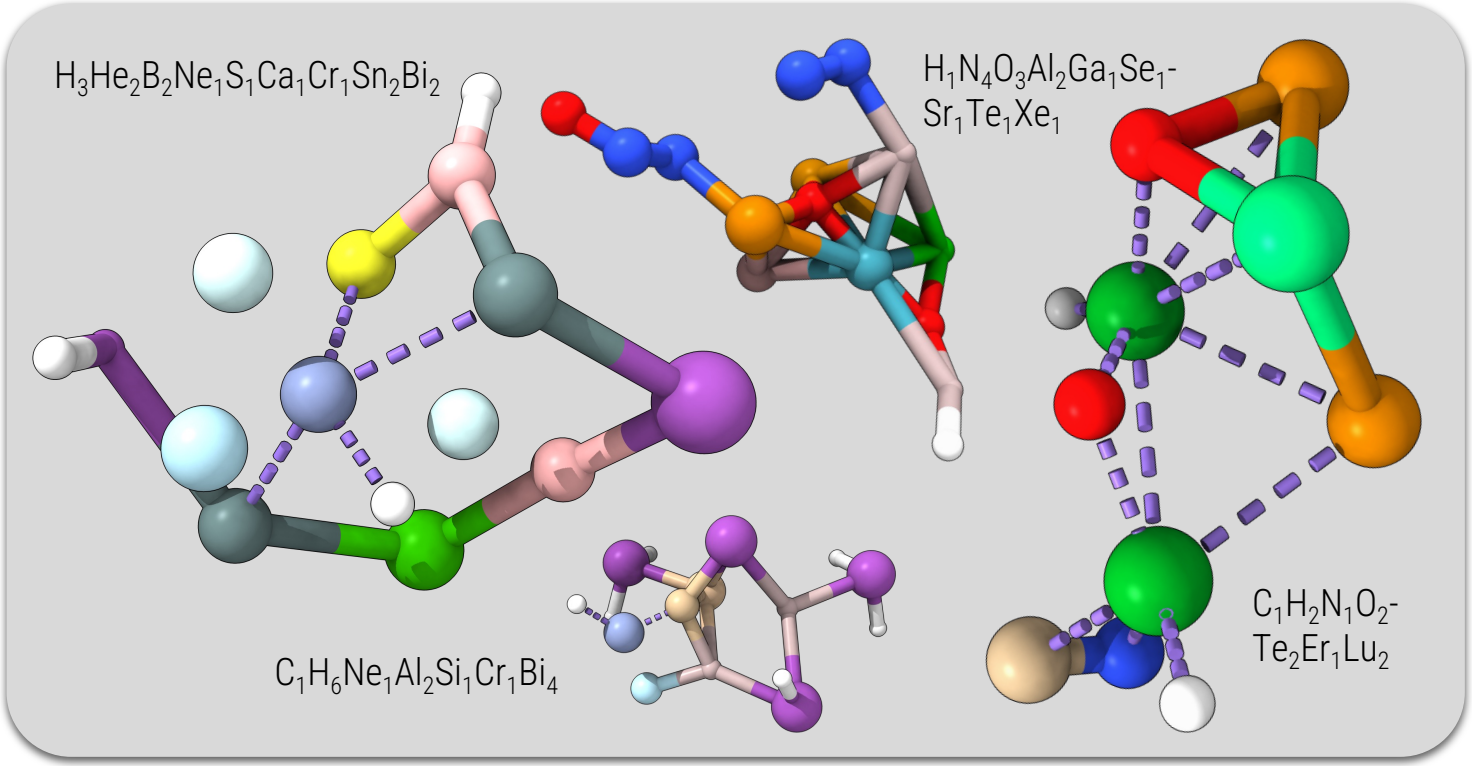
MindlessGen

Generate ”mindless” molecules from scratch!

… powered by xTB and ORCA.




```
Reading configuration from file: '/Users/marcelmueller/projects/mindlessgen/testdir/mindlessgen.toml'

MindlessGen v0.3.1
Semi-Automated Molecule Generator

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General configuration:
                verbosity:   1
                max_cycles:  500
              print_config:  False
                 parallel:   6
            num_molecules:   1
              postprocess:   True

Generate configuration:
                min_num_atoms:   15
                max_num_atoms:   25
           init_coord_scaling:   3.0
                dist_threshold:   1.0
       increase_scaling_factor:   1.1
           element_composition:   {6: (1, 2)}
           forbidden_elements:   [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 3

Orca configuration:
                 orca_path:   orca
                functional:   PBE
                     basis:   def2-SVP
                 gridsize:   1
               scf_cycles:   200

Postprocess configuration:
                    engine:   orca
                opt_cycles:   5
                  optimize:   True
                     debug:   False

Refine configuration:
             max_frag_cycles:   5
                    engine:   xtb
                     debug:   False

Xtb configuration:
                 xtb_path:   /path/to/xtb


Running with 6 cores.
/Users/marcelmueller/source/MindlessGen/src/mindlessgen/generator/main.py:67: UserWarning: Parallelization v
  warnings.warn(
Cycle... ////////////////////////////////
```

Simple but extensive input in **`TOML`** format

```
[generate]
# > Minimum number of atoms in the generated molecule. Option
min_num_atoms = 2
# > Maximum number of atoms in the generated molecule. Option
max_num_atoms = 100
# > Initial coordinate scaling factor. Options: <float>
init_scaling = 3.0
# > Increase in the coordinate scaling factor per trial after
increase_scaling_factor = 1.3
# > Distance threshold for the inital, randomly generated coo
dist_threshold = 1.2
# > Atom types and their minimum and maximum occurrences. For
# > Elements that are not specified are only added by random
# > A star sign (*) can be used as a wildcard for integer val
element_composition = "C:2-10, H:10-20, O:1-5, N:1-*"
# > Atom types that are not chosen for random selection. Form
# > CAUTION: This option is overridden by the 'element_compos
# > I.e., if an element is specified in 'element_composition'
# > Example: forbidden_elements = "18,57-*"
forbidden_elements = "57-71"

[refine]      You, 2 weeks ago • refactored configuration, it
# > Maximum number of fragment optimization cycles. Options:
max_frag_cycles = 100
# > Quantum Mechanics (QM) engine to use. Options: 'xtb', 'or
engine = "xtb"
# > Debug this step. Leads to more verbose output as soon as
# > If `debug` is true, the process is terminated after the f
debug = false

[postprocess]
# > Engine for the post-processing part. Options: 'xtb', 'orc
```

SotA Python code base

- **Detailed atom composition possible**
- **Self-consistent fragment detection**
- **xTB geometry optimization & DFT sanity check**
- **Isomerization reactions**

github.com/grimme-lab/MindlessGen