# Sample application: SimplePDBBrowser

**Overview of the application**

SimplePDBBrowser will be a relatively simple gateway to access Protein Data Bank data. It will allow to search by codes, and for textual data included in PDB headers like, description, techniques used, resolution, source or author. Results of the search will give basic information about the PDB entry and link to the appropriate web pages in the main PDB web site.

**Input data.** *Nature and origin (user input, replicated database, calculation results, etc.). Input validation if necessary. User control, etc.*

User input: User should fill a web form including either a PDB id or some information. Fields available would be:

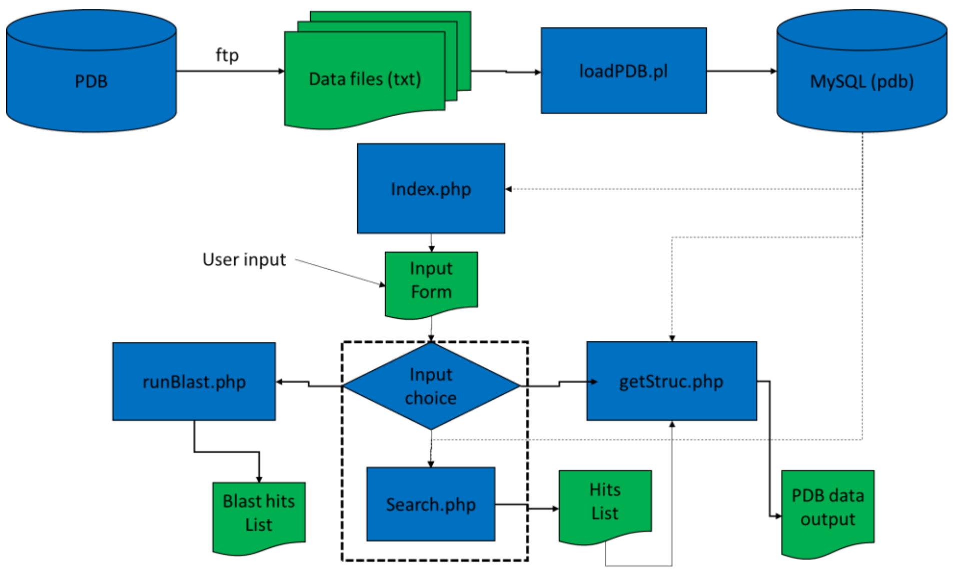
- PDB code (4 letter code). Will direct to a single entry if available
- Search Fields
    - Description, headers, authors, source (text search)
    - Resolution (numeric input)
    - Technique used (selection of possibles, X Ray, NMR, etc)
    - Type of molecule (selection of protein, nucleic acid, complex)
    - Year of submission (numeric input)
- Sequence search: PDB entries will be obtained through a Standard Blast search. Sequence can be provided as text or uploaded file

Data input: Data will be obtained off-line by parsing the index files provided at Protein Data Bank Ftp (/derived_data), and stored in the a database with the appropriate structure.

**Output.** *Data, way of presentation (web/email).*

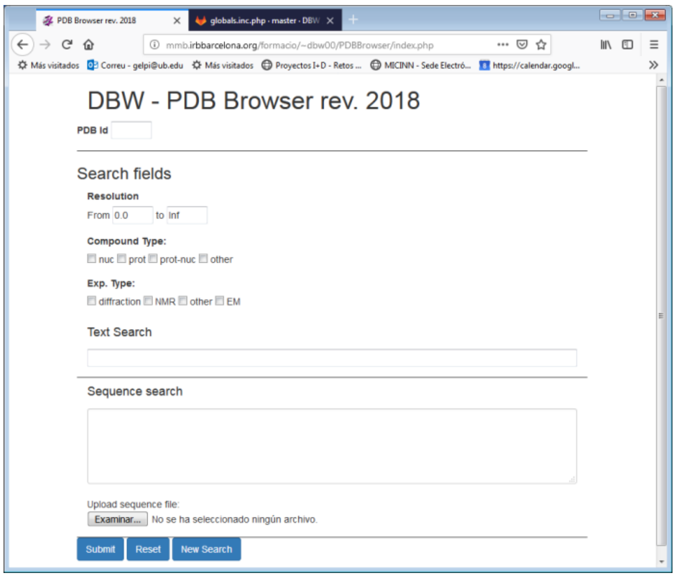
Search/blast search outputs: Output of a search would be a list of the found hits, showing a limited amount of information just to identify the hit: PDB Id, entry description, type of molecule, source. List items will have links to entries data.

Entry data: Complete information available about the entry, links to the PDB main site, and to other related sites with structural information.



**globals.inc.php**
(to be included by any .php script)

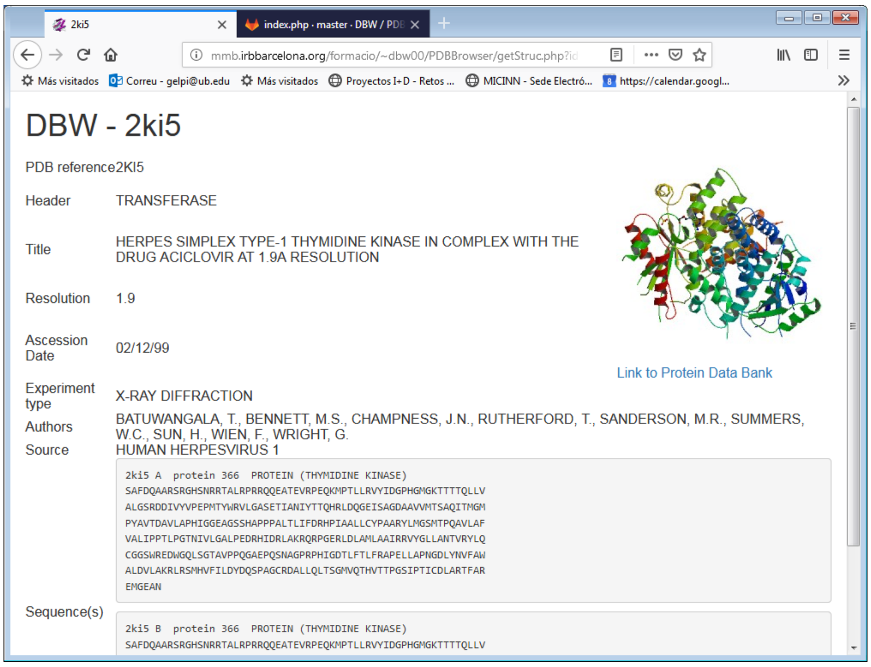
```php
<?php

/*
 * globals.inc.php
 * Global variables and settings
 */
// Base directories
// Automatic, taken from CGI variables.
$baseDir = dirname($_SERVER['SCRIPT_FILENAME']);
#$baseDir = '/home/dbw00/public_html/PDBBrowser';
$baseURL = dirname($_SERVER['SCRIPT_NAME']);

// Temporal dir, create if not exists, however Web server
// may not have the appropriate permission to do so
$tmpDir = "$baseDir/tmp";
if (!file_exists($tmpDir)) {
    mkdir($tmpDir);
}
// Blast details, change to adapt to local settings
// Blast databases should be created using the appropriate programs.
$blastHome = "$baseDir/../../blast";
$blastDbsDir = "$blastHome/DBS";
$blastExe = "$blastHome/bin/blastp";
$blastDbs = array("SwissProt" => "sprot", "PDB" => "pdb");
$blastCmdLine = "$blastExe -db $blastDbsDir/" . $blastDbs['PDB'] . " -evalue 0.001 -max_target_seqs 100 -outfmt \"6 sseqid
stitle evalue\"";

// Include directory
$incDir = "$baseDir/include";

// Load accessory routines
include_once "$incDir/bdconn.inc.php";
include_once "$incDir/libDBW.inc.php";

// Load predefined arrays
// Fulltext search fields
$textFields = Array('e.header', 'e.compound', 'a.author', 's.source', 'sq.header');

// Compounds
$rs = mysqli_query($mysqli, "SELECT * from comptype") or print mysql_error();
while ($rsF = mysqli_fetch_array($rs)) {
    $compTypeArray[$rsF['idCompType']] = $rsF['type'];
}

//expTypes
$rs = mysqli_query($mysqli,"SELECT * from expType") or print mysql_error();
while ($rsF = mysqli_fetch_array($rs)) {
    $expTypeArray[$rsF['idExpType']] = $rsF;
}
//expClasses
$rs = mysqli_query($mysqli,"SELECT * from expClasse") or print mysql_error();
while ($rsF = mysqli_fetch_array($rs)) {
    $expClasseArray[$rsF['idExpClasse']] = $rsF['expClasse'];
}
// Start session to store queries
session_start();
```



**index.php**

Main entry for the application. Uses default values from $_SESSION to reload pass choices

```
<?php
/*
 *  index.php, main form
 */
# Loading global variables and DB connection
include "globals.inc.php";
//
// $_SESSION['queryData'] array holds data from previous forms,
// if empty it should be initialized to avoid warnings, and set defaults
// also a ...?new=1 allows to clean it from the URL.
//
if (isset($_REQUEST['new']) or !isset($_SESSION['queryData'])) {
    $_SESSION['queryData'] = [
        'minRes' => '0.0',
        'maxRes' => 'Inf',
        'query' => ''
    ];
}
print headerDBW("PDB Browser rev. 2018");
#Main Form follows
?>
<form name="MainForm" action="search.php" method="POST" enctype="multipart/form-data">
    <div class="row" style="border-bottom: solid 1px">
        <div class="form-group">
            <label><b>PDB Id</b></label>
            <input type="text" name="idCode" value="<?php print $_SESSION['queryData']['idCode']?>" size="5" maxlength="4"/>
        </div>
    </div>
    <div class="row">
        <h3>Search fields</h3>
    </div>
    <div class="row">
        <div class="col-md-4">
            <div class="form-group">
                <label>Resolution</label>
                <p>  From <input type="text" name="minRes" value="<?php print $_SESSION['queryData']['minRes'] ?>" size="5">
                    to <input type="text" name="maxRes" value="<?php print $_SESSION['queryData']['maxRes'] ?>" size="5" >
                </p>
            </div>
        </div>
    </div>
    <div class="row">
        <div class="col-md-4">
            <div class="form-group">
                <label>Compound Type:</label>
                <div class="form-check">
                    <?php
                    /*
                     * input options from $compTypeArray[] array
                     */
                    foreach (array_keys($compTypeArray) as $idCompType ) {?>
                        <input class="form-check-input" type="checkbox"
                               name="idCompType[<?php print $idCompType ?>]" />  <?php print $compTypeArray[$idCompType]."\n" ?>
                    <?php } ?>
                </div>
            </div>
        </div>
    </div>
    <div class="row">
        <div class="col-md-4">
            <div class="form-group">
                <label>Exp. Type:</label>
                <div class="form-check">
                    <?php
                    /*
                     * input options from $expClasseArray
                     */
                    foreach (array_keys($expClasseArray) as $idExpClasse) { ?>
                        <input class="form-check-input" type="checkbox" name="idExpClasse[<?php print $rsF['idExpClasse'] ?>]" />
<?php print $expClasseArray[$idExpClasse] . "\n" ?>
                    <?php } ?>
                </div>
            </div>
        </div>
    </div>
    <div class="row" style="border-bottom: 1px solid">
        <div class="col-md-6">
            <label><h4> Text Search</h4></label>
            <div class="form-group">
                <input type="text" name="query" value="<?php print $_SESSION['queryData']['query'] ?>" style="width:100%" />
            </div>
        </div>
    </div>
    <div class="row" style="border-bottom: 1px solid">
        <div class="col-md-6">
            <label><h4>Sequence search</h4></label>
            <div class="form-group">
                <textarea class="form-control" name="seqQuery" rows="4" cols="60" style="width:100%"></textarea><br>
                Upload sequence file: <input type="file" name="seqFile" value="" width="50" style="width:100%"/>
            </div>
        </div>
    </div>
    <div class="row">
        <p>
    <button type='submit' class="btn btn-primary">Submit</button>
    <button type='reset' class="btn btn-primary">Reset</button>
    <button class="btn btn-primary" onclick="window.location.href='index.php=?new=1">New Search</button>
    </p>
    </div>
</form>
<?php
print footerDBW();
```


2ki5
index.php · master · DBW / PDE
mmb.irbbarcelona.org/formacio/~dbw00/PDBBrowser/getStruc.php?ic
Más visitados
Correu - gelpi@ub.edu
Más visitados
Proyectos I+D - Retos ...
MICINN - Sede Electró...
https://calendar.googl...

DBW - 2ki5

| | | |
|---|---|---|
| PDB reference | 2KI5 | Link to Protein Data Bank |
| Header | TRANSFERASE | |
| Title | HERPES SIMPLEX TYPE-1 THYMIDINE KINASE IN COMPLEX WITH THE DRUG ACICLOVIR AT 1.9A RESOLUTION | |
| Resolution | 1.9 | |
| Accession Date | 02/12/99 | |
| Experiment type | X-RAY DIFFRACTION | |
| Authors | BATUWANGALA, T., BENNETT, M.S., CHAMPNESS, J.N., RUTHERFORD, T., SANDERSON, M.R., SUMMERS, W.C., SUN, H., WIEN, F., WRIGHT, G. | |
| Source | HUMAN HERPESVIRUS 1 | |
| Sequence(s) | (see below) | |

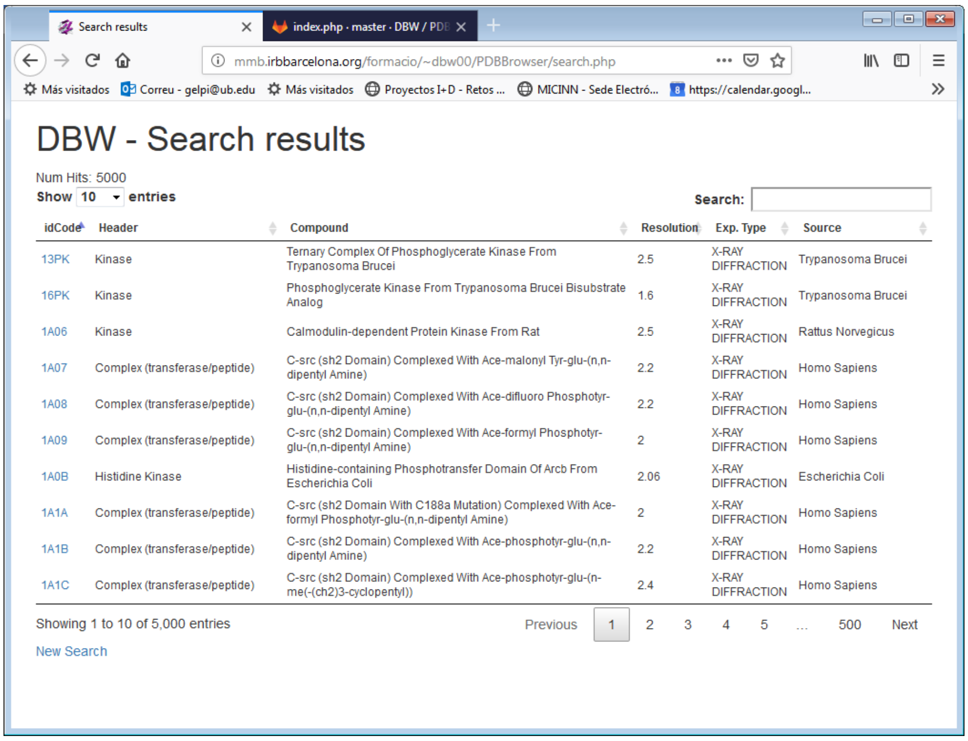
```
2ki5 A  protein 366  PROTEIN (THYMIDINE KINASE)
SAFDQAARSRGHSNRRTALRPRRQQEATEVRPEQKMPTLLRVYIDGPHGMGKTTTTQLLV
ALGSRDDIVYVPEPMTYWRVLGASETIANIYTTQHRLDQGEISAGDAAVVMTSAQITMGM
PYAVTDAVLAPHIGGEAGSSHAPPPALTLIFDRHPIAALLCYPAARYLMGSMTPQAVLAF
VALIPPTLPGTNIVLGALPEDRHIDRLAKRQRPGERLDLAMLAAIRRVYGLLANTVRYLQ
CGGSWREDWGQLSGTAVPPQGAEPQSNAGPRPHIGDTLFTLFRAPELLAPNGDLYNVFAW
ALDVLAKRLRSMHVFILDYDQSPAGCRDALLQLTSGMVQTHVTTPGSIPTICDLARTFAR
EMGEAN
```

```
2ki5 B  protein 366  PROTEIN (THYMIDINE KINASE)
SAFDQAARSRGHSNRRTALRPRRQQEATEVRPEQKMPTLLRVYIDGPHGMGKTTTTQLLV
```

**getStruc.php**
Output view for PDB data (parameters passed using GET)

```
<?php
/*
 * getStruc.php Shows data for a PDB entry
 */
// load global vars and includes
include "globals.inc.php";
//get data for the structure requested
$sql = "SELECT e.* from entry e where e.idCode='" . $_REQUEST['idCode'] . "'";
$rs = mysqli_query($mysqli, $sql) or print mysqli_error($mysqli);
if (!mysqli_num_rows($rs)) { //search is empty
   print errorPage('Not Found', 'The requested structure is not available');
} else {
   $data = mysqli_fetch_assoc($rs);
   print headerDBW($_REQUEST['idCode']);
   ?>
   <table border="0" cellspacing="2" cellpadding="4">
      <tbody>
         <tr>
            <td>PDB reference</td>
            <td><?php print $data['idCode'] ?></td>
            <td rowspan="5">
               <a href="http://www.pdb.org/pdb/explore.do?structureId=<?php print $data['idCode'] ?>">
                  <img src="http://www.pdb.org/pdb/images/<?php print strtolower($data['idCode']) ?>_bio_r_250.jpg" border="0"
width="250" height="250"><br>
                  Link to Protein Data Bank</a>
            </td>
         </tr>
         <tr>
            <td>Header</td>
            <td><?php print $data['header'] ?></td>
         </tr>
         <tr>
            <td>Title</td>
            <td><?php print $data['compound'] ?></td>
         </tr>
         <tr>
            <td>Resolution</td>
            <td>
```

```
                <?php
                if ($data['resolution']) {
                    print $data['resolution'];
                } else {
                    print "N.D.";
                }
                ?>
            </td>
        </tr>
        <tr>
            <td>Ascession Date</td>
            <td><?php print $data['ascessionDate'] ?></td>
        </tr>
        <tr>
            <?php // $expTypeArray is generated in globals.inc.php?>
            <td>Experiment type</td>
            <td colspan="2"><?php print $expTypeArray[$data['idExpType']]['ExpType'] ?></td>
        </tr>
        <tr>
            <td>Authors</td>
            <td colspan="2">
                <?php
                // new DB query to get authors
                $rsA = mysqli_query($mysqli, "SELECT * from author a, author_has_entry ae where ae.idCode='" . $data['idCode'] . "'
and a.idAuthor = ae.idAuthor order by a.author") or print mysqli_error($mysqli);
                if (mysqli_num_rows($rsA)) {
                    $auts = array();
                    while ($rsAF = mysqli_fetch_assoc($rsA))
                        $auts[] = $rsAF['author'];
                    print join(", ", $auts);
                }
                ?>
            </td>
        </tr>
        <tr>
            <td>Source</td>
            <td colspan="2">
                <?php
                // new DB query to get sources
                $rsA = mysqli_query($mysqli, "SELECT * from source s, entry_has_source es where es.idCode='" . $data['idCode'] . "'
and s.idSource = es.idSource order by s.source") or print mysql_error($mysqli);
                if (mysqli_num_rows($rsA)) {
                    $sources = array();
                    while ($rsAF = mysqli_fetch_assoc($rsA))
                        $sources[] = $rsAF['source'];
                    print join(", ", $sources);
                }
                ?>
            </td>
        </tr>
        <tr>
            <td>Sequence(s)</td>
            <td colspan="2">
                <?php
                // new DB query to get sequences, output in FASTA format
                $rsA = mysqli_query($mysqli, "SELECT * from sequence s where s.idCode='" . $data['idCode'] . "' order by s.chain")
                        or print mysqli_error($mysqli);
                if (mysqli_num_rows($rsA)) {
                    while ($sq = mysqli_fetch_assoc($rsA)) {
                        print "<pre>" . $sq['header'] . "\n" . preg_replace("/(.{60})/", "$1\n", $sq['sequence']) . "</pre>";
                    }
                }
                ?>
            </td>
          </tr>
        </tbody>
    </table>
    <?php
    print footerDBW();
}
```


Search results
index.php · master · DBW / PDB
mmb.irbbarcelona.org/formacio/~dbw00/PDBBrowser/search.php
Más visitados
Correu - gelpi@ub.edu
Más visitados
Proyectos I+D - Retos ...
MICINN - Sede Electró...
https://calendar.googl...

## DBW - Search results

Num Hits: 5000

Show 10 entries

Search:

| idCode | Header | Compound | Resolution | Exp. Type | Source |
|---|---|---|---|---|---|
| 13PK | Kinase | Ternary Complex Of Phosphoglycerate Kinase From Trypanosoma Brucei | 2.5 | X-RAY DIFFRACTION | Trypanosoma Brucei |
| 16PK | Kinase | Phosphoglycerate Kinase From Trypanosoma Brucei Bisubstrate Analog | 1.6 | X-RAY DIFFRACTION | Trypanosoma Brucei |
| 1A06 | Kinase | Calmodulin-dependent Protein Kinase From Rat | 2.5 | X-RAY DIFFRACTION | Rattus Norvegicus |
| 1A07 | Complex (transferase/peptide) | C-src (sh2 Domain) Complexed With Ace-malonyl Tyr-glu-(n,n-dipentyl Amine) | 2.2 | X-RAY DIFFRACTION | Homo Sapiens |
| 1A08 | Complex (transferase/peptide) | C-src (sh2 Domain) Complexed With Ace-difluoro Phosphotyr-glu-(n,n-dipentyl Amine) | 2.2 | X-RAY DIFFRACTION | Homo Sapiens |
| 1A09 | Complex (transferase/peptide) | C-src (sh2 Domain) Complexed With Ace-formyl Phosphotyr-glu-(n,n-dipentyl Amine) | 2 | X-RAY DIFFRACTION | Homo Sapiens |
| 1A0B | Histidine Kinase | Histidine-containing Phosphotransfer Domain Of Arcb From Escherichia Coli | 2.06 | X-RAY DIFFRACTION | Escherichia Coli |
| 1A1A | Complex (transferase/peptide) | C-src (sh2 Domain With C188a Mutation) Complexed With Ace-formyl Phosphotyr-glu-(n,n-dipentyl Amine) | 2 | X-RAY DIFFRACTION | Homo Sapiens |
| 1A1B | Complex (transferase/peptide) | C-src (sh2 Domain) Complexed With Ace-phosphotyr-glu-(n,n-dipentyl Amine) | 2.2 | X-RAY DIFFRACTION | Homo Sapiens |
| 1A1C | Complex (transferase/peptide) | C-src (sh2 Domain) Complexed With Ace-phosphotyr-glu-(n-me(-(ch2)3-cyclopentyl)) | 2.4 | X-RAY DIFFRACTION | Homo Sapiens |

Showing 1 to 10 of 5,000 entries

Previous 1 2 3 4 5 … 500 Next

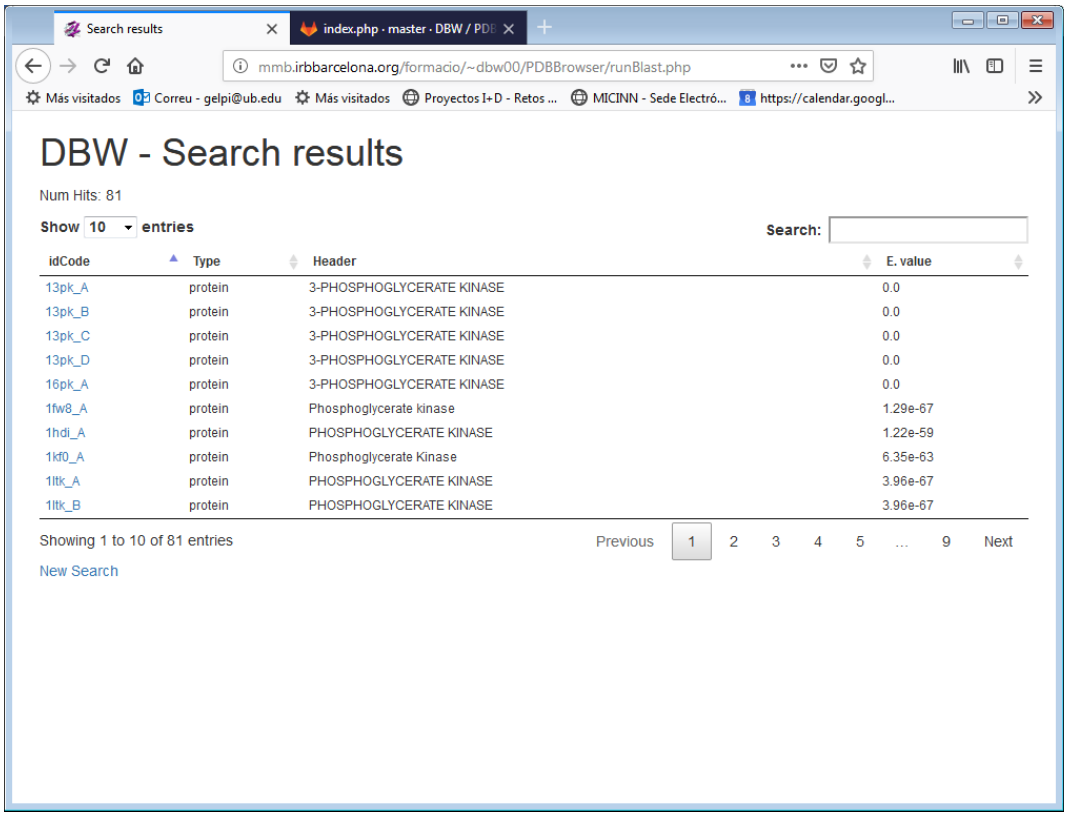
New Search

**search.php**

Search script, includes initial selection of operations

```
<?php
// load global vars and includes
include "globals.inc.php";
// Store input data in $_SESSION to reload initial form if necessary
$_SESSION['queryData'] = $_REQUEST;
// Selection of action to do
// 1. IdCode -> Results page
// 2. Sequence input -> runBlast
// 3. Other -> search on DB
//
// 1. Redirection to the requested entry if code selected
if ($_REQUEST['idCode']) {
   header('Location: getStruc.php?idCode=' . $_REQUEST['idCode']);
   // 2. Sequence input. If uploaded file, this takes preference
} elseif ($_FILES['seqFile']['name'] or $_REQUEST['seqQuery']) {
   if (($_FILES['seqFile']['tmp_name'])) {
      $_SESSION['queryData']['seqQuery'] = file_get_contents($_FILES['seqFile']['tmp_name']);
   }
   // Redirect to Blast if sequence, data is already stored in $_SESSION
   header('Location: runBlast.php');
} else {
   //  3. normal search, Bluiding SQL SELECT from the input form
   //     $ANDConds will contain all SQL conditions found in the form
   $ANDconds = ["True"]; // required to fulfill SQL syntax if form is empty
   //  Resolution, we consider only cases where user has input something
   if (($_REQUEST['minRes'] != '0.0') or ( $_REQUEST['maxRes'] != 'Inf')) {
      if ($_REQUEST['minRes'] != '0.0') {
         $ANDconds[] = "e.resolution >= " . $_REQUEST['minRes'];
      }
      if ($_REQUEST['maxRes'] != 'Inf') {
         $ANDconds[] = "e.resolution <= " . $_REQUEST['maxRes'];
```

```
        }
    }
    //    Compound type $ORconds holds options selected
    if (isset($_REQUEST['idCompType'])) { //should be isset as idCompType come from checkboxes
        $ORconds = [];
        foreach (array_keys($_REQUEST['idCompType']) as $k) {
            $ORconds[] = " e.idCompType = " . $k;
        }
        $ANDconds[] = "(" . join(" OR ", $ORconds) . ")";
    }
    //    Classe of experiment
    if (isset($_REQUEST['idExpClasse'])) {//should be isset as idExpClasse come from checkboxes
        $ORconds = [];
        foreach (array_keys($_REQUEST['idExpClasse']) as $k) {
            $ORconds[] = " et.idExpClasse = " . $k;
        }
        $ANDconds[] = "(" . join(" OR ", $ORconds) . ")";
    }
    //   text query, adapted to use fulltext indexes, $textFields is defined in globals.inc.php and
    // lists all text fields to be searched in.
    if ($_REQUEST['query']) {
        $ORconds = [];
        foreach (array_values($textFields) as $field) {
            $ORconds[] = "MATCH (" . $field . ") AGAINST ('" . $_REQUEST['query'] . "' "
                    . "IN BOOLEAN MODE)";
        }
        $ANDconds[] = "(" . join(" OR ", $ORconds) . ")";
    }
    //   text query without fulltext indexes
    //   if ($_REQUEST['query']){
    //       foreach (split (' ',$_REQUEST['query']) as $wd) {
    //           $ANDconds=array();
    //           foreach (array_values($textFields) as $field) {
    //               $ORconds[] = $field." like '%".$wd."%'";
    //           }
    //           $ANDconds[] = "(".join (" OR ", $ORconds).")";
    //       }
    //   }
    //   main SQL string, make sure that all tables are joint, and relationships included
    // SELECT columns FROM tables WHERE Conditions_from_relationships AND Conditions_from_query_Form
    $sql = "SELECT distinct e.idCode,e.header,e.compound,e.resolution,s.source,et.expType FROM
        expType et, author_has_entry ae, author a, source s, entry_has_source es, entry e, sequence sq WHERE
        e.idExpType=et.idExpType AND
        ae.idCode=e.idCode and ae.idAuthor=a.idAuthor AND
        es.idCode=e.idCode and es.idsource=s.idSource AND
        e.idCode = sq.idCode AND
        " . join(" AND ", $ANDconds);
//   Ordering will be done by the DataTable element using JQuery, if not available can also be done from the SQL
//   switch ($order) {
//       case 'idCode':
//       case 'header':
//       case 'compound':
//       case 'resolution':
//           $sql .= " ORDER BY e." . $order;
//           break;
//       case 'source':
//           $sql .= " ORDER BY s.source";
//           break;
//       case 'expType':
//           $sql .= " ORDER BY et.expType";
//           break;
//   }
    if (!isset($_REQUEST['nolimit'])) {
        $sql .= " LIMIT 5000"; // Just to avoid too long listings when testing
    }
#DEBUG
 print "<p>$sql</p>";
    //     DB query
    $rs = mysqli_query($mysqli,$sql) or print mysqli_error($mysqli);
    //     We check whether there are results to show
    if (!mysqli_num_rows($rs)) {
        print errorPage("Not Found", "No results found.");
    } else {
        //       Results table formated with DataTable
        print headerDBW("Search results");
        print "Num Hits: " . mysqli_num_rows($rs);
        ?>
        <table border="0" cellspacing="2" cellpadding="4" id="dataTable">
            <thead>
                <tr>
                    <th>idCode</th>
                    <th>Header</th>
                    <th>Compound</th>
                    <th>Resolution</th>
                    <th>Exp. Type</th>
                    <th>Source</th>
                </tr>
            </thead>
            <tbody>
                <?php while ($rsF = mysqli_fetch_assoc($rs)) { ?>
                    <tr>
                        <td><a href="getStruc.php?idCode=<?php print $rsF['idCode'] ?>">
                                <?php print $rsF['idCode'] ?></a></td>
                        <td><?php print ucwords(strtolower($rsF['header'])) ?></td>
                        <td><?php print ucwords(strtolower($rsF['compound'])) ?></td>
                        <td><?php print $rsF['resolution'] ?></td>
                        <td><?php print $rsF['expType'] ?></td>
                        <td><?php print ucwords(strtolower($rsF['source'])) ?></td>
                    </tr>
                <?php } ?>
            </tbody>
        </table>
        <p class="button"><a href="index.php?new=1">New Search</a></p>
        <script type="text/javascript">
        <!-- this activates the DataTable element when page is loaded-->
            $(document).ready(function () {
                $('#dataTable').DataTable();
            });
        </script>
        <?php
        print footerDBW();
    }
}
```


Search results
index.php · master · DBW / PDB
mmb.irbbarcelona.org/formacio/~dbw00/PDBBrowser/runBlast.php

DBW - Search results

Num Hits: 81

Show 10 entries

Search:

| idCode | Type | Header | E. value |
|---|---|---|---|
| 13pk_A | protein | 3-PHOSPHOGLYCERATE KINASE | 0.0 |
| 13pk_B | protein | 3-PHOSPHOGLYCERATE KINASE | 0.0 |
| 13pk_C | protein | 3-PHOSPHOGLYCERATE KINASE | 0.0 |
| 13pk_D | protein | 3-PHOSPHOGLYCERATE KINASE | 0.0 |
| 16pk_A | protein | 3-PHOSPHOGLYCERATE KINASE | 0.0 |
| 1fw8_A | protein | Phosphoglycerate kinase | 1.29e-67 |
| 1hdi_A | protein | PHOSPHOGLYCERATE KINASE | 1.22e-59 |
| 1kf0_A | protein | Phosphoglycerate Kinase | 6.35e-63 |
| 1ltk_A | protein | PHOSPHOGLYCERATE KINASE | 3.96e-67 |
| 1ltk_B | protein | PHOSPHOGLYCERATE KINASE | 3.96e-67 |

Showing 1 to 10 of 81 entries

Previous 1 2 3 4 5 … 9 Next

New Search

**runBlast.php**
Blast search

```
<?php
require "globals.inc.php";
// Take data from $_SESSION, loaded in search.php, if empty back to front page
if (!isset($_SESSION['queryData']) or ! $_SESSION['queryData']['seqQuery'])
    header('Location: index.php');
// prepare FASTA file
// Identify file format, ">" as first char indicates FASTA
$p = strpos($_SESSION['queryData']['seqQuery'], '>');
if (!$p and ( $p !== 0)) { // strpos returns False if not found and "0" if first character in the string
    // When is not already FASTA, add header + new line
    $_SESSION['queryData']['seqQuery'] = ">User provided sequence\n" . $_SESSION['queryData']['seqQuery'];
}
// Set temporary file name to a unique value to protect from concurrent runs
$tempFile = $tmpDir . "/" . uniqId('pdb');
// Open temporary file and store query FASTA
$ff = fopen($tempFile . ".query.fasta", 'wt');
fwrite($ff, $_SESSION['queryData']['seqQuery']);
fclose($ff);
// execute Blast, Command line set in globals.inc.php
print $blastCmdLine . " -query " . $tempFile . ".query.fasta -out " . $tempFile . ".blast.out\n";
exec($blastCmdLine . " -query " . $tempFile . ".query.fasta -out " . $tempFile . ".blast.out");
// Read results file and parse hits onto $result[]
$result = file($tempFile . ".blast.out");
if (!count($result)) {
    print errorPage("Not Found", 'No results found. <p class="button" ><a href="index.php?new=1">New Search</a></p>');
} else {
//       Results table
    print headerDBW("Search results");
    ?>
<p>Num Hits: <?php print count($result) ?> </p>
    <table border="0" cellspacing="2" cellpadding="4" id="blastTable">
        <thead
            <tr>
            <th>idCode</th>
            <th>Type</th>
            <th>Header</th>
            <th>E. value</th>
          </tr>
        </thead>
        <tbody>
          <?php
          foreach (array_values($result) as $rr) {
            if (strlen($rr) > 1) {
                        $data = explode ("\t",$rr);
              preg_match('/(....)_(.) mol:([^ ]*) length:([0-9]*) *(.*)/', $data[1], $hits);
              list ($r, $idCode, $sub, $tip, $l, $desc)= $hits;
              $ev = $data[2];
              ?>
              <tr>
                <td>
                  <a href="getStruc.php?idCode=<?php print $idCode ?>"><?php print $idCode . "_$sub" ?></a>
                </td>
                <td><?php print $tip ?></td>
                <td><?php print $desc ?></td>
                <td><?php print $ev ?></td>
              </tr>
              <?php
            }
          }
          ?>
        </tbody>
      </table>
<p class="button"><a href="index.php?new=1">New Search</a></p>
    <?php
    // Cleaning temporary files
    if (file_exists($tempFile . ".query.fasta"))
        unlink($tempFile . ".query.fasta");
//    if (file_exists($tempFile . ".blast.out"))
//        unlink($tempFile . ".blast.out");
    print footerDBW();
}
// DataTable activation
?>
<script type="text/javascript">
    $(document).ready(function () {
        $('#blastTable').DataTable();
    });
</script>
```

**Include/bdconn.inc.php**

```
<?php
/*
 * bdconn.inc.php
 * DB Connection
 */
$host = "localhost";
$dbname = "pdb";
$user = "dbw00";
$password = "dbw2018";
($mysqli = mysqli_connect($host, $user, $password)) or die(mysqli_error());
mysqli_select_db($mysqli, $dbname) or die(mysql_error($mysqli));
```

**Include/libDBW.inc.php**

```
<?php
function headerDBW($title) {
   return "<html lang=\"en\">
<head>
<meta charset=\"utf-8\">
   <meta http-equiv=\"X-UA-Compatible\" content=\"IE=edge\">
   <meta name=\"viewport\" content=\"width=device-width, initial-scale=1\">
<title>$title</title>
      <!-- Bootstrap styles -->
   <link rel=\"stylesheet\" href=\"https://maxcdn.bootstrapcdn.com/bootstrap/3.3.7/css/bootstrap.min.css\"
integrity=\"sha384-BVYiiSIFeK1dGmJRAkycuHAHRg32OmUcww7on3RYdg4Va+PmSTsz/K68vbdEjh4u\"
crossorigin=\"anonymous\">
     <!-- IE 8 Support-->
   <!--[if lt IE 9]>
     <script src=\"https://oss.maxcdn.com/html5shiv/3.7.3/html5shiv.min.js\"></script>
     <script src=\"https://oss.maxcdn.com/respond/1.4.2/respond.min.js\"></script>
   <![endif]-->
      <link rel=\"stylesheet\" href=\"DataTable/jquery.dataTables.min.css\"/>
      <script type=\"text/javascript\" src=\"DataTable/jquery-2.2.0.min.js\"></script>
      <script type=\"text/javascript\" src=\"DataTable/jquery.dataTables.min.js\"></script>

</head>
<body bgcolor=\"#ffffff\">
<div class= \"container\">
<h1>DBW - $title</h1>
";
}

function footerDBW() {
   return '
      </div>
</body>
</html>';
}

function errorPage($title, $text) {
   return headerDBW($title) . $text . footerDBW();
}
```

**loadPDB.pl**
ETL to load database data from PDB text files

```
#!/usr/bin/perl
use DBI;
use strict;
#
require "bdconn.pl";
#
my $dbh=connectDB();
# Clean Tables !!
foreach my $tab ('entry', 'source', 'sequence', 'author', 'author_has_entry', 'expType', 'comptype', 'entry_has_source',
'expClasse') {
  print "Cleaning $tab\n";
  $dbh->do ("DELETE FROM $tab");
}
foreach my $tab ('source','author','expType','comptype','expClasse') {
  $dbh->do ("ALTER TABLE $tab AUTO_INCREMENT=1");
}
#
$dbh->do("SET FOREIGN_KEY_CHECKS=0");
#
print "Authors...";
my %AUTHORS;
my %author_has_entry;
my $sthAuthor=$dbh->prepare ("INSERT INTO author (author) VALUES (?)");
my $sthEntryAuthor=$dbh->prepare("INSERT INTO author_has_entry VALUES (?,?)");
open AUTS, "author.idx";

#author.idx
#IDCODE; AUTHOR
#2NPB ; AACHMANN, F.L.
#2KV1 ; AACHMANN, F.L.

while (<AUTS>) {
  next if !/;/;
  chomp;
  my ($idCode, $author) = split / *; */;
  next if (!$author);
  if ($author && !$AUTHORS{$author}) {
          $sthAuthor->execute ($author);
          $AUTHORS{$author}=$dbh->last_insert_id('','','Author','idAuthor');
  }
  if (!$author_has_entry{"$AUTHORS{$author}-$idCode"}) {
    $sthEntryAuthor->execute ($AUTHORS{$author},$idCode);
    $author_has_entry{"$AUTHORS{$author}-$idCode"}=1;
  }
  print ".";
}
close AUTS;
print "ok\n";
#
#
print "Sources...";
my %SOURCES;
my %Entry_has_source;
my $sthSource =$dbh->prepare("INSERT INTO source (source) VALUES (?)");
my $sthEntrySource = $dbh->prepare("INSERT INTO entry_has_source (idCode,idSource) VALUES (?,?)");
open SOUR, "source.idx";

#source.idx
#IDCODE  SOURCE
#102L      ENTEROBACTERIA PHAGE T4
#102M      PHYSETER CATODON
```

```
while (<SOUR>) {
  chomp;
  my ($idCode,$source) = split ' ', $_, 2;
  next if (!$source) || (length($idCode) != 4);
  foreach my $s (split /; */, $source) {
    if (!$SOURCES{$s}) {
      $sthSource->execute ($s);
             $SOURCES{$s}=$dbh->last_insert_id('','','source','idSource');
    }
    $sthEntrySource->execute($idCode, $SOURCES{$s});
  }
  print ".";
}
close SOUR;
print "ok\n";
#
#
print "Entries...";
open ENTR, "entries.idx";

#entries.idx
# IDCODE, HEADER, ACCESSION DATE, COMPOUND, SOURCE, AUTHOR LIST, RESOLUTION, EXPERIMENT TYPE (IF NOT X-RAY)
#100D       DNA/RNA  12/05/94   CRYSTAL STRUCTURE OF THE HIGHLY DISTORTED CHIMERIC DECAMER R(C)D(CGGCGCCG)R(G)-SPERMINE COMPLEX-SPERMINE
BINDING TO PHOSPHATE ONLY AND MINOR GROOVE TERTIARY BASE-PAIRING                         Ban, C., Ramakrishnan, B., Sundaralingam, M.             1.9
                X-RAY DIFFRACTION
#101D       DNA          12/14/94   REFINEMENT OF NETROPSIN BOUND TO DNA: BIAS AND FEEDBACK IN ELECTRON DENSITY MAP INTERPRETATION
                Goodsell, D.S., Kopka, M.L., Dickerson, R.E.  2.25          X-RAY DIFFRACTION

my $sthEntry = $dbh->prepare ("INSERT INTO entry (idCode, header, ascessionDate, compound, resolution) VALUES (?,?,?,?,?)");
my %ExpTypes;
my $sthExpType = $dbh->prepare ("INSERT INTO expType (ExpType) VALUES (?)");
my $sthEntryExpType = $dbh->prepare ("UPDATE entry SET idExpType=? WHERE idCode=?");
my %expTypesbyCode;
while (<ENTR>) {
  chomp;
  my ($idCode, $header, $ascDate, $compound, $source, $authorList, $resol, $expType) = split /\t/;
  next if (length($idCode) != 4);
  $sthEntry-> execute ($idCode,$header, $ascDate, $compound, $resol);
          if (!$ExpTypes{$expType }) {
                    $sthExpType->execute($expType);
                    $ExpTypes{$expType}=$dbh->last_insert_id('','','ExpType','idExpType');
          }
          $sthEntryExpType->execute($ExpTypes{$expType},$idCode);
          $expTypesbyCode{$idCode}=$expType;
  print ".";
}
close ENTR;
print "ok\n";
#
#
open EXPCL , 'pdb_entry_type.txt';
#pdb_entry_type.txt
#100d       nuc          diffraction
#101d       nuc          diffraction

my %expClasses;
my %compTypes;
my $sthExpClasse=$dbh->prepare('INSERT INTO expClasse (expClasse) VALUES (?)');
my $sthcompType=$dbh->prepare('INSERT INTO comptype (type) VALUES (?)');
my $entryUpdate= $dbh->prepare('UPDATE entry SET idCompType=? WHERE idCode=?');
my $expTypeUpdate=$dbh->prepare('UPDATE expType SET idExpClasse=? where ExpType=?');

while (<EXPCL>) {
  chomp;
		my ($idCode, $compType, $expClass) = split ' ';
		$idCode =~ tr/a-z/A-Z/;
		if (!$expClasses{$expClass}) {
			$sthExpClasse->execute($expClass);
			$expClasses{$expClass}=$dbh->last_insert_id('','','expClasses','idExpClass');
		}
		if (!$compTypes{$compType}) {
			$sthcompType->execute($compType);
			$compTypes{$compType}=$dbh->last_insert_id('','','compType','idCompType');
		}
		$expTypeUpdate->execute($expClasses{$expClass}, $expTypesbyCode{$idCode});
		$entryUpdate->execute($compTypes{$compType},$idCode);
}
#Sequence
print "Sequences...";
my $codes=[];
my %CODES;
my $sthInsert= $dbh->prepare ("INSERT INTO sequence (idCode,chain,sequence,header) VALUES (?,?,?,?)");
open "SEQS", "pdb_seqres.txt";

#pdb_seqres.txt (FASTA)
#>101m_A mol:protein length:154  MYOGLOBIN
#MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHP...
#>...

my $seq;
my $idPdb;
my $chain;
my $header;
while (<SEQS>) {
  chomp;
  if (/^>/) {
		if ($seq) {
			$seq =~ s/\n//g;
			$idPdb =~ tr/a-z/A-Z/;
			$chain =~ s/ //;
			$sthInsert->execute ($idPdb,$chain,$seq, $header) || die $DBI::errstr;
		    $seq="";
		}
		/^>([^_]*)_(.*)mol:(\S*) length:(\S*) (.*)/;
		($idPdb,$chain,$header)=($1,$2,"$1 $2 $3 $4 $5");
		print "$header\n";
  }
  else {$seq .= $_};
};
print "ok\n";
disconnectDB($dbh);
```

**bdconn.pl**
Script to connect to mysql

```
#!/usr/bin/perl
# Connect script for DBI-Mysql
#
use DBI;

1;

sub connectDB {
        my $driver = "mysql";
        my $database = "pdb";
        my $host = "localhost";
        my $user="gelpi";
        my $passwd = "jl12gb";
        my $autoCommit = 1;
        my $dsn = "DBI:$driver:database=$database;host=$host;user=$user;password=$passwd";
        return DBI->connect ($dsn, undef, undef,
                {RaiseError => 1, AutoCommit => $autoCommit});
}

sub disconnectDB {
        my $dbh = shift;
        return $dbh->disconnect;
}
```