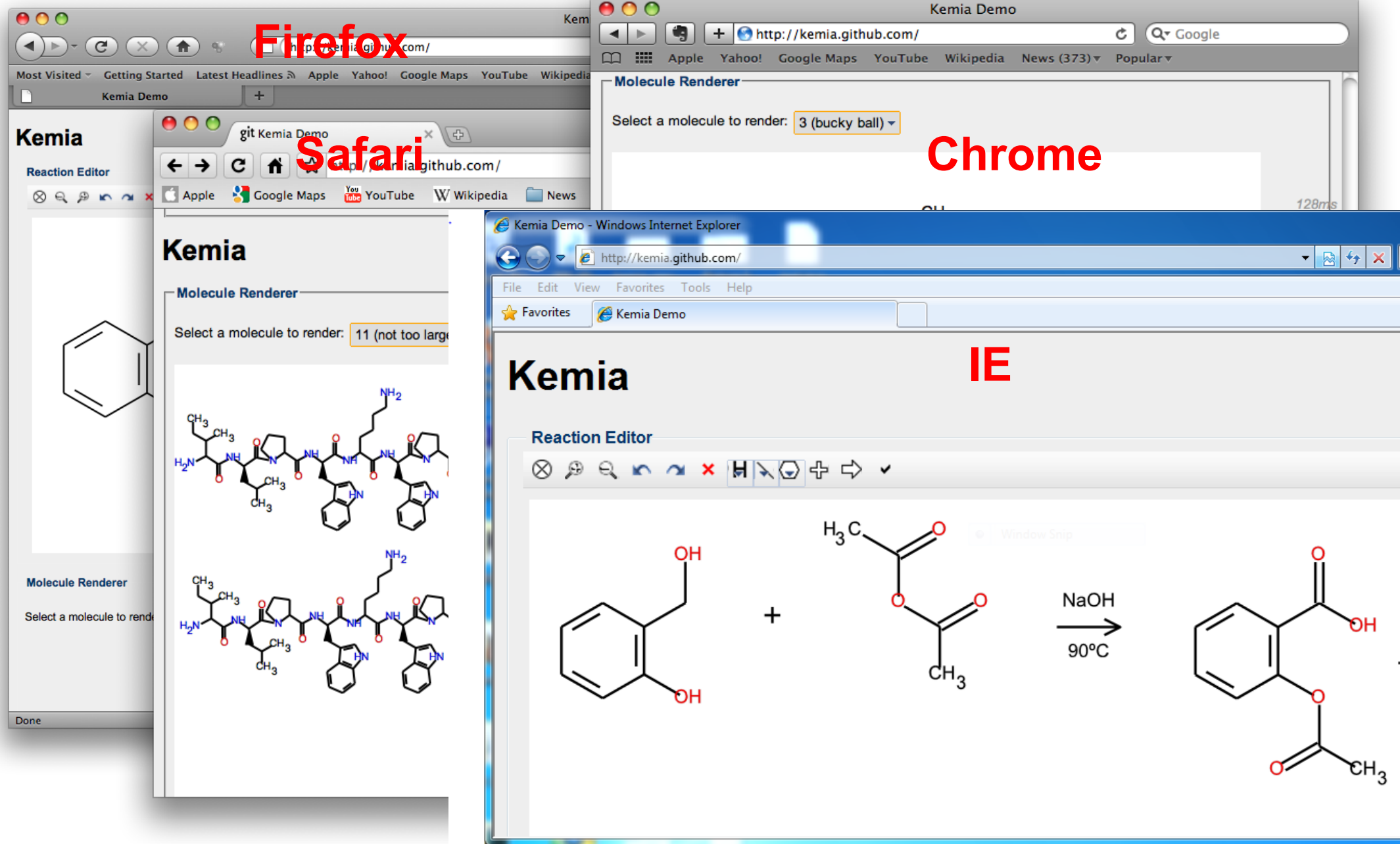


Kemia

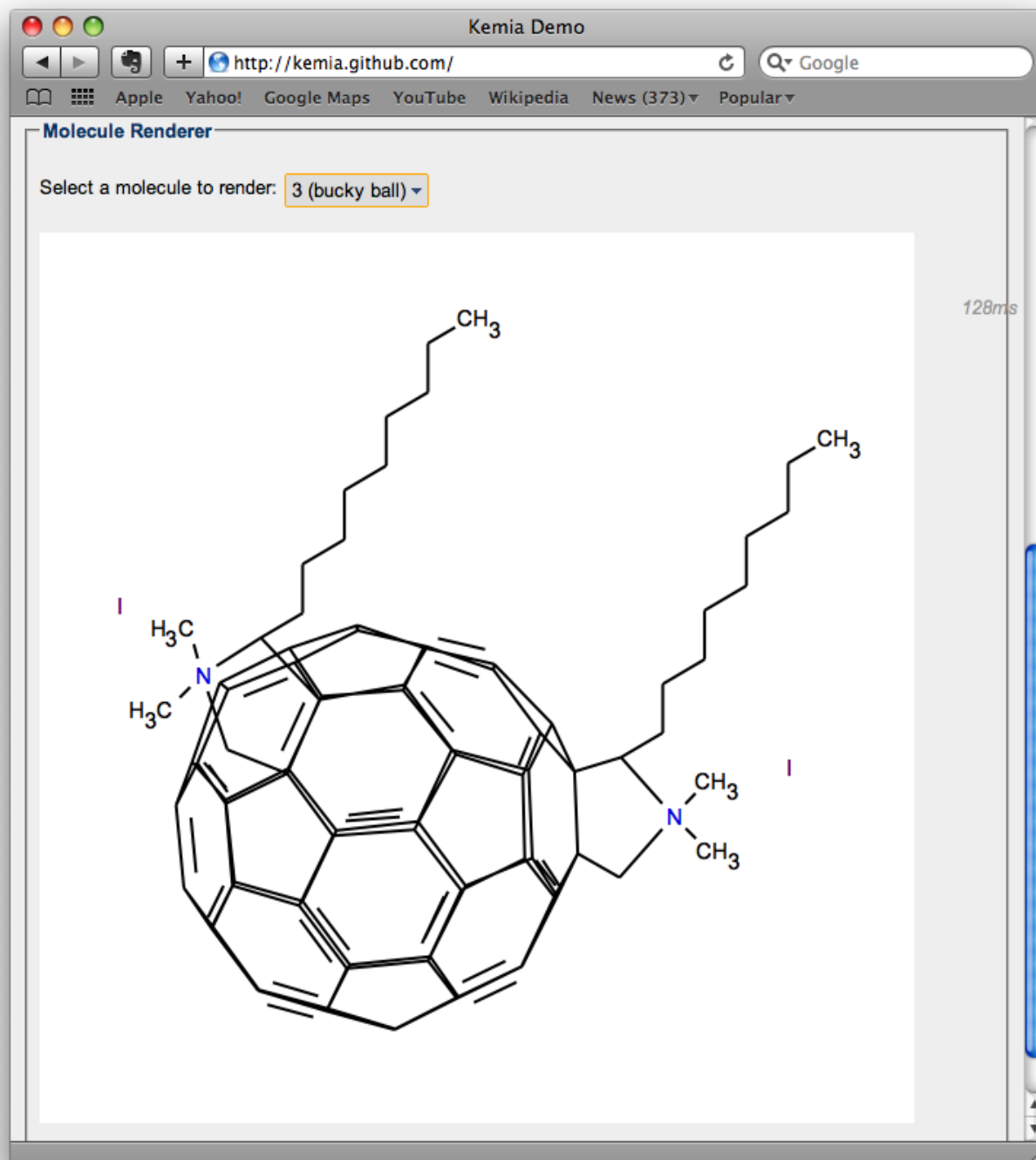
- 100% Javascript
- Cheminformatics Library
- Reaction Editor

<http://kemia.github.com>



works with popular browsers

<http://kemia.github.com>



Fast - buckyball from molfile in 128 ms

<http://kemia.github.com>

git Kemia Demo

http://kemia.github.com/

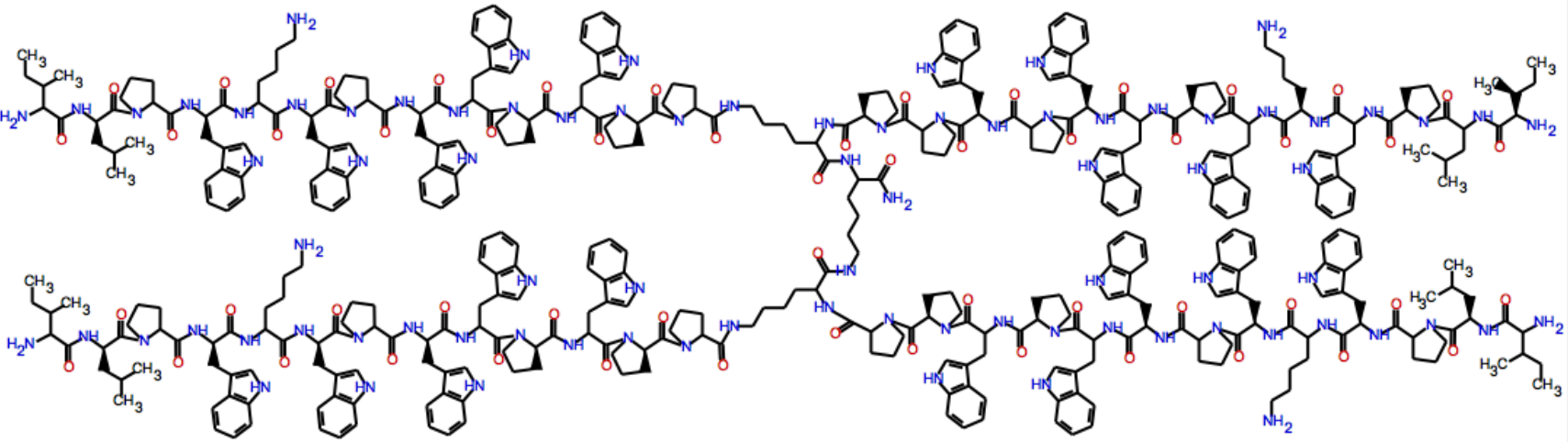
Apple Google Maps YouTube Wikipedia News Popular Closure Library API D Spring It! Other Bookmarks

Kemia

86ms

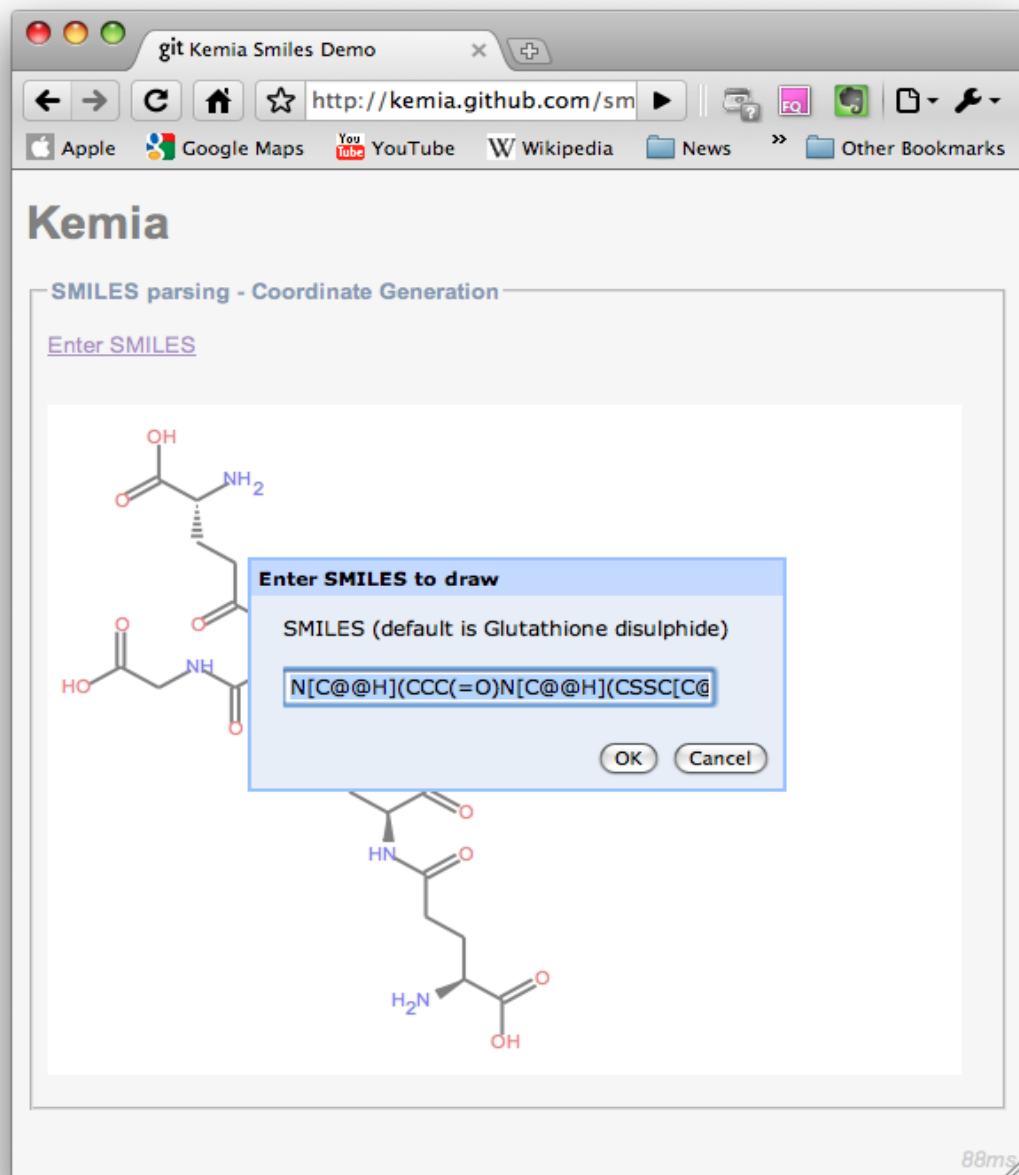
Molecule Renderer

Select a molecule to render: 11 (not too large now!) ▼



The image displays a web browser window with the address bar showing 'http://kemia.github.com/'. The page title is 'git Kemia Demo'. Below the address bar, there are several icons for social media and search engines. The main content area is titled 'Kemia' and features a 'Molecule Renderer' section. A dropdown menu in this section shows '11 (not too large now!)'. Below the dropdown, a large, complex chemical structure is rendered, consisting of multiple repeating units connected by amide bonds, with various side chains including pyrrolidine rings and indole-like structures. The structure is rendered in a 2D format with blue and black colors. The browser's status bar at the bottom shows '86ms'.

<http://kemia.github.com>



Parse SMILES and Generate Coordinates <http://kemia.github.com>

```

1 var mol_renderer;
2 function initPage() {
3     mol_renderer = new kemia.controller.ReactionEditor(goog.dom.getElement('kemia'));
4 }
5
6 var promptHandler = function(smiles) {
7     if (smiles != null) {
8         var timer = goog.now();
9         var mol = kemia.io.smiles.parse(smiles);
10        kemia.layout.CoordinateGenerator.generate(mol);
11        mol_renderer.setModels( [ mol ] );
12        goog.dom.setTextContent(goog.dom.getElement('perf'), (goog.now() - timer) + 'ms');
13    }
14
15    var prompt = new goog.ui.Prompt('Enter SMILES to draw',
16        'SMILES (default is Glutathione disulphide)', promptHandler);
17

```

Sample code for SMILES parsing, coordinate generation and rendering. This is entire script block for <http://kemia.github.com/smiles.html>

Contributors

Paul Novak
Wingu Inc.

Mark Rijnbeek
EBI

Tim Vandermeersch
University of Antwerp Belgium

TJ O'Donnell
gNova Inc.

Duan Lian
EBI