Supplementary Materials

Deep Transfer Learning for Automatic Analysis of Ignitable Liquid Residues in Fire Debris Samples

Ting-Yu Huang[1*], Ph.D.; Jorn Chi Chung Yu[2], Ph.D.

[1]Department of Fire Science, College of Police Science and Technology, Central Police University, Taoyuan City 333322, Taiwan

[2]Department of Forensic Science, College of Criminal Justice, Sam Houston State University, Huntsville, TX 77340, USA

*** tingyuh@mail.cpu.edu.tw**

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Table S1. Information of intra-laboratory samples.

(a) Neat gasoline

Number	SRN	Brand name	Grade	Weathering
1	0105	Phillips 66	Unleaded Regular gasoline	Neat liquid
2	0115	Exxon	Unleaded Regular gasoline	N/A
3	0258	Chevron	Unleaded Regular gasoline	Neat liquid
4	0301	Hess	Unleaded Regular gasoline	Neat liquid
5	0385	BP	Unleaded Regular gasoline	N/A
6	0536	Holiday	Unleaded Regular gasoline	N/A
7	0547	N/A	Unleaded Regular gasoline	N/A
8	0600	Marathon	Unleaded Regular gasoline	N/A
9	0940	Texaco	Unleaded Regular gasoline	Neat liquid
10	1011	Shell	Unleaded Regular gasoline	Neat liquid
11	1075	Murphy USA	Unleaded Regular gasoline	Neat liquid
12	0733	Phillips 66	Unleaded Regular gasoline	25% weathered
13	0734	Phillips 66	Unleaded Regular gasoline	50% weathered
14	0735	Phillips 66	Unleaded Regular gasoline	75% weathered
15	0736	Phillips 66	Unleaded Regular gasoline	90% weathered
16	0737	Phillips 66	Unleaded Regular gasoline	95% weathered
17	0798	Chevron	Unleaded Regular gasoline	25% weathered
18	0799	Chevron	Unleaded Regular gasoline	50% weathered
19	0800	Chevron	Unleaded Regular gasoline	75% weathered
20	0801	Chevron	Unleaded Regular gasoline	90% weathered
21	0802	Chevron	Unleaded Regular gasoline	95% weathered
22	1012	Shell	Unleaded Regular gasoline	25% weathered
23	1013	Shell	Unleaded Regular gasoline	50% weathered
24	1014	Shell	Unleaded Regular gasoline	75% weathered
25	1015	Shell	Unleaded Regular gasoline	90% weathered
26	1016	Shell	Unleaded Regular gasoline	95% weathered
27	1076	Murphy USA	Unleaded Regular gasoline	25% weathered
28	1077	Murphy USA	Unleaded Regular gasoline	50% weathered
29	1078	Murphy USA	Unleaded Regular gasoline	75% weathered
30	1079	Murphy USA	Unleaded Regular gasoline	90% weathered
31	1080	Murphy USA	Unleaded Regular gasoline	95% weathered
32	0941	Texaco	Unleaded Regular gasoline	25% weathered
33	0942	Texaco	Unleaded Regular gasoline	50% weathered
34	0943	Texaco	Unleaded Regular gasoline	75% weathered
35	0944	Texaco	Unleaded Regular gasoline	90% weathered
36	0945	Texaco	Unleaded Regular gasoline	95% weathered

(b) Burned substrates

Number	MRN	Major peaks	Predominant profile	Material composition
1	M0057	naphthalene biphenyl styrene benzaldehyde caprolactam	Cycloalkanes/alkenes	Nylon
2	M0720	styrene alpha methylstyrene 2-ethyl-1-hexanol caprolactam	Cycloalkanes/alkenes	Nylon
3	M0721	styrene alpha methylstyrene caprolactam 1-dodecanol	Cycloalkanes/alkenes	Nylon
4	M0722	styrene alpha methylstyrene 2,4,6-trimethyl-1- nonene caprolactam 2,4,6,8- tetramethyl-1- undecene	Cycloalkanes/alkenes	Nylon
5	M0724	2,4-dimethyl-1- heptene styrene benzaldehyde caprolactam 2,4,6,8- tetramethyl-1- undecene	Cycloalkanes/alkenes	Nylon
6	M0725	styrene caprolactam	Cycloalkanes/alkenes	Nylon
7	M0726	2,4-dimethyl-1- heptene styrene benzaldehyde 2-ethyl-1-hexanol caprolactam	Cycloalkanes/alkenes	Nylon

Number	MRN	Major peaks	Predominant profile	Material composition
8	M0727	styrene caprolactam	Cycloalkanes/alkenes	Nylon
9	M0728	styrene caprolactam	Cycloalkanes/alkenes	Nylon
10	M0800	styrene caprolactam alpha methylstyrene 2,4,6,8-tetramethyl-1-undecene biphenyl	Cycloalkanes/alkenes	Nylon
11	M0801	styrene caprolactam a-terpineol 2,4,6,8-tetramethyl-1-undecene biphenyl	Cycloalkanes/alkenes	Nylon
12	M802	styrene benzaldehyde caprolactam	Cycloalkanes/alkenes	Nylon
13	M804	styrene caprolactam 2,4,6,8-tetramethyl-1-undecene	Cycloalkanes/alkenes	Nylon
14	M805	styrene benzaldehyde caprolactam	Cycloalkanes/alkenes	Nylon
15	M806	2,4-dimethyl-1-heptene styrene benzaldehyde caprolactam 2,4,6,8-tetramethyl-1-undecene	Cycloalkanes/alkenes	Nylon
16	M807	2,4-dimethyl-1-heptene styrene caprolactam	Cycloalkanes/alkenes	Nylon

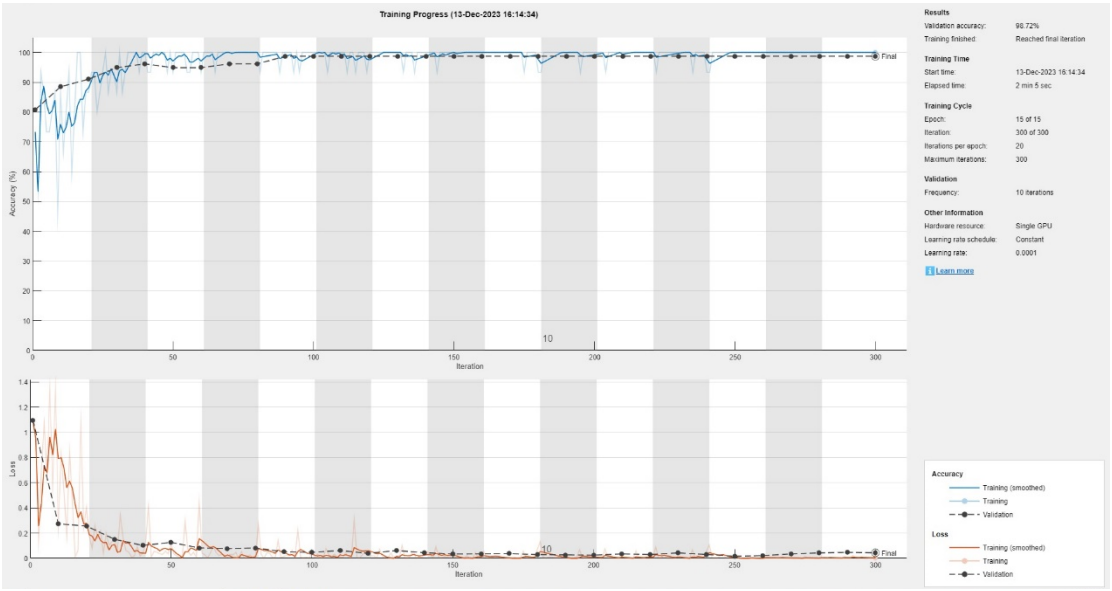
Number	MRN	Major peaks	Predominant profile	Material composition
		2,4,6,8-tetramethyl-1-undecene		
17	M808	caprolactam 2,4,6,8-tetramethyl-1-undecene	Cycloalkanes/alkenes	Nylon

(c) Simulated fire debris samples

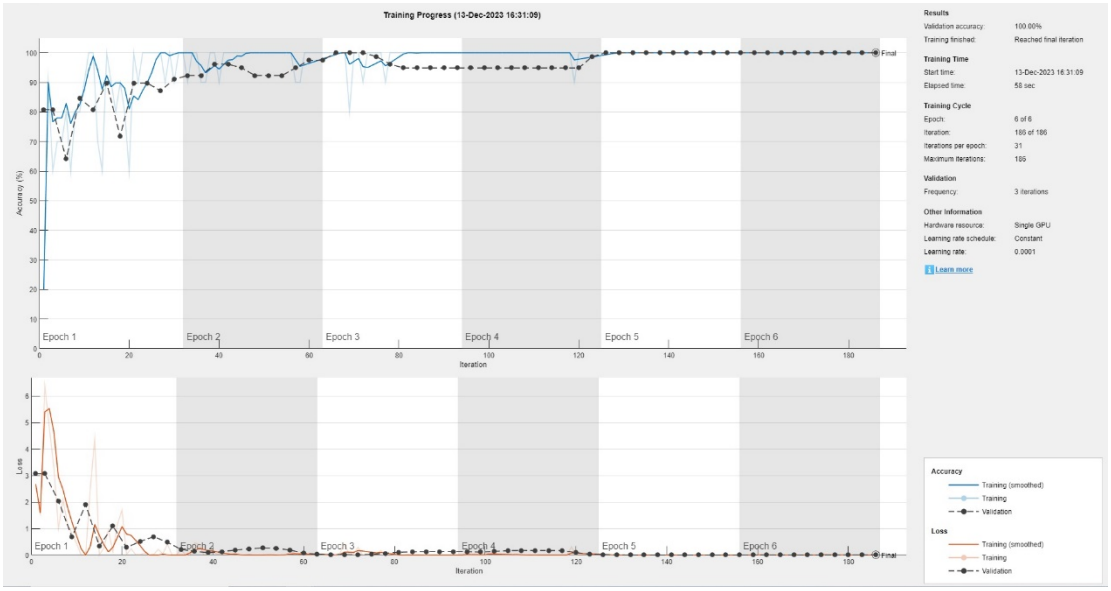
Number	RN	Relative IL contribution	Weathered	Material Class	Subclass
1	0044	Weak	75%	Flooring	Carpet, carpet padding
2	0196	Weak	90%	Flooring, miscellaneous	Vinyl/Linoleum, household material
3	0628	Strong	50%	Miscellaneous, building materials	Household material, ceiling
4	0633	Strong	75%	Miscellaneous, building materials	Household material, ceiling
5	0637	Strong	75%	Miscellaneous	Household material
6	0641	Strong	75%	Miscellaneous	Household material
7	0648	Strong	50%	Miscellaneous, building materials	Household material, ceiling
8	0650	Strong	50%	Miscellaneous, building materials	Household material, ceiling
9	0652	Strong	50%	Miscellaneous, building materials	Household material, Ceiling
10	0653	Strong	70%	Miscellaneous, building materials	Household material, ceiling
11	1298	Weak	50%	Flooring	Carpet, vinyl/linoleum
12	1302	Moderate	50%	Flooring, building materials	Engineered, wood
13	1303	Moderate	50%	Flooring, building materials	Vinyl/linoleum, wood
14	1306	Moderate	50%	Flooring	Hardwood, carpet
15	1307	Moderate	50%	Flooring, paper products	Hardwood, magazines
16	1308	Moderate	75%	Building materials, miscellaneous	Wood, household material
17	1309	Weak	50%	Building materials, flooring	Wood, vinyl/linoleum
18	1310	Moderate	75%	Building materials, paper products	Wood, paper
19	1312	Strong	75%	Building materials, flooring	Adhesives, laminate
20	1314	Strong	75%	Building materials, flooring	Adhesives, carpet

Number	RN	Relative IL contribution	Weathered	Material Class	Subclass
21	1316	Moderate	50%	Building materials, flooring	Adhesives, carpet
22	1320	Moderate	50%	Building materials, flooring	Composite decking, engineered
23	1321	Moderate	75%	Building materials, flooring	Composite decking, vinyl/linoleum
24	1322	Moderate	75%	Building materials, flooring	Adhesives, hardwood
25	1324	Moderate	50%	Building materials, flooring	Pre-treated wood, hardwood
26	1325	Moderate	50%	Building materials, flooring	Siding, hardwood
27	1327	Strong	75%	Flooring, building materials	Carpet padding, wood
28	1397	Strong	75%	Automotive	Floor mat, accessories

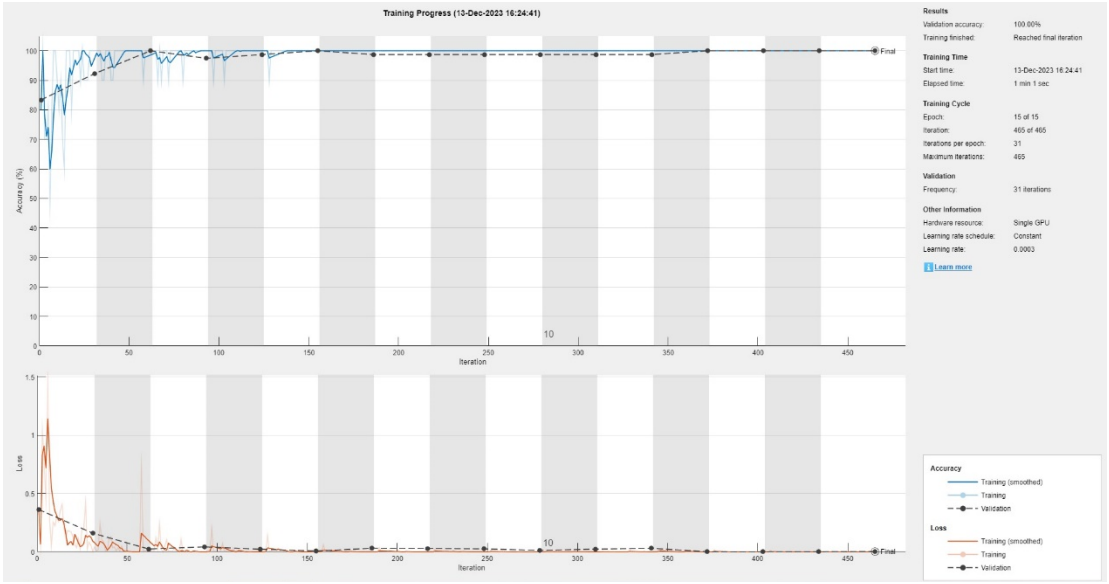
(a) GoogLeNet



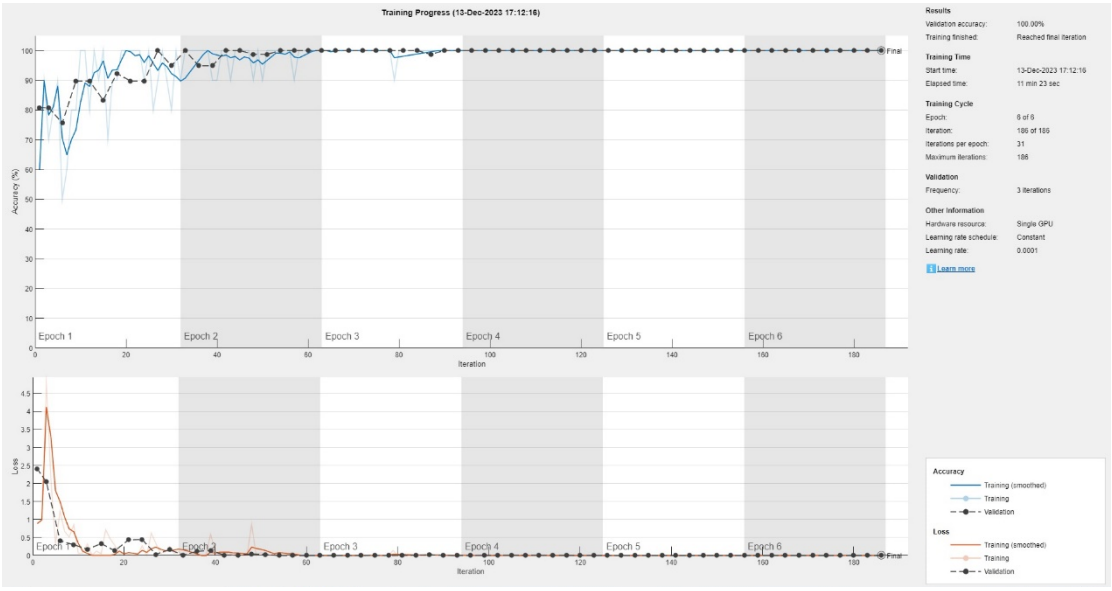
(b) AlexNet



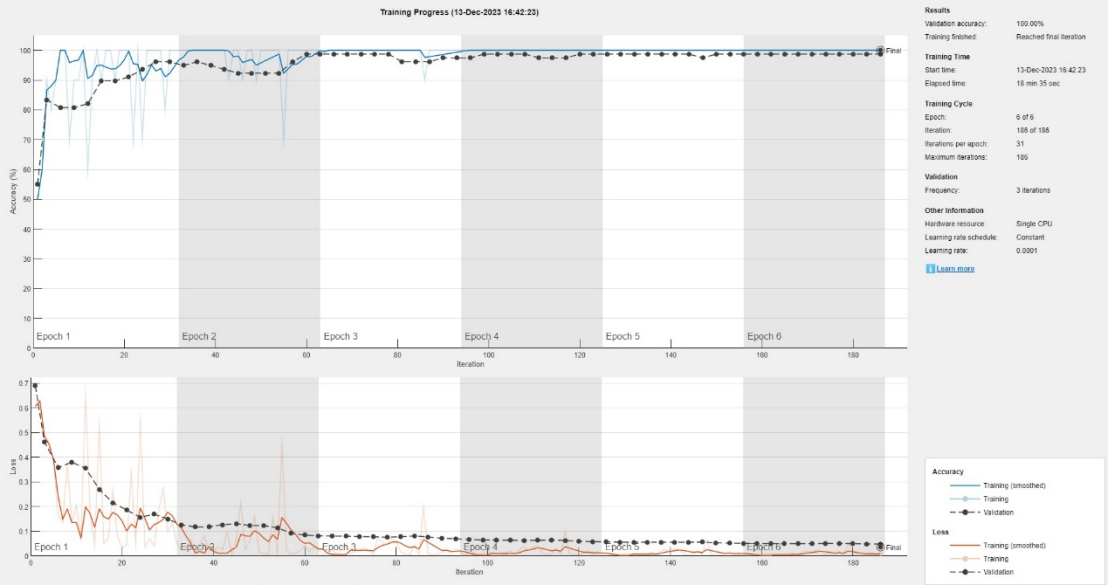
(c) SqueezeNet



(d) VGG-16



(e) ResNet-50



(f) Inception-v3

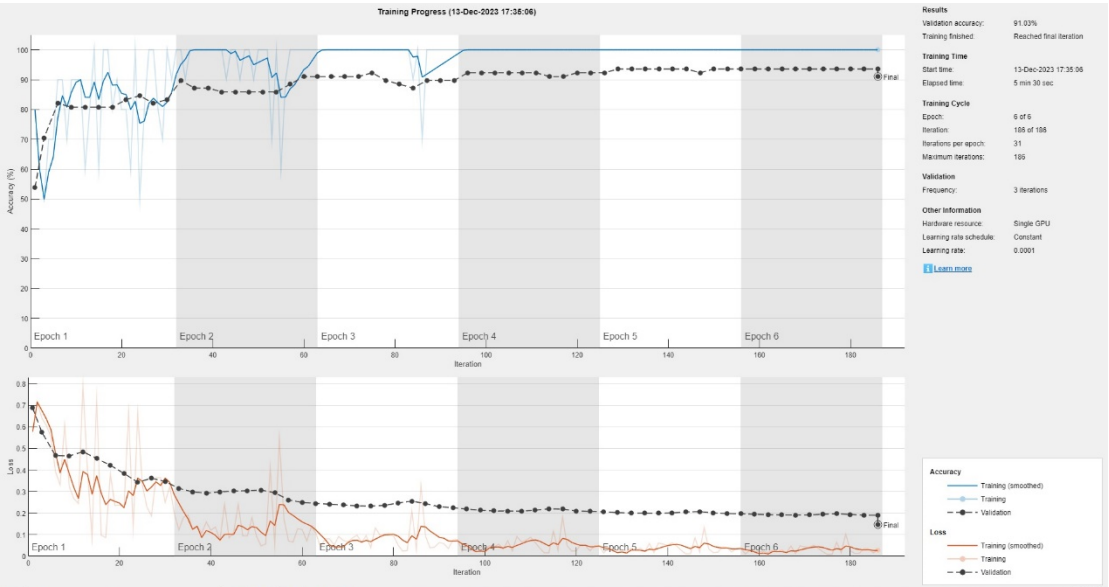
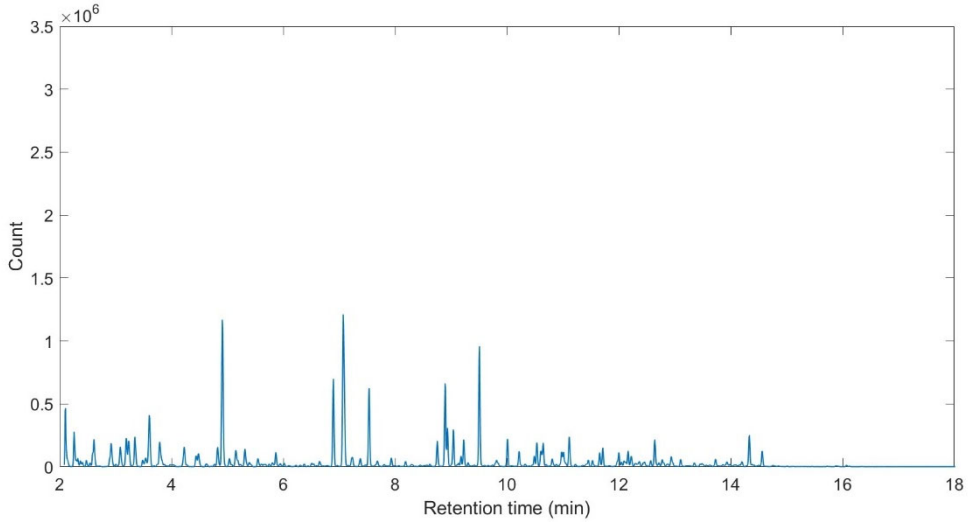


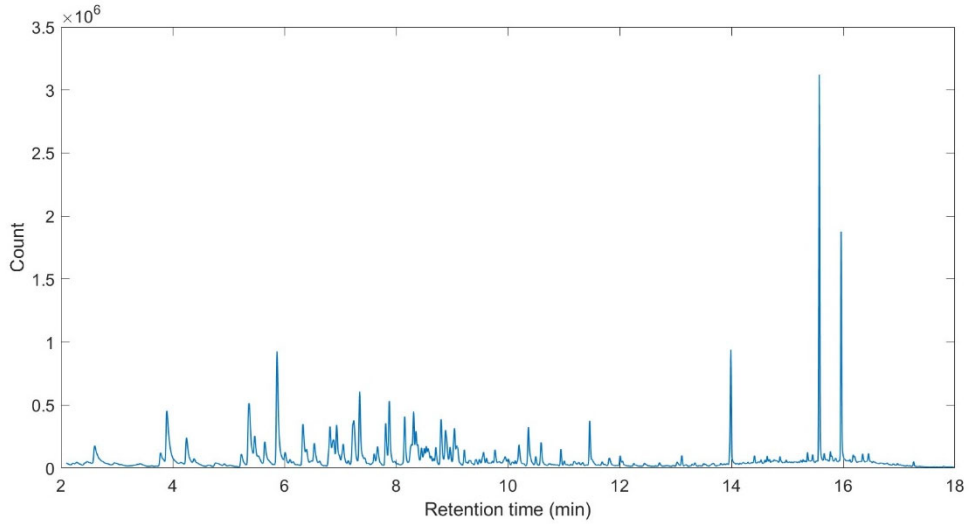
Figure. S1. The training progress of the CNNs.
Note: (a) GoogLeNet; (b) AlexNet; (c) SqueezeNet; (d) VGG-16; (e) ResNet-50; (f) Inception-v3.

(a)

0105.D

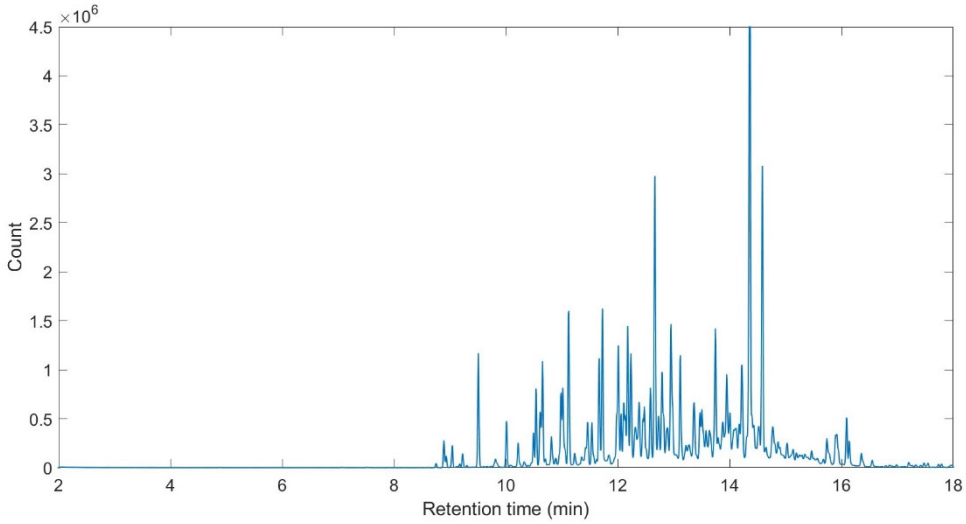


06042022_PDMS_philips66_2500_3.D

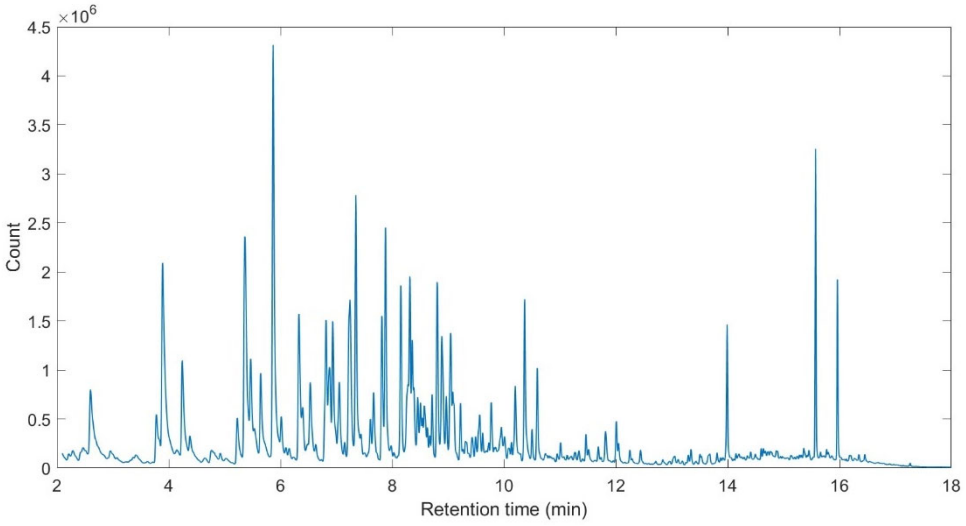


(b)

0737.D



06042022_PDMS_philips66_10000_3.D



(c)

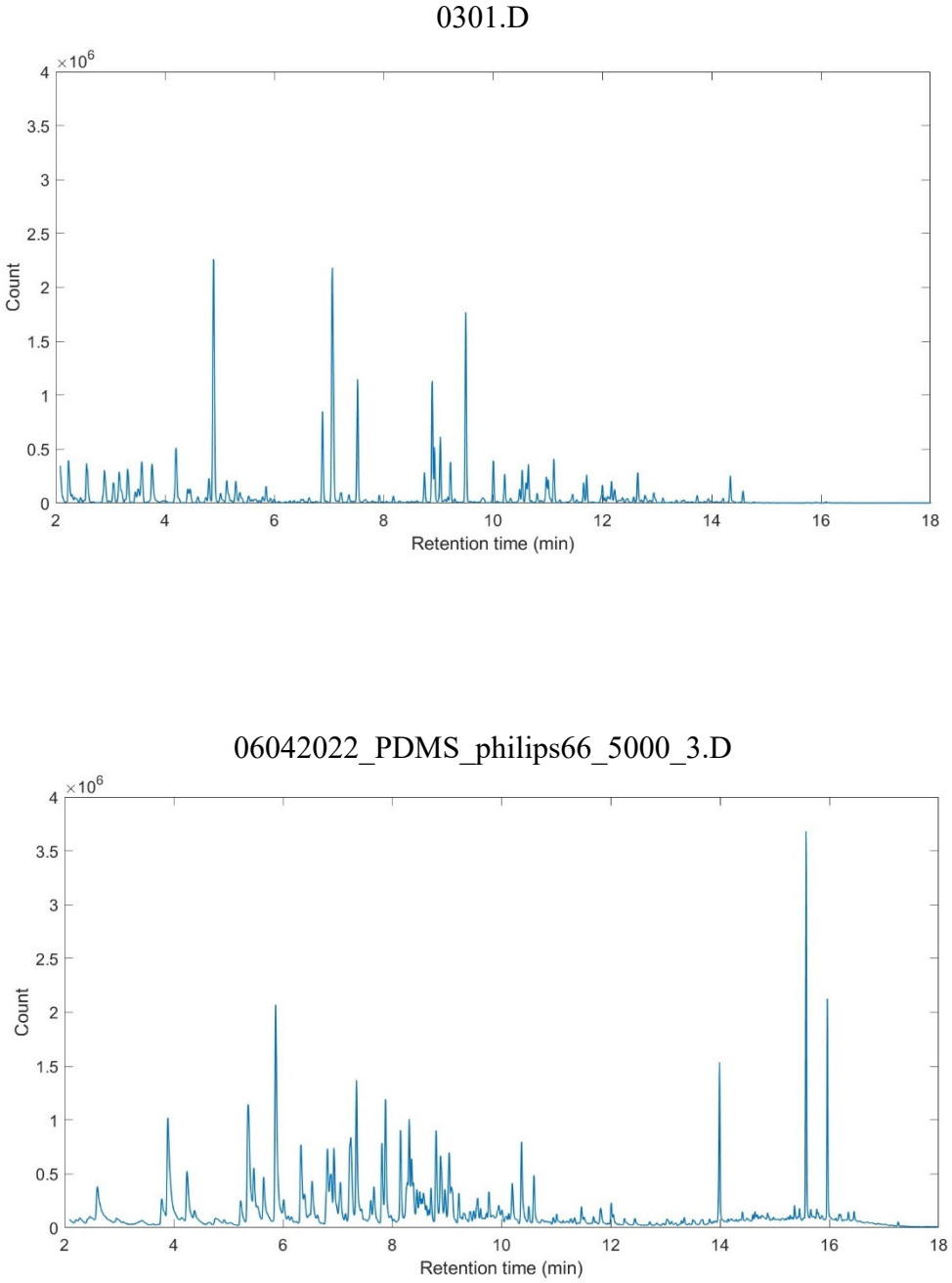


Figure. S2. Comparison of TICs of neat gasoline between lab-made samples and external lab-made samples.

Note: (a) Neat gasoline from same brand; (b) neat gasoline vs. 95% weathered gasoline (same brand); (c) neat gasoline from different brands.