

Special Committee Report
Boston Area Group for Modeling and Informatics

(www.BAGIM.org)

2012 Summary Report to NESACS

Prepared by Kenneth Mattes
15 January 2013

Officers

President:	Andrew Good
VP and Program Chair:	J. Christian Baber
Treasurer	Kenneth Mattes
Communications	Omar Stadella

Advisory council

Lee Herman
Richard Dixon
Ryszard Czerminski

2012 Activity Summary

Fund Raising for 2012

Andrew successfully, through a letter campaign, raised \$1500 from three companies. BAGIM was supported by a ACS Division of Computers in Chemistry grant of up to \$500 on joint CompTogether-BAGIM meetings.

Meetings in 2012

A total of 4 meeting were held (Jan, April, June and Oct) at three different venues. Attendance averaged ca. 15. Details can be found in Appendix 1.

APPENDIX 1: Meeting Details

DATE: January 19, 2012

VENUE: Elephant Walk in Cambridge (free parking and meeting room)
(<http://www.elephantwalk.com/cambridge/index.html>)
2067 Massachusetts Avenue, Cambridge, MA 02140
617-492-6900

AGENDA: 5:30-6:30 Socializing (Cash bar)
6:30 – 7:30 Dinner (3 course, \$30.00)



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7:30 - 7:45 Business meeting
7:45 – 8:30 Presentation and Q&A (open to the public)
8:30 – 9:00 Wrap-up and Departure

TITLE:
Family based scoring and docking constraints in eHiTS

SPEAKER(s):
Drs. Zsolt Zsoldos and Orr Ravitz, SimBioSys Inc (<http://www.simbiosys.ca/>)

DATE: April 26, 2012

VENUE: Harvard Faculty Club (<http://www.hfc.harvard.edu/>)
Theatre Room
20 Quincy St. Cambridge, MA 02138
617 495 5758

AGENDA: 5:30-6:30 Socializing (Cash bar)
6:30 – 7:30 Dinner (\$30.00, or \$25.00 for students and post-docs)



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7:30 - 7:45 Business meeting
7:45 – 8:30 Presentation and Q&A (open to the public)
8:30 – 9:00 Wrap-up and Departure

TITLE:
KNIME - Integrating Data, Tools and Science and Interfacing MOE and KNIME

SPEAKER(s):

Bernd Wiswede, KNIME.com AG, (<http://www.knime.org/>)

Alain Deschenes, Chemical Computing Group (<http://www.chemcomp.com/>)

DATE: June 21, 2012

VENUE: The Chateau
(<http://www.chateaurrestaurant.com/waltham/waltham.asp>)
195 School Street
Waltham, MA 02451
Phone: 781.894.3339
Fax: 781.894.5291

AGENDA: 5:30-6:30 Socializing (Cash bar)
6:30 – 7:30 Dinner (\$20.00))
7:30 - 7:45 Business meeting
7:45 – 8:30 Presentation and Q&A (open to the public)
8:30 – 9:00 Wrap-up and Departure

TITLE:
The Semantic Web: Semantic interoperability for drug discovery

SPEAKER(s):

Tom Plasterer, AstraZeneca R&D Boston

DATE: **October 25, 2012**

VENUE: Elephant Walk in Cambridge (free parking and meeting room)
(<http://www.elephantwalk.com/cambridge/index.html>)
2067 Massachusetts Avenue, Cambridge, MA 02140
617-492-6900

AGENDA: 5:30-6:30 Socializing (Cash bar)
6:30 – 7:30 Dinner (3 course, \$30.00)



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7:30 - 7:45 Business meeting
7:45 – 8:30 Presentation and Q&A (open to the public)
8:30 – 9:00 Wrap-up and Departure

TITLE:
Text Mining for Drug Discovery

SPEAKER(s):
David Milward, Chief Technology Officer, Linguamatics (<http://www.linguamatics.com/>)