

Electronic Supplementary Information

Evaluation of reverse osmosis drinking water treatment of riverbank filtrate by bioanalytical tools and non-target screening

Vittorio Albergamo ^a, Beate I. Escher ^{b,c}, Emma L. Schymanski ^d, Rick Helmus ^a, Milou M.L. Dingemans ^e, Emile R. Cornelissen ^{e,f}, Michiel H. S. Kraak ^a, Juliane Hollender ^{g,h}, Pim de Voogt ^{a,e}

^a Institute for Biodiversity and Ecosystem Dynamics (IBED), University of Amsterdam, 1098 XH Amsterdam, The Netherlands

^b UFZ – Helmholtz Centre for Environmental Research, Department Cell Toxicology, 04318 15 Leipzig, Germany

^c Eberhard Karls University Tübingen, Environmental Toxicology, Center for Applied Geosciences, 2074 Tübingen, Germany

^d Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg, L-4367 Belvaux, Luxembourg

^e KWR Watercycle Research Institute, 3430 BB Nieuwegein, The Netherlands

^f Particle and Interfacial Technology Group, Ghent University, B-9000 Ghent, Belgium

^g Eawag, Swiss Federal Institute of Aquatic Science and Technology, CH-8600 Dübendorf, Switzerland

^h Institute of Biogeochemistry and Pollutant Dynamics, ETH Zürich, 8092 Zürich, Switzerland

S-1. Solid-phase extraction protocols

To comply with pre-established procedures and avoid problems with the biological and chemical analysis, three different solid-phase extraction (SPE) protocols were used, all relying on hydrophilic-lipophilic balance (HLB) sorbent material. The enrichment protocols differed by the sample load and composition of elution solvent as detailed in this section. The same broad range of organic compounds is expected to be covered by the three procedures as (i) there were no differences in the pH of water samples and wash solvents and (ii) organic eluents of comparable polarity were used in all cases.

S-1.1 SPE in preparation for reporter gene assays

For the reporter gene assays, aliquots of 2 L RO feed water (n=2), 1L RO concentrate(n=2) and 2 L RO permeate (n=4) were enriched. Four replicates of 2 L procedural blanks consisting of ultrapure water were extracted to match the number of replicates of the RO permeate. Oasis HLB (500 mg) from Waters were mounted on a vacuum manifold and conditioned with 10 mL ethyl acetate, 10 mL methanol and 10 mL ultrapure water acidified to pH 2-3 with HCl. All samples were acidified to pH 2-3 with HCl, filtered through a Whatman glass microfibre filters (pore size 1.6 µm) and loaded onto the cartridges with the aid of a vacuum. The cartridges were dried by vacuum and eluted with 10 mL methanol and 10 mL ethyl acetate. The eluates were combined, reduced to dryness by a gentle nitrogen flow and reconstituted with methanol to achieve an enrichment factor of 1000x.

S-1.2 SPE in preparation for Ames

For the Ames tests, 2 L of RO feed water, 2 L of RO permeate and 2 L ultrapure water acidified to pH 2-3 by addition of HCl were extracted in duplicate with Oasis HLB cartridges (500 mg) by Waters. An air cleaning system relying on a Sep-Pak C18 SPE cartridge (500 mg) by Waters was used to prevent contamination of the samples. Both extraction and air cleaning SPE columns were conditioned with two times 6 mL of a mixture of acetonitrile:methanol 20:80 (v/v), one time 6 mL of pure methanol and two times acidified ultrapure water. The samples were loaded onto the extraction cartridges with the aid of a vacuum, the cartridges washed with two times 6 mL of acidified ultrapure water and eluted six times with 2.5 mL of acetonitrile:methanol 20:80 (v/v). The eluates were evaporated to almost dryness under a gentle nitrogen flow and reconstituted with 200 µL DMSO, resulting in a final concentration factor of 10000x.

S-1.3 SPE LC-HRMS analysis

Enrichment of the samples for LC-HRMS analysis relied on Oasis HLB cartridges (150 mg) by Waters. Aliquots of 100 mL RO feed water, RO permeate, RO concentrate and ultrapure water (n=3) acidified to pH 2-3 with HCl. The cartridges were placed on a vacuum manifold and conditioned with 5 mL methanol and 5 mL acidified ultrapure water. The samples were loaded with the aid of a vacuum, the cartridges washed with 2 mL of ultrapure water and dried for 15 min. Elution was achieved with 4 times 2.5 mL of MeOH. The eluates were filtered with 0.22 µm PP filters (Filter-Bio, Jiangsu, China) and collected in 15 mL PP falcon tubes before evaporation to 0.2 mL under a gentle nitrogen flow. Prior to UHPLC-q-ToF/MS analysis the concentrated extracts were diluted 5-fold in ultrapure water to be more compatible with the aqueous mobile phase used for chromatographic separation.

S-2. LC-HRMS analysis

Chemical analyses were conducted with an ultrahigh-performance LC system (Nexera Shimadzu, Den Bosch, The Netherlands) coupled to a maXis 4G high resolution quadrupole time-of-flight HRMS (q-ToF/HRMS) upgraded with HD collision cell and equipped with a ESI source (Bruker Daltonics, Wormer, The Netherlands). The chromatographic stationary phase was a polar reversed-phase core-shell Kinetex biphenyl LC column having 1.7 μm particle size, pore size of 100 \AA and dimensions of 150 \times 2.1 mm (Phenomenex, Utrecht, The Netherlands). The mobile phase consisted of (A) pure H_2O and (B) MeOH acidified with 0.05% acetic acid (B). The LC gradient program expressed as B% was 0% from 0 to 2 min, 100% B at 17 min and 100% from 17 to 25 min. The flow rate was 0.3 mL/min. The sample injection volume was 20 μL . The MS detector equipped with an electrospray ionisation source (ESI) was internally calibrated before starting an analysis batch and additionally prior to any injection by infusing a 50 μM sodium acetate solution in $\text{H}_2\text{O}:\text{MeOH}$ (1:1, v/v) with a loop injection of 20 μL and a loop rinse of 20 μL . Positive and negative ESI were achieved in separate runs by acquiring HRMS1 spectra for masses ranging from m/z 50 to 1,000 with a resolving power of 30,000–60,000 at full width at half maximum (FWHM) and with a spray voltage of +3.5 kV and -3.5 kV for positive and negative ESI modes, respectively. The capillary temperature was 300 $^\circ\text{C}$. HRMS2 spectra were recorded in data-dependent acquisition mode with a resolving power of at least 20,000 FWHM.

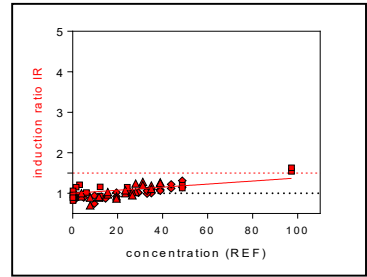
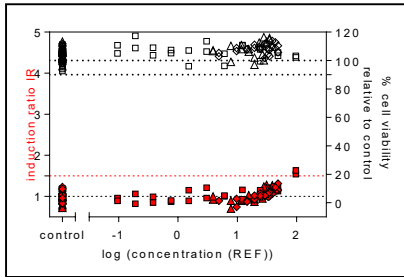
S-3. Concentration-effect curves

On the left, full concentration–response curves for cell viability (empty symbols) and induction (filled symbols). On the right, linear range of the concentration–effect curve at low effect levels from which the $EC_{IR1.5}$ for the AREc32 assay and EC_{10} for the AhR assay were derived (IR 1.5 and 10% effect indicated as dotted lines). Different symbols refer to independent experiments performed on different days.

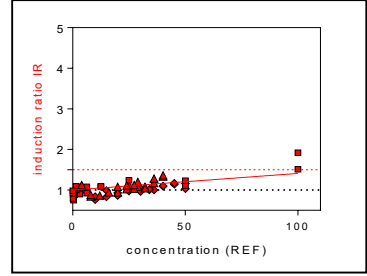
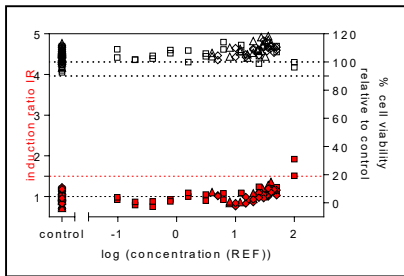
S-3.1. AREc32 assay

SPE Blanks

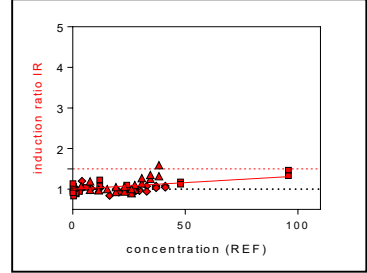
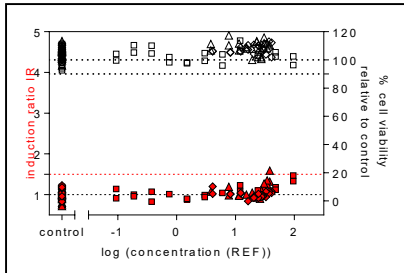
SPE blank 1



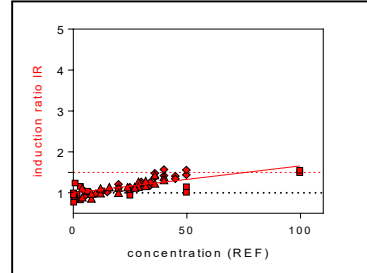
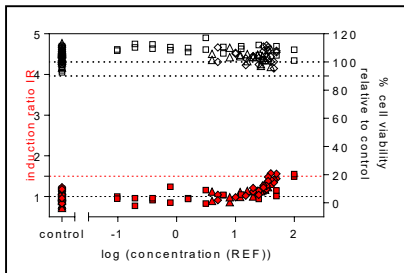
SPE blank 2



SPE blank 3

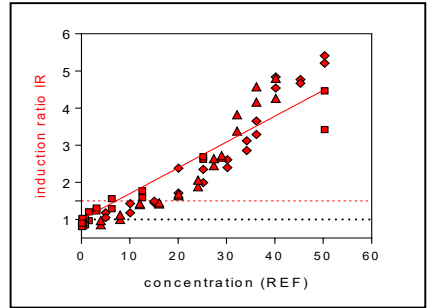
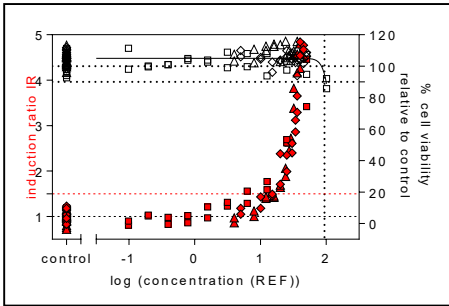


SPE blank 4

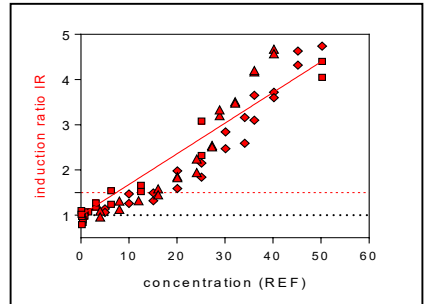
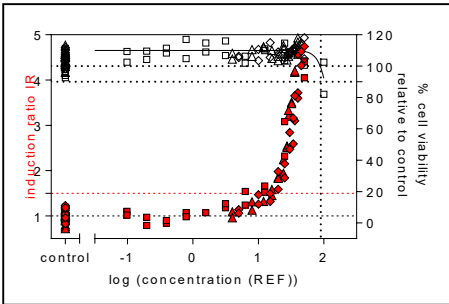


RO feed water

ROF 1

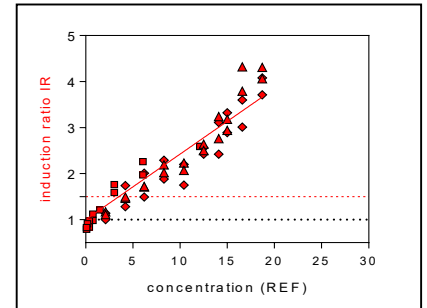
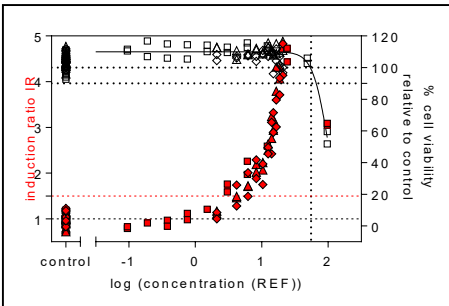


ROF 2

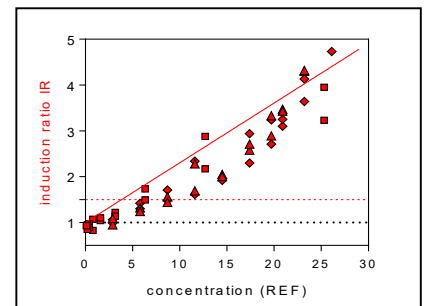
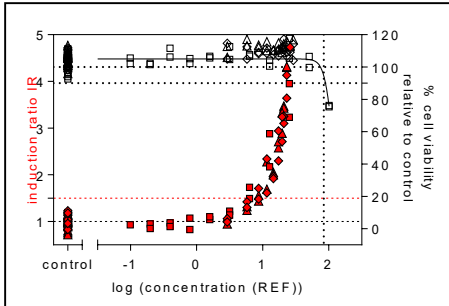


RO concentrate

ROC 1



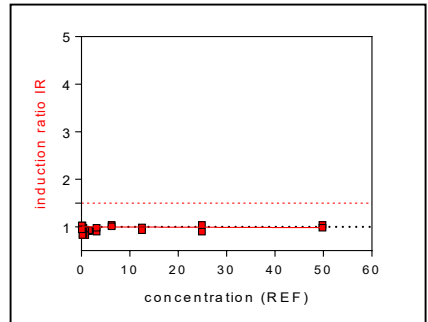
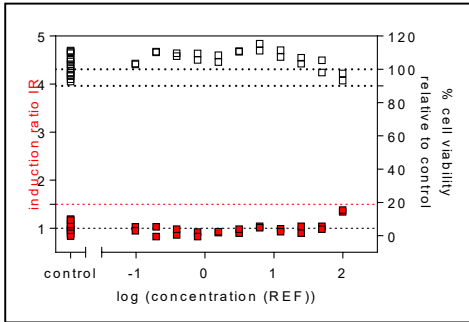
ROC 2



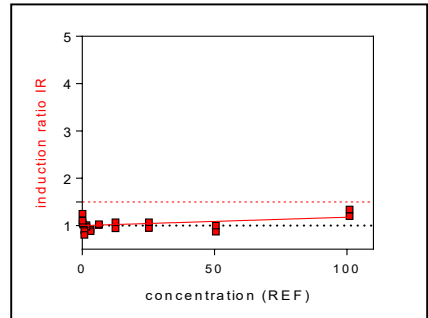
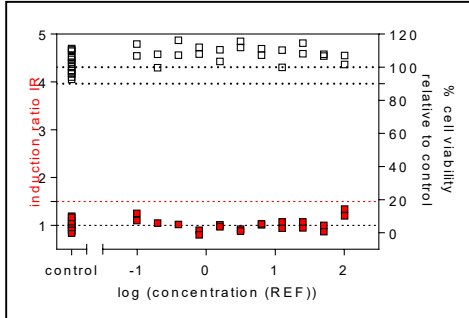
RO permeate

Note: since no activity was detected, the experiments were not repeated.

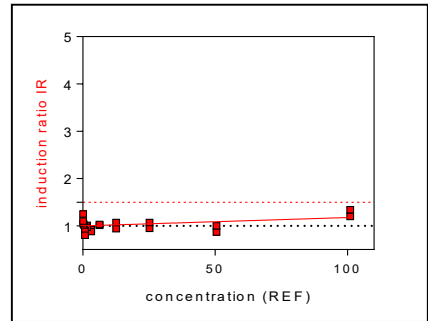
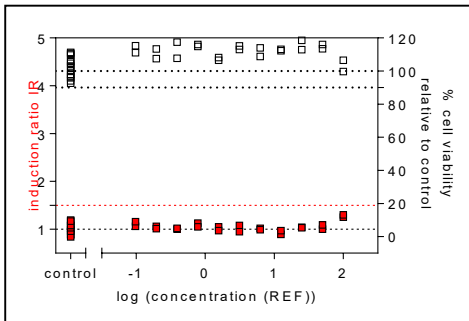
ROP 1



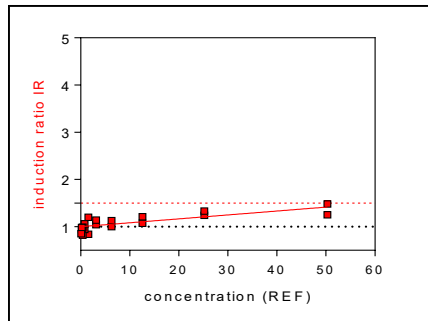
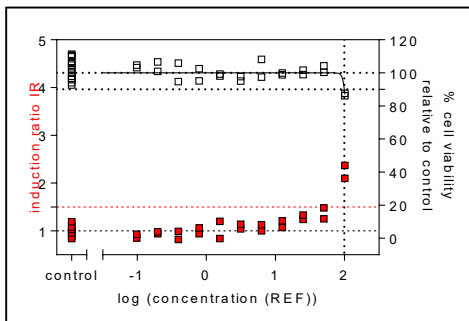
ROP 2



ROP 3



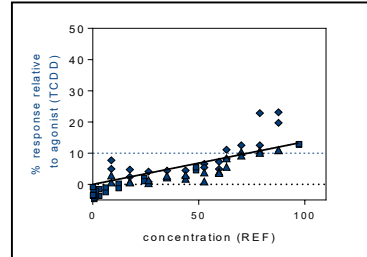
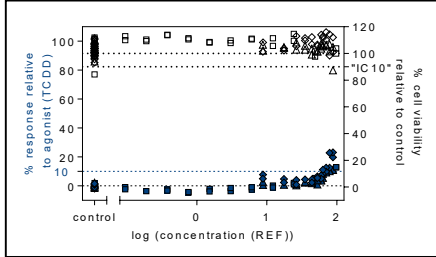
ROP 4



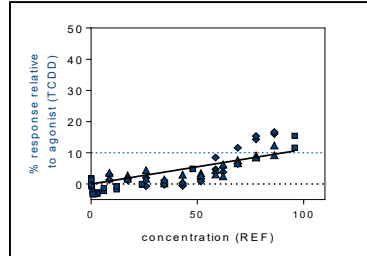
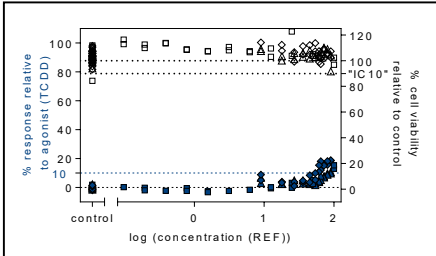
S-3.2. AhR assay

SPE Blanks

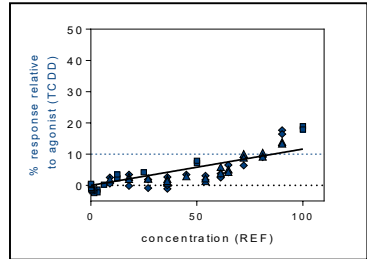
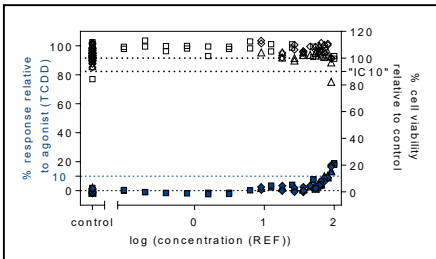
SPE blank 1



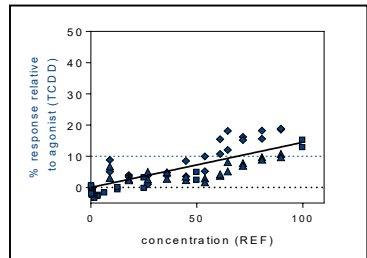
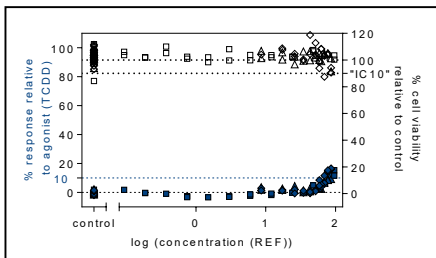
SPE blank 2



SPE blank 3

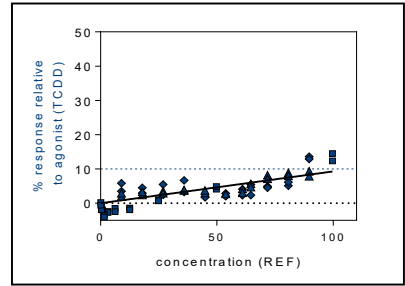
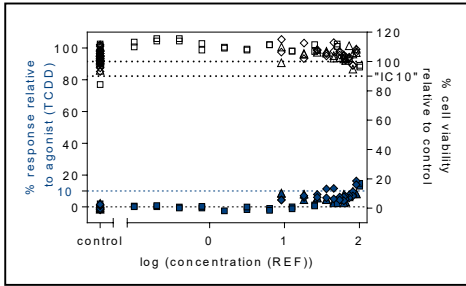


SPE blank 4

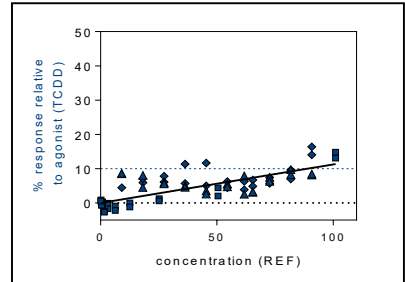
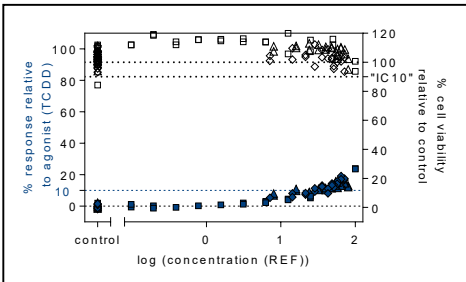


RO permeate

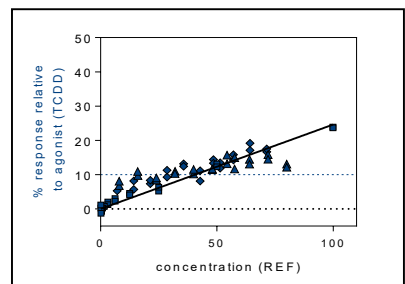
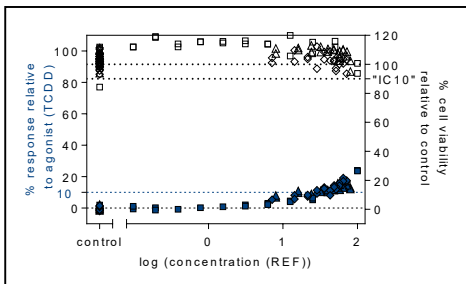
ROP 1



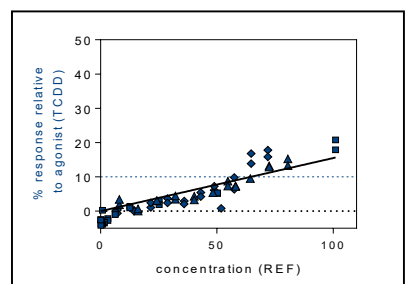
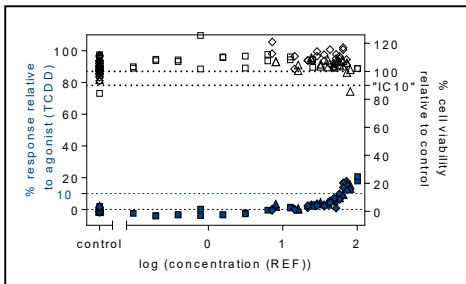
ROP 2



ROP 3

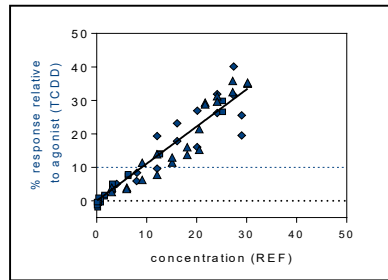
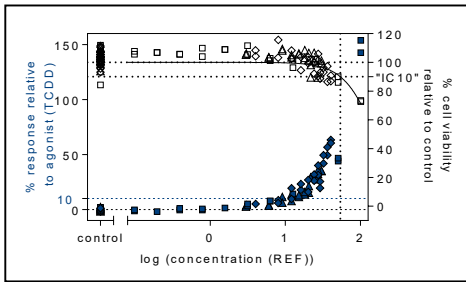


ROP 4

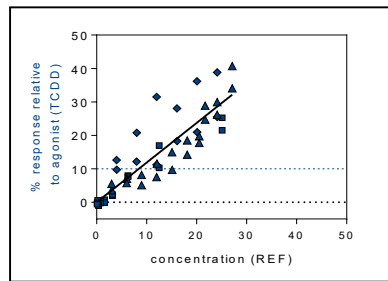
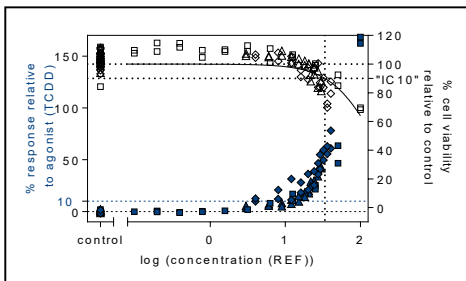


RO feed water

ROF 1

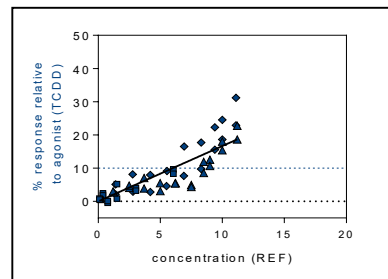
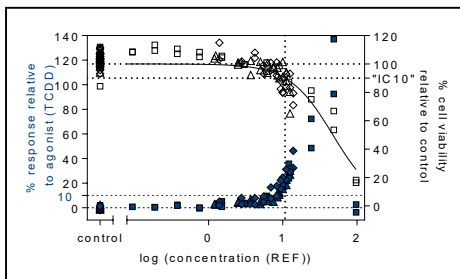


ROF 2

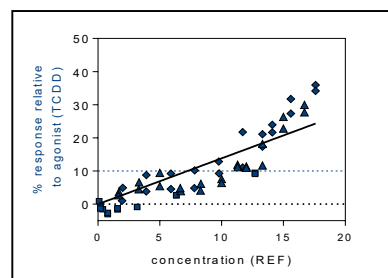
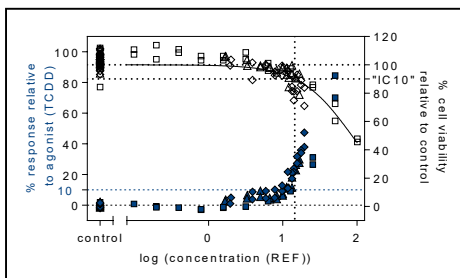


- RO concentrate (n=2)

ROF 3



ROF 4



S-4. Effect concentrations

Table S-4.1. Cytotoxicity (IC₁₀) and effect concentration (EC₁₀ and EC_{IR.15}) values in REF units limited to reporter gene assays that were activated by the RO samples.

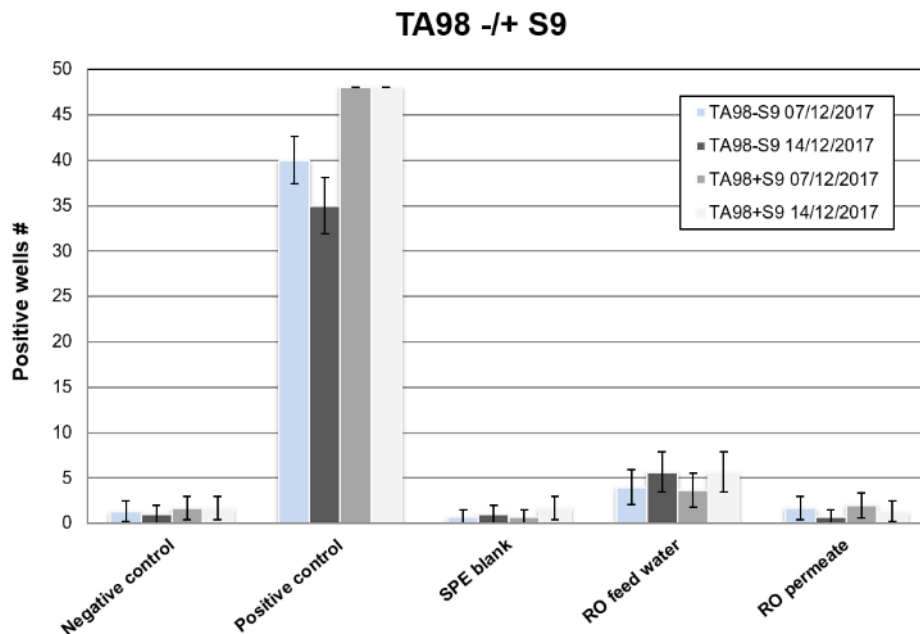
Sample	AhR		AREc32	
	IC ₁₀ [REF]±SE cytotoxicity	EC ₁₀ [REF]±SE induction	IC ₁₀ [REF]±SE cytotoxicity	EC _{IR.15} [REF]±SE induction
ROF1	51.88±1.12	8.06±0.23	92.04±1.16	6.53±0.23
ROF2	31.48±1.13	7.59±0.35	86.90±1.09	6.69±0.21
ROC1	9.84±1.11	5.31±0.25	56.20±1.10	3.14±0.08
ROC2	13.34±1.11	6.51±0.32	82.79±1.51	3.46±0.14
ROP1	NC	NA ^a	NC	NA
ROP2	NC	NA ^a	NC	NA
ROP3	NC	NA ^a	NC	NA
ROP4	NC	NA ^a	NC	60.36±9.54

AhR: aryl hydrocarbon receptor; AREc32: antioxidant response element c32; IC₁₀: inhibitory concentration causing 10% reduction in cell viability; EC₁₀: effect-concentration causing 10% of maximum effect; EC_{IR.15}: concentration causing 50% effect increase compared to negative controls; SE: standard error; ROF: reverse osmosis feed water; ROC: reverse osmosis concentrate; ROP: reverse osmosis permeate; NC: not converged, *i.e.*, IC₁₀ > 100 REF; NA: not active.

^a Considered not active as the derived EC values were comparable or lower to those quantified for the SPE blanks.

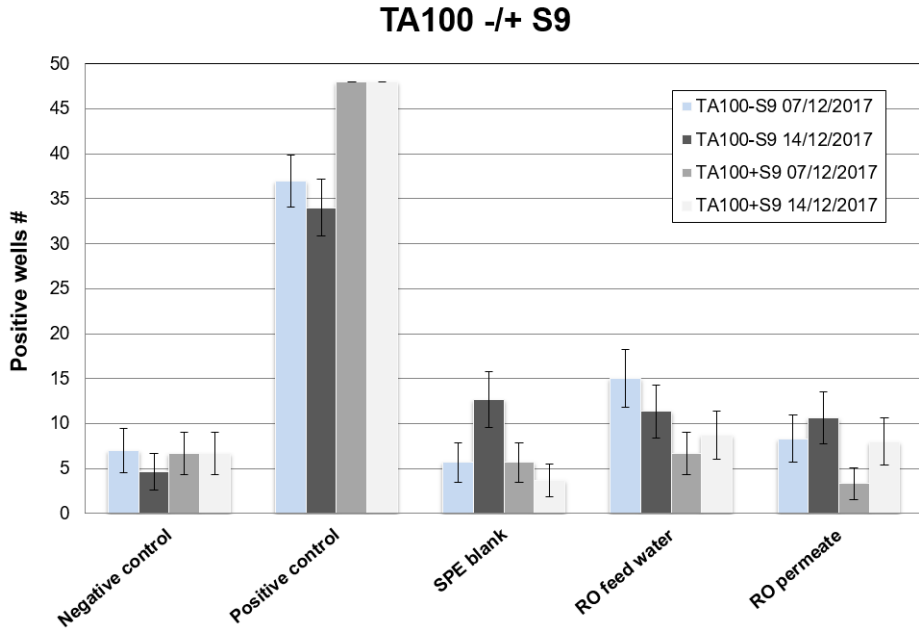
S-5. Ames-fluctuation test results

Figure S-5.1. Results of Ames test for *Salmonella typhimurium* strain TA98 with and without the S9 enzyme mix



- The relative enrichment factor (REF) of the water extracts in the Ames test was 200
- Negative control: dimethyl sulfoxide (CAS No. 67-68-5)
- Positive controls:
 - TA98-S9: 20 mg/L 4-nitroquinoline *N*-oxide (CAS No. 56-57-5)
 - TA98+S9: 5 µg/L 2-aminoanthracene (CAS No. 613-13-8)

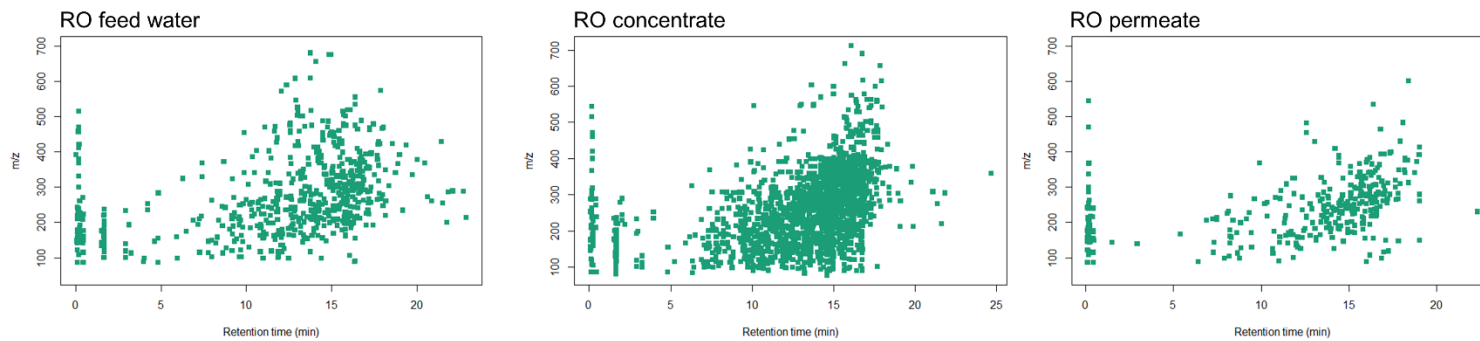
Figure S-5.2 Results of Ames test for *Salmonella typhimurium* strain TA100 with and without the S9 enzyme mix



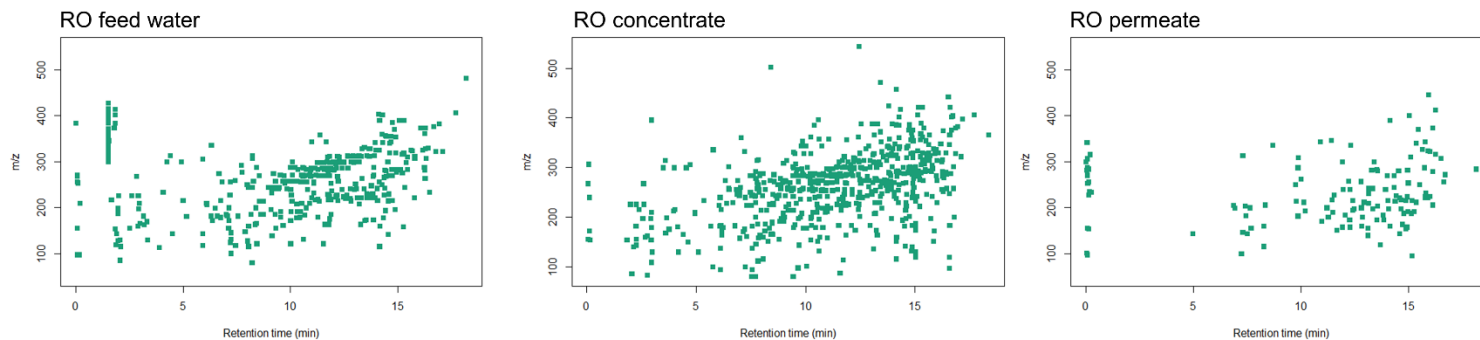
- The relative enrichment factor (REF) of the water extracts in the Ames test was 200
- Negative control: dimethyl sulfoxide (CAS No. 67-68-5)
- Positive controls:
 - TA98-S9: 12.5 mg/L nitrofurantoin (CAS No. 67-20-9)
 - TA98+S9: 5 mg/L 2-aminoanthracene (CAS No. 613-13-8)

Figure S-6.1. Plots of m/z and retention time of the non-target features detected in RO feed water, RO concentrate and RO permeate in positive (top) and negative (bottom) electrospray ionisation mode

Positive Electrospray Ionisation Mode



Negative Electrospray Ionisation Mode



S-7. Confirmed and tentatively identified compounds detected in RO system

Table S-7.1 Results of non-target screening in the positive electrospray ionisation dataset

Compound	Formula	Neutral mass	RT (min)	EPA		TOXCAST		EXPOCAST ^b	ICL ^c
				Dashboard identifier	TOX21SL ^a	TOXCAST ^a	Active (%)		
Phenethylamine	C8H11N	121.0892	9.0	DTXSID5058773	0	0	0	0	3 ¹
Anthranilic acid	C7H7NO2	137.0477	10.3	DTXSID8020094	1	0	0	2.02E-07	3 ¹
4-Hydroxybenzoic acid	C7H6O3	138.0317	11.9	DTXSID3026647	1	1	1.35	3.50E-06	3 ¹
Trimethyl phosphate	C3H9O4P	140.0239	8.2	DTXSID1021403	1	1	0.68	4.11E-08	1
Methyl styryl ketone	C10H10O	146.0732	7.6	DTXSID4025662	1	1	10.44	1.82E-05	3
Benzisothiazolinone	C7H5NOS	151.0092	13.4	DTXSID5032523	1	1	30.62	1.25E-05	2a
Diethyl hydrogen phosphate	C4H11O4P	154.0395	16.4	DTXSID1044699	0	1	0	0	2a
N-(3-Aminophenyl)propanamide	C9H12N2O	164.0950	12.5	DTXSID9044877	1	1	0	1.31E-07	3
4-Toluenesulfonamide	C7H9NO2S	171.0354	16.6	DTXSID8029105	1	1	0	3.50E-06	3
Fusaric acid	C10H13NO2	179.0947	15.4	DTXSID5023085	1	0	1.56	1.23E-07	3 ¹
1,3,5-Triazin-2(1H)-one, 4,6-bis(ethylamino)-	C7H13N5O	183.1121	10.3	DTXSID6062547	0	0	0	0	3 ²
Phenazone	C11H12N2O	188.0950	12.7	DTXSID6021117	1	1	0	1.88E-08	1
2,6-Dichlorobenzamide	C7H5Cl2NO	188.9748	8.2	DTXSID7022170	1	1	1.78	7.42E-08	1
2-Hydroxyatrazine	C8H15N5O	197.1277	11.9	DTXSID6037807	0	0	0	0	3 ²
tert-Butyl phenyl glycidyl ether	C13H18O2	206.1308	10.3	DTXSID1024702	1	0	0.88	3.70E-08	3 ³
tert-Butyl phenyl glycidyl ether	C13H18O2	206.1308	16.4	DTXSID1024702	1	0	0.88	3.70E-08	3 ³
Phosphinic acid, diphenyl-7-Diethylamino-4-methylcoumarin	C12H11O2P	218.0497	9.9	DTXSID70168929	0	0	0	0	2a ⁴
Hydroxyvaleric acid	C14H17NO2	231.1260	9.5	DTXSID9025035	1	1	16.55	3.23E-08	3
	C15H22O3	250.1570	15.0	DTXSID8033564	1	0	0	1.64E-07	3

Table S-7.1 (continued). Results of non-target screening in the positive electrospray ionisation dataset

Compound	Formula	Neutral mass	RT (min)	EPA	TOX21SL ^a	TOXCAST ^a	TOXCAST Active (%)	EXPOCAST ^b	ICL ^c
				Dashboard identifier					
Triphenylphosphine oxide	C18H15OP	278.0861	10.7	DTXSID2022121	1	1	1.78	4.09E-08	2a
4-Androstene-3,17-dione	C19H26O2	286.1934	17.3	DTXSID8024523	1	1	11.52	2.20E-07	3
Thiamethoxam	C8H10ClN5O3S	291.0193	17.4	DTXSID2034962	1	1	0.61	1.25E-08	3
Zearalenone	C18H22O5	318.1468	14.3	DTXSID0021460	1	1	23.84	2.17E-07	3
11-Hydroxy-9-oxo-15,20-cycloprosta-8(12),15,17,19-tetraen-1-oic acid	C20H26O4	330.1832	16.6	DTXSID70615382	0	0	0	0	3
Corticosterone	C21H30O4	346.2145	16.6	DTXSID6022474	1	1	8.91	2.82E-07	3
4-Androstene-3,17-dione	C19H26O2	286.1934	17.3	DTXSID8024523	1	1	11.52	2.20E-07	3
Thiamethoxam	C8H10ClN5O3S	291.0193	17.4	DTXSID2034962	1	1	0.61	1.25E-08	3
Zearalenone	C18H22O5	318.1468	14.3	DTXSID0021460	1	1	23.84	2.17E-07	3
11-Hydroxy-9-oxo-15,20-cycloprosta-8(12),15,17,19-tetraen-1-oic acid	C20H26O4	330.1832	16.6	DTXSID70615382	0	0	0	0	3
Corticosterone	C21H30O4	346.2145	16.6	DTXSID6022474	1	1	8.91	2.82E-07	3

^a Suspect lists: “1” indicates presence of candidate structure in the list, whereas “0” indicates absence; ^b ExpoCast median exposure prediction in mg per kg of body weight per day (mg/kg-bw/day); ^c Identification confidence level by Schymanski et al., 2014a; ¹ Supporting spectral library evidence found, but it was not possible to rule out other isomers; ² Supporting spectral library evidence found, but extra peaks in experimental HRMS2 spectrum suggest (quasi-)isobaric interferences; ³ Possibly isomer of candidate structure exhibiting same fragmentation behaviour, but different retention time; ⁴ Reference spectrum previously measured in house.

Table S-7.2. Results of non-target screening in the negative electrospray ionisation dataset

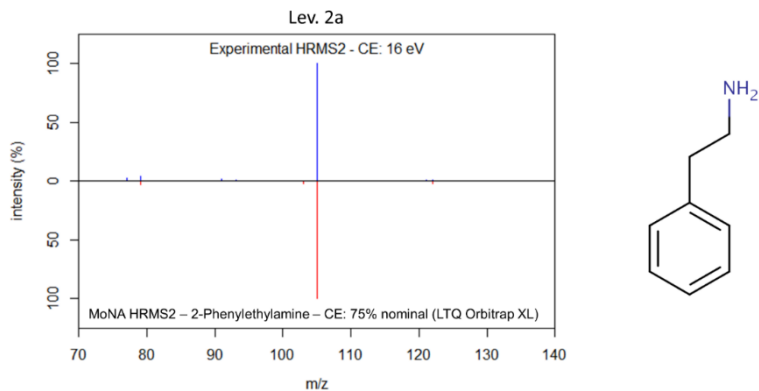
Compound	Formula	Neutral mass	RT (min)	EPA		TOXCAST		EXPOCAST ^b	ICL ^c
				Dashboard identifier	TOX21SL ^a	TOXCAST ^a	Active (%)		
Catechol	C6H6O2	110.0368	3.0	DTXSID3020257	1	1	14.10	4.41E-08	3 ¹
4-Hydroxybenzoic acid	C7H6O3	138.0317	6.1	DTXSID3026647	1	1	1.35	3.50E-06	3 ¹
D-(-)-Mandelic acid	C8H8O3	152.0474	10.6	DTXSID4046523	1	0	1.83	1.03E-07	3 ¹
4-Hydroxy-3-methoxybenzaldehyde	C8H8O3	152.0473	8.3	DTXSID0021969	1	1	4.73	3.08E-05	3
Diethyl hydrogen phosphate	C4H11O4P	154.0395	1.9	DTXSID1044699	0	1	0	0	2a
Acesulfame	C4H5NO4S	162.9939	2.8	DTXSID1030606	1	1	0.34	1.15E-06	1
Acamprosate	C5H11NO4S	181.0409	4.2	DTXSID6047529	1	1	1.77	2.91E-07	2a
Saccharin	C7H5NO3S	182.9990	7.1	DTXSID5021251	1	1	1.35	2.25E-07	2a ²
Naphthalene-2-sulfonic acid	C10H8O3S	208.0194	9.8	DTXSID5044788	1	1	2.03	2.06E-07	3 ¹
Mecoprop	C10H11ClO3	214.0397	14.6	DTXSID9024194	1	1	0.64	7.16E-08	2a
Phosphinic acid, diphenyl-	C12H11O2P	218.0497	11.5	DTXSID70168929	0	0	0	0	2a ²
Bentazone	C10H12N2O3S	240.0569	12.4	DTXSID0023901	1	1	3.34	1.70E-08	1
8-(2-Ethoxyphenyl)-8-oxooctanoic acid	C16H22O4	278.1519	13.2	DTXSID60645436	0	0	0	0	3
10-(4-sulfophenyl)decanoic acid	C16H24O5S	328.1345	13.1	DTXSID80891332	0	0	0	0	3

Table S-7.2 (continued). Results of non-target screening in the negative electrospray ionisation dataset

Compound	Formula	Neutral mass	RT (min)	EPA Dashboard identifier	TOXCAST				
					TOX21SL ^a	TOXCAST ^a	Active (%)	EXPOCAST ^b	ICL ^c
Pencycuron	C19H21ClN2O	328.1343	13.4	DTXSID3042261	1	1	11.21	1.30E-07	3 ³
Pencycuron	C19H21ClN2O	328.1343	13.7	DTXSID3042261	1	1	11.21	1.30E-07	3 ³
Cortisone	C21H28O5	360.1938	14.9	DTXSID5022857	1	1	3.62	2.20E-07	3
Bucolome	C14H22N2O3	266.1631	14.3	DTXSID4048854	1	0	0	1.72E-07	3
4-(4-sulfophenyl)heptanoic acid	C13H18O5S	286.0876	12.4	DTXSID50891662	0	0	0	0	3
Zearalenone	C18H22O5	318.1468	12.3	DTXSID0021460	1	1	23.84	2.17E-07	3
11-Hydroxy-9-oxo-15,20-cycloprosta-8(12),15,17,19-tetraen-1-oic acid	C20H26O4	330.1832	16.4	DTXSID70615382	0	0	0	0	3
Corticosterone	C21H30O4	346.2145	16.6	DTXSID6022474	1	1	8.909	2.82E-07	3
Prednisolone	C21H28O5	360.1938	13.8	DTXSID9021184	1	1	3.62	4.24E-08	3
Methylprednisolone	C22H30O5	374.2094	16.3	DTXSID7023300	1	1	3.98	4.52E-08	3

^a Suspect lists: “1” indicates presence of candidate structure in the list, whereas “0” indicates absence; ^b ExpoCast median exposure prediction in mg per kg of body weight per day (mg/kg-bw/day); ^c Identification confidence level by Schymanski et al., 2014a; ¹ Supporting spectral library evidence found, but it was not possible to rule out other isomers; ² Supporting spectral library evidence found, but extra peaks in experimental HRMS2 spectrum suggest (quasi-)isobaric interferences; ³ Possibly isomer of candidate structure exhibiting same fragmentation behaviour, but different retention time; ⁴ Reference spectrum previously measured in house.

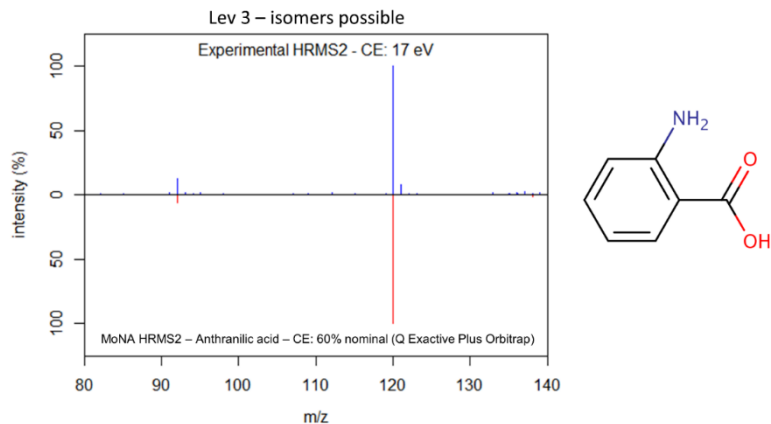
Figure S-8.1. Spectral similarity of m/z 122.0964 \pm 0.002 [M+H]⁺ to library spectrum of 2-phenylethylamine.



Similarity: 0.9989528

Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/UF023309>

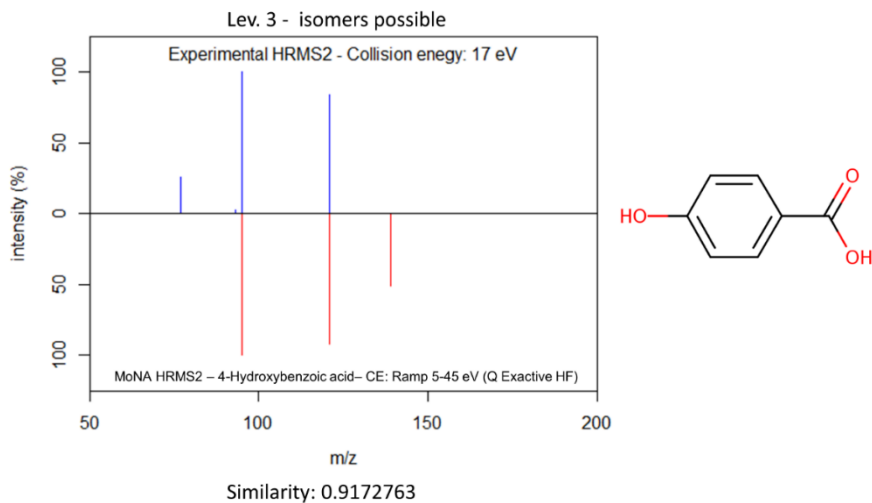
Figure S-8.2. Spectral similarity of m/z 138.0549 \pm 0.002 [M+H]⁺ to library spectrum of anthranilic acid.



Similarity: 0.9917146

Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/SM884401>

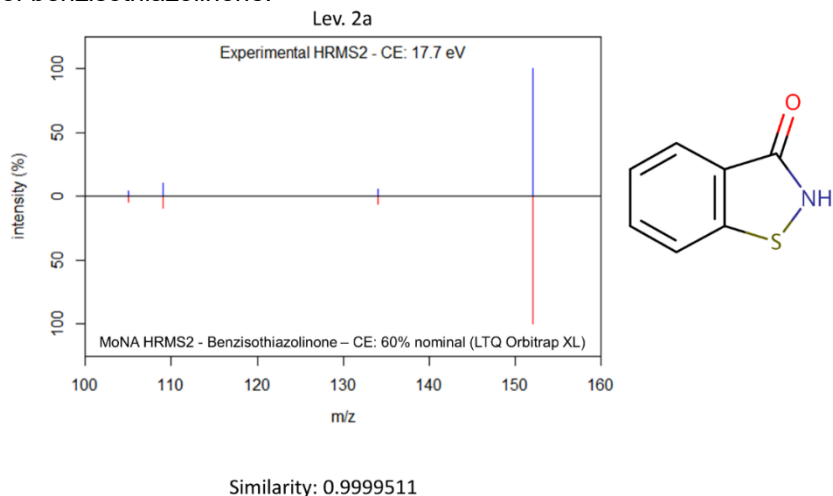
Figure S-8.3. Spectral similarity of m/z 139.0389 \pm 0.002 [M+H]⁺ to library spectrum of 4-hydroxybenzoic acid.



Reference spectrum:

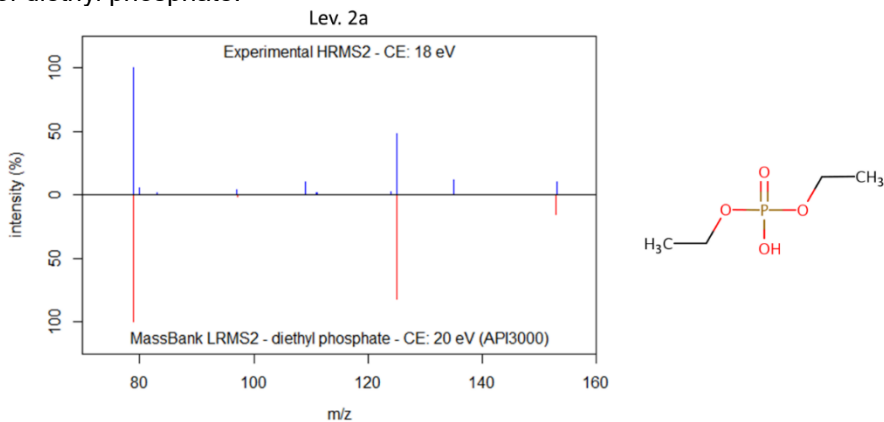
<http://mona.fiehnlab.ucdavis.edu/spectra/display/FiehnHILIC000989>

Figure S-8.4. Spectral similarity of m/z 152.0164 \pm 0.002 [M+H]⁺ to library spectrum of benzisothiazolinone.



Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/EA030111>

Figure S-8.5. Spectral similarity of m/z 155.0467 \pm 0.002 [M+H]⁺ to library spectrum of diethyl phosphate.

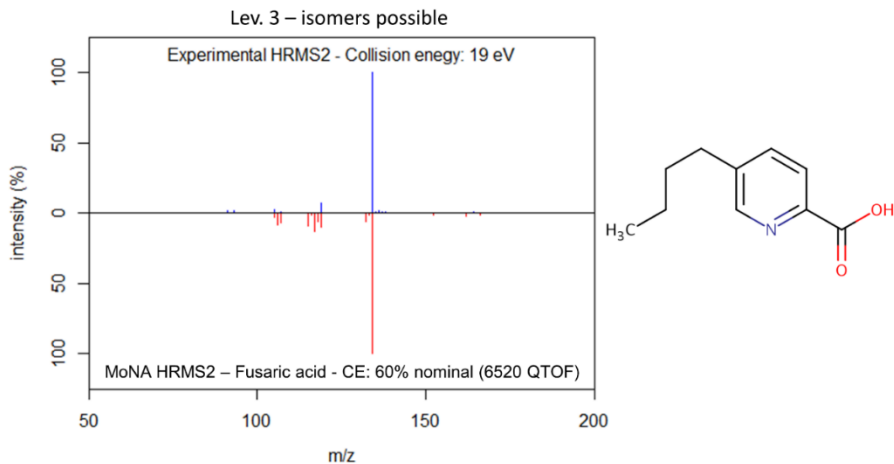


Similarity: 0.9595454

Reference spectrum:

https://massbank.eu/MassBank/RecordDisplay.jsp?id=KO000680&dsn=Keio_Univ

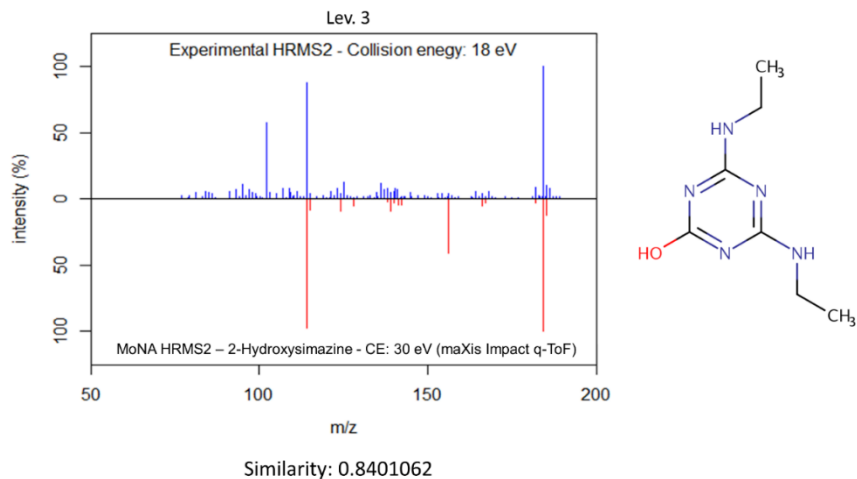
Figure S-8.6. Spectral similarity of m/z 180.1019 \pm 0.002 [M+H]⁺ to library spectrum of fusaric acid.



Similarity: 0.9787027

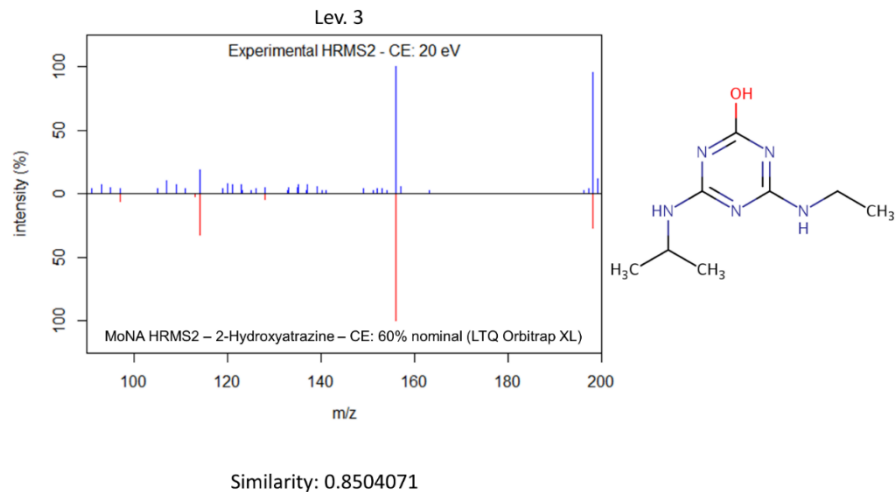
Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/BML00612>

Figure S-8.7. Spectral similarity of m/z 184.1192 \pm 0.002 [M+H]⁺ to library spectrum of 2-hydroxysimazine.



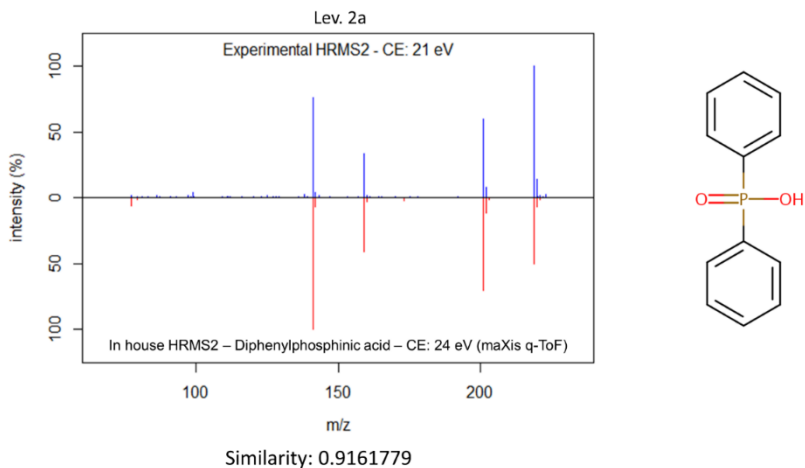
Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/AU207903>

Figure S-8.8. Spectral similarity of m/z 198.1349 \pm 0.002 [M+H]⁺ to library spectrum of 2-hydroxyatrazine.



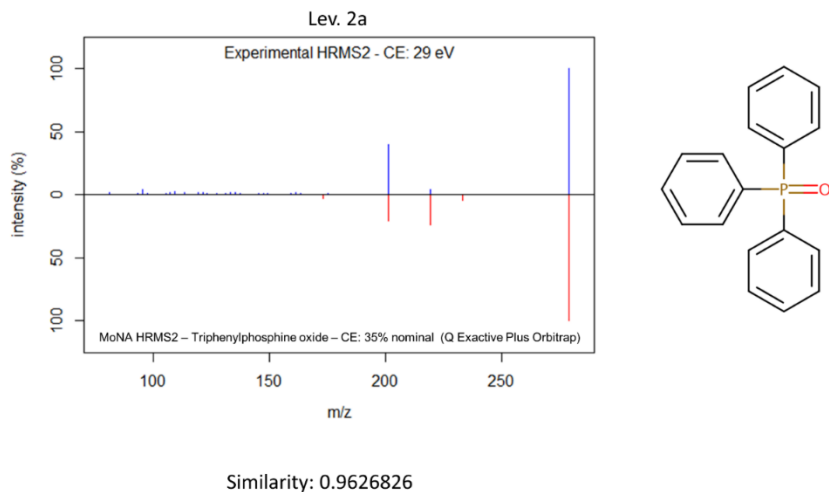
Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/AU207903>

Figure S-8.9. Spectral similarity of m/z 219.0569 \pm 0.002 [M+H]⁺ to library spectrum of diphenylphosphinic acid.



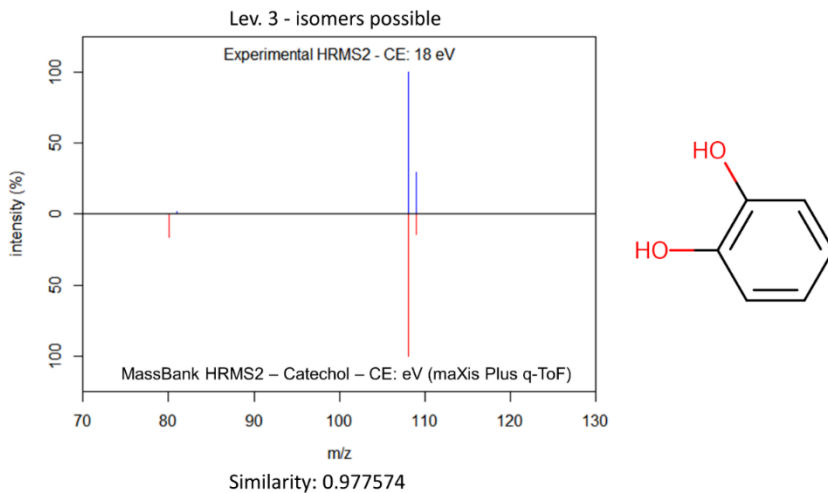
Reference spectrum: *in house standard measurement*

Figure S-8.10. Spectral similarity of m/z 279.0933 \pm 0.002 [M+H]⁺ to library spectrum of triphenylphosphine oxide.



Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/SM825001>

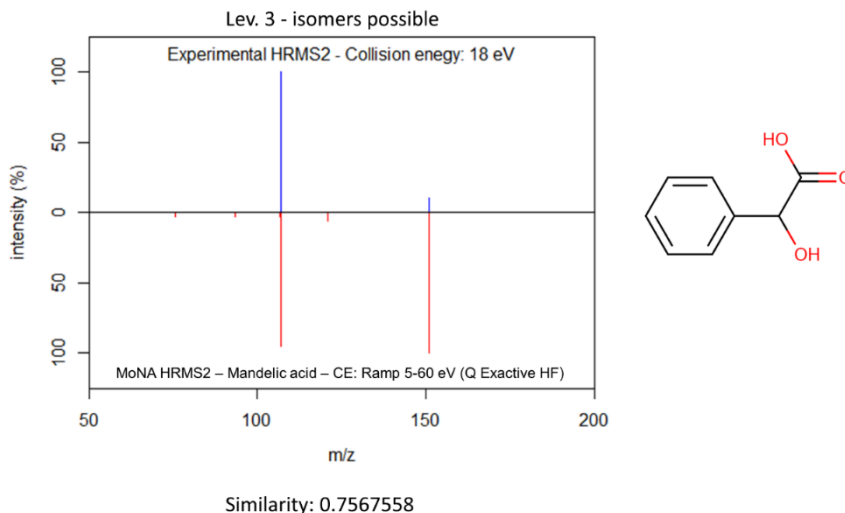
Figure S-8.11. Spectral similarity of m/z 109.0295±0.002 [M-H]⁻ to library spectrum of catechol.



Reference spectrum:

https://massbank.eu/MassBank/RecordDisplay.jsp?id=RP012013&dsn=BGC_Munch

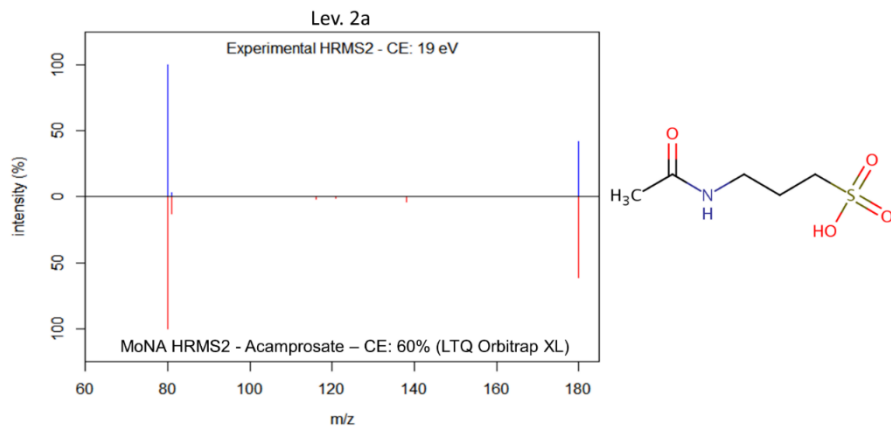
Figure S-8.12. Spectral similarity of m/z 151.0401±0.002 [M-H]⁻ to library spectrum of mandelic acid



Reference spectrum:

<http://mona.fiehnlab.ucdavis.edu/spectra/display/FiehnHILIC001315>

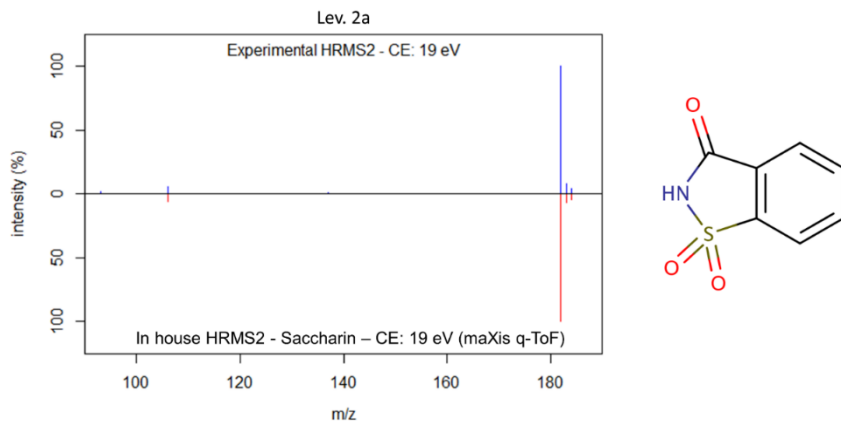
Figure S-8.13. Spectral similarity of m/z 180.0336 \pm 0.002 [M-H]⁻ to library spectrum of acamprosate.



Similarity: 0.9827208

Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/EA284861>

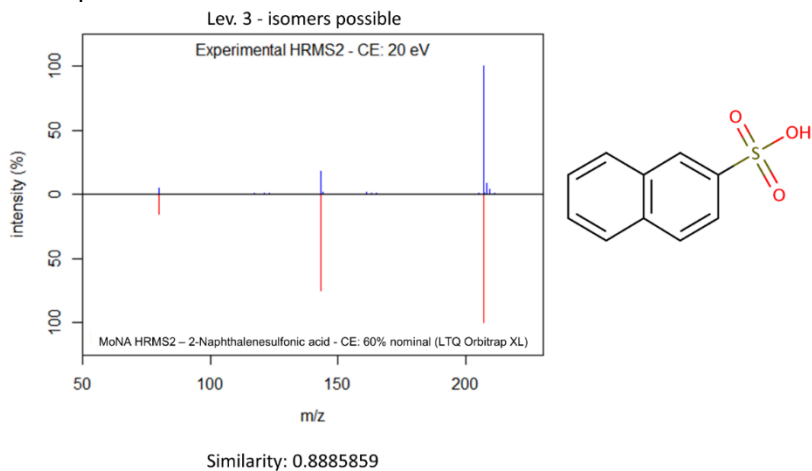
Figure S-8.14. Spectral similarity of m/z 181.9917 \pm 0.002 [M-H]⁻ to library spectrum of saccharin.



Similarity: 0.9999507

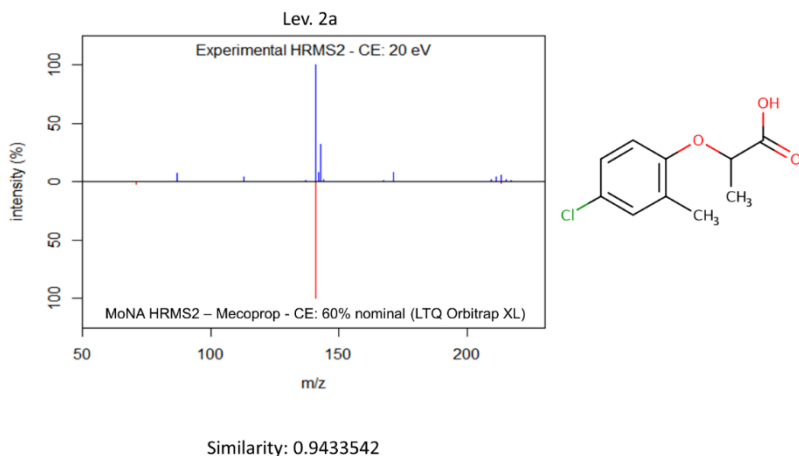
Reference spectrum: *in house standard measurement*

Figure S-8.15. Spectral similarity of m/z 207.0121 \pm 0.002 [M-H]⁻ to library spectrum of 2-naphthalenesulfonic acid.



Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/EA065355>

Figure S-8.16. Spectral similarity of m/z 213.0324 \pm 0.002 [M-H]⁻ to library spectrum of mecoprop.



Reference spectrum: <http://mona.fiehnlab.ucdavis.edu/spectra/display/EA030859>