1. Cation-pi interaction which is an important interaction besides other non-covalent interactions is found to be present in large numbers in the studied toxins revealing the stability of the toxins structures that relates to the proper functioning of the toxins allowing them to cause specific diseases in hosts.

2. Analysis of the toxins Enterotoxin A, exfoliative toxin A, TSST-1 and γ-hemolysin reveals non-homology of the toxins to human proteome and thus no cross reaction would occur when drug is administered in host. Also, the more number of interacting partners of the toxins provides clue for using the same drugs for the toxins involved in the interaction. The absence of drugs for the toxins confirmed by the database search proves the novelty of the drug target and thus emphasizes the need to develop new drugs to inhibit the functions of the toxins.

3. The identified epitopes from the toxin γ-hemolysin of S. aureus could be used as vaccine candidates against the organism for T-cell mediated immune response in host after confirmation with experimental results.

4. Molecular docking analysis of the toxins by Autodock 4.0 with 27 flavonoids obtained through literature reveals that the flavonoids diosmetin, fisetin, apigenin and isoluteolin compounds are identified as potent inhibitors of the toxins enterotoxin A, exfoliative toxin A, TSST-1 and γ-hemolysin respectively based on the low energy values of the complexes indicating stability.

5. The complexes are found to be stable according to their RMS deviations which are less than 0.35 nm during the simulation. An average of 2 hydrogen bonds is formed in all the complexes throughout the simulation of 20 ns production of molecular dynamics simulation which indicates the stability of the complexes.
Appendix

LIST OF ANTI-TARGETS

>gi|13236497|ref|NP_076917.1| 5-hydroxytryptamine receptor 5A [Homo sapiens]
>gi|1168243|sp|P25100.2|ADA1D_HUMAN Alpha-1D adrenergic receptor (Alpha 1D-adrenoreceptor) (Alpha 1D-adrenoceptor) (Alpha-1A adrenergic receptor) (Alpha-adrenergic receptor 1a)
>gi|1168246|sp|P35348.2|ADA1A_HUMAN Alpha-1A adrenergic receptor (Alpha 1A-adrenoreceptor) (Alpha 1A-adrenoceptor) (Alpha-1C adrenergic receptor) (Alpha-adrenergic receptor 1c)
>gi|7690135|gb|AAB31163.2| alpha adrenergic receptor subtype alpha 1a [Homo sapiens]
>gi|547222|gb|AAB31165.1| alpha adrenergic receptor subtype alpha 1c [human, heart, Peptide, 466 aa]
>gi|547221|gb|AAB31164.1| alpha adrenergic receptor subtype alpha 1b [human, heart, Peptide, 516 aa]
>gi|2978556|gb|AAC06138.1| alpha 1A adrenergic receptor isoform 4 [Homo sapiens]
>gi|52000961|sp|P63092.1|GNAS2_HUMAN Guanine nucleotide-binding protein G(s) subunit alpha isoforms short (Adenylate cyclase-stimulating G alpha protein)
>gi|148539879|ref|NP_005151.2| beta adrenergic receptor kinase 2 [Homo sapiens]
>gi|15004694|gb|AAK77197.1|AF395806_1 adrenergic receptor alpha-1a [Homo sapiens]
>gi|111118990|ref|NP_150647.2| alpha-1A-adrenergic receptor isoform 4 [Homo sapiens]
>gi|111118988|ref|NP_150645.2| alpha-1A-adrenergic receptor isoform 3 [Homo sapiens]
>gi|111118986|ref|NP_150646.3| alpha-1A-adrenergic receptor isoform 2 [Homo sapiens]
>gi|4501959|ref|NP_000670.1| alpha-1B-adrenergic receptor [Homo sapiens]
>gi|177807|gb|AAA35496.1| alpha-1A-adrenergic receptor
>gi|117938756|ref|NP_001070950.1| constitutive androstane receptor isoform 1 [Homo sapiens]
>gi|117938754|ref|NP_001070949.1| constitutive androstane receptor isoform 4 [Homo sapiens]
>gi|117938752|ref|NP_001070948.1| constitutive androstane receptor isoform 2 [Homo sapiens]
>gi|117938750|ref|NP_001070947.1| constitutive androstane receptor isoform 10 [Homo sapiens]
>gi|117938748|ref|NP_001070945.1| constitutive androstane receptor isoform 14 [Homo sapiens]
>gi|117938746|ref|NP_001070946.1| constitutive androstane receptor isoform 7 [Homo sapiens]
>gi|117938744|ref|NP_001070944.1| constitutive androstane receptor isoform 13 [Homo sapiens]
>gi|117938742|ref|NP_001070943.1| constitutive androstane receptor isoform 15 [Homo sapiens]
>gi|117938740|ref|NP_001070942.1| constitutive androstane receptor isoform 8 [Homo sapiens]
>gi|117938738|ref|NP_001070941.1| constitutive androstane receptor isoform 12 [Homo sapiens]
>gi|117938736|ref|NP_001070940.1| constitutive androstane receptor isoform 9 [Homo sapiens]
>gi|117938734|ref|NP_001070939.1| constitutive androstane receptor isoform 5 [Homo sapiens]
>gi|117938732|ref|NP_001070938.1| constitutive androstane receptor isoform 11 [Homo sapiens]
>gi|117938729|ref|NP_001070937.1| constitutive androstane receptor isoform 6 [Homo sapiens]
>gi|4826661|ref|NP_005113.1| constitutive androstane receptor isoform 3 [Homo sapiens]
>gi|48869156|gb|AAT47173.1| constitutive androstane receptor SV15 [Homo sapiens]
>gi|48869154|gb|AAT47172.1| constitutive androstane receptor SV14 [Homo sapiens]
>gi|48869152|gb|AAT47171.1| constitutive androstane receptor SV13 [Homo sapiens]
>gi|48869150|gb|AAT47170.1| constitutive androstane receptor SV12 [Homo sapiens]
>gi|48869148|gb|AAT47169.1| constitutive androstane receptor SV11 [Homo sapiens]
>gi|48869142|gb|AAT47166.1| constitutive androstane receptor SV8 [Homo sapiens]
>gi|48869140|gb|AAT47165.1| constitutive androstane receptor SV7 [Homo sapiens]
>gi|48869128|gb|AAT47159.1| constitutive androstane receptor SV1 [Homo sapiens]
>gi|48869168|gb|AAT47179.1| constitutive androstane receptor SV21 [Homo sapiens]
>gi|48869166|gb|AAT47178.1| constitutive androstane receptor SV20 [Homo sapiens]
>gi|48869162|gb|AAT47176.1| constitutive androstane receptor SV18 [Homo sapiens]
>gi|48869146|gb|AAT47168.1| constitutive androstane receptor SV10 [Homo sapiens]
>gi|48869158|gb|AAT47174.1| constitutive androstane receptor SV16 [Homo sapiens]
>gi|48869130|gb|AAT47160.1| constitutive androstane receptor SV2 [Homo sapiens]
>gi|32307128|ref|NP_054790.2| nuclear receptor coactivator 6 [Homo sapiens]
>gi|52630419|ref|NP_001005291.1| sterol regulatory element binding transcription factor 1 isoform a [Homo sapiens]
>gi|22547195|ref|NP_004167.3| sterol regulatory element binding transcription factor 1 isoform b [Homo sapiens]
>gi|119587627|gb|EAW67223.1| dopamine receptor D2, isoform CRA_d [Homo sapiens]
>gi|119587623|gb|EAW67219.1| dopamine receptor D2, isoform CRA_a [Homo sapiens]
>gi|32483397|ref|NP_000788.2| dopamine receptor D4 [Homo sapiens]
>gi|4503383|ref|NP_000785.1| dopamine receptor D1 [Homo sapiens]
>gi|89191861|ref|NP_000787.2| dopamine receptor D3 isoform a [Homo sapiens]
>gi|89191863|ref|NP_387512.3| dopamine receptor D3 isoform e [Homo sapiens]
>gi|7381416|gb|AAF61479.1|AF176812_1 dopamine receptor D2longer [Homo sapiens]
>gi|5921992|ref|NP_000666.2| adenosine A2a receptor [Homo sapiens]
>gi|12548788|ref|NP_068712.1| gamma-aminobutyric acid (GABA) A receptor, beta 3 isoform 2 precursor [Homo sapiens]
>gi|4503867|ref|NP_000805.1| gamma-aminobutyric acid (GABA) A receptor, beta 3 isoform 1 precursor [Homo sapiens]
>gi|157389018|ref|NP_000802.2| gamma-aminobutyric acid A receptor, alpha 6 precursor [Homo sapiens]
>gi|150378528|ref|NP_001092881.1| G protein-coupled receptor associated sorting protein 1 [Homo sapiens]
>gi|4507685|ref|NP_003295.1| transient receptor potential cation channel, subfamily C, member 1 [Homo sapiens]
>gi|20373106|dbj|BAB91222.1| muscarinic acetylcholine receptor M5 [Homo sapiens]
>gi|30425444|ref|NP_848605.1| ankyrin repeat and kinase domain containing 1 [Homo sapiens]
>gi|66933005|ref|NP_001019820.1| calnexin precursor [Homo sapiens]
>gi|4504041|ref|NP_002061.1| guanine nucleotide binding protein (G protein), alpha inhibiting activity polypeptide 2 [Homo sapiens]
>gi|50541890|gb|AAT78421.1| Galphai2 protein [Homo sapiens]
>gi|4885563|ref|NP_005391.1| protein kinase C, epsilon [Homo sapiens]
>gi|96974985|ref|NP_060191.3| coiled-coil and C2 domain containing 1A [Homo sapiens]
KCNQ1_HUMAN Potassium voltage-gated channel subfamily KQT member 1 (Voltage-gated potassium channel subunit Kv7.1) (IKs producing slow voltage-gated potassium channel subunit alpha KvLQT1) (KQT-like 1)

KCNQ4_HUMAN Potassium voltage-gated channel subfamily KQT member 4 (Voltage-gated potassium channel subunit Kv7.4) (Potassium channel subunit alpha KvLQT4) (KQT-like 4)

nicotinic acetylcholine receptor beta 1 subunit precursor [Homo sapiens]

guanine nucleotide binding protein (G protein), q polypeptide [Homo sapiens]

potassium voltage-gated channel KQT-like protein 4 isoform b [Homo sapiens]

PTK2B protein tyrosine kinase 2 beta isoform a [Homo sapiens]

PTK2B protein tyrosine kinase 2 beta isoform b [Homo sapiens]

calcium channel, voltage-dependent, T type, alpha 11 subunit isoform b [Homo sapiens]

calcium channel, voltage-dependent, T type, alpha 11 subunit isoform a [Homo sapiens]

guanine nucleotide binding protein (G protein), alpha 11 (Gq class) [Homo sapiens]

Nuclear receptor subfamily 1 group I member 2 (Orphan nuclear receptor PXR) (Pregnane X receptor) (Orphan nuclear receptor PAR1) (Steroid and xenobiotic receptor) (SXR)

pregnane X receptor isoform 3 [Homo sapiens]

pregnane X receptor isoform 2 [Homo sapiens]

B Chain B, Crystal Structure Of The Human Pregnane X Receptor Lbd In Complex With An Src-1 Coactivator Peptide And T0901317
>gi|14719569|pdb|1ILH|A Chain A, Crystal Structure Of Human Pregnane X Receptor Ligand Binding Domain Bound To Sr12813
>gi|22538457|ref|NP_671756.1| nuclear receptor coactivator 1 isoform 2 [Homo sapiens]
>gi|22538459|ref|NP_671766.1| nuclear receptor coactivator 1 isoform 3 [Homo sapiens]
>gi|22538455|ref|NP_003734.3| nuclear receptor coactivator 1 isoform 1 [Homo sapiens]
>gi|13752550|gb|AAK38720.1|AF364606_1 orphan nuclear receptor PXR.1 [Homo sapiens]
>gi|71725341|ref|NP_001025174.1| hepatocyte nuclear factor 4 alpha isoform e [Homo sapiens]
>gi|71725339|ref|NP_787110.2| hepatocyte nuclear factor 4 alpha isoform d [Homo sapiens]
>gi|71725336|ref|NP_001025175.1| hepatocyte nuclear factor 4 alpha isoform f [Homo sapiens]
>gi|31077209|ref|NP_849181.1| hepatocyte nuclear factor 4 alpha isoform c [Homo sapiens]
>gi|31077207|ref|NP_849180.1| hepatocyte nuclear factor 4 alpha isoform a [Homo sapiens]
>gi|31077205|ref|NP_004483.3| hepatocyte nuclear factor 4 alpha isoform b [Homo sapiens]
>gi|62737968|pdb|1SKX|A Chain A, Structural Disorder In The Complex Of Human Pxr And The Macrolide Antibiotic Rifampicin
>gi|61679486|pdb|1XV9|D Chain D, Crystal Structure Of CarRXR HETERODIMETER BOUND WITH SRC1 Peptide, Fatty Acid, And 5b-Pregnane-3,20-Dione.
>gi|61679485|pdb|1XV9|C Chain C, Crystal Structure Of CarRXR HETERODIMETER BOUND WITH SRC1 Peptide, Fatty Acid, And 5b-Pregnane-3,20-Dione.
>gi|10863829|gb|AAG23345.1|PAR2 [Homo sapiens]
>gi|307180|gb|AAAS9575.1| P-glycoprotein [Homo sapiens]
>gi|386862|gb|AAAAS9576.1| P glycoprotein
>gi|34523|emb|CAA41558.1| P-glycoprotein [Homo sapiens]
>gi|2394178|gb|AAB70218.1| P-glycoprotein [Homo sapiens]  
>gi|2353264|gb|AAB69423.1| P-glycoprotein [Homo sapiens]  
>gi|33307712|gb|AAQ03033.1|AF399931_1 P-glycoprotein [Homo sapiens]  
>gi|37543520|gb|AAM09027.1| P-glycoprotein [Homo sapiens]  
>gi|25990364|gb|AAN76500.1|AF319622_1 P-glycoprotein [Homo sapiens]  
>gi|307181|gb|AAA36207.1| P-glycoprotein  
>gi|41058415|gb|AAR99172.1| P-glycoprotein [Homo sapiens]  
>gi|2506118|sp|P08183.2|MDR1_HUMAN Multidrug resistance protein 1 (ATP-binding cassette sub-family B member 1) (P-glycoprotein 1) (CD243 antigen)  
>gi|126302568|sp|P21439.2|MDR3_HUMAN Multidrug resistance protein 3 (ATP-binding cassette sub-family B member 4) (P-glycoprotein 3)  
>gi|10106242|prf|2111304A P glycoprotein  
>gi|1006663|emb|CAA84542.1| MDR3 P-glycoprotein [Homo sapiens]  
>gi|34525|emb|CAA29547.1| P-glycoprotein (431 AA) [Homo sapiens]  
>gi|6681436|dbj|BAA88711.1| sister p-glycoprotein [Homo sapiens]  
>gi|116242940|sp|Q2M3G0.2|ABCB5_HUMAN ATP-binding cassette sub-family B member 5 (P-glycoprotein ABCB5) (ABCB5 P-gp)  
>gi|40795903|gb|AAR91622.1| P-glycoprotein 1 [Homo sapiens]  
>gi|9961252|ref|NP_061338.1| ATP-binding cassette, subfamily B, member 4 isoform C [Homo sapiens]  
>gi|21536378|ref|NP_003733.2| ATP-binding cassette, sub-family B (MDR/TAP), member 11 [Homo sapiens]  
>gi|4506201|ref|NP_002788.1| proteasome beta 5 subunit [Homo sapiens]  
>gi|47116933|sp|Q9NS86.1|LANC2_HUMAN LanC-like protein 2 (Testis-specific adriamycin sensitivity protein)  
>gi|19913412|ref|NP_005106.2| major vault protein [Homo sapiens]  
>gi|25777707|ref|NP_740753.1| zinc ribbon domain containing 1 [Homo sapiens]  
>gi|66529005|ref|NP_005679.2| ATP-binding cassette, sub-family C, member 5 isoform 1 [Homo sapiens]
>gi|66529093|ref|NP_001018881.1| ATP-binding cassette, sub-family C, member 5 isoform 2 [Homo sapiens]
>gi|40287613|gb|AAR83914.1| unknown [Homo sapiens]
>gi|11545827|ref|NP_071395.1| p53-regulated apoptosis-inducing protein 1 [Homo sapiens]
>gi|121746|sp|P09211.2|GSTP1_HUMAN Glutathione S-transferase P (GST class-pi) (GSTP1-1)
>gi|56549095|ref|NP_001008406.1| B-cell receptor-associated protein BAP29 isoform c [Homo sapiens]
>gi|56549093|ref|NP_001008405.1| B-cell receptor-associated protein BAP29 isoform a [Homo sapiens]
>gi|56549091|ref|NP_061332.2| B-cell receptor-associated protein BAP29 isoform b [Homo sapiens]
>gi|4507811|ref|NP_003349.1| ceramide glucosyltransferase [Homo sapiens]
>gi|19913401|ref|NP_005066.2| organic anion transporting polypeptide A isoform b [Homo sapiens]
>gi|6005747|ref|NP_009143.1| ring finger protein 2 [Homo sapiens]
>gi|5729810|ref|NP_006570.1| emopamil binding protein (sterol isomerase) [Homo sapiens]
>gi|33946329|ref|NP_005393.2| ras related v-ral simian leukemia viral oncogene homolog A [Homo sapiens]
>gi|8923198|ref|NP_060182.1| pyroglutamyl-peptidase I [Homo sapiens]
>gi|19913403|ref|NP_602307.1| organic anion transporting polypeptide A isoform a [Homo sapiens]
>gi|19923262|ref|NP_004153.2| RAB5A, member RAS oncogene family [Homo sapiens]
>gi|2664295|emb|CAA84543.1| multidrug resistance protein 3 [Homo sapiens]
>gi|35553|emb|CAA41416.1| 70kDa peroxisomal membrane protein [Homo sapiens]
>gi|19584229|emb|CAD28599.1| unnamed protein product [Homo sapiens]
potassium channel subunit beta Mink) (Minimal potassium channel) (Delayed rectifier potassium channel subunit IsK)
>gi|19923352|ref|NP_006158.2| NK3 homeobox 1 [Homo sapiens]
>gi|27436978|ref|NP_751951.1| potassium voltage-gated channel, Isk-related family, member 2 [Homo sapiens]
>gi|5803225|ref|NP_006752.1| tyrosine 3/trypotphan 5-monooxygenase activation protein, epsilon polypeptide [Homo sapiens]
>gi|103488986|gb|ABF71886.1| voltage-gated potassium channel KV11.1 transcript variant 1 [Homo sapiens]
>gi|38635441|emb|CAE82156.1| potassium voltage-gated channel, subfamily H (eag-related), member 2 [Homo sapiens]
>gi|26006811|sp|Q9NS40.1|KCNH7_HUMAN Potassium voltage-gated channel subfamily H member 7 (Voltage-gated potassium channel subunit Kv11.3) (Ether-a-go-go-related gene potassium channel 3) (HERG-3) (Ether-a-go-go-related protein 3) (Eag-related protein 3)
>gi|26006810|sp|Q9H252.1|KCNH6_HUMAN Potassium voltage-gated channel subfamily H member 6 (Voltage-gated potassium channel subunit Kv11.2) (Ether-a-go-go-related gene potassium channel 2) (Ether-a-go-go-related protein 2)
>gi|4033376|sp|Q14524.1|SCN5A_HUMAN Sodium channel protein type 5 subunit alpha (Sodium channel protein type V subunit alpha) (Voltage-gated sodium channel subunit alpha Nav1.5) (Sodium channel protein cardiac muscle subunit alpha) (HH1)
>gi|154448884|ref|NP_542402.2| potassium voltage-gated channel, Isk-related family, member 4 [Homo sapiens]
>gi|27886665|ref|NP_775185.1| potassium voltage-gated channel, subfamily H, member 7 isoform 2 [Homo sapiens]
>gi|4885443|ref|NP_005463.1| potassium voltage-gated channel, Isk-related family, member 3 [Homo sapiens]
>gi|27886651|ref|NP_775115.1| potassium voltage-gated channel, subfamily H, member 6 isoform 2 [Homo sapiens]
>gi|6729769|pdb|1BYW|A Chain A, Structure Of The N-Terminal Domain Of The Human-Erg Potassium Channel
>gi|71739466|gb|AAZ40507.1| potassium channel HERG1 [Homo sapiens]
>gi|3452413|emb|CAA09232.1| ether-a-go-go-related protein [Homo sapiens]
LIST OF PUBLICATIONS


