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| Class | Wellington Year 11-12 Chemists |
| Lesson 2 | Recap Skeletal formulae and using computers.  Recap smiles strings |
| Building on | Crude oil is mixture of complex hydrocarbons  Carbon atoms in chains and rings  Fractional distillation  Variation in physical properties  Cracking |
| Last lesson | Students should know that a line indicates two carbons bonded together  Hydrogens are implicit  That alkanes are a homologous series  Names of first 4 alkanes  That a computer can be used to manually draw these molecules  That a computer can be used to generate these images and calculate properties |
| Learning objectives | Students should know that variables can be stored in a list or array  They should be able to use a for loop to iterate over a list or array  Know how to define and extend a string by concatenation  Use this to define SMILES strings for the top n alkanes |
| Requirements: | Jupyter notebook with RDKit, pandas, matplotlib numpy env to work in |
|  | Lessons are an hour long? |
| Starter  5-10 mins | What is a string in python?  Any text, defined using inverted commas ‘text’ or quotation marks “text”  What is a SMILES string?  A machine readable way to describe an organic molecule  What does SMILES stand for? (google if you don’t know)  Simplified Molecular Input Line Entry System  What is the displayed formula of ethane?    What is the structural formula of pentane (five carbons long)?  CH3CH2CH2CH2CH3  What is the skeletal formula of propane?    What is the SMILES string for Pentane?  ‘CCCCC’  Write down any other smiles strings you can think of, together with their displayed formula and molecular weights |
| Strings  10 - 15 mins | Strings in Python  One of the most common and useful variable types in Python is the string.  You can define a string using inverted commas or quotation marks, both work well.  This also allows you to define a string with an apostrophe:  See code blocks 3 and 4.  S = ‘I don’t like cabbage’ returns an error.  Errors are very useful, they tell you where you went wrong in programming, and everyone, even very experienced programmers go wrong.  This error is a SyntaxError, telling you the computer doesn’t understand what you said.  If you change it so there are quotation marks around it in the code block, then run it again,  p = “I don’t like cabbage”  print(p)  works well.  Work down to code block 8, and complete the TODO |
| Arrays  10 mins | We can store the information we generate in a list.  Arrays and lists are defined in Python using square brackets.  An empty list is defined by []  A list has an order.  For example, in code block 9, I have defined a list of names. Please change these names to names you like, add other names if you like too, then run this block.  You can index by using the name of the array e.g. my\_names[0] gives you the first value, my\_names[-1] gives you the last value, my\_names[1] gives the second value, e.t.c..  What happens if you try to index something that isn’t there, i.e. my\_names[9]? – (try it!) IndexError  You can append to an array by using a method on the array itself.  my\_names.append(‘Fred’) adds the name ‘Fred’ to the list.  Work down to code block 14 and complete the TODO there. |
| For Loops  10 mins | If you want to say hello to everyone on the list, it would be annoying to write print(‘Hello ‘ + ‘Alice’ + ‘!’) out for each of the people in the list.  So we use a for loop as a way of repeating the same code again and again.  The syntax is simple: first you put the word for, then you put the variable name that will substitute for each of the members of the array one after the other, then you put in, and last you put the name of the array you will be iterating over.  You can use any array, though be careful if you have different data types, the same code might not work for everything.  You can substitute range(n) for any list of numbers 0 – n.  Run through code blocks 15-18, then work though the TODO in block 19. |
| Using RDKit  20 mins | We can use range to define as many alkanes as we want.  See blocks 20-21.  Complete the TODO in block 22  If you finish that, try to get the skeletal formula for each one to show. You may need to google how to do this.  Try to do the same for other homologous serieses, such as alkenes, alcohols |
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| Summary  2 mins | We have learned more about strings in Python, and been introduced to Lists, which are Python arrays, as well as for loops, which help us reuse code, making it faster and easier to work though a whole series of things. |
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