



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, pI, 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.

INTRODUCTION

Clostridium difficile (kilos-TRID-e-um dif-uh-SEEL), often called *C. difficile* 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*]
MPVTINNFNYPIDNDNIIMPEPPFARGTGRYKAFKITD
RIWIIPERYTFGYKPEDFNKSSGIFNRDV
CEYYDPDYLNTNDKKNIFLQTMIKLFNRIKSKPLGEKLEMI
NGIPYLGDRRVPLEEFNTNIASVTVNK
LISNPGEVEQKKGIFANLIIFGPGPVLNENETIDIGIQNHFAS
REGFGGIMQMKFCPEYVSFVNNVQENK

GASIFNRRGYFSDPALILMHELIHVLHGLYGIKVDDLPIVPNE
KKFFMQSTDTIQAEELYTFGGQDPSII
SPSTDKSIYDKVLQNFRGIVDRLNKLVCISDPNININIKNK
FKDKYKFVEDSEGKYSIDVESFNKLYK
SLMFGFTETNIAENYKIKTRASYFSDSLPPVKIKNLLDNEIYTI
EEGFNISDKNMKGKEYRGQNKAINKQA
YEEISKEHLAVYKIQMCKSVKVPGLICIDVDNENLFFIADKNSF
SDDLKNERVEYNTQNNYINGGFPINE
LILDTDLISKIELPSENTESLTDFNVDPVVEKQPAIKKVFTDE
NTIFQYLYSQTFPLNIRDISLTSSFD
DALLVSSKVYSFFSMDYIKTANKVVEAGLFAGWVKQIVDDF
VIEANKSSTMDKIADISLIVPYIGLALNV
GNETAKGNFESAFEIAGSSILLEFIPELLIPVVGVLLESYIDNK
NKIITIDNALTKRVEKWIDMYGLI
VAQWLSTVNTQFYTIKEMYKALNYQAQALEEIIKYKYNIS
EEEKSNININFNDINSKLNENINQAMDND
INDFINECSVSYLMKKMIPLAVKKLLDFDNTLKKNLLNYIDE
NKLYLIGSVEDEKSKVDKYLKTIIPFDL
SMYTNNEILIKIFNKYNSEILNIIILNRYRDNLLIDLSGYGAK
VEVDGVLKNDKNQFKLTSSADSKIR
VTQNQNIIFNSMFLDFSFSFWIRIPKYRNDIDIQNYIHNEYTII
NCMKNSGWKISIRGNRIIWTLDING
KTKSVFFEYNIREDISEYINRWFFVTITNNLDNAKIYINGTLES
NMDIKDIGEVIINGEITFKLDGDVDR
TQFIWMKYFSIFNTQLNQSNIEIKIYQSYSEYKDFWGNPL
MYNKEYYMFNAGNKNSYIKLVKDDSSVGE
MLIRSKYNQNSNYINRNLIGYGEKFIIRKNSNSQSINDDIVRK
EDYIHLDFVNSNKEWRVYAYKNFKEQE
QKLFLSIYDSNEFYKTIQIKEYDEQPTYSCQLLFKKDEESTDEI
GLIGIHRFYESGLLRKNYKDYFCIS
KWYLKEVKRKPYSNLGCNWQFIPKDEGWTE

NUCLEOTIDE:

>CP006721.1:2697395-2699002 *Clostridium saccharo*
butylicum DSM 13864, complete genome
TTGAGTATTAAGAAAGAACTTATTATTCGTTTTTTGTTT
AATAAGTGTTAAGCTTATCCCAAAAA
TTACGGTACAAGCTGATACTACTGGATGGAAAAATGATA
ATGGTTCATACTACTACTACAAATCAGATAA
TACTAAGGCATTAGGTTGGCTTGAAATAACAACAACACTG
GTACTATTTTAAGGATGACGGAAAAATGGCC
ACTGGATGGATTAATGACAATGGTTTAAATATTATTTTA
AGGATTCTGGCTCTATGGTCAAAGGTTGGT
TTCAATTAATAATCAGTGGTATTATTTTAATGACTCTGG
CTCTATGGCTACTGGCTTTATTGATGATAA
TGTTTCAATCTACTATTTCAATGAATCCGGTACTATGACT
AAAGGATGGATTAATTATAACGGTAAAAAA
TATTATTTTAAAGATTCTGGAATCATGGCACTTGGTTGGC
TTAAATAGATGATAATTGGTATTATTTTA

AGGATTCAGGTGCTATGGCAACAGGGATTGTAAATGATG
GTTCAAATTTATATTATTTCAATGAGTCAGG
AAATATGATGTCTGGAAACGGTTGGACTCAAATTTGAGA
AAAATATTATTACATAGGAGCAAACGGCATT
GTAAAACTGGATGGTTTAAAGATAACTCAAAATGTTATT
ATTTAATGATGATGGTACTATGGCCAAAG
GATGGATTAATCCAGATAAAAAATTGGTACTATATGCAGG
ATGATGGTTCAATGAAATCATCAACTTTCTT
CAATGATAAAAAATAATTGGTACTATTTAGATGAAAATGG
TGTAATGAAAAAATCCGATTGGGCACAAGTT
AATAGTAAGTATTATTACTTTCTGGATAATGGAGTTATGG
CTAAAGGATGGAATAACATTAATGGTTTAT
CTTATTATTTTAAACGACGATGGTTCTATGTATTGTAATGG
CTGGCTGCAATATGATAGTAAATGGTTTTA
CCTTGCAGACAATGGTGTTATGAAGCATTCAATGTGGAT
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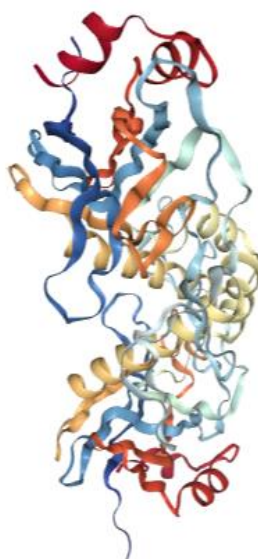
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CCGTGGACAAGATTCTCAAATGAAACAATAGGATATGG
ACATGTTATTGAGGATGGTGAAACATTTACA
AATTTAACGCAGGCTGAAGCCAAATCATTATTGAAAAGC
GACCTTAATATCTATGTTAGTGGAGTTAACG
ATTTAACTCATGAACCTTAACTTAAGTAATCAGTTTGA
TGCTCTTGTTAGTTTTTCTTATAACTGTGG
TATACATGCTTTCACTCAATCTAAATTGTTAAAAGACATT
AAAACAGGTGCTTCTTTAGACACTATAAAA
GATGACTTTTGTCTTTATATACATGTAAGTGAAGTGAAGTG
GTCAACAAATTGAATCGTTAGGTCTATGGC
GAAGAAGAATGGATGAATATGATATATATTCAAAGGTG
ATTACACAAGAGATTACAGAAATCGGTAA
The above show the fast format of protein and
nucleotide sequence of toxin B protein.

2. PDB – STRUCTURAL SIMILARITY SEARCH

5TTA

A 1.85Å X-Ray Structure from *Peptoclostridium difficile* 630 of a Hypothetical Protein

Note: Use your mouse to drag, rotate, and zoom in and out of the structure. Mouse-over to identify atoms and bonds. [Mouse controls documentation](#).



Currently showing 1 - 25 of 100 Page: 1 of 4 Previous Next Displaying 25 Results

View: Detailed Reports: Select a Report Sort: Match score: Higher to Lower Download Files



5TTA

A 1.85Å X-Ray Structure from *Peptoclostridium difficile* 630 of a Hypothetical Protein

[Brunzelle, J.S.](#), [Minasov, G.A.](#), [Anderson, W.F.](#), [Center for Structural Genomics of Infectious Diseases \(CSGID\)](#)

PubMed ID is not available.

Released: 2/1/2017

Method: X-ray Diffraction

Resolution: 1.85 Å

Residue Count: 496

Macromolecule:

Putative exported protein (protein)

Unique Ligands: MSE

Search term match score: 25.77

The above result shows the similarity structure of Toxin B protein

3. AMIGO – GENE ANNOTATION

AmiGO 2 Home Search Browse Tools & Resources Help Feedback About AmiGO 1.8 toxin b Search

Text search document selection

The following results were found for **toxin b** using a general search over all text fields.

To narrow your search, select the type of document that you would like to search for and continue narrowing your search from the linked search page.

Ontology	Gene Ontology Term, Synonym, or Definition.	5
Genes and gene products	Genes and gene products associated with GO terms.	264
Annotations	Associations between GO terms and genes or gene products.	270

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 olopavo	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

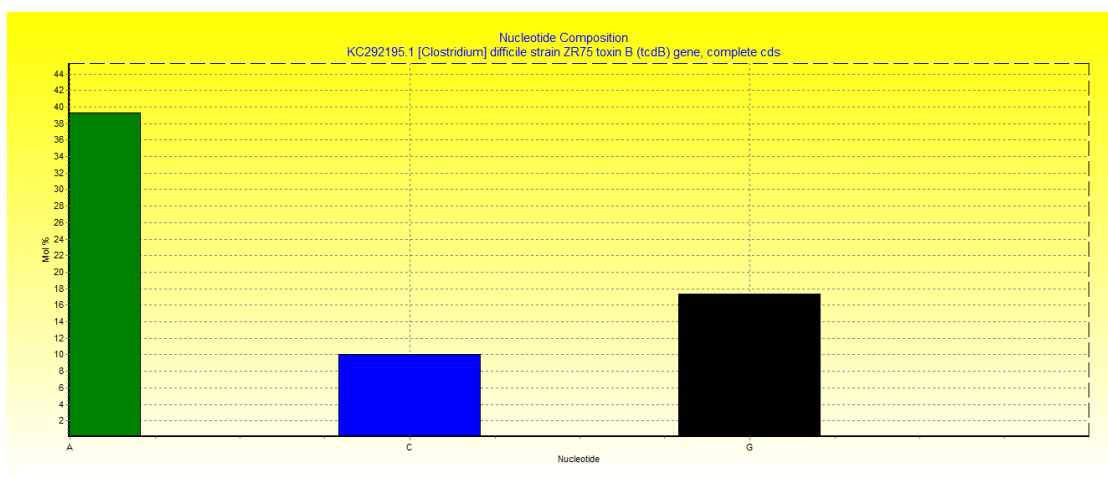
Molecular Weight = 4289457.00 Daltons, double stranded

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

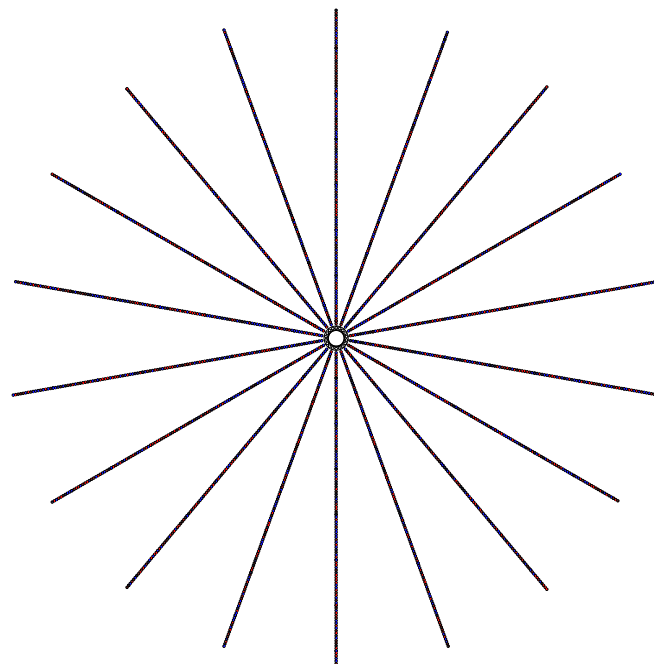
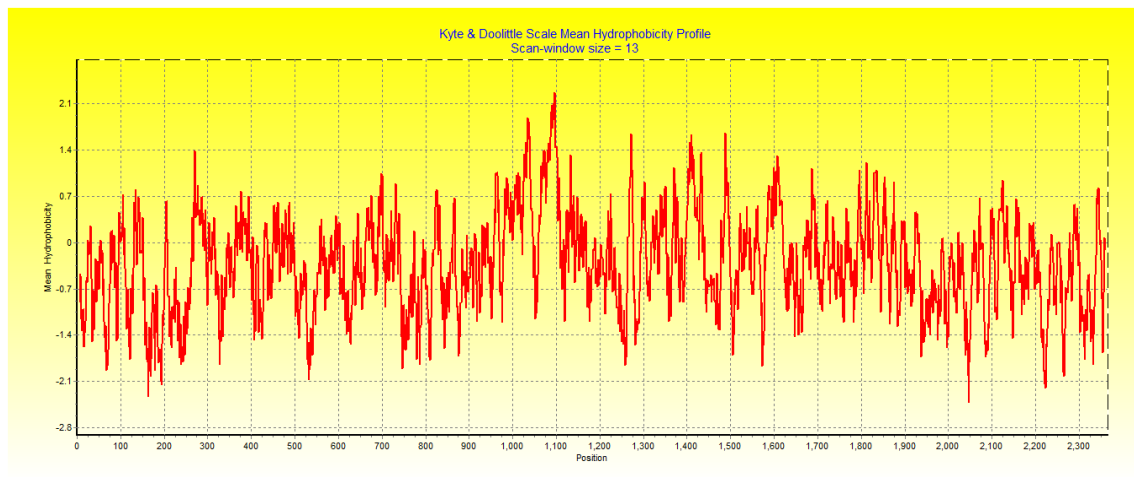
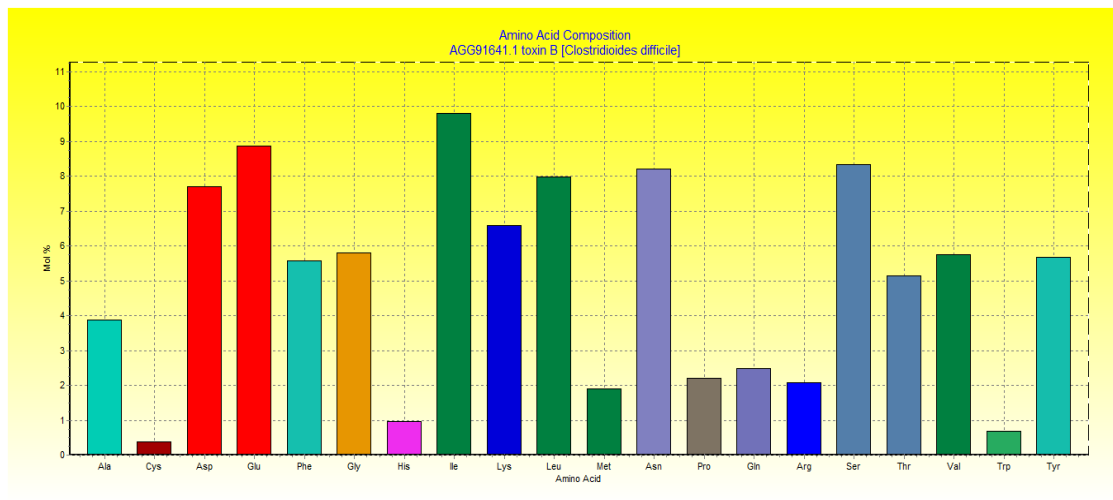
Amino acid composition

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

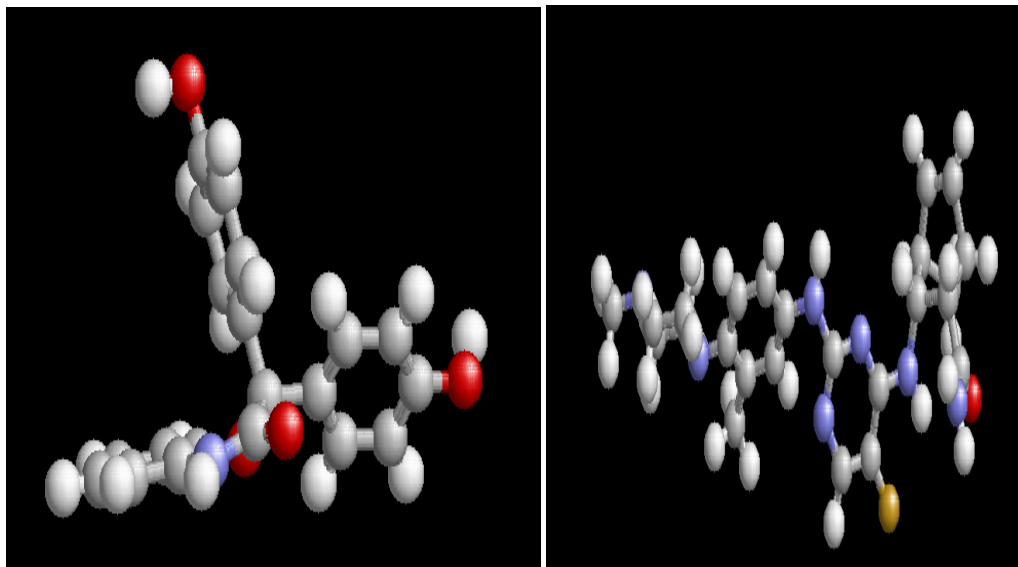
s.no	Drug name	Smiles	Molecule weight
1	Bisoxatin	<chem>OC1=CC=C(C=C1)C1(OC2=CC=CC=C2NC1=O)C1=CC=C(O)C=C1</chem>	Average: 333.343 Monoisotopic: 333.100107967
2	cenisertib	<chem>[H][C@@]12C[C@@]([H])(C=C1)[C@@H]([C@@H]2NC1=C(F)C=NC(NC2=CC=C(N3CCN(C)CC3)C(C)=C2)=N1)C(N)=O</chem>	Average: 451.55 Monoisotopic: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

Table no:3

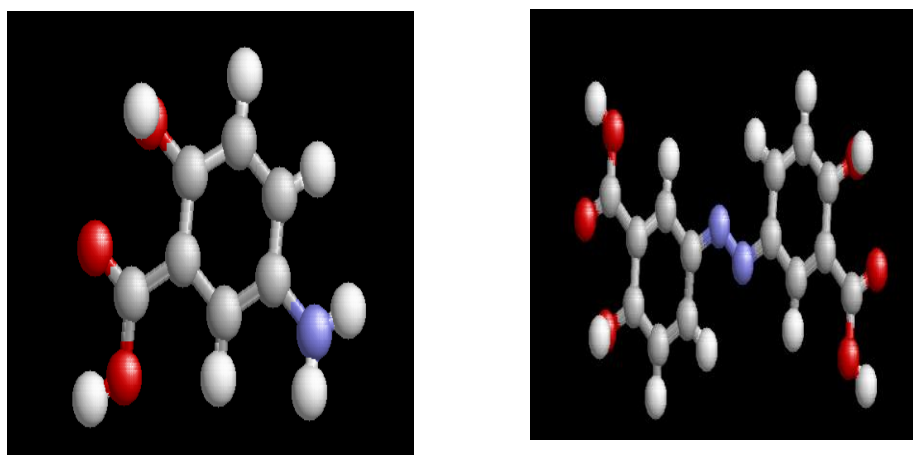
S:NO	DRUG NAME	IUPAC NAME
1	Bisoxatin	2,2-bis(4-hydroxyphenyl)-3,4-dihydro-2H-1,4-benzoxazin-3-on
2	cenisertib	(1S,2S,3R,4R)-3-[(5-fluoro-2-[[3-methyl-4-(4-methylpiperazin-1-yl)phenyl]amino]pyrimidin-4-yl)amino]bicyclo[2.2.1]hept-5-ene-2-carboxamide
3	olsazine	5-[(E)-2-(3-carboxy-4-hydroxyphenyl)diazene-1-yl]-2-hydroxybenzoic 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-pentaoso-7,13-dioxo-21,24,27,41,43-pentaazaocetacyclo[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



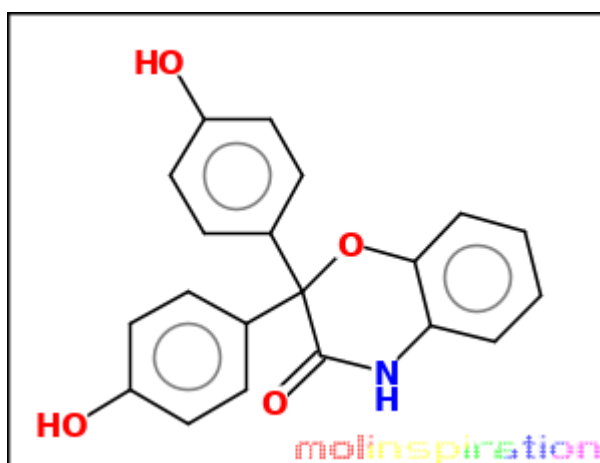
The above result shows the 3 D structure of Bisoxatin and Cenisetib.



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

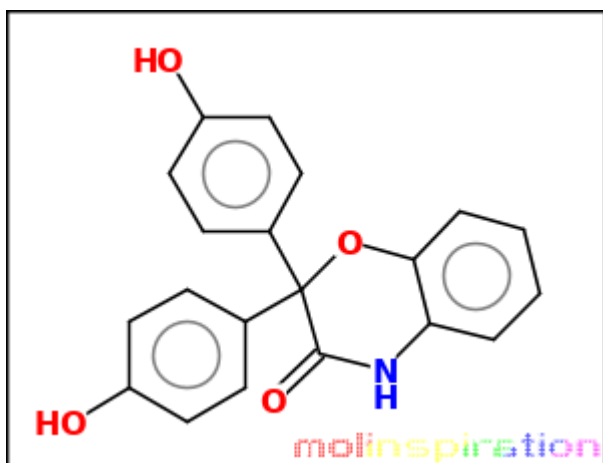
8. MOLINSPRATION SERVER

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



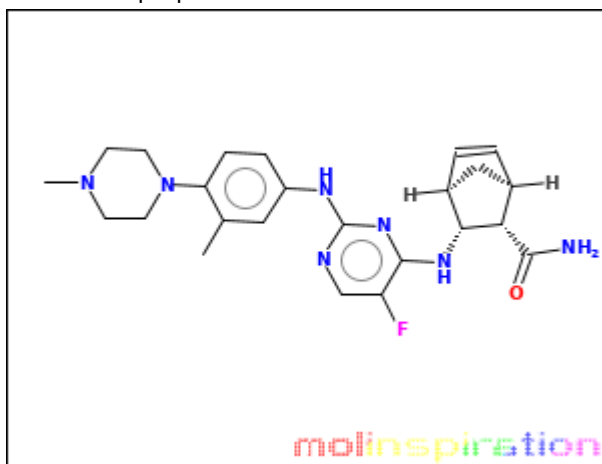
[Molinspiration bioactivity score](#) v2018.03

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

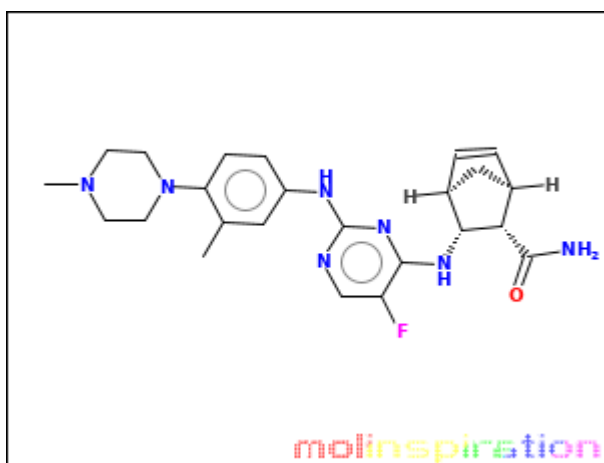
1. Calculate properties



[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



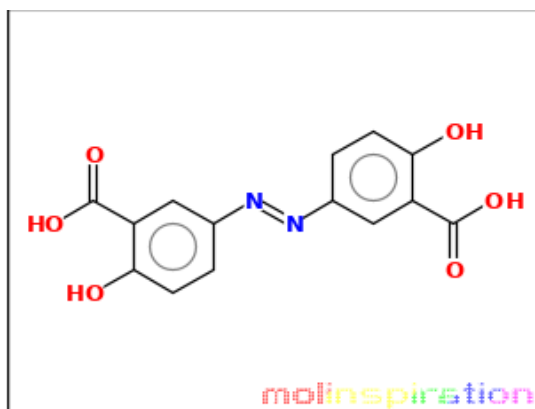
[Molinspiration bioactivity score](#) v2018.03

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

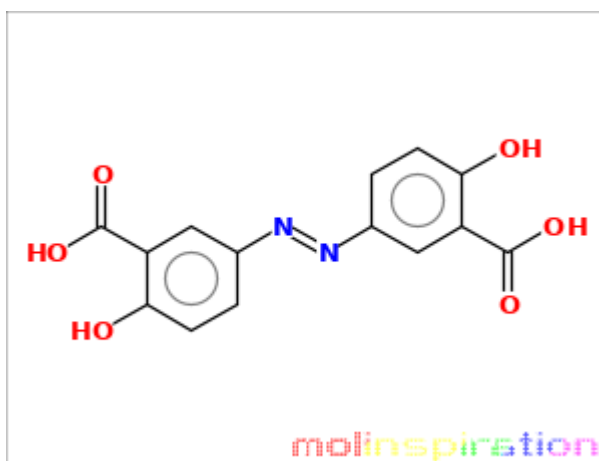
1. Calculate properties



[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



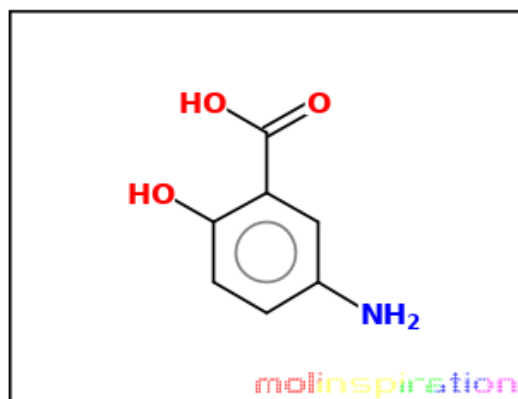
[Molinspiration bioactivity score](#) v2018.03

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 above results shows the bioactivity properties of olsazine drug compound.

4.mesalazine

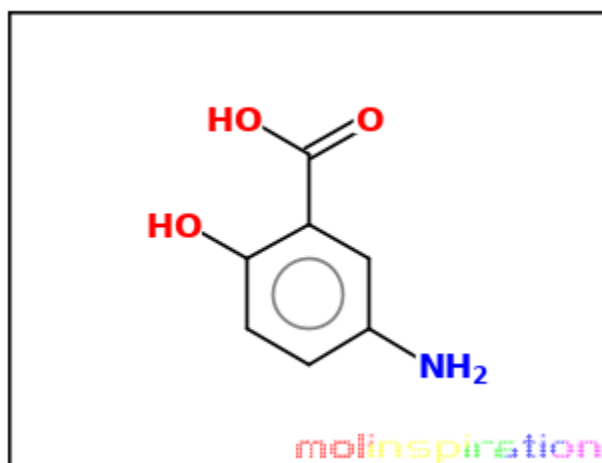
1. Calculate proptis



[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 faeces, 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.

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