enveloped viruses, on the other hand, must enter cells through membrane fusion driven by the hemagglutinin (or HA) protein. This process involves the fusion of the viral and host cell membranes. Harrison explains that enveloped viruses infect cells by inducing the fusion of their membrane with the host cell membrane.

In Part 1 (last month's featured video), Harrison also elaborates on how these viruses infect cells. In his talk, he asks why most non-enveloped viruses and some enveloped viruses are symmetrical in shape. He proceeds to show us images of the structures obtained by X-ray crystallography of numerous viral coat proteins. Deciphering these structures allows scientists to understand how these viruses infect cells. In Part 2 of his talk, Harrison delves deeper into the molecular mechanism of membrane fusion driven by the hemagglutinin (or HA) protein of the influenza virus in Part 2 of his talk. Non-enveloped viruses, on the other hand, must enter cells by undergoing a process called endocytosis.

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- Crystallography in the news
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Science Video of the Month

iBioSeminar by Prof. Stephen Harrison (pt. 2)

Harrison begins his talk by asking why most non-enveloped viruses and some enveloped viruses are symmetrical in shape. He proceeds to show us lovely images of the structures obtained by X-ray crystallography. Deciphering these structures allowed scientists to understand how these viruses infect cells. In Part 2 of his talk, Harrison delves deeper into the molecular mechanism of membrane fusion driven by the hemagglutinin (or HA) protein of the influenza virus. Non-enveloped viruses, on the other hand, must enter cells by undergoing a process called endocytosis.
by a mechanism other than membrane fusion. This is the focus of Part 3. Using rotavirus as a model, Harrison and his colleagues have used a combination of X-ray crystallography and electron cryomicroscopy to decipher how the spike protein on the viral surface changes its conformation and perforates the cell membrane allowing the virus to enter the cell.

**Product spotlight: Compact HomeLab**

Rigaku’s new Compact HomeLab was designed for structural biologists who want a low-maintenance X-ray system that is easy to use, and provides the ultimate in experimental flexibility. From screening crystals prior to a synchrotron trip to solving structures from SAD phasing, the Compact HomeLab provides your group with the tools it needs to carry out structural biology in today’s fast and competitive environment.

Rigaku’s Compact HomeLab brings a new level of capabilities for protein crystallography to your lab. It has the industry’s highest usable flux from a micro-focus sealed tube X-ray source, a comforting three year tube warranty, a new high-gain CCD detector, remote iPad or iPhone control and monitoring, and the unparalleled performance of HKL-3000R instrument control, data processing and structure solution software. The Compact HomeLab gives you everything you need to properly screen crystals in advance of a synchrotron experiment or teach your students the science of solving protein structures. Ask for more information.

**Lab in the spotlight: Southampton Diffraction Centre**

Southampton Diffraction Centre (SDC)
Dr. Simon Coles, Director
Chemical and Life Sciences: Bridging the gap

The vision of the SDC is one of a fully integrated structure-centric research facility where chemists and life scientists work together and learn from each other to progress individual research projects and the field as a whole.

The SDC is an organization that pools facilities and services associated with the analysis of atomic resolution structure from both the Chemical and Life Sciences. The center boasts state-of-the-art instrumentation and exceptional expertise in crystallization, diffraction and thermal analysis of both small and macromolecular-based systems. The UK National Crystallography Service, funded by EPSRC, is housed within the centre and provides a centralized service for chemistry-based academia where advanced facilities are required to answer problems that cannot be solved with local resources. Additionally, our exceptional facilities are accessible to industrial-based research through Southampton Chemistry Analytical Solutions.

**Useful link - new refinement software**

Scientists at the University of Chicago have developed automated software to refine crystallographic, EM, and NMR structures. The server converts moderate- to low-resolution structures at initial (e.g., backbone trace only) or late stages of refinement to structures with increased numbers of hydrogen bonds, improved crystallographic R-factors, and superior backbone geometry. The fully automated method is applicable to DNA-binding and membrane proteins of any size and will aid studies of structural biology by improving model quality and saving considerable effort. It can be applied to the entire structure or just specific regions, and employed multiple times in conjunction with other refinement tools. It can be used with or without electron density and is available on the Godzilla Computing Cluster. Ref. Haddadian, et al. (2011). Automated real-space refinement of protein structures using a realistic backbone move set. Biophys. J. 101, 899. The method was used in Krishnamurthy, H. & Gouaux, E. (2012) Nature 481, p469; Scharff et al. (2010) Immunity 33, p853; Feld et al. (2010) Nat Struct Mol Biol 17, p1383.

**Selected recent crystallographic papers**

This is the first time the American Association for Cancer Research (AACR) Team Science Award has been won outside the US. The AACR said its decision was based on "the tremendous impact this team has had in preclinical and clinical studies of cancer therapeutics."

The Team members are from the Cancer Research UK Cancer Therapeutics Unit at the ICR, which discovers new drugs, and the Drug Development Unit at the ICR and The Royal Marsden, which progresses drug candidates into clinical trials.

**Selected recent crystallographic papers**

- Computing design of a protein crystal. Lanci, Christopher J.; MacDermaid, Christopher M.; Kang, Seung-gu; Acharya, Rudresh; North, Benjamin; Xi Yang; Qi, X. Jade; DeGrado, William F.; Saven, Jeffery G. Proceedings of the National Academy of Sciences of the United States of America, 5/8/2012, **Vol. 109** Issue 19, p7304-7309, 6p; http://dx.doi.org/10.1073/pnas.1121051109
- Exploration of Pirocopic Sulfonamides as Binders of the FK506-Binding Proteins 51 and 52. Gopalakrishnan, Ranganath; Kozany, Christian; Wang, Yongsan; Schneider, Sabine; Hoogeland, Bastiaan; Bracher, Andreas; Hausch, Felix. Journal of Medicinal Chemistry, May 2012, **Vol. 55** Issue 9, p4123-4131, 9p; http://dx.doi.org/10.1021/jm201747c
- X-ray crystallographic structure-based design of selective thienopyrazole inhibitors for interleukin-2-inducible tyrosine kinase. McLean, Larry R.; Zhang, Ying; Zaidi, Nisha; Bi, Xiping; Wang, Rachel; Dharanipragada, Ram; Jurcak, John G.; Gillespy, Timothy A.; Zhao, Zhicheng; Musick, Kwon Y.; Choi, Yong-Mi; Barrague, Matthieu; Peppard, Jane; Smcker, Matthew; Duguid, Mei; Parker, Ashfaq; Fordham, Jeremy; Kominos, Dorothea. Bioorganic & Medicinal Chemistry Letters, May 2012, **Vol. 22** Issue 9, p3296-3300, 5p; http://dx.doi.org/10.1016/j.bmcl.2012.03.016
- In situ macromolecular crystallography using microbeams. Axford, Danny; Owen, Robin L.; Ashima, Jun; Foadi, James; Morgan, Ann W.; Robinson, James I.; Nettleship, Joanne A.; Fleit, Peter; Wilson, Baum, Jake. IUBMB Life, May 2012, **Vol. 64** Issue 5, p370-377, 8p, 2 Diagrams; http://dx.doi.org/10.1002/iub.1014
- Structural biology is such an international field that there are essentially no geographical boundaries. This means that many structural biologists travel on a global basis to attend scientific meetings and visit colleagues. What is your favorite way to pass the time on an international flight?

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<th>Sleep</th>
<th>Watch 5 movies</th>
<th>Read scientific journals</th>
<th>Read something mindless</th>
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## Book review:

**Packing for Mars: The Curious Science of Life in the Void**

by Mary Roach  

In her nonfiction book, *Packing for Mars*, Mary Roach explores the numerous (and often less mainstream) trials and tribulations astronauts in training must undergo before they achieve clearance for travel to outer space.

Roach’s book is chock-full of interesting tidbits of information about NASA and its practices and policies. Roach balances sometimes overwhelming ideas with anecdotal footnotes and a witty, deadpan sense of humor. The ideas themselves are not overwhelming conceptually, but rather overwhelming to the senses. For example, an entire chapter is dedicated to discussing the difficulties and dilemmas of liquid and solid excretion in zero gravity. Roach exhibits an acute attention to detail and an unparalleled inquisitiveness as she digs into the past, present, and future of space travel. Additionally, the book is a fast-paced and energetic read, a means for those with little or no knowledge or experience in extraterrestrial affairs to learn a lot.

Among the topics Roach delves into are: the procedures by which potential Japanese astronauts are assessed and tested for desirable qualities by JAXA (the Japanese equivalent of NASA), both in intellect and personality (think solitary confinement and 1000 origami paper cranes, each methodologically analyzed for signs of psychological deterioration in the test subject); the psychology of isolation and confinement, or how NASA attempts to assess how the human brain reacts to extended periods of forced asocial conditions; the effects of space travel on the psyche, or how a number of former astronauts (think Lisa Nowak) have exhibited signs of mental instability following "out of this world" ventures; the dangers of life in zero gravity and the perpetual plague of motion sickness that afflicts many astronauts-in-training and even those who make it to the Moon (Roach does debunk the myth that barfing in a spacesuit will result in death by vomit; astronauts are not supposed to be intoxicated, as Jimi Hendrix was); the careers of two space chimps, Ham and Enos, who were only two of the many non-human mammalian test subjects used for assessing the effects of space travel on the human body; and the nausea-inducing nature of freeze-dried cuisine (tomato paste anyone?) and other aerospace delicacies (corned beef sandwiches + zero gravity= crumb snowstorm). This is not an exhaustive list, merely a glimpse of the breadth and wealth of material Roach covers in her work.

Perhaps my favorite anecdote is that of the NASA crash test dummy. Unlike the creepy mannequins from car commercials, the National Aeronautics and Space Administration uses cadavers. They are frozen after death, and thawed for several days
prior to testing. These cadavers are used to provide more accurate information concerning the effects of higher G forces applied laterally, longitudinally, and transversely. It is difficult to simulate the effects of a human body in a crash on a mannequin because of the intricacies of organ placement in the abdominal cavity. Also, one of the most important things to study in a crash test is the effect of the crash on the brain (which mannequins do not possess).

All in all, Packing for Mars is an engaging and enjoyable read, appropriate for science enthusiasts and other people of a curious nature.

Jeanette S. Ferrara
Princeton, Class of 2015