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Determination of n-alkanes, polycyclic aromatic hydrocarbons 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
Hexadercane	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
Tritriactotane	C_{33}	464	33	57、85、99	1.3	R^2=0.93	0.56	R^2=0.99
Tetratriactoane	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-Trisnorphopane	TH	370	27	191	5.20E-03	R^2=0.99	3.00E-03	R^2=1.00
αβ-Norhopane (C29αβ-hopane)	C29αβH	398	29	191	5.70E-03	R^2=0.99	3.09E-03	R^2=1.00
αα-+βα-Norhopane (C29αα-+βα-hopane)	C29αα- +βαH	398	29	191	5.70E-03	R^2=0.97	1.92E-03	R^2=1.00
αβ-Hopane (C30αβ-hopane)	C30αβH	398	29	191	3.20E-03	R^2=0.97	3.58E-03	R^2=1.00
αα-Hopane (C30αα-hopane）	C30ααH	412	30	191	3.60E-03	R^2=0.85	2.95E-03	R^2=1.00
βα-Hopane (C30βα-hopane）	C30βαH	412	30	191	3.40E-03	R^2=0.99	4.06E-03	R^2=1.00
αβS-Homohopane (C31αβS-hopane)	C31αβSH	426	31	191	3.90E-03	R^2=0.87	3.01E-03	R^2=1.00
αβR-Homohopane (C31αβR-hopane)	C31αβRH	426	31	191	4.30E-03	R^2=0.81	2.30E-03	R^2=1.00

Table S3 The analytical parameters of organic compounds being tested by two methods.

Compounds	SE method			TD method		
	LOD_{SE} (ng per injection)	**Repeatability r_{SE} (%)**	**Reproducibility R_{SE} (%)**	**LOD_{TD} (ng per sample)**	**Repeatability r_{TD} (%)**	**Reproducibility R_{TD} (%)**
n-Alkanes						
n-Tetradecane (C_{14})	0.73	14.45	9.25	0.81	16.35	10.95
n-Pentadecane (C_{15})	0.42	10.70	7.73	0.63	11.37	12.42
n-Hexadercane(C_{16})	0.68	8.39	6.13	0.36	12.96	6.94
n-Heptadecane(C_{17})	0.47	8.54	4.54	0.54	10.70	6.01
n-Octadecane(C_{18})	0.38	11.52	7.66	0.57	16.21	8.41
n-Nonadecane(C_{19})	0.84	6.99	10.85	0.18	6.91	8.81
n-Eicosane(C_{20})	0.05	8.72	8.15	0.27	9.49	4.14
n-Heneicosane(C_{21})	0.21	10.05	7.61	0.15	5.64	7.35
n-Docosane(C_{22})	0.24	8.54	4.75	0.18	6.98	5.48
n-Tricosane(C_{23})	0.28	9.40	8.72	0.24	8.96	6.01
n-Tetracosane(C_{24})	0.88	7.32	10.36	0.12	4.22	3.34
n-Pentacosane(C_{25})	0.69	8.90	4.48	0.09	3.21	5.08
n-Hexacosane(C_{26})	0.71	5.88	5.44	0.12	4.65	7.48
n-Heptacosane(C_{27})	0.58	4.81	5.54	0.09	3.21	8.15
n-Octacosane(C_{28})	0.60	4.99	7.41	0.15	9.32	9.48
n-Nonacosane(C_{29})	0.92	7.65	8.84	0.15	5.96	10.28
n-Triacontane(C_{30})	0.86	7.20	5.45	0.18	6.31	5.08
n-Hentriacotane(C_{31})	0.73	6.12	4.58	0.18	6.26	12.95
n-Dotriacontane(C_{32})	0.28	7.73	4.32	0.27	9.02	7.35
n-Tritriactotane(C_{33})	0.57	4.78	4.02	0.33	11.40	6.41
n-Tetratriactoane(C_{34})	0.75	6.24	4.43	0.24	8.03	12.15
n-Pentatriacontane(C_{35})	0.42	3.48	2.02	0.48	16.24	11.62
n-Hexatriacontane(C_{36})	0.46	3.85	3.06	0.33	11.63	4.27
n-Heptatriacontane(C_{37})	0.68	6.73	3.58	0.21	7.96	6.28
PAHs						
Acenaphthene	0.78	9.12	3.57	1.86	6.46	5.81
Fluorene	0.33	6.91	1.61	0.42	2.73	4.69
Phenanthrene	0.49	10.59	6.49	0.33	4.09	5.30
Anthracene	0.34	9.35	3.66	0.27	2.84	5.70
Fluoranthene	0.54	5.37	2.58	0.15	4.54	6.11
Pyrene	0.14	5.41	6.02	0.15	9.53	4.95
Benz(a)anthracene	0.11	4.62	4.56	0.12	9.23	6.41
Chrysene	0.08	4.37	5.24	0.12	8.14	7.77
Benzo(b)fluoranthene	0.75	7.81	3.29	0.21	6.25	8.43
Benzo(k)fluoranthene	0.16	7.31	4.39	0.21	7.98	6.97
Benzo(a)pyrene	0.65	7.26	4.50	0.21	5.41	5.45
Indeno(1,2,3-cd)pyrene	0.10	6.52	4.95	0.18	9.13	5.91
Dibenz(a,h)anthracene	0.19	6.95	2.64	0.18	6.58	8.18
Benzo(g,h,i)perylene	0.20	9.61	4.17	0.12	4.16	7.98

Hopanes						
22,29,30-Trisnorphopane	0.35	7.22	5.81	0.21	2.95	1.71
αβ-Norhopane	0.69	6.33	5.25	0.19	5.73	2.81
αα -+βα-Norhopane	1.00	6.00	4.14	0.18	8.35	4.62
αβ -Hopane	0.54	7.67	1.82	0.23	4.54	2.33
αα-Hopane	0.25	3.83	2.07	0.46	2.10	1.12
βα-Hopane	0.46	5.08	2.83	0.61	3.84	2.11
αβS-Homohopane	0.27	3.50	1.16	0.42	2.25	1.13
αβR-Homohopane	0.58	6.00	2.47	0.71	4.75	2.84