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Emissions of intermediate-volatility and semi-volatile organic compounds (I/SVOCs) from different cumulative-mileage diesel vehicles at various ambient temperatures

Shuwen Guo et al.

Correspondence to: Xuan Zheng (x-zheng11@szu.edu.cn)

S1. Description of all organic category names.

Alkane: n-alkane and i-alkane. Alcohol: aliphatic alcohol. Phenol: organics containing one benzene ring and a hydrocarbon group directly attached to the benzene ring. Carbonyls: aliphatic ketone and aliphatic aldehyde. Acid: aliphatic acid. Oxy-PAH & Oxy-benzene: organic compounds containing benzene rings and oxygen-containing groups, except for phenols whose hydroxyl group is directly connected to one benzene ring. PAH_2rings: PAH with 2 benzene rings. PAH_3rings: PAH with 3 benzene rings. PAH_4rings: PAH with 4 benzene rings. Alkene: organics containing carbon double bond(s) without any other function groups. Cycloalkane: organics containing a saturated carbon ring without any other function groups.

S2. Description of the steps for qualitatively identifying organic compounds using mass spectrometry principles.

Taking alkanes as an example, compounds containing hydrocarbon chains give rise to a series of ions separated by 14 Da (-CH2-). As a result, the top ions to identify alkanes would be m/z = 43, m/z = 57, m/z = 71, and m/z = 84 (He et al., 2022a, b). Due to the stability of chemical groups, generally, the abundance of m/z = 57 is highest, followed by m/z = 43 and m/z = 71. When incorporating these rules into the data treatment software (Canvas, version 2.5, J&X Technologies), a few steps need to be taken, as shown in Fig. S1(a). Four built-in features can be deployed. ABUND (X) returns the normalized abundance of the input ion mass; HASMASS (X) returns the value to indicate if the input ion exists; ORDER (X) returns the order of the input ion mass; MASS (X) returns the mass of the input ion's order. Additionally, the function allows two logical operators, "And" and "Or". Then, the cluster of alkanes can be extracted by the following rules:

((MASS(1)=43 && (MASS(2)=57 || MASS(2)=71 || MASS(2)=41)) || (MASS(1)=57 && (MASS(2)=43 || MASS(2)=71 || MASS(2)=41)))

where "&&" and "||" refer to the logical operators "And" and "Or", respectively. Paste the rules in Ion Extractor Editor and the cluster of alkanes can be filtered, as shown in Fig. S1(b).

Table S1. Sets of test cycles.

No.	Vehicle ID	Ambient Temperature	Cold- or Hot-start Cycle	Repetitions
1	D1	23 °C	Cold-start cycle	2
2	D1	23 °C	Hot-start cycle	2
3	D2	23 °C	Cold-start cycle	2
4	D2	23 °C	Hot-start cycle	2
5	D2	0 °C	Hot-start cycle	2
6	D3	23 °C	Cold-start cycle	3
7	D3	23 °C	Hot-start cycle	3
8	D4	23 °C	Cold-start cycle	3
9	D4	23 °C	Hot-start cycle	3
10	D4	0 °C	Hot-start cycle	2

Table S2. The list of 120 external standard curves used in this study.

No.	Groups	Name	Molecular Formula	Cas No.	R^2
1	Alkane	Heptane	C_7H_{16}	142-82-5	0.973
2	Alkane	Octane	C_8H_{18}	111-65-9	0.984
3	Alkane	Nonane	C_9H_{20}	111-84-2	0.996
4	Alkane	Decane	$C_{10}H_{22}$	124-18-5	0.995
5	Alkane	Undecane	$C_{11}H_{24}$	1120-21-4	0.992
6	Alkane	Dodecane	$C_{12}H_{26}$	112-40-3	0.973
7	Alkane	Tridecane	$C_{13}H_{28}$	629-50-5	0.975
8	Alkane	Tetradecane	$C_{14}H_{30}$	629-59-4	0.985
9	Alkane	Pentadecane	$C_{15}H_{32}$	629-62-9	0.987
10	Alkane	Hexadecane	$C_{16}H_{34}$	544-76-3	0.988
11	Alkane	heptadecane	$C_{17}H_{36}$	629-78-7	0.975
12	Alkane	Octadecane	$C_{18}H_{38}$	593-45-3	0.969
13	Alkane	Nonadecane	$C_{19}H_{40}$	629-92-5	0.987
14	Alkane	Eicosane	$C_{20}H_{42}$	112-95-8	0.961
15	Alkane	Heneicosane	$C_{21}H_{44}$	629-94-7	0.962
16	Alkane	Docosane	$C_{22}H_{46}$	629-97-0	0.976
17	Alkane	Tricosane	$C_{23}H_{48}$	638-67-5	0.971
18	Alkane	Tetracosane	$C_{24}H_{50}$	646-31-1	0.973
19	Alkane	Pentacosane	$C_{25}H_{52}$	629-99-2	0.995
20	Alkane	Hexacosane	$C_{26}H_{54}$	630-01-3	0.990
21	Alkane	Heptacosane	$C_{27}H_{56}$	593-49-7	0.977
22	Alkane	Octacosane	$C_{28}H_{58}$	630-02-4	0.982
23	Alkane	Nonacosane	$C_{29}H_{60}$	630-03-5	0.972
24	Alkane	Triacontane	$C_{30}H_{62}$	638-68-6	0.963
25	Alkane	Hentriacontane	$C_{31}H_{64}$	630-04-6	0.971
26	Alkane	Dotriacontane	$C_{32}H_{66}$	544-85-4	0.956
27	Alkane	Tritriacontane	$C_{33}H_{68}$	630-05-7	0.959
28	Alkane	Tetratriactoane	$C_{34}H_{70}$	14167-59-0	0.957
29	Alkane	Pentatriacontane	$C_{35}H_{72}$	630-07-9	0.989
30	Alkane	Hexatriacontane	$C_{36}H_{74}$	630-06-8	0.980
31	Alkane	Heptatriacontane	$C_{37}H_{76}$	7194-84-5	0.989
32	Alkene	Octene	C_8H_{16}	111-66-0	0.992
33	Alkene	Decene	$C_{10}H_{20}$	872-05-9	0.982
34	Alkene	Dodecene	$C_{12}H_{24}$	112-41-4	0.959
35	Alkene	Tetradecene	$C_{14}H_{28}$	1120-36-1	0.976
36	Alkene	Hexadecene	$C_{16}H_{32}$	629-73-2	0.985
37	Alkene	Octadecene	$C_{18}H_{36}$	112-88-9	0.986
38	Alkene	Eicosene	$C_{20}H_{40}$	3452-07-1	0.988
39	Alkene	Docosene	$C_{22}H_{44}$	1599-67-3	0.987
40	Alkyl-PAH	Methylnaphthalene	$C_{11}H_{10}$	90-12-0	0.997
41	Acid	Isobutyric Acid	$C_4H_8O_2$	79-31-2	0.989

No.	Groups	Name	Molecular Formula	Cas No.	R^2
42	Acid	2-Methyl butyric acid	$C_5H_{10}O_2$	116-53-0	0.986
43	Acid	Tetradecanoic acid	$C_{11}H_{22}O_2$	544-63-8	0.981
44	Acid	heptadecanoic acid	$C_{14}H_{28}O_2$	506-12-7	0.984
45	Acid	Undecanoic acid	$C_{17}H_{34}O_2$	112-37-8	0.984
46	Alcohol	Decanol	$C_{10}H_{22}O$	112-30-1	0.982
47	Alcohol	Tridecanol	$C_{13}H_{28}O$	26248-42-0	0.987
48	Alcohol	Hexadecanol	$C_{16}H_{34}O$	36653-82-4	0.961
49	Alcohol	Nonadecanol	$C_{19}H_{40}O$	1454-84-8	0.953
50	Alcohol	Docosanol	$C_{22}H_{46}O$	661-19-8	0.994
51	Aldehyde	Valeraldehyde	$C_5H_{10}O$	110-62-3	0.966
52	Aldehyde	1-Pentanecarbaldehyde	$C_6H_{12}O$	66-25-1	0.996
53	Aldehyde	Octanal	$C_8H_{16}O$	124-13-0	0.995
54	Aldehyde	Decylaldehyde	$C_{10}H_{20}O$	112-31-2	0.994
55	Aldehyde	Dodecanal	$C_{12}H_{24}O$	112-54-9	0.957
56	Aldehyde	Tetradecanal	$C_{14}H_{28}O$	124-25-4	0.978
57	Aldehyde	Hexadecanal	$C_{16}H_{32}O$	629-80-1	0.955
58	Aldehyde	Octadecanone	$C_{18}H_{36}O$	638-66-4	0.968
59	Aldehyde	Icosanal	$C_{20}H_{40}O$	2400-66-0	0.959
60	Aldehyde	Docosanal	$C_{22}H_{44}O$	57402-36-5	0.952
61	Alkyl-PAH	Ethylnaphthalene	$C_{12}H_{12}$	1127-76-0	0.971
62	Amide	Acetamide	C_2H_5NO	60-35-5	1.000
63	Amide	Propanamide	C_3H_7NO	79-05-0	0.960
64	Amide	N,N-Dibutylformamide	$C_9H_{19}NO$	761-65-9	0.952
65	Amine	Triethylamine	$C_6H_{15}N$	121-44-8	0.986
66	Amine	Aniline	C_6H_7N	62-53-3	0.981
67	Amine	2-Aminoaniline	$C_6H_8N_2$	95-54-5	0.997
68	Amine	Dibutylamine	$C_8H_{19}N$	111-92-2	0.990
69	Amine	1-Naphthalenamine	$C_{10}H_9N$	134-32-7	0.962
70	Amine	4-Biphenylamine	$C_{12}H_{11}N$	92-67-1	0.994
71	Aromatic	Ethylbenzene	C_8H_{10}	100-41-4	0.996
72	Aromatic	p-xylene	C_8H_{10}	106-42-3	0.993
73	Aromatic	o-xylene	C_8H_{10}	95-47-6	0.993
74	Aromatic	Isopropylbenzene	C_9H_{12}	98-82-8	0.995
75	Aromatic	4-Ethyltoluene	C_9H_{12}	622-96-8	0.982
76	Aromatic	1,3,5-trimethylbenzene	C_9H_{12}	108-67-8	0.993
77	Aromatic	p-Cymene	$C_{10}H_{14}$	99-87-6	0.966
78	Aromatic	butyl-benzene	$C_{10}H_{14}$	104-51-8	0.993
79	Aromatic	pentyl-benzene	$C_{11}H_{16}$	538-68-1	0.974
80	Aromatic	hexyl-benzene	$C_{12}H_{18}$	1077-16-3	0.973
81	Cycloalkane	Ethyl-cyclohexane	C_8H_{16}	1678-91-7	0.950
82	Cycloalkane	Butyl-cyclohexane	$C_{10}H_{20}$	1678-93-9	0.986
83	Cycloalkane	Hexyl-cyclohexane	$C_{12}H_{24}$	4292-75-5	0.968

No.	Groups	Name	Molecular Formula	Cas No.	R^2
84	Cycloalkane	Octyl-cyclohexane	$C_{14}H_{28}$	1795-15-9	0.950
85	Cycloalkane	Decyl-cyclohexane	$C_{16}H_{32}$	1795-16-0	0.955
86	Cycloalkane	Dodeyl-cyclohexane	$C_{18}H_{36}$	1795-17-1	0.974
87	Cycloalkane	Tetradecyl-cyclohexane	$C_{20}H_{40}$	1795-18-2	0.969
88	Cycloalkane	Hexadecyl-cyclohexane	$C_{22}H_{44}$	6812-38-0	0.979
89	Ester	Butyl acetate	$C_6H_{12}O_2$	123-86-4	0.979
90	Ester	Isoamyl Acetate	$C_7H_{14}O_2$	123-92-2	0.995
91	Ester	Amyl Acetate	$C_7H_{14}O_2$	628-63-7	0.973
92	Furan	Furan	C_4H_4O	110-00-9	0.961
93	Ketone	2-Pentanone	$C_5H_{10}O_2$	107-87-9	0.990
94	Ketone	3-Heptanone	$C_7H_{14}O$	106-35-4	0.995
95	Ketone	2-Nonanone	$C_9H_{18}O$	821-55-6	0.984
96	Ketone	2-Dodecanone	$C_{12}H_{24}O$	6175-49-1	0.972
97	Ketone	Pentadecanone	$C_{15}H_{30}O$	2345-28-0	0.986
98	Oxy-PAH	1,4-naphthoquinone	$C_{10}H_6O_2$	130-15-4	0.994
99	Oxy-PAH	1-naphthaldehyde	$C_{11}H_8O$	66-77-3	0.982
100	Oxy-PAH	9,10-anthraquinone	$C_{14}H_8O_2$	84-65-1	0.992
101	Oxy-PAH	benzo[a]anthracene-7,12-dione	$C_{18}H_{10}O_2$	2498-66-0	0.983
102	PAH	Indene	C_9H_8	95-13-6	0.990
103	PAH	Naphthalene	$C_{10}H_8$	91-20-3	0.997
104	PAH	Acenaphthylene	$C_{12}H_8$	208-96-8	0.996
105	PAH	Acenaphthene	$C_{12}H_{10}$	83-32-9	0.989
106	PAH	Fluorene	$C_{13}H_{10}$	86-73-7	0.997
107	PAH	Phenanthrene	$C_{14}H_{10}$	85-01-8	0.994
108	PAH	Anthracene	$C_{14}H_{10}$	120-12-7	0.992
109	PAH	Pyrene	$C_{16}H_{10}$	129-00-0	0.992
110	PAH	Benz[a]anthracene	$C_{18}H_{12}$	56-55-3	0.973
111	PAH	Chrysene	$C_{18}H_{12}$	218-01-9	0.973
112	PAH	Benzo[b]fluoranthene	$C_{20}H_{12}$	205-99-2	0.961
113	PAH	Benzo[k]fluoranthene	$C_{20}H_{12}$	207-08-9	0.983
114	PAH	Benzo[a]pyrene	$C_{20}H_{12}$	50-32-8	0.967
115	PAH	Indeno[1,2,3-cd]fluoranthene	$C_{22}H_{12}$	193-39-5	0.991
116	Pinene	(+)-alpha-Pinene	$C_{10}H_{16}$	7785-70-8	0.950
117	Pinene	β-Pinene	$C_{10}H_{16}$	18172-67-3	0.991
118	Polyphenyls	Biphenyl	$C_{12}H_{10}$	92-52-4	0.952
119	Polyphenyls	p-terphenyl	$C_{18}H_{14}$	92-94-4	0.967
120	Polyphenyls	p-quaterphenyl	$C_{24}H_{18}$	135-70-6	0.987

Table S3. Average THC, NOx, and CO EFs for LMV and HMV, respectively.

Vehicle	Test Cycle	THC ($mg \cdot km^{-1}$)	NOx ($mg \cdot km^{-1}$)	CO ($mg \cdot km^{-1}$)
LMV (D2)	Hot_23°C	35	6951	600
	Hot_0°C	38	8048	657
HMV (D4)	Hot_23°C	289	2629	359
	Hot_0°C	302	3555	404

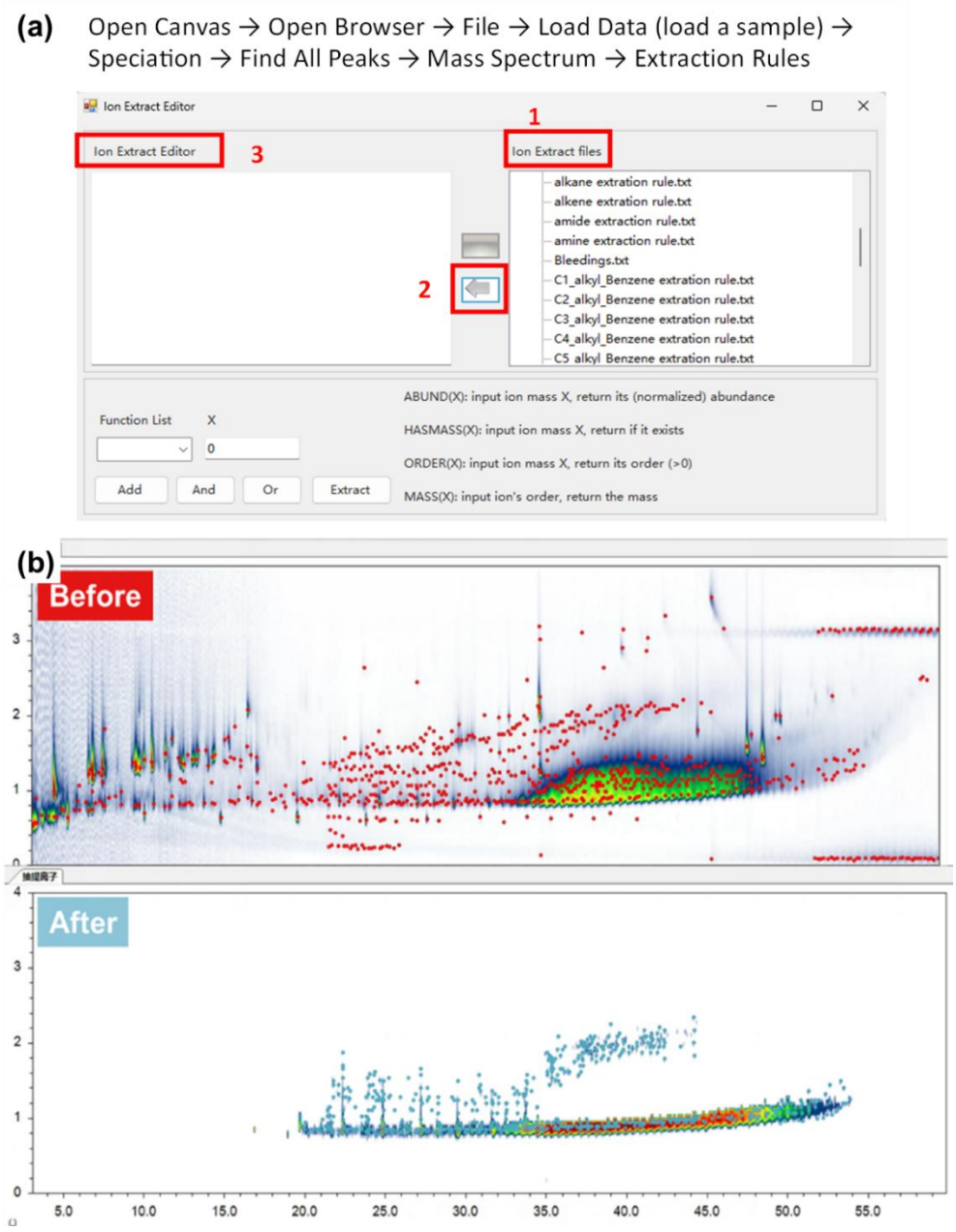

Figure S1. (a) The steps to enable the ion extract function built in Canvas software. Canvas is the supporting software of solid-state modulator (SSM1810, J&X Technologies, China) and is not originally created by the authors of this research. (b) Comprehensive two-dimensional chromatograms before and after screening alkanes. Each red and blue point represents a chromatographic peak.

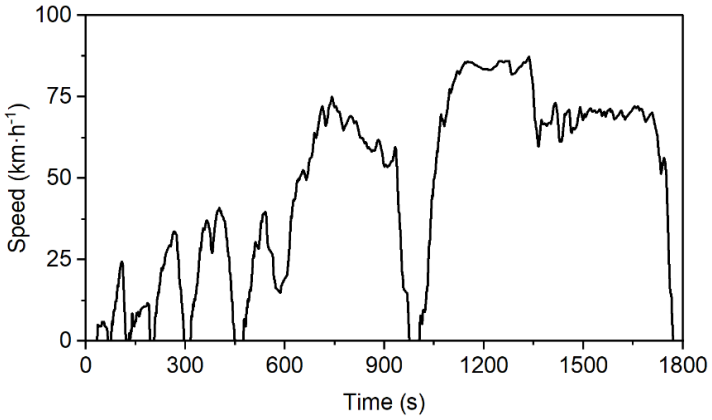

Figure S2. CHTC-TT test cycle for tractor trailers. The cycle lasts 1800 s, with the first 473 s as phase 1 and the last 1327 s as phase 2. The total driving distance is about 23 km, and the maximum speed is 88 km·h^{-1}.

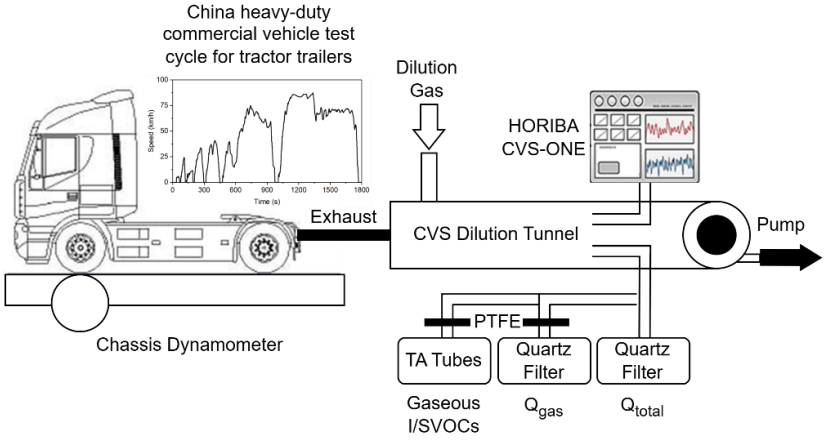

Figure S3. A schematic of the sampling systems.

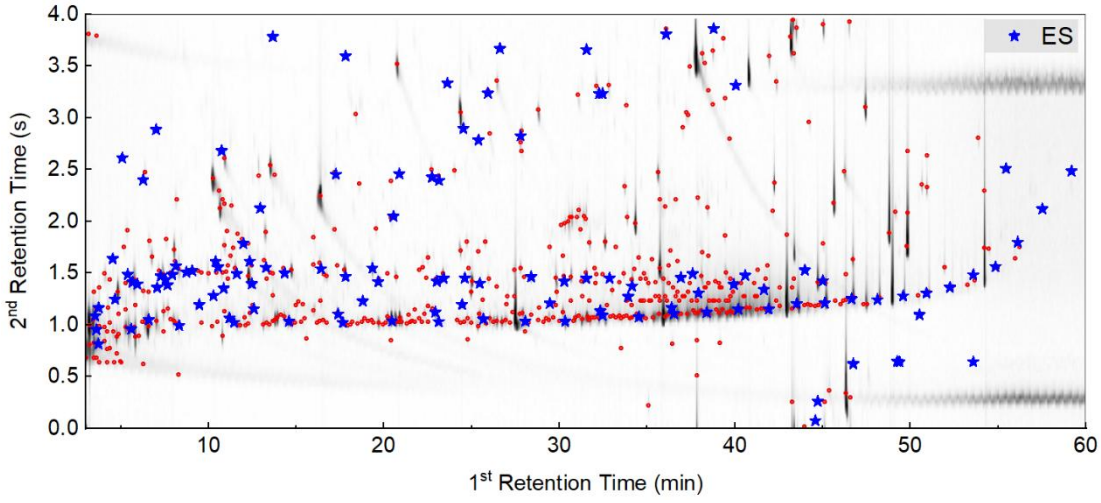

Figure S4. Actual GC×GC chromatogram and sample chromatographic peaks (the red dots). The blue stars represent all ES used in this study including n-alkanes, PAHs, carbonyls, etc. All their detailed information was listed in Table S2.

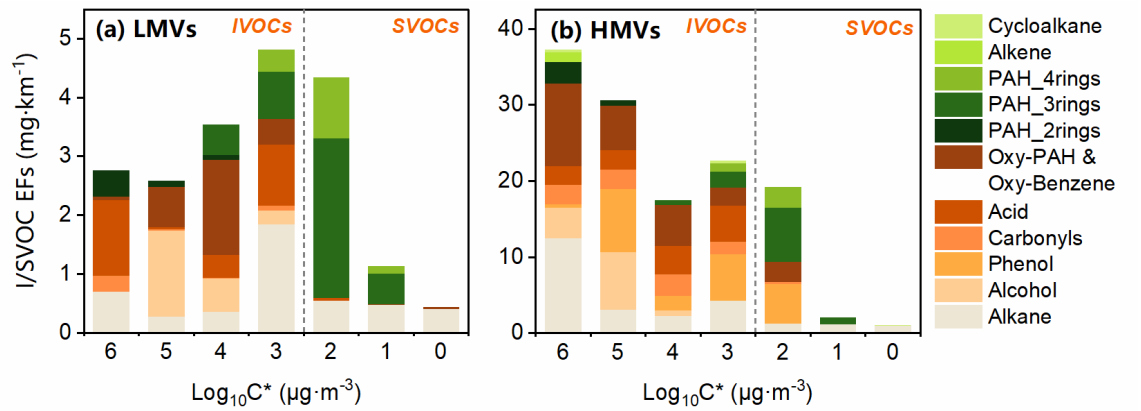

Figure S5. The average volatility distribution of I/SVOCs from the (a) LMVs and (b) HMVs. Different colored bars represent different organic groups.

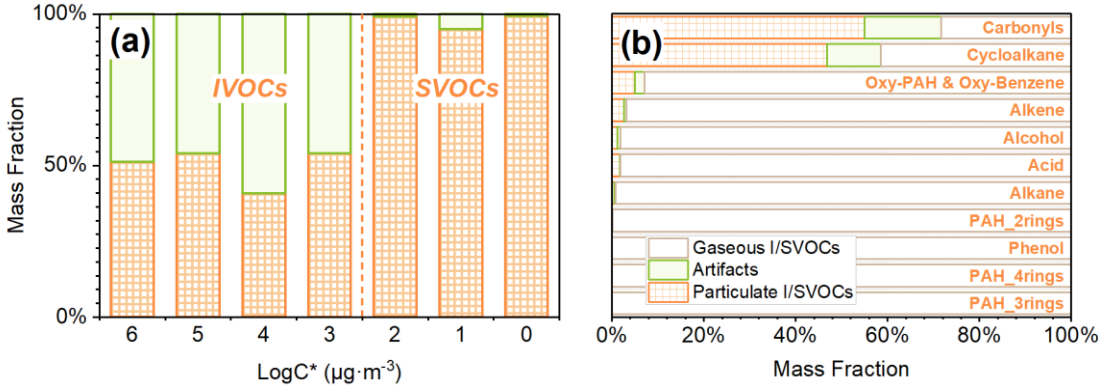

Figure S6.(a) The mass fraction of artifacts and particulate I/SVOCs divided by C* captured by quartz. (b) Gas-particle partition and artifacts of various organic compound groups.

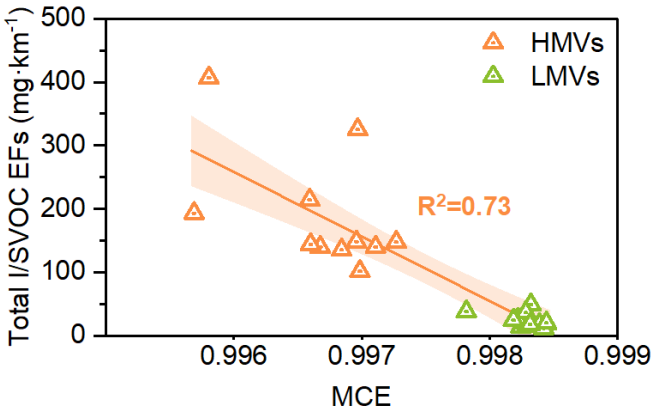

Figure S7. The linear correlation between total I/SVOC EFs and MCE.

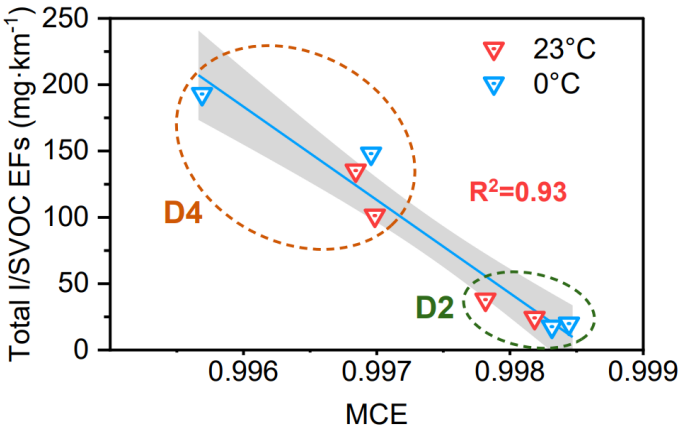

Figure S8. The linear correlation between hot-start cycle I/SVOC EFs and MCE of LMV (D2) and HMV (D4) at different ambient temperatures.

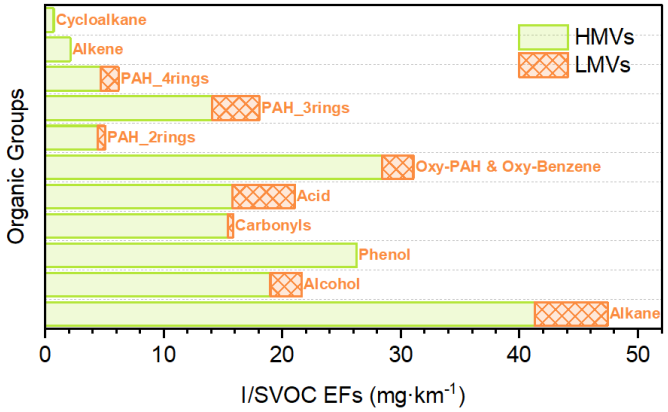

Figure S9. The average organic group distribution of HMVs and LMVs.

References

He, X., Zheng, X., Zhang, S., Wang, X., Chen, T., Zhang, X., Huang, G., Cao, Y., He, L., Cao, X., Cheng, Y., Wang, S., and Wu, Y.: Comprehensive characterization of particulate intermediate-volatility and semi-volatile organic compounds (I/SVOCs) from heavy-duty diesel vehicles using two-dimensional gas chromatography time-of-flight mass spectrometry, Atmos. Chem. Phys., 22, 13935–13947, https://doi.org/10.5194/acp-22-13935-2022, 2022a.

He, X., Zheng, X., You, Y., Zhang, S., Zhao, B., Wang, X., Huang, G., Chen, T., Cao, Y., He, L., Chang, X., Wang, S., and Wu, Y.: Comprehensive chemical characterization of gaseous I/SVOC emissions from heavy-duty diesel vehicles using two-dimensional gas chromatography time-of-flight mass spectrometry, Environ. Pollut., 305, 119284, https://doi.org/10.1016/j.envpol.2022.119284, 2022b.