

Supporting Information

Essential role of sunlight irradiation in aqueous micropollutant transformations: Influence of the water matrix and changes in toxicities

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Text S1 Methodology

Data in this review were collected from literature on MPs photolysis behavior in environment water over the last 20 years, including surface water (river and lake water) and treated wastewater (second effluent and disinfected wastewater). The search strategies used in Scopus and Web of Science are (phototransformation OR photoconversion OR photolysis OR photodegradation NOT photocataly-) AND (sunlight OR solar irradiation). The MPs were chosen if they were under the compatible conditions. As described in the beginning of each section, the concentration of water matrices was environmentally relative and then the corresponding MPs would be summarized. If a MP was investigated in more than one study, the variability between studies were assessed in table S1, and the one which was more environmentally relative (e.g., neutral pH, around 25°C, natural sunlight at midlatitude or xenon light filtered <290 nm) and published lately was selected to be shown in Fig. 1.

Text S2 References in Fig.2, Fig.3 and Fig.4.

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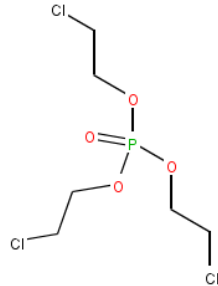
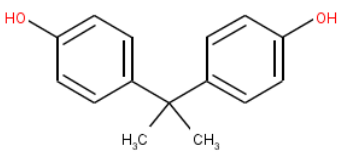
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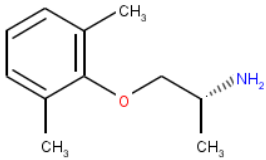
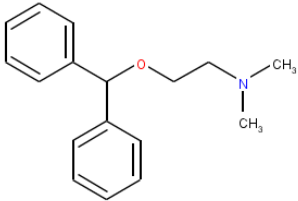
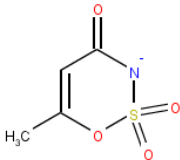
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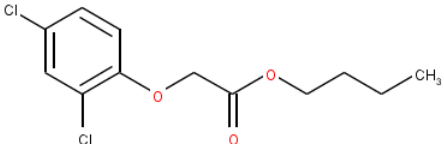
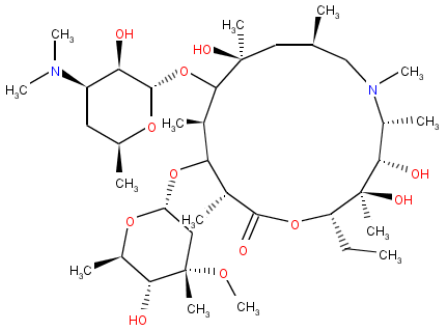
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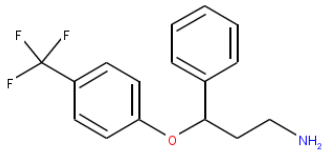
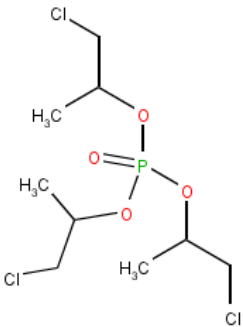
Table S1 MPs observable photodegradation rates in ultrapure water from previous researches, 91 MPs. $t_{1/2}$ refers to the number of days required for 50% attenuation under 8 h of effective solar irradiation per day.

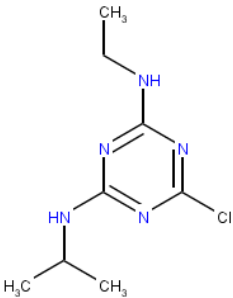
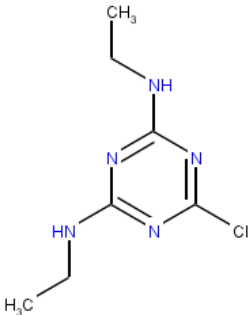
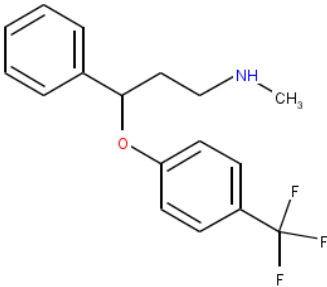
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
Slow group						
1	Atenolol	ATL	<chem>CC(C)NCC(O)COc1ccc(cc1)CC(=O)N</chem>	0^a 0.002^b	a: For $k \sim 0$, merry-go-round reactor (Xujiang Electromechanical Plant, Nanjing, China) equipped with a 290 nm-filtered 1000 W Xe lamp as simulated solar irradiation. $1.12 \times 10^{-7} \text{ Einstein} \cdot \text{L}^{-1} \cdot \text{s}^{-1}$ (290~600nm). Irradiance at the surface of cavettes was 7.9 to 8.3 $\text{W} \cdot \text{m}^{-2}$ at 365 nm that close to that of the sunlight (9.0 W m^{-2}) at noon in Nanjing ($32^\circ 02' \text{N}$). Water pH=6.8, 25°C. b: For $k=0.002 \text{ min}^{-1}$, a suntest (lamp power $765 \text{ W} \cdot \text{m}^{-2}$ with wavelength $> 300 \text{ nm}$; $[\text{MP}]_0 = 10 \mu\text{g} \cdot \text{L}^{-1}$) in a reactor containing pure water. Water pH≈ 7, 40°C.	1,2

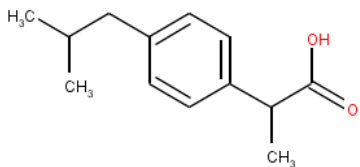
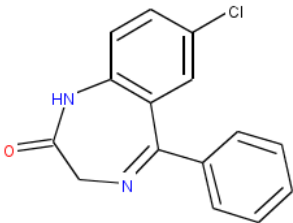
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
2	Tris(2-chloroethyl) phosphate	TCEP		0	Xe-OP lamp (Phillips 1 kW), simulated sunlight. 2.68×10^{-6} Einstein s^{-1} (290–400 nm), 0.17 Einstein s^{-1} in UV-C, pH=6.6, 25°C.	³
3	Bisphenol A	BPA		0	500 W medium mercury vapor lamp, filtered out light <290 nm. $5.25 \text{ W} \cdot \text{m}^{-2}$ at 365 nm. Neutral pure water at room temperature.	⁴

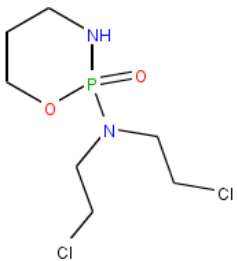
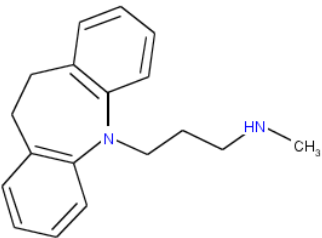
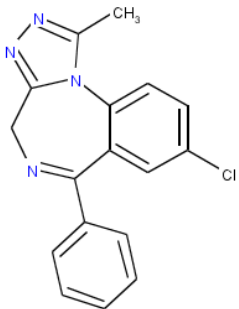
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
4	Mexiletine	MXE		0	A 150W Xenon Short Arc Lamp, filtered out light < 300 nm.	5
5	Diphenhydramine	DPHA		0	Same to NO.4	5
6	Acesulfame	ASF		$0.24 \times 10^{-5} \text{ a}$ $0.18 \times 10^{-5} \text{ b}$	Natural solar irradiation at Tianjin, China (39.13°N, 117.15°E) on 8/8/2013. A sunlight simulator (XPA-7, Nanjing Xujiang China) equipped with a 1 kW xenon lamp and filtered light below 290 nm. 26 ± 3°C. a: pH=7, b: pH=8.	6

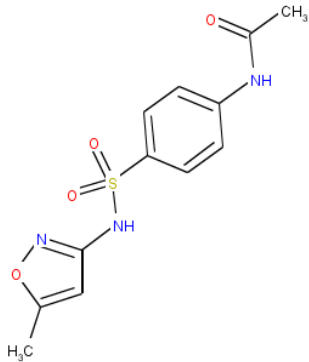
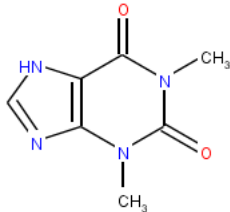
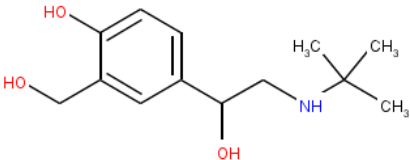
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
7	Butyl 2,4-dichlorophen oxyacetate	2,4-D		1.67×10^{-5a} 4.67×10^{-5b}	a: Outdoor (37.8° S, 145.0° E) solar irradiation at 16~19°C. A solar simulator (Hanau Suntest) equipped with a xenon arc lamp filtered out < 290 nm. $2.65 \times 10^{-4} \text{ Einstein} \cdot \text{m}^{-2} \text{ s}^{-1}$ (290~400 nm). b: Natural sunlight irradiation experiments were performed by exposure of the test systems on the roof of a building at RMIT University, Melbourne, Victoria (37.8° S, 145.0° E). Direct photolysis pathway.	7,8
8	Azithromycin	AZI		0.00010	Same to NO.1 ^b	1

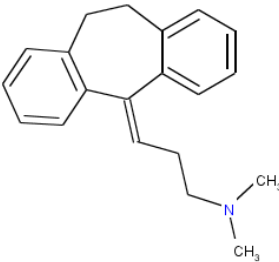
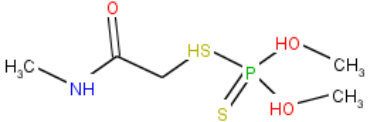
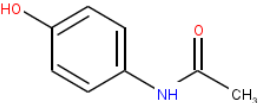
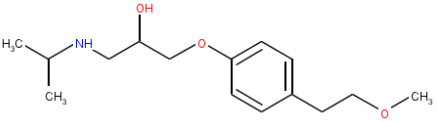
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
9	Norfluoxetine	NFX		0.00012	Same to NO.1 ^b	1
Medium group						
10	Tris(2-chloroisopropyl) phosphate	TCIPP		0.00018	Same as NO.2	3

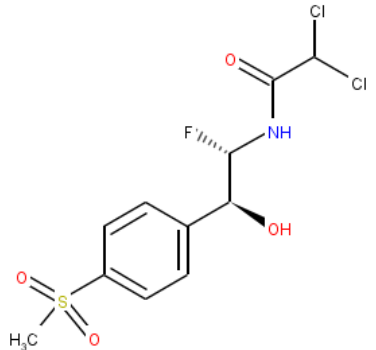
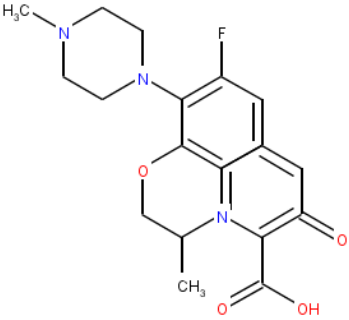
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
11	Atrazine	ATZ		0.00022	Same to NO.1 ^b	1
12	Simazine	SIM		0.00023a 0.00014 ^{b'}	a: Same to NO.1 ^b b': Same to NO.7b	1,8
13	Fluoxetine	FLUOX		0.00025	Same to NO.1 ^b	1

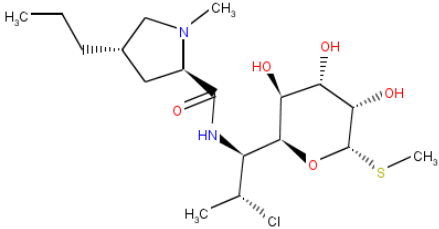
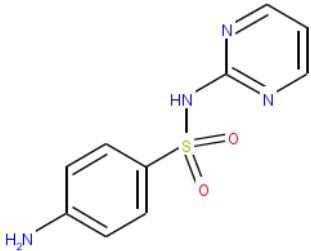
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
14	Ibuprofen	IPF		0.00025^a 0^b	a: A solar simulator (Atlas Suntest CPS+) with 500 W Xenon arc lamp, filtered < 290 nm. Light intensity is similar to natural sunlight at 40° 40 41" N, 83° 40 24" W in June at noon. pH=7 (± 0.1), 25 °C. b: Suntest CPS⁺, Atlas solar simulator, Xe short-arc lamp (1500 W) filtered < 290 nm. The light intensity, I_{lamp}, of the lamp was 765 $\text{W}\cdot\text{m}^{-2}$ and corresponded to 108% of annual average noon-time irradiation in Singapore. 29 °C, the average water temperature in Singapore's surface water. pH=6.	9,10
15	Nordiazepam	NDZ		0.00025	Same to NO.1 ^b	1

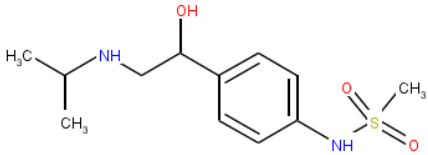
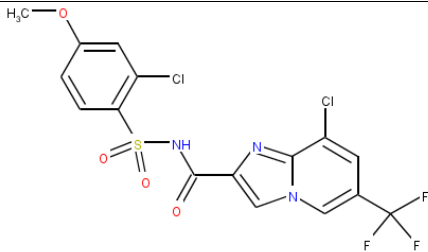
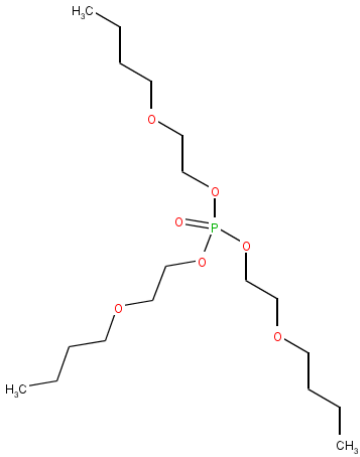
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
16	Cyclophosphamide	CYC		0.00027	Same to NO.1 ^b	1
17	Desipramine	DSP		0.00032	An Atlas Suntest XLS ⁺ solar simulator system (Chicago, USA), xenon arc lamp, $I=500 \text{ W}\cdot\text{m}^{-2}$ which is approximate the average annual conditions in temperate zones (NASA, 2014). Filtered < 290 nm. 25°C.	11
18	Alprazolam	ALP		0.00033	Same to NO.1 ^b	1

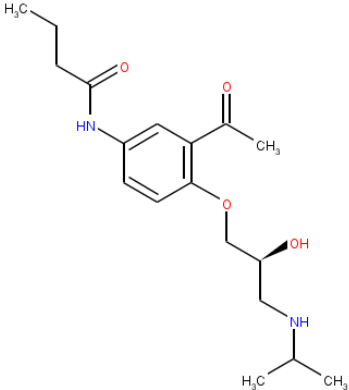
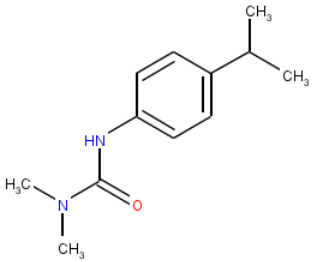
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
19	N-Acetyl Sulfamethoxazole	ASUL		0.00038	Same to NO.1 ^b	1
20	Theophylline	TPL		0.00038	Same to NO.1 ^b	1
21	Salbutamol	SAL		0.00047	Same to NO.1 ^b	1

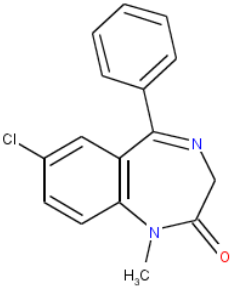
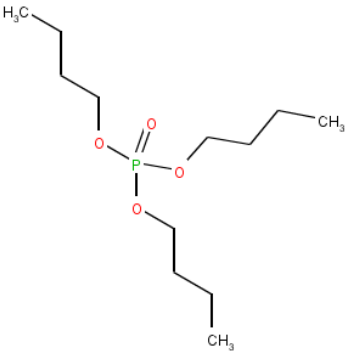
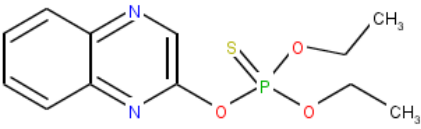
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
22	Amitriptyline	AMI		0.00048	Same to NO.1 ^b	1
23	Dimethoate	DM		0.00050	Same to NO.1 ^b	1
24	Paracetamol	PAT		0.00050 ^a 0.00310 ^b	a: Same to NO.1 ^b b': Solar light simulator, I _{300-800 nm} = 500 W·m ⁻² . k=0.00310 is for photolysis at the first 40 min.	1,12
25	Metoprolol	MTP		0.00053	Same to NO.1 ^b	1

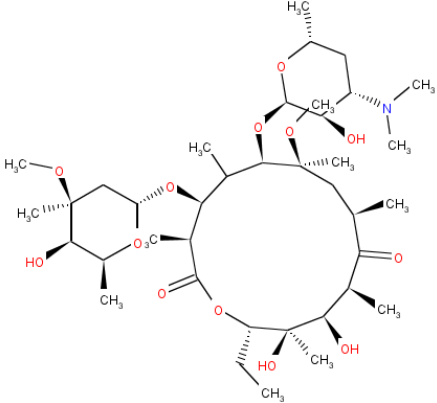
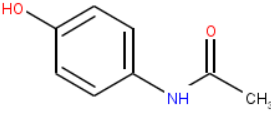
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
26	Florfenicol	FFC		0.00055^a $6.12 \times 10^{-5}^b$	a: Simulated solar irradiation experiments were performed by a XPA-II photochemical reactor (Xujiang Electromechanical Plant, China) equipped with a 1000-W xenon arc lamp. $\lambda < 290 \text{ nm}$ radiopacity. b: Outdoor experiments in Nanjing ($32^\circ 12' \text{ N}$, $118^\circ 95' \text{ E}$) and exposed to sunlight from 9 a.m. to 4 p.m. on sunny days of July.	13
27	Ofloxacin	OFA		0.00055	Same to NO.1 ^b	1

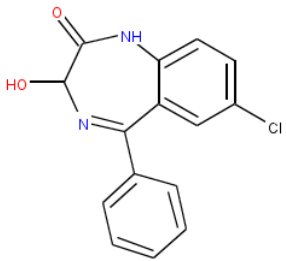
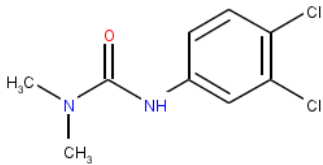
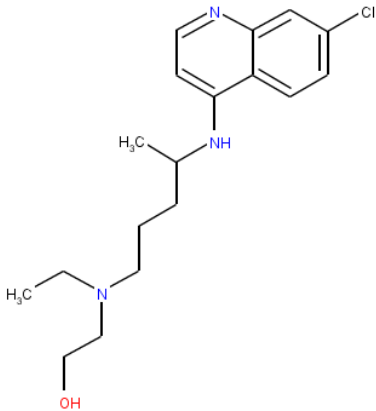
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
28	Clindamycin	CLIN		0.00057	Same to NO.1 ^b	1
29	Sulfadiazine	SDZ		0.00060 ^a 0.00426 ^b	a: A water-refrigerated 500 W Xe lamp surrounded by 290 nm cut-off filters was used as the light source. $pK_{a1} = 2$, $pK_{a2} = 6.5$. $pH=4$ ($k_{pH=9}=30\%k_{pH=4}$). Relative light intensity is similar to local solar irradiation (Oct., 2014, Dalian China). b: Suntest CPS⁺ simulator (Atlas, Germany) equipped with a xenon lamp and temperature sensor was used as the source of artificial sunlight in the wavelength range of 300~800 nm. $250 \text{ W}\cdot\text{m}^{-2}$. $pH=8$. $25\pm 2 \text{ }^{\circ}\text{C}$.	14,15

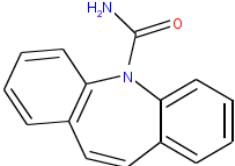
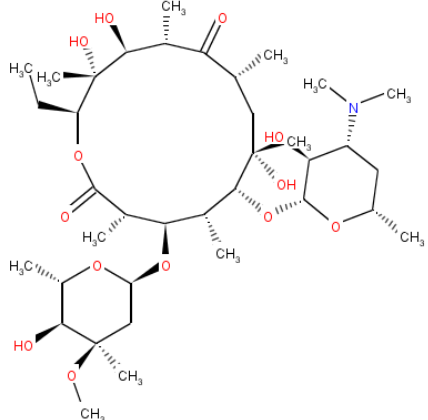
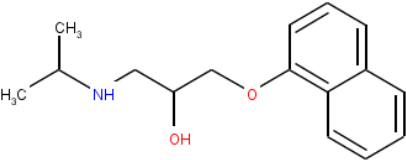
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
30	Sotalol	STL		0.00060	Same to NO.1 ^b	1
31	Fluazaindoline	FZD		0.00061	500W xenon lamp ($\lambda > 290 \text{ nm}$). pH=7.2, 25°C.	16
32	Tris(2-butoxyethyl) phosphate	TBOEP		0.00066	Same as NO.2	3

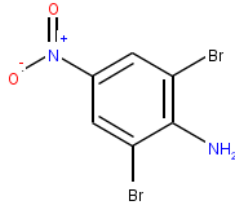
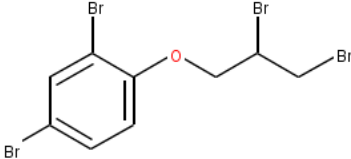
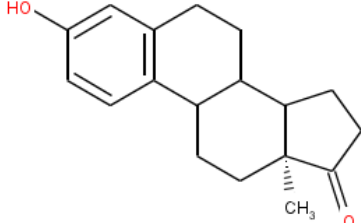
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33	Acebutolol	ACE		0.00067	Same to NO.1 ^b	1
34	Isoproturon	IPT		0.00072	Same to NO.1 ^b	1

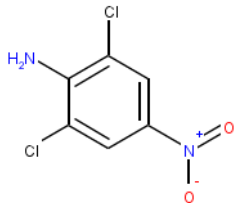
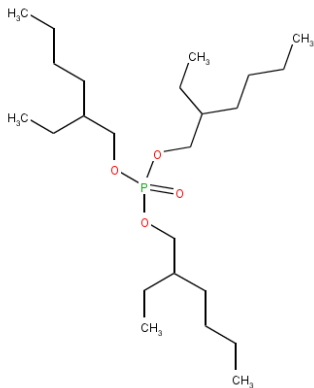
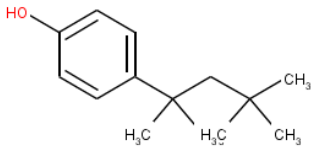
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
35	Diazepam	DZP		0.00073 ^a 0.00042 ^b	a: Same to NO.1 ^b b: Solarbox 1500 (Co.fo.me.gra, Italy), a 1500 W arc xenon lamp filtered light < 290 nm. $I_{290\sim 400 \text{ nm}}=55 \text{ W}\cdot\text{m}^{-2}$.	1,17
36	Tris(butyl) phosphate	TNBP		0.00077	Same as NO.2	3
37	Quinalphos	QP		0.00081	Xenon arc lamp (Suntest CPS ⁺ apparatus), 1500W, $750 \text{ W}\cdot\text{m}^{-2}$, equivalent to $2700 \text{ kJ}\cdot\text{m}^{-2}\cdot\text{h}^{-1}$, filtered < 290 nm. pH=5.35.	18

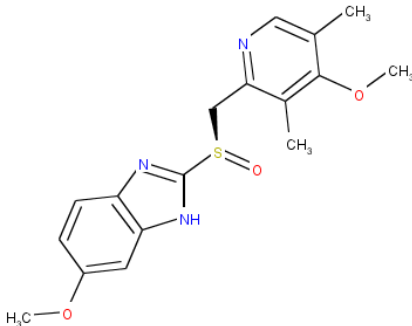
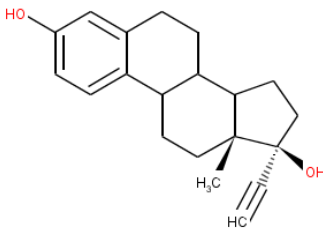
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38	Clarithromycin	CLA		0.00083	Same to NO.1 ^b	1
39	Acetaminophen	AAP		0.00084 ^a 0.05453 ^b	a: solar simulator (Suntest XLS⁺) with a 1700 W xenon lamp and filtered < 290 nm. $I_{300\sim400 \text{ nm}} = 40 \text{ W}\cdot\text{m}^{-2}$. $25 \pm 1 \text{ }^\circ\text{C}$, $\text{DO} = 0.5 \text{ mg}\cdot\text{L}^{-1}$. pH=7. b: 300 W solar simulator, $34 \pm 1 \text{ }^\circ\text{C}$, pH=7.	19,20

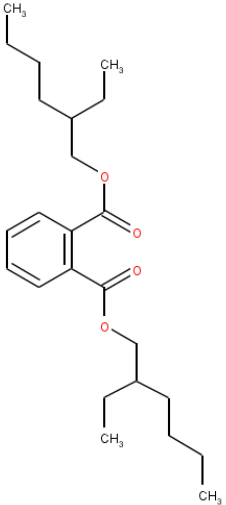
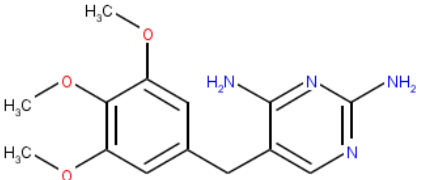
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
40	Oxazepam	OZP		0.00093 ^a 0.00076 ^{b'}	a: Same to NO.1 ^b b: Same to NO.17	1,17
41	Diuron	DU		0.00097 ^a $8.33 \times 10^{-5b'}$	a: Same to NO.1 ^b b': Same to NO.7 ^b	1,8
42	Hydroxychloroquine	HCQ		0.00100	Suntest CPS ⁺ simulator (Atlas, Germany) with a Xe lamp, produces the non-collimated light. $I_{300-800\text{nm}} = 500 \text{ W} \cdot \text{m}^{-2}$, 25 °C, pH=6.43.	21

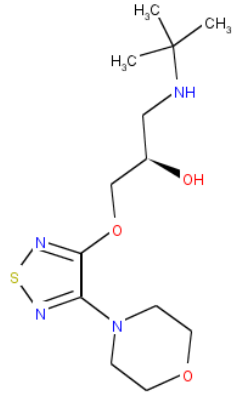
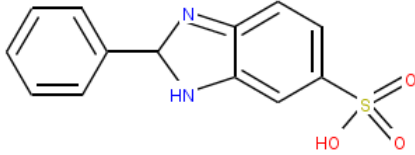
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
43	Carbamazepine	CBZ		0.00110 ^a 0.00012 ^{b'}	a: Same to NO.1 ^b b': Same to NO.7 ^b	1,8
44	Erythromycin	ETM		0.00110	Same to NO.1 ^b	1
45	Propranolol	PPN		0.00115 ^a 0.0017 ^{b'}	a: For $k=0.00115 \text{ min}^{-1}$, same to NO.4 b': For $k=0.0017 \text{ min}^{-1}$, same to NO.1 ^b	1,5

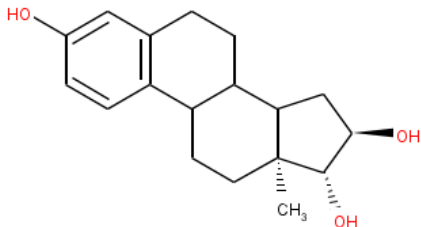
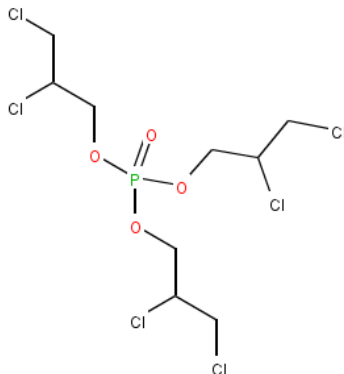
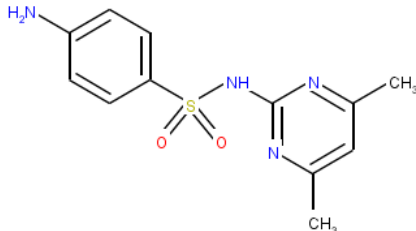
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
46	2,6-dibromo-4-nitroaniline	DBNA		0.00130	$I_{300\sim 400 \text{ nm}} = 65 \text{ W}\cdot\text{m}^{-2}$ and 20% relative humidity. Each hour of exposure in the chamber at this intensity was calculated to be equivalent to approximately 1.8 h of direct sunlight at 30°N latitude during the June summer solstice. 20 °C. Media: distilled water.	22
Fast group						
47	2,3-Dibromopropyl-2,4,6-tribromophenyl ether	DPTE		0.00147	A water-refrigerated 500 W medium-pressure mercury lamp filtered 290 nm, mimicking the UV-A and UV-B portions of sunlight. $I_{\lambda\text{max}}=I_{\lambda 360\text{nm}}=6\times 10^{-2} \text{ Einstein}\cdot\text{m}^{-2} \text{ s}^{-1}$.	23
48	Estrone	E1		0.00150 ^a 0.00190 ^b	a: A Suntest CPS ⁺ solar simulator (Moussy Le Neuf France), 1500 W xenon lamp filtered UV light. $I=250 \text{ W}\cdot\text{m}^{-2}$. Room temperature ($20 \pm 2 \text{ }^{\circ}\text{C}$), $\text{pH}=7.3 \pm 0.1$. b: Solarbox 1500 (Co.fo.me.gra, Italy), 1500W arc xenon lamp	24,25

Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
					filtered < 290 nm. $I_{290\sim 400 \text{ nm}} = 55 \text{ W}\cdot\text{m}^{-2}$.	
49	Dicloran	DL		0.00153	Same to NO.47	22
50	Tris(2-ethylhexyl) phosphate	TEHP		0.00157	Same as NO.2	3
51	p-tert-octylphenol	PTO		0.00160 ^{a'} 0.00290 ^{b'} 0.00360 ^{c'} 0.00420 ^{d'}	Same to NO.14 ^b . a': pH=6, b': pH=7.5, c': pH=9, d': pH=11.	10

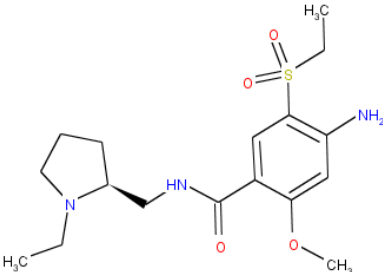
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
52	Omeprazole	OPZ		0.00170^a 0.08530^b	a: Natural irradiation. The average total daily short-wave radiation was 286 and 273 $\text{W}\cdot\text{m}^{-2}$ for July and August, respectively, while the sunshine duration from sunrise to sunset was 10 and 11 h, for the two months respectively. The mean daily air temperature was 23 and 26 °C, with minimum air temperature at 17 and 18 °C and maximum air temperature at 26 and 32 °C, for July and August, respectively. b: Xenon arc lamp (1500 W), 750 $\text{W}\cdot\text{m}^{-2}$. Filtered light < 290 nm. a and b are in distilled water at pH=6.	26
53	17 α -ethinylestradiol	EE2		0.00200^a 0.01665^b	a: Solar simulator (SOL 500, Dr. Hönle, Germany). $I_{\text{UVB}}=2.0 \text{ W}\cdot\text{m}^{-2}$, $I_{\text{UVA}}=31.2 \text{ W}\cdot\text{m}^{-2}$. While sunlight radiation on a sunny afternoon in late June in Gdynia (54 °N), showed corresponding	27,28

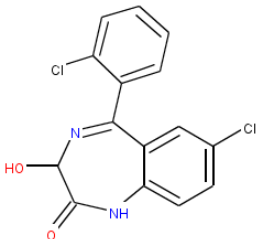
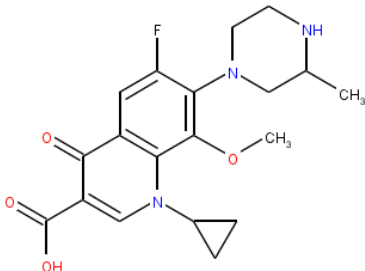
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					values of $2.3 \text{ W}\cdot\text{m}^{-2}$ and $26.8 \text{ W}\cdot\text{m}^{-2}$. b': Same to NO.47b	
54	Bis(2-ethylhexyl) phthalate	DEHP		0.00203	Same as NO.2	3
55	Trimethopri me	TIM		0.00218	Same to NO.1 ^b	1

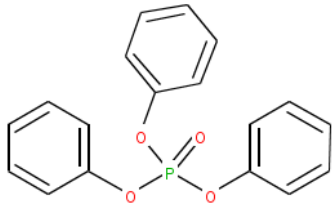
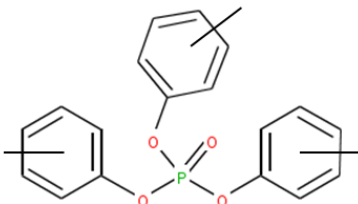
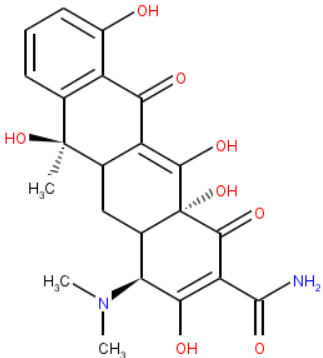
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
56	Timolol	TMO		0.00250	Same to NO.4	29
57	2-phenylbenzimidazole-5-sulfonic acid	PBSA		0.00263	A 125 W high pressure mercury lamp (HPK, Heraeus) filtered < 290 nm. The HPK lamp was turned on preliminarily for 10 min for stabilization. $I_{300\sim 400 \text{ nm}} = 33 \text{ W}\cdot\text{m}^{-2}$, comparable to the midday sunlight in June, Lyon (France; 45°N latitude). The temperature was maintained at $20 \pm 1 \text{ }^{\circ}\text{C}$ by cooling water circulation. pH = 8.	30

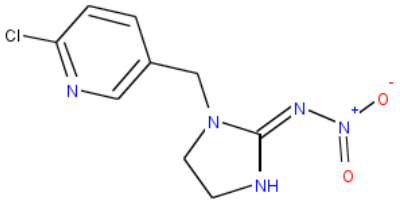
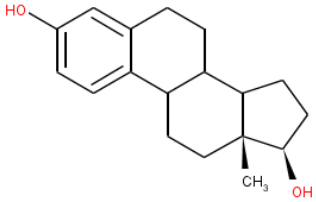
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
58	Estriol	E3		0.00300	A 150 W Xenon Short Arc Lamp (Oriel Optics Corporation, Stamford, CT, USA) filtered <300 nm. $I = 1.68\sim 1.88 \text{ mmol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$. 22~25 °C. pH = 8.	31
59	Tris(2,3-dichloropropyl) phosphate	TDCPP		0.00351	Same as NO.2	3
60	Sulfamethazine	SMT		0.00396	Same to NO.29 ^b	15

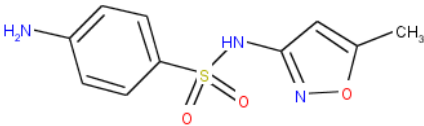
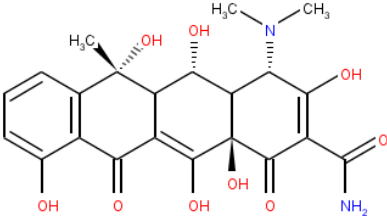
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
61	Caffeine	CAF		0.00400^a $5.67 \times 10^{-5b'}$	a: A solar simulator (Atlas Suntest CPS⁺) with a Xenon arc lamp and lamp energy of 500 W. Filtered light < 290 nm. Compared to chemical actinometry (p-nitroanisole/pyridine system) is 2.83 d⁻¹ over a range of 290–800 nm at noon in June at 40°N, their solar simulator is 10.51 d⁻¹). 25 °C. b': Same to NO.7^b	8,32

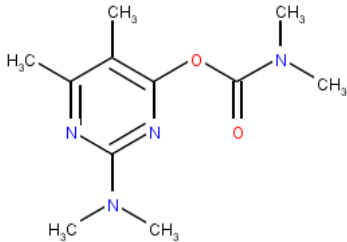
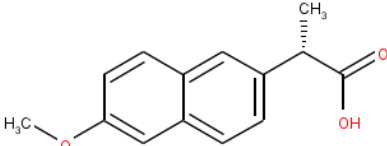
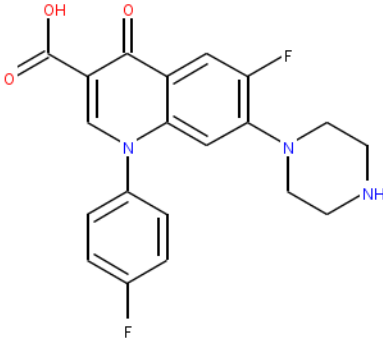
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
62	Amisulpride	ASP		0.00413	Same to NO.17	11

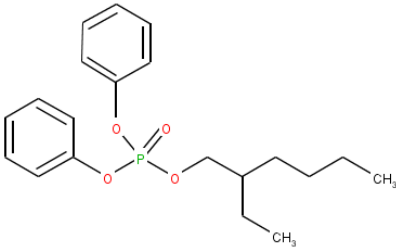
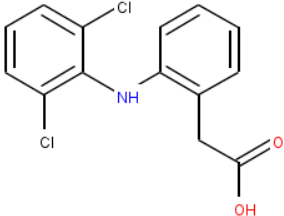
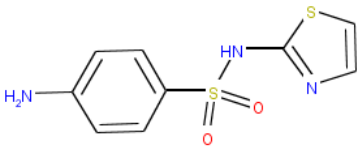
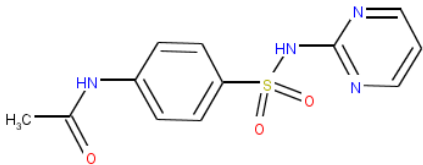
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
63	Lorazepam	LAP		0.00450	Same to NO.36	17
64	Gatifloxacin	GFC		0.00505 0.00630	A merry-go-round photochemical reactor was employed, and a Pyrex well cooled and filtered xenon lamp (1000W) was used to simulate sunlight ($\lambda > 290 \text{ nm}$). For $k = 0.00505 \text{ min}^{-1}$, pH=7 under simulated irradiation. $k = 0.00630 \text{ min}^{-1}$ is under natural sunlight.	33,34

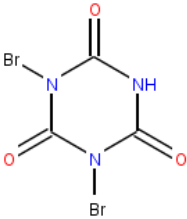
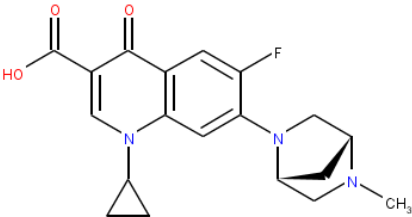
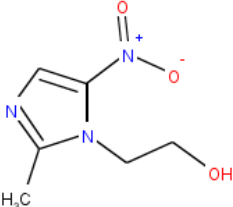
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
65	Tris(phenyl) phosphate	TPHP		0.00717	Same as NO.2	3
66	Tris(methylphenyl) phosphate	TMPP		0.00870	Same as NO.2	3
67	Tetracycline	TC		0.01360	150W Xenon Short Arc Lamp (XBO 150W/CR OFR). The operation current was set at 8.00A in all experiments. Filtered light < 300nm. pH=6.99. 25±0.5 °C	35

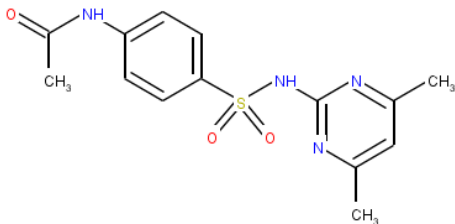
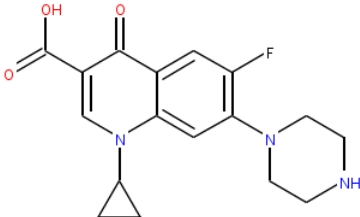
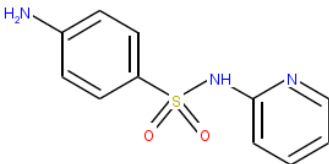
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
68	Imidacloprid	IMI		0.01461	Same to NO.1 ^b	1
69	17 β -estradiol	E2		0.01656 ^a 0.00085 ^{b'}	a: Same to NO.47b. b': A solar simulator (SunTest XLS+; Atlas Inc., Chicago, IL), filtered < 290nm. Exposures lasted 6 h at a constant irradiance of 11040 $\mu\text{mol}\cdot\text{m}^{-2}$ (650 $\text{W}\cdot\text{m}^{-2}$), which is equivalent to the total irradiance received during a typical clear, summer day at 36° N (i.e. central North Carolina, USA).	27,36

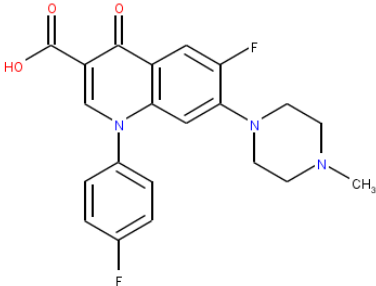
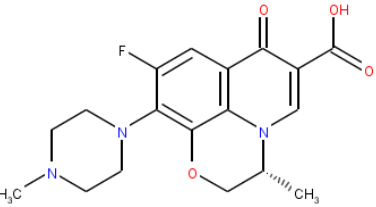
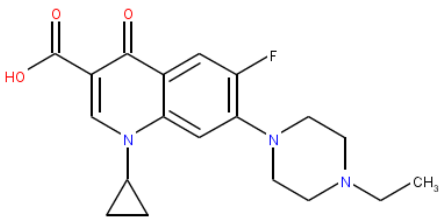
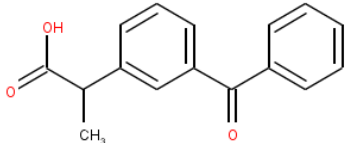
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
70	Sulfamethoxazole	SMA		0.01698	Same to NO.1 ^b	1
71	Oxytetracycline	OTC		0.01730	Irradiation was provided by a Suntest CPS ⁺ sunlight simulator (Atlas, Germany) equipped with a 1.1 kW xenon lamp, $I_{300-800 \text{ nm}}=765 \text{ W}\cdot\text{m}^{-2}$. pH=7.1. 20°C.	37

Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
72	Pirimicarb	PIRI		0.02063	Same to NO.1 ^b	1
73	Naproxen	NPX		0.0227 ^a 0.0636 ^b	a: Same to NO.24b' b: Direct photolysis. An SGY-IIB.Y1 rotary photochemical reactor (Nanjing STO Co. Ltd., China) and a 350W xenon lamp filtered 290 nm. 25 °C. during irradiation. $I = 996\sim1042 \text{ W}\cdot\text{m}^{-2}$ for the full-spectrum.	12,38
74	Sarafloxacin	SFC		0.02660 ^a 0.07010 ^b	a: Same to NO.65 b: Same to NO.65, under sunlight.	33,34

Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
75	2-ethylhexyl diphenyl phosphate	EHDP		0.02671	Same as NO.2	3
76	Diclofenac	DCF		0.03240 ^a 0.01860 ^{b''}	a: Same to NO.1b b'': Same to NO.24b'	1,12
77	Sulfathiazole	STZ		0.03352	A SUNTEST XLS ⁺ sunlight simulator (ATLAS, USA), I _{300–800 nm} =600 W·m ⁻² , filtered light < 285 nm. pH=7.	39
78	N ⁴ -acetylsulfadiazine	Ac-SDZ		0.03637	Same to NO.29 ^b	15

Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
79	1,3,5-Tris-(2,3-dibromopropyl)-1,3,5-triazine-2,4,6-trione	TDTT		0.04100	Same as NO.2	3
80	Danofloxacin	DFN		0.04240 ^a 0.11700 ^b	a: Same to NO.65 b: Same to NO.65, under natural sunlight.	33,34
81	Metronidazole	MTD		0.04278	Same to NO.1 ^b	1

Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
82	N ⁴ -acetylsulfamethazine	Ac-SMT		0.04316	Same to NO.29 ^b	15
83	Ciprofloxacin	CFN		0.04550 ^a 0.11300 ^b	a: Same to NO.65 b: Same to NO.65, under natural sunlight.	33,34
84	Sulfapyridine	SPD		0.05341	XPA-7 photoreactor (Xujiang, China). A water-refrigerated 500 W medium-pressure Hg lamp filtered < 290 nm. I _{300–800 nm} =53 W·m ⁻² . pH=8.3.	40

Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
85	Difloxacin	DIF		0.08330 ^a 0.04920 ^b	a: Same to NO.65 b: Same to NO.65, under natural sunlight.	33,34
86	Levofloxacin	LFN		0.09170 ^a 0.01480 ^b	a: Same to NO.65 b: Same to NO.65, under natural sunlight.	33,34
87	Enrofloxacin	ENF		0.09900 ^a 0.06900 ^b	a: Same to NO.65 b: Same to NO.65, under natural sunlight.	33,34
88	Ketoprofen	KTP		0.11552	Same to NO.1 ^b	1

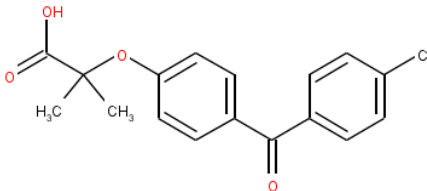
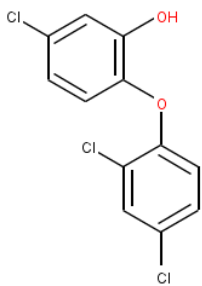
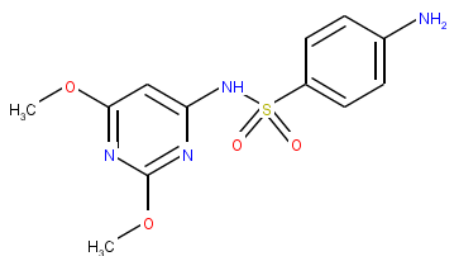
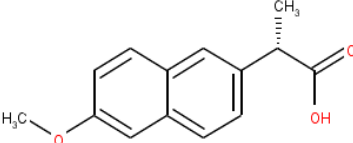
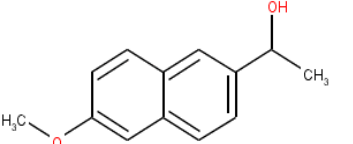
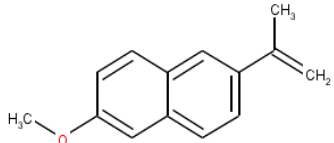
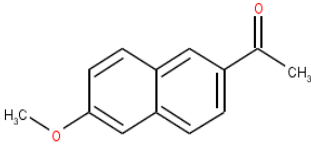
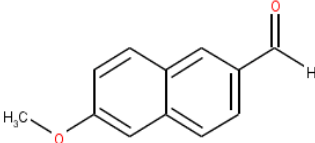
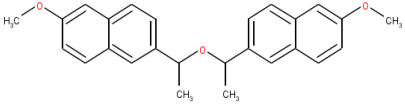
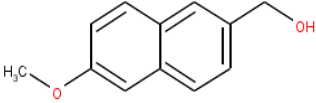
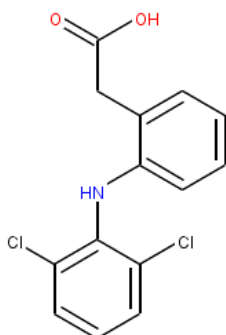
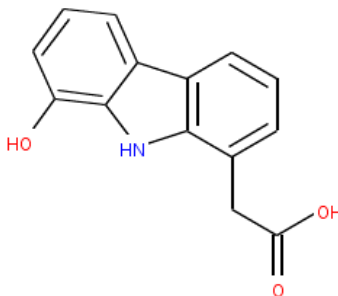
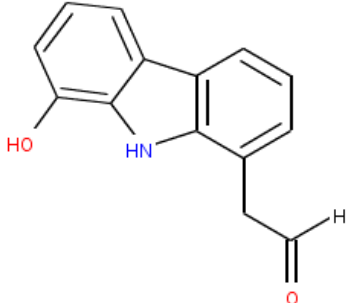
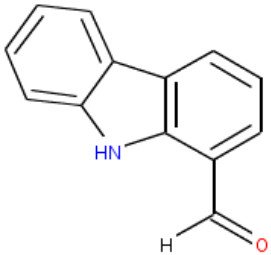
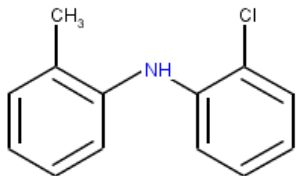
Number	Name	Abbreviation	Structure	$k \text{ min}^{-1}$	Conditions	Reference
89	Fenofibric acid	FFA		0.23105	Same to NO.1 ^b	1
90	Triclosan	TCS		0.27253 ^a 0.00627 ^b	a: An air-cooled Xenon lamp (NXe 1500B, Atlas), 550 W·m ⁻² . 35°C. b: Same to NO.7b	7,41
91	Sulfadimethoxine	SDT		9.58900	Suntest CPS ⁺ (Atlas Devices) solar simulator with a 500 W xenon lamp which operated at 4.5 times the intensity of average sunlight at 40°N at noon in June. 25°C.	42

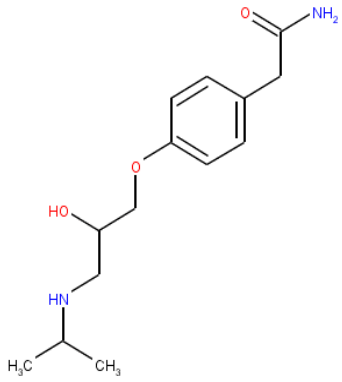
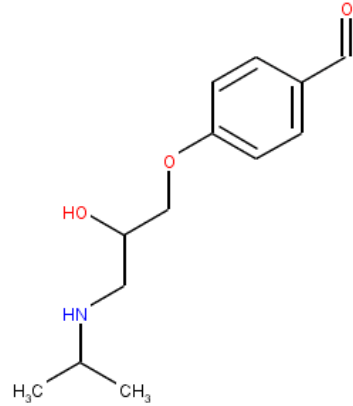
Table S2 Toxicity of parent MPs and product predicted by T.E.S.T. during photodegradation. a: Developmental toxicity value > 0.5 refers to developmental toxicant. b: Mutagenicity>0 refers to be mutagenic.

Number of products	Structure of photodegradation products	Toxicity of photodegradation products				Reference
		<i>Daphnia magna</i> LC ₅₀ (48 h) (mg/L)	Oral rat LD ₅₀ (mg/kg)	Developmental toxicity ^a	Mutagenicity ^b	
1	 Naproxen	30.26	285.03	1.04	0.29	38,43,44
1_1		0.56	1263.40	0.95	0.22	

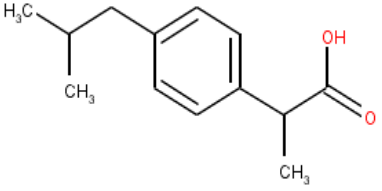
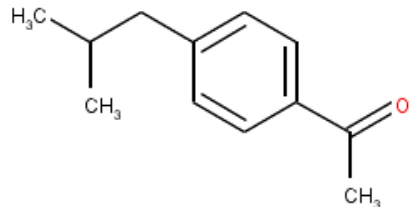
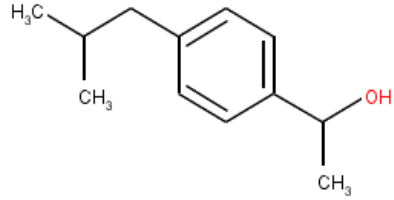
1_2		3.39	841.93	0.71	0.56	
1_3		0.86	527.53	0.85	0.47	
1_4		0.92	n.a.	0.59	1.17	
1_5		0.26	824.20	0.4	0.3	
1_6		0.73	2346.95	0.64	0.47	

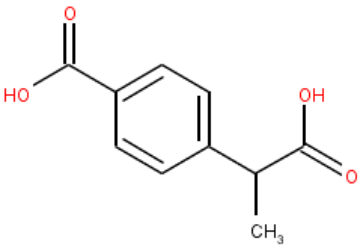
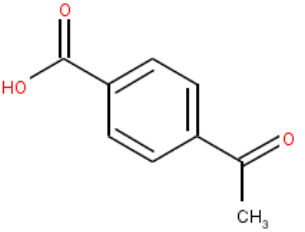
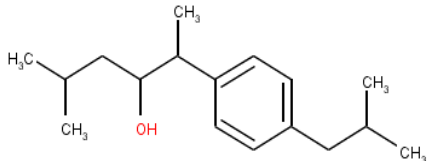
2	 Diclofenac	9.37	228.56	0.91	0.4	45
2_1		1.50	1903.56	1.02	0.12	

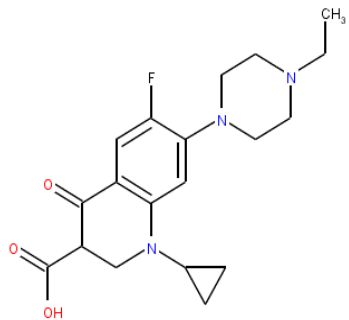
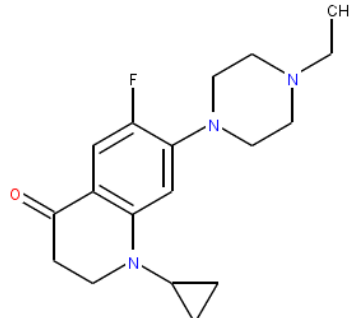
2_2		1.27	n.a.	1.02	0.4	
2_3		3.74	n.a.	0.81	0.88	
2_4		3.33	1362.80	0.46	0.34	

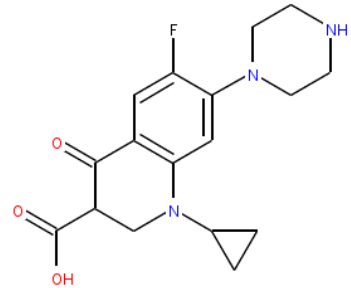
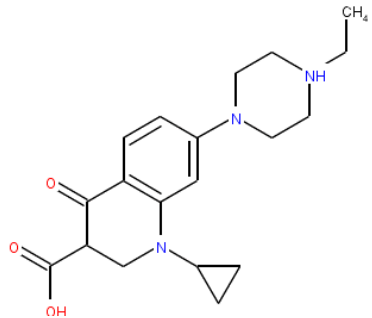
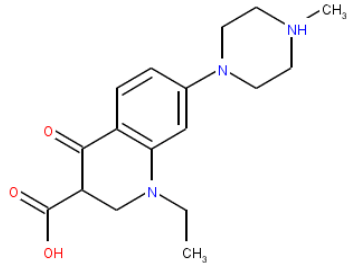
3	 Atenolol	43.75	2063.92	0.65	0.02	46
3_1		81.94	n.a.	0.5	0.02	

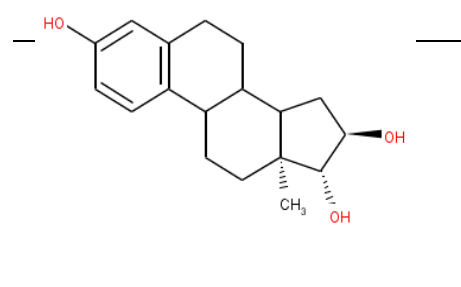
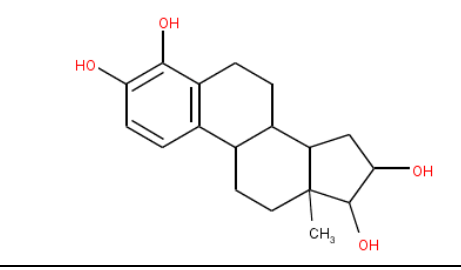
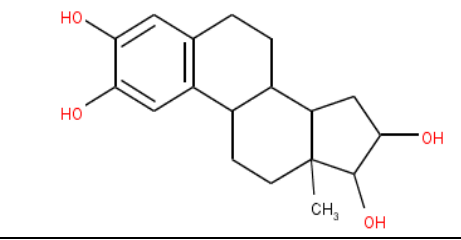
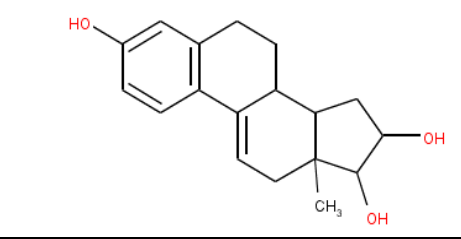
3_2	Chemical structure of 4-(4-hydroxy-3-(2-isopropylaminoethoxy)benzaldehyde). The molecule consists of a benzene ring with a hydroxyl group (OH) at position 4, an isopropylamino group (NH-CH(CH₃)₂) at position 3, and an aldehyde group (CHO) at position 1. The benzene ring is connected to the isopropylamino group via an ether linkage (-O-).	64.28	1789.60	0.64	0.11	
3_3	Chemical structure of 4-(4-hydroxy-3-(2-isopropylaminoethoxy)benzaldehyde). The molecule consists of a benzene ring with a hydroxyl group (OH) at position 4, an isopropylamino group (NH-CH(CH₃)₂) at position 3, and an aldehyde group (CHO) at position 1. The benzene ring is connected to the isopropylamino group via an ether linkage (-O-).	58.87	1757.19	0.52	0.02	
3_4	Chemical structure of 4-(4-hydroxy-3-(2-isopropylaminoethoxy)benzaldehyde). The molecule consists of a benzene ring with a hydroxyl group (OH) at position 4, an isopropylamino group (NH-CH(CH₃)₂) at position 3, and an aldehyde group (CHO) at position 1. The benzene ring is connected to the isopropylamino group via an ether linkage (-O-).	1244.90	2067.78	0.70	0.35	

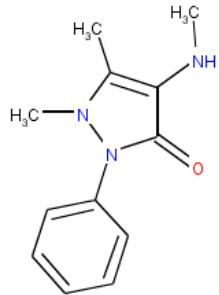
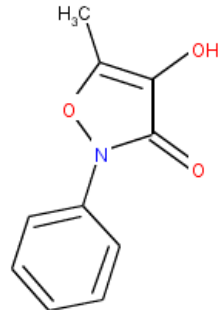
4	 Ibuprofen	6.78	1367.46	0.87	0.09	47
4_1		5.95	1412.26	0.59	0.66	
4_2		3.93	1590.60	0.66	0.18	

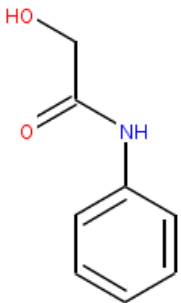
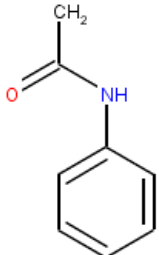
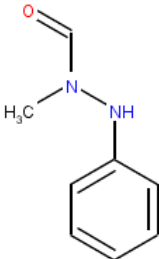
4_3		15.78	3231.71	0.78	0.22	
4_4		91.06	n.a.	0.58	0.29	
4_5		1.94	2485.02	0.50	0.11	

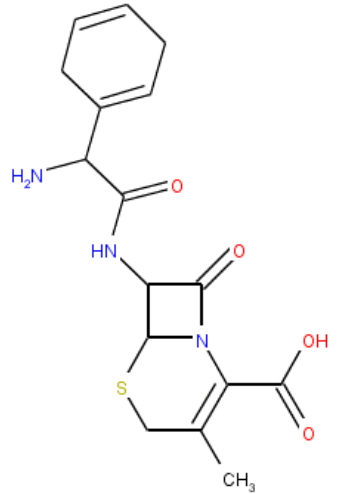
5	 Enrofloxacin	66.92	2092.34	1.13	0.67	48
5_1		2.36	1418.13	1.03	0.65	

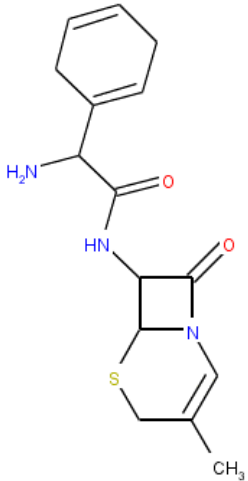
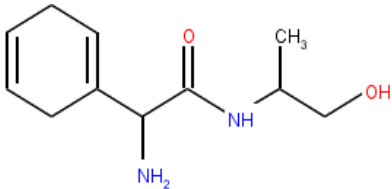
5_2		104.38	3832.45	1.15	0.56	
5_3		20.37	1516.69	1.25	0.52	
5_4		175.39	2332.58	1.19	0.44	

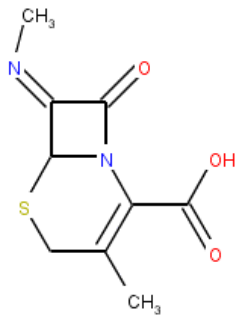
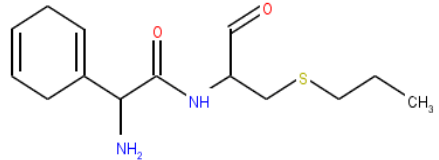
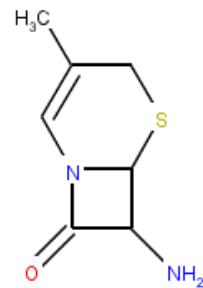
6	 Estriol	5.15	499.14	0.99	0.7	31
6_1		4.63	259.13	0.98	0.27	
6_2		4.74	256.26	0.97	0.31	
6_3		6.75	332.95	1.02	0.59	

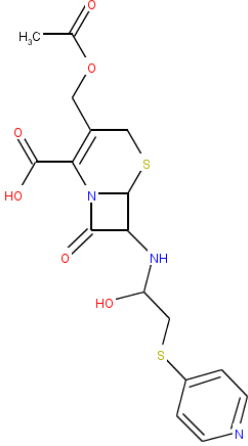
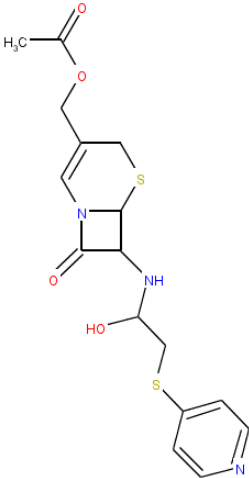
7	 4-methylaminoantipyrine	38.24	724.21	0.52	0.35	49
7_1		n.a.	n.a.	0.85	0.12	

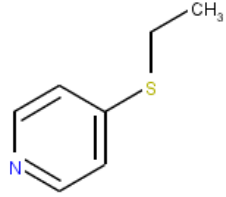
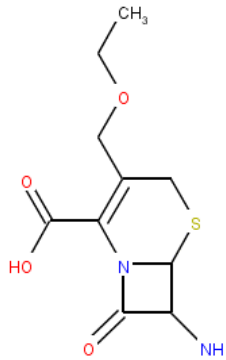
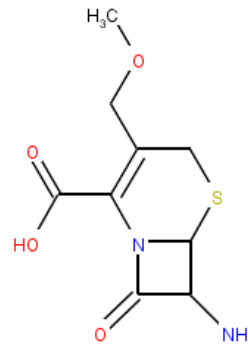
7_2		75.90	1505.42	0.09	0.19	
7_3		2.66	1321.18	0.44	0.07	
7_4		81.22	867.80	0.82	0.64	

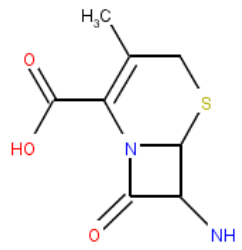
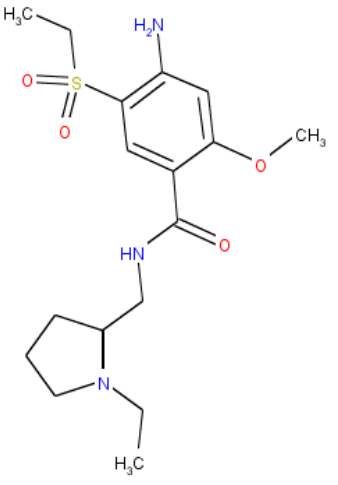
8	 Chemical structure of Cephadrine, a cephalosporin antibiotic. It features a cephadrine nucleus (a 6-membered ring with a sulfur atom and a 4-membered ring fused to it, containing a nitrogen atom). The 4-membered ring has a carbonyl group (=O) and an amide group (-NH-) attached to it. The amide group is further substituted with a phenylacetamido group (-CH(Ph)-C(=O)-NH-). The 6-membered ring has a methyl group (-CH₃) and a carboxylic acid group (-COOH) attached to it. Cephadrine	2640.85	15147.01	0.03	0.13	50
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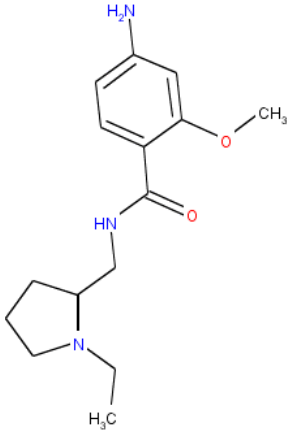
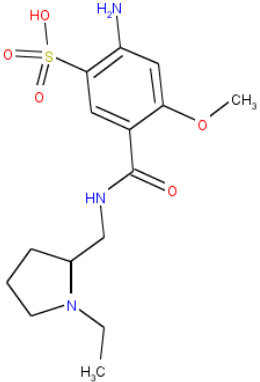
8_1	 <chem>CC1=CC=C(C=C1)C(=O)C(N)NC2=CC3=C(C=C2)S[C@H](C=C3)C(=O)N1</chem>	273.80	15653.15	0.06	0.20	
8_2	 <chem>CC(C)C(O)NC(=O)C(N)Cc1ccccc1</chem>	408.65	628.45	0.56	0.55	

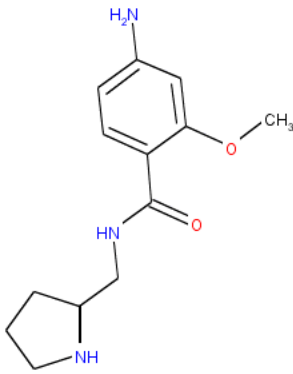
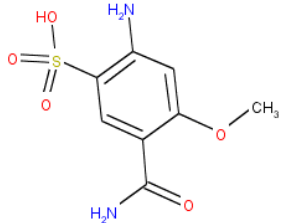
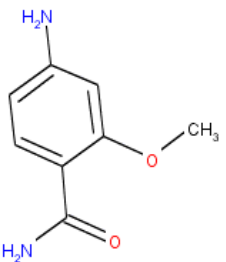
8_3		255.93	1793.90	0.75	0.12	
8_4		15.10	n.a.	0.08	0.05	
8_5		1.80	n.a.	0.8	n.a.	

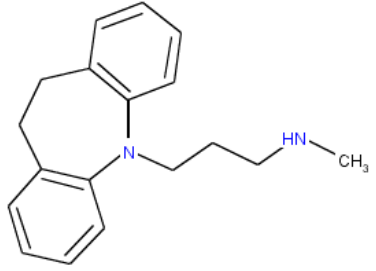
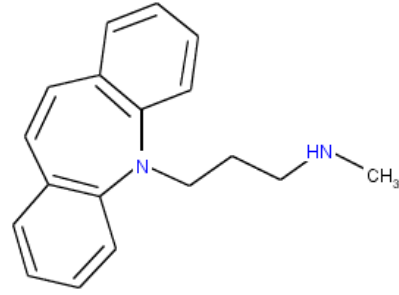
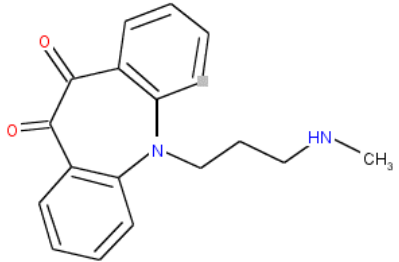
9	 Cephapirin	484.33	6166.53	0.01	0.22	50
9_1		137.22	14864.36	0.04	0.31	

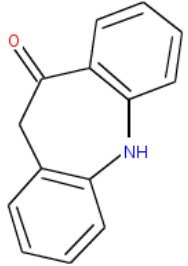
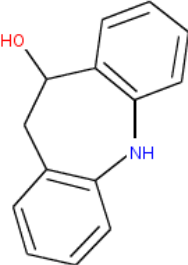
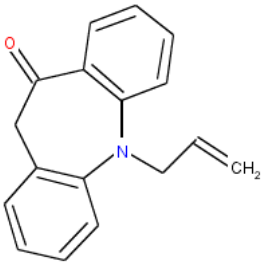
9_2		55.83	1108.74	0.90	0.01	
9_3		6883.42	n.a.	0.59	0.05	
9_4		8392.66	n.a.	0.61	0.12	

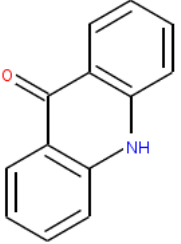
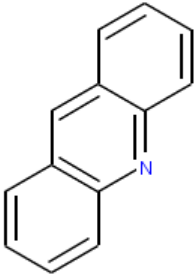
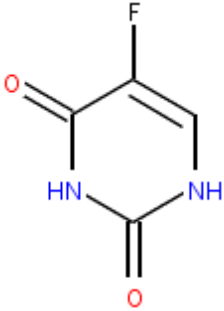
9_5		193.50	n.a.	0.75	0.03	
10	 Amisulpride	19.21	2390.72	0.86	0.31	11

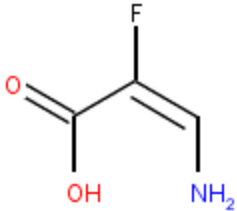
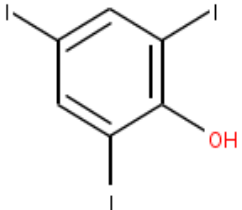
10_1		47.79	823.69	0.52	0.30	
10_2		n.a.	2710.64	1.09	0.36	

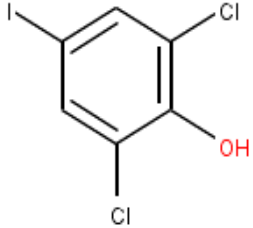
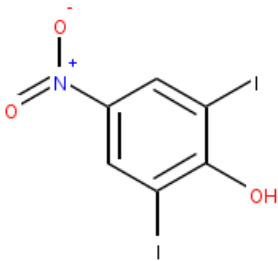
10_3		68.66	499.20	0.73	0.05	
10_4		n.a.	3885.28	1.23	0.31	
10_5		23.48	1258.62	0.61	0.47	

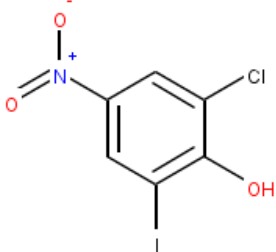
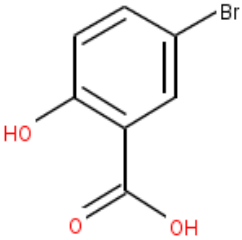
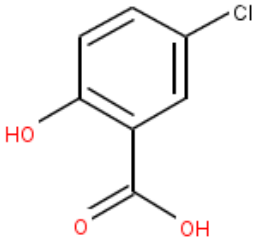
11	 Desipramine	1.90	379.44	0.66	0.19	11
11_1		2.51	267.72	0.48	0.44	
11_2		14.62	228.42	0.79	0.29	

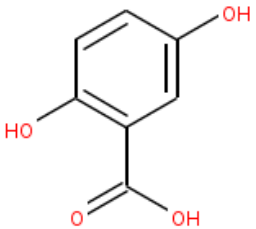
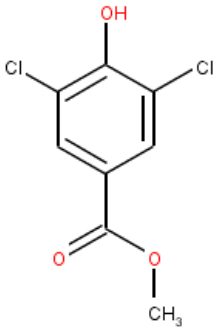
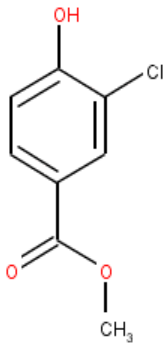
11_3		27.60	480.50	0.72	0.53	
11_4		29.88	675.37	0.73	0.32	
11_5		2.82	n.a.	0.85	0.25	

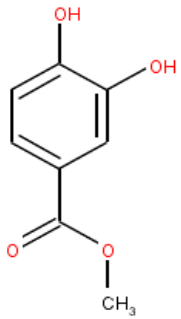
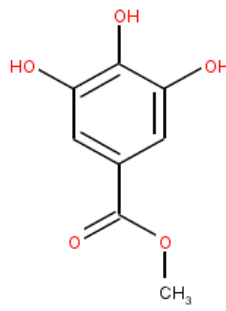
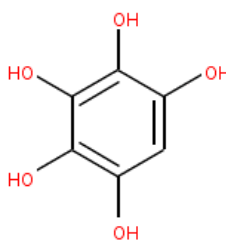
11_6		5.95	1589.86	0.46	0.70	
11_7		5.20	2477.40	0.36	0.78	
12	 5-fluorouracil	30.68	514.22	0.89	0.18	51

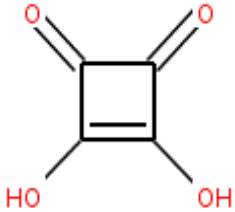
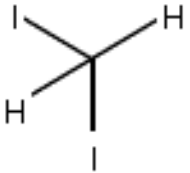
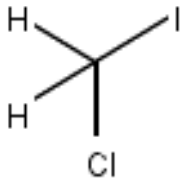
12_1	 <chem>O=C(O)C(F)=CN</chem>	39.83	n.a.	0.55	0.43	
13	 2,4,6-triodophenol	n.a.	148.28	0.36	0.08	52

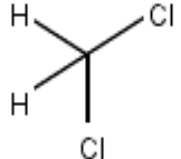
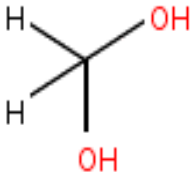
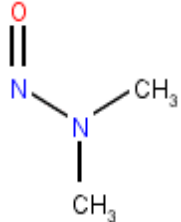
13_1		n.a.	1371.49	0.71	0.10	
14	 2,6-diiodo-4-nitrophenol	n.a.	214.61	0.41	0.30	52

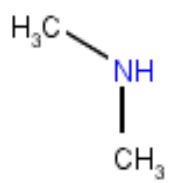
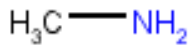
14_1			425.01	0.33	0.54	
15	 5-bromosalicylic acid	77.12	2388.32	0.13	0.07	53
15_1		100.88	404.08	0.17	0.14	

15_2		192.37	1264.35	0.29	0.56	
16	 3,5-Dichloromethylparaben	2.30	360.13	0.62	0.28	54
16_1		4.59	1353.21	0.49	0.46	

16_2	 <chem>COC(=O)c1cc(O)c(O)cc1</chem>	6.15	1878.31	0.70	0.51	
16_3	 <chem>COC(=O)c1cc(O)c(O)c(O)c1</chem>	7.00	n.a.	0.51	0.15	
16_4	 <chem>COC(=O)c1c(O)c(O)c(O)c(O)c1</chem>	68.01	n.a.	0.35	0.02	

16_5		651.12	n.a.	0.43	0.58	
17	 CH ₂ I ₂	0.12	119.30	n.a.	n.a.	55
17_1		0.69	493.02	0.47	0.82	

17_2		185.17	736.49	0.93	0.64	
17_3		5496.07	n.a.	0.96	0.07	
18	 N-Nitrosodimethylamine	71.05	118.27	0.85	0.61	56

18_1		170.73	925.29	0.93	0.07	
18_2		61.66	89.38	0.94	0.02	

n.a. refers to data is not accessible.

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