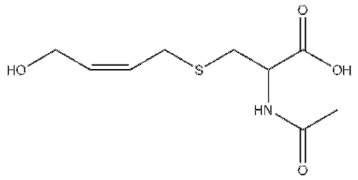
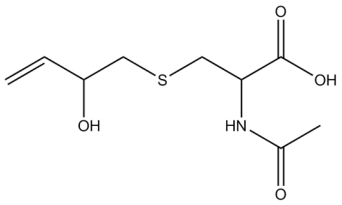
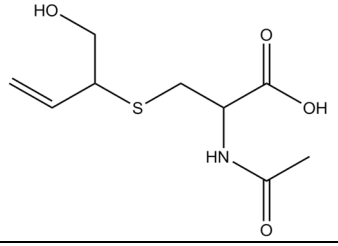
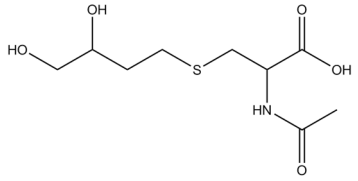
Urinary Volatile Organic Compound Metabolites: Reference Ranges, Chemical Structures and Parent Compounds
Volatile Organic Compounds Laboratory, CDC/DLS/Tobacco and Volatiles Branch

Parent VOC	VOC Metabolite [Common Name] [Analyte Code]	VOC Metabolite Structure	Geometric Mean[1*] (95% conf. interval) (ng/mL)	95th Percentile Intervals[1*] (95% conf. interval) (ng/mL)	LOD (ng/mL)	ULOQ (ng/mL)‡
1,3-Butadiene	N-Acetyl-S-(4-hydroxy-2-buten-1-yl)-L-cysteine [MHBMA3] [MHB3]		Smokers: **57.5** (51.3-64.6) Non-Smokers: **6.99** (6.32-7.73)	Smokers: **257** (230-286) Non-Smokers: **28.3** (25.7-31.2)	0.600	8650
1,3-Butadiene	N-Acetyl-S-(2-hydroxy-3-butenyl)-L-cysteine [MHBMA2] [MHB2]		Smokers: ** Non-Smokers: **	Smokers: **8.99** (7.71-10.0) Non-Smokers: **< LOD**	0.700	760
1,3-Butadiene	N-Acetyl-S-(1-hydroxymethyl-2-propenyl)-L-cysteine [MHBMA1] [MHB1]		Smokers: **< LOD** Non-Smokers: **< LOD**	Smokers: **< LOD** Non-Smokers: **< LOD**	0.700	722
1,3-Butadiene	N-Acetyl-S-(3,4-dihydroxybutyl)-L-cysteine [DHBMA] [DHBM]		Smokers: **333** (293-378) Non-Smokers: **231** (215-248)	Smokers: **1220** (989-1550) Non-Smokers: **730** (666-785)	5.25	20100

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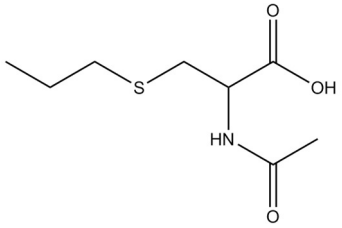
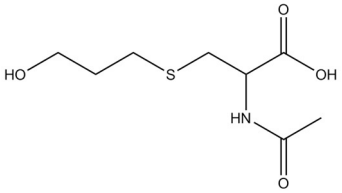
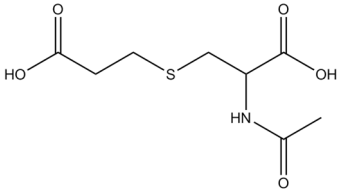
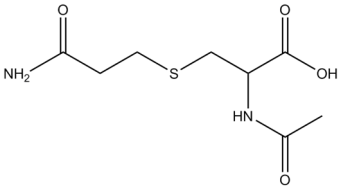
1-Bromopropane	N-Acetyl-S-(n-propyl)-L-cysteine [BPMA] [BPMA]		Smokers: **3.85** (3.23-4.58) Non-Smokers: **4.80** (4.24-5.43)	Smokers: **64.8** (29.9-105) Non-Smokers: **56.1** (35.7-78.6)	1.20	3820
Acrolein	N-Acetyl-S-(3-hydroxypropyl)-L-cysteine [3HPMA or HPMA] [HPMA]		Smokers: **1090** (968-1230) Non-Smokers: **224** (208-241)	Smokers: **5070** (4360-5840) Non-Smokers: **1060** (916-1230)	13.0	64900
Acrolein	N-Acetyl-S-(2-carboxyethyl)-L-cysteine [CEMA] [CEMA]		Smokers: **228** (203-256) Non-Smokers: **80.6** (74.3-87.5)	Smokers: **1030** (869-1320) Non-Smokers: **367** (310-448)	6.96	9490
Acrylamide	N-Acetyl-S-(2-carbamoylethyl)-L-cysteine [AAMA] [AAMA]		Smokers: **111** (95.0-129) Non-Smokers: **36.5** (33.8-39.3)	Smokers: **507** (370-686) Non-Smokers: **157** (137-192)	2.20	5490

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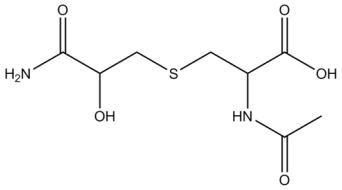
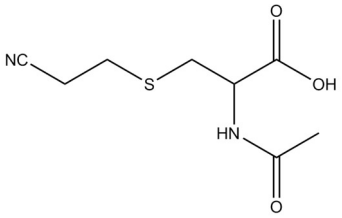
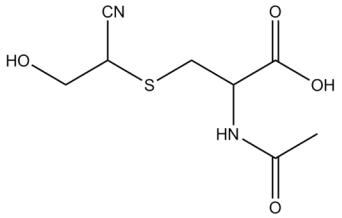
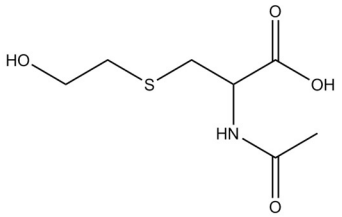
Acrylamide	N-Acetyl-S-(2-carbamoyl-2-hydroxyethyl)-L-cysteine [GAMA] [GAMA]		Smokers: **28.4** (25.2-32.0) Non-Smokers: **12.9** (12.2-13.7)	Smokers: **138** (98.9-169) Non-Smokers: **41.5** (34.8-50.9)	9.40	9410
Acrylonitrile	N-Acetyl-S-(2-cyanoethyl)-L-cysteine [CYMA] [CYMA]		Smokers: **122** (106-141) Non-Smokers: **1.50** (1.35-1.67)	Smokers: **717** (513-827) Non-Smokers: **12.1** (7.05-18.2)	0.500	7980
Acrylonitrile	N-Acetyl-S-(1-cyano-2-hydroxyethyl)-L-cysteine [CYHA] [CYHA]		Smokers: **N/A** Non-Smokers: **N/A**	Smokers: **N/A** Non-Smokers: **N/A**	2.60	13000
Acrylonitrile Vinyl chloride Ethylene oxide	***N-Acetyl-S-(2-hydroxyethyl)-L-cysteine [HEMA] [HEMA]		Smokers: **1.97** (1.74-2.22) Non-Smokers: **	Smokers: **12.5** (9.56-14.4) Non-Smokers: **2.10** (1.77-2.67)	0.791	597

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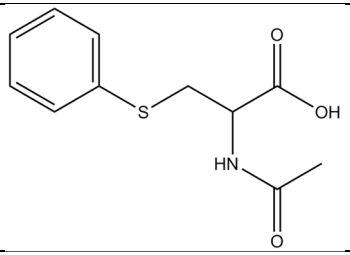
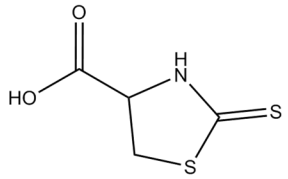
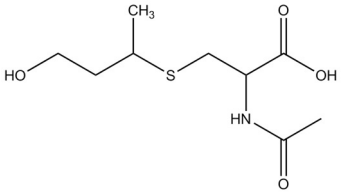
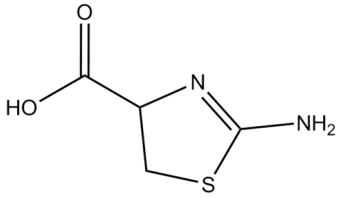
Benzene	N-Acetyl-S-(phenyl)-L-cysteine [PMA] [PMA]		Smokers: ** Non-Smokers: **	Smokers: **3.11** (2.08-3.76) Non-Smokers: **3.08** (2.18-3.79)	0.600	552
Carbon disulfide	2-Thioxothiazolidine-4-carboxylic acid [TTCA] [TTCA]		Smokers: **11.4** (9.99-12.9) Non-Smokers: **8.83** (7.94-9.82)	Smokers: **84.5** (61.2-183) Non-Smokers: **115** (77.0-144)	11.2	17700
Crotonaldehyde	N-Acetyl-S-(3-hydroxypropyl-1-methyl)-L-cysteine [HPMMA] [HPMM]		Smokers: **1790** (1620-1980) Non-Smokers: **334** (315-354)	Smokers: **7910** (7610-8720) Non-Smokers: **1260** (991-1890)	3.00	48000
Cyanide	2-Aminothiazoline-4-carboxylic acid [ATCA] [ATCA]		Smokers: **117** (101-137) Non-Smokers: **95.9** (88.2-104)	Smokers: **608** (491-759) Non-Smokers: **433** (364-501)	15.0	14200

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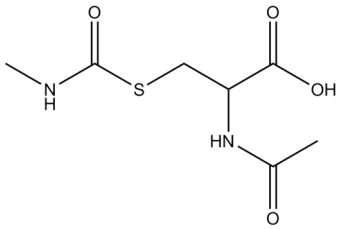
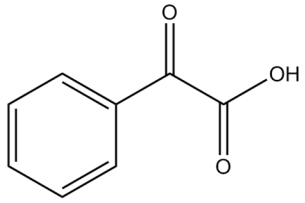
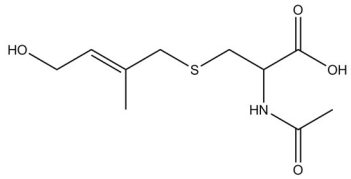
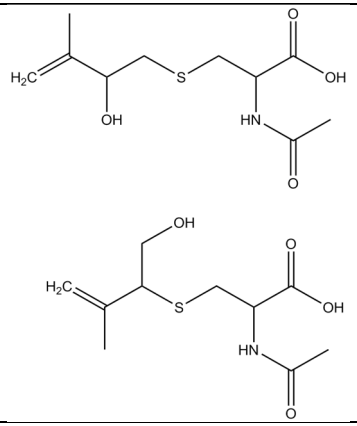
N, N-Dimethylformamide	N-Acetyl-S-(N-methylcarbamoyl)-L-cysteine [AMCC or AMCA] [AMCA]		Smokers: **415** (364-473) Non-Smokers: **109** (102-116)	Smokers: **1810** (1360-2050) Non-Smokers: **468** (402-553)	6.26	18000
Ethylbenzene Styrene	***Phenylglyoxylic acid [PGA] [PHGA]		Smokers: **309** (274-348) Non-Smokers: **160** (146-175)	Smokers: **1140** (973-1530) Non-Smokers: **566** (478-655)	12.0	15900
Isoprene	N-Acetyl-S-(4-hydroxy-2-methyl-2-buten-1-yl)-L-cysteine [IPMA3] [IPM3]		Smokers: **N/A** Non-Smokers: **N/A**	Smokers: **N/A** Non-Smokers: **N/A**	0.740	8430
Isoprene	N-Acetyl-S-(2-hydroxy-3-methyl-3-buten-1-yl)-L-cysteine + N-Acetyl-S-(1-(hydroxymethyl)-2-methyl-2-propen-1-yl)-L-cysteine [IPMA1+IPMA2] [IPM1]		Smokers: **N/A** Non-Smokers: **N/A**	Smokers: **N/A** Non-Smokers: **N/A**	1.43	2250

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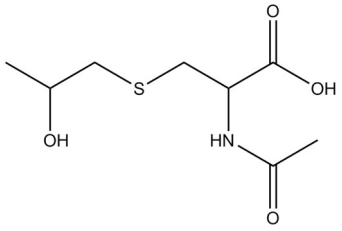
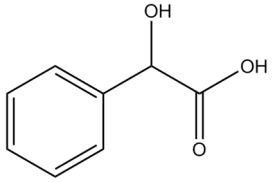
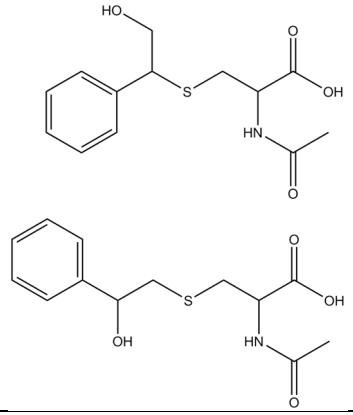
Propylene oxide	N-Acetyl-S-(2-hydroxypropyl)-L-cysteine [2HPMA] [HPM2]		Smokers: **105** (91.4-121) Non-Smokers: **52.6** (47.4-58.3)	Smokers: **552** (401-731) Non-Smokers: **509** (289-717)	5.30	41700
Styrene	Mandelic acid [MA] [MADA]		Smokers: **283** (244-330) Non-Smokers: **129** (118-142)	Smokers: **1200** (969-1420) Non-Smokers: **465** (396-534)	12.0	18900
Styrene	N-Acetyl-S-(1-phenyl-2-hydroxyethyl)-L-cysteine + N-Acetyl-S-(2-phenyl-2-hydroxyethyl)-L-cysteine [PHEMA] [PHEM]		Smokers: **1.21** (1.04-1.41) Non-Smokers: **	Smokers: **6.26** (5.05-8.62) Non-Smokers: **1.87** (1.63-2.16)	0.700	796

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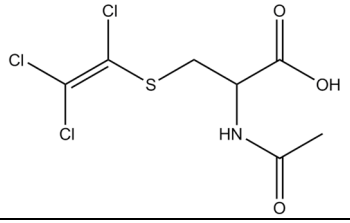
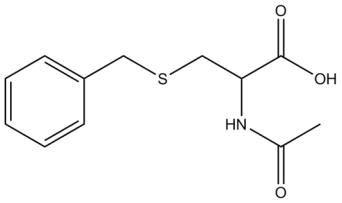
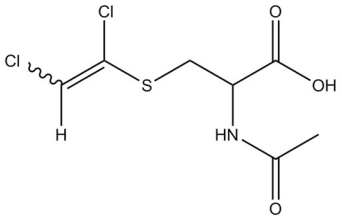
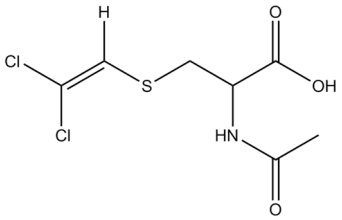
Tetrachloroethylene	N-Acetyl-S-(trichlorovinyl)-L-cysteine [TCVMA] [TCVM]		Smokers: **< LOD** Non-Smokers: **< LOD**	Smokers: **< LOD** Non-Smokers: **< LOD**	3.00	2380
Toluene	N-Acetyl-S-(benzyl)-L-cysteine [BMA] [BMA]		Smokers: **6.47** (5.58-7.51) Non-Smokers: **6.45** (5.91-7.05)	Smokers: **41.8** (28.8-83.4) Non-Smokers: **37.0** (29.5-53.9)	0.500	2200
Trichloroethylene	*N*-Acetyl-S-(1,2-dichlorovinyl)-L-cysteine [1DCVMA] [1DCV]		Smokers: **< LOD** Non-Smokers: **< LOD**	Smokers: **< LOD** Non-Smokers: **< LOD**	12.6	9870
Trichloroethylene	N-Acetyl-S-(2,2-dichlorovinyl)-L-cysteine [2DCVMA] [2DCV]		Smokers: **< LOD** Non-Smokers: **< LOD**	Smokers: **< LOD** Non-Smokers: **< LOD**	4.70	6170

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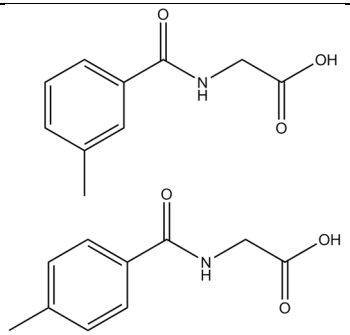
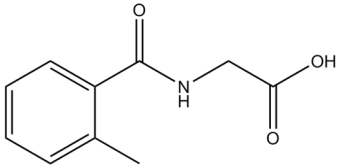
Xylene	3-Methylhippuric acid + 4-Methylhippuric acid [3MHA+4MHA] [34MH]		Smokers: **668** (576-775) Non-Smokers: **173** (158-189)	Smokers: **2850** (2380-3410) Non-Smokers: **1330** (1170-1470)	8.00	33000
Xylene	2-Methylhippuric acid [2MHA] [2MHA]		Smokers: **99.4** (87.4-113) Non-Smokers: **25.9** (23.0-29.0)	Smokers: **408** (337-434) Non-Smokers: **170** (129-211)	5.00	15500

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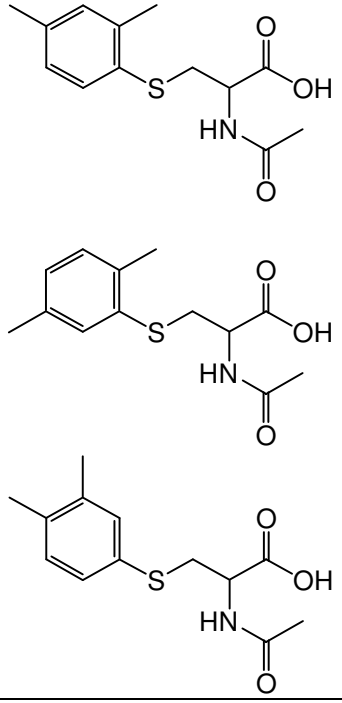
Xylene	N-Acetyl-S-(2,4-dimethylphenyl)-L-cysteine + N-Acetyl-S-(2,5-dimethylphenyl)-L-cysteine + N-Acetyl-S-(3,4-dimethylphenyl)-L-cysteine [DPMA] [DPMA]		Smokers: **< LOD** Non-Smokers: **< LOD**	Smokers: **< LOD** Non-Smokers: **< LOD**	0.500	360

* Values listed are NOT creatinine corrected.
**Not Calculated: Proportion of results below limit of detection was too high to provide a valid result.
***VOC metabolite is common to multiple parent VOCs.
‡ULOQ corresponds to highest calibrator x dilution factor (table shows typical dilution factor of 5x, but method is validated to 20x)
[1]Fourth National Report on Human Exposure to Environmental Chemicals (February 2015), http://www.cdc.gov/biomonitoring/pdf/FourthReport_UpdatedTables_Feb2015.pdf, accessed February 24, 2017.