COMP Executive Committee Meeting August 16, 2008 Philadelphia, PA

Program Meeting

Present: Curt Breneman, Wendy Cornell, Jeffry Madura, Ralph Wheeler, Hanneke Jansen, Emilio Esposito, Ed Sherer, Adrian Roitberg, Irache Visiers, Chris Harwell, Orlando Acevedo, Terry Stouch, Allen Richon

Program Report: Jeffry Madura

- The number of attendees at New Orleans was <13 thousand. COMP had a total of 278 papers with 87 posters, 72 orals, and 119 talks in symposia. At Philadelphia, there were 92 posters, 100 general oral, and 194 symposia talks totaling 386 papers.
- 2) COMP was split geographically from MEDI and PHYS and it was suggested that COMP try and co-locate with one or both of these divisions at future meetings. Adrian was told by ACS that COMP and PHYS being co-located would be a priority in moving ahead.
- 3) The P2C2 is coming up, and it was recommended that Emilio attend. Hanneke will possibly attend the Division Summit. Themes for national meetings are discussed at P2C2. The ACS pays for 2 attendees.
- 4) The question was posed as to whether we could in the future prevent symposia from being split across 5 days. Some organizers are upset that they need to be at the conference for several days. Due to even programming rules, this issue will be discussed further.
- 5) Jeffry noted that this meeting had a high number of withdrawals. The ACS will begin maintaining a list of attendees who consistently submit one or more papers/posters and then do not show up to the meeting.
- 6) It was suggested that we communicate with MEDI in the future to avoid overlap of symposium topics.
- 7) The deadlines for award submissions/nominations are the same as for submission of posters/talks for each meeting.

Web Report: Allen Richon

- 1) The web page has now been transformed, and Allen would like to know what this page will do for COMP, and also is looking for suggestions for content.
- 2) Jeffry mentioned having audio and video of certain talks, and will work with Allen to post this material to the webpage.
- 3) Allen would like to add graphics/images to the webpage, and the committee discussed the idea of having contests where members would submit image content, and a possible award would be given out.
- 4) The possibility of adding member's highlights or bios of COMP members was proposed.
- 5) The website has the capability of providing executive committee members with personal email accounts. This capability might support archiving and/or discussion boards/groups.

- 6) Allen mentioned that Elsevier will allow COMP to place Abstracts from ARCC onto the COMP website.
- 7) The possibility of adding links to books/publications on the website was proposed.
- 8) In a future edition of the newsletter it was suggested to solicit ideas for content from members.

Executive Committee Meeting (for agenda see appendix)

Present: Curt Breneman, Wendy Cornell, Jeffry Madura, Ralph Wheeler, Hanneke Jansen, Emilio Esposito, Ed Sherer, Adrian Roitberg, Irache Visiers, Chris Harwell, Orlando Acevedo, Allen Richon, Carlos Simmerling, Peter Jurs, Chuck Reynolds, Phil Bowen

Guests: Ed King, Sarah Cho (International Affairs Committee), Rigoberto Hernandez (DAC), Terry Stouch, Luke Achene (Virginia Tech)

Secretary's Report: Ed Sherer

- 1) Ed Sherer gave the secretary report in place of John Woolfrey who was unable to attend the meeting. A listing of the action items from the New Orleans executive committee meeting was read. While preliminary, this list will be refined and passed around once minutes and action items from the Philadelphia executive committee meeting are prepared.
- 2) From Jan to Aug 2008, COMP membership has maintained a steady level of 2300-2315 total members.
- 3) Currently, COMP elections are taking place via SurveyMonkey. Not all COMP members have seen the ballot, so an investigation as to why will be underway soon.
- 4) Minutes from the 2007 Boston meeting, 2008 New Orleans meeting, and 2008 Philadelphia meeting are not yet finalized, and this will be a priority for the current secretary/assistant secretary.
- 5) Hanneke agreed to post a note about the current elections on the CCL and COMP webpages.
- 6) The wording of the travel policy will be reworded to incorporate all members of the committee who need funding (i.e., assistants to elected positions).

Treasurer's Report: Curt Breneman

- 1) The treasurer's report can be found as an appendix to the minutes.
- 2) Curt had a request from CINF to pay for the Peter Jurs symposium, he mentioned they also owe us money, so he will work out with them how to balance.
- 3) Wendy would like to see a summary of how much each sponsor is giving annually.
- 4) For the year 2008, our annual allocation increased. Related to this increase, we are awaiting announcement of the revised allocation formula which contains a new way to allocate support for co-sponsorship.

- 5) Curt noted that Schedule B of the tax filings from each year contains information about donors if their gift was in excess of \$5000/year.
- 6) The ACS would like each division to have at least twice their annual programming budget in assets.
- 7) Concerning sponsorship of COMP activities and donor's having their logo on our webpage, it was determined that we would allow any sponsor who has donated more than \$1000/year to have a logo scroll on the front of the COMP webpage.

Regional Meetings: no update

ARCC Discussion: Ralph Wheeler

- 1) The 3rd volume should have been received by all in the past, volume 4 will be ready by the end of the year. There are 5 sections including 12 chapters. Topics are bioinformatics, biological modeling, emerging technologies, physical modeling, and simulation techniques.
- 2) An **action item** is for Ralph to email section editors to solicit new contributors.
- 3) Ralph has only received one bid for advertisement on the inside pages, and would like anyone who has ideas of sponsors/advertisers to email him with suggestions (this is an **action item** for all).
- 4) At the moment, CCG has not given word as to whether they will pick up the back cover again. Ralph mentioned that if CCG backs out of the cover in the future, we will have a deficit when ARCC is printed.
- 5) Current distribution is 2500 members plus a few individuals and libraries. ARCC is currently abstracted in SciFinder.
- 6) An **action item** will be for Ralph to look into having ARCC indexed in PubMed and ISI.
- 7) Authors being asked to contribute to ARCC would like to know whether the papers influence their H-index.
- 8) An **action item** for Ed, Hanneke, and John is to provide Ralph with an official year end list of COMP members.

International Affairs Committee: Ed King

- 1) Ed King, a representative from the IA Committee spoke on behalf of his group to make COMP aware of programs with international ties. He specifically represents the Asia and Pacific Rim.
- 2) He would like COMP to look at ACS international events, and also let him know what conferences outside the US COMP is involved with, and which outside agencies we have ties with
- 3) Sarah Cho, who works with Brad Miller, was in attendance to help bring awareness to international activities of the ACS.
- 4) More or less they would like to start a dialog and collaborate with COMP on international activities
- 5) Wendy brought up interactions with the Brazilian Chemical Society

- 6) The IREU is the International Research Experience for Undergraduates program, there are 18 students going both ways in Germany, France, the UK. These programs are in collaboration with the NSF.
- 7) For the last 14 years there has also been an international program in collaboration with PITTCON covering analytical chemistry.
- 8) Their office is willing to set up staff support of any international programs we are involved in.
- 9) We have an international collaboration between ARCC and JMGM

Program Chair Report: Jeffry Madura

- 1) Jeffry reiterated the information concerning numbers of posters and talks discussed in the program meeting.
- 2) The next ACS national meeting will be in Salt Lake City followed by Washington, D.C.

Mentor Lunches: Wendy on behalf of Rommie Amaro

- 1) Rommie will conduct the fourth series of mentor lunches at the national meetings covering both academic and industrial topics.
- 2) The lunches are being sponsored by BioSolveIT.
- 3) It was recommended that the academic lunch focus on interviewing to get an academic position rather than the academic lifestyle.
- 4) A second suggestion is for academic lunches to focus on why academics do academia; some students may be wondering why one would choose the academic lifestyle.

Newsletter: Orlando Acevedo

- 1) The newsletter is running late, but a draft went out August 25, 2008.
- 2) The goal is to have the newsletter printed and available for the national meetings.
- 3) It might be a good addition to do an update profile on past winners of various COMP related awards.
- 4) It was discussed that the bylaws state that we shall have a newsletter.

Website: Allen Richon

- 1) Allen began by stating that all broken links had been removed from the website, and further alterations will be easier to make.
- 2) Since the website is in need of content, Allen would like the COMP division to get back to him about what we would like the website to do/be.
- 3) Several **action items** for web content were discussed including: obtaining graphics/images; adding biographies of COMP members as human interest stories; adding a search function; adding discussion groups/forums; including the abstracts from ARCC articles on the COMP webpage.

4) An **action item** for all executive committee members is to submit a head shot image for incorporation into the webpage.

Social Networks: Hanneke Jansen

- 1) Hanneke will research tools for helping members network, and the desire is to incorporate these tools into the division and/or webpage. This might lead to the ability to have mentor lunches outside ACS national meetings.
- Rigoberto from the DAC mentioned that an existing ACS tool called the ACS Member Network, more or less chemistry facebook, would do exactly what we are looking for. There was an ad in the Philadelphia program, and information can be obtained from the focus interest group (<u>fig@acs.org</u>).

Council Meeting

1) For the current Council meeting Emilio will replace Andy, and for this reason, Emilio needed to be credentialed to attend.

Councilor Reports: Peter Jurs

- 1) Peter is sitting on two committees, the first of which is Publications. The ACS has an electronic version of C&E News available, and members will be able to get the e-version only, if desired, in the near future.
- 2) A new Publications web page for ACS will be up in September of 2008
- 3) Chuck mentioned that discussions concerning what to do about copyright issues have not yet concluded
- 4) From Nominations and Elections, Peter mentioned that the next presidential election will be an automatic electronic run-off. The committee is currently discussing how much politics should be allowed in national elections.
- 5) Wendy asked whether COMP would like to place a representative on the Committee on Science. The COMP division needs to appoint someone if so.
- 6) An **action item** for all members to email Wendy about possible representatives was issued.

Various Issues: All

- 1) The NIH sent a request to COMP to help in identification of reviewers for a lung health study.
- 2) After discussion, it was decided that an **action item** will be for Wendy to inform the NIH we are not interested in pursuing this work.
- 3) A discussion of how to handle the Boston based BAGIM group was again had. Basically, they would like us to handle their finances, and prior to saying yes or no, we would like to know exactly how many of them are ACS members, and how many are COMP members. This is considered an **action item**. [Irache]

- 4) A second **action item** concerning BAGIM is to investigate the creation of a subdivision of COMP concerning regional activities. Curt mentioned that he will pursue this. [Curt and Phil]
- 5) Action item: To help determine what to do with BAGIM, Hanneke and Irache will work up a plan for how to deal with regional activities/groups.

Regional Meetings: Phil Bowen

- 1) The question was raised as to what the protocol is for getting money out of COMP to support regional activities.
- 2) Curt mentioned that the event must have COMP sponsorship clearly indicated
- 3) It was requested that a form is created and posted to streamline the request for regional support. This could possibly be placed on the webpage. One idea would be to have a cover sheet for a one page proposal for funding.
- 4) As an **action item**, Phil and Curt will put something together in way of a form for regional support by COMP.

Division Allocation Committee: Rigoberto Hernandez

- 1) Rigoberto's first order of business was to tell COMP that there was no negative feedback from the 2007 annual report.
- 2) In the future negative feedback will be reported prior to the division committee meetings
- 3) He mentioned the ACS innovative grant program which is money set aside to go only to divisions, interestingly, 1/3 of divisions could be fully funded with the available cash.
- 4) Each division is eligible for two grants a year totaling \$12,500 where the maximum per grant is \$7,500. Throughout the history of the program the amount of available funds has never been asked for by the divisions.
- 5) Since there were no applications from COMP, we can assume we lost out on \$12,500 according to Rigoberto.
- 6) It is possible to write a grant such that DAC would help support the COMP annual planning retreat.
- 7) The next deadline for innovative grants is 2/1/09 and decisions will be made at the spring meeting in Salt Lake City. The possible decision outcomes are accept, defer, or decline. A deferred grant can be re-submitted the following grant period.
- 8) The money can not be retroactive, but is allotted for the next coming meeting after the decision has been made.
- 9) Each division chair should receive regular announcements of the innovative grant program and deadlines, but it was mentioned that information is available online.
- 10) Recommendations of how to get money were as follows:
 - a. Anything which enhances value to division members
 - b. Anything which is targeted towards students
 - c. Anything for a symposium which might help hook in industry money/interest/support/collaboration

Rosters:			
JAN	2199 RM	89 AM	27 AF 2315 total
FEB	2181 RM	93 AM	27 AF 2301 total
MAR	2182 RM	91 AM	27 AF 2300 total
APR	2183 RM	91 AM	27 AF 2301 total
MAY	2183 RM	91 AM	27 AF 2301 total
JUN	2191 RM	97 AM	27 AF 2315 total
JUL	2191 RM	97 AM	27 AF 2315 total
AUG	2192 RM	97 AM	26 AF 2315 total

RM Real Member, AM Associate Member, AF, Affiliate

Elections:

SurveyMonkey (Pro edition) used. May be used for other surveys, approving minutes, etc.

Number of successful ballots (initial count):2129

Method to determine vote list: July roster 2315 – 26 AF (RM/AM only) -82 RM without email address -3 AM without email address -35 SurveyMonkey Opt Out – 40 returned email (incorrect address?).

<u>Election notes:</u> Final Date: Sept 22, 2008 Return email (graciously set up by Allen Richon): <u>elections@acscomp.org</u> Email forwarded to <u>elections@pharmacophore.com</u> All members requesting ballot will be checked against roster/acsID.