

The background features several molecular models. On the left, a grey wireframe mesh represents a protein structure, with a blue ribbon tracing a path through it. In the top right, a blue ball-and-stick model shows a portion of a carbon nanotube. In the bottom right, there are several smaller molecular models, including one with orange and white spheres and another with a blue sphere and a light blue arrow.

Support for RDKit development

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Software engineering support

- Automated compilation and internal tests allow devs to work with confidence
- Building any tool using a consistent set of options is trickier than you expect
- RDKit had existing and deep automated testing
- Schrodinger has additional experience in releasing and testing software
 - We've found some tools and practices particularly useful

Added instructions for building under anaconda

- Easiest way to build using a consistent toolchain
- Should help new developers contribute more easily to core RDKit
- <https://github.com/rdkit/rdkit/pull/1944>

Helps new developers contribute successfully:

- Who's joining the hackathon?

Addressed compiler warnings

- Why address warnings?
- <https://github.com/rdkit/rdkit/pull/2097>
- <https://github.com/rdkit/rdkit/pull/2318>

Helps developers:

- Catch unused variable problems (and many more)

Addressed existing memory leaks

- Major effort, 80+ commits
- Most leaks were in test code
- There were a few leaks in production code, especially in error conditions
- <https://github.com/rdkit/rdkit/pull/2123>
- <https://github.com/rdkit/rdkit/pull/2305>

Helps users!

```
168         if (!agentMol) {
169             std::string errMsg = "Problems constructing agent from SMARTS: ";
170             errMsg += agentText;
171 +         delete rxn;
172         throw ChemicalReactionParserException(errMsg);
173     }
```

Enabled automatic memory testing

- Enabled automatic memory leak detection (valgrind)
- A test not run automatically is a test not run!
- <https://github.com/rdkit/rdkit/pull/2113>

Helps developers:

- Avoid pushing errors that are easy to make and hard to catch

Run automated tests on Windows

- Switched automated builds to Windows Azure
- Allows automated testing
 - precluded by duration previously
- <https://github.com/rdkit/rdkit/pull/2409>

Helps developers:

- Catch Windows-only execute and runtime linking issues