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

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

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

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

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, ER α , ER β , 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 μ M to 100 μ M; orange, binding predicted at 1 μ M to 10 μ M; red, binding predicted at 100 nM to 1 μ M; brown, binding predicted at 1 nM to 10 nM.

References