

SIG No: 9
Reported Period: 2012-2013
Report Date: 06/08/2018
Reported by: Harry Powell

1. Introduction. (50 words max.)

We are organising a Workshop for younger developers immediately before ECM31 in Oviedo; the popular Software Fayre will be held at ECM31.

2. SIG web site:

SIG 9 url: <http://sig9.ecanews.org/>

3. Number of ECA individual members registered with the SIG according to

(<http://www.xray.cz/eca/im-paymenthtm>)

SIG 9 ecacomsg 287

4. Existence of a SIG mailing list Yes / No No (an informal list is kept by HRP; a list is held on IUCr web server but is defunct)

Address of the mailing list:

Number of members in the SIG mailing list : 96

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate) ~300 (based on the mailing list and knowledge that most researchers in this field are not on the list).

6. List of MS organized by the SIG at the last ECM (as for 2014 report)

[MS 50: Measuring data quality](#)

[MS 52: Computational tools for theoretical chemistry and structure prediction \(joint with 2, 7, 8\)](#)

+ Software Fayre

7. Prizes sponsored/coordinated

8. Past Activities other than Microsymposia at ECM

none this year

For Each Activity

Title:

Number of Participants:

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

endorsed (SIG logo on the web page/leaflets)

Sponsored by ECA?

Yes/ No

Other Sponsors/Organizers:

Short Description: (50 words max.)

9. Future/Programmed Activities.

For Each Activity

Title: Software Fayre at ECM31.

Number of Participants: unknown.

Level of involvement of SIG in the activity:

ECA Individual members registered with the SIG involved in the organizing committee 1

ECA Individual members registered with the SIG involved as lecturers unknown

endorsed (SIG logo on the web page/leaflets) no

Sponsored by ECA?

Yes/ No no

Other Sponsors/Organizers:

no

Short Description: (25 words max.)

Interactive lectures based on use of different software packages.

Title: European Crystallographic Computing Forum (prior to ECM31)

Number of Participants: We have room for ~50 participants (including tutors)

Level of involvement of SIG in the activity:

ECA Individual members registered with the SIG involved in the organizing committee 2

ECA Individual members registered with the SIG involved as lecturers not known

endorsed (SIG logo on the web page/leaflets) yes

Sponsored by ECA?

Yes/ No No

Other Sponsors/Organizers: I will be approaching our usual sponsors, e.g. CCP4, Dectris, Rigaku, Bruker

Short Description: (25 words max.)

An opportunity for younger crystallographic developers (across powder, small molecule and protein crystallography) to meet and discuss their individual software developments and techniques. We will hold it at Universidad de Oviedo, Mieres Campus, a short distance from Oviedo.

10. Other matters. (50 words max.)

Harry Powell will be retiring as SIG9 Chair at ECM31.

It is disappointing that SIG9 has so few MS at ECMs because our MS are usually well attended. While appreciating that each IG wants representative MS, attendance at ECMs is largely dependent on the MS that take place.

11. Brief annual activity report (100 words max.)

None. Martin Lutz held the Software Fayre in Hyderabad at the IUCr, and the IUCr Computing Commission held a computing School in Bangalore before the IUCr in Hyderabad.

12. List SIG officers, name and e-mail, and specify their main function in the SIG:

Chairman - Harry Powell, hrp1000@virginmedia.com

Deputy Chairman - Martin Lutz, m.lutz@uu.nl

Secretary - Andrea Thorn, andrea.thorn@WEB.DE

Committee: Laura Rocas, laura.uniovi@gmail.com

Garib Murshudov, garib@mrc-lmb.cam.ac.uk

Rocco Caliandro rocco.caliandro@ic.cnr.it

Supplementary Materials.

(List of all supplementary materials, if any, related to the SIG report)

- Addendum 1 to n (to be sent in separate files)