# Recommending an Optimal d3.js Visualization Method for Organic Chemistry Reaction Pathways

## 1. Introduction

### 1.1. Context and Significance

Organic chemistry, the science of molecular transformations, presents significant learning challenges due to the complexity and abstract nature of its core concepts, particularly reaction mechanisms and synthesis pathways.[1] Students frequently struggle to grasp the intricate sequences of reactions, the role of reagents, and the underlying principles governing molecular changes.[2] Effective visualization tools are therefore paramount in organic chemistry education and research. Visualizations serve as crucial bridges between abstract chemical models and tangible understanding, making concepts like reaction pathways—the interconversions between functional groups—more concrete [[1], [52]]. Well-designed visualizations can support cognitive processes such as reasoning [[1], facilitate the development of accurate mental models or schemas,, and potentially alleviate the high cognitive load often associated with learning this subject,, [53]]. Given the documented difficulties students face, including misconceptions about reaction pathways and mechanisms,, [[2]], [[50]], and challenges with visuospatial reasoning,, the need for optimized visualization strategies is clear.

### 1.2. Problem Statement

Representing the complex network of organic reactions, often depicted as "reaction maps", [12], poses a significant visualization challenge. Traditional methods or previously explored digital approaches have shown limitations. Standard flowcharts, while useful for depicting linear sequences [4], are often described as merely 'okish' for representing the highly interconnected and potentially cyclic nature of reaction networks.[6] Tree-based visualizations like sunburst diagrams, designed for hierarchical data [8], are perceived as 'messy' and inappropriate for the non-hierarchical structure of these chemical transformations,.[13] An effective visualization must not only display connections but also handle the inherent complexity of the network—including cycles, multiple pathways between functional groups, and associated reaction details (reagents, conditions)—in a way that fosters understanding rather than confusion, [[54]], [[18]].

### 1.3. Objective and Scope

This report provides an expert analysis and recommendation for the most suitable visualization method, implementable using the versatile d3.js JavaScript library [10], for

representing and understanding organic chemistry reaction pathways, specifically the interconversions between functional groups. The analysis involves:

1. Characterizing the structural properties of organic reaction pathway data as a network.
2. Critically evaluating the specific limitations of flowchart and sunburst diagram approaches in this context.
3. Systematically assessing a range of network visualization techniques available within d3.js against criteria relevant to chemical education and data clarity.
4. Justifying the recommended method(s) based on this comparative analysis, focusing on how they address the identified limitations.
5. Providing initial guidance on how key chemical entities (functional groups, reactions, reagents/conditions) can be represented using the recommended d3.js approach.

The scope is confined to visualization methods readily implementable with d3.js, targeting the representation of functional group interconversion networks common in introductory and intermediate organic chemistry.

### 1.4. Visualization and Cognitive Impact

The selection of an appropriate visualization technique extends beyond mere aesthetics or data representation; it directly influences cognitive processing and learning outcomes. An ill-suited visualization can inadvertently increase cognitive load,, [55], hindering the learner's ability to process information effectively within the limits of working memory, [1. Conversely, a well-designed visualization can support the construction of robust mental schemas—interconnected knowledge structures that are crucial for deep understanding in complex domains like organic chemistry, [1],, [56]. Organic chemistry heavily relies on understanding abstract representations and spatial relationships, [1,, areas where students often exhibit difficulties,, [3]. Therefore, the evaluation of visualization methods must prioritize cognitive ergonomics—how well the visualization supports the necessary mental operations without overwhelming the user—alongside the accurate depiction of the chemical network. The goal is to find a representation that not only shows the connections but actively facilitates the cognitive processes needed to understand those connections and build meaningful knowledge structures,.

## 2. Characterizing Organic Reaction Pathway Data

To select an appropriate visualization method, it is essential to first understand the structure and characteristics of the data representing organic reaction pathways. This

data can be conceptualized as a network graph.

### 2.1. Nodes: Chemical Entities

The nodes in this network represent distinct chemical entities. Primarily, these are functional groups (e.g., alkane, alkene, alcohol, ketone, carboxylic acid, amine) which define the chemical character and reactivity of organic molecules [[1], [5], [56]]. In some contexts, nodes might represent specific compound classes or even individual molecules, but for a general reaction map, functional groups provide a suitable level of abstraction.[12] Students' documented difficulties in identifying functional groups underscore the need for clear, unambiguous node representations. These functional groups can be thought of as the "cities" or key locations on a conceptual map of organic chemistry.[12]

### 2.2. Links (Edges): Chemical Reactions

The links or edges connecting these nodes represent the chemical reactions that interconvert one functional group into another [[1], [19]],.[12] These are the "roads" that link the functional group "cities".[12] Key characteristics of these links include:

- **Directionality:** Most organic reactions proceed in a specific direction under given conditions (e.g., oxidation of a primary alcohol yields an aldehyde, which can be further oxidized to a carboxylic acid). This inherent directionality necessitates the use of directed graph representations, where links have a defined source and target.[13]
- **Attributes:** Each reaction (link) is associated with crucial information beyond the simple connection. This includes the reaction name or type (e.g., hydrogenation, esterification, SN2 substitution), the necessary reagents (e.g., $H_2$, $KMnO_4$, NaOH), and specific reaction conditions (e.g., presence of a catalyst like $H_2SO_4$, application of heat (Δ), use of UV light, specific solvent),, [[1], [5], [49]]. Representing these attributes is vital for educational utility, as understanding *how* a transformation occurs is as important as knowing *that* it occurs. However, incorporating these details visually adds significant complexity.

### 2.3. Network Properties

The overall structure formed by these nodes and links exhibits several important properties:

- **High Interconnectivity:** The network is often densely connected. A single functional group can typically be converted to several others, and can often be formed from multiple precursors [[1]],,.[13] Some functional groups, like ketones or alkenes, act as central hubs with numerous connections, while others, like ethers,

might have fewer direct interconversion routes.[12]

- **Presence of Cycles:** Reaction sequences can form cycles, where a series of transformations returns to a previously encountered functional group or compound type.[13] For example, an alkene might be converted to an alcohol, then to an alkyl halide, which is then eliminated back to an alkene. Visualizations must be capable of clearly representing these cyclic pathways, a known weakness of standard flowcharts.[6] While force-directed layouts can display cyclic structures, specific algorithms might be needed for explicit cycle detection and highlighting.[13] Techniques like Sankey diagrams are generally designed for acyclic flows.[16]
- **Multiple Pathways:** Often, multiple distinct sequences of reactions exist to convert a starting functional group to a target functional group,, [5], [19]. For instance, an alcohol might be synthesized from an alkene via direct hydration or via hydroboration-oxidation, leading to different regiochemical outcomes.[17] A useful visualization should ideally allow users to identify, trace, and potentially compare these alternative routes.
- **Non-Hierarchical Structure:** Unlike organizational structures or file directories, the map of organic reactions does not possess a rigid, inherent hierarchy. While specific synthetic sequences are often taught linearly, the overall network of possibilities is fundamentally non-hierarchical, [13], [56]. Any functional group can potentially be reached from many others, and there isn't a single "root" or "top level". This non-hierarchical nature is a primary reason why tree-based visualizations like sunburst diagrams are fundamentally ill-suited for this type of data.[8]

### 2.4. Implications for Learning and Cognition

The characteristics of reaction pathway data directly relate to documented challenges in learning organic chemistry:

- **Complexity and Cognitive Load:** The sheer volume of reactions, reagents, and interconnections contributes significantly to the cognitive load experienced by students [1],,, [55], [1]. Many students resort to rote memorization, which is largely ineffective for developing true understanding or problem-solving skills.[2] An effective visualization should structure this complexity, perhaps facilitating cognitive strategies like "chunking"—grouping related information into manageable units [20]—by visually grouping related reactions or functional groups.
- **Schema Development:** Meaningful learning involves constructing mental schemas or well-organized knowledge structures, [1],,,, [56]. A good visualization should act as an external representation that mirrors and supports the

development of an accurate internal "reaction map", [12], [57]. The use of concept maps in chemistry education highlights the value of network-like representations for fostering connected understanding,, [1].
- **Addressing Student Difficulties:** Students commonly struggle with recalling specific reactions, understanding the underlying mechanisms (the "why" behind the transformation), applying concepts like stereochemistry or regiochemistry correctly, and planning multi-step syntheses,, [2], [5], [50], [19], [58], [59]. The visualization should ideally provide affordances to navigate these difficulties, such as allowing users to filter information, highlight specific pathways, view reaction details on demand, or even link to resources explaining mechanisms or concepts.

The "reaction map" metaphor [12] provides a useful conceptual starting point, but it's crucial to recognize its limitations. Unlike a geographical map where physical distance is a primary attribute, the "distance" between functional groups on a reaction map (i.e., the number of reaction steps) is often less critical than the *feasibility*, *selectivity*, and *conditions* required for each transformation,,. Students often struggle precisely because they focus on start and end points without grasping the nuances of the intermediate steps or the factors governing the reactions.[2] Therefore, the visualization must go beyond simply showing connectivity. It needs to represent a *knowledge graph* of potential transformations, providing mechanisms to access or display information about the nature of each link (reaction details) without implying that all paths are equally viable or easy. This distinguishes it from typical process flow diagrams where the focus is on a single, defined sequence of events.

## 3. Limitations of Flowcharts and Sunburst Diagrams

The user's observation that flowcharts are 'okish' and sunburst diagrams 'messy' for representing organic reaction pathways points to fundamental mismatches between these visualization types and the nature of the data.

### 3.1. Sunburst Diagrams

Sunburst diagrams are specifically designed to visualize hierarchical data, effectively showing how a whole is divided into parts across multiple concentric levels.[8] Each ring represents a level in the hierarchy, and the angular size of segments typically represents proportion or magnitude within that level.

However, organic reaction pathways, as established, constitute a network, not a strict hierarchy, [13], [56]. Attempting to force this interconnected, potentially cyclic network structure into a radial tree format inevitably leads to problems:

- **Structural Mismatch:** The core representation is inappropriate. There is no

natural root node or clear hierarchical progression for the entire set of functional group interconversions.
- **Redundancy and Clutter:** Representing network connections (where a node can have multiple parents or connections outside a strict lineage) within a tree structure often requires duplicating nodes or drawing complex, overlapping links, leading to the perceived "messiness".[8]
- **Inability to Represent Cycles:** Cycles, which are integral to understanding some reaction sequences, cannot be naturally represented in a tree structure.
- **Misleading Proportions:** While sunbursts excel at showing part-to-whole relationships [9], this is not the primary goal when visualizing reaction pathways. The focus is on connectivity and transformation possibilities, not the proportion of reactions belonging to a certain category.
- **Scalability Issues:** Clarity in sunburst diagrams often requires limiting the number of segments per ring [8], which conflicts with the potentially large number of functional groups and reactions in organic chemistry.

The fundamental incompatibility of the hierarchical model with the network structure of reaction pathways renders sunburst diagrams unsuitable for this application.

### 3.2. Flowcharts

Standard flowcharts are powerful tools for representing linear processes, sequential steps, and simple decision points.[4] They are widely used in various fields, including project management and programming, to document workflows.[4]

Their limitations become apparent when applied to complex, highly interconnected systems like organic reaction networks:

- **Handling Complexity:** Flowcharts struggle to clearly represent processes with numerous interconnections, multiple parallel paths, and feedback loops (cycles).[6] Attempting to map the entire network of functional group interconversions often results in a sprawling, visually cluttered diagram with excessive crossing lines, making it difficult to follow and understand the overall structure.[6]
- **Focus on Single Paths:** Flowcharts are inherently better suited for depicting a *single*, specific pathway (e.g., a planned synthesis route or a specific mechanism) rather than the *entire map* of potential transformations.[4] While students might be encouraged to draw flowcharts for specific problems [5], this doesn't address the need for a comprehensive overview visualization.
- **Practical Constraints:** Keeping flowcharts confined to a single page for readability is a common guideline [6], which is often impossible for complex reaction networks. Furthermore, alterations or additions to the network typically

require significant redrawing of the flowchart.[7]

While flowcharts have their place for illustrating specific linear sequences, their inherent limitations in handling network complexity, cycles, and multiple pathways explain why they are only considered 'okish' for representing the broader landscape of organic reaction pathways.

The inadequacy of both sunburst diagrams and flowcharts stems from this fundamental mismatch between their underlying representational models (hierarchy and linear flow, respectively) and the inherent network structure of the data. This strongly suggests that a successful visualization must be based on a network paradigm. The specific user feedback ("messy," "okish") further implies that the chosen network visualization must effectively address challenges of clarity, scalability, and the representation of complex topological features like cycles and multiple paths, while also providing a means to incorporate associated reaction details without causing excessive visual clutter or cognitive overload.

## 4. Evaluation of d3.js Network Visualization Techniques

Given the limitations of sunburst and flowchart methods, the solution lies in network visualization techniques. The d3.js library offers several powerful options for implementing such visualizations.[10] We evaluate candidate techniques based on their suitability for representing organic reaction pathways, considering the criteria outlined previously.

### 4.1. Candidate d3.js Methods

- **(a) Force-Directed Graphs (Node-Link Diagrams):** These visualizations use a physics-based simulation (d3-force) where nodes repel each other and links act as springs, settling into a layout that reflects the network's structure.[23] They are highly flexible and widely used for general network exploration.[25]
- **(b) Sankey Diagrams:** Implemented using the d3-sankey module, these diagrams excel at showing the flow of quantities between nodes, typically arranged in distinct stages or columns.[23] The width of the links is proportional to the flow volume.[16] They are primarily designed for directed, acyclic graphs.[16] Customizations exist for highlighting specific flows.[32]
- **(c) Arc Diagrams:** Nodes are positioned along a single linear axis (horizontal or vertical), and links are represented by arcs connecting them.[23] The visual appearance is highly dependent on the node order.[34] Implementation uses standard SVG path elements, calculating arc coordinates manually or with helper functions [34] (note: d3.arc is for pie/donut chart segments [36]).

- **(d) Adjacency Matrices:** This technique represents the network as a grid, where a colored or sized cell at position (i, j) indicates a connection (link) between node i and node j.[29] They are effective for dense graphs and quickly checking direct connections [38], but path tracing is notoriously difficult.[37] Implementation in d3 involves drawing SVG rectangles or using Canvas.
- **(e) Chord Diagrams:** Using the d3-chord module, nodes are arranged circularly, and relationships or flows are shown as ribbons connecting pairs of nodes.[23] Ribbon width can represent the strength or volume of the connection.[42] They are particularly suited for visualizing relationships within a closed system.
- **(f) Hierarchical Edge Bundling (HEB):** This method requires both network links and an underlying hierarchy for the nodes.[44] Nodes are arranged according to the hierarchy (often radially using d3.cluster), and edges are bundled along the hierarchical paths using curved lines (e.g., d3.curveBundle) to reduce visual clutter.[44]
- **(g) Directed Graphs (with Cycles):** This is not a distinct layout method but a characteristic applicable to others, especially force-directed graphs. It involves adding visual cues for direction (like arrowheads) and using a layout algorithm that can handle cyclic structures.[14] d3-force inherently handles cycles without issue.[15]

### 4.2. Comparative Analysis

We compare these techniques based on the specific requirements for visualizing organic reaction pathways:

| Feature | Force-Directed Graph | Sankey Diagram | Arc Diagram | Adjacency Matrix | Chord Diagram | Hierarchical Edge Bundling |
|---|---|---|---|---|---|---|
| **Key Characteristic** | Physics-based node placement | Flow volume visualization | Linear node layout, arc links | Grid-based connection matrix | Circular layout, ribbon links | Hierarchical layout, bundled edges |
| **Clarity of Connections** | Good for topology, potential clutter [29] | Clear flow paths, less clear topology [47] | No edge crossing, order-dependent [34] | Excellent direct adjacency, poor paths [38] | Good for pairwise, clutter possible [41] | Reduces clutter via hierarchy [46] |

| | | | | | | |
|---|---|---|---|---|---|---|
| **Reaction Detail Rep.** | Interaction (tooltip, labels) [26] | Link width (quantity), interaction [31] | Interaction (tooltip, labels) | Cell color/size, interaction | Ribbon width/color, interaction [41] | Interaction (tooltip, labels) |
| **Overall Network View** | Intuitive structure, clusters [29] | Major flows, stages [30] | Order-dependent patterns [34] | Dense clusters (if ordered), poor paths [37] | Pairwise relationships [40] | High-level patterns via hierarchy [46] |
| **Cycle/Multi-Path Handling** | Handles naturally [15] | Acyclic preferred [16], cycles difficult | Can represent, tracing complex | Requires inference/tracing [39] | Implied cycles, poor path tracing | Can represent, may obscure cycles |
| **Pros for Pathways** | Flexible topology, intuitive structure, handles cycles/paths | Good for yields/fluxes (if primary goal) | Highlights order-based relations | Fast check for direct reaction | Shows mutual interconversions | Reduces clutter in large systems |
| **Cons for Pathways** | Potential clutter, details need interaction | Poor for cycles, less topological insight | Order dependency, arc clutter | Poor path finding, scales poorly for sparse | Poor path finding, clutter risk | Requires meaningful hierarchy |
| **d3 Module(s)** | d3-force [24] | d3-sankey [16] | SVG paths, d3-scale [34] | SVG rects/Canvas | d3-chord [40] | d3-hierarchy, d3-shape [44] |

### 4.3. Synthesis of Evaluation

The comparison reveals distinct trade-offs. Force-directed graphs offer the most natural fit for the general network topology, including cycles and multiple paths. However, their tendency towards visual clutter, especially for dense networks, necessitates interactive features to manage complexity and display reaction details effectively.[29] Sankey diagrams excel at quantitative flow but struggle with cyclic

structures and providing a clear topological overview.[16] Arc diagrams avoid edge crossings but introduce a strong dependency on node order, which may not have inherent meaning for the entire reaction network.[34] Adjacency matrices are poor for the crucial task of understanding reaction *pathways* (sequences).[37] Chord diagrams focus on pairwise relationships, less suited for exploring longer synthetic routes.[41] Hierarchical edge bundling requires imposing a hierarchy, which might be artificial for the overall reaction map, although potentially useful if visualizing reactions within a specific hierarchical classification of compounds.[44]

No single static visualization perfectly captures all aspects—topology, directionality, cycles, multiple paths, and detailed reaction attributes—without compromise. The need to represent detailed information like reagents and conditions, combined with the potential for network complexity, strongly suggests that an interactive approach is superior to a static one. Interactivity allows for progressive disclosure of information, helping to manage cognitive load, [[1] by showing the overall structure first and revealing details only when requested by the user (e.g., via tooltips or highlighting).[26]

## 5. Recommendation and Justification

Based on the analysis of organic reaction pathway data characteristics and the comparative evaluation of d3.js visualization techniques, a primary recommendation emerges.

### 5.1. Primary Recommendation: Force-Directed Graph

The most suitable visualization method implementable in d3.js for representing the general network of organic chemistry reaction pathways is the **Force-Directed Graph (Node-Link Diagram)**, utilizing the d3-force module.[24]

### 5.2. Justification

This recommendation is based on the following key points:

- **Structural Congruence:** Force-directed graphs inherently model network structures. They can naturally represent the high interconnectivity, multiple pathways between functional groups, and critically, the cyclic nature of reaction sequences that are characteristic of organic chemistry.[13] This directly addresses the fundamental structural limitations of the previously considered hierarchical (Sunburst) and linear (Flowchart) methods.[6]
- **Intuitive Topological Representation:** This method provides a visually intuitive overview of the reaction landscape.[29] Users can readily perceive the relationships between functional groups (nodes), identify central or peripheral groups,

recognize clusters of related reactions, and gain a qualitative sense of the overall network connectivity. This aids in building a mental map or schema of reaction possibilities.[12]

- **Flexibility and Customization (d3.js):** d3-force and associated SVG/Canvas rendering offer extensive customization.[48] Nodes can be styled (color, size, shape) to represent functional group categories or properties. Links can be styled (color, thickness, dash patterns) to indicate reaction types, qualitative yields, or specific conditions. Crucially, directionality can be explicitly shown by adding arrowheads to links, essential for understanding reaction flow.[15]
- **Superiority over Alternatives for Pathway Exploration:**
  - It overcomes the acyclic limitation of Sankey diagrams [16] and their focus on flow quantity over network structure.
  - It avoids the arbitrary node ordering dependency of Arc diagrams.[34]
  - It directly visualizes paths, unlike Adjacency Matrices where path tracing is difficult.[37]
  - It is better suited for exploring multi-step pathways than Chord diagrams, which emphasize pairwise connections.[41]
  - It does not require an artificial hierarchy like Hierarchical Edge Bundling.[44]
- **Amenability to Interaction:** Force-directed graphs are exceptionally well-suited for interactive exploration, which is crucial for managing the complexity inherent in reaction networks and mitigating cognitive load, [[60]]. Key interactions include:
  - *Dragging nodes* to manually adjust the layout and untangle specific areas.[26]
  - *Zooming and panning* to navigate large networks effectively.[26]
  - *Hover effects* to display detailed information (reagents, conditions, structures) in tooltips [26] or to highlight connected nodes and pathways.[28]
  - *Filtering mechanisms* to selectively display subsets of the network (e.g., only oxidation reactions, only pathways involving alcohols), reducing clutter and focusing user attention.

### 5.3. Secondary Recommendation (Conditional)

If the *primary* objective is to visualize and compare quantitative aspects of pathways, such as reaction yields, rates, or mass flow through different routes, and the network can be meaningfully represented in stages, then a **Sankey Diagram** [30] could be a valuable supplementary tool. Its ability to represent flow magnitude through link width is its main strength.[16] However, due to its limitations in representing cycles [16] and complex network topology, it is generally unsuitable as the sole or primary visualization for exploring the overall reaction map.

### 5.4. Beyond Layout: The Importance of Interaction

It is crucial to understand that recommending the force-directed layout is only part of the solution. The inherent potential for visual clutter in complex networks [29] means that a static force-directed graph can still be overwhelming and cognitively demanding. Therefore, the true recommendation is for an *interactive system* built upon the d3-force layout. This system must incorporate thoughtful interaction design principles. Features like on-demand detail display (tooltips), highlighting, filtering, and zooming act as forms of cognitive scaffolding,, allowing users to progressively explore the network's complexity at their own pace. This aligns with effective pedagogical strategies that support learners in managing complex information and building understanding incrementally,, [[61]]. The visualization thus transforms from a static map into an interactive learning environment, better equipped to address the cognitive challenges of mastering organic reaction pathways.

## 6. Representing Reaction Pathways in d3.js using a Force-Directed Graph

Implementing the recommended force-directed graph visualization in d3.js involves mapping chemical entities to visual elements and incorporating interactivity for detail and exploration.

### 6.1. Mapping Chemical Entities to Visual Elements

- **Nodes (Functional Groups):**
  - *Representation:* Use standard SVG elements like <circle> or <rect> bound to the node data.[25] Each node object in the data array should have properties like id (e.g., "Alkene", "Ketone") and potentially group (e.g., "Hydrocarbon", "OxygenContaining").[28]
  - *Styling:* Apply styles based on data attributes. fill color can map to the functional group category (e.g., using d3.scaleOrdinal with a color scheme like d3.schemeCategory10 [34]). Node size (r for circles) could be uniform for simplicity or potentially scaled based on a property like frequency or complexity, though this might add clutter.
  - *Labels:* Add SVG <text> elements for each node, displaying the id (functional group name).[27] Careful label placement is critical to avoid overlap. Options include placing labels adjacent to nodes, using force-based label adjustment algorithms (more complex), or showing labels only on hover.
- **Links (Reactions):**
  - *Representation:* Use SVG <line> elements for simple connections or <path> elements if more complex styling (like curves) is desired.[25] Link data objects should specify source and target node IDs, matching the id field of the

nodes.[25]
    - *Styling:* Style links based on reaction properties. stroke color could represent the general reaction type (e.g., red for oxidation, blue for reduction, green for addition [5]). stroke-width can be uniform or perhaps subtly varied to indicate qualitative yield or importance. stroke-dasharray (e.g., "5,5") can indicate specific conditions like photochemical reactions or equilibrium.
    - *Directionality:* Implement arrowheads to show reaction direction. This involves defining an SVG <marker> element (containing a <path> for the arrowhead shape) within a <defs> section and applying it to the marker-end style attribute of the link lines/paths. Examples and discussions on adding arrows to d3 force layouts can be found online.[15]

### 6.2. Incorporating Details via Interactivity

Given the density of information associated with each reaction, relying on interactivity is key to maintaining clarity and managing cognitive load, [62].

- **Tooltips:** Implement hover interactions (.on("mouseover",...) and .on("mouseout",...) [26]).
    - *On Link Hover:* Display a tooltip (e.g., a  positioned near the mouse [26]) showing the specific reaction name (e.g., "Hydroboration-Oxidation"), required reagents (e.g., "1. $BH_3$/THF, 2. $H_2O_2$, NaOH"), conditions (e.g., "Anti-Markovnikov"), and potentially a link to more detailed mechanistic information or literature references.
    - *On Node Hover:* Display the chemical structure of the functional group or representative example molecules.
- **Highlighting:** Use hover events to dynamically change element styles.[28]
    - *On Node Hover:* Increase the stroke width or change the color of the hovered node. Dim or fade non-connected nodes and links. Highlight directly connected nodes and the links connecting them (e.g., by increasing opacity or changing color).
    - *On Link Hover:* Highlight the link itself and its source and target nodes. This helps users visually trace connections within potentially complex layouts.
- **Filtering and Fading:** Provide UI controls (e.g., checkboxes, dropdowns) to allow users to filter the displayed network. For example, users could choose to see only reactions involving alcohols, or only addition reactions. Elements not matching the filter criteria can be hidden (display: none) or faded (reduced opacity). This allows users to focus on specific subsets of the reaction network, reducing extraneous cognitive load. The concept is similar to faded worked examples where complexity is gradually introduced,.

- **Zooming and Panning:** Implement zoom and pan functionality using d3.zoom() applied to the main SVG container or a containing <g> element.[26] This is essential for navigating networks that may be too large to view clearly all at once.
- **Path Exploration (Advanced):** For enhanced analysis, consider implementing functionality where a user selects a starting and ending functional group, and the visualization highlights one or more possible reaction pathways between them. This would require integrating graph traversal algorithms (like Breadth-First Search or Depth-First Search) with the d3 visualization.

Designing these interactive elements should be guided by the goal of reducing cognitive burden while providing necessary information. Displaying all reaction details statically would overwhelm working memory, [63]. By using tooltips and highlighting, information is revealed progressively, allowing users to first grasp the overall structure and then delve into specifics as needed. This approach supports schema construction by allowing learners to build connections incrementally, [1], aligning the technical implementation with sound cognitive and pedagogical principles [1, [1].

## 7. Conclusion

### 7.1. Summary of Findings

The analysis confirms that organic chemistry reaction pathways constitute complex, non-hierarchical, and often cyclic networks. Traditional visualization methods like flowcharts and sunburst diagrams are ill-suited for capturing this structure, leading to representations that are either overly simplistic ('okish') or structurally inappropriate and cluttered ('messy'). Among the network visualization techniques available in the d3.js library, the **Force-Directed Graph (Node-Link Diagram)** emerges as the most suitable foundational approach. Its inherent ability to model network topology, represent cycles and multiple pathways naturally, and its flexibility for customization make it superior to alternatives like Sankey, Arc, Chord, or Adjacency Matrix visualizations for the primary goal of understanding the overall reaction landscape.

### 7.2. The Crucial Role of Interactivity

However, the effectiveness of the force-directed graph approach is critically dependent on the implementation of **thoughtful interactive features**. Due to the potential complexity and information density of comprehensive reaction networks, static representations risk overwhelming users and increasing cognitive load. Interactivity—including tooltips for on-demand detail display, highlighting for tracing connections, filtering mechanisms for managing complexity, and zooming/panning for navigation—is essential. These features transform the visualization from a potentially

cluttered static map into a dynamic and explorable learning environment, allowing users to manage information complexity and focus on specific aspects of the network as needed.

### 7.3. Implications for Teaching and Learning

A well-designed interactive force-directed graph visualization of organic reaction pathways, built with d3.js, holds significant potential to enhance organic chemistry education. By providing a clear, explorable representation of functional group interconversions, it can help students move beyond rote memorization of isolated reactions.[2] It can foster the development of a more integrated understanding—a robust mental schema, [1], [56]—of the relationships between different chemical entities and transformations. Such a tool can support higher-order thinking skills required for understanding reaction mechanisms and planning multi-step syntheses, [1, [18], addressing known areas of student difficulty.[2] It provides a powerful digital realization of the "reaction map" concept central to the discipline.[12]

### 7.4. Future Directions

Potential future enhancements could include integrating quantitative data more explicitly (e.g., scaling node size by compound class prevalence, or link thickness/color by typical reaction yield), linking nodes or edges directly to external chemical databases (like ORD [13]) or detailed mechanism animations, incorporating predictive models [51], or implementing graph algorithms to automatically identify shortest or most efficient synthesis pathways. These extensions could further bridge the gap between educational visualization and tools for chemical research and computer-aided synthesis planning, [13], [64].

Ultimately, the development of such a visualization tool is more than a technical implementation of d3.js; it represents an opportunity to apply principles from chemical education research,, [65], [22] and cognitive science,,, to create a pedagogically sound instrument. By carefully considering how students learn, the difficulties they encounter, and the cognitive processes involved in understanding complex chemical networks, we can design visualizations that truly facilitate mastery of organic chemistry.

### Works cited

1. (PDF) Exploring the Needs for the Development of Organic Reaction Teaching Model: Experts' Collective Opinion - ResearchGate, accessed April 11, 2025, https://www.researchgate.net/publication/350736782_Exploring_the_Needs_for_the_Development_of_Organic_Reaction_Teaching_Model_Experts'_Collective_Opi

nion
2. www.ijese.com, accessed April 11, 2025, https://www.ijese.com/download/examining-some-of-the-challenges-students-face-in-learning-about-rearrangement-reactions-in-organic-13203.pdf
3. Priority and Selectivity Rules To Help Students Predict Organic Reaction Mechanisms | Journal of Chemical Education - ACS Publications, accessed April 11, 2025, https://pubs.acs.org/doi/10.1021/acs.jchemed.2c00950
4. Data Flow Diagram vs Flowchart - What's the difference? - Miro, accessed April 11, 2025, https://miro.com/diagramming/data-flow-diagram-vs-flowchart/
5. Solving Organic Chemistry Reaction Pathways - HSCprep, accessed April 11, 2025, https://hscprep.com.au/hsc-chemistry/organic-chemistry-reaction-pathways
6. Keep it simple & follow these flowchart rules for better diagrams - Nulab, accessed April 11, 2025, https://nulab.com/learn/design-and-ux/keep-it-simple-follow-flowchart-rules-for-better-diagrams/
7. Advantages and Disadvantages of Flowcharts - PlanetTogether, accessed April 11, 2025, https://www.planettogether.com/blog/advantages-and-disadvantages-of-flowcharts
8. What is a sunburst chart? How to create one | Mokkup.ai, accessed April 11, 2025, https://www.mokkup.ai/blogs/sunburst-charts/
9. What is a Sunburst Chart and When to Use a Sunburst Chart in Excel - Simple Sheets, accessed April 11, 2025, https://www.simplesheets.co/blog/sunburst-chart
10. Alternatives to D3.js | JavaScript Chart Comparisons - SciChart, accessed April 11, 2025, https://www.scichart.com/blog/alternatives-to-d3-js/
11. 7 Cool Data Visualizations Using D3 and Vega - Open Data Science, accessed April 11, 2025, https://opendatascience.com/7-cool-data-visualizations-using-d3-and-vega/
12. Organic Chemistry: Building Reaction Maps, accessed April 11, 2025, https://chemistry.coach/knowledge-base/organic-chemistry-building-reaction-maps
13. Creating a Graph of Chemical Reactions - Graph Database & Analytics - Neo4j, accessed April 11, 2025, https://neo4j.com/blog/developer/chemical-reactions-graph/
14. Directed Graph Visualizer | Tom Sawyer Software, accessed April 11, 2025, https://blog.tomsawyer.com/directed-graph-visualizer
15. Find cycles in force directed graph - d3.js - Stack Overflow, accessed April 11, 2025, https://stackoverflow.com/questions/28040182/find-cycles-in-force-directed-graph
16. d3/d3-sankey: Visualize flow between nodes in a directed acyclic network. - GitHub, accessed April 11, 2025, https://github.com/d3/d3-sankey
17. How to Tackle Organic Chemistry Synthesis Questions - Leah4Sci, accessed April 11, 2025,

https://leah4sci.com/how-to-tackle-organic-chemistry-synthesis-questions/
18. How do students work through organic synthesis learning activities? - ResearchGate, accessed April 11, 2025, https://www.researchgate.net/publication/265138673_How_do_students_work_through_organic_synthesis_learning_activities
19. Examining Challenges that Students Face in Learning Organic Chemistry Synthesis, accessed April 11, 2025, https://www.researchgate.net/publication/341608142_Examining_Challenges_that_Students_Face_in_Learning_Organic_Chemistry_Synthesis
20. (PDF) Chunking in Chemistry - ResearchGate, accessed April 11, 2025, https://www.researchgate.net/publication/239524823_Chunking_in_chemistry
21. Organic Chemistry Study Tips: Quick Wins, accessed April 11, 2025, https://www.masterorganicchemistry.com/2010/09/17/quick-wins/
22. An in-depth guide on HSC Chemistry: Breaking down the Modules, Assessments and Final Exams for your success, accessed April 11, 2025, https://kisacademics.com/blog/an-in-depth-guide-on-hsc-chemistry-breaking-down-the-modules-assessments-and-final-exams-for-your-success/
23. Network Graph | the D3 Graph Gallery, accessed April 11, 2025, https://d3-graph-gallery.com/network.html
24. d3-force | D3 by Observable - D3.js, accessed April 11, 2025, https://d3js.org/d3-force
25. Basic network graph in d3.js, accessed April 11, 2025, https://d3-graph-gallery.com/graph/network_basic.html
26. Elevating Network Visualizations: D3-force & Next.js | by Abdul Majeed | Medium, accessed April 11, 2025, https://medium.com/@abdulmajeedamm33/elevating-network-visualizations-d3-force-next-js-2ce1a322d746
27. D3 Force Directed Network Diagram - Sisense Community, accessed April 11, 2025, https://community.sisense.com/t5/knowledge-base/d3-force-directed-network-diagram/ta-p/9108
28. Force-directed graph component / D3 - Observable, accessed April 11, 2025, https://observablehq.com/@d3/force-directed-graph-component
29. Graph Network Visualization | Tom Sawyer Software, accessed April 11, 2025, https://blog.tomsawyer.com/graph-network-visualization
30. Sankey plot | the D3 Graph Gallery, accessed April 11, 2025, https://d3-graph-gallery.com/sankey.html
31. Sankey diagram component / D3 - Observable, accessed April 11, 2025, https://observablehq.com/@d3/sankey-component
32. QinMing/d3-sankey-with-highlighting: "Sankey" Data Visualization with End-to-End Highlighting - GitHub, accessed April 11, 2025, https://github.com/QinMing/d3-sankey-with-highlighting
33. Arc diagram | the D3 Graph Gallery, accessed April 11, 2025, https://d3-graph-gallery.com/arc.html
34. Arc diagram / D3 - Observable, accessed April 11, 2025,

https://observablehq.com/@d3/arc-diagram
35. Vertical arc diagram in d3.js, accessed April 11, 2025, https://d3-graph-gallery.com/graph/arc_vertical.html
36. Arcs | D3 by Observable - D3.js, accessed April 11, 2025, https://d3js.org/d3-shape/arc
37. Computers & Graphics - Hsiang-Yun WU, accessed April 11, 2025, https://yun-vis.net/projects/graph/cg2024.pdf
38. What is better, adjacency lists or adjacency matrices for graph problems in C++?, accessed April 11, 2025, https://stackoverflow.com/questions/2218322/what-is-better-adjacency-lists-or-adjacency-matrices-for-graph-problems-in-c
39. Graffinity: Visualizing Connectivity in Large Graphs - Data Analytics, accessed April 11, 2025, https://analytics.drake.edu/~urness/research/download/2017_eurovis_graffinity.pdf
40. d3/d3-chord: Visualizations relationships or network flow with a circular layout. - GitHub, accessed April 11, 2025, https://github.com/d3/d3-chord
41. d3-chord | D3 by Observable - D3.js, accessed April 11, 2025, https://d3js.org/d3-chord
42. Chords | D3 by Observable - D3.js, accessed April 11, 2025, https://d3js.org/d3-chord/chord
43. d3-chord examples - CodeSandbox, accessed April 11, 2025, https://codesandbox.io/examples/package/d3-chord
44. Hierarchical edge bundling / D3 - Observable, accessed April 11, 2025, https://observablehq.com/@d3/hierarchical-edge-bundling
45. Hierarchical Edge Bundling - React Graph Gallery, accessed April 11, 2025, https://www.react-graph-gallery.com/hierarchical-edge-bundling
46. Hierarchical edge bundling - The D3 Graph Gallery, accessed April 11, 2025, https://d3-graph-gallery.com/bundle.html
47. Sankey vs Sunburst Diagrams: Key Differences Explained, accessed April 11, 2025, https://www.quantummetric.com/blog/sankey-diagram-vs-sunburst-diagram-what-are-the-differences
48. JavaScript Charting Tool Showdown: FusionCharts vs. D3.js, accessed April 11, 2025, https://www.fusioncharts.com/blog/javascript-charting-tool-showdown-fusioncharts-vs-d3-js/
49. Organic Chemistry Reactions Cheatsheet | HSC Chemistry - Learnable Education, accessed April 11, 2025, https://www.learnable.education/organic-chemistry-reactions-cheatsheet-hsc-chemistry/
50. Blooming student difficulties in dealing with organic reaction mechanisms – an attempt at systemization | Request PDF - ResearchGate, accessed April 11, 2025, https://www.researchgate.net/publication/370998405_Blooming_student_difficulties_in_dealing_with_organic_reaction_mechanisms_-_an_attempt_at_systemization

51. Predicting and analyzing organic reaction pathways by combining machine learning and reaction network approaches - Chemical Communications (RSC Publishing) DOI:10.1039/D3CC03890D, accessed April 11, 2025, https://pubs.rsc.org/en/content/articlehtml/2023/cc/d3cc03890d
52. Promoting Understanding of Chemical Representations: Students' Use of a Visualization Tool in the Classroom - Deep Blue Repositories, accessed April 11, 2025, https://deepblue.lib.umich.edu/bitstream/handle/2027.42/34515/1033_ftp.pdf
53. Optimizing Pedagogical Strategies in Organic Chemistry: Examining Students' Conceptual Mastery and Perspectives on the Use of Multimedia-Supported Flipped Classroom Approach in Organic Chemistry | Journal of Chemical Education, accessed April 11, 2025, https://pubs.acs.org/doi/10.1021/acs.jchemed.4c01444
54. Heron: Visualizing and Controlling Chemical Reaction Explorations and Networks | The Journal of Physical Chemistry A - ACS Publications, accessed April 11, 2025, https://pubs.acs.org/doi/10.1021/acs.jpca.4c03936
55. Developing and evaluating an e-learning and e-assessment tool for organic chemistry in higher education - Frontiers, accessed April 11, 2025, https://www.frontiersin.org/journals/education/articles/10.3389/feduc.2024.1355078/full
56. (PDF) Using concept maps in teaching organic chemical reactions - ResearchGate, accessed April 11, 2025, https://www.researchgate.net/publication/228634487_Using_concept_maps_in_teaching_organic_chemical_reactions
57. Concept Maps as a Tool for Teaching Organic Chemical Reactions - ResearchGate, accessed April 11, 2025, https://www.researchgate.net/publication/278791320_Concept_Maps_as_a_Tool_for_Teaching_Organic_Chemical_Reactions
58. “It's Only the Major Product That We Care About in Organic Chemistry”: An Analysis of Students' Annotations of Reaction Coordinate Diagrams | Journal of Chemical Education, accessed April 11, 2025, https://pubs.acs.org/doi/abs/10.1021/acs.jchemed.8b00153?ref=vi_JCE100yr-cer
59. Engaging Health Student in Learning Organic Chemistry Reaction Mechanisms Using Short and Snappy Lightboard Videos | Journal of Chemical Education, accessed April 11, 2025, https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00619
60. Full article: Web-based discussion in teaching and learning organic chemistry: a scoping literature review on its current trends, cognitive, social, and teaching aspects - Taylor and Francis, accessed April 11, 2025, https://www.tandfonline.com/doi/full/10.1080/2331186X.2024.2431947
61. Teaching and Learning Strategies of Organic Reaction Mechanism in Pre-University Chemistry: A Scoping Review - Akademi Sains Malaysia, accessed April 11, 2025, https://www.akademisains.gov.my/asmsj/?mdocs-file=7955
62. How to Memorize Organic Chemistry Mechanisms Through Active Writing - YouTube, accessed April 11, 2025, https://m.youtube.com/watch?v=4dIKg7duilU&t=5s

63. 3D force-directed graph component using ThreeJS/WebGL - GitHub, accessed April 11, 2025, https://github.com/vasturiano/3d-force-graph
64. rNets: A standalone package to visualize reaction networks. - ChemRxiv, accessed April 11, 2025, https://chemrxiv.org/engage/api-gateway/chemrxiv/assets/orp/resource/item/660c5ccae9ebbb4db9378cc1/original/r-nets-a-standalone-package-to-visualize-reaction-networks.pdf
65. High Structure Active Learning Pedagogy for the Teaching of Organic Chemistry: Assessing the Impact on Academic Outcomes | Journal of Chemical Education - ACS Publications, accessed April 11, 2025, https://pubs.acs.org/doi/abs/10.1021/acs.jchemed.6b00663