

Molecular storytelling for online structural biology outreach and education

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ABSTRACT

Knowledge about the structure and function of biomolecules continues to grow exponentially, enabling us to “see” structural snapshots of biomolecular interactions and functional assemblies. At PDB-101, the educational portal of the RCSB Protein Data Bank, we have taken a storytelling approach to make this body of knowledge accessible and comprehensible to a wide community of students, educators, and the general public. For over 20 years, the Molecule of the Month series has utilized a traditional illustrated storytelling approach that is regularly adapted for classroom instruction. Similar visual and interactive storytelling approaches are used to present topical subjects at PDB-101 and full curricular materials and case studies for building a detailed narrative around topics of particular interest. This emphasis on storytelling led to the Video Challenge for High School students, now in its 8th year. In this Article, we will present some of the lessons we have learned for teaching and communicating structural biology using the PDB archive of biomolecular structures.

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INTRODUCTION

What got you interested in science? Chances are, it was a book, a video, or a teacher that brought science to life with a story. Stories are one of the oldest forms of teaching and communicating complex ideas and concepts, and stories are an engaging way to approach education and outreach in science. Looking back to our own childhood influences, storytelling approaches abound. Field guides, such as the Golden Nature Guide series¹ and field guides from the National Audubon Society,² told us stories about the natural history that surrounds us every time we step out the door. Books like Macaulay’s “The Way Things Work”³ did the same for technology, taking us inside the science and engineering of the machines and mechanisms that we encounter every day in our familiar lives. In these examples, the stories tell us about science, but also tell us how science impacts our own lives, inviting us to explore and learn more.

We have taken a storytelling approach in our creation of materials to explore structural biology at PDB-101, the education portal of the RCSB Protein Data Bank (RCSB PDB^{4,5}). Structural biologists explore the shapes and interactions of biological macromolecules, such

as proteins and DNA, to understand their functions. Today, experimentally determined structures of hundreds of thousands of biological macromolecules are freely available from the Protein Data Bank, data resources such as UniProt⁶ and GenBank⁷ place bioinformatics information at our fingertips, and an enormous body of primary literature is instantly available and searchable through PubMed.⁸ However, the information in these resources is often technical and inaccessible to non-expert audiences. Storytelling approaches provide an opportunity to share these accomplishments, to make this body of knowledge accessible and comprehensible to a wide community of students, educators, and the general public. In this editorial, we present some of the lessons we have learned for teaching and communicating structural biology using the PDB archive of open-access biomolecular structures and the freely available educational materials we have created for PDB-101.

MODES OF STORYTELLING

The overarching goal of storytelling is to connect with an audience and hopefully inspire them to learn more and continue their

exploration. It is critical to tailor the storytelling approach for the people who will be reading or viewing the story. At PDB-101, we have employed several aspects of storytelling that have been devised and widely used over the history of science to connect with our user community: narratives, fact-based stories, and to a lesser extent, fiction. We have employed these storytelling approaches in multiple ways, ranging from the traditional mode of stories told by an expert to an audience, to interactive settings where educators build a story in an exploratory dialog with audience members, to settings where students create the stories themselves based on what they have learned.

Narratives build a story around the people impacted by science, in the traditional way that we think of a story or a tale. For example, medical science narratives can focus on case studies of patients, or narratives can follow the scientists themselves, their successes and failures, their collaborations or competitions, or the international fame acquired from a Nobel Prize. Narrative approaches are highly accessible and effective and are widely used in journalism and the popular media when science is presented to a general audience.

Fact-based storytelling is also widely used to dig deeper into science itself. In these stories, the scientific subject is the key player. The two examples given in the Introduction are perfect examples. Nature guides tell stories about birds, bugs, plants, shells, and all of the other living things around us. The stories guide us through where and when we could expect to find them, and what they might be doing when we do. Macaulay's book tells stories about human ingenuity, inviting us to discover for ourselves how technology works and imagine what it would be like to get inside these machines and perhaps invent something like this ourselves.

Fiction is also a powerful way to engage viewers and can incorporate as much or as little science fact as desired. These stories build on narrative and fact-based approaches, but weave in imagined elements. Due to its easy accessibility and appeal in movies and literature, fictional science stories are one of the most common ways that the general public encounters science and scientists. It may not be ideal, but many people base much of their knowledge of astronomy on what they have seen in *Star Trek*, and *Jurassic Park* and *Big Bang Theory* have inspired whole generations of future scientists.

MOLECULE OF THE MONTH

For 20 years, the *Molecule of the Month* series has utilized a traditional fact-based storytelling approach to present monthly "molecular portraits" of entries in the PDB archive.^{9,10} The series is intended as an easily accessible introduction to a molecule and its role in our lives, to invite additional exploration at the archive. Each feature is designed with engaging figures to entice readers and a brief format for easy reading. Typically, there are three sections. The first section begins with a hook that describes the role of the molecule in our daily lives, addressing the question "Why do we care?" An illustration and description of an exemplar entry from the archive presents how structural biology can answer this question. Many of these features are health-related given the central role of structural biology in the discovery of new approaches to fighting disease. Other hooks are related to the central mechanisms of molecular biology, such as the intrinsic story of protein synthesis embodied in the expressome (Fig. 1),¹¹ or related to bioenergy, the environment, nanotechnology, or a host of other topics. Narrative elements may also be employed, for example, in structures related to Nobel Prizes.

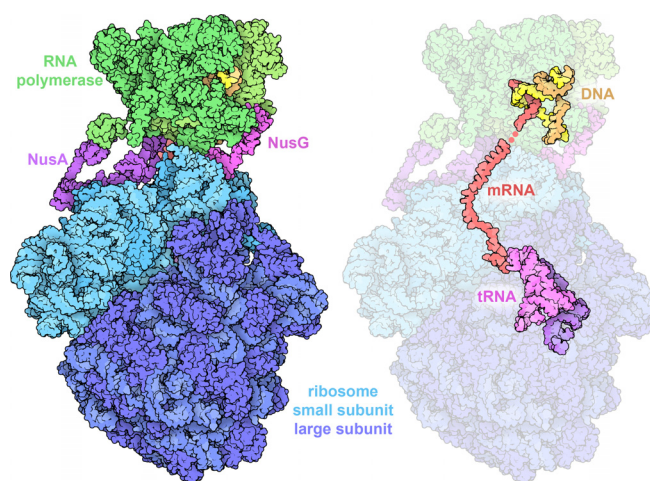


FIG. 1. The expressome, featured as the Molecule of the Month in January 2021, is a structure that tells an entire story. The complex shows the "Central Dogma" of molecular biology, with a small piece of DNA being unwound and transcribed into mRNA by RNA polymerase and an associated ribosome aligning tRNA and translating the mRNA into protein. Two small transcription factors, NusA and NusG, hold the whole assembly in place. Reproduced with permission from D. S. Goodsell, "Epressome," in PDB-101 (2021). Copyright 2021 Author, licensed under a Creative Commons CC-BY-4.0 license.

Following this introduction, a secondary topic is presented, adding additional depth to the story. This topic describes interactions of the exemplar molecule with other molecules, or related molecules in other organisms, or how medical science is using the knowledge of the structure and function of the molecule to design new diagnostic and therapeutic approaches. The goal is to show that none of these molecules act in isolation—they are part of the rich, interconnected environment of cells and organisms, and often we need to explore many molecules to understand their function and roles in life.

The feature finishes with an "Exploring the Structure" section that allows users to use interactive graphics to explore the functional details of a molecule first-hand. This is an interactive Jmol¹² that is designed to focus attention on one key property, for example, revealing the allosteric motions of hemoglobin when oxygen binds or exploring multiple rotational states of ATP synthase. An additional goal of this section is to provide a worked example of how to use interactive molecular graphics to understand the relationship between structure and function, to empower users when they use these tools to explore additional structures from the archive themselves.

The 250+ Molecule of the Month features are self-contained stories that showcase exemplar structures from the PDB archive. Since these articles are intended to be accurate representations of the science, factual accuracy is paramount, and features are reviewed by external structural biologists for accuracy. The Molecule of the Month series has proven to be an effective mode of engaging visitors, as evidenced by the $\sim 1 \times 10^6$ visits to the archive of articles annually. In addition, these articles are regularly adapted for classroom instruction, as evidenced by the continued high access for articles on key topics such as hemoglobin and catalase for many years after their publication on the PDB-101 site.

CURRICULAR MODULES AND MOLECULAR CASENET

Interactive storytelling employs audience participation in the storytelling process to deepen engagement with the subject. This poses an immediate challenge: in order to participate, audience members need to be familiar with the setting, vocabulary, tools, and resources for the subject. To reduce the barriers that limit audience participation, we have organized workshops and developed educational materials to familiarize students (and educators) with the PDB archive, visualization tools, and bioinformatics resources used in developing molecular stories. Developing molecular stories can be time consuming and challenging, especially for educators who are new to the field of structural biology. We have undertaken two collaborative projects to engage high school/community college students and undergraduate students in interactive molecular storytelling.

In response to requests from educators, the RCSB PDB faculty collaborated with high school and community college educators, students, scientists, and clinicians to launch a series of curriculum development workshops in 2014. The purpose of these workshops was to develop ready-to-use exercises around global health topics such as HIV/AIDS and diabetes, publish them on PDB-101 (<http://pdb101.rcsb.org/teach/overview>),¹³ and use them to engage students in learning about the molecular basis of these biomedical topics. The main focus of these exercises is to introduce students (and educators) to PDB data and help them practice molecular visualization and integration of information from relevant bioinformatics data resources. Continuing this work, we recently published a curricular module that enables the exploration of COVID-19 topics in molecular detail (<http://pdb101.rcsb.org/teach/covid-19>). Besides guided exercises, the

curricular modules include learning materials, assessment suggestions, exercise keys, and teaching notes to support teachers in guiding classroom discussions. The exercises are freely available online, and teachers can access accompanying notes and keys by requesting an account. All curricular materials meet the Next Generation Science Standards (NGSS, <https://www.nextgenscience.org>).¹⁴ As of this writing, ~600 educators world-wide have requested and received access to teaching notes for these curricular materials. Several educators have also provided feedback after they used these materials in their classrooms.

In 2018, a new NSF-funded project was initiated for developing molecular case studies to engage undergraduate students (and educators) in molecular storytelling. The main aim of these case studies is to enable the exploration of biomolecular structure–function relationships since these structures from the PDB archive are perfectly positioned at the interface between biology and chemistry. Each case in the Molecular CaseNet project (<https://molecular-casenet.rcsb.org/>) completes a “Molecular Case Study Cycle” at least once. For example, Figure 2 presents how a molecular case study cycle uses an NIH-produced video about Nicholas, a teenager living with sickle cell anemia, to explore the biology of hemoglobin and discuss the molecular basis for Nicholas’s pain crisis.¹⁵ These cycles include four major elements: (a) a hook related to the case theme (such as a video, narrative, image, story, or report), to engage students in the case with a specific question; (b) a process for guiding students to the structure(s) of key molecular players (or main characters) in the story and identifying relevant structures/complexes in the PDB archive to study; (c) molecular exploration to visualize and analyze selected PDB structures to understand the system and find answers to the case question(s); and (d) modeling to help

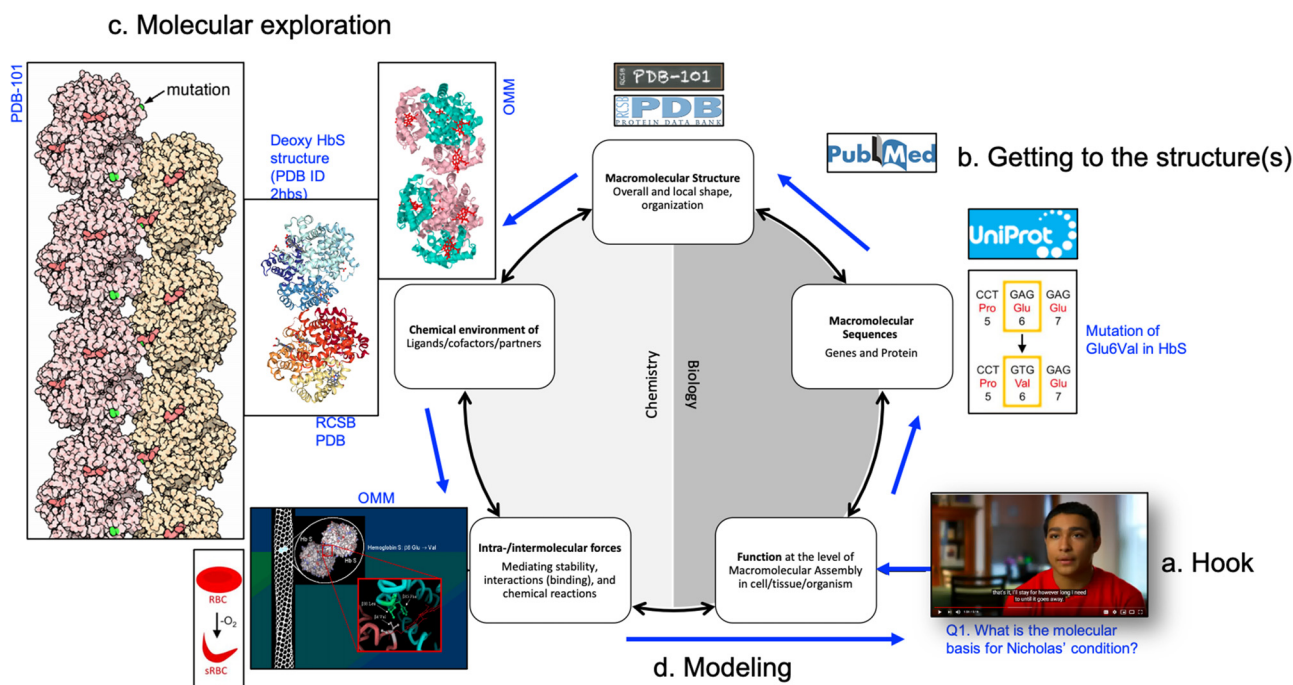


FIG. 2. Molecular Case Study Cycle for Nicholas’ Story. The four components of the cycle are listed with labels (a)–(d). The biomolecular structures at the heart of the case are positioned at the interface of biology and chemistry. Adapted with permission from Dutta *et al.*, Nicholas’ Story, Molecular CaseNet Faculty Mentoring Network (QUBES Educational Resources, 2020). Copyright 2020 Authors, licensed under a Creative Commons CC-BY-4.0.

students integrate information from the literature and various bioinformatics resources (such as the Online Macromolecular Museum, http://earth.callutheran.edu/Academic_Programs/Departments/BioDev/omm/exhibits.htm) and knowledge of molecular shapes and interactions to answer the case question(s). While the key players in the case study represent the main characters of the story, the molecular exploration and modeling present opportunities to examine the conflict (or question) in the story and its resolution.

In the past two years, ~25 undergraduate educators have participated in developing molecular case studies on a variety of different topics and piloted them in different curricular contexts as part of the QUBES Faculty Mentoring Networks (<https://qubeshub.org/community/fmns>). In collaboration with undergraduate educators, the Molecular CaseNet is developing a variety of foundational educational materials that can be used by students and educators while discussing molecular case studies and also help educators meet the various biology and chemistry professional society standards for undergraduate education. In the next five years of this project, we plan to develop many more case studies and accompanying educational materials in collaboration with students and educators to facilitate interactive molecular storytelling.

ANNUAL HIGH SCHOOL VIDEO CHALLENGE

Often, the best way to teach is to have students tell their own stories about the subject. In order to tell their own story, students need to have a deep knowledge of the subject and then make it intelligible to other students. The PDB-101 Annual Video Challenge for High School students, now in its 8th year, invites teams of students to create short videos on a yearly topic (<http://pdb101.rcsb.org/events/video-challenge>). For example, we are currently focusing on topics related to drugs and the brain, with the 2020 topic of the “Molecular Mechanisms of Opioid Action” and the upcoming 2021 topic of “Molecular Mechanisms of Drugs for Mental Disorders.” The challenge provides the core of a biennial theme that is used to integrate instructional materials that are created and deployed at PDB-101.

The creativity of the participants is truly remarkable, and all manner of storytelling is employed, often with fictional elements. Three award-winning videos from the 2020 contest are good examples (Fig. 3). “Saving Hector’s Friend from Opioids” takes a case-study approach to overdose treatment, telling the story with animated toys. “Fighting Opioids One Punch at a Time” focuses on the molecules themselves, using cute cartoon characters for each of the molecules. “Opioid Busters” employs a cast of superheroes to intervene, tell us about the dangers, and save us from the crisis. In all cases, the result is a story that presents the science, but couched in elements that keep us watching and help us make connections between the structural biology and global health challenges.

INSIGHTS AND BEST PRACTICES

The Protein Data Bank archive was established in 1971¹⁶ as the first open access digital data resource in all of biology and medicine.¹⁷ The PDB provides access to 3D structure data for large biological molecules (proteins, DNA, and RNA) studied by X-ray crystallography, NMR, and 3D electron microscopy. Each structure is a story in itself, as knowing the shape of a biological macromolecule is essential for understanding its role in health and disease, energy, and fundamental biology. The PDB has grown to

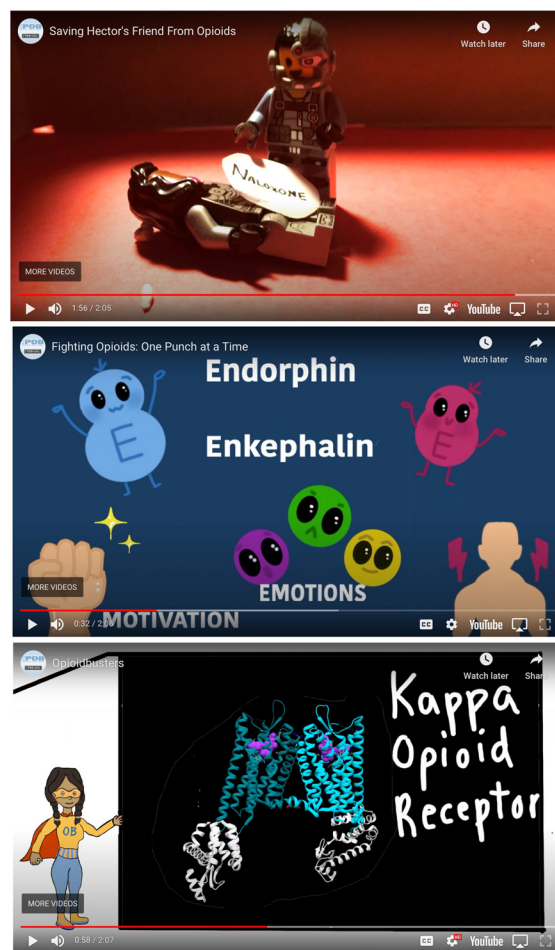


FIG. 3. Award-winning student videos from the 2020 RCSB PDB Video Challenge for High School Students on “Molecular Mechanisms of Opioid Action.” Adapted with permission from the RCSB PDB, see <http://pdb101.rcsb.org/events/video-challenge/2020-awards>. Copyright 2020 Authors, licensed under a Creative Commons CC-BY-4.0.

encompass over 170 000 structural entries from researchers that circle the globe. It will be celebrating its 50th year in 2021 with symposia and resources (<http://rcsb.org/pdb50>).

PDB-101 (<http://pdb101.rcsb.org>) was created in 2011 to serve as a complementary portal to the main RCSB PDB site, streamlining access for users not actively engaged in structural biology research. A variety of materials, including the ones described here, are freely available online at the site for use and reuse by all. We have gathered feedback from users from multiple sources, including questions from the help desk and conferences, questionnaires, and our own teaching. Based on this feedback, we have garnered insights about the aspects of our molecular stories that resonate with our user community. They boil down to three major insights: finding the context, showing a process, and reducing jargon.

Finding the Context is often the most important and also the most challenging aspect of scientific storytelling. Most of our molecular stories seek to answer the question “Why do we care?” This

information is often difficult to find, particularly for fact-driven molecular portrait stories, because much of the scientific literature is highly focused on the details of a particular subject. The introduction sections of technical papers often nod to this information, but typically, it takes extensive sleuthing to find sources to support descriptions of the general biology and implications of the structure/function relationships of individual structures to their larger physiological consequences. Higher-level descriptions also often require speculation and may have to be based on foundational knowledge about the discipline, multidisciplinary scientific concepts, and familiarity with scientific practices. This is especially true with newly discovered systems, since many aspects may not be well studied. For example, in the 2014 Molecule of the Month on Ebola virus proteins (Fig. 4), we wanted to present a comprehensive illustration of the entire virus to put the individual molecular structures in context.¹⁸ Considerable speculation was required to integrate the available structures and electron micrographs, for example, with the domains that are not included in the structure determinations and specifics of the connections between different parts of the virion.

Showing a Process is a great way to bring a molecule to life for viewers. Instead of showing a single structure, providing only a snapshot of a protein, it is often better to employ a series of structures that show structural transitions or to describe how a molecule interacts with one or more partners while playing its functional role. We use this approach in nearly all installments of the Molecule of the Month, in particular, through the secondary topics. For example, the feature on adenyl cyclase starts with a structure of the enzyme activated by a

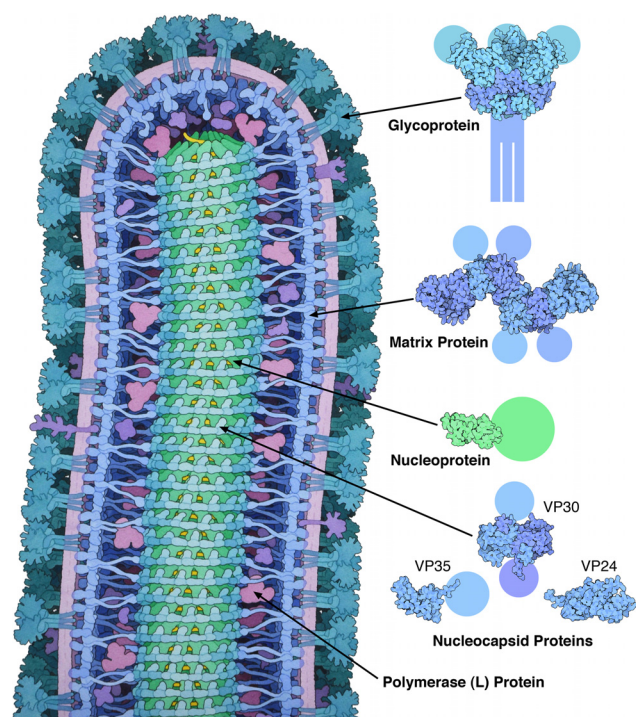


FIG. 4. Ebola virus proteins. The atomic structures are shown at right, with portions that were not determined schematically. An artistic conception on the left shows the context of each protein within the entire Ebola virion. Reproduced with permission from D. S. Goodsell, "Ebola virus proteins," in PDB-101 (2014). Copyright 2014 Author, licensed under a Creative Commons CC-BY-4.0.

G-protein, showing the cyclization reaction, and then presents one of the channels that is activated by cAMP as the secondary topic.¹⁹ Mechanistic discussions are also central to the hands-on visualization exercises in the various curricular modules and the molecular case studies. These presentations of entire processes are intended to inspire questions like "What happens next?" or "What happens if you change the molecular structure or its environment?" and to invite visitors to keep exploring the topic.

Finally, and perhaps most important, *Reducing Jargon* is essential if the story is intended for anyone other than a structural biologist. Jargon can be visual, written, or even conceptual. The scientific language used for writing and the scientific conventions and assumptions used for figures are complex for a reason: they are meant to be specific and unambiguous when presenting results that will be used as evidence in the scientific record. This, however, is not the goal of scientific outreach and education. Our goal is rather to generate excitement, give an overall understanding of a topic, and bridge any knowledge gaps to enable easy navigation through a molecular story. So, general, high-level writing and simplified image conventions are generally most effective in this context. For example, in the Molecule of the Month, we use a cartoony non-photorealistic style that omits much of the atomic detail, but presents the overall shape, form, and interaction of the molecules.²⁰ The writing is similarly simplified, avoiding detailed descriptions of individual amino acids and domains, and instead focusing on the broader strokes of the structure/function relationships with plain language. We are also constantly aware of the prior exposure and experience of our readers and pitch the molecular stories at the appropriate level. If needed, audiences with limited or no prior exposure to structural biology are referred to PDB-101 resources that present foundational concepts.

CONCLUSIONS

The PDB archive represents a seminal body of knowledge gathered by and for the global structural biology community.²¹ In our experience, molecular storytelling has provided an effective method for engaging, serving, and growing the community of users of this information. Molecular stories allow students and educators to explore the basic concepts of molecular biology, empowering them to utilize the actual primary data in which these concepts were discovered. These molecular stories are also intended to spark interest in these remarkable molecular machines and underscore the importance of this research in the health and welfare of the general public.

Box: Selected Online Resources with Biomolecular Storytelling
Molecule of the Month and Video Challenge at PDB-101 (RCSB PDB) <http://pdb101.rcsb.org>
Molecular CaseNet (RCSB PDB) <https://molecular-casenet.rcsb.org>
Protein Spotlight (UniProtKB) <https://www.proteinspotlight.org>
Protein Focus (InterPro, legacy) <https://www.ebi.ac.uk/interpro/legacy/protein-focus>
Proteopedia (Weizmann Institute of Science) <http://proteopedia.org>

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