Supplementary Materials:

Developing an intelligent data analysis approach for marine sediments

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Table S1. Factor loadings

Factor Loadings (Varimax normalized) Extraction: Principal components (Marked loadings are significant)				
Variables	**Factor 1**	**Factor 2**	**Factor 3**	**Factor 4**
Humidity	0.025	**0.483**	-0.234	**0.453**
Loss on ignition	0.322	**0.635**	0.091	-0.425
N-tot	0.072	0.160	-0.130	**0.561**
P-tot	0.118	**0.634**	0.143	0.029
Cr -lab.	0.095	**0.916**	-0.020	-0.155
Zn-lab.	0.340	**0.828**	0.053	-0.104
Cu-lab.	0.163	**0.883**	-0.098	-0.162
Ni-lab.	0.194	**0.920**	-0.064	-0.174
Pb- lab.	0.491	**0.787**	-0.031	-0.024
As-tot	0.026	**0.709**	0.002	0.206
Cr-tot	0.234	**0.933**	-0.110	-0.048
Zn-tot	0.203	**0.805**	-0.066	-0.048
Cu-tot	0.056	**0.892**	-0.042	0.024

Ni-tot	0.093	**0.810**	-0.103	0.035
Pb-tot	0.383	**0.832**	-0.062	0.091
Naphthalene	0.074	0.066	0.382	0.598
Acenaphthylene	**0.690**	0.030	0.010	0.332
Acenaphthene	**0.646**	0.385	0.366	0.231
Fluorene	**0.881**	0.179	0.031	0.158
Phenanthrene	**0.728**	0.306	0.280	0.090
Anthracene	**0.773**	-0.083	0.022	0.243
Benzo(a)anthracene	**0.937**	0.211	0.026	-0.015
Chrysene	**0.872**	0.381	0.068	-0.140
Benzo(b)fluoranthene	**0.906**	0.268	-0.081	-0.220
Benzo(k)fluoranthene	**0.809**	0.142	-0.013	-0.176
Benzo(a)pyrene	**0.840**	0.105	-0.005	-0.292
Indeno(1,2,3, -cd)pyrene	**0.795**	0.236	-0.037	-0.319
Benzo(g, h, i)perylene	**0.869**	0.258	-0.068	-0.174
SPAHs	**0.859**	0.265	0.253	0.201
PCB 101	0.139	0.021	**0.790**	0.109
PCB 138	0.014	-0.056	**0.961**	0.140
PCB 153	0.099	-0.067	**0.951**	0.018
PCB 180	-0.042	-0.070	**0.900**	0.024
S PCB	0.027	-0.070	**0.982**	0.053
Expl.Var %	28.2	28.1	14.2	8.1

Table S2. Factor loadings

Factor Loadings (Varimax normalized):Principal components (Marked loadings are significant)				
Variable	**Factor1**	**Factor2**	**Factor3**	**Factor4**
Humidity	0.056	-0.013	0.294	0.198
Loss on ignition	0.074	0.037	0.322	0.205
N-tot	0.085	0.035	0.088	-0.294
P-tot	0.168	0.035	0.009	-0.077
Cr -lab.	0.133	0.047	0.235	-0.405
Zn-lab.	-0.027	-0.100	**0.691**	0.090
Cu-lab.	0.119	-0.027	**0.712**	-0.024
Ni-lab.	0.054	0.022	**0.709**	-0.383
Pb- lab.	-0.169	-0.107	**0.677**	-0.040

As-tot	-0.028	-0.007	0.191	-0.229
Cr-tot	0.058	0.054	**0.711**	-0.166
Zn-tot	-0.125	0.070	0.077	-0.021
Cu-tot	-0.019	0.015	-0.002	0.058
Ni-tot	0.001	0.032	0.484	0.011
Pb-tot	-0.167	-0.109	**0.639**	-0.177
Naphthalene	0.013	0.067	0.207	0.191
Acenaphthylene	**0.655**	0.037	-0.128	0.057
Acenaphthene	0.015	-0.011	0.048	**0.826**
Fluorene	0.151	0.015	0.146	**0.899**
Phenanthrene	0.433	-0.013	0.184	**0.747**
Anthracene	0.379	0.070	-0.031	**0.772**
Benzo(a)anthracene	**0.895**	0.049	-0.033	0.213
Chrysene	**0.920**	-0.028	0.018	0.134
Benzo(b)fluoranthene	**0.910**	0.094	0.217	0.061
Benzo(k)fluoranthene	**0.678**	0.041	0.245	0.031
Benzo(a)pyrene	**0.768**	0.027	-0.194	-0.067
Indeno(1,2,3, -cd)pyrene	**0.720**	-0.007	0.302	-0.182
Benzo(g, h, i)perylene	0.276	0.039	**0.610**	0.028
SPAHs	**0.786**	0.041	0.253	0.594
PCB 101	-0.028	**-0.713**	0.059	-0.028
PCB 138	-0.063	**-0.905**	0.037	0.090
PCB 153	-0.062	**-0.938**	0.047	-0.065
PCB 180	0.008	**-0.774**	-0.025	-0.091
S PCB	-0.048	**-0.973**	0.012	-0.014
Expl.Var %	25.8	18.3	11.1	10.1

Table S3. Decoded variables tables

Variables	Code
Humidity	**V1**
Loss on ignition	**V2**
N-tot	**V3**

P-tot	**V4**
Cr -lab.	**V5**
Zn-lab.	**V6**
Cu-lab.	**V7**
Ni-lab.	**V8**
Pb- lab.	**V9**
As-tot	**V10**
Cr-tot	**V11**
Zn-tot	**V12**
Cu-tot	**V13**
Ni-tot	**V14**
Pb-tot	**V15**
Naphthalene	**V16**
Acenaphthylene	**V17**
Acenaphthene	**V18**
Fluorene	**V19**
Phenanthrene	**V20**
Anthracene	**V21**
Benzo(a)anthracene	**V22**
Chrysene	**V23**
Benzo(b)fluoranthene	**V24**
Benzo(k)fluoranthene	**V25**
Benzo(a)pyrene	**V26**
Indeno(1,2,3, -cd)pyrene	**V27**
Benzo(g, h, i)perylene	**V28**
SPAHs	**V29**
PCB 101	**V30**
PCB 138	**V31**
PCB 153	**V32**
PCB 180	**V33**
S PCB	**V34**

Descriptive Statistics (Spreadsheet1)					
	Valid N	**Mean**	**Minimum**	**Maximum**	**Std.Dev.**
Humidity	174	17.7037	4.3800	27.000	3.7995
Loss on ignition	174	0.3138	0.0400	1.770	0.1868
N-tot	174	791.9195	103.0000	2926.000	453.3002
P-tot	174	267.4551	144.9700	984.340	109.3148
Cr -lab.	174	0.7511	0.1250	4.383	0.4805
Zn-lab.	174	2.6744	0.7631	12.085	1.2883
Cu-lab.	174	0.4495	0.1250	5.596	0.5566
Ni-lab.	174	0.4336	0.1250	5.383	0.4745
Pb- lab.	174	1.8978	0.6517	5.503	0.6969
As-tot	174	0.9731	0.6250	5.050	0.6861
Cr-tot	174	2.6900	1.2400	19.540	1.7015
Zn-tot	174	8.7082	2.3710	59.330	6.4428
Cu-tot	174	0.9081	0.1250	45.000	3.4560
Ni-tot	174	1.4799	0.3808	11.820	1.2644
Pb-tot	174	2.5138	0.9624	7.404	0.8271
Naphthalene	174	0.0017	0.0005	0.053	0.0052
Acenaphthylene	174	0.0006	0.0005	0.002	0.0002
Acenaphthene	174	0.0009	0.0005	0.012	0.0010
Fluorene	174	0.0014	0.0005	0.007	0.0012
Phenanthrene	174	0.0028	0.0005	0.010	0.0019
Anthracene	174	0.0007	0.0005	0.006	0.0005
Benzo(a)anthracene	174	0.0010	0.0005	0.006	0.0010
Chrysene	174	0.0011	0.0005	0.005	0.0009
Benzo(b)fluoranthene	174	0.0020	0.0005	0.013	0.0020
Benzo(k)fluoranthene	174	0.0007	0.0005	0.003	0.0004
Benzo(a)pyrene	174	0.0006	0.0005	0.003	0.0003
Indeno(1,2,3, -cd)pyrene	174	0.0012	0.0005	0.009	0.0013
PCB 28	174	0.0009	0.0005	0.005	0.0008
PCB 52	174	0.0179	0.0005	0.086	0.0163
PCB 101	174	0.0001	0.0001	0.000	0.0000

PCB 138	174	0.0002	0.0001	0.001	0.0002
PCB 153	174	0.0001	0.0001	0.001	0.0001
PCB 180	174	0.0002	0.0001	0.001	0.0002
S PCB	174	0.0006	0.0001	0.004	0.0006

Table S4. Factor loadings for zone C

Factor Loadings (Varimax normalized)) Extraction: Principal components (Marked loadings are significant				
Variables	**Factor1**	**Factor2**	**Factor3**	**Factor4**
Humidity	-0.228	-0.185	-0.078	-0.019
Loss on ignition	0.102	**0.720**	0.113	0.210
N-tot	0.177	**0.797**	0.131	-0.088
P-tot	-0.026	0.047	0.423	**-0.729**
Cr -lab.	0.014	0.473	0.020	**-0.795**
Zn-lab.	0.186	**0.745**	0.589	0.194
Cu-lab.	0.188	0.354	**0.742**	-0.009
Ni-lab.	0.168	**0.724**	0.464	-0.428
As-tot	0.123	0.231	**0.698**	0.021
Pb- lab.	0.148	0.122	**0.766**	-0.127
Cr-tot	0.081	0.109	**0.698**	-0.070
Zn-tot	0.100	-0.044	**0.683**	0.450
Cu-tot	-0.062	0.302	0.188	**0.684**
Ni-tot	-0.095	0.066	0.374	**0.750**
Pb-tot	0.058	0.286	**0.770**	-0.221
Naphthalene	0.046	-0.153	**0.701**	0.250
Acenaphthylene	**0.777**	0.060	-0.139	-0.297
Acenaphthene	0.241	-0.180	**0.701**	0.253
Fluorene	0.628	-0.191	**0.700**	0.137
Phenanthrene	**0.715**	-0.110	0.507	0.010
Anthracene	0.242	**0.683**	0.178	-0.033
Benzo(a)anthracene	**0.847**	0.092	0.335	-0.234

Chrysene	**0.800**	0.159	0.471	0.012
Benzo(b)fluoranthene	**0.736**	0.206	0.511	0.165
Benzo(k)fluoranthene	**0.846**	0.397	0.143	-0.138
Benzo(a)pyrene	**0.781**	0.179	0.351	0.309
Indeno(1,2,3, -cd)pyrene	**0.686**	0.399	0.396	0.175
Dibenzo(a, h)anthracene	**0.777**	0.060	-0.139	-0.297
Benzo(g, h, i)perylene	**0.625**	-0.302	0.033	0.320
SPAHs	**0.725**	0.034	0.629	0.169
PCB 138	**0.627**	0.373	-0.344	0.368
PCB 153	0.102	0.419	0.195	-0.139
PCB 180	**0.687**	0.555	-0.307	-0.213
S PCB	0.466	**0.742**	-0.226	-0.028
Expl.Var %	24.1	19.7	13.8	10.6