

QSAR Models for Cytotoxicity of Chlorinated Alkanes

R.Suganya, S.Bharanidharan, R.Velavan

Abstract: Knowledge on the degree of toxicity of aliphatic hydrocarbons and their derivatives has become essential for environmental safety and security. In the present study, an effort has been put forth to analyze the toxicity of aliphatic hydrocarbons. This work focuses on development of new QSAR models with various DFT based descriptors. Cytotoxicity of Chlorinated alkanes with experimental activity log EC₅₀ Values are utilized to obtain QSTR models.

Key words: QSAR/ QSTR, DFT electrophilicity index (ω), polarizability (α), chemical potential (μ), and hardness (η)

I. INTRODUCTION

Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Toxicity Relationship (QSTR) have seen recent upsurge of interest because of their ability in predicting various activities and properties of complex molecules. QSAR is a powerful research tool to successfully establish / predict activity models and evaluate the toxicity of those chemicals introduced or not introduced into the markets. Such theoretical evaluation of toxicity of chemicals reduces the experimental efforts in identifying its effect on living forms. [8],[10],[12]

A QSAR model has to satisfy a number of conditions related to the different aspects of the model (Wold et al 1983, Eriksson et al 2001). The biological activity/toxicity of a series of compounds should be related to the physico-chemical properties being considered. Also, the activities of the compounds should be elicited by common and relevant mechanism. Related chemical structures are not strictly required but structures with unknown mechanism of action are not encouraged. Hence, chemically similar compounds with same mechanism of action are used for generating QSAR models. [7],[9],[11]

A mathematical formulation on “the principle for toxicity” was first coined by Ferguson (1939). It has been observed that the toxicity of aliphatic and aromatic hydrocarbons to mammals is extremely variable, depending on the species, compound, and environmental conditions (UNEP 2006). Alkanes are a class of aliphatic hydrocarbons having very low (aquatic) toxicity. The introduction of chlorine atoms into the hydrocarbon chain alters properties such as

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solubility, density, volatility, and toxicity (NRC 1993). Several studies have highlighted the acute toxicity of chlorinated alkanes.

Quantum chemical descriptors based on density functional theory (DFT) (Parr & Yang 1989; Chattaraj 2009; Chattaraj & Giri 2009) have become quite successful in explaining physicochemical properties (Giri et al 2008) and toxicity (Roy et al 2006, Padmanabhan et al 2006) of diverse classes of chemical compounds and drug molecules. [1],[3],[5]

II. COMPUTATIONAL DETAILS

The three-dimensional conformation of the compounds and their derivatives are built using Cerius2 package and are optimized using the semi empirical quantum chemical method, Austin Method 1 (AM1) to obtain the stable conformation. The conformational energy and the atomic / molecular orbital energies (EHOMO and ELUMO) have been obtained by calculating the single point energy at B3LYP/6-31G* level. Using this method, a series of quantum chemical indices, [2],[4],[6] such as Hartree Fock energy HF (E), the LUMO energy (L), electrophilicity index (ω), polarizability (α), chemical potential (μ), and hardness (η) have been obtained. Relationship between these parameters has been analyzed to identify whether the activity of these compounds have any influence over these parameters and hence these parameters can be used as a controlling factor for its activity and vice versa. The quantum calculations have been performed using GAUSSIAN98W package and the structures of studied compounds has been modeled using Silicon Graphics workstation [13],[15],[17]

III. RESULT AND DISCUSSION

The QSAR analysis on aliphatic and aromatic hydrocarbons have been performed to highlight inhibitor-enzyme interaction mechanisms based on the *in silico* derived toxicity, which would eventually provide additional information for future molecular design of compounds belonging to this category.

A set of 77 chlorinated alkanes with cytotoxicity activity (log EC₅₀) (Zvinavashe et. al.2008) have been selected for this analysis. The studied

chlorinated alkanes have been classified into two categories based on their hardness values. [32],[34]

Compounds having hardness value greater than 0.15 are listed in Table 1.1a (16 compounds) and those having lesser than 0.15 are listed in Table 1.1b (61 compounds). Majority of the compounds in the first set have long hydrocarbon chain (up to ten carbons) with chlorine in the first position. The second set of compounds are shorter in length (< 10 carbons) and are more chlorinated (~ 3 to 7 chlorines). The parameters such as chemical potential (μ), electrophilicity index (ω), dipole moment (DP), polarizability, hydrophobicity (logP) and relative energy (RE) are used for deriving QSAR equations. [14],[16], [18]

Table 1.1a: List of compounds classified as set 1

S.NO	1) Compound
A1	1,3-dichloropropane
A2	1,2-dichloropropane
A3	1,1,2-trichloroethane
A4	1,2-dichlorobutane
A5	1-chloro-2,2-dimethylpropane
A6	1-chloro-2-methylbutane
A7	1-chloropentane
A8	1,6-dichlorohexane
A9	1-chlorohexane
a) A10	1,1-dichloro-3,3 dimethylbutane
A11	1-chloroheptane
A12	1,8-dichlorooctane
A13	1-chlorooctane
A14	1,9-dichlorononane
A15	1-chlorononane
A16	1-chlorodecane

Table 1.1b: List of compounds classified as set 2

S.NO	Compound
B1	1, 2, 3-trichloropropane
B2	1-chlorobutane
B3	1, 5-dichloropentane
B4	Pentachloroethane
B5	1, 1, 1, 2, 2, 2, 3-heptachloropropane
B6	Hexachloroethane
B7	1, 1-dichloroethane
B8	1, 3-dichloro-2,2-bis(chloromethyl)propane
B9	Trichloromethane
B10	1-chloropropane

B11	2-chloropropane
B12	1, 3-dichlorobutane
B13	1, 4-dichlorobutane
B14	1, 1-dichloropropane
B15	2, 2-dichloropropane
B16	1, 2, 3-trichloro-2-methylpropane
B17	1, 2-dichloro-2-methylpropane
B18	1-chloro-2-methylpropane
B19	2-chloro-2-methylpropane
B20	1, 1, 1-trichloroethane
B21	1, 2, 3, 4-tetrachlorobutane
B22	2, 3-dichlorobutane
B23	2-chlorobutane
B24	1, 1, 3-trichlorobutane
B25	1, 1, 2, 3-tetrachloropropane
B26	1, 2, 2, 3-tetrachloropropane
B27	1, 1, 2-trichloropropane
B28	1, 2, 2-trichloropropane
B29	1, 3-dichloro-3-methylbutane
B30	Tetrachloroethane
B31	1, 1, 1, 3-tetrachloropropane
B32	1, 1-dichlorobutane
B33	2, 2-dichlorobutane
B34	1, 1, 3, 3-tetrachlorobutane
B35	1-chloro-3-methylbutane
B36	2-chloro-2-methylbutane
B37	Trichloropropane
B38	1, 1, 1, 2-tetrachloroethane
B39	2, 3-dichloropentane
B40	2-chloropentane
B41	3-chloropentane
B42	1, 1, 2, 2, 3-pentachloropropane
B43	1, 1, 1, 3-tetrachlorobutane
B44	1-chloro-3,3-dimethylbutane
B45	1, 1, 1-trichlorobutane
B46	1, 1, 1, 2-tetrachloropropane
B47	1, 1, 1, 3, 3-pentachlorobutane
B48	2-chlorohexane
B49	3-chlorohexane
B50	2-chloro-2, 3, 3-trimethylbutane
B51	2, 5-dichloro-2, 5-dimethylhexane
B52	2-chloroheptane
B53	3-chloroheptane
B54	1, 1, 1, 3-tetrachloro-4-methylpentane
B55	1-chloro-2, 2, 4-trimethylpentane

B56	3-(chloromethyl)heptane
B57	2-chlorooctane
B58	3-chlorooctane
B59	4-chlorooctane
B60	1, 1, 2, 2 - tetrachloroethane
B61	Carbon tetrachloride

An attempt has been made to elucidate a QSAR model considering the Number of Carbon Atoms (NCA) and the Number of Chlorine Atoms (NCIA). [31],[33],[35]

Table 1.1c lists the experimentally reported log EC₅₀ values, dipole moment and

log EC ₅₀ (vitro)= 14.39* RE + 0.18 * DP - 0.25* NCA - 0.91681 n=16 with R ² = 0.91 and S D = 0.19	(1.1)
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relative energy derived at B3LYP/6-31G*, NCA and the predicted activity. From the table 1.1c, it is clear that the considered descriptors have significant role in predicting the cytotoxicity of the studied chlorinated alkanes and is evidenced by the QSAR equation 1.1 [19],[21],[23]

Table 1.1c The relative energy RE, Dipole Moment DP, number of carbon atom NCA values calculated for compounds classified as set 1 along with their experimental and predicted cytotoxicity values of selected 16 compounds.

S. NO	Compound	log EC ₅₀	RE	DP	NCA	Predicted log EC ₅₀
1	1, 3-dichloropropane	2.99	0.27	3.61	3	2.88
2	1, 2-dichloropropane	3.03	0.29	2.84	3	3.06
3	1, 1, 2-trichloroethane	3.04	0.29	1.31	2	3.03
4	1, 2-dichlorobutane	2.61	0.28	2.75	4	2.64
5	1-chloro-2, 2-dimethylpropane	2.30	0.28	1.96	5	2.21
6	1-chloro-2-methylbutane	2.30	0.28	1.96	5	2.21
7	1-chloropentane	2.24	0.28	2.07	5	2.26
8	1, 6-dichlorohexane	2.02	0.28	3.21	6	2.16
9	1-chlorohexane	2.24	0.28	2.01	6	1.98
10	1, 1-dichloro-3, 3 dimethylbutane	1.67	0.28	1.93	6	1.90
11	1-chloroheptane	1.73	0.28	2.06	6	1.98
12	1, 8-dichlorooctane	1.72	0.29	3.27	8	1.85
13	1-chlorooctane	1.43	0.29	2.02	8	1.65
14	1, 9-dichlorononane	1.78	0.29	3.84	9	1.69
15	1-chlorononane	1.35	0.29	2.07	9	1.40
16	1-chlorodecane	1.44	0.29	2.02	10	1.12

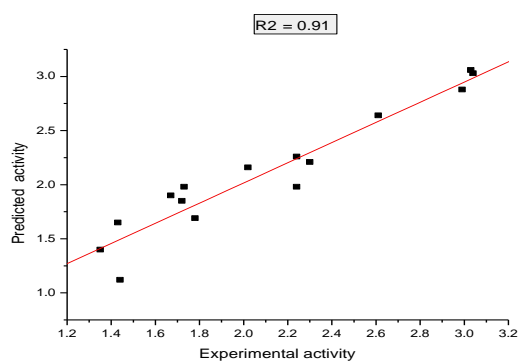


Fig. 1.1a. A plot generated from a linear regression model, using simulated data, with a high value of R² for the compounds listed in Table 1.1a.

The experimental and predicted cytotoxicity values for the second set of compounds (Table 1.1b) have been predicted using the descriptors such as electrophilicity index, dipole moment and NCA is given in Table 1.1d and the corresponding QSAR equation is given in Equation. 1.2. In this set, presence of more chlorine directly does not give a better QSAR equation than NCA whereas it indirectly

changes the descriptor (RE) to electrophilicity index (ω).
[20],[22], [24]

$\log EC_{50} \text{ (vitro)} = 14.58 * \omega + 0.05 * DP - 0.199 * NCA - 4.4543$ $n=59 \text{ with } R^2 = 0.70 \text{ and } SD = 0.20$	(1.2)
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Table 1.1d The electrophilicity index ω , Dipole Moment DP, number of carbon atom NCA values calculated for compounds classified as set 2 along with their experimental and predicted cytotoxicity values of selected 59 compounds

S.NO	Compound	log EC ₅₀	ω	DP	NCA	Predicted log EC ₅₀
1	1,2,3-trichloropropane	2.8	0.09	3.94	3	2.69
2	1-chlorobutane	2.56	0.08	2.01	4	2.57
3	1,5-dichloropentane	2.45	0.09	3.76	5	2.38
4	pentachloroethane	2.07	0.13	1.00	2	2.27
5	1,1,1,2,2,2,3-heptachloropropane	1.57	0.13	0.88	3	1.96
6	hexachloroethane	1.63	0.13	0.00	2	2.14
7	1,1-dichloroethane	2.89	0.09	2.13	2	2.84
8	1,3 – dichloro - 2, 2 –bis (chloromethyl) propane	2.82	0.09	0.00	5	2.12
9	trichloromethane	2.81	0.12	1.21	3	2.16
10	1-chloropropane	2.8	0.08	2.06	3	2.75
11	2-chloropropane	2.8	0.08	2.16	3	2.74
12	1,3-dichlorobutane	2.69	0.08	3.66	4	2.62
13	1,4-dichlorobutane	2.69	0.09	3.13	4	2.55
14	1,1-dichloropropane	2.66	0.09	2.11	3	2.68
15	2,2-dichloropropane	2.66	0.09	2.33	3	2.71
16	1,2,3-trichloro-2-methylpropane	2.62	0.09	4.18	4	2.54
17	1,2-dichloro-2-methylpropane	2.62	0.09	2.99	4	2.50
18	1-chloro-2-methylpropane	2.62	0.08	2.04	4	2.53
19	2-chloro-2-methylpropane	2.62	0.08	2.17	4	2.53
20	1,1,1-trichloroethane	2.58	0.11	1.89	2	2.49
21	1,2,3,4-tetrachlorobutane	2.57	0.10	0.00	4	2.26
22	2,3-dichlorobutane	2.56	0.08	0.00	4	2.48
23	2-chlorobutane	2.56	0.08	2.10	4	2.56
24	1,1,3-trichlorobutane	2.55	0.09	2.72	4	2.53
25	1,1,2,3-tetrachloropropane	2.54	0.10	1.23	3	2.44
26	1,2,2,3-tetrachloropropane	2.54	0.11	2.22	3	2.43
27	1,1,2-trichloropropane	2.53	0.09	1.40	3	2.56
28	1,2,2-trichloropropane	2.53	0.09	1.63	3	2.56
29	1,3-dichloro-3-methylbutane	2.51	0.09	2.55	5	2.30
30	Tetrachloroethane	2.51	0.10	0.00	1	2.77
31	1,1,1,3-tetrachloropropane	2.47	0.12	2.07	3	2.28
32	1,1-dichlorobutane	2.42	0.09	2.03	4	2.51
33	2,2-dichlorobutane	2.42	0.09	2.25	4	2.48
34	1,1,3,3-tetrachlorobutane	2.41	0.09	3.50	4	2.51
35	1-chloro-3-methylbutane	2.38	0.08	1.92	5	2.35
36	2-chloro-2-methylbutane	2.38	0.08	2.12	5	2.34
37	Trichloropropane	2.34	0.09	3.94	3	2.69
38	1,1,1,2-tetrachloroethane	2.33	0.12	1.53	2	2.35
39	2,3-dichloropentane	2.33	0.09	2.78	5	2.31
40	2-chloropentane	2.32	0.08	2.04	5	2.37
41	3-chloropentane	2.32	0.08	2.02	5	2.36

42	1,1,2,2,3-pentachloropropane	2.27	0.11	1.24	3	2.28
43	1,1,1,3-tetrachlorobutane	2.24	0.11	2.27	4	2.10
44	1-chloro-3,3-dimethylbutane	2.2	0.09	2.28	6	2.12
45	1,1,1-trichlorobutane	2.11	0.11	2.14	4	2.15
46	1,1,1,2-tetrachloropropane	2.1	0.12	1.97	3	2.25
47	1,1,1,3,3-pentachlorobutane	2.1	0.12	1.51	4	1.98
48	2-chlorohexane	2.09	0.08	2.08	6	2.17
49	3-chlorohexane	2.09	0.08	1.95	6	2.17
50	2-chloro-2,3,3-trimethylbutane	2.03	0.08	2.06	7	1.96
51	2,5-dichloro-2,5-dimethylhexane	1.86	0.09	3.58	8	1.75
52	2-chloroheptane	1.85	0.08	2.02	7	1.97
53	3-chloroheptane	1.85	0.08	2.00	7	1.97
54	1,1,1,3-tetrachloro-4-methylpentane	1.82	0.11	2.45	6	1.75
55	1-chloro-2,2,4-trimethylpentane	1.79	0.08	2.07	8	1.73
56	3-(chloromethyl)heptane	1.67	0.08	1.87	8	1.75
57	2-chlorooctane	1.62	0.08	2.07	8	1.77
58	3-chlorooctane	1.62	0.08	1.94	8	1.77
59	4-chlorooctane	1.62	0.08	1.92	8	1.78

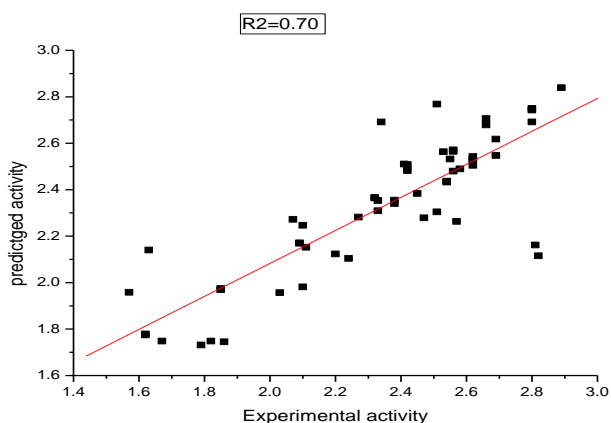


Figure 1.1b Plot illustrating the experimental cytotoxicity against the predicted values for the compounds listed in Table 3.1b with a high value of R^2 .

IV. CONCLUSION

From the QSAR analysis of the chlorinated alkanes, [26],[28],[30]it is clear that the compounds having a greater number of C-atoms gives better prediction with relative energy than the electrophilicity index, whereas, for the more chlorinated compounds, the electrophilicity index influences the QSAR model. [25],[27],[29]

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