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MGFp: An Open Mascot Generic Format Parser Library Implementation

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Received February 6, 2010

Abstract: Despite the efforts of the mass spectrometry (MS) community to migrate data representation toward modern file formats, legacy text formats still play an important role in MS data processing workflows. We provide a formal grammar and a portable, efficient C++ implementation for a Mascot Generic Format (MGF) parser. Software and technical documentation are available from http://software.steenlab.org/mgfp/.

Keywords: mass spectrometry • Mascot Generic Format • MGF

Despite significant efforts in the mass spectrometry community to define, implement, and motivate XML-based open data formats such as mzXML,¹ mzML,² pepXML,³ protXML,⁴ and mzIdentXML,⁵ legacy text formats are still widely used. A particular example is the Mascot Generic Format (MGF).⁶ MGF is the *de facto* standard for MS2 data storage and peptide/protein search submission in existing mass spectrometry data analysis workflows. As a consequence, the complete transition from MGF to a modern file format is likely to be a lengthy process during and after which it will be necessary to maintain backward compatibility for tools and processing pipelines.

Given the importance of MGF, it is surprising to see that: (i) MGF is not a rigorously defined format, that is, there is no formal grammar;⁶ (ii) there exist no efficient, openly available parser implementations for compiled languages (e.g., C++ or the .NET environment). Current analysis software needs to include *ad hoc* MGF parser implementations that support the MGF subset necessary for the analysis task at hand.

As illustrated in Figure 1, we have derived a formal grammar from the MGF format description and have implemented the grammar using the bison/flex parser generators.^{7,8} We have defined and implemented an efficient, intuitive

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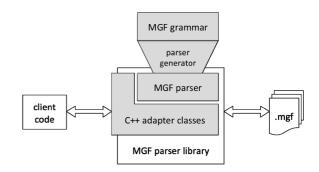


Figure 1. Schematic overview of the MGFp library components. The formal MGF grammar is translated into a bison/flex^{7,8} parser which is encapsulated in a C++ interface. The library is capable of reading and writing MGF files and provides convenient data access for client code.

C++ library interface which can easily be integrated into existing C++ projects, adapted to managed code environments (e.g., .NET) or bridged to scripting languages such as Python⁹ or R.¹⁰ The library is portable and has been tested successfully on Linux, MacOS, and MS Windows platforms. Binaries and source code are freely available under a BSD license and can be downloaded from http://software.steenlab. org/mgfp.

Acknowledgment. We thank Bernhard X. Kausler, and Thorben Kroeger for code contributions and Anna Kreshuk, Wiebke Timm, Bernhard Y. Renard, Michael Hanselmann, Xinghua Lou, and Ullrich Koethe for helpful discussions.

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PR100118F