Investigating the use of software for Chemists Survey

Study Information

Study title: Investigating the use of software for Chemists Survey
Researcher name: Samantha Kanza
Study reference: iSurvey 16857
Ethics reference: Ergo 17642 – Chemistry Tools Survey

Participant Information

Please read this information carefully before deciding to take part in this research. If you are happy to participate you will be asked to check the consent form box.

What is the research about?
This research is for my PhD in Computer Science and Chemistry. I am coming to the end of the first year of my PhD and I am looking to investigate the use of chemistry tools to better understand what type of tools chemists actually use. This is a very simple survey that asks what type of chemist you are, and what types of tools you use, and if applicable which specific tools of that type you use. This PhD is part of the Web Science CDT and is funded by EPSRC.

Why have I been chosen?
You have been chosen because you work in chemistry.

What will happen to me if I take part?
This is a short survey that is being conducted to get a better idea of the usage of chemistry tools.

Are there any benefits in my taking part?
This survey will form part of a body of research aimed to improve the understanding of how chemists use technology to assist their work.

Are there any risks involved?
There are no risks involved.

Will my participation be confidential?
Your participation will be confidential. The only personal data that will be collected is what type of chemist you are. The data will be coded and stored securely on a password protected computer.

What happens if I change my mind?
If you change your mind you can withdraw at any point.

What happens if something goes wrong?
In the unlikely case of concern or complaint please contact:

Research Governance Manager (02380 595058, rgoinfo@soton.ac.uk)

Where can I get more information?

If you wish to receive more information please contact:

Samantha Kanza (sk11g08@soton.ac.uk)

Consent

By consenting to this survey you are agreeing to the following:

- I have read and understood the participant information (above) and have had the opportunity to ask questions about the study.
- I agree to take part in this research project and agree for my data to be used for the purpose of this study
- I understand my participation is voluntary and I may withdraw at any time without my legal rights being affected

Data Protection

I understand that information collected about me during my participation in this study will be stored on a password protected computer and that this information will only be used for the purpose of this study. All files containing any personal data will be made anonymous.

Section 1. Demographics

Question 1.1

Please select all the types of Chemist that you feel apply to you

- [ ] Analytical
- [ ] Environmental
- [ ] Industrial
- [ ] Inorganic
- [ ] Material
- [ ] Organic
- [ ] Physical

Question 1.2

How many years of chemistry research experience have you had?

Section 2. Molecular Modelling & Simulation

This section is about your usage of molecular modelling & simulation software

Question 2.1

Have you ever used molecular modelling & simulation software?

- Yes
- No

Section 3. Molecular Modelling & Simulation Software

This section is about your usage of molecular modelling & simulation software programs

Question 3.1

Please state how often you have used these types of molecular modelling & simulation software

Abalone			
ACEMD			
ADUN			
AMBER			
Ascalaph Designer			
Automated Topology Builder			
Avogadro			
BALLVIEW			
Biskit			
Blaze			
BOSS			
CHARMM			
CHEMKIN			
Cosmos			
CP2K			
Culgi			
Deneb			
Desmond			
Discovery Studio			
DOCK			
Extensible Computational Chemistry			
Environment			
FastROCS			
Firefly			
FoldX			
Gabedit			
Ghemical			
GOMC			
GPIUTMD			

GROMACS	○	○	○
GROMOS	○	○	○
HALMD	○	○	○
HOOMD	○	○	○
ICM Suite	○	○	○
LAMMPS	○	○	○
Lead Finder	○	○	○
MacroModel	○	○	○
Maestro	○	○	○
MAPS	○	○	○
Materials Studio	○	○	○
MedeA Gibbs	○	○	○
MCCCS Towhee	○	○	○
MDynaMix	○	○	○
MOE	○	○	○
MOIL	○	○	○
Molden	○	○	○
NAB	○	○	○
NAMD + VMD	○	○	○
Newton-X	○	○	○
NWChem	○	○	○
Octopus	○	○	○
ORAC	○	○	○
oxDNA	○	○	○
Packmol	○	○	○
pi-qmc	○	○	○
Prime	○	○	○
Protein Local Optimization Program	○	○	○
Q	○	○	○
Qwalk	○	○	○
SCIGRESS	○	○	○
Spartan	○	○	○
StruMM3D	○	○	○
TeraChem	○	○	○
TINKER	○	○	○
Tremolo-X	○	○	○
UCSF Chimera	○	○	○
VASP	○	○	○
VEGA ZZ	○	○	○
VLifeMDS	○	○	○
WHAT IF	○	○	○
YASARA	○	○	○

Section 4. Molecular Editor

This section is about your usage of molecular editor software

Question 4.1

Have you ever used molecular editor software?

- Yes
- No

Section 5. Molecular Editor Software

This section is about your usage of molecular editor software programs

Question 5.1

Please state how often you have used these types of molecular editor software

3D Molecules Editor			
Accelrys Draw			
ACD / ChemSketch			
Amira			
ArgusLab			
Ascalaph Designer			
Avogadro			
BALLView			
Bioeclipse			
BKChem			
Chem3D			
ChemDoodle			
ChemDraw			
chemicalize.org			
ChemJuice			
ChemTool			
ChemWindow			
ChemWriter			
Chirys Draw / Chirys Sketch			
CLC Workbench			
Deneb			
Elemental			
ICEDIT			
JChemPaint			

JME Molecule Editor	○	○	○
JMol	○	○	○
JSDraw	○	○	○
JSME	○	○	○
JSMol	○	○	○
KnowItAll	○	○	○
Marvin (MarvinSketch, MarvinSpace)	○	○	○
MedChem Designer	○	○	○
Molecular Editor Software and Image Sharer	○	○	○
MolEditor	○	○	○
Molinspiration	○	○	○
molsKetch	○	○	○
MolView	○	○	○
ODYSSEY	○	○	○
PubChem	○	○	○
Rastop	○	○	○
SketchEl	○	○	○
Smormo-Ed	○	○	○
Spartan	○	○	○
StruMM3D	○	○	○
Vimol	○	○	○
XDrawChem	○	○	○

Section 6. Quantum Chemistry

This section is about your usage of quantum chemistry software

Question 6.1

Have you ever used quantum chemistry software?

- ○ Yes
- ○ No

Section 7. Quantum Chemistry Software

This section is about your usage of quantum chemistry software programs

Question 7.1

Please state how often you have used these types of quantum chemistry software

ACES	○	○	○
ADF	○	○	○

AIMAll	○	○	○
AMPAC	○	○	○
Atomistix ToolKit (ATK)	○	○	○
BigDFT	○	○	○
CADPAC	○	○	○
Car-Parrinello (CPMD)	○	○	○
CASINO	○	○	○
CASTEP	○	○	○
CFOUR	○	○	○
COLUMBUS	○	○	○
CP2K	○	○	○
CRUNCH	○	○	○
Crystal	○	○	○
DACAPO	○	○	○
DALTON	○	○	○
DeMon2k	○	○	○
DFTB	○	○	○
DFT++	○	○	○
DIRAC	○	○	○
DMol3	○	○	○
ELK	○	○	○
Empire	○	○	○
ErgoSCF	○	○	○
ERKALE	○	○	○
EXCITING	○	○	○
FHI-aims	○	○	○
Firefly	○	○	○
FreeON	○	○	○
GAMESS(UK)	○	○	○
GAMESS(US)	○	○	○
Gaussian	○	○	○
Ghemical	○	○	○
GPAW	○	○	○
HiLAPW	○	○	○
HORTON	○	○	○
ICM Suite	○	○	○
Jaguar	○	○	○
JDFTx	○	○	○
LOWDIN	○	○	○
MADNESS	○	○	○
MOLCAS	○	○	○
MOLPRO	○	○	○

MOPAC	○	○	○
MPQC	○	○	○
NWChem	○	○	○
Octopus	○	○	○
ONETEP	○	○	○
OpenAtom	○	○	○
OpenMX	○	○	○
ORCA	○	○	○
PARSEC	○	○	○
PSI	○	○	○
PyQuante	○	○	○
PySCF	○	○	○
Q-Chem	○	○	○
QSite	○	○	○
Quantemol-N	○	○	○
Quantum ESPRESSO	○	○	○
RMG	○	○	○
SCIGRESS	○	○	○
Spartan	○	○	○
Siam Quantum	○	○	○
SIESTA	○	○	○
TB-LMTO	○	○	○
TeraChem	○	○	○
TURBOMOLE	○	○	○
VASP	○	○	○
VB2000	○	○	○
WIEN2k	○	○	○
XMVB	○	○	○
Yambo Code	○	○	○

Section 8. Organic Synthesis

This section is about your usage of organic synthesis software

Question 8.1

Have you ever used organic synthesis software?

- ○ Yes
- ○ No

Section 9. Organic Synthesis Software

This section is about your usage of organic synthesis software programs

Question 9.1

Please state how often you have used these types of organic synthesis software

CHIRON	○	○	○
ICSynth	○	○	○
SYLVIA	○	○	○
WODCA	○	○	○

Section 10. Nanostructure Modelling

This section is about your usage of nanostructure modelling software

Question 10.1

Have you ever used nanostructure modelling software?

- ○ Yes
- ○ No

Section 11. Nanostructure Modelling Software

This section is about your usage of nanostructure modelling software programs

Question 11.1

Please state how often you have used these types of nanostructure modelling software

Ascalaph Designer	○	○	○
Atomistix ToolKit (ATK)	○	○	○
Atomistix Virtual NanoLab	○	○	○
CST STUDIO SUITE	○	○	○
CoNTub	○	○	○
Deneb	○	○	○
Nanohub	○	○	○
Ninithi	○	○	○
Nanotube Modeller	○	○	○
Materials Design MedeA	○	○	○
Materials Studio	○	○	○
Quantum DotLab	○	○	○
SCIGRESS	○	○	○
Tubegen	○	○	○
Wrapping	○	○	○

Section 12. Chemical Kinetics & Process Simulator

This section is about your usage of chemical kinetics & process simulator software

Question 12.1

Have you ever used chemical kinetics & process simulator software?

- Yes
- No

Section 13. Chemical Kinetics & Process Simulator Software

This section is about your usage of chemical kinetics & process simulator software programs

Question 13.1

Please state how often you have used these types of chemical kinetics & process simulator software

Cantera			
ChemCollective			
Chemical Workbench			
COSILAB			
DWSIM			
Khimera			
ReactLab KINETICS			

Section 14. Chemical Database & Informatics

This section is about your usage of chemical database & informatics software

Question 14.1

Have you ever used chemical database & infomatics software?

- Yes
- No

Section 15. Chemical Database & Informatics Software

This section is about your usage of chemical database & informatics software programs

Question 15.1

Please state how often you have used these types of chemical database & informatics software

ASU Physical, Chemical and Other Property Data	○	○	○
ChemBioFinder	○	○	○
ChemExper	○	○	○
ChemFinder	○	○	○
ChemIDPlus	○	○	○
Chemical Development Kit	○	○	○
Chem Spider	○	○	○
Chemical Workbench	○	○	○
Chemical Theasaurus	○	○	○
IUPAC-NIST Solubility Database	○	○	○
OpenBabel	○	○	○
Organic Reactions	○	○	○
Organic Syntheses	○	○	○
PubChem	○	○	○
NIST Chemistry WebBook	○	○	○
NIST Chemical Kinetics Database	○	○	○
NIST Physical Reference Data	○	○	○
Reaxys Database	○	○	○
RDKit	○	○	○
Sigma-Aldrich Reaction Database	○	○	○
ZINC	○	○	○

Section 16. Chemistry Bibliographic Database

This section is about your usage of chemical bibliographic database software

Question 16.1

Have you ever used chemistry bibliographic database software?

- ○ Yes
- ○ No

Section 17. Chemistry Bibliographic Database Software

This section is about your usage of chemical bibliographic database software programs

Question 17.1

Please state how often you have used these types of chemistry bibliographic database software

Analytical Abstracts Database	○	○	○
OJOSE: Online JOurnal Search Engine	○	○	○
Synthesis Reviews	○	○	○

Section 18. Computer Based Chemical Terminology (Semantic Web)

This section is about your usage of computer based chemical terminology (semantic web) software

Question 18.1

Have you ever used any computer based chemical terminology (semantic web) software?

- Yes
- No

Section 19. Computer Based Chemical Terminology (Semantic Web) Software

This section is about your usage of computer based chemical terminology (semantic web) software programs

Question 19.1

Please state how often you have used these types of computer based chemical terminology (semantic web) software

Avogadro	○	○	○	○
ChEBI - The Database & Ontology of Chemical Entities of Biological Interest	○	○	○	○
Chemical Tagger	○	○	○	○
CHEMINF - Chemical Information Ontology	○	○	○	○
CMO - Chemical Methods Ontology	○	○	○	○
MOP - Molecular Processes Ontology	○	○	○	○
NanoParticle Ontology	○	○	○	○
RXNO - Name Reaction Ontology	○	○	○	○

Section 20. Other

This section is about your usage of other chemistry software

Question 20.1

Have you ever used any other types of chemistry software?

- Yes
- No

Section 21. Other Software

This section is about your usage of other chemistry software programs

Question 21.1

Please state how often you have used these other types of chemistry software

A More Accurate Fourier Transform	○	○	○
APBS	○	○	○
Aqion	○	○	○
CIF2Cell	○	○	○
DISCUS	○	○	○
GaussSum	○	○	○
GenX	○	○	○
Insensitive	○	○	○
OpenChrom	○	○	○
PyMca	○	○	○
RubyChem	○	○	○
spgLib	○	○	○
ToxTree	○	○	○

Section 22. Future Tools

Question 22.1

What tool would you most like to be created?

Thank you for taking this questionnaire.