

Supplementary Data

This supplementary data is a part of a paper entitled “Non-Target Screening of Chemical Migrants from Paper-Based Tea Bags: A Preliminary Investigation for Food Safety Assessment”.

Table S1. Tentative identifications from ESI- and ESI+ mass spectrometry datasets

Component name	Formula	Observed <i>m/z</i>	Code	Positive samples
Candidate Mass C ₃ H ₂ F ₈ N ₂ O ₂	C ₃ H ₂ F ₈ N ₂ O ₂	248.9926 [M-H] ⁻	U-1	SPL10, SPL9
Candidate Mass C ₃ H ₅ F ₅ N ₂ O ₅ P ₂	C ₃ H ₅ F ₅ N ₂ O ₅ P ₂	304.9521 [M-H] ⁻	U-2	SPL9, SPL10
Candidate Mass C ₉ H ₇ F ₂ N ₂ O ₉ PS ₂	C ₉ H ₇ F ₂ N ₂ O ₉ PS ₂	418.9224 [M-H] ⁻	U-3	SPL1, SPL2
Candidate Mass C ₃ H ₉ F ₇ N ₄ OP ₆	C ₃ H ₉ F ₇ N ₄ OP ₆	434.9037 [M-H] ⁻	U-4	SPL2, SPL1
Candidate Mass C ₃ H ₆ F ₇ N ₄ O ₇ P ₃	C ₃ H ₆ F ₇ N ₄ O ₇ P ₃	434.9263 [M-H] ⁻	U-5	SPL9, SPL10
Candidate Mass C ₂ HF ₄ N ₂ OP	C ₂ HF ₄ N ₂ OP	174.9687 [M-H] ⁻	U-6	SPL2, SPL3
Candidate Mass CHF ₄ N ₄ P	CHF ₄ N ₄ P	174.9789 [M-H] ⁻	U-7	SPL10, SPL11
Candidate Mass C ₂ H ₁₀ FN ₄ O ₃ P ₃	C ₂ H ₁₀ FN ₄ O ₃ P ₃	248.9888 [M-H] ⁻	U-8	SPL7, SPL8
Candidate Mass C ₃ H ₆ F ₁₁ N ₈ O ₈ P	C ₃ H ₆ F ₁₁ N ₈ O ₈ P	520.978 [M-H] ⁻	U-9	SPL10, SPL11
Candidate Mass C ₃ H ₉ F ₁₀ N ₈ O ₉ P ₃	C ₃ H ₉ F ₁₀ N ₈ O ₉ P ₃	582.9453 [M-H] ⁻	U-10	SPL6, SPL7
Candidate Mass C ₃ H ₃ F ₅ NOPS	C ₃ H ₃ F ₅ NOPS	225.9511 [M-H] ⁻	U-11	SPL7, SPL8
<i>N</i> -[2-(1 <i>H</i> -Tetrazol-1-yl)ethyl]sulfuric diamide	C ₃ H ₈ N ₆ O ₂ S	191.035 [M-H] ⁻	U-12	SPL3, SPL2
1-(2,2-Dinitropropyl)urea	C ₄ H ₈ N ₄ O ₅	191.0415 [M-H] ⁻	U-13	SPL6, SPL7, SPL9
Candidate Mass C ₉ H ₁₅ F ₅ N ₄ O ₂	C ₉ H ₁₅ F ₅ N ₄ O ₂	305.1042 [M-H] ⁻	U-14	SPL9, SPL8
Candidate Mass C ₃ H ₈ F ₆ N ₆	C ₃ H ₈ F ₆ N ₆	241.0633 [M-H] ⁻	U-15	SPL8, SPL9
4-Fluorostyrene	C ₈ H ₇ F	121.0458 [M-H] ⁻	U-16	SPL11, SPL10
Diethylphosphinic acid	C ₄ H ₁₁ O ₂ P	121.0436 [M-H] ⁻	U-17	SPL8, SPL6
<i>N</i> ''-(2,2,2-Trifluoroethylidene)carbonohydrazonic diamide	C ₃ H ₅ F ₃ N ₄	153.0376 [M-H] ⁻	U-18	SPL8, SPL9
Candidate Mass C ₂₃ H ₄₆ FN ₂ O ₃ P	C ₂₃ H ₄₆ FN ₂ O ₃ P	491.1799 [M-H] ⁻	U-19	SPL8, SPL9, SPL8
Candidate Mass C ₆ H ₃₀ FN ₁₆ P	C ₆ H ₃₀ FN ₁₆ P	375.2479 [M-H] ⁻	U-20	SPL9, SPL8, SPL7
Candidate Mass C ₃ HCl ₃ OP ₂ S ₇	C ₃ HCl ₃ OP ₂ S ₇	442.6556 [M-H] ⁻	U-21	SPL3, SPL1, SPL2
Candidate Mass C ₁₄ H ₃₄ N ₈ O ₂	C ₁₄ H ₃₄ N ₈ O ₂	345.2744 [M-H] ⁻	U-22	SPL11, SPL9, SPL7
Candidate Mass C ₂₀ H ₄₈ N ₁₄ O	C ₂₀ H ₄₈ N ₁₄ O	499.4061 [M-H] ⁻	U-23	SPL3, SPL4
Candidate Mass CH ₂ ClF ₄ N ₃ OP ₂	CH ₂ ClF ₄ N ₃ OP ₂	243.9228 [M-H] ⁻	U-24	SPL5, SPL4
Candidate Mass C ₂ HClF ₄ NO ₄ P	C ₂ HClF ₄ NO ₄ P	243.919 [[M-H] ⁻	U-25	SPL2, SPL3
Candidate Mass C ₃ H ₃ ClFN ₃ O ₃ P ₂	C ₃ H ₃ ClFN ₃ O ₃ P ₂	243.9252 [[M-H] ⁻	U-26	SPL6, SPL7
Candidate Mass CHF ₂ N ₃ O	CHF ₂ N ₃ O	110.0158 [M+H] ⁺	U-27	SPL5, SPL4
Candidate Mass C ₂ H ₅ FNPS	C ₂ H ₅ FNPS	125.9945 [M+H] ⁺	U-28	SPL3, SPL6, SPL5
Candidate Mass CH ₃ F ₂ N ₃ O ₂	CH ₃ F ₂ N ₃ O ₂	128.0273 [M+H] ⁺	U-29	SPL3, SPL5, SPL6
Candidate Mass C ₂ H ₇ N ₄ O ₂ P	C ₂ H ₇ N ₄ O ₂ P	151.0372 [M+H] ⁺	U-30	SPL1, SPL10
<i>N</i> -Carbamoyl-2,2-dihydroxyhydrazinecarboxamide	C ₂ H ₆ N ₄ O ₄	151.0445 [M+H] ⁺	U-31	SPL5, SPL4
2,2-Bis(difluoroamino)-2-fluoroethanol	C ₂ H ₃ F ₅ N ₂ O	167.0228 [M+H] ⁺	U-32	SPL3, SPL5, SPL4
Candidate Mass 110.0121	-	110.0121 [M+H] ⁺	U-33	SPL7, SPL8
Candidate Mass CH ₅ NO ₂ P ₂	CH ₅ NO ₂ P ₂	125.9883 [M+H] ⁺	U-34	SPL1, SPL9

Component name	Formula	Observed m/z	Code	Positive samples
Candidate Mass $C_2H_2F_2NOP$	$C_2H_2F_2NOP$	125.9911 $[M+H]^+$	U-35	SPL2, SPL7
Candidate Mass $C_3H_8N_2O_2P_2$	$C_3H_8N_2O_2P_2$	167.015 $[M+H]^+$	U-36	SPL1, SPL9
Candidate Mass $C_3H_6F_4N_6$	$C_3H_6F_4N_6$	203.0654 $[M+H]^+$	U-37	SPL3, SPL5, SPL4
Candidate Mass $C_{10}H_{36}N_{16}O_4$	$C_{10}H_{36}N_{16}O_4$	445.3187 $[M+H]^+$	U-38	SPL4, SPL3
2-Bromo- <i>N,N</i> -didecylacetamide	$C_{22}H_{44}BrNO$	418.2682 $[M+H]^+$	U-39	SPL7, SPL1
4-(2-Methyl-2-propanyl)-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane	$C_8H_{15}O_3P$	191.084 $[M+H]^+$	U-40	SPL3, SPL4
2-Methylquinoxaline	$C_9H_8N_2$	145.0751 $[M+H]^+$	U-41	SPL3, SPL4
(2 <i>R</i> ,6 <i>S</i>)-6-Methyl-2-[(1 <i>E</i>)-1-propen-1-yl]-5,6-Dihydro-2 <i>H</i> -1,2-oxaphosphinine 2-oxide	$C_8H_{13}O_2P$	173.072 $[M+H]^+$	U-42	SPL4, SPL3
1-Butoxy-3-methyl-2,5-dihydro-1 <i>H</i> -phosphole 1-oxide	$C_9H_{17}O_2P$	189.104 $[M+H]^+$	U-43	SPL3, SPL4
9-Vinylanthracene	$C_{16}H_{12}$	205.0997 $[M+H]^+$	U-44	SPL4, SPL3
3-Fluoro-4-piperazin-1-yl-benzonitrile	$C_{11}H_{12}FN_3$	206.1081 $[M+H]^+$	U-45	SPL3, SPL4
Candidate Mass $C_8H_{18}FN_4P$	$C_8H_{18}FN_4P$	221.1327 $[M+H]^+$	U-46	SPL3, SPL4
Candidate Mass $C_4H_{11}F_3N_6O_2$	$C_4H_{11}F_3N_6O_2$	233.0964 $[M+H]^+$	U-47	SPL3, SPL4
Candidate Mass $C_7H_{19}F_2N_4OP$	$C_7H_{19}F_2N_4OP$	245.1339 $[M+H]^+$	U-48	SPL3, SPL4
3-Sulfanyl- <i>N</i> -(5-tetrazolidinyl)propanamide	$C_4H_{11}N_5OS$	178.0776 $[M+H]^+$	U-49	SPL2, SPL6
Glufosinate	$C_5H_{12}NO_4P$	182.0577 $[M+H]^+$	U-50	SPL3, SPL5
Candidate Mass $C_3H_{12}N_7O_2P$	$C_3H_{12}N_7O_2P$	210.0879 $[M+H]^+$	U-51	SPL5, SPL6
<i>N</i> -[(Dodecylsulfanyl)methyl]- <i>N</i> -ethylethanamine	$C_{17}H_{37}NS$	288.2724 $[M+H]^+$	U-52	SPL3, SPL4
Candidate Mass $C_3H_9F_2N_{11}O$	$C_3H_9F_2N_{11}O$	254.104 $[M+H]^+$	U-53	SPL9, SPL10
5-(1-Amino-2-hydroxypropyl)-1,2,4-oxadiazolidine-3-carboxylic acid	$C_6H_{13}N_3O_4$	192.0971 $[M+H]^+$	U-54	SPL3, SPL4
Candidate Mass $C_3H_9N_5O_6$	$C_3H_9N_5O_6$	212.0644 $[M+H]^+$	U-55	SPL2, SPL7
Candidate Mass $C_{11}H_{28}N_6O_2$	$C_{11}H_{28}N_6O_2$	277.2343 $[M+H]^+$	U-56	SPL3, SPL4
4-(Difluoromethylene)-4'-propyl-1,1'-Bi(cyclohexyl)	$C_{16}H_{26}F_2$	257.2073 $[M+H]^+$	U-57	SPL4, SPL3
Candidate Mass $C_8H_{21}N_7O_4$	$C_8H_{21}N_7O_4$	280.1731 $[M+H]^+$	U-58	SPL4, SPL3
Candidate Mass $C_3H_8FN_9$	$C_3H_8FN_9$	190.0959 $[M+H]^+$	U-59	SPL2, SPL6
Candidate Mass $C_{10}H_{19}N_{11}$	$C_{10}H_{19}N_{11}$	294.1896 $[M+H]^+$	U-60	SPL3, SPL4
<i>N</i> -[2-[[2-[[2-[(2-Aminoethyl)amino]ethyl]amino]ethyl]amino]ethyl]octanamide	$C_{16}H_{37}N_5O$	316.3052 $[M+H]^+$	U-61	SPL4, SPL3
Candidate Mass 228.2479	-	228.2479 $[M+H]^+$	U-62	SPL3, SPL4, SPL5
<i>tert</i> -Butyl 3,3-difluoro-5-(hydroxymethyl)piperidine-1-carboxylate	$C_{11}H_{19}F_2NO_3$	252.1406 $[M+H]^+$	U-63	SPL3, SPL4
5-(Nitroamino)-1,2,4-triazolidine-3-carboxylic acid	$C_3H_7N_5O_4$	178.0584 $[M+H]^+$	U-64	SPL6, SPL7
Candidate Mass $C_5H_{13}NP_2$	$C_5H_{13}NP_2$	150.0591 $[M+H]^+$	U-65	SPL8, SPL7
Candidate Mass $C_3H_7F_2N_5$	$C_3H_7F_2N_5$	152.0755 $[M+H]^+$	U-66	SPL6, SPL7
Candidate Mass $C_6H_{32}N_{20}$	$C_6H_{32}N_{20}$	385.3181 $[M+H]^+$	U-67	SPL3, SPL4
Candidate Mass $C_{17}H_{49}N_{13}O_2$	$C_{17}H_{49}N_{13}O_2$	468.4209 $[M+H]^+$	U-68	SPL3, SPL4

Component name	Formula	Observed m/z	Code	Positive samples
5-[2-({1-[Isopropyl(methyl)amino]-2-propanyl}amino)ethyl)-4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one	C ₁₂ H ₂₅ N ₅ O	256.2148 [M+H] ⁺	U-69	SPL6, SPL7
2,2'-(2,6-Pyridinediyl)bis(<i>N,N,N',N'</i> -tetramethyl-1,3-propanediamine)	C ₁₉ H ₃₇ N ₅	336.3127 [[M+H] ⁺	U-70	SPL3, SPL4
Candidate Mass C ₂₄ H ₄₈ FN ₃ O	C ₂₄ H ₄₈ FN ₃ O	414.3848 [M+H] ⁺	U-71	SPL3, SPL4
Candidate Mass 283.2824	-	283.2824 [M+H] ⁺	U-72	SPL3, SPL4