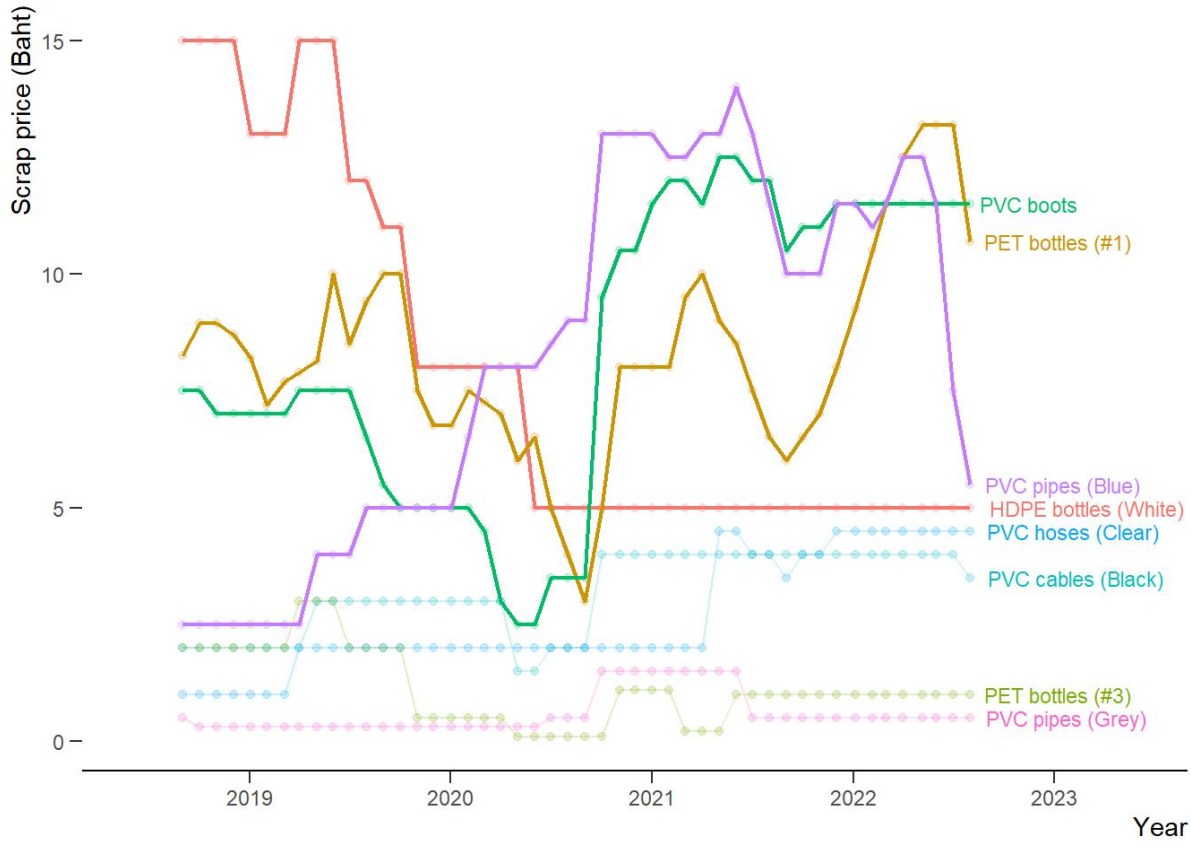
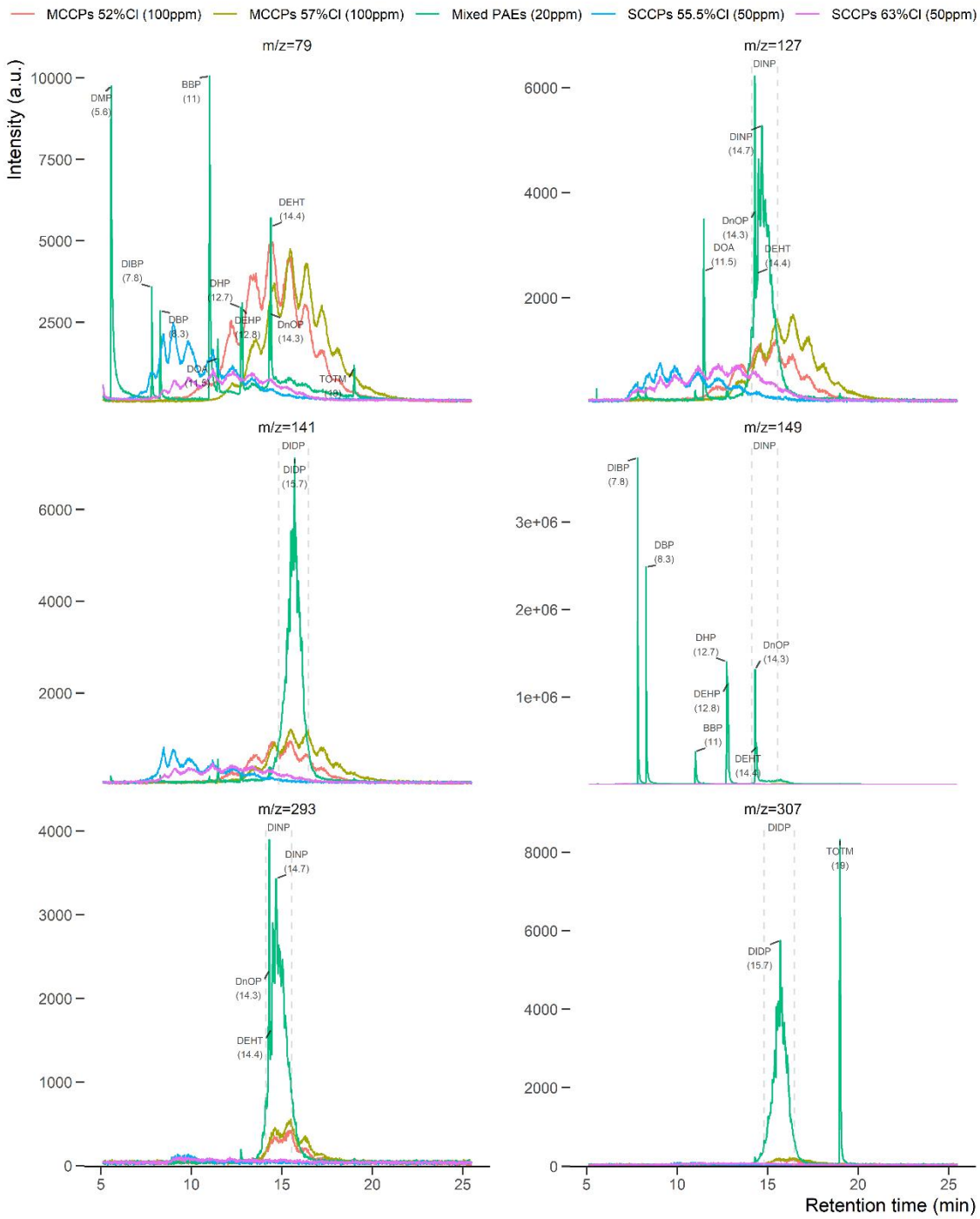
# Supplementary Materials: Circular economy without chemicals controls? Evidence of recirculated toxic plasticizers in flexible PVC products

**Supplementary Figure 1.** Buying prices of selected plastic scraps over the past 5 years, showing relatively high prices for flexible PVC scraps.

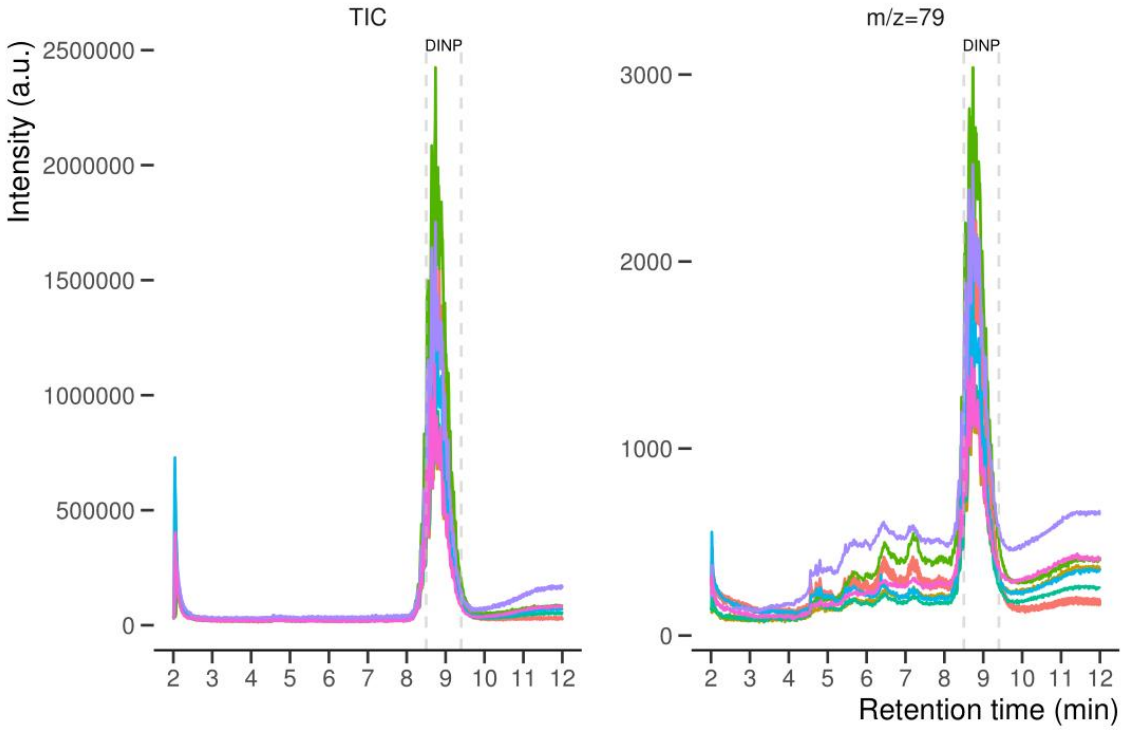



Data source: Wongpanit International, 2022, “Scrap Retail Price.” http://www.wongpanit.com/list_history_price/

**Supplementary Figure 2.** Reference GC-MS chromatograms (overlaid, without normalization) obtained from 5 reference solutions (13-plasticizer mixed solution, 2 SCCPs standard solutions, and 2 MCCPs standard solutions) at m/z = 79, 127, 141, 149, 293, and 307.



**Supplementary Figure 3.** Py/TD-GC-MS SIM-mode chromatograms (total ion current (TIC) and m/z = 79) from 7 repeated tests of homemade PVC samples containing 29% DINP and 1% MCCPs.



## Supplementary Table 1: Measurement conditions for Py/TD-GC-MS analysis

| | |
|---|---|
| **Pyrolyzer** | Frontier; Py-2020ID; Single shot mode |
| **Sample Mass** | 0.5 ± 0.3 mg |
| **Furnace temperature** | 340 °C, hold 1 minute |
| **Py/GC interface temperature** | 300 °C |
| **GC** | Shimadzu QP2010 |
| **Column** | Rtx-1614, 5% diphenyl/95% dimethyl polysiloxane 15 m × 0.25 mm × 0.1 μm |
| **Injection mode** | Split (split ratio: 1/300) |
| **Inlet port temperature** | 300 °C |
| **Carrier gas** | He (99.999%), 52.1 cm/s Constant linear flow |
| **Oven temperature program** | 80 °C no hold, to 300 °C at 20 °C /min and hold for 5 min |
| **MS** | Shimadzu QP2010 |
| **Solvent Delay** | 2 min |
| **Ion source temperature** | 230 °C |
| **Interface temperature** | 320 °C |
| **Detector voltage** | Abs 0.85 kV |
| **Ionization method** | EI, 70 eV |
| **SCAN range** | 50-1000 amu |

## Supplementary Table 2: MS characteristics for the simultaneous identification of plasticizers by Py/TD-GC-MS

| Compound | Retention time (min) | Identifying ion (m/z)* |
|---|---|---|
| **DMP** | 2.86 | 163, 77, 135, 94 |
| **DEP** | 3.56 | 147, 177, 65 |
| **MCCPs** | 4.0-9.0 | 79, 89, 91, 105, 115, 125, 151 |
| **DAP** | 4.42 | 149, 104, 189, 63 |
| **DIBP** | 5.02 | 149, 57, 104, 223 |
| **DBP** | 5.45 | 149, 205, 223 |
| **DPP** | 6.37 | 149, 55, 104, 237 |
| **BBP** | 7.13 | 149, 91, 104, 206 |
| **DOA** | 7.37 | 129, 57, 147 |
| **DCHP** | 7.82 | 149, 55, 83, 249 |
| **DHP** | 7.91 | 147, 57, 265 |
| **DEHP** | 7.94 | 149, 57, 113, 279 |
| **DINCH** | 8.10-9.00 | 155, 127, 281 |
| **DINP** | 8.25-9.75 | 149, 71, 85, 293 |
| **DnOP** | 8.63 | 149, 57, 279 |
| **DEHT** | 8.68 | 70, 112, 261 |
| **DIDP** | 8.75-10.00 | 149, 57, 85, 307 |
| **TOTM** | 6.77 | 70, 83, 175 |
| | 10.9 | 305, 57, 193, 113 |

Note: (*) Based on results from Type-B samples in conjunction with built-in MS library.

## Supplementary Table 3. GC-MS measurement conditions applied for solvent-extracted samples

| | |
|---|---|
| **GC** | Shimadzu QP2010 |
| **Column** | Rtx-1614, 5% diphenyl/95% dimethyl polysiloxane 15 m × 0.25 mm × 0.1 μm |
| **Injection mode** | Splitless |
| **Inlet port temperature** | 280 °C |
| **Carrier gas** | He (99.999%), Column Flow 3.38 mL/min |
| **Injection volume** | 1μL |
| **Oven temperature program** | 50 °C for 1 min, to 200 °C at 20 °C /min and hold for 2 min, to 300 °C at 30 °C /min and hold for 5 min |
| **MS** | Shimadzu QP2010 |
| **Solvent delay** | 5 min |
| **Ion source temperature** | 230 °C |
| **Interface temperature** | 300 °C |
| **Detector voltage** | Abs 0.95 kV |
| **Ionization method** | EI, 70 eV |
| **SCAN range** | 59-500 amu |

# Supplementary Table 4. MS characteristics for the simultaneous identification of solvent-extracted plasticizers by GC-MS

| Compound | Retention time (min) | Identifying ion (m/z) | Reference |
|---|---|---|---|
| **DMP*** | 5.57 | 163, 77, 194 | (1) |
| **SCCPs*,**** | 6.50-17.25 | 79, 89, 91 | (2) |
| **MCCPs*,**** | 7.25-20.00 | | |
| **DIBP*** | 7.82 | 149, 57, 223 | (1) |
| **DBP*** | 8.28 | 149, 205, 223 | (1) |
| **BBP*** | 11.00 | 149, 91, 206 | (1) |
| **DOA*** | 11.48 | 129, 112, 147 | (1) |
| **DHP*** | 12.73 | 149, 265, 247 | (1) |
| **DEHP*** | 12.82 | 149, 167, 279 | (1) |
| **DINCH*,**** | 13.15-16.00 | 155, 281, 127 | (3,4) |
| **DINP*** | 14.12-15.55 | 149, 293, 127 | (3-5) |
| **DnOP*** | 14.32 | 149, 279, 261 | (1) |
| **DEHT*** | 14.40 | 261, 112, 149 | (3-5) |
| **DIDP*** | 14.82-16.48 | 307, 149, 167 | (4) |
| **TOTM*** | 19.00 | 305, 193, 323 | (1) |

Note: (*) Mass fragments were verified with published sources; (**) From built-in MS library.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2. Yanagisawa H, Maruyama F, Fujimaki S. Journal of Analytical and Applied Pyrolysis Verification of simultaneous screening for major restricted additives in polymer materials using pyrolyzer / thermal desorption gas - chromatography mass spectrometry ( Py / TD-GC-MS ). Journal of Analytical and Applied Pyrolysis [Internet]. 2019;137(November 2018):37-42. Available from: https://doi.org/10.1016/j.jaap.2018.11.004

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4. Gimeno P, Thomas S, Bousquet C, Civade C, Brenier C, Bonnet P. Identification and quantification of 14 phthalates and 5 non-phthalate plasticizers in PVC medical devices by GC - MS. 2014;950:99-108.

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**Supplementary Table 5. Py/TD-GC-MS analysis results for all samples. Twenty percent of all samples were randomly subjected to confirmation by solvent extraction and GC-MS analysis.**

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | SPT027 | Boots | Black | Yes | | | | | Py&E | | | | | | | |
| 2 | SPT083 | Boots | White | | | Py | | Py | | | | | | Py | | |
| 3 | SPT201 | Boots | Blue | | | | | Py | | | | | | | | |
| 4 | SPT208 | Boots | Black | | | | | | Py | | | | Py | Py | | |
| 5 | SPT209 | Boots | Black | | | | Py | Py | | | | | | | | |
| 6 | SPT220 | Boots | Black | | | Py | | Py | | | | | Py | | Py | |
| 7 | SPT286 | Boots | Black | Yes | | Py&E | E | Py&E | Py&E | | | | E | Py&E | E | |
| 8 | SPT476 | Boots | Black | | | | | Py | Py | | | | Py | Py | Py | |
| 9 | SPT478 | Boots | Black | | | Py | | Py | | | | | Py | | | |
| 10 | SPT479 | Boots | Yellow | | | | | Py | | | | | | | | |
| 11 | SPT480 | Boots | Green | | | | | Py | Py | | | | Py | | | |
| 12 | SPT481 | Boots | Blue | | | | | Py | | | | | Py | | Py | |
| 13 | SPT482 | Boots | Black | | | | | Py | Py | | | | Py | | | |
| 14 | SPT483 | Boots | Orange | | | | | Py | | | | Py | | | Py | |
| 15 | SPT484 | Boots | C-GRN | Yes | | Py&E | | Py&E | | | | | Py&E | Py&E | E | |
| 16 | SPT485 | Boots | Purple | | | | | Py | | | | | Py | | | |
| 17 | SPT486 | Boots | White | | | | | Py | | | | | | | | |
| 18 | SPT487 | Boots | Blue | | | | | Py | | | | | Py | | Py | |
| 19 | SPT488 | Boots | Blue | | | | | Py | | | | | | | | |
| 20 | SPT489 | Boots | Clear | | | | | Py | Py | | | | Py | | | |
| 21 | SPT490 | Boots | Black | Yes | | Py&E | Py&E | Py&E | Py&E | | | | Py&E | E | E | |
| 22 | SPT491 | Boots | Brown | | | Py | Py | Py | | Py | | | | | | |

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23 | SPT492 | Boots | Green | | | | Py | Py | Py | | | | Py | | | |
| 24 | SPT493_1 | Boots | Blue | Yes | | | E | Py&E | | | | | | | E | DINP(T) |
| 25 | SPT493_2 | Boots | Blue | Yes | | Py&E | | Py&E | | | | | Py&E | | | DEHT(T) |
| 26 | SPT494_1 | Boots | Blue | | | | | Py | | | | | Py | | Py | |
| 27 | SPT494_2 | Boots | Blue | | | Py | | Py | | | | | Py | | | |
| 28 | SPT495_1 | Boots | Blue | | | Py | | | | | | | Py | | | |
| 29 | SPT495_2 | Boots | Blue | | | | | Py | | | | | | | | |
| 30 | SPT496_1 | Boots | Green | | | | | Py | Py | | | | Py | | | |
| 31 | SPT496_2 | Boots | Green | Yes | | | | Py&E | Py&E | | | | Py&E | | E | |
| 32 | SPT497_1 | Boots | Blue | Yes | | | | Py&E | | | | | Py&E | Py&E | Py&E | DBP(T) |
| 33 | SPT497_2 | Boots | Blue | Yes | | | Py&E | Py&E | E | | | E | Py&E | Py&E | Py&E | |
| 34 | SPT498_1 | Boots | Green | | | | | Py | | | | | Py | | | |
| 35 | SPT498_2 | Boots | White | Yes | | | | Py&E | Py&E | | | | Py&E | Py&E | E | DBP(T) |
| 36 | SPT499_1 | Boots | Green | | | Py | | Py | | | | | | | | |
| 37 | SPT499_2 | Boots | White | | | Py | | Py | | | | | | | | |
| 38 | SPT500_1 | Boots | Green | | | | | Py | | | | | Py | | | |
| 39 | SPT500_2 | Boots | Green | | | | | Py | | | | | Py | | | |
| 40 | SPT501_2 | Boots | Black | Yes | | Py&E | Py&E | Py&E | Py&E | | | | Py&E | Py&E | Py&E | |
| 41 | SPT502_2 | Boots | Brown | | | | | Py | | | | | | | | |
| 42 | SPT503_2 | Boots | Brown | | | | | Py | | | | | Py | | | |
| 43 | SPT504_2 | Boots | White | Yes | | | | Py&E | | | | | Py&E | | E | |
| 44 | SPT055 | Cables | BRO/WHT | | | Py | | | | | | | Py | | | |
| 45 | SPT056 | Cables | BLU/WHT | | | Py | | | | | | | Py | | | |
| 46 | SPT057 | Cables | White | | | Py | | | | | | | Py | | | |
| 47 | SPT078 | Cables | Gray | | | | Py | Py | | | Py | | Py | | Py | |
| 48 | SPT079 | Cables | White | | | | | Py | | | Py | | | | Py | |
| 49 | SPT146 | Cables | Black | | | | | Py | | | | | Py | | Py | |

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 50 | SPT147 | Cables | Gray | | | Py | Py | Py | | | | | Py | | | |
| 51 | SPT234 | Cables | White | | | Py | | | | | | | Py | | | |
| 52 | SPT235 | Cables | Red | | | Py | | Py | | | | | Py | | | |
| 53 | SPT236 | Cables | Green | | | | | Py | | | | | Py | | | |
| 54 | SPT237 | Cables | BLU/WHT | | | Py | | | | | | | Py | | | |
| 55 | SPT238 | Cables | BRO/WHT | Yes | | Py&E | | | | | | | Py&E | | | DEHP(T), DEHT(T) |
| 56 | SPT239 | Cables | Black | | | Py | | Py | | | Py | | Py | | | |
| 57 | SPT240 | Cables | White | | | Py | | | | | | | Py | | | |
| 58 | SPT241 | Cables | RED/WHT | | | Py | | | | | | | Py | | | |
| 59 | SPT242 | Cables | GRN/WHT | | | Py | | | | | | | Py | | | |
| 60 | SPT243 | Cables | Green | | | | | Py | | | | | Py | | | |
| 61 | SPT244 | Cables | BLK/WHT | | | Py | | | | | | | Py | | | |
| 62 | SPT245 | Cables | Gray | Yes | | Py&E | | Py&E | | | | | | | | DINP(T) |
| 63 | SPT246 | Cables | BLU/WHT | | | Py | | | | | | | Py | | | |
| 64 | SPT247 | Cables | Yellow | | | Py | | | | | | | Py | | | |
| 65 | SPT248 | Cables | RED/WHT | | | Py | Py | Py | | | | | | | | |
| 66 | SPT249 | Cables | GRN/WHT | | | Py | | Py | | | | | Py | | | |
| 67 | SPT250 | Cables | White | Yes | | Py&E | | Py&E | | | | | E | | | |
| 68 | SPT251 | Cables | White | | | Py | | Py | Py | | | | | | | |
| 69 | SPT252 | Cables | Black | | | | | | Py | | | | | | | |
| 70 | SPT253 | Cables | Gray | | | | | | Py | | | | | | | |
| 71 | SPT254 | Cables | Black | | | Py | | | | | | | Py | | | |
| 72 | SPT255 | Cables | GRN/WHT | | | Py | | | | | | | Py | | | |
| 73 | SPT256 | Cables | Black | | | Py | | | | | | | Py | | | |
| 74 | SPT257 | Cables | Black | | | Py | | | | | | | Py | | | |
| 75 | SPT292 | Cables | Black | | | | | | Py | | | | | | | |

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 76 | SPT293 | Cables | Black | | | | | | Py | | | | | | | |
| 77 | SPT294 | Cables | Black | Yes | | Py&E | Py&E | Py&E | Py&E | Py&E | | | Py&E | E | E | |
| 78 | SPT295 | Cables | Black | Yes | | Py&E | Py&E | Py&E | Py&E | | | | Py&E | E | Py&E | |
| 79 | SPT296 | Cables | Black | | | | | | Py | | | | | | Py | |
| 80 | SPT297 | Cables | Black | Yes | | | E | | Py&E | | | | | | Py&E | CPs(T) |
| 81 | SPT298 | Cables | Black | | | Py | Py | Py | Py | Py | | | Py | Py | | |
| 82 | SPT300 | Cables | White | | | Py | Py | Py | Py | | | | Py | Py | | |
| 83 | SPT427 | Cables | Black | | | Py | Py | | | | | | Py | | | |
| 84 | SPT428 | Cables | Black | Yes | | Py&E | | Py&E | | | | | Py&E | E | Py&E | DBP(T) |
| 85 | SPT429 | Cables | Blue | | | Py | | Py | | | | | Py | | | |
| 86 | SPT430 | Cables | BRO/WHT | | | Py | | Py | | | | | Py | | | |
| 87 | SPT431 | Cables | BRO/WHT | | | Py | | Py | | | | | Py | | | |
| 88 | SPT432 | Cables | GRA/WHT | | | Py | | Py | | | | | Py | | | |
| 89 | SPT433 | Cables | GRN/WHT | | | Py | | Py | | | | | Py | | | |
| 90 | SPT434 | Cables | GRN/WHT | | | Py | | Py | | | | | Py | | | |
| 91 | SPT435 | Cables | Green | | | Py | | | | | | | Py | | | |
| 92 | SPT436 | Cables | GRN/WHT | Yes | | Py&E | | E | E | | | | Py&E | | E | |
| 93 | SPT437 | Cables | Blue | Yes | | Py&E | | Py&E | | | | | Py&E | | E | DEHT(T) |
| 94 | SPT438 | Cables | BLU/WHT | | | Py | | | | | | | Py | | | |
| 95 | SPT439 | Cables | White | | | Py | | Py | | | | | | | | |
| 96 | SPT440 | Cables | ORN/WHT | | | Py | | | | | | | Py | | | |
| 97 | SPT441 | Cables | YEL/WHT | | | | | Py | | | | | | | | |
| 98 | SPT442 | Cables | Black | | | Py | | Py | | | | | Py | | Py | |
| 99 | SPT443 | Cables | BLK/WHT | | | Py | | Py | | | | | Py | | | |
| 100 | SPT001 | Floorings | Mx/GRA | | Py | | | Py | | | | | | | | |
| 101 | SPT002 | Floorings | Mx/GRA | | Py | | | Py | | | | | | | | |
| 102 | SPT003 | Floorings | Mx/GRA | Yes | Py&E | | | Py&E | E | | | | E | | | |

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 103 | SPT004 | Floorings | Mx/GRA | Yes | | | | Py&E | | | | | E | | | TOTM(T) |
| 104 | SPT258 | Floorings | Mx/GRA | | | Py | | Py | | | | | Py | | | |
| 105 | SPT259 | Floorings | Mx/GRA | | | Py | | Py | | | | | Py | | | |
| 106 | SPT260 | Floorings | Mx/GRA | | | Py | | Py | Py | | | | Py | | | |
| 107 | SPT444 | Floorings | Mx/GRA | | | Py | | Py | Py | | | | Py | | | |
| 108 | SPT445 | Floorings | Mx/GRA | Yes | | Py&E | | Py&E | Py&E | | | | Py&E | E | E | |
| 109 | SPT446 | Floorings | Mx/GRA | | | | | Py | | | | | | | | |
| 110 | SPT447 | Floorings | Mx/GRA | | | Py | | Py | Py | | | | Py | | | |
| 111 | SPT448 | Floorings | Mx/GRA | | | | | Py | | | | | | | | |
| 112 | SPT449 | Floorings | Mx/GRA | | | Py | | Py | Py | | | | Py | | | |
| 113 | SPT450 | Floorings | Mx/GRA | Yes | | Py&E | | Py&E | | | | | Py&E | | E | DEHT(T) |
| 114 | SPT451 | Floorings | Mx/GRA | | | Py | | Py | | | | | Py | | | |
| 115 | SPT452 | Floorings | Mx/GRA | | | Py | | Py | | | | | Py | | | |
| 116 | SPT453 | Floorings | Mx/GRA | | | | | Py | | | | | | | | |
| 117 | SPT454 | Floorings | Mx/GRA | | | | | Py | | | | | Py | | | |
| 118 | SPT455 | Floorings | Mx/GRA | | | Py | | Py | Py | | | | Py | | | |
| 119 | SPT456 | Floorings | Mx/GRA | | | Py | Py | Py | | | | | Py | | | |
| 120 | SPT457 | Floorings | Mx/GRA | Yes | | Py&E | | Py&E | Py&E | | | | Py&E | E | E | |
| 121 | SPT458 | Floorings | Mx/GRA | | | Py | | Py | | | | | Py | | | |
| 122 | SPT459 | Floorings | Mx/GRA | | | Py | | Py | | | | | Py | | | |
| 123 | SPT460 | Floorings | Mx/GRA | | | | | Py | Py | | | | Py | | | |
| 124 | SPT033 | Hoses | Clear | | | | | Py | | | | | Py | | | |
| 125 | SPT042 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 126 | SPT043 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 127 | SPT142 | Hoses | YEL/BLK | | | Py | | Py | | | | | | | | |
| 128 | SPT143 | Hoses | Mx/BLK | | | Py | Py | Py | | | | | | Py | | |
| 129 | SPT144 | Hoses | Clear | | | Py | | Py | | | | | | | | |

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 130 | SPT145 | Hoses | Clear | | | | | Py | | | | | | | | |
| 131 | SPT219 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 132 | SPT271 | Hoses | Blue | | | Py | | Py | | | | | | | | |
| 133 | SPT272 | Hoses | GRN/BLK | Yes | | Py&E | | Py&E | | | | | Py&E | | E | DBP(T) |
| 134 | SPT273 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 135 | SPT274 | Hoses | Clear | Yes | | Py&E | Py&E | | | | | | | | | |
| 136 | SPT275 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 137 | SPT276 | Hoses | GRN/BLK | | | | | Py | | | | | Py | | | |
| 138 | SPT277 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 139 | SPT278 | Hoses | Clear | Yes | | Py&E | E | Py&E | | Py&E | | | | | | |
| 140 | SPT279 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 141 | SPT280 | Hoses | GRN/BLK | | | Py | | Py | | | | | | | | |
| 142 | SPT281 | Hoses | Blue | Yes | | Py&E | | Py&E | | | | | E | E | | DBP(T) |
| 143 | SPT282 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 144 | SPT283 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 145 | SPT284 | Hoses | Clear | Yes | | Py&E | | Py&E | | | | | | | | DOA(T) |
| 146 | SPT285 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 147 | SPT316 | Hoses | Clear | | | Py | | Py | | Py | | | | | | |
| 148 | SPT462 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 149 | SPT463 | Hoses | Blue | Yes | | Py&E | Py&E | E | | | | | | | | |
| 150 | SPT464 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 151 | SPT465 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 152 | SPT466 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 153 | SPT467 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 154 | SPT468 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 155 | SPT469 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 156 | SPT470 | Hoses | GRN/BLK | | | Py | | Py | | | Py | | Py | | Py | |

| No | Sample ID | Product | Color | Conf. | BBP | CPs | DBP | DEHP | DEHT | DIBP | DIDP | DINCH | DINP | DOA | TOTM | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 157 | SPT471 | Hoses | GRN/BLK | | | | | Py | | | | | Py | | | |
| 158 | SPT472 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 159 | SPT473 | Hoses | Blue | Yes | | Py&E | | Py&E | | | | | | | | |
| 160 | SPT474 | Hoses | Clear | | | Py | | Py | | | | | | | | |
| 161 | SPT475 | Hoses | White | | | Py | | Py | | | | | Py | | | |
| Total | | | | 33 | 3 | 106 | 23 | 131 | 35 | 5 | 4 | 2 | 99 | 19 | 32 | |
| Frequency of detection | | | | 20% | 2% | 65% | 14% | 81% | 22% | 3% | 2% | 1% | 61% | 12% | 20% | |

Note: (*) Confirmed by solvent extraction followed by GC-MS analysis; Py: Identified by Py/TD-GC-MS; E: Identified by solvent extraction followed by GC-MS; Py&E: Identified by both methods; (T): Trace, as identified by extraction GC-MS.
Double ordering system: Color (outside layer)/Color (inside layer); BLK: Black; BLU: Blue; BRO: Brown; RED: Red; GRN: Green; ORG: Orange; YEL: Yellow; GRA: Gray; PUR: Purple; Mx:Mixed color.

## Supplementary Table 6: Indicators for the analysis of Py/TD-GC-MS performance

| Indicator | Description | Formular |
|---|---|---|
| **Accuracy** | Accuracy of Py/TD-GC-MS for identifying a particular substance is the ratio of the number of similar identifications provided by both methods to the total number of identifications. | $Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$ |
| **Precision** | Precision of Py/TD-GC-MS for identifying a particular substance is the ratio of the number of positive identifications provided by both methods to the total number of positive identifications identified by Py/TD-GC-MS. | $Precision = \frac{TP}{TP + FP}$ |
| **Sensitivity (also known as Recall)** | Sensitivity of Py/TD-GC-MS for identifying a particular substance is the ratio of the number of positive identifications provided by both methods to the total number of positive identifications identified by GC-MS | $Sensitivity = \frac{TP}{TP + FN}$ |
| **Specificity** | Specificity of Py/TD-GC-MS for identifying a particular substance is the ratio of the number of negative identifications provided by both methods to the total number of negative identifications identified by GC-MS. FP rate is also given by (1 - specificity). | $Specificity = \frac{TN}{TN + FP}$ |
| **F1 score** | The F1 score is defined as the harmonic mean of the method's precision and sensitivity. | $F1\ score = \frac{2}{\frac{1}{Precision} + \frac{1}{Sensitivity}} = \frac{2 \times Precision \times Sensitivity}{Precision + Sensitivity}$ |