ONLINE ISSN : 1349-0923
PRINT ISSN : 1348-589X

Journal of Pesticide Science
Vol. 31 (2006) , No. 3 pp.273-281

Structure–activity relationships and pathway analysis of biological degradation processes

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(Received: May 29, 2006)

Abstract:
(Q)SARs estimate biological activity; however these models are insufficient to fully understand and predict the ADME-Tox processes of small molecules in biological systems. By integrating (Q)SARs with biological databases, the predictive capability of these models can be significantly improved. However, the techniques and methods for integrated analysis have not yet been sufficiently developed for these combined systems. In this review, we discuss standard (Q)SAR methods and biological database construction as well as provide an example of how SAR and metabolic pathway analysis can be combined to examine the biological degradation processes of endocrine disrupting chemicals.

Keywords:
structure–activity relationships, pathway analysis, biodegradation, 1,1,1-trichloro-2,2-bis (*p*-chlorophenyl)ethane, 1,1-dichloro-2,2-bis(*p*-chlorophenyl)ethylene

processes”. *J. Pestic. Sci.* Vol. **31**, pp.273-281 (2006) .

doi:10.1584/jpestics.31.273
JOI JST.JSTAGE/jpestics/31.273