**Web Technology for bioinformatics**

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**Aim :**

To create a web app for symmetry equivalent molecules generation using PHP.

**Procedure:**

1. Load a CIF molecule in the server using HTML form.
2. Input the Symmetry operation using the Input box.
3. Develop a PHP script in a web server for finding the symmetry equivalent molecules.

**Program:**

**The code below is written in a html:**

**<!DOCTYPE html>**

**<head>**

**<title>Upload file</title>**

**</head>**

**<body>**

**<!-- name : Dharineesh K S**

**regno : 123013012 -->**

**<form method="post" action="sym.php" enctype="multipart/form-data" autocomplete="off">**

**<center>**

**<label>Upload file</label>**

**<input type="file" name="upload" autofocus required>**

**<br />**

**<br />**

**<label><b>Enter Symmetry operation</b></label>**

**<input type="search" name="symopr" list="sym" autofocus required placeholder="x y z">**

**<datalist id="sym">**

**<option value="x 1/2-y 1/2+z"></option>**

**<option value="x y z"></option>**

**<option value="-x -y -z"></option>**

**<option value="-x 1/2+y 1/2-z"></option>**

**</datalist>**

**<br />**

**<br />**

**<input type="submit" value="upload file" autofocus>**

**</center>**

**</form>**

**</body>**

**</html>**

**The code below is written in a php file:**

**<?php**

**echo "**

**<html>**

**<head>**

**<title>Symmetry operation</title>**

**<style type=\"text/css\">**

**body {**

**font-family: \"Times New Roman\";**

**}**

**table {**

**width: 50%;**

**}**

**tr:nth-child(even) {**

**background-color: #f2f2f2 ;**

**}**

**</style>**

**</head> ";**

**echo"<body>";**

**$new = "";**

**$filename = $\_FILES['upload']['name'];**

**// $file\_temp\_loc = $\_FILES['upload']['tmp\_name'];**

**move\_uploaded\_file($\_FILES['upload']['tmp\_name'],"uploads/$filename");**

**$sym = $\_POST['symopr'];**

**$symopr = explode(",",$sym);**

**$symopr[0] = preg\_replace("/1\/2/","0.5",$symopr[0]);**

**$symopr[1] = preg\_replace("/1\/2/","0.5",$symopr[0]);**

**$symopr[2] = preg\_replace("/1\/2/","0.5",$symopr[0]);**

**$tt = fopen("new.cif","w");**

**$file\_cif = array();**

**$cif\_syml = array();**

**$cif\_header = array();**

**$cif\_atom = array();**

**$handle = fopen("uploads/$filename","r");**

**$bb = "";**

**$entirefile = "";**

**while (!feof($handle))**

**{**

**$buffer1 = fgets($handle);**

**if (preg\_match("/^[\_\d#a-z]/",$buffer1))**

**{**

**$new = $new.$buffer1;**

**}**

**if (preg\_match("/^[A-Z]/",$buffer1))**

**{**

**$bb = $bb.$buffer1;**

**preg\_match\_all("/[A-Z][a-z]?[\d{1}]?[\d{1}]?\s?[A-Z]?\s?[A-Z]?\s?/",$buffer1,$dy);**

**$firstpart = $dy[0][0];**

**preg\_match\_all("/-?\d{1,2}\.\d+/",$buffer1,$d2);**

**$x1 = $d2[0][0];**

**$y1 = $d2[0][1];**

**$z1 = $d2[0][2];**

**if($x1!="" && $y1!="" && $z1!="")**

**{**

**$xcc = preg\_replace("/x/",$x1,$symopr[0]);**

**$ycc = preg\_replace("/y/",$x1,$symopr[1]);**

**$zcc = preg\_replace("/z/",$x1,$symopr[2]);**

**$xcc1 = preg\_replace("/--/","+",$xcc);**

**$ycc1 = preg\_replace("/--/","+",$ycc);**

**$zcc1 = preg\_replace("/--/","+",$zcc);**

**$xdd = eval("return ". $xcc1 .";");**

**$ydd = eval("return ". $ycc1 .";");**

**$zdd = eval("return ". $zcc1 .";");**

**$new .= "".$firstpart."".$xdd." ".$ydd." ".$zdd."\n";**

**}**

**}**

**}**

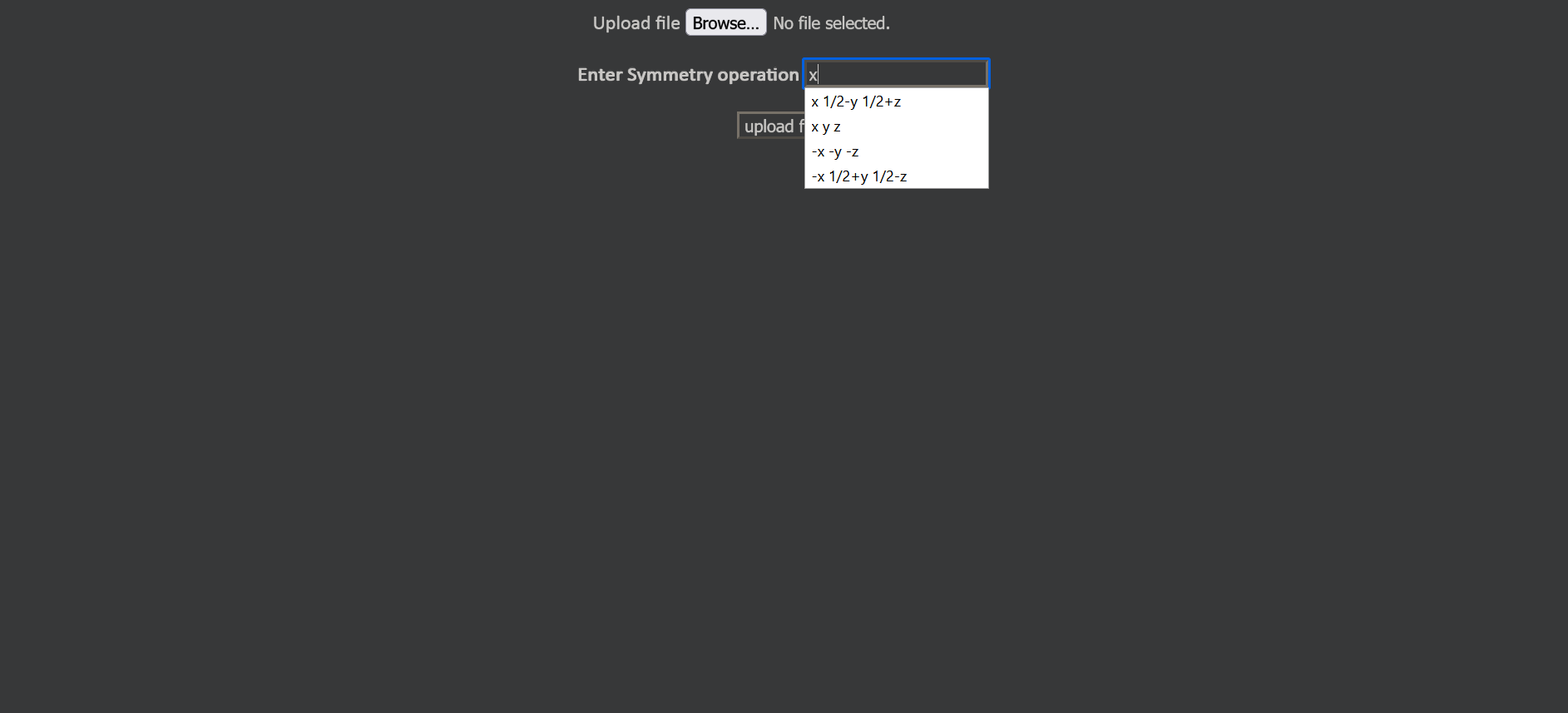
**echo "<br>After Symmetry Operation <br>textarea rows=10 cols=90>$new</textarea><br>";**

**echo"</body>";**

**echo"</html>";**

**?>**

**Output:**

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