

Supplemental Information for

Determination of n-alkanes, PAHs and hopanes in atmospheric aerosol: evaluation and comparison of thermal desorption GC-MS and solvent extraction GC-MS approaches

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Table S1 The description of aerosol samples used in this study.

city	Longitude, Latitude	Site Description	Sampling type	Number of samples	Sampling rate (m ³ min ⁻¹)	Sampling duration (h)
Beijing (BJ)	39.9°N, 116.4°E	Urban residential	high volume	12	1.05	24
Guangzhou (GZ)	23.1°N, 113.2°E	Urban residential	high volume	11	1.05	24
Shanghai (SH)	31.2°N, 121.4°E	Industrial & commercial	high volume	11	1.05	24
Chengdu (CD)	30.7°N, 104.1°E	Urban residential	high volume	11	1.05	24

*24 h integrated PM samples were collected every second day.

Table S2 The calibration parameters of organic compounds being tested by two methods

	abbreviation	MW	Cn	quantification Ion	Slope-SE	R ² -SE	Slope-TD	R ² -TD
n-Alkanes								
Tetradecane	C ₁₄	198	14	57、85、99	0.38	R ² =0.94	0.39	R ² =1.00
Pentadecane	C ₁₅	212	15	57、85、99	0.45	R ² =0.92	0.52	R ² =1.00
Hexadecane	C ₁₆	226	16	57、85、99	0.63	R ² =0.96	0.46	R ² =1.00
Heptadecane	C ₁₇	240	17	57、85、99	0.99	R ² =1.00	0.49	R ² =1.00
Octadecane	C ₁₈	254	18	57、85、99	1.3	R ² =1.00	0.51	R ² =1.00
Nonadecane	C ₁₉	268	19	57、85、99	1.1	R ² =0.97	0.51	R ² =1.00
Eicosane	C ₂₀	282	20	57、85、99	1.3	R ² =0.98	0.55	R ² =0.99
Heneicosane	C ₂₁	296	21	57、85、99	1.3	R ² =0.97	0.59	R ² =1.00
Docosane	C ₂₂	310	22	57、85、99	1.5	R ² =1.00	0.71	R ² =1.00
Tricosane	C ₂₃	324	23	57、85、99	1.3	R ² =1.00	1.8	R ² =1.00
Tetracosane	C ₂₄	338	24	57、85、99	1.4	R ² =0.99	1.3	R ² =1.00
Pentacosane	C ₂₅	352	25	57、85、99	1.5	R ² =0.98	0.75	R ² =1.00
Hexacosane	C ₂₆	366	26	57、85、99	1.3	R ² =0.98	0.89	R ² =1.00
Heptacosane	C ₂₇	380	27	57、85、99	1.3	R ² =0.99	0.72	R ² =1.00
Octacosane	C ₂₈	394	28	57、85、99	1.3	R ² =0.99	0.71	R ² =1.00
Nonacosane	C ₂₉	408	29	57、85、99	1.4	R ² =0.99	0.63	R ² =1.00
Triacontane	C ₃₀	422	30	57、85、99	1.3	R ² =0.98	0.67	R ² =1.00
Hentriacotane	C ₃₁	436	31	57、85、99	1.2	R ² =0.97	0.70	R ² =0.99
Dotriacontane	C ₃₂	450	32	57、85、99	1.2	R ² =0.92	0.66	R ² =1.00
Tritriacontane	C ₃₃	464	33	57、85、99	1.3	R ² =0.93	0.56	R ² =0.99
Tetraactotane	C ₃₄	478	34	57、85、99	1.2	R ² =0.89	0.57	R ² =0.99
Pentatriacontane	C ₃₅	492	35	57、85、99	1.6	R ² =0.87	0.52	R ² =0.99
Hexatriacontane	C ₃₆	506	36	57、85、99	1.6	R ² =0.93	0.47	R ² =0.99
Heptatriacontane	C ₃₇	520	37	57、85、99	1.6	R ² =0.87	0.36	R ² =1.00

PAHs

Acenaphthene	Ace	154	12	152、153、154	0.20	R ² = 1.00	0.12	R ² =1.00
Fluorene	Fl	166	13	165、166、167	1.1	R ² = 1.00	0.97	R ² =0.99
Phenanthrene	Phe	178	14	176、178、179	1.3	R ² = 1.00	1.3	R ² =0.98
Anthracene	Ant	178	14	176、178、180	2.0	R ² = 1.00	1.4	R ² =0.99
Fluoranthene	Fla	202	16	101、202、203	0.43	R ² = 1.00	0.91	R ² =0.99
Pyrene	Pyr	202	16	101、202、204	0.47	R ² = 1.00	1.5	R ² =0.99
Benz(a)anthracene	BaA	228	18	226、228、229	1.3	R ² = 1.00	1.6	R ² =0.99
Chrysene	Chry	228	18	226、228、230	1.5	R ² = 1.00	1.3	R ² =0.99
Benzo(b)fluoranthene	BbF	252	20	126、252、253	2.4	R ² = 1.00	1.0	R ² =1.00
Benzo(k)fluoranthene	BkF	252	20	126、252、254	1.7	R ² = 1.00	1.8	R ² =1.00
Benzo(a)pyrene	BaP	252	20	126、252、255	1.6	R ² =0.99	0.62	R ² =1.00
Indeno(1,2,3-cd)pyrene	IcdP	276	22	138、276、277	0.70	R ² =0.99	0.40	R ² =1.00
Dibenz(a,h)anthracene	DahA	278	22	139、278、279	0.17	R ² =0.98	0.75	R ² =1.00
Benzo(g,h,i)perylene	BghiP	276	22	138、276、277	0.63	R ² =0.99	0.83	R ² =1.00

Hopanes

22,29,30-Trisnorhopane	TH	370	27	191	5.20E-03	R ² =0.99	3.00E-03	R ² =1.00
$\alpha\beta$ -Norhopane (C29 $\alpha\beta$ -hopane)	C29 $\alpha\beta$ H	398	29	191	5.70E-03	R ² =0.99	3.09E-03	R ² =1.00
$\alpha\alpha$ -+ $\beta\alpha$ -Norhopane (C29 $\alpha\alpha$ -+ $\beta\alpha$ -hopane)	C29 $\alpha\alpha$ - + $\beta\alpha$ H	398	29	191	5.70E-03	R ² =0.97	1.92E-03	R ² =1.00
$\alpha\beta$ -Hopane (C30 $\alpha\beta$ -hopane)	C30 $\alpha\beta$ H	398	29	191	3.20E-03	R ² =0.97	3.58E-03	R ² =1.00
$\alpha\alpha$ -Hopane (C30 $\alpha\alpha$ -hopane)	C30 $\alpha\alpha$ H	412	30	191	3.60E-03	R ² =0.85	2.95E-03	R ² =1.00
$\beta\alpha$ -Hopane (C30 $\beta\alpha$ -hopane)	C30 $\beta\alpha$ H	412	30	191	3.40E-03	R ² =0.99	4.06E-03	R ² =1.00
$\alpha\beta$ S-Homohopane (C31 $\alpha\beta$ S-hopane)	C31 $\alpha\beta$ SH	426	31	191	3.90E-03	R ² =0.87	3.01E-03	R ² =1.00
$\alpha\beta$ R-Homohopane (C31 $\alpha\beta$ R-hopane)	C31 $\alpha\beta$ RH	426	31	191	4.30E-03	R ² =0.81	2.30E-03	R ² =1.00