Electronic Supplementary Material (ESI) for Analytical Methods.

SUPPLEMENTARY MATERIAL

In-situ Dissolved Polypropylene Prediction by Raman and ATR-IR Spectroscopy for its Recycling

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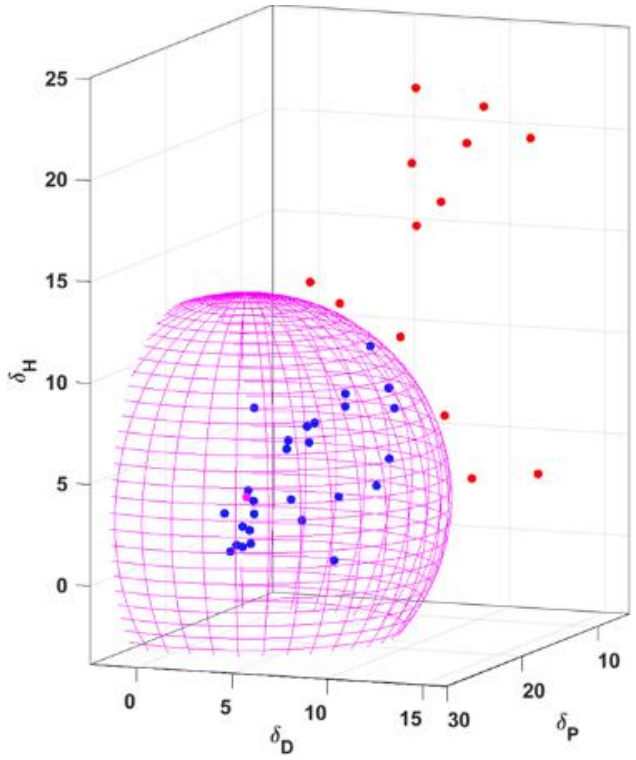

Figure S1 Hansen solubility model of PP and the four selected solvents. The pink dot represents PP, the pink grid represents the Hansen sphere, the blue dots represent good solvents which falls inside the sphere and the red dots represent the bad solvents which falls outside the sphere.

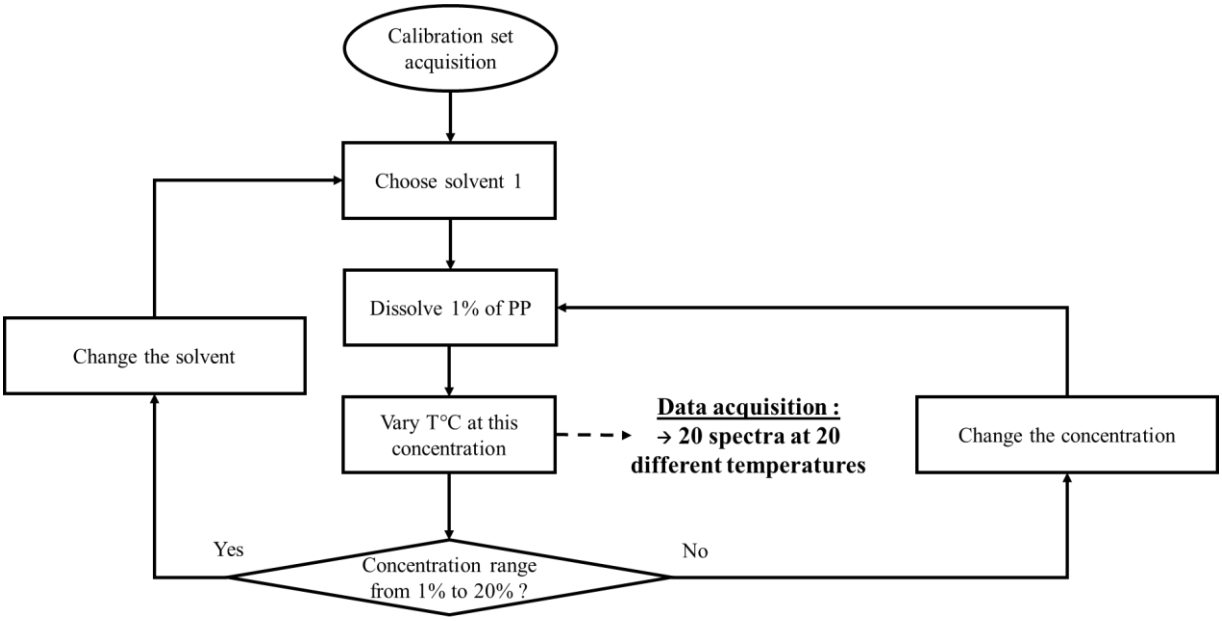

Figure S2 Flow diagram for the construction of the calibration set.

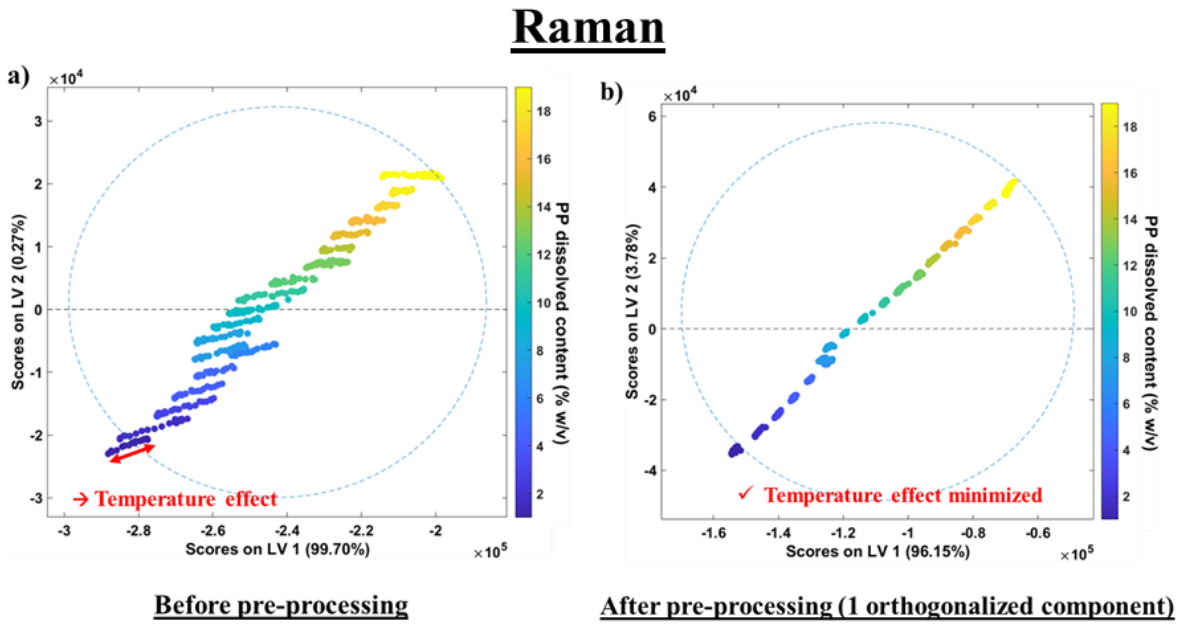

Figure S3 PCA scores plot on the two first latent variables of the Raman calibration set in TCB (a) before pre-processing and (b) after EPO pre-processing.

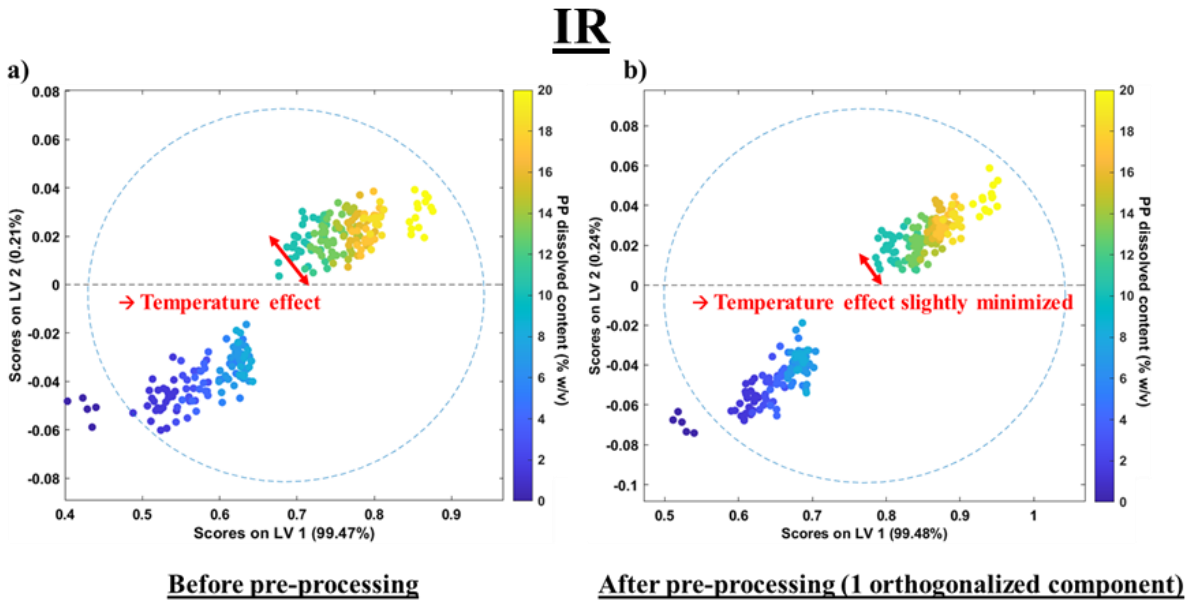

Figure S4 PCA scores plot on the two first latent variables of the Raman calibration set in TCB (a) before pre-processing and (b) after EPO pre-processing.

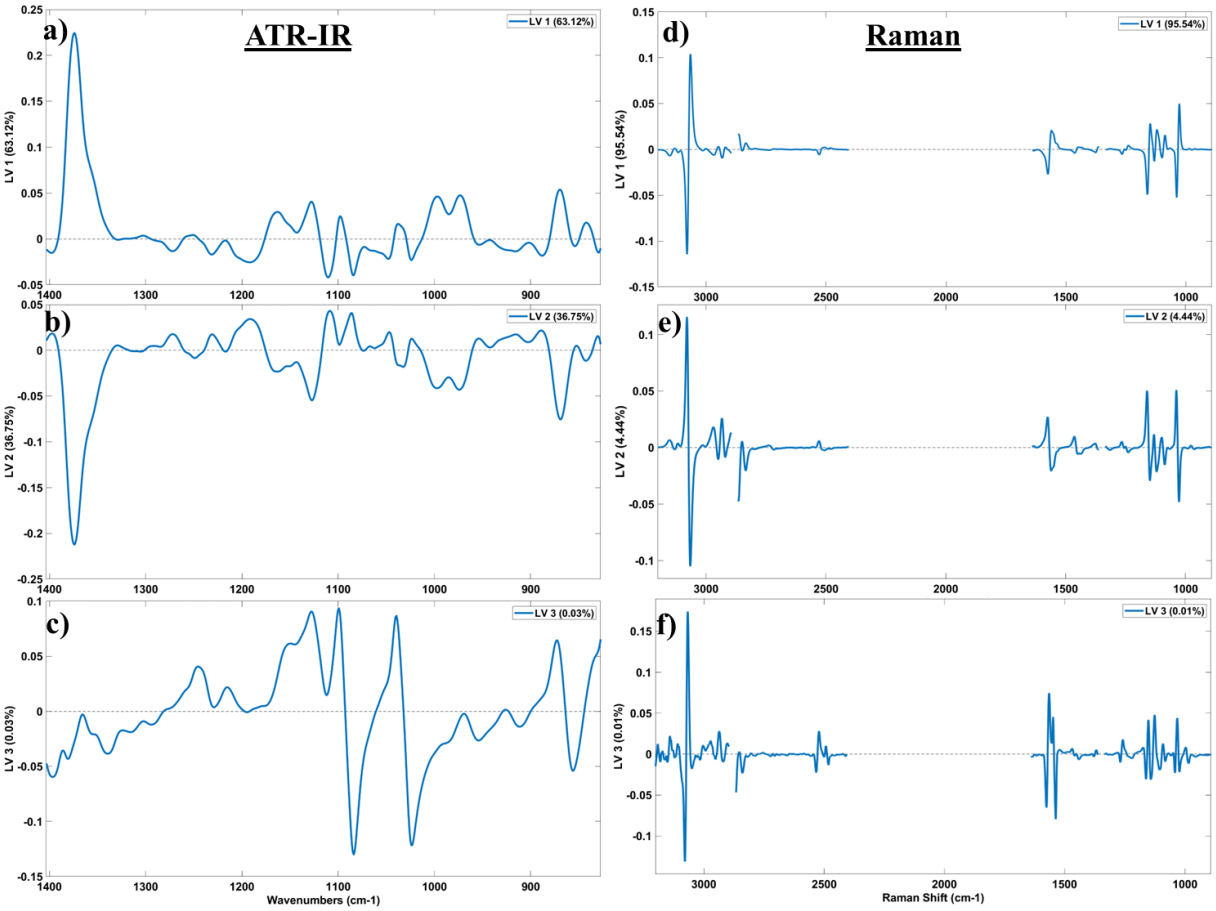

Figure S5 PLS model loadings for: a) ATR-IR 1st latent variable, b) ATR-IR 2nd latent variable c) ATR-IR 3rd latent variable d) Raman 1st latent variable, e) Raman 2nd latent variable and f) Raman 3rd latent variable of the TCB models.

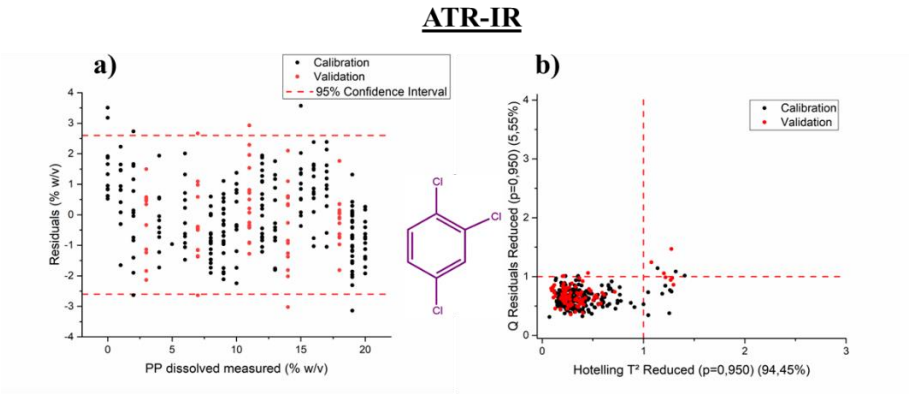

Figure S6 a) Residuals and b) Q Residuals reduced versus Hotelling T^2 of polypropylene concentration in TCB for ATR-IR model.

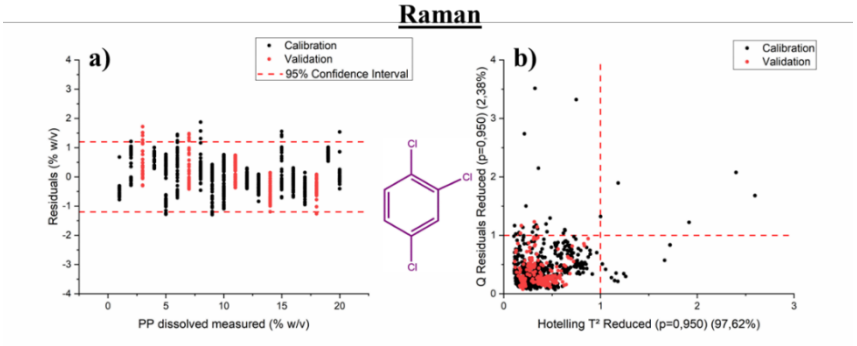

Figure S7 a) Residuals and b) Q Residuals reduced versus Hotelling T^2 of polypropylene concentration in TCB for Raman model.

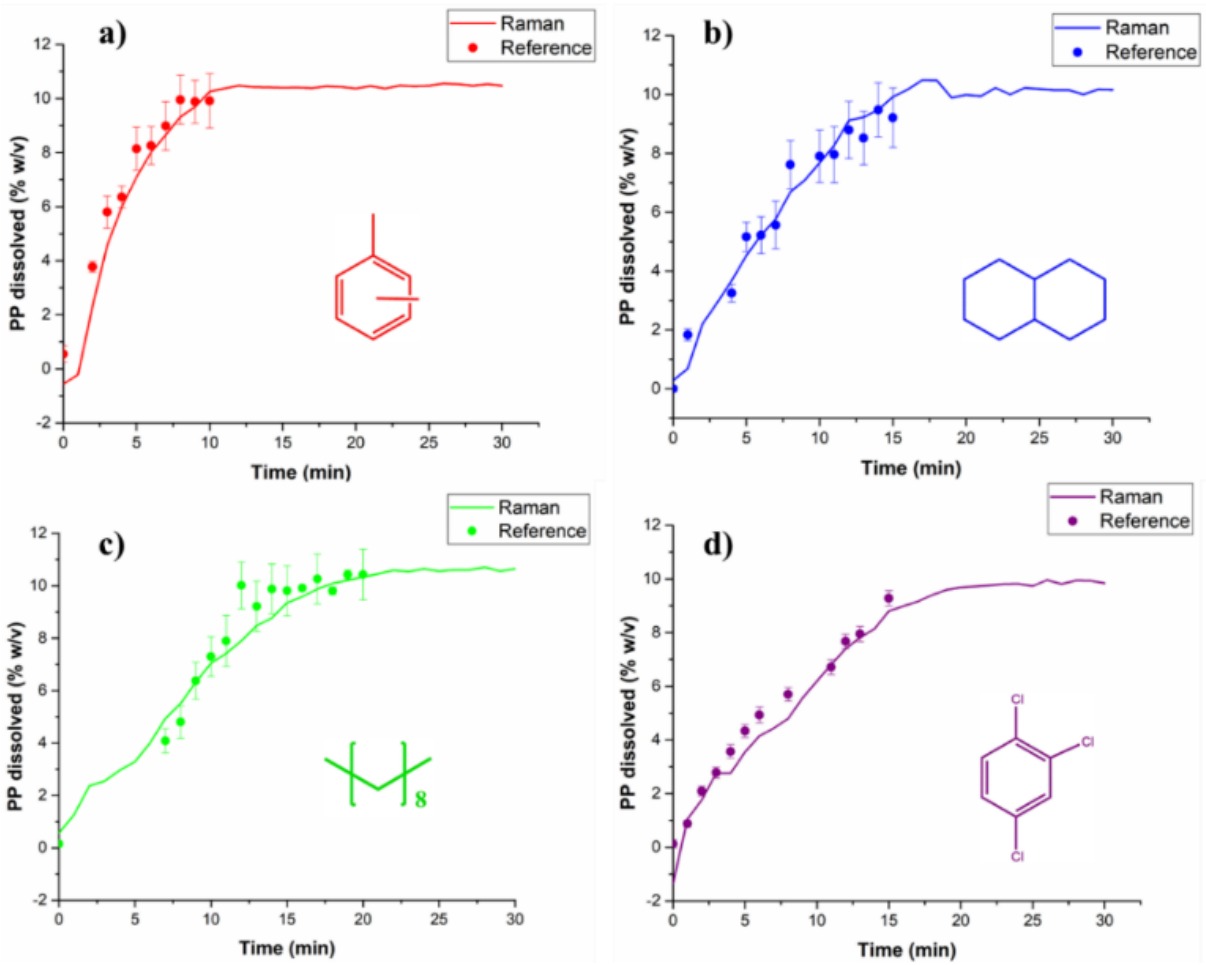

Figure S8 Prediction of the dissolved polymer content dissolved in a) Xylene, b) Decalin, c) Decane and d) TCB.

Table. S1 Values of Hansen solubility parameters of polypropylene and various solvents

	δd	δp	δh
Polypropylene	18	1	2.8
Solvent	δd	δp	δh
toluene	18	1.4	2
trichloroethylene	18	3.1	5.3
chlorobenzene	19	4.3	2
chloroform	17.8	3.1	5.7
cyclohexane	16.8	0	0.2
benzene	18.4	0	2
o-dichlorobenzene	19.2	6.3	3.3
butyl acetate	15.8	3.7	6.3
hexane	14.9	0	0
ethyl acetate	15.8	5.3	7.2
diethyl ether	14.5	2.9	5.1
1,4-dioxane	19	1.8	7.4
tetrahydrofuran	16.8	5.7	8
nitrobenzene	20	8.6	4.1
xylene	17.8	1	3.1
cyclohexanone	17.8	8.4	5.1
amyl acetate	15.8	3.3	6.1
isopropyl benzene (cumene)	18.1	1.2	1.2
Tetrahydronaphthalene (Tetralin)	19.6	2	2.9
Decahydronaphthalene (Decalin)	17.6	0	0
Decane	16	0	0
Methyl Cyclopentane	16	0	1
n-Butyl Acetate	15.8	3.7	6.3
isophorone	16.6	8.2	7.4
diethyl maleate	16.1	7.7	8.3
butoxy ethoxy propanol	15.5	6.5	10.2
trichlorobenzene	20.2	4.2	3.2
tetrachloroethylene	18.3	5.7	0
nitroethane	16	15.5	4.5
ethanolamine	17	15.5	21.2
acetone	15.5	10.4	7
methanol	15.1	12.3	22.3
2-nitropropane	16.2	12.1	4.1
dipropylene glycol	16.6	12	20.7
ethanol	15.8	8.8	19.4

Table. S2 Chemical properties of the selected solvent in this study

Solvent	Purity	Molar mass	Density	Viscosity @20 °C	Molar volume
	(%)	(g mol^{-1})	(g cm^{-3})	(mPa.s)	(cm^3 mol^{-1})
Xylene	99	106.17	0.87	0.591	122.3
Decahydronaphthalene (decalin)	98	138.25	0.88	1.788	154.8
n-Decane	99	142.29	0.74	0.850	196.0
1,2,4-Trichlorobenzene	99	181.46	1.45	0.306	123.6