

# Minutes of the Programming Meeting

## COMP National ACS Meeting April 6, 2013 – New Orleans, LA

### Present

Kennie Merz, Ed Sherer, Jeffrey Madura, Terry Stouch, Emilio Esposito, Scott Wildman, Ralph Wheeler, Jane Tseng, Eric Patterson, Veer Shanmugasundaram, Hannake Jansen, Adrian Roitberg

- 1) Background on NO meeting: 431 abstracts, 141 posters, 290 talks (48 sessions)
- 2) Poster session Tuesday night: Hall A section D
- 3) Undergrad poster session – 44 COMP – Mon 12-230 PM Hall D
  - a. From Philadelphia – 2012: Peter makes a motion that COMP awards up to 10% of the undergraduate posters submitted (and tagged as COMP) to include ribbon, ARCC, COMP membership for 1 year, cash of \$100, and award will be called: "COMP Undergraduate Poster Award" where name can be amended in future with sponsors, etc.
- 4) Graduate reception 7-830 Section B/C Hall A
- 5) Scott will arrange for the undergraduate posters in COMP to get rewarded as laid out from last Exec meeting, details below

## ACTION ITEMS

- 1) Ed to post Philadelphia minutes to web page
- 2) Jeffery, Ralph, and Terry to draft a document to list specific requirements for moving ARCC to a different publishing model so that vendors can provide level quotes.
- 3) Hanneke and Ed will follow up with Chris/Sara to determine if \$4K for TDT round 2 is an acceptable level of funding
- 4) Terry and Jeffery to provide Kennie with needed information relative to ACS Fellow nominations which are due April 22
- 5) Elections subcommittee of COMP needs to meet to determine slate of candidates. Kennie to provide ballot to Ed for voting. Election to start on June 1
- 6) Petrina to work with Adrian, Jeffrey and Carlos concerning CCG award application process.
- 7) Scott- will make sure undergraduate poster awards will be given to about 4 posters

# **Minutes of the Executive Meeting**

## **COMP National ACS Meeting April 6, 2013 – New Orleans, LA**

### **Present**

Kennie Merz, Ed Sherer, Jeffry Madura, Terry Stouch, Emilio Esposito, Scott Wildman, Ralph Wheeler , Jane Tseng, Eric Patterson, Veer Shanmugasundaram, Hannake Jansen, Adrian Roitberg, Peter Jurs, Petrina Kamyra (CCG), Luke Achenie, Rigoberto Hernandez, Wendy Cornell

### **1) Secretary Report (10 mins, Ed Sherer)**

#### **Election for 2013**

The division will need to elect the following positions:

Chair-Elect 2014 = Chair 2015

Councilor 2014-2016 (currently Emilio)

Alternate Councilor 2014-2016 (currently Patrick)

#### **Vote on acceptance of meeting minutes**

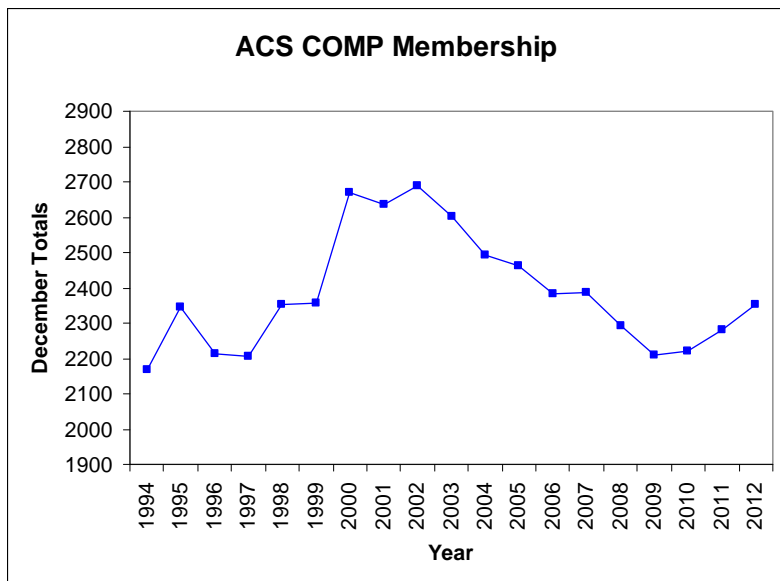
All previous minutes have been posted to the web page.

The division will need to vote to approve the minutes from the Fall ACS meeting in Philadelphia (2012).

The division voted to accept these minutes.

#### **Membership Update 2013**

All demographics reports have been posted to the web page.



Annual Report 2012- Completed and available

## 2) Treasurer Report (15 mins, Sara Nichols/Chris Harwell (in absentia))

Owing to travel changes a treasurer's report was not provided during the executive meeting.

## 3) Programming Report (20 mins, Emilio Esposito/Scott Wildman)

The programming for NO is strong; unfortunately the Indianapolis meeting does not have a strong poster submission.

At the NO meeting this Spring, there will be a session involving the use of mobile devices for chemistry applications. This was a session picked up in C&E News.

## 4) MPPG Report (10 mins, Luke Achenie)

List of COMP based applicants was supplied for selection as a theme organizer.

Themes for future meetings are points of discussion at these planning meetings.

## **5) ARCC (15 mins, Ralph Wheeler/Jeffry Madura)**

The publication of ARCC is a growing expense. Can we move to a different publication model to save money? For instance JMGM single annual issue. Move to Springer also a possibility. Cost for single issue access of JMGM via Elsevier would be about \$30K, where current cost of hard copy is \$22K plus shipping where cost was \$8/issue before shipping – total up to about \$33-36K. Access would then be only electronic and not print. Springer would do a special issue of JCAMD, which would be \$3K for open access per paper, thus dependent on 8-15 papers per issue of ARCC. The papers are indexed by SciFinder, but not other indices.

The COMP survey from 2011 indicated that 40% of members wanted both electronic/hard copy, 20% wanted hard copy, and 30% wanted electronic.

Eliminating shipping cost would be the largest savings.

Rigoberto brought up the issue of the current ARCC issues do not have good DOIs.

## **6) Awards Nomination (15 mins Terry Stouch)**

Nominations for ACS Fellows due April 22, COMP has three candidates to nominate.

All COMP members should consider nominating members for the computers in pharmaceutical chemistry award. Nominations last for 3 consecutive years.

Additional discussion was had concerning awards and whether you would need to always give money or is the award itself recognition enough.

## **7) CCG Awards (15 mins, Petrina Kamy) with Carlos Simmerling (TC)**

Discussion of the management of the awards and visibility of CCG in the process. CCG is interested in getting an idea of the number of applicants which COMP gets for this award. Would it help to make the requirements more stringent?

CCG considering dropping number of awards from 5 to 3. Largely driven by a numbers game, meaning, if we just had a few applicants are the odds very good to get an award, do we need to make it more difficult to apply?

Often times about 50-60 applications

Adrian Roitberg is willing to help out with logistics of application submission via a web link, such that an applicant would submit material and then an email gets sent to the respective award administrator.

Nvidia award will be starting this year. The award will be administered by Nvidia.

Other awards are Kollman and OpenEye awards.

## **8) TDT (15 mins, Hanneke Jansen) w/ Wendy Cornell, Jane Tseng, and Rommie Amaro**

This year Pat Walters and Emilio Esposito will be joining the team to help manage TDT.

One overall winner, one runner up and 4 honorable mentions were awarded. The SBDD project on malaria was the overall winner and the project led to a selection of compounds which we purchased in and are being screened now.

Areas to discuss:

- 1) Need for increased submissions – how can communication be expanded
  - a. Already on twitter, LinkedIn and facebook
  - b. What about blogs
- 2) What would be needed for your/are labs to contribute to the submission of proposals
- 3) Should we restrict the social TDT events to COMP membership – deemed to be difficult
  - a. Signing up members to be COMP as well is difficult on site
  - b. Possibility to get a OCR reader/scanner from ACS to monitor attendees
- 4) Will COMP co-sponsor an event for round 2? Jeffrey motions that we support TDT for round 2 in the amount of \$4000 after confirmation from the COMP treasurer that COMP is in the position to fund to this extent. Motion seconded. Vote – unanimous vote

## **9) Counselors (15 mins, Peter Jurs, Emilio Esposito)**

Technical program for ACS costs \$70K to print. Try and download PDF if you can.

Councilors for NO – Emilio, Peter, Veer (for Mel), Ralph

Peter is on the council policy committee which runs the council meeting – organizational structure of ACS

Ralph – committee on science, he is also on policy subcommittee

## **10) Update on last year initiatives (10 mins, Jeffry Madura)**

## **11) Closing Comments (5 mins, Kennie Merz)**