Supporting Information

Optimization of Fluorescence Humification Index Calculation for Low-Concentration Dissolved Organic Matter Solutions

Jin Liao,[*a] Xiaofan Wang, [b] Xiuli Li, [c] Guangning Liu, [a] and Chaoyong Hu [b,c]

a. Wuhan Center, China Geological Survey, Wuhan, 430205, China.

b. Hubei Key Laboratory of Regional Ecology and Environmental Change, School of Geography and Information Engineering, China University of Geosciences, Wuhan 430074, China.

c. State Key Laboratory of Geomicrobiology and Environmental Changes, China University of Geosciences, Wuhan, 430074, China.

[*] Corresponding author: Jin Liao, Ph.D.

Wuhan Center, China Geological Survey, Wuhan, 430205, China

E-mail: liaojin_earth@163.com

Table S1. Categorization of fluorophore types utilizing fluorescence regional integration

Region	Fluorophore Type	Excitation Range (nm)	Emission Range (nm)
I	Tyrosine-like	200-250	280-330
II	Tryptophan-like	200-250	330-380
III	Fulvic-like	200-250	380-550
IV	Microbial protein-like	250-400	280-380
V	Humic-like	250-400	380-550

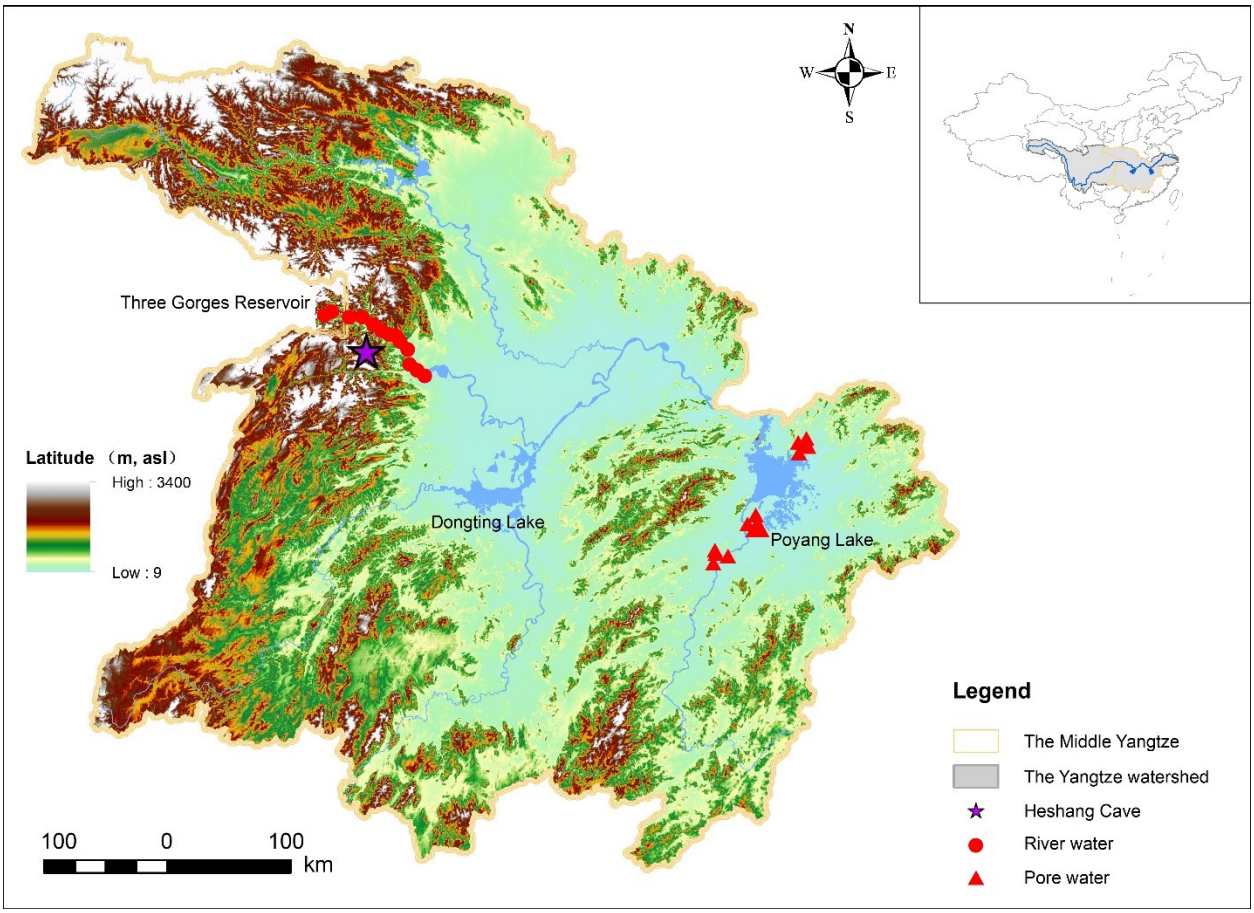

Figure S1. Location of the four types of natural samples. Soil leachate samples and karst dripwater samples are both from Heshang Cave site.

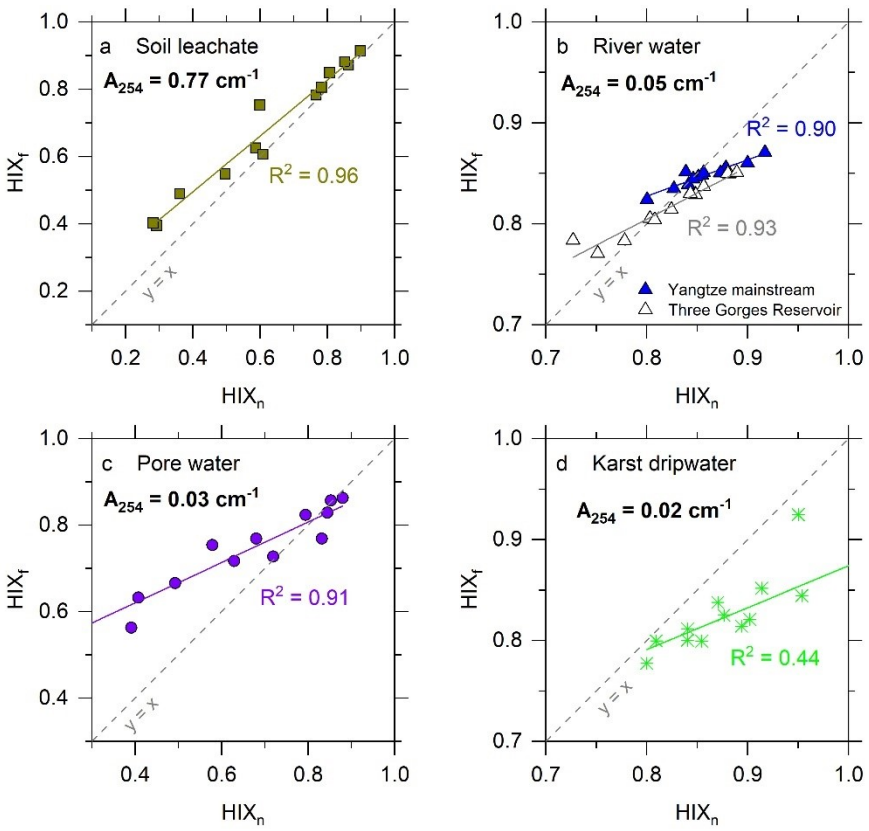

Figure S2. Relationships between HIX_n and HIX_f derived from four natural solutions: (a) Soil leachate; (b) River water; (c) Pore water; (d) Karst dripwater.

Table S2 Original spectral results obtained from four different natural solutions.

Types	A_{254} (cm^{-1})	$I_{300-345}$ (R.U.)	$I_{435-480}$ (R.U.)	HIX_n	FRI_{IV} (R.U.)	FRI_V (R.U.)	∑FRI (R.U.)	HIX_f
Soil leachate	0.645	42.96	140.90	0.77	9035	32639	49020	0.78
	0.209	23.52	147.60	0.86	5863	39656	52078	0.87
	0.330	41.47	61.95	0.60	4791	14631	24924	0.75
	0.193	15.22	8.59	0.36	2075	1992	4658	0.49
	0.049	15.12	63.11	0.81	2723	15355	20827	0.85
	0.468	41.02	58.14	0.59	7170	12009	23163	0.63
	1.257	79.92	124.39	0.61	41550	64034	113711	0.61
	2.655	456.33	448.96	0.50	135560	164511	341253	0.55
	1.814	49.88	439.40	0.90	9772	104294	132931	0.91
	0.054	14.72	6.09	0.29	2081	1360	3940	0.40
	0.370	30.12	108.81	0.78	6241	25854	37442	0.81
	0.839	35.48	203.06	0.85	6667	49749	65291	0.88
	1.149	263.90	103.72	0.28	37840	25492	74240	0.40
River Water	0.042	3.72	19.31	0.84	814	4667	6392	0.85
	0.046	4.93	19.77	0.80	1009	4725	6706	0.82
	0.050	5.06	24.15	0.83	1112	5628	7905	0.84
	0.059	4.44	49.06	0.92	1046	7047	10006	0.87
	0.049	4.83	43.49	0.90	1088	6710	9537	0.86
	0.057	4.00	28.92	0.88	949	5623	7826	0.86
	0.043	3.74	25.71	0.87	878	4994	6993	0.85
	0.042	3.62	19.19	0.84	859	4461	6235	0.84
	0.045	3.43	20.15	0.85	867	4840	6661	0.85
	0.042	3.55	20.31	0.85	829	4579	6362	0.85
	0.051	3.24	18.52	0.85	805	4451	6128	0.85
	0.042	3.23	19.23	0.86	804	4583	6287	0.85
	0.044	3.69	20.30	0.85	896	4865	6718	0.84
Pore water	0.009	0.34	1.68	0.83	143	475	806	0.77
	0.035	4.09	23.65	0.85	979	5852	8007	0.86
	0.015	1.94	4.97	0.72	449	1199	1990	0.73
	0.017	3.62	7.67	0.68	550	1832	2838	0.77
	0.008	1.34	0.86	0.39	160	206	516	0.56
	0.008	1.71	2.34	0.58	154	473	864	0.75
	0.046	6.79	36.83	0.84	1700	8255	12021	0.83
	0.058	11.79	45.56	0.79	2314	10811	15417	0.82
	0.013	2.36	3.99	0.63	378	959	1634	0.72
	0.044	16.68	11.47	0.41	2334	4022	7272	0.63
	0.006	1.45	0.28	0.16	109	121	387	0.53
	0.033	2.77	20.34	0.88	796	5011	6825	0.86
	0.047	16.47	15.97	0.49	2333	4649	8037	0.67
Karst dripwater	0.010	0.84	3.34	0.80	246	861	1290	0.78
	0.022	0.95	4.06	0.81	258	1031	1509	0.80
	0.010	0.36	3.82	0.91	183	1050	1417	0.85
	0.018	0.47	8.87	0.95	177	2178	2658	0.92
	0.010	0.56	3.78	0.87	183	947	1318	0.84
	0.021	0.22	4.50	0.95	218	1184	1639	0.84
	0.014	0.84	4.42	0.84	284	1139	1668	0.80
	0.019	0.48	3.41	0.88	191	902	1267	0.83
	0.013	0.84	4.42	0.84	257	1103	1609	0.81
	0.021	0.43	3.63	0.89	204	893	1290	0.81
	0.009		3.12	1.01	147	774	1076	0.84
	0.020	0.64	3.73	0.85	232	924	1362	0.80
	0.009	0.31	2.87	0.90	158	727	1034	0.82

Table S3 Original spectral results at varying dilution ratios for a river water sample.

Dilution Ratios	A_{254} (cm^{-1})	$I_{300-345}$ (R.U.)	$I_{435-480}$ (R.U.)	HIX_n	FRI_{IV} (R.U.)	FRI_V (R.U.)	∑FRI (R.U.)	HIX_f
	0.036	7.14	17.83	0.71	1384	4394	6708	0.76
	0.038	7.22	18.46	0.72	1450	4520	6916	0.76
	0.037	7.33	18.23	0.71	1419	4448	6807	0.76
	0.036	7.70	18.53	0.71	1502	4521	6995	0.75
	0.038	7.71	18.66	0.71	1498	4517	6991	0.75
1	0.038	7.53	18.68	0.71	1462	4515	6940	0.76
	0.038	7.39	18.41	0.71	1473	4506	6935	0.75
	0.038	7.68	18.61	0.71	1462	4528	6965	0.76
	0.039	7.34	18.71	0.72	1463	4529	6961	0.76
	0.039	7.31	18.71	0.72	1461	4532	6960	0.76
	0.038	7.23	18.36	0.72	1453	4504	6918	0.76
	0.013	2.44	4.39	0.64	404	1023	1719	0.72
	0.012	2.24	4.51	0.67	383	1023	1690	0.73
	0.010	1.79	3.97	0.69	356	980	1579	0.73
	0.012	2.32	4.46	0.66	383	1021	1681	0.73
	0.012	1.97	4.48	0.70	379	1016	1661	0.73
5	0.012	2.18	4.28	0.66	377	1008	1653	0.73
	0.012	2.23	4.54	0.67	380	1014	1673	0.73
	0.012	2.12	4.46	0.68	389	1016	1674	0.72
	0.012	2.17	4.49	0.67	381	1017	1661	0.73
	0.012	2.14	4.46	0.68	388	1017	1681	0.72
	0.012	2.37	4.40	0.65	393	1020	1691	0.72
	0.007	2.91	2.40	0.45	279	546	1038	0.66
	0.006	1.78	2.17	0.55	227	487	872	0.68
	0.006	1.75	2.09	0.55	226	494	875	0.69
	0.007	2.55	2.16	0.46	253	509	939	0.67
	0.007	1.62	2.04	0.56	215	477	853	0.69
10	0.007	1.62	2.05	0.56	222	487	860	0.69
	0.007	1.94	2.01	0.51	223	487	863	0.69
	0.007	1.73	2.04	0.54	226	487	869	0.68
	0.007	1.73	1.95	0.53	222	477	844	0.68
	0.007	1.87	2.10	0.53	226	488	871	0.68
	0.006	1.81	2.05	0.53	228	487	870	0.68
	0.003	0.54	1.22	0.69	110	299	494	0.73
	0.003	0.67	1.22	0.65	114	294	493	0.72
	0.003	0.41	1.11	0.73	109	287	468	0.72
	0.003	0.25	1.31	0.84	98	297	474	0.75
	0.003	0.67	1.15	0.63	107	289	482	0.73
15	0.003	0.55	1.14	0.68	105	296	483	0.74
	0.003	0.33	1.15	0.78	100	296	478	0.75
	0.002	0.56	1.20	0.68	110	306	498	0.73
	0.003	0.45	1.20	0.73	110	298	486	0.73
	0.003	0.55	1.18	0.68	107	292	478	0.73
	0.003	0.36	1.19	0.77	103	293	478	0.74
	0.001	0.43	0.82	0.66	80	213	366	0.73
	0.003	0.44	0.93	0.68	94	211	373	0.69
	0.003	0.15	0.87	0.85	78	212	349	0.73
	0.002	0.36	0.75	0.68	81	205	353	0.72
	0.002	0.12	0.83	0.87	77	204	343	0.73
20	0.002	0.38	0.78	0.67	77	207	342	0.73
	0.002	\	0.90	\	72	203	330	0.74
	0.002	0.20	0.86	0.81	78	211	356	0.73
	0.003	0.23	0.76	0.77	77	205	340	0.73
	0.003	0.27	0.88	0.76	82	206	346	0.72
	\	0.34	0.96	0.74	85	212	370	0.71