Scripting system

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1 Summary

1.1 Description

High platforms team leverage enthusiastically high infrastructures utilize convergence functionalized action capital. Than growth multimedia viral alternative emerging infrastructures e-enable sucking fashion capital niches standards. Extensible "organic" team re-engineer reinvent quality leading-edge paradigms cultivate infrastructures energistically dynamic. Art holisticly covalent leverage initiatives enterprise interoperable empowerment actualize collaborative invested chains utilize expedite corporate. Improvements potentialities results energistically streamline completely positioning brand adaptive team visualize of holistic infrastructures.

1.2 File Structure

- NOTES:
  - ***`bolded-italicized`*** files/directories need to be created by the user
  - **`bolded`** files/directories/names need to be modified by the user
  - *`italicized`* files and directories are created by scripts
  - `plain` files and directories do not (and should not) by modified
  - `$ command` indicates a command line command in the terminal
  - directories and files (and parts of file names) in lower case must included exactly as indicated
  - directories and files in all caps should be named appropriately to the proteins and dockings in question

- ***base_dir*** – The root of the system is the base directory, containing all other files (probably best not to put anything else in this folder but what's indicated below)
  - `Readme.md` –This file
  - ***Dockings.csv*** – A spreadsheet containing master docking parameters
  - ***Gridboxes.csv*** – A spreadsheet specifying all the grid box parameters
  - `ligsets/` –A directory containing all the sets of ligands
    - ***ligsets/LIGSET/*** – for each set, the there should be a directory within the `ligsets/` directory, whose name is the name of the ligand set. Substitute `LIGSET` for some appropriate name (e.g. `ligsets/my_awesome_ligset/`)
      - ***ligsets/LIGSET/pdbqts/*** –a directory containing a PDBQT file for each ligand in the set (whose name is `LIG.pdbqt`, with `LIG` being exactly the same as in `ligsets/LIGSET/LIGSET_list.txt`) [may be scripted later]
      - ***ligsets/LIGSET/LIGSET_list.txt*** –a text file containing a list of all the ligands (one on each line) and nothing else
        - you can create this easily on the command line using: `$ cd base_dir/ligsets/; for l in $(ls LIGSET/pdbqts | sed 's/.pdbqt//'); do echo $l >> LIGSET/LIGSET_list.txt ; done` (appropriately substituting `base_dir` and `LIGSET`, and assuming the PDBQTs are already made)
      - [optional/preliminary] `ligsets/LIGSET/LIGSET.cdxml/` or `ligsets/LIGSET/LIGSET.mol/`– one file to show all the ligands in one page for presentations, PDFmaking and such.
      - [optional/preliminary] `/mols/` and `ligsets/LIGSET/pdbs/` – directories for preparing the initial PDBQT files. Will either be optional, or more scripts will be written.
  - `parameters_csvs/` –A directory containing small CSV files specifying the docking parameters for each individual docking (needed for scripts, at least as of now). Generated by `scripts/write_params_csv.R` from information in `Gridboxes.csv`
    - They will be named **`parameters_csvs/DOCKING_parameters.csv`**, where `DOCKING` is the docking ID
  - `vina_submit_shs/` – A directory containing the submission files for

Vina jobs on the (Wesleyan) cluster. Generated by `write_vina_submit` function of `docking_data_assembly.py`

- **`vina_submit_shs/vina_submit_DOCKING.sh`** –for a docking of 20 models or less, a single submission script is written (and submitted using `$ bsub < vina_submit_DOCKING.sh`, see submission instructions below)
- **`vina_submits_DOCKING/`** –dockings of more than 20 models need to be submitted with multiple scripts (because Vina will not generate more than 20 poses). In this case, the `write_vina_submit` function will create a directory called `vina_submits_DOCKING/` containing n scripts **`vina_submit_DOCKING.1.sh`** , **`vina_submit_DOCKING.2.sh`** through **`vina_submit_DOCKING.n.sh`** . This script is set up to write each n submission scripts, where each of which script has a model number of 20 and n is the number of models divided by 20. Therefore, if greater than 20, the number of models should always be a multiple of twenty, or things will get messed up. (These are submitted used `$ for s in $(ls vina_submits_DOCKING); do bsub < $s; done$`, see instructions below)

◦ ***`PROTEIN/`*** , etc. – A directory for *each* protein, whose name is the name of the protein, the reference name/abbreviation used throughout, it just needs to be consistent (e.g. I primarily dock the proteins HepI and p300 and have the directories `hepi/` and `p300/` in my `base_dir/`)

- ***`PROTEIN/PROTEIN.pdbqt`*** – the PDBQT file to be used for docking (`PROTEIN` must be *exactly* the same for the directory/file names and in the `Dockings.csv` and `Gridboxes.csv` entries for the protein's dockings) [may be scripted later, from `PROTEIN.pdb`]
- [optional/preliminary] `PROTEIN.pdb` – the original PDB file
- **`PROT/DOCKING/`** – for every docking, there should be a directory whose name in the docking ID (the same as in `Dockings.csv`). Note: the user shouldn't make this folder, it is made by `vina_submit_DOCKING.sh`.
  - This will eventually contain
- ***`PROT/binding_sites/`*** – a directory containing binding site PDBs:
  - To do binding site scoring by residues contacted (which is detected by the AutoDockTools script `process_VinaResult.py`),

There must be one or more `PROT/binding_sites/BINDING_SITE.pdb` files. These are subsets of the original `PROTEIN.pdb` (I originally created mine by grabbing the residues within $5\AA$ of the bound ligands that came with the crystal structure, but it could be done many other ways).

- `scripts/` – all the scripts needed to use this set up
  - `write_params_csv.R` – writes `DOCK_parameters.csv` using information in `Dockings.csv` and `Gridboxes.csv`
  - `load_parameters.sh` – loads parameters from `DOCKING_parameters.csv` (used in the next script)
  - `separate_vina_results.sh` – runs Vina result PDBQTs through the AutoDockTools script `process_VinaResult.py`, which separates the poses into separate files and extracts the receptor contacts. The resulting files ended up in `DOCKING/processed_pdbqts/`, named `DOCKING_LIGAND_mMODEL.pdbqt`, where MODEL is the particular pose represented by the file. (A docking with l ligands and with Vina set to produce m models will therefore end up having $l \times m$ files after this script runs.)
  - `cleanup_processed_vina_results.sh` – cleans up processed PDBQTs (`DOCKING/processed_pdbqts/DOCKING_LIGAND_mMODEL.pdbqt`) and converts then to PDBs using the AutoDockTools script `pdbqt_to_pdb.py`
  - `parse_pdb.py` – defines a object class called `Pdb` for parsing PDB and PDBQT files for their 3D coordinates and in the case of processed Vina results, their binding energy, protein contacts, and other data generated by Vina. (Necessary for `docking_data_assembly.py`.)
  - `aiad_icpd.py` – defines functions to calculate the AIAD (averaged inter–atomic distance) and ICPD (inter–centerpoint distance) between two `Pdb` objects, two useful parameters for determining where a pose is binding on a protein and clustering poses together based on proximity. (Necessary for these functions in `docking_data_assembly.py`.)
  - `docking_data_assembly.py` – defines an object class called `Docking` for preparation and analysis of dockings. Contains several important functions:
    - `write_vina_submit` – prepares Vina job submission scripts
    - `assemble_dic` – assembles a data dictionary that contains all

the mined data from the Vina results
    - `score_binding_sites` – scores each pose for the proportion of residues contacted in each reference binding site
    - `assess_all_resis` – uses binding scores to determine a True/-False for each pose binding in at each binding site (based on a threshold score, currently 0.1 or 10%)
    - (`aiad_icpd_binding_sites`) – calculates AIAD and ICPD scores for each pose compared to each binding site
    - `write_alldata_csv` – writes the data dictionary to a CSV file called `DOCKING_alldata.csv`
    - `cluster_poses` [`prepare_clustering_csv.py`] – calculates AIAD scores for every pose compared to every other pose, for cluster analysis later on
- `pre_and_post_control.py` – links to all of the above scripts to coordinate their function, providing the global variables required to run this system on different computers.
- **Other scripts that may or may not be added:**
    - A script to add an entry to `Dockings.csv` or `Gridboxes.csv` with use input

1.3 Complete listing of included files

- **Notes**:
    - ... indicates more of the same kind of file or directory
    - .py files (except for the control script) may have a compiled .pyc file with them
    - (files) are optional (for now)
    - [files] are works in progress and may not be included ultimately
    - [[files]] need to be made

```
/path/to/base_dir/
  Readme.md
  Dockings.csv
  Gridboxes.csv
  ligsets/
    LIGSET1/
      LIGSET1_list.txt
      (LIGSET1.cdxml)
      (mols/...)
      (pdbs/...)
```

```
          pdbqts/
            LIG1_1.pdbqt
            LIG1_2.pdbqt
            LIG1_3.pdbqt
            ...
        LIGSET2/
          LIGSET1_list.txt
          (mols/...)
          (pdbs/...)
          pdbqts/
            LIG2_1.pdbqt
            LIG2_2.pdbqt
            LIG2_3.pdbqt
            ...
        ...
      vina_submit_shs/
        vina_submit_A1.sh
        vina_submits_A2/
          vina_submit_A2.1.sh
          vina_submit_A2.2.sh
          vina_submit_A2.3.sh
          ...
        vina_submit_B1.sh
        ...
      PROT_A/
        (PROT_A.pdb)
        PROT_A.pdbqt
        binding_sites/
          BINDING_SITE_ALPHA1.pdb
          BINDING_SITE_ALPHA2.pdb
          BINDING_SITE_ALPHA3.pdb
          ...
        A1/
        A2/
        A3/
        ...
      PROT_B/
        (PROT_B.pdb)
        PROT_B.pdbqt
        binding_sites/
          BINDING_SITE_BETA1.pdb
          ...
        B1/
        B2/
        ...
```

```
      ...
      scripts/
        [new_grid_or_dock_entry.R]
        [[write_ligset_list_txt.sh]]
        load_parameters.sh
        [[ligand, protein preparation]]
        separate_vina_results.sh
        cleanup_processed_vina_results.sh
        parse_pdb.py
        aiad_icpd.py
        [[prepare_clustering_csv.py]]
        docking_data_assembly.py
        pre_and_post_control.py
        [[post_docking_graphs.R]]
        [[clustering_graphs.R]]
        [[R cript to select poses to view in PyMol]]
        [[Py script to load PyMol sessions from lists]]
```

1.3.1 After docking post-processing:

```
      PROTEIN/
        (PROTEIN.pdb)
        PROTEIN.pdbqt
        binding_sites/
          SITE1.pdb
          SITE1.pdb
          SITE1.pdb
          ...
        DOCKING/
          result_pdbqts/
            DOCKING_LIG1_results.pdbqt
            DOCKING_LIG2_results.pdbqt
            DOCKING_LIG3_results.pdbqt
            ...
          processed_pdbqts/
            DOCKING_LIG1_m1.pdbqt
            DOCKING_LIG1_m2.pdbqt
            DOCKING_LIG1_m3.pdbqt
            ...
            DOCKING_LIG2_m1.pdbqt
            DOCKING_LIG2_m2.pdbqt
            DOCKING_LIG2_m3.pdbqt
```

```
            ...
            DOCKING_LIG3_m1.pdbqt
            DOCKING_LIG3_m2.pdbqt
            DOCKING_LIG3_m3.pdbqt
            ...
          processed_pdbs/
            DOCKING_LIG1_m1.pdb
            DOCKING_LIG1_m2.pdb
            DOCKING_LIG1_m3.pdb
            ...
            DOCKING_LIG2_m1.pdb
            DOCKING_LIG2_m2.pdb
            DOCKING_LIG2_m3.pdb
            ...
            DOCKING_LIG3_m1.pdb
            DOCKING_LIG3_m2.pdb
            DOCKING_LIG3_m3.pdb
            ...
          DOCKING_alldata.csv
          DOCKING.p
          DOCKING_clustering.csv [[DOCKING_pose_pose_aiads.csv]]
          [[DOCKING_best_aiad_pairs.csv]]
          [[graphs/]]
            [[...graphs...]]
```

1.4 Example Dockings.csv file

```
Docking ID,Date,Protein,Ligset,Grid box,Exhaustiveness,Number of Models,Number
     of CPUs,Notes
A1,20160301,PROTA,LIGS1,AAS,20,10,2,looking at active size of protein A
A2,20160308,PROTA,LIGS2,AWP,50,400,4,high volume docking of whole protein A
B1,20160308,PROTB,LIGS3,BWP,8,20,1,initial docking of whole protein B
```

1.5 Example Gridboxes.csv file

```
Gridbox Name,Protein,Size in x-dimension,Size in y-dimension,Size in z-
    dimension,Center in x-dimension,Center in y-dimension,Center in z-
    dimension,Notes
```

Docking ID	Date	Protein	Ligset	Grid box	Exhaustiveness	Number of Models	Number of CPUs	Notes
A1	20160301	PROTA	LIGS1	AAS	20	10	2	looking at active size of protein A
A2	20160308	PROTA	LIGS2	AWP	50	400	4	high volume docking of whole protein A
B1	20160308	PROTB	LIGS3	BWP	8	20	1	initial docking of whole protein B

```
AAS,PROTA,60,72,88,41.89,2.69,-1.85,active site of protein A
AWP,PROTA,126,126,126,41.89,2.69,-1.85,all of protein A
BWP,PROTB,126,126,126,4.89,-5.27,12.0,all of protein B
```

Gridbox Name	Protein	Box size (x)	Box size (y)	Box size (z)	Box center (x)	Box center (y)	Box center (z)	Notes
AAS	PROTA	60	72	88	41.89	2.69	-1.85	active site of protein A
AWP	PROTA	126	126	126	41.89	2.69	-1.85	all of protein A
BWP	PROTB	126	126	126	4.89	-5.27	12.0	all of protein B

2 Scripts

- constants.py (*,**)
- new_grid_or_dock_entry.py (*)
- create_docking_object.py (*)
- write_vina_submit_sh.py (*)
- read_alldata.py (*)
- cleanup_processed_vina_results.sh [pr]
- separate_vina_results.sh [pr]
- parse_pdb.py (*, sa)
- mine_vina_data.py (*)
- aiad_icpd.py (*, sa)
- binding_site_analysis.py (*)
- energies_properties.py (*, sa)
- get_pose_energies_properties.py (*)
- write_alldata.py (*)
- correlations.py (*)
- [postdocking_summary.R]
- postdocking_graphs.R (nc)
- pre_and_post_control.py

2.1 `constants.py`

2.1.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
### Module-wide constants
# (c) Zarek Siegel
# v1 3/11/16
# v2 3/15/16

base_dir="/Users/zarek/GitHub/TaylorLab/zvina"
AutoDockTools_dir="/Library/MGLTools/latest/MGLToolsPckgs/AutoDockTools"
AutoDockTools_pythonsh_binary="/Library/MGLTools/latest/bin/pythonsh"

python_binary="/anaconda/envs/python27/bin/python"
Rscript_binary="/usr/bin/Rscript"
openbabel_binaries_dir="/usr/local/bin"

cluster_base_dir="/home/zsiegel"
cluster_vina_binary="/share/apps/autodock/autodock_vina_1_1_2_linux_x86/bin/
    vina"
cluster_AutoDockTools_dir="/home/apps/CENTOS6/mgltools/1.5.6/MGLToolsPckgs/
    AutoDockTools"
cluster_AutoDockTools_pythonsh_binary="/home/apps/CENTOS6/mgltools/1.5.6/bin/
    pythonsh"

# base_dir="/home/zsiegel"
# AutoDockTools_dir="/home/apps/CENTOS6/mgltools/1.5.6/MGLToolsPckgs/
    AutoDockTools"
# AutoDockTools_pythonsh_binary="/home/apps/CENTOS6/mgltools/1.5.6/bin/
    pythonsh"
#
# python_binary="/share/apps/python/2.7.2/bin/python"
# Rscript_binary="/share/apps/R/3.1.0/bin/Rscript"
# openbabel_binaries_dir="/share/apps/openbabel/2.2.1/bin"
```

/Users/zarek/lab/zvina/scripts/constants.py

2.2 `new_grid_or_dock_entry.py`

2.2.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Write a new entry to Dockings.csv or Gridboxes.csv
# (c) Zarek Siegel
# v1 3/10/16
# v1.1 3/11/16

import csv, re, argparse, time, datetime
from constants import *

class Timestamp():
  def __init__(self):
    time_obj = time.time()
    self.display = datetime.datetime.fromtimestamp(time_obj).strftime('%Y-%m-%d %H:%M:%S')
    self.eightdigit = datetime.datetime.fromtimestamp(time_obj).strftime('%Y%m%d')

def new_docking_entry():
  # Hello
  print("\n\tWelcome! This script will add an entry to Dockings.csv\n")

  # Dockings.csv columns:
  # Docking ID
  # Date
  # Protein
  # Protein File
  # Ligset
  # Gridbox
  # Exhaustiveness
  # Number of Models
  # Number of CPUs
  # Notes

  # Going through each variable, taking user input
  dock_input = raw_input("\t\tDocking identifier: ")
  print("\t\t>>> dock set to: {}\n".format(dock_input))

```

```
37  current_time = Timestamp()
38  date_input = raw_input("\t\tDate (enter 'd' to default to {}): ".format(
      current_time.eightdigit))
39  if date_input == "d": date_input = current_time.eightdigit
40  print("\t\t>>> date set to: {}\n".format(date_input))
41
42  prot_input = raw_input("\t\tProtein: ")
43  print("\t\t>>> prot set to: {}\n".format(prot_input))
44
45  prot_file_input = raw_input("\t\tSpecific protein file (without the .pdbqt):
       ")
46  print("\t\t>>> prot_file set to: {}\n".format(prot_file_input))
47
48  ligset_input = raw_input("\t\tLigset identifier: ")
49  print("\t\t>>> ligset set to: {}\n".format(ligset_input))
50
51  box_input = raw_input("\t\tGridbox identifier: ")
52  print("\t\t>>> box set to: {}\n".format(box_input))
53
54  exhaust_input = raw_input("\t\tExhaustiveness: ")
55  print("\t\t>>> exhaust set to: {}\n".format(exhaust_input))
56
57  n_models_input = raw_input("\t\tNumber of models: ")
58  print("\t\t>>> n_models set to: {}\n".format(n_models_input))
59
60  n_cpus_input = raw_input("\t\tNumber of CPUs: ")
61  print("\t\t>>> n_cpus set to: {}\n".format(n_cpus_input))
62
63  notes_input = raw_input("\t\tAny notes (with no commas): ")
64  if notes_input == "":
65    notes_input = "Entered by new_grid_or_dock_entry.py {}".format(
      current_time.display)
66  else:
67    notes_input = "{} (Entered by new_grid_or_dock_entry.py {})".format(
68      notes_input, current_time.display)
69  print("\t\t>>> notes set to: {}\n".format(notes_input))
70
71  # New row as a dictionary
72  new_row = {
73    'Docking ID' : dock_input,
74    'Date' : date_input,
75    'Protein' : prot_input,
76    'Protein File' : prot_file_input,
77    'Ligset' : ligset_input,
78    'Gridbox' : box_input,
```

```
    'Exhaustiveness' : exhaust_input,
    'Number of Models' : n_models_input,
    'Number of CPUs' : n_cpus_input,
    'Notes': notes_input
  }

  # Print confirmation of all entered variabled
  print("\t>>> The new row will be\n\n\
    Docking ID: {dock}\n\
    Date: {date}\n\
    Protein: {prot}\n\
    Protein File: {prot_file}\n\
    Ligset: {ligset}\n\
    Gridbox: {box}\n\
    Exhaustiveness: {exhaust}\n\
    Number of Models: {n_models}\n\
    Number of CPUs: {n_cpus}\n\
    Notes: {notes}\n".format(
              dock = dock_input,
              date = date_input,
              prot = prot_input,
              prot_file = prot_file_input,
              ligset = ligset_input,
              box = box_input,
              exhaust = exhaust_input,
              n_models = n_models_input,
              n_cpus = n_cpus_input,
              notes = notes_input
            )
  )

  # Don't write row without confirmation
  proceed = raw_input("\tWrite this as a new docking entry? [y/n] ")
#   print("\t{}".format(new_row))

  # If "y" is entered, write the row, otherwise don't
  if proceed == "y":
    dockings_csv = "{b_d}/Dockings.csv".format(b_d=base_dir)
    dockings_headers = ["Docking ID", "Date", "Protein", "Protein File",
      "Ligset", "Gridbox", "Exhaustiveness", "Number of Models",
      "Number of CPUs", "Notes"]
    with open(dockings_csv, 'a') as f:
      appender = csv.DictWriter(f, fieldnames=dockings_headers)
      appender.writerow(new_row)
    print("\n\t>>> New row appended to Dockings.csv:\n\topen {}\n".format(
```

```
    dockings_csv))
  else:
    print("\n\t>>> No docking entry written\n")

def new_gridbox_entry():
  # Hello
  print("\n\tWelcome! This script will add an entry to Gridboxes.csv\n")

  # Gridboxes.csv columns:
  # Gridbox Name
  # Protein File
  # Size in x-dimension
  # Size in y-dimension
  # Size in z-dimension
  # Center in x-dimension
  # Center in y-dimension
  # Center in z-dimension
  # Notes

  # Going through each variable, taking user input
  box_input = raw_input("\t\tGridbox Name: ")
  print("\t\t>>> box set to: {}\n".format(box_input))

  prot_file_input = raw_input("\t\tSpecific protein file (without the .pdbqt):
     ")
  print("\t\t>>> prot_file set to: {}\n".format(prot_file_input))

  box_size_x_input = raw_input("\t\tSize in x-dimension: ")
  print("\t\t>>> box_size_x set to: {}\n".format(box_size_x_input))

  box_size_y_input = raw_input("\t\tSize in y-dimension: ")
  print("\t\t>>> box_size_y set to: {}\n".format(box_size_y_input))

  box_size_z_input = raw_input("\t\tSize in z-dimension: ")
  print("\t\t>>> box_size_z set to: {}\n".format(box_size_z_input))

  box_center_x_input = raw_input("\t\tCenter in x-dimension: ")
  print("\t\t>>> box_center_x set to: {}\n".format(box_center_x_input))

  box_center_y_input = raw_input("\t\tCenter in y-dimension: ")
  print("\t\t>>> box_center_y set to: {}\n".format(box_center_y_input))

  box_center_z_input = raw_input("\t\tCenter in z-dimension: ")
  print("\t\t>>> box_center_z set to: {}\n".format(box_center_z_input))

```

```
current_time = Timestamp()
notes_input = raw_input("\t\tAny notes (with no commas): ")
if notes_input == "":
  notes_input = "Entered by new_grid_or_dock_entry.py {}".format(
  current_time.display)
else:
  notes_input = "{} (Entered by new_grid_or_dock_entry.py {})".format(
    notes_input, current_time.display)
print("\t\t>>> notes set to: {}\n".format(notes_input))

# New row as a dictionary
new_row = {
  'Gridbox Name' : box_input,
  'Protein File' : prot_file_input,
  'Size in x-dimension' : box_size_x_input,
  'Size in y-dimension' : box_size_y_input,
  'Size in z-dimension' : box_size_z_input,
  'Center in x-dimension' : box_center_x_input,
  'Center in y-dimension' : box_center_y_input,
  'Center in z-dimension' : box_center_z_input,
  'Notes' : notes_input
}

# Print confirmation of all entered variabled
print("\t>>> The new row will be\n\n\
  Gridbox Name: {box}\n\
  Protein File: {prot_file}\n\
  Size in x-dimension: {box_size_x}\n\
  Size in y-dimension: {box_size_y}\n\
  Size in z-dimension: {box_size_z}\n\
  Center in x-dimension: {box_center_x}\n\
  Center in y-dimension: {box_center_y}\n\
  Center in z-dimension: {box_center_z}\n\
  Notes: {notes}\n".format(
            box = box_input,
            prot_file = prot_file_input,
            box_size_x = box_size_x_input,
            box_size_y = box_size_y_input,
            box_size_z = box_size_z_input,
            box_center_x = box_center_x_input,
            box_center_y = box_center_y_input,
            box_center_z = box_center_z_input,
            notes = notes_input
          )
)
```

```
211
212   # Don't write row without confirmation
213   proceed = raw_input("\tWrite this as a new grid box entry? [y/n] ")
214
215   # If "y" is entered, write the row, otherwise don't
216   if proceed == "y":
217     gridboxes_csv = "{b_d}/Gridboxes.csv".format(b_d=base_dir)
218     gridboxes_headers = ["Gridbox Name", "Protein File", "Size in x-dimension"
      ,
219       "Size in y-dimension", "Size in z-dimension", "Center in x-dimension",
220       "Center in y-dimension", "Center in z-dimension", "Notes"]
221     with open(gridboxes_csv, 'a') as f:
222       appender = csv.DictWriter(f, fieldnames=gridboxes_headers)
223       appender.writerow(new_row)
224     print("\n\t>>> New row appended to Gridboxes.csv:\n\topen {}\n".format(
      gridboxes_csv))
225   else:
226     print("\n\t>>> No grid box entry written\n")
227
228 # Stuff below is commented because this script is being used as a module
229
230 # def main():
231 #   parser = argparse.ArgumentParser(
232 #     description='Write a new entry to Dockings.csv or Gridboxes.csv')
233 #
234 #   parser.add_argument('-b', '--base_dir', metavar='BASE_DIR', type=str,
      nargs=1,
235 #     help='The base directory containing Docking.csv and Gridboxes.csv')
236 #   parser.add_argument('-d', '--new_docking', action='store_true', default=
      False,
237 #     help='New set of docking parameters (written to Dockings.csv)')
238 #   parser.add_argument('-g', '--new_gridbox', action='store_true', default=
      False,
239 #     help='New set of grid box parameters (written to Gridboxes.csv)')
240 #
241 #   args = vars(parser.parse_args())
242 #   global base_dir
243 #   base_dir = str(args['base_dir'][0])
244 #   new_docking = args['new_docking']
245 #   new_gridbox = args['new_gridbox']
246 #
247 #   if new_docking: new_docking_entry()
248 #   elif new_gridbox: new_gridbox_entry()
249 #
250 # if __name__ == "__main__": main()
```

/Users/zarek/lab/zvina/scripts/new_grid_or_dock_entry.py

2.3 `create_docking_object.py`

2.3.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Putting together all parsed data from processed vina results
# (c) Zarek Siegel
# v1 3/5/16 (as assemble_alldata.py)
# v2 3/6/16

from __future__ import print_function
import csv, re, os, subprocess
from constants import *

### A class for docking data, for sourcing, reading, and analyzing
class Docking():
  # Basic docking parameters are contained in CSV file in .../base/
    parameters_csvs/
  def load_parameters(self):
    # Basic docking parameters are stored in base_dir/Dockings.csv
    dockings_csv = "{}/Dockings.csv".format(base_dir)
    with open(dockings_csv) as f:
      reader = csv.DictReader(f)
      for row in reader:
        if row['Docking ID'] == self.dock:
          self.dockings_csv_row = row
    # Source the parameters as class attributes
    self.prot = self.dockings_csv_row['Protein']
    self.prot_file = self.dockings_csv_row['Protein File']
    self.ligset = self.dockings_csv_row['Ligset']
    self.box = self.dockings_csv_row['Gridbox']
    self.exhaust = self.dockings_csv_row['Exhaustiveness']
    self.n_models = int(self.dockings_csv_row['Number of Models'])
    self.n_cpus = self.dockings_csv_row['Number of CPUs']
    self.notes = self.dockings_csv_row['Notes']
    self.date = self.dockings_csv_row['Date']

    # Grid box parameters are stored in base_dir/Gridboxes.csv
    gridboxes_csv = "{}/Gridboxes.csv".format(base_dir)
    with open(gridboxes_csv) as f:
      reader = csv.DictReader(f)
```

```
      for row in reader:
        if row['Gridbox Name'] == self.box and row['Protein File'] == self.
    prot_file:
          self.gridboxes_csv_row = row

    # Source the grid box parameters as class attributes
    self.box_center_x = self.gridboxes_csv_row['Center in x-dimension']
    self.box_center_y = self.gridboxes_csv_row['Center in y-dimension']
    self.box_center_z = self.gridboxes_csv_row['Center in z-dimension']
    self.box_size_x = self.gridboxes_csv_row['Size in x-dimension']
    self.box_size_y = self.gridboxes_csv_row['Size in y-dimension']
    self.box_size_z = self.gridboxes_csv_row['Size in z-dimension']
    self.box_notes = self.gridboxes_csv_row['Notes']

    # Some useful directories
    self.prot_dir = "{b_d}/{p}".format(b_d=base_dir, p=self.prot)
    self.dock_dir = "{b_d}/{p}/{d}".format(b_d=base_dir, p=self.prot, d=self.
    dock)

    self.parameters_loaded = True
    print("   > Loaded docking parameters")

  # Retrieve the list of ligands in the set
  def get_ligset_list(self):
    # If there is a ligset text file; source it;
    # else write it by looking at the files in LIGSET/pdbqts
    self.ligset_list_txt = "{b_d}/ligsets/{ls}/{ls}_list.txt".format(
      b_d=base_dir,ls=self.ligset)
    if os.path.isfile(self.ligset_list_txt):
      with open(self.ligset_list_txt, 'r') as f:
        self.ligset_list = f.read().splitlines()
      print("   > Ligset list sourced from .../{ls}/{ls}_list.txt".format(
        ls=self.ligset))
    else:
      self.ligset_dir = "{b_d}/ligsets/{ls}/pdbqts".format(
        b_d=base_dir,ls=self.ligset)
      self.ligset_list = subprocess.Popen(["ls", self.ligset_dir], stdout=
    subprocess.PIPE)
      self.ligset_list = self.ligset_list.communicate()[0]
      self.ligset_list = re.sub('.pdbqt', '', self.ligset_list)
      self.ligset_list = re.split('\n', self.ligset_list)
      for l in self.ligset_list:
        if l == '' or l == ' ':
          self.ligset_list.remove(l)
      print(("   > Ligset list sourced by looking at files in .../{ls}/pdbqts\
```

```
    n"
80          "         and saved as .../{ls}/{ls}_list.txt".format(ls=self.
    ligset)))
81      with open(self.ligset_list_txt, 'w') as f:
82        for l in self.ligset_list:
83          f.write("{}\n".format(l))
84    self.ligset_list_str = str(self.ligset_list)
85    self.ligset_list_str = re.sub('[\'|\[|\]|,]', '', self.ligset_list_str)
86
87    self.ligset_list_gotten = True
88    print("   > Retrieved ligset list")
89
90  #Create blank alldata dictionary
91  def create_data_dic(self):
92    self.data_dic = {}
93    self.keys = []
94    for lig in self.ligset_list:
95      for m in range(1, self.n_models + 1):
96        key = "{}_{}_m{}".format(self.dock, lig, m)
97        self.data_dic[key] = {
98          'key' : key,
99          'lig' : lig,
100         'model' : m
101       }
102       self.keys.append(key)
103
104   self.is_data_dic_created = True
105   print("   > Created empty data dictionary")
106
107 def print_parameters(self):
108   print("dock=\'{}\'".format(self.dock))
109   print("prot=\'{}\'".format(self.prot))
110   print("prot_file=\'{}\'".format(self.prot_file))
111   print("ligset=\'{}\'".format(self.ligset))
112   print("box=\'{}\'".format(self.box))
113   print("exhaust={}".format(self.exhaust))
114   print("n_models={}".format(self.n_models))
115   print("n_cpus={}".format(self.n_cpus))
116   print("box_center_x={}".format(self.box_center_x))
117   print("box_center_y={}".format(self.box_center_y))
118   print("box_center_z={}".format(self.box_center_z))
119   print("box_size_x={}".format(self.box_size_x))
120   print("box_size_y={}".format(self.box_size_y))
121   print("box_size_z={}".format(self.box_size_z))
122   print("ligset_list=\'{}\'".format(self.ligset_list_str))
```

```
    print("notes=\'{}\'".format(self.notes))
    print("date={}".format(self.date))
    print("box_notes=\'{}\'".format(self.box_notes))

  def export_parameters_to_environment(self):
    os.environ['dock'] = "{}".format(self.dock)
    os.environ['prot'] = "{}".format(self.prot)
    os.environ['prot_file'] = "{}".format(self.prot_file)
    os.environ['ligset'] = "{}".format(self.ligset)
    os.environ['box'] = "{}".format(self.box)
    os.environ['exhaust'] = "{}".format(self.exhaust)
    os.environ['n_models'] = "{}".format(self.n_models)
    os.environ['n_cpus'] = "{}".format(self.n_cpus)
    os.environ['box_center_x'] = "{}".format(self.box_center_x)
    os.environ['box_center_y'] = "{}".format(self.box_center_y)
    os.environ['box_center_z'] = "{}".format(self.box_center_z)
    os.environ['box_size_x'] = "{}".format(self.box_size_x)
    os.environ['box_size_y'] = "{}".format(self.box_size_y)
    os.environ['box_size_z'] = "{}".format(self.box_size_z)
    os.environ['ligset_list'] = "{}".format(self.ligset_list_str)
    os.environ['notes'] = "{}".format(self.notes)
    os.environ['date'] = "{}".format(self.date)
    os.environ['box_notes'] = "{}".format(self.box_notes)

    self.parameters_exported_to_environment = True
    print("   > Exported parameters to shell environment")


  def set_recordkeeping_parameters(self):
    self.parameters_loaded = False
    self.ligset_list_gotten = False
    self.parameters_exported_to_environment = False
    self.is_data_dic_created = False

    self.vina_data_mined = False
    self.binding_sites_list_gotten = False
    self.binding_sites_scored = False
    self.aiad_icpd_calcd = False
    self.all_resis_assessed = False

    self.is_csv_written = False
    self.energies_props_gotten = False
    self.are_poses_clustered = False
    self.is_pickled = False

```

```
168   def __init__(self, d):
169     self.dock = d
170
171     print("---> Creating docking object for docking {}...".format(self.dock))
172
173     self.set_recordkeeping_parameters()
174     self.load_parameters()
175     self.get_ligset_list()
176     self.create_data_dic()
177
178     print("")
```

/Users/zarek/lab/zvina/scripts/create_docking_object.py

2.4 `write_vina_submit_sh.py`

2.4.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Putting together all parsed data from processed vina results
# (c) Zarek Siegel
# v1 3/5/16 (as assemble_alldata.py)
# v2 3/6/16

from __future__ import print_function
import subprocess, os, sys
from constants import *
from create_docking_object import * # Docking

def write_vina_submit_sh(self):
  # (no need for batch submission)
  if self.n_models <= 20:
    batch_submission = False
    vina_submit_sh = "{b_d}/vina_submit_shs/vina_submit_{d}.sh".format(
      b_d=base_dir, d=self.dock)
    if os.path.isfile(vina_submit_sh):
      print(">>> Vina submission script already exists at")
      print("\t{}".format(vina_submit_sh))
      overwrite = raw_input("\n\t>>> Enter 'y' or enter to overwrite, 'n' to
    exit: ")

      if overwrite == "y" or \
         overwrite == "yes" or \
         overwrite == "Y" or \
         overwrite == "Yes" or \
         overwrite == "":
        subprocess.call(["rm", "-f", vina_submit_sh])
        print("")
      else: sys.exit("\n\t> OK, exiting this script\n")

  # (batch submission)
  elif self.n_models > 20:
    batch_submission = True
    vina_submits_dir = "{b_d}/vina_submit_shs/vina_submits_{d}/".format(
      b_d=base_dir, d=self.dock)
```

```
    if os.path.isdir(vina_submits_dir):
      print(">>> Vina submission scripts already exist at")
      print("\t{}".format(vina_submits_dir))
      overwrite = raw_input("\n\t>>> Enter 'y' or enter to overwrite, 'n' to exit: ")

      if overwrite == "y" or \
         overwrite == "yes" or \
         overwrite == "Y" or \
         overwrite == "Yes" or \
         overwrite == "":
        subprocess.call(["rm", "-rf", vina_submits_dir])
        print("")
      else: sys.exit("\n\t> OK, exiting this script\n")

  else: print("! ! ! bad n_models")

  template = (
    "#BSUB -q hp12\n"
    "#BSUB -n {self.n_cpus}\n"
    "#BSUB -N\n"
    "#BSUB -o {cluster_base_dir}/bsub_logs/vina_{subdock}_log.txt\n"
    "#BSUB -J vina_{subdock}\n"
    "\n"
    "# Parameters"
    "dock={self.dock}\n"
    "ligset={self.ligset}\n"
    "ligset_list=\"{self.ligset_list_str}\"\n"
    "\n"
    "# Create the docking and output directories\n"
    "mkdir {cluster_base_dir}/{self.prot}/{self.dock}/\n"
    "mkdir {cluster_base_dir}/{self.prot}/{self.dock}/result_pdbqts\n"
    "\n"
    "vina_start_time=$(date \"+%Y%m%d%H%M%S\")\n"
    "printf '\\n~~~> Vina docking %s started %s' \"$dock\" \"$vina_start_time\"\n"
    "\n"
    "# Vina command\n"
    "for lig in $ligset_list\n"
    "do\n"
    " lig_start_time=$(date \"+%Y%m%d%H%M%S\")\n"
    " printf '\\n\\n> Docking ligand <%s> starting at %s\\n' \"$lig\" \"$lig_start_time\"\n"
    " /share/apps/autodock/autodock_vina_1_1_2_linux_x86/bin/vina \\\n"
    " --receptor {cluster_base_dir}/{self.prot}/{self.prot_file}.pdbqt \\\n"
```

```
    " --ligand {cluster_base_dir}/ligsets/{self.ligset}/pdbqts/$lig.pdbqt \\\n"
    " --out {cluster_base_dir}/{self.prot}/{self.dock}/result_pdbqts/{subdock}_$lig\_results.pdbqt \\\n"
    " --center_x {self.box_center_x} \\\n"
    " --center_y {self.box_center_y} \\\n"
    " --center_z {self.box_center_z} \\\n"
    " --size_x {self.box_size_x} \\\n"
    " --size_y {self.box_size_y} \\\n"
    " --size_z {self.box_size_z} \\\n"
    " --cpu {self.n_cpus} \\\n"
    " --num_modes {self.n_models} \\\n"
    " --exhaustiveness {self.exhaust}\n"
    " lig_end_time=$(date \"+%Y%m%d%H%M%S\")\n"
    " printf '> Finished at %s' \"$lig_start_time\"\n"
    " lig_duration=$(bc <<< \"$lig_end_time - $lig_start_time\")\n"
    " printf '\\n> Docking of ligand %s took %s seconds' \"$lig\" \"$lig_duration\"\n"
    "done\n"
    "\n"
    "vina_end_time=$(date \"+%Y%m%d%H%M%S\")\n"
    "printf '\\n\\n---> Vina job finished %s\\n' \"$vina_end_time\"\n"
    "\n"
    "vina_duration=$(bc <<< \"$vina_end_time - $vina_start_time\")\n"
    "printf '\\n---> Docking %s of ligset %s took %s seconds \\n\\n' \"$dock\" \"$lig\" \"$vina_duration\"\n"
)

template = template.format(
  cluster_base_dir = cluster_base_dir,
  self=self,
  n_models = '{n_models}',
  dock = '{dock}',
  subdock = '{subdock}'
)

# (no need for batch submission)
if not batch_submission:
  template_filled = template.format(
    n_models = self.n_models, dock = self.dock, subdock = self.dock)
  with open(vina_submit_sh, 'w') as f:
    f.write(template_filled)
  print("---> Vina submission script for docking {} has been created. It can be found at:".format(self.dock))
  print("\t{}".format(vina_submit_sh))
```

```
120   # (batch submission)
121   elif batch_submission:
122     subprocess.call(['mkdir', vina_submits_dir])
123     n_batches = self.n_models / 20
124     for b in range(1, n_batches + 1):
125       subdock = "{d}.{b}".format(d = self.dock, b = b)
126       template_filled = template.format(
127         n_models = 20, dock = self.dock, subdock = subdock)
128       vina_submit_sh = "{v_s_d}/vina_submit_{sd}.sh".format(
129         v_s_d = vina_submits_dir, sd = subdock)
130       with open(vina_submit_sh, 'w') as f:
131         f.write(template_filled)
132     print("---> Vina submission scripts for docking h11 have been created.
      They can be found in:")
133     print("\t{}".format(vina_submits_dir))
134
135 Docking.write_vina_submit_sh = write_vina_submit_sh
```

/Users/zarek/lab/zvina/scripts/write_vina_submit_sh.py

2.5 read_alldata.py

2.5.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Output all the data mined and analyzed into a CSV file
# (c) Zarek Siegel

import os, sys
import cPickle as pickle
from create_docking_object import * # Docking


def read_alldata_csv(self):
  self.alldata_csv = "{d_d}/{d}_alldata.csv".format(d_d=self.dock_dir, d=self.
    dock)

  print("---> Reading alldata.csv\n")
  with open(self.alldata_csv, 'r') as csvfile:
    reader = csv.DictReader(csvfile)
    for row in reader:
      self.data_dic[row['key']] = row
  print("! ! ! Warning, it is better to load from the whole object pickled
    versus just the data from a CSV")


Docking.read_alldata_csv = read_alldata_csv

# Save the data dictionary as a pickled file (i.e. in native python format)
def read_docking_pickled(self):
  self.docking_obj_pickled = "{d_d}/{d}.p".format(d_d=self.dock_dir, d=self.
    dock)

  print("---> Reading docking.p\n")
  self = pickle.load(open(self.docking_obj_pickled, 'rb'))

Docking.read_docking_pickled = read_docking_pickled
```

/Users/zarek/lab/zvina/scripts/read_alldata.py

2.6 `cleanup_processed_vina_results.sh`

2.6.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/bin/bash

### Converting and cleaning up processed vina result pdbqts
# (c) Zarek Siegel
# v1 3/5/16
# v1.2 3/6/16

### Required input
dock=$1
# Set scripts directory to the directory containing this script
scripts_dir="$( cd "$( dirname "${BASH_SOURCE[0]}" )" && pwd )"
# Set base directory to the one containing scripts_dir
base_dir="$( cd $scripts_dir && cd .. )"
# Source # AutoDockTools Directory and MGLTools Python binary paths from
    constants.py
source $scripts_dir/constants.py
# Location of pdbqt_to_pdb
q2b_py="$AutoDockTools_dir/Utilities24/pdbqt_to_pdb.py"

# Retrieve the parameters for this docking
# source $base_dir/scripts/load_parameters.sh $dock

# Relevant directories
processed_pdbqts_dir=$base_dir/$prot/$dock/processed_pdbqts
cleanedup_processed_pdbqts_dir=$base_dir/$prot/$dock/
    cleanedup_processed_pdbqts
processed_pdbs_dir=$base_dir/$prot/$dock/processed_pdbs

# Check if already done
if [ -d $processed_pdbs_dir ]; then
  echo "  ! Results already cleaned up (processed_pdbs exists), exiting this
    step"
  exit 1
fi

# Create a directory for cleaned up files and pdb converts
mkdir $cleanedup_processed_pdbqts_dir
mkdir $processed_pdbs_dir
```

```
36
37 # Retrieve ligset list
38 ligset_list_txt=$base_dir/ligsets/$ligset/$ligset\_list.txt
39 ligset_list=$(for l in $(cat $ligset_list_txt); do echo $l; done)
40
41 # The clean-up step
42 for lig in $ligset_list; do
43   for ((m=1;m<=$n_models;m++)); do
44     processed_pdbqt=$processed_pdbqts_dir/$dock\_$lig\_m$m.pdbqt
45     cleanedup_processed_pdbqt=$cleanedup_processed_pdbqts_dir/$dock\_$lig\_m$m
       .pdbqt
46     processed_pdb=$processed_pdbs_dir/$dock\_$lig\_m$m.pdb
47
48     # The clean-up step
49     cat $processed_pdbqt | \
50       sed 's/^\(HETATM..........\).....\1LIG L/g' \
51       > $cleanedup_processed_pdbqt
52
53     # The PDBQT > PDB Conversion step
54     $AutoDockTools_pythonsh_binary $q2b_py -f $cleanedup_processed_pdbqt \
55                           -o $processed_pdb \
56                           1 > /dev/null
57
58     echo "---> processed ligand $lig model $m"
59   done
60 done
61
62 # Overwrite pre-clean-up pvr'd pdbqts with cleaned up ones
63 rm -rf $processed_pdbqts_dir
64 mv $cleanedup_processed_pdbqts_dir $processed_pdbqts_dir
```

/Users/zarek/lab/zvina/scripts/cleanup_processed_vina_results.sh

2.7 `separate_vina_results.sh`

2.7.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/bin/bash

### process_VinaResult and a bit of organization
# (c) Zarek Siegel
# v1 3/5/16
# v1.2 3/6/16
# v2 3/6/16 (batch separation)
# v3 3/11/16

### Required input
dock=$1
# Set scripts directory to the directory containing this script
scripts_dir="$( cd "$( dirname "${BASH_SOURCE[0]}" )" && pwd )"
# Set base directory to the one containing scripts_dir
base_dir="$( cd $scripts_dir && cd .. )"
# Source # AutoDockTools Directory and MGLTools Python binary paths from
    constants.py
source $scripts_dir/constants.py
# Location of process_VinaResult.py
pvr_py="$AutoDockTools_dir/Utilities24/process_VinaResult.py"

# Retrieve the parameters for this docking
# source $base_dir/scripts/load_parameters.sh $dock
#
# # Retrieve ligset list
# ligset_list_txt=$base_dir/ligsets/$ligset/$ligset\_list.txt
# ligset_list=$(for l in $(cat $ligset_list_txt); do echo $l; done)

# Exit if already done
if [ -e $base_dir/$prot/$dock/processed_pdbqts/ ]; then
  echo "  ! Results already separated"
  echo "    ($prot/$dock/processed_pdbqts/ exists),"
  echo "  -> exiting this step"
  exit 1
fi

# Relevant directories
result_pdbqts_dir=$base_dir/$prot/$dock/result_pdbqts
```

```
processed_pdbqts_dir=$base_dir/$prot/$dock/processed_pdbqts

# Create a directory for processed files
mkdir $processed_pdbqts_dir

# The actual process_VinaResult step
receptor_pdbqt=$base_dir/$prot/$prot_file.pdbqt
batch_size=20
# No batches
n_models=$(echo $n_models | sed 's/[^0-9]//')
if [[ "n_models" -le "$batch_size" ]]; then
  for lig in $ligset_list; do
    result_pdbqt=$result_pdbqts_dir/$dock\_$lig\_results.pdbqt
    processed_pdbqt_stem=$processed_pdbqts_dir/$dock\_$lig\_m
    $AutoDockTools_pythonsh_binary $pvr_py -r $receptor_pdbqt \
                         -f $result_pdbqt \
                         -o $processed_pdbqt_stem \
                         1 > /dev/null
    echo "  processed ligand $lig"
  done
# Batches
elif [[ "n_models" -gt "$batch_size" ]]; then
  n_batches=$(bc <<< "$n_models / $batch_size")
  for ((b=1;b<=$n_batches;b++)); do
    echo "  processing batch $b"
    for lig in $ligset_list; do
      result_pdbqt=$result_pdbqts_dir/$dock\.$b\_$lig\_results.pdbqt
      processed_pdbqt_stem=$processed_pdbqts_dir/$dock\.$b\_$lig\_m
      $AutoDockTools_pythonsh_binary $pvr_py -r $receptor_pdbqt \
                           -f $result_pdbqt \
                           -o $processed_pdbqt_stem \
                           1 > /dev/null
      # Rename the processed pdbqts
      for ((m=1;m<=$batch_size;m++)); do
        old_processed_pdbqt=$processed_pdbqts_dir/$dock\.$b\_$lig\_m$m.pdbqt
        new_m=$(bc <<< "(( $b - 1 ) * $batch_size ) + $m")
        new_processed_pdbqt=$processed_pdbqts_dir/$dock\_$lig\_m$new_m.pdbqt
        mv $old_processed_pdbqt $new_processed_pdbqt
      done
      echo "    processed ligand $lig"
    done
  done
else
  echo "! ! ! Error in batch processing (n_models is weird)"
fi
```

```
83
84 # *** check for results, prot.pdb, params
85 # *** check if already pvr'd
```

/Users/zarek/lab/zvina/scripts/separate_vina_results.sh

2.8 `parse_pdb.py`

2.8.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Parsing data from processed pdbqt result files
# (c) Zarek Siegel
# v1 3/5/16

import re

### A class for residues and residue atoms
#   (input is a string of form 'RES123' or 'RES123_A1')

class Residue:
  def __init__(self, str):
    # String
    self.str = str
    # Atom & Residue String
    if re.search(r'^[A-Z]+[0-9]+$', self.str):
      self.atom = None
      self.res_str = self.str
    elif re.search(r'^[A-Z]+[0-9]+_.+$', self.str):
      self.atom = re.sub(r'^[A-Z]+[0-9]+_', '', self.str)
      self.res_str = re.sub(r'_[A-Z0-9]+$', '', self.str)
    else: self.atom = None
    # Residue Index
    self.resi = re.sub(r'^[A-Z]+|_?[^_]*$', '', self.str)
    try:
      self.resi = int(self.resi)
    except ValueError:
      self.resi = None
    # Residue Name
    self.resn = re.sub(r'[0-9]+_?[^_]*$', '', self.str)
    # Dictionary of Props
    self.dic = {'str' : self.str, 'res_str' : self.res_str,
      'resi' : self.resi, 'resn' : self.resn, 'atom' : self.atom}
  def __str__(self):
    return self.str

### A class for molecules, including ones with data from process_VinaResult.py
```

```
#   (input is a .pdb or .pdbqt file address which may or may not be pvr'd)

class Pdb:
  def get_pdb_coords(self):
    _coords = []
    for line in self.pdb_lines:
      if re.search('HETATM|ATOM', line) or (re.search('ATOM', line)):
        _dic = {
          'atomi' : int(line[6:11]),
          'atomn' : line[12:16].replace(" ", ""),
          'resn' : line[17:20].replace(" ", ""),
          'resi' : line[22:26].replace(" ", ""),
          'x' : float(line[30:38].replace(" ", "")),
          'y' : float(line[38:46].replace(" ", "")),
          'z' : float(line[46:54].replace(" ", "")),
          'xyz' : (float(line[30:38].replace(" ", "")),
            float(line[38:46].replace(" ", "")),
            float(line[46:54].replace(" ", "")) ),
          'atom_type' : line[76:78].replace(" ", ""),
          'charge' : line[78:80].replace(" ", "") # element
        }
        _coords.append(_dic)
    self.coords = _coords

  def get_pdbqt_coords(self):
    _coords = []
    for line in self.pdb_lines:
      if re.search('HETATM|ATOM', line) or (re.search('ATOM', line)):
        _dic = {
          'atomi' : int(line[6:11]),
          'atomn' : line[12:16].replace(" ", ""),
          'resn' : line[17:20].replace(" ", ""),
          'resi' : line[22:26].replace(" ", ""),
          'x' : float(line[30:38].replace(" ", "")),
          'y' : float(line[38:46].replace(" ", "")),
          'z' : float(line[46:54].replace(" ", "")),
          'xyz' : (float(line[30:38].replace(" ", "")),
            float(line[38:46].replace(" ", "")),
            float(line[46:54].replace(" ", "")) ),
          'charge' : line[70:76].replace(" ", ""), # partial charge
          'atom_type' : line[77:79].replace(" ", "") # AD4 atom type
        }
        _coords.append(_dic)
    self.coords = _coords

```

```
  def mine_pvr_data(self): # mine data from pvrd file
    contacts = []
    for line in self.pdb_lines:
      # Binding Energy
      if re.search('REMARK VINA RESULT: ', line):
        self.E = re.sub( r'^REMARK VINA RESULT:[ ]+|[ ]+[^ ]+[ ]+[^ ]+$' ,
          r'' , line.replace('\n', '')) # [23:31].replace(" ", ""))
        self.E = float(self.E)
      # RMSD Lower Bound
      if re.search('REMARK VINA RESULT: ', line):
        self.rmsd_lb = re.sub( r'^REMARK VINA RESULT:[ ]+[^ ]+[ ]+|[ ]+[^ ]+$'
     ,
          r'' , line.replace('\n', ''))
        self.rmsd_lb = float(self.rmsd_lb)
      # RMSD Upper Bound
      if re.search('REMARK VINA RESULT: ', line):
        self.rmsd_ub = re.sub( r'^REMARK VINA RESULT:[ ]+[^ ]+[ ]+[ ]+[^ ]+' ,
          r'' , line.replace('\n', ''))
        self.rmsd_ub = float(self.rmsd_ub)
      # Ligand Efficiency (whatever that means...)
      if re.search('USER  AD>  ligand efficiency', line):
        self.pvr_effic = re.sub( r'USER  AD>  ligand efficiency' ,
          r'' , line.replace('\n', ''))
        self.pvr_effic = float(self.pvr_effic)
      # Model Number
      if re.search(r'USER  AD> .+ of .+ MODELS', line):
        self.pvr_model = re.sub( r'USER  AD>| of [0-9]+ MODELS' ,
          r'' , line.replace('\n', ''))
        self.pvr_model = int(self.pvr_model)
      # Torsional Degrees of Freesom
      if re.search('REMARK .+ active torsions:', line):
        self.torsdof = re.sub( r'REMARK|active torsions:' ,
          r'' , line.replace('\n', ''))
        self.torsdof = int(self.torsdof)
      # Number of Contacts
      if re.search('USER  AD> macro_close_ats:', line):
        self.macro_close_ats = re.sub( r'USER  AD> macro_close_ats:' ,
          r'' , line.replace('\n', ''))
        self.macro_close_ats = int(self.macro_close_ats)
      # Contacts
      if re.search(r'^USER  AD> [^ ]+:[^ ]+:[^ ]+:[^ ,]+$', line):
        contacts.append(line.replace('\n', '').replace('USER  AD> ', ''))

    # Contacts Processing
    self.pvr_resis_objs = []
```

```
    self.pvr_resis = []
    self.pvr_resis_atoms = []
    for c in contacts:
      self.pvr_resis_objs.append(Residue(re.sub(r'^[^:]+:[^:]+:', '',
        c).replace(':', '_')))

    for r in self.pvr_resis_objs:
      if r.atom != None:
        self.pvr_resis_atoms.append(r.str)
        self.pvr_resis.append(r.res_str)
      else:
        self.pvr_resis_atoms.append(None)
        self.pvr_resis.append(r.res_str)

    self.pvr_resis_objs = list(set(self.pvr_resis_objs)) # remove duplicates
    self.pvr_resis = list(set(self.pvr_resis))
    self.pvr_resis_atoms = list(set(self.pvr_resis_atoms))

    self.pvr_data = {
      'E' : self.E,
      'rmsd_ub' : self.rmsd_ub,
      'rmsd_lb' : self.rmsd_lb,
      'pvr_resis' : self.pvr_resis,
      'pvr_resis_atoms' : self.pvr_resis_atoms,
      'pvr_resis_objs' : self.pvr_resis_objs,
      'torsdof' : self.torsdof,
      'macro_close_ats' : self.macro_close_ats,
      'pvr_model' : self.pvr_model
    }

  def get_types(self):
    # Detect if its been through ADT process_VinaResult.py
    self.is_pvrd = False # by default
    try:
      for line in self.pdb_lines:
        if re.search('REMARK VINA RESULT: ', line):
          self.mine_pvr_data()
          self.is_pvrd = True
    except AttributeError:
      print("! ! ! AttributeError while trying to read PDB lines")

    # Determine file type PDB/PDBQT (they are slightly different)
    if self.pdb_file_in[-5:] == 'pdbqt':
      self.get_pdbqt_coords()
      self.file_type = 'pdbqt'
```

```
173     elif self.pdb_file_in[-3:] == 'pdb':
174       self.get_pdb_coords()
175       self.file_type = 'pdb'
176     else:
177       print("!!! BAD FILETYPE !!!")
178 
179   def __init__(self, pdb_file_in):
180     # Specify input file
181     self.pdb_file_in = pdb_file_in
182     # Try to read it, else error
183     try:
184       pdb_file_open = open(pdb_file_in)
185       with pdb_file_open as f:
186         self.pdb_lines = f.readlines()
187     except IOError:
188       print("! ! ! IOError while trying to read PDB lines")
189       pass
190     # Determine if PDB or PDBQT, and whether it has been through
      process_VinaResult.py
191     self.get_types() # this also mines the actual data
```

/Users/zarek/lab/zvina/scripts/parse_pdb.py

2.9 `mine_vina_data.py`

2.9.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Mine data from processed vina results, add to data dictionary
# (c) Zarek Siegel

from parse_pdb import * # Pdb
from create_docking_object import * # Docking

# Mine Vina result for data (actual mining is in parse_pdb.py, acting via the Pdb class)
def mine_vina_data(self):
  print("---> Mining data from processed vina result PDBQTs...")
  ## ** check if proper files exist
  for lig in self.ligset_list:
    for m in range(1, self.n_models + 1):
      key = "{}_{}_m{}".format(self.dock, lig, m)
      processed_pdbqt = "{d_d}/processed_pdbqts/{key}.pdbqt".format(
        d_d=self.dock_dir, key=key)
      if os.path.isfile(processed_pdbqt):
        try: pose = Pdb(processed_pdbqt)
        except: print("! ! ! Error while trying to read PDB for {}".format(key))
        try:
          pose_dic = {
            'E' : pose.E,
            'rmsd_ub' : pose.rmsd_ub,
            'rmsd_lb' : pose.rmsd_lb,
            'pvr_resis' : pose.pvr_resis,
            'pvr_resis_atoms' : pose.pvr_resis_atoms,
            'pvr_resis_objs' : pose.pvr_resis_objs,
            'torsdof' : pose.torsdof,
            'pvr_n_contacts' : pose.macro_close_ats,
            'pvr_model' : pose.pvr_model,
            'pvr_effic' : pose.pvr_effic,
            'coords' : pose.coords,
            'pvr_obj' : pose,
            'pdbqt_address' : processed_pdbqt,
            'pdb_address' : re.sub('pdbqt', 'pdb', processed_pdbqt)
```

```
37            }
38          except AttributeError:
39            print("! ! ! pose {} failed, check for the processed PDBQT".format(
      key))
40        else: print("! ! ! processed_pdbqt does not exist for {}".format(key))
41
42        self.data_dic[key] = dict(self.data_dic[key].items() + pose_dic.items())
43
44    self.vina_data_mined = True
45    print("   > Data dictionary filled with data from process_VinaResult.py\n")
46
47  Docking.mine_vina_data = mine_vina_data
```

/Users/zarek/lab/zvina/scripts/mine_vina_data.py

2.10 `aiad_icpd.py`

2.10.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Calculating average inter-atomic distance
# (c) Zarek Siegel
# v1 3/6/16

from parse_pdb import *
from math import sqrt
# from numpy import mean

def mean(list):
  list_mean = float(sum(list)) / len(list)
  return list_mean

class Molecule():
  def list_coords(self):
    self.coord_triples = []
    for atom in self.pdb.coords:
      self.coord_triples.append(atom['xyz'])

  def get_centerpoint(self):
    x_coords = []
    y_coords = []
    z_coords = []
    for triple in self.coord_triples:
      x_coords.append(triple[0])
      y_coords.append(triple[1])
      z_coords.append(triple[2])
    self.centerpoint = (mean(x_coords), mean(y_coords), mean(z_coords))

  def __init__(self, pdb):
    self.pdb = pdb
    self.list_coords()
    self.get_centerpoint()

def threeD_distance(triple1, triple2):
  x1 = triple1[0]
  y1 = triple1[1]
```

```
  z1 = triple1[2]
  x2 = triple2[0]
  y2 = triple2[1]
  z2 = triple2[2]
  distance = sqrt( ((x2 - x1)**2) + ((y2 - y1)**2) + ((z2 - z1)**2) )
  return distance

def caclulate_aiad(pdb1, pdb2):
  molc1 = Molecule(pdb1)
  molc2 = Molecule(pdb2)
  dist_list = []
  for triple1 in molc1.coord_triples:
    dists_from_t1 = []
    for triple2 in molc2.coord_triples:
      dist = threeD_distance(triple1, triple2)
      dists_from_t1.append(dist)
    dist_list.append(min(dists_from_t1))
  return mean(dist_list)

def calculate_icpd(pdb1, pdb2):
  molc1 = Molecule(pdb1)
  molc2 = Molecule(pdb2)
  return threeD_distance(molc1.centerpoint, molc2.centerpoint)

def main():
  # m1_p = Pdb("/Users/zarek/lab/Docking/p300/p27/res_pdbqts_cleaned/p27_s3_m4
    .pdbqt")
#   m2_p = Pdb("/Users/zarek/lab/Docking/p300/p27/res_pdbqts_cleaned/
    p27_s2_m142.pdbqt")
#   m1 = Molecule(m1_p)
#   m2 = Molecule(m2_p)
#   caclulate_aiad(m1_p, m2_p)
  pass

if __name__ == "__main__": main()
```

/Users/zarek/lab/zvina/scripts/aiad_icpd.py

2.11 `binding_site_analysis.py`

2.11.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Mine data from processed vina results, add to data dictionary
# (c) Zarek Siegel

from __future__ import print_function
import re
from operator import itemgetter
from create_docking_object import * # Docking
from parse_pdb import * # Pdb
from aiad_icpd import *


# Create a list of the binding sites previously prepared for the protein
def get_binding_sites_list(self):
  if not self.vina_data_mined: self.mine_vina_data()

  binding_sites_dir = "{b_d}/binding_sites/{p_f}".format(
    b_d=base_dir, p_f=self.prot_file)
  self.binding_sites_list = []
  self.binding_sites_objs = {}
  for root, dirs, files in os.walk(binding_sites_dir):
    for file in files:
      self.binding_sites_list.append(re.sub('.pdb', '', file))
      try: self.binding_sites_objs[re.sub('.pdb', '', file)] = Pdb("{}/{}".
    format(root, file))
      except: print("! ! ! Error while trying to read PDB for {}".format(file)
    )

  self.bs_resis_lists = {}
  self.bs_resis_atoms_lists = {}

  for bs, bso in self.binding_sites_objs.items():
    bs_resis = []
    if self.evaluate_resis_atoms:
      bs_resis_atoms = []
    for atom in bso.coords:
      bs_resis.append("{}{}".format(atom['resn'], atom['resi']))
```

```
      if self.evaluate_resis_atoms:
        bs_resis_atoms.append("{}{}_{}".format(atom['resn'], atom['resi'], atom['atomn']))
    self.bs_resis_lists[bs] = list(set(bs_resis))
    if self.evaluate_resis_atoms:
      self.bs_resis_atoms_lists[bs] = list(set(bs_resis_atoms))

  self.binding_sites_list_gotten = True
  print("   > Retrieved binding sites")

Docking.get_binding_sites_list = get_binding_sites_list

# Score the binding sites in terms of the residues they contact
# relative to those contained in the reference PDB
def score_binding_sites(self):
  if not self.vina_data_mined: self.mine_vina_data()
  print("---> Scoring poses against binding sites by ratio of residues contacted...")
  if not self.binding_sites_list_gotten: self.get_binding_sites_list()

  print("   > Scoring binding sites for pose ", end="")
  char_count = 31
  for pose in self.keys:
    if char_count <= 76:
      print(pose, end=" ")
      char_count = char_count + len(pose) + 1
    else:
      print("\n\t{}".format(pose), end = " ")
      char_count = len(pose) + 1
    for bs in self.binding_sites_list:
      resis_union = ( set(self.bs_resis_lists[bs]) & set(self.data_dic[pose]['pvr_resis']) )
      self.data_dic[pose]["{}_fraction".format(bs)] = float(len(resis_union)) / float(len(self.bs_resis_lists[bs]))
      if self.evaluate_resis_atoms:
        resis_atoms_union = ( set(self.bs_resis_atoms_lists[bs]) & set(self.data_dic[pose]['pvr_resis_atoms']) )
        self.data_dic[pose]["{}_atoms_fraction".format(bs)] = float(len(resis_atoms_union)) / float(len(self.bs_resis_atoms_lists[bs]))

  self.binding_sites_scored = True
  print("\n   > Done scoring binding sites\n")

Docking.score_binding_sites = score_binding_sites

```

```
# Score binding sites by average inter-atomic distance
# and inter-centerpoint difference
# Acting via aiad_icpd.py
def aiad_icpd_binding_sites(self):
  if not self.binding_sites_list_gotten: self.get_binding_sites_list()

  print("---> Scoring poses against binding sites by AIAD and ICPD...")
  print("   > Scoring AIAD and ICPD for pose ", end="")
  char_count = 31
  for pose in self.keys:
    if char_count <= 76:
      print(pose, end=" ")
      char_count = char_count + len(pose) + 1
    else:
      print("\n\t{}".format(pose), end = " ")
      char_count = len(pose) + 1
    for bs, bso in self.binding_sites_objs.items():
      aiad = caclulate_aiad(self.data_dic[pose]['pvr_obj'], bso)
      self.data_dic[pose]["{}_aiad".format(bs)] = aiad
      icpd = calculate_icpd(self.data_dic[pose]['pvr_obj'], bso)
      self.data_dic[pose]["{}_icpd".format(bs)] = icpd

  self.aiad_icpd_calcd = True
  print("\n   > Done calculating AIAD and ICPD for binding sites\n")

Docking.aiad_icpd_binding_sites = aiad_icpd_binding_sites

# Add attributes for whether the ligand contacts each residue of the protein
def assess_all_resis(self):
  if not self.vina_data_mined: self.mine_vina_data()

  print("---> Evaluating residues contacted for each pose")
  self.prot_pdbqt = "{p_d}/{p_f}.pdbqt".format(p_d=self.prot_dir, p_f=self.
    prot_file)
  try: self.prot_obj = Pdb(self.prot_pdbqt)
  except: print("! ! ! Error while trying to read PDB for {}".format(file))
  self.prot_resis_list = []
  if self.evaluate_resis_atoms:
    self.prot_resis_atoms_list = []
  for atom in self.prot_obj.coords:
    self.prot_resis_list.append((atom['resn'], atom['resi']))
    if self.evaluate_resis_atoms:
      self.prot_resis_atoms_list.append((atom['resn'], atom['resi'], atom['
    atomn']))
    # self.prot_resis_list.append("{}{}".format(atom['resn'], atom['resi']))
```

```
119     # self.prot_resis_atoms_list.append("{}{}_{}".format(atom['resn'], atom['
        resi'], atom['atomn']))
120   self.prot_resis_list = list(set(self.prot_resis_list))
121   self.prot_resis_list = sorted(self.prot_resis_list, key=itemgetter(1))
122   self.prot_resis_list = ["{}{}".format(r[0], r[1]) for r in self.
        prot_resis_list]
123   if self.evaluate_resis_atoms:
124     self.prot_resis_atoms_list = list(set(self.prot_resis_atoms_list))
125     self.prot_resis_atoms_list = sorted(self.prot_resis_atoms_list, key=
        itemgetter(1,2))
126     self.prot_resis_atoms_list = ["{}{}_{}".format(r[0], r[1], r[2]) for r in
        self.prot_resis_atoms_list]
127     # self.prot_resis_atoms_list = list(set(self.prot_resis_atoms_list))
128
129   for pose in self.data_dic:
130     for res in self.prot_resis_list:
131       if res in self.data_dic[pose]['pvr_resis']:
132         self.data_dic[pose][res] = 1
133       else:
134         self.data_dic[pose][res] = 0
135     if self.evaluate_resis_atoms:
136       for atom in self.prot_resis_atoms_list:
137         if atom in self.data_dic[pose]['pvr_resis_atoms']:
138           self.data_dic[pose][atom] = 1
139         else:
140           self.data_dic[pose][atom] = 0
141
142   self.all_resis_assessed = True
143   print("   > Residues contacted added to data dictionary\n")
144
145 Docking.assess_all_resis = assess_all_resis
```

/Users/zarek/lab/zvina/scripts/binding_site_analysis.py

2.12 energies_properties.py

2.12.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

###
# (c) Zarek Siegel
# v1 3/16/16

import subprocess, re, sys
from constants import *

##########

def get_energies(molc_in):
  obenergy_binary = "{}/obenergy".format(openbabel_binaries_dir)

  obenergy_out = subprocess.Popen([obenergy_binary, molc_in],
    stdout=subprocess.PIPE, stderr=subprocess.PIPE)
  obenergy_out = obenergy_out.communicate()[0]
  obenergy_out = re.split('\n', obenergy_out)

  #      TOTAL BOND STRETCHING ENERGY =   28.617 kJ/mol
  #      TOTAL ANGLE BENDING ENERGY =   18.099 kJ/mol
  #      TOTAL TORSIONAL ENERGY =   62.835 kJ/mol
  #      TOTAL VAN DER WAALS ENERGY =  104.782 kJ/mol
  #
  # TOTAL ENERGY = 214.33290 kJ/mol

  obenergy_dic = {}

  def extract_energy_value(search_str):
    for row in obenergy_out:
      if re.search(search_str, row):
#         print(row)
        value = (re.sub(r'^\s*([\w ]+)=\s*(-?\d+\.\d+)\s+(.+)$', r'\2', row))
        units = (re.sub(r'^\s*([\w ]+)=\s*(-?\d+\.\d+)\s+(.+)$', r'\3', row))
    return value#, units

  search_str_list = [
    "TOTAL BOND STRETCHING ENERGY",
```

```
    "TOTAL ANGLE BENDING ENERGY",
    "TOTAL TORSIONAL ENERGY",
    "TOTAL ENERGY"
  ]

  for search_str in search_str_list:
    parameter = search_str.lower()
    parameter = re.sub(' ', '_', parameter)
    obenergy_dic[parameter] = extract_energy_value(search_str)

  return obenergy_dic
##########

##########

def get_properties(molc_in):
  obprop_binary = "{}/obprop".format(openbabel_binaries_dir)

  obprop_out = subprocess.Popen([obprop_binary, molc_in],
    stdout=subprocess.PIPE, stderr=subprocess.PIPE)
  obprop_out = obprop_out.communicate()[0]
  obprop_out = re.split('\n', obprop_out)

  # name             /Users/zarek/GitHub/TaylorLab/zvina/ligsets/hls1/pdbs/ab.
    pdb 1
  # formula          C6H12O6
  # mol_weight       180.156
  # exact_mass       180.063
  # canonical_SMILES OC[C@H]1O[C@@H](O)[C@@H]([C@H]([C@H]1O)O)O
  #
  # InChI            InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2
    /t2-,3+,4+,5-,6-/m1/s1
  #
  # num_atoms        24
  # num_bonds        24
  # num_residues     1
  # sequence         LIG
  # num_rings        1
  # logP             -3.2214
  # PSA              110.38
  # MR               35.736

  obprop_dic = {}

  def extract_property_value(search_str):
```

```
    for row in obprop_out:
      if re.search(search_str, row):
    #     print(row)
        value = (re.sub(r'^(\w+)\s+(\S+)\s?\S?$', r'\2', row))
    return value

  search_str_list = [
    "name", "formula", "mol_weight",
    "exact_mass", "canonical_SMILES", "num_atoms",
    "num_bonds", "num_rings", "logP", "PSA", "MR"
  ]

  for search_str in search_str_list:
    parameter = search_str
    obprop_dic[parameter] = extract_property_value(search_str)

  return obprop_dic
##########

def get_combined_dic(molc_in):
  combined_dic = dict(get_energies(molc_in).items() + \
    get_properties(molc_in).items())
  return combined_dic

def print_energies_properties(molc_in):
  print("\n{0:.<36}{v}".format("PROPERTY", v="VALUE"))
  for prop, value in get_combined_dic(molc_in).items():
    print("{0:.<36}{v}".format(prop, v=value))

def main():
  print_energies_properties(sys.argv[1])

if __name__ == "__main__": main()
```

/Users/zarek/lab/zvina/scripts/energies_properties.py

2.13 `get_pose_energies_properties.py`

2.13.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

###
# (c) Zarek Siegel

from __future__ import print_function
from energies_properties import *
from create_docking_object import * # Docking

def get_pose_energies_properties(self):
  if not self.vina_data_mined: self.mine_vina_data()

  print("---> Assessing molecular properties and energies for pose...")
  # Properties are gathered once per ligand
  #   But energies are gathered for each pose
  print("   > Evaluating pose ", end="")
  for lig in self.ligset_list:
    first_pose = "{}_{}_m{}".format(self.dock, lig, "1")
    first_pdbqt = self.data_dic[first_pose]['pdbqt_address']

    char_count = 24
    pose_properties_dic = get_properties(first_pdbqt)
    for m in range(1, self.n_models + 1):
      pose = "{}_{}_m{}".format(self.dock, lig, m)
      if char_count <= 76:
        print(pose, end=" ")
        char_count = char_count + len(pose) + 1
      else:
        print("\n\t{}".format(pose), end = " ")
        char_count = len(pose) + 1
      pdbqt = self.data_dic[pose]['pdbqt_address']
      pose_energies_dic = get_energies(pdbqt)
      combined_dic = dict(pose_properties_dic.items() +
        pose_energies_dic.items())
#       print(combined_dic)
      self.data_dic[pose] = dict(self.data_dic[pose].items() + combined_dic.
    items())

```

```
38    self.energies_props_gotten = True
39
40    print("\n   > Done\n")
41
42  Docking.get_pose_energies_properties = get_pose_energies_properties
```

/Users/zarek/lab/zvina/scripts/get_pose_energies_properties.py

2.14 `write_alldata.py`

2.14.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Output all the data mined and analyzed into a CSV file
# (c) Zarek Siegel

import os, sys
import cPickle as pickle
from create_docking_object import * # Docking

def get_fieldnames(self):
  # Determine which headers to write to the CSV

  # Choose from these groups
  self.alldata_fieldnames = ['key', 'lig', 'model'] # basics
#   energies_properties_fieldnames = self.energies_dic.keys() + self.
    properties_dic.keys()

  if self.vina_data_mined:
    pvr_fieldnames = ['E', 'rmsd_lb', 'rmsd_ub', 'pvr_effic',
      'pvr_n_contacts', 'torsdof', 'pdbqt_address', 'pdb_address'] # (
    processed vina results)
    self.alldata_fieldnames = self.alldata_fieldnames + pvr_fieldnames

  if self.energies_props_gotten:
    energies_properties_fieldnames = [
      'total_bond_stretching_energy', 'total_angle_bending_energy',
      'total_torsional_energy', 'total_energy',
      'name', 'formula', 'mol_weight', 'exact_mass', 'canonical_SMILES',
      'num_atoms', 'num_bonds', 'num_rings', 'logP', 'PSA', 'MR'
    ]
    self.alldata_fieldnames = self.alldata_fieldnames +
    energies_properties_fieldnames

  if self.binding_sites_scored:
    binding_site_fieldnames = []
    for bs in self.binding_sites_list:
      binding_site_fieldnames.append("{}_fraction".format(bs))
      binding_site_fieldnames.append("{}_atoms_fraction".format(bs))
```

```
    self.alldata_fieldnames = self.alldata_fieldnames +
    binding_site_fieldnames

  if self.aiad_icpd_calcd:
    aiad_icpd_fieldnames = []
    for bs in self.binding_sites_list:
      aiad_icpd_fieldnames.append("{}_aiad".format(bs))
      aiad_icpd_fieldnames.append("{}_icpd".format(bs))
    self.alldata_fieldnames = self.alldata_fieldnames + aiad_icpd_fieldnames

  if self.all_resis_assessed:
    self.alldata_fieldnames = self.alldata_fieldnames + self.prot_resis_list
    if self.evaluate_resis_atoms:
      self.alldata_fieldnames = self.alldata_fieldnames + self.
    prot_resis_atoms_list

Docking.get_fieldnames = get_fieldnames

def write_alldata_csv(self):
  self.alldata_csv = "{d_d}/{d}_alldata.csv".format(d_d=self.dock_dir, d=self.
    dock)

  # If the CSV already exists, ask to overwrite
  if os.path.isfile(self.alldata_csv):
    print(">>>> Docking CSV file already exists at")
    print("\t{}".format(self.alldata_csv))
    overwrite = raw_input("\n\t>>>> Enter 'y' or enter to overwrite, 'n' to
    exit: ")
    if overwrite == "y" or \
       overwrite == "yes" or \
       overwrite == "Y" or \
       overwrite == "Yes" or \
       overwrite == "":
      subprocess.call(["rm", "-f", self.alldata_csv])
      print("")
    else: sys.exit("\n\t> OK, exiting this script\n")

  self.get_fieldnames()

  print("---> Writing alldata.csv...")
  with open(self.alldata_csv, 'w') as csvfile:
    writer = csv.DictWriter(csvfile, fieldnames=self.alldata_fieldnames)
    writer.writeheader()
    for key in self.keys:
      row = {}
```

```
      for f in self.alldata_fieldnames:
        try: row[f] = self.data_dic[key][f]
        except KeyError:
          print("! ! ! KeyError while trying to write {}".format(f))
          row[f] = "!Err!"
      writer.writerow(row)

  self.is_csv_written = True
  print("   > Completed alldata.csv is located at:\n\t{}\n".format(self.
    alldata_csv))

Docking.write_alldata_csv = write_alldata_csv

# Save the data dictionary as a pickled file (i.e. in native python format)
def write_docking_pickled(self):
  self.docking_obj_pickled = "{d_d}/{d}.p".format(d_d=self.dock_dir, d=self.
    dock)

  # If the pickled dictionary already exists, ask to overwrite
  if os.path.isfile(self.docking_obj_pickled):
    print(">>>> Pickled docking object file already exists at")
    print("\t{}".format(self.docking_obj_pickled))
    overwrite = raw_input("\n\t>>>> Enter 'y' or enter to overwrite, 'n' to
    exit: ")
    if overwrite == "y" or \
       overwrite == "yes" or \
       overwrite == "Y" or \
       overwrite == "Yes" or \
       overwrite == "":
      subprocess.call(["rm", "-f", self.docking_obj_pickled])
      print("")
    else: sys.exit("\n\t> OK, exiting this script\n")

  print("---> Pickling docking object...")
  pickle.dump(self, open(self.docking_obj_pickled, 'wb'))

  self.is_pickled = True
  print("   > Pickled docking object located at:\n\t{}\n".format(self.
    docking_obj_pickled))

Docking.write_docking_pickled = write_docking_pickled
```

/Users/zarek/lab/zvina/scripts/write_alldata.py

2.15 `correlations.py`

2.15.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
#!/usr/bin/env python

### Output all the data mined and analyzed into a CSV file
# (c) Zarek Siegel

from scipy.stats.stats import pearsonr
from operator import itemgetter
from create_docking_object import * # Docking
from write_alldata import get_fieldnames

def correlations(self):

  self.get_fieldnames()

  not_quant = ['key', 'lig', 'model', 'pdbqt_address', 'pdb_address',
    'name', 'formula', 'canonical_SMILES']
  correl_vars = [var for var in self.alldata_fieldnames if var not in
    not_quant]

  correl_var_lists = {}
  for var in correl_vars:
    correl_var_lists[var] = []
    for pose in self.keys:
      try: correl_var_lists[var].append(self.data_dic[pose][var])
      except KeyError: correl_var_lists[var].append(None)

  correls = []
  for var1 in correl_vars:
    print(var1)
    for var2 in correl_vars:
      pearson = pearsonr(correl_var_lists[var1], correl_var_lists[var2])
      correls.append(
        {
          'var1' : var1,
          'var2' : var2,
          'correl' : pearson[0],
          'cor_mag' : abs(pearson[0]),
          'p' : pearson[1]
```

```
        }
      )


  sig_correls = [c for c in correls if c['p'] < 0.05]

  print(len(correls))
  print(len(sig_correls))
  for c1 in sig_correls:
    # print(c1)
    if (c1['var1'] == c1['var2']):
        sig_correls.remove(c1)
    for c2 in sig_correls:
      # print(c2)
      if (c2['var1'] == c2['var2']):
        sig_correls.remove(c2)
      elif (c1['var1'] == c2['var2']) and (c1['var2'] == c2['var1']):
        sig_correls.remove(c2)

      else:
        continue
  print(len(correls))
  print(len(sig_correls))
  sig_correls = sorted(sig_correls, key=itemgetter('cor_mag', 'p', 'var1'))

  # Don't print correlations between two residues
  for c in sig_correls:
    if not (c['var1'] in self.prot_resis_list) and (c['var2'] in self.
    prot_resis_list):
      print("{:<30}{:<30}{:<30}{:<30}".format(c['var1'], c['var2'], c['correl'
    ], c['p']))




#   print("{} = {}".format("parameters_loaded", self.parameters_loaded))
#   print("{} = {}".format("ligset_list_gotten", self.ligset_list_gotten))
#   print("{} = {}".format("parameters_exported_to_environment", self.
    parameters_exported_to_environment))
#   print("{} = {}".format("is_data_dic_created", self.is_data_dic_created))
#
#   print("{} = {}".format("vina_data_mined", self.vina_data_mined))
#   print("{} = {}".format("binding_sites_list_gotten", self.
    binding_sites_list_gotten))
```

```
#   print("{} = {}".format("binding_sites_scored", self.binding_sites_scored))
#   print("{} = {}".format("aiad_icpd_calcd", self.aiad_icpd_calcd))
#   print("{} = {}".format("all_resis_assessed", self.all_resis_assessed))
#
#   print("{} = {}".format("is_csv_written", self.is_csv_written))
#   print("{} = {}".format("energies_props_gotten", self.energies_props_gotten
    ))
#   print("{} = {}".format("are_poses_clustered", self.are_poses_clustered))
#   print("{} = {}".format("is_pickled", self.is_pickled))



Docking.correlations = correlations


# pvr_fieldnames = ['E', 'rmsd_lb', 'rmsd_ub', 'pvr_effic',
#       'pvr_n_contacts', 'torsdof', 'pdbqt_address', 'pdb_address'] # (
    processed vina results)
#     self.alldata_fieldnames = self.alldata_fieldnames + pvr_fieldnames
#
#   if self.energies_props_gotten:
#     energies_properties_fieldnames = [
#       'total_bond_stretching_energy', 'total_angle_bending_energy',
#       'total_torsional_energy', 'total_energy',
#       'name', 'formula', 'mol_weight', 'exact_mass', 'canonical_SMILES',
#       'num_atoms', 'num_bonds', 'num_rings', 'logP', 'PSA', 'MR'
```

/Users/zarek/lab/zvina/scripts/correlations.py

2.16 postdocking_graphs.R

2.16.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

```
### Docking data graphs (hepi and p300 - pls1a and hls1)
#   2/14/16 Zarek Siegel
#   2/21/16 up to full ggplot2 replacement
#   2/23/16 more density plots, p300 and hepi compatible
# v1.0 3/16/16 lots stuff

rm(list=ls(all=TRUE)) # clear out old variables
library(foreign) # for reading csv
library(ggplot2)
library(reshape2)

### Command line arguments

args <- commandArgs()
script_path <- args[4]
script_path <- sub("--file=", "", script_path)
base_dir <- sub("/scripts/postdocking_graphs.R", "", script_path)
# base_dir <- "/Users/zarek/GitHub/TaylorLab/zvina"
dock <- args[6]



### Basic parameters
# dock <- "p7b" # docking id
# if(substr(dock,0,1) == "p") {prot <- "p300"} # p300 dockings are labeled p##
# if(substr(dock,0,1) == "h") {prot <- "hepi"} # hepi dockings are labeled h##
# assumptions
#   -dockings have a docking id of the form d##,
#     where d represents the protein and ## is a number
#   -inallo the home docking directory,
#     there is a directory with the protein's name (e.g. .../p300/).
#     (this is what I mean by 'dock directory')
#   -inallo the protein directory directory,
#     there is a directory with the docking id (e.g. .../p300/p27/)
#   -inallo the docking directory,
#     threre is a CSV file called d##_alldata.csv (** see zarek or a sample
    for details)

```

```
# docks.xlsx <- "/Users/zarek/lab/Docking/docks.xlsx"
# dock.params <- read.xlsx2(docks.xlsx, sheetName = prot)
#
# ligset <- as.character(dock.params$ligSET[dock.params$DOCK == dock])
#
# all.ligsets <- read.xlsx2(docks.xlsx, sheetName = "ligsets")
# ligset_list <- as.character(all.ligsets$lig_list[all.ligsets$name == ligset
    ])
# ligset_list <- unlist(strsplit(ligset_list, "[ ]"))

# ### System directories
# docking.base.dir <- "/Users/zarek/lab/Docking/"
# dock.dir <- paste(docking.base.dir, prot, "/", dock, "/", sep = "")
# graphs_dir <- paste(dock.dir, "graphs/", sep="")
# if(dir.exists(graphs_dir)) {
#   print("graphs directory was not created because it already exists")
# } else {dir.create(graphs_dir)}
#
# ### Read in alldata.csv
# alldata.csv <- paste(dock.dir, dock, "_alldata.csv", sep="")
# data <- read.csv(alldata.csv)
#
# ### Look up ligset
# # ** add this**, this (below) is temporary
#
# # ligset_list <- c("adph", "fdla", "ab", "gb", "aam",
# #                  "abm", "gam", "gbm", "ab3", "gb3",
# #                  "ab6", "gb6", "ab7", "gb7", "aa8",
# #                  "ab8", "ga8", "gb8", "gb8y", "aa10",
# #                  "ab10", "ga10", "gb10")
#
# ### Look up ligset
# #**KLUDGE* ** add this**, this (below) is temporary
# if(prot == "hepi") {
#   binding_sites <- c("adph", "fdla", "allo")
#   #***# Order levels
#   ncs.sugargrouped <- c("adph", "fdla",
#                         "ab", "aam", "abm", "ab3", "ab6",
#                         "ab7", "aa8", "ab8", "aa10", "ab10",
#                         "gb", "gam", "gbm", "gb3", "gb6",
#                         "gb7", "ga8", "gb8", "gb8y",
#                         "ga10", "gb10")
#   ligset_list <- ncs.sugargrouped
# }
# if(prot == "p300") {
```

```r
#   binding_sites <- c("lys", "coa", "side", "allo1", "allo2") # "coa_adpp", "coa_pant",
#   ligset_list <- c("Garcinol", "CTB", "EGCG", "CTPB", "C646")
# }
# ##**##
#
# ### Recode variables with more convenient names
# if(is.element(dock, c("p28", "p29", "p30"))) {
#   ligset.coded <- c("ng", "s2", "ne", "s1", "s3")
#   ligset.names <- factor(c("Garcinol", "CTB", "EGCG", "CTPB", "C646"))
#   data$lig <- ligset.names[match(data$lig, ligset.coded)]
#   data$lig <- factor(data$lig, levels = ligset.names)
# }
# if(is.element(dock, c("p27", "p31"))) {
#   ligset.names <- factor(c("Garcinol", "CTB", "EGCG", "CTPB", "C646"))
#   data$lig <- factor(data$lig, levels = ligset.names)
# }


dockings_csv <- paste0(base_dir, "/", "Dockings.csv")
dockings_df <- read.csv(dockings_csv)

prot <- as.character(dockings_df$Protein[dockings_df$Docking.ID == dock])
date <- as.character(dockings_df$Date[dockings_df$Docking.ID == dock])
prot_file <- as.character(dockings_df$Protein.File[dockings_df$Docking.ID == dock])
ligset <- as.character(dockings_df$Ligset[dockings_df$Docking.ID == dock])
box <- as.character(dockings_df$Gridbox[dockings_df$Docking.ID == dock])
exhaust <- as.character(dockings_df$Exhaustiveness[dockings_df$Docking.ID == dock])
n_models <- as.integer(dockings_df$Number.of.Models[dockings_df$Docking.ID == dock])
n_cpus <- as.integer(dockings_df$Number.of.CPUs[dockings_df$Docking.ID == dock])
notes <- as.character(dockings_df$Notes[dockings_df$Docking.ID == dock])

gridboxes_csv <- paste0(base_dir, "/", "Gridboxes.csv")
gridboxes_df <- read.csv(gridboxes_csv)

box_center_x <- as.numeric(gridboxes_df$Center.in.x.dimension[gridboxes_df$Gridbox.Name == box])
box_center_y <- as.numeric(gridboxes_df$Center.in.y.dimension[gridboxes_df$Gridbox.Name == box])
box_center_z <- as.numeric(gridboxes_df$Center.in.z.dimension[gridboxes_df$Gridbox.Name == box])
```

```r
box_size_x <- as.numeric(gridboxes_df$Size.in.x.dimension[gridboxes_df$Gridbox.Name == box])
box_size_y <- as.numeric(gridboxes_df$Size.in.y.dimension[gridboxes_df$Gridbox.Name == box])
box_size_z <- as.numeric(gridboxes_df$Size.in.z.dimension[gridboxes_df$Gridbox.Name == box])
box_notes <- as.character(gridboxes_df$Notes[gridboxes_df$Gridbox.Name == box])

ligset_list_txt <- paste0(base_dir, "/ligsets/", ligset, "/", ligset, "_list.txt")
ligset_list <- read.delim(ligset_list_txt, header = F, sep = "\n")
ligset_list <- as.character(unlist(ligset_list))
ligset_list <- factor(ligset_list, levels = ligset_list)

### Read in alldata.csv
dock_dir <- paste0(base_dir, "/", prot, "/", dock)

dock_alldata_csv <- paste0(dock_dir, "/", dock, "_alldata.csv")
data <- read.csv(dock_alldata_csv)

### Recode variables with more convenient names
if(ligset == "pls1a") {
# ligset.coded <- c("ng", "s2", "ne", "s1", "s3")
# ligset.names <- factor(c("Garcinol", "CTB", "EGCG", "CTPB", "C646"))
  pls1a_coded <- c("ng", "s2", "ne", "s1", "s3")
  pls1a_renamed <- factor(c("Garcinol", "CTB", "EGCG", "CTPB", "C646"))
  data$lig <- pls1a_renamed[match(data$lig, pls1a_coded)]
  data$lig <- factor(data$lig, levels = pls1a_renamed)
  ligset_list <- pls1a_renamed
}

binding_sites_dir <- paste0(base_dir, "/binding_sites/", prot_file)
binding_sites <- list.files(path = binding_sites_dir)
binding_sites <- sub(".pdb", "", binding_sites)

### Create binds_in_SITE rows (T/F depending on score fraction)
binding.threshold <- 0.10 # threshold for binding fraction
for(bs in binding_sites) {
# data[, paste("binds_in_", bs, sep = "")] <- rep(NA, nrow(data))
# data[, paste("binds_in_", bs, sep = "")][data[,paste("resis_score_fraction_", bs, sep = "")] >= binding.threshold] <- T
# data[, paste("binds_in_", bs, sep = "")][data[,paste("resis_score_fraction_", bs, sep = "")] < binding.threshold] <- F
  bindsin_bs <- paste0("binds_in_", bs)
```

```r
  bs_fraction <- paste0(bs, "_fraction")
  data[, bindsin_bs] <- rep(NA, nrow(data))
  data[, bindsin_bs][data[,bs_fraction] >= binding.threshold] <- T
  data[, bindsin_bs][data[,bs_fraction] < binding.threshold] <- F
}


### Create analysis data frame
analysis <- data.frame(row.names = ligset_list)

# Build column headers for averages, minimums, standard deviations, distribution fractions
analysis.columns <- c("AvgE", "MinE", "StdevE", paste("Num_", binding_sites, sep = ""),
                      paste("DistribFrac_", binding_sites, sep = ""),
                      paste("AvgE_", binding_sites, sep = ""), paste("MinE_", binding_sites, sep = ""))
for(c in analysis.columns) {
  analysis[,c] <- rep(NA, length(ligset_list))
}

# Fill in analysis data
for(l in ligset_list) {
  analysis[l, "lig"] <- l
  analysis[l, "AvgE"] <- mean(data$E[data$lig == l]) # Overall average energy for lig
  analysis[l, "MinE"] <- min(data$E[data$lig == l]) # Overall minimum energy for lig
  analysis[l, "StdevE"] <- sd(data$E[data$lig == l]) # Overall standard deviation of energies for lig
  DistribFrac_Denom <- 0
  for(bs in binding_sites) {
    num_in_site <- length(data$E[data$lig == l & data[, paste("binds_in_", bs, sep = "")] == T])
    analysis[l, paste0("Num_", bs)] <- num_in_site # Number binding in each site
    DistribFrac_Denom <- DistribFrac_Denom + num_in_site
    if(analysis[l, paste0("Num_", bs)] > 0) {
      analysis[l, paste0("AvgE_", bs)] <-  # Average energy for ligs binding in site
        mean(data$E[data$lig == l & data[, paste0("binds_in_", bs)] == T])
      analysis[l, paste0("MinE_", bs)] <- # Minimum energy for ligs binding in site
        min(data$E[data$lig == l & data[, paste0("binds_in_", bs)] == T])
    } else { # otherwise it will return Inf's
```

```
      analysis[l, paste0("AvgE_", bs)] <- NA
      analysis[l, paste0("MinE_", bs)] <- NA
    }
  }
  for(bs in binding_sites) { # fraction of bindings in site from count
    analysis[l, paste("DistribFrac_", bs, sep = "")] <-
      analysis[l, paste("Num_", bs, sep = "")] / DistribFrac_Denom
  }
}

analysis_csv = paste0(dock_dir, "/", dock, "_summary.csv")

write.csv(analysis, file = analysis_csv)
print(paste0("Created summary CSV"))

#
    ##############################################################################

#
    ##############################################################################

#
    ##############################################################################



### Graphs!!!!!!!
# setwd(graphs_dir) # needed for pdf names below
# bs.colors <- brewer.pal(length(binding_sites), "Set1")
# lig.colors <- brewer.pal(length(ligset_list), "Set2")
# lig.palette <- "Greys"

graphs_dir <- paste0(dock_dir, "/graphs/")
if(dir.exists(graphs_dir)) {
  print("graphs directory was not created because it already exists")
} else {dir.create(graphs_dir)}
setwd(graphs_dir)

####################
### Box plot of binding energies (in all sites) by ligand
boxplots_energy_vs_lig_allsites <- ggplot(data=data, aes(x=lig, y=E)) +
  geom_boxplot(aes(fill=lig)) +
  scale_fill_hue(name="Ligands") + # legend
  scale_x_discrete(limits=ligset_list) +
  xlab("Ligand") +
```

```
  ylab("Binding energy (kcal/mol)") +
  ggtitle("Binding Energies by Ligand (All binding sites)") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
boxplots_energy_vs_lig_allsites

graph_name <- "boxplots_energy_vs_lig_allsites"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
print(paste0("Created ", graph_name))

####################

####################
### Density of dockings over energy range
# All ligands combined
densities_energy_by_lig_allcombined <- ggplot(data=data, aes(x=E)) +
  geom_density() +
  xlab("Binding energy (kcal/mol)") +
  ggtitle("Overall Density of Dockings versus Binding Energy") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
densities_energy_by_lig_allcombined

graph_name <- "densities_energy_by_lig_allcombined"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
print(paste0("Created ", graph_name))

# Separate charts for each ligand, arranged in a grid
#   OK fine it actually wraps but whatever
densities_energy_by_lig_grid <- ggplot(data=data, aes(x=E, color=lig, group=
    lig)) +
  geom_density() +
  scale_color_hue(name="Ligands") +
  xlab("Binding energy (kcal/mol)") +
  ggtitle("Density of Dockings versus Binding Energy by Ligand (All Binding
    Sites)") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold")) +
  facet_wrap(~lig)
densities_energy_by_lig_grid

graph_name <- "densities_energy_by_lig_grid"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
print(paste0("Created ", graph_name))

```

```r
# *A*
# Same thing but overlayed
densities_energy_by_lig_overlay <- ggplot(data=data, aes(x=E, color=lig)) +
  geom_density() +
  scale_color_hue(name="Ligands") +
  scale_x_reverse(limits=c(max(data$E), min(data$E))) +
  xlab("Binding energy (kcal/mol)") +
  ylab("Probability density") +
  ggtitle("Density of Dockings versus Binding Energy (All Binding Sites)") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
densities_energy_by_lig_overlay

graph_name <- "densities_energy_by_lig_overlay"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=6, height=4)
print(paste0("Created ", graph_name))

####################

####################
### Create a new melted data frame for energies with one unique entry per bidning site placement
data.E.bs.melted <- melt(data,
                         id.vars=c("key", "E", "lig"), # ID variables - all the variables to keep but not split apart on
                         measure.vars=paste0("binds_in_", binding_sites) # The source columns
)
# This new variable will simply be name of the site
data.E.bs.melted$binding.placement <-  rep(NA, nrow(data.E.bs.melted))
data.E.bs.melted$binding.placement <- sub("binds_in_", "", data.E.bs.melted$variable) # data.E.bs.melted$variable is binds_in_SITE
data.E.bs.melted <- data.E.bs.melted[data.E.bs.melted$value, c("key", "E", "lig", "binding.placement")] # data.E.bs.melted$value is T/F
### A density plot for all ligands with separate traces for each binding site
densities_energy_by_site_overlay <- ggplot(data=data.E.bs.melted, aes(x=E, color=binding.placement)) +
  geom_density() +
  scale_color_hue(name="Binding Site", labels=binding_sites) +
  xlab("Binding energy (kcal/mol)") +
  ggtitle("Density of Dockings versus Binding Energy by Binding Site (All Ligands)") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
densities_energy_by_site_overlay
```

```
312
313 graph_name <- "densities_energy_by_site_overlay"
314 ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
315 print(paste0("Created ", graph_name))
316
317 ### A grid of density plots (lig vs. site) with single energy traces for each
        box
318 densities_energy_by_lig_and_site_grid <- ggplot(data=data.E.bs.melted, aes(x=E
        , color=binding.placement, group=lig)) +
319   geom_density() +
320   facet_grid(binding.placement ~ lig) +
321   scale_color_hue(name="Binding Site", labels=binding_sites) +
322   xlab("Binding energy (kcal/mol)") +
323   ggtitle("Density of Dockings versus Binding Energy by Binding Site and
        Ligand") +
324   theme(legend.title=element_text(face="bold"),
325         plot.title=element_text(face="bold"))
326 densities_energy_by_lig_and_site_grid
327
328 graph_name <- "densities_energy_by_lig_and_site_grid"
329 ggsave(paste0(dock, "_", graph_name, ".pdf"), width=1.75*(length(ligset_list)
        +2), height=2*length(binding_sites))
330 print(paste0("Created ", graph_name))
331
332 ####################
333
334
335
336
337
338
339
340
341
342
343
344
345 # *A*
346 data$combined.sites <- rep(NA, nrow(data))
347 binding_sites.capitalized <- c("Lys", "CoA", "Side", "Allo1", "Allo2")
348
349 for(r in 1:nrow(data)) {
350   combined.sites <- NA
351   # for(bs in binding_sites) {
352   for(bs in binding_sites.capitalized) {
```

```
    # if(data[r, paste0("binds_in_", bs)]) {combined.sites <- c(combined.sites, bs) }
    if(data[r, paste0("binds_in_", tolower(bs))]) {combined.sites <- c(combined.sites, bs) }
  }
  data[r, "combined.sites"] <- paste(na.omit(combined.sites), collapse=" + ")
}
data$combined.sites[data$combined.sites == ""] <- "No site placement"

barplot_bindingdist_by_lig_combinedsites <- ggplot(data=data) +
  geom_bar(aes(x=lig, fill=combined.sites), color="black", width=0.8) +
  scale_x_discrete(limits=ligset_list) +
#   scale_fill_hue(name="Binding Site(s)") +
#   scale_fill_manual(values=c("orchid", "mediumpurple", "greenyellow", "mediumaquamarine", "grey"), name="Binding Site(s)") +
  scale_fill_brewer(palette="Set2", name="Binding Site(s)") +
  xlab("Ligand") +
  ylab("Number of Ligands in Site") +
  ggtitle("Binding Site Placement Distribution by Ligand") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
barplot_bindingdist_by_lig_combinedsites

graph_name <- "barplot_bindingdist_by_lig_combinedsites"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=6, height=4)
print(paste0("Created ", graph_name))









####################
### Bar plot of binding distribution in each binding site by ligand
# Make a data frame with only the binding site numbers
analysis.bindingsites <- analysis[c(paste("Num_", binding_sites, sep=""))]
analysis.bindingsites$bs_cat <- row.names(analysis.bindingsites)
# Melt this data frame for graphing
melted.analysis.bindingsites <- melt(analysis.bindingsites, id.vars = "bs_cat")
barplot_bindingdist_by_lig <- ggplot(data=melted.analysis.bindingsites, aes(x=bs_cat, y=value, fill=variable)) +
  geom_bar(stat="identity", color="black") +
```

```
  scale_x_discrete(limits=ligset_list) +
  scale_fill_hue(name="Binding Site", labels=binding_sites) +
  xlab("Ligand") +
  ylab("Number of Ligands in Site") +
  ggtitle("Binding Distribution by Ligand") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
barplot_bindingdist_by_lig

graph_name <- "barplot_bindingdist_by_lig"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
print(paste0("Created ", graph_name))

####################

####################
### Bar plot of average binding energy in each binding site per ligand
# Make a data frame with only the binding site numbers
analysis.avgenergies <- analysis[c(paste("AvgE_", binding_sites, sep=""))]
analysis.avgenergies$bs_cat <- row.names(analysis.avgenergies)
# Melt this data frame for graphing
melted.analysis.avgenergies <- melt(analysis.avgenergies, id.vars = "bs_cat")
barplot_avge_vs_lig_by_bs <- ggplot(data=melted.analysis.avgenergies, aes(x=bs
    _cat, y=value, fill=variable, width=0.75)) +
  geom_bar(stat="identity", color="black", position=position_dodge()) +
  scale_x_discrete(limits=ligset_list) +
  scale_fill_hue(name="Binding Site", labels=binding_sites) +
  xlab("Ligand") +
  ylab("Binding energy (kcal/mol)") +
  ggtitle("Average Energy by Binding Site") +
  theme(legend.title=element_text(face="bold"),
        plot.title=element_text(face="bold"))
barplot_avge_vs_lig_by_bs

graph_name <- "barplot_avge_vs_lig_by_bs"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
print(paste0("Created ", graph_name))

####################

####################

counts.max <- max(analysis[, paste0("Num_", binding_sites)])
### 'Stripcharts' for energy by ligand
# Overall
```

```
vertbarplots_energy_by_lig_allsites <- ggplot(data=data, aes(x=E, fill=lig,
    group=lig)) +
  geom_bar(width=0.1) +
  coord_flip() +
  scale_fill_hue(guide=FALSE) +
  xlab("Binding energy (kcal/mol)") +
  scale_x_reverse(limits=c(max(data$E), min(data$E))) +
  ylim(0, counts.max) +
  ggtitle("Binding Affinity Frequencies by Ligand (All binding sites)") +
  theme(plot.title=element_text(face="bold"),
        legend.title=element_text(face="bold")) +
  facet_grid(. ~ lig, drop=F)
vertbarplots_energy_by_lig_allsites

graph_name <- "vertbarplots_energy_by_lig_allsites"
ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
print(paste0("Created ", graph_name))

### For each binding site
# HepI:
if(prot == "hepi") {
  # ADPH
  vertbarplots_energy_by_lig_adphsite <- ggplot(data=subset(data, binds_in_
    adph), aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (ADPH Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_adphsite

  graph_name <- "vertbarplots_energy_by_lig_adphsite"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

  # FDLA
  vertbarplots_energy_by_lig_fdlasite <- ggplot(data=subset(data, binds_in_
    fdla), aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
```

```
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (FDLA Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_fdlasite

  graph_name <- "vertbarplots_energy_by_lig_fdlasite"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

  # ALLO
  vertbarplots_energy_by_lig_allosite <- ggplot(data=subset(data, binds_in_
    allo), aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (ALLO Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_allosite

  graph_name <- "vertbarplots_energy_by_lig_allosite"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))



  ### Dan's Percent Inhibition data
  dan.data <- read.csv("/Users/zarek/lab/Resources/Dans_Percent_Inhib_Data.csv
    ", header = T)
  dan.data$Ligand <- factor(dan.data$Ligand, levels = ncs.sugargrouped)
  dan_percent_inhib_barplot <- ggplot(data=dan.data, aes(x=Ligand, y=Percent.
    Inhibition, fill=Ligand)) +
    geom_bar(stat="identity") +
    scale_fill_discrete(guide=F) +
    xlab("Ligand") +
    ylab("Percent Inhibition") +
    ggtitle("In Vitro Percent Inhibition by Ligand (from Dan)") +
    theme(legend.title=element_text(face="bold"))
  dan_percent_inhib_barplot
```

```
  ggsave("dan_percent_inhib_barplot.pdf", width=12, height=8)
}
# p300:
if(prot == "p300") {
  # lys
  vertbarplots_energy_by_lig_lyssite <- ggplot(data=subset(data, binds_in_lys)
    , aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    ylim(0, counts.max) +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ggtitle("Binding Affinity Frequencies by Ligand (lys Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_lyssite

  graph_name <- "vertbarplots_energy_by_lig_lyssite"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

  # coa
  vertbarplots_energy_by_lig_coasite <- ggplot(data=subset(data, binds_in_coa)
    , aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (coa Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_coasite

  graph_name <- "vertbarplots_energy_by_lig_coasite"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

  # side
  vertbarplots_energy_by_lig_sidesite <- ggplot(data=subset(data, binds_in_
    side), aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
```

```
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (side Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_sidesite

  graph_name <- "vertbarplots_energy_by_lig_sidesite"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

  # allo1
  vertbarplots_energy_by_lig_allo1site <- ggplot(data=subset(data, binds_in_
    allo1), aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (allo1 Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_allo1site

  graph_name <- "vertbarplots_energy_by_lig_allo1site"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

  # allo2
  vertbarplots_energy_by_lig_allo2site <- ggplot(data=subset(data, binds_in_
    allo2), aes(x=E, fill=lig, group=lig)) +
    geom_bar(width=0.1) +
    coord_flip() +
    scale_fill_hue(guide=FALSE) +
    xlab("Binding energy (kcal/mol)") +
    scale_x_reverse(limits=c(max(data$E), min(data$E))) +
    ylim(0, counts.max) +
    ggtitle("Binding Affinity Frequencies by Ligand (allo2 Binding Site)") +
    theme(legend.title=element_text(face="bold")) +
    facet_grid(. ~ lig, drop=F)
  vertbarplots_energy_by_lig_allo2site

```

```r
  graph_name <- "vertbarplots_energy_by_lig_allo2site"
  ggsave(paste0(dock, "_", graph_name, ".pdf"), width=12, height=8)
  print(paste0("Created ", graph_name))

}
####################



# Multiple plot function
#
# ggplot objects can be passed in ..., or to plotlist (as a list of ggplot
    objects)
# - cols:   Number of columns in layout
# - layout: A matrix specifying the layout. If present, 'cols' is ignored.
#
# If the layout is something like matrix(c(1,2,3,3), nrow=2, byrow=TRUE),
# then plot 1 will go in the upper left, 2 will go in the upper right, and
# 3 will go all the way across the bottom.
#

# multiplot <- function(..., plotlist=NULL, file, cols=1, layout=NULL) {
#   library(grid)
#
#   # Make a list from the ... arguments and plotlist
#   plots <- c(list(...), plotlist)
#
#   numPlots = length(plots)
#
#   # If layout is NULL, then use 'cols' to determine layout
#   if (is.null(layout)) {
#     # Make the panel
#     # ncol: Number of columns of plots
#     # nrow: Number of rows needed, calculated from # of cols
#     layout <- matrix(seq(1, cols * ceiling(numPlots/cols)),
#                      ncol = cols, nrow = ceiling(numPlots/cols))
#   }
#
#   if (numPlots==1) {
#     print(plots[[1]])
#
#   } else {
#     # Set up the page
#     grid.newpage()
#     pushViewport(viewport(layout = grid.layout(nrow(layout), ncol(layout))))
```

```
#
#     # Make each plot, in the correct location
#     for (i in 1:numPlots) {
#       # Get the i,j matrix positions of the regions that contain this
    subplot
#       matchidx <- as.data.frame(which(layout == i, arr.ind = TRUE))
#
#       print(plots[[i]], vp = viewport(layout.pos.row = matchidx$row,
#                                       layout.pos.col = matchidx$col))
#     }
#   }
# }



# barplot_bindingdist_by_lig_combinedsites
# vertbarplots_energy_by_lig_allsites
# densities_energy_by_lig_overlay

# combined_bar_bySite_and_density_byLig <- multiplot(barplot_bindingdist_by_
    lig_combinedsites,
#                                                    densities_energy_by_lig_
    overlay, cols=2)
# print(paste0(dock, "_", "combined_bar_bySite_and_density_byLig", ".pdf"))#,
    width=12, height=4)

# combined_bar_bySite_and_histograms_byLig <- multiplot(barplot_bindingdist_by
    _lig_combinedsites,
#                                                       vertbarplots_energy_by
    _lig_allsites, cols=2)
# print(paste0(dock, "_", "combined_bar_bySite_and_histograms_byLig", ".pdf"))
    #, width=12, height=4)









####################
```

```
688 ### Save data tables for % Distribution
689 distrib.table <- analysis[paste0("DistribFrac_", binding_sites)]
690 for(bs in binding_sites) {
691   distrib.table[, bs] <- round(distrib.table[paste0("DistribFrac_", bs)] *
      100, 2)
692 }
693 distrib.table <- distrib.table[binding_sites]
694 distrib_table_csv <- paste0(dock_dir, "/", dock, "_binding_site_distribution_
      table.csv")
695
696 write.csv(distrib.table, file=distrib_table_csv)
697 print(paste0("Created ", "binding_site_distribution_table"))
698
699 ####################
700
701
702
703
704
705
706
707 #
      ################################################################################
708 print("All done, graphs can found in:")
709 print(graphs_dir, quote=F)
```

/Users/zarek/lab/zvina/scripts/postdocking_graphs.R

2.17 `pre_and_post_control.py`

2.17.1 Function

Transcompiler picojava pseudolanguage java ee regular expression syntactic sugar eclipse rust bug. Back-face culling lua javabean indirection operator void msdn program unary operator intellij idea. Bug tracking library softwar

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#!/usr/bin/env python

### One script to control them AAAAAALLLLL!!!!
# (c) Zarek Siegel
# v1 3/6/16

import argparse, subprocess, os
import new_grid_or_dock_entry
from constants import *
from create_docking_object import * # Docking
from write_vina_submit_sh import * # write_vina_submit_sh
from get_pose_energies_properties import * # get_pose_energies_properties
from mine_vina_data import * # mine_vina_data
from binding_site_analysis import * # get_binding_sites_list
# from binding_site_analysis import * # score_binding_sites
# from binding_site_analysis import * # aiad_icpd_binding_sites
# from binding_site_analysis import * # assess_all_resis
from write_alldata import * # write_alldata_csv, write_docking_pickled
from read_alldata import * # read_alldata_csv, read_docking_pickled
from correlations import * # correlations

# from docking_data_assembly import *


def main():
  print("")
  print("->-> hi")

  parser = argparse.ArgumentParser(description='Pre- and post-Vina file fun
    times')
  parser.add_argument('-d', '--dock', metavar='DOCK', type=str, nargs='?',
    help='the ID for this docking')

  parser.add_argument('-nd', '--new_docking', action='store_true', default=
    False,
    help='Write a new set of docking parameters to Dockings.csv')
  parser.add_argument('-ng', '--new_gridbox', action='store_true', default=
    False,
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    help='Write a new set of grid box parameters to Gridboxes.csv')
  parser.add_argument('-v', '--vina', action='store_true', default=False,
    help='write the Vina job submission script')
  parser.add_argument('-p', '--print', action='store_true', default=False,
    help='print docking parameters')

  parser.add_argument('-s', '--separate', action='store_true', default=False,
    help='execute the bash script to separate row Vina results')
  parser.add_argument('-n', '--clean', action='store_true', default=False,
    help='execute the bash script to clean up processed Vina results')

  parser.add_argument('-rc', '--read_csv', action='store_true', default=False,
    help='load data from alldata CSV file')
  parser.add_argument('-ri', '--read_pickle', action='store_true', default=
    False,
    help='load data from pickled object')

  parser.add_argument('-bs', '--binding_sites', action='store_true', default=
    False,
    help='score binding sites by fraction of binding site residues contacted')
  parser.add_argument('-ai', '--aiad_icpd', action='store_true', default=False
    ,
    help='score binding sites by AIAD and ICPD')
  parser.add_argument('-ar', '--all_resis', action='store_true', default=False
    ,
    help='asses contacts with all residues')
  parser.add_argument('--atoms', action='store_true', default=False,
    help='assess poses against all atoms (not just residues) for -bs and -ar')

  parser.add_argument('-l', '--cluster', action='store_true', default=False,
    help='create cluster CSV files (all lig x lig AIADs)')
  parser.add_argument('-co', '--correls', action='store_true', default=False,
    help='find correlations between all quantitative variables')
  parser.add_argument('-c', '-wc', '--write_csv', action='store_true', default
    =False,
    help='generate and save the alldata CSV file')
  parser.add_argument('-i', '-wi', '--write_pickle', action='store_true',
    default=False,
    help='save the entire docking as a pickled object')

  parser.add_argument('-ep', '--en_props', action='store_true', default=False,
    help='Write a new set of docking parameters to Dockings.csv')
  parser.add_argument('-o', '--post_proc', action='store_true', default=False,
    help='Perform all post-processing steps (separate, clean, csv, cluster,
    pickle)')
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parser.add_argument('-g', '--graphs', action='store_true', default=False,
  help='Generate graphs for this docking')

args = vars(parser.parse_args())


if args['new_docking']:
  print("---> Write new set of docking parameters to Dockings.csv...")
  new_grid_or_dock_entry.new_docking_entry()
elif args['new_gridbox']:
  print("---> Write new set of grid box parameters to Gridboxes.csv...")
  new_grid_or_dock_entry.new_gridbox_entry()
else:
  dock = str(args['dock'])
  d = Docking(dock)
  if args['print']:
    d.print_parameters()
  if args['vina']:
    print("---> Writing Vina submission script")
    d.write_vina_submit_sh()
  if args['separate']:
    print("---> Processing raw Vina output PDBQTs")
    d.export_parameters_to_environment()
    subprocess.call(["{b_d}/scripts/separate_vina_results.sh".format(b_d=
  base_dir), dock])
  if args['clean']:
    print("---> Cleaning up processed PDBQTs and converting to PDBs")
    d.export_parameters_to_environment()
    subprocess.call(["{b_d}/scripts/cleanup_processed_vina_results.sh".
  format(b_d=base_dir), dock])
  if args['read_csv']: d.read_alldata_csv()
  if args['read_pickle']: d.read_docking_pickled()
  if args['en_props']:
    print("---> Getting molecular energies and properties for all poses")
    d.get_pose_energies_properties()
  if args['atoms']: d.evaluate_resis_atoms = True
  else: d.evaluate_resis_atoms = False
  if args['binding_sites']: d.score_binding_sites()
  if args['aiad_icpd']: d.aiad_icpd_binding_sites()
  if args['all_resis']: d.assess_all_resis()
  if args['cluster']: d.cluster_poses()
  if args['write_csv']: d.write_alldata_csv()
  if args['correls']: d.correlations()
  if args['write_pickle']: d.write_docking_pickled()
  if args['graphs']:
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      print("---> Generating graphs")
      subprocess.call([Rscript_binary, "{b_d}/scripts/postdocking_graphs.R".format(b_d=base_dir), dock])
    if args['post_proc']:
      print("---> Processing raw Vina output PDBQTs")
      subprocess.call(["{b_d}/scripts/separate_vina_results.sh".format(b_d=base_dir),
        dock, base_dir, AutoDockTools_dir, AutoDockTools_pythonsh_binary])
      print("---> Cleaning up processed PDBQTs and converting to PDBs")
      subprocess.call(["{b_d}/scripts/cleanup_processed_vina_results.sh".format(b_d=base_dir),
        dock, base_dir, AutoDockTools_dir, AutoDockTools_pythonsh_binary])
      d.write_alldata_csv()
      d.cluster_poses()
      d.save_pickled_docking_obj()

  print("->-> All done!!!!!!!!!!!!!!!")
  print("")

if __name__ == "__main__": main()









# print("{} = {}".format("parameters_loaded", self.parameters_loaded))
# print("{} = {}".format("ligset_list_gotten", self.ligset_list_gotten))
# print("{} = {}".format("parameters_exported_to_environment", self.parameters_exported_to_environment))
# print("{} = {}".format("is_data_dic_created", self.is_data_dic_created))
#
# print("{} = {}".format("vina_data_mined", self.vina_data_mined))
# print("{} = {}".format("binding_sites_list_gotten", self.binding_sites_list_gotten))
# print("{} = {}".format("binding_sites_scored", self.binding_sites_scored))
# print("{} = {}".format("aiad_icpd_calcd", self.aiad_icpd_calcd))
# print("{} = {}".format("all_resis_assessed", self.all_resis_assessed))
#
# print("{} = {}".format("is_csv_written", self.is_csv_written))
# print("{} = {}".format("energies_props_gotten", self.energies_props_gotten))
# print("{} = {}".format("are_poses_clustered", self.are_poses_clustered))
# print("{} = {}".format("is_pickled", self.is_pickled))
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/Users/zarek/lab/zvina/scripts/pre_and_post_control.py