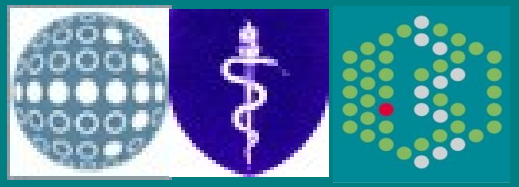
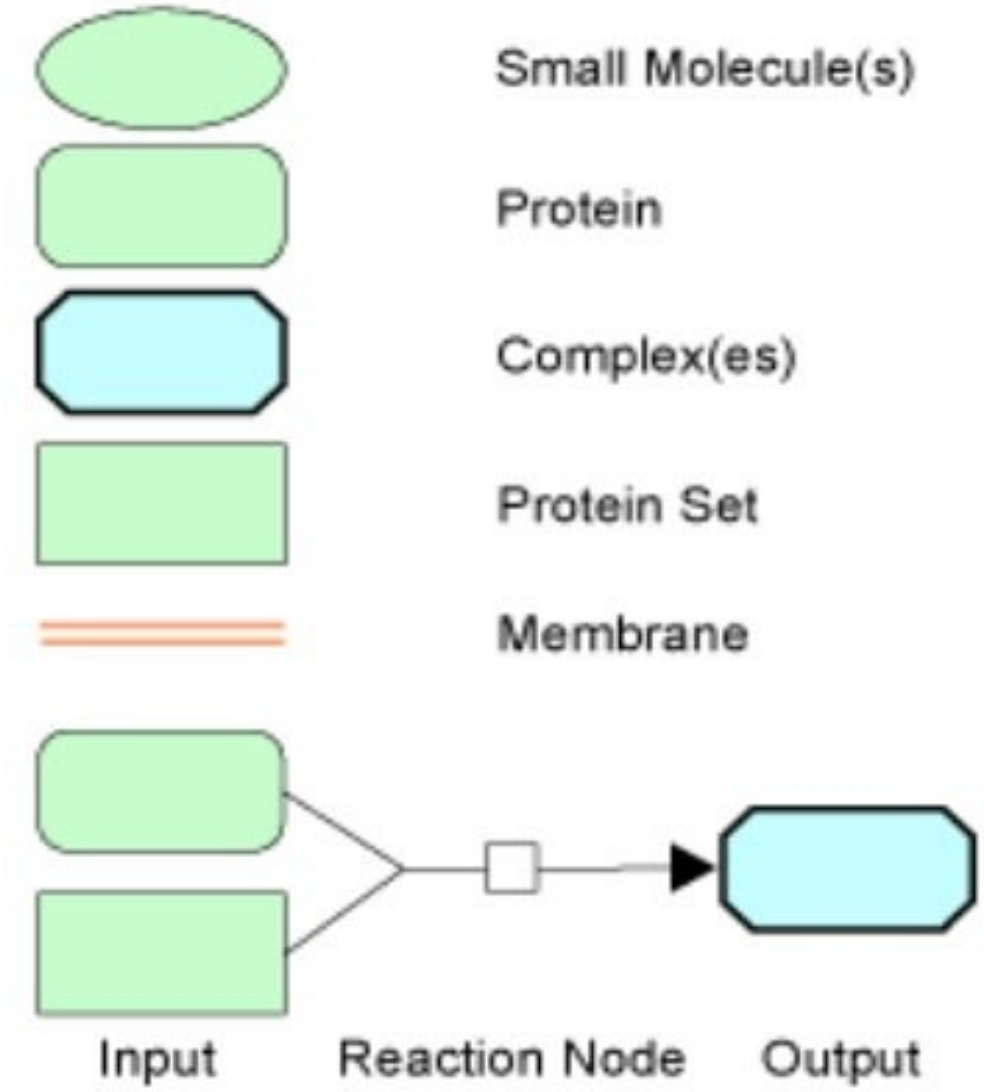
Reactome and libSBGN

How we generate SBGN-ML and how it renders

David Croft



Reactome's glyphorium



Mapping Reactome's data model to SBGN 1

The following are extracted from Reactome's diagrams:

- Compartments
- Entities (proteins, complexes, compounds, complexes)
- Reactions
- Edges

Mapping Reactome's data model to SBGN 2

For reactions:

- All dimensions multiplied by 3
- Only 1 reaction type
- Reactome stores reaction type, so we could use this in future

Mapping Reactome's data model to SBGN 3

For entities:

- All dimensions multiplied by 3
- Most SBGN entity types recognised: protein, DNA, RNA, complex and small molecule.
- Sets and complexes annotated with a list of constituent names, using a callout
- mt: decorations used to distinguish between protein, DNA and RNA.

Mapping Reactome's data model to SBGN 4

For edges:

- All dimensions multiplied by 3
- Most SBGN arc types recognised: protein, consumption, production, catalysis, inhibition and stimulation.
- All arcs start and end at nodes, no hyperarcs are used.

Mapping Reactome's data model to SBGN 5

For compartments:

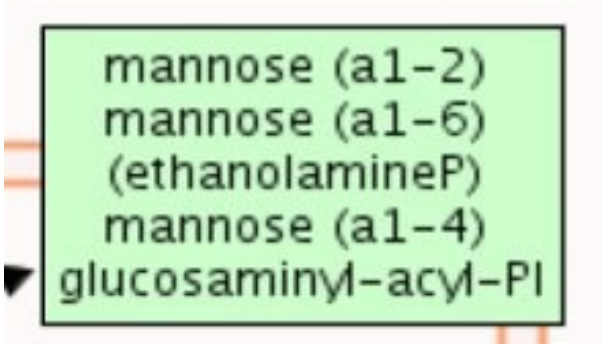
- All dimensions multiplied by 3
- Name label inserted in top left corner.

```
<sbgn xmlns="http://sbgn.org/libsbgn/0.2"><map language="process descripti
on"><glyph class="compartment" id="compartmentVertex_7660_555067"><label t
```

Reactome sets

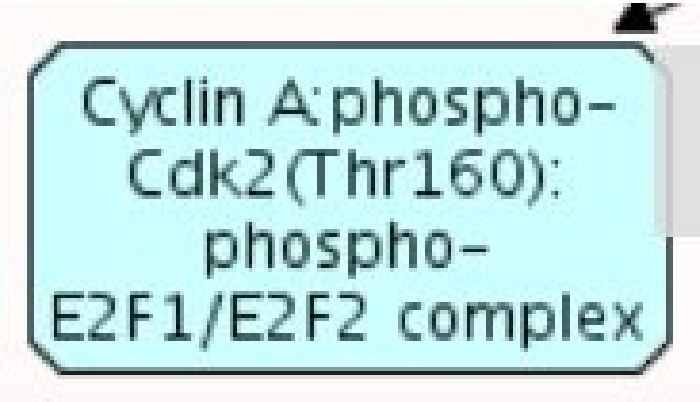
Three different types of set:

- **CandidateSet**. Entities that are hypothesised to do the job.
- **DefinedSet**. Any one of the set members can do the job.
- **OpenSet**. A set of example entities, where the number of possible entities is very large, e.g. alcohols.



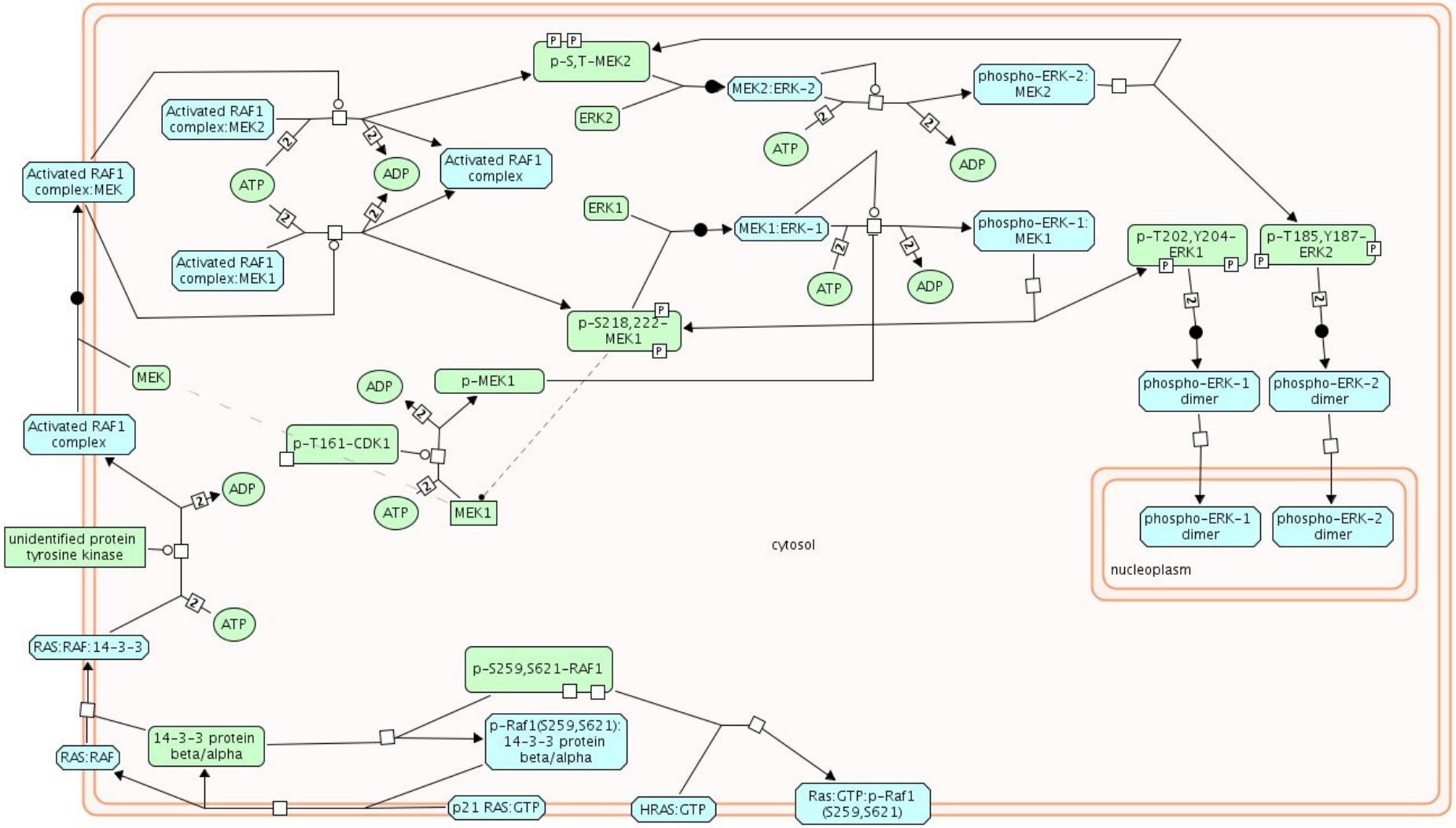
Reactome complexes

- Any type of entity can be combined into a complex.
- Complexes can be nested.
- Only a simple glyph used for complexes in pathway diagrams – no detail shown.

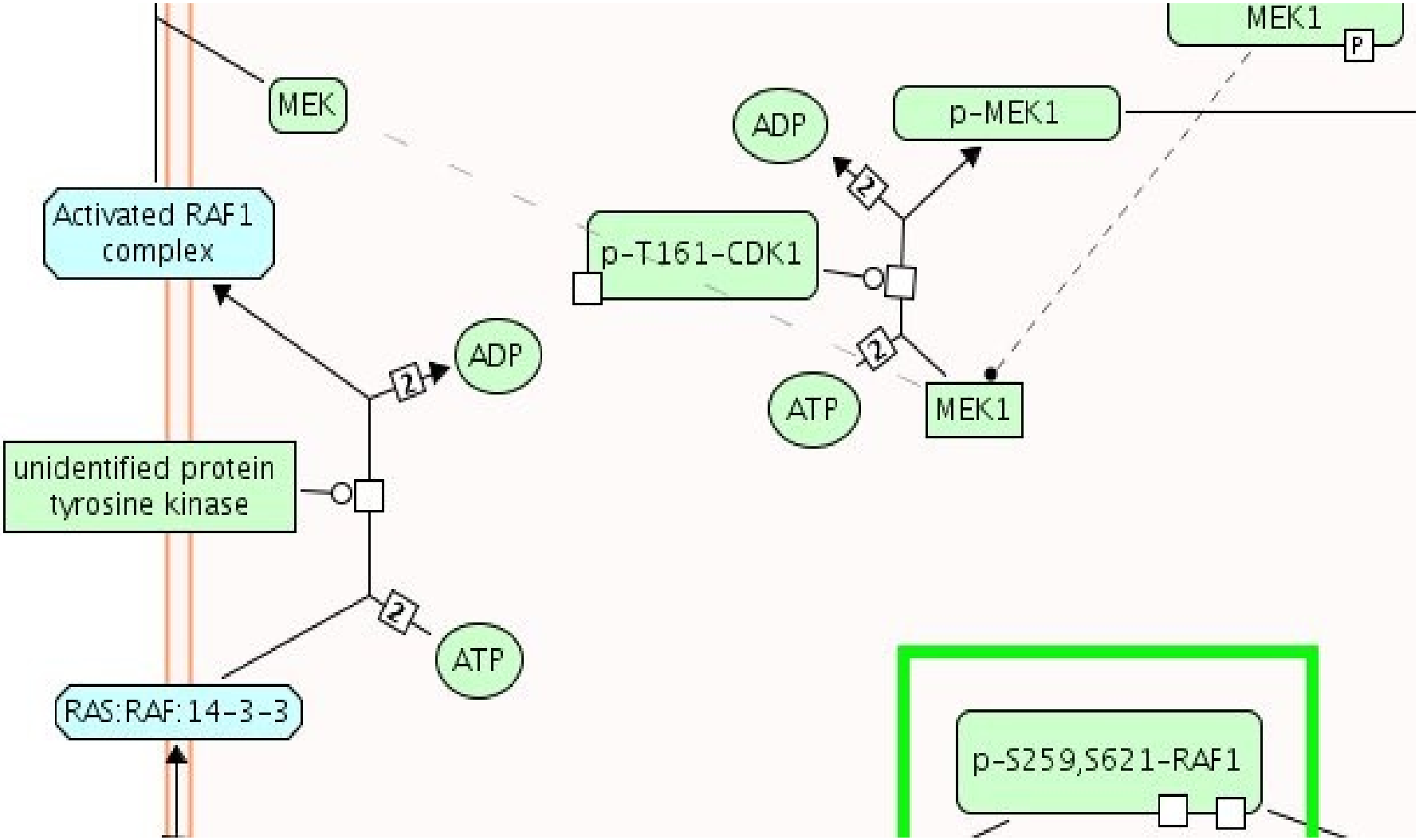


Reactome: RAF/MAP kinase cascade

www.reactome.org/cgi-bin/eventbrowser?ID=109869

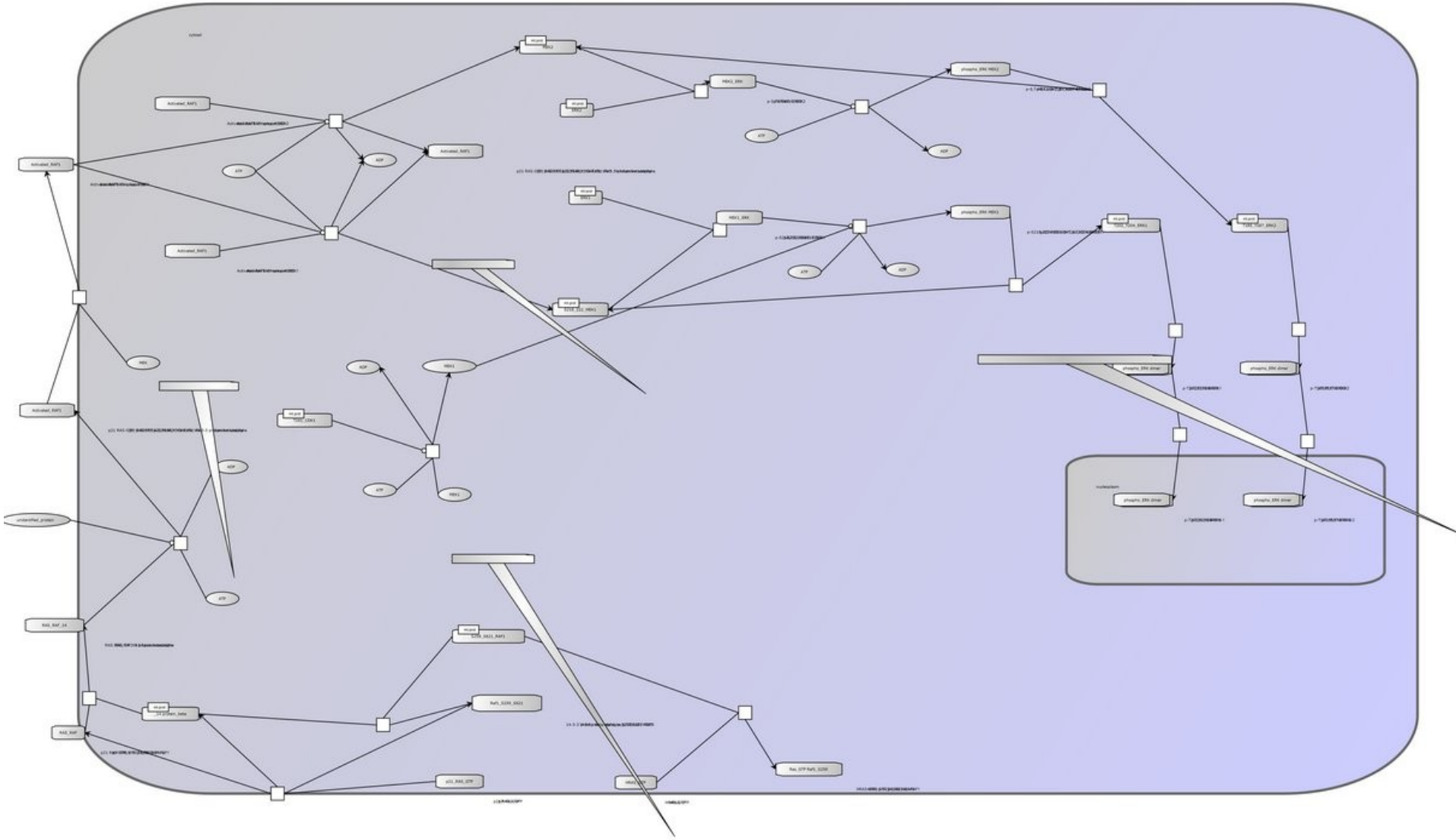


Reactome: closeup

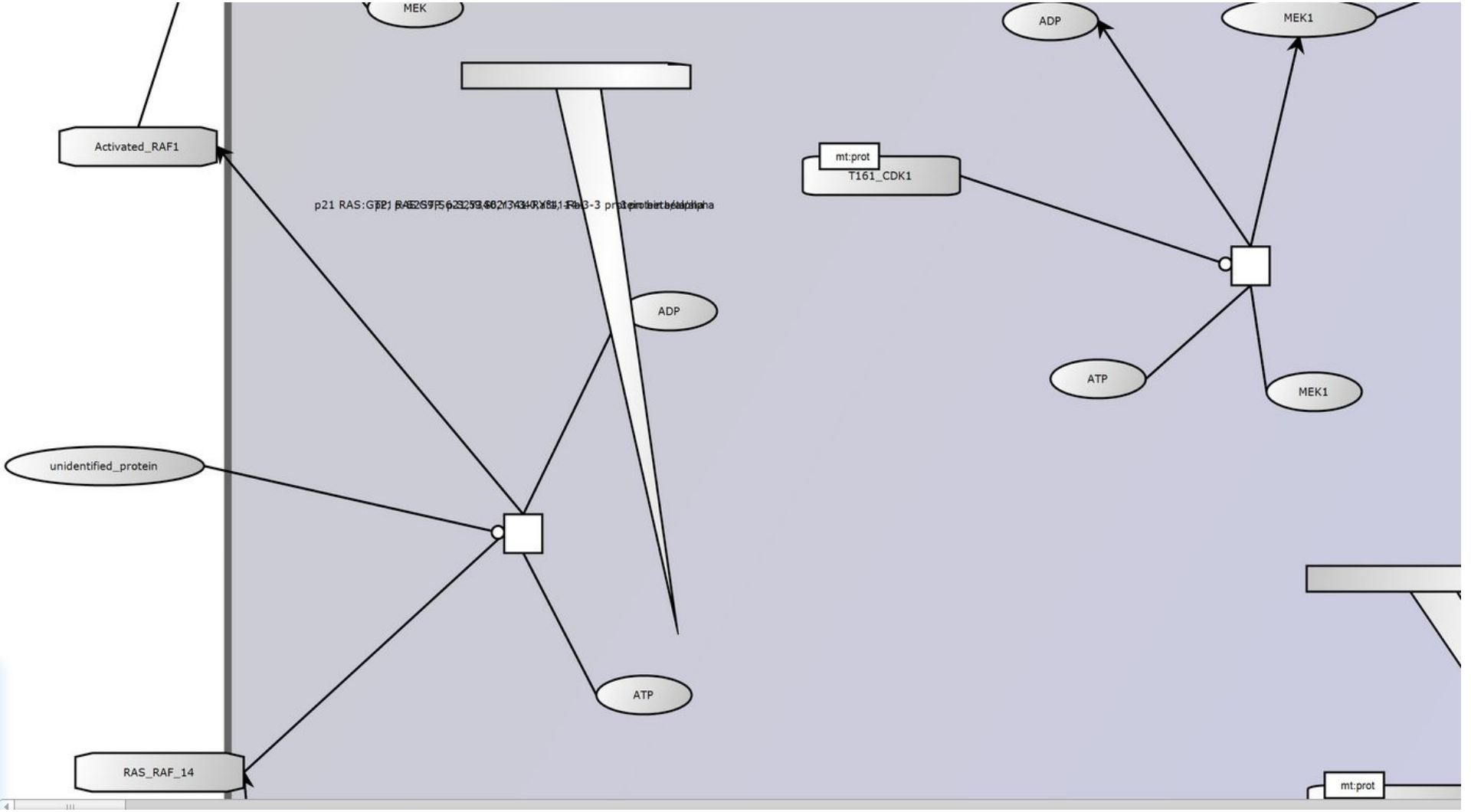


Render Comparison: RAF/MAP kinase cascade

sysbioapps.dyndns.org/RenderComparison/Home/UploadFile

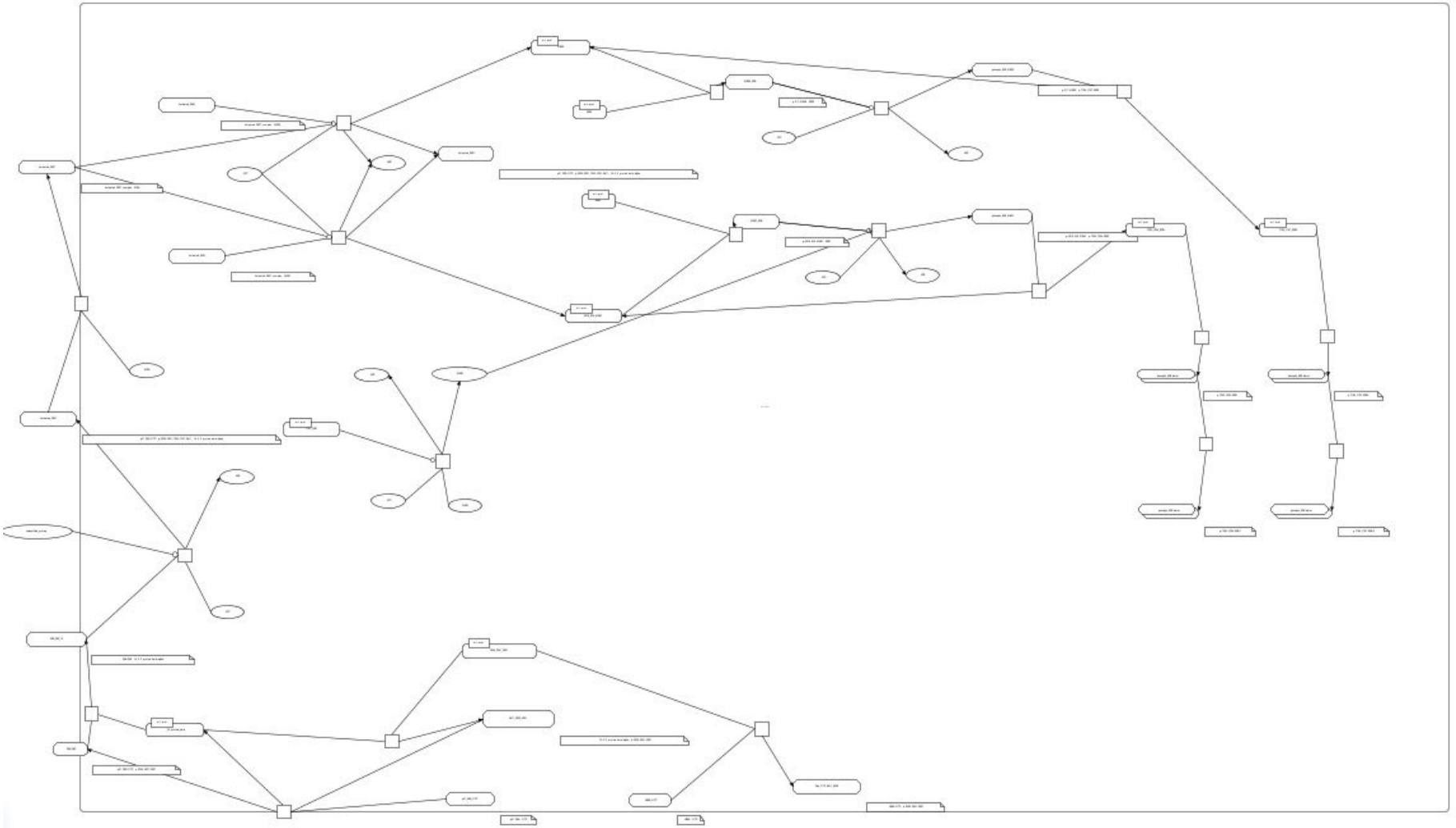


Render Comparison: closeup

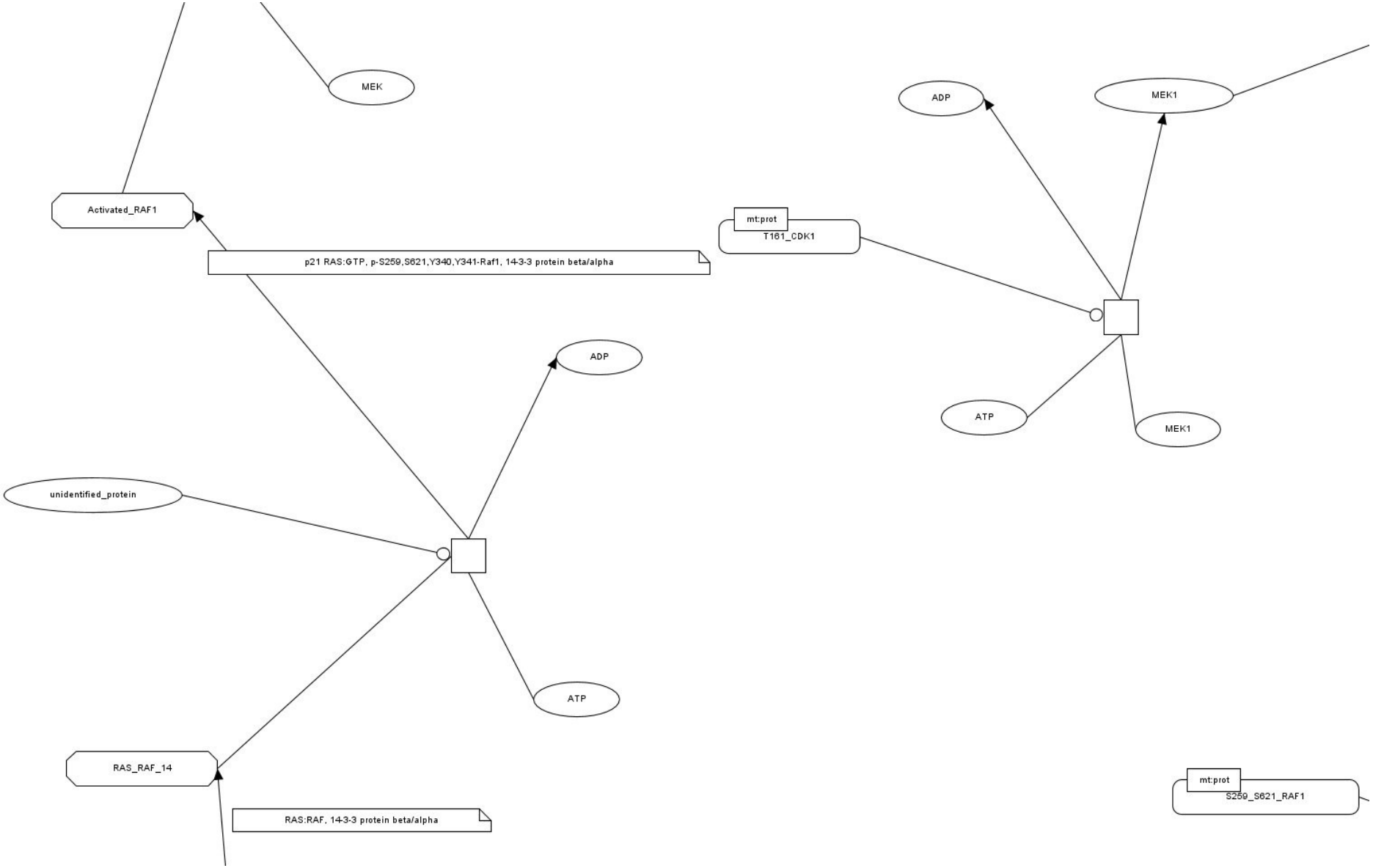


PathVisio: RAF/MAP kinase cascade

www.pathvisio.org/webstart/sbgn/SBGN.jnlp

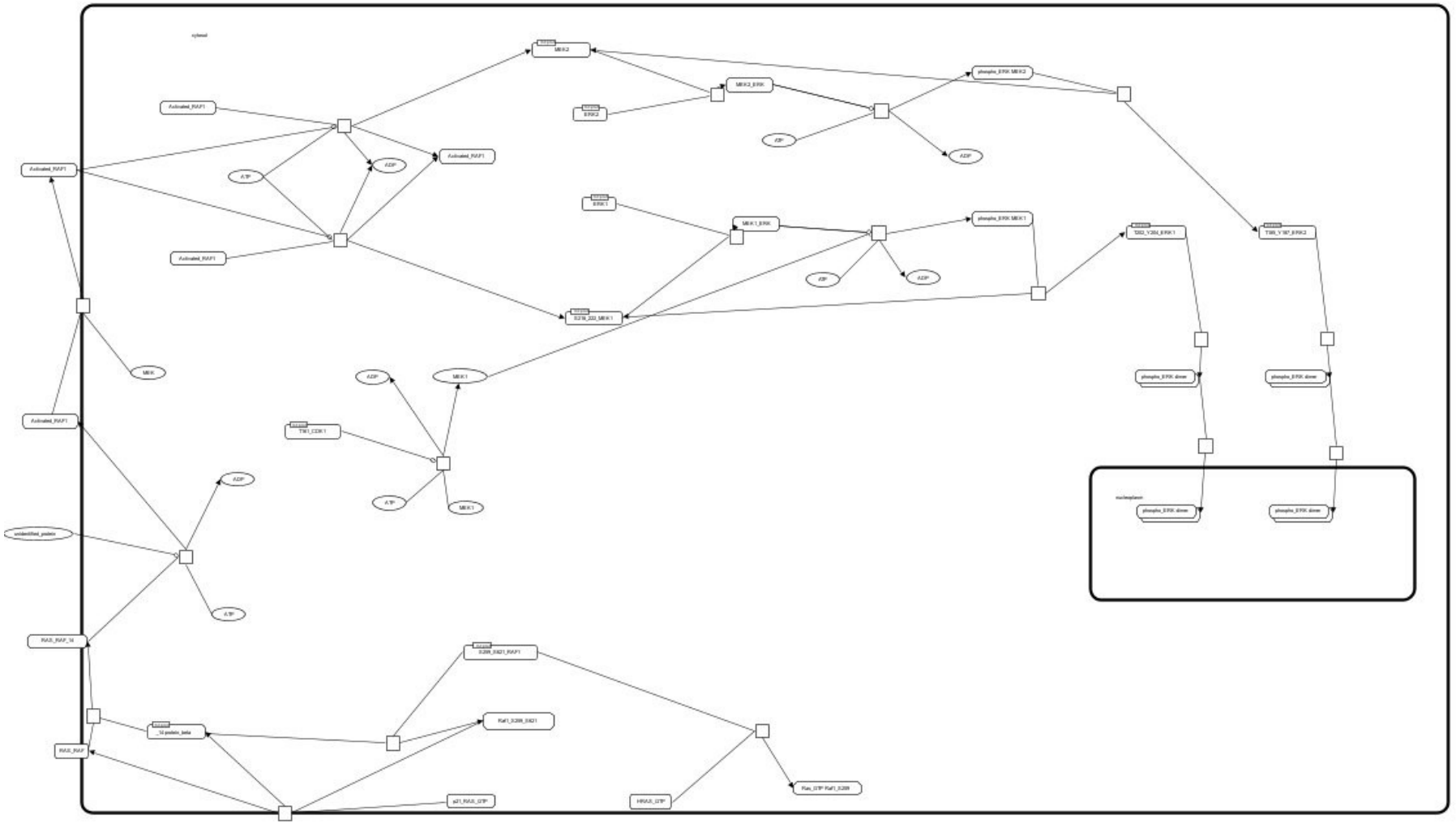


PathVisio: closeup



SBGN-ED: RAF/MAP kinase cascade

vanted.ipk-gatersleben.de/addons/sbgn-ed/



SBGN-ED: closeup