I. Research Overview and Outcome

**Concept**

Protein docking web servers are one of the online tools used by biochemists to research the geometry of proteins when a ligand (smaller entity) binds with them. The web servers accept one ligand and one protein as input to do the calculations that result in a file or files that describe the geometry of binding sites of the ligand on the protein. My research consisted of designing an interface that could accept one ligand and up to six proteins and submit them in pairs to up to seven protein docking web servers simultaneously. Each web server receives up to six pairs, one ligand paired with each of the six proteins.

**Methodology**

- Research which languages have libraries for handling post requests.
- Use online tools to determine the parameters required by the target website to submit posts.
- Choose a language and find out how to write the POST requests in that language using its libraries.
- Create the interface form.
- Write the code to prepare and assemble the parameters needed for the requests.
- Write the code to submit the request.
- Test the code. Things we need to find (once the researcher prepares correct protein and ligand files):
  - Does our code post successfully to each protein docking web server?
  - Does the protein docking web server produce an output file or files?
- Gather output into a repository
- Test and debug against each server
- Write the code to submit the request.
- Write the code to prepare and assemble the parameters needed for the POST requests.
- Write the code to submit the request.
- Test the code. Things we need to find (once the researcher prepares correct protein and ligand files):
  - Does our code post successfully to each protein docking web server?
  - Does the protein docking web server produce an output file or files?

**Web Server | Response from server | Errors**

<table>
<thead>
<tr>
<th>Web Server</th>
<th>Response from server</th>
<th>Errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>ClusPro</td>
<td>not logged in</td>
<td>Closing connection #0</td>
</tr>
<tr>
<td>3DGarden</td>
<td>unknown</td>
<td>Closing connection #0</td>
</tr>
<tr>
<td>PatchDock</td>
<td>results will be mailed</td>
<td>Closing connection #0</td>
</tr>
</tbody>
</table>

**Developmental Resources**

- Language
  - PHP
  - cURL
- Library
  - cURL
- Web
  - XAMPP server (local to web)
  - Apache server (web to web)

**CURL functions used**

- `curl_init()`
- `curl_setopt()`
- `curl_exec()`
- `curl_close()`

II. International Experience

Thanks to PIRE I had the opportunity to be in Spain to witness the fervor of the people of this beautiful country when celebrating three international sporting events: the European Soccer Cup, the World Cup of Soccer, and the Valencia Formula Circuit. I was able also to participate in two local patron saint celebrations: the sardine beach cookout and the "Fiesta de San Juan". I learned that traveling to research sites abroad should be part of a researcher's agenda, and that collaboration with researchers of different cultures not only enriches us culturally but it nurtures and expands our intellect.

III. Acknowledgement

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