**MANUSCRIT SUPPLEMENTAL INFORMATION (SI)**

## SI-A. Experimental LDPE-Lipid Partition coefficients ($P_{ldpe/lipid}$)

Table SI-A tabulates the measured LDPE-lipid partition coefficients and their physicochemical properties [42-47]. The data by Ref [47] are used in the LDPE-lipid model construction (Section 2.2).

**Table S1. Tabulation of Analytes with Measured Partition coefficients ($P_{ldpe/lipid}$) and Their Physicochemical Properties**

| Ref # | # | Analytes | CAS # | MW | SMILES | E | S | A | B | V | $P_{ldpe/lipid}$ | $log_{10}P_{o/w}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| [47][a] | 1 | Hexachloro-1,3-butadiene | 87-68-3 | 260.8 | C(=C(Cl)Cl)(C(=C(Cl)Cl)Cl)Cl | 0.9964 | 0.4721 | -0.001 | 0.1348 | 1.3206 | 0.26 | 4.72 |
| | 2 | Pentachlorobenzene | 608-93-5 | 250.3 | C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl | 1.3262 | 0.9105 | 0.0368 | 0.0069 | 1.3284 | 0.252 | 4.92 |
| | 3 | Hexachlorobenzene | 118-74-1 | 284.8 | C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)Cl | 1.4616 | 0.8233 | 0.0136 | 0.0502 | 1.4508 | 0.309 | 5.40 |
| | 4 | PCB 18 | 37680-65-2 | 257.5 | C1=CC=C(C(=C1)C2=C(C=CC(=C2)Cl)Cl)Cl | 1.7467 | 1.352 | 0.0003 | 0.1689 | 1.6914 | 0.088 | 5.51 |
| | 5 | PCB 28 | 7012-37-5 | 257.5 | C1=CC(=CC=C1C2=C(C=C(C=C2)Cl)Cl)Cl | 1.7603 | 1.332 | 0.0006 | 0.1557 | 1.6914 | 0.114 | 5.59 |
| | 6 | PCB 31 | 16606-02-3 | 257.5 | C1=CC(=CC=C1C2=C(C=CC(=C2)Cl)Cl)Cl | 1.7758 | 1.3344 | 0.0016 | 0.1526 | 1.6914 | 0.094 | 5.60 |
| | 7 | PCB 44 | 41464-39-5 | 292 | C1=CC(=C(C(=C1)Cl)Cl)C2=C(C=CC(=C2)Cl)Cl | 1.8891 | 1.4854 | 0.0013 | 0.148 | 1.8138 | 0.0756 | 5.99 |
| | 8 | PCB 49 | 41464-40-8 | 292 | C1=CC(=C(C=C1Cl)Cl)C2=C(C=CC(=C2)Cl)Cl | 1.8888 | 1.4834 | 0.0013 | 0.148 | 1.8138 | 0.0852 | 5.99 |
| | 9 | PCB 52 | 35693-99-3 | 292 | C1=CC(=C(C=C1Cl)C2=C(C=CC(=C2)Cl)Cl)Cl | 1.8975 | 1.4797 | 0.001 | 0.1494 | 1.8138 | 0.079 | 6.00 |
| | 10 | PCB 101 | 37680-73-2 | 326.4 | C1=CC(=C(C=C1Cl)C2=CC(=C(C=C2Cl)Cl)Cl)Cl | 2.0379 | 1.6143 | 0.0004 | 0.1285 | 1.9362 | 0.0855 | 6.47 |
| | 11 | PCB 118 | 31508-00-6 | 326.4 | C1=CC(=C(C=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl | 2.0606 | 1.5793 | 0.0004 | 0.1122 | 1.9362 | 0.0952 | 6.58 |
| | 12 | PCB 138 | 35065-28-2 | 360.9 | C1=CC(=C(C(=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl)Cl | 2.1798 | 1.7379 | 0.0014 | 0.1076 | 2.0586 | 0.0864 | 6.96 |
| | 13 | PCB 153 | 35065-27-1 | 360.9 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl | 2.1657 | 1.7331 | -0.0009 | 0.1081 | 2.0586 | 0.097 | 6.96 |
| | 14 | PCB 170 | 35065-30-6 | 395.3 | C1=CC(=C(C(=C1C2=CC(=C(C(=C2Cl)Cl)Cl)Cl)Cl)Cl)Cl | 2.3255 | 1.8739 | 0.0011 | 0.0894 | 2.181 | 0.086 | 7.43 |
| | 15 | PCB 180 | 35065-29-3 | 395.3 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl | 2.3102 | 1.8708 | 0.0025 | 0.0894 | 2.181 | 0.0995 | 7.42 |
| | 16 | PCB 187 | 52663-68-0 | 395.3 | C1=C(C(=CC(=C1Cl)Cl)Cl)C2=C(C(=CC(=C2Cl)Cl)Cl)Cl | 2.2923 | 1.8701 | 0.0015 | 0.0925 | 2.181 | 0.0978 | 7.40 |
| | 17 | PCB 77 | 32598-13-3 | 292 | C1=CC(=C(C=C1C2=CC(=C(C=C2)Cl)Cl)Cl)Cl | 1.9438 | 1.4515 | -0.0007 | 0.1132 | 1.8138 | 0.0903 | 6.18 |
| | 18 | PCB 81 | 70362-50-4 | 292 | C1=CC(=CC=C1C2=CC(=C(C(=C2)Cl)Cl)Cl)Cl | 1.9365 | 1.4411 | 0.001 | 0.1124 | 1.8138 | 0.106 | 6.19 |
| | 19 | PCB 105 | 32598-14-4 | 326.4 | C1=CC(=C(C=C1C2=C(C(=C(C=C2)Cl)Cl)Cl)Cl)Cl | 2.0585 | 1.5862 | 0.0005 | 0.1136 | 1.9362 | 0.0877 | 6.56 |
| | 20 | PCB 114 | 74472-37-0 | 326.4 | C1=CC(=CC=C1C2=CC(=C(C(=C2Cl)Cl)Cl)Cl)Cl | 2.0508 | 1.5726 | 0.0022 | 0.1129 | 1.9362 | 0.1096 | 6.58 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 21 | PCB 123 | 65510-44-3 | 326.4 | C1=CC(=C(C=C1Cl)Cl)C2=CC(=C(C(=C2)Cl)Cl)Cl | 2.0466 | 1.594 | 0.0016 | 0.1164 | 1.9362 | 0.1003 | 6.54 |
| | 22 | PCB 126 | 57465-28-8 | 326.4 | C1=CC(=C(C=C1C2=CC(=C(C(=C2)Cl)Cl)Cl)Cl)Cl | 2.0908 | 1.5723 | 0 | 0.0975 | 1.9362 | 0.0878 | 6.65 |
| | 23 | PCB 156 | 38380-08-4 | 360.9 | C1=CC(=C(C=C1C2=CC(=C(C(=C2Cl)Cl)Cl)Cl)Cl)Cl | 2.199 | 1.7251 | 0.0018 | 0.0955 | 2.0586 | 0.0952 | 7.03 |
| | 24 | PCB 157 | 69782-90-7 | 360.9 | C1=CC(=C(C(=C1C2=CC(=C(C(=C2)Cl)Cl)Cl)Cl)Cl)Cl | 2.1945 | 1.7315 | 0.0008 | 0.0957 | 2.0586 | 0.0954 | 7.02 |
| | 25 | PCB 167 | 52663-72-6 | 360.9 | C1=C(C=C(C(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl | 2.2059 | 1.7223 | 0.0018 | 0.0941 | 2.0586 | 0.1034 | 7.04 |
| | 26 | PCB 169 | 32774-16-6 | 360.9 | C1=C(C=C(C(=C1Cl)Cl)Cl)C2=CC(=C(C(=C2)Cl)Cl)Cl | 2.2158 | 1.7063 | -0.0006 | 0.077 | 2.0586 | 0.0911 | 7.12 |
| | 27 | PCB 189 | 39635-31-9 | 395.3 | C1=C(C=C(C(=C1Cl)Cl)Cl)C2=CC(=C(C(=C2)Cl)Cl)Cl | 2.2158 | 1.7063 | -0.0006 | 0.077 | 2.0586 | 0.1023 | 7.12 |
| | 28 | Naphthalene | 91-20-3 | 128.169 | C1=CC=C2C=CC=CC2=C1 | 1.3366 | 0.8919 | 0.0001 | 0.2135 | 1.0854 | 0.191 | 3.30 |
| | 29 | Acenaphthylene | 208-96-8 | 152.19 | C1=CC2=C3C(=C1)C=CC3=CC=C2 | 1.7787 | 1.1599 | 0.0025 | 0.2276 | 1.2156 | 0.161 | 3.71 |
| | 30 | Acenaphthene | 83-92-9 | 154.12 | C1CC2=CC=CC3=C2C1=CC=C3 | 1.5673 | 1.0467 | 0.0009 | 0.2235 | 1.2586 | 0.1853 | 3.89 |
| | 31 | Fluorene | 86-73-7 | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C31 | 1.6647 | 1.1123 | 0.0018 | 0.2299 | 1.3565 | 0.165 | 4.23 |
| | 32 | Phenanthrene | 85-01-8 | 178.23 | C1=CC=C2C(=C1)C=CC3=CC=CC=C32 | 2.1518 | 1.2906 | 0.0024 | 0.2907 | 1.4544 | 0.152 | 4.48 |
| | 33 | Anthracene | 120-12-7 | 178.23 | C1=CC=C2C=C3C=CC=CC3=CC2=C1 | 2.2331 | 1.3285 | 0.0019 | 0.2868 | 1.4544 | 0.188 | 4.50 |
| | 34 | Fluoranthene | 206-44-0 | 202.25 | C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4 | 2.4081 | 1.5199 | 0.0005 | 0.2388 | 1.5846 | 0.183 | 5.06 |
| | 35 | Pyrene | 129-00-0 | 202.25 | C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2 | 2.7868 | 1.6865 | 0.003 | 0.2873 | 1.5846 | 0.203 | 4.93 |
| | 36 | Benz[a]anthracene | 56-55-3 | 228.3 | C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32 | 3.0436 | 1.7468 | 0.0038 | 0.3368 | 1.8234 | 0.1777 | 5.75 |
| | 37 | Chrysene | 218-01-9 | 228.3 | C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43 | 2.9849 | 1.7055 | 0.0031 | 0.3459 | 1.8234 | 0.217 | 5.73 |
| | 38 | Benzo[b]fluoranthene | 205-99-2 | 252.3 | C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1 | 3.2109 | 1.8598 | 0.0045 | 0.3737 | 1.9536 | 0.233 | 6.09 |
| | 39 | Benzo[k]fluoranthene | 207-08-9 | 252.3 | C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1 | 3.1981 | 1.9031 | 0.0024 | 0.3613 | 1.9536 | 0.35 | 6.08 |
| | 40 | Benzo[a]pyrene | 50-32-8 | 252.3 | C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3 | 3.6746 | 1.9325 | 0.003 | 0.3826 | 1.9536 | 0.361 | 6.24 |
| | 41 | Benzo[ghi]perylene | 191-24-2 | 276.3 | C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2 | 4.0694 | 1.9435 | 0.0035 | 0.4497 | 2.0838 | 0.37 | 6.72 |
| | 42 | Dibenz[a,h]anthracene | 53-70-3 | 278.3 | C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32 | 3.9752 | 2.1385 | 0.0024 | 0.4396 | 2.1924 | 0.299 | 6.91 |
| | 43 | Indeno[1,2,3-cd]pyrene | 193-39-5 | 276.3 | C1=CC=C2C(=C1)C3=C4C2=CC5=CC=CC6=C5C4=C(C=C6)C=C3 | 3.6831 | 1.9726 | 0.0013 | 0.4404 | 2.0838 | 0.517 | 6.50 |
| | 44 | cis-Chlordane | 5103-71-9 | 409.8 | C1[C@H]2[C@@H]([C@H]([C@H]1Cl)Cl)[C@]3(C(=C([C@@]2(C3(Cl)Cl)Cl)Cl)Cl)Cl | 2.1033 | 1.3174 | -0.0055 | 0.5104 | 2.128 | 0.059 | 6.23 |
| | 45 | trans-Chlordane | 5103-74-2 | 409.8 | C1[C@H]2[C@@H]([C@H]([C@@H]1Cl)Cl)[C@]3(C(=C([C@@]2(C3(Cl)Cl)Cl)Cl)Cl)Cl | 2.1033 | 1.3174 | -0.0055 | 0.5104 | 2.128 | 0.058 | 6.23 |
| | 46 | alfa-HCH | 58-89-9 | 290.8 | C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl | 1.4642 | 0.8751 | -0.0012 | 0.6766 | 1.5798 | 0.056 | 3.67 |
| | 47 | beta-HCH | 58-89-9 | 290.8 | C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl | 1.4642 | 0.8751 | -0.0012 | 0.6766 | 1.5798 | 0.0281 | 3.67 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 48 | gamma-HCH | 58-89-9 | 290.8 | C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl | 1.4642 | 0.8751 | -0.0012 | 0.6766 | 1.5798 | 0.052 | 3.67 |
| | 49 | delta-HCH | 58-89-9 | 290.8 | C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl | 1.4642 | 0.8751 | -0.0012 | 0.6766 | 1.5798 | 0.0318 | 3.67 |
| | 50 | 2,4'-DDD | 53-19-0 | 320 | C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl | 1.7859 | 1.7242 | 0.0756 | 0.2549 | 2.0956 | 0.0484 | 6.39 |
| | 51 | 2,4'-DDE | 3424-82-6 | 318 | C1=CC=C(C(=C1)C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 1.8681 | 1.4832 | 0.0171 | 0.1805 | 2.0526 | 0.0794 | 6.78 |
| | 52 | 2,4'-DDT | 789-02-6 | 354.5 | C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl)Cl | 1.8356 | 1.7212 | 0.0016 | 0.2342 | 2.218 | 0.0656 | 6.95 |
| | 53 | 4,4'-DDD | 72-54-8 | 320 | C1=CC(=CC=C1C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl | 1.7684 | 1.7109 | 0.0582 | 0.2412 | 2.0956 | 0.0331 | 6.44 |
| | 54 | 4,4'-DDE | 72-55-9 | 318 | C1=CC(=CC=C1C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl | 1.8368 | 1.4274 | 0.0381 | 0.1498 | 2.0526 | 0.085 | 6.93 |
| | 55 | 4,4'-DDT | 50-29-3 | 354.5 | C1=CC(=CC=C1C(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl)Cl | 1.8195 | 1.7235 | 0.0036 | 0.1956 | 2.218 | 0.039 | 7.08 |
| | 56 | Aldrin | 309-00-2 | 354.9 | C1[C@@H]2C=C[C@H]1[C@H]3[C@@H]2[C@]4(C(=C([C@@]3(C4(Cl)Cl)Cl)Cl)Cl)Cl | 2.0831 | 1.0454 | 0.0071 | 0.4613 | 2.0134 | 0.121 | 6.24 |
| | 57 | Dieldrin | 60-57-1 | 380.9 | C1[C@@H]2[C@H]3[C@@H]([C@H]1[C@H]4[C@@H]2O4)[C@]5(C(=C([C@@]3(C5(Cl)Cl)Cl)Cl)Cl)Cl | 2.0833 | 1.5199 | -0.001 | 0.6885 | 2.0065 | 0.078 | 4.93 |
| | 58 | Endrin | 72-20-8 | 380.9 | C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl | 2.0833 | 1.5199 | -0.001 | 0.6885 | 2.0065 | 0.0745 | 4.93 |
| | 59 | Isodrin | 465-73-6 | 364.9 | C1[C@@H]2C=C[C@H]1[C@@H]3[C@H]2[C@@]4(C(=C([C@]3(C4(Cl)Cl)Cl)Cl)Cl)Cl | 2.0831 | 1.0454 | 0.0071 | 0.4613 | 2.0134 | 0.11 | 6.24 |
| | 60 | Telodrin | 297-78-9 | 411.7 | C12C(C(OC1Cl)Cl)C3(C(=C(C2(C3(Cl)Cl)Cl)Cl)Cl)Cl | 2.171 | 1.0184 | -0.0164 | 0.6512 | 2.0458 | 0.0752 | 5.78 |
| | 61 | Heptachlor | 75-44-8 | 373.3 | C1=CC(C2C1C3(C(=C(C2(C3(Cl)Cl)Cl)Cl)Cl)Cl)Cl | 2.0589 | 1.0303 | -0.0002 | 0.5136 | 1.9626 | 0.0831 | 5.87 |
| | 62 | Heptachlor epoxide | 1024-57-3 | 389.3 | C12C(C(C3C1O3)Cl)C4(C(=C(C2(C4(Cl)Cl)Cl)Cl)Cl)Cl | 2.1067 | 1.2216 | -0.001 | 0.5955 | 1.9557 | 0.0556 | 5.38 |
| | 63 | beta-Endosulfan | 959-98-8 | 406.9 | C1[C@@H]2[C@H](COS(=O)O1)[C@@]3(C(=C([C@]2(C3(Cl)Cl)Cl)Cl)Cl)Cl | 2.2042 | 1.0337 | -0.0067 | 1.0144 | 2.0819 | 0.0449 | 4.67 |
| | 64 | Endosulfan sulfate | 1031-07-8 | 422.9 | C1C2C(COS(=O)(=O)O1)C3(C(=C(C2(C3(Cl)Cl)Cl)Cl)Cl)Cl | 2.1653 | 1.3662 | 0.0306 | 1.1089 | 2.1406 | 0.0345 | 4.19 |
| | 65 | Biphenyl-d10 (PRC) | 1486-01-7 | 164.27 | [2H]C1=C(C(=C(C(=C1[2H])[2H])C2=C(C(=C(C(=C2[2H])[2H])[2H])[2H])[2H])[2H])[2H] | 1.4149 | 1.4044 | 0.0334 | 0.492 | 1.3242 | 0.1293 | 2.75 |
| | 66 | PCB 1 (PRC) | 2051-60-7 | 188.65 | C1=CC=C(C=C1)C2=CC=CC=C2Cl | 1.4964 | 1.0731 | 0.0018 | 0.2006 | 1.4466 | 0.124 | 4.62 |
| | 67 | PCB2 (PRC) | 2051-61-8 | 188.65 | C1=CC=C(C=C1)C2=CC(=CC=C2)Cl | 1.515 | 1.061 | 0.0027 | 0.1815 | 1.4466 | 0.1166 | 4.71 |
| | 68 | PCB 3 (PRC) | 2051-62-9 | 188.65 | C1=CC=C(C=C1)C2=CC=C(C=C2)Cl | 1.4994 | 1.0625 | 0.0016 | 0.1815 | 1.4466 | 0.1289 | 4.70 |
| | 69 | PCB 10 (PRC) | 33146-45-1 | 223.09 | C1=CC=C(C=C1)C2=C(C=CC=C2Cl)Cl | 1.6255 | 1.2085 | 0.0001 | 0.1963 | 1.569 | 0.115 | 5.03 |
| | 70 | PCB 14 (PRC) | 34883-41-5 | 223.09 | C1=CC=C(C=C1)C2=CC(=CC(=C2)Cl)Cl | 1.6341 | 1.1783 | 0.0008 | 0.1648 | 1.569 | 0.1228 | 5.18 |
| | 71 | PCB 21 (PRC) | 55702-46-0 | 257.5 | C1=CC=C(C=C1)C2=C(C(=C(C=C2)Cl)Cl)Cl | 1.7801 | 1.3462 | 0.0006 | 0.1572 | 1.6914 | 0.1135 | 5.58 |
| | 72 | PCB 30 (PRC) | 35693-92-6 | 257.5 | C1=CC=C(C=C1)C2=C(C=C(C=C2Cl)Cl)Cl | 1.7485 | 1.3373 | 0.0017 | 0.166 | 1.6914 | 0.1265 | 5.54 |
| | 73 | PCB 50 (PRC) | 62796-65-0 | 292 | C1=CC=C(C(=C1)C2=C(C=C(C=C2Cl)Cl)Cl)Cl | 1.8648 | 1.4865 | 0.001 | 0.1559 | 1.8138 | 0.116 | 5.95 |
| | 74 | PCB 55 (PRC) | 74338-24-2 | 292 | C1=CC(=CC(=C1)Cl)C2=C(C(=C(C=C2)Cl)Cl)Cl | 1.9124 | 1.4621 | 0.001 | 0.1346 | 1.8138 | 0.0966 | 6.07 |
| | 75 | PCB 78 (PRC) | 70362-49-1 | 292 | C1=CC(=CC(=C1)Cl)C2=CC(=C(C(=C2)Cl)Cl)Cl | 1.9408 | 1.4436 | 0.0012 | 0.1142 | 1.8138 | 0.0868 | 6.18 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 76 | PCB104 (PRC) | 56558-16-8 | 326.4 | C1=CC(=C(C(=C1)Cl)C2=C(C=C(C=C2Cl)Cl)Cl)Cl | 1.9876 | 1.6143 | 0.0009 | 0.1346 | 1.9362 | 0.107 | 6.42 |
| | 77 | PCB 145 (PRC) | 74472-40-5 | 360.9 | C1=CC(=C(C(=C1)Cl)C2=C(C(=C(C=C2Cl)Cl)Cl)Cl)Cl | 2.1408 | 1.7426 | 0.0022 | 0.1131 | 2.0586 | 0.103 | 6.91 |
| | 78 | PCB 204 (PRC) | 74472-52-9 | 429.8 | C1=C(C=C(C(=C1Cl)C2=C(C(=C(C(=C2Cl)Cl)Cl)Cl)Cl)Cl)Cl | 2.4527 | 2.0034 | 0.004 | 0.0637 | 2.3034 | 0.156 | 7.92 |
| [43][b] | A1 | Styrene | 100-42-5 | 104.2 | C=CC1=CC=CC=C1 | 0.8537 | 0.6515 | -0.0032 | 0.1704 | 0.9552 | 0.058 | 2.93 |
| | A2 | Benzophenone | 119-61-9 | 182.2 | C1=CC=C(C=C1)C(=O)C2=CC=CC=C2 | 1.3721 | 1.3408 | 0.0015 | 0.5071 | 1.4808 | 0.117 | 3.34 |
| | A3 | 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester (ATBC) | 77-90-7 | 402.5 | CCCCOC(=O)CC(CC(=O)OCCCC)(C(=O)OCCCC)OC(=O)C | 0.3401 | 1.9108 | 0.0015 | 1.7801 | 3.2242 | 0.302 | 4.40 |
| | A4 | 1-Octene | 111-66-0 | 112.2 | CCCCCCC=C | 0.1009 | 0.0853 | 0.0007 | 0.0741 | 1.1928 | 0.319 | 4.35 |
| | A5 | trans,trans-1,4-Diphenyl-1,3-butadiene (DPBD) | 538-81-8 | 206.3 | C1=CC=C(C=C1)/C=C/C=C/C2=CC=CC=C2 | 1.655 | 1.1325 | 0.0127 | 0.4075 | 1.8018 | 0.054 | 5.29 |
| | A6 | bis(2-Ethylhexyl) adipate (DEHA) | 103-23-1 | 370.6 | CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC | 0.0285 | 1.0921 | -0.006 | 1.0898 | 3.3572 | 1.548 | 7.99 |
| | A7 | 2,2'-(2,5-Thienediyl)bis[5-(2-methyl-2-propanyl)-1,3- benzoxazole] (Uvitex OB) | 7128-64-5 | 430.6 | CC(C)(C)C1=CC2=C(C=C1)OC(=N2)C3=CC=C(S3)C4=NC5=C(O4)C=CC(=C5)C(C)(C)C | 3.0035 | 2.3222 | 0.0341 | 1.1392 | 3.2795 | 0.148 | 7.90 |
| [44, 45][C] | B1 | Triacetine | 102-76-1 | 218.2 | CC(=O)OCC(COC(=O)C)OC(=O)C | 0.1395 | 1.2957 | 0.0011 | 1.3044 | 1.5999 | 0.036 | 0.39 |
| | B2 | styrene | 100-42-5 | 104.15 | C=CC1=CC=CC=C1 | 0.8537 | 0.6515 | -0.0032 | 0.1704 | 0.9552 | 0.080 | 2.93 |
| | B3 | benzophenone | 119-61-9 | 182.22 | C1=CC=C(C=C1)C(=O)C2=CC=CC=C2 | 1.3721 | 1.3408 | 0.0015 | 0.5071 | 1.4808 | 0.200 | 3.34 |
| | B4 | diphenylphthalate, | 84-62-8 | 318.3 | C1=CC=C(C=C1)OC(=O)C2=CC=CC=C2C(=O)OC3=CC=CC=C3 | 1.8788 | 1.8829 | -0.0142 | 1.1163 | 2.3626 | 0.063 | 4.31 |
| | B5 | limonene | 5989-27-5 | 136.23 | CC1=CC[C@@H](CC1)C(=C)C | 0.5312 | 0.2923 | 0.0001 | 0.2266 | 1.323 | 0.224 | 4.34 |
| | B6 | acetyl tributyl citrate | 77-90-7 | 402.5 | CCCCOC(=O)CC(CC(=O)OCCCC)(C(=O)OCCCC)OC(=O)C | 0.3401 | 1.9108 | 0.0015 | 1.7801 | 3.2242 | 0.100 | 4.40 |
| | B7 | 1,4- diphenyl-1,3-butadiene | 538-81-8 | 206.28 | C1=CC=C(C=C1)/C=C/C=C/C2=CC=CC=C2 | 1.655 | 1.1325 | 0.0127 | 0.4075 | 1.8018 | 0.200 | 5.29 |
| | B8 | 2,6-di-tert-butyl-4-methylphenol | 128-37-0 | 220.35 | CC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C | 0.8384 | 0.8908 | 0.2013 | 0.5123 | 2.0432 | 0.112 | 5.65 |
| | B9 | 1-octene | 124-18-5 | 142.48 | CCCCCCCCCC | 0.0103 | 0.002 | -0.0002 | 0.002 | 1.5176 | 0.200 | 5.87 |
| | B10 | Chimassorb 81 | 1843-05-6 | 326.4 | CCCCCCCCOC1=CC(=C(C=C1)C(=O)C2=CC=CC=C2)O | 1.5611 | 1.8107 | 0.4373 | 0.917 | 2.7254 | 0.036 | 6.29 |
| | B11 | bis(2-ethylhexyl)adipate | 103-23-1 | 370.6 | CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC | 0.0285 | 1.0921 | -0.006 | 1.0898 | 3.3572 | 0.178 | 7.99 |
| | B12 | dinonylphthalate | 84-76-4 | 418.6 | CCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC | 0.6287 | 1.3116 | -0.001 | 1.0457 | 3.6832 | 0.317 | 9.49 |
| | B13 | Irganox 1076 | 2082-79-3 | 530.9 | CCCCCCCCCCCCCCCCCCOC(=O)CCC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C | 0.724 | 1.254 | 0.3116 | 0.9171 | 4.9356 | 0.159 | 14.83 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | B14 | Irgafos 168 | 31570-04-4 | 646.9 | CC(C)(C)C1=CC(=C(C=C1)OP(OC2=C(C=C(C=C2)C(C)(C)C)C(C)(C)C)OC3=C(C=C(C=C3)C(C)(C)C)C(C)(C)C)C(C)(C)C | 2.1032 | 1.8939 | 0.0207 | 1.2519 | 5.6943 | 1.000 | 16.66 |
| [42][d] | C1 | n-decane | 124-18-5 | 142.48 | CCCCCCCCCC | 0.0103 | 0.002 | -0.0002 | 0.002 | 1.5176 | 2.500 | 5.87 |
| | C2 | d-limonene | 5989-27-5 | 136.23 | CC1=CC[C@@H](CC1)C(=C)C | 0.5312 | 0.2923 | 0.0001 | 0.2266 | 1.323 | 0.900 | 4.34 |
| | C3 | ethyl caproate | 123-66-0 | 144.21 | CCCCCC(=O)OCC | 0.0493 | 0.5714 | -0.0003 | 0.4547 | 1.3102 | 0.550 | 2.94 |
| | C4 | hexanal | 66-25-1 | 100.16 | CCCCCC=O | 0.1563 | 0.6515 | -0.0013 | 0.4452 | 0.9697 | 0.130 | 1.65 |
| | C5 | n-hexanol | 111-27-1 | 102.17 | CCCCCCO | 0.2145 | 0.4142 | 0.3692 | 0.4872 | 1.0127 | 0.170 | 1.96 |
| | C6 | 2-phenylethanol | 60-12-8 | 122.16 | C1=CC=C(C=C1)CCO | 0.8213 | 0.9278 | 0.3278 | 0.6568 | 1.0569 | 0.100 | 1.34 |

[a]Used for construction of the predictive models.
[b,c]LDPE-olive oil partition system.
[d]LDPE-sunflower oil partition system.

## SI-B Tabulation of Experimentally Measured and Reported LDPE Extractables by Solvent Extraction (Total 76)

Table SI-B tabulates the collected LDPE extractables and their physicochemical properties by organic solvent extractions [77-83].

**Table S2. Tabulation of LDPE Extractables with Their Physicochemical Properties**

| # | LDPE Extractables | CAS # | MW | SMILES | E | S | A | B | V | $Log(P_{o/w})$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Nonane | 111-84-2 | 128.25 | CCCCCCCCC | 0.0083 | 0.0002 | 0 | 0.0014 | 1.3767 | 5.34 |
| 2 | Decane | 124-18-5 | 142.28 | CCCCCCCCCC | 0.0103 | 0.002 | -0.0002 | 0.002 | 1.5176 | 5.87 |
| 3 | Dodecane | 112-40-3 | 170.33 | CCCCCCCCCCCC | 0.0111 | 0.0046 | 0.0003 | 0.0037 | 1.7994 | 6.94 |
| 4 | Tetradecane | 629-59-4 | 198.39 | CCCCCCCCCCCCCC | 0.0098 | 0.0044 | 0.0008 | 0.0027 | 2.0812 | 8.02 |
| 5 | Hexadecane | 544-76-3 | 226.44 | CCCCCCCCCCCCCCCC | 0.0085 | 0.004 | 0.0006 | 0.0029 | 2.363 | 9.09 |
| 6 | Octadecane | 593-45-3 | 254.5 | CCCCCCCCCCCCCCCCCC | 0.0076 | 0.0016 | -0.0001 | 0.0039 | 2.6448 | 10.16 |
| 7 | Icosane | 112-95-8 | 282.5 | CCCCCCCCCCCCCCCCCCCC | 0.0078 | 0.0017 | -0.0004 | 0.0033 | 2.9266 | 11.24 |
| 8 | Docosane | 629-97-0 | 310.6 | CCCCCCCCCCCCCCCCCCCCCC | 0.0059 | 0.0011 | -0.0005 | 0.0017 | 3.2084 | 12.32 |
| 9 | Tetracosane | 646-31-1 | 338.7 | CCCCCCCCCCCCCCCCCCCCCCCC | 0.0062 | 0.0016 | -0.0004 | 0.0003 | 3.4902 | 13.40 |
| 10 | Hexacosane | 630-01-3 | 366.7 | CCCCCCCCCCCCCCCCCCCCCCCCCC | 0.0044 | -0.0039 | -0.0006 | -0.0017 | 3.772 | 14.49 |
| 11 | Octacosane | 630-02-4 | 394.8 | CCCCCCCCCCCCCCCCCCCCCCCCCCCC | 0.0039 | -0.0032 | -0.0016 | -0.0041 | 4.0538 | 15.57 |
| 12 | Triacontane | 638-68-6 | 422.8 | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 0.0022 | -0.0021 | -0.0027 | -0.0033 | 4.3356 | 16.64 |
| 13 | Dotriacontane | 544-85-4 | 450.59 | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 0.0008 | -0.0001 | -0.0027 | -0.0029 | 4.6174 | 17.71 |
| 14 | Benzenamine | 62-53-3 | 93.13 | C1=CC=C(C=C1)N | 0.9518 | 0.9636 | 0.2643 | 0.4027 | 0.8162 | 1.34 |
| 15 | Cyclododecane | 294-62-2 | 168.32 | C1CCCCCCCCCCC1 | 0.5602 | 0.0969 | 0.0003 | -0.0004 | 1.6908 | 6.75 |
| 16 | Squalene | 111-02-4 | 410.7 | CC(=CCC/C(=C/CC/C(=C/CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)/C)/C)C | 0.7136 | 0.4893 | 0.0174 | 0.626 | 4.0776 | 13.36 |
| 17 | Triacetine | 102-76-1 | 218.2 | CC(=O)OCC(COC(=O)C)OC(=O)C | 0.1395 | 1.2957 | 0.0011 | 1.3044 | 1.5999 | 0.39 |
| 18 | 2,4-Di-t-butyl phenol | 96-76-4 | 206.32 | CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C | 0.829 | 0.9203 | 0.4259 | 0.4997 | 1.9023 | 5.12 |
| 19 | Tris(2,4-di-tert-butylphenyl) phosphate | 95906-11-9 | 662.9 | CC(C)(C)C1=CC(=C(C=C1)OP(=O)(OC2=C(C=C(C=C2)C(C)(C)C)C(C)(C)C)OC3=C(C=C(C=C3)C(C)(C)C)C(C)(C)C)C(C)(C)C | 2.2882 | 3.3927 | 0.1795 | 2.1477 | 5.753 | 12.32 |
| 20 | Irgafos 168 | 31570-04-4 | 646.9 | CC(C)(C)C1=CC(=C(C=C1)OP(OC2=C(C=C(C=C2)C(C)(C)C)C(C)(C)C)OC3=C(C=C(C=C3)C(C)(C)C)C(C)(C)C)C(C)(C)C | 2.1032 | 1.8939 | 0.0207 | 1.2519 | 5.6943 | 16.66 |
| 21 | 3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid | 20170-32-5 | 278.4 | CC(C)(C)C1=CC(=CC(=C1O)C(C)(C)C)CCC(=O)O | 0.9848 | 1.4518 | 0.9454 | 0.9321 | 2.3994 | 5.07 |
| 22 | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester | 6386-38-5 | 292.4 | CC(C)(C)C1=CC(=CC(=C1O)C(C)(C)C)CCC(=O)OC | 0.8607 | 1.3668 | 0.2313 | 0.8408 | 2.5403 | 5.92 |
| 23 | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,1'-[2,2- | 36913-60-7 | 656.9 | CC(C)(C)C1=CC(=CC(=C1O)C(C)(C)C)CCC(=O)OCC(CO)(CO)COC(=O)CCC2=CC(=C(C(=C2)C(C)(C)C)O)C(C)(C)C | 2.3765 | 2.9458 | 1.1761 | 3.0486 | 5.5121 | 8.83 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | bis(hydroxymethyl)-1,3-propanediyl] ester | | | | | | | | | |
| 24 | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,1'-[2-[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl] -1-oxopropoxy]methyl]-2-(hydroxymethyl)-1,3-propanediyl] ester | 84633-54-5 | 917.3 | CC(C)(C)C1=CC(=CC(=C1O)C(C)(C)C)CCC(=O)OCC(CO)(COC(=O)CCC2=CC(=C(C(=C2)C(C)(C)C)O)C(C)(C)C)COC(=O)CCC3=CC(=C(C(=C3)C(C)(C)C)O)C(C)(C)C | 2.9832 | 3.3889 | 1.1729 | 3.1361 | 7.7442 | 16.92 |
| 25 | Irganox 1010 | 6683-19-8 | 1176.6 | CC(C)(C)C1=CC(=CC(=C1O)C(C)(C)C)CCC(=O)OCC(COC(=O)CCC2=CC(=C(C(=C2)C(C)(C)C)O)C(C)(C)C)(COC(=O)CCC3=CC(=C(C(=C3)C(C)(C)C)O)C(C)(C)C)COC(=O)CCC4=CC(=C(C(=C4)C(C)(C)C)O)C(C)(C)C | 3.0745 | 3.6829 | 0.8855 | 2.8173 | 9.9763 | 26.27 |
| 26 | Octylphenol ethoxylate | 9002-93-1 | 250.38 | CC(C)(C)CC(C)(C)C1=CC=C(C=C1)OCCO | 0.8327 | 0.9862 | 0.2826 | 0.956 | 2.2428 | 4.77 |
| 27 | Heptadecanamide, N,N'-1,2-ethanediylbis- | 63059-78-9 | 593 | CC(C)CCCCCCCCCCCCCCCC(=O)NCCNC(=O)CCCCCCCCCCCCCCC(C)C | 0.6013 | 2.0269 | 0.5262 | 1.6155 | 5.6938 | 14.43 |
| 28 | Diisooctyl phthalate | 131-20-4 | 390.6 | CC(C)CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCC(C)C | 0.631 | 1.2706 | -0.0012 | 1.0119 | 3.4014 | 8.58 |
| 29 | Diisobutyl phthalate | 84-69-5 | 278.34 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | 0.6794 | 1.2212 | 0.0043 | 0.9613 | 2.2742 | 4.53 |
| 30 | α-tocopherol | 2074-53-5 | 430.71 | CC1=C(C2=C(CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C)C(=C1O)C)C | 1.098 | 1.1256 | 0.4575 | 0.6958 | 3.9659 | 12.25 |
| 31 | BHT | 128-37-0 | 220.35 | CC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C | 0.8384 | 0.8908 | 0.2013 | 0.5123 | 2.0432 | 5.65 |
| 32 | 2-Butanone | 78-93-3 | 72.11 | CCC(=O)C | 0.1615 | 0.6911 | 0.0055 | 0.5124 | 0.6879 | 0.30 |
| 33 | Pentanamide | 626-97-1 | 101.15 | CCCCC(=O)N | 0.4392 | 1.2986 | 0.5349 | 0.653 | 0.9286 | 0.27 |
| 34 | Octinoxate | 5466-77-3 | 290.4 | CCCCC(CC)COC(=O)/C=C/C1=CC=C(C=C1)OC | 0.9795 | 1.2577 | 0.0069 | 0.8584 | 2.4973 | 5.87 |
| 35 | DEHP | 117-81-7 | 390.6 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | 0.6401 | 1.252 | -0.0012 | 1.0286 | 3.4014 | 8.54 |
| 36 | (Z)-Hexanedioic acid, bis(2-ethylhexyl) ester | 103-23-1 | 370.6 | CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC | 0.0285 | 1.0921 | -0.006 | 1.0898 | 3.3572 | 7.99 |
| 37 | Methyl 10-trans,12-cis-octadecadienoate | 21870-97-3 | 295.4 | CCCCC/C=C\C=C\CCCCCCCCC(=O)OC | 0.2676 | 0.6531 | -0.0001 | 0.6856 | 2.7741 | 7.76 |
| 38 | Nonaoic acid | 24323-21-5 | 172.26 | CCCCCCCC(C)C(=O)O | 0.1384 | 0.5834 | 0.5966 | 0.4588 | 1.592 | 4.06 |
| 39 | Oleamide | 301-02-0 | 281.5 | CCCCCCCC/C=C\CCCCCCCC(=O)N | 0.5345 | 1.1532 | 0.4509 | 0.8595 | 2.7173 | 6.58 |
| 40 | 11-Eicosenamide, (11Z)- | 10436-08-5 | 309.5 | CCCCCCCC/C=C\CCCCCCCCCC(=O)N | 0.5261 | 1.1526 | 0.4606 | 0.8811 | 2.9991 | 7.57 |
| 41 | Erucamide | 112-84-5 | 337.6 | CCCCCCCC/C=C\CCCCCCCCCCCC(=O)N | 0.5198 | 1.1538 | 0.4685 | 0.8979 | 3.2809 | 8.59 |
| 42 | Octanal | 124-13-0 | 128.21 | CCCCCCCC=O | 0.1444 | 0.6557 | -0.0002 | 0.4531 | 1.2515 | 2.68 |
| 43 | Nonanoic acid, methyl ester | 1731-84-6 | 172.26 | CCCCCCCCC(=O)OC | 0.0649 | 0.6079 | 0.0004 | 0.456 | 1.592 | 3.98 |
| 44 | 9-Octadecenenitrile | 61041-55-2 | 263.5 | CCCCCCCCC=CCCCCCCCC#N | 0.2726 | 0.8671 | 0.0088 | 0.4711 | 2.6156 | 7.67 |
| 45 | 9-Octadecenamide | 3322-62-1 | 281.5 | CCCCCCCCC=CCCCCCCCC(=O)N | 0.5337 | 1.1528 | 0.4512 | 0.8596 | 2.7173 | 6.58 |
| 46 | Nonanal | 124-19-6 | 142.24 | CCCCCCCCC=O | 0.1395 | 0.6521 | 0.0006 | 0.4526 | 1.3924 | 3.22 |
| 47 | Tetradecanoic acid, methyl ester | 124-10-7 | 242.4 | CCCCCCCCCCCCCC(=O)OC | 0.0336 | 0.6313 | -0.0004 | 0.4516 | 2.2965 | 6.64 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | N,N'-(1,2-Ethanediyl)bis(pentadecanamide) | 5518-18-3 | 508.9 | CCCCCCCCCCCCCCC(=O)NCCNC(=O)CCCCCCCCCCCCCC | 0.5986 | 2.0326 | 0.5231 | 1.6181 | 4.8484 | 11.19 |
| 49 | Hexadecanamide | 629-54-9 | 255.44 | CCCCCCCCCCCCCCCC(=O)N | 0.3876 | 1.0779 | 0.4448 | 0.7297 | 2.4785 | 6.11 |
| 50 | Hexadecanamide, N,N'-1,2-ethanediylbis- | ?? | 536.9 | CCCCCCCCCCCCCCCC(=O)NCCNC(=O)CCCCCCCCCCCCCCC | 0.6088 | 2.0329 | 0.5209 | 1.6203 | 5.1302 | 12.27 |
| 51 | Palmitic acid | 57-10-3 | 256.2 | CCCCCCCCCCCCCCCC(=O)O | 0.0415 | 0.6735 | 0.6103 | 0.4544 | 2.4374 | 7.15 |
| 52 | Hexadecanoic acid, methyl ester | 112-39-0 | 270.5 | CCCCCCCCCCCCCCCC(=O)OC | 0.0233 | 0.6213 | -0.0001 | 0.4527 | 2.5783 | 7.71 |
| 53 | Stearamide | 124-26-5 | 283.5 | CCCCCCCCCCCCCCCCCC(=O)N | 0.371 | 1.0582 | 0.4472 | 0.7492 | 2.7603 | 7.13 |
| 54 | Stearic acid | 57-11-4 | 284.5 | CCCCCCCCCCCCCCCCCC(=O)O | 0.022 | 0.6706 | 0.6109 | 0.4528 | 2.7192 | 8.22 |
| 55 | Octadecanoic acid, methyl ester | 112-61-8 | 298.5 | CCCCCCCCCCCCCCCCCC(=O)OC | 0.0135 | 0.6057 | -0.0011 | 0.4534 | 2.8601 | 8.80 |
| 56 | 1-Nonadecene | 18435-45-5 | 266.5 | CCCCCCCCCCCCCCCCCC=C | 0.0782 | 0.0867 | 0.0034 | 0.0747 | 2.7427 | 10.24 |
| 57 | 2-Methyltetracosane | 112-95-8 | 282.5 | CCCCCCCCCCCCCCCCCCCCCCC(C)C | -0.0357 | 0.0181 | -0.0015 | -0.0313 | 3.6311 | 14.01 |
| 58 | (Z)-Dotriacontane | 1560-78-7 | 352.7 | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 0.0008 | -0.0001 | -0.0027 | -0.0029 | 4.6174 | 17.71 |
| 59 | Tetrapentacontane | 544-85-4 | 450.9 | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 0.0284 | 0.0017 | 0.0041 | 0.0079 | 7.7172 | 29.51 |
| 60 | Octacosanol | 5856-66-6 | 759.4 | CCCCCCCCCCCCCCCCCCCCCCCCCCCCO | 0.1598 | 0.369 | 0.358 | 0.4737 | 4.1125 | 13.85 |
| 61 | 1-Heptacosanol | 557-61-9 | 410.8 | CCCCCCCCCCCCCCCCCCCCCCCCCCCO | 0.1545 | 0.3772 | 0.3588 | 0.4721 | 3.9716 | 13.30 |
| 62 | n-Tetracosanol-1 | 2004-39-9 | 396.7 | CCCCCCCCCCCCCCCCCCCCCCCCO | 0.1438 | 0.4037 | 0.3649 | 0.4738 | 3.5489 | 11.65 |
| 63 | N,N-Bis(2-hydroxyethyl) octadecylamine | 506-51-4 | 354.7 | CCCCCCCCCCCCCCCCCCN(CCO)CCO | 0.4119 | 0.9276 | 0.6079 | 1.5143 | 3.4256 | 7.19 |
| 64 | Irganox 1076 | 10213-78-2 | 357.6 | CCCCCCCCCCCCCCCCCCOC(=O)CCC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C | 0.724 | 1.254 | 0.3116 | 0.9171 | 4.9356 | 14.83 |
| 65 | (Z)-1-Hexadecanol | 2082-79-3 | 530.9 | CCCCCCCCCCCCCCCCO | 0.1584 | 0.42 | 0.3688 | 0.4819 | 2.4217 | 7.32 |
| 66 | Hexadecyl 2-ethylhexanoate | 36653-82-4 | 242.44 | CCCCCCCCCCCCCCCCOC(=O)C(CC)CCCC | -0.0238 | 0.5651 | -0.0072 | 0.5089 | 3.5646 | 11.31 |
| 67 | N,N-Bis(2-hydroxyethyl) hexadecylamine | 59130-69-7 | 368.6 | CCCCCCCCCCCCCCN(CCO)CCO | 0.4131 | 0.9705 | 0.6086 | 1.4121 | 2.862 | 5.35 |
| 68 | Myristyl myristate | 18924-66-8 | 301.5 | CCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCC | -0.0409 | 0.5688 | 0.0017 | 0.459 | 4.1282 | 13.62 |
| 69 | Tridodecylamine | 3234-85-3 | 424.7 | CCCCCCCCCCCN(CCCCCCCCCCCC)CCCCCCCCCCC | -0.0182 | 0.1477 | 0.0031 | 0.8304 | 5.2808 | 17.19 |
| 70 | N,N-Bis(2- hydroxyethyl) dodecylamine | 102-87-4 | 522 | CCCCCCCCCCCN(CCO)CCO | 0.415 | 0.9869 | 0.6079 | 1.3645 | 2.5802 | 4.42 |
| 71 | Dilauryl-3,3'-thiodipropionate (Irganox PS 800) | 1541-67-9 | 273.45 | CCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCC | 0.4803 | 1.45 | -0.0038 | 1.3069 | 4.6479 | 12.03 |
| 72 | Dibutyl amine | 123-28-4 | 514.799 | CCCCNCCCC | 0.1127 | 0.2901 | 0.0791 | 0.6886 | 1.3356 | 2.56 |
| 73 | Dibutyl phthalate | 111-92-2 | 129.24 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | 0.6941 | 1.2622 | -0.0013 | 0.9447 | 2.2742 | 4.55 |
| 74 | Ethanol, 2-(2-butoxyethoxy), acetate | 84-74-2 | 278.34 | CCCCOCCOCCOC(=O)C | 0.0655 | 0.9153 | -0.0004 | 1.2556 | 1.7094 | 1.34 |
| 75 | Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]- | 124-17-4 | 204.26 | CCCCOCCOCCOCCO | 0.1782 | 0.9365 | 0.268 | 1.4457 | 1.7524 | 0.89 |
| 76 | Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propanoate Benzenepropanoic acid, 3,5-bis(1,1- | 143-22-6 | 206.28 | CCOC(=O)CCC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C | 0.8247 | 1.3733 | 0.2739 | 0.8732 | 2.6812 | 6.32 |

Note: LDPE  extractables not by organic solvent extractions are not included in the collection, because they may not be relevant in the chemical characterization studies.

## SI-C Correlation Matrix of Descriptors of Solutes with Measured $P_{ldpe/lipid}$ (n=78)

| Table S3. Correlation Matrix of Descriptors of Measured Solutes | | | | | |
|---|---|---|---|---|---|
| | ***Column 1 (E)*** | ***Column 2 (S)*** | ***Column 3 (A)*** | ***Column 4 (B)*** | ***Column 5 (V)*** |
| ***Column 1 (E)*** | 1 | | | | |
| ***Column 2 (S)*** | 0.726 | 1 | | | |
| ***Column 3 (A)*** | -0.133 | 0.089 | 1 | | |
| ***Column 4 (B)*** | 0.147 | -0.269 | -0.039 | 1 | |
| ***Column 5 (V)*** | 0.510 | 0.684 | 0.043 | 0.088 | 1 |

## SI-D Correlation Matrix of Observed LDPE Extractables Descriptors (n=76)

| Table S4. Correlation Matrix of Descriptors of LDPE Extractables | | | | | |
|---|---|---|---|---|---|
| | ***Column 1 (E)*** | ***Column 2 (S)*** | ***Column 3 (A)*** | ***Column 4 (B)*** | ***Column 5 (V)*** |
| ***Column 1 (E)*** | 1 | | | | |
| ***Column 2 (S)*** | 0.874 | 1 | | | |
| ***Column 3 (A)*** | 0.575 | 0.621 | 1 | | |
| ***Column 4 (B)*** | 0.790 | 0.927 | 0.653 | 1 | |
| ***Column 5 (V)*** | 0.545 | 0.487 | 0.307 | 0.495 | 1 |

## SI-E Tabulation of Over Extraction Data

Table SI-G tabulates the over extraction data, compiled from literatures [14,15,20,22,34,40,41,87,95–98]. The derivation of these values is described in Section 2.8.

**Table S5. Tabulation of Over Extraction Data**

| # | Material[a] | Solvent | Extractables[b] | Temperature (°C) | Over Ext. | Comment[c] |
|---|---|---|---|---|---|---|
| 1 | BPE | n-Heptane | n-C32H66 alkane | 30 | 15.6 | By diffusion coef. to corn oil |
| 2 | BPE | n-Heptane | BHT | 30 | 15.7 | By diffusion coef. to corn oil |
| 3 | BPE | n-Heptane | BHT | 30 | 13.3 | By diffusion coef. to corn oil |
| 4 | BPE | n-Heptane | BHT | 30 | 48.3 | By diffusion coef. to corn oil |
| 5 | BPE | n-Heptane | n-C32H66 alkane | 60 | 9.2 | By diffusion coef. to corn oil |
| 6 | BPE | n-Heptane | BHT | 60 | 7.4 | By diffusion coef. to corn oil |
| 7 | BPE | n-Heptane | BHT | 60 | 6.7 | By diffusion coef. to corn oil |
| 8 | BPE | n-Heptane | BHT | 60 | 23.0 | By diffusion coef. to corn oil |
| 9 | BPE | n-Heptane | Overall | 70 | 7.8 | By total amount to ethanol (=oil) |
| 10 | LDPE | Cyclohexane | Irganox 1076 | 40 | 8.5 | By diffusion coef. to olive oil |
| 11 | LDPE | Isooctane | BHT | 10 | 5.2 | By diffusion coef. to 95% ethanol |
| 12 | LDPE | Isooctane | BHT | 20 | 4.5 | By diffusion coef. to 95% ethanol |
| 13 | LDPE | Isooctane | BHT | 40 | 4.1 | By diffusion coef. to 95% ethanol |
| 14 | LDPE | Isooctane | DBP | 10 | 3.0 | By diffusion coef. to 95% ethanol |
| 15 | LDPE | Isooctane | DBP | 20 | 3.4 | By diffusion coef. to 95% ethanol |
| 16 | LDPE | Isooctane | DBP | 40 | 2.9 | By diffusion coef. to 95% ethanol |
| 17 | LDPE | Isooctane | ATBC | 10 | 3.0 | By diffusion coef. to 95% ethanol |
| 18 | LDPE | Isooctane | ATBC | 20 | 3.2 | By diffusion coef. to 95% ethanol |
| 19 | LDPE | Isooctane | ATBC | 40 | 4.3 | By diffusion coef. to 95% ethanol |
| 20 | LDPE | Isooctane | Di-n-butyl phthalate | 25 | 4.8 | By diffusion rate, ethanol as oil |
| 21 | LDPE | Hexane | Dodecane | 23 | 6.2 | By diffusion coef. to ethanol |
| 22 | LDPE | Hexane | Tetradecane | 23 | 7.5 | By diffusion coef. to ethanol |
| 23 | LDPE | Hexane | Hexadecane | 23 | 7.7 | By diffusion coef. to ethanol |
| 24 | LDPE | Hexane | Octadecane | 23 | 7.7 | By diffusion coef. to ethanol |
| 25 | LDPE | Hexane | Eicosane | 23 | 6.9 | By diffusion coef. to ethanol |
| 26 | LDPE | Hexane | Docosane | 23 | 7.2 | By diffusion coef. to ethanol |
| 27 | LDPE | Isooctane | Irganox 1076 | 5 | 11.3 | By specific amount to retified oil |
| 28 | LDPE | Isooctane | Irganox 1076 | 25 | 4.6 | By specific amount to retified oil |
| 29 | LDPE | Isooctane | Irganox 1076 | 40 | 2.1 | By specific amount to retified oil |
| 30 | LDPE (0.1) | Isooctane | Global | 40 | 2.1 | By total amount to olive oil |
| 31 | LDPE (0.25) | Isooctane | Global | 40 | 2.1 | By total amount to olive oil |

| | | | | | | |
|---|---|---|---|---|---|---|
| 32 | LDPE (0.50) | Isooctane | Global | 40 | 7.6 | By total amount to HB307 |
| 33 | LDPE (4.40) | Isooctane | Global | 40 | 2.9 | By total amount to HB307 |
| 34 | LDPE (4.5) | Isooctane | Global | 40 | 7.6 | By total amount to HB307 |
| 35 | LLDPE | Heptane | Hexanal | 22 | 4.0 | By measured data, heptane to oil |
| 36 | LLDPE | Heptane | Ethyl caproate | 22 | 0.8 | By measured data, heptane to oil |
| 37 | LLDPE | Sunfower Oil | Phenylethanol | 22 | 0.2 | By measured data, heptane to oil |
| 38 | LPE | n-Heptane | n-C32H66 | 30 | 24.0 | By diffusion coef. to corn oil |
| 39 | LPE | n-Heptane | BHT | 30 | 38.1 | By diffusion coef. to corn oil |
| 40 | LPE | n-Heptane | BHT | 30 | 50.5 | By diffusion coef. to corn oil |
| 41 | LPE | n-Heptane | n-C32H66 alkane | 60 | 30.0 | By diffusion coef. to corn oil |
| 42 | LPE | n-Heptane | BHT | 60 | 12.6 | By diffusion coef. to corn oil |
| 43 | LPE | n-Heptane | BHT | 60 | 15.5 | By diffusion coef. to corn oil |
| 44 | LPE | n-Heptane | Overall | 70 | 5.9 | By total amount to ethanol (=oil) |
| 45 | ABS(0.60) | Isooctane | Global | 40 | 0.9 | By total amount to olive oil |
| 46 | ABS(0.60) | Isooctane | Global | 40 | 17.8 | By total amount to HB307 |
| 47 | HDPE | n-Heptane | Ionox 341 | 20 | 14.3 | By specific amount to olive oil |
| 48 | HDPE and PP | 1-pentanol | Irganox 1010 | 48.9 (120 F) | 4.5 | By specific amount, pentanol to oil |
| 49 | HDPE-0.05 | Isooctane | Irganox 1076 | 60 | 1.2 | By specific amount to olive oil |
| 50 | HDPE-0.25 | Isooctane | Irganox 1076 | 60 | 2.0 | By specific amount to olive oil |
| 51 | HIPS-0.11 | Isooctane | Irganox 1076 | 60 | 4.3 | By specific amount to olive oil |
| 52 | PP | n-Heptane | n-C32H66 | 30 | 76.4 | By diffusion coef. to corn oil |
| 53 | PP | n-Heptane | n-C32H66 | 60 | 19.1 | By diffusion coef. to corn oil |
| 54 | PP | Isooctane | BHT | 40 | 17.4 | By specific amount to ethanol as oil |
| 55 | PP | Isooctane | Ionox 220 | 40 | 64.8 | By specific amount to ethanol as oil |
| 56 | PP | Isooctane | Uvinul 3039 | 40 | 163.8 | By specific amount to ethanol as oil |
| 57 | PP | Isooctane | TBAC | 40 | 10.1 | By specific amount to ethanol as oil |
| 58 | PP | Isooctane | TOTM | 40 | 16.5 | By specific amount to ethanol as oil |
| 59 | PP-0.05 | Isooctane | Irganox 1076 | 60 | 4.8 | By specific amount to olive oil |
| 60 | PP-0.25 | Isooctane | Irganox 1076 | 60 | 6.9 | By specific amount to olive oil |

[a]Material Notation:
BPE: branched polyethylene (=LDPE)
LLDPE: linear low-density polyethylene
LPE: linear polyethylene (=HDPE)
ABS: Acrylonitrile butadiene styrene
PP: polyethylene
HIPS: High Impact Polystyrene

[b]Extractables Notation:
DBP: Dibutyl phthalate
ATBC: Acetyl tributyl citrate
TOTM: Trioctyl Trimellitate
[c]HB307: a fat simulant in food industries. It is a mixture of synthetic triglycerides, primarily $C_{10}$, $C_{12}$, and $C_{14}$.

## SI-F Time-Dependent HDPE Extractables Release Profiles by Different Solvents

The kinetic extractables profiles from HDPE materials by different solvents are shown in Figure SI-1 to SI-3. Three extractables were studied, and they were butylated hydroxytoluene (BHT, SI-1), octadecane (C18, SI-2), and dotriacontane (C32, SI-3) [46].

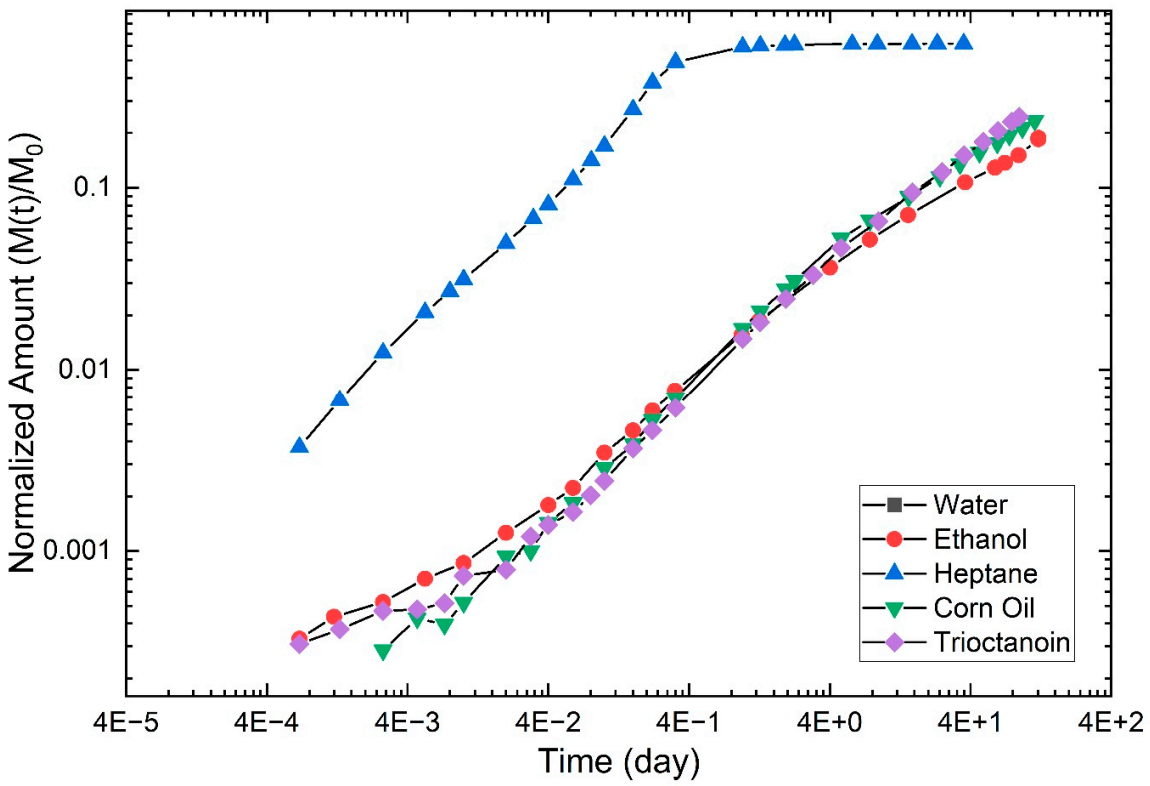


**Figure S1: Time-Dependent BHT Release Profiles by Different Solvents from HDPE Material**

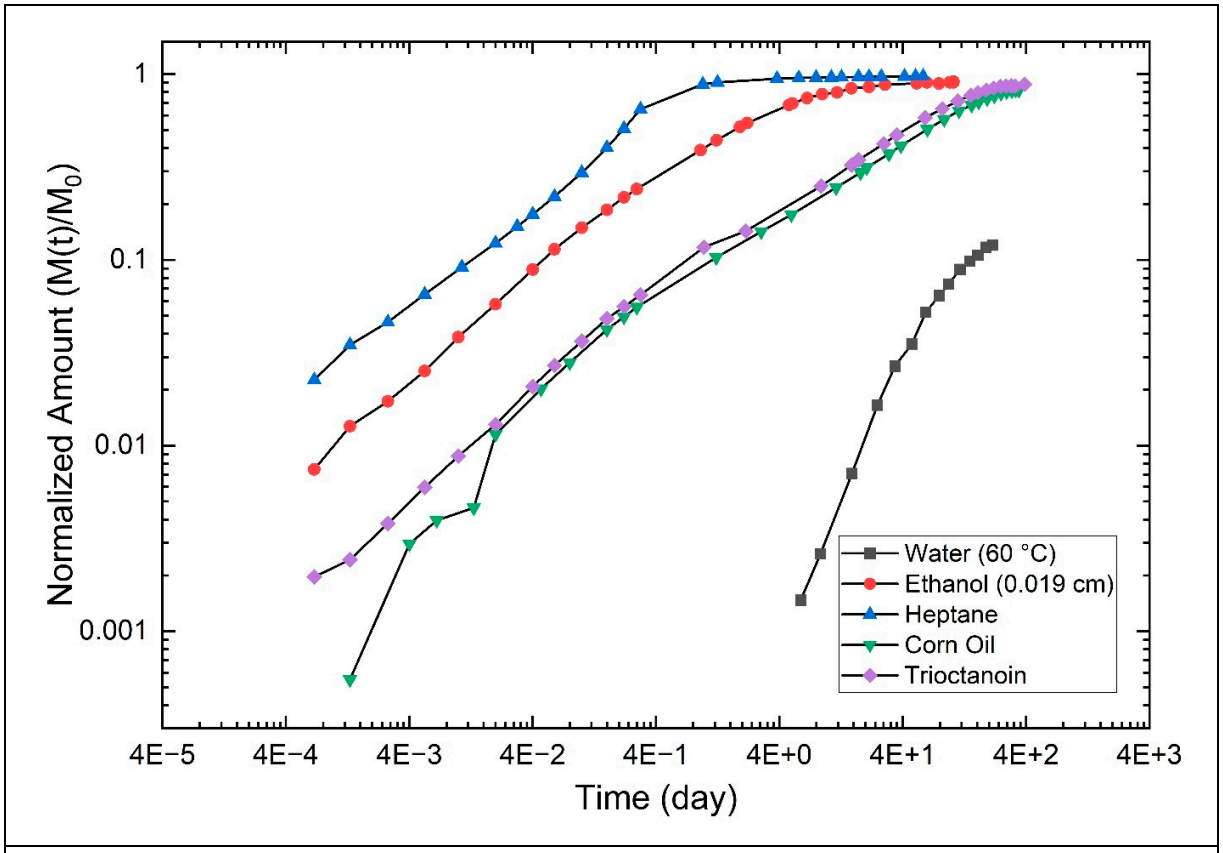


**Figure S2: Time-Dependent C18 Release Profiles by Different Solvents from HDPE Material**

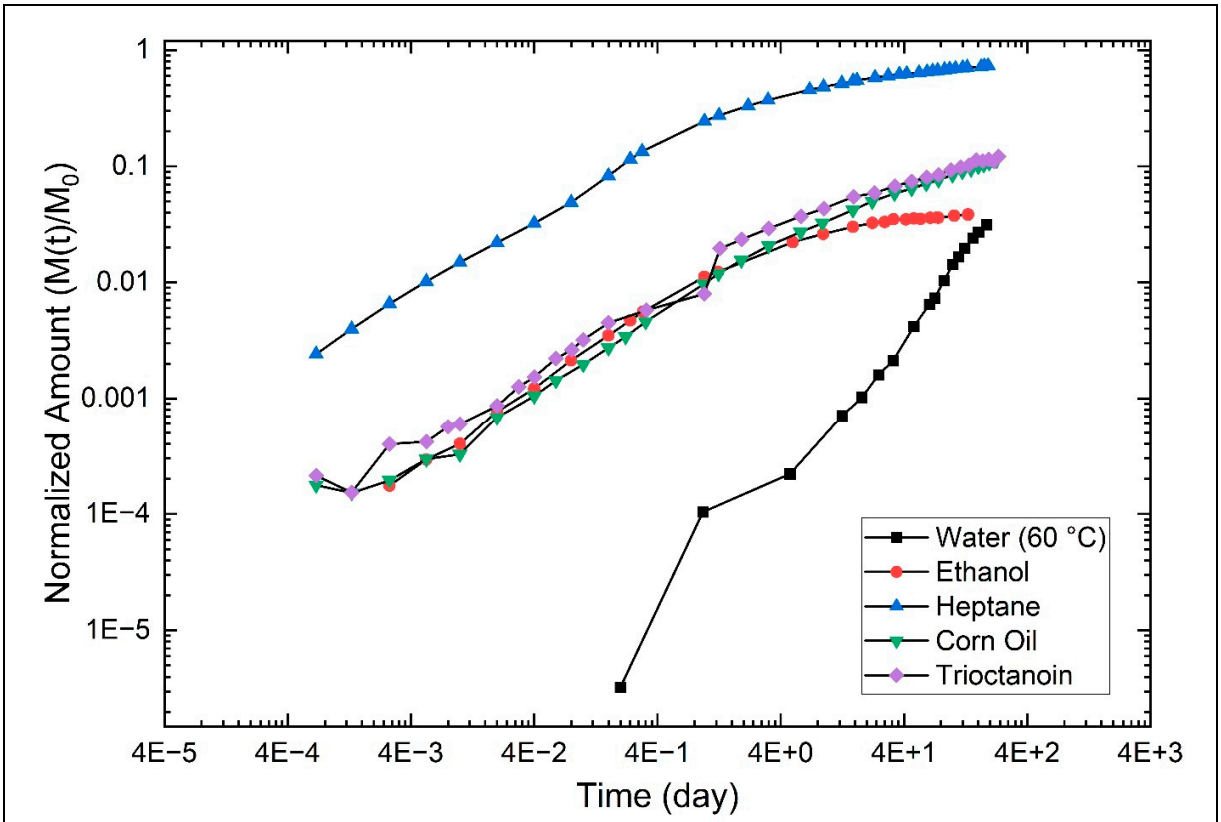


**Figure S3: Time-Dependent C32 Release Profiles by Different Solvents from HDPE Material**

The conclusions from the three figures by HDPE materials are the same as those for LDPE materials in Section 4.8.2. The extraction kinetics by heptane is much faster than those by oils/ethanol, and ethanol has the same release kinetics as the oils.

## SI-G Dependence of LDPE-Solvent Partition Coefficient on $log_{10}P_{o/w}$ of Extractables

The dependence of LDPE (and HDPE)-solvent partition coefficient, $P_{LDPE/S}$, on $log_{10}P_{o/w}$ is examined in Figure SI-4 for additional (extraction) solvents, including methanol, ethanol, acetone [22,23].

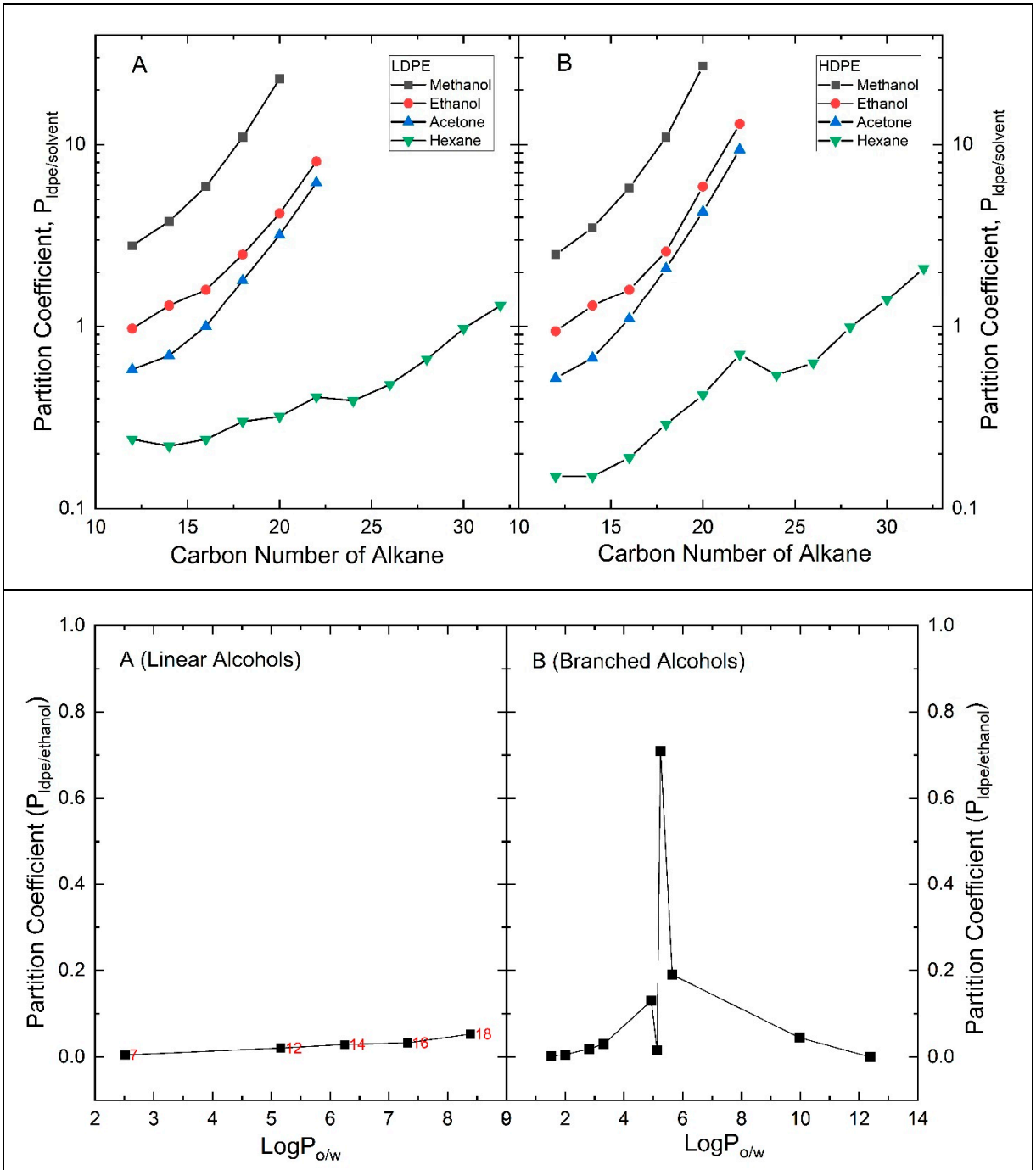


**Figure S4: Illustration of the Dependence of LDPE (or HDPE)-Solvent Partition Coefficient on $log_{10}P_{o/w}$ of Extractables.** Top graph (plot A): LDPE-solvent partition coefficient vs. the number of carbons (as the hydrophobicity) in extractables alkanes. Top graph (plot B): same as plot A, but the material is HDPE. The solvents in top graph are methanol, ethanol, acetone, and hexane. The bottom graph (plot A): LDPE-ethanol partition coefficient vs. the number of carbons (as the hydrophobicity) of linear alcohol extractables. The bottom graph (plot B)

shows LDPE-ethanol partition coefficient of branched alcohol extractables against the hydrophobicity by $log_{10}P_{o/w}$, calculated by Eq.6. All data are adopted from ref [22,23].

It is seen in the figure (top graph plot A) that, while the extraction solvent changes from semipolar to nonpolar hexane, the partition coefficient increases with the carbon # for both materials. As the hydrophobicity of alkane extractables is related to number of carbons, the top plot in Figure SI-1 shows a positive dependence of partition coefficient on hydrophobicity.

The bottom graph in the figure shows the partition coefficient (LDPE-ethanol) of different extractables, linear and branched long-chain alcohols, extracted by ethanol. Again, the LDPE-ethanol partition coefficient in general increases slowly with the number of carbons in the linear alcohols or hydrophobicity. However, the change in the partition coefficient for branched alcohols is far from linear with $log_{10}P_{o/w}$, because they don't have the same reference phase [33].

Overall, the data in Figure SI-1 clearly indicate that, if the LDPE-solvent partition coefficients of all extractables are included, specific relationship may not be expected between the LDPE-solvent partition coefficients and $log_{10}P_{o/w}$ for semipolar and nonpolar solvents [33].