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Multi-site non-methane hydrocarbon source apportionment and ozone insights in Southern Taiwan using positive matrix factorization

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Table S1. Summary of selected NMHC compounds with MDL, MIR values, and S/N ratio-classified

No.	Compounds	MDL	MIR	S/N ratio-classified	No.	Compounds	MDL	MIR	S/N ratio-classified
1	Ethane	0.52	3.41	STRONG	28	2,3-Dimethylpentane	0.19	1.34	BAD
2	Ethylene	0.43	3.41	STRONG	29	3-Mehtylhexane	0.21	1.61	BAD
3	Acetylene	0.83	3.41	STRONG	30	2,2,4-Trimethylpentane	0.18	1.26	BAD
4	Propylene	0.18	11.66	STRONG	31	Heptane	0.45	1.07	BAD
5	Propane	0.28	0.49	STRONG	32	Methylcyclohexane	0.19	1.7	BAD
6	Isobutane	0.09	1.23	STRONG	33	2,3,4-Trimethylpentane	0.06	1.03	BAD
7	1-Butene	0.25	9.37	BAD	34	Toluene	0.41	4	STRONG
8	n-Butane	0.23	1.51	STRONG	35	2-Methylheptane	0.16	1.07	BAD
9	t-2-Butene	0.22	15.16	BAD	36	3-Methylheptane	0.16	1.24	BAD
10	cis-2-Butene	0.25	14.24	BAD	37	n-Octane	0.15	0.9	BAD
11	Isopentane	0.14	1.45	STRONG	38	Ethylbenzene	0.23	3.04	WEAK
12	1-Pentene	0.15	7.21	BAD	39	m,p-Xylene	0.24	7.795	STRONG
13	n-Pentane	0.12	1.31	STRONG	40	Styrene	0.17	1.73	BAD
14	Isoprene	0.17	10.61	WEAK	41	o-Xylene	0.3	7.64	BAD
15	t-2-Pentene	0.17	10.56	BAD	42	n-Nonane	0.12	0.78	BAD
16	cis-2-Pentene	0.27	10.38	BAD	43	Isopropylbenzene	0.24	2.52	BAD
17	2,2-Dimethylbutane	0.17	1.17	BAD	44	n-Propylbenzene	0.14	2.03	BAD
18	Cyclopentane	0.09	2.39	WEAK	45	m-Ethyltoluene	0.15	7.39	WEAK
19	2,3-Dimethylbutane	0.11	0.97	BAD	46	p-Ethyltoluene	0.23	4.44	BAD
20	2-Methylpentane	0.16	1.5	WEAK	47	1,3,5-Trimethylbenzene	0.42	11.76	BAD
21	3-Methylpentane	0.2	1.8	BAD	48	o-Ethyltoluene	0.22	5.59	BAD
22	n-Hexane	0.43	1.24	WEAK	49	1,2,4-Trimethylbenzene	0.14	8.87	STRONG
23	Methylcyclopentane	0.13	2.19	STRONG	50	n-Decane	0.09	0.68	BAD
24	2,4-Dimethylpentane	0.15	1.55	BAD	51	1,2,3-Trimethylbenzene	0.15	11.97	BAD
25	Benzene	0.57	0.72	WEAK	52	m-Diethylbenzene	0.16	7.1	BAD
26	Cyclohexane	0.3	1.25	WEAK	53	p-Diethylbenzene	0.21	4.43	BAD
27	2-Methylhexane	0.15	1.19	WEAK	54	n-Unecane	0.16	0.61	BAD

Table S2. Sensitivity of CPF directional patterns to percentile thresholds. Acetylene, whose source direction is well established as primarily originating from the northern industrial area, was used as a reference factor for this evaluation. CPF patterns were consistent between the 0.60 and 0.70 quantiles but became unstable above 0.75, as higher thresholds yielded fewer valid samples per sector and less coherent directional features. Therefore, the 0.70 quantile was determined to be the most appropriate solution, effectively filtering out moderate events while retaining sufficient data for statistically stable and interpretable CPF results.

Wind sector	CPF-0.6	CPF-0.65	CPF-0.7	CPF-0.75	CPF-0.8	CPF-0.85
1	1	1	1	1	1	0.895
2	0.803	0.799	0.799	0.747	0.631	0.486
3	0.379	0.379	0.379	0.268	0.172	0.111
4	0.202	0.191	0.169	0.135	0.079	0.034
5	0.140	0.116	0.093	0.093	0.093	0.047
6	0.233	0.178	0.068	0.041	0.027	0.014
7	0.287	0.207	0.069	0.023	0.011	0.011
8	0.319	0.181	0.026	0	0	0
9	0.595	0.214	0.048	0	0	0
10	0.308	0.192	0.077	0.077	0.038	0.038
11	0.367	0.306	0.245	0.143	0.122	0.082
12	0.181	0.111	0.056	0.028	0.014	0.014
13	0.170	0.112	0.076	0.054	0.036	0.022
14	0.545	0.545	0.545	0.500	0.455	0.364
15	0.900	0.900	0.900	0.900	0.800	0.700

Table S3. Statistical data of annual mean NMHC concentrations

Station	Mean ± SD (ppb)	Median (ppb)	Remove elevated period in August Mean ± SD (ppb)	Median (ppb)
Xiaogang	18.90 ± 11.85	13.68	–	–
Linyuan	28.20 ± 37.28	10.92	–	–
Chaozhou	9.88 ± 6.92	6.92	9.97 ± 5.82	7.10

Table S4. Summary and brief description of the eight distinct sources

Source	Key Species	Description
Petro I	Ethylene	Ethylene is the most important feedstock in the synthetic organic chemical manufacturing industry
Petro II	Propylene	Propylene is a critical precursor in producing various petrochemical products.
Refinery	C_3–C_5 alkanes	Associated with petroleum refining processes; distinct from petrochemical sources due to C_3–C_5 dominance and stability
Industrial fugitive emissions	n-Pentane, Isopentane	Isopentane and n-pentane are recognized tracers of natural gas or gasoline vapor emissions. The ratio of iC_5/nC_5 that smaller than 1, leading to the signs of downstream petrochemical operations, gasoline/fuel storage
Mixed factor	Toluene, Benzene, Ethylbenzene, m,p-Xylene, Cyclopentane, 2-methylpentane, methylcyclopentane, acetylene, n-hexane, and 1,2,4-trimethylbenzene	Combination of vehicle and solvent emissions; difficult to separate due to overlapping NMHCs
Aged air mass	Ethane, Propane, Acetylene, Benzene	Long-lived NMHCs from regional transport; representing secondary and transported sources
Biogenic	Isoprene	Vegetation emissions, sensitive to temperature and sunlight; local to agricultural areas (Chaozhou)
Acetylene	Acetylene	Local industrial source (cylinder filling); distinct single-species source at Linyuan
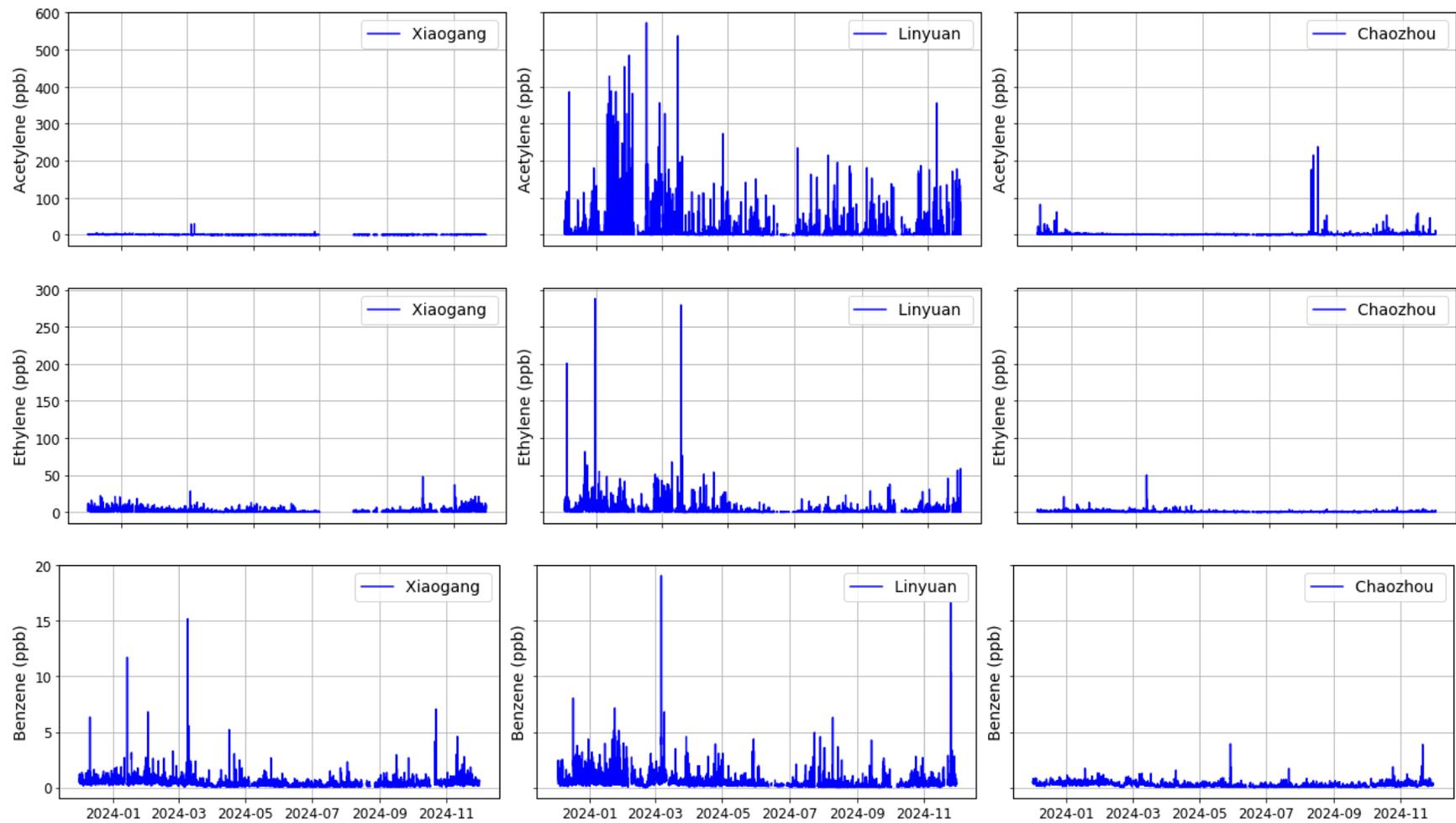
Figure S1 High-temporal-resolution PAMS data (01/12/2023 – 30/11/2024). Examples of acetylene, ethylene, and benzene species
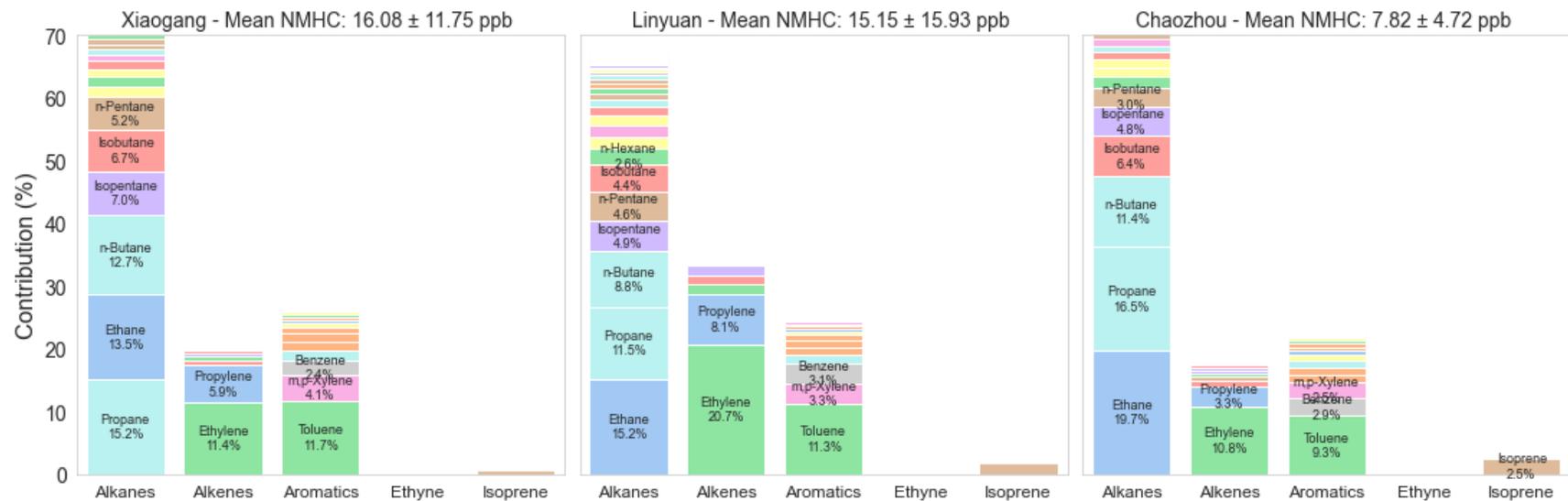
Figure S2 Mean NMHC concentrations (ppb) and percentage contributions of individual compounds within major chemical groups after removing acetylene
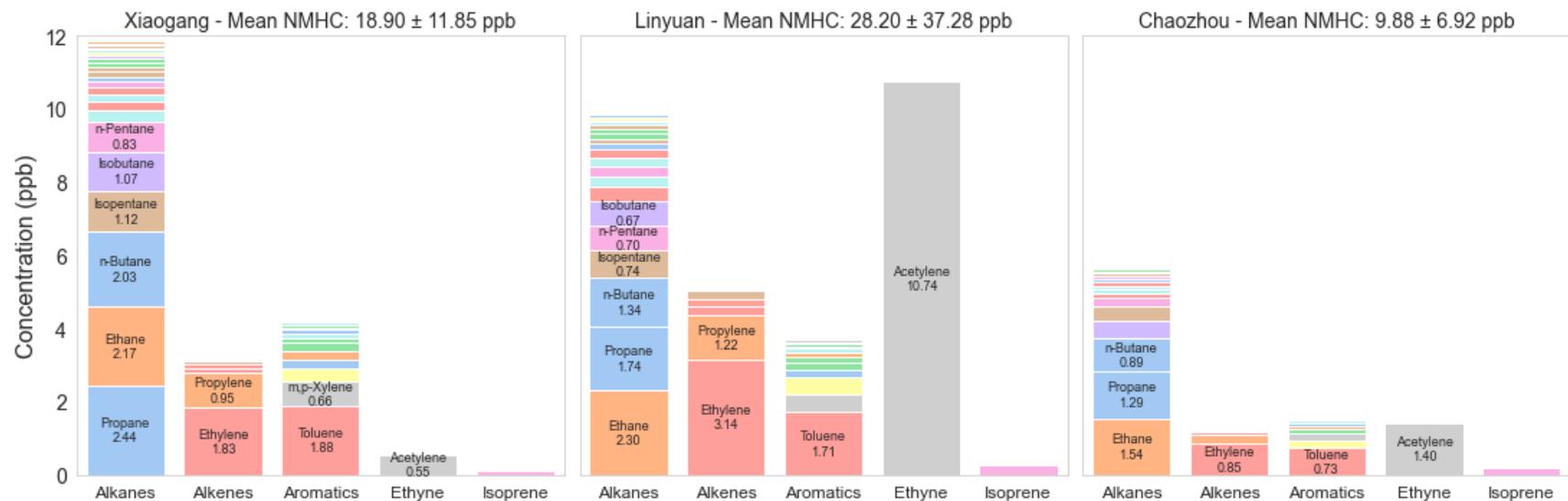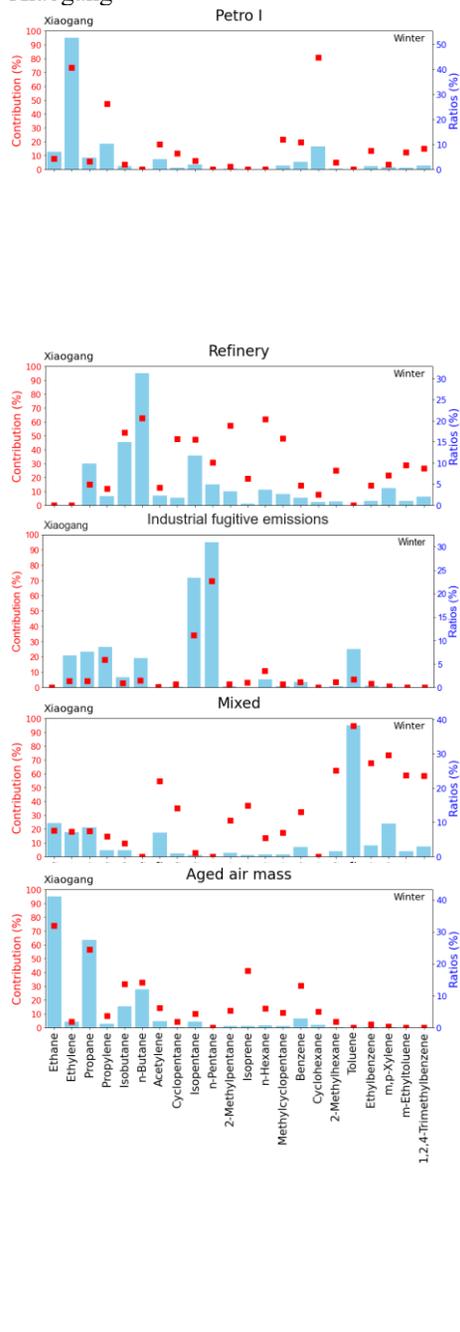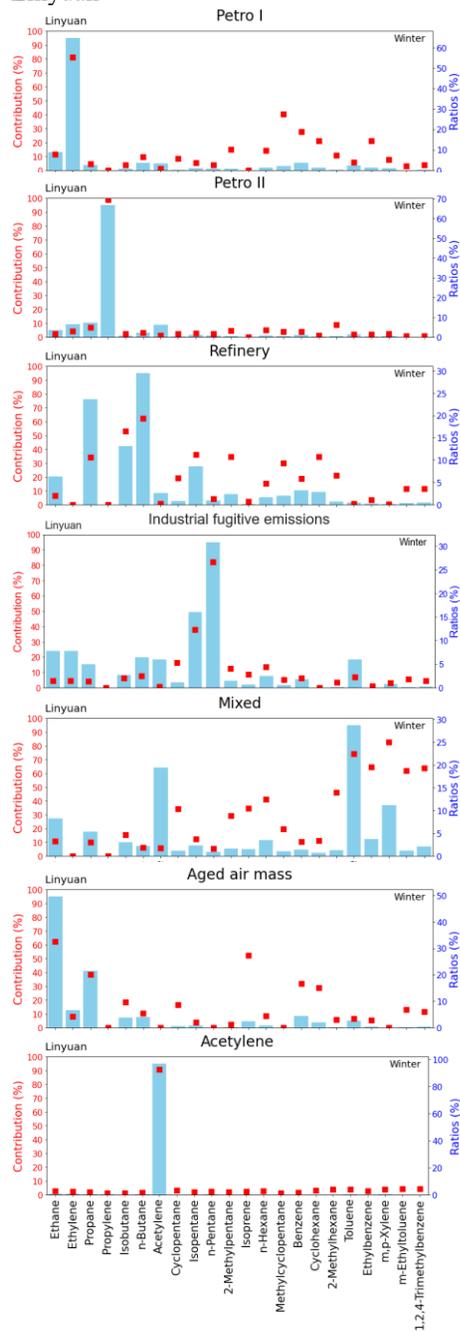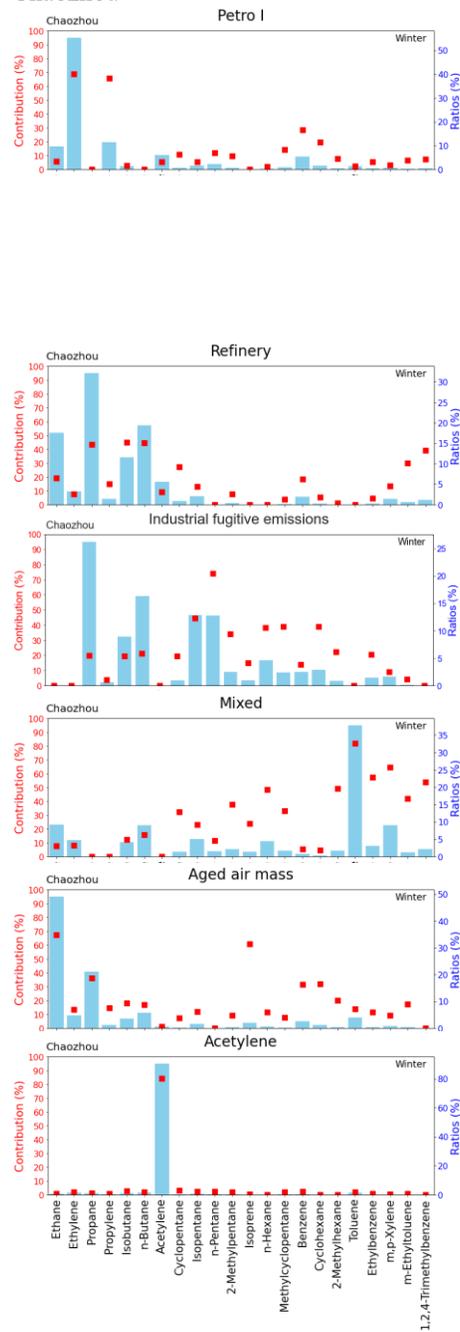

Figure S3 Annual mean of notable NMHC species

(a) PMF-resolved factor profiles in Winter

(b) PMF-resolved factor profiles in Spring
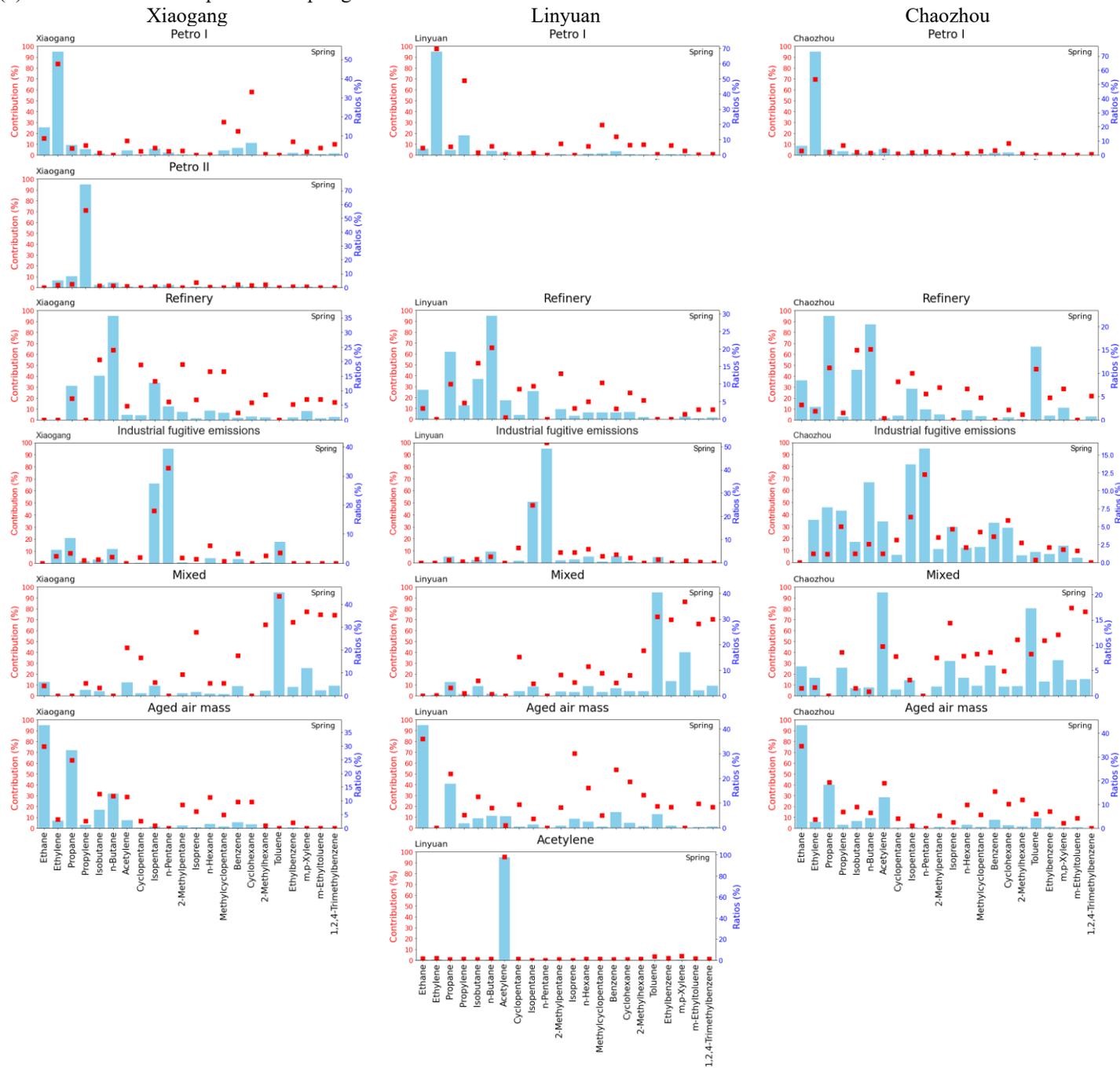
(c) PMF-resolved factor profiles in Summer
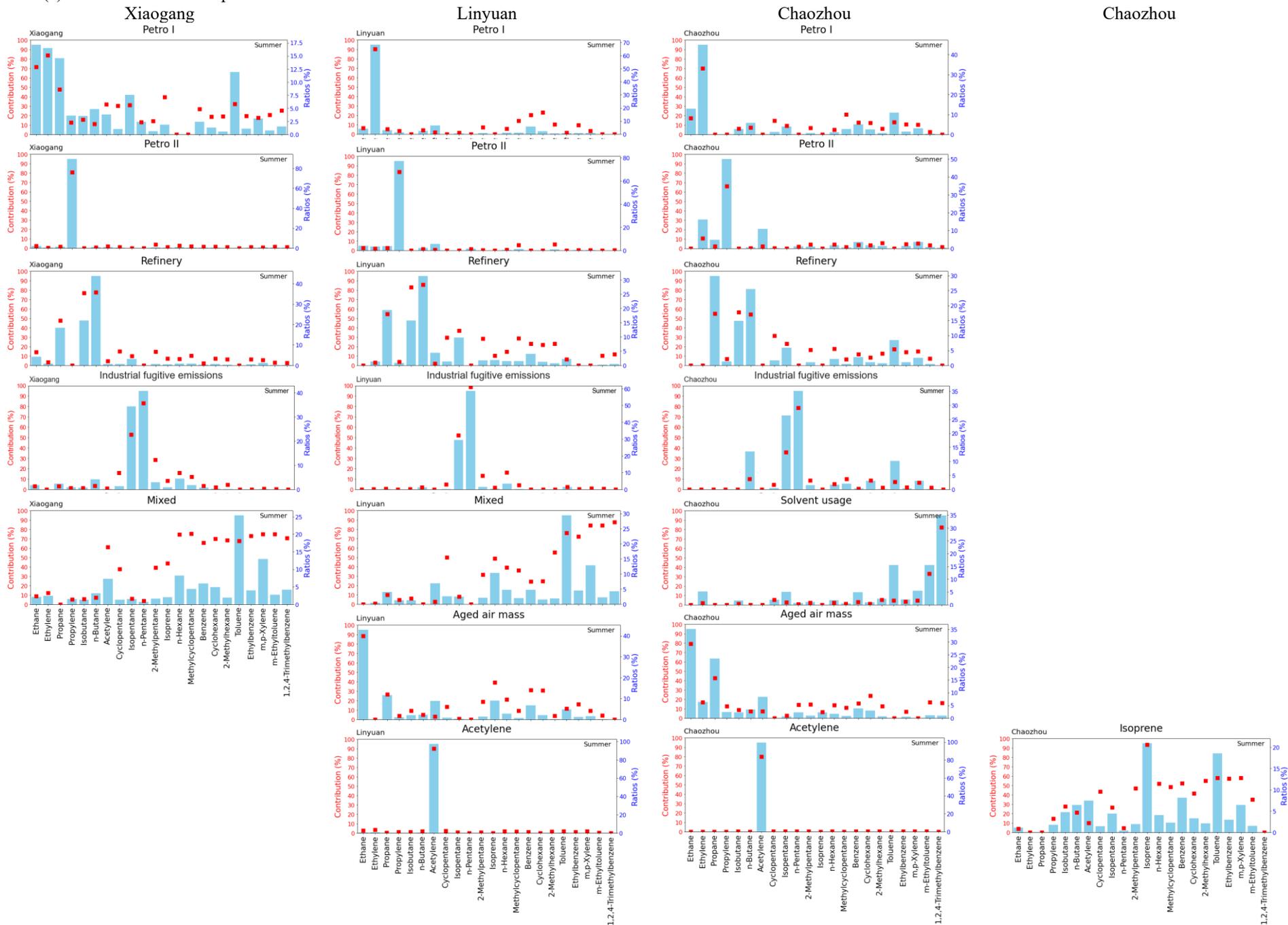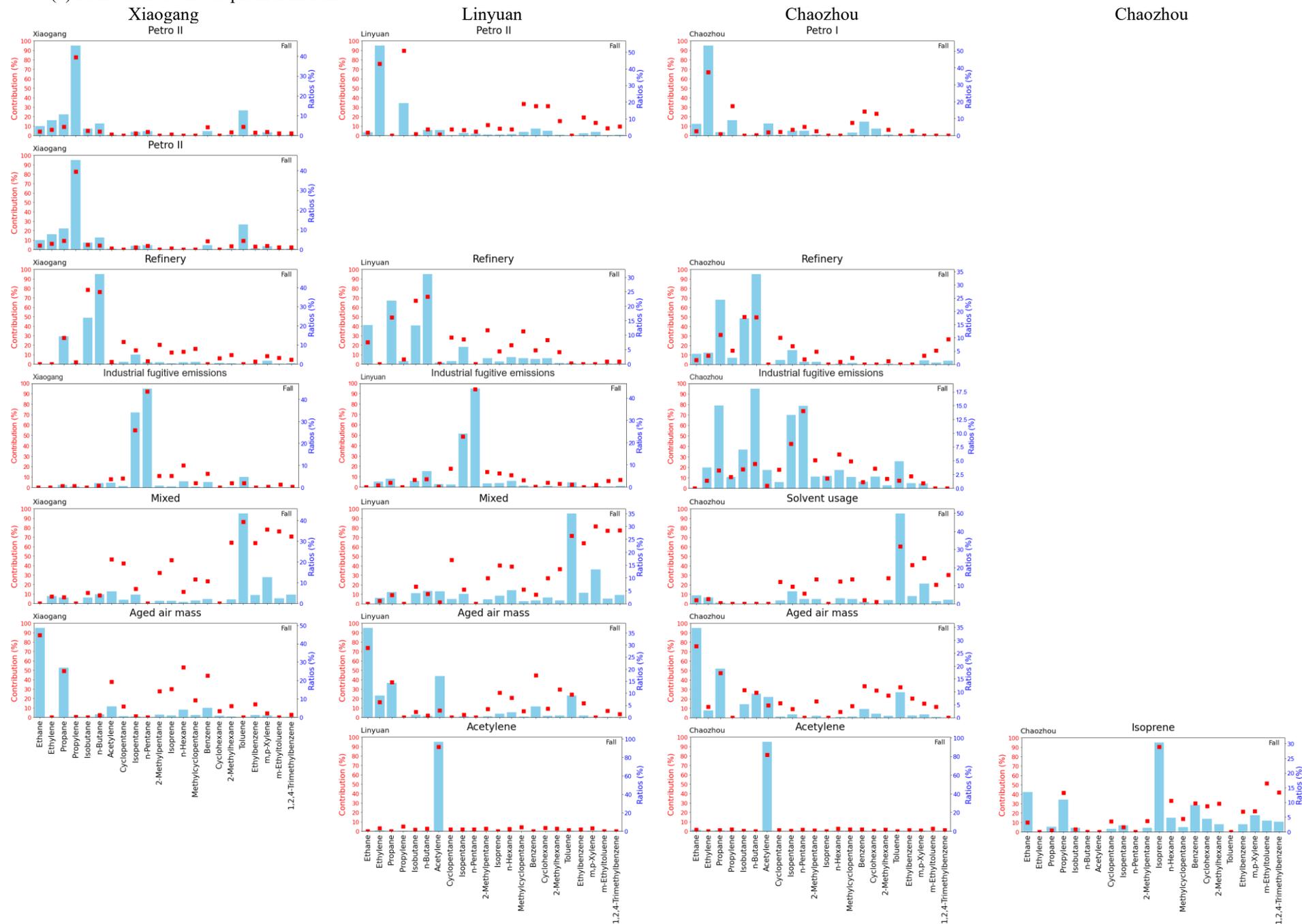
Figure S4 Seasonal PMF-resolved factor profiles at the study sites (a) winter, (b) spring, (c) summer, and (d) fall. Panels correspond to PAMS sites. Percentage contributions reflect relative patterns within each site; therefore, similar percentages do not necessarily correspond to similar absolute acetylene levels or emission characteristics. Species contribution in the factor profile is denoted by the red dot.
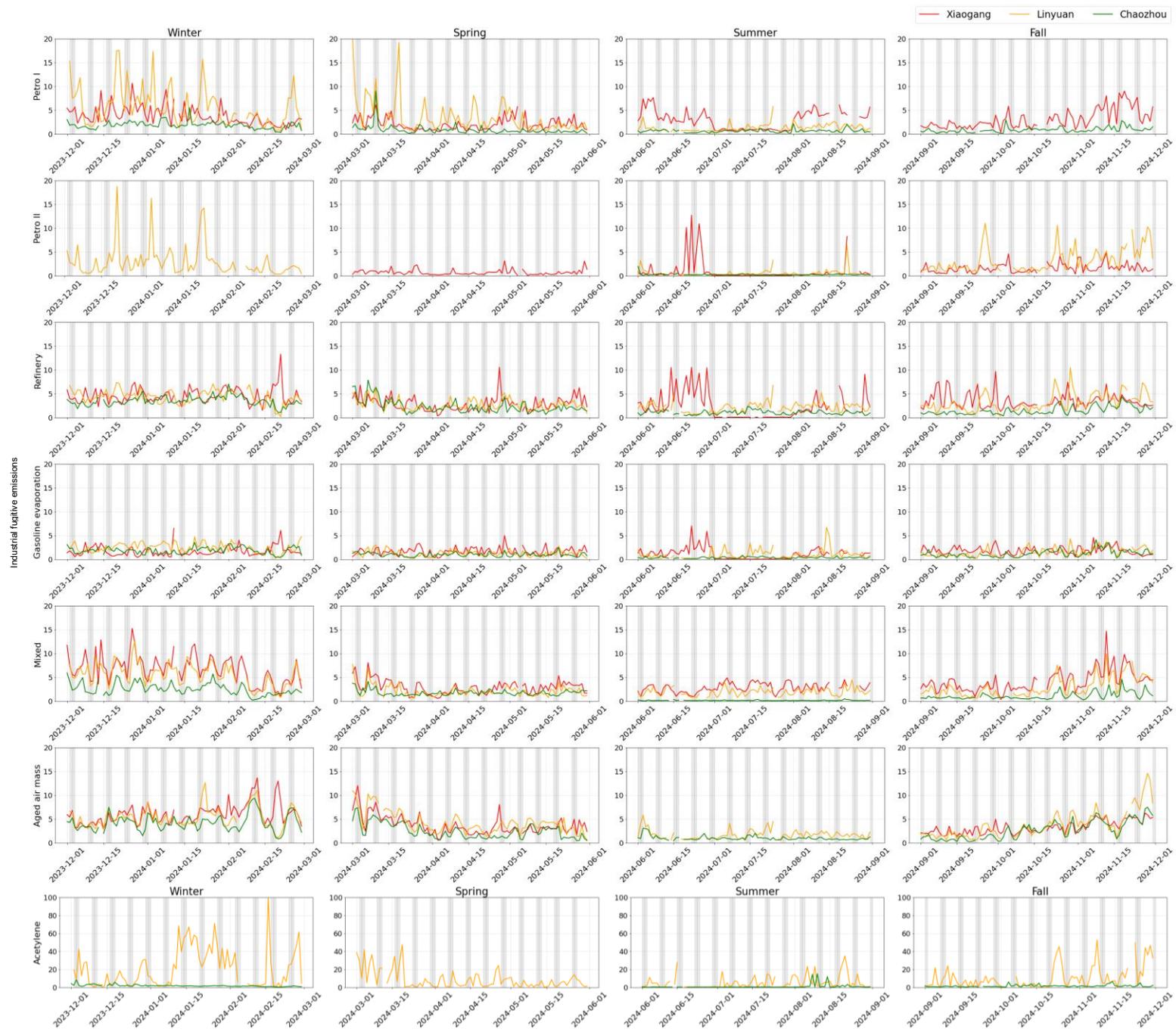
Figure S5 Seasonal variation of daily mean contributions of NMHC concentration from PMF-resolved factors. This figure illustrates the daily variability of identified source factors (Petro I, Petro II, Refinery, Industrial fugitive emissions, Mixed, Aged air mass, and Acetylene) over the course of a year at three monitoring sites: Xiaogang (red), Linyuan (orange), and Chaozhou (green). To interpret this figure, follow the trends of the lines for each site within each season to observe how a specific source factor changes over time and reveal episodic emission events that indicate the changes in source activity. Shaded columns represent weekends.
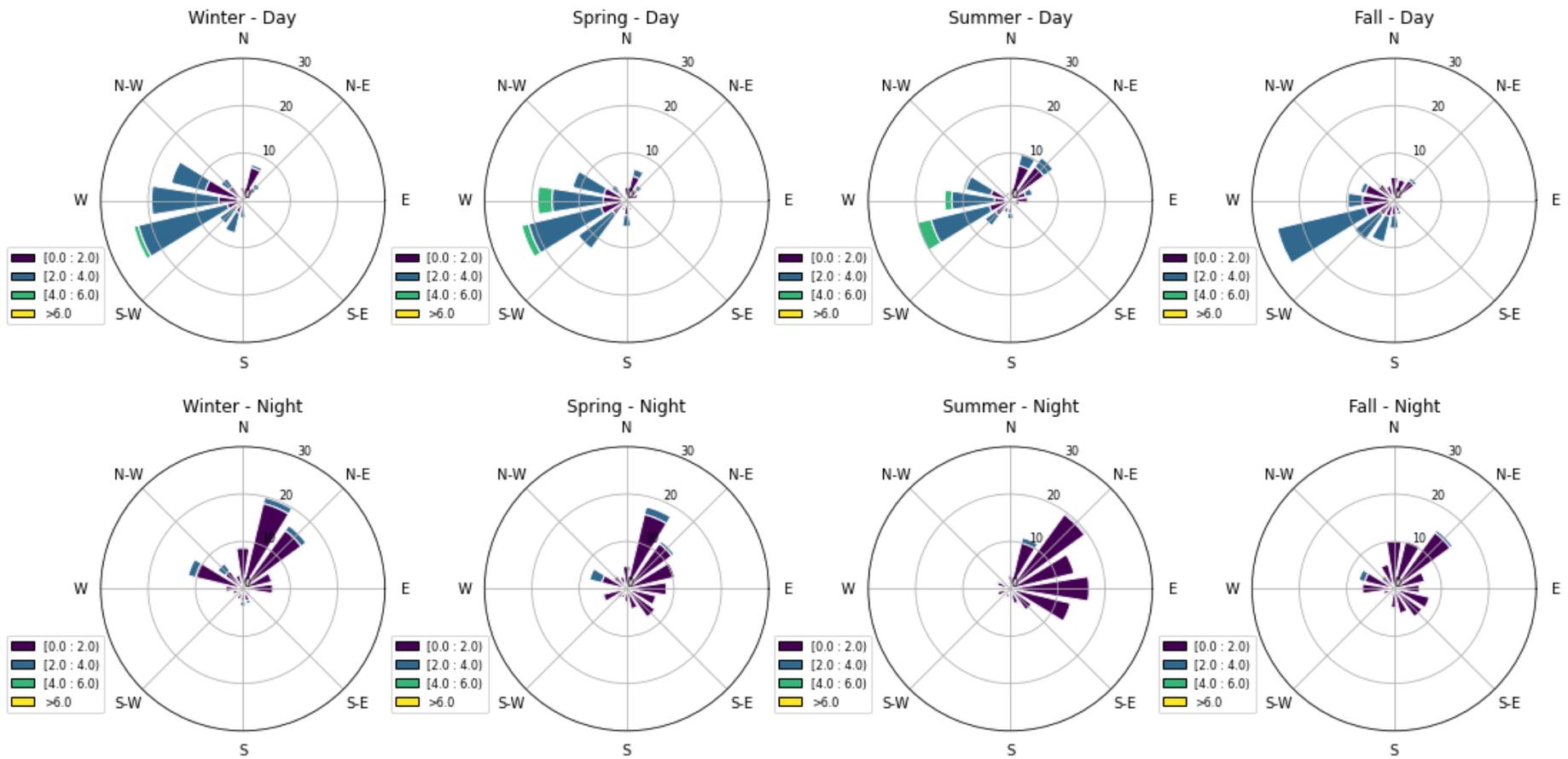
Figure S6 Day-Night wind profile for aged air mass factor at Chaozhou over the seasons with the top 30% contribution
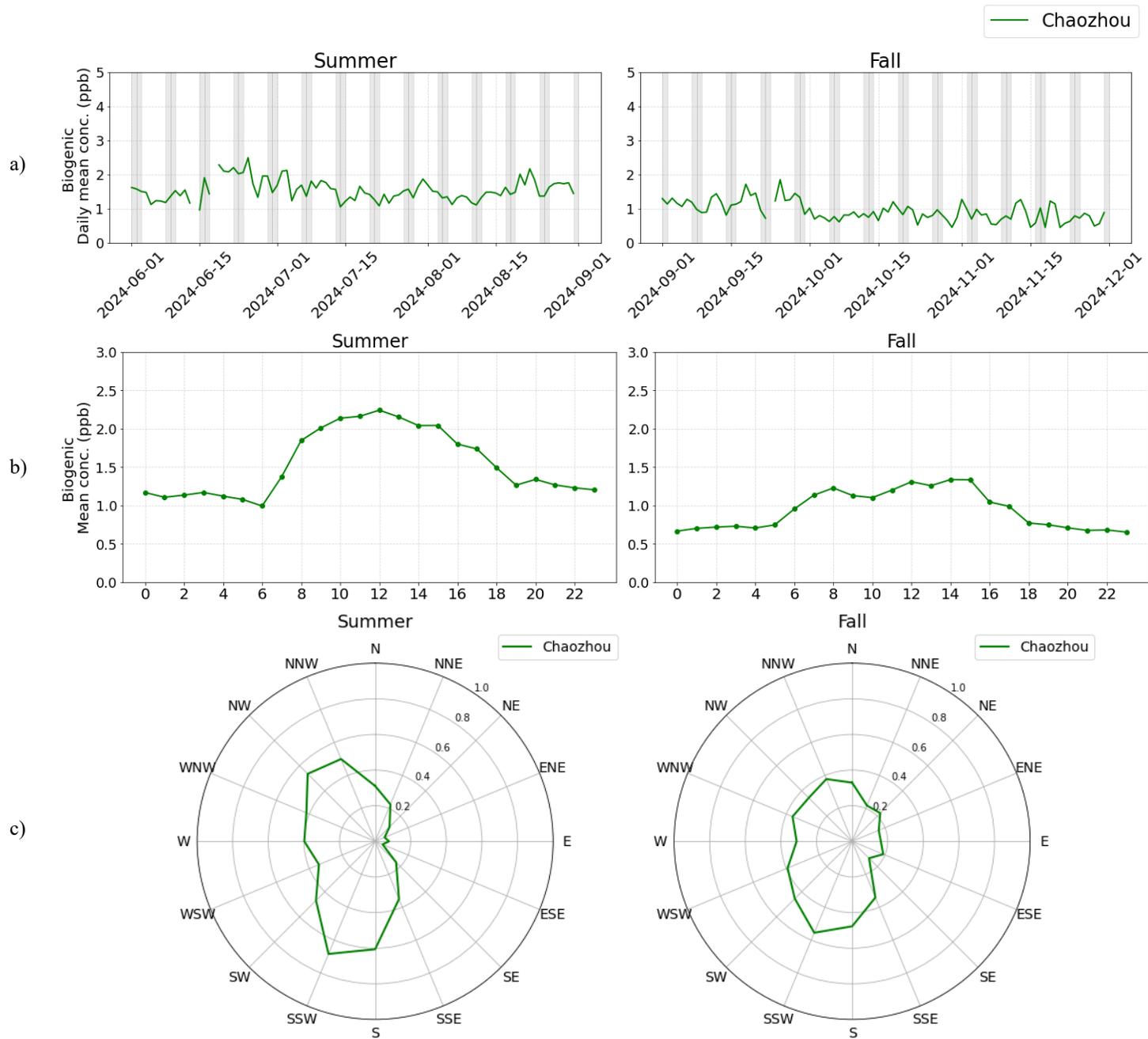
Figure S7 Temporal variation and CPF analysis for biogenic factors over the seasons, a) Timeseries of daily average factor contribution, b) Diurnal variation, and c) CPF analysis
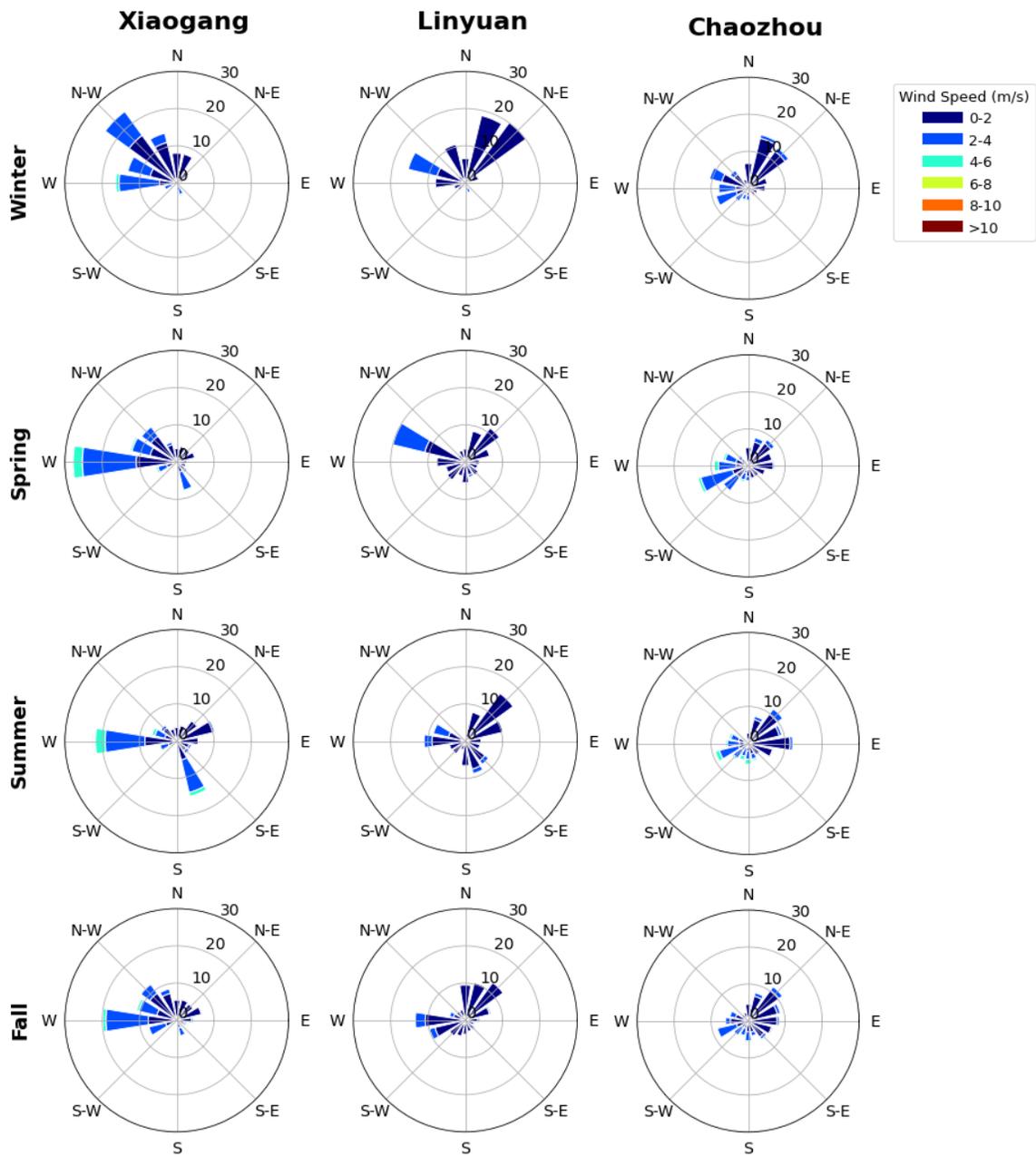
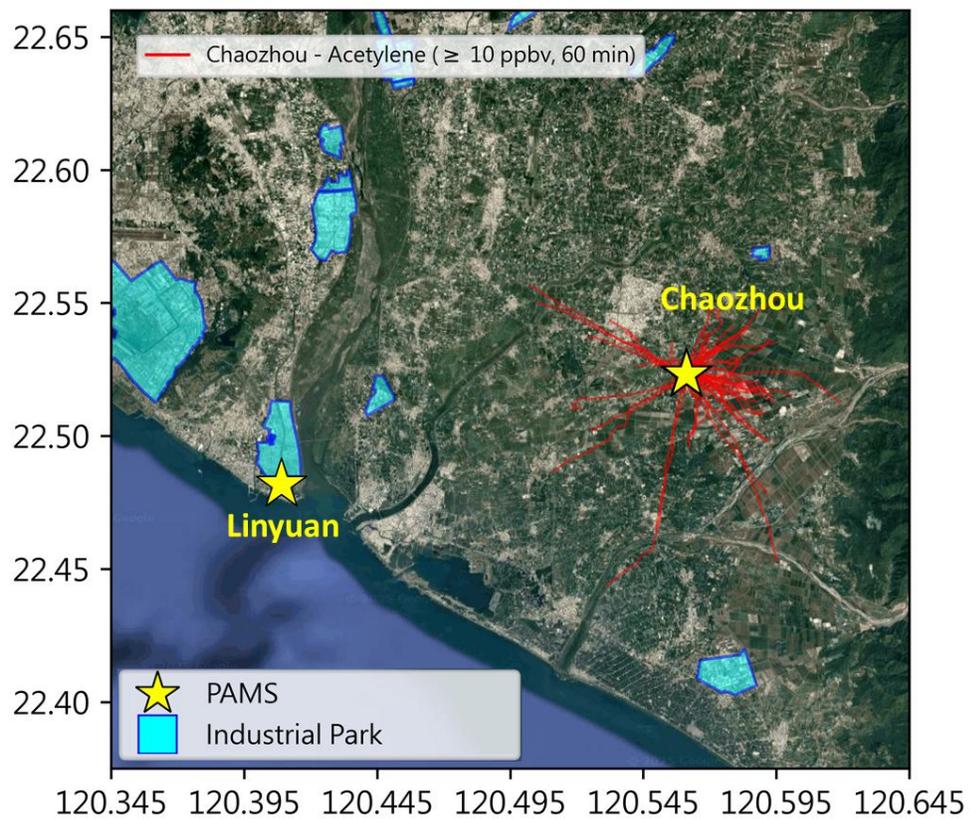**Figure S8** Seasonal wind profile at the three PAMS sites

Figure S9 Triggered back trajectory analysis of spike levels in Chaozhou. Base map from Google Maps (Map data ©2025 Google).
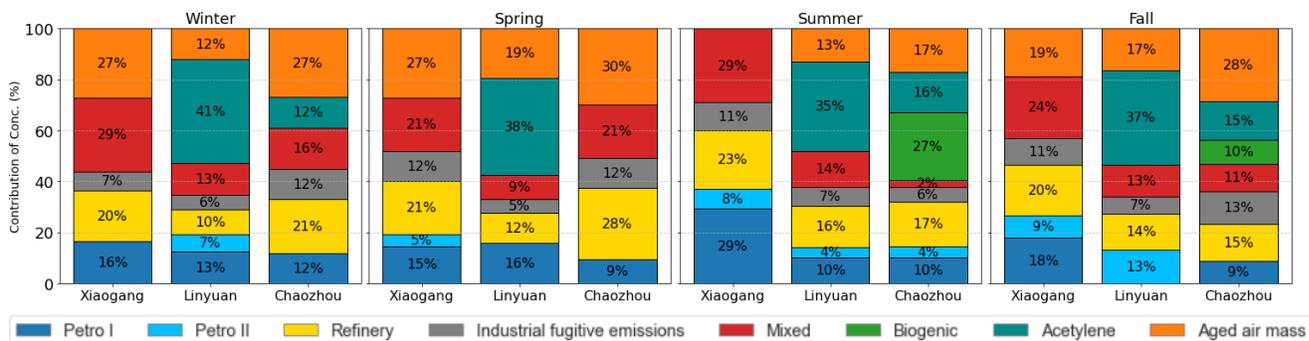
Figure S10 Contribution of concentration from eight resolved source factors. Xiaogang tends to have a relatively balanced influence among mixed, refinery, and aged air mass sources, suggesting complex source-receptor dynamics at this site. This reflects Xiaogang's transitional setting between industrial clusters and transportation hubs, where port activity, on-road emissions, and solvent-use industries intersect, producing overlapping chemical signals captured under the mixed factor.
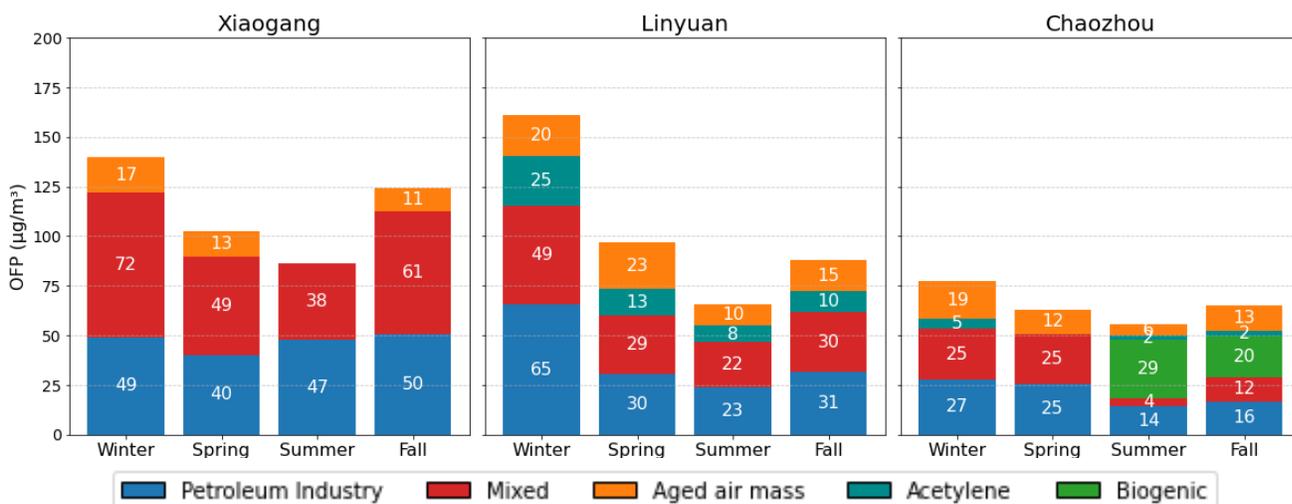

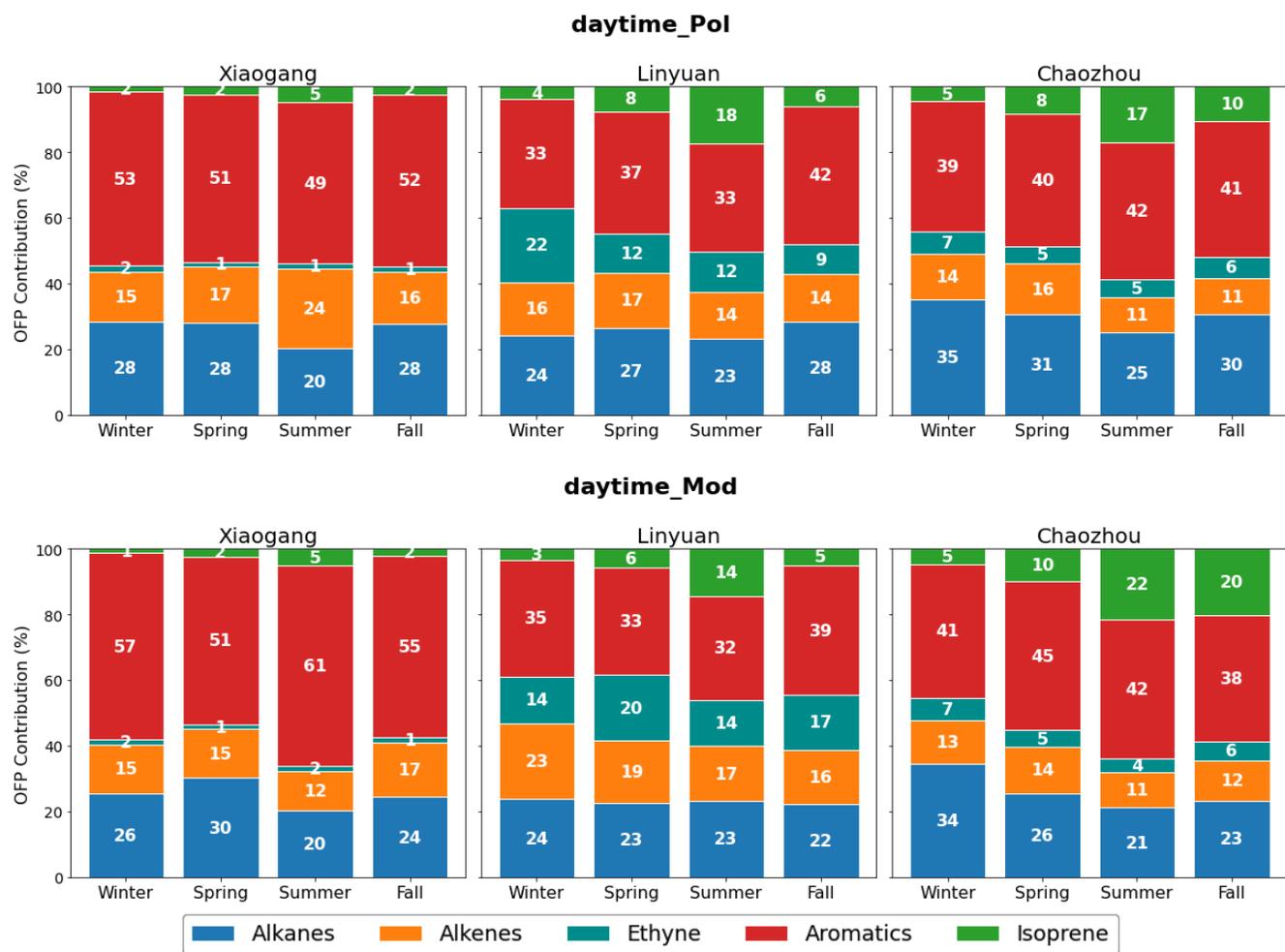**Figure S11** Ozone formation potential in the context of seasonal variation

Figure S12 Ozone formation potential in the context of species group variation during ozone pollution and moderate pollution days