Water solubilities and subcooled vapor pressures for chloronaphthalene congeners determined by neural network (NN) computational technique

Tomasz Puzyn, Jerzy Falandysz, Agata Wilczyńska - Piliszek, Sławomir Piliszek

Introduction

Polychlorinated naphthalenes (PCNs) are known persistent organic pollutants, contaminating natural ecosystems in effect of technical human activity[1-6]. Subcooled vapour pressures and water solubility are important properties in many practical applications. Vapour pressures and water solubility are commonly used for assessing the mass distribution of chemical in the environment. A quantitative structure-property relationships (QSPR) methodology based on neural network was developed for prediction of the subcooledvapour pressure and water solubility for chloronaphthalenes. Neural networks have gained popularity in recent years as a technique for developing of QSPR models. The advantage of neural networks over the regression analysis methods is their inherent ability to incorporate nonlinear relationships between descriptors and physicochemical properties[7-9].

The aim of this study was determination of water solubility and subcooled vapor pressure using quantum chemical molecular descriptors and neural network technique.

Materials and Methods

Initially, a set of structural descriptors was computed for each of 75 chloronaphthalene congeners and based on the level of the density functional theory using B3LYP hybrid functional and 6-311++G** basis set[10]. To characterize water solubility we used six descriptors but to characterized the subcooledvapour pressure we used seventeen descriptors. To characterize water solubility we used descriptors such as the number of chlorine atoms connected with second ring (nClp2), standard heat of formation (dH), entropy (S), molecular refraction (MR), solvent-accessible surface area (water) (SASw) and the total energy of electrostatic hydratation (TEESolw)[11-14].To characterize subcooledvapour pressures we used descriptors such as the number of chlorine atoms in molecule (nCL), the number of chlorine atoms in a-positions (nClalpha), the number of chlorine atoms in b-positions (nClbeta), bond valencebehind C1-C-C8 (CCC(1-8)), total dipole moment of the molecule (D), diagonalized average polarizability (A), the most positive partial charge on atoms ($MaxQ^+$), energy of the highest occupied molecular orbital (HOMO), energy of the lowest unoccupied molecular orbital (LUMO), chemical hardness (Hard), ionization potential (IP), electron affinity (EA), thermal energy (Et), standard heat of formation (dH), thermal capacity (Cv), molar volume (MVOL) and the index of sumeinteratomic distance chlorine atoms (T(Cl-Cl))[11-13].

Next, we constructed a model for subcooledvapour pressures based on 17-8-1 perceptorn architecture, and for water solubility based on 6-3-1 architecture. Both networks were learned using back-propagation technique and experimental data taken from available literature.

Results and Discussion

The models findings (Figure 1 and 2) in own research predict with less error then similar model for other groups of chemical. The values of root mean square error of prediction (RMSEP) for both neural networks were calculated to be 0.078 for subcooled vapour pressure and to be 0.155 for water solubility.

Goll and Jurs[15] predicted the vapour pressures at 25 ^oC for selected 353 hydrocarbons (include chloroorganic compounds). The values are between -1.00 to 6.65 logarythmic units Pa. The value for 7-3-1 neural network model of RMSEP (root mean square error of prediction) was calculated to be 0.209. The similar McClelland and Jurs[16] predict for 420 differents organic compounds take advantage of experimentals results with 10-4-1 neural network model. The RMSEP value was calculated to be 0.33. Beck *et al.*[17] create a 10-8-1 neural network model make use of semi-empirical calculation using the AM1 method for 551 organic compounds. Standard deviation for that model (validation data) was calculated to s = 0.68.

The subcooledvapour pressure and the water solubility for each PCNs subset from -4.23 to 0.43 logarythmic units Pa and from -1.01 to 3.30 logarythmicunits μg/dm^3. Only monochloronaftalens are characterized by positive values of logarythmic subcooled vapour pressure (from 0.43 to 0.37). Similar results findings experimentally Lei*et al.*[18]. Only monochloronaphtalens are liquids in room temperature. The other congeners in the same conditions occure how solid state. Determined subcooled vapour pressure and water solubility are presented in Table 1.

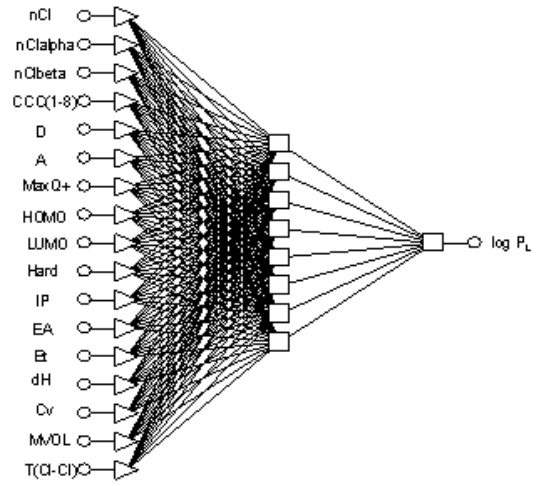

Figure 1. The 17-8-1 neural network architecture model for predicted log P_L

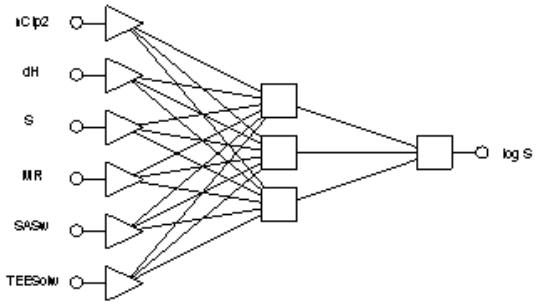

Figure 2. The 6-3-1 neural network architecture model for predicted log S

The values subcooled vapour pressures for monochloronaphtalenes are similarity for non-*ortho*monochlorobiphenyls and two rings PAHs. Di-, tri-, and tetrachloronaphtalens was characterized by vapour pressures approach to hexachlorocyclohexan, dieldrin, polychlorinated biphenyls with two to four chloride atoms, monochlorodibenzo-*p*-dioxins, furans and three rings PAHs.

Table 1. Minimum and maximum predicted values of subcooled vapour pressures and water solubility

Congeners of CN	Water solubility log S [μg/dm^3]		Subcooled vapour pressure log P_L [Pa]	
	Min	Max	Min	Max

Mono-	3.23	3.30	0.37	0.43
Di-	2.44	2.76	-0.79	-0.01
Tri-	1.53	1.81	-1.31	-0.84
Tetra-	0.62	1.81	-1.73	-1.53
Penta-	-0.24	0.74	-2.48	-2.12
Hexa-	-0.74	0.05	-3.17	-2.63
Hepta-	-0.94	-0.66	-3.73	-3.67
Octa-	-1.01	-	-4.23	-

Penta-, hexa-, and heptachloronaphtalens are characterized by volatility similar to DDT and their derivatives (DDD, DDE, DDMU), also to chlordane, congeners PCBs with four to eight atom of chlorine, PCDDs/Fs with two to four atom of chlorine and four rings PAHs. Subcooled vapour pressure for octachloronaphtalene are near to bornans and high chlorinated biphenyls, dibenzo-*p*-dioxins, dibenzofurans and largest PAHs such as benzo[a]piren.

The present study demonstrates that neural network/QSPR and QSAR can be applied to describe subcooled vapour pressure and water solubility.

Acknowledgements

This study was supported by the Polish Ministry of Science and Informatics under grant no. KBN 1128/T09/2003/24. Computations were carried out using computers in the TASK – Academic Computer Center in Gdańsk.

References

1. Falandysz J., Kawano M., Ueda M., Matsuda M., Kannan K., Giesy J.P. and Wakimoto T. (2000) J. Environ. Sci. HealthA. 35(3): 281-298.
2. Falandysz J. and Rappe C. (1996) Environ Sci. Technol. 30: 3362-3370.
3. Harner T., Lee R.G.M. and Jones K.C. (2000) Environ. Sci. Technol. 34: 3137-3142.
4. Helm P.A. and Bidleman T.F. (2003) Environ. Sci. Technol. 37: 1075-1082.
5. Horii Y., Falandysz J., Hanari N., Rostkowski P., Puzyn T., Okada M., Amano K., Naya T., Taniyasu S. and Yamashita N. (2004) J. Environ. Sci. Health 39A: 587-609.
6. Yamashita N., Taniyasu S., Hanari N., Horii Y. and Falandysz J. (2003) J. Environ. Sci. Health 38A: 1745-1759.
7. Beck B., Breindl A. and Clark T. (2000) J. Chem. Inf. Comp. Sci. 40: 1046-1051.
8. Goll E.S. and Jurs P.C. (1999) J. Chem. Inf. Comp. Sci. 39: 1081-1089.
9. McClelland H.E. and Jurs P.C. (2000) J. Chem. Inf. Comp. Sci. 40: 967-975.
10. FrishM.J.*et al*. (2003) GAUSSIAN 03, Gaussian Inc., Pittsburgh.
11. Curtiss L.A., Raghavachari K., Redfern P.C. and Pople J.A. (1997) J. Chem. Phys. 106: 1063-1079.
12. OchterskiJ.W. (2000) Thermochemistry in Gaussian. Gaussian Inc. http://gaussian.com
13. Todeschini R. and Consonni V. (2000) Handbook of molecular descriptors. Wiley- VCH Verlag, Weinheim.
14. Tomasi J. and Persico M. (1994) Chem. Rev. 94: 2027-2094.
15. Goll E.S. and Jurs P.C. (1999) J. Chem. Inf. Comp. Sci. 39: 1081-1089.
16. McClelland H.E. and Jurs P.C. (2000) J. Chem. Inf. Comp. Sci. 40: 967-975.
17. Beck B., Breindl A. and Clark T. (2000) J. Chem. Inf. Comp. Sci. 40: 1046-1051.
18. Lei Y.D., Wania F. and Shiu W.Y. (1999) J. Chem. Eng. Data. 44: 577-582.