

**PROPOSED ASSESSMENT RUBRIC FOR BIOMACROMOLECULAR 3D LITERACY (updated 8/8/09)**

	<b>Introductory Biology (Novice level)</b>	<b>Biochemistry/Cell Biology (Amateur level)</b>	<b>Structural biology graduate student (Expert level)</b>
<b>Alternate Renderings</b>	Views alternate renderings as different molecules or giving different properties to molecule	Sees alternate renderings as different views of the same molecule. Understands basic information conveyed by each.	Understands the limitations and information to be gained by each type of molecular rendering
<b>Kinematics</b>	Sees animation as cartoon rather than as structural motion	Recognition of molecular hinges and movement of both backbone and sidechains during conformational change	Understands the limitations and information to be gained by various types of animations. Creates and evaluates animations.
<b>Structure-Function Relationship</b>	Vague notion of active/binding sites or functional groups. Can visualize nucleic acid grooves.	Recognition of the role the structure of the binding site plays in function. Can reasonably predict the effect of a mutation on function. Sees relationships between structurally homologous binding sites which may not have sequence homology	Sees beyond the binding site to the role of the overall structure in function. Can extract information and relationships from figures in publications or presentations.
<b>Structural Model Skepticism</b>	Acceptance of physical or graphic structure as portrayed	Understands fundamental limitations of models derived from either experimental or theoretical means	Is able to query model with visual inspection and validation tools to identify flaws
<b>Atomic Geometry</b>	Unable to recognize problematic bond angles or gain information from them	Recognizes obvious problems with bond angles and geometries. Is able to measure dihedral angles and identify secondary structures.	Is able to propose alternative structural interpretations that may resolve problems Recognizes relationship of metal ligand geometry to redox state and potential function
<b>Symmetry/Asymmetry Recognition</b>	Able to see simple rotational axes of symmetry.	Able to orient molecule to illustrate axes of symmetry. Recognizes helical handedness and dipoles.	Recognizes symmetry in oligomers as well as monomers (eg fused gene duplications). Recognizes significant charge asymmetries.
<b>Topology and Connectivity</b>	Able to see overall shape of molecule and general chain winding.	Able to determine chain direction from visual inspection. Able to draw a linear topology map illustrating secondary structure sequencing	Able to draw a 2D topology map of supersecondary structure from a 3D structural model. Recognizes common protein folds and possible evolutionary relationships.
<b>Molecular Interactions</b>	Able to discern key intramolecular interactions such as hydrogen bonding or charge interactions.	Able to recognize specific intermolecular interactions (H bonding, salt bridges, etc)	Able to recognize nonspecific forces at interfaces, i.e. packing and hydrophobic interactions
<b>Construction and Annotation</b>	Able to build only the simplest molecular model	Able to construct a macromolecular model from a coordinate set and provide brief annotation	Able to read a PDB file and construct a detailed, labeled model making appropriate use of color, animations, and alternate renderings from it.
<b>Monomer Recognition</b>	Able to distinguish between dissimilar monomers	Recognizes all native monomer groups and their physical properties	Recognizes unusual or modified monomer groups and surmises their physical and functional properties
<b>Het Group Recognition</b>	Does not recognize significant additions to the biopolymer chain	Recognizes common het groups such as common metals and glycans	Recognizes unusual/unexpected het groups and surmises their physical and functional properties

## Definition of Terms:

**Alternate Renderings:** Rendering of a macromolecular structure such as a protein or nucleic acid structure in various ways from the simplest possible way (connections between alpha carbons) to illustration of secondary structure (ribbons) to surface rendering and space filling.

**Kinematics:** Animated motion simulating conformational changes involved in ligand binding or catalysis, or other molecular motion/dynamics.

**Structure-Function Relationship:** Active/binding sites, microenvironments, nucleophiles, redox centers, etc.

**Structural Model Skepticism:** Recognition of the limitations of models to describe the structure of macromolecules

**Atomic Geometry:** three atom and four atom (dihedral) angles, metal size and metal-ligand geometries, steric clashes

**Symmetry Recognition:** recognition of symmetry elements within both single chain and oligomeric macromolecules

**Topology and Connectivity:** Following the chain direction through the molecule, translating between 2D topology mapping and 3D rendering

**Intermolecular Interactions:** covalent and noncovalent bonding governing ligand binding and subunit-subunit interactions

**Construction and Annotation:** ability to build macromolecular models, either physical or computerized, and, where possible, add commentary, either written or verbal, to tell a molecular story

**Monomer Recognition:** recognition of both native and modified amino acids, nucleotides, sugars, and other biomonomer units. Understanding of their physical and chemical properties, particularly regarding functional groups.

**Het Group Recognition:** metals and metal clusters, posttranslational additions such as glycosylation, phosphorylation, lipid attachment, etc.

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