# Nit MAP

# (Nitrilase Mining and Prediction Database)

Project report submitted in partial fulfillment of the requirement for the degree of Bachelor of Technology

In

# **Bioinformatics**

By

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Under the supervision of

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&

# Dr.Narendra Kumar

To



# **BONAFIDE CERTIFICATE**

This is to certify that this project report entitled "**NitMaP:Nitrilase Mining and Prediction Tool**", submitted to Jaypee University of Information Technology, Waknaghat, is a bonafide record of work done by "**Dhruv Gaur(141502), Shaurya Mehta(141505)**" for the degree of B.Tech Bioinformatics has been carried out under my supervision.

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# **Declaration by Authors**

This is to affirm that this report title "**NitMaP: Nitrilase Mining and Prediction Tool**" has been written by us i.e. Dhruv Gaur(141502) and Shaurya Mehta(141505) under the supervision of Late Dr. Chittaranjan Rout And Dr. Narendra Kumar. No part of the report has been plagiarized from other sources. All information included from other sources have been duly acknowledged. I aver that if any part of the report is found to be plagiarized, I shall take full responsibility for it.

Dhruv Gaur(141502)

Shaurya Mehta(141505)

Place:

Date:

# **ACKNOWLEDGEMENTS**

We have taken efforts in this project. However, it would not have been possible without the kind support and help of many individuals. We would like to extend our sincere thanks to all of them. We are highly indebted to our guide Late **Dr. Chittaranjan Rout**, for his guidance and constant supervision as well as also for his support in completing the project.

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Thanking You

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# **List of Abbreviations**

NCBI-National Center for Biotechnology Information

PDB-Protein Data Bank

HTML-Hypertext Markup Language

JS-Java Script

CSS-Cascading Style Sheets

PHP-Hypertext Preprocessor

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# CHAPTER 1

### **INTRODUCTION**

The protein nitrilase was first portrayed by Thimann and Mahadevan (1964). The catalyst, which was confined from grain leaves, catalyzed the change of indoleacetonitrile (IAN) to indoleacetic corrosive (IAA) and was at first called indoleacetonitrilase. Substrate investigation with cleansed compound on 26 nitriles demonstrated that the protein had a wide substrate extend. The rate of hydrolysis was eight times more noteworthy with 3-cyanopyridine than with IAN. The protein was in this manner renamed nitrilase to demonstrate the wide substrate scope of the chemical (Thimann and Mahadevan 1964).

The main bacterial nitrilase was disengaged from a dirt bacterium (perhaps a Pseudomonas species) by choice for development on the normally happening nitrile, ricinine (N-methyl-3-cyano-4-methoxy-2-pyridone), as a sole carbon source (Hook and Robinson 1964; Robinson and Hook 1964). This chemical catalyzed the hydrolysis of a scope of 2-pyridones with rates in the vicinity of 0 and 118% in respect to ricinine (100%).

The biotechnological capability of nitrile hydrolysing chemicals has prompted the separation of a scope of microorganisms and growths equipped for hydrolysing nitriles. A large portion of these were disengaged based on utilizing a specific nitrile as a carbon or potentially nitriogen source. The catalysts concentrated to date demonstrate an exceptionally various scope of biochemical qualities. Specifically substra qte specificity of the compounds fluctuates generally. Beginning examinations proposed that nitrilases were particular for sweet-smelling nitriles and nitrile hydratases for aliphatic nitriles yet this refinement must be reexamined in the light of the developing assortment of data on both nitrilases and nitrile hydratases.

While it isn't conceivable to give a total investigation of substrate extend for every one of the chemicals the most prominent highlights for every protein are given and the relative rate of benzonitrile hydrolysis is given where accessible. None of the catalysts demonstrate indistinguishable properties. The most outstanding contrasts between the compounds are in substrate specificity, local structure and collection properties, and pH optima.

Cyanide and nitrile hydrolysing catalysts have been examined in an extensive variety of microbial species, and progressively, in plants. The enzymatic change of HCN/nitrile to the relating corrosive can occur by a one-advance process as exemplified by nitrilases and cyanide dihydratases (CDH) or by a two-advance process with an amide middle of the road similar to the case with nitrile hydratases and cyanide hydratases (CH).

As on today in excess of 5000 prokaryotic genomes have been totally sequenced and the arrangement information are accessible openly space databases. Subsequently there is sufficient extension for in silico screening of these microbial genomes to discover novel wellsprings of nitrilases. Bioinformatics devices have made it simple to dig genome information for new catalysts. The preserved succession themes in the quality/protein groupings of chemicals are utilized for genome mining or in silico screening for seeking novel wellsprings of the coveted catalysts. Keeping in see the extension and impediments the accompanying database NitMAP has been created to gather data relating to nitrilases.

# **CHAPTER 2**

# 2.1 Collection of Information from various databases

- **PDB-** Protein Data Bank is a crystallographic database which contains the data for the three-dimensional structures of large biological molecules, such as proteins, nucleic acids and complex assemblies, that helps to understand all the aspects of biomedicine and agriculture, protein synthesis to health and diesease. The protein data bank can be accessed free on the Internet via the websites (PDBe , PDBj, and RCSB). The PDB is operated or maintained by an organization called the Worldwide Protein Data Bank, (wwPDB). X-ray crystallography and NMR spectroscopy as submitted by biochemists and structural biologists done experimently, are the basis for the data present in the protein data bank. The file format initially used by the PDB was called the PDB file format.
- $\Rightarrow$  **Piece of work**: Template for protein modeling
  - NCBI- National center for biotechnology information is operated and maintained by United states library of medicine(NLM) relevant to biotechnology and biomedicine and is an important resource for bioinformatics tools and services. Major databases include GenBank for DNA sequences and PubMed, a bibliographic database for the biomedical literature. Other databases include the NCBI Epigenomics database. All these databases are available online through the Entrez search engine.
- $\Rightarrow$  **Piece of work**: Retrieval of taxonomical data

# 2.2 Use of computational language HTML and Java

# 2.2.1 Languages used

 $\Rightarrow$  HTML - HTML stands for Hyper Text Markup Language, which is the most widely used language to develop web applications, HTML describes the structure of web pages using markup and is the main back-end language used for our database.

```
-->
<html>
    <head>
       <title>database</title>
       <meta http-equiv="content-type" content="text/html; charset=utf-8" />
       <meta name="description" content="" />
       <meta name="keywords" content="" />
       <link href='http://fonts.googleapis.com/css?family=Roboto:400,100,300,700,500,900'</pre>
       <script src="http://ajax.googleapis.com/ajax/libs/jquery/1.11.0/jquery.min.js"></s</pre>
       <script src="js/skel.min.js"></script>
       <script <pre>src="js/skel-panels.min.js"></script>
       <script <pre>src="js/init.js"></script>
        <noscript>
           <link rel="stylesheet" href="css/skel-noscript.css" />
           k rel="stylesheet" href="css/style.css" />
           <link rel="stylesheet" href="css/style-desktop.css" />
       </noscript>
    </head>
    <body class="homepage">
    <!-- Header -->
       <div id="header">
            <div id="nav-wrapper">
               <!-- Nav -->
               <nav id="nav">
                   <a href="index.html">HOME</a>
                   <a href="Taxonomy.html">TAXONOMY</a>
                   <a href="Protein models.html">PROTEIN MODELS</a>
                   <a href="Our work.html">OUR WORK AND RESEARCH</a>
                   <a href="References.html">REFERENCES AND ACKNOWLEDGEMENT</a>
                   </11>
               </nav>
            </div>
```

# Figure:2.1 HTML File for Home Page

 CSS- stands for Cascading Style Sheets.CSS describes how HTML elements are to be displayed on screen, paper, or in other media.CSS saves a lot of work. It can control the layout of multiple web pages all at once. External stylesheets are stored in .CSS files.

```
accordin,
article
ł
    clear: both;
    margin: 2em 0 2em 0 !important;
}
section > :first-child,
article > :first-child
{
    margin-top: 0 !important;
}
section:first-child,
article:first-child
{
    margin-top: 0 !important;
}
```

Figure:2.2 Code for CSS

⇒ JavaScript - JavaScript is one of the three core technologies of World Wide Web content production. It is used to make webpages interactive and provide online programs, including video games. The majority of websites employ it, and all modern web browsers support it without the need for plug-ins by means of a built-in +JavaScript engine.

```
var locationPath = filterPath(location.pathname);
var scrollElem = scrollableElement('html', 'body');
$('a[href*=#]:not(a.mobile-btn)').each(function() {
  var thisPath = filterPath(this.pathname) || locationPath;
  if ( locationPath == thisPath
  && (location.hostname == this.hostname || !this.hostname)
  && this.hash.replace(/#/,'') ) {
    var $target = $(this.hash), target = this.hash;
    if (target) {
      var targetOffset = $target.offset().top;
      $(this).click(function(event) {
        event.preventDefault();
        $(scrollElem).animate({scrollTop: targetOffset}, 400, function() {
          location.hash = target;
       });
      });
   }
  3
});
```

# Figure: 2.3 Code for JS

# 2.2.2 Software's and databases used

⇒ SWISS-MODEL: Swiss model is a fully automated protein structure homologymodelling server, accessible via the ExPASy web server, or from the program DeepView (Swiss Pdb-Viewer). The purpose of this server is to make Protein Modelling accessible to all biochemists and molecular biologists worldwide.

Piece of work: Protein modelling

⇒ IMG/ER: The mission of the Integrated Microbial Genomes & Expert Review (IMG/ER) system is to support the annotation, analysis and distribution of microbial genome and microbiome datasets sequenced at DOE's Joint Genome Institute (JGI).

IMG/ER is also open to scientists worldwide for the annotation, analysis, and distribution of their own genome and microbiome datasets, as long as they agree with the IMG/M data release policy and follow the metadata requirements for integrating data into IMG/ER.

Piece of work: Organism detailing.

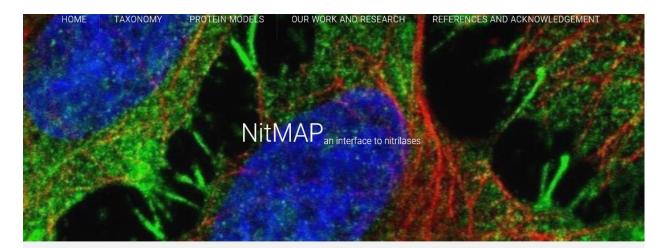
# CHAPTER 3

# **RESULTS AND DISCUSSION**

In the wake of experiencing all the previously mentioned convention we built up a database in namely NitMAP. NitMAP abbreviates for Nitrilase Mining And Prediction Database. A far reaching database has been created for mapping and characterizing some potential nitrilase sources, successions, structures and their scientific categorization Nitrilases have been generally recognized as critical other options to chemical catalysts, as they have been demonstrated to change a massive assortment of nitriles frequently delivered by mechanical procedures.

The content of the NitMAP database as follows :

# **3.1** Page 1: Introductory page for nitrilases describing pathway and the major generas of organisms producing nitrilases.



# INTRODUCTION TO NitMAP

NitMAP abrreviates for <u>Nit</u>rilase <u>Mining And Prediction Database</u>. A comprehensive database has been developed for mapping and defining some potential nitrilase sources, sequences, structures and their taxonomy. Chemical compounds containing cyano (- CN) functional groups are called nitriles. Nitrilases have been widely acknowledged as important alternatives to chemical catalysts, as they have been proved to transform an immense variety of nitriles often produced by industrial processes. They are synthesized naturally as well as xenobiotically. Nitrilases are nitrile-degrading enzymes and belong to nitrilase superfamily. They convert nitriles into corresponding carboxylic acids in a single step pathway.

### MECHANISM OF ACTION OF NITRILASE

Members of nitrile superfamily are present in both prokaryotes and eukaryotes and have characteristics  $\alpha\beta\beta\alpha$  fold.

Figure: 3.1.1 View of Home Page

```
<!DOCTYPE html>
<!--[if lt IE 8 ]><html class="ie ie7" lang="en"> <![endif]-->
<!--[if IE 8 ]><html class="ie ie8" lang="en"> <![endif]-->
<!--[if (gte IE 8)|!(IE)]><!--><html lang="en"> <!--<![endif]-->
<head>
  <!--- Basic Page Needs
  ---->
   <meta charset="utf-8">
   <title> Our work and Research</title>
  <meta name="description" content="">
  <meta name="author" content="">
  <!-- Mobile Specific Metas
 --->
   <meta name="viewport" content="width=device-width, initial-scale=1, maximum-scale=1">
  <!-- CSS
  <link rel="stylesheet" href="css/base.css">
  k rel="stylesheet" href="css/layout.css">
  <!--[if lt IE 9]>
      <script src="http://html5shim.googlecode.com/svn/trunk/html5.js"></script>
   <![endif]-->
  <!-- Favicons
   k rel="shortcut icon" href="favicon.ico">
</head>
<body class="narrow">
  <!-- Header
  -->
  <header id="top" class="static">
    </div>
```

<nav id="nav-wrap">

# Figure: 3.1.2 Code For Home Page 1

```
<a class="mobile-btn" href="#nav-wrap" title="Show navigation">Show navigation</a>
           <a class="mobile-btn" href="#" title="Hide navigation">Hide navigation</a>
          <a href="index.html">Home</a>
              <a href="Our work.html">Our Work and Research</a>
           </nav>
     </div>
</header> <!-- Header End -->
<!-- Post
 --->
<article class="post">
   <div class="row">
     <div class="col entry-header cf">
        <h1>Our work and research</h1>
<div class="post-meta">
          <span class="sep">/</span><a href="G:\Database\workflow.html">Workflow</a>
             <span class="sep">/</span><a href="G:\Database\Research.html">Ongoing Research</a>
          </div>
     </div>
     <div class="col post-image">
        <img src="images/Our work.jpg" alt="post-image" title="post-image"width="100%" height ="300">
     </div>
```

### Figure: 3.1.3 Code for referencing to other tab.

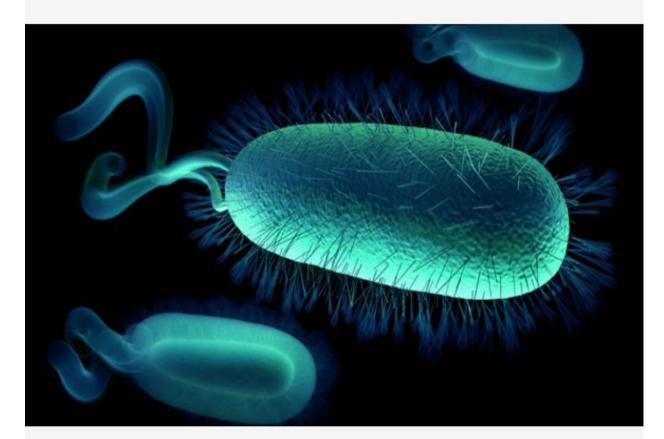
<div class="col post-content offset-2"> <h3>Till now we have achieved</h3> <br> Collection of the datasets for nitrile-degrading enzymes along with their microbial sources. Retrieval of protein sequences of microbial nitrilases. Protein modelling of nitrilase(s) using Swiss Model First with template --> template used by us: <a href="http://www.rcsb.org/pdb/explore.do?">http://www.rcsb.org/pdb/explore.do?</a> structureId=3WUY">Synechocystis sp.(PDB ID:3WUY)</a> >then without template (automated modelling to validate the modelling results by comparing the identity scores)</or> Start developing the database using the preffered languages (we have used HTML, CSS, JAVA and PHP).  $\langle ol \rangle \langle br \rangle$ <h6>We have provided the whole workflow of this study as well as the ongoing research for the same.(You can explore the links from the top of the page)</h6> </div> </body> </article> </html> </div> </body> </article>

</html>

### Figure: 3.1.3 Code Contd.

3.2 Page 2: Taxonomy which gives the overall hierarchical details of organisms.

# **Taxonomical studies**



The taxonomical studies reveal a great biological significance of the organism(s) which serves as a source of nitrilase.

(Click on the name of the organism to be redirected to the related taxonomical data)

Serial No.	Organism	Electron microscopic view

Figure:3.2.1 Images used in Web Pages.

```
<!DOCTYPE html>
<!--[if lt IE 8 ]><html class="ie ie7" lang="en"> <![endif]-->
<!--[if IE 8 ]><html class="ie ie8" lang="en"> <![endif]-->
<!--[if (gte IE 8)|!(IE)]><!--><html lang="en"> <!--<![endif]-->
<head>
  <!--- Basic Page Needs
  <meta charset="utf-8">
   <title> Taxonomy</title>
   <meta name="description" content="">
   <meta name="author" content="">
  <!-- Mobile Specific Metas
 --->
   <meta name="viewport" content="width=device-width, initial-scale=1, maximum-scale=1">
   <!-- CSS
   --->
  k rel="stylesheet" href="css/base.css">
   k rel="stylesheet" href="css/layout.css">
   <!--[if lt IE 9]>
      <script src="http://html5shim.googlecode.com/svn/trunk/html5.js"></script></script></script></script></script>
   <![endif]-->
  <!-- Favicons
   ----
   k rel="shortcut icon" href="favicon.ico">
</head>
<body class="narrow">
  <!-- Header
   -->
  <header id="top" class="static">
     </div>
          <nav id="nav-wrap">
```

# Figure: 3.2.2 Code For HTML Page

```
<a class="mobile-btn" href="#nav-wrap" title="Show navigation">Show navigation</a>
<a class="mobile-btn" href="#" title="Hide navigation">Hide navigation</a>
            <a href="index.html">HOME</a>
                class="active"><a href="Taxonomy.html">TAXONOMY</a>
            </nav>
       </div>
  </header> <!-- Header End -->
  <!-- Post
  --->
  <article class="post">
    <div class="row">
       <div class="col entry-header cf">
          <h1>Taxonomical studies </h1>
        </div>
 <div class="col post-image">
         <img src="<u>images/org.jpg</u>" alt="post-image" title="post-image"width="100%" height ="100">
       </div>
       <div class="col post-content offset-2">
<h4>The taxonomical studies reveal a great biological significance of the organism(s) which serves as a source of nitrilase.</h4> <br>
<caption align="top"><b>(Click on the name of the organism to be redirected to the related taxonomical data)</b>
           Serial No. Organism
              Electron microscopic view
```

# Figure: 3.2.3 Code for HTML Page

>		
<td th="" v<=""><th>idth="100" align=" center"&gt;1</th></td>	<th>idth="100" align=" center"&gt;1</th>	idth="100" align=" center">1
<td th="" v<=""><th><pre>idth="100"align="center"&gt;<a href="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=155978"><i>Acaryochloris marina</i> MBIC11017<!--/r--></a></pre></th></td>	<th><pre>idth="100"align="center"&gt;<a href="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=155978"><i>Acaryochloris marina</i> MBIC11017<!--/r--></a></pre></th>	<pre>idth="100"align="center"&gt;<a href="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=155978"><i>Acaryochloris marina</i> MBIC11017<!--/r--></a></pre>
<td th="" v<=""><th>/idth="100" align="center"&gt;<img alt="post-image" height="10%" src="&lt;u&gt;images/Acaryochloris marina.jpg&lt;/u&gt;" title="post-image" width="50%"/></th></td>	<th>/idth="100" align="center"&gt;<img alt="post-image" height="10%" src="&lt;u&gt;images/Acaryochloris marina.jpg&lt;/u&gt;" title="post-image" width="50%"/></th>	/idth="100" align="center"> <img alt="post-image" height="10%" src="&lt;u&gt;images/Acaryochloris marina.jpg&lt;/u&gt;" title="post-image" width="50%"/>
<td td="" v<=""><td>ridth="100" align=" center"&gt;2</td></td>	<td>ridth="100" align=" center"&gt;2</td>	ridth="100" align=" center">2
	idth="100"align="center"×a href ="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=634457"×i>Acetobacter pasteurianus IFO 3283-32<	
	<pre>idth="100" align="center"&gt;<img alt="post-image" height="10%" src="images/Acetobacter pasteurianus.jpg" title="post-image" width="50%"/> </pre>	
	idth="100" align=" center">3	
	idth="100"align="center"> <a href="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=762376"><i>Ahromobacter xylosoxidans</i> A8</a>	
<td td="" v<=""><td><pre>idth="100" align="center"&gt;<img alt="post-image" height="10%" src="&lt;u&gt;images/Achromobacter xylosoxidans1.jpg&lt;/u&gt;" title="post-image" width="50%"/> </pre></td></td>	<td><pre>idth="100" align="center"&gt;<img alt="post-image" height="10%" src="&lt;u&gt;images/Achromobacter xylosoxidans1.jpg&lt;/u&gt;" title="post-image" width="50%"/> </pre></td>	<pre>idth="100" align="center"&gt;<img alt="post-image" height="10%" src="&lt;u&gt;images/Achromobacter xylosoxidans1.jpg&lt;/u&gt;" title="post-image" width="50%"/> </pre>
	<pre>idth="100" align=" center"&gt;4</pre>	
	<pre>inter=""""""""""""""""""""""""""""""""""""</pre>	
	idth="100" align="center">img src="imges/22.ipg" alt="post-imges" title="cost-imges" idth="50%" height ="10%"> //td>	
	ancie too arrele view are a mobeliner 188 are host twole crite host twole wrether and views	
<td td="" v<=""><td>ridth="100" align=" center"&gt;5</td></td>	<td>ridth="100" align=" center"&gt;5</td>	ridth="100" align=" center">5
	idth="100"align="center"> <a href="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=351607"><i>Acidothermus cellulolyticus </i></a>	
	idth="100" align="center"> <img alt="post-image" height="10%" src="images/Acidothermus cellulolyticus 118.jpg" title="post-image" width="50%"/>	
>		
<td td="" v<=""><td>ridth="100" align=" center"&gt;6</td></td>	<td>ridth="100" align=" center"&gt;6</td>	ridth="100" align=" center">6
	<pre>idth="100"align="center"&gt;<a href="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=905"><i>Acidaminococcus fermentans </i>VR4</a></pre>	
	idth="100" align="center"> <img alt="post-image" height="10%" src="images/Acidaminococcus fermentans vr4.jpg" title="post-image" width="50%"/>	
>		
<td td="" v<=""><td>ridth="100" align=" center"&gt;7</td></td>	<td>ridth="100" align=" center"&gt;7</td>	ridth="100" align=" center">7
	<pre>idth="100"align="center"&gt;<a hef="https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi?id=930169"><i>Alcanivorax dieselolei</i> B5</a></pre>	
	idth="100" align="center"> <img alt="post-image" height="10%" src="images/Alcanivorax dieselolei 85.jpg" title="post-image" width="50%"/>	

# Figure: 3.2.4 Code contd. For HTML Page

**3.3.** Page 3: Information regarding protein models from their amino acid sequence of each organism, sequence identity, displays the modelled cartoon structures attached to their Swiss model reports.

including Amino acid Sequence and the protein models.				
338aa				
Serial no.	Name	Amino acid	Cartoon	Sequence
		Sequence	structure	identity%
				(reports
				attached)
			A CONTRACTOR	
1	Acaryochloris marina	a 332aa		80.77
	MBIC11017			
2	Acetobacter	324aa		68.09
	<i>pasteurianus</i> IFO			
	3283-32			
3	Achromobacter	319aa		31.41
	xylosoxidans			

Figure: 3.3.1 Protein Model Info from aa sequence.

36	<i>Desulfomonile tiedjei</i> DCB1	342aa	35.34	
37	<i>Halanaerobium</i> praevalens DSM 2228	318aa	35.34	
38	<i>Hyphomicrobium</i> sp. MC1	327aa	35.34	
39	<i>Saccharomonospora</i> <i>viridis</i> DSM 43017	331aa	35.34	
40	Runella slithyformis	310aa	35.64	

# Figure: 3.3.2 Protein Model Info from aa sequence contd. .

```
<!DOCTYPE html>
<!--[if lt IE 8 ]><html class="ie ie7" lang="en"> <![endif]-->
<!--[if IE 8 ]><html class="ie ie8" lang="en"> <![endif]-->
<!--[if (gte IE 8)|!(IE)]><!--><html lang="en"> <!--<![endif]-->
<head>
  <!--- Basic Page Needs
  --->
   <meta charset="utf-8">
   <title> models</title>
   <meta name="description" content="">
   <meta name="author" content="">
  <!-- Mobile Specific Metas
 <meta name="viewport" content="width=device-width, initial-scale=1, maximum-scale=1">
  <!-- CSS
  --->
  <link rel="stylesheet" href="css/base.css">
   <link rel="stylesheet" href="css/layout.css">
   <!--[if lt IE 9]>
      <script src="http://html5shim.googlecode.com/svn/trunk/html5.js"></script></script></script>
   <![endif]-->
  <!-- Favicons
   --->
   <link rel="shortcut icon" href="favicon.ico">
</head>
<body class="narrow">
  <!-- Header
  --->
  <header id="top" class="static">
     </div>
```

<nav id="nav-wrap">

# Figure: 3.3.3 Code for CSS.

```
<h4> Further are the results of the whole protocol followed including amino acid sequence and the protein models. </h4>
>
              Serial no.width="200" align="left"> Namewidth="200" align="left"> Amino acid Sequence

              Cartoon structure 

              Sequence identity% (reports attached)
         >
             </d width="100" align=" center">1
</d width="100"align="center">1
</d width="100"align="center"><i>Acaryochloris marina </i>MBIC11017
</d width="100" align="center"><a href ="images\Acaryochloris marina.fasta">332aa 
</d>
</d>

             <img src="images\prot1 Acaryochloris marina 2017-06-13.png" alt="post-image" title="post-i

              <a href="images\prot1_Acaryochloris_marina_2017-06-13.html"> 80.77
         >
             2 
             <i>Acetobacter pasteurianus</i> IFO 3283-32
             <a href ="images\Acetobacter pasteurianus.fasta">324aa 

             <img src="images\prot2_Acetobacter pasteurianusIF0_328332_2017-06-13.png" alt="post-image"
="20%"> 

              <a href="images\prot2_Acetobacter_pasteurianusIF0_328332_2017-06-13.html"> 68.09
             >
             3 
             <i>Achromobacter xylosoxidans</i>

<i>Achromobacter xylosoxidans</i>

<i>Achromobacter xylosoxidans

             <img src="images\prot3_Achromobacter_xylosoxidans_2017-06-13.png" alt="post-image" title="</pre>
```

# Figure: 3.3.4 Code for CSS.

**3.4.** Page 4: Details about the research and protocol carried out for designing the database.



# Till now we have achieved

- 1. Collection of the datasets for nitrile-degrading enzymes along with their microbial sources.
- 2. Retrieval of protein sequences of microbial nitrilases.
- 3. Protein modelling of nitrilase(s) using Swiss Model
  - 1. First with template --> template used by us: Synechocystis sp.(PDB ID:3WUY)
  - 2. Then without template (automated modelling to validate the modelling results by comparing the identity scores)

# Figure: 3.4.1 Protocol For Db Design.

```
<!DOCTYPE html>
<!--[if lt IE 8 ]><html class="ie ie7" lang="en"> <![endif]-->
<!--[if IE 8 ]><html class="ie ie8" lang="en"> <![endif]-->
<!--[if (gte IE 8)|!(IE)]><!--><html lang="en"> <!--<![endif]-->
<head>
       <!--- Basic Page Needs
        <meta charset="utf-8">
         <title> Our work and Research</title>
         <meta name="description" content="">
          <meta name="author" content="">
       <!-- Mobile Specific Metas
     <meta name="viewport" content="width=device-width, initial-scale=1, maximum-scale=1">
         <!-- CSS
         --->
       <link rel="stylesheet" href="css/base.css">
         k rel="stylesheet" href="css/layout.css">
         <!--[if lt IE 9]>
                     <script src="http://html5shim.googlecode.com/svn/trunk/html5.js"></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></script></scr
          <![endif]-->
       <!-- Favicons
          <link rel="shortcut icon" href="favicon.ico">
</head>
<body class="narrow">
       <!-- Header
        <header id="top" class="static">
              </div>
                              <nav id="nav-wrap">
```

# Figure: 3.4.2Code for CSS.

```
<a class="mobile-btn" href="#nav-wrap" title="Show navigation">Show navigation</a>
           <a class="mobile-btn" href="#" title="Hide navigation">Hide navigation</a>
          <a href="index.html">Home</a>
              <a href="Our work.html">Our Work and Research</a>
           </nav>
     </div>
</header> <!-- Header End -->
<!-- Post
<article class="post">
   <div class="row">
     <div class="col entry-header cf">
        <h1>Our work and research</h1>
<div class="post-meta">
          <span class="sep">/</span><a href="G:\Database\workflow.html">Workflow</a>
             <span class="sep">/</span><a href="G:\Database\Research.html">Ongoing Research</a>
          </div>
     </div>
     <div class="col post-image">
        <img src="images/Our work.jpg" alt="post-image" title="post-image"width="100%" height ="300">
     </div>
```

# Figure: 3.4.3 Code contd. for CSS.

The two additional pages display the

 $\Rightarrow$  Workflow: The sequential display of the steps followed.

# Workflow opted for studying nitrilases

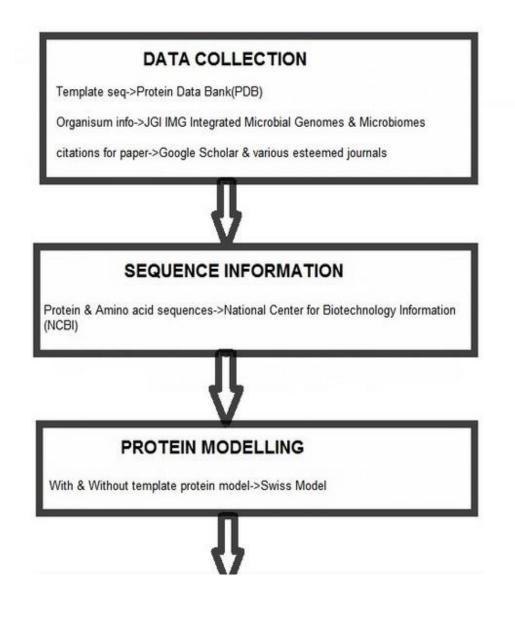


Figure: 3.4.4 Image showing the Work Flow

 $\Rightarrow$  Ongoing research: Till date all the information pertaining to nitrilases from various organisms has been collected and deposited.

```
<!DOCTYPE html>
<!--[if lt IE 8 ]><html class="ie ie7" lang="en"> <![endif]-->
<!--[if IE 8 ]><html class="ie ie8" lang="en"> <![endif]-->
<!--[if (gte IE 8)|!(IE)]><!--><html lang="en"> <!--<![endif]-->
<head>
  <!--- Basic Page Needs
  --->
   <meta charset="utf-8">
   <title>Workflow</title>
   <meta name="description" content="">
   <meta name="author" content="">
  <!-- Mobile Specific Metas
 <meta name="viewport" content="width=device-width, initial-scale=1, maximum-scale=1">
   <!-- CSS
  --->
  k rel="stylesheet" href="css/base.css">
   k rel="stylesheet" href="css/layout.css">
   <!--[if lt IE 9]>
      <script src="http://html5shim.googlecode.com/svn/trunk/html5.js"></script></script></script>
   <![endif]-->
  <!-- Favicons
   --->
   k rel="shortcut icon" href="favicon.ico">
</head>
<body class="narrow">
  <!-- Header
  --->
  <header id="top" class="static">
    </div>
```

Figure: 3.4.5 Code for CSS.

<nav id="nav-wrap">

## 3.5 Page 5: References and acknowledgements:

# **Our data referred following articles**Mining of Microbial Genomes for the Novel Sources of Nitrilases (Sharma N, Thakur N, Raj T, Savitri, Bhalla TC , 2017). Nitrilases - An attractive nitrile degrading biocatalyst (Agarwal A, Nigam V K and Vidyarthi A S, 2012). Nitrilase and its application as a 'Green' catalyst (Singh R, Sharma R, Tewari N, Geetanjali, Rawat D S, 2006). Nitrilase II. Substrate specificity and possible mode of action (Mahadevan S, Thimann K V, 1964). Nitrilase enzymes and their role in plant-microbe interactions (Howden A J M and Preston G M, 2009). The nitrilase superfamily: classification, structure and function (Pace H C and Brenner C, 2001).

# ACKNOWLEDGEMENTS

We have put enough efforts in concieving and designing NitMAP database. However, it would not have been possible without the kind support and help of many individuals. We would like to extend our sincere thanks to all of them.

# Figure: 3.5.1 References

In future the following improvements/changes are proposed

• To add more and latest information pertaining to sequence, structure and some important physiochemical properties.

• To add the created database on the University website and also in public domain for wider acceptability of nitrilases.

# CHAPTER 5

- Nitrilases An attractive nitrile degrading biocatalyst (Agarwal A, Nigam V K and Vidyarthi A S).
- 2. Nitrilase and its application as a 'Green' catalyst (Singh R, Sharma R, Tewari N, Geetanjali, Rawat D S).
- **3.** Nitrilase: II. Substrate specificity and possible mode of action (Mahadevan S, Thimann K V).
- **4.** Nitrilase enzymes and their role in plant–microbe interactions (Howden A J M and Preston G M).
- **5.** The nitrilase superfamily: classification, structure and function (Pace H C and Brenner C).