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## Volume One

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- 19 Acrylamide  
CAS No. 79-06-1
- 20 Glycidamide  
CAS No. 486-56-6

### Tobacco Smoke

- 21 Cotinine  
CAS No. 486-56-6
- 24 Hydroxycotinine
- 25 NNAL  
CAS No. 76014-81-8

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- 29 Bromodichloromethane  
CAS No. 75-27-4
- 31 Dibromochloromethane (Chlorodibromomethane)  
CAS No. 124-48-1
- 33 Tribromomethane (Bromoform)  
CAS No. 75-25-2
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CAS No. 67-66-3

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- 37 Benzophenone-3  
CAS No. 131-57-7
- 41 Bisphenol A  
CAS No. 80-05-7
- 45 Bisphenol F
- 47 Bisphenol S
- 49 4-*tert*-Octylphenol  
CAS No. 140-66-9
- 51 Triclocarban  
CAS No. 101-20-2
- 53 Triclosan  
CAS No. 3380-34-5
- 57 Butyl paraben  
CAS No. 94-26-8

- 61 Ethyl paraben  
CAS No. 120-47-8
- 65 Methyl paraben  
CAS No. 99-76-3
- 69 *n*-Propyl paraben  
CAS No. 94-13-3
- 73 2,4-Dichlorophenol  
CAS No. 120-83-2
- 77 2,5-Dichlorophenol  
CAS No. 583-78-8

#### Flame Retardant Metabolites

- 81 Bis(1-chloro-2-propyl) phosphate (BCPP)
- 83 Bis(2-chloroethyl) phosphate (BCEtP)
- 85 Bis(1,3-dichloro-2-propyl) phosphate (BDCPP)
- 87 Dibenzyl phosphate (DBzP)
- 89 Dibutyl phosphate (DBuP)
- 91 Di-*o*-cresylphosphate (DoCP)
- 93 Di-*p*-cresylphosphate (DpCP)
- 95 Diphenyl phosphate (DPhP)
- 97 2,3,4,5-Tetrabromobenzoic acid (TBBA)

#### Fungicides and Metabolites

- 99 *ortho*-Phenylphenol  
CAS No. 90-43-7
- 101 Ethylene thiourea  
CAS No. 96-45-7
- 103 Pentachlorophenol  
CAS No. 87-86-5
- 105 Propylene thiourea  
CAS No. 2122-19-2

#### Herbicides and Metabolites

- 107 Atrazine  
CAS No. 1912-24-9
- 109 Atrazine mercapturate  
CAS No. 138722-96-0
- 111 Desethyl atrazine  
CAS No. 6190-65-4
- 113 Desisopropyl atrazine  
CAS No. 1007-28-9
- 115 Desisopropyl atrazine mercapturate  
CAS No. 1007-28-9
- 117 Diaminochlorotriazine
- 119 2,4-Dichlorophenoxyacetic acid  
CAS No. 94-75-7
- 123 2,4,5-Trichlorophenoxyacetic acid  
CAS No. 93-76-5

#### Sulfonyl Urea Herbicides

- 127 Bensulfuron-methyl  
CAS No. 83055-99-6

- 129 Chlorsulfuron  
CAS No. 64902-72-3
- 131 Ethametsulfuron-methyl  
CAS No. 97780-06-8
- 133 Foramsulfuron  
CAS No. 173159-57-4
- 135 Halosulfuron  
CAS No. 135397-30-7
- 137 Mesosulfuron-methyl  
CAS No. 208465-21-8
- 139 Metsulfuron-methyl  
CAS No. 74223-64-6
- 141 Nicosulfuron  
CAS No. 111991-09-4
- 143 Oxasulfuron  
CAS No. 144651-06-9
- 145 Primisulfuron-methyl  
CAS No. 86209-51-0
- 147 Prosulfuron  
CAS No. 94125-34-5
- 149 Rimsulfuron  
CAS No. 122931-48-0
- 151 Sulfometuron-methyl  
CAS No. 74222-97-2
- 153 Sulfosulfuron  
CAS No. 141776-32-1
- 155 Thifensulfuron-methyl  
CAS No. 79277-27-3
- 157 Triasulfuron  
CAS No. 82097-50-5
- 159 Triflurosulfuron-methyl  
CAS No. 126535-15-7

#### **Insect Repellent and Metabolites**

- 161 N,N-Diethyl-*meta*-toluamide (DEET)  
CAS No. 134-62-3
- 165 3-(Diethylcarbamoyl) benzoic acid (DCBA)  
CAS No. 858981-15-4
- 169 N,N-Diethyl-3-(hydroxymethyl) benzamide (DHMB)  
CAS No. 72236-22-7

#### **Carbamate Pesticide Metabolites**

- 173 Carbofuranphenol  
CAS No. 1563-38-8
- 175 2-Isopropoxyphenol  
CAS No. 4812-20-8

#### **Organochlorine Pesticide Metabolites**

- 177 2,4,5-Trichlorophenol  
CAS No. 95-95-4
- 179 2,4,6-Trichlorophenol  
CAS No. 88-06-2

### Organophosphorus Insecticides: Specific Metabolites

- 181 Acephate  
CAS No. 30560-19-1
- 183 Dimethoate  
CAS No. 60-51-5
- 185 Methamidophos  
CAS No. 10265-92-6
- 187 Omethoate  
CAS No. 1113-02-6
- 189 Malathion dicarboxylic acid  
CAS No. 1190-28-9
- 191 2-Isopropyl-4-methyl-pyrimidinol  
CAS No. 2814-20-2
- 193 *para*-Nitrophenol  
CAS No. 100-02-7
- 195 3,5,6-Trichlor-2-pyridinol  
CAS No. 6515-38-4

### Organophosphorus Insecticides: Dialkyl Phosphate Metabolites

- 197 Diethylphosphate (DEP)  
CAS No. 598-02-7
- 201 Dimethylphosphate (DMP)  
CAS No. 813-78-5
- 205 Diethylthiophosphate (DETP)  
CAS No. 5871-17-0
- 209 Dimethylthiophosphate (DMTP)  
CAS No. 59401-04-6
- 213 Diethyldithiophosphate (DEDTP)  
CAS No. 298-06-6
- 217 Dimethyldithiophosphate (DMDTP)  
CAS No. 756-80-9

### Pyrethroid Metabolites

- 221 *trans*-3-(2,2-Dichlorovinyl)-2,2-dimethylcyclopropane carboxylic acid  
CAS No. 55701-05-8
- 225 *cis*-3-(2,2-Dibromovinyl)-2,2dimethylcyclopropane carboxylic acid
- 227 4-Fluoro-3-phenoxybenzoic acid  
CAS No. 77279-89-1
- 229 3-Phenoxybenzoic acid  
CAS No. 3739-38-6

### Metals and Metalloids

- 231 Antimony  
CAS No. 7440-36-0
- 237 Arsenic, Total  
CAS No. 7440-38-2
- 241 Inorganic-related Arsenic Species
- 245 Arsenic (V) acid
- 249 Arsenobetaine  
CAS No. 64436-13-1
- 253 Arsenocholine  
CAS No. 96055-45-7
- 257 Arsenous (III) acid  
CAS No. 13464-58-9

- 261 Dimethylarsinic acid  
CAS No. 917-76-0
- 265 Monomethylarsonic acid  
CAS No. 65513-69-1
- 269 Trimethylarsine oxide  
CAS No. 4964-14-1
- 273 Barium  
CAS No. 81-25-4
- 279 Beryllium  
CAS No. 7440-41-7
- 283 Cadmium  
CAS No. 81271-94-5
- 292 Cesium  
CAS No. 7440-46-2
- 298 Chromium
- 299 Cobalt
- 306 Copper  
CAS No. 7440-50-8
- 307 Lead  
CAS No. 7439-92-1
- 316 Manganese  
CAS No. 8075-39-6
- 319 Mercury  
CAS No. 92786-62-4
- 330 Molybdenum  
CAS No. 7439-98-7
- 336 Platinum  
CAS No. 7740-106-4
- 340 Selenium  
CAS No. 7782-49-2
- 342 Strontium  
CAS No. 7440-24-6
- 344 Thallium  
CAS No. 7440-28-0
- 350 Tin  
CAS No. 7440-31-5
- 352 Tungsten  
CAS No. 7440-33-7
- 358 Uranium  
CAS No. 7440-61-1
- 364 Zinc  
CAS No. 7440-66-6

#### **Perchlorate and Other Anions**

- 365 Nitrate  
CAS No. 84145-82-4
- 369 Perchlorate  
CAS No. 14797-73-0
- 375 Thiocyanate  
CAS No. 302-04-5

#### **Perfluoroalkyl and Polyfluoroalkyl Substances: Surfactants**

- 379 Perfluorobutane sulfonic acid (PFBS)  
CAS No. 375-73-5

- 383 Perfluorodecanoic acid (PFDA)  
CAS No. 335-76-2
- 387 Perfluorododecanoic acid (PFDoA)  
CAS No. 307-55-1
- 391 Perfluoroheptanoic acid (PFHpA)  
CAS No. 375-85-9
- 395 Perfluorohexane sulfonic acid (PFHxS)  
CAS No. 355-46-4
- 399 Perfluorononanoic acid (PFNA)  
CAS No. 375-95-1
- 403 Perfluorooctanoic acid (PFOA)  
CAS No. 335-67-1
- 407 *n*-Perfluorooctanoic acid (*n*-PFOA)
- 409 Branched Perfluorooctanoic isomers (Sb-PFOA)
- 411 Perfluorooctane sulfonic acid (PFOS)  
CAS No. 1763-23-1
- 415 *n*-Perfluorooctane sulfonic acid (*n*-PFOS)
- 417 Perfluoromethylheptane sulfonic acid isomers (Sm-PFOS)
- 419 Perfluorooctane sulfonamide (PFOSA or FOSA)  
CAS No. 754-91-6
- 423 2-(*N*-Ethyl-perfluorooctane sulfonamido) acetic acid (EtFOSAA)  
CAS No. 2991-50-6
- 427 2-(*N*-Methyl-perfluorooctane sulfonamido) acetic acid (MeFOSAA)  
CAS No. 2355-31-9
- 431 Perfluoroundecanoic acid (PFUnDA)  
CAS No. 2058-94-8

#### Phthalate and Phthalate Alternative Metabolites

- 435 Mono-benzyl phthalate (MBzP)  
CAS No. 2528-16-7
- 441 Mono-3-hydroxybutyl phthalate (MHBP)
- 443 Mono-*n*-butyl phthalate (MnBP)  
CAS No. 131-70-4
- 449 Mono-isobutyl phthalate (MiBP)  
CAS No. 30833-53-5
- 455 Mono-2-methyl-2-hydroxypropyl phthalate (MHiBP)
- 457 Mono-cyclohexyl phthalate (MCHP)  
CAS No. 7517-36-4
- 461 Mono-ethyl phthalate (MEP)  
CAS No. 863029-89-4
- 467 Mono-2-ethylhexyl phthalate (MEHP)  
CAS No. 4376-20-9
- 473 Mono-(2-ethyl-5-hydroxyhexyl) phthalate (MEHHP)  
CAS No. 40321-99-1
- 479 Mono-(2-ethyl-5-oxohexyl) phthalate (MEOHP)  
CAS No. 40321-98-0
- 485 Mono-(2-ethyl-5-carboxypentyl) phthalate (MECPP)  
CAS No. 40809-41-4
- 489 Mono-(carboxynonyl) phthalate (MCNP)  
CAS No. 1373125-93-9
- 493 Mono-isononyl phthalate (MiNP)  
CAS No. 297182-83-3

- 499 Mono-(carboxyoctyl) phthalate (MCOP)  
CAS No. Di-isononyl phthalate (DNP)
- 503 Mono-methyl phthalate (MMP)  
CAS No. 4376-18-5
- 509 Mono-(3-carboxypropyl) phthalate (MCP)P  
CAS No. 66851-46-5
- 515 Mono-*n*-octyl phthalate (MOP)  
CAS No. 5393-19-1
- 519 Cyclohexane-1,2-dicarboxylic acid mono(hydroxy-isononyl ester) (MHNCH)

#### Phytoestrogens and Metabolites

- 521 Daidzein  
CAS No. 486-66-8
- 525 Enterodiol  
CAS No. 80226-00-2
- 529 Enterolactone  
CAS No. 77756-20-8
- 533 Equol  
CAS No. 531-95-3
- 537 Genistein  
CAS No. 446-72-0
- 541 O-Desmethylangolensin  
CAS No. 21255-69-6

#### Polycyclic Aromatic Hydrocarbon Metabolites

- 545 2-Hydroxyfluorene  
CAS No. 2443-58-5
- 551 3-Hydroxyfluorene  
CAS No. 6344-67-8
- 557 9-Hydroxyfluorene  
CAS No. 1689-64-1
- 563 1-Hydroxyphenanthrene  
CAS No. 2433-56-9
- 569 2-Hydroxyphenanthrene  
CAS No. 605-55-0
- 575 3-Hydroxyphenanthrene  
CAS No. 605-87-8
- 581 2 + 3-Hydroxyphenanthrene
- 583 4-Hydroxyphenanthrene  
CAS No. 7657-86-7
- 587 1-Hydroxypyrene  
CAS No. 5315-79-7
- 593 1-Hydroxynaphthalene (1-Naphthol)  
CAS No. 90-15-3
- 599 2-Hydroxynaphthalene (2-Naphthol)  
CAS No. 135-19-3

#### Heterocyclic Amines

- 605 3-Amino-1,4-dimethyl-5H-pyrido[4,3-b]indole (Trp-P-1)
- 607 2-Amino-3-methyl-9H-pyrido[2,3-b]indole (MeA- $\alpha$ -C)
- 609 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (Ph1P)
- 611 2-Amino-9H-pyrido[2,3-b]indole (A- $\alpha$ -C)

- 613 2-Amino-3-methylimidazo[4,5-f]quinoline (IQ)
- 615 2-Amino-6-methyldipyrido[1,2-a:3',2'-d]imidazole (Glu-P1)
- 617 2-Aminodipyrido[1,2-a:3',2'-d]imidazole (GLU-P2)
- 619 Harman
- 621 1-Methyl-3-amino-5H-pyrido[4,3-b]indole (Trp-P-2)
- 623 Norharman

#### **Volatile Organic Compounds (VOCs)**

- 625 1,1,1-Trichloroethane (Methyl chloroform)  
CAS No. 71-55-6
- 627 1,1,1,2-Tetrachloroethane  
CAS No. 79-34-5
- 629 1,1,2,2-Tetrachloroethane  
CAS No. 79-34-5
- 631 1,1,2-Trichloroethane  
CAS No. 79-00-5
- 633 1,2,3-Trichloropropane  
CAS No. 96-18-4
- 635 1,1-Dichloroethane  
CAS No. 75-34-3
- 637 1,1-Dichloroethene (Vinylidene chloride)  
CAS No. 75-34-3
- 639 1,2-Dibromo-3-chloropropane (DBCP)  
CAS No. 96-12-8
- 640 1,2-Dibromoethane  
CAS No. 106-93-4
- 642 1,2-Dichlorobenzene (*o*-Dichlorobenzene)  
CAS No. 95-50-1
- 644 1,2-Dichloroethane (Ethylene dichloride)  
CAS No. 107-06-2
- 646 *cis*-1,2-Dichloroethene  
CAS No. 156-59-2
- 648 *trans*-1,2-Dichloroethene  
CAS No. 156-60-5
- 650 1,2-Dichloropropane  
CAS No. 78-87-5
- 652 1,3-Dichlorobenzene (*m*-Dichlorobenzene)  
CAS No. 95-50-1
- 654 1,4-Dichlorobenzene (Paradichlorobenzene)  
CAS No. 106-46-7
- 656 1,4-Dioxane
- 658 2,5-Dimethylfuran  
CAS No. 625-86-5
- 660 Benzene  
CAS No. 71-43-2
- 662 Chlorobenzene (Monochlorobenzene)  
CAS No. 108-90-7
- 664 Chloroethane
- 665 Cyclohexane
- 666 Dibromomethane  
CAS No. 74-95-3



- 668 Dichloromethane (Methylene chloride)  
CAS No. 75-09-2
- 670 Ethyl acetate
- 671 Diethylether
- 672 Ethylbenzene  
CAS No. 100-41-4
- 674 Furan  
CAS No. 110-00-9
- 676 Heptane
- 677 Hexachloroethane  
CAS No. 67-72-1
- 679 Hexane
- 681 Isopropylbenzene (Cumene)  
CAS No. 98-82-8
- 683 Methyl-*tert*-butyl ether (MTBE)  
CAS No. 1634-04-4
- 685 Methylcyclopentane
- 686 Nitrobenzene  
CAS No. 98-95-3
- 688 Nitromethane  
CAS No. 75-52-5
- 689 Octane
- 690 Styrene  
CAS No. 100-42-5
- 691 Tetrachloroethene (Perchloroethylene)  
CAS No. 127-18-4
- 693 Tetrachloromethane (Carbon tetrachloride)  
CAS No. 56-23-5
- 695 Tetrahydrofuran
- 696 Toluene  
CAS No. 108-88-3
- 698 Trichloroethene (Trichloroethylene)  
CAS No. 79-01-6
- 700  $\alpha\alpha\alpha$ -Trifluorotoluene
- 701 Vinyl bromide
- 702 *m*-/*p*-Xylene  
CAS No. 108-38-3/106-42-3
- 704 *o*-Xylene  
CAS No. 95-47-6

#### **Volatile Organic Compound (VOC) Metabolites**

- 706 N-Acetyl-S-(2-carboxyethyl)-L-cysteine  
CAS No. 51868-61-2
- 710 N-Acetyl-S-(3-hydroxypropyl)-L-cysteine  
CAS No. 23127-40-4
- 714 N-Acetyl-S-(2-carbamoyl-ethyl)-L-cysteine  
CAS No. 81690-92-8
- 718 N-Acetyl-S-(2-carbamoyl-2-hydroxyethyl)-L-cysteine
- 722 N-Acetyl-S-(2-cyanoethyl)-L-cysteine  
CAS No. 74514-75-3
- 726 N-Acetyl-S-(2-hydroxyethyl)-L-cysteine  
CAS No. 15060-26-1

- 730 N-Acetyl-S-(phenyl)-L-cysteine  
CAS No. 4775-80-8
- 734 N-Acetyl-S-(*n*-propyl)-L-cysteine
- 738 N-Acetyl-S-(3,4-dihydroxybutyl)-L-cysteine  
CAS No. 144889-50-9
- 742 N-Acetyl-S-(1-hydroxymethyl-2-propenyl)-L-cysteine
- 746 N-Acetyl-S-(2-hydroxy-3-butenyl)-L-cysteine  
CAS No. 159092-64-5
- 750 N-Acetyl-S-(4-hydroxy-2-butenyl)-L-cysteine  
CAS No. 159092-65-6
- 754 2-Thioxothiazolidine-4-carboxylic acid  
CAS No. 20933-67-9
- 758 N-Acetyl-S-(3-hydroxypropyl-1-methyl)-L-cysteine  
CAS No. 33164-70-4
- 762 2-Aminothiazoline-4-carboxylic acid  
CAS No. 40283-41-8
- 766 N-Acetyl-S-(N-methylcarbamoyl)-L-cysteine  
CAS No. 103974-29-4
- 770 Phenylglyoxylic acid  
CAS No. 611-73-4
- 774 N-Acetyl-S-(2-hydroxypropyl)-L-cysteine  
CAS No. 923-43-3
- 778 N-Acetyl-S-(phenyl-2-hydroxyethyl)-L-cysteine
- 782 Mandelic acid  
CAS No. 90-64-2, 611-71-2 (R), 17199-29-0 (S)
- 786 N-Acetyl-S-(trichlorovinyl)-L-cysteine  
CAS No. 111348-61-9
- 790 N-Acetyl-S-(benzyl)-L-cysteine  
CAS No. 19542-77-9
- 794 N-Acetyl-S-(1,2-dichlorovinyl)-L-cysteine  
CAS No. 2148-31-4
- 798 N-Acetyl-S-(2,2-dichlorovinyl)-L-cysteine  
CAS No. 126543-43-9
- 802 N-Acetyl-S-(dimethylphenyl)-L-cysteine
- 806 2-Methylhippuric acid  
CAS No. 42013-20-7
- 810 3- and 4-Methylhippuric acid  
CAS No. 27115-49-7, 27115-50-0

## Appendices

- 814 Appendix A
- 818 Appendix C
- 833 Appendix D

## Volume Two

### *Special Analysis of Pooled Samples for Select Chemicals*

- 1 Special Analysis of Pooled Samples for Select Chemicals

### Organochlorine Pesticides and Metabolites (Pooled Samples after 2004)

- 3 Aldrin  
CAS No. 309-00-2
- 5 Dieldrin  
CAS No. 60-57-1
- 7 Endrin  
CAS No. 72-20-8
- 9 Heptachlor epoxide  
CAS No. 1024-57-3
- 11 Oxychlordan  
CAS No. 27304-13-8
- 19 *trans*-Nonachlor  
CAS No. 39765-80-5
- 27 *p,p'*-DDT  
CAS No. 50-29-3
- 35 *p,p'*-DDE  
CAS No. 72-55-9
- 43 *o,p'*-DDT
- 45 Hexachlorobenzene  
CAS No. 118-74-1
- 53 *beta*-Hexachlorocyclohexane  
CAS No. 319-85-7
- 61 *gamma*-Hexachlorocyclohexane
- 69 Mirex  
CAS No. 2385-85-5

### Polybrominated Diphenyl Ethers and PBB 153 (Pooled Samples after 2004)

- 79 2,2',4'-Tribromodiphenyl ether (BDE 17)  
CAS No. 147217-75-2
- 83 2,4,4'-Tribromodiphenyl ether (BDE 28)  
CAS No. 41318-75-6
- 87 2,2',4,4'-Tetrabromodiphenyl ether (BDE 47)  
CAS No. 5436-43-1
- 91 2,3',4,4'-Tetrabromodiphenyl ether (BDE 66)  
CAS No. 189084-61-5
- 95 2,2',3,4,4'-Pentabromodiphenyl ether (BDE 85)  
CAS No. 182346-21-0
- 99 2,2',4,4',5-Pentabromodiphenyl ether (BDE 99)  
CAS No. 60328-60-9
- 103 2,2',4,4',6-Pentabromodiphenyl ether (BDE 100)  
CAS No. 189084-64-8
- 107 2,2',4,4',5,5'-Hexabromodiphenyl ether (BDE 153)  
CAS No. 68631-49-2
- 111 2,2',4,4',5,6'-Hexabromodiphenyl ether (BDE 154)  
CAS No. 207122-15-4
- 115 2,2',3,4,4',5,6'-Heptabromodiphenyl ether (BDE 183)  
CAS No. 207122-16-5
- 119 2,2',3,3',4,4',5,5',6,6'-Decabromodiphenyl ether (BDE 209)  
CAS No. 1163-19-5
- 122 2,2',4,4',5,5'-Hexabromobiphenyl (PBB 153)  
CAS No. 59080-40-9

### Polychlorinated Dibenzo-*p*-dioxins (Pooled Samples after 2004)

- 126 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin (HpCDD)

- 134 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin (HxCDD)  
CAS No. 39227-28-6
- 142 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin (HxCDD)  
CAS No. 57653-85-7
- 150 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin (HxCDD)  
CAS No. 19408-74-3
- 158 1,2,3,4,6,7,8,9-Octachlorodibenzo-*p*-dioxin (OCDD)  
CAS No. 3268-87-9
- 166 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin (PeCDD)  
CAS No. 40321-76-4
- 174 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin (TCDD)  
CAS No. 1746-01-6

#### Polychlorinated Dibenzofurans (Pooled Samples after 2004)

- 182 1,2,3,4,6,7,8-Heptachlorodibenzofuran (HpCDF)  
CAS No. 67562-39-4
- 190 1,2,3,4,7,8,9-Heptachlorodibenzofuran (HpCDF)  
CAS No. 55673-89-7
- 198 1,2,3,4,7,8-Hexachlorodibenzofuran (HxCDF)  
CAS No. 70648-26-9
- 206 1,2,3,6,7,8-Hexachlorodibenzofuran (HxCDF)  
CAS No. 57117-44-9
- 214 1,2,3,7,8,9-Hexachlorodibenzofuran (HxCDF)  
CAS No. 72918-21-9
- 222 2,3,4,6,7,8-Hexachlorodibenzofuran (HxCDF)  
CAS No. 60851-34-5
- 230 1,2,3,4,6,7,8,9-Octachlorodibenzofuran (OCDF)  
CAS No. 39001-02-0
- 238 1,2,3,7,8-Pentachlorodibenzofuran (PeCDF)  
CAS No. 57117-41-6
- 246 2,3,4,7,8-Pentachlorodibenzofuran (PeCDF)  
CAS No. 57117-31-4
- 254 2,3,7,8-Tetrachlorodibenzofuran (TCDF)  
CAS No. 51207-31-9

#### Dioxin-like Polychlorinated Biphenyls: coplanar PCBs (Pooled Samples after 2004)

- 262 3,4,4',5'-Tetrachlorobiphenyl (PCB 81)  
CAS No. 70362-50-4
- 270 3,3',4,4',5'-Pentachlorobiphenyl (PCB 126)  
CAS No. 57465-28-8
- 278 3,3',4,4',5,5'-Hexachlorobiphenyl (PCB 169)  
CAS No. 32774-16-6

#### Dioxin-like Polychlorinated Biphenyls: mono-*ortho*-substituted PCBs (Pooled Samples after 2004)

- 286 2,3,3',4,4'-Pentachlorobiphenyl (PCB 105)  
CAS No. 32598-14-4
- 294 2,3,3',4,4'-Pentachlorobiphenyl (PCB 114)  
CAS No. 74472-37-0
- 300 2,3',4,4',5-Pentachlorobiphenyl (PCB 118)  
CAS No. 31508-00-6
- 308 2',3,4,4',5-Pentachlorobiphenyl (PCB 123)  
CAS No. 65510-44-3
- 312 2,3,3',4,4',5-Hexachlorobiphenyl (PCB 156)  
CAS No. 38380-08-4

- 320 2,3,3',4,4',5'-Hexachlorobiphenyl (PCB 157)  
CAS No. 69782-90-7
- 328 2,3',4,4',5,5'-Hexachlorobiphenyl (PCB 167)  
CAS No. 52663-72-6
- 336 2,3,3',4,4',5,5'-Heptachlorobiphenyl (PCB 189)  
CAS No. 39635-31-9

**Polychlorinated Biphenyls: Non-Dioxin-Like (Pooled Samples after 2004)**

- 344 2,4,4'-Trichlorobiphenyl (PCB 28)  
CAS No. 7012-37-5
- 352 2,2',3,5'-Tetrachloro biphenyl (PCB 44)  
CAS No. 41464-39-5
- 358 2,2',4,5'-Tetrachloro biphenyl (PCB 49)  
CAS No. 41464-40-8
- 364 2,2',5,5'-Tetrachlorobiphenyl (PCB 52)  
CAS No. 35693-99-3
- 370 2,3',4,4'-Tetrachlorobiphenyl (PCB 66)  
CAS No. 33025-41-1
- 378 2,4,4',5-Tetrachlorobiphenyl (PCB 74)  
CAS No. 32690-93-0
- 386 2,2',3,4,5'-Pentachlorobiphenyl (PCB 87)  
CAS No. 41464-51-1
- 392 2,2',4,4',5-Pentachlorobiphenyl (PCB 99)  
CAS No. 38380-02-8
- 400 2,2',4,5,5'-Pentachlorobiphenyl (PCB 101)  
CAS No. 37680-73-2
- 406 2,3,3',4',6-Pentachlorobiphenyl (PCB 110)  
CAS No. 74472-35-8
- 412 2,2',3,3',4,4'-Hexachlorobiphenyl (PCB 128)  
CAS No. 38380-07-3
- 418 2,2',3,4,4',5' and 2,3,3',4,4',6-Hexachlorobiphenyl (PCB 138 & 158)  
CAS No. 52712-04-6 and 74472-42-7
- 426 2,2',3,4',5,5'-Hexachlorobiphenyl (PCB 146)  
CAS No. 51908-16-8
- 434 2,2',3,4',5',6-Hexachlorobiphenyl (PCB 149)  
CAS No. 38380-04-0
- 440 2,2',3,5,5',6-Hexachlorobiphenyl (PCB 151)  
CAS No. 52663-63-5
- 446 2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153)  
CAS No. 35065-27-1
- 454 2,2',3,3',4,4',5-Heptachlorobiphenyl (PCB 170)  
CAS No. 35065-30-6
- 462 2,2',3,3',4,5,5'-Heptachlorobiphenyl (PCB 172)  
CAS No. 52663-74-8
- 468 2,2',3,3',4,5',6'-Heptachlorobiphenyl (PCB 177)  
CAS No. 40186-70-7
- 474 2,2',3,3',5,5',6-Heptachlorobiphenyl (PCB 178)  
CAS No. 52663-67-9
- 482 2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB 180)  
CAS No. 35065-29-3
- 490 2,2',3,4,4',5',6-Heptachlorobiphenyl (PCB 183)  
CAS No. 52663-69-1
- 498 2,2',3,4',5,5',6-Heptachlorobiphenyl (PCB 187)  
CAS No. 52663-68-0

- 506 2,2',3,3',4,4',5,5'-Octachlorobiphenyl (PCB 194)  
CAS No. 35694-08-7
- 514 2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB 195)  
CAS No. 52663-78-2
- 520 2,2',3,3',4,4',5,6' and 2,2',3,4,4',5,5',6-Octachlorobiphenyl (PCB 196 & 203)  
CAS No. 42740-50-1 and 52663-76-0
- 528 2,2',3,3',4,5,5',6-Octachlorobiphenyl (PCB 199)  
CAS No. 52663-73-7
- 536 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB 206)  
CAS No. 40186-72-9
- 544 2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl (PCB 209)  
CAS No. 2051-24-3

***Exposure to Chemicals Found in Cigarette Smoke in U.S. Adults***

- 551 Exposure to Chemicals Found in Cigarette Smoke in U.S. Adults: Analysis of Select Chemicals in a Special Sample

**Metals and Metalloids (Special Sample: Adult Smokers & Nonsmokers)**

- 552 Antimony  
CAS No. 7440-36-0
- 554 Arsenic, Total  
CAS No. 7440-38-2
- 556 Arsenic (V) acid
- 558 Arsenobetaine  
CAS No. 64436-13-1
- 560 Arsenocholine  
CAS No. 96055-45-7
- 562 Arsenous (III) acid  
CAS No. 13464-58-9
- 564 Dimethylarsinic acid  
CAS No. 917-76-0
- 566 Monomethylarsonic acid  
CAS No. 65513-69-1
- 568 Trimethylarsine oxide  
CAS No. 4964-14-1
- 570 Barium  
CAS No. 81-25-4
- 572 Cadmium  
CAS No. 81271-94-5
- 574 Cesium  
CAS No. 7440-46-2
- 576 Cobalt  
CAS No. 7440-48-4
- 578 Lead  
CAS No. 7439-92-1
- 580 Manganese  
CAS No. 8075-39-6
- 582 Molybdenum  
CAS No. 7439-98-7
- 584 Strontium  
CAS No. 7440-24-6
- 586 Thallium  
CAS No. 7440-28-0
- 588 Tin  
CAS No. 7440-31-5

590 Tungsten  
CAS No. 7440-33-7

592 Uranium  
CAS No. 7440-61-1

#### Perchlorate and Other Anions (Special Sample: Adult Smokers & Nonsmokers)

594 Nitrate  
CAS No. 84145-82-4

596 Perchlorate  
CAS No. 14797-73-0

598 Thiocyanate  
CAS No. 302-04-5

#### Polycyclic Aromatic Hydrocarbon Metabolites (Adult Cigarette Smokers & Nonsmokers: Special Sample)

600 2-Hydroxyfluorene  
CAS No. 2443-58-5

602 3-Hydroxyfluorene  
CAS No. 6344-67-8

604 9-Hydroxyfluorene  
CAS No. 1689-64-1

606 1-Hydroxyphenanthrene  
CAS No. 2433-56-9

608 2-Hydroxyphenanthrene  
CAS No. 605-55-0

610 3-Hydroxyphenanthrene  
CAS No. 605-87-8

612 4-Hydroxyphenanthrene  
CAS No. 7657-86-7

614 1-Hydroxypyrene  
CAS No. 5315-79-7

616 1-Hydroxynaphthalene (1-Naphthol)  
CAS No. 90-15-3

618 2-Hydroxynaphthalene (2-Naphthol)  
CAS No. 135-19-3

#### Heterocyclic Amines

620 3-Amino-1,4-dimethyl-5H-pyrido[4,3-b]indole (Trp-P-1)

622 2-Amino-3-methyl-9H-pyrido[2,3-b]indole (MeA- $\alpha$ -C)

624 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (Ph1P)

626 2-Amino-9H-pyrido[2,3-b]indole (A- $\alpha$ -C)

628 2-Amino-3-methylimidazo[4,5-f]quinoline (IQ)

630 2-Amino-6-methyldipyrido[1,2-a:3',2'-d]imidazole (Glu-P1)

632 2-Aminodipyrido[1,2-a:3',2'-d]imidazole (GLU-P2) Harman

634 1-Methyl-3-amino-5H-pyrido[4,3-b]indole (Trp-P-2)

636 Norharman

#### Volatile Organic Compounds (VOC)

640 1,1,1-Trichloroethane (Methyl chloroform)  
CAS No. 71-55-6

641 1,1,1,2-Tetrachloroethane  
CAS No. 79-34-5

642 1,2,3-Trichloropropane  
CAS No. 96-18-4

- 643 1,2-Dibromoethane  
CAS No. 106-93-4
- 644 1,2-Dichlorobenzene (*o*-Dichlorobenzene)  
CAS No. 95-50-1
- 645 1,2-Dichloroethane (Ethylene dichloride)  
CAS No. 107-06-2
- 646 1,3-Dichlorobenzene (*m*-Dichlorobenzene)  
CAS No. 95-50-1
- 647 1,4-Dichlorobenzene (Paradichlorobenzene)  
CAS No. 106-46-7
- 648 1,4-Dioxane
- 649 2,5-Dimethylfuran  
CAS No. 625-86-5
- 650 Benzene  
CAS No. 71-43-2
- 651 Bromodichloromethane
- 652 Chlorobenzene (Monochlorobenzene)  
CAS No. 108-90-7
- 653 Chloroethane
- 654 Cyclohexane
- 655 Dibromochloromethane
- 656 Dichloromethane (Methylene chloride)  
CAS No. 75-09-2
- 657 Diethylether
- 658 Ethyl acetate
- 659 Ethylbenzene  
CAS No. 100-41-4
- 660 Furan  
CAS No. 110-00-9
- 661 Heptane
- 662 Hexane
- 663 Isopropylbenzene (Cumene)  
CAS No. 98-82-8
- 664 Methyl-*tert*-butyl ether (MTBE)  
CAS No. 1634-04-4
- 665 Methylcyclopentane
- 666 Nitrobenzene  
CAS No. 98-95-3
- 667 Octane
- 668 Tetrachloroethene (Perchloroethylene)  
CAS No. 127-18-4
- 669 Tetrachloromethane (Carbon tetrachloride)  
CAS No. 56-23-5
- 670 Tetrahydrofuran
- 671 Toluene  
CAS No. 108-88-3
- 672 Tribromomethane (Bromoform)
- 673 Trichloroethene (Trichloroethylene)  
CAS No. 79-01-6
- 674 Trichloromethane (Chloroform)



675  $\alpha\alpha\alpha$ -Trifluorotoluene

676 Vinyl bromide

677 *m*-/*p*-Xylene

CAS No. 108-38-3/106-42-3

678 *o*-Xylene

CAS No. 95-47-6

**Volatile Organic Compound (VOC) Metabolites (Special Sample: Adult Smokers & Nonsmokers)**

679 N-Acetyl-S-(2-carboxyethyl)-L-cysteine

CAS No. 51868-61-2

681 N-Acetyl-S-(3-hydroxypropyl)-L-cysteine

CAS No. 23127-40-4

683 N-Acetyl-S-(2-carbamoyl-ethyl)-L-cysteine

CAS No. 81690-92-8

685 N-Acetyl-S-(2-carbamoyl-2-hydroxyethyl)-L-cysteine

687 N-Acetyl-S-(2-cyanoethyl)-L-cysteine

CAS No. 74514-75-3

689 N-Acetyl-S-(2-hydroxyethyl)-L-cysteine

CAS No. 15060-26-1

691 N-Acetyl-S-(phenyl)-L-cysteine

CAS No. 4775-80-8

693 N-Acetyl-S-(*n*-propyl)-L-cysteine

695 N-Acetyl-S-(3,4-dihydroxybutyl)-L-cysteine

CAS No. 144889-50-9

697 N-Acetyl-S-(1-hydroxymethyl-2-propenyl)-L-cysteine

699 N-Acetyl-S-(2-hydroxy-3-butenyl)-L-cysteine

CAS No. 159092-64-5

701 N-Acetyl-S-(4-hydroxy-2-butenyl)-L-cysteine

CAS No. 159092-65-6

703 2-Thioxothiazolidine-4 carboxylic acid

CAS No. 20933-67-9

705 N-Acetyl-S-(3-hydroxypropyl-1-methyl)-L-cysteine

CAS No. 33164-70-4

707 2-Aminothiazoline-4-carboxylic acid

CAS No. 40283-41-8

709 N-Acetyl-S-(*N*-methylcarbamoyl)-L-cysteine

CAS No. 103974-29-4

711 Phenylglyoxylic acid

CAS No. 611-73-4

713 N-Acetyl-S-(2-hydroxypropyl)-L-cysteine

CAS No. 923-43-3

715 N-Acetyl-S-(phenyl-2-hydroxyethyl)-L-cysteine

717 Mandelic acid

CAS No. 90-64-2, 611-71-2 (R), 17199-29-0 (S)

719 N-Acetyl-S-(trichlorovinyl)-L-cysteine

CAS No. 111348-61-9

721 N-Acetyl-S-(benzyl)-L-cysteine

CAS No. 19542-77-9

723 N-Acetyl-S-(1,2-dichlorovinyl)-L-cysteine

CAS No. 2148-31-4

725 N-Acetyl-S-(2,2-dichlorovinyl)-L-cysteine

CAS No. 126543-43-9