International Journal of Advanced Research in Biological Sciences
ISSN: 2348-8069
www.ijarbs.com
(A Peer Reviewed, Referred, Indexed and Open Access Journal)
DOI: 10.22192/ijarbs Coden: IJARQG (USA) Volume 9, Issue 5 -2022

Research Article

Special Issue on Potential Applications of Bioinformatics in Biological Sciences - PABBS 2022

DOI: http://dx.doi.org/10.22192/ijarbs.2022.09.05.01.017

In silico QSAR studies on Indian medicinal plant of *Coriandrum sativam* (Coriander) and *Centella asiatica* (Gotu Kola) as fungal inhibitors.

Mahendran Radha[1]*, Jyothsana Madhavan, K. Eswaramoorthy, A. Jyotsna, Jeyabaskar Suganya, R. Priya, M.Vinoth, Nishandhini. M.
Department of Bioinformatics, School of Life Sciences, VISTAS, Chennai-600117, Tamil Nadu,India.
*Corresponding Author
E-mail: *mahenradha@gmail.com, hodbioinfo@velsuniv.ac.in*

Abstract

The era of defining antibiotics for the treatment of bacterial endemic conditions was the beginning of the emergence of fungal infections as a common threat to people's health. Infections caused by fungi are superficial, cutaneous and sub-cutaneous infections, further cutaneous infections are of 'superficial' and 'deep' forms. Medicinal plants being reservoir of small molecules, tracking the plant's activity and identifying the efficient bioactive compounds might help in the discovery of right candidate inhibitors. .Coriander (Coriandrum sativum L.) is an aromatic, aromatic annual herbaceous plant in the family Coriaceae .Centella asiaticais an herbaceous perennial plant belonging to the family Umbelliferae and medicinal properties such as anti-inflammatory, anti-hemorrhagic, antibacterial, and memory enhancing properties. QSAR studies were performed for the plants Coriandrumsativam and Centellaasiatica and the results were predicted.

Keywords: QSAR Analysis, Coriandrum sativam Centella asiatica, Build QSAR, Molinspiration,

Introduction

The era of defining antibiotics for the treatment of bacterial endemic conditions was the beginning of the emergence of fungal infections as a common threat to people's health. Infections caused by fungi are superficial, cutaneous and sub-cutaneous infections, further cutaneous infections are of 'superficial' and 'deep' forms. The existing antifungal agents are polyenes, azoles, pyrimidines, allylamines, candins and the drug griseofulvin, each targeting the fungal cell with their unique mode of action. In general, natural plant products are recognized as healthier than manufactured drugs. Medicinal plants being reservoir of small molecules, tracking the plant's activity and identifying the efficient bioactive compounds might help in the discovery of right candidate inhibitors[1].Coriander (Coriandrumsativum L.) is an aromatic, aromatic annual herbaceous plant in the family Coriaceae. Coriander is one of the oldest spices in recorded history, with evidence Its use dates back more than 5,000 years. Its use has been mentioned in Egyptian, Sanskrit and Roman literature. The Egyptians called this herb the the spice of happiness. The herb in the form of young plants is used to make curries, soups, salads and sauces, while the fruit is mainly used as a seasoning for pickles, cold cuts, confectionery products and mixes. Spice.[2]Centellaasiatica is one of the most common herbs found in abundant amounts China, Japan, Italy, Sri Lanka, Iran, India, Madagascar, USA, Australia, South Africa, Indonesia and Malaysia. It is a herbaceous perennial plant belonging to the family Umbelliferae and medicinal properties such as anti-inflammatory, anti-hemorrhagic, antibacterial, and memory enhancing properties.[3]

Materials and Methods

PubChem Database:

PubChem is a database of chemical molecules and their activities against biological assays. The system is maintained by the National Center for Biotechnology Information (NCBI), a component of the National Library of Medicine, which is part of the United States National Institutes of Health (NIH).[4] The Pubchem ID were retrieved from Pubchem Database.

Molinspiration:

Lipinski's rule of five: To evaluate druglikeness or determine if a chemical compound with a certain pharmacological or biological activity has chemical properties and physical properties that would make it a likely orally active drug in humans.[5] The Molecular properties and Bioactivity calculation are analysed by Molinspiration.

Build QSAR:

Quantitative structure-activity relationship methods are important for prediction of biological effect of chemical compounds based on mathematical and statistical relations. Quantitative structure-property relationship approaches determine the physiochemical properties based on the molecular features of various compounds.[6] The ADME properties were performed by Build QSAR software.

Results and Discussion

DESCRIPTORS FOR THE QSAR MODELS AND MLR ANALYSIS

- The independent variables along with dependent variables were calculated usingQED (quantitative estimation of drug likeness) and Molinspirationserver.
- The compounds inhibitory activity (Descriptors) was manually incorporated to the software Build QSAR. And various QSAR models were generated by correlating 1/log P values against any one of the independent variables in MLR analysis.

QSAR MODEL GENERATION

- The various models were generated by both independent variables (all descriptors) against the dependent variable 1/logP. Finally the

identification of best QSAR model between 1/log P values and structural descriptors could be the major molecular factor are associated with the activity of drug molecule.

➢ Further these models were validated using leave-one-out method in MLR analysis. The graphical analysis for the QSAR model has been plotted between the predicted value from the model X-axis and the predicted 1/log P values in Y-axis.

➢ The graph depicts that, the compounds aligned on and near the diagonal line displayed the good correlation between predicted 1/log P values and structural descriptors (antifungal activity)

Coriandrum sativam plants

Table 1a: Dependent and Independent variables (descriptors) used in QSAR models

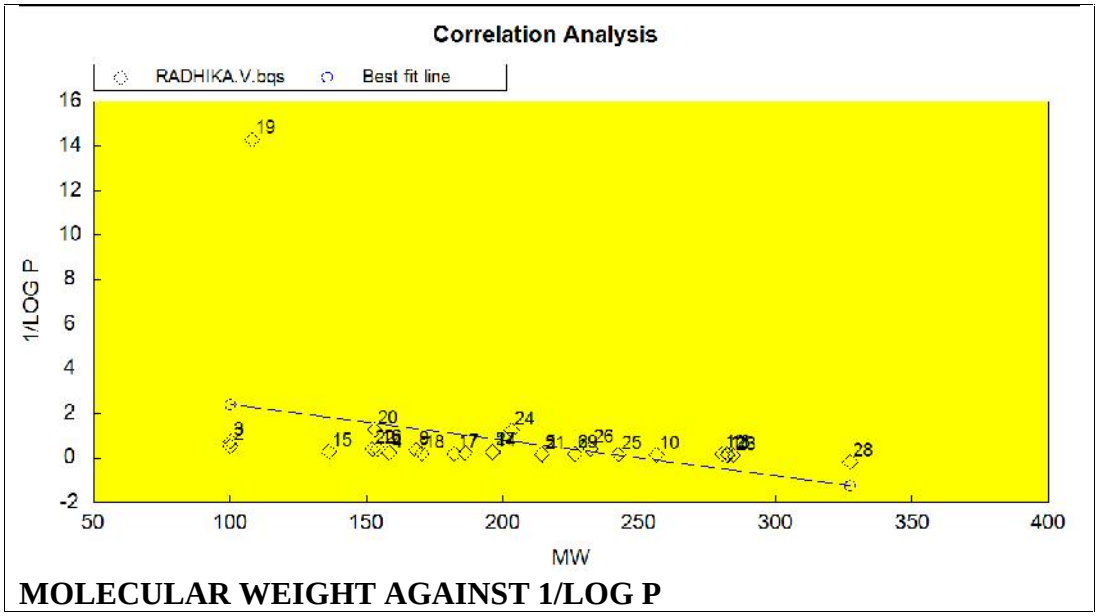
S.NO	COMPOUNDS NAME	PUBCHEM ID	DEPENDENT	INDEPENDENT				
			1/LOG P	MW	K+MW	HBD	K+HBD	HBA	K+HBA
1	neryl acetate	1549025	0.255754476	196.29	196.29	0	0	2	2
2	2-hexen-l-ol	5318042	0.531914894	100.16	100.16	1	1	1	1
3	3-hexen-l-ol	5284503	0.740740741	100.16	100.16	1	1	1	1
4	n-decanol	8174	0.240963855	158.28	158.28	1	1	1	1
5	tridecanoic acid	12530	0.180505415	214.35	214.35	1	1	2	2
6	E-11-Tetradecenoic acid	5362745	0.189753321	226.36	226.36	1	1	2	2
7	undecanoic acid	8180	0.220750552	186.29	186.29	1	1	2	2
8	2E-decenal	6442990	0.36101083	168.24	168.24	0	0	2	2
9	decanol	8174	0.36101083	168.24	168.24	1	1	1	1
10	palmitic acid	985	0.141643059	256.43	256.43	1	1	2	2
11	oleic acid	445639	0.131926121	282.47	282.47	1	1	2	2
12	linoleic acid	5280450	0.173340267	280.445	280.445	1	1	2	2

13	petroselinic acid	5281125	0.168123739	282.461	282.461	1	1	2	2
14	geranyl acetate	1549026	0.255754476	196.29	196.29	0	0	2	2
15	limonene	22311	0.276243094	136.24	136.24	0	0	0	0
16	borneol	64685	0.425531915	154.25	154.25	1	1	1	1
17	2E-dodecenal	5283361	0.186567164	182.31	182.31	0	0	1	1
18	undecanal	8186	0.195694716	170.3	170.3	0	0	1	1
19	m-phenylenediamine	7935	14.28571429	108.14	108.14	4	4	0	0
20	4-nitro-o-phenylenediamine (NOP)	5111791	1.265822785	153.14	153.14	4	4	2	2
21	n-tetradecanol	8209	0.162074554	214.39	214.39	1	1	1	1
22	cis-pihydrocarvone	24473	0.406504065	152.24	152.24	0	0	1	1
23	octadecanoic acid	100914606	0.123915737	284.48	284.48	1	1	2	2
24	phenols	2151	1.234567901	203.25	203.25	2	2	1	1
25	pentadecanoic acid	91929149	0.152671756	242.4	242.4	2	2	2	2
26	dihydocoriandrin	351388	0.418410042	232.24	232.24	0	0	0	0
27	myorelaxant	728948	0.288184438	196.29	196.29	0	0	2	2
28	antihypertensive	461549	-0.183150183	327.31	327.31	0	0	7	7
29	E-11-Tetradecenoic acid	5362745	0.189753321	226.36	226.36	1	1	2	2

QSAR MODEL GENERATION:

The various models were generated by both independent variables(all descriptors) against the dependent variable 1/logP. Finally the identification of best QSAR model between 1/log P values and structural descriptors could be the major molecular factor are associated with the activity of drug molecule. Further these models were validated using leave-one-out mehod in MLR analysis. The graphical analysis for the QSAR model has been plotted between the predicted value from the model X-axis and the predicted 1/log P values in Y-axis (image1). The graph depicts that, the compounds aligned on and near the diagonal line displayed the good correlation between predicted 1/log P values and structural descriptors (antifungal activity)

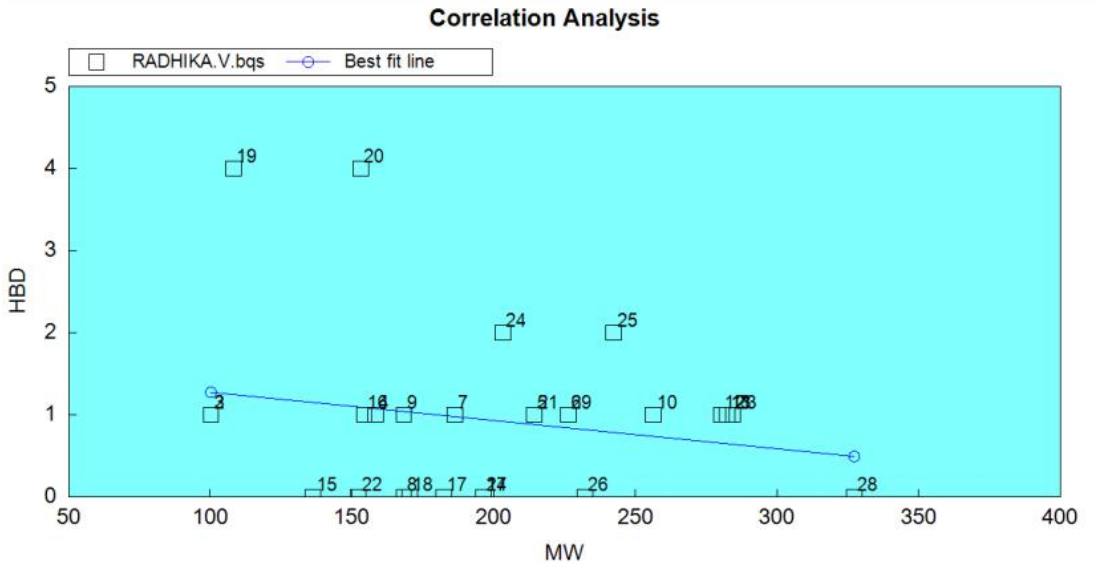
IMAGE 1:-Graph(a) depicted that 3 compounds were occupied on the regression line and 10 compounds near the line. Thus the 13 predicted Compounds were found to be best inhibitors. Graph (b) showed that 3 compounds were occupied on the regression line and 4 compounds near the line. Thus the 7 predicted Compounds were found to be best inhibitors. Graph(c) depicted that 4 compounds were occupied on the regression line and 8 compounds near the line. Thus the 15 predicted Compounds were found to be best inhibitors And. Graph (d) showed that 4 compounds were occupied on the regression line and 5 compounds near the line. Thus the 16 predicted Compounds were found to be best inhibitors.



MOLECULAR WEIGHT AGAINST 1/LOG P

S.NO	COMPOUND NAME	MW AGAINST 1/LOG P
1	undecanoic acid	7
2	palmitic acid	9
3	limonene	14
4	2E-dodecenal	16
5	oleic acid	10
6	dihydocoriandrin	25
7	E-11-Tetradecenoic acid	29
8	tridecanoic acid	6
9	4-nitro-o-phenylenediamine (NOP)	20

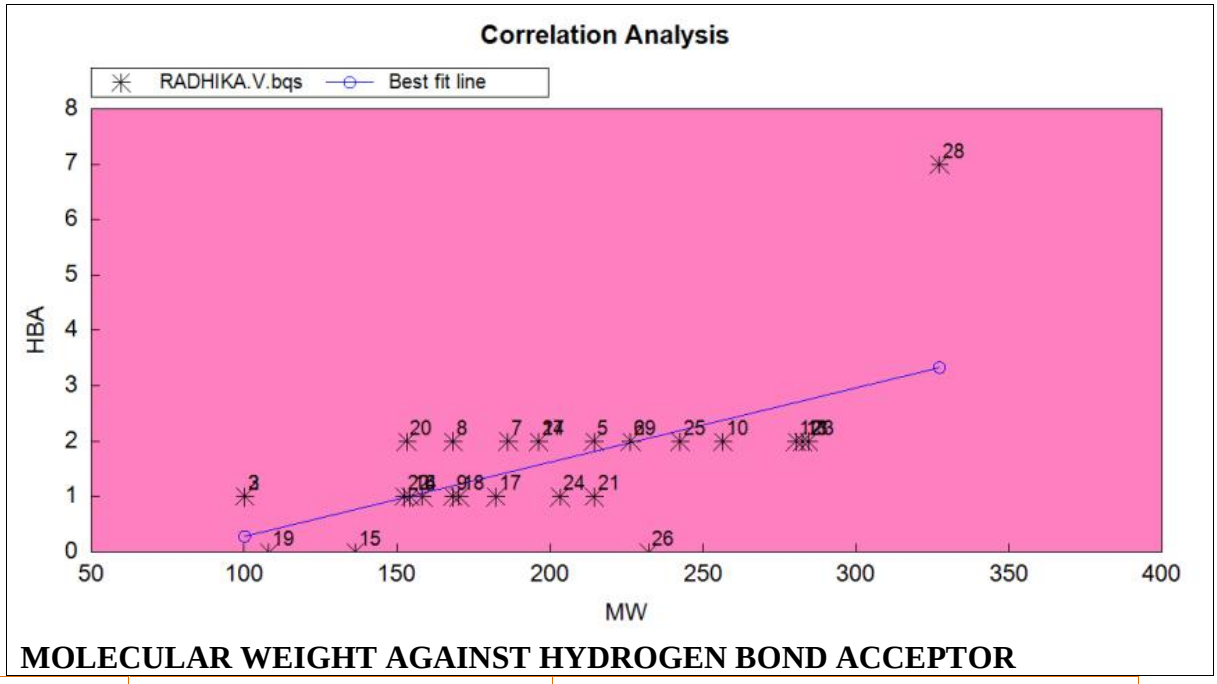
IMAGE 2 Graph(a)depicted that 3 compounds were occupied on the regression line and 6 compounds near the line. Thus the 9 predicted Compounds were found to be best inhibitors. Graph (b) showed that 2 compounds were occupied on the regression line and 5 compounds near the line. Thus the 7 predicted Compounds were found to be best inhibitors. And Graph(c) showed that 2 compounds were occupied on the regression line and 4 compounds near the line. Thus the 9 predicted Compounds were found to be best inhibitors.



MOLECULAR WEIGHT AGAINST HYDROGEN BOND DONAR

S.NO	COMPOUND NAME	MOLECULAR WEIGHT AGAINST HBD
1	undecanoic acid	7
2	palmitic acid	9
3	limonene	14
4	2E-dodecenal	16

IMAGE 3: Graph(a)depicted that 3 compounds were occupied on the regression line and 6 compounds near the line. Thus the 9 predicted Compounds were found to be best inhibitors. Graph (b) showed that 2 compounds were occupied on the regression line and 5 compounds near the line. Thus the 7 predicted Compounds were found to be best inhibitors. And Graph(c) showed that 2 compounds were occupied on the regression line and 4 compounds near the line. Thus the 4 predicted Compounds were found to be best inhibitors.



MOLECULAR WEIGHT AGAINST HYDROGEN BOND ACCEPTOR

S.NO	COMPOUND NAME	MOLECULAR WEIGHT AGAINST HBA
1	pentadecanoic acid	25
2	E-11-Tetradecenoic acid	29
3	tridecanoic acid	5
4	palmitic acid	9
5	cis-pihydrocarvone	22
6	2E-dodecenal	16

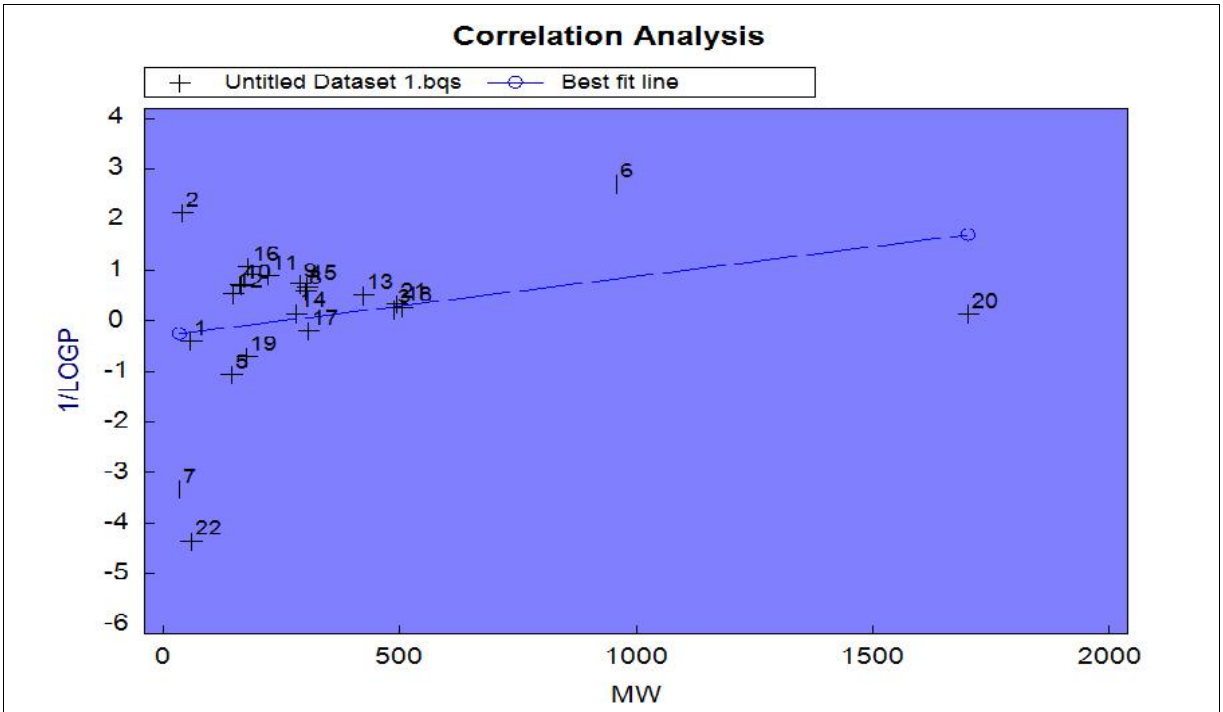
Centella asiatica plants

Table 1: Dependent and Independent variables (descriptors) used in QSAR models

S.NO	COMPOUNDS NAME	PUBCHEM ID	DEPENDENT	INDEPENDENT				
			1/LOG P	MW	K+MW	HBD	K+HBD	HBA	K+HBA
1	Ferric thiocyanate	165185	-0.393700787	58.09	58.09	0	0	1	1

2	Acetonitrile	6342	2.127659574	41.05	41.05	0	0	1	1
3	Asiatic acid	119034	0.212765957	488.71	488.71	4	4	5	5
4	Trichloroacetic acid	6421	0.709219858	163.39	163.39	1	1	2	2
5	Thiobarbituric acid	2723628	-1.063829787	144.16	144.16	2	2	3	3
6	Asiaticoside	108062	2.702702703	959.13	959.13	12	12	19	19
7	Hydroperoxide	784	-3.333333333	34.01	34.01	2	2	2	2
8	Quercetin	5280343	0.595238095	302.24	302.24	5	5	7	7
9	Catechin	9064	0.729927007	290.27	290.27	5	5	6	6
10	p-coumaric acid	637542	0.699300699	164.16	164.16	2	2	3	3
11	isobutylmethylxanthine	3758	0.892857143	222.25	222.25	1	1	3	3
12	Cinnamic acid	444539	0.523560209	148.16	148.16	1	1	2	2
13	Phosphatidic acid	24978512	0.507614213	423.46	423.46	1	1	8	8
14	Linoleic acid	5280450	0.145772595	280.45	280.45	1	1	2	2
15	Chloroauric acid	44134746	0.675675676	303.33	303.33	0	0	0	0
16	Caffeic acid	689043	1.063829787	180.16	180.16	3	3	4	4
17	Glutathione	124886	-0.201207243	307.33	307.33	7	7	6	6
18	Madecassic acid	73412	0.264550265	504.71	504.71	5	5	6	6
19	Ascorbic acid	54670067	-0.714285714	176.12	176.12	4	4	6	6
20	Tannic acid	16129778	0.141643059	1701.21	1701.21	25	25	46	46
21	Phenolic acid		0.332225914	494.45	494.45	7	7	10	10
22	Glacial acetic acid	176	-4.347826087	60.05	60.05	1	1	0	0

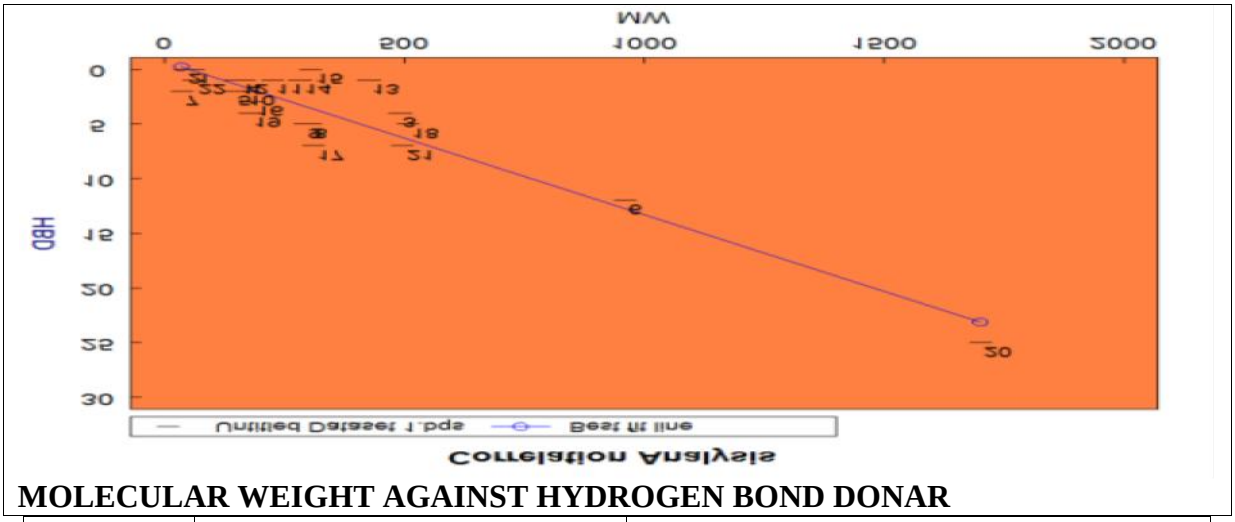
IMAGE.1:-Graph(a) depicted that 3 compounds were occupied on the regression line and 10 compounds near the line. Thus the 13 predicted Compounds were found to be best inhibitors.Graph (b) showed that 3 compounds were occupied on the regression line and 4 compounds near the line. Thus the 7 predicted Compounds were found to be best inhibitors. Graph(c) depicted that 4 compounds were occupied on the regression line and 8 compounds near the line. Thus the 12 predicted Compounds were found to be best inhibitors And. Graph (d) showed that 4 compounds were occupied on the regression line and 5 compounds near the line. Thus the 10 predicted Compounds were found to be best inhibitors.



MOLECULAR WEIGHT AGAINST HYDROGEN BOND ACCEPTOR

S.NO	COMPOUND NAME	MW AGAINST 1/LOG P
1	Ferric thiocyanate	1
2	Glutathione	5
3	Asiatic acid	6
4	Madecassic acid	9
5	Betulinic acid	12

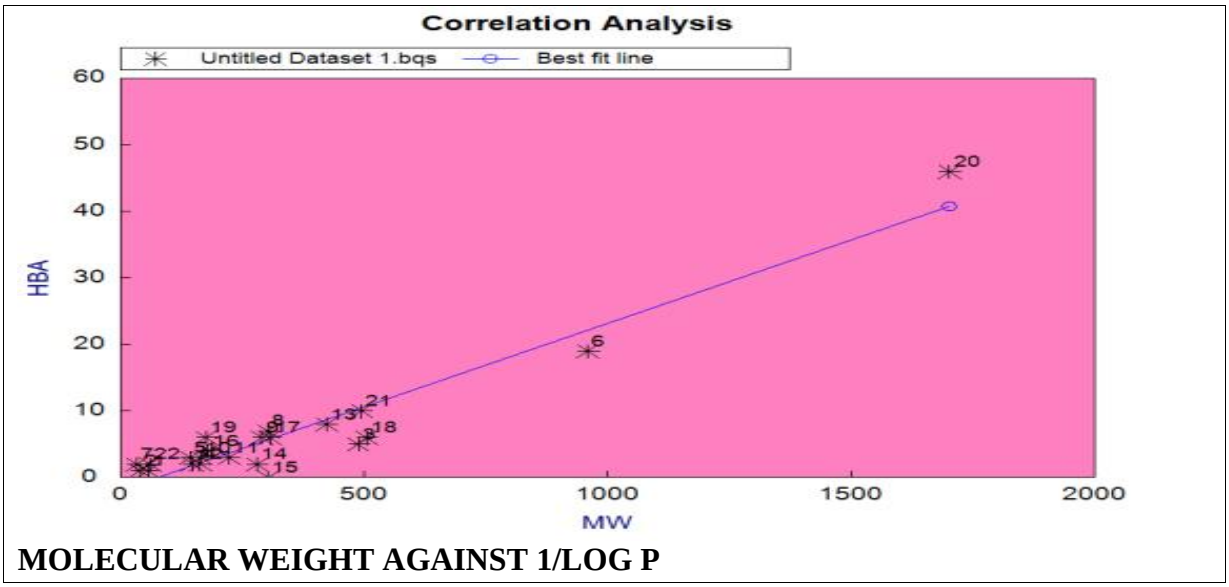
IMAGE 2: Graph (a) depicted that 3 compounds were occupied on the regression line and 6 compounds near the line. Thus the 9 predicted Compounds were found to be best inhibitors. Graph (b) showed that 2 compounds were occupied on the regression line and 5 compounds near the line. Thus the 7 predicted Compounds were found to be best inhibitors. And Graph(c) showed that 2 compounds were occupied on the regression line and 4 compounds near the line. Thus the 6 predicted Compounds were found to be best inhibitors.



MOLECULAR WEIGHT AGAINST HYDROGEN BOND DONAR

S.NO	COMPOUND NAME	MOLECULAR WEIGHT AGAINST HBD
1	Phenolic acid	21
2	isobutylmethylxanthine	11
3	Cinnamic acid	12

IMAGE 3:Graph(a)depicted that 3 compounds were occupied on the regression line and 6 compounds near the line. Thus the 9 predicted Compounds were found to be best inhibitors. Graph (b) showed that 2 compounds were occupied on the regression line and 5 compounds near the line. Thus the 7 predicted Compounds were found to be best inhibitors. And Graph(c) showed that 2 compounds were occupied on the regression line and 4 compounds near the line. Thus the 6 predicted Compounds were found to be best inhibitors.



MOLECULAR WEIGHT AGAINST 1/LOG P

S.NO	COMPOUND NAME	MOLECULAR WEIGHT AGAINST HBA
1	Phenolic acid	21
2	Phosphatidic	13
3	Glutathion	17
4	Catechi	9
5	isobutylmethylxanthine	11
6	Trichloroacetic acid	4

Conclusion

QSAR study was employed to determine the antifungal activity of the compounds from the plants Coriandrum sativam and Centella asiatica. The compounds were analyzed whether to obey Lipinski's rule of five, predicted through QED and molinspiration. Among 100 compounds, only 52 showed drug-likeness. Further on QSAR analysis, the compounds obtusin, thymohydroquinone and aloe emodin demonstrated antifungal property based on the descriptors molecular volume, molecular weight, polar surface area, number of rotatable bonds, number of aromatic rings, hydrogen donor and acceptor. These three compounds would be explored for future perspectives like docking studies and pharmacophore mapping.

Conflict of interest:

The authors declare they have no competing interests.

Acknowledgments

We acknowledge Vels Institute of Science, Technology and Advanced Studies (VISTAS) for providing us with required infrastructure and support system needed.

References

1) Saab R1, Rodriguez-Galindo C, Matmati K, Rehg JE, Baumer SH, Khoury JD, Billups C, Neale G, Helton KJ, Skapek SXp18Ink4c and p53 Act as tumor suppressors in cyclin D1-driven primitive neuroectodermal tumor. 1Children's Cancer Center of Lebanon, American University of Beirut Medical Center, Beirut, Lebanon.

2. Chahal, Khushminder& Singh, Ravinder& Kumar, A. & Bhardwaj, Urvashi. (2017). Chemical composition and biological activity of coriandrumsativum l.: A review. Indian Journal of Natural Products and Resources. 8. 193-203.

3. FarhanaNaziraIdris and MasrinaMohdNadzir . Comparative Studies on Different Extraction Methods of Centellaasiatica and Extracts Bioactive Compounds Effects on Antimicrobial Activities. 2021, 10, 457.

4. Kim S, Thiessen PA, Bolton EE, Chen J, Fu G, Gindulyte A, Han L, He J, He S, Shoemaker BA, Wang J, Yu B, Zhang J, Bryant SH. PubChem Substance and Compound databases. Nucleic Acids Res. 2016 Jan 4;44(D1):D1202-13.

5 Thangavelu, Rajkumar& .P, Shirisha& Faisal, Saima&Hussain, Shaik&Nagaiah, T &Sulthana, Ayesha &Rajkumar, Mr. (2016). PREDICTION OF MOLECULAR PROPERTIES, BIOACTIVITY & DOCKING OF NOVEL HYDRAZINES.International Journal of Trends in Pharmacy and Life Sciences. 2. 757-768.

6. Sadeghian-Rizi, S., Sakhteman, A., &Hassanzadeh, F. (2016). A quantitative structure-activity relationship (QSAR) study of some diaryl urea derivatives of B-RAF inhibitors. Research in pharmaceutical sciences, 11(6)

Access this Article in Online	
	Website: www.ijarbs.com
Quick Response Code	Subject: Bioinformatics
DOI:10.22192/ijarbs.2022.09.05.01.017	

How to cite this article:
Mahendran Radha, Jyothsana Madhavan, K. Eswaramoorthy, A. Jyotsna, Jeyabaskar Suganya, R. Priya, M.Vinoth, Nishandhini. M. (2022). *In silico* QSAR studies on Indian medicinal plant of Coriandrum sativam (Coriander) and Centellaasiatica (Gotu Kola) as fungal inhibitors. Int. J. Adv. Res. Biol. Sci. 9(5): Special Issue 1: 173-184.
DOI: http://dx.doi.org/10.22192/ijarbs.2022.09.05.01.017