

Supporting Information

Title: General Suspect Screening of Maternal Serum to Identify New Environmental Biomonitoring Targets using Quadrupole Time-Of-Flight Mass Spectrometry

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Table S1 . Relative sensitivity of LC-QTOF/MS (Agilent LC1260-QTOF/MS 6550) and LC-MS/MS (Agilent LC1260-AB Sciex 5500) platforms.

Compound	Limit of Detection (ng/mL)	
	LC-QTOF/MS	LC-MS/MS
Bisphenol A-d16	0.2	0.05
Bisphenol A	0.2	0.05
Methyl paraben	0.1	0.01
Monobutyl phthalate	0.2	0.02
Perfluorooctanoic acid	0.25	0.02
4-Amino-2-nitrophenol	1	0.025

Table S2. Reproducibility of data collected from five consecutive test sample runs on the Agilent LC1260 -QTOF/MS 6550

Sample	% Similarity
1	74
2	90
3	85
4	82
5	87

Table S3. LC-MS/MS recoveries obtained for low and high concentrations of four representative analytes.

Compound	Recovery	
	Low Concentration (1 ng/mL)	High Concentration (40 ng/mL)
Bisphenol A-d16	80%	87%
Bisphenol A	82%	90%
Monobutyl phthalate	85%	90%
Perfluorooctanoic acid	82%	88%

Table S4. Detection frequencies of 282 environmental organic acids detected in 20 pregnant women sera

Compound Name	Formula	Chemical Class	Count
1,4-Dichlorobenzene metabolite or 2,3-Dichlorophenol or 2,4-Dichlorophenol or 2,5-Dichlorophenol or 2,6-Dichlorophenol or 3,4-Dichlorophenol	C6 H4 Cl2 O	Pesticide metabolite - phenol	20
1,4-Dichlorobenzene metabolite or 2,3-Dichlorophenol or 2,4-Dichlorophenol or 2,5-Dichlorophenol or 2,6-Dichlorophenol or 3,4-Dichlorophenol	C6 H4 Cl2 O	Pesticide metabolite - phenol	2
1,7-bis(4-Hydroxyphenylthio)-3,5-dioxaheptane	C17 H20 O4 S2	Phenol	1
2-(1,1-Dimethylethyl)phenol or 2-sec-Butylphenol or 4-Butylphenol or 4-sec-Butylphenol or 4-tert-Butylphenol	C10 H14 O	Phenol	17
2-(1,1-Dimethylethyl)phenol or 2-sec-Butylphenol or 4-Butylphenol or 4-sec-Butylphenol or 4-tert-Butylphenol	C10 H14 O	Phenol	13
2-(1,1-Dimethylethyl)phenol or 2-sec-Butylphenol or 4-Butylphenol or 4-sec-Butylphenol or 4-tert-Butylphenol	C10 H14 O	Phenol	4
2-(1,1-Dimethylethyl)phenol or 2-sec-Butylphenol or 4-Butylphenol or 4-sec-Butylphenol or 4-tert-Butylphenol	C10 H14 O	Phenol	2
2-(2H-benzotriazol-2-yl)-4,6-bis(1-	C30 H29 N3 O	Phenol	2

methyl-1-phenylethyl)phenol			
2-(N-ethylperfluorooctane sulfonamido) acetate (Et-PFOSA-AcOH)	C12 H8 F17 N O4 S	PFC	3
2-(N-methyl-perfluorooctane sulfonamido) acetate (Me-PFOSA-AcOH)	C11 H6 F17 N O4 S	PFC	11
2-Bromo-4-cyclohexylphenol	C12 H15 Br O	Phenol	1
2-Chloro-4-methylphenol or 4-Chloro-2-methylphenol or 4-Chloro-3-methylphenol	C7 H7 Cl O	Phenol	1
2-Chloro-4-methylphenol or 4-Chloro-2-methylphenol or 4-Chloro-3-methylphenol	C7 H7 Cl O	Phenol	1
2-Chlorophenol or 3-Chlorophenol or 4-Chlorophenol	C6 H5 Cl O	Phenol	7
2-Chlorophenol or 3-Chlorophenol or 4-Chlorophenol	C6 H5 Cl O	Phenol	2
2-Cyclohexylphenol or 4-Cyclohexylphenol	C12 H16 O	Phenol	20
2-Cyclohexylphenol or 4-Cyclohexylphenol	C12 H16 O	Phenol	13
2-Ethylphenol or 3-Ethylphenol or 4-Ethylphenol	C8 H10 O	Phenol	5
2-Ethylphenol or 3-Ethylphenol or 4-Ethylphenol	C8 H10 O	Phenol	1
2-Ethylphenol or 3-Ethylphenol or 4-Ethylphenol	C8 H10 O	Phenol	1
2-Hydroxy-4-methoxybenzophenone or PHBB	C14 H12 O3	Phenol	10
2-Hydroxy-4-methoxybenzophenone or PHBB	C14 H12 O3	Phenol	4
2-Isopropoxyphenol or 4-Propoxyphenol	C9 H12 O2	Phenol	17
2-Isopropoxyphenol or 4-Propoxyphenol	C9 H12 O2	Phenol	9
2-Methylphenol or 4-Methylphenol	C7 H8 O	Phenol	19
2-Methylphenol or 4-Methylphenol	C7 H8 O	Phenol	9

2-Phenylphenol or 3-Phenylphenol or 4-Phenylphenol or Biphenyl metabolite	C12 H10 O	Pesticide - phenolic	4
2-Phenylphenol or 3-Phenylphenol or 4-Phenylphenol or Biphenyl metabolite	C12 H10 O	Pesticide - phenolic	2
2-Phenylphenol or 3-Phenylphenol or 4-Phenylphenol or Biphenyl metabolite	C12 H10 O	Pesticide - phenolic	1
2-sec-Pentylphenol or 4- Isopentylphenol or 4-Pentylphenol or 4-sec-Pentylphenol or 4-tert-Pentylphenol	C11 H16 O	Phenol	19
2-sec-Pentylphenol or 4- Isopentylphenol or 4-Pentylphenol or 4-sec-Pentylphenol or 4-tert-Pentylphenol	C11 H16 O	Phenol	16
2-sec-Pentylphenol or 4- Isopentylphenol or 4-Pentylphenol or 4-sec-Pentylphenol or 4-tert-Pentylphenol	C11 H16 O	Phenol	15
2-sec-Pentylphenol or 4- Isopentylphenol or 4-Pentylphenol or 4-sec-Pentylphenol or 4-tert-Pentylphenol	C11 H16 O	Phenol	14
2-sec-Pentylphenol or 4- Isopentylphenol or 4-Pentylphenol or 4-sec-Pentylphenol or 4-tert-Pentylphenol	C11 H16 O	Phenol	14
2,3,4-Trichlorophenol or 2,3,6- Trichlorophenol or 2,4,5-Trichlorophenol or 2,4,6-Trichlorophenol	C6 H3 Cl3 O	Phenol	1
2,3,6-Trimethylphenol or 4- Propylphenol	C9 H12 O	Phenol	14
2,3,6-Trimethylphenol or 4- Propylphenol	C9 H12 O	Phenol	8

2,4-bis(1-Methyl-1-phenylethyl)phenol	C24 H26 O	Phenol	6
2,4-bis(1,1-Dimethylethyl)phenol or 2,6-bis(1,1-Dimethylethyl)phenol or 4-Octylphenol or 4-tert-Octylphenol	C14 H22 O	Phenol	20
2,4-bis(1,1-Dimethylethyl)phenol or 2,6-bis(1,1-Dimethylethyl)phenol or 4-Octylphenol or 4-tert-Octylphenol	C14 H22 O	Phenol	16
2,4-bis(1,1-Dimethylethyl)phenol or 2,6-bis(1,1-Dimethylethyl)phenol or 4-Octylphenol or 4-tert-Octylphenol	C14 H22 O	Phenol	16
2,4-bis(1,1-Dimethylethyl)phenol or 2,6-bis(1,1-Dimethylethyl)phenol or 4-Octylphenol or 4-tert-Octylphenol	C14 H22 O	Phenol	12
2,4-bis(1,1-Dimethylpropyl)phenol	C16 H26 O	Phenol	13
2,4-Dibromophenol	C6 H4 Br2 O	Phenol	3
2,4-Dihydroxyphenone or Methyl paraben or Phenoxyacetic acid	C8 H8 O3	Phenol	19
2,4-Dihydroxyphenone or Methyl paraben or Phenoxyacetic acid	C8 H8 O3	Phenol	15
2,4-Dihydroxyphenone or Methyl paraben or Phenoxyacetic acid	C8 H8 O3	Phenol	2
2,4-Dinitrophenol	C6 H4 N2 O5	Phenol	18
2,4,4'-Trichloro-2'-hydroxyphenyl ether or Hydroxy trichlorobiphenyl	C12 H7 Cl3 O2	Phenol	12
2,4,4'-Trichloro-2'-hydroxyphenyl ether or Hydroxy trichlorobiphenyl	C12 H7 Cl3 O2	Phenol	1
2,4,6-Tribromophenol	C6 H3 Br3 O	Phenol	2
2,4,6-tris(1,1-Dimethylethyl)phenol or 2,6-bis(1,1-Dimethylethyl)-4-(1-methylpropyl)phenol or 4-Dodecylphenol or 4-Isododecylphenol	C18 H30 O	Phenol	20
2,4'- Dichlorophenylmethane metabolite or 4,4-Dichlorophenylmethane metabolite	C13 H10 Cl2 O	Pesticide metabolite - phenol	1

or 4,4'-Dichlorophenylmethane metabolite			
2H-Perfluoro-2-decenoic acid (FOUEA)	C10 H2 F16 O2	PFC	2
2H-Perfluoro-2-octenoic acid FHUEA	C8 H2 F12 O2	PFC	1
3-Hydroxyphenone or 4-Hydroxyphenone	C8 H8 O2	Phenol	14
3-Hydroxyphenone or 4-Hydroxyphenone	C8 H8 O2	Phenol	8
3-Trifluoromethyl-4-nitrophenol	C7 H4 F3 N O3	Phenol	4
3,5-Di-tert-Butylsalicylic acid	C15 H22 O3	Phenol	20
4-(Imidazol-1-yl)phenol	C9 H8 N2 O	Phenol	4
4-(Phenylazo)phenol or Fenazox	C12 H10 N2 O	Phenol	1
4-Butoxyphenol	C10 H14 O2	Phenol	20
4-Chloro-3,5-dimethylphenol	C8 H9 Cl O	Phenol	1
4-Cyclopentylphenol	C11 H14 O	Phenol	19
4-Heptyloxyphenol	C13 H20 O2	Phenol	20
4-Hexyloxyphenol	C12 H18 O2	Phenol	20
4-Hexylphenol	C12 H18 O	Phenol	20
4-Hydroxycoumarin	C9 H6 O3	Phenol	5
4-Nitrophenol	C6 H5 N O3	Phenol	20
4-Nonylphenol or 4-tert-Nonylphenol	C15 H24 O	Phenol	17
4-Nonylphenol or 4-tert-Nonylphenol	C15 H24 O	Phenol	16
4-Pentyloxyphenol	C9 H13 N	Phenol	1
4-Phenethylphenol	C14 H14 O	Phenol	2
4-Phenoxyphenol or 4,4'-Biphenol	C12 H10 O2	Phenol	5
4-Phenoxyphenol or 4,4'-Biphenol	C12 H10 O2	Phenol	1
4,4'-(Octahydro-4,7-methano-5H-inden-5-ylidene) bisphenol	C22 H24 O2	Phenol	1
4,4'-butylidenebis[2-(1,1-dimethylethyl)-5-methylphenol]	C26 H38 O2	Phenol	3
4,4'-Cyclohexylidenebisphenol or	C18 H20 O2	Phenol	2

Bisphenol Z			
4,4'-Cyclohexylidenebisphenol or Bisphenol Z	C18 H20 O2	Phenol	1
4,4'-Ethylene diphenol	C14 H14 O2	Phenol	14
4,4'-Methylenebis(phenol) or Bisphenol F	C13 H12 O2	Phenol	3
4,4'-Methylenebis(phenol) or Bisphenol F	C13 H12 O2	Phenol	2
4,4'-Thiodiphenol	C12 H10 O2 S	Phenol	5
4,4'-Isopropylidenebis(2-phenylphenol) or Bisphenol PH	C27 H24 O2	Phenol	3
4,4'-Isopropylidenebis(2-phenylphenol) or Bisphenol PH	C27 H24 O2	Phenol	2
6:2 Fluorotelomer sulfonic acid (6:2 FTS)	C8 H5 F13 O3 S	PFC	3
Aclonifen metabolite	C12 H9 Cl N2 O4	Pesticide metabolite - phenol	4
Ancymidol metabolite	C15 H16 N2 O3	Pesticide metabolite - phenol	1
Azamethiphos metabolite	C9 H10 Cl N2 O6 P S	Pesticide metabolite - phenol	3
Bendiocarb metabolite or Dioxacarb metabolite	C11 H13 N O5	Pesticide metabolite - phenol	1
Bendiocarb metabolite or Dioxacarb metabolite	C11 H13 N O5	Pesticide metabolite - phenol	1
Benfuracarb metabolite	C20 H30 N2 O6 S	Pesticide metabolite - phenol	1
Benomyl metabolite	C14 H18 N4 O4	Pesticide metabolite - phenol	1
Bentazone artifact 2	C10 H14 N2 O2	Pesticide metabolite - phenol	1
Benzadox	C9 H9 N O4	Pesticide-acid	1
Benzophenone-1	C13 H10 O3	Phenol	6
Bioresmethrin metabolite or Resmethrin metabolite	C22 H26 O4	Pesticide metabolite - phenol	12
Bioresmethrin metabolite or Resmethrin metabolite	C22 H26 O4	Pesticide metabolite - phenol	2
Bisphenol A	C15 H16 O2	Phenol	19
Bisphenol A diglycidyl ether	C21 H26 O5	Phenol	1
Bisphenol A ethoxylate diacrylate	C25 H28 O6	Phenol	4
Bisphenol AF	C15 H10 F6 O2	Phenol	1
Bisphenol AP	C20 H18 O2	Phenol	5

Bisphenol BP	C25 H20 O2	Phenol	1
Bisphenol C	C17 H20 O2	Phenol	1
Bisphenol G	C21 H28 O2	Phenol	10
Bisphenol M or Bisphenol P	C24 H26 O2	Phenol	1
Bisphenol S	C12 H10 O4 S	Phenol	10
Bisphenol TMC	C21 H26 O2	Phenol	2
Bitertanol metabolite	C20 H23 N3 O3	Pesticide metabolite - phenol	7
Bromoxynil	C7 H3 Br2 N O	Pesticide - phenolic	14
BTUM	C27 H24 N4 O6 S2	Phenol	5
Butacarb metabolite	C16 H25 N O3	Pesticide metabolite - phenol	1
Butyl paraben	C11 H14 O3	Phenol	18
Butylated hydroxyanisole	C11 H16 O2	Phenol	20
Carbofuran (-C2H3NO) metabolite	C10 H12 O3	Pesticide metabolite - phenol	19
Carbofuran metabolite	C12 H15 N O4	Pesticide metabolite - phenol	13
Carbofuran or Eugenol	C10 H12 O2	Pesticide - phenolic	16
Carbofuran or Eugenol	C10 H12 O2	Pesticide - phenolic	6
Carbosulfan metabolite	C20 H32 N2 O4 S	Pesticide metabolite - phenol	2
Chlorbufam metabolite	C11 H10 Cl N O3	Pesticide metabolite - phenol	2
Chlordimeform metabolite	C10 H13 Cl N2 O	Pesticide metabolite - phenol	2
Chlorotoluron metabolite	C10 H13 Cl N2 O2	Pesticide metabolite - phenol	3
Chlorpropham metabolite	C10 H12 Cl N O3	Pesticide metabolite - phenol	6
Ciodrin metabolite	C14 H19 O7 P	Pesticide metabolite - phenol	5
Coumithoate metabolite	C17 H21 O6 P S		1
Cyphenothrin metabolite	C24 H25 N O4	Pesticide metabolite - phenol	1
D-8	C15 H16 O4 S	Phenol	11
Daidzein	C15 H10 O4	Phenol	5
DEET metabolite or Diethyltoluamide metabolite	C12 H17 N O2	Pesticide metabolite - phenol	4
Desmedipham metabolite or Phenmedipham metabolite	C16 H16 N2 O5	Pesticide metabolite - phenol	1
Desmedipham metabolite or Phenmedipham metabolite	C16 H16 N2 O5	Pesticide metabolite - phenol	1
Diazinon (Dimpylate) metabolite	C12 H21 N2 O4 P S	Pesticide metabolite - phenol	2

Dicamba or Dichlorophenoxyacetic acid	C8 H6 Cl2 O3	Pesticide-acid	1
Dichlobenil metabolite	C7 H3 Cl2 N O	Pesticide metabolite - phenol	9
Diethquinalphione metabolite or Phoxim metabolite or Quinalphos metabolite	C12 H15 N2 O4 P S	Pesticide metabolite - phenol	1
Difenoxuron metabolite	C16 H18 N2 O4	Pesticide metabolite - phenol	11
Difenzoquate metabolite	C17 H17 N2 O	Pesticide metabolite - phenol	1
Diflunisal	C14 H8 F2 O3	Phenol	1
Dinoseb or Dinoterb or Subitex	C10 H12 N2 O5	Pesticide - phenolic	18
Dinoseb or Dinoterb or Subitex	C10 H12 N2 O5	Pesticide - phenolic	7
Dinoseb or Dinoterb or Subitex	C10 H12 N2 O5	Pesticide - phenolic	1
Dinoseb-acetate metabolite	C12 H14 N2 O7	Pesticide metabolite - phenol	1
Dinoterb metabolite or Subitex metabolite	C10 H12 N2 O6	Pesticide metabolite - phenol	1
Dioxacarb artifact or Ethyl-p-hydroxybenzoate (Ethyl paraben)	C9 H10 O3	Phenol	17
Dioxacarb artifact or Ethyl-p-hydroxybenzoate (Ethyl paraben)	C9 H10 O3	Phenol	5
Diphenolic acid	C17 H18 O4	Phenol	9
DNOC (2,4-Dinitro-o-kresol)	C7 H6 N2 O5	Pesticide - phenolic	12
Enterodiol	C18 H22 O4	Phenol	18
Enterolactone	C18 H18 O4	Phenol	8
Equol	C15 H14 O3	Phenol	14
Estragole	C10 H12 O	Phenol	19
Estrone	C18 H22 O2	Phenol	19
Ethametsulfuron-methyl metabolite or Nicosulfuron metabolite	C15 H18 N6 O7 S	Pesticide metabolite - phenol	2
Ethofumesate metabolite	C13 H18 O6 S	Pesticide metabolite - phenol	12
Etrimfos metabolite	C10 H17 N2 O5 P S	Pesticide metabolite - phenol	2
Fenarimol metabolite	C17 H12 Cl2 N2 O2	Pesticide metabolite - phenol	2
Fenoxycarb metabolite or Furalaxyl metabolite	C17 H19 N O5	Pesticide metabolite - phenol	8

Fenoxycarb metabolite or Furalaxyl metabolite	C17 H19 N O5	Pesticide metabolite - phenol	4
Fenzaflor metabolite	C15 H7 Cl2 F3 N2 O3	Pesticide metabolite - phenol	1
Fluorotelomer hexanoic acid	C7 H3 F13 O2	PFC	4
Fluridone metabolite	C19 H14 F3 N O2		1
Fluvalinate metabolite	C26 H22 Cl F3 N2 O4	Pesticide metabolite - phenol	3
Foramsulfuron metabolite	C17 H20 N6 O8 S	Pesticide metabolite - phenol	4
Formetanate metabolite	C11 H15 N3 O3	Pesticide metabolite - phenol	15
Genistein	C15 H10 O5	Phenol	2
Glyphosate	C3 H8 N O5 P	Pesticide-acid	1
Hymecromone	C10 H8 O3	Pesticide - phenolic	2
Imazalil metabolite	C32 H40 N4 O7	Pesticide metabolite - phenol	3
Imazapyr or Pyrolan metabolite	C13 H15 N3 O3	Pesticide-acid	8
Imazapyr or Pyrolan metabolite	C13 H15 N3 O3	Pesticide-acid	6
Isofenphos metabolite	C15 H24 N O5 P S	Pesticide metabolite - phenol	1
Isoproturon metabolite	C12 H18 N2 O2	Pesticide metabolite - phenol	1
Isoxaben metabolite	C18 H24 N2 O5	Pesticide metabolite - phenol	5
Jasmolin I	C21 H30 O3	Pesticide-acid	8
Jasmolin II	C22 H30 O5	Pesticide-acid	7
Karbutilate metabolite	C14 H21 N3 O4	Pesticide metabolite - phenol	2
Kresoxim-methyl metabolite	C18 H19 N O5	Pesticide metabolite - phenol	4
Lambast metabolite	C12 H23 N5 O3 S	Pesticide metabolite - phenol	3
MBHA or O-Desmethylangolensin	C15 H14 O4	Phenol	3
MBHA or O-Desmethylangolensin	C15 H14 O4	Phenol	3
Medinoterbacetate metabolite	C13 H16 N2 O7	Pesticide metabolite - phenol	10
Metalaxyl metabolite	C15 H21 N O5	Pesticide metabolite - phenol	1
Methoxychlor (-HCl) metabolite	C16 H14 Cl2 O3	Pesticide metabolite - phenol	1
Methoxyphenone metabolite	C16 H16 O3	Pesticide metabolite - phenol	5
Methyl eugenol	C11 H14 O2	Phenol	14
Metsulfuron-methyl metabolite	C14 H15 N5 O7 S	Pesticide metabolite - phenol	1
MNFA metabolite metabolite	C13 H12 F N O2	Pesticide metabolite - phenol	5
Monalide metabolite or Pentanochlor metabolite	C13 H18 Cl N O2	Pesticide metabolite - phenol	1

Monalide metabolite or Pentanochlor metabolite	C13 H18 Cl N O2	Pesticide metabolite - phenol	1
Mono (2-carboxymethylhexyl) phthalate or Mono (2-ethyl-5-carboxypentyl) phthalate or Monocarboxyheptyl phthalate or Monocarboxyisoheptyl phthalate	C16 H20 O6	Phthalate metabolite	13
Mono (2-carboxymethylhexyl) phthalate or Mono (2-ethyl-5-carboxypentyl) phthalate or Monocarboxyheptyl phthalate or Monocarboxyisoheptyl phthalate	C16 H20 O6	Phthalate metabolite	6
Mono (2-ethyl-5-oxohexyl) phthalate	C16 H20 O5	Phthalate metabolite	12
Mono (2-ethylhexyl) phthalate or Monoisooctyl phthalate or Monooctyl phthalate	C16 H22 O4	Phthalate metabolite	18
Mono (2-ethylhexyl) phthalate or Monoisooctyl phthalate or Monooctyl phthalate	C16 H22 O4	Phthalate metabolite	16
Mono (2-ethylhexyl) phthalate or Monoisooctyl phthalate or Monooctyl phthalate	C16 H22 O4	Phthalate metabolite	8
Mono (2-ethylhydroxyhexyl) phthalate	C16 H22 O5	Phthalate metabolite	4
Mono (2-propylheptyl) phthalate or Monodecyl phthalate or Monoisodecyl phthalate	C18 H26 O4	Phthalate metabolite	16
Mono (2-propylheptyl) phthalate or Monodecyl phthalate or Monoisodecyl phthalate	C18 H26 O4	Phthalate metabolite	11
Mono (2-propylheptyl) phthalate or Monodecyl phthalate or Monoisodecyl phthalate	C18 H26 O4	Phthalate metabolite	8
Mono (4-methyl-7-carboxyheptyl)phthalate or Monocarboxyisooctyl phthalate	C17 H22 O6	Phthalate metabolite	6
Mono (4-methyl-7-carboxyheptyl)phthalate or Monocarboxyisooctyl phthalate	C17 H22 O6	Phthalate metabolite	5
Mono (4-methyl-7-oxo-octyl)phthalate or Monooxoisononyl	C17 H22 O5	Phthalate metabolite	6

phthalate			
Mono 3-carboxypropyl phthalate	C12 H12 O6	Phthalate metabolite	3
Monoallyl phthalate	C11 H10 O4	Phthalate metabolite	17
Monobenzyl phthalate	C15 H12 O4	Phthalate metabolite	3
Monobutyl phthalate or Monoisobutyl phthalate	C12 H14 O4	Phthalate metabolite	18
Monobutyl phthalate or Monoisobutyl phthalate	C12 H14 O4	Phthalate metabolite	5
Monocarboxyisononyl phthalate	C18 H24 O6	Phthalate metabolite	4
Monocyclohexyl phthalate	C14 H16 O4	Phthalate metabolite	5
Monoethyl phthalate	C10 H10 O4	Phthalate metabolite	1
Monoheptyl phthalate or Monoisoheptyl phthalate	C15 H20 O4	Phthalate metabolite	19
Monoheptyl phthalate or Monoisoheptyl phthalate	C15 H20 O4	Phthalate metabolite	15
Monohydroxyisononyl phthalate	C17 H24 O5	Phthalate metabolite	4
Monoisohexyl phthalate or Monohexyl phthalate	C14 H18 O4	Phthalate metabolite	19
Monoisohexyl phthalate or Monohexyl phthalate	C14 H18 O4	Phthalate metabolite	16
Monoisononyl phthalate	C17 H24 O4	Phthalate metabolite	15
Monoisotridecyl phthalate	C21 H32 O4	Phthalate metabolite	19
Monoisoundecyl phthalate or Monoundecyl phthalate	C19 H28 O4	Phthalate metabolite	18
Monopentyl phthalate	C13 H16 O4	Phthalate metabolite	4
Monopropyl phthalate	C11 H12 O4	Phthalate metabolite	7
Myclobutanil metabolite	C15 H17 Cl N4 O	Pesticide metabolite - phenol	6
Naphthoxyacetic acid	C12 H10 O3	Pesticide-acid	3
Nitraline metabolite	C13 H19 N3 O7 S		1
Nitrofen metabolite	C12 H7 Cl2 N O4	Pesticide metabolite - phenol	2
Nonylphenol diethoxylate	C19 H32 O3	Phenol	18
Nonylphenol monoethoxylate	C17 H28 O2	Phenol	20
Nuarimol metabolite	C17 H12 Cl F N2 O2	Pesticide metabolite - phenol	3
Octylphenol diethoxylate	C18 H30 O3	Phenol	20

Octylphenol monoethoxylate	C16 H26 O2	Phenol	20
Oryzalin metabolite	C12 H18 N4 O7 S	Pesticide metabolite - phenol	2
Oxadixyl metabolite	C14 H18 N2 O5	Pesticide metabolite - phenol	8
Oxycarboxin metabolite	C12 H13 N O5 S	Pesticide metabolite - phenol	1
paraquat metabolite	C12 H14 N2 O	Pesticide metabolite - phenol	4
Parathion metabolite	C10 H14 N O6 P S	Pesticide metabolite - phenol	1
Pentachlorophenol	C6 H Cl5 O	Phenol	16
Perfluoro-3,7-bis(trifluoromethyl)- octanoic acid or Perfluorodecanoic acid	C10 H F19 O2	PFC	15
Perfluorodecane sulfonic acid	C10 H F21 O3 S	PFC	2
Perfluorodecyl ethanoic acid	C12 H3 F21 O2	PFC	17
Perfluoroheptadecanoic acid (PFHpDA)	C17 H F33 O2	PFC	3
Perfluoroheptane sulfonic acid	C7 H F15 O3 S	PFC	19
Perfluoroheptanoic acid	C7 H F13 O2	PFC	5
Perfluorohexanesulfonic acid	C6 H F13 O3 S	PFC	19
Perfluorohexyl ethanoic acid	C8 H3 F13 O2	PFC	7
Perfluorononanoic acid	C9 H F17 O2	PFC	20
Perfluorooctane sulfonic acid	C8 H F17 O3 S	PFC	20
Perfluorooctanoic acid	C8 H F15 O2	PFC	18
Perfluorooctyl ethanoic acid	C10 H3 F17 O2	PFC	4
Perfluoropentane sulfonic acid (PFPS)	C5 H F11 O3 S	PFC	4
Perfluoropentanoic acid	C5 H F9 O2	PFC	13
Perfluorotridecanoic acid	C13 H F25 O2	PFC	4
Perfluoroundecanoic acid	C11 H F21 O2	PFC	6
Phenol red	C19 H14 O5 S	Phenol	1
Phenol, styrenated	C10 H10 O	Phenol	5
Phenothrin metabolite	C23 H26 O4	Pesticide metabolite - phenol	4
Phenyl isocyanate metabolite	C7 H5 N O2	Pesticide metabolite - phenol	9
Phosmet metabolite	C11 H12 N O5 P S2	Pesticide metabolite - phenol	2
Primisulfuron-methyl metabolite	C15 H12 F4 N4 O8 S	Pesticide metabolite - phenol	2

Prodiamine metabolite	C13 H17 F3 N4 O5	Pesticide metabolite - phenol	18
Promecarb metabolite	C12 H17 N O3	Pesticide metabolite - phenol	20
Propargite metabolite	C19 H26 O5 S	Pesticide metabolite - phenol	15
Propham metabolite	C10 H13 N O3	Pesticide metabolite - phenol	20
Propiconazole metabolite	C15 H17 Cl2 N3 O3	Pesticide metabolite - phenol	3
Prosulfocarb metabolite	C14 H21 N O2 S	Pesticide metabolite - phenol	8
Prosulfuron metabolite	C15 H16 F3 N5 O5 S	Pesticide metabolite - phenol	2
Proximpham metabolite	C10 H12 N2 O3	Pesticide metabolite - phenol	1
Pyracarbolid metabolite	C13 H15 N O3	Pesticide metabolite - phenol	3
Pyrethrin II	C22 H28 O5	Pesticide-acid	15
Pyrocatechol	C6 H6 O2	Pesticide - phenolic	20
Quinoamide metabolite	C12 H6 Cl3 N O4	Pesticide metabolite - phenol	4
Quintiofos metabolite	C17 H16 N O3 P S	Pesticide metabolite - phenol	1
Siduron metabolite	C14 H20 N2 O2	Pesticide metabolite - phenol	4
Sorbic acid	C6 H8 O2		1
Tebutam metabolite	C15 H23 N O2	Pesticide metabolite - phenol	1
Tecnazene metabolite	C6 H Cl4 N O3	Pesticide metabolite - phenol	3
Tralkoxydime metabolite	C20 H27 N O4		1
trans-Methacrifos	C7 H13 O5 P S	Pesticide-acid	1
Trichlophenidine metabolite	C16 H13 Cl5 N2 O	Pesticide metabolite - phenol	1
Triclocarban	C13 H9 Cl3 N2 O	Phenol	1
Tricyclazole metabolite	C9 H7 N3 O S	Pesticide metabolite - phenol	1
Trifloxystrobin metabolite	C20 H19 F3 N2 O5	Pesticide metabolite - phenol	9
Trimethacarb metabolite	C11 H15 N O3	Pesticide metabolite - phenol	1

Figure S1. Comparison of the number of EOA hits obtained from two different methods of sample preparation: protein precipitation (PP) (n=110) and solid phase extraction (SPE) (n=135)

