```
Welcome to the CHN Program for Elemental Analysis

Sample Name: lisinopril
Molecular formula Input

How many Carbons ? 21

How many Hydrogens ? 31

How many Nitrogens ? 3

How many Oxygens ? 5

How many Chlorines ?

How many Fluorines ?

Other Elements? [N]

CHN Analysis Report - 06-Dec-2019 02:07 PM
lisinopril
C2 H3 N3 O5
MW: 405.49
Monoisotopic Mass: 405.22637
+---------+-------------------------+
| Element | Theoretical Percentage |
+---------+-------------------------+
|    C    |         62.20          |
|    H    |          7.71          |
|    N    |         10.36          |
|    O    |         19.73          |
+---------+-------------------------+

1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 4

Filename: [chn_results.txt]

1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 2
```

You can enter as long as a sample code and/or description as needed.

Add integers for each specified element, hit return if there are none of the specified element.

You'll have the option, to enter less common elements by symbol. Hit return for none.

Printing to file for documentation. Enter file name or hit return to accept the default.

Choosing to enter experimental data.

```
Enter experimental determined percentages

%C: 57.12

%H: 7.98

%N: 9.53
```

Enter experimentally determined percentages. Sulfur will be included if it's in your molecular formula.

```
CHN Analysis Report - 06-Dec-2019 02:08 PM
lisinopril
C2 H3 N3 O5
MW: 405.49
Monoisotopic Mass: 405.22637
```

Element	Theoretical Percentage	Experimental	Difference
C	62.20	57.12	-5.08
H	7.71	7.98	0.27
N	10.36	9.53	-0.83
O	19.73		

```
1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 4

Filename: [chn_results.txt]

1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 3

Molar Ratio : 1
```

Printing will append an existing file.

Selecting Add Water of hydration and entering the molar ratio.

```
CHN Analysis Report - 06-Dec-2019 02:08 PM
lisinopril
C2 H3 N3 O5  * 1.0H2O
MW: 405.49 (free)
FW: 423.50
Monoisotopic Mass: 405.22637
```

A formula weight is added to incorporate the weight of the hydrate.

Element	Theoretical Percentage	Experimental	Difference
C	59.56	57.12	-2.44
H	7.85	7.98	0.13
N	9.92	9.53	-0.39
O	22.67		

```
1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 4

Filename: [chn_results.txt]

1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 3

Molar Ratio : 2
```

Updating the hydration molar ratio to 2; in this case more closes matches the experimental data.

```
CHN Analysis Report - 06-Dec-2019 02:09 PM
lisinopril
C2 H3 N3 O5  * 2.0H2O
MW: 405.49 (free)
FW: 441.52
Monoisotopic Mass: 405.22637
```

Element	Theoretical Percentage	Experimental	Difference
C	57.13	57.12	-0.01
H	7.99	7.98	-0.01
N	9.52	9.53	0.01
O	25.37		

```
1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 4

Filename: [chn_results.txt]

1)Enter new MF
2)Enter experimental data
3)Add Water of hydration
4)Print to file
5)Exit Program

Input a menu option number : 5
Done.
```

Printing to file again. See included chn_results.txt file for a consolidated elemental analysis report.