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Supplementary Material

Analysis of commonly prescribed analgesics using *in-silico* processing of spectroscopic signals: application to surface water and industrial effluents, and comparative study via green and white assessments

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Analysis of Commonly Prescribed Analgesics Using In-silico Processing of Spectral Signals: Application to Surface water and industrial effluents, and Comparative Study Via Green and White Assessments

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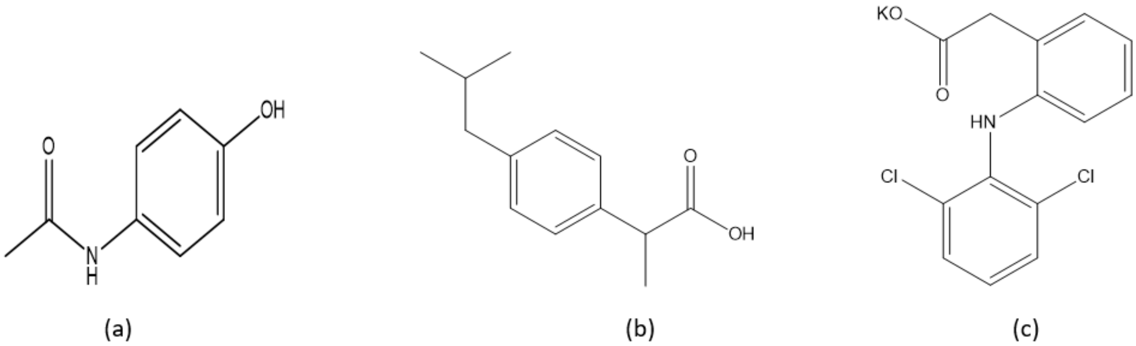

Fig 1SM. chemical structure of (a)PCM, (b) IBU and (c) DCF

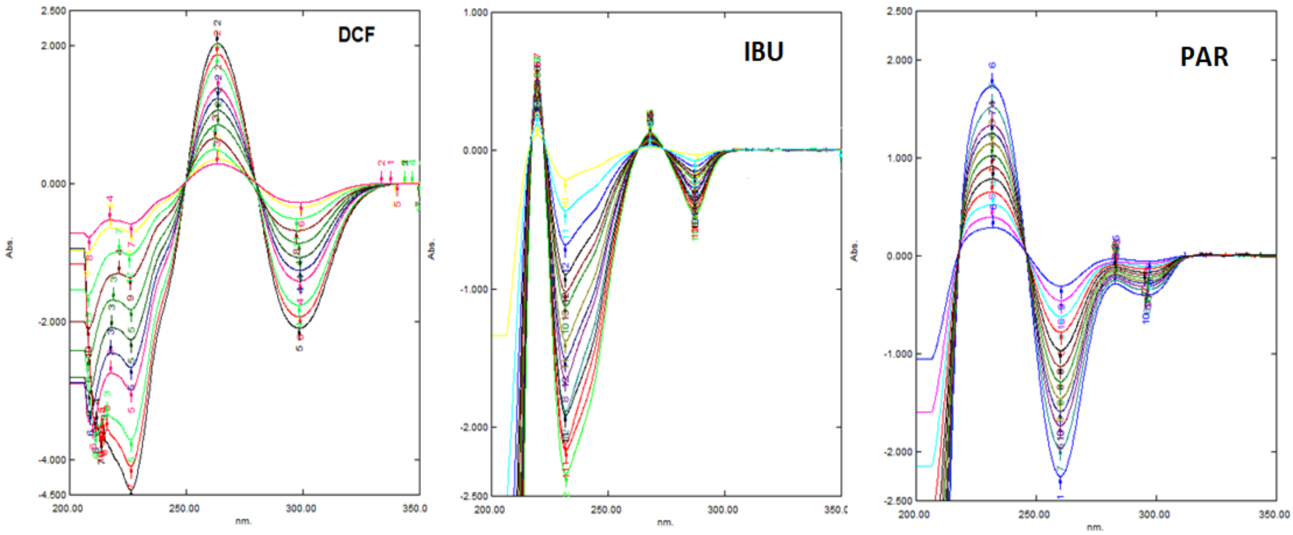

Fig.2SM. D[1] first derivative spectra of DCF (4-30 µg/ml), IBU (1-10 µg/ml) and PAR (2-14 µg/ml).

Table 1SM. The 12 principles of GAC

1	Direct analytical techniques should be applied to avoid sample treatment.
2	Minimal sample size and minimal number of samples are goals
3	In situ measurements should be performed.
4	Integration of analytical processes and operations saves energy and reduces the use of reagents.
5	Automated and miniaturized methods should be selected.
6	Derivatization should be avoided.
7	Generation of a large volume of analytical waste should be avoided and proper management of analytical waste should be provided.
8	Multi-analyte or multi-parameter methods are preferred versus methods using one analyte at a time.
9	The use of energy should be minimized.
10	Reagents obtained from renewable source should be preferred.
11	Toxic reagents should be eliminated or replaced.
12	The safety of the operator should be increased.

Table 2SM. The calculated penalty points (PPs) and Eco-scales of the reported methods versus the proposed ones.

	Santos et al	Aguilar-Arteaga et al	Weigel et al	Caban et al	Diuzheva et al	Yehia et al	proposed methods
Reagent							
methanol	6	12	12	12	6	18	
ethanol							8
acetonitrile	8				4		
Hexane	8	8	16	8			
ethyl acetate	4	4	8	4	4		
toluene			6	6			6
chloroform					4		
acetone				4			4
Sulfuric acid		2					
Triethylamine			6				
dichloromethane				8			
formic acid					5		
Energy	1	2	2	2	2	1	0
Occupational hazards	3	3	3	3	3	3	3
Waste	8	8	8	8	8	8	8
Total PPs	38	39	61	55	36	30	29
Eco scale	62	61	39	45	64	70	**71**

Table 3SM. AGREE reports for the reported methods versus the proposed ones.

	Santos et al	Aguilar-Arteaga et al	Weigel et al	Caban et al	Diuzheva et al	Yehia et al	Proposed methods
Sample treatment	external sample pre- and treatment and batch analysis - reduced number of steps (0.3)	external sample pre- and treatment and batch analysis - reduced number of steps (0.3)	external sample pre- and treatment and batch analysis (large number of steps) 0.0	external sample pre- and treatment and batch analysis - reduced number of steps (0.3)	external sample pre- and treatment and batch analysis - reduced number of steps (0.3)	external sample pre- and treatment and batch analysis - reduced number of steps (0.3)	external sample pre- and treatment and batch analysis - reduced number of steps (0.3)
Sample size	-0.33090125	-0.429328149	-0.33090125	-0.23247435	0.664961193	-0.23247435	0.323032917
	macroanalysis (1000 mL)	macroanalysis (2000 mL)	macroanalysis (1000 mL)	500 ml	0.9 ml	500 ml	10 ml
in-situ measure	automatic, not miniaturized (0.5)	at-line (0.33)	at-line (0.33)	at-line (0.33)	at-line (0.33)	at-line (0.33)	at-line (0.33)
No. of steps	4 (0.8)	4 (0.8)	7 (0.2)	5 (0.7)	3 (1)	4 (0.8)	3 (1)
Automation and Miniaturization	automatic, not miniaturized (0.5)	automatic, not miniaturized (0.5)	semi-automatic, not miniaturized (0.25)	automatic, not miniaturized (0.5)	semi-automatic, miniaturized (0.75)	automatic, miniaturized (1)	semi-automatic, miniaturized (0.5)
Derivatization	none (1)	none (1)	methyl chloro-methanoate	DIMETRIS, BSTFA	none	none	none
Waste	0.070332732	-0.233955247	-0.074962427	-0.140811037	0.386053598	-0.147223744	0.373282033
	45.5 ml + 60 mg (0.1)	0.2	0.2	0.2	10 ml	535	11
Multianalyte	-0.0517	0.11666545	-0.0517	-0.0517	-0.0517	0.11666545	0.2854
No. of analytes / hr	1 sample (0)	2 samples	1 sample / 14 analyte	1 sample / 8 analyte	1 sample/ 11 analyte	2 sample / 3 analyte	4 sample / 3 analyte
Energy	HPLC - UV- FL (0.5)	HPLC - UV (0.5)	GC-MS (0)	GC-MS (0)	HPLC / MS-MS (0)	SPE/Spectro	Spectro
Bio-based sources	0	0	0	0	0	0	0
Toxic solvents	0.087655371	0.08153694	0.094023602	0.338727686	0.37353808	0.122465765	0.446858646
Threats	0.8	0.8	0.8	0.8	0.6	0.8	0.8
Cost/sample	20 $	20 $	40 $	40 $	45 $	7 $	5 $
LOD (µg/mL)	2.0	1.0	0.2	0.2	3.3	0.4	0.4
Accuracy (R%)	71 to 103 %	94-100 %	74 – 87 %	82 – 107 %	80-102 %	88-114 %	85-97 %
Precision (RSD%)	7.3 %	2.1 %	5.0 %	6.5 %	4.2 %	3.2 %	3.5 %

Table 4SM. Evaluation of White assessment of the proposed methods using RGB-12 algorithms.

RED PRINCIPLES (analytical performance)			R1: Scope of application		R2: LOD and LOQ			R3: Precision			R4: Accuracy		
	Method no.	Method name	Linearity	0-100	LOD	LOQ	0-100	RSD% (repeatability)	RSD% (reproducibility)	0-100	Relative error (%)	Recovery (%)	0-100
	1	AAC	2-10.5, 4-30	90	0.267	0.805	100	0.598	0.830	100	1.77	92.26	80
	2	MCR	3-10.5, 4-30	80	0.353	1.070	80	0.754	1.006	90	2.23	92.68	70
	3	SDS	1-10.5, 4-30	100	0.299	0.906	95	0.863	1.045	80	1.98	94.62	90
	4	CWT	2-10.5, 5-30	80	0.350	1.062	85	1.330	1.581	70	2.17	90.31	60

GREEN PRINCIPLES (green chemistry)			G1: Toxicity of reagents (impact and biodegradation)		G2: Amount of reagents and waste			G3: Consumption of energy and other media	G4: Direct impacts (safety, use of animals and GMOs)			
	Method no.	Method name	Total number of pictograms	0-100	Reagent consumption	Waste production	0-100	1-100	Occupational hazards	Safety of users (0-100)	Use of animals (0 if no, 1 if yes)	Use of GMO (0 if no, 1 if yes)
	1	AAC	8	70	5	15	75	85	3	85	0	0
	2	MCR	8	70	5	15	75	85	3	85	0	0
	3	SDS	8	70	5	15	75	85	3	85	0	0
	4	CWT	8	70	5	15	75	85	3	85	0	0

BLUE PRINCIPLES (practical side)			B1: Cost-efficiency		B2: Time-efficiency		B3: Requirements				B4: Operational simplicity		
	Method no.	Method name	Total cost	0-100	Speed of analysis	0-100	Sample consumption	Sample consumption (0-100)		Other needs: advanced instrument, skills, (0-100)	Miniaturization (0-100)	Integration and automation (0-100)	Portability (0-100)
	1	AAC	very low	90	15 minutes	70	10 ml	70	software/excel	90	90	70	75
	2	MCR	very low	90	15 minutes	70	10 ml	70	Matlab	80	80	70	75
	3	SDS	very low	90	15 minutes	70	10 ml	70	software/excel	90	90	70	75
	4	CWT	very low	90	15 minutes	70	10 ml	70	Matlab	80	80	70	75