Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supplementary Information

1. Method MIB/Geosmin and benzene

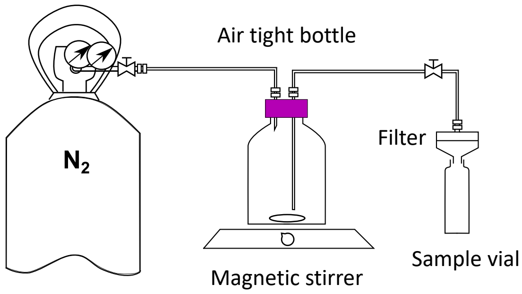


Figure SI 1 : Air-tight setup for benzene adsorption experiments and sampling

Table SI 1 : Analytical methods parameters and validation data

Pollutant	Desorption parameters (TDU-CIS)	GC gradient	Sample extraction	Injection mode	Quantification ions (*m/z*)	Internal standards	LOD (ng/L)
Geosmin and MIB	TDU: 30°C (1 min) rate 720°C/min to 280°C (3 min); CIS: 12°C/min to 280°C (5 min)	50°C (2 min); 10°C/min to 200°C; 25°C/min to 280°C; 280°C (2 min)	10 g NaCl; stir bar placed into the sample (50 mL) at 1200 rpm during 1h	Venting mode	*m/z* 95 for geosmin and *m/z* 112 for MIB	cis-decahydro-1-naphtol	0.8 ng/L for MIB and 0.4 ng/L for geosmin
Benzene	TDU: 20°C (1 min) rate 720°C/min to 280°C (2 min); CIS: 12°C/min to 280°C (5 min)	35°C (5 min); 5°C/min to 70°C, 30°C/min to 220°C, 80°C/min to 280°C (2 min)	Stir bar placed into the gas phase. Sample (50 mL) was stirred at 1750 rpm	Splitless mode	*m/z* 78	d^6-benzene	21 ng/L

Table SI 2 : Parameters obtained during the method development for MIB/Geosmin and benzene analysis

Compounds	LOD (ng/L)	R2	Repeatability at 50 ng/L (%)	Reproducibility (%)	Accuracy (%)

Geosmin	0.8	0.992	5	8	13
MIB	0.4	0.999	3	7	13
Benzene	21	0.998	15	18	15

Stir bar sorptive extraction coupled to GC-MS (SBSE-GC-MS) has been widely used to extract off flavour compounds from water samples.[1-3] Benanou et al. have developed a method with this technique that showed good linearity over the concentration range 5-40 ng/L for MIB/geosmin.[4] The development of this method was inspired by this publication. Method parameters and validation control measurements for all target compounds can be found in Table SI 1 and Table SI 2.

For method validation: A five-point calibration curve was obtained by spiking surface water samples at 1, 5, 10, 50, 100 and 250 $ng \cdot L^{-1}$ of MIB/geosmin. The method limit of detection (LOD) and method limit of quantification (LOQ) were determined as 3.3 and 10 times, respectively, the standard deviation of the y intercept divided by the slope of the calibration curve in the matrix sample. A deuterated benzene internal standard (IS) was used to correct the signal variation of benzene and a homologous compound was used to correct the MIB/geosmin signal. Thus, concentrations of geosmin, MIB and benzene were calculated using the ratio of the target compounds area to that of the labelled IS. In each set of samples, the IS were added to the samples before the extraction step. Repeatability (intra-day precision) was calculated by analysing the same spiked and extracted samples at two different concentrations (50 and 250 $ng \cdot L^{-1}$) on a single workday (n = 5) and was expressed as a relative standard deviation (RSD - %). Reproducibility (inter-day precision) was also evaluated by analysing spiked and extracted samples at two different concentrations (50 and 250 $ng \cdot L^{-1}$) for two days (n = 5 each days) and prepared daily. Accuracy was determined by the relative error (%) and precision values were calculated as the RSD (%).

2. Correlations between iodine number and carbon characteristics

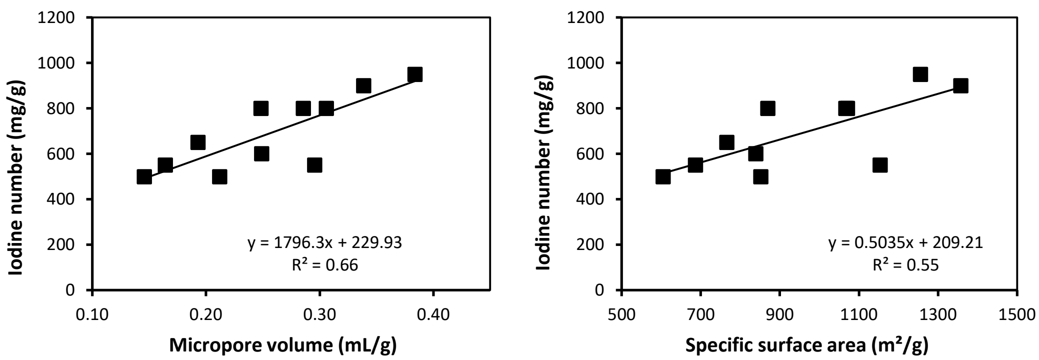


Figure SI 2: Iodine number as a function of micropore volume and specific surface area

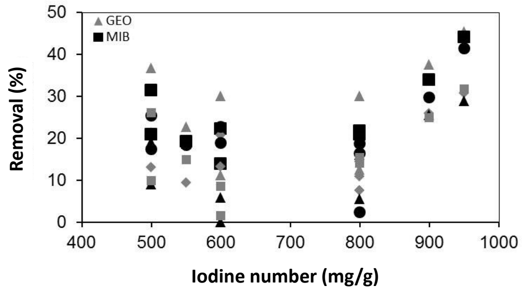


Figure SI 3: Removal of MIB and geosmin as a function of iodine number

3. Performance data of the tested PACs in different water types

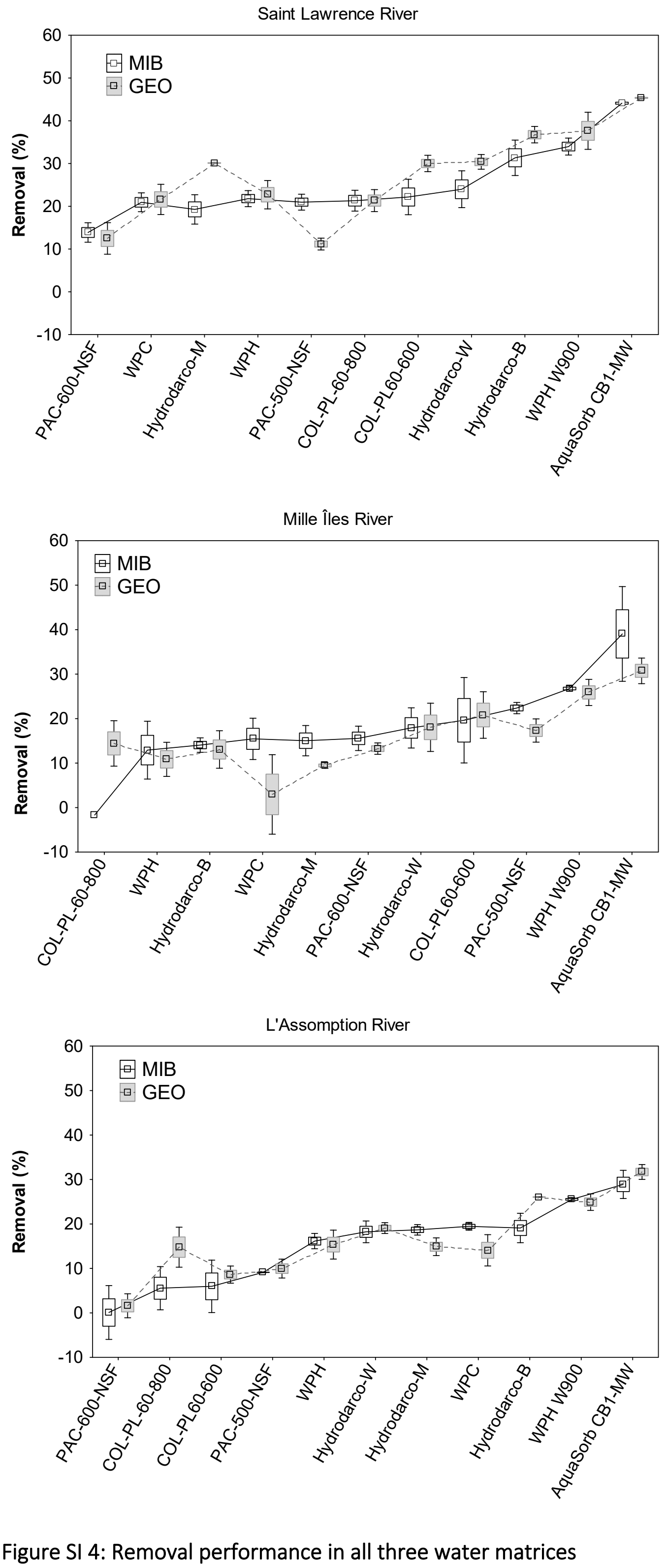


Figure SI 4: Removal performance in all three water matrices

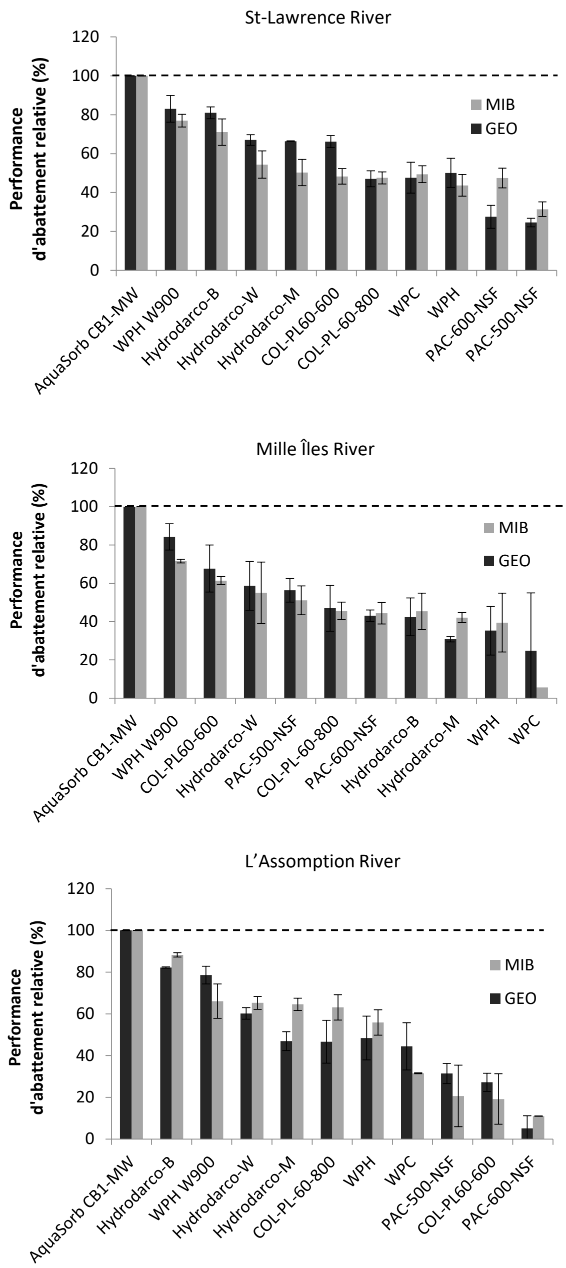


Figure SI 5: Relative removal performance of MIB and geosmin in water from the St-Lawrence and Mille Îles River

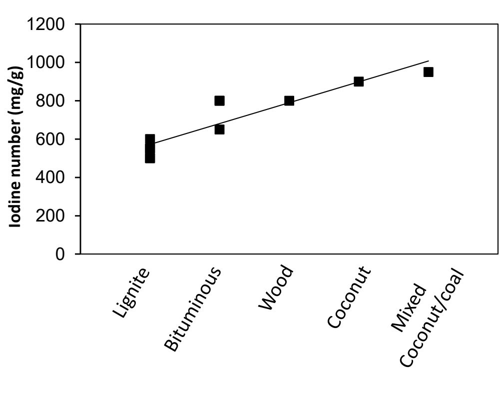


Figure SI 6: Iodine numbers of PAC with different base material.

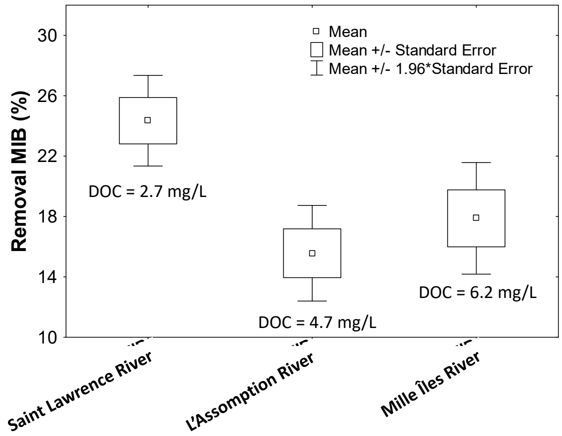


Figure SI 7: Removal of MIB in three tested water matrices

4. Carbon characteristics

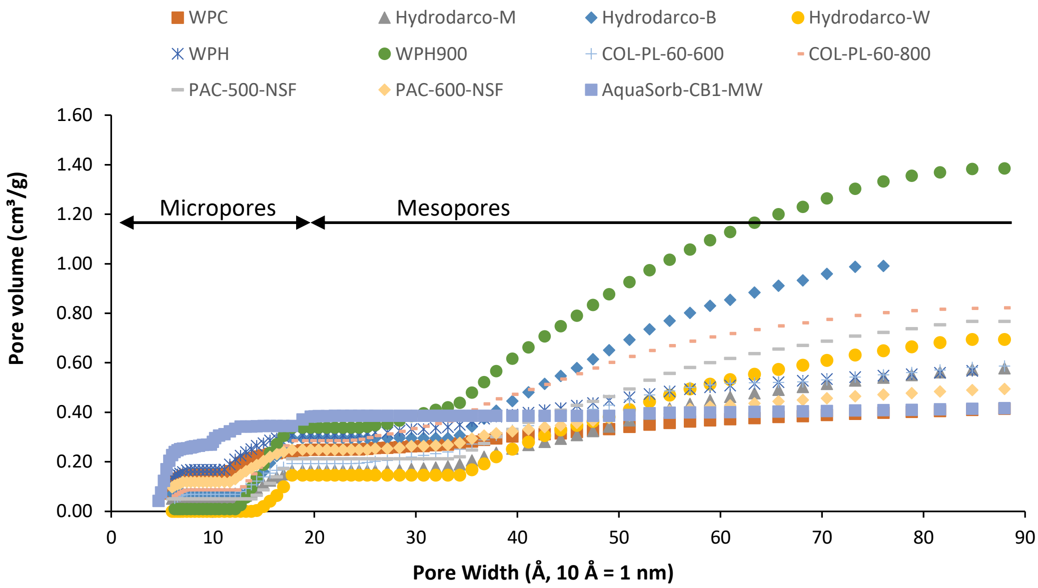
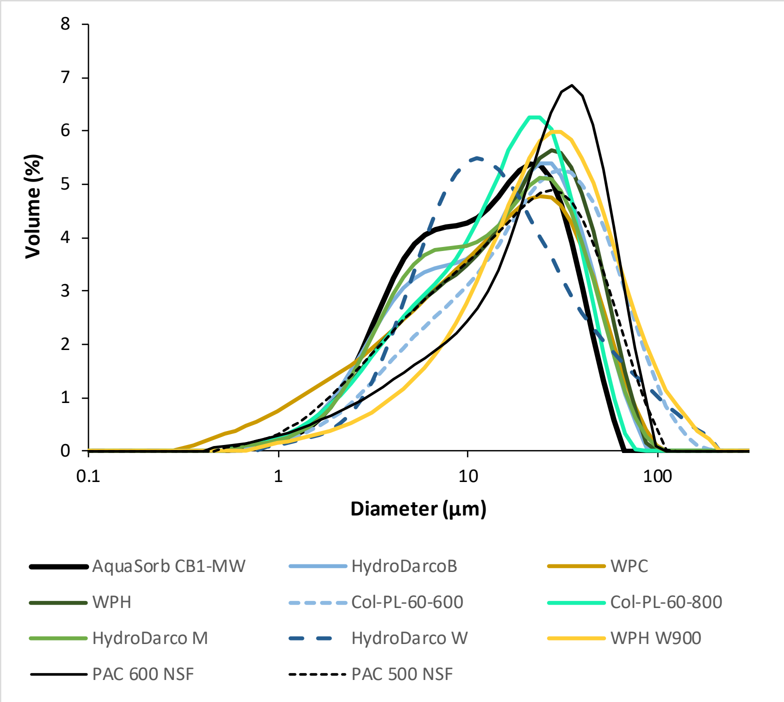


Figure SI 8: Pore size distributions of all tested carbons



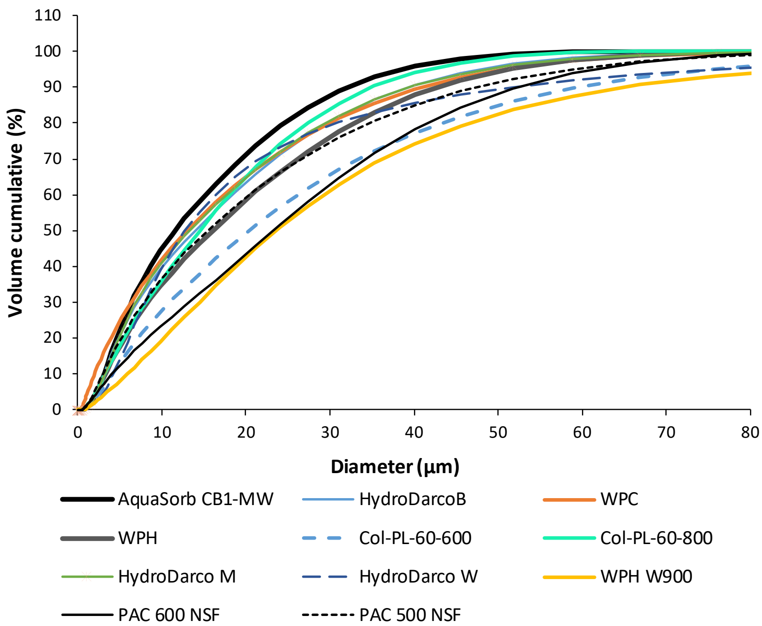


Figure SI 9: Particle size distributions of PACs as (a) frequency distribution and (b) cumulative curve

Table SI 3: General linear models tested

Model	Predictors	Predictor type	Levels	P-values	R^2	Adjusted R^2
1	Micropore Vol Uniformity Coeff D50 Matrix Pollutant	Continuous Continuous Continuous Categorical Categorical	- - - 3 2	0.003 0.003 < 0.001 < 0.001 0.860	0.425	0.367
2	Micropore Vol Uniformity Coeff Matrix D50	Continuous Continuous Categorical Continuous	- - 3 -	0.003 0.002 < 0.001 0.084	0.425	0.377
3	Micropore Vol Uniformity Coeff Matrix	Continuous Continuous Categorical	- - 3	0.005 < 0.001 < 0.001	0.395	0.355
4	Micropore Vol Uniformity Coeff Total LMW NOM	Continuous Continuous Continuous	- - -	0.006 0.003 < 0.001	0.355	0.324
5	Micropore Vol Uniformity Coeff DOC	Continuous Continuous Continuous	- - -	0.008 0.004 0.004	0.300	0.267
6	Micropore Vol Uniformity Coeff UVA254	Continuous Continuous Continuous	- - -	0.008 0.004 0.002	0.310	0.277
7	Micropore Vol Uniformity Coeff Matrix Micropore Vol x Uniformity Coeff Micropore Vol x Matrix Uniformity Coeff x Matrix	Continuous Continuous Categorical	- - 3	0.019 0.138 0.511 0.045 0.746 0.770	0.448	0.359
8	Micropore Vol Uniformity Coeff Matrix Micropore Vol x Uniformity Coeff	Continuous Continuous Continuous	- - -	0.017 0.129 < 0.001 0.040	0.437	0.390

References

1. N. Ochiai, K. Sasamoto, M. Takino, S. Yamashita, S. Daishima, A. Heiden and A. Hoffman, *Determination of trace amounts of off-flavor compounds in drinking water by stir bar sorptive extraction and thermal desorption GC-MS, Analyst*, 2001, **126**, 1652-1657.
2. S. Nakamura, N. Nakamura and S. Ito, *Determination of 2-methylisoborneol and geosmin in water by gas chromatography-mass spectrometry using stir bar sorptive extraction, Journal of Separation Science*, 2001, **24**, 674-677.
3. J. D. Carmi, I. Olivares, P. Grossi and F. M. Lancas, *Refrigerated Sorptive Extraction: Determination of BTEX in Water Samples, Journal of Chromatographic Science*, 2009, **47**, 812-816.
4. D. Benanou, F. Acobas and M.-R. de Roubin, *Optimization of stir bar sorptive extraction applied to the determination of odorous compounds in drinking water, Water Science and Technology*, 2004, **49**, 161-170.