关于虎纹阵痛肽-I的讨论

车南颖(10311029)
第一组:abc04a05

一.对蜘蛛毒素及其中一种毒素(虎纹阵痛肽)的简介

蜘蛛是古老的动物,最早的化石记录显示在3亿年前的石炭纪蜘蛛就已经存在于地球了.相对于蜘蛛的漫长的进化时间而言,蜘蛛形态上的分化不是非常显著.这可能与它们很早就有毒液有关.毒液的主要作用是麻痹和杀死猎物,遇到其他肉食性动物时的防御作用,以及可能的预消化作用.蜘蛛毒素成分复杂,组成上来看,粗毒主要成分是蛋白质和多肽类神经毒素,还含有多胺类神经毒素、多种酶类、激肽类似物、溶血物质、凝聚素、抗菌肽、氨基酸、ATP、核苷酸、单胺类等活性物质.

虎纹阵痛肽-I(HWTX-I)是从中国稀有的蜘蛛物种虎纹捕鸟蛛(Selenocosmia huwena Wang)中分离纯化出来的神经毒素,是突触前膜N型钙离子通道的阻断剂.

HWTX-I 由33个氨基酸组成,含有三对二硫键,现已确定是以I-IV,II-V,III-VI的方式配对,三对二硫键配合三股反平行的β折叠形成一个非常致密稳定的结构.采用核磁共振二维氢谱的方法解析出来的HWTX-1的空间结构是典型的抑制剂胱氨酸结结构模体(Inhibitor Cystine Knot motif, ICK模体).

蜘蛛毒素cDNA结构:5′非翻译区域 + 富含疏水性氨基酸的信号肽区域(pre区)(与蜘蛛毒素分泌特性有关) + 富含Glu等酸性氨基酸的信号肽与成熟蛋白之间的间隔区域(pro区) + 成熟蛋白区域 + 间隔区(pro区) + 3′非翻译区域.

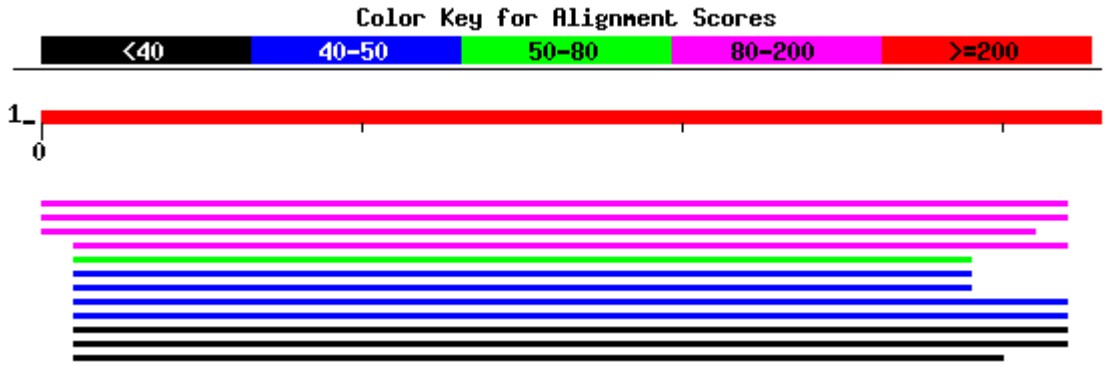
HWTX-I 前体蛋白由81个氨基酸组成,而经过剪切后的成熟蛋白只有33个氨基酸组成.

二.HWTX-I的PROTEIN-PROTEIN BLAST结果

一.用 HWTX-I 的 mature chain 做 protein-protein Blast 结果(CBI TOOL):

Query= hwtx-1
(33 letters)

Distribution of 12 Blast Hits on the Query Sequence



Scor
e E
Sequences producing significant alignments:
(bits) Value

pir||A37479 huwentoxin-I - Chinese bird spider >gi|451267|g... 85
3e-16
sp|P56676|TXH1_SELHU Huwentoxin-I precursor (HwTx-I) >gi|30... 85
3e-16
pdb|1QK6|A Chain A, Solution Structure Of Huwentoxin-I By Nmr 84
8e-16
gb|AAF25774.1|AF157504_1 huwentoxin-I [Selenocosmia huwena] 84
8e-16
sp|P83464|TXN3_SELHA Hainantoxin-III (HnTx-III) 63
1e-09
sp|P83591|TXN1_SELHA Hainantoxin-I (HnTx-I) 47
8e-05
pdb|1NIX|A Chain A, Three Dimensional Solution Structure Of... 47
8e-05
sp|P83471|TXN4_SELHA Hainantoxin-IV (HnTx-IV) 41
0.004
pdb|1NIY|A Chain A, Three Dimensional Solution Structure Of... 41
0.004
sp|P83303|TXH4_SELHU Huwentoxin-IV (HwTx-IV) >gi|23200501|p... 39
0.017
gb|AAP33074.1| huwentoxin-IV precursor [Ornithoctonus huwena] 39
0.017

sp|P83480|TX1_THRPR Toxin ProTx-I 34
0.72

>pir||A37479 huwentoxin-I - Chinese bird spider
 gb|AAB28456.1| huwentoxin-I=neurotoxin [Selenocosmia huwena=Chinese bird
spiders, venom, Peptide, 33 aa]
Length = 33

 Score = 85.1 bits (209), Expect = 3e-16
 Identities = 33/33 (100%), Positives = 33/33 (100%)

Query: 1 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL
Sbjct: 1 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33

>sp|P56676|TXH1_SELHU Huwentoxin-I precursor (HwTx-I)
 gb|AAP33078.1| huwentoxin-I precursor [Ornithoctonus huwena]
Length = 81

 Score = 85.1 bits (209), Expect = 3e-16
 Identities = 33/33 (100%), Positives = 33/33 (100%)

Query: 1 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL
Sbjct: 49 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 81

>pdb|1QK6|A Chain A, Solution Structure Of Huwentoxin-I By Nmr
Length = 33

 Score = 83.6 bits (205), Expect = 8e-16
 Identities = 32/32 (100%), Positives = 32/32 (100%)

Query: 2 CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL
Sbjct: 2 CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33

>gb|AAF25774.1|AF157504_1 huwentoxin-I [Selenocosmia huwena]
Length = 32

 Score = 83.6 bits (205), Expect = 8e-16
 Identities = 32/32 (100%), Positives = 32/32 (100%)

Query: 1 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWK 32

```
            ACKGVFDACTPGKNECCPNRVCSDKHKWCKWK
Sbjct: 1    ACKGVFDACTPGKNECCPNRVCSDKHKWCKWK 32
```

>sp|P83464|TXN3_SELHA Hainantoxin-III (HnTx-III)

```
            Length = 33

 Score = 62.8 bits (151), Expect = 1e-09
 Identities = 23/29 (79%), Positives = 24/29 (82%)

Query: 2    CKGVFDACTPGKNECCPNRVCSDKHKWCK 30
            CKG  D+CTPGKNECCPN  CS KHKWCK
Sbjct: 2    CKGFGDSCTPGKNECCPNYACSSKHKWCK 30
```

>sp|P83591|TXN1_SELHA Hainantoxin-I (HnTx-I)

```
            Length = 33

 Score = 47.0 bits (110), Expect = 8e-05
 Identities = 16/29 (55%), Positives = 19/29 (65%)

Query: 2    CKGVFDACTPGKNECCPNRVCSDKHKWCK 30
            CKG   +C PGKNECC    C+ + KWCK
Sbjct: 2    CKGFGKSCVPGKNECCSGYACNSRDKWCK 30
```

>pdb|1NIX|A Chain A, Three Dimensional Solution Structure Of Hainantoxin-I By

```
            2d 1h-Nmr
            Length = 34

 Score = 47.0 bits (110), Expect = 8e-05
 Identities = 16/29 (55%), Positives = 19/29 (65%)

Query: 2    CKGVFDACTPGKNECCPNRVCSDKHKWCK 30
            CKG   +C PGKNECC    C+ + KWCK
Sbjct: 2    CKGFGKSCVPGKNECCSGYACNSRDKWCK 30
```

>sp|P83471|TXN4_SELHA Hainantoxin-IV (HnTx-IV)

```
            Length = 35

 Score = 41.2 bits (95), Expect = 0.004
 Identities = 15/34 (44%), Positives = 21/34 (61%), Gaps = 2/34 (5%)

Query: 2    CKGVFDACTPGKNECCP--NRVCSDKHKWCKWKL 33
            C G    C P  ++CC   N VCS KH+WCK+++
Sbjct: 2    CLGFGKGCNPSNDQCCKSSNLVCSRKHRWCKYEI 35
```

>pdb|1NIY|A Chain A, Three Dimensional Solution Structure Of Hainantoxin-Iv
By 2d 1h-Nmr
Length = 36

Score = 41.2 bits (95), Expect = 0.004
Identities = 15/34 (44%), Positives = 21/34 (61%), Gaps = 2/34 (5%)

```
Query: 2  CKGVFDACTPGKNECCP--NRVCSDKHKWCKWKL 33
          C G    C P  ++CC   N VCS KH+WCK+++
Sbjct: 2  CLGFGKGCNPSNDQCCKSSNLVCSRKHRWCKYEI 35
```

>sp|P83303|TXH4_SELHU Huwentoxin-IV (HwTx-IV)
pdb|1MB6|A Chain A, Three Dimensional Solution Structure Of Huwentoxin-Iv By
2d 1h-Nmr
Length = 35

Score = 39.3 bits (90), Expect = 0.017
Identities = 14/34 (41%), Positives = 22/34 (64%), Gaps = 2/34 (5%)

```
Query: 2  CKGVFDACTPGKNECCPNR--VCSDKHKWCKWKL 33
          C  +F AC P  ++CC +   VCS K +WCK+++
Sbjct: 2  CLEIFKACNPSNDQCCKSSKLVCSRKTRWCKYQI 35
```

>gb|AAP33074.1| huwentoxin-IV precursor [Ornithoctonus huwena]
Length = 89

Score = 39.3 bits (90), Expect = 0.017
Identities = 14/34 (41%), Positives = 22/34 (64%), Gaps = 2/34 (5%)

```
Query: 2  CKGVFDACTPGKNECCPNR--VCSDKHKWCKWKL 33
          C  +F AC P  ++CC +   VCS K +WCK+++
Sbjct: 54 CLEIFKACNPSNDQCCKSSKLVCSRKTRWCKYQI 87
```

>sp|P83480|TX1_THRPR Toxin ProTx-I
Length = 35

Score = 33.9 bits (76), Expect = 0.72
Identities = 12/30 (40%), Positives = 17/30 (56%), Gaps = 1/30 (3%)

```
Query: 2  CKGVFDACTPGKNECCPNRVCSDKHKWCKW 31
          C+     C+ G+  CC + VCS +H WC W
```

Sbjct: 2 CRYWLGGCSAGQT-CCKHLVCSRRHGWCVW 30

Database: All non-redundant GenBank CDS translations+PDB+SwissProt+PIR+PRF
Posted date: Aug 28, 2003 12:45 AM
Number of letters in database: 486,132,453
Number of sequences in database: 1,509,571

Lambda	K	H
0.325	0.140	0.576

Gapped

Lambda	K	H
0.267	0.0410	0.140

Matrix: BLOSUM62
Gap Penalties: Existence: 11, Extension: 1
Number of Hits to DB: 39,692,228
Number of Sequences: 1509571
Number of extensions: 762311
Number of successful extensions: 2280
Number of sequences better than 10.0: 12
Number of HSP's better than 10.0 without gapping: 8
Number of HSP's successfully gapped in prelim test: 4
Number of HSP's that attempted gapping in prelim test: 2268
Number of HSP's gapped (non-prelim): 12
length of query: 33
length of database: 486,132,453
effective HSP length: 9
effective length of query: 24
effective length of database: 472,546,314
effective search space: 11341111536
effective search space used: 11341111536
T: 11
A: 40
X1: 15 (7.0 bits)
X2: 38 (14.6 bits)
X3: 64 (24.7 bits)
S1: 40 (21.6 bits)
S2: 67 (30.4 bits)

二.用 HWTX-I 的 mature chain 做的 protein-protein blast 结果(NCBI TOOL):

50	Pairwise	Semiauto	web	yes
100	10	None	All organisms	Alignment
Format_page_11	HTML	on	100	0.005
TwoWindows	0	0	on	Proteins
1766	Blast_Results_	1093657223-176	18	on
on	1	2	2	Get
50	Pairwise	Semiauto	web	yes
100	10	None	All organisms	Alignment
Format_page_11	HTML	on	100	0.005
TwoWindows	0	0	on	Proteins
1766	Blast_Results_	1093657223-176	18	on
on	1	2	Get	

BLASTP 2.2.9 [May-01-2004]

Reference:
Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schäffer, Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997), “Gapped BLAST and PSI-BLAST: a new generation of protein database search
programs”, Nucleic Acids Res. 25:3389-3402.

RID: 1093657223-1766-18917342593.BLASTQ4

Query= hwtx-I

(33 letters)

Database: All non-redundant GenBank CDS

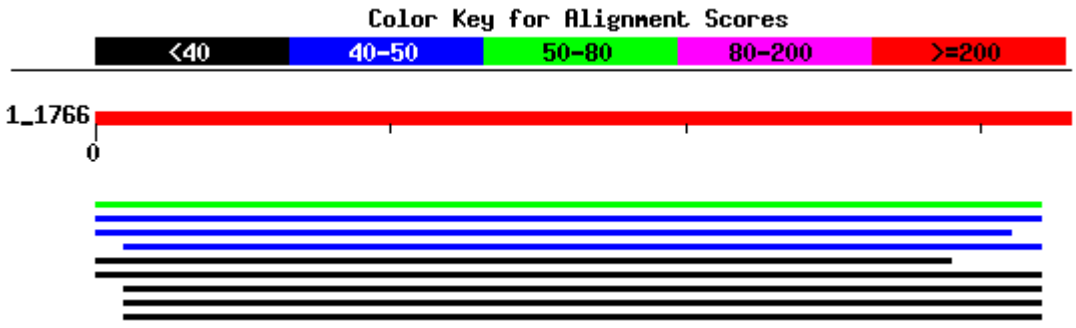
translations+PDB+SwissProt+PIR+PRF excluding environmental samples

1,995,204 sequences; 669,608,501 total letters

If you have any problems or questions with the results of this search please refer to the BLAST FAQs

Taxonomy reports

Distribution of 9 Blast Hits on the Query Sequence



Related Structures

Score E

Sequences producing significant alignments:
(bits) Value

gi|32363504|sp|P56676|TXH1_ORNHU Huwentoxin-I precursor (Hw... 67
9e-11
gi|476777|pir||A37479 huwentoxin-I — Chinese bird spider >g...
47 1e-04
gi|6708032|gb|AAF25774.1| huwentoxin-I [Selenocosmia huwena] 46
3e-04
gi|5822307|pdb|1QK6|A Chain A, Solution Structure Of Huwent... 46
3e-04
gi|24638300|sp|P83464|TXN3_SELHA Hainantoxin-III (HnTx-III) 37
0.15
gi|42559580|sp|P83745|TX1_THEBL Theraphotoxin 1 (T1Tx1) 34
0.74
gi|42559582|sp|P83747|TX3_THEBL Theraphotoxin 3 (T1Tx3) 32
3.4
gi|30575584|gb|AAP33074.1| huwentoxin-IV precursor [Ornitho... 32
3.7
gi|42559581|sp|P83746|TX2_THEBL Theraphotoxin 2 (T1Tx2) 32
4.2

Alignments

>gi|32363504|sp|P56676|TXH1_ORNHU Huwentoxin-I precursor (HwTx-I)
gi|30575612|gb|AAP33078.1| huwentoxin-I precursor [Ornithoctonus huwena]
Length = 81

Score = 67.4 bits (163), Expect = 9e-11
Identities = 33/33 (100%), Positives = 33/33 (100%)

Query: 1 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL
Sbjct: 49 ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 81

>gi|476777|pir||A37479 huwentoxin-I — Chinese bird spider
gi|451267|gb|AAB28456.1| huwentoxin-I=neurotoxin [Selenocosmia huwena=Chinese bird
spiders, venom, Peptide, 33 aa]
Length = 33

Score = 47.0 bits (110), Expect = 1e-04

Identities = 33/33 (100%), Positives = 33/33 (100%)

```
Query: 1  ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
          ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL
Sbjct: 1  ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
```

>gi|6708032|gb|AAF25774.1| huwentoxin-I [Selenocosmia huwena]

Length = 32

Score = 45.8 bits (107), Expect = 3e-04
Identities = 32/32 (100%), Positives = 32/32 (100%)

```
Query: 1  ACKGVFDACTPGKNECCPNRVCSDKHKWCKWK 32
          ACKGVFDACTPGKNECCPNRVCSDKHKWCKWK
Sbjct: 1  ACKGVFDACTPGKNECCPNRVCSDKHKWCKWK 32
```

>gi|5822307|pdb|1QK6|A Chain A, Solution Structure Of Huwentoxin-I By Nmr

Length = 33

Score = 45.8 bits (107), Expect = 3e-04
Identities = 32/32 (100%), Positives = 32/32 (100%)

```
Query: 2  CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
          CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL
Sbjct: 2  CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
```

>gi|24638300|sp|P83464|TXN3_SELHA Hainantoxin-III (HnTx-III)

Length = 33

Score = 36.6 bits (83), Expect = 0.15
Identities = 23/30 (76%), Positives = 24/30 (80%)

```
Query: 1  ACKGVFDACTPGKNECCPNRVCSDKHKWCK 30
           CKG  D+CTPGKNECCPN  CS KHKWCK
Sbjct: 1  GCKGFGDSCTPGKNECCPNYACSSKHKWCK 30
```

>gi|42559580|sp|P83745|TX1_THEBL Theraphotoxin 1 (TlTx1)

Length = 35

```
 Score = 34.3 bits (77), Expect = 0.74
 Identities = 20/33 (60%), Positives = 27/33 (81%)

Query: 1  ACKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
          AC G+F++C P  ++CCPNR C+ KHKWCK+KL
Sbjct: 2  ACLGMFESCDPNNDKCCPNRECNRKHKWCKYKL 34
```

>gi|42559582|sp|P83747|TX3_THEBL Theraphotoxin 3 (T1Tx3)

```
          Length = 35

 Score = 32.3 bits (72), Expect = 3.4
 Identities = 17/32 (53%), Positives = 24/32 (75%)

Query: 2  CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
          C G+F +C P  ++CCPNRVC  + +WCK+KL
Sbjct: 3  CLGMFSSCDPNNDKCCPNRVCRVRDQWCKYKL 34
```

>gi|30575584|gb|AAP33074.1| huwentoxin-IV precursor

```
[Ornithoctonus huwena]
          Length = 89

 Score = 32.0 bits (71), Expect = 3.7
 Identities = 14/34 (41%), Positives = 22/34 (64%), Gaps = 2/34 (5%)

Query: 2  CKGVFDACTPGKNECCPNR--VCSDKHKWCKWKL 33
          C  +F AC P  ++CC +   VCS K +WCK++
Sbjct: 54 CLEIFKACNPSNDQCCKSSKLVCSRKTRWCKYQI 87
```

>gi|42559581|sp|P83746|TX2_THEBL Theraphotoxin 2 (T1Tx2)

```
          Length = 35

 Score = 32.0 bits (71), Expect = 4.2
 Identities = 17/32 (53%), Positives = 24/32 (75%)

Query: 2  CKGVFDACTPGKNECCPNRVCSDKHKWCKWKL 33
          C G+F +C P  ++CCPNRVC  + +WCK+KL
Sbjct: 3  CLGMFSSCDPKNDKCCPNRVCRSRDQWCKYKL 34
```

窗体底端

窗体顶端

Database: All non-redundant GenBank CDS translations+PDB+SwissProt+PIR+PRF excluding environmental samples
Posted date: Aug 25, 2004 2:14 AM
Number of letters in database: 669,608,501
Number of sequences in database: 1,995,204

Lambda	K	H
0.325	0.139	0.576

Gapped

Lambda	K	H
0.267	0.0410	0.140

Matrix: BLOSUM62
Gap Penalties: Existence: 11, Extension: 1
Number of Hits to DB: 14,665,808
Number of Sequences: 1995204
Number of extensions: 297778
Number of successful extensions: 1053
Number of sequences better than 10.0: 18
Number of HSP's better than 10.0 without gapping: 11
Number of HSP's successfully gapped in prelim test: 7
Number of HSP's that attempted gapping in prelim test: 1035
Number of HSP's gapped (non-prelim): 18
length of query: 33
length of database: 669,608,501
effective HSP length: 8
effective length of query: 25
effective length of database: 653,646,869
effective search space: 16341171725
effective search space used: 16341171725
T: 11
A: 40
X1: 15 (7.0 bits)
X2: 38 (14.6 bits)
X3: 64 (24.7 bits)
S1: 40 (21.6 bits)
S2: 68 (30.8 bits)

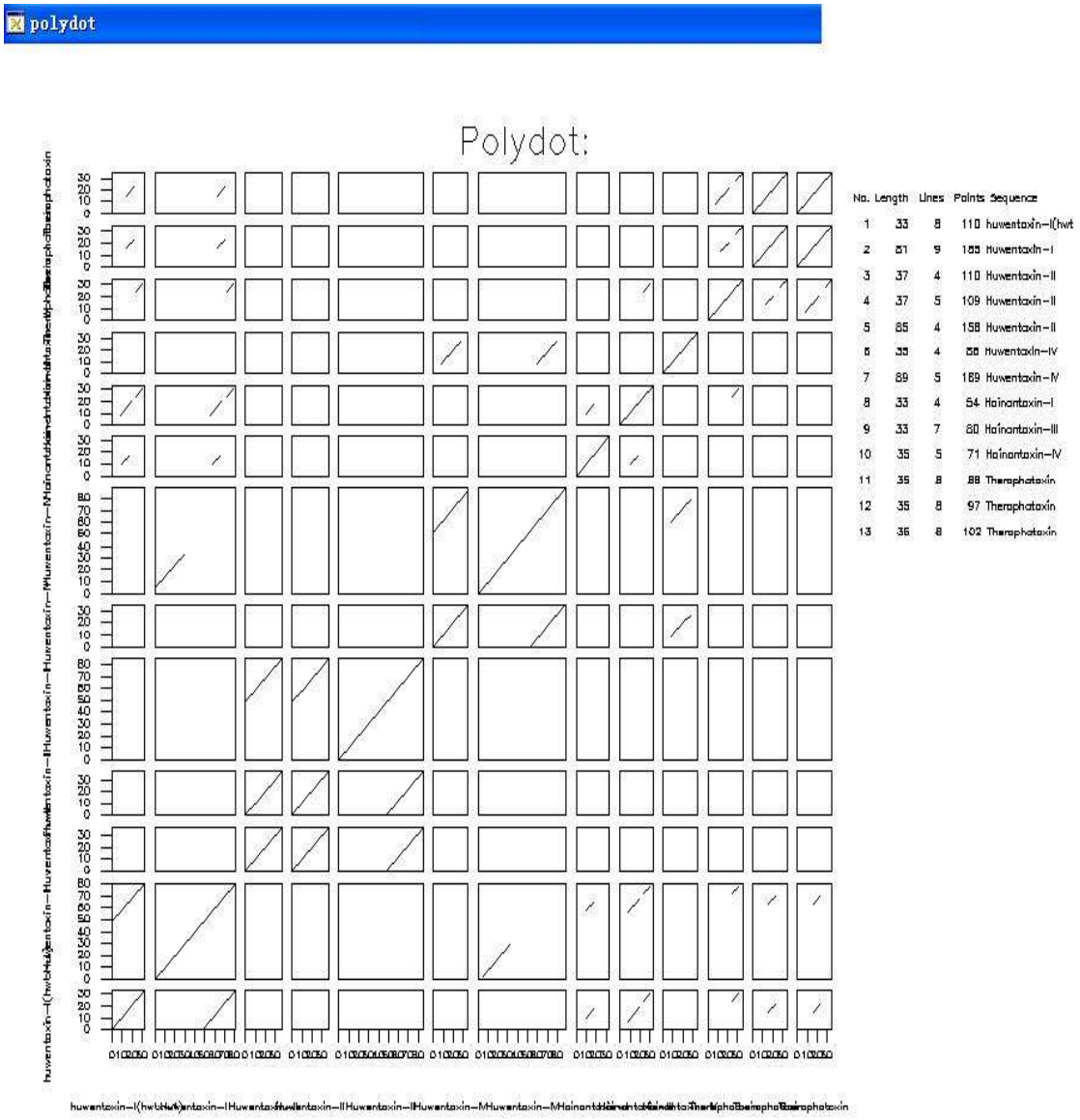
三.与 HWTX-I 有较大相似度的蛋白的序列比较

1.有来自三种不同种类的蜘蛛的蜘蛛毒素蛋白序列(from NCBI):
第一种:Ornithoctonus huwena:
1.huwentoxin-I(hwtx-1): (33 AA)
ackgvfdact pgkneccpnr vcsdkhkwck wkl
2.Huwentoxin-I precursor: (81 AA)
mrasmflala glvllfvvcy aseseekefp rellfkffav ddfkgeerac kgvfdactpg kneccpnrvc sdkhkwckwk l
3. Huwentoxin-II isoform 1 (HwTx-II): (37 AA)
lfecsfscei ekegdkpckk kkckggwkck fnmcvkv
4. Huwentoxin-II isoform 2 (HwTx-II): (37 AA)
lfecsfsceq ekegdkpckk kkckggwkck fnmcvkv
5.Huwentoxin-II precursor: (85 AA)
mkvtliailt caavlvlhtt aaeeleaesq lmevgmpdte laavdeerlf ecsfsceiek egdkpckkkk ckggwkckfn mcvkv
6.Huwentoxin-IV (HwTx-IV): (35 AA)
ecleifkacn psndqcckss klvcsrktrw ckyqi
7. Huwentoxin-IV precursor: (89 AA)
mvnmkasmfl alaglvllfv vcyaseseek efsnellssv lavddnskge erecleifka cnpsndqcck ssklvcsrkt rwckyqigk

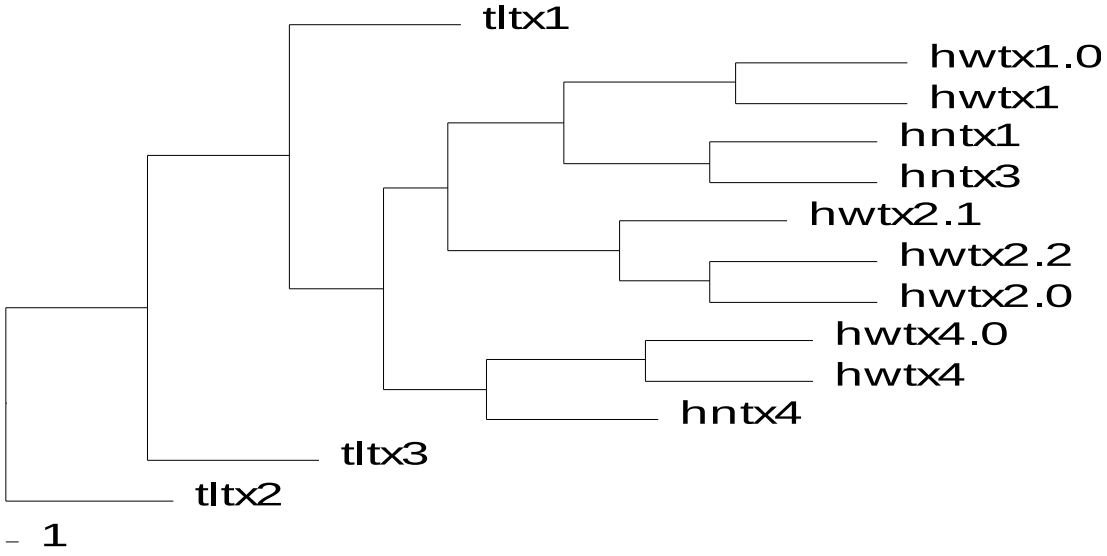
第二种:Ornithoctonus hainana:
1.Hainantoxin-I (HnTx-I): (33 AA)
eckgfgkscv pgkneccsgy acnsrdkwck vll
2.Hainantoxin-III (HnTx-III): (33 AA)
gckgfgdsct pgkneccpny acsskhkwck vyl
3.Hainantoxin-IV (HnTx-IV): (35 AA)
eclgfgkgcn psndqcckss nlvcsrkhrw ckyei

第三种:Theraphosa blondi:
1.Theraphotoxin 1 (TlTx1): (35 AA)
aaclgmfesc dpnndkccpn recnrkhkwc kyklw
2.Theraphotoxin 2 (TlTx2): (35 AA)
ddclgmfssc dpkndkccpn rvcrsrdqwc kyklw
3.Theraphotoxin 3 (TlTx3): (35 AA)
ddclgmfssc dpnndkccpn rvcrvrdqwc kyklw

2.polydot 结果:

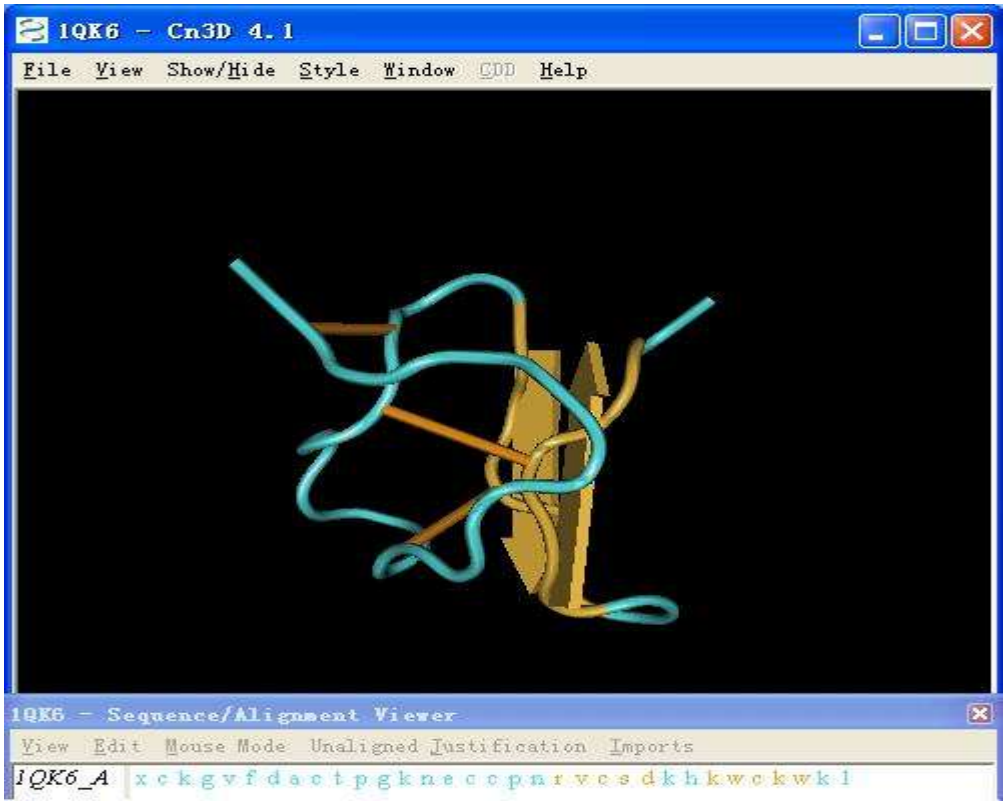


3. 建立树-序列相似的蛋白之间的关系:

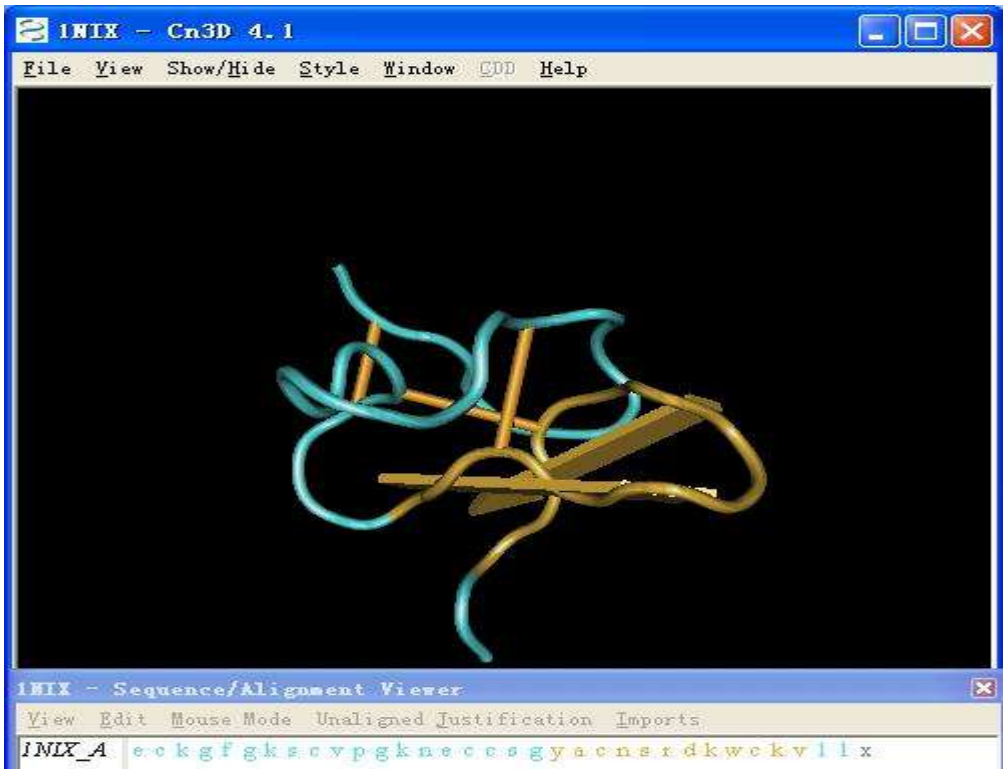


四.与 HWTX-I 有较大相似度的蛋白中已发表的蛋白结构图

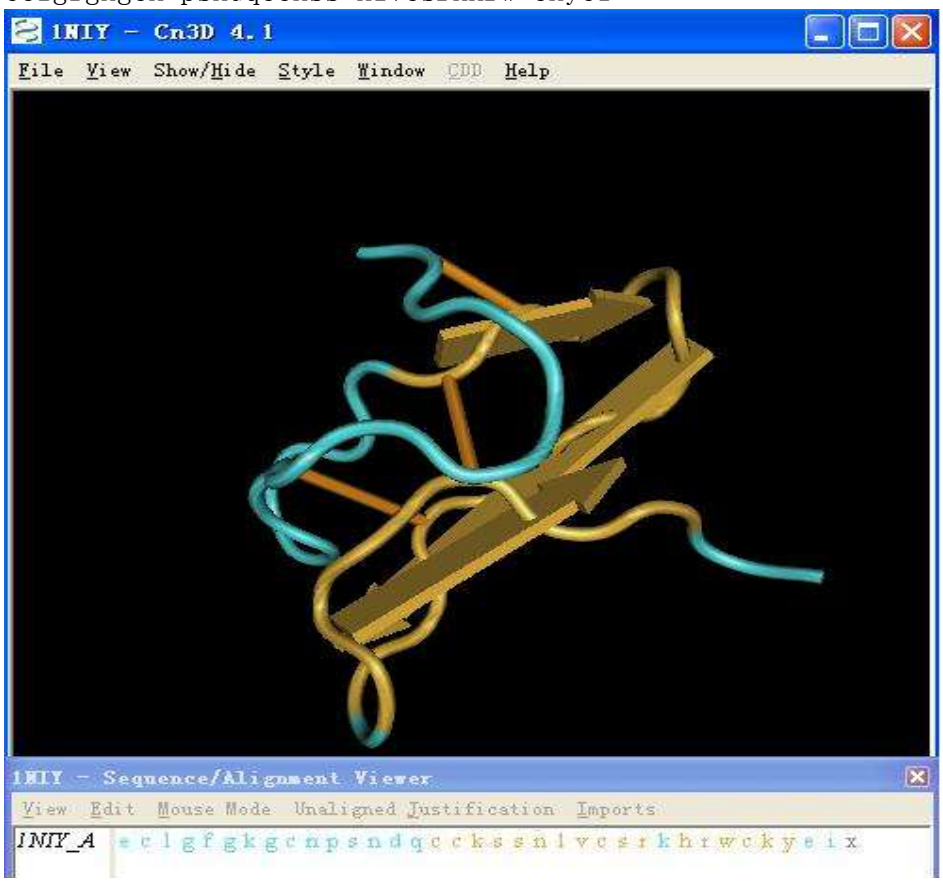
huwentoxin-I(hwtx-1): (33 AA)
ackgvfdact pgkneccpnr vcsdkhkwck wkl



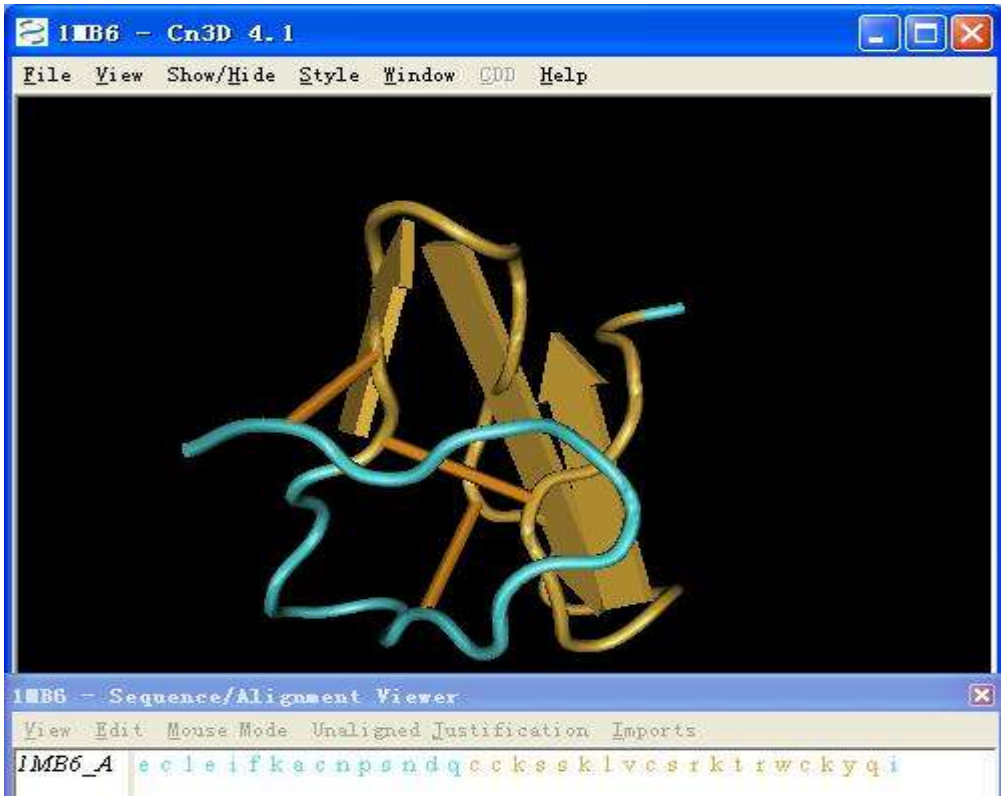
Hainantoxin-I (HnTx-I): (33 AA)
eckgfgkscv pgkneccsgy acnsrdkwck vll



Hainantoxin-IV (HnTx-IV): (35 AA)
eclgfgkgcn psndqcckss nlvcsrkhrw ckyei



Huwentoxin-IV (HwTx-IV): (35 AA)
ecleifkacn psndqcckss klvcsrktrw ckyqi



五. HWTX-I 的其他信息

1.HWTX-I 前体蛋白序列如下所示**:**

mrasmflala glvllfvvcy aseseekefp rellfkffav ddfkgeerac kgvfdactpg kneccpnrvc sdkhkwckwk l

1-21:信号肽　22-48:间隔区　49-81:成熟链

disulfide bond: (50,65) (57,70) (64,77)

Hydrogen bonded turn: 59-62

Beta-strand region: 68-70　77-79

2. HWTX-I 前体蛋白的蛋白序列分析(PEPSTATS):

PEPSTATS of Huwentoxin-I precursor from 1 to 81

Molecular weight = 9318.90　　Residues = 81

Average Residue Weight = 115.048　　Charge = 1.5

Isoelectric Point = 7.6918

A280 Molar Extinction Coefficient = 12660

A280 Extinction Coefficient 1mg/ml = 1.36

Improbability of expression in inclusion bodies = 0.559

Residue	Number	Mole%	DayhoffStat
A = Ala	7	8.642	1.005
B = Asx	0	0.000	0.000
C = Cys	7	8.642	2.980
D = Asp	4	4.938	0.898
E = Glu	8	9.877	1.646
F = Phe	8	9.877	2.743
G = Gly	4	4.938	0.588
H = His	1	1.235	0.617
I = Ile	0	0.000	0.000
K = Lys	9	11.111	1.684
L = Leu	8	9.877	1.335
M = Met	2	2.469	1.452
N = Asn	2	2.469	0.574
P = Pro	3	3.704	0.712
Q = Gln	0	0.000	0.000
R = Arg	4	4.938	1.008
S = Ser	4	4.938	0.705
T = Thr	1	1.235	0.202

V = Val 6 7.407 1.122

W = Trp 2 2.469 1.899

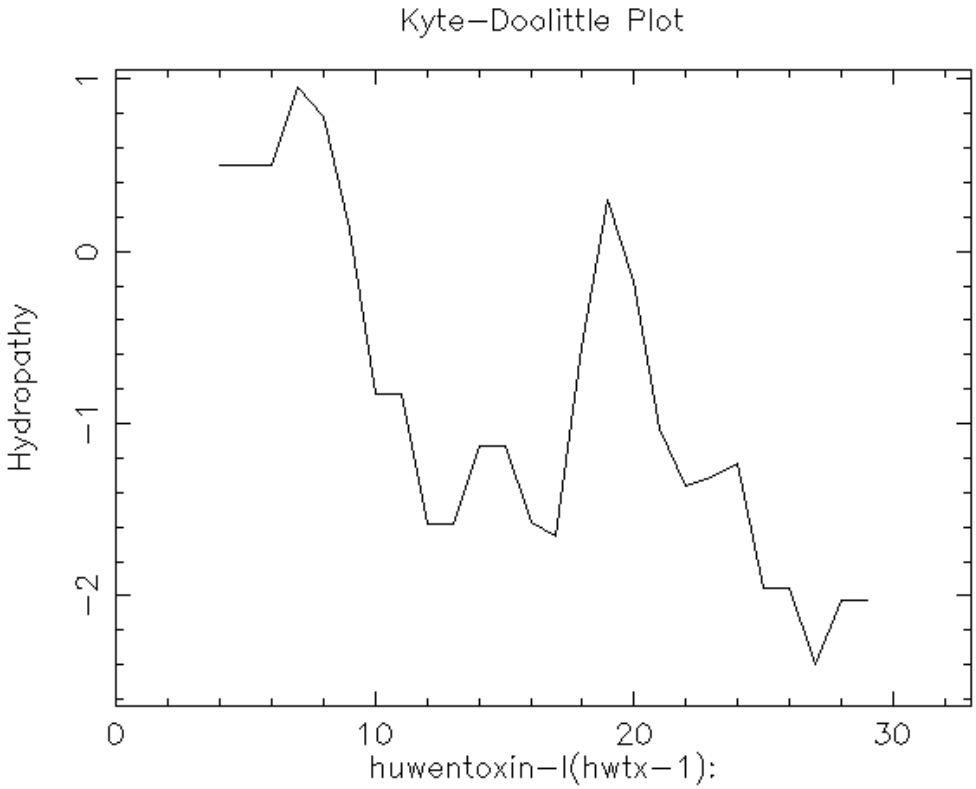
X = Xaa 0 0.000 0.000

Y = Tyr 1 1.235 0.363

Z = Glx 0 0.000 0.000

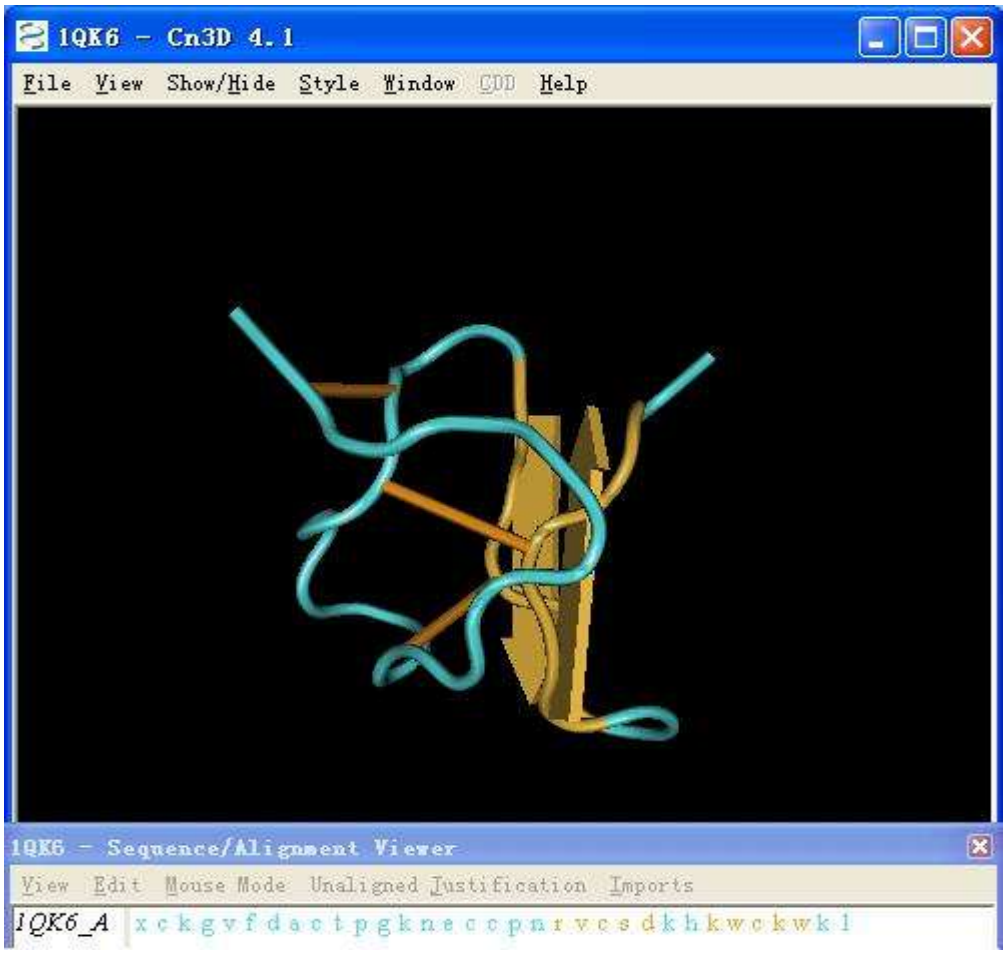
Property	Residues	Number	Mole%
Tiny	(A+C+G+S+T)	23	28.395
Small	(A+B+C+D+G+N+P+S+T+V)	38	46.914
Aliphatic	(I+L+V)	14	17.284
Aromatic	(F+H+W+Y)	12	14.815
Non-polar	(A+C+F+G+I+L+M+P+V+W+Y)	48	59.259
Polar	(D+E+H+K+N+Q+R+S+T+Z)	33	40.741
Charged	(B+D+E+H+K+R+Z)	26	32.099
Basic	(H+K+R)	14	17.284
Acidic	(B+D+E+Z)		

3. HWTX-I 疏水性区域分析**(PEPWINDOW):**



4.HWTX-I 的空间构象**:**

huwentoxin-I(hwtx-1): (33 AA)
ackgvfdact pgkneccpnr vcsdkhkwck wkl



六. 总结

除了昆虫, 蜘蛛是陆地上最成功的无脊椎动物. 现在世界上约有 40000 种蜘蛛, 从海滩到雪线以上的高山, 从沙漠到热带雨林, 都有蜘蛛的存在. 我国估计有不少于 4000 种. 虽然蜘蛛种类繁多, 但是最后蜘蛛一般都注入毒液来麻醉或杀死列物; 然后分泌消化液, 经猎物伤口注入体内. 蜘蛛一般都是先进行体外消化, 分解猎物的软组织后再吸入体内.

从上面的各种结果可以得出以下几个结论:

1. 蜘蛛毒素有效成分很多是小分子的多肽

2. 这些小肽都富含二硫键, 虽然只有几十个氨基酸, 但是都具有三到四对二硫键. 这使它们具有特定的空间结构.

3. 虽然一些毒素是来自不同种类, 甚至不同属的蜘蛛, 但是它们蛋白序列之间还是有很大的同源性, 说明进化过程中这些毒素起着非常重要的作用.

4. 属于同一属的蜘蛛毒素亲源关系近, 属于不同属的蜘蛛毒素亲源关系远.

5. 蜘蛛毒素成分构成比较相似. 比如从建树的结果中可以看出 HWTX-I 和 HNTX-I、HNTX-III 之间相似; HWTX-II 和 HNTX-II 之间相似; HWTX-IV 和 HNTX-IV 之间相似。从蛋白质的空间构象图比较中也可以看出这一点。

6. 从 HWTX-I 的前体蛋白序列中有信号肽，这与它的分泌性相吻合。从 HWTX-I 的序列分析，构想分析中可以看到三对二硫键配合三股反平行的 β 折叠

形成一个非常致密稳定的结构是典型的抑制剂胱氨酸结结构模体.