

# TOPPAS: A graphical workflow editor for the analysis of high-throughput proteomics data

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## Supplemental Material

### Integration of External Tools

Listing 1 shows an example TTD file shipped with TOPPAS. The external tool itself is listed in the *path* tag. A full path is required unless the tool is in the system path. Parameters exposed in TOPPAS are listed in the *ini\_param* tag. The values of these parameters are assembled into a command line, where *cloptions* serves as template. The mapping between internal and external parameters can be found in *mappings*. Special placeholders like %TMP or %BASENAME allow

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to modify paths and filenames. A complete documentation and all pre-installed TTD files can be found in *[OpenMS]\share\OpenMS\TOOLS\EXTERNAL* for WindowsOS, or in the equivalent shared directory for Linux- and MacOS. *[OpenMS]* refers to the OpenMS installation directory, for example *c:\Program Files\OpenMS1.9\*. Custom TTD files can be added by just copying them to the *EXTERNAL* directory and restarting TOPPAS. New external tools will be available immediately.

## Listing 1: msconvert.ttd example

```
<ttd>
  <tool status="external">
    <category>Misc</category>
    <type>RAWFileConvert</type>
    <external>
      <text>
        <onstartup>Calling PWiz' 'msconvert'</onstartup>
        <onfail>Something went wrong. Is 'msconvert' in your PATH?</onfail>
        <onfinish>Tool finished successfully.</onfinish>
      </text>
      <e_category>FileConversion</e_category>
      <cloptions>-o "%1" --mzML "%2"</cloptions>
      <path>msconvert</path>
      <mappings>
        <mapping id="1" cl="%TMP" />
        <mapping id="2" cl="%%in" />
        <file_post location="%TMP/%BASENAME[%%in].mzML" target="out" />
      </mappings>
      <ini_param>
        <ITEM name="in" value="" type="string"
          description="input file in RAW format"
          restrictions="*.RAW" tags="input file" />
        <ITEM name="out" value="" type="string"
          description="output file in mzML format"
          restrictions="*.mzML" tags="output file" />
      </ini_param>
    </external>
  </tool>
</ttd>
```