

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 m/z	Code	Positive samples
Candidate Mass $C_3H_2F_8N_2O_2$	$C_3H_2F_8N_2O_2$	248.9926 [M-H] ⁻	U-1	SPL10, SPL9
Candidate Mass $C_3H_5F_5N_2O_5P_2$	$C_3H_5F_5N_2O_5P_2$	304.9521 [M-H] ⁻	U-2	SPL9, SPL10
Candidate Mass $C_9H_7F_2N_2O_9PS_2$	$C_9H_7F_2N_2O_9PS_2$	418.9224 [M-H] ⁻	U-3	SPL1, SPL2
Candidate Mass $C_3H_9F_7N_4OP_6$	$C_3H_9F_7N_4OP_6$	434.9037 [M-H] ⁻	U-4	SPL2, SPL1
Candidate Mass $C_3H_6F_7N_4O_7P_3$	$C_3H_6F_7N_4O_7P_3$	434.9263 [M-H] ⁻	U-5	SPL9, SPL10
Candidate Mass $C_2HF_4N_2OP$	$C_2HF_4N_2OP$	174.9687 [M-H] ⁻	U-6	SPL2, SPL3
Candidate Mass CHF_4N_4P	CHF_4N_4P	174.9789 [M-H] ⁻	U-7	SPL10, SPL11
Candidate Mass $C_2H_{10}FN_4O_3P_3$	$C_2H_{10}FN_4O_3P_3$	248.9888 [M-H] ⁻	U-8	SPL7, SPL8
Candidate Mass $C_3H_6F_{11}N_8O_8P$	$C_3H_6F_{11}N_8O_8P$	520.978 [M-H] ⁻	U-9	SPL10, SPL11
Candidate Mass $C_3H_9F_{10}N_8O_9P_3$	$C_3H_9F_{10}N_8O_9P_3$	582.9453 [M-H] ⁻	U-10	SPL6, SPL7
Candidate Mass $C_3H_3F_5NOPS$	$C_3H_3F_5NOPS$	225.9511 [M-H] ⁻	U-11	SPL7, SPL8
<i>N</i> -[2-(1 <i>H</i> -Tetrazol-1-yl)ethyl]sulfuric diamide	$C_3H_8N_6O_2S$	191.035 [M-H] ⁻	U-12	SPL3, SPL2
1-(2,2-Dinitropropyl)urea	$C_4H_8N_4O_5$	191.0415 [M-H] ⁻	U-13	SPL6, SPL7, SPL9
Candidate Mass $C_9H_{15}F_5N_4O_2$	$C_9H_{15}F_5N_4O_2$	305.1042 [M-H] ⁻	U-14	SPL9, SPL8
Candidate Mass $C_3H_8F_6N_6$	$C_3H_8F_6N_6$	241.0633 [M-H] ⁻	U-15	SPL8, SPL9
4-Fluorostyrene	C_8H_7F	121.0458 [M-H] ⁻	U-16	SPL11, SPL10
Diethylphosphinic acid	$C_4H_{11}O_2P$	121.0436 [M-H] ⁻	U-17	SPL8, SPL6
<i>N</i> '-(2,2,2-Trifluoroethylidene)carbonohydrazonic diamide	$C_3H_5F_3N_4$	153.0376 [M-H] ⁻	U-18	SPL8, SPL9
Candidate Mass $C_{23}H_{46}FN_2O_3P$	$C_{23}H_{46}FN_2O_3P$	491.1799 [M-H] ⁻	U-19	SPL8, SPL9, SPL8
Candidate Mass $C_6H_{30}FN_{16}P$	$C_6H_{30}FN_{16}P$	375.2479 [M-H] ⁻	U-20	SPL9, SPL8, SPL7
Candidate Mass $C_3HCl_3OP_2S_7$	$C_3HCl_3OP_2S_7$	442.6556 [M-H] ⁻	U-21	SPL3, SPL1, SPL2
Candidate Mass $C_{14}H_{34}N_8O_2$	$C_{14}H_{34}N_8O_2$	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 $CH_2ClF_4N_3OP_2$	$CH_2ClF_4N_3OP_2$	243.9228 [M-H] ⁻	U-24	SPL5, SPL4
Candidate Mass $C_2HClF_4NO_4P$	$C_2HClF_4NO_4P$	243.919 [[M-H] ⁻	U-25	SPL2, SPL3
Candidate Mass $C_3H_3ClFN_3O_3P_2$	$C_3H_3ClFN_3O_3P_2$	243.9252 [[M-H] ⁻	U-26	SPL6, SPL7
Candidate Mass CHF_2N_3O	CHF_2N_3O	110.0158 [M+H] ⁺	U-27	SPL5, SPL4
Candidate Mass C_2H_5FNPS	C_2H_5FNPS	125.9945 [M+H] ⁺	U-28	SPL3, SPL6, SPL5
Candidate Mass $CH_3F_2N_3O_2$	$CH_3F_2N_3O_2$	128.0273 [M+H] ⁺	U-29	SPL3, SPL5, SPL6
Candidate Mass $C_2H_7N_4O_2P$	$C_2H_7N_4O_2P$	151.0372 [M+H] ⁺	U-30	SPL1, SPL10
<i>N</i> -Carbamoyl-2,2-dihydroxyhydrazinecarboxamide	$C_2H_6N_4O_4$	151.0445 [M+H] ⁺	U-31	SPL5, SPL4
2,2-Bis(difluoroamino)-2-fluoroethanol	$C_2H_3F_5N_2O$	167.0228 [M+H] ⁺	U-32	SPL3, SPL5, SPL4
Candidate Mass 110.0121	-	110.0121 [M+H] ⁺	U-33	SPL7, SPL8
Candidate Mass $CH_5NO_2P_2$	$CH_5NO_2P_2$	125.9883 [M+H] ⁺	U-34	SPL1, SPL9

Component name	Formula	Observed m/z	Code	Positive samples
Candidate Mass C ₂ H ₂ F ₂ NOP	C ₂ H ₂ F ₂ NOP	125.9911 [M+H] ⁺	U-35	SPL2, SPL7
Candidate Mass C ₃ H ₈ N ₂ O ₂ P ₂	C ₃ H ₈ N ₂ O ₂ P ₂	167.015 [M+H] ⁺	U-36	SPL1, SPL9
Candidate Mass C ₃ H ₆ F ₄ N ₆	C ₃ H ₆ F ₄ N 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 ₈ H ₁₅ O ₃ P	191.084 [M+H] ⁺	U-40	SPL3, SPL4
2-Methylquinoxaline	C ₉ H ₈ N 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 ₈ H ₁₃ O ₂ P	173.072 [M+H] ⁺	U-42	SPL4, SPL3
1-Butoxy-3-methyl-2,5-dihydro-1 <i>H</i> -phosphole 1-oxide	C ₉ H ₁₇ O ₂ P	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 ₈ H ₁₈ FN ₄ P	C ₈ H ₁₈ FN ₄ P	221.1327 [M+H] ⁺	U-46	SPL3, SPL4
Candidate Mass C ₄ H ₁₁ F ₃ N ₆ O ₂	C ₄ H ₁₁ F ₃ N ₆ O ₂	233.0964 [M+H] ⁺	U-47	SPL3, SPL4
Candidate Mass C ₇ H ₁₉ F ₂ N ₄ OP	C ₇ H ₁₉ F ₂ N ₄ OP	245.1339 [M+H] ⁺	U-48	SPL3, SPL4
3-Sulfanyl- <i>N</i> -(5-tetrazolidinyl)propanamide	C ₄ H ₁₁ N ₅ OS	178.0776 [M+H] ⁺	U-49	SPL2, SPL6
Glufosinate	C ₅ H ₁₂ NO ₄ P	182.0577 [M+H] ⁺	U-50	SPL3, SPL5
Candidate Mass C ₃ H ₁₂ N ₇ O ₂ P	C ₃ H ₁₂ N ₇ O ₂ P	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 ₃ H ₉ F ₂ N ₁₁ O	C ₃ H ₉ F ₂ N ₁₁ O	254.104 [M+H] ⁺	U-53	SPL9, SPL10
5-(1-Amino-2-hydroxypropyl)-1,2,4-oxadiazolidine-3-carboxylic acid	C ₆ H ₁₃ N ₃ O ₄	192.0971 [M+H] ⁺	U-54	SPL3, SPL4
Candidate Mass C ₃ H ₉ N ₅ O ₆	C ₃ H ₉ N ₅ O ₆	212.0644 [M+H] ⁺	U-55	SPL2, SPL7
Candidate Mass C ₁₁ H ₂₈ N ₆ O ₂	C ₁₁ H ₂₈ N ₆ O 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 ₈ H ₂₁ N ₇ O ₄	C ₈ H ₂₁ N ₇ O ₄	280.1731 [M+H] ⁺	U-58	SPL4, SPL3
Candidate Mass C ₃ H ₈ FN ₉	C ₃ H ₈ FN 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 ₅ O	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 ₂ NO ₃	252.1406 [M+H] ⁺	U-63	SPL3, SPL4
5-(Nitroamino)-1,2,4-triazolidine-3-carboxylic acid	C ₃ H ₇ N ₅ O ₄	178.0584 [M+H] ⁺	U-64	SPL6, SPL7
Candidate Mass C ₅ H ₁₃ NP ₂	C ₅ H ₁₃ NP ₂	150.0591 [M+H] ⁺	U-65	SPL8, SPL7
Candidate Mass C ₃ H ₇ F ₂ N ₅	C ₃ H ₇ F ₂ N ₅	152.0755 [M+H] ⁺	U-66	SPL6, SPL7
Candidate Mass C ₆ H ₃₂ N ₂₀	C ₆ H 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(N,N,N',N'-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