

BioPAX Work Group
December 1, 2004 Conference Call Minutes

Participants: Gary Bader, Gabriel Berriz, Michael Cary, Frank Gibbons, Geeta Joshi-Tope, Joanne Luciano, Jonathan Rees, Vincent Yau, Jeremy Zucker

Summary:

1. Recent releases
 - a. Level 1, version 1.2 released on Nov. 19
 - i. Adds several restrictions, disjointedness, sub-properties
 - ii. Old version available in the <http://biopax.org/Downloads/> directory
 - b. Level 2, version 0.5 (draft) released on Nov. 23; Adds support for:
 - i. Molecular interactions
 1. Incorporated bulk of PSI spec
 - ii. Black-box & hierarchical pathways
 1. Added inputs and outputs to pathways
 - a. What about variable outputs?
 - i. E.g. Protein degradation
 - ii. Can't handle yet, would need generic class (e.g. "polypeptide fragments")
 - iii. Good issue for consideration in Level 3
 2. Difference between conversion and pathway?
 - a. Conversions have no physical entity intermediates (that would normally be captured in BioPAX as individual physical entities); whereas pathways do
 - b. Jeremy suggested removing the distinction between pathways and conversions; Mike, Joanne, and Geeta disagreed, stating that most databases make a distinction between the two and we should adhere to the major trends in existing pathway data.
 - iii. Sequence features
 1. Represent binding domains, post-translational modifications, DNA modifications, etc.
 2. Attached to physical entity participants
 3. FEATURE-TYPE slot can point to SO (Sequence Ontology)
 - a. Jeremy suggested using SO directly instead of via the openCV wrapper; this would be a test-case for ontology cross-pointing in OWL
 - iv. Evidence
 1. Support class has slot for evidence codes
 - a. The ontology cross-pointing issue (above) is also relevant for evidence codes
 2. Support subclasses represent experimental information
2. Level 2 TO-DO
 - a. Review draft proposal

- i. Hierarchical & black-box pathways - Jeremy will look into these and post an email to the discuss list
 - ii. Sequence features - Mike will ask Emek if he will evaluate the draft Level 2 representation
 - iii. Pointing to external OWL ontologies – Jonathan Rees will examine feasibility of this (instead of wrapping terms with openCV class)
 - 1. Evidence - Mike suggested Peter or Suzanne as reviews, possibly another PSI developer
 - b. Develop examples
 - i. PSI example: Frank volunteered to translate a small PSI dataset into BioPAX Level 2
 - ii. Sequence features example: metabolic pathways involving post-translational modifications?
 - 1. Reactome creates a different sequence entity for each different PTM; each sequence entity points to a parent reference entity from which it is derived
 - a. Mike said this was similar to the BioPAX representation (reference entity = physicalEntity; physicalEntityParticipant = sequence entity)
 - 2. Geeta will send out some Reactome data that includes PTMs for manual translation into BioPAX
 - a. E.g. involving p53
 - 3. Geeta asked how the proposed mechanism would work with flux balance analysis
 - a. Mike said that in order to do it, the sequence feature would need to point to a physical entity (e.g. a small molecule called “phosphate”)
 - b. Gary said that most people just use controlled vocabularies to represent chemical modifications on large molecules because it is much easier
 - c. Jeremy suggested discussing this more on the biopax-discuss list
 - iii. Black-box & hierarchical pathways example
 - 1. Geeta will send some examples of pathways that interact with each other; Jeremy will look at them
 - c. Update documentation; write BioPAX paper
 - i. Need to make Level 2 docs self-sufficient
 - ii. BioPAX paper
 - 1. ISMB deadline is Jan 14
 - 2. Need to write it, then discuss where to submit
 - 3. Will likely need 2+ DBs in BP format to get published
 - a. Reactome: mapping done
 - i. Jeremy said Reactome could annotate their SBML with BioPAX
3. Lib-BioPAX
 - a. Yuhong Ming contributed two implementations of BioPAX API

- i. One from Jsave, the other from Kazuki (See SF CVS)
 - b. Jeremy and Joanne generating unit tests
 - c. Recent Boston meeting – Joanne and Jeremy will generate and send out minutes
- 4. Data Conversion
 - a. Reactome - Gary has been in contact with Geeta, he will provide them with help on the Reactome conversion if they need it
 - b. aMAZE - They will start work on a converter in January
 - c. WIT - Jeremy and Joanne talked to Liz, Mustafa may attend the Jan 21 meeting (he cannot work on WIT→BioPAX until January)
 - d. KEGG - Jeremy loaded KEGG into BioWarehouse
 - i. Need to query it with appropriate Lib-BioPAX Java classes to generate BioPAX
 - ii. Gary will test it
- 5. Next meeting
 - a. Location – still not determined (either SRI or NYC)
 - i. Jeremy said he favored SRI, no one objected
 - ii. ADDENDUM: Chris cannot attend meeting if it is held at SRI
 - b. Duration
 - i. Formal meeting all day Friday, January 21
 - 1. With possible hack sessions the day before or day after
 - c. Agenda
 - i. Discuss and ratify new features of Level 2
 - ii. Plan Level 3
 - iii. Not focusing on lib-biopax
 - 1. Possible lib-biopax meeting in Boston in February
 - d. Budget allows four international participants
 - i. Mike and Gary will send out invitations