Data and Molecular Visualization

Visualization

J. D. Madura

Department of Chemistry and Biochemistry
Center for Computational Chemistry
Duquesne University

June 11, 2015
Schedule of Lectures

Lecture 1

- Visualization (VMD, PyMol, MOE)
- Introduction to R
- Plotting using R
- Examples

Lecture 2

- IMF
- Force-fields
- Molecular Dynamics (MD)
- Simulation of a protein (in vacuo and in solution)

Lecture 3

- Enhanced Sampling (aMD, ABF, metadynamics)
- Simulation of a simple system using metadynamics
- Examples

Lecture 4

- Free Energy Perturbation Method (FEP)
- Simulation of protein-ligand system
- Examples
Lecture Objectives

- Learn how to create scientific plots using R
- Learn how to visualize (bio)molecular using VMD, MOE, PyMol, etc.
Introduction

Overview

- Why is visualization important?
- Data versus Molecular visualization.

Data

Molecular

![Simple Plot](image)

![Molecular Visualization](image)
### An Example

Which of the following is more appropriate?

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>q</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>-2.076665</td>
<td>-0.450512</td>
<td>0.113719</td>
<td>0.31</td>
</tr>
<tr>
<td>6</td>
<td>-1.303573</td>
<td>-1.578362</td>
<td>0.018659</td>
<td>-0.25</td>
</tr>
<tr>
<td>6</td>
<td>0.052338</td>
<td>-1.468019</td>
<td>-0.25975</td>
<td>-0.24</td>
</tr>
<tr>
<td>6</td>
<td>0.632158</td>
<td>-0.225992</td>
<td>-0.442758</td>
<td>-0.07</td>
</tr>
<tr>
<td>6</td>
<td>-0.168762</td>
<td>0.907155</td>
<td>-0.343817</td>
<td>-0.23</td>
</tr>
<tr>
<td>6</td>
<td>-1.510177</td>
<td>0.802410</td>
<td>-0.068220</td>
<td>0.38</td>
</tr>
<tr>
<td>1</td>
<td>-1.744472</td>
<td>-2.546830</td>
<td>0.156610</td>
<td>0.24</td>
</tr>
<tr>
<td>1</td>
<td>0.650035</td>
<td>-2.354561</td>
<td>-0.336670</td>
<td>0.24</td>
</tr>
<tr>
<td>1</td>
<td>0.240234</td>
<td>1.886524</td>
<td>-0.485182</td>
<td>0.26</td>
</tr>
<tr>
<td>8</td>
<td>-2.290785</td>
<td>1.925857</td>
<td>0.025961</td>
<td>-0.76</td>
</tr>
<tr>
<td>1</td>
<td>-3.206353</td>
<td>1.679199</td>
<td>0.218002</td>
<td>0.42</td>
</tr>
<tr>
<td>8</td>
<td>-3.438723</td>
<td>-0.428600</td>
<td>0.384651</td>
<td>-0.76</td>
</tr>
<tr>
<td>1</td>
<td>-3.824804</td>
<td>-1.304988</td>
<td>0.485354</td>
<td>0.40</td>
</tr>
<tr>
<td>6</td>
<td>2.118392</td>
<td>-0.091134</td>
<td>-0.700641</td>
<td>-0.42</td>
</tr>
<tr>
<td>1</td>
<td>2.509992</td>
<td>-0.977440</td>
<td>-1.182030</td>
<td>0.24</td>
</tr>
<tr>
<td>1</td>
<td>2.306003</td>
<td>0.750995</td>
<td>-1.358991</td>
<td>0.21</td>
</tr>
<tr>
<td>6</td>
<td>2.894472</td>
<td>0.113603</td>
<td>0.615320</td>
<td>-0.17</td>
</tr>
<tr>
<td>1</td>
<td>2.490833</td>
<td>0.979069</td>
<td>1.138684</td>
<td>0.19</td>
</tr>
<tr>
<td>1</td>
<td>2.737549</td>
<td>-0.751163</td>
<td>1.246935</td>
<td>0.22</td>
</tr>
<tr>
<td>7</td>
<td>4.334095</td>
<td>0.211951</td>
<td>0.325333</td>
<td>-0.80</td>
</tr>
<tr>
<td>1</td>
<td>4.587156</td>
<td>1.050440</td>
<td>-0.167043</td>
<td>0.29</td>
</tr>
<tr>
<td>1</td>
<td>4.922120</td>
<td>0.072153</td>
<td>1.126572</td>
<td>0.30</td>
</tr>
</tbody>
</table>

**Explanation...**
Visualizing Data

“Assessments of change, dynamics, and cause and effect are at the heart of thinking and explanation. To understand is to know what cause provokes what effect, by what means, at what rate. How then is such knowledge to be represented?”¹

The goal is to design “...proper arrangement in space and time images, words, numbers – for presenting information about motion, process, mechanism, cause, and effect.”¹

Therefore visualization, in our case molecular visualization, is extremely important since it is an extremely effective method to convey information.

Visualizing Data

“Excellence in statistical graphics consists of complex ideas communicated with clarity, precision, and efficiency.” A quote from Edward R. Tufte

Therefore graphical data should

- show that data
- induce the viewer to think about the substance rather than about the methodology
- avoid distorting what the data have to say
- make large datasets coherent
- encourage the eye to compare different pieces of data
- reveal that data at several levels of detail, from a broad overview to the fine structure
- serve a reasonably clear purpose: description, exploration, tabulation, or decoration
- be closely integrated with the statistical and verbal description of a data set.
Graphical Example
Consider the following data

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>Y</td>
<td>X</td>
<td>Y</td>
<td>X</td>
</tr>
<tr>
<td>---</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
</tr>
<tr>
<td>10.0</td>
<td>8.04</td>
<td>10.0</td>
<td>9.14</td>
<td>10.0</td>
</tr>
<tr>
<td>8.0</td>
<td>6.95</td>
<td>8.0</td>
<td>8.14</td>
<td>8.0</td>
</tr>
<tr>
<td>13.0</td>
<td>7.58</td>
<td>13.0</td>
<td>8.74</td>
<td>13.0</td>
</tr>
<tr>
<td>9.0</td>
<td>8.81</td>
<td>9.0</td>
<td>8.77</td>
<td>9.00</td>
</tr>
<tr>
<td>11.0</td>
<td>8.33</td>
<td>11.0</td>
<td>9.26</td>
<td>11.0</td>
</tr>
<tr>
<td>14.0</td>
<td>9.96</td>
<td>14.0</td>
<td>8.10</td>
<td>14.0</td>
</tr>
<tr>
<td>6.0</td>
<td>7.24</td>
<td>6.0</td>
<td>6.13</td>
<td>6.0</td>
</tr>
<tr>
<td>4.0</td>
<td>4.26</td>
<td>4.0</td>
<td>3.10</td>
<td>4.0</td>
</tr>
<tr>
<td>12.0</td>
<td>10.84</td>
<td>12.0</td>
<td>9.13</td>
<td>12.0</td>
</tr>
<tr>
<td>7.0</td>
<td>4.82</td>
<td>7.0</td>
<td>7.26</td>
<td>7.0</td>
</tr>
<tr>
<td>5.0</td>
<td>5.68</td>
<td>5.0</td>
<td>4.74</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Table: $N = 11$; mean of $X'$s = 9.0; mean of $Y'$s = 7.5; equation of regression line: $Y = 3 + 0.5X$; standard error of estimate of slope = 0.118; $t = 4.24$; sum of squares $X - \bar{X} = 110.0$; regression sum of square = 27.50; residual sum of squares of $Y = 13.75$; correlation coefficient = 0.82; and $r^2 = 0.67$. 
Graphical Example Visualized

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Another Example

![Data Visualization Graphs](image_url)
One More Example

![Graphs showing Mg²⁺ in 42 H₂O shell over time](image-url)
Proper Figure Guidelines

Characteristics of a quality graph / plot

• Use complete and consistent axis labels
  • Label each axis with the parameter or variable being measured and the units of measure in parentheses.
  • Use initial capital letters only, not all capitals: Time (min), Reaction Temperature (°C), Thickness (µm).
  • Place all labels outside and parallel to the axes. Numbers and letters on the abscissa and ordinate should read from left to right and from bottom to top, respectively
  • Do not place arrowheads on the ends of the axis lines.
  • Label the tick marks on an axis in type that is one or two points smaller than the axis labels (but not smaller than 7 points in general, 5 points for ACS journals).

• Use symbols for discrete data points while lines are used for continuous data, e.g. plotting a function.

• Axes should be ±10% larger than the min/max of the data.

Consult the ACS Style Guide, chapter 15, for complete details
Proper Figure Guidelines, cont.

Every figure must have a caption that includes the figure number and a brief, informative description, preferably in nonsentence format. Good examples of figure captions:

- Figure 2. Mass spectrum obtained when laboratory ambient air containing 2.5 ppm of \( \text{1} \) was introduced into the MS system.

- Figure 4. Change in carotenoid contents during maturation of three varieties of grapes: (A) Concord grapes; (B) Thompson seedless; and (C) Chilean red.

- Figure 7. Reaction rate constants as a function of proton afFnity for the reactions shown in eqs 5–7: \( k_{\text{exp}} \), experimental; \( k_c \), calculated.

If more information is necessary, use complete sentences and standard punctuation. The caption should be understandable without reference to the text.
Introduction to \texttt{R}

\texttt{R} is a statistical and graphics program.

You can download the program from http://cran.r-project.org.

It has a simple language to facilitate the input and output of your data and the results.

A nice introduction to \texttt{R} can be found in the book “\textit{Computer Simulation and Data Analysis in Molecular Biology and Biophysics: An Introduction Using R}” by Victor Bloomfield.

YouTube is an excellent source of videos instructing the viewer on how to install and use \texttt{R}. See the YouTube video on installation at http://www.youtube.com/watch?v=WJDrYUqNrHg
Simple Plot

```r
x = c(1, 2, 3, 4, 5)
y = c(1, 2, 3, 4, 5)
plot(x, y, xlab = "x data", ylab = "y data")
```
Improved Simple Plot

Make the x and y axis labels larger.

```r
x = c(1, 2, 3, 4, 5)
y = c(1, 2, 3, 4, 5)
par(cex=1.5)
plot(x, y, xlab="x data", ylab="y data")
```
Improved Simple Plot, cont.

Change the tick marks to be inside the plot.

```r
x=c(1,2,3,4,5)
y=c(1,2,3,4,5)
par(cex=1.5,tck=0.025)
plot(x,y,xlab="x data",ylab="y data")
```
Improved Simple Plot, cont.

Add some color to the data points.

```r
x=c(1,2,3,4,5)
y=c(1,2,3,4,5)
par(cex=1.5,tck=0.025)
plot(x,y,xlab="x data",ylab="y data",
 + col="red")
```
Improved Simple Plot, cont.

Add a second set of data points.

```r
x=c(1,2,3,4,5)  
y=c(1,2,3,4,5)  
z=c(1,4,9,16,25)  
par(cex=1.5,tck=0.025)  
plot(x,y,xlab="x data",ylab="y data", +  col="red",ylim=c(min(y,z),max(y,z)))  
points(x,z,col="blue")
```
Improved Simple Plot, cont.

Add a legend.

```r
x = c(1, 2, 3, 4, 5)
y = c(1, 2, 3, 4, 5)
z = c(1, 4, 9, 16, 25)
par(cex = 1.5, tck = 0.025)
plot(x, y, xlab = "x data", ylab = "y data",
    + col = "red", ylim = c(min(y, z), max(y, z)))
points(x, z, col = "blue")
legend(2, 20, c("red data", "blue data"),
    + col = c("red", "blue"), pch = c(1, 1), bty = "n")
```
Improved Simple Plot

Annotations and saving the plot to a file.

```r
x=c(1,2,3,4,5)
y=c(1,2,3,4,5)
z=c(1,4,9,16,25)
png(file="simple07.png")
par(cex=1.5,tck=0.025)
plot(x,y,xlab="x data",ylab="y data",
    col="red",ylim=c(min(y,z),max(y,z)),
    main="Red versus Blue")
points(x,z,col="blue")
legend(1,25,c("red data","blue data"),
    col=c("red","blue"),pch=c(1,1),bty="n")
axis(3,labels=FALSE)
axis(4,labels=FALSE)
arrows(2,15,3,9)
text(2,16,"This one")
dev.off()
```
Fitting Data

One of the skills you will need is fitting your data to some type of equation. The most common fitting is linear least squares. Everyone is familiar with the ideal gas law $PV = nRT$. Consider the following data collected for 1.0 mol of CO$_2$ at 298.15 K.

<table>
<thead>
<tr>
<th>$P$/bar</th>
<th>V/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>99.1076</td>
</tr>
<tr>
<td>0.50</td>
<td>49.5538</td>
</tr>
<tr>
<td>0.75</td>
<td>33.0359</td>
</tr>
<tr>
<td>1.00</td>
<td>24.7769</td>
</tr>
<tr>
<td>5.00</td>
<td>4.9554</td>
</tr>
<tr>
<td>10.00</td>
<td>2.4777</td>
</tr>
</tbody>
</table>

Use this data to determine a value for $R$. 
The Solution using \texttt{R}

\begin{verbatim}
P = c(0.25, 0.5, 0.75, 1.0, 5.0, 10.0)
V = c(99.1076, 49.5538, 33.0359, 24.7769, 4.9554, 2.4777)
png(file = "idgfit.png")
par(cex=1.75)
plot(1/P, V,
    + xlab=expression(paste("P"^"-1"," / (bar"^-1","))
    , ylab="V / (L)")
x = 1/P
fit = lm(V ~ x)
abline(fit, col = "red")
text(1, 80, bquote(paste("slope = ",
    + .(fit$coefficients[2])))
dev.off()
\end{verbatim}
Nonlinear Data Fitting

Occasionally one encounters a situation in which the expression you need to fit the data is non-linear. Consider the following scenario. You collect the following data for an enzyme (5 µM) 298.15 K.

<table>
<thead>
<tr>
<th>[Substrate] / mM</th>
<th>( v_0 / \text{mM/s} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>10.83</td>
</tr>
<tr>
<td>0.04</td>
<td>18.57</td>
</tr>
<tr>
<td>0.07</td>
<td>26.76</td>
</tr>
<tr>
<td>0.10</td>
<td>32.50</td>
</tr>
<tr>
<td>0.15</td>
<td>39.00</td>
</tr>
<tr>
<td>0.20</td>
<td>43.33</td>
</tr>
<tr>
<td>0.30</td>
<td>48.75</td>
</tr>
<tr>
<td>0.50</td>
<td>54.17</td>
</tr>
<tr>
<td>0.70</td>
<td>56.88</td>
</tr>
</tbody>
</table>

which must be fit to the following expression.

\[
v = \frac{V_{\text{max}}[S]}{K_M + [S]}
\]
The Solution using \texttt{R} \\

\begin{verbatim}
S=c(0.02,0.04,0.07,0.10,0.15,0.20,0.30,0.50,0.70)
v0=c(10.83,18.57,26.76,32.50,39.00,43.33,48.75,54.17,56.88)
png(file ="mmenzyme.png")
par(cex=1.75)
plot(S,v0,xlab=expression([S] / mM),
+ ylab=expression(paste("v"[0]," / mM s"\(^{-1}\))))
KM=0.5
Vmax=50
fit = nls(v0 ~ ((Vmax*S)/(KM+S)),
+ start=list(KM=KM,Vmax=Vmax))
yfit=fitted(fit)
points(S,yfit,type="l",col="red")
text(0.3,30,bquote(paste("K"[M]," = ",
+ .(signif(coef(fit)[1],digits=2))))
text(0.3,25,bquote(paste("V"[max]," = ",
+ .(signif(coef(fit)[2],digits=2))))
dev.off()
\end{verbatim}
Plotting Data

A classic example of a hydrogen bond is the water dimer.

Using Gaussian we can generate a potential energy scan for the energy versus distance between the oxygen atoms.

```
%chk=dimer.chk

# hf/sto-3g opt=z-matrix

Water dimer potential energy scan

0 1
h
o 1 roh
h 2 rho 1 hoh
o 2 roo 1 ooh 3 0.0
h 4 rho1 3 hoh1 1 d1
h 4 rho1 3 hoh1 1 -d1

roh 0.988
rho 0.9897
roo 2.3 s 50 0.05
rho1 0.9871
hoh 100.3585
ooh 100.4281
hoh1 110.4991
d1 124.5952
```
Water Dimer

After running the Gaussian calculation for the water dimer look in the output file for

Summary of Optimized Potential Surface Scan

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eigenvalues</td>
<td>−149.91807</td>
<td>−149.92838</td>
<td>−149.93180</td>
<td>−149.93492</td>
<td>−149.93730</td>
</tr>
<tr>
<td>roh</td>
<td>0.98800</td>
<td>0.98710</td>
<td>0.98660</td>
<td>0.98671</td>
<td>0.98701</td>
</tr>
<tr>
<td>rho</td>
<td>0.96936</td>
<td>0.97592</td>
<td>0.97671</td>
<td>0.97884</td>
<td>0.98162</td>
</tr>
<tr>
<td>roo</td>
<td>2.30000</td>
<td>2.35000</td>
<td>2.40000</td>
<td>2.45000</td>
<td>2.50000</td>
</tr>
<tr>
<td>rho1</td>
<td>0.98471</td>
<td>0.98552</td>
<td>0.98532</td>
<td>0.98549</td>
<td>0.98579</td>
</tr>
<tr>
<td>hoh</td>
<td>102.28153</td>
<td>102.90172</td>
<td>102.38682</td>
<td>101.62750</td>
<td>101.23188</td>
</tr>
<tr>
<td>ooh</td>
<td>123.21440</td>
<td>126.89952</td>
<td>115.20560</td>
<td>106.64471</td>
<td>103.93286</td>
</tr>
<tr>
<td>hoh1</td>
<td>106.38848</td>
<td>105.50372</td>
<td>108.04529</td>
<td>110.58072</td>
<td>111.11540</td>
</tr>
<tr>
<td>d1</td>
<td>126.66192</td>
<td>126.70510</td>
<td>125.41616</td>
<td>124.05844</td>
<td>123.83537</td>
</tr>
</tbody>
</table>
|       |                | 6              | 7              | 8              | 9              | 10
| Eigenvalues | −149.93900     | −149.94014     | −149.94083     | −149.94117     | −149.94124     |
| roh   | 0.98729        | 0.98755        | 0.98772        | 0.98792        | 0.98810        |

Using this data create a file, e.g. dimer.dat, with two columns. The first column is the number of the frame and the second column is the Eigenvalue. For example

1, −149.91807
2, −149.92838
Water Dimer Plot

The \texttt{R}-code to generate the water dimer plot

data=read.table("dimer.dat",header=F,sep=",")
x=2.3+(data[,1]−1)∗0.05
y=(data[,2]−2∗(−74.9659012))∗627.51
png("dimerplt.png")
par(cex=1.5,mgp=c(2,0.75,0),tck=0.025)
plot(x,y,type="l",main="Relative Potential Energy",
+ xlab=expression(r[oo]/\text{A}),
+ ylab=expression(paste("Potential Energy / (kcal \text{ \text{mol}}\ -(1))")
+ axes=F,frame.plot=T)
axis(1,at=seq(min(x),max(x),0.5))
axis(2,at=seq(−6,8,1))
axis(3,at=seq(min(x),max(x),0.5),labels=F)
axis(4,at=seq(−6,8,1),labels=F)
abline(h=0,lty=3,col="red")
dev.off()
VMD Overview

- Visual Molecular Dynamics
- Open-source program
- Performs visualization, analysis, and interfaces with several external programs.
  - NAMD
  - APBS
  - MSMS
- Extended using Tcl/Tk

The program, VMD, can be freely downloaded from http://www.ks.uiuc.edu/Research/vmd/

There are several VMD tutorials examples on this webpage.
Opening Screen

Dialog Box

Description

- 3D Window
- GUI
  - File
  - Molecule
  - Graphics
  - Display
  - Mouse
  - Extensions
  - Help
- Terminal window

Description

- 3D Window
- GUI
  - File
  - Molecule
  - Graphics
  - Display
  - Mouse
  - Extensions
  - Help
- Terminal window
Molecule Input Screen

Dialog Box

Description

- File types / extensions
  - PDB
  - COOR
  - DCD
  - PQR
  - MOL2

Description

- File types / extensions
  - PDB
  - COOR
  - DCD
  - PQR
  - MOL2
Representations

Screen

Description

- Coloring Method
- Drawing Method
- Material
Coloring Method

Dialog Box

- Type
- Element
- ResName
- ResType
- Chain
- Conformation
- Secondary Structure
- ColorID
- Volume
Dialog Box

Drawing Method

Description

- Lines
- Bonds
- VDW
- CPK
- Trace
- Ribbons
- Cartoon
- Surf
- Isosurface
Representations

Example 1

Example 2

Example 3
Analysis

Description

- APBS Electrostatics
- Contact Map
- NAMD Energy
- NAMD Plot

- Ramachandran Plot
- RMSD Calculator
- Sequence Viewer

Screen
Modeling

Dialog Box

Description

- Add Ions
- Add Solvation Box
- Automatic PSF Builder
- Membrane Builder
- Mutate Residue
Simulation

Dialog Box

Description

- AutoIMD
- IMD Connect
- NAMD Graphical Interface
- QM Tool
Dialog Box

Description

- Clipping Plane Tool
- Color Scale Bar
- Movie Maker
- Multiple Molecule Animation
- Ruler
Under the File Menu

Dialog Box

Description

• Save State
• Render
  • Snapshot
  • Tachyon
  • POV3
  • Postscript
Animation

Protein in Water
MOE Overview

- **Molecular Operating Environment**
- Commercial software
- Integrated visualization, computation and analysis
- Can connect to 3rd party software (e.g. Gaussian, MOPAC, NAMD, APBS, etc.)
- Written in SVL (Scientific Vector Language) and can be extended.

MOE is a commercial program. You can access the program while using the campus network. To install and get the appropriate license file see Scott Boesch.
Opening Screen

MOE 3D Screen

Description

- Menu items across the top
- Buttons down the right side
- 3D viewing
- Bottom right corner
Build

Dialog Box

Description

- Build by atoms
- Build by groups
- Build using SMILES
- Assign ionization state
- Assign stereochemistry
- Set a geometric parameter
Dialog Box

Description

- Numerous file types can be read
  - PDB
  - MOL2
  - moe
  - Fasta
- Text edit the file
Render

Screen

Description

- View
- Hide
- Show
- Atoms
- Ribbons
- Draw
Commands

- Invert - inverts the current selection
- Extend - extends the current selection based on selected criteria
- Ligand - selects the ligand
- Pocket - selects the pocket
- Receptor - selects the receptor
- Solvent - selects the solvent
- Potential - selects to force-field to be used
- Atom Selector - selects atoms based on certain criteria
### Atom Selection

**Description**

- Works on selected subsets of atoms
- Save selection sets
- Pick by Element
- Pick based on proximity
- Extends to complete groups, e.g. residues
- Picks based on connectivity
Computations Available

- Potential Energy
- Site Preparation
- Protonate 3D
- Partial Charges
- Energy Minimize
- Site Finder
- Surfaces and Maps
- Ligand Interactions
- Conformations (e.g. Conformational Search, Dihedral Energy Plot)
- Biopolymer (e.g. Residue pKa, Align, Superpose, Homology Modeling)
- Simulations (e.g. Dock, SCF Calculations, Dynamics, etc.)
Atom Selection

Dialog Box

Visual
Ligand Interaction

LIE

3D

Visualisation
J. D. Madura

Schedule of Lectures
Lecture Objectives
Introduction
Data Visualization
Introduction
Scientific Plots
Introduction to R
Water Dimer Example
Molecular Visualization
VMD
Input
Graphics
Extensions
Saving and Capturing Graphics
Movie Making
MOE
Input
Graphics
Selection
Compute
Learning Outcomes
Stereoview
Outcomes

You should be able to

- create a simple plot of (x,y) pairs of data and properly label the plot using R.
- describe the basic features of VMD and know how to use them.
- describe the basic features of MOE.