**Python**

**How to make a multiplication in Python**

**>>> 2+3\*4**

**14**

**How to print variables in python**

**>>> name = “Andrew”**

**>>> name**

**Andrew**

**How to concatenate and print**

**>>> print “Hello”, name**

**Hello Andrew**

**How to create a list**

**>>> names = [“Ben”,”Chen”,”Yaqin”]**

**How to get the length of a list**

**>>> len(names)**

**3**

**How to get an item from the list**

**>>> names[0]**

**‘Ben’**

**How to get an item from the list using negative values**

**>>> names[-1]**

**‘Yaqin’**

**How to use slice to get substring**

**>>> smiles=”C(=N)(N)N.C(=O)(O)O”
>>> smiles[1:5]**

**(=N)**

**>>> smiles[10:-4]**

**C(=O)**

**How to find the location of an element
>>> smiles.find(“(O”))**

**15
>>> smiles.find(“.”)**

**9**

**>>> smiles.find(“.”,10)**

**-1 #nt found**

**>>> smiles.split(“.”)**

**[‘C(=N)(N)N’,’C(=O)(O)O’]**

**How to check if a string is inside another**

**if “Br” in “Brother”:**

 **print “contains brother”**

**Remove whitespace like chomp**

**>>> line ‘ This is a comment \n”**

**>>> line.strip()**

**‘This is a comment line’**

**Check if a string starts with**

**>>> email = ‘ceorge@hotmail.com’**

**>>> email.startswith(“c”)**

**True**

**Check if string ends with**

**>>> email = ‘ceorge@hotmail.com’**

**>>> email.startswith(“m”)**

**False**

**Turns list into string
>>> names =[“Ben”,”Chen”,”Yaqin”]**

**>>> “,” .join(names)**

**‘Ben , Chen, Yaqin’**

**Turn a string into upper case**

**>>> “chen”.upper()
CHEN**

**Change the char of a string
>>> s = “andrew”**

**>>> s[0] = “A” #Doesn’t work**

**>>> s = “A” + s[1:]**

**>>> s**

**Andrew**

**Append element to a list**

**>>> ids = [“9pti”,”2plv”,”1crn”]**

**>>> ids.append(“1alm”)**

**>>> ids**

**[‘9pti’,’2plv,’1crn’,’1alm’]**

**Delete element from list**

**>>> del ids[0]**

**>>> ids**

**[‘2plv’,’1crn’,’1alm’]**

**Sort elements from list**

**>>> ids.sort()**

**>>> ids**

**[‘1alm’,’1crn’,’2plv’]**

**Reverse elements from list**

**>>> ids.reverse()**

**>>> ids**

**[‘2plv’,’1crn’,’1alm’]**

**Insert element to list at a specific location**

**>>> ids.insert(0,”9pti”)**

**>>> ids**

**[‘9pti,’2plv’,’1crn’,’1alm’]**

**Zipping lists together**

**>>> names**

**[‘ben’,’chen’,’yaqin’]**

**>>> gender = [0,0,1]**

**>>> zip(names, gender)**

**[(‘ben,0),(‘chen’,0),(‘yaqin,1)]**

**How to create a dictionary (hash) in python**

**symbol\_to\_name = {**

**“H”: “Hydrogen”,**

**“He”: “Helium”,**

**“Li”: “Lithium”,**

**“C”: “Carbon”,**

**“O”: “Oxygen”,
“N”: “Nitrogen”**

**}**

 **How to get a value of a given key of a dictionary**

**>>> Symbol\_to\_name[“C”]**

**‘carbon’**

**How to check if a value of a given key of a dictionary exists**

**>>> “O” in symbol\_to\_name**

**True**

**>>> “U” in symbol\_to\_name**

**False**

**How to list all the keys of a given dictionary**

**>>> symbol\_to\_name.keys()
[‘C’,’H’,’O’,’N’,’Li’,’He]**

**How to list all the values of a given dictionary**

**>>> symbol\_to\_name.values()**

**[‘carbon’, ‘hydrogen’,’oxygen’,’nitrogen’,’lithium’,’helium’]**

**How to update a value from a given dictionary**

**>>> symbol\_to\_name.update({“P”:”phosphorous”,”S”: “sulfut”})**

**How to print keys and values of a given dictionary**

**>>> symbol\_to\_name.items()**

**[(‘C’, ‘carbon’),( ‘H’, ‘hydrogen’),(‘O’,’oxygen’),(’N’, nitrogen’),(‘L’, ’lithium’),(‘H’, ’helium’)]**

**How to delete a key of a given dictionary**

**del symbol\_to\_name[‘C’]**

**[( ‘H’, ‘hydrogen’),(‘O’,’oxygen’),(’N’, nitrogen’),(‘L’, ’lithium’),(‘H’, ’helium’)]**

**How to use bool in python**

**>>> smiles =”Hello world!”
>>> bool(smiles)**

**True**

**>>> not bool(smiles)**

**False**

**How to use if in python**

**>>> if not smiles**

 **print “The SMILES string is empty”**

**How to use elif in python**

**Mode =”absolute”**

**If mode = “canonical”:**

 **smiles = “canonical”**

**elif mode ==” simoeric”:**

**else:**

**do it.**

**>>> smiles**

**‘absolute’**

**How to use For in python**

**>>> names = [“Ben”,”Chen”,”Yaqin”]**

**>>> for ame in names:**

 **print name**

**Ben
Chen
Yaqin**

**How to assign tuple in for loops**

**Data = [ (“C20H2003”,”308.371”),**

**(“C20H200k”,”316.393”),**

**(“C20H200i”,”416.6”)]**

**for (formula, mw) in data:**

 **print “The molecular weight of %s is %s” % (formula, mw)**

**The molecular weight of C20H2003 is 308.371.**

**The molecular weight of C20H200k is 316.393.**

**The molecular weight of C20H200i is 416. 6.**

**Break, continue**

**Break: stop the for loop
Continue: stop the current for loop and restart**

**How to use range**

**>>> range(5)**

**[0,1,2,3,4]**

**range(5,10)**

**[5,6,7,8,9]**

**range(0,10,2)**

**[0,2,4,6,8]**

**How to read a file**

**>>> f = open(“names.txt”)**

**>>> f.readline()**

**Yaqin\n**

**How to create file output in python**

**Input\_file = open(“in.txt”)**

**Output\_file = open(“out.txt,”w”)**

**for line in input\_file:**

 **output\_file.write(line)**

**Common file read/write:**

**“w”: write mode**

**“a”: append mode
“wb”: write in binary”**

**“r”: read mode (default)**

**“rb”: “read in binary”**

**“U” = “read files with Unix”**

**Math:**

**>>> import math**

**>>> math.pi**

**3.14234234234234**

**>>> math.cos(0)**

**1.0**

**>>> math.cos(math.pi)**

**-1.0**

**>>> dir(math)**

**[‘doc’os…..]**

**>>> help(math)
>>> help (math.cos)**