

## Investigation of Alkyl Phthalates and Other Estrogenic Endocrine Disruptors on “The Organic Conceptual Diagram”

Kikuo Takeda\*, Taketoshi Fujimoto, Makoto Imai, Tatsuo Nonaka, Toshikazu Taira, Hiroyuki Iida, Yasuko Sakamoto, Ayumi Hasegawa, Yasuko Yoshida, Yoshio Koda<sup>1</sup>, Masatoshi Morita<sup>2</sup>

Sumika Chemical Analysis Service, Ltd., <sup>1</sup>Research Institute of Environmental Chemistry, <sup>2</sup>National Institute for Environmental Studies, Japan

**Introduction :** A variety of the chemical compounds are suspicious as endocrine disruptors. To summarize and obtain outlook (bird's-eye view) about these endocrine disruptors is of not only scientific but also practical interest. The use of “The Organic Conceptual Diagram” is also an attractive application in this purpose. By locating many contaminants which are deterrent to semiconductor production process on “The Organic Conceptual Diagram”, understanding the behaviors and properties of the contaminants was of considerable practical significance. In this paper, the alkyl phthalates and the other compounds were located on the diagram and compared to the other endocrine disruptors.

**Result and discussion:** Dibutyl phthalate (DBP) having remarkable estrogenic activity was located in the region of estrogen. On the other hand, di-(2-ethylhexyl) phthalate (DOP) was located away from the estrogen region. DOP was also away from the region of compounds having xenobiotic responsive element (XRE) abnormality such as dioxins. Estrogen-like substances can be divided into two types: (1) one is the type to bond to estrogen receptor, and (2) the other is the type to form complex with dioxin receptor (AhR), to connect with Ah receptor nuclear translocator (Arnt) and to accelerate transcription by connecting with XRE. Many of estrogen-like substances were located almost near the region of estrogen. Agricultural chemicals and dioxins were located away from the region of estrogen. This region corresponded to the region of substances having hardly- decomposition, accumulation, and bio-concentration properties. This fact corresponds to (1) and (2) described above. Benomyl was not located in the region of (1) and (2) above.

**Conclusion:** The use of “The Organic Conceptual Diagram” is an attractive application in the purpose of investigating the substances showing abnormal behavior, predicting of mechanism and magnitude of the affect, and deciding the order of priority order of investigation.

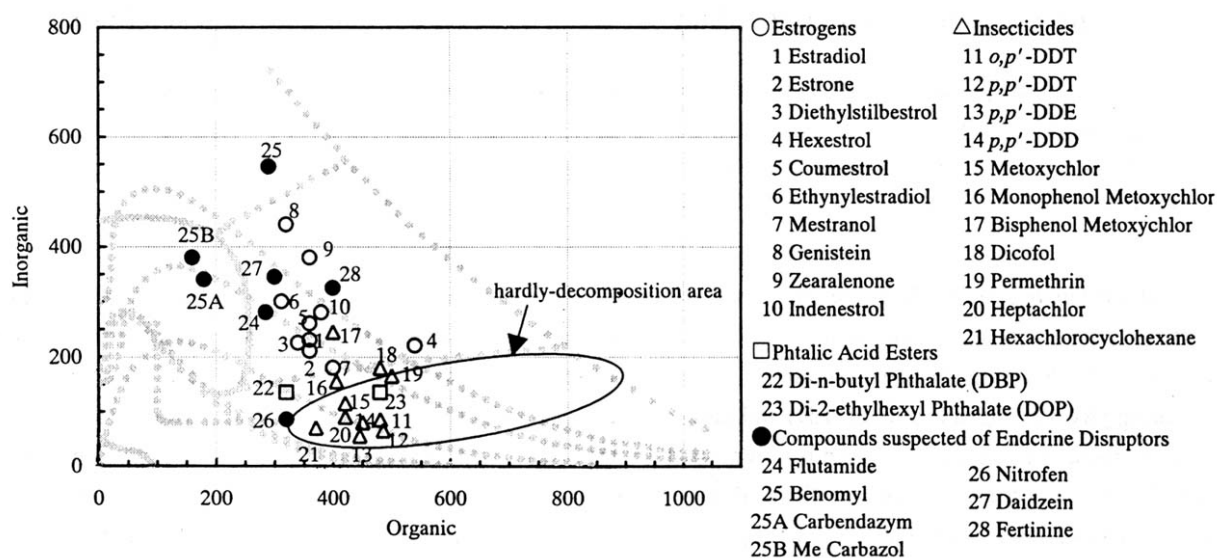


Fig.1 The location of estrogenic endocrine disruptors on “The Organic Conceptual Diagram”