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REVIEW ARTICLE

QSPR Studies of Non Cyclic Polyether

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Abstract
This paper deals with a Quantitative Structure Property relationship (QSPR) study on a large set of Podands (non cyclic polyether) using a combination of topological indices. The regression analysis has been carried out assuming linear relationship between ClogP and topological indices. The analysis of the data has indicated that an excellent model is obtained when these topological indices are combined with some classical descriptor. The obtained model is further supported through cross validation.

Keywords: QSPR / Topological Indices / lipophilicity / Podands

INTRODUCTION:-
Quantitative Structure Property Relationships i.e. QSPR is a relationship between structure and property. Lipophilicity has been recognized for its importance in QSPR. Lipophilicity is defined by the partitioning of a compound between an aqueous and a non-aqueous phase. The logarithm of the partition coefficient (P) between octanol and water (logP) is an important physiochemical parameter widely used in medicinal chemistry [1-3], and is closely related to the transport properties of drugs and their interaction with receptor. Efforts have been made to determine the logP values of a number of compounds.
Lipophilicity is very important property for podands because main application of podands is in transportation, Extraction and its capacity of extraction can explain by lipophilicity. Drug action, Pharmacology and phase catalysis studies also deals with the portioning attitude of podands in lipophilic and aqueous phase.[4]
The basic assumption in the present work is that the lipophilicity of the compound may be related to their structural descriptor as a multilinear function. In the present study, we have used 61 podands for modeling of lipophilicity using topological indices and structural descriptor

Experimental
Molecular graphs:
The molecular graphs used for the calculation of topological indices were carbon-hydrogen as well as hetero atom hydrogen suppressed graphs.

ClogP:
The value of lipophilicity calculated by Cambridge computer software for the set of 61 podands.

Topological Indices[5-7]
The topological indices: Connectivity indices (0χ, $0\chi Av$ and $3\chi A$), kappa index (S2k), Polarity number (P2), D_{min}/D_{max} (D/D), Wms used in the present investigation were calculated by topological graphs of compounds.

Indicator parameters[8]
Indicator parameter is not a QSPR parameter. It is dummy parameter used to indicate the significance of any particular group or species in a given series of drug. In the present study two indicator parameter are used. Indicator parameter nCl stands for no. of Chlorine atom and nBnz stands for no. of benzene ring present in that compound. They assume only numerical value of the number of atoms present in the structure.

Statistical Parameters:
Regression analysis is a statistical method which has been found to be a versatile technique for QSAR/QSPR studies. The regression analysis was performed using maximum-R^2 method by the SPSS software. The cross-validation method evaluates the validity of a model by how well it fits data. (Table 3)

Result and Discussion
The chemical names of the podands are given in table 1along with the estimated topological indices along with structural descriptor used in modeling. To obtain statistically significant model for modeling of lipophilicity we have used maximum R^2 method.

Quantitative structure activity / property relationships

(QSAR/QSPR) are mathematical models obtain via statistical regression analysis aiming at predicting properties of molecules from their structure. Molecular activity and properties obtained experimentally are digital values but structures are in graphical form. Thus molecular topology involves the translation of molecular structure in to characteristic numerical descriptors which are known as topological indices. In chemical graph theory and topology, atoms are treated as vertices and the bonds edges. When certain condition are imposed on vertices, edges, or both a number is obtain which is called the topological index used in the modeling of physicochemical properties, biological activities and toxicity of organic compounds.[9-15]

To develop appropriate model we should know the relation between independent variables (topological indices and indicator parameter) and the dependent variables (ClogP). The correlation matrix obtained in the present study is given in table-2. The correlation matrix shows that the topological indices nBnz, 0χAv, 0χ, D/D, nCl, S2k, 3χA, Wms, P2 are highly correlated. Thus a model containing any combination of these indices may suffer from the defect due to collinearities. To overcome this difficulty we have used the recommendations of Randic[16].

Initial statistical analysis has indicated that no statistically significant single linear regressions are possible for modeling lipophilicity of the compounds. This indicates that the ClogP i.e. lipophilicity is a function of more than one property and we have to choose more than one Ties that have been tried for good result and correlation of the several 4-parametric models, the one which is the best is given below:

ClogP = -11.904 – 2.90E-02 * **D/D** + 0.723 * **0χ** + 11.472 * **0χAv** + 0.876 * **nBnz** **(1)**

k= 4, **SE** = 0.643, **R** = 0.911, **R²adj** = 0.818, **F** = 55.621

In above model, the value of initial statistical parameters is good but not significant for the correlation. However with a hope of obtaining still better results we have carried out 5-parametric regression analysis by addition of nCl. Which is the best in several 5-parametric model and is given below:

ClogP *= -11.461 - 2.79E-02 * **D/D** + 0.686 * **0χ** + 11.179 * **0χAv** + 0.948 * **nBnz** + 0.295 * **nCl*** **(2)**

k= 5, **SE** = 0.603, **R** = 0.923, **R²adj** = 0.839, **F** = 59.678

For the aforementioned model, the value of statistical parameter is good but not significant for the correlation. Looking to such an excellent result we add S2k.

ClogP *= -10.6948 + 0.924 * **nBnz** – 0.0223 * **D/D** + 0.621 * **0χ** + 11.935 * **0χAv** + 0.269 * **nCl** – 0.124 * **S2k*** **(3)**

k= 6, **SE** = 0.570, **R** = 0.933, **R²adj** = 0.856, **F** = 60.732

Addition of the parameter 3χA during the stepwise regression analysis yielded a 7-parametric regression expression with improved statistics, the resulted 7-parametric model is given below

ClogP *= 13.8327 + 0.974 * **nBnz** - 0.0246 * **D/D** + 0.716 * **0χ** + 11.932 * **0χAv** + 0.279 * **nCl** – 0.186 * **S2k** + 12.119 * **3χA*** **(4)**

k= 7, **SE** = 0.549, **R** = 0.939, **R²adj** = 0.867, **F** = 63.689

When Wms is added to eq.4, great improvement observed in the statistics and the obtained 8-paramertic model is given below:

ClogP *= -14.117 + 0.933 * **nBnz** – 0.0318 * **D/D** + 0.742 * **0χ** +12.736 * **0χAv** + 0.299 * **nCl** – 0.216 * **S2k** + 12.205 * **3χA** + 0.001 * **Wms*** **(5)**

k= 8, **SE** = 0.526, **R** = 0.945, **R²adj** = 0.875, **F** = 65.987

The significant improvement in the statistics indicates its favorable role in the modeling of lipophilicity. 9-parameric model having the best statistics than those described above. This model was containing nBnz, 0χAv, 0χ, D/D, nCl, S2k, 3χA, Wms, P2 as correlating parameters and is given below:

ClogP *= -13.792 + 0.939 * **nBnz** – 0.031 * **D/D** + 0.774 * **0χ** +12.601 * **0χAv** + 0.296 * **nCl** – 0.224 * **S2k** + 11.186 * **3χA** + 0.001 * **Wms** – 0.015 * **P2*** **(6)**

k= 9, **SE** = 0.517, **R** = 0.948, **R²adj** = 0.881, **F** = 68.431

In the regression equation 6 some Ties have positive coefficient and some have negative coefficient. This means in some cases ClogP increase with magnitude of Ties with positive coefficient and vice versa. The initial statistics SE, R, R²adj and F statistics that the model 6 is found to be far superior than the other proposed model based on eq.1,2,3,4 and 5.

The statistical parameters that deem to be good for the modeling of lipophilicity is discussed one by one. Firstly we have used quality factor (Q) for establishing the quality of the proposed models. This quality factor is defined as the ratio of correlation coefficient R and the standard error estimation SEE i.e. Q=R/SEE. Thus higher the value of R, lower the SEE and the larger will be quality of the model. The value of Q for model 6 is suggested that the model 6 is better than other 5 models. (Table 3)

Several cross-validation parameters were calculated and the meanings of these parameters are given in experi-

mental section and their values are presented in table-3. PRESS is a good estimate of the real prediction error of the model. If PRESS is smaller than the model predicts can be considered statistically significant. On the basis of this all 6 models proposed by us are good and model-6 is the best one. All cross-validation parameters PSE, R^2cv, Q, Spress, and PRESS are in favour of model-6.

Finally the predictive potential of the model is confirmed by calculating predictive correlation coefficient of the model (R^2press), (fig-1) 0.899, for the expressed model-6 (equation 6). Thus R^2pred indicates that our improved model as expressed by equation-6 is the best.

Table 1- Structural details, calculated lipophilicity value, topological indices and structural indicators for compounds

Comp No.	Compound Structure	*Clog P*	*nBnz*	*D/D*	*0χ*	*0χAv*	*nCl*	*S2k*	*3χA*	*Wms*	*P2*
1	Diphenyl 2, 2′-oxydiacetate	2.268	2	159.554	14.916	0.535	0	8.072	0.21	648.676	27
2	2, 2′-[oxybis (ethane-2, 1-diyloxy)] diphenol	2.336	2	150.1902	14.916	0.55	0	8.515	0.21	708.109	27
3	1, 1′-[ethane-1, 2-diylbis (oxyethane-2, 1-diyloxy)] dibenzene	1.38	2	181.91	15.296	0.575	0	10.933	0.222	706.249	26
4	[Oxybis (ethane-2, 1-diyloxypyridine-2, 3-diyl)] dimethanol	1.441	0	179.335	16.33	0.553	0	9.998	0.204	865.067	31
5	1, 2, 3, 4-tetrahydroquinolin-8-yl (2-methoxyphenoxy) acetate	2.93	2	139.383	16.071	0.554	0	7.31	0.187	613.446	33
6	Bis (2-methylphenyl) 2, 2′-oxydiacetate	3.266	2	186.482	16.656	0.568	0	8.345	0.205	763.422	31
7	2, 2′-[ethane-1, 2-diylbis (oxyethane-2, 1-diyloxy)] diphenol	2.2	2	211.382	17.037	0.558	0	10.884	0.214	580.304	30
8	Pyridin-2-yl pyridin-3-yl pyridine-2, 6-dicarboxylate	0.944	0	177.123	16.778	0.514	0	7.337	0.196	654.996	34
9	2, 2′-[ethane-1, 2-diylbis (oxy-2, 1-phenyleneoxy)] diethanol	1.56	2	184.182	17.037	0.558	0	10.884	0.2	823.855	60
10	Diphenyl pyridine-2, 6-dicarboxylate	3.007	2	177.123	16.778	0.524	0	7.425	0.196	706.304	34
11	2, 2′-[(methylimino) bis (ethane-2, 1-diyloxy)] biscyclohepta-2, 4, 6-trien-1-one	1.741	0	187.381	17.2	0.576	0	9.734	0.212	882.246	31
12	2-{2-[2-(2-nitrophenoxy) ethoxy] ethoxy} benzoic acid	3.105	2	211.753	18.0707	0.5316	0	6.619	0.195	1018.243	33
13	2-{2-[2-(quinolin-8-yloxy) ethoxy] ethoxy} benzonitrile	3.83	2	182.433	17.322	0.549	0	8.911	0.192	1017	34
14	2, 2′-[1, 4-phenylenebis (methyleneoxy)] biscyclohepta-2, 4, 6-trien-1-one	2.956	1	201.61	18.192	0.543	0	8.863	0.203	1026.735	36
15	2-(2-{2-[2-(2-aminophenoxy) ethoxy] ethoxy} ethoxy) benzoic acid	2.329	2	246.015	18.6147	0.555	0	11.489	0.205	1364.074	33
16	2, 2′-{pyridine-2, 6-diylbis [methylenenitrilo (*E*) methylylidene]} diphenol	3.647	2	211.825	18.192	0.544	0	8.817	0.201	1070.822	36
17	Benzaldehyde *O*, *O′*-[pyridine-2, 6-diylbis (methylene)] oxime	2.839	2	225.422	17.866	0.547	0	9.996	0.207	1239.511	34
18	Bis (2-nitrophenyl) 2, 2′-oxydiacetate	1.794	2	253.302	19.811	0.504	0	9.272	0.13	1078.12	37

Continue…….

Comp No.	Compound Structure	*Clog P*	*nBnz*	*D/D*	*0χ*	*0χAv*	*nCl*	*S2k*	*3χA*	*Wms*	*P2*
19	2-(2-{2-[2-(2-nitrophenoxy) ethoxy] ethoxy} ethoxy) benzoic acid	2.969	2	283.368	20.192	0.54	0	11.927	0.199	1596.804	36
20	2, 2′-[ethane-1, 2-diylbis (oxyethane-2, 1-diyloxy)] dibenzoic acid	2.739	2	283.368	20.192	0.543	0	12.103	0.199	1596.804	36
21	2-hydroxybenzaldehyde *O*, *O*′-[pyridine-2, 6-diylbis (methylene)] oxime	1.505	2	258.231	19.606	0.535	0	10.21	0.203	1433.064	38
22	Bis (2-nitrophenyl) pyridine-2, 6-dicarboxylate	2.533	2	274.896	21.673	0.499	0	8.803	0.185	1146.297	44
23	Pyridine-2, 6-diylbis {*N*-[(1*E*)-(4-nitrophenyl) methylene] methanamine}	2.665	2	314.283	21.347	0.526	0	9.817	0.2	1742.949	42
24	*N*, *N*′-[pyridine-2, 6-diylbis (methylene)] bis (4-nitrobenzamide	0.569	2	363.779	20.087	0.517	0	10.142	0.198	1843.54	46
25	*N*, *N*′-[pyridine-2, 6-diylbis (methylene)] bis (2-nitrobenzamide	2.369	2	329.067	23.087	0.517	0	10.142	0.188	1564.975	46
26	Dimethyl pyridine-2, 6-dicarboxylate	1.047	0	88.934	11.966	0.577	0	6.108	0.202	242.533	20
27	Pyridine-2, 6-diylbis (methylene) diacetate	0.281	0	90.234	11.966	0.577	0	6.108	0.21	270.253	76
28	Bis (2-chloroethyl) pyridine-2, 6-dicarboxylate	1.173	0	117.534	13.38	0.606	2	8.163	0.207	359.667	22
29	2, 6-bis [(*tert*-butylthio) methyl] aniline	4.785	1	128.85	14.682	0.772	0	6.556	0.199	387.041	28
30	{2, 6-bis [(*tert*-butylthio) methyl] phenyl}(Hydroxy) methylsulfonium	4.521	1	154.489	16.259	0.798	0	7.673	0.185	419.307	31
31	1, 3-bis [(*tert*-butylthio) methyl]-2-nitrobenzene	5.695	1	154.489	16.259	0.731	0	7.065	0.185	368.769	31
32	Bis (2, 2, 2-trifluoroethyl) pyridine-2, 6-dicarboxylate	0.575	0	185.878	16.966	0.477	0	6.866	0.202	597.069	32
33	Bis (2, 2, 2-trichloroethyl) pyridine-2, 6-dicarboxylate	4.605	0	185.878	16.966	0.683	6	8.303	0.202	597.069	32
34	Bis (2, 2, 2-tribromoethyl) pyridine-2, 6-dicarboxylate	5.445	0	185.878	16.966	0.91	0	9.132	0.202	597.069	32
35	(2*Z*, 2′Z)-Butane-2, 3-dione 2, 2′-{O^2, *O*2′-[1, 2-phenylenebis (methylene)] oxime	2.688	1	179.394	16.535	0.602	0	8.983	0.22	693.769	28
36	(2*E*)-Butane-2, 3-dione *O*-{4-[({[(1*E*)-1-methyl-2-oxopropylidene] amino} oxy) methyl] benzyl} oxime	2.738	1	199.907	16.535	0.602	0	8.983	0.226	842.619	28

Continue……

Comp No.	Compound Structure	*Clog P*	*nBnz*	*D/D*	*0χ*	*0χAv*	*nCl*	*S2k*	*3χA*	*Wms*	*P2*
37	(2*Z*, 2′Z)-Butane-2, 3-dione 2, 2′-{*O*², *O2′*-[1, 3-phenylenebis (methylene)] oxime}	1.591	1	188.704	16.535	0.602	0	8.983	0.224	765.588	28
38	(2*E*, 2′E)-Butane-2, 3-dione 2, 2′-{*O*², *O2′*-[(2-methoxy-1, 3-phenylene)bis (methylene)] oxim	2.605	1	217.162	18.113	0.608	0	9.835	0.21	789.971	31
39	(2*Z*)-Butane-2, 3-dione *O*-{3-[({[(1*Z*)-1-methyl-2-oxopropylidene] amino} oxy) methyl]-2-nitrobenzyl} oxime	2.321	1	233.372	18.983	0.577	0	9.53	0.204	823.84	33
40	8, 8′-[1, 3-phenylenebis (methyleneoxy)] diquinoline	6.041	3	211.578	20.175	0.545	0	8.421	0.181	1156.048	46
41	2-[2-(2-nitrophenoxy) ethoxy] ethanol	1.015	1	87.952	11.803	0.542	0	6.904	0.205	290.566	19
42	2-{2-[2-(2-methoxyethoxy) ethoxy] ethoxy} phenol	0.942	1	125.389	13.054	0.591	0	9.996	0.226	541.628	20
43	8-[2-(2-methoxyethoxy) ethoxy] quinoline	2.077	1	89.811	12.632	0.581	0	7.065	0.195	397.601	23
44	2-{2-[2-(2-nitrosophenoxy) ethoxy] ethoxy} ethanol	1.098	1	121.195	13.054	0.56	0	9.68	0.218	544.392	22
45	2-(3, 6, 9, 12-tetraoxatridec-1-yloxy) phenol	0.807	1	181.547	15.176	0.593	0	12.707	0.23	908.871	23
46	1, 2-bis [2-(2-methoxyethoxy) ethoxy] benzene	1.308	1	181.276	15.883	0.61	0	13.636	0.219	831.771	24
47	3*Z*)-4-hydroxy-6-{3-[(4*Z*)-5-hydroxy-3-oxohex-4-en-1-yl] phenyl} hex-3-en-2-one	2.086	1	188.194	16.535	0.591	0	9.086	0.206	734.819	28
48	2-({2-[(2*S*)-2-hydroxy-2-(7-oxocyclohepta-1, 3, 5-trien-1-yl) ethyl] benzyl} oxy) cyclohepta-2, 4, 6-trien-1-one	2.906	1	180.11	18.192	0.543	0	8.863	0.199	834.243	36
49	1, 1′-[1, 2-phenylenebis (methyleneoxy)] bis(2-nitrobenzene)	4.992	3	222.508	19.933	0.525	0	8.872	0.187	980.084	38
50	Dimethyl glutarate	0.779	0	55	8.69	0.614	0	6.014	0.278	126.782	11
51	2, 5, 9, 13-tetrathiatetradecane	2.952	0	91	10.485	0.897	0	14.403	0.269	274.167	11
52	(3*Z*, 12Z)-3, 13-dimethyl-5, 8, 11-trioxa-4, 12-diazapentadeca-3, 12-diene-2, 14-Dione	0.92	0	171	14.673	0.619	0	10.502	0.255	668.392	21
53	(3Z)-4-hydroxy-7-{[(5Z)-6-hydroxy-4-oxohept-5-en-1-yl] oxy} hept-3-en-2-one	0.368	0	171	14.673	0.606	0	10.62	0.23	643.918	21
54	Ethyl 4, 8, 11-trioxo-3, 6, 9, 12-tetraoxatetradecan-1-oate	0.654	0	210	16.088	0.567	0	12.263	0.239	1349.725	23

Comp No.	Compound Structure	*Clog P*	*nBnz*	*D/D*	*0χ*	*0χAv*	*nCl*	*S2k*	*3χA*	*Wms*	*P2*
55	(3Z, 15Z)-3, 16-dimethyl-5, 8, 11, 14-tetraoxa-4, 15-diazaoctadeca-3, 15-diene-2, 17-Dione	0.784	0	231	16.795	0.618	0	13.225	0.254	1085.589	24
56	4-*tert*-butyl-2-(hydroxymethyl) phenol	2.163	1	53.264	10.061	0.641	0	3.483	0.196	115.7949	19
57	4-*tert*-butyl-2-(hydroxymethyl)-6-methylphenol	2.612	1	61.75	10.931	0.661	0	3.716	0.191	131.121	21
58	Ethyl 8-hydroxyquinoline-7-carboxylate	3.149	1	59.634	11.544	0.55	0	4.393	0.183	227.617	21
59	Ethane-1, 2-diyl dimorpholine-4-carboxylate	0.51	0	140.523	14.209	0.577	0	8.414	0.209	545.2	26
60	2-(3-morpholin-4-yl-3-oxopropoxy) ethyl morpholine-4-carboxylate	0.374	0	179.024	15.623	0.583	0	9.998	0.211	934.775	29
61	2-[2-(2-phenoxyphenoxy) phenoxy] phenol	6.819	4	201.673	19.184	0.532	0	8.611	0.189	895.767	41

Table 2- Correlation Matrix of Structural descriptor for proposed model

	ClogP	*nBnz*	*D/D*	*0χ*	*0χAv*	*nCl*	*S2k*	*3χA*	*Wms*	*P2*
ClogP	1									
nBnz	0.514	1								
D/D	0.098	0.447	1							
0χ	0.326	0.549	0.932	1						
0χAv	0.316	-0.414	-0.368	-0.384	1					
nCl	0.151	-0.207	-0.033	-0.013	0.153	1				
S2k	-0.185	0.038	0.54	0.388	0.037	-0.055	1			
3χA	-0.418	-0.488	-0.24	-0.446	0.293	-0.025	0.391	1		
Wms	0.033	0.467	0.932	0.848	-0.451	-0.105	0.56	-0.182	1	
P2	0.18	0.401	0.489	0.581	-0.333	-0.024	0.007	-0.469	0.445	1

Table 3- Cross-validation parameters for the proposed models

Model	*No. of Parameters*	*PRESS*	*PSE*	*R^2cv*	*Spress*	*Q*
1	4	22.036	0.601	0.838	0.627	1.516
2	5	19.172	0.561	0.859	0.59	1.645
3	6	17.149	0.53	0.874	0.317	1.76
4	7	15.681	0.507	0.884	0.295	1.852
5	8	14.421	0.486	0.894	0.277	1.953
6	9	13.667	0.443	0.901	0.246	2.045

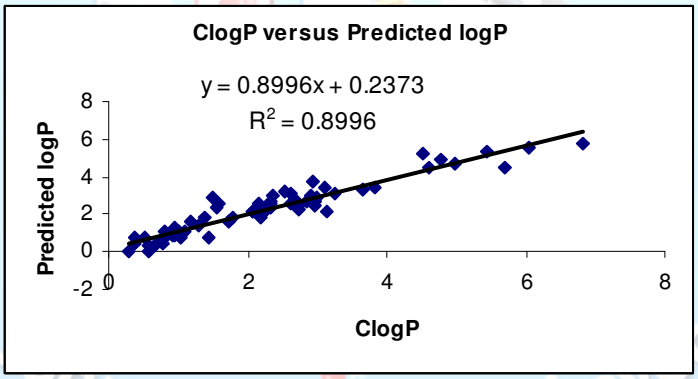

Table 4- Comparison between ClogP and Predicted logP values for Model-6

Compound No	ClogP	Predicted logP	Residuals	Compound No	ClogP	Predicted logP	Residuals
1	2.268	2.212	0.055	32	0.575	0.393	0.181
2	2.336	2.67	-0.334	33	4.605	4.448	0.156
3	1.38	1.88	-0.5	34	5.445	5.343	0.101
4	1.441	0.725	0.715	35	2.688	2.687	0.001
5	2.93	3.762	-0.832	36	2.738	2.281	0.456
6	3.266	3.078	0.187	37	1.591	2.522	-0.931
7	2.2	1.786	0.414	38	2.605	2.551	0.053
8	0.944	0.858	0.086	39	2.321	2.33	-0.009
9	1.56	2.315	-0.755	40	6.041	5.606	0.435
10	3.007	2.904	0.102	41	1.015	1.124	-0.109
11	1.741	1.602	0.138	42	0.942	1.351	-0.408
12	3.105	3.461	-0.355	43	2.077	2.116	-0.038
13	3.83	3.468	0.362	44	1.098	1.046	0.051
14	2.956	2.631	0.324	45	0.807	1.068	-0.261
15	2.329	2.527	-0.197	46	1.308	1.4	-0.091
16	3.647	3.3	0.346	47	2.086	2.138	-0.052
17	2.839	2.691	0.147	48	2.906	3.038	-0.132
18	1.794	1.83	-0.036	49	4.992	4.7	0.291
19	2.969	2.44	0.528	50	0.779	0.672	0.106
20	2.739	2.431	0.299	51	2.952	2.686	0.266
21	1.505	2.922	-1.417	52	0.92	0.917	0.002
22	2.533	3.216	-0.682	53	0.368	0.418	-0.049
23	2.665	2.741	-0.076	54	0.654	0.332	0.322
24	0.569	0.0441	0.524	55	0.784	0.476	0.307
25	2.369	3.023	-0.654	56	2.163	2.578	-0.415
26	1.047	0.792	0.255	57	2.612	3.114	-0.502
27	0.281	-0.003	0.284	58	3.149	2.132	1.017
28	1.173	1.643	-0.47	59	0.51	0.722	-0.212
29	4.785	4.939	-0.154	60	0.374	0.759	-0.384
30	4.521	5.259	-0.738	61	6.819	5.742	1.076
31	5.695	4.49	1.204				

Conclusion

From above mention result and discussion it is conclude that models which obtained by the combination of topological indices and structural descriptor have better predictivity and quality.

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