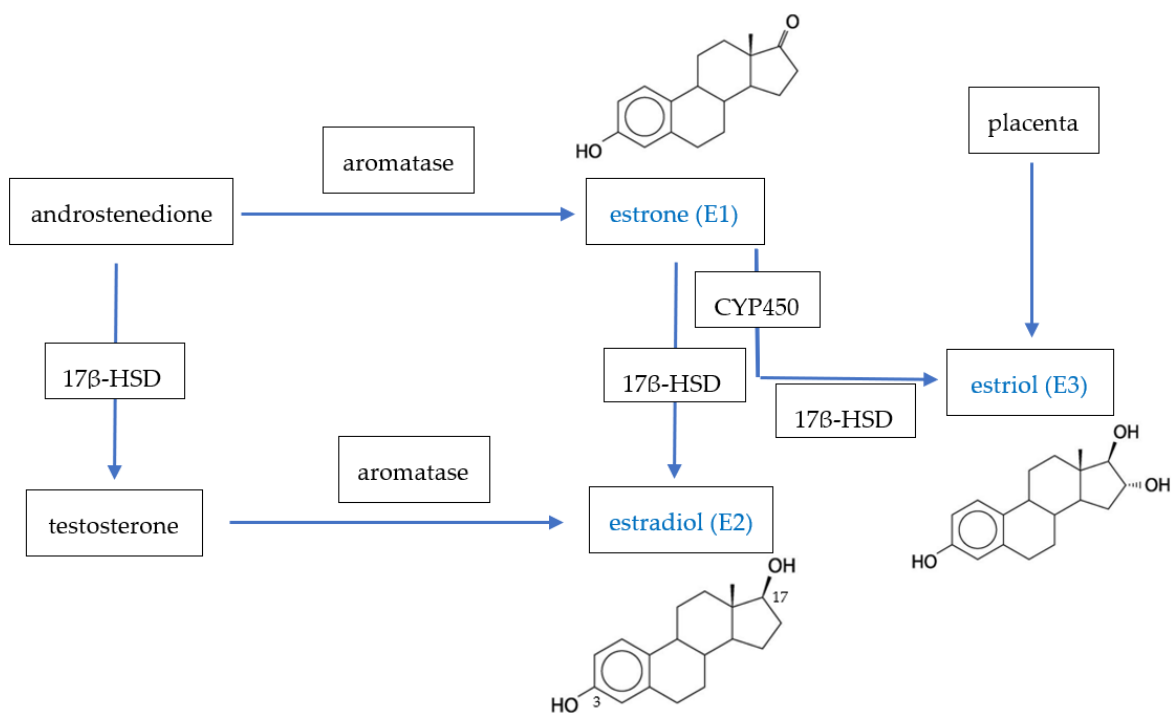


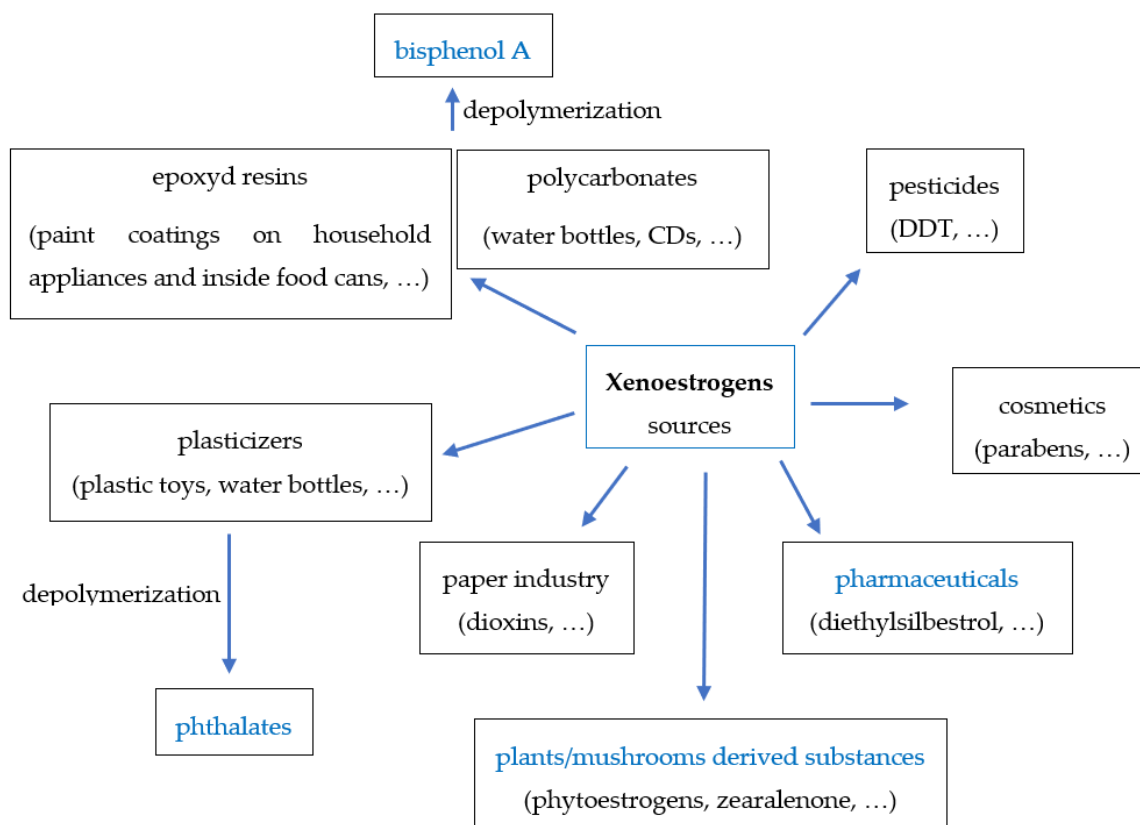


## Supplementary Materials



**Figure S1.** Mutual metabolic dependence between E1, E2, E3 and their structures. In E2 structure, carbon C3 and C17 have been marked. Based on:

Tofovic S.P.; Jackson E.K. Estradiol Metabolism: Crossroads in Pulmonary Arterial Hypertension. *Int J Mol Sci.* 2019, 21(1). pii: E116. doi: 10.3390/ijms21010116.



**Figure S2.** Main sources and types of xenoestrogens. In blue have been marked the ones frequently investigated with the application of *in silico* methods and, consequently, the ones mentioned in the main part of this review. Based on:

1. Cotterill, J.V.; Palazzolo, L.; Ridgway, C.; Price, N.; Rorije, E.; Moretto, A.; Peijnenberg, A.; Eberini, I. Predicting estrogen receptor binding of chemicals using a suite of *in silico* methods – Complementary approaches of (Q)SAR, molecular docking and molecular dynamics. *Toxicology and Applied Pharmacology* **2019**, 114630. doi:10.1016/j.taap.2019.114630.
2. Kerdivel, G.; Habauzit, D.; Pakdel, F. Assessment and Molecular Actions of Endocrine-Disrupting Chemicals That Interfere with Estrogen Receptor Pathways. *International Journal of Endocrinology* **2013**, 1–14. doi:10.1155/2013/501851.