# Science for diplomats (Introduction)

# Scientific discovery and technology development: trends and topics for the CWC policy-maker

*Brought to you by the Office of Strategy and Policy*

26 June 2014
OPCW Headquarters
The Hague, The Netherlands

Jonathan E. Forman
Science Policy Adviser
Office of Strategy and Policy
Organisation for the Prohibition of Chemical Weapons

# From The Convention

- **The Conference of States Parties Shall:**
  - **"Review scientific and technological developments that could affect the operation of this Convention** and, in this context, direct the Director General to establish a Scientific Advisory Board to enable him, in the performance of his functions, to render specialized advice in areas of science and technology relevant to this Convention, to the Conference, the Executive Council or States Parties."
  - *CWC Article VIII, Section B, paragraph 21(h)*

# The Third Review Conference

- "**Conviction** that the provisions of the Convention are mutually reinforcing and that the full, effective, and non-discriminatory implementation of all of its provisions, taking into account relevant developments in science, technology and industry, is of critical importance;"

  *RC-3/3* paragraph 9.4*

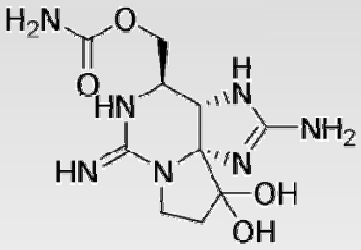
- "**Recognition** that new challenges related to the Convention continue to arise and that its implementation may need to be improved to continue to achieve the object and purpose of the Convention and to stay abreast of developments in science and technology;"

  *RC-3/3*, paragraph 9.9*

ORGANISATION FOR THE
PROHIBITION OF CHEMICAL WEAPONS

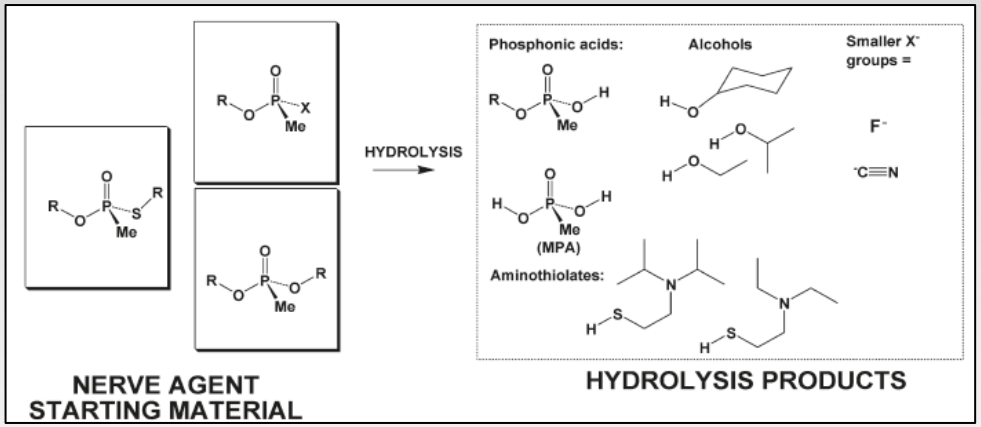
*Working together for a world free of chemical weapons*

# Science and Technology Underpin the CWC




**Article II**

**Article III**



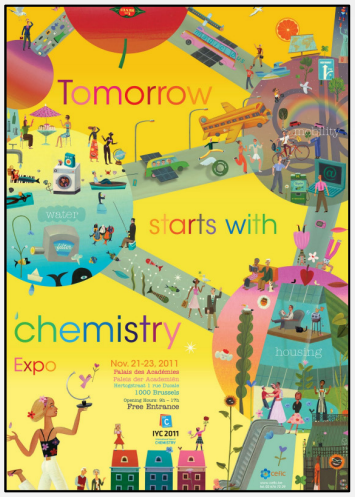

**Articles IV and V**

**Article VI**

**Article VIII**

**Articles IX and X**


**Article VII**




**Article XI**

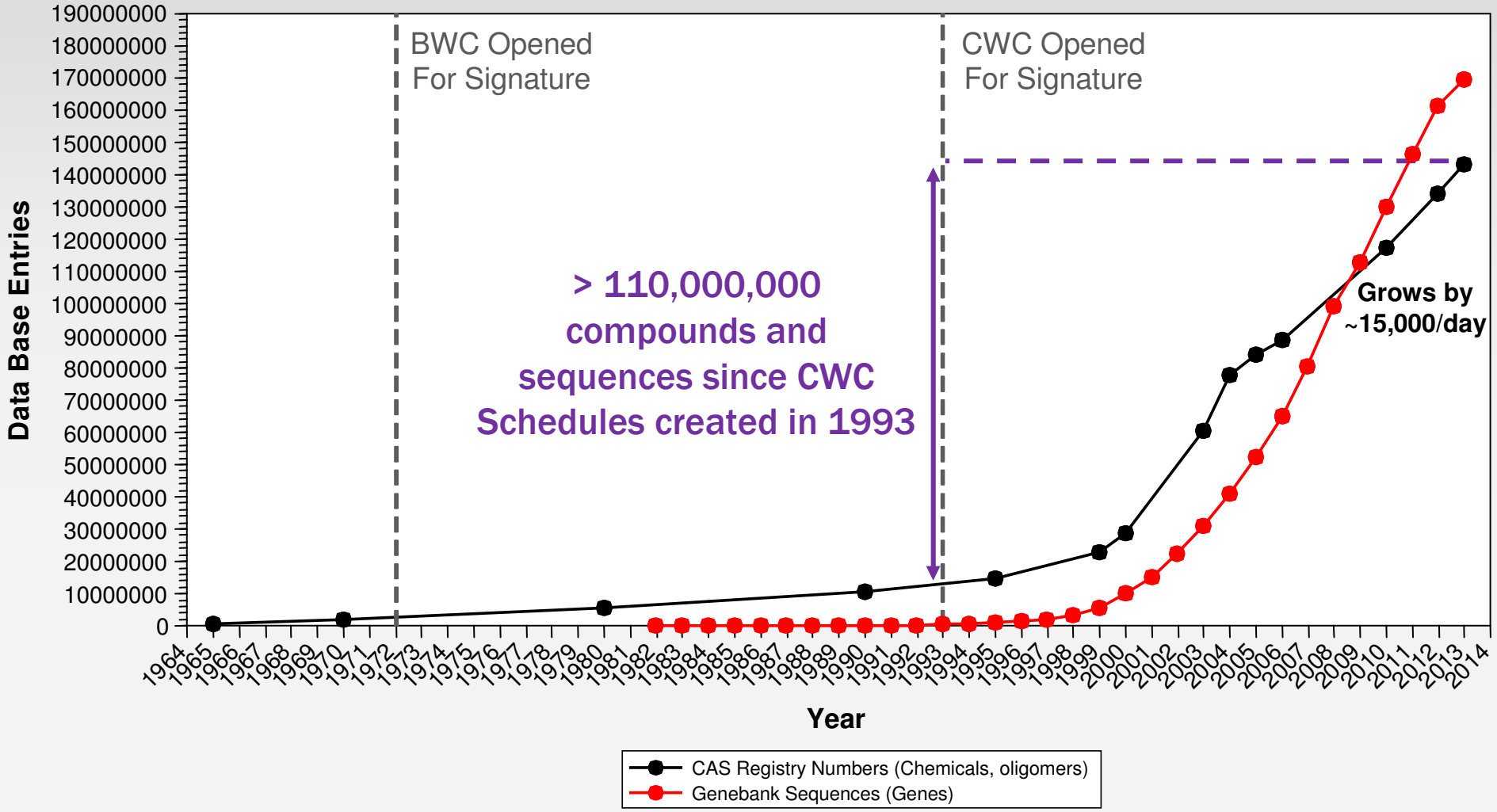
# SAB Report of the Developments in S&T to The Third review Conference

## (RC-3/DG.1, Dated 29 October 2012)

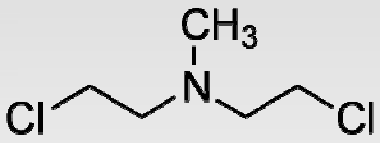
# Director General's Recommendations

## (RC-3/DG.2, Dated 31 January 2013)

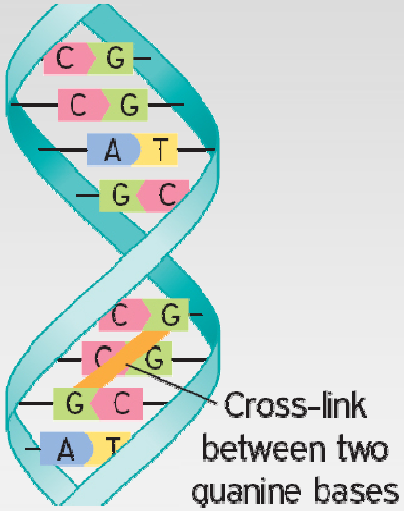
# Monitoring Science



# Chemicals Have Multiple Uses




***Nitrogen Mustard***
***Schedule 1A***





***and Anti-Cancer Drug***
***(as a salt)***

# Research On Toxic Substances

## THE BACTERIAL TOXIN TOOLKIT

*Giampietro Schiavo* and F. Gisou van der Goot‡*

Pathogenic bacteria and higher eukaryotes have spent a long time together, leading to a precise understanding of one another's way of functioning. Through rapid evolution, bacteria have engineered increasingly sophisticated weapons to hit exactly where it hurts, interfering with fundamental host functions. However, toxins are not only useful to the bacteria — they have also become an essential asset for life scientists, who can now use them as toolkits to explore cellular processes.

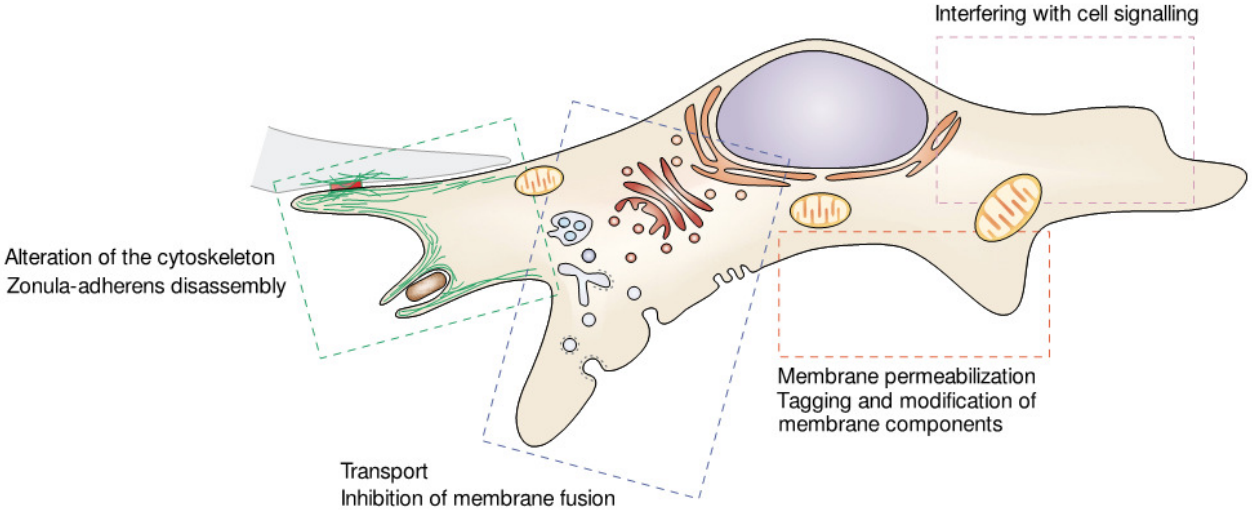


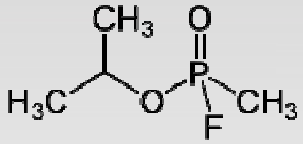

Figure 1 | **Cellular processes targeted by bacterial toxins.** These have been subdivided into four classes, each represented by examples in FIGS 2 to 5.

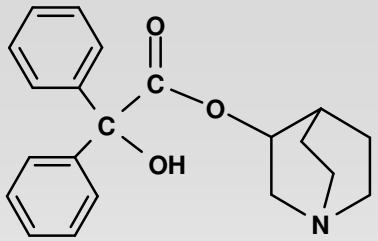
*From: Nature Reviews, Molecular cell Biology, 2001, 531-537*

# Can This Be Easily Discussed?

# What Defines a Chemical?

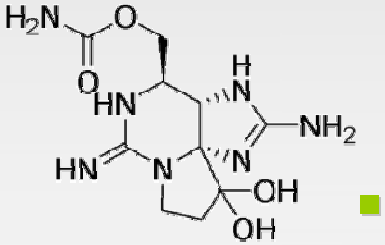
# Understanding Chemicals

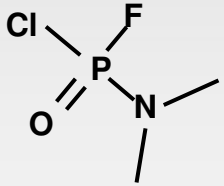




- **> 140 Million CAS Numbers!**
- **How Many Possible Scheduled Chemicals?**

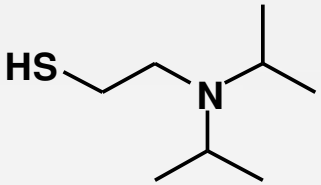
***Infinite number of possibilities!***
***(generic structures in Schedule 1 and Schedule 2)***

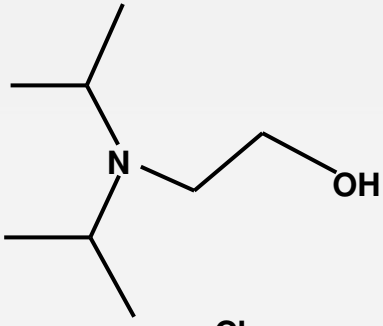




- **How Many Actual Scheduled Chemicals**

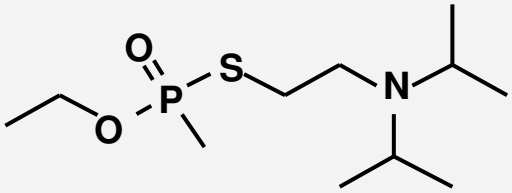
***~35,000 CAS Numbers Reported***

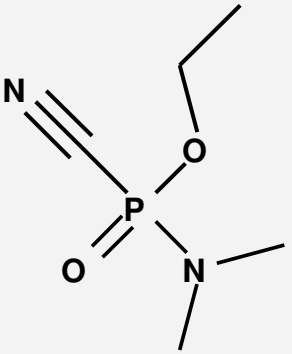


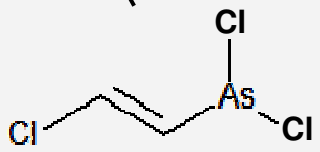


- **How Many Mass Spectra in OCAD?**

***~5,000***

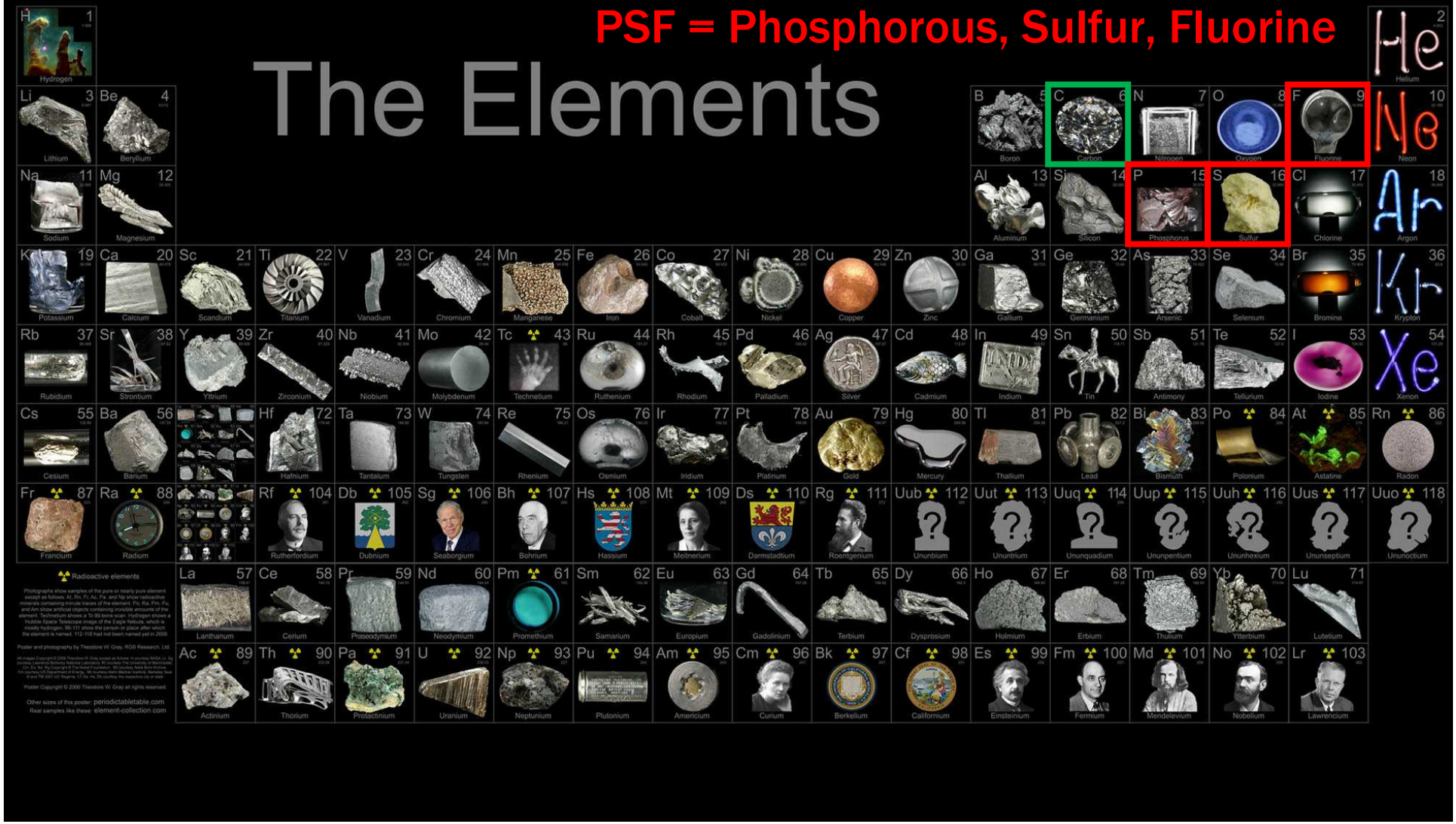






# Organic chemicals: A broad class of substances containing carbon

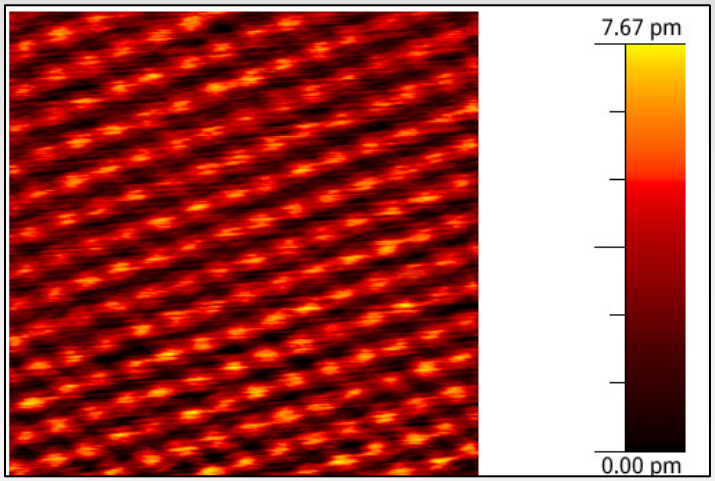
**PSF = Phosphorous, Sulfur, Fluorine**



# From Atoms to Compounds

- **Atoms are the building blocks**

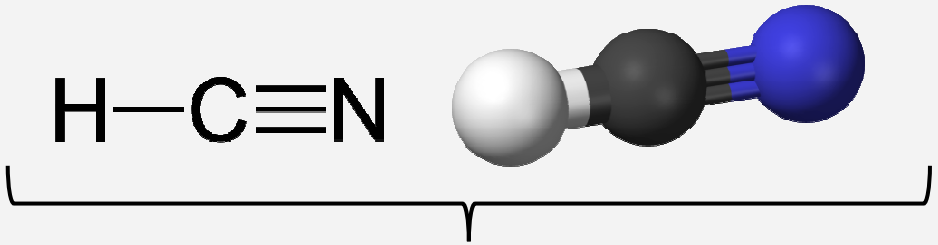
**Silver (Ag) atoms in a crystal**



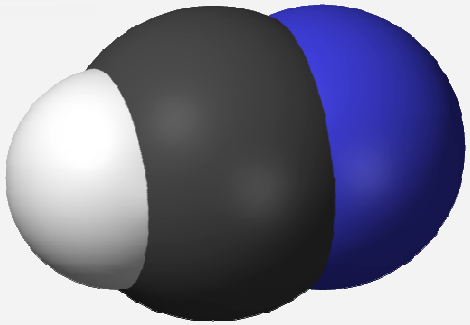

$$1\ \text{pm} = \frac{1\ \text{meter}}{1{,}000{,}000{,}000{,}000}$$

- **Atoms combine to form molecules**

**HCN**
Hydrogen (H)
Carbon (C)
Nitrogen (N)



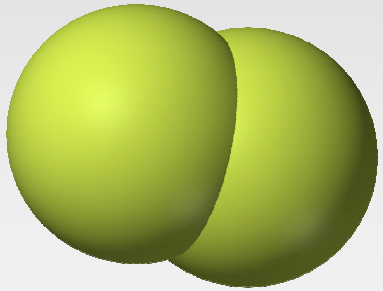

Depiction of how atoms are bonded to one another



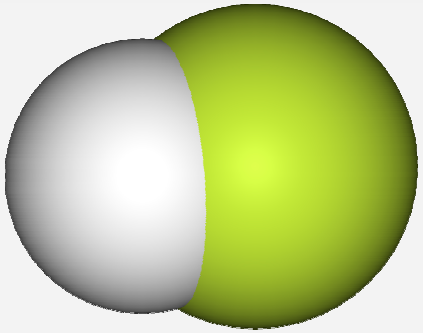
3D Representation showing relative sizes of atoms

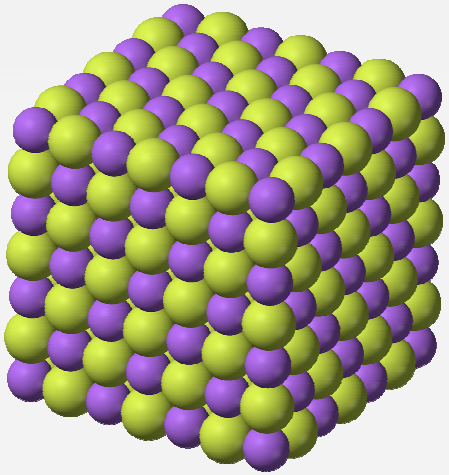
# Some Definitions

- **Elements can be described as atoms or molecules**
  - Fluorine atom (F)
  - Fluorine molecule ($F_2$)



- **Compounds are composed of multiple elements**
  - Hydrogen Fluoride (HF)
  - Sodium Fluoride (NaF)

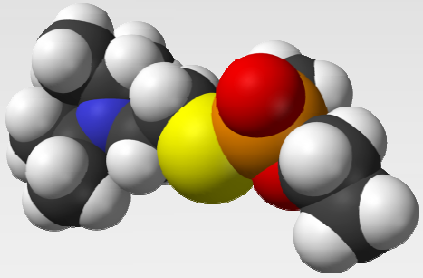




# Scheduled Chemicals Span a Broad Range of Properties

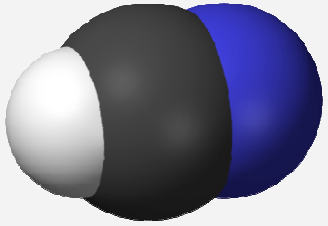
**<u>*O*-ethyl-*S*-[2(diisopropylamino)ethyl] methylphosphonothiolate (VX)</u>**

43 atoms ($C_{11}H_{26}NO_2PS$)
Schedule 1
liquid
Molecular mass = 267



**<u>Hydrogen Cyanide (HCN)</u>**

3 atoms
Schedule 3
Gas
Molecular mass = 27



**<u>Ricin</u>**

A sequence of
> 520 amino acids
Schedule 1
Solid
Molecular mass ~62,000
(~260X larger than VX)

# The Convergence of Chemistry and Biology

# Chemistry Underpins Biology

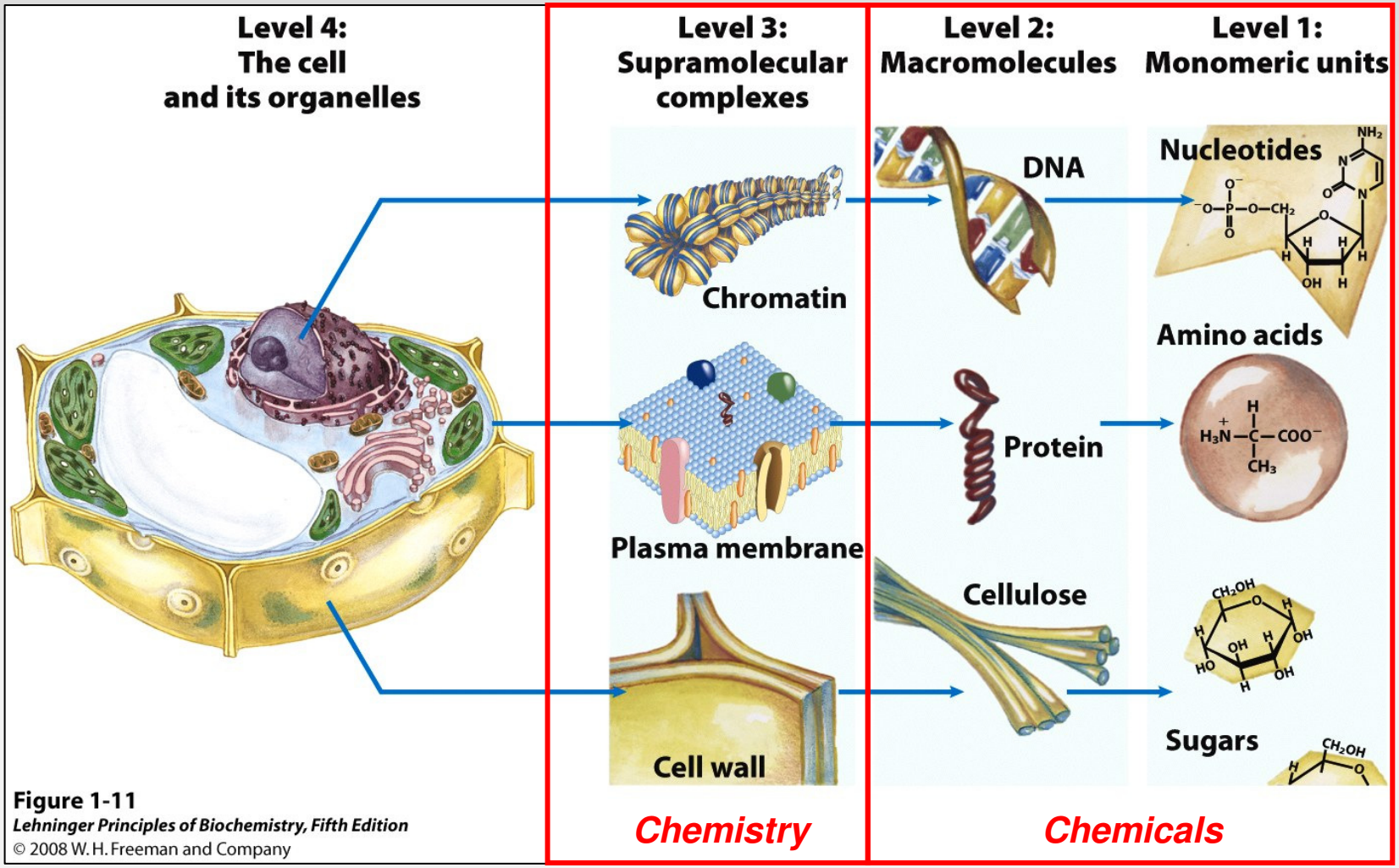
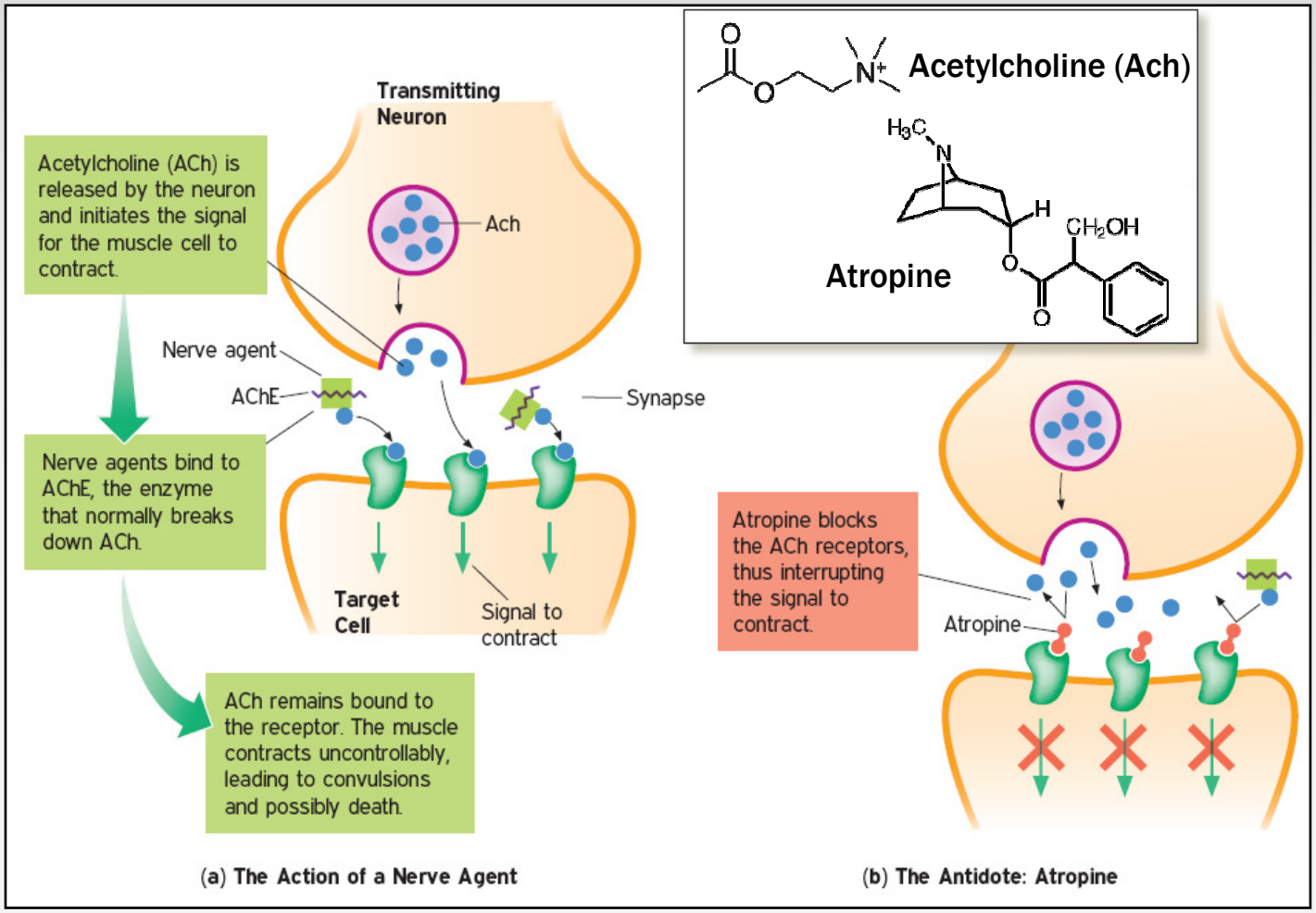



**Figure 1-11**
***Lehninger Principles of Biochemistry, Fifth Edition***

# Chemicals Influence Biology



# Chemical Production

# Chemistry is a Science of Change

# Technology is the Integration of functional components into Multifunctional Tools

# Production Technology: Production by Synthesis?

**From Petroleum**

**Distillation**

**Reactor**

**Separation**

**Raw Material *(Bulk Chemical)***

**Pre-Process**

**Chemical Formation (Synthesis?)**

**Separate (Purify)**

**Product *(Bulk Chemical)***

**From Biomass**

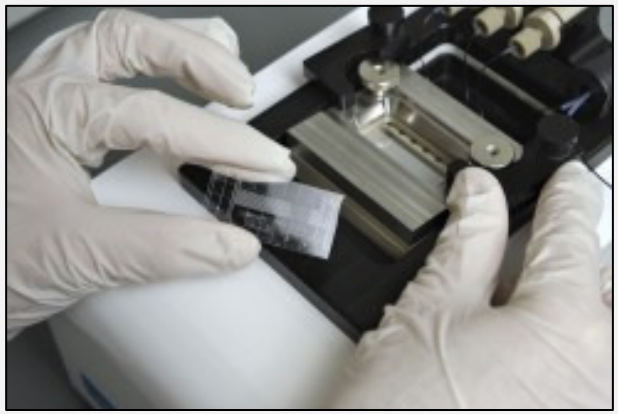
**Milling Mashing Digestion**

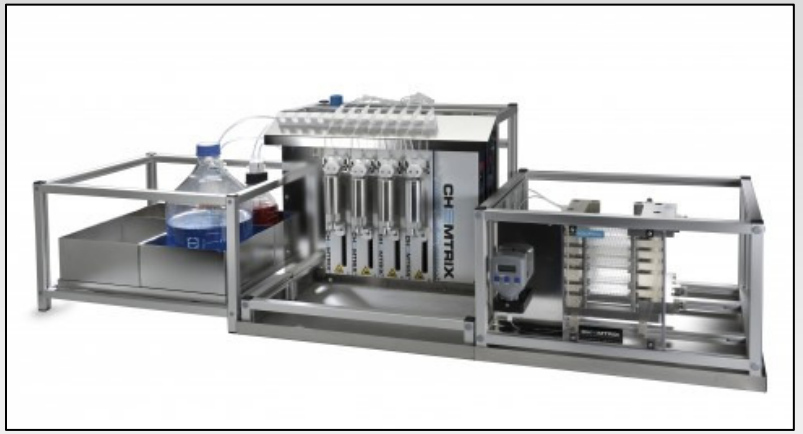
**and/or Fermentor**

**DOC**

# Continuous Flow Technologies

**Microreactor**
**1 metric tonne ~700,000 days**






**Larger "Microreactor"**
**1 metric tonne ~1,070 days**
**"number up" to increase throughput**

# Production Scale Continuous Flow System

# Scientific and Technological Development

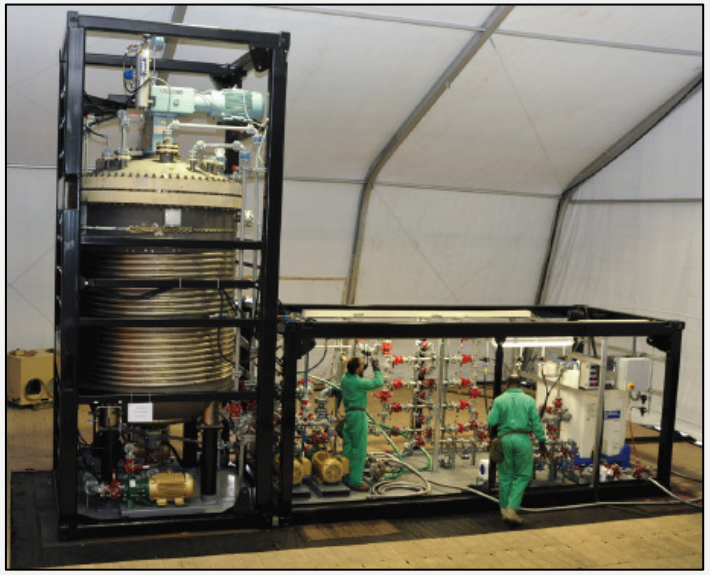
# Basic Research vs. Fieldable Applications


***Clever ideas – but are they practical and effective?***

*~150,000/ml ~ 200 rpm mechanical stirring in 15 ml volume using $H_2O_2$ as both fuel for stirrers and neutralization agent*

*Angewandte Chemie International Edition, 2013, 50, p13276*

**Portable systems adopted for use in 2013**



# How Do Ideas and Research Results Become Realities?

?



# Converging Science is the Norm, Not the Exception!

**Chemistry – Biology – Physics – Engineering – Informatics and More…**

# Deciphering Technical Reports

# What Does It Mean and How Applicable Is it?

# Scrutinizing Technical Reports

- Differences and chance cause variation
- No measurement is exact
- Bias is rife
- Bigger is usually better for sample size
- Correlation does not imply causation
- Regression to the mean can mislead
- Extrapolating beyond the data is risky
- Beware the base-rate fallacy
- Controls are important
- Randomization avoids bias
- Seek replication, not pseudoreplication
- Scientists are human
- Significance is significant
- Separate no effect from non-significance
- Effect size matters
- Study relevance limits generalizations
- Feelings influence risk perception
- Dependencies change the risks
- Data can be dredged or cherry picked
- Extreme measurements may mislead

From: "Twenty tips for interpreting scientific claims", *Nature*, 2013, 503,p337

# Summary and Future Discussion

# From The Director General's Recommendations to RC-3

## (RC-3/DG.2, Dated 31 January 2013)

- Monitoring S&T Developments (paras 7, 8, 29, 37)
- Verification (paras 12, 13, 14, 17, 18, 20, 21, 22)
  - Includes recommendations on Transfer Notifications (para 11) and
  - Incapacitating Agents (paras 15, 16)
- Laboratory Capabilities and Analysis (paras 24, 25, 26, 30, 32)
- Expertise, Training and Knowledge (paras 34, 36, 37)
- Assistance and Protection (para 35)
- Education and Outreach (para 28)

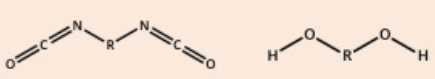
# S & T For Diplomats: A Series of Discussions

- 9 July (On the margins of EC-76)
  - **S&T for Diplomats (1): Chemical analysis in verification**
    - SAB Laboratory recommendations
    - Sampling and analysis
- October (On the margins of EC-77, To be confirmed)
  - **S&T for Diplomats (2): Biological processes and chemical production**
    - SAB convergence related recommendations
    - Production by synthesis
- **Other topics to be scheduled**

# THE CHEMISTRY OF THE WORLD CUP BALL

## POLYURETHANE COVERING

The surface covering of a football is composed of synthetic leather; in professional footballs, this is made from polyurethane polymers. The World Cup ball is made from six polyurethane panels, which are thermally bonded together. This covering protects the ball and minimises water absorption. In cheaper footballs, the coating can be made from PVC.

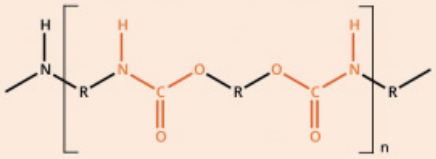


ISOCYANATE



POLYOL

R represents the portion of the organic molecule that can be varied depending on the specific polyurethane that is being synthesised.

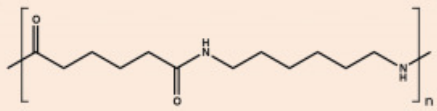


POLYURETHANE
(urethane linkages in orange)

Polyurethane is a polymer - a very large molecule built up from many smaller units bonded together. The basic synthesis of polyurethanes involves the addition reaction of isocyanate and polyol molecules to form urethane groups.


## NYLON LINING

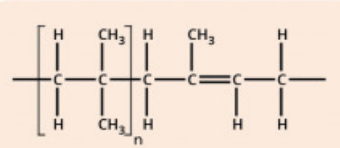
Several layers of lining are used between the covering of the football and the bladder to improve the bounce and strength of the ball. This lining is made of nylon, another class of polymers also known as polyamides. Polyesters can also be used for this purpose.



NYLON 6-6

## BUTYL BLADDER

The bladder is the part of the ball in which the air is contained. Butyl rubber is often used because it retains the air better than the other option, latex. However, latex bladders can provide better surface tension.



BUTYL RUBBER