

# Supplementary Information

## $^1\text{H}$ qNMR and Chemometric Analyses of Urban Wastewater

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Compounds identified in untreated and treated wastewater samples

Two-dimensional (2D) NMR experiments were acquired using the standard spectrometer library pulse sequences.  $^1\text{H}$ - $^1\text{H}$  COSY experiments were obtained with spectral width of 18,028.1 Hz in both dimensions;  $4\text{k} \times 256$  data matrix; 48 scans *per* t1 increment and relaxation delay of 1.0 s. One-bond  $^1\text{H}$ - $^{13}\text{C}$  HSQC experiments were acquired

with an evolution delay of 1.7 ms for an average  $^1J(\text{C},\text{H})$  of 145 Hz;  $4\text{k} \times 256$  data matrix; 96 scans *per* t1 increment; spectral widths of 18,028.1 Hz in f2 and 36,057.7 Hz in f1 and relaxation delay of 1.0 s. Long-range  $^1\text{H}$ - $^{13}\text{C}$  HMBC experiments were recorded with an evolution delay of 50.0 ms for  $^{LR}J(\text{C},\text{H})$  of 10 Hz;  $4\text{k} \times 256$  data matrix; 160 scans *per* t1 increment; spectral width 18,028.8 Hz in f2 and 14,529.3 Hz in f1 and relaxation delay of 1.0 s.

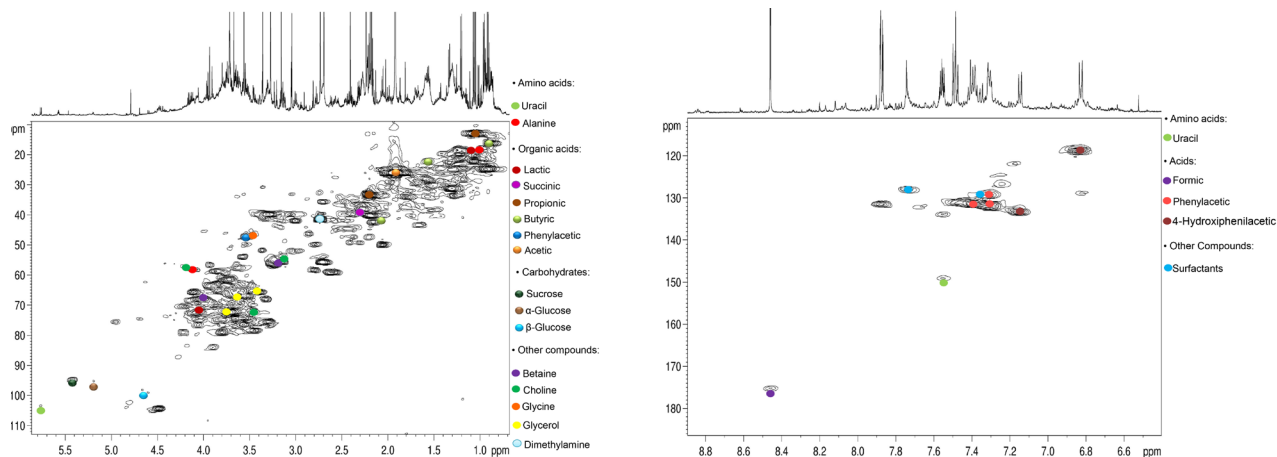
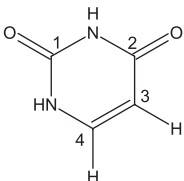
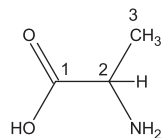
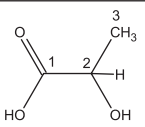
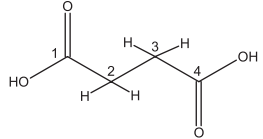
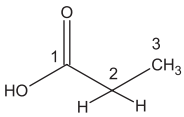
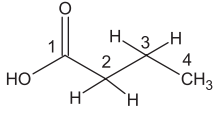
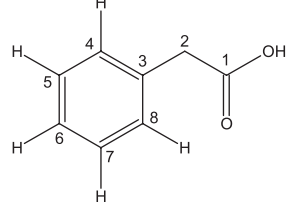
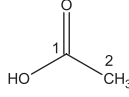
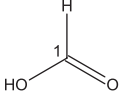
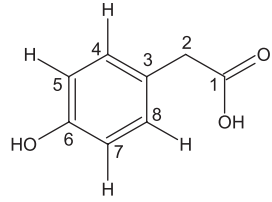


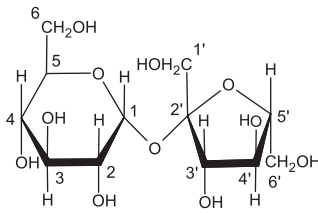
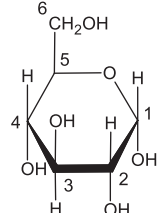
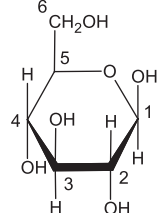
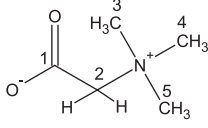
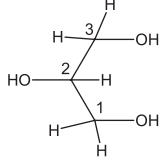
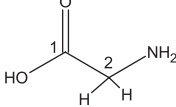
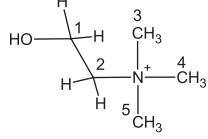
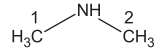
Figure S1. Expansions showing  $^1\text{H}$ - $^{13}\text{C}$  NMR direct correlations of the organic compounds from wastewater samples.

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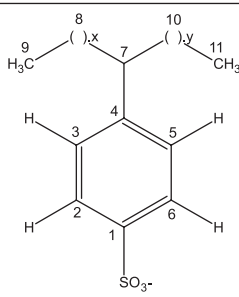
**Table S1.** Compounds identified in untreated and treated wastewater samples from STP of São Carlos-SP, Brazil

Structure	Structure position	$\delta$ <sup>1</sup> H (multiplicity, <sup>a</sup> J in Hz)	HSQC ( $\delta$ <sup>13</sup> C)	
Amino acid				
Uracil		3 4	5.76 (d, 7.40) 7.55 (m)	103.4 148.8
Alanine		2 3	4.12 (q, 6.90) 1.20 (d, 6.90)	57.5 21.1
Organic acid				
Lactic		2 3	4.06 (q, 7.30) 1.33 (d, 7.30)	71.1 21.1
Succinic		2;3	2.41 (m)	37.5
Propionic		2 3	2.17 (q, 7.41) 1.06 (t, 7.41)	33.4 13.0
Butiric		2 3 4	2.16 (t, 7.41) 1.56 (sex) 0.90 (t, 7.41)	42.1 21.9 16.1
Phenylacetic		2 4;6;8 5;7 1	3.53 (s) 7.31 (m) 7.38 (m) –	47.2 129.1; 131.5 131.4
Acetic		2	1.92 (s)	26.0
Formic		1	8.46 (s)	173.5
4-Hydroxyphenylacetic		4;8 5;7	7.15 (d, 8.53) 6.83 (d, 8.53)	133.4 119.0

**Table S1.** Compounds identified in untreated and treated wastewater samples from STP of São Carlos-SP, Brazil (cont.)

Structure	Structure position	$\delta^1\text{H}$ (multiplicity, <sup>a</sup> <i>J</i> in Hz)	HSQC ( $\delta^{13}\text{C}$ )
Carbohydrate			
 Sucrose	1	5.41 (d, 3.89)	94.9
	2	3.56 (m)	73.9
	3	3.76 (m)	75.2
	4	3.47 (m)	71.9
	5	3.84 (m)	75.1
	6	3.81 (m)	62.9
	1'	3.67 (m)	64.1
	2'	–	104.7
	3'	4.22 (m)	79.1
	4'	4.05 (m)	76.5
5'	3.89 (m)	84.0	
6'	3.82 (m)	65.1	
 $\alpha$ -Glucose	1	5.24 (d, 3.70)	94.7
	2	3.47 (m)	71.8
	3	3.77 (m)	75.0
	4	3.56 (m)	73.8
	5	3.74 (m)	63.1
	6	3.85 (m)	74.9
 $\beta$ -Glucose	1	4.60 (d, 7.90)	99.0
	2	3.30 (m)	75.2
	3	3.74 (m)	63.1
	4	3.44 (m)	78.3
	5	3.47 (m)	71.8
	6	3.92 (m)	63.1
 Glycine betaine	2	3.99 (m)	68.0
	3;4;5	3.26 (s)	54.6
 Glycerol	1	3.52 (m)	66.8
	2	3.80 (m)	71.9
	3	3.62 (m)	66.7
 Glycine	2	3.54 (s)	47.1
 Choline	1	4.06 (m)	58.3
	2	3.48 (m)	71.9
	3;4;5	3.13 (s)	55.6
 Dimethylamine	1;2	2.73 (s)	41.1

**Table S1.** Compounds identified in untreated and treated wastewater samples from STP of São Carlos-SP, Brazil (cont.)

Structure	Structure position	$\delta$ <sup>1</sup> H (multiplicity, <sup>a</sup> <i>J</i> in Hz)	HSQC ( $\delta$ <sup>13</sup> C)	
Carbohydrate				
C <sub>10</sub> , C <sub>11</sub> , C <sub>12</sub> and C <sub>13</sub> 4-LAS surfactants		2;6	7.73 (m)	128.0
		3;5	7.40 (m)	131.3

<sup>a</sup>s: singlet; d: doublet; t: triplet; q: quadruplet; sex: sextet; m: multiplet.