# Supplementary Material:

# Migration modeling as a valuable tool for exposure assessment and risk characterization of polyethylene terephthalate oligomers

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**Table S1. SMILES and CAS Registry Numbers (CAS RN) of PET oligomers used for migration predictions.** Abbreviations: C (cyclic), L (linear), TPA (terephthalic acid), EG (ethylene glycol), DEG (diethylene glycol).
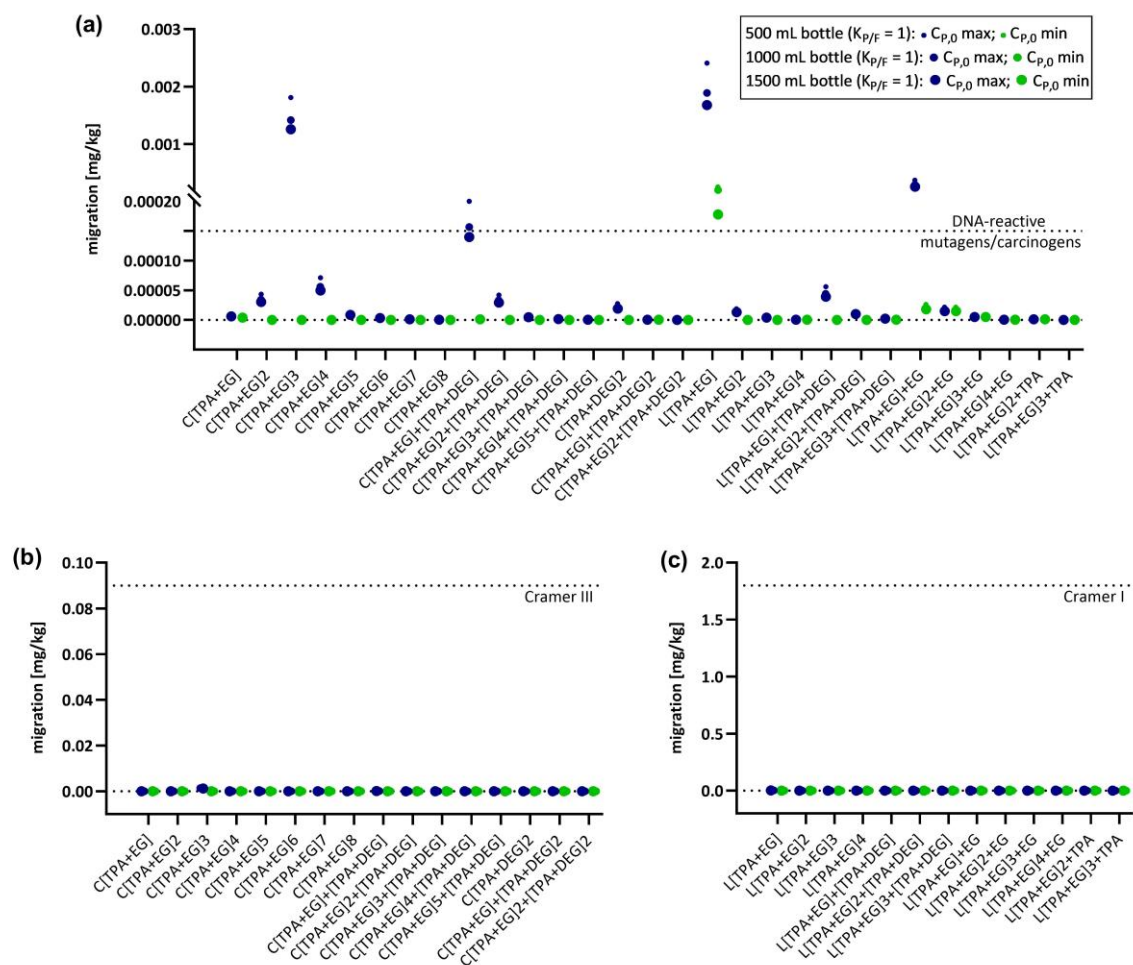
| PET oligomer (CAS RN) | SMILES |
|---|---|
| C[TPA+EG] (7337-79-3) | O=C1OCCOC(=O)C2=CC=C1C=C2 |
| C[TPA+EG]2 (24388-68-9) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C1C=C3 |
| C[TPA+EG]3 (7441-32-9) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C1C=C4 |
| C[TPA+EG]4 (16104-96-4) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C1C=C5 |
| C[TPA+EG]5 (16104-97-5) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C(C=C5)C(=O)OCCOC(=O)C6=CC=C1C=C6 |
| C[TPA+EG]6 (29644-29-9) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C(C=C5)C(=O)OCCOC(=O)C6=CC=C(C=C6)C(=O)OCCOC(=O)C7=CC=C1C=C7 |
| C[TPA+EG]7 (29668-12-0) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C(C=C5)C(=O)OCCOC(=O)C6=CC=C(C=C6)C(=O)OCCOC(=O)C7=CC=C(C=C7)C(=O)OCCOC(=O)C8=CC=C1C=C8 |
| C[TPA+EG]8 (42245-76-1) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C(C=C5)C(=O)OCCOC(=O)C6=CC=C(C=C6)C(=O)OCCOC(=O)C7=CC=C(C=C7)C(=O)OCCOC(=O)C8=CC=C(C=C8)C(=O)OCCOC(=O)C9=CC=C1C=C9 |
| C[TPA+DEG] (18189-01-0) | O=C1OCCOCCOC(=O)C2=CC=C1C=C2 |
| C[TPA+EG]+[TPA+DEG] (29278-57-7) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOCCOC(=O)C3=CC=C1C=C3 |
| C[TPA+EG]2+[TPA+DEG] (873422-64-1) | O=C1OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C1C=C4 |
| C[TPA+EG]3+[TPA+DEG] (2222729-29-3) | O=C(C1=CC=C(C(OCCOCCOC(C(C=C2)=CC=C2C(OCCOC(C3=CC=C4C=C3)=O)=O)=O)=O)=O)C=C1)OCCOC(C(C=C5)=CC=C5C(OCCOC4=O)=O)=O |
| C[TPA+EG]4+[TPA+DEG] (not available) | O=C(C1=CC=C(C(OCCOCCOC(C(C=C2)=CC=C2C(OCCOC(C3=CC=C4C=C3)=O)=O)=O)=O)=O)C=C1)OCCOC(C(C=C5)=CC=C5C(OCCOC(C(C=C6)=CC=C6C(OCCOC4=O)=O)=O)=O)=O)=O |
| C[TPA+EG]5+[TPA+DEG] (not available) | O=C(OCCOC(C1=CC=C(C=C1)C(OCCOC(C2=CC=C(C=C2)C(OCCOC(C3=CC=C(C=C3)C(OCCOC(C4=CC=C(C=C4)C(OCCO5)=O)=O)=O)=O)=O)=O)=O)=O)C(C=C6)=CC=C6C(OCCOCCOC(C(C=C7)=CC=C7C5=O)=O)=O |
| C[TPA+DEG]2 (16104-98-6) | O=C1OCCOCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOCCOC(=O)C3=CC=C1C=C3 |
| C[TPA+EG]+[TPA+DEG]2 (not available) | O=C(C1=CC=C(C2=O)C=C1)OCCOC(C3=CC=C(C(OCCOCCOC(C4=CC=C(C(OCCOCCO2)=O)C=C4)=O)=O)C=C3)=O |
| C[TPA+EG]2+[TPA+DEG]2 (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOCCOC(C3=CC=C4C=C3)=O)=O)C=C2)=O)=O)C=C1)OCCOC(C5=CC=C(C(OCCOCCOC4=O)=O)C=C5)=O |
| C[TPA+EG]3+[TPA+DEG]2 (not available) | O=C(OCCOCCOC(C1=CC=C(C(OCCOCCOC(C2=CC=C(C3=O)C=C2)=O)=O)C=C1)=O)C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOC(C6=CC=C(C(OCCO3)=O)C=C6)=O)=O)C=C5)=O)=O)C=C4 |
| C[TPA+EG]4+[TPA+DEG]2 (not available) | O=C(C1=CC=C(C=C1)C(OCCOC(C2=CC=C(C=C2)C(OCCOC(C3=CC=C4C=C3)=O)=O)=O)=O)OCCOCCOC(C5=CC=C(C=C5)C(OCCOCCOC(C6=CC=C(C=C6)C(OCCOC(C(C=C7)=CC=C7C(OCCOC4=O)=O)=O)=O)=O)=O)=O)=O |
| C[TPA+EG]+[TPA+DEG]3 (not available) | O=C(C1=CC=C(C(OCCOCCOC(C2=CC=C(C(OCCOC(C3=CC=C4C=C3)=O)=O)C=C2)=O)=O)C=C1)OCCOCCOC(C(C=C5)=CC=C5C(OCCOCCOC4=O)=O)=O |
| L[TPA+EG] (1137-99-1) | O=C(O)C1=CC=C(C=C1)C(=O)OCCO |
| L[TPA+EG]2 (23186-89-2) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCO |
| L[TPA+EG]3 (16958-96-6) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCO |
| L[TPA+EG]4 (1497479-05-6) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCO |
| L[TPA+EG]5 (51799-34-9) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C(C=C5)C(=O)OCCO |
| L[TPA+EG]6 (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOC(C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOC(C6=CC=C(C(OCCO)=O)C=C6)=O)=O)C=C5)=O)=O)C=C4)=O)=O)C=C3)=O)=O)C=C2)=O)=O)C=C1)O |
| L[TPA+EG]7 (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOC(C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOC(C6=CC=C(C(OCCOC(C7=CC=C(C(OCCO)=O)C=C7)=O)=O)C=C6)=O)=O)C=C5)=O)=O)C=C4)=O)=O)C=C3)=O)=O)C=C2)=O)=O)C=C1)O |
| L[TPA+EG]8 (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOC(C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOC(C6=CC=C(C(OCCOC(C7=CC=C(C(OCCOC(C8=CC=C(C(OCCO)=O)C=C8)=O)=O)C=C7)=O)=O)C=C6)=O)=O)C=C5)=O)=O)C=C4)=O)=O)C=C3)=O)=O)C=C2)=O)=O)C=C1)O |
| L[TPA+DEG] (65087-23-2) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOCCO |

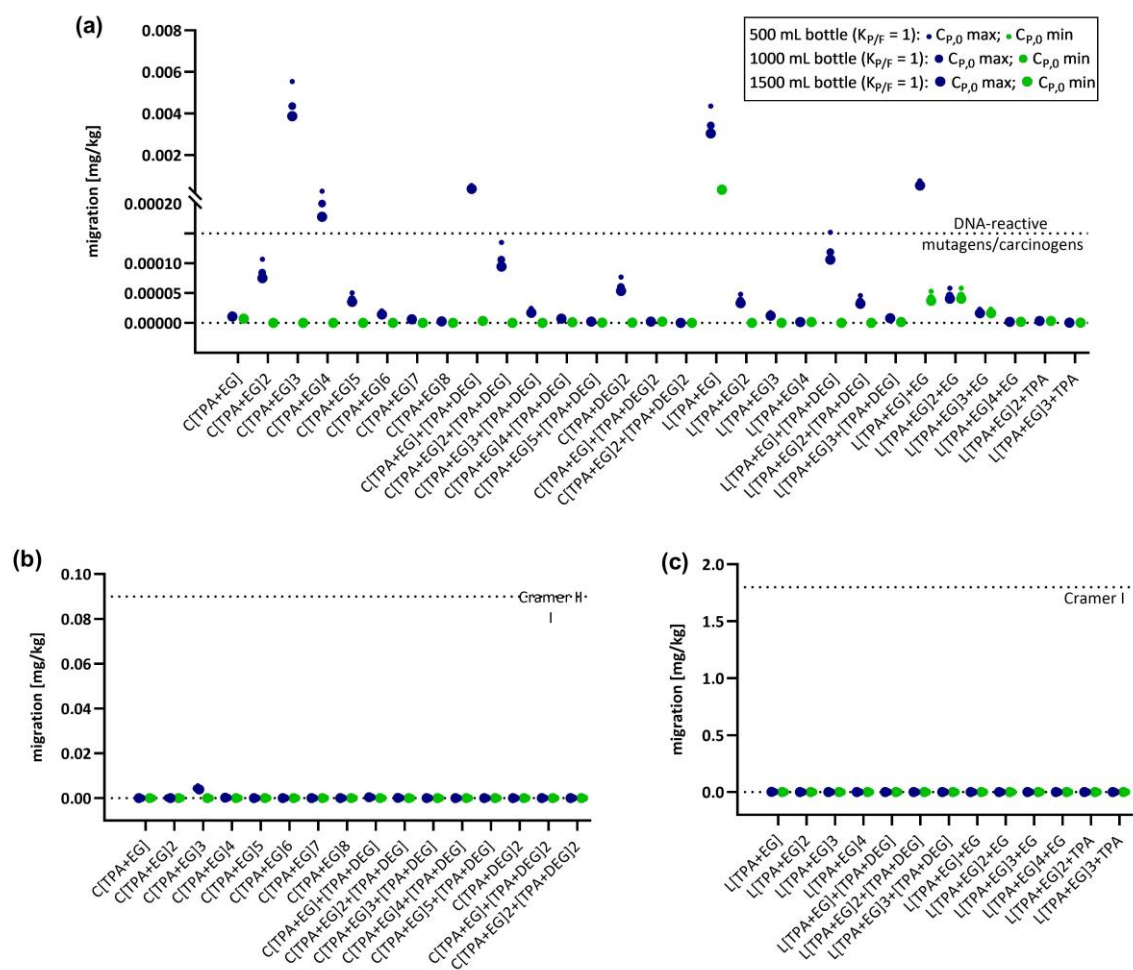| PET oligomer | SMILES |
|---|---|
| L[TPA+DEG]+EG (65133-69-9) | OCCOC(C1=CC=C(C(OCCOCCO)=O)C=C1)=O |
| L[TPA+EG]+[TPA+DEG] (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOCCO)=O)C=C2)=O)=O)C=C1)O |
| L[TPA+EG]2+[TPA+DEG] (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)OCCOC(C3=CC=C(C(OCCOCCO)=O)C=C3)=O |
| L[TPA+EG]3+[TPA+DEG] (not available) | O=C(OCCOC(C1=CC=C(C=C1)C(OCCOC(C2=CC=C(C=C2)C(OCCOCCO)=O)=O)=O)=O)C3=CC=C(C=C3)C(OCCOC(C4=CC=C(C=C4)C(O)=O)=O)=O |
| L[TPA+EG]4+[TPA+DEG] (not available) | O=C(OCCOC(C1=CC=C(C(OCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)=O)C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOCCO[H])=O)C=C5)=O)=O)C=C4)=O)=O)C=C3 |
| L[TPA+EG]5+[TPA+DEG] (not available) | O=C(OCCOC(C1=CC=C(C(OCCOCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)=O)C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOC(C6=CC=C(C(OCCO[H])=O)C=C6)=O)=O)C=C5)=O)=O)C=C4)=O)=O)C=C3 |
| L[TPA+DEG]2 (not available) | [H]OCCOCCOC(C1=CC=C(C(OCCOCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)=O |
| L[TPA+EG]+[TPA+DEG]2 (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)OCCOCCOC(C3=CC=C(C(OCCOCCO)=O)C=C3)=O |
| L[TPA+EG]2+[TPA+DEG]2 (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)OCCOC(C3=CC=C(C(OCCOCCOC(C4=CC=C(C(OCCOCCO)=O)C=C4)=O)=O)C=C3)=O |
| L[TPA+EG]3+[TPA+DEG]2 (not available) | O=C(OCCOC(C1=CC=C(C(OCCOC(C2=CC=C(C(O)=O)C=C2)=O)=O)C=C1)=O)C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOCCOC(C5=CC=C(C(OCCOCCO[H])=O)C=C5)=O)=O)C=C4)=O)=O)C=C3 |
| L[TPA+EG]4+[TPA+DEG]2 (not available) | O=C(C1=CC=C(C=C1)C(OCCOC(C2=CC=C(C=C2)C(OCCOC(C3=CC=C(C=C3)C(OCCO)=O)=O)=O)=O)=O)OCCOCCOC(C4=CC=C(C=C4)C(OCCOCCOC(C5=CC=C(C=C5)C(OCCOC(C(C=C6)=CC=C6C(O)=O)=O)=O)=O)=O)=O |
| L[TPA+EG]+EG (959-26-2) | O=C(OCCO)C1=CC=C(C=C1)C(=O)OCCO |
| L[TPA+EG]2+EG (2144-69-6) | O=C(OCCO)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCO |
| L[TPA+EG]3+EG (16033-73-1) | O=C(OCCO)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCO |
| L[TPA+EG]4+EG (34298-51-6) | O=C(OCCO)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCO |
| L[TPA+EG]5+EG (85122-18-5) | O=C(OCCO)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)OCCOC(=O)C5=CC=C(C=C5)C(=O)OCCO |
| L[TPA+EG]6+EG (85122-19-6) | O=C(C1=CC=C(C=C1)C(OCCOC(C2=CC=C(C=C2)C(OCCOC(C3=CC=C(C=C3)C(OCCOC(C4=CC=C(C=C4)C(OCCO)=O)=O)=O)=O)=O)=O)=O)OCCOC(C5=CC=C(C=C5)C(OCCOC(C6=CC=C(C=C6)C(OCCO)=O)=O)=O)=O)=O |
| L[TPA+EG]+TPA (2225-05-0) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)O |
| L[TPA+EG]2+TPA (1855-25-0) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)O |
| L[TPA+EG]3+TPA (122295-57-2) | O=C(O)C1=CC=C(C=C1)C(=O)OCCOC(=O)C2=CC=C(C=C2)C(=O)OCCOC(=O)C3=CC=C(C=C3)C(=O)OCCOC(=O)C4=CC=C(C=C4)C(=O)O |
| L[TPA+EG]4+TPA (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOC(C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(O)=O)C=C5)=O)=O)C=C4)=O)=O)C=C3)=O)=O)C=C2)=O)=O)C=C1)O |
| L[TPA+EG]5+TPA (not available) | O=C(C1=CC=C(C(OCCOC(C2=CC=C(C(OCCOC(C3=CC=C(C(OCCOC(C4=CC=C(C(OCCOC(C5=CC=C(C(OCCOC(C6=CC=C(C(O)=O)C=C6)=O)=O)C=C5)=O)=O)C=C4)=O)=O)C=C3)=O)=O)C=C2)=O)=O)C=C1)O |
| L[TPA+EG]6+TPA (not available) | O=C(C1=CC=C(C=C1)C(OCCOC(C2=CC=C(C=C2)C(OCCOC(C3=CC=C(C=C3)C(OCCOC(C4=CC=C(C=C4)C(O)=O)=O)=O)=O)=O)=O)=O)OCCOC(C5=CC=C(C=C5)C(OCCOC(C6=CC=C(C=C6)C(OCCOC(C7=CC=C(C(O)=O)C=C7)=O)=O)=O)=O)=O)=O |

**Table S2. Reported concentrations ($C_{P,0}$) for PET oligomers in food contact materials.** Collected information on $C_{P,0}$ values, corresponding literature source, and information if concentration was reported for the isomer as described in **Table S1** or if isomers were not defined. For values were standard deviation was available, only the mean value was captured. In case several values have been determined, the highest and lowest value were captured as a range. The highest concentration ($C_{P,0}$ max) used for migration predictions is marked in blue and the lowest concentration ($C_{P,0}$ min) is marked in green. Abbreviations: (cyclic), L (linear), TPA (terephthalic acid), EG (ethylene glycol), DEG (diethylene glycol).

| PET oligomer | $C_{P,0}$ value(s) correspond(s) to isomer described in Table S1 | Reported $C_{P,0}$ [mg/kg] | Literature source |
|---|---|---|---|
| C[TPA+EG] | yes | 0.18 – 0.27 | [2] |
| C[TPA+EG]2 | yes | 34 | [3] |
| | | 0.18 – 1.2 | [2] |
| | | $4.0 \times 10^{-4}$ – $1.5 \times 10^{-3}$ | [4] |
| | | 0.40 – 25 | [5] |
| | | 30 | [6] |

| | | | |
|---|---|---|---|
| C[TPA+EG]3 | yes | 2922 | [3] |
| | | 3000 – 6700 | [7] |
| | | 3000 – 4830 | [8] |
| | | 0.66 – 7.0 | [2] |
| | | 0.60 – 3.5 | [4] |
| | | 7951 – 9592 | [9] |
| | | 5150 – 8100 | [10] |
| | | 1400 – 5700 | [11] |
| | | 2.8 – 6039 | [5] |
| | | 5380 – 5680 | [6] |
| C[TPA+EG]4 | yes | 749 | [3] |
| | | 0.61 – 0.85 | [2] |
| | | $1.0 \times 10^{-3}$ – 0.4 | [4] |
| | | 450 – 1477 | [5] |
| | | 430 | [6] |
| C[TPA+EG]5 | yes | 303 | [3] |
| | | 0.18 – 0.17 | [2] |
| | | $1.0 \times 10^{-3}$ – $1.5 \times 10^{-3}$ | [4] |
| | | 205 – 749 | [5] |
| | | 66 | [6] |
| C[TPA+EG]6 | yes | 155 | [3] |
| | | 0.10 – 1.80 | [4] |
| | | 149 – 643 | [5] |
| | | 15 | [6] |
| C[TPA+EG]7 | yes | $1.6 \times 10^{-3}$ – $2.3 \times 10^{-3}$ | [12] |
| | | 84 – 551 | [5] |
| C[TPA+EG]8 | yes | 53 – 424 | [5] |
| C[TPA+EG]+[TPA+DEG] | yes | 281 | [3] |
| | | 2.5 – 19 | [2] |
| | | 174 – 240 | [5] |
| | | 100 | [6] |
| C[TPA+EG]2+[TPA+DEG] | yes | 157 | [3] |
| | | 0.34 – 2.2 | [2] |
| | | 72 – 334 | [5] |
| | | 140 | [6] |
| C[TPA+EG]3+[TPA+DEG] | yes | 124 | [3] |
| | | 0.18 – 0.59 | [2] |
| | | 37 – 185 | [5] |
| | | 9 | [6] |
| C[TPA+EG]4+[TPA+DEG] | yes | 84 | [3] |
| | | 32 – 189 | [5] |
| C[TPA+EG]5+[TPA+DEG] | yes | 21 – 130 | [5] |
| C[TPA+DEG]2 | yes | 65 | [3] |
| | | 0.69 – 4.8 | [2] |
| C[TPA+EG]+[TPA+DEG]2 | yes | 11 /11 | [3] |
| C[TPA+EG]2+[TPA+DEG]2 | *Isomer unclear | 0.18 – 1.1* | [2] |
| L[TPA+EG] | yes | 12.5 – 34.4 | [9] |
| | | 18 – 118 | [5] |
| L[TPA+EG]2 | yes | 0.18 – 0.51 | [2] |
| | | 19 | [6] |
| L[TPA+EG]3 | yes | 0.18 – 0.70 | [2] |
| | | 35 | [6] |
| L[TPA+EG]4 | yes | 14/14 | [6] |
| L[TPA+EG]+[TPA+DEG] | yes *Isomer unclear | 0.18 – 7.7 | [2] |
| | | 16 – 99* | [5] |
| L[TPA+EG]2+[TPA+DEG] | *Isomer unclear | 0.18 – 1.4* | [2] |
| | | 26 – 131* | [5] |
| L[TPA+EG]3+[TPA+DEG] | *Isomer unclear | 18 – 96* | [5] |
| L[TPA+EG]+EG | yes | 18 – 49 | [9] |
| | | 3.5 – 50 | [5] |
| L[TPA+EG]2+EG | yes | 38/38 | [6] |
| L[TPA+EG]3+EG | yes | 66/66 | [6] |
| L[TPA+EG]4+EG | yes | 25/25 | [6] |
| L[TPA+EG]2+TPA | yes | 7/7 | [6] |
| L[TPA+EG]3+TPA | | 3/3 | [6] |

**Figure S1. Graphical representation of predicted migrations using the $E_A$-based model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET bottles (500 – 1500 mL) under long-term storage condition (25 °C, 365 d) and evaluated for the exceeding different safety thresholds. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.
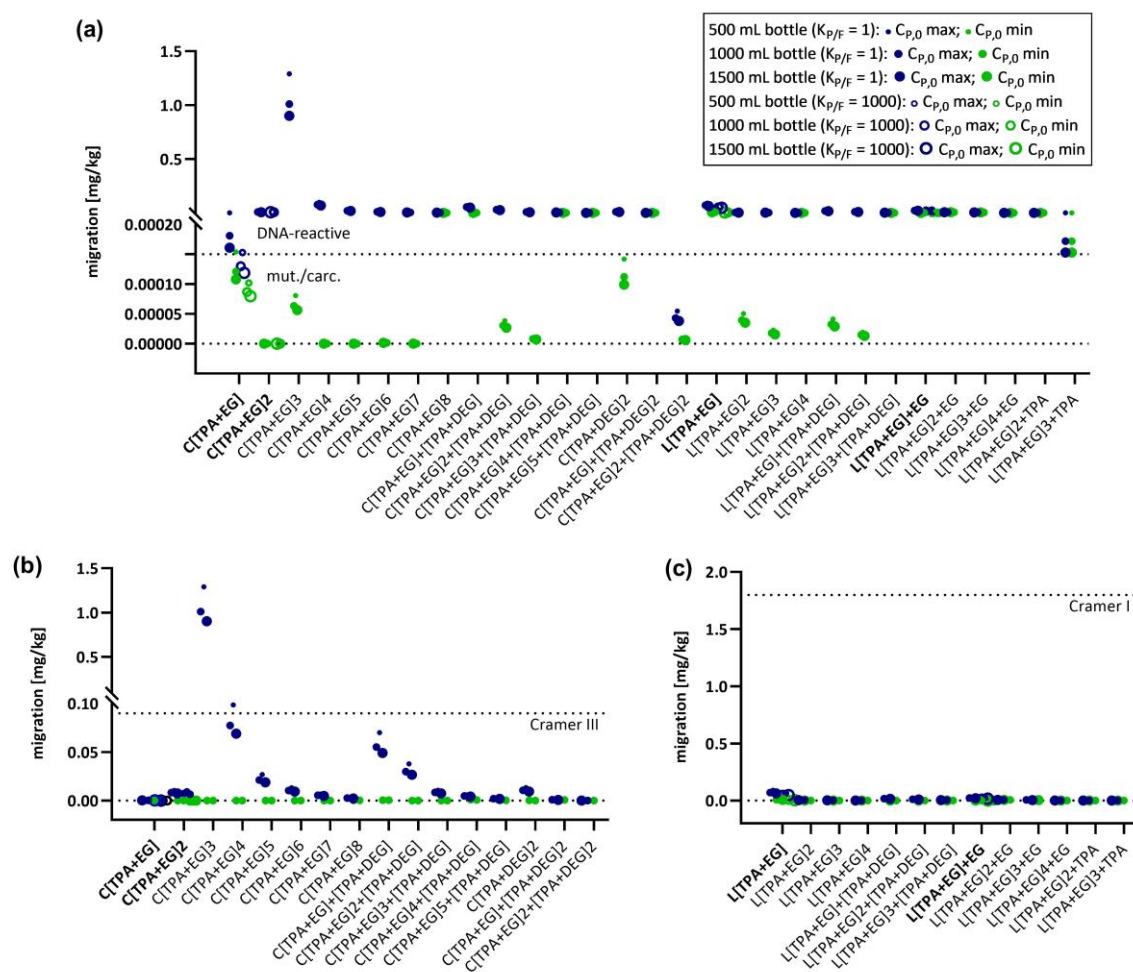
**Figure S2. Graphical representation of predicted migrations using the $E_A$-based model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET bottles (500 – 1500 mL) under short-term non-controlled/extreme summer storage condition (40 °C, 60 d) and evaluated for the exceeding different safety thresholds. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.
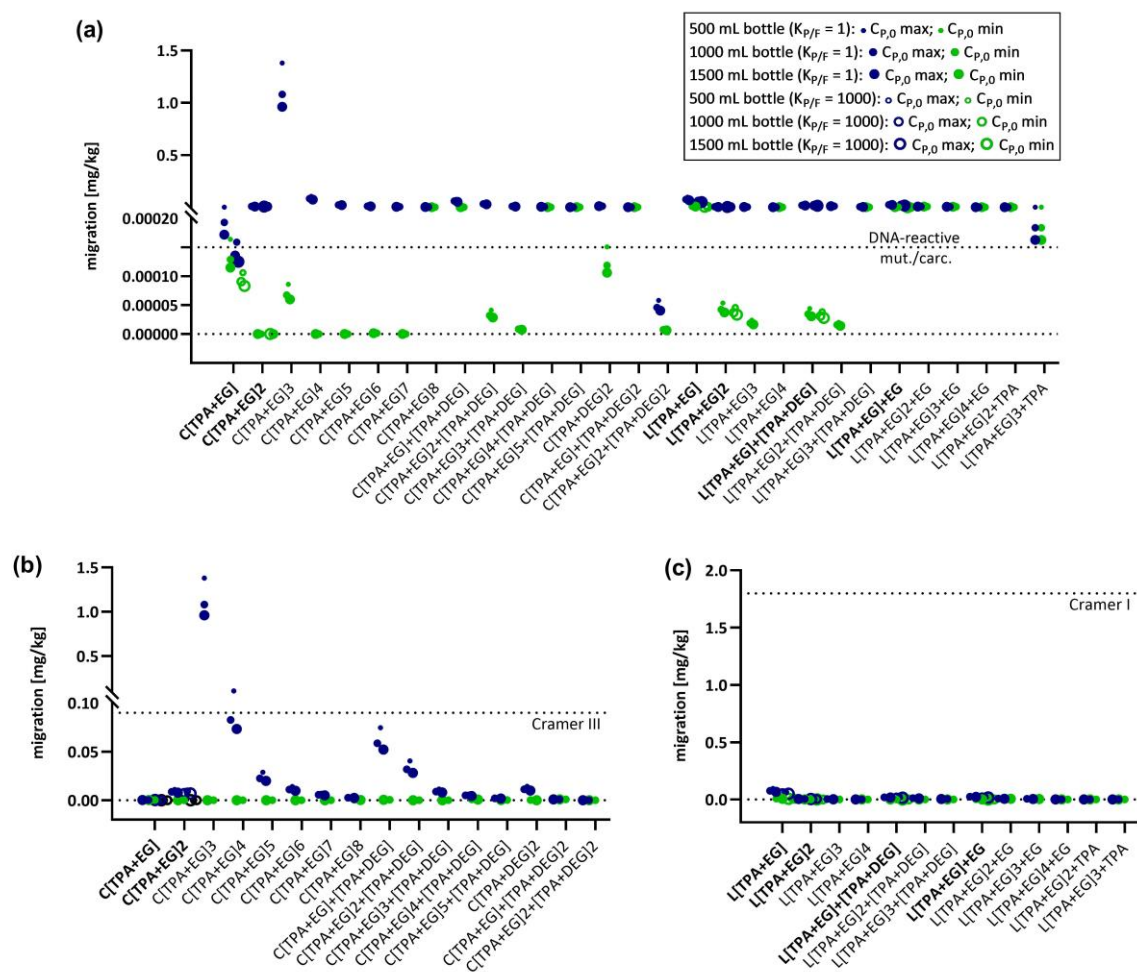
**Figure S3. Graphical representation of predicted migrations using the $E_A$-based model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET trays (rectangular and round) under short-term heating condition (70 °C, 30 min) and evaluated for the exceeding different safety thresholds. Oligomer names in bold represent molecules for which both $K_{P/F} = 1$ and $K_{P/F} = 1000$ were used for predictions. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.

**Figure S4. Graphical representation of predicted migrations using the $E_A$-based model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET trays (rectangular and round) under short-term heating condition (100 °C, 10 min) and evaluated for the exceeding different safety thresholds. Oligomer names in bold represent molecules for which both $K_{P/F} = 1$ and $K_{P/F} = 1000$ were used for predictions. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.
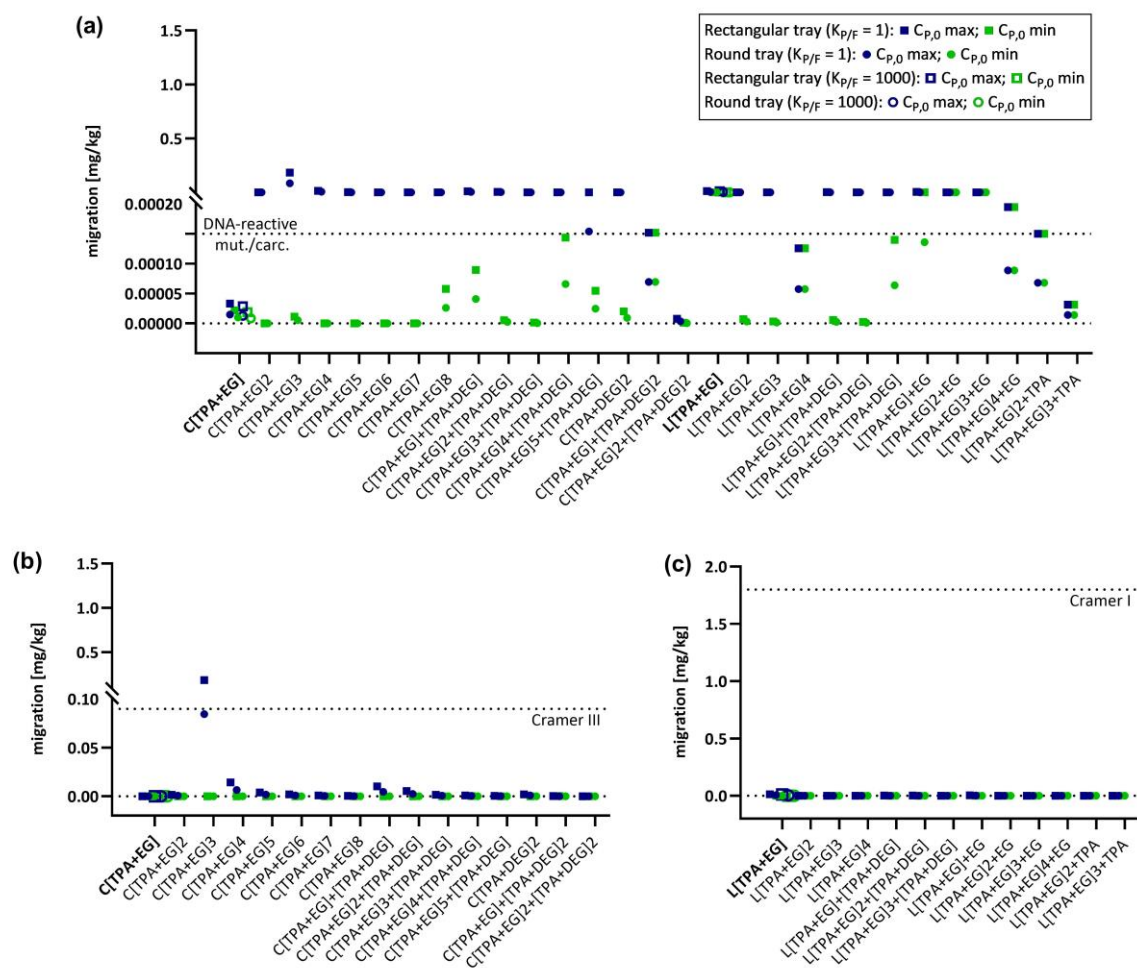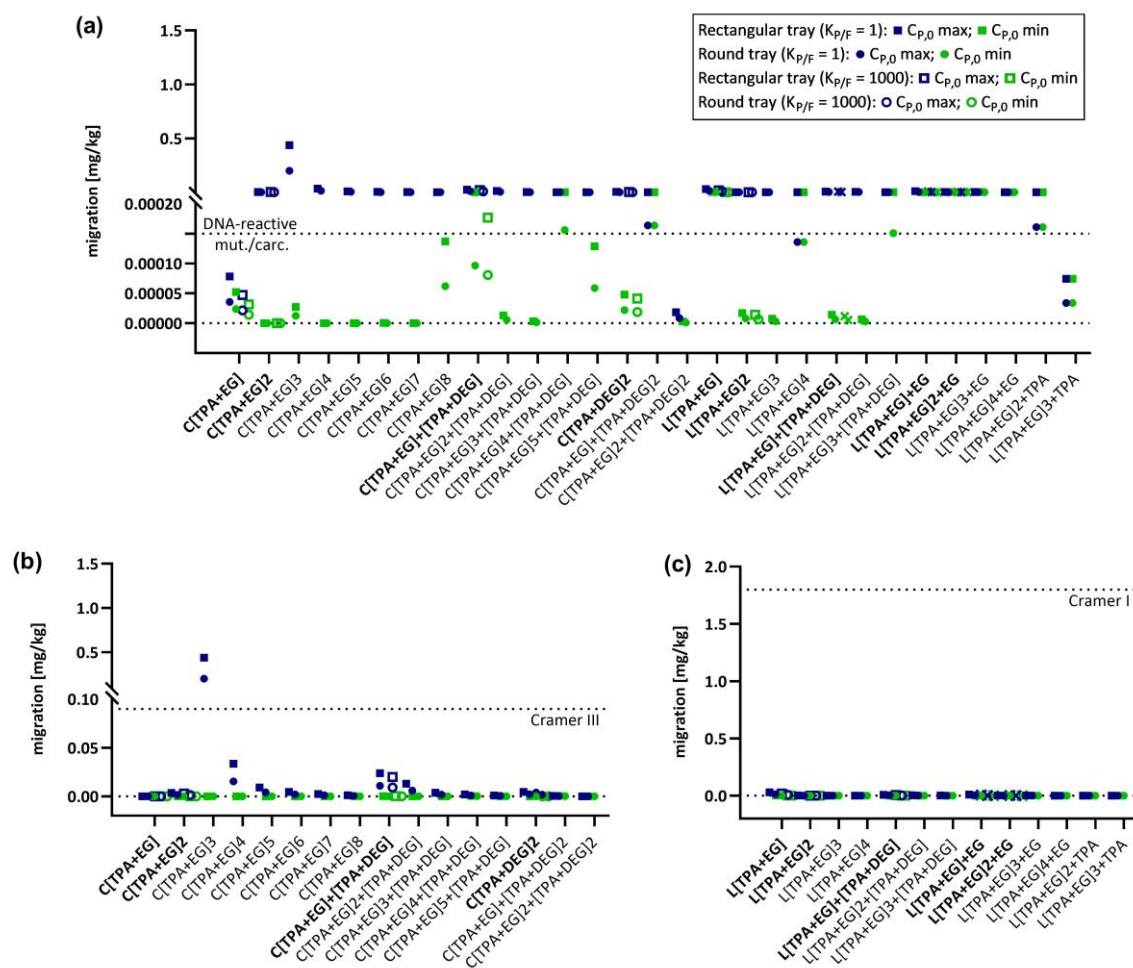
**Figure S5. Graphical representation of predicted migrations using the $A_P$ model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET bottles (500 – 1500 mL) under long-term storage condition (25 °C, 365 d) and evaluated for the exceeding different safety thresholds. Oligomer names in bold represent molecules for which both $K_{P/F} = 1$ and $K_{P/F} = 1000$ were used for predictions. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.
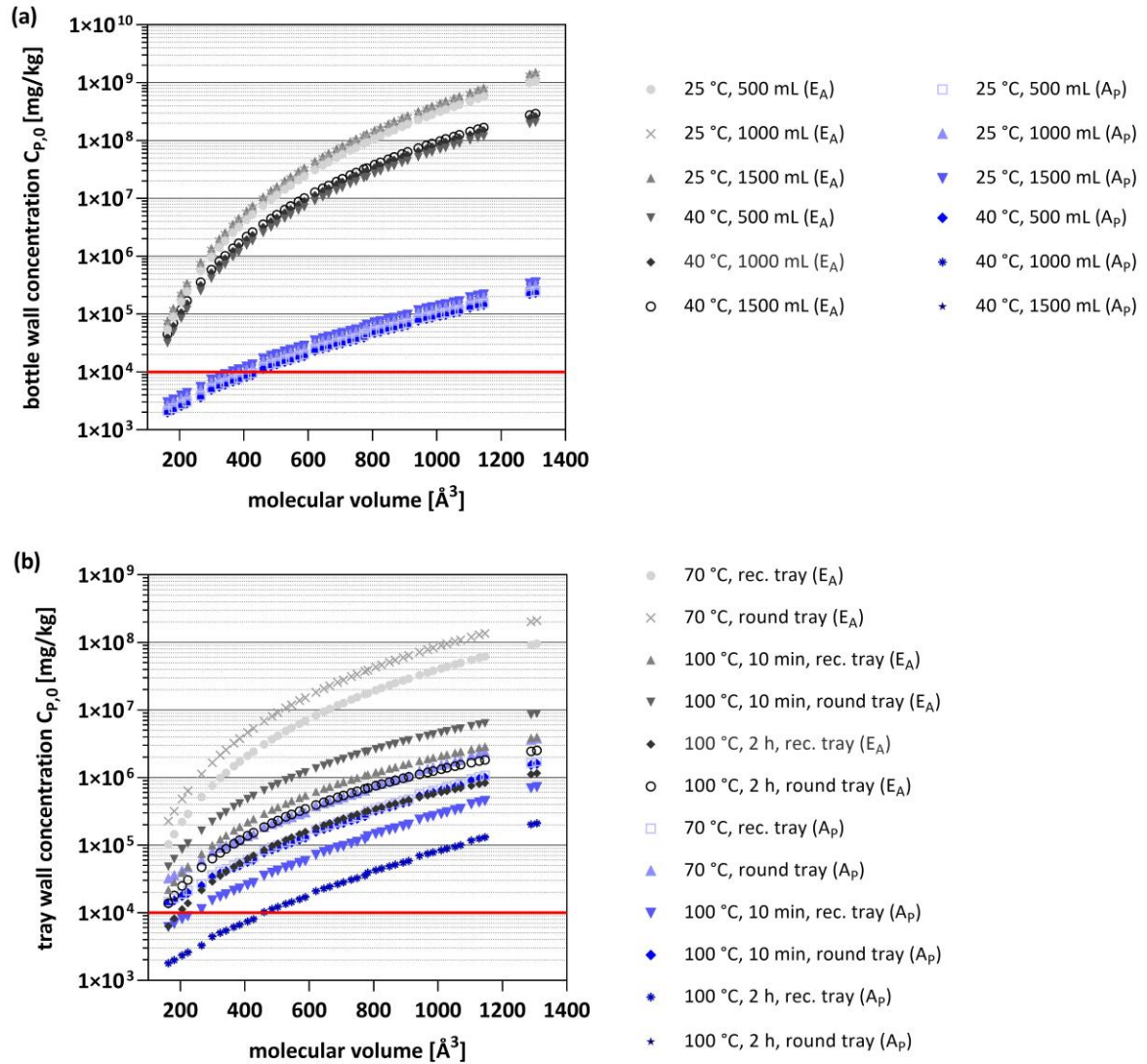
**Figure S6. Graphical representation of predicted migrations using the $A_P$ model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET bottles (500 – 1500 mL) under short-term non-controlled/extreme summer storage condition (40 °C, 60 d) and evaluated for the exceeding different safety thresholds. Oligomer names in bold represent molecules for which both $K_{P/F} = 1$ and $K_{P/F} = 1000$ were used for predictions. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.

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**Figure S7. Graphical representation of predicted migrations using the $A_P$ model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET trays (rectangular and round) under short-term heating condition (70 °C, 30 min) and evaluated for the exceeding different safety thresholds. Oligomer names in bold represent molecules for which both $K_{P/F} = 1$ and $K_{P/F} = 1000$ were used for predictions. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.

**Figure S8. Graphical representation of predicted migrations using the $A_P$ model.** Migration of PET oligomers for which $C_{P,0}$ values were available was predicted for PET trays (rectangular and round) under short-term heating condition (100 °C, 10 min) and evaluated for the exceeding different safety thresholds. Oligomer names in bold represent molecules for which both $K_{P/F} = 1$ and $K_{P/F} = 1000$ were used for predictions. **(a)** Modeled migration of all 29 PET oligomers and their evaluation against the DNA-reactive mutagens/carcinogens safety threshold of 0.15 µg/kg. **(b)** Modeled migration of cyclic PET oligomers and their evaluation against the Cramer Class III threshold of 90 µg/kg. **(c)** Modeled migration of linear PET oligomers and their evaluation against the Cramer Class I threshold of 1.8 mg/kg.

**(a)**

**(b)**

**Figure S9. Maximum bottle and tray wall concentrations ($C_{P,0}$) of all oligomers corresponding to a migration of 1.8 mg/kg, calculated for the $E_A$-based model (grey, ($E_A$)) and the $A_P$ model (blue, ($A_P$)).** **(a)** $C_{P,0}$ concentrations for 500, 1000, and 1500 mL bottle at 25 °C for 365 d and 40 °C for 60 d. **(b)** $C_{P,0}$ concentrations for rectangular (rec.) and round trays at 70 °C for 30 min and 100 °C for 10 min or 2 h. Red line indicates a $C_{P,0}$ concentration of 1% (w/w).

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