

# MetalMine Tutorial

## 3. BLAST Search

MetalMine database contains the list of metal coordinating residues. By performing a BLAST sequence search against a set of sequences that contain metal binding sites, and check the matching with the metal coordinating residues, MetalMine answers if there is any known metal binding residues, in the query sequence. The BLAST database only contains the amino acid sequences of metal binding proteins, so the search is pretty fast.

To perform the analysis, first click on the “BLAST” in top menu, then a text box and a couple of buttons appear.

**BLAST Search**  
Input Amino Acid Sequence (Fasta format) in the text box and press Execute

```
>gil157837117|pdb16PCYIA Chain A, Crystal Structure Analyses Of Reduced (Cu) Poplar PlastoCytochrome b6/f complex subunit L  
IDVLLGADGDSLAFVPSSEFSISPGEKIVFKNNAGFPHNIVFDEDSIPSGVDASKISMSEEDLLNAKGETFEVALSNKGEY  
SFYCSFHOGAGMVGKVTVN
```

Reset Form Execute

show raw output from BLAST.

Put a query amino acid sequence in the text box, and press “Execute Button”, to run the BLAST search. There is also a checkbox for an optional raw BLAST output.

IDVLLGADGDSLAFVPSSEFSISPGEKIVFKNNAGFPHNIVFDEDSIPSGVDASKISMSEEDLLNAKGETFEVALSNKGEY | 80  
SFYCSFHOGAGMVGKVTVN | 100

List of High Reliability Match

1	H37 matches with	Cupredoxin/Multicopperoxidase (Blue Copper Site)	coppermine	32
2	C84 matches with	Cupredoxin/Multicopperoxidase (Blue Copper Site)	coppermine	33
3	H87 matches with	Cupredoxin/Multicopperoxidase (Blue Copper Site)	coppermine	33
4	M92 matches with	Cupredoxin/Multicopperoxidase (Blue Copper Site)	coppermine	32

A typical output is shown at the bottom of previous page. First your query sequence is re-displayed with matched residues highlighted with magenta. The

numbers at right indicates the residue number of the last residue of each line. Also, every ten'th residues is slightly darker.

Following the query sequene is a list of matches. In this example, Histidines at 37 and 87, Cysteins at 84 and Methionines at 92 positions match with Blue Copper Site of Cupredoxin or Multicopper oxidases.

Sometimes, BLAST outputs alignment with very low probability of homology. Matches in such an alignment may have lower significance as a result. The match with this low reliability is displayed as light cyan color in the sequence and a separate list of matches, as is demonstrated in the following search result, for a fragment of nitrite reductase.

**MetalMine: A Database of Functional Metal ion Binding Sites in Proteins**

Home
About
BLAST
Tutorial
Contact

<b>MetalMines</b>	GLRDEKQPLTYDKIYYVGEQDFYVPKDEAGNYKKYETPGEAYEDAVKAMRTLTPTHIVFNGAVGALTGDHALTAAVGER   80
Cobalt	VLVVHSQANR <b>D</b> TRPHLIGGHGDYVWATGKFRNPPDLQETWLI PGGTAGAAFYTRQPGVYAYVNNLIEAFELGAAGHF   160
Copper	KVTGEWDDLMTSVVKPASM   181
Manganese	<b>List of High Reliability Match</b>
Molybdenum	<b>1</b> H146 matches with Nitrite Reductase Interdomain Site Mononuclear coppermine <b>15</b>
Nickel	<b>There found match with low reliability.</b>
Vanadium	<b>List of Low Reliability Match (e-value higher than 0.0001)</b>
Tungsten	<b>1</b> H71 matches with Arginase manganese <b>1</b>
In Preparation	<b>2</b> D91 matches with Arginase manganese <b>1</b>
Iron	
Iron(hem)	
Iron(Sulfur)	
Zinc	
Magnesium	
Calcium	

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