

# Analysis of PET Cyclic Oligomers Migrated in Olive Oil and Food Simulants Using UHPLC-qTOF-MS

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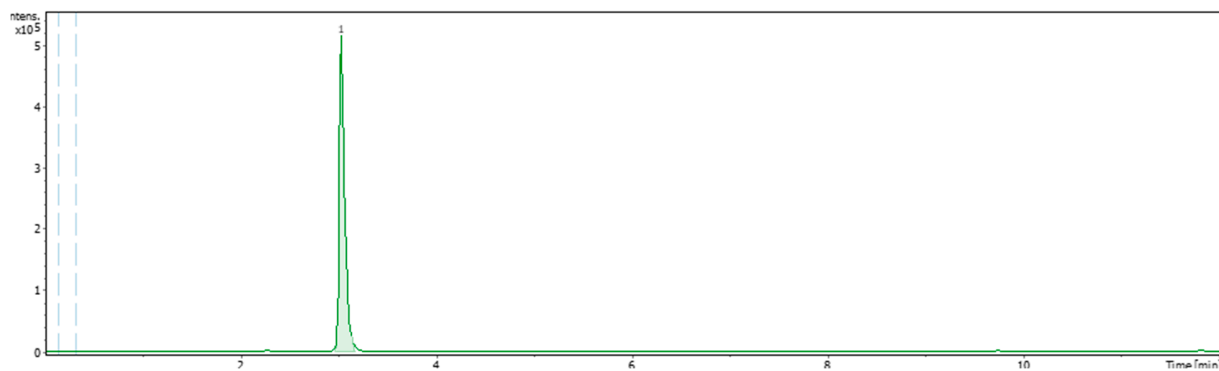
## Supplementary information

**Table S1.** Tentative quantification results ( $\mu\text{g L}^{-1}$ ) of PET linear oligomers from recycled and virgin PET in food simulants D2. Linear oligomers were identified based on monoisotopic molecular mass in accordance with Tsochatzis et al. (2020), unless otherwise stated.

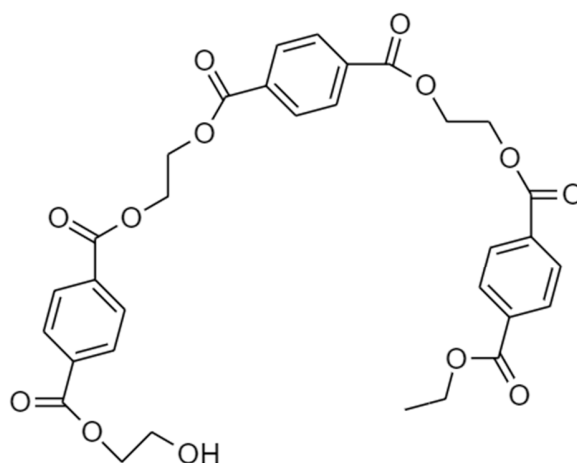
Linear oligomer code	Precursor ion (m/z)	Retention time (min)	rPET		vPET	
			Sample no.1	Sample no.2	Sample no.1	Sample no.2
H-[TPA-EG] <sub>2</sub> -H	387.1924	2.5	39.36±0.21	35.51±1.23	113.4±7.12	102.2±5.32
H-[TPA-EG] <sub>2</sub> -OH	403.1016	1.8	41.33±2.31	40.81±5.67	61.14±3.98	47.22±3.45
H-[TPA-EG] <sub>3</sub> -OH	594.1593	3.2	3953±32.34	2845±54.43	738.2±18.56	378.7±8.88
H-[TPA-EG] <sub>3</sub> -OC <sub>2</sub> H <sub>5</sub> *	623.1744	3.1	4282±56.21	3994±39.76	822.4±11.56	645.1±9.67
H-[TPA-EG] <sub>3</sub> -EG-OH	639.1697	2.2	83.52±6.54	80.78±4.87	24.98±1.95	19.17±0.65

\* Identification based on monoisotopic molecular mass.

(A)



(B)



**Figure S1.** (A) UHPLC-qTOF-MS extracted ion chromatogram of ionic mass 623.1744 Da of a representative D2 solvent and (B) the corresponding molecular structure identified as H-[TPA-EG]<sub>3</sub>-O-C<sub>2</sub>H<sub>5</sub>.



**Figure S2.** Representative TICs of food simulants D2 from (A) nPET and (B) rPET bottles after their storage in accelerated conditions.