Supporting Information I

Comparison of Trace Organic Chemical Removal Efficiencies between Aerobic and Anaerobic Membrane Bioreactors Treating Municipal Wastewater

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PRINCIPAL COMPONENT ANALYSIS

Principal component analysis (PCA) was conducted as a QSPR approach to determine if physical-chemical properties or molecular descriptors predicted percent change of the 351 tentatively identifiable compounds. Two groups of potential mechanistically significant descriptors were separately assessed: 1) 16 physical-chemical properties (listed in Table S20) and 2) 12 molecular descriptors (listed in Table S21). For the group 1 descriptors, the proportion of variance explained by principal component 1 (PC1) and principal component 2 (PC2) was 31% and 16%, respectively. Due to the low proportions of explained variance, PCA was unable to predict compound removal based on these physical-chemical properties. For the group 2 descriptors, the proportion of variance explained by PC1 and PC2 was 68% and 10%, respectively.

For the group 2 descriptors, we investigated one step further to evaluate the correlation of PC1 and percent removal, for the compounds that were removed and had a coefficient of variation less than 30%. Here, removal was defined as the percent decrease change in peak area before and after MBR treatment. All correlations between percent removal and PC1 across the experimental treatment cycles were found to be non-significant ($p>0.05$, Figure S3).

Note in our prior study of centralized and decentralized WWTFs the compounds removed across all three WWTFs had significantly higher numbers of hydrogen bond acceptors-1, fraction of rotatable bonds, and number of atoms than the compounds that persisted.[18] In the present study, we additionally assessed these individual descriptors against percent removal using linear regression and no significant correlations were observed ($p>0.05$). The difference between study results may be due to the much greater number of compounds identified in our study, which may reduce spurious correlations.

In order to check if excluding the transformation products from the PCA would change the result, two additional principal component analyses were conducted in the same way except this time only on the removed compounds for each treatment type, specifically, 1) on the compounds removed by AeMBR and 2) on the compounds removed by AnMBR. First, PCA was conducted on the tentatively identified compounds (n=129) removed by AeMBR in all three treatment cycles. The proportion of variance represented by principal component 1 (PC1) and PC2 for group 1 descriptors were PC1 = 34.3% and PC2 = 28.0%; and for group 2 descriptors were PC1= 67.3% and PC2= 11.7%. Then, PCA was run on the tentatively identified compounds (n=167) removed by AnMBR in all three treatment cycles. The proportion of variance represented by PC1 and PC2 for group 1 descriptors were PC1 =33.9% and PC2 =24.2%; and for group 2 descriptors were PC1= 69.4% and PC2= 11.2%.

The results of the additional PCA analyses on only the compounds that were removed were very similar to the results that included all 351 tentatively identified compounds. In all cases for group 1 descriptors, PCA was unable to predict compound removal based on these physical-chemical properties due to the low proportions of explained variance. For each case examined for group 2 descriptors, PC1 and PC2 ranged from 67-69% and 10-12%, respectively. Although there was a greater degree of the proportion of variance explained for group 2, when further investigated, correlations between percent removal and PC1 were still found to be non-significant ($p > 0.05$) across the three treatment cycles.

VOLATILE ORGANIC COMPOUNDS

Volatilization can be one important removal pathway, especially for highly volatile compounds,[1] and it can be unrelated to the aerobic or anaerobic biological processes but related to the physical aeration in both the aeration and membrane tanks of the AeMBR system. In this experiment, rates of compound volatilization were expected to be the same in the membrane tanks because air and N_2 sparging rates were the same for both membranes. There was, however, greater opportunity for volatilization in the aeration tank of the AeMBR system, which was absent in the ABR of the AnMBR system. To evaluate the influence of volatilization on TOrC removal in the AeMBR system, we compared the removal of 65 compounds that are considered volatile organic compounds (VOCs), defined as having a molecular weight less than 200 g/mol and a Henry's law constant greater than 1×10–5 atm-m3/mol,[2] in the AeMBR and AnMBR systems. We found that the average percent removal of VOCs (in terms of their individual peak abundances) was higher for AnMBR than AeMBR (46% and 14%, respectively), however the difference was not significant (student's t-test). Additionally, although there were a greater number of VOCs completely removed in the AeMBR treatment than in the AnMBR treatment (11 VOCs versus 6 VOCs, respectively), there were 18 VOCs that increased in average peak area in the AeMBR, from 15% up to 850% change. The AnMBR showed less of an increase for only 13 VOCs, which ranged from 1% to 113%. Therefore, we conclude that volatilization was not a major driving factor in the difference of losses observed between the AeMBR and AnMBR. It is important to note that in this study, the GC method including the injection method and GC oven temperature program detects volatile and semi-volatile compounds but does not cover highly volatile compounds, which requires a different GC method.

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Table S16: The 113 tentatively identified persistent compounds and potential transformation products. Persistent compounds were defined as compounds that had less than 90% percent peak area decrease from influent to membrane permeate.

Table S17: The 30 tentatively identified compounds unique to the aerobic membrane permeate samples.

Table S18: The 18 tentatively identifiable compounds unique to the anaerobic membrane permeate samples.

Table S19: Compounds confirmed with analytical standards and a comparison of their treatment efficiencies in Mladenov et al. (2021)[3] to the AeMBR and AnMBR.

Table S20: The 16 physicochemical properties assessed by principal component analysis.

Table S21: Twelve molecular descriptors assessed by principal component analysis.

Table S22: Database of all 102 tentatively identified compounds containing at least one nitrogen atom which were common among all the influents (from treatment cycle I, II, and III).

Table S23: Database of the 30 tentatively identified compounds containing at least one sulfur atom which were common among all the influents (from treatment cycle I, II, and III).

Table S24: Index of the EPA Comptox databases used to define each product use category.

Table S25: Sixty-five tentatively identifiable compounds identified in the United States (US) Environmental Protection Agency (EPA) High Production Volume List.

ADDITIONAL FIGURES

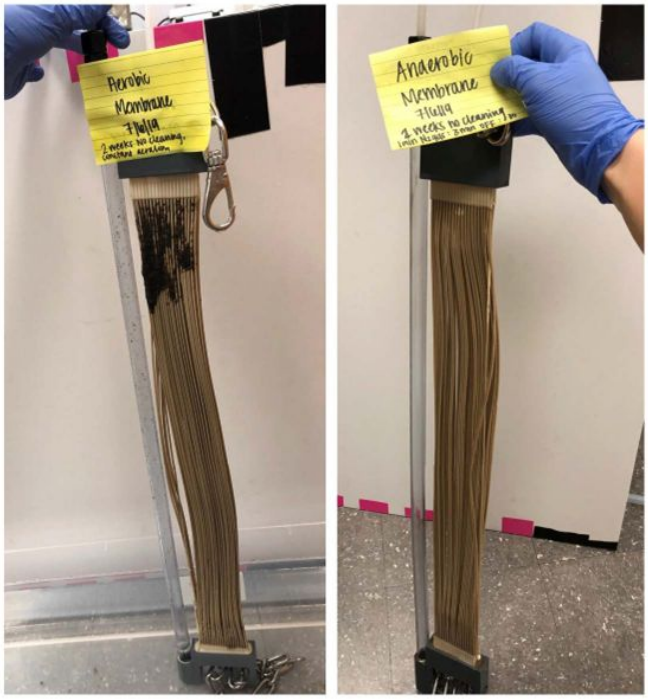

Figure S1. Aerobic (left) and anaerobic (right) membranes, before cleaning, after running two treatment cycles on 100% municipal wastewater.

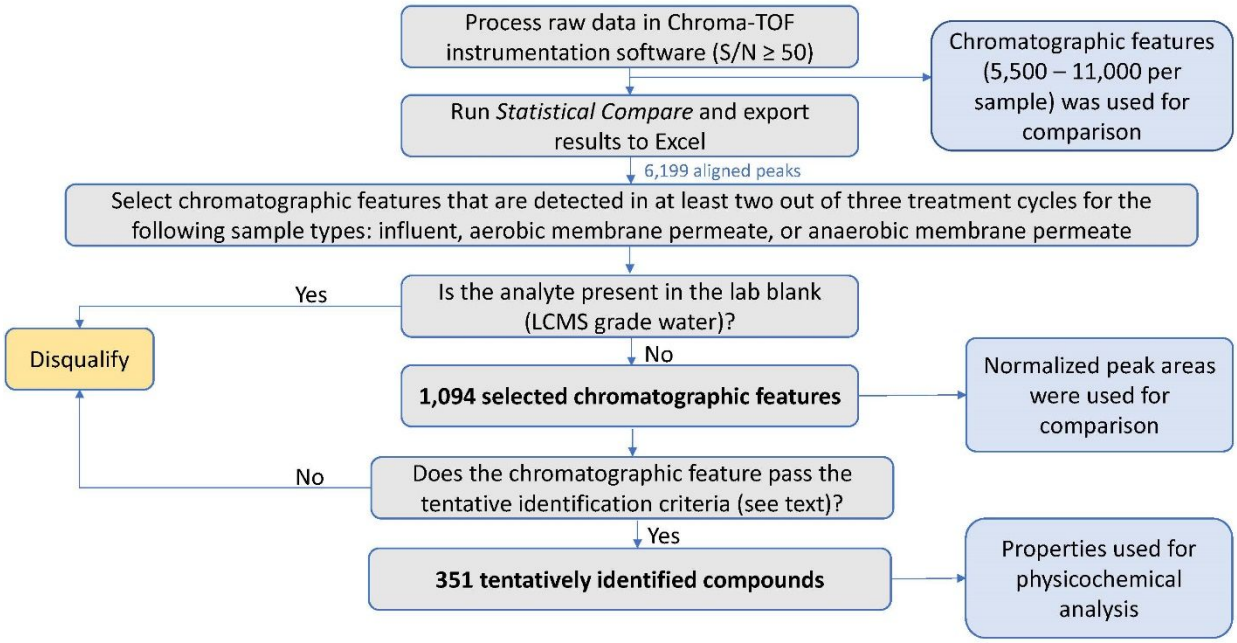

Figure S2. Non-targeted data analysis flow chart. The selected chromatographic features and tentatively identified compounds are used for comparing AeMBR and AnMBR treatment of TOrCs.

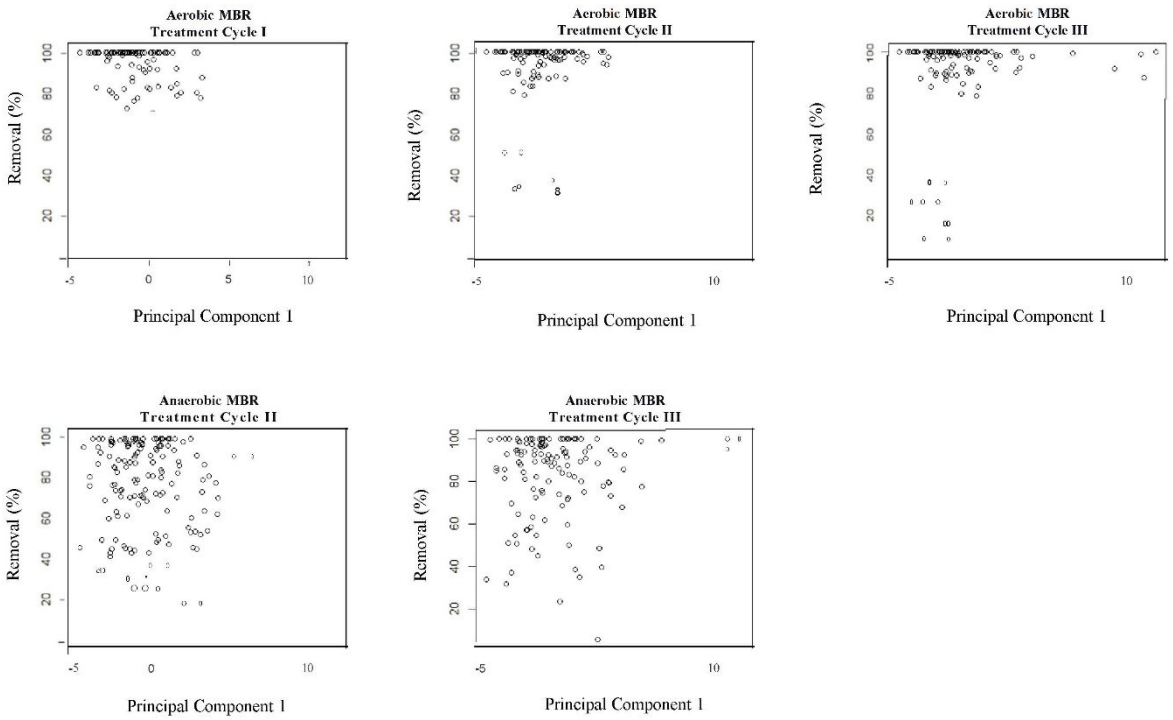

Figure S3. Correlation of principal component 1 (x-axis), for group 2 descriptors, against percent removal (y-axis) for each treatment cycle (I, II, and III).

ADDITIONAL TABLES

Table S1. Operating parameters of aerobic and anaerobic MBRs and average concentrations and % reduction of chemical oxygen demand and total suspended solids.

Operating parameter/ constituent	**Untreated WW Influent (n=3)**	**Aerobic MBR (n=3)**	**Anaerobic MBR (n=2)**
Total suspended solids (TSS) of influent and permeate (mg/L)	83 ± 16.0	3 ± 2.8 (97 ± 2.7 % Removal)	8 ± 1.7 (89 ± 0.7 % Removal)
Chemical oxygen demand of influent and permeate (mg/L)	358 ± 20.8	42 ± 3.5 (88 ± 0.00 % Removal)	65 ± 7.0 (83 ± 0.02 % Removal)
Solids retention time* in bioreactor (d	-	3.97	~960
Aerobic tank mixed liquor suspended solids (MLSS) (mg/L)	-	1174 ± 855	-
ABR sludge blanket TSS* (mg/L)	-	-	1780 ± 1414
Flow rate (mL/min)	-	30	13.9
Hydraulic retention time (HRT) for bioreactors (h)	-	24	48

Note: * For the AnMBR, no wasting was needed due to low sludge production. Therefore, solid retention time is estimated based on a conservative value of 1L wasted per 30 d. Because the ABR does not have a mixed liquor the TSS concentration of the sludge blanket is given instead of a MLSS concentration.

Table S2. Mean and relative standard deviations of total peak area and total number of peaks detected per sample type.

Sample Type	N	Average Total Peak Area*	Standard Deviation of Total Peak Area	Relative Standard Deviation (RSD) of Total Peak Area	Average Total No. of Peaks*	Standard Deviation of Total No. of Peaks	Relative Standard Deviation (RSD) of Total No. of Peaks
Influent	3	9.60E+06	2.00E+06	21%	10,009	1,393	13.9 %
AeMBR	3	1.55E+06	2.14E+05	14%	5,357	421	7.9 %
AnMBR	3**	1.98E+06	1.04E+06	53%	6,529	2,865	43.9 %
AnMBR	2***	2.71E+06	2.14E+05	8%	8,533	730	8.56 %

RSD = (100% × standard deviation) ÷ average.

* Individual peak areas were normalized to the sample volume before calculating summing all peak areas to calculate the total peak area.

** N=3, includes AnMBR samples from treatment cycle I, II, and III. N=2

*** N=2, includes AnMBR samples from treatment cycles II and III. Samples from treatment cycle I was excluded from TOrC removal analysis due to the substantially higher relative standard deviations and its mis-collection, given the sample was only collected for 24-hr as opposed to how the samples from treatment cycle II and III were collected for 48-hrs. The 24-hr composite sample is not representative of the entire process since the total hydraulic retention time of the AnMBR system is 48-hrs.

Table S3. Water quality data summary of averages over the three treatment cycles.

Sample	n	pH	Conductivity (mS)	TDS (ppt)	Temperature (ºC)	DO (%)	DO (mg/L)	Turbidity (FAU)
Influent grab 1 (t=0 hr)	3	7.75 ± 0.13	3.08 ± 0.06	1.53 ± 0.04	23.27 ± 1.06	2.53 ± 0.38	0.22 ± 0.03	161.67 ± 46.46
Influent grab 2 (t=24 hr)	3	7.49 ± 0.07	2.53 ± 0.01	1.27 ± 0.01	24.57 ± 1.37	2.40 ± 0.75	0.20 ± 0.06	249.67 ± 21.03
Aerobic bioreactor effluent	6	7.72 ± 0.17	2.61 ± 0.31	1.30 ± 0.15	23.98 ± 0.64	64.35 ± 4.93	5.42 ± 0.47	56 ± 18.9
Aerobic sludge	3	7.55 ± 0.06	2.36 ± 0.27	1.18 ± 0.13	23.80 ± 1.56	64.15 ± 1.15	5.47 ± 0.09	69 ± 0
Aerobic membrane tank	6	6.39 ± 0.74	2.65 ± 0.25	1.32 ± 0.15	24.6 (n=1)	89.6 (n=1)	7.45 (n=1)	5 ± 1
Anaerobic baffled reactor effluent	4	8.09 ± 0.09	2.34 ± 0.1	1.12 ± 0.07	24.00 ± 0.66	2 ± 0.27	0.17 ± 0.03	69 ± 0.66
Anaerobic sludge	2	7.78 ± 0.04	2.42 ± 0.29	1.19 ± 0.17	25.65 ± 1.25	2.17 ± 0.34	0.18 ± 0.03	O.D. L
Anaerobic membrane tank	6	8.81 ± 0.10	2.44 ± 0.07	1.22 ± 0.01	25.10 ± 0.50 (n=2)	2.25 ± 0.45 (n=2)	0.19 ± 0.04 (n=2)	14.25 (n=2)

Note: “TDS” – total dissolved solids. “DO” – dissolved oxygen. “O.D.L.” - The value was over the detection limit.

Table S4. GC×GC/TOF-MS instrument conditions for sample analysis.

GC×GC-TOF/MS Parameters	
1D Column	Rtx-5 (35 m x 0.25 mm x 0.25 μm)
Maximum Temperature	350 °C
2D Column	Rtx-17 (0.79 m x 0.10 mm x 0.10 μm)
Maximum Temperature	360 °C
Injection Volume	2 μL
Inlet Temperature	300 °C
Carrier Gas Flow	1 mL/min (constant)
1D Oven Program	Initial Temp at 60 °C (1 min hold), 60°C to 300°C at 10°C/min (15 min hold)
2D Oven Program	Initial Temp at 80 °C (1 min hold), 80°C to 320°C at 10°C/min (15 min hold)
Modulator Temperature Offset	10 °C
Modulation Time	3.50 s
Hot Pulse Time	0.90 s
Cold Time	0.85 s
Transfer Line Temperature	300 °C
Ion Source Temperature	250 °C
Ionization	EI
Electron Energy	-70 eV
Detector Voltage	1700
Mass Range	50-1000
Scan Speed	151.51 spectra/s
Total Run Time	2400 s

Table S5. Number of chromatographic features per sample.

Treatment Cycle	Sample Type	Total Number of Chromatographic Features per Sample Type	Sample Volume	Composite description (hours)
I	Influent	8,461	500	48
II	Influent	10,407	500	48
III	Influent	11,160	500	48
I	Aerobic Membrane Permeate	4,876	1000	24
II	Aerobic Membrane Permeate	5,663	1000	24
III	Aerobic Membrane Permeate	5,531	1000	24
II	Anaerobic Membrane Permeate	8,016	1000	48
III	Anaerobic Membrane Permeate	9,049	1000	48

Table S6. Comparing mean number of chromatographic features using one-way ANOVA.

	Sum of Squares	df	Mean Square	F	Sig.
Between Groups	33553436.042	2	16776718.021	17.592	.005
Within Groups	4768325.833	5	953665.167		
Total	38321761.875	7			

Table S7. Multiple comparisons of mean number of chromatographic features for influent and the membrane permeates, using Bonferroni-adjusted post hoc test.

					95% Confidence Interval	
(I) id	(J) id	Mean Difference (I-J)	Std. Error	Sig.	Lower Bound	Upper Bound
INF	AeMP	4652.667*	797.356	.006	1834.72	7470.61
	AnMP	1476.833	891.471	.475	-1673.72	4627.39
AeMP	INF	-4652.667*	797.356	.006	-7470.61	-1834.72
	AnMP	-3175.833*	891.471	.049	-6326.39	-25.28
AnMP	INF	-1476.833	891.471	.475	-4627.39	1673.72
	AeMP	3175.833*	891.471	.049	25.28	6326.39

Note: "*" - The mean difference is significant at the 0.05 level. INF = influent; AeMP = aerobic membrane permeate; AnMP = anaerobic membrane permeate

Table S8. Comparing mean sum of the peak areas (normalized to the sample volume) for all chromatographic features per sample type using one-way ANOVA.

	Sum of Squares	df	Mean Square	F	Sig.
Between Groups	103204139537838.220	2	51602069768919.110	22.967	.003
Within Groups	11233737640860.906	5	2246747528172.181		
Total	114437877178699.120	7			

Table S9. Multiple comparisons of the mean sum of peak areas (normalized to the sample volume) for all chromatographic features per sample type, using Bonferroni-adjusted post hoc test.

		Mean Difference			95% Confidence Interval	
(I) sampletype	(J) sampletype	(I-J)	Std. Error	Sig.	Lower Bound	Upper Bound
INF	AeMP	7.82636E+006*	1.22386E+006	.004	3.5011E+006	1.2152E+007
	AnMP	6.66106E+006*	1.36832E+006	.014	1.8253E+006	1.1497E+007
AeMP	INF	-7.82636E+006*	1.22386E+006	.004	-1.2152E+007	-3.5011E+006
	AnMP	-1.16530E+006	1.36832E+006	1.000	-6.0011E+006	3.6705E+006
AnMP	INF	-6.66106E+006*	1.36832E+006	.014	-1.1497E+007	-1.8253E+006
	AeMP	1.16530E+006	1.36832E+006	1.000	-3.6705E+006	6.0011E+006

Note: "*" -The mean difference is significant at the 0.05 level. INF = influent; AeMP = aerobic membrane permeate; AnMP = anaerobic membrane permeate

Table S10. Data processing and statistical compare conditions.

Conditions	Value
Data Processing:	
S/N	50
Statistical Compare:	
Analyte Similarity Required to Match (0-999)	600
1^{st} Dimension Retention Time Difference (s)	7
2^{nd} Dimension Retention Time Difference (s)	0.5
Percent of Samples in Class Containing Analyte	50

Table S11. List of the 351 tentatively identifiable compounds, their normalized peak areas, and their average percent change in AeMBR and AnMBR systems.

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
20189-42-8	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	4.89 E-06	6.06 E-05	2.47 E-05	4.49 E-06	1.66 E-05	1.29 E-05	1.46 E-05	2.43 E-05	-43%	-39%	P-both
99-92-3	Acetophenone, 4'-amino-	5.34 E-05	0.00 0287	0.00 0221	1.36 E-05	2.76 E-05	2.74 E-05	3.37 E-05	3.99 E-05	-84%	-85%	P-both
7006-52-2	Benzenamine, 3-chloro-N-methyl-	3.77 E-05	0.00 0222	1.14 E-05	0.00 0125	0.000 156	4.82 E-05	0.000 308	0.000 0392	175 %	141 %	TP-both
499-75-2	Phenol, 2-methyl-5-(1-methylethyl)-	0.00 1174	0.00 4711	0	2.74 E-05	4.39 E-05	0	0	0.001 156	-98%	-100 %	R-both
270-91-7	5H-1-Pyrindine	0.00 8315	0.07 8582	0.04 532	0.00 0134	0.000 266	0.000 22	0.001 17	0.000 483	-99%	-99%	R-both
5910-89-4	Pyrazine, 2,3-dimethyl-	6.18 E-06	2.84 E-05	0	6.84 E-05	0.000 119	0.000 118	4.59 E-05	5.84 E-05	663 %	62%	TP-both
497-23-4	2(5H)-Furanone	4.09 E-05	0.00 0183	0	6.61 E-05	0.000 177	0.000 156	6.13 E-05	8.55 E-05	29%	-67%	TP-Ae, P-An
1487-99-6	Oxepine, 2,7-dimethyl-	2.69 E-05	0.00 0103	0.00 0116	2.37 E-05	5.08 E-05	3.44 E-05	1.70 E-05	1.84 E-05	-44%	-84%	P-both
5842-53-5	3-Penten-1-ol, 2,2,4-trimethyl-	4.94 E-05	0.00 0113	6.28 E-05	0.00 012	0.000 14	0.000 148	0.000 13	0.000 0912	101 %	30%	TP-both
103-65-1	Benzene, propyl-	0.00 0137	0.00 0416	0.00 1824	0.00 0532	0.000 11	0.000 196	0.000 21	0.000 0722	42%	-73%	TP-Ae, P-An
4436-75-3	3-Hexene-2,5-dione	0.00 0306	0.00 0676	0.00 0816	0.00 1433	0.002 039	0.002 136	0.001 143	0.000 989	244 %	45%	TP-both
95-14-7	1H-Benzotriazole	1.74 E-05	1.05 E-05	7.57 E-06	0.00 0251	0.000 237	0.000 231	2.56 E-05	1.92 E-05	2150 %	149 %	TP-both
10264-55-8	3-Ethylcyclopentanone	1.99 E-05	0.00 0164	4.73 E-05	5.00 E-05	3.44 E-05	0.000 149	4.19 E-05	1.89 E-04	96%	113 %	TP-both
622-96-8	Benzene, 1-ethyl-4-methyl-	0.00 0455	0.00 0936	0.00 1024	0.00 2317	0.000 507	0.000 785	0.000 909	0.000 337	113 %	-35%	TP-Ae, P-An
100-52-7	Benzaldehyde	0.00 0375	0.00 1043	0.00 1612	0.00 051	0.000 691	0.000 564	0.000 321	0.000 488	-21%	-69%	P-both
3658-80-8	Dimethyl trisulfide	0.00 2289	0.01 6494	0.00 7594	4.81 E-05	0.000 205	0.000 168	0.000 309	0.000 122	-98%	-98%	R-both
108-95-2	Phenol	0	0.02 7408	0.00 8669	0.00 2466	0.000 489	0.000 59	0.001 151	0.001 622	-96%	-89%	R-Ae, P-An
62-53-3	Aniline	0.00 0895	0.00 2341	0.00 1505	0.00 0141	0.000 238	0.000 452	0.002 137	0.001 499	-81%	-5%	P-both
100-47-0	Benzonitrile	2.67 E-05	0.00 0172	0.00 0138	6.99 E-05	8.57 E-05	4.71 E-05	5.27 E-05	9.64 E-05	15%	-50%	TP-Ae, P-An
695-98-7	Pyridine, 2,3,5-trimethyl-	4.70 E-06	4.45 E-05	2.90 E-05	2.94 E-05	4.21 E-05	3.50 E-05	5.58 E-05	1.03 E-04	180 %	140 %	TP-both
526-73-8	Benzene, 1,2,3-trimethyl-, isomer 1	0.00 0307	0.00 0713	0.00 0495	0.00 1598	0.000 354	0.000 624	0.000 63	0.000 268	132 %	-29%	TP-Ae, P-An
541-73-1	Benzene, 1,3-dichloro-	2.56 E-05	5.06 E-05	3.17 E-05	5.67 E-05	7.44 E-05	2.13 E-05	6.37 E-05	9.65 E-06	45%	-22%	TP-Ae, P-An
527-84-4	o-Cymene	0.00 0163	0.00 04	0.00 1071	0.00 0125	7.72 E-05	7.72 E-05	8.23 E-05	7.78 E-05	-66%	-86%	P-both
470-82-6	Eucalyptol	0.00 0343	0.00 1299	0.00 0794	5.26 E-06	0	7.46 E-06	0.000 365	0.000 159	-99%	-76%	R-Ae, P-An
1193-79-9	2-Acetyl-5-methylfuran	2.90 E-05	4.70 E-05	0.00 024	5.51 E-05	9.48 E-05	7.23 E-05	5.46 E-05	1.12 E-04	41%	-19%	TP-Ae, P-An

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeM P-I	AeM P-II	AeM P-III	AnM P-II	AnM P-III	AeM BR Avg. %C	AnM BR Avg. %C	R/P/TP/new TP
766-39-2	2,5-Furandione, 3,4-dimethyl-	4.25 E-06	2.37 E-05	3.64 E-05	8.22 E-05	0.000157	9.14 E-05	1.60 E-05	4.23 E-05	849 %	-8%	TP-Ae, P-An
0-00-0	2,4,6-Cycloheptatrien-1-one, 4-methyl-	8.15 E-05	0.000545	0	0.000116	0.000212	0.000171	0.000114	0.000154	-9%	-79%	P-both
872-50-4	2-Pyrrolidinone, 1-methyl-	1.60 E-05	0	2.51 E-05	7.40 E-05	9.45 E-05	3.15 E-05	0.000115	0.0000286	194 %	14%	TP-both
6124-79-4	4-Methyl-5H-furan-2-one	1.36 E-05	5.03 E-05	0	7.26 E-05	0.000109	8.68 E-05	2.53 E-05	4.75 E-05	275 %	-50%	TP-Ae, P-An
1193-18-6	2-Cyclohexen-1-one, 3-methyl-	5.38 E-05	0.000252	0.000142	2.39 E-05	4.85 E-05	4.20 E-05	0.000143	0.000272	-69%	24%	P-Ae, TP-An
1072-83-9	Ethanone, 1-(1H-pyrrol-2-yl)-	6.76 E-05	0.000421	0	5.72 E-06	1.97 E-05	1.39 E-05	0.000178	0.000298	-93%	-58%	R-Ae, P-An
93-53-8	Benzeneacetaldehyde, à-methyl-	1.66 E-05	0	4.81 E-05	6.92 E-05	1.61 E-05	2.54 E-05	3.44 E-05	1.95 E-05	135 %	-59%	TP-Ae, P-An
98-86-2	Acetophenone	0.000323	0.000896	0.000966	0.000488	0.000653	0.000619	0.000711	0.001194	-4%	1%	P-Ae, TP-An
8/8/3709	2(3H)-Furanone, dihydro-3,3-dimethyl-	1.39 E-05	6.08 E-05	0	7.75 E-05	0.00024	0.000705	5.40 E-05	7.92 E-05	376 %	-11%	TP-Ae, P-An
616-45-5	2-Pyrrolidinone	3.20 E-05	0.000239	0.000205	9.17 E-05	0.000128	0.000178	5.59 E-05	3.11 E-05	42%	-81%	TP-Ae, P-An
17312-83-3	Undecane, 5,7-dimethyl-	8.99 E-05	0.000017	0.000183	0.000115	0.000135	8.48 E-05	6.09 E-05	4.93 E-05	-15%	-69%	P-both
100-53-8	Benzenemethanethiol	0.000113	0.001277	0.002891	1.93 E-05	2.19 E-05	3.11 E-05	0.000295	0.000318	-93%	-83%	R-Ae, P-An
90-05-1	Phenol, 2-methoxy-	0.00008	0.004861	0.003496	0.000163	0.000251	0.000371	3.45 E-05	7.74 E-05	-88%	-99%	P-Ae, R-An
526-75-0	Phenol, 2,3-dimethyl-	0	4.99 E-05	3.61 E-05	6.29 E-06	1.04 E-05	1.04 E-05	8.19 E-06	3.01 E-05	-75%	-50%	P-both
106251-09-6	1H-Pyrazole, 4,5-dihydro-5,5-dimethyl-4-isopropylidene-	2.91 E-05	0.000192	0.000248	4.24 E-05	0.000107	0.000117	0.000104	0.000257	-17%	-21%	P-both
104-88-1	Benzaldehyde, 4-chloro-	3.01 E-05	6.29 E-05	9.67 E-05	9.34 E-05	7.23 E-05	6.35 E-05	3.69 E-05	4.78 E-05	64%	-46%	TP-Ae, P-An
10468-64-1	Benzene, 1-isocyano-2-methyl-	8.45 E-05	0.000358	0.000277	3.21 E-06	1.03 E-05	9.43 E-06	1.10 E-05	1.91 E-05	-97%	-95%	R-both
824-22-6	1H-Indene, 2,3-dihydro-4-methyl-	4.06 E-05	9.70 E-06	3.24 E-05	4.34 E-05	1.10 E-05	2.14 E-05	1.36 E-05	1.29 E-05	-5%	-10%	P-both
1125-21-9	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	0.000137	0.000678	0.00005	0.000459	0.000764	0.000728	0.000186	0.000388	98%	-47%	TP-Ae, P-An
23747-48-0	5H-5-Methyl-6,7-dihydrocyclopentapyrazine	0	8.32 E-06	9.53 E-06	1.86 E-05	3.31 E-05	3.13 E-05	8.30 E-06	2.43 E-05	263 %	77%	TP-both
28564-83-2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	1.19 E-06	2.67 E-05	4.34 E-06	6.61 E-06	3.77 E-05	4.03 E-05	1.34 E-05	3.02 E-05	442 %	273 %	TP-both
464-48-2	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	0.000402	0.001738	0	2.03 E-05	2.19 E-05	5.26 E-05	0.000769	0.000948	-97%	-56%	R-Ae, P-An
622-76-4	Benzene, 1-butynyl-	0.000222	0.001568	0.001321	4.91 E-05	7.83 E-05	7.56 E-05	0	0.002237	-89%	-15%	P-both
20547-99-3	1,4-Cyclohexanedione, 2,2,6-trimethyl-	1.24 E-05	6.22 E-05	4.26 E-05	1.55 E-05	2.69 E-05	2.78 E-05	2.72 E-05	5.19 E-05	-22%	-17%	P-both
15677-15-3	Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	0.000177	1.79 E-05	4.52 E-05	0.000196	2.05 E-05	6.48 E-05	4.65 E-05	2.34 E-05	23%	56%	TP-both
87-62-7	2,6-Xylidine	2.56 E-06	3.71 E-05	4.31 E-05	1.00 E-05	1.53 E-05	1.66 E-05	9.56 E-06	1.85 E-05	57%	-66%	TP-Ae, P-An
4748-78-1	Benzaldehyde, 4-ethyl-	9.24 E-06	5.80 E-05	0	3.87 E-05	5.18 E-05	0.000182	1.14 E-05	1.34 E-05	154 %	-80%	TP-Ae, P-An
1438-94-4	1H-Pyrrole, 1-(2-furanylmethyl)-	1.08 E-05	4.92 E-05	0	2.04 E-05	3.65 E-05	4.43 E-05	1.96 E-05	2.62 E-05	32%	-60%	TP-Ae, P-An

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
0-00-0	4-Phenylbut-3-ene-1-yne	0.000592	0.000329	0.000444	0.001078	0.00029	0.000338	0.000309	0.000304	15%	-19%	TP-Ae, P-An
101-48-4	Benzene, (2,2-dimethoxyethyl)-	9.90E-05	0.000555	0.000374	8.44E-05	0.000123	9.38E-05	0.000316	0.000706	-56%	23%	P-Ae, TP-An
2628-16-2	Phenol, 4-ethenyl-, acetate	0.000145	0.000433	0.000444	2.40E-05	5.14E-05	4.17E-05	8.04E-05	6.19E-05	-87%	-84%	P-both
95-16-9	Benzothiazole	0.000159	0.000704	0.000599	0.000367	0.0006	0.000532	0.000279	0.000271	35%	-58%	TP-Ae, P-An
6485-40-1	(-)-Carvone	0.000269	0.001395	0.000983	5.54E-05	8.75E-05	0.000103	7.16E-05	9.61E-05	-88%	-93%	P-Ae, R-An
77-67-8	Ethosuximide	0.000244	6.09E-05	0.000115	7.66E-05	0.000154	7.83E-05	0.000184	0.000861	17%	425%	TP-both
1/2/3637	Ethanone, 1-(3,4-dimethylphenyl)-	1.27E-05	5.11E-05	6.37E-05	3.85E-05	4.75E-05	0.000129	1.67E-05	2.44E-05	100%	-65%	TP-Ae, P-An
5306-85-4	D-Glucitol, 1,4:3,6-dianhydro-2,5-di-O-methyl-	0.001805	0.004064	0.000919	0.000758	0.005274	0.005561	0.005817	0.00426	159%	203%	TP-both
18344-37-1	Heptadecane, 2,6,10,14-tetramethyl-	0.000113	0	0.000219	0.000115	0.000202	0.000115	8.43E-05	2.83E-05	-23%	-87%	P-both
0-00-0	Tricyclo[5.2.1.0(2,6)]dec-3-en-10-one	7.32E-05	0.000035	0.000357	2.95E-05	5.81E-05	0.000137	0.000334	0.001537	-68%	163%	P-Ae, TP-An
50918-26-8	Acetic acid, 2-(5-methyl-1,3,4-thiadiazol-2-ylthio)-	1.96E-06	4.57E-06	0	0.000357	0.000184	3.82E-05	1.40E-05	9.96E-05	1102%	206%	TP-both
42966-64-3	2-Pentanamine, N-ethyl-4-methyl-	1.82E-05	0.000569	0.000333	0.00005	0.000449	0.000366	0.000285	0.000979	879%	72%	TP-both
264-09-5	Benzocycloheptatriene	3.98E-05	9.17E-05	0.000104	7.79E-05	5.70E-05	4.32E-05	6.02E-05	5.71E-05	0%	-40%	P-both
7786-61-0	2-Methoxy-4-vinylphenol	0.000107	0.000623	0.00054	7.64E-05	0.000177	0.000112	1.72E-05	4.03E-05	-60%	-95%	P-Ae, R-An
102-76-1	Triacetin	0.000305	0.000132	5.64E-05	0.00044	0.001633	0.000153	0.000705	0.000793	451%	237%	TP-both
334-48-5	n-Decanoic acid	0.000445	0	0.009361	0.000234	0.000285	0.000636	0.000465	0	-70%	-100%	P-Ae, R-An
87-41-2	1(3H)-Isobenzofuranone	3.69E-05	0.000199	0.000135	4.71E-05	4.58E-05	3.13E-05	7.25E-05	7.93E-05	-42%	-52%	P-both
123-08-0	Benzaldehyde, 4-hydroxy-	0.000307	0.000773	0.000802	5.61E-05	7.17E-05	6.44E-05	0.000112	0.000604	-88%	-89%	P-both
41446-68-8	3-Tetradecene, (E)-	1.01E-05	4.66E-05	0	1.18E-05	1.61E-05	1.37E-05	3.66E-05	8.36E-06	-24%	-21%	P-both
56718-71-9	4-(2-Methoxyethyl)phenol	0	0.000142	0.000157	2.35E-05	1.89E-05	1.41E-05	0.000105	0.000263	-89%	21%	P-Ae, TP-An
88-04-0	Chloroxylenol	0.000432	0.000226	0.001833	2.75E-05	5.11E-05	7.12E-05	0.000509	0.000962	-96%	-62%	R-Ae, P-An
95-20-5	1H-Indole, 2-methyl-	0.002252	0.001044	0.006282	2.29E-05	6.20E-05	7.02E-05	0.000121	0.000172	-99%	-98%	R-both
80-46-6	Phenol, 4-(1,1-dimethylpropyl)-	5.98E-05	0.001584	0.000313	0.000725	6.42E-05	2.71E-05	0.001869	0.004599	308%	694%	TP-both
121-71-1	Ethanone, 1-(3-hydroxyphenyl)-	0	0.000432	0.000326	2.75E-05	4.43E-05	3.71E-05	4.74E-05	1.35E-04	-89%	-74%	P-both
644-08-6	1,1'-Biphenyl, 4-methyl-	0.000119	0.000175	0.000457	3.27E-05	4.44E-05	4.06E-05	4.78E-05	7.31E-05	-79%	-78%	P-both
614-60-8	2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	0.000123	0.000905	0.001095	8.18E-06	2.08E-05	1.85E-05	2.69E-05	8.26E-05	-96%	-95%	R-both
93-04-9	Naphthalene, 2-methoxy-	0.000142	0	0.001139	2.33E-05	2.64E-05	3.52E-05	1.95E-05	4.16E-05	-90%	-96%	R-both
128-37-0	Butylated Hydroxytoluene	0.000211	0.000693	0.000772	0.000149	0.000153	0.000148	0.000274	0.000882	-63%	-75%	P-both

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
7779-30-8	1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	5.04E-05	0.000255	0.000212	5.66E-05	0.000127	0.000115	3.88E-05	1.03E-04	-28%	-68%	P-both
23676-09-7	Benzoic acid, 4-ethoxy-, ethyl ester	0.000153	0.000831	0.000856	0.001976	0.001169	0.001305	0.001606	0.000558	428%	29%	TP-both
135-19-3	2-Naphthalenol	1.02E-05	8.84E-05	0.000115	5.69E-05	1.15E-05	1.14E-05	0.000849	0.0000317	94%	394%	TP-both
90-43-7	o-Hydroxybiphenyl	0.003863	0.001329	0.000265	0.000168	5.07E-05	1.93E-05	0.000864	0.002027	-95%	315%	R-Ae, TP-An
14667-55-1	Pyrazine, trimethyl-	1.01E-05	7.09E-05	3.06E-05	9.10E-06	8.85E-06	0	5.53E-05	8.15E-05	-66%	72%	P-Ae, TP-An
60142-96-3	Gabapentin	4.93E-06	4.06E-05	2.33E-05	9.71E-05	0.000126	0.000137	2.09E-05	8.38E-05	856%	106%	TP-both
29878-31-7	1H-Benzotriazole, 4-methyl-	3.72E-05	0	5.71E-05	5.96E-05	5.65E-05	4.09E-05	4.33E-05	1.05E-04	16%	84%	TP-both
84-66-2	Diethyl Phthalate	0.000142	0.000882	0.008148	0.000224	0.000585	0.000423	0.002146	0.001623	-71%	32%	P-Ae, TP-An
119-61-9	Benzophenone	0.000494	0.002739	0.002003	0.001279	0.001832	0.002076	0.001699	0.003772	43%	25%	TP-both
88-19-7	Benzenesulfonamide, 2-methyl-	3.41E-06	4.15E-05	3.26E-05	4.03E-05	6.21E-05	7.19E-05	2.28E-05	5.64E-05	417%	14%	TP-both
77-93-0	Triethyl citrate	0.000685	0.000586	0.005373	0.000072	0.001514	0.001643	0.000482	0.000344	31%	-56%	TP-Ae, P-An
1077-56-1	Benzenesulfonamide, N-ethyl-2-methyl-	5.07E-05	0.000451	0.000207	0.000221	0.000309	0.000376	0.000214	0.000433	129%	28%	TP-both
46048-64-0	2,7(1H,3H)-Naphthalenedione, hexahydro-	1.94E-05	0.000141	1.22E-05	5.40E-05	0.000106	6.70E-05	4.09E-05	8.22E-05	201%	251%	TP-both
70-55-3	Benzenesulfonamide, 4-methyl-	2.17E-06	2.96E-05	2.93E-05	2.83E-05	5.10E-05	6.64E-05	1.64E-05	4.39E-05	468%	3%	TP-both
115-96-8	Tri(2-chloroethyl) phosphate	4.02E-05	0.000772	0.000249	0.000561	0.000749	0.001105	0.000048	0.000827	545%	97%	TP-both
1620-98-0	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	4.14E-05	0.000168	0.000132	7.54E-05	0.000121	9.73E-05	9.04E-05	6.83E-05	9%	-47%	TP-Ae, P-An
120-51-4	Benzyl Benzoate	2.13E-05	0.000142	0.000266	5.70E-05	7.34E-05	5.22E-05	3.98E-05	2.34E-05	13%	-82%	TP-Ae, P-An
13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	0.000257	0.001405	0.001068	0.000838	0.00172	0.002191	0.000988	0.002247	118%	40%	TP-both
85-01-8	Phenanthrene	7.13E-05	0.000237	0.000263	0.000151	0.000184	0.000147	0.000178	0.000134	15%	-37%	TP-Ae, P-An
28705-96-6	Carbamic acid, (3-chloro-4-hydroxyphenyl)-, 1-methylethyl ester	2.04E-05	0.000123	5.14E-05	1.41E-05	2.10E-05	1.01E-05	4.41E-05	9.32E-05	-65%	9%	P-Ae, TP-An
104-66-5	Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-	1.34E-06	1.02E-05	6.62E-06	1.45E-06	1.50E-06	1.14E-06	2.42E-06	3.99E-06	-53%	-58%	P-both
4534-50-3	Benzene, (1-butylnonyl)-	3.65E-05	0.000107	0	4.32E-05	5.50E-05	3.73E-05	8.34E-05	1.48E-04	-15%	-22%	P-both
260-94-6	Acridine	9.26E-06	2.35E-05	4.27E-05	6.26E-05	0.000109	4.75E-05	1.13E-05	4.42E-05	317%	-24%	TP-Ae, P-An
1196-69-6	Indole-5-aldehyde	5.18E-05	0.000288	0.000155	8.67E-06	4.79E-05	4.10E-06	1.13E-05	1.18E-05	-88%	-94%	P-Ae, R-An
1222-05-5	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	0.000153	0.000838	0.001242	1.73E-05	2.20E-05	3.61E-05	0.000109	0.0000684	-94%	-91%	R-both
21145-77-7	Tonalid	1.44E-05	8.85E-05	9.52E-05	1.02E-05	8.55E-06	5.59E-06	1.63E-05	7.14E-06	-71%	-87%	P-both

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
3531-24-6	2-Propenenitrile, 3,3-diphenyl-	2.06E-05	0.000152	7.55E-05	4.52E-05	0.000157	0.000576	7.36E-05	1.34E-04	262%	13%	TP-both
707-07-3	Benzene, (trimethoxymethyl)-	1.56E-05	4.00E-05	3.12E-05	4.12E-05	5.26E-05	6.15E-05	2.63E-05	4.24E-05	98%	1%	TP-both
1421-49-4	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-	0	6.69E-06	2.89E-06	0.000169	0.000279	0.000288	1.06E-05	2.89E-05	6968%	479%	TP-both
728-40-5	Bayer 28,589	9.00E-06	2.41E-05	2.36E-05	5.87E-06	9.35E-06	1.27E-05	1.08E-05	1.70E-05	-47%	-42%	P-both
82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	3.40E-05	0.000133	0	0.000152	0.000228	0.000255	0.000135	0.000172	209%	2%	TP-both
37398-23-5	Acetamide, N-[4-hydroxy-3-(methylthio)phenyl]-	0.000195	0.001084	0.000597	3.05E-05	3.04E-05	1.91E-05	3.77E-05	7.43E-05	-93%	-92%	R-both
6386-38-5	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-	8.26E-06	0	3.38E-05	4.55E-05	4.95E-05	5.76E-05	4.76E-05	4.28E-05	261%	27%	TP-both
7206-76-0	Propanediamide, 2-ethyl-2-phenyl-	8.97E-06	1.55E-05	3.96E-05	4.36E-05	4.14E-05	0.000117	7.21E-06	4.62E-05	250%	-18%	TP-Ae, P-An
55591-05-4	1H-Indene-4-acetic acid, 6-(1,1-dimethylethyl)-2,3-dihydro-1,1-	5.70E-06	3.69E-05	8.79E-06	3.41E-05	4.74E-05	5.48E-05	2.99E-05	2.46E-05	350%	80%	TP-both
606-28-0	Benzoic acid, 2-benzoyl-, methyl ester	5.50E-05	0.000241	0.000231	0.000113	0.000281	0.000175	0.000174	0.000123	33%	-37%	TP-Ae, P-An
13401-18-8	2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-	0.000303	0.001832	0.001015	1.56E-06	5.79E-06	4.38E-06	5.67E-05	2.96E-05	-100%	-97%	R-both
20170-32-5	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	1.05E-05	8.23E-05	4.20E-05	0.000258	0.00035	0.00028	8.07E-05	1.91E-04	1083%	176%	TP-both
613-73-0	1,2-Benzenediacetonitrile	2.81E-05	8.92E-05	5.83E-05	9.40E-05	0.000125	0.000101	5.06E-05	1.22E-04	116%	33%	TP-both
16489-90-0	6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline	2.87E-06	3.29E-05	3.35E-05	2.30E-05	3.14E-05	5.52E-05	1.45E-05	1.50E-04	254%	146%	TP-both
131-57-7	Oxybenzone	0.000164	0.002046	0.001796	2.99E-05	4.98E-05	3.41E-05	3.23E-05	7.12E-05	-92%	-97%	R-both
0-00-0	Acridine-9-carbaldehyde	8.32E-06	0	1.07E-05	0.000571	0.00033	0.000235	8.70E-06	3.80E-05	4430%	255%	TP-both
3380-34-5	Triclosan	3.06E-05	0.000149	7.92E-05	6.80E-05	7.30E-05	3.94E-05	7.84E-05	4.87E-05	7%	-43%	TP-Ae, P-An
1/1/4640	Benzene, 4-chloro-1-(2,4-dichlorophenoxy)-2-methoxy-	1.90E-05	6.88E-05	2.49E-05	6.09E-05	5.88E-05	4.08E-05	6.52E-05	1.74E-05	90%	-18%	TP-Ae, P-An
3678-72-6	Pyridine, 4-(diphenylmethyl)-	1.09E-05	3.74E-05	0.000157	2.36E-05	8.96E-06	4.03E-05	1.95E-05	2.71E-05	-11%	-65%	P-both
86386-73-4	Fluconazole	3.71E-05	0.000132	7.05E-05	0.000246	0.000259	0.000178	6.30E-05	1.66E-04	271%	42%	TP-both
74401-03-9	4-(2-(4-Formylphenyl)ethenyl)pyridine	6.89E-06	5.48E-05	8.07E-05	2.88E-05	6.80E-05	9.59E-05	9.41E-06	2.02E-05	120%	-79%	TP-Ae, P-An
2309-49-1	1,3,7,9-Tetramethyluric acid	7.90E-06	4.34E-05	4.27E-05	1.40E-05	7.84E-06	6.43E-06	2.31E-05	4.57E-05	-30%	-20%	P-both
33374-28-6	1,2-Benzenedicarboxylic acid, 2-butoxyethyl butyl ester	4.23E-05	0.000167	0	4.43E-05	6.87E-05	0.000166	4.92E-06	0.00E+00	-27%	-97%	P-Ae, R-An
125-33-7	Primidone	2.70E-05	5.82E-05	9.36E-05	8.63E-05	0.000128	0.000133	2.20E-05	9.13E-05	127%	-32%	TP-Ae, P-An
78-43-3	1-Propanol, 2,3-dichloro-, phosphate (3:1)	5.65E-05	0.000289	0.000357	0.000124	0.000194	0.000298	0.000123	0.000254	23%	-43%	TP-Ae, P-An
1235-74-1	Methyl dehydroabietate	4.14E-06	1.78E-05	2.58E-05	3.72E-06	5.52E-06	4.25E-06	5.98E-06	5.85E-06	-54%	-72%	P-both

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeM P-I	AeM P-II	AeM P-III	AnM P-II	AnM P-III	AeM BR Avg. %C	AnM BR Avg. %C	R/P/TP/new TP
15521-04-7	2,6-Diphenyl-4-methyl-1,4-dihydropyridine-3,5-dicarbonitrile	3.96 E-06	1.75 E-05	1.22 E-05	3.13 E-05	4.88 E-05	2.22 E-05	3.85 E-06	3.92 E-06	317 %	-73%	TP-Ae, P-An
103-23-1	Hexanedioic acid, bis(2-ethylhexyl) ester	0.00 0153	0.00 0565	0.00 0561	4.15 E-05	8.66 E-05	6.48 E-05	0.000 12	0.000 0287	-82%	-87%	P-both
78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	0.00 0169	0.00 0389	0.00 02	2.16 E-05	1.69 E-05	1.48 E-05	0.000 192	0.000 387	-92%	21%	R-Ae, TP-An
298-46-4	Carbamazepine	4.20 E-06	2.56 E-05	8.96 E-06	3.45 E-05	3.30 E-05	4.24 E-05	5.71 E-06	2.86 E-05	375 %	71%	TP-both
115-86-6	Triphenyl phosphate	2.69 E-06	1.60 E-05	1.47 E-05	2.72 E-06	2.57 E-06	2.16 E-06	2.75 E-06	7.59 E-06	-56%	-66%	P-both
57-41-0	Phenytoin	3.75 E-06	2.30 E-05	1.76 E-05	2.66 E-05	3.52 E-05	3.09 E-05	7.88 E-06	2.70 E-05	246 %	-6%	TP-Ae, P-An
94-28-0	Triethylene glycol di(2-ethylhexoate)	1.70 E-05	3.51 E-05	0.00 0393	3.26 E-06	5.19 E-06	3.87 E-06	4.48 E-06	4.02 E-06	-88%	-93%	P-Ae, R-An
5756-24-1	Tetrasulfide, dimethyl	0.00 0289	0.00 6301	0.00 3875	0	7.42 E-06	2.58 E-06	0.000 137	0.000 204	-100 %	-96%	R-both
1948-33-0	t-Butylhydroquinone	0.00 0165	0.00 0872	0.00 0546	0	0.000 114	0.000 102	0.000 22	0.000 0714	-89%	-81%	P-both
118-79-6	Phenol, 2,4,6-tribromo-	0	3.41 E-06	5.44 E-06	0	4.36 E-06	6.55 E-06	1.87 E-06	1.92 E-06	24%	-55%	TP-Ae, P-An
83-67-0	Theobromine	5.08 E-05	0.00 0255	0.00 0727	0	3.78 E-06	4.48 E-06	3.09 E-05	2.76 E-05	-99%	-92%	R-both
54340-85-1	Benzene, 1-(2-butenyl)-2,3-dimethyl-	1.83 E-05	0.00 0173	7.87 E-05	0	5.79 E-05	1.89 E-05	3.32 E-05	2.25 E-05	-81%	-76%	P-both
32624-67-2	10,18-Bisnorabieta-8,11,13-triene	2.42 E-06	3.08 E-05	0	0	5.45 E-06	1.59 E-06	2.37 E-06	1.71 E-06	-91%	-92%	R-both
100-44-7	Benzyl chloride	5.60 E-05	0	0.00 028	1.74 E-05	3.55 E-05	4.52 E-05	0.000 16	0.000 0827	-76%	-70%	P-both
765-70-8	1,2-Cyclopentanedione, 3-methyl-	3.07 E-05	0.00 0168	0.00 0106	1.15 E-05	1.67 E-05	1.24 E-05	0.000 109	0.000 0665	-80%	-36%	P-both
1193-22-2	4-Amino-6-hydroxypyrimidine	9.04 E-06	3.69 E-05	3.03 E-05	2.36 E-05	4.01 E-05	4.04 E-05	2.42 E-05	2.07 E-05	68%	-33%	TP-Ae, P-An
617-94-7	Benzenemethanol, à,à-dimethyl-	5.36 E-05	0.00 0316	0.00 0239	0.00 0247	0.000 273	0.000 135	0.000 302	0.000 495	101 %	51%	TP-both
13679-74-8	2-Acetyl-5-methylthiophene	9.74 E-06	8.04 E-05	7.39 E-05	3.81 E-06	1.18 E-05	7.03 E-06	2.30 E-05	3.18 E-05	-79%	-64%	P-both
119-65-3	Isoquinoline	1.38 E-05	8.82 E-05	5.29 E-05	2.52 E-05	3.54 E-05	3.88 E-05	4.27 E-05	4.88 E-05	-1%	-30%	P-both
21494-57-5	1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	0.00 0109	0.00 0592	0.00 0453	0.00 0192	0.000 387	0.000 269	0.000 171	0.000 301	0%	-52%	TP-Ae, P-An
50868-73-0	2-Methoxy-6-methylaniline	3.31 E-05	0.00 0185	0.00 014	3.17 E-05	9.29 E-05	6.20 E-05	7.71 E-05	1.19 E-04	-37%	-37%	P-both
6574-97-6	2,3-Dichlorobenzonitrile	1.30 E-05	5.19 E-05	6.26 E-05	9.34 E-05	0.000 113	0.000 107	3.08 E-05	8.77 E-05	269 %	0%	TP-Ae, P-An
2809-64-5	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	8.33 E-05	0.00 0144	0.00 0122	4.71 E-05	9.50 E-05	9.82 E-05	8.93 E-05	1.44 E-04	-32%	-10%	P-both
2078-54-8	Propofol	9.40 E-05	0.00 0232	0.00 0167	0.00 012	6.97 E-05	2.84 E-05	0.000 167	0.000 526	-42%	93%	P-Ae, TP-An
88-06-2	Phenol, 2,4,6-trichloro-	3.27 E-06	2.72 E-05	0	1.97 E-06	7.75 E-06	1.22 E-05	9.01 E-06	2.28 E-05	-56%	-67%	P-both
643-79-8	1,2-Benzenedicarboxaldehyde	1.87 E-05	0.00 0114	4.59 E-05	7.34 E-06	1.22 E-05	7.20 E-06	2.95 E-05	8.70 E-05	-78%	8%	P-Ae, TP-An
492-86-4	p-Chloromandelic acid	5.50 E-06	3.07 E-05	2.96 E-05	0	1.46 E-05	1.80 E-05	5.84 E-06	2.41 E-05	-64%	-50%	P-both

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one	7.90E-05	0.000034	0.000129	8.17E-05	0.000105	0.000141	0.000156	0.000241	-19%	16%	P-Ae, TP-An
59-48-3	2H-Indol-2-one, 1,3-dihydro-	0.000341	0.001153	0.002349	0	3.80E-05	4.84E-05	0.000447	0.000142	-98%	-78%	R-Ae, P-An
96-76-4	2,4-Di-tert-butylphenol	0.000329	0.000495	0.000288	0.000285	0.000307	0.000258	0.000404	0.000592	-21%	44%	P-Ae, TP-An
0-00-0	Benzamide, 3-methyl-N-methyl-N-propyl-	0	0.009149	0.003196	3.21E-05	0.000145	0.000267	0.002656	0.005524	-95%	1%	R-Ae, TP-An
39711-79-0	Cyclohexanecarboxamide, N-ethyl-5-methyl-2-(1-methylethyl)-	7.32E-05	0.000452	0.000314	0.000413	0.000558	0.000622	0.00021	0.000554	195%	11%	TP-both
615-22-5	2-(Methylmercapto)benzothiazole	5.59E-05	0.000259	0.000218	0.000265	0.000303	0.000182	7.34E-05	5.22E-04	125%	34%	TP-both
122-40-7	Cinnamaldehyde, à-pentyl-	0	7.38E-06	4.05E-05	9.48E-07	0	4.55E-06	3.15E-05	3.82E-05	-94%	161%	R-Ae, TP-An
6066-49-5	3-Butylisobenzofuran-1(3H)-one	5.28E-05	0.000314	0.000338	4.53E-05	6.86E-05	6.16E-05	8.48E-05	1.69E-04	-58%	-61%	P-both
6957-19-3	2,3,6,7-Tetramethylquinoxaline	1.86E-06	1.11E-05	0	1.21E-05	1.76E-05	2.74E-05	1.28E-05	6.37E-05	305%	15%	TP-both
490-91-5	Thymoquinone	5.06E-05	0.000536	0.000176	7.82E-05	0.000151	0.000101	9.14E-05	2.02E-04	-20%	-34%	P-both
17190-29-3	Benzenepropanenitrile, á-hydroxy-	4.07E-05	0.000173	0.000158	3.09E-05	5.27E-05	8.31E-05	4.20E-05	1.23E-04	-47%	-49%	P-both
0-00-0	6-Methylenebicyclo[3.2.0]hept-3-en-2-one	1.41E-05	5.32E-05	3.71E-05	2.63E-05	3.53E-05	3.08E-05	2.70E-05	3.23E-05	12%	-31%	TP-Ae, P-An
1689-64-1	9H-Fluoren-9-ol	0	5.57E-05	4.24E-05	1.40E-05	1.33E-05	2.49E-05	1.89E-05	6.50E-05	-59%	-6%	P-both
151805-12-8	(1S,4S,9aS)-4-Allyl-1-ethyloctahydro-1H-quinolizine	3.60E-06	2.46E-05	1.35E-05	1.72E-05	3.45E-05	2.68E-05	6.09E-05	1.66E-04	172%	639%	TP-both
3550-21-8	Benzhydryl isothiocyanate	2.69E-05	0.000016	7.15E-05	8.15E-05	0.000198	0.000273	0.000139	0.000339	170%	181%	TP-both
118-23-0	Amodryl	0.000114	0	0.001152	0.000978	0.001671	0.001382	0.0026	0.003982	389%	246%	TP-both
25812-30-0	Gemfibrozil	4.70E-05	7.92E-05	0.000291	8.63E-06	4.53E-06	2.70E-05	2.44E-05	3.98E-04	-89%	-16%	P-both
899028-28-3	2(5H)-Furanone, 4-methyl-3,5,5-tris(2-methyl-2-propenyl)-	2.12E-05	0.000139	0.000114	0.00011	0.000176	0.000226	6.37E-05	1.90E-04	181%	6%	TP-both
127-63-9	Diphenyl sulfone	0.000118	0.000612	0.000554	0.000036	0.000631	0.00073	0.000299	0.000688	80%	-13%	TP-Ae, P-An
486-16-8	Carbinoxamine	5.91E-05	0.000547	0	0.000814	0.00109	0.000885	0.0004	0.000821	688%	-27%	TP-Ae, P-An
0-00-0	Norharmane, N-acetyl-	6.72E-06	5.73E-05	4.93E-05	3.71E-06	7.29E-06	6.03E-06	1.02E-05	4.35E-05	-73%	-47%	P-both
2651-34-5	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10aoctahydro-	2.69E-05	0.000128	0.000164	2.34E-05	3.54E-05	6.54E-05	3.78E-05	1.26E-05	-48%	-81%	P-both
80-05-7	Phenol, 4,4'-(1-methylethylidene)bis-	0.000117	0.000607	0.000546	2.30E-05	2.87E-05	6.88E-06	0.000278	0.000703	-91%	-13%	R-Ae, P-An
0-00-0	Adipic acid, 2-decyl isobutyl ester	5.14E-06	1.66E-05	1.80E-05	1.84E-05	5.95E-05	2.88E-05	1.30E-05	7.01E-06	192%	-41%	TP-Ae, P-An
137-89-3	1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	7.64E-05	0.000238	0	9.48E-05	6.20E-05	5.12E-05	8.57E-05	5.35E-05	-25%	-64%	P-both
95906-11-9	Tris(2,4-di-tert-butylphenyl) phosphate	0.000661	0.002381	0	0.001536	0.001755	0.001226	0.000628	0.000821	53%	-74%	TP-Ae, P-An

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeM P-I	AeM P-II	AeM P-III	AnM P-II	AnM P-III	AeM BR Avg. %C	AnM BR Avg. %C	R/P/TP/new TP
110-93-0	5-Hepten-2-one, 6-methyl-	2.53 E-05	0	5.17 E-05	6.52 E-06	1.89 E-05	1.98 E-05	5.06 E-05	5.18 E-05	-68%	0%	P-both
2445-93-4	2-Pentenoic acid, ethyl ester	5.76 E-05	3.95 E-05	0.00 0203	8.78 E-06	3.11 E-05	1.40 E-05	9.28 E-05	1.92 E-05	-66%	22%	P-Ae, TP-An
6452-49-9	Benzene, 1-chloro-3-phenoxy-	4.19 E-06	2.12 E-05	1.05 E-05	1.10 E-05	1.33 E-05	6.29 E-06	2.94 E-05	2.94 E-06	28%	-17%	TP-Ae, P-An
873-94-9	Cyclohexanone, 3,3,5-trimethyl-	8.08 E-05	0.00 0706	0.00 0577	8.60 E-05	0.000 269	0.000 48	0.000 525	0.001 169	-24%	38%	P-Ae, TP-An
98-53-3	Cyclohexanone, 4-(1,1-dimethylethyl)-	6.48 E-05	0.00 0384	0.00 0348	5.09 E-06	1.06 E-05	4.89 E-05	0.000 12	0.000 803	-92%	31%	R-Ae, TP-An
73200-73-4	3-Phenylpyrazin-2-ol	2.43 E-05	0.00 0148	7.11 E-05	0.00 0117	0.000 163	8.22 E-05	0.000 111	0.000 293	136 %	144 %	TP-both
72189-24-3	4-Hexen-2-one, 3-methyl-	4.46 E-06	3.68 E-05	1.44 E-05	5.13 E-06	5.52 E-06	0	5.15 E-06	5.31 E-06	-57%	-75%	P-both
693-54-9	2-Decanone	0.00 0483	0.00 2832	0.00 1797	3.54 E-05	2.39 E-05	0.000 133	0.000 32	0.000 108	-95%	-91%	R-both
78-70-6	Linalool	0.00 0137	0.01 0573	0.00 7663	1.04 E-05	1.43 E-05	1.75 E-05	0.000 369	0.000 463	-97%	-95%	R-both
29393-32-6	2(3H)-Furanone, 5-acetyldihydro-	7.47 E-05	0.00 0439	0.00 0278	0.00 0161	0.000 355	0.000 218	6.09 E-05	3.35 E-05	25%	-87%	TP-Ae, P-An
4819-67-4	Amyl cyclopentenone	4.00 E-05	0.00 0254	0.00 0168	1.35 E-05	3.33 E-05	2.59 E-05	4.21 E-05	4.67 E-05	-79%	-78%	P-both
121-33-5	Vanillin	4.93 E-05	0.00 0552	0	4.37 E-05	0.000 195	4.46 E-05	2.34 E-05	3.11 E-05	-38%	-96%	P-Ae, R-An
65050-80-8	Pent-1-yn-3-ene, 4-methyl-3-phenyl-	4.39 E-06	3.08 E-05	0	1.52 E-05	1.21 E-05	1.29 E-05	1.44 E-05	8.83 E-06	93%	-53%	TP-Ae, P-An
121-00-6	3-tert-Butyl-4-hydroxyanisole	3.10 E-05	0.00 0192	0.00 0152	3.95 E-05	7.58 E-05	4.53 E-05	2.97 E-05	6.12 E-05	-34%	-72%	P-both
58-08-2	Caffeine	0.02 9485	0.13 9785	0.09 2725	5.22 E-05	0.000 136	0.000 308	0.002 834	0.009 916	-100 %	-94%	R-both
2854-40-2	Cyclo(L-prolyl-L-valine)	0	0.00 0513	0.00 0353	2.99 E-06	3.88 E-06	0	1.05 E-05	2.30 E-05	-100 %	-96%	R-both
58-55-9	Theophylline	0.00 0129	0.00 0536	0.00 0279	1.69 E-05	3.62 E-05	2.79 E-05	4.24 E-05	6.79 E-05	-90%	-84%	R-Ae, P-An
0-00-0	Adipic acid, 3-heptyl isobutyl ester	0.00 0113	0.00 0659	0.00 0455	0.00 0208	0.000 481	0.000 568	0.000 1	0.000 15	27%	-76%	TP-Ae, P-An
1/3/2781	1,3,6-Trioxocane, 2-methyl-	2.47 E-05	6.98 E-05	7.13 E-05	3.13 E-05	2.74 E-05	0	1.81 E-05	0.00 E+00	-45%	-87%	P-both
3777-69-3	Furan, 2-pentyl-	0.00 0468	0.00 2634	0.00 3126	4.24 E-05	8.36 E-05	4.83 E-05	0.000 482	0.000 361	-95%	-85%	R-Ae, P-An
1195-32-0	Benzene, 1-methyl-4-(1-methylethenyl)-	6.94 E-05	0.00 0178	0.00 0865	3.98 E-06	1.99 E-05	1.51 E-05	1.60 E-05	2.18 E-05	-94%	-94%	R-both
122-00-9	Ethanone, 1-(4-methylphenyl)-	7.82 E-05	0.00 0437	0.00 0548	3.12 E-05	5.15 E-05	4.86 E-05	0.000 127	0.000 248	-80%	-63%	P-both
101-84-8	Diphenyl ether	1.87 E-05	8.09 E-05	8.54 E-05	2.94 E-06	2.12 E-06	0	6.73 E-06	7.45 E-06	-94%	-91%	R-both
60593-11-5	S-(+)-5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one	0.00 0113	0.00 0428	0.00 0418	8.29 E-06	1.24 E-05	1.18 E-05	5.08 E-05	1.10 E-04	-96%	-81%	R-Ae, P-An
131-11-3	Dimethyl phthalate	3.13 E-05	0	0.00 0217	1.49 E-05	3.22 E-05	3.07 E-05	3.78 E-05	2.84 E-05	-69%	-87%	P-both
114933-28-7	3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	0.00 0141	0.00 0786	0.00 0817	2.00 E-05	1.35 E-05	1.68 E-05	0.000 103	0.000 0765	-94%	-89%	R-Ae, P-An
14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	2.67 E-05	0.00 0149	0.00 0163	4.22 E-06	4.79 E-06	8.05 E-06	8.30 E-06	1.75 E-05	-92%	-92%	R-both

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
13757-90-9	6,7-Dodecanedione	5.92 E-06	4.39 E-05	6.09 E-05	1.21 E-05	2.79 E-05	0	1.17 E-05	1.24 E-05	-11%	-76%	P-both
50-78-2	Aspirin	2.62 E-05	0	0.000673	5.88 E-05	3.91 E-05	3.85 E-05	5.14 E-05	2.77 E-05	15%	-96%	TP-Ae, R-An
6938-51-8	2-Octyl benzoate	4.39 E-05	0.000219	0.000382	6.22 E-05	6.45 E-05	5.07 E-05	8.19 E-05	5.43 E-05	-39%	-74%	P-both
12/6/4537	Benzene, (1-propylheptyl)-	4.55 E-05	0.000134	0.001311	2.07 E-05	3.04 E-05	2.69 E-05	8.49 E-05	1.45 E-04	-77%	-63%	P-both
68039-35-0	Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-	7.96 E-06	5.09 E-05	5.85 E-05	1.64 E-06	3.22 E-06	4.27 E-06	1.05 E-05	1.21 E-05	-89%	-79%	P-both
0-00-0	Salicylic acid, 2-methylbutyl ether, 2-methylbutyl ester	5.16 E-05	0.000642	0.000187	2.36 E-05	2.61 E-05	2.09 E-05	6.40 E-05	2.13 E-05	-83%	-94%	P-Ae, R-An
5466-77-3	2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	3.08 E-05	0.000195	0.000521	2.67 E-06	6.78 E-06	3.27 E-06	1.69 E-05	4.17 E-06	-96%	-95%	R-both
20384-05-8	(S,E)-2,5-Dimethyl-4-vinylhexa-2,5-dien-1-yl acetate	3.84 E-05	2.94 E-05	6.73 E-05	5.83 E-05	1.83 E-05	3.27 E-05	2.90 E-05	3.34 E-05	-12%	-26%	P-both
638-53-9	Tridecanoic acid	0.000419	0.000171	0	1.94 E-05	1.31 E-05	3.56 E-05	8.32 E-05	4.31 E-05	-94%	-51%	R-Ae, P-An
91-56-5	1H-Indole-2,3-dione	0.001297	0.000267	0.002678	0.000012	0.000153	9.36 E-05	0.000189	0.000127	-77%	-62%	P-both
3251-55-6	3-Methoxyparacetamol	0.000281	0.000349	0.000724	8.78 E-06	1.40 E-05	0	2.02 E-05	3.32 E-05	-98%	-95%	R-both
526-73-8	Benzene, 1,2,3-trimethyl-, isomer 2	1.20 E-05	2.22 E-05	0	4.63 E-05	8.57 E-06	1.83 E-05	2.16 E-05	6.95 E-06	112%	-3%	TP-Ae, P-An
13788-35-8	Bis(3-chloro-1-propyl)(1-chloro-2-propyl)phosphate	7.56 E-06	4.39 E-05	4.48 E-05	2.50 E-05	5.25 E-05	5.62 E-05	2.71 E-05	5.93 E-05	92%	-3%	TP-Ae, P-An
106-44-5	p-Cresol	0	0.03421	0.017279	0.001059	7.09 E-05	9.56 E-05	0.000453	0.000968	-100%	-97%	R-both
611-74-5	Benzamide, N,N-dimethyl-	3.82 E-05	0.000131	0.000172	3.47 E-05	6.09 E-05	0.000588	2.67 E-05	1.82 E-05	60%	-85%	TP-Ae, P-An
123-56-8	Succinimide	1.39 E-05	9.77 E-05	7.87 E-05	0.000168	8.87 E-05	0.000123	1.84 E-05	1.06 E-05	385%	-84%	TP-Ae, P-An
101-86-0	Octanal, 2-(phenylmethylene)-	6.36 E-05	0.000374	0	3.84 E-05	3.08 E-05	4.05 E-05	0	0.00015	-66%	-100%	P-Ae, R-An
18612-99-2	8,9-Dehydrothymol	4.42 E-06	5.00 E-05	7.04 E-06	6.12 E-06	0	6.39 E-06	1.42 E-05	3.71 E-05	-24%	178%	P-Ae, TP-An
98-82-8	Benzene, (1-methylethyl)-	0.000101	0.000292	0	0.000303	0.000101	0.000146	0.000138	0.0000833	67%	-53%	TP-Ae, P-An
496-11-7	Indane	0	3.43 E-05	4.73 E-05	7.10 E-05	2.67 E-05	5.12 E-05	3.40 E-05	1.97 E-05	-7%	-30%	P-both
19715-19-6	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-2-hydroxy-	1.04 E-05	2.80 E-05	5.47 E-05	0.000163	0.000351	0.00051	1.97 E-05	3.31 E-05	1151%	-35%	TP-Ae, P-An
2000-43-3	2,2,2-Trichloro-1-phenylethanol	0	0.000466	0.000346	6.35 E-05	0.000143	4.19 E-05	0	0	-79%	-100%	P-Ae, R-An
19037-58-2	Syringylacetone	1.03 E-05	0.000131	8.56 E-05	5.85 E-06	1.87 E-05	6.38 E-06	0	0	-74%	-100%	P-Ae, R-An
2033-89-8	Phenol, 3,4-dimethoxy-	2.91 E-05	0.000122	0.000104	3.31 E-06	1.51 E-05	7.32 E-06	0	0	-90%	-100%	P-Ae, R-An

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
59121-24-3	Butanenitrile, 4-(methylthio)-	0.000257	0.001271	0.000926	0	0	0	0.000135	0.000177	-100%	-85%	R-Ae, P-An
931-20-4	2-Piperidinone, 1-methyl-	1.50E-06	1.90E-05	0	0	0	0	1.30E-05	6.37E-06	-100%	-32%	R-Ae, P-An
24050-09-7	Thiazolidine, 2-ethyl-	8.51E-06	6.48E-05	5.55E-05	0	0	0	2.35E-05	1.06E-04	-100%	14%	R-Ae, TP-An
53547-60-7	6-Methyl-2-pyridinecarbaldehyde	1.14E-05	2.18E-05	5.96E-05	0	0	0	4.93E-06	3.70E-06	-100%	-86%	R-Ae, P-An
122-99-6	Ethanol, 2-phenoxy-	0	0.000165	6.35E-05	0	0	0	1.65E-05	7.57E-05	-100%	-35%	R-Ae, P-An
501-94-0	Benzeneethanol, 4-hydroxy-	0.001527	0.008865	0.005575	0	0	0	9.11E-05	1.79E-04	-100%	-98%	R-both
1677-27-6	3H-1,2-Benzodithiol-3-one	7.21E-05	0.000414	0.000811	0	0	0	3.70E-05	4.38E-05	-100%	-93%	R-both
7661-55-4	Quinoline, 5-methyl-	2.57E-05	0.000182	5.60E-05	0	0	0	9.92E-05	9.84E-05	-100%	15%	R-Ae, TP-An
17233-71-5	Hexathiepane	5.63E-05	0.000622	0.000112	0	0	0	3.80E-05	5.84E-05	-100%	-71%	R-Ae, P-An
611-59-6	1,7-Dimethylxanthine	0.000165	0.003336	0.001882	0	0	0	1.79E-05	3.24E-05	-100%	-99%	R-both
86-96-4	2,4(1H,3H)-Quinazolinedione	4.45E-06	1.45E-05	3.79E-05	0	0	0	5.55E-06	9.01E-06	-100%	-69%	R-Ae, P-An
0-00-0	1H-Tetrazole, 5-(1,5-dimethyl-1H-pyrrol-2-yl)-	3.11E-05	0	5.23E-05	0	0	0	3.50E-05	4.40E-05	-100%	-16%	R-Ae, P-An
101-72-4	1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-	3.02E-06	2.02E-05	1.51E-05	0	0	0	3.76E-05	1.53E-05	-100%	44%	R-Ae, TP-An
0-00-0	Phthalazin-1(2H)-one, 2-ethenyl-	1.59E-05	0.000104	0	0	0	0	9.65E-06	1.96E-05	-100%	-91%	R-both
13679-75-9	1-(2-Thienyl)-1-propanone	5.08E-06	3.53E-05	3.09E-05	0	0	0	1.09E-05	3.83E-05	-100%	-23%	R-Ae, P-An
108-43-0	Phenol, 3-chloro-	3.98E-05	0.000187	0.000142	0	0	0	9.40E-05	6.96E-05	-100%	-50%	R-Ae, P-An
2219-73-0	Phenol, 4-ethyl-2-methyl-	5.42E-06	2.20E-05	1.82E-05	0	0	0	2.27E-05	5.39E-05	-100%	100%	R-Ae, TP-An
35029-03-9	1,3-Cyclopentanedione, 4-methyl-	8.80E-06	4.71E-05	0	0	0	0	3.40E-05	3.37E-05	-100%	-28%	R-Ae, P-An
6/7/5257	Formamide, N-(2-acetylphenyl)-	8.05E-05	0.000489	0.000218	0	0	0	0.000231	0.000209	-100%	-28%	R-Ae, P-An
10375-96-9	Benzene, 1,4-dimethyl-2,5-bis(1-methylethyl)-	0	2.39E-05	1.57E-05	0	0	0	1.72E-05	8.92E-06	-100%	-36%	R-Ae, P-An
88-26-6	3,5-di-tert-Butyl-4-hydroxybenzyl alcohol	2.95E-06	3.31E-05	7.11E-06	0	0	0	1.81E-05	3.34E-05	-100%	162%	R-Ae, TP-An

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
92-69-3	p-Hydroxybiphenyl	1.54E-05	0.000152	3.97E-05	0	0	0	0.000122	0.0000303	-100%	-22%	R-Ae, P-An
53874-66-1	Benzene, 1-(chloromethyl)-3-phenoxy-	0	3.86E-06	4.04E-06	0	0	0	2.85E-06	4.68E-06	-100%	-5%	R-Ae, P-An
0-00-0	3H-Cyclopenta[c]pyridazin-3-one, 2,5,6,7-tetrahydro-	0	9.77E-06	7.73E-06	0	0	0	3.88E-06	1.17E-05	-100%	-4%	R-Ae, P-An
17619-36-2	Trisulfide, methyl propyl	0	5.19E-05	3.02E-05	0	0	0	3.61E-06	1.03E-06	-100%	-95%	R-both
877-65-6	Benzenemethanol, 4-(1,1-dimethylethyl)-	0	0.000118	9.11E-05	0	0	0	6.05E-06	2.87E-05	-100%	-82%	R-Ae, P-An
150-13-0	4-Aminobenzoic acid	3.73E-06	3.78E-05	1.35E-05	0	0	0	2.02E-05	2.27E-05	-100%	11%	R-Ae, TP-An
33996-58-6	Etiracetam	7.41E-05	0.000527	0.000272	0	0	0	0.000293	0.000227	-100%	-30%	R-Ae, P-An
94-13-3	Propylparaben	0.000448	0.002652	0.002222	0	0	0	0.000236	0.000374	-100%	-87%	R-Ae, P-An
131-56-6	Methanone, (2,4-dihydroxyphenyl)phenyl-	3.91E-05	0.000697	0.000271	0	0	0	2.46E-05	4.89E-05	-100%	-89%	R-Ae, P-An
288-26-6	3H-1,2-Dithiole	0	7.95E-06	1.14E-05	0	0	0	4.31E-06	7.54E-06	-100%	-40%	R-Ae, P-An
7210-64-2	2(5H)-Thiophenone, 5-methyl-	4.17E-06	2.64E-05	2.29E-05	0	0	0	3.31E-06	3.29E-06	-100%	-87%	R-Ae, P-An
116664-30-3	5-Methyl-1,2,3,4-tetrathiane	4.41E-05	0.000173	0.00017	0	0	0	1.19E-05	1.20E-05	-100%	-93%	R-both
4792-78-3	2-(2-Hydroxyethoxy)phenol	0.000102	0.000417	0.000469	0	0	0	9.21E-05	1.19E-04	-100%	-76%	R-Ae, P-An
93-35-6	7-Hydroxycoumarin	0.000105	0.000413	0.000585	0	0	0	1.36E-05	6.32E-05	-100%	-93%	R-both
145344-72-5	2-(2',4',4',6',6',8',8'-Heptamethyltetrasiloxan-2'-yloxy)-2,	1.60E-06	1.07E-05	0.000206	0	0	0	3.60E-06	1.03E-06	-100%	-83%	R-Ae, P-An
0-00-0	3-pyridinecarbonitrile, 2-amino-1,6-dihydro-1,4-dimethyl-6-oxo-	1.32E-05	2.63E-05	2.66E-05	0	0	0	6.40E-06	1.49E-05	-100%	-60%	R-Ae, P-An
1436-27-7	2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	3.43E-06	3.30E-05	1.34E-05	0	0	0	2.75E-06	2.97E-06	-100%	-85%	R-Ae, P-An
290354-70-0	Thiophene, 2-formyl-2,3-dihydro-	2.27E-06	3.82E-05	7.49E-06	0	0	0	0	0	-100%	-100%	R-both
501-92-8	Phenol, 4-(2-propenyl)-	2.62E-05	7.38E-05	0	0	0	0	0	0	-100%	-100%	R-both
56630-95-6	Bicyclo[3.3.1]nonan-2-one, 1-methyl-9-(1-methylethylidene)-	8.83E-06	1.52E-05	2.25E-05	0	0	0	0	0	-100%	-100%	R-both
108-46-3	Resorcinol	0.000189	0.000923	0.001139	0	0	0	0	0	-100%	-100%	R-both

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
829-99-2	Benzene, 1-heptenyl-	2.96 E-06	4.85 E-05	0.000327	0	0	0	0	0	-100 %	-100 %	R-both
1203-08-03	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	5.38 E-06	1.49 E-05	1.80 E-05	0	0	0	0	0	-100 %	-100 %	R-both
274-40-8	Indolizine	1.99 E-05	6.26 E-05	2.86 E-05	0	0	0	0	0	-100 %	-100 %	R-both
2941-72-2	Benzothiazole, 6-methoxy-2-methyl-	2.81 E-06	2.31 E-05	1.11 E-05	0	0	0	0	0	-100 %	-100 %	R-both
489-84-9	Azulene, 1,4-dimethyl-7-(1-methylethyl)-	1.20 E-06	5.39 E-06	2.42 E-05	0	0	0	0	0	-100 %	-100 %	R-both
13410-15-6	1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-, (R)-	3.65 E-06	3.16 E-05	1.66 E-05	0	0	0	0	0	-100 %	-100 %	R-both
50899-59-7	Indole-2,3-dione, 1-(hydroxymethyl)-	4.41 E-06	2.60 E-05	8.09 E-05	0	0	0	0	0	-100 %	-100 %	R-both
830-96-6	1H-Indole-3-propanoic acid	2.67 E-05	6.05 E-05	2.40 E-05	0	0	0	0	0	-100 %	-100 %	R-both
5037-75-2	2,5-Piperazinedione, 3-(phenylmethyl)-	1.15 E-05	8.40 E-05	4.28 E-05	0	0	0	0	0	-100 %	-100 %	R-both
1086-80-2	Lumichrome	1.21 E-06	1.58 E-05	4.89 E-05	0	0	0	0	0	-100 %	-100 %	R-both
644511-76-9	2-(4-(But-2-yl)phenyl)propanoic acid	2.31 E-05	0	8.50 E-06	0	0	0	0	0	-100 %	-100 %	R-both
552700-48-9	5-Ethoxy-2-methyl-pyridine	2.24 E-05	4.54 E-05	1.55 E-05	0	0	0	0	0	-100 %	-100 %	R-both
29267-67-2	2-Methoxyresorcinol	4.18 E-05	0.000301	8.29 E-06	0	0	0	0	0	-100 %	-100 %	R-both
72777-88-9	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-	0	0.000118	6.08 E-05	0	0	0	0	0	-100 %	-100 %	R-both
486-21-5	Isofraxidin	1.54 E-06	1.38 E-05	6.83 E-06	0	0	0	0	0	-100 %	-100 %	R-both
116664-29-0	4-Methyl-1,2,3-trithiolane	4.61 E-06	2.05 E-05	2.04 E-05	0	0	0	0	0	-100 %	-100 %	R-both
28715-26-6	Benzofuran, 4,7-dimethyl-	9.82 E-06	4.58 E-05	0.000129	0	0	0	0	0	-100 %	-100 %	R-both
0-00-0	5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde	2.24 E-05	4.14 E-05	0.000162	0	0	0	0	0	-100 %	-100 %	R-both
4842-89-1	3-Pyridinol, 6-methyl-, acetate (ester)	0	2.05 E-05	0.000503	0	0	0	0	0	-100 %	-100 %	R-both
0-00-0	1,4-diazabicyclo[4.3.0]nonan-2,5-dione, 3-methyl	9.00 E-06	5.79 E-05	0	0	0	0	0	0	-100 %	-100 %	R-both
930-88-1	N-Methylmaleimide	0	0	0	1.49 E-05	1.46 E-05	8.30 E-06	0	0	n/a	n/a	new TP-AeMBR

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
14657-22-8	Silane, trimethyl-1,2-propadienyl-	0	0	0	0	2.56 E-05	1.61 E-05	0	0	n/a	n/a	new TP-AeMBR
1635-02-05	3-Hexen-2-one, 3,4-dimethyl-	0	0	0	7.74 E-06	6.03 E-06	6.57 E-06	0	0	n/a	n/a	new TP-AeMBR
2949-92-0	S-Methyl methanethiosulphonate	0	0	0	1.21 E-05	8.96 E-06	1.02 E-05	0	0	n/a	n/a	new TP-AeMBR
637-88-7	1,4-Cyclohexanedione	0	0	0	3.72 E-06	7.84 E-06	9.89 E-06	0	0	n/a	n/a	new TP-AeMBR
42786-06-1	4H-1,2,4-Triazol-3-amine, 4-ethyl-	0	0	0	1.26 E-05	1.13 E-05	6.97 E-06	0	0	n/a	n/a	new TP-AeMBR
1125-11-7	1,3-Cyclohexanedione, 2,5,5-trimethyl-	0	0	0	3.48 E-05	2.65 E-05	0.000142	0	0	n/a	n/a	new TP-AeMBR
21450-56-6	1,2,3,4-Tetramethoxybenzene	0	0	0	7.49 E-06	1.39 E-05	1.49 E-05	0	0	n/a	n/a	new TP-AeMBR
1008-89-5	Pyridine, 2-phenyl-	0	0	0	3.16 E-06	3.76 E-06	4.68 E-06	0	0	n/a	n/a	new TP-AeMBR
55092-18-7	2,7:3,6-Dimethano-2H-1-benzopyran, octahydro-	0	0	0	1.31 E-05	1.94 E-05	1.48 E-05	0	0	n/a	n/a	new TP-AeMBR
55103-64-5	2H-Benzocyclohepten-2-one, decahydro-4a-methyl-, trans-	0	0	0	1.55 E-06	3.29 E-06	5.51 E-06	0	0	n/a	n/a	new TP-AeMBR
3866-16-8	Benzene, 1-azido-3-methoxy-	0	0	0	0.000128	0.000395	0.000263	0	0	n/a	n/a	new TP-AeMBR
55720-37-1	Naphthalene, 1,3,7-trichloro-	0	0	0	7.53 E-06	5.42 E-05	0	0	0	n/a	n/a	new TP-AeMBR
10103-06-7	Naphthalene, 2,3-dimethoxy-	0	0	0	8.11 E-06	1.21 E-05	1.56 E-05	0	0	n/a	n/a	new TP-AeMBR
3483-18-9	Sydnone, 3-(2-methylphenyl)-	0	0	0	5.16 E-06	7.48 E-06	6.95 E-06	0	0	n/a	n/a	new TP-AeMBR
14035-34-8	2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol	0	0	0	2.73 E-05	7.39 E-05	5.36 E-05	0	0	n/a	n/a	new TP-AeMBR
22518-27-0	4-(4-Chlorophenyl)-2-pyrrolidinone	0	0	0	5.22 E-06	3.14 E-05	2.46 E-05	0	0	n/a	n/a	new TP-AeMBR
84922-05-4	cis-1-(4-Isopropylphenyl)-3-(2-furyl)cyclopropane	0	0	0	4.36 E-06	7.73 E-06	5.78 E-06	0	0	n/a	n/a	new TP-AeMBR
3902-71-4	Trioxsalen	0	0	0	6.90 E-06	2.99 E-05	1.25 E-05	0	0	n/a	n/a	new TP-AeMBR
484-18-4	Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-	0	0	0	1.26 E-05	9.80 E-06	5.86 E-06	0	0	n/a	n/a	new TP-AeMBR
93007-54-6	5-Isopropyl-3,8-dimethylazulene-1-carbonitrile	0	0	0	4.77 E-06	1.11 E-05	4.62 E-06	0	0	n/a	n/a	new TP-AeMBR
0117-10-2	Danthron	0	0	0	3.08 E-06	6.52 E-06	9.02 E-06	0	0	n/a	n/a	new TP-AeMBR
28721-07-5	Oxcarbazepine	0	0	0	1.56 E-05	2.63 E-05	2.16 E-05	0	0	n/a	n/a	new TP-AeMBR
21651-53-6	(4aR,7S,7aS)-4,7-Dimethyl-5,6,7,7a-tetrahydrocyclopenta[c]pyran-1(4aH)-one	0	0	0	3.83 E-06	5.06 E-06	1.60 E-05	0	0	n/a	n/a	new TP-AeMBR

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
69745-73-9	2-Cyclopenten-1-one, 4-hydroxy-2-methyl-3-phenyl-	0	0	0	4.00E-05	3.99E-05	2.20E-05	0	0	n/a	n/a	new TP-AeMBR
67652-84-0	3,5-Octadiene, 4,5-diethyl-	0	0	0	4.80E-06	8.05E-06	7.56E-06	0	0	n/a	n/a	new TP-AeMBR
38205-55-9	5-Acetyl-4-methylthiazole	0	0	0	0.000192	0.000258	0.000168	0	0	n/a	n/a	new TP-AeMBR
108562-69-2	2,1-Benzisoxazole, 7-ethyl-3-methyl-	0	0	0	3.99E-06	9.77E-06	8.08E-06	0	0	n/a	n/a	new TP-AeMBR
29927-08-0	2-Benzothiazolamine, 5,6-dimethyl-	0	0	0	4.34E-06	6.07E-06	5.16E-06	0	0	n/a	n/a	new TP-AeMBR
619-62-5	4-Isopropyl-1-methylcyclohex-2-enol	0	0	0	2.95E-05	3.66E-05	6.69E-05	0	0	n/a	n/a	new TP-AeMBR
13618-88-7	5,6,7,8-Tetrahydroindolizine	0	0	0	3.80E-06	7.23E-06	1.29E-05	0	0	n/a	n/a	new TP-AeMBR
15001-27-1	3,4-Dimethoxybenzylideneacetone	0	0	0	5.76E-06	9.81E-06	1.28E-05	0	0	n/a	n/a	new TP-AeMBR
718-25-2	Benzene, 1-fluoro-4-(2-phenylethenyl)-, (E)-	0	0	0	0	3.40E-06	7.58E-06	0	0	n/a	n/a	new TP-AeMBR
536-78-7	Pyridine, 3-ethyl-	0	0	0	0	0	0	0.000437	0.000816	n/a	n/a	new TP-AnMBR
0350-03-08	Ethanone, 1-(3-pyridinyl)-	0	0	0	0	0	0	2.97E-06	8.75E-06	n/a	n/a	new TP-AnMBR
1121-25-1	3-Pyridinol, 2-methyl-	0	0	0	0	0	0	4.35E-05	3.36E-05	n/a	n/a	new TP-AnMBR
13623-12-6	2-tert-Butylthiazole	0	0	0	0	0	0	4.91E-06	1.84E-05	n/a	n/a	new TP-AnMBR
514-95-4	1,5,5-Trimethyl-6-methylene-cyclohexene	0	0	0	0	0	0	0	0.000499	n/a	n/a	new TP-AnMBR
137-00-8	5-Thiazoleethanol, 4-methyl-	0	0	0	0	0	0	0.000547	0.000317	n/a	n/a	new TP-AnMBR
18951-85-4	(R)-(+)-Citronellic acid	0	0	0	0	0	0	0.000371	0.000699	n/a	n/a	new TP-AnMBR
1780-19-4	Quinoline, 1,2,3,4-tetrahydro-2-methyl-	0	0	0	0	0	0	4.16E-05	1.18E-04	n/a	n/a	new TP-AnMBR
28785-06-0	Benzaldehyde, 4-propyl-	0	0	0	0	0	0	4.79E-06	7.63E-06	n/a	n/a	new TP-AnMBR
2033-30-9	5,6-Dimethyl-2-benzimidazolinone	0	0	0	0	0	0	2.49E-05	1.22E-04	n/a	n/a	new TP-AnMBR
22319-31-9	4-Hepten-3-one, 4-methyl-	0	0	0	0	0	0	6.99E-06	1.63E-05	n/a	n/a	new TP-AnMBR
0-00-0	Carbonic acid, monoamide, N-butyl-, allyl ester	0	0	0	0	0	0	1.99E-05	5.38E-05	n/a	n/a	new TP-AnMBR
62056-54-6	2,2-Dimethyl-N-phenethylpropionamide	0	0	0	0	0	0	0.000219	0.000218	n/a	n/a	new TP-AnMBR
0-00-0	5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid	0	0	0	0	0	0	4.15E-05	1.91E-04	n/a	n/a	new TP-AnMBR
22105-12-0	4H-1-Benzopyran-4-one, 6-hydroxy-2-methyl-	0	0	0	0	0	0	7.31E-06	1.50E-05	n/a	n/a	new TP-AnMBR

CAS No.	Compound Name	Inf.-I	Inf.-II	Inf.-III	AeMP-I	AeMP-II	AeMP-III	AnMP-II	AnMP-III	AeMBR Avg. %C	AnMBR Avg. %C	R/P/TP/new TP
0-00-0	2-(2-Oxo-2H-pyridin-1-yl)benzoic acid	0	0	0	0	0	0	3.30 E-06	1.57 E-05	n/a	n/a	new TP-AnMBR
5191-80-0	L-Cysteine, S-(diphenylmethyl)-	0	0	0	0	0	0	5.56 E-06	1.62 E-05	n/a	n/a	new TP-AnMBR
0-00-0	4,8,12,16-tetraoxaeicosan-1-ol	0	0	0	0	0	0	8.77 E-05	1.66 E-04	n/a	n/a	new TP-AnMBR
1002-84-2	Pentadecanoic acid	0	0	0	2.37 E-05	2.02 E-05	5.04 E-05	0	0.000 128	n/a	n/a	new TP-both

Note: R = Removed; P = Persistent; TP = the peak area abundance increased >0% from influent to permeate; new TP = compounds that were not detected in the influent, that newly appeared in the permeate; Ae = AeMBR; An = AnMBR. The reported peak areas were normalized to the sample volume and the peak area of the internal standard, phenanthrene-d10.

Table S12. Description of the 15 selected compounds confirmed with their authentic standards.

CAS No.	Compound name	Vendor
59121-25-4	Pentanenitrile, 5-(methylthio)-	Enamine Building Blocks, Cincinnati, OH
54-11-5	Nicotine	Cambridge Isotope Laboratories, Tewksbury, MA
140-29-4	Benzyl cyanide	Accustandard, New Haven, CT
611-59-6	1,7-Dimethylxanthine	Cambridge Isotope Laboratories, Tewksbury, MA
2785-89-9	Phenol, 4-ethyl-2-methoxy-	Enamine Building Blocks, Cincinnati, OH
7786-61-0	2-Methoxy-4-vinylphenol	AA Blocks, San Diego, CA
122-48-5	2-Butanone, 4-(4-hydroxy-3-methoxyphenyl)-	Enamine Building Blocks, Cincinnati, OH
5651-47-8	Benzoic acid, 3-(1-methylethyl)-	Enamine Building Blocks, Cincinnati, OH
100-53-8	Benzenemethanethiol	Enamine Building Blocks, Cincinnati, OH
138-87-4	Terpineol	Sigma Aldrich, Saint Louis, MO
92-61-5	Scopoletin	TCI America, Portland, OR
80-05-7	Bisphenol A	Accustandard, New Haven, CT
131-56-6	Methanone, (2,4-dihydroxyphenyl)phenyl-	Enamine Building Blocks, Cincinnati, OH
94-62-2	Piperine	Enamine Building Blocks, Cincinnati, OH
3380-34-5	Triclosan	Accustandard, New Haven, CT

Table S13. Comparison of the number of compounds treated at various efficiencies by AeMBR vs AnMBR.

Percent Peak Area Change	AeMBR	AnMBR
-100%	161	92
< -95%	165	108
< -90%	193	137
< -85%	204	163
< -75%	225	198
< -50%	255	270
< -25%	281	313
< -10%	296	337
< 0%	306	356
> 0%	220	193
> 10%	212	188
> 25%	200	182
> 50%	187	177
> 75%	180	177
> 100%	176	177
> 200%	170	172
> 500%	168	171
> 1,000%	167	171
Newly formed	165	171

Note: Compounds which were detected across all influent experimental replicates were isolated (N=493), then sorted into a percent peak area change category between "-100%" and ">1,000%". Where a -100% change refer to the compounds that were detected in the influents, but not in the permeates. Newly formed compounds (the compounds that were not detected in the influents but were detected in the permeates) comprise their own category.

Table S14. The 34 tentatively identifiable compounds that were commonly removed by aerobic and anaerobic membrane bioreactor treatment.

Peak	CAS No.	AeMBR			AnMBR	
		A (%C)	B (%C)	C (%C)	B (%C)	C (%C)
1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-, (R)-	13410-15-6	-100	-100	-100	-100	-100
1H-Indole-3-propanoic acid	830-96-6	-100	-100	-100	-100	-100
2,5-Piperazinedione, 3-(phenylmethyl)-	5037-75-2	-100	-100	-100	-100	-100
2-Methoxyresorcinol	29267-67-2	-100	-100	-100	-100	-100
4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	1203-08-3	-100	-100	-100	-100	-100
4-Methyl-1,2,3-trithiolane	-	-100	-100	-100	-100	-100
5-Ethoxy-2-methyl-pyridine	55270-48-9	-100	-100	-100	-100	-100
5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde	-	-100	-100	-100	-100	-100
Azulene, 1,4-dimethyl-7-(1-methylethyl)-	489-84-9	-100	-100	-100	-100	-100
Benzene, 1-heptenyl-	829-99-2	-100	-100	-100	-100	-100
Benzofuran, 4,7-dimethyl-	28715-26-6	-100	-100	-100	-100	-100
Benzothiazole, 6-methoxy-2-methyl-	2941-72-2	-100	-100	-100	-100	-100
Bicyclo[3.3.1]nonan-2-one, 1-methyl-9-(1-methylethylidene)-	56630-95-6	-100	-100	-100	-100	-100
Cyclic octaatomic sulfur	10544-50-0	-100	-100	-100	-100	-100
Indole-2,3-dione, 1-(hydroxymethyl)-	50899-59-7	-100	-100	-100	-100	-100
Indolizine	274-40-8	-100	-100	-100	-100	-100
Isofraxidin	486-21-5	-100	-100	-100	-100	-100
Lumichrome	1086-80-2	-100	-100	-100	-100	-100
Resorcinol	108-46-3	-100	-100	-100	-100	-100
Thiophene, 2-formyl-2,3-dihydro-	290354-70-0	-100	-100	-100	-100	-100
1,7-Dimethylxanthine	611-59-6	-100	-100	-100	-99	-98
Benzeneethanol, 4-hydroxy-	501-94-0	-100	-100	-100	-99	-97
5-Methyl-1,2,3,4-tetrathiane	116664-30-3	-100	-100	-100	-93	-93
3H-1,2-Benzodithiol-3-one	1677-27-6	-100	-100	-100	-91	-95
2-Acetyl-5-methylthiophene	5756-24-1	-100	-100	-100	-98	-95
2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-	13401-18-8	-99	-100	-100	-97	-97
5H-1-Pyrindine	270-91-7	-98	-100	-100	-99	-99
1H-Indole, 2-methyl-	95-20-5	-99	-99	-99	-99	-97
Dimethyl trisulfide	3658-80-8	-98	-99	-98	-98	-98
3-Methoxyparacetamol	3251-55-6	-97	-96	-100	-94	-95
Linalool	78-70-6	-92	-100	-100	-97	-94
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	5466-77-3	-91	-99	-100	-95	-100
Benzene, 1-isocyano-2-methyl-	10468-64-1	-96	-97	-97	-97	-93
2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	614-60-8	-93	-98	-98	-97	-92

Table S15. The 21 tentatively identifiable compounds that were removed by AeMBR treatment and not AnMBR treatment.

Compound Name	CAS No.	AeMBR				AnMBR		
		A (%C)	B (%C)	C (%C)	Avg. (%C)	B (%C)	C (%C)	Avg. (%C)
o-Hydroxybiphenyl	90-43-7	-96	-96	-93	-95	-35	666	316
3,5-di-tert-Butyl-4-hydroxybenzyl alcohol	88-26-6	-100	-100	-100	-100	-45	371	163
Phenol, 4-ethyl-2-methyl-	2219-73-0	-100	-100	-100	-100	3	196	100
1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-	101-72-4	-100	-100	-100	-100	86	1	44
Quinoline, 5-methyl-	7661-55-4	-100	-100	-100	-100	-46	76	15
Thiazolidine, 2-ethyl-	24050-09-7	-100	-100	-100	-100	-64	92	14
4-Aminobenzoic acid	150-13-0	-100	-100	-100	-100	-46	67	10
p-Hydroxybiphenyl	92-69-3	-100	-100	-100	-100	-20	-24	-22
1-(2-Thienyl)-1-propanone	13679-75-9	-100	-100	-100	-100	-69	24	-23
Formamide, N-(2-acetylphenyl)-	-	-100	-100	-100	-100	-53	-4	-28
Etiracetam	33996-58-6	-100	-100	-100	-100	-44	-16	-30
Phenol, 3-chloro-	108-43-0	-100	-100	-100	-100	-50	-51	-50
3-pyridinecarbonitrile, 2-amino-1,6-dihydro-1,4-dimethyl-6-oxo-	-	-100	-100	-100	-100	-76	-44	-60
Chloroxylenol	88-04-0	-94	-98	-96	-96	-77	-48	-62
2,4(1H,3H)-Quinazolinedione	86-96-4	-100	-100	-100	-100	-62	-76	-69
Eucalyptol	470-82-6	-98	-100	-99	-99	-72	-80	-76
2-(2-Hydroxyethoxy)phenol	4792-78-3	-100	-100	-100	-100	-78	-75	-76
S-(+)-5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one	-	-93	-97	-97	-96	-88	-74	-81
Furan, 2-pentyl-	3777-69-3	-91	-97	-98	-95	-82	-88	-85
Butanenitrile, 4-(methylthio)-	59121-24-3	-100	-100	-100	-100	-89	-81	-85
2(5H)-Thiophenone, 5-methyl-	7210-64-2	-100	-100	-100	-100	-87	-86	-87

Note: "Avg." = Average

Table S16. The 113 tentatively identified persistent compounds and potential transformation products. Persistent compounds were defined as compounds that had less than 90% percent peak area decrease from influent to membrane permeate.

Compound Name	CAS No.	AeMBR				AnMBR		
		A (%C)	B (%C)	C (%C)	Avg. (%C)	B (%C)	C (%C)	Avg. (%C)
1H-Benzotriazole	95-14-7	1342	2147	2949	2146	143	154	148
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-2-hydroxy-	19715-19-6	1474	1150	831	1152	-30	-40	-35
3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	20170-32-5	2349	325	567	1080	-2	355	176
2-Pentanamine, N-ethyl-4-methyl-	-	2650	-21	10	880	-50	194	72
Gabapentin	60142-96-3	1871	209	489	857	-48	260	106
2,5-Furandione, 3,4-dimethyl-	766-39-2	1833	564	151	849	-32	16	-8
Tri(2-chloroethyl) phosphate	115-96-8	1296	-3	344	546	-38	233	97
Benzenesulfonamide, 4-methyl-	70-55-3	1208	72	127	469	-45	50	2
Triacetin	102-76-1	44	1140	171	452	435	40	238
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	28564-83-2	455	41	829	442	-50	595	272
Benzoic acid, 4-ethoxy-, ethyl ester	23676-09-7	1195	41	52	429	93	-35	29
Benzenesulfonamide, 2-methyl-	88-19-7	1082	49	120	417	-45	73	14
Succinimide	123-56-8	1111	-9	57	386	-81	-86	-84
Carbamazepine	298-46-4	721	29	373	374	-78	219	71
1H-Indene-4-acetic acid, 6-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-`	-	498	28	523	350	-19	180	81
2,6-Diphenyl-4-methyl-1,4-dihydropyridine-3,5-dicarbonitrile	-	691	179	82	318	-78	-68	-73
Acridine	260-94-6	576	362	11	316	-52	4	-24
Fluconazole	86386-73-4	562	96	153	270	-52	136	42
2,3-Dichlorobenzonitrile	61593-48-4	619	119	71	270	-41	40	0
2-Propenenitrile, 3,3-diphenyl-	3531-24-6	119	4	663	262	-51	77	13
6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline	16489-90-0	700	-5	65	253	-56	348	146
Propanediamide, 2-ethyl-2-phenyl-	7206-76-0	386	167	195	249	-54	17	-19
Phenytoin	57-41-0	609	53	76	246	-66	54	-6
3-Hexene-2,5-dione	4436-75-3	368	202	162	244	69	21	45
2,7(1H,3H)-Naphthalenedione, hexahydro-	-	179	-25	448	201	-71	573	251
Cyclohexanecarboxamide, N-ethyl-5-methyl-2-(1-methylethyl)-	39711-79-0	464	24	98	195	-53	77	12
Adipic acid, 2-decyl isobutyl ester	-	258	259	60	192	-21	-61	-41
2(5H)-Furanone, 4-methyl-3,5,5-tris(2-methyl-2-propenyl)-	-	416	27	98	180	-54	67	6
Pyridine, 2,3,5-trimethyl-	695-98-7	525	-5	21	180	25	255	140
Benzenamine, 3-chloro-N-methyl-	7006-52-2	231	-30	324	175	39	245	142
(1S,4S,9aS)-4-Allyl-1-ethyloctahydro-1H-quinolizine	-	377	40	99	172	147	1130	639
Benzhydryl isothiocyanate	3550-21-8	203	24	282	170	-13	375	181
D-Glucitol, 1,4:3,6-dianhydro-2,5-di-O-methyl-	5306-85-4	-58	30	505	159	43	363	203
3-Phenylpyrazin-2-ol	-	381	10	16	136	-25	313	144
Benzene, 1,2,3-trimethyl-	526-73-8	420	-50	26	132	-12	-46	-29
Benzenesulfonamide, N-ethyl-2-methyl-	1077-56-1	336	-32	82	129	-53	109	28
Primidone	125-33-7	220	121	43	128	-62	-2	-32
2-(Methylmercapto)benzothiazole	615-22-5	374	17	-17	125	-72	140	34
4-(2-(4-Formylphenyl)ethenyl)pyridine	-	318	24	19	120	-83	-75	-79
2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	226	22	105	118	-30	111	40
1,2-Benzenediacetonitrile	613-73-0	235	40	74	116	-43	110	33

Compound Name	CAS No.	AeMBR				AnMBR		
		A (%C)	B (%C)	C (%C)	Avg. (%C)	B (%C)	C (%C)	Avg. (%C)
Benzene, 1-ethyl-4-methyl-	622-96-8	410	-46	-23	114	-3	-67	-35
Benzenemethanol, à,à-dimethyl-	617-94-7	360	-14	-43	101	-4	107	51
3-Penten-1-ol, 2,2,4-trimethyl-	5842-53-5	142	24	136	101	15	45	30
Ethanone, 1-(3,4-dimethylphenyl)-	3637-01-2	203	-7	103	100	-67	-62	-64
Benzene, (trimethoxymethyl)-	707-07-3	165	32	97	98	-34	36	1
2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	235	13	46	98	-73	-22	-47
3-Ethylcyclopentanone	10264-55-8	151	-79	215	96	-75	300	113
Bis(3-chloro-1-propyl)(1-chloro-2-propyl)phosphate	137888-35-8	230	20	25	92	-38	32	-3
Benzene, 4-chloro-1-(2,4-dichlorophenoxy)-2-methoxy-	4640-01-1	220	-15	64	90	-5	-30	-18
Diphenyl sulfone	127-63-9	206	3	32	80	-51	24	-13
4-Amino-6-hydroxypyrimidine	1193-22-2	161	9	33	68	-34	-32	-33
Benzaldehyde, 4-chloro-	104-88-1	211	15	-34	64	-41	-51	-46
Benzamide, N,N-dimethyl-	611-74-5	-9	-54	241	59	-80	-89	-85
2,6-Xylidine	87-62-7	291	-59	-62	57	-74	-57	-66
Benzene, 1,3-dichloro-	541-73-1	122	47	-33	45	26	-70	-22
Benzophenone	119-61-9	159	-33	4	43	-38	88	25
2-Pyrrolidinone	616-45-5	187	-46	-13	42	-77	-85	-81
2-Acetyl-5-methylfuran	1193-79-9	90	101	-70	40	16	-54	-19
Benzothiazole	95-16-9	131	-15	-11	35	-60	-55	-58
Benzoic acid, 2-benzoyl-, methyl ester	606-28-0	105	17	-24	32	-28	-47	-37
1H-Indene, 2,3-dihydro-4-methyl-	824-22-6	18	66	1	28	139	-63	38
Benzene, 1-chloro-3-phenoxy-	6452-49-9	161	-37	-40	28	39	-72	-17
Adipic acid, 3-heptyl isobutyl ester	-	84	-27	25	27	-85	-67	-76
2(3H)-Furanone, 5-acetyldihydro-	29393-32-6	116	-19	-22	25	-86	-88	-87
Benzocycloheptatriene	-	156	-33	-51	24	-35	-52	-43
1-Propanol, 2,3-dichloro-, phosphate (3:1)	78-43-3	119	-33	-16	23	-58	-29	-43
Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	15677-15-3	11	15	43	23	160	-48	56
Ethosuximide	77-67-8	-69	153	-32	18	202	650	426
4-Phenylbut-3-ene-1-yne	-	82	-12	-24	16	-6	-31	-19
Benzonitrile	100-47-0	162	-50	-66	15	-69	-30	-50
Phenanthrene	85-01-8	111	-23	-44	15	-25	-49	-37
6-Methylenebicyclo[3.2.0]hept-3-en-2-one	-	87	-34	-17	12	-49	-13	-31
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	82	-28	-27	9	-46	-48	-47
Triclosan	3380-34-5	122	-51	-50	7	-47	-39	-43
1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	21494-57-5	76	-35	-41	0	-71	-34	-52
Isoquinoline	119-65-3	82	-60	-27	-1	-52	-8	-30
Acetophenone	98-86-2	51	-27	-36	-4	-21	24	1
Pyridine, 4-(diphenylmethyl)-	3678-72-6	116	-76	-74	-12	-48	-83	-65
(S,E)-2,5-Dimethyl-4-vinylhexa-2,5-dien-1-yl acetate	-	52	-38	-51	-12	-1	-50	-26
Undecane, 5,7-dimethyl-	17312-83-3	27	-21	-54	-16	-64	-73	-69
1H-Pyrazole, 4,5-dihydro-5,5-dimethyl-4-isopropylidene-	106251-09-6	45	-45	-53	-17	-46	4	-21
2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one	10396-80-2	3	-69	9	-19	-54	87	17
Thymoquinone	490-91-5	55	-72	-42	-20	-83	15	-34
2,4-Di-tert-butylphenol	96-76-4	-13	-38	-11	-21	-19	105	43
Benzaldehyde	100-52-7	36	-34	-65	-21	-69	-70	-69
1,4-Cyclohexanedione, 2,2,6-trimethyl-	20547-99-3	25	-57	-35	-22	-56	22	-17
Cyclohexanone, 3,3,5-trimethyl-	873-94-9	6	-62	-17	-24	-26	102	38
1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	7779-30-8	12	-50	-46	-28	-85	-51	-68
1,3,7,9-Tetramethyluric acid	2309-49-1	77	-82	-85	-30	-47	7	-20
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	2809-64-5	-44	-34	-20	-32	-38	18	-10
3-tert-Butyl-4-hydroxyanisole	121-00-6	28	-61	-70	-34	-85	-60	-72
2-Methoxy-6-methylaniline	50868-73-0	-4	-50	-56	-37	-58	-15	-37
2-Octyl benzoate	6938-51-8	42	-71	-87	-39	-63	-86	-74

Compound Name	CAS No.	AeMBR				AnMBR		
		A (%C)	B (%C)	C (%C)	Avg. (%C)	B (%C)	C (%C)	Avg. (%C)
Propofol	2078-54-8	27	-70	-83	-42	-28	216	94
1(3H)-Isobenzofuranone	87-41-2	28	-77	-77	-42	-64	-41	-52
1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	20189-42-8	-8	-73	-48	-43	-76	-2	-39
Oxepine, 2,7-dimethyl-	1487-99-6	-12	-51	-70	-44	-83	-84	-84
Benzenepropanenitrile, á-hydroxy-	17190-29-3	-24	-70	-47	-47	-76	-22	-49
Bayer 28,589	728-40-5	-35	-61	-46	-47	-55	-28	-42
Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-	104-66-5	8	-85	-83	-53	-76	-40	-58
Methyl dehydroabietate	1235-74-1	-10	-69	-84	-54	-66	-77	-72
Benzene, (2,2-dimethoxyethyl)-	101-48-4	-15	-78	-75	-56	-43	89	23
Triphenyl phosphate	115-86-6	1	-84	-85	-56	-83	-48	-66
3-Butylisobenzofuran-1(3H)-one	6066-49-5	-14	-78	-82	-58	-73	-50	-61
Butylated Hydroxytoluene	128-37-0	-29	-78	-81	-63	-61	-89	-75
Carbamic acid, (3-chloro-4-hydroxyphenyl)-, 1-methylethyl ester	28705-96-6	-31	-83	-80	-65	-64	81	9
Tricyclo[5.2.1.0(2,6)]dec-3-en-10-one	-	-60	-83	-62	-68	-5	331	163
2-Cyclohexen-1-one, 3-methyl-	1193-18-6	-55	-81	-70	-69	-43	91	24
Norharmane, N-acetyl-	-	-45	-87	-88	-73	-82	-12	-47
1,2-Benzenedicarboxaldehyde	643-79-8	-61	-89	-84	-78	-74	90	8
Amyl cyclopentenone	4819-67-4	-66	-87	-85	-79	-83	-72	-78
Aniline	62-53-3	-84	-90	-70	-81	-9	0	-5

Note: “Avg.” = Average

Table S17. The 30 tentatively identified compounds unique to the aerobic membrane permeate samples.

Compound Name	**CAS No.**
(4aR,7S,7aS)-4,7-Dimethyl-5,6,7,7a-tetrahydrocyclopenta[c] pyran-1(4aH)-one	21651-53-6
1,2,3,4-Tetramethoxybenzene	21450-56-6
1,3-Cyclohexanedione, 2,5,5-trimethyl-	1125-11-7
1,4-Cyclohexanedione*	637-88-7
2,1-Benzisoxazole, 7-ethyl-3-methyl-	108562-69-2
2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol	14035-34-8
2,7:3,6-Dimethano-2H-1-benzopyran, octahydro-	-
2-Benzothiazolamine, 5,6-dimethyl-**	29927-08-0
2-Cyclopenten-1-one, 4-hydroxy-2-methyl-3-phenyl-	-
2H-Benzocyclohepten-2-one, decahydro-4a-methyl-, trans-	-
3,4-Dimethoxybenzylideneacetone	-
3,5-Octadiene, 4,5-diethyl-	-
3-Hexen-2-one, 3,4-dimethyl-	-
4-(4-Chlorophenyl)-2-pyrrolidinone	22518-27-0
4H-1,2,4-Triazol-3-amine, 4-ethyl-	42786-06-1
4-Isopropyl-1-methylcyclohex-2-enol	619-62-5
5,6,7,8-Tetrahydroindolizine	-
5-Acetyl-4-methylthiazole	38205-55-9
5-Isopropyl-3,8-dimethylazulene-1-carbonitrile	93007-54-6
Benzene, 1-azido-3-methoxy-	3866-16-8
cis-1-(4-Isopropylphenyl)-3-(2-furyl)cyclopropane	84922-05-4
Danthron**	117-10-2
Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-	484-18-4
Naphthalene, 2,3-dimethoxy-	10103-06-7
N-Methylmaleimide*	930-88-1
Oxcarbazepine**	28721-07-5
Pyridine, 2-phenyl-*	1008-89-5
S-Methyl methanethiosulphonate*	2949-92-0
Sydnone, 3-(2-methylphenyl)-	3483-18-9
Trioxsalen**	3902-71-4

Table S18. The 18 tentatively identifiable compounds unique to the anaerobic membrane permeate samples.

Compound Name	**CAS ID**
(R)-(+)-Citronellic acid	18951-85-4
2-(2-Oxo-2H-pyridin-1-yl)benzoic acid	-
2,2-Dimethyl-N-phenethylpropionamide	62056-54-6
2-tert-Butylthiazole	13623-12-6
3-Pyridinol, 2-methyl-	1121-25-1
4,8,12,16-tetraoxaeicosan-1-ol	-
4H-1-Benzopyran-4-one, 6-hydroxy-2-methyl-	-
4-Hepten-3-one, 4-methyl-	22319-31-9
5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid	763109-71-3
5,6-Dimethyl-2-benzimidazolinone	2033-30-9
5-Thiazoleethanol, 4-methyl-**	137-00-8
Benzaldehyde, 4-propyl-*	28785-06-0
Carbonic acid, monoamide, N-butyl-, allyl ester	-
Ethanone, 1-(3-pyridinyl)-	-
L-Cysteine, S-(diphenylmethyl)-	5191-80-0
Pyridine, 3-ethyl-*	536-78-7
Quinoline, 1,2,3,4-tetrahydro-2-methyl-	-

Table S19. Compounds confirmed with analytical standards and a comparison of their treatment efficiencies in Mladenov et al. (2021)[3] to the AeMBR and AnMBR.

Alternate name	CAS No.	% Change US-C	% Change SA-D	% Change SA-C	Avg. % Change AeMBR	Avg. % Change AnMBR
4-(4-Hydroxy-3-methoxyphenyl)-2-butanone	122-48-5	-100 %	-100 %	-100 %	-100 ± 0 %	-100 ± 0 %
4-Ethyl-2-methoxyphenol	2785-89-9	-100 %	-100 %	-100 %	-100 ± 0 %	-100 ± 0 %
Piperine	94-62-2	-100 %	-100 %	-100 %	-100 ± 0 %	-100 ± 0 %
Scopoletin	92-61-5	-100 %	-100 %	-100 %	-100 ± 0 %	-100 ± 0 %
Benzyl cyanide	140-29-4	-94 %	-98 %	-96 %	-97 ± 0 %	-95 ± 2%
2,4-Dihydroxy benzophenone	131-56-6	-100 %	-100 %	-100 %	-100 ± 0 %	-89 ± 7 %
5-(Methylsulfanyl) pentanenitrile	59121-25-4	-100 %	-100 %	-100 %	-100 ± 0 %	-87 ± 3 %
1,7-Dimethylxanthine	611-59-6	-100 %	-100 %	-100 %	-100 ± 0 %	-77 ± 19 %
Benzoic acid, 3-(1-methylethyl)-	5651-47-8	-100 %	-100 %	-100 %	-100 ± 0 %	-67 ± 1 %
Nicotine	23950-04-1	-100 %	-100 %	-100 %	-99 ± 1 %	-68 ± 20 %
Benzenemethanethiol	100-53-8	-100 %	-100 %	-100 %	-93 ± 7 %	-83 ± 6 %
beta-Terpineol	138-87-4	-99 %	-100 %	29 %	-99 ± 0 %	-94 ± 2 %
Bisphenol A	80-05-7	-57 %	-87 %	-100 %	-91 ± 8 %	-13 ± 41 %
2-Methoxy-4-vinylphenol	7786-61-0	-66 %	-98 %	-81 %	-60 ± 22 %	-95 ± 2 %
Triclosan	3380-34-5	-89 %	-89 %	-93 %	7 ± 81 %	-43 ± 4 %

Note: "SA-C" = South Africa – Centralized Wastewater Treatment Plant; "SA-D" = South Africa – Decentralized Wastewater Treatment Plant; "US-C" = United States Centralized Wastewater Treatment Plant

Table S20. The 15 physicochemical properties assessed by principal component analysis.

Molecular Weight
Density [a] (g/cm^3)
Surface Tension [a] (dyn/cm)
Viscosity [a] (cP)
Atmospheric Hydroxylation Rate [b] (cm^3/ molecule*sec)
Bioconcentration Factor [b]
Biodegradation Half-Life (day)[b]
Boiling Point [b] (ºC)
Henry's Law Constant [b] (atm-m^3/mol)
Fish Biotransformation Half-Life [b] (K_M/day)
Octanol Air Partition Coefficient [b] (Log K_{OA})
Soil Adsorption Coefficient [b], K_{OC} (L/kg)
Octanol Water Partition Coefficient [b] (Log P)
Melting Point [b] (ºC)
Vapor Pressure [b] (mmHg)
Water Solubility [b] (mol/L)

Note: a. TEST prediction; TEST = Toxicity Estimation Software Tool; b. OPERA prediction; OPERA = Open Structure-activity/property Relationship App

Table S21. Twelve molecular descriptors assessed by principal component analysis.

Fraction of Rotatable Bonds
Number of Atoms
Number of Bonds
Molar Refractivity
Polar Surface Area
Geometrical Diameter
Geometrical Radius
Geometrical Shape Coefficient
Kier Shape 1
Kier Shape 2
Zagreb Group Index 1
Zagreb Group Index 2

Note: Retrieved from JoeLib, ChemMine Tools

Table S22. Database of all 102 tentatively identified compounds containing at least one nitrogen atom which were common among all the influents (from treatment cycle I, II, and III).

Compound Name	Log(P)	No. of N Atoms	AeMBR			AnMBR	
			I (%C)	II (%C)	III (%C)	II (%C)	III (%C)
*Indolizine	2.49	1	-100	-100	-100	-100	-100
*Benzothiazole, 6-methoxy-2-methyl-	2.25	1	-100	-100	-100	-100	-100
*Indole-2,3-dione, 1-(hydroxymethyl)-	0.87	1	-100	-100	-100	-100	-100
*1H-Indole-3-propanoic acid	1.75	1	-100	-100	-100	-100	-100
*2,5-Piperazinedione, 3-(phenylmethyl)-	1.61	2	-100	-100	-100	-100	-100
*Lumichrome	1.93	4	-100	-100	-100	-100	-100
*5-Ethoxy-2-methyl-pyridine	1.64	1	-100	-100	-100	-100	-100
*1,7-Dimethylxanthine	-0.22	4	-100	-100	-100	-99	-98
*2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	0.87	2	-100	-100	-100	-92	-78
*Butanenitrile, 4-(methylthio)-	0.32	1	-100	-100	-100	-89	-81
*6-Methyl-2-pyridinecarbaldehyde	0.61	1	-100	-100	-100	-77	-94
*3-pyridinecarbonitrile, 2-amino-1,6-dihydro-1,4-dimethyl-6-oxo-	-	3	-100	-100	-100	-76	-44
Thiazolidine, 2-ethyl-	1.43	1	-100	-100	-100	-64	91
*2,4(1H,3H)-Quinazolinedione	0.77	2	-100	-100	-100	-62	-76
Formamide, N-(2-acetylphenyl)-	-	1	-100	-100	-100	-53	-4
4-Aminobenzoic acid	0.82	1	-100	-100	-100	-47	68
Quinoline, 5-methyl-	2.38	1	-100	-100	-100	-46	76
Etiracetam	-0.82	2	-100	-100	-100	-44	-16
1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-	3.23	2	-100	-100	-100	86	1
*Theobromine	-0.77	4	-100	-99	-99	-88	-96
*2H-Indol-2-one, 1,3-dihydro-	1.16	1	-100	-97	-98	-61	-94
*Caffeine	-0.07	4	-100	-100	-100	-98	-89
*2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-	0.05	4	-99	-100	-100	-97	-97
*1H-Indole, 2-methyl-	2.53	1	-99	-99	-99	-99	-97
*5H-1-Pyrindine	1.65	1	-98	-100	-100	-99	-99
*3-Methoxyparacetamol	0.97	1	-97	-96	-100	-94	-95
*Benzene, 1-isocyano-2-methyl-	1.95	1	-96	-97	-97	-97	-93
1H-Indole-2,3-dione	0.83	1	-91	-43	-97	-29	-95
*Theophylline	-0.02	4	-87	-93	-90	-92	-76
*Acetamide, N-[4-hydroxy-3-(methylthio)phenyl]-	1.62	1	-84	-97	-97	-97	-88
Aniline	0.90	1	-84	-90	-70	-9	0
*Indole-5-aldehyde	1.82	1	-83	-83	-97	-96	-92
*Acetophenone, 4'-amino-	0.83	1	-75	-90	-88	-88	-82
Ethosuximide	0.38	1	-69	153	-32	203	650
Norharmane, N-acetyl-	-	2	-45	-87	-88	-82	-12
Bayer 28,589	4.20	1	-35	-61	-46	-55	-28
Carbamic acid, (3-chloro-4-hydroxyphenyl)-, 1-methylethyl ester	1.98	1	-31	-83	-80	-64	81
Benzenepropanenitrile, á-hydroxy-	1.43	1	-24	-70	-47	-76	-22
Pyrazine, trimethyl-	0.95	2	-10	-88	-100	-22	166
Benzamide, N,N-dimethyl-	0.62	1	-9	-54	241	-80	-89
1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	0.23	1	-8	-73	-48	-76	-2
2-Methoxy-6-methylaniline	1.40	1	-4	-50	-56	-58	-15
1H-Pyrazole, 4,5-dihydro-5,5-dimethyl-4-isopropylidene-	2.01	2	46	-45	-53	-46	4
1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	0.86	1	76	-35	-41	-71	-34
1,3,7,9-Tetramethyluric acid	-0.08	4	77	-82	-85	-47	7
Isoquinoline	2.08	1	83	-60	-27	-52	-8
Pyridine, 4-(diphenylmethyl)-	4.77	1	117	-76	-74	-48	-83
2-Propenenitrile, 3,3-diphenyl-	3.22	1	119	4	663	-51	77
Benzothiazole	2.01	1	131	-15	-11	-60	-55
4-Amino-6-hydroxypyrimidine	-0.87	3	161	9	33	-34	-32

Compound Name	Log(P)	No. of N Atoms	AeMBR			AnMBR	
			I (%C)	II (%C)	III (%C)	II (%C)	III (%C)
Benzonitrile	1.56	1	162	-50	-66	-69	-30
2-Pyrrolidinone	-0.85	1	187	-46	-13	-77	-85
Benzhydryl isothiocyanate	5.09	1	203	24	282	-13	374
Primidone	0.91	2	220	121	43	-62	-2
Benzenamine, 3-chloro-N-methyl-	2.11	1	231	-30	323	39	244
1,2-Benzenediacetonitrile	1.94	2	235	40	74	-43	110
2,6-Xylidine	1.84	1	291	-59	-61	-74	-57
4-(2-(4-Formylphenyl)ethenyl)pyridine	-	1	318	24	19	-83	-75
Benzenesulfonamide, N-ethyl-2-methyl-	1.62	1	336	-32	82	-53	109
2-(Methylmercapto)benzothiazole	3.15	1	374	17	-17	-72	140
(1S,4S,9aS)-4-Allyl-1-ethyloctahydro-1H-quinolizine	-	1	378	40	99	148	1127
3-Phenylpyrazin-2-ol	-	2	380	10	16	-25	313
Propanediamide, 2-ethyl-2-phenyl-	0.13	2	386	167	195	-53	17
Cyclohexanecarboxamide, N-ethyl-5-methyl-2-(1-methylethyl)-	3.89	1	464	24	98	-53	77
Pyridine, 2,3,5-trimethyl-	1.35	1	526	-5	21	25	255
Fluconazole	0.50	6	562	96	153	-52	136
Acridine	3.40	1	576	362	11	-52	4
Phenytoin	2.36	2	609	53	76	-66	53
2,3-Dichlorobenzonitrile	2.93	1	618	118	71	-41	40
2,6-Diphenyl-4-methyl-1,4-dihydropyridine-3,5-dicarbonitrile	-	3	690	179	82	-78	-68
6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline	3.95	1	701	-5	65	-56	347
Carbamazepine	2.45	2	721	29	373	-78	219
Benzenesulfonamide, 2-methyl-	0.84	1	1082	50	121	-45	73
Succinimide	-0.67	1	1107	-9	57	-81	-87
Benzenesulfonamide, 4-methyl-	0.82	1	1204	72	127	-45	50
1H-Benzotriazole	1.44	3	1342	2157	2947	144	154
Gabapentin	-1.10	1	1870	209	489	-49	260
2-Pentanamine, N-ethyl-4-methyl-	-	1	2649	-21	10	-50	194
5-Isopropyl-3,8-dimethylazulene-1-carbonitrile	3.88	1	New	New	New	n.d.	n.d.
Pyridine, 2-phenyl-	2.63	1	New	New	New	n.d.	n.d.
2-Benzothiazolamine, 5,6-dimethyl-	2.17	2	New	New	New	n.d.	n.d.
Sydnone, 3-(2-methylphenyl)-	1.49	2	New	New	New	n.d.	n.d.
4H-1,2,4-Triazol-3-amine, 4-ethyl-	0.03	4	New	New	New	n.d.	n.d.
2,1-Benzisoxazole, 7-ethyl-3-methyl-	2.79	1	New	New	New	n.d.	n.d.
N-Methylmaleimide	-0.58	1	New	New	New	n.d.	n.d.
5,6,7,8-Tetrahydroindolizine	NA	1	New	New	New	n.d.	n.d.
Oxcarbazepine	2.17	2	New	New	New	n.d.	n.d.
4-(4-Chlorophenyl)-2-pyrrolidinone	2.25	1	New	New	New	n.d.	n.d.
5-Acetyl-4-methylthiazole	1.15	1	New	New	New	n.d.	n.d.
Benzene, 1-azido-3-methoxy-	1.63	3	New	New	New	n.d.	n.d.
Pyridine, 3-ethyl-	1.66	1	n.d.	n.d.	n.d.	New	New
Ethanone, 1-(3-pyridinyl)-	NA	1	n.d.	n.d.	n.d.	New	New
3-Pyridinol, 2-methyl-	0.03	1	n.d.	n.d.	n.d.	New	New
2-tert-Butylthiazole	3.1	1	n.d.	n.d.	n.d.	New	New
5-Thiazoleethanol, 4-methyl-	1.06	1	n.d.	n.d.	n.d.	New	New
Quinoline, 1,2,3,4-tetrahydro-2-methyl-	NA	1	n.d.	n.d.	n.d.	New	New
5,6-Dimethyl-2-benzimidazolinone	0.71	2	n.d.	n.d.	n.d.	New	New
Carbonic acid, monoamide, N-butyl-, allyl ester	NA	1	n.d.	n.d.	n.d.	New	New
2,2-Dimethyl-N-phenethylpropionamide	1.13	1	n.d.	n.d.	n.d.	New	New
5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid	2.13	1	n.d.	n.d.	n.d.	New	New
2-(2-Oxo-2H-pyridin-1-yl)benzoic acid	NA	1	n.d.	n.d.	n.d.	New	New
L-Cysteine, S-(diphenylmethyl)-	2.46	1	n.d.	n.d.	n.d.	New	New

Note: "*" – The compound was one of the 25 nitrogen-containing compounds meeting selection criteria described in text. "NA" – A Log P value was not available in the U.S. EPA Comptox Dashboard.; "New" – The compound was not detected in the influents but was detected in the permeate.; "n.d." – The compound was not detected.

Table S23. Database of the 30 tentatively identified compounds containing at least one sulfur atom which were common among all the influents (from treatment cycle I, II, and III).

Compound Name	Log(P)	No. of S Atoms	AeMBR			AnMBR	
			I (%C)	II (%C)	III (%C)	II (%C)	III (%C)
*Thiophene, 2-formyl-2,3-dihydro-	1.49	1	-100	-100	-100	-100	-100
*Benzothiazole, 6-methoxy-2-methyl-	2.25	1	-100	-100	-100	-100	-100
*4-Methyl-1,2,3-trithiolane	NA	3	-100	-100	-100	-100	-100
*Cyclic octaatomic sulfur	NA	8	-100	-100	-100	-96	-99
Hexathiepane	2.58	6	-100	-100	-100	-94	-48
*5-Methyl-1,2,3,4-tetrathiane	3.33	4	-100	-100	-100	-93	-93
*3H-1,2-Benzodithiol-3-one	2.73	2	-100	-100	-100	-91	-95
*Butanenitrile, 4-(methylthio)-	0.32	1	-100	-100	-100	-89	-81
*2(5H)-Thiophenone, 5-methyl-	-0.06	1	-100	-100	-100	-87	-86
1-(2-Thienyl)-1-propanone	2.13	1	-100	-100	-100	-69	24
Thiazolidine, 2-ethyl-	1.43	1	-100	-100	-100	-64	91
*Tetrasulfide, dimethyl	3.34	4	-100	-100	-100	-98	-95
*Dimethyl trisulfide	2.75	3	-98	-99	-98	-98	-98
*Acetamide, N-[4-hydroxy-3-(methylthio)phenyl]-	1.62	1	-84	-97	-97	-97	-88
*Benzenemethanethiol	2.45	1	-83	-98	-99	-77	-89
*2-Acetyl-5-methylthiophene	2.09	1	-61	-85	-90	-71	-57
Benzothiazole	2.01	1	131	-15	-11	-60	-55
Benzhydryl isothiocyanate	5.09	1	203	24	282	-13	374
Diphenyl sulfone	2.40	1	206	3	32	-51	24
Benzenesulfonamide, N-ethyl-2-methyl-	1.62	1	336	-32	82	-53	109
2-(Methylmercapto)benzothiazole	3.15	2	374	17	-17	-72	140
Benzenesulfonamide, 2-methyl-	0.84	1	1082	50	121	-45	73
Benzenesulfonamide, 4-methyl-	0.82	1	1204	72	127	-45	50
2-Benzothiazolamine, 5,6-dimethyl-	2.17	1	New	New	New	n.d.	n.d.
S-Methyl methanethiosulphonate	1.6	2	New	New	New	n.d.	n.d.
5-Acetyl-4-methylthiazole	1.15	1	New	New	New	n.d.	n.d.
2-tert-Butylthiazole	3.1	1	n.d.	n.d.	n.d.	New	New
5-Thiazoleethanol, 4-methyl-	1.06	1	n.d.	n.d.	n.d.	New	New
5-(Thiophen-2-yl)-1,2-oxazole-3-carboxylic acid	2.13	1	n.d.	n.d.	n.d.	New	New
L-Cysteine, S-(diphenylmethyl)-	2.46	1	n.d.	n.d.	n.d.	New	New

Note: "*" – The compound was one of the 13 sulfur-containing compounds meeting selection criteria described in text. "NA" – A Log P value was not available in the U.S. EPA Comptox Dashboard.; "New" – The compound was not detected in the influents but was detected in the permeate.; "n.d." – The compound was not detected.

Table S24. Index of the EPA Comptox databases used to define each product use category.

Product Use Category	Title of EPA Comptox List
Metabolite/Transformation Product	MTox700; NISTSRM1950; WETMORE2015; HSDBTPS; MSMLS; SOLNSLMCTPS; METABWKBEN; METXBIODB
Odorant/Aroma Compound	VOLATILOME; FLAVORNET; POLYPHENOLS; PHENOLEXP; FOODVOLATILES
Plastic Related	BISPHENOLS; ECHAPLASTICS; FOODPLASTICS; CPPDBLISTA; CSSEXTRACTS; CECTOYS; CPPDBLISTB; PLASTICMAP
Consumer Product	EPACONS
Food Contact Substance	FDACEDI; FOODCONTACTSDB; FOODPLASTICS
Cosmetic Ingredient	HAIRDYES; TATTOOINK; COSMOSDB; EUCOSMETICS
Pharmaceutical/Drug	FDAMDD; ANTIBIOTICS; ITNANTIBIOTIC; FDAORANGE; GREEKPHARMA; LUXPHARM; ANTUPHTW; PSYCHOCANNAB; TRANSPORTAL; UOATARGPHARMA; VETDRUGPCDL; VETDRUGS; WIKINSAIDSHIGHRESNPS; SWISSPHARMA; DRUGBANKSWG; DRUGV2
Inert Ingredient	PESTINERTS; INERTNONFOOD
Food Additive	WIKIFLAVORS; FDAFOODSUBS
Phermones/Semiochemicals	PHEROBASE
Toxin	MYCOTOX2; NATOXAQ; HUMANBLOOD; PHYTOTOXINS; T3DB
Solvent	WIKISOLVENTS; PARISIII
Pesticide/Biocide/Insect Repellant/Antifungal	EDSP21LIST1; EUBIOCIDES; LUXPEST; PESTHHBS; SWISSPEST; WIKIANTIFUNGALS; WIKIINSECTICIDES; EPABIOPESTICIDES; PPDB; SWISSPEST19; EPAOPPIN; EPAPCS; NPINSECT
Oil Related (hydraulic fracturing, oil field additive, motor fuel ingredient)	CALWATERBDS; MOTORFUELS; EPAHFRTABLE2; EPAHFR; PRODWATER
Tobacco/Cigarette/Vaping Related	VAPETERPENES; VATERPENES; SLTChemDB; THSMOKE; UNCTCORS; CIGARETTES
Extractable or Leachable from Pharmaceutical Product	ELSIE
Other	NISTSRM2585; PEROXIDESB; CIDYES; STORAGETANKS; PAHLIST; PEROXIDESD; SWISSLIPIDS2022; LIPIDMAPSv2
Disinfection Byproduct	DBP; CHLORINETPS
Detected in Recycled Tire Crumb	TIRECRUMB
Water Distribution Leachable Substance	EXTRACTPIPES
Flame Retardant	FLAMERETARD; FRFULLLIST; FRLIKELY; OFRLIKELY
Antimicrobial	ANITMICROB2; ANTIMICROBIALS; WIKIANTISEPTICS
Antioxidant	PHENANTIOX; WIKIANTIOXIDANTS
Surfactant	ALLSURFACTANTS; EIUBASURF
Industrial Chemical or Manufacturing Waste	HUMANNEUROTOX

Table S25. Sixty-five tentatively identifiable compounds identified in the United States (US) Environmental Protection Agency (EPA) High Production Volume List

CAS No.	Compound Name
95-14-7	1,2,3-Benzotriazole
622-96-8	4-Ethyltoluene
100-52-7	Benzaldehyde
108-95-2	Phenol
62-53-3	Aniline
100-47-0	Benzonitrile
541-73-1	1,3-Dichlorobenzene
872-50-4	N-Methyl-2-pyrrolidone
98-86-2	Acetophenone
616-45-5	2-Pyrrolidinone
100-53-8	Benzenemethanethiol
90-05-1	2-Methoxyphenol
526-75-0	2,3-Dimethylphenol
104-88-1	4-Chlorobenzaldehyde
87-62-7	2,6-Dimethylaniline
95-16-9	Benzothiazole
102-76-1	Triacetin
334-48-5	Decanoic acid
80-46-6	4-(2-Methylbutan-2-yl)phenol
128-37-0	Butylated hydroxytoluene
135-19-3	2-Naphthalenol
90-43-7	2-Phenylphenol
84-66-2	Diethyl phthalate
119-61-9	Benzophenone
88-19-7	o-Toluenesulfonamide
70-55-3	4-Toluenesulfonamide
115-96-8	Tris(2-chloroethyl) phosphate
120-51-4	Benzyl benzoate
13674-84-5	Tris(2-chloroisopropyl)phosphate
104-66-5	1,2-Diphenoxyethane
1222-05-5	1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethylcyclopenta[g]-2-benzopyran
21145-77-7	Tonalide
6386-38-5	Methyl 3,5-bis(tert-butyl)-4-hydroxyhydrocinnamate
131-57-7	2-Hydroxy-4-methoxybenzophenone
3380-34-5	Triclosan
103-23-1	Bis(2-ethylhexyl)hexanedioate
78-51-3	Tris(2-butoxyethyl) phosphate
298-46-4	Carbamazepine
115-86-6	Triphenyl phosphate

CAS No.	Compound Name
57-41-0	5,5-Diphenylhydantoin
94-28-0	Triethylene glycol bis(2-ethylhexanoate)
1948-33-0	tert-Butylhydroquinone
118-79-6	2,4,6-Tribromophenol
83-67-0	Theobromine
100-44-7	Benzyl chloride
88-06-2	2,4,6-Trichlorophenol
96-76-4	2,4-Di-tert-butylphenol
122-40-7	alpha-Amyl cinnamaldehyde
80-05-7	Bisphenol A
110-93-0	6-Methyl-5-hepten-2-one
873-94-9	3,3,5-Trimethylcyclohexanone
78-70-6	Linalool
121-33-5	4-Hydroxy-3-methoxybenzaldehyde
58-08-2	Caffeine
58-55-9	Theophylline
101-84-8	Diphenyl oxide
131-11-3	Dimethyl phthalate
50-78-2	Aspirin
5466-77-3	Octinoxate
106-44-5	p-Cresol
101-86-0	2-(Phenylmethylene)octanal
98-82-8	Cumene
122-99-6	2-Phenoxyethanol
101-72-4	N-Isopropyl-N'-phenyl-p-phenylenediamine
108-46-3	Resorcinol

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