

# Supporting Information

## Target Screening of Chemicals of Concern in Recycled Water

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**Table S1. Summary of the chemicals targeted in post RO and post UV treated water at Beenyup AWRP.**

Chemical (labelled surrogate)	CAS-Nr.	Formula	Exact mass	Ionisation mode	LOQ	metabolite of/ sub-group
<b>PESTICIDES</b>						
2,4-D (2,4-D <sup>13</sup> C <sub>6</sub> )	94-75-7	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	219.9689	-	5	herbicide
Acetochlor	34256-82-1	C <sub>14</sub> H <sub>20</sub> ClNO <sub>2</sub>	269.1177	+	100	herbicide
Alachlor (Alachlor-d <sub>13</sub> )	15972-60-8	C <sub>14</sub> H <sub>20</sub> ClNO <sub>2</sub>	269.1177	+	100	herbicide
Aldicarb (Aldicarb-d <sub>3</sub> )	116-06-3	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> N <sub>2</sub> S	190.0776	+	10	insecticide
Asulam	3337-71-1	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> S	230.0356	+	20	herbicide
Atraton	1610-17-9	C <sub>9</sub> H <sub>17</sub> N <sub>5</sub> O	211.1428	+	1	herbicide
Atrazine (Atrazine-d <sub>5</sub> )	1912-24-9	C <sub>8</sub> H <sub>14</sub> ClN <sub>5</sub>	215.0932	+	1	herbicide
Azoxystrobin	131860-33-8	C <sub>22</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub>	403.1163	+	1	fungicide
Bentazone (Bentazone-d <sub>6</sub> )	25057-89-0	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> S	240.0563	-	0.5	herbicide
Bromazil	314-40-9	C <sub>9</sub> H <sub>13</sub> BrN <sub>2</sub> O <sub>2</sub>	260.0155	+	3	herbicide
Bromoxynil	1689-84-5	C <sub>7</sub> H <sub>3</sub> Br <sub>2</sub> NO	276.8561	-	1	herbicide
Carbetamide	16118-49-3	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	236.1155	-	1	herbicide
Chloridazon (Chloridazon-d <sub>5</sub> )	1698-60-8	C <sub>10</sub> H <sub>8</sub> ClN <sub>3</sub> O	221.035	+	2	herbicide
Chlortoluron (Chlorotoluron-d <sub>6</sub> )	15545-48-9	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O	212.0711	+	0.5	herbicide
Clomazone	81777-89-1	C <sub>12</sub> H <sub>14</sub> ClNO <sub>2</sub>	239.0708	+	1	herbicide
Cymoxanil	57966-95-7	C <sub>7</sub> H <sub>10</sub> N <sub>4</sub> O <sub>3</sub>	198.0753	+	10	fungicide
Cyproconazole	94361-06-5	C <sub>15</sub> H <sub>18</sub> ClN <sub>3</sub> O	291.1133	+	10	fungicide
Cyprodinil	121552-61-2	C <sub>14</sub> H <sub>15</sub> N <sub>3</sub>	225.126	+	10	fungicide
Desmedipham	13684-56-5	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	300.1105	+	20	herbicide
Diazinon (hydrolized)(Diazinon-d <sub>10</sub> )	333-41-5	C <sub>12</sub> H <sub>21</sub> N <sub>2</sub> O <sub>3</sub> PS	304.1005	+	n.q.	insecticide
Dicamba (Dicamba-d <sub>3</sub> )	1918-00-9	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	219.9699	-	20	herbicide
Dichlorprop (Dichlorprop-d <sub>6</sub> )	120-36-5	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub> Cl <sub>2</sub>	233.9845	-	5	herbicide
Diflufenican (Diflufenican-d <sub>3</sub> )	83164-33-4	C <sub>19</sub> H <sub>11</sub> F <sub>5</sub> N <sub>2</sub> O <sub>2</sub>	394.0735	+	70	herbicide
Dimethachlor	50563-36-5	C <sub>13</sub> H <sub>18</sub> ClNO <sub>2</sub>	255.1021	+	0.5	herbicide
Dimethenamid	87674-68-8	C <sub>12</sub> H <sub>18</sub> ClNO <sub>2</sub> S	275.0741	+	0.5	herbicide
Dinoseb	88-85-7	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>	240.0741	-	5	herbicide
Epoxyconazole	133855-98-8	C <sub>17</sub> H <sub>13</sub> ClFN <sub>3</sub> O	329.0726	+	10	fungicide
Ethofumesat	26225-79-6	C <sub>13</sub> H <sub>18</sub> O <sub>5</sub> S	286.0869	+	10	herbicide
Fenpropimorph	67306-03-0	C <sub>20</sub> H <sub>33</sub> NO	303.2557	+	1	fungicide
Fipronil	120068-37-3	C <sub>12</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>4</sub> O <sub>1</sub> S	435.9387	+	1	insecticide

Fluazifop (free acid)	69335-91-7	C15H12F3NO4	327.0724	-	1	herbicide
Fludioxonil	131341-86-1	C12H6F2N2O2	248.0392	-	0.5	fungicide
Flufenacet	142459-58-3	C14H13F4N3O2S	363.067	+	2.5	herbicide
Fluroxypyr (free acid)	69377-81-7	C7H5Cl2FN2O3	253.9667	-	5	herbicide
Flusilazole	85509-19-9	C16H15F2N3Si	315.0998	+	15	fungicide
Foramsulfuron	173159-57-4	C17H20N6O7S	452.1114	+	10	herbicide
Hexazinon	51235-04-2	C12H20N4O2	252.1581	+	0.5	herbicide
Imidacloprid	138261-41-3	C9H10ClN5O2	255.0523	+	3	insecticide
loxynil	1689-83-4	C7H3I2NO	370.8299	-	5	herbicide
Isoproturon (Isoproturon-d6)	34123-59-6	C12H18N2O	206.1414	+	0.5	herbicide
Kresoxim-methyl	143390-89-0	C18H19NO4	313.1309	+	2.5	fungicide
Linuron	330-55-2	C9H10Cl2N2O2	248.0114	+	2.5	herbicide
MCPA (MCPA-d6)	94-74-6	C9H9ClO3	200.0235	-	1	herbicide
MCPB	94-81-5	C11H13ClO3	228.0553	-	10	herbicide
Mecoprop (Mecoprop-d6)	93-65-2	C10H11ClO3	214.0391	-	1	herbicide
Mesotrione (Mesotrione-d3)	104206-82-8	C14H13NO7S	339.0407	-	25	herbicide
Metalaxyl	57837-19-1	C15H21NO4	279.1465	+	2.5	fungicide
Metamitron	41394-05-2	C10H10N4O	202.086	+	25	herbicide
Metazachlor	67129-08-2	C14H16ClN3O	277.0976	+	1	herbicide
Metolachlor (Metolachlor-d6)	51218-45-2	C15H22ClNO2	283.1334	+	0.5	herbicide
Metribuzin	21087-64-9	C8H14N4OS	214.0883	+	5	herbicide
Metsulfuron-methyl	74223-64-6	C14H15N5O6S	381.0738	+	3	herbicide
Monuron	150-68-5	C9H11ClN2O	198.0554	+	0.5	herbicide
Napropamid	15299-99-7	C17H21NO2	271.1567	+	0.5	herbicide
Nicosulfuron	111991-09-4	C15H18N6O6S	410.1003	+	5	herbicide
Orbencarb	34622-58-7	C12H16ClNOS	257.0647	+	10	herbicide
Pethoxamid	106700-29-2	C16H22ClNO2	295.1334	+	1	herbicide
Phenmedipham	13684-63-4	C16H16N2O4	300.1116	+	25	herbicide
Pirimicarb	23103-98-2	C11H18N4O2	238.143	+	1	insecticide
Prochloraz	67747-09-5	C15H16Cl3N3O2	375.0303	+	200	fungicide
Prometon	1610-18-0	C10H19N5O	225.1584	+	0.5	herbicide
Propachlor	1918-16-7	C11H14ClNO	211.0758	+	0.5	herbicide
Propaquizafop	111479-05-1	C22H22ClN3O5	443.1242	+	100	herbicide
Prosulfocarb (Surrogate: Propiconazole-d5)	52888-80-9	C14H21NOS	251.1349	+	5	herbicide
Pyraclostrobin	175013-18-0	C19H18ClN3O4	387.0986	+	7.5	fungicide

Pyrimethanil	53112-28-0	C12H13N3	199.1109	+	1	fungicide
Rimsulfuron	122931-48-0	C14H17N5O7S2	431.0564	+	25	herbicide
Simazine (Simazine-d5)	122-34-9	C7H12ClN5	201.0776	+	1	herbicide
Simeton	673-04-1	C8H15N5O	197.1271	+	0.25	herbicide
Spiroxamine	118134-30-8	C18H35N1O2	297.2668	+	2.5	fungicide
Sulcotrione (Sulcotrione-d3)	99105-77-8	C14H13Cl1O5S	328.0167	+	20	herbicide
Tebuconazole	107534-96-3	C16H22ClN3O	307.1446	+	15	fungicide
Tebutam (Tebutam-d4)	35256-85-0	C15H23NO	233.1774	+	2.5	herbicide
Terbumeton	33693-04-8	C10H19N5O	225.1584	+	0.5	herbicide
Terbutylazine (Terbutylazine-d5)	5915-41-3	C9H16ClN5	229.1089	+	2	herbicide
Thifensulfuron-methyl	79277-27-3	C12H13N5O6S2	387.0302	-	5	herbicide
Trinexapac-ethyl	95266-40-3	C13H16O5	252.0992	+	3	growth regulator
Tritosulfuron	142469-14-5	C13H9F6N5O4S	445.0279	+	5	herbicide

#### PESTICIDE METABOLITES

2,4-dimethylphenylformamide	60397-77-5	C9H11NO	149.0835	+	20	Amitraz
2,6-Dichlorobenzamide	2008-58-4	C7H5Cl2NO	188.9743	+	3	Dichlobenil Thifensulfuron-methyl
2-Amino-4-methoxy-6-methyl-1,3,5 triazine	1668-54-8	C5H8N4O	140.0693	+	2.5	Metsulfuron-methyl
3,5,6-Trichloro-2-pyridinole	6515-38-4	C5H2Cl3NO	196.9202	-	1	Chlorpyrifos
3,5-dibromo-4-hydroxybenzoic acid	3337-62-0	C7H4Br2O3	293.8533	-	2	Bromoxynil
3-Phenoxybenzoic acid	3739-38-6	C13H10O3	214.0624	-	5	Permethrin
Acetochlor-ESA	187022-11-3	C14H21NO5S	315.1135	-	1	Acetochlor
Acetochlor-OXA	194992-44-4	C14H19NO4	265.132	-	1	Acetochlor
Alachlor-ESA	142363-53-9	C14H21NO5S	315.1135	-	1	Alachlor
Alachlor-OXA	171262-17-2	C14H19NO4	265.132	-	1	Alachlor
Atrazin-Desethyl (Atrazin-desethyl-15N3)	6190-65-4	C6H10ClN5	187.0619	+	2.5	Atrazine
Atrazin-Desisopropyl (Atrazine-desisopropyl-d5)	1007-28-9	C5H8ClN5	173.0463	+	5	Atrazine
Atrazine-2-Hydroxy (Atrazine-2-Hydroxy-d5)	2163-68-0	C8H15N5O	197.1271	+	1	Atrazine
Atrazine-desethyl-2-hydroxy	19988-24-0	C6H11N5O	169.0958	+	2	Prometon/Atrazine
Azoxystrobinic acid	N/A	C21H15N3O5	389.1012	+	3	Azoxystrobin
Bifenoic acid	53774-07-5	C13H7Cl2NO5	326.9707	-	1	Bifenox
Chloridazon-desphenyl (Chloridazon-desphenyl- <sup>15</sup> N2)	6339-19-1	C4H4ClN3O	145.0047	+	200	Chloridazon
Chloridazon-methyl-desphenyl	17254-80-7	C5H6ClN3O	159.0199	+	0.5	Chloridazon
Dimethachlor-ESA	N/A	C13H19NO5S	301.0978	-	1	Dimethachlor

Dimethachlor-OXA	1086384-49-7	C13H17NO4	251.1158	-	5	Dimethachlor
Dimethenamide-ESA	205939-58-8	C12H19N1O5S2	321.0699	-	1	Dimethenamide
Dimethenamide-OXA	380412-59-9	C12H17NO4S	271.0873	-	1	Dimethenamide
N,N-Dimethylaminosulfanilid (DMSA)	4710-17-2	C8H12N2O2S	200.0614	+	1.5	Dichlofluanid
Fipronil-sulfide	120067-83-6	C12H4Cl2F6N4S	419.9438	-	1	Fipronil
Fipronil-sulfon	120068-36-2	C12H4Cl2F6N4O2S	451.9336	-	2.5	Fipronil
Flufenacet-ESA	201668-32-8	C11H14FNO4S	275.0622	-	1	Flufenacet
Flufenacet-OXA	201668-31-7	C11H12FNO3	225.0796	-	1	Flufenacet
Isoproturon-didemethyl	56046-17-4	C10H14N2O	178.1101	+	1	Isoproturon
Isoproturon-monodemethyl	34123-57-4	C11H16N2O	192.1257	+	1	Isoproturon
Mesotrione-MNBA	110964-79-9	C8H7NO6S	244.9989	-	75	Mesotrion
Metamitron-Desamino	36993-94-9	C10H9N3O	187.0746	+	1.5	Metamitron
Metazachlor-ESA	172960-62-2	C14H17N3O4S	323.0934	-	5	Metazachlor
Metazachlor-OXA	N/A	C14H15N3O3	273.1108	-	5	Metazachlor
Metolachlor-ESA	171118-09-5	C15H23NO5S	329.1291	-	1	Metolachlor
Metolachlor-Morpholinon	120375-14-6	C14H19NO2	233.141	+	1	Metolachlor
Metolachlor-OXA	152019-73-3	C15H21NO4	279.1465	-	1.5	Metolachlor
Metribuzin-Desamino	35045-02-4	C8H13N3OS	199.0774	+	0.5	Metribuzin
Metribuzin-Diketo	56507-37-0	C7H12N4O2	184.0966	+	25	Metribuzin
N-(2,4-dimethylphenyl)-N-methylformamidin	33089-74-6	C10H14N2	162.1152	+	5	Amitraz
N,N-dimethyl-N'-(4-methylphenyl)-sulfamid	66840-71-9	C9H14N2O2S	214.077	+	0.5	Tolyfluanid
Propachlor-ESA	123732-85-4	C11H15NO4S	257.0716	-	1	Propachlor
Propachlor-OXA	70628-36-3	C11H13N1O3	207.089	-	3	Propachlor
Propazine-2-hydroxy	7374-53-0	C9H17N5O	211.1428	+	5	Propazine
Pyrimidinole	2814-20-2	C8H12N2O	152.095	+	30	Diazinon
Simazine-2-hydroxy	2599-11-3	C7H13N5O	183.1115	+	1	Simazine
Sulcotrione-CMBA	53250-83-2	C8H7Cl1O4S	233.9748	-	20	Sulcotrione
Terbutylazine-2-hydroxy	66753-07-9	C9H17N5O	211.1428	+	5	Terbutylazine
Terbutylazine-desethyl	30125-63-4	C7H12Cl1N5	201.0776	+	0.5	Terbutylazine
Terbutylazine-desethyl-2-hydroxy	30125-63-4	C7H13N5O	183.1115	+	1	Terbutylazine

#### PHARMACEUTICALS

4-Dimethylaminoantipyrine	58-15-1	C13H17N3O	231.1366	+	5	
Albuterol	18559-94-9	C13H21NO3	239.1521	+	2	
Amisulpride (Amisulpride-d5)	71675-85-9	C17H27N3O4S	369.1722	+	0.5	
Amitriptylin	50-48-6	C20H23N	277.183	+	2	

Atenolol (Atenolol-d7)	29122-68-7	C14H22N2O3	266.1625	+	1
Atomoxetine (Atomoxetine-d3)	83015-26-3	C17H21NO	255.1623	+	1
Atorvastatine	134523-03-8	C33H35FN2O5	558.253	+	50
Azithromycin (Azithromycin-d3)	83905-01-5	C38H72N2O12	748.508	+	2.5
Bezafibrate (Bezafibrate-d4)	41859-67-0	C19H20ClNO4	361.1075	+	2.5
Bicalutamide	90357-06-5	C18H14F4N2O4S	430.061	-	10
Bupropion	34911-55-2	C13H18ClNO	239.1077	+	1
Candesartan	139481-59-7	C24H20N6O3	440.1597	+	10
Carbamazepine (Carbamazepine- <sup>13</sup> C, d2)	298-46-4	C15H12N2O	236.0944	+	1
Cetirizine	83881-52-1	C21H25ClN2O3	388.1554	+	15
Cilastatin	82009-34-5	C16H26N2O5S	358.1562	+	n.q.
Citalopram (Citalopram-d6)	59729-33-8	C20H21FN2O	324.1638	+	1
Clarithromycin (Clarithromycin-d3)	81103-11-9	C38H69NO13	747.4763	+	5
Clindamycin	18323-44-9	C18H33ClN2O5S	424.1798	+	5
Clopidogrel (Clopidogrel-d4)	144457-28-3	C15H14ClNO2S	307.0439	+	5
Clozapine (Clozapine-d8)	5786-21-0	C18H19ClN4	326.1298	+	10
Cyclophosphamide (Cyclophosphamide-d4)	50-18-0	C7H15Cl2N2O2P	260.0248	+	10
Cytarabine	147-94-4	C9H13N3O5	243.085	+	10
Dexamethasone	50-02-2	C22H29FO5	392.1999	+	5
Dextromethorphan	125-71-3	C18H25NO	271.1936	+	2.5
Diclofenac (Diclofenac-d4)	15307-86-5	C14H11Cl2NO2	295.0161	+	5
Dronedarone	141626-36-0	C31H44N2O5S	556.2971	+	n.q.
Ephedrine	299-42-3	C10H15NO	165.2345	+	2
Eprosartan (Eprosartan-d3)	133040-01-4	C23H24N2O4S	424.1457	+	5
Ethambutole	1070-11-7	C10H24N2O2	204.1838	+	n.q.
Exemestane	107868-30-4	C20H24O2	296.1771	+	1
Fenofibrate (Fenofibrate-d6)	49562-28-9	C20H21Cl1O4	360.1123	+	100
FK-506 (Tacrolimus)	104987-11-3	C44H69NO12	803.482	-	50
Fluconazole (Fluconazole-d4)	86386-73-4	C13H12F2N6O	306.1035	+	10
Fluoxetine (Fluoxetine-d5)	54910-89-3	C17H18F3NO	309.1335	+	2
Furosemide (Furosemide-d5)	54-31-9	C12H11ClN2O5S	330.0077	-	30
Gabapentin (Gabapentin-d4)	60142-96-3	C9H17NO2	171.1259	+	50
Gemcitabine (Gemcitabine- <sup>13</sup> C, d2)	95058-81-4	C9H11F2N3O4	263.0718	+	50
Hydrochlorothiazide	58-93-5	C7H8ClN3O4S2	296.9645	-	10
Ibuprofen (Ibuprofen-d3)	15687-27-1	C13H18O2	206.1301	+	25

Ifosfamide	3778-73-2	C7H15Cl2N2O2P	260.0248	+	3
Indomethacin (Indomethacin-d4)	53-86-1	C19H16ClNO4	357.0768	+	10
lobitridol	136949-58-1	C20H28I3N3O9	834.896	+	2000
Iohexol	66108-95-0	C19H26I3N3O9	820.8798	+	1000
Iopromide	73334-07-3	C18H24I3N3O8	790.8692	+	100
Ketamine	6740-88-1	C13H16ClNO	237.092	+	0.5
Ketoprofen	22071-15-4	C16H14O3	254.0937	+	25
Lamotrigine (Surrogate: Atrazine-desethyl-d5)	84057-84-1	C9H7Cl2N5	255.0079	+	1
Levamisole	14769-73-4	C11H12N2S	204.0721	+	2.5
Levetiracetam (Levetiracetam-d3)	102767-28-2	C8H14N2O2	170.1055	+	5
Lidocaine (Lidocaine-d10)	137-58-6	C14H22N2O	234.1732	+	1.5
Mefenamic acid (Mefenamic acid-d3)	61-68-7	C15H15NO2	241.1097	+	2.5
Metformin (Metformin-d6)	657-24-9	C4H11N5	129.1014	+	20
Methylprednisolone (Methylprednisolone-d4)	83-43-2	C22H30O5	374.2093	+	5
Metoclopramide	7232-21-5	C14H22ClN3O2	299.1401	+	1
Metoprolol (Metoprolol-d7)	37350-58-6	C15H25NO3	267.1829	+	1
Metronidazole	443-48-1	C6H9N3O3	171.0638	+	5
Moclobemide	71320-77-9	C13H17ClN2O2	268.0979	+	1
Mycophenolic acid	24280-93-1	C17H20O6	320.126	+	10
Naltrexon	16590-41-3	C20H23NO4	341.1627	+	1
Naproxen (Naproxen-d3)	22204-53-1	C14H14O3	230.0937	+	10
Oseltamivir	196618-13-0	C16H28N2O4	312.2044	+	2.5
Paracetamol (Paracetamol-d4)	103-90-2	C8H9NO2	151.0628	+	10
Phenazone (Phenazone-d3)	60-80-0	C11H12N2O	188.0944	+	0.5
Pravastatin (Pravastatin-d3)	81093-37-0	C23H36O7	424.2461	-	20
Prednisolon	50-24-8	C21H28O5	360.1937	+	15
Primidone (Primidone-d5)	125-33-7	C12H14N2O2	218.105	+	5
Propranolol (Propranolol-d7)	525-66-6	C16H21NO2	259.1567	+	0.5
Ranitidine (Ranitidine-d6)	66357-35-5	C13H22N4O3S	314.1407	+	5
Ritonavir (Ritonavir-d6)	155213-67-5	C37H48N6O5S2	720.3128	+	10
Rosuvastatin	287714-41-4	C22H28FN3O6S	481.1683	+	5
Roxithromycin	80214-83-1	C41H76N2O15	836.524	+	5
Sitagliptin	486460-32-6	C16H15F6N5O	407.1181	+	10
Sotalol (Sotalol-d6)	3930-20-9	C12H20N2O3S	272.1189	+	5
Sulfadiazine (Sulfadiazine-d4)	68-35-9	C10H10N4O2S	250.0519	+	5

Sulfadimethoxine (Sulfadimethoxine-d4)	122-11-2	C12H14N4O4S	310.073	+	2.5
Sulfamethazine (Sulfamethazine- <sup>13</sup> C6)	57-68-1	C12H14N4O2S	278.0832	+	3
Sulfamethoxazole (Sulfamethoxazole-d4)	723-46-6	C10H11N3O3S	253.0516	+	5
Sulfapyridine (Sulfapyridine-d4)	144-83-2	C11H11N3O2S	249.0566	+	5
Sulfathiazole (Sulfathiazole-d4)	72-14-0	C9H9N3O2S2	255.0131	+	5
Telmisartan	144701-48-4	C33H30N4O2	514.2369	+	100
Thiopental	76-75-5	C11H18N2O2S	242.1089	-	15
Tramadol (Tramadol-d6)	27203-92-5	C16H25NO2	263.1885	+	1
Trimethoprim (Trimethoprim-d9)	738-70-5	C14H18N4O3	290.1373	+	2
Trimipramin	739-71-9	C20H26N2	294.2096	+	1
Tylosin	1401-69-0	C46H77NO17	915.5186	+	50
Valsartan (Valsartan- <sup>15</sup> N, <sup>13</sup> C5)	137862-53-4	C24H29N5O3	435.227	+	5
Venlafaxine (Venlafaxine-d6)	93413-69-5	C17H27NO2	277.2036	+	0.5
Verapamil (Verapamil-d6)	152-11-4	C27H38N2O4	454.2826	+	2

#### PHARMACEUTICAL METABOLITES

2',3'-di-O-acetyl-5'-desoxy-5-fluorocytidine	161599-46-8	C13H16FN3O6	329.1023	+	10	Capecitabin
4-(Trifluoromethyl)phenol	402-45-9	C7H5F3O	162.0287	-	50	Fluoxetine
4-Acetamidoantipyrine	83-15-8	C13H15N3O2	245.117	+	1	Aminopyrine/Metamizol
4-Formylaminoantipyrine	1672-58-8	C12H13N3O2	231.1008	+	1.5	Aminopyrine/Metamizol
AMDOPH	519-65-3	C13H17N3O3	263.127	+	0.5	Aminopyrine
Atenolol-desisopropyl	81346-71-6	C11H16N2O3	224.1161	+	50	Atenolol
Atenololic acid (Atenolol acid-d5)	56392-14-4	C14H21N1O4	267.1465	+	1	Atenolol/Metoprolol
Carbamazepine-10,11-dihydro-10,11-dihydroxy	58955-93-4	C15H14N2O3	270.1004	+	5	Carbamazepine
Carbamazepine-10,11-epoxide (Carbamazepine 10, 11-Epoxide- <sup>13</sup> C, d2)	36507-30-9	C15H12N2O2	252.0899	+	1	Carbamazepine
Clofibric acid (Clofibric acid-d4)	882-09-7	C10H11ClO3	214.0391	-	1	Clofibrate
D617	34245-14-2	C17H26N2O2	290.1994	+	0.5	Verapamil
Fenofibrinic acid	42017-89-0	C17H15ClO4	318.0653	+	2.5	Fenofibrate
Iminostilbene	256-96-2	C14H11N	193.0892	+		Carbamazepine
N,N-Didesvenlafaxine	93413-77-5	C15H23N1O2	249.1729	+	5	Venlafaxine
N,O-Didesvenlafaxine	135308-74-6	C15H23N1O2	249.1729	+	5	Venlafaxine
N4-Acetyl-Sulfadiazine	127-74-2	C12H12N4O3S	292.0625	+	5	Sulfadiazine
N4-Acetyl-Sulfadimethoxine	24341-30-8	C14H16N4O5S	352.0836	+	4	Sulfadimethoxine
N4-Acetyl-Sulfamethazine	100-90-3	C14H16N4O3S	320.0938	+	2.5	Sulfamethazine
N4-Acetyl-Sulfamethoxazole (N4-Acetyl-	21312-10-7	C12H13N3O4S	295.0621	+	3	Sulfamethoxazole



Sulfamethoxazole-d5)						
N4-Acetyl-Sulfathiazole (N4-Acetyl-Sulfathiazole-d4)	127-76-4	C11H11N3O3S2	297.0236	+	10	Sulfathiazole
N-Desvenlafaxine	149289-30-5	C16H25N1O2	263.1885	+	0.5	Venlafaxine
O-Desvenlafaxine	93413-62-8	C16H25N1O2	263.1885	+	1	Venlafaxine
Oseltamivir-carboxylate	187227-45-8	C14H24N2O4	284.1731	+	10	Oseltamivir
Ranitidine-N-oxide	738557-20-2	C13H22N4O4S	330.1362	+	2	Ranitidine
Ranitidine-S-oxide	73851-70-4	C13H22N4O4S	330.1362	+	20	Ranitidine
Ritalinic acid (Ritalinic acid-d10)	19395-41-6	C13H17NO2	219.1254	+	5	Methylphenidat Valsartan, Losartan, Candesartan,
Valsartan acid (Valsartan acid-d4)	164265-78-5	C14H10N4O2	266.0804	+	5	Irbesartan

#### BIOCIDES and METABOLITES

2-Aminobenzimidazol	934-32-7	C7H7N3	133.0634	+	5	Carbendazim
2-n-Octyl-4-isothiazolin-3-on	26530-20-1	C11H19NOS	213.1182	+	1	
4,5-Dichloro-2-n-octyl-isothiazol-3(2H)-on	64359-81-5	C11H17Cl2NOS	281.0402	+	25	
Carbendazim (Carbendazim-d4)	10605-21-7	C9H9N3O2	191.0689	+	3	
Diuron (Diuron-d6)	330-54-1	C9H10Cl2N2O	232.0165	+	1	
Diuron-desdimethyl	2327-02-8	C7H6Cl2N2O	203.9852	+	5	Diuron
Diuron-desmonomethyl	3567-62-2	C8H8Cl2N2O	218.0008	+	5	Diuron
Irgarol (Irgarol-d9)	28159-98-0	C11H19N5S	253.1356	+	2	
Irgarol-descyclopropyl	N/A	C8H15N5S	213.1043	+	1	Irgarol
N,N-diethyl-3-methylbenzamid	134-62-3	C12H17NO	191.1305	+	1	
Prometryn	7287-19-6	C10H19N5S	241.1356	+	0.5	
Propiconazole (Propiconazole-d5)	60207-90-1	C15H17Cl2N3O2	341.0692	+	5	
Terbutryn (Terbutryn-d5)	886-50-0	C10H19N5S	241.1356	+	0.5	
Triclosan (Triclosan-d3)	3380-34-5	C12H7Cl3O2	287.9506	-	25	

#### ILLICIT DRUGS and METABOLITES

1-(3-Chlorophenyl)-piperazine	6640-24-0	C10H13ClN2	196.0767	+	5	
1-(3-Trifluoromethylphenyl)-piperazine	15532-75-9	C11H13F3N2	230.1031	+	20	
1-Benzylpiperazine	2759-28-6	C11H16N2	176.1313	+	50	
Amphetamine	300-62-9	C9H13N	135.1048	+	3	
Benzoyllecgonine	519-09-5	C16H19NO4	289.1314	+	2.5	Cocaine
Cocaine	50-36-2	C17H21NO4	303.1471	+	1	
Codeine (Codeine- <sup>13</sup> C, d3)	76-57-3	C18H21NO3	299.1521	+	1	

Diazepam (Diazepam-d5)	439-14-5	C16H13CIN2O	284.0716	+	1	
2-Ethyliden-1,5-dimethyl-3,3-diphenylpyrrolidine	30223-73-5	C20H23N	277.183	+	5	Methadone
Mephedrone	1189805-46-6	C11H15NO	177.1154	+	5	
Methadone	76-99-3	C21H27NO	309.2093	+	0.5	
Methamphetamine	537-46-2	C10H15N	149.1204	+	1	
Morphine (Morphine-d3)	57-27-2	C17H19NO3	285.1359	+	2.5	
Oxazepam (Oxazepam-d5)	604-75-1	C15H11CIN2O2	286.048	+	2.5	
<b>FOOD ADDITIVES (Artificial Sweeteners)</b>						
Acesulfame (Acesulfame-d4)	55589-62-3	C4H5NO4S	162.9939	-	1	
Aspartame (Aspartame-d5)	22839-47-0	C14H18N2O5	294.121	+	70	
Cyclamate (Cyclamate-d11)	100-88-9	C6H13NO3S	179.0616	-	1.5	
Neotame (Neotane-d3)	165450-17-9	C20H30N2O5	378.2155	+	5	
Saccharine (Saccharine <sup>13</sup> C6)	81-07-2	C7H5NO3S	182.999	-	1	
Sucralose (Sucralose-d6)	56038-13-2	C12H19Cl3O8	396.0146	-	4	
<b>INDUSTRIAL CHEMICALS</b>						
1,2-Bis-(4,4'-dinitro-2,2'-disulfonic acid)-phenylethylenoxide	128-42-7	C14H10N2O10S2	429.9771	-	200	
2-Naphthalinsulfonic acid	120-18-3	C10H8O3S	208.0189	-	30	
4,4'-Diaminostilben-2,2'-disulfonic acid	81-11-8	C14H14N2O6S2	370.0288	-	20	
N-(4-Aminophenyl)-N-methyl-acetamide	119-63-1	C9H12N2O	164.0944	+	5	
N-Methylacetanilide	579-10-2	C9H11NO	149.0835	+	1	
<b>CORROSION INHIBITORS</b>						
1-Hydroxy-Benzotriazole	2592-95-2	C6H5N3O	135.0433	+	40	Benzotriazole
1-Methyl-Benzotriazole	13351-73-0	C7H7N3	133.0635	+	1	Benzotriazole
4 + 5-Methyl-Benzotriazole (5-Methyl-Benzotriazole-d6)	136-85-6	C7H7N3	133.0635	+	50	
4-Hydroxy-Benzotriazole	26725-51-9	C6H5N3O	135.0433	+	40	Benzotriazole
Benzotriazole (Benzotriazole-d4)	95-14-7	C6H5N3	119.0478	+	25	
<b>OTHERS</b>						
Benzophenone	131-57-7	C14H12O3	228.0781	+	10	Personal care product
Caffeine (Caffeine-d9)	58-08-2	C8H10N4O2	194.0798	+	50	Tracer
Climbazole	38083-17-9	C15H17CIN2O2	292.0979	+	50	Personal care product
Galaxolidon (Surrogate: Propiconazole-d5)	256393-37-0	C18H24O2	272.1771	+	10	Metabolite of Galaxolide
NN-Dimethyldicylamin N-oxide	2605-79-0	C12H27NO	201.2093	+	2	Disinfectant

In addition to the surrogate standards indicated in the table, the following surrogates were also used: N,N-diethyl-3-methylbenzamide-d7; octilinone-d17; propazine-d6; 2',2'-difluoro-2-deoxyuridine-<sup>13</sup>C,<sup>15</sup>N2; 5-fluorouracil-<sup>15</sup>N2; bisphenol-A-d16; ciprofloxacin-d8; erythromycin-<sup>13</sup>C2; irbesartan-d3; N,O-didesmethylvenlafaxin-d3; N-desmethylvenlafaxin-d3; nelfinavir-d3; norfloxacin-d5; O-desmethylvenlafaxin-d6; oxcarbazepine-d4.

**Table S2. Summary of ESI and HRMS parameters used for analysis of Beenyup AWRP samples.**

<b>Parameter</b>	<b>positive (+eV)</b>	<b>negative (-eV)</b>
Source Voltage (kV)	4	3
Capillary Temp (°C)	350	350
Sheath Gas Flow (Arb)	40	40
Aux Gas Flow (Arb)	10	10
Sweep Gas Flow (Arb)	0	0
Gas Heater Temp	50	50
S-Lense-RF (V)	50	50
Quadrupole scan range ( <i>m/z</i> )	100-1000	100-1000
FTMS Full AGC Target	5E5	5E5
FTMS MS2 AGC Target	5E5	5E5
Ion Trap and FT Micro Scans	1	1
Dynamic exclusion for MS2 (sec)	8	8
FTMS Full Max Ion Time (ms)	250	250
FTMS MSn Max Ion Time (ms)	250	250
MS2 Isolation window ( <i>m/z</i> )	1	1

*Arb: arbitrary units; ms: milli seconds*

**Table S3. Summary of the enviMass1.2 parameters adopted for quantitative screening of target substances.**

<b>EnviMass Parameter</b>	<b>Value</b>
<b>blank subtraction</b>	
<i>m/z</i> tolerance	10 ppm
RT window	0.4 min
Safety factor	4
<b>before recalibration</b>	
<i>m/z</i> tolerance for internal standard	10 ppm
RT tolerance	1 min
<b>after recalibration</b>	
<i>m/z</i> tolerance for targets	4 ppm
RT tolerance	1 min
RT tolerance for isotopic/adduct peak	0.3 min
Isotopic abundance tolerance	50%
Intensity cut-off	5000

*RT: retention time; m/z: mass-to-charge ration*

**Table S4. Summary of the Formulator parameters adopted for quantitative screening of target substances.**

<b>Formulator Parameter</b>	<b>Value</b>
Average by scan	3
<i>m/z</i> tolerance	±5 ppm
RT tolerance	1 min
MassChromatogram S/N	0.85
Signal threshold S/N	10
RT window	0.5 - 20 min
Average by scan	3
<i>m/z</i> tolerance	± 5 ppm

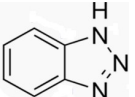
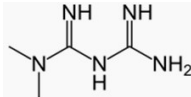
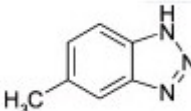
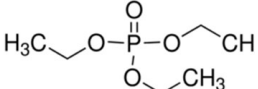
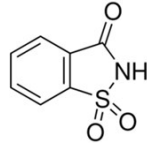
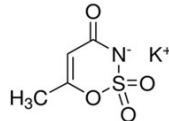
*RT: retention time; S/N: signal-to-noise ratio; m/z: mass-to-charge ration*

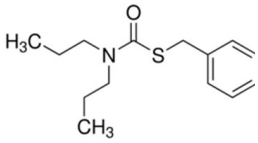
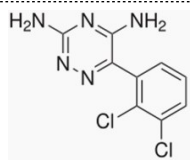
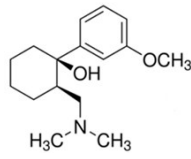
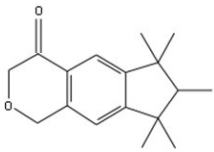
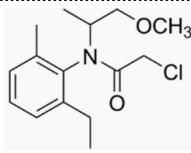
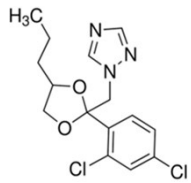
**Table S5. Summary of the recovery percentages from a 100 ng spike. Recoveries are presented only for the 13 compounds which were subsequently detected in the post RO and post UV water samples.**

<b>Chemical</b>	<b>RO water + 100 ng spike (ng in vial)</b>	<b>RO water Blank (ng in vial)</b>	<b>Relative recovery %</b>	<b>Ultrapure water blank</b>
5-Methyl benzotriazole*	1700	1300	N/A	<LOD
Benzotriazole*	2200	1600	N/A	<LOD
Galaxolidone	170	40	130%	<LOD
Lamotrigine	100	5	95%	<LOD
Metholachor	125	30	95%	<LOD
Metformin	325	220	105%	<LOD
Propiconazol	115	30	85%	<LOD
Prosulfocarb	110	25	85%	<LOD
Tramadol	110	1	109%	<LOD
Acesulfam	170	55	115%	<LOD
Saccharin	115	14	101%	<LOD
Sucralose	110	15	95%	<LOD

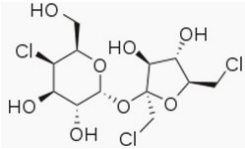
*\*outside linearity range*

**Table S6: Main physical-chemical properties of the chemicals that were detected in post RO and post UV water at Beenyup AWRP. Chemicals have been ordered by molecular weight.**

Chemical	Molecular structure	Chemical type/ classification	Molecular weight (Da)	pKa	Log Kow	ChemSpider ID	Estimated RO rejection
Benzotriazole		Various household and industrial uses/ corrosion inhibitor	119	8.2	1.23	6950	Very poor <sup>1-3</sup>
Metformin		Pharmaceutical/ diabetes treatment	129	12.4	-1.43	3449	Very poor <sup>1,2</sup>
4 + 5 methyl benzotriazole		Various household and industrial uses/ corrosion inhibitor	133	8.7	1.89	109219	Very poor <sup>1-3</sup>
Triethyl phosphate		Flame retardant	182	19	0.80	6287	Very poor <sup>1,2</sup>
Saccharin		Food additive/ artificial sweetener	183	2.32	0.91	4959	Very poor <sup>1,2</sup>
Acesulfame-K		Food additive/ artificial sweetener	201	3.2	-1.33	55940	Very poor <sup>1,2</sup>

Chemical	Molecular structure	Chemical type/ classification	Molecular weight (Da)	pKa	Log Kow	ChemSpider ID	Estimated RO rejection
Prosulfocarb		Pesticide/ herbicide	251	...	4.65	55867	Good <sup>1,2</sup>
Lamotrigine		Pharmaceutical/ antiepileptic	255	5.7	-0.19	3741	Moderate to good <sup>1,2</sup>
Tramadol		Pharmaceutical/ analgesic	263	9.41	2.51	5322	Good <sup>1,2</sup>
Galaxolidone		Polycyclic musk fragrance/ personal care product	272	...	5.50	28290252	Good <sup>2</sup>
Metolachlor		Pesticide/ herbicide	283		3.00	4025	Moderate to good <sup>1,2</sup>
Propiconazole		Biocide/ fungicide	341	~1	3.88	39402	Moderate to good <sup>1,2</sup>



Chemical	Molecular structure	Chemical type/ classification	Molecular weight (Da)	pKa	Log Kow	ChemSpider ID	Estimated RO rejection
Sucralose		Food additive/ artificial sweetener	396	11.8	0.68	64561	Good <sup>1,2</sup>

1. C. Bellona, J. E. Drewes, P. Xu and G. Amy, *Water Res.*, 2004, **38**, 2795-2809.
2. J. E. Drewes, D. Sedlak, S. Snyder and E. Dickenson, *Development of Indicators and Surrogate for Chemical Contaminant Removal during Wastewater Treatment and Reclamation*, WateReuse Foundation, Alexandria, VA, 2008.
3. C. Loi, F. Buseti, K. L. Linge and C. Joll, *J. Chrom. A*, 2013, **1299**, 48-57.