

Tool name	Tool type	First released	Latest known release	Preservation of data and software	Version control - maintainance	Licensing and legal	Community engagement	Testing against benchmarks	Containerization	Workflow management system	Manual, documentation, logging, reporting	Standardized inputs and outputs	FAIR principles	Reproducibility level
MSGF+	Command Line	2014	2023	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
Comet	Command Line	2013	2023	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
X! Tandem	Command Line	2003	2017	Archived tool and data	No version control – tool still works	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
OMSSA	Command Line	2004	2022	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
SearchGUI	Command line, GUI	2010	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Frequent testing done with updates	Containerized	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
MSFragger	GUI	2017	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
Skyline	GUI	2010	2022	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
OpenMS	Command Line	2008	2023	Archived data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
MSstats	GUI	2014	2023	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized	A workflow management system is used	Full manual, documentation, logging, and reporting	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
PeptideShaker	GUI	2015	2023	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
MSCConvert	Command Line	2012	2023	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Testing done on initial tool publication	Containerized	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
ThermoRawFileParser	Command Line	2019	2023	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Testing done on initial tool publication	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
DIA-Umpire	Command Line	2016	2022	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Testing done on initial tool publication	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
Skyline	GUI	2009	2023	Archived tool and data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Frequent testing done with updates	Containerized	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
OpenSWATH	Command Line	2017	2019	Archived tool and data	No version control – tool still works	Fully open-source and the code is available	Community engagement - >1 platform	Testing done on initial tool publication	Containerized	A workflow management system is used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3
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DIA-NN	Command Line	2018	2022	Archived tool and data	Complete version control	Fully open-source and the code is available	Community engagement - >1 platform	Frequent testing done with updates	Containerized	A workflow management system is used	Full manual, documentation, logging, and reporting	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	3