

## Supporting Information

### **Occurrence of N-nitrosamines and their precursors in Spanish drinking water treatment plants and distribution systems**

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**Table S1:** Water quality parameters measured during sampling campaign 1 (January 2018). IN=sample taken at the inlet of the DWTP, TR=treated water sample before disinfection, F=treated water after disinfection, DIS=sample taken at the distribution system

| DWTP      | conductivity ( $\mu\text{S/cm}$ ) | pH  | N-NO <sub>2</sub> (mgN/L) | N-NO <sub>3</sub> (mgN/L) | Cl <sup>-</sup> (mg/L) | N-NH <sub>4</sub> (mgN/L) | TOC (mg/L) | TN (mg/L) |
|-----------|-----------------------------------|-----|---------------------------|---------------------------|------------------------|---------------------------|------------|-----------|
| DWTP1_IN  | 81                                | 6.7 | <LOQ                      | 0.4                       | 7.7                    | <LOQ                      | 3.2        | 0.7       |
| DWTP1_TR  | 112                               | 7.0 | <LOQ                      | 0.7                       | 11.7                   | <LOQ                      | 1.5        | 0.8       |
| DWTP1_F   | 131                               | 6.0 | <LOQ                      | 0.7                       | 13.8                   | 0.2                       | 1.5        | 1.0       |
| DWTP1_DIS | 167                               | 6.9 | 0.003                     | 0.4                       | 19.8                   | 0.2                       | 1.9        | 0.9       |
| DWTP2_IN  | 200                               | 6.7 | 0.008                     | 0.1                       | 24.6                   | 0.4                       | 4.7        | 1.0       |
| DWTP2_TR  | 213                               | 6.5 | <LOQ                      | 0.2                       | 29.7                   | <LOQ                      | 2.5        | 0.4       |
| DWTP2_F   | 245                               | 6.3 | 0.005                     | 0.2                       | 32.0                   | 0.3                       | 3.4        | 0.7       |
| DWTP2_DIS | 248                               | 6.8 | 0.005                     | 0.2                       | 31.7                   | 0.3                       | 3.3        | 0.8       |
| DWTP4_IN  | 44                                | 6.8 | <LOQ                      | 0.1                       | 3.6                    | <LOQ                      | 3.5        | 0.4       |
| DWTP4_TR  | 68                                | 6.8 | <LOQ                      | 0.1                       | 6.2                    | <LOQ                      | 2.2        | 0.2       |
| DWTP4_F   | 90                                | 7.1 | <LOQ                      | 0.1                       | 8.5                    | 0.3                       | 2.3        | 0.7       |
| DWTP4_DIS | 84                                | 7.5 | <LOQ                      | 0.1                       | 7.2                    | 0.2                       | 2.2        | 0.5       |
| DWTP5_IN  | 98                                | 6.9 | 0.005                     | 0.3                       | 5.8                    | 0.2                       | 3.5        | 0.8       |
| DWTP5_TR  | 138                               | 7.1 | <LOQ                      | 0.3                       | 11.7                   | 0.1                       | 1.4        | 0.5       |
| DWTP5_F   | 167                               | 6.7 | <LOQ                      | 0.3                       | 13.2                   | 0.5                       | 1.2        | 0.7       |
| DWTP5_DIS | 165                               | 7.8 | <LOQ                      | 0.2                       | 13.0                   | 0.3                       | 1.1        | 0.7       |

| DWTP      | conductivity (μS/cm) | pH  | N-NO <sub>2</sub> (mgN/L) | N-NO <sub>3</sub> (mgN/L) | Cl <sup>-</sup> (mg/L) | N-NH <sub>4</sub> (mgN/L) | TOC (mg/L) | TN (mg/L) |
|-----------|----------------------|-----|---------------------------|---------------------------|------------------------|---------------------------|------------|-----------|
| DWTP6_F   | 123                  | 7.0 | <LOQ                      | 0.2                       | 16.3                   | 0.2                       | 1.1        | 0.6       |
| DWTP6_DIS | 126                  | 7.2 | <LOQ                      | 0.2                       | 15.9                   | 0.2                       | 1.0        | 0.5       |
| DWTP7_F   | 107                  | 6.8 | <LOQ                      | 0.1                       | 14.1                   | 0.2                       | 1.9        | 0.5       |
| DWTP7_DIS | 199                  | 6.8 | 0.003                     | 0.2                       | 25.6                   | 0.2                       | 2.2        | 0.6       |
| DWTP8_F   | 121                  | 6.9 | <LOQ                      | 0.2                       | 14.6                   | 0.2                       | 1.7        | 0.7       |
| DWTP8_DIS | 122                  | 7.4 | <LOQ                      | 0.2                       | 14.8                   | 0.2                       | 1.9        | 0.6       |
| DWTP9_F   | 125                  | 7.5 | 0.003                     | 0.20                      | 16.6                   | 0.28                      | 1.8        | 0.7       |
| DWTP11_F  | 187                  | 7.6 | 0.003                     | 0.48                      | 27.6                   | 0.17                      | 3.7        | 1.1       |

LOQ: 0.003 mg N-NO<sub>2</sub>/L, 0.002 mg N-NO<sub>3</sub>/L, 0.025 mg Cl/L, 0.001 mgN-NH<sub>4</sub>/L, 0.05 mg/L TOC, 0.05 mg/L TN, Br<sup>-</sup> was not measured above 0.01mg/L.

**Table S2:** Water quality parameters during sampling campaign 2 (October 2018). IN=sample taken at the inlet of the DWTP, TR=treated water sample before disinfection, F=treated water after disinfection, DIS=sample taken at the distribution system

| DWTP      | conductivity ( $\mu\text{S/cm}$ ) | pH   | N-NO <sub>2</sub><br>(mgN/L) | N-NO <sub>3</sub><br>(mgN/L) | Cl <sup>-</sup> (mg/L) | N-NH <sub>4</sub><br>(mgN/L) | TOC<br>(mg/L) | TN<br>(mg/L) |
|-----------|-----------------------------------|------|------------------------------|------------------------------|------------------------|------------------------------|---------------|--------------|
| DWTP2_IN  | 188.4                             | 5.9  | 0.006                        | 0.4                          | 27.8                   | 0.02                         | 4.9           | 0.8          |
| DWTP2_TR  | 251.3                             | 6.2  | <LOQ                         | 0.1                          | 32.9                   | 0.02                         | 2.2           | 0.3          |
| DWTP2_F   | 252.5                             | 6.4  | 0.008                        | 0.1                          | 34.8                   | 0.20                         | 2.2           | 0.5          |
| DWTP2_DIS | 244.1                             | 6.5  | 0.010                        | 0.1                          | 33.3                   | 0.19                         | 2.2           | 0.5          |
| DWTP3_IN  | 128.8                             | 6.4  | <LOQ                         | 0.08                         | 28.0                   | 0.02                         | 2.3           | 0.3          |
| DWTP3_TR  | 141.4                             | 6.27 | <LOQ                         | 0.07                         | 29.3                   | <LOQ                         | 1.3           | 0.2          |
| DWTP3_F   | 154.8                             | 6.8  | <LOQ                         | 0.08                         | 29.9                   | 0.3                          | 1.3           | 0.5          |
| DWTP3_DIS | 174.4                             | 7.2  | <LOQ                         | <LOQ                         | 34.2                   | 0.3                          | 1.4           | 0.5          |
| DWTP4_IN  | 45.7                              | 5.23 | <LOQ                         | 0.09                         | 4.6                    | 0.03                         | 3.8           | 0.3          |
| DWTP4_TR  | 67.1                              | 5.55 | <LOQ                         | 0.09                         | 6.7                    | 0.01                         | 2.3           | 0.2          |
| DWTP4_F   | 80.9                              | 6.45 | <LOQ                         | 0.09                         | 7.6                    | 0.3                          | 2.4           | 0.5          |
| DWTP5_IN  | 86.0                              | 6.9  | <LOQ                         | <LOQ                         | 5.7                    | 0.1                          | 2.7           | 0.3          |
| DWTP5_TR  | 129.6                             | 6.9  | 0.003                        | 0.06                         | 9.8                    | <LOQ                         | 1.7           | 0.2          |
| DWTP5_F   | 3291.6                            | 8.9  | 0.002                        | 0.06                         | 12.9                   | 0.3                          | 1.3           | 0.6          |
| DWTP5_DIS | 158.9                             | 7.4  | 0.002                        | 0.07                         | 13.5                   | 0.2                          | 0.9           | 0.4          |

| DWTP       | conductivity (µS/cm) | pH  | N-NO <sub>2</sub><br>(mgN/L) | N-NO <sub>3</sub><br>(mgN/L) | Cl <sup>-</sup> (mg/L) | N-NH <sub>4</sub><br>(mgN/L) | TOC<br>(mg/L) | TN<br>(mg/L) |
|------------|----------------------|-----|------------------------------|------------------------------|------------------------|------------------------------|---------------|--------------|
| DWTP6_F    | 135.2                | 7.3 | 0.002                        | 0.5                          | 18.5                   | 0.27                         | 1.6           | 0.9          |
| DWTP6_DIS  | 138.7                | 7.2 | 0.038                        | 0.5                          | 18.6                   | 0.22                         | 1.7           | 0.9          |
| DWTP7_F    | 108.1                | 7.1 | <LOQ                         | 0.2                          | 15.4                   | 0.30                         | 2.3           | 0.7          |
| DWTP8_F    | 129.0                | 7.2 | <LOQ                         | 0.3                          | 17.6                   | 0.23                         | 1.9           | 0.7          |
| DWTP8_DIS  | 126.3                | 7.4 | 0.003                        | 0.2                          | 16.9                   | 0.27                         | 1.9           | 0.7          |
| DWTP9_F    | 88.5                 | 7.8 | <LOQ                         | 0.1                          | 12.1                   | 0.26                         | 2.7           | 0.6          |
| DWTP9_DIS  | 95.5                 | 8.2 | 0.004                        | 0.2                          | 12.7                   | 0.26                         | 1.8           | 0.6          |
| DWTP10_DIS | 81.0                 | 7.8 | <LOQ                         | 0.08                         | 10.6                   | 0.27                         | 2.2           | 0.6          |
| DWTP11_DIS | 183.9                | 7.3 | 0.021                        | 0.3                          | 30.4                   | 0.14                         | 2.8           | 0.6          |

LOQ: 0.003 mg N-NO<sub>2</sub>/L, 0.002 mg N-NO<sub>3</sub>/L, 0.025 mg Cl/L, 0.001 mgN-NH<sub>4</sub>/L, 0.05 mg/L TOC, 0.05 mg/L TN, Br<sup>-</sup> was not measured above 0.01mg/L.

**Table S3.** Water quality parameters measured during additional sampling campaigns at DWTP2 (June 2015)

| Sample code         | pH  | Conductivity<br>( $\mu$ S/cm) | TOC<br>(mgC/L) | TN (mgN/L) | N-NO <sub>2</sub><br>(mg N/L) | N-NO <sub>3</sub><br>(mg N/L) | N-NH <sub>4</sub><br>(mgN/L) | NDMA FP<br>(ng/L) | St dev<br>(NDMA<br>FP) |
|---------------------|-----|-------------------------------|----------------|------------|-------------------------------|-------------------------------|------------------------------|-------------------|------------------------|
| S1-inlet            | 7.2 | 307                           | 5.6            | 1.9        | 0.008                         | 1.6                           | 0.01                         | 39.2              | 3.3                    |
| S2-inlet            | 7.0 | 305                           | 5.6            | 1.9        | 0.007                         | 1.6                           | <LOQ                         | 45.9              | 2.4                    |
| S3- pre-ozone       | 6.8 | 346                           | 3.8            | 1.8        | <LOQ                          | 1.5                           | 0.04                         | 14.3              | 1.3                    |
| S4-prechlorine      | 6.5 | 334                           | 3.2            | 1.7        | <LOQ                          | 1.5                           | 0.00                         | 12.3              | 1.1                    |
| S5- sand filtration | 6.4 | 339                           | 3.3            | 1.8        | <LOQ                          | 1.5                           | 0.01                         | 16.3              | 1.5                    |
| S6- GAC             | 6.4 | 334                           | 3.0            | 1.8        | <LOQ                          | 1.5                           | 0.01                         | 13.3              | 1.5                    |
| S7-final            | 6.6 | 359                           | 2.7            | 2.1        | <LOQ                          | 1.6                           | 0.34                         | 10.3              | 0.2                    |

LOQ: 0.003 mg N-NO<sub>2</sub>/L, 0.002 mg N-NO<sub>3</sub>/L, 0.025 mgCl/L, 0.001 mgN-NH<sub>4</sub>/L.

**Table S4.** Water quality parameters measured during additional sampling campaigns at DWTP2 (September 2015)

| Sample code        | pH  | Conductivity<br>( $\mu$ S/cm) | TOC<br>(mgC/L) | TN (mgN/L) | N-NO <sub>2</sub><br>(mg<br>N/L) | N-NO <sub>3</sub><br>(mg<br>N/L) | N-NH <sub>4</sub><br>(mgN/L) | NDMA FP<br>(ng/L) | St dev<br>(NDMA<br>FP) |
|--------------------|-----|-------------------------------|----------------|------------|----------------------------------|----------------------------------|------------------------------|-------------------|------------------------|
| S1-inlet           | 5.4 | 332                           | 7.1            | 1.5        | <LOQ                             | 0.00                             | 0.81                         | 34.4              | 3.4                    |
| S2- pre-ozone      | 7.1 | 335                           | 6.7            | 1.6        | <LOQ                             | 0.02                             | 0.81                         | 14.0              | 0.6                    |
| S3-coag.           | 6.6 | 361                           | 4.8            | 1.1        | <LOQ                             | 0.01                             | 0.76                         | 14.4              | 0.2                    |
| S4-sand filtration | 6.1 | 375                           | 4.7            | 0.4        | <LOQ                             | 0.02                             | 0.01                         | 14.3              | 0.8                    |
| S6- GAC            | 5.6 | 369                           | 4.2            | 0.4        | <LOQ                             | 0.03                             | 0.03                         | 10.7              | 1.1                    |
| S7-final           | 5.8 | 381                           | 3.9            | 0.9        | <LOQ                             | 0.03                             | 0.54                         | 11.9              | 0.7                    |
| S7_B- final no FP  | 5.8 | 381                           | 3.9            | 0.9        | <LOQ                             | 0.03                             | 0.54                         | 1.2               | 0.3                    |

LOQ: 0.003 mg N-NO<sub>2</sub>/L, 0.002 mg N-NO<sub>3</sub>/L, 0.025 mgCl/L, 0.001 mgN-NH<sub>4</sub>/L.

**Table S5.** Water quality parameters measured during additional sampling campaigns at DWTP2 (September 2015)

| Sample code                      | pH  | Conductivity<br>( $\mu$ S/cm) | TOC<br>(mgC/L) | TN (mgN/L) | N-NO <sub>2</sub><br>(mg N/L) | N-NO <sub>3</sub><br>(mg<br>N/L) | N-NH <sub>4</sub><br>(mgN/L) | NDMA FP<br>(ng/L) | St dev<br>(NDMA<br>FP) |
|----------------------------------|-----|-------------------------------|----------------|------------|-------------------------------|----------------------------------|------------------------------|-------------------|------------------------|
| S1-inlet                         | 8.0 | 314                           | 8.6            | 1.0        | 0.008                         | 0.02                             | 0.30                         | 26.5              | 0.5                    |
| S2- preozone                     | 8.9 | 325                           | 8.1            | 0.9        | 0.004                         | 0.02                             | 0.23                         | 12.7              | 0.5                    |
| S3- coag.+ClO <sub>2</sub> +filt | 7.4 | 345                           | 4.6            | 0.3        | <LOQ                          | 0.03                             | <LOQ                         | 20.1              | 1.3                    |
| S4- main ozone                   | 6.6 | 354                           | 4.5            | 0.4        | <LOQ                          | 0.04                             | 0.07                         | 17.4              | 0.5                    |
| S5- GAC                          | 6.0 | 355                           | 4.0            | 0.4        | <LOQ                          | 0.04                             | 0.04                         | 11.1              | 0.8                    |

LOQ: 0.003 mg N-NO<sub>2</sub>/L, 0.002 mg N-NO<sub>3</sub>/L, 0.025 mgCl/L, 0.001 mgN-NH<sub>4</sub>/L.