Decisions and Loops

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In Terminal, open new screen

Open a Python Interactive prompt

$ **python**

```
Python 2.6.1 (r261:67515, Aug  2 2010, 20:10:18)
[GCC 4.2.1 (Apple Inc. build 5646)] on darwin
Type "help", "copyright", "credits" or "license" for
more information.
>>> dna = 'atcgatc'
```

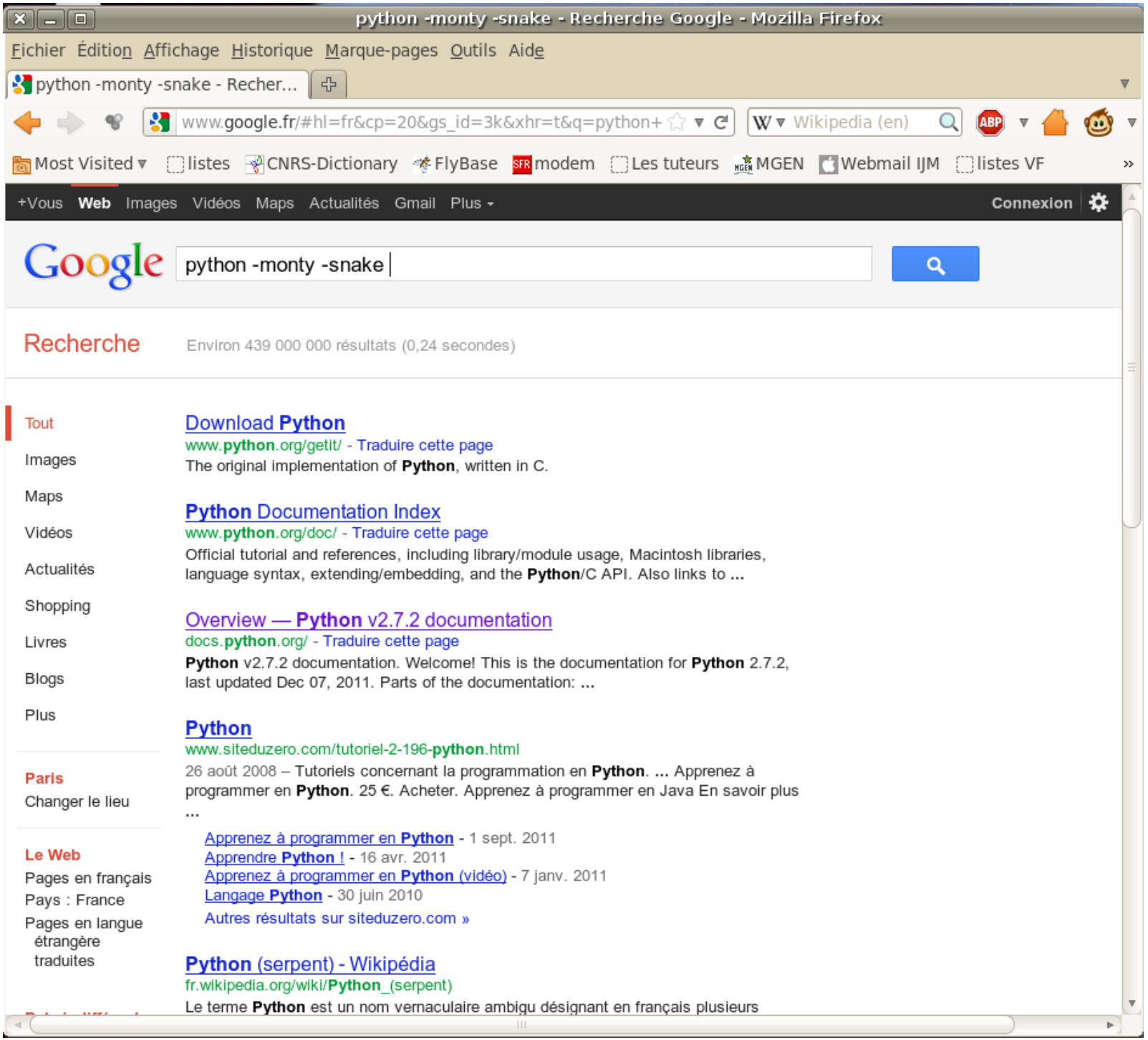
>>> dir(dna) shows all “methods” for use with strings

Methods are functions built into each type of variable. “dot notation”

```
>>> dna.count('atc')
2
```

>>> help(strg) shows all commands for use with strings

Ctrl+D to quit Python Interactive prompt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www.siteduzero.com/tutoriel-2-196-python.html
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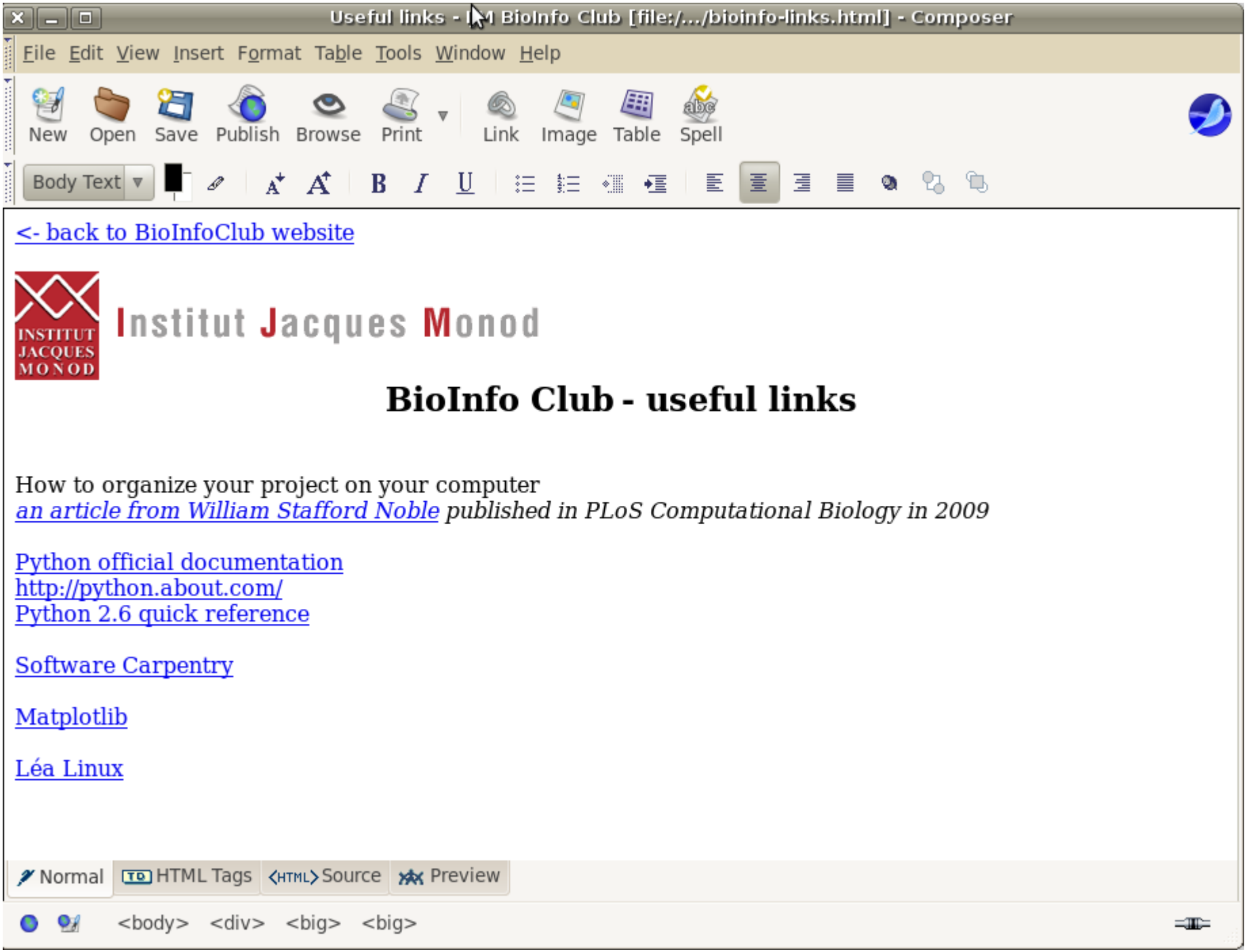
Autres résultats sur siteduzero.com »
Python (serpent) - Wikipédia
fr.wikipedia.org/wiki/Python_(serpent)
Le terme Python est un nom vernaculaire ambigu désignant en français plusieurs


Useful links - IJM BioInfo Club [file:/.../bioinfo-links.html] - Composer
File Edit View Insert Format Table Tools Window Help
New Open Save Publish Browse Print Link Image Table Spell
Body Text
<- back to BioInfoClub website
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Institut Jacques Monod
BioInfo Club - useful links
How to organize your project on your computer
an article from William Stafford Noble published in PLoS Computational Biology in 2009
Python official documentation
http://python.about.com/
Python 2.6 quick reference
Software Carpentry
Matplotlib
Léa Linux
Normal HTML Tags Source Preview
<body> <big> <big>

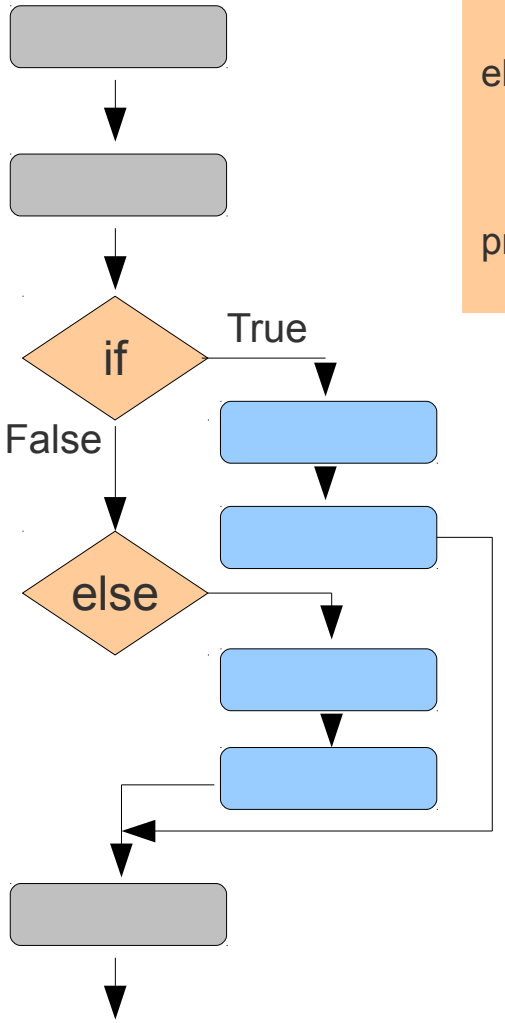
Goal:

calculate melting temperature of a given DNA sequence

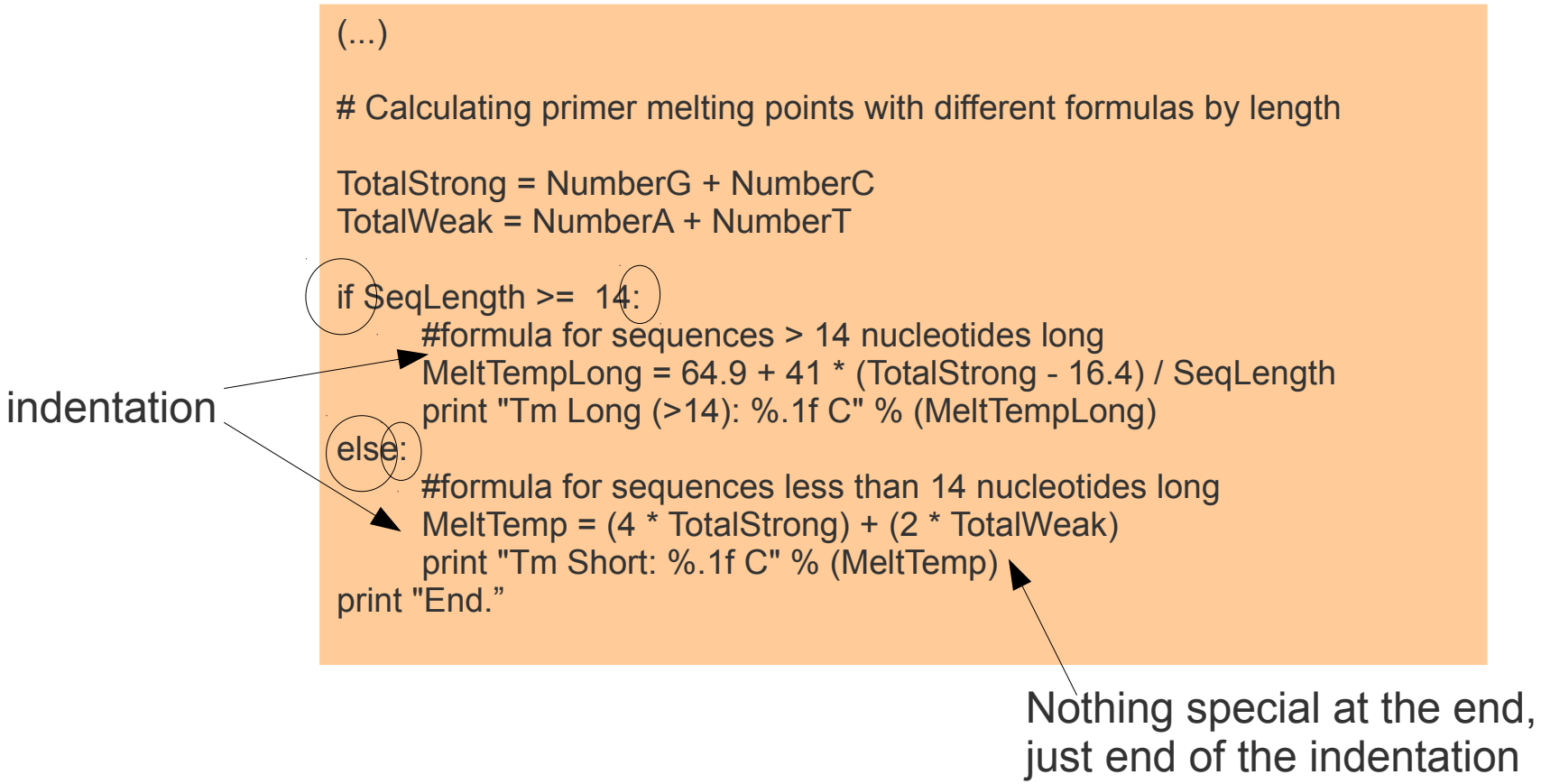
Open the dnacalc1.py file

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

DNASeq = "ATGTCTCATTCAAAGCA"

# gather user input for sequence
# this overrides the definition of DNASeq above
# DNASeq = raw_input("Enter a sequence: ")
DNASeq = DNASeq.upper()  # convert to uppercase for .count() function
DNASeq = DNASeq.replace(" ","") # remove spaces

print 'Sequence:', DNASeq

# below are nested functions: first find the length, then make it float

SeqLength = float(len(DNASeq))

print "Sequence Length:", SeqLength

NumberA = DNASeq.count('A')
NumberC = DNASeq.count('C')
NumberG = DNASeq.count('G')
NumberT = DNASeq.count('T')

# Old way to output the Numbers
# print "A:", NumberA/SeqLength
# print "C:", NumberC/SeqLength
# print "G:", NumberG/SeqLength
# print "T:", NumberT/SeqLength

# Calculate percentage and output to 1 decimal
print "A: %.1f" % (100 * NumberA / SeqLength)
print "C: %.1f" % (100 * NumberC / SeqLength)
print "G: %.1f" % (100 * NumberG / SeqLength)
print "T: %.1f" % (100 * NumberT / SeqLength)

# End of Chapter 8
```

'if-else' statement




```
(...)

# Calculating primer melting points with different formulas by length

TotalStrong = NumberG + NumberC
TotalWeak = NumberA + NumberT

if SeqLength >=  14:
        #formula for sequences > 14 nucleotides long
        MeltTempLong = 64.9 + 41 * (TotalStrong - 16.4) / SeqLength
        print "Tm Long (>14): %.1f C" % (MeltTempLong)
else:
        #formula for sequences less than 14 nucleotides long
        MeltTemp = (4 * TotalStrong) + (2 * TotalWeak)
        print "Tm Short: %.1f C" % (MeltTemp)
print "End."
```



Indentation is a requirement in Python.

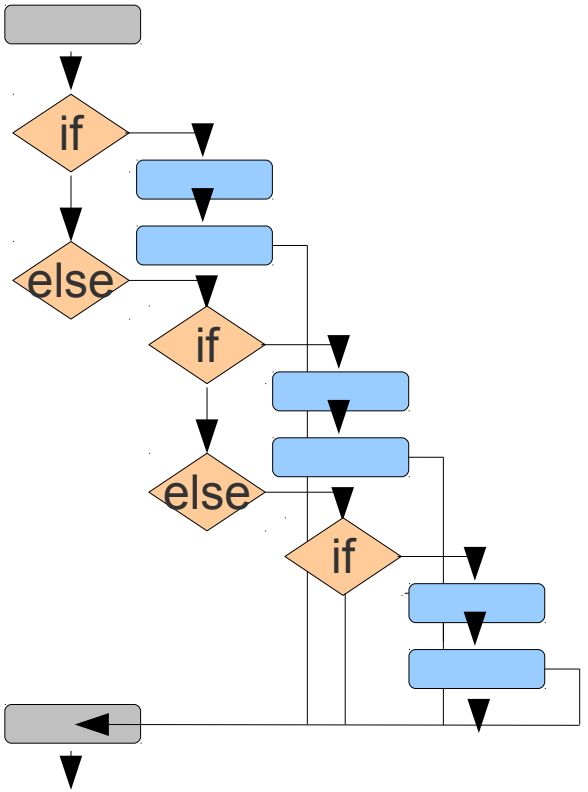
Either spaces (always same number, typically four) or tab.

	Operators	Is true if...
Comparison operators	X == y	X is equal to y
	X != y	X is not equal to y
	X > y	X is greater than y
	X >= y	X is greater than or equal to y
Logical operators	A and B	Both A and B are true
	A or B	Either A or B are true
	not B	B is false (inverts the value of B)
	(not A) or B	A is false or B is true
	not (A or B)	A and B are both false

Be careful not to put a single = sign in an “if” statement

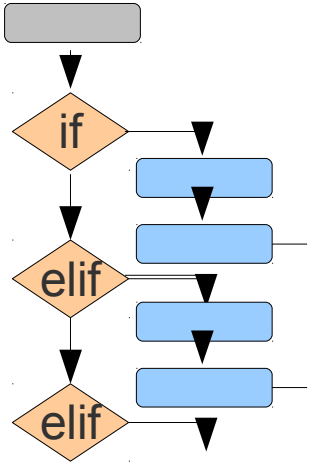
Many indentations when there are 3 cases

```
If X == 1:
        Value = “one”
else:
                if X == 2:
                                Value=”two”
                else:
                                if X == 3:
                                                Value=”three”
```



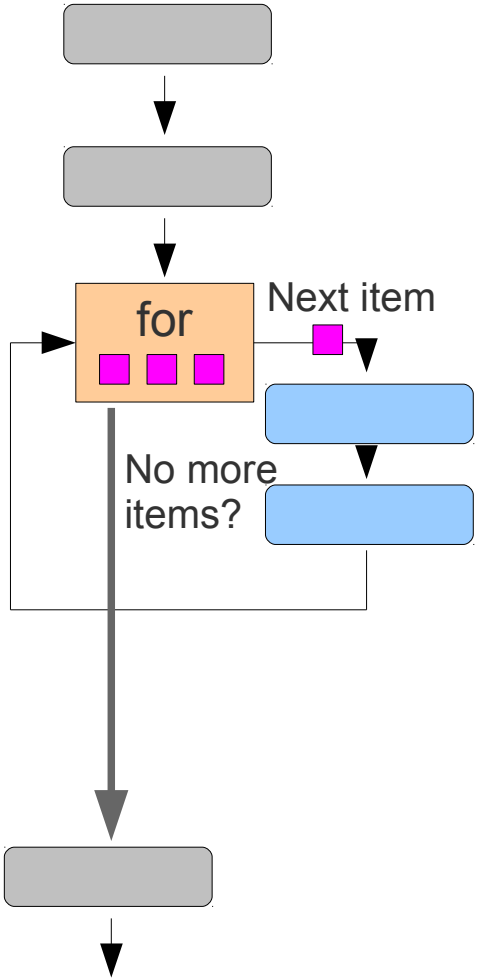
Better = use elif

```
If X == 1:
        Value = “one”
elif X == 2:
        Value=”two”
elif X == 3:
        Value=”three”
```



Goal:
calculate molecular weight of a given protein sequence

We will use the for loop



We will use a list

```
MyCollection= [1,2,3,4,5]
MyCollection=['A','T','G','C','T']
MyCollection=list('ATGCT')
```

In Python, the for loop can operate directly on each character of a string without conversion to a list.

Write a new script entitled proteincalcTEST.py

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

ProteinSeq="FDILSATFTYGNR"

for Aa in ProteinSeq:
        print Aa
        print '-'
```

What does it do?

We will generate a dictionary with each amino acid's single letter code and its corresponding molecular weight.

```
MyDictionary = {key1:value1, key2:value2}

MyDictionary = {'A':89,09, 'R':174,20, 'N':...}

MyDictionary = {
'A':89.09,
'R':174.20,
'N':
(…)
'X':0,
'-':0,
'*':0 }
```

(1) use the aminoacid.html file that can be found on the web (also in your example folder).

(2) copy only the useful lines into your text editor

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```
<tr><td>Alanine</td><td>Ala</td><td>A</td><td>89.09</td></tr>
<tr><td>Arginine</td><td>Arg</td><td>R</td><td>174.20</td></tr>
<tr><td>Asparagine</td><td>Asn</td><td>N</td><td>132.12</td></tr>
<tr><td>Aspartic acid</td><td>Asp</td><td>D</td><td>133.10</td></tr>
<tr><td>Cysteine</td><td>Cys</td><td>C</td><td>121.15</td></tr>
<tr><td>Glutamine</td><td>Gln</td><td>Q</td><td>146.15</td></tr>
<tr><td>Glutamic acid</td><td>Glu</td><td>E</td><td>147.13</td></tr>
<tr><td>Glycine</td><td>Gly</td><td>G</td><td>75.07</td></tr>
<tr><td>Histidine</td><td>His</td><td>H</td><td>155.16</td></tr>
<tr><td>Isoleucine</td><td>Ile</td><td>I</td><td>131.17</td></tr>
<tr><td>Leucine</td><td>Leu</td><td>L</td><td>131.17</td></tr>
<tr><td>Lysine</td><td>Lys</td><td>K</td><td>146.19</td></tr>
<tr><td>Methionine</td><td>Met</td><td>M</td><td>149.21</td></tr>
<tr><td>Phenylalanine</td><td>Phe</td><td>F</td><td>165.19</td></tr>
<tr><td>Proline</td><td>Pro</td><td>P</td><td>115.13</td></tr>
<tr><td>Serine</td><td>Ser</td><td>S</td><td>105.09</td></tr>
<tr><td>Threonine</td><td>Thr</td><td>T</td><td>119.12</td></tr>
<tr><td>Tryptophan</td><td>Trp</td><td>W</td><td>204.23</td></tr>
<tr><td>Tyrosine</td><td>Tyr</td><td>Y</td><td>181.19</td></tr>
<tr><td>Valine</td><td>Val</td><td>V</td><td>117.15</td></tr>
<tr><td>Unknown</td><td>Xaa</td><td>X</td><td>0.0</td></tr>
<tr><td>Gap</td><td>Gap</td><td>-</td><td>0.0</td></tr>
<tr><td>Stop</td><td>End</td><td>*</td><td>0.0</td></tr>
```

(3) use regular expressions to change this text into:

HINT: use [\d\.]+
The beginning of your query should be:
.+(.)

```
'A':89.09,
'R':174.20,
'N':132.12,
'D':133.10,
'C':121.15,
'Q':146.15,
'E':147.13,
'G':75.07,
'H':155.16,
'I':131.17,
'L':131.17,
'K':146.19,
'M':149.21,
'F':165.19,
'P':115.13,
'S':105.09,
'T':119.12,
'W':204.23,
'Y':181.19,
'V':117.15,
'X':0.0,
'-':0.0,
'*':0.0,
```

(2) copy only the useful lines into your text editor

```
<tr><td>Alanine</td><td>Ala</td><td>A</td><td>89.09</td></tr>
<tr><td>Arginine</td><td>Arg</td><td>R</td><td>174.20</td></tr>
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<tr><td>Tryptophan</td><td>Trp</td><td>W</td><td>204.23</td></tr>
<tr><td>Tyrosine</td><td>Tyr</td><td>Y</td><td>181.19</td></tr>
<tr><td>Valine</td><td>Val</td><td>V</td><td>117.15</td></tr>
<tr><td>Unknown</td><td>Xaa</td><td>X</td><td>0.0</td></tr>
<tr><td>Gap</td><td>Gap</td><td>-</td><td>0.0</td></tr>
<tr><td>Stop</td><td>End</td><td>*</td><td>0.0</td></tr>
```

Search for:

```
.+(.)</td><td>([\d\.]+)</td></tr>
```

Replace by:

```
'$1':$2,
```

(3) use regular expressions to change this text into:

```
'A':89.09,
'R':174.20,
'N':132.12,
'D':133.10,
'C':121.15,
'Q':146.15,
'E':147.13,
'G':75.07,
'H':155.16,
'I':131.17,
'L':131.17,
'K':146.19,
'M':149.21,
'F':165.19,
'P':115.13,
'S':105.09,
'T':119.12,
'W':204.23,
'Y':181.19,
'V':117.15,
'X':0.0,
'-':0.0,
'*':0.0,
```

HINT: use [\d\.]+
The beginning of your query should be:
.+(.)

(4) copy and paste in your script file

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

ProteinSeq="FDILSATFTYGNR"

AminoDict={
'A':89.09,
'R':174.20,
'N':132.12,
(…)
'-':0.0,
'*':0.0}

for Aa in ProteinSeq:
    print Aa, AminoDict[Aa]

MolWeight = 0
for Aa in ProteinSeq:
    MolWeight = MolWeight + AminoDict[Aa]
Print “Molecular Weight: %.1f” % (MolWeight)
```

Improvements

Use the .get() function so that unknown characters are taken into account

`AminoDict.get('A')` is equivalent to **`AminoDict['A']`**
Here use **`AminoDict.get(Aa,0.0)`**

The .keys() and .values() functions might be useful as well.

`print AminoDict.values()` return them in an unpredictable order
use `sorted(AminoDict.values())` for the alphabetical order

Check the compositioncalc1.py file

What does it do?

```
#! /usr/bin/env python
DNASeq = "ATGTCTCATTCAAAGCA"
SeqLength = float(len(DNASeq))

BaseList = list(set(DNASeq))
for Base in BaseList:
    Percent = 100 * DNASeq.count(Base) / SeqLength
    print "%s: %4.1f" % (Base,Percent)
```