Looking for β3 integrin family selectivity: The use of snake venom disintegrin as a tool for molecular modeling approach

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In the hemostasis and angiogenesis several cell adhesion molecules and transmembrane receptors are of great importance for the functioning those processes



R&D System, http://http://www.rndsystems.com/BIObrief_s07.aspx

B3 Integrins family

Platelets aggregation





Angiogenesis

 $\alpha_v \beta_3$



Disintegrins and drug design



Aims

in silico analysis

Structure activity relationship (SAR) of disintegrins;

Selective profile of disintegrins against integrins receptors.

Disintegrins Alignment of ...

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BarbourinaPAGEECDCGSPENPCCDAATCKLRPGAQCADGLCCDCCREMKGTVCRVV KGL NNDDTCTGCSADCPRNGFYGUssuristatina-1GEECDCGAPANPCCDAATCKLRPGQCAEGLCCDCREMKGTVCRV KGL NNDDTCTGCSADCPRNGFYGSalmosina-2EAGKECDCGAPANPCCDAATCKLRPGQCAEGLCCDCREMKEGTCOEKGL NNDDTCTGCSADCPRNGFYGUssuristatina-2EAGEECDCGAPANPCCDAATCKLRPGQCAEGLCCDCCREMKEGTCOEKGL NNDDTCTGCSADCPRNGFYGHalystatinaEAGEECDCGAPANPCCDAATCKLRPGQCAEGCCCDCCREMKEGTCORKGL NNDDTCTGCSADCPRNGHalystatinaEAGEECDCGAPANPCCDAATCKLRPGQCAEGCCDCCCREMKEGTVCREKGL NNDDTCTCGSADCPRNGAcostatina-betaETGEESDFDAPANPCCDAATCKLTGSCADGLCDCCKEMKEGTVCREKGL NDDYCNGISAGCPRNPFHAContortrostatinaETGEESDFDAPANPCCDAATCKLTGSCADGLCDCCKEMKEGTVCREKGL LDDYCNGISAGCPRNPFHAApWMZETGEESDFDAPANPCCDAATCKLTREGQCAEGLCCDCCKEMKEGTVCREKGL LDDYCNGISAGCPRNPFHAPiscivostatina-betaETGEESDFDAPANPCCDAATCKLTREGQCAEGLCCDCCKEMKEGTVCREKGL LDDYCNGISAGCPRNPFHAJerdonitinaETGEESDFDAPANPCCDAATCKLTPGSQCAEGLCCDCCSEMKEGTVCREKGL LDDYCNGISAGCPRNPFHAJerdonitinaEYGEDCDCGPPANCONPCCDAATCKLTPGSQCAEGLCCDCCSEMKEGTVCREKGL LDDYCNGISAGCPRNPFHATrigramina-alphaEAGEECDCGFPGNPCCDAATCKLIPGAQCAEGLCCDCCSEMKEGTVCREKGL LDDYCNGISAGCPRNPFHABiVI IIGAGEECDCGFPGNPCCDAATCKLIPGAQCAEGLCCDCCSEMKEGTVCREKGL LDDYCNGISAGCPRNPFHAJarastatinaEAGEECDCGFPGNPCCDAATCKLIPGAQCAEGLCCDCCREMKEGTVCREKGL LDDYCNGISAGCPRNPFHABaMP IGAGEECDCGFPGNPCCDAATCKLIPGAQCAEGLCCDCCREMKEGTVCREKGL LDDYCNGISAGCPRNPFHABAHY	Cerastina	EAGEECDCGTPE	NPCCDAATCKLRPGAÕCADGLCCDÕCREMKKGTVCRVI RGE NNDDTCTGÕSADCPRNGLYG
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GhMP I EAGKECD CGAPA NPCCDAETCKLRPCQCAEGLCDOCREMKECTIOQE KGT VNDTCNGTSAGCPRNGFYG Ussuristatina-2 EAGKECD CGAPA NPCCDAATCKLRPCQCAEGLCDOCREMKECTIOQE KGT VNDTCTGOSADCPRNGFYG Halystatina EAGEECD CGAPA NPCCDAATCKLRPCQCAEGLCDOCREMKECTIOQE KGT VNDTCTGOSADCPRNGFYG Halystatina EAGEECD CGAPA NPCCDAATCKLRPCQCAEGLCDOCREMKECTIOQE KGT VNDTCTGOSADCPRNGF Acostatina-beta ETGEESDEDAPA NPCCDAATCKLRPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA ApMP II ETGEESDEDAPA NPCCDAETCKLRPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA ApVMZ ETGEESDEDAPA NPCCDAETCKLRPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA Agkistina EYGEDCD CGPPANCONPCCDAETCKLRPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA Jerdonitina EYGEDCD CGPPANCONPCCDAATCKLTPCSOCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA Trigramina-alpha EYGEDCD CGPPANCONPCCDAATCKLTPCSOCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA Trigramina-alpha EAGEDCD CGSPA NPCCDAATCKLIPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA Trigramina-alpha EAGEDCD CGSPA NPCCDAATCKLIPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA Trigramina-alpha EAGEDCD CGSPA NPCCDAATCKLIPCQCAEGLCDOCREMKECTVCRR KGT UDDYCNGTSAGCPRNPEHA	Ussuristatina-1	GEECDCGSPG	NPCCDAATCKLRPGAQCAEGLCCEQCRFIKAGTVCRV/RGT/NDDKCTGQSADCPRNGFYG
Salmosina-2 BAGKCDCCGAPA NPCCDAATCKLRPEGCAEGICCDCCRPMKEGTICRE KGD KNDTCTGOSADCPRNGE Halystatina BAGECDCGAPA NPCCDAATCKLRPGACAEGICCDCCRPMKEGTICRE KGD KNDTCTGOSADCPRNGE Halystatina BAGEDCDCGAPA NPCCDAATCKLRPGACAEGICCDCCRPMKEGTICRE KGD KNDTCTGOSADCPRNGE Acostatina-beta ETGEESDEDAPA NPCCDAATCKLTTCSCADGLCCDCCKEMKEGTICRE RGD JDDYCNGISAGCPRNEPHA ApMP II ETGEESDEDAPA NPCCDAATCKLTTCSCADGLCCDCCKEMKEGTICRE RGD JDDYCNGISAGCPRNEPHA ApVMZ ETGEESDEDAPA NPCCDAATCKLTPESCAEGICCDCCKEMKEGTUCHE KGD JDDYCNGISAGCPRNEPHA Agkistina ETGEESDEDAPA NPCCDAATCKLTPESCAEGICCDCCKEMKEGTUCHE KGD JDDYCNGISAGCPRNEPHA Agkistina EVGEDCDCGPPANCONCCDAATCRLTPESCAEGICCDCCKEMKEGTUCHE KGD JDDYCNGISAGCPRNEPHA Trigramina-beta EAGKDCDCGSPA NPCCDAATCKLIPESCAEGICCDCCSFMKEGTUCRE RGD JDDYCNGISAGCPRNEPHA Trigramina-alpha EAGKDCDCGSPA NPCCDAATCKLIPESCAEGICCDCCSFMKEGTUCRE RGD JDDYCNGISAGCPRNEPHA Jaraštatina BAGEECDCCTPG NPCCDAATCKLIPESCAEGICCDCCREMKEGTUCRE RGD JDDYCNGISAGCPRNEPHA Jaraštatina BAGEECDCCTPG NPCCDAATCKLIPESCAEGICCDCCREMKEGTUCRE RGD JDDYCNGISAGCPRNEPHA Jaraštatina BAGEECDCCTPG NP	GhMP_I	EAGKECDCGAPA	NPCC <mark>DAE</mark> TCKLRPGQQCAEGLCCDQCRFMKEGTICQ <mark>E</mark> /KGD/NDDTCNGISAGCPRNGFYG
Description DAGEECOCGAPA NPCCDAATCKIRPCAQCAECOCCGCREVKECTVCRE RCDINDTCTCGSADCPRNCI Halystatina EAGEECOCGAPA NPCCDAATCKIRPCAQCAECOCCCCREVKECTVCRE RCDINDTCTCGSADCPRNCI Acostatina-beta ETCEESDFDAPA NPCCDAATCKIFTCSQCADGLCCDCCKEMKECTVCRE RCDINDTCTCGSADCPRNEPHA ApMP II ETCEESDFDAPA NPCCDAATCKIFTCSQCADGLCCDCCKEMKECTVCRE RCDINDTCTGSACPRNEPHA ApVMZ ETCEESDFDAPA NPCCDAATCKIFTCSQCAEGLCCDCCKEMKECTVCRE KCDINDTVCGISACCPRNEPHA Agkistina ETCEESDFDAPA NPCCDAATCKIFTCSQCAEGLCCDCCKEMKECTVCRE KCDINDTVCGISACCPRNEPHA Agkistina ETCEESDFDAPA NPCCDAATCKIFTCSQCAEGLCCDCCKEMKECTVCRE KCDINDTVCGISACCPRNEPHA Agkistina EVCEDCDCCGPPANCONPCCDAATCKIFTCSQCAEGLCCDCCKEMKECTVCRE KCDINDTVCGISACCPRNEPHA Trigramina-alpta EAGECCCCSPA NPCCDAATCKIFTCSQCAEGLCCDCCSFMKECTVCRE RCDINDTVCGISACCPRNEPHA Tigramina-alpta EAGEECCCCSPA NPCCDAATCKIFTCSQCAEGLCCDCCSFMKECTVCRE RCDINDTVCGISACCPRNEPHA Jarastatina EAGEECCCCSFG NPCCDAATCKIFTCSQCAEGLCCDCCSFMKECTVCRE RCDINDTVCGISACCPRNEPHA Jarastatina EAGEECCCCSFG NPCCDAATCKIFTCSQCAEGLCCDCCSFMKECTVCRE RCDINDTVCGISACCPRNEPHA Jarastatina EAGEECCCCSFG NPCC	Salmosina-2	EAGKECDCGAPA	NPCCDAATCKLRPGEQCAEGLCCDQCRFMKEGTICQE KGD vNDDTCTGQSADCPRNGFYG
HalystatinaDAGEDCDCGAPA PCCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCADGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCKEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCCEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCCEINAGTVCRRNECTAGENDCPRACE NECCDATCKLTFGSCACGLCDQCCEINAGTVCRRNECCDATCKLTFGSCACGGCCDQCSEINAGTVCRRNECCDATCKLTFGSQCACGGCCDQCSEINAGTVCRRNECCDATCKLTFGSQCACGGCCDQCSEINAGTVCRRNECCDATCKLTFGSQCACGGCCDQCSEINAGTTCRI	Ussuristatina-2	DAGDDCDCGAPA	NPCCDAATCKLRPGAQCABGDCCBQCREVKBGTVCRE KGL VNDDSCTGQSADCPRNG
Active StatinaEndeside DepartEndeside DepartEndeside DepartEndeside DepartApWP IIEndes SpipAPANPCCDAATCKINTGSQCADGLCCDQCKEMKEGTVCRRKGD JLDDYCNGISAGCPRNPFHAApVM2Endes SpipAPANPCCDAETCKINPGAQCAEGLCCDQCKEMKEGTVCRRKGD JLDDYCNGISAGCPRNPFHAAgkistinaEndes SpipAPANPCCDAATCKINPGAQCAEGLCCDQCKEMKEGTVCRRKGD JLDDYCNGISAGCPRNPFHAAgkistinaEvGEDCDCGPPARQNPCCDAATCKINPGSQCAEGLCCDQCKEMKEGTVCRRKGD JLDDYCNGISAGCPRNPFHAAgkistinaEvGEDCDCGPPARQNPCCDAATCKINPGSQCAEGLCCDQCSEMKKGTICRIRGD JLDDYCNGISAGCPRNPFHAJerdonitinaEvGEDCDCGPPARQNPCCDAATCKINPGSQCAEGLCCDQCSEMKKGTICRIRGD JLDDYCNGISAGCPRNPFHATrigramina-betaEAGEDCDCGSPANPCCDAATCKINPGAQCGEGLCCDQCSEMKKGTICRIRGD JLDDYCNGISAGCPRNPFHAJarastatinaEAGEDCDCGSPANPCCDAATCKINPGAQCAEGLCCDQCSEMKKGTICRIRGD JLDDYCNGISAGCPRNPFHABjVM IIGAGEECDCGTPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTVCRIRGD MDDYCNGISAGCPRNPFHABaMP IEAGEECDCGTPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTVCRIRGD MDDYCNGISAGCPRNPFHABaMP IEAGEECDCGSPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTVCRIRGD MDDYCNGISAGCPRNPFHABaMP IEAGEECDCGSPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTVCRIRGD MDDYCNGISAGCPRNPFHAHalysinaEAGEECDCGSPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTVCRIRGD MDDYCNGISAGCPRNPFHAHalystatina-1EAGEECDCGSPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTVCRIRGD MDDYCNGISAGCPRNPFHASalmosinaEAGEECDCGSPGNPCCDAATCKINPGAQCAEGLCCDQCREMKEGTICRNRGD JDDYCNGISAGCPRNPFHAApplaginaEAGEECDC	Haiystatina	EAGEDCDCGAPA	
Control <t< td=""><td>Contortrostatina</td><td>ETCER SDEDADA</td><td>NPCCDAATCALIIGSQCADGLCCDQCAFMARGCIVCAR, AGD JLDDICAGISAGCPANPETA</td></t<>	Contortrostatina	ETCER SDEDADA	NPCCDAATCALIIGSQCADGLCCDQCAFMARGCIVCAR, AGD JLDDICAGISAGCPANPETA
ApVM2ETGEESDEDAPANPCCDAETCKLRPGAQCAEGLCCDQCKEMKEGTVCHRKGTDLDDYCNGISAGCPRNPFHAPiscivostatina-betaETGEESDEDAPANPCCDAATCKLTPGSQCAEGLCCDQCKEMKEGTVCHRKGTDLDDYCNGISAGCPRNPFHAAgkistinaEVGEDCDCGPPANCONPCCDAATCKLTPGSQCAEGLCCDQCREMKEGTVCRLRGTDLDDYCNGISAGCPRNPFHAAgkistinaEVGEDCDCGPPANCONPCCDAATCKLTPGSQCAEGLCCDQCREMKEGTICRRRGTDLDDYCNGISAGCPRNPFHATrigramina-alphaEVGEDCDCGSPANPCCDAATCKLTPGSQCAEGLCCDQCREMKEGTICRRRGTDLDDYCNGRSAGCPRNPFHATrigramina-alphaEAGEDCDCGSPANPCCDAATCKLTPGAQCGEGCCDQCSEMKKGTICRRRGTDLDDYCNGRSAGCPRNPFHAJarastatinaEAGEDCDCGSPANPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRTRGTDLDDYCNGRSAGCPRNPFHAJarastatinaEAGEECDCGTPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRTRGTMDDYCNGISAGCPRNPFHAJarastatinaEAGEECDCGTPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRTRGTMDDYCNGISAGCPRNPFHAJarastatinaEAGEECDCGTPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRTRGTMDDYCNGISAGCPRNPFHAJayinaEAGEECDCGSPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRTRGTMDDYCNGISAGCPRNPFHAHalysinaEAGEECDCGSPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRTRGTMDDYCNGISAGCPRNPFHAHalystatina-1EAGEECDCGSPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTUCRTRGTMDDYCNGISAGCPRNPFHASalmosinaEAGEECDCGSPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRRRGTDDDYCNGISAGCPRNPFHAApplaginaEAGEECDCGSPGNPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRMRGTNDDYCNGISAGCPRNPFHA </td <td>ApMP II</td> <td>ETCEESDEDAPA</td> <td>NPCCDAETCKL RPGAOCAEGLCCDOCK EMKEGTVCHR, KGT SLDDYCNGT SAGCPRNPEHA</td>	ApMP II	ETCEESDEDAPA	NPCCDAETCKL RPGAOCAEGLCCDOCK EMKEGTVCHR, KGT SLDDYCNGT SAGCPRNPEHA
Piscivostatina-betaETGEESDEDAPANPCCDAATCKLTPGSOCAEGLCCDOCKEMKEGTVCHRKGTLDDYCNGISAGCPRNPFHAAgkistinaEVGEDCDCGPPANCONPCCDAATCRLTPGSOCAEGLCCDOCKEMKEGTVCHTKGTLDDYCNGISAGCPRNPFHAJerdonitinaEVGEDCDCGPPANCONPCCDAATCRLTPGSOCAEGLCCDOCSEMKEGTICRRKGTLDDYCNGISAGCPRNPFHAJerdonitinaEAGEDCDCGSPANPCCDAATCKLTPGSOCAEGLCCDOCSEMKKGTICRRKGTLDDYCNGISAGCPRNPFHATrigramina-alphaEAGEDCDCGSPANPCCDAATCKLTPGAOCGEGLCCDOCSEMKKGTICRRKGTLDDYCNGRSAGCPRNPFHABjVM IIGAGEECDCGTPGNPCCDAATCKLRPGAOCAEGLCCDOCREMKEGTVCRTKGTDDDYCNGISAGCPRNPFHABaMP IEAGEECDCGTPGNPCCDAATCKLRPGAOCAEGLCCDOCREMKEGTVCRTKGTDDDYCNGISAGCPRNPFHABaMP IEAGEECDCGTPGNPCCDAATCKLRPGAOCAEGLCCDOCREMKEGTVCRTKGTDDDYCNGISAGCPRNPFHAJssurinaEAGEECDCGTPGNPCCDAATCKLRPGAOCAEGLCCDOCREMKEGTVCRTKGTDDDYCNGISAGCPRNPFHAHalysinaEAGEECDCGSPGNPCCDAATCKLRPGAOCAEGLCCDOCREMKEGTVCRTKGTDDDYCNGISAGCPRNPFHAHalystatina-1EAGEECDCGSPGNPCCDAATCKLRQGAOCAEGLCCDOCREMKEGTVCRTKGTDDDYCNGISAGCPRNPFHAAgnosinaEAGEECDCGSPGNPCCDAATCKLRQGAOCAEGLCCDOCREMKEGTICRRRGTDDDYCNGISAGCPRNPFHAApplaginaEAGEECDCGSPGNPCCDAATCKLRQGAOCAEGLCCDOCREMKEGTICRRRGTDDDYCNGISAGCPRNPFHAApplaginaEAGEECDCGSPGNPCCDAATCKLRQGAOCAEGLCCDOCREMKEGTICRRRGTDDDYCNGISAGCPRNPFHAAsaxatilinaEAGEECDCGAPANPCCDAATCKLRPGAOCAEGLCCDOCREMKEGTICRRRGTDDDYCNGISAGCPRNPFHAApplagina <t< td=""><td>ApVM2</td><td>TGPESDEDAPA</td><td>NPCCDAFTCKLRPGAOCAPGLCCDOCKEMKPGTVCHR, KGL DLDDYCNGI SAGCPRNPEHA</td></t<>	ApVM2	TGPESDEDAPA	NPCCDAFTCKLRPGAOCAPGLCCDOCKEMKPGTVCHR, KGL DLDDYCNGI SAGCPRNPEHA
AgkistinaEVGEDCDCGPPANCQNPCCDAATCRLTPGSQCAEGLCCEQCSEMKEGTVCRLTRGTLDDYCNGISAGCPRNPSHAJerdonitinaEVGEDCDCGPPANCQNPCCDAATCRLTPGSQCADGLCDQCREMKKGTICRLTRGTLDDYCNGISAGCPRNPSHATrigramina-betaEAGEDCDCGSPANPCCDAATCRLTPGSQCADGLCCDQCSEMKKGTICRLTRGTLDDYCNGISAGCPRNPFHATrigramina-alphaEAGEDCDCGSPANPCCDAATCRLTPGSQCAEGLCCDQCSETLEGTVCRLTRGTLDDYCNGISAGCPRNPFHABjVM_IIGAGEECDCGTPGNPCCDAATCRLTPGAQCAEGLCCDQCREMKEGTVCRTRRGTNDDYCNGISAGCPRNPFHABaMP_IEAGEECDCGTPGNPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRTRRGTMDDYCNGISAGCPRNPFHABaMP_IEAGEECDCGTPGNPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRTRRGTMDDYCNGISAGCPRNPFHABaMP_IEAGEECDCGTPGNPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRTRRGTMDDYCNGISAGCPRNPFHAUssurinaEAGEECDCGSPGNPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRTRRGTMDDYCNGISAGCPRNPFHAHalysinaEAGEECDCGSPGNPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTVCRTRRGTMDDYCNGISAGCPRNPFHAHalystatina-1EAGEECDCGSPGNPCCDAATCRLRQGAQCAEGLCCDQCREMKRGTVCRTRRGTMDDYCNGISAGCPRNPFHASalmosinaEAGEECDCGSPGNPCCDAATCRLRQGAQCAEGLCCDQCREMKRGTVCRTRRGTNDDYCNGISAGCPRNPFHAApplaginaEAGEECDCGSPGNPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTICRRRNDDYCNGISAGCPRNPFHAApplaginaEAGEECDCGSPGNPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTICRRRNDDYCNGISAGCPRNPFHAAsaxatilinaEAGEECDCGAPANPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTICRRRNDDYCNGISAGCPRNPFHAHalystatina-2EAGEECDCGAPANPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTICRRRNDDYCNGISAGCPRNPFHAKt-dEAGEECDCGAPA </td <td>Piscivostatina-beta</td> <td>ETGEE SDFDAPA</td> <td>NPCCDAATCKLTPGSQCAEGLCCDQCKFMKEGTVCHR KGD DLDDYCNGISAGCPRNPFHA</td>	Piscivostatina-beta	ETGEE SDFDAPA	NPCCDAATCKLTPGSQCAEGLCCDQCKFMKEGTVCHR KGD DLDDYCNGISAGCPRNPFHA
Jerdonitina EVGEDCDCGPPANCQNPCCDAATCRLTPGSQCADGLCCDQCREMKKGTICRI RGD LDDYCNGISAGCPRNPFHA Trigramina-beta EAGKDCDCGSPA NPCCDAATCRLTPGSQCADGLCCDQCSEMKKGTICRI RGD LDDYCNGRSAGCPRNPFHA BjVM_II GAGEECDCGFPG NPCCDAATCRLTPGAQCGEGLCCDQCSEMKEGTVCRI RGD LDDYCNGRSAGCPRNPFHA BjVM_II GAGEECDCGFPG NPCCDAATCRLTPGAQCGEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA BaMP_I EAGEECDCGFPG NPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA BaMP_I EAGEECDCGFPG NPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA Jusaina EAGEECDCGFPG NPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA Jusuina EAGEECDCGFPG NPCCDAATCRLRPGAQCAEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA Jusuina EAGEECDCGSPG NPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA Halysina EAGEECDCGSPG NPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTVCRI RGD MDDYCNGISAGCPRNPFHA Halysina EAGEECDCGSPG NPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTUCRI RGD MDDYCNGISAGCPRNPFHA Mt-b EAGEECDCGSPG NPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTUCRI RGD MDDYCNGISAGCPRNPFHA Salmosina EAGEECDCGSPG NPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTUCRI RGD MDDYCNGISAGCPRNPFHA Applagina EAGEECDCGSPG NPCCDAATCRLRQGAQCAEGLCCDQCREMKEGTUCRN RGD MDDYCNGISAG	Agkistina	EVGEDCDCGPPANC	ONPCCDAATCRLTPGSQCAEGLCCEQCSFMKEGTVCRL RGDLDDYCNGISAGCPRNPSHA
Trigramina-betaEAGEDCDCGSPANPCCDAATCKLIPGAQCGEGPCCDQCSPMKKGTICRRRGD JLDDYCNGRSAGCPRNPFHATrigramina-alphaEAGEDCDCGSPANPCCDAATCKLIPGAQCGEGLCCDQCSFIEGTVCRLRGD JLDDYCNGRSAGCPRNPFHABjVM IIGAGEECDCGTPGNPCCDAATCKLIPGAQCAEGLCCDQCRFMKEGTVCRRRGD JLDDYCNGRSAGCPRNPFHAJaraātatinaEAGEECDCGTPGNPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTVCRRRGD JMDYCNGISAGCPRNPFHABaMP_IEAGEECDCGTPGNPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTVCRLRGD JMDYCNGISAGCPRNPFHAJaraātatinaEAGEECDCGSPGNPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTVCRLRGD JMDYCNGISAGCPRNPFHAAdinbitorEAGEECDCGSPGNPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTVCRLRGD JMDYCNGISAGCPRNPFHAHalysinaEAGEECDCGSPGNPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRLRGD JMDYCNGISAGCPRNPFHAHalystatina-1EAGEECDCGSPGNPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRLRGD JMDYCNGISAGCPRNPFHASalmosinaEAGEECDCGSPGNPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRLRGD JLDDYCNGISAGCPRNPFHAApplaginaEAGEECDCGSPGNPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRRRGD JLDDYCNGISAGCPRNPFHAAgplaginaEAGEECDCGSPGNPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRRRGD JLDDYCNGISAGCPRNPFHASaxatilinaEAGEECDCGAPANPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRMRGD JMDYCNGISAGCPRNPFHASaxatilinaEAGEECDCGAPANPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRMRGD JMDYCNGISAGCPRNPFHASaxatilinaEAGEECDCGAPANPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRMRGD JMDYCNGISAGCPRNPFHAHalystatina-2EAGEECDCGAPANPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRMRGD JMDYCNGISAGCPRNPFHA	Jerdonitina	EVGEDCDCGPPANC	QNPCCDAATCRLTPGSQCADGLCCDQCRFMKKGTICRI RGD)LDDYCNGISAGCPRNPFHA
Trigramina-alpha DAGEDCOCCSEA NPCCDAATCKLIPGAQCASCLCCDQCSPLEEGTVCRIFRCDJADYCNGRSAGCPRNPFHA BjVM II GAGEECDCGTPG NPCCDAATCKLRPGAQCAEGLCCDQCRPMKEGTVCRIFRCDJADYCNGISAGCPRNPFHA BaMP I EAGEECDCGTPG NPCCDAATCKLRPGAQCAEGLCCDQCRPMKEGTVCRIFRCDJADDYCNGISAGCPRNPFHA BaMP I EAGEECDCGTPG NPCCDAATCKLRPGAQCAEGLCCDQCRPMKEGTVCRIFRCDJADDYCNGISAGCPRNPFHA BaMP I EAGEECDCGTPG NPCCDAATCKLRPGAQCAEGLCCDQCRPMKEGTVCRIFRCDJADDYCNGISAGCPRNPFHA Adinbitor EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRPMKEGTVCRIFRCDJADDYCNGISAGCPRNPFHA Halysina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRPMKKGTVCRIFRCDJADDYCNGISAGCPRNPFHA Halystatina-1 EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRPMKKGTVCRIFRCDJADDYCNGISAGCPRNPFHA Halystatina-1 EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRIFRCDJADDYCNGISAGCPRNPFHA Salmosina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR DDDYCNGISAGCPRNPFHA Applagina EAGEECDCGSPE NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD JDDYCNGISAGCPRNPFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD JDDYCNGISAGCPRNPFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR NDDYCNGISAGCPRNPFHA Saxatilina <	Trigramina-beta	EAGKDCDCGSPA	NPCCDAATCKLLPGAQCGEGPCCDQCSFMKKGTICRR.RGD_LDDYCNGRSAGCPRNPFHA
BJW_11 CAGEECDUCGTPG NPCCDAVTCALRPGACAEGLCCDUCKEMAEGTVCKK KG DMDPCNGISAGCPKNPHA BaMP_I EAGEECDUCGTPG NPCCDAATCKLRPGACAEGLCCDUCKEMKEGTVCKI KG DMDPCNGISAGCPKNPFHA BaMP_I EAGEECDUCGTPG NPCCDAATCKLRPGACAEGLCCDUCKEMKEGTVCKI KG DMDPCNGISAGCPKNPFHA Jussufina EAGEECDUCSPG NPCCDAATCKLRPGACAEGLCCDUCKEMKEGTVCKI KG DMDPCNGISAGCPKNPFHA Halysina EAGEECDUCSPG NPCCDAATCKLRQGACAEGLCCDUCKEMKEGTVCKI KG DMDPCNGISAGCPKNPFHA Halysina EAGEECDUCSPG NPCCDAATCKLRQGACAEGLCCDUCKEMKKGTVCKI KG DMDPCNGISAGCPKNPFHA Halystatina-1 EAGEECDUCGSPG NPCCDAATCKLRQGACAEGLCCDUCKEMKKGTVCKI KG DMDPCNGISAGCPKNPFHA Halystatina-1 EAGEECDUCSPG NPCCDAATCKLRQGAUCAEGLCCDUCKEMKKGTVCKI KG DMDPCNGISAGCPKNPFHA Salmosina EAGEECDUCSPG NPCCDAATCKLRQGAUCAEGLCCDUCKEMKEGTICKK KG DLDDYCNGISAGCPKNPFHA Applagina EAGEECDUCSPG NPCCDAATCKLRQGAUCAEGLCCDUCKEMKEGTICKK KG DLDDYCNGISAGCPKNPFHA Applagina EAGEECDUCGAPA NPCCDAATCKLRQGAUCAEGLCCDUCKEMKEGTICKK KG DLDDYCNGISAGCPKNPFHA Saxatilina EAGEECDUCGAPA NPCCDAATCKLRQGAUCAEGLCCDUCKEMKEGTICKM KG DMDDYCNGISAGCPKNPFHA Saxatilina EAGEECDUCGAPA NPCCDAATCKLRQGAUCAEGLCCDUCKEMKEGTICKM KG MDDYCNGISAGCPKNPFHA Halystatina-2 EAGEECDUCGAPA NPCCDAATCKLRQGAUCAEGLCDUCKEMKEG	Trigramina-alpha	DAGDDCDCGSPA	NPCCDAATCKLIPGAQCGEGLCCDQCSETEEGTVCRLIRGEDLDDYCNGRSAGCPRNPEHA
Datastatina DAGEBCOCGEPG NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCNN KGT JEDDYCNGISAGCPNPFHA Ussurina EAGEECDCGSPG NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTVCRI KGT JMDDYCNGISAGCPNPFHA Adinbitor EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTVCRI KGT JMDDYCNGISAGCPNPFHA Halysina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKKGTVCRI KGT JMDDYCNGISAGCPNPFHA Halysina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKKGTVCRI KGT JMDDYCNGISAGCPNPFHA Mt-b EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKKGTVCRI KGT JMDDYCNGISAGCPNPFHA Mt-b EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRK KGT JMDDYCNGISAGCPNPFHA Salmosina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRK KGT JMDDYCNGISAGCPRNPFHA Applagina EAGEECDCGSPE NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRK KGT JMDYCNGISAGCPRNPFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRK KGT JMDYCNGISAGCPRNPFHA Halystatina-2 EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM KGT JMDYCNGISAGCPRNPFHA	BJVM II	GAGEECDCGTPG	NPCCDAVTCKLRPGAQCABGLCDQCRPMREGTVCRR RGLMDDYCNGI SAGCPRNPPHA
Dame	Band T	TAGERCDCGTPG	NPCCDAATCNIRPGAQAACGICCDQCRIMRACTVCRR RGLMDDYCNGI SAGCPRNPHHA
Adinbitor EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRL RGD MDDYCNGISAGCPRNFHA Halysina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRL RGD MDDYCNGISAGCPRNFHA Halystatina-1 EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRL RGD MDDYCNGISAGCPRNFHA Kt-b EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRL RGD MDDYCNGISAGCPRNFHA Salmosina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD LDDYCNGISAGCPRNFHA Applagina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD DDYCNGISAGCPRNFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRR RGD DDYCNGISAGCPRNFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDDYCNGISAGCPRNFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDDYCNGISAGCPRNFHA Halystatina-2 EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDDYCNGISAGCPRNFHA	Ussurina	EAGEECDCDSPG	NPCCDAATCKLRPGAOCAEGLCCEOCREMKEGTVCRU RGDMDDYCNGTSAGCPRNPFHA
Halysina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRI RGD MDDYCNGISAGCPRNFHA Halystatina-1 EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRI RGD MDDYCNGISAGCPRNFHA Mt-b EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRI RGD MDDYCNGISAGCPRNFHA Salmosina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD MDDYCNGISAGCPRNFHA Applagina EAGEECDCGSPE NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD MDYCNGISAGCPRNFH Mt-d EAGEECDCGSPE NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDYCNGISAGCPRNFH Mt-d EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDYCNGISAGCPRNFH Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDYCNGISAGCPRNFHA Halystatina-2 EAGEDCDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCRFMKEGTICRM RGD MDYCNGISAGCPRNFHA	Adinbitor	EAGEECDCGSPG	NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRL RGD MDDYCNGISAGCPRNPFHA
Halystatina-1 EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTUCRI RCD MDDYCNGISAGCPRNFHA Mt-b EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRR RCD LDDYCNGISAGCPRNFHA Salmosina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRR RCD LDDYCNGISAGCPRNFHA Applagina EAGEECDCGSPE NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRR RCD LDDYCNGISAGCPRNFH Mt-d EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRR RCD DDYNYCNGISAGCPRNFH Mt-d EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RCD MDDYCNGISAGCPRNFH Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RCD MDDYCNGISAGCPRNFHA Halystatina-2 EAGEDCDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RCD MDDYCNGISAGCPRNFHA	Halysina	EAGEECDCGSPG	NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRLIRGDMDDYCNGISAGCPRNPFHA
Mt-b EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRN RCD LDDYCNGISAGCPRNFHA Salmosina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRN RCD LDDYCNGISAGCPRNFHA Applagina EAGEECDCGSPG NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRN RCD LDDYCNGISAGCPRNFHA Mt-d EAGVECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRN RCD MDDYCNGISAGCPRNFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRN RCD MDDYCNGISAGCPRNFHA Halystatina-2 EAGEDCDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRN RCD MDDYCNGISAGCPRNFHA ***** **::* **::* **::* **::* **:*	Halystatina-1	EAGEECDCGSPG	NPCCDAATCKLRQGAQCAEGLCCDQCRFMKKGTVCRLIRGD MDDYCNGISAGCPRNPFHA
Salmosina PAGEBCDCGSPE NPCCDAATCKLRQGAQCAEGLCCDQCREMKEGTICRN RGD LDDYCNGISAGCPRNPFHA Applagina EAGEECDCGSPE NPCCDAATCKLRQGAQCAEGLCCDQCKEMKEGTICRN RGD NDDYCNGISAGCPRNPFHA Mt-d EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RGD NDDYCNGISAGCPRNPFHA Saxatilina EAGEECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RGD MDDYCNGISAGCPRNPFHA Halystatina-2 EAGEDCDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RGD MDDYCNGISAGCPRNPFHA	Mt-b	EAG <mark>EE</mark> CDCGSPG	NPCC <mark>D</mark> AATCKLRQGAQCA <mark>E</mark> GLCCDQCRFMKEGTICRR(RGE)LDDYCNGISAGCPRNPFHA
Applagina DAGENECDOGSPM NPCCDAATCKLRPGAQCANGLCCDQCKEMKEGTVCR-7 RED DVNDYCNGISAGCPRNPFH Mt-d DAGVECDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RGD DMDYCNGISAGCPRNPFHA Saxatilina DAGECCDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RGD DMDYCNGISAGCPRNPFHA Halystatina-2 DAGECCDCGAPA NPCCDAATCKLRPGAQCAEGLCCDQCREMKEGTICRM RGD DMDYCNGISAGCPRNPFHA ***** **:: **:: **:: **:: :*:: :*::	Salmosina	EAGEECDCGSPG	NPCCDAATCKLRQGAQCAEGLCCDQCRFMKEGTICRR RGD)LDDYCNGISAGCPRNPFHA
MC-G DAGVBCDUCGAPA NPCCDAATCKLRPCAQCADGCCDQCRPMKEGTICKM RED MDDYCNGISAGCPRNPFHA Saxatilina DAGECDCGAPA NPCCDAATCKLRPCAQCADGCCDQCRPMKEGTICKM RED MDDYCNGISAGCPRNPFHA Halystatina-2 DAGECDCGAPA NPCCDAATCKLRPCAQCADGCCDQCRPMKEGTICKM RED MDDYCNGISAGCPRNPFHA When the state of	Applagina		NPCCDAATCKLRPGAQCAEGLCCDQCKFMKEGTVCR-/RGDDVNDYCNGISAGCPRNPFH
Halystatina-2 AGEDCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCCCAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCDCGAPA KAGEDCCCAPA KAGECCAPA KAGECCCAPA KAGECCAPA KA	MT-a Caratilina		NPCCDAATCKLIKPGAQCAEGLCCDQCRFMKEGTICRM RGD MDDYCNGISAGCPRNPFHA
	Baratilia Halvstatina-9	FACEDCDCCAPA	NPCCDAATCKLRPGAOCAEGLCCDOCREMKECTICRM RGI MDDYCNGISAGCPRNPFHA
	marystatina z	CONFA	**** **:: **:* ** ** :: :*: :*:

C-terminal

Phylogenetic tree



Selected disintegrins of each subgroup



Disintegrins 3D alignment



Docking complexes





Docking with $\alpha_{IIb}\beta_3$

SUBGROUP 2

SUBGROUP 1

GREEN – Common to all disintegrins RED – Common only to subgroup BLLUE – Only in the specific disintegrin

SUBGROUP 3



Docking with $\alpha_v \beta_3$

SUBGROUP 2

GREEN – Common to all disintegrins RED – Common only to subgroup BLLUE – Only in the specific disintegrin

SUBGROUP 1

SUBGROUP 3







With the propose of confirming the interaction profile degree of interaction a theoretical analysis binding energy among the integrins and disintegrins was performed.

Two disintegrins studied by my group JARASTATIN (SUBGROUP2) and JARARACIN (SUBGROUP 4) for the study of molecular dynamics were selected.

- Strategies used in the analysis of MD simulations ::
 - Physic-chemical properties of the system:
 - Pressure
 - Volume
 - Density

Indicate stability the simulation system

- Energies
 - Total energy, Kinetic energy and Potential energy
 - Interaction Energy (amino acids, ligand, receptor, solvent, ions)
- RMSD > Root-mean-square deviation at all amino acids in the simulation
- RMSF → Root-mean-square fluctuation at all amino acids in the simulation
- Radius of gyration
 Refers to the distribution of the components of an object around an axis.

RMSF with disintegrins binding with $\alpha_{IIb}\beta_3$ during the 10ns.



RMSF with disintegrins binding with $\alpha_{v}\beta_{3}$ during the 10ns.



Energy Studies

	Energia total	Energia de Lennard-Jones	Energia de Coulomb	Energia de Interação
Jararacina isolada	-1,28×10 ⁵	-1,87 _x 10 ³	-1,76×10 ⁵	-
Jararacina/α _{llb} β₃	-1,6×10 ⁶	-2,04×10 ⁶	-2,23×10 ⁶	-4,27×10 ⁶
Jararacina/α _ν β₃	-1,38×10 ⁶	-1,77×10 ⁶	-1,89×10 ⁶	-3,66×10 ⁶
Jarastatina isolada	-1,27×10 ⁵	-2,04 _x 10 ³	-1,73×10 ⁵	-
Jarastatina/α _{llb} β₃	-1,39×10 ⁶	-1,96×10 ⁶	-2,11×10 ⁶	-4,07×10 ⁶
Jarastatina/α _ν β₃	-1,5×10 ⁶	-1,91×10 ⁶	-2,04×10 ⁶	-3,95×10 ⁶

Differences of interaction energy between the disintegrins

Jararacina/ $\alpha_{IIb}\beta_3$ — Jarastatina/ $\alpha_{IIb}\beta_3$ = -2,0 x 10⁵ kJ/mol

Jarastatina/ $\alpha_{\nu}\beta_{3}$ — Jararacina/ $\alpha_{\nu}\beta_{3}$ = -2,9 x 10⁵ kJ/mol

Conclusões (in silico)

Within the group of PII - medium size disintegrins, we can subdivide on some distinct subgroups. That being Subgroup 4 (jararacin and kistrin) still could be more divided.

Subgroups 1 and 3 that are in the transition of the phylogenetic tree exhibit high affinity for αIIbβ3 and αvβ3 integrins; while one subgroup shows more affinity for αVβ3 and subgroup 4 (jararacina) more affinity for αIIbβ3.

Molecular Dynamics corroborated the data showing that the rigid docking jararacin (subgroup 4) has a higher affinity for αIIbβ3, in contrast to jarastatina (subgroup 2) showed higher affinity for αvβ3.

Greetings

To my collaborators: Prof^a. Lina B. Zingali (UFRJ) e Prof^a. Helena C. Castro (UFF) **Prof. Rodolpho Albano (UERJ) Prof. Hugo Verli (UFRGS)** Dr^a. Ana Moura (Butantã Institut – SP) **Prof. Carlos R. Rodrigues (UFRJ)** To the technical support Aninha, Dione and Augusto To all of my group in UEMP lab., LabHemoVen e LaBioMol.

Financial supports:





