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Supplemental Material

Triclocarban, Triclosan, Bromochlorophene, Chlorophene, and Climbazole Effects on Nuclear Receptors: An *in Silico* and *in Vitro* Study

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Figure S1. Combined binding probabilities of the 56 preservatives tested grouped according to each of the nuclear receptors (see main text for abbreviations). **(A)** Endocrine Disruptome docking data for 12 nuclear receptors (as indicated). Binding probabilities for AR, ERα, ERβ, and GR are shown separately for agonist and antagonist conformations of each receptor. Threshold values, depending on the binding affinity of the ligands are as follows: red (sensitivity < 0.25) for high binding probability of the ligand; orange (0.25 < sensitivity < 0.5) for moderate binding probability; yellow (0.5 < sensitivity < 0.75) for low binding probability and green (sensitivity > 0.75) for very low binding probability. **(B)** VirtualToxLab-based data for 10 nuclear receptors (as indicated). Green, no predicted interactions; yellow, binding predicted at 10 μM to 100 μM; orange, binding predicted at 1 μM to 10 μM; red, binding predicted at 100 nM to 1 μM; brown, binding predicted at 1 nM to 10 nM.

References

Table S1. Annex V (European Parliament 2009) preservatives with Endocrine Disruptome (ED)-predicted binding to respective nuclear receptors.

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number	AR	ARan	ERα	ERαan	ERβ	ERβan	GR	GRan.	LXRα	LXRβ	PPARα	PPARβ	PPARγ	RXRα	TRα	TRβ
1	Benzoic acid	Benzoic acid	65-85-0	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	Propionic acid	Propionic acid	79-09-4	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
3	Salycilic acid	Salicylic acid	69-72-7	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4	Hexa-2,4-dienoic acid	Sorbic acid	110-44-1	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	Formal-dehyde	Formaldehyde	50-00-0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
7	Biphenyl-2-ol	o-Phenylphenol	90-43-7	2	3	1	1	1	1	2	1	1	1	1	1	1	1	2	1
8	Pyrithione zinc	Zinc pyrithione	13463-41-7	2	3	1	1	1	1	2	1	1	1	1	1	1	1	2	2
11	Chlorobutanol	Chlorobutanol	57-15-8	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
12	4-Hydroxybenzoic acid	4-Hydroxybenzoic acid	99-96-7	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
13	3-Acetyl-6-methylpyran-2,4 (3H)-dione	Dehydroacetic acid	520-45-6	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
14	Formic acid	Formic acid	64-18-6	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
15	3,3'-Dibromo-4,4'-hexamethylenedioxydi-benzamidine	Dibromohexamidine	93856-83-8	1	2	1	1	1	1	2	1	1	1	1	1	1	1	1	2
18	Undec-10-enoic acid	Undecylenic acid	112-38-9	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
19	5- Pyrimidinamine, 1,3-bis (2-ethylhexyl) hexahydro-5-methyl-	Hexetidine	141-94-6	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
20	5-Bromo-5-nitro-1,3-dioxane	5-Bromo-5-nitro-1,3-dioxane	30007-47-7	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
21	Bronopol	2-Bromo-2-nitropropane-1,3- diol	52-51-7	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
22	2,4-Dichlorobenzyl alcohol	Dichlorobenzyl Alcohol	1777-82-8	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
23	1-(4-Chlorophenyl)-3-(3,4-dichlorophenyl) urea	Triclocarban	101-20-2	1	3	3	1	2	4	2	1	1	1	1	1	1	1	2	2
24	Chlorocresol	p-Chloro-m-Cresol	59-50-7	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
25	5-Chloro-2- (2,4-dichlorophe-noxy)	Triclosan	3380-34-5	1	2	1	1	1	1	2	1	1	1	1	1	1	1	2	2

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number	AR	ARan	ERα	ERαan	ERβ	ERβan	GR	GRan.	LXRα	LXRβ	PPARα	PPARβ	PPARγ	RXRα	TRα	TRβ
	phenol																		
26	Chloro-xylenol	Chloroxylenol	88-04-0	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
27	N,N''-methylenebis[N'-[3-(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]urea]	Imidazolidinyl urea	39236-46-9	2	3	1	1	1	1	2	1	1	1	1	1	1	1	1	2
29	2-Phenoxyethanol	Phenoxyethanol	122-99-6	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
30	Methenamine	Methenamine	100-97-0	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
32	1-(4-Chlorophenoxy)-1-(imidazol-1-yl)-3,3-dimethylbutan-2-one	Climbazole	38083-17-9	1	3	1	1	1	1	1	1	1	1	1	1	1	1	2	2
33	1,3-Bis (hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione	DMDM Hydantoin	6440-58-0	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
34	Benzyl alcohol	Benzyl alcohol	100-51-6	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
35	1-Hydroxy-4-methyl-6-(2,4,4-trimethylpentyl) 2-pyridon	1-Hydroxy-4-methyl-6-(2,4,4-trimethylpentyl) 2-pyridon	50650-76-5	2	1	1	1	1	1	1	1	1	1	1	1	1	1	2	2
37	2,2'-methylenebis(6-bromo-4-chlorophenol)	Bromochlorophene	15435-29-7	1	2	1	1	1	1	2	1	1	1	1	1	1	1	2	1
38	4-Isopropyl-m-cresol	o-Cymen-5-ol	3228-02-2	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
39	5-Chloro-2-methyl-isothiazol-3(2H)-one	Methylchloroisothiazolinone	26172-55-4	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
39	2-Methyl-2H-isothiazol-3-one	Methylisothiazolinone	2682-20-4	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
40	2-Benzyl-4-chlorophenol	Chlorophene	120-32-1	2	3	1	1	1	1	2	1	1	1	1	1	1	1	2	2
41	2-Chloroacetamide	Chloroacetamide	79-07-2	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
42	N,N''-bis(4-chlorophenyl)-3,12-diimino-2,4,11,13-tetraazatetradecanediamidine	Chlorhexidine	55-56-1	1	2	2	1	1	1	2	1	1	1	2	1	1	1	1	1
43	1-Phenoxypropan-2-ol	Phenoxyisopropanol	770-35-4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number	AR	ARan	ERα	ERαan	ERβ	ERβan	GR	GRan.	LXRα	LXRβ	PPARα	PPARβ	PPARγ	RXRα	TRα	TRβ
45	4,4-Dimethyl-1,3-oxazolidine	Dimethyl Oxazolidine	51200-87-4	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
46	N-(Hydroxymethyl)-N-(dihydroxymethyl-1,3-dioxo-2,5-imidazolidinyl-4)-N'-(hydroxymethyl) urea	Diazolidinyl Urea	78491-02-8	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
47	Benzenecarboximidamide	Hexamidine	3811-75-4	1	3	2	1	1	2	2	1	1	1	1	1	1	1	2	2
48	Glutaraldehyde (Pentane-1,5-dial)	Glutaral	111-30-8	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
49	5-Ethyl-3,7-dioxa-1-azabicyclo [3.3.0] octane	7-Ethylbicyclooxazolidine	7747-35-5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
50	3-(p-Chlorophenoxy)-propane-1,2 diol	Chlorphenesin	104-29-0	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
51	Sodium hydroxymethylamino acetate	Sodium Hydroxymethylglycinate	70161-44-3	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
53	Benzenemethanaminium, N,N-dimethyl-N-[2-[2-[4-(1,1,3,3,-tetramethylbutyl)phenoxy] ethoxy] ethyl]-, chloride	Benzethonium Chloride	121-54-0	1	2	2	1	1	1	2	1	1	1	1	1	1	1	1	2
54	Benzalkonium chloride	Benzalkonium chloride	8001-54-5	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
55	Methanol, (phenylmethoxy-)	Benzylhemiformal	14548-60-8	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
56	3-Iodo-2-propynylbutylcarbamate	Iodopropynyl butylcarbamate	55406-53-6	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Note: Binding probabilities were obtained with the Endocrine Disruptome (ED) tool and are designated by numbers 1-4 as follows: 1 – class green (sensitivity > 0.75) in ED corresponds to very low probability of binding; 2 – class yellow (0.5 < sensitivity < 0.75) in ED corresponds to low probability of binding; 3 – class orange (0.25 < sensitivity < 0.5) in ED corresponds to moderate probability of binding; 4 – class red (sensitivity < 0.25) in ED corresponds to high

probability of binding. AR – agonist conformation of androgen receptor; ARan – antagonist conformation of androgen receptor; ERα – agonist conformation of estrogen receptor α; ERαan – antagonist conformation of estrogen receptor α; ERβ – agonist conformation of estrogen receptor β; ERβan – antagonist conformation of estrogen receptor β; GR – agonist conformation of glucocorticoid receptor; GRan – antagonist conformation of glucocorticoid receptor; LXRα – liver X receptor α; LXRβ – liver X receptor β; PPARα – peroxisome proliferator activated receptor α; PPARβ – peroxisome proliferator activated receptor β; PPARγ – peroxisome proliferator activated receptor γ; RXRα – retinoid X receptor α ; TRα – thyroid receptor α; TRβ – thyroid receptor β.

Table S2. Annex V (European Parliament 2009) preservatives with VirtualToxLab (VTL)-predicted binding to respective nuclear receptors.

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number	AR	ERα	ERβ	GR	LXR	MR	PPARγ	PR	TRα	TRβ
1	Benzoic acid	Benzoic acid	65-85-0	0	0	0	0	60.3 μM	0	0	54.6 μM	63.0 μM	23.6 μM
2	Propionic acid	Propionic acid	79-09-4	0	0	0	0	0	0	0	0	0	0
3	Salycilic acid	Salicylic acid	69-72-7	0	0	0	0	0	0	0	0	0	90.4 μM
4	Hexa-2,4-dienoic acid	Sorbic acid	110-44-1	0	0	0	0	0	0	0	0	0	0
7	Biphenyl-2-ol	o-Phenylphenol	90-43-7	2.28 μM	32.0 μM	5.14 μM	32.6 μM	0	0	0	0	0	0
11	Chlorobutanol	Chlorobutanol	57-15-8	33.8 μM	0	36.9 μM	0	0	0	0	0	0	0
12	4-Hydroxybenzoic acid	4-Hydroxybenzoic acid	99-96-7	0	0	0	0	20.6 μM	0	0	99.4 μM	0	0
13	3-Acetyl-6-methylpyran-2,4 (3H)-dione	Dehydroacetic acid	520-45-6	0	0	0	0	0	0	0	0	0	0
14	Formic acid	Formic acid	64-18-6	0	0	0	0	0	0	0	0	0	0
15	3,3'-Dibromo-4,4'-hexamethylenedioxydi-benzamidine	Dibromohexamidine	93856-83-8	0	43.8 μM	0	0	0	0	0	0	0	0
18	Undec-10-enoic acid	Undecylenic acid	112-38-9	0	0	0	43.1 μM	63.2 μM	0	0	1.58 μM	52.5 μM	12.9 μM
19	5- Pyrimidinamine, 1,3-bis (2-ethylhexyl) hexahydro-5-methyl-	Hexetidine	141-94-6	0	0	0	409 nM	0	0	0	4.69 μM	0	0
20	5-Bromo-5-nitro-1,3-dioxane	5-Bromo-5-nitro-1,3-dioxane	30007-47-7	92.2 μM	0	27.9 μM	28.5 μM	0	0	0	16.9 μM	0	0
21	Bronopol	2-Bromo-2-nitropropane-1,3- diol	52-51-7	518 nM	71.5 μM	908 nM	36.9 μM	0	0	0	46.4 μM	0	0
22	2,4-Dichlorobenzyl alcohol	Dichlorobenzyl Alcohol	1777-82-8	7.19 μM	55.2 μM	11.1 μM	0	0	12.6 μM	0	0	0	0
23	1-(4-Chlorophenyl)-3-(3,4-dichlorophenyl) urea	Triclocarban	101-20-2	0	81.4 μM	47.6 μM	633 nM	0	3.62 μM	0	0	0	0
24	Chlorocresol	p-Chloro-m-Cresol	59-50-7	0	0	60.9 μM	0	0	0	0	0	0	0
25	5-Chloro-2- (2,4-dichlorophe-noxy) phenol	Triclosan	3380-34-5	6.22 μM	79.5 μM	6.01 μM	7.36 μM	32.6 μM	4.82 μM	37.6 μM	646 nM	190 nM	368 nM
26	Chloro-xylenol	Chloroxylenol	88-04-0	0	0	0	0	0	0	0	0	0	0
27	N,N''-methylenebis[N'-[3-	Imidazolidinyl urea	39236-46-9	0	0	0	0	0	0	0	0	0	0

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number	AR	ERα	ERβ	GR	LXR	MR	PPARγ	PR	TRα	TRβ
	(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]urea]												
29	2-Phenoxyethanol	Phenoxyethanol	122-99-6	44.3 μM	0	82.3 μM	0	0	51.1 μM	0	0	0	0
30	Methenamine	Methenamine	100-97-0	0	0	0	0	0	0	0	0	0	0
32	1-(4-Chlorophenoxy)-1-(imidazol-1-yl)-3,3-dimethylbutan-2-one	Climbazole	38083-17-9	856 nM	0	10.5 μM	3.19 μM	0	18.3 μM	60.7 μM	647 nM	95.2 μM	0
33	1,3-Bis (hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione	DMDM Hydantoin	6440-58-0	0	0	0	0	0	0	0	0	0	0
34	Benzyl alcohol	Benzyl alcohol	100-51-6	0	0	0	0	0	94.1 μM	0	0	0	0
35	1-Hydroxy-4-methyl-6-(2,4,4-trimethylpentyl) 2-pyridon	1-Hydroxy-4-methyl-6-(2,4,4-trimethylpentyl) 2-pyridon	50650-76-5	0	0	0	79.9 μM	0	0	0	13.0 μM	79.6 μM	34.5 μM
37	2,2'-methylenebis(6-bromo-4-chlorophenol)	Bromochlorophene	15435-29-7	1.98 nM	67.8 nM	1.89 μM	3.52 μM	0	23.9 μM	1.43 μM	16.5 μM	219 nM	516 nM
38	4-Isopropyl-m-cresol	o-Cymen-5-ol	3228-02-2	94.8 μM	0	0	0	0	0	0	0	0	0
39	5-Chloro-2-methyl-isothiazol-3(2H)-one	Methylchloroisothiazolinone	26172-55-4	0	0	0	0	0	0	0	0	0	0
39	2-Methyl-2H-isothiazol-3-one	Methylisothiazolinone	2682-20-4	0	0	0	0	0	0	0	0	0	0
40	2-Benzyl-4-chlorophenol	Chlorophene	120-32-1	592 nM	1.30 μM	829 nM	14.4 μM	0	5.12 μM	0	10.5 μM	50.9 μM	21.1 μM
41	2-Chloroacetamide	Chloroacetamide	79-07-2	0	0	0	0	0	0	0	0	0	0
42	N,N''-bis(4-chlorophenyl)-3,12-diimino-2,4,11,13-tetraazatetradecanediamidine	Chlorhexidine	55-56-1	0	0	0	0	0	0	0	0	0	0
43	1-Phenoxypropan-2-ol	Phenoxyisopropanol	770-35-4	64.0 μM	0	77.9 μM	0	0	99.4 μM	0	0	0	0
45	4,4-Dimethyl-1,3-oxazolidine	Dimethyl Oxazolidine	51200-87-4	0	0	0	0	0	0	0	0	0	0
46	N-(Hydroxymethyl)-N-(dihydroxymethyl-1,3-dioxo-2,5-imidazolidinyl-4)-N'-	Diazolidinyl Urea	78491-02-8	0	0	0	0	0	0	0	0	0	0

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number	AR	ERα	ERβ	GR	LXR	MR	PPARγ	PR	TRα	TRβ
	(hydroxymethyl) urea												
47	Benzenecarboximidamide	Hexamidine	3811-75-4	0	65.5 μM	0	0	0	0	0	0	0	0
48	Glutaraldehyde (Pentane-1,5-dial)	Glutaral	111-30-8	0	0	0	0	0	0	0	0	0	0
49	5-Ethyl-3,7-dioxa-1-azabicyclo [3.3.0] octane	7-Ethylbicyclooxazolidine	7747-35-5	0	0	0	0	0	0	0	0	0	0
50	3-(p-Chlorophenoxy)-propane-1,2 diol	Chlorphenesin	104-29-0	19.2 μM	3.04 μM	17.7 μM	66.8 μM	0	24.0 μM	0	99.5 μM	10.3 μM	0
51	Sodium hydroxymethylamino acetate	Sodium Hydroxymethylglycinate	70161-44-3	0	0	0	0	0	0	0	0	0	0
55	Methanol, (phenylmethoxy-)	Benzylhemiformal	14548-60-8	0	0	66.8 μM	0	0	31.9 μM	0	51.8 μM	0	0
56	3-Iodo-2-propynylbutylcarbamate	Iodopropynyl butylcarbamate	55406-53-6	0	0	39.1 μM	0	0	39.4 μM	0	0	0	0

0 – not binding, AR – androgen receptor; ERα – estrogen receptor α; ERβ – estrogen receptor β; ERβ – antagonist conformation of estrogen receptor β; GR – glucocorticoid receptor; LXR – liver X receptor; MR – mineralocorticoid receptor; PPARγ – peroxisome proliferator activated receptor γ; PR – progesterone receptor; TRα – thyroid receptor α; TRβ – thyroid receptor β.

Table S3. Items listed in Annex V (European Parliament 2009) that could not be screened with *in-silico* programs.

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number
6	Moved or deleted		
5	Formal-dehyde	Formaldehyde	50-00-0
8	Pyrithione zinc	Zinc pyrithione	13463-41-7
9	Inorganic sulphites and hydrogen- sulphites	Sodium sulfite, ammonium bisulfite, ammonium sulfite, potassium sulfite, potassium hydrogen sulfite, sodium bisulfite, sodium metabisulfite, potassium metabisulfite	7757-83-7, 10192-30-0, 10196-04-0, 10117-38-1, 7773-03-7, 7631-90-5, 7681-57-4, 16731-55-8
10	Moved or deleted		
16	Thiomersal	Thiomersal	54-64-8
17	Phenylmercuric salts (including borate)	Phenyl Mercuric Acetate, Phenyl Mercuric Benzoate	62-38-4, 94-43-9
28	Poly(methylene),.alpha.,.omega.-bis[[[(aminoiminomethyl)amino]iminomethyl] amino]-, dihydrochloride	Polyaminopropyl biguanide	70170-61-5, 28757-47-3, 133029-32-0
31	Methenamine 3-chloroallylochloride	Quaternium-15	99-96-7
36	Moved or deleted		
44	Alkyl (C 12-22) trimethyl ammo- nium bromide and chloride	Behentrimonium chloride, cetri- monium bromide, cetrimonium chloride, laurtrimonium bro- mide, laurtrimonium chloride,	17301-53-0, 57-09-0, 112- 02-7, 1119-94-4, 112-00-5, 1120-02-1, 112-03-8

Reference number	Chemical name/INN	Name of Common Ingredients Glossary	CAS number
		steartrimonium bromide, steart- rimonium chloride	
52	Silver chloride deposited on titanium dioxide	Silver chloride	7783-90-6
53	Benzenemethanaminium, N,N- dimethyl-N-[2-[2-[4-(1,1,3,3,- tetramethylbutyl)phenoxy] ethoxy] ethyl]-, chloride	Benzethonium Chloride	121-54-0
54	Benzalkonium chloride	Benzalkonium chloride	8001-54-5

Table S4. Endocrine Disruptome (ED) binding probability classes and respective binding free energy (kcal/mol) thresholds for each nuclear receptor.

Class designation in table S2	Binding probability	Sensitivity	Color output	Binding free energy thresholds (kcal/mol)															
				AR	ARan	ERα	ERαan	ERβ	ERβan	GR	GRan.	LXRα	LXRβ	PPARα	PPARβ	PPARγ	RXRα	TRα	TRβ
1	High	< 0.25	red	> -8.6	> -8.4	> -9.3	> -10.7	> -9.2	> -9	> -10.7	> -9.8	> -11.9	> -12.1	> -10	> -10.5	> -10.3	> -12.1	> -10.2	> -10.5
2	Moderate	0.25 – 0.5	orange	> -8.1	> - 7.6	> -8.8	> -9.5	> -8.7	> -8.6	> -9.7	> -9.2	> -10.7	> -11.3	> -9.4	> -10.1	> -9.6	> -10.8	> -9.2	> -9.4
3	Low	0.5 – 0.75	yellow	> -7.4	> -3.1	> -8.2	> -8.6	> -8	> - 8.3	> -7.3	> -8.5	> -9.8	> -10.3	> -8.9	> -9.6	> -8.9	> -10	> -7.2	> -7.8
4	Very low/no binding	> 0.75	green	< -7.4	< -3.1	< -8.2	< -8.6	< -8	< -8.3	< -7.3	< -8.5	< -9.8	< -10.3	< -8.9	< -9.6	< -8.9	< -10	< -7.2	< -7.8

AR – agonist conformation of androgen receptor; ARan – antagonist conformation of androgen receptor; ERα – agonist conformation of estrogen receptor α; ERαan – antagonist conformation of estrogen receptor α; ERβ – agonist conformation of estrogen receptor β; ERβan – antagonist conformation of estrogen receptor β; GR – agonist conformation of glucocorticoid receptor; GRan – antagonist conformation of glucocorticoid receptor; LXRα – liver X receptor α; LXRβ – liver X receptor β; PPARα – peroxisome proliferator activated receptor α; PPARβ – peroxisome proliferator activated receptor β; PPARγ – peroxisome proliferator activated receptor γ; RXRα – retinoid X receptor α ; TRα – thyroid receptor α; TRβ – thyroid receptor β.

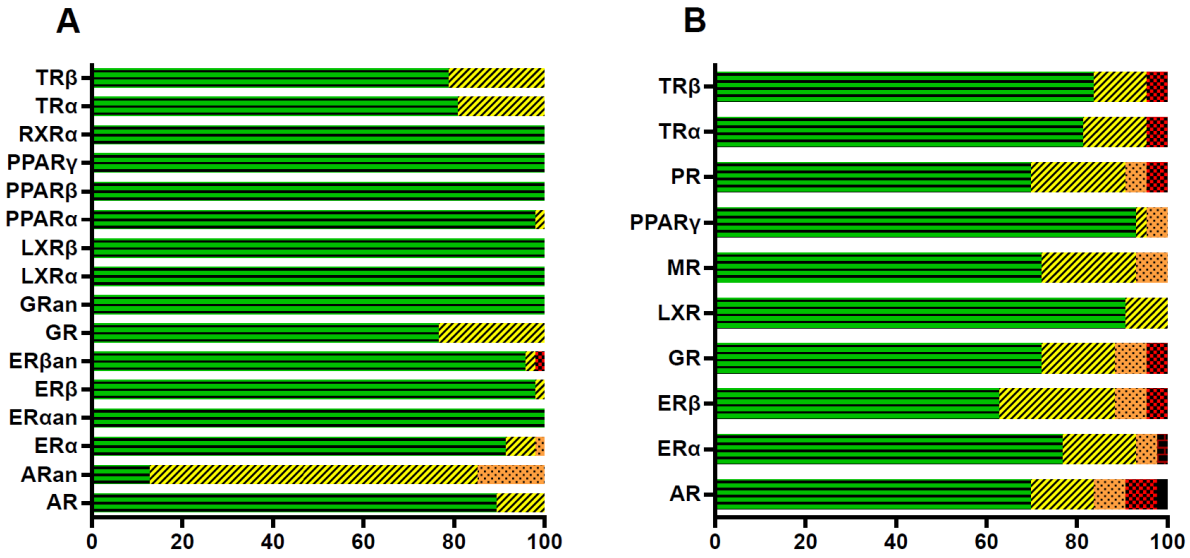

Figure S1. Combined binding probabilities of the 56 preservatives tested grouped according to each of the nuclear receptors (see main text for abbreviations). **(A)** Endocrine Disruptome docking data for 12 nuclear receptors (as indicated). Binding probabilities for AR, ERα, ERβ, and GR are shown separately for agonist and antagonist conformations of each receptor. Threshold values, depending on the binding affinity of the ligands are as follows: red (sensitivity < 0.25) for high binding probability of the ligand; orange (0.25 < sensitivity < 0.5) for moderate binding probability; yellow (0.5 < sensitivity < 0.75) for low binding probability and green (sensitivity > 0.75) for very low binding probability. **(B)** VirtualToxLab-based data for 10 nuclear receptors (as indicated). Green, no predicted interactions; yellow, binding predicted at 10 µM to 100 µM; orange, binding predicted at 1 µM to 10 µM; red, binding predicted at 100 nM to 1 µM; brown, binding predicted at 1 nM to 10 nM.

References

European Parliament Council of the EU. 2009. Regulation (EC) No 1223/2009 of the European Parliament and of the Council of 30 November 2009 on cosmetic products.