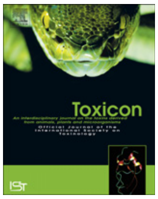
Toxicon 56 (2010) 644–647

Contents lists available at ScienceDirect

Toxicon

journal homepage: www.elsevier.com/locate/toxicon



Short communication

ATDB 2.0: A database integrated toxin-ion channel interaction data

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ARTICLE INFO

Article history:
Received 24 March 2010
Received in revised form 23 May 2010
Accepted 25 May 2010
Available online 1 June 2010

Keywords:
Interaction network
Toxin
Ion channel
Toxin Ontology
Ion channel ontology

ABSTRACT

We have developed an updated version of the Animal Toxin Database (ATDB 2.0) that provides a new bioinformatics resource for analyzing toxin-channel (T-C) interactions. Data on more than 54,000 T-C interactions, including 9193 high-confidence interactions, has been extracted, formatted and mapped to toxin and ion channel databases. The interaction data can be accessed easily through a new network browser on the website at http://protchem.hunnu.edu.cn/toxin. This resource may be useful for sequence pattern recognition and prediction of the function of new toxins.

The Animal Toxin Database (ATDB) (He et al., 2008) is an integrative database of animal toxins. In recent two years, we have updated the database continually and taken great efforts to build an integrated platform for the toxin–target interaction data. It now contains more than 54,000 T-C interactions between 817 toxins and 1013 ion channels, including 9193 high-confidence interactions with active site information, as core dataset. These data are categorized carefully by species, toxin/ion channel types as well as interaction types (e.g., inhibition or activation). To facilitate the easy accessibility to these data, we built a new network browser. Other advanced features, such as an upgraded search engine, on-line 3D structural views and new sequence analysis tools are also available for more accurate analysis and less time consuming.

1. Data construct of ATDB 2.0

ATDB 2.0 consists of three parts of data: toxin, ion channel and toxin–channel interaction (Fig. 1A). The protein and nucleic acid sequences of ion channel were extracted from UniProtKB/Swiss-Prot, TrEMBL (Boeckmann et al., 2003), NCBI-nucleotide (Pruitt et al., 2007). Domain architectures of ion channel were determined by HMMER software based on the deposit of HMM models of PFAM (Finn et al., 2006) database version 23 with default parameters. 3D structure models were downloaded from PDB database (Berman et al., 2000). Pictures of more than 200 animal species were collected from internet. At last, 5097 protein sequences, 8396 nucleic acid sequences and 525 structure models of ion channels from 299 species were deposited in the dataset.

Because ion channels have complex features, it is necessary to create a hierarchic controlled term system (ion channel ontology) (Camerino et al., 2007; Catterall et al., 2005a,b; Clapham and Garbers, 2005; Clapham et al., 2005; Goldstein et al., 2005; Gutman et al., 2005; Hofmann et al., 2005; Kubo et al., 2005; Wei et al., 2005; Yu et al., 2005; Wood et al., 2009) to annotate and classify them.

The ion channel ontology (IO) contains 507 unique terms and was designed to answer six biological questions about ion channels (detailed information in http://protchem.hunnu.edu.cn/toxin/Ontology/Introduction.jsp).

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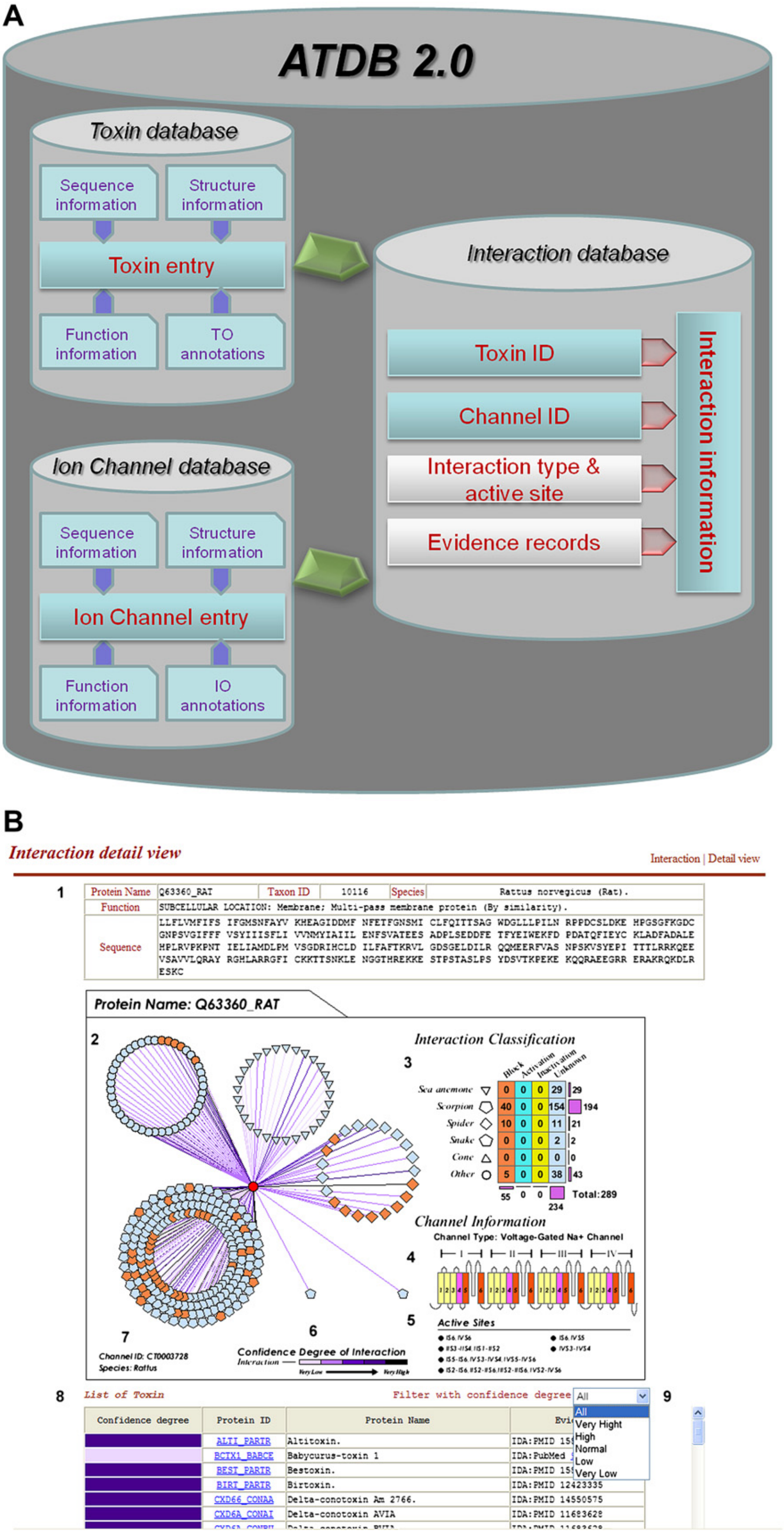
doi:10.1016/j.toxicon.2010.05.013



Interaction detail view

Protein Name	Q63360_RAT	Taxon ID	10116	Species	Rattus norvegicus (Rat).
Function	SUBCELLULAR LOCATION: Membrane; Multi-pass membrane protein (By similarity).				
Sequence	LLFLVMFIFS IFGMSNFAYV KHEAGIDDMF NFETFGNSMI CLFQITTSAG WDGLLLPILN RPPDCSLDKE HPGSGFKGDC GNPSVGIFFF VSYIIISFLI VVNMYIAIIL ENFSVATEES ADPLSEDDFE TFYEIWEKFD PDATQFIEYC KLADFADALE HPLRVPKPNT IELIAMDLPM VSGDRIHCLD ILFAFTKRVL GDSGELDILR QQMEERFVAS NPSKVSYEPI TTTLRRKQEE VSAVVLQRAY RGHLARRGFI CKKTTSNKLE NGGTHREKKE STPSTASLPS YDSVTKPEKE KQQRAEEGRR ERAKRQKDLR ESKC				

Protein Name: Q63360_RAT

Interaction Classification

		Block	Activation	Inactivation	Unknown	
Sea anemone	▽	0	0	0	29	29
Scorpion	⬠	40	0	0	154	194
Spider	◇	10	0	0	11	21
Snake	⬠	0	0	0	2	2
Cone	△	0	0	0	0	0
Other	○	5	0	0	38	43
		55	0	0	234	Total:289

Channel Information

Channel Type: Voltage-Gated Na+ Channel

Active Sites

- IS6, IVS6
- IS6, IVS5
- IIS3-IIS4, IS1-IIS2
- IVS3-IVS4
- IS5-IS6, IVS3-IVS4, IVS5-IVS6
- IS2-IS6, IIS2-IIS6, IIIS2-IIIS6, IVS2-IVS6

Confidence Degree of Interaction

Interaction

Channel ID: CT0003728
Species: Rattus

List of Toxin

Filter with confidence degree All

- All
- Very Hight
- High
- Normal
- Low
- Very Low

Confidence degree	Protein ID	Protein Name	Evi
■	ALTI_PARTR	Altitoxin.	IDA:PMID 15
□	BCTX1_BABCE	Babycurus-toxin 1	IDA:PubMed
■	BEST_PARTR	Bestoxin.	IDA:PMID 15
■	BIRT_PARTR	Birtoxin.	IDA:PMID 12423335
■	CXD66_CONAA	Delta-conotoxin Am 2766.	IDA:PMID 14550575
■	CXD6A_CONAI	Delta-conotoxin AVIA	IDA:PMID 11683628