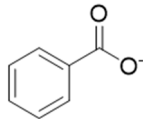
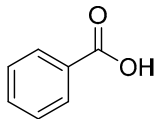

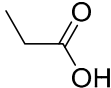
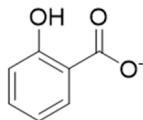
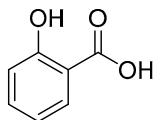
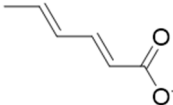
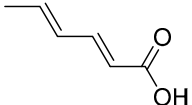
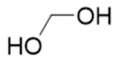
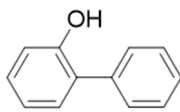
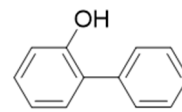
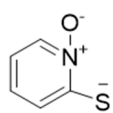
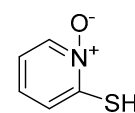
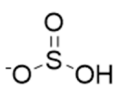

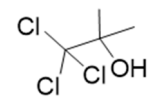
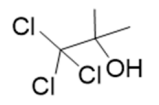
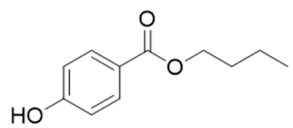
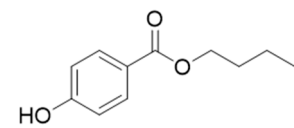
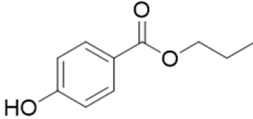
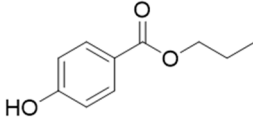
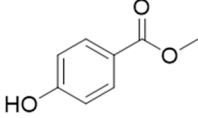
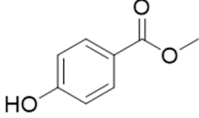
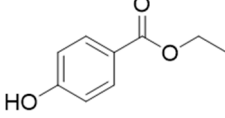
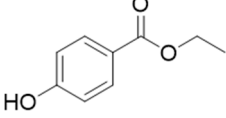
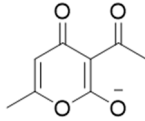
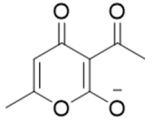

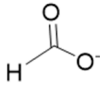
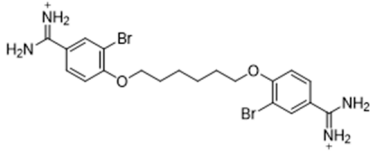
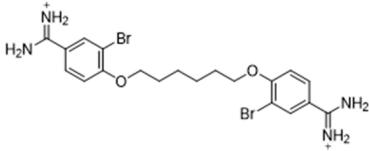
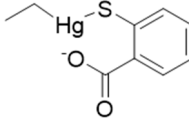



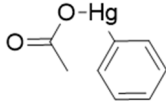
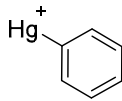
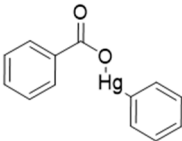
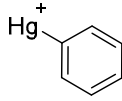
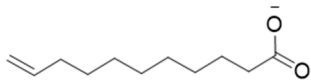
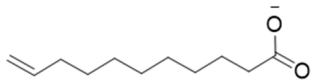
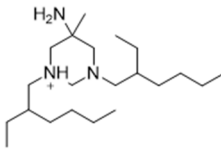
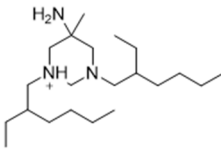
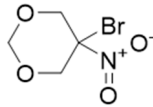
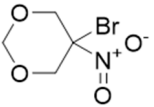
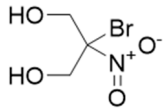
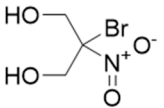
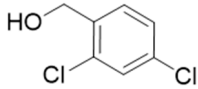
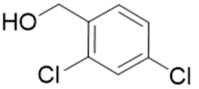
## Supporting Information Table S1

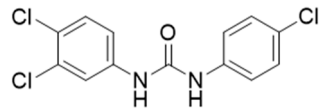
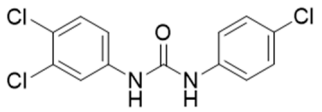
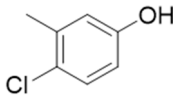
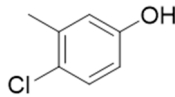
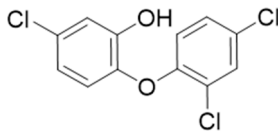
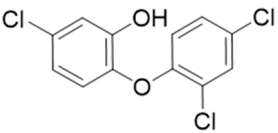
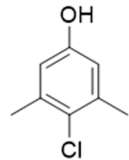
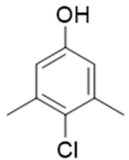
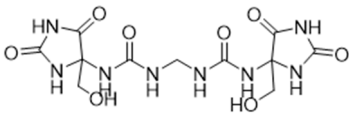

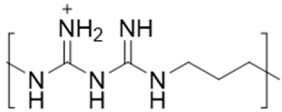
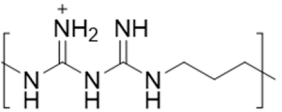
**Table S1.** List of Annex V substances, acceptance of underlying antimicrobial mechanism-of-action, and structures of predominant and active species which were used for calculation of molecular characteristics.

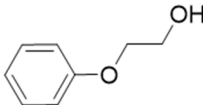
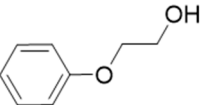
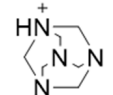

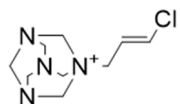

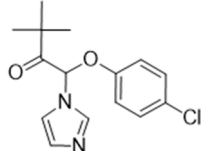
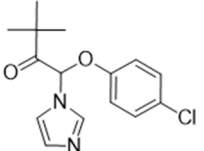
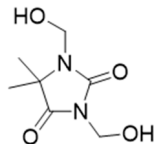

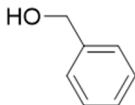
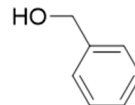
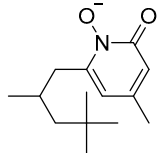
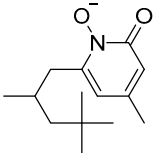
Annex V ID	Substances	Acceptance of Mechanism-of-action?	pKa (conjugated acid)	Predominant species structure	Active species structure
1	Benzoic acid and its salts	<i>accepted</i>	pKa=4.2		
2	Propionic acid and its salts	<i>accepted</i>	pKa=4.9		
3	Salicylic acid and its salts	<i>accepted</i>	pKa(COOH)=3.0 pKa(OH)=13.6		
4	Sorbic acid and its salts	<i>accepted</i>	pKa=4.8		

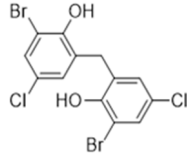
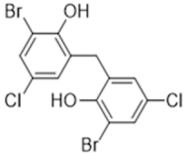
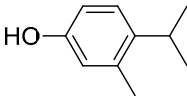
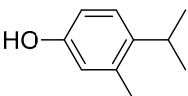
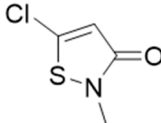
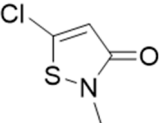
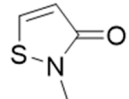
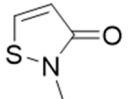
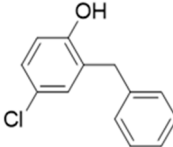
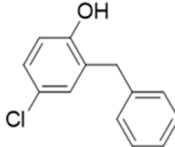
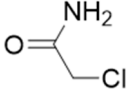
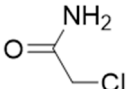
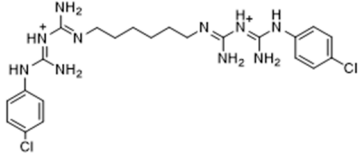
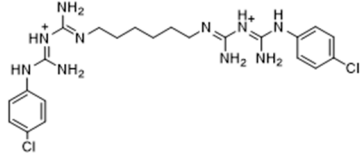
5	Formaldehyde, paraformaldehyde	<i>not accepted</i>	pKa=13.7 (methanediol)		$=O$
7	Biphenyl-2-ol	<i>accepted</i>	pKa=9.5		
8	Pyrithione zinc [here: pyrithione]	<i>accepted</i>	Formation constant log Kt = 5.3; pH<4.5 dissociates to pyrithione. pH>9.5 hydrolyzes to ionic pyrithione and zincate.		
9	Inorganic sulphites and hydrogensulphites	<i>not accepted</i>	pKa=2.0 pKa=7.0		
11	Chlorobutanol	<i>accepted</i>	-		
12 bis	Butyl 4-hydroxybenzoate	<i>accepted</i>	pKa=8.4		

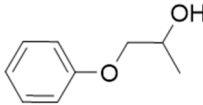
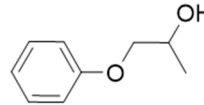
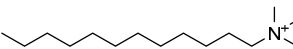
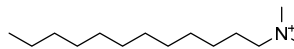
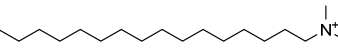
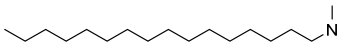
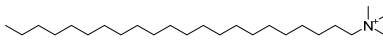
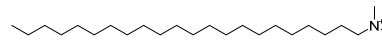
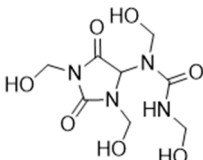
12 bis	Propyl 4-hydroxybenzoate	<i>accepted</i>	pKa=8.7		
12	Methylparaben	<i>accepted</i>	pKa=8.4		
12	Ethylparaben	<i>accepted</i>	pKa=8.2		
13	Dehydroacetic acid and its salts	<i>accepted</i>	pKa=5.3		
14	Formic acid and its salts	<i>accepted</i>	pKa=3.7		
15	Dibromohexamidine and its salts	<i>accepted</i>	pKa~12		
16	Thiomersal	<i>not accepted</i>	-		

17	Phenyl mercuric acetate	<i>not accepted</i>	-		
17	Phenyl mercuric benzoate	<i>not accepted</i>	-		
18	Undec-10-enoic acid and its salts	<i>accepted</i>	pKa=4.9		
19	Hexetidine	<i>accepted</i>	pKa=8.3		
20	5-Bromo-5-nitro-1,3-dioxane (Bronidox)	<i>not accepted</i>	pKa=9.6		
21	2-Bromo-2-nitropropane-1,3-diol (Bronopol)	<i>not accepted</i>	pKa=9.6		
22	2,4-Dichlorobenzyl alcohol	<i>accepted</i>	pKa=13.5		

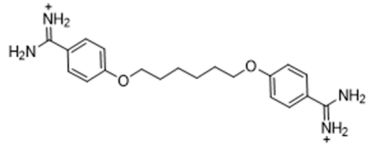
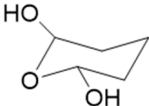
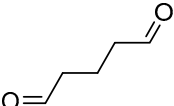
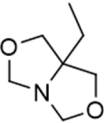
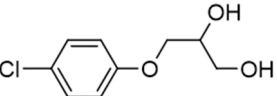
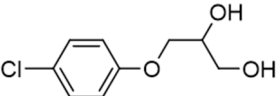
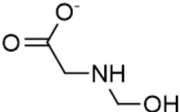
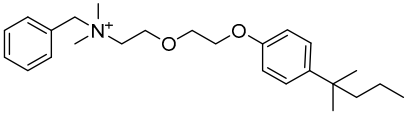
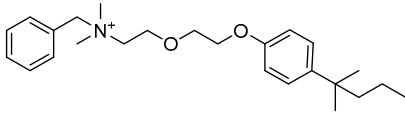
23	1-(4-Chlorophenyl)-3-(3,4-dichlorophenyl)urea (Triclocarban)	<i>accepted</i>	pKa=12.7		
24	Chlorocresol (4-Chlor-3-methylphenol) (PCMC)	<i>accepted</i>	pKa=9.6		
25	5-Chloro-2-(2,4-dichlorophenoxy)phenol (Triclosan)	<i>accepted</i>	pKa=8.1		
26	Chloroxylenol	<i>accepted</i>	pKa=9.8		
27	N,N''-Methylenebis[N'-(3-(hydroxymethyl)-2,5-dioximidazolidin-4-yl)urea] (Imidazolidinyl Urea)	<i>not accepted</i>	-		
28	Polyaminopropyl biguanide; N-Hexylimidodicarbonimidic diamide HCl (1:1); (SCCS: MW <sub>av</sub> ~4000; 22 monomers/chain)	<i>accepted</i>	pKa=2-3 (conj. acid) pKa=10.5-11.1 (conj. acid)		

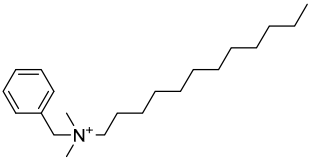
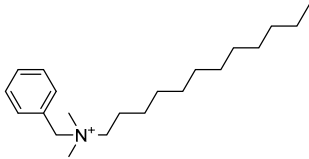
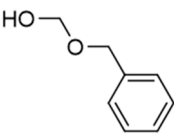

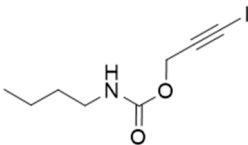
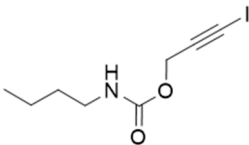
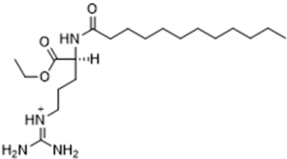
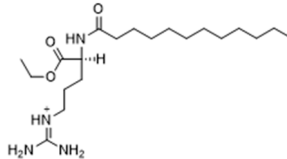
29	2-Phenoxyethanol	<i>accepted</i>	pKa=15.1		
30	Methenamine	<i>not accepted</i>	pKa=8.5		
31	Methenamine 3-chloroallylochloride (Quaternium-15)	<i>not accepted</i>	pKa=3.7		
32	1-(4-Chlorophenoxy)-1-(imidazol-1-yl)-3,3-dimethylbutan-2-one (Climbazol)	<i>accepted</i>	pKa=5.2 (conj. acid)		
33	1,3-Bis(hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione (DMDM Hydantoin)	<i>not accepted</i>	pKa=-3.5 (conj. acid) pKa=-2.0. (conj. acid)		
34	Benzyl alcohol	<i>accepted</i>	pKa=15.4		
35	1-Hydroxy-4-methyl-6-(2,4,4-trimethylpentyl)-2-pyridon and its monoethanolamine salt	<i>accepted</i>	pKa=5.9		

37	2,2'-Methylenebis(6-bromo-4-chlorophenol) (Bromochlorophen)	<i>accepted</i>	-		
38	4-Isopropyl-m-cresol (IPMP)	<i>accepted</i>	pKa=10.3		
57	2-Methyl-2H-isothiazol-3-one (MIT)	<i>not accepted</i>	-		
39	Methylchloroisothiazolinone (Annex V/39: mixture with MIT)	<i>not accepted</i>	-		
40	2-Benzyl-4-chlorophenol (Chlorophene)	<i>accepted</i>	pKa=9.8		
41	2-Chloroacetamide	<i>not accepted</i>	pKa=-2.4 (conj. acid) pKa=13.3		
42	Chlorhexidin and its salts	<i>accepted</i>	pKa=10.8 (conj. Acid) pKa=10.8		

43	1-Phenoxypropan-2-ol	<i>accepted</i>	-		
44	Alkyl (C12-C22) trimethyl ammonium bromide and chloride; [here: C12]	<i>accepted</i>	-		
44	Alkyl (C12-C22) trimethyl ammonium bromide and chloride; [here: C16]	<i>accepted</i>	-		
44	Alkyl (C12-C22) trimethyl ammonium bromide and chloride; [here: C22]	<i>accepted</i>	-		
45	4,4-Dimethyl-1,3-oxazolidine	<i>not accepted</i>	pKa=9.3		
46	N-(Hydroxymethyl)-N-(dihydroxymethyl-1,3-dioxo-2,5-imidazolidinyl-4)-N'-(hydroxymethyl)urea (Diazolidinyl Urea)	<i>not accepted</i>	-		



47	Hexamidine and its salts	<i>accepted</i>	pKa=12.5 (conj. acid)		
48	Glutaraldehyde	<i>not accepted</i>	-		
49	5-Ethyl-3,7-dioxo-1-azabicyclo[3.3.0] octane (7-Ethylbicyclooxazolidine)	<i>not accepted</i>	pKa=4.0 (conj. acid)		
50	3-(p-Chlorophenoxy)-propane-1,2-diol (Chlorphenesin)	<i>accepted</i>	pKa=13.6		
51	Sodium hydroxymethylamino acetate	<i>not accepted</i>	pKa=2.3 (COOH) pka=10.3		
52	Silver Chloride on TiO2 [here: silver AgCl]	<i>not accepted</i>	-	AgCl	Ag <sup>+</sup>
53	Benzethonium chloride	<i>accepted</i>	-		

54	Benzalkonium salts (C8-C18) [here: C12]	<i>accepted</i>	-		
55	Benzylhemiformal	<i>not accepted</i>	-		
56	3-Iodo-2-propynylbutylcarbamate (Iodocarb)	<i>accepted</i>	-		
58	Ethyl Lauroyl Arginate Hydrochloride	<i>accepted</i>	pKa=13.6		
59	Citric acid & silver chloride [here: silver chloride; see also entry No 52]	<i>not accepted</i>	-	AgCl	Ag <sup>+</sup>