Differences in dissolved organic matter composition between rivers and estuaries is conserved across freshwater and saltwater coastal regions

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Table S1: Site level metadata for each sampling location. Additional metadata is available at Pennington et al., 2023

ID	Latitude	Longitude	System	Region	Water Type (Consortium Reported)	Water Type
K004	41.502	-83.0435	Great Lakes	Great Lakes	Tidal River	Riverine
K008	41.3824	-82.5147	Great Lakes	Great Lakes	Lacestuary	Estuarine
K009	41.3754	-82.5164	Great Lakes	Great Lakes	Lacestuary	Estuarine
K010	41.3734	-82.5091	Great Lakes	Great Lakes	Lacestuary	Estuarine
K011	41.3772	-82.51	Great Lakes	Great Lakes	Lacestuary	Estuarine
K012	43.5831	-83.688	Great Lakes	Great Lakes	Tidal Stream	Riverine
K013	43.9688	-83.8603	Great Lakes	Great Lakes	Lake	Estuarine
K015	37.4147	-76.7161	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine
K016	37.3044	-76.5539	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine
K017	37.5678	-76.8867	Chesapeake Bay	Mid-Atlantic	Tidal River	Riverine
K018	37.2192	-76.4136	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine
K019	46.6533	-92.2266	Great Lakes	Great Lakes	Lacestuary	Estuarine
K021	41.6056	-83.1526	Great Lakes	Great Lakes	Lacestuary	Estuarine
K022	41.4629	-82.9971	Great Lakes	Great Lakes	Lacestuary	Estuarine
K023	38.8014	-76.7033	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K024	38.2087	-75.8044	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine
K025	38.8873	-76.5621	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K026	37.7106	-75.6117	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K029	39.4188	-75.3786	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K030	39.0884	-75.4374	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K033	47.1041	-88.5153	Great Lakes	Great Lakes	Lacustuary	Estuarine
K034	38.7746	-75.9752	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine

K035	38.5922	-76.1307	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine
K036	39.0412	-76.2218	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine
K037	37.5569	-76.9731	Chesapeake Bay	Mid-Atlantic	Tidal River	Riverine
K038	37.3264	-77.2078	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K040	37.4559	-75.8335	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K041	37.4557	-75.8334	Chesapeake Bay	Mid-Atlantic	Tidal River	Riverine
K042	39.8816	-75.2665	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K043	39.062	-75.394	Delaware Bay	Mid-Atlantic	Estuary	Estuarine
K045	39.9886	-74.8467	Delaware Bay	Mid-Atlantic	Tidal River	Riverine
K046	39.0892	-75.4365	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K047	43.4162	-86.3489	Great Lakes	Great Lakes	Lacestuary	Estuarine
K048	39.8803	-75.2667	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K049	42.6708	-86.2107	Great Lakes	Great Lakes	Lake	Estuarine
K050	37.3344	-77.2072	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K051	38.5747	-76.2191	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K052	38.1595	-75.7905	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K053	38.812	-76.7083	Chesapeake Bay	Mid-Atlantic	Tidal Stream	Riverine
K054	38.9677	-75.3703	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K055	39.8055	-75.2077	Delaware Bay	Mid-Atlantic	Tidal stream	Riverine
K056	39.1838	-74.8511	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K058	39.2576	-75.0905	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K059	38.4292	-76.2374	Chesapeake Bay	Mid-Atlantic	Open Water	Estuarine
K060	39.3259	-75.4749	Delaware Bay	Mid-Atlantic	Estuary	Estuarine
K061	39.2157	-75.4618	Delaware Bay	Mid-Atlantic	Tidal Stream	Riverine
K062	38.8753	-76.5513	Chesapeake Bay	Mid-Atlantic	Estuary	Estuarine

Table S2: Site-level data for dissolved organic carbon (DOC), pH, salinity, alkalinity, total suspended solids (TSS), total dissolved nitrogen (TDN), and redox potential (ORP)

ID	DOC (mg/L)	pH	Salinity (psu)	TDN (mg/L	TSS (mg/L)	Alkalinity (mg/L CaCO3)	ORP (mV)
K004	7.31	7.69	0.25	2.54	45	102	360
K008	2.97	7.74	0.20	0.43	31	111	315
K009	7.03	7.58	0.26	0.67	221	166	305
K010	7.20	7.57	0.30	1.24	78	170	291
K011	3.28	7.83	0.20	0.54	39	108	262
K012	15.01	6.81	0.27	2.29	1234	164	350
K013	7.73	7.69	0.31	2.58	296	199	296
K015	4.50	7.29	16.05	0.56	63	67	334
K016	5.06	7.12	20.51	0.58	50	74	311
K017	5.08	7.07	2.70	0.44	89	33	328
K018	3.17	7.77	20.46	0.43	37	73	314
K019	7.62	7.90	0.18	0.49	5	105	322
K021	30.37	7.52	0.27	1.96	56	167	298
K022	27.65	7.28	0.22	1.74	17	126	322
K023	3.58	7.03	0.20	0.47	12	52	311
K024	7.63	6.87	12.93	0.56	18	63	325
K025	5.78	6.44	2.65	0.74	28	40	334
K026	6.33	7.38	31.86	1.44	382	131	347
K029	5.07	6.62	5.01	0.77	133	106	301
K030	7.00	6.70	13.31	0.85	51	76	354

K033	4.25	7.55	0.15	0.44	4	89	322
K034	5.89	6.92	1.75	0.83	19	57	180
K035	4.21	7.07	10.96	0.54	18	66	308
K036	4.04	7.97	6.60	0.57	12	86	300
K037	5.94	6.67	0.41	0.38	9	28	348
K038	4.50	7.07	0.10	0.34	34	48	350
K040	3.00	7.67	32.62	0.36	30	131	283
K041	6.50	7.29	33.34	0.54	54	124	265
K042	3.40	6.75	0.28	1.25	15	113	339
K043	3.91	7.52	20.62	0.72	137	107	289
K045	8.47	6.42	0.09	0.90	7	17	315
K046	7.96	6.73	15.84	0.93	180	111	304
K047	4.84	7.23	0.31	0.58	4	172	329
K048	3.36	6.98	0.27	1.29	9	94	321
K049	7.54	7.66	0.14	0.60	5	128	279
K050	5.26	6.08	0.06	0.66	24	18	357
K051	8.37	6.60	12.19	0.70	20	51	290
K052	7.03	6.92	15.06	0.60	25	92	263
K053	4.47	7.02	0.22	0.50	15	62	330
K054	10.01	7.00	10.30	1.64	616	192	150
K055	3.42	7.17	0.16	1.07	15	46	292
K056	8.84	6.89	18.38	0.96	206	175	-164
K058	6.43	6.90	15.76	0.54	31	95	285

K059	6.14	7.14	12.52	0.49	55	85	327
K060	3.56	7.17	7.38	1.16	162	77	277
K061	7.26	6.98	12.04	1.44	73	197	87
K062	6.08	7.22	7.54	0.99	53	133	244

Table S3: Site-level optical data including specific UV absorbance at 254 nm (SUVA) and the relative proportions of each PARAFAC component

ID	$SUVA_{254}$	PercC1	PercC2	PercC3	PercC4	PercC5
K004	3.39	41.97	32.63	11.25	11.16	2.98
K008	1.89	39.35	30.95	9.88	18.46	1.36
K009	3.19	37.51	30.74	9.73	17.23	4.79
K010	2.78	39.39	32.47	9.96	14.04	4.15
K011	2.15	39.49	30.87	10.18	17.55	1.91
K012	5.37	43.64	31.51	10.67	10.59	3.59
K013	3.22	41.67	30.70	12.92	9.90	4.82
K015	2.98	42.58	32.09	11.59	12.54	1.20
K016	2.78	40.10	30.22	11.27	16.60	1.81
K017	3.23	44.05	33.01	10.52	9.94	2.49
K018	2.23	38.94	32.05	9.98	19.03	0.00
K019	3.42	47.42	32.86	10.39	8.50	0.83
K021	3.44	38.85	32.38	8.75	16.15	3.88
K022	3.57	44.72	31.85	10.44	9.21	3.79
K023	4.25	35.15	29.44	10.30	14.93	10.18
K024	3.33	44.09	31.71	12.36	9.41	2.43
K025	4.55	37.34	30.65	10.36	13.50	8.15
K026	3.56	36.81	27.12	14.35	14.40	7.32
K029	5.13	41.94	27.70	14.97	7.93	7.46

K030	3.84	40.20	29.13	14.04	8.69	7.94
K033	3.74	42.44	28.23	14.95	6.86	7.52
K034	3.38	43.57	31.49	11.48	9.09	4.37
K035	2.76	39.75	31.19	11.72	14.99	2.35
K036	3.14	40.88	29.51	12.53	14.95	2.14
K037	2.97	43.18	31.17	10.70	10.14	4.82
K038	3.34	41.08	30.10	9.93	14.47	4.41
K040	2.45	41.51	30.52	11.71	14.28	1.97
K041	3.05	41.93	30.39	12.19	11.67	3.82
K042	10.43	29.85	31.04	10.00	20.71	8.40
K043	2.29	39.08	30.80	10.87	16.27	2.98
K045	6.03	45.52	24.45	13.89	7.37	8.78
K046	4.28	40.21	28.64	14.17	9.83	7.15
K047	3.97	43.66	31.62	10.83	10.89	3.00
K048	3.50	34.20	32.28	8.88	18.71	5.93
K049	2.65	44.13	32.92	8.85	13.62	0.48
K050	4.63	42.43	28.01	11.68	8.62	9.25
K051	3.21	41.82	29.37	12.37	10.13	6.32
K052	3.16	43.41	31.21	11.95	11.21	2.23
K053	3.79	35.40	29.46	10.39	13.95	10.80
K054	4.23	43.22	27.54	15.18	7.08	6.98
K055	3.48	40.54	30.37	10.28	12.14	6.68

K056	3.96	40.65	28.85	14.49	9.25	6.76
K058	3.60	43.22	30.60	12.85	8.34	4.99
K059	3.04	44.20	32.18	11.17	10.89	1.56
K060	3.00	41.26	31.47	11.12	12.50	3.65
K061	3.81	41.64	29.63	13.95	7.49	7.29
K062	3.15	41.35	31.36	10.88	10.59	5.81

Table S4: Site-level FTICR-MS data including the mean carbon (C), hydrogen (H), oxygen (O), nitrogen (N), sulfur (S), double bond equivalents (DBE), modified aromaticity index (Almode), nominal oxidation state of carbon (NOSC), oxygen to carbon ratio (OC), hydrogen to carbon ratio (HC) and the relative proportions of identified formula identified as CHO, CHON, and CHOS

ID	Mass	C	H	O	N	S	Almod	DBE	NOSC	OC	HC	CHO	CHON	CHOS
K004	457.88	20.30	22.12	11.40	0.23	0.22	0.29	10.36	0.15	0.58	1.08	34.43	29.37	21.99
K008	457.36	20.43	24.12	11.23	0.33	0.10	0.22	9.56	0.03	0.57	1.18	36.11	36.72	13.92
K009	468.11	20.93	23.63	11.51	0.28	0.18	0.28	10.26	0.09	0.57	1.11	36.55	32.42	18.41
K010	461.99	20.86	23.44	11.20	0.33	0.15	0.29	10.32	0.07	0.55	1.11	34.67	35.63	16.06
K011	444.47	19.84	23.61	10.88	0.34	0.11	0.22	9.23	0.03	0.57	1.18	36.10	35.91	14.73
K012	447.07	19.71	21.30	11.14	0.32	0.22	0.30	10.22	0.17	0.58	1.07	32.56	31.52	20.17
K013	453.45	20.47	22.73	11.03	0.37	0.11	0.29	10.30	0.07	0.55	1.11	37.68	38.76	11.85
K015	446.81	19.82	22.19	10.99	0.28	0.22	0.28	9.88	0.11	0.57	1.11	32.76	30.97	20.58
K016	441.31	19.56	22.53	10.72	0.27	0.27	0.25	9.45	0.07	0.57	1.14	31.98	28.19	22.90
K017	460.69	20.56	22.50	11.44	0.22	0.17	0.30	10.44	0.12	0.57	1.09	36.89	30.34	19.47
K018	440.24	19.66	23.56	10.61	0.34	0.18	0.22	9.07	0.01	0.56	1.19	32.64	33.01	18.95
K019	477.58	21.20	22.03	12.25	0.18	0.09	0.33	11.29	0.19	0.59	1.03	41.85	31.98	15.98
K021	454.80	20.94	24.88	10.56	0.38	0.14	0.26	9.70	-0.05	0.52	1.17	34.37	35.39	15.67
K022	451.91	20.08	21.81	11.07	0.29	0.26	0.30	10.33	0.14	0.57	1.07	32.26	30.02	20.30
K023	446.58	20.10	23.03	10.63	0.27	0.23	0.27	9.75	0.02	0.54	1.14	34.96	29.65	21.47
K024	398.10	18.15	20.38	9.39	0.33	0.14	0.29	9.15	0.03	0.53	1.11	41.98	35.30	16.86
K025	461.19	20.62	23.27	11.31	0.24	0.19	0.27	10.13	0.07	0.56	1.12	34.92	31.58	19.93
K026	432.86	19.14	21.14	10.46	0.31	0.32	0.28	9.74	0.13	0.56	1.10	30.79	26.81	23.29
K029	445.75	19.73	21.09	11.08	0.22	0.25	0.31	10.30	0.16	0.58	1.06	37.08	25.78	23.07
K030	389.81	17.75	19.72	9.40	0.25	0.11	0.31	9.02	0.05	0.54	1.10	53.97	29.61	14.85

K033	460.57	20.57	22.22	11.69	0.17	0.06	0.30	10.56	0.12	0.58	1.08	53.04	29.36	11.37
K034	464.68	20.88	22.25	11.50	0.27	0.14	0.33	10.90	0.14	0.57	1.05	36.03	33.42	16.56
K035	444.96	19.96	23.22	10.71	0.32	0.20	0.26	9.52	0.04	0.55	1.15	33.80	32.60	18.83
K036	457.90	20.55	22.88	11.21	0.27	0.17	0.29	10.26	0.09	0.56	1.10	35.11	32.17	17.74
K037	468.70	21.30	23.19	11.49	0.22	0.10	0.31	10.82	0.09	0.56	1.07	39.67	33.09	14.82
K038	460.27	20.81	23.64	11.27	0.20	0.11	0.27	10.12	0.04	0.56	1.13	42.73	30.38	15.56
K040	426.86	19.28	22.72	10.15	0.32	0.18	0.25	9.10	0.00	0.54	1.17	37.09	30.47	18.92
K041	450.58	20.13	22.41	10.94	0.24	0.26	0.28	10.05	0.09	0.56	1.10	33.23	27.93	21.48
K042	455.06	21.13	24.98	10.29	0.25	0.26	0.26	9.78	-0.09	0.50	1.17	33.60	29.76	21.40
K043	450.79	20.10	22.74	10.96	0.32	0.21	0.25	9.91	0.09	0.56	1.12	32.31	31.39	19.14
K045	476.14	21.40	22.37	12.01	0.13	0.10	0.33	11.30	0.15	0.57	1.04	45.16	28.76	16.01
K046	408.57	18.74	20.68	9.37	0.32	0.23	0.30	9.59	0.03	0.52	1.11	36.56	33.38	19.37
K047	452.34	20.55	22.24	10.98	0.26	0.13	0.32	10.57	0.08	0.55	1.07	39.34	33.02	16.32
K048	455.85	21.04	24.57	10.49	0.24	0.24	0.26	9.89	-0.06	0.52	1.16	34.53	30.38	19.95
K049	468.12	21.12	22.79	11.64	0.29	0.06	0.32	10.88	0.13	0.57	1.06	40.16	38.57	10.70
K050	473.45	21.32	23.61	11.73	0.19	0.10	0.29	10.63	0.08	0.57	1.10	41.77	31.56	14.83
K051	475.39	21.55	23.86	11.53	0.21	0.18	0.30	10.74	0.06	0.55	1.09	36.10	29.46	18.51
K052	458.76	20.49	22.61	11.21	0.26	0.24	0.29	10.32	0.11	0.56	1.09	33.50	30.08	20.63
K053	443.11	19.96	22.88	10.53	0.24	0.25	0.27	9.67	0.02	0.54	1.14	35.55	29.38	21.37
K054	453.63	20.24	21.55	11.08	0.24	0.27	0.32	10.60	0.14	0.56	1.06	33.51	27.12	21.37
K055	455.12	20.31	22.15	11.28	0.22	0.18	0.29	10.36	0.12	0.57	1.09	37.40	29.91	19.28
K056	450.68	20.19	21.83	10.76	0.27	0.32	0.30	10.43	0.11	0.55	1.08	31.81	24.69	22.16
K058	457.87	20.58	22.36	11.20	0.24	0.20	0.31	10.52	0.11	0.56	1.08	35.19	29.72	18.96

K059	459.10	20.57	22.68	11.23	0.23	0.22	0.29	10.35	0.10	0.56	1.09	33.98	29.11	20.26
K060	460.27	20.64	22.55	11.36	0.23	0.16	0.30	10.49	0.11	0.57	1.08	36.82	31.20	17.80
K061	448.26	19.94	21.53	10.88	0.28	0.31	0.31	10.32	0.13	0.56	1.07	31.64	26.95	21.89
K062	457.64	20.87	23.50	10.97	0.27	0.15	0.29	10.26	0.03	0.54	1.11	35.94	32.52	16.75

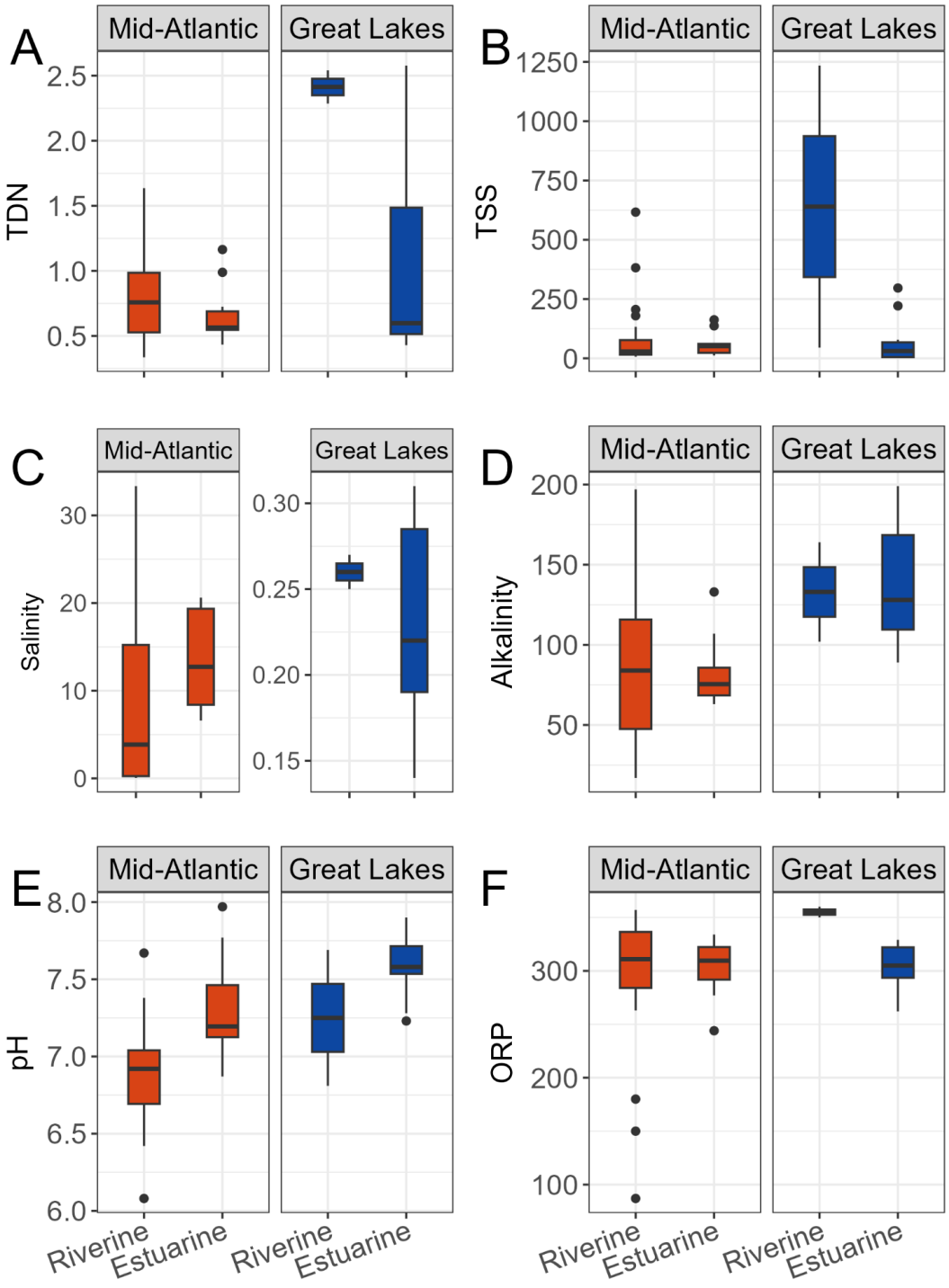

Figure S1: Boxplots displaying regional trends in water type for various water quality parameters including A) total dissolved nitrogen (TDN, mg/L), B) total suspended solids (TSS, mg/L), C) salinity (psu), D) alkalinity (mg/L $CaCO_3$), E) pH and F) redox potential (ORP, mv)

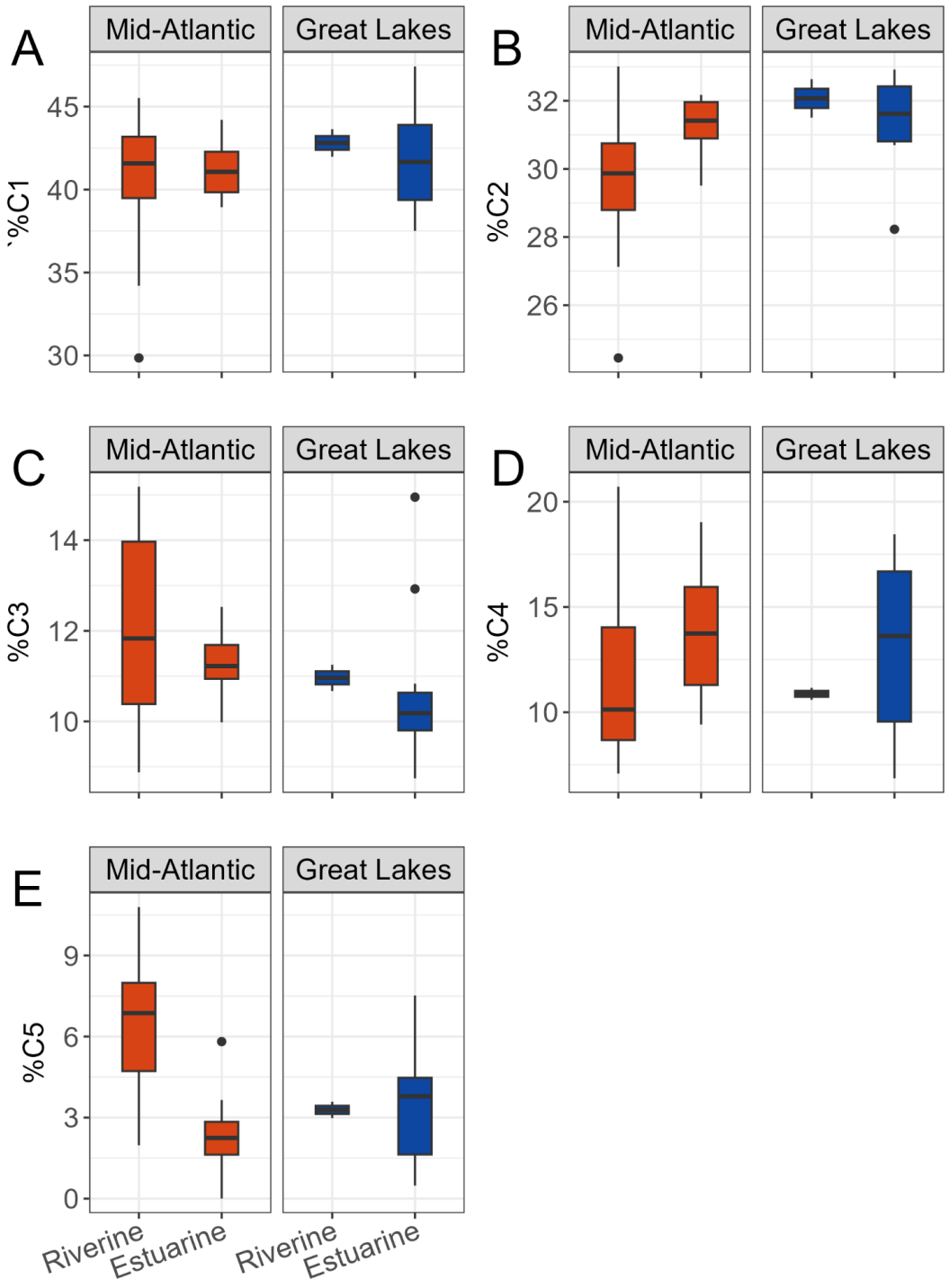

Figure S2: Boxplots displaying regional trends in water type for relative contributions of PARAFAC components including A) %C1, B) %C2, C) %C3, D) %C4, and E) %C5

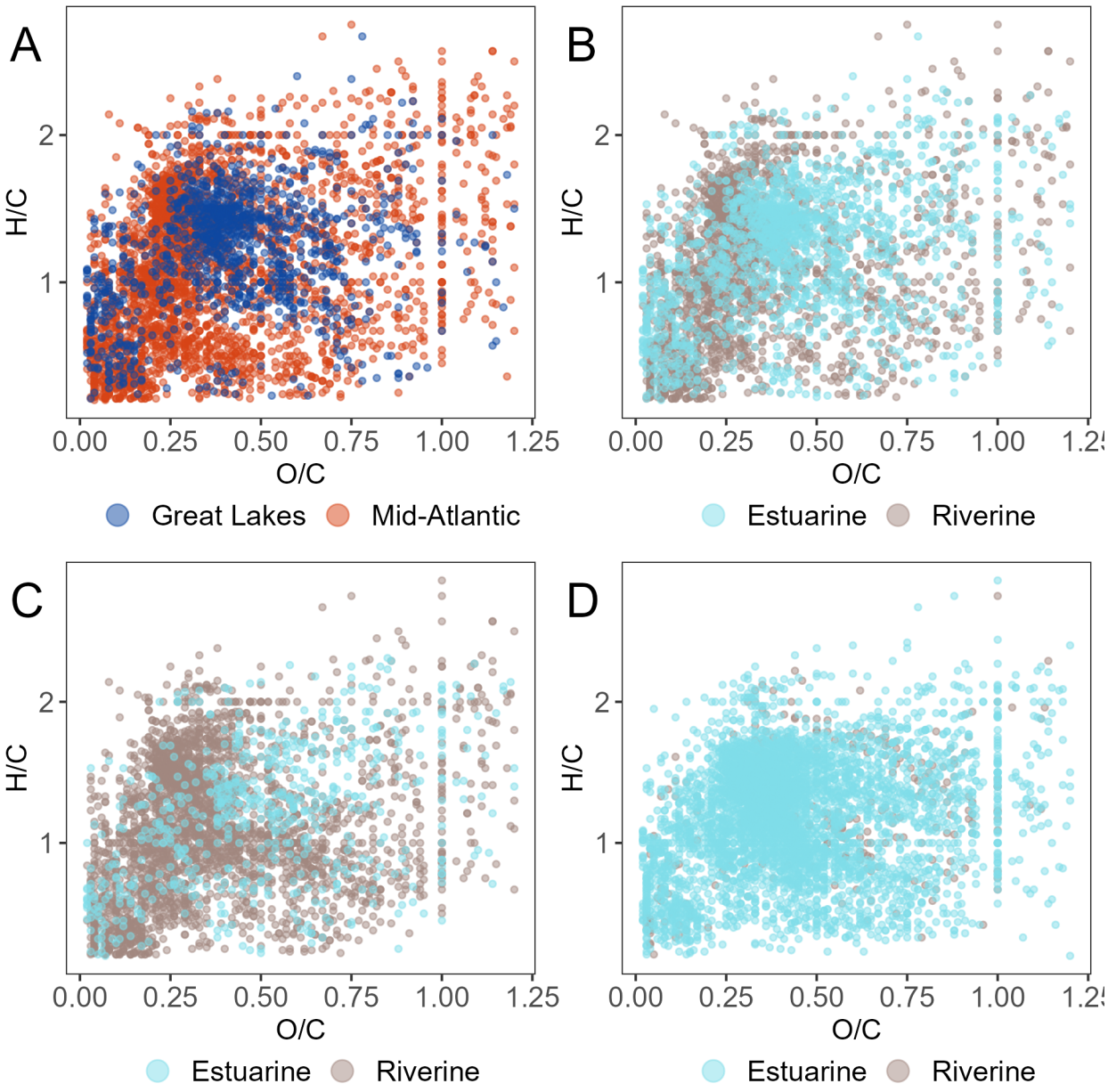

Figure S3: van Krevelen diagrams showing the unique formula across a) regions, b) water type, c) water type within the mid-Atlantic region, and D) water type within the Great Lakes region

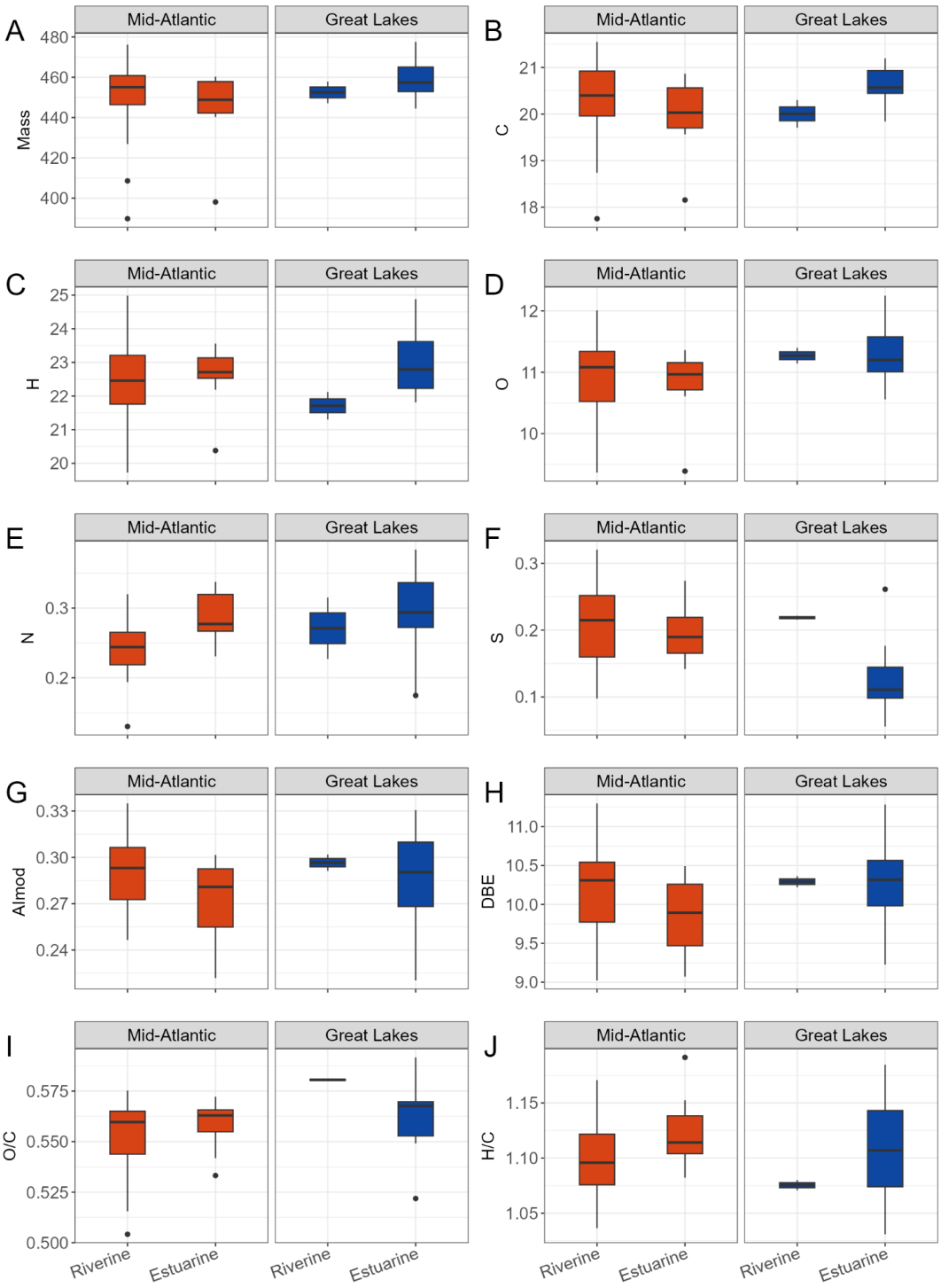

Figure S4: Boxplots displaying regional trends in water type for mean FTICR-MS molecular properties including A) mass (m/z), B) Carbon (C), C) hydrogen (H), D) oxygen (O), E) nitrogen (N), F) sulfur (S), G) modified aromaticity index (AImod), H) double bond equivalents (DBE), I) oxygen to carbon ratio (O/C), and J) hydrogen to carbon ratio (H/C)