsu, S., Yonemoto, R., Masuda, K., Katsu, T., Asanuma, M., Kamata, T., Katagi, M., Tsuchihashi, H., Kumamoto, T., Ishikawa, T., Naito, S., Yamano, S., Hanioka, N., 2008. Oxidation of 5-methoxy-N,N-diisopropyltryptamine in rat liver microsomes and recombinant cytochrome P450 enzymes. Biochem. Pharmacol. 75, 752–760. doi:10.1016/j.bcp.2007.09.019

Reid, M.J., Derry, L., Thomas, K. V., 2014. Analysis of new classes of recreational drugs in sewage: Synthetic cannabinoids and amphetamine-like substances. Drug Test. Anal. 6, 72–79. doi:10.1002/dta.1461

Reid, M.J., Langford, K.H., Mørland, J., Thomas, K. V., 2011. Analysis and interpretation of specific ethanol metabolites, ethyl sulfate, and ethyl glucuronide in sewage effluent for the quantitative measurement of regional alcohol consumption. Alcohol. Clin. Exp. Res. 35, 1593–1599. doi:10.1111/j.1530-0277.2011.01505.x

Rodríguez-Álvarez, T., Racamonde, I., González-Mariño, I., Borsotti, A., Rodil, R., Rodríguez, I., Zuccato, E., Quintana, J.B., Castiglioni, S., 2015. Alcohol and cocaine co-consumption in two European cities assessed by wastewater analysis. Sci. Total Environ. 536, 91–8. doi:10.1016/j.scitotenv.2015.07.016

Senta, I., Gracia-Lor, E., Borsotti, A., Zuccato, E., Castiglioni, S., 2015a. Wastewater analysis to monitor use of caffeine and nicotine and evaluation of their metabolites as biomarkers for population size assessment. Water Res. 74, 23–33. doi:10.1016/j.watres.2015.02.002

Senta, I., Krizman, I., Ahel, M., Terzic, S., 2015b. Multiresidual analysis of emerging amphetamine-like psychoactive substances in wastewater and river water. J. Chromatogr. A 1425, 204–212. doi:10.1016/j.chroma.2015.11.043

Sundström, M., Pelander, A., Angerer, V., Hutter, M., Kneisel, S., Ojanperä, I., 2013. A high-sensitivity ultra-high performance liquid chromatography/high-resolution time-of-flight mass spectrometry (UHPLC-HR-TOFMS) method for screening synthetic cannabinoids and other drugs of abuse in urine. Anal. Bioanal. Chem. 405, 8463–74. doi:10.1007/s00216-013-7272-8

Tang, M.H.Y., Ching, C.K., Lee, C.Y.W., Lam, Y.H., Mak, T.W.L., 2014. Simultaneous detection of 93 conventional and emerging drugs of abuse and their metabolites in urine by UHPLC-MS/MS. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 969, 272–284. doi:10.1016/j.jchromb.2014.08.033

Thai, P.K., Lai, F.Y., Edirisinghe, M., Hall, W., Bruno, R., O’Brien, J.W., Prichard, J., Kirkbride, K.P., Mueller, J.F., 2016. Monitoring temporal changes in use of two cathinones in a large urban catchment in Queensland, Australia. Sci. Total Environ. 545–546, 250–255. doi:10.1016/j.scitotenv.2015.12.038

Tscharke, B.J., Chen, C., Gerber, J.P., White, J.M., 2016. Temporal trends in drug use in Adelaide, South Australia by wastewater analysis. Sci. Total Environ. 565, 384–391. doi:10.1016/j.scitotenv.2016.04.183

Wohlfarth, A., Scheidweiler, K.B., Chen, X., Liu, H., Huestis, M.A., 2013. Qualitative Confirmation of 9 Synthetic Cannabinoids and 20 Metabolites in Human Urine Using LC–MS/MS and Library Search. Anal. Chem. 85, 3730–3738.

Wurst, F.M., Dresen, S., Allen, J.P., Wiesbeck, G., Graf, M., Weinmann, W., 2006. Ethyl sulphate: A direct ethanol metabolite reflecting recent alcohol consumption. Addiction 101, 204–211. doi:10.1111/j.1360-0443.2005.01245.x

Table S2. Literature summary of exposure biomarkers from environment and food

Class/ *Family*	**Parent Compound**/*Metabolite*	**Acronym**	**Excretion rate (%)**	**Stability in urine**	**Stability in WW**	**Detected in IWW**	**Reference**
Pesticides/*Carbamates*	**Carbofuran**	CFP					(Yusa et al., 2015)
	3-hydroxycarbofuran						(Yusa et al., 2015)
	Propoxur						(Yusa et al., 2015)
	2-isopropoxyphenol	2-IPP					(Yusa et al., 2015)
	Propineb						(Yusa et al., 2015)
	Propylenethiourea	PETU					(Yusa et al., 2015)
	ethylene bisdithiocarbamates: mancozeb, maneb, metiram, nabam, zineb						(Yusa et al., 2015)
	Ethylenethiourea	ETU					(Yusa et al., 2015)
	Propoxur						(Yusa et al., 2015)
Pesticides/*Triazine and Chloroacetanilid*	**Atrazine**	ATZ			6% decrease at 4°C or frozen	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Desisopropyl atrazine	DIA			Small increase at 4°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Atrazine mercapturate	ATZM			Small increase at 4°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Hydroxiatrazine	HA					(Yusa et al., 2015)
	Desethyl atrazine	DEA					(Yusa et al., 2015)
	Desethylatrazine mercapturate	DEAM					(Yusa et al., 2015)
	Diaminochloroatrazine	DACT					(Yusa et al., 2015)
	Diaminochloroatrazine	DACT					(Yusa et al., 2015)
	Acetochlor						(Yusa et al., 2015)
	Acetochlormercapturate	ACM					(Yusa et al., 2015)
	Alachlor						(Yusa et al., 2015)
	Alachlormercapturate	ALM					(Yusa et al., 2015)
	Metalochlor						(Yusa et al., 2015)
	metolachlormercapturate	MET					(Yusa et al., 2015)
	2-methyl-6-ethylaniline	2,6 EA					(Yusa et al., 2015)
	Terbuthylazine						(Yusa et al., 2015)
	Terbuthylazine desethyl	DES			Small increase at 4°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Simazine						(Yusa et al., 2015)
	Desisopropyl atrazine						(Yusa et al., 2015)
	Diaminochloroatrazine						(Yusa et al., 2015)
	Terbuthylazine						(Yusa et al., 2015)
	Desisopropyl atrazine						(Yusa et al., 2015)
	Diaminochloroatrazine						(Yusa et al., 2015)
	Propazine						(Yusa et al., 2015)
	Desisopropyl atrazine						(Yusa et al., 2015)
	Diaminochloroatrazine						(Yusa et al., 2015)
Pesticides/*Insect repellents*	**n,n-diethyl-m-toluamide**	DEET					(Yusa et al., 2015)
	n,ndiethyl-3-hydroxymethylbenzamide	DHMB					(Yusa et al., 2015)
	3-(diethylcarbamoyl)benzoicacid	DCBA					(Yusa et al., 2015)
Pesticides/*Neonicotinoid insecticides*	**Imidacloprid**						
	6-chloronicotinic acid	6CN					(Yusa et al., 2015)
	Thiamethoxam						
	2-chloro-1,3-thiazole-5-carboxylic acid	2CTCA					(Yusa et al., 2015)
	Dinotefuran						

	3-furoic acid						
	Acetamiprid						
	n-desmethylacetamiprid						(Yusa et al., 2015)
	Acetamiprid						
	5-(N-Acetyl-N-methylaminomethyl)-2-chloropyridine	5-AMAM-2-CP					
	5-(N-acetylaminomethyl)-2-chloropyridine-2-chloropyridine	5-AAM-2-CP					
	2-chloropyridine-2-chloropyridine						
	Nitenpyram						
	6-chloronicotinic acid	6CN					
	Thiacloprid						
	6-chloronicotinic acid	6CN					
	Acetamiprid						
	6-chloronicotinic acid	6CN					
	Thiamethoxam						
	2-chloro-1,3-thiazole-5-carboxylic acid	2CTCA					
Pesticides/*Organophosphates*	**Dimethoate**						
	Omethoate						
	Acephate						
	Methamidophos						
	Methyl parathion						
	Fenthion						
	Chlorpyrifos	CPF				✓	(Rousis et al., 2016; Yusa et al., 2015)
	Chlorpyrifos methyl	CPF-MET				✓	(Rousis et al., 2016; Yusa et al., 2015)
	3,5,6-trichloro-2-pyridinol	TCPY	70			✓	(Nolan et al., 1984; Rousis et al., 2016; Yusa et al., 2015)
	Malathion						
	Malathion monocarboxylic acid	MMA	36			✓	(Bouchard et al., 2003; Rousis et al., 2016)
	Malathion dicarboxylic acid	MDA	9				(Bouchard et al., 2003; Rousis et al., 2016)
	Diazinon						
	2-isopropyl-6-methyl-4-pyrimidinol	IMPY			24% increase in room	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Common alkyl phosphate metabolite						
	Diethyl phosphate	DEP			Stable at 4°C or -20°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	o,o-diethyl thiophosphate	DETP			Stable at 4°C or -20°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Dimethyl phosphate	DMP			Stable at 4°C or -20°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Dimethyl thiophosphate	DMTP			Stable at 4°C or -20°C	✓	(Rousis et al., 2016; Yusa et al., 2015)
	Dimethyldithiophosphate	DMDTP					(Yusa et al., 2015)
	Parathion						(Yusa et al., 2015)
	p-Nitrophenol	PNP					(Yusa et al., 2015)
	Pirimiphos methyl						(Yusa et al., 2015)
	2-Diethylamino-6-methyl-4-pyrimidinol	DEAMPY					(Yusa et al., 2015)
	Coumaphos						(Yusa et al., 2015)
	3-Chloro-7-hydroxy-4-methylcoumarin (3-Chloro-4-methylumbelliferone)	CMHC					(Yusa et al., 2015)
	Azinphos-methyl						(Yusa et al., 2015)
	1,2,3-Benzotriazin-4-one	BTA					(Yusa et al., 2015)
	Fenitrothion						(Yusa et al., 2015)
	3-Methyl-4-nitrophenol	MNP					(Yusa et al., 2015)

Pesticides/ *Phenoxyacid herbicides*	*2,4-dichlorophenoxyacid*	2,4D					(Yusa et al., 2015)
	2,4,5-trichlorophenoxyacetic acid	2,4,5-T					(Yusa et al., 2015)
	20 common pyrethroids						
	3-phenoxybenzoic acid	3-PBA				✓	(Barr, 2008; Rousis et al., 2016; Yusa et al., 2015)
	Permetrin, cypermetrin & cyflutrin						
	cis/trans- 3-(2,2-dichlorovinyl)-2,2-dimethyl-(1-cyclopropane)carboxylic acid	DCCA	19-78		-100% even while frozen	✓	(Eadsforth et al., 1988; Eadsforth and Baldwin, 1983; Ratelle et al., 2015a,
	Cyfluthrin						
	4-Fluoro-3-phenoxybenzoic acid	4-F-3-PBA	47				(Aylward et al., 2009)
	Deltamethrin						
	cis-3-(2,2-Dibromovinyl)-2,2-dimethylcyclopropane carboxylic acid	DBCA	46				(Sams and Jones, 2012)
	Allethrin						
	Chrysanthemumdicarboxylic acid						(Yusa et al., 2015)
	Bifenthrin						
	2-Methyl-3-phenylbenzoic acid	MPA					(Yusa et al., 2015)
	Lambda-cyhalothrin						
	3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylic acid	HCBA					(Yusa et al., 2015)
	Esfenvalerate						
	s-Fenvalerate acid	sFA					(Yusa et al., 2015)
Pesticides/ *Quaternary ammomium com*	**Paraquat**	PQ					(Yusa et al., 2015)
	Diquat	DQ					(Yusa et al., 2015)
Pesticides/ *Sulfonylurea herbicides*	**Chlorsulfuron**						(Yusa et al., 2015)
	Foramsulfuron						(Yusa et al., 2015)
	Halosulfuron methyl						(Yusa et al., 2015)
	Mesosulfuron						(Yusa et al., 2015)
	Nicosulfuron						(Yusa et al., 2015)
	Oxasulfuron						(Yusa et al., 2015)
	Triasulfuron						(Yusa et al., 2015)
Other pesticides	**Thiabendazole**						(Yusa et al., 2015)
	5-hydroxythiabendazole						(Yusa et al., 2015)
	Chlormequat (chlorocholine chloride)	CCC					(Yusa et al., 2015)
	Diuron						(Yusa et al., 2015)
	3,4-dichloroaniline	3,4-DCA					(Yusa et al., 2015)
	Linuron						(Yusa et al., 2015)
	3,4-dichloroaniline	3,4-DCA					(Yusa et al., 2015)
	Neburon						(Yusa et al., 2015)
	3,4-dichloroaniline	3,4-DCA					(Yusa et al., 2015)
	Prorpanil						(Yusa et al., 2015)
	3,4-dichloroaniline	3,4-DCA					(Yusa et al., 2015)
	Vinclozolin						(Yusa et al., 2015)
	3,5-dichloroaniline	3,5-DCA					(Yusa et al., 2015)
	Iprodione						(Yusa et al., 2015)
	3,5-dichloroaniline	3,5-DCA					(Yusa et al., 2015)
	Procymidone						(Yusa et al., 2015)
	3,5-dichloroaniline	3,5-DCA					(Yusa et al., 2015)
	Chozolinate						(Yusa et al., 2015)

	3,5-dichloroaniline	3,5-DCA					(Yusa et al., 2015)
Mycotoxins	**Aflatoxin M1**	AFM1					(Fromme et al., 2016)
	Ochratoxin A	OTA					(Fromme et al., 2016)
	Deoxynivalenol						(Fromme et al., 2016)
	3-Acetyldeoxynivalenol	3-AcDON					
	Nivalenol	NIV					(Fromme et al., 2016)
	Fumonisin B1	FB1					(Fromme et al., 2016)
	Zearalenone	ZON				✓	(Fromme et al., 2016; Laganà et al., 2004)
	Beauvericin	BEA					
Parabens	**All parabens**						
	4-hydroxybenzoic acid						(Moos et al., 2015)
	Methylparaben						
	Methylparaben sulphate		10.6				(Moos et al., 2015)
	Methylparaben glucuronide		5.1				(Moos et al., 2015)
	Ethylparaben						
	Ethylparaben glucuronide						(Abbas et al., 2010)
	Propylparaben						
	Propylparaben sulphate		43				(Ye et al., 2006)
	Propylparaben glucuronide		55				(Ye et al., 2006)
	n-Butylparaben						
	3-OH-n-Butylparaben		5.8 (of which 63.7 % as glucuronide and 34.2 % as				(Moos et al., 2015)
	n-Butylparaben sulphate		0.7				(Moos et al., 2015)
	n-Butylparaben glucuronide		4.9				(Moos et al., 2015)
	Iso-Butylparaben						
	2-OH-iso-Butylparaben		15.8 (of which 46 % as glucuronide and 53.3 % as				(Moos et al., 2015)
	Iso-Butylparaben sulphate		0.8				(Moos et al., 2015)
	Iso-Butylparaben		6				(Moos et al., 2015)
	Benzylparaben						
	Benzylparaben glucuronide						(Abbas et al., 2010)
UV-filters	**Benzophenone-3**						
	Benzophenone-3-sulphate		6				(Ye et al., 2006)
	Benzophenone-3-glucuronide		84.6				(Ye et al., 2006)
	3-(4-Methylbenzylidene)camphor						
	3-(4-carboxybenzylidene)camphor		0.07-0.1				(Schauer et al., 2006)
Plasticizers	**DINCH**						
	MINCH						(Fromme et al., 2016)
	OH-MINCH						(Fromme et al., 2016)
	cx-MINCH						(Fromme et al., 2016)
	oxo-MINCH						(Fromme et al., 2016)
	DEHA		6.0-12.0				(Loftus et al., 1993)
	2-ethylhexanoic acid	EHA					
	Dimethyl phthalate	DMP					(Frederiksen et al., 2007)
	Monomethyl phthalate	MMP					(Frederiksen et al., 2007)
	Diethyl phthalate	DEP					(Frederiksen et al., 2007)
	Monoethyl phthalate	MEP					(Frederiksen et al., 2007)

	Di-n-butylphthalate	DBP					(Frederiksen et al., 2007)
	Mono-n-butyl phthalate	MBP					(Frederiksen et al., 2007; Silva et al., 2007)
	mono(4-hydroxybutyl) phthalate	*MHBP*	9.2				(Frederiksen et al., 2007; Silva et al., 2007)
	Di(2-ethylhexyl) phthalate	DEHP					
	Mono(2-ethylhexyl) phthalate	MEHP					(Frederiksen et al., 2007; Herrero et al., 2015)
	Mono(2-ethyl-5-hydroxyhexyl) phthalate	MEHHP or 5OH-MEHP					(Frederiksen et al., 2007; Herrero et al., 2015)
	Mono(2-ethyl-5-oxohexyl) phthalate	MEOHP or 5oxo-MEHP					(Frederiksen et al., 2007; Herrero et al., 2015)
	Mono(2-ethyl-5-carboxypentyl) phthalate	MECPP or 5cx-MEPP					(Frederiksen et al., 2007; Herrero et al., 2015)
	Mono(2-carboxy-hexyl) phthalate	MCMHP or 2cx-MMHP					(Frederiksen et al., 2007; Guo et al., 2011)
Flame retardants	**Organophosphate flame retardants (PFRs)**						
	Bis(2-chloroethyl) phosphate	BCEP					(Van den Eede et al., 2015)
	Bis(1-chloro-2-propyl) phosphate	BCIPP					(Van den Eede et al., 2015)
	Bis(1,3-dichloro-2-propyl) phosphate	BDCIPP					(Van den Eede et al., 2015)
	Bis(2-butoxyethyl) phosphate	BBOEP					(Van den Eede et al., 2015)
	Bis(2-butoxyethyl) 3´-hydroxy2-butoxyethyl phosphate	HO-TBOEP					(Van den Eede et al., 2015)
	2-hydroxyethyl bis(2-butoxyethyl) phosphate	BBOEHEP					(Van den Eede et al., 2015)
	Dibutyl phosphate	DBP					(Van den Eede et al., 2015)
	Diphenyl phosphate	DPHP					(Van den Eede et al., 2015)
	4-hydroxyphenyl diphenyl phosphate	HO-TPHP					(Van den Eede et al., 2015)
	4-hydroxyphenyl diphenyl phosphate	HO-TPHP					(Van den Eede et al., 2015)

References

Abbas, S., Greige-Gerges, H., Karam, N., Piet, M.-H., Netter, P., Magdalou, J., 2010. Metabolism of parabens (4-hydroxybenzoic acid esters) by hepatic esterases and UDP-glucuronosyltransferases in man. Drug Metab. Pharmacokinet. 25, 568–577. doi:10.2133/dmpk.DMPK-10-RG-013

Aylward, L.L., Hays, S.M., Gagné, M., Krishnan, K., 2009. Derivation of Biomonitoring Equivalents for di(2-ethylhexyl)phthalate (CAS No. 117-81-7). Regul. Toxicol. Pharmacol. 55, 249–258. doi:10.1016/j.yrtph.2009.09.001

Barr, D.B., 2008. Biomonitoring of exposure to pesticides. J. Chem. Heal. Saf. 15, 20–29. doi:10.1016/j.jchas.2008.07.001

Bouchard, M., Gosselin, N.H., Brunet, R.C., Samuel, O., Dumoulin, M.J., Carrier, G., 2003. A toxicokinetic model of malathion and its metabolites as a tool to assess human exposure and risk through measurements of urinary biomarkers. Toxicol. Sci. 73, 182–194. doi:10.1093/toxsci/kfg061

Eadsforth, C.V., Baldwin, M.K., 1983. Human dose-excretion studies with the pyrethroid insecticide, cypermethrin. Xenobiotica 13, 67–72.

Eadsforth, C.V., Bragt, P.C., Van Sittert, N.J., 1988. Human dose-excretion studies with pyrethroid insecticides cypermethrin and alphacypermethrin: Relevance for biological monitoring. Xenobiotica 15, 603–614.

Frederiksen, H., Skakkebæk, N.E., Andersson, A.M., 2007. Metabolism of phthalates in humans. Mol. Nutr. Food Res. 51, 899–911. doi:10.1002/mnfr.200600243

Fromme, H., Gareis, M., Völkel, W., Gottschalk, C., 2016. Overall internal exposure to mycotoxins and their occurrence in occupational and residential settings – An overview. Int. J. Hyg. Environ. Health 219, 143–165. doi:http://dx.doi.org/10.1016/j.ijheh.2015.11.004

Guo, Y., Alomirah, H., Cho, H.-S., Minh, T.B., Mohd, M.A., Nakata, H., Kannan, K., 2011. Occurrence of phthalate metabolites in human urine from several Asian countries. Environ. Sci. Technol. 45, 3138–44. doi:10.1021/es103879m

Herrero, L., Calvarro, S., Fernández, M.A., Quintanilla-López, J.E., González, M.J., Gómara, B., 2015. Feasibility of ultra-high performance liquid and gas chromatography coupled to mass spectrometry for accurate determination of primary and secondary phthalate metabolites in urine samples. Anal. Chim. Acta 853, 625–636. doi:10.1016/j.aca.2014.09.043

Laganà, A., Bacaloni, A., De Leva, I., Faberi, A., Fago, G., Marino, A., 2004. Analytical methodologies for determining the occurrence of endocrine disrupting chemicals in sewage treatment plants and natural waters. Anal. Chim. Acta 501, 79–88. doi:10.1016/j.aca.2003.09.020

Loftus, N.J., Laird, W.J.D., Steel, G.T., Wilks, M.F., Woollen, B.H., 1993. Metabolism and pharmacokinetics of deuterium-labelled di-2-(ethylhexyl) adipate (DEHA) in humans. Food Chem. Toxicol. 31, 609–614. doi:10.1016/0278-6915(93)90042-W

Moos, R.K., Angerer, J., Dierkes, G., Brüning, T., Koch, H.M., 2015. Metabolism and elimination of methyl, iso- and n-butyl paraben in human urine after single oral dosage. Arch. Toxicol. 1–11. doi:10.1007/s00204-015-1636-0

Nolan, R.J., Rick, D.L., Freshour, N., Saunders, J.H., 1984. Chlorpyrifos: pharmacokinetics in human volunteers. Toxicol. Appl. Pharmacol. 73, 8–15.

Ratelle, M., Côté, J., Bouchard, M., 2015a. Time profiles and toxicokinetic parameters of key biomarkers of exposure to cypermethrin in orally exposed volunteers compared with previously available kinetic data following permethrin exposure. J Appl Toxicol 35, 1586–1593.

Ratelle, M., Côté, J., Bouchard, M., 2015b. Toxicokinetics of permethrin biomarkers of exposure in orally exposed volunteers. Toxicol. Lett. 232, 369–375. doi:10.1016/j.toxlet.2014.12.003

Rousis, N.I., Zuccato, E., Castiglioni, S., 2016. Monitoring population exposure to pesticides based on liquid chromatography-tandem mass spectrometry measurement of their urinary metabolites in urban wastewater: a novel biomonitoring approach. Sci. Total Environ. 571, 1349–1357. doi:10.1016/j.scitotenv.2016.07.036

Sams, C., Jones, K., 2012. Biological monitoring for exposure to deltamethrin: A human oral dosing study and background levels in the UK general population. Toxicol. Lett. 213, 35–38. doi:10.1016/j.toxlet.2011.04.014

Schauer, U.M.D., Völkel, W., Heusener, A., Colnot, T., Broschard, T.H., von Landenberg, F., Dekant, W., 2006. Kinetics of 3-(4-methylbenzylidene)camphor in rats and humans after dermal application. Toxicol. Appl. Pharmacol. 216, 339–346. doi:10.1016/j.taap.2006.05.011

Silva, M.J., Samandar, E., Reidy, J.A., Hauser, R., Needham, L.L., Calafat, A.M., 2007. Metabolite profiles of Di-n-butyl phthalate in humans and rats. Environ. Sci. Technol. 41, 7576–7580. doi:10.1021/es071142x

Van den Eede, N., Heffernan, A.L., Aylward, L.L., Hobson, P., Neels, H., Mueller, J.F., Covaci, A., 2015. Age as a determinant of phosphate flame retardant exposure of the Australian population and identification of novel urinary PFR metabolites. Environ. Int. 74, 1–8. doi:10.1016/j.envint.2014.09.005

Woollen, B.H., Marsh, J.R., Laird, W.J., Lesser, J.E., 1992. The metabolism of cypermethrin in man: differences in urinary metabolite profiles following oral and dermal administration. Xenobiotica 22, 983–991.

Table S3. Literature summary of health biomarkers

Class/ *Family*	**Parent Compound**/*Metabolite*	**Excretion rate (%)**	**Reference**	**Stability in urine**	**Stability in WW**	**Detected in IWW**	**Reference**
Antibiotics/ *Penicillins*	**Amoxicillin**	30–70	(Petrie et al., 2015)			✓	(Mutiyar and Mittal, 2013)
		80–90	(Hirsch et al., 1999)				
	Ampicillin	30–60	(Hirsch et al., 1999)				
	Penicillin V	~40	(Hirsch et al., 1999)				
	Oxacillin	~40	(Hirsch et al., 1999)				
	Penicillin G	50–70	(Hirsch et al., 1999)			✓	(Gulkowska et al., 2008)
	Dicloxacillin	~65					
Antibiotics/*Macrolides–lincosamides*	**Erythromycin**	5	(Petrie et al., 2015)			✓	(Jelic et al., 2012)
		>60	(Hirsch et al., 1999)				
	Clarithromycin	>60	(Hirsch et al., 1999)			✓	(Gracia-Lor et al., 2012b; Jelic et al., 2012)
	Roxithromycin	>60	(Hirsch et al., 1999)			✓	(Gros et al., 2010)
	Metronidazole	20	(Petrie et al., 2015)			✓	(Kasprzyk-Hordern et al., 2009)
	Azithromycin					✓	(Gros et al., 2010)
Antibiotics/*Quinolones*	**Ofloxacin**	65–80	(Petrie et al., 2015)			✓	(Gracia-Lor et al., 2012b)
	Norfloxacin					✓	(Gracia-Lor et al., 2012b; Jelic et al., 2012)
	Ciprofloxacin					✓	Gracia-Lor et al., 2012; Jelic et al., 2012)
	Chloramphenicol	8–12	(Petrie et al., 2015)			✓	(Kasprzyk-Hordern et al., 2009)
		5–10					
Antibiotics/*Sulphonamides And Trimethoprim*	**Sulfamethoxazole**	30	(Petrie et al., 2015)			✓	(Leung et al., 2012)
		~15	(Hirsch et al., 1999)				(Gracia-Lor et al., 2012b; Jelic et al., 2012; Kasprzyk-Hordern et al., 2009)
	Sulfapyridine	<10	(Petrie et al., 2015)				(Petrie et al., 2015)
	Sulfasalazine	15	(Petrie et al., 2015)				(Petrie et al., 2015)
	Sulfathiazole					✓	(Gracia-Lor et al., 2012b)
	Trimethoprim	80	(Petrie et al., 2015)			✓	(Verlicchi et al., 2014)
		~60					(Hirsch et al., 1999)
Antibiotics/*Tetracyclines*	**Oxytetracycline**	30	(Petrie et al., 2015)			✓	
		>80	(Hirsch et al., 1999)				(Gros et al., 2010)
	Chlortetracyline	>70	(Hirsch et al., 1999)			✓	(Yang et al., 2005)
	Tetracycline	80–90	(Hirsch et al., 1999; Kühne et al., 2000)			✓	(Gros et al., 2010; Yang et al., 2005)
	Minocycline	~60	(Hirsch et al., 1999)				(Verlicchi et al., 2014)
	Doxycycline	>70	(Hirsch et al., 1999)			✓	(Verlicchi et al., 2014; Yang et al., 2005)
Pharmaceuticals	**Acetaminophen (paracetamol)**	54	(Riva et al., 2015)			✓	(Gracia-Lor et al., 2012b; O'Brien et al., 2014; Riva et al., 2015)
		20	(Petrie et al., 2015)				
	Acetylsalicylic acid						
	Salicylic acid					✓	(O'Brien et al., 2014)
	Allopurinol						
	Oxypurinol	80	(Funke et al., 2015)				
	Atenolol	82	(Riva et al., 2015)			✓	
		50	(Petrie et al., 2015)				
	Bezafibrate	40	(Huschek et al., 2004)			✓	
	Carbamazepine	2-3	(Clara et al., 2004; Petrie et al., 2015)			✓	(Dickenson et al., 2011; Dsikowitzky et al., 2004; Gasser et al., 2010;
	Carbamazepine-10,11-epoxide						(Kahle et al., 2009)

Clindamycine	10	(Jjemba, 2006)				
Clofibrate						(Dsikowitzky et al., 2004)
Clofibric acid						
Codeine	64-70	(Petrie et al., 2015)			✓	(Terzic et al., 2010)
Etofibrate						(Dsikowitzky et al., 2004)
Clofibric acid						
Etofyllinclofibrate						(Dsikowitzky et al., 2004)
Clofibric acid						
Codeine	64-70	(Petrie et al., 2015)			✓	(Bruno et al., 2014; Dickenson et al., 2011)
Codeine-6-glucuronide						
Norcodeine	10-20	(Petrie et al., 2015)				
Crotamiton						(Nakada et al., 2008)
Diatrizoic acid						(Scheurer et al., 2011)
Diclofenac	61	(Riva et al., 2015)				(Dickenson et al., 2011; Gracia-Lor et al., 2012b; Riva et al., 2015)
Dilantin						(Dickenson et al., 2011)
Diltiazem	2-4	(Petrie et al., 2015)				
Diphenhydramine						(Dickenson et al., 2011)
Fluoxetine	17-25	(Brooks et al., 2003)			✓	(Dickenson et al., 2011; Petrie et al., 2016)
	11	(Petrie et al., 2015)				
Norfluoxetine					✓	(Petrie et al., 2016)
Furosemide	78	(Riva et al., 2015)			✓	(O'Brien et al., 2014; Riva et al., 2015)
	Little	(Petrie et al., 2015)				
Gabapentin	78.5	(Baselt, 2004)			✓	(Baselt, 2004; O'Brien et al., 2014)
Gemfibrozil	76	(Huschek et al., 2004)				(Dickenson et al., 2011; Huschek et al., 2004)
Hydrochlorothiazide	82	(Lienert et al., 2007)			✓	(Lienert et al., 2007; O'Brien et al., 2014)
Hydrocodone					✓	(Castrignanò et al., 2016; Dickenson et al., 2011)
Ibuprofen	12	(Riva et al., 2015)			✓	(Dickenson et al., 2011; Gracia-Lor et al., 2012b; O'Brien et al., 2014; Riva et
Iopromide	94	(Huschek et al., 2004)			✓	(Dsikowitzky et al., 2004; Huschek et al., 2004; O'Brien et al., 2014)
Meprobamate						(Dickenson et al., 2011)
Metamizole/ dipyrone						
4-methylaminoantipyrine						
4-aminoantipyrine						(Ibanez et al., 2012)
4-formylaminoantipyrine						(Ibanez et al., 2012)
4-acetylaminoantipyrine						(Ibanez et al., 2012)
Metoprolol	5-10	(Huschek et al., 2004)				(Dickenson et al., 2011; Huschek et al., 2004)
	10-30	(Petrie et al., 2015)				
Naproxen	70	(Riva et al., 2015)			✓	(Dickenson et al., 2011; Gracia-Lor et al., 2012a; O'Brien et al., 2014; Riva et
	<1	(Petrie et al., 2015)				
Nifedipine						
Dehydronifedipine						
Primidone						(Dickenson et al., 2011; Kahle et al., 2009)
Propranolol						(Dickenson et al., 2011; Fono and Sedlak, 2005)
Propyphenazone	1	(Huschek et al., 2004)				(Dsikowitzky et al., 2004; Huschek et al., 2004)
Sulfapyridine						(Dickenson et al., 2011)
Metformin	79	(Riva et al., 2015)				

	Venlafaxine	4.7	(Howell et al., 1993)			✓	(Howell et al., 1993)
	Valsartan	80	(Petrie et al., 2015)				
Benzodiazepines	**Alprazolam**			<-6.8[a]		✓	(Borova et al., 2014; Fernández et al., 2014; Racamonde et al., 2014)
	α-hydroxy-alprazolam						
	Bromazepam			<-6.8[a]		✓	(Borova et al., 2014; Fernández et al., 2014)
	Chlordiazepoxide	6.9	(Baker et al., 2014)		-14,4		(Baker et al., 2014)
	Demoxepam						
	Nordazepam						
	Clobazam					✓	(Borova et al., 2014)
	Clonazepam						
	7-aminoclonazepam						(Herrero et al., 2015)
	Clorazepate						
	Demoxepam						
	Nordazepam						
	Diazepam	1	(Smith-Kielland et al., 2001)	<-6.8[a]	-3	✓	(Borova et al., 2014; Castrignanò et al., 2016; Herrero et al., 2015; Kosiek
		Trace	(Petrie et al., 2015)				
	Oxazepam	33		<-6.8[a]	2,4	✓	(Baker et al., 2014; Borova et al., 2014; Castrignanò et al., 2016;
	Nordazepam						
	Flunitrazepam			<-6.8[a]			
	7-aminoflunitrazepam			<-6.8[a]			
	Flurazepam			<-6.8[a]			
	2-hydroxy-ethyl flurazepam						
	Lorazepam					✓	(Borova et al., 2014; Castrignanò et al., 2016; Fernández et al., 2014;
	Lormetazepam						(Fernández et al., 2014; Racamonde et al., 2014)
	Medazepam						
	Nordazepam						
	Midazolam			<-6.8[a]		✓	(Borova et al., 2014)
	Nitrazepam	1.2	(Baker et al., 2014)		-61,9	✓	(Baker et al., 2014; Castrignanò et al., 2016)
	7-aminonitrazepam	37,2	(Baker et al., 2014)		29,8	✓	(Baker et al., 2014; Castrignanò et al., 2016)
	Nordazepam	~7		<-6.8[a]	15,6	✓	(Baker et al., 2014; Borova et al., 2014; Castrignanò et al., 2016;
	Pinazepam						
	Nordazepam						
	Prazepam					✓	
	Nordazepam						
	Temazepam	75	(Petrie et al., 2015)	<-6.8[a]	19,4	✓	(Baker et al., 2014; Borova et al., 2014; Castrignanò et al., 2016;
	Oxazepam	33		<-6.8[a]	2,4		(Baker et al., 2014; Borova et al., 2014; Hummel et al., 2006; Kosiek et
	Tetrazepam					✓	(Fernández et al., 2014)
	Triazolam						
	α-hydroxy-triazolam						

[a] between -0.42 and -6.8% after 90 days at -20°C, for 40 days at 5°C and at room temperature for 12 hours and after three freeze-thaw cycles (Karampela, 2012)

References

Baker, D.R., Barron, L., Kasprzyk-Hordern, B., 2014. Illicit and pharmaceutical drug consumption estimated via wastewater analysis. Part A: Chemical analysis and drug use estimates. Sci. Total Environ. 487, 629–641. doi:10.1016/j.scitotenv.2013.11.107

Baselt, R.C., 2004. Disposition of toxic drugs and chemicals in man., 7th ed. Biochemical Publications (California, USA).

Borova, V.L., Maragou, N.C., Gago-Ferrero, P., Pistos, C., Thomaidis, N.S., 2014. Highly sensitive determination of 68 psychoactive pharmaceuticals, illicit drugs, and related human metabolites in wastewater by liquid chromatography-tandem mass spectrometry. Anal. Bioanal. Chem. 406, 4273–4285. doi:10.1007/s00216-014-7819-3

Brooks, B.W., Foran, C.M., Richards, S.M., Weston, J., Turner, P.K., Stanley, J.K., Solomon, K.R., Slattery, M., La Point, T.W., 2003. Aquatic ecotoxicology of fluoxetine. Toxicol. Lett. 142, 169–183. doi:10.1016/S0378-4274(03)00066-3

Bruno, R., Hall, W., Kirkbride, K.P., Lai, F.Y., O'Brien, J.W., Prichard, J., Thai, P.K., Mueller, J.F., 2014. Commentary on Ort etal. (2014): What next to deliver on the promise of large scale sewage-based drug epidemiology? Addiction 109, 1353–1354. doi:10.1111/add.12651

Castrignanò, E., Lubben, A., Kasprzyk-Hordern, B., 2016. Enantiomeric profiling of chiral drug biomarkers in wastewater with the usage of chiral liquid chromatography coupled with tandem mass spectrometry. J. Chromatogr. A 1438, 84–99. doi:10.1016/j.chroma.2016.02.015

Clara, M., Strenn, B., Kreuzinger, N., 2004. Carbamazepine as a possible anthropogenic marker in the aquatic environment: Investigations on the behaviour of Carbamazepine in wastewater treatment and during groundwater infiltration. Water Res. 38, 947–954. doi:10.1016/j.watres.2003.10.058

Dickenson, E.R. V, Snyder, S.A., Sedlak, D.L., Drewes, J.E., 2011. Indicator compounds for assessment of wastewater effluent contributions to flow and water quality. Water Res. 45, 1199–1212. doi:10.1016/j.watres.2010.11.012

Dsikowitzky, L., Schwarzbauer, J., Littke, R., 2004. The anthropogenic contribution to the organic load of the Lippe River (Germany). Part II: Quantification of specific organic contaminants. Chemosphere 57, 1289–1300. doi:10.1016/j.chemosphere.2004.08.053

Fernández, P., Regenjo, M., Fernández, A.M., Lorenzo, R.A., Carro, A.M., 2014. Optimization of ultrasound-assisted dispersive liquid-liquid microextraction for ultra performance liquid chromatography determination of benzodiazepines in urine and hospital wastewater. Anal. Methods 6, 8239–8246. doi:10.1039/c4ay01348d

Fono, L.J., Sedlak, D.L., 2005. Use of the chiral pharmaceutical propranolol to identify sewage discharges into surface waters. Environ. Sci. Technol. 39, 9244–9252. doi:10.1021/es047965t

Funke, J., Prasse, C., Eversloh, C.L., Ternes, T.A., 2015. Oxypurinol - A novel marker for wastewater contamination of the aquatic environment. Water Res. 74, 257–265. doi:10.1016/j.watres.2015.02.007

Gasser, G., Rona, M., Voloshenko, A., Shelkov, R., Tal, N., Pankratov, I., Elhanany, S., Lev, O., 2010. Quantitative evaluation of tracers for quantification of wastewater contamination of potable water sources. Environ. Sci. Technol. 44, 3919–3925. doi:10.1021/es100604c

Gracia-Lor, E., Martínez, M., Sancho, J. V., Puñuela, G., Hernández, F., 2012a. Multi-class determination of personal care products and pharmaceuticals in environmental and wastewater samples by ultra-high performance liquid-chromatography-tandem mass spectrometry. Talanta 99, 1011–1023. doi:10.1016/j.talanta.2012.07.091

Gracia-Lor, E., Sancho, J. V., Serrano, R., Hernández, F., 2012b. Occurrence and removal of pharmaceuticals in wastewater treatment plants at the Spanish Mediterranean area of Valencia. Chemosphere 87, 453–462. doi:10.1016/j.chemosphere.2011.12.025

Gros, M., Petrović, M., Ginebreda, A., Barceló, D., 2010. Removal of pharmaceuticals during wastewater treatment and environmental risk assessment using hazard indexes. Environ. Int. 36, 15–26. doi:10.1016/j.envint.2009.09.002

Gulkowska, A., Leung, H.W., So, M.K., Taniyasu, S., Yamashita, N., Yeung, L.W.Y., Richardson, B.J., Lei, A.P., Giesy, J.P., Lam, P.K.S., 2008. Removal of antibiotics from wastewater by sewage treatment facilities in Hong Kong and Shenzhen, China. Water Res. 42, 395–403. doi:10.1016/j.watres.2007.07.031

Herrero, L., Calvarro, S., Fernández, M.A., Quintanilla-López, J.E., González, M.J., Gómara, B., 2015. Feasibility of ultra-high performance liquid and gas chromatography coupled to mass spectrometry for accurate determination of primary and secondary phthalate metabolites in urine samples. Anal. Chim. Acta 853, 625–636. doi:10.1016/j.aca.2014.09.043

Hirsch, R., Ternes, T., Haberer, K., Kratz, K.L., 1999. Occurrence of antibiotics in the aquatic environment. Sci. Total Environ. 225, 109–118. doi:10.1016/S0048-9697(98)00337-4

Howell, S.R., Husbands, G.E., Scatina, J.A., Sisenwine, S.F., 1993. Metabolic disposition of 14C-venlafaxine in mouse, rat, dog, rhesus monkey and man. Xenobiotica 23, 349–359.

Hummel, D., Löffler, D., Fink, G., Ternes, T. a, 2006. Simultaneous determination of psychoactive drugs and their metabolites in aqueous matrices by liquid chromatography mass Spectrometry. Environ. Sci. Technol. 40, 7321–8.

Huschek, G., Hansen, P.D., Maurer, H.H., Krengel, D., Kayser, A., 2004. Environmental risk assesssment of medicinal products for human use according to European Commission recommendations. Environ. Toxicol. 19, 226–240. doi:10.1002/tox.20015

Ibañez, M., Gracia-Lor, E., Sancho, J. V., Hernández, F., 2012. Importance of MS selectivity and chromatographic separation in LC-MS/MS-based methods when investigating pharmaceutical metabolites in water. Dipyrone as a case of study. J. Mass Spectrom. 47, 1040–1046. doi:10.1002/jms.3050

Jelic, A., Gros, M., Petrovic, M., Ginebreda, A., Barceló, D., 2012. Occurrence and elimination of pharmaceuticals during conventional wastewater treatment. Emerg. Prior. Pollut. Rivers 1–23. doi:10.1007/978-3-642-25722-3

Jjemba, P.K., 2006. Excretion and ecotoxicity of pharmaceutical and personal care products in the environment. Ecotoxicol. Environ. Saf. 63, 113–130. doi:10.1016/j.ecoenv.2004.11.011

Kahle, M., Buerge, I.J., Müller, M.D., Poiger, T., 2009. Hydrophilic anthropogenic markers for quantification of wastewater contamination in ground- and surface waters. Env. Toxicol Chem. 28, 2528–2536.

Karampela, S., Vardakou, I., Papoutsis, I., Dona, A., Spiliopoulou, C., Athanaselis, S., Pistos, C., 2012. Direct urine analysis for the identification and quantification of selected benzodiazepines for toxicology screening. J. Chromatogr. B Anal. Technol. Biomed. Life Sci. 902, 42–46. doi:10.1016/j.jchromb.2012.06.012

Kasprzyk-Hordern, B., Dinsdale, R.M., Guwy, A.J., 2009. The removal of pharmaceuticals, personal care products, endocrine disruptors and illicit drugs during wastewater treatment and its impact on the quality of receiving waters. Water Res. 43, 363–380. doi:10.1016/j.watres.2008.10.047

Kosjek, T., Perko, S., Zupanc, M., Zanoški Hren, M., Landeka Dragičević, T., Žigon, D., Kompare, B., Heath, E., 2012. Environmental occurrence, fate and transformation of benzodiazepines in water treatment. Water Res. 46, 355–368. doi:10.1016/j.watres.2011.10.056

Kühne, M., Ihnen, D., Möller, G., Agthe, O., 2000. Stability of tetracycline in water and liquid manure. J. Vet. Med. A. Physiol. Pathol. Clin. Med. 47, 379–384. doi:10.1046/j.1439-0442.2000.00300.x

Leung, H.W., Minh, T.B., Murphy, M.B., Lam, J.C.W., So, M.K., Martin, M., Lam, P.K.S., Richardson, B.J., 2012. Distribution, fate and risk assessment of antibiotics in sewage treatment plants in Hong Kong, South China. Environ. Int. 42, 1–9. doi:10.1016/j.envint.2011.03.004

Lienert, J., Güdel, K., Escher, B., 2007. Screening method for ecotoxicological hazard assessment of 42 pharmaceuticals considering human metabolism and excretory routes. Environ. Sci. Technol. 41, 4471–4478.

Mutiyar, P.K., Mittal, A.K., 2013. Occurrences and fate of an antibiotic amoxicillin in extended aeration-based sewage treatment plant in Delhi, India: a case study of emerging pollutant. Desalin. Water Treat. 51, 6158–6164.

Nakada, N., K, K., H, S., A, H., K, K., S, T., H, T., 2008. Evaluation of pharmaceuticals and personal care products as water-soluble molecular markers of sewage. Env. Sci Technol. 42, 6347–6353.

O'Brien, J.W., Thai, P.K., Eaglesham, G., Ort, C., Scheidegger, A., Carter, S., Lai, F.Y., Mueller, J.F., 2014. A Model to Estimate the Population Contributing to the Wastewater Using Samples Collected on Census Day. Environ. Sci. Technol. 48, 517–525. doi:10.1021/es403251g

Petrie, B., Barden, R., Kasprzyk-Hordern, B., 2015. A review on emerging contaminants in wastewaters and the environment: Current knowledge, understudied areas and recommendations for future monitoring. Water Res. 72, 3–27. doi:10.1016/j.watres.2014.08.053

Petrie, B., Youdan, J., Barden, R., Kasprzyk-Hordern, B., 2016. New Framework To Diagnose the Direct Disposal of Prescribed Drugs in Wastewater - A Case Study of the Antidepressant Fluoxetine. Environ. Sci. Technol. 50, 3781–3789. doi:10.1021/acs.est.6b00291

Racamonde, I., Rodil, R., Quintana, J.B., Villaverde-de-Sáa, E., Cela, R., 2014. Determination of benzodiazepines, related pharmaceuticals and metabolites in water by solid-phase extraction and liquid-chromatography-tandem mass spectrometry. J. Chromatogr. A 1352, 69–79. doi:10.1016/j.chroma.2014.05.064

Riva, F., Zuccato, E., Castiglioni, S., 2015. Prioritization and analysis of pharmaceuticals for human use contaminating the aquatic ecosystem in Italy. J. Pharm. Biomed. Anal. 106, 71–78. doi:10.1016/j.jpba.2014.10.003

Scheurer, M., Storck, F.R., Graf, C., Brauch, H.J., Ruck, W., Lev, O., Lange, F.T., 2011. Correlation of six anthropogenic markers in wastewater, surface water, bank filtrate, and soil aquifer treatment. J Env. Monit. 13, 966–973.

Smith-Kielland, A., Skuterud, B., Olsen, K.M., Mørland, J., 2001. Urinary excretion of diazepam metabolites in healthy volunteers and drug users. Scand J Clin Lab Invest 61, 237–246.

Suzuki, T., Kosugi, Y., Hosaka, M., Nishimura, T., Nakae, D., 2014. Occurrence and behavior of the chiral anti-inflammatory drug naproxen in an aquatic environment. Env. Toxicol Chem. 33, 2671–2678.

Terzic, S., Senta, I., Ahel, M., 2010. Illicit drugs in wastewater of the city of Zagreb (Croatia) - Estimation of drug abuse in a transition country. Environ. Pollut. 158, 2686–2693. doi:10.1016/j.envpol.2010.04.020

Verlicchi, P., Al Aukidy, M., Jelic, A., Petrovi??, M., Barcel??, D., 2014. Comparison of measured and predicted concentrations of selected pharmaceuticals in wastewater and surface water: A case study of a catchment area in the Po Valley (Italy). Sci. Total Environ. 470–471, 844–854. doi:10.1016/j.scitotenv.2013.10.026

Yang, S., Cha, J., Carlson, K., 2005. Simultaneous extraction and analysis of 11 tetracycline and sulfonamide antibiotics in influent and effluent domestic wastewater by solid-phase extraction and liquid chromatography-electrospray ionization tandem mass spectrometry. J. Chromatogr. A 1097, 40–53. doi:10.1016/j.chroma.2005.08.027

Table S4. Literature summary of population biomarkers

Class/ *Family*	**Parent Compound/** *Metabolite*	**Acronym**	**Excretion rate (%)**	**Stability in urine**	**Stability in WW**	**Detected in IWW**	**Reference**
Artificial Sweeteners	**Acesulfame**	ACE	100% in urine		Stable	✓	(Lai et al., 2015; O'Brien et al., 2014; Ordóñez et al., 2012; Tran et al.,
	Alitame	ALI	7-22% in faeces				
	Aspartame	ASP			70-80% loss over 24 hours in WW		(Tran et al., 2013)
	Cyclamate	CYC	100% in urine		Stable	✓	(Ordóñez et al., 2012; Tran et al., 2013)
	Neotame	NEO	< 2% un urine				
	N -[*N* -(3,3-dimethylbutyl)-L-*alpha* -aspartyl]-L-phenylalanine						
	Neohesperidin dihydrochalcone	NHDC			90% loss in WW at 4°C in 24 hours		(Tran et al., 2013)
	Saccharin	SAC	100% in urine		Stable	✓	(Ordóñez et al., 2012; Tran et al., 2013)
	Sucralose	SUC	78 - 92% in faeces, 8 -22% in urine as sucrolose or		Stable	✓	(Ordóñez et al., 2012; Tran et al., 2013)
Endogenous Compounds	**Creatine**	CR			100% loss over 24 hours	✓	(Thai et al., 2014)
	Creatinine						
	Cholesterol						
	Coprostanol	COP					
	Cortisol				100% loss over 48 hours	✓	(Chen et al., 2014)
	Androstenedione				100% loss over 48 hours	✓	(Chen et al., 2014)
	1-aminopropan-2-one	APR			Appears to increase in wastewater, further investigation required		
	Serotonin						
	5-hydroxyindoleacetic acid	5-HIAA			Stable	✓	(Chen et al., 2014)
	Ammonia						
	Ammonium	NH_4^+				✓	(Been et al., 2014)
	α-fetoprotein						
	Isoprostanes						
	Eicosanoids						

References

Been, F., Rossi, L., Ort, C., Rudaz, S., Delémont, O., Esseiva, P., 2014. Population normalization with ammonium in wastewater-based epidemiology: Application to illicit drug monitoring. Environ. Sci. Technol. 48, 8162–8169. doi:10.1021/es5008388

Chen, C., Kostakis, C., Gerber, J.P., Tscharke, B.J., Irvine, R.J., White, J.M., 2014. Towards finding a population biomarker for wastewater epidemiology studies. Sci. Total Environ. 487, 621–628. doi:10.1016/j.scitotenv.2013.11.075

Lai, F.Y., Anuj, S., Bruno, R., Carter, S., Gartner, C., Hall, W., Kirkbride, K.P., Mueller, J.F., O'Brien, J.W., Prichard, J., Thai, P.K., Ort, C., 2015. Systematic and day-to-day effects of chemical-derived population estimates on wastewater-based drug epidemiology. Environ. Sci. Technol. 49, 999–1008. doi:10.1021/es503474d

O'Brien, J.W., Thai, P.K., Eaglesham, G., Ort, C., Scheidegger, A., Carter, S., Lai, F.Y., Mueller, J.F., 2014. A Model to Estimate the Population Contributing to the Wastewater Using Samples Collected on Census Day. Environ. Sci. Technol. 48, 517–525. doi:10.1021/es403251g

Ordóñez, E.Y., Quintana, J.B., Rodil, R., Cela, R., 2012. Determination of artificial sweeteners in water samples by solid-phase extraction and liquid chromatography-tandem mass spectrometry. J. Chromatogr. A 1256, 197–205. doi:10.1016/j.chroma.2012.07.073

Thai, P.K., O'Brien, J., Jiang, G., Gernjak, W., Yuan, Z., Eaglesham, G., Mueller, J.F., 2014. Degradability of creatinine under sewer conditions affects its potential to be used as biomarker in sewage epidemiology. Water Res. 55, 272–279. doi:10.1016/j.watres.2014.02.035

Tran, N.H., Hu, J., Ong, S.L., 2013. Simultaneous determination of PPCPs, EDCs, and artificial sweeteners in environmental water samples using a single-step SPE coupled with HPLC-MS/MS and isotope dilution. Talanta 113, 82–92. doi:10.1016/j.talanta.2013.03.072