Operation	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
Protein Identification and Peptide Identification	MaxQuant	GUI (Graphical User Interface) and CLI	2008	2022	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	A workflow management system is used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	Mascot	Web Browser (Web-based interface), GUI	1999	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	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	2
	Proteome Discoverer	GUI	2007	Unknown	Archived data	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	Sequest	Command Line, GUI	1994	2008	Archived data	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	PEAKS Studio	GUI	2012	2021	Archived data	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	Byonic	GUI	2012	2023	Not archived	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	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
	MyriMatch	Command Line	2007	Unknown	Archived tool and data	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Containerized as part of another tool or pipeline	A workflow management system is used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	2
	Andromeda	GUI	2011	2020	Archived tool and data	Complete version control	Open-source but with limited usage or code is not 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, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	pFind	Command Line, GUI	2005	2023	Not archived	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	MASCOT Distiller	GUI	2003	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	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	2
	ProteinPilot	GUI	2007	2018	Archived data	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1

Category	Tool	Interface	Year created	Year updated	Archived	Version control	Open-source	Community	Testing	Containerization	Workflow	Documentation	Formats	FAIR	Score
	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
Quantification and Labeling	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
	Scaffold	GUI	2010	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	Progenesis QI	GUI	2012	2017	Not archived	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	TPP (Trans-Proteomic Pipeline)	Command Line	2005	2023	Not archived	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	1
	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
	Progenesis LC-MS	GUI	2012	Unknown	Not archived	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	IsoQuant	(Tool not specified)	2012	Unknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	FreeQuant	(Tool not specified)	2010	2015	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	Spectronaut	GUI	2012	2023	Archived data	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Frequent testing done with updates	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	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
	XPRESS	(Tool not specified)	2001	Unknown	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	ASAPRatio	(Tool not specified)	2003	Unknown	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	PIQMIe	GUI	2014	2015	Archived tool and data	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	RAAMS	(Tool not specified)	2003	Uknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	IsobariQ	(Tool not specified)	2011	Uknown	Not archived	No version control – tool is deprecated	Open-source but with limited usage or code is not available	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1

	Tool	Interface	Created	Updated	Archived	Version control	Open source	Community	Testing	Containerized	Workflow	Documentation	Formats	FAIR	Score
	RelEx	(Tool not specified)	2003	Unknown	Not archived	No version control – tool is deprecated	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	PQPQ	(Tool not specified)	2011	Unknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	proBAMsuite	(Tool not specified)	2016	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	No workflow management system 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	2
	proStaR	(Tool not specified)	2017	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	No workflow management system 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	2
	QuaMeter	(Tool not specified)	2012	Unknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
Post translational modification analysis	PhosphoSiteAnalyzer	Web Browser (Web-based interface)	2011	2013	Archived tool and data	No version control – tool still works	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	PhosCalc	Web Browser (Web-based interface)	2008	2008	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	PhosphoRS	Web Browser (Web-based interface)	2011	Unknown	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	Motif-X	Web Browser (Web-based interface)	2011	Unknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	PTMProphet	Web Browser (Web-based interface)	2019	Unknown	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	PTMiner	GUI	2019	2022	Not archived	Complete version control	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	PhosphoPep	(Tool not specified)	2007	Unknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	Modiro	Web Browser (Web-based interface)	2007	Unknown	Not archived	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	PhosSA	Web Browser (Web-based interface)	2012	Unknown	Not archived	No version control – tool is deprecated	Unknown	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	GPQuest	(Tool not specified)	2015	2019	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	STRING	Web Browser (Web-based interface)	2003	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	Not containerized at all	No workflow management system 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	2
	Cytoscape	GUI	2003	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	No workflow management system 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	2

Category	Tool	Interface	Year	Year	Archival	Version Control	Open-source	Community	Testing	Containerization	Workflow	Documentation	Formats	FAIR	Score
Protein-Protein Interaction Analysis	SAINT	Web Browser (Web-based interface)	2011	2018	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	Not containerized at all	No workflow management system 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	2
	Biogrid	Web Browser (Web-based interface)	2006	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	Not containerized at all	No workflow management system 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	2
	Interactome3D	Web Browser (Web-based interface)	2013	2020	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	Not containerized at all	No workflow management system 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	2
	CoExpress	Web Browser (Web-based interface)	2012	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	Not containerized at all	No workflow management system 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	2
	PSICQUIC	Web Browser (Web-based interface)	2011	Unknown	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	FunCoup	Web Browser (Web-based interface)	2009	Unknown	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	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	APID	Web Browser (Web-based interface)	2006	2019	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Unknown	Not containerized at all	No workflow management system 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	2
	IntAct	Web Browser (Web-based interface)	2004	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	Not containerized at all	No workflow management system 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	2
	Mentha	Web Browser (Web-based interface)	2013	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	Not containerized at all	No workflow management system 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	2
Protein Structure Analysis	PyMOL	GUI	2002	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	Not containerized at all	No workflow management system 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	2
	Chimera	GUI	2004	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	Not containerized at all	No workflow management system 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	2
	VMD (Visual Molecular Dynamics)	GUI	2000	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	Not containerized at all	No workflow management system 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	2
	MODELLER	Command Line	2000	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	Not containerized at all	No workflow management system 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	2
	Rosetta	Command Line	1998	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	Not containerized at all	No workflow management system 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	2
	Swiss-PdbViewer	GUI	1996	2023	Not archived	Complete version control	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system 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	2

Category	Tool	Interface	Year Created	Year Last Updated	Archiving	Version Control	Open-source	Community Engagement	Testing	Containerization	Workflow Management	Documentation	Standardized Formats	FAIR Principles	Score
	MMTSB	Command Line	2004	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	Not containerized at all	No workflow management system 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	2
	FoldX	Command Line	2005	2023	Not archived	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	Full manual, documentation, logging, and reporting	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	2
Peptide Spectrum Matching and Visualization	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 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
	ProteoIQ	GUI	2010	Unknown	Not archived	Unknown	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	Peptigram	Web Browser (Web-based interface)	2016	2023	Not archived	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system 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	2
	ProteoMapper	Web Browser (Web-based interface)	2018	2023	Not archived	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Containerized as part of another tool or pipeline	No workflow management system 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	2
Mass Spectrometry Data Processing	FragPipe	GUI	2017	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	No workflow management system 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	2
	ProteoWizard	Command Line	2008	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	No workflow management system 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	2
	MSConvert	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
	RawConverter	Command Line	2015	Unknown	Archived tool and data	Complete version control	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	msalign	Command Line	2007	Unknown	Not archived	Unknown	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	MSBlender	Command Line	2016	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	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	Thermo XCalibur	GUI	Unknown	2019	Not archived	No version control – tool still works	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	MZmine	GUI	2006	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	Not containerized at all	No workflow management system 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	2
	MassChroQ	GUI	2009	2018	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	Not containerized at all	No workflow management system 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	2
	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

Category	Tool	Interface	Year	Year	Archived	Version Control	Open-source	Community	Testing	Containerization	Workflow	Documentation	Formats	FAIR	Score
Data Visualization and Statistical Analysis	Perseus	GUI	2012	2023	Not archived	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	1
	DanteR	GUI	2008	Unknown	Not archived	No version control – tool still works	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	ProRata	GUI	2010	2013	Not archived	No version control – tool is deprecated	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Possibly follows some or all standards – not mentioned in the literature	1
	HiQuant	GUI	2018	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	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	InfernoRDN	Command Line	2017	2021	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	Not containerized at all	No workflow management system 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	2
	SuperHirn	GUI	2007	2009	Not archived	No version control – tool is deprecated	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Possibly follows some or all standards – not mentioned in the literature	1
	pRoloc	GUI	2021	2014	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	Not containerized at all	No workflow management system 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	2
	maSigPro	Command Line	2006	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	Not containerized at all	No workflow management system 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	2
	MultiQuant	GUI	2013	2022	Not archived	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	Multi-Q	GUI	2020	2022	Archived tool and data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system 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	2
	MRMPilot	GUI	2007	Unknown	Not archived	Unknown	Proprietary – requires payment or sign-up fees/ free trial	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	SQID	GUI	2012	Unknown	Not archived	Unknown	Open-source but with limited usage or code is not available	No community engagement	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Possibly follows some or all standards – not mentioned in the literature	1
	Pep2D	Web Browser	2019	Unknown	Not archived	Unknown	Open-source but with limited usage or code is not available	Community engagement - 1 platform	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	Spectrum Mill	GUI	Unknown	Unknown	Not archived	Unknown	Proprietary – requires payment or sign-up fees/ free trial	Community engagement - 1 platform	Unknown	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Unknown	Unknown or does not follow FAIR principles	1
	PatternLab	GUI	2008	2021	Not archived	Complete version control	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	2
	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

Category	Tool	Interface	Year	Last Updated	Archiving	Version Control	Licensing	Community	Testing	Containerization	Workflow	Documentation	Formats	FAIR	Score
DIA (Data-Independent Acquisition) Analysis	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
	MSPLIT-DIA	Command Line	2010	Unknown	Not archived	Unknown	Open-source but with limited usage or code is not available	No community engagement	Testing done on initial tool publication	Not containerized at all	No workflow management system used	No manual, little documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Possibly follows some or all standards – not mentioned in the literature	1
	SWATH2Stats	Command Line	2016	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	Not containerized at all	No workflow management system 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	2
	OpenMS	Command Line	2017	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
	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
	EncyclopeDIA	Web Browser (Web-based interface)	2018	2023	Not archived	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Testing done on initial tool publication	Not containerized at all	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	2
	SpectraST	Command Line	Unknown	Unknown	Not archived	Unknown	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
Web-Based Tools and Resources	PRIDE Archive	Database	Unknown	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
	MassIVE	Database	Unknown	2023	Archived data	Complete version control	Proprietary – requires payment or sign-up fees/ free trial	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system used	No manual, good documentation, reporting or logging	Formats can be converted to standardized inputs and outputs	Unknown or does not follow FAIR principles	2
	PeptideAtlas	Database	2006	2022	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
	MassBank	Database	2014	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
	ProteomeXchange	Database	Unknown	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
	GPMDB (Global Proteome Machine Database)	Database	Unknown	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
	Human Protein Atlas	Database	2005	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2

neXtProt	Database	2011	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
UniProt	Database	2010	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
PIR (Protein Information Resource)	Database	1999	2018	Archived data	No version control – tool still works	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2
ExPASy	Database	1993	2023	Archived data	Complete version control	Open-source but with limited usage or code is not available	Community engagement - >1 platform	Unknown	Not containerized at all	No workflow management system 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	2