Table S1. Concentrations of DCA and C_2 (ng m^{-3}) at different types of sampling sites.

Site type	Site	Sample type	Period	DCA	C_2	Reference
Urban	China, Shangdong	$PM_{2.5}$	January to February, 2017	1415 ± 899	817 ± 544	(Meng et al., 2020)
		$PM_{2.5}$	January to February, 2020	369 ± 112	210 ± 88	(Meng et al., 2023)
	China, Xi'an	TSP	2009 summer	1350 ± 247	1291 ± 120	(Wang et al., 2012)
			2009 winter	2053 ± 1097	1887 ± 586	
	China, Beijing	$PM_{2.5}$	January 2017	1068.7	440.9	(Yu et al., 2021)
			April 2017	601.5	228.2	
			July 2017	1471.7	756	
			October 2017	1046.9	519.4	
	14 cities of China	$PM_{2.5}$	2003 summer	892 ± 457	513 ± 285	(Ho et al., 2007)
			2003 winter	904 ± 480	558 ± 351	
	Mongolia, Ulaanbaatar	$PM_{2.5}$	November 2007 to January 2008	536 ± 156	107 ± 28	(Jung et al., 2010)
	India, Raipur	$PM_{2.1}$	2012-2013 winter	1072 ± 375	545 ± 231	(Deshmukh et al., 2016)
	USA, Fairbanks	$PM_{2.5}$	June to September, 2009	73.6 ± 70.4	36.6 ± 35.6	(Deshmukh et al., 2018)
Coast	China, Shanghai	$PM_{2.5}$	May to August 2018	359 ± 277	213 ± 177	(Ding et al., 2021)
	China, Shanghai	$PM_{2.5}$	December 2018 to January 2019	360 ± 233	199 ± 151	(Du et al., 2022)
	East China Sea	$PM_{2.5}$	2002 winter	193 ± 164	92.6 ± 94.5	(Zhang et al., 2016)
Mountain	China, MT. Hua	PM_{10}	2019 winter	638 ± 377	399 ± 261	(Meng et al., 2014)
			2019 summer	744 ± 340	522 ± 261	
	China, MT. Tai	$PM_{2.5}$	July to August, 2016	354 ± 239	213±162	(Meng et al., 2018)
	Japan, Fuji	TSP	July to August, 2009	308 ± 102	160 ± 37	(Kunwar et al., 2019)
Marine	Bay of Bengal	$PM_{2.5}$	December 2008 to January 2009	154 ± 84	116 ± 65	(Bikkina et al., 2017)
	North Pacific	TSP	August to September 2008 (MBA)	58 ± 45	26.1 ± 15.9	(Bikkina et al., 2014)
			August to September 2008 (LBA)	15 ± 6	10.3 ± 4.8	

Table S2. Information on target organic compounds and internal standards

	Compounds	Internal standards
Dicarboxylic acid	Succinic acid (C_4)	Lauric acid-D_{23}
	Glutaric acid (C_5)	Lauric acid-D_{23}
	Adipic acid (C_6)	Lauric acid-D_{23}
	Pimelic acid (C_7)	Lauric acid-D_{23}
	Suberic acid (C_8)	Lauric acid-D_{23}
	Azelaic acid (C_9)	Lauric acid-D_{23}
	Sebacic acid (C_{10})	Lauric acid-D_{23}
	Phthalic acid (Ph)	Phthalic acid 3,4,56-D_4
	Terephthalic acid (tPh)	Phthalic acid 3,4,56-D_4
Hopanes	17α(H)-22,29,30-trisnorhopane ($C_{27\alpha}$)	$C_{24}D_{50}$
	17α(H),21β(H)-30-norhopane ($C_{29\alpha\beta}$)	$C_{24}D_{50}$
	17α(H),21β(H)-30-hopane ($C_{30\alpha\beta}$)	$C_{24}D_{50}$
	17α(H),21β(H)-22R-homohopane ($C_{31\alpha\beta}R$)	$C_{24}D_{50}$
	17α(H),21β(H)-22S-homohopane ($C_{31\alpha\beta}S$)	$C_{24}D_{50}$
	Levoglucosan	levoglucosan-C_{13}
	Octadecanoic acid	hexadecanoic acid-d_{31}
	Picene	Perylene-D_{12}
	Citramalic acid	lauric acid-d_{23}
	Malic acid	lauric acid-d_{23}

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Table S3. Meteorological parameters, PM2.5 main components, organic molecular tracers, diacids, pH, and ALWC in the PRD (2007–2018).

	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
I. Meteorological parameters												
Temperature (°C) [a]	22.2 ± 2.1	17.2 ± 2.9	17.0 ± 3.1	19.7 ± 3.2	19.9 ± 3.8	22.1 ± 1.4	20.9 ± 1.1	20.2 ± 4.4	25.1 ± 2.4	23.8 ± 3.8	21.3 ± 3.2	22.4 ± 2.9
Relative humidity (%) [a]	57 ± 11	47 ± 12	67 ± 13	64 ± 11	57 ± 11	61 ± 7	50 ± 13	57 ± 14	63 ± 8	67 ± 7	56 ± 13	63 ± 12
Solar radiation (W m^{-2}) [a]	161.3 ± 41.3	156.5± 28.3	135.2 ± 36.3	141.8 ± 51.4	134.7 ± 36.9	101.2 ± 40.4	125.2 ± 46.2	95.3 ± 49.1	149.0 ± 36.2	122.4 ± 44.0	128.9 ± 53.1	122.2 ± 39.9
Boundary layer height (m) [b]	624 ± 124	572 ± 141	633 ± 105	635 ± 183	555 ± 167	550 ± 121	515 ± 88	586 ± 146	591 ± 115	577 ± 165	540 ± 142	532 ± 107
II. Molecular tracers (ng m^{-3})												
Levoglucosan	203 ± 77	422 ± 301	333 ± 259	264 ± 170	208 ± 152	48 ± 43	257 ± 140	205 ± 131	110 ± 66	92 ± 44	143 ± 63	63 ± 33
Hopanes	2.81 ± 1.05	6.20 ± 3.30	3.38 ± 2.57	2.69 ± 2.36	2.61 ± 1.53	0.86 ± 0.65	1.09 ± 0.64	1.11 ± 0.59	0.70 ± 0.39	1.08 ± 0.74	0.86 ± 0.47	0.71 ± 0.30
Octadecanoic acid	38.5 ± 8.1	41.8 ± 29.6	30.8 ± 11.1	28.4 ± 17.3	24.3 ± 14.2	23.9 ± 10.1	53.1 ± 20.8	26.8 ± 13.8	23.6 ± 10.6	16.3 ± 15.0	14.6 ± 7.8	17.9 ± 14.7
Picene	0.13 ± 0.07	0.29 ± 0.25	0.19 ± 0.15	0.21 ± 0.17	0.29 ± 0.20	0.19 ± 0.10	0.22 ± 0.11	0.18 ± 0.11	0.17 ± 0.08	0.24 ± 0.11	0.26 ± 0.14	0.12 ± 0.07
Terephthalic acid (tPh)	32.9 ± 23.6	58.9 ± 30.5	22.7 ± 12.0	34.4 ± 17.6	26.1 ± 35.6	39.1 ± 30.3	103.1 ± 59.5	62.3 ± 31.3	52.8 ± 29.1	51.8 ± 43.6	31.3 ± 16.4	17.4 ± 8.7
Phthalic acid (Ph)	51.9 ± 14.9	36.9 ± 10.9	23.6 ± 12.1	24.1 ± 10.0	18.3 ± 12.1	22.4 ± 12.1	47.6 ± 18.1	53.3 ± 21.0	31.1 ± 15.7	28.3 ± 16.6	20.5 ± 8.0	16.7 ± 5.7
2,3-dihydroxy-4-oxopentanioic acid (DHOPA)	1.85 ± 1.35	2.30 ± 2.50	1.15 ± 1.25	2.10 ± 1.70	2.11 ± 2.16	0.44 ± 0.41	2.15 ± 1.59	2.64 ± 2.37	2.42 ± 2.53	1.21 ± 1.02	2.07 ± 1.57	1.05 ± 0.88
Malic acid	24.2 ± 19.4	14.1 ± 17.8	2.5 ± 2.7	9.4 ± 7.3	15.6 ± 18.9	4.57 ± 3.4	14.3 ± 12.9	17.9 ± 16.8	27.9 ± 21.7	10.7 ± 8.3	15.2 ± 10.0	5.9 ± 4.9
III. Aliphatic Diacids (ng m^{-3})												
Oxalic acid (C_2)	692 ± 243	460 ± 171	NA	386 ± 168	357 ± 161	317 ± 191	526 ± 274	432 ± 200	468 ± 205	361 ± 208	404 ± 208	274 ± 114
Succinic acid (C_4)	106.8 ± 51.5	47.3 ± 61.3	29.8 ± 34.1	20.5 ± 12.9	18.4 ± 14.6	13.4 ± 10.7	34.8 ± 20.4	41.0 ± 25.3	23.8 ± 16.7	30.0 ± 22.0	22.1 ± 13.8	10.9 ± 5.8
Glutaric acid (C_5)	24.9 ± 11.2	6.6 ± 9.4	5.8 ± 5.3	6.2 ± 3.7	5.1 ± 3.5	1.9 ± 1.7	9.6 ± 5.1	9.8 ± 5.6	1.4 ± 1.3	9.7 ± 7.9	6.3 ± 4.6	3.5 ± 1.9
Adipic acid (C_6)	8.7 ± 3.6	4.3 ± 4.5	3.8 ± 2.7	4.8 ± 2.9	3.8 ± 2.6	2.3 ± 1.8	9.9 ± 4.4	7.2 ± 3.5	2.2 ± 1.3	5.5 ± 2.9	4.8 ± 2.8	4.1 ± 2.4
Pimelic acid (C_7)	2.0 ± 0.5	1.5 ± 1.3	1.3 ± 0.9	0.9 ± 0.5	1.0 ± 0.7	1.1 ± 0.6	2.8 ± 1.7	2.2 ± 1.0	1.5 ± 0.8	1.9 ± 1.5	1.2 ± 0.5	1.1 ± 0.4
Suberic acid (C_8)	2.7 ± 0.5	2.0 ± 1.5	3.4 ± 2.4	1.5 ± 2.8	1.8 ± 1.3	1.9 ± 1.0	5.1 ± 2.8	3.1 ± 1.7	2.4 ± 0.9	3.4 ± 2.2	1.7 ± 0.8	2.4 ± 0.9

Table S3. (continued)

	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
Azelaic acid (C_9)	8.5 ± 1.8	8.6 ± 6.1	18.7 ± 13.2	6.7 ± 3.7	7.3 ± 5.5	9.6 ± 4.8	27.3 ± 14.3	16.8 ± 8.6	11.6 ± 4.9	17.8 ± 10.9	7.5 ± 3.1	11.4 ± 4.0
Sebacic acid (C_{10})	1.1 ± 0.2	1.1 ± 0.8	2.8 ± 2.3	1.1 ± 0.8	1.1 ± 0.9	1.7 ± 0.8	3.6 ± 2.1	2.2 ± 1.3	2.0 ± 0.8	2.9 ± 2.1	1.2 ± 0.6	1.5 ± 0.5
Subtotal	864 ± 283	532 ± 202	NA	427 ± 156	396 ± 181	352 ± 194	610 ± 305	527 ± 173	529 ± 227	416 ± 238	452 ± 226	307 ± 122
IV. Other species												
pH [a]	1.51 ± 1.07	2.60 ± 0.71	1.94 ± 0.29	1.97 ± 1.00	2.54 ± 0.37	2.55 ± 0.43	2.69 ± 0.42	2.29 ± 0.33	2.13 ± 0.33	2.05 ± 0.46	2.60 ± 0.45	2.66 ± 0.37
ALWC (μg m^{-3}) [a]	20.6 ± 10.0	11.3 ± 7.9	28.8 ± 11.4	22.0 ± 10.8	19.3 ± 9.9	13.5 ± 5.6	12.0 ± 7.5	10.8 ± 5.4	12.5 ± 6.2	12.0 ± 7.3	9.9 ± 6.5	11.0 ± 6.7
O_x (μg m^{-3})	113 ± 31	136 ± 29	123 ± 39	119 ± 29	113 ± 26	NA	NA	125 ± 24	128 ± 46	100 ± 43	127 ± 44	114 ± 32

[a] These data were reported by our previous study (He et al., 2025). [b] The boundary layer height (BLH) data used in this study were obtained from the ERA5 reanalysis dataset provided by the European Centre for Medium-Range Weather Forecasts (ECMWF) via the Copernicus Climate Data Store (CDS, https://cds.climate.copernicus.eu/datasets/). The dataset has a spatial resolution of 0.25° × 0.25° and an hourly temporal resolution. BLH represents the height of the planetary boundary layer, defined as the atmospheric layer affected by surface friction and turbulence. 'NA' means the data are not available in this study.

Table S4. Meteorological parameters, PM2.5 main components, organic molecular tracers, diacids, pH, and ALWC in the PRD (IT0-IT4).

	IT0	IT1	IT2	IT3	IT4
I. Meteorological parameters					
Temperature (°C)	20.2 ± 2.9	21.5 ± 3.6	21.6 ± 3.4	22.8 ± 3.1	20.8 ± 4.8
Relative humidity (%)	56 ± 12.4	56 ± 13	62 ± 10	67 ± 9	66 ± 7
Solar radiation (W m^{-2})	148.0 ± 43.9	145.6 ± 42.6	118.0 ± 46	115.5 ± 43.4	112.0 ± 50.5
Boundary layer height (m)	578 ± 159	578 ± 134	613 ± 167	583 ± 142	626 ± 154
II. Molecular tracers (ng m^{-3})					
Levoglucosan	333 ± 225	194 ± 131	114 ± 79	96 ± 74	63 ± 34
Hopanes	3.4 ± 2.6	2.0 ± 1.6	1.3 ± 1.9	0.88 ± 0.70	0.54 ± 0.30
Octadecanoic acid	37.5 ± 21.0	28.4 ± 17.2	22.3 ± 14.8	17.3 ± 8.7	11.3 ± 0.93
Picene	0.26 ± 0.20	0.22 ± 0.15	0.18 ± 0.11	0.17 ± 0.10	0.10 ± 0.04
Terephthalic acid	50.0 ± 46.8	48.9 ± 30.7	32.1 ± 31.3	27.9 ± 27.1	14.5 ± 12.4
Phthalic acid	40.3 ± 17.8	29.2 ± 16.0	22.7 ± 10.2	19.6 ± 10.1	14.1 ± 8.8
DHOPA	2.52 ± 2.28	2.27 ± 2.07	1.42 ±1.06	1.05 ± 1.01	0.78 ± 0.43
Malic acid	19.0 ± 19.0	16.6 ± 16.4	9.6 ± 8.3	7.4 ± 6.1	3.9 ± 2.3
III. Aliphatic Diacids (ng m^{-3})					
Oxalic acid (C_2)	619 ± 290	483 ± 200	329 ± 158	293 ± 125	189 ± 102
Succinic acid (C_4)	55.0 ± 49.5	29.3 ± 28.5	18.5 ± 14.2	16.7 ± 12.7	12.9 ± 12.1
Glutaric acid (C_5)	12.5 ± 10.5	6.4 ± 5.9	4.8 ± 2.7	4.2 ± 4.2	4.5 ± 5.6
Adipic acid (C_6)	7.1 ± 4.2	4.9 ± 3.4	4.0 ± 2.7	3.4 ± 2.5	2.9 ± 2.6
Pimelic acid (C_7)	1.9 ± 1.3	1.4 ± 0.8	1.1 ± 0.7	1.1 ± 0.9	0.7 ± 0.5
Suberic acid (C_8)	3.0 ± 2.2	2.5 ± 1.5	2.2 ± 1.3	2.0 ± 1.3	1.4 ± 1.0
Azelaic acid (C_9)	13.5 ± 12.3	11.9 ± 8.3	10.4 ± 7.0	9.6 ± 6.1	6.7 ± 3.8
Sebacic acid (C_{10})	2.0 ± 1.8	1.7 ± 1.2	1.6 ± 1.3	1.5 ± 1.1	1.0 ± 0.9
Subtotal	734 ± 337	540 ± 218	358 ± 163	325 ± 135	208 ± 67
IV. Other species					
pH	2.04 ± 0.96	2.40 ± 0.61	2.48 ± 0.43	2.36 ± 0.58	2.11 ± 0.71
ALWC (μg m^{-3})	20.9 ± 11.0	15.1 ± 9.9	13.1 ± 6.9	13.1 ± 8.0	7.2 ± 3.0
O_x (μg m^{-3})	136.7 ± 31.7	134.9 ± 34.4	111.9 ± 27.1	98.5 ± 25.0	72.7 ± 19.1

Table S5. Impact factor (%) of individual factor under different pollution conditions

	IT0	IT1	IT2	IT3	IT4
Levoglucosan	3 ± 3	4 ± 4	5 ± 5	7 ± 4	4 ± 2
Hopanes	10 ± 5	9 ± 6	10 ± 6	10 ± 5	5 ± 4
Octadecanoic acid	3 ± 2	2 ± 2	2 ± 2	2 ± 2	1 ± 1
Picene	1 ± 1	1 ± 1	2 ± 2	1 ± 1	1 ± 0
Terephthalic acid	9 ± 7	7 ± 5	9 ± 5	8 ± 6	9 ± 3
O_x	24 ± 14	31 ± 10	32 ± 10	33 ± 14	48 ± 12
ALWC	19 ± 11	22 ± 11	20 ± 12	21 ± 13	13 ± 9
pH	16 ± 15	9 ± 11	9 ± 6	11 ± 12	7 ± 6
Temp	9 ± 7	9 ± 7	7 ± 5	7 ± 6	9 ± 8
RH	3 ± 3	2 ± 1	2 ± 2	1 ± 1	2 ± 1
SR	2 ± 2	1 ± 1	2 ± 2	1 ± 1	1 ± 0

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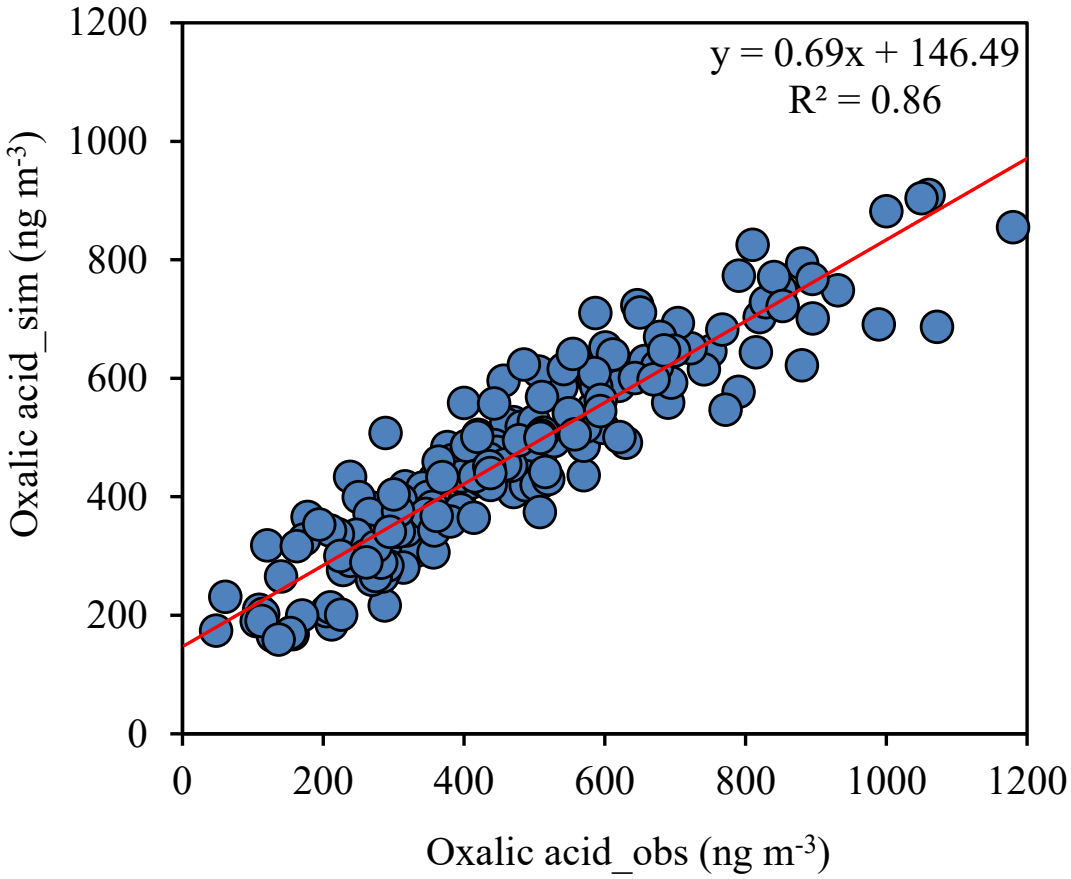

Figure S1. Observations and simulations of oxalic acid.

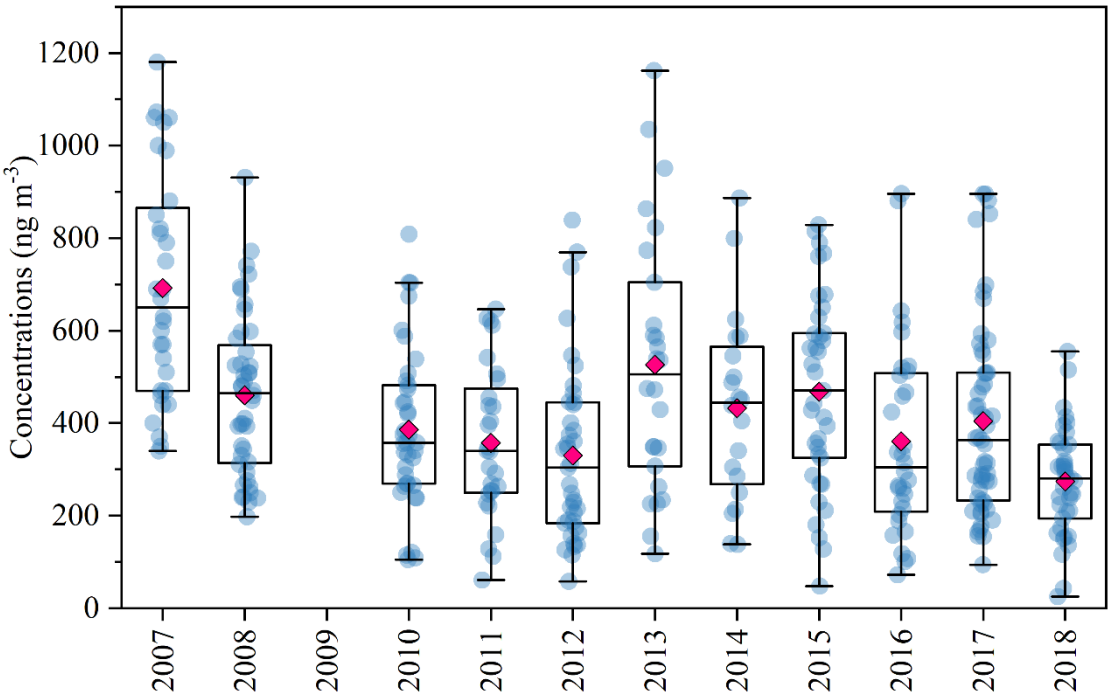

Figure S2. Annual variations in oxalic acid between 2007 and 2018 in the PRD.

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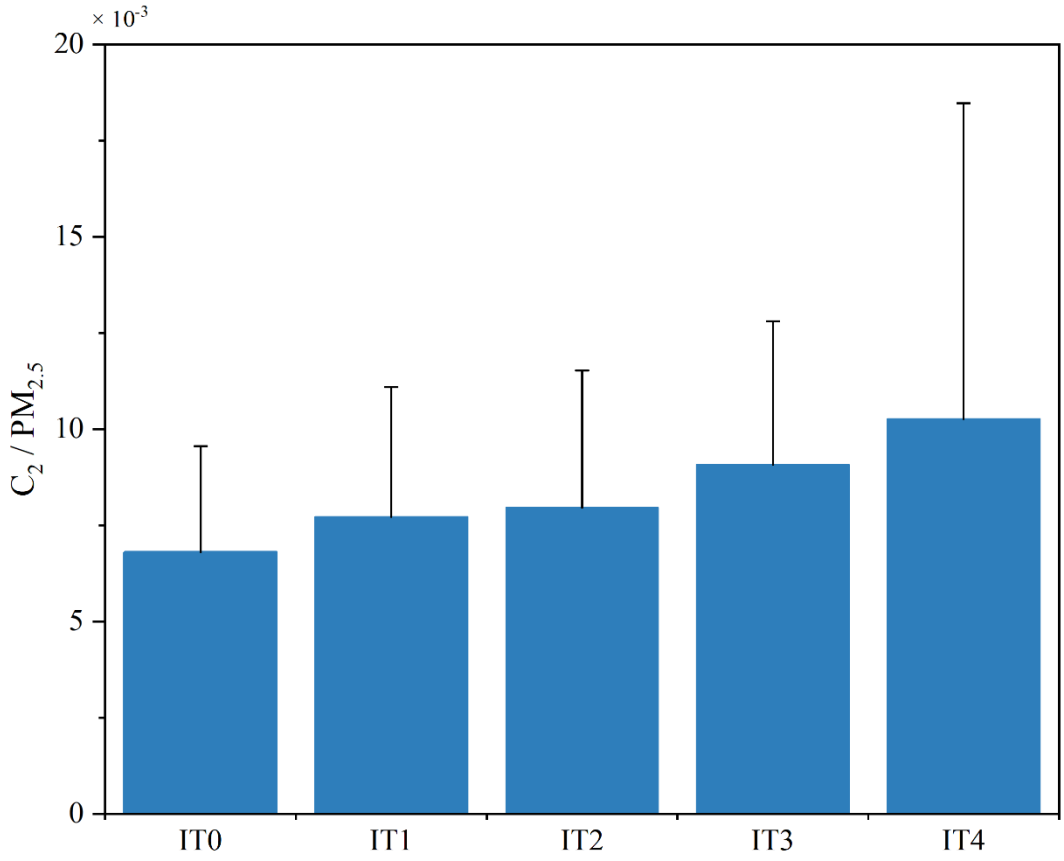

Figure S3. The ratio of C_2 to $PM_{2.5}$ under different pollution conditions.

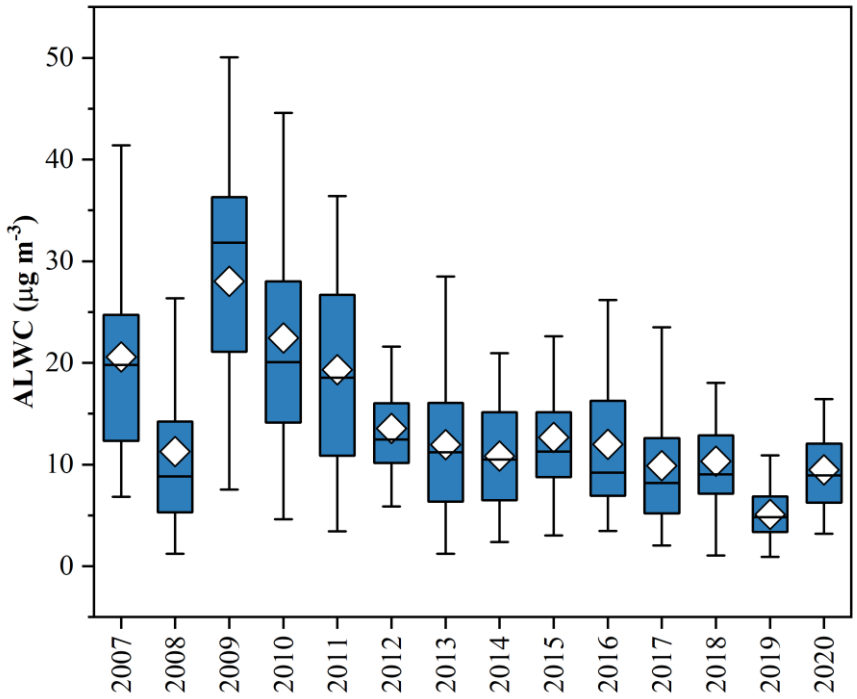

Figure S4. The variations in ALWC from 2007 to 2018 in the PRD (He et al., 2025).

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