

# Supporting Information: Biodiversity drives micropollutant biotransformation in freshwater phytoplankton assemblages

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41 pages, 10 figures and 11 tables

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## S1. Methods

### S1.1. Experiment

#### Culture medium.

Growth medium (Woods Hole Combo (WC) medium, modified after Guillard and Lorenzen<sup>1</sup>) was prepared from deionized water, 10x TES (2-[[1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl]amino]ethanesulfonic acid) buffer stock solution, and 1000x stock solutions of all other constituents to a final concentration of 1 mM NaNO<sub>3</sub>, 250 µM CaCl<sub>2</sub>, 150 µM MgSO<sub>4</sub>, 150 µM NaHCO<sub>3</sub>, 50 µM K<sub>2</sub>HPO<sub>4</sub>, 390 µM H<sub>3</sub>BO<sub>3</sub>, 11.7 µM Na<sub>2</sub>EDTA, 11.7 µM FeCl<sub>3</sub>, 10 nM CuSO<sub>4</sub>, 76.5 nM ZnSO<sub>4</sub>, 42 nM CoCl<sub>2</sub>, 910 nM MnCl<sub>2</sub>, 26 nM Na<sub>2</sub>MoO<sub>4</sub>, 98 nM Na<sub>3</sub>VO<sub>4</sub>, 0.5 mM TES. The medium was sterilized by autoclaving (30 min at 121°C). Alternative versions of the growth medium additionally contained 100 µM Na<sub>2</sub>O<sub>3</sub>Si (WC+Si medium), 50 µM Na<sub>2</sub>O<sub>3</sub>Si (WC+0.5Si medium) or 5% heat-killed bacteria (WC+Bac medium). WC+Bac medium was prepared immediately before use by adding heat-killed bacteria to regular WC medium under the sterile hood. Heat-killed bacteria were prepared as follows: From frozen stock aliquots, 500 µL each of *Bacillus subtilis* (cat. no. 154865, Carolina, Burlington, NC, USA), *Bacillus brevis* (cat. no. 154921, ibid.) and *Serratia fonticuli* (cat. no. DSM 4576, DSMZ, Braunschweig, Germany) were added to 250 mL WC medium in a 500-mL Schott bottle and incubated 48 h at room temperature. The culture was visibly turbid at this point. The culture bottle was incubated for 3 h at 80°C in a heating oven before an aliquot of the heat-killed bacteria culture was added to the WC+Bac medium.

#### Growth inhibition tests

Five species (one for each taxonomic class; CHR: *Poterioochromonas malhamensis*, CYA: *Aphanizomenon flos-aquae*, DIA: *Cyclotella cf. glomerata*, CRY: *Cryptomonas* sp., CHL: *Chlorella* sp.) were diluted into fresh medium and incubated in duplicate with 2.5 µg/L or 10 µg/L (concentration per compound) of the 36-compound chemical mixture in 20-mL glass vials (culture volume: 4 mL). Samples (200 µL) were taken at 0h, 72h, 112h, 163h or 0h, 54h, 95h, 146h, and optical density at 750 nm (OD<sub>750</sub>) was measured.

**Table S1.** Experimental design: Number of combinations at each CR and SR level.

SR	CR		
	1	3	5
	5	7 × 2 *	5 × 2
	8		5 × 2
		11	5 × 2

„×2“ indicates duplication for each combination. (\*): Not for all taxonomic classes 5 species were available. For CHR, 3 species were used; for CRY, 4 species. In addition, a 3 species combination was added for both CYA and CHL.

**Table S2.** Algal strains used in the experiment, with growth media (see text) and source. “WC/WC+Bac”: Medium was cycled between WC and WC+Bac.

Code	Species name	Strain	Source	Functional group	Medium
<b>CHL1</b>	<i>Ankistrodesmus bibarianus</i>	NIVA 179	NIVA	Chlorophyta	WC
<b>CHL2</b>	<i>Chlamydomonas reinhardtii</i>		in-house	Chlorophyta	WC
<b>CHL3</b>	<i>Chlorella</i> sp.	NIVA 170	NIVA	Chlorophyta	WC
<b>CHL4</b>	<i>Kirchneriella subcapitata</i>		in-house	Chlorophyta	WC
<b>CHL5</b>	<i>Pediastrum</i> sp.	SCCAP K-1033	SCCAP	Chlorophyta	WC
<b>CHR1</b>	<i>Chrysocapsa epiphytica</i>	SAG 20.88	SAG	Chrysophyta	WC+Si
<b>CHR2</b>	<i>Ochromonas danica</i>	SAG 933-7	SAG	Chrysophyta	WC/WC+Bac
<b>CHR3</b>	<i>Poterioochromonas malhamensis</i>	SAG 933-1a	SAG	Chrysophyta	WC/WC+Bac
<b>CRY1</b>	<i>Chroomonas</i> sp.	SAG 980-1	SAG	Cryptophyta	WC
<b>CRY2</b>	<i>Cryptomonas</i> sp.		in-house	Cryptophyta	WC
<b>CRY3</b>	<i>Komma</i> sp.	SCCAP K-1622	SCCAP	Cryptophyta	WC
<b>CRY4</b>	<i>Rhodomonas</i> sp.	CCAC 0194	CCAC	Cryptophyta	WC/WC+Bac
<b>CYA1</b>	<i>Anabaena flos-aquae</i>	NIVA 269/6	NIVA	Cyanobacteria	WC
<b>CYA2</b>	<i>Aphanizomenon flos-aquae</i>	NIVA 693	NIVA	Cyanobacteria	WC
<b>CYA3</b>	<i>Microcystis aeruginosa</i>	PCC 7806	PCC	Cyanobacteria	WC
<b>CYA4</b>	<i>Planktothrix rubescens</i>	SCCAP K-0576	SCCAP	Cyanobacteria	WC
<b>CYA5</b>	<i>Synechococcus</i> sp.		in-house	Cyanobacteria	WC
<b>DIA1</b>	<i>Asterionella formosa</i>	NIVA BAC-3	NIVA	Diatom	WC+Si
<b>DIA2</b>	<i>Fragilaria crotonensis</i>	SAG 28.96	SAG	Diatom	WC+Si
<b>DIA3</b>	<i>Nitzschia</i> sp.	SCCAP K-1905	SCCAP	Diatom	WC+Si
<b>DIA4</b>	<i>Synedra rumpens var. familiaris</i>	NIVA BAC-18	NIVA	Diatom	WC+Si
<b>DIA5</b>	<i>Tabellaria</i> sp.	CCAC 3717 B	CCAC	Diatom	WC+Si

SCCAP Scandinavian Culture Collection of Algae and Protozoa, University of Copenhagen, Copenhagen, Denmark, now NIVA, Oslo, Norway; SAG Culture Collection of Algae at Göttingen University, Georg-August-Universität Göttingen, Göttingen, Germany; CCAC Culture Collection of Algae at the University of Cologne, Cologne, Germany; NIVA Norwegian Institute for Water Research Culture Collection of Algae, Oslo, Norway

**Table S3.** Mixture of micropollutants used in the experiment.

Name	Compound class	Formula	Molecular weight [Da]	Exact mass [Da]	log Kow	CAS	Vendor	Ion	m/z	Retention time [min]	
<b>Amisulpride</b>	Pharmaceutical	C <sub>17</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S	369.4811	369.1722	1.06	[2]	71675-85-9	[M+H] <sup>+</sup>	370.1795	12.2	
<b>Atenolol</b>	Pharmaceutical	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	266.3374	266.1630	0.16	[2]	29122-68-7	[M+H] <sup>+</sup>	267.1703	9.9	
<b>Azoxystrobin</b>	Fungicide	C <sub>22</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub>	403.3894	403.1168	2.5	[1]	131860-33-8	Fluka	[M+H] <sup>+</sup>	404.1241	21.2
<b>Benzotriazole</b>	Corrosion inhibitor	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub>	119.1246	119.0483	1.44	[5]	95-14-7	Fluka	[M+H] <sup>+</sup>	120.0556	15.4
<b>Bezafibrate</b>	Pharmaceutical	C <sub>19</sub> H <sub>20</sub> ClNO <sub>4</sub>	361.8213	361.1081	4.25	[4]	41859-67-0	Sigma-Aldrich	[M+H] <sup>+</sup>	362.1154	21.6
<b>Boscalid</b>	Fungicide	C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O	343.2086	342.0327	2.96	[1]	188425-85-6	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	343.0399	21.7
<b>Caffeine</b>		C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>	194.1914	194.0804	-0.07	[6]	58-08-2	Fluka	[M+H] <sup>+</sup>	195.0877	14.3
<b>Carbamazepine</b>	Pharmaceutical	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O	236.2699	236.0950	2.45	[2]	298-46-4	Sigma-Aldrich	[M+H] <sup>+</sup>	237.1022	19.9
<b>Carbendazim</b>	Fungicide	C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	191.1875	191.0695	1.48	[1]	10605-21-7	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	192.0768	12.6
<b>Chlorpyrifos</b>	Insecticide	C <sub>9</sub> H <sub>11</sub> Cl <sub>3</sub> NO <sub>3</sub> PS	350.5882	348.9263	4.7	[1]	2921-88-2	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	349.9336	24.9
<b>Citalopram</b>	Pharmaceutical	C <sub>20</sub> H <sub>21</sub> FN <sub>2</sub> O	324.3937	324.1638	3.5	[2]	59729-33-8	TRC Canada	[M+H] <sup>+</sup>	325.1711	16.8
<b>Climbazole</b>	Fungicide / Pharmaceutical	C <sub>15</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>	292.7622	292.0979	3.76	[1]	38083-17-9	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	293.1051	18.7
<b>Cyprodinil</b>	Fungicide	C <sub>14</sub> H <sub>15</sub> N <sub>3</sub>	225.2903	225.1266	4	[1]	121552-61-2	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	226.1339	22.2
<b>Dimethoate</b>	Insecticide	C <sub>5</sub> H <sub>12</sub> NO <sub>3</sub> PS <sub>2</sub>	229.2589	228.9996	0.7	[1]	60-51-5	Riedel-de Haën	[M+H] <sup>+</sup>	230.0069	16.5
<b>Fexofenadine</b>	Pharmaceutical	C <sub>32</sub> H <sub>39</sub> NO <sub>4</sub>	501.6592	501.2879	5.6	[2]	83799-24-0	TRC Canada	[M+H] <sup>+</sup>	502.2952	18.1
<b>Fipronil</b>	Insecticide	C <sub>12</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>4</sub> OS	437.1497	435.9387	3.75	[1]	120068-37-3	Dr. Ehrenstorfer	[M-H] <sup>-</sup>	434.9314	22.6
<b>Fludioxonil</b>	Fungicide	C <sub>12</sub> H <sub>6</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	248.1861	248.0397	4.12	[1]	131341-86-1	Fluka	[M-H] <sup>-</sup>	247.0325	21.7
<b>Hydrochlorothiazide</b>	Pharmaceutical	C <sub>7</sub> H <sub>8</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>	297.7410	296.9645	-0.07	[2]	58-93-5	Sigma-Aldrich	[M-H] <sup>-</sup>	295.9572	11.5
<b>Imidacloprid</b>	Insecticide	C <sub>9</sub> H <sub>10</sub> ClN <sub>5</sub> O <sub>2</sub>	255.6621	255.0523	0.57	[1]	138261-41-3	Riedel-de Haën	[M+H] <sup>+</sup>	256.0596	15.3
<b>Iopromide</b>	X-ray contrast medium	C <sub>18</sub> H <sub>24</sub> I <sub>3</sub> N <sub>3</sub> O <sub>8</sub>	791.1135	790.8698	-2.49	[4]	73334-07-3	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	791.877	11.3
<b>Ketoconazole</b>	Fungicide / Pharmaceutical	C <sub>26</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub>	531.4337	530.1488	4.35	[2]	65277-42-1	Sigma-Aldrich	[M+H] <sup>+</sup>	531.156	18.5

<b>Kresoxim-methyl</b>	Fungicide	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	313.3494	313.1314	3.4	[1]	143390-89-0	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	314.1387	23.0
<b>Lamotrigine</b>	Pharmaceutical	C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>5</sub>	256.0926	255.0079	2.5	[2]	84057-84-1	TRC Canada	[M+H] <sup>+</sup>	256.0151	14.9
<b>Mefenamic acid</b>	Pharmaceutical	C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub>	241.2864	241.1103	5.12	[2]	61-68-7	Sigma-Aldrich	[M+H] <sup>+</sup>	242.1176	24.0
<b>Methoxyfenozide</b>	Insecticide	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	368.4713	368.2100	3.72	[1]	161050-58-4	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	369.2173	22.0
<b>Metoprolol</b>	Pharmaceutical	C <sub>15</sub> H <sub>25</sub> NO <sub>3</sub>	267.3653	267.1834	1.88	[2]	37350-58-6	Sigma-Aldrich	[M+H] <sup>+</sup>	268.1907	14.4
<b>Oxazepam</b>	Pharmaceutical	C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>	286.7146	286.0509	2.24	[2]	604-75-1	Lipomed AG	[M+H] <sup>+</sup>	287.0582	20.7
<b>Propamocarb</b>	Fungicide	C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	188.2682	188.1525	0.84	[1]	24579-73-5	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	189.1598	10.5
<b>Sucratose</b>	Artificial sweetener	C <sub>12</sub> H <sub>19</sub> Cl <sub>3</sub> O <sub>8</sub>	397.6352	396.0146	-1	[4]	56038-13-2	Dr. Ehrenstorfer	[M+FA] <sup>-</sup>	441.0128	15.1
<b>Sulfamethoxazole</b>	Pharmaceutical	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S	253.2791	253.0521	0.89	[2]	723-46-6	Sigma-Aldrich	[M+H] <sup>+</sup>	254.0594	14.8
<b>Tebuconazole</b>	Fungicide	C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O	307.8201	307.1451	3.7	[1]	107534-96-3	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	308.1524	23.2
<b>Thiamethoxam</b>	Insecticide	C <sub>8</sub> H <sub>10</sub> ClN <sub>5</sub> O <sub>3</sub> S	291.7162	291.0193	-0.13	[1]	153719-23-4	Dr. Ehrenstorfer	[M+H] <sup>+</sup>	292.0266	13.9
<b>Torasemide</b>	Pharmaceutical	C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>3</sub> S	348.4220	348.1256	2.3	[2]	56211-40-6	TRC Canada	[M+H] <sup>+</sup> , [M-H] <sup>-</sup>	349.1329, 347.1183	17.8
<b>Valsartan</b>	Pharmaceutical	C <sub>24</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>	435.5210	435.2270	5.8	[2]	137862-53-4	LGC Standards	[M+H] <sup>+</sup>	436.2343	21.7
<b>Venlafaxine</b>	Pharmaceutical	C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub>	277.4033	277.2042	3.28	[3]	93413-69-5	TRC Canada	[M+H] <sup>+</sup>	278.2115	16.3
<b>Vildagliptin</b>	Pharmaceutical	C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>	303.4009	303.1947	0.79	[4]	274901-16-5	TRC Canada	[M+H] <sup>+</sup>	304.202	9.9

[1]: Data from Pesticide Properties Database <sup>7</sup>

[2]: Data from DrugBank <sup>8</sup>

[3]: Data from PubChem (CID: 5656) <sup>9</sup>

[4]: No experimental value for the log K<sub>ow</sub> could be found; the used value is calculated using EPI-Suite <sup>10</sup>

[5]: Data from PubChem (CID: 7220) <sup>11</sup>

[6]: Data from PubChem (CID: 2519) <sup>12</sup>

**Table S4.** Culture selections

<b>Selection 1</b>	<b>CR = 5</b>	<b>SR = 3 (CHR)</b>	<b>Selection 7</b>	<b>CR = 5</b>	<b>SR = 11</b>
<b>chemical-negative control</b>					
CHR1		<i>Chrysocapsa epiphytica</i>	CHL3		<i>Chlorella</i> sp.
CHR3		<i>Poteroiochromonas malhamensis</i>	CHL4		<i>Kirchneriella subcapitata</i>
CHR2		<i>Ochromonas danica</i>	CYA5		<i>Synechococcus</i> sp.
			CYA1		<i>Anabaena flos-aquae</i>
			CYA2		<i>Aphanizomenon flos-aquae</i>
<b>Selection 2</b>	<b>CR = 1</b>	<b>SR = 3 (CHL)</b>	CRY2		<i>Cryptomonas</i> sp.
CHL1		<i>Ankistrodesmus bibarianus</i>	CRY1		<i>Chroomonas</i> sp.
CHL5		<i>Pediastrum</i> sp.	DIA5		<i>Tabellaria</i> sp.
CHL2		<i>Chlamydomonas reinhardtii</i>	DIA4		<i>Synedra rumpens var. familiaris</i>
			CHR3		<i>Poteroiochromonas malhamensis</i>
			CHR2		<i>Ochromonas danica</i>
<b>Selection 3</b>	<b>CR = 5</b>	<b>SR = 8</b>			
CHL3		<i>Chlorella</i> sp.	<b>Selection 8</b>	<b>CR = 5</b>	<b>SR = 4 (CRY)</b>
CYA5		<i>Synechococcus</i> sp.	<b>chemical-negative control</b>		
CYA4		<i>Planktothrix rubescens</i>	CRY2		<i>Cryptomonas</i> sp.
		<i>Chroomonas</i>	CRY1		<i>Chroomonas</i> sp.
CRY1		sp.	CRY3		<i>Komma</i> sp.
CRY3		<i>Komma</i> sp.	CRY4		<i>Rhodomonas</i> sp.
DIA5		<i>Tabellaria</i> sp.			
DIA1		<i>Asterionella formosa</i>	<b>Selection 9</b>	<b>CR = 5</b>	<b>SR = 5</b>
CHR1		<i>Chrysocapsa epiphytica</i>	CHL2		<i>Chlamydomonas reinhardtii</i>
			CYA4		<i>Planktothrix rubescens</i>
<b>Selection 4</b>	<b>CR = 5</b>	<b>SR = 5 (DIA)</b>	CRY2		<i>Cryptomonas</i> sp.
<b>chemical-negative control</b>			DIA5		<i>Tabellaria</i> sp.
DIA5		<i>Tabellaria</i> sp.	CHR2		<i>Ochromonas danica</i>
DIA2		<i>Fragilaria crotonensis</i>			
DIA1		<i>Asterionella formosa</i>	<b>Selection 10</b>	<b>medium control</b>	
DIA3		<i>Nitzschia</i> sp.			
DIA4		<i>Synedra rumpens var. familiaris</i>	<b>Selection 11</b>	<b>CR = 5</b>	<b>SR = 11</b>
<b>Selection 5</b>	<b>CR = 5</b>	<b>SR = 5 (DIA)</b>	CHL1		<i>Ankistrodesmus bibarianus</i>
DIA5		<i>Tabellaria</i> sp.	CHL2		<i>Chlamydomonas reinhardtii</i>
DIA2		<i>Fragilaria crotonensis</i>	CYA3		<i>Microcystis aeruginosa</i>
DIA1		<i>Asterionella formosa</i>	CRY1		<i>Chroomonas</i> sp.
DIA3		<i>Nitzschia</i> sp.	CRY3		<i>Komma</i> sp.
DIA4		<i>Synedra rumpens var. familiaris</i>	CRY4		<i>Rhodomonas</i> sp.
			DIA5		<i>Tabellaria</i> sp.
<b>Selection 6</b>	<b>CR = 5</b>	<b>SR = 8</b>	DIA1		<i>Asterionella formosa</i>
CHL5		<i>Pediastrum</i> sp.	CHR1		<i>Chrysocapsa epiphytica</i>
CYA1		<i>Anabaena flos-aquae</i>	CHR3		<i>Poteroiochromonas malhamensis</i>
CRY1		<i>Chroomonas</i> sp.	CHR2		<i>Ochromonas danica</i>
CRY3		<i>Komma</i> sp.			
CRY4		<i>Rhodomonas</i> sp.	<b>Selection 12</b>	<b>CR = 5</b>	<b>SR = 5</b>
DIA3		<i>Nitzschia</i> sp.	CHL5		<i>Pediastrum</i> sp.
DIA4		<i>Synedra rumpens var. familiaris</i>	CYA1		<i>Anabaena flos-aquae</i>
CHR2		<i>Ochromonas danica</i>	CRY2		<i>Cryptomonas</i> sp.
			DIA1		<i>Asterionella formosa</i>
			CHR3		<i>Poteroiochromonas malhamensis</i>

**Table S4.** (continued)

<b>Selection 13</b>	<b>CR = 5</b>	<b>SR = 5</b>	<b>Selection 19</b>	<b>CR = 5</b>	<b>SR = 8</b>
CHL4		<i>Kirchneriella subcapitata</i>	CHL1		<i>Ankistrodesmus bibarianus</i>
CYA5		<i>Synechococcus</i> sp.	CHL5		<i>Pediastrum</i> sp.
CRY3		<i>Komma</i> sp.	CHL2		<i>Chlamydomonas reinhardtii</i>
DIA5		<i>Tabellaria</i> sp.	CYA1		<i>Anabaena flos-aquae</i>
CHR1		<i>Chrysocapsa epiphytica</i>	CRY1		<i>Chroomonas</i> sp.
			CRY4		<i>Rhodomonas</i> sp.
<b>Selection 14</b>	<b>CR = 5</b>	<b>SR = 5 (CYA)</b>	DIA2		<i>Fragilaria crotonensis</i>
chemical-negative control			CHR2		<i>Ochromonas danica</i>
CYA5		<i>Synechococcus</i> sp.			<b>Selection 20</b>
CYA1		<i>Anabaena flos-aquae</i>			<b>medium control</b>
CYA4		<i>Planktothrix rubescens</i>			
CYA3		<i>Microcystis aeruginosa</i>	<b>Selection 21</b>	<b>CR = 5</b>	<b>SR = 11</b>
CYA2		<i>Aphanizomenon flos-aquae</i>	CHL4		<i>Kirchneriella subcapitata</i>
			CYA5		<i>Synechococcus</i> sp.
<b>Selection 15</b>	<b>CR = 5</b>	<b>SR = 11</b>	CYA4		<i>Planktothrix rubescens</i>
CHL1		<i>Ankistrodesmus bibarianus</i>	CRY2		<i>Cryptomonas</i> spec.
CHL2		<i>Chlamydomonas reinhardtii</i>	CRY3		<i>Komma</i> sp.
CYA5		<i>Synechococcus</i> sp.	CRY4		<i>Rhodomonas</i> sp.
CYA1		<i>Anabaena flos-aquae</i>	DIA5		<i>Tabellaria</i> sp.
CYA4		<i>Planktothrix rubescens</i>	DIA1		<i>Asterionella formosa</i>
CYA3		<i>Microcystis aeruginosa</i>	DIA4		<i>Synedra rumpens</i> var. <i>familiaris</i>
CYA2		<i>Aphanizomenon flos-aquae</i>	CHR3		<i>Poterioochromonas malhamensis</i>
CRY1		<i>Chroomonas</i> sp.	CHR2		<i>Ochromonas danica</i>
CRY3		<i>Komma</i> sp.			<b>Selection 22</b>
DIA4		<i>Synedra rumpens</i> var. <i>familiaris</i>	CHR1	<b>CR = 5</b>	<b>SR = 3 (CHR)</b>
CHR3		<i>Poterioochromonas malhamensis</i>	CHR3		<i>Chrysocapsa epiphytica</i>
			CHR2		<i>Poterioochromonas malhamensis</i>
<b>Selection 16</b>	<b>CR = 5</b>	<b>SR = 5 (CHL)</b>			<i>Ochromonas danica</i>
CHL1		<i>Ankistrodesmus bibarianus</i>			<b>Selection 23</b>
CHL3		<i>Chlorella</i> sp.	CHL5	<b>CR = 3</b>	<b>SR = 5</b>
CHL5		<i>Pediastrum</i> sp.	CHL2		<i>Pediastrum</i> sp.
CHL4		<i>Kirchneriella subcapitata</i>	CRY3		<i>Chlamydomonas reinhardtii</i>
CHL2		<i>Chlamydomonas reinhardtii</i>	CHR3		<i>Komma</i> sp.
			CHR2		<i>Poterioochromonas malhamensis</i>
<b>Selection 17</b>	<b>CR = 5</b>	<b>SR = 5</b>			<i>Ochromonas danica</i>
CHL1		<i>Ankistrodesmus bibarianus</i>			<b>Selection 24</b>
CYA2		<i>Aphanizomenon flos-aquae</i>	CYA5	<b>CR = 5</b>	<b>SR = 5 (CYA)</b>
CRY1		<i>Chroomonas</i> sp.	CYA1		<i>Synechococcus</i> sp.
DIA3		<i>Nitzschia</i> sp.	CYA4		<i>Anabaena flos-aquae</i>
CHR2		<i>Ochromonas danica</i>	CYA3		<i>Planktothrix rubescens</i>
			CYA2		<i>Microcystis aeruginosa</i>
<b>Selection 18</b>	<b>CR = 5</b>	<b>SR = 8</b>			<i>Aphanizomenon flos-aquae</i>
CHL2		<i>Chlamydomonas reinhardtii</i>			<b>Selection 25</b>
CYA2		<i>Aphanizomenon flos-aquae</i>	CHL1	<b>CR = 3</b>	<b>SR = 5</b>
CRY3		<i>Komma</i> sp.	CHL3		<i>Ankistrodesmus bibarianus</i>
DIA1		<i>Asterionella formosa</i>	CYA4		<i>Chlorella</i> sp.
DIA3		<i>Nitzschia</i> sp.	CYA2		<i>Planktothrix rubescens</i>
DIA4		<i>Synedra rumpens</i> var. <i>familiaris</i>	CHR3		<i>Aphanizomenon flos-aquae</i>
CHR1		<i>Chrysocapsa epiphytica</i>			<i>Poterioochromonas malhamensis</i>
CHR3		<i>Poterioochromonas malhamensis</i>			

**Table S4.** (continued)

<b>Selection 26</b>	<b>CR = 5</b>	<b>SR = 8</b>	<b>Selection 33</b>	<b>CR = 5</b>	<b>SR = 5</b>
CHL4		<i>Kirchneriella subcapitata</i>	CHL3		<i>Chlorella</i> sp.
CHL2		<i>Chlamydomonas reinhardtii</i>	CYA3		<i>Microcystis aeruginosa</i>
CYA4		<i>Planktothrix rubescens</i>	CRY4		<i>Rhodomonas</i> sp.
CYA3		<i>Microcystis aeruginosa</i>	DIA5		<i>Tabellaria</i> sp.
CRY1		<i>Chroomonas</i> sp.	CHR3		<i>Poterioochromonas malhamensis</i>
CRY4		<i>Rhodomonas</i> sp.			
DIA4		<i>Synedra rumpens</i> var. <i>familiaris</i>	<b>Selection 34</b>	<b>bacterial control 1</b>	
CHR3		<i>Poterioochromonas malhamensis</i>	CHL1-CHL5 and CYA1-CYA4		filtrate
<b>Selection 27</b>	<b>CR = 3</b>	<b>SR = 5</b>	<b>Selection 35</b>	<b>CR = 5</b>	<b>SR = 11</b>
CYA4		<i>Planktothrix rubescens</i>	CHL1		<i>Ankistrodesmus bibarianus</i>
CYA2		<i>Aphanizomenon flos-aquae</i>	CHL4		<i>Kirchneriella subcapitata</i>
CRY2		<i>Cryptomonas</i> sp.	CYA1		<i>Anabaena flos-aquae</i>
DIA1		<i>Asterionella formosa</i>	CYA4		<i>Planktothrix rubescens</i>
DIA4		<i>Synedra rumpens</i> var. <i>familiaris</i>	CYA3		<i>Microcystis aeruginosa</i>
			CRY2		<i>Cryptomonas</i> sp.
<b>Selection 28</b>	<b>CR = 5</b>	<b>SR = 5 (CHL)</b>	CRY3		<i>Komma</i> sp.
<b>chemical-negative control</b>			DIA2		<i>Fragilaria crotonensis</i>
CHL1		<i>Ankistrodesmus bibarianus</i>	CHR1		<i>Chrysocapsa epiphytica</i>
CHL3		<i>Chlorella</i> sp.	CHR3		<i>Poterioochromonas malhamensis</i>
CHL5		<i>Pediastrum</i> sp.	CHR2		<i>Ochromonas danica</i>
CHL4		<i>Kirchneriella subcapitata</i>			
CHL2		<i>Chlamydomonas reinhardtii</i>	<b>Selection 36</b>	<b>bacterial control 2</b>	
<b>Selection 29</b>	<b>CR = 5</b>	<b>SR = 4 (CRY)</b>	CHR1-CHR3		filtrate
CRY2		<i>Cryptomonas</i> sp.	CRY1-CRY4		filtrate
CRY1		<i>Chroomonas</i> sp.	DIA1-DIA5		filtrate
CRY3		<i>Komma</i> sp.			
CRY4		<i>Rhodomonas</i> sp.			
<b>Selection 30</b>	<b>CR = 3</b>	<b>SR = 5</b>			
CHL4		<i>Kirchneriella subcapitata</i>			
CYA5		<i>Synechococcus</i> sp.			
CYA2		<i>Aphanizomenon flos-aquae</i>			
DIA5		<i>Tabellaria</i> sp.			
DIA3		<i>Nitzschia</i> sp.			
<b>Selection 31</b>	<b>CR = 1</b>	<b>SR = 3 (CYA)</b>			
CYA1		<i>Anabaena flos-aquae</i>			
CYA4		<i>Planktothrix rubescens</i>			
CYA2		<i>Aphanizomenon flos-aquae</i>			
<b>Selection 32</b>	<b>CR = 3</b>	<b>SR = 5</b>			
CRY1		<i>Chroomonas</i> sp.			
CRY3		<i>Komma</i> sp.			
DIA2		<i>Fragilaria crotonensis</i>			
DIA4		<i>Synedra rumpens</i> var. <i>familiaris</i>			
CHR3		<i>Poterioochromonas malhamensis</i>			

**Table S5.** Biovolumes per culture in each selection.

	Replicate:	Biovolume [x 2*10 <sup>5</sup> µg/L]			Replicate:	Biovolume [x 2*10 <sup>5</sup> µg/L]	
		1	2			1	2
<b>Selection</b>	<b>1</b>	<b>3.30</b>	<b>3.30</b>	Species	CHL2	0.93	0.11
Species	CHR1	0.46	0.10	Species	CHR2	1.87	2.39
Species	CHR2	1.63	1.90	Species	CRY2	0.05	0.24
Species	CHR3	1.20	1.29	Species	CYA4	0.34	0.29
<b>Selection</b>	<b>2</b>	<b>3.30</b>	<b>3.30</b>	Species	DIA5	0.11	0.08
Species	CHL1	1.78	2.86	<b>Selection</b>	<b>11</b>	<b>3.30</b>	<b>3.30</b>
Species	CHL2	0.89	0.13	Species	CHL1	0.64	0.72
Species	CHL5	0.63	0.31	Species	CHL2	0.32	0.03
<b>Selection</b>	<b>3</b>	<b>3.30</b>	<b>2.49</b>	Species	CHR1	0.18	0.04
Species	CHL3	1.34	1.32	Species	CHR2	0.64	0.71
Species	CHR1	0.37	0.08	Species	CHR3	0.47	0.48
Species	CRY1	0.06	0.11	Species	CRY1	0.03	0.05
Species	CRY3	0.15	0.22	Species	CRY3	0.07	0.10
Species	CYA4	0.23	0.18	Species	CRY4	0.09	0.03
Species	CYA5	1.03	0.16	Species	CYA3	0.80	0.93
Species	DIA1	0.05	0.37	Species	DIA1	0.03	0.17
Species	DIA5	0.07	0.05	Species	DIA5	0.04	0.03
<b>Selection</b>	<b>4</b>	<b>1.68</b>	<b>2.43</b>	<b>Selection</b>	<b>12</b>	<b>3.30</b>	<b>3.22</b>
Species	DIA1	0.08	0.59	Species	CHL5	0.84	0.26
Species	DIA2	0.42	0.31	Species	CHR3	1.77	1.62
Species	DIA3	0.25	0.52	Species	CRY2	0.06	0.24
Species	DIA4	0.83	0.93	Species	CYA1	0.53	0.51
Species	DIA5	0.11	0.08	Species	DIA1	0.09	0.59
<b>Selection</b>	<b>5</b>	<b>1.68</b>	<b>2.43</b>	<b>Selection</b>	<b>13</b>	<b>3.30</b>	<b>3.30</b>
Species	DIA1	0.08	0.59	Species	CHL4	1.64	2.60
Species	DIA2	0.42	0.31	Species	CHR1	0.38	0.11
Species	DIA3	0.25	0.52	Species	CRY3	0.15	0.30
Species	DIA4	0.83	0.93	Species	CYA5	1.05	0.22
Species	DIA5	0.11	0.08	Species	DIA5	0.08	0.07
<b>Selection</b>	<b>6</b>	<b>3.30</b>	<b>3.28</b>	<b>Selection</b>	<b>14</b>	<b>3.30</b>	<b>3.30</b>
Species	CHL5	0.47	0.16	Species	CYA1	0.22	0.33
Species	CHR2	1.35	1.49	Species	CYA2	0.88	0.59
Species	CRY1	0.06	0.11	Species	CYA3	1.23	2.03
Species	CRY3	0.15	0.22	Species	CYA4	0.18	0.18
Species	CRY4	0.19	0.07	Species	CYA5	0.79	0.16
Species	CYA1	0.30	0.32	<b>Selection</b>	<b>15</b>	<b>3.30</b>	<b>3.30</b>
Species	DIA3	0.18	0.32	Species	CHL1	0.53	0.75
Species	DIA4	0.59	0.58	Species	CHL2	0.27	0.03
<b>Selection</b>	<b>7</b>	<b>3.30</b>	<b>3.30</b>	Species	CHR3	0.40	0.50
Species	CHL3	0.53	0.57	Species	CRY1	0.02	0.05
Species	CHL4	0.63	0.82	Species	CRY3	0.06	0.11
Species	CHR2	0.51	0.64	Species	CYA1	0.12	0.16
Species	CHR3	0.38	0.44	Species	CYA2	0.48	0.28
Species	CRY1	0.02	0.05	Species	CYA3	0.67	0.97
Species	CRY2	0.01	0.06	Species	CYA4	0.10	0.09
Species	CYA1	0.11	0.14	Species	CYA5	0.43	0.08
Species	CYA2	0.45	0.25	Species	DIA4	0.23	0.29
Species	CYA5	0.40	0.07	<b>Selection</b>	<b>16</b>	<b>3.30</b>	<b>3.30</b>
Species	DIA4	0.22	0.25	Species	CHL1	0.80	1.00
Species	DIA5	0.03	0.02	Species	CHL2	0.40	0.05
<b>Selection</b>	<b>8</b>	<b>0.78</b>	<b>1.08</b>	Species	CHL3	0.83	0.87
Species	CRY1	0.11	0.21	Species	CHL4	0.99	1.27
Species	CRY2	0.06	0.30	Species	CHL5	0.28	0.11
Species	CRY3	0.27	0.44	<b>Selection</b>	<b>17</b>	<b>3.30</b>	<b>3.30</b>
Species	CRY4	0.34	0.14	Species	CHL1	1.07	1.25
<b>Selection</b>	<b>9</b>	<b>3.30</b>	<b>3.11</b>	Species	CHR2	1.08	1.23
				Species	CRY1	0.05	0.09

		Biovolume [x 2*10 <sup>5</sup> µg/L]			Biovolume [x 2*10 <sup>5</sup> µg/L]		
	Replicate:	1	2		Replicate:	1	2
Species	CYA2	0.96	0.47	Species	CHR3	0.54	0.57
Species	DIA3	0.14	0.27	Species	CRY1	0.03	0.06
<b>Selection</b>	<b>18</b>	<b>3.30</b>	<b>3.24</b>	Species	CRY4	0.10	0.04
Species	CHL2	0.53	0.07	Species	CY43	0.91	1.10
Species	CHR1	0.30	0.08	Species	CY44	0.13	0.10
Species	CHR3	0.78	1.02	Species	DIA4	0.32	0.33
Species	CRY3	0.12	0.22	<b>Selection</b>	<b>27</b>	<b>3.30</b>	<b>2.96</b>
Species	CYA2	0.94	0.57	Species	CRY2	0.06	0.24
Species	DIA1	0.04	0.37	Species	CY42	1.87	0.92
Species	DIA3	0.14	0.32	Species	CY44	0.38	0.29
Species	DIA4	0.46	0.58	Species	DIA1	0.08	0.59
<b>Selection</b>	<b>19</b>	<b>3.30</b>	<b>3.30</b>	Species	DIA4	0.91	0.93
Species	CHL1	0.95	1.27	<b>Selection</b>	<b>28</b>	<b>3.30</b>	<b>3.30</b>
Species	CHL2	0.47	0.06	Species	CHL1	0.80	1.00
Species	CHL5	0.33	0.14	Species	CHL2	0.40	0.05
Species	CHR2	0.95	1.26	Species	CHL3	0.83	0.87
Species	CRY1	0.04	0.09	Species	CHL4	0.99	1.27
Species	CRY4	0.13	0.06	Species	CHL5	0.28	0.11
Species	CY41	0.21	0.27	<b>Selection</b>	<b>29</b>	<b>0.78</b>	<b>1.08</b>
Species	DIA2	0.21	0.16	Species	CRY1	0.11	0.21
<b>Selection</b>	<b>21</b>	<b>3.30</b>	<b>3.30</b>	Species	CRY2	0.06	0.30
Species	CHL4	0.86	1.02	Species	CRY3	0.27	0.44
Species	CHR2	0.69	0.80	Species	CRY4	0.34	0.14
Species	CHR3	0.51	0.54	<b>Selection</b>	<b>30</b>	<b>3.30</b>	<b>3.30</b>
Species	CRY2	0.02	0.08	Species	CHL4	1.31	2.09
Species	CRY3	0.08	0.12	Species	CY42	0.95	0.63
Species	CRY4	0.10	0.04	Species	CY45	0.84	0.17
Species	CY44	0.12	0.10	Species	DIA3	0.14	0.35
Species	CY45	0.55	0.09	Species	DIA5	0.06	0.06
Species	DIA1	0.03	0.20	<b>Selection</b>	<b>31</b>	<b>3.30</b>	<b>3.30</b>
Species	DIA4	0.30	0.31	Species	CY41	0.57	0.98
Species	DIA5	0.04	0.03	Species	CY42	2.28	1.77
<b>Selection</b>	<b>22</b>	<b>3.30</b>	<b>3.30</b>	Species	CY44	0.46	0.55
Species	CHR1	0.46	0.10	<b>Selection</b>	<b>32</b>	<b>3.30</b>	<b>3.30</b>
Species	CHR2	1.63	1.90	Species	CHR3	1.57	1.58
Species	CHR3	1.20	1.29	Species	CRY1	0.10	0.17
<b>Selection</b>	<b>23</b>	<b>3.30</b>	<b>3.30</b>	Species	CRY3	0.24	0.34
Species	CHL2	0.61	0.08	Species	DIA2	0.47	0.30
Species	CHL5	0.43	0.18	Species	DIA4	0.92	0.91
Species	CHR2	1.22	1.66	<b>Selection</b>	<b>33</b>	<b>3.30</b>	<b>3.30</b>
Species	CHR3	0.90	1.13	Species	CHL3	1.06	0.98
Species	CRY3	0.14	0.24	Species	CHR3	0.76	0.76
<b>Selection</b>	<b>24</b>	<b>3.30</b>	<b>3.30</b>	Species	CRY4	0.15	0.05
Species	CY41	0.22	0.33	Species	CY43	1.28	1.47
Species	CY42	0.88	0.59	Species	DIA5	0.06	0.04
Species	CY43	1.23	2.03	<b>Selection</b>	<b>35</b>	<b>3.30</b>	<b>3.30</b>
Species	CY44	0.18	0.18	Species	CHL1	0.53	0.55
Species	CY45	0.79	0.16	Species	CHL4	0.65	0.70
<b>Selection</b>	<b>25</b>	<b>3.30</b>	<b>3.30</b>	Species	CHR1	0.15	0.03
Species	CHL1	0.86	1.09	Species	CHR2	0.53	0.55
Species	CHL3	0.89	0.94	Species	CHR3	0.39	0.37
Species	CHR3	0.63	0.73	Species	CRY2	0.01	0.05
Species	CY42	0.77	0.41	Species	CRY3	0.06	0.08
Species	CY44	0.15	0.13	Species	CY41	0.12	0.12
<b>Selection</b>	<b>26</b>	<b>3.30</b>	<b>3.30</b>	Species	CY43	0.66	0.72
Species	CHL2	0.36	0.04	Species	CY44	0.09	0.07
Species	CHL4	0.90	1.07	Species	DIA2	0.12	0.07

## S1.2. Data acquisition

### Phytoplankton flow cytometry and data processing.

Culture sample was diluted 1:10 in 0.25% glutaraldehyde / H<sub>2</sub>O, and particle properties were determined using a scanning flow cytometer (CytoSense, CytoBuoy b.v., Woerden, Netherlands) with a flow velocity of 1 µL/s, and triggering on sideway scattering (SWS) of 32, at a beam width of 5 and core speed of 1.47. Particles were measured for a maximum of 300 s or until ca. 15000 particles were counted. If the particle count exceeded 1000 particles/µL, then the sample was remeasured at higher dilution to avoid instrument saturation. Using the software CytoUSB (CytoBuoy b.v., Woerden, Netherlands), concentration and pressure sensor data and all measured single-particle parameters (Listmode particle parameters) were exported in CSV format. Using the statistical software R, a noise cutoff for total red fluorescence (FL Red Total) was determined, and biovolume per particle (in µm<sup>3</sup>) was determined from the total forward scattering per particle (FWS Total) with the following equation <sup>2,3</sup>:

$$B = \sqrt{0.0017 FWS\ Total - 0.0133} [1]$$

Total biovolume (per culture volume, µg / L) was obtained by summing particle biovolumes and adjusting for measured volume and dilution.

### Bacteria counting flow cytometry.

5 µL of fixed sample was diluted 1:100 in Evian water. 5 µL of SYBR® Green I (Invitrogen AG, Basel, Switzerland) working solution (1:100 in anhydrous dimethylsulfoxide) was added to the sample. The sample was briefly vortexed and incubated at 37 °C for 10 min. Flow cytometric measurements were performed on a BD Accuri C6 flow cytometer (BD Accuri, Belgium). The instrument was equipped with a 50 mW laser emitting at a wavelength of 488 nm. Settings were as follows: Run with limits, 50 µL; Fluidics, fast; Threshold, 800 on FL1-H. Data analysis was performed using CFlow® software (BD Accuri, Belgium). Bacteria were counted using electronic gating on the density plots of green fluorescence (FL1; 533 nm) and red fluorescence (FL3; > 670 nm).

### Chemical analysis: Online solid-phase extraction and chromatography

The instrumentation for online solid phase extraction and liquid chromatography and the online solid phase extraction cartridge used for online solid-phase extraction was described previously <sup>4,5</sup>. For online solid-phase extraction, 80 µL 0.5M citric acid buffer (pH 7) were added to 20 mL sample. The entire sample was loaded into a sample loop and enriched on an online SPE cartridge (loading solvent: 2 mM ammonium acetate in H<sub>2</sub>O, pH 7). Separation was performed with an Atlantis T3 column (3 µm, 3.0 mm x 150 mm; Waters, Milford, USA). For chromatography, a gradient was formed by mixing water (A, H<sub>2</sub>O / 0.1% formic acid (FA)) and organic solvent (B, MeOH / 0.1% FA) delivered by two separate pumps (total flow rate: 300 µL/min, gradient: 13.3% B (0-4 min), 13.3 to 95% B (4-20 min), 95% B (20-28 min), 95 to 13.3% B (28-28.2 min), 13.3% B (28.2-32.3 min; reconditioning)). For 5 min, solvent B ran over the SPE cartridge (elution of enriched analytes) before mixing with A (dilution before analytical column). During cartridge elution, the sample loop was washed with acetonitrile (0.5 min, 2 mL/min). During chromatography, the cartridge was washed with acetonitrile (7.5 min, 0.4 mL/min) and reconditioned with loading solvent (6.5 min, 0.4 mL/min), and subsequently the next sample was enriched on the cartridge (11.5 min, 2 mL/min).

Detection was performed using a quadrupole-Orbitrap mass spectrometer (Q-Exactive, Thermo Scientific, Bremen) with a heated electrospray (H-ESI) source. Data was acquired in

polarity-switching mode with data-independent MS<sup>2</sup> acquisition. For positive and negative mode each, a full scan (*m/z* range: 70-1050, resolution: 70'000, maximum injection time: 50 ms, automatic gain control (AGC) target:  $1 \times 10^6$ , profile mode) was followed by three data-independent high-energy collision-induced fragmentation events (resolution: 35'000, maximum injection time: 50 ms, AGC target:  $2 \times 10^5$ , profile mode; isolation windows: *m/z* range: 70-330, normalized collision energy (NCE): 30; *m/z* range: 320-680, NCE: 50; *m/z* range: 670-1030, NCE: 70). Source parameters were set as follows: spray voltage: 4 kV (positive mode), 3 kV (negative mode); capillary temperature: 350 °C, sheath gas: 40; auxiliary gas: 10; spare gas: 0; probe heater temperature: 50 °C.

Quantification of the analytes was performed using the internal standard method with TraceFinder EFS (version 3.2.368.22, Thermo Scientific, Bremen). The mass tolerance was set to 5 ppm. Peak integration was performed with the ICIS algorithm, and integrated peaks were reviewed by hand. If available, the isotope-labeled analyte was used as internal standard; otherwise, an internal standard close in retention time and structure was used.

### S1.3. Data analysis

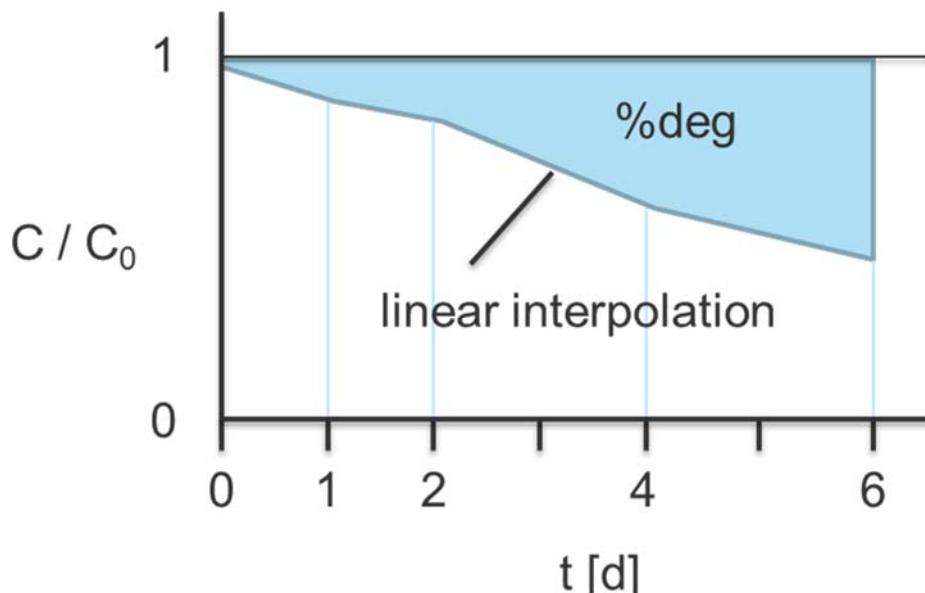
#### Degradation assessment

The degradation integral %deg was determined by 1) determining the average measured starting concentration of the compound  $C_0$  across all samples, 2) linearly interpolating compound concentrations  $C(t)$  between the five measurement points at  $t = 0, 1, 2, 4, 6$  d; 3) integrating the difference between  $C_0$  and  $C(t)$ , i.e., the amount of compound degraded from 0 to 6 days, and 4) dividing by 6 (the experiment duration). The measure is illustrated in Fig. S1 and described by equation 2, where  $C(t)$  is the piecewise linear approximation function between the measured data points.

$$\% \text{ deg} = \frac{1}{6d} \left( \int_{t=0}^{6d} C_0 - C(t) \right) [2]$$

The biomass integral  $B$  was computed in analogy as the area under the curve of the optical density at 750 nm ( $OD_{750}$ ) corrected by background ( $OD_{750,\text{blank}}$ ).  $OD_{750}$  was interpolated between the five measurement points at  $t=0, 1, 2, 4, 6$  d, integrated over 0 to 6 days, and divided by 6. The measure is described by the equation 3, where  $OD_{750}(t)$  is the piecewise linear approximation between the measured data points.

$$B = \frac{1}{6} \left( \int_{t=0}^6 OD_{750}(t) - OD_{750,\text{blank}} \right) [3]$$



**Figure S1.** Determination of %deg, illustrated.

#### Taxonomic class composition

The influence of specific classes on %deg for each compound, #TC and MPMF was analyzed by linear regression of the response variable against 5 dummy variables encoding presence/absence of each taxonomic class (CHL, CHR, CRY, CYA, DIA), using the function *lm* from the statistical package R. Note that the inclusion of CR=5 experiments effectively only includes data for one specific combination of classes (all classes are present).

In analogy to Tilman et al.<sup>6</sup>, the explanatory power of community composition versus CR on %deg for each compound, #TC and MPMF was analyzed with (nested) ANOVA of the response variable against a factor encoding CR (1, 3 or 5 classes) and a factor encoding

community composition (11 combinations for presence/absence of each class: 5 single-class combinations, 5 combinations with CR=3, one combination with CR=5.) Note that community composition is nested within CR.

### **Transformation product screening**

For 13 compounds (atenolol, metoprolol, venlafaxine, mefenamic acid, cyprodinil, carbendazim, tebuconazole, benzotriazole, climbazole, azoxystrobin, fludioxonil, kresoxim-methyl, and sulfamethoxazole), a list of TP candidates was generated from the parent mass and likely modification reactions using the open-source workflow RMassScreening (<https://github.com/meowcat/RMassScreening>). First, a list of compound-specific reactions (Table S6) dependent on the chemical structure (e.g., dechlorination if a chlorine was present in the structure) was applied recursively (i.e., first reactions are applied to the parent, and subsequently follow-up reactions were applied until all reactions were processed).

Subsequently a list of general reactions (Table S7) was applied on all parents and generated TP candidates as specified by the reaction count (e.g., for hydroxylation with count 3, for every parent and TP candidate three new candidates with 1, 2, or 3 hydroxylations were generated), and all generated products were added to the candidate list for the next reaction. Finally, all reactions specified “F” in Table S7 were applied to the parents and candidate list without recursion.

Whereas this generates a large reaction list, during the screening process higher-generation TPs were only considered when the respective precursor was observed and the chemical reaction was plausible.

**Table S6.** Transformation product candidate generation: reactions applied to specific parent compounds.

Parent	Reaction	Loss	Gain
<b>Atenolol (ATE)</b>			
ATE	deisopropylation	C3H7	H
ATE	sidechain loss	C6ONH14	H
ATE	hydrolysis (TP1)	NH2	OH
ATE TP1	decarboxylation	CO2H	H
<b>Metoprolol (MPL)</b>			
MPL	deme	CH3	H
MPL	deipr	C3H7	H
<b>Venlafaxine (VFX)</b>			
VFX	deme	CH3	H
<b>Mefenamic acid (MEF)</b>			
MEF	C8H9 aryl loss (TP1)	C8H9	H
MEF TP1	deamination	NH2	H
MEF	decarboxylation	CO2H	H
MEF	C6H5 aryl loss (TP2)	C6H5	H
MEF TP2	deamination	NH2	H
<b>Cyprodinil (CPD)</b>			
CPD	decyclopropyl	C3H5	H
CPD	C8H9 aryl loss (TP1)	C8H9	H
CPD TP1	deamination	NH2	H
<b>Carbendazim (CBDZ)</b>			
CBDZ	demethylation	CH3	H
CBDZ	urea hydrolysis	C2O2H3	H
<b>Tebuconazole (TEB)</b>			
TEB	dechlorination (reductive)	Cl	H
TEB	dechlorination (oxidative)	Cl	OH
TEB	demethylation	CH3	H
TEB	deethylation	C2H5	H
TEB	depropylation	C3H7	H
TEB	debutylation	C4H9	H
TEB	triazole ring loss	C2N3H2	NH2
TEB	C6H4Cl aryl loss	C6H4Cl	H
<b>Benzotriazole (BTA)</b>			
none (all expected BTA reactions are within the general reactions)			
<b>Climbazole (CLI)</b>			
CLI	demethylation	CH3	H
CLI	deethylation	C2H5	H
CLI	depropylation	C3H7	H
CLI	debutylation	C4H9	H
CLI	decarbox	CO2H	H
CLI	imidazole ring loss (TP1)	C3N2H3	NH2
CLI	ether cleavage 1	C8H8N2O	
CLI	ether cleavage 2	C6H3Cl	
CLI TP1	deamination	NH2	H
CLI and all			
TP	dechlorination (reductive)	Cl	H
CLI and all			
TP	dechlorination (oxidative)	Cl	OH
<b>Fludioxonil (FDX)</b>			
FDX	defluorination (reductive)	F	H
FDX	defluorination (oxidative)	F	OH
FDX	didefluorination (reductive)	F2	H2
FDX	CF2 loss	CF2	H2
FDX	CN oxidation to COOH (TP1)	CN	CO2H
FDX TP1	decarboxylation	CO2H	H

**Kresoxim-methyl (KME)**

KME	demethylation (TP1)	CH3	H
KME	didemethylation (TP2)	C2H6	H2
KME	methoxy loss (TP3)	CH3O	H
KME	methoxy loss + demethylation	C2H6O	H
KME	strobilurin moiety loss	C4O3NH6	H
KME TP1-3	decarboxylation	CO2H	H
KME	ether cleavage 1	C7H7	H
KME	ether cleavage 1 (incl. O)	C7H7O	H
KME	ether cleavage 2	C11H11NO3	
KME	ether cleavage 2 (incl. O)	C11H11NO4	H

**Azoxystrobin (AZY)**

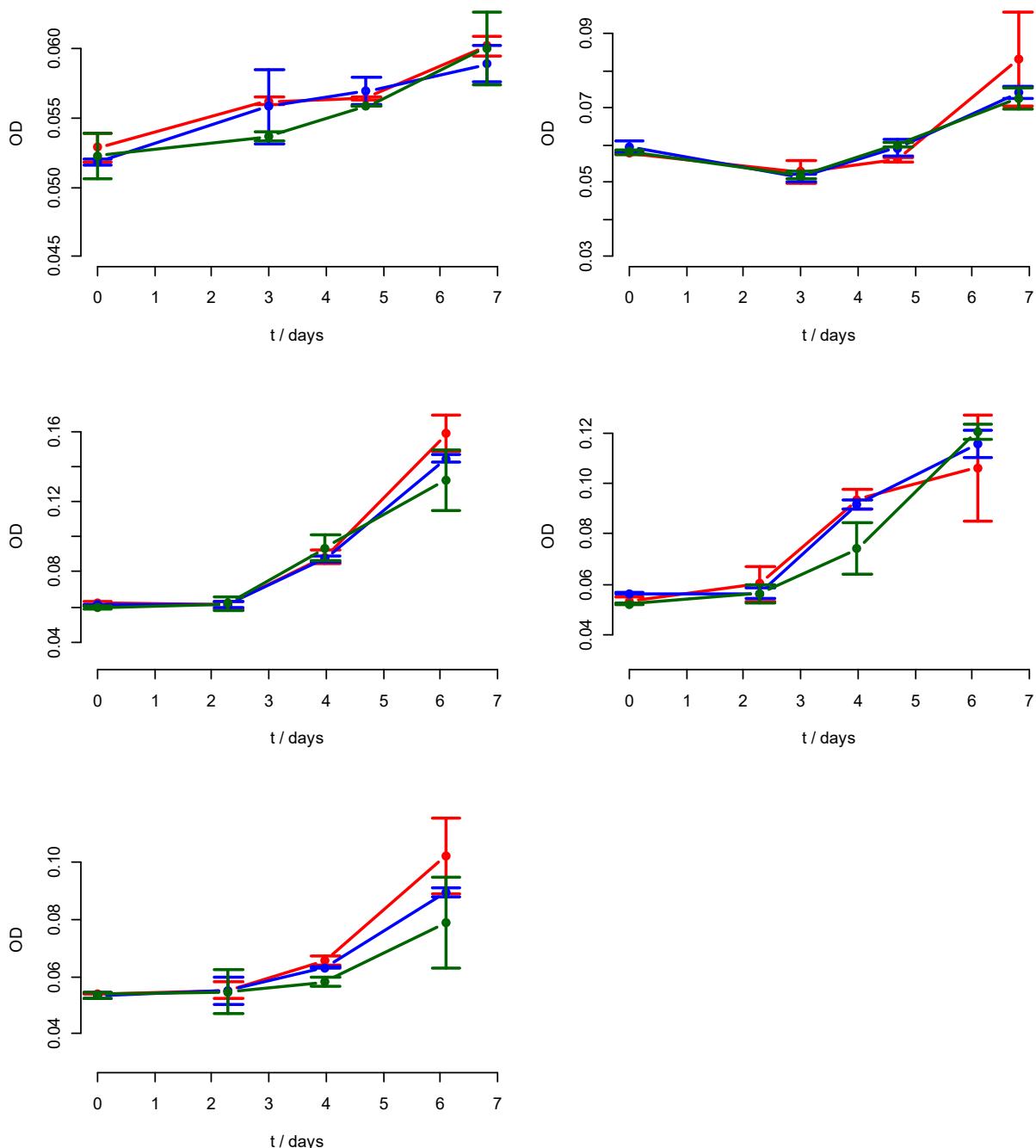
AZY	demethylation (TP1)	CH3	H
AZY	didemethylation (TP2)	C2H6	H2
AZY	methoxy loss (TP3)	CH3O	H
AZY	methoxy loss + demethylation	C2H6O	H
AZY	strobilurin moiety loss (TP4)	C5H7O3	H
AZY TP1-3	decarboxylation	CO2H	H
AZY TP4	ether cleavage 1	C6H5	H
AZY TP4	ether cleavage 1 (incl. O)	C6H5O	H
AZY	ether cleavage 2	C7H5N	H
AZY	ether cleavage 2 (incl. O; TP5)	C7H5NO	H
AZY TP5	ether cleavage 3	C4H2N2	H
AZY	CN oxidation to COOH (TP6)	CN	CO2H
AZY TP6	decarboxylation	COOH	H

**Table S7.** Transformation product candidate generation: reactions applied to all parent compounds.

Reaction	Loss	Gain	Count
hydroxylation	H	OH	3
oxidation	H2		2
reduction		H2	2
methyl to COOH oxidation	CH3	CO2H	2
formylation		CO	F
glucuronidation		C6H8O6	F
sulfate conjugation		SO3	F
taurine conjugation		C2H5NO2S	F
glutathione conjugation		C10H15N3O6S	F
cysteine conjugation		C3H5NO2S	F
acetylation		C2H2O	F
acetyl cysteine conjugation		C5H7NO3S	F
glucose conjugation		C6H10O5	F
glutamate conjugation	H2O	C5H9NO4	F
glycine conjugation	H2O	C2H5NO2	F
aspartate conjugation	H2O	C4H7NO4	F
methylation	H	CH3	F
carboxylation	H	CO2H	F
propanoic acid	H	C3H5O2	F

## S2. Results

### S2.1. Chemical mixture assessment

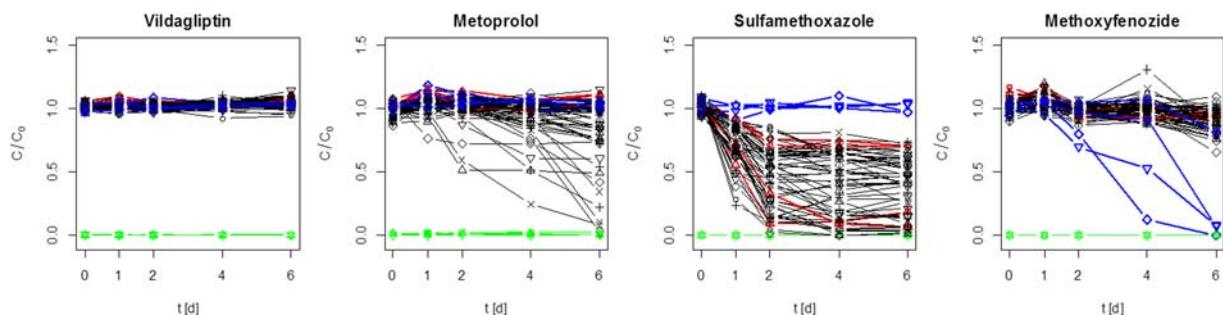


**Figure S2.** Chemical mixture assessment. Growth of 5 species (top left: *Poterioochromonas malhamensis*, top right: *Aphanizomenon flos-aquae*, mid left: *Cyclotella cf. glomerata*, mid right: *Cryptomonas* sp., bottom: *Chlorella* sp. under control conditions (red), 2.5 µg/L (blue) or 10 µg/L (green) chemical mixture concentration

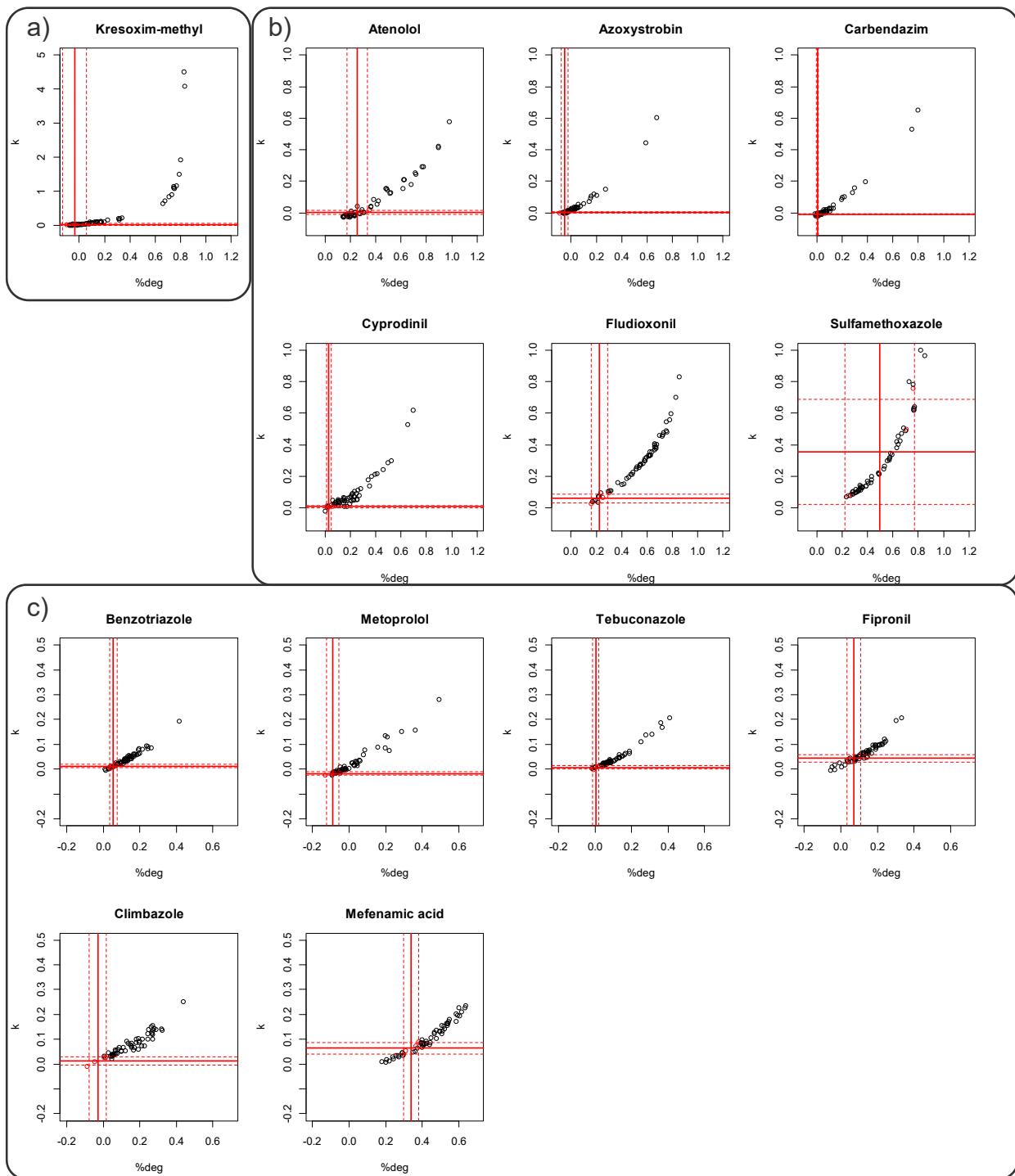
## S2.2. Degradation assessment

For compounds with a maximal %deg of 0.2 or above in cultures, degradation was compared with bacterial controls to verify that the observed degradation was not primarily bacterial. The mean and standard deviation (SD) of the bacterial control samples were calculated, and a cutoff was set to one SD around the mean. The exceedances in negative and positive directions were compared: a one-sided sign test compared the positive exceedances (degradation) to the total exceedances, and a one-sided t-test compared the absolute deviations from the control mean for positive and negative exceedances (when a sufficient number of negative exceedances was present). A compound was classified as degrading if three out of four statistical tests (t test and sign test for k or %deg) were significant on a  $p < 0.05$  level (or no t-tests could be performed for lack of negative exceedances).

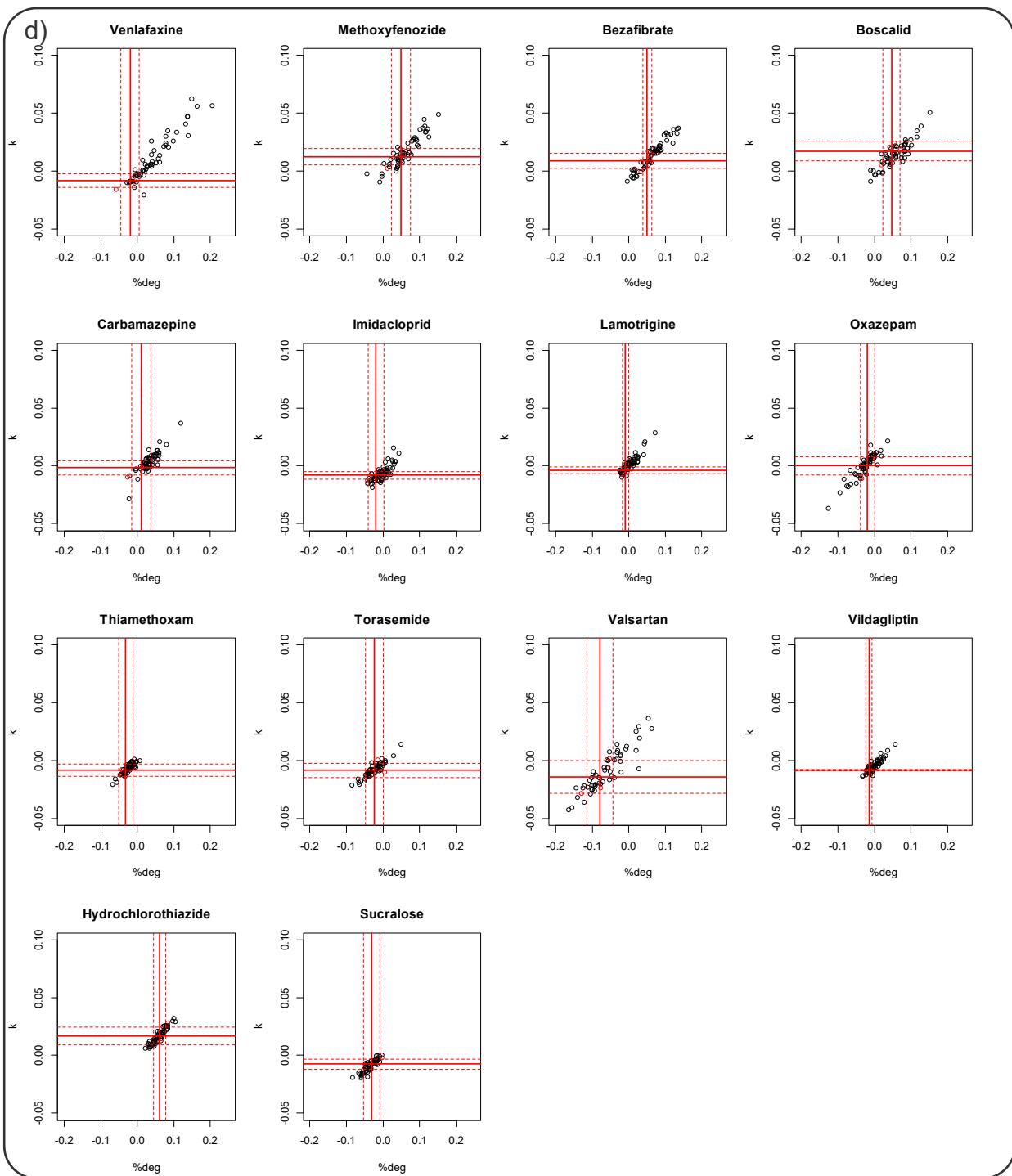
Note: the compounds vildagliptin and lamotrigine showed significant numbers of samples with transformation stronger than bacterial control, but very marginal extent of transformation (maximal %deg of <0.1), making their classification uncertain. We excluded them from the final analysis, however the analyses were run also including the two compounds, confirming the results.



**Figure S3.** Degradation assessment. Examples of corrected concentration time profiles ( $C/C_0$  over time) for a compound persistent in the experiment (vildagliptin), degraded in cultures (metoprolol), degraded by cultures and bacteria (sulfamethoxazole), and degraded exclusively in medium controls (methoxyfenozide). *Black*, phytoplankton communities; *red*, bacterial control; *blue*, medium control; *green*, chemical-free control.



**Figure S4.** Plot of degradation rates versus integrals for 27 compounds (continued on next page)



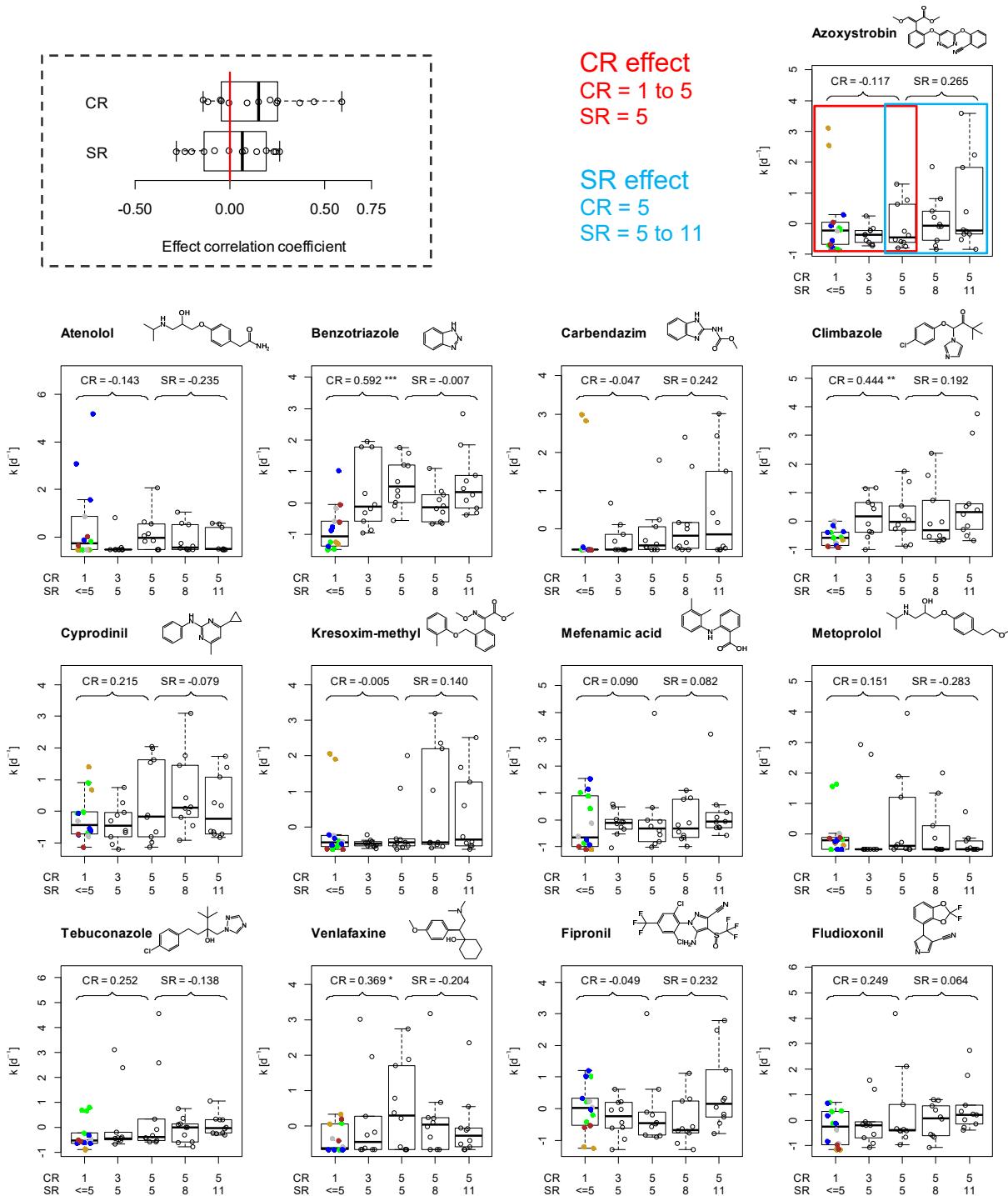
**Figure S4.** Plot of degradation rates versus integrals for 27 compounds. a) Kresoxim-methyl (maximal rate:  $k=4.8$ ), b) compounds with maximal  $k$  of 0.5 to 1, c) compounds with maximal  $k$  of 0.25 to 0.5. Red, bacterial controls; black, phytoplankton communities; red solid lines, mean of bacterial controls; red dotted lines, mean plus/minus one standard deviation of bacterial controls.

**Table S8.** Transformation/persistence assessment of 36 substances.

Substance	Transformation by cultures	bacterial control	stable medium	unreliable analytics
Atenolol	X			
Azoxystrobin	X		X	
Benzotriazole	X			
Carbendazim	X			
Cyprodinil	X			
Kresoxim-methyl	X		X	
Metoprolol	X			
Tebuconazol	X		X	
Venlafaxin	X			
Fipronil	X		X	
Fludioxonil	X			
Climbazole	X	(X) <sup>1</sup>	X	
Mefenamic acid	X	(X) <sup>1</sup>		
Sulfamethoxazole	X	X		
Methoxyfenozide			X	
Bezafibrate			X	
Boscalid			X	
Carbamazepine			X	
Imidacloprid			X	
Lamotrigine			X	
Oxazepam			X	
Thiamethoxam			X	
Torasemide			X	
Valsartan			X	
Vildagliptin			X	
Hydrochlorothiazide			X	
Sucratose			X	
Chlorpyrifos	(X) <sup>2</sup>	(X) <sup>2</sup>	(X) <sup>2</sup>	X
Ketoconazole	(X) <sup>2</sup>	(X) <sup>2</sup>	(X) <sup>2</sup>	X
Amisulpride			(X) <sup>2</sup>	X
Citalopram			(X) <sup>2</sup>	X
Caffeine			(X) <sup>2</sup>	X
Dimethoate			(X) <sup>2</sup>	X
Propamocarb			(X) <sup>2</sup>	X
Fexofenadine		(X) <sup>2</sup>		X
Iopromide				X

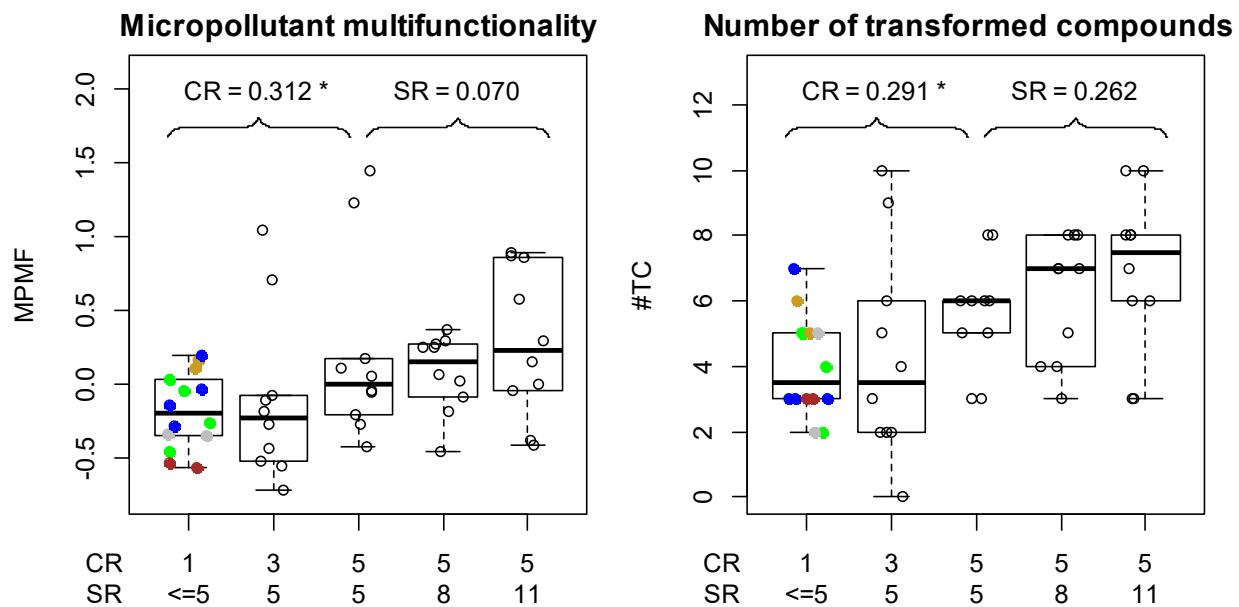
<sup>1</sup>microbial degradation present but to an extent smaller than in culture samples<sup>2</sup>analytics are unreliable or not sensitive enough, therefore degradation or stability assessment is tentative.

### S2.3. Influence of class and species richness on single compound transformation.



**Figure S5.** Richness effects on degradation rates ( $k$ ). Top left: Distribution of class richness (CR) and species richness (SR) effect slopes for all compounds for degradation rates ( $k$ ). Red line indicates the zero effect line. Top right and below: Distribution of degradation rates ( $k$ ) for each compound, separated by SR and CR, and Pearson correlation coefficients for CR and SR effects (top right, illustrated example for azoxystrobin). On top: Pearson correlation coefficient for CR and SR effects, respectively. \*:  $p < 0.05$ ; \*\*:  $p < 0.01$ ; \*\*\*:  $p < 0.001$ . Colors for classes, and boxplot margins are as specified in Fig. 1.

## S2.4. Influence of class and species richness on overall compound transformation.



**Figure S6.** Influence of CR and SR on micropollutant multifunctionality (MPMF, left) and number of compounds transformed (#TC, right), determined from transformation rates ( $k$ ). On top Pearson correlation coefficient for CR and SR effects, respectively (n=34 and n=30 for CR and SR effect, respectively.). \*:  $p < 0.05$  \*\*:  $p < 0.01$ . Colors for classes, and boxplot margins are as specified in Fig. 1.

## S2.5. Influence of class identity

The effect of CR might, for single compounds, be caused by changes in community composition, rather than the actual number of algal groups present. (i.e., sampling effect)<sup>13</sup>. The single-group transformation rates (Fig. 1) suggest the importance of community composition and group identity in cases such as tebuconazole and metoprolol (CHL), mefenamic acid (CYA), azoxystrobin, and carbendazim (CHR). Given the high activity observed for single algal groups and many compounds, we investigated the effect of community composition in more detail. To this end, we studied the effect of presence or absence of each group on %deg of individual compounds, as well as on MPMF and #TC. For all experiments with 1 or 3 CR, multiple regressions for %deg values, MPMF or TC were conducted against five binary variables encoding presence or absence of CHL, CYA, CHR, CRY, and DIA. The results are shown in Table S9.

Five compounds each showed positive effects of CHL, CHR, or CYA presence, respectively, and 2 for CRY presence. By contrast, CHR and CHL presence had a negative effect in one case, CRY presence in two cases and DIA presence in 4 cases. For 5 compounds, significant positive effects were observed for multiple algal groups. In summary, this shows that single classes can be significantly important for the transformation of individual compounds but overall there is no single group that dominates the total community effect. DIA presence showed only significant negative effects, suggesting that their presence contributed to a lower fraction of biomass being active in transformation; also, the DIA strains exhibited overall slow growth. Therefore, all examined groups except DIA contribute to the CR effect on micropollutants biotransformation. This is also reflected in the MPMF, where CHL, CHR, and CYA contribute positively. The same evaluation was conducted including the 5 CR and 5 SR experiments, yielding similar results (Table S10). Overall, we conclude that multiple algal groups contributed to the overall CR effect.

To compare community composition and CR effects, an ANOVA was conducted for the individual compound %deg and multifunctionality (MPMF and #TC) measures against CR and composition. The results (Table S11) varied depending on different compounds, showing significance for CR (2 compounds: climbazole and cyprodinil), community composition (3 compounds: atenolol, azoxystrobin, and carbendazim) or both (2 compounds, benzotriazole and venlafaxine); #TC was affected by both, whereas for MPMF, only by CR. Overall this supports the conclusions above, that community composition is only part of the explanation for the observed CR effects.

**Table S9.** Influence of class identity at CR = 1 or 3. p-values for multiple linear regressions (n=24 for each compound) of %deg values per compound, #TC, and MPMF against presence/absence of the classes CHL, CHR, CRY, CYA, DIA in experiments with CR= 1 or 3. Colors depict the direction of significant effects (i.e. slope of the significant linear regression fits ( $p < 0.05$ ): green, positive effect; red, negative effect).

	CHL	CHR	CRY	CYA	DIA
<b>Atenolol</b>	0.07	0.42	0.85	0.08	0.08
<b>Azoxystrobin</b>	0.02	0.005	0.02	0.35	0.71
<b>Benzotriazole</b>	0.15	0.07	0.05	0.05	0.61
<b>Carbendazim</b>	0.14	<0.0001	0.006	0.56	0.35
<b>Climbazole</b>	0.006	0.0008	0.02	0.008	0.41
<b>Cyprodinil</b>	0.005	0.02	0.96	0.12	0.01
<b>Kresoxim-methyl</b>	0.07	0.64	0.35	0.04	0.001
<b>Mefenamic acid</b>	0.04		0.34	0.24	0.09
<b>Metoprolol</b>	0.06	0.71	0.30	0.94	0.47
<b>Tebuconazole</b>	0.005		0.22	0.64	0.22
<b>Venlafaxine</b>	0.69	0.001	0.19	0.29	0.82
<b>Fipronil</b>	0.18	0.0003	0.005	0.14	0.0006
<b>Fludioxonil</b>	0.006		0.76	0.66	0.008
<b>#TC</b>	0.33	0.01	0.95	0.24	0.03
<b>MPMF</b>	0.05	0.01	0.99	0.006	0.007

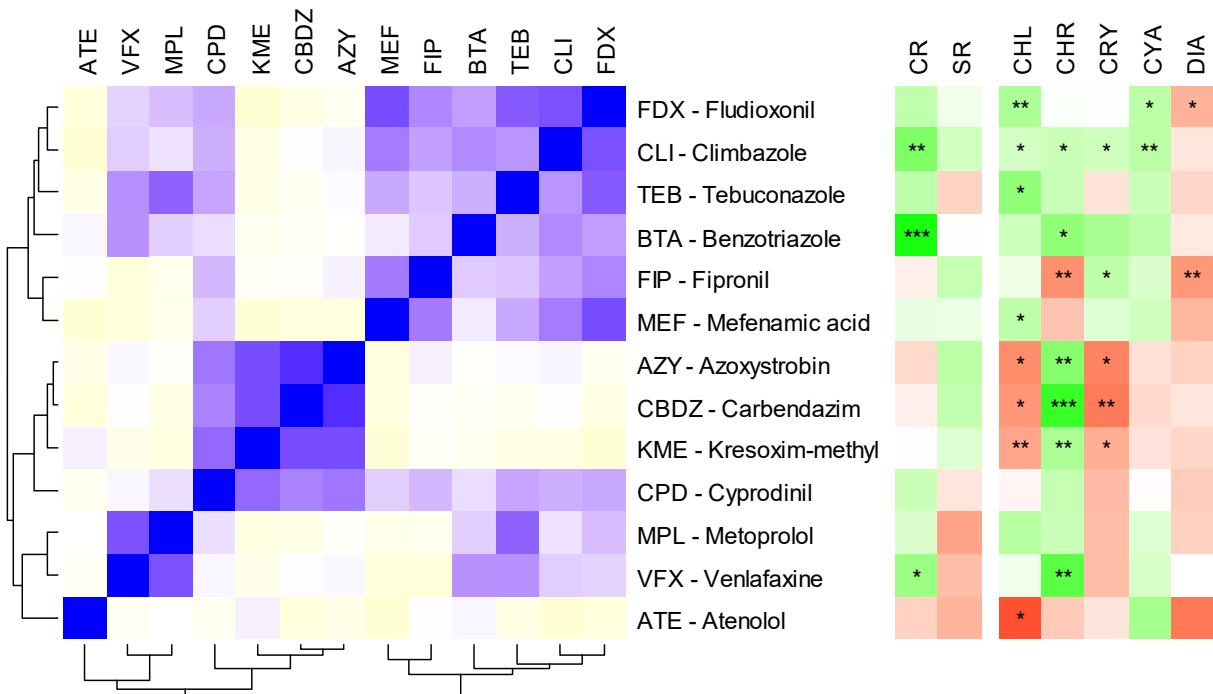
**Table S10.** Influence of class identity at SR≤5. p values for multiple linear regressions (n=34 for each compound) of %deg values per compound, #TC, and MPMF against presence/absence of the classes CHL, CHR, CRY, CYA, DIA in experiments with CR 1, 3 or 5 and SR≤5. Colors depict the direction of significant effects (i.e. slope of the significant linear regression fits;  $p < 0.05$ , green, positive effect, red, negative effect)

	CHL	CHR	CRY	CYA	DIA
<b>Atenolol</b>	0.18	0.78	0.65	0.006	0.16
<b>Azoxystrobin</b>	0.08	0.001	0.06	0.80	0.86
<b>Benzotriazole</b>	0.35	0.15	0.11	0.11	0.28
<b>Carbendazim</b>	0.20	<0.0001	0.01	0.48	0.46
<b>Climbazole</b>	0.14	0.03	0.23	0.18	0.25
<b>Cyprodinil</b>	0.05	0.14	0.77	0.24	0.27
<b>Kresoxim-methyl</b>	0.52	0.48	0.31	0.06	0.07
<b>Mefenamic acid</b>	0.17	0.52	0.47	0.18	0.25
<b>Metoprolol</b>	0.05		0.63	0.43	0.89
<b>Tebuconazole</b>	0.03		0.44	0.62	0.44
<b>Venlafaxine</b>	0.73	0.003	0.22	0.33	0.85
<b>Fipronil</b>	0.19	0.02	0.03	0.16	0.03
<b>Fludioxonil</b>	0.08		0.92	0.76	0.09
<b>#TC</b>	0.18	0.006	0.85	0.12	0.05
<b>MPMF</b>	0.12	0.06	0.87	0.03	0.08

**Table S11.** ANOVA of CR versus community composition. p values for individual ANOVAs (n=34 for each compound) of %deg values per compound, #TC, and MPMF against CR (1, 3 or 5 classes) and community composition (presence/absence of each class, 11 total combinations: 5 combinations with CR=1, 5 combinations with CR=3, one combination with CR=5)

	CR	Community composition
<b>Atenolol</b>	0.10	0.005
<b>Azoxystrobin</b>	0.27	0.0004
<b>Benzotriazole</b>	0.0002	0.01
<b>Carbendazim</b>	0.08	0.0001
<b>Climbazole</b>	0.0006	0.18
<b>Cyprodinil</b>	0.03	0.43
<b>Kresoxim-methyl</b>	0.39	0.54
<b>Mefenamic acid</b>	0.70	0.77
<b>Metoprolol</b>	0.65	0.15
<b>Tebuconazole</b>	0.22	0.07
<b>Venlafaxine</b>	0.010	0.010
<b>Fipronil</b>	0.58	0.11
<b>Fludioxonil</b>	0.41	0.47
<b>#TC</b>	0.02	0.03
<b>MPMF</b>	0.03	0.10

## S2.6. Transformation patterns of compounds

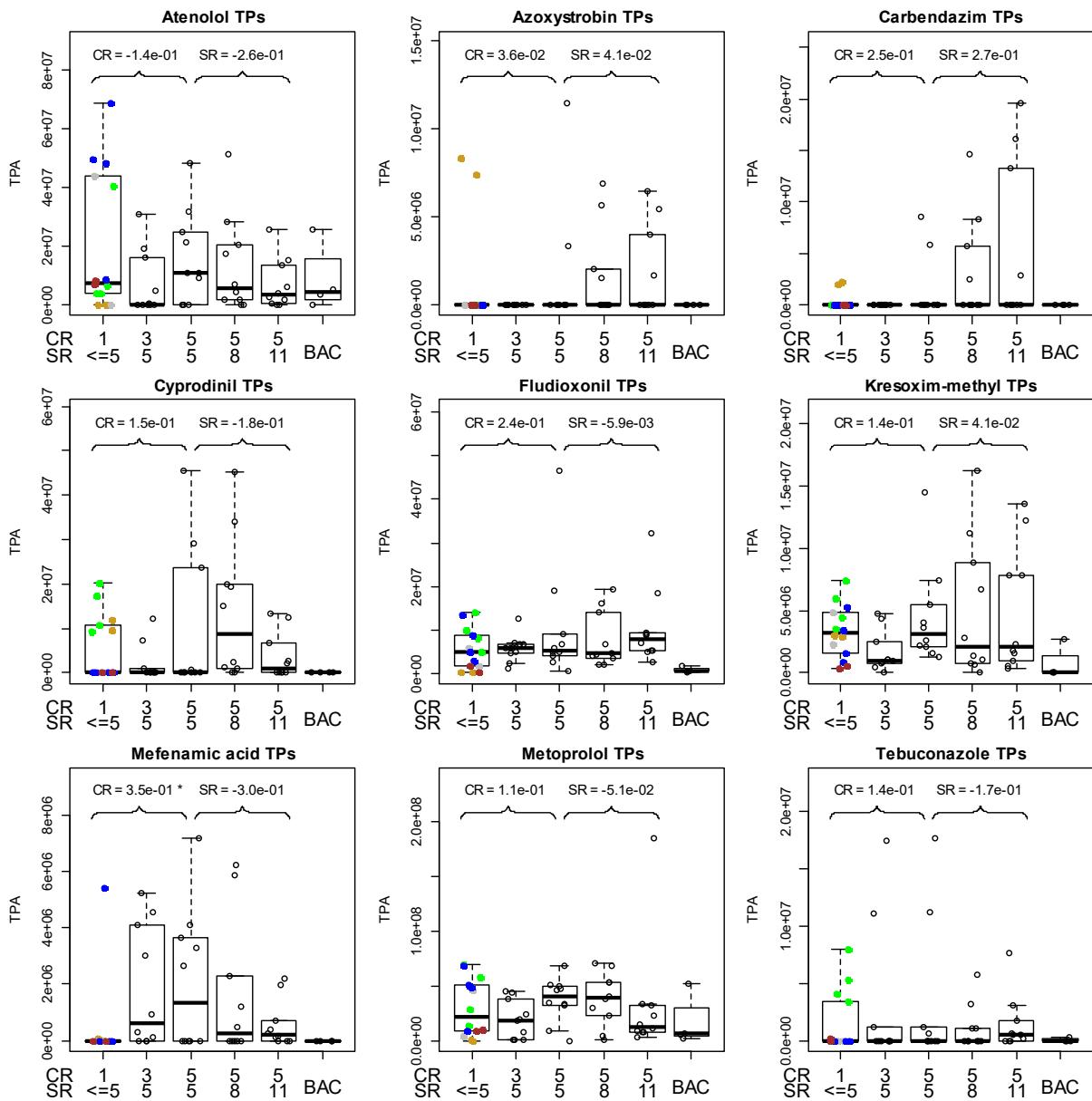


**Figure S7.** Transformation patterns of compounds from transformation rates (k). Left: Hierarchical clustering of Pearson correlation coefficients between compound transformation rates (k) across all samples. Column names are the compound name abbreviations as specified in rows. *Blue*, positive correlation; *white*, no correlation; *yellow*, negative correlation. Right: Effect of CR and SR (as from Fig. 1), and effect of presence/absence of individual classes in CR=1 and CR=3 samples. *Green*, positive effect; *white*, no effect; *red*, negative effect. \*: p<0.05; \*\*: p<0.01; \*\*\*: p<0.001.

## S2.7. The influence of biodiversity on transformation products

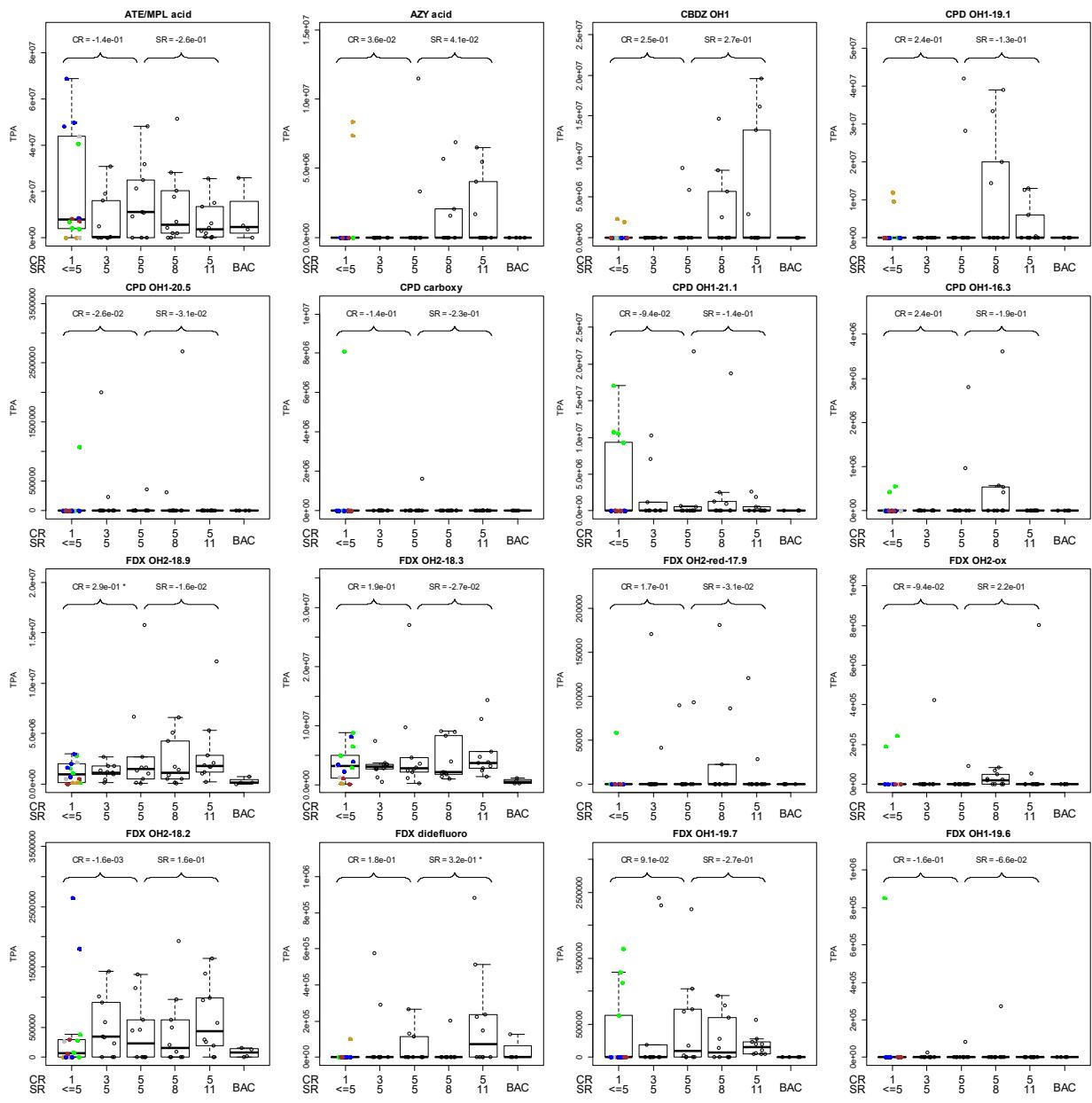
To examine the behavior of individual parent compounds, the total peak area of all potential TPs for each parent were summed and evaluated for CR and SR effects (Fig. S8). The trends were compared to the parent substance trends (Fig. 1). For carbendazim and azoxystrobin (with only a single observed TP), as well as for kresoxim-methyl (2 TPs), the observed TPs appear to match the general trend observed for the parent's transformation. No clear trend is apparent for fludioxonil, metoprolol and tebuconazole. The atenolol (and metoprolol) TP (ATE/MPL acid) shows a moderate negative trend for high SR, resembling the trend for atenolol parent, but is not clearly interpretable since there is also bacterial formation.

By contrast, the TPs for mefenamic acid and cyprodinil show a strong decrease for high species diversity which is not observed for the parents. These examples show that “further biotransformation” at high diversity levels can occur at the level of individual compounds, and the effects of diversity are more complex than an additive view would suggest.

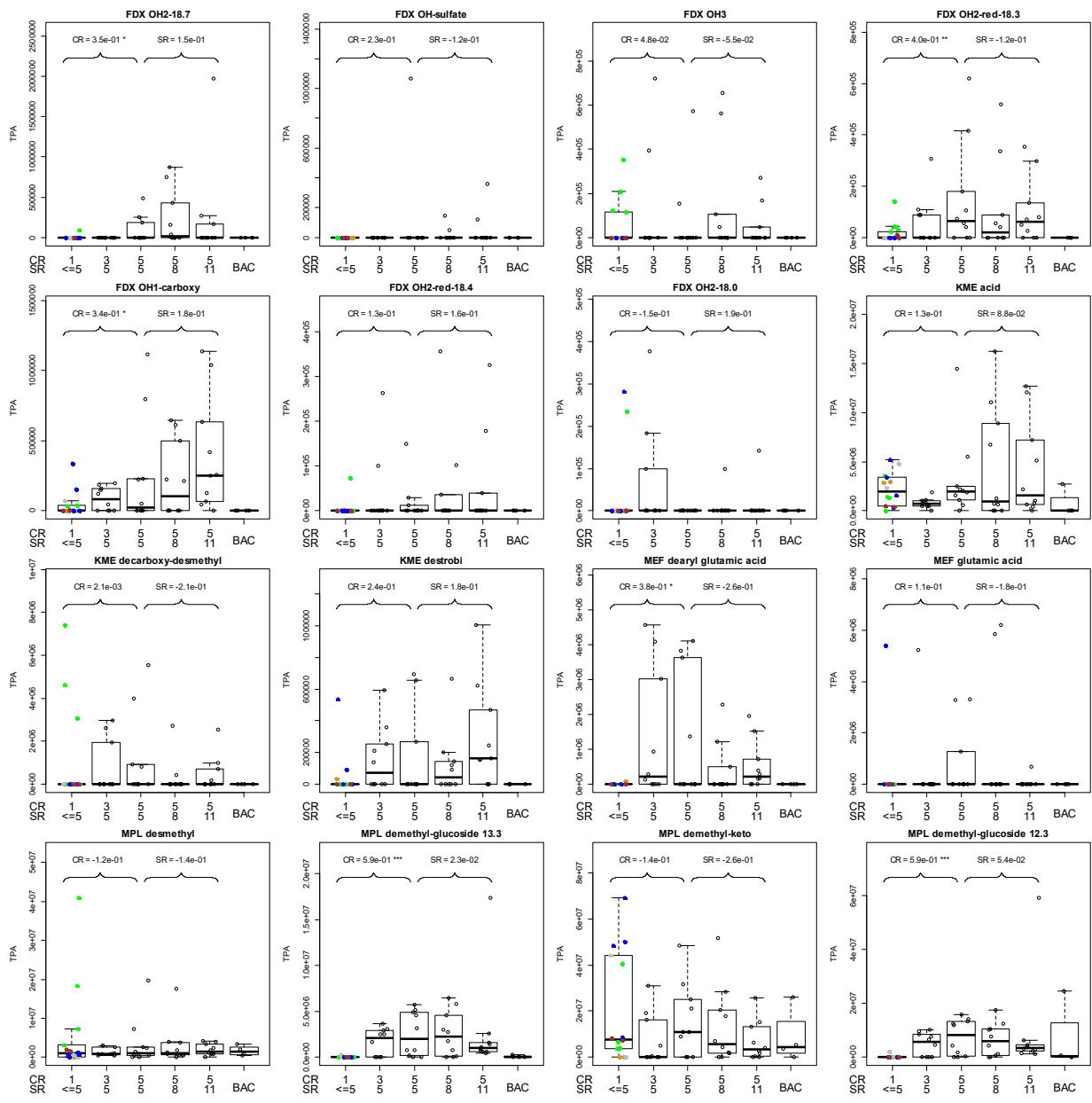


**Figure S8.** Richness effects on total TPs per compound. For 10 parent compounds, sum of total peak areas (TPA) of all observed TP, for assembled communities by CR and SR, and for bacterial controls. Atenolol and metoprolol are evaluated in combination, since they share the important TP atenolol acid. BAC, bacterial control. On top: Pearson correlation coefficient for CR and SR effects, respectively.

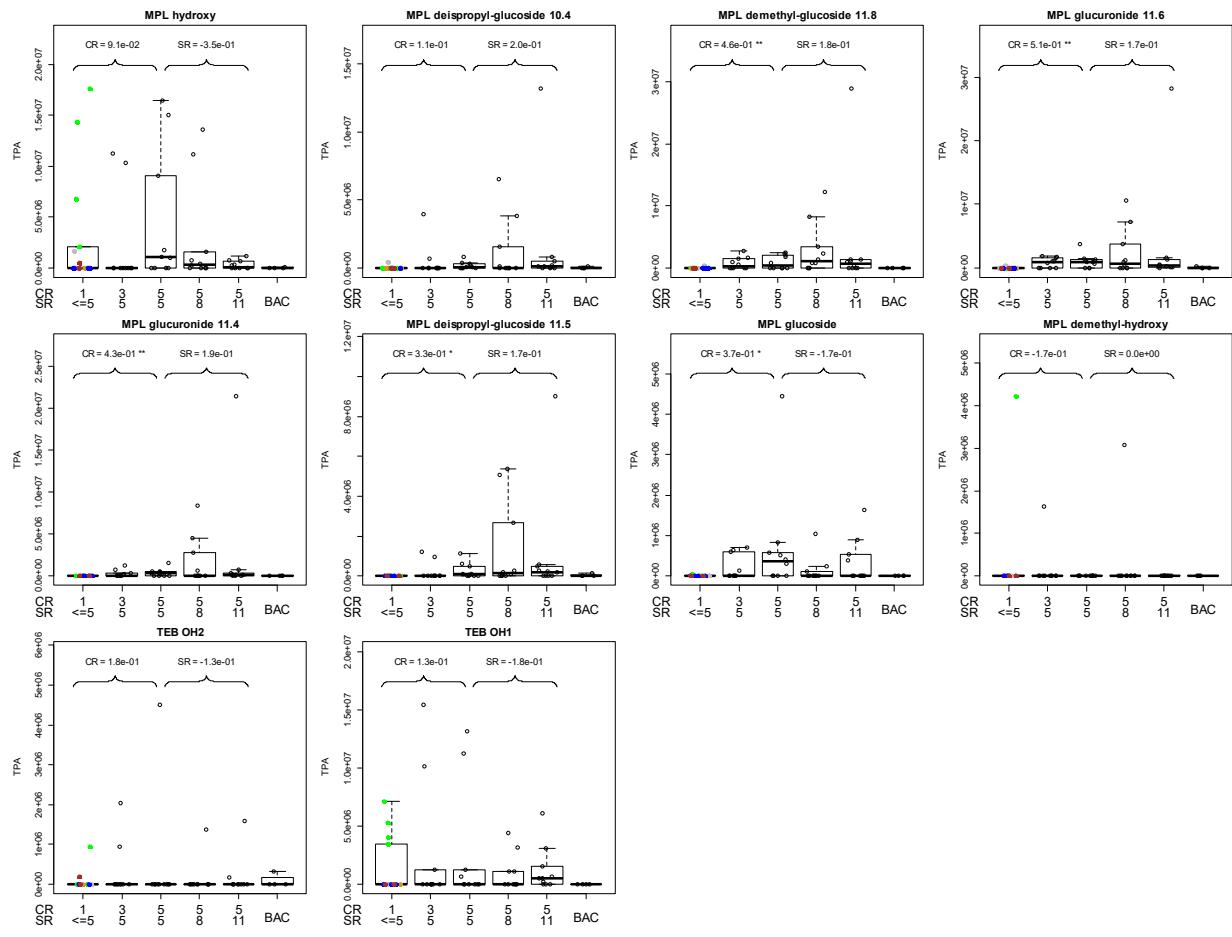
\*: p<0.05; \*\*: p<0.01; \*\*\*: p<0.001. Colors for classes, and boxplot margins are as specified in Fig. 1.



**Figure S9.** Richness effects on individual TPs (continued on next page)

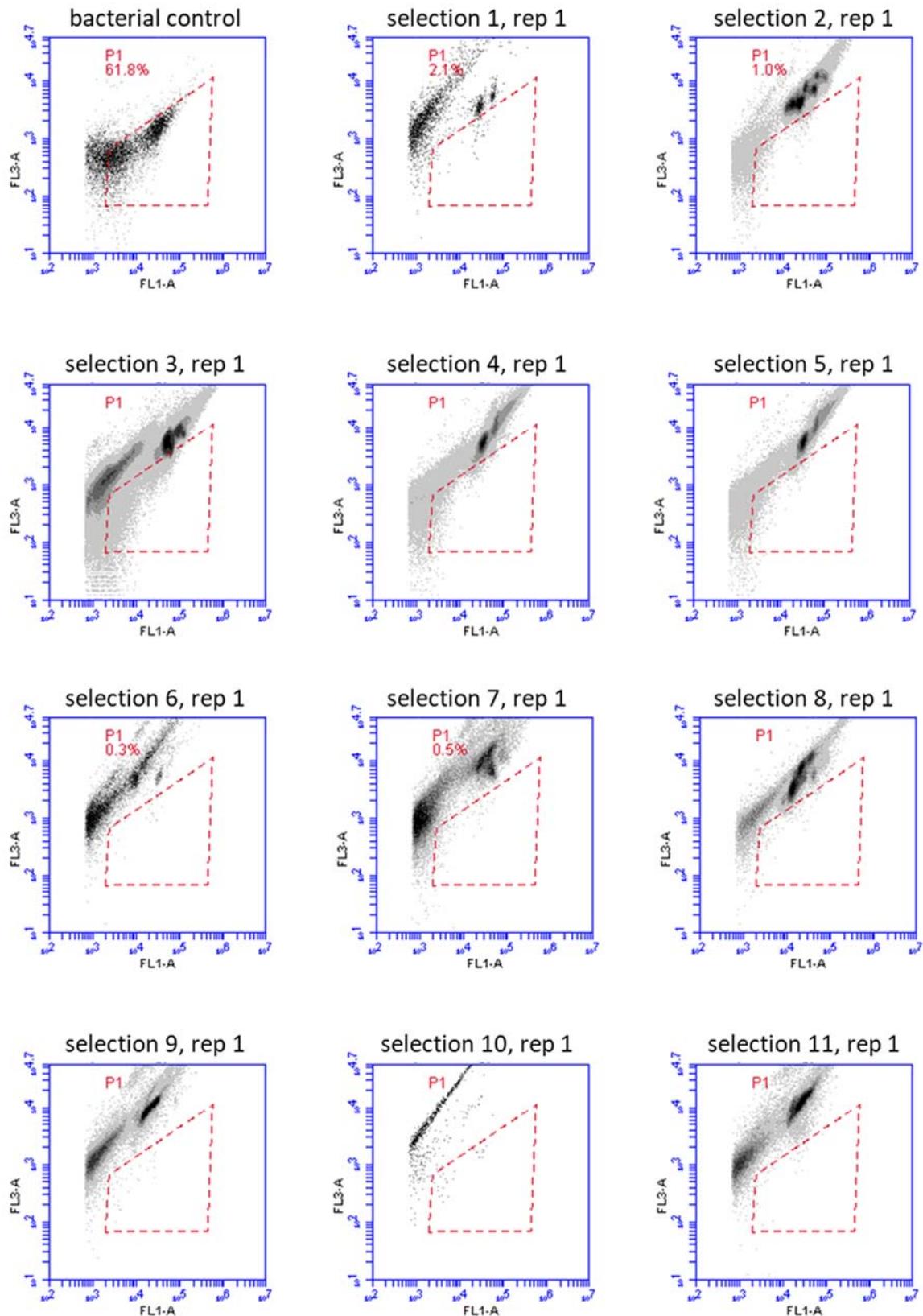


**Figure S9.** (continued on next page)

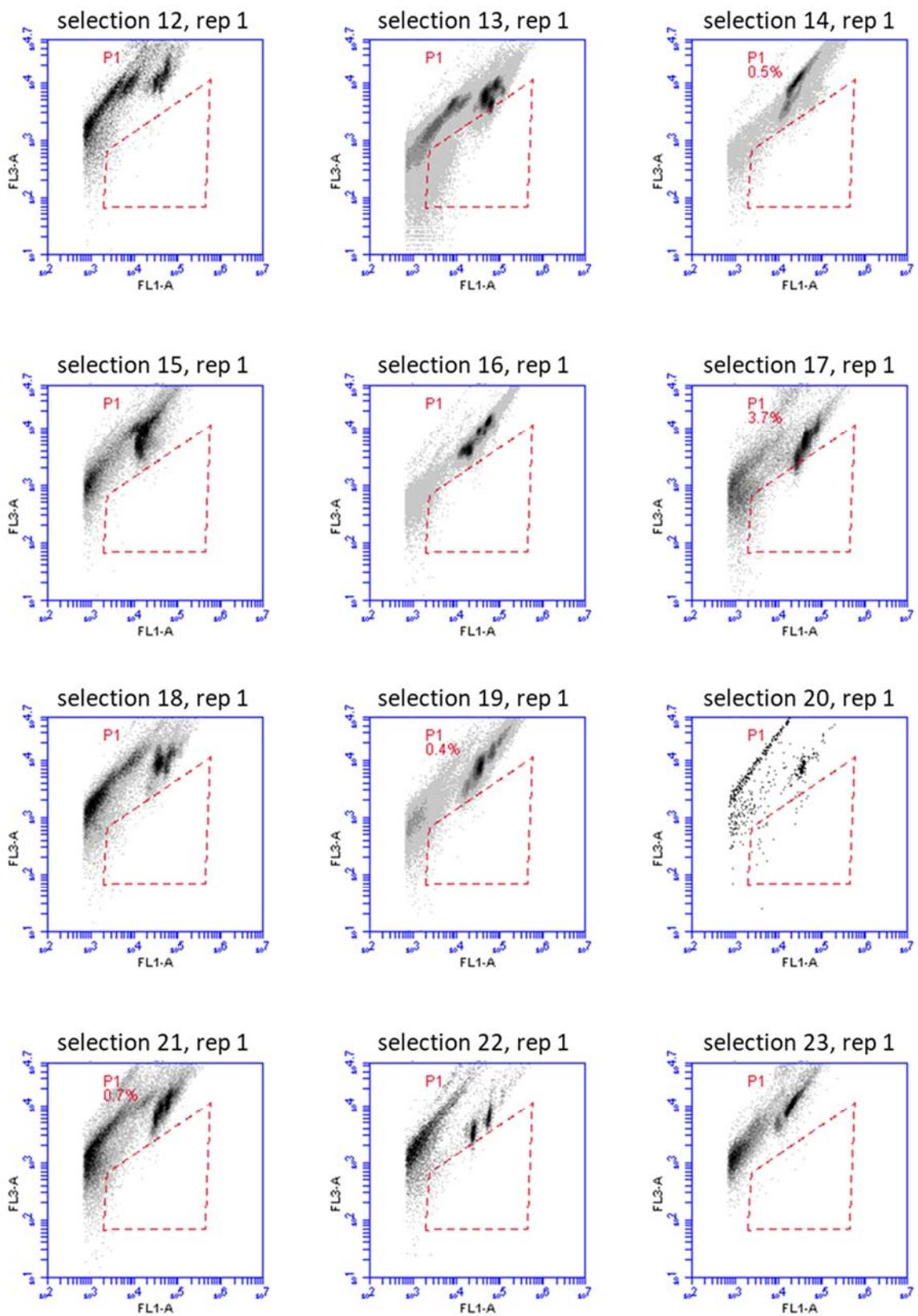


**Figure S9.** Richness effects on individual TPs (continued) For 46 TP candidates, total peak areas (TPA) for assembled communities by CR and SR, and for bacterial controls (BAC). . On top: Pearson correlation coefficient for CR and SR effects, respectively. \*:  $p<0.05$ ; \*\*:  $p<0.01$ ; \*\*\*:  $p<0.001$ . Colors for classes, and boxplot margins are as specified in Fig. 1. *ATE*, atenolol; *MPL*, metoprolol; *MEF*, mefenamic acid; *CPD*, cyprodinil; *CBDZ*, carbendazim; *TEB*, tebuconazole; *AZY*, azoxystrobin; *FDX*, fludioxonil; *KME*, kresoxim-methyl; *SMZ*, sulfamethoxazole. Numbers after TP candidate name indicate the retention time in case of isobaric compounds.

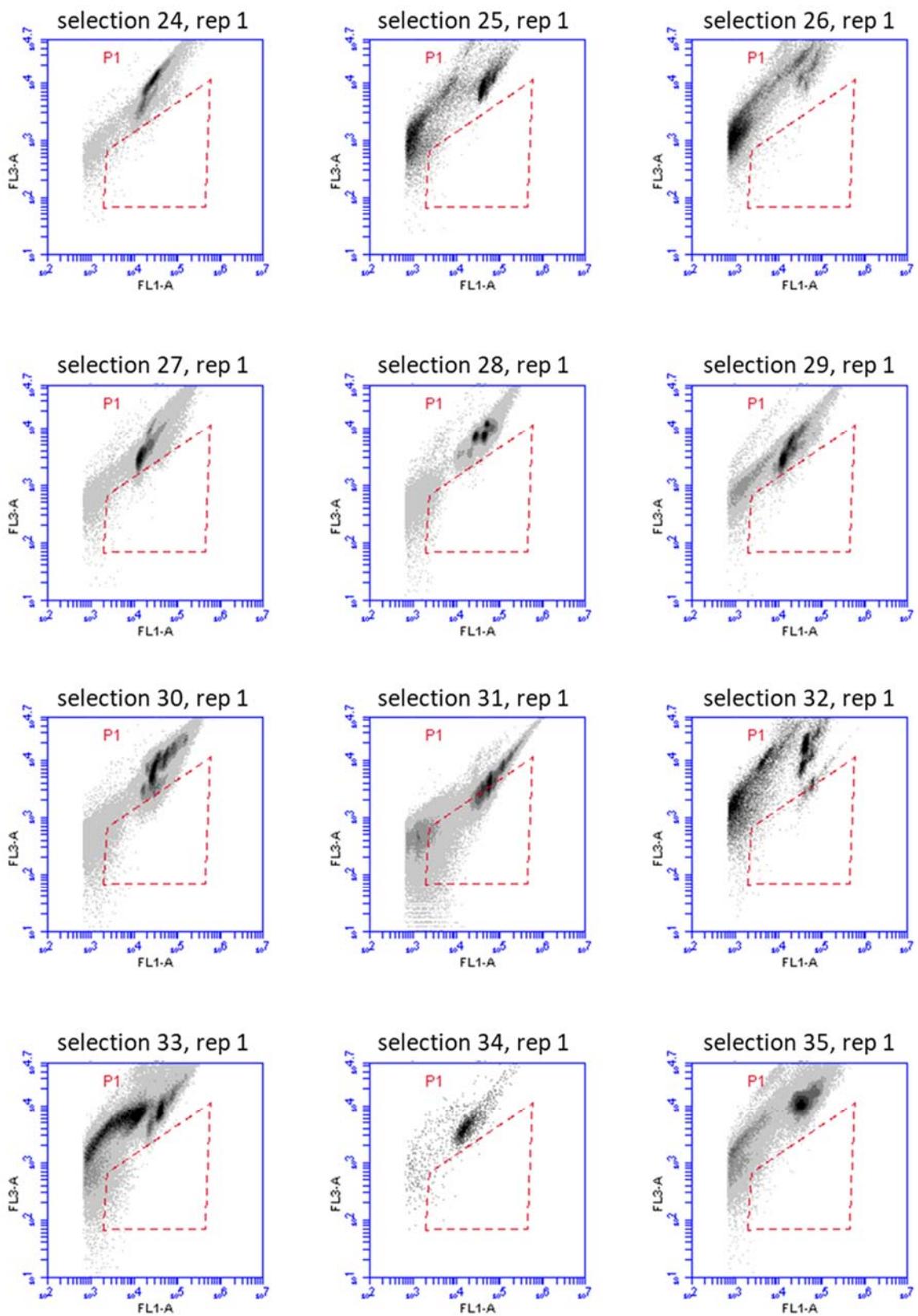
## S2.8. Bacterial growth in experimental samples



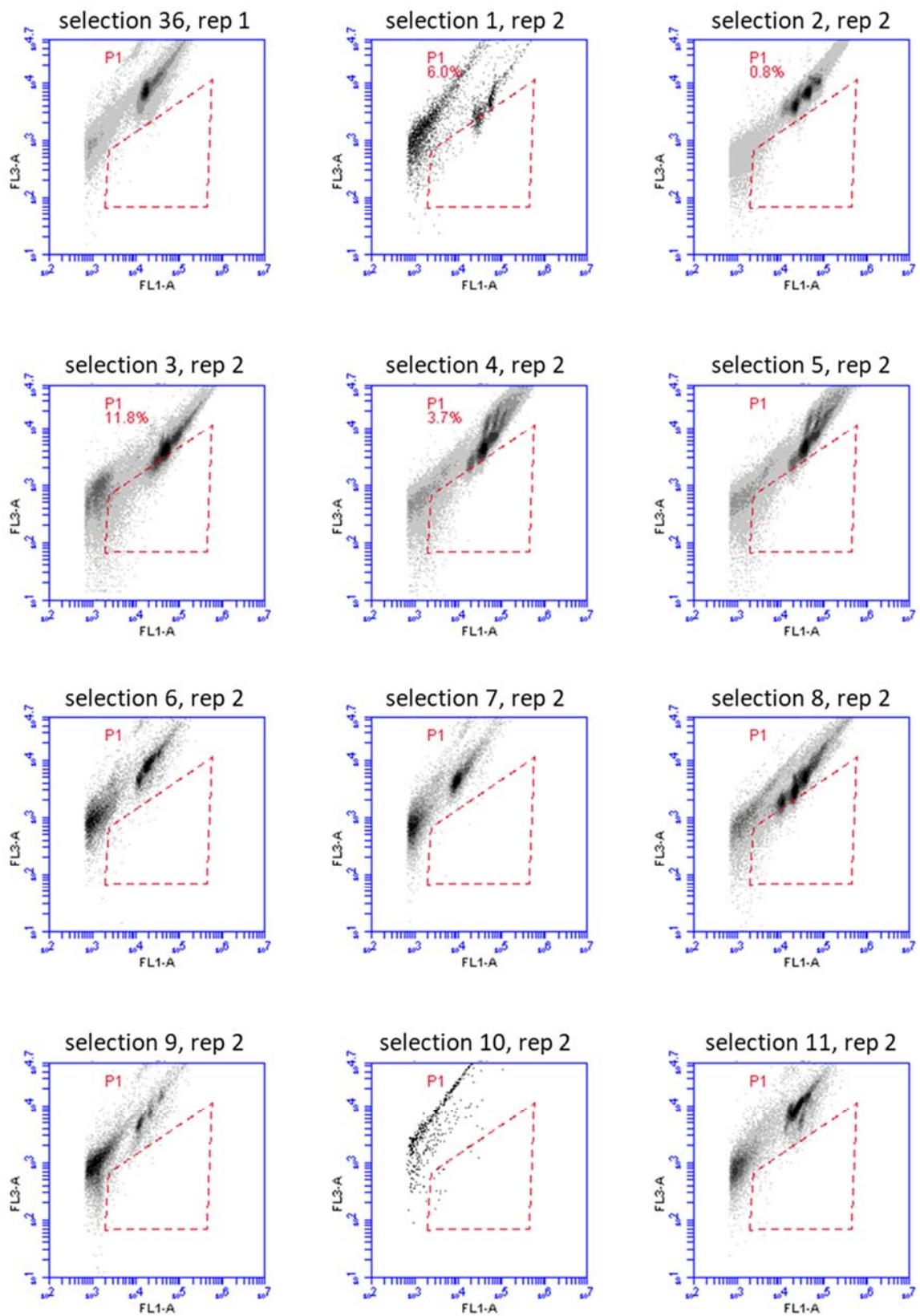
**Figure S10.** Flow cytometry of fixed samples (continued on next page)



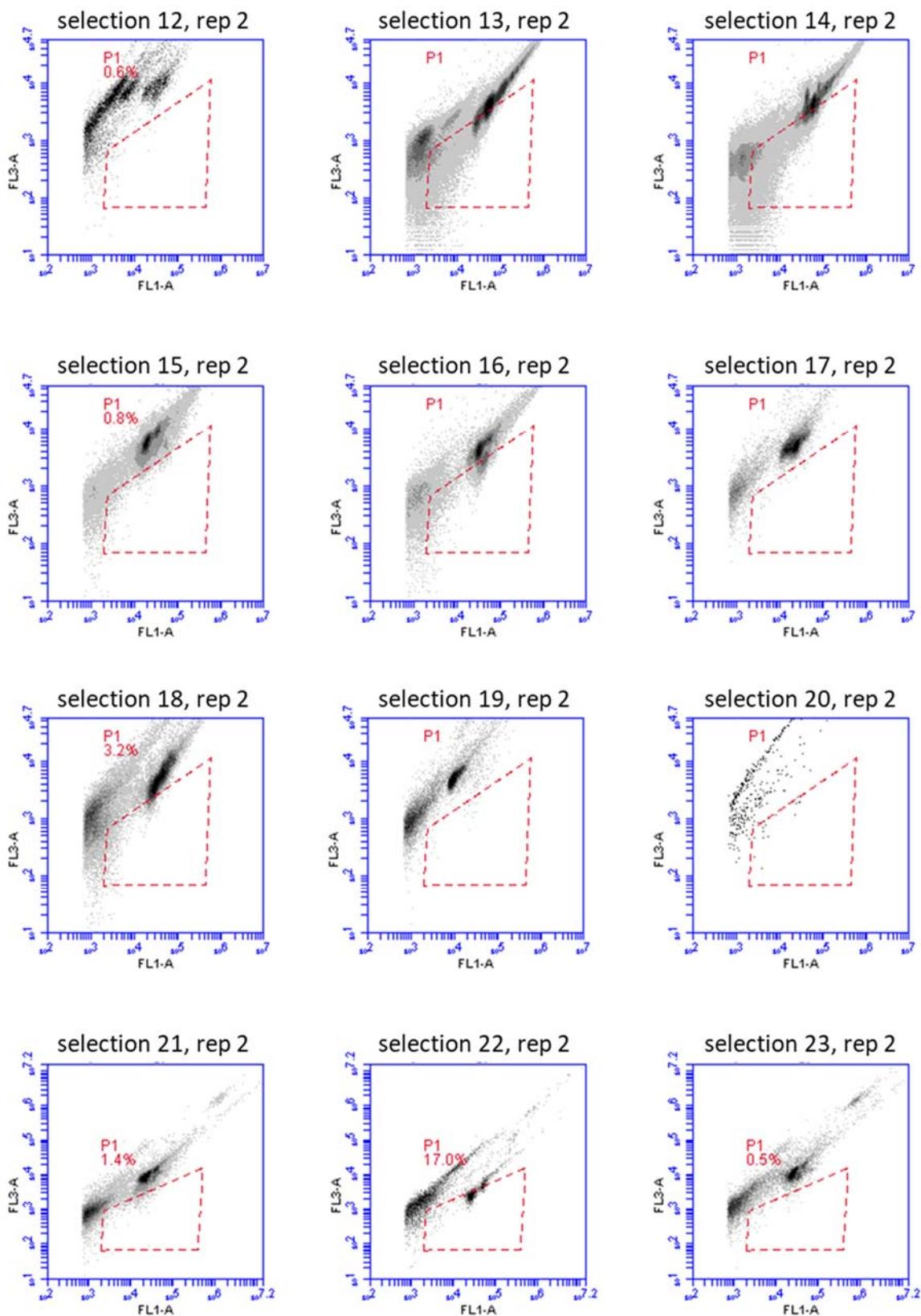
**Figure S10.** (continued on next page)



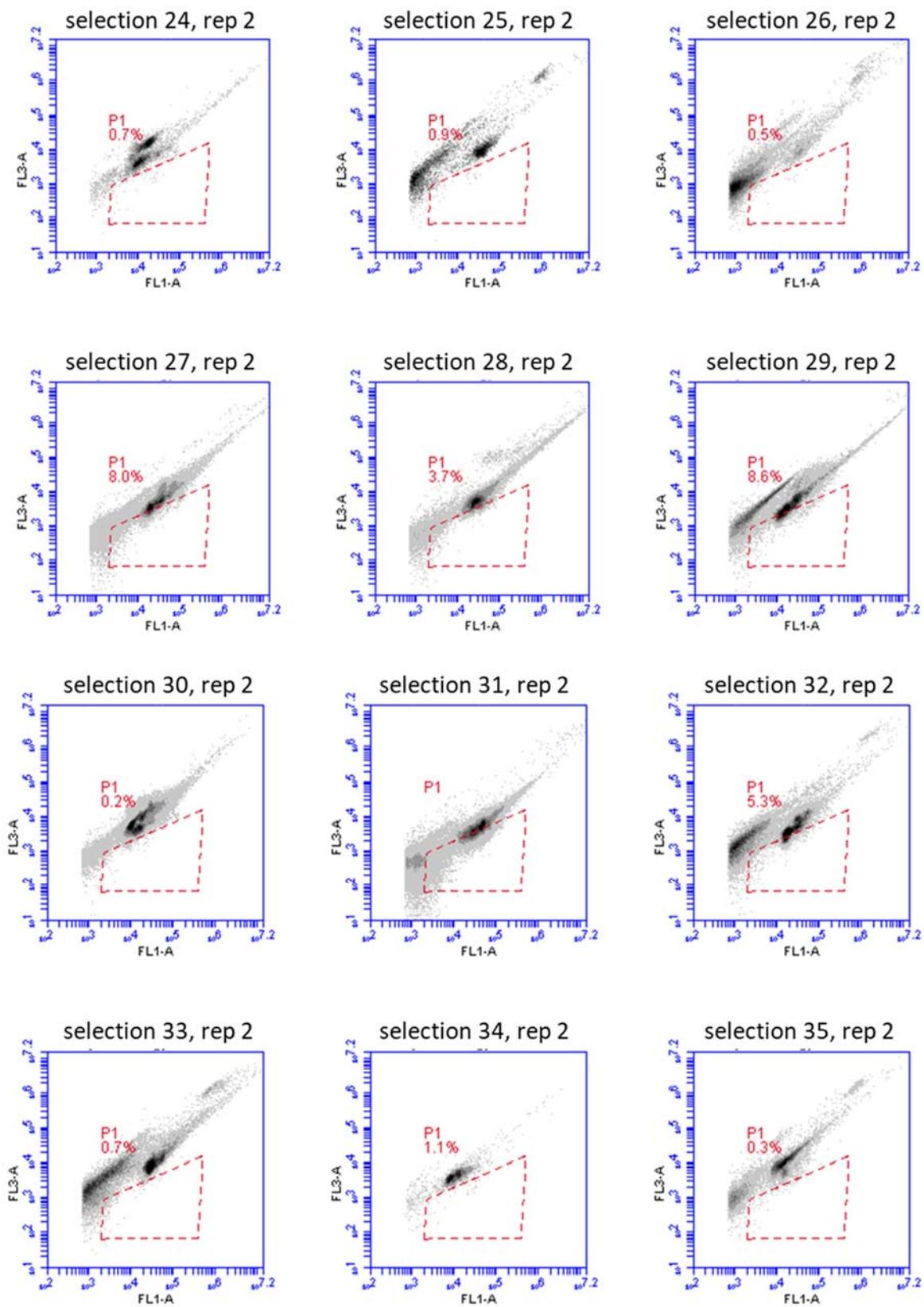
**Figure S10.** (continued on next page)



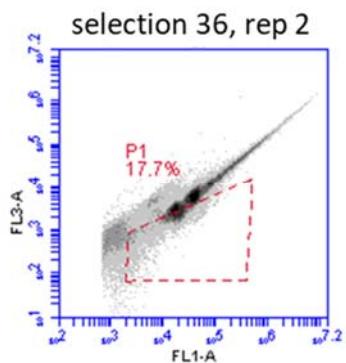
**Figure S10.** (continued on next page)



**Figure S10.** (continued on next page)



**Figure S10.** (continued on next page)



**Figure S10.** Flow cytometry of fixed samples. FL1-A: green fluorescence, FL3-A: red fluorescence. Red shape: electronic gate corresponding to bacteria. Clusters with center above the gate which extend into the gate are likely cyanobacteria. First plot: drinking water sample with bacteria; plots 2..37: 6-day timepoint samples of first experimental replicate; plots 38..73: 4-day timepoint samples of second experimental replicate. Labels on top: selection and replicate (rep). Note that while not all plots are scaled identically, the gating is the same.

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