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Sequence Analysis and Drug Like Properties Studies on Toxin B in *Clostridium difficile*

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Abstract
C. difficile infection among people traditionally not considered high risk, such as younger and healthy individuals without a history of antibiotic use or exposure to health care facilities. Each year in the United States, about a half million people get sick from C. difficile, and in recent years, C. difficile infections have become more frequent, severe and difficult to treat. Toxin B (TcdB) is a cytotoxin that has a molecular weight of 270 kDa and an isoelectric point, pl, of 4.1. Toxin B has four different structural domains: catalytic, cysteine protease, translocation, and receptor binding. The sequence analysis of Toxin B protein retrieved from [NCBI] in fasta format. The structural analysis of Toxin B was carried out by using bioinformatics tools, like ncbi, pdb, amigo, drug bank, clustal w, online smiles translator.

Keywords
C. difficile, cytotoxin, Toxin B, NCBI, pdb , amigo, drug bank, clustal w.

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INTRODUCTION
Clostridium difficult (kilos-TRID-e-um dif-uh-SEEL), often called C. difficult or C. diff, is a bacterium that can cause symptoms ranging from diarrhea to life-threatening inflammation of the colon. illness from *C. difficile* most commonly affects older adults in hospitals or in long-term care facilities and typically occurs after use of antibiotic medications. However, studies show increasing rates of C. *difficile* infection among people traditionally not considered high risk, such as younger and healthy individuals without a history of antibiotic use or exposure to health care facilities. Each year in the United States, about a half million people get sick from C. *difficile,* and in recent years, *C. difficile* infections have become more frequent, severe and difficult to treat. *C. difficile* bacteria are found throughout the environment — in soil, air, water, human and animal feces, and food products, such as processed meats. A small number of healthy people naturally carry the bacteria in their large intestine and don't have ill effects from the infection. C. *difficile* infection is most commonly associated with health care and recent antibiotic use, occurring in hospitals and other health care facilities where a much higher percentage of people carry the bacteria. However, studies show increasing rates of community-associated *C. difficile* infection, which occurs among populations traditionally not considered high risk, such as children and people without a history of antibiotic use or recent hospitalization. Spores from C. *difficile* bacteria are passed in feces and spread to food, surfaces and objects when people who are infected don't wash their hands thoroughly. These spores can persist in a room for weeks or months. If you touch a surface contaminated with *C. difficile* spores, you may then unknowingly swallow the

bacteria. Your intestines contain about 100 trillion bacterial cells and up to 2,000 different kinds of bacteria, many of which help protect your body from infection. When you take an antibiotic to treat an infection, these drugs tend to destroy some of the normal, helpful bacteria in addition to the bacteria causing the infection. Without enough healthy bacteria to keep it in check, *C. difficile* can quickly grow out of control. The antibiotics that most often lead to C. difficile infections include fluoroquinolones, cephalosporins, penicillins and clindamycin. Once established, *C. difficile* can produce toxins that attack the lining of the intestine. The toxins destroy cells and produce patches (plaques) of inflammatory cells and decaying cellular debris inside the colon and cause watery diarrhea.

METHODOLOGY

Target protein of Toxin B in *Clostridium difficile* were retrieved from NCBI database. The sequence is submitted to PDB database for similarity search of Toxin B. The retrieved sequence is submitted to the amigo server for annotation analysis of Toxin B protein. The retrieved sequence is submitted to the JCAT server for gene expression analysis of annotated sequence with Toxin B proteins. The retrieved sequence is submitted to the Clustal-W server for multiple sequence alignment of annotated sequence with Toxin B protein. The retrieved sequence is submitted to bioedit server for sequence analysis of Toxin B protein. Based upon the bioavailability of drug ,drug compound were selected and drug like properties of the selected compound were analyzed using tools like online smiles translator and molinspiration server.

RESULT AND DISCUSSION

1. SEQUENCE RETRIVEL:

NCBI:

PROTEIN:

>AIW54888.1 botulinum neurotoxin type B, BoNT/B (plasmid) [Clostridium botulinum]

MPVTINNFNYNDPIDNDNIIMMEPPFARGTGRYYKAFKITD
RIWIIPERYTFGYKPEDFNKSSGIFNRDV
CEYYDPDYLNTNDKKNIFLQTMIKLFNRIKSKPLGEKLLEMII
NGIPYLGDRRVPLEEFNTNIASVTVNK
LISNPGEVEQKKGIFANLIIFGPGPVLNENETIDIGIQNHFAS
REGFGGIMQMKFCPEYVSVFNNVQENK
GASIFNRRGYFSDPALILMHELIHVLHGLYGIKVDDLPIVPNE
KKFFMQSTDTIQAEELYTFGGQDPSII
SPSTDKSIYDKVLQNFRGIVDRLNKVLVCISDPNININIYKNK
FKDKYKFVEDSEGKYSIDVESFNKLYK
SLMFGFTETNIAENYKIKTRASYFSDSLPPVKIKNLLDNEIYTI
EEGFNISDKNMGKEYRGQNKAINKQA
YEEISKEHLAVYKIQMCKSVKVPGICIDVDNENLFFIADKNSF
SDDLSKNERVEYNTQNNYIGNGFPINE
LILDTDLISKIELPSENTESLTDFNVDVPVYEKQPAIKKVFTDE
NTIFQYLYSQTFPLNIRDISLTSSFD
DALLVSSKVYSFFSMDYIKTANKVVEAGLFAGWVKQIVDDF
VIEANKSSTMDKIADISLIVPYIGLALNV
GNETAKGNFESAFEIAGSSILLEFIPELLIPVVGVFLLESYIDNK
NKIIKTIDNALTKRVEKWIDMYGLI
VAQWLSTVNTQFYTIKEGMYKALNYQAQALEEIIKYKYNIYS
EEEKSNININFNDINSKLNEGINQAMDN
INDFINECSVSYLMKKMIPLAVKKLLDFDNTLKKNLLNYIDE
NKLYLIGSVEDEKSKVDKYLKTIIPFDL
SMYTNNEILIKIFNKYNSEILNNIILNLRYRDNNLIDLSGYGAK
VEVYDGVKLNDKNQFKLTSSADSKIR
VTQNQNIIFNSMFLDFSVSFWIRIPKYRNDDIQNYIHNEYTII
NCMKNNSGWKISIRGNRIIWTLIDING
KTKSVFFEYNIREDISEYINRWFFVTITNNLDNAKIYINGTLES
NMDIKDIGEVIINGEITFKLDGDVDR
TQFIWMKYFSIFNTQLNQSNIKEIYKIQSYSEYLKDFWGNPL
MYNKEYYMFNAGNKNSYIKLVKDSSVGE
MLIRSKYNQNSNYINYRNLYIGEKFIIRRKSNSQSINDDIVRK
EDYIHLDFVNSNKEWRVYAYKNFKEQE
QKLFLSIIYDSNEFYKTIQIKEYDEQPTYSCQLLFKKDEESTDEI
GLIGIHRFYESGLLRKNYKDYFCIS
KWYLKEVKRKPYKSNLGCNWQFIPKDEGWTE

NUCLEOTIDE:

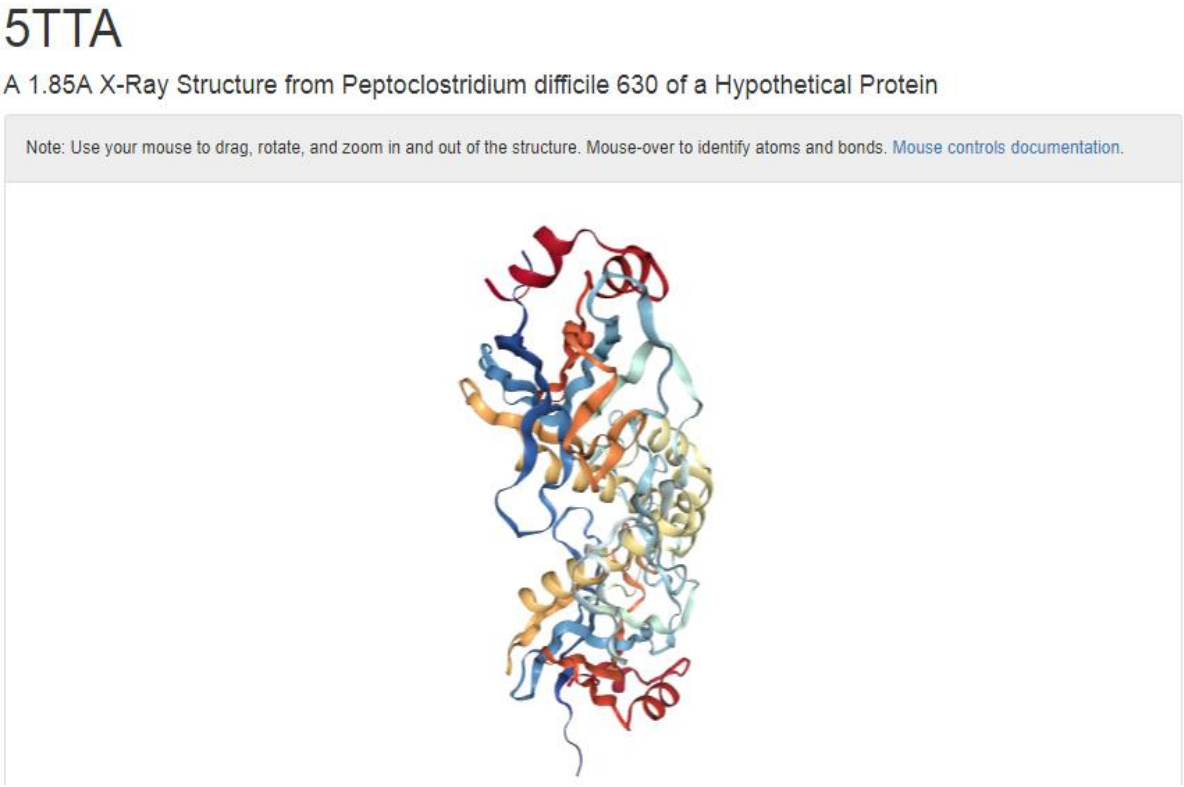
>CP006721.1:2697395-2699002 Clostridium saccharo butylicum DSM 13864, complete genome

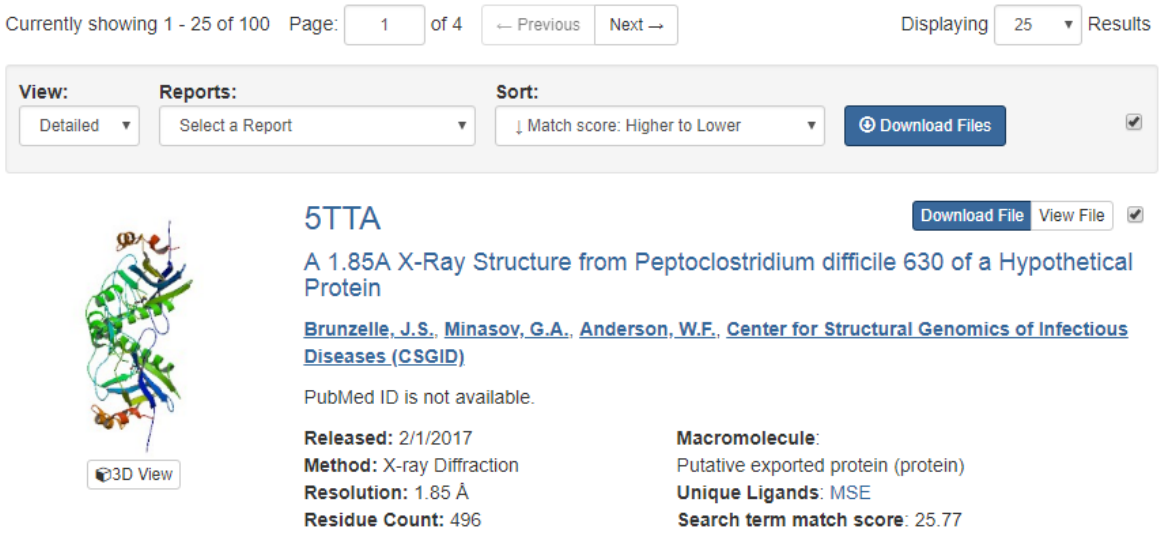
TTGAGTATTAAAAAGAAACTTATTATTTCGTTTTTTTGTTT
AATAAGTGTGTTAAGCTTATTCCCAAAAA
TTACGGTACAAGCTGATACTACTGGATGGAAAAATGATA
ATGGTTCATACTACTACTACAAATCAGATAA
TACTAAGGCATTAGGTTGGCTTGAAATAAACAACAACTG
GTACTATTTTAAGGATGACGGAAAAATGGCC
ACTGGATGGATTAATGACAATGGTTTAAAATATTATTTTA
AGGATTCTGGCTCTATGGTCAAAGGTTGGT
TTCAATTAAATAATCAGTGGTATTATTTTAATGACTCTGG
CTCTATGGCTACTGGCTTTATTGATGATAA
TGGTTCAATCTACTATTTCAATGAATCCGGTACTATGACT
AAAGGATGGATTAATTATAACGGTAAAAAA
TATTATTTTAAAGATTCTGGAATCATGGCACTTGGTTGGC
TTAAAATAGATGATAATTGGTATTATTTTA

AGGATTCAGGTGCTATGGCAACAGGGATTGTAAATGATG
GTTCAAATTTATATTATTTCAATGAGTCAGG
AAATATGATGTCTGGAAACGGTTGGACTCAAATTTCAGA
AAAATATTATTACATAGGAGCAAACGGCATT
GTTAAAACTGGATGGTTTAAAGATAACTCAAAATGTTATT
ATTTTAATGATGATGGTACTATGGCCAAAG
GATGGATTAATCCAGATAAAAATTGGTACTATATGCAGG
ATGATGGTTCAATGAAATCATCAACTTTCTT
CAATGATAAAAATAATTGGTACTATTTAGATGAAAATGG
TGTAATGAAAAAATCCGATTGGGCACAAGTT
AATAGTAAGTATTATTACTTTCTGGATAATGGAGTTATGG
CTAAAGGATGGAATAACATTAATGGTTTAT
CTTATTATTTTAACGACGATGGTTCTATGTATTGTAATGG
CTGGCTGCAATATGATAGTAAATGGTTTTA
CCTTGCAGACAATGGTGTTATGAAGCATTCAATGTGGAT
ATCTGTTGATGATAAATGGTATTACTTAAAT
GAAGATGGTACCATGGCAACTAATACTTCTATCGATGGT
TGGATAATAGATGAAAGTGGCGTTGGTACTA
AAAACCACCAAATTTCAGATAAAGGTATAAAGTTTATAG
CCGACTATGAAGCTTATTACCCTACGGCCTA
CCGTGGACAAGATTCTCAAAATGAAACAATAGGATATGG
ACATGTTATTCAGGATGGTGAAACATTTACA
AATTTAACGCAGGCTGAAGCCAAATCATTATTGAAAAGC
GACCTTAATATCTATGTTAGTGGAGTTAACG
ATTTAACTCATGAACTTAACTTAACTAGTAATCAGTTTGA
TGCTCTTGTTAGTTTTTCTTATAACTGTGG
TATACATGCTTTCACTCAATCTAAATTGTTAAAAGACATT
AAAACAGGTGCTTCTTTAGACACTATAAAA
GATGACTTTTGTCTTTATATACATGTAACTGATGCAAGTG
GTCAACAAATTGAATCGTTAGGTCTATGGC
GAAGAAGAATGGATGAATATGATATATATTCAAAAGGTG
ATTACACAAGAGATTACAGAAATCGGTAA

The above show the fast format of protein and nucleotide sequence of toxin B protein.

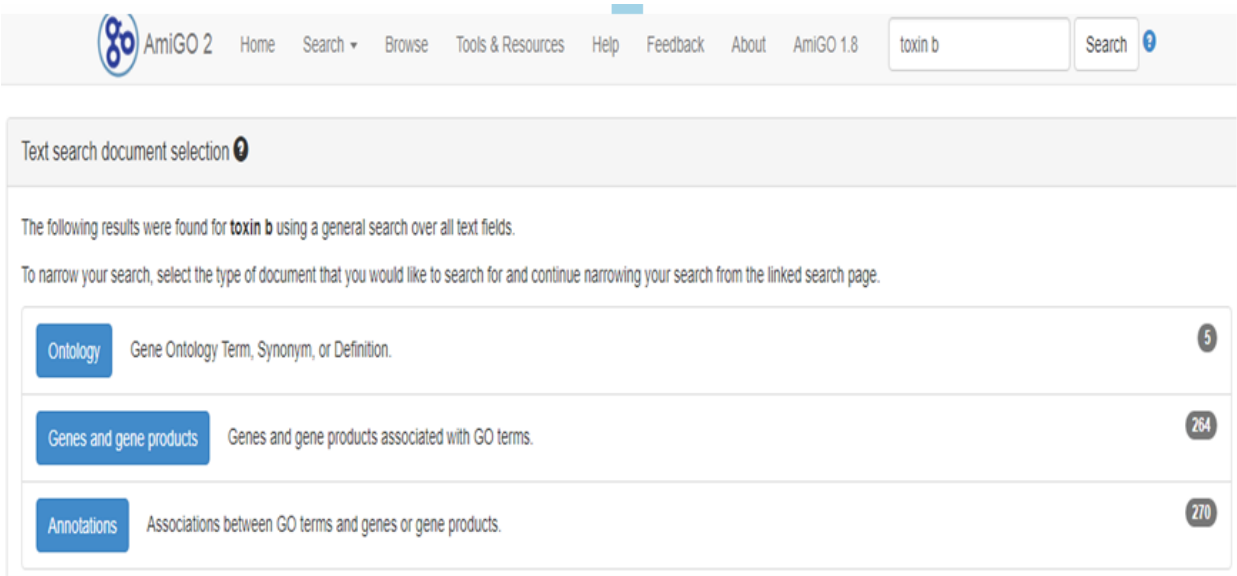
2. PDB – STRUCTURAL SIMILARITY SEARCH





The above result shows the similarity structure of Toxin B protein

3. AMIGO – GENE ANNOTATION



The above result shows the functional annotation Toxin B.

4. JCAT – GENE EXPRESSION ANALYSIS

Table no: 1 CAI VALUES

S:NO	SEQUENCE	CAI – value
1	Meleagris ollopavo	0.9568
2	Clostridium difficilice	0.9536
3	Gallus gallus	0.9546

The above results show the gene expression analysis of annotated sequences with Toxin B Protein.

5. BIO DEIT: SEQUENCE ANALYSIS

Nucleotide sequence analysis

DNA molecule: KC292195.1 [Clostridium] difficile strain ZR75 toxin B (tcdB) gene, complete cds

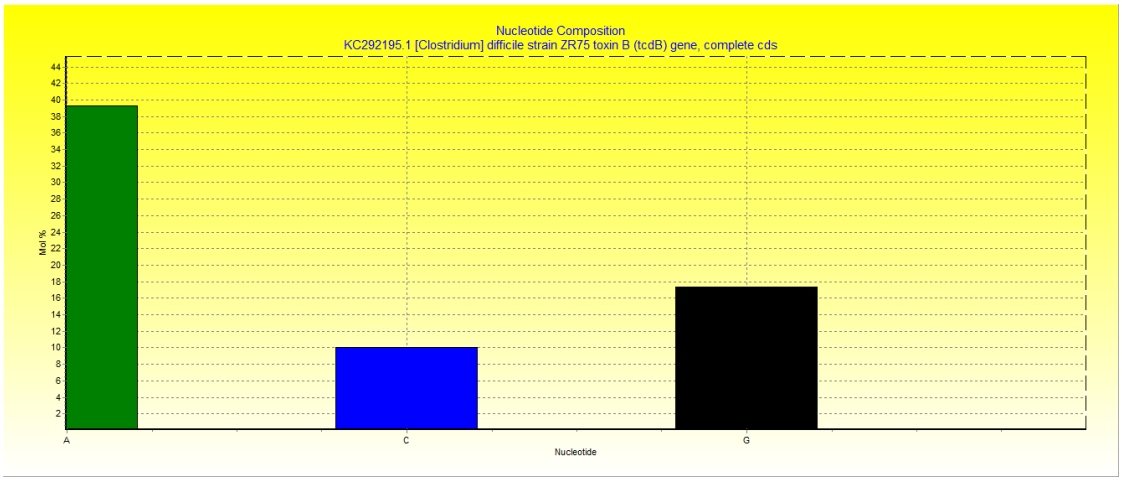
Length = 7101 base pairs

Molecular Weight = 2139656.00 Daltons, single stranded

Molecular Weight = 4289457.00 Daltons, double stranded

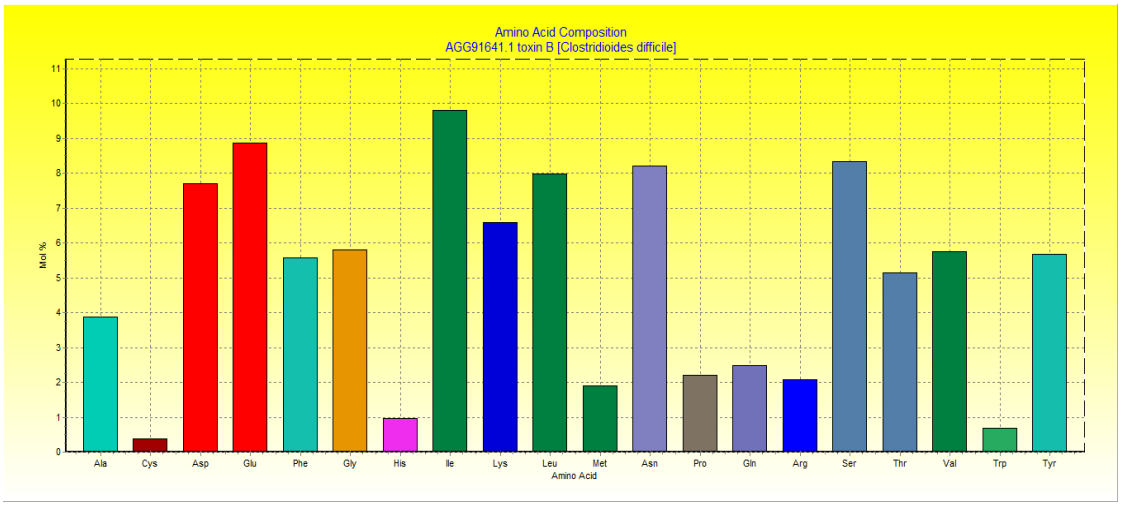
G+C content = 27.40%
A+T content = 72.60%

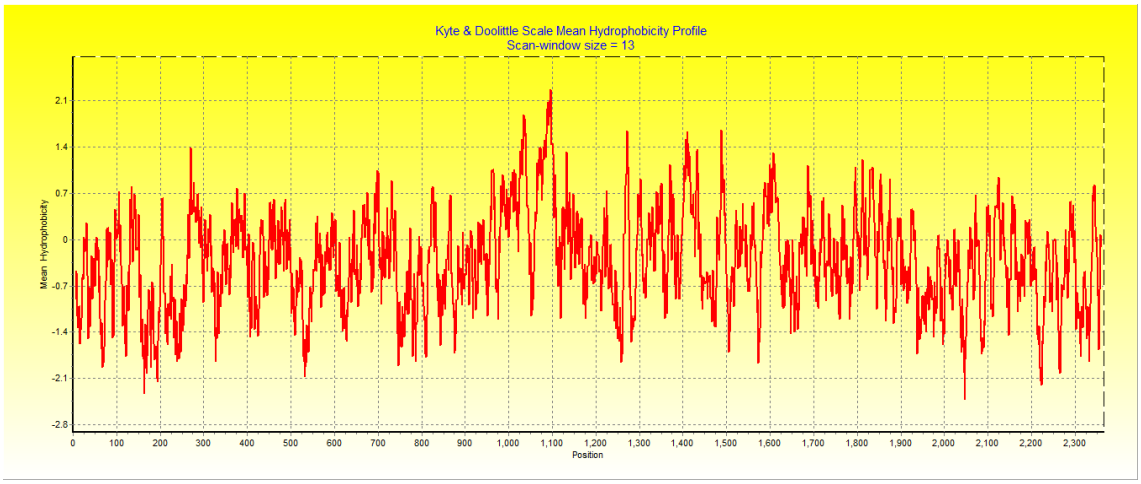
Nucleotide	Number	Mol%
A	2789	39.28
C	714	10.05
G	1232	17.35
T	2366	33.32

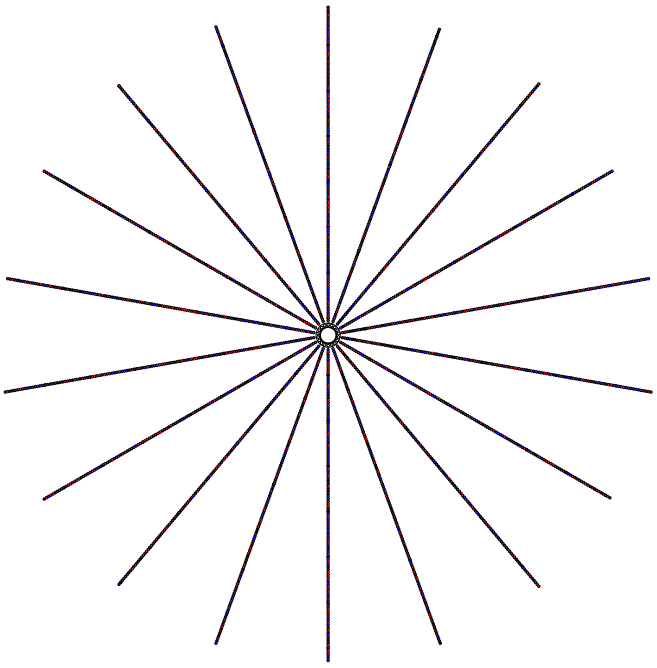


Protein sequence analysis
Amino acid composition
Protein: AGG91641.1 toxin B [Clostridioides difficile]
Length = 2366 amino acids
Molecular Weight = 269683.37 Daltons

Amino Acid	Number	Mol%
Ala A	92	3.89
Cys C	9	0.38
Asp D	182	7.69
Glu E	210	8.88
Phe F	132	5.58
Gly G	137	5.79
His H	23	0.97
Ile I	232	9.81
Lys K	156	6.59
Leu L	189	7.99
Met M	45	1.90
Asn N	194	8.20
Pro P	52	2.20
Gln Q	59	2.49
Arg R	49	2.07
Ser S	197	8.33
Thr T	122	5.16
Val V	136	5.75
Trp W	16	0.68
Tyr Y	134	5.66







The above result shows the helical wheel structure of Toxin B protein.

6. DRUG BANK

Table no:2

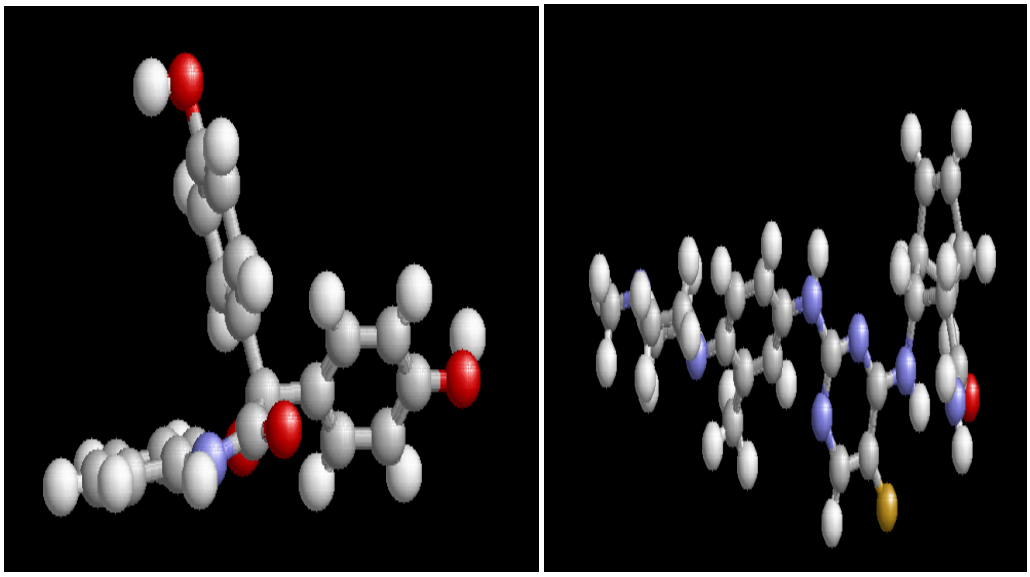
s.no	Drug name	Smiles	Molecule weight
1	Bisoxatin	OC1=CC=C(C=C1) C1(OC2=CC=CC=C2NC1=O)C1=CC=C(O)C=C1	Average: 333.343 Monoisotopic: 333.100107967
2	cenisertib	[H][C@@]12C[C@@]([H])(C=C1)[C@@H]([C@@H]2NC1=C(F)C=NC(NC2=CC=C(N3CCN(C)CC3)C(C)=C2)=N1)C(N)=O	Average: 451.55 Monoisotopic: 451.249586777
3	olsalazine	OC(=O) C1=CC(=CC=C1O)\N=N\C1=CC=C(O)C(=C1)C(O)=O	Average: 302.239 Monoisotopic: 302.053886062
4	vancomycin	CN[C@H](CC(C)C)C(=O)N[C@@H]1[C@H](O)C2=CC=C(OC3=C(O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O[C@H]4C[C@](C)(N)[C@H](O)[C@H](C)O4)C4=CC(=C3)[C@@H](NC(=O)[C@H](CC(N)=O)NC1=O)C(=O)N[C@@H]1C3=CC(=C(O)C=C3)C3=C(O)C=C(O)C=C3[C@H](NC(=O)[C@@H](NC1=O)[C@H](O)C1=CC(Cl)=C(O4)C=C1)C(O)=O)C(Cl)=C2	Average: 1449.254 Monoisotopic: 1447.430199787
5	mesalazine	NC1=CC(C(O)=O)=C(O)C=C1	Average: 153.1354 Monoisotopic: 153.042593095
6	linsitinib	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=CN=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	Average: 421.504 Monoisotopic: 421.190260381

Table no:3

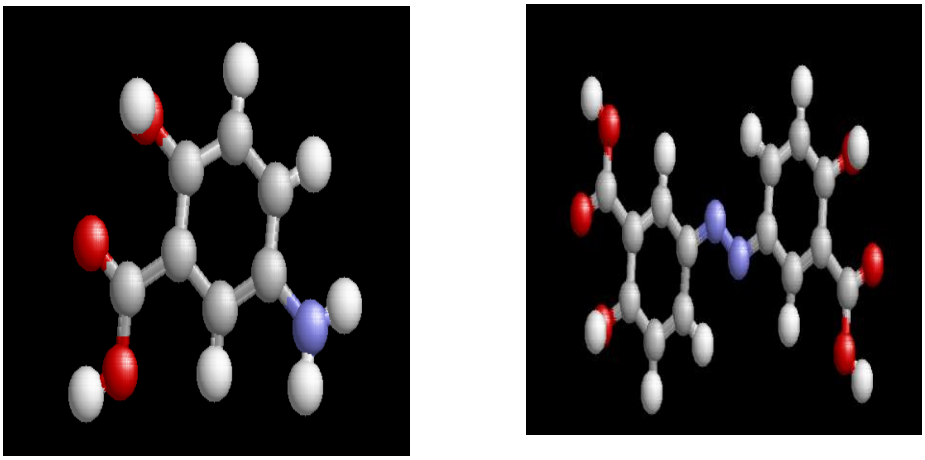
S:NO	DRUG NAME	I UPAC NAME
1	Bisoxatin	2,2-bis(4-hydroxyphenyl)-3,4-dihydro-2H-1,4-benzoxazin-3-on
2	cenisertib	(1S,2S,3R,4R)-3-[(5-fluoro-2-{[3-methyl-4-(4-methylpiperazin-1-yl) phenyl] amino} pyrimidin-4-yl) amino] bicyclo[2.2.1]hept-5-ene-2-carboxamide
3	olsazine	5-[(E)-2-(3-carboxy-4-hydroxyphenyl) diazen-1-yl]-2-hydroxybenzoic acid
4	ancomycin	(1S,2R,18R,19R,22S,25R,28R,40S)-48-{[(2S,3R,4S,5S,6R)-3-{[(2S,4S,5S,6S)-4-amino-5-hydroxy-4,6-dimethyloxan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-22-(carbamoylmethyl)-5,47-dichloro-2,18,32,35,37-pentahydroxy-19-[(2R)-4-methyl-2-(methylamino)pentanamido]-20,23,26,42,44-pentaoxo-7,13-dioxa-21,24,27,41,43-pentaazaoctacyclo[26.14.2.2^{3,6}.2^{14,17}.1^{8,12}.1^{29,33}.0^{10,25}.0^{34,39}]pentaconta-3,5,8,10,12(48),14,16,29(45),30,32,34,36,38,46,49-pentadecaene-40-carboxylic acid
5	mesalazine	5-amino-2-hydroxybenzoic acid
6	Linsitinib	(1s,3r)-3-[8-amino-1-(2-phenylquinolin-7-yl) imidazo[1,5-a] pyrazin-3-yl]-1-methylcyclobutan-1-ol

The above Table shows the drug like properties selected drug.

7. ONLINE SMILE TREANSLATOR



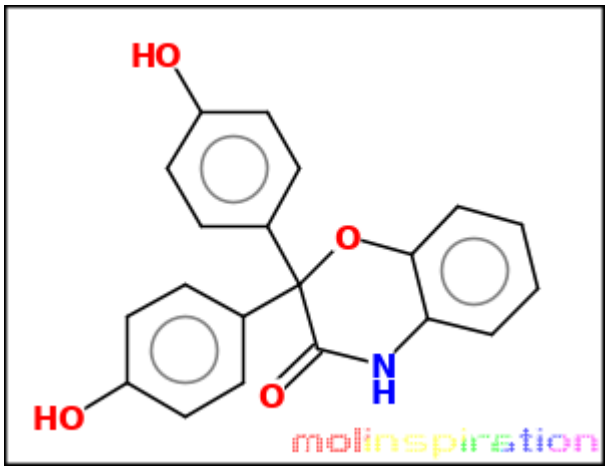
The above result shows the 3 D structure of Bisoxatin and Cenisertib.



The above result shows the 3 D structure of mesalazine and olsalazine.

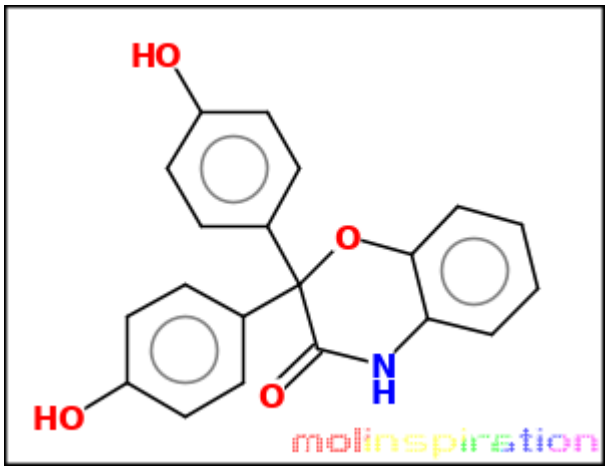
8. MOLINSPRATION SERVER

1. Bisoxatin



Molinspiration property engine v2018.10

miLogP	2.65
TPSA	78.79
natoms	25
MW	333.34
nON	5
nOHNH	3
nviolations	0
nrotb	2
volume	288.93



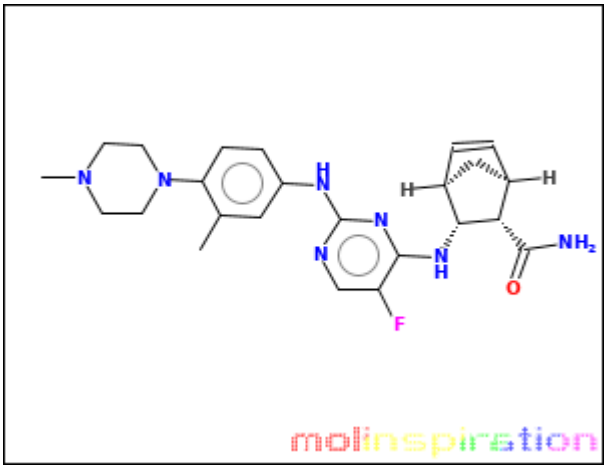
Molinspiration bioactivity score v2018.03

GPCR ligand	0.00
Ion channel modulator	-0.15
Kinase inhibitor	-0.27
Nuclear receptor ligand	-0.01
Protease inhibitor	-0.12
Enzyme inhibitor	-0.09

The above results show the bioactivity properties of Bisoxatin drug compound.

2. cenisertib

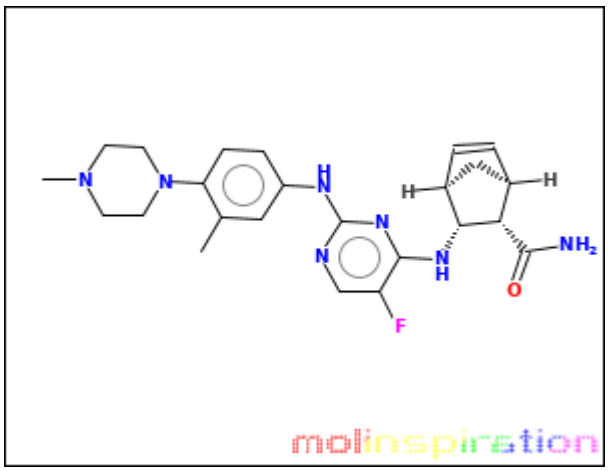
1. Calculate properties



Molinspiration property engine v2018.10

miLogP	3.33
TPSA	99.41
natoms	33
MW	451.55
nON	8
nOHNH	4
nviolations	0
nrotb	6
volume	412.05

2. Predict bioactivity



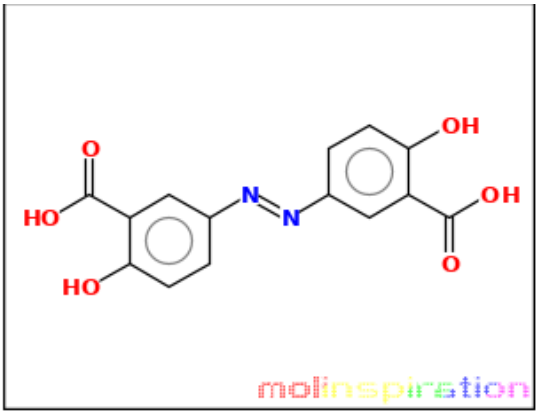
Molinspiration bioactivity score v2018.03

GPCR ligand	0.16
Ion channel modulator	-0.18
Kinase inhibitor	0.26
Nuclear receptor ligand	-0.42
Protease inhibitor	-0.18
Enzyme inhibitor	0.05

The above results shows the bioactivity properties of cenisertib drug compound.

3. olsalazine

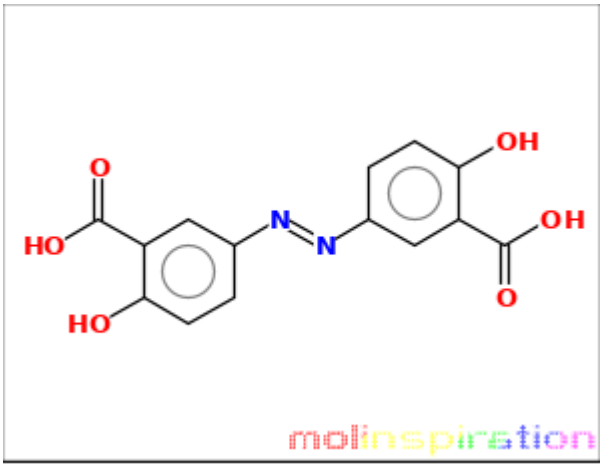
1.Calculate properties



Molinspiration property engine v2018.10

miLogP	3.95
TPSA	139.78
natoms	22
MW	302.24
nON	8
nOHNH	4
nviolations	0
nrotb	4
volume	244.59

2.predict bioactivity



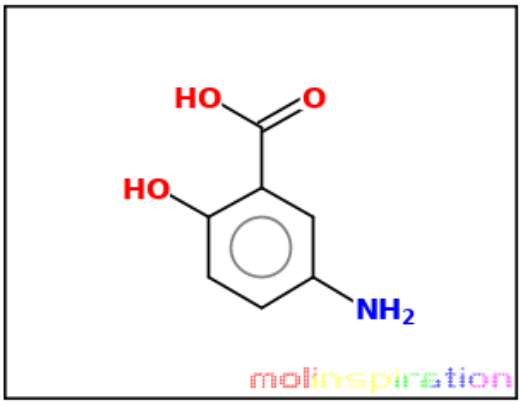
Molinspiration bioactivity score v2018.03

GPCR ligand	-0.03
Ion channel modulator	-0.03
Kinase inhibitor	0.02
Nuclear receptor ligand	-0.19
Protease inhibitor	-0.07
Enzyme inhibitor	0.06

The obove results shows the bioactivity properties of olsazine drug compound.

4.mesalazine

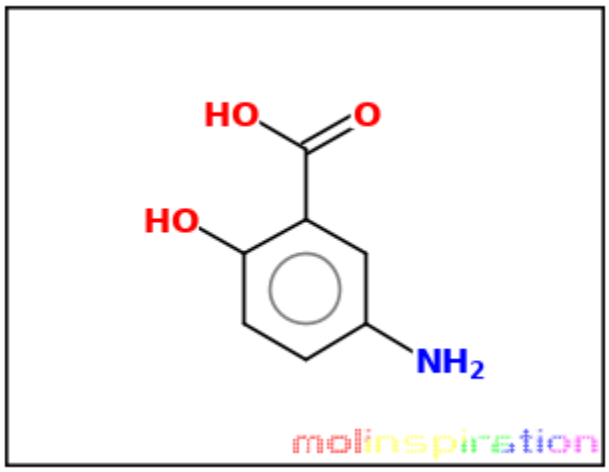
1. Calclulate proprtis



Molinspiration property engine v2018.10

miLogP	0.92
TPSA	83.55
natoms	11
MW	153.14
nON	4
nOHNH	4
nviolations	0
nrotb	1
volume	130.35

2. Predict bioactivity



Molinspiration bioactivity score v2018.03	
GPCR ligand	-0.80
Ion channel modulator	-0.25
Kinase inhibitor	-0.81
Nuclear receptor ligand	-0.81
Protease inhibitor	-0.86
Enzyme inhibitor	-0.18

The above results show the bioactivity properties mesalazine drug compound.

CONCLUSION

The main source of transmission is patients with symptomatic infection. These people shed large numbers of *C.* difficile spores and bacteria in the faces, resulting in widespread contamination of their skin, bed linen and nearby environmental surfaces. The spores are resistant to drying and the usual chemical cleaning agents and can therefore remain in the environment for weeks or months. Spores can then be picked up on the hands of patients and healthcare workers. The glycosylation activity of toxin B occurs in the N-terminal catalytic region (residues 1–544). This region glycosylates substrates independent of any cytotoxic activity.[6] However, a small deletion of the receptor binding region causes attenuation of toxin B activity.[6]The translocation region contains a hydrophobic stalk-like structure, which may help residues 958–1130 in forming membrane spanning pores. The sequence of Toxin B protein retrieved from NCBI database in fasta format. The Sequential analysis of Toxin B protein were carried out by using bioinformatic tools, like NCBI, pdb, amigo, Clustal w. In future toxin B will have more application in the field of pharmacology.

REFERENCES

Aggarwal S1,, Somani VK1,3, Gupta S1, Garg R1,4, Bhatnagar R5,6Development of a novel multiepitope chimeric vaccine against anthrax. Med Microbiol Immunol. 2019 Jan 22. doi: 10.1007/s00430-019-00577-x.

Bellon G, Venturin A, Masiero S, Del Felice A.Intra-articular botulinum toxin injection 11 Complex Regional Pain Syndrome: case report and review of the literature. Toxicon. 2019 Jan 17. pii: S0041-0101(19)30013-3. doi: 10.1016/j.toxicon.2019.01.002.

Dubberke ER, Carling P, Carrico R, Donskey CJ, Loo VG, McDonald LC, Maragakis LL, Sandora TJ, Weber DJ, Yokoe DS, Gerding DN (Jun 2014). "Strategies to PreventClostridium difficile Infections in Acute Care Hospitals: 2014 Update". Infection Control and Hospital Epidemiology (Submitted manuscript). .

Hebsibah Elsie B, Subashini.G, Nithya.G and Shoba.K. (2018); Purification and Identification of Antioxidant Peptides from the Skin Protein Hydrolysate of Marine Fish (Aurigequula Fasciata). European journal of Pharmaceutical and Medical Research.5 (10). 371 – 378.Issn No 2394-3211.

Hudson SL,Arnoczy G Gibson H, Thurber C, Lee J, Kessell AProbiotic use as prophylaxis for Clostridium difficile-associated diarrhea in a community hospital. Am J Infect Control. 2019 Jan 18. pii:

S0196-6553(18)31181-7. doi: 10.1016/j.ajic.2018.12.018.

Kalpana K., Manjuvani S., Shoba K. In Silico Comparative Modeling of Maturase K Protein in Cymbopogon martinii Plant. Research & Reviews: A Journal of Bioinformatics. 2018; 5(3): 30–36p.

Mora Pinzon MC, Buie R, Liou JI, Shirley DK, Evans CT, Ramanathan S, Poggensee L, Safdar NOutcomes of Community and Healthcare-onset Clostridium difficileInfections.Clin Infect Dis. 2018 Aug 23. doi: 10.1093/cid/ciy715.

Pulse ME, Weiss WJ, Kers JA, DeFusco AW, Park JH, Handfield MPharmacological, Toxicological and Dose-Range Assessment of OG716, a Novel Lantibiotic for the Treatment of Clostridium difficile Associated Infection (CDI). Antimicrob Agents Chemother. 2019 Jan 22. pii: AAC.01904-18. doi: 10.1128/AAC.01904-

Revathi G, Shoba K, Hebsibah Elsie B, "Gene Expression and Structural analysis of NADH Dehydrogenase subunit 2 protein in Sargassum Muticum", IJRAR - International Journal of Research and Analytical Reviews (IJRAR), Volume.6, Issue 1, Page No pp.720-733, February-2019, E-ISSN 2348-1269, P- ISSN 2349-5138.

Schadt EE, Argmann C, Dubinsky M, Kasarskis A, Sands B, Faith JJGut microbiota density influences host physiology and is shaped by host and microbial factors. Elife. 2019 Jan 22;8. pii: e40553. doi: 10.7554/eLife.40553

Shoba K. , Sowmiya S and Dr. Mazher sultana, World Journal of Pharmaceutical and Life Sciences, ISSN 2454-2229, Vol. 3, Issue 1, 427-436.

Shoba K. , Manjuladevi M , Dr. Mazher sultana, Biochemical analysis and gene expression profiling on collagenase protein in fiddler crab, World journal of pharmacy and pharmaceutical sciences, issn 2278 – 4357, volume 6, issue 3, 747-756

Shoba K., Hebsibah Elsie B. And Bavyasri S. Insilico Peptide Modeling Stuidies And Structural Analysis on Ribulose -1, 5 Bisphosphate Carboxylase In GracilariaEdulis, World Journal Of Pharmacy And Pharmaceutical Sciences, 2018, Volume 7, Issue 3, 1086-1095, Issn 2278 – 4357.

Shoba K., Kalpana K., Protein Modeling and Drug Docking Studies on Potential Protein Target (E. coli–dosP) and Compound Aldehyde (Sumatriptan) using Bioinformatics Tools. Research & Reviews: A Journal of Bioinformatics. 2018; 5(3): 9–18p.

Shoba. K, Hebsibah Elsie. B and Jayakumari. S. Sathya. R. (2018); Insilico Structural Analysis and Drug Docking Stuidies On Ribulose -1, 5 Bisphosphate Carboxylase In Gracilaria Edulis. International journal of advanced research. 6 (9). 159-165] (ISSN 2320-5407).

Shoba. K, Nithy.G and Deepa.L. (2018); Biochemical Analysis and Peptide Modeling of Lysozyme in Indian Fenneropenaeus indicus shrimp species. International journal of advanced research. 6 (9). 159-165] (ISSN 2320-5407).

Shoba.K, Hebsibahelsie.B, insilico homology modeling ofribulose-1, 5-bisphosphate carboxylase protein in gracilariaedulis, world journal of pharmacy and pharmaceutical sciences, 2017,volume 6, issue 8, 396-406, issn 2278 – 4357.

Shoba.K, Lavanya.G, Identification Of De Novo Peptide And Motif Prediction On Porphyria Protein (Hmbs) Using Insilico Tools, Universal Journal Of Pharmacy ,2018, Volume 8, Issue 1, Issn2320-303x.

Shoba.K, Lavanya.G, Tertiary Structural Prediction And Drug Binding Studies On Mutated Gene (Hmbs) In Human Porphyria,International Journal Of Novel Trends In Pharmaceutical Science,2018,Issn 2277 -2782,Volume 8,Issue 1

Usha.K and Shoba.K, Functional analysis & pepptide structure modeling of sphyastatin protein in scylla paramamosain, International Journal of Current Science and Technology, Volume 7, Issue, 01(A), pp. 666-669, January 2019, ISSN: 2320-8090.

Wilkins LE1, Badi N2, Du Prez F2, Gibson MI1,3. Double-Modified Glycopolymers from Thiolactones to Modulate Lectin Selectivity and Affinity. ACS Macro Lett. 2018 Dec 18;7(12):1498-1502. doi: 10.1021/acsmacrolett.8b00825. Epub 2018 Dec 6.