Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Table S1 List of volatile organic compounds (VOCs) in Photochemical Assessment Monitoring System standards.

VOCs	Molecular formula	CAS NO.	Molecular weight	Detection Limit ($\mu g/m^3$)	Classification	
					WHO (IARC)	U.S.EPA (IRIS)
Ethene+Acetylene+Ethane	C2H4;C2H2;C2H6	74851;74862;74840	28.05;26.04;30.07	1.09	-	-
Propene (Propylene)	C3H6	115-07-1	42.08	0.10	3	-
Propane	C3H8	74-98-6	44.10	0.22	-	-
Isobutane	C4H10	75-28-5	58.12	0.12	-	-
1-Butene	C4H8	106-98-9	56.11	0.16	-	-
Butane	C4H10	106-97-8	58.12	0.38	-	-
Trans-2-Butene	C4H8	624-64-6	56.10	0.25	-	-
Cis-2-Butene	C4H8	590-18-1	56.10	0.21	-	-
Isopentane	C5H12	78-78-4	72.15	0.15	-	-
1-Pentene	C5H10	109-67-1	70.13	0.14	-	-
Pentane	C5H12	109-66-0	72.15	0.15	-	-
Isoprene	C5H8	78-79-5	68.12	0.39	2B	-
Trans-2-Pentene	C5H10	646-04-8	70.13	0.14	-	-
Cis-2-Pentene	C5H10	627-20-3	70.13	0.14	-	-
2,2-Dimethylbutane	C6H14	75-83-2	86.17	0.18	-	-
Cyclopentane	C5H10	287-92-3	70.13	0.14	-	-
2,3-Dimethylbutane	C6H4	79-29-8	86.17	0.21	-	-
2-Methylpentane	C6H14	107-83-5	86.17	0.18	-	-
3-Methylpentane	C6H14	96-14-0	86.17	0.18	-	-
1-Hexene	C6H12	592-41-6	84.16	0.17	-	-
Hexane	C6H14	110-54-3	86.17	0.18	-	-
2,4-Dimethylpentane	C7H16	108-08-7	100.2	0.20	-	-
Benzene	C6H6	71-43-2	78.11	1.02	1	A
Cyclohexane	C6H12	110-82-7	84.16	0.17	-	-
2,3-Dimethylpentane	C7H16	565-59-3	100.2	0.20	-	-
3-Methylhexane	C7H16	589-34-4	100.2	0.20	-	-
2,2,4-Trimethylpentane	C8H18	540-84-1	114.2	0.23	-	-
Heptane	C7H16	142-82-5	100.2	0.70	-	-
Methylcyclohexane	C7H14	108-87-2	98.19	0.20	-	-
Toluene	C6H5CH3	108-88-3	92.14	1.02	3	-
2-Methylheptane	C8H18	592-27-8	114.2	0.23	-	-
3-Methylheptane	C8H18	589-81-1	114.2	0.23	-	-

n-Octane	C8H18	111-65-9	114.2	0.23	-	-
Ethylbenzene	C6H5C2H5	100-41-4	106.2	0.22	2B	D
m / p-Xylene	C6H4(CH3)2	108-38-3;106-42-3	106.2	0.22	3	-
Styrene	C6H5CH=CH2	100-42-5	104.2	0.21	2B	-
o-Xylene	C6H4(CH3)2	95-47-6	106.2	0.22	3	-
n-Nonane	C9H20	111-84-2	128.3	0.26	-	-
Cumene (Isopropylbenzene)	C9H12	98-82-8	120.2	1.33	2B	D
n-Propylbenzene	C9H12	103-65-1	120.2	0.25	-	-
m-Ethyltoluene	C9H12	620-14-4	120.2	0.25	-	-
p-Ethyltoluene	C9H12	622-96-8	120.2	0.25	-	-
1,3,5-Trimethylbenzene	C6H3(CH3)3	108-67-8	120.2	0.25	-	-
o-Ethyltoluene	C9H12	611-14-3	120.2	0.25	-	-
1,2,4-Trimethylbenzene	C6H3(CH3)3	95-63-6	120.2	0.25	-	-
n-Decane	C10H22	124-18-5	142.3	0.29	-	-
1,2,3-Trimethylbenzene	C9H12	526-73-8	120.2	0.25	-	-
m-Diethylbenzene	C10H14	141-93-5	134.2	0.27	-	-
p-Diethylbenzene	C10H14	105-05-5	134.2	0.27	-	-
n-Undecane	C11H24	1120-21-4	156.3	0.32	-	-
Dodecane	C12H26	112-40-3	170.3	0.35	-	-

WHO (IARC)	U.S.EPA (IRIS)
Group 1:the agent is carcinogenic to humans	Group A: human carcinogen
Group 2A:the agent is probably carcinogenic to humans	Group B1: probable carcinogen, limited human evidence
Group 2B:the agent is possibly carcinogenic to humans	Group B2: probable carcinogen, sufficient evidence in animals
Group 3:the agent is not classifiable with respect to its carcinogenicity to humans	Group C: possible human carcinogen
	Group D: not classifiable as to human carcinogenicity
Group 4:the agent is probably not carcinogenic to humans	Group E: evidence of non-carcinogenicity for humans

Supplementary Table S2 List of volatile organic compounds (VOCs) in Urban Air Toxics standards.

VOCs	Molecular formula	CAS NO.	Molecular weight	Detection Limit (μg/m^3)	Classification	
					WHO (IARC)	U.S.EPA (IRIS)
Dichlorodifluoromethane	CCl2F2	75-71-8	120.9	0.79	-	-
Chloromethane	Ch3Cl	74-87-3	50.49	0.41	3	D
1,2-Dichlorotetrafluoroethane	C2Cl2F4	76-14-2	170.9	1.33	-	-
Vinyl chloride (Chloroethene)	H2C=CHCl	75-01-4	62.50	0.41	1	A
1,3-Butadiene	H2C=CHCH=CH2	106-99-0	54.09	0.44	1	B2
Bromomethane	CH3Br	74-83-9	94.94	0.82	3	D
Chloroethane	CH2ClCH3	75-00-3	64.52	0.98	3	-
Trichlorofluoromethane	CCl3F	75-69-4	137.4	1.01	-	-
Acetone (2-Propanone)	C3H6O	67-64-1	58.08	0.81	-	-
1,1-Dichloroethene	H2C=CCl2	75-35-4	96.94	0.67	3	C
Carbon Disulfide	CS2	75-15-0	76.14	0.40	-	-
Dichloromethane (Methylene Chloride)	CH2Cl2	75-09-2	84.93	0.52	2B	B2
112-Trichloro-122-Trifluoroethane	CF2ClCFCl2	76-13-1	187.4	1.23	-	-
Trans-1,2-Dichloroethene	C2H2Cl2	156-60-5	96.94	0.52	-	-
1,1-Dichloroethane	ClCH2CH2Cl	75-34-3	98.96	0.65	-	C
2-Methoxy-2-Methyl-Propane (MTBE)	C5H12O	1634-04-4	88.15	0.54	3	-
Vinyl Acetate	C4H6O2	108-05-4	86.09	0.49	2B	-
2-Butanone (MEK)	C4H8O	78-93-3	72.11	0.91	-	-
cis-1,2-Dichloroethene	ClCH=CHCl	156-59-2	96.94	0.59	-	-
Chloroform	CHCl3	67-66-3	119.4	0.73	2B	B2
Ethyl Acetate (EAC)	C4H8O2	141-78-6	88.11	0.58	-	-
Tetrahydrofuran (THF)	C4H8O	109-99-9	72.11	0.83	-	-
1,2-Dichloroethane	ClCH2CH2Cl	107-06-2	98.96	0.40	2B	B2
1,1,1-Trichloroethane	CH3CCl3	71-55-6	133.4	0.38	3	-
Carbon Tetrachloride	CCl4	56-23-5	153.8	0.94	2B	B2
1,2-Dichloropropane	CH3CH(Cl)CH2Cl	78-87-5	113.0	0.97	3	-
Bromodichloromethane	CHBrCl2	75-27-4	163.8	1.34	2B	-
Trichloroethene	ClCH=CCl2	79-01-6	131.4	1.02	1	A
1,4-Dioxane	C4H8O2	123-91-1	88.11	0.90	2B	B2
Cis-1,3-Dichloropropene	ClCH2CH=CHCl	10061-01-5	111.0	1.04	-	-

4-Methyl-2-Pentanone (MIBK)	C6H12O	108-10-1	100.2	0.74	2B	-
Trans-1,3-Dichloropropene	ClCH2CH=CHCl	10061-02-6	111.0	0.73	-	-
1,1,2-Trichloroethane	ClCH2CHCl2	79-00-5	133.4	0.98	3	C
Dibromochloromethane	CHBrCl2	124-48-1	208.3	1.62	3	-
2-Hexanone	C6H12O	591-78-6	100.2	0.94		-
1,2-Dibromoethane	CH2BrCH2Br	106-93-4	187.9	1.23	2A	B2
Tetrachloroethylene	Cl2C=CCl2	127-18-4	165.8	1.15	2A	B2
Chlorobenzene	C6H5Cl	108-90-7	112.6	0.78	-	D
Bromoform	CHBr3	75-25-2	252.7	1.76	3	B2
1,1,2,2-Tetrachloroethane	Cl2CHCHCl2	79-34-5	167.9	1.65	2B	C
1,3-Dichlorobenzene	C6H4Cl2	541-73-1	147.0	0.90	3	-
Benzyl chloride	C7H7Cl	100-44-7	126.6	1.60	2A	B2
1,4-Dichlorobenzene	C6H4Cl2	106-46-7	147.0	1.74	2B	-
1,2-Dichlorobenzene	C6H4Cl2	95-50-1	147.0	1.38	3	D
1,2,4-Trichlorobenzene	C6H3Cl3	120-82-1	181.5	2.23	4	D
Hexachlorobutadiene	Cl2C=CClCCl=CCl2	87-68-3	260.8	4.26	3	C

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	Group E: evidence of non-carcinogenicity for humans

Supplementary Table S3 Ratios of BTEXs normalized by ethylene and benzene, and weather condition in Taoyuan and Zhongli on sampling dates (9 a.m. to 3 p.m.)

Sampling dates	Area	Ratios of BTEXs									Weather condition			
		B/E	T/E	m/p-X/E	O/E	X/E	T/B	m/p-X/B	O/B	X/B	Temperature (°C)	Relative humidity (%)	Wind Direction (°)	Wind Speed (m/s)
2010/08/26	Taoyuan	2.27	35.8	1.02	0.82	1.84	15.7	0.45	0.36	0.81	31.36	68.70	252.6	0.59
	Zhongli	0.00	9.69	2.08	1.17	3.25	-	-	-	-	31.20	66.17	331.9	0.91
2010/10/13	Taoyuan	0.00	26.1	2.53	1.13	3.65	-	-	-	-	29.38	73.51	187.0	0.40
	Zhongli	0.00	11.9	3.18	1.37	4.55	-	-	-	-	28.56	75.57	281.8	0.54
2010/11/19	Taoyuan	-	-	-	-	-	-	-	-	-	22.10	84.12	189.7	0.72
	Zhongli	0.00	12.8	3.41	1.37	4.78	-	-	-	-	20.83	89.11	265.3	0.33
2010/12/24	Taoyuan	0.00	11.7	2.04	1.15	3.19	-	-	-	-	20.33	71.68	79.33	2.37
	Zhongli	0.00	13.1	3.10	1.40	4.50	-	-	-	-	19.56	70.75	161.0	0.26
2011/02/25	Taoyuan	0.00	35.9	2.11	1.21	3.33	-	-	-	-	20.76	76.52	86.21	2.76
	Zhongli	0.00	13.4	1.81	1.31	3.12	-	-	-	-	19.97	79.10	307.0	0.28
2011/04/01	Taoyuan	0.00	48.0	1.69	0.00	1.69	-	-	-	-	23.56	58.72	214.4	0.83
	Zhongli	4.90	21.1	2.37	1.10	3.47	4.30	0.48	0.22	0.71	22.30	59.15	285.6	0.37
2011/05/18	Taoyuan	-	-	-	-	-	-	-	-	-	27.86	63.21	177.1	1.04
	Zhongli	-	-	-	-	-	-	-	-	-	26.51	63.94	294.7	0.31
2011/06/24	Taoyuan	-	-	-	-	-	-	-	-	-	32.12	58.49	91.59	3.84
	Zhongli	-	-	-	-	-	-	-	-	-	32.22	58.57	213.7	0.58

Note: B: benzene; T: toluene; E: ethylbenzene; X: xylenes.

SUPPLEMENTARY FIGURE LEGENDS

Figure S1 Locations of sampling sites in (a) Taoyuan (sites T1-T4) and (b) Zhongli (sites Z1 and Z2)

Figure S2 Boxplots for concentrations of alkane, ketone, and aromatics by sampling season from August 2010 to June 2011

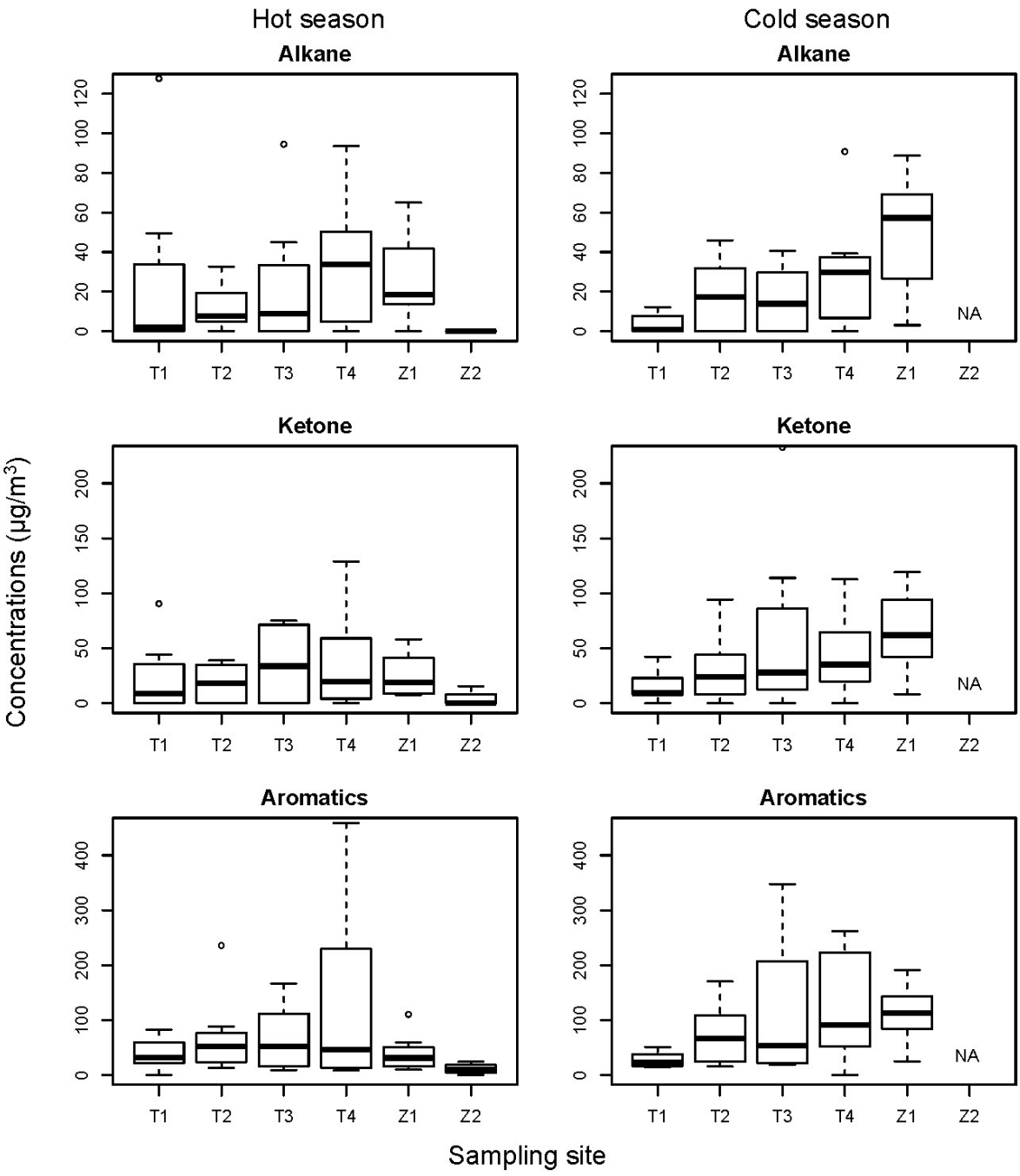
Figure S3 Boxplots for concentrations of alkane, ketone, and aromatics by sampling time period (9-11 AM and 13-15 PM) from August 2010 to June 2011

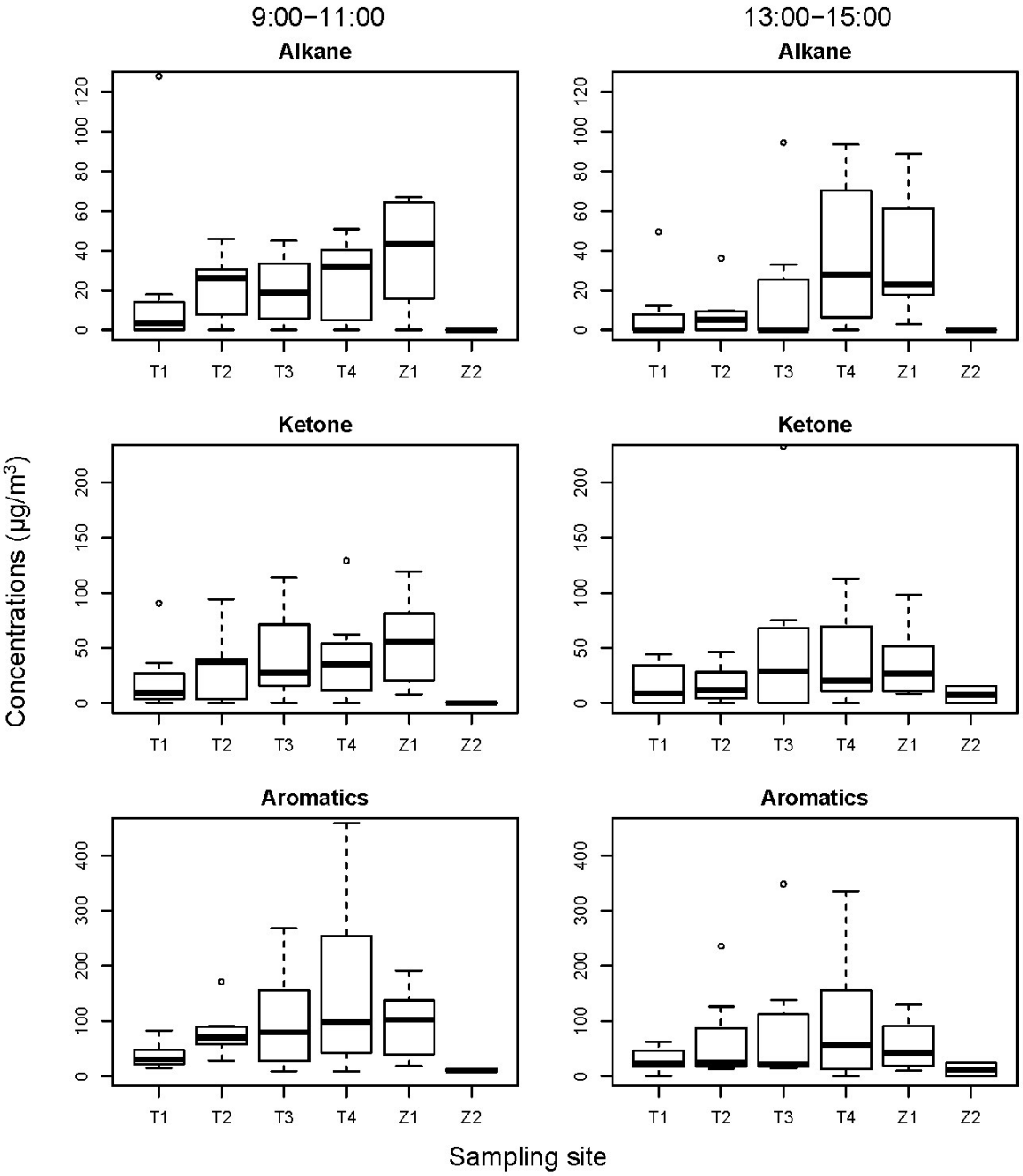
Figure S4 Pollution roses for ambient alkane, aromatics, and ketone by sampling sites from August 2010 to June 2011

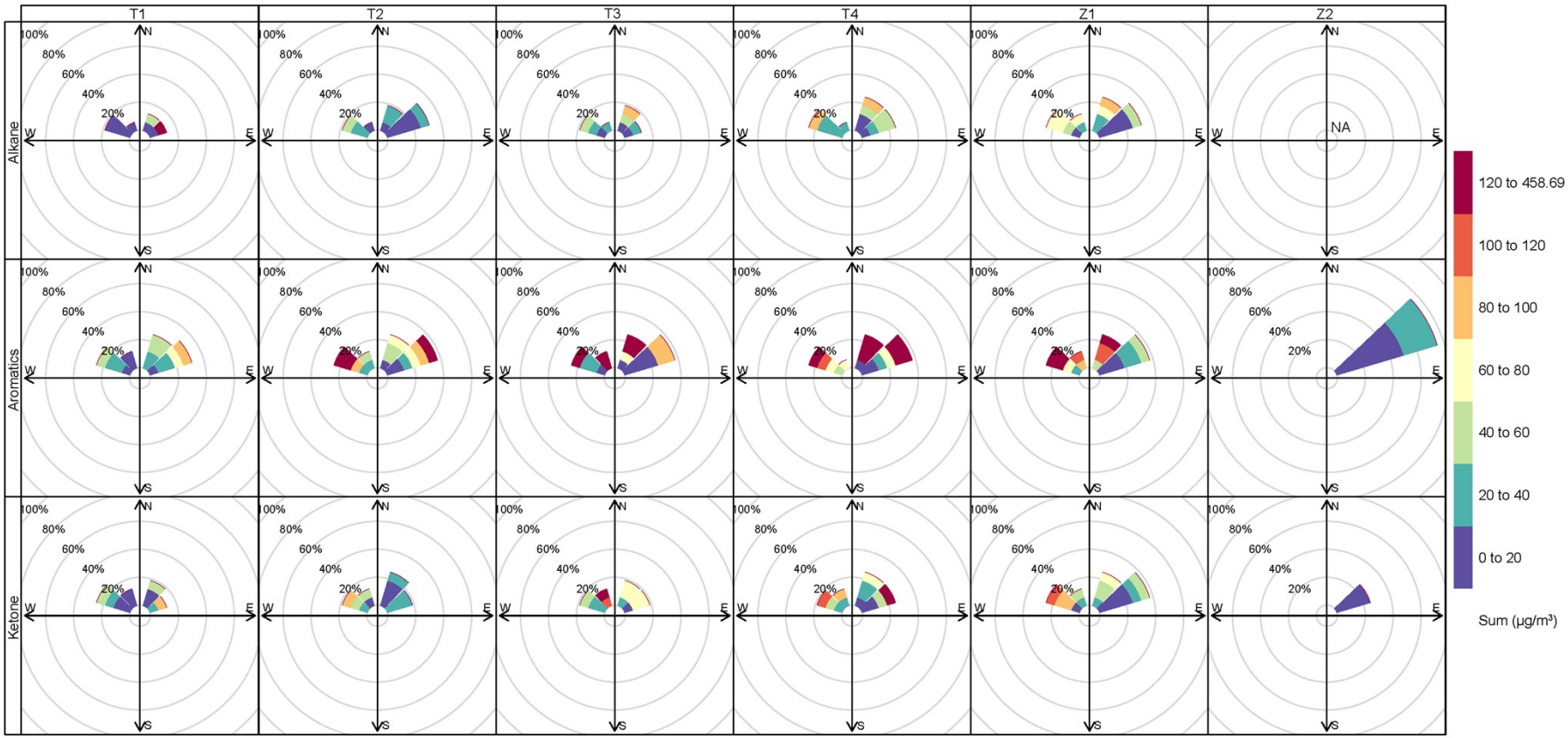
Figure S5 Pollution roses for ambient alkene, ester, and ether by sampling sites from August 2010 to June 2011

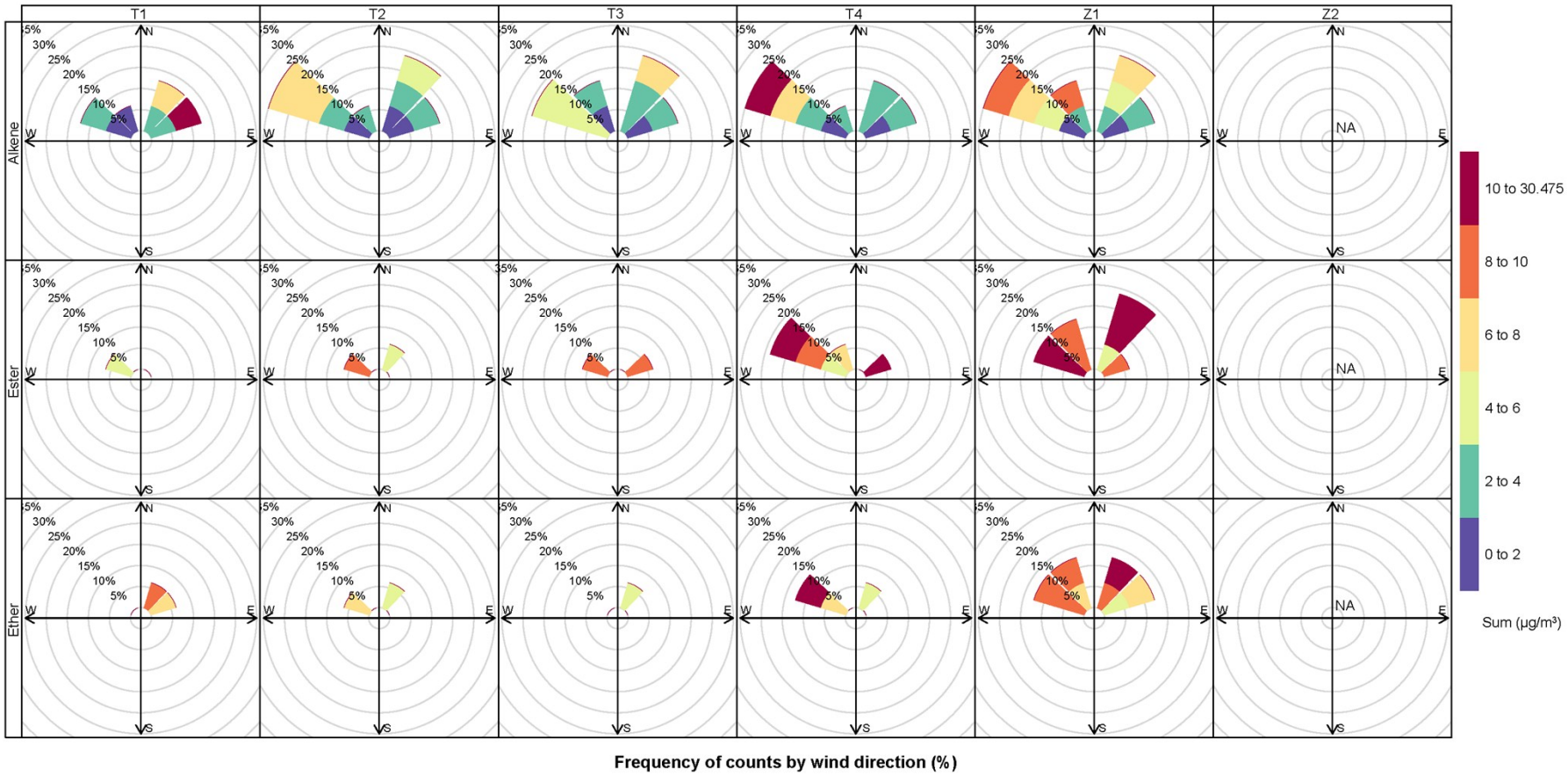
Figure S6 Pollution roses for ambient toluene, 2-butanone, and acetone by sampling sites from August 2010 to June 2011.

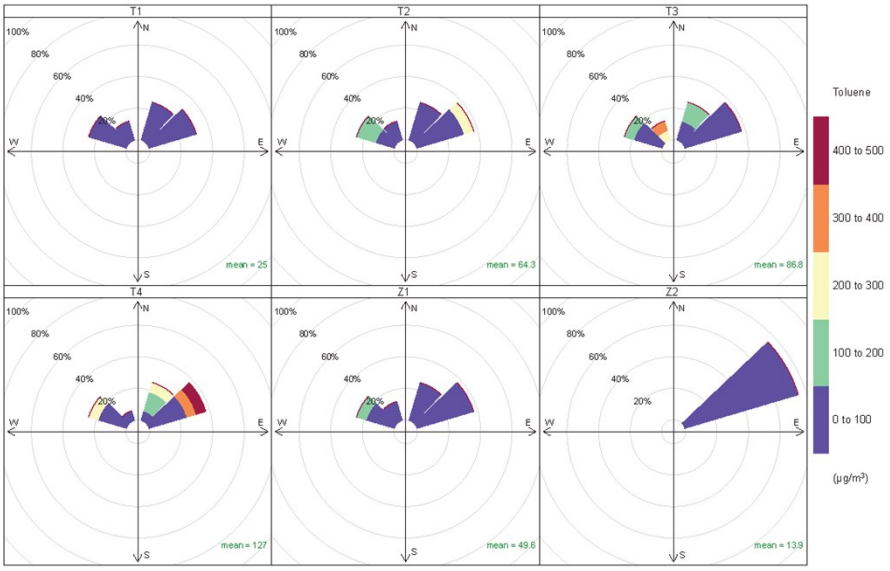

(a)
N
Sun Yat-sen Freeway
T1
Taoyuan Refinery Plant
T2
T4
T3
0 0.45 0.9 km
25°3'0"N
25°2'30"N
25°2'0"N
25°1'30"N
25°1'0"N
121°17'30"E
121°18'0"E
121°18'30"E
(b)
N
Sun Yat-sen Freeway
Z1
Z2
0 0.45 0.9 km
24°58'0"N
24°57'30"N
24°57'0"N
24°56'30"N
121°11'30"E
121°12'0"E
121°12'30"E
121°13'0"E
N


Hot season
Cold season
Alkane
Ketone
Aromatics
Concentrations (µg/m3)
Sampling site
T1
T2
T3
T4
Z1
Z2
NA

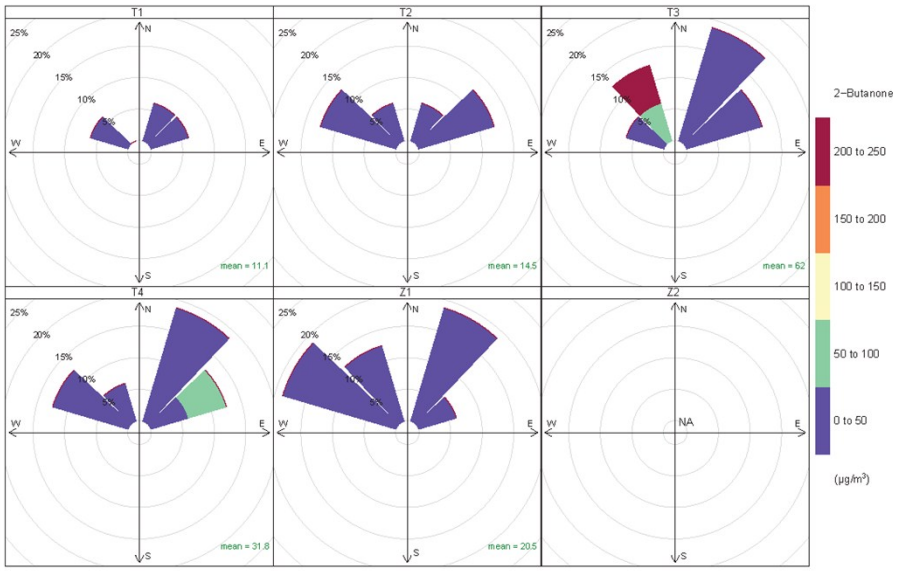

9:00−11:00
13:00−15:00
Alkane
Ketone
Aromatics
Concentrations (μg/m3)
Sampling site
T1
T2
T3
T4
Z1
Z2


T1
T2
T3
T4
Z1
Z2
Alkane
Aromatics
Ketone
100%
80%
60%
40%
20%
N
S
W
E
NA
120 to 458.69
100 to 120
80 to 100
60 to 80
40 to 60
20 to 40
0 to 20
Sum (μg/m³)
Frequency of counts by wind direction (%)

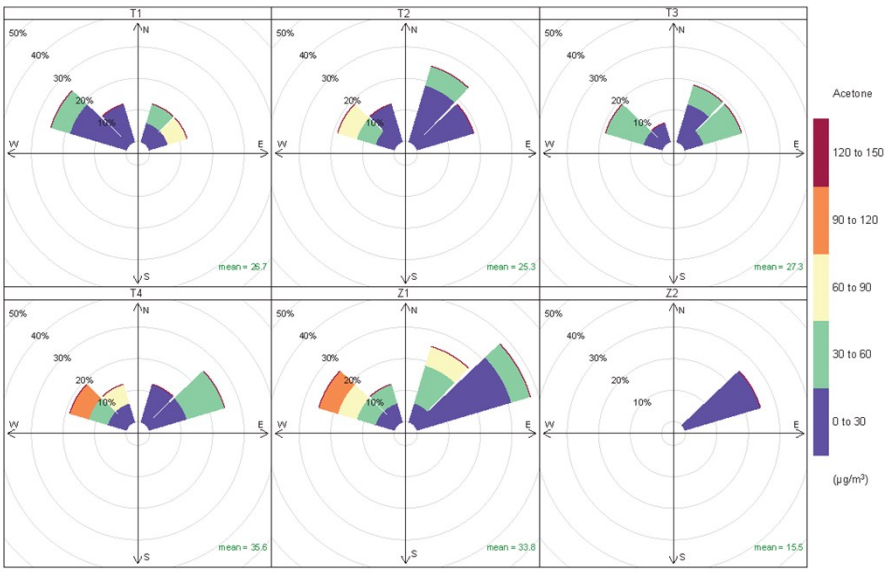

T1
T2
T3
T4
Z1
Z2
Alkene
Ester
Ether
N
S
W
E
5%
10%
15%
20%
25%
30%
NA
10 to 30.475
8 to 10
6 to 8
4 to 6
2 to 4
0 to 2
Sum (µg/m³)
Frequency of counts by wind direction (%)



Frequency of counts by wind direction (%)



Frequency of counts by wind direction (%)



Frequency of counts by wind direction (%)