End-to-end Solution for Accessible Chemical Diagrams

Volker Sorge

Scientific Document Analysis Group
School of Computer Science
University of Birmingham

Progressive Accessibility Solutions
Birmingham, UK
progressiveaccess.com

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joint work with Mark G. Lee and Sandy Wilkinson

Motivation

- Accessibility to STEM material is important issue for inclusive education
- Diagrams are an important teaching means in STEM
- Chemical diagrams (depictions of molecules) are ubiquitous in teaching from GCSE and A-levels teaching to undergrad curriculum chemistry, biosciences, life sciences.

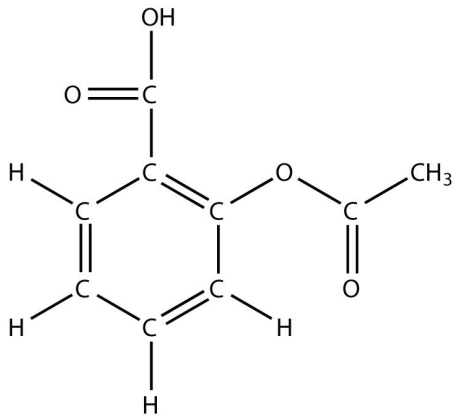
- Previous work on assistive technology for chemical diagrams
  - Require diagrams to be drawn in particular way or authoring environment
  - Need for specialist software to access and interact with diagrams
- Additional hurdles for both authors and readers

Goals

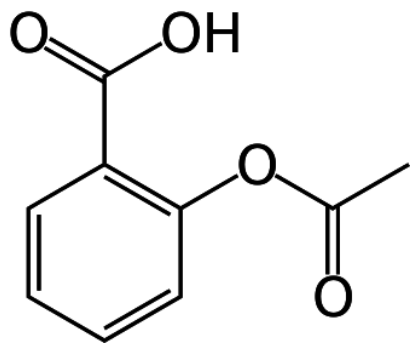
- Make regular teaching material accessible
- From inaccessible image to support for independent learning
- Source independence
  - Do not rely on the benevolent, educated author
- Platform independence
  - Use standard web technology (HTML5)
  - Accessible with all browsers, screen readers
- Provide a seamless user experience without/very little interface
- Support diverse material, for novices and experts alike

Examples

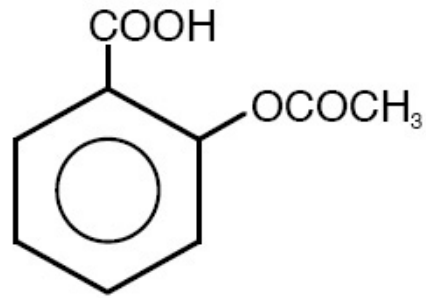
- Different representations of Aspirin molecule.



Displayed formula.



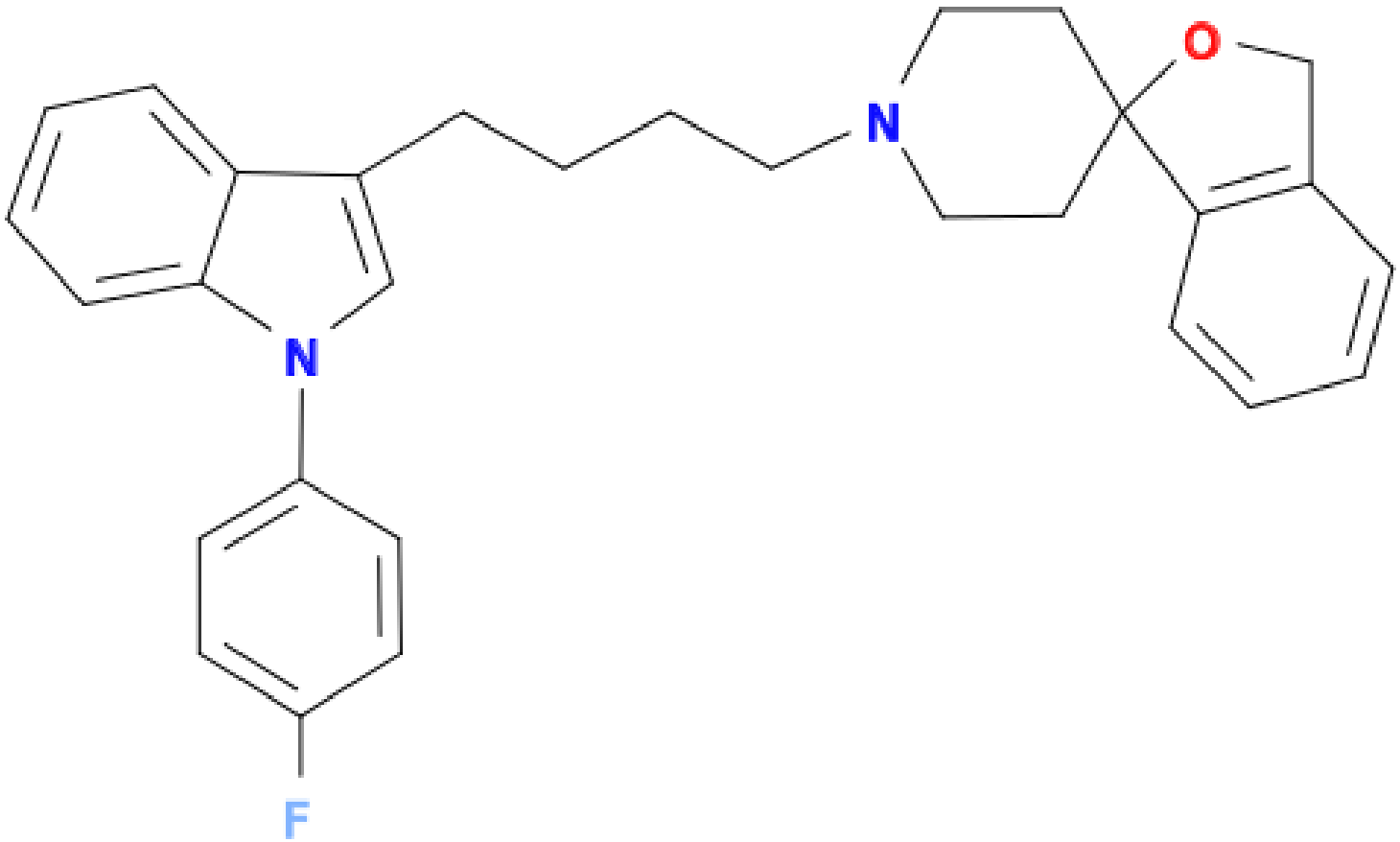
Skeletal formula.



Structural formula.

Examples

- Or somewhat more complex.



Procedure

Input: A bitmap image of a molecule diagram

1. Image analysis and recognition
2. Generation of annotated SVG
3. Semantic enrichment
4. Accessible diagram via browser front-end

Image Segmentation

MolRec system implemented for diagram recognition on patent databases

- Initial preprocessing: Binarisation, noise reduction...
- Connected component extraction and labelling
- Optical Character recognition and removal
- Separation of bond elements
  - Walk skeleton diagram structure
  - Identify and break junction points
- Result is a set of geometric primitives:
  Character groups, lines, circles, triangles

Diagram Recognition

- Rule based system
- Rewrites bag of geometric primitives into a graph representation
- Example:
  1. Let l_1, l_2 be distinct line segments of a minimum length.
  2. If l_1 is nearly parallel to and in a neighbourhood of l_2.
  3. No other line segment is nearly parallel to l_1 or l_2.

  $\Rightarrow$ Then (l_1, l_2) form a double bond.

single double triple wedge dashed wedge wavy

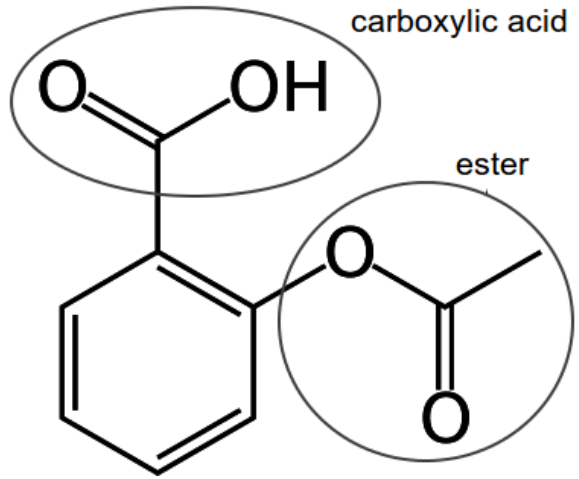
- Result is a Chemical Markup File (CML or MOL)

SVG Generation

- Many solutions for generating SVG from chemical markup
- But they only draw!
- And in the process destroy any structure or chemical knowledge
- Build our own SVG generator with emphasis on
  - Grouping meaningful units together (e.g., double bonds)
  - Retaining names given to components in the chemical markup (IDs of atoms, bonds, etc.)
- Result annotated and grouped SVG

Semantic Enrichment

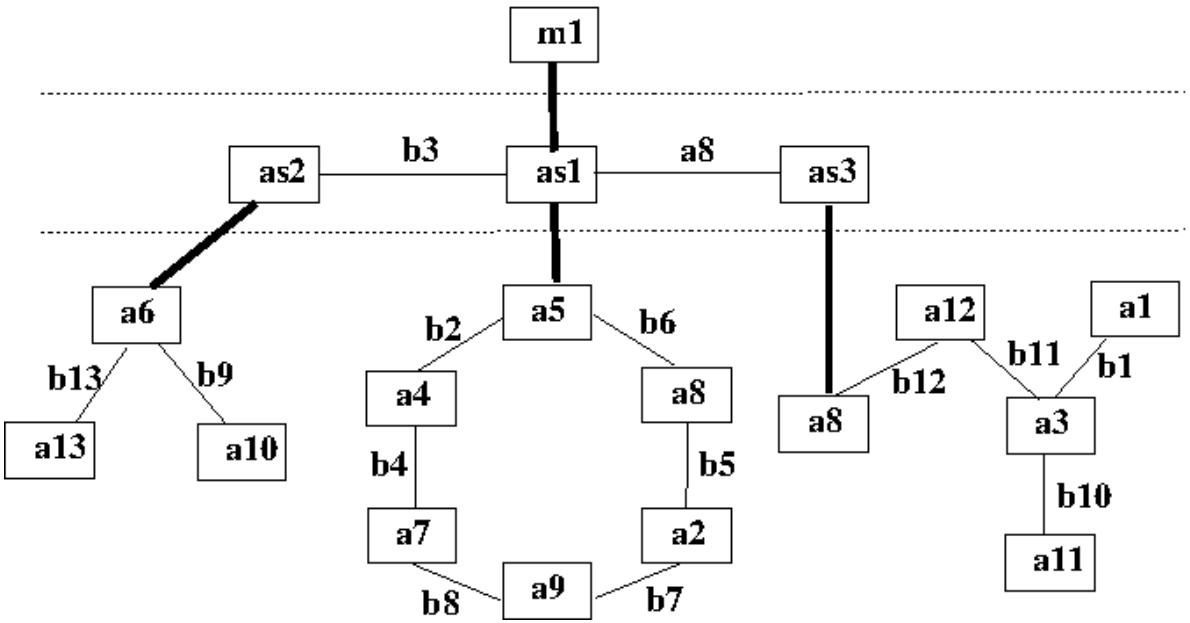
- Take basic chemical markup: Enrich it with derived knowledge and structure it accordingly
- Detect major building blocks of the molecule
  - Aliphatic chains
  - Ring systems: Isolated and fused
  - Functional groups



- Order blocks and atoms by chemical conventions
- Naming and description
  - Cactus webservice
  - Basic descriptions via atoms, bonds, substitutions

Abstraction Graph

- Represent molecule as multi-layered graph
- 3-4 layers of abstraction



- Molecule
- Block
- Atom

- Additional layer in case of fused ring systems
- Result semantically enriched CML File

Accessibility Support

- Graph structure can serve as the bases for interacting with the molecule
- Very simple navigation model: down/up, right/left
- Screen Reader Support:
  - Generate speech output from CML annotations on different levels
  - Display of speech output using subtitling
- Low Vision/Learning Disability Support:
  - Highlighting of inspected components
  - Optional zooming and magnification of components
  - Changing contrast, colour configurations

Browser Front-end

Generic browser front-end using standard web technology:

- Ajax service to import
  - annotated SVG
  - enriched CML as XML object
- Some JavaScript to tie it all together.
- WAI-ARIA and CSS to implement interactive exploration
  - Speech output by updating ARIA live regions
  - Zooming by changing SVG view port
  - Colour/contrast changes by rewriting CSS properties

User Feedback and Testing

Ongoing stake holder involvement throughout development

- input from blind chemist (Duncan Bell)
- explanations tested in regular classroom teaching
- "Phone-experiments" with chemistry researchers
- "Molimod testing" with students at various levels in specialist college (NCW)
- Low vision support testing with A-level students
- Testing with educators for visually impaired children.

Conclusions and Future Work

- End-to-end procedure from images to accessible diagrams
- Don't need to rely on author cooperation
- Integrates seamlessly without need for bespoke tools
- Demo of web front end tomorrow or `http://progressiveaccess.com/chemistry`

Next steps:

- Tactile diagrams, 3D printing, Localisation
- Other STEM subjects: Physics (circuit diagrams), Maths (geometry, bearings), Biology (phylogenetic trees), Computer Science (flow charts)

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