Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry
Volume 42, Issue 6, 1 June 2003, Pages 1368-1378

QSAR modeling of polychlorinated aromatic compounds

Caprioara, M., Diudea, M.V.

Fac. of Chem./Chemical Engineering, Babes-Bolyai University, 3400 Cluj, Romania

Abstract

Polychlorinated aromatic compounds viz., dibenzofurans (PCDFs), dibenzo-p-dioxins (PCDDs) and biphenyls (PCBs) have been characterized on the basis of topological descriptors. A quantitative structure-activity relationship (QSAR) study is performed in order to emphasize the relation between some topochemical and electronic parameters and their binding affinity to the aryl hydrocarbon receptor (AhR). The models reveal that the main feature influencing the binding activity of these compounds is a partial charge-based descriptor, a measure of the molecular electronic properties derived using the correlation weights of these local invariants. The linear regression equations enable to predict correctly the binding affinity of the polychlorinated derivatives. The present model shows good agreement with the literature data.

References (29)

1. Basak, S.C., Grunwald, G.D., Gute, B.D., Balasubramanian, K., Opitz, D. (2000) *J Chem Inf Comput Sci*, 40 p. 885 Cited 31 times
Abstract + Refs View at Publisher

2. Basak, S.C. (1990) *Practical Applications of Quantitative Structure-Activity Relationships QSAR in Environmental Chemistry and Toxicology*, p. 83 edited by W Karcher & J Devillers (Kluwer Academic Publishers, Dordrecht, The Netherlands)

3. Gombar, K.V., Enslein, K., Blake, B.W. (1995) *Chemosphere*, 31 p. 2499 Cited 10 times
Abstract + Refs View at Publisher

4. Basak, S.C., Gute, B.D., Grunwald, G.D. (1999) *QSAR Environ SAR Res*, 10 p. 117

5. Hawkins, D., Bask, S.C., Shi, X. (2001) *J Chem Inf Comput Sci*, 41 p. 663 Cited 13 times
Abstract + Refs View at Publisher

6. Tysklind, M., Lundgren, K., Rappe, C., Eriksson, L., Jonsson, Sjostrom, M. (1993) *Environ Toxicol Chem*, 12 p. 659 Cited 13 times
Abstract + Refs

7. Safe, S. (1987) *Chemosphere*, 16 p. 791 Cited 51 times
Abstract + Refs View at Publisher

8. Safe, S.

(1990) *Crit Rev Toxicol*, 21 (1) p. 50 Cited 3 times

9. Mekemyan, O.G., Veith, G.D., Call, D.J., Ankley, G.T.
(1996) *Environ Health Perspect*, 104 p. 1302 Cited 36 times
Abstract + Refs

10. Bhandiera, S., Sawyer, T., Romkes, M., Zmudzka, B., Safe, L., Mason, G., Keys, B., Safe, S.
(1984) *Toxicology*, 32 p. 131 Cited 25 times
Abstract + Refs View at Publisher

11. Mason, G., Farrell, K., Keys, B., Piskorska-Pliszczynska, J., Safe, L., Safe, S.
(1986) *Toxicology*, 41 p. 21 Cited 43 times
Abstract + Refs View at Publisher

12. Mc Gregor, D.B., Partensky, C., Wilbourn, J., Rice, J.M.
(1998) *Envir Health Perspect*, 106 (SUPPL. 2) p. 755 Cited 46 times
Abstract + Refs

13. Beger, R.D., Wilkes, J.G.
(2001) *J Chem Inf Comput Sci*, 41 p. 1322 Cited 17 times
Abstract + Refs View at Publisher

14. Bandiera, S., Safe, S., Okey, A.B.
(1982) *Chem-Biol Interact*, 39 p. 259 Cited 50 times
Abstract + Refs View at Publisher

15. Poland, A., Knutson, J.C.
(1982) *Annu Rev Pharmacol Toxicol*, 22 p. 517 Cited 695 times
Abstract + Refs

16. Poland, A., Glover, E., Kende, A.S.
(1976) *J Biol Chem*, 251 p. 493

17. Safe, S.
(1984) *Crit Rev Toxicol*, 13 p. 319 Cited 185 times
Abstract + Refs

18. Safe, S.H.
(1986) *Annu Rev Pharmacol Toxicol*, 26 p. 371 Cited 219 times
Abstract + Refs

19. Diudea, M.V., Ursu, O.
(2002) *TOPOCLUJ*, Cited 2 times
Copyright Babes-Bolyai Univ. Cluj

20. Diudea, M.V., Gutman, I., **Jantschi**, L.
(2001) *Molecular Topology*, Cited 13 times
NOVA SCIENCE, Huntington, New York

21. Diudea, M.V., Ursu, O.
Indian J Chem A,
In press

22. *HyperChem [TM]*,
release 4.5 for SGI, © 1991-1995, Hypercube, Inc

23. Rios-Santamaria, I., Garcia-Domenech, R., Cortijo, J., Santamaria, P., Morcillo, E.J., Galvez, J.
(2002) *Internet Electron J Mol Design*, 1 p. 70 Cited 8 times
http://www.biochempress.com

24. Galvez, J., Garcia-Domenech, R., Salabert, M.T., Soler, R.
(1994) *J Chem Inf Comput Sci*, 34 p. 520 Cited 99 times
Abstract + Refs View at Publisher

25. Toropov, A.A., Toropova, A.P.
(2002) *Internet Electron J Mol Design*, 1 p. 108 Cited 13 times
http://www.biochempress.com

26. Marino, D.J.G., Peruzzo, P.J., Castro, E.A., Toropov, A.A.
(2002) *Internet Electron J Mol Design*, 1 p. 115 Cited 12 times
http://www.biochempress.com

27. Diudea, M.V., Ivanciuc, O.

(1995) *Topologie Moleculara*, Cited 5 times
Ed. COMPREX, Cluj

28. Randic, M., Basak, S.C.
(2001) *J Chem Inf Comput Sci*, 41 p. 650 Cited 8 times
Abstract + Refs View at Publisher

29. Viswanadhan, N.V., Mueller, G.A., Basak, S.C., Weistein, J.N.
(2001) *J Chem Inf Comput Sci*, 41 p. 505 Cited 19 times
Abstract + Refs View at Publisher

Caprioara, M.; Fac. of Chem./Chemical Engineering, Babes-Bolyai University, 3400 Cluj, Romania;

Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry
Volume 42, Issue 6, 1 June 2003, Pages 1368-1378