This journal is © The Royal Society of Chemistry 2023

Supplementary Materials for

Development of Diffusive Gradients in Thin-films with Mixed

Binding Gel for in-situ Monitoring of Artificial Sweeteners in

Waters

Hussain Ijaz^{† #}, Jin-Xin Zi^{† #}, Si-Si Liu^{† *}, Qi-Si Cai[†], Sheng-Ming Cheng[†], Zhong-Xi

Zhao[†], Guang-Guo Ying[†], Andy J. Sweetman[‡], Chang-Er Chen[†]*

† Environmental Research Institute/School of Environment, Guangdong Provincial Key

Laboratory of Chemical Pollution and Environmental Safety & MOE Key Laboratory of

Theoretical Chemistry of Environment, South China Normal University, Guangzhou 510006,

China.

[‡] Lancaster Environment Centre, Lancaster University, Lancaster LA1 4YO, U.K.

these authors contributed equally to this work.

* To whom correspondence should be addressed:

CE Chen: changer.chen@m.scnu.edu.cn, +86 20 3931 1529

SS Liu: sisi.liu@m.scnu.edu.cn, +86 20 3931 1582

MS Conditions for Chemical Analysis:

Source temperature: 120 °C; Desolvation gas temperature: 300 °C; Desolvation gas:

800 L/h; Cone gas: 150 L/h; Scan mode: MRM; Ionization: ESI positive; Capillary

voltage: 2.0 kV; Sampling cone: 40 V.

Extraction Procedures for Wastewater Samples from WWTP:

All the water samples were filtered using 0.7 μ m glass fiber filters (GF/F, Whatman) before extraction, and the filtered samples were subsequently spiked with the relevant internal standard before. Final extracts were filtered using a 0.22 μ m membrane filter and stored at -18 °C before analysis.

Chromabonds HR-X SPE cartridges (500 mg, 6 mL) were applied for the extraction of ASs. The SPE cartridges were preconditioned with 6 mL of methanol and 6 mL of Milli-Q water. Then, 500 mL of water samples were adjusted to pH =2 and passed through the cartridges at a flow rate of approximately 10 mL/min. Subsequently, the cartridges were rinsed with 10 mL of Milli-Q water and dried for 2 h under a vacuum. Finally, the SPE cartridges were eluted with methanol (2 × 5 mL). The eluent was evaporated to dryness and re-dissolved with 1 mL methanol.

Table S1 Basic information of selected Artificial Sweeteners.

Compound	CAS Number	Formula	Molecular Weight	pK_a	$Log K_{OW}$
Saccharin, SAC	82385-42-0	C ₇ H ₅ NO ₃ S	182.99	1.31	0.91
Acesulfame, ACE	33665-90-6	C ₄ H ₄ NO ₄ S	162.99	2.00	-1.33
Cyclamate, CYC	139-05-9	$C_6H_{12}NO_3S$	178.05	1.71	-1.61
Sucralose, SUC	56038-13-2	$C_{12}H_{19}Cl_3O_8$	396.01	-3.0/11.8	-1.00

Table S2 Physical and chemical properties parameters of commonly used resins.

		XAD18	XDA1	WAX	MAX	HLB
	Physical Properties					
	Matrix	Macroporous, Crosslinked DVB	Macroporous, crosslinked PDVB	PS/DVB	PS/DVB	PNVP/DVB
	Type	Adsorbent	Adsorbent	Ion exchange	Ion exchange	Adsorbent
	Physical Form	White, opaque, spherical beads	Red brown, spherical particles	White, particles	White or yellowish, particles	White, particles
	Nitrogen BET	-				
Typical Properties	Surface Area	$\sim 700 \text{ m}^2/\text{g}$	$\sim 1100 \text{ m}^2/\text{g}$	$\sim 600 \text{ m}^2/\text{g}$	$\sim 600 \text{ m}^2/\text{g}$	$\sim 600 \text{ m}^2/\text{g}$
	Pore Diameter	~150 Å	~90 Å	~300 Å	~300 Å	~300 Å
	Exchange Intensity	-	-	0.6 meq/g	0.9 meq/g	-
	Particle Size					
	Particle Diameter	$425\pm50~\text{um}$	$750 \pm 50 \text{ um}$	$50 \pm 5 \text{ um}$	$50 \pm 5 \text{ um}$	$40 \pm 5 \text{ um}$
	Variable Coefficient	≤ 1.7%	-	< 5%	< 5%	< 5%
	Particle Density	1.03 g/mL	0.75 g/mL	-	0.3 g/mL	-
Suggested Operating	Maximum Operating Temperature	150°C (302°F)	150°C (302°F)	60°C (140°F)	60°C (140°F)	60°C (140°F)
Conditions	pH Range (Application)	1-14	1-14	1-14	1-14	1-14
	pK_a	-	-	~6	>18	-
	Storage Condition	room temperature	room temperature	room temperature	room temperature	room temperature

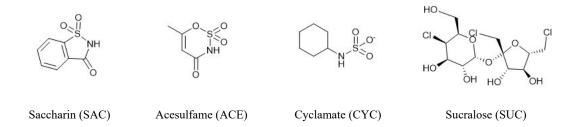


Fig S1. Structures of four ASs investigated in the present study.

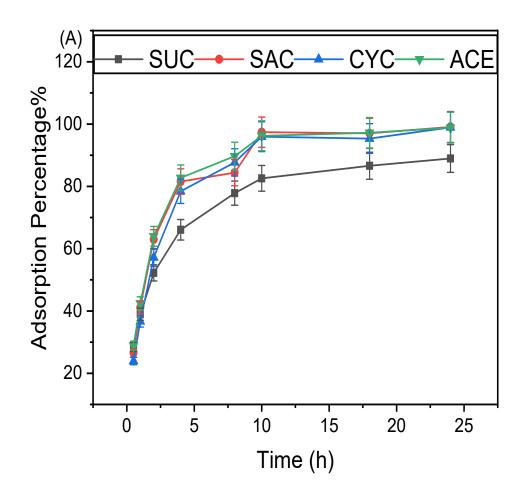


Fig. S2. Plot A: Uptake kinetics of SUC, SAC, CYC, and ACE onto WAX: XDA1 gels over the corresponding time in ASs solutions of 100 μg L⁻¹ 10 mL.

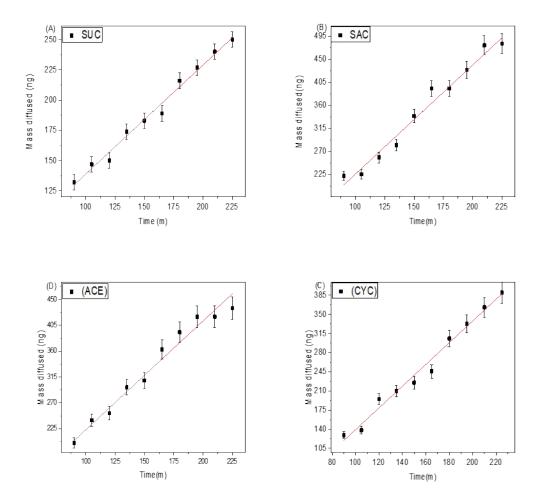


Fig. S3. AS masses diffused through PES (filter membrane) and Agarose (diffusive gel) at different intervals of time at 23°C, and ionic strength of 0.01 M. Error bars was calculated from the standard deviations of three replicates.