

**SIG No:** 9  
**Reported Period:** 2012-2013  
**Report Date:** 06/07/2017  
**Reported by:** Harry Powell

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**1. Introduction.** (50 words max.)

We are organising a Workshop for younger developers immediately before ECM31 in Oviedo.

**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                      279

**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 does not seem to elicit any replies)

**Address of the mailing list:**

**Number of members in the SIG mailing list :**                      166

**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: Advanced Software Development for Crystallographers Workshop (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, Agilent, 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 plan to hold it in Mieres, a short distance from Oviedo.

**10. Other matters.** ( 50 words max.)

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

Very little, since this year is a non-ECM year. Martin Lutz will be holding the Software Fayre in Hyderabad at the IUCr, and the IUCr Computing Commission will be holding 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, [harry@mrc-lmb.cam.ac.uk](mailto:harry@mrc-lmb.cam.ac.uk) or [hrp1000@cam.ac.uk](mailto:hrp1000@cam.ac.uk)

**Deputy Chairman** - Martin Lutz, [m.lutz@uu.nl](mailto:m.lutz@uu.nl)

**Secretary** - Andrea Thorn, [andrea.thorn@WEB.DE](mailto:andrea.thorn@WEB.DE)

Committee: Laura Rocas, [laura.uniovi@gmail.com](mailto:laura.uniovi@gmail.com)

Garib Murshudov, [garib@mrc-lmb.cam.ac.uk](mailto:garib@mrc-lmb.cam.ac.uk)

Rocco Caliandro [rocco.caliandro@ic.cnr.it](mailto: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)