Research Article **ISSN: 2349 – 4492**

Asian Journal of Research in Biological and Pharmaceutical Sciences

Journal home page: www.ajrbps.com

ANALYZING THE NOVEL CHEMICAL CONSTITUENT FITNESS FOR THE DISEASE INFLUENZA

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ABSTRACT

Influenza is an acute highly contagious infection of the respiratory tract which is spread by influenza viruses. Influenza virus's proteins are the main target for the anitiviral drugs which produce adverse side effects like anti-pyretics, anti-inflammatory. So the scientists turned the attention to powerful herbal medicines. We list out some of the best practiced antiviral herbs chemical composition like Eugenol, Ursolic acid, Carvacrol, Gingerol, Zingeberene, Shogoal, Allyl propyl sulfide, Dially sulfide and Allicin. Their fitness is evaluated through Lipinski rule of five and Wienner index Calculator. From this the highly referenced herbs chemical constituents like Eugenol, Gingerol and Allicin are taken for our further study. They are taken as ligands. Moreover the receptors Neuraminidase and M2 ion give their best active site cavities. The binding ability and the distance calculation predict allicin, gingerol and eugenol optimized result. So it is recommended that these drugs can be used to control influenza.

KEYWORDS

Influenza type A, Antiviral herbs, Fitness, Binding ability and Active site.

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INTRODUCTON

Influenza, often called the flu, is an acute, highly contagious infection of the respiratory tract. It affects the people of all ages. Influenza spreads around the world as seasonal epidemics resulting in the deaths of hundreds of thousands annually (Who.int, 2014)[1]. People such as older people, young children and people with certain health conditions, are at high risk for serious flu complications (Cdc.gov, 2014)[2]. People who have the flu are most likely to pass it to someone else

from 1 day before to 5 days after symptoms develop. Children may be infectious for up to 6 days before symptoms develop (Cdc.gov, 2014)[2]. Children are much more infectious than adults and shed virus from just before they develop symptoms until two weeks after infection (Carrat F, 2006[3] and Mitamura K, 2006)[4].

Viruses in the family orthomyxoviridae cause influenza. There are three genera of influenza viruses: *influenza virus A, influenza virus B and influenza virus C* (ICTV, 2003)[5]. These viruses are also called type A, type B and type C influenza viruses. Mutations make the influenza viruses to change over time. Hence the genetic materials also undergo changes and new subtypes are evolved (The Gale Group Inc, 2003)[6]. The most effective way to prevent the disease or severe outcomes form the illness is vaccination (Who.int, 2014)[1].

The World Health Organization (WHO) in assisted with the National Influenza Centers (NIC) makes recommendation for two different vaccine formulations every year; one for the Northern and one for the Southern Hemisphere (Who.int, 2014)[1]. Vaccine preparation remains challenging for the scientist. The reason for this the strains of flu viruses change from year to year and this new strain often replaces the older strain (Wolf, 2006)[7].

Antiviral drugs have a role in the prevention and treatment of mainly influenza type a infection. Currently, there are four antiviral drugs available. They are amantadine, rimantadine, zanamivir and oseltamivir. In 2006, the CDC recommended that neither amantadine nor rimantadine be used for prevention of influenza A as resistance to these drugs had developed. The 2007-2008 Advisory Committees on Immunization Practices (ACIP) recommends that only zanamivir and oseltamivir can be used in the U.S for treatment or prevention until influenza a susceptibility to the other drugs is reestablished. Antiviral medication may be effective, if given early, but some strains of influenza can show resistance to the standard antiviral drugs and there is concern about the quality of the research (Hurt AC *et al*, 2006)[8].

The conventional therapies are focused on the temporary symptoms and also produce adverse side effects like anti-pyretics, anti-inflammatory. This makes the scientists turned the attention to powerful herbal medicines. For this purpose number of patients seeking alternate and herbal therapy is growing exponentially. Herbal medicines are now in great demand in the developing world. Since they are have better cultural acceptability, better compatibility with the human body and minimum side effects. Beside this the immune stimulant drug can support the body's natural defenses potentially (Kalra M *et al*, 2011)[9].

Complementary and traditional medicines have been utilized for several years in various parts of the world to alleviate human disease (Rajesh arora *et al*, 2011)[10]. For all these medicines plants are the rich source. Several antiviral agents including polyphenols, flavonoids, saponines, glucosides and alkaloids have been isolated from plants and are used in pharmacological studies (X Wang *et al*, 2006)[11].

Drug design is one of the active components in the field of Bioinformatics. The activity of the drug is best notified by the preferred orientation of binding with the receptor. Docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex (Lengauer T, and Rareu M, 1996)[12] and also predict the binding orientation of small molecule drug to their protein targets (Kitcher D B *et al*, 2004)[13]. Prior to docking the active site of the receptor is analyzed and the ligands are evaluated for their efficiency. Docking software is used to find out the binding site of the receptor and ligand. The close distance between the bindings modes of the complex describe their native structure.

MATERIAL AND METHODS

Antiviral herbs chemical constituent and its conversion

The required antiviral herbs chemical constituent like Eugenol, Ursolic acid, Carvacrol, Gingerol, Zingeberene, Shogoal, Allyl propyl sulfide, Dially sulfide, Allicin are selected form the chemspider database. For the purpose of further analyzing the chemical constituents in mol extension are converted into pdb file extension by using the chemspider database (Table No.1).

Efficiency analyzing

The selected antiviral herbs chemical constituent efficacies are analyzed by the database SCFBIO-

LIPINSKI Rule of five and Wiener index calculator (Table No.2 and 3).

Selection of test set

From the PDB database the required receptor neuraminidase (2htv.pdb) M2 ion channel (3bkd.pdb) and the ligands Eugenol, Gingerol and Allicin are selected (Table No.4).

Active site prediction

The receptor active sites are predicted by using SCFBIO-Active site prediction server (Table No. 5 and 6).

Docking studies

The servers namely HEX is used for docking studies. To these servers the following receptor and highly preferred selective ligands like Eugenol (Hu Ge *et al,* 2010)[14], Gingerol and Allicin (Feng T, 2011[15] and Shubham S *et al,* 2017)[16] are fed for to analyze their binding mode (Table No.7).

Binding distance calculation

After docking the binding distance between the complexes are calculated by using swiss PDB Viewer (Table No.8 and 9).

RESULTS AND DISCUSSION

Analyzing efficiency

The chemical constituent Dially sulfide shows the best efficiency values in both Lipinski rule of five and Wienner index calculator.

Active site

The receptor neuraminidase shows 108 cavities as their active site whereas the receptor M2 ion channel shows 28 cavities as their active site. Both receptors give their best active site cavities.

Docking studies

Docking is the process by which two molecules fit together in 3D space (Mehrotra *et al*, 2005)[17] and its ultimate goal is to predict the structure of the resulting complex (Brindha devi and Chandraskaran, 2013)[18]. The receptor and ligand molecules are fed into the software HEX. It show the neuraminidase receptor and the ligand Eugenol, Gingerol and Allicin have high Angstrom value and for the receptor M2 ion channel and the ligands Eugenol, Gingerol and Allicin have low Angstrom value.

The docked output structures are submitted to SPDBV for the calculation of their various binding mode. The neuraminidase docked complexes have greater angstrom value (Table No.8) than the M2 ion channel docked complex (Table No. 9).

Based on the distance calculation methodology of Brindha devi *et al*, 2014[19] the M2 ion channel suggested to have the best binding mode. As per this the M2 ion channel docked complex distance measurement is further analyzed. The docked complex residues are classified into three major areas as interface area, contact area and near native structure (Table No.10,11 and 12) (Brindha Devi *et al*, 2013[18], Morelli *et al*, 2000[20], Wenfen 2005[21], Palma *et al*[22], 2000, Li *et al*, 2003)[23].

Table No.1: Antiviral herbs chemical constituent conversion from mol to pdb

S.No	Ligand name	Chemspider ID	PDB id
1	Eugenol	13876130.Mol	Eugenol.pdb
2	Ursolic Acid	58472.Mol	ursolic acid.pdb
3	Carvacrol	21105867.Mol	carvacrol.pdb
4	Gingerol	391126.Mol	gingerol.pdb
5	Zingeberene	83751.Mol	zingeberene.pdb
6	Shogoal	445106.Mol	shogoal.pdb
7	Allyl Propyl Sulfide	89217.Mol	allyl propyl sulfide.pdb
8	Dially Sulfide	11128.Mol	dially sulfide.pdb
9	Allicin	58548.Mol	allicin.pdb

Table No.2: Antiviral herbs chemical constituent Lipinski values

		LIPINSKI RULE OF FIVE				
S.No	**Antiviral herbs chemical constituent name**	**Mass**	**H bond donor**	**H bond acceptor**	**LOGP**	**Molar Refractivity**
1	Eugenol	164.000000	1	2	2.129300	48.559792
2	Ursolic Acid	455.000000	1	3	5.754800	129.982758
3	Carvacrol	150.000000	1	1	2.824019	46.932793
4	Gingerol	294.000000	2	4	3.233799	82.752571
5	Zingeberene	204.000000	0	0	4.891299	68.832977
6	Shogoal	276.000000	1	3	4.038999	81.268776
7	Allyl Propyl Sulfide	116.000000	0	0	2.315600	37.812992
8	Dially Sulfide	114.000000	0	0	2.091600	37.718994
9	Allicin	163.000000	1	1	2.097900	47.712791

Table No.3: Antiviral herbs chemical constituent wiener index values

S.No	**Antiviral herbs chemical constituent**	**Wiener index**
1	Eugenol	153.833
2	Ursolic Acid	2516.75
3	Carvacrol	120.417
4	Gingerol	1037.33
5	Zingeberene	391
6	Shogoal	894.042
7	Allyl Propyl Sulfide	54.9375
8	Dially Sulfide	35.625
9	Allicin	38.625

Table No.4: Receptor and ligand selection from Pdb

S.No	**Receptor name**	**PDB ID**	**Ligand name**	**PDB ID**
1	Neuraminidase	2htv.pdb	Eugenol	eugenol.pdb
2	M2 Ion channel	3bkd.pdb	Gingerol	gingerol.pdb
3	----------	----------	Allicin	allicin.pdb

Table No.5: Neuraminidase active site (cavities)

cavity_1_TESKRWGPDFINVAYQL	cavity_2_QSVFTLRWPNIGKDEYAM
cavity_3_LDKSIFAQVWPTGRNMEY	cavity_4_TESKGWRILNPVDFYQAH
cavity_5_LIWTMERKDGQVSPFYN	cavity_6_QSVRPTGLWKDEIYANF
cavity_7_RNGKCPTQVSDWYLEFAI	cavity_8_FESDTKWVNIGMPRLAQ
cavity_9_AWSNGVDQFTRIKEPML	cavity_10_FVLCYASTGQEKRWNPDI
cavity_11_GVEITRPCNSWYFALKD	cavity_12_FSRGVNKDTEPIMLYW
cavity_13_VICFLDATPWQGSKNMR	cavity_14_SLRFANGPIKWDMETQ
cavity_15_SVAPDTCRNGQKFWLYEI	cavity_16_RGENSIVPADLCKFWTM
cavity_17_SNIVPARGEDCKLWFTY	cavity_18_NGKDCRSPLTEVYWAFQ
cavity_19_NKGERTDCIPLSVYFWAQ	cavity_20_WDSINFVKTRGELPYM
cavity_21_PYCDKVNGWSAFTQIRE	cavity_22_IRSNLKFAGPWDME
cavity_23_WTGQDKNFVERYSILAM	cavity_24_PNEIGCSLRTAVDYFWQK
cavity_25_LDSYEGVNIFCRAWQ	cavity_26_PALWQTSFIKGVDNEMR
cavity_27_GADSPNKIEVMRLWFT	cavity_28_NGQKCPDVWFLYSIAR
cavity_29_WGNTAQPSFIVDREKL	cavity_30_EGSDNQRLYVFWIC
cavity_31_INGWKVTREFPSMLQA	cavity_32_FRSVMTPLWIEQGDKAHN

cavity_33_HIVESKPFYNTCGRWA	cavity_34_RSFGINTKEQVPLW
cavity_35_ECLRPINTVGSWFKAD	cavity_36_CEPRNSGDWVAYTMKL
cavity_37_RDPITSEWVLNGQKA	cavity_38_PNRSEFVCWIGKYTL
cavity_39_KPYNGTCSIWERAVFM	cavity_40_DSNRLIGFAPKVWQTME
cavity_41_PRVNEICWSTGLYKH	cavity_42_DIGTLKAVERFSPW
cavity_43_IKHYESRLGCDVPQFN	cavity_44_PSFAEVQIGLRHNDWK
cavity_45_QDFYSEGKVNCLRWI	cavity_46_NQSDRYGFEWVICPAT
cavity_47_PLVDNFHKIGASTQWR	cavity_48_SEDGNKRTCQPLIVYW
cavity_49_RTCNIVYKSWDFLAGPQ	cavity_50_RMLTWKVYGNDPFAQI
cavity_51_ESPLVDRFHGATQ	cavity_52_CYFKWDRVQAIPGNS
cavity_53_ITKGVDALMSW	cavity_54_RVGENPSYDKWQAI
cavity_55_RTIGQVLEAHNFSDWKP	cavity_56_GIKSLWPCTAVDRFNQ
cavity_57_ETGIRHYSNKCPDQVL	cavity_58_FTKQVPSRLWDGEA
cavity_59_DCRPSLTNIGVYKWAFQ	cavity_60_IGWCPFNYTVSQRD
cavity_61_FITGKEVPSWDAL	cavity_62_KVDYIPAFWTGQ
cavity_63_VNERWSIGPYKHCTL	cavity_64_HSEFDGKVNYQRILCPT
cavity_65_VKTGSAEPWNRIDFQ	cavity_66_VSIKLDTWF
cavity_67_RDATMISENGWPKYFQ	cavity_68_ENRYDGPVFKAQIWCS
cavity_69_IGRVDANWQSKCYFTP	cavity_70_REGPLDSVNFHKIAQWT
cavity_71_PNGSWERCKATIFVM	cavity_72_IGRVLDFKPMWNSCYT
cavity_73_HIVSFEDKPYNCGT	cavity_74_RIDSVNLFAGPWKE
cavity_75_TLGISCRVADNKPWY	cavity_76_WPATNFSGIDQVKER
cavity_77_DNSYQKLRVFWICGPA	cavity_78_PGQSERWNDAYK
cavity_79_RSEGNIVLAPDCKF	cavity_80_HISEDGNVKRPTCQYF
cavity_81_NEVCWSRIPTGYLKQ	cavity_82_NSIVEPARGFDLCKTWM
cavity_83_EYKTRGLCSNWPFAQ	cavity_84_DVKSYILW
cavity_41_PRVNEICWSTGLYKH	cavity_42_DIGTLKAVERFSPW
cavity_43_IKHYESRLGCDVPQFN	cavity_44_PSFAEVQIGLRHNDWK
cavity_45_QDFYSEGKVNCLRWI	cavity_46_NQSDRYGFEWVICPAT
cavity_47_PLVDNFHKIGASTQWR	cavity_48_SEDGNKRTCQPLIVYW
cavity_49_RTCNIVYKSWDFLAGPQ	cavity_50_RMLTWKVYGNDPFAQI
cavity_51_ESPLVDRFHGATQ	cavity_52_CYFKWDRVQAIPGNS
cavity_53_ITKGVDALMSW	cavity_54_RVGENPSYDKWQAI
cavity_55_RTIGQVLEAHNFSDWKP	cavity_56_GIKSLWPCTAVDRFNQ
cavity_57_ETGIRHYSNKCPDQVL	cavity_58_FTKQVPSRLWDGEA
cavity_59_DCRPSLTNIGVYKWAFQ	cavity_60_IGWCPFNYTVSQRD
cavity_61_FITGKEVPSWDAL	cavity_62_KVDYIPAFWTGQ
cavity_63_VNERWSIGPYKHCTL	cavity_64_HSEFDGKVNYQRILCPT
cavity_65_VKTGSAEPWNRIDFQ	cavity_66_VSIKLDTWF
cavity_67_RDATMISENGWPKYFQ	cavity_68_ENRYDGPVFKAQIWCS
cavity_69_IGRVDANWQSKCYFTP	cavity_70_REGPLDSVNFHKIAQWT
cavity_71_PNGSWERCKATIFVM	cavity_72_IGRVLDFKPMWNSCYT
cavity_73_HIVSFEDKPYNCGT	cavity_74_RIDSVNLFAGPWKE
cavity_75_TLGISCRVADNKPWY	cavity_76_WPATNFSGIDQVKER
cavity_77_DNSYQKLRVFWICGPA	cavity_78_PGQSERWNDAYK
cavity_79_RSEGNIVLAPDCKF	cavity_80_HISEDGNVKRPTCQYF

cavity_81_NEVCWSRIPTGYLKQ	cavity_82_NSIVEPARGFDLCKTWM
cavity_83_EYKTRGLCSNWPFAQ	cavity_84_DVKSYILW
cavity_85_CWSFYGVRNKDETP	cavity_86_ETPVFLSDGNICRWQ
cavity_87_IHKSEGQPYRCFTVWA	cavity_88_KVTDGPIALRMSW
cavity_89_KWFGTANPREISD	cavity_90_CGFEKRSDVNYTMPIW
cavity_91_KIDVFYLSN	cavity_92_VNIETPGSCRHYK
cavity_93_FTKGWERVDISCN	cavity_94_DNSLKIFPVWTERGQ
cavity_95_ETWFKPDLSRYIGMQ	cavity_96_FSCPTVGQLRWDEYK
cavity_97_DYVGWNASTQKR	cavity_98_KSLINPWTCAVFMQG
cavity_99_EFVYSKNQILCDPTA	cavity_100_NSRVFEGYPLC
cavity_101_ATSFGEWKPLRID	cavity_102_VCFLPAWQGTSIKDM
cavity_103_WVNYGISRADKCT	cavity_104_GSKYLCERVIQPFN
cavity_105_PMFIRTWESYKVGND	cavity_106_EKVYINGDTCW
cavity_107_INGYKTVCD	cavity_108_YIFDVCGWPANR
cavity_85_CWSFYGVRNKDETP	cavity_86_ETPVFLSDGNICRWQ
cavity_87_IHKSEGQPYRCFTVWA	cavity_88_KVTDGPIALRMSW
cavity_89_KWFGTANPREISD	cavity_90_CGFEKRSDVNYTMPIW
cavity_91_KIDVFYLSN	cavity_92_VNIETPGSCRHYK
cavity_93_FTKGWERVDISCN	cavity_94_DNSLKIFPVWTERGQ
cavity_95_ETWFKPDLSRYIGMQ	cavity_96_FSCPTVGQLRWDEYK
cavity_97_DYVGWNASTQKR	cavity_98_KSLINPWTCAVFMQG
cavity_99_EFVYSKNQILCDPTA	cavity_100_NSRVFEGYPLC
cavity_101_ATSFGEWKPLRID	cavity_102_VCFLPAWQGTSIKDM
cavity_103_WVNYGISRADKCT	cavity_104_GSKYLCERVIQPFN
cavity_105_PMFIRTWESYKVGND	cavity_106_EKVYINGDTCW
cavity_107_INGYKTVCD	cavity_108_YIFDVCGWPANR

Table No.6: m2 ion channel active site (Cavities)

cavity_1_PLRDVAIWSHG	cavity_2_VPSAILGHWDR
cavity_3_PVLDIASGHWR	cavity_4_RLDWIAHGSVP
cavity_5_LRPDWIHGA	cavity_6_ISALGHWDR
cavity_7_PDSLVRAIWGH	cavity_8_IHLGAWSRDVP
cavity_9_LPRDWAIHSGV	cavity_10_VLSAIGHWDR
cavity_11_HWLIGASVPD	cavity_12_RDWLHIGAS
cavity_13_LPAVISGHWDR	cavity_14_SDVPALRIWGH
cavity_15_RWDLHIGASVP	cavity_16_RDWLHIGASV
cavity_17_SDPVLRWIAH	cavity_18_RDWHILGAS
cavity_19_WIHLGASVP	cavity_20_SDPVLRAIWGH
cavity_21_PVLIASGHWR	cavity_22_PLDVAISGHW
cavity_23_SPDVLARIG	cavity_24_AISLVPD
cavity_25_LIASVPD	cavity_26_SPDVLIAG
cavity_27_IASLGHWDR	cavity_28_SPDVLAI

Table No.7: List of receptor and ligand used for docking

S.No	Receptor name	Ligand name
1	Neuraminidase (2htv.pdb)	Eugenol (eugenol.pdb)
2	Neuraminidase (2htv.pdb)	Gingerol (gingerol.pdb)
3	Neuraminidase (2htv.pdb)	Allicin (allicin.pdb)
4	M2ion channel (3bkd.pdb)	Eugenol (eugenol.pdb)
5	M2ion channel (3bkd.pdb)	Gingerol (gingerol.pdb)
6	M2ion channel (3bkd.pdb)	Allicin (allicin.pdb)

Table No.8: Receptor Neuraminidase residues and their ligand RMSD values

S.No	Neuraminidase residues	Eugenol	Gingerol	Allicin
1	CYS 92	133.22	-	133.22
2	GLY 88	126.17	-	126.17
3	ILE 126	136.62	-	136.62
4	ILE 210	136.60	-	136.10
5	ILE 211	134.95	-	134.95
6	HIS S4	130.15	-	130.15
7	LYS 150	-	198.03	-
8	LYS 219	-	205.45	-
9	GLY 414	-	197.39	-
10	ASPP 452	-	142.44	-
11	TRP 378	-	134.10	-

Table No.9: Receptor M2 ion channel residues and their ligand RMSD values

S.No	M2 ion channel residues	Eugenol	Gingerol	Allicin
1	SER 31	2.80	-	-
2	ILE 35	3.52	5.90	-
3	ALA 30	3.96	-	-
4	BOG 702	3.94	-	-
5	ALA 29	3.94	3.91	-
6	HIS 37	-	4.15	-
7	LEU 43	-	5.56	-
8	ILE 39	-	5.49	-
9	ILE 32	-	-	4.11
10	BOG 71	-	-	5.32
11	LEU 38	-	-	3.21
12	BOG 701	-	-	2.97
13	MSE 33	-	-	1..65

Table No.10: Distance calculation of the receptor M2 ion channel and the ligand eugenol

S.No	Angstrom value (RMSD)	Interface area (≤ 10Å)	Contact area (≤ 5Å)	Near native structure (< 4Å)
1	2.80	-	-	SER 31
2	3.52	-	-	ILE 35
3	3.96	-	-	ALA 30
4	3.94	-	-	BOG 702
5	3.94	-	-	ALA 29

Table No.11: Distance calculation of the receptor M2 ion channel and the ligand gingerol

S.No	Angstrom value	Interface area (≤ 10Å)	Contact area (≤ 5Å)	Near native structure (< 4Å)
1	5.90	ILE 35	-	-
2	4.15	-	HIS 37	-
3	5.56	LEU 43	-	-
4	3.91	-	-	ALA 29
5	5.49	ILE 39	-	-

Table No.12: Distance calculation of the receptor M2 ion channel and the ligand allicin

S.No	Angstrom value	Interface area (≤ 10Å)	Contact area (≤ 5Å)	Near native structure (< 4Å)
1	4.11	-	ILE 32	-
2	5.32	BOG 71	-	-
3	3.21	-	-	LEU 38
4	2.97	-	-	BOG 701
5	1.65	-	-	MSE 33

CONCLUSION

According to the concept lower the angstrom value give better binding orientation (Brindha Devi *et al,* 2014)[19] we observed all the residues of eugenol are in near native structure whereas for the ligand gingerol the residues ILE 35, LEU 43 and ILE 39 are in interface area HIS 37 residue is in contact area, ALA 29 is in near native structure. For the ligand Allicin BOG 71 residue is in interface area ILE 32 is in contact area, the residues LEU 38, BOG 701, MSE 33 are in near native structure. On comparing all the ligands the lowest Angstrom value 1.65 is observed in Allicin. Hence we suggest and conclude that the docked complex M2 ion channel with the ligands Eugenol and allicin show more residues in the near native structure. So it is recommended that these drugs can have better potency than others to control influenza.

ACKNOWLEDGMENT

The authors wish to express their sincere gratitude to Department of Biotechnology, Marudu Pandiyar College, Thanjavur, Tamil Nadu, India for providing necessary facilities to carry out this research work.

CONFLICT OF INTEREST

We declare that we have no conflict of interest.

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Please cite this article in press as: Brindha Devi A *et al*. Analyzing the novel chemical constituent fitness for the disease influenza, *Asian Journal of Research in Biological and Pharmaceutical Sciences,* 7(1), 2019, 15-23.