Supplement 2:

Program	**Code Base**	**Primary Focus**	**Statistical Analysis Capabilities**	**Putative Identification**	**Comments**
MetaboLyzer	Open source Writen in Python/R	Post-processed analysis	Extensive	KEGG HMDB BioCyc Lipid Maps	Only workflow to eschew missing value imputation for alternative methods
XCMS	Open source Written in R Web server	Chromatogram deconvolution	Limited	Metlin	Its suggested workflow may bias peak picking
MetaboAnalyst	Web server	Post-processed analysis	Extensive	HMDB DrugBank T3DB SMPDB	Very thorough workflow, but output can contain too much statistical information that can seem superfluous to biologists
FIEmspro	Open Source Written in R	Post-processed analysis	Extensive	None	Very thorough workflow, however lacks putative identification capabilities
Sieve	Proprietary (Thermo Scientific)	Chromatogram deconvolution	Limited	ChemSpider	Commercial software; proprietary algorithms
MPP	Proprietary (Agilent)	Chromatogram deconvolution	Limited	Metlin	Commercial software; proprietary algorithms
MarkerLynx	Proprietary (Waters)	Chromatogram deconvolution	Limited	ChemSpider	Commercial software; proprietary algorithms
MZmine	Open Source Written in Java	Chromatogram deconvolution	Limited	PubChem KEGG METLIN HMDB	Excellent graphical user interface and cross platform compatibility

Table S-1. A table outlining the major software suites utilized in metabolomics. The majority of programs available for analyzing metabolomics data focus on the pre-processing stage. Only a handful of programs are especially designed for post-processed statistical analysis.