Supplementary Materials

Occurrence and health risks of tire-derived chemicals in urban road dust

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Supplementary Table 1. The detail information of the 30 selected tire-derived chemicals (TDCs)

Compounds	Full name	CAS/CID	Formula	MW	Supplier	class
DNPD	1-*N*,4-*N*-dinaphthalen-2-ylbenzene-1,4-diamine	93-46-9	$C_{26}H_{20}N_2$	360.4	Tokyo Chemical Industry	PPDs
6PPD	4-*N*-(4-methylpentan-2-yl)-1-*N*-phenylbenzene-1,4-diamine	793-24-8	$C_{18}H_{24}N_2$	268.4	Tokyo Chemical Industry	PPDs
DPPD	1-*N*-cyclohexyl-4-*N*-phenylbenzene-1,4-diamine	74-31-7	$C_{18}H_{16}N_2$	260.3	AccuStandard	PPDs
DTPD	2-(cyclohexylamino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione	27417-40-9	$C_{20}H_{20}N_2$	288.4	Toronto Research Chemicals	PPDs
CPPD	2-anilino-5-(4-methylpentan-2-ylamino)cyclohexa-2,5-diene-1,4-dione	101-87-1	$C_{18}H_{22}N_2$	266.4	ChemService	PPDs
IPPD	1-*N*,4-*N*-diphenylbenzene-1,4-diamine	101-72-4	$C_{15}H_{18}N_2$	226.32	Tokyo Chemical Industry	PPDs
6PPD-Q	2,5-dianilinocyclohexa-2,5-diene-1,4-dione	154926030 (CID)	$C_{18}H_{22}N_2O_2$	298.4	Toronto Research Chemicals	PPD-Qs
CPPD-Q	4-*N*-(2-methylphenyl)-1-*N*-(4-methylphenyl)benzene-1,4-diamine	68054-78-4	$C_{18}H_{20}N_2O_2$	296.4	HPC standards Gmbh	PPD-Qs
DTPD-Q	1-*N*-phenyl-4-*N*-propan-2-ylbenzene-1,4-diamine	100944018 (CID)	$C_{20}H_{18}N_2O_2$	318.4	HPC standards Gmbh	PPD-Qs
IPPD-Q	2-anilino-5-(propan-2-ylamino)cyclohexa-2,5-diene-1,4-dione	12413088 (CID)	$C_{15}H_{16}N_2O_2$	256.3	HPC standards Gmbh	PPD-Qs
2-Me-BTH	2-methyl-1,3-benzothiazole	120-75-2	C_8H_7NS	149.21	TLC Pharmaceutical Standards	BTs
2-ABTH	1,3-benzothiazol-2-amine	136-95-8	$C_7H_6N_2S$	150.2	Toronto Research Chemicals	BTs
2-Me-S-BTH	2-methylsulfanyl-1,3-benzothiazole	615-22-5	$C_8H_7NS_2$	181.3	Sigma Aldrich	BTs
2-OH-BTH	3H-1,3-benzothiazol-2-one	934-34-9	C_7H_5NOS	151.19	Sigma Aldrich	BTs

BTH	1,3-benzothiazole	95-16-9	C_7H_5NS	135.19	Toronto Research Chemicals	BTs
BT	2H-benzotriazole	95-14-7	$C_6H_5N_3$	119.12	Sigma Aldrich	BTs
CBS	*N*-(1,3-benzothiazol-2-ylsulfanyl)cyclohexanamine	95-33-0	$C_{13}H_{16}N_2S_2$	264.4	Toronto Research Chemicals	BTs
DCBS	*N*-(1,3-benzothiazol-2-ylsulfanyl)-*N*-cyclohexylcyclohexanamine	4979-32-2	$C_{19}H_{26}N_2S_2$	346.6	International Laboratory	BTs
NOBS	4-(1,3-benzothiazol-2-ylsulfanyl)morpholine	102-77-2	$C_{11}H_{12}N_2OS_2$	252.4	Tmstandard	BTs
TBBS	*N*-(1,3-benzothiazol-2-ylsulfanyl)-2-methylpropan-2-amine	95-31-8	$C_{11}H_{14}N_2S_2$	238.4	Alfa Aesar	BTs
DM	2-(1,3-benzothiazol-2-yldisulfanyl)-1,3-benzothiazole	120-78-5	$C_{14}H_8N_2S_4$	332.5	Tmstandard	BTs
BLE	9,9-dimethyl-10H-acridine	6267-02-3	$C_{15}H_{15}N$	209.29	Aladdin	BTs
4-HDPA	4-anilinophenol	122-37-2	$C_{12}H_{11}NO$	185.22	TLC Pharmaceutical Standards	others
DCU	1,3-dicyclohexylurea	2387-23-7	$C_{13}H_{24}N_2O$	224.34	Dr. Ehrenstorfer	others
DPU	1,3-diphenylurea	102-07-8	$C_{13}H_{12}N_2O$	212.25	Dr. Ehrenstorfer	others
HMMM	2-*N*,2-*N*,4-*N*,4-*N*,6-*N*,6-*N*-hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamin	3089-11-0	$C_{15}H_{30}N_6O_6$	390.44	TLC Pharmaceutical Standards	others
RD	2,2,4-trimethyl-1H-quinoline	147-47-7	$C_{12}H_{15}N$	173.25	Macklin	others
TMTD	dimethylcarbamothioylsulfanyl *N*,*N*-dimethylcarbamodithioate	137-26-8	$C_6H_{12}N_2S_4$	240.4	AccuStandard	others
DPG	1,2-diphenylguanidine	102-06-7	$C_{13}H_{13}N_3$	211.26	CATO	others
DCA	*N*-cyclohexyl-*N*-methylcyclohexanamine	2387-23-7	$C_{13}H_{24}N_2O$	224.34	Dr. Ehrenstorfer	others

Supplementary Table 2. Basic information on sampling

Sampling sites	Classification	Sampling date	Number	Geographical location (E, N)
B1	Business district	2023.4.14	B1-1	113.348684, 23.007663
		2022.9.25	B1-2	
B2		2023.4.14	B2-1	113.323084, 23.122272
		2022.10.17	B2-2	
B3		2023.4.14	B3-1	113.333944, 23.132429
		2022.10.17	B3-2	
B4		2023.3.20	B4-1	113.372927, 23.054674
		2022.9.6	B4-2	
C1	Urban village	2023.3.20	C1-1	113.36029, 23.056601
		2022.9.6	C1-2	
C2		2023.4.14	C2-1	113.345523, 22.966942
		2022.9.25	C2-2	
D1	Green space	2023.3.20	D1-1	113.380806, 23.052137
		2022.9.6	D1-2	
D2		2023.4.14	D2-1	113.381639, 23.06685
		2022.9.6	D2-2	
D3		2023.4.14	D3-1	113.33303, 22.981062
		2022.9.25	D3-2	
E1	Residential area	2023.4.14	E1-1	113.384647, 23.061477
		2022.9.25	E1-2	
E2		2023.4.14	E2-1	113.330081, 23.139502

E3	2022.10.17	E2-2	113.359293, 23.139445
	2023.4.14	E3-1	
	2022.10.17	E3-2	

Supplementary Table 3. The detail information of gradient elution

Time（min）	%A	%B
0	70	30
1	30	70
1.5	20	80
2	0	100
4	0	100
5.5	30	70
6.5	30	70

Supplementary Table 4. Mass transitions and retention times for target compounds in HPLC-MS/MS

Chemicals	RT (min)	Precursor ions (m/z)	Production ions (m/z)	Dwell (s)	Cone (V)	Collision (V)	Internal standard
DNPD	2.63	360.4	217.19 232.93	0.03	40	32	6PPD-Q-d5
6PPD	1.72	269.05	183.9 212	0.03	40	25	6PPD-Q-d5
DPPD	2.32	261	167.9 183.8	0.03	40	20	6PPD-Q-d5
DTPD	2.58	289	180.8 197.9	0.03	20	24	6PPD-Q-d5
CPPD	1.69	267.03	92.7 183.9	0.03	40	24	6PPD-Q-d5
IPPD	1.47	227.03	92.6 107	0.03	40	33	6PPD-Q-d5
6PPD-Q	2.34	299.28	99.97 186.9	0.03	6	20	6PPD-Q-d5
CPPD-Q	2.28	297.31	97.93 186.99	0.03	28	22	6PPD-Q-d5
DTPD-Q	2.27	319.3	117.95 128.19	0.03	40	34	6PPD-Q-d5
IPPD-Q	1.90	227.03	92.6 107	0.03	40	33	6PPD-Q-d5
2-Me-BTH	1.80	150.05	65.07 117.03	0.03	28	28	BT-D4
2-ABTH	1.04	151.04	64.88 123.87	0.03	16	26	BT-D4
2-Me-S-BTH	2.10	182.06	90.89 108.84	0.03	14	28	BT-D4
2-OH-BTH	1.24	151.97	80.03 119	0.03	78	20	BT-D4
BTH	1.63	136.03	64.88 76.91	0.03	20	26	BT-D4
BT	1.25	120.03	51.02 64.88	0.03	46	22	BT-D4
CBS	2.55	265	165.7 182.7	0.03	40	13	BT-D4
DCBS	3.16	347.07	138 180	0.03	40	13	BT-D4
NOBS	2.10	253.07	85.6 165.6	0.03	40	15	BT-D4
TBBS	2.32	239.02	165.6 182.8	0.03	40	15	BT-D4

DM	2.69	333.28	90.87 108.75	0.03	2	52	BT-D4
BLE	2.37	210	193.9 210.1	0.03	40	20	BT-D4
4-HDPA	1.71	186	65.07 80.21	0.03	72	34	Atrazine-d5
DCU	2.00	225.34	82.9 100	0.03	40	20	Atrazine-d5
DPU	1.80	213.03	77.03 94	0.03	2	30	Atrazine-d5
HMMM	1.77	391	177 207	0.03	40	10	Atrazine-d5
RD	2.36	174.03	117.9 131.8	0.03	40	15	Atrazine-d5
TMTD	2.33	241.15	167.78 184.81	0.03	30	18	Atrazine-d5
DPG	1.18	212.1	65.06 93.99	0.03	98	10	Atrazine-d5
DCA	1.25	196.12	41.07 55.11	0.03	88	32	Atrazine-d5
Atrazine-d5	1.84	221.01	78.84 100.88	0.03	40	22	
6PPD-Q-d5	2.33	304.35	191.96 219.98	0.03	14	24	
BT-d4	1.24	124	68.6 95.8	0.03	40	20	

Supplementary Table 5. The recoveries (mean (%) ± standard deviation (%), n=3), method limit of detection (LOD, ng/g), and limit of quantification (LOQ, ng/g) of the 30 tire-derived chemicals in road dust

Compounds	Recovery (%)	LOD (ng/g)	LOQ (ng/g)
DNPD	50%±6.53	0.02	0.06
6PPD	110%±8.12	0.54	1.8
DPPD	58%±5.21	0.42	1.4
DTPD	107%±3.45	2.25	7.5
CPPD	102±15.9	0.15	0.5
IPPD	102±16.9	0.11	0.36
6PPD-Q	103%±6.88	0.18	0.6
CPPD-Q	91%±7.41	0.29	0.96
DTPD-Q	93%±2.24	0.09	0.31
IPPD-Q	102%±6.56	0.04	0.12
2-Me-BTH	66%±3.13	13.17	43.9
2-ABTH	124%±7.36	0.42	1.4
2-Me-S-BTH	58%±4.32	1.02	3.4
2-OH-BTH	113%±6.67	3.45	11.5
BTH	87%±3.54	1.71	5.7
BT	94%±6.45	0.18	0.6
CBS	85%±2.57	0.18	0.6
DCBS	71%±12.3	0.51	1.7
NOBS	84%±6.74	0.18	0.6
TBBS	62%±3.45	0.02	0.06
DM	57%±10.4	0.32	1.08
BLE	65.1±8.85	0.04	0.13
4-HDPA	87%±4.56	0.03	0.10
DCU	100%±9.89	2.19	7.3
DPU	70%±7.89	0.15	0.5
HMMM	123%±10.9	0.18	0.6
RD	51%±5.43	0.18	0.6
TMTD	70%±6.73	0.18	0.6
DPG	65%±2.45	0.03	0.12
DCA	104±9.3	0.32	1.05

Supplementary Table 6. Parameters used to estimate daily intake rates via dust ingestion($EDI_{ingestion}$) and dermal absorption (EDI_{dermal}) for the local population

	Adults	Children	Reference Source
IGR(Dust ingestion rate)	100 mg/day	200 mg/day	[1]
SA(Skin surface area available for contact)	2145 cm2/day	1150 cm2/day	[1]
AF(Dust to skin adherence factor)	0.07 mg/cm2	0.20 mg/cm2	[1]
ABS(Absorption factor)	13%	13%	[1]
EF(Exposure frequency)	365 days/year	365 days/year	[1]
BW(Body weight)	58.55 kg	16.58 kg	[1]

Supplementary Table 7. Patterns of 30 selected tire-derived chemicals in various functional areas

Compounds	Business district（ng/g)				Urban village(ng/g)				Green space(ng/g)				Residential area(ng/g)			
	Mean	Median	Range	DF (%)	Mean	Median	Range	DF (%)	Mean	Median	Range	DF (%)	Mean	Median	Range	DF (%)
DNPD	0.59	0.70	ND-0.70	60	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	0.73	0.70	ND-1.37	83
6PPD	322	165	86.0-730	100	209	95.0	70.0-462	100	257	90.3	6.00-1082	100	240	225	54.0-509	100
DPPD	32.7	32.7	4.33-61.0	40	5.67	5.67	4.67-6.67	67	5.00	4.33	4.33-6.33	60	5.73	4.50	ND-6.67	83
DTPD	136	136	128-145	60	16.8	16.8	ND-30.3	33	3.33	0	ND-16.6	20	12.9	12.3	ND-15.3	50
CPPD	9.61	10.5	4.00-20.3	100	5.00	2.00	0.67-12.3	100	3.73	0.33	ND-20.0	60	5.19	4.50	0.5-12.7	100
IPPD	20.3	8.33	ND-79.8	83	18.4	10.5	6.17-38.5	100	12.2	5.83	ND-30.2	80	33.8	16.3	ND-104	60
6PPD-Q	63.4	60.3	16.5-148	100	57.4	28.2	16.5-128	100	39.4	14.8	0.50-159	100	56.5	49.3	11.5-107	100
CPPD-Q	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0
DTPD-Q	1.67	1.67	0.33-3.00	60	0.33	0	ND-1.00	33	0.40	0	ND-2.00	0	1.33	1.33	ND-2.33	67
IPPD-Q	1.78	1.67	1.33-2.33	60	1.00	0.67	0.67-1.67	100	<MDL	<MDL	ND	0	2.00	2.17	ND-3.67	67
2-Me-BTH	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0
2-ABTH	25.6	22.7	ND-42.7	80	13.2	13.2	10.3-16.0	100	10.5	10.7	6.00-17.7	100	20.1	17.2	5.67-43.7	100
2-Me-S-BTH	22.0	22.0	ND-27.3	40	<MDL	<MDL	ND	0	19.3	19.3	11.7-27.0	40	15.6	15.7	11.0-20.0	67
2-OH-BTH	323	325	ND-483	80	244	244	143-345	100	205	132	38.0-578	100	313	298	32.3-607	100
BTH	108	108	ND-145	80	88.5	88.5	41.0-136	100	101	51.7	20.0-351	100	132	125	ND-254	83
BT	16.8	16.5	ND-20.7	80	5.33	5.33	3.00-7.67	100	5.56	3.67	ND-9.67	60	10.6	10.3	ND-15.3	83
CBS	3.83	3.83	ND-7.67	20	<MDL	<MDL	ND	0	0.40	0	ND-2.00	20	2.67	2.67	ND-2.67	50
DCBS	3.50	3.50	ND-7.00	20	<MDL	<MDL	ND	0	1.47	0	ND-7.33	20	0.00	<MDL	ND	0
NOBS	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0
TBBS	0.17	0.17	ND-0.33	20	<MDL	<MDL	ND	0	0.27	0	ND-1.33	20	<MDL	<MDL	ND	0
DM	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0
BLE	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0

4-HDPA	54.6	66.0	4.33-77.3	100	40.9	30.7	19.3-72.7	100	60.5	10.7	4.00-265	100	38.3	40.0	3.50-70.7	100
DCU	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0	<MDL	<MDL	ND	0
DPU	20.5	22.7	2.03-32.7	100	18.9	13.4	7.70-35.7	100	6.63	4.70	1.70-6.70	100	18.4	15.0	6.37-32.7	100
HMMM	23.7	25.0	5.00-38.0	100	39.6	35.0	16.7-67.0	100	10.3	5.33	2.00-28.7	100	63.9	40.3	2.67-231	100
RD	156	73.0	3.67-524	100	419	58.0	43.0-1156	100	63.4	26.3	ND-188	80	117	78.2	4.00-296	100
TMTD	1.67	2.00	ND-2.33	80	28.2	28.2	8.67-47.7	67	4.00	4.00	3.67-4.33	40	2.89	2.33	ND-4.33	50
DPG	3354	3270	208-6206	100	2931	688	444-7661	100	1409	581	236-4696	100	2396	2470	647-4168	100
DCA	16.8	18.8	ND-30.2	83	8.50	7.17	3.83-14.5	100	10.6	4.17	ND-43.8	60	12.0	6.83	3.83-34.2	100

DF: Detection frequency; ND: Not detected; <MDL:Below instrumental detection limit.

Supplementary Table 8. Prediction of potential toxicity of 30 tire-derived chemicals using ProTox-3.0

Potential	Hepatotoxicity		Neurotoxicity		Carcinogenicity		Immunotoxicity		Mutagenicity		Cytotoxicity	
toxicity	Value	Probability	Value	Probability	Value	Probability	Value	Probability	Value	Probability	Value	Probability
DNPD	-	0.56	+	0.63	-	0.85	-	0.97	+	0.63	-	0.79
6PPD	-	0.73	+	0.66	-	0.59	-	0.97	-	0.86	-	0.75
DPPD	-	0.57	+	0.65	-	0.85	-	0.99	+	0.71	-	0.79
DTPD	-	0.60	+	0.74	+	0.61	-	0.99	+	0.68	-	0.76
CPPD	-	0.77	+	0.77	-	0.88	-	0.99	-	0.52	-	0.75
IPPD	-	0.59	+	0.60	-	0.62	-	0.99	+	0.51	-	0.78
6PPD-Q	-	0.65	+	0.57	-	0.56	-	0.67	-	0.71	-	0.70
CPPD-Q	-	0.74	+	0.66	-	0.63	-	0.91	-	0.58	-	0.66
DTPD-Q	-	0.50	+	0.62	+	0.60	-	0.95	+	0.65	-	0.71
IPPD-Q	-	0.53	+	0.52	-	0.53	-	0.88	-	0.51	-	0.68
2-Me-BTH	+	0.63	-	0.63	-	0.50	-	0.99	-	0.94	-	0.84
2-ABTH	+	0.77	+	0.62	+	0.52	-	0.99	-	0.81	-	0.71
2-Me-S-BTH	+	0.63	-	0.63	-	0.50	-	0.99	-	0.94	-	0.84
2-OH-BTH	+	0.66	+	0.55	+	0.54	-	0.99	-	0.81	-	0.80
BTH	+	0.65	-	0.61	+	0.53	-	0.99	-	0.95	-	0.82
BT	+	0.62	+	0.65	-	0.76	-	0.99	+	0.67	-	0.86
CBS	+	0.52	+	0.66	-	0.64	-	0.98	-	0.58	-	0.69
DCBS	-	0.55	+	0.64	-	0.64	-	0.81	-	0.57	-	0.75
NOBS	-	0.64	+	0.65	-	0.78	-	0.99	-	0.83	-	0.69
TBBS	+	0.55	-	0.53	-	0.61	-	0.98	-	0.70	-	0.77
DM	+	0.67	-	0.59	-	0.83	-	0.99	+	0.74	-	0.85
BLE	-	0.60	+	0.59	-	0.68	-	0.99	-	0.69	-	0.84
4-HDPA	-	0.50	+	0.66	-	0.62	-	0.99	-	0.65	-	0.84

DCU	-	0.75	+	0.68	-	0.87	-	0.99	-	0.88	-	0.71
DPU	+	0.64	+	0.69	-	0.75	-	0.99	-	0.94	-	0.66
HMMM	-	0.79	+	0.65	+	0.55	-	0.99	-	0.63	-	0.69
RD	-	0.63	+	0.53	-	0.66	-	0.95	-	0.91	-	0.82
TMTD	-	0.57	-	0.54	-	0.97	-	0.99	+	0.67	-	0.69
DPG	-	0.53	-	0.51	-	0.67	-	0.99	+	0.66	-	0.71
DCA	-	0.75	+	0.68	-	0.87	-	0.99	-	0.88	-	0.71

Supplementary Table 8. Prediction of potential toxicity of 30 tire-derived chemicals using ProTox-3.0 (Continued)

Potential toxicity	AhR Value	AhR Probability	AR Value	AR Probability	ER Value	ER Probability	TTR Value	TTR Probability	Acute 0ral toxicity LD_{50}(mg/kg)
DNPD	+	1	-	0.99	-	0.76	-	0.66	4500
6PPD	-	0.54	-	0.99	-	0.99	-	0.97	271
DPPD	+	0.68	-	1	-	0.91	-	0.59	244
DTPD	+	0.75	-	0.99	-	0.80	-	0.54	330
CPPD	-	0.6	-	0.97	-	0.87	-	0.79	2000
IPPD	-	0.75	-	0.99	-	0.85	-	0.66	720
6PPD-Q	-	0.65	-	0.95	-	0.85	-	0.97	1000
CPPD-Q	-	0.84	-	0.94	-	0.85	-	0.77	338
DTPD-Q	+	0.61	-	0.90	-	0.72	+	0.61	215
IPPD-Q	-	0.56	-	0.93	-	0.79	+	0.51	215
2-Me-BTH	-	0.72	-	0.99	-	0.98	+	0.60	900
2-ABTH	+	1	-	0.99	-	0.90	-	0.65	1000
2-Me-S-BTH	-	0.72	-	0.99	-	0.98	+	0.60	631
2-OH-BTH	-	0.50	-	0.98	-	0.85	+	0.78	540
BTH	-	0.50	-	0.99	-	0.97	+	0.61	380
BT	-	0.97	-	1	-	0.98	-	0.52	560
CBS	+	1	-	0.97	-	0.91	-	0.77	400
DCBS	+	1	-	0.99	-	0.96	-	0.75	1077
NOBS	+	0.85	-	0.99	-	0.92	-	0.88	1870
TBBS	+	1	-	0.99	-	0.94	-	0.64	6000
DM	-	0.70	-	0.98	-	0.93	+	0.58	7000
BLE	-	0.67	-	0.99	-	0.62	-	0.64	2140
4-HDPA	+	0.78	-	0.99	+	0.99	+	0.73	380

DCU	-	0.96	-	0.99	-	0.83	-	0.83	1600
DPU	+	0.99	-	0.99	+	1	-	0.59	3440
HMMM	-	0.91	-	0.98	-	0.97	-	0.79	1800
RD	-	0.85	-	0.99	-	0.93	-	0.63	1450
TMTD	-	0.85	-	1	-	0.96	-	0.78	560
DPG	+	0.51	-	1	-	0.81	-	0.84	880
DCA	-	0.96	-	0.99	-	0.83	-	0.83	1600

+/–: Non–detected risk/Detected risk; AhR: Aryl hydrocarbon receptor; AR: Androgen receptor; ER: Estrogen receptor alpha; TTR: Transtyretrin.

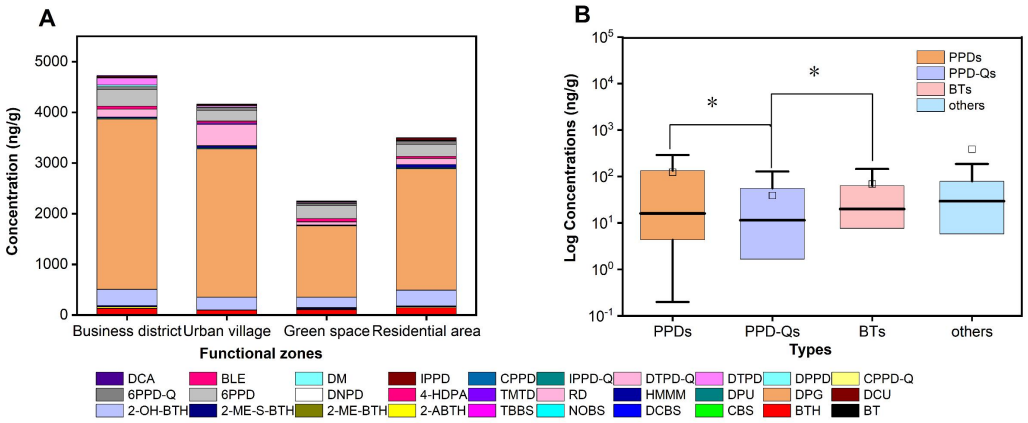
Supplementary Table 9. Estimated daily intake of target compounds by oral dust ingestion and dermal exposure for adults and children

Compounds	EDI (ng/kg bw/day)							
	Business District		Urban Village		Green Space		Residential Area	
	Adults	children	Adults	children	Adults	children	Adults	children
DNPD	0.0012	0.0082	0	0	0	0	0.0015	0.01
6PPD	0.66	4.5	0.43	2.9	0.52	3.6	0.49	3.3
DPPD	0.067	0.45	0.012	0.079	0.01	0.069	0.012	0.079
DTPD	0.28	1.9	0.034	0.23	0.0068	0.046	0.026	0.18
CPPD	0.02	0.13	0.020	0.069	0.0076	0.052	0.011	0.072
IPPD	0.041	0.28	0.038	0.25	0.025	0.17	0.069	0.47
6PPD-Q	0.13	0.88	0.12	0.8	0.08	0.55	0.12	0.78
CPPD-Q	0	0	0	0	0	0	0	0
DTPD-Q	0.0034	0.023	0.00067	0.0046	0.00082	0.0055	0.0027	0.018
IPPD-Q	0.0036	0.025	0.002	0.014	0	0	0.0041	0.028
2-Me-BTH	0	0	0	0	0	0	0	0
2-ABTH	0.052	0.35	0.027	0.18	0.021	0.15	0.041	0.28
2-Me-S-BTH	0.045	0.31	0	0	0.039	0.27	0.032	0.22
2-OH-BTH	0.66	4.5	0.5	3.4	0.42	2.8	0.64	4.3
BTH	0.22	1.5	0.18	1.2	0.21	1.4	0.27	1.8
BT	0.034	0.23	0.011	0.074	0.011	0.077	0.022	0.15
CBS	0.0078	0.053	0	0	0.00082	0.0055	0.0055	0.037
DCBS	0.0071	0.049	0	0	0.003	0.02	0	0
NOBS	0	0	0	0	0	0	0	0
TBBS	0.00035	0.0024	0	0	0.00055	0.0037	0	0
DM	0	0	0	0	0	0	0	0
BLE	0	0	0	0	0	0	0	0
4-HDPA	0.11	0.76	0.083	0.57	0.12	0.84	0.078	0.53
DCU	0	0	0	0	0	0	0	0
DPU	0.042	0.28	0.039	0.26	0.014	0.092	0.038	0.26
HMMM	0.048	0.33	0.081	0.55	0.021	0.14	0.13	0.89
RD	0.32	2.2	0.86	5.8	0.13	0.88	0.24	1.6
TMTD	0.0034	0.023	0.058	0.39	0.0082	0.055	0.0059	0.04
DPG	6.8	47	6	41	2.9	20	4.9	33
DCA	0.034	0.23	0.027	0.12	0.022	0.15	0.024	0.17
Sum	9.49	65.4	8.44	57.5	4.52	31	7.06	47.5

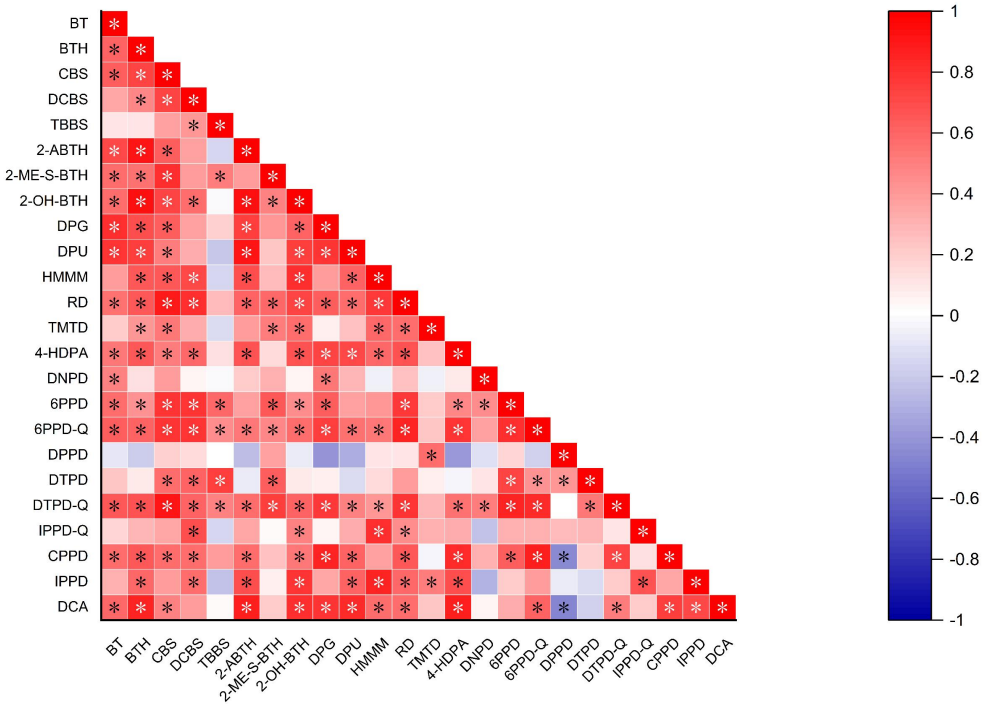
Note: All parameters in this table are calculated from the parameters in Table 6 using Eqs. (1)–(3) in the main text.

Supplementary Table 10. Comprehensive Risk Assessment of 30 TDCs: LD_{50}, Reference Doses (RfDs), Estimated Daily Intakes (EDIs), Hazard Quotients (HQs), and Priority Ranking

Compounds	LD_{50}(mg/kg)	RfD(mg/kg.day)	EDI(ng/kg bw/day)	HQ	Rank
DPG	880	0.88	20.2	2.29545E-05	1
6PPD	271	0.271	2.05	7.56458E-06	2
2-OH-BTH	540	0.54	2.1525	3.98611E-06	3
BTH	380	0.38	0.8475	2.23026E-06	4
RD	1450	1.45	1.50375	1.03707E-06	5
DTPD	330	0.33	0.33785	1.02379E-06	6
4-HDPA	380	0.38	0.386375	1.01678E-06	7
6PPD-Q	1000	1	0.4325	4.325E-07	8
DPPD	244	0.244	0.09725	3.98566E-07	9
IPPD	720	0.72	0.167875	2.3316E-07	10
2-Me-S-BTH	631	0.631	0.1145	1.81458E-07	11
HMMM	1800	1.8	0.27375	1.52083E-07	12
2-ABTH	1000	1	0.137625	1.37625E-07	13
BT	560	0.56	0.076125	1.35938E-07	14
TMTD	560	0.56	0.0729375	1.30246E-07	15
DCA	1600	1.6	0.097125	6.07031E-08	16
IPPD-Q	215	0.215	0.0095875	4.4593E-08	17
DPU	3440	3.44	0.128125	3.72456E-08	18
CBS	400	0.4	0.0137025	3.42563E-08	19
DTPD-Q	215	0.215	0.00733625	3.41221E-08	20
CPPD	2000	2	0.0477	2.385E-08	21
DCBS	1077	1.077	0.0098875	9.18059E-09	22
DNPD	4500	4.5	0.0026125	5.80556E-10	23
TBBS	6000	6	0.000875	1.45833E-10	24
CPPD-Q	338	0.338	0	0	-
2-Me-BTH	900	0.9	0	0	-
NOBS	1870	1.87	0	0	-
DM	7000	7	0	0	-
BLE	2140	2.14	0	0	-
DCU	1600	1.6	0	0	-

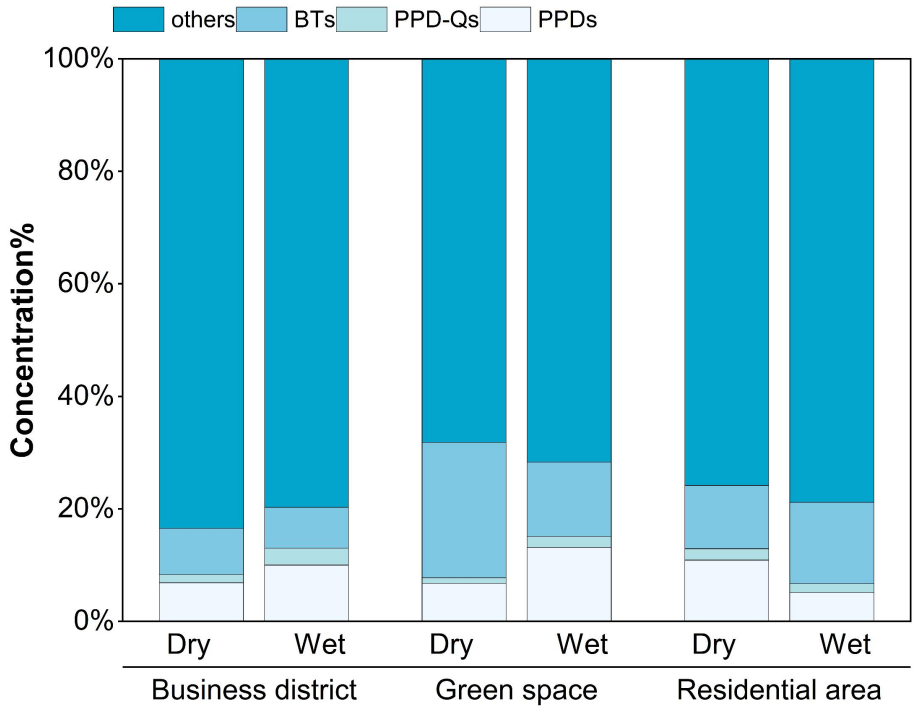


Supplementary Figure 1. (A) The mean concentrations of 30 types of tire-derived chemicals (TDCs) in the road dust at different functional areas. (B) The concentration of 4 different types of TDCs. PPDs: p-phenylenediamine types; PPD-Qs: quinone conversion products of p-phenylenediamine types; BTs: benzothiazole types; Others: other TDCs. The box represents the interquartile range (IQR) from the 25th to the 75th percentile; the black line inside the box denotes the median; the open square (□) indicates the mean; and the asterisk (*) represents significant differences at the levels of $p < 0.05$.

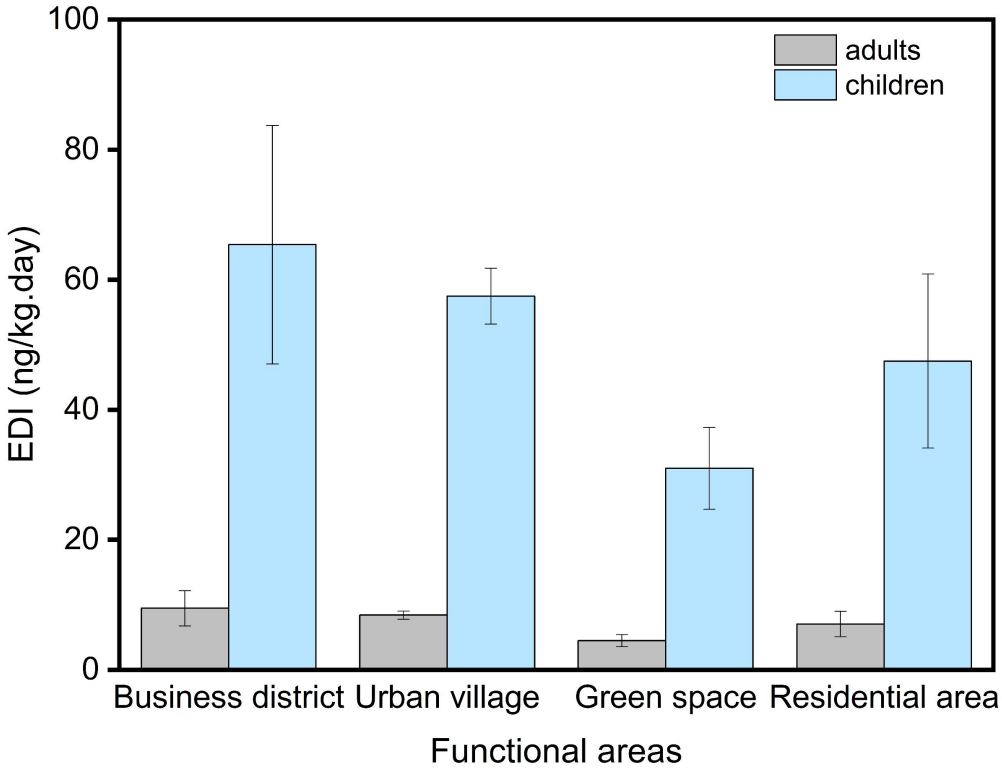


* p<=0.05

Supplementary Figure 2. Correlation analysis of 24 tire-derived chemicals (TDCs) in road dust from various functional areas. Six substances (CPPD-Q, 2-Me-BTH, NOBS, DCU, BLE, and DM) are not included as they were not detected at any sampling site. An asterisk (*) indicates a statistically significant difference at $p < 0.05$.



Supplementary Figure 3. The composition and distribution of four types of Tire-Derived Chemicals (TDCs) in road dust during different seasons.



Supplementary Figure 4. Exposure assessment for different populations in different functional areas. Error bars represent the standard error of the mean (SEM).

Reference

1. Jin, R.H.; Wu, Y.; He, Q.; et al. Ubiquity of amino accelerators and antioxidants in road dust from multiple land types: targeted and nontargeted analysis. *Environ. Sci. Technol.* **2023**, *57*, 10361−10372. DOI: 10.1021/acs.est.3c01448