Supplemental Material

Toward the Systematic Identification of Microplastics in the Environment: Evaluation of a New Independent Software Tool (siMPle) for Spectroscopic Analysis

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Paragraph S1: File format for Single Spectra Correlation

The file must be saved as .csv file containing the entries WaveNumber (in cm^{-1}) and Spectrum (absorbance value at the assigned WaveNumber) separated by a ",". Please keep in mind that the format is currently case sensitive. Afterwards follows the spectrum starting from the lowest wavenumber and the measured absorbance for (FTIR) or counts (for Raman).

Example:

WaveNumber,Spectrum

1249.5058,0

1251.43405,0.00269

1253.3623,0.02026

1255.29055,0.03502

etc.

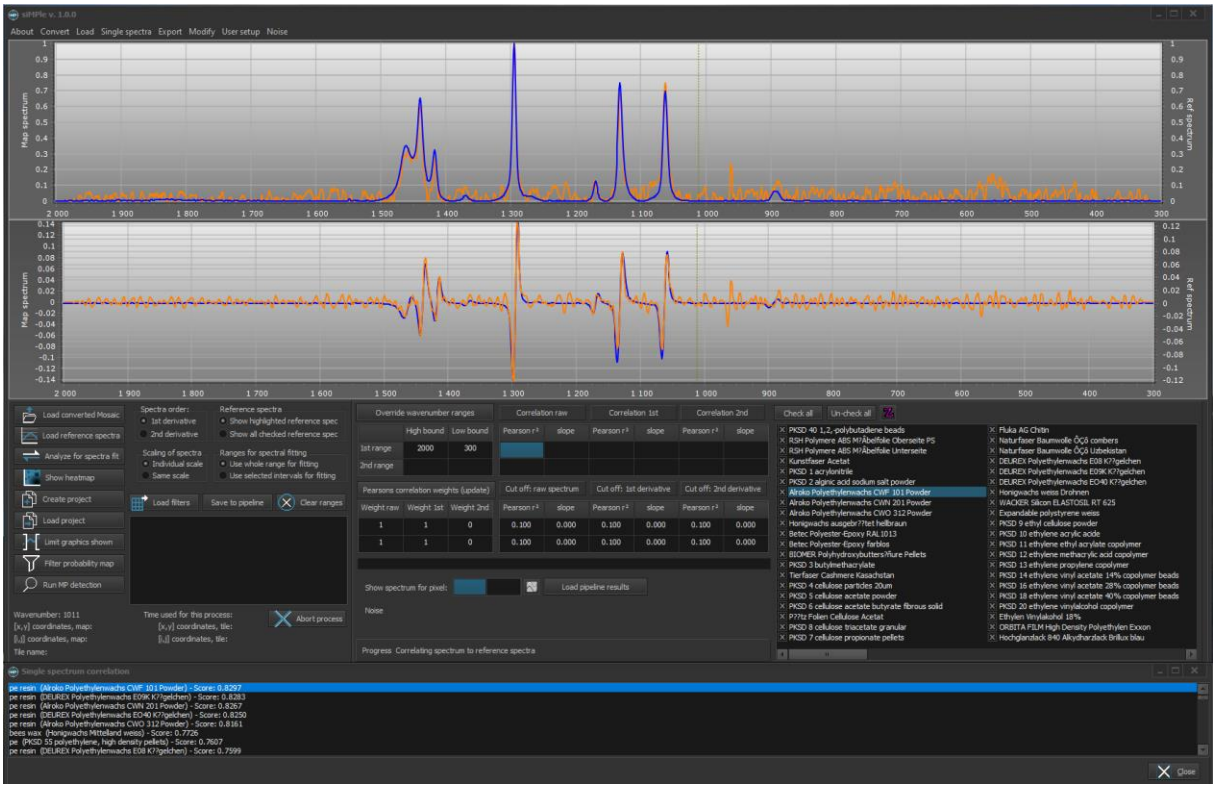

Figure S1. Exemplary processed Raman spectrum identified using siMPle S_d = 0.8292 for polyethylene.

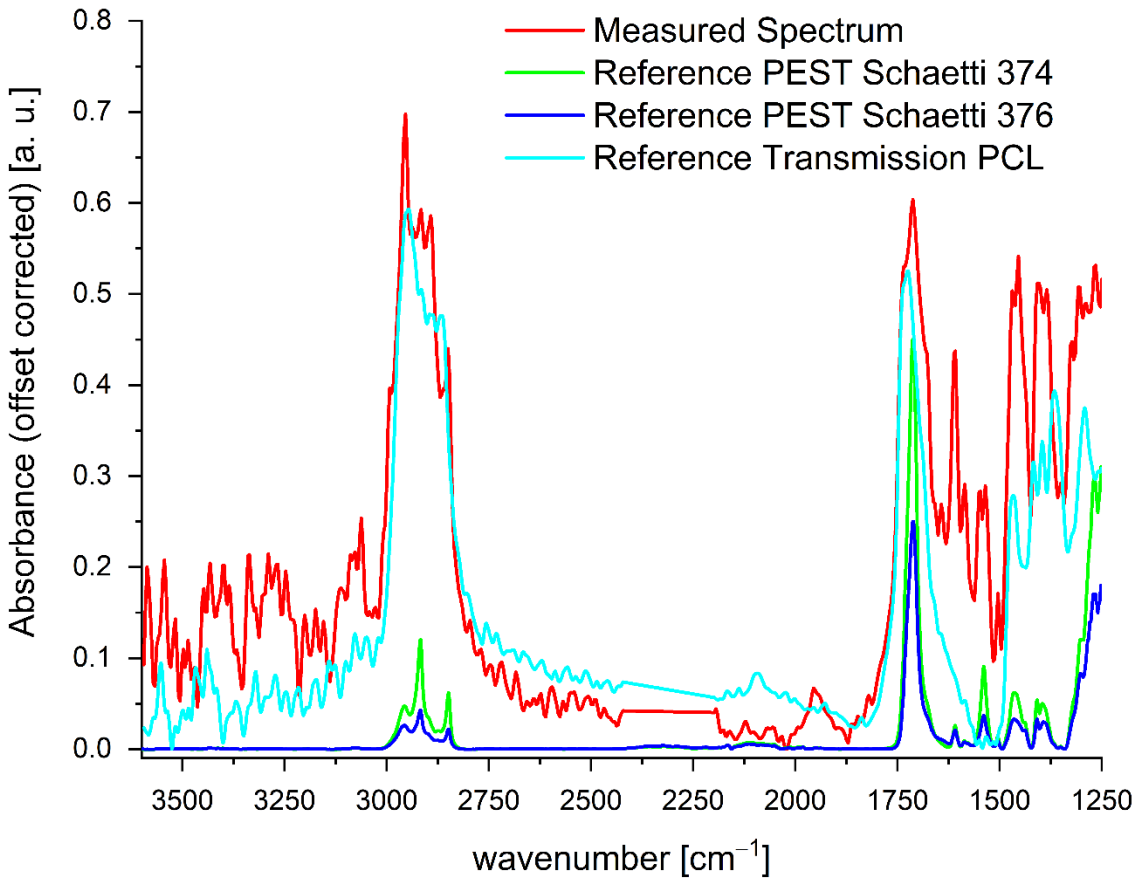

Figure S2. Comparison between a measured spectrum assigned to polycaprolactone (PCL), the polyester (PEST) added to the sample from the manufacturer Schaetti and the spectrum of PCL causing the assignment measured in transmission.

Table S1. Spectrum based polymer type identification rates using OPUS and siMPle on sample RefEnv1.

Polymer type	RefEnv1 OPUS	RefEnv1 siMPle	RefEnv2 OPUS	RefEnv2 siMPle*

Polyethylene	45	46	7114	7579
Polyethylene oxidized	0	0	7	0
Polyethylene-chlorinated	0	0	47	93
Polypropylene	753	794	54934	54965
Polystyrene	152	170	4	3
Polycarbonate	1	2	2	0
Polyamide	33	33	65	80
Polyvinylchloride	30	32	1	6
Cellulose chemical modified	0	0	163	163
Polyester	4	4	179	198
Acrylates/polyurethanes/varnish	430	450	3001	3860
Animal fur/natural polyamides	126	180	685	1151
Plant fibers/ cellulose	4520	13750	82563	141833
Sand	10	1	7348	6808
Polysulfone	495	508	2	1
Polychloroprene	1	0	401	105
Chitin	10	7	3756	4382
Polycaprolactone	0	0	180	285
Ethylene-Vinyl-Acetate	1	2	522	334
Polyoxymethylene	3	1	12	20
Rubber type 1	0	1	26	0
Charcoal	0	1	1	1
Coal	0	11	1	6
Rubber type 3	112	302	683	1067

*Please note that the export for siMPle could only be performed for a fieldsize of 85*85 FPA fields by combing 2 x 2 FPA fields to a larger one, an export of each field was not possible because the Marco stop working due to unknown reasons. The dataset misses 42910 spectra and mainly PP assignments as it was part of the outer region also visualized in Figure XY.

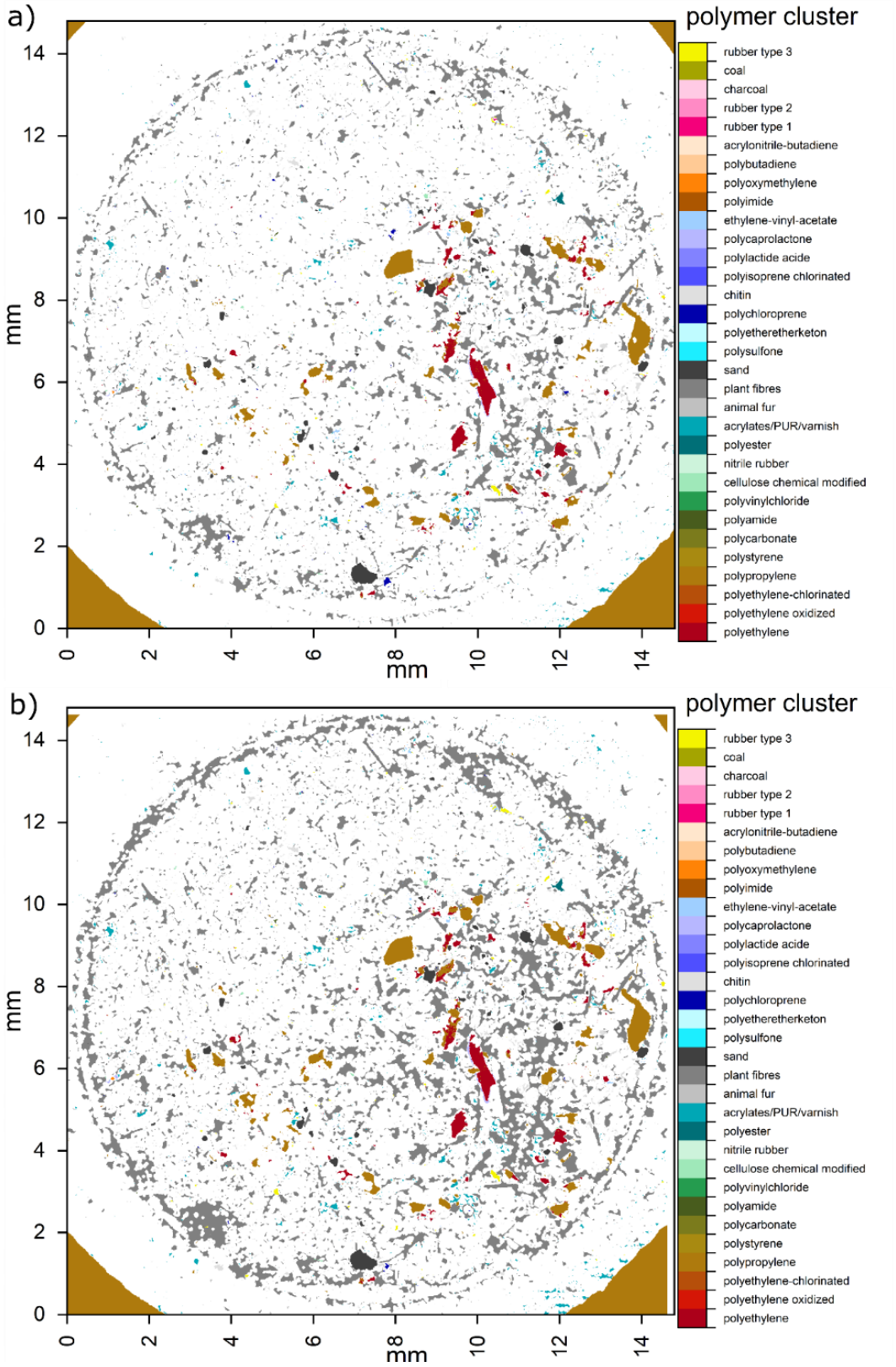

Figure S3. False color overview images from the analysis of the sample RefEnv2 via OPUS (a) and siMPle (b). Please note that the export for siMPle could only be performed for

RefEnv2 (field size of 85*85 FPA fields) by combing 2 x 2 FPA fields to a larger one, an export of each field was not possible because the Marco stop working due to unknown reasons. The dataset misses 42910 spectra visible as white area at the top and right side.

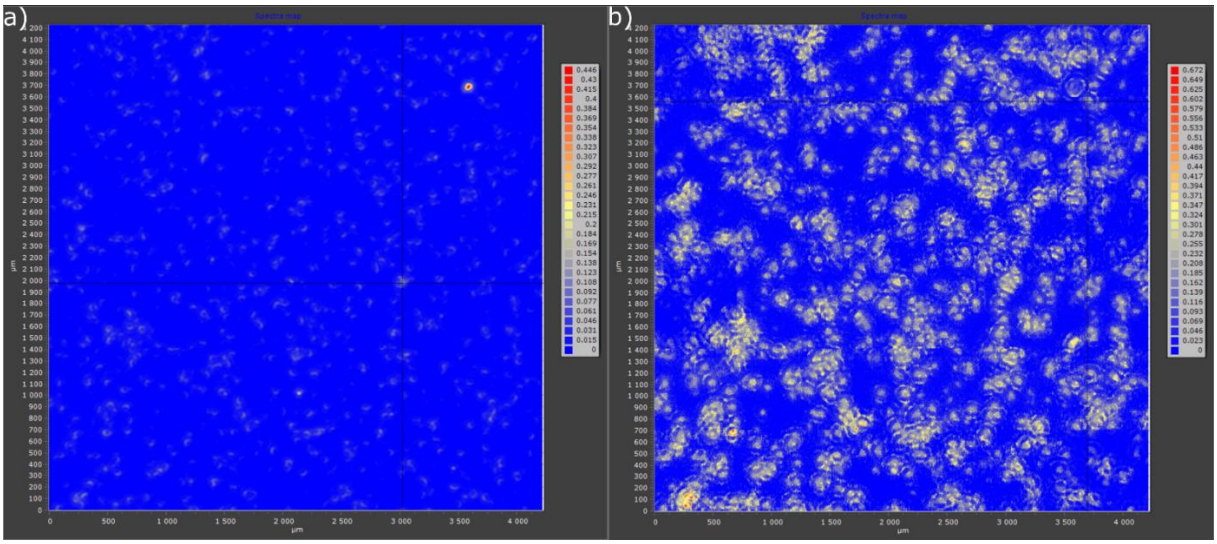

Figure S4. Algae cells (*Raphidocelis subcapitata*) placed on CaF_2 measured using the Agilent system. (a) General Heatmap based on the highest Peak in the spectrum. (b) Visualization of the particles using spectral comparison against the database entry algae *fucus serratus*.