

# Supplementary\_7:Venom variation and evolution in populations of montane pitvipers (*Viperidae* :*Cerrophidion*).

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2022 May 23

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## Query "4733" for ramsesr@g.clemson.edu submitted to webserver.
##
##   Probe radius   :   1.400
##   Residue       Total   Apolar   Backbone Sidechain Ratio(%) In/Out
## MET           1    234.49   189.17    69.60    164.89    100.0    o
## ARG           2    208.61    96.44    21.88    186.73     95.5    o
## THR           3    101.30    77.08    13.23    88.07     82.9    o
## LEU           4    102.15    82.13    20.02    82.13     56.2    o
## TRP           5    132.23   108.43     7.00   125.22     55.8    o
## ILE           6     11.00    11.00     0.00    11.00      7.5    i
## VAL           7      0.00     0.00     0.00     0.00      0.0    i
## ALA           8      0.00     0.00     0.00     0.00      0.0    i
## VAL           9    10.23    10.23     0.00    10.23      8.4    i
## LEU          10    45.41    45.41     0.00    45.41     31.1
## LEU          11   120.18   118.66     1.98   118.20     80.8    o
## VAL          12    29.62    29.62     0.85    28.76     23.5
## VAL          13     3.63     3.63     0.00     3.63      3.0    i
## VAL          14    60.00    56.49     7.60    52.40     42.8
## GLU          15   101.41    33.86     5.38    96.02     68.0    o
## GLY          16      0.00     0.00     0.00     0.00      0.0    i
## SER          17    36.49    23.17     3.59    32.90     42.5
## PRO          18     1.00     1.00     0.00     1.00      1.0    i
## VAL          19     5.27     5.27     0.00     5.27      4.3    i
## GLU          20    51.10     6.87     0.00    51.10     36.2
## PHE          21    53.35    50.40     5.35    47.99     26.6
## GLU          22     4.35     2.79     3.24     1.11      0.8    i
## THR          23      0.00     0.00     0.00     0.00      0.0    i
## LEU          24    75.35    73.12     2.23    73.12     50.0    o
## ILE          25   132.69   130.85     5.65   127.03     86.2    o
## MET          26    41.60    29.67    19.03    22.57     14.3    i
```

##	LYS	27	188.42	149.28	31.28	157.13	95.5	o
##	ILE	28	114.22	95.26	21.93	92.28	62.7	o
##	ALA	29	44.51	44.51	15.17	29.34	45.2	
##	GLY	30	29.66	19.30	29.66	0.00	34.0	
##	ARG	31	6.51	1.21	0.07	6.45	3.3	i
##	SER	32	44.10	18.90	0.29	43.81	56.6	o
##	GLY	33	5.98	5.57	5.98	0.00	6.9	i
##	VAL	34	116.61	105.49	11.12	105.49	86.3	o
##	TRP	35	133.94	125.97	4.11	129.83	57.8	o
##	TYR	36	38.58	18.64	0.00	38.58	20.0	i
##	TYR	37	10.76	9.82	0.00	10.76	5.6	i
##	GLY	38	22.18	17.78	22.18	0.00	25.4	
##	SER	39	47.92	21.41	5.25	42.67	55.1	o
##	TYR	40	0.00	0.00	0.00	0.00	0.0	i
##	GLY	41	4.43	0.00	4.43	0.00	5.1	i
##	CYS	42	4.99	0.54	4.71	0.28	0.3	i
##	TYR	43	12.91	10.79	0.73	12.18	6.3	i
##	CYS	44	3.33	0.36	3.06	0.27	0.3	i
##	GLY	45	27.83	11.56	27.83	0.00	31.9	
##	ALA	46	106.38	88.29	31.69	74.69	100.0	o
##	GLY	47	62.51	53.74	62.51	0.00	71.7	o
##	GLY	48	33.90	4.88	33.90	0.00	38.9	
##	GLN	49	82.32	16.39	1.46	80.85	56.3	o
##	GLY	50	1.53	1.51	1.53	0.00	1.8	i
##	TRP	51	137.31	119.06	2.40	134.91	60.1	o
##	PRO	52	5.11	1.45	3.66	1.45	1.4	i
##	GLN	53	76.85	8.40	27.47	49.38	34.4	
##	ASP	54	33.99	32.15	15.69	18.30	16.2	i
##	ALA	55	38.57	36.86	11.00	27.57	42.5	
##	SER	56	1.42	0.54	0.00	1.42	1.8	i
##	ASP	57	0.00	0.00	0.00	0.00	0.0	i
##	ARG	58	71.74	29.94	0.00	71.74	36.7	
##	CYS	59	0.59	0.36	0.58	0.01	0.0	i
##	CYS	60	7.48	4.73	2.14	5.35	5.2	i
##	PHE	61	8.74	8.74	0.00	8.74	4.9	i
##	GLU	62	89.47	32.74	1.13	88.34	62.6	o
##	HIS	63	18.49	11.65	2.49	16.01	10.4	i
##	ASP	64	54.99	23.10	3.30	51.69	45.7	
##	CYS	65	8.04	7.22	0.28	7.76	7.6	i
##	CYS	66	33.76	29.38	1.56	32.20	31.5	
##	TYR	67	20.90	18.75	2.15	18.75	9.7	i
##	ARG	68	133.96	67.21	11.66	122.31	62.6	o
##	LYS	69	156.36	103.96	33.76	122.60	74.5	o
##	VAL	70	21.49	21.49	5.29	16.20	13.2	i
##	THR	71	113.83	69.40	25.05	88.78	83.6	o
##	GLY	72	85.10	52.01	85.10	0.00	97.6	o
##	CYS	73	20.43	3.55	6.64	13.79	13.5	i

##	ASP	74	67.99	37.11	6.19	61.80	54.7	o
##	PRO	75	31.31	31.31	0.00	31.31	29.8	
##	LYS	76	113.12	69.02	0.48	112.64	68.5	o
##	LEU	77	126.42	122.64	7.38	119.04	81.4	o
##	ASP	78	31.30	12.01	8.18	23.11	20.5	
##	VAL	79	114.65	106.65	8.00	106.65	87.2	o
##	TYR	80	11.80	1.86	11.80	0.00	0.0	i
##	THR	81	58.04	32.38	6.40	51.65	48.6	
##	TYR	82	59.13	24.71	13.61	45.52	23.6	
##	ARG	83	133.16	45.63	6.57	126.59	64.8	o
##	GLU	84	74.67	18.67	24.90	49.77	35.2	
##	GLU	85	80.26	10.16	10.57	69.69	49.4	
##	ASN	86	145.85	51.38	24.79	121.06	100.0	o
##	GLY	87	42.56	30.54	42.56	0.00	48.8	
##	ASP	88	55.23	35.51	0.17	55.06	48.7	
##	MET	89	3.15	0.63	2.52	0.63	0.4	i
##	ILE	90	64.23	64.23	0.11	64.12	43.5	
##	CYS	91	1.45	0.00	1.45	0.00	0.0	i
##	GLY	92	3.90	3.90	3.90	0.00	4.5	i
##	GLY	93	23.03	14.09	23.03	0.00	26.4	
##	ASP	94	68.73	14.15	28.88	39.84	35.3	
##	ASP	95	81.74	16.67	2.33	79.42	70.3	o
##	PRO	96	88.21	88.21	0.00	88.21	83.9	o
##	CYS	97	42.91	10.04	0.86	42.05	41.1	
##	GLU	98	17.60	1.18	0.00	17.60	12.5	i
##	LYS	99	14.68	1.86	0.00	14.68	8.9	i
##	GLN	100	62.98	23.63	0.70	62.27	43.3	
##	ILE	101	0.00	0.00	0.00	0.00	0.0	i
##	CYS	102	1.12	0.00	0.00	1.12	1.1	i
##	GLU	103	72.55	21.44	0.00	72.55	51.4	o
##	CYS	104	8.29	3.29	3.84	4.45	4.4	i
##	ASP	105	0.08	0.08	0.00	0.08	0.1	i
##	LYS	106	51.52	44.88	0.40	51.12	31.1	
##	ALA	107	60.77	58.59	9.18	51.59	79.5	o
##	ALA	108	5.78	5.78	4.08	1.70	2.6	i
##	ALA	109	0.00	0.00	0.00	0.00	0.0	i
##	ILE	110	57.68	57.68	0.00	57.68	39.2	
##	CYS	111	33.05	15.60	4.69	28.36	27.7	
##	PHE	112	11.67	10.75	1.04	10.63	5.9	i
##	ARG	113	103.32	31.44	3.27	100.05	51.2	o
##	ASP	114	104.70	19.96	15.87	88.83	78.6	o
##	ASN	115	23.99	0.00	0.00	23.99	21.0	
##	LYS	116	35.05	22.32	4.48	30.57	18.6	i
##	ASP	117	129.13	61.33	42.36	86.77	76.8	o
##	THR	118	48.87	25.41	20.15	28.72	27.0	
##	TYR	119	26.27	7.62	18.64	7.62	3.9	i
##	ASP	120	34.53	13.39	1.59	32.94	29.1	

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## ILE      121      116.03      116.03      0.00      116.03      78.8      o
## LYS      122      166.83      110.64      19.29      147.54      89.7      o
## TYR      123       44.37       20.36       0.00       44.37      23.0
## TRP      124       69.11       66.12       0.00       69.11      30.8
## PHE      125      104.31       92.22      12.51       91.80      51.0      o
## PHE      126       38.39       32.89       6.04       32.35      18.0      i
## PRO      127       88.87       88.87      11.44       77.43      73.6      o
## ALA      128       44.65       41.74       3.03       41.62      64.1      o
## LYS      129      182.99      132.63      20.01      162.99      99.1      o
## GLU      130       98.06       23.76      10.74       87.31      61.8      o
## CYS      131       13.83        3.86      10.28        3.56       3.5      i
## GLN      132      135.99       40.09      13.29      122.70      85.4      o
## GLU      133      143.10       56.79      34.33      108.77      77.0      o
## GLU      134      136.49       65.15      16.17      120.32      85.2      o
## SER      135       58.82       33.81       9.75       49.07      63.4      o
## GLU      136       28.86        7.01       7.77       21.09      14.9      i
## PRO      137      107.63      101.94      13.90       93.73      89.1      o
## CYS      138       81.09        1.58      41.33       39.76      38.9
## -----
## POLAR   area/energy      =      2937.05
## APOLAR  area/energy      =      4992.47
## UNKNOW  area/energy      =         0.00
## -----
## Total   area/energy      =      7929.53
## -----
## Number of surface atoms  =         642
## Number of buried atoms   =         448
## Number of atoms with ASP=0 =          0
## *** Thanks for using Getarea. Please visit us again. http://curie.utmb.edu/***

```

PeptideCutter

PeptideCutter

The sequence to investigate:

10 20 30 40 50 60  
MRTLWIVAVL LVVVEGSPVE FETLIMKIAG RSGVWYYGSY GCYCGAGGQG WPQDASDRCC  
70 80 90 100 110 120  
FEHDCCYRKV TGCDPKLDVY TYREENGDMI CGGDDPCEKQ ICECDKAAAI CFRDNKDTYD  
130  
IKYWFFPAKE CQEESEPC

The sequence is 138 amino acids long.

Available enzymes

The enzyme(s) that you have chosen:

- Chymotrypsin

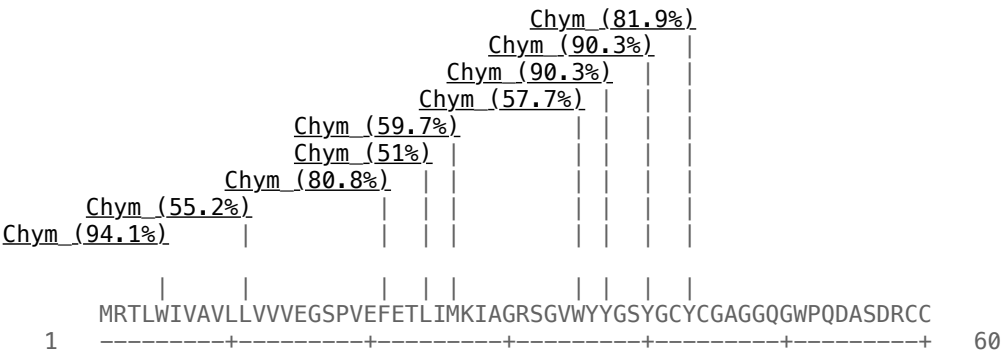
You have chosen to display all possible cleaving enzymes.

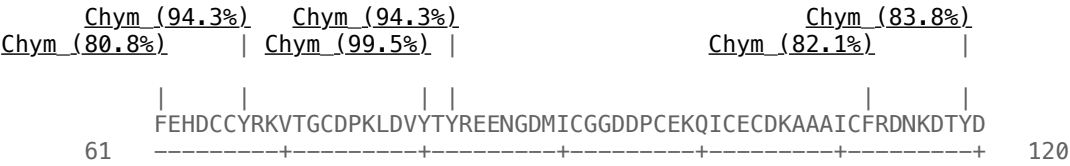
These enzymes cleave the sequence:

Name of enzyme	No. of cleavages	Positions of cleavage sites
Chymotrypsin	17	5 (94.1%) 11 (55.2%) 21 (80.8%) 24 (51%) 26 (59.7%) 35 (57.7%) 37 (90.3%) 40 (90.3%) 43 (81.9%) 61 (80.8%) 67 (94.3%) 80 (99.5%) 82 (94.3%) 112 (82.1%) 119 (83.8%) 124 (70.4%) 125 (59.4%)

These are the cleavage sites of the chosen enzymes and chemicals mapped onto the entered protein sequence:

- You have chosen a block size of 60 for the map.
- Please note that the cleavage occurs at the **right side** (C-terminal direction) of the marked amino acid.
- You have the possibility to display the results of a single enzyme by **mouseclicking** on the respective enzyme name in the map.





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