Supplementary Data for manuscript titled

Comparison of two rapid automated analysis tools for large FTIR microplastic data sets

Authors: Sonya R. Moses[1]*, Lisa Roscher[2]*, Sebastian Primpke[2+], Benedikt Hufnagl[3,4], Martin G. J. Löder[1+], Gunnar Gerdts[2+#], Christian Laforsch[1+#]

*joint first authorship

#joint senior authorship

[+]corresponding authors:
sebastian.primpke@awi.de
martin.loeder@uni-bayreuth.de
gunnar.gerdts@awi.de
christian.laforsch@uni-bayreuth.de

Affiliations

[1] Department of Animal Ecology I and BayCEER, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

[2] Alfred-Wegener-Institute Helmholtz Centre for Polar and Marine Research, Biologische Anstalt Helgoland, Kurpromenade 201, 27498 Helgoland, Germany

[3] Institute of Chemical Technologies and Analytics, Vienna University of Technology, A 1060 Vienna, Austria

[4] Purency GmbH, Walfischgasse 8/34, A 1010 Vienna, Austria

Content:

Figures

Tables

Tab. S 1 Background information including suspended particulate matter (SPM) on subsamples reanalysed in the present study, originating from samples collected in the catchment area of the River Weser (A-01 – A-10) and transition to the North Sea (B-01 – B-10) in the framework of previous studies (Roscher et al. [1], Moses et al. (unpublished data))

Sample ID	Sampling area	North	East	SPM [mg/L]
A-01	Fulda	50°35.91	09°38.34	3.7
A-02	Eder	51°02.98	08°17.05	1.3
A-03	Eder	51°07.52	09°17.70	1.8
A-04	Fulda	51°19.46	09°31.70	6.6
A-05	Werra	51°24.99	09°40.20	5.5
A-06	Weser	51°25.81	09°38.33	6.0
A-07	Große Aue	52°34.64	09°02.29	9.6
A-08	Leine	52°41.01	09°36.12	16.5
A-09	Örtze	52°44.33	10°02.01	11.5
A-10	Wümme	53°04.54	09°12.33	7.6
B-01	Jade Bay	53°29.94	08°14.18	147.6
B-02	Jade Bay	53°27.87	08°14.00	85.6
B-03	Lower Weser	53°21.86	08°30.19	29.7
B-04	Lower Weser	53°25.46	08°29.88	47.1
B-05	Outer Weser	53°32.74	08°33.43	54.0
B-06	Outer Weser	53°35.22	08°31.12	14.3
B-07	Outer Weser	53°37.75	08°28.01	35.7
B-08	Outer Weser	53°39.27	08°24.32	29.9
B-09	North Sea	53°52.78	07°39.42	0.8
B-10	North Sea	53°59.53	07°50.61	12.8

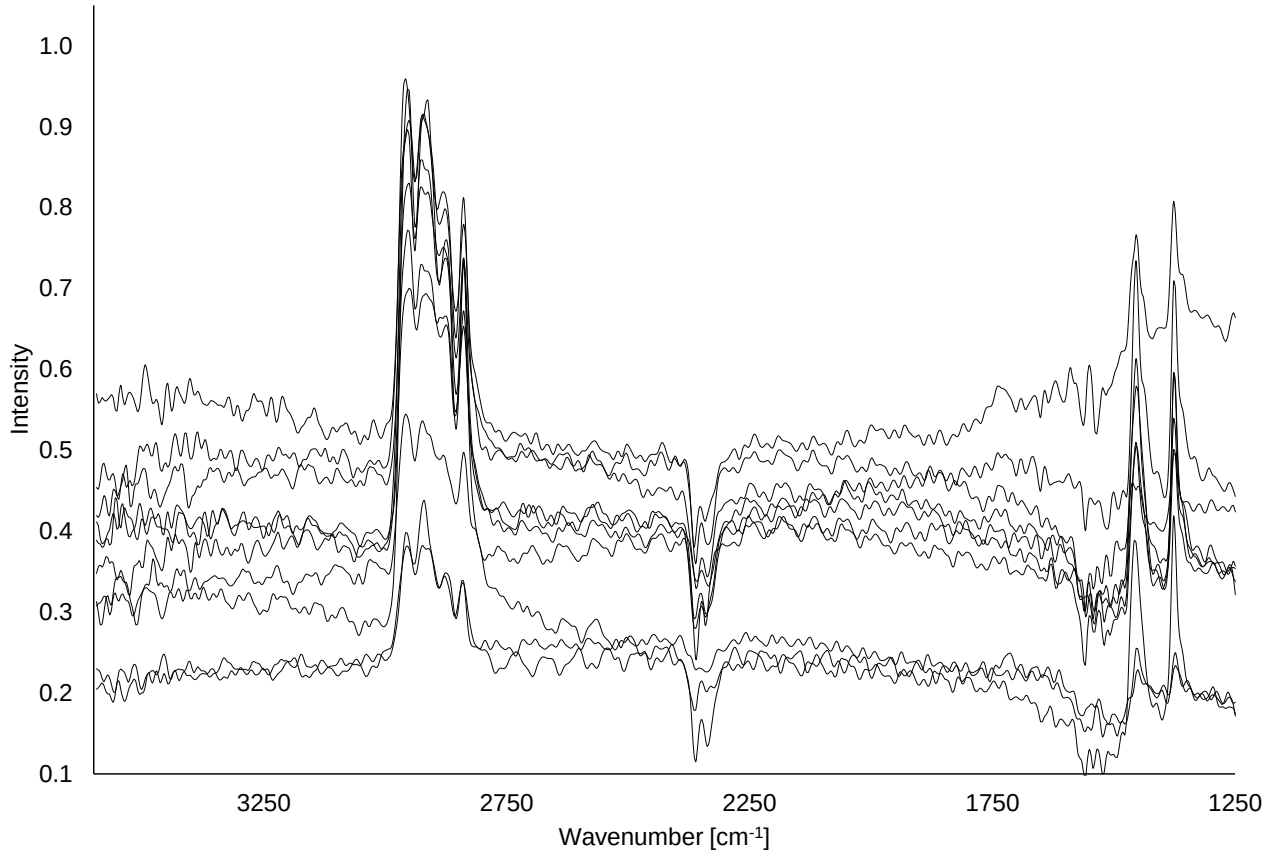

Fig. S 1 Randomly selected PP-spectra (n=10) from siMPle analysis of sample B-06

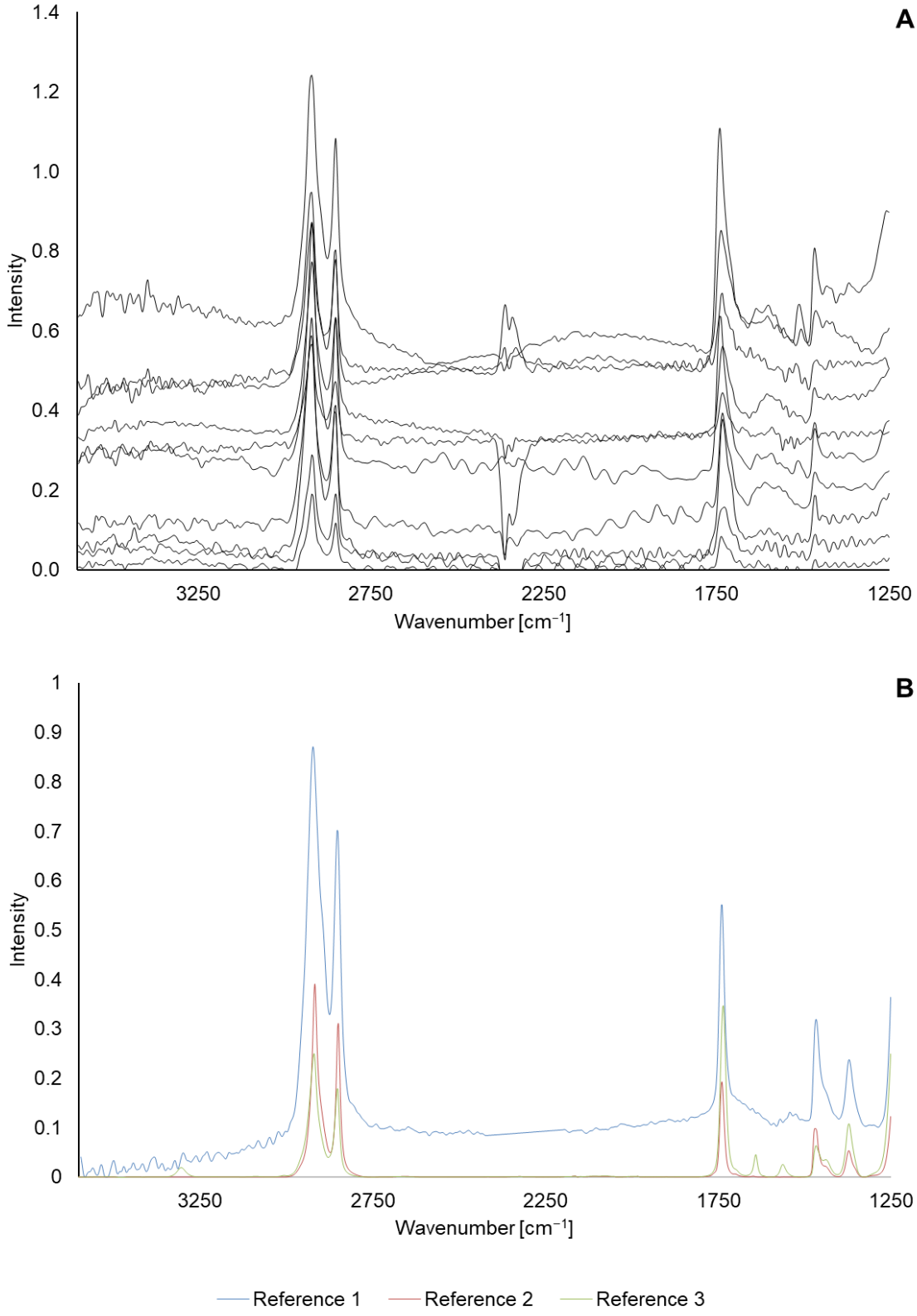

Fig. S 2 A. Ten randomly selected EVA spectra, extracted from siMPle analysis (sample set A and B) and manually evaluated. B. EVA reference spectra included in siMPle database

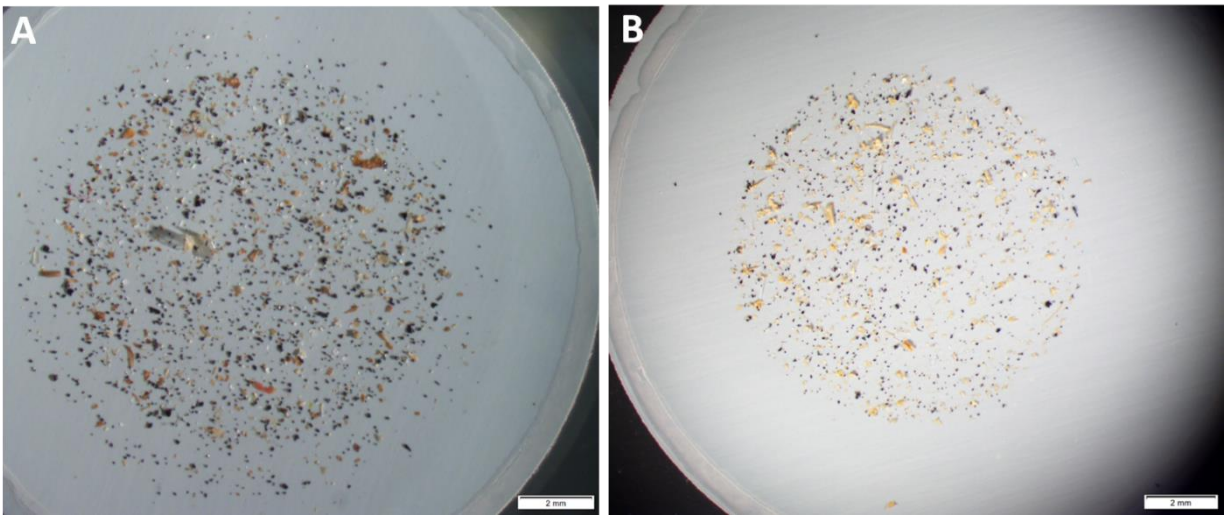

Fig. S 3 Microscopy image of Anodisc filter with sample B-03 (A) and A-08 (B), showing high amounts of material with biogenic appearance

Tab. S 2 MP count of polymer types detected in sample set A after analysis with siMPle/MPAPP. The clusters A/PUR/V, CA and EVA were excluded from analysis. For abbreviations refer to Table 1 in main manuscript

	PE	PP	PS	PC	PA	PVC	CA	PEST	A/PUR/V	PSU	PEEK	EVA	POM	∑	∑ without A/PUR/V	∑ without A/PUR/V, CA and EVA
A-01	1	4	0	0	0	0	0	0	91	0	0	4	0	100	9	5
A-02	0	1	0	0	0	0	0	1	60	0	0	1	0	63	3	2
A-03	0	11	0	0	0	0	0	0	59	0	0	1	0	71	12	11
A-04	5	8	1	0	1	0	0	0	85	1	0	2	0	103	18	16
A-05	5	9	1	0	2	1	0	4	69	0	0	2	0	93	24	22
A-06	6	14	1	0	1	0	0	4	121	0	0	7	0	154	33	26
A-07	0	3	0	0	0	0	0	0	6	0	0	0	0	9	3	3
A-08	11	76	0	0	4	0	0	5	252	0	0	25	0	373	121	96
A-09	0	3	0	0	2	0	0	1	158	0	0	5	0	169	11	6
A-10	0	3	0	0	0	0	0	1	185	0	0	8	0	197	12	4
∑	28	132	3	0	10	1	0	16	1086	1	0	55	0	1332	246	191

Tab. S 3 MP count of polymer types detected in sample set A after analysis with BPF. The clusters A/PUR/V, CA and EVA were excluded from analysis. For abbreviations refer to Table 1 in main manuscript

	PE	PP	PS	PC	PA	PVC	CA	PEST	A/PUR/V	PSU	PEEK	EVA	POM	∑	∑ without A/PUR/V	∑ without A/PUR/V, CA and EVA
A-01	3	3	0	0	0	0	0	0	3	0	0	0	0	9	6	6
A-02	0	2	0	0	0	0	0	0	0	0	0	0	0	2	2	2
A-03	0	11	0	0	0	0	0	0	1	0	0	0	0	12	11	11
A-04	0	5	1	0	0	0	0	0	0	0	0	0	0	6	6	6
A-05	1	10	1	0	0	2	0	0	0	0	0	0	1	15	15	15
A-06	2	14	2	0	0	0	0	0	0	0	0	0	0	18	18	18
A-07	0	3	0	0	0	1	0	0	0	0	0	0	0	4	4	4
A-08	8	47	1	0	3	1	0	9	0	0	0	0	0	69	69	69
A-09	0	4	0	0	0	0	0	0	0	0	0	0	0	4	4	4
A-10	0	4	0	0	0	1	0	0	0	0	0	0	0	5	5	5
∑	14	103	5	0	3	5	0	9	4	0	0	0	1	144	140	140

Tab. S 4 MP count of polymer types detected in sample set B after analysis with siMPle. The clusters A/PUR/V, CA and EVA were excluded from analysis. For abbreviations refer to Table 1 in main manuscript

	PE	PP	PS	PC	PA	PVC	CA	PEST	A/PUR/V	PSU	PEEK	EVA	POM	∑	∑ without A/PUR/V	∑ without A/PUR/V, CA and EVA
B-01	3	2	4	0	1	0	0	2	15	0	0	0	0	27	12	12
B-02	1	0	1	0	14	0	0	1	10	0	0	0	0	27	17	17
B-03	14	14	3	0	20	0	0	2	393	0	0	39	0	485	92	53
B-04	7	21	9	0	2	1	0	1	78	1	0	3	0	123	45	42
B-05	3	5	6	1	6	0	0	1	53	6	1	4	0	86	33	29
B-06	1	9	2	0	1	0	0	1	13	3	0	1	0	31	18	17
B-07	5	12	4	0	0	3	0	0	61	0	0	7	0	92	31	24
B-08	1	4	1	0	1	0	0	2	60	0	0	1	0	70	10	9
B-09	0	0	0	0	1	1	0	0	7	0	0	0	0	9	2	2
B-10	0	0	1	0	1	0	14	1	326	0	0	0	0	343	17	3
∑	35	67	31	1	47	5	14	11	1016	10	1	55	0	**1293**	**277**	**208**

Tab. S 5 MP count of polymer types detected in sample set B after analysis with BPF. The clusters A/PUR/V, CA and EVA were excluded from analysis. For abbreviations refer to Table 1 in main manuscript

	PE	PP	PS	PC	PA	PVC	CA	PEST	A/PUR/V	PSU	PEEK	EVA	POM	∑	∑ without A/PUR/V	∑ without A/PUR/V, CA and EVA
B-01	0	0	0	0	0	0	0	0	5	0	0	0	0	5	0	0
B-02	0	0	0	0	0	0	0	1	5	0	0	0	0	6	1	1
B-03	0	0	0	0	0	0	0	1	42	0	0	0	0	43	1	1
B-04	7	16	9	0	0	2	0	2	3	1	0	0	0	40	37	37
B-05	1	0	0	0	12	2	0	0	10	1	0	0	0	26	16	16
B-06	7	0	0	0	2	0	0	0	2	1	0	0	0	12	10	10
B-07	17	0	0	0	0	2	0	0	11	0	0	0	0	30	19	19
B-08	0	0	0	0	1	0	0	3	6	0	0	0	0	10	4	4
B-09	0	0	0	0	0	0	0	0	9	0	0	0	0	9	0	0
B-10	0	0	0	0	0	0	0	0	15	0	0	0	0	15	0	0
∑	32	16	9	0	15	6	0	7	108	3	0	0	0	196	88	88

References supplementary

1. Roscher L, Fehres A, Reisel L, Halbach M, Scholz-Böttcher B, Gerriets M, et al. Microplastic pollution in the Weser estuary and the German North Sea. Environ Pollut. 2021;288:117681. https://doi.org/10.1016/j.envpol.2021.117681