

Looking back at 20 years of the MOLECULE OF THE MONTH website

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The Internet/World Wide Web has been with us for just over 20 years and it is commonplace to say that it has revolutionised the ways in which we communicate with each other.

Nearly 20 years ago a group of chemistry academics in the UK were thinking about ways to use these new media to communicate the wonder of chemistry to a wider audience. The original idea came from Henry Rzepa of Imperial College London, who brought together Karl Harrison of the University of Oxford and Paul May of the University of Bristol to try to produce regular, monthly articles showcasing important chemical substances, and hosting them on their department's website. The website linking these articles together became known as the Molecule of the Month (MOTM) website [1], with the first molecule (mauveine) appearing in January 1996 (which is so early that it's actually before many University Chemistry departments even had their own departmental website!).

Sucrose
Table sugar

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So, sucrose is sugar?

Someone's table sugar. The name comes from the Greek word for sugar (sacchar). It might be odd to think now, but until about 200 years ago sugar was very rare in the Western world. It was so rare that it was considered to be a very valuable luxury.

So how was food sweetened?

People usually added honey, but this doesn't work well for baking, and it's tricky to add to drinks like coffee or tea. Once sugar became available, and people found out how useful, convenient and tasty it was, the demand grew hugely. Within a few years in the late 1700s it had gone from being a luxury to an important food item. In the US, molasses (made from sugar cane) and treacle (made from sugar beets) were used to sweeten drinks at the period from 1800 to 1850. Sugar was so valuable that when it was brought over across the Caribbean islands and piracy was rife, the standard coin of the Royal Navy (and of pirates) used to be rum, made from molasses. The sugar trade was so important that it led to the 'triangular trade' between Europe, Africa and the Americas. Sugar is also an essential ingredient in manufacturing alcohol, which is why many famous beverages were invented in the 18th & early 19th centuries. Indeed, in the 19th century some workers were partly paid in alcohol allowance rather than cash. It could be argued that sugar was so influential it changed the course of world history.

Really, how?

Sugar cane grows best in hot, humid climates, such as the island in the Caribbean. So from the beginning of the 18th Century a race began among European countries to colonise these areas as fast as possible, and set up sugar plantations. In 1665 the first sugar plantation was set up in Barbados, and this led to the first sugar plantation in the Americas. In the West Indies, sugar was so valuable that when it was brought over across the Caribbean islands and piracy was rife, the standard coin of the Royal Navy (and of pirates) used to be rum, made from molasses. The sugar trade was so important that it led to the 'triangular trade' between Europe, Africa and the Americas. Sugar is also an essential ingredient in manufacturing alcohol, which is why many famous beverages were invented in the 18th & early 19th centuries. Indeed, in the 19th century some workers were partly paid in alcohol allowance rather than cash. It could be argued that sugar was so influential it changed the course of world history.

What exactly is sucrose?

Sucrose is a disaccharide, which means it is made up of two monosaccharides (simple sugars) joined together. The two monosaccharides in sucrose are glucose and fructose. The chemical structure of sucrose is shown below. The chemical structure of sucrose is shown below. The chemical structure of sucrose is shown below.

O[C@@H]1[C@H](O[C@@H]2[C@@H](CO)O[C@H](CO)O2)O[C@H](CO)O[C@H](CO)O1

The MOTM page for May 2014 was about sucrose.

The original idea was that the 3 founders would each only write the occasional MOTM article; most of the content (it was hoped) would be written for us by willing volunteers from around the world. This was broadly true for the first 5 years or so, with contributions coming from a whole range of authors drawn from across the globe. Most have been from the University sector, but some have been written by chemists in industry, and some by schoolteachers and students, the youngest being 15 year old Layth Hendow, of Hull Collegiate School, Yorkshire, who wrote about Teflon [2]. Some of the earliest MOTM articles were short and rather basic. But the more recent ones have been quite detailed

essays, with scientific diagrams, videos, synthetic reactions schemes, more reminiscent of mini-review papers than web pages.

Other ‘molecule’ sites followed in their wake, such as one based at Virginia Commonwealth University in the USA, or at Prous in Spain, but gradually many of these have fallen by the wayside. Others have grown up in the blogging sector. One of the issues that began to emerge around 2000 was that of legal liability for the content of the sites. At Oxford and Bristol, we were getting undergraduate students to write small MOTM pages as web projects (originally sponsored with prizes by the RSC as part of their *Exemplarchem project*), the best of which were then becoming that month’s official MOTM. An example of this is the MOTM page about capsaicin, written by the then Bristol undergraduate Matt Bellringer [3]. The issue was that the university was effectively publishing scientific documents that had been written by students, and potentially full of errors. Even back then, the university lawyers began to worry whether the university might be laying itself open to litigation if someone read a factually incorrect MOTM written by a student, and then acted on this false information, e.g. if they tried to follow a synthesis recipe which led to an accident, or ingested a chemical they’d read was non-toxic, only to find the author hadn’t checked their facts properly! In light of these worries, Karl Harrison decided to take all the Oxford MOTM pages off the Oxford University server, and place them onto an independent server operated by the company 3dchem.com [4], and ensuring that all content was verified by him. The main MOTM site, however, carried on regardless, except that all content became much more carefully vetted. In fact, the only MOTM page that was ever withdrawn was one about sarin nerve gas (March 1999) because it contained rather too much detail about the precursors and the synthesis procedure than was deemed expedient – even though those details were freely available in the scientific literature (and still are available on Wikipedia and the wider internet).

As time passed, some of the innovations that accompanied the early web – like Chime or VRML (which allowed 3D structures to be displayed inside webpages) – have faded into history, but HTML versions have been the backbone of the Bristol site. Even though some users might not have Chime or Java installed to help them visualise some of the graphics, there has always been a HTML version “open to all”.

Hemoglobin



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Also available: Chem-enhanced, PDF, and VML versions.

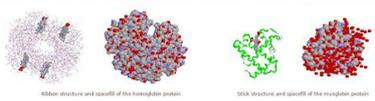
Myoglobin and Hemoglobin - the Oxygen Carriers

Most living organisms perform respiration, the breakdown of food products to release energy in the presence of oxygen. However oxygen is not very soluble in water, and so in order for animals to convey oxygen from the lungs (or gills) to the muscles they needed to evolve an efficient oxygen-carrying molecule. In vertebrates, these molecules are the proteins myoglobin and hemoglobin.



Red blood cells (above) contain hemoglobin. Blood is high red (left), due to the presence of oxy-hemoglobin.

Hemoglobin (or haemoglobin, frequently abbreviated as Hb), which is contained in red blood cells, serves as the oxygen carrier in blood. The name hemoglobin comes from **heme** and **globin**, since each subunit of hemoglobin is a globular protein with an embedded heme (or haem) group. Each heme group contains an iron atom, and this is responsible for the binding of oxygen. The presence of hemoglobin in blood increases the oxygen-carrying ability of a litre of blood from 3 to 200 ml. Hemoglobin also plays a major role in the transport of carbon dioxide from the tissues back to the lungs. Myoglobin, on the other hand, is located in muscle, and serves as a reserve supply of oxygen and also facilitates the movement of O₂ within muscle.



HbMon structure and spawill of the hemoglobin protein. MbMon structure and spawill of the myoglobin protein.

The Heme Porphyrin

Although the hemoglobin and myoglobin molecules are very large, complex proteins, the active site is actually a non-protein group called heme. The heme consists of a flat organic ring surrounding an iron atom. The organic part is a porphyrin ring based on porphyrin (a tetrapyrrole ring), and in the back of a number of other important biological molecules, such as chlorophyll and cytochrome. The ring contains a large number of conjugated double bonds, which allows the molecule to absorb light in the visible part of the spectrum. The iron atom and the attached protein chain modify the wavelength of the absorption and gives hemoglobin its characteristic colour. Oxygenated hemoglobin (found in blood from arteries) is bright red, but without oxygen present (as in blood from veins), hemoglobin turns a darker red. Venous blood is often depicted as low in colour in medical diagrams, and veins sometimes look blue when seen through the skin. The appearance of blood as dark blue is a wavelength phenomenon of light, having to do with the reflection of blue light away from the outside of venous tissue if the vein is ~0.02 inches deep or more.



Porphyrin: the building block of heme.

The MOTM page for February 2006 was about hemoglobin.

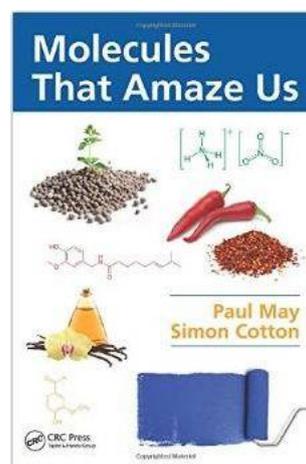
The emergence of Wikipedia has seen that develop as a free repository of factual information about chemicals, and there are also readily available databases of spectroscopic data (such as the Spectral Database for Organic Compounds, SDBS [5]). Not long after Wikipedia became established, we saw a large drop in MOTM hits, and a reluctance for authors to write new MOTM pages. After all, why would anyone bother reading a MOTM page when all the facts you could ever possibly want about every molecule are on Wikipedia?

Original MOTMs often featured research advances of interest to the authors, and the style could be rather academic. What was needed was a change of style, to differentiate a MOTM article from a Wikipedia entry. This was brought about by Simon Cotton's first MOTM about tetraethyl lead in Jan 2001 [6]. The innovation was to write the article in a question-and-answer style, which chunked the information up into a series of short paragraphs, in the form of a curious student asking questions of a knowledgeable, patient, but long-suffering teacher. Simon's background as a "long-suffering" schoolteacher was ideal for this, and this style let a breath of fresh air into the tired MOTM format. Nearly all the MOTMs nowadays use this style, and the MOTM articles have continued to be posted monthly, not a bad achievement after 20 years! We try to aim at a level that is readily understood by a motivated 18-year old, and experience (and feedback) tells us that many adults from a non-scientific, even arts background find interesting content that they had not expected to encounter. So many molecules are fantastic in terms of what they do. The MOTM site compasses a vast range of them, found everywhere from foodstuffs to medicines; explosives to toxins. It exists to convey a little of our contributors' wonderment to a wide readership. We don't just concentrate on the facts, but try to weave an interesting story about the history of that month's molecule, its role in modern society (including references

to rock/pop music, Hollywood films/filmstars, TV programmes, historical figures, *etc.*) and its good and bad points. For controversial molecules (DDT, thiomersal, bisphenol A, *etc.*) we try to remain neutral, tell both sides of the story, and let the reader make up their own mind. After all, molecules are morally neutral until humans start to interact with them or use them.

Even within the first 5 years of the website, we'd started to notice that articles contributed by external authors and hosted on their websites were not as permanent as we'd hoped. MOTMs would disappear, either because in the years since the article had been written the host server had been replaced, or the author had moved jobs, or in two cases because the authors had died and their webpages (and our precious MOTM article) deleted! Luckily we'd made local backups of these pages, so simply switched the link. But it made us worry about the permanency of the MOTM project. After 20 years, we have nearly 240 MOTM articles, which include a wealth of data and information that would be a shame to lose, if say, Bristol University decided it no longer wished to host the site in future.

Partly to get around this legacy issue, we decided to publish our favourite 60 or so MOTMs in a more long-lasting format – a paper book! Selected articles were rewritten (in the Q&A style) to make them more accessible to a general audience, with less detailed chemistry (synthetic recipes, *etc.*) and more interesting anecdotes, 'fun facts', cartoons, and pictures, and these were collated and published in a book called '*Molecules that Amaze Us*' [7].



The cover of the book.

We were originally concerned that people would not buy a book if a large part of its content was already freely available online, but we needn't have worried. It seems that the book has actually inspired readers to come back to the website, with hits increasing from 2,500 to nearly 10,000 per month in the year since the book was published. (Okay, it's not at the same level as a Youtube video of a piano-playing cat, but for a factual scientific site, that's not bad). So, it's turned full circle – the website inspired the book, which inspired people to view the web site. So far in 20 years the MOTM pages have had over 4 million hits, which is nearly 20,000 readers per MOTM article (which is far more than any of our Journal scientific papers could ever achieve).

So where will the MOTM project go in the next 10 years? There are still plenty of interesting molecules to write about, and judging from the number of hits, the readership still seem keen to read about them. The original goal of having the MOTM content written by numerous external contributors didn't really pan out. Nowadays, only about 2-3 MOTMs per year are written by volunteers, with the remainder being written alternately by the authors of this article. We'd be keen on getting feedback from readers as to how to

improve the site, or how to get more general engagement, particularly from authors (or volunteers to write a MOTM or two!). Are there any new display technologies we should adopt (noting that most of the previous ones didn't last long)? Or should we forego the transient webpage format entirely, and stick to the tried-and-tested permanency of a book?

[1]. MOTM website at Bristol University - <http://www.chm.bris.ac.uk/motm/motm.htm>

[2] *Teflon* (MOTM June 2009) - <http://www.chm.bris.ac.uk/motm/teflon/teflonh.htm>

[3]. *Capsaicin* (MOTM April 2001) - <http://www.chm.bris.ac.uk/motm/chilli/>

[4]. www.3dchem.com

[5]. http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

[6]. *Tetraethyl lead* (MOTM January 2001) - <http://www.chm.bris.ac.uk/motm/leadtet/leadh.htm>

[7]. P.W. May & S.A. Cotton, *Molecules that Amaze Us* (2014, Taylor and Francis, New York)