



Corrigendum to: A Tutorial on AGREEprep an Analytical Greenness Metric for Sample Preparation[☆]

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The authors have noticed that the parameter assigned in Criterion 3 (Target sustainable, reusable, and renewable materials) during the evaluation of the second method involving SPME was not correct. As a result, the assessment results appearing in Fig. 3 were also not correct. The parameter assigned for this Criterion should have been “Only sustainable and renewable materials are used several times” with a score=1.0, rather than “< 25% of reagents and materials are sustainable or renewable and can only be used once” with a score=0.0. The latter parameter was not correct nor in accordance with a past report published by the same authors (<https://doi.org/10.1016/j.trac.2022.116553>).

The correct versions of Fig. 3 and S3A–S3C are given below and the discussion concerning Scenario 2 in the second evaluated method involving SPME should be as follows:

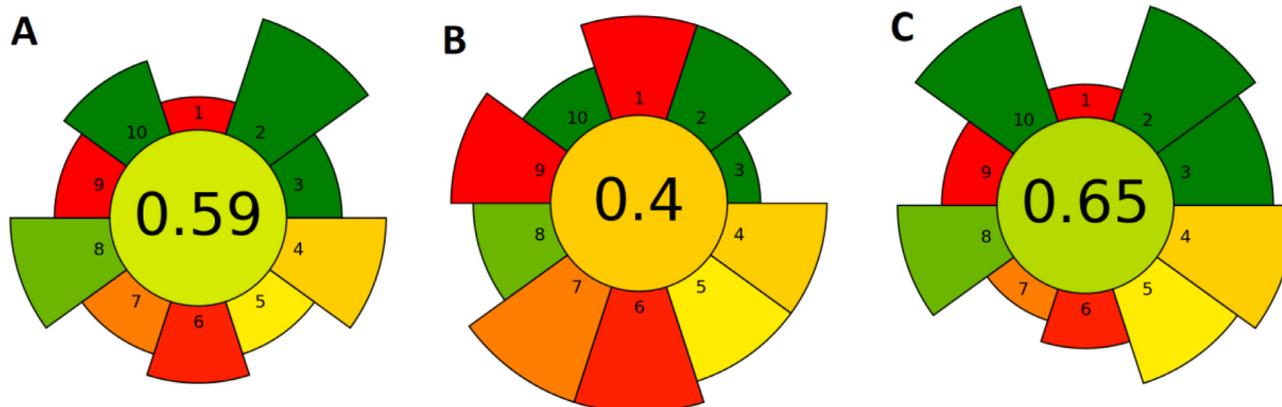


Fig. 3. Comparison of the assessment results on the SPME method used for screening organic pollutants in water [15] after applying the (A) default weights, (B) Scenario 1 weights promoting a simple, automated systems, (C) Scenario 2 weights promoting safe chemicals/materials.

“On the other hand, the final score of Scenario 2 (promoting safe chemicals/materials) was superior to the one obtained when applying the default weights, mainly due to the absence of non-sustainable materials and the green and “safe” features inherent to the SPME technology.”

The authors apologize for any inconvenience caused.

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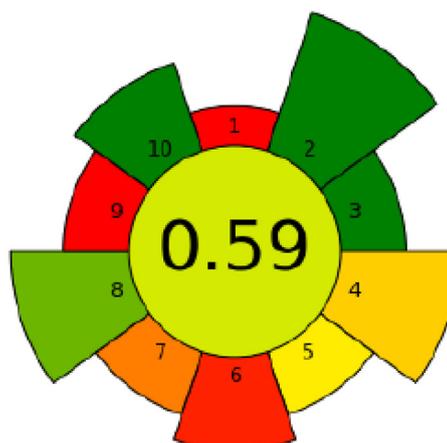
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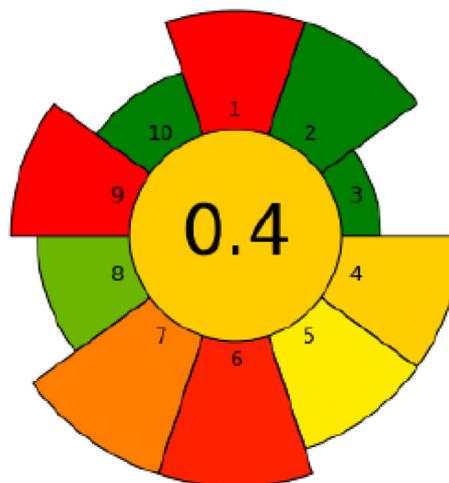
#	Criterion	Score	Weight
1.	Sample preparation placement Sample preparation placement: Ex situ	0.0	1
2.	Hazardous materials Mass [g] or volume [mL] of problematic materials: 0	1.0	5
3.	Sustainability and renewability of materials Only sustainable and renewable materials are used several times	1.0	2
4.	Waste Mass [g] or volume [mL] of waste: 4	0.41	4
5.	Size economy of the sample Mass [g] or volume [mL] of the sample: 4	0.47	2
6.	Sample throughput Hourly sample throughput: 1.3333	0.07	3
7.	Integration and automation No. of sample prep. steps: 2 steps or fewer; degree of automation: Manual systems	0.25	2
8.	Energy consumption Approximate energy consumption per analysis [W]: 22.5	0.79	4
9.	Post-sample preparation configuration for analysis Advanced MS with high energy and/or noble gas consumption: ICP-OES, ICP-MS, etc.	0.0	2
10.	Operator's safety No. of distinct hazards: No hazards or no exposure	1.0	3

Fig. S3A. Evaluation report of the AGREEprep assessment of the method described in Ref [15] (<https://doi.org/10.1021/ac071551b>) using the default weights.

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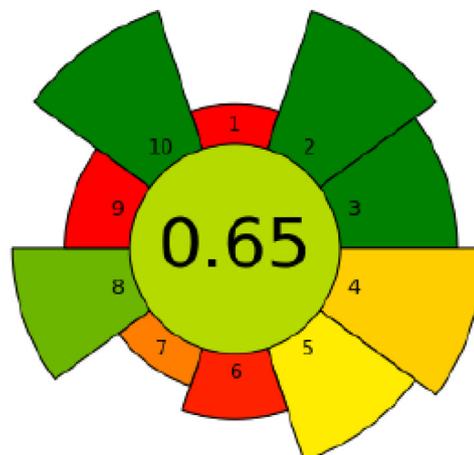
#	Criterion	Score	Weight
1.	Sample preparation placement	0.0	4
	Sample preparation placement: Ex situ		
2.	Hazardous materials	1.0	4
	Mass [g] or volume [mL] of problematic materials: 0		
3.	Sustainability and renewability of materials	1.0	1
	Only sustainable and renewable materials are used several times		
4.	Waste	0.41	4
	Mass [g] or volume [mL] of waste: 4		
5.	Size economy of the sample	0.47	4
	Mass [g] or volume [mL] of the sample: 4		
6.	Sample throughput	0.07	5
	Hourly sample throughput: 1.3333		
7.	Integration and automation	0.25	5
	No. of sample prep. steps: 2 steps or fewer; degree if automation: Manual systems		
8.	Energy consumption	0.79	3
	Approximate energy consumption per analysis [W]: 22.5		
9.	Post-sample preparation configuration for analysis	0.0	4
	Advanced MS with high energy and/or noble gas consumption: ICP-OES, ICP-MS, etc.		
10.	Operator's safety	1.0	2
	No. of distinct hazards: No hazards or no exposure		

Fig. S3B. Evaluation report of the AGREEprep assessment of the method described in Ref [15] (<https://doi.org/10.1021/ac071551b>) using the hypothetical Scenario 1 weights promoting simple and automated methods.

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#	Criterion	Score	Weight
1.	Sample preparation placement Sample preparation placement: Ex situ	0.0	1
2.	Hazardous materials Mass [g] or volume [mL] of problematic materials: 0	1.0	5
3.	Sustainability and renewability of materials Only sustainable and renewable materials are used several times	1.0	4
4.	Waste Mass [g] or volume [mL] of waste: 4	0.41	5
5.	Size economy of the sample Mass [g] or volume [mL] of the sample: 4	0.47	4
6.	Sample throughput Hourly sample throughput: 1.3333	0.07	2
7.	Integration and automation No. of sample prep. steps: 2 steps or fewer; degree if automation: Manual systems	0.25	1
8.	Energy consumption Approximate energy consumption per analysis [W]: 22.5	0.79	4
9.	Post-sample preparation configuration for analysis Advanced MS with high energy and/or noble gas consumption: ICP-OES, ICP-MS, etc.	0.0	2
10.	Operator's safety No. of distinct hazards: No hazards or no exposure	1.0	5

Fig. S3C. Evaluation report of the AGREEprep assessment of the method described in Ref [15] (<https://doi.org/10.1021/ac071551b>) using the hypothetical Scenario 2 weights promoting safe chemicals/materials.