



Report of "Workshop Series on Software in Chemical Science" (WSSCS-2020)

Department of Chemistry, Uka Tarsadia University organized GUJCOST sponsored "Workshop Series on Software in Chemical Science" (WSSCS-2020) on 18-20th Dec 2020. This workshop was organized online using licensed version of ZOOM with live broadcast on Facebook. Total of more than 350 registrations were received from around the world while Six invited speakers from India and USA provided hands on training on various software, used in chemical science, during this three-day online workshop.





As this was an online workshop all the moderators, speakers were at their respective places and joined the meeting through online platform. The workshop was divided into total six session where in each session the invited speaker provided valuable

information and demo to the participants on a particular software for 1 and half hour. The live broadcast of the workshop was started at 11 am IST on 18th of Dec-2020. At the start of the conference the moderator Dr. Sachinkumar Modha, Asst. Prof at Department of Chemistry welcomed all the guest and participants and requested Dr. Paresh N. Patel,

Assistant Professor and I/c director of Department of Chemistry, Uka Tarsadia University to give a short introduction of the department and university to all. Dr. Paresh N. Patel presented a brief profile of department and university to all.



1st Session

The video of this session, along with the starting remarks, is available on the following

https://www.facebook.com/dchemistrv.utu/videos/2772632816318296

The moderator introduced the invited speaker Prof. T. Saravanan from University of Hyderabad, India and invited him to present his talk titled "Role of SciFinder in Chemical Science". Saravanan presented a brief introduction of SciFinder and later he focused on the different features available in SciFinder search engine, e.g., search through keywords, structure search, reaction search, sorting of results, saving the results, etc. He



also pointed out the latest features of new version of SciFinder. After completion of the talk the moderator opened the session for question answers. Couple of questions were asked by penal members and some selected questions from participant; who posted their questions on

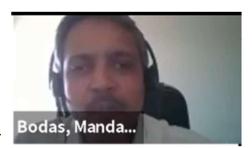
Facebook comment box; were asked by moderator. Moderator then thanked the speaker and concluded the session.

2nd Session

The video of this session is available online on the following link. https://www.facebook.com/dchemistry.utu/videos/238620000992869

The live broadcast of this 2nd session was started at 3 pm IST on 18th of Dec-2020. The moderator Dr. Sachinkumar Modha introduced the invited speaker Dr. Mandar Bodas, Elsevier, Bangalore, India and requested him to present his talk. Mandar presented his talk titled "Reaxys: An Innovative Data Analytics Tool for Chemistry and Pharmacy Researchers". He briefly introduced various products developed by Elsevier and then moved on to Reaxys search engine. Mandar provided an in-depth and thorough introduction of various features of Reaxys, how to use them properly, keywords search,

structure search, reaction search, documents search, author search, etc. Sorting options, suppliers' details, chemical details, retrosynthesis, etc were also highlighted thoroughly. The presentation was followed by question answer session. The moderator thanked the speakers of this session and concluded the 2nd session.



3rd Session

The video of this session is available online on the following link. https://www.facebook.com/dchemistry.utu/videos/460451615351402

The live broadcast of this 3rd session was started at 11 am IST on 19th of Dec-2020. The moderator Dr. Sachinkumar Modha introduced the invited speaker Dr. Md Kausar Raza from California Institute of Technology, USA. Md Kausar presented his talk titled "Topspin software for NMR spectral analysis". He provided a brief introduction of NMR theory and principle followed by step wise use of topspin software. He highlighted the



features of the software and how to open the fid file, process, integration, peak-picking, font change, overlap spectra, etc. Md. Kaushar then explained all the above with few examples of proton and carbon NMR spectra. After completion of the talk and question answers the session was concluded.

4th Session

The video of this session is available online on the following link. https://www.facebook.com/dchemistry.utu/videos/210069543925872

The live broadcast of this 4th session was started at 3 pm IST on 19th of Dec-2020. The moderator Dr. Sachinkumar Modha introduced the invited speaker Dr. Paresh N. Patel from the Uka Tarsadia University, Surat, Gujarat, India. Paresh presented his talk titled "Mestrenove software for NMR spectral analysis". He provided a brief introduction

of NMR instrument and theory behind it. He then went through various features available in the Mestrenova software for NMR spectral analysis for which few spectra were used for demonstration. The talk was followed by question answers and the session was concluded after that.



5th Session

The video of this session is available online on the following link. https://www.facebook.com/dchemistry.utu/videos/144749230762919

The live broadcast of this 5th session was started at 11 am IST on 20th of Dec-2020. The moderator Dr. Paresh N. Patel introduced the invited speaker Dr. Sutapa Mondal Roy from the Uka Tarsadia University, Surat, Gujarat, India. Sutapa presented her talk titled "Use of OriginPro® for Different Chemical Analysis" with brief introduction of OriginPro

software in the beginning followed by in-depth presentation of various features that are available in the software. Various published results were used to demonstrate practical



applications of OriginPro software for design and plotting of various type of graphs and charts. At the end of the talk moderator asked questions to the speaker on behalf of the participants. This session was concluded after that.

6th Session

The video of this session is available online on the following link. https://www.facebook.com/dchemistry.utu/videos/3568746689871767

The live broadcast of this 6th session was started at 3 pm IST on 20th of Dec-2020. The moderator Dr. Paresh N. Patel introduced the invited speaker Dr. Gopala Ram Bhadu from the CSIR-CSMCRI Bhavnagar, Gujarat, India. Gopala presented his talk titled "Introduction to Microscopy & data analysis using GATAN Software". He first introduced the participants to types of Microscope instruments and different ways in which one can

measure a sample using these instruments. He then presented the use of GATAN microscopy suit to analyze and represent the data obtained from electron microscope with examples of raw data and analyzed data. After completion of the talk moderator asked few questions on behalf of the participants.



After conclusion of the talk the moderator requested Dr. Bhavin Patel, Assistant professor, Department of Chemistry, Uka Tarsadia University to give vote of thanks.

Bhavin thanked all the resource persons, authorities of Uka Tarsadia University, organizing committee members and all who contributed directly or indirectly to make this workshop a success. Moderator then concluded the session and the workshop after thanking all



the participants for their positive responses and support.

Organizing committee:

Dr. Sachikumar G. Modha, Organizing Secretary

Dr. Paresh N. Patel, Coordinator

Dr. Sutapa Mondal Roy, Coordinator

