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| Class | Wellington Year 11-12 Chemists |
| SOW | Course within a Course  Computing for chemists |
| Building on | Crude oil is mixture of complex hydrocarbons  Carbon atoms in chains and rings  Fractional distillation  Variation in physical properties  Cracking  GCSE Chemistry |
| Aims: | Show how Python is used in Chemistry  Learn basic programming – Variables, loops and arrays.  Use RDKit to calculate values and display molecular structures  Learn about chemical data |
| Lesson 1 | What is a homologous series?  Alkanes: first four names  Displayed, structural and skeletal formulae  Smiles strings  With prewritten code to support learning of molecular and skeletal formula, and calculation of molecular weights.  Main acitivty:  Draw up a table of the first four alkanes, with molecular, structural, and skeletal formula as well as molecular weight and a photo of the molymod sturcture  Requirements:  Molymods  Jupyter notebook with RDKit, pandas, matplotlib numpy env to work in |
| Lesson 2 | More programming:  Strings, defining, concatenation  Arrays, defining, indexing and appending  For loops to iterate over arrays and reuse code  Using examples of names, then SMILES strings.  Reusing code from lesson 1 inside a for loop  Main Activity:  Writing code snippets supported with other bits of code  Producing images of arrays of molecules generated by for loops  Requirements:  Jupyter notebook with RDKit, pandas, matplotlib numpy env to work in |
| Lesson 3 | Data in chemistry and programming  Plotting graphs, manipulating arrays, numpy  Graph of boiling points, melting points |
| Lesson 4 | Getting data about molecules  Reading in data, plotting graphs |
| Lesson 5 |  |
| Lesson 6 |  |
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