

Detection and Occurrence of *N*-Nitrosamines in Archived Biosolids from the 2006-7 Targeted National Sewage Sludge Survey of the U.S. Environmental Protection Agency

Arjun K. Venkatesan, Benny F.G. Pycke, Rolf U. Halden

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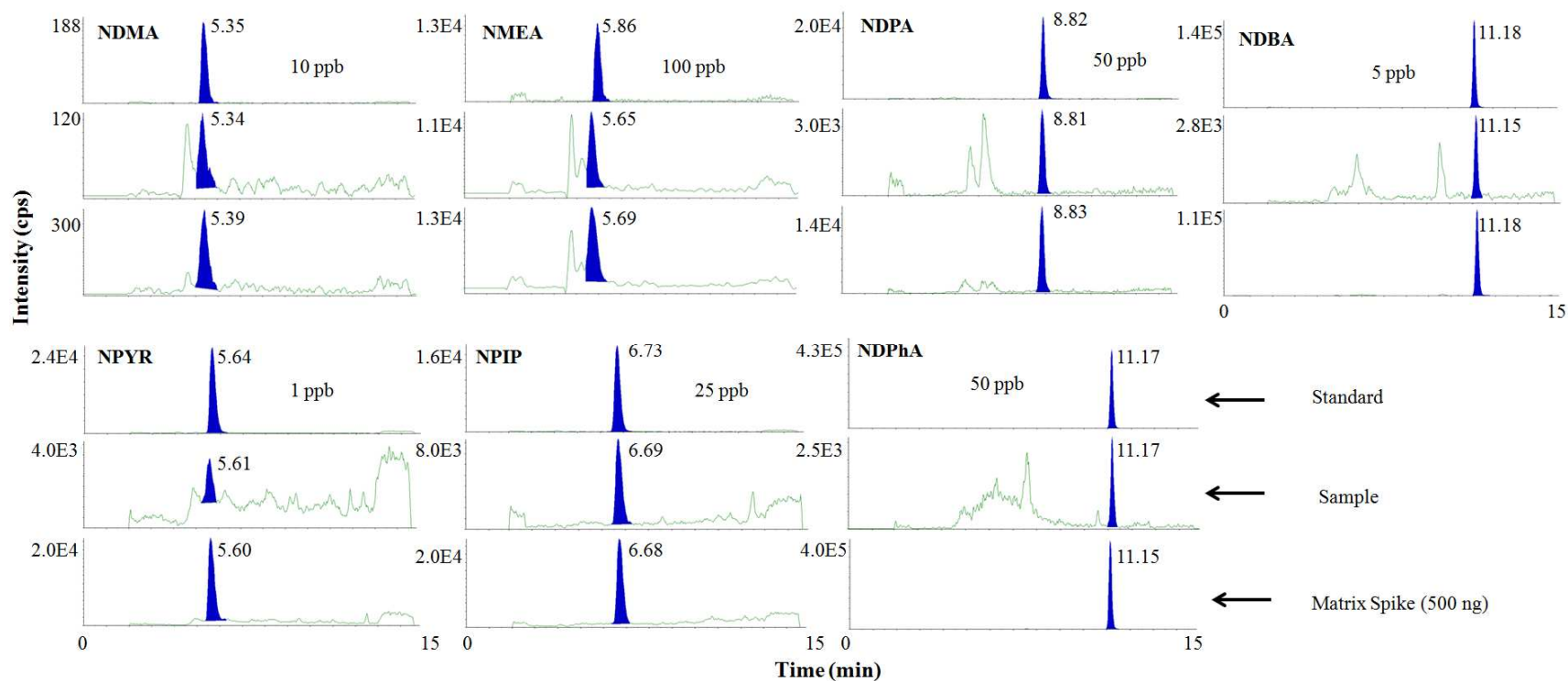


Figure S1. LC-MS/MS chromatograms of standards, sample extracts and matrix spike samples of seven detected *N*-nitrosamines. Number next to the peak represent the retention time of the analyte in minutes.

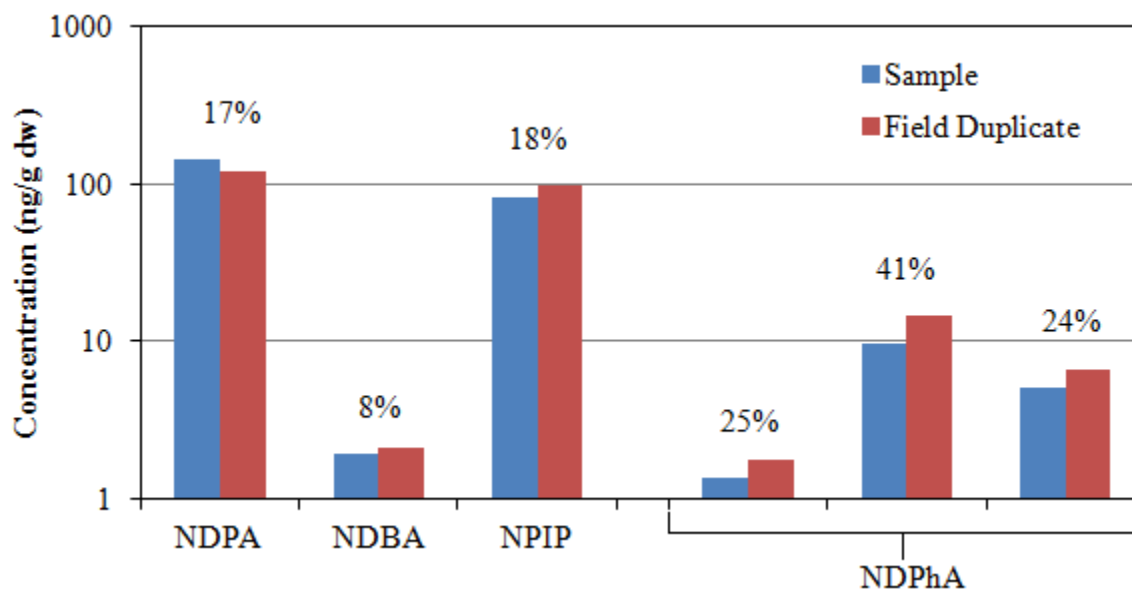


Figure S2. Concentrations of nitrosamines detected in samples and field duplicates. The percentage above the bar is the relative percentage difference (RPD) of the respective analyte concentration between sample and field duplicate.

Table S1. List of wastewater treatment plants (WWTPs) sampled for the targeted national sewage sludge survey by U.S. EPA

| WWTP | Flow (F) in MGD | City | State |
|--|------------------------|----------------|--------------|
| Sugar Creek WWTP | 1<F<10 | Alexander City | AL |
| Aldridge Creek WWTP | 1<F<10 | Huntsville | AL |
| Phoenix WWTP | 10<F<100 | Phoenix | AZ |
| Valley Sanitary District STP | 1<F<10 | Indio | CA |
| San Francisco | F>100 | San Francisco | CA |
| El Estero WWTP | 1<F<10 | Santa Barbara | CA |
| Santa Rosa | 1<F<10 | Santa Rosa | CA |
| Stockton Water Quality Plant | F>100 | Stockton | CA |
| Los Angeles County Sanitation District | 10<F<100 | Whittier | CA |
| Boulder WWTP | 1<F<10 | Boulder | CO |
| South Windsor | 1<F<10 | South Windsor | CT |
| Three Oaks WWTF | 1<F<10 | Estero | FL |
| Orange County Northwest WRF | 1<F<10 | Orlando | FL |
| Tampa | 1<F<10 | Tampa | FL |
| Albany | 10<F<100 | Albany | GA |
| Americus-Mill Creek | 1<F<10 | Americus | GA |
| Boone STP | 1<F<10 | Boone | IA |
| Calumet Water Reclamation Plant | F>100 | Chicago | IL |
| Plainfield WWTP | 1<F<10 | Plainfield | IL |
| Lake County DPW, New Century STP | 1<F<10 | Vernon Hills | IL |
| Dupage County-Knollwood STP | 1<F<10 | Wheaton | IL |
| Blucher Poole WWTP | 1<F<10 | Bloomington | IN |
| William Ross Edwin WWTP | 10<F<100 | Richmond | IN |
| Parsons | 1<F<10 | Parsons | KS |
| Topeka | 10<F<100 | Topeka | KS |
| Mayfield WWTP | 1<F<10 | Mayfield | KY |
| Eunice | 1<F<10 | Eunice | LA |
| Jefferson Parish East Bank WWTP | 1<F<10 | Marrero | LA |
| Nantucket | 1<F<10 | Nantucket | MA |
| Salisbury | 1<F<10 | Salisbury | MD |
| Mechanic Falls Treatment Plant | 1<F<10 | Mechanic Falls | ME |
| Benton Harbor-St. Joseph WWTP | 1<F<10 | St. Joseph | MI |
| Wixom WTP | 1<F<10 | Wixom | MI |
| Festus Crystal City STP | 1<F<10 | Crystal City | MO |
| Elizabeth City WWTP | 1<F<10 | Elizabeth City | NC |
| Hillsborough WWTP | 1<F<10 | Hillsborough | NC |
| Beatrice | 1<F<10 | Beatrice | NE |

| | | | |
|---|----------|----------------------|----|
| Wildwood Lower WTF | 10<F<100 | Cape May Court House | NJ |
| Middlesex County Utility Authority WRC | F>100 | Sayreville | NJ |
| Verona TWP DPW | 1<F<10 | Verona | NJ |
| Buffalo | F>100 | Buffalo | NY |
| Canajoharie WWTP | 1<F<10 | Canajoharie | NY |
| Geneva A-C Marsh Creek STP | 1<F<10 | Geneva | NY |
| NYC DEP - Jamaica WPCP | 10<F<100 | New York City | NY |
| North Tonawanda STP | 1<F<10 | North Tonawanda | NY |
| Clermont County Commissioners | 1<F<10 | Batavia | OH |
| Bedford | 1<F<10 | Bedford | OH |
| Metropolitan Sewer District Little Miami | 10<F<100 | Cincinnati | OH |
| Northeast Ohio Regional Sewerage District Southerly | F>100 | Cleveland | OH |
| Delaware County Alum Creek WWTP | 1<F<10 | Delaware | OH |
| Mingo Junction STP | 1<F<10 | Mingo Junction | OH |
| Duncan Public Utilities Authority | 1<F<10 | Duncan | OK |
| City of Klamath Falls WWTF | 1<F<10 | Klamath Falls | OR |
| Western Westmoreland Municipal Authority | 1<F<10 | Irwin | PA |
| Allegheny County Sanitary Authority | 1<F<10 | Pittsburgh | PA |
| Greater Pottsville Area Sewer Authority | 1<F<10 | Pottsville | PA |
| Punxsutawney | 1<F<10 | Punxsutawney | PA |
| South Kingstown WWTF | 1<F<10 | Narragansett | RI |
| Plum Island WWTP | 10<F<100 | Charleston | SC |
| Lawson Fork WTP | 1<F<10 | Spartanburg | SC |
| Elizabethton | 1<F<10 | Elizabethton | TN |
| Amarillo | 10<F<100 | Amarillo | TX |
| Dallas Southside WWTP | F>100 | Dallas | TX |
| Trinity River Authority of Texas | 1<F<10 | Ellis County | TX |
| Fredericksburg | 1<F<10 | Fredericksburg | TX |
| Odo J. Riedel Regional WWTP | 1<F<10 | Schertz | TX |
| Wagner Creek WWTP | 1<F<10 | Texarkana | TX |
| Tyler Southside WTP | 1<F<10 | Tyler | TX |
| Spanish Fork City Corporation | 1<F<10 | Spanish Fork | UT |
| Buena Vista | 1<F<10 | Buena Vista | VA |
| Everett City SVC Center MVD | 10<F<100 | Everett | WA |
| Beaver Dam | 1<F<10 | Beaver Dam | WI |
| Elkins WWTP | 1<F<10 | Elkins | WV |
| Huntington | 10<F<100 | Huntington | WV |

Table S2. LC-ESI-MS/MS parameters for analysis of *N*-nitrosamines

| MS/MS parameter | |
|------------------------|----------------------------------|
| Ion source | Positive electrospray ionization |
| Collision Gas | 6 |
| Curtain Gas | 50 |
| Ion source Gas 1 | 80 |
| Ion Source Gas 2 | 70 |
| Ion Spray Voltage | 4500 V |
| Source Gas Temperature | 700 °C |

| Analyte | Parent ion (m/z) | Product ion (m/z) | Declustering potential (V) | Exit Potential (V) | Collision Energy (V) | Collision Cell Exit Potential (V) | Retention Time (min) |
|----------------------------|-------------------------|--------------------------|-----------------------------------|---------------------------|-----------------------------|--|-----------------------------|
| NDMA | 75 | 43 | 51 | 10 | 25 | 2 | 5.34 |
| NMEA | 89 | 61 | 51 | 10 | 17 | 10 | 5.86 |
| NDEA | 103 | 75 | 51 | 10 | 17 | 12 | 6.65 |
| NDPA ^a | 131 | 89 | 51 | 10 | 17 | 8 | 8.82 |
| | 131 | 43 | | | | | |
| NDBA ^a | 159 | 103 | 56 | 10 | 17 | 8 | 11.18 |
| | 159 | 57 | | | | | |
| NPYR | 101 | 55 | 61 | 10 | 23 | 8 | 5.64 |
| NPIP ^a | 115 | 69 | 61 | 10 | 23 | 12 | 6.73 |
| | 115 | 41 | | | | | |
| NDPhA ^a | 199 | 169 | 56 | 10 | 17 | 8 | 11.16 |
| | 199 | 168 | | | | | |
| Deuterated isotopes | | | | | | | |
| NDMA-d ₆ | 81 | 46 | 51 | 10 | 25 | 2 | 5.35 |
| NDPA-d ₁₄ | 145 | 50 | 51 | 10 | 17 | 8 | 8.76 |
| NPIP-d ₁₀ | 125 | 78 | 61 | 10 | 23 | 12 | 6.70 |
| NDPhA-d ₆ | 205 | 175 | 56 | 10 | 17 | 8 | 11.11 |

^aTwo different transitions were used for these analytes for quantification and identification

Table S3. Octanol-water partitioning coefficient of nitrosamines (source: SciFinder).

| Compound | Log K_{ow} |
|-----------------|--------------------------------|
| NDMA | -0.5 |
| NMEA | 0.01 |
| NDEA | 0.51 |
| NDPA | 1.54 |
| NDBA | 2.56 |
| NPYR | -0.1 |
| NPIP | 0.44 |
| NDPhA | 3.13 |