

Article

Direct mass spectrometry with online headspace sample pretreatment for continuous water quality monitoring

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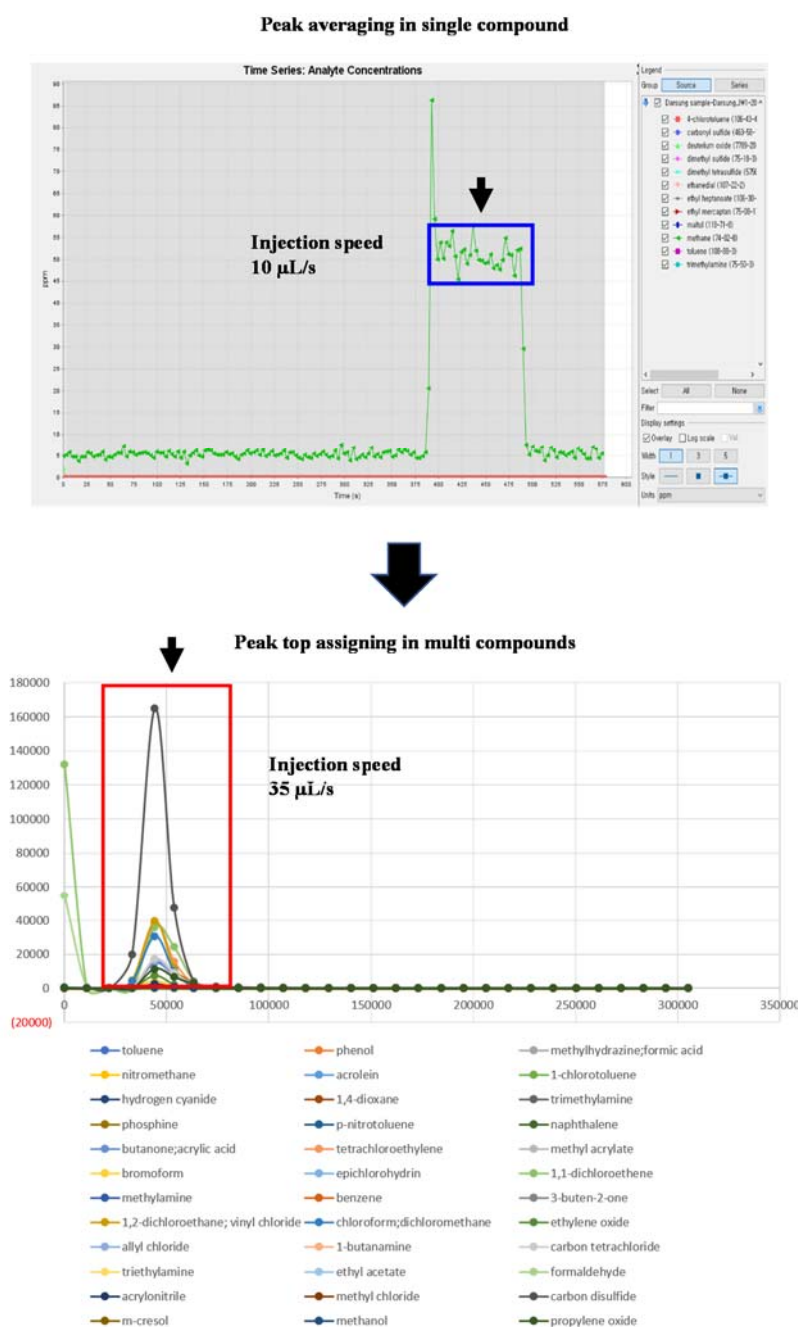


Figure S1. Data assignment under headspace extraction and injection conditions(upper: single compound injection, lower: multi compound injection).

Table S1. Physico/chemical properties of target compounds for chemical accidents and leakages.

Compounds	CAS no	Elemental composition	Molecular weight	Vapor pressure (mmHg) @ 25°C	Solubility (mg/L) @ 25°C
Toluene	108-88-3	C ₇ H ₈	92.14	28.4	526
Phenol	108-95-2	C ₆ H ₆ O	94.11	0.35	82 800
Formic acid	64-18-6	CH ₂ O ₂	46.025	42.59 (extrapolated)	1 000 000
Nitromethane	75-52-5	CH ₃ NO ₂	61.04	35.8	111 000
Acrolein	107-02-8	C ₃ H ₄ O	56.06	274	212 000
Benzyl chloride	100-44-7	C ₇ H ₇ Cl	126.58	1.23	525
Acrylamide	79-06-1	C ₃ H ₅ NO	71.08	0.007	2 040 000
1,4-dioxane	123-91-1	C ₄ H ₈ O ₂	88.11	38.1	800 000
Trichloroethylene	79-01-6	C ₂ HCl ₃	131.38	69	1 280
p-nitrotoluene	99-99-0	C ₇ H ₇ NO ₂	137.14	0.0157 (extrapolated)	361
Naphthalene	91-20-3	C ₁₀ H ₈	128.17	0.085	31
Methyl ethyl ketone	78-93-3	C ₄ H ₈ O	72.11	90.6	223 000
Tetrachloroethene	127-18-4	C ₂ Cl ₄	165.8	18.5	206
Methyl acrylate	96-33-3	C ₄ H ₆ O ₂	86.09	86.6	49 400
Bromoform	75-25-2	CHBr ₃	252.73	5.4 (estimated)	3 100
1,1-dichloroethylene	75-35-4	C ₂ H ₂ Cl ₂	96.94	600	2 420
Benzene	71-43-2	C ₆ H ₆	78.11	94.8	17 900
Methyl vinyl ketone	78-94-4	C ₄ H ₆ O	70.09	152	100 000
Vinyl chloride	75-01-4	C ₂ H ₃ Cl	62.5	2980	8 800
Dichloromethane	75-09-2	CH ₂ Cl ₂	84.93	435	13 200
Ethylene oxide	75-21-8	C ₂ H ₄ O	44.05	1310	237
Allyl chloride	107-05-1	C ₃ H ₅ Cl	76.52	368	3.37
Carbon tetrachloride	56-23-5	CCl ₄	153.82	115	793
Ethyl acetate	141-78-6	C ₄ H ₈ O ₂	88.11	93.2	80 000
Formaldehyde	50-00-0	CH ₂ O	30.03	10.5	400 000 @ 20°C

Acrylonitrile	107-13-1	C ₃ H ₃ N	53.06	109	74 500
Methyl chloride	74-87-3	CH ₃ Cl	50.49	4300	5 040
Carbon disulfide	75-15-0	CS ₂	76.14	359	2 160
m-cresol	108-39-4	C ₇ H ₈ O	108.14	0.11	22 700
Methanol	67-56-1	CH ₃ OH	32.04	127	1 000 000
Propylene oxide	75-56-9	C ₃ H ₆ O	58.08	538	590 000

Table S2. Reaction ion, mass, theoretical and measured reaction ratio of target compounds.

Compounds	Reaction Ion	m/z	Reaction ratio	Compounds	Reaction Ion	m/z	Reaction ratio	Compounds	Reaction Ion	m/z	Reaction ratio
Toluene	H ₃ O ⁺	93*	1	Naphthalene	H ₃ O ⁺	129*	1	Ethylene oxide	H ₃ O ⁺	45*	1
	NO ⁺	92	1		NO ⁺	128*	1		O ₂ ⁺	44*	1
	O ₂ ⁺	92*	1		O ₂ ⁺	128	1	Allyl chloride	H ₃ O ⁺	41*	0.87
Phenol	H ₃ O ⁺	95*	1	Butanone	H ₃ O ⁺	73	1			59*	0.13
	NO ⁺	94	1		NO ⁺	102*	1		O ₂ ⁺	41*	0.65
	O ₂ ⁺	94	1		O ₂ ⁺	72*	0.3			76*	0.3
Formic acid	H ₃ O ⁺	47	0.9	Tetrachloroethylene	O ₂ ⁺	166*	0.42	Tetrachloromethane	H ₃ O ⁺	119*	0.48
	NO ⁺	46	0.35			164*	0.32			117*	0.52
	O ₂ ⁺	45*	0.4			168*	0.21		O ₂ ⁺	117	0.52
Nitromethane	H ₃ O ⁺	62*	1	Methyl acrylate	H ₃ O ⁺	87*	1	Ethyl acetate	H ₃ O ⁺	89*	1
	NO ⁺	61*	0.9		NO ⁺	116*	0.9		O ₂ ⁺	88*	0.2
Acrolein	H ₃ O ⁺	57*	1		O ₂ ⁺	85*	0.4	Formaldehyde	H ₃ O ⁺	31*	1
	NO ⁺	55*	0.6	Bromoform	H ₃ O ⁺	173*	0.5		O ₂ ⁺	31*	1
		86*	0.4		O ₂ ⁺	175*	0.25	Acrylonitrile	H ₃ O ⁺	54	1
Benzyl chloride	NO ⁺	91*	1			173*	0.5		O ₂ ⁺	83*	1
	O ₂ ⁺	91	0.6	1,1-dichloroethylene	H ₃ O ⁺	97*	0.57	Methyl chloride	O ₂ ⁺	49*	0.76
		126	0.3			99*	0.37			51*	0.24
Acrylamide	H ₃ O ⁺	72*	1								

	NO ⁺	101*	1		O ₂ ⁺	96	0.57	Carbon disulfide	H ₃ O ⁺	77	1
	O ₂ ⁺	71	0.55			98	0.37		O ₂ ⁺	76*	1
1,4-Dioxane	H ₃ O ⁺	89*	1	Benzene	H ₃ O ⁺	79*	1	m-cresol	H ₃ O ⁺	109	1
	NO ⁺	88*	0.45		NO ⁺	108*	0.24		NO ⁺	108*	1
	O ₂ ⁺	88	0.65		O ₂ ⁺	78*	1		O ₂ ⁺	108	1
Trichloroethylene	H ₃ O ⁺	131*	0.42	Methyl vinyl ketone	H ₃ O ⁺	71*	1	Methanol	H ₃ O ⁺	33*	1
		133	0.42		NO ⁺	100*	1		NO ⁺	62	1
	O ₂ ⁺	130	0.42		O ₂ ⁺	70*	0.5		O ₂ ⁺	31	0.5
		132	0.42	Vinyl chloride	O ₂ ⁺	62*	0.75			32	0.5
p-nitrotoluene	H ₃ O ⁺	138*	1			64*	0.25	Propylene oxide	H ₃ O ⁺	59*	1
	NO ⁺	167	1	Dichloromethane	O ₂ ⁺	83*	0.56		NO ⁺	57*	0.35
	O ₂ ⁺	137	1			85*	0.38			88	0.65

* : mass-to-charge ratio (m/z) chosen for quantification and qualification of each compound.