class06HW

AUTHOR
Rogelio Castro

First we got to make sure that we install the necessary packages to be able to answer Q6.

```
# Set a specific CRAN mirror
options(repos = "https://cloud.r-project.org")

# Install the bio3d package
install.packages("bio3d")
```

```
The downloaded binary packages are in
    /var/folders/tb/h1gqvy1s2mb813g1qkdm08340000gn/T//RtmpuqtkWg/downloaded_packages
```

```
# Install the bio3d package with dependencies
install.packages("bio3d", dependencies = TRUE)
```

```
Warning: dependencies 'msa', 'Biostrings' are not available
```

```
The downloaded binary packages are in
    /var/folders/tb/h1gqvy1s2mb813g1qkdm08340000gn/T//RtmpuqtkWg/downloaded_packages
```

> Q6. How would you generalize the original code above to work with any set of input protein structures?

```
library(bio3d)

plot_protein_drug_interactions <- function(pdb_path, protein_name) {

pdb <- read.pdb(pdb_path)
protein <- atom.select(pdb, "protein and chain A","pdb")
pockets <- pocket(protein, "fpocket")
drug_binding_residues <- pockets$fpocket$pdb
plot.drug2res(protein, drug_binding_residues, name = protein_name)

}
```