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DFT based QSAR Study of Non- Peptidic Cyclic Urea Derivatives

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Abstract

The AIDS [1,2] (Acquired Immune Deficiency Syndrome) chemotherapy now depends on the identification of the molecular events critical to virus replication, and thus depends on the detailed knowledge of the structure and the life cycle of the virus. We have confined our work on QSAR studies of non-peptidic inhibitors. In this work we have presented QSAR studies of cyclic urea derivatives which are known HIV-1-Pr inhibitor. The QSAR study has been made on 38 cyclic urea derivative cyclic urea derivatives with the setup new descriptors [3] which are illustrated below –

1. Heat of formation
2. Molecular weight
3. Chemical potential (μ) [4]
4. Electronegativity (χ) [5]
5. Absolute Hardness (η) [6,7]
6. Global Softness (S) [8]
7. HOMO [9] and LUMO [10,11] energies- εLUMO, εHOMO

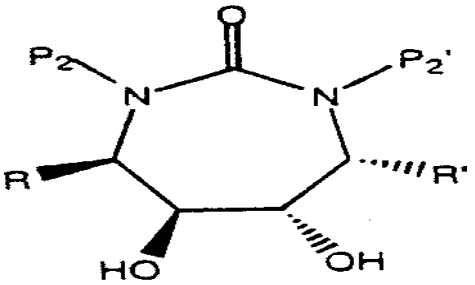
Semi-empirical calculations with the help of AM1[12], PM3[13] and PM5 was made and the QSAR models has been drawn. In recent years density functional theory has been found to provide valuable theoretical information useful for drug design and QSAR studies. DFT based calculations of the above parameters was made on the compounds under study with the help of MOPAC and Cache Software and their relationship with the known activity of the inhibitors has been studied and QSAR model has been developed. A comparison of the QSAR results obtained by AM1, PM3 and DFT has been studied. The values of the descriptors was used to prepare the regression equation and the predicted activity as obtained from the regressing equation has been compared with the known activity. The correlation coefficient and cross validation coefficient [14] has been evaluated and compared with the known activity, the quality of relationship has been found dependable, the basis of correlation coffecient and the combination of descriptors providing that relation, a new series of drugs can be predicted and put to clinical trial.

Keywords: QSAR Studies, Cyclic urea derivatives, Semi-empirical Calculations, AM1[12], PM3[13] and PM5

Introduction

Cyclic urea based PR inhibitors[15] have been extensively studied. The enzyme inhibition constant (Ki) and antiviral potency (IC90) for three different series have been reported [16,17].

The Ki data of cyclic urea derivatives against HIV protease are presented in Table-1. This Table enlist all the derivatives of cyclic ureas studied by us. The parent structure of cyclic urea is given below in fig –1.



The QSAR study of the derivatives above mentioned parent compound has been made by us and the results are presented in this chapter.

Aim of the Study

This work is confined on QSAR (Quantitative structure–activity relationship models) STUDIES OF non-peptidic inhibitors in which we presented QSAR studies of cyclic urea derivatives which are known HIV1-prinhibitor. QSAR models summarize a supposed relationship between chemical structures and biological activity in a data-set of chemicals. QSAR models are mathematical relationships linking chemical structure and pharmacological activity in a quantitative manner for a series of compounds.

The main objective of QSAR models is to allow the prediction of biological activities of untested or novel compounds to provide insight into relevant and consistent chemical properties which defines the biological activity.

The aim of this study is the comparison of correlation coefficient and cross validation coefficient has been evaluated and compared with the known activity, the quality of relationship has been found dependable. On the basis of correlation coefficient and the combination of descriptors providing that relation, a new series of drugs can be predicted and put to clinical trial.

Material and Methods

The study material of this chapter are 38 derivatives of the compound shown in fig.-1. the substituents R/R' consist of an aromatic moiety (ortho substituent), and P2/P2' substituents are either benzyl or CH2-Cy-Pr. All the derivatives are listed in table -1.

The 3D modeling and geometry optimization of all the compounds listed in Table-1, have been done with the help Cache Pro software fujitsu using PM3 hamiltonian. The MOPAC calculations have been performed with MOPAC-2000 software. All the values required for determination of the value of descriptors have been determined from this software by solving the equations given in methodology (39-42).

Results and Discussion

The 38 derivatives of cyclic urea, and their inhibition constant data (Ki) are presented in Table-1. The QSAR study of these compounds have been made with the help of following descriptors:

1. Heat of formation
2. Molecular weight
3. Total energy
4. HOMO energy
5. LUMO energy
6. Electronegativity
7. Absolute hardness

The values of above descriptors have been evaluated with the help of MOPAC calculation on Win- MOPAC 7.21 software by applying keywords change=0, Gnoum=0.1, Bonds, Geo-ok, Vector density. The results are presented in Table-2. the values of various descriptors in different combination has been used for MLR analysis. The combination that has been tried are described below:

Description of descriptors in different combinations

90 QSAR models from the above mentioned have been attempted but only 37 models have been found successful, because they have correlation coefficient value above 0.50 , The rest have lower values hence are treated as not reliable for prediction. The 37 such models are included in table -14 in decreasing order of their merit. The 90 QSAR models that have been attempted are listed below-

90 QSAR MODELS

PA1=-0.00554038*Hf+0.00742233*Mw+3.78412 rCV^2=0.93707 r^2=0.943281 PA2=-0.0059747*Hf+3.56581*TE+7.94816 rCV^2=0.706762 r^2=0.725075

PA3=-0.00556615*Hf+0.968009*HOMO+16.3289 rCV^2=0.729421 r^2=0.759689 PA4=-0.00579413*Hf-0.836653*LUMO+7.59945 rCV^2=0.725223 r^2=0.742545 PA5=-0.00573749*Hf-1.51921*En+14.4404 rCV^2=0.786119 r^2=0.827002 PA6=-0.00561634*Hf+0.00965985*Ah+7.65619 rCV^2=0.591815 r^2=0.640035 PA7=0.00811882*Mw-1.08624*TE+3.44945 rCV^2=0.294456 r^2=0.327819

PA8=0.00703409*Mw+0.232796*HOMO+6.20986 rCV^2=0.268168 r^2=0.325916

PA9=0.00778659*Mw+0.0606384*LUMO+3.72631 rCV^2=0.284166 r^2=0.321393 PA10=0.00723348*Mw-0.157783*En+4.7205 rCV^2=0.24462 r^2=0.322112 PA11=0.00762541*Mw+0.248604*Ah+4.92927 rCV^2=0.287926 r^2=0.324465 PA12=0.428211*TE+0.982619*HOMO+16.6318 rCV^2=-0.0942923 r^2=0.132744 PA13=0.232708*TE-0.641736*LUMO+7.75945 rCV^2=0.0360406 r^2=0.0661017 PA14=-1.31768*TE-1.6216*En+14.9078 rCV^2=0.0179104 r^2=0.168602 PA15=2.01785*TE+0.405585*Ah+9.76649 rCV^2=-0.104145 r^2=0.0314262 PA16=0.915378*HOMO-0.514861*LUMO+15.9796 rCV^2=0.100565 r^2=0.169408 PA17=0.400517*HOMO-1.02972*En+15.9796 rCV^2=0.100565 r^2=0.169408 PA18=1.43024*HOMO-1.02972*Ah+15.9796 rCV^2=0.100565 r^2=0.169408 PA19=0.400517*LUMO-1.83076*En+15.9796 rCV^2=0.100565 r^2=0.169408 PA20=-1.43024*LUMO+1.83076*Ah+15.9796 rCV^2=0.100565 r^2=0.169408 PA21=-1.43024*En+0.400517*Ah+15.9796 rCV^2=0.100565 r^2=0.169408

PA22=-0.00564332*Hf+0.00698063*Mw+0.982137*TE+4.10436 rCV^2=0.940345 r^2=0.948659 PA23=-0.0055351*Hf+0.00690563*Mw+0.200364*HOMO+5.85478 rCV^2=0.939407 r^2=0.946938 PA24=-0.00558242*Hf+0.00697648*Mw-0.177311*LUMO+4.0113 rCV^2=0.939898 r^2=0.946792 PA25=-0.00558463*Hf+0.00635309*Mw-0.419859*En+6.2226 rCV^2=0.942183 r^2=0.951269 PA26=-0.00554219*Hf+0.00742277*Mw-0.0137824*Ah+3.72173 rCV^2=0.935401 r^2=0.943292 PA27=0.00747206*Mw-1.24584*TE+0.27827*HOMO+6.2731 rCV^2=0.192733 r^2=0.334726 PA28=0.00803158*Mw-1.18241*TE-0.0519276*LUMO+3.48464 rCV^2=0.257904 r^2=0.32807 PA29=0.00731694*Mw-1.57198*TE-0.400524*En+5.61723 rCV^2=0.163571 r^2=0.333756 PA30=0.00805922*Mw-0.967979*TE+0.18501*Ah+4.32544 rCV^2=0.265548 r^2=0.329669

PA31=-1.11223*TE+0.976787*HOMO-0.632022*LUMO+16.4239 rCV^2=-0.0353193 r^2=0.175074 PA32=-1.11223*TE+0.344765*HOMO-1.26404*En+16.4239 rCV^2=-0.0353193 r^2=0.175074 PA33=-1.11223*TE+1.60881*HOMO-1.26404*Ah+16.4239 rCV^2=-0.0353193 r^2=0.175074 PA34=-5*HOMO+5*LUMO-12*En+16.7362 rCV^2=0.0268142 r^2=0.131782 PA35=?*HOMO+?*LUMO+?*Ah+? rCV^2=? r^2=?

PA36=3.125*LUMO-4.25*En-2.5*Ah+15.6189 rCV^2=-0.11308 r^2=0.158334

PA37=0.00714279*Mw+0.228183*HOMO+0.0386357*LUMO+6.11266 rCV^2=0.228502 r^2=0.326082

PA38=0.00714279*Mw+0.266819*HOMO+0.0772713*En+6.11266 rCV^2=0.228502 r^2=0.326082

PA39=0.00714279*Mw+0.189548*HOMO+0.0772713*Ah+6.11266 rCV^2=0.228502 r^2=0.326082
PA40=0.00714279*Mw+0.266819*LUMO-0.456367*En+6.11266 rCV^2=0.228502 r^2=0.326082

PA41=0.00714279*Mw-0.189548*LUMO+0.456367*Ah+6.11266 rCV^2=0.228502 r^2=0.326082 PA42=0.00714279*Mw-0.189548*En+0.266819*Ah+6.11266 rCV^2=0.228502 r^2=0.326082 PA43=-1.11223*TE+0.344765*LUMO-1.95357*En+16.4239 rCV^2=-0.0353193 r^2=0.175074 PA44=-1.11223*TE-1.60881*LUMO+1.95357*Ah+16.4239 rCV^2=-0.0353193 r^2=0.175074 PA45=-1.11223*TE-1.60881*En+0.344765*Ah+16.4239 rCV^2=-0.0353193 r^2=0.175074 PA46=-0.00581864*Hf+2.42303*TE+0.782714*HOMO+14.8884 rCV^2=0.761546 r^2=0.794574 PA47=-0.00595334*Hf+2.08311*TE-0.602551*LUMO+7.79915 rCV^2=0.74705 r^2=0.763543 PA48=-0.00581269*Hf+0.860702*TE-1.37991*En+13.8953 rCV^2=0.792025 r^2=0.830385 PA49=-0.0059559*Hf+3.68056*TE+0.229351*Ah+8.99333 rCV^2=0.703269 r^2=0.727936
PA50=-0.00571997*Hf+0.832269*HOMO-0.694897*LUMO+15.0957 rCV^2=0.778285 r^2=0.828055 PA51=-0.00571997*Hf+0.137372*HOMO-1.38979*En+15.0957 rCV^2=0.778285 r^2=0.828055
PA52=-0.00579848*Hf+0.963881*TE+1.37374*HOMO-1.19167*Ah+14.6985 rCV^2=0.784387 r^2=0.832186 PA53=-0.00571997*Hf+0.137372*LUMO-1.66454*En+15.0957 rCV^2=0.778285 r^2=0.828055
PA54=-0.00571997*Hf-1.52717*LUMO+1.66454*Ah+15.0957 rCV^2=0.778285 r^2=0.828055 PA55=-0.00571997*Hf-1.52717*En+0.137372*Ah+15.0957 rCV^2=0.778285 r^2=0.828055 PA56=2.375*HOMO+1.125*En-1.9375*Ah+15.3359 rCV^2=-0.103822 r^2=0.16663
PA57=-0.00562825*Hf+0.00659395*Mw+0.880438*TE+0.167681*HOMO+ 5.8041 rCV^2=0.941234 r^2=0.951163
PA58=-0.00564802*Hf+0.00680338*Mw+0.789501*TE-0.104946*LUMO+4.17601 rCV^2=0.941444 r^2=0.949682
PA59=-0.00563579*Hf+0.00631451*Mw+0.57495*TE-0.333477*En+5.90839 rCV^2=0.942721 r^2=0.952774 PA60=-0.00564009*Hf+0.00696581*Mw+1.01166*TE+0.0480466*Ah+4.33148 rCV^2=0.939101 r^2=0.948784
PA61=-0.00558164*Hf+0.00634508*Mw+0.22383*HOMO-0.198861*LUMO+6.35208 rCV^2=0.939802 r^2=0.951303
PA62=-0.00558164*Hf+0.00634508*Mw+0.0249695*HOMO-0.397721*En+6.35208 rCV^2=0.939802 r^2=0.951303
PA63=-0.00558164*Hf+0.00634508*Mw+0.422691*HOMO-0.397721*Ah+6.35208 rCV^2=0.939802 r^2=0.951303
PA64=-0.00558164*Hf+0.00634508*Mw+0.0249695*LUMO-0.44766*En+6.35208 rCV^2=0.939802 r^2=0.951303
PA65=-0.00558164*Hf+0.00634508*Mw-0.422691*LUMO+0.44766*Ah+6.35208 rCV^2=0.939802 r^2=0.951303
PA66=-0.00558164*Hf+0.00634508*Mw-0.422691*En+0.0249695*Ah+6.35208 rCV^2=0.939802 r^2=0.951303
PA67=0.00724548*Mw-1.4551*TE+0.298644*HOMO-0.106685*LUMO+6.55212 rCV^2=0.132791 r^2=0.335747
PA68=0.00724548*Mw-1.4551*TE+0.191958*HOMO-0.213371*En+6.55212 rCV^2=0.132791 r^2=0.335747
PA69=0.00724548*Mw-1.4551*TE+0.405329*HOMO-0.213371*Ah+6.55212 rCV^2=0.132791 r^2=0.335747
PA70=0.00724548*Mw-1.4551*TE+0.191958*LUMO-0.597287*En+6.55212 rCV^2=0.132791 r^2=0.335747
PA71=0.00724548*Mw-1.4551*TE-0.405329*LUMO+0.597287*Ah+6.55212 rCV^2=0.132791 r^2=0.335747
PA72=0.00724548*Mw-1.4551*TE-0.405329*En+0.191958*Ah+6.55212 rCV^2=0.132791 r^2=0.335747
PA73=-1.11223*TE-5*HOMO+5*LUMO-14*En+25.6212 rCV^2=0.00787302 r^2=-0.303633
PA74=2.5*TE-1.1259e+015*HOMO-8.44425e+014*LUMO+2.2518e+015*Ah+3.04521e+012 rCV^2=-0.00701611 r^2=-1.16747e+028
PA75=-1.11223*TE+2.375*HOMO+0.625*En-1.4375*Ah+19.7302 rCV^2=0.00810453 r^2=0.154454
PA76=2*HOMO+2.5*LUMO-1*En-7*Ah-1.27536 rCV^2=0.0890579 r^2=-0.349017
PA77=-0.00579848*Hf+0.963881*TE+0.777909*HOMO-0.595834*LUMO+14.6985 rCV^2=0.784387 r^2=0.832186
PA78=-0.00579848*Hf+0.963881*TE+0.182075*HOMO-1.19167*En+14.6985 rCV^2=0.784387 r^2=0.832186
PA79=-0.00201587*Hf-0.00350203*TE+1.64093*HOMO-1.6642*Ah-2.1452 rCV^2=-0.233293 r^2=0.242577 PA80=-0.00579848*Hf+0.963881*TE+0.182075*LUMO-1.55582*En+14.6985 rCV^2=0.784387 r^2=0.832186 PA81=-0.00579848*Hf+0.963881*TE-1.37374*LUMO+1.55582*Ah+14.6985 rCV^2=0.784387 r^2=0.832186
PA82=?*Hf+?*HOMO+?*LUMO+?*En+? rCV^2=? r^2=?
PA83=-0.00571997*Hf-0.75*HOMO-2.75*LUMO+2*Ah+9.84207 rCV^2=0.383785 r^2=0.651069
PA84=-0.00561761*Hf+7.61263 rCV^2=0.622195 r^2=0.64003 PA85=0.00763466*Mw+3.80406 rCV^2=0.306948 r^2=0.320978
PA86=1.80512*TE+7.91803 rCV^2=-0.00822257 r^2=0.0224571 PA87=1.01499*HOMO+16.882 rCV^2=0.0691337 r^2=0.131614 PA88=-0.668405*LUMO+7.73672 rCV^2=0.0626537 r^2=0.0658333 PA89=-1.40605*En+14.0657 rCV^2=0.139541 r^2=0.160405 PA90=0.276302*Ah+8.98923 rCV^2=-0.119643 r^2=0.00430722

The predicted activity obtained by the solution of above equations are presented in Table- 4,to13 . Each table contains 9 predicted values. The predicted values that have been found close to observed biological activity are only 37. They are PA1-PA6, PA22-PA26, PA50-PA66, PA77, PA78,
PA80, PA81, PA83, PA84. they are placed in Table- 14 in decreasing order of their predicted power. The predicted values are very close to the observed activity.

Conclusion

The values of cross validation coefficient and correlation coefficient are presented in Table -14. The values show that PA59, PA61-66, PA25, PA51 have the correlation coefficient value above 0.95, it means very close to observed activity. They are thus the very good QSAR models. In all these cases the first descriptor is Heat of Formation. The second common descriptor is Molecular Weight.

The next best combination provides correlation coefficient above 0.94. The QSAR models providing these values are PA58, PA60, PA22, PA23, PA24, PA26 and PA1. The most common descriptor in these cases is again Heat Of Formation.

The third best QSAR models are PA52, PA77, PA78, PA80, PA81, PA48, PA50, PA51, PA53- PA55, PA5. The coefficient value is above 0.82. The most common descriptor is again Heat of Formation.

All the above sets of QSAR models have high predictive power as they are above 0.82 . These models can be used for prediction of biological activity, that is inhibition constant (Ki) very reliably.

The last set of QSAR model has correlation

coefficient value above 0.64. They are PA46, PA47, PA3, PA4, PA49, PA2, PA83, PA6 and PA84. The correlation value of these models is good but not as reliable as in above three cases. The most common descriptor is again Heat of Formation.

Fig. -1

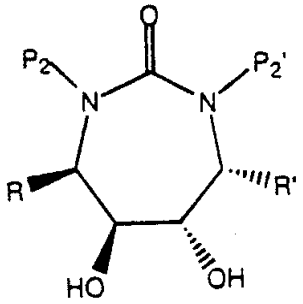


Table- 1
List of 38 Compounds along With Inhibition Constant

No.	R/R'	obsd	calcd	▼	MGVol	Ia	Io
1.	$CH_2C_6H_5$(A)[a]	8.47	8.48	-0.01	4.03	1.00	0.00
2	Me(A)	5.30	5.13	0.18	2.82	0.00	0.00
3	$CH_2C_6H_4$-4$CHMe_2$(A)	8.96	8.10	0.86	4.88	1.00	0.00
4	$CH_2C_6H_4$-3$CHMe_2$(A)	8.47	8.29	0.18	4.64	1.00	0.00
5	CH_2CHMe_2(A)	5.77	5.98	-0.21	3.66	0.00	0.00
6	CH(Me)SMe(A)	5.96	6.00	-0.04	3.71	0.00	0.00
7	CH_2-3indolyl(A)[a]	6.24	8.38	-2.14	4.49	1.00	0.00
8	CH_2-Cy-C_6H_{11}(A)[a]	7.55	6.05	1.50	4.29	0.00	0.00
9	$CH_2CH_2C_6H_5$(A)[a]	6.50	8.45	-1.95	4.31	1.00	0.00
10	CH_2-2-naphthyl(A)	8.01	8.19	-0.18	4.77	1.00	0.00
11	CH_2-3-furanyl(A)	8.08	8.38	-0.31	3.67	1.00	0.00
12	CH_2C6H_4-3-SMe(A)	8.60	8.29	0.31	4.64	1.00	0.00
13	CH_2C6H4-4-SO_2-Me-(A)	8.60	8.10	0.51	4.88	1.00	0.00
14	$CH_2C_6H_4$-2-OMe-(A)	7.22	7.25	-0.03	4.43	1.00	0.00
15	$CH_2C_6H_4$-2-OH(A)	7.46	7.32	0.13	4.15	1.00	1.00
16	$CH_2C_6H_4$-3-OMe(A)	8.33	8.41	-0.08	4.43	1.00	0.00
17	$CH_2C_6H_4$-4-OMe(A)	8.07	8.41	-0.34	4.43	1.00	0.00
18	$CH_2C_6H_4$-4-OH(A)	8.96	8.48	0.48	4.15	1.00	0.00
19	$CH_2C_6H_4$-3-NH_2(A)	8.55	8.47	0.09	4.23	1.00	0.00
20	$CH_2C_6H_4$-3-NMe_2(A)	8.37	8.17	0.20	4.80	1.00	0.00
21	$CH_2C_6H_4$-4-NH_2(A)	8.07	8.47	-0.40	4.23	1.00	0.00
22	C_6H_4-4-NH2-2Cl(A)	8.15	8.47	-0.32	4.23	1.00	0.00
23	$CH_2C_6H_4$-4-NMe_2(A)	7.34	8.17	-0.83	4.80	1.00	0.00
24	CH_2-4-pyridyl(A)	7.66	8.47	-0.82	3.95	1.00	0.00
25	3-2,5-Me-pyrolyl)-$CH_2C_6H_4$ (A)	6.80	7.21	-0.41	5.53	1.00	0.00
26	$CH_2C_6H_4$-3,4-(-OCH_2O-)(A)	8.89	8.44	0.44	4.33	1.00	0.00
27	$CH_2C_6H_5$(B)[b]	8.72	8.24	0.48	3.45	1.00	0.00
28	CH_2CHMe_2(B)[c]	7.07	5.48	1.59	3.07	0.00	0.00
29	$CHMe_2$(B)[c]	6.60	5.09	1.51	2.79	0.00	0.00
30	CH(Me)SMe(B)	5.60	5.09	1.51	2.79	0.00	0.00
31	$CH_2C_6H_4$-4-F(B)	8.24	8.27	-0.03	3.48	1.00	0.00
32	$CH_2C_6H_4$-2-OMe(B)	7.19	7.29	-0.11	3.84	1.00	1.00
33	$CH_2C_6H_4$-3-OMe(B)	9.06	8.45	0.61	3.84	1.00	0.00
34	$CH_2C_6H_4$-3-OH(B)	7.89	8.32	-0.44	3.56	1.00	0.00
35	$CH_2C_6H_4$-4-OMe(B)	8.54	8.45	0.09	3.84	1.00	0.00
36	CH_2naphthyl(B)	8.37	8.48`	-0.11	4.18	1.00	0.00
37	$CH_2C_6H_3$-3,5-OMe(B)	8.57	8.47	0.10	4.24	1.00	0.00
38	CH_2-2-thienyl(B)	8.04	8.12	-0.07	3.29	1.00	0.00

Table-2 Values of Various Descriptors Data

Comp.	Heat of Formation	Mole. Weight	Total Energy	HOMO Energy	LUMO Energy	Electr-onegat-ivity	Absolute Hardness	Activity
T1C1	-183.7	506.64	-0.007	-9.366	0.144	4.755	-4.611	8.47
T1C2	233.63	354.45	-0.133	-9.625	0.03	4.827	-4.797	5.3
T1C3	-152.5	590.8	-0.084	-9.229	0.079	4.654	-4.575	8.96
T1C4	-51.45	590.8	-0.082	-9.259	0.001	4.63	-4.629	8.47
T1C5	234.12	438.61	-0.16	-8.967	0.175	4.571	-4.396	5.77
T1C6	213.26	474.68	-0.093	-9.116	-0.189	4.463	-4.652	5.96
T1C7	124.68	438.53	-0.039	-9.514	-0.08	4.717	-4.797	6.24
T1C8	12.441	518.74	-0.179	-9.26	0.33	4.795	-4.465	7.55
T1C9	132.33	534.7	-0.052	-9.372	0.11	4.741	-4.631	6.5
T1C10	21.6	606.76	0.034	-8.687	-0.654	4.016	-4.67	8.01
T1C11	-62.75	486.57	-0.1	-9.222	0.152	4.687	-4.535	8.08
T1C12	18.651	598.82	0.03	-8.489	-0.167	4.161	-4.328	8.6
T1C13	12.27	662.81	0.02	-8.935	-1.112	3.912	-5.024	8.6
T1C14	82.112	566.7	-0.147	-9.027	-0.019	4.504	-4.523	7.22
T1C15	-6.846	538.64	-0.17	-9.068	-0.093	4.487	-4.581	7.46
T1C16	-84.05	566.7	-0.134	-9.01	0.096	4.553	-4.457	8.33
T1C17	-78.87	566.7	-0.126	-8.829	0.026	4.428	-4.402	8.07
T1C18	-197.4	538.64	-0.171	-8.943	0.002	4.473	-4.47	8.96
T1C19	-114.5	536.67	-0.023	-8.63	0.109	4.37	-4.261	8.55
T1C20	-7.246	592.78	-0.012	-7.993	0.357	4.175	-3.818	8.37
T1C21	-18.71	536.67	-0.03	-8.451	0.07	4.26	-4.19	8.07
T1C22	25.136	577.51	0.04	-8.229	-0.537	3.846	-4.383	8.15
T1C23	176.43	592.78	-0.041	-8.348	0.162	4.255	-4.093	7.34
T1C24	8.908	508.62	0.014	-9.426	-0.383	4.521	-4.905	7.66
T1C25	239.54	590.8	-0.063	-9.31	0.204	4.757	-4.553	6.8
T1C26	-122.1	594.66	-0.195	-8.78	-0.187	4.297	-4.483	8.89
T1C27	-295.8	434.58	-0.057	-9.316	-0.013	4.652	-4.664	8.72
T1C28	-121.5	366.54	-0.194	-9.276	1.009	5.142	-4.133	7.07
T1C29	-125.6	338.49	-0.2	-9.204	1.107	5.156	-4.049	6.6
T1C30	210.17	402.61	-0.16	-9.107	-0.028	4.539	-4.567	5.6
T1C31	-110.4	470.56	-0.176	-9.187	-0.287	4.45	-4.737	8.24
T1C32	102.26	494.63	-0.163	-8.985	0.049	4.517	-4.468	7.19
T1C33	-212	494.63	-0.178	-9.076	0.082	4.579	-4.497	9.06
T1C34	-123.4	466.58	-0.197	-9.107	0.021	4.564	-4.543	7.89
T1C35	-263.5	494.63	-0.165	-8.987	-0.001	4.493	-4.494	8.54
T1C36	-111.3	534.7	0.032	-8.583	-0.69	3.946	-4.637	8.37
T1C37	-178.2	554.68	-0.284	-8.927	0.158	4.542	-4.384	8.57
T1C38	-114	446.62	-0.022	-9.277	-0.443	4.417	-4.86	8.04

Table-3 Combination of Descriptors For M.L.R. Analysis

	First descriptor	Second descriptor	Third descriptor	Fourth descriptor
PA1	Heat of Formation	Molecular Weight		
PA2	Heat of Formation	Total Energy		
PA3	Heat of Formation	HOMO Energy		
PA4	Heat of Formation	LUMO Energy		
PA5	Predicted Activity	Electronegativity		
PA6	Heat of Formation	Absolute Hardness		
PA7	Molecular Weight	Total Energy		
PA8	Molecular Weight	HOMO Energy		
PA9	Molecular Weight	LUMO Energy		
PA10	Molecular Weight	Electronegativity		
PA11	Molecular Weight	Absolute Hardness		
PA12	Total Energy	HOMO Energy		
PA13	Total Energy	LUMO Energy		
PA14	Total Energy	Electronegativity		
PA15	Total Energy	Absolute Hardness		
PA16	HOMO Energy	LUMO Energy		
PA17	HOMO Energy	Electronegativity		
PA18	HOMO Energy	Absolute Hardness		
PA19	LUMO Energy	Electronegativity		
PA20	LUMO Energy	Absolute Hardness		
PA21	Electronegativity	Absolute Hardness		
PA22	Heat of Formation	Molecular Weight	Total Energy	
PA23	Heat of Formation	Molecular Weight	HOMO Energy	
PA24	Heat of Formation	Molecular Weight	LUMO Energy	
PA25	Heat of Formation	Molecular Weight	Electronegativity	
PA26	Heat of Formation	Molecular Weight	Absolute Hardness	
PA27	Molecular Weight	Total Energy	HOMO Energy	
PA28	Molecular Weight	Total Energy	LUMO Energy	
PA29	Molecular Weight	Total Energy	Electronegativity	
PA30	Molecular Weight	Total Energy	Absolute Hardness	
PA31	Total Energy	HOMO Energy	LUMO Energy	
PA32	Total Energy	HOMO Energy	Electronegativity	
PA33	Total Energy	HOMO Energy	Absolute Hardness	
PA34	HOMO Energy	LUMO Energy	Electronegativity	
PA35	HOMO Energy	LUMO Energy	Absolute Hardness	
PA36	LUMO Energy	Electronegativity	Absolute Hardness	
PA37	Molecular Weight	HOMO Energy	LUMO Energy	
PA38	Molecular Weight	HOMO Energy	Electronegativity	
PA39	Molecular Weight	HOMO Energy	Absolute Hardness	
PA40	Molecular Weight	LUMO Energy	Electronegativity	
PA41	Molecular Weight	LUMO Energy	Absolute Hardness	
PA42	Molecular Weight	Electronegativity	Absolute Hardness	
PA43	Total Energy	LUMO Energy	Electronegativity	
PA44	Total Energy	LUMO Energy	Absolute Hardness	
PA45	Total Energy	Electronegativity	Absolute Hardness	
PA46	Heat of Formation	Total Energy	HOMO Energy	
PA47	Heat of Formation	Total Energy	LUMO Energy	

PA48	Heat of Formation	Total Energy	Electronegativity	
PA49	Heat of Formation	Total Energy	Absolute Hardness	
PA50	Heat of Formation	HOMO Energy	LUMO Energy	
PA51	Heat of Formation	HOMO Energy	Electronegativity	
PA52	Heat of Formation	Total Energy	HOMO Energy	Absolute Hardness
PA53	Heat of Formation	LUMO Energy	Electronegativity	
PA54	Heat of Formation	LUMO Energy	Absolute Hardness	
PA55	Heat of Formation	Electronegativity	Absolute Hardness	
PA56	HOMO Energy	Electronegativity	Absolute Hardness	
PA57	Heat of Formation	Molecular Weight	Total Energy	HOMO Energy
PA58	Heat of Formation	Molecular Weight	Total Energy	LUMO Energy
PA59	Heat of Formation	Molecular Weight	Total Energy	Electronegativity
PA60	Heat of Formation	Molecular Weight	Total Energy	Absolute Hardness
PA61	Heat of Formation	Molecular Weight	HOMO Energy	LUMO Energy
PA62	Heat of Formation	Molecular Weight	HOMO Energy	Electronegativity
PA63	Heat of Formation	Molecular Weight	HOMO Energy	Absolute Hardness
PA64	Heat of Formation	Molecular Weight	LUMO Energy	Electronegativity
PA65	Heat of Formation	Molecular Weight	LUMO Energy	Absolute Hardness
PA66	Heat of Formation	Molecular Weight	Electronegativity	Absolute Hardness
PA67	Molecular Weight	Total Energy	HOMO Energy	LUMO Energy
PA68	Molecular Weight	Total Energy	HOMO Energy	Electronegativity
PA69	Molecular Weight	Total Energy	HOMO Energy	Absolute Hardness
PA70	Molecular Weight	Total Energy	LUMO Energy	Electronegativity
PA71	Molecular Weight	Total Energy	LUMO Energy	Absolute Hardness
PA72	Molecular Weight	Total Energy	Electronegativity	Absolute Hardness
PA73	Molecular Weight	Total Energy	LUMO Energy	Electronegativity
PA74	Molecular Weight	Total Energy	LUMO Energy	Absolute Hardness
PA75	Total Energy	HOMO Energy	Electronegativity	Absolute Hardness
PA76	HOMO Energy	LUMO Energy	Electronegativity	Absolute Hardness
PA77	Heat of Formation	Total Energy	HOMO Energy	LUMO Energy
PA78	Heat of Formation	Total Energy	HOMO Energy	Electronegativity
PA79	Heat of Formation	Total Energy	HOMO Energy	Absolute Hardness
PA80	Heat of Formation	Total Energy	LUMO Energy	Electronegativity
PA81	Heat of Formation	Total Energy	LUMO Energy	Absolute Hardness
PA82	Heat of Formation	HOMO Energy	LUMO Energy	Electronegativity
PA83	Heat of Formation	HOMO Energy	LUMO Energy	Absolute Hardness
PA84	Heat of Formation			
PA85	Molecular Weight			
PA86	Total Energy			
PA87	HOMO Energy			
PA88	LUMO Energy			
PA89	Electronegativity			
PA90	Absolute Hardness			

Table-4 Predicted Activity by Solution Of Qsar Equation

Comp.	PA1	PA2	PA3	PA4	PA5	PA6	PA7	PA8	PA9
T1C1	8.562	9.019	8.285	8.544	8.271	8.643	7.571	7.593	7.68
T1C2	5.121	6.077	5.712	6.221	5.766	6.298	6.472	6.462	6.488
T1C3	9.014	8.561	8.244	8.417	8.245	8.469	8.337	8.217	8.331
T1C4	8.454	7.963	7.652	7.897	7.701	7.9	8.335	8.21	8.327
T1C5	5.743	5.98	6.346	6.097	6.153	6.299	7.184	7.208	7.152
T1C6	6.126	6.343	6.318	6.522	6.436	6.413	7.404	7.427	7.411
T1C7	6.348	7.063	6.425	6.944	6.559	6.91	7.053	7.08	7.136
T1C8	7.565	7.235	7.296	7.251	7.084	7.543	7.856	7.703	7.786
T1C9	7.02	6.974	6.52	6.741	6.478	6.868	7.847	7.789	7.896
T1C10	8.168	7.942	7.8	8.022	8.215	7.49	8.338	8.456	8.411
T1C11	7.743	7.966	7.751	7.836	7.68	7.965	7.508	7.485	7.524
T1C12	8.125	7.943	8.008	7.631	8.012	7.51	8.279	8.446	8.379
T1C13	8.636	7.945	7.611	8.459	8.428	7.539	8.809	8.792	8.82
T1C14	7.535	6.934	7.133	7.14	7.127	7.151	8.21	8.095	8.138
T1C15	7.82	7.382	7.589	7.717	7.663	7.65	8.008	7.888	7.915
T1C16	8.456	7.973	8.074	8.006	8.005	8.085	8.196	8.098	8.145
T1C17	8.427	7.971	8.221	8.035	8.166	8.057	8.187	8.141	8.141
T1C18	8.876	8.517	8.771	8.741	8.778	8.722	8.009	7.917	7.921
T1C19	8.402	8.55	8.612	8.171	8.459	8.258	7.832	7.976	7.912
T1C20	8.224	7.95	8.632	7.343	8.14	7.66	8.275	8.519	8.364
T1C21	7.871	7.954	8.253	7.649	8.076	7.721	7.839	8.018	7.909
T1C22	7.931	7.941	8.223	7.903	8.453	7.473	8.095	8.356	8.191
T1C23	7.206	6.749	7.266	6.441	6.964	6.626	8.306	8.436	8.352
T1C24	7.51	7.946	7.155	7.869	7.521	7.559	7.563	7.593	7.663
T1C25	6.842	6.292	5.983	6.041	5.839	6.267	8.315	8.198	8.339
T1C26	8.874	7.984	8.509	8.463	8.613	8.299	8.489	8.349	8.345
T1C27	8.649	9.512	8.958	9.324	9.071	9.273	7.04	7.098	7.109
T1C28	7.178	7.984	8.026	7.459	7.325	8.299	6.636	6.629	6.642
T1C29	6.992	7.985	8.118	7.401	7.328	8.322	6.415	6.448	6.429
T1C30	5.608	6.123	6.344	6.405	6.338	6.432	6.892	6.922	6.86
T1C31	7.888	7.98	8.05	8.479	8.314	8.23	7.461	7.381	7.373
T1C32	6.889	6.756	7.062	6.966	6.992	7.039	7.642	7.598	7.581
T1C33	8.63	8.578	8.723	8.759	8.7	8.803	7.659	7.576	7.583
T1C34	7.931	7.984	8.2	8.297	8.214	8.306	7.451	7.372	7.361
T1C35	8.915	8.934	9.096	9.127	9.126	9.093	7.644	7.597	7.578
T1C36	8.37	8.729	8.64	8.822	9.084	8.237	7.755	7.973	7.848
T1C37	8.888	8	8.68	8.5	8.562	8.615	8.261	8.033	8.055
T1C38	7.731	8.55	7.984	8.631	8.384	8.249	7.1	7.192	7.177

Table-5. Predicted Activity By Solution Of Qsar Equation

Comp.	PA10	PA11	PA12	PA13	PA14	PA15	PA16	PA17	PA18
T1C1	7.635	7.646	7.425	7.666	7.207	7.881	7.332	7.332	7.332
T1C2	6.523	6.439	7.117	7.709	7.255	7.552	7.154	7.154	7.154
T1C3	8.26	8.297	7.527	7.689	7.471	7.742	7.491	7.491	7.491
T1C4	8.263	8.284	7.498	7.74	7.507	7.724	7.503	7.503	7.503
T1C5	7.172	7.181	7.752	7.61	7.706	7.662	7.681	7.681	7.681
T1C6	7.45	7.392	7.635	7.859	7.793	7.692	7.733	7.733	7.733
T1C7	7.148	7.081	7.266	7.801	7.31	7.742	7.312	7.312	7.312
T1C8	7.716	7.775	7.456	7.506	7.368	7.594	7.333	7.333	7.333
T1C9	7.84	7.855	7.4	7.677	7.288	7.784	7.344	7.344	7.344
T1C10	8.476	8.395	8.111	8.187	8.35	7.942	8.365	8.365	8.365

T1C11	7.501	7.512	7.527	7.639	7.439	7.725	7.459	7.459	7.459
T1C12	8.395	8.42	8.303	7.873	8.121	8.071	8.295	8.295	8.295
T1C13	8.898	8.735	7.86	8.478	8.539	7.768	8.373	8.373	8.373
T1C14	8.109	8.126	7.699	7.738	7.798	7.636	7.726	7.726	7.726
T1C15	7.909	7.898	7.649	7.78	7.856	7.565	7.727	7.727	7.727
T1C16	8.101	8.142	7.721	7.667	7.701	7.688	7.682	7.682	7.682
T1C17	8.121	8.156	7.902	7.714	7.893	7.728	7.884	7.884	7.884
T1C18	7.911	7.925	7.771	7.718	7.881	7.608	7.792	7.792	7.792
T1C19	7.913	7.962	8.142	7.684	7.852	7.992	8.023	8.023	8.023
T1C20	8.35	8.5	8.773	7.528	8.153	8.195	8.48	8.48	8.48
T1C21	7.93	7.98	8.315	7.708	8.039	8.007	8.208	8.208	8.208
T1C22	8.291	8.243	8.563	8.113	8.618	8.07	8.723	8.723	8.723
T1C23	8.337	8.432	8.412	7.646	8.061	8.025	8.254	8.254	8.254
T1C24	7.686	7.588	7.376	8.009	7.558	7.806	7.549	7.549	7.549
T1C25	8.244	8.302	7.457	7.614	7.277	7.793	7.352	7.352	7.352
T1C26	8.344	8.349	7.921	7.834	8.197	7.555	8.039	8.039	8.039
T1C27	7.13	7.084	7.454	7.754	7.44	7.76	7.459	7.459	7.459
T1C28	6.56	6.697	7.434	7.067	6.824	7.699	6.969	6.969	6.969
T1C29	6.355	6.504	7.502	7.002	6.811	7.721	6.984	6.984	6.984
T1C30	6.917	6.864	7.615	7.74	7.757	7.592	7.658	7.658	7.658
T1C31	7.422	7.34	7.53	7.903	7.924	7.49	7.718	7.718	7.718
T1C32	7.586	7.59	7.733	7.69	7.798	7.625	7.73	7.73	7.73
T1C33	7.576	7.583	7.638	7.665	7.718	7.583	7.63	7.63	7.63
T1C34	7.375	7.358	7.599	7.7	7.765	7.527	7.632	7.632	7.632
T1C35	7.589	7.584	7.73	7.722	7.839	7.611	7.753	7.753	7.753
T1C36	7.966	7.854	8.212	8.21	8.465	7.951	8.478	8.478	8.478
T1C37	8.016	8.069	7.739	7.592	7.917	7.415	7.727	7.727	7.727
T1C38	7.254	7.127	7.507	8.039	7.775	7.75	7.716	7.716	7.716

Table-6. Predicted Activity By Solution Of Qsar Equation

Comp.	PA19	PA20	PA21	PA22	PA23	PA24	PA25	PA26	PA27
T1C1	7.332	7.332	7.332	8.67	8.494	8.546	8.471	8.564	7.462
T1C2	7.154	7.154	7.154	5.129	5.081	5.175	5.143	5.124	6.409
T1C3	7.491	7.491	7.491	9.007	8.93	8.971	8.874	9.016	8.224
T1C4	7.503	7.503	7.503	8.438	8.364	8.42	8.319	8.456	8.213
T1C5	7.681	7.681	7.681	5.688	5.791	5.733	5.783	5.74	7.254
T1C6	7.733	7.733	7.733	6.123	6.126	6.166	6.173	6.127	7.399
T1C7	7.312	7.312	7.312	6.423	6.287	6.389	6.332	6.352	6.951
T1C8	7.333	7.333	7.333	7.479	7.513	7.502	7.436	7.565	7.796
T1C9	7.344	7.344	7.344	7.04	6.937	6.983	6.89	7.021	7.725
T1C10	8.365	8.365	8.365	8.252	8.185	8.24	8.271	8.17	8.347
T1C11	7.459	7.459	7.459	7.757	7.714	7.729	7.696	7.744	7.467
T1C12	8.295	8.295	8.295	8.208	8.186	8.114	8.176	8.123	8.348
T1C13	8.373	8.373	8.373	8.681	8.574	8.764	8.723	8.643	8.715
T1C14	7.726	7.726	7.726	7.453	7.505	7.51	7.473	7.535	8.178
T1C15	7.727	7.727	7.727	7.736	7.795	7.824	7.799	7.821	7.987
T1C16	7.682	7.682	7.682	8.403	8.428	8.417	8.381	8.455	8.167
T1C17	7.884	7.884	7.884	8.382	8.436	8.4	8.404	8.426	8.207
T1C18	7.792	7.792	7.792	8.81	8.875	8.871	8.869	8.876	8.023

T1C19	8.023	8.023	8.023	8.474	8.465	8.375	8.437	8.398	7.91
T1C20	8.48	8.48	8.48	8.272	8.387	8.124	8.276	8.215	8.493
T1C21	8.208	8.208	8.208	7.927	7.971	7.847	7.948	7.867	7.969
T1C22	8.723	8.723	8.723	8.033	8.055	7.995	8.136	7.93	8.248
T1C23	8.254	8.254	8.254	7.207	7.299	7.133	7.217	7.2	8.43
T1C24	7.549	7.549	7.549	7.619	7.429	7.578	7.506	7.515	7.433
T1C25	7.352	7.352	7.352	6.815	6.743	6.76	6.641	6.842	8.175
T1C26	8.039	8.039	8.039	8.753	8.878	8.875	8.879	8.874	8.516
T1C27	7.459	7.459	7.459	8.751	8.627	8.697	8.683	8.651	6.999
T1C28	6.969	6.969	6.969	7.159	7.2	7.068	7.071	7.173	6.672
T1C29	6.984	6.984	6.984	6.979	7.043	6.878	6.91	6.986	6.49
T1C30	7.658	7.658	7.658	5.572	5.647	5.652	5.701	5.608	6.946
T1C31	7.718	7.718	7.718	7.839	7.875	7.961	7.96	7.892	7.452
T1C32	7.73	7.73	7.73	6.82	6.904	6.883	6.898	6.888	7.672
T1C33	7.63	7.63	7.63	8.578	8.625	8.631	8.626	8.63	7.666
T1C34	7.632	7.632	7.632	7.865	7.935	7.952	7.96	7.932	7.47
T1C35	7.753	7.753	7.753	8.882	8.928	8.933	8.95	8.915	7.674
T1C36	8.478	8.478	8.478	8.497	8.444	8.486	8.584	8.372	7.84
T1C37	7.727	7.727	7.727	8.703	8.883	8.848	8.835	8.887	8.288
T1C38	7.716	7.716	7.716	7.843	7.711	7.842	7.842	7.736	7.057

Table-7. Predicted Activity By Solution Of QSAR Equation

Comp.	PA28	PA29	PA30	PA31	PA32	PA33	PA34	PA35	PA36
T1C1	7.555	7.432	7.563	7.193	7.193	7.193	7.227	Failed	7.388
T1C2	6.487	6.487	6.423	7.152	7.152	7.152	7.081	Failed	7.19
T1C3	8.325	8.208	8.321	7.452	7.452	7.452	7.428	Failed	7.524
T1C4	8.327	8.214	8.31	7.47	7.47	7.47	7.476	Failed	7.517
T1C5	7.187	7.247	7.201	7.732	7.732	7.732	7.594	Failed	7.729
T1C6	7.417	7.449	7.38	7.743	7.743	7.743	7.81	Failed	7.69
T1C7	7.057	6.998	7.01	7.225	7.225	7.225	7.302	Failed	7.314
T1C8	7.846	7.774	7.853	7.37	7.37	7.37	7.146	Failed	7.434
T1C9	7.834	7.712	7.828	7.257	7.257	7.257	7.254	Failed	7.391
T1C10	8.351	8.394	8.318	8.314	8.314	8.314	8.704	Failed	8.182
T1C11	7.503	7.457	7.505	7.431	7.431	7.431	7.362	Failed	7.511
T1C12	8.268	8.285	8.322	8.204	8.204	8.204	8.414	Failed	8.233
T1C13	8.843	8.87	8.719	8.377	8.377	8.377	8.913	Failed	8.079
T1C14	8.211	8.191	8.198	7.782	7.782	7.782	7.728	Failed	7.725
T1C15	8.017	8.029	7.984	7.815	7.815	7.815	7.762	Failed	7.708
T1C16	8.189	8.151	8.198	7.711	7.711	7.711	7.63	Failed	7.711
T1C17	8.183	8.188	8.2	7.923	7.923	7.923	7.881	Failed	7.887
T1C18	8.013	8.036	8.005	7.878	7.878	7.878	7.791	Failed	7.793

T1C19	7.817	7.83	7.885	7.951	7.951	7.951	7.997	Failed	8.04
T1C20	8.241	8.301	8.408	8.404	8.404	8.404	8.387	Failed	8.536
T1C21	7.827	7.885	7.904	8.159	8.159	8.159	8.216	Failed	8.207
T1C22	8.103	8.239	8.13	8.68	8.68	8.68	9.044	Failed	8.552
T1C23	8.285	8.314	8.385	8.212	8.212	8.212	8.226	Failed	8.274
T1C24	7.573	7.506	7.503	7.444	7.444	7.444	7.694	Failed	7.467
T1C25	8.294	8.134	8.305	7.271	7.271	7.271	7.222	Failed	7.422
T1C26	8.501	8.553	8.477	8.182	8.182	8.182	8.143	Failed	7.983
T1C27	7.043	7.024	7.02	7.396	7.396	7.396	7.433	Failed	7.471
T1C28	6.605	6.544	6.702	6.941	6.941	6.941	6.451	Failed	7.25
T1C29	6.382	6.344	6.498	6.956	6.956	6.956	6.425	Failed	7.288
T1C30	6.908	6.996	6.88	7.724	7.724	7.724	7.657	Failed	7.658
T1C31	7.487	7.555	7.412	7.828	7.828	7.828	7.837	Failed	7.652
T1C32	7.647	7.684	7.643	7.798	7.798	7.798	7.703	Failed	7.745
T1C33	7.664	7.683	7.653	7.706	7.706	7.706	7.579	Failed	7.657
T1C34	7.463	7.512	7.436	7.733	7.733	7.733	7.608	Failed	7.645
T1C35	7.652	7.696	7.64	7.829	7.829	7.829	7.75	Failed	7.755
T1C36	7.777	7.898	7.745	8.44	8.44	8.44	8.843	Failed	8.281
T1C37	8.267	8.303	8.259	7.921	7.921	7.921	7.652	Failed	7.769
T1C38	7.121	7.151	7.047	7.668	7.668	7.668	7.903	Failed	7.613

Table-8. Predicted Activity By Solution Of Qsar Equation

Comp.	PA37	PA38	PA39	PA40	PA41	PA42	PA43	PA44	PA45
T1C1	7.6	7.6	7.6	7.6	7.6	7.6	7.193	7.193	7.193
T1C2	6.449	6.449	6.449	6.449	6.449	6.449	7.152	7.152	7.152
T1C3	8.23	8.23	8.23	8.23	8.23	8.23	7.452	7.452	7.452
T1C4	8.22	8.22	8.22	8.22	8.22	8.22	7.47	7.47	7.47
T1C5	7.206	7.206	7.206	7.206	7.206	7.206	7.732	7.732	7.732
T1C6	7.416	7.416	7.416	7.416	7.416	7.416	7.743	7.743	7.743
T1C7	7.071	7.071	7.071	7.071	7.071	7.071	7.225	7.225	7.225
T1C8	7.718	7.718	7.718	7.718	7.718	7.718	7.37	7.37	7.37
T1C9	7.798	7.798	7.798	7.798	7.798	7.798	7.257	7.257	7.257
T1C10	8.439	8.439	8.439	8.439	8.439	8.439	8.314	8.314	8.314
T1C11	7.49	7.49	7.49	7.49	7.49	7.49	7.431	7.431	7.431
T1C12	8.446	8.446	8.446	8.446	8.446	8.446	8.204	8.204	8.204
T1C13	8.765	8.765	8.765	8.765	8.765	8.765	8.377	8.377	8.377
T1C14	8.1	8.1	8.1	8.1	8.1	8.1	7.782	7.782	7.782
T1C15	7.887	7.887	7.887	7.887	7.887	7.887	7.815	7.815	7.815
T1C16	8.108	8.108	8.108	8.108	8.108	8.108	7.711	7.711	7.711
T1C17	8.147	8.147	8.147	8.147	8.147	8.147	7.923	7.923	7.923
T1C18	7.92	7.92	7.92	7.92	7.92	7.92	7.878	7.878	7.878

T1C19	7.981	7.981	7.981	7.981	7.981	7.981	7.951	7.951	7.951
T1C20	8.537	8.537	8.537	8.537	8.537	8.537	8.404	8.404	8.404
T1C21	8.02	8.02	8.02	8.02	8.02	8.02	8.159	8.159	8.159
T1C22	8.339	8.339	8.339	8.339	8.339	8.339	8.68	8.68	8.68
T1C23	8.448	8.448	8.448	8.448	8.448	8.448	8.212	8.212	8.212
T1C24	7.58	7.58	7.58	7.58	7.58	7.58	7.444	7.444	7.444
T1C25	8.216	8.216	8.216	8.216	8.216	8.216	7.271	7.271	7.271
T1C26	8.35	8.35	8.35	8.35	8.35	8.35	8.182	8.182	8.182
T1C27	7.091	7.091	7.091	7.091	7.091	7.091	7.396	7.396	7.396
T1C28	6.653	6.653	6.653	6.653	6.653	6.653	6.941	6.941	6.941
T1C29	6.473	6.473	6.473	6.473	6.473	6.473	6.956	6.956	6.956
T1C30	6.909	6.909	6.909	6.909	6.909	6.909	7.724	7.724	7.724
T1C31	7.366	7.366	7.366	7.366	7.366	7.366	7.828	7.828	7.828
T1C32	7.597	7.597	7.597	7.597	7.597	7.597	7.798	7.798	7.798
T1C33	7.578	7.578	7.578	7.578	7.578	7.578	7.706	7.706	7.706
T1C34	7.368	7.368	7.368	7.368	7.368	7.368	7.733	7.733	7.733
T1C35	7.595	7.595	7.595	7.595	7.595	7.595	7.829	7.829	7.829
T1C36	7.947	7.947	7.947	7.947	7.947	7.947	8.44	8.44	8.44
T1C37	8.044	8.044	8.044	8.044	8.044	8.044	7.921	7.921	7.921
T1C38	7.169	7.169	7.169	7.169	7.169	7.169	7.668	7.668	7.668

Table-9. Predicted Activity by Solution of QSAR Equation

Comp.	PA46	PA47	PA48	PA49	PA50	PA51	PA52	PA53	PA54
T1C1	8.608	8.791	8.395	9.002	8.252	8.252	8.385	8.252	8.252
T1C2	5.673	6.112	5.761	6.011	5.728	5.728	5.71	5.728	5.728
T1C3	8.349	8.485	8.288	8.544	8.232	8.232	8.276	8.232	8.232
T1C4	7.742	7.934	7.734	7.936	7.683	7.683	7.714	7.683	7.683
T1C5	6.121	5.968	6.09	6.003	6.172	6.172	6.108	6.172	6.172
T1C6	6.288	6.45	6.417	6.314	6.421	6.421	6.394	6.421	6.421
T1C7	6.621	7.023	6.627	7.006	6.52	6.52	6.584	6.52	6.52
T1C8	7.134	7.153	7.052	7.236	7.088	7.088	7.054	7.088	7.088
T1C9	6.658	6.838	6.54	6.953	6.462	6.462	6.525	6.462	6.462
T1C10	8.047	8.136	8.257	7.92	8.197	8.197	8.239	8.197	8.197
T1C11	7.793	7.873	7.706	7.959	7.674	7.674	7.701	7.674	7.674
T1C12	8.207	7.85	8.07	7.999	8.04	8.04	8.115	8.04	8.04
T1C13	7.871	8.437	8.443	7.84	8.362	8.362	8.358	8.362	8.362
T1C14	6.989	7.016	7.077	6.927	7.126	7.126	7.07	7.126	7.126
T1C15	7.418	7.542	7.597	7.357	7.653	7.653	7.576	7.653	7.653
T1C16	8	7.963	7.985	7.979	8.011	8.011	7.99	8.011	8.011
T1C17	8.132	7.991	8.136	7.991	8.18	8.18	8.151	8.18	8.18
T1C18	8.623	8.616	8.724	8.514	8.78	8.78	8.72	8.78	8.78

T1C19	8.744	8.367	8.511	8.613	8.492	8.492	8.561	8.492	8.492
T1C20	8.647	7.603	8.167	8.118	8.237	8.237	8.299	8.237	8.237
T1C21	8.311	7.806	8.1	8.034	8.121	8.121	8.163	8.121	8.121
T1C22	8.398	8.056	8.476	7.986	8.476	8.476	8.509	8.476	8.476
T1C23	7.23	6.567	6.963	6.855	7.026	7.026	7.046	7.026	7.026
T1C24	7.493	8.007	7.617	7.868	7.466	7.466	7.557	7.466	7.466
T1C25	6.055	6.119	5.885	6.29	5.836	5.836	5.885	5.836	5.836
T1C26	8.255	8.233	8.509	7.976	8.617	8.617	8.5	8.617	8.617
T1C27	9.18	9.449	9.147	9.475	9.043	9.043	9.119	9.043	9.043
T1C28	7.866	7.511	7.339	8.056	7.37	7.37	7.4	7.37	7.37
T1C29	7.93	7.463	7.339	8.076	7.384	7.384	7.414	7.384	7.384
T1C30	6.151	6.232	6.272	6.107	6.334	6.334	6.258	6.334	6.334
T1C31	7.914	8.263	8.245	7.917	8.281	8.281	8.194	8.281	8.281
T1C32	6.866	6.822	6.928	6.76	6.999	6.999	6.93	6.999	6.999
T1C33	8.586	8.64	8.655	8.568	8.698	8.698	8.647	8.698	8.698
T1C34	8.002	8.111	8.145	7.963	8.207	8.207	8.127	8.207	8.207
T1C35	8.987	9.025	9.085	8.925	9.123	9.123	9.076	9.123	9.123
T1C36	8.896	8.946	9.125	8.712	9.069	9.069	9.11	9.069	9.069
T1C37	8.25	8.173	8.419	8.004	8.576	8.576	8.42	8.576	8.576
T1C38	8.237	8.698	8.444	8.476	8.335	8.335	8.386	8.335	8.335

Table-10. Predicted Activity By Solution Of Qsar Equation

Comp.	PA55	PA56	PA57	PA58	PA59	PA60	PA61	PA62	PA63
T1C1	8.252	7.375	8.602	8.639	8.553	8.667	8.467	8.467	8.467
T1C2	5.728	7.203	5.095	5.16	5.143	5.117	5.137	5.137	5.137
T1C3	8.232	7.517	8.937	8.983	8.899	9.003	8.871	8.871	8.871
T1C4	7.683	7.523	8.365	8.421	8.338	8.432	8.315	8.315	8.315
T1C5	6.172	7.699	5.735	5.693	5.743	5.694	5.787	5.787	5.787
T1C6	6.421	7.721	6.124	6.147	6.162	6.118	6.171	6.171	6.171
T1C7	6.52	7.341	6.364	6.433	6.379	6.413	6.325	6.325	6.325
T1C8	7.088	7.389	7.444	7.459	7.412	7.479	7.436	7.436	7.436
T1C9	6.462	7.383	6.968	7.014	6.928	7.035	6.887	6.887	6.887
T1C10	8.197	8.272	8.257	8.278	8.299	8.247	8.267	8.267	8.267
T1C11	7.674	7.493	7.731	7.746	7.714	7.756	7.695	7.695	7.695
T1C12	8.04	8.241	8.25	8.186	8.214	8.22	8.181	8.181	8.181
T1C13	8.362	8.249	8.625	8.748	8.731	8.658	8.71	8.71	8.71
T1C14	7.126	7.727	7.436	7.454	7.438	7.45	7.473	7.473	7.473
T1C15	7.653	7.723	7.724	7.755	7.754	7.73	7.797	7.797	7.797
T1C16	8.011	7.694	8.385	8.39	8.365	8.403	8.381	8.381	8.381
T1C17	8.18	7.876	8.394	8.375	8.382	8.385	8.407	8.407	8.407
T1C18	8.78	7.789	8.817	8.82	8.832	8.809	8.869	8.869	8.869

T1C19	8.492	8.01	8.52	8.444	8.472	8.487	8.443	8.443	8.443
T1C20	8.237	8.447	8.403	8.203	8.294	8.306	8.294	8.294	8.294
T1C21	8.121	8.177	8.005	7.902	7.965	7.944	7.956	7.956	7.956
T1C22	8.476	8.61	8.126	8.051	8.154	8.042	8.141	8.141	8.141
T1C23	7.026	8.226	7.284	7.163	7.215	7.228	7.228	7.228	7.228
T1C24	7.466	7.539	7.54	7.637	7.57	7.603	7.496	7.496	7.496
T1C25	5.836	7.398	6.735	6.771	6.666	6.813	6.639	6.639	6.639
T1C26	8.617	8.004	8.769	8.777	8.807	8.75	8.879	8.879	8.879
T1C27	9.043	7.481	8.722	8.76	8.736	8.745	8.678	8.678	8.678
T1C28	7.37	7.1	7.179	7.097	7.082	7.176	7.079	7.079	7.079
T1C29	7.384	7.12	7.023	6.914	6.919	7.001	6.92	6.92	6.92
T1C30	6.334	7.663	5.608	5.605	5.661	5.57	5.701	5.701	5.701
T1C31	8.281	7.701	7.833	7.892	7.917	7.826	7.955	7.955	7.955
T1C32	6.999	7.735	6.84	6.83	6.856	6.821	6.899	6.899	6.899
T1C33	8.698	7.645	8.58	8.589	8.597	8.576	8.626	8.626	8.626
T1C34	8.207	7.643	7.875	7.89	7.915	7.86	7.959	7.959	7.959
T1C35	9.123	7.753	8.896	8.899	8.923	8.88	8.95	8.95	8.95
T1C36	9.069	8.374	8.546	8.541	8.615	8.494	8.582	8.582	8.582
T1C37	8.576	7.74	8.718	8.715	8.737	8.702	8.837	8.837	8.837
T1C38	8.335	7.689	7.816	7.887	7.885	7.829	7.834	7.834	7.834

Table-11. Predicted Activity By Solution Of Qsar Equation

Comp.	PA64	PA65	PA66	PA67	PA68	PA69	PA70	PA71	PA72
T1C1	8.467	8.467	8.467	7.421	7.421	7.421	7.421	7.421	7.421
T1C2	5.137	5.137	5.137	6.437	6.437	6.437	6.437	6.437	6.437
T1C3	8.871	8.871	8.871	8.19	8.19	8.19	8.19	8.19	8.19
T1C4	8.315	8.315	8.315	8.187	8.187	8.187	8.187	8.187	8.187
T1C5	5.787	5.787	5.787	7.266	7.266	7.266	7.266	7.266	7.266
T1C6	6.171	6.171	6.171	7.424	7.424	7.424	7.424	7.424	7.424
T1C7	6.325	6.325	6.325	6.954	6.954	6.954	6.954	6.954	6.954
T1C8	7.436	7.436	7.436	7.771	7.771	7.771	7.771	7.771	7.771
T1C9	6.887	6.887	6.887	7.691	7.691	7.691	7.691	7.691	7.691
T1C10	8.267	8.267	8.267	8.374	8.374	8.374	8.374	8.374	8.374
T1C11	7.695	7.695	7.695	7.453	7.453	7.453	7.453	7.453	7.453
T1C12	8.181	8.181	8.181	8.33	8.33	8.33	8.33	8.33	8.33
T1C13	8.71	8.71	8.71	8.776	8.776	8.776	8.776	8.776	8.776
T1C14	7.473	7.473	7.473	8.178	8.178	8.178	8.178	8.178	8.178
T1C15	7.797	7.797	7.797	8.005	8.005	8.005	8.005	8.005	8.005
T1C16	8.381	8.381	8.381	8.152	8.152	8.152	8.152	8.152	8.152
T1C17	8.407	8.407	8.407	8.201	8.201	8.201	8.201	8.201	8.201
T1C18	8.869	8.869	8.869	8.033	8.033	8.033	8.033	8.033	8.033

T1C19	8.443	8.443	8.443	7.885	7.885	7.885	7.885	7.885	7.885
T1C20	8.294	8.294	8.294	8.439	8.439	8.439	8.439	8.439	8.439
T1C21	7.956	7.956	7.956	7.953	7.953	7.953	7.953	7.953	7.953
T1C22	8.141	8.141	8.141	8.278	8.278	8.278	8.278	8.278	8.278
T1C23	7.228	7.228	7.228	8.396	8.396	8.396	8.396	8.396	8.396
T1C24	7.496	7.496	7.496	7.443	7.443	7.443	7.443	7.443	7.443
T1C25	6.639	6.639	6.639	8.122	8.122	8.122	8.122	8.122	8.122
T1C26	8.879	8.879	8.879	8.542	8.542	8.542	8.542	8.542	8.542
T1C27	8.678	8.678	8.678	7.003	7.003	7.003	7.003	7.003	7.003
T1C28	7.079	7.079	7.079	6.612	6.612	6.612	6.612	6.612	6.612
T1C29	6.92	6.92	6.92	6.429	6.429	6.429	6.429	6.429	6.429
T1C30	5.701	5.701	5.701	6.985	6.985	6.985	6.985	6.985	6.985
T1C31	7.955	7.955	7.955	7.505	7.505	7.505	7.505	7.505	7.505
T1C32	6.899	6.899	6.899	7.685	7.685	7.685	7.685	7.685	7.685
T1C33	8.626	8.626	8.626	7.676	7.676	7.676	7.676	7.676	7.676
T1C34	7.959	7.959	7.959	7.497	7.497	7.497	7.497	7.497	7.497
T1C35	8.95	8.95	8.95	7.692	7.692	7.692	7.692	7.692	7.692
T1C36	8.582	8.582	8.582	7.889	7.889	7.889	7.889	7.889	7.889
T1C37	8.837	8.837	8.837	8.302	8.302	8.302	8.302	8.302	8.302
T1C38	7.834	7.834	7.834	7.097	7.097	7.097	7.097	7.097	7.097

Table-12. Predicted Activity by Solution of QSAR Equation

Comp.	PA73	PA74	PA75	PA76	PA77	PA78	PA79	PA80	PA81
T1C1	6.61	4E+13	7.095	7.875	8.385	8.385	8.385	8.385	8.385
T1C2	6.459	1E+13	6.933	8.304	5.71	5.71	5.71	5.71	5.71
T1C3	7.098	3E+13	7.39	7.835	8.276	8.276	8.276	8.276	8.276
T1C4	7.191	3E+12	7.379	7.982	7.714	7.714	7.714	7.714	7.714
T1C5	7.515	5E+13	7.787	7.43	6.108	6.108	6.108	6.108	6.108
T1C6	7.872	-5E+13	7.661	8.124	6.394	6.394	6.394	6.394	6.394
T1C7	6.796	-2E+13	7.022	8.358	6.584	6.584	6.584	6.584	6.584
T1C8	6.641	1E+14	7.352	7.49	7.054	7.054	7.054	7.054	7.054
T1C9	6.714	3E+13	7.149	7.932	6.525	6.525	6.525	6.525	6.525
T1C10	9.518	-2E+14	8.285	8.393	8.239	8.239	8.239	8.239	8.239
T1C11	6.984	5E+13	7.387	7.719	7.701	7.701	7.701	7.701	7.701
T1C12	8.943	-4E+13	8.358	7.464	8.115	8.115	8.115	8.115	8.115
T1C13	9.953	-3E+14	8.154	9.328	8.358	8.358	8.358	8.358	8.358
T1C14	7.769	-2E+12	7.771	7.781	7.07	7.07	7.07	7.07	7.07
T1C15	7.862	-2E+13	7.773	7.933	7.576	7.576	7.576	7.576	7.576
T1C16	7.557	3E+13	7.732	7.591	7.99	7.99	7.99	7.99	7.99
T1C17	8.05	1E+13	7.995	7.515	8.151	8.151	8.151	8.151	8.151
T1C18	7.921	4E+12	7.903	7.664	8.72	8.72	8.72	8.72	8.72

T1C19	8.168	3E+13	8.115	7.191	8.561	8.561	8.561	8.561	8.561
T1C20	8.936	1E+14	8.858	6.182	8.299	8.299	8.299	8.299	8.299
T1C21	8.614	2E+13	8.38	7.071	8.163	8.163	8.163	8.163	8.163
T1C22	10.191	-1E+14	8.845	7.759	8.509	8.509	8.509	8.509	8.509
T1C23	8.646	5E+13	8.492	6.829	7.046	7.046	7.046	7.046	7.046
T1C24	7.521	-1E+14	7.204	8.725	7.557	7.557	7.557	7.557	7.557
T1C25	6.664	6E+13	7.207	7.729	5.885	5.885	5.885	5.885	5.885
T1C26	8.651	-5E+13	8.224	7.785	8.5	8.5	8.5	8.5	8.5
T1C27	7.078	-5E+11	7.281	8.059	9.119	9.119	9.119	9.119	9.119
T1C28	5.267	3E+14	7.071	6.486	7.4	7.4	7.4	7.4	7.4
T1C29	5.221	3E+14	7.135	6.268	7.414	7.414	7.414	7.414	7.414
T1C30	7.641	-5E+12	7.682	7.873	6.258	6.258	6.258	6.258	6.258
T1C31	8.018	-8E+13	7.698	8.342	8.194	8.194	8.194	8.194	8.194
T1C32	7.736	2E+13	7.818	7.637	6.93	6.93	6.93	6.93	6.93
T1C33	7.504	3E+13	7.7	7.677	8.647	8.647	8.647	8.647	8.647
T1C34	7.583	9E+12	7.702	7.8	8.127	8.127	8.127	8.127	8.127
T1C35	7.831	3E+12	7.837	7.713	9.076	9.076	9.076	9.076	9.076
T1C36	9.799	-2E+14	8.441	8.344	9.11	9.11	9.11	9.11	9.11
T1C37	7.769	5E+13	7.987	7.415	8.42	8.42	8.42	8.42	8.42
T1C38	7.979	-1E+14	7.47	8.666	8.386	8.386	8.386	8.386	8.386

Table-13. Predicted Activity By Solution Of QSAR Equation

Comp.	PA82	PA83	PA84	PA85	PA86	PA87	PA88	PA89	PA90
T1C1	Failed	8.3	8.644	7.672	7.905	7.376	7.641	7.38	7.715
T1C2	Failed	6.047	6.3	6.51	7.677	7.113	7.717	7.278	7.664
T1C3	Failed	8.269	8.47	8.315	7.767	7.514	7.684	7.522	7.725
T1C4	Failed	7.82	7.902	8.315	7.77	7.484	7.736	7.555	7.71
T1C5	Failed	5.956	6.297	7.153	7.63	7.78	7.62	7.639	7.775
T1C6	Failed	6.675	6.415	7.428	7.75	7.63	7.863	7.79	7.704
T1C7	Failed	6.89	6.912	7.152	7.847	7.225	7.79	7.433	7.664
T1C8	Failed	6.879	7.543	7.764	7.595	7.483	7.516	7.324	7.756
T1C9	Failed	6.55	6.869	7.886	7.825	7.369	7.663	7.4	7.71
T1C10	Failed	8.692	7.491	8.436	7.98	8.065	8.174	8.419	7.699
T1C11	Failed	7.63	7.965	7.519	7.738	7.521	7.635	7.475	7.736
T1C12	Failed	7.905	7.508	8.376	7.972	8.266	7.848	8.215	7.793
T1C13	Failed	9.484	7.544	8.864	7.953	7.813	8.48	8.566	7.601
T1C14	Failed	7.15	7.151	8.131	7.653	7.719	7.75	7.733	7.739
T1C15	Failed	7.778	7.651	7.916	7.611	7.678	7.799	7.757	7.724
T1C16	Failed	7.902	8.085	8.131	7.676	7.736	7.673	7.664	7.758
T1C17	Failed	8.04	8.056	8.131	7.691	7.92	7.719	7.84	7.773
T1C18	Failed	8.732	8.722	7.916	7.609	7.805	7.735	7.777	7.754
T1C19	Failed	8.148	8.256	7.901	7.876	8.122	7.664	7.922	7.812
T1C20	Failed	7.261	7.653	8.33	7.897	8.77	7.498	8.196	7.934
T1C21	Failed	7.714	7.718	7.901	7.864	8.305	7.69	8.076	7.831
T1C22	Failed	8.58	7.471	8.213	7.99	8.529	8.095	8.658	7.778
T1C23	Failed	6.462	6.621	8.33	7.845	8.409	7.628	8.083	7.858
T1C24	Failed	8.106	7.563	7.687	7.944	7.315	7.993	7.709	7.634
T1C25	Failed	5.788	6.267	8.315	7.804	7.432	7.601	7.377	7.731
T1C26	Failed	8.672	8.299	8.344	7.567	7.97	7.861	8.024	7.75
T1C27	Failed	9.227	9.274	7.122	7.815	7.427	7.745	7.525	7.701
T1C28	Failed	6.452	8.295	6.602	7.568	7.467	7.062	6.835	7.847
T1C29	Failed	6.322	8.318	6.388	7.557	7.54	6.997	6.817	7.871
T1C30	Failed	6.412	6.432	6.878	7.63	7.639	7.755	7.683	7.727
T1C31	Failed	8.679	8.233	7.397	7.601	7.558	7.929	7.809	7.68
T1C32	Failed	6.926	7.038	7.58	7.624	7.763	7.704	7.715	7.755

T1C33	Failed	8.642	8.803	7.58	7.596	7.67	7.682	7.628	7.747
T1C34	Failed	8.234	8.306	7.366	7.563	7.638	7.722	7.648	7.734
T1C35	Failed	9.104	9.093	7.58	7.62	7.76	7.737	7.748	7.747
T1C36	Failed	9.541	8.238	7.886	7.977	8.17	8.198	8.517	7.708
T1C37	Failed	8.354	8.614	8.039	7.405	7.822	7.631	7.679	7.778
T1C38	Failed	8.95	8.253	7.214	7.878	7.466	8.033	7.856	7.646

Table-14. 37 Qsar Models In Decreasing Order Of Co-Relation Coefficient Value

Pred. Activity	rCV^2	r^2
PA59	0.942721	0.952774
PA61	0.939802	0.951303
PA62	0.939802	0.951303
PA63	0.939802	0.951303
PA64	0.939802	0.951303
PA65	0.939802	0.951303
PA66	0.939802	0.951303
PA25	0.942183	0.951269
PA57	0.941234	0.951163
PA58	0.941444	0.949682
PA60	0.939101	0.948784
PA22	0.940345	0.948659
PA23	0.939407	0.946938
PA24	0.939898	0.946792
PA26	0.935401	0.943292
PA1	0.937070	0.943281
PA52	0.784387	0.832186
PA77	0.784387	0.832186
PA78	0.784387	0.832186
PA80	0.784387	0.832186
PA81	0.784387	0.832186
PA48	0.792025	0.830385
PA50	0.778285	0.828055
PA51	0.778285	0.828055
PA53	0.778285	0.828055
PA54	0.778285	0.828055
PA55	0.778285	0.828055
PA5	0.786119	0.827002
PA46	0.761546	0.794574
PA47	0.747050	0.763543
PA3	0.729421	0.759689
PA4	0.725223	0.742545
PA49	0.703269	0.727936
PA2	0.706762	0.725075
PA83	0.383785	0.651069
PA6	0.591815	0.640035
PA84	0.622195	0.640030

Endnotes

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