Supplementary Information

Leaching of chemicals and DOC from tire particles under simulated marine conditions

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Table of Contents

Table S1. Selected organic compounds analyzed by LC-MS

Abbreviation	CAS	Name	Sum Formula	RT [min]	Exact mass (m/z, $[M+H]^+$ or M-H]-)	standard for quantification	LOQ ng/ml	Supplier	Purity grade
DPG	102-06-7	Diphenylguanidine	$C_{13}H_{13}N_3$	4.83	121.119	yes	0.1	Merck (Darmstadt, germany)	97%
PG	2002-16-6	Phenylguanidine	$C_7H_9N_3$	2.62	136.087	yes	0.03	BLD pharm	97%
Aniline	62-53-3	Benzenamine	$C_6H_5NH_2$	1.34	194.066	yes	0.3	Sigma-aldrich (Schnelldorf, Germany)	97%
MBT	149-30-4	Mercaptobenzothiazole	$C_7H_5NS_2$	7.31	176.994	yes	0.3	Sigma-aldrich (Schnelldorf, Germany)	97%
MTBT	615-22-5	2-(Methylthio)benzothiazole	$C_8H_7NS_2$	9.52	182.01	yes	0.3	abcr GmbH (Karlsruhe, Germany)	98%
NH_2-BT	136-95-8	2-Aminobenzothiazole	$C_7H_6N_2S$	3.82	151.033	yes	0.03	Sigma-aldrich (Schnelldorf, Germany)	97%
BT	95-16-9	Benzothiazole	C_7H_5NS	7.07	136.022	yes	1	Sigma-aldrich (Schnelldorf, Germany)	96%
OBS	4225-26-7	2-(4-morpholinyl)benzothiazole	$C_{11}H_{12}N_2OS$	8.39	221.075	yes	1	abcr GmbH (Karlsruhe, Germany)	95%
CBS*	95-33-0	N-Cyclohexyl-2-benzothiazolesulfenamide	$C_{13}H_{16}N_2S_2$	11.43	265.083	yes	1	abcr GmbH (Karlsruhe, Germany)	94%
2-OHBT	934-34-9	2-Hydroxybenzothiazole	C_7H_5NOS	6.88	152.017	yes	0.03	Sigma-aldrich (Schnelldorf, Germany)	98%
BTSA	941-57-1	Benzothiazole-2-sulfonic acid	$C_7H_5NO_3S_2$	4.96	213.9633 (-)	yes	0.1	Sigma-aldrich (Schnelldorf, Germany)	98%
BTCA*	3622-35-3	Benzothiazolecarboxylic acid	$C_8H_5NO_2S$	6.07	177.9963 (-)	yes	0.3	Alfa Aesar (Kandel, Germany)	96%
6-PPD*	793-24-8	N-(1,3-dimethylbutyl)-N′-phenyl-1,4-phenylenediamine	$C_{18}H_{24}N_2$	8.39	269.202	yes	0.3	abcr GmbH (Karlsruhe, Germany)	98%
4-HDPA	122-37-2	4-Hydroxydiphenylamine	$C_{12}H_{11}NO$	7.85	186.0919	yes	0.03	Alfa Aesar (Kandel, Germany)	98%
4-ADPA	101-54-2	4-Aminodiphenylamine	$C_{12}H_{12}N_2$	4.95	186.0919	yes	1	Sigma-aldrich (Schnelldorf, Germany)	98%
6-PPDQ	8026-48-0	6-PPD-quinone	$C_{18}H_{22}N_2O_2$	10.96	299.176	yes	0.02	HPC Standards GmbH (Borsforf, Germany)	99%
DPPD	74-31-7	N,N′-Diphenyl-p-phenylenediamine	$C_{18}H_{16}N_2$	10.72	260.1313	yes	0.1	Sigma-aldrich (Schnelldorf, Germany)	98%
TPG	101-01-9	Triphenylguanidine	$C_{19}H_{17}N_3$	7.25	288.149	yes	0.1	J&K Scientific	98%
NO-DPA	86-30-6	Nitroso-diphenylamine	$C_{12}H_{10}N_2O$	8.8	199.089	yes	0.1	abcr GmbH (Karlsruhe, Germany)	95%
MDCH	7560-83-0	Methyldicyclohexylamine	$C_{13}H_{25}N$	5.72	196.2061	yes	0.03	Sigma-aldrich (Schnelldorf, Germany)	98%
HMMM	3089-11-0	Hexamethoxymethylmelamine	$C_{15}H_{30}N_6O_6$	8.63	413.2125	yes	0.03	abcr GmbH (Karlsruhe, Germany)	98%
DCH	101-83-7	Dicyclohexylamine	$C_{12}H_{23}N$	5.79	182.1909	no	0.1	Sigma-aldrich (Schnelldorf, Germany)	99%

**concentration values < LOQ, therefore not further considered.*

Table S2. List of tires types and brands used for the cryo-milled tire tread mixture

Sample	Season	Details
TP1	all-season	Falken outside Euroall Season 225/50 R17 98 V
TP2	winter	WINTEC PN150 165/65 R15 91T M+S
TP3	winter	Goodyear Vector 5+ M+S 185/65 R15 88T
TP4	winter	Fulda Kristall Montero 2 M+S 195/60 R15 88T
TP5	winter	Continental ContiWinter Contact TS830 205/55 R16
TP6	summer	tire rubber summer (typical mixture)
TP7	winter	tire rubber winter (typical mixture)
TP8	not specified	Continental Germany
TP9	not specified	Triangle, China
TP10	not specified	Wanlitire, China
TP11	not specified	Cheng Shin, China
TP12	summer	Bridgestone DriveGuard 225/40R18 92Y DRGSFZ 67854 VRT7
TP13	winter	Pirelli Sottozero 3 225/40 R18 92Y M+S extra load studless tubeless
TP14	winter	Fulda Kristall Montero 3 205/65 R15 94T M+S
TP15	all-season	Continental VancoFourSeason 2 235/65 R16 C
TP16	summer	Dunlop SP Sport Maxx GT 235/65 R17
TP17	summer	Sava intensa uhp 225/50 R16 92W
TP18	summer	Continental ContiSportContact 5 235/45 R17 94W
TP19	summer	Hankook VentusPrime 3 205/55R16 91V
TP20	summer	Semperit Speed-Life 195/50 R15 82H alpine proven

Table S3. Concentration values of the 19 target compounds found in the leachates

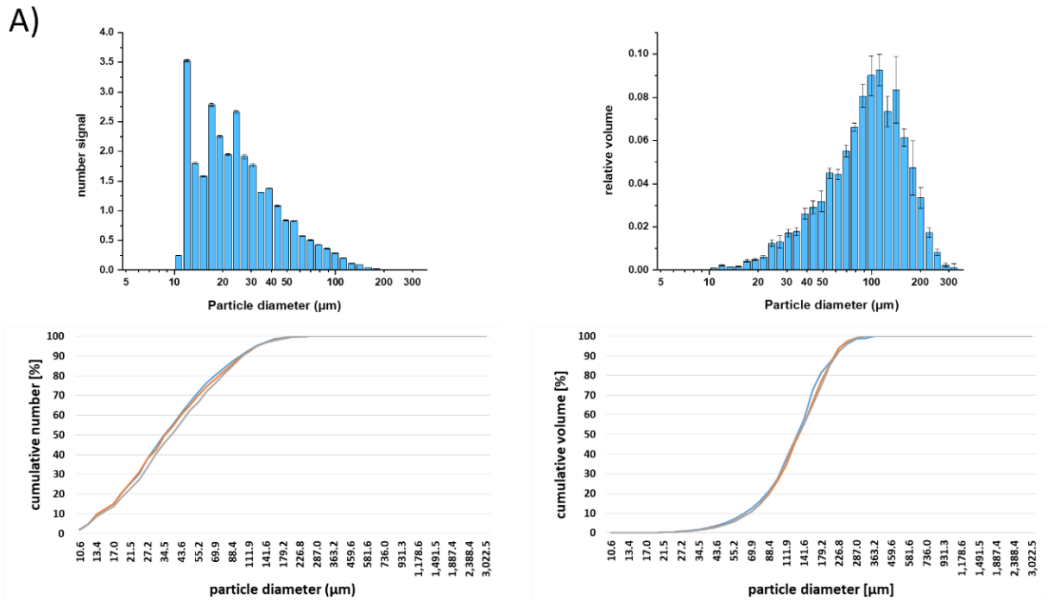
Please see Excel-table "Table S3: Target compounds"

Table S4. List of the 23 DPG transformation products found in the leachates

Please see Excel-table "Table S4: DPG TPs"

Table S5. List of the 5 DCH isomeric transformation products detected in the leachates

Please see Excel-table "Table S5: DCH TPs"



B)

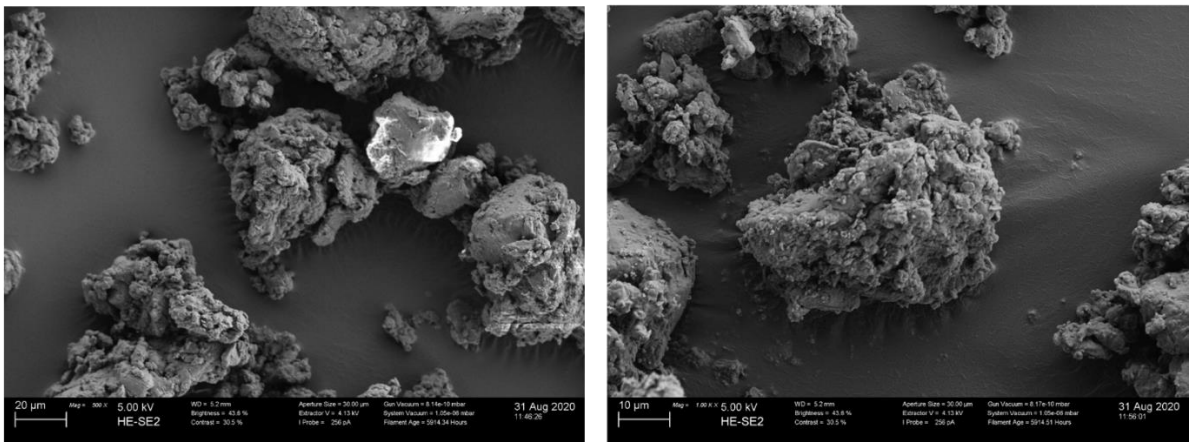


Figure S1. (A) The CMTT particle size range in number (left) and volume (right) distribution, and (B) the SEM images at 250X (left) and 1000X (right) magnification.

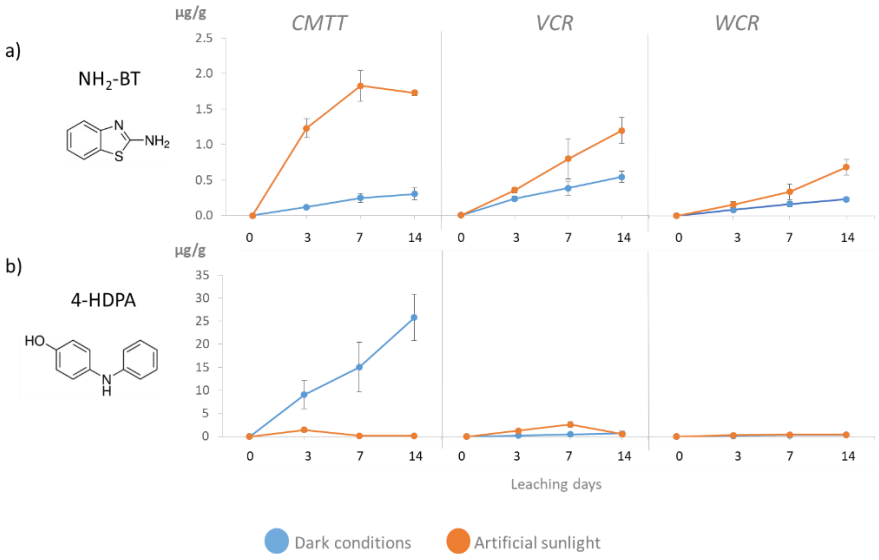


Figure S2. Amounts of a) 2-Aminobenzothiazole (NH_2-BT), b) benzothiazole (BT), c) benzothiazole-2-sulfonic acid (BTSA), d) 4-Hydroxydiphenylamine (4-HDPA) released from CMTT, VCR and WCR by leaching over 14 days in the dark (blue lines) and under artificial sunlight. Error bars represent standard deviation (n=3) of independent replicates.

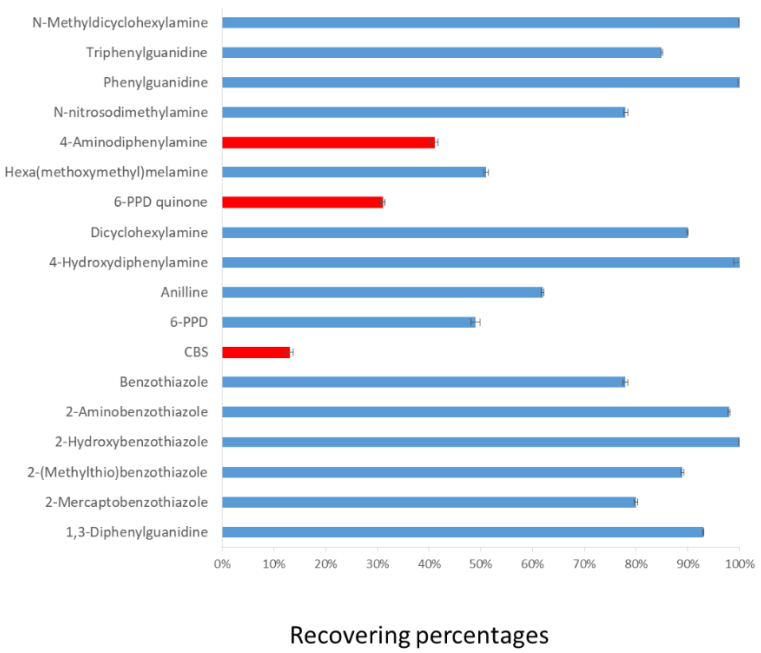


Figure S3. Recoveries of the filter test performed with a standard mixture by applying the same filtration system, volume and water medium.