BIOINFORMATION

open access

Supplementary material:

Table 1: The dataset of VVSPs used in the analysis. In total 185 VVSP sequences were collected from the protein sequence databases and 11 sequences were obtained from relevant literature (indicated as 'not reported' under accession number category). The name of snake, NCBI accession number and the short reference code for each sequence is given in the table

Viper Species	Accession number	Reference code	Viper Species	Accession number	Reference code
Agkistrodon bileatus	Q9PSN3	AB-BL		ADI47557	EP-SP2
Agkistrodon contortrix contortrix	P82981	AC-CN	*Gloydius blomhoffi*	P81176	GB-HY
	P09872	AC-AN		Q9PT51	GB-BV
Agkistrodon piscivorus leucostoma	ADP88562	AP-PC	*Gloydius blomhoffi brevicaudus*	AAD01624	GBB-PA
	ADP88561	AP-PA		Q9YGJ9	GBB-H2
	ADW77220	AP-TL		P85109	GBB-KA
Bitis gabonica rhinoceros	AAR24534	BG-SP1		Q9PTL3	GBB-SL
	CBM40645	BG-RHIN2	*Gloydius halys*	Q9YGI6	GH-P2
	CBM40646	BG-RHIN3		O93421	GH-PS
	CBM40647	BG-RHIN4		Q802F0	GH-PT
	CBM40648	BG-RHIN5	*Gloydius halys*	Q9YGJ2	GH-PL
Bothrops alternatus	Q6IWF1	BAl-BT		AAC61838	GH-SL
	P0CG03	BAl-BH		P81176	GH-H
Bothrops asper	Q072L6	BAs-SPL	*Gloydius saxatilis*	Q7SZE1	GSa-DE
Bothrops atrox	P04971	BAt-BT	*Gloydius shedaoensis*	Q6T5L0	GSh-SH
	AAA48553	BAt-BAT		P0C5B4	GSh-GL
Bothrops insularis	Q8QG86	BI-SP	*Gloydius ussuriensis*	Q7SZE2	GU-BRE
Bothrops jararaca	Q5W959	BJa-HP2		Q8UUJ2	GU-TUI
	P81824	BJa-PABJ		Q91053	GU-TC
	O13069	BJa-KN		Q8UUJ1	GU-TUA
	Q9PTU8	BJa-SPA		O42207	GU-CPI
	P81661	BJa-BT		Q8UVX1	GU-TG
	Q5W960	BJa-HP1		P86171	GU-KR
	Q5W958	BJa-HP3		Not reported	GU-GS
Bothrops jararacussu	Q2PQJ3	BJu-SP1	*Lachesis muta muta*	Q27J47	LMM-PA
	Q7T229	Bju-SPH		P33589	LMM-GY
Calloselasma rhodostoma	P26324	CR-AN	*Lachesis stenophrys*	Q072L7	LS-TLE
	P47797	CR-A	*Macrovipera lebetina*	Q9PT41	ML-FVA
	CAA01526	CR-ALP4		Q9PT40	ML-P2
	CAA01525	CR-ALP1		Q8JH85	ML-AF
	CAA01524	CR-ALP2		Q8JH62	ML-BF
	CAA01523	CR-ALP3		Not reported	ML-P3
Cerastes cerastes	Q7SYF1	CC-CR		Not reported	ML-P4
Crotalus adamanteus	Q8UUK2	CAd-SP		ADN04917	ML-BFP
	Not reported	CAd-CR		ADN04916	ML-SP1
	AEJ32000	CAd-SP6		ADN04918	ML-SP3
	AEJ31999	CAd-SP5	*Protobothrops mucrosquamatus*	Q9DG84	PM-S2
	AEJ31998	CAd-SP4		Q91511	PM-M5
	AEJ31997	CAd-SP3		Q91507	PM-M1
	AEJ31996	CAd-SP2		Q91510	PM-M4
	AEJ31995	CAd-SP1		AAB01070	PM-PT
Crotalus atrox	Q8QHK2	CAt-CT2		Q9DG83	PM-SK
	Q8QHK3	CAt-CT1		Q91509	PM-M3
Crotalus durissus terrificus	Q58G94	CDT-G21		Q91508	PM-M2
	ABY65929	CDT-G13	*Sistrurus catenatus edwardsi*	ABG26969	SCE-SP3
	ABY65930	CDT-G14		ABG26970	SCE-SP4
	ABY65931	CDT-G17		ABG26974	SCE-SP8
Crotalus durissus durissus	Q2QA04	CDD-SP		ABG26975	SCE-SP9
Cryptelytrops albolabris	Not reported	CAl-AF		ABG26967	SCE-SP1
	Not reported	CAl-PA		ABG26977	SCE-SP11
	ABS12074	CAl-TL1		ABG26968	SCE-SP2
	ABS12075	CAl-TL2		ABG26972	SCE-SP6
Daboia russelli siamensis	P18965	DR-VG		ABG26976	SCE-SP10
	P18964	DR-VA		ABG26973	SCE-SP7
	ADP88560	DR-SB		ABG26971	SCE-SP5
	ADP88559	DR-SA	*Protobothrops elegans*	Not reported	PE-PI
	ADP88558	DR-VGP		P84787	PE-EL2
	3SBK_A	DR-VS		P84788	PE-EL1
Deinagkistrodon acutus	AAW56608	DA-TL1	*Trimeresurus flavoviridis*	P05620	TF-TLE
	AAW56633	DA-TL2		1405260A	TF-FL
	AAW56609	DA-TL3		O13057	TF-SP2
	ABK91854	DA-TL4		O13058	TF-SP3
	ABK91856	DA-TL5	*Trimeresurus gramineus*	O13059	TG-SP1
	ABK97625	DA-TL6		O13062	TG-SP2C
	ABK97628	DA-TL7		O13063	TG-SP3
	ABK91852	DA-TL8		O13060	TG-SP2A
	AAK52506	DA-TL10		O13061	TG-SP2B
	ABK97627	DA-TL11	*Trimeresurus jerdonii*	Q9DF66	TJ-SP3
	ABK91853	DA-TL12		Q9DF67	TJ-SP2
	ABK97626	DA-TL13		Q9DF68	TJ-SP1
	1OP2_A	DA-ASII		B0ZT25	TJ-SPH
	1OP0_A	DA-ASI	*Viridovipera stejnegeri*	Q8AY79	VS-S2
	AAD19350	DA-DF		Q71QH7	VS-PA
	Q9I8X0	DA-DK		1BQY_A	VS-VPA
	Q9I8W9	DA-DX		Q8AY82	VS-SPH1
	CAC00530	DA-AC2		Q71QJ1	VS-KN9
	CAB46431	DA-AC		Q71QI8	VS-KN10
	Q9I8X2	DA-AT		Q71QJ3	VS-KN1
	ACF17164	DA-VY		Q71QH5	VS-KN8
	Not reported	DA-P1		Q71QI5	VS-KN3
	Not reported	DA-P7		Q71QI7	VS-KN11
	Not reported	DA-P8		Q71QI4	VS-KN5
	Not reported	DA-P9		Q71QJ4	VS-KNH4
	ABV89584	DA-TL		Q71QI1	VS-KN12

Echis coloratus	ADI47576	EC-SP1		Q71QH6	VS-KN13
	ADI47574	EC-SP2		Q8AY80	VS-S1
	ADI47566	EC-SP3		Q8AY78	VS-SP5
	ADI47562	EC-SP4		Q8AY81	VS-SJ
	ADI47559	EC-SP5		AAQ02901	VS-C3
	ADI47552	EC-SP6		AAQ02898	VS-C1
	ADI47549	EC-SP7		Q71QI3	VS-C5
Echis ocellatus	ADE45141	EO-SP		AAQ02909	VS-C4
	ADC52861	EO-SP1		Q71QI2	VS-C2
	ADE45139	EO-SP2		Q71QI0	VS-KNH7
	ADE45140	EO-SP3		Q71QJ0	VS-KN2
	CAQ72889	EO-SP4		Q71QJ2	VS-KN6
	ADI47555	EO-SP5		Q71QH9	VS-KN14
Echis pyramidum leakeyi	ADI47558	EP-SP1	*Vipera nikolskii*	CBW30778	VN-NI

Table 2: VVSPs with substitutions for cysteine residues involved in the formation of disulphide linkages. The VVSPs and their substituted residue (blue) in the appropriate positions are shown in table. The positions of two corresponding cysteine residues which form disulphide linkage are placed next to each other to indicate the missing disulphide linkage due to substitution. VVSPs normally contain 6 disulphide linkages; C22-C157, C42-C58, C91-C245e, C136-C201, C168-C182 and C191-C220. X indicates the substituted residue and – indicates a deletion.

Name of VVSP	22	157	42	58	91	245e	136	201	168	182	191	220
BAI-BH	C	C	C	C	X	C	C	C	C	C	C	C
CAd-SP5	C	C	C	C	C	X	C	C	C	C	C	C
CC-CR	C	C	X	C	C	C	C	C	C	C	C	C
DA-DK	C	C	C	C	C	C	C	X	C	C	C	C
DA-TL4	C	C	C	X	C	C	C	C	C	C	C	C
DA-TL7	C	C	C	C	C	C	C	X	C	C	C	C
EO-SP2	C	C	C	C	C	X	C	C	C	C	C	C
EO-SP5	C	C	C	C	C	-	C	C	C	C	C	C
EO-SP6	C	C	C	C	C	X	C	C	C	C	C	C
GBB-SL	C	C	C	C	X	C	C	C	C	C	C	C
VS-KN5	C	C	X	C	C	C	C	C	C	C	C	C
VS-KN6	C	C	X	C	C	C	C	C	C	C	C	C
VS-KN14	C	C	X	C	C	C	C	C	C	C	C	C

Table 3: VVSPs with substituted catalytic triad residues. VVSPs with various substitutions (blue) for their catalytic triad residues are shown in table. Normally VVSPs contain H57, D102 and S195 in their catalytic triad.

Name of VVSP	57	102	195	Name of VVSP	57	102	195
BGSP1	R	D	N	ML-P2	R	D	N
BG-RHIN2	R	D	N	ML-P3	H	D	N
BG-RHIN3	R	D	N	ML-P4	R	D	S
BAI-BH	N	T	S	TF-SP2	R	D	S
Bas-SPL	N	D	S	TG-SP2A	R	D	S
BJa-HP3	Q	D	S	TJ-SP1	R	D	P
BJu-SPH	N	D	S	TJ-SPH	R	D	S
CAd-SP6	H	D	A	VS-SPH1	R	D	S
EC-SP4	R	D	T	VS-KNH4	R	D	S
EC-SP5	R	D	T	VS-KNH7	R	D	S
EO-SP	R	D	T				

Table 4: VVSPs with substituted primary specificity pocket residues. VVSPs with various substitutions (blue) for their specificity pocket residues are shown in table. Normally VVSPs contain D189, G216 and G/A226 in their specificity pocket.

Name of VVSP	189	216	226	Name of VVSP	189	216	226
AP-PA	D	R	G	DA-TL12	G	G	G
BG-SP1	D	E	A	DR-SA	G	G	S
BG-RHIN2	D	E	A	DR-SB	G	G	V
BG-RHIN3	D	E	A	EC-SP6	G	G	G
BG-RHIN4	G	A	G	EC-SP7	G	V	G
BG-RHIN5	G	A	G	EP-SP1	G	G	V
BJa-HP3	D	R	G	EP-SP2	G	G	V
CAd-SP3	G	G	G	EO-SP1	G	V	G
CR-ALP2	S	G	A	EO-SP2	G	S	G
CDD-SP	G	G	E	ML-AF	G	G	G
DA-AC	G	G	G	ML-BF	G	G	V
DA-AC2	G	G	G	SCE-SP9	S	G	S
DA-TL5	G	G	G	SCE-SP5	S	G	G
DA-TL6	G	G	G	TF-SP3	G	G	G
DA-TL7	G	G	G	TG-SP3	D	G	N
DA-TL8	G	G	G	VS-C2	G	T	A
DA-TL10	G	G	G	VS-KN8	D	G	V
DA-TL11	G	G	G				