ijpbs 2020; doi 10.22376/ijpbs.2020.11.3.p56-62

International Journal of Pharma and Bio Sciences

Original Research Article

Pharmaceutical chemistry for better medicinal drug

QSAR Studies of Some Pharmacologically important Compoundsfor SARS CoV

Veena Saluja[1], Pradeep Kumar Gupta[2], Yashaswina Arora[3] and Kishor Arora[*2]

[1]Ex- Faculty, The City College, Gwalior, Madhya Pradesh, India.

[2] Department of Chemistry, Government Postgraduate College (Autonomous); Datia - 475 661, Madhya Pradesh, India.

[3] Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER); Raibareli, Uttar Pradesh, India.

Abstract: Currently, the outbreak of the novel human respiratory coronavirus, also popularly known as COVID-19, has sought the attention of the scientific community across the world and stresses on the need for new therapeutic alternatives in order to cease the global health crisis and fight the pandemic. The situation, therefore, calls out for new researchcentred on targeting the pathogen. A number of studies reveal the potential of different chemical moieties that could possibly act against the virus. In our work, we report the semi-empirical based 3D -QSAR 3D-quantitaive structure and activity relationship / QSAR studies of 3 series of compounds viz. Ethacrynic Acid Derivatives (E1-E3), Isatin (2,3-oxindole) Inhibitors (I1-I7) and Flavonoid and Biflavonoid Derivatives (F1-F7) on the basis of their reported activities against SARS Co-V. The studies are carried out on Hyperchem 8.0 version software using AM1 and PM3 methods. Selected QSAR/ 3D-QSAR equations including different physical parameters of these series are reported.

Keywords: Semi-empirical / QSAR and 3D- QSAR/Pharmacological compounds/Ethacrynic Acid derivatives/Isatin (2,3-q oxindole)Inhibitors/Flavonoid and Bioflavonoid Derivatives.

Article History	Date of Receiving	18 May 2020	Date of Revision	17 June 2020
	Date of Acceptance	24 June 2020	Date of Publishing	02 July 2020

***Corresponding Author**

Kishor Arora , Professor, Department of Chemistry, Government Postgraduate College (Autonomous); Datia - 475 661, Madhya Pradesh, India.

Funding This research did not receive any specific grant from any funding agencies in the public, commercial or not for profit sectors.

CItation Veena Saluja, Pradeep Kumar Gupta, Yashaswina Arora and Kishor Arora , QSAR Studies of Some Pharmacologically important Compounds for SARS CoV.(2020).Int J Pharm Sci.11(3), P56-62 http://dx.doi.org/10.22376/ijpbs.2020.11.3.p56-62

Int J Pharma Bio Sci., Volume11., No 3 (July) 2020, pp P56-62

1. INTRODUCTION

Since the beginning of the 21st century, Coronaviruses have caused an outbreak of a fatal form of pneumonia in humans. Initially, in 2003, severe acute respiratory syndrome coronavirus (SARS-CoV) broke out in 5 continents followed by a second outbreak in the Arabian peninsula in 2012, which came to be known as middle-east respiratory syndrome coronavirus (MERS-CoV). The SARS Covid-19 outbreak is the highlight of 2020, which emerged in Asia late last year and gradually became a major health problem killing numerous people and upending people's lives across the globe[1-16]. Till date, no vaccine or drug has been approved for treatment of the human coronaviruses and the battle is based solely on symptomatic relief. Hence, getting rid of it at the earliest is the call of the hour for every nation in order to minimize the threat posed by this virus to humankind. A number of studies are being carried out which give a detailed account of the pathophysiology of the disease, highlighting the ways to target it and have enabled the members of the scientific community to recognize different strategies for development of new drugs including testing the existing broad-spectrum antivirals and use of existing molecular databases for screening of molecules that might be effective against coronavirus. A number of studies have reported activities of a different series of compounds based on different sets of experiments. A recent study by Pillaiyar et al. [17]highlighted series of different peptidomimetic and small molecule inhibitors of Covid-19. In the present work, we pick 3 series from the reported series of molecules for 3D QSAR/QSAR studies including Ethacrynic Acid derivatives ,Isatin inhibitors and flavonoid and biflavonoid derivatives. The structures of the compounds selected for studies are shown in Figure 1-3 .

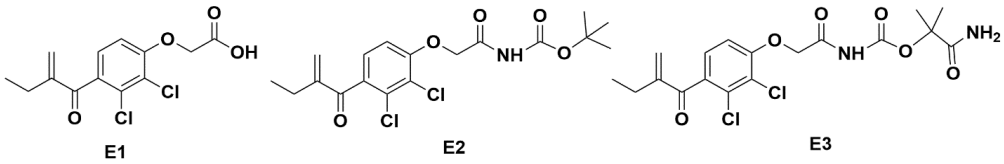
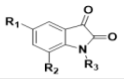


Fig1.Ethacrynic Acid Derivatives (E1-E3)



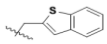
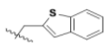
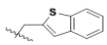
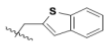
Str.	R_1	R_2	R_3
I-1	CN	H	
I-2	I	H	
I-3	H	NO_2	
I-4	H	Br	
I-5	F	H	
I-6	I	H	
I-7		H	

Fig 2.Isatin (2,3-oxindole) Inhibitors compounds (I1-I7)

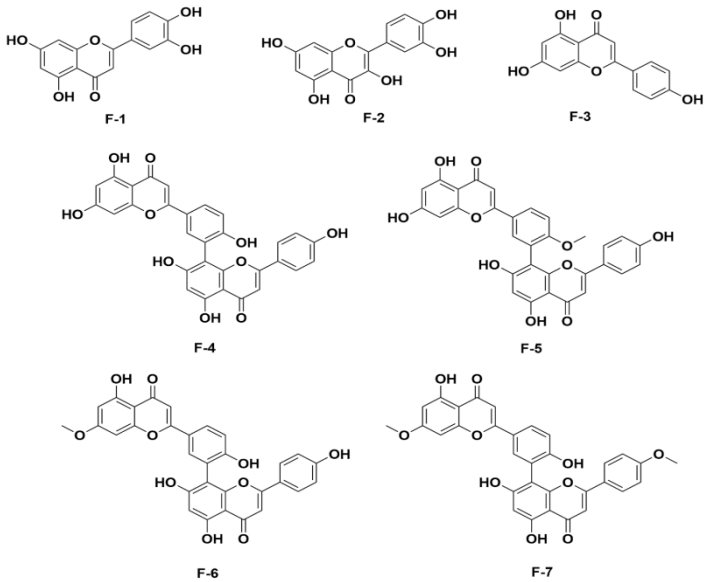


Fig 3.Flavonoid and Bioflavonoid Derivative compounds (F1-F7)

2. METHODS

For the purpose of our study, the following protocol was adopted:

(i) Drawing structures of the compounds/ series of the compounds under study
(ii) Optimization of their geometries
(iii) Recording physical parameters along with vibration spectral parameters for these compounds.
(iv) Recording QSAR parameters of the compounds under study.

All the above-mentioned steps were carried out on the HYPERCHEM 8.0 professional software on the basis of semi-empirical calculations using AM1 and PM3 methods on the PC/ machine Pentium core-2 duo machine with the following configuration: Intel ® core TM 2 Duo CPUT5450@1.66GHz982 MHz 896 MB RAM, 150 GB HDD. Structures of the series of compounds are drawn using Chembio draw 14.0 version.

3. STATISTICAL ANALYSIS

Statistical calculations were carried out to obtain 3D-QSAR/QSAR equations based on the properties recorded in the above step on the PC/ computer with configuration: Intel ® core ™ 2 Duo CPU,T5450 @ 1.66 GHZ,2 GB RAM,250 GB HDD with windows Microsoft windows XP software operating system.

4. RESULTS AND DISCUSSIONS

The reported activities[17] viz. Ki, IC_{50} or EC_{50}have been used as such and are reported in the tables 1-6. The other computed parameters/ properties for the compounds under study are also listed in the table 1-6. These parameters include total energy (TE), electronic energy (EE), core –core interaction (C-C interaction),heat of formation (HF), dipole moment(DM) and zero point energy (ZPE)along with their computed QSAR parameters viz. partial charge(partial charge), surface area approx. (SAA), surface area grid (SAG), volume (Vol), hydration energy(HE), log P (log P), refractivity (Ref), polarizability (POL) and mass (Mass) are also reported in the tables 1-6. These parameters though are physical parameters but have a vital role in the designing of a drug. Therefore their QSAR studies have importance. In order to carry out these studies, the computed parameters as mentioned above were then subjected to linear regression analysis using MS-Excel to obtain 3D-QSAR/QSAR equations for the series of compounds under study[18-20]. The generated QSAR model was selected on the basis of various statistical parameters such as correlation coefficient which is relative measure of quality of fit, Fischer's value (F-test) which represent F-ratio between the variance of calculated and observed activity, standard error, representing absolute measure of quality of fit respectively. The 3D-QSAR/QSAR equations are given after the tables 1-6 along with the graphs between observed/ reported and computed activities.

Table 1. AM1 Computed QSAR properties of compounds E1 –E3

Compounds	Ki	Partial charge	SAA	SAG	VOL	HE	Log P	REF	POL	Mass
E1	375	0	493.46	489.03	808.93	-8.78	1.22	76.2	28.58	305.16
E2	45.8	0	572.69	559.56	934.79	-6.7	0.82	89.02	33.5	360.19
E3	35.3	0	591.67	646.58	1071.58	-11.97	-0.16	101.73	38.33	401.25

Table1A. AM1 computed other physical parameters of the compounds E1 –E3

Compounds	TE	EE	C-C Interaction	HF	DM	ZPE
E1	-89633.43	-523364.52	433731.08	-162.34	1.524	161.15
E2	-107967	-666659.65	558692.64	-137.08	2.615	182.12
E3	-119607.26	-805175.92	685568.66	-137.83	3.000	215.07

Table 2. PM3 Computed QSAR properties of compounds E1 –E3

Compounds	Ki	Partial charge	SAA	SAG	VOL	HE	Log P	REF	POL	Mass
E1	375	0	493.3	487.59	807.14	-8.65	1.22	76.2	28.58	305.16
E2	45.8	0	565.44	571.54	943.34	-6.87	0.82	89.02	33.5	360.19
E3	35.3	0	602.31	651.36	1075.75	-12.2	-0.16	101.73	38.33	401.25

Table2A. PM3 computed other physical parameters of the compounds E1 –E3

Compounds	TE	EE	C-C Interaction	HF	DM	ZPE
E1	-82205.3	-513511.25	431305.94	-163.96	1.7	156.18
E2	-98514.7	-663617.88	565103.15	-168.05	1.96	174.3
E3	-108774	-787284.28	678509.85	-147.36	1.84	205.85

Table 3. AM1 Computed QSAR properties of compounds I1 –I7

Compounds	IC50	Partial charge	SAA	SAG	VOL	HE	Log P	REF	POL	Mass
I1	7.2	0	402.92	494.25	830.66	-4.65	-0.36	84.4	30.85	283.33
I2	9.4	0	424.59	491.32	819.71	-1.88	0.69	93.46	33.21	415.59
I3	2	0	397.64	516.89	874.94	-13.9	-3.89	99.95	34.68	340.35
I4	0.98	0	389.56	497.9	836.95	-3	-0.18	100.6	34.68	372.24

I5	4.98	0	390.07	486.33	809.94	-3.34	-0.83	93.19	31.96	311.33
I6	0.95	0	433.96	524.79	880.64	-3.27	0.29	105.39	37.08	419.24
I7	1.04	0	492.15	608.94	1061.94	-6.73	1.64	114.15	41.04	380.44

Table3A. AM1 computed other physical parameters of the compounds I1 –I7

Compounds	TE	EE	C-C Interaction	HF	DM	ZPE
I1	-81683.4	-560914	479230.9	22.93	7.3	197.02
I2	-94150.7	-549026	454875.3	-19.26	4.6	128.34
I3	-97482.1	-673219	575737.4	12.22	4.84	170.88
I4	-85495.8	-555488	469991.8	41.16	4.03	148.22
I5	-88536.1	-551784	463248.2	-9.63	4.2	149.77
I6	-85359.3	-543602	458242.5	50.69	4.28	147.96
I7	-111660	-883426	771765.9	-89.69	5.56	275.36

Table 4. PM3 Computed QSAR properties of compounds I1 –I7

Compounds	IC50	Partial charge	SAA	SAG	VOL	HE	Log P	REF	POL	Mass
I1	7.2	0	397.28	494.15	826.99	-4.91	-0.36	84.4	30.85	283.33
I2	9.4	0	430	492.17	816.55	-1.55	0.69	93.46	33.21	415.59
I3	2	0	395.26	511.43	867.37	-15.9	-3.89	99.95	34.68	340.35
I4	0.98	0	384.97	495.69	834.24	-2.9	-0.18	100.6	34.68	372.24
I5	4.98	0	386.11	484.12	809.91	-3.33	-0.83	93.19	31.96	311.33
I6	0.95	0	430.81	519.29	879.14	-3.28	0.29	105.39	37.08	419.24
I7	1.04	0	484.68	607.6	1010.74	-7.04	1.64	114.15	41.04	380.44

Table 4A. PM3 computed other physical parameters of the compounds I1 –I7

Compounds	TE	EE	C-C Interaction	HF	DM	ZPE
I1	-74511.3	-552345	477834	-17.68	6.65	190.91
I2	-85197	-532399	447201.8	-36.43	4.03	123.67
I3	-89479.3	-656832	567352.8	-4.14	2.99	164.02
I4	-79689	-544535	464845.6	23.79	3.25	142.91
I5	-81694.6	-540914	459219.3	-29.97	3.5	144.19
I6	-78196.1	-532716	454519.5	34.39	3.57	142.69
I7	-103224	-874584	771360.2	-122.93	5.97	266.35

Table 5. AM1 Computed QSAR properties of compounds F1 –F7

Compounds	EC50	Partial charge	SAA	SAG	VOL	HE	Log P	REF	POL	Mass
F1	10.6	0	367.28	463.25	750.94	-27.9	-3.11	81.49	27.9	286.24
F2	83.4	0	368.64	468.82	766.01	-31.31	-4.01	83.17	28.54	302.24
F3	280	0	362.67	450.6	730.81	-22.31	-2.09	79.88	27.27	270.24
F4	8.3	0	566.6	727.83	1298.28	-36.18	-5.16	157.33	53.76	538.47
F5	72.3	0	604.19	734.42	1354.64	-33.14	-5.13	162.09	55.6	552.49
F6	32.7	0	644.81	779.58	1409.63	-29.35	-5.1	166.86	57.43	566.52
F7	38.4	0	623.58	747.13	1414.19	-23.53	-5.07	171.63	59.27	580.55

Table 5A. AM1 computed other physical parameters of the compounds F1 –F7

Compounds	TE	EE	CC	HF	DM	ZPE
F1	-91766.13	-543352.41	451586.28	-166.82	4.22	146.57
F2	-99157.48	-601250.07	502092.58	-209.03	5.14	149.45
F3	-84373.33	-494365.71	4-9992.38	-123.16	3.83	143.92
F4	-168112.17	-1426241.7	1258129.6	-241.64	6.49	275.67
F5	-171692.31	-1516081.3	1344389	-234.94	6.07	293.82
F6	-175272.81	-1577234	1401961.2	-228.6	5.82	311.77
F7	-178851.74	-1667227	1488375.3	-22.68	6.5	330.01

Table 6. PM3 Computed QSAR properties of compounds F1 –F7

Compounds	EC50	Partial charge	SAA	SAG	VOL	HE	Log P	REF	POL	Mass
F1	10.6	0	367.72	461.54	749.87	-28.02	-3.11	81.49	27.9	286.24
F2	83.4	0	370.63	475.51	771.92	-31.59	-4.01	83.17	28.54	302.24
F3	280	0	362.35	453.75	731.78	-22.37	-2.09	79.88	27.27	270.24
F4	8.3	0	560.39	723.33	1291.44	-36.52	-5.16	157.33	53.76	538.47

F5	72.3	0	598.13	743.16	1344.48	-32.47	-5.13	162.09	55.6	552.49
F6	32.7	0	657.65	773.35	1399.75	-28.73	-5.1	166.86	57.43	566.52
F7	38.4	0	665.11	794.58	1441.55	-22.85	-5.07	171.63	59.27	580.55

Table 6A. PM3 computed other physical parameters of the compounds F1 –F7

Compounds	TE	EE	C-C Interaction	HF	DM	ZPE
F1	-85145.3903	-533066.546	447923.5	-175.275	4.444	143.7462
F2	-91919.1564	-590017.433	498098.3	-219.372	4.707	146.9689
F3	-78370.3618	-485069.403	406699	-134.727	3.821	140.7368
F4	-156035.583	-1413409.61	1257374	-271.471	6.664	270.9022
F5	-159471.512	-1494753.2	1335282	-264.278	3.603	287.5016
F6	-162907.328	-1557622.94	1394716	-256.972	4.032	303.9892
F7	-166343.497	-1628124.05	1461781	-250.02	4.42	320.4813

These selected 3D-QSAR equations so obtainedgiven as follows:

Isatin (2,3-oxindole) Inhibitors compounds (I1-I7)/AM1 computed
Act = -0.0259444(SAG) - 0.862623(REF) + 1.9558655(POL) + 34.34578
N= 7, SE= 2.689735, R= 0.833881, F= 2.282549

Isatin (2,3-oxindole) Inhibitors compounds (I1-I7)/PM3 computed
Act = -0.03065(VOL) - 0.975431(REF) + 2.542850(POL) + 38.11805
N= 7, SE= 2.591939, R= 0.846822, F= 2.534929

Flavonoid and Bioflavonoid Derivative compounds (F1-F7)/ AM1 computed
Act = 0.41593263(SAG) + 0.67196135(HE) + 100.944972(LogP) + 262.760817
N= 7, SE= 83.4344468, R= 0.78231969, F= 1.57748

Flavonoid and Bioflavonoid Derivative compounds (F1-F7)/ PM3 computed
Act = -0.55273(HE) + 116.7531(LogP) + 0.549207(Mass) + 311.0076
N= 7, SE= 81.86627, R= 0.791499, F= 1.67717

Graphs between observed and computed activities are also plotted which are given in the figure 4-5 for these series of compounds viz. Isatin (2,3-oxindole) inhibitors compounds (I1-I7) and Flavonoid and Bioflavonoid derivative compounds (F1-F7).In the case of Ethacrynicacid Derivatives (E1-E3)series, selected QSAR equations that are obtained are given as below followed by the graphs obtained between observed and computed activities, in figure 6.

Ethacrynic Acid Derivatives (E1-E3)./AM1 Computed
Act = -3.66298 (SAA) + 2176.222
N= 3, SD= 42.4461, CC= 0.98785, F-Test= 0.135599

Ethacrynic Acid Derivatives (E1-E3)./PM3 Computed
Act = -3.31583(SAA) + 1987.953
N= 3, SD= 83.78907, CC= 0.9518, F-Test= 0.152248

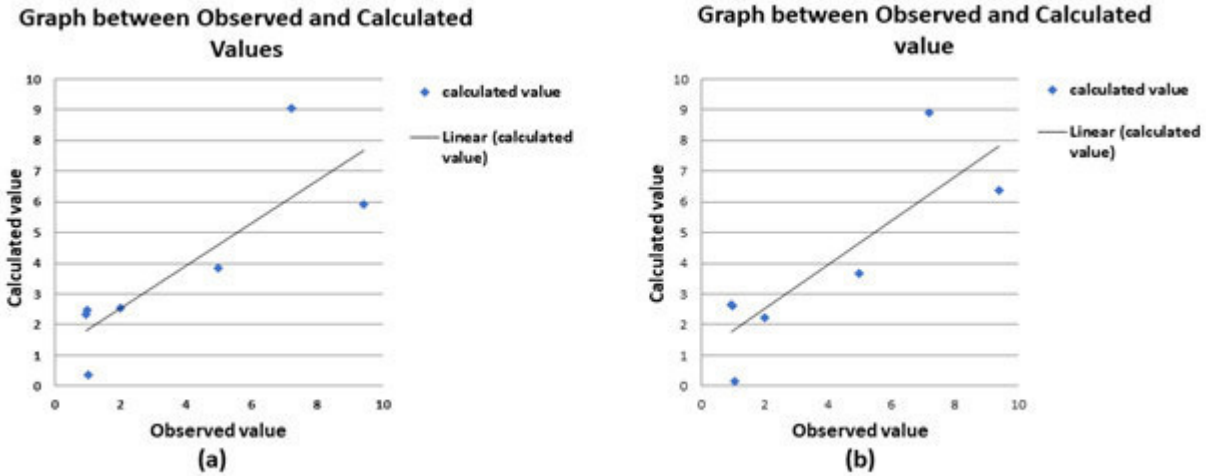


Fig 4. (a) Graph between AM1 computed activities and observed activities for Isatin (2,3-oxindole) Inhibitors compounds (I1-I7), (b) Graph between PM3 computed activities and observed activitiesfor Isatin (2,3-oxindole) Inhibitors compounds (I1-I7)

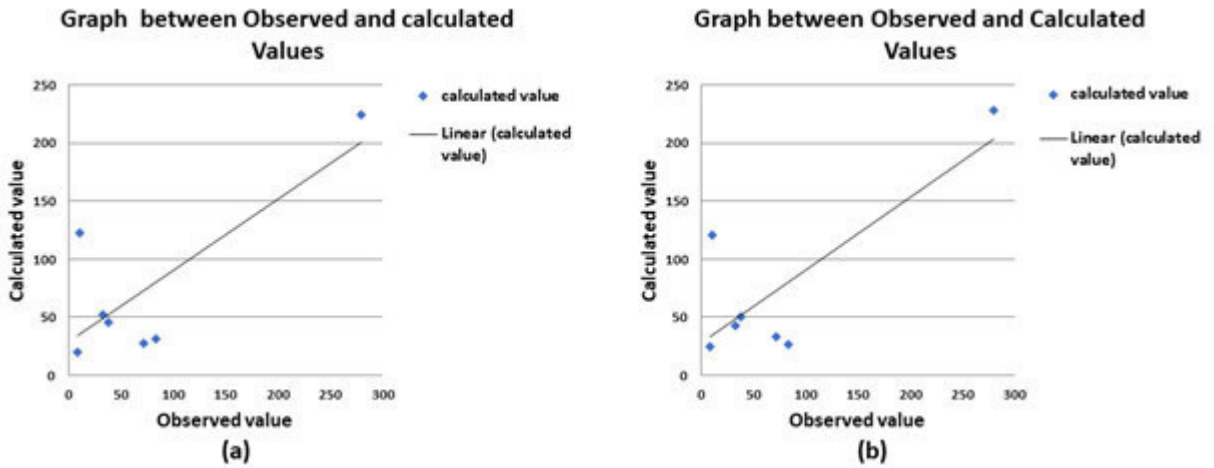


Fig 5. (a) Graph between AM1 computed activities and observed activities for Flavonoid and Bioflavonoid Derivative compounds (F1-F7), (b) Graph between PM3 computed activities and observed activities for Flavonoid and Bioflavonoid Derivative compounds (F1-F7)

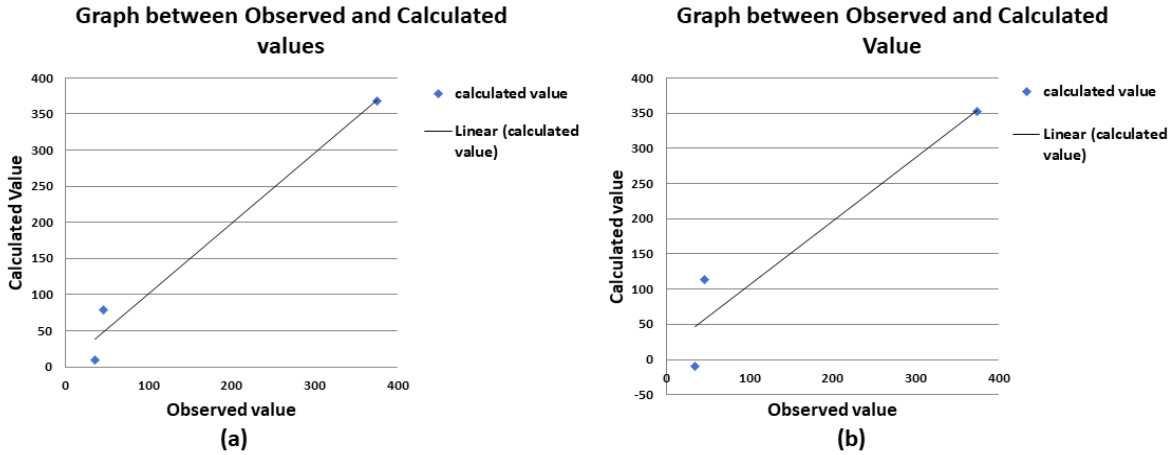


Fig 6. (a) Graph between AM1 computed activities and observed activities for Ethacrynic Acid Derivatives (E1-E3), (b) Graph between PM3 computed activities and observed activities for Ethacrynic Acid Derivatives (E1-E3)

Though QSAR/3D QSAR studies of these series of compounds reveal that standard error values are little bit high for the equations so obtained. Those equations are selected and reported here which have comparative less standard error value.So far as correlation coefficient is concerned, only those equations are selected and presented here which have comparatively high correlation coefficient values[18-20].It is quite obvious from these equations which are framed on the basis of this study, that following parameters/ properties impart the effect on the activities of the series of compounds selected for the studies [18-20]and reported in this paper.

Isatin (2,3-oxindole) Inhibitors compounds (I1-I7)/AM1:- SAG, REF and POL
Isatin (2,3-oxindole) Inhibitors compounds (I1-I7)/PM3 :- VOL, REF, and POL
Flavonoid and Bioflavonoid Derivative compounds (F1-F7)/ AM1:- SAG, HE and LOG P
Flavonoid and Bioflavonoid Derivative compounds (F1-F7)/ PM3:- HE, LOG P and MASS
QSAR/ Ethacrynic Acid Derivatives (E1-E3)./AM1 :- SAA
QSAR/ Ethacrynic Acid Derivatives (E1-E3)./PM3 :- SAA

5. CONCLUSION

In our findings, we conclude that the AM1 method seems to be more effective and precise among these two methods which are adopted by our group for this study[18-20]. Secondly, theoretically computed properties/ parametersas mentioned in the results and discussion part may contribute towards improvement of the activities of these compounds under study as per mentioned in the respective QSAR/3D -QSAR equations so obtained. These parameters which have effective impact on the basis of QSAR / 3D-QSAR studies for the different series of compounds under studies are listed in the results and discussion part.

6. AUTHORS CONTRIBUTION STATEMENT

Kishor Arora conceptualized and gathered the related data with extensive literature survey. Pradeep Gupta helped in this task. Kishor Arora performed computational work on PC using a semi-empirical package. Statistical calculations were performed by Veena Saluja on PC using MS Excel. She also helped in framing the QSAR/3D-QSAR equations. Yashaswina Arora analyzed the results so obtained and helped in the designing of structures of the compounds under study along with writing of the complete manuscript. All authors discussed the methodology and results contributed to the final manuscript.

7. CONFLICT OF INTEREST

Conflict of interest declared none.

8. REFERENCES

1. Yao X, Ye F, Zhang M, Cui C, Huang B, Niu P, Liu X, Zhao L, Dong E, Song C, Zhan S, Lu R, Li H, Tan W, Liu D. In vitro antiviral activity and projection of optimized dosing design of hydroxychloroquine for the treatment of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Clin Infect Dis. 2020Mar9. doi: 10.1093/cid/ciaa237, PMID 32150618.
2. Macfarlane DE, Manzel L. Antagonism of immune stimulatory CpG-oligodeoxynucleotides by quinacrine, chloroquine, and structurally related compounds. J Immunol. 1998Feb1;160(3):1122-31. PMID 9570525.
3. Teengam P, Siangproh W, Tuantranont A, Vilaivan T, Chailapakul O, Henry CS. Multiplex paper-based colorimetric DNA sensor using pyrrolidinyl peptide nucleic acid-induced AgNPs aggregation for detecting MERS-CoV, MTB, and HPV oligonucleotides. Anal Chem. 2017May16;89(10):5428-35. doi: 10.1021/acs.analchem.7b00255, PMID 28394582.
4. Baig AM, Khaleeq A, Ali U, Syeda H. Evidence of the COVID-19 virus targeting the CNS: tissue distribution, Host-Virus Interaction, and Proposed Neurotropic Mechanisms. ACS Chem Neurosci. 2020Mar13;11(7):995-8. doi: 10.1021/acschemneuro.0c00122, PMID 32167747.
5. Liu C, Zhou Q, Li Y, Garner LV, Watkins SP, Carter LJ, Smoot J, Gregg AC, Daniels AD, Jervey S, Albaiu D. Research and development on therapeutic agents and vaccines for COVID-19 and related human coronavirus diseases. ACS Cent Sci. 2020;6(3):315-31. doi: 10.1021/acscentsci.0c00272, PMID 32226821.
6. Huang C, Qi J, Lu G, Wang Q, Yuan Y, Wu Y, Zhang Y, Yan J, Gao GF. Putative receptor binding domain of bat-derived coronavirus HKU9 spike protein: evolution of Beta coronavirus receptor binding Motifs. Biochemistry. 2016Nov1;55(43):5977-88. doi: 10.1021/acs.biochem.6b00790, PMID 27696819.
7. Kvach MV, Barzak FM, Harjes S, Schares HAM, Jameson GB, Ayoub AM, Moorthy R, Aihara H, Harris RS, Filichev VV, Harki DA, Harjes E. Inhibiting APOBEC3 activity with single-stranded DNA containing 2′-Deoxyzebularine analogues. Biochemistry. 2019Nov12;58(5):391-400. doi: 10.1021/acs.biochem.8b00858, PMID 30418757.
8. Xiang DF, Bigley AN, Desormeaux E, Narindoshvili T, Raushel FM. Enzyme-catalyzed kinetic resolution of chiral precursors to antiviral pro drugs. Biochemistry. 2019Jul3;58(29):3204-11. doi: 10.1021/acs.biochem.9b00530, PMID 31268686.
9. Łoczechin A, Séron K, Barras A, Giovanelli E, Belouzard S, Chen YT, Metzler-Nolte N, Boukherroub R, Dubuisson J, Szunerits S. Functional carbon quantum dots as medical countermeasures to human coronavirus. ACS Appl Mater Interfaces. 2019Oct21;11(46):42964-74. doi: 10.1021/acsami.9b15032, PMID 31633330.
10. Xu J, Shi PY, Li H, Zhou J. Broad spectrum antiviral agent niclosamide and its therapeutic potential. ACS Infect Dis. 2020Mar10;6(5):909-15. doi: 10.1021/acsinfecdis.0c00052, PMID 32125140.
11. Lin SM, Lin SC, Hsu JN, Chang CK, Chien CM, Wang YS, Wu HY, Jeng US, Kehn-Hall K, Hou MH. Structure-based stabilization of non-native protein–protein interactions of coronavirus nucleocapsid proteins in antiviral drug design. J Med Chem. 2020Feb27;63(6):3131-41. doi: 10.1021/acs.jmedchem.9b01913, PMID 32105468.
12. Zhang L, Lin D, Kusov Y, Nian Y, Ma Q, Wang J, Von Brunn A, Leyssen P, Lanko K, Neyts J, De Wilde A, Snijder EJ, Liu H, Hilgenfeld R. α-Ketoamides as broad-spectrum inhibitors of coronavirus and enterovirus replication: structure-based design, synthesis, and activity assessment. J Med Chem. 2020Feb24;63(9):4562-78. doi: 10.1021/acs.jmedchem.9b01828, PMID 32045235.
13. Rao L, Tian R, Chen X. Cell-membrane-mimicking nanodecoys against infectious diseases. ACS Nano. 2020Mar4;14(3):2569-74. doi: 10.1021/acsnano.0c01665, PMID 32129977.
14. Mehellou Y, Rattan HS, Balzarini J. The Pro Tide pro drug technology: from the concept to the clinic. J Med Chem. 2018;61(6):2211-26. doi: 10.1021/acs.jmedchem.7b00734, PMID 28792763.
15. Wang C, Zhao L, Xia S, Zhang T, Cao R, Liang G, Li Y, Meng G, Wang W, Shi W, Zhong W, Jiang S, Liu K. De novo design of α-helical lipopeptides targeting viral fusion proteins: A promising strategy for relatively broad-spectrum antiviral drug discovery. J Med Chem. 2018Sep7;61(19):8734-45. doi: 10.1021/acs.jmedchem.8b00890, PMID 30192544.
16. Yoon JS, Kim G, Jarhad DB, Kim HR, Shin YS, Qu S, Sahu PK, Kim HO, Lee HW, Wang SB, Kong YJ, Chang TS, Ogando NS, Kovacikova K, Snijder EJ, Posthuma CC, van Hemert MJ, Jeong LS. Design, synthesis, and anti-RNA virus activity of 6′-fluorinated-aristeromycin analogues. J Med Chem. 2019Jun7;62(13):6346-62. doi: 10.1021/acs.jmedchem.9b00781, PMID 31244113.
17. Pillaiyar T, Manickam M, Namasivayam V, Hayashi Y, Jung SH. An overview of severe acute respiratory syndrome–coronavirus (SARS-CoV) 3CL protease inhibitors: peptidomimetics and small molecule chemotherapy. J Med Chem. 2016Jul28;59(14):6595-628. doi: 10.1021/acs.jmedchem.5b01461, PMID 26878082.
18. Arora K. 3D-QSAR studies for some pyrazolones against a pathogen. J Chem Pharm Res.2014;6(11):117-28.
19. Arora K. Semi empirical based 3D-QSAR studies of some pharmacological important compounds. Int J Pharm BiolSci. 2013;4(2):244-54.
20. Arora K. 3D-QSAR studies for some Schiff bases against bacterial pathogen. Int J Pharm BiolSci.2014;5(3):402-21.