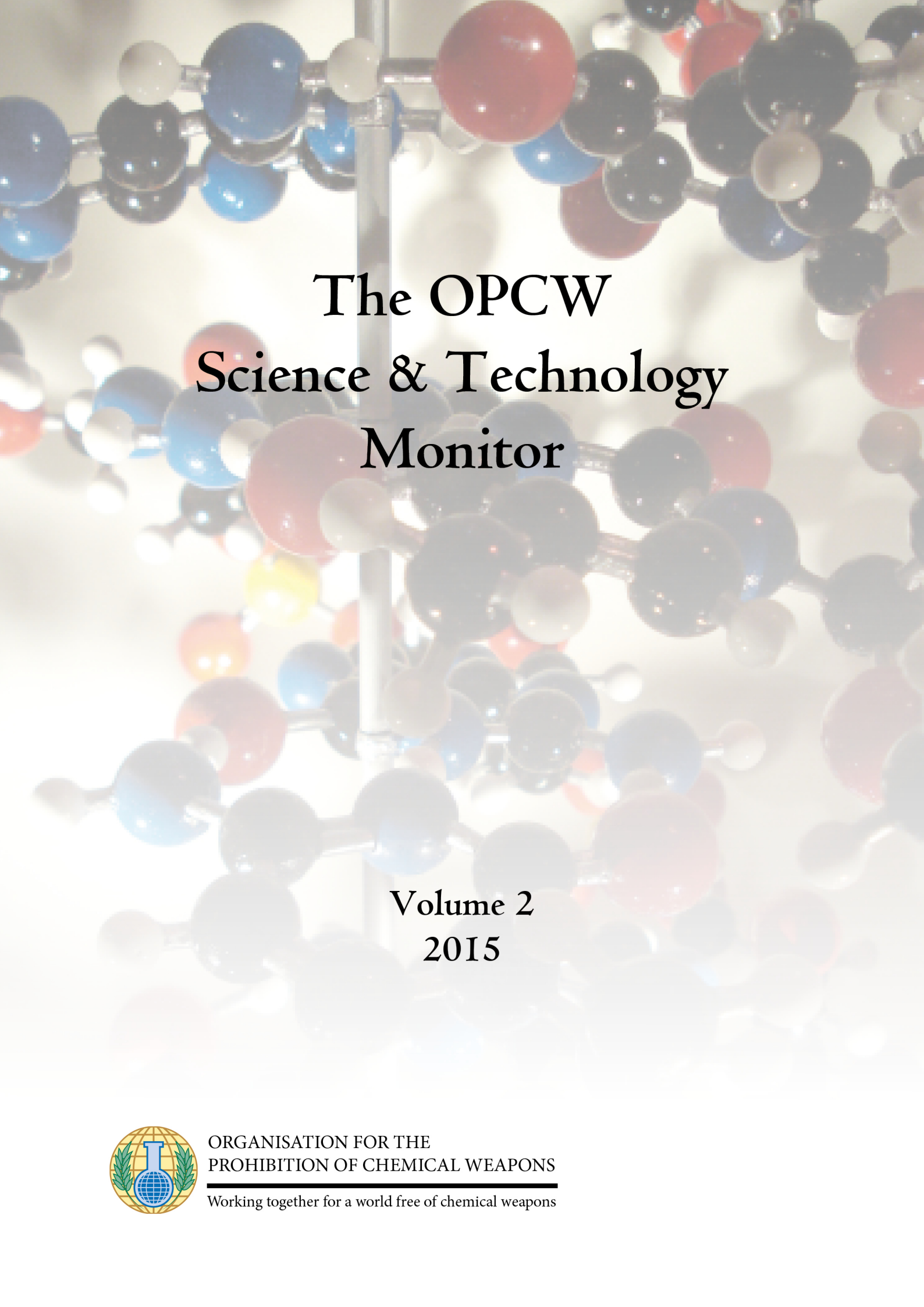

The OPCW Science & Technology Monitor

Volume 2
2015

ORGANISATION FOR THE
PROHIBITION OF CHEMICAL WEAPONS

Working together for a world free of chemical weapons

The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention (CWC)

A compilation of volume 2 (2015 edition) of the *OPCW Science & Technology Monitor* produced by the Office of Strategy and Policy. Original issues can be downloaded from the OPCW website: www.opcw.org/special-sections/science-technology/science-technology-monitor/

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Printing: OPCW Reprographic Centre

Foreword

Bringing the S&T Monitor to life in 2015!

The OPCW Science and Technology Monitor

We are fortunate to be living in an era of unprecedented scientific advancement and technological innovation. Technologies once confined to the realm of science fiction are today a reality, with breakthroughs and new discoveries continuing to capture our imagination and find their way into our daily lives. Recognising where new technologies benefit our work or present new challenges is an important on-going activity at the OPCW. As we keep abreast of advances in S&T, we find many interesting (as well as entertaining) examples of new discoveries and innovations that we share through our Science & Technology Monitor.

The OPCW Science and Technology Monitor began as an intern project in the Office of Strategy and Policy to provide updates on recent scientific developments and events. Through the efforts of all those involved, the project has evolved into a platform for both keeping abreast of science and science communication. We present this compilation of the materials produced in 2015 to celebrate the efforts of our intern staff and the support they have received by our subscribers.

Archives from past OPCW Science and Technology Monitor issues are available from the OPCW Website at:

www.opcw.org/special-sections/science-technology/science-technology-monitor/

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A sampling of Science & Technology relevant to the Chemical Weapons Convention

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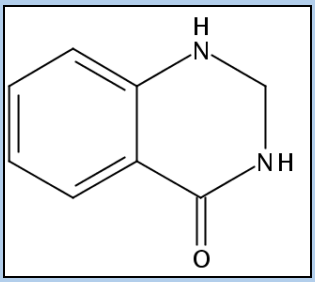
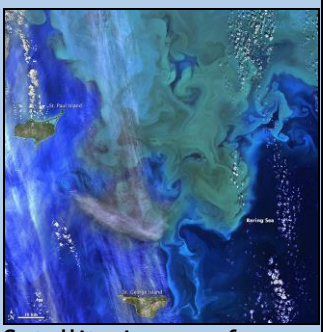


Derivatives of 2,3-dihydroquinazolin-4(1H) for blocking the toxic effects of ricin.



Satellite image of a phytoplankton bloom near Alaska's Pribilof Islands (image from NASA). Algae blooms are a potential source of saxitoxin!

Welcome

Welcome to our first *OPCW Science and Technology Monitor* of 2015, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Office of Strategy and Policy (on our portal or by request).

Friday 23 January 2015 marks the 119th the anniversary of the x-ray image of the hand of Albert von Köllikers, obtained as part of the presentation of Wilhelm Conrad Röntgen to the Wurzburg Physical Medical Society. Today x-rays are an important tool for understanding bimolecular structure. We mark the day with an S&T contribution to the OPCW digital diplomacy initiative by going live on Twitter, follow us @OPCW_ST!

The S&T Puzzle

Congratulations to Arjan Louter (once again from VER) for finding all the pictures (with face hidden and visible) of Amir Imani (of both OSP and IVB) in the Port Annual Report. Puzzle stats now stand at VER 3, OCS 1.

For our next challenge, we are looking for the total number of patent grants that include examples and/or claims related to Schedule 1 chemicals from 1946 – 2014. Closest estimate wins the prize of choosing our next featured topic, designing the next puzzle or a gift of a special beverage hand selected by the Science Policy Adviser. Good luck!

In addition to the puzzle, we offer one more chance at the prize. With our foray into social media, we are in need of an avatar that creatively ties Science and Technology to the OPCW. Got any good doodles, catchy phrases or flashy graphics that you would like to see starring in future newsletters? Send it to us at SciTech@OPCW.org. Best submission (as chosen by our staff) wins!

In this issue:

Science Fun:

How are you keeping up with your 2015 New Year's resolutions? How do your resolutions compare to those of world-renown scientists?

Fans of the Back to the Future movies should find 2015, the year in which the 2nd film of the series took place, to be quite special. Take a look at how well the 1989 film predicted the future.

Other attempts at predicating 2015 came from the world of think tanks (see how well they did in the complete report).

Of course, both the movie and the think tank report neglected to mention that 2015 will be one second longer than previous years. No need to panic, there is a mitigation strategy in place.

As the year unfolds, you may want to see how good these science predictions for 2015 (based on the best data available from 2014) turn out.

For a bit of inspiration, take a look at some of the cool science we might expect to see in 2015 and beyond!

One thing we do know will hold true in 2015 is our love of gadgets! Yet, some fear these same gadgets may be infringing on our

News and Updates

Recently Published Reports:

Dstl scientists have edited and contributed to an issue of *Best Synthetic Methods* devoted to organophosphorus (V) chemistry.

2015 Chemical Outlook by Region and by Market from *Chemical and Engineering News*.

A User's Guide for Evaluating Learning Outcomes from Citizen Science.

Mobile Apps

A mobile app for biodetection technology information from PNNL.

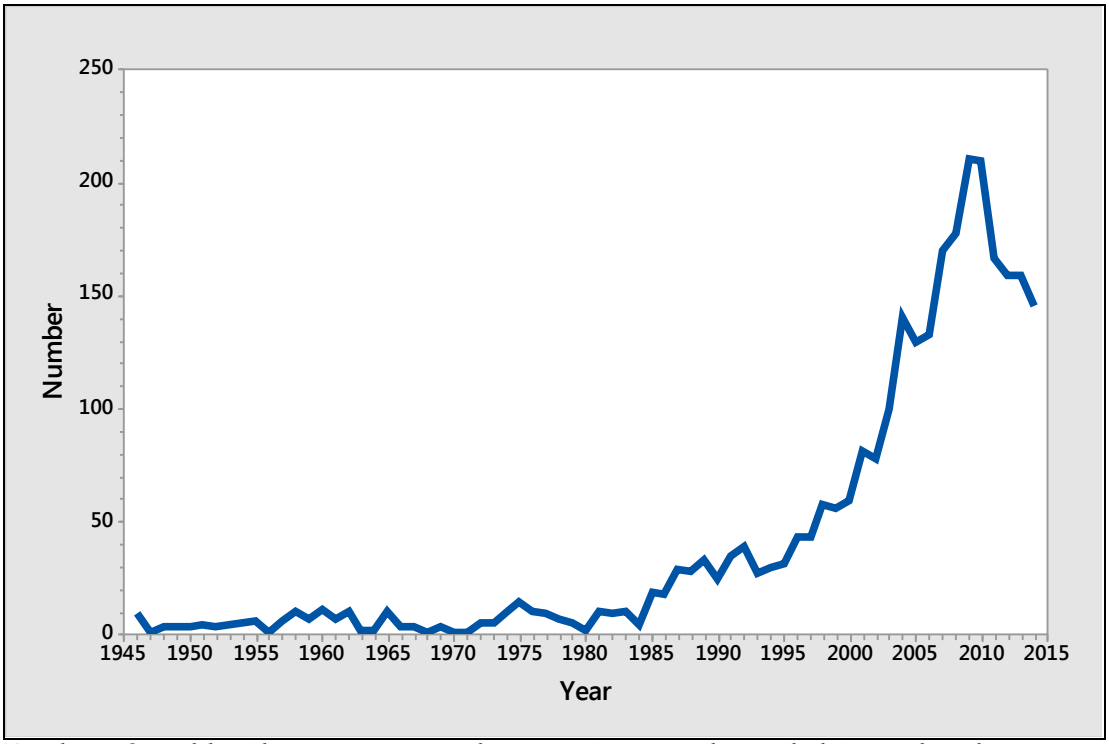
Mobile apps for science from AAAS.

Making News in Chemistry:

From 28 December 2014 - 3 January 2015; from 4 -10 January 2015; and from 11 -17 January 2015.

Schedule 1 Chemicals in 2014 Patent Grants

The references to patents containing examples and claims related to Schedule 1 chemicals in previous issues of the *S&T Monitor* generated significant interest (even surprise) from our readers. Yet, these types of patents are not unusual; see for example, the chart below showing the number of patent grants related to Schedule 1 chemicals from 1946 – 2014 (data was collected using SciFinder®).



Number of world-wide patent grants that contain examples and claims related to Schedule 1 chemicals from 1946 – 2014.

privacy or even compromising our security! Not to mention that our own possessions may be spying on us!

Leave it to technology to save us from technology! For example, worried about the security of data transfer between devices? Technologies now exist that allow data transfer through your body to reduce the risk! Privacy can also be protected by means of biometrics, some which you may not have yet heard of.

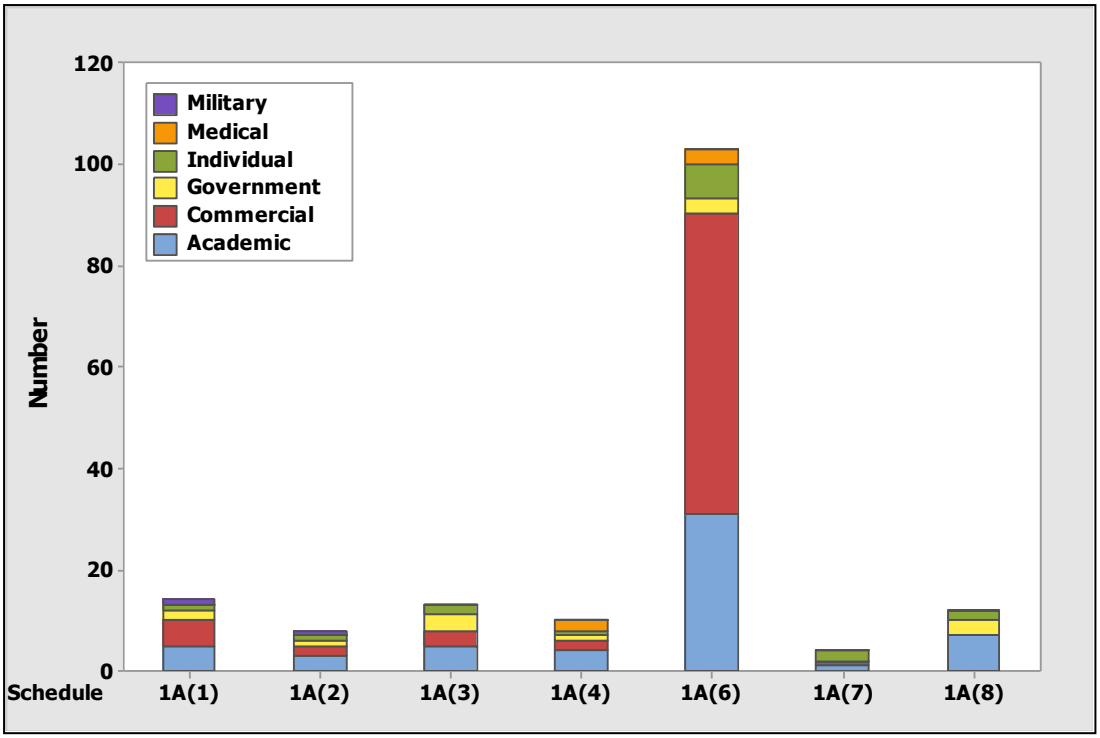
A simple solution to the privacy issues could be to just not use gadgets, but don't be so sure... Even your own biology can give you away, as demonstrated by a chewing gum collecting artist! On the bright side, the artist sells a perfume to allow you to cover your genetic tracks! One can even learn the details of your diet, centuries after your last meal!

It appears that 2015 is off to a very good start, we may not be flying on hoverboards (well most of us that is), but there are all kinds of enabling and fun technologies available to us. Of particular interest to those of you living in The Netherlands, we offer wheels and handlebars for your bicycle.

As observed in the figure, the majority of these patents were actually granted after the entry into force of the Chemical Weapons Convention in 1997! Of course, these patents fall under section titles (scientific areas of inquiry as defined by SciFinder®) not prohibited by the Convention. For patents represented in the chart, > 50% are related to nitrogen mustard, Schedule 1A(6), and > 60% have a medical or toxicological context.

As of 21 January 2015, we were able to identify 146 patents granted during calendar year 2014 with examples and/or claims related to Schedule 1 chemicals (there may be still more as the final publications from 2014 are updated into searchable databases). The patented inventions include many examples of sensors and analytical equipment that can detect chemical warfare agents, along with health care related methodology (such as identifying biomarkers for disease diagnosis and therapy).

The Schedules covered by the patents and the types of organisations to which the patent grants have been assigned are provided in the chart below. For those readers interested in more specific information on individual patents, a detailed summary table is available upon request.



Number of patents granted in calendar year 2014 shown by Schedule (columns) and the type of organisation represented by the patent grant assignee (stacked colours). Note that many patents cover chemicals from multiple schedules (there is some overlap of the individual patents described in the chart between the plotted categories).

2014 Patents Containing Examples and/or Claims from Schedules 1A(1), 1A(2), and/or 1A(3)

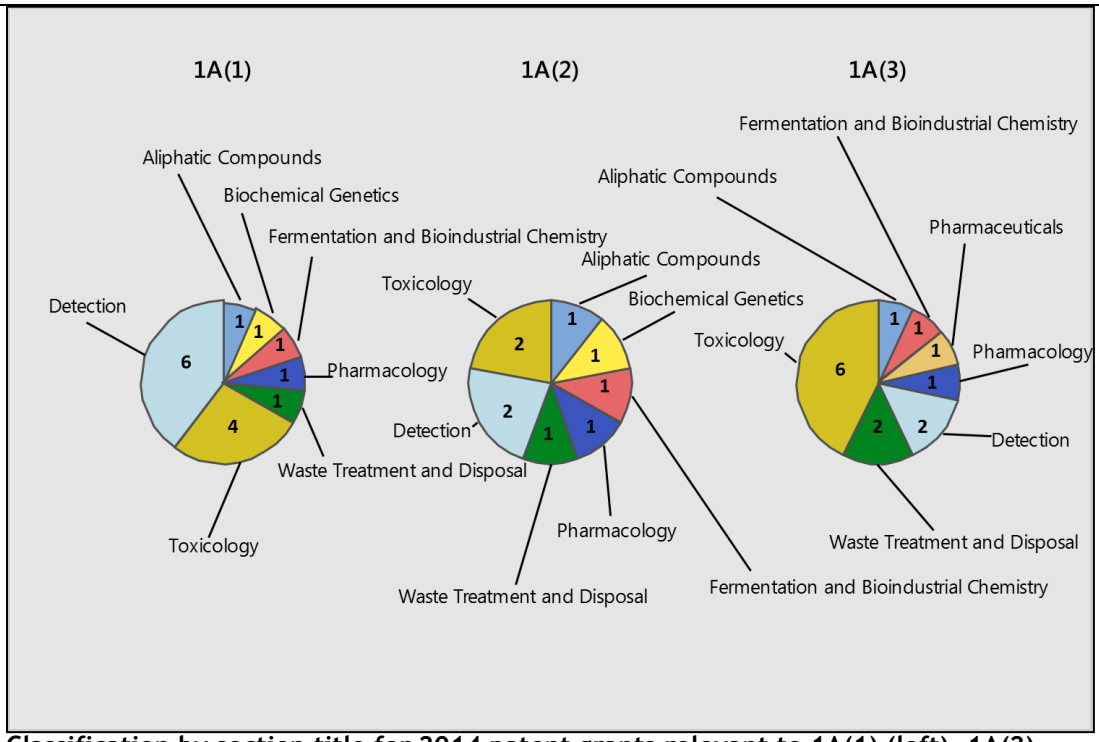
Individual patents encompassing work on organophosphorus nerve agents generally include all three of the Schedules 1A(1), 1A(2) and 1A(3) in the examples and claims. To reflect this, the following word cloud and pie charts summarise the text of the combined abstracts and section titles of the relevant 2014 patents.

Crowdsourcing:

Call for contributions to an African Moon Mission. (details here).

Have you taken any nice wildlife photographs recently? Interested in using them to help scientists understand animal migration?

And one final crowd source for today, this time for the *S&T Monitor*. Have a hidden photographer or artist within you? Here's a chance to showcase your talent! We are looking for photos we can use for our (in progress) OPCW S&T webpage and in conjunction with our S&T social media activities. If you have pictures relevant to S&T and OPCW that you can share, please send them (with photo credits and caption) to SciTech@OPCW.org.



Classification by section title for 2014 patent grants relevant to 1A(1) (left), 1A(2) (centre), and 1A(3) (right) chemicals.

Word cloud derived from abstracts of 2014 patent grants relevant to Schedule 1A(1), 1A(2), and 1A(3) chemicals.

As nerve agents disrupt neurological function by targeting the enzyme Acetylcholinesterase, much of the terminology in the word cloud relates to such processes. Patents were also found to contain examples and claims involving thrombopoietin (a regulator of platelet production) and Thrombopoeiten mimetics. These substances can increase platelet production to treat bone marrow injury induced by exposure to chemical agents or radiation. Thrombopoetin also appears in many of the patents related to sulphur mustards as illustrated below for 1A(4) chemicals.

2014 Patents Containing Examples and/or Claims from Schedule 1A(4) (Sulphur Mustards)

Relevant inventions related to sulphur mustard include methods of detecting aerosolised agents and detoxification.

Upcoming S&T Related Events:

28 - 29 January 2015
5th Meeting of the Scientific Advisory Board's Temporary Working Group on Verification. The Hague

4 - 6 February 2015
The Unmanned Systems Expo 2015. The Hague

12 - 16 February 2015
AAAS Annual Meeting 2015: Innovations, Information, and Imaging. San Jose, California, USA.

21 - 26 March 2015
249th American Chemical Society (ACS) National Meeting & Exposition. Denver, Colorado, USA.

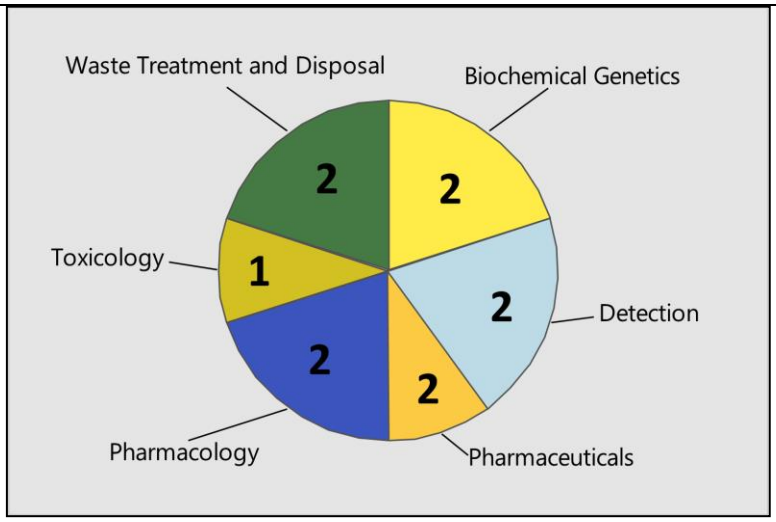
During the open session of the ACS Board of Directors meeting, the 2013 Nobel Peace Prize recipient, the OPCW will be honoured for its work in finding peaceful applications of chemical sciences worldwide.

6 - 7 May 2015
6th Meeting of the Scientific Advisory Board's Temporary Working Group on Verification. The Hague

22 - 26 June 2015
CTBT Science and Technology Conference (SnT2015)
Vienna, Austria

14 - 26 July 2015
19th Annual Green Chemistry and Engineering Conference.
Bethesda, ML, USA.

19 - 22 July 2015
12th World Congress on Industrial Biotechnology.
Montreal, Canada.

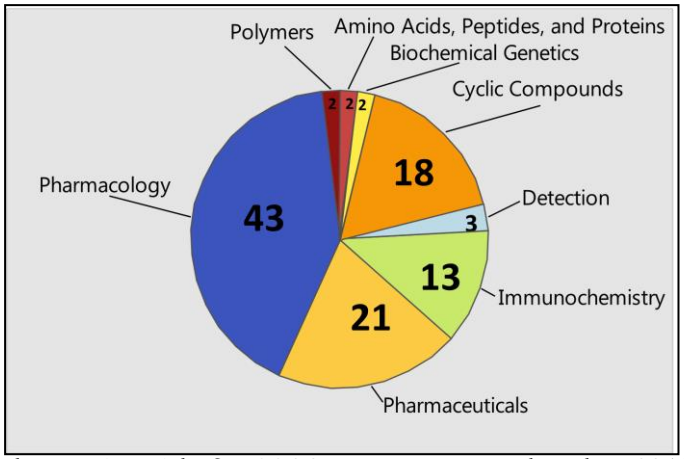


Classification by section title for 2014 patent grants related to 1A(4) chemicals.

Word cloud derived from abstracts of 2014 patent grants relevant to Schedule 1A(4) chemicals.

2014 Patents Containing Examples and/or Claims from Schedule 1A(6) (Nitrogen Mustards)

Nitrogen mustard itself is very familiar for use in chemotherapy; mustard agents were actually the first drugs used in chemotherapy. Inventions included claims related to anti-body drug conjugates and the use of 1A(6) chemicals as linkers for polymers. Other inventions were methods for the early detection and treatment of cancer.



Classification by section title for 2014 patent grants related to 1A(6) chemicals.

6 - 13 August 2015
IUPAC 2015
48th General Assembly
45th World Chemistry Congress. Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

27 September - 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering)

ECAB3 (3rd European Congress of Applied Biotechnology)

EPIC5 (5th European Process Intensification Conference)

Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

16 - 19 November 2015

Malta Conference.
Rabat, Morocco.

18 - 21 November 2015

16th Asian Chemical Congress. Dhaka, Bangladesh.

15 - 20 December 2015

Pacifichem 2015.
Honolulu, Hawaii, USA.

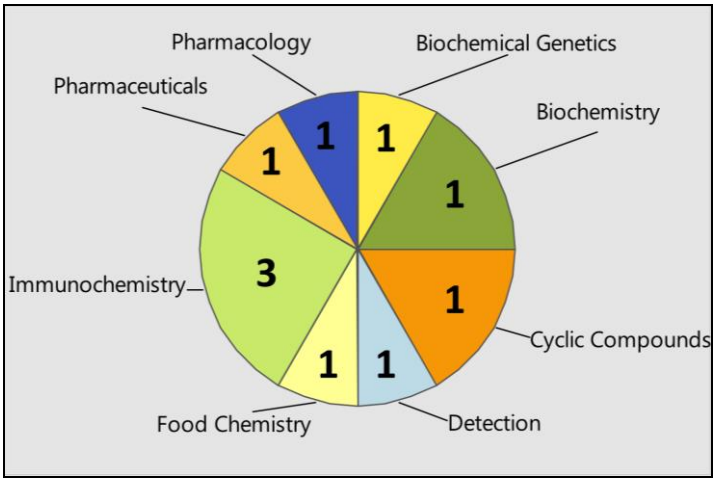
Word cloud derived from abstracts of 2014 patent grants relevant to Schedule 1A(6) chemicals.

2014 Patents Containing Examples and/or Claims from Schedule 1A(7) (Saxitoxin)

There were a total of six patent grants mentioning saxitoxin. The inventions included disease detecting diagnostic devices and even the treatment of neuropathies. We are not including a word cloud summary here as not all the patents actually included saxitoxin in the claims and several were only available without abstracts (the publications are included in our 2014 patent report for those interested).

2014 Patents Containing Examples and/or Claims from Schedule 1A(8) (Ricin)

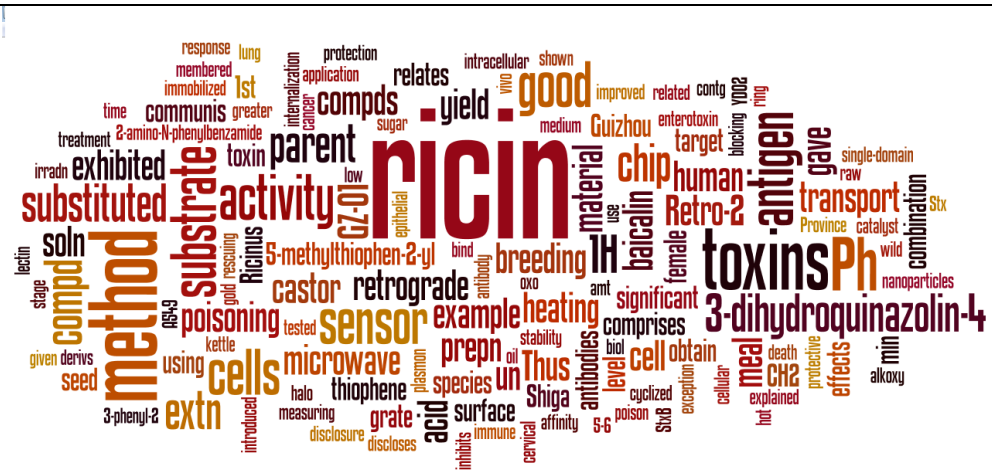
The naturally occurring toxin ricin comes from the seeds of the castor plant. As with many toxins, the biological activity provides a way to understand important intra-cellular mechanisms effecting life processes that may lead to discoveries with medicinal value. Inventions from 2014 include compounds such as derivatives of 2,3-dihydroquinazolin-4(1H) which can block the intracellular route of the toxin.



Classification by section title for 2014 patent grants related to 1A(8) (Ricin).

Contact:

Questions, comments, suggestions, or want to make a contribution? Or simply to be added to the mailing list, please contact the Science Policy Adviser in the OPCW Office of Strategy and Policy



Word cloud derived from abstracts of 2014 patent grants relevant to Schedule 1A(8) (Ricin).

Saxitoxin, Paralytic Shellfish Poisoning and Algae Blooms

While saxitoxin may not have appeared in many of the patent grants of 2014, we are alerted to scientific publications related to this toxin every week! The reason for so much attention: food safety due to the risk of, paralytic shellfish poisoning (PSP).

Saxitoxin can be produced by freshwater cyanobacteria such as *Cylindrospermopsis raciborskii* or by dinoflagellates such as *Alexandrium* which are associated with harmful algae blooms (HABs, also called red tides). The toxin commonly accumulates in shellfish coexisting with the saxitoxin producing microorganisms.

Cyanobacteria can be found in many regions of the planet; some recent publications describe testing for and detection of saxitoxin (and other cyanobacertia produced toxins) in Alaska, Croatia, Greece, Great Britain, Italy, New Zealand, and the North Eastern USA. These observations have prompted the testing of shellfish for saxitoxin in some countries. The extent to which cyanobacteria forms and toxins are expressed can be influenced by environmental conditions such as environmental nitrogen/phosphorous ratios and elevated carbon dioxide levels.

Monitoring of cyanobacteria and their associated toxins is necessary for public health purposes and new methods for quicker detection and tracking are continually being evaluated; including molecular diagnostic approaches (some of which are being patented) and analytical tools based on planar waveguides and microarrays.

Recent examples of methodologies to remove harmful cyanobacteria include the use of filtration methods and hydrogen peroxide. There are also ultrasound based methods in development that have shown both positive and mixed results.

The OPCW Science & Technology Monitor

A sampling of Science & Technology relevant to the Chemical Weapons Convention

6 February 2015 **Volume 2, Number 2**

Featured Content:

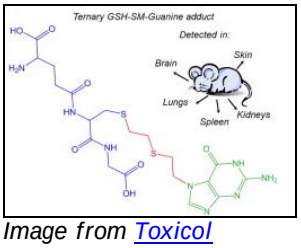


Image from Toxicol Lett.2015, 223 (1), pp 1-7.

A guanine ethylthio-ethylglutathione adduct as a major DNA lesion in skin exposed to sulfur mustard.

Image from Anal. Chem., 2015, 87 (1), pp 394–398.

Temporary paper based tattoo measures blood glucose levels.

Science Fun:

While the OPCW works toward its goal of eliminating the declared chemical weapon stock-piles on Earth, much has been happening away from Earth too!

In 2014 a Schedule 3 chemical was found on a comet. Now in 2015 on Mars, we found the long lost Beagle 2 at its crash site and organic molecules! Methane to be precise. A sign of life? Maybe the new NASA drone will confirm if something lives there.

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Office of Strategy and Policy (on our portal or by request).

Today's issue of the *S&T Monitor* arrives on the 129th anniversary of the discovery of the element germanium by Clement Winkler. Today germanium can be used as a detector in neutron beam devices for the underwater identification of toxic chemicals.

The S&T Puzzle

Congratulations to Stephane Hohn (again from VER) for his estimate of 2750 patent grants in our puzzle plot - closest estimate to the actual value of 2769! Many thanks to the others who plotted their own graphs, weighed paper or used other clever means to come to similar (but not quite close enough) estimates. We also congratulate Alexander Kelle (OSP, yes that's right) for his winning submission of the "OPCW S&T" logo. Puzzle statistics now stand at: VER 4, OCS 1, OSP 1.

For this weeks puzzle, we go beyond our newsletter and ask you to think about OPCW S&T information from across our communication channels. Have you ever wondered how many chemical substances are known? Closest estimate of the total number of chemical substances with CAS numbers (at the start of 2015) wins the prize: a choice of either choosing our next featured topic, designing the next puzzle, or a gift of a special beverage hand selected by the Science Policy Adviser. Good luck!

In this issue:

We hope so, because as observed on Earth, sometimes drones need friends who are fast on their feet!

That's not all! A space probe launched in 2006, New Horizons, has travelled over 3 billion miles to wake up at Pluto's doorstep. Meanwhile an exoplanet, with rings 200 times larger than those of Saturn, was just reported!

With such a fantastic universe, perhaps you might be interested in a vacation? Take a look at these travel posters for a few suggestions. Even if there is no life at these destinations, we may have already found alien life here on Earth! Take a closer look at these bacteria that eat and breathe electricity. To be on the safe side, one should be clean and hygienic, even on a spacecraft. To that end, take this advice for using a wash cloth.

Another handy tool to have in space is a 3D printer. Here are the tools that have been produced in zero gravity and even more 3D printable tools that have been designed to make space station life better! That 3D printer may also provide shelter upon arrival at the exoplanet! As you are more likely to gain access to 3D printers here on Earth, we offer this simple chart to help find the right one for your needs!

While you read this, you may want to prepare and enjoy an espresso – also available in space!

We now leave you with the science images of January. Over and out!

News and Updates

Recently published reports:

European Chemical Agency's (ECHA's) REACH 2018 Roadmap (full document)

CEFIC 2014 Facts and Figures for the European Chemical Industry

Results of a survey on scientists and the public from the Pew Research Center in collaboration with the American Association for the Advancement of Science (complete report here).

Presentations from the Centre for Defence Enterprise (CDE) networking event for science and technology (London, January 2015).

A blessing in the skies? A report on UAVs from The Hague Security Delta.

The Global Risks report 2015 from the World Economic Forum.

A summary report from the meeting on "Creating an Environment to Support Investment and Innovation in Synthetic Biology" (hosted by the UK Synthetic Biology Leadership Council and US National Academies' Forum on Synthetic Biology, October 2014).

From our Laboratory: A look at the novel sample-preparation methods and strategies of the Mobile Laboratory of OPCW.

e-learning:

Courseware from Project 10 of the EU CBRN Centre of Excellence Initiative.

News from other S&T relevant organisations:

Issue 26 of Dstl's *Insight*.

January 2015 Issue of PNNL's *Currents*.

Making news in chemistry:

From the weeks of 18 – 24 and 25 – 31 January 2015.

Biomarkers for Sulphur Mustard Exposure

Sulphur mustard (HD, commonly called mustard gas due to its weaponisation in aerosolized form), is a powerful vesicant and

Crowdsourcing:

A recent discovery of a new antibiotic using an "iChip" that allowed cultivation of bacteria not previously grown in lab conditions has sparked great interest in looking across a wide range of soil samples for possibly even more new antibiotics. Want to contribute some dirt? Sign up here.

How about a $1,000,000 digitization competition? Beware it might be a little buggy!

With all the science fun of the universe, perhaps you are interested in helping scientists to learn about Mars? NASA invites you to take part in a citizen science project by becoming a Martian! Or play the Cerebus game and actually map real planets!

Finally, how about some feedback for us – we are looking for suggestions for newsletter format and layout as well as any pictures that can be shared of subject matter relevant to S&T and OPCW, please send it all! (Please include credits and captions with photos).

Upcoming S&T Related Events:

12 – 16 February 2015
AAAS Annual Meeting 2015: Innovations, Information, and Imaging. San Jose, California, USA.

16 – 18 March 2015
CBRN – Research and innovation. Antibes - Juan-les-Pins, France.

biologically cytotoxic agent with a well characterised toxicological profile. "Mustard poisoning" is brought about by inhalation or exposure to the eyes and skin. First used as a chemical warfare agent in 1917, sulphur mustard was also an important chemical in the early development of cancer chemotherapy drugs.

Sulphur mustard containing munitions, the legacy of wars from the 20th century, continue to pose a hazard in several parts of the world. Injuries from sulphur mustard have also been reported at chemical weapon storage facilities. On the positive side, clean up of abandoned chemical weapon sites has produced technology to help keep workers safe from exposure (details here).

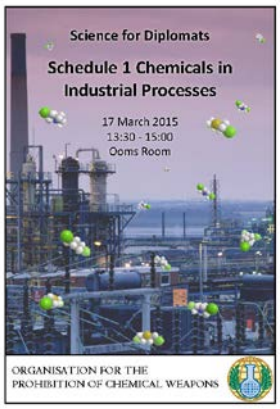
For medical purposes, recognizing exposure to sulphur mustard is important to ensure victims are properly treated. Evidence of exposure can be determined through analysis of hydrolysis/oxidation products, ß-lyase metabolites, DNA adducts and hemoglobin adducts from biomedical samples. Biomarkers (i.e. substances that can act as indicators of some biological state or condition) indicative of sulphur mustard exposure include guanine-ethylthioethyl-glutathione adducts and other DNA adducts in exposed skin, and plasma proteins obtained from blood samples. It is also possible to detect exposure using hair. To ensure the safety of those that study toxicity of sulphur mustard in animal models, customised vapour inhalers are needed for controlling dosage and thorough training in decontamination too!

Exposure to sulphur mustard can induce long-term health problems. Clinical studies on injured veterans have demonstrated changes in serum cytokine, albumin and metalloproteinase levels compared to control groups; along with other haematological complications. Other studies have looked at gene expression and substance P levels in veterans with sulphur mustard induced lung injury.

Paper

Paper, something very familiar to us, was invented about 2000 years ago

17 March 2015
Science for Diplomats side event at EC-78. "Schedule 1 Chemicals in Industrial Processes". Ooms Room, 13:30-15:00.



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14 - 26 July 2015
19th Annual Green Chemistry and Engineering Conference. Bethesda, ML, USA.

19 - 22 July 2015
12th World Congress on Industrial Biotechnology. Montreal, Canada.

in China and today around 400 million tonnes of it are produced worldwide each year! In the twenty-first century we talk about a "paperless" world, yet many people won't give up their paper! Even a Smartphone diagnostic system requires the use of paper!

Paper also has uses relevant to our work, for example: detecting chemical warfare agents and as a platform for biosensors. In fact, paper can be used for a variety of microfluidic applications and as a platform in drug discovery. To see the potential, consider these reports on biosensors containing synthetic gene networks that can detect small molecules and viruses, paper strips for disease detection (details here) and temporary tattoos that can measure blood-glucose levels (details here).

With some redox dyes and UV light, rewritable paper can be prepared. Paper integrated with "nanowire" ink may eventually lead to the development of inexpensive medical tools. One can convert paper into a memory device with a sequence of ink-jet and screen-printing techniques. Bendable batteries based on paper platforms are even possible (details here).

Despite all the possibilities for electronic devices, there are times where only the absorptive properties of a material are required such as in expansion microscopy (details here). Likewise, paper will always have a place in hands-on science teaching and in art (especially origami)!

Bioactive Peptides

Peptides (short chains of amino acids linked by amide bonds) are one of the many types of molecules that can be defined as bioregulators (see the report of the TWG on the convergence of chemistry and biology for a more detailed definition).

Due to the bioactivity (bioregulation) of these substances, they have potential for use as therapeutics, including those aimed at preventing

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48th General Assembly
45th World Chemistry Congress. Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
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SOLVE.
Cambridge, MA, USA.

31 October - 2 November 2015
The Port Hackathon.
CERN

16 - 19 November 2015

Malta Conference. Rabat, Morocco.

18 - 21 November 2015

16th Asian Chemical Congress. Dhaka, Bangladesh.

15 - 20 December 2015

Pacifichem 2015.
Honolulu, Hawaii, USA.

diseases associated with mental health as well as for the treatment of central nervous system disorders. For example, Substance P has been proposed for use in the treatment of Alzheimer's Disease and brain tumours. Peptides with antihypertensive, antioxidative, anticoagulant, anticancer, anti-HIV and other useful properties have been identified. Bioactive peptides have also been considered for use in nutritional and food packing/preservation applications (an area of much current interest).

Sources of bioactive peptides include muscle sources, fish, milk, eggs, plants, seaweed, bacteria and fungi. Identification of therapeutic targets employ "omics" (especially "peptidomics" of endogenous bioactive peptides and their proteolysis products) and high-throughput screening technologies. Peptides, as well as some proteins, can also be chemically synthesized.

Peptides can also be used in the design of drugs for targeted delivery as binding sites on specific types of cells may recognize unique peptide sequences, enabling the possibility of non-invasive delivery routes. Yet, there are still challenges to overcome with oral delivery and ensuring adequate bioavailability of the administered drug.

Research on bioactive compounds continues to identify numerous candidates with potential medical uses, however, developing new pharmaceuticals is a lengthy, complex and (often) highly regulated process and many candidate drugs are eliminated from consideration before ever reaching a clinical trial.

Gas Masks

A chemical weapons inspector carries quite a variety of things while travelling on mission, protective equipment being the most vital for those involved in the hands on work of Chemical Weapons Convention Implementation. Perhaps the most critical piece of equipment is the gas mask. Respiratory protective equipment (e.g. gas masks) have actually been around for thousands of years, although World War I is

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For more frequent updates, Follow us on Twitter at @OPCW_ST.

where we often look to the origins of their development. School children were regularly given instructions on how to use gas masks in times of war (and some designers gave consideration to soothing fear). Gas masks can be fabricated at home with the right materials and these DIY instructions were originally published in 1942! Here is some further information on how gas masks work.

Gas mask technology has continued to advance throughout the 20th century and beyond, thanks to developments in materials chemistry. Methods for designing improved filters and for testing have continued to evolve. A more recent patent shows how designers are working towards filter canisters with convex shapes to better conform to the face of the wearer and the integration with other safety equipment (such as a helmet). There are also systems for the indication of remaining life of cartridges and canisters as well as demonstrations of masks that incorporate sensors for chemical detection. Some new gas mask designs look like they belong in a science fiction movie, and we certainly expect to see gas mask wireless devices in our future! Cleaning your mask, however, may still be quite effective with low tech methodology.

The OPCW Science & Technology Monitor

A sampling of Science & Technology relevant to the Chemical Weapons Convention

26 February 2015 **Volume 2, Number 3**

Featured Content:

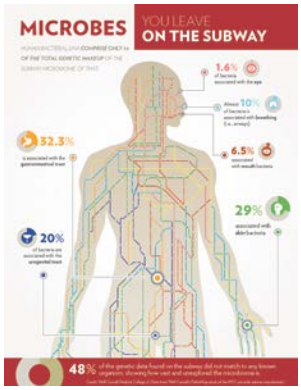


Image from Weill Cornell medical college.

The microbiome of the New York subway system.

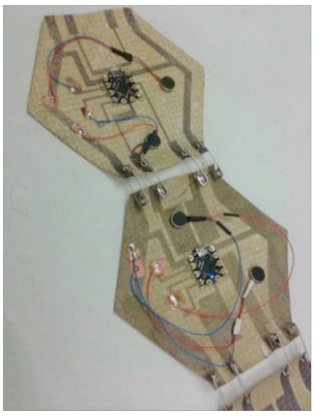


Image from geek.com

Smart scarf developed by Microsoft.

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Office of Strategy and Policy (on our portal or by request).

Today's issue of the *S&T Monitor* arrives on the anniversary of the opening of the first pneumatic powered subway line in New York City in 1870. Today, one-hundred and forty-five years later, the New York subway system uses newer technology and is home to hundreds of known and unknown microorganisms as identified by a citywide metagenomics study (details here).

The S&T Puzzle

Congratulations to Alexander Kelle (OSP) for winning the most recent puzzle with his estimate of 155,555,060 CAS numbers (closest to the reported value of >156,920,778). For those of you who were not sure where to look for the correct answer, it had been previously revealed through one of our social media posts. Puzzle statistics now stand at: VER 4, OSP 2, OCS 1.

For our next puzzle, can you guess what analysis is being performed and on what sample (in the image on the left)?

The first person to correctly answer wins the prize: a choice of either choosing our next featured topic, designing the next puzzle, or a gift of a special beverage hand selected by the Science Policy Adviser. Send your answers by email or tweet to #OPCWST. Good luck!

In this issue:

Science Fun:

The headline read: "science has great news for beer lovers", so how could we possibly not run with this for the latest instalment of science fun?

The great news is of course that the hops used to make beer contain a compound that has neuroprotective properties against oxidative-stress-induced neuronal cell damage (in other words, a chemical that can help fend off Alzheimer's and Parkinson's disease (details here). For those that don't like beer, we offer hop flavoured candy.

Empirical evidence tells us that despite neuro-protective chemicals; too much beer will adversely affect your balance. No need to worry, because it turns out that it is easier to spill coffee than beer. For those that wish to do their own experiments, be aware that magnets can be used to control the foaminess of your beverages (details here).

Even genomics has studied beer (and alcohol consumption in hominids, details here) in its quest to advance our knowledge. All this beer analysis helps us make sense of historical finds too!

Beer inspires inventions; the beer can (which celebrates its 80th birthday in 2015), for example, has enabled the production of sun tracking cameras and barbeques!

Other beverages can be scientifically interesting too. Tequila for growing

News and Updates

We are pleased to announce that funding has been received for Project III: Science and Technology from EU Council Decision (CFSP) of 17 February 2015. This was in support of the activities of the Organisation for the Prohibition of Chemical Weapons (OPCW) for the framework of the implementation of the EU Strategy against Proliferation of Weapons of Mass Destruction.

Recently Published Reports:

Report on growing a digital social innovation ecosystem for Europe.

Mobile Technologies and Empowerment: Enhancing human development through participation and innovation from United Nations Development Programme (UNDP).
The Hague Security Delta's Achievements in 2014.
January 2015 edition of *Horizon 2020 Projects Portal*.

Science and Technology Resources:

100 years of chemical weapons from *Chemical and Engineering News*.

Infographics describing G- and V- type nerve agents.

Learn chemistry and perform virtual laboratory experiments with the ChemCrafter App.

Statistics resources for biologists (and useful for chemists too!).

Easy access to Dstl innovation (details here).

A collection of images to teach and promote safe vaccine transport.

Making News in Science and Technology:

In chemistry from the weeks of 1 - 7, 8 – 14 and 15 – 21 February 2015.

A look at what are being called the top breakthrough technologies of 2015 from the *MIT Technology Review*.

Finalists for the UAE Drones for Good Award.

Winners of the 2015 science and engineering visualisation challenge (The Vizzies).
2015 marks the 85th anniversary of the discovery of Pluto.

Analytical Tools

For sampling and analysis related to the CWC, gas chromatography/mass

diamond films, wine for studying brain function, Scotch whiskey to produce art, cider to study fermentation, and the energetics of turning water into wine to teach physics (details here), just to name a few!

There is still the problem of the after effect of alcohol consumption, but science is trying to solve that too (details here)!

Crowdsourcing:

Cancer researchers need help analysing genetic information. You can contribute by playing the game, Genes in Space.

Are you good at visualising complex data? Take a look at the UNDP Human Development Data Visualization Competition.

Have any clever ideas about intravenous sustained release drug delivery technologies?

spectrometry has long been the most suitable method for routine use. As a testament to those who developed protocols and methods, OPCW proficiency tests have been recognised as a model for inter-laboratory testing. Laboratories also have access to a variety of methodology that employs mass spectrometry and other analytical tools. Mass spectrometry coupled with appropriate separation techniques can enable complex sample analysis and characterisation, as demonstrated by a recent collection of papers on global metabolic profiling.

Raman spectroscopy is another tool that has found use in chemical weapon analysis. The methodology also finds applications that include: art and archaeology, analysis of lichens, analysis of hair (details here), identifying cancer cells during brain surgery (details here), and the analysis of biomedical samples (including urine and blood). To improve the reliability of analysis, application specific automatic standardization methods are being developed.

Everyday we read about new analytical tools and methods with a broad range of chemical applications – often identified as potential tools for chemical weapons detection (as in the case of infrared-terahertz double-resonance spectroscopy and tetrahertz gas phase spectroscopy). Tetrahertz waves can also sequence short strands of DNA (details here).

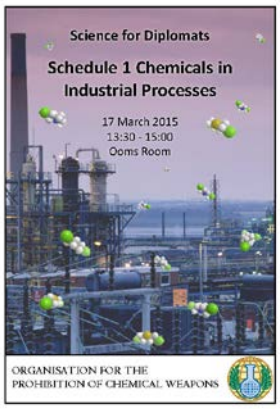
A device that exploits the semiconducting properties of a two dimensional metal-organic framework (MOF) to detect gases has been prepared for the first time (details here). MOF materials can also be used to degrade toxic chemicals. Nanotechnology based sensors with chemical weapons applications and nanosensors for explosives detection have also been demonstrated.

Other inventive approaches to detecting chemical agents use electronic "noses" and "tongues". These devices can be both bio-inspired and based on silicon devices. "Organs on chip" can be used to study the biological response to a chemical agent. The use of biological components that respond to or recognise the presence of selected chemicals is the principle behind a biosensor (these are typically

Upcoming S&T Related Events:

16 – 18 March 2015
CBRN – Research and innovation. Antibes - Juan-les-Pins, France.

17 March 2015
Science for Diplomats side event at EC-78. "Schedule 1 Chemicals in Industrial Processes". Ooms Room, 13:30-15:00.



21 - 26 March 2015
249th American Chemical Society (ACS) National Meeting & Exposition. Denver, Colorado, USA.

During the open session of the ACS Board of Directors meeting, the 2013 Nobel Peace Prize recipient, the OPCW will be honoured for its work in finding peaceful applications of chemical sciences worldwide.

19 – 24 April 2015
ALLData2015. Barcelona, Spain.

6 – 7 May 2015
6th Meeting of the Scientific Advisory Board's Temporary Working Group on Verification. The Hague.

10 – 13 May 2015
4th International Conference on Bio-Sensing Technology. Lisbon, Portugal.

integrated into microfluidic devices). Two examples of biosensor detection methods that have been applied to toxins are quantum dot fluorescence and surface acoustic waves (including Love-waves); the later with integration of the biosensor into a microfluidic device. Did you know that living plants can also be used as chemical weapon detectors (details here)?

There may be many interesting technologies out there, but one should not forget the less exotic approaches. Consider the use of imaging techniques in forensics, image analysis of sea dumped chemical weapons and detecting chemical weapons with colour (details here).

Wearable Technologies

Advancements in technology have allowed devices to become smarter and smaller! Combining cloud computing and data collection, a wealth of wearable devices are now available to consumers, especially fitness trackers. Devices such as smart belts and smart scarves may seem like novelty items, but could actually be helpful for people with disabilities; while telescopic contact lenses and wearable air pollution monitors may have scientific applications. Computers themselves can be produced in button size and still maintain Bluetooth, low-energy radio and motion sensor capabilities.

While in the consumer world, smart glasses (Google Glass for example) have had a rocky reception, these technologies can be used to make colorimetric measurements of chlorophyll levels in plants (details here). For applications, consider that Chlorophyll has been used as a detector for chemical agent exposure.

The power of wearables lies in their combination with other devices (especially Smartphones), allowing for collection and transmission of data with temporal and geospatial information in real time; applications include monitoring crowds and pollution. Accessories to turn Smartphones into personal environmental monitors are commercially available. Health monitors based on Smartphone platforms are being developed. A miniature spectrometer for chemical analysis of food will

7 - 12 June 2015
2015 AAAS-TWAS Course on Science Diplomacy, Trieste, Italy.

8 - 12 June 2015
22nd Session of the OPCW Scientific Advisory Board. The Hague

22 – 26 June 2015
CTBT Science and Technology Conference (SnT2015)
Vienna, Austria

14 – 26 July 2015
19th Annual Green Chemistry and Engineering Conference.
Bethesda, ML, USA.

19 – 22 July 2015
12th World Congress on Industrial Biotechnology.
Montreal, Canada.

6 – 13 August 2015
IUPAC 2015
48th General Assembly
45th World Chemistry Congress. Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering)

ECAB3 (3rd European Congress of Applied Biotechnology)

EPIC5 (5th European Process Intensification Conference)

Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

31 October – 2 November 2015
The Port Hackathon.
CERN

be developed if they can procure their crowd funding.

Wearables consume energy and it should come as no surprise that wearable energy sources are also being developed. We have seen solar arm bands, energy generating shoes (details here), batteries that can be spun into clothing (details here) and batteries inspired by jewelry makers. Producing power from bodily fluids with bioelectrodes (details here) is another option (for medical implants as well as wearables!).

Despite the push for miniaturization, some wearables, such as mass spectrometer backpacks and robotic devices, may always be large in size. Miniaturization of smart clothing may also create a disadvantage. Consider, for example, nanomaterials that blur faces in photographs, adhesive tape for infrared invisibility, and adaptive optoelectronic camouflage. Smart helmets enabling reduction of stress (involving a Smartphone of course), measurement of brainwaves (for mapping "fun" bicycle routes) or "bat vision" would likewise need to remain large enough to fit your head (although this could be overcome with brain-computer interfaces).

Continuous Flow Chemical Production

When we think of a chemical production facility, we often envision stirrer tanks and large volume reactors in which a "batch" of material would be produced. An accompanying "continuous flow" process might be distillation. As with many things in the world, even this is changing as continuous flow systems for chemical production are finding their way into manufacturing processes, especially for pharmaceutical applications.

Continuous flows devices may be more familiar when called "microreactors", although larger scale devices are used for industrial scale production (microreactors themselves are best suited to research applications). Continuous flow chemical synthesis has many applications for pharmaceuticals and fine chemicals. Ibuprofen production has served as a model case, with optimisation of reaction conditions leading to significant reduction of process time (details

16 – 19 November 2015
Malta Conference.
Rabat, Morocco.

18 – 21 November 2015
16th Asian Chemical Congress.
Dhaka, Bangladesh.

22 - 27 November 2015
2nd African Conference on research in Chemical Education (ACRICE).
University of Venda, South Africa.

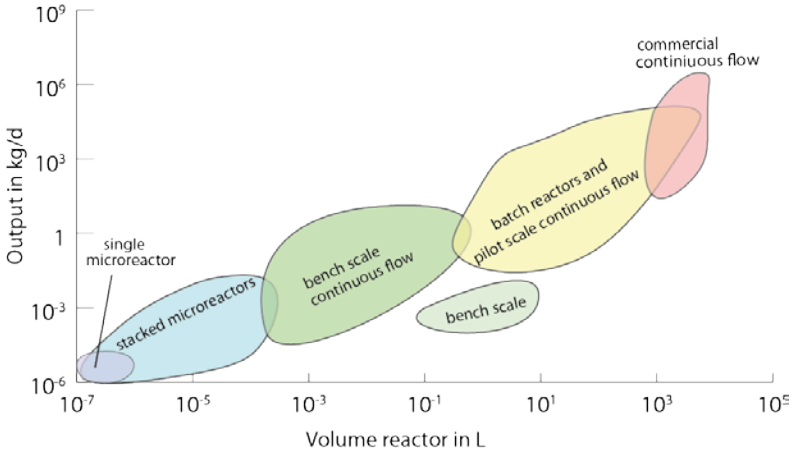
15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

here). As these synthetic methods become more integrated into research, applications for a variety of organic and inorganic chemicals, and even nanoparticles have been found. Examples of reactivity patterns that change from batch to microscale flow reactors have been reported and polymerisation processes are also possible.

Flow reactors can be customised for temperature control, gas-liquid transformations or combined with sonicators and microwave devices. When combined with analytical devices (including NMR, details here), reaction conditions can optimized in real time. Reactors can be used to flow substrate solution over stationary catalysts (details here) and with their narrow dimensions, they offer advantages for photochemical processes.

Continuous flow reactors will continue to develop and enable more chemistry, however, it is perhaps the benefits they provide to chemical safety that truly make these technologies valuable. This has been demonstrated with scaling up hazardous reactions and handling hazardous reagents.

The chart below compares the scales of chemical production from laboratory (research) to industrial batch processes, to illustrate how continuous flow systems compare with batch reactors for production capability. The size of the bubbles are illustrative not exact.



Chemical Safety and Security

Chemical safety and security (and dual-use chemicals) are topics of much interest to us, and like so many of the themes and issues we think

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about, they have strong science and technology components.

In regards to safety, we can learn much and continue to improve process safety by examining historical chemical plant disasters. Likewise, surveying safety management, collaboration and work environment in the chemical industry is a valuable way to prevent accidents from occurring. Inherent safety is an important concept that helps to mitigate hazards on a chemical plant; it is valuable to consider amongst the many factors one evaluates in plant design. Hazard identification is another important tool, as illustrated in a recent report on LNG regasification technologies. While safety management may generate bureaucracy, this is not always a bad thing. In regards to the importance of safety awareness, it has been suggested that ignorance is no form of defence!

While chemical safety looks to prevent accidents, chemical security is a more complex issue as it looks to prevent intentional and unexpected harm. Chemical supply chains are of particular interest for security considerations; their complexity lends itself to modelling with game theory. Concerns about security have prompted specialised laws and regulations in some nations and considerable discussions on chemical terrorism, vulnerability of chemical sites and analysis of how chemical weapons might still used in a 21st century world.

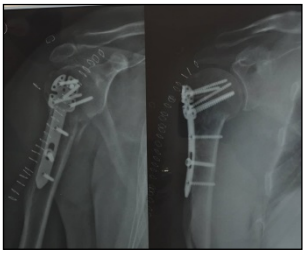
Chemical safety and security extends beyond those that work in laboratories or at chemical production facilities. Emergency responders and medical personnel must be trained on how to deal with patients exposed to toxic chemicals in case of an incident. In this regard, the February 2015 issue of *Emergency Medicine Clinics of North America* has an informative collection of articles on the management of hazardous material emergencies. For training, of course we want innovative approaches, perhaps virtual reality platforms are just that!

The OPCW Science & Technology Monitor

A sampling of Science & Technology relevant to the Chemical Weapons Convention

17 March 2015 **Volume 2, Number 4**

Featured Content:



(Bio)Materials for healing and recovery from injury.

Image from 3D Printing magazine.

Science and technology of food.

In this issue:

Welcome

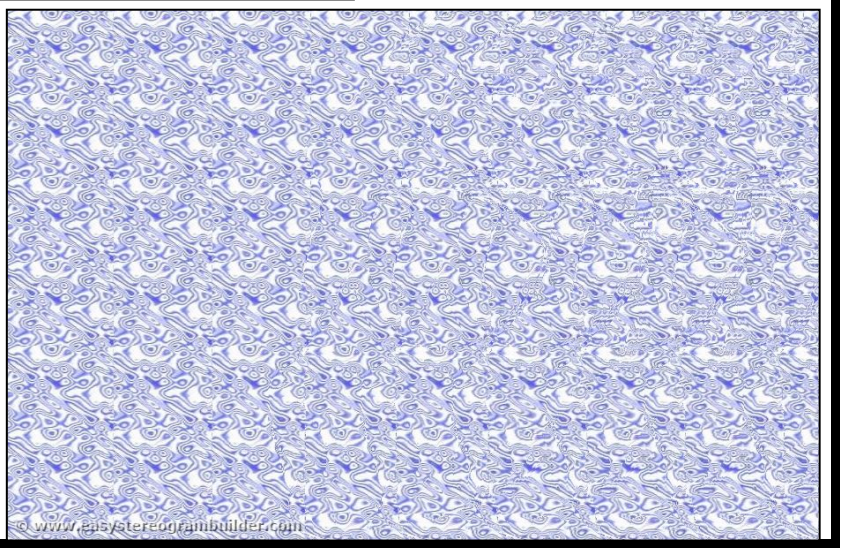
Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are now available from the Science and Technology special section of the OPCW website.

Today marks the 65th anniversary of the discovery of the element Californium at the University of California at Berkeley. Californium-252 has been used as a neutron source in devices for non-destructive identification of chemical warfare agents. As residents of California, are more likely to recognize 17 March for being St. Patricks Day; we offer them a home science experiment with a "green" theme.

The S&T Puzzle

We have our first non-OPCW winner! Congratulations go to a subscriber from the CTBTO, who recognized the ultrasonic pulse echo analysis on a single container of a chemical agent (photo revealed on the left). Statistics now stand at: VER 4, OCS 1, OSP 2 and CTBTO 1.

For the next puzzle, we ask you to identify the familiar item depicted in the image to on the right. First person to correctly answer can choose a featured topic, design a puzzle, or receive a beverage hand selected by the Science Policy Adviser. Send answers by email or tweet to #OPCWST. Good luck!



Science Fun:

As our colleague from the Lab (shown below) constantly reminds us, what could possibly be more fun than toys?

We also know that toys are valuable tools for science. They can be used to encourage career paths, teach math and physics (details here), build 3D printers, provide hours of intense study when combined with a washing machine or inspire real-world smart building materials; and all of that can be done just with LEGO®!

There are certainly other science toys to be found including 3D printing pens! Like so many of the objects that surround us, toys too can be controlled by apps on Smartdevices. You might even want to try controlling marionettes with drones (not for commercial purposes though because this has already been patented)!

Moving from toys to games, one can learn how to create devices with synthetic biology or simulate (and figure out the best way to survive) a zombie apocalypse (play for yourself here). Machines can also learn

News and Updates

Recently published reports and newsletters:

Industrialization of Biology: A Roadmap to Accelerate the Advanced Manufacturing of Chemicals from the National Academies Press (can be read online).

Final Report of the Expert Panel of Technology and Innovation in UN Peacekeeping.

Issue 20 of *inno4dev* (UNDP Innovation News Update).

January-February 2015 OECD news on innovation, science, technology and industry.

Hospital and Healthcare Security (Sixth Edition).

Report on Global Strategic Trends out to 2045 from the UK Ministry of Defence.

Science resources:

Visualisation tools for geographic data.

After school science resources from AAAS.

Science teacher resources from Science Friday.

Celebrate "Brain Awareness Week" with this collection of educational materials.

Some news from world of science:

From the weeks of 22 – 28 February; and 1 – 7 and 8 – 14 March 2015 in chemistry.

Enjoy the science images of the month from *Nature* and the 2015 Wellcome Trust best science images.

Biomaterials

It is not always easy to remain injury free (just ask our science adviser), but there is good news to be found from scientific developments in the field of biomaterials. Historically, many materials employed in injury recovery have seemed a bit barbaric (nuts and bolts really)! However, modern biomaterials are being engineered to interact with components of living systems to impart therapeutic benefits.

3D Printing has been an enabling technology in the field of biomaterials:

to play games, unfortunately this may result in an unbeatable poker player (details here).

Inevitably, the combining of Smartdevices with toys has created some legal questions. For those that prefer simpler ways to have fun, hovering Styrofoam or a collection of science toys from before the days of Smartphones may be of greater interest.

Crowdsourcing:

Want to develop mobile applications, software, hardware, data visual-ization and/or platform solutions to contribute to space exploration and improve life on Earth? Join the International Space Apps Challenge.

Seeking a wearable alcohol biosensor! As a reference point, here's how a breathalyzer works.

Develop a diagnostic test to combat antibiotic resistance (and win a one million Euro prize!).

Upcoming S&T Related Events:

21 - 26 March 2015
249th American Chemical Society (ACS) National Meeting & Exposition. Denver, Colorado, USA.

During the open session of the ACS Board of Directors meeting, the 2013 Nobel Peace Prize recipient, the OPCW will be honoured for its work in finding peaceful applications of chemical sciences worldwide.

commonly implantable materials, such as titanium can be printed into pelvic and shoulder bones; and in the engineering of tissues and artificial organs, water-based gels containing synthetic DNA and peptides (details here) along with the use of DNA strands as a glue to hold biocompatible materials together (details here) offer great promise.

The use of hydrogels (such as those described in the 3D printing references) may also enable advances for implantable devices (such as heart valves and devices to treat hearing disorders).

Nanofibers derived from collagen (obtained from fish skin) have been demonstrated to aid in skin regeneration (details here) and there are "Smart" bandages that can deliver medicines (details here) and monitor vital signs. Simple methods to create nanoparticle based antibacterial and antifungal tapes have also been reported (details here).

Injectable materials with wound healing properties are another area of interest; these include platelet mimicking nanoparticles and compounds that stop wounds from bleeding (details here). Similar principles have aided the healing of injured grape vines (details here).

Food and Science

Like so many of the day to day things we experience in the world, our food has highly complex science behind it and there is much to learn by studying food. Consider the field of "foodomics" – an area of study that employs omics methodologies across the food life cycle (e.g. from raising plants and animals, to processing and cooking, and all the way to the metabolism of your meal). This field seeks to improve understanding of food and nutrition and presents a variety of complex technical challenges.

Health concerns have required the development of a multitude of methods for analysing food samples and additives. Examples include the identification of arsenolipids in canned cod liver, determination of aflatoxin in milk, enzymatic tests for the caffeine content of beverages and fluorescent probes for the fat content of milk. Playing with your food (or drink in this case) can also provide insights into bacterial transfer. There is also the topic of food safety, from which concerns about supply chains have prompted the development of tracers that can be added to food and used to ensure product authenticity.

Familiar chemical analytical tools such as ^{1}H NMR have been used to distinguish beef from horse meat, identify the country of origin of coffee beans, and to identify organically grown tomatoes. Gas Chromatography/Mass Spectrometry, another familiar technique, finds valuable use for the quality control of Japanese Sake.

Scientific advances are creating many new applications in food. Molecular biology is enabling new approaches to producing food, such as lab grown meat (details here); 3D Printing is providing new means of preparing food; materials science underpins molecular gastronomy; sensors that detect food odours can be used in analysis; and even Big Data is used in food studies. We have seen informatics studies of Indian recipes looking for the spices that make it taste

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27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering); ECAB3 (3rd European Congress of Applied Biotechnology); and EPIC5 (5th European Process Intensification Conference)
Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

best (details here) and chemometrics techniques for identifying production methods, geographical origin and species authentication of shrimp.

Chemical components of common spices are known to have antimicrobial properties that can be used to better understand pathogenicity and even to develop antimicrobial surfaces (think about "cutting boards", details here).

We now give you two examples of modern technology and the kitchen: satellite technology for cooking steaks and a recipe for powdered alcohol (see video here); and end with a reminder that sometimes a simple look at complex science is valuable, as illustrated by chocolate and garlic.

Big Data

Have you ever considered how much data is generated every minute, how that data might be visualized, who could possibly analyze it all or what it might actually be used for? This topic seems to come up more and more as we look across the horizon at developments in science and technology. This has of course raised many questions regarding potential security implications (and how to think about them) as well as privacy implications (and how to address them, details here). Reports of how marketing data might be collected don't always ease these concerns!

Data science expertise has developed into an extremely important asset to any organisation. It has application across a broad range of fields: biology, chemistry, linguistics (including the influence of language of publication on fame), geo-information, transportation (details here), behavioural sciences, unemployment, agriculture and more.

Big data has proved to be valuable in regard to public health. Certain internet search terms might be indicators for spreading of the flu and possibly other diseases, and there are indications of negative comments on social media correlating to heart disease (details here). Yet, there is still significant work to be done to ensure these methods are reliable. Still, the ability to share information and the use of text messages and/or social media can help improve public health (and this in turn generates more data to analyze). Data collected from the Ebola outbreak has informed studies on the risk assessment of the spread of disease, provided insights into the effectiveness of surveillance and intervention, and lead to predictions on when the epidemic might end (details here). Data collection for public health has also generated its own ethical challenges.

A wealth of data comes from communication, as can be seen in this real-time tweet map and the Big Data of social (and professional) networks can tell us much about how effective (or problematic, details here) and far reaching our communication networks really are. Take a look at the twitter networks of foreign ministries and international organisations. For those of you who like to use Twitter, we share some tips on the use of hashtags and assessing content.

31 October – 2 November 2015
The Port Hackathon.
CERN

16 – 19 November 2015
Malta Conference. Rabat, Morocco.

18 – 21 November 2015
16th Asian Chemical Congress. Dhaka, Bangladesh.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

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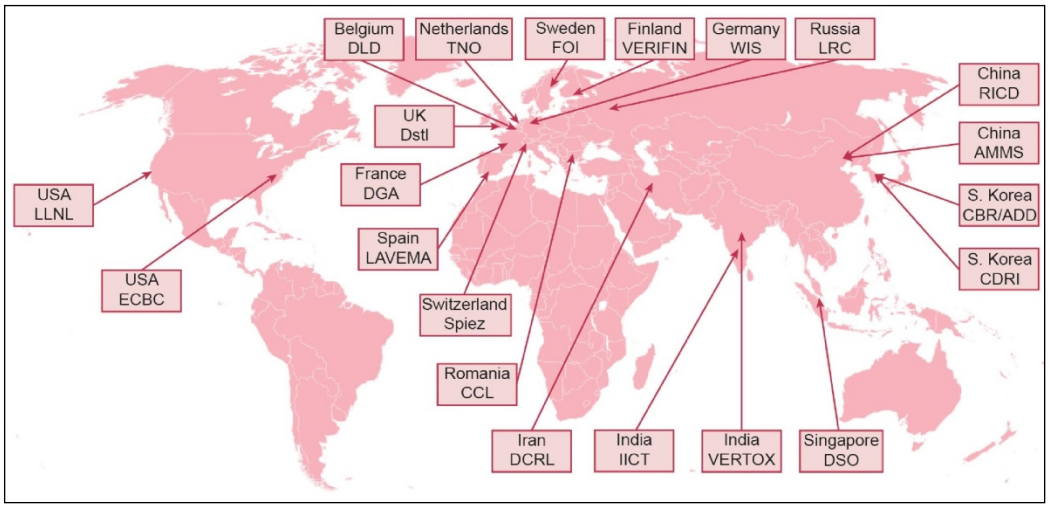
For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

Designated Laboratories

The Designated Laboratory network forms a key part of the verification regime of the Chemical Weapons Convention (CWC) by providing laboratories with proven expertise in off-site analysis of CWC-related samples. Theses laboratories provide a high degree of confidence that the chemical analyses needed to determine issues occurring during OPCW inspections or allegations of use of chemical weapons can be carried out unambiguously. On 27 August 2014, the network consisted of twenty-one laboratories in seventeen States Parties; these are illustrated on the map below.

Many scientists from the designated laboratories are currently serving as or have previously been members of the OPCW Scientific Advisory Board (as well as its Temporary Working Groups). We thank these individuals for the vital role they play in providing specialised advice to the Director-General on a variety of technical issues.



The designated laboratories also publish a variety of high quality scientific papers and reports. To learn more about the individual laboratories we present an appendix with links to public websites and recent publications from across the laboratory network. Please note that some of the materials are only available in the national language of the State Party.

Country	Laboratory	Links to Recent Publications
	Defence Laboratories Department	- Rapid and Efficient Filtration-Based Procedure for Separation and Safe Analysis of CBRN Mixed Samples
	The Laboratory of Analytical Chemistry, Research Institute of Chemical Defence	- Study on the N-terminal valine adducts in hemoglobin after exposing to mustard gas by mass spectrometry
	Laboratory of Toxicant Analysis, Institute of Pharmacology and Toxicology, Academy of Military Medical Sciences	- Determination of nerve agent metabolites in human urine by isotope-dilution gas chromatography-tandem mass spectrometry after solid phase supported derivatization - A novel approach for high sensitive determination of sulfur mustard by derivatization and isotope-dilution LC-MS /MS analysis
	VERIFIN, Finnish Institute for Verification of the Chemical Weapons Convention	- Verification and quantification of saxitoxin from algal samples using fast and validated hydrophilic interaction liquid chromatography-tandem mass spectrometry method - Development and validation of efficient stable isotope dilution LC-HESI-MS/MS method for the verification of ß-lyase metabolites in human urine after sulfur mustard exposure
	DGA Maîtrise NRBC, Département d'analyses chimiques	- Effects of Repeated Low-Dose Exposure of the Nerve Agent VX on Monoamine Levels in Different Brain Structures in Mic
	Bundeswehr Research Institute for Protective Technologies and NBC Protection	- Analysis of chemical warfare agents-searching for molecule
	Vertox Laboratory, Defence Research & Development Establishment	- A highly selective and sensitive "turn-on" fluorescence chemodosimeter for the detection of mustard gas

	Council of Scientific and Industrial Research, Centre for Analysis of Chemical Toxins, Indian Institute of Chemical Technology	- Rapid screening of N-oxides of chemical warfare agents degradation products by ESI-tandem mass spectrometry - Mass spectral characterization of the CWC-related isomeric dialkyl alkylphosphonothiolates /alkylphosphonothionates under gas chromatography/mass spectrometry conditions
	Defense Chemical Research Laboratory (DCRL)	- Determination of lewisite metabolite 2-chlorovinylarsonous acid in urine by use of dispersive derivatization liquid-liquid microextraction followed by gas chromatography-mass spectrometry - Photoassisted and photocatalytic degradation of sulfur mustard using TiO2nanoparticles and polyoxometalates
	TNO Defence, Security and Safety	- Verification of Exposure to Cholinesterase Inhibitors: Generic Detection of OPCW Schedule 1 Nerve Agent Adducts to Human Butyrylcholinesterase - December 2015 issue of *TNOTIME*
	Chemical Analysis Laboratory, CB Department, Agency for Defence Development	
	The Chemical Defence Research Institute	- Armed Forces Institute of Chemical Defense, has been accredited by the Organization for the Prohibition of Chemical Weapons Lab
	Chemical Analysis and Testing Laboratory, Scientific Research Center for CBRN Defense and Ecology	- Encapsulation of highly toxic organic compounds: Novelly functionalized nanoparticles for the safe storage of pollutants and their by-products
	Laboratory for Chemical and Analytical Control, Military Research Centre	- Dilute-and-shoot' RSLC-MS-MS method for fast detection of nerve and vesicant chemical warfare agent metabolites in urine

	Verification Laboratory, Defence Medical and Environmental Research Institute, DSO National Laboratories	- Chemical analysis of bleach and hydroxide-based solutions after decontamination of the chemical warfare agent O-ethyl S-2-diisopropylaminoethyl methylphosphonothiolate (VX) - *Creating Disruptive Capabilities* DSO brochure
	Laboratorio de Verificación de Armas Químicas (LAVEMA), Instituto Tecnológico "La Marañosa"	
	FOI, CBRN Defence and Security, Swedish Defence Research Agency	- Detection and monitoring of CWA and BWA using LIBS
	Spiez Laboratory, Swiss NBC Defence Establishment	- Identification of sulfur mustard hydrolysis products by LC-UV-SPE NMR - Spiez Convergence Workshop Report 2014
	Defence Science and Technology Laboratory, Chemical and Biological Systems, Porton Down	- Potency of irritation by benzylidenemalononitriles in humans correlates with TRPA1 ion channel activation - Detection of the organophosphorus nerve agent VX and its hydrolysis products in white mustard plants grown in contaminated soil - Issue 27 of Dstls *insight*
	Edgewood Chemical and Biological Forensic Analytical Center	- Quantitation of five organophosphorus nerve agent metabolites in serum using hydrophilic interaction liquid chromatography and tandem mass spectrometry - Purity analysis of hydrogen cyanide, cyanogen chloride and phosgene by quantitative (13)C NMR spectroscopy - 2014 Annual Report
	Lawrence Livermore National Laboratory	- Derivatization of pinacolyl alcohol with phenyldimethylchlorosilane for enhanced detection by gas chromatography-massspectrometry - 2014 Annual Report - January-February 2015 issue of LLNL's *Science and Technology Review*

The OPCW Science & Technology Monitor

A sampling of Science & Technology relevant to the Chemical Weapons Convention

14 April 2015 **Volume 2, Number 5**

Featured Content:

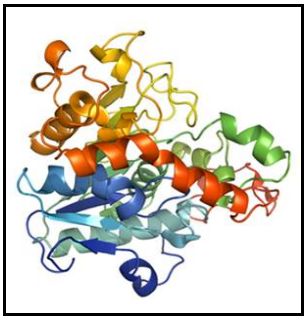


*Image from Green Chem, 2015,**17**, 1756-1766.*

Solvent free catalysis using enzymes immobilized in thin films.

*Image from Soft Matter, 2015,**11**,1667-1676.*

From insects to reptiles: technological advances discovered by studies across some of the "creepier" citizens of the animal kingdom.

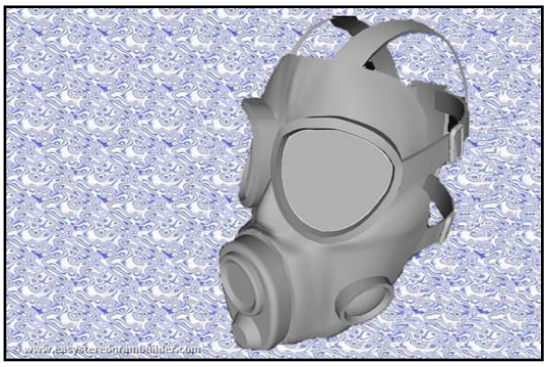
In this issue:

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

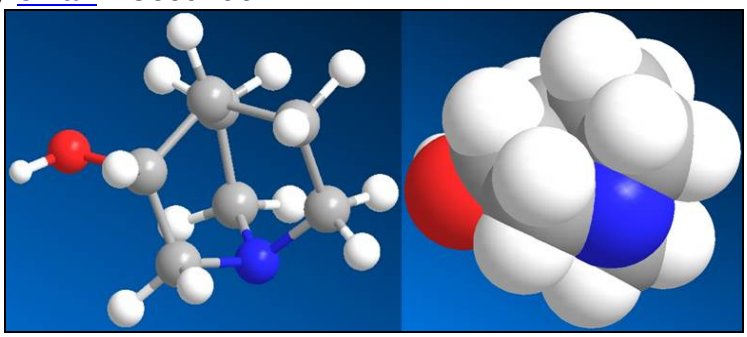
Today marks the 12th anniversary of the completion of the Human Genome Project. Tools and methods developed for studying genomics have applications for studying chemical warfare agents. Published studies include gene expression in survivors of sulphur mustard exposure and analysis of single-nucleotide polymorphisms of the genes involved in organophosphate detoxification.

The S&T Puzzle



Congratulations to Janaina Teixeira Pires do Couto from the Inspectorate, who was quickest to recognize the gas mask in our stereogram (look left for what you will see when viewing it correctly). Statistics now stand at: VER 4, OSP 2, OCS 1, INS 1, and CTBTO 1.

Moving on to this edition of the puzzle and considering all of our S&T communication channels, do you recognize the molecule below? Can you name it? Identify if it is on a Schedule (and if so, which one)? And tell us why it has relevance to the Chemical Weapons Convention? First person to correctly answer can choose a featured topic, design a puzzle, or receive a beverage hand selected by the Science Policy Adviser. Send answers by email. Good luck!



Science Fun:

With Koningsdag (Kings Day) fast approaching, we thought it only fitting to look at some of the science and technology that underpins life here in the Netherlands.

We are fortunate to live in a country with so much science to be observed, for example: innovative developments in water technologies, windmills (and continued development in wind and other renewables), greenhouses, laser armed trains, gouda cheese (a scientifically interesting food), solar powered bicycle paths (night photos here), wooden shoes and people whose average height has increased by 20 cm over the last 200 years (details here)!

Photo of Keukenhof.

Tulips: a dual-use biological material?

Perhaps more relevant to our Chemical Weapons Convention is the Tulip, a flower that was originally introduced to The Netherlands during the mid 16th Century. Tulips contain the chemicals Tulipalin A and B, which render these flowers toxic to dogs and cats and can induce dermatitis or eczema in humans. The bulbs also contain proteins capable

News and Updates

Recently published reports and newsletters:

Nature Index 2015 on Science in the Asia-Pacific Region.

Algae as a Potential Source of Food and Energy in Developing Countries.

Issue 27 of Dstl's *Insight*.

March 2015 Issue of PNNL's *Currents*.

Atoms for Peace and Development, Volume 56 Issue 1 from the IAEA.

Third issue of NASA's *Digital Technology Innovation Magazine*.

Issue 7 of *UNDP Skopje: Innovation Stories* (Innovation News Update).

2014 Intellectual property facts and figures from WIPO.

Documents from the commemorative event for the 40th Anniversary of entry into force of the Biological Weapons Convention.

Behind the Curve: New Technologies, New Control Challenges; report from the Small Arms Survey.

Defense Advanced Research Projects Agency (DARPA) report on *Breakthrough Technologies for National Security*.

2015 AAAS Science and Human Rights Report.

Science resources:

GLEAMviz a tool for modelling and visualizing epidemics.

Introduction to Ebola for journalists from the WFSJ.

Games that can be used to teach public health.

Infographic guides to scientific evidence and evaluating scientific work.

How good is your knowledge of scientific glassware? Answers can be found in this infographic visual guide.

Some news from world of science:

From the weeks of 15 – 21 and 22 – 28 March; 29 March – 4 April; and 5 - 11 April 2015 in chemistry.

New Technology for Chemical Production and Discovery

We pay considerable attention to devices and technologies for analyzing chemicals, but before we can identify and detect a chemical, it must somehow be prepared (whether by nature or in a lab).

of inhibiting DNA synthesis.

Of course biological materials and the chemicals they contain have multiple uses. These Tulip derived chemicals have anti-bacterial, cosmetic and biopolymer applications.

Finally, we can't ignore the fact that The Netherlands is a country of bicycles, a form of transportation that continues to evolve with technological innovation, lends itself to becoming a smart device and drives invention to keep riders safe. And we all know that if we can make our bicycles smarter and safer, we can also make them faster!

Crowdsourcing:

Do you have any photographs that convey the role Power Africa and energy innovation are playing in powering Africa?

Interested in designing a mobile app to educate children about good hygiene practices and sanitation?

Our crowd sourcing feature has primarily focused on alerting our readers to crowd source opportunities they can participate in. Have you ever wondered how good the crowd can be for providing information? Here are some reports on going to the "crowd" to detect clinical features of an eye condition from digital photography and to rank adverse drug reactions.

Not surprisingly, new concepts and technologies to make organic synthesis more efficient are changing the laboratory as chemists work toward the development of a "synthesis machine". Automated synthesis of peptides and nucleic acids has been accessible for many years, and we are now seeing machines that automate the assembly of a variety of small molecules (details here).

New chemistry to form carbon-carbon bonds employing boronate esters and functionalized olefin coupling under mild conditions are opening up new routes to synthesis. New approaches to using biological molecules in synthesis continue to emerge as well, such as enzymes that can be engineered to catalyse reactions not found in nature, the use of DNA to catalyse enantioselective reactions (details here) and solventless reactions using enzymes in thin films (details here).

To help contain the ever increasing cost of pharmaceutical development, enabling tools such as Computer-Aided Drug Design (CADD) to better identify drug leads (details here) and other computational methods for exploring "small molecule space" along with "Robot Scientists" that streamline drug discovery are being adopted (details here). These methods are themselves augmented by new ways to combine computational and functional studies with analytical tools in identifying and screening drug function (such as reduced risk of pain-killer dependency).

New methods for producing materials are likewise being invented, as demonstrated by a simple yet high volume method recently reported for graphene.

From Worms to Reptiles: Nature Inspired Science

We've spent considerable time thinking about the convergence of chemistry and biology, with much focus on the manipulation of microorganisms and plants. Yet, it is much more than just chemistry and biology that has converged and a significant amount of bio-inspired science and technology has developed from observations of multicellular organisms across the animal kingdom. Bio-inspired materials and venom component derived drugs are just two of the topical areas that can be explored in the scientific literature. We present here a sampling of convergent science inspired by observing some of natures less charismatic creatures.

Starting with invertebrates, "worms in space" are informing astronauts how to mitigate bone and muscle loss in zero gravity. Moving to the world of molluscs, the stretchy material that makes up the teeth of a limpet was recently discovered to be one of the strongest materials in nature (details here). Cephalopods are masters at camouflage, their associated chemical and biological processes have inspired interesting reflective coatings. A recent scientific article accused cone snails of using "chemical weapons", perhaps not quite a concern for the CWC, but of interest to those who study insulin.

Upcoming S&T Related Events:

19 – 23 April 2015
ALLData2015 - The First International Conference on Big Data, Small Data, Linked Data and Open Data. Barcelona, Spain.

30 April - 1 May 2015
2015 AAAS Forum on Science and Technology Policy. Washington DC, USA.

6 – 7 May 2015
6th Meeting of the Scientific Advisory Board's Temporary Working Group on Verification. The Hague

26 – 30 May 2015
International Conference on Robotics and Automation. Seattle, Washington, USA. The Amazon Robot Contest will take place at this event.

7 – 12 June 2015
2015 AAAS-TWAS Course on Science Diplomacy. Trieste, Italy.

8 – 12 June 2015
Twenty-Second Session of the OPCW Scientific Advisory Board. The Hague, Netherlands.

15 – 19 June 2015
ACHEMA – World Forum for Chemical Engineering and the Process Industries. Frankfurt am Main, Germany.

22 – 26 June 2015
CTBT Science and Technology Conference (SnT2015) Vienna, Austria.

14 – 26 July 2015
19th Annual Green Chemistry and Engineering Conference. Bethesda, ML, USA.

Silk from insect cocoons has molecular properties that can be used to generate electricity or even dissipate energy (details here). Other insect inspired materials include antireflective coating discovered by studying moth eyes (more details here). Insect neural systems can be manipulated with technologies that produce "cyborg" drones (controllable by Smartphones, details here); actual non-hybrid drones inspired by butterflies and ants exist too. Spiders quite naturally have also inspired drone technologies.

Other examples of arachnid science focus on spider webs, a fascinating area of materials science that has inspired 3D printer design and breakthroughs in nanofiber and 3D cell printing (for tissue engineering) research. Sensors can also be designed to mimics a spider's sensory system to detect vibrations (such as those produced from the motion of an insect's wing; a video is available here). Looking to other arachnids, scorpion venom has shown potential for treating bacterial infections and in chemotherapy. Molecular components of arachnid venoms have been identified as drug development scaffolds and insect specific insecticides. Venom from ants, centipedes (details here), and other arthropods are studied for similar purposes.

Fish and reptiles have also contributed to scientific development in similar ways to many of the invertebrates already described. Consider oil repellent materials for diving goggles inspired by fish (and flowers too, details here) and potential therapeutics identified in the blood of alligators (details here). Perhaps the chameleon (details here) can give those cephalopods a bit of competition in camouflage too?

We'll end this survey of somewhat scary creatures and their scientific contributions with a plea to be kind to rats and a reminder that interesting discoveries inspired by nature often come from unexpected places (even slime molds, details here).

Codes of Conduct and Ethics in Chemistry

Codes of conduct and ethics in chemistry received renewed attention at OPCW when the Nineteenth Conference of States Parties to the Chemical Weapons Convention welcomed an initiative for a text of ethical guidelines for chemical professionals related to the Convention (see C-19/5, dated 5 December 2014, paragraph 23.3). In support of this initiative, 19 scientists participated in a workshop on 11 March to discuss the issue and think about how it might be taken forward. Participants included members of the American Chemical Society (ACS), Bangladesh Chemical Society (BCS), European Chemical Industry Council (Cefic), European Association for Chemical and Molecular Sciences (EuCheMS), Federation of Asian Chemical Societies (FACS), Gesellschaft Deutscher Chemiker – the German Chemical Society (GDCh), Indian Chemical Council (ICC), International Union of Pure and Applied Chemistry (IUPAC), Ministry of Industry and Information Technology of the People's Republic of China, The National Academies and the National Engineering & Scientific Commission – Pakistan (NESCOM). Those involved in the workshop are continuing their considerations and we are sure to hear more in the next few months.

19 – 22 July 2015
12th World Congress on Industrial Biotechnology.
Montreal, Canada.

6 – 13 August 2015
IUPAC 2015
48th General Assembly
45th World Chemistry Congress. Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering);
ECAB3 (3rd European Congress of Applied Biotechnology); and
EPIC5 (5th European Process Intensification Conference)
Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

15 October 2015
Smart Manufacturing Summit. Livermore, California, USA.

31 October - 2 November 2015
The Port Hackathon.
CERN

16 – 19 November 2015
Malta Conference. Rabat, Morocco.

18 – 21 November 2015
16th Asian Chemical Congress. Dhaka, Bangladesh.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

During the workshop a number of presentations were made on past, present, and on-going initiatives in developing ethical codes and this is where our focus for this feature comes in. As part of the discussion, a first pass text analytics study that encompassed sixty-three existing codes of conduct and ethics for chemistry (and/or broader scientific professionals that include chemists and chemical engineers). For those interested, the text of these codes is available upon request from us here at the *S&T Monitor*.

The study was meant to be insightful, not comprehensive. The codes in the data set represent international and regional organisations as well as organisations specific to the countries shown in Figure 1. The types and number of these organisations in the data set are reported in Figure 2. In some cases (several of the South American countries for example, the national chemical society was using a translated version of a code already included in the data set from another chemical society; in this instance we did not include the duplicate code).

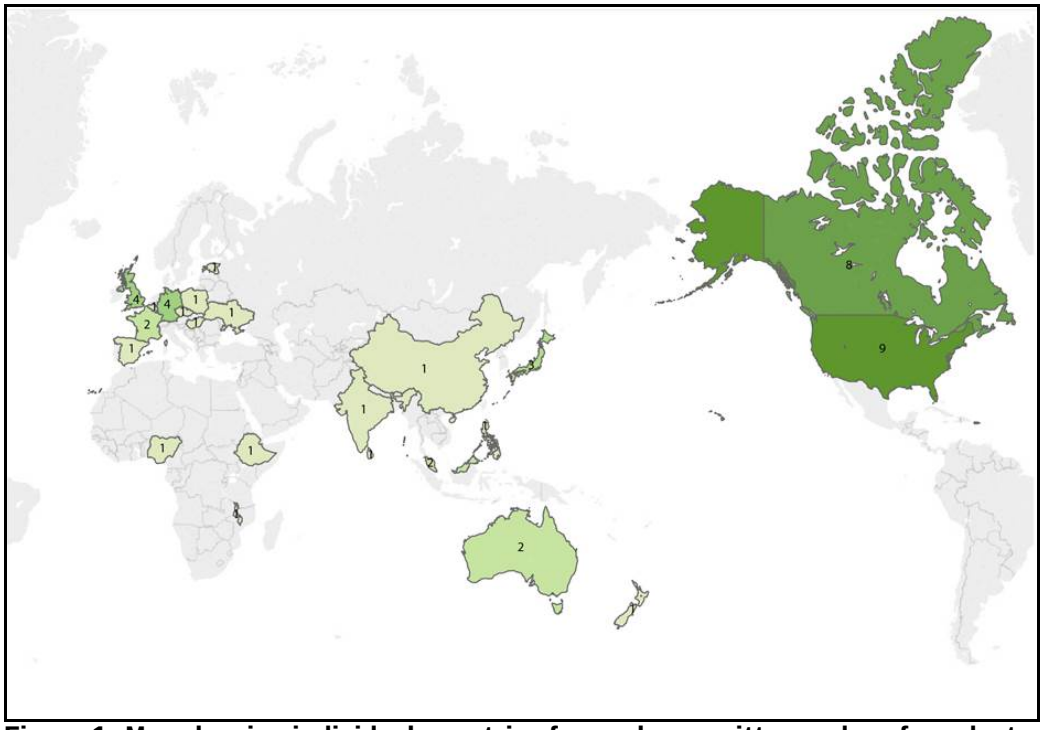


Figure 1: Map showing individual countries from where written codes of conduct or ethics in chemistry and chemical engineering were available (and how many codes came from each country). In addition there were eight codes from organisations that represented regional and international scientific organisations and some national societies used identical codes (which were not duplicated in the data set).

The analysis sought to discover patterns in the existing codes to provide an in-depth insight. The analysis was performed using Provalis QDA Miner software (available in OSP and the OPCW the Library). In this feature we report an introductory summary of the cluster analysis that was performed. Cluster analysis is a data reduction method by which a large number of items are grouped into a number of clusters of similar items. When applied to textual data, cluster analysis can be used to identify themes or broad classes of concepts that are common between documents placed into their respective clusters (groups). For purposes of this summary, one can think of all the codes found in the same

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For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

cluster to have text that is similar to one another and divergent from the text of the documents in the other clusters. Additionally the closer the distance between the codes within a cluster, the more similar the documents actually are. Figure 3 illustrates the first pass cluster analysis, indicating the documents considered to be (by their authors) codes of conduct or codes of ethics).

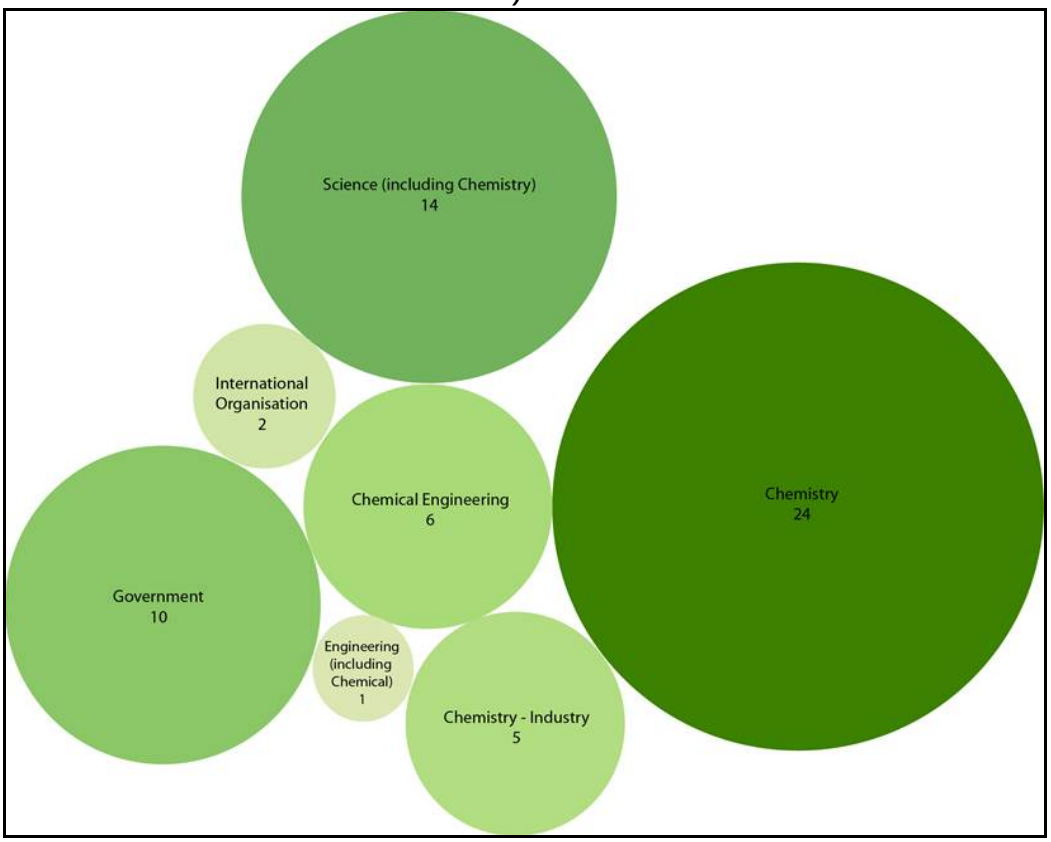


Figure 2: Illustration of number and types of organisations represented by the codes used in the analysis.

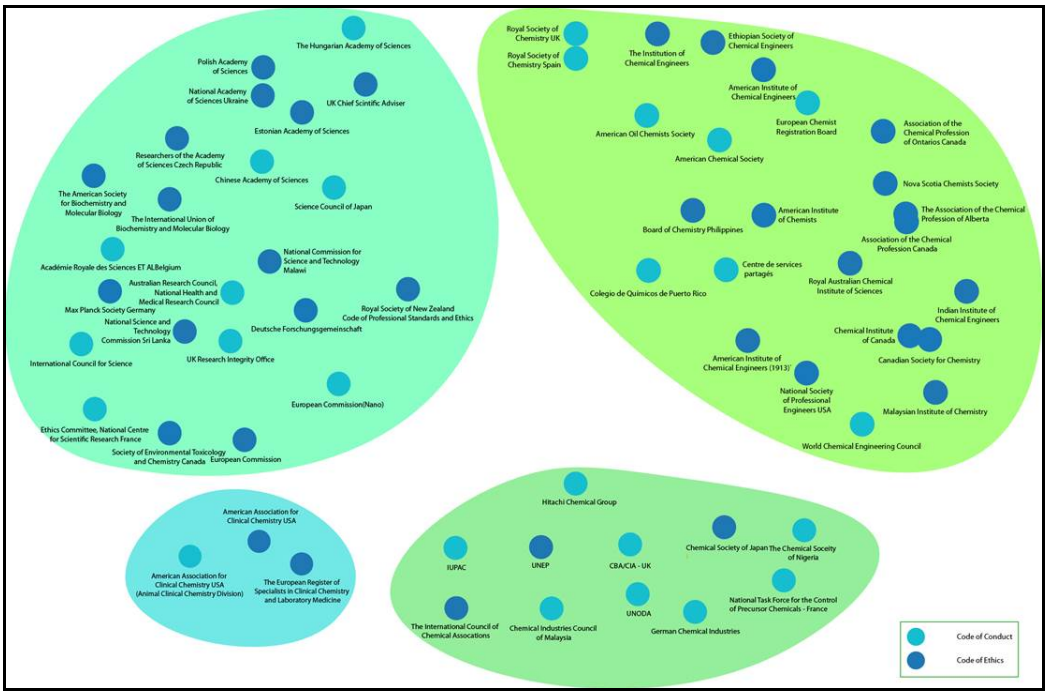


Figure 3: The codes separated into four clusters (groups of documents with similar text content). The cluster here is visualised with each code indicating if it is a code of conduct or a code of ethics (as defined by its authors and purpose).

There are several observations from Figure 3 to point out. First, the

smallest cluster (bottom left in Figure 3) containing only three codes represents clinical chemistry organisations – all of whose codes contain similar text and whose organisations have a clinical focus that is not represented by organisations found in other clusters. Next, the actual written codes do not distinguish themselves within the clusters by whether they represent codes of conduct or codes of ethics. Figure 4 delves into other unique factors represented by the codes and organisations to further compare the content.

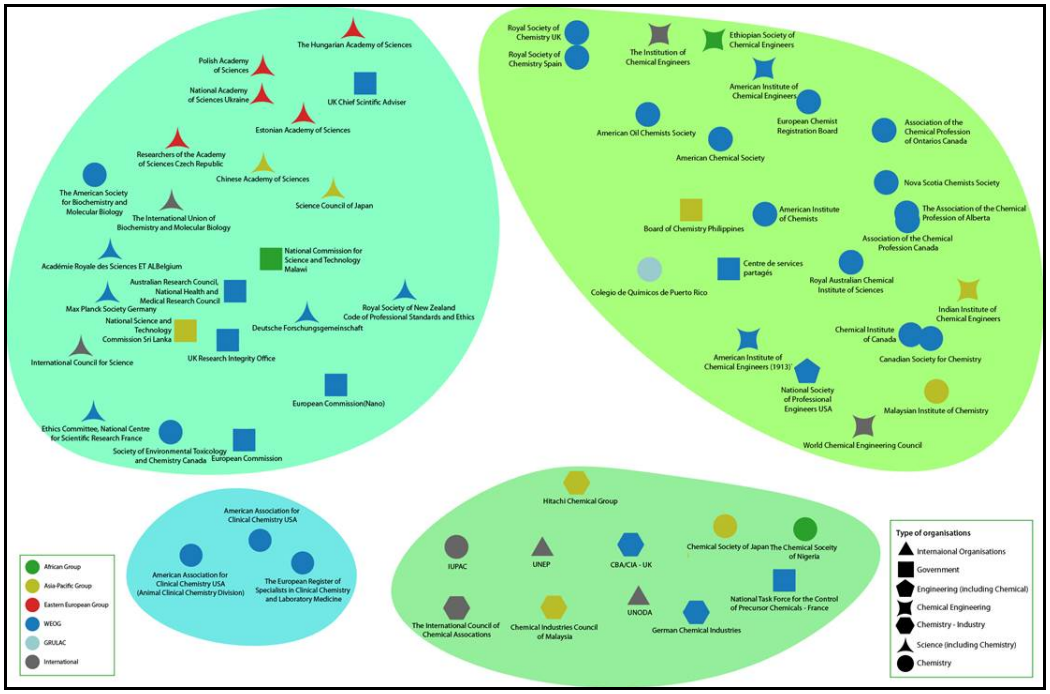


Figure 4: Visualisation of the codes within each cluster indicating the regional affiliation and type of organisation represented by the code.

In Figure 4, the clusters also do not segregate themselves by region. The majority of codes come from countries in the Western Regional Group and these codes are found in every cluster. Despite smaller representation over the sixty-three codes, Asian and African Regional organisations also appear in all clusters not representing clinical organisations (there are no clinical organisations from these regions in the data set). The only region which falls into a single cluster is Eastern Europe (top left in Figure 4). However, on closer inspection it can be seen that all the organisations from this regions are Academies of Science and all the Academies of Science from across the data set fall into this same cluster.

Other organisational groupings observed within the clusters are the chemical engineering organisations all in the top right cluster; and international and industrial organisations in the bottom right cluster (showing that international organisation and industrial codes distinguish themselves from the other types of organisations represented in the data set). The major attribute which appears to define to which cluster a document belongs, is the type of organisation that the code is written for, not the geographical region, nor the type of document (e.g. a code of ethics vs. a code of conduct).

To explore the relationship between significant words within the documents and the types of organisations (the most prominent distinction between the clusters), a cross-tabulation analysis was performed. Figure 5 summarises the observations of highest word frequency across the codes.

Figure 5 illustrates the most common words found across the documents and it is noteworthy to point out that terms such as Chemical Weapons Convention, Biological Weapons Convention, Weapons of Mass Destruction, Dual-use, Multiple-use, and Security are observed in a very small number of codes. The heat-map indicates the most frequent topics in the codes of this data set focus on safety, health, and welfare. It also indicates that not all types of organisations are concerned equally about these issues.

The workshop participants are following up on their meeting to identify key elements of CWC relevant ethical guidelines, principles and best practices for drafting ethical guidelines and how they might establish synergy with other similar initiatives (both past and present). The text analysis study presented here, while by no means comprehensive, may usefully inform their work. A more detailed publication (with more codes included) is currently being considered as a follow up.

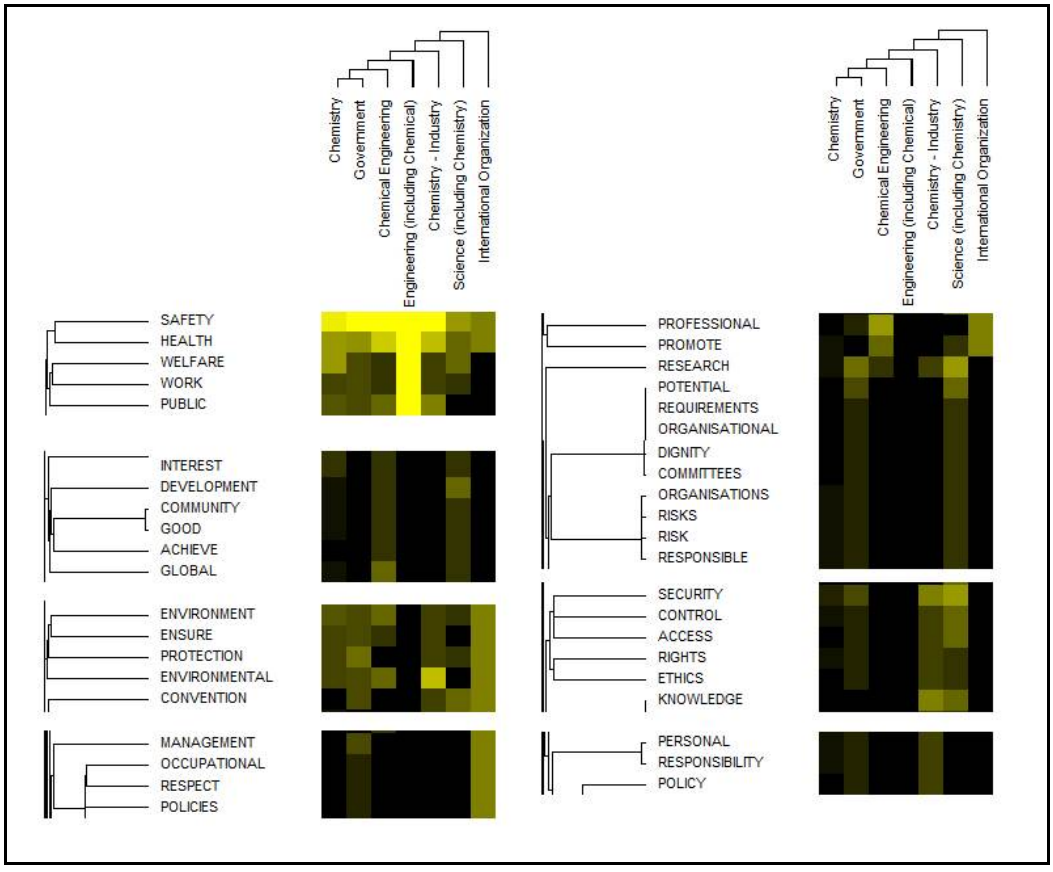


Figure 5: Heat map of word associations and frequencies across data set organised by the type of organisation represented by the code. Brighter colour indicates higher frequency of a specific word or word association across the documents.

VOLUME 2 NUMBER 6

The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

12 May 2015

In This Issue

Featured content

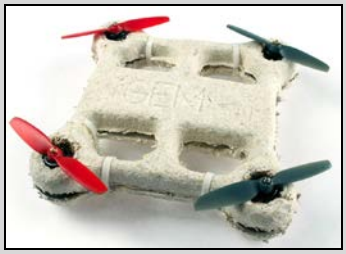


Image from wired magazine

Self-destructing biodrones are one of the many developments in the world of UAVs.

OPCW Inspectors during an Article VI Inspection.

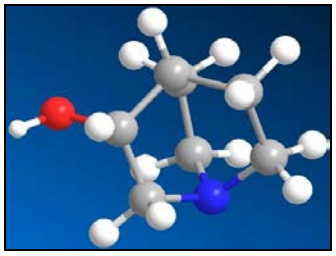
Inherent safety concepts applied to chemical production.

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

Today marks the 105th anniversary of the birth of Dorothy Crowfoot Hodgkin (1910 – 1994), who was awarded the 1964 Nobel Prize in Chemistry "for her determinations by X-ray techniques of the structures of important biochemical substances". We have previously highlighted the importance of X-Rays in understanding biomolecular structure; a relevant example to the CWC comes from work in the development of bioscavengers against nerve agents.

The S&T Puzzle



We congratulate our colleagues at the CTBTO, who were quickest to recognize 3-quinuclidinole (shown on the left), a schedule 2.B.09 chemical that is a key precursor to BZ (3-quinuclidinole benzilate, schedule 2.A.03). Thanks to all you who submitted answers!

This was by far the largest puzzle participation we have yet seen! Puzzle statistics now stand at: VER 4, OSP 2, OCS 1, INS 1, and CTBTO 2.

Our next puzzle is a combination scavenger hunt and text analysis. We are looking for the five most frequently spoken words by our Director-General in public addresses from January to April 2015 (commonly used words such as "and", "the", etc. do not count). Without giving too much away, this covers 8 statements and 1717 words! Highest number of correct words identified in the top 5 wins the prize: a choice of requesting a featured topic, designing a puzzle, or receiving a beverage hand selected by the Science Policy Adviser. Send answers by email. There is also a bonus prize for the "best" visualisation of the Director-General's words. Good luck!

News and Updates

Recently published reports and newsletters:

Handbook of Toxicology of Chemical Warfare Agents (Second Edition); table of contents and abstracts can be viewed online.

Science Fun:

May is a month of many celebrations that inspire ideas for fun science which leads to hours of debate on what should fill the pages of science fun. The obvious choice for a May newsletter arrived (with great fanfare) on this months first Monday, greeting us with "May the 4th be with You!" in celebration of "Star Wars Day". Now, 38 years after the original movie was released, we take a look at the science of Star Wars and how far from reality it is today. While we encourage questioning of the science behind what we see on film (for example, laser physics and slow digestive processes), don't snicker: planets like Tatooine may actually exist (and not just one, but many), the force may already be with us and you might even be able to purchase some of it!

Was R2-D2 using technology based on graphene? Image: Screenshot from Star Wars/Lucasfilm/20th Century Fox (through *Science Alert*).

Following the original storyline, we begin with droids: here is one you can build at home (with simple instructions). With an appropriate neural network, you may be able to add Artificial Intelligence (AI) as an upgrade. Is there need for an emotion accessory too? Add some graphene, and the ability to generate 3D holograms could be the next addition (details here). Alternately, given all the wearable and implantable gadgets we cherish, should the droids receive the most enabling technologies?

Spiez Laboratory 2014 Annual Report.

A report on The Global Pandemic of Falsified Medicines: Laboratory and Field Innovations and Policy Perspectives.

Science and technology roadmap for graphene (details here).

The World Academy of Sciences (TWAS) Newsletter: The Power of Science Diplomacy.

United Nations Global Pulse 2014 Annual Report (highlighting Big Data innovation projects in sustainable development).

Reports on the use of Twitter by international organisations and world leaders.

April 2015 issue of International Council for Science (ICSU) Newsletter.

Science and education resources:

Celebrating Chemistry from the American Chemical Society (Earth Day Edition).

Infographic on CRISPR/CAS9 Targeted Genome Editing.

Open Labware: 3-D Printing Your Own Lab Equipment.

Disarmament education resources from the United Nations Office of Disarmament Affairs (UNODA).

Some news from world of science:

From the weeks of 12 – 18 and 19 – 26 April, 27 April – 3 May and 3 – 10 May in chemistry.

Images to celebrate 25 years of the Hubbel telescope.

Drones

The development of unmanned autonomous vehicles (UAVs), whether terrestrial, aerial, or aquatic (and combinations thereof) has experienced significant growth in recent years for personal, economic and utilitarian purposes. We are continually seeing proposals of new applications and demonstrations of capabilities. Examples include drone-based deliveries (where delivery locations might update in real-time using the addressees Smartphone as a locator), aerial drones for security, delivery of blood to critically injured patients, delivering life preservers to struggling swimmers, tracking stray dogs and even sheep herding.

The majority of drone based measurements that we have seen involve photography and video; applications include mapping, high resolution 3D imaging and search operations where aerial surveillance may have limitations.

What about all those fantastic vehicles? How fast do the land speeders really go? This question is being addressed in a most scientific manner. Can you determine if the calculations are accurate? For most of us, the prospect of owning a space craft is only realistic if we build it from Lego®. Although with a sufficient budget, a Tie Fighter engine can be had! Achieving light speed capability however, may remain difficult.

We often hear about science fiction predicting the future, is it true, or is it a case of science fiction inspiring people to build what they see? No matter the answer, we can be sure that in another 38 years, science can only become more fun!

The ambulance drone that could save your life. Photo from *Daily Mail Online*.

As sensors become smaller, integration of devices (Smartphones for example) is a foregone conclusion (and there are many potentially portable and miniaturised devices available). This concept has appeared in patent literature for many years (with some patents focusing on CBRN specific applications). Agriculture is another sector where we are seeing UAV platforms integrated with sensors and other technologies; examples include evaluating leaf water use efficiency and applying pesticides. Other examples involve pollution and environmental monitoring, and environmental sample collection.

With the proliferation of UAVs into more and more everyday uses, a need for "air traffic control", miniaturized radar and advanced autopilot systems is critical for collision free sky (and there are certainly other unforeseen situations that may arise). UAVs can challenge regulations, prompting policy-makers to review existing laws and propose UAV specific measures. Self-driving cars have prompted conceptually similar discussions. There are also security concerns that have lead to net carrying interceptor drones to counter potential threats from small UAVs. Privacy concerns have likewise emerged, with calls for no fly zones over private property.

We end this feature by noting that UAVs have not been spared from the list of technologies converging with biology, as demonstrated by a "biological UAV" that is intended to self-destruct and dissolve upon impact. It was designed to avoid leaving behind litter in pristine eco-systems. Interested in creating your own "biodrone"? The inventors have made the procedure available.

Chemical Weapons Inspectors and Industry Verification

When we reflect on the work of the OPCW and its accomplishments in demilitarisation and non-proliferation, we rarely hear directly from OPCW inspectors. Yet without them, these accomplishments would not have been possible. Likewise, OPCWs demilitarisation activities (representing more than 13,000 inspector days in 2014) overshadow another important aspect of the Chemical Weapons Convention verification regime: the inspection of industrial chemical facilities (Article VI Verification). In 2014, OPCW inspectors conducted 241 Article VI missions adding up to nearly 3,000 inspector days; this amounts to about 8 OPCW inspectors on mission somewhere in the world where declared (and inspectable) Article VI facilities exist (see Figure 2) on any given day of the year!

For this feature, we sat down with a few Inspection Team Leaders (ITLs), Chemical Production Technologists (CPTs) and an Analytical Chemist from the OPCW Inspectorate to learn about them and their work in Article VI verification activities. For those with further interest in the facts and figures presented, we refer you to OPCW Annual Reports.

Crowdsourcing:

The IUPAC Committee on Chemistry Education seeks a new logo. If you are a chemistry student with a flair for design, they need your help!

How do we establish a sustainable human presence on Mars? NASA is looking for proposals (while this may not get you on a flight, creative ideas might win you a cash award).

Interested in a Smartphone App that can help save lives of children born prematurely? Your photographs of newborn babies feet, eyes and ears could turn it into a reality.

Crowdsourcing to verify social media information for emergency response? Here's what is being done in Nepal following the recent earthquake.

Upcoming S&T Related Events:

26 – 30 May 2015
International Conference on Robotics and Automation. Seattle, Washington, USA.
The Amazon Robot Contest will take place at this event.

7 – 12 June 2015
2015 AAAS-TWAS Course on Science Diplomacy.
Trieste, Italy.

8 – 12 June 2015
Twenty-Second Session of the OPCW Scientific Advisory Board.
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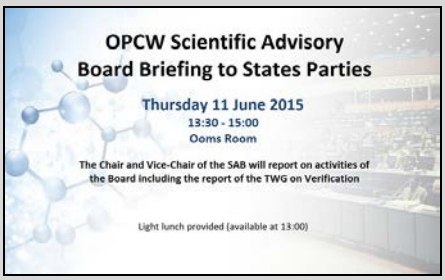

Figure 1: OPCW Inspectors at a chemical production facility (Article VI inspection).

The current staff of the OPCW Inspectorate Division numbers 163. This includes inspectors, Inspectorate management and support staff; they collectively make up 55 unique nationalities (which means up to 86 different "official" languages might be heard as you walk down the hallway). Inspectors join OPCW from a wide range of professional backgrounds. Some are former military or come to OPCW from governmental and/or international agencies; while others draw their experience from the chemical industry, manufacturing plants and/or science and engineering laboratories.

Many have backgrounds in chemistry (especially analytical chemistry), chemical engineering (including the division director) and other science/engineering disciplines. Several inspectors also hold an MBA.

Article VI inspections are intended to build confidence amongst the States Parties to the CWC through verifying the absence of undeclared Schedule 1 Chemicals (chemicals with limited or no use for peaceful purposes) and activities banned by the Chemical Weapons Convention. The broad expertise within the inspectorate is necessary to be able to inspect facilities that span a wide spectrum of declared purposes (this is illustrated by the product group codes in Appendix 4 of the *Declarations Handbook*). Knowledge about scheduled and non-scheduled chemicals, chemical synthesis and, methods and equipment for producing chemicals are needed. As is a sufficient level of familiarity with the laboratory equipment, production equipment, safety (containment) infrastructure and other features of the inspection site in order to recognise consistency with declared purpose. Some missions (a total of nine in 2014) include Sampling and Analysis (S&A), where training in analytical chemistry is required. The work of an inspection team may provide an unusual degree of access to a plant site, requiring that operating procedures concerning confidentiality are strictly followed (as described in the Confidentially Annex of the CWC).

22 – 26 June 2015
CTBT Science and Technology Conference (SnT2015)
Vienna, Austria.

8 July 2015
"Science for Diplomats". The science of medical countermeasures.
13:30 – 15:00 Ooms Room
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12th World Congress on Industrial Biotechnology.
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6 – 13 August 2015
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48th IUPAC General Assembly and 45th World Chemistry Congress.
Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering); ECAB3 (3rd European Congress of Applied Biotechnology); and EPIC5 (5th European Process Intensification Conference)
Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

15 October 2015
Smart Manufacturing Summit.
Livermore, California, USA.

31 October - 2 November 2015
The Port Hackathon.
CERN

16 – 19 November 2015
Malta Conference.
Rabat, Morocco.

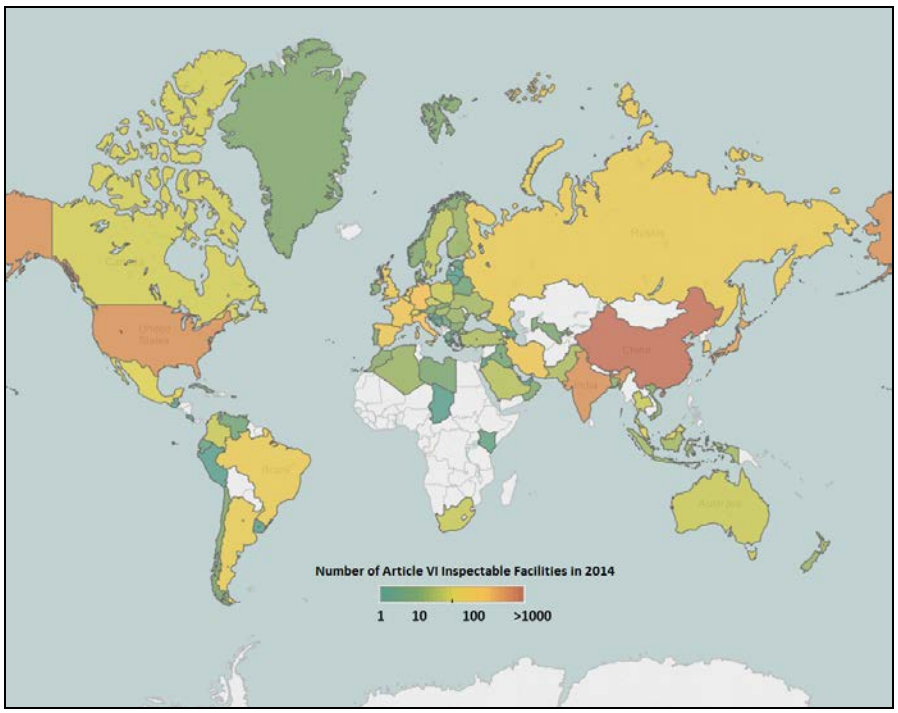


Figure 2: Declared and inspectable facilities under Article VI in 2014.

Team size and mission duration for Article VI inspections vary with the types of facilities inspected and whether or not S&A is to be performed. Schedule 1 and 2 facilities typically require three to five inspectors, while facilities producing unscheduled Discrete Organic Chemicals (DOCs) typically have inspections teams of two to four; in cases where a plant site has multiple inspectable facilities, larger teams might be dispatched. On S&A missions, teams of five are normally required (an ITL with two CPTs and two ACs).

Missions involving S&A are the most demanding. In preparation of the mission, ACs must ensure their instruments are calibrated and in some cases they may need to synthesise relevant chemical standards and controls (to ensure the highest levels of accuracy, this may include known and anticipated components/impurities of the samples to be tested – another example of where knowledge of chemistry becomes important). A mobile laboratory that includes a GC/MS (gas chromatograph/mass spectrometer), generators, portable fume hoods, sample preparation equipment and a variety of laboratory supplies (20 pieces taking up more than 5 m^3 and weighing more than a ton, see Figure 3), is shipped and assembled at the inspection site. Number and locations of sampling points at a chemical facility are negotiated with the inspected States Party prior to the analysis; they can include key points in a chemical production process along with random sampling points such as a waste water stream. As an S&A mission is typically three days in duration, the inspectors have limited time to assemble the lab, collect samples (see Figure 4) and run their analysis, making the logistical aspects of these missions critical for success.

18 – 21 November 2015
16th Asian Chemical Congress.
Dhaka, Bangladesh.

22 – 27 November 2015
2nd African Conference on Research in Chemical Education (ACRICE)
University of Venda,
Thohoyandou, South Africa.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

Contact Us:

Questions, ideas, comments, suggestions, want to make a contribution, or be added to the mailing list? Please contact us through the OPCW Office of Strategy and Policy (OSP).

For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

Figure 3: Sample collection at an industrial chemical facility.

As S&A missions are labour intensive, chemists from OPCW have developed improved methods for sample collection (from liquids and air), derivitization and sample desorption from solid supports to streamline the analysis. The work-horse on-site analytical tool is the GC/MS; in Article VI inspections, the primary analysis is the comparison of measured mass spectra and GC Retention Indexes to reference data contained in the OPCW Central Analytical Data Base (OCAD; see chapter 7 of Chemical Weapons Convention Chemical Analysis).

The OCAD only contains reference data for scheduled chemicals. For routine analysis, chemicals in collected samples are only identified if there is a match to data contained within OCAD. This allows verification of the presence or absence of scheduled chemicals while maintaining confidentiality on sensitive information related to industrial (i.e. commercial) facilities. Further information on the OCAD can be found in the October 2014 *S&T Monitor* feature on the "40th Meeting of the OPCW Validation Group". A report from the 41st Meeting of the Validation Group is also available.

Figure 4: The OPCW Mobile Laboratory.

In addition to the technical skills and knowledge just described, "soft skills" that aid in negotiations and promote team work are equally important. One might say that the ITL is a "technical diplomat", requiring a thorough understanding of the Chemical Weapons Convention (what is and what is not allowed during an inspection), the necessary technical knowledge to perform the inspection and the ability to maintain a cooperative interaction with the teams escorts (National Authorities and staff of the inspected facility).

Several of the team leaders have been known to prepare presentations to explain the purpose of the inspection and bring awareness of the CWC and its goals. In effect, some of our greatest assets for the OPCWs Education and Outreach work are the inspectors themselves; OPCW staff who regularly interact with people involved at an operational level in chemistry, chemical production and chemistry commerce.

Inherent Safety

Through the Chemical Weapons Convention (CWC), the OPCW works toward a world free of chemical weapons, a world that becomes more secure in the process. Chemical security is another means to strengthen this drive toward a chemical weapon free world and receives much attention within security focused communities. Just as the OPCW inspects industrial facilities for security reasons, industrial facilities are inspected with high frequency for safety reasons. Chemical safety seeks to ensure the safety of people, the environment and property from harmful chemicals. We often describe the focus of chemical safety as preventing accidents rather than addressing the potential of intentional misuse; yet, chemical safety compliments (and benefits) chemical security.

Chemical and chemical engineering societies (such as the ACS and AIChE) place great importance on chemical and process safety. Both are important to keep people safe who work in chemistry laboratories or chemical production plants (occupational safety). There are many aspects to ensuring the safety of people handling chemicals, personal protective equipment (PPE) is critical (with more hazardous chemicals requiring more effective protection).

Of course, many hazards surround us in our day to day life. The gasoline (something all of us with motor vehicles are exposed to) is a chemical hazard and the speed at which you ride your bike can be a hazard if you don't pay attention to those around you. For an engineer on a chemical facility, potential hazards include toxic chemicals and industrial equipment. This is where the concept of inherent safety comes into the picture. The goal of inherent safety is to reduce hazards, and by doing it also promotes good practices for chemical safety and security.

We are all aware of a number of tragic events involving accidents in chemistry laboratories and high profile industrial incidents such as Bhopal and the Flixborough. While we can learn from past accidents, we must also strive to prevent future incidents. Toward this end, in 1977 Trevor Kletz defined the concept of *Inherent Safety* as a response to 1974 Flixborough Disaster where on a Saturday afternoon, 1st of June 1974, a loud explosion occurred at the Nypro site at Flixborough, United Kingdom. The incident was triggered by a cyclohexane leak that found a source of ignition. After investigating the incident, it was found one of the reactors (number 5) had a crack and in order to continue production, a temporary bypass assembly was placed between reactors 4 and reactor 6. Unfortunately, the bypass failed releasing a cloud of cyclohexane vapour. Twenty eight workers were killed that day, had it been a weekday, the number of casualties would likely have been higher.

Key principles of inherent safety are substitution, minimization, moderation and simplicity.

Substitution is the replacement of hazardous chemical with a less hazardous material in a process. The use of water based paint instead of solvent based paint for example; the substitution reduces a fire hazard and the water based paint is less toxic and more environmental friendly.

Minimization is the reduction in quantity of hazardous materials. For example, in processes where hazardous materials must be used, reducing pipe diameters can help minimize the amount of material that spills from an unexpected leak.

Moderation is reducing safety risk for processes utilizing hazardous materials. This could be the running a reaction at less severe process conditions or the dilution of a hazardous material to a concentration range that provides an acceptable safety and environmental risk. Interested readers may wish to read a report on the application of the dilution principle using hydrazine as an example.

Simplicity is a reduction in the complexity of plant design. Using less complex equipment for certain critical processes, for example, in order to minimize the number of possible failure modes. The use of gravity flow systems in place of electric or mechanical pumps (where process tolerance permits) would be an example of simplicity.

Inherent safety is an important concept in plant design and there are a number of publications illustrating specific case studies of the application of its principles, including for batch and semi-batch processes in pharmaceuticals.

Adopting the concepts of inherent safety is only one aspect of building an effective safety culture. Keeping informed on new developments and maintaining proper safety training are equally important. Many resources are available to help promote chemical safety (and bring with it benefits to chemical security).

High quality inspections can eliminate potential safety risks in production plants. Photograph Copyright by BASF (used here under a creative commons license).

VOLUME 2 NUMBER 7

The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

1 June 2015

In This Issue

Featured content

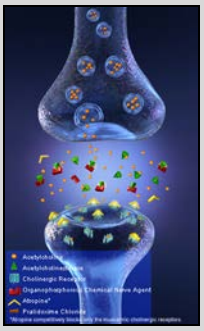


Image from DuoDote®

Medical countermeasures at work in a synapse.

Fingerprinting chemicals.

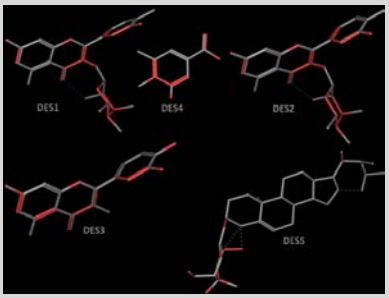


*Image from PLoS One. **2013** Nov. 8(11)*

Drug discovery research in OPCW Supported Research Projects

Welcome

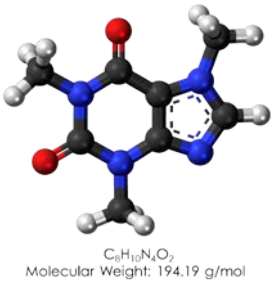
Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

Thanks to all of you who have taken our survey. For those who have not yet responded, the survey is still open (click here). There are only six questions, all easier than the puzzle (we promise) and all responses are anonymous. Your feedback is highly appreciated!

Today marks the 25th anniversary of the signing of the 1990 Chemical Weapons Accord by the United States of America and the Soviet Union. This agreement, which pre-dated the CWC, marks one of many steps taken in the journey toward a world free of chemical weapons. Steps taken in chemical disarmament have been supported by the science of chemistry itself; a scientific field that provides opportunities for international collaborations and brings forth new developments with peaceful economic and technological benefits. As we move into the future, we look forward to a wealth of new discoveries from this evolving scientific field.

The S&T Puzzle

We once again congratulate our colleagues at the CTBTO, whose entry correctly recognized four of the top five spoken words of the Director-General in the eight statements delivered from 22 January to 29 April 2015 (in case you were wondering, they missed "States"). The prize for best visualisation of the words of the Director-General, however, goes unclaimed as no submissions (except our own, below) were received. Puzzle statistics now stand at: VER 4, OSP 2, OCS 1, INS 1 and CTBTO 3.



For this edition of the puzzle, we look at the multiple uses of a cup of coffee. Can you tell us the identity and LD_{50} (that's right, the median lethal dose) of the most abundant chemical in the cup; the molarity (M) of caffeine (molecule above); and the LD_{50} of coffee itself? To keep this simple, assume this coffee is made with Arabica beans and brewed by a certified procedure (for

Science Fun:

As much fun as we have with *Science Fun*, we have found that it is not always fun trying to research and identify suitable material to use in each new issue! So where do inspiration and ideas come from? We've previously seen reports that certain beverages can help (when properly consumed of course); one of our favorites is prepared from a material containing more than 1500 chemicals! With so many chemical components, we needed a part one and a part two of reference articles to describe it! Given the worldwide consumption of this beverage, you are probably already quite familiar with it and its most familiar ingredient, 1,3,7-trimethylxanthine. Are you genetically predisposed to enjoy this beverage? If unsure, you might check get a DNA test. If yes, then we invite you to sit down with a cup and learn about the science of coffee (and if no, we won't mind if you choose to drink something more compatible with your personal genome!).

Preparing to draft the next issue of the *S&T Monitor*.

Coffee cultivation covers more than 11 million hectares of the planet! Anything so important requires study in the most advanced laboratory settings, and the study of coffee has revealed a genome that has evolved to produce caffeine and all those aroma producing components! One area of current interest is the economic viability of coffee cultivation in relation to climate change (take example, ISO 6668:2008) and our "cup" holds 250 ml (to ensure we stay below the LD_{50}). The first person to give us the correct answers (highest number of the four questions) wins the prize: a choice of requesting a featured topic, designing a puzzle, or receiving a beverage hand selected by the Science Policy Adviser. Send answers by email. Good luck!

News and Updates

Recent reports and publications:

Presentations (videos and slides) from the Continuing Innovation in Information Technology Workshop (held on 5 March at the National Academy of Sciences, Washington DC, USA).

A look at EU funded projects producing advanced analysis and visualisation tools for archaeology and restoration. Such tools could benefit other types of investigations.

Advances in optical fibres are helping make laser based weapons a reality.

The Epigenome Roadmap, a collection of research papers describing the main findings of the NIH Roadmap Epigenomics Program.

Have you ever wondered how to describe the complexity of a chemical structure and if that complexity description is reduced by advances in synthetic chemistry? Read about a new tool for assessing the "current complexity" of organic molecules.

Which factors influence international mobility of research scientists? Report from OECD.

Report from the workshop on ethical guidelines in the practice of chemistry (held on 11 March at OPCW).

Making It Happen: Technology, Finance and Statistics for Sustainable Development in Asia and the Pacific. Report from UNDP.

Science and education resources:

Card games to learn science: Retrosynthetic Rummy, Ion (use ions to make compounds), Evolve and Linkage (games to explore relationships between RNA and DNA).

POPs Hunter: A Smartphone game to learn about pollutants.

Some news from world of science and technology:

From the weeks of 10 – 16, 17 – 23 and 24-30 May in chemistry.

Spectrometers, magnetometers, thermometers and more. The science instruments of NASA's Europa mission.

The United Nations turns 70 this year. Here's a look at 10 innovative programmes and projects that it has initiated.

for example this study that indicates coffee crop yields would decrease in current regions of production with a global temperature rise). Today, scientists are using big data to develop actionable solutions for the future the world's morning beverage of choice.

For those of us who prefer to drink coffee rather than grow it or manipulate its genome, it is good to recognize the health implications of coffee consumption; although it may be what you take with your coffee that needs to be watched! Did you know that pent coffee grounds are a potential source for bioactive compounds (and also biodiesel)? The issue of water quality and temperature must also be considered when talking about the difference between a good and perfect cup! Like so many of the food and beverages we enjoy, drinking coffee is a sensory experience (especially with espresso), we enjoy the smell and the taste, but what about the sound of coffee? Did you know that roasting coffee is both a chemical and an acoustic process? For those who prefer an espresso to that garden variety cup of coffee, make sure you get these three critical steps correct!

In our world of fancy gadgets, even the tried and true coffee maker has evolved with the times, one was recently installed on the International Space Station (requiring a special zero-gravity cup)! Of course, a cup of coffee can still be produced in a low-tech manner for those in a bind, using three light bulbs and some sandpaper for example. If necessary, a robot can help operate your coffee machine too. Finally, we point out that even coffee making has been assimilated by convergent science and technology: coffee machines have become valuable tools in chemistry laboratories for performing hot-water extractions, just what you need to brew up natural products.

Medical Countermeasures

Critical for response to a chemical attack is access to countermeasures to treat victims and protect emergency responders. The OPCW Scientific Advisory Board has produced reports on treatments for nerve and blister agent exposure; and on adjunct agents and new trends in the treatment of nerve agent poisoning. Despite published recommendations for treatment and availability of countermeasures, a number of limitations and challenges still remain. In this feature we reference recent publications relevant to medical countermeasures to inform interested readers about ongoing work in the field. It is notable that a number of these reports make reference to events in the Syrian Arab Republic from 2013.

Starting with countermeasures to organophosphorus poisoning, there are the familiar autoinjectors that contain atropine and an oxime (such as obidoxime, pralidoxime, TMB-4 or HI-6); as effectiveness can vary with the nerve agent of exposure, we have seen studies to identify additional oximes. The autoinjector is designed to deliver antidotes to muscle where the primary effect of the nerve agent occurs, however, nerve agent exposure can also produce neurodegenration. For mitigation of neurodegeneration, anticonvulsants are combined with atropine and oximes; typically diazepam, lorazepam or midazolam (and a number of other suitable substances have been reported). The psychoactive drug ketamine, may also have neuroprotective benefits (and has been studied for controlling epileptic seizures). Oximes that can cross the blood-brain-barrier and provide neuroprotective benefits continue to be an active area of study.

The enzyme butyrylcholinesterase can be used to scavenge nerve agents and prevent inhibition of acetylcholinesterase (a "bioscanvenger"). Combinations of butyrylcholinesterase with oximes have been studied to enable catalytic bioscavenging (studies have also been conducted using acetylcholinesterase mutants), while other approaches involve combining bioscavengers with hyaluronan-degrading enzymes. Modified cyclodextrins have also been proposed as potential catalytic scavengers.

Pre-treatments to nerve agent exposure that rely on carbamates or topical skin protectants are also known (see for example these studies on the effectiveness of topical protectants against VX and soman). As pre-treatments must be applied before exposure; emergency responders would need to recognize nerve agent presence prior to deployment (in this context, it has been suggested that social media could be used as a tool to help evaluate clinical syndromes). Research continues on additional options for supplementary drug treatments and possible alternatives to atropine and oximes.

Therapeutic strategies for sulphur mustard exposure have focused on anti-inflammatory compounds, antioxidants, protease inhibitors and antiapoptotic compounds. Combination anti-inflammatory and anti-cholinergic skin treatments have also

Crowdsourcing:

Map the 3D neural circuits that make vision possible by playing a game. With 84 million neurons in a human brain, your help really is needed!

Do you have clever designs for 3D printed objects? Are you a student? Do you live in India? Yes, yes, and yes? Then take a look at this 3D Printing Design contest.

Interested in education and outreach to build public awareness and involvement in protecting water resources? Participate in the World Water Monitoring Challenge™ (a truly global crowdsource as can be seen by the data collected thus far).

Crowdsourcing the world for emergency medicine – insights from two recent studies.

Upcoming S&T Related Events:

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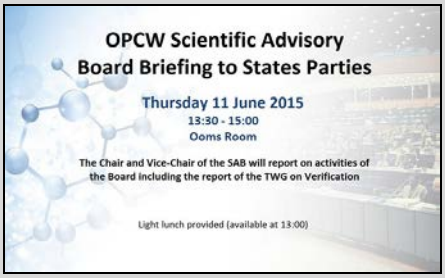

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Vienna, Austria.

show therapeutic potential. Other treatments of interest include the use of the catalytic antioxidant AEOL 10150, a compound previously studied for treatment of chlorine gas inhalation, as a possible countermeasure against sulphur mustard skin exposure. The peptide Rlip76, known to reduce oxidative stress in cells, may also have countermeasure potential as seen in a recent patent application. Finally, tissue plasminogen activator (tPA) can help to prevent airway obstruction (a possible consequence of sulphur mustard exposure). For topical treatments, fatty acids and cholesterol have been studied as a means to modulate skin adsorption.

While we've focused on nerve and blister agents, as there are far too many agents and countermeasures for a comprehensive review, the following reports may also be of interest: nitrocobinamide as an anti-cyanide antidote, antibodies that inhibit the transport of Ricin in cells and the use of polymers as antidotes for toxins.

Chemical Forensics

We thank our colleagues from the OPCW Laboratory for their major contribution and input to this feature

The ability to obtain unique signatures such as fingerprints and DNA to identify individuals or the marks left on a fired bullet to identify the firearm that shot it, to compare with reference materials (such as a fingerprint obtained from a suspect) are among the most powerful forensic tools available to law enforcement. Chemical signatures that indicate drug use or gender can even be collected from fingerprints.

Chemical samples can also have unique signatures that might reflect how and where they originated. For the Chemical Weapons Convention, one might ask, questions such as: What kind of molecular signatures exists for chemical warfare agents and toxic chemicals that may have been used in an incident under investigation, what kind of reference samples are required for comparison and what kind of forensic information can be obtained with such information?

Impurity profiling is the determination of types and quantities of impurities within a chemical sample (a type of analysis with important pharmaceutical and illicit drug law enforcement related applications). As molecules are made up of atoms of different elements connected in a specific way by chemical bonds it is tempting to think that this cannot be the source of a unique signature that could allow tracing back the origin of the chemical. However, chemicals are almost never absolutely pure. That is they contain impurities, which in the case of toxic chemicals and warfare agents, might be: side products of the reaction that produced the toxic chemical; side products originating from earlier reactions leading to precursors used to produce the toxic chemical; intermediate and final products of degradation reactions; and/or additives and stabilizers deliberately added to a toxic chemical.

8 July 2015
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13:30 – 15:00 Ooms Room
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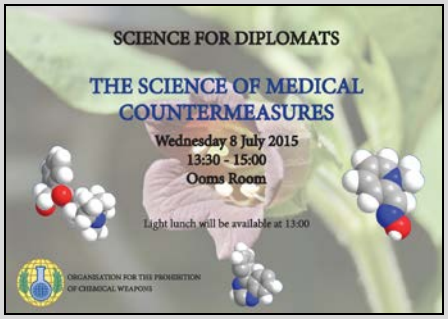

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Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

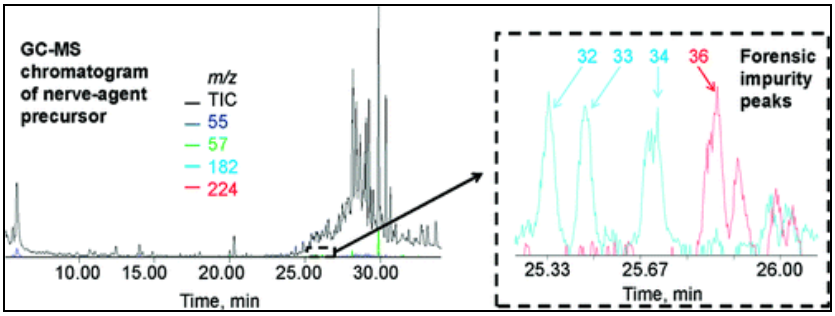
16 – 20 August 2015-05-25
250th American Chemical Society National Meeting and Exhibition.
Boston, MA, USA.

31 August – 4 September 2015
Sixth Summer Programme on Disarmament and Non-Proliferation of Weapons of Mass Destruction (WMD) in a Changing World. Asser Institute, The Hague, The Netherlands.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering); ECAB3 (3rd European Congress of Applied Biotechnology); and EPIC5 (5th European Process Intensification Conference)
Nice, France.

The chemicals that constitute the impurities can be indicative of the source of the chemical, the location from where it was collected, the process used to prepare or purify the chemical, or even a unique preparation (batch) of the chemical sample.

In addition to the presence of the impurities themselves, their relative amounts constitute another important signature. Some impurities will be stable under storage or reaction conditions or even in the environment after a chemical agent has been deployed, others will react further to produce other chemicals. "Stable" impurities are of high value for a signature as they potentially carry information from different steps in the preparation process. In situations where the sample is a mixture of several chemicals (or isomers of a given chemical), ratios of components can also be informative.



Impurity Profiling of a Nerve Agent from Researchers at the Pacific Northwest National Laboratory (Figure Copyright © 2011 American Chemical Society).

Most (but not all) chemical elements are composed of more than one stable (that is non-radioactive) isotope. For example carbon exists as two stable isotopes, ^{12}C (carbon with an atomic mass of 12) and ^{13}C (carbon with a mass of 13). On average, there will be 98.93% ^{12}C and 1.07% ^{13}C. However this ratio is not constant and will vary slightly in the environment. The range for ^{12}C is from 98.85% to 99.04% and that for ^{13}C 0.96% to 1.15%. This ratio of stable isotopes, which can be measured using a special (isotope ratio) mass spectrometer, can be used as a molecular signature. Stable isotope analysis can potentially be used to identify the source or supplier of certain chemical compounds. In drug forensics, stable isotope ratios have been successfully used to determine geographical origins of plant derived drugs such as heroin and cocaine. There are also applications in authentication of foods with protected designation of origin. This type of information can be valuable in conjunction with other information on proliferation channels and resource networks.

A significant challenge in chemical forensic analysis is the availability of appropriate reference materials for comparison. The exact nature of the required reference materials depends on the question that is being asked. If a unique molecular signature is used to confirm the origin of a chemical, known samples from the same origin are necessary for comparison; to link a toxic agent with a production batch requires that a sample of this batch is available; to link a chemical agent to certain precursors, reference samples of the precursors must be

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

15 October 2015
Smart Manufacturing Summit.
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available; similarly to show that the same agent from the same batch was used in incidents at several locations, samples from all of these locations must be obtained and compared. Without the availability of the right reference samples the possible information that can be obtained from the determination of chemical signatures can be severely limited. One possible (but not absolute) exception is that it an impurity pattern can indicate a certain type of production process. This need for suitable reference sets for attribution of samples is quite evident in other forensic analysis as well, microbial forensics for example. Furthermore, inhomogeneous chemical profiles across samples can limit the ability to establish links between them.

Impurity profiling and stable isotope analysis are important techniques in law enforcement, as illustrated by many of the references presented. However, chemical forensics as applied to chemical warfare agents is still an area of active and on-going research, not a set of routine techniques. In regard to warfare agents, we have presented a number of proof-of-principle references. To our knowledge there are no reports involving the use of these methods for investigation of warfare agents in an actual case study. We will report on future developments in the field as they come to our attention.

OPCW Research Projects Support Programme

Guest contribution from our colleagues in the International Cooperation Branch

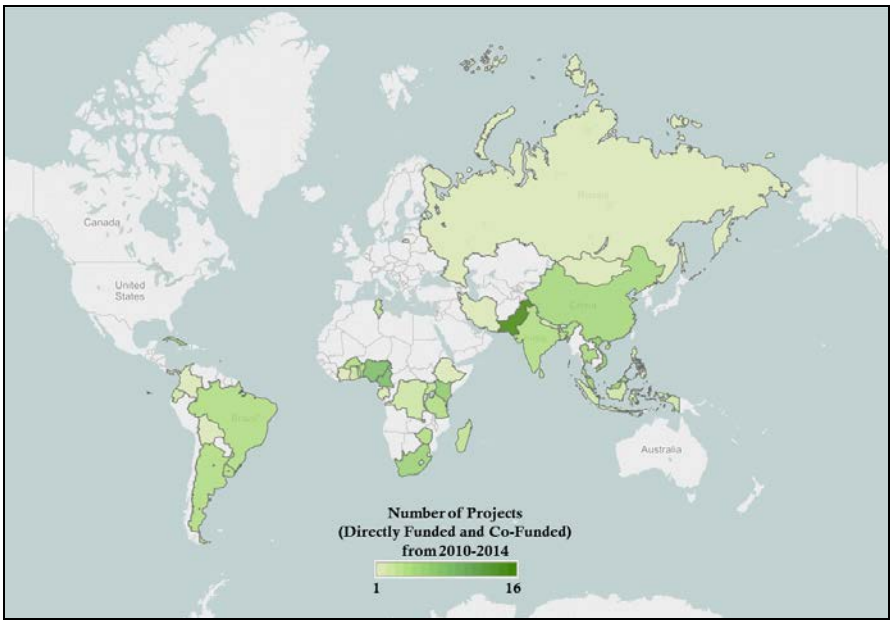


Figure 1: Funded and co-funded research projects through the OPCW Research Project Support Programme from 2010 – 2014.

Chemistry as a scientific discipline has always been central to the Convention. As the destruction of declared stockpiles of chemical weapons moves closer to its conclusion, the work of the OPCW in promoting research, as well as economic and technological development in the field of chemistry, becomes even more important. By supporting scientific research, the OPCW seeks to balance the numerous obligations that the Convention imposes on its Member States and their chemical industries.

For the last 15 years, the OPCW has been supporting small-scale research projects to Member States of the OPCW who fall under the category of developing countries or countries with economies in transition. These projects receive funds to cover auxiliary expenditures, such as consumables, maintenance, and small labware, with the aim of promoting research in the peaceful applications of chemistry hence contributing to economic and technological development of the recipient countries. Figure 1 illustrates the projects that have been funded (both directly and as a cofounder with the International Foundation for Science, IFS) from 2010 – 2014. For more information on the programme and how to apply, see Note S/1258/2015 available on the OPCW public website.

The projects funded from 2010–2014 have been distributed across the African, Asian, and the Latin American and Caribbean group (GRULAC) regions (and a single project was also funded in Eastern Europe) as indicated in Figure 1. Figure 2 illustrates the gender make up of the principle investigators and Figure 3 the areas of research focus.

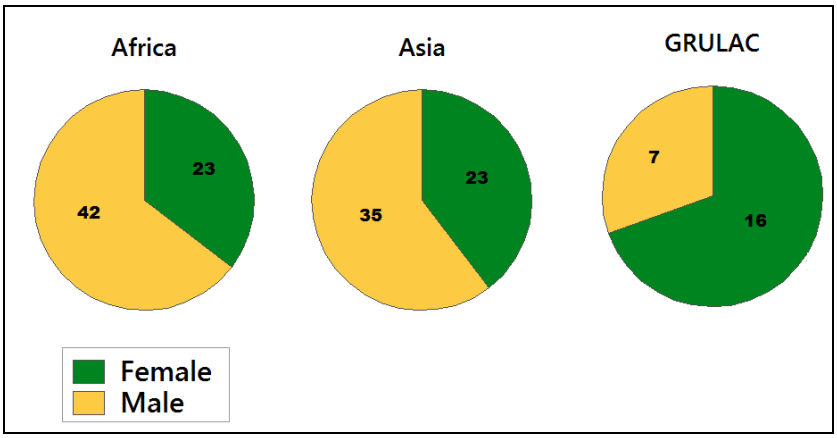


Figure 2: Gender make up of principle investigators in projects funded from 2010-2014.

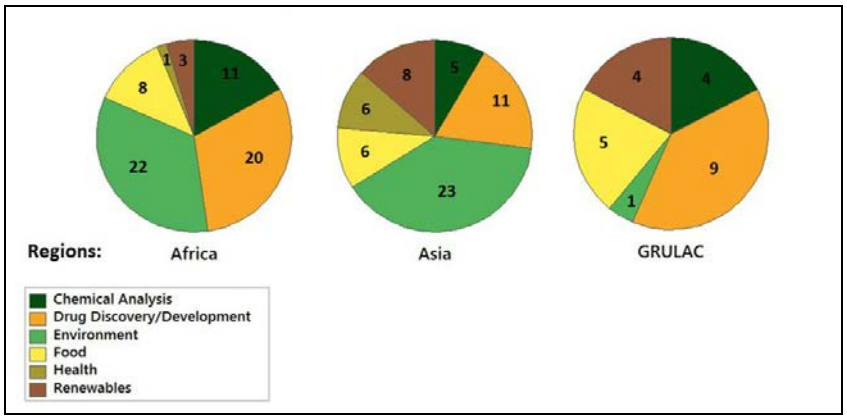


Figure 3: Areas of focus for research projects funded from 2010-2014.

Green chemistry represents an additional dimension to the research areas illustrated in Figure 3. The principles of this field give rise to innovative chemical transformations with high industrial interest and low environmental impact; low toxicity to humans; sustainable uses of energy and resources; and other social and economic sustainability benefits. Clean up and destruction of toxic materials, new analytical methods, reduction of the use and presence of toxic chemicals, and scientific collaborations that result from work in Green Chemistry compliments the core activities of the OPCW (destruction of chemical weapons, non-proliferation, assistance and protection from toxic chemicals, and international cooperation).

The 2010-2014 funding period saw 57 scientific publications go to print in a variety of peer reviewed scientific journals. For those interested in receiving OPCW funding through this programme, the areas noted below (and Green Chemistry projects falling under all of these thematic areas) are of particular interest.

Chemical Analysis: analysis, characterization, and detection of chemicals, including and modelling distributions of measured chemicals in the environment. Recent publications:

- *Confined gold nanoparticles enhance the detection of small molecules in label-free impedance aptasensors*
- *Spatial Variation and Source Distribution of Organic Contaminants in Langat River Basin, Malaysia Using Chemometric Techniques*
- *Structure-fragmentation relationship and rapid dereplication of Buxussteroidal alkaloids by electrospray ionization-quadrupole time-of-flight mass spectrometry*

Drug Discovery: drug design (including *in silico*), drug synthesis and bioactivity of natural substances (*in vitro* and *in vivo*); and, **Health**: medical treatments, prophylactics, protection and the health effects of chemicals. Recent publications:

- *New Antimalarial Hits from Dacryodes edulis (Burseraceae) - Part I: Isolation, In Vitro Activity, In Silico "drug-likeness" and Pharmacokinetic Profiles*
- *Oxindole Derivatives: Synthesis and Antiglycation Activity*
- *Solid-Phase Total Synthesis of Cherimolacyclopeptide E and Discovery of More Potent Analogues by Alanine Screening*

Environmental: pollution monitoring; destruction, remediation, detoxification and prevention; and, health effects of pollutants on humans and ecosystems. Recent publications:

- *Composite nanofloral clusters of carbon nanotubes and activated alumina: An efficient sorbent for heavy metal removal*
- *Nickel and manganese release in serpentine soil from the Ussangoda Ultramafic Complex, Sri Lanka*
- *Pesticide potential dermal exposure during the manipulation of concentrated mixtures at small horticultural and floricultural production units in Argentina: The formulation effect*
- *Structural characteristics and flammability of fire retarding EPDM/layered double hydroxide (LDH) nanocomposites*

Food: chemicals and organisms that have impact and improve food (crops and livestock) production. A recent publication:

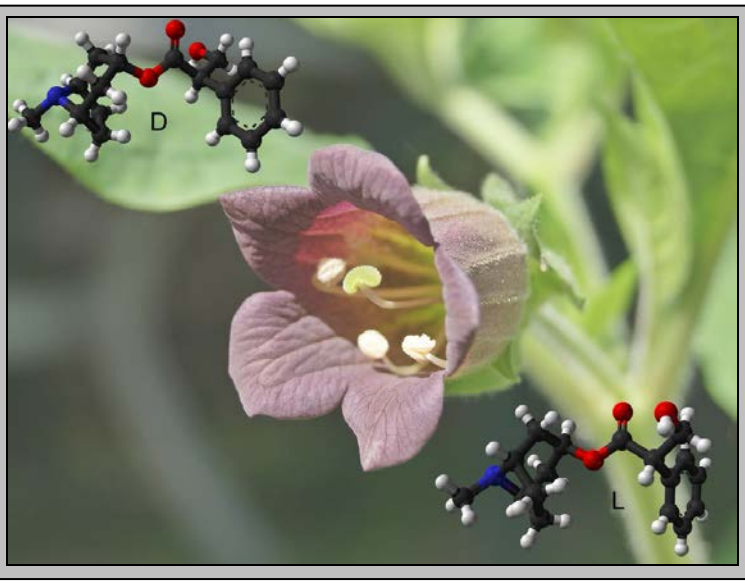
- *Chemical Composition and Phenolic Compound Profile of Mortiño (*Vaccinium floribundum *Kunth)*

Renewables: biomass and natural substances for chemicals and energy. A recent publication:

- *Development of novel in situ nickel-doped, phenolic resin-based micro–nano-activated carbon adsorbents for the removal of vitamin B-12*

Did You Know?

Atropine, a nerve agent countermeasure, was isolated from *atropa belladonna*?



VOLUME 2 NUMBER 8

The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

10 July 2015

In This Issue

Featured content

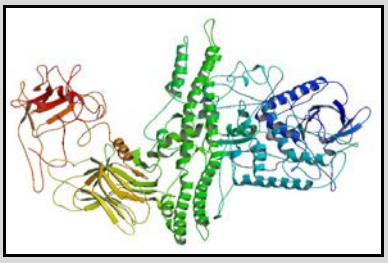
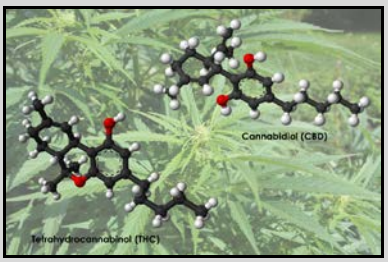


Image from Protein Data Bank (structure 3BTA).

Protein structure of botulinum toxin

Image from beautynz.

Chemistry of cosmetics



Cannabinoids

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

Today marks the birthday of Edward Lowe (1920-1995), the accidental inventor of "kitty litter"; an absorbent material that is now found in cat boxes around the world. We highlight this inventor for his support of new and unusual ideas, and we point out that absorbent materials are routinely used to protect us from and to collect samples of chemical agents. Absorbent materials can also be used to capture toxic chemicals from the environment.

The S&T Puzzle

In the tightest contest yet for winning the prize, our friends at the CTBTO submitted their correct answers a mere minute ahead of a member of the OPCW staff! These answers were of course: LD_{50} of water = 0.08 liter/kg bodyweight, Molarity of Caffeine in a cup of coffee falls in the range of 0.0016 – 0.0021 mol/liter, and LD_{50} of coffee itself = 1.57 cups/kg bodyweight). Congratulations for a job well done! Puzzle statistics now stand at: VER 4, OSP 2, OCS 1, INS 1 and CTBTO 4.

For this edition of the puzzle, we ask you to find the collection of words that make up the section titles of the *S&T Monitor* in the word search puzzle below (twenty-five words in all). Circle the words and send us an image of the completed puzzle, whoever finds the most correct words wins the prize: a choice of requesting a featured topic, designing a puzzle, or receiving a beverage hand selected by the Science Policy Adviser. Send answers by email. Good luck!

G	R	Z	Y	C	S	U	T	S	H	Q	W	N	C	C
D	G	D	R	R	C	B	P	O	A	A	R	O	A	O
N	M	N	O	V	I	P	K	D	X	I	N	I	N	S
O	G	U	S	L	E	L	S	G	A	I	S	S	N	M
C	I	F	I	T	N	E	I	C	S	T	N	S	A	E
E	W	F	V	Q	C	A	F	Y	C	M	E	E	B	T
S	K	H	D	Q	E	Y	R	U	L	U	W	S	I	I
S	B	O	A	R	D	T	D	X	T	N	S	U	N	C
C	R	O	W	D	S	O	U	R	C	I	N	G	O	S
W	C	P	O	I	R	D	E	T	A	L	E	R	I	W
C	I	R	M	P	U	Z	Z	L	E	U	V	J	D	N
Q	P	E	R	S	O	N	A	L	N	T	E	B	S	N
D	H	W	E	L	C	O	M	E	V	O	N	R	X	A
C	G	N	I	M	O	C	P	U	B	B	T	B	A	K
Y	T	N	E	W	T	H	B	Z	A	M	S	P	B	C

Science Fun:

Through today's edition of *Science Fun*, we congratulate our colleagues here at the OPCW on a series of birth announcements that all took place within the past few weeks! Do we have future scientists? Future diplomats? Or perhaps future motorcycle racers or beer brewers? Only time will tell, and we look forward to watching them all grow. To celebrate, we look at some of the science of babies!

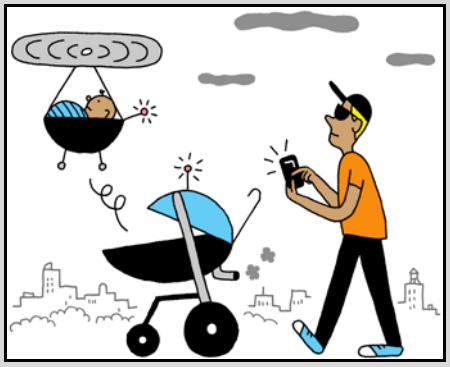


Image from The New York Times. (Fatherhood Has Its Rewards, Like That $1,700 Stroller).

Do you remember the milestones you reached in the first hour after birth? Perhaps not (and for good reason), so here is a little reminder! You probably don't remember what the world looked like as new-born either; but you can experience it again with the help of computers as shown by a recent study. Does a baby's behaviour have a scientific basis? Studies suggest that new-borns who recognise familiar smells and experience skin to skin contact may be more adept at finding their favourite sources of nutrition! Babies even produce their own smells to help their parents too!

Parents might also want to talk to their babies to help boost brain power which is an especially important job for parents of premature babies.

News and Updates

Recent reports and publications:

Report of the Second Meeting of the United Nations Secretary-General's Scientific Advisory Board and summary of the Third Meeting.

A look at the good, the bad and the unknown of the DNA-Editing technology CRISPR.

Nature Index 2015 Global.

Report from the Workshop on lessons learned from the international maritime operation for the removal and transport of Syrian chemical materials.

June 2015 issue of Dstl's *Insight*.

IAEA Bulletin Volume 56-2 (June 2015).

The ABCs of Sustainable Production and Consumption from UNEP.

The *Social Innovation Lab Guide* from Waterloo Institute for Social Innovation and Resilience.

The report on the public attitudes to chemistry study in the United Kingdom from the Royal Society of Chemistry.

Is there a link between political party and views on science? Take a look at Americans, Politics and Science Issues.

Report from Geneva: The Biological Weapons Convention Fortieth Anniversary of the Entry into Force.

Science and education resources:

Examples of the use of new technologies for treaty verification from the James Martin Center for Non-Proliferation Studies.

Project Ignite. 3D Printing resources for teachers and schools.

Test your knowledge of chemical hazard symbols and pictograms with this quiz.

How to give a science flash talk – some tips and advice for science communication.

Some news from world of science and technology:

From the weeks of 31 May – 6 June, 7 – 13 June, 14 – 20 June, 21 - 27 June and 28 June – 4 July in chemistry.

Did you know that babies recognize the sound of their mothers voices and heartbeat before birth? For those of you thinking about what to say to a baby, consider if you should be speaking in "parentese" (which includes dialects such as "motherese" and "fatherese") or standard speech – it could influence future language development! Bilingual babies can even teach adults a thing or two! Does Music help? It may, but it depends on who you ask!

We all know that parents play a vital role in the development of a child, yet we always hear that there is no manual, but we have found some online lessons (and some resources for science minded parents). For those who would like to see their babies contribute to science, there are plenty of science experiments that can be done at home and babies can contribute to global scientific knowledge just by laughing! There is plenty of science and technology to keep parents (especially fathers) occupied too, and the new gadgets are much less terrifying than some of the options available in the 20th century.

Crowdsourcing:

Contribute to saving lives and promoting clean energy uptake throughout Africa (and win a reward) by submitting your ideas on recycling liquid petroleum gas cylinders.

Do you have any innovative and environmentally sustainable ideas? If so, submit a proposal to the Green and Sustainable Chemistry Challenge!

Do you have a talent for visualising science and engineering? Submit your work to the Vizzies!

Twenty-Second Session of the OPCW Scientific Advisory Board

We thank the Secretary to the SAB for his contributions to this feature

The OPCW Scientific Advisory Board (SAB) held its Twenty-Second session from 8 to 12 June 2015 at OPCW Headquarters in The Hague under the chairmanship of Dr Christopher Timperley (United Kingdom and Northern Ireland), with Mr Cheng Tang (China) serving as Vice-Chair. Deputy Director-General, Ambassador Grace Asirwatham, delivered the opening statement on behalf of the OPCW Director-General, noting that "Science and technology are ingrained in the Chemical Weapons Convention".

During the session, the SAB endorsed the report received from its Temporary Working Group (TWG) on verification and submitted a report with further advice on medical countermeasures for exposure to nerve agents (this report was further discussed at the July Science for Diplomats briefing). Commenting on the reports, Dr Timperley noted, "Verification is at the heart of the Chemical Weapons Convention, and we hope our advice will better inform the OPCW's efforts to achieve a world free of chemical weapons." A briefing by the Chair and Vice-Chair to OPCW States Parties on the activities of the SAB was also held.

A call for evidence-informed ideas to provide new insights in international responses to new threats and challenges to peace, security, and development.

Upcoming S&T Related Events:

14 – 26 July 2015
19th Annual Green Chemistry and Engineering Conference.
Bethesda, ML, USA.

19 – 22 July 2015
12th World Congress on Industrial Biotechnology.
Montreal, Canada.

28 – 30 July 2015
International Society for the Philosophy of Chemistry (ISPC 2015).
Rio de Janeiro, Brazil.

6 – 13 August 2015
48th IUPAC General Assembly and 45th World Chemistry Congress.
Busan, Republic of Korea.

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

16 – 20 August 2015-05-25
250th American Chemical Society National Meeting and Exhibition.
Boston, MA, USA.

24 – 27 August 2015
FinMedChem 2015.
Helsinki, Finland.

31 August – 4 September 2015
Sixth Summer Programme on Disarmament and Non-Proliferation of Weapons of Mass Destruction (WMD) in a Changing World. Asser Institute, The Hague, The Netherlands.

3 – 4 September 2015
The International Conference On Chemical Sciences And Engineering (CHEMSCIE 2015).
Veracruz, Mexico.

The session included contributions from three guest speakers: Professor Åke Sellström on lessons identified from the 2013 United Nations Investigation into Alleged Uses of Chemical Weapons in the Syria Arab Republic, which he led; Dr Istvan Gyarmati in his capacity as Chairperson of the Advisory Board of the Secretary-General of the United Nations on Disarmament Matters; and Dr Daan Noort (The Netherlands Organisation for Applied Scientific Research) on chemical forensics.

Developments related to the convergence of chemistry and biology (including green chemistry), and education and outreach were also discussed during the session. To prepare its comprehensive report to the Fourth Review Conference of the Chemical Weapons Convention, the SAB will meet twice in 2016 and in 2017. A report on the 22nd session of the SAB will be issued shortly, followed by the Director-General's response.

We thank the SAB for their contributions to the work of the OPCW and leave you messages of science and peace from some of our SAB members.

Botulinum Toxin

Botulinum toxin is a potent neurotoxin that is produced by *Clostridium Botulinum* (an anaerobic, Gram-positive, spore-forming rod-shaped bacteria). The toxin causes paralysis by blocking the action of the neurotransmitter acetylcholine. *Clostridium botulinum* is found in soils and sediments; in intestinal tracts of fish and mammals; and in gills and viscera of shellfish. Under certain (low oxygen) conditions toxins may be produced; such conditions include improperly canned foods, minimally heated chilled food that has not been adequately refrigerated, and contaminated wounds. *Clostridium botulinum* produces serologically distinct botulinum toxin types (A, B, C_1, C_2, D, E, F and G). Human botulism is caused primarily by toxin types A, B, or E and rarely F.

With a Median Lethal Dose (LD_{50}) approximately 100,000 times smaller than that of sarin and historical examples of botulinum toxin produced for state sponsored biological warfare programmes, concerns have been raised over the possibility

13 – 16 September
1st International Workshop on Mobile Learning (WmL'15).
Lodz, Poland.

20 – 24 September 2015
9th International Conference on Instrumental Methods of Analysis-Modern Trends and Applications (IMA2015). Kalamata, Greece.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering); ECAB3 (3rd European Congress of Applied Biotechnology); and EPIC5 (5th European Process Intensification Conference)
Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

6 October 2015
"Science for Diplomats". Data Analytics and the CWC: An Introduction to OCPF Site Selection Methodology. 13:30 – 15:00 Ooms Room
OPCW Headquarters, The Hague, Netherlands.

15 October 2015
Smart Manufacturing Summit.
Livermore, California, USA.

31 October - 2 November 2015
The Port Hackathon.
CERN

4 – 7 November
World Science Forum.
Budapest, Hungary.

16 – 19 November 2015
Malta Conference.
Rabat, Morocco.

18 – 21 November 2015
16th Asian Chemical Congress.
Dhaka, Bangladesh.

22 – 27 November 2015
2nd African Conference on Research in Chemical Education (ACRICE)
University of Venda, Thohoyandou, South Africa.

botulinum toxin might be used as a biological weapon. For example, the potential for an intentional botulinum contamination of milk has been mathematically modelled, the subject of newspaper editorials and actually experimentally tested.

Despite how often it is referred to as one of the most poisonous biological substances known, botulinum toxin finds use in a number of clinical treatments and even in cosmetics (BOTOX® for example); a convergence of medicine and neurotoxins! Clinical conditions that can be treated with botulinum toxin include lower urinary tract function; tetanus; migraine and other chronic pain; and neurological disorders.

Cosmetic use involves the injection of very low doses of the type A toxin under the skin; usually on the face to smooth out wrinkles. Formulations for cosmetic use continue to be patented and can include claims that cover use of alternate neurotoxins (saxitoxin for example) in the formulation. Botulinum toxin therapeutics and cosmetics are generally considered safe; however, reports of adverse effects are not unknown.

Chemistry of Personal Care Products and Cosmetics

We thank Julie Foucqueteau, Kyungsin Kim and Diana Pyrikova from OPCWs Media and Public Affairs Branch for their contributions to this feature and interest in learning a bit of chemistry. We wish all of them the best of luck as they move onward from their OPCW internships.

While it is a strange thought that a substance as toxic as botulinum is a common cosmetic treatment, the use of toxic substances in cosmetics is nothing new. Beauty practices from the ancient world give an all new meaning to the age old saying "beauty is pain". Toxic lead based chemicals seem to have been popular: Laurionite (PbOHCl) and phosgenite ($Pb_2Cl_2CO_3$) applied as eyeliner in ancient Egypt (which may have actually had a health benefit for warding off disease) and lead face power in the European royal courts of the 17th century just to name a few. Today beauty products are a multi-billion dollar industry that has maintained an average growth rate of 4.5% per year over the past two decades!

Given the history of toxic substances in personal care products, we thought it might be worth a look at some of the modern chemicals we wilfully treat ourselves with. In the 21st century, personnel care often starts out with soap, shampoo and fluoride containing toothpaste. Soap is especially important for health and hygiene (details here).

14 - 18 December 2015
Biological Weapons Convention Meeting of States Parties.
Geneva, Switzerland.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

Contact Us:

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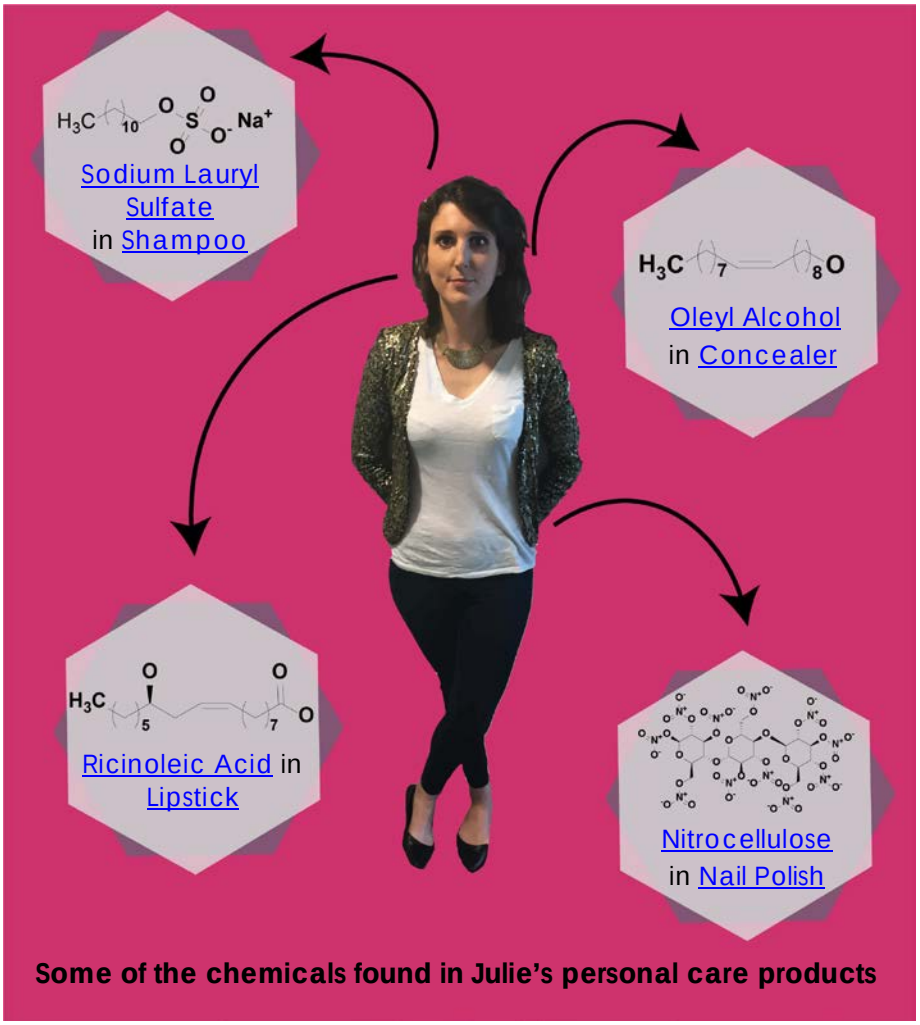
For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.



Some of the chemicals found in Julie's personal care products

Some of us go on to apply shaving cream (which can contain the Schedule 3 chemical triethanolamine) and/or hair gel; and perhaps beauty products such as lipstick (which might contain castor oil, an oil that comes from the same plant that gives us ricin) and/or nail polish (which might leave behind flakes that can link a person to a crime scene). If your make-up kit includes body paint and you find yourself on an investigation of alleged use, you might be interested in learning how latex body paints can be used to sample chemical agents.

For hair, longer lasting cosmetic treatments (hair dying) may be preferred, However, be very careful how you treat your hair, all it takes is surface-enhanced-Raman-spectroscopy (SERS) to identify not only if your hair is dyed, but also what brand of dye you used!

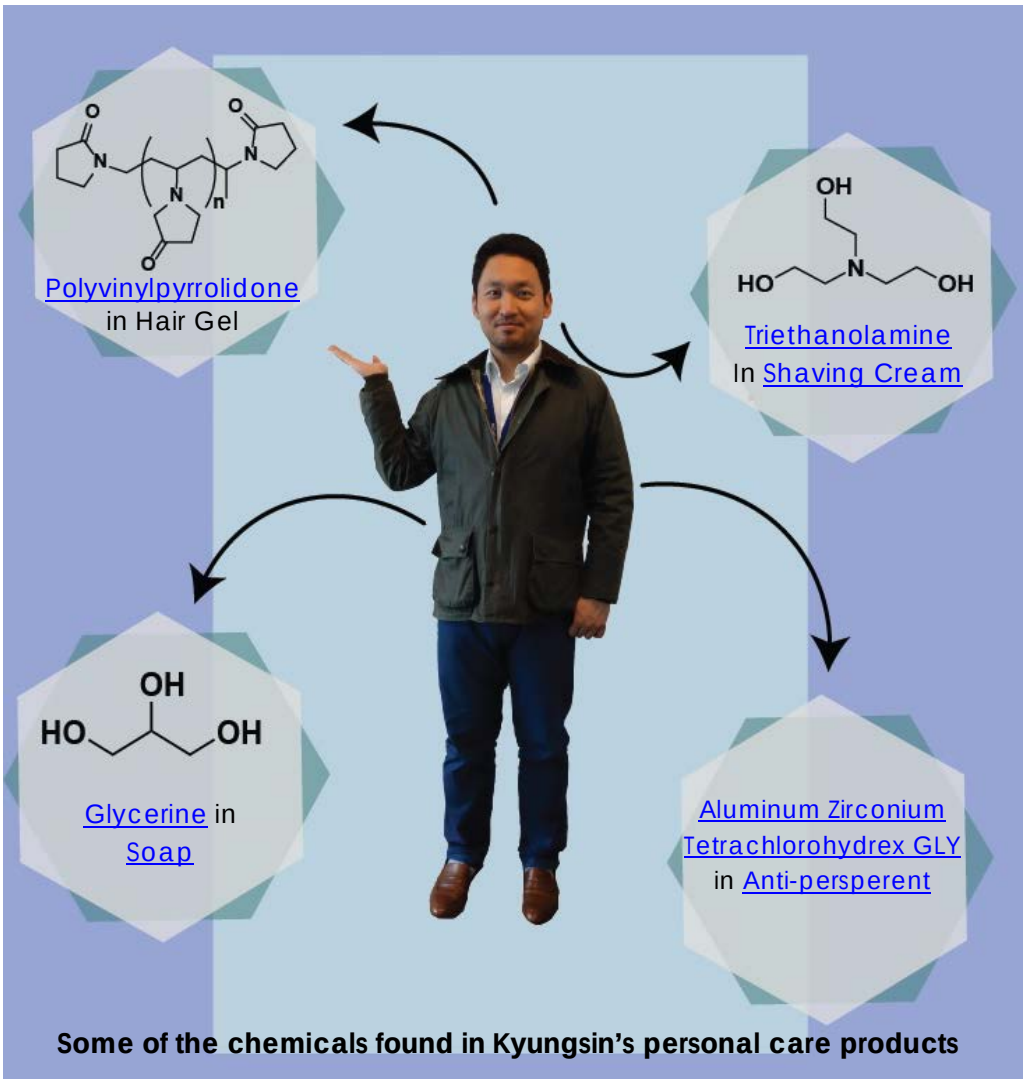
Protection from sun exposure employs sunscreens that contain titanium dioxide (for absorbing and scattering UV light) mixed with organic compounds (that absorb specific wavelengths of UV). UV absorbing compounds can also be generated through metabolic processes in some species of fish (and these metabolic processes can be transferred into to yeast for production of cosmetic components). Tanning without UV is also possible through chemistry.

Spending time in the sun can induce sweating, a process associated with foul odours which has created a market for deodorants. Scientists are of course working to solve the odour problem; using for example, ionic liquids that are applied to the skin where they emit pleasant smells when exposed to perspiration. Sweat may actually have redeeming qualities, such as energy production!

The beauty industry invests heavily in R&D, always in search of something that will set a company apart from its competition. One such innovation is nail polish that detects incapacitating agents through a colour change (a method to ensure no one has spiked your drink!); conceptually, this is similar to paint on vehicles (and UAVs) that changes colour when exposed to a chemical agent.

Personal care product R&D might also help solve sanitation issues in the developing world, as demonstrated by fragrance chemistry and latrines.

At the end of the day when the personal care products on our bodies are removed, they still end up somewhere. The degradation of these products in waste treatment facilities and their environmental fate can involve a series of complex mechanisms; calling for large research initiatives for assessment.



Some of the chemicals found in Kyungsin's personal care products

Cannabinoids

A growing number of countries are legalizing marijuana for medical purposes (see Figure 1), sparking increased interest in cannabis-derived compounds (cannabinoids) for clinical use. Given that cannabinoids can be considered as a central nervous system (CNS) acting chemical, we take a look at chemistry and clinical reports related to cannabis.

Conditions for which therapeutic use have been considered include: nausea and vomiting (due to chemotherapy), appetite stimulation for HIV/AIDS patients, chronic pain, spasticity, depression, anxiety, sleep disorder, psychosis, glaucoma, and Tourette syndrome. An analysis of published studies has yielded mixed results for the quality of evidence supporting the benefits of medical marijuana. Never the less, other studies suggest there may be benefits from the use of cannabis (and/or cannabinoids) for conditions that include pain modulation, especially in combination with opioids; inflammatory bowel disease; reducing insulin-resistance in HIV-HCV infected patients; Parkinson's Disease; Alzheimer's Disease; and pediatric treatment resistant epilepsy.

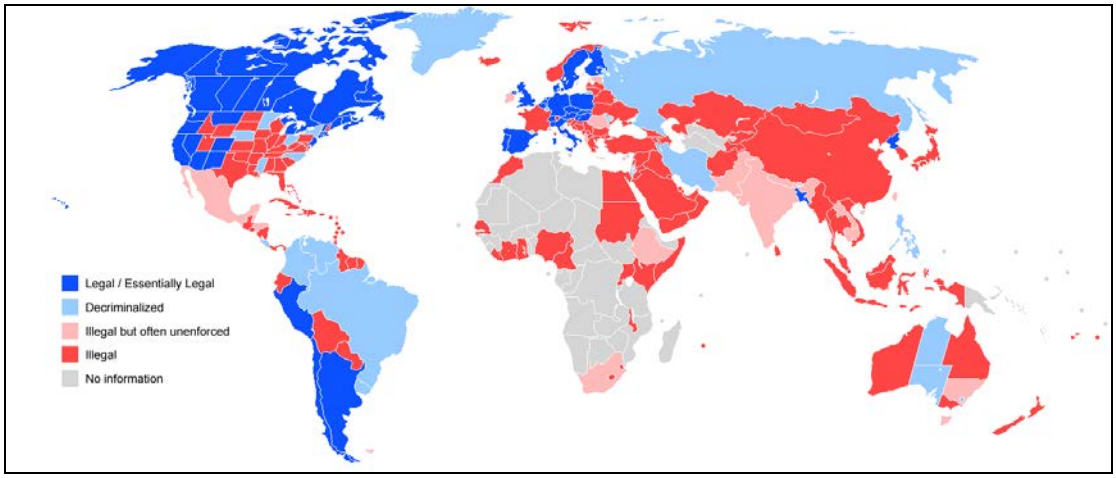


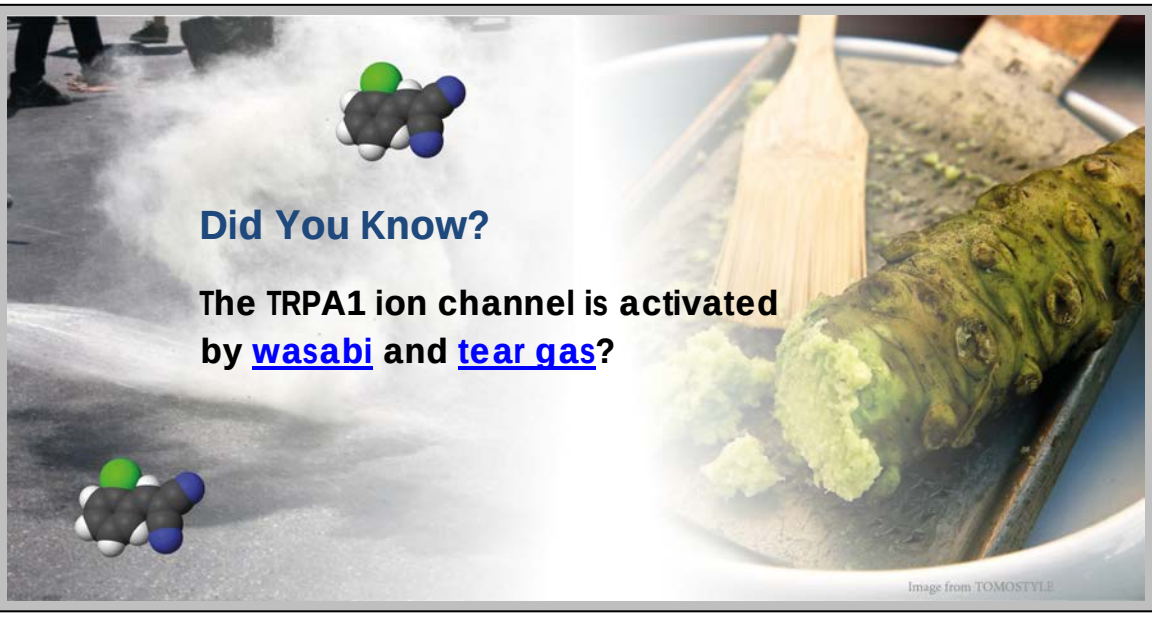
Figure 1: Status of Medical Marijuana as of 7 May 2014, *Image courtesy of Trinitresque*

There is also interest in the use of cannabinoids for chemotherapy, however, no solid proof exists that cannabinoids would be effective in this application. Given studies that cannot produce conclusive data, and concerns about unintended complications, more clinical studies have been recommended.

As cannibus and cannabinoids become more available (whether for medical purposes or the recreational use of marijuana and/or synthetic cannabinoids), so does the potential for their misuse; for instance, poison control centers in the United States reported a greater than 200% increase in the number of calls related to synthetic cannabinoid use for January - May 2015. Long-term effects, particularly in relation to smoking and lung health, are also a concern.

With both a higher visibility and prevalence of use, issues related to how to ensure legal marijuana is safe; primary care of users and education for medical practitioners; potency of the method of administration; combined effects with alcohol and other drugs; and fitness to drive have received greater attention.

Not surprisingly, technology developers have also seized upon opportunities, such as the marketing of a 3D printable herb garden, resulting from all the interest in cannabis.



VOLUME 2 NUMBER 9

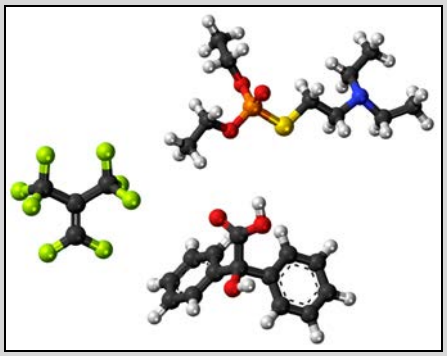
The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

13 August 2015

In This Issue

Featured content



Schedule 2 Chemicals

Image from World Water Monitoring Challenge.

Global science experiments

Image from Sparkfun.

A Carbon monoxide sensor

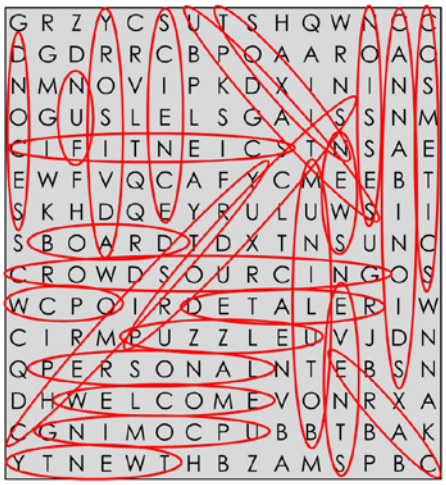
Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

Today marks the 55th anniversary of the first two-way telephone conversation by satellite (a balloon satellite called Echo 1) in 1960. One of many steps that have taken our communication technologies to where they are today and enabling so many opportunities for collecting and communicating information. To, further remind us of how far we have come, today is also the 126th anniversary of an 1889 patent for a coin-operated telephone, and we are certain that there will be many more telecommunication innovations to come.

The S&T Puzzle

We once again congratulate our friends at the CTBTO for finding all 25 words in last issues puzzle. The answers are shown below. Puzzle statistics now stand at: VER 4, OSP 2, OCS 1, INS 1 and CTBTO 5.



For this edition of the puzzle, we take inspiration from the "Astrobiological Periodic Table" and seek your inputs for a "Chemical Weapons Convention Periodic Table". We ask you to tell us how the elements of the periodic table are relevant in this context. Identify a link to the CWC for as many or as few elements as you like; points, equal to the sum of the atomic numbers of the elements identified, will be awarded. No points will be given for any element that is reported as having no relevance. Highest number of points scored wins the prize: a choice of requesting a featured topic, designing a puzzle, or receiving a beverage hand selected by the Science Policy Adviser. Send answers by email. Good luck!

Science Fun:

Hello Pluto! Last month, after a nine and a half year, 3 billion mile (that's 4.8 billion km) journey, astronomers celebrated as an unmanned vehicle called New Horizons reached Pluto, the last major *terra incognito* of our solar system (and how much do you know about pre-flyby Pluto?). The flyby took place on 14 July, fifty years to the day after another unmanned vehicle had been the first to reach Mars (that's right, we just celebrated the 50th anniversary of the first Mars flyby!). New Horizons represents everything we look for in an unmanned vehicle: fast (the average speed to get to Pluto was nearly 60,000 km/hour), capable of making chemical measurements and communicating with us from afar!

Image from Nasa.

Why do the images of Pluto appear red? Perhaps a consequence of the large amount of methane that is found there; cosmic rays and solar ultraviolet light can interact with this hydrocarbon to ultimately form tholins, which would explain the colour of the images.

Pluto is one of the coldest places in the solar system, with surface temperatures below -225ºC; plains covered by frozen nitrogen, methane and carbon monoxide; and mountains (some as high as 3500 meters) made of frozen water (and shorter mountain ranges have also been observed).

News and Updates

Recent reports and publications:

Report of the Twenty-Second Session of the OPCW Scientific Advisory Board.

UN Security Council Resolution 2235 (Adopted 7 August 2015) to establish a UN-OPCW Joint Investigative Mechanism.

Innovation and Diffusion of Green Technologies: The Role of Intellectual Property and Other Enabling Factors; a report on intellectual property and green technology from WIPO.

Bioenergy & Sustainability: Bridging The Gaps, report from Scientific Committee on Problems of the Environment (SCOPE).

Application of Modern Toxicology Approaches for Predicting Acute Toxicity for Chemical Defense, report from the US NAS.

Reimagining Human Health: 30 Innovations to Save Lives report from the IC2030 Initiative.

Reproducibility in life science research is an on-going issue, one with significant economic consequences. Improving inter-laboratory communication is recommended in one report; and guidelines for reporting have been created, however some scientists suggest these guidelines need more flexibility.

Science magazine special report on artificial intelligence.

July 2015 issue of Dstl's *inSIGHT*.

World Academy of Sciences (TWAS) newsletter, Volume 26 Issue 4.

Top 50 global chemical companies of 2014.

The game changing effect of new technology on finance. Report from the World Economic Forum.

An efficient and practical approach to biosecurity from the Centre for Biosecurity and Bioprepardness (Denmark).

Science and education resources:

Effective communication, to technical and non-technical audiences, is critical for productive engagement on science. Here are some tips for memorable presentations.

Building the 21st Century Scientist, the promise and challenges of bringing science, technology, engineering and mathematics (STEM) education in line with the lessons of education research.

Some news from world of science and technology:

From the weeks of 5 – 11, 12 – 18, 19 – 25 July, 26 July – 1 August and 2 – 8 August in chemistry.

Images show a large heart-shaped plain (of frozen carbon monoxide) alongside and the high frozen water mountains noted above; these features were named the Tombaugh Regio in honor of Pluto's discoverer Clyde Tombaugh.

The icy plains are scarred with long polygonal marks, dark streaks and rolling hills; challenging assumptions about geological activity on icy worlds; internal geological activity may be a possibility as heat appears to be coming from somewhere. Another intriguing feature of both Pluto and its largest moon, Charon, is their "youthful appearance" (crater free) which may have resulted from a collision between the two bodies.

Images reveal flowing glaciers of nitrogen and a haze extending over 130 km above the surface of the planet; a planet that appears to be "leaking nitrogen" at 500 tons per hour (from an atmosphere that reaches over 1,600 km above the surface). As New Horizons moves beyond Pluto, the spacecraft has already observed components of Pluto's atmosphere, carried off by solar winds, thousands of miles away.

There is much more is to look forward to over the next sixteen months (the time required to download all the data that has been collected), and even more fantastic discoveries are sure to follow as New Horizons moves onward. For those of you who can't wait the sixteen months, if you have a few minutes to spare to learn more about Pluto, take a look at the "Pluto in a Minute" video series.

July 2015 was quite a month for NASA: the Pluto flyby, the 50th anniversary of the 1st Mars flyby and no less significant, the 46th anniversary of the 1969 moon landing on 20 July (here's an article published in the 14 July 1969 issue of *Chemical and* Engineering News about the

Schedule 2 Chemicals

When we discuss chemicals relevant to the Chemical Weapons Convention (CWC), those falling under Schedule 1 tend to receive the most attention; yet, the number of possible chemical structures covered under Schedule 2 represents more chemicals than have actually been reported in the scientific literature! One just has to look at Schedule 2B(4) to see this. Have you ever wondered about the chemicals that fall under Schedule 2, why they are CWC relevant and what they are used for? Illustrating the importance of these chemicals beyond the CWC, in 2014, 1048 scientific journal articles and 1348 patents (applications and grants) involving Schedule 2 chemicals were published. Figure 1 summarises the publications, which were collected by SciFinder® searches through 1 June 2015. Figure 2 displays the collective abstracts in a word cloud to illustrate the words and themes across the publications.

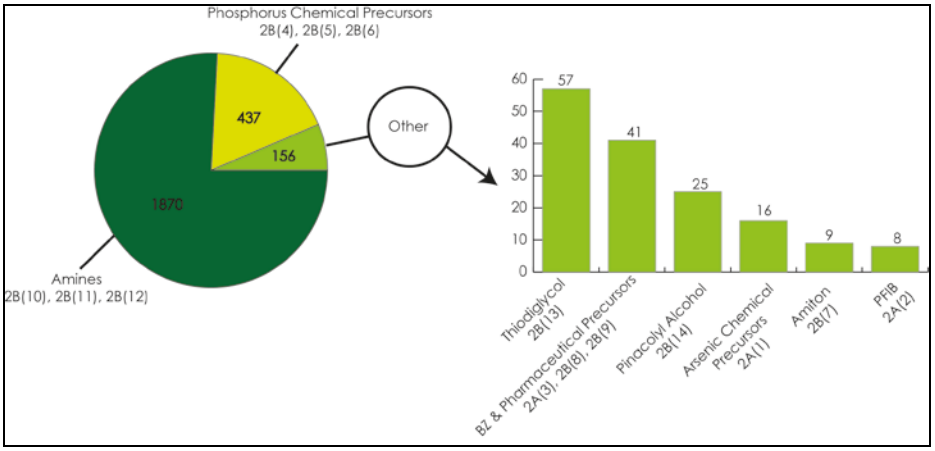


Figure 1: Number of publications (journal articles and patents) involving Schedule 2 Chemicals from 2014 (note that some publications concern more than one class of Schedule 2 chemicals – this has been corrected for within categories but not across categories).

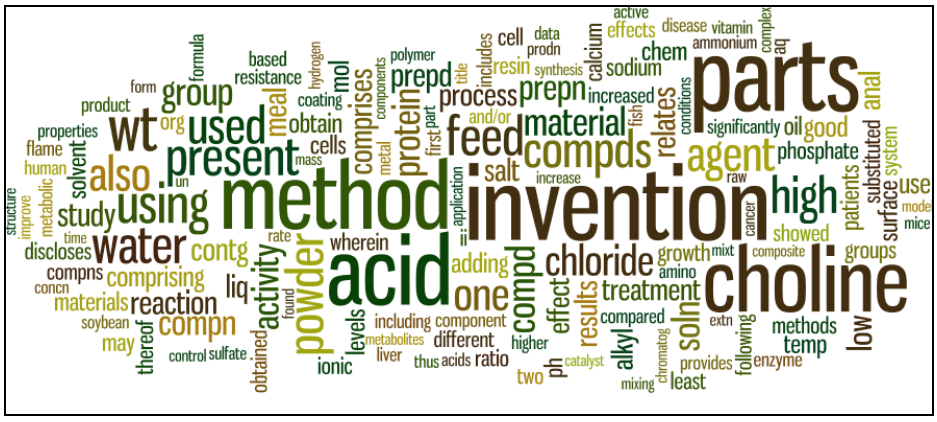


Figure 2: Word cloud of abstracts from journal articles and patents involving Schedule 2 chemicals published in 2014.

The following criteria are taken into account to consider whether or not toxic chemicals not listed in Schedule 1 and pre-cursors to chemicals in Schedule 1 or Schedule 2, part A would be listed in Schedule 2:

1. It poses a significant risk to the object and purpose of the Convention Weapons Convention because it possesses such lethal or incapacitating toxicity as well as other

Apollo 11 mission). We can only look forward to what comes next, no matter what it will be (perhaps a colony on the moon?), it is sure to capture the imagination.

Crowdsourcing:

Looking for a scanner that can recognise harmful ingredients in food. Do you have any ideas on how to build one? Take the food scanner challenge for a chance to win a European Union Horizon Prize.

Do you have ideas for a methodology that can identify the early indication of a climate or water event (such as a floods or drought) in one location triggering direct or indirect impacts in another location?

Help build a sustainable food system by creating an app with data from the USDA. This will help researchers, consumers and farmers understand the food supply, economic demand and remote sensing data.

Help NASA identify the features of Mars.

News from the (Twitter) crowd: an examination of civic media systems in wartime. To strengthen use of Twitter data to draw conclusions, this method of quantifying "controversy" might also be helpful.

Upcoming S&T Related Events:

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.
Daily reports are now available.

16 – 20 August 2015
250th American Chemical Society National Meeting and Exhibition.
Boston, MA, USA.

properties that could enable it to be used as a chemical weapon;

2. It may be used as a precursor in one of the chemical reactions at the final stage of formation of a chemical listed in Schedule 1 or Schedule 2, part A;

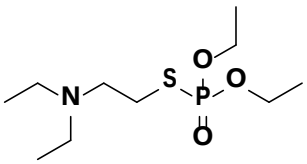
3. It poses a significant risk to the object and purpose of the Chemical Weapons Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;

4. It is not produced in large commercial quantities for purposes not prohibited under the Chemical Weapons Convention.

We continue with an overview of Schedule 2, parts A (Toxic Chemicals) and B (Precursors). In regard to uses of these chemicals for purposes not prohibited under the Chemical Weapons Convention, Figures 3 and 4 categorize the 2014 publications by topical area.

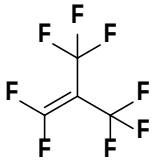
Schedule 2 Part A, Toxic Chemicals

Schedule 2A(1): Amiton (VG, *O*,*O*-Diethyl *S*-[2-(diethylamino)ethyl] phosphorothiolate) and its corresponding alkylated or protonated salts. Amiton was originally produced as an insecticide, but was later determined to be too toxic for agricultural use.



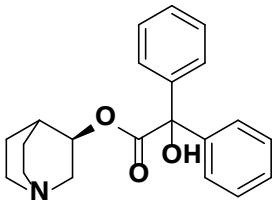
Amiton
2A(1)

Schedule 2A(2): 1,1,3,3,3-Penta-fluoro-2-(trifluoromethyl)-1-propene (PFIB), a lung toxic agent that has seen development for use as a chemical weapon.



PFIB
2A(2)

Schedule 2A(3): 3-Quinuclidinyl benzilate (BZ), an anticholinergic agent that was developed as a psychomimetic chemical weapon in the 1960s. This bioactive chemical can also be used as a building block for other more complex therapeutic compounds.



(R)-(-)-3-Quinuclidinyl benzilate
2A(3)

Schedule 2 Part B, Precursors

Schedule 2B(4): This Schedule covers chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms. There are an infinite number of possible structures that can fit this description. Compounds that are precursors and degradation products (methylphosphonic acid for example) of Schedule 1 nerve agents fall under this Schedule. The Schedule makes an exemption for Fonofos, an insecticide that was widely used on corn at the time the convention was signed.

24 – 27 August 2015
FinMedChem 2015.
Helsinki, Finland.

31 August – 4 September 2015
Sixth Summer Programme on Disarmament and Non-Proliferation of Weapons of Mass Destruction (WMD) in a Changing World Disarmament and Non-Proliferation of Weapons of Mass Destruction (WMD) in a Changing World. Asser Institute, The Hague, The Netherlands.

3 – 4 September 2015
The International Conference On Chemical Sciences And Engineering (CHEMSCIE 2015).
Veracruz, Mexico.

6 - 10 September 2015
The European Conference on Analytical Chemistry (EUROANALYSIS 2015)
Bordeaux, France

9 - 11 September 2015
Wait What? A Future Technology Forum. Saint Louis, MO, USA.

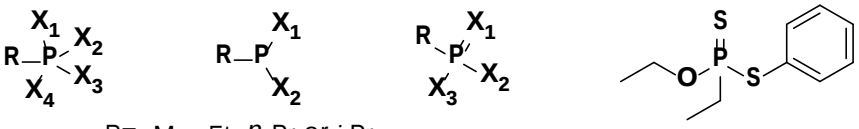
13 - 15 September
Trends Symposium IAP Biosecurity Working Group. Warsaw, Poland

13 – 16 September
1st International Workshop on Mobile Learning (WmL'15).
Lodz, Poland.

20 – 24 September 2015
9th International Conference on Instrumental Methods of Analysis-Modern Trends and Applications (IMA2015). Kalamata, Greece.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering); ECAB3 (3rd European Congress of Applied Biotechnology); and EPIC5 (5th European Process Intensification Conference)
Nice, France.

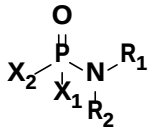
5 - 8 October 2015
SOLVE. Cambridge, MA, USA.



R= Me, Et, *n*-Pr or *i*-Pr
X_1, X_2, X_3, X_4 = Any group not attached to the Phosphorous atom through a Carbon

2B(4) Fonofos

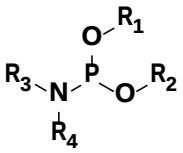
Schedule 2B(5): *N*,*N*-Dialkyl (Me, Et, *n*-Pr or *i*-Pr) phosphoramidic dihalides; compounds that can serve as intermediates in the preparation of nerve agents.



R_1, R_2= Me, Et, *n*-Pr or *i*-Pr
X_1, X_2= Halogens

2B(5)

Schedule 2B(6): Dialkyl (Me, Et, *n*-Pr or *i*-Pr) *N*,*N*-dialkyl (Me, Et, *n*-Pr or *i*-Pr)-phosphoramidates; compounds that are formed as co-products in the synthesis of Tabun class nerve agents. Compounds in this Schedule, as well as those of 2B(5), are of interest for their fire resistant properties.

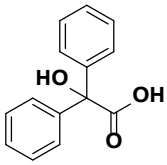


R_1, R_2'R_3, R_4= Me, Et, *n*-Pr or *i*-Pr

2B(6)

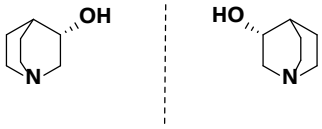
Schedule 2B(7): Arsenic trichloride ($ASCl_3$), a compound that can be used as a precursor for lewisites and other arsenic containing chemicals; including fluorescent probes (which can be attached to quantum dots and surfaces) for protein analytics.

Schedules 2B(8), 2,2-Diphenyl-2-hydroxyacetic acid; and **2(B)9,** Quinuclidin-3-ol; are precursors of BZ and other bioactive compounds. Quinuclidin-3-ol has also been used to prepare amine mixtures for carbon dioxide capture.



2,2-Diphenyl-2-hydroxyacetic acid

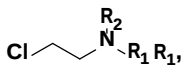
2B(8)



(S)-(+)-3-Quinuclidinol (R)-(+)-3-Quinuclidinol

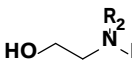
2B(9)

Schedules 2B(10), *N*,*N*-Dialkyl (Me, Et, *n*-Pr or *i*-Pr) aminoethyl-2-chlorides and corresponding protonated salts; **2B(11),** *N*,*N*-Dialkyl (Me, Et, *n*-Pr or *i*-Pr) aminoethane-2-ols and corresponding protonated salts; and **2B(12),** *N*,*N*-Dialkyl (Me, Et, *n*-Pr or *i*-Pr) aminoethane-2-thiols and corresponding protonated salts; are amino compounds that can be both pre-cursors and degradation products of Schedule 1 chemical agents. These compounds make up over 75% of the 2014 publications illustrated in Figure 1; their uses spanning a broad range of applications (as shown in Figures 3 and 4). *N*,*N*-Dimethyl- and *N*,*N*-Diethyl-aminoethanol and their corresponding protonated salts are exempted from Schedule 2B(11).



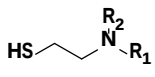
R_2= Me, Et, *n*-Pr or *i*-Pr

2B(10)



R_1, R_2= Me, Et, *n*-Pr or *i*-Pr

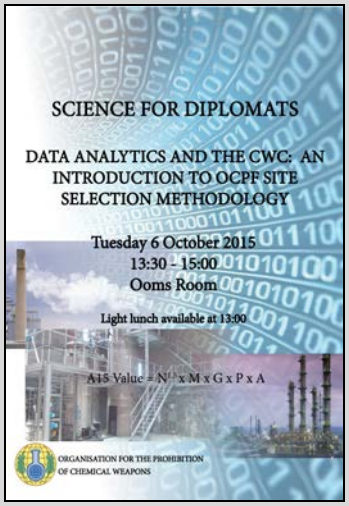
2B(11)



R_1, R_1= Me, Et, *n*-Pr or *i*-Pr

2B(12)

6 October 2015
"Science for Diplomats".
OPCW Headquarters, The Hague, Netherlands.



15 October 2015
Smart Manufacturing Summit.
Livermore, California, USA.

31 October - 2 November 2015
The Port Hackathon.
CERN

4 – 7 November
World Science Forum.
Budapest, Hungary.

16 – 19 November 2015
Malta Conference.
Rabat, Morocco.

18 – 21 November 2015
16th Asian Chemical Congress.
Dhaka, Bangladesh.

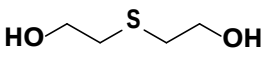
22 – 27 November 2015
2nd African Conference on Research in Chemical Education (ACRICE)
University of Venda,
Thohoyandou, South Africa.

23 – 25 November 2015
XIIIth International Symposium on Environment, Catalysis and Process Engineering (ECGP'13)
Hammamet, Tunisia.

14 – 18 December 2015
Biological Weapons Convention Meeting of States Parties.
Geneva, Switzerland.

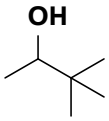
15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

Schedule 2B(13): Thiodiglycol, the precursor (and also a hydrolysis product) of sulphur mustard. Uses of this compound include inks and dyes. A recent patent made use of this chemical in a process to render tissue samples trans-parent.



Thiodiglycol: Bis(2-hydroxyethyl)sulfide
2B(13)

Schedule 2B(14): Pinacolyl alcohol, a precursor for soman. This alcohol may also have applications in the stabilization of gas hydrates, making it a candidate for use in carbon dioxide sequestration.



Pinacolyl alcohol
2B(14)

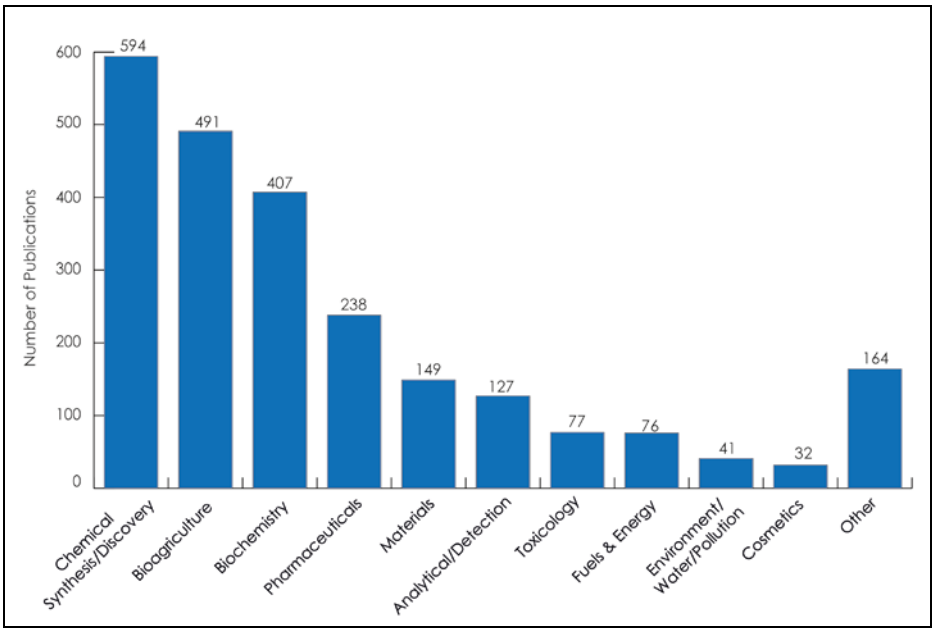


Figure 3: The number of publications from 2014 concerning Schedule 2 chemicals categorized by topical area.

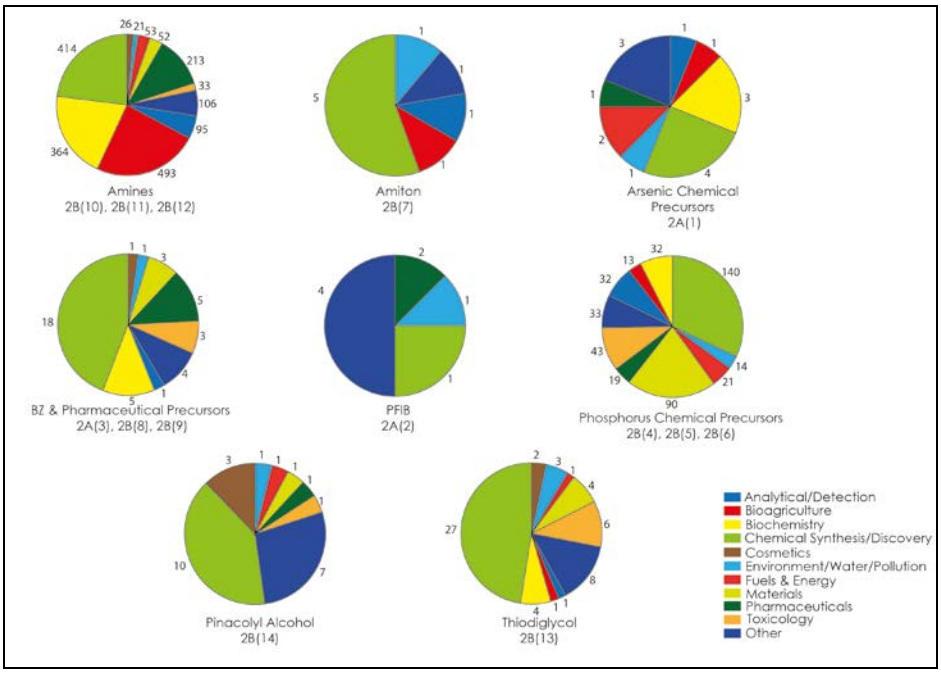


Figure 4: 2014 publications categorized by topical area for individual (and similar) classes of Schedule 2 chemicals.

Contact Us:

Questions, ideas, comments, suggestions, want to make a contribution, or be added to the mailing list? Please contact us through the OPCW Office of Strategy and Policy (OSP).

For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

Citizen Science

Our world is increasingly more "connected" through devices that make measurements, store data, facilitate communication and open up untold possibilities for how we live and work. A connected world facilitates new and more global ways to collaborate, to harness the power of "the crowd" and to participate in scientific endeavours without needing a specialised degree or even access to a laboratory. In effect, anyone can collect and analyse data, and participate in the scientific process. Scientific projects that involve the crowd strategy, generally relying on volunteer participation, are often called "Citizen Science". The crowd sourced approach can even be implemented through engagement of those involved in activities such as biking and surfing! Using citizens and smartdevices to monitor the structural health of urban infrastructure has also been proposed.

"Crowds" have been engaged for observing weather, astronomy (including projects where space agencies provide data to citizens), preventative medical research, studying biodiversity (building distribution models of animal species for example), monitoring bees, reporting of invasive species, mapping radiation levels, water and other environmental monitoring (by recording observations and/or making chemical or physical measurements). Crowd based projects can serve as a platform for education and awareness raising of environmental issues such as water quality (with global reach); some environmental projects have actually resulted in the creation of monitoring networks, identification of violators of pollution laws and when combined with other data sources have resulted in legal initiatives. Citizen science projects can also provide mechanisms to accelerate digitization and archiving of scientific collections.

There have always been opportunities for citizens to participate in scientific pursuits. Our connected world has opened up such opportunities by making them more accessible to a broader spectrum of people. Organisations such as the Citizen Science Association, the European Citizen Science Association and Citizen Science Network Australia provide forums for practitioners to engage with one another. Zooniverse, CitSci.org, Wildbook and SciStarter provide infrastructure to host projects and connect scientists with citizens. There are also forums focused on specific activities including sensor based projects and teaching citizens how to engage in environmental monitoring. Science museums and governmental bodies (the European Union for example) also organise citizen science projects; if interested we encourage you to seek out opportunities, especially with science museums, in your local area.

As with any scientific activity, questions concerning qualifications of participants (and how these vary), validity of the data collection method, validity of the data itself and the robustness of the conclusions all need to be addressed. Data management is very important to think through, prompting some to call for the standardization of metadata language to facilitate more efficient sharing of information across projects. To help, practitioners have taken the lessons learned from previous studies and produced guides, manuals and recommendations for best practices, as well as guidelines for data quality and ethical considerations.

The availability of tools to make measurements is key to successful crowd engagement. In this regard, simply having a Smartphone (or multiple Smartphones) opens up opportunities. Examples include Smartphone microscopes and Apps for ecology. As new Smartphone capabilities come forth (ultrasonic fingerprint reading for example, details here), citizen science projects will certainly find clever ways to employ them.

For environmental monitoring, a wealth of possibilities are now available through low cost sensor

technologies (using kits to build customised sensors or by using commercially available devices), which we will further elaborate in the feature that follows.

The ability to miniaturize analytical tools has generated interest in portable scanners for food (to detect allergens), with monetary awards available for working tools and companies developing products.

For health related projects, infectious disease surveillance data can easily be collected in rural locations with Smartphones, and a project like ResearchKit provides Apps for iPhones to gather medical data. Of course, the growing trend in personal health and wearable fitness monitors is generating questions about measurement accuracy (which are especially important in regard to concerns raised about do-it-yourself healthcare).

We have previously looked at the use of Smartphones as scientific instruments and diagnostic tools. However, more advanced cellular, biomolecular or clinical measurements require laboratory training, laboratory equipment and/or specialty reagents, which are impractical for many citizen science initiatives. Providing passive sampling devices that absorb chemicals and are sent to a lab for analysis (wearable wristbands for example) provide a means to overcome such limitations. Likewise, the idea of volunteers sending samples to laboratories for analysis has seen use in commercial endeavours for product development.

Gamification can be an effective method for engaging the crowd. This is the use of games which are designed to be fun and to remove the barriers to understanding the underlying science. In effect, scientific knowledge can be generated simply by aligning coloured blocks to perform multiple sequence alignment or looking at the connectivity of tangled objects to map the brain.

Open source scientific tools, internet based communities and even access to 3D printing provide additional opportunities for low cost science resources (telescopes for example). Other projects are enabled through sharing of ideas and expertise across participants – take for example a project for monitoring biodiversity of a lake involving scientists, naturalists and drone technology developers.

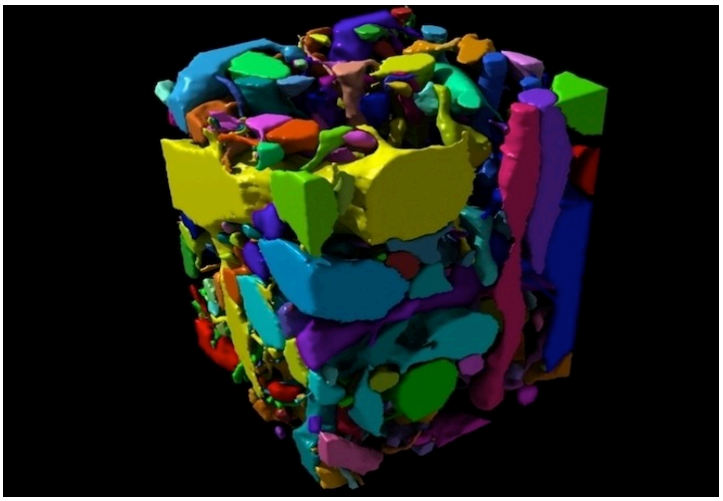


Image from EyeWire.

We conclude by pointing out that the crowd can also be engaged to fund science projects, through resources such as Experiment or Kickstarter (infamous in some circles for the glowing plant project of 2013).

A recent example, related to sensors and citizen science: a university project combining gas sensors with small drones for pollution monitoring.

Sensors for Citizens

Of all the tools employed in citizen science projects, simple and low cost environmental sensors (specifically for air and water sampling) are of the most interest to us; these types of sensors being relevant to the chemical informatics project under EU Council Decision (CFSP) of 17 February 2015 Project III. Mobile sensors with the ability to collect and transmit data can augment environmental data collected across networks of more traditional expensive (and non-mobile) systems; a concept that has been described in reports from the United States Environmental Protection Agency (EPA). The EPA website includes resources on both air and water monitoring.

For those who like to tinker, open-source electronics are ideal. There are a wealth of do-it-yourself options and guide books for making and programming sensors available. Open-source electronics

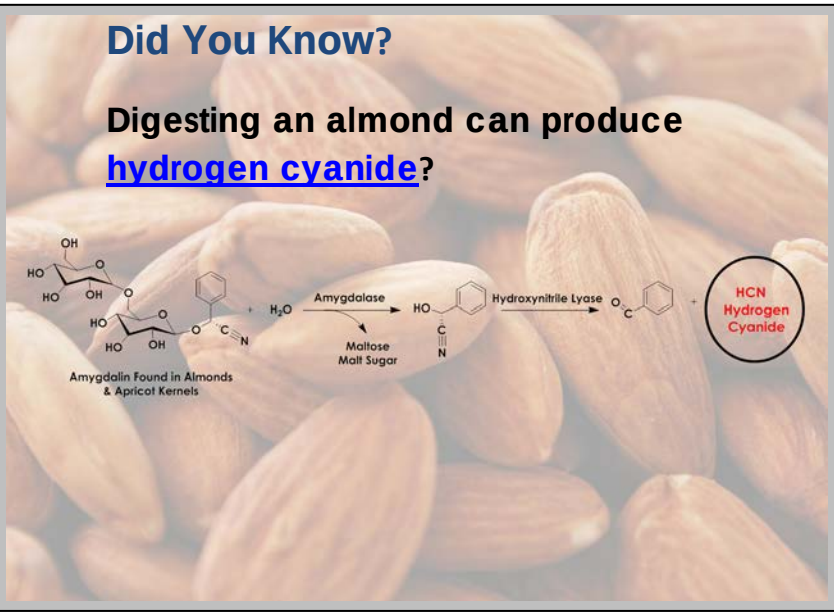
can also create gadgets to act as sensor platforms (likewise, cars can be used in this capacity too). Arduino (often in combination with Raspberry Pi computers) is one of the more popular platforms for open-source electronic prototyping (with kits and components are available from vendors such as Adafruit and Sparkfun). Arduino systems have been used to produce air sensors, pH meters for ocean water studies and microspectrometers. They also can be integrated with more complex analytical chemistry equipment (automation to assist mass spectrometry for example). With the proper tools, electrochemical sensors are also possible (details here). Home automation and the "internet of things" may offer additional capabilities that can be combined into sensor systems.

For those who prefer to buy ready to use technology, an appendix with a table containing examples of portable commercially available sensors is attached. The accuracy, precision and reliability of these devices will vary with how they are used; what makes them valuable is the easy access they provide for citizen science and educational initiatives related to chemical measurement. Guidebooks for evaluating and choosing suitable sensors for various applications are available.

In regard to chemistry education, measurement of chemicals in air pollution or of water quality parameters can generate data sets with signal, temporal and geographic dimensions. Such data could be compared to independently measured data sets with similar (or identical) temporal and geospatial information. The source of comparison data might be from an environmental monitoring system (for those of us in The Hague, this could be the air quality network of the Netherlands).

Airqualityegg, a commercial air monitor lets you connect to a global data monitoring system

There is no expectation for the data sets to correlate, however, the measurements and their comparisons could be integrated into laboratory coursework intended to introduce and explain important concepts in analytical science: accuracy, precision, uncertainty, correlation, differences between measuring devices (and/or locations) as well as statistical treatments of measurement data. Low cost sensors are ideally suited for these purposes; with the open-source electronics platforms expanding the educational potential.



Appendix to *OPCW Science & Technology Monitor* Volume 2, Number 9: Examples of commercially available portable chemical sensors.

Sensor	Sampling	Sensor Used for Chemical Measurements*	Chemical Measurements	Description
Hydrolab DS5	Water	Optical light scattering fluoresce Electrochemical	ammonium nitrate chloride rhodamine WT chlorophyll a total dissolved gas (TDG)	 Profiling or unattended long term data collection.
Hydrolab MS5	Water	Optical light scattering fluoresce Electrochemical	ammonium nitrate chloride rhodamine WT chlorophyll a total dissolved gas (TDG)	 Profiling or unattended long term data collection
Hydrolab Quanta G	Water	Electrochemical Conductivity	Dissolved oxygen pH	 Measures 8 different water quality parameters.
smarTROLL	Water	Electrochemical Conductivity	Dissolved oxygen pH	 Works with mobile device and measures other physical parameters.
Seneye Reef	Water	Electrochemical Conductivity	ammonia pH	 Aquarium monitor.

***Some of the devices may also measure temperature, humidity, particulates and/or light exposure. Sensors for these measurements are not listed.**

Appendix to *OPCW Science & Technology Monitor* Volume 2, Number 9: Examples of commercially available portable chemical sensors.

Sensor	Sampling	Sensor Used for Chemical Measurements*	Chemical Measurements	Description
MQ Gas Sensors	Air	Metal oxide semiconductor	carbon monoxide hydrogen hydrogen sulfide alcohol volatile organic compounds (VOC)	 Multiple sensors that interface with Arduino kits are available(MQ-7 Carbon monoxide sensor shown above)
Aeroqual series 500	Air	Multiple types of sensors are available	30 different gas sensors are available	
NEXTtoME	Air	Electrochemical Optical	carbon monoxide alcohol	 Can be linked to mobile devices via Bluetooth.
Q-trak Indoor AQM	Air	Electrochemical Non-dispersive infrared (NDIR)	carbon dioxide carbon monoxide volatile organic compounds (VOC)	

***Some of the devices may also measure temperature, humidity, particulates and/or light exposure. Sensors for these measurements are not listed.**

Appendix to *OPCW Science & Technology Monitor* Volume 2, Number 9: Examples of commercially available portable chemical sensors.

Sensor	Sampling	Sensor Used for Chemical Measurements*	Chemical Measurements	Description
Cube	Air	Electrochemical	carbon monoxide	
Foobot	Air	Metal oxide semiconductor	carbon dioxide carbon monoxide volatile organic compounds (VOC)	 Signal processing converts VOC levels to CO_2 equivalents. Links to mobile devices.
Airqualityegg	Air	Metal oxide semiconductor	carbon monoxide nitrogen dioxide ozone	 Connects to an existing global monitoring system
Langan DataBear T15v	Air	Electrochemical	carbon monoxide	
SCIO Spectrometer	Multiple	Near Infrared Spectrometer	750 nm - 950 nm	 Links to mobile devices.

***Some of the devices may also measure temperature, humidity, particulates and/or light exposure. Sensors for these measurements are not listed.**

VOLUME 2 NUMBER 10

The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

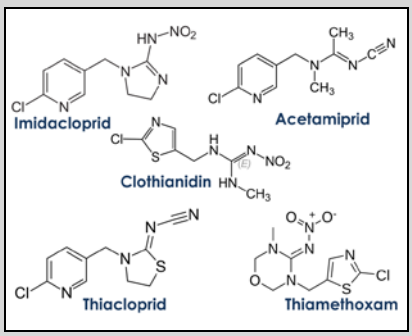
16 October 2015

In This Issue

Featured content

From D. Endy, S. Galanie, C. D. Smolke.
http://dx.doi.org/10.1101/024299
Fermentation of opiates

Image from FNIH.
Genomics



Neonicotinoids

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

We begin this issue with a round of applause for the 2015 Nobel Prize winners. In physics: Takaaki Kajita and Arthur B. McDonald "for the discovery of neutrino oscillations, which shows that neutrinos have mass". In physiology or medicine, a tale of anti-parasite drugs: William C. Campbell and Satoshi Ōmura "for their discoveries concerning a novel therapy against infections caused by roundworm parasites"; and Youyou Tu "for her discoveries concerning a novel therapy against Malaria". In chemistry: Tomas Lindahl, Paul Modrich and Aziz Sancar "for mechanistic studies of DNA repair". In economic sciences: Angus Deaton "for his analysis of consumption, poverty, and welfare". In literature: Svetlana Alexievich "for her polyphonic writings, a monument to suffering and courage in our time". Last but not least, the Nobel Prize of Peace was awarded to the Tunisian National Dialogue Quartet "for its decisive contribution to the building of a pluralistic democracy in Tunisia in the wake of the Jasmine Revolution of 2011". Congratulations to all!

The S&T Puzzle

Our periodic table puzzle finally ended the CTBTO winning streak! One of our own Industry Verification Officers accumulated 458 points by identifying CWC relevant examples of elements: H, C, N, O, F, Na, Si, P, S, Cl, Ti, Cr, Mn, Fe, Co, Ni, As, Mo, I and W. Puzzle statistics now stand at: VER 5, OSP 2, OCS 1, INS 1 and CTBTO 5.

In this edition of the puzzle, we ask you to identify differences between the images on the left. The first person to correctly list all of them wins the prize: a choice of requesting a featured topic or designing a puzzle or a hand selected beverage courtesy of the Science Policy Adviser.

A bonus prize if you can tell us which of our Office of Strategy & Policy colleagues is under the mask. Send answers by email.

Science Fun:

For this edition of Science Fun, we looked for commonality amongst neonicotinoids, fermentation, and genomes: we found a food that does not spoil and is produced on an economically viable scale by an insect (an insect adept at chemistry and whose genome tells us, originated in Asia). The food is not the insect itself, but the honey it produces!

Honey is produced from plant nectar by honey bees. It contains carbohydrates (sugars), proteins, free amino acids, vitamins, minerals, anti-oxidants and other chemicals; the chemical composition reflects the type of nectar collected (DNA sequencing helps too). The geographical origin can be determined by the chemical composition and isotope ratio analysis (a technique used in chemical forensics) can identify adulterated samples.

Photograph from Pixapay.

Making honey is quite the effort: it requires flying more than 176,00 km and visiting more than 5.7 million flowers, just to make 1 kg of the stuff. Worker bees go off into the world and collect nectar from flowers and store it in a "honey stomach", where sugar (sucrose) in the nectar is enzymatically broken down into glucose and fructose. On returning to the hive, the worker bee regurgitates its payload and sends it off to a house bee. The house bee continues the enzymatic breakdown process started by the worker bee (by repeatedly drinking and regurgitating the nectar). Once suitably processed, the nectar is deposited into a honeycomb.

News and Updates

Recent reports and publications:

Briefing to States Parties by OPCW Scientific Advisory Board Chair from EC-80.

Evaluation of the Results of the 37th Official OPCW Laboratory Proficiency Test and Status of Laboratories Designated for the Analysis of Authentic Samples.

September 2015 issue of Dstl's *inSIGHT*.

Converging sciences – the extent of interdisciplinary research and why it matters.

How to avoid bias in research and other challenges in irreproducibility from *Nature*.

A look at editing mischief for contentious scientific topics on Wikipedia (details here).

2015 Global Innovation Index.

Verification handbook - a definitive guide for verifying digital content for emergency coverage.

Ambassadors on twitter and best practices for Ambassadorial tweeting.

Science, education and industry resources:

The Hague Ethical Guidelines provide a set of key elements related to the practice of chemistry under the norms of the CWC. These guidelines have also been translated into Spanish.

A 3D Printing Database.

Recipes for Biomedical & Life Sciences Researchers from Springer.

An app for counting elephants toenails to learn math!

The ESCom Package - Key process for the successful implementation of REACH.

A collection of A0 printable OPCW S&T related Posters is online: biomedical sample analysis, physicochemical properties of chemical agents, mechanism of action of nerve agents, mechanism of action of blister agents, mechanism of action of choking agents, mechanism of action of blood agents and WWI gas mask development timeline.

Some news from world of science and technology:

From the weeks of 9 – 15, 16 – 22, and 23 – 29 August; 30 August – 5 September; 6 – 12, 13 – 19 and 20 – 26 September; 27 September – 4 October; and 4 – 10 October in chemistry.

A dehydration process takes place to bring the water content of the honey below 18% (nectar can contain over 70% water); higher water content can actually allow yeast to ferment the honey. Bees accelerate the evaporation process by fanning with their wings. In the end, it takes several days to convert watery nectar to syrupy nectar, and here is one of the secrets behind honey not spoiling – low water content combined with low water activity (e.g. limited water available to support bacterial growth and the low water content promotes the dehydration of bacteria).

There is of course more to the story than simply limited water. Honey contains a number of acids (including gluconic acid, the result of enzymes acting on glucose) and typically has a pH around 4. The formation of gluconic acid will also produce hydrogen peroxide – a chemical that increases the antibacterial properties of honey! Did you know that honey has antimicrobial and antibiofilm applications? It has been used in traditional medicine for treating skin wound infections and disease; there are even commercially available anti-bacterial wound dressings. It turns out honey finds use in burn treatment, treatment of athlete's foot, as an anti-inflammitory and an anti-oxidant. Compounds found in honey even may have applications in chemotherapy (as well as mitigating side effects of chemotherapy agents). This would appear to indicate that honey is a microorganism free product, but alas some of the microrganisms in our world are quite resilient and can survive in honey (and they may not always be benign!).

As most of us probably don't think of honey as a medicinal substance; we are likely to be more familiar with its use in cooking and baking. Perhaps it could be thought of as a sweetener with medicinal

Fermentation

As a means of producing chemicals, fermentation has been used for centuries, the method is particularly valuable for producing protein based and other biopharmaceuticals. For those watching trends in modern chemical production, fermentation has attracted considerable attention in relation to the bioeconomy and a blurring distinction between certain industrial chemical and biological processes (as illustrated by the production of organic acids as platform chemicals).

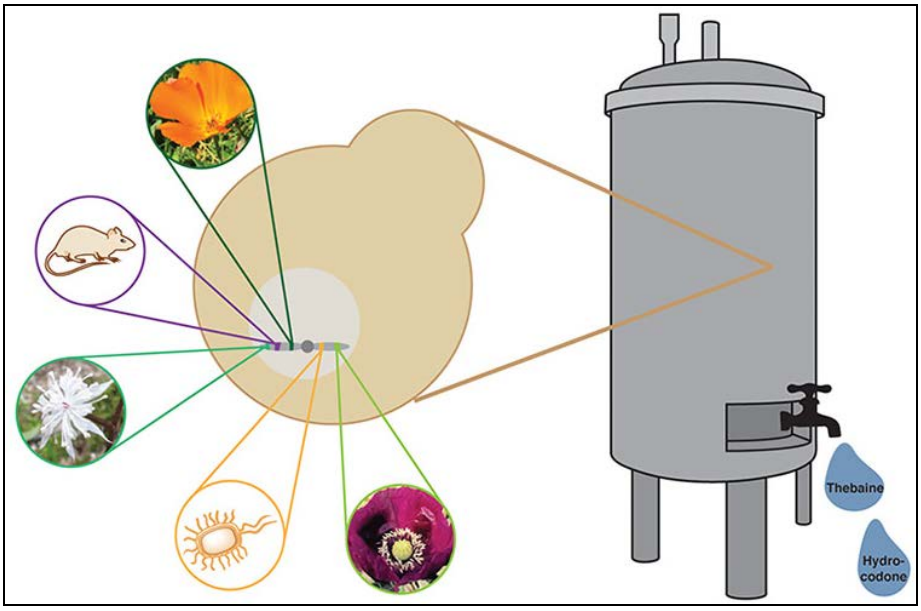


Image from Stanford News.

A bioengineering team engineered more than 20 genes from five different organisms into the genome of baker's yeast; the result: a yeast capable of converting glucose into hydrocodone.

Much has been written on large volume biobased chemical production, the engineering of microorganisms, complexity and limitations of metabolic engineering, and the adoption of biotechnology for chemical production. We have also been alerted to challenges facing industrial biotechnology for commodity chemical production resulting from low oil prices and oil price volatility. As oil prices stay low, the expense associated with some biobased processes to produce fuels (from algal biomass for example) requires co-production of additional biochemicals with economic value; requiring engineering microorganisms capable of accumulating multiple products and coculture systems. The use of fermentation to produce speciality and fine (bio)chemicals, such as flavours, fragrances, cosmetic ingredients and isoprenoids is an active area of growth. This is exemplified by the shift of synthetic biology based companies to these sectors; more information on the types of products emerging from synthetic biology companies can be found here). With this in mind, we take this opportunity to look at some recent developments in speciality (bio)chemicals arising from microbial fermentation processes.

The wealth of information resulting from breakthroughs in genomics has enabled a broad spectrum of metabolic engineering opportunities and approaches. Examples include producing and screening new forms of antibiotics (details here);

properties? Of course, the ability of honey to produce products for human consumption goes well beyond sweets, as demonstrated by its use in fermentation!

When thinking about all this honey, ask yourself how important it is to have the honey removed from the insect. If you are looking for sweet honey mixed with protein, perhaps the honey pot ant is a more desirable treat?

"HoneyAnt" photogtaph by Greg Hume at en.wikipedia..

Crowdsourcing:

The City of The Hague invites students and organisations to submit ideas to solve global challenges such as safety & security, energy, climate and food to The Hague Innovators Challenge 2016. Prizes worth 5,000 to 35,000 euros will be awarded to the best submissions.

The Humanitarian Innovation Fund is looking for a lightweight, portable, simple, efficient, and durable incinerator for medical waste. Must be suitable for use in humanitarian emergencies!

Reimagine CO_2 by converting emissions into high value products in the $20M NRG COSIA Carbon XPRIZE.

Do you have a world-changing invention that you would like to see in the pages of *Popular Science* Magazine? If yes, enter your creation in the 2016 Invention Awards

Need some tools to help with social innovation projects? Take a look at the DIY (Development

eliminating the need to milk poisonous snakes to produce anti-coagulants (details here); and "brewing" perfumes or silk proteins.

Recent examples with implication for pharmaceutical production include modifying yeast strains with genes from plants to enable production of opiates (details here) or cannabinoids (details here) starting from glucose. The prospect of yeast strains producing narcotics has received attention in the popular press and prompted calls for regulation. Suggestions were made that a home brewing kit might be used to produce drugs of abuse; however, in an attempt at home brewing pharmaceuticals, researchers failed to detect opiates in their ale.

The ale kit example reminds us that developing an engineered microbe based production process requires combinatorial approaches to metabolic engineering and high-throughput screening processes to identify strains capable of performing in desired process conditions and scales; highly automated microfluidic systems are an integral part of this work (details here). This can require screening millions of strains, as illustrated in a recent article about the company Amyris, Inc., in order to identify single digit numbers of strains capable of performing at commercial scale. Additionally, tolerances of the microbes to process conditions (thermally and in regard to toxicity of the metabolites being produced for example) must be considered; requiring suitable means of strain evolution.

Given the broad ranges of natural and unnatural chemical products obtainable through fermentation, the methodology is well suited for sustainable chemical production initiatives; as described in a recently published roadmap to accelerate the advanced manufacturing of chemicals.

Genomics

The Human Genome Project (HGP), one of biology's first "Big Science" projects, celebrated its twenty-fifth birthday last month; twenty-five years in which the field of genomics, the study of the complete set of DNA within a single cell or an organism, has seen enormous technological development. Genomics has opened up new possibilities for applications in healthcare, helped scientists identify the genes that make a person more attractive to mosquitos (the genes producing certain body odours), better understand the evolution of octopus cleverness (details here) and provided a means to study historical livestock by sequencing historical documents. With the "next generation sequencing" market expected to grow to over 27 billion USD by 2022, there will be continued investment and further discoveries to come.

Today, the amount of genomic data that is produced doubles every seven months; should this continue, expect there to be more genomic data in 2025 than astronomy, YouTube and Twitter data combined! Thus begging the question, should we replace the term "astronomical" with "genomical"? It is

Impact and You) Toolkit.

Upcoming S&T Related Events:

19 - 23 October
International Conference on Global Emergency Preparedness and Response
Vienna, Austria.

31 October - 2 November 2015
The Port Hackathon
CERN

3 November
The 6th edition of the Intelligent Sensor Network Conference
High Tech Campus, Eindhoven, The Netherlands.

4 – 7 November
World Science Forum
Budapest, Hungary.

16 – 19 November 2015
Malta Conference
Rabat, Morocco.

18 – 21 November 2015
16th Asian Chemical Congress
Dhaka, Bangladesh.

22 – 27 November 2015
2nd African Conference on Research in Chemical Education (ACRICE)
University of Venda, Thohoyandou, South Africa.

23 – 25 November 2015
XIIIth International Symposium on Environment, Catalysis and Process Engineering (ECGP'13)
Hammamet, Tunisia.

30 November 2015
Emerging Technologies and the CWC: Autonomous Systems and Artificial Intelligence CSP-20 side event organised by UNICRI, Hague Security Delta and OPCW
World Forum, The Hague, Netherlands.

genomics (combined with other "Omics" technologies) that are enabling the large scale metabolic engineering of microbes and expanding the potential of the fermentation based chemical production methods described in the previous feature.

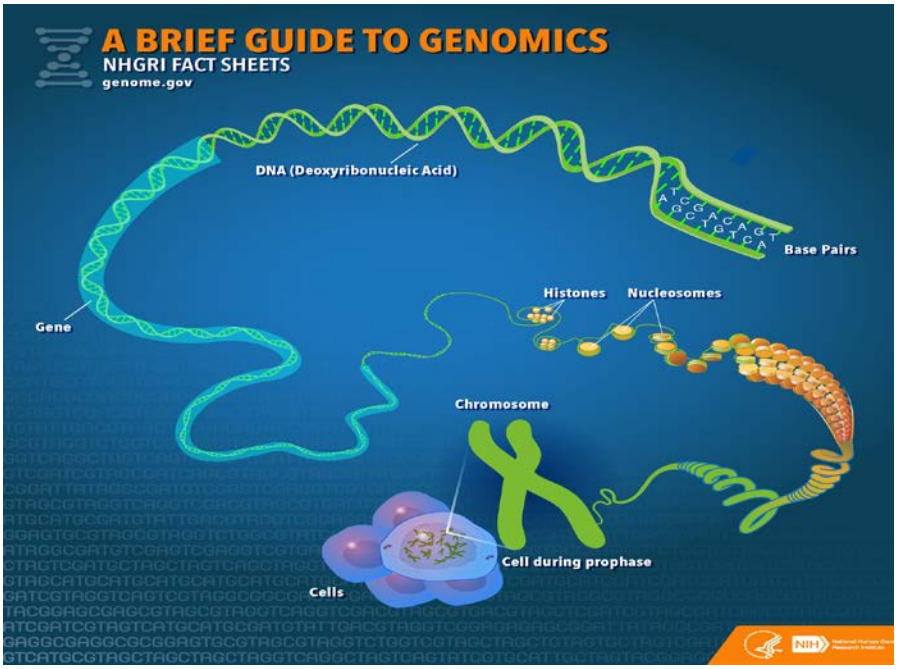


Image from the *National Human Genome Research Institute*.

DNA sequencing, effectively a chemical analysis of the building blocks of DNA (**A**denine, **G**uanine, **C**ytosine and **T**hymine) has become a powerful tool for studying biological systems. Examples of large scale studies include sequencing of entire human populations (including ancient populations using DNA extracted from archaeological samples) and large scale microbial mapping studies of urban areas (such as New York City; see also erratum). The actual cost of sequencing has dropped to the point that companies can now charge1000 USD for the sequencing of a complete human genome! In the case of large scale industrial metabolic engineering, high-throughput methods have been (and continue to be) developed.

The tools employed for DNA sequencing continue to advance and miniaturized devices are commercially available. Nanopore sequencers for example, have been used in real-time analysis of salmonella outbreaks in a hospital, viral pathogen detection in clinical samples and in West Africa for rapid Ebola testing.

Sequencing microbial populations in wounds or the eyes of individuals (the ocular microbiome); or in areas where bacteria thrive such as an athletic facility (details here) are three examples of how sequencing can provide information that helps to prevent the spread of infection.

Of relevance to the world of safety and security, sequencing can be used to rapidly detect pathogens, elucidate the origin and transmission of viral outbreaks (Ebola), to detect foodborne illnesses and for precision emergency medical treatment.

Data handling and informatics is a key aspect of the use of

2 December 2015
"Science for Diplomats": Chemical Forensics.
CSP-20 side event
World Forum, The Hague, Netherlands.

14 – 18 December 2015
Biological Weapons Convention Meeting of States Parties.
Geneva, Switzerland.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii
United States of America

2 – 4 February 2016
The Unmanned Systems Expo (TUSE)
The World Forum, The Hague
The Netherlands.

6 – 10 March 2016
Pittconn 2016
Atlanta, GA
United States of America

13 – 17 March 2016
251st American Chemical Society National Meeting & Exposition
San Diego, CA
United States of America

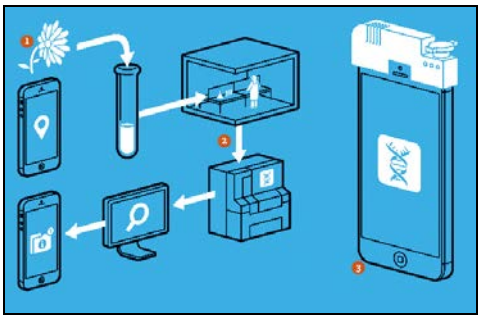
6 – 8 April 2016
XXI IUPAC CHEMRAWN Conference
Solid Urban Waste Management
Rome, Italy.

21 July 2016
2016 Spring ConfChem
Science, Disarmament, and Diplomacy in Chemical Education: The Example of the Organisation for the Prohibition of Chemical Weapons.

15 – 20 August 2016
24th IUPAC International Conference on Chemistry Education (ICCE 2016)
Kuching, Sarawak.
Malaysia.

4 – 7 September 2016
52nd Congress of the European Societies of Toxicology (EUROTOX2016)
Istanbul, Turkey

sequencing technologies. Detection and identification of pathogens requires matching data to reference sequences in databases, in this respect the data used in analysis is not limited to genomic data. For example, organisms that produced a detected protein sequence can potentially be identified by recognising the DNA sequence required to express that protein (and genomic data can be validated by comparison to proteome data, a technique used in proteogenomics). A pitfall to this type of analytical approach is the need for databases free of "contaminated" sequence information. These proteogenomic approaches are valuable tools for the study of toxins and other natural products.



Can DNA be sequenced by iPhone? (Apps already exist!). *Image from United Hemisphere.*

We are very familiar with how chemistry influences biology, to further illustrate this phenomena consider a new set of nucleobases created by chemists (**Z**, 6-amino-5-nitro-2(1*H*)-pyridone and **P**, 2-amino-imidazo[1,2-*a*]-1,3,5-triazin-4(8*H*)one) and how much additional information a 6-nucleotide based genome would contain!

Without adding new nucleobases, there is plenty of sequencing work to be done as our biosphere already contains enough DNA to fill an estimated one billion standard shipping containers (details here). Just in case we do run out of samples, the work won't stop as arrangements are already being made to bring sequencing to the stars!

Neonicotinoids

Since their introduction in the 1990's, neonicotinoids have become the most widely used class of agricultural insecticides in the world; imidacloprid, clothianidin, acetamiprid, thiacloprid and thiamethoxam represent the most common of these compounds. These insecticides have received much attention due to concerns of their effect on bee colonies. Hundreds of scientific studies have been carried out to address this issue: providing evidence that can both support claims and raise uncertainties. Further complicating this issue is an observation that bees may actually prefer neonicotinoid-laced nectar!

Neonicotinoids are systemic, being taken up by the plants and transported to leaves, flowers, roots, stems, pollen and nectar. The insecticide remains active in the plant for weeks, protecting the crop throughout a growing season. The insecticides are often applied as seed coatings, with large scale use on crops such as maize, soy and cotton. The insecticides also find use in

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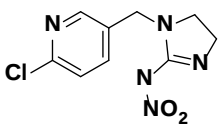
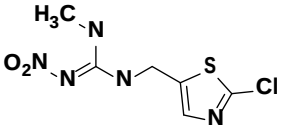
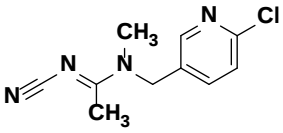
Questions, ideas, comments, suggestions, want to make a contribution, or be added to the mailing list? Please contact us through the OPCW Office of Strategy and Policy (OSP).

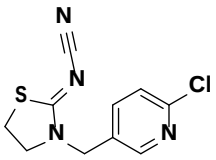
For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

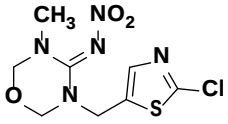
the treatment of turf, as foliar sprays in orchards, in soil treatment of trees and potted plants, and in a range of greenhouse crops.


Imidacloprid


Clothianidin


Acetamiprid


Thiacloprid


Thiamethoxam

Neonicotinoids selectively target the nicotinic acetylcholine receptor in insects. The compounds bind to this receptor, stimulating nerve excitation which leads to paralysis and death. While mammals also have nicotinic acetylcholine receptors, structural differences between the insect and mammalian receptors (creating selectivity for the types of chemicals they bind) result in toxicity to insects but not mammals. Examples of neonicotinoid toxicity to other invertebrates (aquatic invertebrates and earthworms) have also been reported Reports of acute human poisoning from neonicotinoid exposure are rare; however, concerns about potential health impacts to humans from neonicotinoid metabolites is an area of current research.

With such wide scale use of neonicotinoids, understanding environmental risk and fate (including under varying soil conditions); persistence and concentrations in farm soil (including farms employing conservation practices); and the residual levels in the crops themselves are important. Available studies include soil applied insecticides in irrigated agricultural systems, and the use of insecticide mixtures. Neonicotinoid residues from agricultural activities have been detected in streams and other surface waters (global reviews and regionally focused studies are available), prairie wetlands, wild flowers, snow melt and soil dust. All of these studies remind us of the importance of analytical chemistry and sampling and analysis for pesticides.

The presence of neonicotinoids and their breakdown products in the environment raises the potential for direct and in-direct (food chain) effects in wildlife ecosystems (an active area of research especially in regard to the concerns on neonicotinoid impact on pollinators). Bioremediation of neonicotinoid contamination is possible and photocatylictic and oxidation-based methods for neonicotinoid degradation have also been tested.

As environmental effects of neonicotinoids and possible impacts on benign insect populations continue to spark debate, scientists continue to explore alternative chemistry that may have use in pest control. Recent studies have identified candidate chemicals that include terpenes (details here), butyl anthranilate (a compound found in fruit, details here) and spider venom.

Science & Technology at the Biological Weapons Convention Meeting of Experts

The Biological Weapons Convention (BWC) Meeting of Experts was held from 10 – 14 August 2015. Under the advances in science and technology standing agenda item, papers were submitted by Iran (statement here), Switzerland (on convergence and on reviewing developments), the United Kingdom (on response to infectious disease outbreaks – statement here and on production and delivery - statement here) and the United States (on production and delivery, and tacit knowledge).

The Chair of the OPCW Scientific Advisory Board (SAB) presented the work of the SAB in plenary and in an S&T side event. Switzerland (on CRISPR/CAS9) and the Georgia Institute of Technology (on vaccines) provided additional S&T presentations; and statements on science and technology were delivered by The Inter Academy Panel (IAP), India, The Netherlands and Russia (in Russian). The S&T side event featured contributions from Biosecure, IAP, and the Research Group for Biological Arms Control (who also presented a poster).

Additional side events with science and technology dimensions were held on microbial forensics (supporting and use in attribution analysis) and the UN Secretary-General's Mechanism (training and analysis network). Of relevance to sampling and analysis from the poster session: a description of real-time detection of biological aerosols from the Swedish Defense Research Agency.

Biosecurity education featured prominently in the Meeting of Experts. A side event on safeguarding science included presentations on biosecurity textbooks (also in the poster session), the gain-of-function debate, biosecurity in Denmark and contributions to biosecurity from scientific organisations. In a second side-event organised by the Netherlands, biosecurity awareness raising to students, professionals and the synthetic biology community was discussed along with biosecurity self-assessment.

An advance meeting report is available.

As the BWC prepares for its 8th Review Conference in 2016, assessment of bioweapons threats and advances in science and technology with BWC implications are receiving significant attention. A pertinent question: can BWC governance keep pace with technological change? To help move these assessments forward, a symposium (with participation from scientific experts) was held from 13-15 September in Warsaw. A report of this symposium is forthcoming.

2015 BWC Meeting of Experts. Photo by Filippa Lentzos

BWC Trends Symposium (Polish Academy of Sciences)

Did You Know?

Brazilian wasp (*Polybia paulista*) venom can selectively kill cancer cells?

VOLUME 2 NUMBER 11

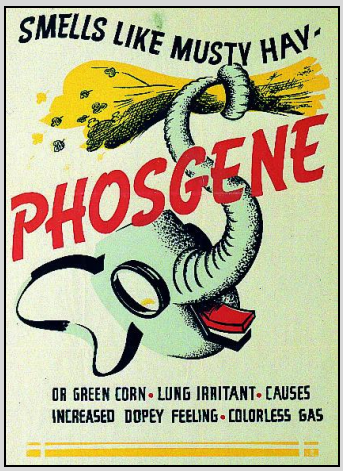
The OPCW Science & Technology Monitor

A sampling of Science & Technology
Relevant to the Chemical Weapons Convention

10 December 2015

In This Issue

Featured content



Schedule 3 Chemicals; Phosgene identification poster from World War II.

Image from allelopathylisacooley.
Allelopathy

Image from Pixapay.
The Internet of Things

Welcome

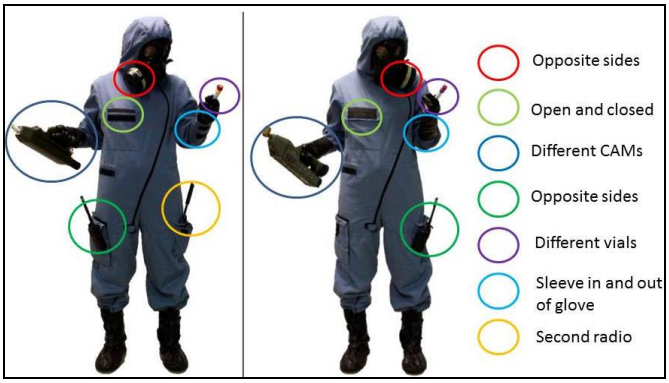
Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

We begin this last newsletter of 2015 with an acknowledgement of the people who have contributed all of the time, ideas, and effort that makes the *S&T Monitor* possible. Our intern staff continues to raise the bar on both form and substance and we wish them the best of luck as they move onward in their careers. We have been lucky to have such a talented group of individuals choosing to spend time in our office this year. Thank you: Edoxie Allier-Gagneur, Wesam Alwan, Wardah Amir, Natalie Childress, Thomas Faria, Beatrice Maneshi, Johannes Niemeier and Inam Siraj.

Today marks the one-hundred fourteenth anniversary of the first Nobel Prize Award ceremony held in 1901 in accordance with Alfred Nobel's will. This day, 10 December is also the anniversary of Nobel's death in 1896. In 1901, the physics prize was awarded to to Wilhelm Röntgen for the discovery of X-rays; the chemistry prize went to Jacobus Henricus van 't Hoffwork for work on chemical dynamics and osmotic pressure; the physiology or medicine prize was given to Emil von Behring for his work on serum therapy, particularly for its use in the treatment of diphtheria; poet Sully Prudhomme was awarded the prize in literature; and the very first Nobel Peace Prize was jointly awarded to Jean Henry Dunant and Frédéric Passy.

The S&T Puzzle

We once again congratulation our friends at CTBTO, the first to spot the differences in the photos of our masked colleague Edoxie Allier-Gagneur (who was not identified for the bonus prize).



The main differences (aside from s ubtle changes in body position) are illustrated above. Puzzle statistics now stand at: VER 5, OSP 2, OCS 1, INS 1 and CTBTO 6.

Science Fun:

In our last issue of *Science Fun* we learned about the secrets of honey and why it does not go bad. That was fifteen days before Halloween 2015, a day known amongst many of us for candy! Now, with more sweets to be consumed for the upcoming end of year holidays (for which we hope you are fully recovered from any October candy induced stomach pains), we explore the chemistry of candy (and taste a few cookies too).

Candy has a rich history in human societies, starting from tree sap in prehistoric times (not so strange if you think about maple syrup) to figs and dates and on to the introduction in Europe of a new spice called "sugar" in 1000 AD. There is a rich chemistry to be found across the world of candy. Did you know that chocolate contains more than 600 chemicals, is toxic to dogs and tastes better when prepared with beer yeast? Did you know that understanding crystal structures and crystallisation methods is important for preparing rock candy (and other candies, even chocolate)? Did you know that Candy can store significant amounts of energy? Or that Candy Canes contain chemicals that bind to TRPM8 receptors? For those who like lab work, you might want to try your own candy chemistry experiments.

Image from Wikipedia.

Making candy is a scientific process that relies heavily on technology as illustrated by the need for an industrial revolution, before it became possible to make cotton candy!

			2	6		7		1
6	8			7			9	
1	9				4	5		
8	2		1				4	
		4	6		2	9		
	5				3		2	8
		9	3				7	4
	4			5			3	6
7		3		1	8			

In this edition of the puzzle, we ask you to first complete the Sudoko puzzle on the left, then use the sum of the numbers in each coloured section to find the symbol of an element in the periodic table. The element symbols can be arranged to spell the name of a Schedule 1 chemical. Be the first to tell us the chemical and you win the prize: your choice of requesting a featured topic, designing a puzzle or receiving a beverage hand selected by the Science Policy Adviser. Send answers by email. Good luck!

News and Updates

Recent reports and publications:

The OPCWs *Practical Guide for Medical Management of Chemical Warfare Casualties*.

A *Handbook on chemical and biological waste management*.

Tear gassing by remote control: The development and promotion of remotely operated means of delivering or dispersing riot control agents.

Wilson Center report on *U.S. Trends in Synthetic Biology Research Funding*.

The report of the Blue Ribbon Study Panel on Biodefense.

CNS Occasional Paper *#21 Biotechnology E-commerce: A Disruptive Challenge to Biological Arms Control*.

Wilton Park Report, *Compliance with the BTWC: strategies towards the 2016 Review Conference*.

WHO *World Health Statistics 2015* and Antibiotic resistance: Multi-country public awareness survey.

2015 World Intellectual Property Report and a *Guide to Using Patent Information* from the World Intellectual Property Organisation (WIPO).

Report on the *Top 10 Urban Innovations of 2015*.

UNESCO Science Report: Towards 2030.

The *Nature Index 2015* looks at global scientific collaborations.

OCED Policy Paper, *Scientific Advice for Policy Making: The Role and Responsibility of Expert Bodies and Individual Scientists*.

Industrialisation also gave us the modern lollipop, which when studied with lasers can generate knowledge of shape dynamics and scaling laws for bodies dissolving in fluid flow. Our readers however, might be more interested in knowing how many licks it takes to get to the chewy chocolate center of a Tootsie pop (a question that requires statistics to answer)! Technological development in candy making continues marching forward with 3D printing now enabling production of visually interesting and tasty treats! Candy not only uses technology, it helps to advance it; as demonstrated by a contribution to the field of soft silicon microstructures (although it took a failure in the kitchen in order to make this discovery).

Science is also important for making that perfect cookie (3D printing helps too, and there are open source recipes). As for chemistry, did you know that baking gingerbread cookies produces a chemical called zingerone? This chemical is not actually present in ginger until it is cooked!

Maybe candy and cookies are not your thing? Not to worry, ice cream also has interesting (and complicated) chemistry to explore! We'll have to come back to that one next summer!

Crowdsourcing:

Compete for the Open Science Prize and enable discoveries for health by harnessing the innovative power of open data.

An app to allow your smartphone to process data and advance cancer research while you sleep.

Have any ideas for a minimally invasive skin biopsy technique for gene expression measurements? Take a look at this reduction-to-practice challenge.

Interested in initiating a citizen science project? Take a look a CitSci.org: a platform for

National Science Foundation special report, *Cybersecurity: Tech, Tools, and Training to safeguard the future*.

October 2015 issue of Dstl's *inSIGHT*.

November 2015 issue of PNNL's *Currents*.

October 2015 issue of *Biocoder*.

September 2015 issue of ICSU Newsletter.

UN Security Council report on OPCW Fact Finding Missions.

Science, education and industry resources:

Creative Technologies in the Classroom.

Presentation files from the Science and Technology for Nonproliferation and Terrorism Studies course at the Middlebury Institute of International Studies at Monterey.

The American Chemical Society Division of Chemistry Education Committee on Computers in Chemistry Education (ACS CHED CCCE) fall newsletter features articles on 21st Century Chemical Education, the use of Google Forms for lab reports, the PubChem Laboratory Chemical Safety Summary, online science and education resources from the OPCW, the Marvin Live application for online chemistry collaboration, Conservation and Art Materials Encyclopedia Online, the ChemWiki, the online biochemical and life sciences collection published by Henry Stewart, MolView, and a look back at 20 Years of the MOLECULE OF THE MONTH Website.

Some news from world of science and technology:

From the weeks of 11 – 17, 18 – 24, and 25 – 31 October; 1 – 6, 7 – 14, 15 – 21 and 22 - 28 November; and 29 November – 5 December; in chemistry.

Schedule 3 Chemicals

We began 2015 with a look at Schedule 1 chemicals in patents, provided statistics on Schedule 2 chemicals in scientific publications in August and now we leave 2015 with a look at the chemicals of Schedule 3.

From the Chemical Weapons Convention, the following criteria are taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

(**a**) It has been produced, stockpiled or used as a chemical weapon;

(**b**) It poses otherwise a risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that might enable it to be used as a chemical weapon;

managing, documenting, and sharing citizen science data.

Upcoming S&T Related Events:

OPCW Calendar of Events October to December 2015.

14 – 18 December 2015
Biological Weapons Convention Meeting of States Parties
Geneva, Switzerland.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii
United States of America

25 January - 4 February 2016
Science and Diplomacy for Peace and Security: The CTBT @ 20
Vienna, Austria

2 – 4 February 2016
The Unmanned Systems Expo (TUSE)
The World Forum, The Hague
The Netherlands

16 – 18 February 2016
7th International Conference on Drug Discovery and Therapy
University of Sharjah, Sharjah, UAE

23 - 25 February 2016
NCT CBRNe Europe
Amsterdam, The Netherlands

6 – 10 March 2016
Pittconn 2016
Atlanta, GA
United States of America

13 – 17 March 2016
251st American Chemical Society National Meeting & Exposition
San Diego, CA, USA.
United States of America

16 – 19 March 2016
16th Asian Chemical Congress
Dhaka, Bangladesh.

21 - 23 March 2016
Biomarker Summit 2016
San Diego, CA, USA.

6 – 8 April 2016
XXI IUPAC CHEMRAWN Conference Solid Urban Waste Management
Rome, Italy.

(**c**) It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, part B;

(**d**) It may be produced in large commercial quantities for purposes not prohibited under this Convention.

Figure 1 illustrates the relationship between the three Schedules, showing how sulphur mustard (a Schedule 1 chemical warfare agent) is formed by treating its Schedule 2 pre-cursor (thiodiglycol) with a Schedule 3 reagent (thionyl chloride, a commonly used chlorinating agent for organic chemistry).

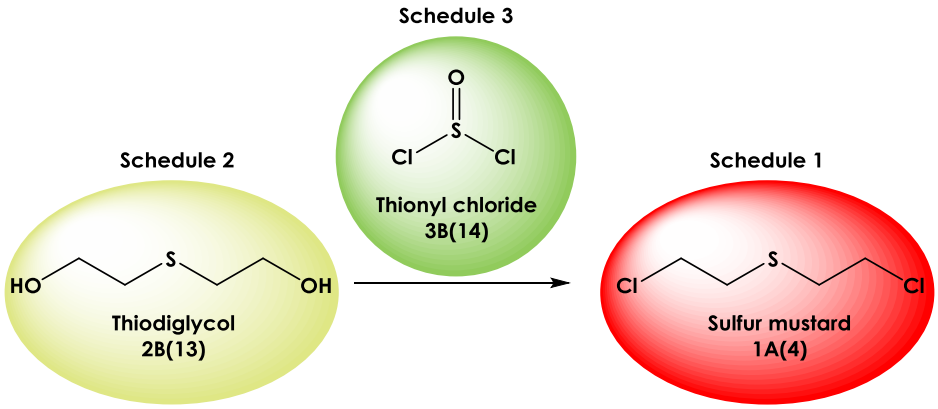


Figure 1: Illustration of the relationship between Schedule 1, 2 and 3 chemicals in the preparation of sulphur mustard.

Schedule 3 is the smallest of the Schedules (only 17 chemicals are listed), yet Schedule 3 chemicals, most notably hydrogen cyanide and triethanolamine, appear in more scientific reports (journal articles and patents) than both Schedule 1 and 2 chemicals combined. As of 3 November 2015, we identified over 330,000 journal articles and patents published from 1900 – 2014 that make reference to Schedule 3 chemicals using SciFinder® (see Figure 2). Figure 3 shows a breakdown of the individual Schedules appearing in publications in 2014.

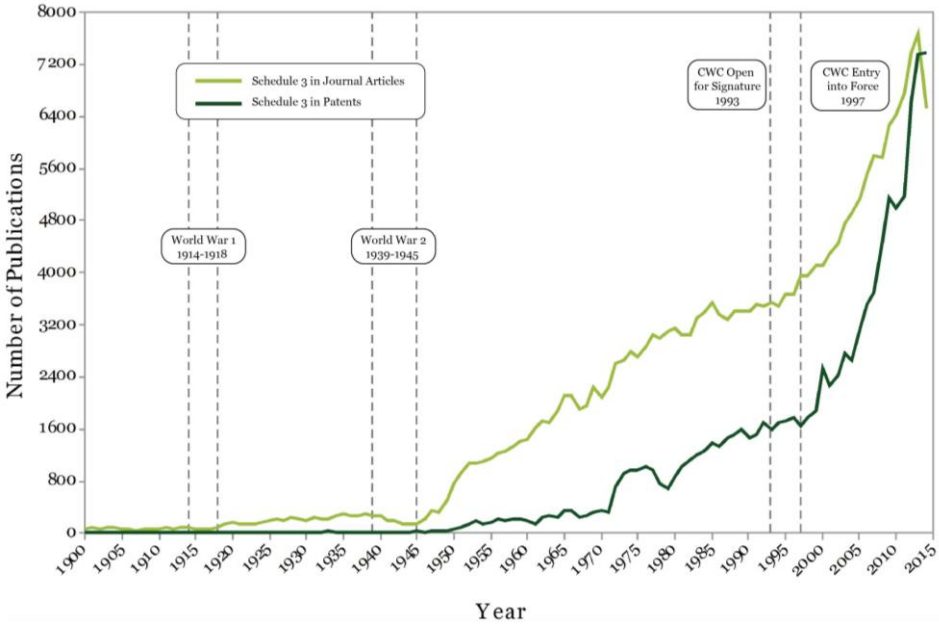


Figure 2: Number of journal articles and patents referencing Schedule 3 Chemicals from 1900-2014 (from SciFinder® as of 3 November 2015).

2 – 4 May 2016
The International Day for the 19th Anniversary of the Foundation of the OPCW.
2016 theme: *"Chemical Safety and Security in a Technologically Evolving World"*
OPCW Headquarters, The Hague
The Netherlands

6 May 2016
2016 Spring ConfChem
Science, Disarmament, and Diplomacy in Chemical Education: The Example of the Organisation for the Prohibition of Chemical Weapons.

24 – 26 May 2016
Innorobo 2016
Paris, France

26 - 28 May 2016
23rd Symposium on Chemical and Science Education
TU Dortmund University, Germany

6 – 9 June 2016
2016 BIO International Convention
San Francisco, California, USA

18 – 22 July 2016
The International Conference on Pure and Applied Chemistry (ICPAC 2016)
"Emerging Trends in Chemical Sciences" Mauritius

15 – 20 August 2016
24th IUPAC International Conference on Chemistry Education (ICCE 2016)
Kuching, Sarawak.
Malaysia

4 – 7 September 2016
52nd Congress of the European Societies of Toxicology (EUROTOX2016)
Istanbul, Turkey

4 – 8 September 2016
6th IUPAC Green Conference (ICGC 2016)
Venice, Italy

7 – 10 September 2016
European Conference on Research in Chemistry Education (ECRICE 2016)
Barcelona, Spain

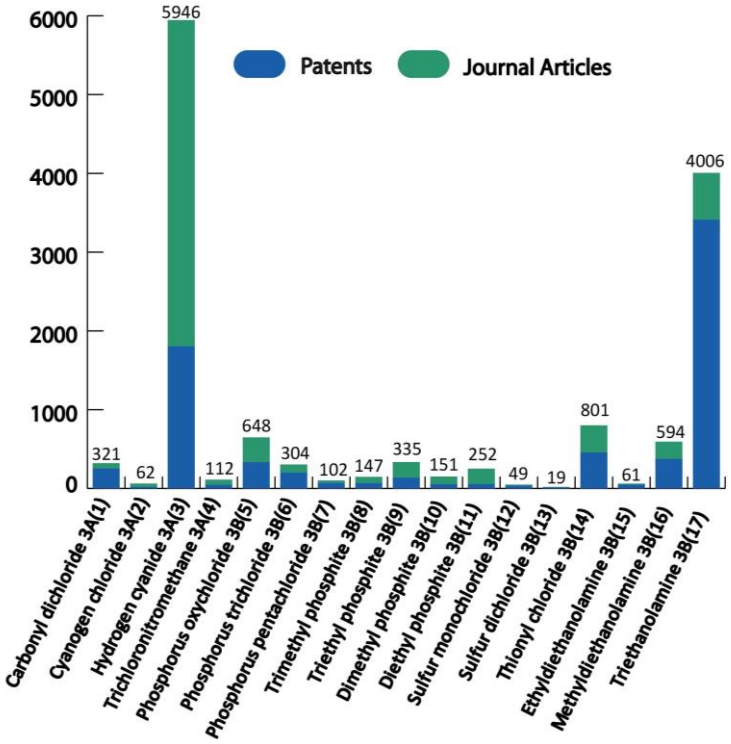
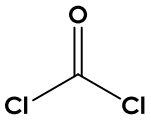


Figure 3: The number of publications (journal articles and patents) referencing Schedule 3 chemicals in 2014 (from SciFinder® as of 3 November 2015).

We continue this feature with a look at the chemicals of Schedule 3, parts A (Toxic Chemicals) and B (Precursors), in regard to uses of these chemicals for purposes not prohibited under the Chemical Weapons Convention:

Schedule 3 Part A, Toxic Chemicals


Phosgene:
Carbonyl dichloride 3A(1)

Schedule 3A(1): Phosgene (Carbonyl dichloride) was used as a chemical weapon in World War 1. Today, phosgene plays a role in the manufacture of a variety of products found in everyday life. These include flexible and rigid foam materials, thermoplastic polyurethanes, coatings, adhesives, sealants, elastomers, polycarbonate plastics, and a wide variety of pharmaceuticals, agricultural chemicals, and specialty chemical intermediates. A set of safe practice guidelines is available for those who work with phosgene.


Cyanogen chloride
3A(2)

Schedule 3A(2): Cyanogen chloride (CK) is volatile liquid and a highly toxic blood agent. The chemical has a number of uses in organic synthesis that include formation of aliphatic carbamates and addition of cyano groups to double bonds double bonds. Trace amounts of cyanogen chloride can actually form if uric acid is introduced into a swimming pool (details here).


Hydrogen cyanide
3A(3)

Schedule 3A(3): Hydrogen cyanide (prussic acid) is a colourless, extremely poisonous liquid that boils slightly above room temperature. The chemical is industrially

Contact Us:

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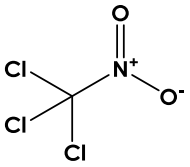
For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

important as precursor to chemical compounds ranging from polymers to pharmaceuticals. It is also used to produce cyanide salts for mining and electroplating. The chemical is known to exist in interstellar space and can actually be found in seeds and nuts that contain cyanogenic glycosides (bitter almonds for example).

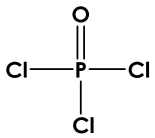
Schedule 3A(4): Chloropicrin (trichloronitromethane) is used as a soil fumigant where it acts on a wide range of species that include fungi, bacteria, nematodes and insects.



Chloropicrin: Trichloronitromethane
3A(4)

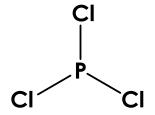
Schedule 3 Part B, Precursors

Schedule 3B(5): Phosphorus oxychloride is a colourless liquid mainly used to produce triarylphosphate esters. These are compounds that find use in flame retardants and plasticisers.



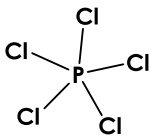
Phosphorus oxychloride
3B(5)

Schedule 3B(6): Phosphorus trichloride is an important industrial chemical used in the synthesis of organophosphorus compounds.

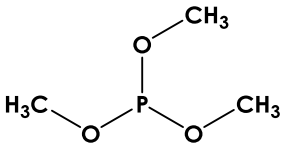


Phosphorus trichloride
3B(6)

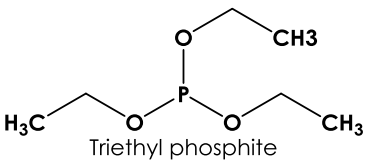
Schedule 3B(7): Phosphorus pentachloride finds use as a chlorinating agent in organic chemistry. **Schedules 3B(8)** trimethyl phosphite and **3B(9)** triethyl phosphite are compounds that are often used as ligands in organometallic chemistry. These trialkylphopshates can also be used in organic synthesis of phosphate esters.



Phosphorus pentachloride
3B(7)

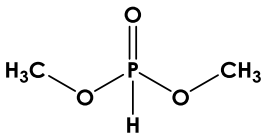


Trimethyl phosphite
3B(8)

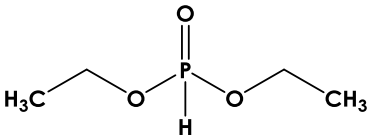


Triethyl phosphite
3B(9)

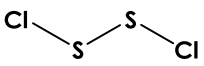
Schedules 3B(10) dimethyl phosphite and **3B(11)** diethyl phosphite are compounds that can be used to produce phosphate esters. **Schedules 3B(12)** sulphur monochloride, **3B(13)** sulphur dichloride and **3B(14)** thionyl chloride are chlorinating agents with many applications in organic chemistry.



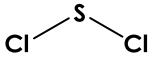
Dimethyl phosphite
3B(10)



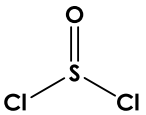
Diethyl phosphite
3B(11)



Sulfur monochloride
3B(12)

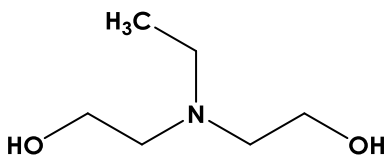


Sulfur dichloride
3B(13)

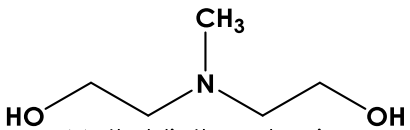


Thionyl chloride
3B(14)

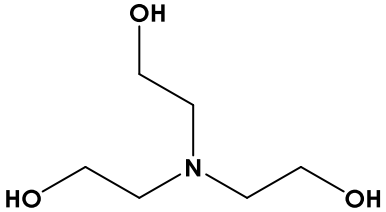
Schedule 3B(15): Ethyldiethanolamine, has applications in CO_2 capture. **Schedule 3B(16):** Methyldiethanolamine is broadly used as a sweetening agent to remove hydrogen sulfide from natural gas. **Schedule 3B(17):** Triethanolamine (TEA) is widely used as an emulsifier in personal care products.



Ethyldiethanolamine
3B(15)



Methyldiethanolamine
3B(16)



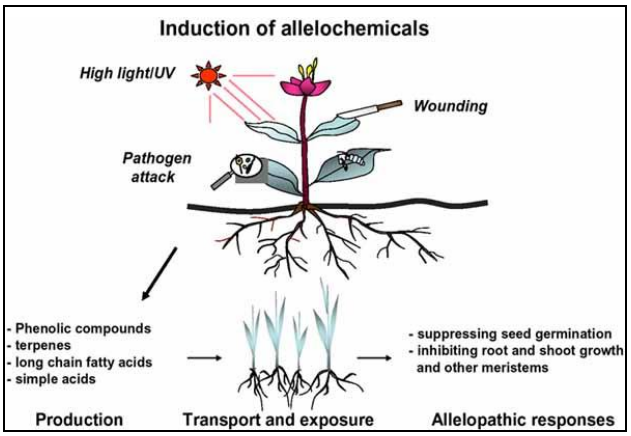
Triethanolamine
3B(17)

Allelopathy

Chemicals emitted by plants are familiar to us from the scents and smells of flowers. The volatile chemicals that produce these scents play an important role in plant reproduction and not surprisingly, this has inspired biotechnological engineering projects. Plant biochemistry has many more dimensions than insect attracting scent chemicals, including potential to produce economically valuable chemicals and the ability to produce and deploy bioregulatory chemicals that influence other plants around them. The release of biochemicals to produce both harmful and beneficial effects on other plants, is called allelopathy; one could think about allelopathy as a botanical use of chemical agents and a potential chemical defence against invasive species!

Allelopathy involves the release of "allelochemicals" into the environment through a variety of processes such as leaching, root extraction, residue decomposition and volatilization. Plants employ volatile chemicals to fend off herbivores, mobilize insects (or parasitic species to insects) in response to herbivore infestations and to inhibit other plant species competing for resources! Allelopathy has also been observed in fungi and marine organisms that include diatoms and sponges (fresh water sponges too).

As the complexity of the biochemical interactions of plants and their ecological systems is better understood, scientists have recognized opportunities to breed plants that use naturally produced chemicals as pesticides (details here) or herbicides ("organic weed management"). This has relevance for the reduction of use of more toxic and/or environmentally persistent agricultural chemicals. There is much work to be done in this field, as the complexity of plant interaction with environment can be influenced by adverse environmental conditions or soil additives.



Inducing allelochemcials (from "The importance of allelopathy in breeding new cultivars").

The Internet of Things (IoT)

Have you ever considered how many devices are currently connected to the internet? Current estimates are about 15 billion (and that's only 1% of what is possible) with 50 billion devices expected to be online by 2020! What we now refer to as the Internet of Things (IoT) is the continually growing network of connected devices that began to emerge in 2008. Who would have imagined that the few connected nodes of ARPANET gave way to the possibility of 1.5 trillion connected devices; potentially revolutionizing how we approach menial and complicated tasks, transforming businesses, daily activities and even our personal health management.

For businesses, the IoT can help to optimize the working environment in real-time, making offices more efficient. Take for example, the Edge building in Amsterdam, which can give individual workers different daily working environments according to their needs and schedules (including temperature preferences throughout the building), while at the same time producing and conserving energy through smart management of the buildings solar panels and climatic controls. Shopping districts could potentially track consumer bounce rates (how long customers stay in a store and which stores they visit) and contribute to security monitoring.

Urban infrastructure can be fitted with sensors to generate data that helps make cities "smarter". For example, "smart parking" can reduce congestion and vehicle exhaust emissions; and, "smart street lamps" can guide citizens out for a nightly stroll to well-lit areas. We have also seen solar and wind powered lamppost concepts in developing countries that trap dengue fever carrying mosquitoes (more details here)!

Sensors that analyse microbes and chemicals can measure sewer water to generate data relevant to public health. In a hospital, IoT devices can more accurately predict the location of patients and the amount of services they receive. This will provide more accurate analysis of drug application, immediate response to emergency situations and external monitoring systems that can trigger immediate response. There are already a wealth of health tracking wearable devices; going forward we can expect these sensors to improve rates of data retrieval and incorporate more functions.

For your home, the same sensors that make buildings smart can be applied to household needs. The concept of a "Smart Fridge" is often brought up, that is a refrigerator that will order food items from a store as they are consumed. However, it may be a while before fridges are indeed smart since the IoT is not about one connected object, but a wide network of objects with sensors. For those interested, there are many DIY home smartsensors available.

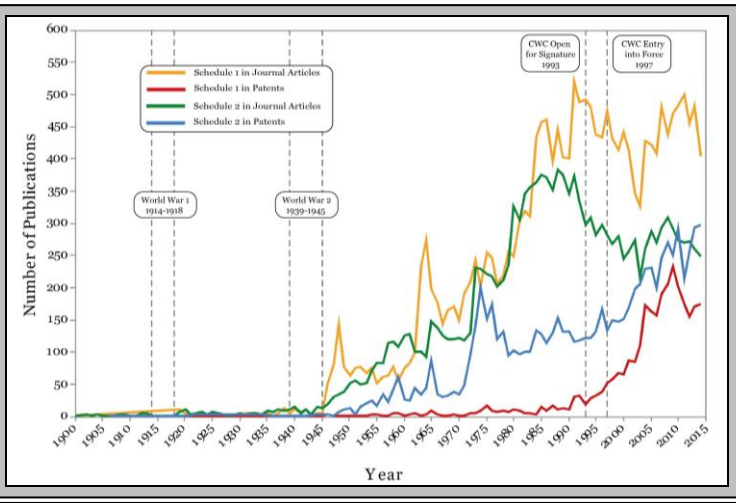
Other applications of the IoT may surprise you, for example the connected cow (with both ear and gut connected to the internet). What purpose does connecting a cow serve? It allows one to detect when an animal is sick, when it is in heat and allows the monitoring of its gut microbiome to ensure production of good quality milk! In regard to chemical security, the IoT is a potentially valuable tool for sniffing out hazardous substances.

As incredible as it all sounds, there are still issues to solve, especially in regard to the capacity to handle the incredible amount of data that would be generated (and consider the size of a daily internet scan) and a need for "the cloud" for worldwide communication. Many solutions have been proposed, such as the use of fog computing, mobile devices as temporary data gateways and the use of data fusion techniques.

What we can expect from all of these developments is a rethinking of our relationship to tools, consumption, services, manufacturing and perhaps even governance. In the meantime, we are privileged to be able to watch this new connected world evolve and perhaps make our own contributions to it!

Did You Know?

There are over 45,000 journal articles and patents published between 1900 and 2014 that make reference to Schedule 1 and Schedule 2 chemicals.



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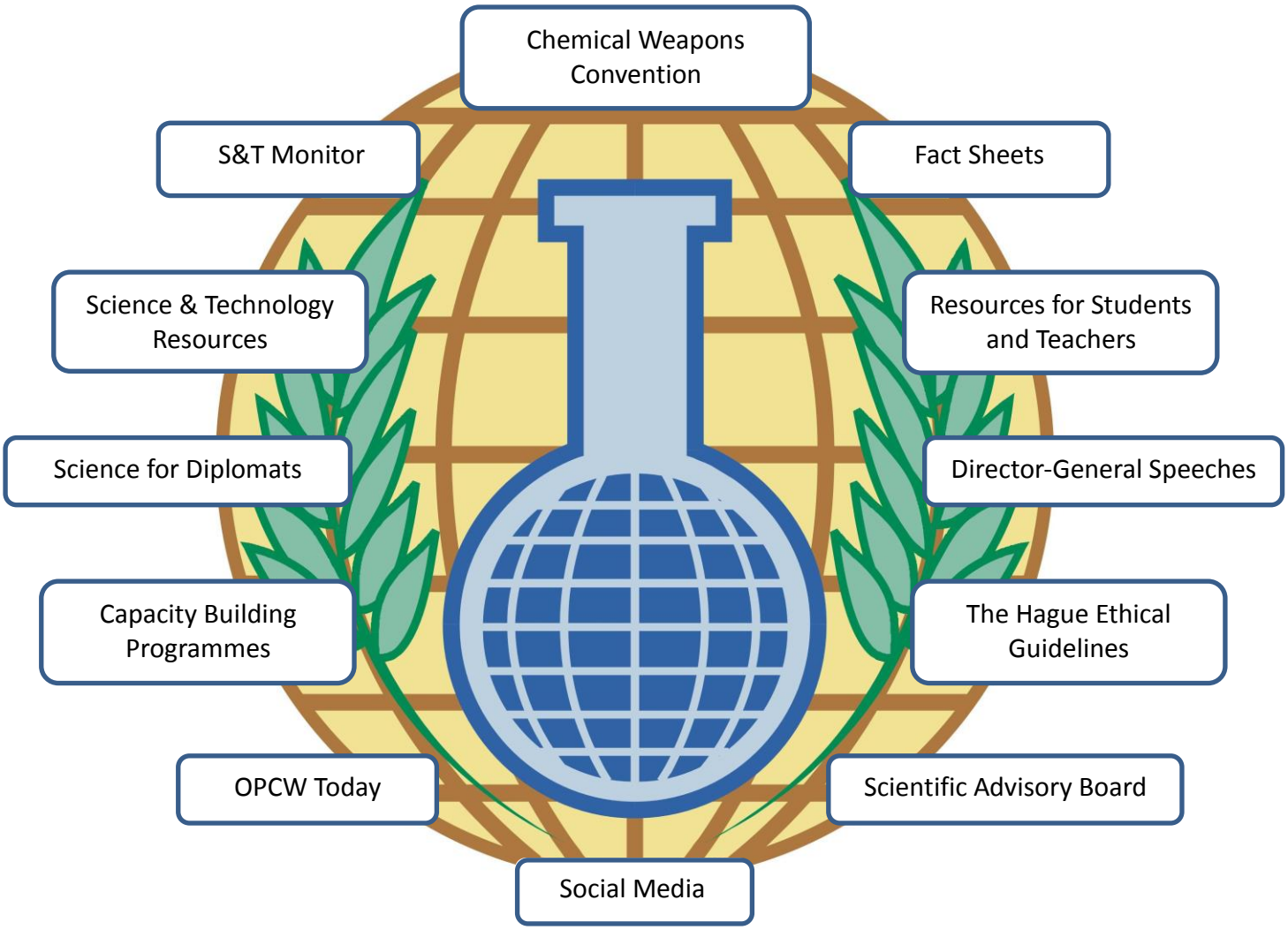

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