

**COMP Division Programming Meeting
248th (Fall) National Meeting
Esplanade Ballroom 301 - Moscone Center, South Building
San Francisco, CA August 9, 2014**

Present: Emilio Esposito, Jeffry Madura, Sara Nichols Swift, Ed Sherer, Terry Stouch, Lorena Tribe, Petrina Kamyra, Adrian Roitberg, Jane Tseng, Patrick Lee, Scott Wildman

- 1) Discussion of withdrawn posters and talks again, continue to monitor this
- 2) Boston agenda is full for COMP, Fall 2015
- 3) Denver Spring 2015
- 4) PACS being replaced with MAPS
- 5) Need judges for undergraduate posters (only 3 posters) Monday afternoon. This year only 1 will be awarded
- 6) Need judges for emerging technologies
- 7) Need judges for GPU session on Tuesday (NVIDIA at poster session)

ACTION ITEMS

- 1) **Action item:** Ed will talk to Hanneke about taking over COMP together for 1 year
- 2) **Action Item** – Ed will organize a COMP together event for NJ
- 3) **ACTION ITEM:** Ed will transition electronic archive from Google DOCS to Jane's server
- 4) **ACTION ITEM:** Emilio to update COMP web site mission statement to: "The Computers in

Chemistry Division of the American Chemical Society promotes an interdisciplinary forum for those interested in developing and applying computational tools in the chemical, biological and materials sciences."

- 5) **ACTION ITEM:** Ed to update travel policy and post to website. "The Chair, Chair-Elect, Secretary, Asst Secretary, Treasurer, Asst Treasurer, Program Chair, and Program vice-Chair will be reimbursed by the Division for travel to each national meeting up to the cap set by ACS for travel reimbursement to councilors." Added in Dallas – member will perform duties they are attending meeting for (their position). Make a substantial contribution to the running of the COMP division effort at the national meeting. Request to include detail about how you will contribute.
- 6) **ACTION ITEM:** Mel will contact Schrodinger for funding possibilities (off line discussion needed for how much and what will money go for?)
- 7) **ACTION ITEM:** Chair should send an annual email to membership which details what COMP does, and what links, etc are available: web, linkedin, etc.
- 8) **ACTION ITEM:** Adrian will look into the possibility of adding in a video series of COMP interviews detailing why people are in COMP and what they get out of it
- 9) **ACTION ITEM:** Sara to make sure CCL is linked on COMP web page
- 10) **ACTION ITEM:** Sara to add links to all relevant blogs and forums for COMP content on the web page
- 11) **ACTION ITEM:** Emilio and Lee will develop a system of contacts for information gathering in a blog/wiki style resource on the COMP web page
- 12) **ACTION ITEM:** Adrian will look into building a COMP website-hosted version of the list of minorities and women job seekers in COMP related fields
- 13) **ACTION ITEM:** From Indianapolis: Jeffry/Terry/Kennie will follow up with past winners of the Computers in Pharmaceutical Research for a discussion with ACS about continuing this national award
- 14) **ACTION ITEM:** Emilio to investigate moving emailing of members from the current system to emailchimp
- 15) **ACTION ITEM:** Terry to gather nominations for ACS fellows 2014
- 16) **ACTION ITEM:** Ed to update list of COMP benefits on web page
- 17) **ACTION ITEM:** Ed/Lee/Adrian/Veer to put list of available COMP based speakers on the website. Pair it with a list of undergraduate focused groups in COMP.
- 18) **ACTION ITEM:** Scott to list the undergraduate poster award on the web site
- 19) **ACTION ITEM:** Patrick to attend ACS 2014 Communications and Publications retreat
- 20) **ACTION ITEM:** Ed to post minutes from Fall 2013 ACS, and Spring 2014
- 21) **ACTION ITEM:** COMP to contact Chris and Laura about women in COMP
- 22) **ACTION ITEM:** Carlos, Terry, Kennie, and Adrian will post the guidelines for awards onto the website by San Francisco meeting
- 23) **ACTION ITEM:** Adrian and Peter will put together a scoring metric for the award judging

Votes held during the Executive meeting

- 1) Motion made by Ed to approve minutes from 2014 Spring Meeting, Terry seconded, passed unanimous.
- 2) Ralph made a motion to accept either the option from Elsevier or JMGM for publication of ARCC. (as opposed to accepting neither). Ed seconded. Unanimous vote to accept one of the options.
- 3) Ralph motioned that we accept the offer from JMGM. Adrian seconded the motion to accept the offer. 2 oppose, 6 abstain, 11 support the publication of ARCC to JMGM.
- 4) Terry made a motion to support TdT round 3 for \$4000. A portion (\$500) of this money from COMPs budget would come from the Merck pass through. Ed seconded the motion. Vote passed unanimously.

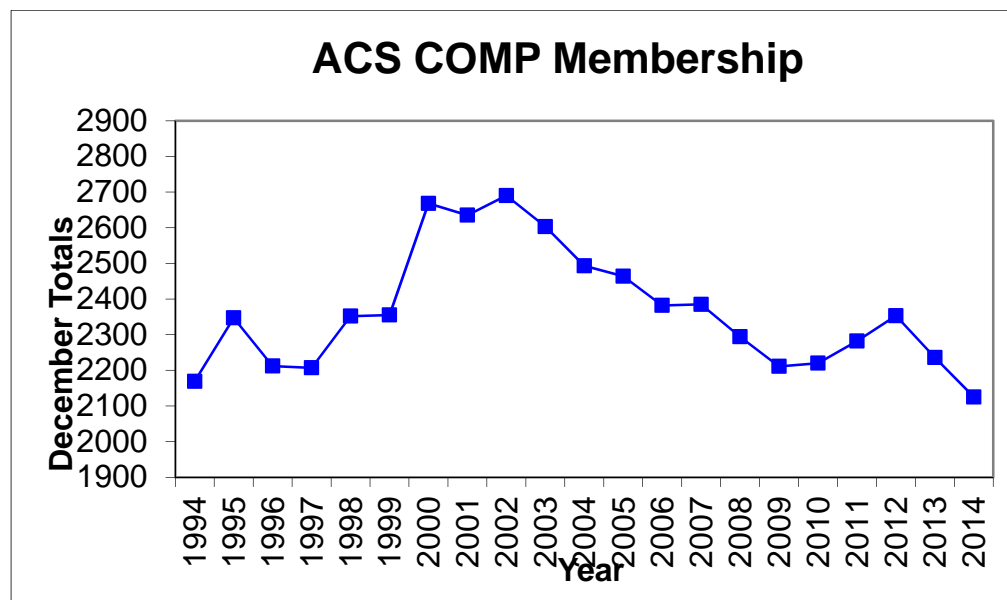
COMP Division Executive Meeting San Francisco, CA August 9, 2014

Present: Emilio Esposito, Jeffry Madura, Sara Nichols Swift, Ed Sherer, Terry Stouch, Petrina Kamyra, Adrian Roitberg, Jane Tseng, Patrick Lee, Peter Jurs, Ralph Wheeler, Hanneke Jansen, Curt Breneman, Carlos Simmerling, Lewis Whitehead, Daniela Kohen (Calrton College), Kennie Merz, Luke Achenie, Scott Wildman

ACTION ITEM: Ed to work with Jane to move Exec email list over to the current comp web server

1) Secretary Report – Ed Sherer

- a. Mentor Lunch (Tuesday), Ed, Sara, 12pm, meet at COMP rooms – Adrian or Ralph
- b. Membership continues to decline, ACS is eyeing the last three years and asking if we need help increasing our membership. Over the last several years we have lost about 600 members, or 20%



- c. Vote on Minutes from Spring meeting

Motion made by Ed to approve minutes, Terry seconded, passed unanimous. Action Item – Ed to post minutes to web page.

- d. Electronic archive issues – will move to Jane’s COMP website

- a. Action Item – Ed to post files to this site
- e. This year’s COMP election: 2016 COMP Chair: Ed Sherer; 2015-2018 Comp Secretary: Veer Shanmugasundaram; 2015-2017 Comp Councilor (Ralph Wheeler) and Alternate Councilor (Luke Achenie); Appointment to Assistant Secretary: Petrina Kamyia
- f. Candidate write-ins may be useful for bringing in new volunteers or executive members: So Hirata, Charles Kyte, Lei Ming, Pat Walters, Jeff Evanseck, Stephen Johnson, Will Noid, Charles Kyte, Shaomeng Wang, Greg Warren, Jeffry Madura, Stephen Johnson, Emilio Esposito, Wei Yang. George Bush, Charles Kyte, Sandor Lovas, Alex McKerrel, Whitney Kellet

2) Treasurer Report - Sara Nichols Swift

- a. Lewis Whitehead will be taking over as assistant treasurer
- b. Increase in checking account balance and savings balance in relation to last year
- c. Division allocation down from 2013
- d. Division retreat cost down from 2013

3) Programming Report – Emilio Esposito / Scott Wildman

See details above, COMP poster session Tuesday night

4) Councilors’ Reports – Peter, Ralph, Melissa, Emilio.

Peter – Sits on the council policy oversight committee.

Ralph – Serves on the policy subcommittee, one a new policy document on fracking, one on science and technology funding

Emilio – sits on meetings and expositions

Patrick – served on communications and PR committee

Mel – not at the Saturday meeting, but will be at the Council meeting

5) Outreach Events in SF: Mentor lunches / Graduate and Postdoc reception / Undergrad speed networking / TDT Happy Hour

Scott, Ed, Terry will attend the PostDoc mixer

Jeffry will do the undergrad speed network 4-530, Monday

TdT will be Monday night as an event and COMP together

Action Item – Ed & Sara will confirm that money has come from Merck via ACS for 2014 and 2013, to complete the assignment of \$\$ for the TdT event in Fall 2014 **DONE** – yes, Merck has a rolling entry in our ledgers

6) Judging posters for Awards- Ed

Stickers, 6 judges, split posters by people, each judge returns 1-2 posters and then ranking and follow up if needed

7) Poster session awards presentation policies and procedures – Adrian

Adrian would like to showcase the COMP division to a greater extent and have the announcement of the awards be a bit more structured. Possibly the Chair would give an overall intro and background. Then hand offs to the award givers. More formalized photo sessions. Make sure sponsors are properly announced.

8) ARCC status & JMGM relationship - Ralph, Jeff, Adrian

The previous/current contract is with Elsevier, new contract would be with Elsevier monographs. Inquired about JMGM electronic copy only. Could print copies if desired to extend proposed contract. Not open access initially but could be after time X. JMGM is slightly more expensive, and would need us to host the articles. Would be indexed under DOI. Historically, ACS was given the option to publish but declined. JMGM option would be peer reviewed. JMGM option would be a name. Either option is less money then was being spent, a large savings on shipping.

Ralph makes a motion to accept either the option from Elsevier or JMGM. (as opposed to accepting neither). Ed seconds. Unanimous vote to accept one of the options.

Ralph motions that we accept the offer from JMGM. Adrian seconds the motion to accept the offer. 2 oppose, 6 abstain, 11 support the movement to JMGM.

9) TDT / COMP together – Hanneke

It would be good to try and get some new organizers for events in areas other than the common event locations of Boston and San Francisco

Should we have a bigger push for events at national meetings.

Hanneke would like to pass the organization of COMP together on to someone else. This could be a role on the Exec committee.

The exec committee will attempt to identify a COMP together champion. Possibly the chair-elect should take over this roll. If no other person is identified, then Ed will perform this roll.

Action item: Ed will talk to Hanneke about taking over COMP together for 1 year

Action Item – Ed will organize a COMP together event for NJ

For TdT, Hanneke requests continued support for the initiative. In 2013, COMP sponsored \$4000. The next highest sponsor for this initiative is \$2000.

Terry makes a motion to support TdT round 3 for \$4000. A portion (\$500) of this money from COMPs budget would come from the Merck pass through. Ed seconds the motion. Vote passes unanimously.

Merck pass through money normally covers the COMP poster session to some extent.

COMP Together outlook & questions: Events have happened in multiple areas, but most consistently in the Boston and San Francisco Bay areas. There may be a need for a new push to engage some of the local champions in areas other than those two. The list we just received this week of #COMP members per local section could be a useful tool to identify areas to target. The COMP Together network has also been used to advertise networking events at the National Meetings, most notably the mentoring lunches and TDT networking events. It could be used for additional events at national (and regional) meetings which would require a small group to champion. Do we want to recruit such a group? Is there someone who would like to take on the overall champion role for COMP Together? Do we need to change or expand the initiative?

TDT outlook & questions: The second round of the TDT competition saw a significantly increased level of participation (16 submissions vs 6 in round-1). We are presenting 5 awards at the award & networking event on Monday the 11th and we'll have an Award symposium on Tuesday the 12th. We are still waiting for papers to be finished by the winners of the first round of the competition, which will describe the models, the workflows, the held-out data (binding mode of an inhibitor) and the effectiveness of the models to enrich a screening set that was acquired with TDT sponsorship money and screened by the academic collaborator. While most of the compounds that were confirmed as hits are close analogues to known anti-Malaria compounds, 5 compounds can be considered novel! We will also push for publication of the work coming out of round-2. The TDT steering committee has started to discuss timing and content of round-3. Would COMP be willing to sponsor again?

Teach-Discover-Treat ("TDT")

The goal of the Teach-Discover-Treat ("TDT") initiative is to provide high quality computational chemistry tutorials that impact education and drug discovery for neglected diseases. The tutorials and models are solicited through a competition and materials are made available through the TDT website. Collaborations have been established with academic collaborators to provide held-

out test-data for the competition and to follow-up on winning submissions with actual drug discovery activities. The initiative also has as an objective to strengthen the community of scientists involved in open source drug discovery for neglected diseases and computational chemistry, through networking and outreach events. The initiative was launched in 2012 and the first competition was completed with an Award symposium in 2013. The second round is about to be completed with an Award symposium planned for Tuesday. The international steering committee consists of six leaders in the COMP community that work in academia and the pharmaceutical industry. There is a separate judging panel, chaired by one of the steering committee members. The initiative received IPG funding and relies on the COMP Treasurer and Assistant Treasurer to receive sponsorship money from external parties (software vendors, pharma) for TDT awards & expenses and then issuing award money to winners and reimbursing the steering committee members for actual expenses out of that sponsorship money. The COMP Division has also provided financial sponsorship for both round-1 and round-2 to cover expenses for the networking events and for compound acquisition for the actual drug discovery activities. The COMP Division received a ChemLuminary Award for this effort in 2013 in the category “Innovation and Outstanding Service to Members of a Division”.

What is the relationship between COMP Together & TDT? Are both of these COMP initiatives?

Both initiatives were launched under the COMP umbrella and they both received IPG funding. They also both use COMP Treasurer resource to manage sponsorship monies. The two initiatives have very different goals but the TDT initiative has used the COMP Together network to advertise networking events. COMP Together is a very clear COMP initiative that came out of the strategic planning process and has as explicit purpose to strengthen the scientific community. It would be hard to imagine COMP Together operating separate from COMP. The TDT initiative is currently also a COMP initiative, although it could become independent if either TDT or COMP decided that would be preferred. For now, TDT relies on COMP to handle the sponsorship monies and host the Award symposia.

10) Protocols for reimbursements, meeting contributions, and other requests made of the Treasurer - Sara and Chris

Requested protocols for reimbursements:

- a. We should vote on the grant requests in a more formal fashion at the exec meetings, a note will be made on the web page about this protocol
- b. There is a form to request money for the events being requested
- c. Form available on the COMP web page
- d. Any event getting money needs to submit a report to be used for COMP summaries
- e. We target about 5 per year at the \$500 level

- f. Request form should be sent to Secretary, both application and report summary
- g. Treasurer needs a more formal set of documents and receipts for all reimbursements.
- h. There is no per diem, and COMP does not cover internet in hotels
- i. Total for councilors for year is \$2874 and \$1437 per meeting. They get 75% reimbursement from ACS prior to COMP funding.

11) Conference support: How do we decide? Should we target some conferences/symposia?

12) Criteria for voting - What percentage do we need for yes or no; How do we vote? Survey monkey? What do we do about absentee? How much time to we allow? - Sara and Ed

13) NTS (Nomenclature, Terminology, and Symbols) Committee - Albert Censullo - introduction to NTS and what they can do for COMP - 5 min as per email

See full notes below

Do not need to be a councilor to be a member. If any COMP members are interested please let us know.

14) Awards procedures: Carlos

15) Sponsors and their recognition (Merck sponsorship)

Taken care of, see notes above.

16) Fund raising – Curt

- a. Alumni, parents, students as potential donors
- b. Trying to cultivate a pyramid of support
- c. COMP should be aware of not diluting its BRAND
- d. Can give people the option of funding specific items
- e. Special events for specific sponsors
- f. Could do a campaign
- g. At the moment we do not have a plan/goal/need for money
 - i. What proposals can we come up with?
- h. Increasing value of COMP will increase membership?
- i. Endowment of awards would be nice

- j. Need to take this discussion to the retreat
- 17) Funds: (How much do we want/need to raise? What will we use it for? What recognition will we provide? Of what advantage is it to the sponsors?)
 - 18) Webpage discussions: webpage modifications and additions / new URL- Sara and Jane
 - 19) Generic emails for EC officers and email archives - Terry, Jane
 - 20) Public Relations Chair position is open
 - 21) Awards nominations (e.g. Computers in Chemical and Pharmaceutical Research, ACS Fellows, Kavli, others?) – Veer
 - 22) Status of our sponsorship of the ACS National ACS Award for Computers in Chemical and Pharmaceutical Research
 - 23) Newsletter or equivalent status
 - 24) Committee on Science (ComSci) nominations for election for two Division Representatives who will serve on the committee for the 2015-2017 term
 - 25) 2014 accomplishments to-date

Guest speaker from committee on nomenclature, terminology and symbols

Dear Division Chairs,

According to its charter, the Committee on NTS examines problems and monitors developments in nomenclature, terminology, symbols, and units, coordinates the activities of divisional and other committees dealing with such matters within the Society, advises and consults with editors of Society publications, acts for the Council in the consideration and action on such documents and proposals presented to the Society, acts for the Council in providing liaison in matters of these issues with non-Society organizations, and makes recommendations to the Council in matters related to these issues.

NTS committee membership consists of experts in various fields of nomenclature, terminology, symbols, and units as well as individuals active at all academic education levels. Through joint membership with national and international terminology committees, NTS provides leadership, cooperation, support, and guidance for ACS membership and publications (including C&EN).

To better serve various ACS Division members, the Committee on NTS wishes to determine if your Division could use or benefit from the expertise available within NTS to address issues and/or items of concern.

A representative from the NTS committee would be happy to provide a five minute presentation about its services and functions at one of your Division meetings either at the next national ACS conference in San Francisco (August 10-14, 2014) or the following meeting in Denver (March 22-26, 2015). In addition, briefing materials can be sent electronically for inclusion in your Division agenda book.

We request that you respond no later than June 30, 2014 to Al Censullo (acensull@calpoly.edu) or 805.541.0636.

The Committee on NTS wishes to thank you for taking your valuable time to consider the potential advantages of future interactions on items of mutual interest. Please contact us any time you desire additional information.

Best wishes,

Al Censullo
Chair, Committee on NTS