MAKING PORTABLE APPLICATIONS WITH RDKIT

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- Chemistry application or chemistry library
  - Written in C++ and using RDKit
  - Self-contained in a single file on your computer
  - Will work on all versions of Windows from XP onwards

- Why? Super-portable!
  - No deployment problems – will just work

NAMERXN

- Commandline application that names reactions

```
C:\NameRxn\Release> namerxn.exe C:\ReactionsFromPatents.rsmi
US20010000038A1 : 10.1.1 Bromination [Halogenation]
US20010000038A1 : 10.1.1 Bromination [Halogenation]
US20010000038A1 : 0.0 Unrecognized [Unassigned]
US20010000038A1 : 9.7.27 Chloro to hydroxy [Other functional group
interconversion]
US20010000038A1 : 1.7.0 Ethyl esterification [O-substitution]
```

COMPILE WITH MSVC++

- Use Cygwin's Cygcheck to look at dependencies

```
C:\NameRxn\Release> C:\Cygwin\bin\cygcheck.exe ./namerxn.exe
C:\NameRxn\Release\namerxn.exe
  ...
  ...
  ...
  C:\Windows\system32\MSVCP110.dll
    C:\Windows\system32\MSVCR110.dll
```

- Depends on MSVC++ dlls which may not be present on the user's machine
  - Would have to bundle somehow with the application

- Solution: Use the MinGW compiler
  - GCC, Open source

MINGW AND RDKIT APPLICATIONS

- Need to build everything from the bottom-up with MinGW
  - Boost
  - RDKit
  - Any other dependencies (e.g. zlib, cairo)

- Finally build your own application
  - Statically link any dependencies

COMPILE WITH MINGW

- Use Cygwin's Cygcheck to look at dependencies

```
C:\NameRxn\Release> C:\Cygwin\bin\cygcheck.exe ./namerxn.exe
C:\NameRxn\namerxn.exe
  ...
  ...
  ...
  C:\MinGW\bin\libgcc_s_dw2-1.dll
  C:\MinGW\bin\libstdc++-6.dll
```

- Same problem as with MSVC++, but this time there is a solution

  – Use special compile and link flags:

  "-static-libgcc" "-static-libstdc++" and "-s"

- Removes the dependency on MinGW dlls

END RESULT

- Portable namerxn.exe
- Also portable SWIG bindings
  - Python, .NET, Java ("-Wl,--kill-at")

- Python modules: one .py file, one .pyd
- Java library: one jar file, one dll
- .NET: one .NET dll, one C++ dll
  - Used to create NameRxn Plugin for Accelrys Draw