

## SUPPORTING INFORMATION

### RAPID AND COST-EFFECTIVE MULTIRESIDUE ANALYSIS OF PHARMACEUTICALS, PERSONAL CARE PRODUCTS AND ANTIFOULING BOOSTER BIOCIDES IN MARINE SEDIMENTS USING MATRIX SOLID PHASE DISPERSION

Karina Lotz Soares<sup>a,b,c</sup>, Adrià Sunyer-Caldú<sup>d</sup>, Sergiane Caldas Barbosa<sup>a,c</sup>, Ednei Gilberto Primel<sup>a,c</sup>, Gilberto Fillmann<sup>a,b,c</sup>, M. Silvia Diaz Cruz<sup>d\*</sup>

<sup>a</sup>*Instituto de Oceanografia, Universidade Federal do Rio Grande (IO -FURG). Av. Itália s/n, Campus Carreiros, C.P. 474, 96201-900, Rio Grande, RS, Brazil.* <sup>b</sup>*PPG em Oceanologia, Universidade Federal do Rio Grande (PPGO-FURG). Av. Itália s/n, Campus Carreiros, 96203-900, Rio Grande, RS, Brazil.* <sup>c</sup>*PPG em Química Tecnológica e Ambiental, Universidade Federal do Rio Grande (PPGQTA-FURG). Av. Itália s/n, Campus Carreiros, 96203-900, Rio Grande, RS, Brazil.* <sup>d</sup>*Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA), Severo Ochoa Excellence Center. Consejo Superior de Investigaciones Científicas (CSIC), Jordi Girona 18 - 26, 08034 Barcelona, Spain.*

#### **Content:**

Table 1S: Analyte name, respective acronym, class, Log Kow (octanol-water partition constant), solubility in water at 25 °C (S) (from [ChemSpider](#); [DrugBank](#); [Pubchem](#)).

Figure 1S: Total ion chromatogram of the target compounds monitored in positive ionization mode (ESI +).

Figure 2S: Total chromatogram of the target compounds monitored in negative ionization mode (ESI -).

TABLE 1S

	Analyte	Acronym	Class	Log Kow	S (mg mL <sup>-1</sup> )	Corresponding IS
UV filters	2-hydroxy-4-methoxybenzophenone	BP3	Benzophenone	3.79	0.128	BP3-d5
	2,4-dihydroxybenzophenone	BP1	Benzophenone	3.17	0.39	BP3-d5
	2,2',4,4'-tetrahydroxybenzophenone	BP2	Benzophenone	2.78	0.09842	BP3-d5
	5-benzoyl-4-hydroxy-2-methoxybenzene sulfonic acid	BP4	Benzophenone	0.39	0.214	Gemfibrozil-d6
	4-hydroxybenzophenone	4HB	Benzophenone	3.82	N.f	BP3-d5
	4,4'-dihydroxybenzophenone	4DHB	Benzophenone	3.02	0.41	BP3-d5
	2,2'-dihydroxy-4-methoxybenzophenone	DHMB	Benzophenone	2.55	0.60	BP3-d5
	1-(4-tert-butylphenyl)-3-(4- methoxyphenyl)propane-1,3-dione	AVO	Benzophenone	N.f	N.f	BP3-d5
UV filters	3-(4-methylbenzilidene)camphor	4MBC	Camphor derivative	4.50	0.00015	4MBC-d4
	2-ethylhexyltrans-4-methoxycinnamate	EHMC	Cinnamate derivative	4.95	0.00510	4MBC-d4
	ethyl-4- aminobenzoate	EtPABA	<i>p</i> -aminobenzoic acid derivatives	1.86	131	4MBC-d4
	1,2,3-benzotriazole	BZT	Benzotriazoles	1.23	20	BZT-d4
	4-methyl-1H-benzotriazole	MeBZT	Benzotriazoles	1.89	5	BZT-d4
	5,6-dimethyl-1H-benzotriazole monohydrate	DMBZT	Benzotriazoles	2.06	N.f	BZT-d4
	2-(2-benzotriazolyl- <i>p</i> -cresol	UVP	Benzotriazole derivates	3.24	0.01359	BZT-d4
						BePB-d4

	Analyte	Acronym	Class	Log Kow	S (mg mL <sup>-1</sup> )	Corresponding IS
Parabens	benzyl-4-hydroxybenzoate	BePB	Parabens	N.f	N.f	
	butyl-4-hydroxybenzoate	BuPB	Parabens	N.f	N.f	BePB-d4
	propyl-4-hydroxybenzoate	PrBP	Parabens	N.f	N.f	BePB-d4
	methyl-4-hydroxybenzoate	MePB	Parabens	N.f	N.f	BePB-d4
Pharmaceuticals	9-fluoro-5-methyl-1-oxo-1,5,6,7-tetrahydropyrido[3,2,1-ij]quinoline-2-carboxylic aci	FLU	Fluoroquinolones	N.f	2.19	Flumequine-13C
	9-fluoro-3-methyl-10(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	ofloxacin	Fluoroquinolones	1.41	0.1	Sulfametazine-d4
	1-cyclopropyl-6-fluoro-4-oxo-7-piperazin-1-ylquinoline-3-carboxylic acid	ciprofloxacin	Fluoroquinolones	N.f	N.f	Trimethoprim-d3
	1-ethyl-7-methyl-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid	nalidixic acid	Quinolones	N.f	0.0514	Flumequine-13C
	5-ethyl-8-oxo-5,8-dihydro-[1,3]dioxolo[4,5-g]quinoline-7-carboxylic acid	oxolinic acid	Quinolones	N.f	0.077	Flumequine-13C
Pharmaceuticals	4-oxo-4-[4-(1,3-thiazol-2-ylsulfamoyl)anilino]butanoic acid	succinyl-Sulfatiazole	Sulfonamides	N.f	N.f	Sulfametazine-d4
	4-amino-N-pyrimidin-2-ylbenzenesulfonamide	SDZ	Sulfonamides	N.f	0.202 (at 20 °C)	Sulfametazine-d4
	N-[4-(pyrimidin-2-	acSDZ	Sulfonamides	N.f	>0.046	Sulfametazine-d4

	Analyte	Acronym	Class	Log Kow	S (mg mL <sup>-1</sup> )	Corresponding IS
Pharmaceuticals	4-amino-N-(4-methylpyrimidin-2-yl)benzenesulfonamide	SMR	Sulfonamides	N.f	N.f	Sulfametazine-d4
	N-[4-(4-methylpyrimidin-2-yl)sulfamoyl]phenyl]acetamide	acSMR	Sulfonamides	N.f	0.61 (at 37 °C)	Sulfametazine-d4
	4-amino-N-(6-methoxyimidazo[4,5-b]pyridin-3-yl)benzenesulfonamide	SMZ	Sulfonamides	N.f	N.f	Sulfametazine-d4
	N-[4-[(4,6-dimethylimidazo[4,5-b]pyridin-2-yl)sulfamoyl]phenyl]acetamide	acSMZ	Sulfonamides	N.f	N.f	Sulfametazine-d4
	4-amino-N-(5-methyl-1,2-oxazol-3-yl)benzenesulfonamide	SMX	Sulfonamides	N.f	0.268	Sulfametazine-d4
	4-acetylamino-N-(5-methyl-3-isoxazolyl)benzenesulfonamide	acSMX	Sulfonamides	N.f	N.f	Sulfametazine-d4
	4-amino-N-(6-methoxyimidazo[4,5-b]pyridin-3-yl)benzenesulfonamide	SMPZ	Sulfonamides	1.68	0.0075	Sulfametazine-d4
	4-amino-N-pyridin-2-ylbenzenesulfonamide	SPY	Sulfonamides	0.05	0.373	Sulfametazine-d4
Pharmaceuticals	N-[4-(pyridine-2-yl)sulfamoyl]phenyl]acetamide	acSPY	Sulfonamides	N.f	N.f	Sulfametazine-d4
	4-amino-N-quinoxalin-2-ylbenzenesulfonamide	SQX	Sulfonamides	N.f	0.343	Sulfametazine-d4
	4-amino-N-(1,3-thiazol-2-yl)benzenesulfonamide	STZ	Sulfonamides	0.91	0.4	Sulfametazine-d4
	4-amino-N-(2,6-dimethylpyrimidin-4-yl)benzenesulfonamide	sulfisomidin	Sulfonamides	N.f	14	Sulfametazine-d4

Analyte	Acronym	Class	Log Kow	S (mg mL <sup>-1</sup> )	Corresponding IS
yl)benzenesulfonamide 4-amino-N-(2,6-dimethoxypyrimidin-4-yl)benzenesulfonamide	SDM	Sulfonamides	0.16	13.3	Sulfametazine-d4
5-[(3,4,5-trimethoxyphenyl)methyl]pyrimidine-2,4-diamine	trimethoprim	Lipid regulators	4.77	0.0278	Trimetoprim-d3
5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoic acid	gemfibrozil	Lipid regulators	N.f	0.0213	Gemfibrozil-d6
2-(2,3-dimethylanilino)benzoic acid	mefenamic acid	Analgesics	N.f	0.02 (at 30 °C)	Mefenamic acid - d3
(2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid	naproxen	Anti-inflammatorys	3.18	0.0159	Naproxen-d3
2-[4-(2-methylpropyl)phenyl]propanoic acid	IBU	Anti-epileptics	2.45	0.0177	IBU-d3
2-(3-benzoylphenyl)propanoic acid	ketoprofen	Analgesic	N.f	N.f	BP3-d5
diclofenac soduim salt	diclofenac	Anti-depressants	N.f	N.f	Diclofenac-d4
N-(4-hydroxyphenyl)acetamide	acetaminophen	Anti-inflammatorys	-0.39	0.0283	Trimetoprim-d3
benzo[b][1]benzazepine-11-carboxamide	CBZ	Anti-epileptics	-0.07	21.6	Carbamazepine-d10
3-oxa-11-azatetracyclo[10.4.0.02,4.05,10]hexadeca-1(16),5,7,9,12,14-hexaene-11-carboxamide	CBZ-10,11-epoxy	Anti-epileptics	0.28	30 (at 20 °C)	Carbamazepine-d10

	Analyte	Acronym	Class	Log Kow	S (mg mL <sup>-1</sup> )	Corresponding IS
	2-[4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl]acetamide	atenolol	B-blocker	N.f	N.f	Trimethoprim-d3
	3-phenyl-3-[4-trifluoromethyl)phenoxy]propan-1-amine	Nor-FXT	Anti-depressive	N.f	N.f	Trimethoprim-d3
	N-desmethylvenlafaxine	N-desVFX	Anti-depressive	N.f	N.f	Trimethoprim-d3
	2-hydroxybenzoic acid	Salicylic acid	Anti-septic	N.f	N.f	Salicylic acid-d6
biocides	3-(3,4-dichlorophenyl)-1,1-dimethylurea	diuron	Triazines	2.85	36.4	BP3-d5
	2-N-tert-butyl-4-N-cyclopropyl-6-methylsulfanyl-1,3,5-triazine-2,4-diamine	irgarol	Triazines	3.95	7	BZT-d4
Booster	4,5-dichloro-2-n-octyl-3-(2H)-isothiazolin-3-one	DCOIT	Organochlorine	2.85	0.0065	BP3-d5
	N-[dichloro(fluoro)methyl]sulfanyl-N-(dimethylsulfamoyl)aniline	dichlofluanid	Organochlorine	3.70	0.0060	Carbamazepine-d10

FIGURE 1S

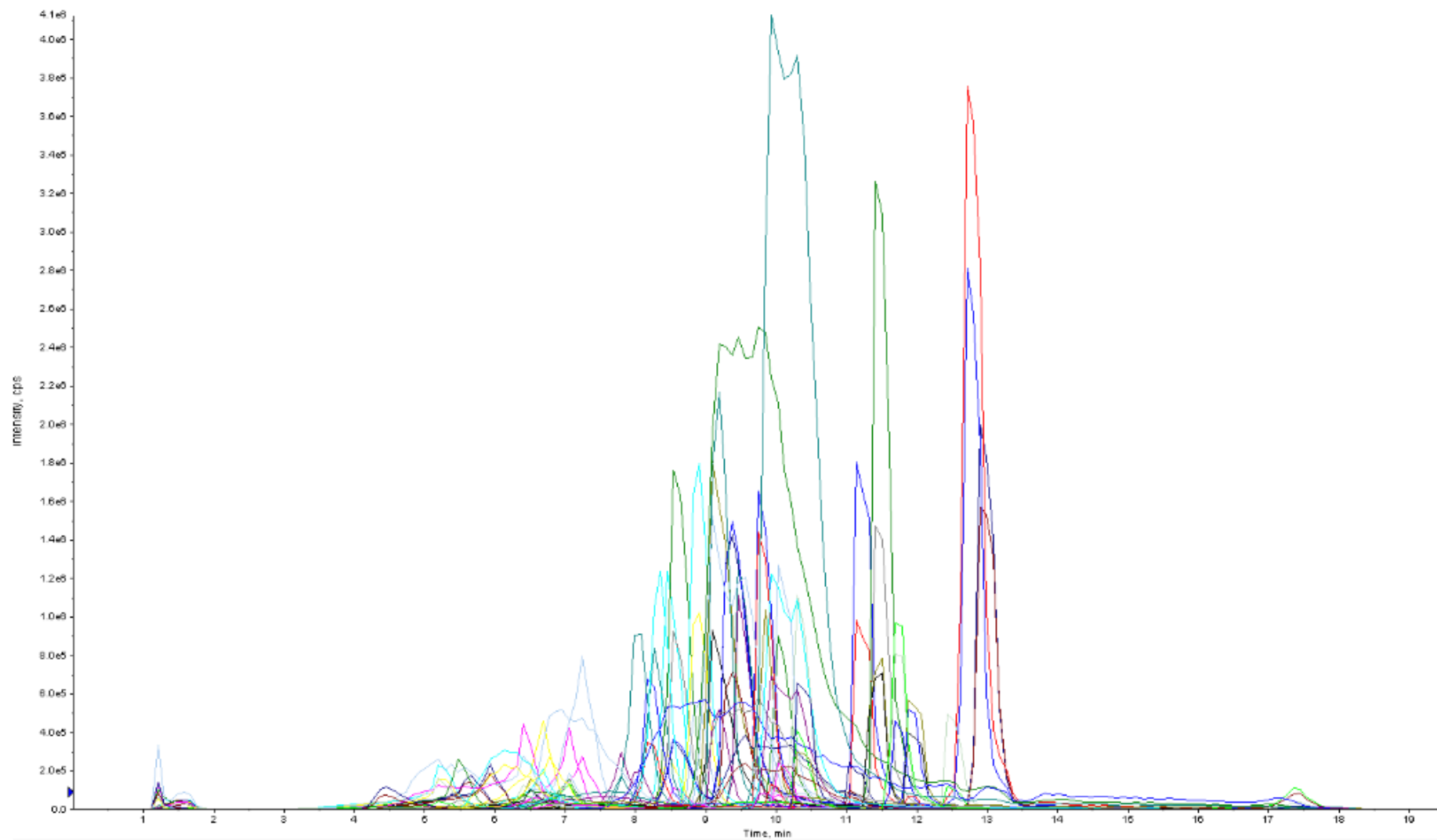


FIGURE 2S

