



禁止化学武器组织



ORGANISATION FOR
THE PROHIBITION OF
CHEMICAL WEAPONS



ОРГАНИЗАЦИЯ ПО
ЗАПРЕЩЕНИЮ
ХИМИЧЕСКОГО ОРУЖИЯ



ORGANISATION POUR
L'INTERDICTION
DES ARMES CHIMIQUES



منظمة حظر
الأسلحة الكيميائية



OP



ON POUR
L'INTERDICTION
DES ARMES CHIMIQUES



منظمة حظر
الأسلحة الكيميائية



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ORGANIZACIÓN PARA
LA PROHIBICIÓN DE
LAS ARMAS QUÍMICAS



禁止化学武器组织



ORGANISATION FOR
THE PROHIBITION OF
CHEMICAL WEAPONS

Emerging Technology and the work of the OPCW Scientific Advisory Board

Emerging Technologies and the CWC:

Mobile Data Collection, Big Data and Artificial Intelligence

21st Conference of the States Parties of the Chemical Weapons Convention

28 November 2016

Jonathan E. Forman, Ph.D.

Science Policy Adviser and Secretary to the Scientific Advisory Board



ON FOR
L'INTERDICTION
DES ARMES CHIMIQUES



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LA PROHIBICIÓN DE
LAS ARMAS QUÍMICAS



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ORGANIZACIÓN PARA
LA PROHIBICIÓN DE



禁止化学武器组织



ORGANISATION FOR
THE PROHIBITION OF



ОРГАНИЗАЦИЯ ПО
ЗАПРЕЩЕНИЮ



ORGANISATION
L'INTERDICTION



OPCW

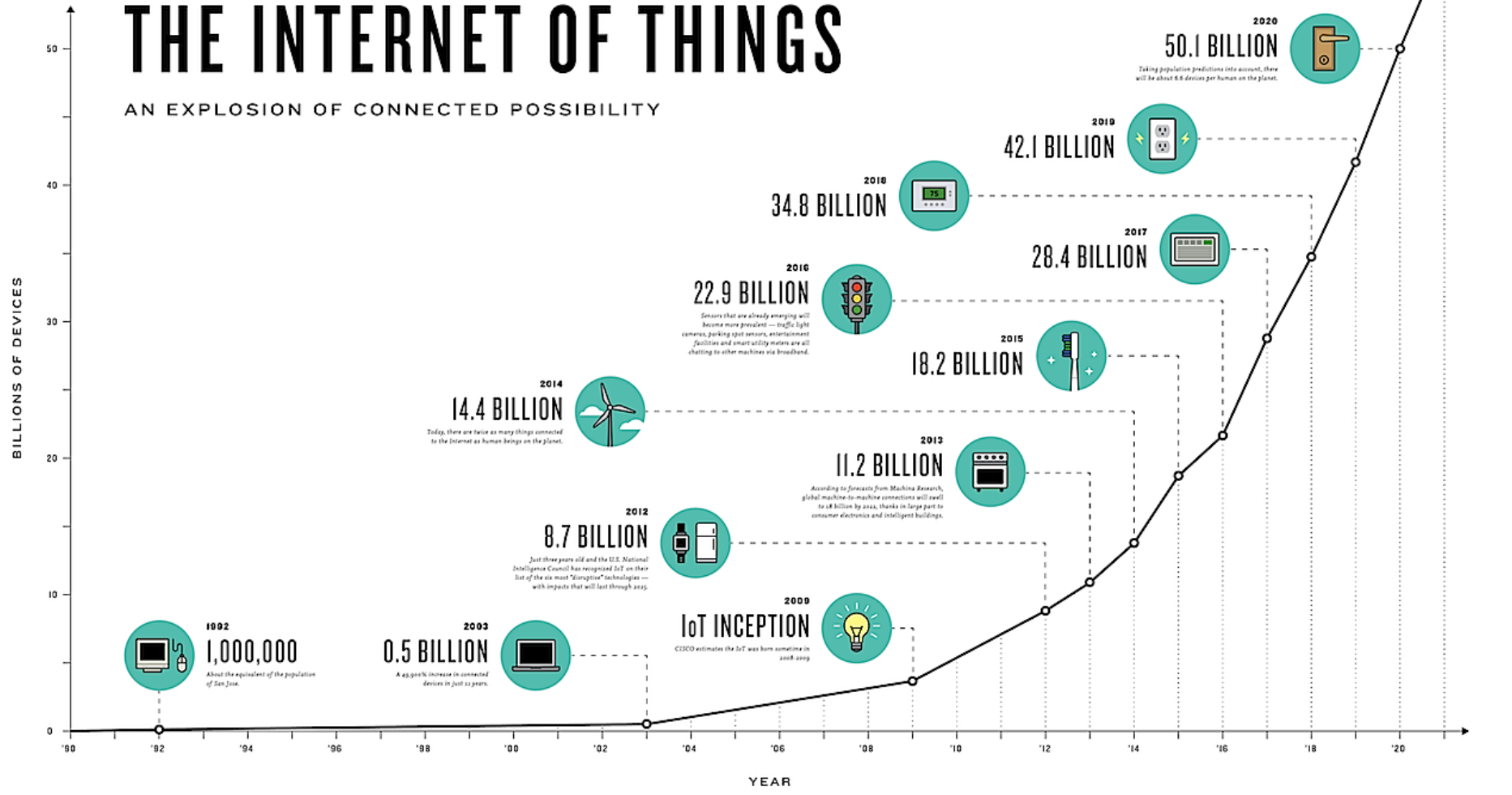
Data Collection and Sharing has Never Been Easier



Data Collection and Sharing has Never Been Easier

THE INTERNET OF THINGS

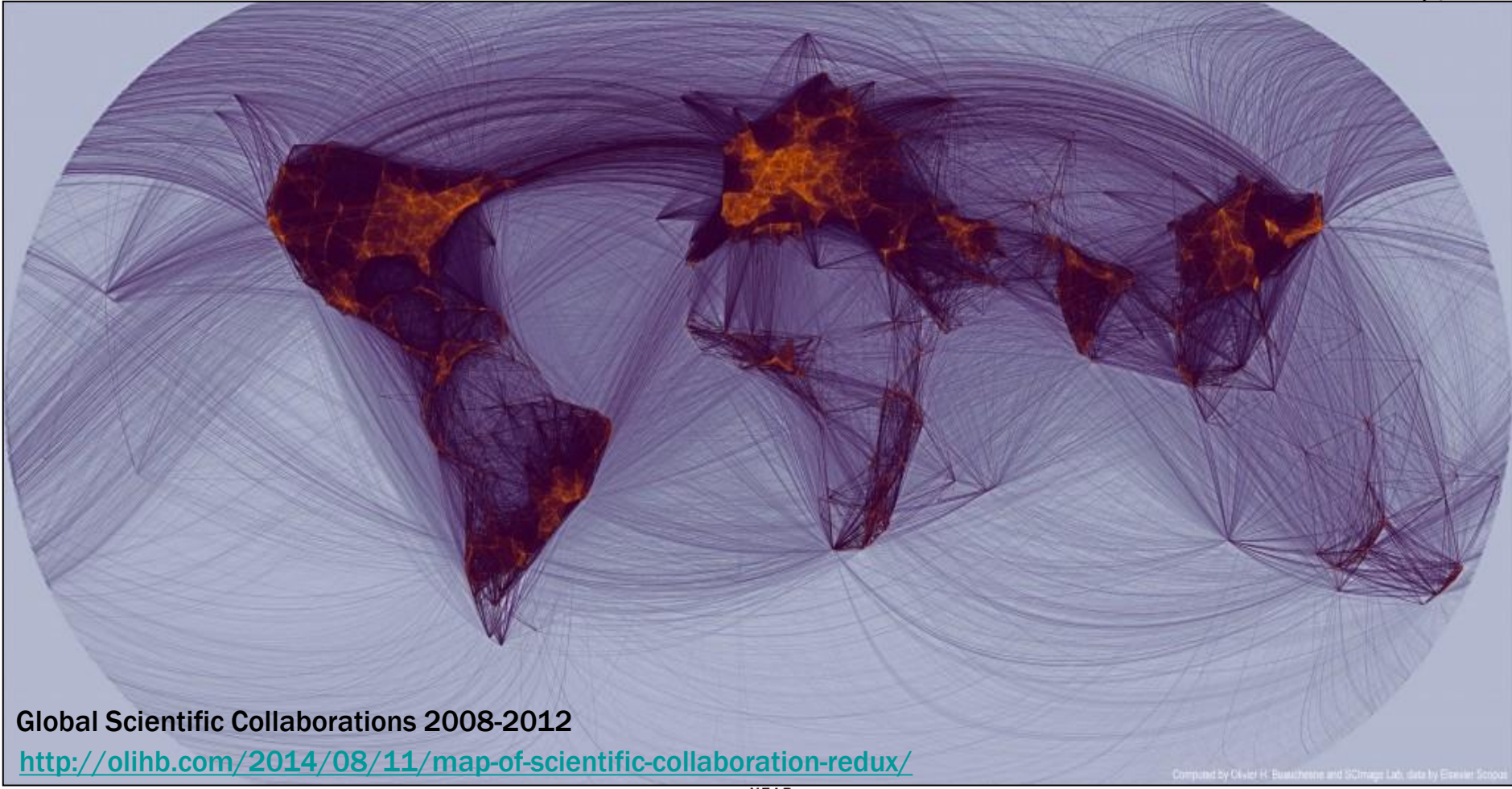
AN EXPLOSION OF CONNECTED POSSIBILITY





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Data Collection and Sharing has Never Been Easier



Global Scientific Collaborations 2008-2012

<http://olihb.com/2014/08/11/map-of-scientific-collaboration-redux/>

Computed by Olivier H. Buachehe and SICImage Lab; data by Elsevier Scopus

YEAR



OPCW

All of this Advanced Science and Technology with Misuse Potential and...

- **Allegations of use of Chlorine Gas and Sulphur Mustard**



Image from bellingcat



Image circulating on social media, August 2015



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All of this Advanced Science and Technology with Misuse Potential and...

- Allegations of use of Chlorine Gas and Sulphur Mustard



Image

C&EN
CHEMICAL & ENGINEERING NEWS

FEBRUARY 23, 2015

FINE CHEMICALS
Nonpharma business rules
InformEx show **P.24**

PITTCON IN N'AWLINS
Analytical conference will
draw thousands **P.50**

CHEMICAL WEAPONS IN WWI
How poison gas set a dark precedent 100 years ago **P.8**

 PUBLISHED BY THE AMERICAN CHEMICAL SOCIETY

<http://chemicalweapons.cenmag.org/>



OPCW

All of this Advanced Science and Technology with Misuse Potential and...

- Allegations of use of Chlorine Gas and Sulphur Mustard

- Diseases found in nature

- Nature does not sign or honour treaties!





OPCW

Disarmament Cannot Afford to be Scientifically or Technologically Illiterate

■ Maintain Critical Knowledge

- Analytical capabilities
- Protection and treatment
- Agents
- Production methods
- Delivery methods

■ Science and Technology

- *Recognize opportunities*
- *Understand concerns*
- *Evolve with technology*





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Opportunities Abound for Chemistry

GC/MS



GC/FTIR



GC/FPD



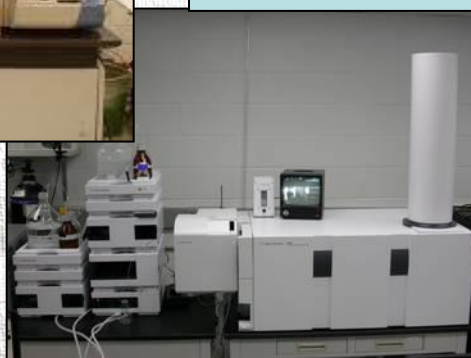
LC/MS



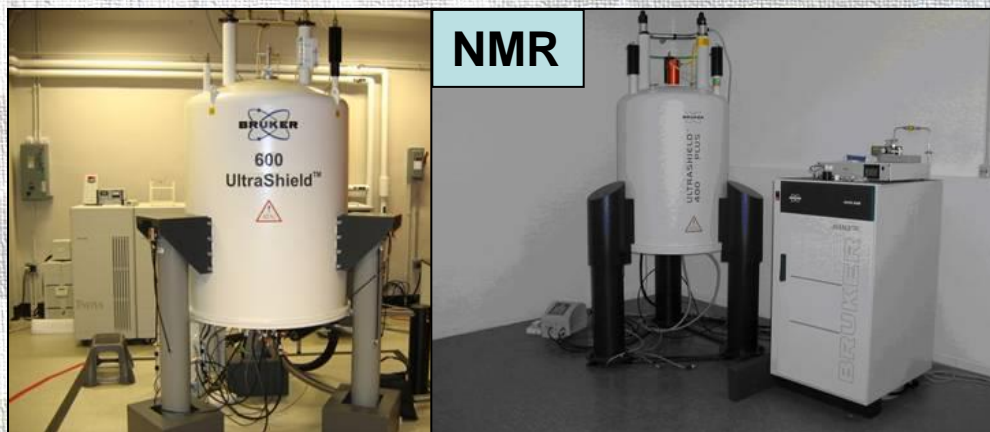
GC/AED



LC/HRMS



NMR





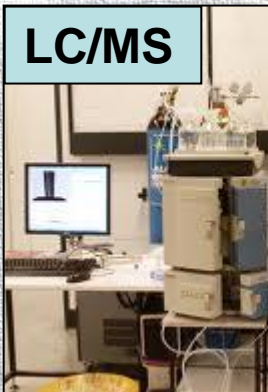
OPCW

Opportunities Abound for Chemistry

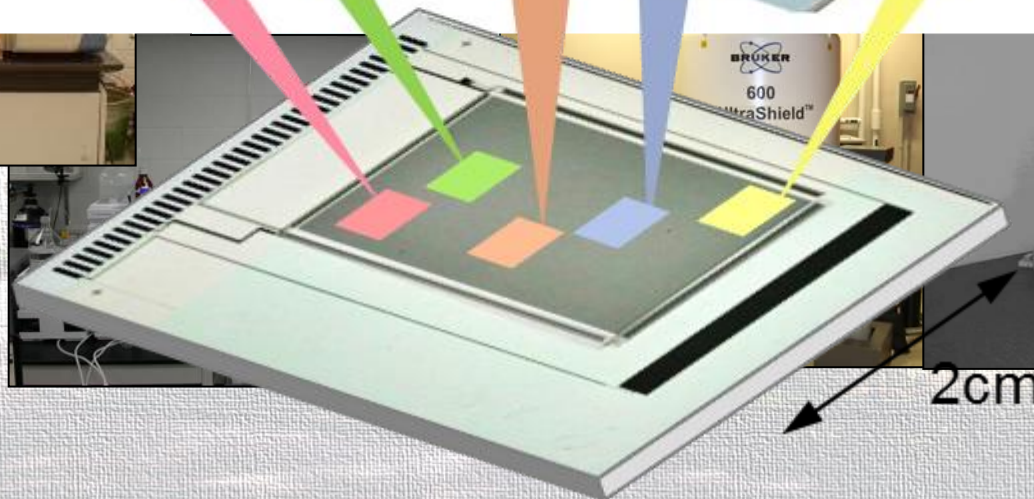
GC/MS



LC/MS



FPD



2cm



The Elusive Tricorder...



OPCW



The Elusive Tricorder...



OPCW

QUALCOMM
TRICORDER XPRIZE®

ABOUT

NEWS

TEAMS

**FINAL WINNERS FOR
THE \$10 MILLION
TRICORDER XPRIZE TO
BE ANNOUNCED EARLY
2017**

Next phase of consumer testing to start in
September 2016

PHYSICIAN CONTACTED
MEDICATION RECOMMENDED
10ML (2TSP) ACETAMINOPHEN
PULSE: 110 BPM
TEMPERATURE: 102°

The Elusive Tricorder...



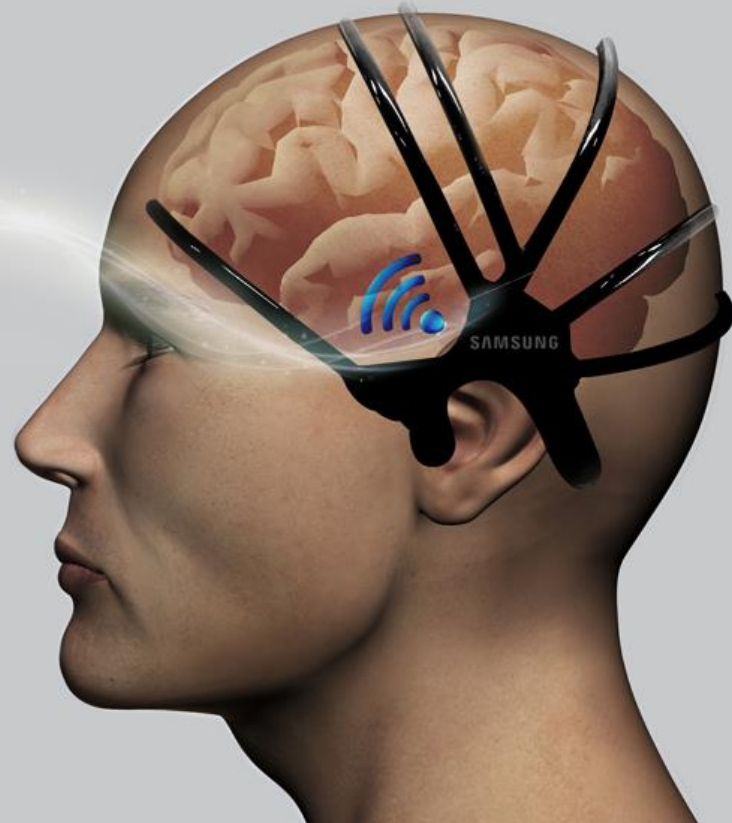
OPCW

QUALCOMM
TRICORDER

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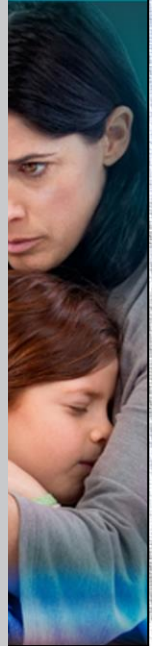
Next phase
September

EARLY DETECTION SENSOR & ALGORITHM PACKAGE (EDSAP)



SAMSUNG TOMORROW

TEAMS



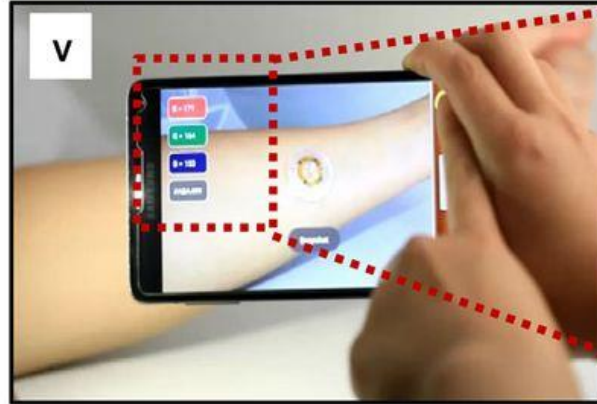
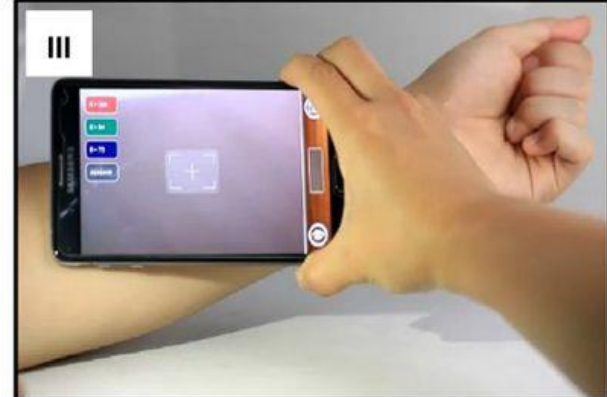
The Elusive Tricorder...

QUALCOMM
TRICORDER

EARLY DETECTION SENSOR &

TEAMS

A



SAMSUNG TOMORROW

Mobile Laboratories

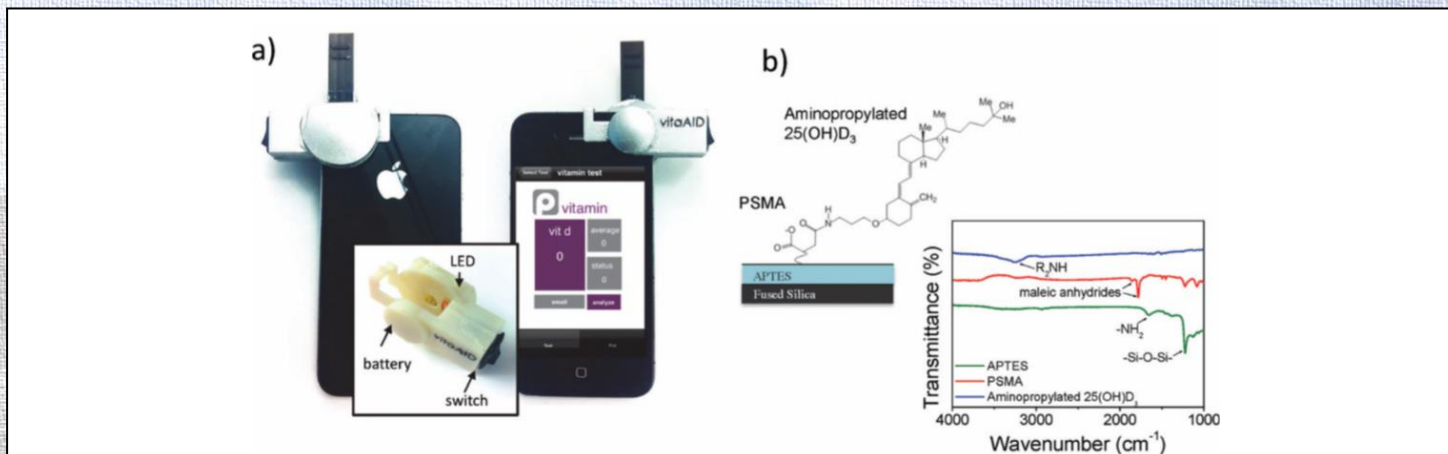


Fig. 1 a) vitaAID accessory on a iPhone with the inset showing the components of the accessory b) FT-IR spectra showing the chemical composition of the APTES, maleic anhydride and aminopropylated 25(OH)D₃ layers that constitute the detection area.

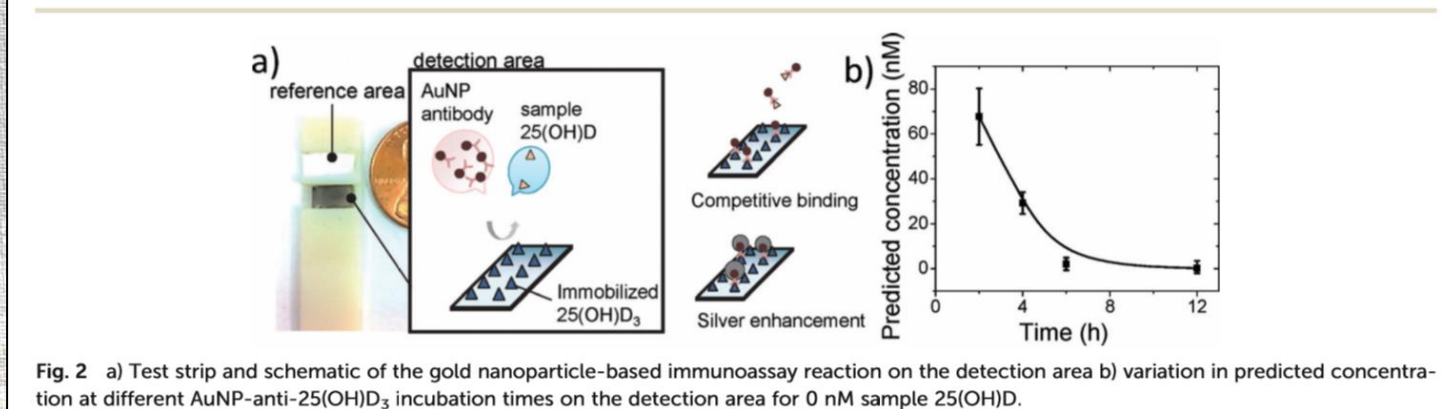


Fig. 2 a) Test strip and schematic of the gold nanoparticle-based immunoassay reaction on the detection area b) variation in predicted concentration at different AuNP-anti-25(OH)D₃ incubation times on the detection area for 0 nM sample 25(OH)D.



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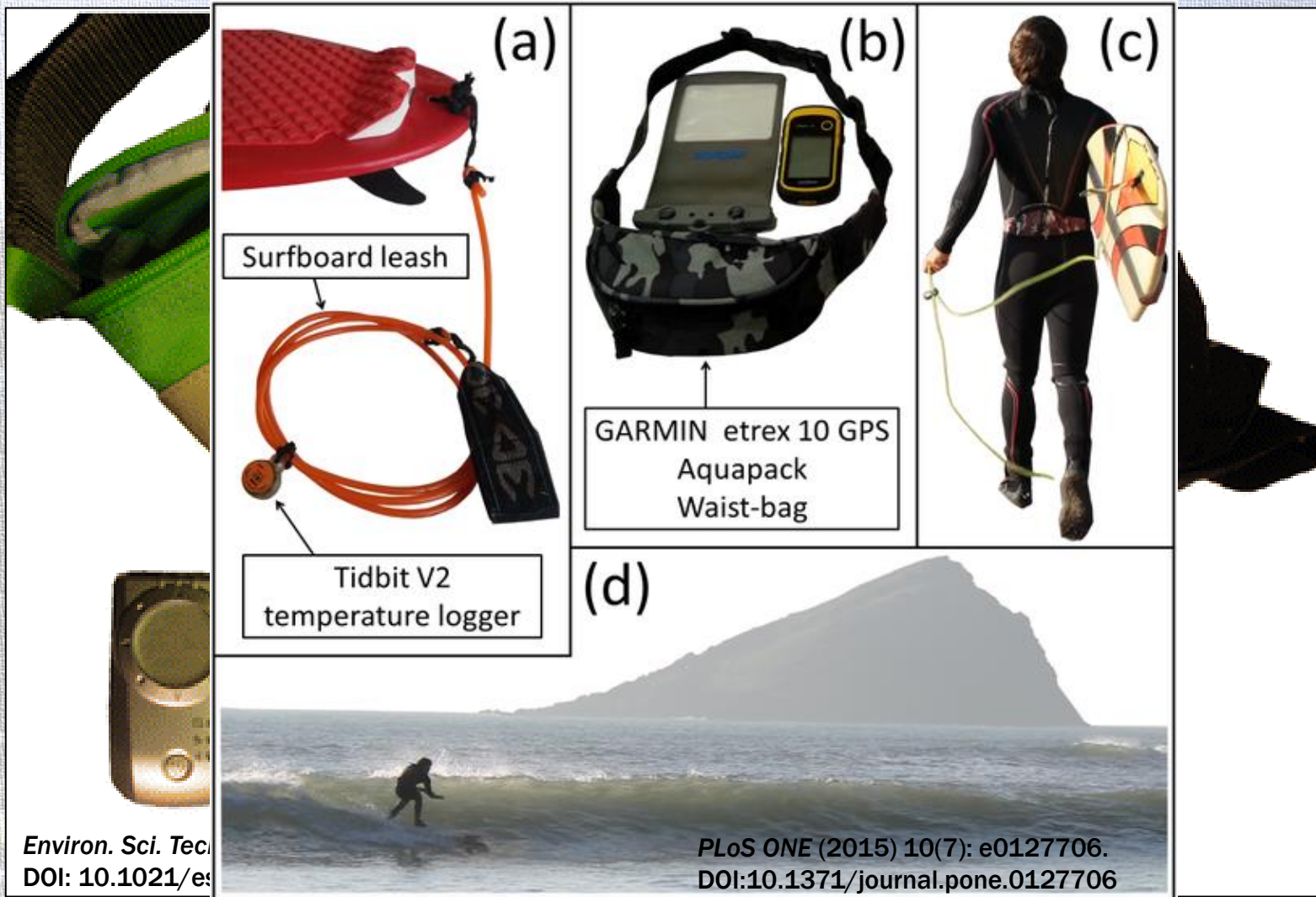
Mobile Laboratories



Environ. Sci. Technol. (2015), 49 , 2977–2982
DOI: 10.1021/es505362x



Mobile Laboratories





OPCW

Mobile Laboratories

Maps of city air.
Streets of people aware.

Denver Test:
3 cars
750 driving hours
150 million air quality data points



Google Earth Outreach



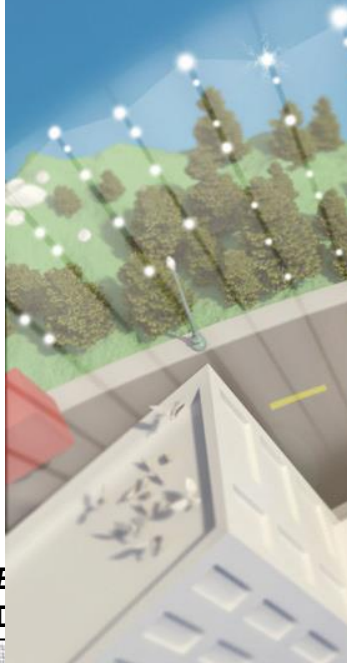
© 2015 aClima Inc



OPCW

Mobile Laboratories

Maps of city
Streets of p



FROM HEAD TO TOE WEARABLE TECHNOLOGY

SHIRT

Conductive thread means a computer is literally built into the fabric of the shirt, providing the processing power for all the other wearable gadgets.

WRISTBAND

A sensor that tracks movement to determine the number of steps taken through the day – 10,000 is ideal – and how much sleep the wearer gets at night.

TROUSERS

Also made with conductive thread, the trousers take the energy generated by movement and use it to power the other gadgets.



GLASSES

Overlays navigation directions and information about points of interest directly on to the wearer's field of vision.

WRISTWATCH

Vibrates when a message arrives and displays it on the watch face. Tells the time too.

HAND

Embedded under the skin is a chip containing medical records, passport data and credit records. Information is transferred by waving the hand over a suitable scanner.

SHOES

GPS chip provides directions using LED lights in each shoe: the left shoe indicates direction, while the right shows distance.

GRAPHIC: JOHN BRADLEY

points

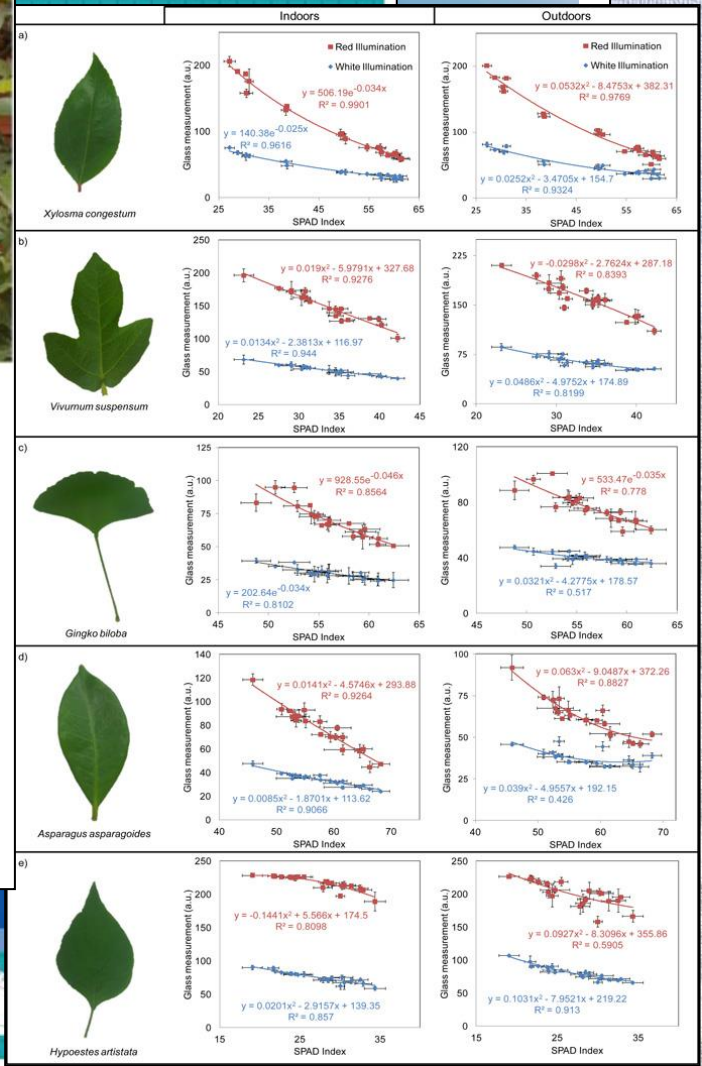
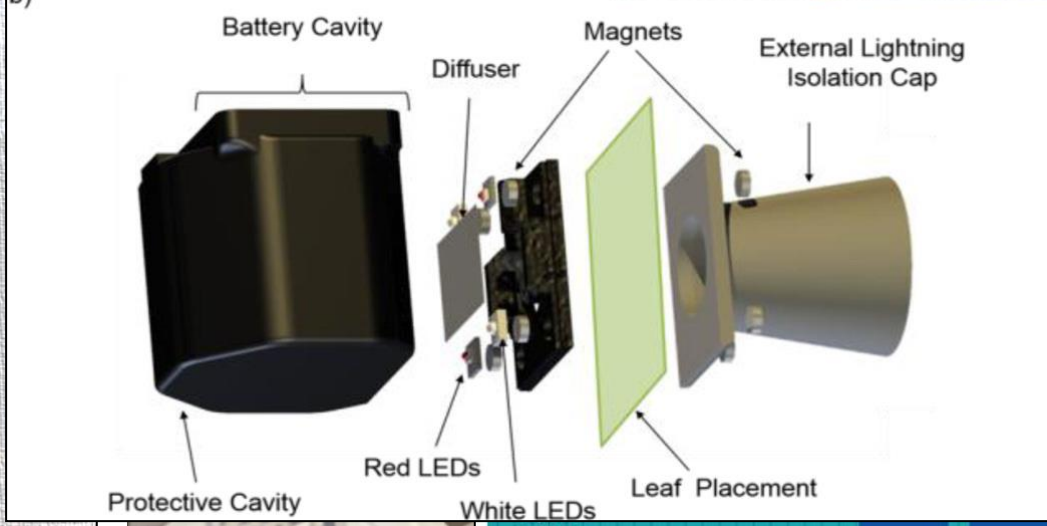
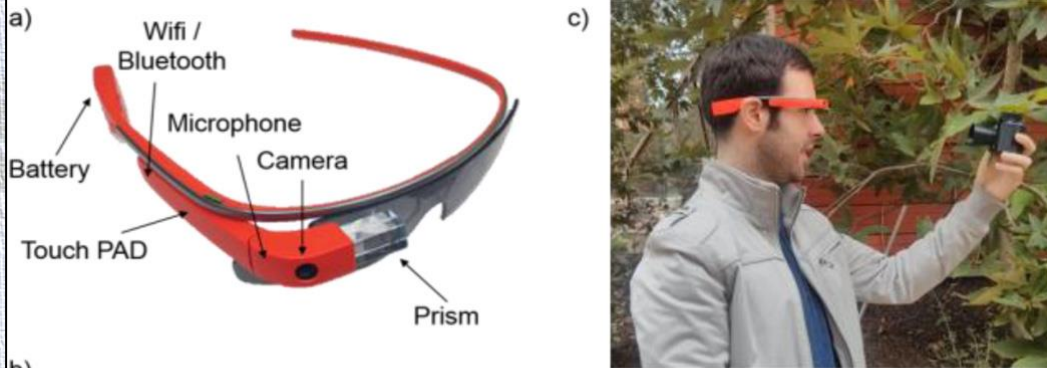




OPCW

Mobile Laboratories

FROM HEAD TO TOE WEARABLE TECHNOLOGY



Lab Chip. 2015 Apr 7; 15(7): 1708–1716

www.ncbi.nlm.nih.gov/pmc/articles/PMC4366296/



Environmental Chemical Signatures

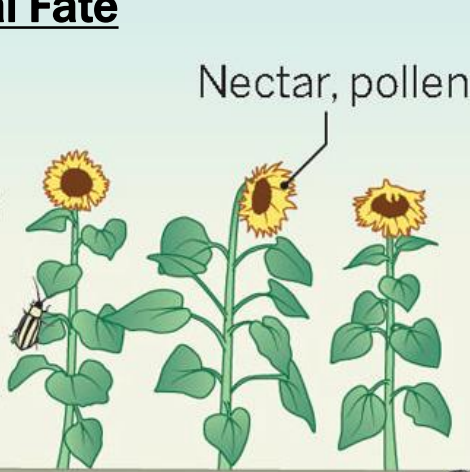
Environmental Fate

Target pests

- Sap sucking
- Burrowing
- Leaf miners

Plant uptake

2 to 20%



Nectar, pollen



Nontarget organisms



Direct poisoning



Food source depletion

Runoff

Seeds

Soil biota



Surface waters

Aquatic arthropods (insect larvae)

Leaching

Soil
80 to 98%



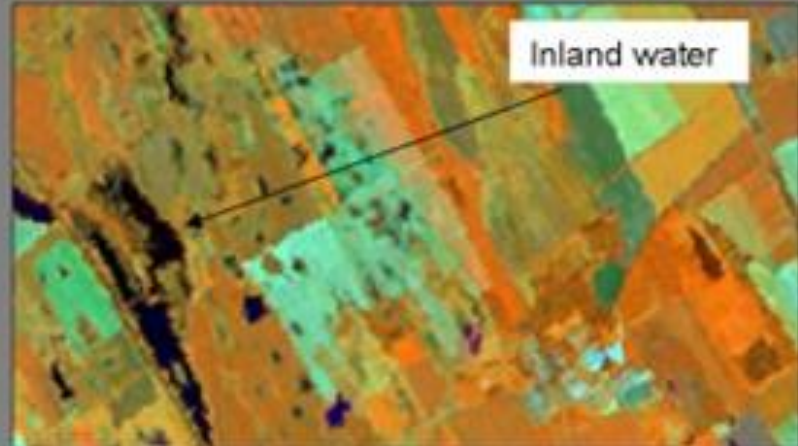
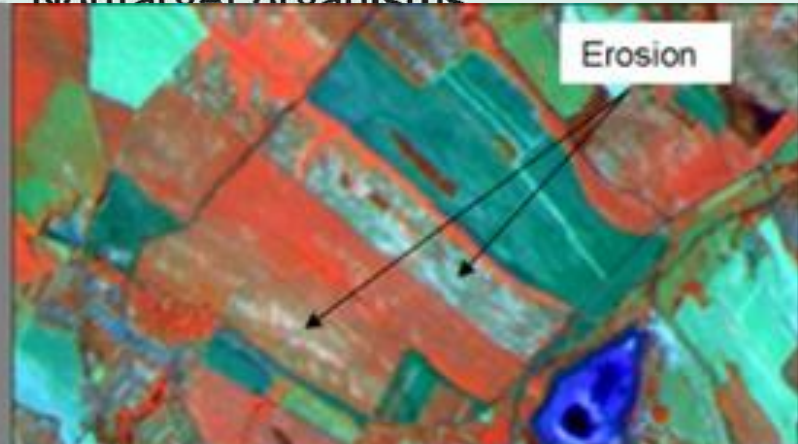
OPCW

Environmental Chemical Signatures

Environmental Fate



Nontarget organisms



http://www.tankonyvtar.hu/en/tartalom/tamop425/0027_DAI6/ch01s05.html



OPCW

Environmental Chemical Signatures

Environmental Fate



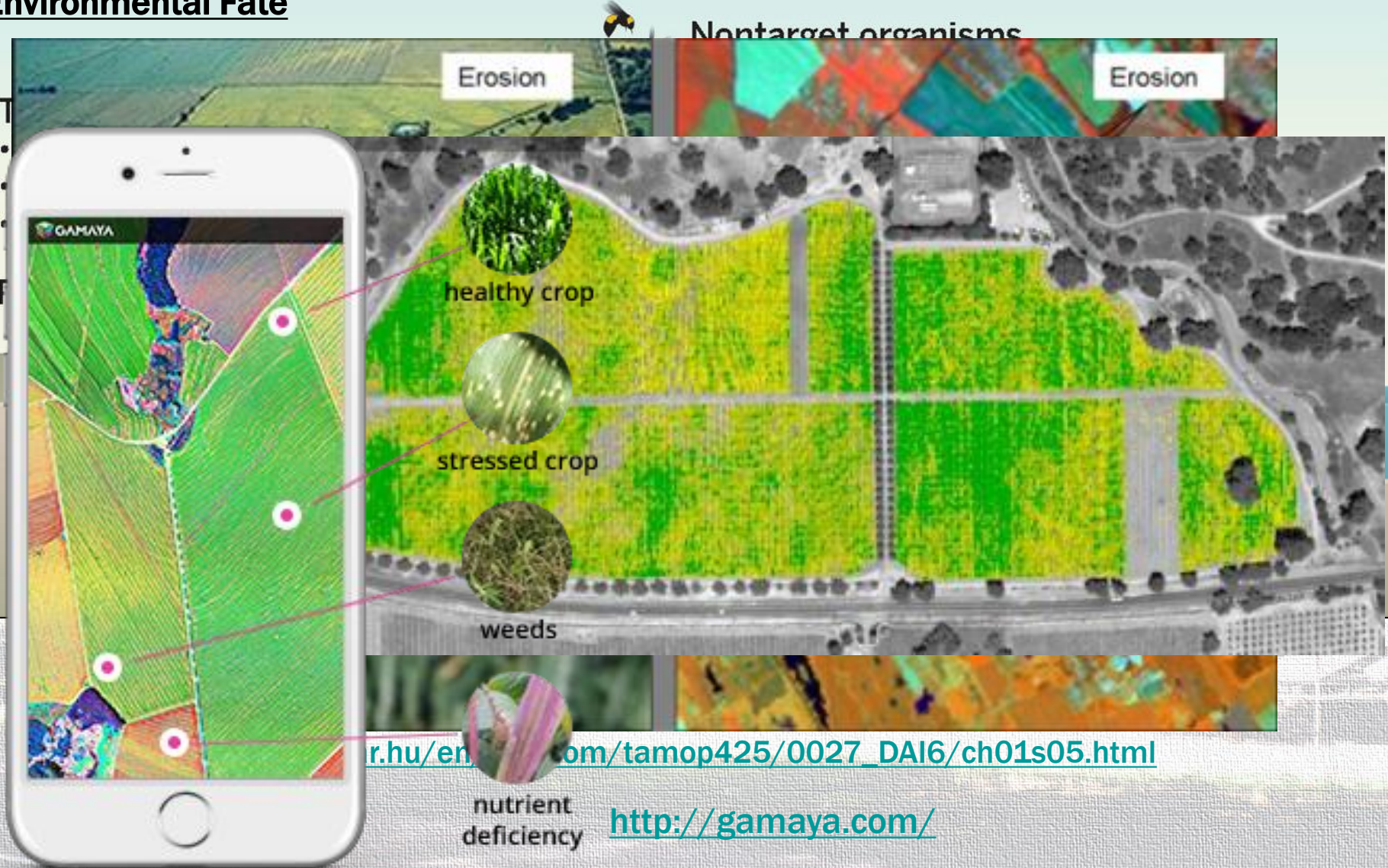
http://www.tankonyvtar.hu/en/tartalom/tamop425/0027_DAI6/ch01s05.html



OPCW

Environmental Chemical Signatures

Environmental Fate





OPCW

Environmental Chemical Signatures

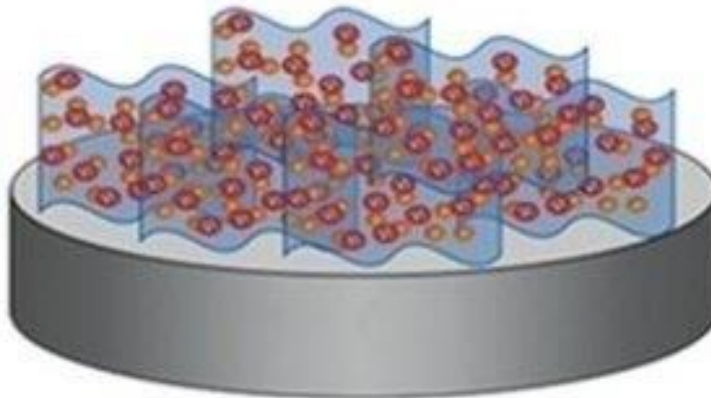
Environmental Fate



Nontarget organisms



Plant based biosensor for OP pesticides



Graphene nanosheets

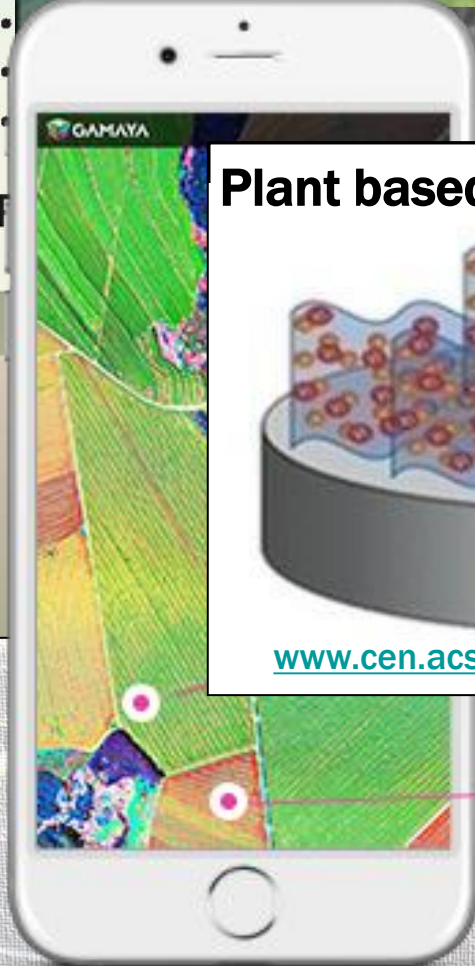


Gold nanoparticles



Plant esterase

www.cen.acs.org/articles/93/web/2015/12/Potentially-Cheaper-Way-Test-Food.html



www.gamaya.com/tamop425/0027_DAI6/ch01s05.html

nutrient
deficiency

<http://gamaya.com/>



OPCW

If Plants Could Talk...



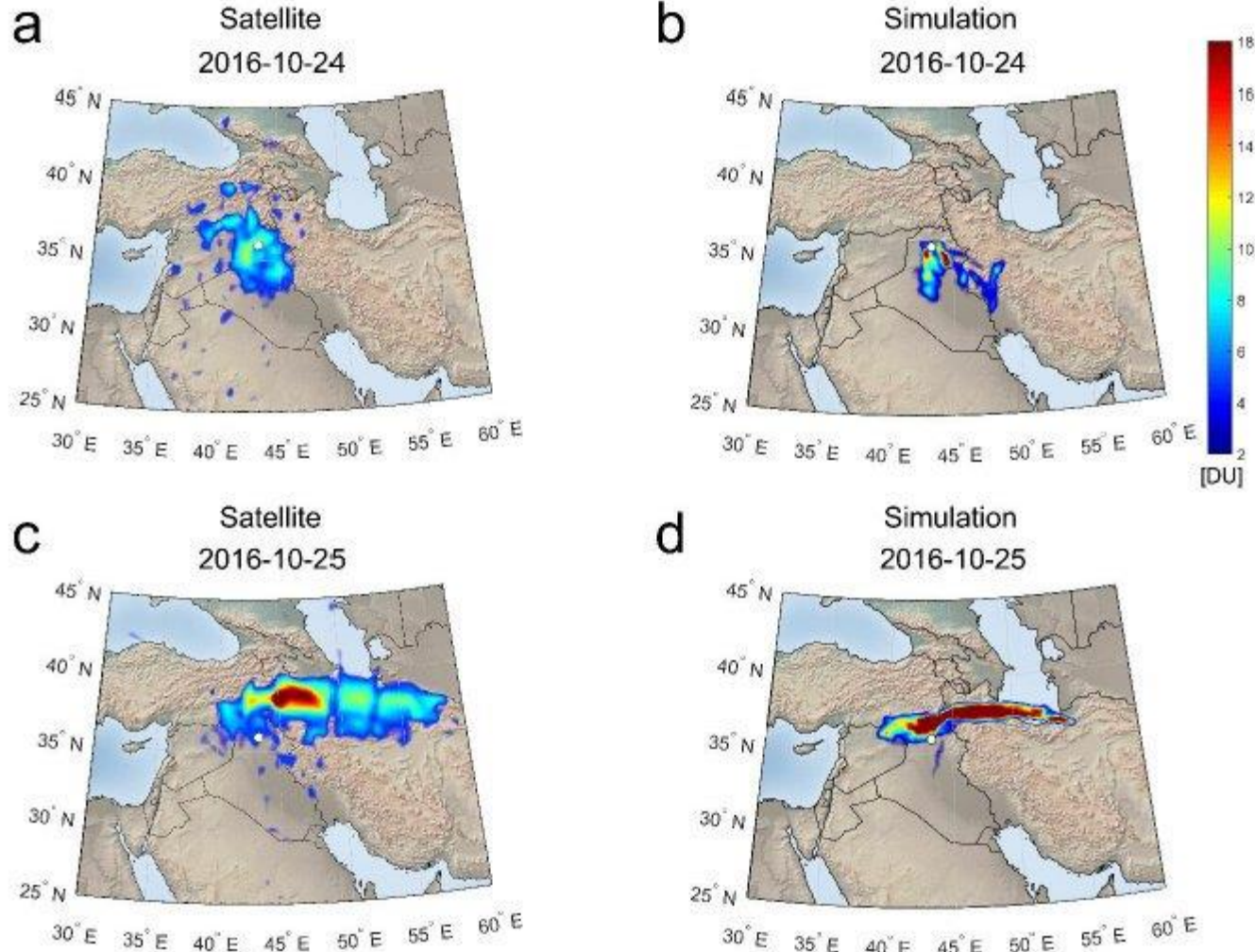
“The signs are that the bombs were made with the windows open but the net curtains taped to the walls to avoid being seen. The fumes had killed off the tops of plants just outside the windows”

- Report of the Official Account of the Bombings in London on 7th July 2005



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Monitoring Chemical Release by Satellite



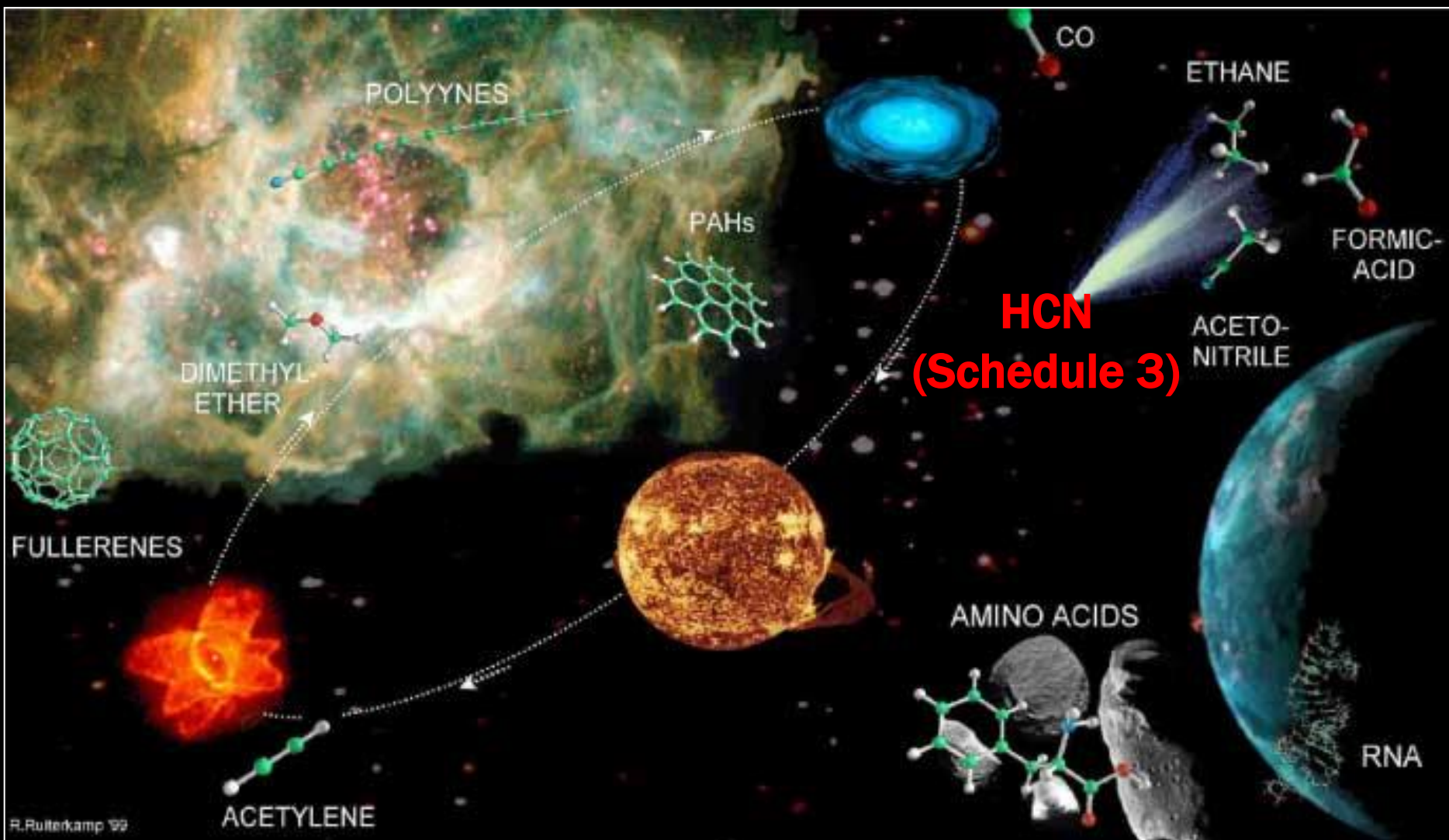
The 2016 Al-Mishraq sulphur plant fire: source and risk area estimation

<https://arxiv.org/abs/1611.03837>



OPCW

Decades of Detecting (Bio)Chemicals Across The Universe!





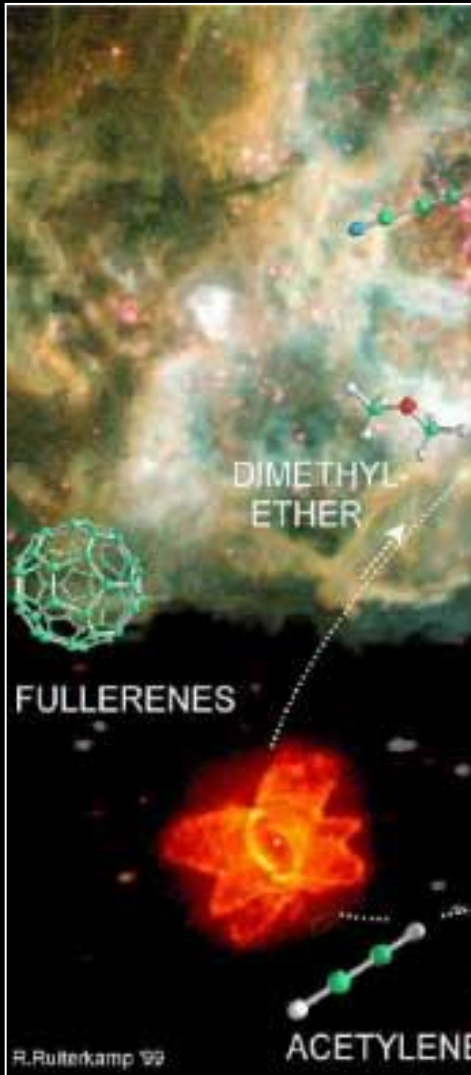
OPCW

Decades of Detecting (Bio)Chemicals Across The Universe!

3 Prospects for Observing Civilisation Destruction

<http://arxiv.org/ftp/arxiv/papers/1507/1507.08530.pdf>

Death Channel	Detection Method	Signature of Active Civilisation	Signature of Dead Civilisation	Detection Timescale (yr)
Nuclear Detonation	Gamma ray detection, Transit spectroscopy	Y	Y	0-5 years
Bioterrorism	Transit spectroscopy	Y	Y	1-30 years
Grey Goo	Transit spectroscopy and photometry	N	Y	>1,000 years
Stellar Pollution	Asteroseismology, stellar abundance studies	Y	Y	>100,000 years (depending on stellar convection)
Planetary Pollution	Transit spectroscopy (IR)	Y	Y	10-100,000 years
Orbital Pollution (Kessler Syndrome)	Transit spectroscopy and photometry	Y	Y	<100,000 years
Total Planetary Destruction	Debris Disk Imaging (IR)	Y	Y	<100,000 years





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Hyperspectral Images and Chemical Sensing: Satellites not required

AVAILABLE SENSORS

DR1000

Sensor ID	Chemical	Range	Lowest Detection	Resolution (ppm)
CD1	Carbon Dioxide - High Concentration	5,000 to 900,000 ppm	5000 ppm	100 ppm
CD2	Carbon Dioxide - Low Concentration	0-5000ppm	0 ppm	15 ppm
CO1	Carbon Monoxide (low Concentration)	500 ppm	15 ppm	5 ppm
CO2	Carbon Monoxide (high concentration)	10000 ppm	250 ppm	20 ppm
C11	Chlorine	20 ppm	200 ppb	20 ppb
E1	Ethylene Oxide	0-100 ppm	1 ppm	0.1 ppm
H1	Hydrogen	0-5000 ppm	1 ppm	0.8 ppm
HCL1	Hydrogen Chloride	100 ppm	0.1 ppm	0.1 ppm
HCY1	Hydrogen Cyanide	100 ppm	0.1 ppm	0.1 ppm
AM1	Ammonia	100 ppm	0 ppm	1 ppm
ON1	Ozone and Nitrogen Dioxide	O3- 20; NO2- 20 ppm	0 ppb	15 ppb
PH1	Phosphine (low Concentration)	10 ppm	0 ppm	30 ppb
PH2	Phosphine (high Concentration)	2000 ppm	5 ppm	2 ppm
HS1	Hydrogen Sulfide (low Concentration - ppb)	1 ppm	3 ppb	1 ppb
HS2	Hydrogen Sulfide (high Concentration - ppm)	2000 ppm	1 ppm	1 ppm
NO1	Nitrogen Oxide	100	0 ppm	0.1 ppm
CH1	Carbon Monoxide and Hydrogen Sulfide	CO 0-1000, H2S 0 - 100 ppm	0 ppm	CO 1, H2S 0.25 ppm
E2	Ethanol	0-500 ppm	0 ppm	1 ppm
MT1	Methane (LEL)	0-100% LEL	0 ppm	1% LEL
NC1	Nitric Oxide (low Concentration)	20 ppm	0 ppm	80 ppb
NC2	Nitric Oxide (High Concentration)	5000 ppm	0 ppm	1 ppm
ND1	Nitrogen Dioxide (Low Concentration)	20 ppm	0 ppm	0.02 ppm
ND2	Nitrogen Dioxide (high Concentration)	200 ppm	0 ppm	0.1 ppm
O1	Oxygen	0-20%	0 ppm	0.10%
O2	Oxygen	0-100%	0 ppm	1%
PD1	Total VOCs (ppb) - PID	50 ppm (isobutylene)	0 ppm	1 (ppb isobutylene)
PD2	Total VOCs (ppm) - PID	300 ppm (isobutylene)	1 ppm	0.1 (ppm isobutylene)
SD1	Sulfur Dioxide (high Concentration)	2000 ppm	0 ppm	2 ppm
SD2	Sulfur Dioxide (low Concentration)	20 ppm	0 ppb	20 ppb
FM1	Formaldehyde	10 ppm	0.01 ppm	0.01 ppm
PM 1-10	Particulate PM 1, 2.5, 10	0-10,000 Particles/Sec	PM 1	N/A





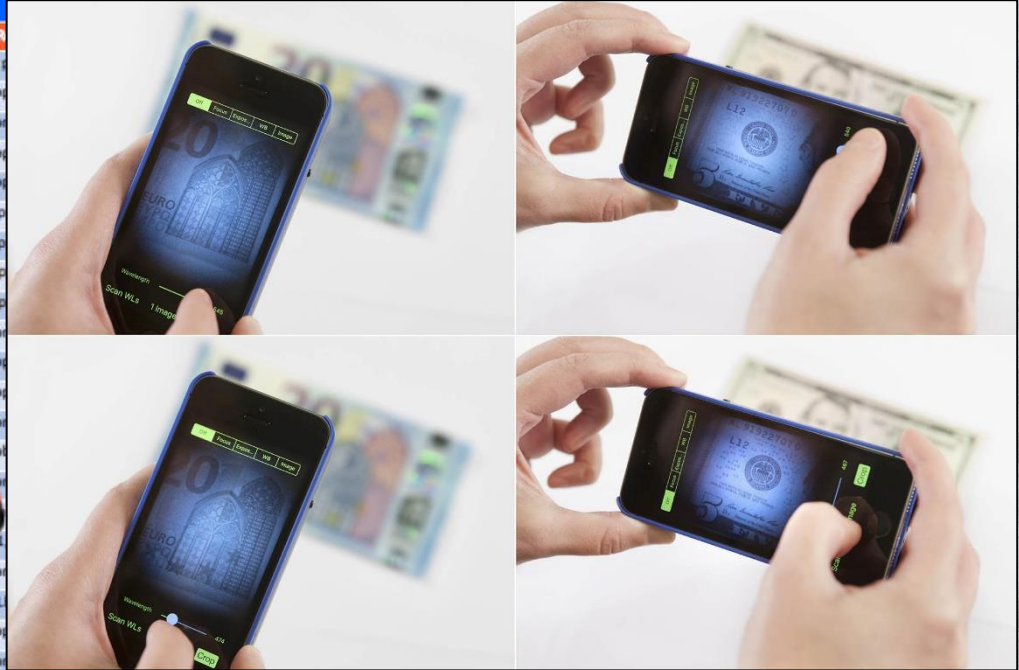
Hyperspectral Images and Chemical Sensing: Satellites not required

AVAILABLE SENSORS DR1000

Sensor ID	Chemical	Range	Lowest Detection	Resolution
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CO1	Carbon Monoxide (low Concentration)	500 ppm	15 ppm	5 ppm
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H1	Hydrogen	0-5000 ppm	1 ppm	0.8 ppm
HCL1	Hydrogen Chloride	100 ppm	0.1 ppm	0.1 ppm
HCY1	Hydrogen Cyanide	100 ppm	0.1 ppm	0.1 ppm
AM1	Ammonia	100 ppm	0 ppm	1 ppm
ON1	Ozone and Nitrogen Dioxide	0.3- 20; NO	0 ppb	15 ppm
PH1	Phosphorus (atmospheric)	10 ppm	30 ppm	30 ppm
PH2	Phosphorus (soil)	20 ppm	2 ppm	2 ppm
HS1	Hydrogen Sulfide (atmospheric - ppb)	20 ppm	1 ppm	1 ppm
HS2	Hydrogen Sulfide (soil - ppm)	20 ppm	1 ppm	1 ppm
NO1	Nitrogen Dioxide (atmospheric - ppb)	20 ppm	1 ppm	1 ppm
NO2	Nitrogen Dioxide (soil - ppm)	20 ppm	1 ppm	1 ppm
NC1	Nitrate (atmospheric - ppb)	20 ppm	1 ppm	1 ppm
NC2	Nitrate (soil - ppm)	20 ppm	1 ppm	1 ppm
ND1	Nitrate (atmospheric - ppb)	20 ppm	0.02 ppm	0.02 ppm
ND2	Nitrate (soil - ppm)	20 ppm	0.1 ppm	0.1 ppm
O1	Oxygen	15-20%	0 ppm	0.10%
O2	Oxygen	0-100%	0 ppm	1%
PD1	Total VOCs (ppb) - Formaldehyde	50 ppm (isobutylene)	0 ppm	1 (ppb isobutylene)
PD2	Total VOCs (ppm) - Formaldehyde	300 ppm (isobutylene)	1 ppm	0.1 (ppm isobutylene)
SD1	Sulfur Dioxide (high Concentration)	2000 ppm	0 ppm	2 ppm
SD2	Sulfur Dioxide (low Concentration)	20 ppm	0 ppb	20 ppb
FM1	Formaldehyde	10 ppm	0.01 ppm	0.01 ppm
PM 1-10	Particulate PM 1, 2.5, 10	0-10,000 Particles/Sec	PM 1	N/A



DR1000

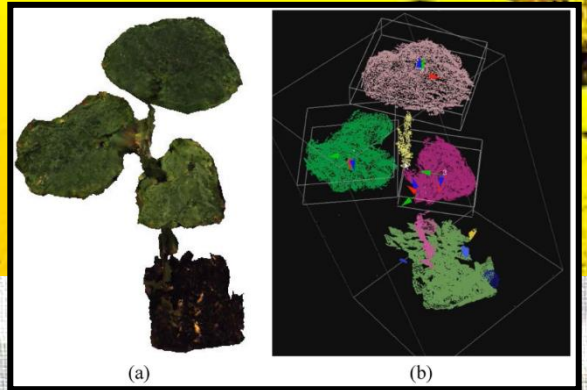
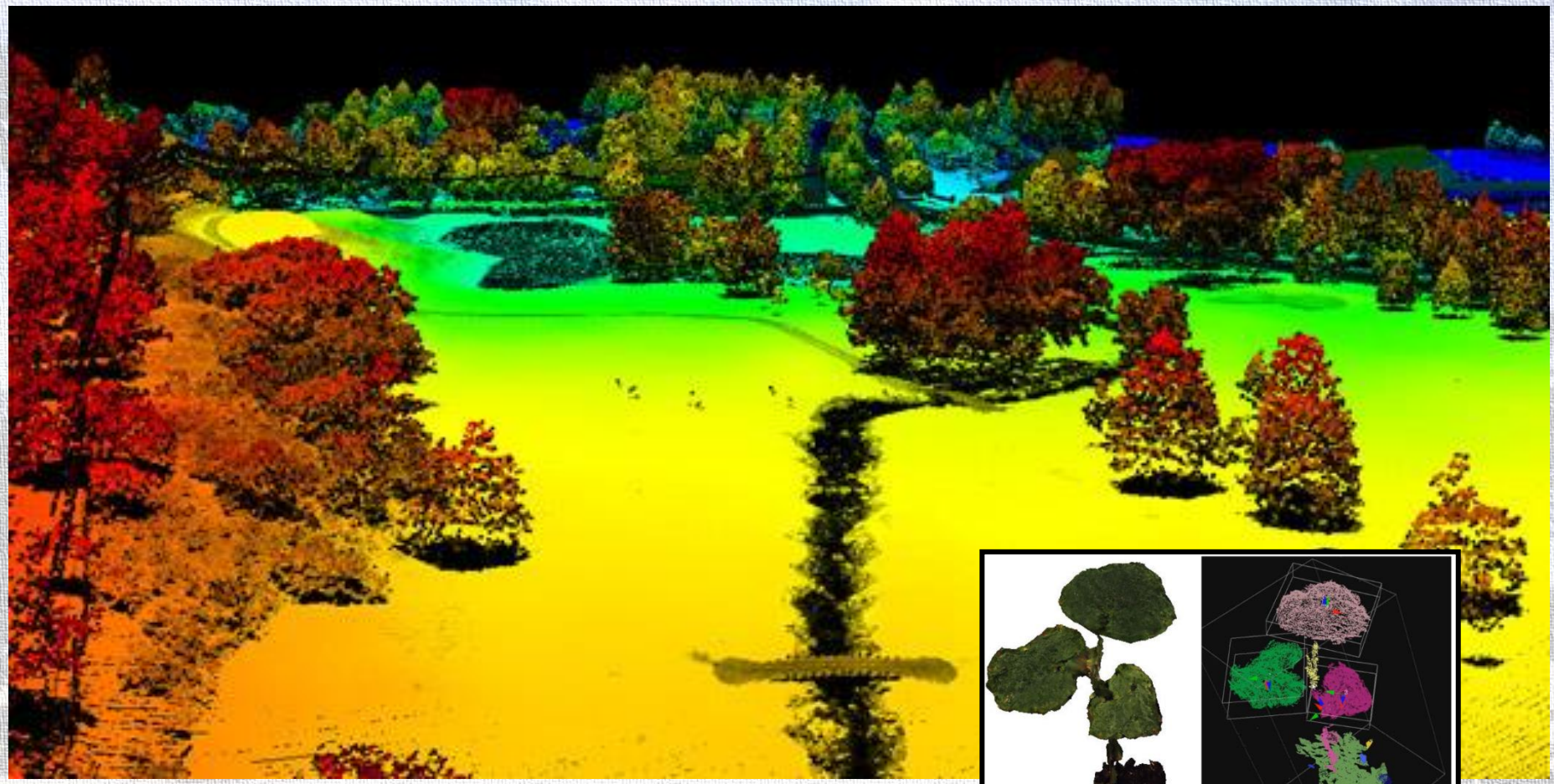


<http://www.vttresearch.com/>

[https://www.parrot.com/fr/solutions-pro/parrot-sequoia#parrot-sequoia-](https://www.parrot.com/fr/solutions-pro/parrot-sequoia#parrot-sequoia)

Integrated Data Streams

(3D and visual images, sensor data, spectral data, external databases)

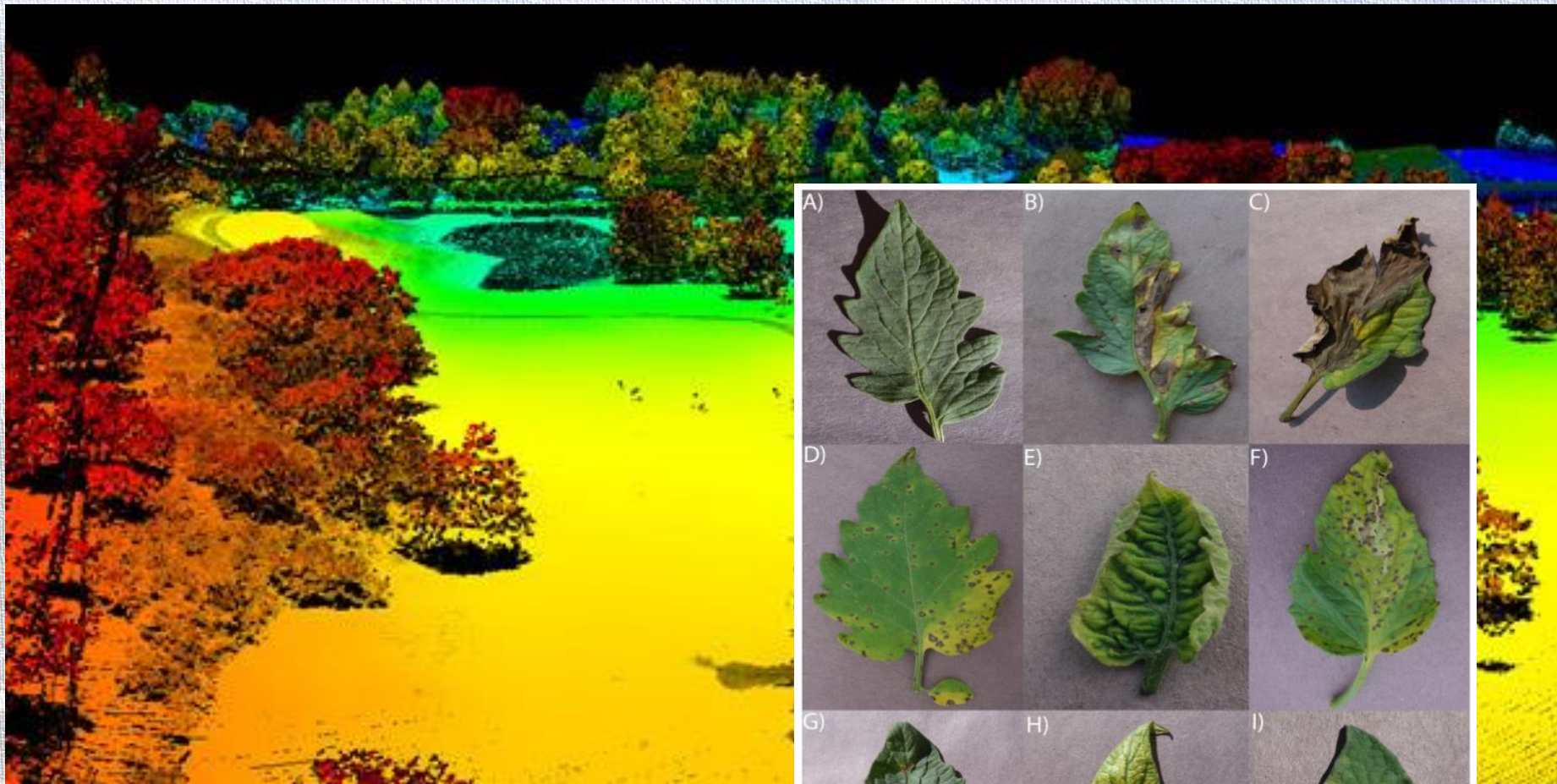




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Integrated Data Streams

(3D and visual images, sensor data, spectral data, external databases)



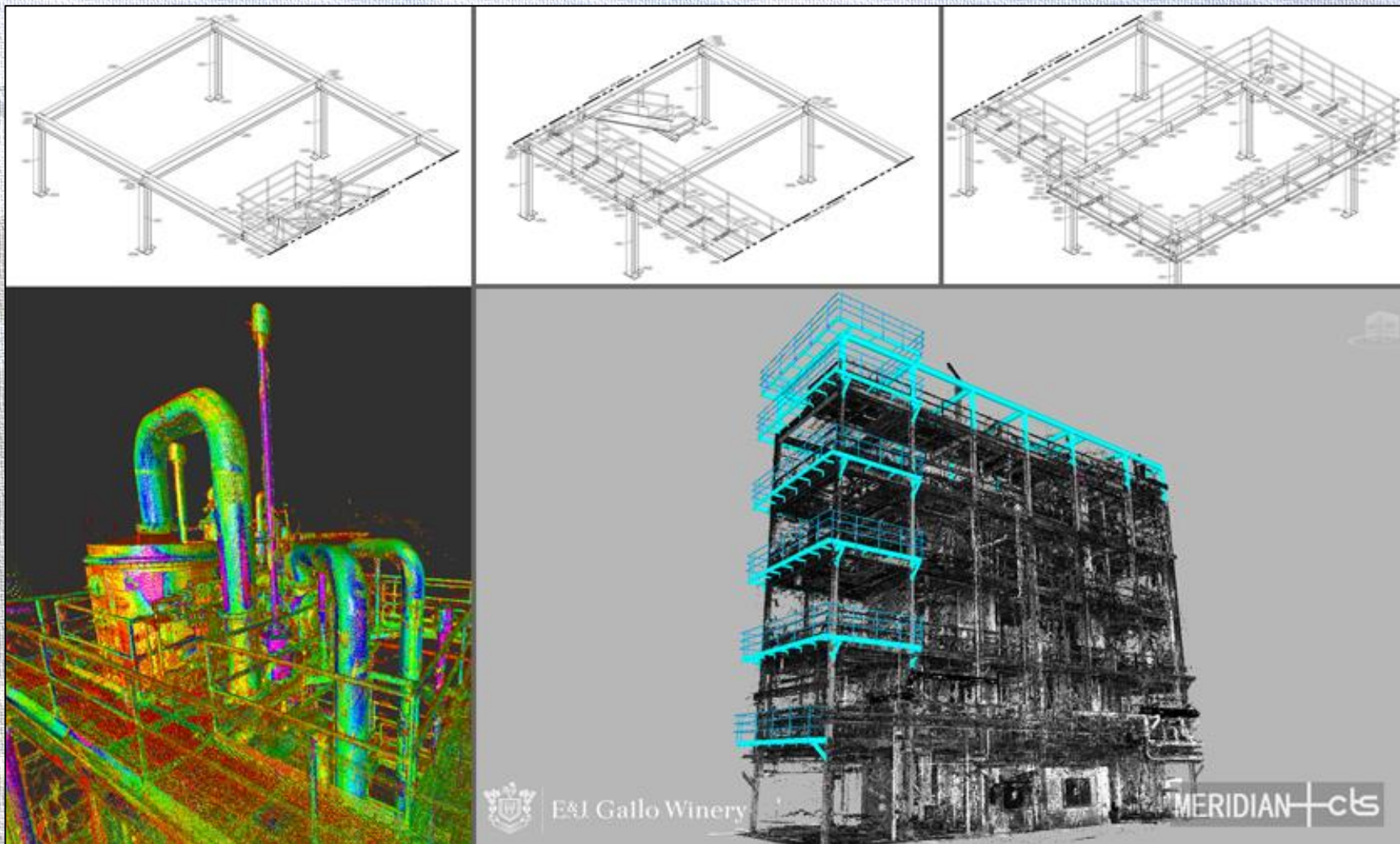
An open access repository of images on plant health to enable the development of mobile disease diagnostics

<https://arxiv.org/abs/1511.08060>



OPCW

Imaging of Complex Structures



E&J Gallo Winery

MERIDIAN+cts



OPCW

Imaging of Complex Structures and a capability to Inspect

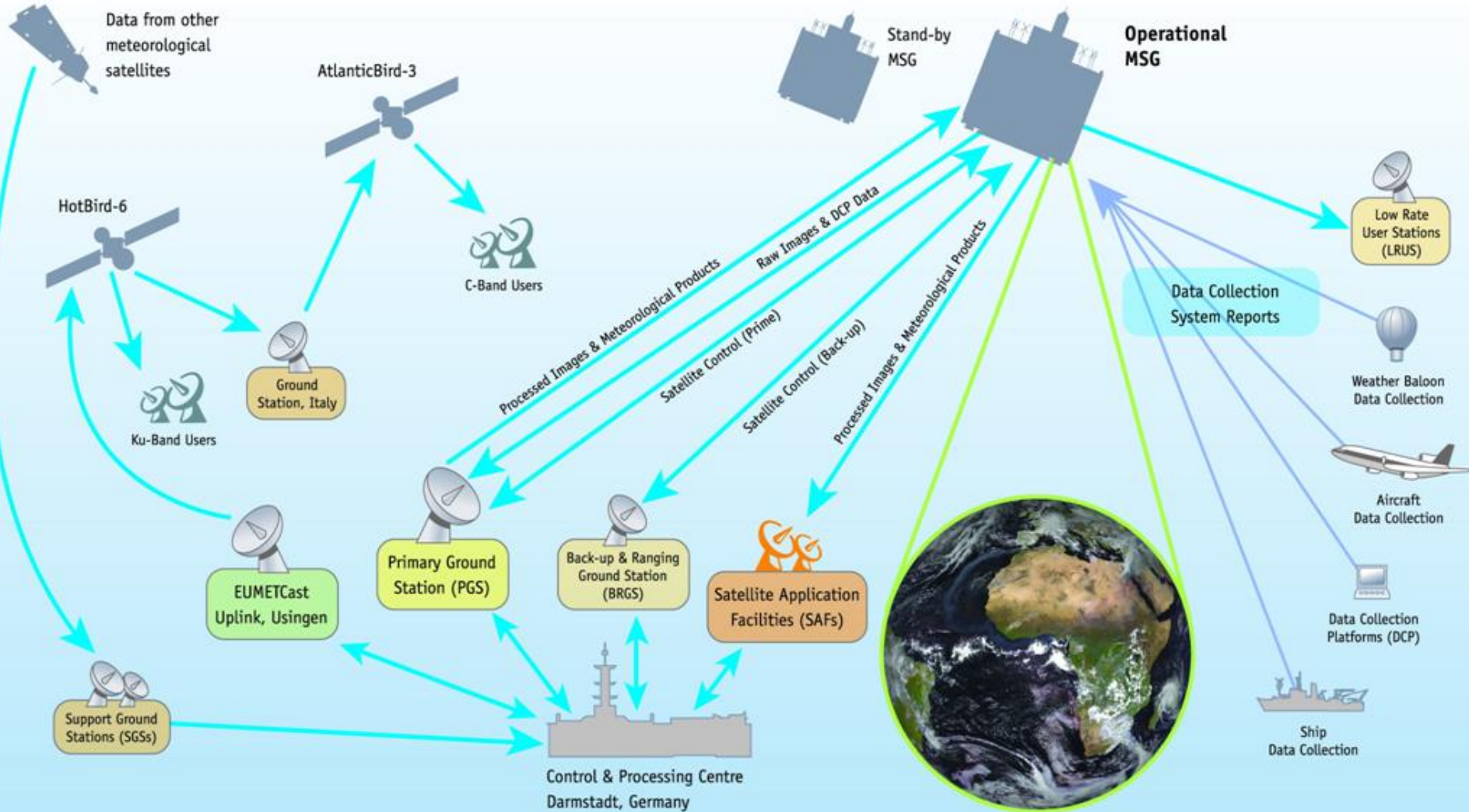


Ed. Gano winery

MENDIAN

cts

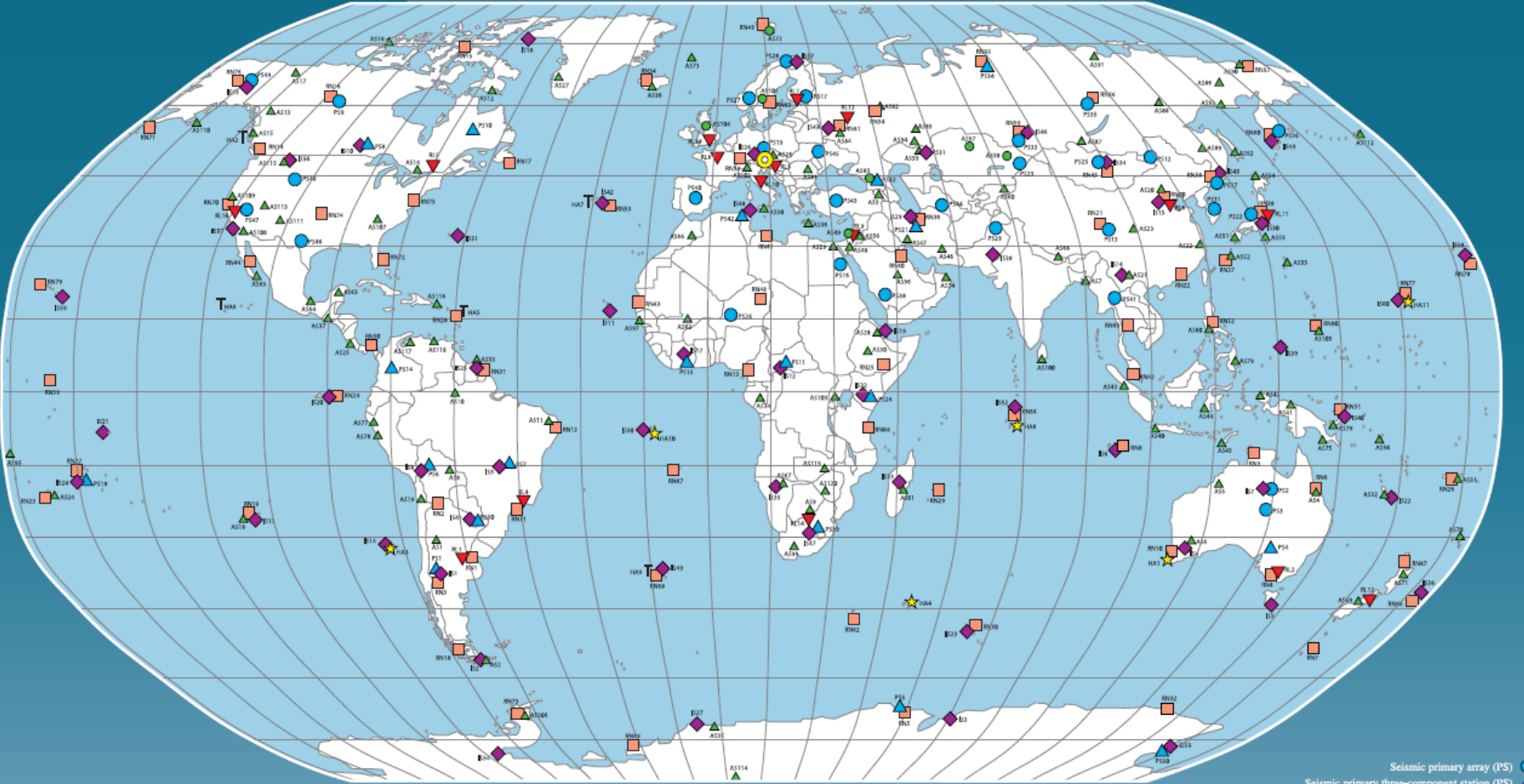
Data Collection on Global Scale





OPCW

Data Collection on Global Scale



The Comprehensive Nuclear-Test-Ban Treaty (CTBT) of 1996 bans nuclear explosions in all environments. Explosions in the atmosphere, under water and in outer space were banned in 1963. CTBT prohibits them underground as well.

Under CTBT, a global system of monitoring stations, using four complementary technologies, is being established to record data necessary to verify compliance with the Treaty. Supported by 16 radionuclide laboratories, this network of 321 monitoring stations will be capable of registering shock waves emanating from a nuclear explosion underground, in the seas and in the air, as well as detecting radioactive debris released into the atmosphere. The location of the stations has been carefully chosen for optimal and cost-effective global coverage.

The monitoring stations will transmit, via satellite, the data to the International Data Centre (IDC) within CTBTO PrepCom in Vienna, where the data will be used to detect, locate and characterize events.

These data and IDC products will be made available to the States Signatories for final analysis.

Overleaf is a listing of the 337 facilities of the international monitoring system and brief descriptions of their characteristics and capabilities.

- Seismic primary array (PS)
- Seismic primary three-component station (PS)
- Seismic auxiliary array (AS)
- Seismic auxiliary three-component station (AS)
- Hydroacoustic (hydrophone) station (HA)
- Hydroacoustic (T-phase) station (HA)
- Infrasound station (IS)
- Radionuclide station (RN)
- Radionuclide laboratory (RL)
- International Data Centre, CTBTO PrepCom, Vienna

The boundaries and presentation of material on this map do not imply the expression of any opinion on the part of the Provisional Technical Secretariat of the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO PrepCom) concerning the legal status of any country, territory, city or area or its authorities, or concerning the delimitation of its frontiers or boundaries.



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Data with Chemical (and Biological) Relevance is Collected too



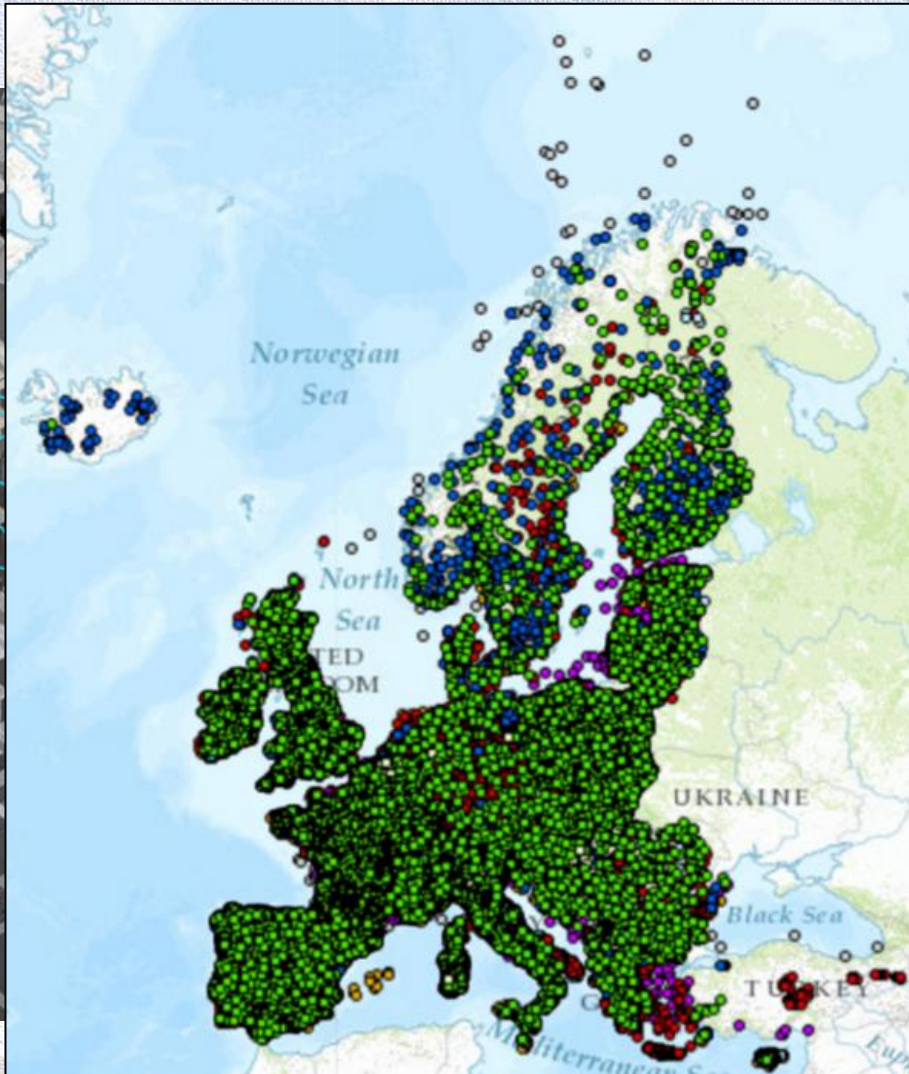
The Array of Things

<https://arrayofthings.github.io/>



OPCW

Data with Chemical (and Biological) Relevance is Collected too



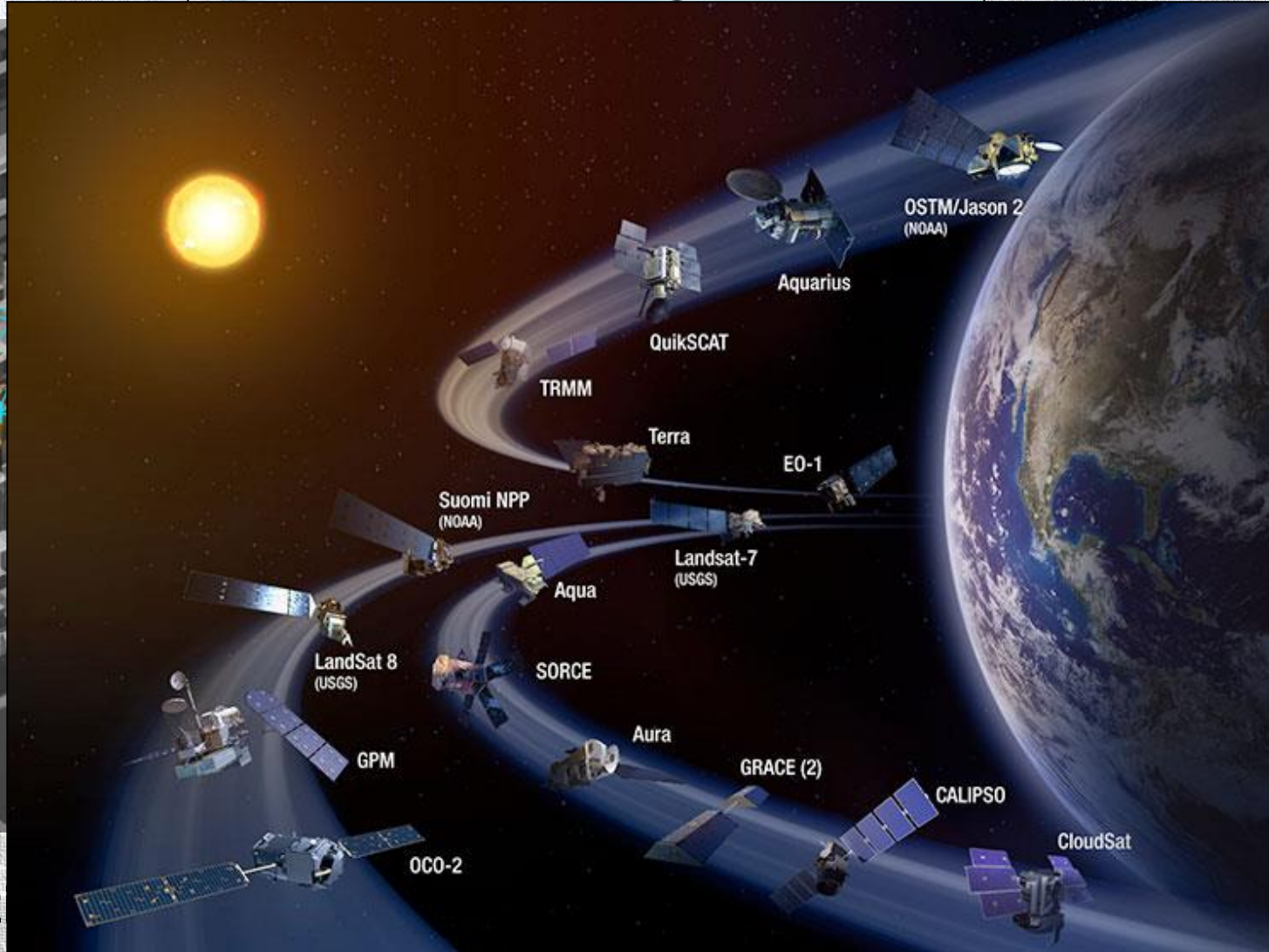
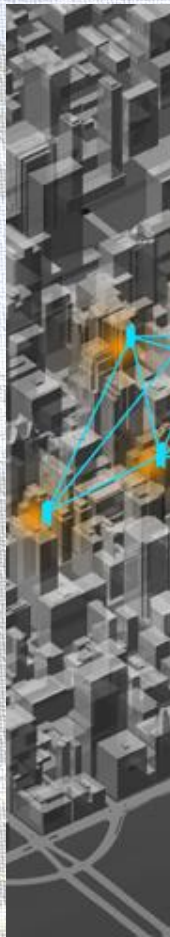
Array of Things

arrayofthings.github.io/

Stations reporting water quality data in 2016 in the EU

<http://www.eea.europa.eu/themes>

Data with Chemical (and Biological) Relevance is Collected too

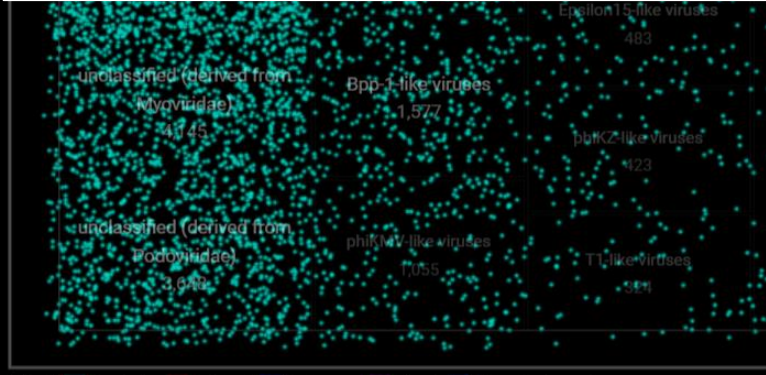
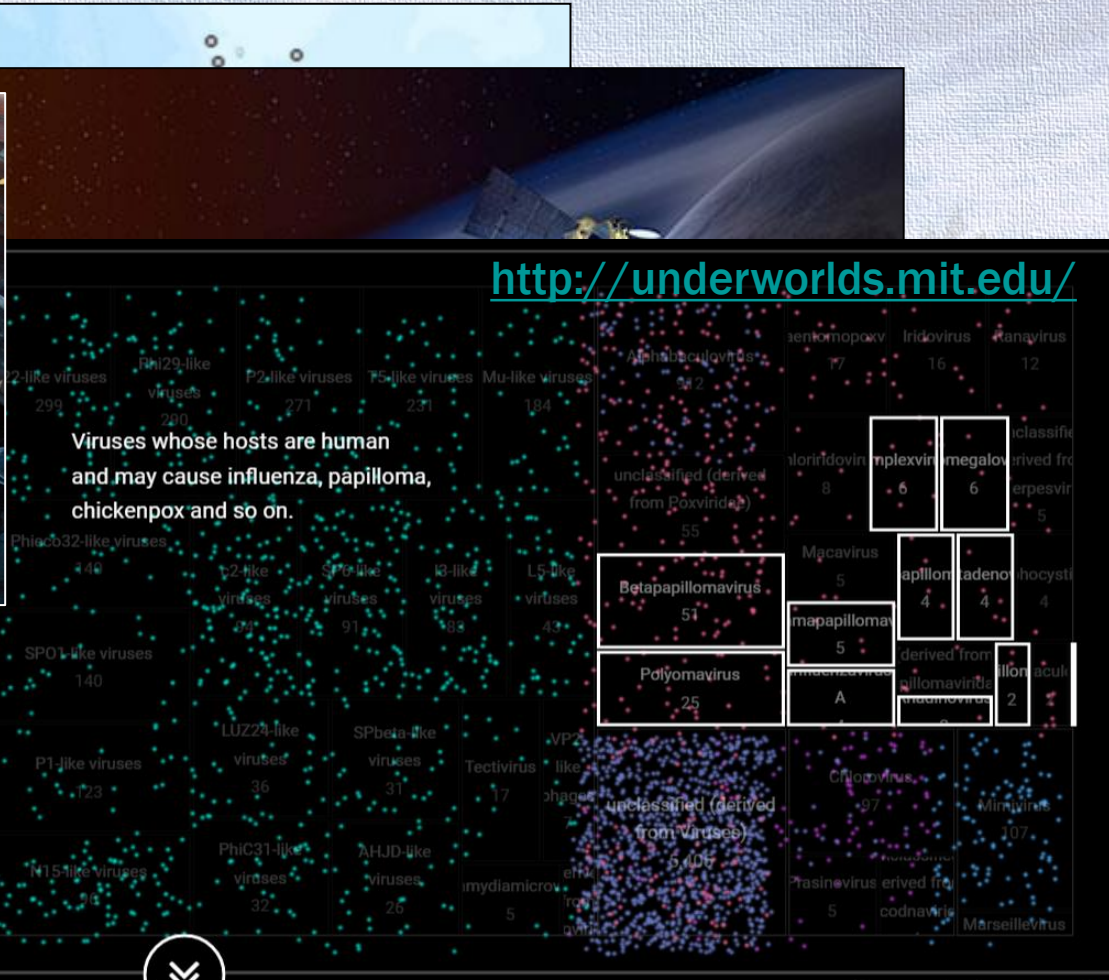


Stat

<http://www.eea.europa.eu/themes>

<http://www.eea.europa.eu/themes>

Data with Chemical (and Biological) Relevance is Collected too



Host ■ Bacteria ■ Animal ■ Unknown ■ Plant ■ Other Eukaryote



In a sample of sewage water

Virus Treemap

Human Virus

Stat



OPCW

The Value is the Data





OPCW

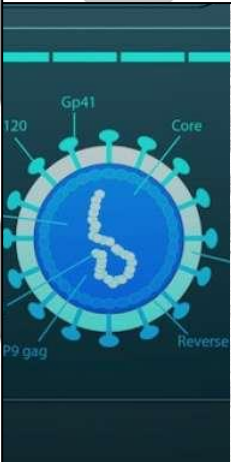
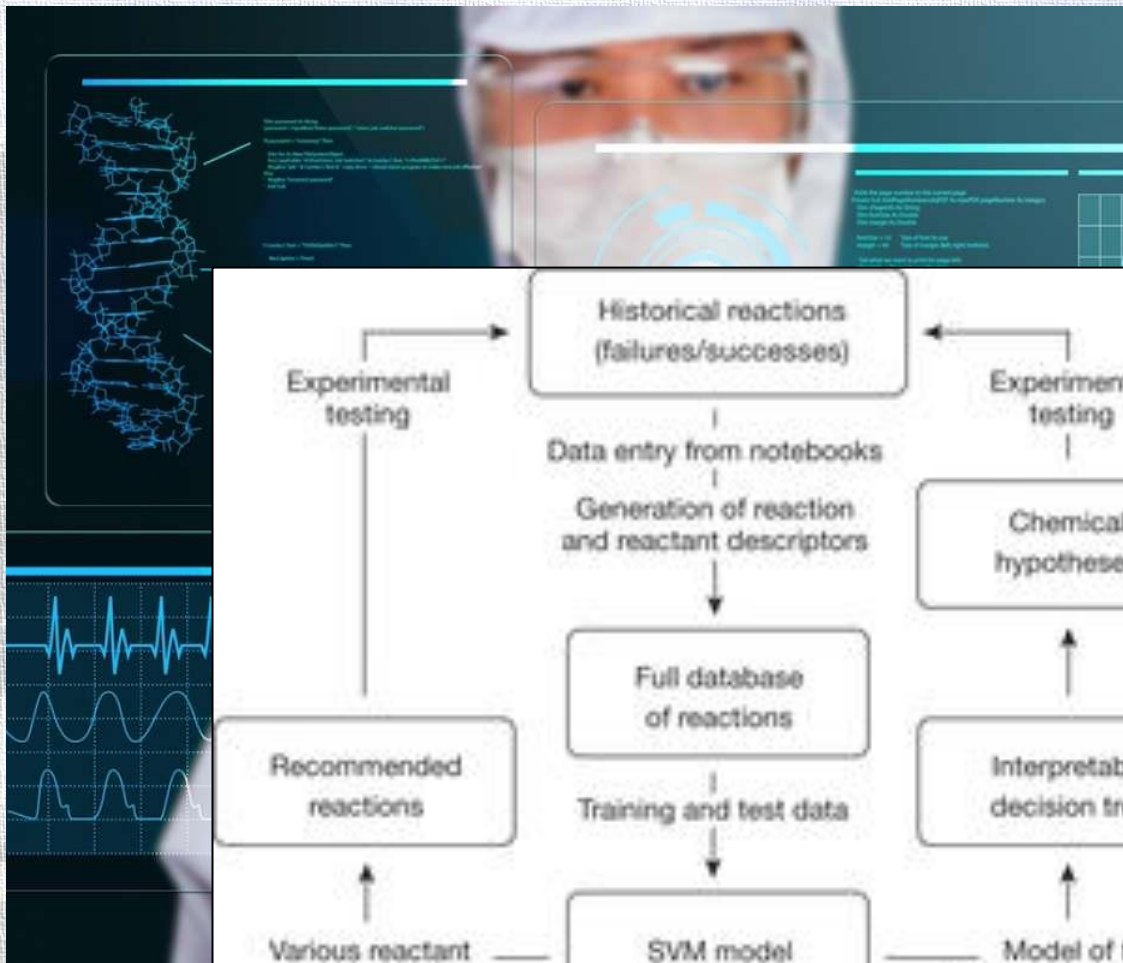
To Make Use of it All, Data Streams Must be Harnessed and Integrated



Artificial Intelligence, Chemistry, Life Sciences and Medicine

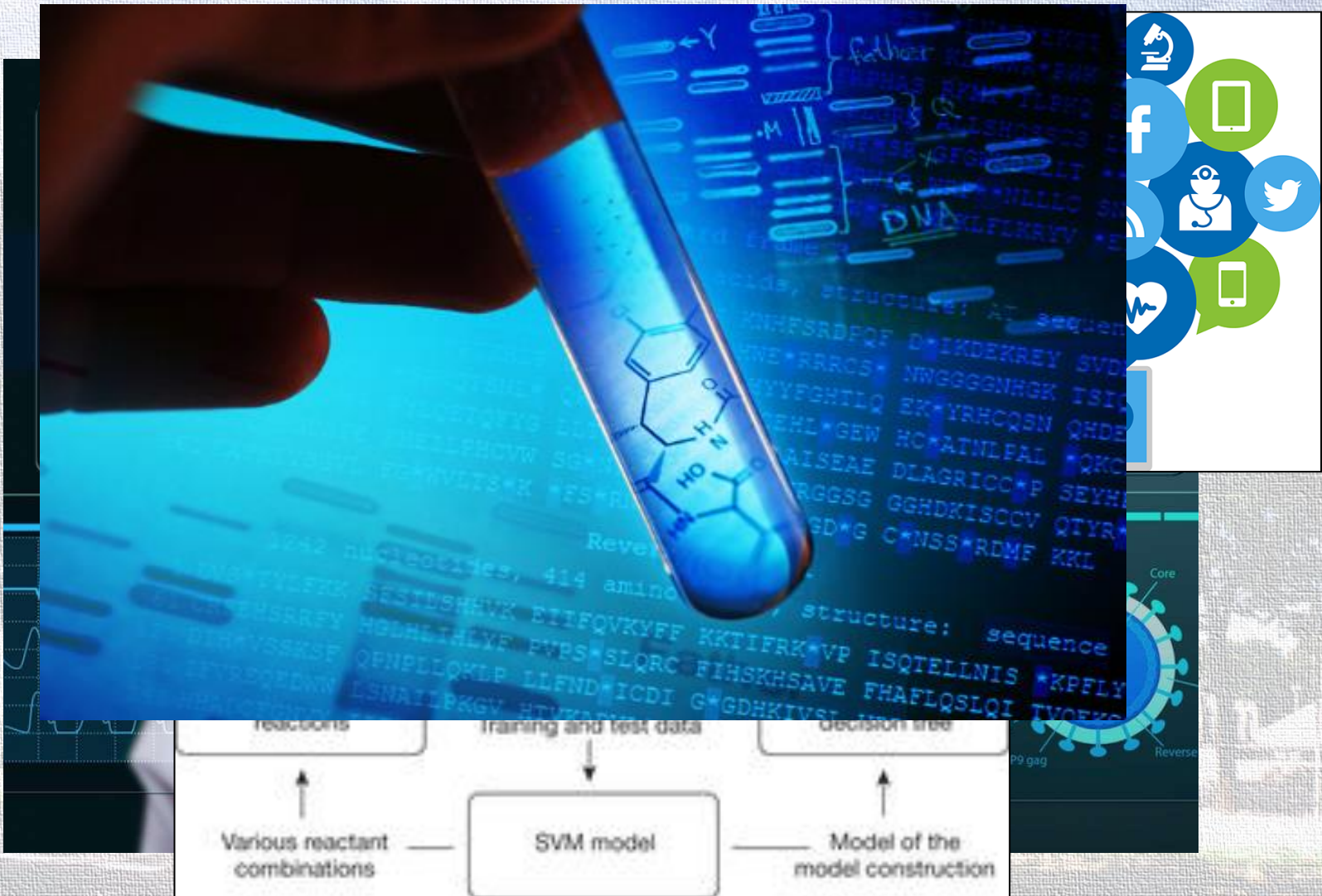


Artificial Intelligence, Chemistry, Life Sciences and Medicine



<http://www.nature.com/nature/journal/v533/n7601/full/nature17439.html>

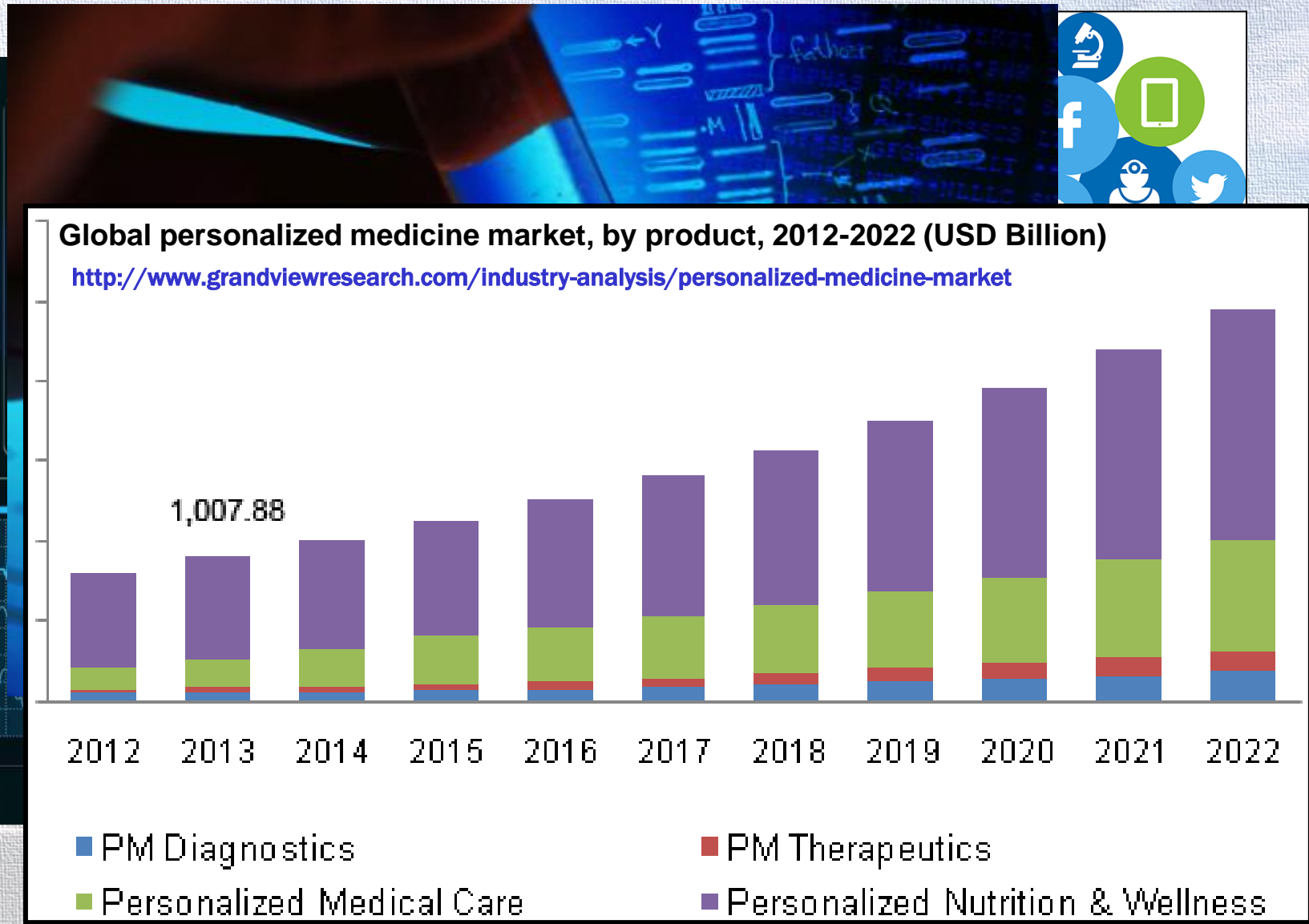
Artificial Intelligence, Chemistry, Life Sciences and Medicine



The image features a hand holding a test tube with a chemical structure overlaid on it. The background is a collage of scientific data, including DNA sequences and chemical structures. To the right, there is a vertical strip of social media icons (Facebook, Twitter, etc.) and a diagram of a virus. Below the main image is a flowchart illustrating the process of model construction and training.

```
graph TD; A[Various reactant combinations] --> B[reactions]; B --> C[training and test data]; C --> D[SVM model]; D --> E[Model of the model construction]; E --> F[Decision area];
```

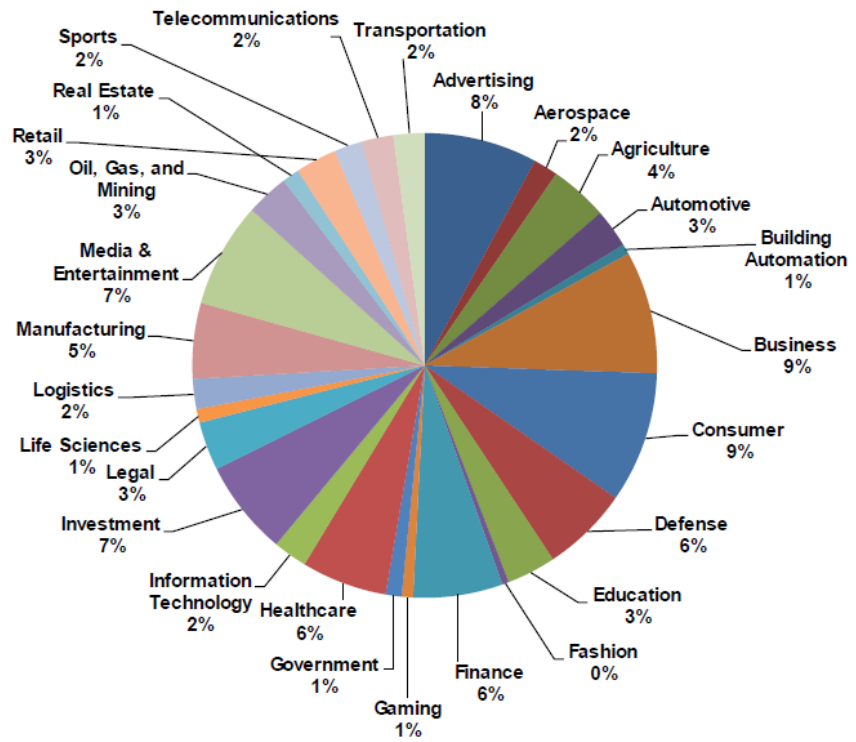
Artificial Intelligence Chemistry, Life Sciences and Medicine



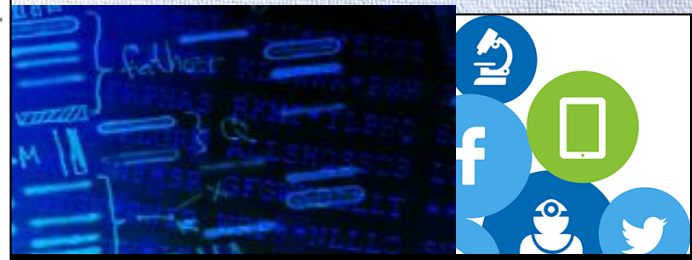
Artificial Intelligence, Chemistry, Life Sciences and Medicine



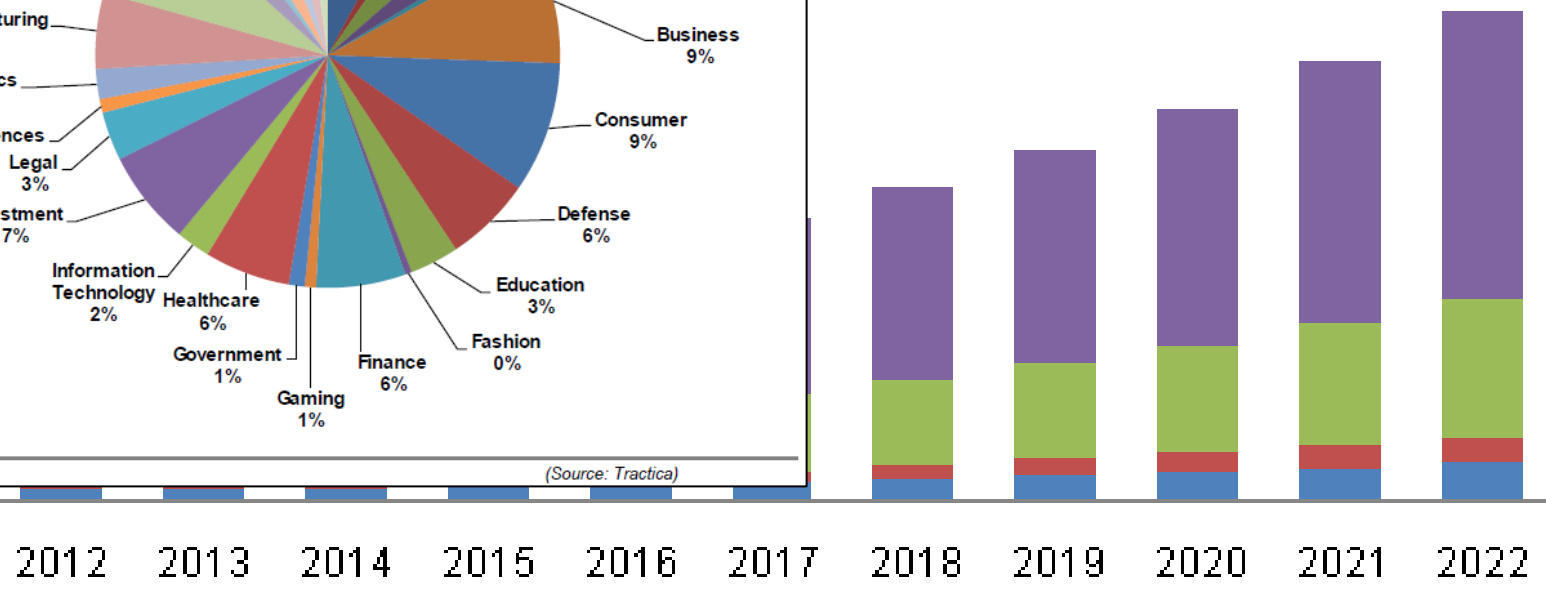
Chart 2.5 Artificial Intelligence Revenue Share by Industry, World Markets: 2025



(Source: Tractica)



Product, 2012-2022 (USD Billion)
Personalized-medicine-market



■ PM Diagnostics

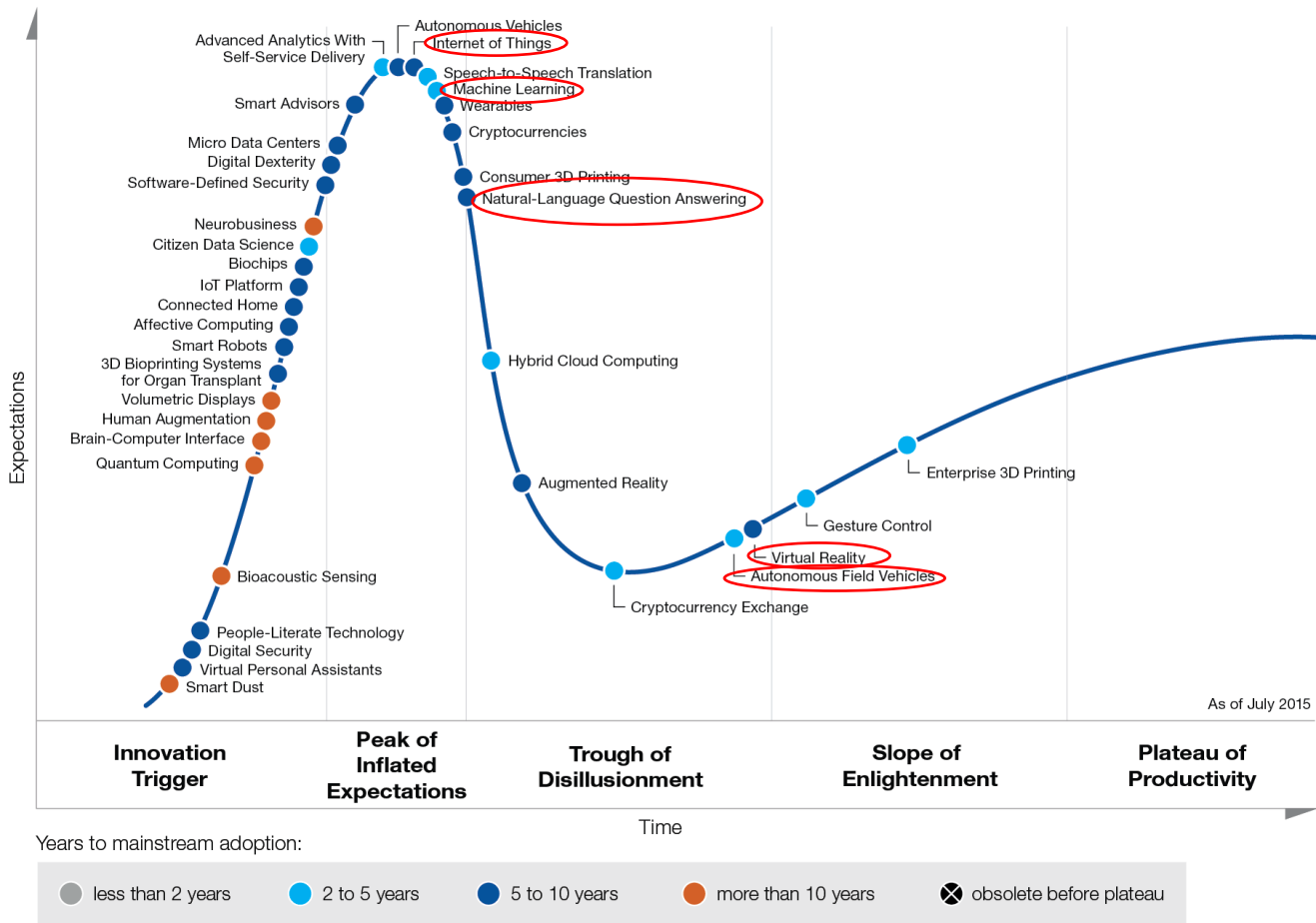
■ PM Therapeutics

■ Personalized Medical Care

■ Personalized Nutrition & Wellness

Beneficial or Challenging: How Much of This Should we Really Believe?

Emerging Technology Hype Cycle





OPCW

OPCW Scientific Advisory Board 2017 Emerging Technology Workshop

- **In support of report to Fourth Review Conference**
- **Co-organised with IUPAC**
 - **EU Funding**
- **Participation from experts in**
 - **Recognizing (bio)chemical change (environment, process, etc.)**
 - **Mobile and wearable technologies**
 - **Point-of-care technologies**
 - **Sample collection and analysis**
 - **Artificial intelligence in the chemical sciences**
- **More to follow...**