SIG7

Reported Period: 2009 Report Date: 12 July 2010 Reported by: Susan Bourne

1. Introduction. (50 words max.)

Established in 1999, SIG7 (Molecular Interaction & Recognition) covers the complete spectrum of theoretical, general and applicative fields of MIR. Activity includes organising sessions at ECMs and specialist meetings. Because of its interdisciplinary nature, SIG7 has established collaboration with SIG#1 (Macromolecular Crystallography), SIG#2 (Charge, Spin and Momentum Densities) and SIG#13 (Molecular Structure and Chemical Properties) to organise ECM microsymposia.

2. SIG web site:

SIG7 NO (under discussion)

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

SIG7 Molecular Interaction and Recognition

4. Existence of a SIG mailing list: No

Address of the mailing list:

Number of members in the SIG mailing list:

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)

6. List of MS organized by the SIG at the last ECM

At the *ECM25* (Istanbul, 16-21 August 2009) MIRSIG promoted:

two Plenary Lectures:

- PL1. Piero Ugliengo: "Modelling of biomaterials: molecular recognition at the surfaces of bioactive glasses"
- PL2. Christer B. Aakeroy: "Engineering co-crystals using molecular sense and supramolecular sensibility"

and five Microsymposia:

- FA1-MS7 Molecular recognition and drug design (with SIG 1) (Chair: Wolfram Saenger Co-chair: Richard Pauptit)
- FA4-MS2 Design and properties of functional molecular materials (Chair: Jürg Hulliger Co-chair: Giuseppe Resnati)
- FA4-MS3 Multicomponent crystals
 - (Chair: Kinga Suwinska Co-chair: Andrew D. Bond)
- FA4-MS4 Supramolecular architectures: from structure to function (Chair: Leonard J. Barbour Co-chair: Matyas Czugler)
- FA4-MS11 Crystal energy landscapes: computation and uses

(Chair: Sarah L. Price - Co-chair: Martin U. Schmidt)

7. Prizes sponsored/coordinated

8. Past Activities other than Microsymposia at ECM

For Each Activity

Title: Indaba6: Structure & Properties, Kruger Park, South Africa. 30 August-4 September 2009.

Number of Participants: 120 (limited to this number by size of venue)

Level of involvement of SIG in the activity:

O ECA Individual members registered with the SIG involved in the organizing committee : Catharine Esterhuysen, Melanie Rademeyer, Demi Levendis, Dave Billing, Manuel Fernandes

O ECA Individual members registered with the SIG involved as lecturers : Alessia Bacchi, Dave Billing, Susan Bourne.

O endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? No

Other Sponsors/Organizers: IUCr (Structural Chemistry commission), University of the Witwatersrand, Royal Society of Chemistry, Oxford Diffraction, Bruker (South Africa), Accelrys. Short Description: (25 words max.) Indaba6 examined progress in first-principle understanding of molecular science: structure, dynamics, activity and function. The symposium attracted molecular scientists from chemistry, biology, physics, materials science and from crystallography, spectroscopy and catalysis.

Title: ISIC12: 12th International Seminar on Inclusion Compounds, Stellenbosch, South Africa. 4-9 April 2009

Number of Participants: 100

Level of involvement of SIG in the activity:

O ECA Individual members registered with the SIG involved in the organizing committee : Luigi Nassimbeni, Susan Bourne, Catharine Esterhuysen, Tanya le Roex

O ECA Individual members registered with the SIG involved as lecturers: Paola Gilli, Demi Levendis, Kinga Suwinska, Tanya le Roex

O endorsed (SIG logo on the web page/leaflets): Yes

Sponsored by ECA? No

Other Sponsors/Organizers: University of Stellenbosch, Cape Peninsula University of Technology, Royal Society of Chemistry.

Short Description: (25 words max.) Held outside Eastern Europe for the first time, ISIC12 considered the state of the art in molecular recognition processes and inclusion compounds.

9. Future/Programmed Activities.

For Each Activity

Title: **Indaba 7, 2012**

Number of Participants: anticipated to be limited to 120

Level of involvement of SIG in the activity:

O ECA Individual Members registered with the SIG involved in the organizing committee : Len Barbour, Susan Bourne, Catharine Esterhuysen

O ECA Individual Members registered with the SIG involved as lecturers: unknown at this stage

O endorsed (SIG logo on the web page/leaflets) Yes

Sponsored by ECA? Possibly (application will be made in 2011)

Other Sponsors/Organizers: unknown at this stage

Short Description: (50 words max.) The next in this successful series of meetings considering all aspects of molecular processes in the solid state, Indaba 7 is likely to move away from the Kruger Park. Venues near Cape Town are currently under consideration. An organising committee has been established and an advisory committee is being set up.

10. Other matters. (50 words max.)

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

SIG7 has been actively involved in its prime purpose – to organise discussions, sessions and microsymposia relating to molecular interactions and recognition processes at a variety of conferences around the world. A new committee of officers were elected at ECM25 and they are working together to arrange a SIG7 mailing list and website.

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

A new MIRSIG Board was elected during ECM25 (Istanbul) in August 2009. Office bearers from 2009-2012 are

Chairman: Susan Bourne (Cape Town) <susan.bourne@uct.ac.za> Co-Chairman: Carl-Henrik Gorbitz (Oslo) <c.h.gorbitz@kjemi.uio.no>

Secretary: Paola Gilli (Ferrara) <paola.gilli@unife.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)