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Supplementary material (SI)

for

Development of a SPE-UHPLC-MS/MS methodology for the determination of non-steroidal anti-inflammatory and analgesic pharmaceuticals in seawater

Paula Paíga^a, Aleksandar Lolić^{a,b}, Floris Hellebuyck^a, Lúcia H.M.L.M. Santos^{a,c},
Manuela Correia^{a,*}, Cristina Delerue-Matos^a

^aREQUIMTE, Instituto Superior de Engenharia do Porto, Instituto Politécnico do Porto, Rua Dr. António Bernardino de Almeida, 431, 4200-072 Porto, Portugal

^bFaculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11158 Belgrade, Serbia

^cCIIMAR/CIMAR - Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Rua dos Bragas 289, P 4050-123 Porto, Portugal

* Corresponding Author:

Manuela Correia

Tel.: +351 228340500

Fax: +351 228321159

E-mail: mmb@isep.ipp.pt

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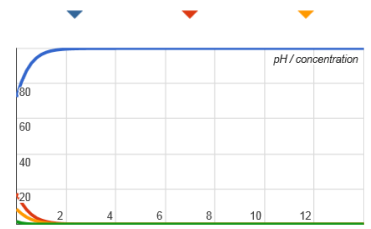
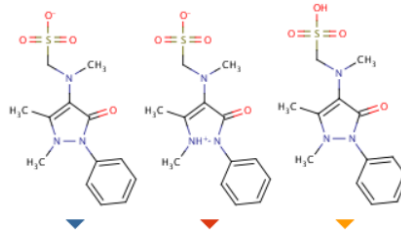
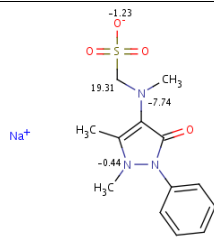
Table S1 – Study of the effect of the SPE sorbents and sample pH in the extraction of the selected pharmaceuticals (n≥2).

SPE cartridge	Pharmaceuticals	Sample pH 2		Without pH adjust		Sample pH 7	
		Recovery (%)	RSD (%)	Recovery (%)	RSD (%)	Recovery (%)	RSD (%)
Strata-X polymeric reversed phase	Dipyron	n.d.		n.d.		n.d.	
	Acetaminophen glucuronide	18.1	9.5	n.d.		n.d.	17
	Acetylsalicylic acid	79.0	3.7	12.3	20	6.30	6.8
	Acetaminophen	70.6	1.2	76.7	5.3	77.2	4.7
	Carboxyibuprofen	65.3	5.6	51.1	32	43.6	69
	Hydroxyibuprofen	82.2	2.1	77.4	13	80.7	15
	<i>p</i> -Aminophenol	n.d.		n.d.		n.d.	
	Ketoprofen	86.5	2.4	72.3	15	76.1	15
	Naproxen	91.9	1.7	81.5	12	84.8	8.5
	Nimesulide	85.9	4.0	89.6	1.0	91.2	0.70
	Diclofenac	76.9	4.9	110	5.2	115	5.1
Ibuprofen	83.8	1.8	106	6.6	103	5.2	
Strata X-AW weak anion exchange	Dipyron	n.d.		36.1	2.8	n.d.	
	Acetaminophen glucuronide	n.d.		66.8	5.5	74.8	14
	Acetylsalicylic acid	n.d.		n.d.		n.d.	
	Acetaminophen	18.1	28	79.7	5.0	70.3	11
	Carboxyibuprofen	7.60	9.9	54.8	5.2	56.0	24
	Hydroxyibuprofen	n.d.		76.6	3.0	78.6	16
	<i>p</i> -Aminophenol	n.d.		n.d.		n.d.	
	Ketoprofen	33.4	7.6	75.0	4.6	74.3	7.8
	Naproxen	36.1	8.7	86.7	3.2	85.8	3.3
	Nimesulide	94.4	6.6	90.8	9.9	92.2	0.58
	Diclofenac	86.6	8.5	103	4.6	108	2.9
Ibuprofen	86.9	4.4	101	0.60	99.7	5.8	
Strata-X-A strong anion exchange	Dipyron	n.d.		n.d.		n.d.	
	Acetaminophen glucuronide	n.d.		n.d.		n.d.	
	Acetylsalicylic acid	61.3	5.1	59.0	7.1	52.8	2.3
	Acetaminophen	112	12	107	5.1	82.9	3.1
	Carboxyibuprofen	51.3	3.2	45.4	5.3	49.3	4.6
	Hydroxyibuprofen	66.0	7.7	65.4	2.9	79.0	0.62
	<i>p</i> -Aminophenol	n.d.		n.d.		n.d.	
	Ketoprofen	58.3	4.2	37.4	1.7	58.1	0.66
	Naproxen	68.2	5.4	38.9	4.1	36.6	14
	Nimesulide	88.7	6.1	63.8	4.9	60.7	4.4
	Diclofenac	85.7	4.7	51.6	9.1	51.7	0.34
Ibuprofen	53.6	4.7	55.2	0.67	65.6	10	
Strata X-C weak cation exchange	Dipyron	n.d.		n.d.		n.d.	
	Acetaminophen glucuronide	46.5	16	n.d.		n.d.	
	Acetylsalicylic acid	33.4	32	13.7	35	26.7	31
	Acetaminophen	76.7	0.012	85.8	1.2	87.5	2.3
	Carboxyibuprofen	48.4	3.2	59.3	4.6	48.7	5.2
	Hydroxyibuprofen	68.0	4.6	83.2	3.9	75.4	5.3
	<i>p</i> -Aminophenol	n.d.		n.d.		n.d.	
	Ketoprofen	87.5	3.1	82.3	4.2	78.1	5.3
	Naproxen	88.3	3.1	87.7	2.7	85.3	2.9
	Nimesulide	92.2	4.5	88.1	5.3	89.6	4.9
	Diclofenac	83.9	3.4	87.6	3.6	85.2	3.1
Ibuprofen	81.1	4.0	81.9	4.3	82.1	3.8	

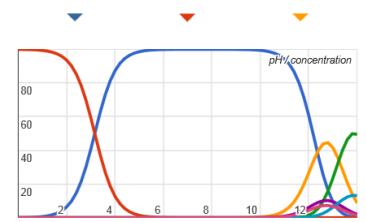
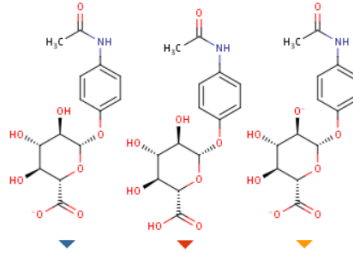
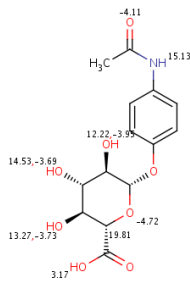
n.d. not detected

Table S2 - Physico-chemical data for the studied pharmaceuticals (adapted from [28]).

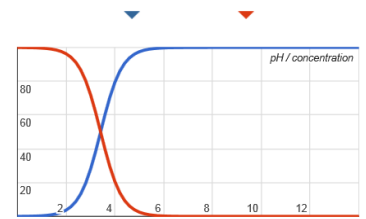
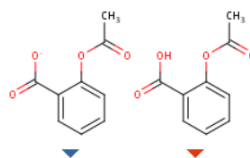
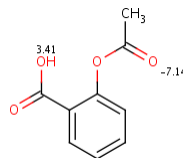
Dipyron
pka=-0.44, -1.23



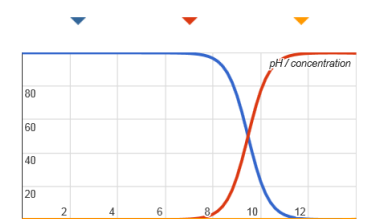
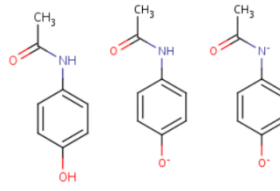
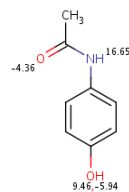
Acetaminophen glucuronide
pka=3.17; 12.22



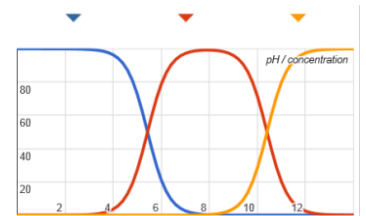
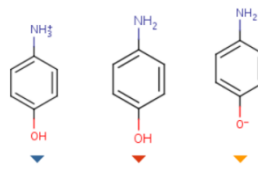
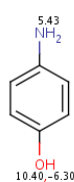
Acetylsalicylic acid
pka=3.41



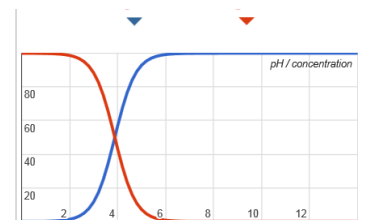
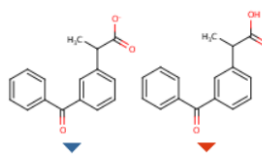
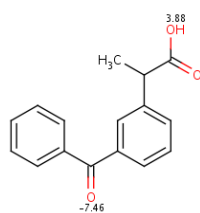
Acetaminophen
pka=9.46



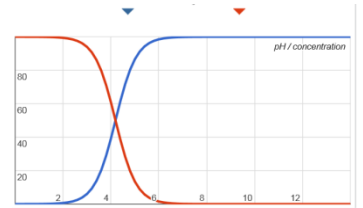
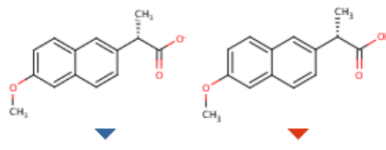
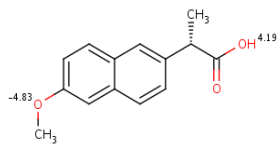
p-Aminophenol
pka=5.43



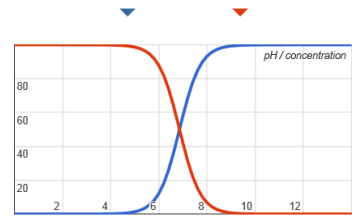
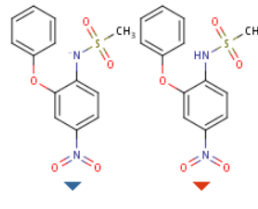
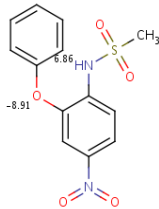
Ketoprofen
pka=3.88



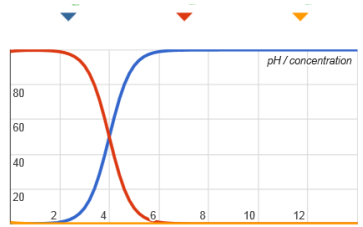
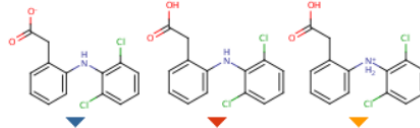
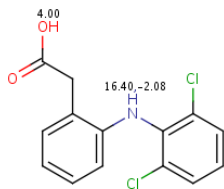
Naproxen
pKa=4.19



Nimesulide
pKa=6.86



Diclofenac
pKa=4.00



Ibuprofen
pKa=4.85

