

Characterization of the *Deltaproteobacteria* in contaminated and uncontaminated stream sediments and identification of potential mercury methylators

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Supplement 1. Detailed data and statistical analyses for biological, physical and geochemical parameters for the 6 sampling sites

Table S1A. Stream water chemical and physical parameters from each site from the May 2008 sampling event. Sedimentary Hg was the only sediment parameter analyzed; all other measurements were of dissolved aqueous species. Site HCK20.6 is viewed as uncontaminated, while sites EFK6.3, EFK13.8, EFK23.4, BCK12.3 and WCK3.9 are contaminated. Bk: samples taken near bank; Ch: samples taken mid-channel; DO: dissolved oxygen; DIC: dissolved inorganic carbon; NTRU: nephelometric turbidity ratio units; ND: below detection limits

	HCK20.6		EFK6.3		EFK13.8		EFK23.4		BCK12.3		WCK3.9	
	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch
<i>Physical parameters</i>												
Conductivity (mS cm ⁻¹)	0.52	0.52	0.63	0.63	0.56	0.55	0.54	0.54	1.84	1.83	0.59	0.57
DIC (mg l ⁻¹)	38.90	39.00	35.30	34.20	34.10	34.50	32.80	31.70	59.00	60.40	36.20	34.30
DO (mg l ⁻¹)	9.00	8.70	8.00	8.00	8.40	8.40	9.00	9.10	9.90	9.40	9.20	9.20
pH	7.87	7.93	8.00	7.83	7.95	7.93	8.08	8.08	7.88	7.91	8.10	8.06
Temperature (C)	14.30	14.60	16.80	16.80	17.10	17.30	18.70	18.70	14.80	14.70	18.80	18.70
Turbidity (NTRU)	10.70	9.90	4.30	8.50	6.60	10.50	7.00	8.60	12.60	12.60	3.90	4.30
<i>Hg</i>												
Hg sediment (ng mg ⁻¹)	0.11	0.00	11.30	20.20	15.60	15.10	30.40	33.20	1.50	1.60	4.00	2.50
Hg dissolved (ng l ⁻¹)	2.30	1.30	22.50	40.10	45.80	82.00	75.00	54.60	5.00	5.60	11.30	9.70
MeHg dissolved (ng l ⁻¹)	ND	0.11	0.51	0.71	0.31	0.38	0.83	0.45	0.10	0.11	ND	ND

<i>Ions</i>												
Cl ⁻ (mg l ⁻¹)	0.22	0.22	0.53	0.54	0.29	0.34	0.34	0.33	2.60	2.60	0.42	0.41
NO ₃ ⁻ (mg l ⁻¹)	0.15	0.14	0.83	0.71	0.26	0.28	0.31	0.32	14.20	15.00	0.00	0.04
SO ₄ ²⁻ (mg l ⁻¹)	0.86	0.86	1.70	1.80	1.60	1.80	1.70	1.70	1.90	1.90	1.80	1.70
<i>Trace metals</i>												
Al (mg l ⁻¹)	0.07	0.11	0.12	0.07	0.12	0.14	0.10	0.06	0.05	0.03	0.40	0.33
Ba (mg l ⁻¹)	0.07	0.08	0.04	0.05	0.06	0.05	0.06	0.05	0.23	0.23	0.06	0.06
Ca (mg l ⁻¹)	39.40	43.90	42.60	44.60	40.20	42.60	39.30	39.00	142.00	139.00	42.20	43.50
Fe (mg l ⁻¹)	0.11	0.15	0.17	0.13	0.14	0.16	0.14	0.12	0.29	0.27	0.31	0.32
Mg (mg l ⁻¹)	14.30	14.90	11.50	10.20	12.20	12.30	12.90	12.80	19.80	19.80	13.10	13.40
Mn (mg l ⁻¹)	0.01	0.01	0.03	0.03	0.02	0.03	0.04	0.03	0.01	0.01	0.01	0.03
Na (mg l ⁻¹)	4.70	4.60	14.80	15.20	8.60	8.70	10.10	10.20	40.40	40.80	11.20	11.00
Sr (mg l ⁻¹)	0.11	0.11	0.13	0.12	0.14	0.14	0.15	0.15	0.53	0.55	0.12	0.13
U (µg l ⁻¹)	0.19	0.13	5.50	3.70	6.60	10.50	7.60	7.10	187.00	175.00	0.24	0.38
Zn (µg l ⁻¹)	2.10	1.40	6.00	5.50	3.00	3.40	11.20	15.60	2.60	1.50	16.40	30.10

Table S1B. Stream water chemical and physical parameters from each site from the July 2008 sampling event. Sedimentary Hg was the only sediment parameter analyzed; all other measurements were of dissolved aqueous species. Site HCK20.6 is viewed as uncontaminated, while sites EFK6.3, EFK13.8, EFK23.4, BCK12.3 and WCK3.9 are contaminated. Bk: samples taken near bank; Ch: samples taken mid-channel; DO: dissolved oxygen; DIC: dissolved inorganic carbon; NTRU: nephelometric turbidity ratio units; ND: below detection limits; NS: not sampled (samples lost)

	HCK20.6		EFK6.3		EFK13.8		EFK23.4		BCK12.3		WCK3.9	
	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch
<i>Physical parameters</i>												
Conductivity (mS cm ⁻¹)	0.35	0.35	0.44	0.44	0.33	0.33	0.34	0.34	1.17	1.17	0.39	0.39
DIC (mg l ⁻¹)	48.80	48.70	40.80	40.80	37.70	37.60	36.70	36.90	75.90	74.90	43.10	43.10
DO (mg l ⁻¹)	7.80	7.80	8.00	8.00	9.00	9.00	10.10	10.20	8.50	8.50	8.40	8.30
pH	7.87	7.87	8.00	7.83	7.95	7.95	8.08	8.08	7.86	7.86	8.90	8.84
Temperature (C)	20.70	20.70	21.50	21.50	21.40	21.30	19.90	19.80	20.60	20.40	20.70	20.70
Turbidity (NTRU)	24.80	25.40	11.70	14.00	23.70	16.60	3.60	5.80	3.20	3.00	4.03	3.69
<i>Hg</i>												
Hg sediment (ng mg ⁻¹)	0.07	0.06	11.90	10.60	11.90	17.20	47.00	46.50	1.70	1.60	11.80	15.10
Hg dissolved (ng l ⁻¹)	1.30	1.10	13.40	13.30	14.10	25.90	73.10	122.00	4.50	4.40	ND	ND
MeHg dissolved (ng l ⁻¹)	ND	ND	1.10	2.50	0.23	0.28	0.42	0.39	ND	ND	0.44	0.91
<i>Ions</i>												
Cl ⁻ (mg l ⁻¹)	0.23	0.18	0.55	0.57	0.25	0.23	0.27	0.27	2.04	2.04	0.83	0.64
NO ₃ ⁻ (mg l ⁻¹)	0.15	0.13	0.69	0.76	0.27	0.27	0.36	0.36	13.30	13.30	0.46	0.26
SO ₄ ²⁻ (mg l ⁻¹)	0.81	0.76	2.20	2.40	1.70	1.70	1.90	1.90	2.40	2.40	4.90	3.70

Trace metals

Al (mg l ⁻¹)	0.31	0.79	1.17	0.66	0.12	0.19	0.17	0.12	0.06	0.05	1.99	0.40
Ba (mg l ⁻¹)	0.07	0.08	0.04	0.05	0.06	0.05	0.06	0.05	0.23	0.23	0.07	0.06
Ca (mg l ⁻¹)	39.40	43.90	42.60	44.70	40.20	42.60	39.30	39.00	142.00	139.00	42.20	43.50
Fe (mg l ⁻¹)	0.36	0.82	0.92	0.56	0.15	0.18	0.22	0.20	0.20	0.20	0.33	0.45
Mg (mg l ⁻¹)	14.20	14.10	11.30	11.90	12.20	10.90	11.90	11.90	20.20	19.50	16.60	16.40
Mn (mg l ⁻¹)	0.03	0.13	3.77	2.47	1.84	0.02	0.03	0.01	0.05	0.05	NS	NS
Sr (mg l ⁻¹)	0.10	0.10	0.12	0.13	0.13	0.13	0.14	0.14	0.46	0.46	0.15	0.14
U (µg l ⁻¹)	4.80	4.80	8.50	9.90	6.80	7.40	7.80	7.00	266.00	268.00	0.34	0.51
Zn (µg l ⁻¹)	3.40	5.60	12.70	14.20	3.80	6.20	16.90	22.60	3.40	3.60	12.70	26.00

Table S1C. Stream water chemical and physical parameters from each site from the September 2008 sampling event. Sedimentary Hg was the only sediment parameter analyzed; all other measurements were of dissolved aqueous species. Site HCK20.6 is viewed as uncontaminated, while sites EFK6.3, EFK13.8, EFK23.4, BCK12.3 and WCK3.9 are contaminated. Note: MeHg data were not available for the September 2008 sampling date. Bk: samples taken near bank; Ch: samples taken mid-channel; DO: dissolved oxygen; DIC: dissolved inorganic carbon; NTRU: nephelometric turbidity ratio units; ND: below detection limits

	HCK20.6		EFK6.3		EFK13.8		EFK23.4		BCK12.3		WCK3.9	
	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch	Bk	Ch
<i>Physical parameters</i>												
Conductivity (mS cm ⁻¹)	0.40	0.40	0.46	0.44	0.35	0.35	0.36	0.36	1.30	1.30	0.40	0.40
DIC (mg l ⁻¹)	59.60	60.30	40.00	39.00	40.90	42.20	40.30	39.30	65.80	68.70	42.80	44.80
DO (mg l ⁻¹)	7.00	7.10	8.30	8.20	9.00	9.10	9.70	9.70	8.30	8.40	8.80	8.80
pH	7.80	7.90	7.60	7.90	7.90	8.00	8.20	8.30	7.70	7.90	8.10	8.20
Temperature (C)	19.20	19.20	19.40	19.30	18.70	18.70	19.30	19.30	19.10	19.10	22.10	22.00
Turbidity (NTRU)	10.00	10.90	7.20	8.10	8.60	13.00	19.40	14.50	1.70	1.50	5.00	5.20
<i>Hg</i>												
Hg sediment (ng mg ⁻¹)	0.07	0.06	11.60	14.00	16.00	17.70	36.40	39.80	1.80	1.40	4.20	3.80
Hg dissolved (ng l ⁻¹)	0.60	0.55	14.50	14.00	21.50	24.30	138.00	129.00	3.18	3.30	8.80	7.60
<i>Ions</i>												
Cl ⁻ (mg l ⁻¹)	0.20	0.20	0.72	0.70	0.31	0.31	0.36	0.37	2.69	2.65	0.52	0.51
NO ₃ ⁻ (mg l ⁻¹)	ND	ND	0.37	0.47	ND	ND	0.07	0.18	18.50	18.10	ND	ND
SO ₄ ²⁻ (mg l ⁻¹)	0.87	0.87	2.30	2.20	1.70	1.70	1.70	1.70	2.10	2.10	2.10	2.10
<i>Trace metals</i>												
Al (mg l ⁻¹)	1.08	0.19	0.37	1.32	3.61	2.83	0.16	0.26	0.04	0.04	1.08	0.98
Ba (mg l ⁻¹)	1.00	0.06	0.04	0.05	0.06	0.05	0.04	0.05	0.18	0.18	0.06	0.06
Ca (mg l ⁻¹)	44.30	43.80	45.90	45.90	42.70	40.80	42.40	41.30	151.00	154.00	45.90	44.50
Fe (mg l ⁻¹)	0.62	0.25	0.31	0.69	1.70	1.40	0.27	0.31	0.26	0.25	0.79	0.75

Mg (mg l^{-1})	19.00	18.50	12.30	12.30	12.30	11.90	12.60	12.00	25.10	25.50	14.00	14.10
Mn (mg l^{-1})	0.15	0.03	0.02	0.03	0.21	0.04	0.07	0.08	0.01	0.01	0.04	0.02
Na (mg l^{-1})	3.70	3.60	17.70	17.30	9.00	8.90	10.20	10.10	49.20	50.20	13.20	13.30
Sr (mg l^{-1})	121.00	117.00	140.00	139.00	140.00	143.00	144.00	143.00	525.00	536.00	138.00	138.00
U ($\mu\text{g l}^{-1}$)	ND	ND	ND	ND	ND	ND	ND	ND	202.00	201.00	ND	ND
Zn (mg l^{-1})	8.10	6.50	7.70	11.50	18.50	16.90	22.60	32.90	6.50	6.50	38.50	37.80

Fig. S1. Triplot of the redundancy analysis (RDA) for bacterial taxa from the 36 stream sediments at 6 sites located on or near the Oak Ridge Reservation with forward selection of predictor variables followed by Monte Carlo permutations. Solid arrows represent predictor (geochemical) variables significantly associated ($p < 0.05$) with the variation in the bacterial community structure. Dashed arrows represent individual taxa ($|r| > 0.6$) significantly associated with the variation among samples. The length of the arrow is correlated with the degree of relation between the response variables. The arrows point in the direction of the maximum change for the associated variable. Open symbols: midchannel; closed: near bank

