Report as of FY2006 for 2006DC77B: "Nutrient flow and biological dynamics in the Anacostia River"

Publications

Project 2006DC77B has resulted in no reported publications as of FY2006.

Report Follows

Nutrient flow and biological dynamics in the Anacostia River
Progress Report
June 18, 2007

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I. Problem and Research Objectives:

Rivers are longitudinally linked systems with processes occurring in the upper reaches impacting downstream reaches and processes occurring in downstream reaches impacting upstream reaches through biological migration. The Anacostia River is an important link between the terrestrial and aquatic regions of the Potomac watershed and the larger Chesapeake Bay system. Although the health of the Potomac Estuary has been improving in recent years (Walker et al. 2004; Carter and Rybioki 1986), the Anacostia River, which runs into the estuary, remains a seriously stressed system with high levels of PAHs, PCBs, pesticides, and heavy metals (Phelps 2004). Researchers have also observed elevated concentrations of *Aeromonas* spp. during the summer months in Anacostia waters relative to concentrations observed in most natural waters (Cavari 1981). The effects of the degraded condition have been far reaching on the biological communities with high mortality rates of filter feeding bivalves (Phelps 1993, 2004); high tumor incidence among resident bullhead catfish (Sakaris et al. 2005, Pinkney et al. 2004), and adverse impacts on the populations of invertebrate macrofauna (Phelps 1985). These effects may impact the microbial community as well. Microbial DNA isolated from sediment from several locations on the Anacostia River reflecting a pollution gradient of heavy metals and organics (see Velinsky et al. 1994 and Wade et al. 1994 for sites), was found to have unique signatures in different regions of the river (Bushaw-Newton, Adams, and Velinsky, unpublished data). Despite increased attention on the Anacostia's environmental degradation, improvements have been marginal (Hall et al. 2002). Benthic organisms remain rare; Asiatic clams experience extremely low survival and have not established resident populations; fish remain unsafe to eat; and over 100 million gallons of raw waste entered the river in the past two years (Washington Post 2005). While studies have concentrated on the larger, macrofauna, little attention has been paid to the microbial and the macroinvertebrate communities. Yet, the structure and function of these two communities often plays a key role in dictating the structure and function of the larger biological community as well as the chemical components of the system. Therefore in order to best improve and protect the ecological function of the rivers, it is imperative to understand the role of the microbial community within that system.

Our objectives were to evaluate the microbial and macroinvertebrate communities of several sites within the upper reaches of the Anacostia River, upstream and downstream of the combined sewage outflow are in Bladensburg Maryland.
Specifically we wished to 1) establish seasonal changes in biological oxygen demand, developing profiles of demand versus depth, 2) evaluate nutrient sources to bacteria, algae, invertebrates and characterize the origins of particulate organic matter through the use of the stable isotopes of sulfur, carbon and nitrogen, 3) characterize the composition of microbial communities at the different sites by DNA analysis, fatty acid profile and standard microbiological techniques.

The following is a progress report on our progress thus far and is being submitted to WRRI pending a full analysis, which will be provided at a later date (a 6 month co-cost extension was granted 2/28/2007).

II. Fatty acid Community Profiling:

Background

Fatty acid profiling was used to determine the dominant sources of carbon in the sediment and water column at our research sites. Freshwater algae and bacteria both synthesize 18:1 fatty acids however the dominant isomer is different for each, algae have a greater abundance of 18:1D9 and bacteria have a greater abundance of 18:1D7. Bacteria also have odd and branched fatty acids, which algae do not (Lechevalier 1982). Bacteria do not have fatty acids larger than 18 carbon atoms long, which is sharply different from fatty acid profiles of the eukaryotic freshwater algae (Delong and Yayanos 1986). These and other characteristics make fatty acid analysis a robust tool for differentiating carbon sources in freshwater. Several studies have effectively shown that specific fatty acids are diagnostic of certain carbon sources. 18:1D7 is diagnostic of freshwater cyanobacteria (Fredrickson et al. 1986), 18:1D15 is diagnostic of green algae (Napolitano et al. 1994) 20:5D17 is diagnostic of freshwater diatoms and 17:1D11 and iso17:0 are diagnostic of sulfate reducing bacteria (Boon et al. 1996).

Fatty acid results and analysis.

July 2006 sediment and water column FAME profiles

Soils at Bladensburg (7/20/06) show a number of both odd-number and branched fatty acids, indicating bacterial origins. These unusual fatty acids made up approximately 9% of all the fatty acids. 16:0, 16:1 and 18:1 were the dominant fatty acids in the Bladensburg sediments and these are probably derived from photosynthesis. The soil samples also showed Filtered material from the water column for this date and site showed several short chain fatty acids and the sample was dominated by trans-4,4-dimethyl-2-pentenoic acid, which may indicate bacteria (the cis was also present, but a much lower amount).

November 2006 sediment and water column FAME profiles

Soils at the Navy Yard and site Waterpark (11/16/06) did not show a wide range of fatty acids, mostly 16:0, 18:0, 18:1 and 18:2 (navy yard only), which are not characteristic of bacteria. Interestingly, the dominant fatty at the Navy Yard (5x greater than any other fatty acid) was 2-oxo-hexadecanoic acid, a fatty acid metabolite (Appendix A, Tables 9 and 11). This acid was absent from the Aquatic Garden. Sediment at the Waterpark 11/16/06 didn't show a diverse group of FAs, and the dominant groups were 16 and 18 carbon saturated and single unsaturated species. Fatty acids were not obtained in sufficient quantity for analysis in filtered water from the Aquatic Gardens, probably because of lower productivity in the water column in November relative to the summer. Sediment and GFF from the Navy Yard on 11/16/07 also failed to show any distinctive bacterial FAs (Appendix A, Tables 11 and12). Sediment FA profiles were similar to those at the Waterpark and only a single relatively short chain FA was detected within the water column filtrate (Appendix A, Table 12).

III. Nutrient Source Assessment: isotope characterization with season and site:

Background.

Stable isotope analyses of carbon, nitrogen and sulfur have become important tools for determining the relative contributions of different nutrient sources in aquatic ecosystems. While it is expected that a stream such as the Anacostia will derive most of its organic carbon from allochthonous sources, which, will be fairly depleted in 13C relative to autochthonous steams, nitrogen and sulfur isotopes have the potential to yield interesting information at the Bladensburg sites. Enriched 15N in organic matter is often associated with human sewage impact (Aravena et al. 1993; Wayland and Hobson 2001) and sulfur isotopes have recently been shown to be a very effective tracer of nutrients from different geographical areas (Krouse and Tabatabai, 1986, MacAvoy et al. 1998, 2000). Unlike carbon and nitrogen isotopes, sulfur isotope signature is derived from sulfur in local minerals and atmospheric deposition (Krouse and Tabatabai, 1986). This has allowed researchers to use sulfur to trace sewage into estuarine ecosystems (Sweeney et al. 1980a;b).

Source assessment.

In July 2006 very negative d13C values for water column filtrate suggest that a pulse of terrestrial (allochthonous) production not bacterial or autocthonous processes dominate (particularly at the downstream site) (Appendix B). Within the sediment there appears to be a draw down of nitrogen (lower C/N ratios. Appendix B) than other sites resulting in lower d15N although higher d15N values appear within the well mixed water column organic matter. The same sediments at the waterpark (middle) site show negative d34S values, suggesting sulfate reduction in the sediments. This is consistent with lower oxygen at this site during the summer.

During the November 2006, uniform water column filtrate d15N values reflect a low level of microbiological activity. Soils show a distinct clustering of d13C and d15N. The Navy Yard and waterpark overlap in d13C but are approximately 3‰ apart in d15N. The elevated d15N at the Navy Yard is unusually high for autotrophic production (whether autocthonous or allochthonous). This suggests that heterotrophs may have excreted 15N-enriched material, which accumulated as the river continued downstream (there is a sediment d15N increase as one progresses downstream) (Appendix B). The waterpark has substantially more 13C-enriched sediments, possibly indicating that benthic production is more important at this site during November than the others.

IV. Biological and Chemical Studies:

In July and November, replicate water and sediment samples were taken from three sites representing an upstream to downstream gradient in the Anacostia River. The upstream site (US) is located at Bladensburg, MD, while the middle stream site (MS) is located by Kenilworth Marsh, and the downstream site (DS) is located underneath the 11th street bridge. For the water samples, water was collected in acid-washed HDPE bottles and placed on ice for transport. Triplicate sediment samples were collected using a Stainless steel Petit Ponar, which was rinsed between samples. Surface sediment was collected from the ponar in whirl pak bags and placed on ice for transport. Several biological and

chemical analyses have been conducted on the collected samples to determine the linkages between microorganisms, their activities, and their environment.

V. Chemical Analyses-Sediment:

Microbes rely heavily upon the organic matter to provide the carbon and nutrients necessary to carryout reactions. Triplicate sediment samples were taken at all sites, except the DS site in November, for organic matter content analysis. At the DS site, main channel sediment samples were not obtainable due to the high concentration of rocks and gravel in the sediment. To determine organic matter content, sediment samples were analyzed for ash free dry mass. Sediment samples were weighed, dried, and re-weighed before muffling at 500ºC for 2 h.

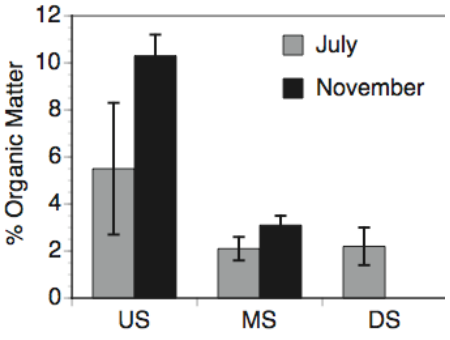

Figure 1. Percent Organic Matter for Sediment of the Anacostia River (n=3 ±SD)

Preliminary results demonstrate that the sediment for the Anacostia River has low organic matter content ranging from 2% at the MS site in July to 10% at the US site in November (Figure 1). Overall concentrations are higher at the US site most likely reflecting higher inputs of leaf litter.

VI. Chemical Analyses-Water:

in situ Measurements

At each site, *in situ* measurements were conducted to provide information on several parameters. Using a YSI environmental probe, temperature, conductivity, dissolved oxygen concentrations and pH (Table 1). As expected temperature decreased from July to November at all sites from 30ºC to 13ºC. Conductivity also decreased though the reasons for this are not clear as concentrations of nutrients such as nitrate which can influence conductivity were higher in November than July (Table 2). Dissolved oxygen levels were similar at all sites in July but highly varied in the November samples. Given the lower temperatures in November, one would expect oxygen saturation. The lower levels in the MS and DS sites compared with the US site may be reflective of biological activity or potentially, chemical oxygen consumption in those areas. For July vs November, pH was elevated. November samples probably have increased acidity due to leaf litter leachates (e.g., humic acids) and lower activities of algae and plants which drawdown carbon dioxide levels in water.

Table 1. Measurement of temperature, conductivity, oxygen concentrations and pH for three areas of the Anacostia River using a YSI Environmental Probe

Station	Temperature (ºC)	Conductivity (mS cm^{-1})	% Dissolved Oxygen	Dissolved Oxygen (mg L^{-1})	pH

July					
US	27.4	0.376	69.2	5.46	6.85
MS	30.27	0.326	62.5	4.7	6.79
DS	30.21	0.317	67.2	5.06	7.1
November					
US	12.85	0.272	94.1	9.9	5.06
MS	13.32	0.312	72.9	7.6	6.19
DS	12.81	0.215	38.9	4.08	6.17

Nutrient concentrations

Within a few hours of collection, triplicate (July) or duplicate (November) water samples were filtered through muffled glass fiber filters and frozen at -20ºC. Ammonium and Soluble Reactive Phosphate (SRP) measurements were done spectrophotometrically using standard methods. All other nitrogen components (NO_3^- + NO_2^-, and Dissolved Organic nitrogen (DON) were analyzed using an Alpkem autoanalyzer by the Academy of Natural Sciences Philadelphia using standard methods. Dissolved organic carbon (DOC) was measured using a total organic carbon analyzer (Shimadzu Corp) by the Academy of Natural Sciences Philadelphia using standard methods.

In both July and November, nitrate and ammonium levels increase with downstream movement (Table 2). These concentrations are less than 1 mg L nitrate which means that for classification purposes this system is not seen as very anthropogenically influenced. Ammonium levels are much lower than nitrate levels at all sites. This is expected as nitrate is readily absorbed in the watershed and nitrate is highly soluble in soil systems. Nitrate and ammonium levels are higher in November than July which is most likely represents lower biological uptake and higher concentrations in the water column. DON concentrations represent half of the nitrogen pool in these system though its biological availability is not determined in these studies. As will all freshwater systems, SRP levels are 20 to 60x lower than nitrogen concentrations. Phosphorus is most likely limiting in these systems. DOC concentrations range from 8.6 mg C L^{-1} at the US site in July to 16.8 mg C L^{-1} at the DS site in November. DOC measures all organic carbon in these system and while a portion of this organic carbon comes from natural sources, it is not clear if other pollutants are contributing to the carbon pool. In November, the leaching of leaf litter may be responsible for the overall increases in DOC concentrations compared with July.

Table 2. Nutrient concentrations for three areas of the Anacostia River, for July n=3 (±SD), for November n=2(±SD)

Station	NO_3^- + NO_2^- (mg L^{-1})	NH_4 (mg L^{-1})	DON (mg L^{-1})	SRP (mg L^{-1})	DOC (mg L^{-1})

July					
US	0.320 (0.228)	0.029 (0.004)	0.205 (0.071)	0.014 (0.001)	8.6 (2.8)
MS	0.447 (0.011)	0.066 (0.016)	0.481 (0.053)	0.015 (0.002)	13.7 (0.32)
DS	0.556 (0.094)	0.140 (0.002)	0.391 (0.038)	0.021 (0)	12.2 (1.0)
November					
US	0.434 (0.124)	0.085 (0.003)	0.319 (0.042)	0.008 (0)	10 (1.0)
MS	0.532 (0.003)	0.186 (0.001)	0.411 (0.033)	0.010 (0.001)	11.9 (1.1)
DS	0.606 (0.006)	0.195 (0.008)	0.420 (0.02)	0.011 (0.001)	16.8 (0.71)

VII. Biological Analyses-Water:

Oxygen Consumption Rates

Table 3. Rates of oxygen consumption representing whole community and the microbial fraction (filtered through 3 μM nominal pore size filters) for three sections of the Anacostia River.

	Oxygen Consumption Rate (mg O_2 L^{-1} h^{-1})	**r^2**
US	0.0203	0.90
US-Filtered	0.0134	0.99
MS	0.0307	0.96
MS-Filtered	0.0133	0.98
DS	0.0355	0.95
DS-Filtered	0.0184	0.97
Distilled Water	0.0007	0.08

Microbes represent an important component of the total biological community in aquatic environments. For the July samples, biological oxygen demand was measured in both whole water and filtered (3 μm nominal pore size) water samples to determine the relative contributions of the microbial communities to overall metabolic activities. Triplicate 60 ml BOD bottles were filled with either whole or filtered water samples and incubated in the dark. To determine oxygen demand, triplicate samples were sacrificed over a period of 5 days and oxygen concentrations were calculated using the Winkler method. Distilled water was used as a control. To determine relative rates of oxygen consumption, linear regression analyses were done for each data set and correlations calculated (r^2, Table 3).

Microbial respiration in the water column (Filtered samples) was shown to be an important component of total community respiration at all sites (Table 3). Similar to nutrient concentrations, respiration rates increased in a downstream direction from 0.0203 mg O_2 L^{-1} h^{-1} for the US site to 0.0355 mg O_2 L^{-1} h^{-1} for the DS site. This increase may be attributed to higher availability of nutrients and carbon in the water column.

Bacterial utilization of different carbon sources

Biolog plates-These analyses are ongoing.

Concentrations of Bacteria
Enumeration of bacteria using direct count method-These analyses are ongoing.

VIII. Microbial Community Analyses-Sediment and Water:

The diversity of the microbial community can be determined using molecular techniques. For both water and sediment samples, microbial DNA was extracted using ~100-200 ml of water or ~0.25 g of sediment. Extracted DNA is currently being amplified using primers for total community (16S rRNA) or specific communities of PCB or PAH degraders (TMOA gene) (see Figure 2 for a representative example).

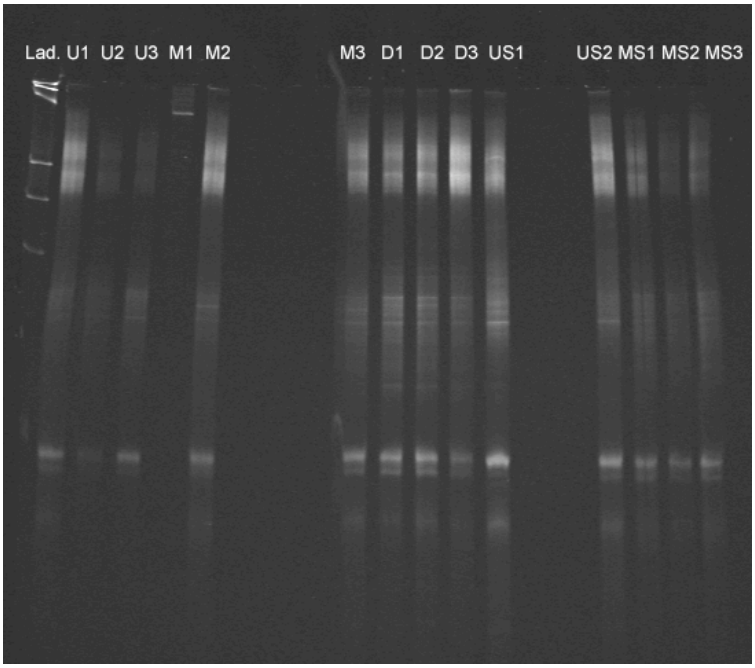

Figure 2. Total microbial diversity based on 16S rRNA genes using Denaturing gradient gel electrophoresis for July and November sediment samples. Each band represents a potential species of bacteria.

Our results, thus far demonstrate that while some strains are found throughout the river system, other strains are unique to one area of the system versus another area.

Literature cited:

Aravena, R., Evans, M.L., Cherry, J.A. 1993. Stable isotopes of oxygen and nitrogen in source identification of nitrate from septic systems. Ground Water 31(2):180-186.

Boon PI, Virtue P, Nichols PD. 1996. Microbial consortia in wetland sediments: a biomarker analysis of the effects of hydrological regime, vegetation and season on benthic microbes. Mar. Freshwat. Res. 47:27-41.

Carter V, Rybicki N. 1986. Resurgence of submersed aquatic macrophytes in the Tidal Potomac River, Maryland, Virginia, and the District of Columbia. Estuaries 9(4b): 368-375.

Cavari, BZ, Allen DA, Colwell RR. 1981. Effect of temperature on growth activity of Aeromonas spp. mixed bacterial populations in the Anacostia River. Applied and Environmental Microbiology 41(4):1052-1054.

Delong EF, Yayanos AA. 1986. Biochemical function and ecological significance of novel bacterial lipids in deep-sea procaryotes. Applied Environmental Microbiology 51:730-737.

Fredrickson HL, Cappenberg TE, Leeuw JW. 1986. Polar lipid ester-linked fatty acids composition of Lake Vechten seston: an ecological application of lipid analysis. FEMS Microbiological Ecology 38:381-396.

Hall LW, Anderson RD, Alden RW. 2002. A ten year summary of concurrent ambient water column and sediment toxicity tests in the chesapeake bay watershed: 1990-1999. Environmental Monitoring and Assessment 76:311-352.

Krouse HR and MA Tabatai. 1986. Stable Sulfur Isotopes. In Sulfur in Agriculture; 27th in the series Agronomy ed MA Tabatai.

Lechevalier H, Lechevalier MP. 1982. Lipids in bacterial taxonomy. In: Laskin AI and Lechevalier HA eds. CRC Handbook of Microbiology. Boca Raton FL. CRC Press Inc. p. 435-541.

Napolitano GE, Hill WR, Guckert JB, Stewart AJ, Nold SC, White DC. 1994. Changes in periphyton fatty acids composition in chlorine polluted streams. Journal of the North American Bethological Association 13:237-249.

Phelps HL. 1993. Sediment toxicity of the Anacostia River estuary, Washington DC. Bull. Environmental Contaminant Toxicology 51:582-587.

Phelps HL. 2004. Sources of Bioavailable Toxic Pollutants in the Anacostia Watershed. Part III, DC Water Resources Research Center Report 2003DC34B, Washington DC. 12p.

Pinkney, AE, Harshbarger JC, May EB, Reichert WL. 2004. Tumor prevalence and biomarkers of exposure and response in brown bullheads (Ameiurus nebulosus) from the Anacostia River, Washington. DC and Tuckahoe River, Maryland, USA.

Sakaris PC, Jensien RV, Pinkney AE. 2005. Brown Bullhead as an indicator species: seasonal movement patterns and home ranges within the Anacostia River, Washington, D.C. Transactions of the American Fisheries Society 134:1262-1270.

Sweeney, R.E., E.K. Kalil, I.R. Kaplan. 1980. Characterization of domestic and industrial sewage in Southern California coastal sediments using nitrogen, carbon, sulfur and uranium tracers. Marine Environmental Research 3:225-243.

Sweeney, R.E. and I.R. Kaplan. 1980. Tracing flocculent industrial and domestic sewage transport on San Pedro Shelf, Southern California, by nitrogen and sulphur isotope ratios. Marine Environmental Research 3:215-224.

Velinsky, D. J., T. L. Wade, C. E. Schlekat, B. L. McGee, and B. J. Presley. 1994. Tidal river sediments in the Washington, D.C. area. I. distribution and sources of trace metals. Estuaries 17: 305-320.

Wade, T. L. , D. J. Velinsky, E. Reinharz, and C.E. Schlekat. 1994. Tidal river sediments in the Washington, D.C. area. II. distribution and sources of organic contaminants. Estuaries 17: 321-333.

Walker SE, Dickhut RM, Chisholm-Brause C. 2004. Polycyclic aromatic hydrocarbons in a highly industrialized urban estuary: inventories and trends. Environmental toxicology and chemistry 23(11):2655-2664.

Wayland, M., K.A. Hobson. 2001. Stable carbon, nitrogen and sulfur isotope ratios in riparian food webs on rivers receiving sewage and pulp-mill effluents. Canadian Journal of Zoology 79:5-15.

Washington Post. 2005. WSSC Agrees to Pay Fines, Make Repairs. 7/27 by David Fahrenthold.

Appendix A, Fatty Acid methyl esters (FAMES) and related compounds
Drs. MacAvoy and Bushaw-Newton
June 18, Progress Report

Table 1: 6/8/06 Sediment Navy Yard

MS Data File = FM36475.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.	FAMES	Area %
181	80994	methyl isobutyl ketone (MIBK)	100		12.96659
186	24941	methyl ester of 3-methylbutanoic acid	116		3.992885
196	2301	toluene	92		0.368375
206	375	2-methyl-3-pentanone	100		0.060035
225	928	2-hexanone	100		0.148567
275	1520	n-nonane	128		0.243342
291	6819	4-methyl-2-pentanol	102		1.091676
300	328	methyl hexanoate	130	6:0	0.052511
311	1151	3-hexanol	102		0.184267
316	269	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis)	142		0.043065
328	1400	2-hexanol	102		0.224131
332	1029	1-methylcyclopentanol	100		0.164736
341	1304	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142		0.208762
346	693				0.110945
353	120				0.019211
357	30				0.004803
363	8599	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		1.376642
367	639				0.1023
371	876	methyl ester of 3-methyl-2-heptenoic acid	156		0.140242
379	89				0.014248
386	4211	2-propenyl ester of 2-methyl, 2-butenoic acid	140		0.674153
391	2188	2-propenyl ester of 3-methyl butanoic acid	142		0.350284
398	640	?			0.10246
404	2752	?	130		0.440577
411	1816	?	130		0.290729
417	7345	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174		1.175885
429	11187	possibly methyl ester of 4-butoxybutyric acid	174		1.790963
437	531	methyl octanoate	158	8:0	0.08501
444	114984	?	172		18.40816
456	10774	possibly methyl ester of 4-butoxybutyric acid	174		1.724845
461	1850	?	182		0.296172
467	2829	?	182		0.452904
472	5024	?			0.804308

478	510	?			0.081648
485	10184	3-butyl-3-octen-2-one	182		1.63039
490	181				0.028977
498	2078	methyl nonanoate	172	9:00	0.332674
507	27489	?	182		4.400803
524	1736	?	152		0.277922
545	1482	?			0.237258
558	2802	methyl decanoate	186	10:0	0.448581
563	70				0.011207
567	731	methyl benzoate	136		0.117028
571	4532	?	144		0.725543
584	775	?			0.124072
588	3718	?			0.595227
595	129				0.020652
601	1698	2,4,4-trimethylbut-2-enolide	126		0.271838
607	6938	?			1.110727
613	6635	?			1.062219
627	644	? lactone			0.1031
632	2752	? cyclohexenone derivative	180		0.440577
646	12726	?	208		2.037347
651	327	? cyclohexenone derivative	180		0.05235
656	321	?	194		0.05139
662	2325	methyl dodecanoate	214	12:0	0.372217
674	955	artifact			0.152889
679	13709	dodecadione	198		2.194718
707	1140	?	192		0.182506
711	2439	methyl tridecanoate	228	13:0	0.390467
716	3465	?	208		0.554723
722	9894	? cyclohexenone derivative	194		1.583962
732	26278	?	226		4.20693
735	1886	?			0.301936
738	1296	?			0.207481
743	4914	?	166		0.786698
753	17318	tridecadione	212		2.772495
758	3480	methyl tetradecanoate	242	14:0	0.557124
772	1920	?			0.307379
782	937	methyl pentadecanoate (branched)	256	15:0	0.150007
788	1045	methyl pentadecanoate (branched)	256	15:0	0.167297
802	2053	methyl pentadecanoate	256	15:0	0.328671
816	19705	?	168		3.154637
825	7736	methyl hexadecanoate (branched)	270	16:0	1.238481
828	6065				0.970965
835	211	methyl hexadecanoate (branched)	270	16:0	0.03378
842	2684	?	222		0.42969
846	14063	methyl hexadecanoate	270	16:0	2.251391
857	8863	methyl hexadecenoate	268	16:1	1.418906
869	2691	methyl octadecanoate (branched)	298	18:0	0.430811
877	1126	?	192		0.180265
880	2159	?			0.345641

886	1472	methyl octadecanoate (branched)	298	18:0	0.235657
896	4193	?	192		0.671271
927	9806	methyl octadecanoate	298	18:0	1.569874
935	14531	methyl oleate	296	18:1	2.326315
952	4442	methyl linoleate	294	18:2	0.711134
972	3610	methyl linolenate	292	18:2	0.577937
1006	6244	methyl eicosanoate	326	20:0	0.999622
1015	8280	methyl eicosenoate	324	20:1	1.325572
1104	8467	methyl eicosanoate	326	20:0	1.355509
1117	11987	methyl eicosenoate	324	20:1	1.919038

Table 2: 7/20/06 Sediment Bladensburg

MS Data File = FM36470.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
178	4390	methyl isobutyl ketone (MIBK)	100		0.622577
186	12472	methyl ester of 3-methylbutanoic acid	116		1.768742
300	324	methyl hexanoate	130	6:0	0.045949
311	217	3-hexanol	102		0.030774
328	360	2-hexanol	102		0.051054
333	269	1-methylcyclopentanol	100		0.038149
341	139	methyl ester of 4,4-dimethyl-2-pentenoic acid	142		0.019713
363	6684	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		0.947905
371	219	methyl heptanoate	144	7:0	0.031058
378	187	2-propenyl ester of 2-butenoic acid	126		0.02652
386	235	?			0.033327
416	343	methyl ester of 3-methyl-2-heptenoic acid	156		0.048643
428	1099	possibly methyl ester of 4-butoxybutyric acid	174		0.155857
437	470	methyl octanoate	158	8:0	0.066654
442	20215	?	172		2.866831
451	15				0.002127
455	779	?	158		0.110475
484	624	?	182		0.088494
497	1359	2-ethylhexyl alcohol	130		0.192729
505	1549	?	182		0.219675
516	338	methyl ester of 2-hydroxy-4-methylpentanoic acid	146		0.047934
556	1481	methyl decanoate	186	10:0	0.210031
567	305	methyl benzoate	136		0.043254
571	1356	?	144		0.192304
589	3091	?	144		0.438356
607	3820	?	144		0.541741
613	5136	?	144		0.728372
627	624	methyl-4-oxooctanonate	174		0.088494
633	4853	?	180		0.688238
646	7855	?	208		1.113973
662	4331	methyl dodecanoate	214	12:0	0.614209
678	4695	dodecadione	198		0.665831
688	467	methyl tridecanoate (branched isomer)	228	13:0	0.066229
695	455	methyl tridecanoate (branched isomer)	228	13:0	0.064527
707	498	?	192		0.070625
711	1379	methyl tridecanoate	228	13:0	0.195566
722	705	? cyclohexenone derivative	194		0.099981
731	4827	?	226		0.684551
736	2462	methyl tetradecanoate (branched isomer)	242	14:0	0.349153
752	4381	tridecadione	212		0.6213

759	26805	methyl tetradecanoate	242	14:0	3.801405
762	963	methyl hexadecanoate (branched isomer)	270	16:0	0.13657
769	1608	methyl tetradecenoate	240	14:1	0.228042
782	9081	methyl pentadecanoate (branched isomer)	256	15:0	1.28784
789	7541	methyl pentadecanoate (branched isomer)	256	15:0	1.069442
803	7996	methyl pentadecanoate	256	15:0	1.133969
809	1040	?	250		0.14749
813	3877	methyl pentadecenoate	254	15:1	0.549825
816	2662	?			0.377517
826	4399	methyl hexadecanoate (branched isomer)	270	16:0	0.623853
850	122891	methyl hexadecanoate	270	16:0	17.42803
858	29857	methyl hexadecenoate	268	16:1	4.234231
863	6363	methyl heptadecanoate (branched isomer)	284	17:0	0.902382
868	6123	methyl heptadecanoate (branched isomer)	284	17:0	0.868346
874	3736	methyl heptadecanoate (branched isomer)	284	17:0	0.529828
887	7632	methyl heptadecanoate	284	17:0	1.082347
896	5240	methyl heptadecenoate	282	17:1	0.743121
908	6714	methyl octadecanoate (branched isomer)	298	18:0	0.952159
923	4703	?	278		0.666965
929	44217	methyl octadecanoate	298	18:0	6.270723
937	87867	methyl oleate	296	18:1	12.46104
953	29575	methyl linoleate	294	18:2	4.194238
957	3735	methyl nonadecanoate	312	19:0	0.529687
978	8117	methyl linolenate	292	18.3	1.151129
1007	14571	methyl eicosanoate	326	20:0	2.066416
1016	17261	methyl eicosenoate	324	20:1	2.447904
1051	5664	methyl heneicosanoate	340	21:0	0.803252
1106	23782	methyl docosanoate	354	22:0	3.372692
1119	23180	methyl docosenoate	352	22:1	3.287318
1167	6621	methyl tricosanoate	368	23:0	0.93897
1230	20219	methyl ester of 10-hydroxyoctadecanoic acid	314		2.867398
1236	5293	glyceryl monopalmitate	330		0.750637
1245	21594	methyl tetradocosanoate	382	24:0	3.062397
1256	4748	methyl abietate (wood rosin ester)	314		0.673347
1264	4313	methyl tetracoasenoate	380	24:1	0.611657
1331	5089	methyl pentadocosanoate	396	25:0	0.721707
1368	11130	?	330		1.578423
1395	3919	?	336		0.555781
	705134	Total			100

Table 3, 7/20/06 GFF Bladensburg

MS Data File = FM36471.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
186	23468	methyl ester of 3-methylbutanoic acid	116		1.901672
253	570	methyl 4-methyl-2-pentenoate	128		0.046189
270	863	methyl hexanoate	130	6:0	0.069931
290	28067	methyl methacrylate	100		2.274341
304	1307	methyl cyclohexanecarboxylate	142		0.10591
311	1171	3-hexanol	102		0.094889
325	5734	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis)	142		0.464641
328	1656	2-hexanol	102		0.13419
333	1358	1-methylcyclopentanol	100		0.110042
345	51025	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142		4.134686
365	40017	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		3.24268
385	896	methyl ester of 3-methyl-2-heptenoic acid	156		0.072605
406	1348	2-methylcyclopentanol	100		0.109232
418	22602	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174		1.831498
429	1333	methyl ester 3-hydroxybutanoic acid	118		0.108016
436	1510	n-undecane	156		0.122359
442	19678	?	172		1.594559
456	30047	possibly methyl ester of 4-butoxybutyric acid	174		2.434785
492	2569	?	166		0.208173
505	12576	methyl, 3-hydroxy-3-methylbutyrate	132		1.019065
514	2660	methyl, 2-hydroxy-4-methylpentanoate	146		0.215547
531	19620	methyl, 6-oxo-octanoate	174		1.589859
547	2528	methyl, 10-oxooctanoate	174		0.20485
609	27175	?			2.20206
615	34313	?			2.78047
626	31131	some type of lactone			2.522624
633	4235	?	180		0.343173
640	4915	?	180		0.398275
645	8443	?	194		0.684158
667	31136	?			2.523029
674	60392	?			4.893718
679	9915	dodecadione	198		0.803438
711	5280	?	192		0.427852
725	58456	? cyclohexenone derivative	194		4.736839
734	15762	?	226		1.277235
739	15732	?	206		1.274804
755	53887	tridecadione	212		4.366601
758	3100	methyl tetradecanoate	242	14:0	0.251201
769	5085	?	252		0.412051
779	4755	?			0.38531

786	17015	?	182		1.378769
789	6059	dimethyl nonanedioate	216		0.490976
809	5343	?	236		0.432957
813	6192	?	176		0.501754
818	6088	?	252		0.493326
830	4459	?	252		0.361324
847	19444	methyl hexadecanoate	270	16:0	1.575597
855	18788	methyl hexadecenoate	268	16:1	1.52244
858	13526	?	224		1.096046
870	36652	?	224		2.970005
878	6106	?			0.494785
882	6763	?			0.548023
897	9576	?	192		0.775968
900	3118	?			0.252659
906	7376	?			0.597696
912	63030	?	252		5.107482
921	16554	methyl octadecanoate	298	18:0	1.341413
938	23640	methyl oleate	296	18:1	1.915609
946	26257	?	278		2.127672
953	10073	?	278		0.816241
960	13910	?	278		1.127163
964	11648	?	328		0.943867
1003	64130	?	310		5.196617
1009	19288	?	306		1.562956
1056	16580	?			1.34352
1071	29274	?			2.372147
1097	5514	?	330		0.446813
1196	38161	?	330		3.092283
1228	17094	?			1.38517
1259	9691	?	364		0.785286
1270	26556	?	330		2.1519
1308	11809	?	336		0.956913
1320	18043	?	336		1.46207
	1E+06	Total			100

Table 4, 7/20/06 sediment Waterpark

MS Data File = FM36473.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
178	61072	methyl isobutyl ketone (MIBK)	100		10.20222
185	10298	methyl ester of 3-methylbutanoic acid	116		1.720304
193	5418	toluene	92		0.905089
204	4873	2-methyl-3-pentanone	100		0.814046
223	4279	2-hexanone	100		0.714817
236	2049	?			0.34229
274	532	n-nonane	128		0.088872
289	3073	methyl methacrylate	100		0.513352
299	244	methyl hexanoate	130	6:0	0.040761
309	1546	3-hexanol	102		0.258263
315	701	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis)	142		0.117104
327	2209	2-hexanol	102		0.369018
331	1921	1-methylcyclopentanol	100		0.320907
341	2398	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142		0.400591
361	4922	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		0.822231
367	1705	2-propenyl ester of 2-butenoic acid	126		0.284824
372	3604	methyl ester of 3-methyl-2-heptenoic acid	156		0.602056
385	1911	2-propenyl ester of 2-methyl, 2-butenoic acid	140		0.319237
390	3533	2-propenyl ester of 3-methyl butanoic acid	142		0.590196
397	3753	?			0.626947
404	1686	2-methylcyclopentanol	100		0.28165
417	48608	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174		8.120077
428	5324	possibly methyl ester of 4-butoxybutyric acid	174		0.889386
435	5593	n-undecane	156		0.934323
442	86202	?	172		14.40024
456	73379	possibly methyl ester of 4-butoxybutyric acid	174		12.25813
466	1320	?	182		0.220509
472	7540	?	182		1.259574
484	4232	3-butyl-3-octen-2-one	182		0.706965
491	650	dihydrojasmone	166		0.108584
496	4626	2-ethylhexyl alcohol	130		0.772784
505	13504	?	182		2.255874
543	1029	? cyclohexenone derivative	138		0.171897
556	1346	? cyclohexenone derivative	138		0.224852
570	4840	?	144		0.808533
582	2806	?			0.468749
587	3515	?			0.587189
590	3561	?			0.594873
601	16942	2,4,4-trimethylbut-2-enolide	126		2.8302
606	2822	?			0.471422

611	4991	?			0.833758
623	2650	? lactone			0.442689
631	3345	? cyclohexenone derivative	180		0.55879
637	894	? cyclohexenone derivative	180		0.149345
643	6487	?	194		1.083668
664	2112	methyl dodecanoate	214	12:0	0.352814
670	6388	artifact			1.06713
677	14263	dodecadione	198		2.382667
705	496	?	192		0.082858
722	36457	? cyclohexenone derivative	194		6.090225
729	4313	?	226		0.720496
736	4710	?	206		0.786816
752	41825	tridecadione	212		6.986962
787	2193	dimethyl nonanedioate	216		0.366346
814	6915	?	168		1.155167
818	3129	?	238		0.522707
828	1289	?	238		0.21533
843	1386	methyl hexadecanoate (branched)	270	16:0	0.231534
853	5635	?	224		0.94134
867	10106	?	224		1.68823
894	2057	?	192		0.343627
906	1249	?	252		0.208648
918	926	?	252		0.15469
921	1077	?	192		0.179915
929	314	methyl octadecanoate	298	18:0	0.052454
932	1264	methyl oleate	296	18:1	0.211154
957	535	methyl linoleate	294	18:2	0.089373
984	2901	methyl linolenate	292	18:2	0.484619
1006	1947	?	306		0.325251
1046	2489	phenanthrene or anthracene	178		0.415793
1067	3987	?	306		0.666037
1192	3008	?	330		0.502493
1254	1529	methyl abietate (wood rosin)	314		0.255423
1285	2024	?	336		0.338114
1315	2008	?	336		0.335441
1354	2150	pyrene or fluoranthene	202		0.359162
	598615	Total			100

Table 5, 7/20/06 GFF Waterpark

MS Data File = FM36474.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
477	843	?			3.462012
520	761	artifact			3.125257
557	1272	artifact			5.223819
632	148	?	180		0.607803
645	220	?	208		0.903491
661	187	methyl dodecanoate	214	12:0	0.767967
677	368	dodecadione	198		1.511294
699	1739	artifact			7.141684
715	223	?	192		0.915811
721	583	? cyclohexenone derivative	194		2.394251
730	1504	?	226		6.176591
752	942	tridecadione	212		3.868583
757	2235	methyl tetradecanoate	242	14:0	9.178645
781	251	methyl hexadecanoate (branched)	270	16:0	1.030801
802	517	methyl hexadecanoate (branched)	270	16:0	2.123203
826	1440	artifact			5.913758
845	7398	methyl hexadecanoate	270	16:0	30.38193
857	1082	?	196		4.443532
886	288	methyl octadecanoate (branched)	298	18:0	1.182752
925	2137	methyl octadecanoate	298		8.776181
933	212	methyl oleate	296	18:1	0.870637
	24350	Total			100

Table 6, 7/20/06 Sediment Navy Yard

MS Data File = FM36472.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
179	27923	methyl isobutyl ketone (MIBK)	100		3.474341
186	33001	methyl ester of 3-methylbutanoic acid	116		4.106175
224	5645	3-heptanone	114		0.702384
269	401	methyl hexanoate	130	6:0	0.049895
290	6867	methyl methacrylate	100		0.854432
310	1090	3-hexanol	102		0.135624
324	616	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis)	142		0.076646
328	1266	2-hexanol	102		0.157523
332	1533	1-methylcyclopentanol	100		0.190745
342	5477	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142		0.68148
363	19985	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		2.486649
373	802	methyl heptanoate	144	7:0	0.099789
385	2116	2-propenyl ester of 2-butenoic acid	126		0.263285
398	1162	?			0.144583
403	1931	methyl ester of 3-methyl-2-heptenoic acid	156		0.240266
411	831	2-methylcyclopentanol	100		0.103398
417	18187	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174		2.262932
428	7302	possibly methyl ester of 4-butoxybutyric acid	174		0.908557
436	5978	n-undecane	156		0.743817
443	76230	?	172		9.484977
456	26575	possibly methyl ester of 4-butoxybutyric acid	174		3.306615
460	850	?	182		0.105762
466	599	?	182		0.074531
471	1960	?	142		0.243875
484	3207	3-butyl-3-octen-2-one	182		0.399033
491	1369	dihydrojasmone	166		0.170339
497	2235	2-ethylhexyl alcohol	130		0.278092
505	10553	?	182		1.313065
512	278	? cyclohexenone derivative	138		0.03459
515	1229	methyl, 2-hydroxy-4-methylpentanoate	146		0.152919
523	948	methyl ester of 3,4,4-trimethyl-5-oxo-2-hexenoic acid	152		0.117956
543	732	? cyclohexenone derivative	138		0.09108
555	1515	methyl decanoate	186		0.188505
567	517	methyl benzoate	136		0.064328
571	2272	?	144		0.282695
583	1244	methyl ester of 2-ethyl, 2-propyl hexanoic acid	200		0.154786
601	5098	2,4,4-trimethylbut-2-enolide	126		0.634323
607	7857	?			0.977613
613	10607	?			1.319784
624	3768	? lactone			0.468836
632	9631	? cyclohexenone derivative	180		1.198345

646	28621	?	194		3.56119
661	4482	methyl dodecanoate	214	12:0	0.557676
672	3162	artifact			0.393434
678	14604	dodecadione	198		1.817114
683	1790	methyl tridecanoate (branched isomer)	228	13:0	0.222722
707	1271	?	192		0.158145
710	2655	methyl tridecanoate	228	13:0	0.33035
717	5174	? cyclohexenone derivative	194		0.643779
722	33389	? cyclohexenone derivative	194		4.154452
731	12839	?	226		1.597503
737	3686	?	206		0.458633
741	2556	?	226		0.318032
754	51508	tridecadione	212		6.408923
757	5411	methyl tetradecanoate	242	14:0	0.673268
762	650	?	252		0.080877
768	1357	methyl pentadecanoate (branched)	256	15:0	0.168846
776	2505	?	214		0.311687
781	2023	methyl pentadecanoate (branched)	256	15:0	0.251713
784	724	?	182		0.090084
788	5382	dimethyl nonanedioate	216		0.66966
796	1989	2-isopropylphenol	136		0.247483
802	3033	methyl pentadecanoate	256	15:0	0.377383
808	637	?	236		0.079259
812	4782	?	176		0.595004
815	2571	?	168		0.319899
824	1950	methyl hexadecanoate (branched)	270	16:0	0.24263
829	3704	?	238		0.460873
836	1074	?			0.133633
846	31518	methyl hexadecanoate	270	16:0	3.921652
854	24286	methyl hexadecenoate	268	16:1	3.021804
869	21845	methyl heptadecanoate (branched)	284	17:0	2.718081
873	1258	methyl heptadecanoate (branched)	284	17:0	0.156528
876	3018	?	192		0.375517
879	3673	?	238		0.457016
886	2688	methyl heptadecanoate	284	17:0	0.334456
896	17661	?	192		2.197484
909	6705	methyl octadecanoate (branched)	298	18:0	0.834275
919	3177	?			0.395301
922	1601	?	252		0.199206
926	13708	methyl octadecanoate	298	18:0	1.705629
934	22026	methyl oleate	296	18:1	2.740602
942	3151	?	304		0.392066
951	4304	methyl linoleate	294	18:2	0.535529
963	2720	?	312		0.338438
973	2777	?	310		0.34553
977	2198	?	306		0.273488
985	5195	methyl linolenate	292	18:2	0.646392
1000	6481	?			0.806403
1007	11559	methyl eicosanoate	326	20:0	1.438238

1018	10258	?	306		1.27636
1019	11391	methyl eicosenoate	324	20:1	1.417334
1103	7395	methyl docosanoate	354	22:0	0.920129
1111	3757	?	276		0.467468
1117	11758	methyl docosenoate	352	22:1	1.462998
1166	5264	methyl tricosanoate	368	23:0	0.654977
1193	11807	?	330		1.469095
1242	6319	methyl tetradocosanoate	382	24:0	0.786246
1255	7553	methyl abietate (wood rosin)	314		0.939788
1266	3391	?	330		0.421928
1277	3487	?	330		0.433873
1305	5590	?	336		0.69554
1317	7099	?	336		0.883299
1336	2158	methyl pentacosanoate	396	25:0	0.268511
	803692	Total			100

Table 7, 11/16/06 sediment Bladensburg

MS Data File = FM36477.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.	Area %
180	110747	methyl isobutyl ketone (MIBK)	100	3.634973
187	2964	methyl ester of 3-methylbutanoic acid	116	0.097285
206	539	2-methyl-3-pentanone	100	0.017691
225	3258	2-hexanone	100	0.106935
238	2449	?		0.080382
275	1734	n-nonane	128	0.056914
290	4866	4-methyl-2-pentanol	102	0.159713
311	5775	3-hexanol	102	0.189549
317	1239	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis)	142	0.040667
329	8375	2-hexanol	102	0.274887
333	8213	1-methylcyclopentanol	100	0.26957
341	1597	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142	0.052417
346	556			0.018249
357	2555	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156	0.083861
363	2950	methyl ester of 3-methyl-2-heptenoic acid	156	0.096826
369	2223	3-ethyl-4-methyl-3-penten-2-one	126	0.072964
374	10855	?	156	0.356286
387	6244	2-propenyl ester of 2-methyl, 2-butenoic acid	140	0.204943
393	8252	2-propenyl ester of 3-methyl butanoic acid	142	0.27085
406	7947	?	130	0.260839
421	185133	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174	6.076493
451	305808	?	172	10.03733
460	176473	possibly methyl ester of 4-butoxybutyric acid	174	5.792252
470	6099	?	182	0.200183
476	61492	?	182	2.01831
487	22931	3-butyl-3-octen-2-one	182	0.752648
494	5211	dihydrojasmone	166	0.171037
499	3448	2-ethylhexyl alcohol	130	0.113171
509	74082	?	182	2.431543
514	4232	?	138	0.138904
521	2801	?	156	0.091935
525	4360	?	152	0.143105
533	3383	?	144	0.111038
544	8738	?	138	0.286801
558	2117	?	150	0.069485
568	3558	?		0.116782
573	1786	?		0.058621
585	14842	?		0.487149
589	5489	?		0.180162
592	12077	?	170	0.396395
603	52078	2,4,4-trimethylbut-2-enolide	126	1.70932
607	15874	?		0.521021

614	15001	?		0.492367
621	814	? lactone		0.026717
626	11863	? cyclohexenone derivative	180	0.389371
636	83849	? cyclohexenone derivative	180	2.752118
641	5637	?		0.185019
649	81670	?	194	2.680598
653	6427	possibly methyl ester of 2-propylheptanoic acid	170	0.210949
664	4503	?	184	0.147799
668	1732	?	180	0.056848
675	40717	artifact		1.336426
682	98638	dodecadione	198	3.237527
685	7954	?	224	0.261069
694	709	?	180	0.023271
699	737	?	192	0.02419
728	206862	? cyclohexenone derivative	194	6.789689
735	107315	?	226	3.522326
742	39592	?	206	1.299501
757	162126	tridecadione	212	5.32135
761	43779	?	196	1.436928
773	10889	?	206	0.357402
781	5433	?	238	0.178324
791	42016	dimethyl nonanedioate	216	1.379062
796	7012	?		0.23015
817	58844	?	168	1.931396
821	37364	?	238	1.226373
832	33833	?	238	1.110477
842	17290	?	238	0.567498
847	20895	?	238	0.685822
857	82482	?	224	2.70725
873	121087	?	224	3.974355
878	15655	?	206	0.513833
882	16357	?	238	0.536875
896	11835	?	192	0.388452
925	32599	?	278	1.069975
936	9500	?	238	0.311812
944	22781	?	304	0.747725
967	18531	?	304	0.60823
980	19189	?	292	0.629827
1010	42774	?	306	1.403942
1017	24743	?	306	0.812122
1047	11585	?	306	0.380246
1053	13985	?	306	0.45902
1072	72548	?	324	2.381193
1122	14974	?	314	0.491481
1144	10817	?	408	0.355039
1195	26438	?	330	0.867756
1232	17145	?	336	0.562739
1254	29904	?	388	0.981518
1268	11168	?	330	0.36656

1289	26091	?	336	0.856367
1309	17484	?	336	0.573865
1322	36792	?	336	1.207598
1333	11750	?	336	0.385662
1361	9643	?	402	0.316506
	3E+06	Total		100

Table 8, 11/16/06 GFF Bladensburg

MS Data File = FM36476.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.	Area %
178	10182	methyl isobutyl ketone (MIBK)	100	1.398761
185	10380	methyl ester of 3-methylbutanoic acid	116	1.425961
224	2232	2-hexanone	100	0.306623
290	480	methyl methacrylate	100	0.06594
310	248	3-hexanol	102	0.034069
328	271	2-hexanol	102	0.037229
332	309	1-methylcyclopentanol	100	0.042449
342	384	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142	0.052752
362	689	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156	0.094652
373	367	methyl ester of 3-methyl-2-heptenoic acid	156	0.050417
386	409	2-propenyl ester of 2-methyl, 2-butenoic acid	140	0.056187
391	625	2-propenyl ester of 3-methyl butanoic acid	142	0.08586
397	138	?		0.018958
404	270	?	130	0.037091
411	228	?	130	0.031322
418	21569	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174	2.96306
436	2250	n-undencane	156	0.309096
443	36065	?	172	4.95446
457	34054	possibly methyl ester of 4-butoxybutyric acid	174	4.678197
460	1158	?	182	0.159081
466	2035	?	182	0.27956
472	1957	?		0.268845
485	6157	3-butyl-3-octen-2-one	182	0.845823
491	695	dihydrojasmone	166	0.095476
506	19115	?	182	2.625939
513	788	?	138	0.108252
524	390	?	152	0.053577
571	2409	?	144	0.330938
583	1301	?		0.178726
588	795	?		0.109214
591	1412	?	170	0.193975
601	1197	2,4,4-trimethylbut-2-enolide	126	0.164439
606	1694	?		0.232715
616	893	?		0.122677
625	1557	? lactone		0.213894
633	8646	? cyclohexenone derivative	180	1.187752
639	2265	? cyclohexenone derivative	180	0.311156
645	25112	?	194	3.449782
652	651	possibly methyl ester of 2-propylheptanoic acid	170	0.089432
659	623	?	184	0.085585
663	741	?	180	0.101796

672	6483	artifact		0.890608
678	8786	dodecadione	198	1.206984
688	728	?	224	0.10001
701	1003	?	180	0.137788
707	1678	?	192	0.230517
725	114211	? cyclohexenone derivative	194	15.68983
733	31202	?	226	4.286401
739	8426	?	206	1.157529
744	1513	?		0.20785
750	812	?	166	0.111549
756	113987	tridecadione	212	15.65906
772	2186	?	196	0.300304
779	1767	?	206	0.242743
785	1194	?	238	0.164027
790	9327	dimethyl nonanedioate	216	1.281305
813	5328	?	218	0.731939
820	6996	?	294	0.961081
825	1188	?		0.163203
830	5217	?	238	0.71669
837	1924	?	294	0.264311
840	1468	?	238	0.201668
845	2763	?	238	0.379569
856	24566	?	224	3.374775
860	5916	?		0.812716
871	46584	?	224	6.399516
877	5165	?	206	0.709546
880	3637	?	238	0.499636
896	4132	?	192	0.567637
931	2525	?	238	0.346874
964	4736	?	304	0.650612
986	4507	?	306	0.619153
1009	21539	?	306	2.958938
1016	5954	?	306	0.817936
1033	1565	?	306	0.214993
1071	24186	?	324	3.322572
1121	2481	?	314	0.340829
1193	7304	?	330	1.003393
1230	4894	?	336	0.672317
1252	4109	?	336	0.564477
1266	2322	?	336	0.318987
1288	3770	?	336	0.517907
1306	5281	?	336	0.725482
1319	11829	?	336	1.625019
	727930	Total		100

Table 9, 11/16/06 sediment waterpark

MS Data File = FM36469.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
187	421468	methyl isobutyl ketone (MIBK)	100		14.15267
190	26173	methyl ester of 3-methylbutanoic acid	116		0.878875
223	5859	3-heptanone	114		0.196742
242	9930	5-methyl-3-hexen-2-one	112		0.333444
248	793	2,4,4-trimethylbut-2-enolide	126		0.026629
270	563	methyl hexanoate	130	6:0	0.018905
275	935	n-nonane	128		0.031397
290	38138	propylene glycol, monomethacrylate	144		1.280653
301	442				0.014842
304	1417	?	142		0.047582
311	2514	3-hexanol	102		0.084419
316	2354	3-methyl-3-hepten-2-one	126		0.079046
325	3887	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis isomer)	142		0.130523
328	3015	2-hexanol	102		0.101242
333	2254	1-methylcyclopentanol	100		0.075688
344	36986	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans isomer)	142		1.24197
356	2182	?	156		0.07327
365	49957	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		1.677529
369	5478	?	126		0.183948
374	10587	methyl ester of 3-methyl-2-heptenoic acid	156		0.355506
379	10933	2-propenyl ester of 2-butenoic acid	126		0.367124
386	7462	dimethyl ester of 3,3-dimethylpentadioate	188		0.25057
392	7763	2-propenyl ester of 3-methylbutanoic acid	142		0.260677
406	4159	?			0.139657
422	166497	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174		5.590879
429	580				0.019476
438	29335	n-undecane	156		0.985053
448	212572	?	172		7.138053
461	168045	possibly methyl ester of 4-butoxybutyric acid	174		5.64286
468	3391	?	182		0.113868
474	15259	2,6-dimethyl-4-heptanone	142		0.512389
486	12048	3-butyl-3-octen-2-one	182		0.404565
492	5472	dihydrojasmone	166		0.183747
498	1467	?	170		0.049261
507	44115	?	182		1.481358
516	7054	? cyclohexenone derivative	138		0.23687
520	3101	?	156		0.10413
523	2492	?	156		0.08368
526	1570				0.05272
531	10114	methyl ester of a C11 branched fatty acid	200		0.339623
546	10124	methyl ester of a C12 branched fatty acid	214		0.339958

559	9692	?			0.325452
572	16564	?	144		0.55621
585	8501	?	184		0.285459
589	32480	?	154		1.090661
604	70029	2,4,4-trimethylbut-2-enolide	126		2.351536
609	17999	?			0.604397
614	27430	methyl ester of 4-oxooctanoate	174		0.921085
620	969				0.032538
625	21229	?			0.712858
634	29214	methyl ester of butanoic acid, 4-(2-methoxy-1-methyl-2-oxoetho	188		0.98099
640	7315	? cyclohexenone derivative	180		0.245634
645	35158	?	194		1.180587
674	45434	artifact			1.525649
680	48846	dodecadione	198		1.640222
728	194232	? cyclohexenone derivative	194		6.522206
733	41466	?	226		1.392406
740	47112	?	206		1.581995
759	211010	tridecadione	212		7.085602
777	22535	?	242		0.756713
790	18442	dimethyl nonanedioate	216		0.619272
795	5500	?	210		0.184687
813	16530	?	176		0.555068
816	16870	?	168		0.566485
820	21020	?	294		0.70584
830	14761	?	238		0.495666
847	20616	methyl hexadecanoate	270	16:0	0.692274
856	58796	?	224		1.974338
871	89900	?	224		3.018793
878	23049	?	306		0.773973
897	15108	?	192		0.507318
911	35838	?	252		1.203421
921	40858	?			1.37199
926	8220	methyl stearate	298	18:0	0.276023
931	5340	?			0.179314
937	15029	?			0.504666
943	19110	methyl oleate	296	18:1	0.641703
986	17489	?			0.587271
1001	28577	?	310		0.9596
1009	41963	?	306		1.409095
1071	70356	?	324		2.362516
1195	34509	?	330		1.158794
1231	7917	?	336		0.265849
1254	16680	?	336		0.560105
1269	15162	?	330		0.509132
1289	11479	?	336		0.385459
1308	17723	?	336		0.595129
1323	46648	?	336		1.566415
1334	8821	?	336		0.296204
	3E+06	Total			100

Table 10, 11/16/06 GFF waterpark

MS Data File = FM36466.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.	Area %
179	151552	methyl isobutyl ketone (MIBK)	100	13.50322
221	2058	3-heptanone	114	0.183367
236	1072	artifact		0.095515
241	11307	5-methyl-3-hexen-2-one	112	1.007449
256	179	artifact		0.015949
274	360	n-nonane	128	0.032076
290	2830	2-hexanol	102	0.252152
317	415	methyl butanedioic acid (monomethyl succinate)	132	0.036976
328	652	2-heptanol	116	0.058093
332	616	1-methylcyclopentanol	100	0.054885
340	422	3-methyl-3-hepten-2-one	126	0.0376
355	1251	methyl ester of 4,4-dimethyl-2-pentenoic acid	142	0.111464
373	4517	methyl ester of 3-methyl-2-heptenoic acid	156	0.402463
377	3110	2-propenyl ester of 2-butenoic acid	126	0.2771
384	2471	dimethyl ester of 3,3-dimethylpentadioate	188	0.220165
390	1334	2-propenyl ester of 3-methylbutanoic acid	142	0.118859
418	79101	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174	7.047864
436	9759	n-undecane	156	0.869523
442	58760	?	172	5.23549
457	109364	possibly methyl ester of 4-butoxybutyric acid	174	9.744284
465	1736	?	182	0.154677
471	4251	2,6-dimethyl-4-heptanone	142	0.378762
484	5067	3-butyl-3-octen-2-one	182	0.451467
491	1262	dihydrojasmone	166	0.112444
504	16416	?	182	1.462658
511	2173	? cyclohexenone derivative	138	0.193613
568	2289	?	144	0.203949
580	3237	?		0.288415
588	8002		170	0.712975
599	19226	2,4,4-trimethylbut-2-enolide	126	1.713028
603	321			0.028601
608	2477	possibly a methyl ester of 4-oxooctanoate		0.2207
613	1690	?		0.150578
622	1166	?	194	0.10389
627	7521	methyl ester of butanoic acid, 4-(2-methoxy-1-methyl-2-oxoetho	188	0.670118
636	2041	? cyclohexenone derivative	180	0.181852
642	12213	?	194	1.088173
669	9830	artifact		0.875849
675	3372	dodecadione	198	0.300444

722	137369	? cyclohexenone derivative	194	12.23952
728	10259	?	226	0.914072
736	23847	?	206	2.124757
739	1156	?		0.102999
752	131465	tridecadione	212	11.71347
776	3644	?	206	0.324679
786	4400	dimethyl nonanedioate	216	0.392038
803	1527	?	252	0.136055
809	3309	?	178	0.29483
817	7197	?	294	0.64125
827	3761	?	238	0.335103
852	31857	?	224	2.838445
867	60553	?	224	5.395246
1005	24216	?	306	2.157635
1067	26976	?	324	2.40355
1192	15304	?	330	1.36358
1228	6970	?	336	0.621024
1249	11139	?	336	0.99248
1264	10275	?	330	0.915498
1283	11489	?	336	1.023665
1303	13365	?	336	1.190816
1316	30010	?	336	2.673878
1328	6832	?	336	0.608728
	1E+06	Total		100

Table 11, 11/16/06 sediment Navy Yard

MS Data File = FM36468.dat;1

MS Scan #	Area Integrat	Peak Assignment	M.W.		Area %
596	815	methyl 3-methylbutyrate	116		0.17469
631	454	?	180		0.097312
645	1858	?	208		0.398251
661	203	methyl-2-methylhexanoate	130		0.043512
671	1031	artifact			0.220989
677	2883	dodecadione	198		0.617953
721	22045	? cyclohexenone derivative	194		4.725211
730	12492	?	226		2.677584
737	1709	?	206		0.366314
753	56392	tridecadione	212		12.08728
775	3101	?	242		0.66468
784	3707	?	182		0.794573
788	7392	dimethyl nonanedioate	216		1.58443
812	5153	?	176		1.104514
818	3622	?	238		0.776354
829	5099	?	238		1.09294
835	1432	?	294		0.30694
844	8023	methyl hexadecanoate (methyl palmitate)	270	16:0	1.719681
853	8238	?	224		1.765765
858	8131	?	238		1.74283
868	30698	?	238		6.579929
877	12321	?	206		2.640931
888	4135	?			0.886312
896	6886	?	192		1.475972
904	2974				0.637459
909	28680	?	252		6.147383
919	13359	?	270		2.86342
922	12818	?	278		2.74746
925	3611	methyl stearate	298	18:0	0.773996
929	2394	?	318		0.513139
935	8456	?	318		1.812492
941	7959	methyl oleate	296	18:1	1.705963
951	8506	methyl linoleate	294	18:2	1.823209
985	11131	?			2.385862
999	12401	?	320		2.658079
1006	16540	?	306		3.545248
1015	16856	?	306		3.612981
1068	53958	methyl ester of 2-oxo-hexadecanoic acid	286		11.56557
1194	24459	?	330		5.242637
1226	5722	dimethyl ester of bicyclo 2.2.2 oct-2-ene-2,3-dicarboxylic acid, 1	324		1.226476

1278	10669	?	288	2.286835
1305	8178	?	336	1.752904
1316	10049	?	336	2.153942
	466540	Total		100

Table 12, 11/16/06 GFF Navy Yard

MS Data File = FM36478.dat;1

MS Scan #	Area Integ.	Peak Assignment	M.W.		Area %
185	10885	methyl ester of 3-methylbutanoic acid	116		2.52761
205	4092	2-methyl-3-pentanone	100		0.950205
224	4435	2-hexanone	100		1.029853
288	2845	methyl methacrylate	100		0.660638
310	307	3-hexanol	102		0.071289
315	214	cyclohexanone	98		0.049693
324	340	methyl ester of 4,4-dimethyl-2-pentenoic acid (cis)	142		0.078952
327	522	2-hexanol	102		0.121214
332	493	1-methylcyclopentanol	100		0.11448
342	4311	methyl ester of 4,4-dimethyl-2-pentenoic acid (trans)	142		1.001059
363	15234	? methyl ester possibly a cyclopropane carboxylic acid derivativ	156		3.537493
370	182	methyl ester of 3-methyl-2-heptenoic acid	156		0.042262
384	298	2-propenyl ester of 2-methyl, 2-butenoic acid	140		0.069199
391	144	2-propenyl ester of 3-methyl butanoic acid	142		0.033438
405	582	?	130		0.135146
417	15575	dimethyl ester of 2-oxo-pentanedioic acid (dimethyl ketoglutarat	174		3.616676
436	955	n-undecane	156		0.221761
442	26080	?	172		6.056046
456	28465	possibly methyl ester of 4-butoxybutyric acid	174		6.609868
460	207	?	182		0.048068
465	239				0.055498
471	469	?	182		0.108907
484	1461	3-butyl-3-octen-2-one	182		0.339259
491	314	dihydrojasmone	166		0.072914
498	142	2-ethylhexyl alcohol	130		0.032974
505	5243	?	182		1.217479
512	389	?	138		0.09033
515	1802	methyl, 2-hydroxy-4-methylpentanoate	146		0.418443
519	139	?	156		0.032277
525	636	?	152		0.147686
530	857	?			0.199004
544	2223	?	138		0.516204
557	2244	methyl decanoate	186	10:0	0.52108
571	3969		144		0.921643
583	1047				0.243124
588	5417	?	116		1.257884
591	1570	?	170		0.36457
607	6990	?	144		1.62315
613	10296	?	144		2.390838
624	4129	lactone			0.958797
633	10335	? cyclohexenone derivative	180		2.399894

639	869	? cyclohexenone derivative	180	0.201791
644	6047	?	194	1.404176
655	714	?	214	0.165798
661	438	?	184	0.101708
663	445	?	180	0.103334
672	7130	artifact		1.65566
678	8889	dodecadione	198	2.064118
683	618	?	224	0.143506
701	691	?	180	0.160457
707	291	?	192	0.067573
710	672	? cyclohexenone derivative	194	0.156045
716	1932	?	208	0.44863
723	43478	? cyclohexenone derivative	194	10.09604
731	7236	?	226	1.680274
738	4579	?	206	1.063291
754	47701	tridecadione	212	11.07667
771	392	?	196	0.091026
776	2546	?	214	0.591208
784	523	?	238	0.121446
788	1832	dimethyl nonanedioate	216	0.425409
794	719	?	210	0.166959
812	2076	?	218	0.482069
819	3254	?	238	0.755613
830	2612	?	238	0.606533
836	546	?	238	0.126787
844	3412	?	238	0.792302
854	7369	?	224	1.711158
869	19462	?	224	4.519278
877	3843	?	206	0.892384
889	361	?	238	0.083828
895	4438	?	192	1.03055
910	4065	?	252	0.943935
920	8572	?	252	1.990507
923	2310	?	278	0.536406
1007	10902	?	306	2.531557
1069	11728	?	324	2.723363
1098	12191	?	364	2.830877
1193	6632	?	330	1.540019
1326	13052	?	426	3.03081
	430644	Total		100

Appendix B. Stable isotope data, micrograms carbon, nitrogen and C/N ratios. Means and standard deviations included where possible for each site and time point
Anacostia Samples
Macavoy, biology dept. American University

Date	item	number	mg sample	Micro g N	**d15N**	Micro g C	**d13C**	C/N	**d34S**
6/8/06	sed 1	navy yard	113.8	10.3	**5.27**	182.5	**-19.53**	17.7	**10.90**
6/8/06	sed 2	navy yard	103.6	9.5	**5.62**	171.4	**-18.02**	18.0	**1.93**
7/20/06	sed 1	bladensburg	23.4	16.3	**1.83**	268.2	**-26.23**	16.5	**-3.54**
7/20/06	sed2	bladensburg	28.4	21.0	**2.07**	320.4	**-27.04**	15.2	**-5.65**
7/20/06	sed 3	bladensburg	33	18.5	**2.35**	279.4	**-26.35**	15.1	
		means			2.08		-26.54	15.61	-4.60
		s.d.			0.26		0.44	0.76	1.49
7/20/06	GFF	bladensburg 1	6.1	26.2	**3.38**	198.7	**-27.71**	7.6	**3.92**
7/20/06	GFF	bladensburg 2	7.4	26.4	**3.44**	202.4	**-27.98**	7.7	
7/20/06	sed	1 water park	13.3	9.1	**3.79**	159.3	**-26.04**	17.5	**-3.18**
7/20/06	sed	2 water park	14.7	4.8	**-2.68**	58.6	**-26.27**	12.1	**-5.45**
7/20/06	sed	3 water park	14.4	2.7	**-5.45**	25.0	**-23.81**	9.4	**-2.28**
		means			-1.45		-25.37	13.01	-3.64
		s.d.			4.74		1.36	4.08	1.63
7/20/06	GFF	water park 1	10.7	38.2	**4.10**	250.8	**-31.16**	6.6	
7/20/06	GFF	water park 2	?	55.5	**4.05**	352.7	**-31.08**	6.4	**2.59**
7/20/06	GFF	water park 3	6.3	39.6	**3.72**	249.6	**-31.11**	6.3	**2.85**
		means			3.96		-31.12	6.41	2.72
		s.d.			0.21		0.04	0.14	0.18
7/20/06	sed 1	Navy Yard 1	27.4	9.3	**3.24**	155.9	**-24.67**	16.8	
7/20/06	sed 2	Navy Yard 2	26.9	8.8	**1.95**	157.0	**-24.49**	17.9	
7/20/06	sed 3	Navy Yard 3	30.3	8.7	**3.86**	180.5	**-26.46**	20.7	**-0.68**
		means			3.02		-25.21	18.43	
		s.d.			0.97		1.09	2.00	
7/20/06	GFF 1	Navy Yard 1	7.2	24.5	**4.70**	196.3	**-31.69**	8.0	**3.21**
7/20/06	GFF 2	Navy Yard 2	12.6	35.6	**4.83**	294.7	**-31.74**	8.3	
		means			4.77		-31.71	8.15	
		s.d.			0.09		0.04	0.19	

			mg sample	Micro g N	**d15N**	Micro g C	**d13C**	C/N	**d34S**
11/16/06	soil	bladensburg 1	31.9	19.6	**3.24**	347.7	**-26.17**	17.7	**2.24**
11/16/06	soil	bladensburg 2	36.8	28.7	**3.21**	429.7	**-26.45**	15.0	**0.67**
11/16/06	soil	bladensburg 3	35	30.1	**3.77**	522.8	**-26.04**	17.4	
		means			3.41		-26.22	16.69	1.46
		s.d.			0.32		0.21	1.49	1.11
11/16/06	GFF	bladensburg 1	0.0052	11.4	**4.55**	134.1	**-26.94**	11.8	
11/16/06	GFF	bladensburg 2	0.0037	19.3	**4.74**	260.8	**-24.79**	13.5	
		means			4.65		-25.86	12.63	
		s.d.			0.14		1.52	1.23	
11/16/06	sed	waterpark 1	58.3	49.2	**4.90**	687.9	**-23.31**	14.0	**0.55**
11/16/06	sed	waterpark 2	46.2	42.4	**5.04**	617.2	**-23.36**	14.6	**0.23**
11/16/06	sed	waterpark 3	40.9	41.3	**4.59**	581.2	**-24.30**	14.1	
		means			4.84		-23.66	14.20	0.39
		s.d.			0.23		0.56	0.32	0.23
11/16/06	GFF extra	waterpark 1	0.0073	11.9	**3.59**	229.7	**-18.37**	19.3	
11/16/06	GFF not e	waterpark 2	0.0101	24.9	**5.23**	720.2	**-14.79**	28.9	
		means			4.41		-16.58	24.09	
		s.d.			1.15		2.53	6.77	
11/16/06	sed	navy yard 1	76.7	42.4	**5.69**	901.5	**-26.14**	21.3	**3.47**
11/16/06	sed	navy yard 2	63.9	17.3	**5.07**	407.3	**-26.36**	23.5	
11/16/06	sed	navy yard 3	63.5	18.9	**5.23**	336.5	**-25.96**	17.8	
		means			5.33		-26.15	20.86	3.47
		s.d.			0.32		0.20	2.86	
11/16/06	GFF	navy yard 1	0.015	71.7	**3.87**	953.7	**-24.80**	13.3	