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TopoIBase: a comprehensive database dedicated to type IA DNA-topoisomerases

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TopolBase : a comprehensive database dedicated to type IA DNA-topoisomerases.

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Topoisomerases

- Proteins discovered in 1971 (Wang et al., 1971)
- Function : stabilization of the DNA topology

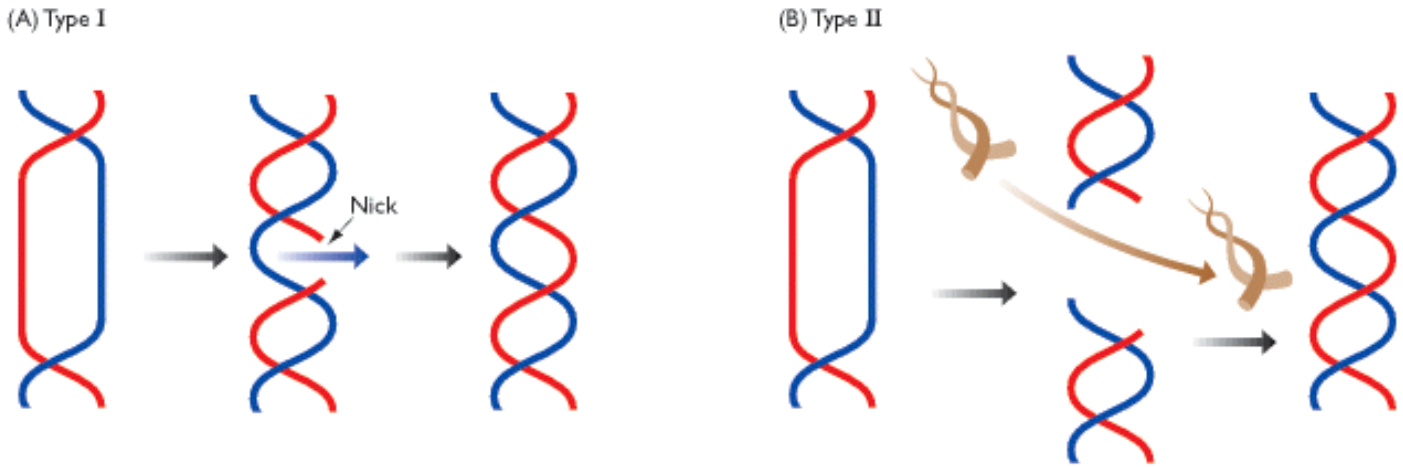


Figure: Mechanisms of action of type I et II topoisomerases.

Diversity

- Many types et sub-types of differents origins
- Different activities and dependancies
- Topoisomerases IA.

Topoisomerases			Caracteristics			Activities			
Types	Sub-types	Name	Mg2+	ATP	Cut	Releases negative supercoiling	Releases positive supercoiling	Insets negative supercoiling	Insets positive supercoiling
I	IA	I	+	-	Simple strand	+	-	-	-
		TopR	+	+	Simple strand	+	-	-	+
	IB	TopoIB	-	-	Simple strand	+	+	-	-
II	IIA (bact.)	Gyrase	+	+	Double strand	-	+	+	-
	IIA (euca.)	Topo2	+	+	Double strand	+	+	-	-
	IIB (arch.)	TopoIV	+	+	Double strand	+	+	-	-

Figure: Types and sub-types of topoisomerases and enzymatic activity variations.

Objectives

- Topoisomerases IA are difficult to study
- Lack of protein database dedicated to topoisomerases
- Objective : develop an expertised database dedicated to topoisomerases
- Expertise : data selection, VLD (Variable Length Decoding : Didier et al., 2012 [1]) classification and annotations

[1] Didier, G., Corel, E., Laprevotte, I., Grossmann, A., and Devauchelle, C. (2012). Variable length local decoding and alignment free sequence comparison.
Theoretical Computer Science, 462:1–11

Model

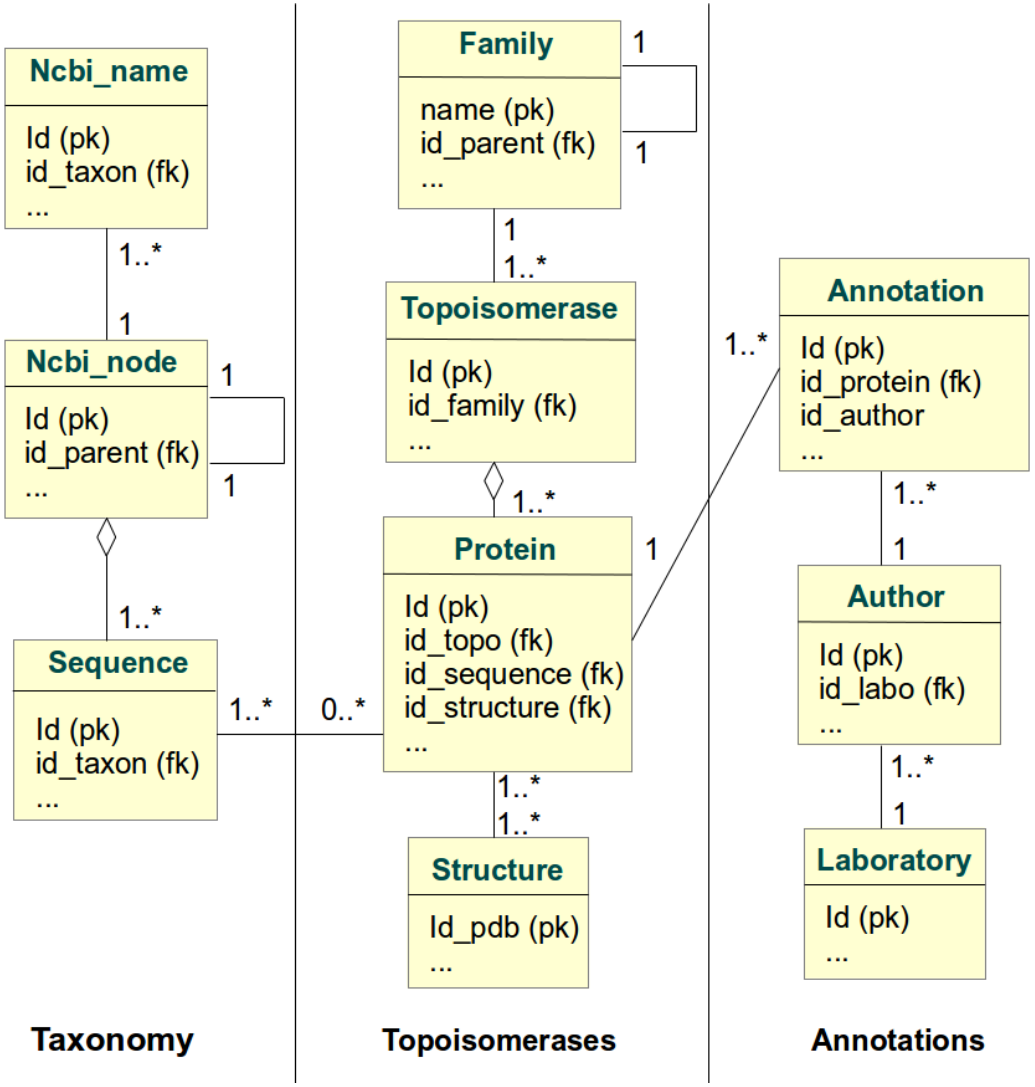


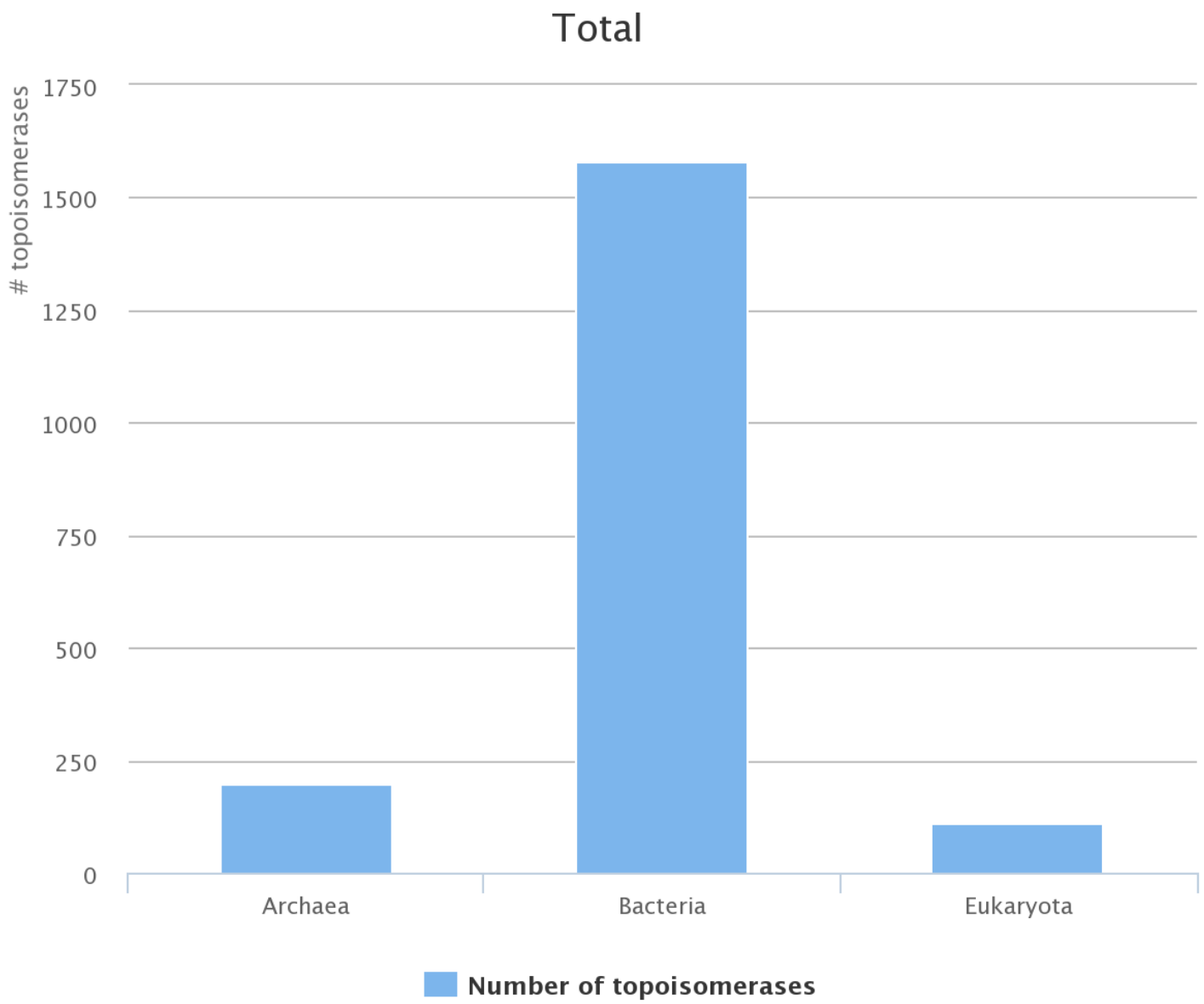
Figure: Simplified UML diagram of the database.

Data selection and expertise

- Topoisomerases : TBLASTN on fully sequenced genomes
- Classification : VLD (Didier et al. 2012 [1]) + hierarchical ascendant clustering
- Annotations by experts

[1] Didier, G., Corel, E., Laprevotte, I., Grossmann, A., and Devauchelle, C. (2012). Variable length local decoding and alignment free sequence comparison.
Theoretical Computer Science, 462:1–11

Database statistics



Database statistics (2)

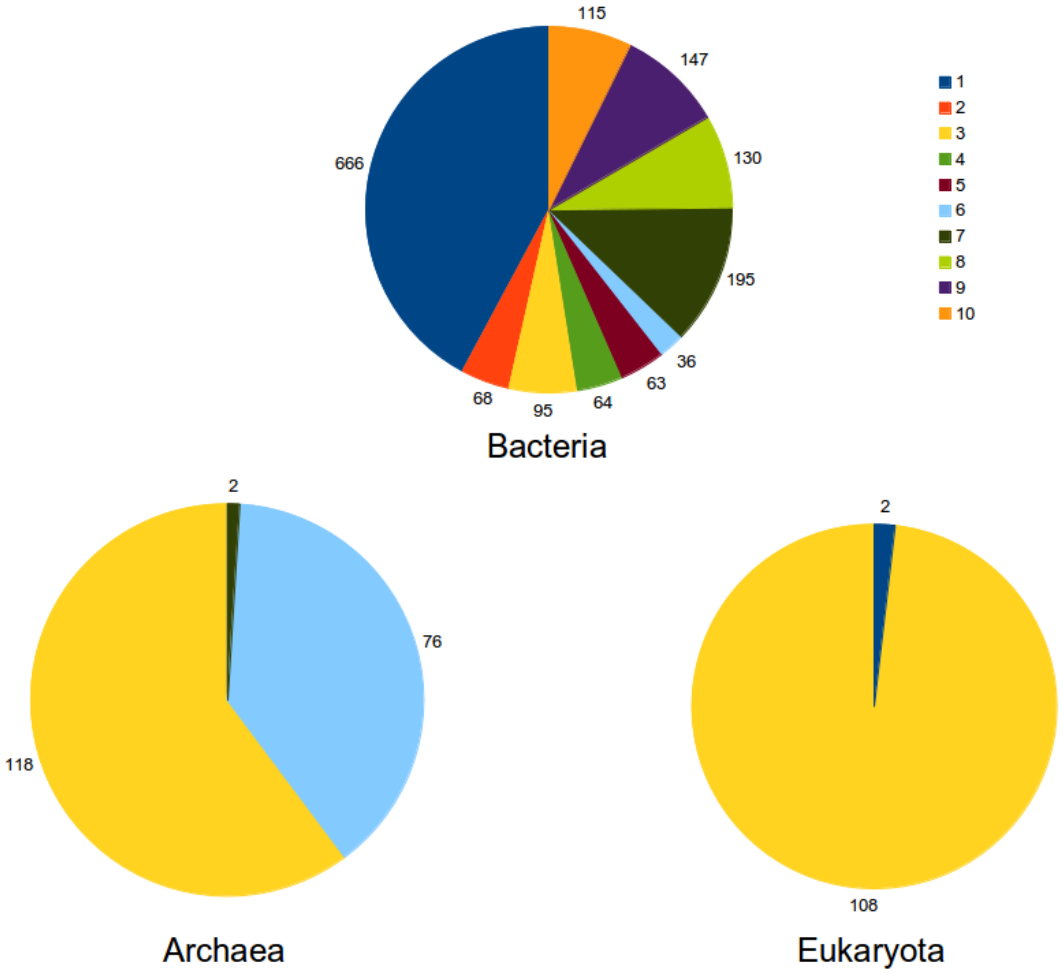


Figure: Topoisomerases distribution in domains.

Graphical interface

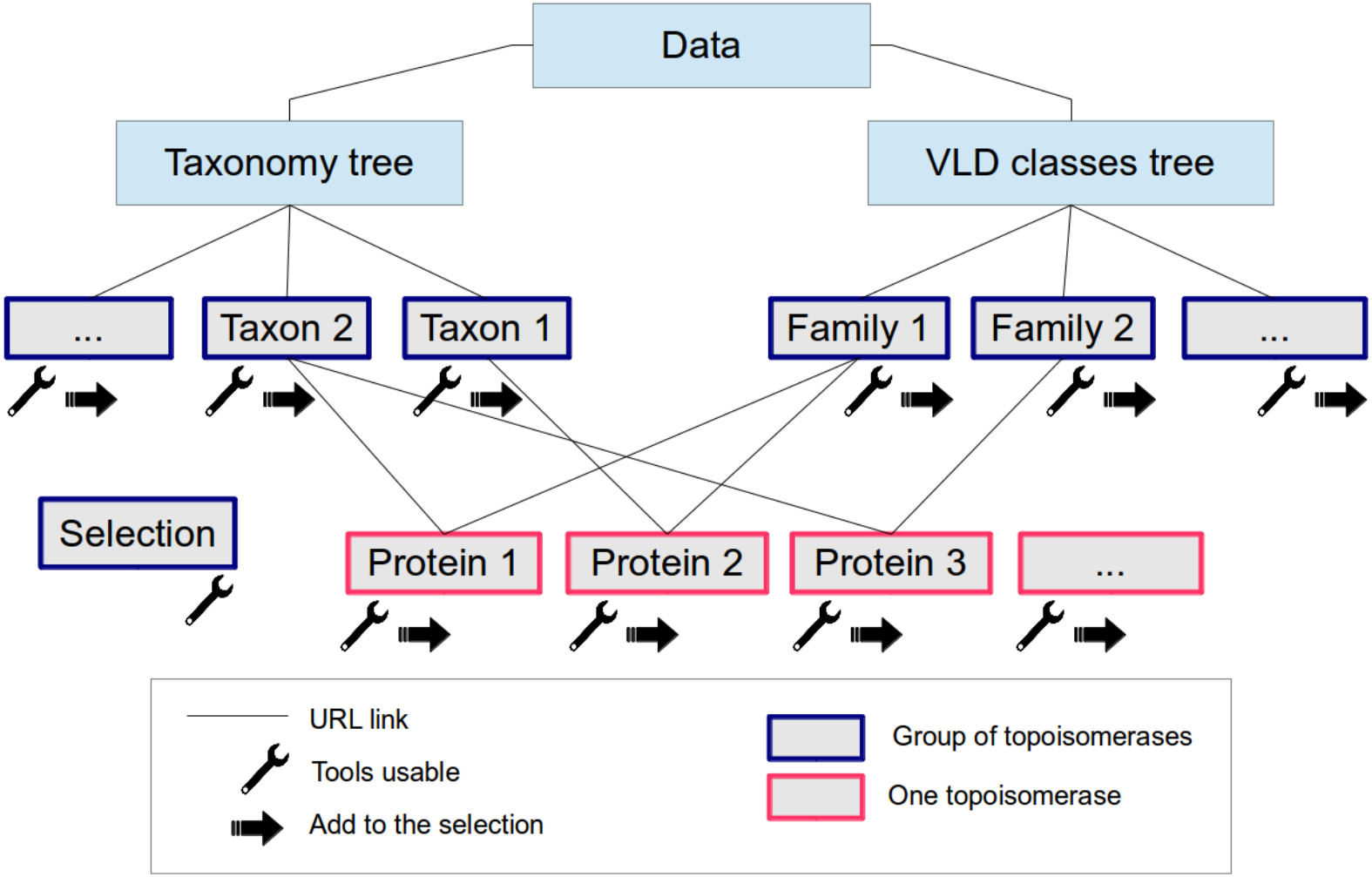


Figure: Data browsing on the interface.

Taxonomy

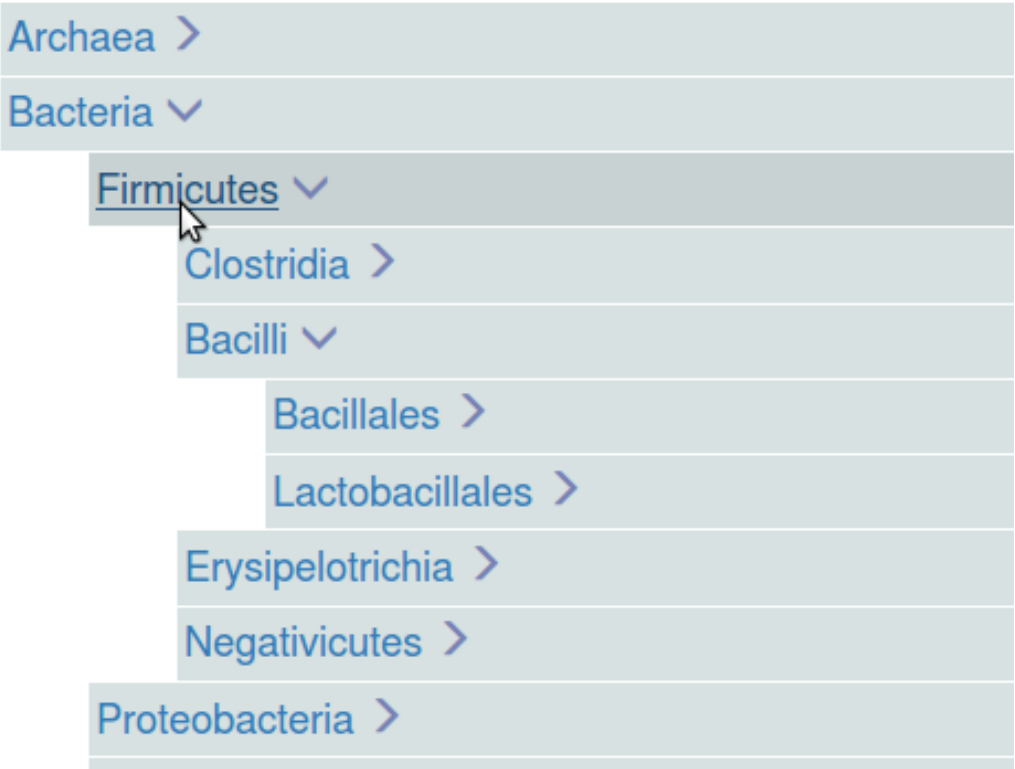


Figure: Part of the taxonomy tree.

Taxonomy

Download | Blast | Muscle | VLD | Add to selection

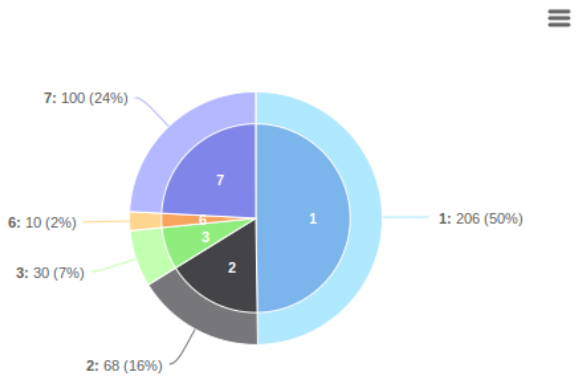
Taxon : Firmicutes

Select all ☑	Name	Family	Sequence
☑	(937) Putative DNA topoisomerase [Lactobacillus brevis]	3	MSIVVLTEKSSQIDPYAKALGTPKKKQGSVWVHSALL NADVQFVAASGHLFKLDGPEDYNDAWRDRSNYEQL PMVPQKFKARIKDARARASFNRIKQAITAADFVILATD
☑	(809) DNA topoisomerase 1 [Lactobacillus acidophilus NCFM]	1	MPTKAKSKSKTKKRKKILVIVESPAKAKTIEKYLGRNY HVIASKGHIRDLPKSQMGIDFEDNYKPKYISIRGKGDT IKELKSEAKKAKEVYLASDPDREGEAIAWHVAHALDL
☑	(276) Reverse gyrase [Caldicellulosiruptor saccharolyticus DSM 8903]	6	MATGAKYYHSCINCGGINSDTRNQKGLPCEKCLPFE NNMNILESLKEHNSLKDYAYFWNFQNEYKEFEKFFV SKVGKPMTGYQRLWARRLLLSKSFTLIAPTGLGKTTF

Showing 1 to 10 of 414 entries

Previous 1 2 3 4 5 … 42 Next

Family distribution



Taxonomy tree

- Firmicutes
  - Clostridia
  - Bacilli
  - Erysipelotrichia
  - Negativicutes

Figure: Taxon page.

Selections

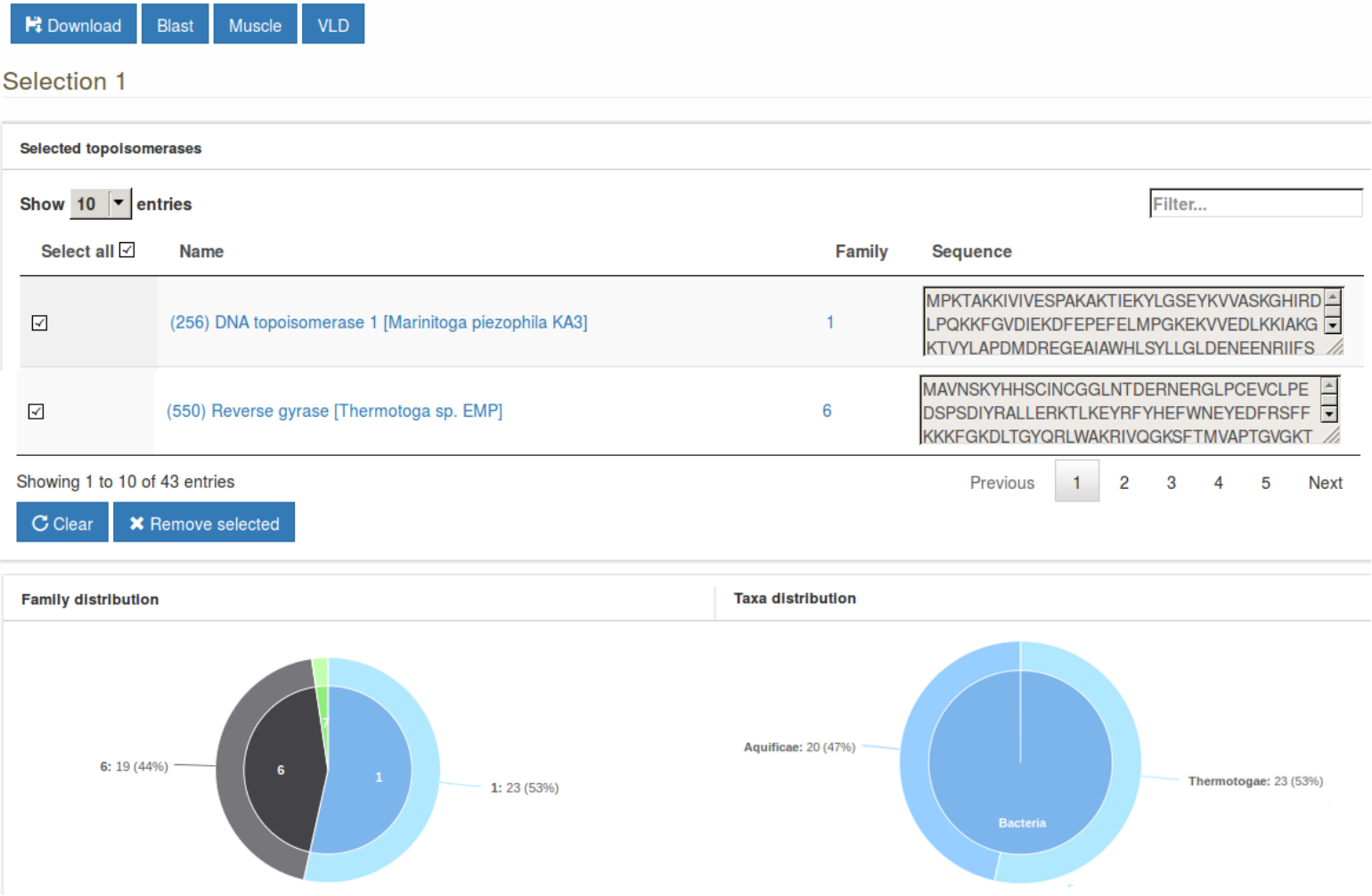


Figure: Selection page.

BLASTP

```
>90|DNA topoisomerase 1|1|AAA68949.1|P46799
MSKKVKKYIVVESPAKAKTIKSILGNEYEVFASMGHIIDLPKSKFGVDLEKDFEPEFAVI
KGKEKVVEKLKDLAKKGELLIASDMDREGEAIAWHIARVTNTLGRKNRIVFSEITPRVIR
EAVKNPREIDMKKVRAQLARRILDRIVGYSLSPVLWRNFKSNLSAGRVQSATLKLVCDRE
REILRFVPKKYHRITVNFDGLTAEIDVKEKKFFDAETLKEIQSIDELVVEEKKVSVKKFA
PPEPFKTSTLQQEAYSKLGFSVSKTMMIAQQLYEGVETKDGHIAFITYMRTDSTRVSDYA
KEEARNLITEVFGEEYVGSKRERRKSNAKIQDAHEAIRPTNVFMTPEEAGKYLNSDQKKL
YELIWKRFLASQMKPSQYEETRFVLRTKDGKYRFKGTVLKKIFDGYEKVWKTERNTGEFP
FEEGESVKPVVVKIEEQETKPKPRYTEGSLVKEMERLGIGRPSTYASTIKLLLNRGYIKK
IRGYLYPTIVGSVVMDYLEKKYSDVVSVSFTAEMEKDLDEVEQGKKTDKIVLREFYESFS
SVFDRNDRIVVDFPTNQKCSCGKEMRLSFGKYGFYLKCECGKTRSVKNDEIAVIDDGKIF
LGRKDSESGSPDGRSVEGKGNLSEKRRKGKKGS
>91|DNA topoisomerase 1|1|AAD35346.1|P46799
MSKKVKKYIVVESPAKAKTIKSILGNEYEVFASMGHIIDLPKSKFGVDLEKDFEPEFAVI
KGKEKVVEKLKDLAKKGELLIASDMDREGEAIAWHIARVTNTLGRKNRIVFSEITPRVIR
EAVKNPREIDMKKVRAQLARRILDRIVGYSLSPVLWRNFKSNLSAGRVQSATLKLVCDRE
REILRFVPKKYHRITVNFDGLTAEIDVKEKKFFDAETLKEIQSIDELVVEEKKVSVKKFA
PPEPFKTSTLQQEAYSKLGFSVSKTMMIAQQLYEGVETKDGHIAFITYMRTDSTRVSDYA
KEEARNLITEVFGEEYVGSKRERRKSNAKIQDAHEAIRPTNVFMTPEEAGKYLNSDQKKL
YELIWKRFLASQMKPSQYEETRFVLRTKDGKYRFKGTVLKKIFDGYEKVWKTERNTGEFP
FEEGESVKPVVVKIEEQETKPKPRYTEGSLVKEMERLGIGRPSTYASTIKLLLNRGYIKK
```

Load sample data

Parameters

Blast program	BLASTP
E-value	
Bank	selection1
Submit	Browse... No files selected.

Figure: BLASTP interface.

Other use-cases

- Taxa and VLD distribution of topoisomerases containing a specific amino acid sequence
- Analysis of a list of uniprot IDs of topoisomerases
- Classification of a new protein compared to stored topoisomerases

Perspectives

- Extension of the database to type IB and II topoisomerases
- Visualization of neighbors genomic elements
- Binding to other databases

Thank you for your attention
`stat.genopole.cnrs.fr/topodb`

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