

IUCr-UNESCO Bruker OpenLab Uruguay 2
“Resolución de estructuras cristalinas por difracción de rayos X de monocristal”
Montevideo, Uruguay, 23rd – 29st February, 2016

<http://cryssmat.fq.edu.uy/OpenLab/index.html>

The second Edition of the Bruker OpenLab Uruguay was held in sunny Montevideo last February taking advantage of the Bruker D8 Venture diffractometer installed in 2014 at Facultad de Química, Universidad de la República. It was organized by Leopoldo Suescun, Mario Macías and Natalia Alvarez from Laboratorio de Cristalografía, Química del Estado Sólido y Materiales (Cryssmat-Lab), Cátedra de Física, DETEMA and DEC Facultad de Química, and was supported by the IUCr (through the IYCr2014 Legacy Fund), Bruker, Comisión Académica de Posgrado (CAP) of Universidad de la República and Teclab company (Bruker representative in Uruguay). The event brought together 44 participants (young professors, PhD, MSc and undergraduate students) from Argentina (4), Bolivia (1), Brazil (4), Chile (3), Costa Rica (2), Perú (2) and Uruguay (28) that had the chance to learn the fundamentals of crystallography and application to single crystal x-ray diffraction. All participants had the chance to experience all the process of SC-XRD, from crystal selection and mounting to CIF preparation, with practice samples and data. They were also provided with temporary licenses to Bruker APEX3 software and the Cambridge Structural Database to complete their structural analysis and learn about databases. Additionally, 17 very excited participants, brought single crystals and were able to select and mount them, collect their own data, and performed the structure determination and refinement of the structures by themselves with the assistance of Tutors, Lecturers and fellow participants. One structure solved and refined during the OpenLab has already been submitted to the CSD and included in a manuscript submitted to Tetrahedron Letters (Victoria de la Sovera, et al).



Left: Prof. Javier Ellena (Brazil) lecturing on the use of CSD-Search software. Center: A group of participants (L. Martínez, A. Peixoto, V. de la Sovera, A. Burgueño, C. Rojas, J. Franco, F. Luzardo y D. Fernández) discuss with Prof. J. Ellena during Sunday morning problem solving session. Right: Participants Brayan Solano (Costa Rica), Carlos Rojas (Uruguay) [back], Mario Pacheco, Victoria Pereyra (Uruguay), Naviana Leiva (Bolivia) [middle], María Bardanca and Daiana Ferreira (Uruguay) following explanations by Bruce Noll on the use of APEX3 software at the diffractometer room.

The OpenLab program included 18 hours of Lectures and 12 hours of Practical sessions on fundamentals of crystallography, taught in Spanish, by the local Lecturers Prof. Leopoldo Suescun, Prof. Álvaro W. Mombrú and Prof. Ricardo Faccio from Facultad de Química, and Professor Javier Ellena from Instituto de Física de Sao Carlos, Universidade de Sao Paulo, Brazil and English by Professor Hamilton B. Napolitano from Universidade Estadual de Goiás, Brazil. Additionally, it included 3 hours of Lectures and 2 of practice on crystallization and single crystal selection and mounting, taught by Prof. Iván Brito of Universidad de Antofagasta, Chile, and 14 hours of Lectures and 10 hours of Practical sessions on application of single crystal diffractometry taught by Dr. Bruce Noll from Bruker AXS, USA. 3 hours of the program were also devoted to advanced applications of SC-XRD to characterization of materials taught by Prof. Serena Tarantino from Università di Pavia, Italy and Michele Zema from U. di Pavia and IUCr, representative. B. Noll and the Tutors Mario Macías and Natalia Alvarez devoted many hours helping the participants select and mount their crystals, performing crystal evaluation and data collection setup and guiding the data processing and structure determination process of organic, metal-organic and mineral samples. The intense program included a welcome reception invited by Teclab and Juan Carrau Winehouse (maker of Cristalizado, the wine of the IYCr2014).



Left: Participant Sebastián Martínez (Uruguay) finishing his presentation on the structure he solved during the OpenLab. Right: Organizers and five of the six international lecturers during the closing of the OpenLab M. Zema (Italy, IUCr), S. Tarantino (Italy), M. Macías (Organizer), L. Suescun (Organizer), B. Noll (Bruker, USA), H. Napolitano (Lecturer, Brazil), N. Alvarez (Organizer), I. Brito (Lecturer, Chile).

Sunday morning was devoted to solving-problem where all Lecturers and Tutors sat with students to finalize their refinements and prepare their CIF files. Sunday afternoon was also a busy afternoon with more than 20 participants and tutors worked on their problems until the evening. The final day of the program was devoted to student presentations by 15 of the students that solved their own problems and an exam taken by 21 participants that will receive academic credit for the participation in the OpenLab. An anonymous evaluation form was submitted for the students to give their opinions on different aspect of the OpenLab. Except for the unanimous feeling that the course was very intense, most comments are positive and some helpful remarks were given that will help organize future schools of this kind in Latin America. A detailed report of the opinions of participants given in the evaluation form of the OpenLab can be obtained from (<http://cryssmat.fq.edu.uy/OpenLab/evaluationbyparticipants2.pdf>).



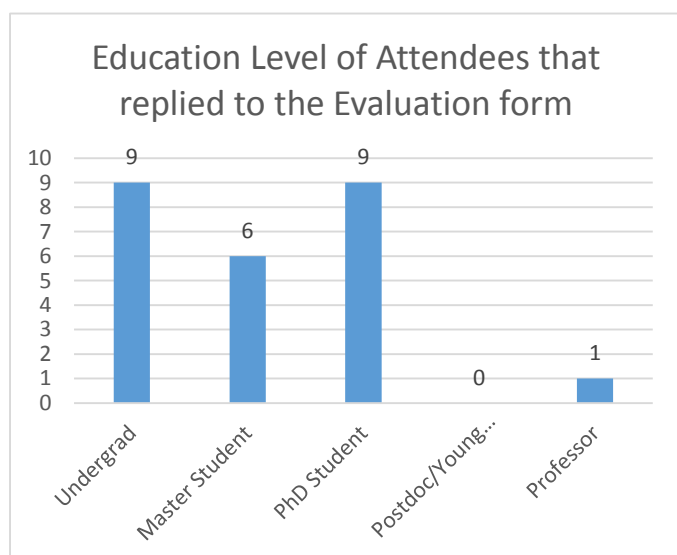
Participants of the IUCr-UNESCO Bruker OpenLab Uruguay 2.

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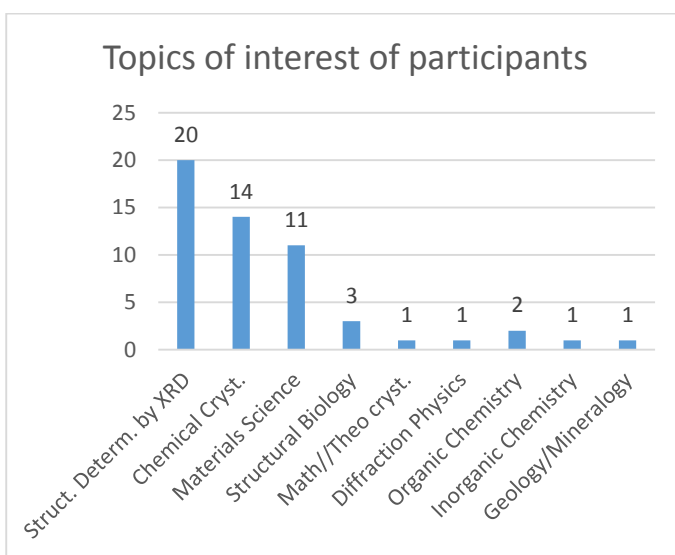
Evaluation by Participants
IUCr-UNESCO Bruker OpenLab Uruguay 2
Montevideo, Uruguay, 23rd – 29st February 2016

The 44 registered participants ([see participants list here](#)) in the IUCr-UNESCO Bruker OpenLab Uruguay 2 listed in the table below were requested to reply to a set of questions to obtain their opinions on the event and gather suggestions on what could be improved for future events. A total of 25 participants replied the questionnaire that is listed below. For clarity purposes, results are shown in a graphical format; in some cases, a transcription of the answers was made. Some of the replies were in Spanish and their translation to English is shown below the original text.

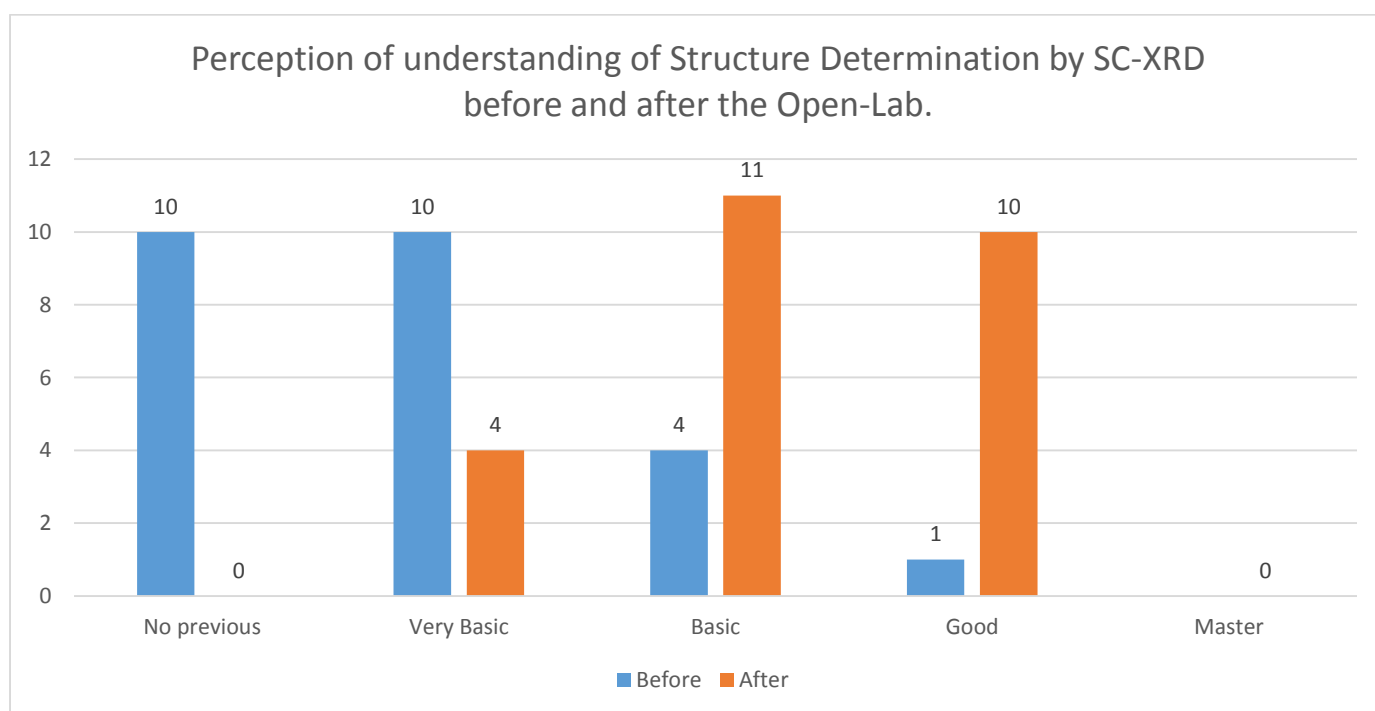
1- Please select your education level



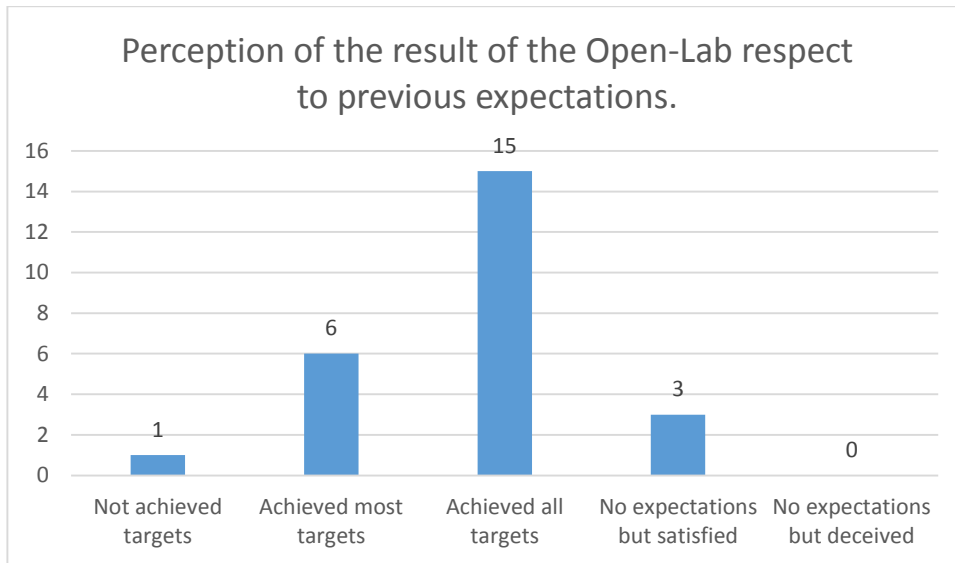
2- What are your research interests?



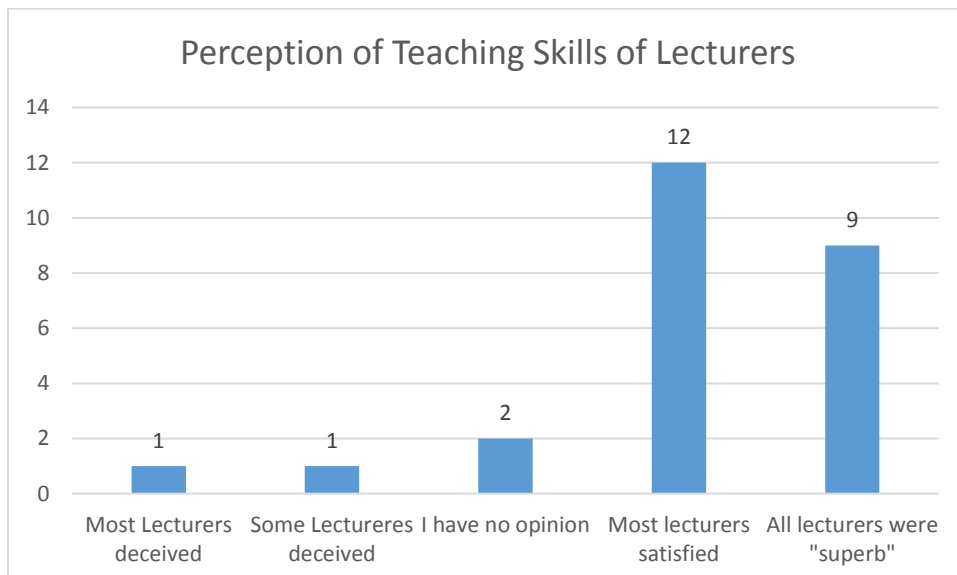
3/4- How would you estimate your level of knowledge about Single Crystal X-ray Diffraction before/after the OpenLab?



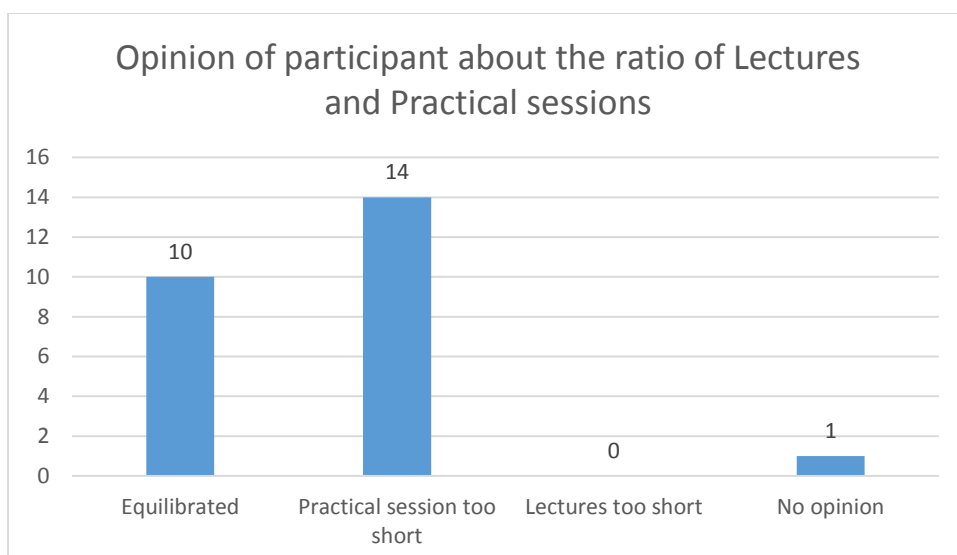
5- Have you reached the targets you expected to reach when you decided to participate in Bruker OpenLab Uruguay 2?



6- How do you find the Lecturers level at the school?



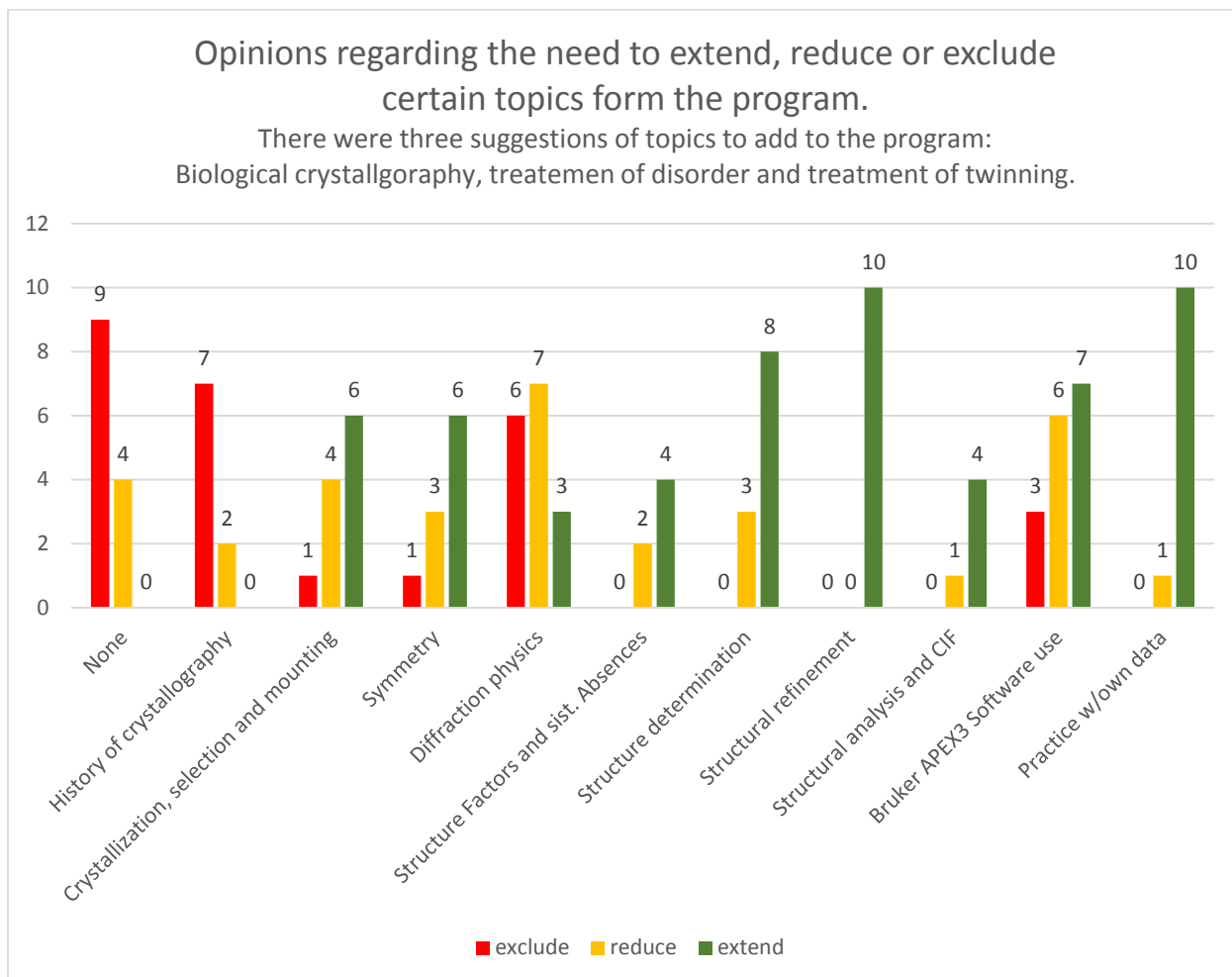
7- How do you find the distribution of lectures vs. exercises?



8- What topics (if any) you think should not have been included in the program?

9- What topics (if any) you think should be treated in more extension?

10- What topics (if any) you think were treated too extensively?



11- What is your opinion about the proportion of Lectures and Practice sessions?

"It was very well organized."

"Much more theoretical than practical aspects. "

"They were well distributed."

"Would be very helpful if each lecture or topic addressed, had an exercise to be done in class"

"Very Good."

"I think we should have more exercise classes"

"I would like to have had more practice when we were learning to use the software to solve structures."

"It was good, but perhaps lacking more exercises to better understand the technique itself"

"Symmetry: relation between lectures and exercises was good. Diffraction physics good: I think more exercises would be better.

Phase problem: relation between lectures and exercises was good. Structure refinement: relation between lectures and

exercises was good. Bruker software: relation between lectures and exercises was good"

"It was good, but I think it would have been better to have more exercises and lees physics"

"The distribution is decanted to theoretical explanations about the physics, or the commands/use behind the X-Ray diffractometer. I think, it is ok, but the OpenLab has to be more extensive (perhaps three to five additional days), to a better assimilation of the ""hard"" topics, which include some physics, the symmetry explanations, and the diffractometer use. "

"Personally, I am very satisfied with the lectures, especially those by *****, ***** and *****. ***** was superb, he has excellent teaching skills, especially when you sit with him, in the refinement of structures, or in the sample mounting. "

"Everything was very well planned. The use of computer programs and the experimental part were very well executed."

"Excellent"

“Me hubiera gustado en general que se incluyeran más ejercicios o ejemplos prácticos. En mi caso, al contar con muy pocos conocimientos previos de los temas dictados, más ejercicios concretos que ejemplificaran las temáticas/problemas tratados hubieran facilitado entender y fijar algunos conceptos. “ “I would have loved, in general, that more exercises or practical examples were included. In my case, counting with very low knowledge on the topics discussed, more exercises or examples of the topics/problems included would have facilitated to fix certain concepts”

“It was accordingly.”

“I saw that most of lectures “

“I'd rather have had more practical exercises”

“I would have preferred to practice much more the knowledge acquired in order to fix the theoretical lectures, to apply what we saw in class.”

“Very Good.”

“I would have preferred to have more exercise lessons in order to consolidate some concepts, and I found that all software lessons should have been practical (with its corresponding explanation at the time, not lectures).”

“I understand that the theory was necessary but I hoped that the hours spent in practice were more than theoretical hours.”

“This distribution is good”

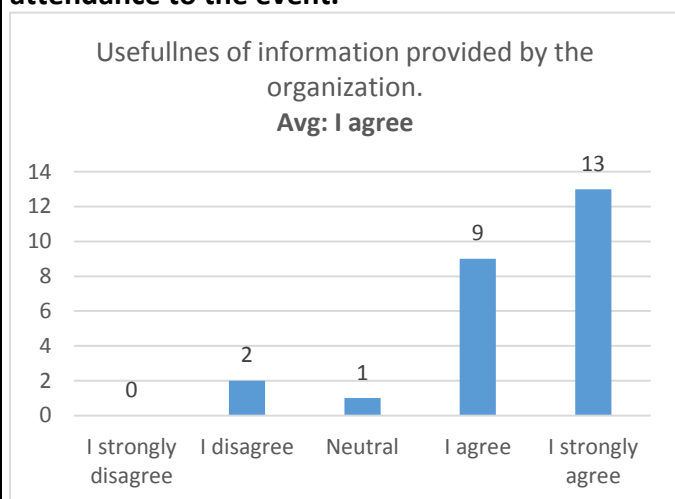
“Good in all cases”

“Very well distributed both, lectures and exercises”

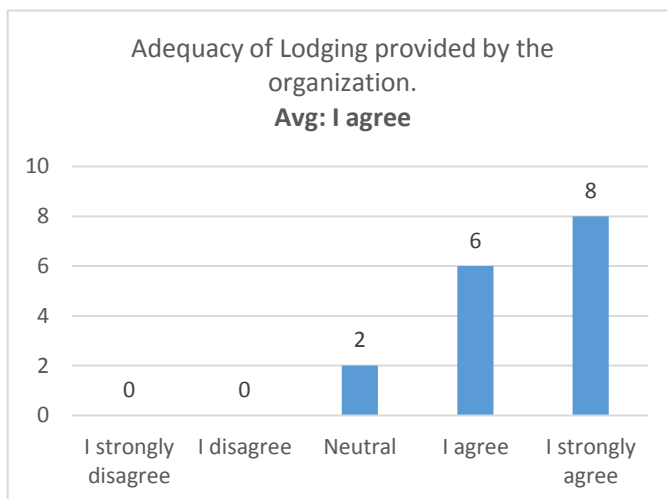
12- What topics (if any) you would have added?

Structural Biology, Disorder, Twinning

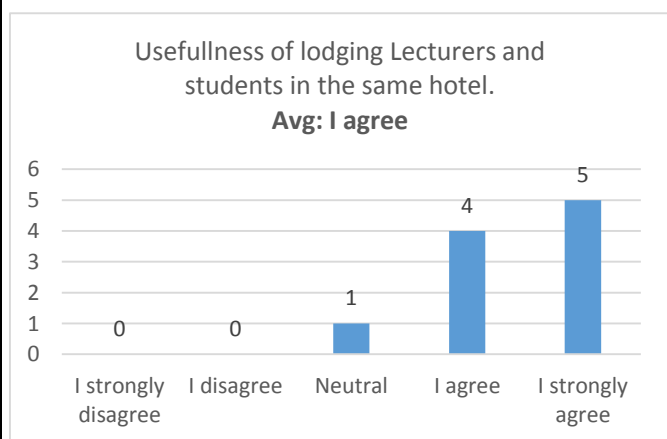
13- The information provided by the organization before the event was accurate and useful for my attendance to the event.



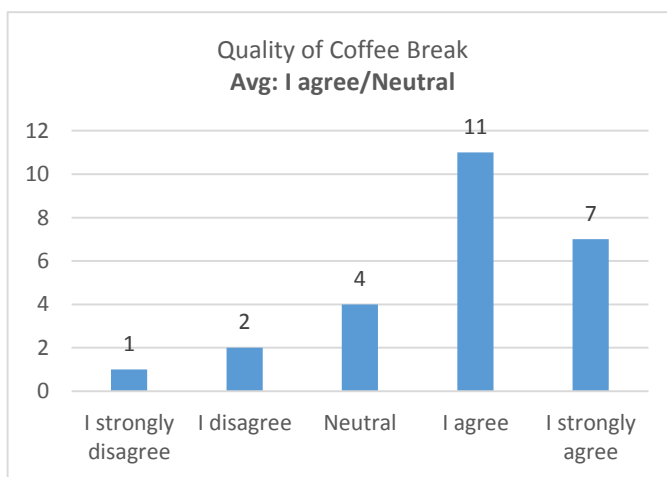
14- The lodging provided by the organization was within my expectations and needs.



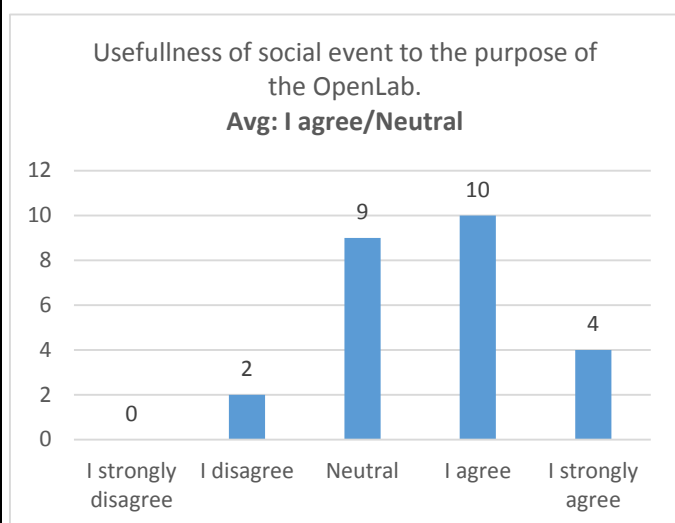
15- The lodging of participants and lecturers in the same hotel was beneficial for my participation in the event.



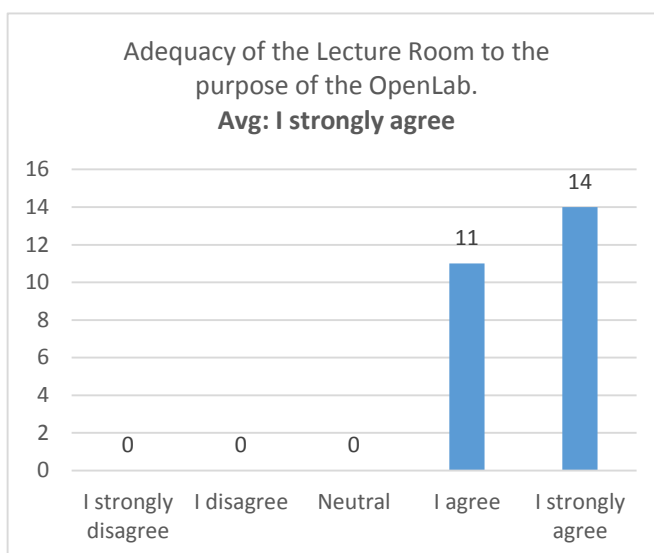
16- The coffee breaks provided by the organization were in general satisfactory



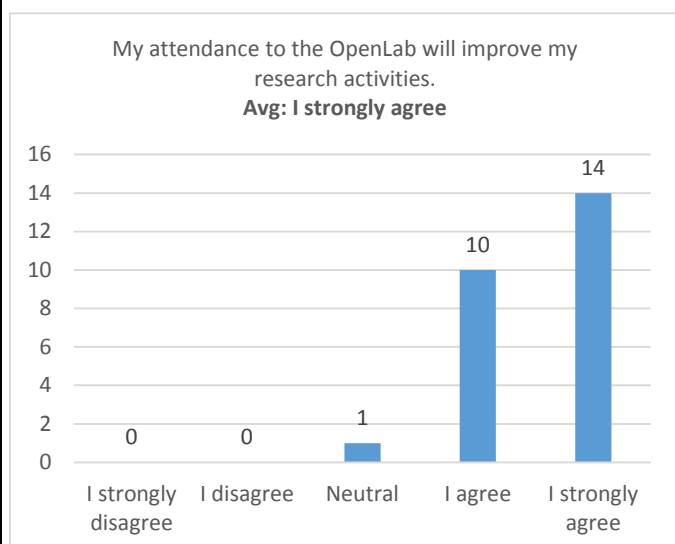
17- The social events organized during the OpenLab collaborated to the objectives of the school.



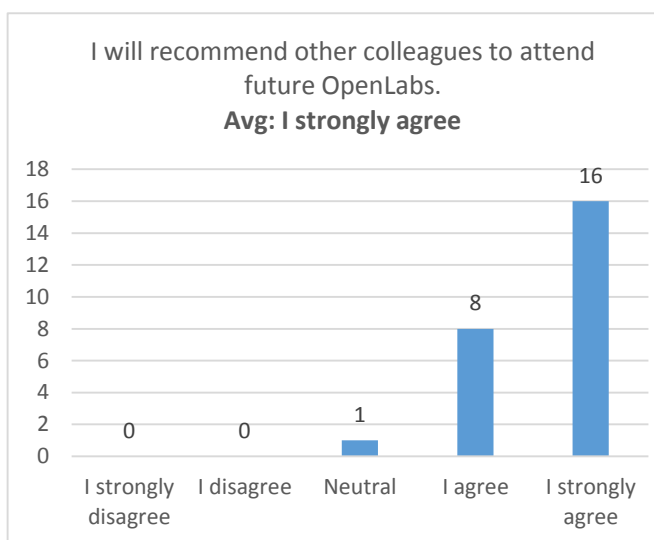
18- The lecture room and services were adequate for the event.



19- My attendance to the Bruker OpenLab Uruguay 2 will improve my research activities



20- I will recommend other students or co-workers to attend a similar OpenLabs in Latin America.



21- Please, describe how your participation in the OpenLab may improve your research activities

“Now I know more about crystallography”

“Now I'm capable to mount my own crystals, do the DRX experiment and try to solve the structure by myself. That's fair enough for one week of lectures!”

“Now I am able to sort some small crystallographic problems in my structures and understand the results.”

“The knowledge gained apply directly to my research, it will be used”

“It will make me independent in the use of x-ray single crystal diffraction instrumental and will give me an improve on the structural resolution and data analysis with a deeper theoretical baggage.”

“The X-ray diffraction is very important for my research activities, because, after obtaining a crystal, I can go to the diffractometer, and then process my data.”

“By starting to solve structures myself.”

“It lets me know how the technique works and in which cases is useful for my research”

“I am currently doing my PhD and for my work it is very important to obtain crystalline structures of certain pharmaceutical compounds. Topics covered on the OpenLab will help me to obtain better crystals, and will also facilitate me the structure resolution and refinement of those compounds”

“By giving me a basic knowledge on how to get better crystals and how the data processing it's done in order to “
“As a synthetic chemist, the structure determination, refining and crystal growing lessons will improve my activities without a doubt. Also, I can mount, measure, and refine my own data!”
“I work in structural biology. For me it is very important to know the mathematical and physical foundations of crystallography and that is why I applied to Bruker OpenLab. This course gave me excellent knowledge about the mathematical and physical foundations of crystallography. I am very grateful for that.”
“El Openlab me presentó una herramienta muy poderosa para la determinación de la estructura de moléculas con los cuales trabajo” The OpenLab showed me a very powerful tool for the determination of the structures of the molecules I work with”
“It will improve by better collecting and handling of data.”
“If I get a new glass having good properties and its application in materials science that will be a great contribution to know other techniques apart from the Powder Diffraction. “
“I will incorporate a previously unknown technique for the structural determination of my synthesis products”
“It's a tool that provides me with accurate information that no other tool can. In my case, I usually have stereocentres and this is a fantastic tool to confirm every chiral center. It's really useful for my area!”
“The understanding of this technique is very useful materials science, so it's important for my research activity.”
“It gave me some useful tips, and introduced me to a technique which I did not understand at all. Now I have a basic understanding and I hope someday I will be able to solve structures on my own “
“It improved my ability to interpret the data obtained, and my understanding of the data collection.”
“Given the area where I work and take out my thesis on crystallography plays a fundamental role, deepen the knowledge of the discipline it is essential.”
“To elucidate crystal structures and studying new compounds”
“It provided me a better understanding of the equipment to be used during my research”

22- Please, give your general impression about the event

“It was very useful and interesting”
“Very nice event, well organized.”
“All lectures were helpful, but the distribution of time was not well done, finishing too late.”
“It was an excellent event with competent and experienced professionals”
“Amazing.”
“The event was excellent, but I think we should have more exercise classes”
“Very good, but the journeys were too long”
“It was good overall; however I think that the days were too long not allowing seizing correctly. I also think that should be clarified that the current level will be given that certain knowledge is required to understand and take advantage of the conference.”
“The topics covered on the event were very helpful for working on monocrystal diffraction. The event was well organized and the lectures were very good, although some of them were basic for people who had a basic understanding on the technique, and others were too difficult for people who did not have a previous understanding”
“It was very good but it was aimed to people with previous knowledge on the subject”
“The event was superb, also a bit intense! I learned a lot, and I think I got a good practical and theoretical base to continue learning!”
“The course was very well organized. The level of teachers is very high and the classes were very good level. The atmosphere was very friendly and nice.”
“El evento fue muy bueno. Se apreciaron las ganas y la buena disposición de los organizadores y todos los participantes. Muy recomendable.” “The event was very good. The willingness and disposition of all participants was evident. I will recommend it”
“It was well organized and it help me a lot to refresh and learn new things about X-ray. “
“It was a learning new analysis techniques with highly trained and dedicated to the subject teachers, organization and staff treatment was for good rest and above all the willingness to collaborate and interact with other Latin American countries in similar research topics for need to know which other techniques outside the traditional and also the ability to access collaboration with other teachers to collaborate, sharing the same information from teachers to students.”
“Great. Good lectures Good practices”
“I enjoyed the event but my previous background in this area was not enough. I would like to have had more practice in choosing crystals, taking samples and analyzing them.”
“Very nice.”
“As I said before, I really liked it. I came with no idea about crystallography, and now I have some notions of it, which I consider really useful”
“I had an excellent impression, but I would like to have more practice hours.”
“I have a good impression in general, but I think I could more practical classes.

"I am very satisfied and would like to continue learning the subject"

"Very well organized with excellent lecturers"

23- Please, indicate what organizational aspects of the next event (if any) should be modified to improve the school

"It should have more social events"

"Maybe, more practical sessions with the programs involved in data collection and solve structure/ refinement "

"The time of finish each day, was 18:45 in the program, but in the reality we have class until around 20. Some social event. At least free water. And more information about how to get to the hotel from airport."

"Because it is an international event I believe that the English language should be adopted as the official language of the event"

"The same amount of lectures but with more days to internalize and understand the concepts in a more natural way."

"More exercise and practical classes. "

"Make the school in more days and less hours a day."

"The organization was very good. The only thing that would change is the duration of the conference."

"I think it would be easier to participate if more time were given between the announcement and the realization of the event. It should have more practice and less physics lessons"

"I think the organizational aspect was satisfying! "

"I think all aspects of the course were successfully covered. I think it would be a very good idea to invite some (a Nobel Prize for example) important scientific personality to share their experience regarding the use of crystallography high-impact research."

"Sería bueno proporcionar material de apoyo/nivelación previo al inicio del Openlab para aquellos participantes que no están formados en el área, de manera que sea más aprovechable y más fácil de seguir luego el desarrollo de la escuela." "It would be good to have some material prior to the beginning of the OpenLab for those participants that have no previous knowledge on the area, this way the school will be easier to follow"

"Please include as I mentioned previously some topics regarding disorder and twinning handling. That would be great!"

"Could be considered that not only will have two breaks, as much information at once and in itself no longer taken into account due to mental fatigue, could be considered the maximum theoretical classes until 4 pm or 5 not more."

"None"

"Any"

"The order of the lessons."

"I would say that the sessions were pretty long, perhaps it should have taken more days and less hours per day. It was really tiring, But it worth it"

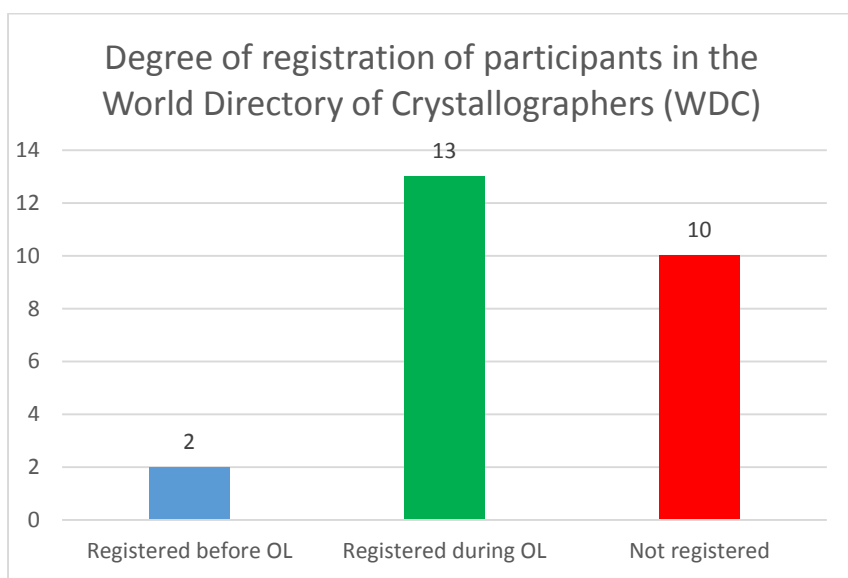
"Increase the practical hours."

"The organization in general don't need modifications"

"More Focus on the part of refinement crystallographic structures and work with tables"

"None"

24- Are you registered in the World Directory of Crystallographers WDC (<http://www.iucr.org/people/wdc/>)?



Results of Final Exam:

| Nombre | Nota Examen |
|--------------------------------------|-------------|
| Sollier, Brenda Maria del Valle | 8 |
| Gaztañaga, Pablo Ernesto | 12 |
| Movilla, Federico | 12 |
| Custodio, Jean Marcos Ferreira | 7 |
| Vaz, Wesley F. | 10 |
| Vilca Morales, Adimir Italo | 3 |
| Zambrano, Pablo Andrés | 4 |
| Solano, Brayán | 11 |
| Medina Sandoval, Rosa Julia | 3 |
| Rojas, Carlos | 10 |
| Martínez, Sebastián | 12 |
| Mendoza, Carolina | 5 |
| Imer Rocha Pita, Marcos Ramon | 12 |
| Pignanelli Abreu, Fernando Francisco | 8 |
| Posada, Laura | 3 |
| Franco, Jaime | 5 |
| Igoa, Fernando | 5 |
| Esteves Martin | 5 |
| Queirolo, Rodolfo | 4 |
| Peixoto de Abreu Lima, Alejandro | 3 |
| Ferreira Biancuyo, Daiana Marcia | 9 |

| Escala | Aprobados |
|--------|-----------|
| 3 | RRR |
| 4 | RRB |
| 5 | BBR |
| 6 | BBB |
| 7 | BBMB |
| 8 | MBMBB |
| 9 | MBMBMB |
| 10 | MBMBS |
| 11 | SSMB |
| 12 | SSS |