

References

- [1] Macedo S, Teixeira E, Gaspar TB, Boaventura P, Soares MA, Miranda-Alves L, et al. Endocrine-disrupting chemicals and endocrine neoplasia: A forty-year systematic review. *Environmental Research*. 2023;218:114869.
- [2] Predieri B, Alves CAD, Iughetti L. New insights on the effects of endocrine-disrupting chemicals on children. *Jornal de Pediatria*. 2022;98:S73–85.
- [3] Toporova L, Balaguer P. Nuclear receptors are the major targets of endocrine disrupting chemicals. *Molecular and Cellular Endocrinology*. 2020;502:110665.
- [4] Browne P, Van Der Wal L, Gourmelon A. OECD approaches and considerations for regulatory evaluation of endocrine disruptors. *Molecular and Cellular Endocrinology*. 2020;504:110675.
- [5] European Chemical Agency (ECHA) and European Food Safety Authority (EFSA). Guidance for the identification of endocrine disruptors in the context of Regulations (EU) No 528/2012 and (EC) No 1107/2009. <https://data.europa.eu/doi/10.2903/j.efsa.2018.5311>. Accessed 20 November 2025.
- [6] Servien R, Mamy L, Li Z, Rossard V, Latrille E, Bessac F, et al. TyPol – A new methodology for organic compounds clustering based on their molecular characteristics and environmental behavior. *Chemosphere*. 2014;111:613–22.
- [7] Maglic JB, Lavendomme R. *MoloVol* : an easy-to-use program for analyzing cavities, volumes and surface areas of chemical structures. *J Appl Crystallogr*. 2022;55(4):1033–44.
- [8] Bonnot K, Benoit P, Hoyau S, Mamy L, Patureau D, Servien R, et al. Accuracy of Computational Chemistry Methods to Calculate Organic Contaminant Molecular Properties. *ChemistrySelect*. 2022;7(48):e202203586.
- [9] Borgert CJ, Baker SP, Matthews JC. Potency matters: Thresholds govern endocrine activity. *Regulatory Toxicology and Pharmacology*. 2013;67(1):83–8.
- [10] Judson R, Houck K, Paul Friedman K, Brown J, Browne P, Johnston PA, et al. Selecting a minimal set of androgen receptor assays for screening chemicals. *Regul Toxicol Pharmacol*. 2020;117:104764.
- [11] Adamovsky O, Groh KJ, Białk-Bielińska A, Escher BI, Beaudouin R, Mora Lagares L, et al. Exploring BPA alternatives – Environmental levels and toxicity review. *Environment International*. 2024;189:108728.
- [12] Braun G, Escher BI. Prioritization of mixtures of neurotoxic chemicals for biomonitoring using high-throughput toxicokinetics and mixture toxicity modeling. *Environment International*. 2023;171:107680.
- [13] Najjar A, Wilm A, Meinhardt J, Mueller N, Boettcher M, Ebmeyer J, et al. Evaluation of new alternative methods for the identification of estrogenic, androgenic and steroidogenic effects: a comparative in vitro/in silico study. *Arch Toxicol*. 2024;98(1):251–66.
- [14] Malakhov G, Pogodin P. Dataset of drugs, their molecular scaffolds and medical indications with interactive visualization. *Data in Brief*. 2024;54:110417.