

## Supplementary Information

### **Simultaneous ozonation of 90 organic micropollutants including illicit drugs and their metabolites in different water matrices**

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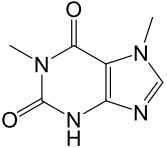
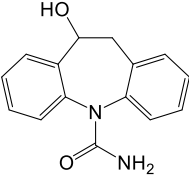
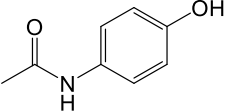
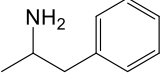
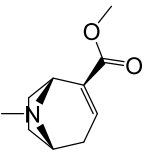
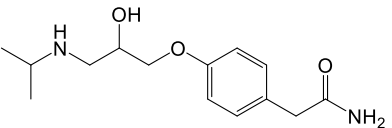
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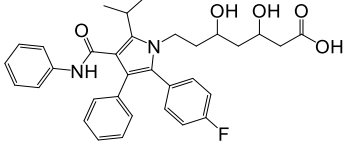
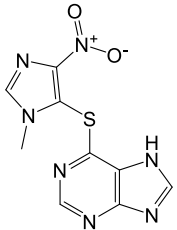
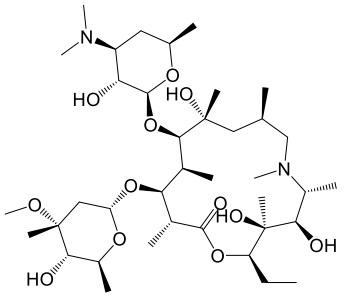
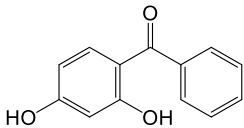
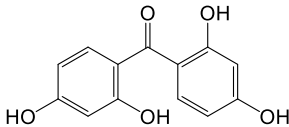
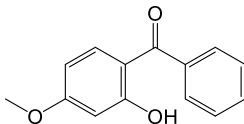
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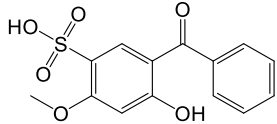
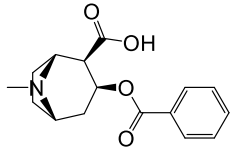
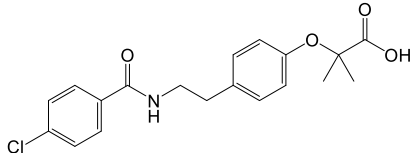
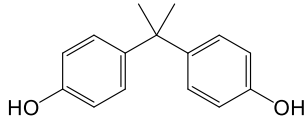
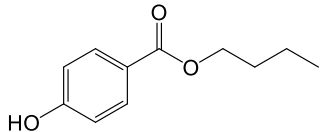
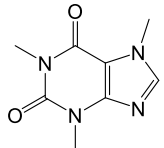
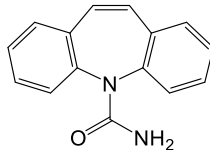
<sup>7</sup> School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen AB10 7GJ, UK

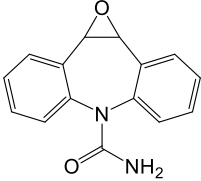
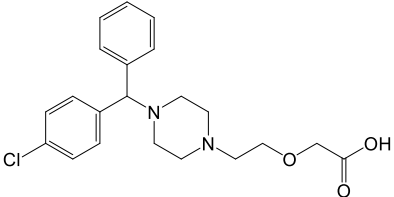
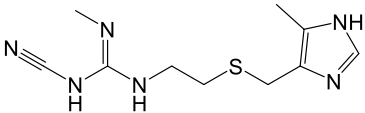
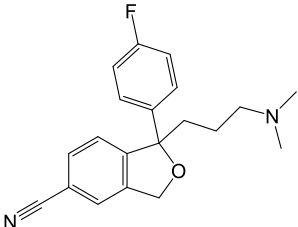
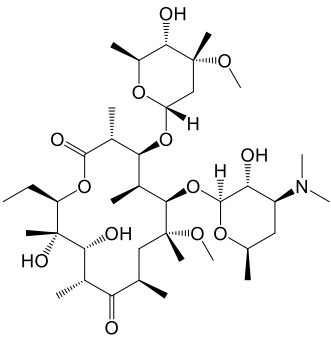
\*j.h.wenk@bath.ac.uk

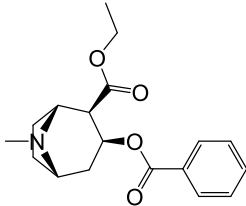
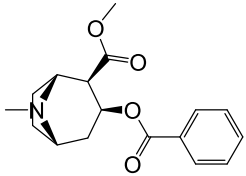
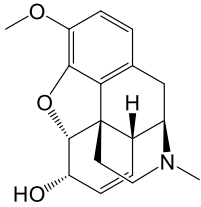
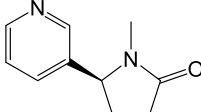
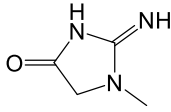
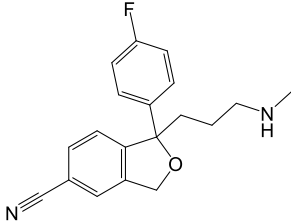
Table S1. Molecular structure and additional information about the 90 OMPs (in alphabetical order). LC-MS performance data was obtained from Petrie et al. [1], where more parameters can also be found (linearity range, precision, accuracy).

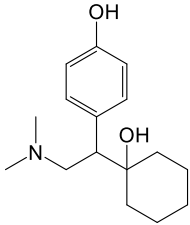
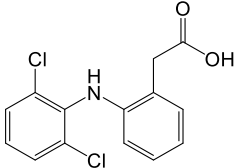
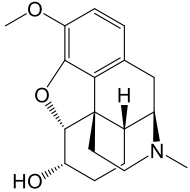
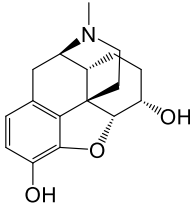
Chemical	CAS number	Molecular weight (g mol <sup>-1</sup> )	Molecular formula	Molecular structure	Instrument detection limit (ng mL <sup>-1</sup> )	Instrument quantification limit (ng mL <sup>-1</sup> )
1,7 dimethylxanthine	611-59-6	180.15	C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>		0.30	1.00
10,11 dihydro 10 hydroxycarbamazepine	29331-92-8	254.28	C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>		0.05	0.50
Acetaminophen	103-90-2	151.17	C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>		0.11	0.54
Amphetamine	300-62-9	135.21	C <sub>9</sub> H <sub>13</sub> N		0.03	0.10
Anhydroecgonine methylester	43021-26-7	181.23	C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>		0.10	0.50
Atenolol	29122-68-7	266.34	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>		0.03	0.10

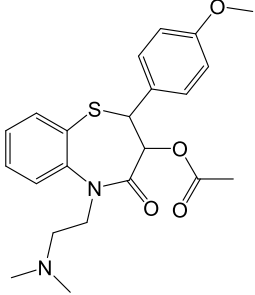
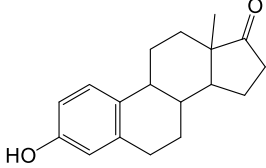
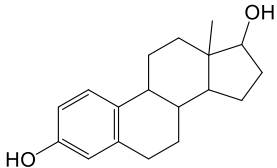
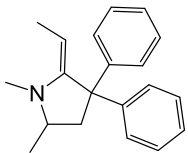
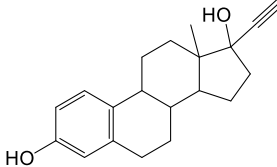
Atorvastatin	134523-00-5	558.64	C <sub>33</sub> H <sub>35</sub> FN <sub>2</sub> O <sub>5</sub>		0.01	0.05
Azathioprine	446-86-6	277.26	C <sub>9</sub> H <sub>7</sub> N <sub>7</sub> O <sub>2</sub> S		0.03	0.10
Azithromycin	83905-01-5	749	C <sub>38</sub> H <sub>72</sub> N <sub>2</sub> O <sub>12</sub>		0.03	0.11
Benzophenone-1	131-56-6	214.22	C <sub>13</sub> H <sub>10</sub> O <sub>3</sub>		0.01	0.06
Benzophenone-2	131-55-5	246.22	C <sub>13</sub> H <sub>10</sub> O <sub>5</sub>		0.01	0.05
Benzophenone-3	131-57-7	228.25	C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>		0.01	0.05

Benzophenone-4	4065-45-6	308.31	C <sub>14</sub> H <sub>12</sub> O <sub>6</sub> S		0.31	1.01
Benzoyllecgonine	519-09-5	289.33	C <sub>16</sub> H <sub>19</sub> NO <sub>4</sub>		0.01	0.05
Bezafibrate	41859-67-0	361.83	C <sub>19</sub> H <sub>20</sub> ClNO <sub>4</sub>		0.03	0.10
Bisphenol A	80-05-7	228.29	C <sub>15</sub> H <sub>16</sub> O <sub>2</sub>		0.03	0.10
Butylparaben	94-26-8	194.23	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>		0.01	0.06
Caffeine	58-08-2	194.19	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>		0.10	0.50
Carbamazepine	298-46-4	236.28	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O		0.01	0.05

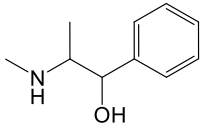
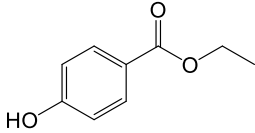
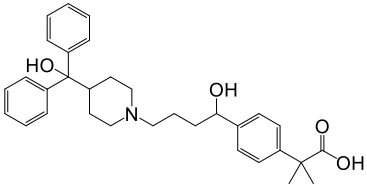
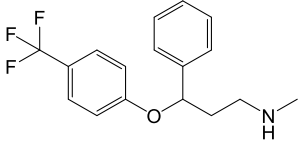
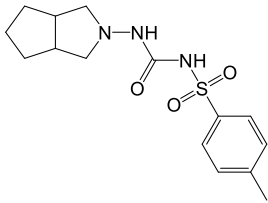
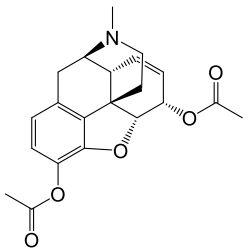
Carbamazepine 10,11 epoxide	36507-30-9	252.27	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>		0.03	0.10
Cetirizine	83881-51-0	388.9	C <sub>21</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>		0.02	0.08
Cimetidine	51481-61-9	252.34	C <sub>10</sub> H <sub>16</sub> N <sub>6</sub> S		0.10	0.52
Citalopram	59729-33-8	324.4	C <sub>20</sub> H <sub>21</sub> FN <sub>2</sub> O		0.05	0.50
Clarithromycin	81103-11-9	747.97	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>		0.01	0.06

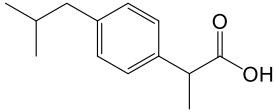
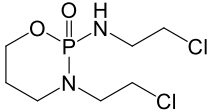
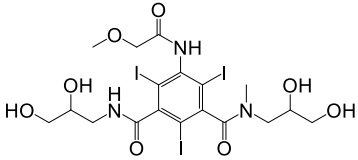
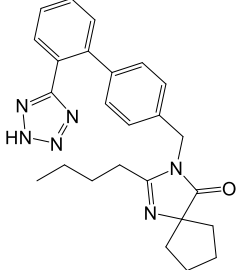
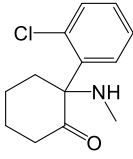
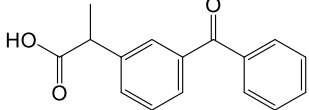
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Cocaine	50-36-2	303.36	C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub>		0.01	0.05
Codeine	76-57-3	299.37	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>		0.10	0.50
Cotinine	486-56-6	176.22	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O		0.01	0.05
Creatinine	60-27-5	113.12	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O		0.30	1.00
Desmethylcitalopram	62498-67-3	310.37	C <sub>19</sub> H <sub>19</sub> FN <sub>2</sub> O		0.01	0.05

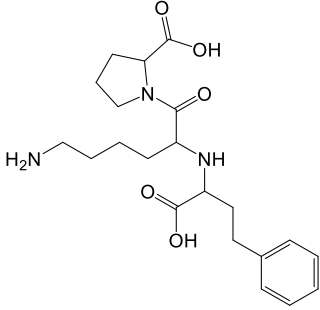
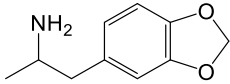
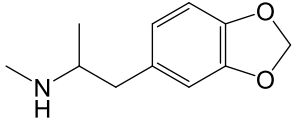
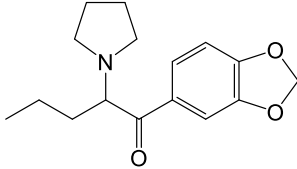
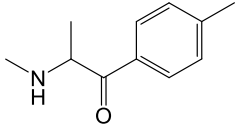
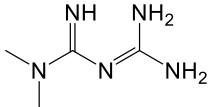
Desmethylvenlafaxine	93413-62-8	263.38	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>		0.03	0.10
Diclofenac	15307-86-5	296.15	C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>		0.03	0.10
Dihydrocodeine	125-28-0	301.39	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>		0.03	0.10
Dihydromorphine	509-60-4	287.36	C <sub>17</sub> H <sub>21</sub> NO <sub>3</sub>		0.01	0.05

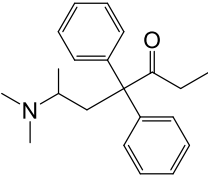
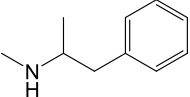
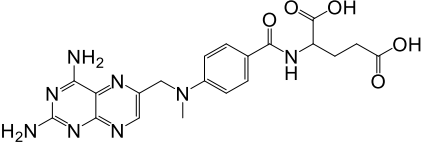
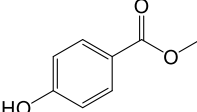
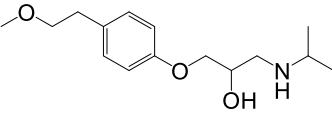
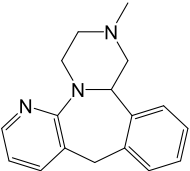
Diltiazem	42399-41-7	414.52	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S		0.01	0.05
E1	53-16-7	270.37	C <sub>18</sub> H <sub>22</sub> O <sub>2</sub>		0.10	0.49
E2	50-28-2	272.39	C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>		0.09	0.47
EDDP	30223-73-5	277.4	C <sub>20</sub> H <sub>23</sub> N		0.01	0.05
EE2	57-63-6	296.41	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>		0.10	0.48

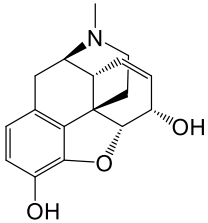
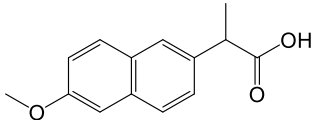
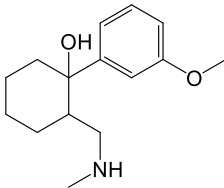
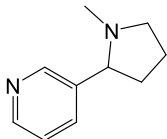
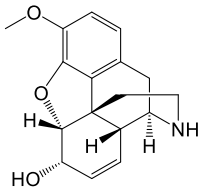
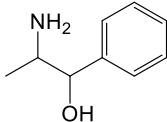


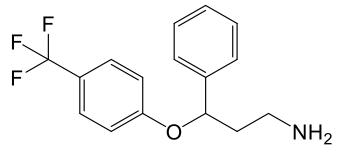
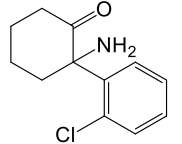
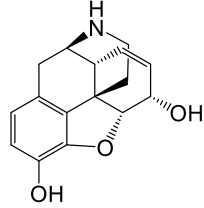
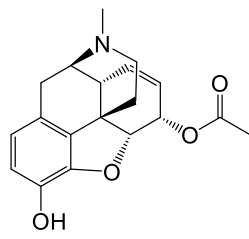
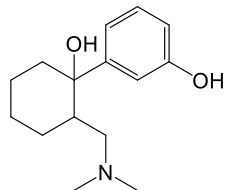
Ephedrine/pseudoephedrine	299-42-3	165.24	C <sub>10</sub> H <sub>15</sub> NO		0.03	0.10
Ethylparaben	120-47-8	166.18	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>		0.03	0.11
Fexofenadine	83799-24-0	501.67	C <sub>32</sub> H <sub>39</sub> NO <sub>4</sub>		0.03	0.09
Fluoxetine	54910-89-3	309.33	C <sub>17</sub> H <sub>18</sub> F <sub>3</sub> NO		0.01	0.05
Gliclazide	21187-98-4	323.41	C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S		0.01	0.05
Heroin	561-27-3	369.42	C <sub>21</sub> H <sub>23</sub> NO <sub>5</sub>		0.10	0.50

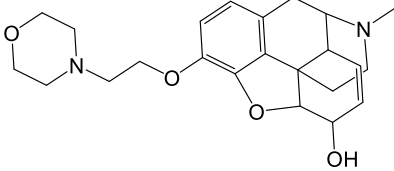
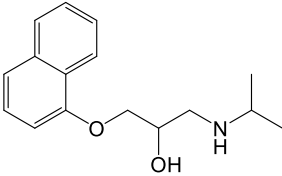
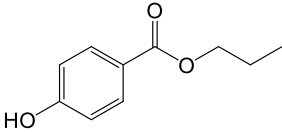
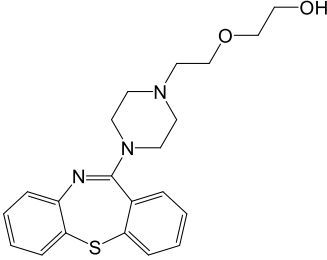
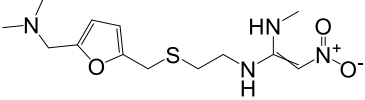
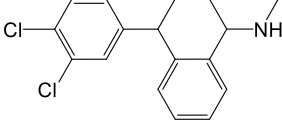
Ibuprofen	15687-27-1	206.29	C <sub>13</sub> H <sub>18</sub> O <sub>2</sub>		0.01	0.05
Ifosfamide	3778-73-2	261.09	C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> P		0.01	0.05
Iopromide	73334-07-3	791.12	C <sub>18</sub> H <sub>24</sub> I <sub>3</sub> N <sub>3</sub> O <sub>8</sub>		1.16	5.79
Irbesartan	138402-11-6	428.53	C <sub>25</sub> H <sub>28</sub> N <sub>6</sub> O		0.10	0.50
Ketamine	6740-88-1	237.73	C <sub>13</sub> H <sub>16</sub> ClNO		0.01	0.05
Ketoprofen	22071-15-4	254.29	C <sub>16</sub> H <sub>14</sub> O <sub>3</sub>		0.11	0.54

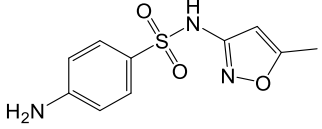
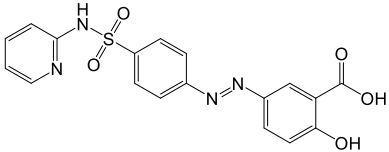
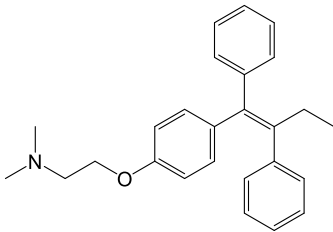
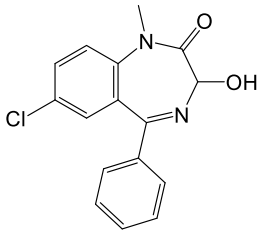
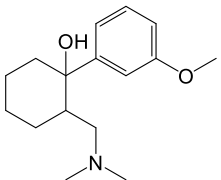
Lisinopril	76547-98-3	405.5	C <sub>21</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub>		0.09	0.93
MDA	4764-17-4	179.22	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>		0.03	0.10
MDMA	42542-10-9	193.25	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>		0.01	0.05
MDPV	687603-66-3	275.34	C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>		0.01	0.50
Mephedrone	1189805-46-6	177.24	C <sub>11</sub> H <sub>15</sub> NO		0.01	0.05
Metformin	657-24-9	129.17	C <sub>4</sub> H <sub>11</sub> N <sub>5</sub>		0.09	0.43

Methadone	76-99-3	309.46	C <sub>21</sub> H <sub>27</sub> NO		0.11	0.56
Methamphetamine	537-46-2	149.24	C <sub>10</sub> H <sub>15</sub> N		0.03	0.10
Methotrexate	59-05-2	454.45	C <sub>20</sub> H <sub>22</sub> N <sub>8</sub> O <sub>5</sub>		0.28	0.92
Methylparaben	99-76-3	152.15	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>		0.01	0.06
Metoprolol	51384-51-1	267.37	C <sub>15</sub> H <sub>25</sub> NO <sub>3</sub>		0.01	0.05
Mirtazapine	85650-52-8	265.35	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub>		0.01	0.05

Morphine	57-27-2	285.35	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>		0.30	1.00
Naproxen	22204-53-1	230.27	C <sub>14</sub> H <sub>14</sub> O <sub>3</sub>		0.10	0.49
N-desmethyltramadol	75377-45-6	249.35	C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>		0.01	0.05
Nicotine	54-11-5	162.24	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>		0.30	1.00
Norcodeine	467-15-2	285.35	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>		0.30	1.00
Norephedrine	492-39-7	151.21	C <sub>9</sub> H <sub>13</sub> NO		0.01	0.50

Norfluoxetine	83891-03-6	295.3	C <sub>16</sub> H <sub>16</sub> F <sub>3</sub> NO		0.01	0.05
Norketamine	35211-10-0	233.7	C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O		0.03	0.10
Normorphine	466-97-7	271.32	C <sub>16</sub> H <sub>17</sub> NO <sub>3</sub>		0.30	1.00
O-6-MAM	2784-73-8	327.37	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>		0.03	0.10
O-desmethyltramadol	185453-02-5	249.35	C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>		0.01	1.00

Pholcodine	509-67-1	398.51	C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>4</sub>		0.35	1.14
Propranolol	525-66-6	259.35	C <sub>16</sub> H <sub>21</sub> NO <sub>2</sub>		0.03	0.09
Propylparaben	94-13-3	180.21	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>		0.04	0.12
Quetiapine	111974-69-7	384.52	C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub> S		0.01	0.05
Ranitidine	66357-35-5	314.41	C <sub>13</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub> S		1.03	5.17
Sertraline	79617-96-2	306.24	C <sub>17</sub> H <sub>17</sub> Cl <sub>2</sub> N		0.01	0.05

Sulfamethoxazole	723-46-6	253.28	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S		0.03	0.10
Sulfasalazine	599-79-1	398.4	C <sub>18</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub> S		0.27	0.90
Tamoxifen	10540-29-1	371.53	C <sub>26</sub> H <sub>29</sub> NO		0.01	0.03
Temazepam	846-50-4	300.75	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>		0.01	0.05
Tramadol	27203-92-5	263.38	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>		0.01	1.00



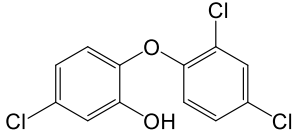
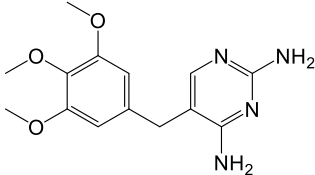
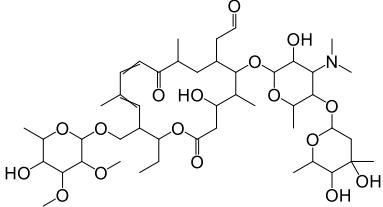
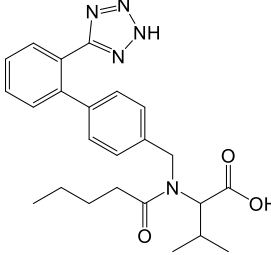
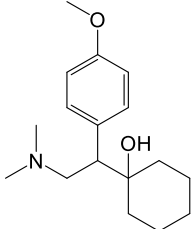
Triclosan	3380-34-5	289.55	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub> O <sub>2</sub>		0.34	1.13
Trimethoprim	738-70-5	290.32	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>		0.03	0.10
Tylosin	1401-69-0	916.12	C <sub>46</sub> H <sub>77</sub> NO <sub>17</sub>		0.01	0.10
Valsartan	137862-53-4	435.53	C <sub>24</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>		0.34	1.12
Venlafaxine	93413-69-5	277.41	C <sub>17</sub> H <sub>27</sub> N <sub>1</sub> O <sub>2</sub>		0.01	0.04

Table S2. Second order rate constants for the reaction of 40 OMPs with OH radicals. Experimentally determined, unless otherwise specified (QSAR: Quantitative structure–activity relationship).

<b>Compound</b>	<b><math>k_{OH}</math> (<math>M^{-1} s^{-1}</math>)</b>	<b>Reference</b>
Acetaminophen	$2.2 \times 10^9$	[2]
Atenolol	$8.0 \times 10^9$	[3]
Atorvastatin	$1.9 \times 10^{10}$	[4]
Azathioprine	$1.86 \times 10^9$	[5]
Azithromycin	$2.9 \times 10^9$	[6]
Benzophenone-3	$2.97 \times 10^{10}$	[7]
Benzoylcegonine	$5.13 \times 10^9$	[8]
Bezafibrate	$7.4 \times 10^9$	[9]
Bisphenol A	$1.02 \times 10^{10}$	[10]
Butylparaben	$9.2 \times 10^9$	[11]
Caffeine	$5.9 \times 10^9$	[12]
Carbamazepine	$8.8 \times 10^9$	[9]
Cimetidine	$6.5 \times 10^9$	[13]
Diclofenac	$7.5 \times 10^9$	[9]
E1	$2.6 \times 10^{10}$	[14]
E2	$1.41 \times 10^{10}$	[10]
EE2	$1.08 \times 10^{10}$	[10]
Ethylparaben	$7.7 \times 10^9$	[11]
Fluoxetine	$9 \times 10^9$	[15]
Ibuprofen	$7.4 \times 10^9$	[9]
Ifosfamide	$3.6 \times 10^9$	[16]
Iopromide	$3.3 \times 10^9$	[9]
Ketoprofen	$8.4 \times 10^9$	[17]
Metformin	$1.4 \times 10^9$	[16]
Methamphetamine	$7.9 \times 10^9$	[18]
Methotrexate	$8.7 \times 10^9$	[19]
Methylparaben	$6.8 \times 10^9$	[11]
Metoprolol	$7.3 \times 10^9$	[3]
Morphine	$10^{10}$ (QSAR)	[20]
Naproxen	$9.6 \times 10^9$	[21]
Propranolol	$1.0 \times 10^{10}$	[3]
Propylparaben	$8.6 \times 10^9$	[11]
Ranitidine	$1.5 \times 10^{10}$	[13]
Sulfamethoxazole	$5.5 \times 10^9$	[9]
Tramadol	$6.3 \times 10^9$	[22]
Triclosan	$5.4 \times 10^9$	[23]
Trimethoprim	$6.9 \times 10^9$	[6]
Tylosin	$8.2 \times 10^9$	[6]
Valsartan	$10^{10}$ (QSAR)	[20]
Venlafaxine	$8.8 \times 10^9$	[16]

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