

D. Software Categories

In Question 10 of the survey, the participants were asked what other software they used. We took these results and split them up into individual pieces of software, and removed all duplicates. From this we had a list of 209 pieces of software. We categorised these using the categories from our previous software research and identified new categories from the remaining items. Table D. 1 shows a full alphabetised list of the categories and the pieces of software within these categories.

Table D. 1: Full categorised list of software from PSDI Survey Question 10

Category	Software
CAD Software	Autodesk inventor
CAD Software	onshape.com
Chemical Database & Informatics Software	Chemistry Open Database
Chemical Database & Informatics Software	CSD (Cambridge Structural Database)
Chemical Database & Informatics Software	dragon
Chemical Database & Informatics Software	icsd
Chemical Database & Informatics Software	mordred
Chemical Database & Informatics Software	NIST
Chemical Database & Informatics Software	nomad
Chemical Database & Informatics Software	openbabel
Chemistry Bibliographic Databases	JabRef
Chemistry Bibliographic Databases	Mendeley
Chemistry Bibliographic Databases	SciFinder
Chemistry Bibliographic Databases	Zenodo
Chemistry Bibliographic Databases	Zotero
Coding software	Anaconda
Coding Software	debuggers
Coding Software	docker engine/swarm
Coding Software	expo
Coding software	Fortran
Coding Software	Git
Coding Software	jax
Coding Software	kubernetes
Coding Software	MATLAB
Coding Software	p4merge
Coding Software	pandoc Vue.js for building GUIs FastAPI/pydantic
Coding Software	pymol
Coding Software	Python
Coding Software	NumPy
Coding Software	SciPy
Coding Software	PyTorch
Coding Software	R
Coding Software	R-chis
Coding Software	RDkit

Coding Software	ruby and crystal programming languages
Coding Software	Spyder
Coding Software	Visual Studio Code
Communication Software	Gmail
Communication Software	Signal
Communication Software	Slack
Communication Software	Zoom
Crystallographic Software	apex4
Crystallographic Software	ConQuest
Crystallographic Software	Crystal17
Crystallographic Software	Crystaldiffract
Crystallographic Software	Crystalexplorer
Crystallographic Software	CrystalisPro
Crystallographic Software	CrystalMaker
Crystallographic Software	CrystalOptimizer
Crystallographic Software	CrystalPredictor
Crystallographic Software	dash
Crystallographic Software	DMACRYS
Crystallographic Software	encifer
Crystallographic Software	gsas
Crystallographic Software	IsoDistort (web based, https://stokes.byu.edu/iso/isodistort.php)
Crystallographic Software	Jana2006
Crystallographic Software	Match
Crystallographic Software	Olex2
Crystallographic Software	platon
Crystallographic Software	Gsas-II
Crystallographic Software	Powder diffraction analysis (GSAS, GSASII, FullProf)
Crystallographic Software	PowDLL
Crystallographic Software	profex
Crystallographic Software	Shelx suite
Crystallographic Software	Topas
Crystallographic Software	webcsd
Crystallographic Software	wingx
Data Visualisation & Analysis	ACD analytical software
Data Visualisation & Analysis	CellProfiler
Data Visualisation & Analysis	CYLView
Data Visualisation & Analysis	DataWarrior
Data Visualisation & Analysis	gnuplot
Data Visualisation & Analysis	Grace
Data Visualisation & Analysis	Gwyddion
Data Visualisation & Analysis	JMP
Data Visualisation & Analysis	Mantid
Data Visualisation & Analysis	MiniTab
Data Visualisation & Analysis	Origin

Data Visualisation & Analysis	POV-ray
Data Visualisation & Analysis	Spotfire Analyst
Data Visualisation & Analysis	super flip
Data Visualisation & Analysis	VESTA
Data Visualisation & Analysis	Veusz
Data Visualisation & Analysis	Virscidian LC-MS (and more) software
Data Visualisation & Analysis	WebPlot Digitizer
Data Visualisation & Analysis	xmgrace
Database Software	ArangoDB
Database Software	Apache Jena Fuseki
Database Software	MongoDB
Database Software	MySQL
Database Software	SQL
General document processing	Flare
General document processing	emacs
General document processing	Google Docs
General document processing	jEdit
General document processing	LaTeX
General document processing	Libreoffice
General document processing	Lyx
General document processing	MS Excel
General document processing	MS 365 Suite
General document processing	MS PowerPoint
General document processing	MS Word
General document processing	OneNote (and on ipad)
General document processing	Overleaf
General document processing	PDF Xchange editor
General document processing	tex/latex
General document processing	LaTeXIt
General document processing	TeXStudio
General document processing	TexShop
Image processing Software	Adobesuite
Image processing Software	AIPS (Astronomical Image Processing System)
Image processing Software	CORELDraw
Image processing Software	FIJI
Image processing Software	GIMP
Image processing Software	ImageJ
Image processing Software	Inkscape
Image processing Software	paint.NET
Image processing Software	PaintShopPro
Instrument Control	ChemStation
Instrument Control	LabVIEW
Instrument Control	Mettler-Toledo iC software suite
Instrument Control	trios

Instrument Control	Unchained Labs Automation Studio and associated viewers
Machine Learning	scikit-learn
Machine Learning	Tensorflow
Molecular Editor Software	ChemDraw
Molecular Editor Software	marvin
Molecular Editor Software	Mercury
Molecular Modelling & Simulation Software	Atomic Simulation environment
Molecular Modelling & Simulation Software	Autodock vina
Molecular Modelling & Simulation Software	BioSimSpace
Molecular Modelling & Simulation Software	Charmm-Gui
Molecular Modelling & Simulation Software	ChimeraX
Molecular Modelling & Simulation Software	DL_Poly
Molecular Modelling & Simulation Software	Geant4
Molecular Modelling & Simulation Software	gromacs
Molecular Modelling & Simulation Software	GULP
Molecular Modelling & Simulation Software	Gypsum-DL
Molecular Modelling & Simulation Software	Lammps (classical MD)
Molecular Modelling & Simulation Software	Materials Studio
Molecular Modelling & Simulation Software	MDAnalysis
Molecular Modelling & Simulation Software	molten
Molecular Modelling & Simulation Software	nwchem
Molecular Modelling & Simulation Software	OpenEye
Molecular Modelling & Simulation Software	OpenMM
Molecular Modelling & Simulation Software	Ovito (visualisation)
Molecular Modelling & Simulation Software	SnapGene
Molecular Modelling & Simulation Software	tinker
Molecular Modelling & Simulation Software	VASP
Molecular Modelling & Simulation Software	VMD
Nanostructures Modelling Software	Aztec
Nanostructures Modelling Software	Quantum Espresso
Organisational Software	DropBox
Organisational software	Google drive
Organisational software	iCloud
Organisational Software	Mural
Organisational Software	Project management
Organisational Software	slurm
Organisational Software	Trello
Other	Adobe Acrobat
Other	Agilent
Other	CASA (Common Astronomy Software Applications)
Other	EIMS online mode solver
Other	Cytoscape
Other	In-house/custom software
Other	KLayout

Other	MadGraph
Other	RNAppbees
Other	TeamViewer
Other	UnityMol
Other	Wolfram Alpha
Other	Wolfram Mathematica
Quantum Chemistry and Solid State Physics Software	AlmaBTE
Quantum Chemistry and Solid State Physics Software	Amber
Quantum Chemistry and Solid State Physics Software	BoltzTraP(2)
Quantum Chemistry and Solid State Physics Software	CASTEP
Quantum Chemistry and Solid State Physics Software	chemshell
Quantum Chemistry and Solid State Physics Software	Delphes
Quantum Chemistry and Solid State Physics Software	Density functional theory (DFT) codes
Quantum Chemistry and Solid State Physics Software	ELK
Quantum Chemistry and Solid State Physics Software	FHI-aims
Quantum Chemistry and Solid State Physics Software	gamess
Quantum Chemistry and Solid State Physics Software	Gaussian
Quantum Chemistry and Solid State Physics Software	hybrid qm/mm
Quantum Chemistry and Solid State Physics Software	Lumerical
Quantum Chemistry and Solid State Physics Software	Molpro
Quantum Chemistry and Solid State Physics Software	multiwfn
Quantum Chemistry and Solid State Physics Software	Orca
Quantum Chemistry and Solid State Physics Software	siesta
Quantum Chemistry and Solid State Physics Software	Quantum mechanics software
Quantum Chemistry and Solid State Physics Software	ShengBTE
Quantum Chemistry and Solid State Physics Software	wxmacmolpld
Quantum Chemistry and Solid State Physics Software	xtb
Simulation (non-chemical)	Cluspro
Simulation (non-chemical)	COMSOL
Simulation (non-chemical)	COPASI
Simulation (non-chemical)	Pythia
Simulation (non-chemical)	RNA fold
Spectroscopic Software	CasaXPS
Spectroscopic Software	diffract.eva
Spectroscopic Software	iNMR
Spectroscopic Software	MassHunter
Spectroscopic Software	MestreNova NMR
Spectroscopic Software	mMass
Spectroscopic Software	Regress Pro
Spectroscopic Software	spectragryph
Spectroscopic Software	topspin
Spectroscopic Software	turbo mass
Workflow software	knime