

Supplemental information

Determination of Volatile Organic Compounds in Child Care Centers by Thermal Desorption Gas Chromatography-Mass Spectrometry

D. C. Vu^{a,b}, T.L. Ho^c, P. H. Vo^a, G. Carlo^d, J.A. McElroy^e, A. N. Davis^f, S.C. Nagel^g, and C.-H. Lin^{*a,b}

^a Center for Agroforestry, School of Natural Resources, University of Missouri, Columbia, MO, USA.

* Email: linchu@missouri.edu

^b Department of Forestry, School of Natural Resources, University of Missouri, Columbia, MO, USA.

^c Center of Core Facilities, Cuu Long Delta Rice Research Institute, Vietnam.

^d Center for Children and Families Across Cultures, Department of Human Development and Family Science, University of Missouri, Columbia, MO, USA

^e Department of Family and Community Medicine, University of Missouri, Columbia, MO, USA

^f Department of Individual, Family, and Community Education, University of New Mexico, NM, USA

^g Department of Obstetrics, Gynecology and Women's Health, School of Medicine, University of Missouri

Table S1. Summary of volatile organic compounds screened in the study

No.	Compounds	Substance group	Classification of toxicity		Emission sources and uses
			Toxicity*	Sources**	
1	1,1,1-Trichloroethane	Halogenated alkane	neurotoxic to humans	ATSDR	solvent for inks, paints
2	1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113a)	Halogenated alkane	ozone depleting chemical	EPA	used as a refrigerant
3	1,1,2-Trichloroethane	Halogenated alkane	possible human carcinogen	EPA	solvent
4	1,1-Dichloroethane	Halogenated alkane	possible human carcinogen	EPA	used as a solvent, cleaning agent
5	1,1-Dichloroethene	Halogenated alkene	potential occupational carcinogen	CDC	used in the productions of PVC, polyacrylonitrile
6	1,2,3-Trimethylbenzene	Aryl hydrocarbon	health hazard	ATSDR	used in jet fuel
7	1,2,4-Trimethylbenzene	Aryl hydrocarbon	toxic to aquatic life	CDC	solvent for industrial coatings, sealants
8	1,2-Dibromo-3-chloropropane	Halogenated alkane	possible human carcinogen; endocrine disruptor	IARC TEDX	soil fumigant, pesticide ingredient
9	1,2-Dibromoethane	Halogenated alkane	probable human carcinogen; endocrine disruptor	EPA TEDX	fumigant for log treatment

10	1,2-Dichloro-1,1,2,2-tetrafluoroethane (R-114)	Halogenated alkane	ozone depleting chemical	EPA	used as a refrigerant
11	1,2-Dichlorobenzene	Halogenated aryl	endocrine disruptor	TEDX	fumigant, insecticide
12	1,2-Dichloroethane	Halogenated alkane	possible human carcinogen	IARC	used as a degreaser and paint remover
13	1,2-Dichloroethene	Halogenated alkene	health hazard	ATSDR	solvent for dyes, lacquers
14	1,2-Dichloropropane	Halogenated alkane	human carcinogen	IARC	industrial solvent in paint strippers, vanishes
15	1,3,5-Trimethylbenzene	Aryl hydrocarbon	toxic to aquatic life	CDC	solvent for industrial coatings, sealants
16	1,3-Butadiene	Alkyne	human carcinogen	IARC	used in synthetic rubber production
17	1,3-Dichlorobenzene	Halogenated aryl	endocrine disruptor	TEDX	fumigant and insecticide
18	1,4-Dichlorobenzene	Halogenated aryl	possible human carcinogen	EPA	room deodorizers, toilet deodorants
19	1,4-Dioxane	Heterocyclic ether	possible human carcinogen	IARC	component of dye baths, paints
20	1-Butanol	Alcohol	not classified		paint thinner
21	1-Dodecanesulfonyl chloride	Alkyl sulfonyl halide	not classified		surfactant

22	1-Eicosanol	Fatty alcohol	not classified		emollient in cosmetics
23	1-Hexadecanol	Fatty alcohol	not classified		emollient in cosmetics
24	1-Octadecanol	Fatty alcohol	not classified		component in skin care and hair care products
25	2-(2-Ethoxyethoxy)ethanol (22EE)	Glycol ether	not classified		used ink, toner, and colorant products
26	2-(2-Methoxyethoxy)ethanol (22MEE)	Glycol ether	endocrine disruptor	TEDX	textile dye paste, solvent for wood stains
27	2-Butanone (MEK)	Ketone	endocrine disruptor	TEDX	used in dry eraser makers
28	2-Butoxyethanol	Glycol ether	endocrine disruptor	TEDX	solvent for inks, paints, surface coatings
29	2-Butyl-1-octanol	Alcohol	not classified		humectant in cosmetics
30	2-Ethylhexanol-1	Alcohol	endocrine disruptor	TEDX	used in manufacture of styrene
31	2-Ethylhexyl salicylate	Hydroxyaryl ester	not classified		sunscreen ingredient
32	2-Ethyltoluene	Aryl hydrocarbon	health hazard; toxic to aquatic life	PubChem	solvent
33	2-Hexanone (MBK)	Ketone	health hazard; neurotoxic to animals	ATSDR	industrial solvent, ingredient in paint
34	2-Propanol	Alcohol	not classified		solvent for coatings

35	3-Carene	Cyclic terpene	not classified		constituent of turpentine
36	3-Ethyltoluene	Aryl hydrocarbon	health hazard; toxic to aquatic life	PubChem	solvent
37	4-Ethyltoluene	Aryl hydrocarbon	health hazard	PubChem	solvent
38	4-Methyl-2-pentanone	Ketone	possible human carcinogen	IARC	solvent for resins and paints
39	Acetone	Ketone	endocrine disruptor	TEDX	component in nail removers, superglue removers
40	Acetophenone	Aryl ketone	not classified		components of inks and coatings
41	Acrolein	Aldehyde	not classified		herbicide
42	Acrylonitrile	Nitrile compound	probable human carcinogen	EPA	used in manufacture of plastics, resins, rubber
43	Allyl chloride	Halogenated alkene	possible human carcinogen	EPA	used in manufacture of pesticides
44	α -Pinene	Cyclic terpene	not classified		lube oil additives, flavoring odorant
45	Benzaldehyde	Aryl aldehyde	endocrine disruptor	TEDX	food additive, cosmetic ingredient
46	Benzene	Aryl hydrocarbon	human carcinogen	EPA	household product ingredient; solvent
47	Benzothiazole	Aromatic	not classified		rubber accelerator,

		heterocyclic			antimicrobial agent
48	Benzyl chloride	Halogenated aryl	probable human carcinogen; endocrine disruptor	EPA TEDX	used in manufacture of dyes, pharmaceutical and perfume products
49	Bromodichloromethane	Halogenated alkane	possible human carcinogen	CDC	solvent for fats and waxes, flame retardant
50	Bromoform	Halogenated alkane	hazardous to environment; probable human carcinogen	EPA	solvent
51	Butanal	Aldehyde	not classified		solvent
52	Butyl acetate	Ester	not classified		used as synthetic fruit flavoring
53	Carbon disulfide	Sulfide	endocrine disruptor	TEDX	used in manufacture of rayon
54	Carbon tetrachloride	Halogenated alkane	probable human carcinogen; endocrine disruptor	EPA TEDX	once used as a dry clean solvent, refrigerant
55	Chlorobenzene	Halogenated aryl	health hazard	CDC	industrial solvent
56	Chloroethane	Halogenated alkane	not classified		used as a blowing agent in foamed plastics
57	cis-1,3-Dichloropropene	Halogenated alkene	possible human carcinogen	IARC	preplanting fumigant
58	Cyclohexane	Cycloalkane	health hazard; toxic to aquatic life	CDC	organic solvent in laboratory

59	Decamethylcyclopentasiloxane	Organosilicon	endocrine disruptor	TEDX	personal care products, cosmetic ingredient
60	Decanal	Aldehyde	not classified		used in fragrances and flavoring
61	Decane	Alkane	health hazard; toxic to aquatic life	CDC	component of fuels
62	Dibromochloromethane	Halogenated alkane	not classified		solvent, once used as flame retardant
63	Dichlorodifluoromethane	Halogenated alkane	ozone depleting chemical	EPA	once used as a refrigerant
64	D-Limonene	Cyclic terpene	not classified		cleaning and furnishing care products
65	Dodecane	Alkane	health hazard; toxic to aquatic life	PubChem	component of fuels
66	Ethyl acetate	Ester	health hazard	CDC	used in nail vanish removers
67	Ethylbenzene	Aryl hydrocarbon	possible human carcinogen; endocrine disruptor	IARC TEDX	solvent for paints, adhesives, household degreasing cleaners
68	<i>g</i> -Terpinene	Cyclic terpene	not classified		used in cosmetics and food industries
69	Heptanal	Aldehyde	not classified		used in production of perfumes

70	Heptane	Alkane	health hazard	CDC	used in paints, coatings
71	Heptanoic acid	Carboxylic acid	not classified		an additive in cigarette
72	Hexachlorobutadiene	Halogenated alkadiene	toxic to aquatic life; possible human carcinogen	CDC EPA	solvent
73	Hexadecane	Alkane	health hazard	PubChem	component of fuels
74	Hexanal	Aldehyde	not classified		used in flavor industry
75	Hexane	Alkane	health hazard; toxic to aquatic life	CDC	used in leather productions, vegetable oil extraction
76	Homomenthyl salicylate	Hydroxyaryl ester	endocrine disruptor	TEDX	sunscreen ingredient
77	Isopropylbenzene (Cumene)	Aryl hydrocarbon	possible human carcinogen toxic to aquatic life	IARC CDC	thinner for paints, solvent for resins
78	<i>m</i> -Diethylbenzene	Aryl hydrocarbon	health hazard; toxic to aquatic life	PubChem	solvent
79	<i>o</i> -Diethylbenzene	Aryl hydrocarbon	health hazard; toxic to aquatic life	CDC	solvent
80	<i>m</i> -Xylene	Aryl hydrocarbon	endocrine disruptor; toxic to aquatic life	TEDX CDC	industrial solvent, cleaning agent
81	<i>p</i> -Xylene	Aryl hydrocarbon	endocrine disruptor; toxic to aquatic life	TEDX CDC	industrial solvent, cleaning agent

82	Methyl methacrylate	Ester	health hazard; toxic to aquatic life	CDC	used in inks, toners, paints and coatings, personal care products
83	Methyl tert-butyl ether	Ether	endocrine disruptor	TEDX	component in furnishing care, foam seating, bedding products
84	Methylene chloride	Halogenated alkane	possible human carcinogen; toxic to aquatic life	CDC	solvent in paint strippers, adhesives
85	Naphthalene	Aryl hydrocarbon	possible human carcinogen; endocrine disruptor	IARC TEDX	moth repellent, household fumigant
86	<i>n</i> -Butyl ether	Ether	health hazard; toxic to aquatic life	CDC	solvent, used in manufacture of pesticides
87	<i>n</i> -Butylbenzene	Aryl hydrocarbon	endocrine disruptor	TEDX	additive in rubber/plastic industries
88	<i>n</i> -Nonane	Alkane	health hazard; toxic to aquatic life	CDC PubChem	fuel additive
89	Nonanal	Aldehyde	not classified		component of perfumes
90	<i>n</i> -Propylbenzene	Aryl hydrocarbon	health hazard; toxic to aquatic life	PubChem	used as solvent, fuel additive
91	Octanal	Aldehyde	not classified		component of perfumes

92	Octane	Alkane	health hazard; toxic to aquatic life	CDC	component of gasoline
93	<i>o</i> -Xylene	Aryl hydrocarbon	endocrine disruptor; toxic to aquatic life	TEDX CDC	solvent in printing, rubber and leather industries
94	<i>p</i> -Diethylbenzene	Aryl hydrocarbon	health hazard; toxic to aquatic life	PubChem	solvent
95	Styrene	Aryl hydrocarbon	possible human carcinogen; endocrine disruptor	IARC TEDX	household product ingredient
96	Tetrachloroethylene	Halogenated alkene	probable human carcinogen; endocrine disruptor	IARC TEDX	household product ingredient, solvent, dry cleaning agent
97	Tetradecane	Alkane	health hazard	PubChem	component of fuels
98	Tetrahydrofuran	Heterocyclic ether	health hazard	CDC	used in adhesives and sealants
99	Toluene	Aryl hydrocarbon	endocrine disruptor; toxic to aquatic life	TEDX CDC	solvent for paints, adhesives
100	<i>trans</i> -1,3-Dichloropropene	Halogenated alkene	possible human carcinogen	IARC	preplanting fumigant
101	Trichloroethene	Halogenated alkane	human carcinogen	IARC	solvent for paints; drying cleaning agent
102	Trichlorofluoromethane	Halogenated alkane	ozone depleting chemical	EPA	refrigerant

103	Tridecane	Alkane	health hazard	PubChem	component of fuels
104	Undecane	Alkane	health hazard; toxic to aquatic life	PubChem	component of fuels
105	Vinyl acetate	Ester	possible human carcinogen; endocrine disruptor	IARC TEDX	used in water-based paints, adhesives, glues
106	Vinyl chloride	Halogenated alkene	human carcinogen	IARC	used in manufacture of PVC
107	α -Methylstyrene	Aryl hydrocarbon	possible human carcinogen	IARC	used in production of plasticizers

*: toxicity of volatile organic compounds

** : sources from which data are cited

ATSDR: Agency for Toxic Substances and Disease Registry - the United States Department of Health and Human Services

CDC: Centers for Disease Control and Prevention

EPA: United States Environmental Protection Agency

IARC: International Agency for Research on Cancer – World Health Organization

PubChem: Open Chemistry Database - the United States National Institutes of Health (NIH) (<https://pubchem.ncbi.nlm.nih.gov/>)

TEDX: the Endocrine Disruption Exchange (<https://endocrinedisruption.org/>)