

**SIG No:** 9  
**Reported Period:** 2015-2016  
**Report Date:** 17/08/2016  
**Reported by:** Harry Powell

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

We are organising a Workshop for potential developers immediately before ECM30.

**2. SIG web site:**

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

**3. Number of ECA individual members registered with the SIG according to**  
**(<http://ecanews.org/mwp/groups/>)**

SIG 9            ecacomsg            164

**4. Existence of a SIG mailing list**  Yes /  No  
kept by HRP)

Yes (an additional informal list is

Address of the mailing list:

managed on <http://ecanews.org>

Number of members in the SIG mailing list :

164 (+98 on informal list)

**5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)** ~260 (based on the two mailing lists).

**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 (organised by Deputy Chairman, Martin Lutz).

**7. Prizes sponsored/coordinated**

Poster prize sponsored by OlexSys - first awarded at ECM28

**8. Past Activities other than Microsymposia at ECM**

Title: **Advanced Software Development for Crystallographers Workshop (prior to ECM29)**

Number of Participants: 33 registered (21/07/2015)

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 ~5

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

Sponsored by ECA?

Yes/  No

No

Other Sponsors/Organizers: 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.

Title: **Software Fayre at ECM29.**

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 presentations on many different software packages.

### 9. Future/Programmed Activities.

For Each Activity

Title: **Software Fayre at ECM30.**

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 presentations on eleven (11) different software packages.

Title: **Methods in Crystallographic Computing** (prior to ECM30)

Number of Participants: 24 registered (17/08/2016)

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 ~5

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

Sponsored by ECA?

Yes/  No No

Other Sponsors/Organizers: CCP4, Dectris, Bruker

Short Description: (25 words max.)

An opportunity for potential crystallographic developers (across powder, small molecule and protein crystallography) to meet and discuss their individual software developments and techniques.

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

Although there are apparently over 260 people who have registered an interest in SIG9, requests for feedback from them has largely fallen on deaf ears; only one reply in the last year. The Committee is defunct, none of the members replied to anything.

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

Organised computing workshop prior to ECM30 in Freudenstadt, Germany; decided to organise registration separately from ECM30 to save on fees from conference organisers in order to

encourage registration, but we organised things very late so this may have resulted in reduced numbers.

**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)

**Supplementary Materials.**

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

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