Isolation, characterisation and structural elucidation of polybutylene terephthalate cyclic oligomers and purity assessment by a ^{1}H qNMR method

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Supplementary information

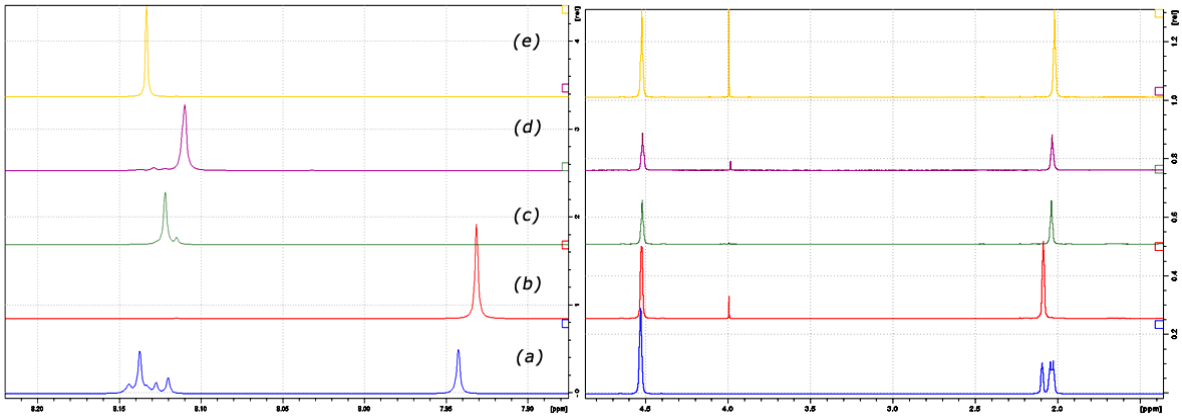

Figure S1. ^{1}H NMR spectrum of **FCM 885** and **4 PBT cyclic** dimer, trimer, tetramer and pentamer; (a) Mixture, (b) PBT dimer, (c) PBT trimer, (d) PBT tetramer, (e) PBT pentamer.

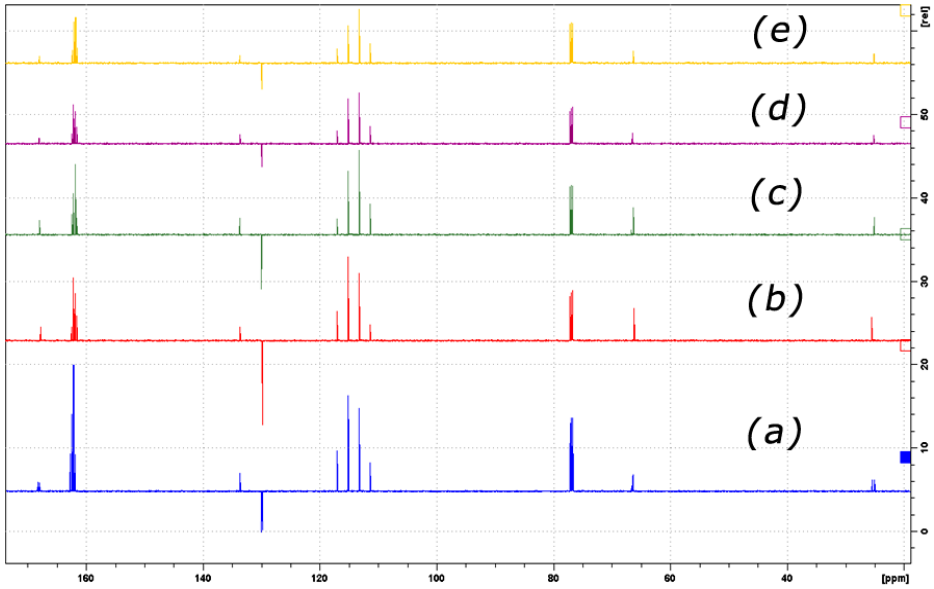

Figure S2. ^{13}C NMR spectrum of **FCM 885** and **4 PBT cyclic** dimer, trimer, tetramer and pentamer; (a) Mixture, (b) PBT dimer, (c) PBT trimer, (d) PBT tetramer, (e) PBT pentamer.

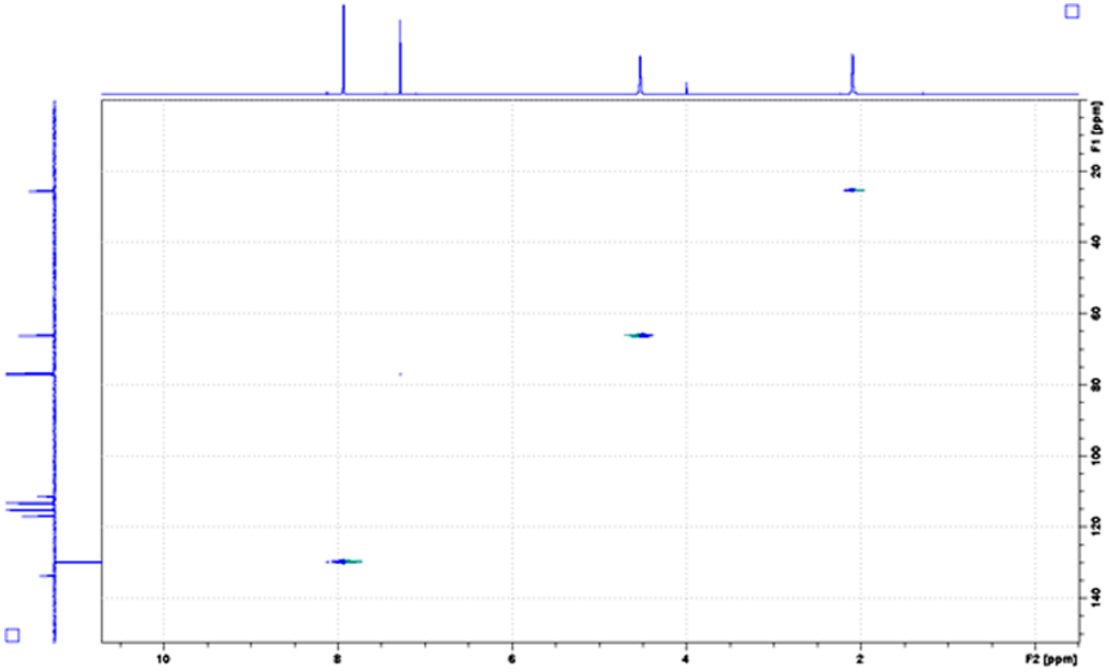

Figure S3: Monodimensional ^{13}C-NMR and ^{1}H-NMR of PBT cyclic dimer

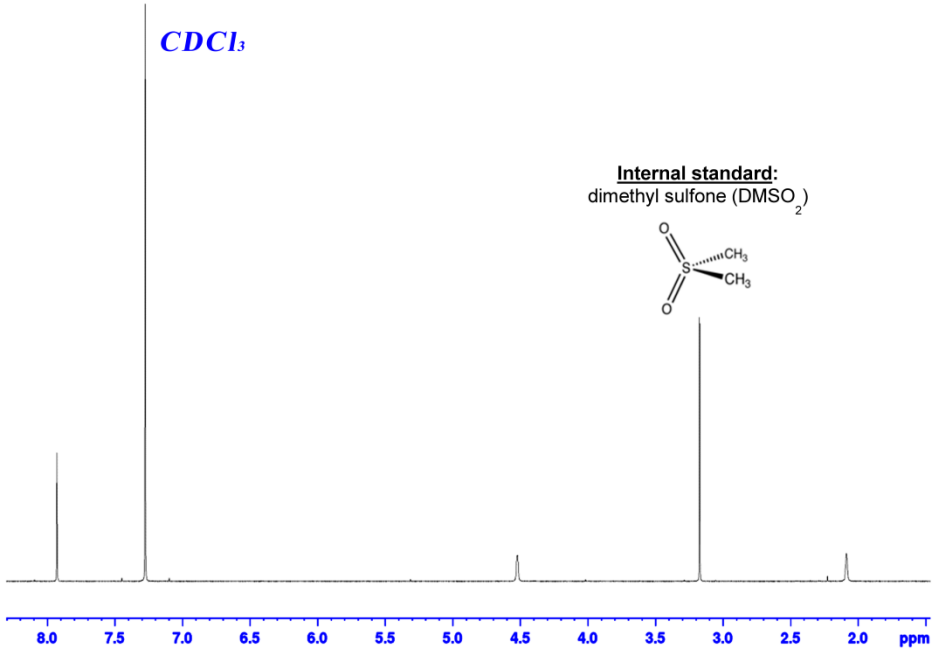

Figure S4. qNMR spectra of the PBT cyclic dimer, using dimethyl sulfone as internal standard.

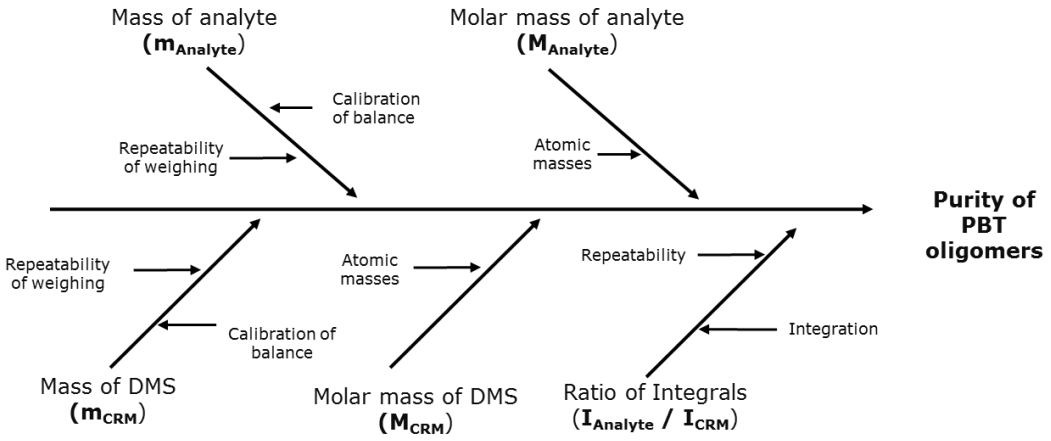

Figure S5. Cause-effect diagram of uncertainty contributions.

Table S1. Purity and expanded uncertainty assessment for the isolated PBT cyclic oligomers by qNMR.

	PBT Cyclic dimer		PBT Cyclic trimer		PBT Cyclic tetramer		PBT Cyclic pentamer	
	Value	**u (%)**	**Value**	**u (%)**	**Value**	**u (%)**	**Value**	**u (%)**
$I_{Analyte}/I$	9.9 (±0.05)	0.5 %	9.9 (±0.04)	0.4 %	10.4 (±0.05)	0.5	10.0 (±0.04)	0.4
I_{CRM}*	18.3 (±0.08)	0.4 %	14.2 (±0.06)	0.4 %	14.6 (±0.05)	0.3	10.8 (±0.05)	0.5
N_{CRM}	6	0	6	0	6	0	6	0
$N_{Analyte}$	4	0	4	0	4	0	4	0
m_{CRM} (mg)	1.0	0.1	1.1	0.1	1.1	0.1	1.1	0.042 %
$m_{ANALYTE}$ (mg)	2.0	0.1	2.7	0.1	2.7	0.1	3.6	0.042 %
$M_{Analyte}$ (g/mol)	440.441	0.015 %	660.662	0.013 %	880.882	0.012 %	1101.103	0.011 %
M_{CRM} (g/mol)	94.13	0.001 %	94.13	0.001 %	94.13	0.001 %	94.13	0.001 %
P_{CRM} (DMS)%	99.96	0.15 %	99.96	0.15 %	99.96	0.15 %	99.96	0.15 %
Purity (%)	96.5		97.0		96.1		96.4	
Relative Uncertainty (k=2); U (%)	1.3 %		1.1 %		1.2 %		1.3 %	