Molecular Storytelling Supplemental Material

# Background

Atoms and molecules are invisible, so in research and education about biomolecules, they must be conceptualized and appropriately represented. Depending on the purpose of communication, atoms and molecules may be represented by conceptual constructs (see Supp. Table 1A) - represented by abstract drawings, symbols, physical models, or even auditory notes. A variety of experimental measures are also used to indicate their presence and/or attributes (see Supp. Table 1B) - that highlight specific properties of the molecule. While conceptual representations are often used across disciplines, measures of molecular attributes are usually highly discipline-specific and often tightly connected to a particular experimental method or technology. Interpreting information presented by both these types of representations requires significant amounts of reasoning, domain knowledge, and instructional support to learn. The properties of representations listed in Supp. Tables 1A and B are often tacit knowledge for disciplinary experts and researchers, while non-experts and students may find it challenging to understand their implications and use them. Sometimes, these representations may be filtered or modified to make it easier for novice learners to navigate through and interpret their significance.

Supp. Table 1A: A sampling of conceptual representations of molecules, commonly used in chemistry, biology, and related sciences.

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| Representation | What is presented | Common Use |
| Chemical symbols | Unique set of alphabets for each element | To recognize chemical and physical/chemical properties |
| Chemical formula | Lists type and number of atoms in a single molecule | To search for and compare molecules in Chemistry |
| Chemical Descriptors (SMILES, InChI) | Lists type and number of atoms along with specific chemical linkages between them | To search for and compare molecules in Chemistry |
| Chemical drawing | A 2-dimensional figure showing atom types and chemical bonding between them | To visualize, search for, compare, and communicate chemical and physical properties in Chemistry and Biology |
| Chemical component identifiers | Abbreviated names of molecules, including building blocks of polymers (such as TRP, AMP or W, A) | To recognize and refer to polymer building blocks inside and outside polymer sequences. Certain physical and chemical properties of these components are implied. Used in chemistry, biology, bioinformatics and more. |
| Polymer sequences in: 3-letter abbreviations; 1-letter code or FASTA format | Order of building blocks in proteins (amino acids) and nucleic acids such as DNA, RNA (nucleotides) with standard linkages connecting them together. | To search for, compare, and analyze polymer sequences for proteins and nucleic acids. Used in biology, genetics, and bioinformatics. |
| Sequence using Symbolic Nomenclature for Glycans (SNFG) | Order of glycan building blocks (monosaccharides) and their specific linkages connecting them. | To search for and compare the sequences of linear and branched carbohydrate polymers. Used in glycobiology, and biochemistry. |
| Polymer names | Protein or gene name, abbreviations of name, names of signature domains and motifs in polymers such as proteins and nucleotides | To search for biomolecules and imply some interactions, and functions in biology |
| Molecular shape and structure using various visual representations | Plotting of 3D coordinates of atoms in the structures showing   * Polymer backbone structure (cartoon/ribbons) * All atoms shown as spheres connected by bonds shown as sticks (ball and stick) * Packing between atoms in a molecule (spacefill) * Surface features of the molecule (molecular surface) | To visualize, analyze, and compare the shapes, properties, and interactions of biological molecules. Used in biology, chemistry, and its sub-disciplines. |
| Intermolecular interactions | Plotting lines (solid/dashed) showing types of interactions between atoms and/or molecules. Sometimes these interactions are implied with no actual lines shown. | To show interactions e.g., solid lines for covalent bonds, dotted or dashed lines for non-covalent interactions. Hydrophobic and ionic interactions are often just implied. |
| Schematic (biomolecules/ assemblies) | Geometric shapes and/or drawings resembling the shapes or representations of molecular properties shown with textual descriptions denoting relationships connecting the shapes. | To show a process or phenomenon with multiple players and/or interactions. |

Supp. Table 1B: A sampling of molecular attributes for learning about their properties.

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| Representation | What is presented | Common Use |
| Gel electrophoresis band | Images of the biomolecule in the gel identified by specific staining with a dye, radiative, fluorescent, or chemical tags, shown alongside markers and controls. | To denote the presence of a biomolecule, estimate its size and/or charge, interactions with other molecules |
| Chromatography peak | Plot of the elution profile of the chromatography showing where the molecule of interest eluted. | To denote the presence, purity, and concentration/quantity of the molecule of interest |
| Fluorescent micrograph | Image of a tissue, cell, or organelle showing the location of specific components that are tagged with fluorescent molecules. | To denote the location of a specific biomolecule at a specific time in the cell. It may also be used to track the movement of specific molecules in the cell from one compartment to another over a period of time or in response to a specific event. |
| Peaks of an NMR spectrum | Images of the NMR spectrum showing peaks representing the chemical composition of molecules | To identify the presence of specific chemical groups and how they interact with atoms in their neighborhood, at a given time or over a period of time |
| Binding curve | Plots showing proportions of different forms of the molecule (e.g., bound to free) over times or in different conditions of the experiment | To understand the functions and properties of a biomolecule in different contexts. |