



OPCW

Organisation for the Prohibition of Chemical Weapons

# The Chemical Universe: Scheduled and Unscheduled

*Science for Diplomats at EC-88  
The Hague, 10 July 2018*

Cheng Tang,; 2019 SAB Chair Elect

Christopher Timperley, Ph.D.; SAB Chair

Jonathan E. Forman, Ph.D.; Science Policy Adviser and SAB Secretary

Mr Joel De Saint Ours, Ms Siqing Sun, and Mr Vivek Suri  
Support Staff, Office of Strategy and Policy

# Scheduled Chemicals under the Chemical Weapons Convention (CWC)

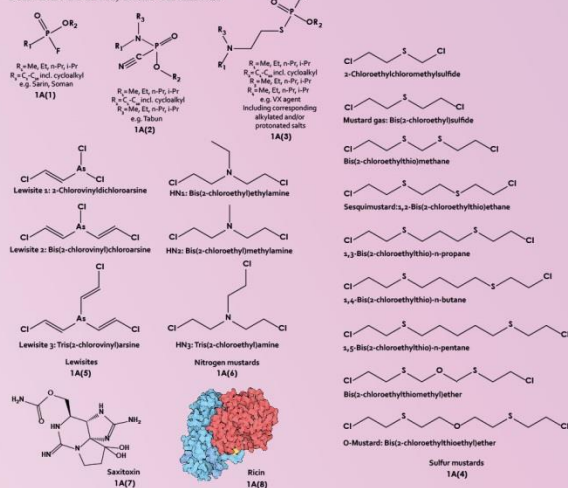
## Schedule 1

### Guidelines for Schedule 1

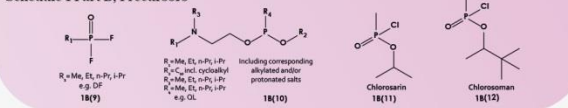
The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

- It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:
  - It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparable properties;
  - It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;
  - It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;
- It has little or no use for purposes not prohibited under this Convention.

#### Schedule 1 Part A, Toxic Chemicals



#### Schedule 1 Part B, Precursors



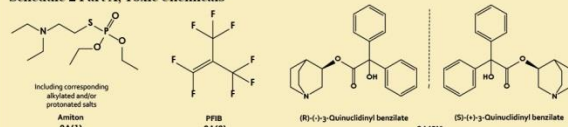
## Schedule 2

### Guidelines for Schedule 2

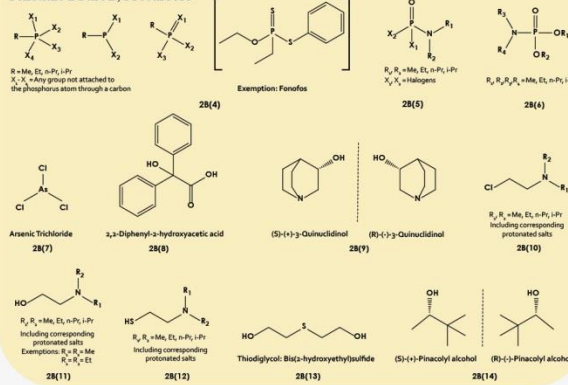
The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:

- It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;
- 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;
- It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;
- It is not produced in large commercial quantities for purposes not prohibited under this Convention.

#### Schedule 2 Part A, Toxic Chemicals



#### Schedule 2 Part B, Precursors



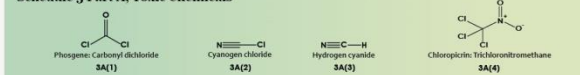
## Schedule 3

### Guidelines for Schedule 3

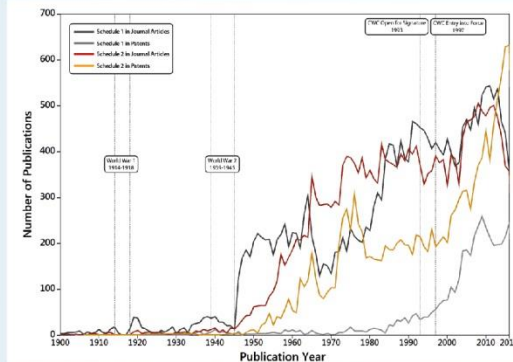
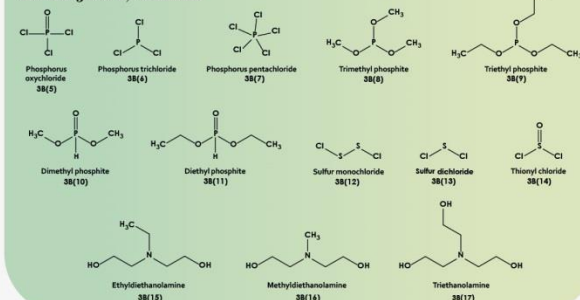
The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

- It has been produced, stockpiled or used as a chemical weapon;
- 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;
- 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;
- It may be produced in large commercial quantities for purposes not prohibited under this Convention.

#### Schedule 3 Part A, Toxic Chemicals



#### Schedule 3 Part B, Precursors



Scheduled chemicals, including those in schedules 1 and 2, can have scientifically and economically important uses. This chart captures the number of yearly scientific publications that refer to them.



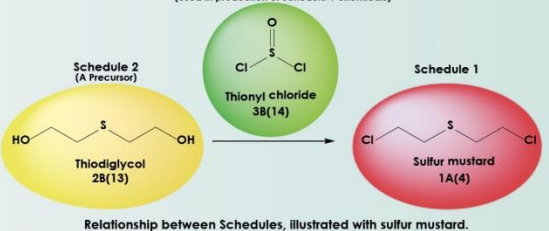
ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

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#### Schedule 3 (Used in production of Schedule 1 chemicals)





# Scheduled Chemicals under the Chemical Weapons Convention (CWC)

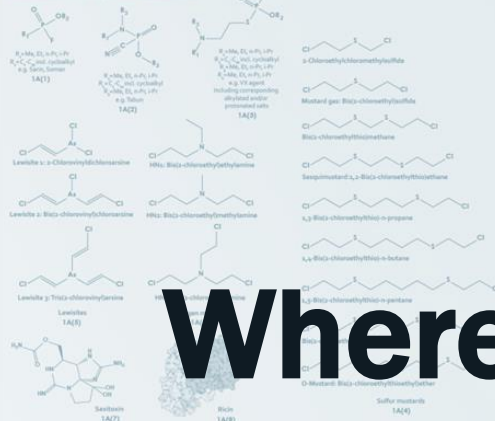
## Schedule 1

### Guidelines for Schedule 1

The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

- (a) It has been developed, produced, stockpiled or defined in Article I;
- (b) It poses otherwise a high risk to the object and virtue of its high potential for use in actual or potential chemical warfare; or
- (c) It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;
- (d) It has little or no use for purposes not prohibited under this Convention.

#### Schedule 1 Part A, Toxic Chemicals



#### Schedule 1 Part B, Precursors



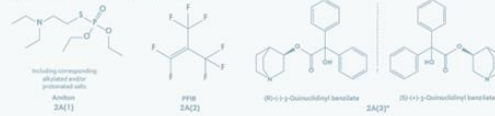
## Schedule 2

### Guidelines for Schedule 2

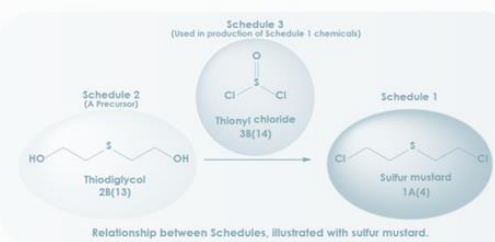
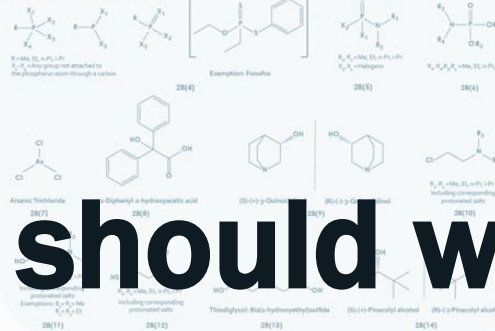
The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1, or a precursor of a Schedule 1 chemical or a chemical listed in Schedule 2, should be included in Schedule 2:

- (a) It is a toxic chemical or precursor of a Schedule 1 chemical or a chemical listed in Schedule 2, or is otherwise a chemical which is developed, produced, stockpiled or defined in Article I;
- (b) 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;
- (c) It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;
- (d) It is not produced in large commercial quantities for purposes not prohibited under this Convention.

#### Schedule 2 Part A, Toxic Chemicals



#### Schedule 2 Part B, Precursors



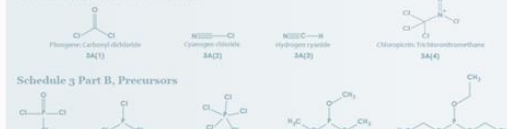
## Schedule 3

### Guidelines for Schedule 3

The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

- (a) It is a toxic chemical or precursor of a Schedule 1 chemical or a chemical listed in Schedule 2, or is otherwise a chemical which is developed, produced, stockpiled or defined in Article I;
- (b) It poses otherwise a high risk to the object and purpose of this Convention because it might enable it to be used as a chemical weapon; or
- (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.

#### Schedule 3 Part A, Toxic Chemicals



#### Schedule 3 Part B, Precursors



# Where should we start?

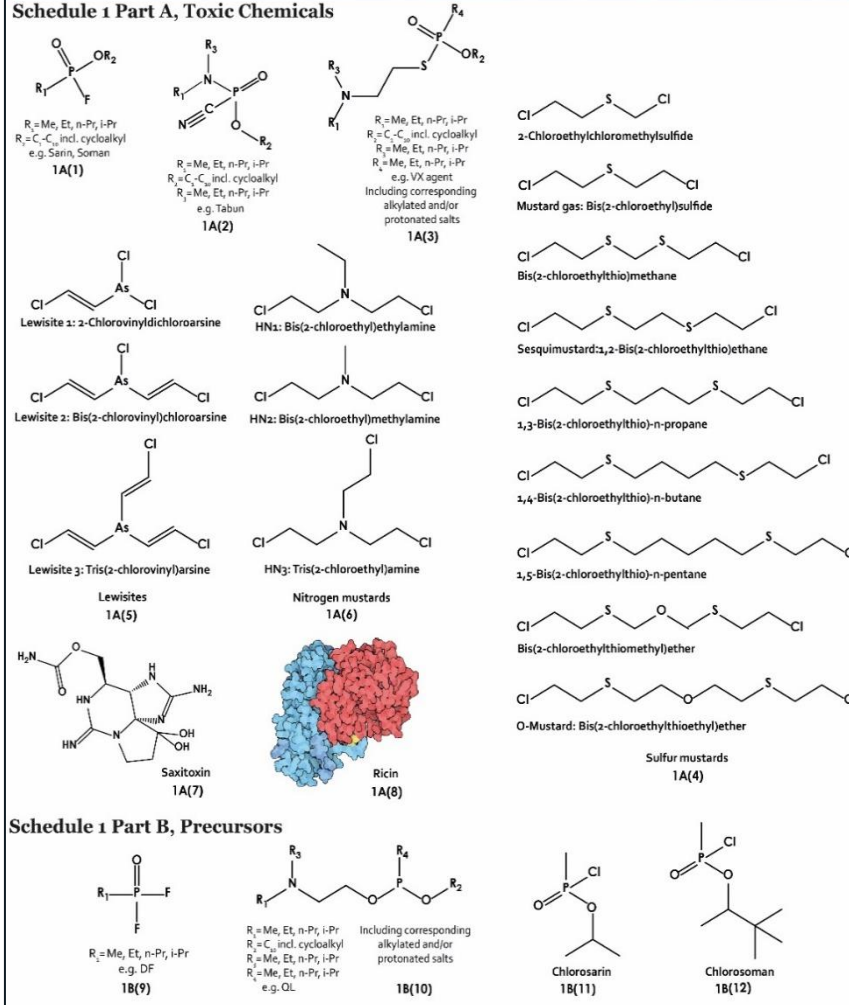


**ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS**  
 Working Together for a World Free of Chemical Weapons

# Schedule 1

## Schedule 1

### Schedule 1 Part A, Toxic Chemicals

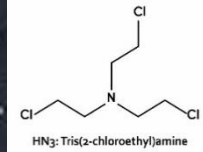
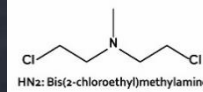
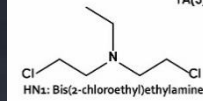
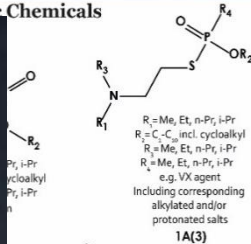


### Schedule 1 Part B, Precursors

# Schedule 1

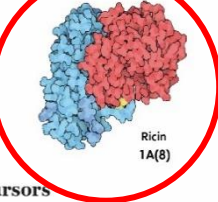
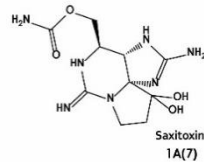
## Schedule 1

### Schedule 1 Part A, Toxic Chemicals

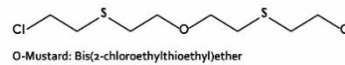
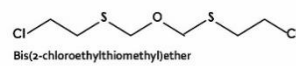
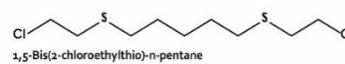
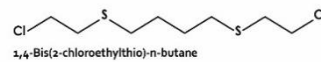
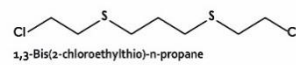
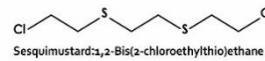
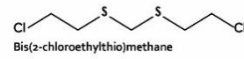
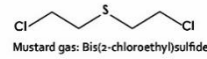
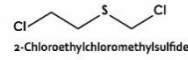
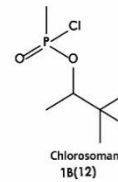
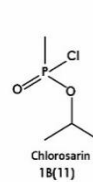
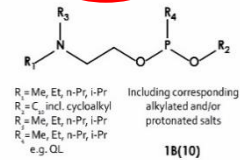
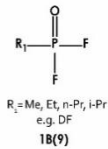


#### Nitrogen mustards

1A(6)



### Schedule 1 Part B, Precursors



#### Sulfur mustards

1A(4)



# Schedule 1

Placement of RSS bar code to read as UPC number

67386 911 51

**DANGER:** Contact Poison: Avoid contact with skin, mucous membranes, or eyes. Do not inhale the dust or vapor. In case of skin contact, wash with copious amounts of water for at least 15 minutes, followed by 2% sodium thiosulfate solution. See PRECAUTIONS and DOSAGE AND ADMINISTRATION in accompanying package insert. Store at controlled room temperature, 15-30°C (59-86°F). Protect from light and humidity.

**NDC 67386-911-51**      **1 Vial**

**Trituration of Mustargen®**      **℞ only**  
(mechlorethamine HCl for injection)

**10 mg**

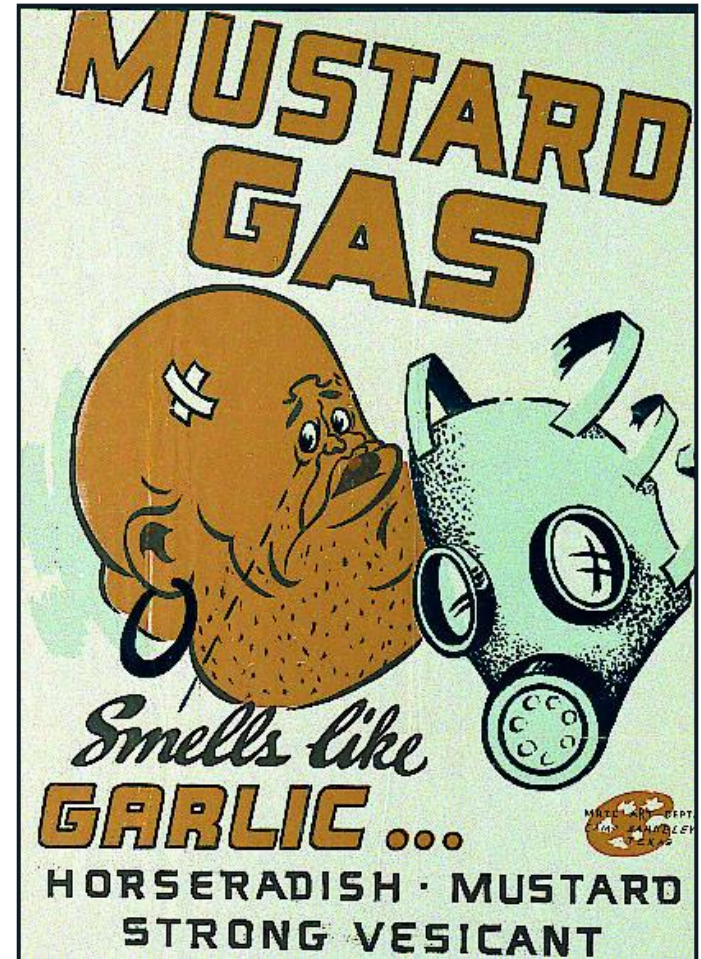
A Nitrogen Mustard – POISON  
This vial contains 10 mg of mechlorethamine hydrochloride with sodium chloride q.s. 100 mg

Lundbeck Inc.  
Deerfield, IL 60015, U.S.A.

Lot:      Exp:      ▶

780-03008-1

Nitrogen mustard



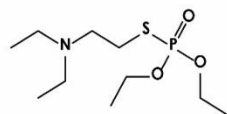
Sulfur mustard



# Schedule 2

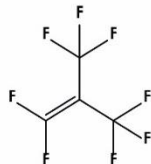
## Schedule 2

### Schedule 2 Part A, Toxic Chemicals

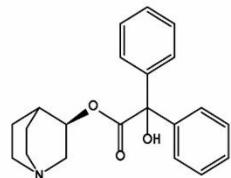


Including corresponding alkylated and/or protonated salts

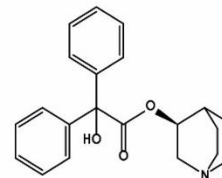
Amiton  
2A(1)



PFIB  
2A(2)

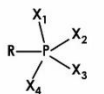


(R)-(-)-3-Quinuclidinyl benzilate  
2A(3)\*



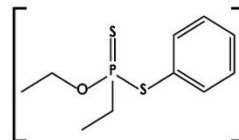
(S)-(-)-3-Quinuclidinyl benzilate

### Schedule 2 Part B, Precursors

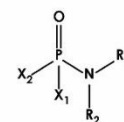


R = Me, Et, n-Pr, i-Pr  
X<sub>1</sub>-X<sub>4</sub> = Any group not attached to the phosphorus atom through a carbon

2B(4)

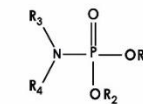


Exemption: Fonofos



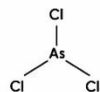
R<sub>1</sub>, R<sub>2</sub> = Me, Et, n-Pr, i-Pr  
X<sub>1</sub>, X<sub>2</sub> = Halogens

2B(5)

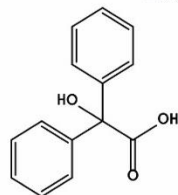


R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>4</sub> = Me, Et, n-Pr, i-Pr

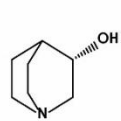
2B(6)



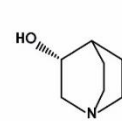
Arsenic Trichloride  
2B(7)



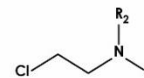
2,2-Diphenyl-2-hydroxyacetic acid  
2B(8)



(S)-(+)-3-Quinuclidinol  
2B(9)

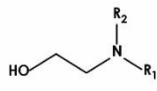


(R)-(-)-3-Quinuclidinol  
2B(9)



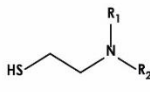
R<sub>1</sub>, R<sub>2</sub> = Me, Et, n-Pr, i-Pr  
Including corresponding protonated salts

2B(10)



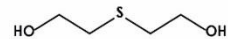
R<sub>1</sub>, R<sub>2</sub> = Me, Et, n-Pr, i-Pr  
Including corresponding protonated salts  
Exemptions: R<sub>1</sub> = R<sub>2</sub> = Me  
R<sub>1</sub> = R<sub>2</sub> = Et

2B(11)



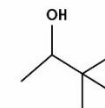
R<sub>1</sub>, R<sub>2</sub> = Me, Et, n-Pr, i-Pr  
Including corresponding protonated salts

2B(12)



Thiodiglycol: Bis(2-hydroxyethyl)sulfide

2B(13)



Pinacolyl alcohol

2B(14)





# Schedule 2

Chemical warfare agent precursors and ...



Pharmaceutical precursors



Fire retardants

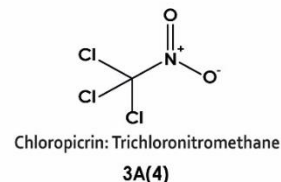
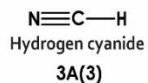
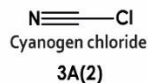
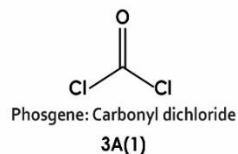


OPCW

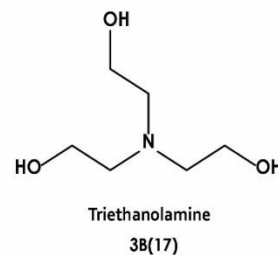
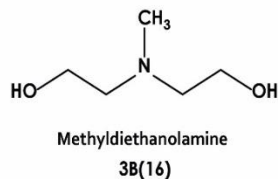
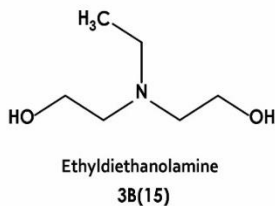
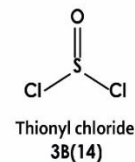
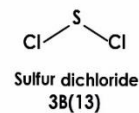
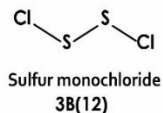
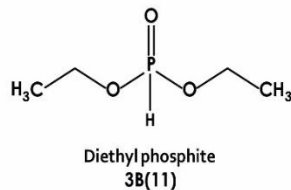
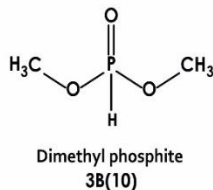
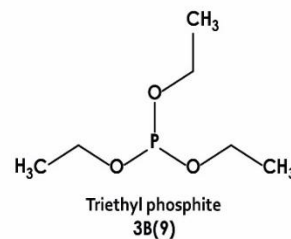
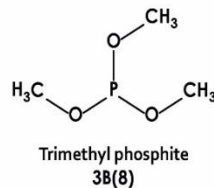
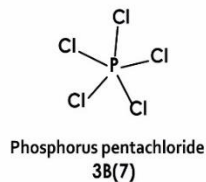
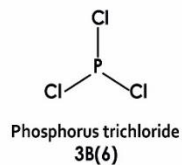
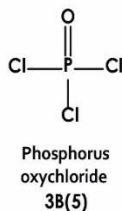
# Schedule 3

## Schedule 3

### Schedule 3 Part A, Toxic Chemicals



### Schedule 3 Part B, Precursors



Industrial  
dual-use  
chemicals



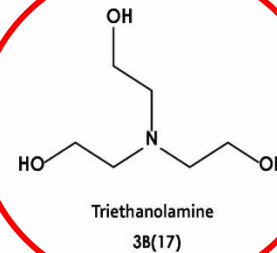
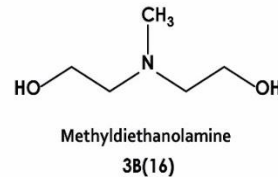
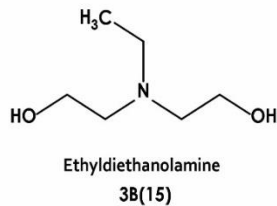
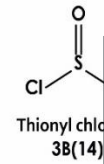
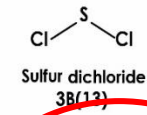
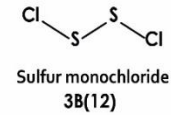
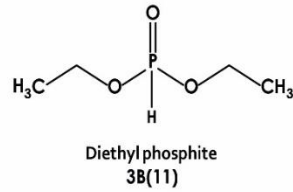
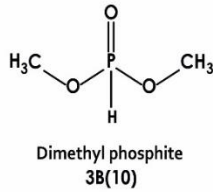
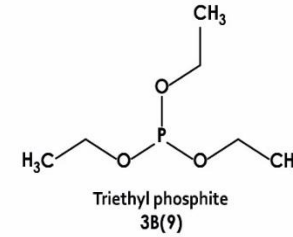
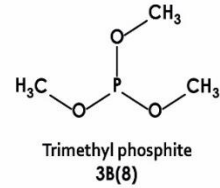
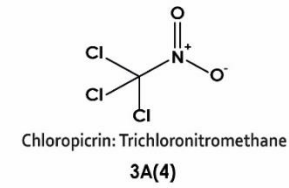
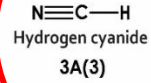
# Schedule 3

## Schedule 3

### Schedule 3 Part A, Toxic Chemicals



3B(5)



# Schedule 3

**“Given the substantial changes in chemistry and chemical industry since the schedules were finalised a quarter century ago, a review of the schedules should be considered to assess whether: (a) the chemicals currently listed are in the appropriate Schedule, and (b) any toxic chemicals or specific precursors should be added to or removed from the Schedules. In this connection, it should be considered whether it is technically feasible to accurately monitor Schedule 3 chemicals that are produced in very large quantities (e.g. over 100,000 tons/year).”**

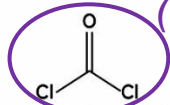


# Schedule 3

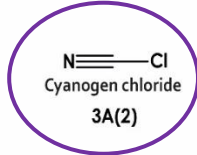
## Schedule 3

### Schedule 3 Part A, Toxic Chemicals

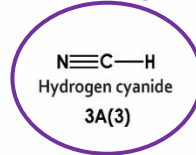
*(isocyanates derived from phosgene)*



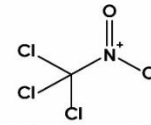
Phosgene: Carbonyl dichloride  
3A(1)



Cyanogen chloride  
3A(2)

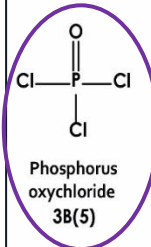


Hydrogen cyanide  
3A(3)

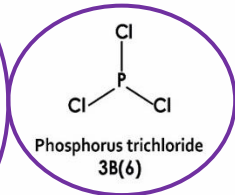


Chloropicrin: Trichloronitromethane  
3A(4)

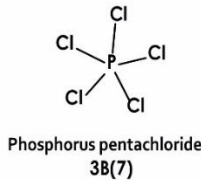
### Schedule 3 Part B, Precursors



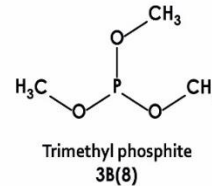
Phosphorus oxychloride  
3B(5)



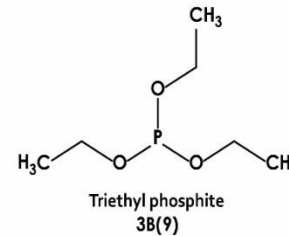
Phosphorus trichloride  
3B(6)



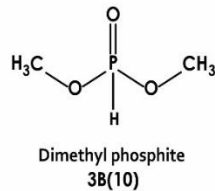
Phosphorus pentachloride  
3B(7)



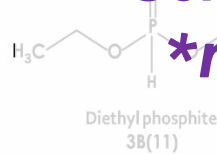
Trimethyl phosphite  
3B(8)



Triethyl phosphite  
3B(9)

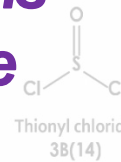


Dimethyl phosphite  
3B(10)

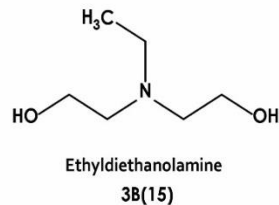


Diethyl phosphite  
3B(11)

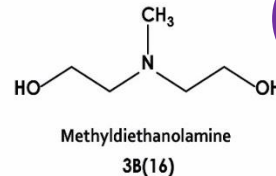
**Some of these chemicals  
\*might\* qualify for the  
> 100,000 club?**



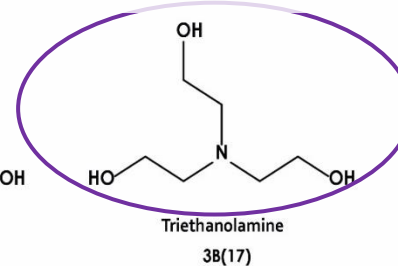
Thionyl chloride  
3B(14)



Ethyldiethanolamine  
3B(15)



Methyl-diethanolamine  
3B(16)



Triethanolamine  
3B(17)



**The Scheduled chemicals explicitly specified in the Convention for monitoring purposes, include chemical warfare agents and their key precursors**

**Scheduled chemicals are associated with historical chemical warfare programmes – *this does not mean they are chemical weapons...***

### ***A Chemical Weapon:***

***Toxic chemicals and their precursors, except where intended for purposes not prohibited under this Convention as long as the types and quantities are consistent with such purposes (Article II).***

# MOST TRADED SCHEDULED CHEMICALS 2017



ORGANISATION FOR THE PROHIBITION  
OF CHEMICAL WEAPONS

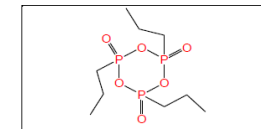
## Most Traded Scheduled Chemicals ordered by Schedule

Schedule 2	CAS RN	Chemical Name	Page
2B04	129788-86-9	Product from the reaction of Methylphosphonic acid and 1,3,5-Triazine-2,4,6-triamine	1
2B04	170836-68-7	Mixture of (5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate (CAS RN 41203-81-0) and Bis[(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl]methylphosphonate (CAS RN 42595-45-9)	2
2B04	18755-43-6	Dimethyl propylphosphonate	3
2B04	294675-51-7	Phosphonic acid, methyl-, polyglycol ester (Exolit OP 560 TP)	4
2B04	3001-98-7	3,9-Dimethyl-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane 3,9-dioxide	5
2B04	363626-50-0	Bis(polyoxyethylene) methylphosphonate	6
2B04	41203-81-0	(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate	7
2B04	42595-45-9	Bis[(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl] methylphosphonate	8
2B04	4708-04-7	Propylphosphonic dichloride	9
2B04	63747-58-0	Poly(1,3-phenylene methyl phosphonate)	10
2B04	663176-00-9	Phosphonic acid, methyl-, polyglycol ester (Exolit OP 560)	11
2B04	676-97-1	Methylphosphonic dichloride	12

Page 13

<b>Chemical Name:</b>	2,4,6-Tripropyl-1,3,5,2,4,6-trioxatriphosphinane 2,4,6-trioxide
<b>CAS RN:</b>	68957-94-8
<b>Schedule:</b>	2B04
<b>HS code:</b>	2931.35
<b>Molecular Formula:</b>	C <sub>9</sub> H <sub>21</sub> O <sub>6</sub> P <sub>3</sub>
<b>CAS Index Name:</b>	1,3,5,2,4,6-Trioxatriphosphorinane, 2,4,6-tripropyl-, 2,4,6-trioxide
<b>IUPAC Name:</b>	2,4,6-Tripropyl-1,3,5,2,4,6-trioxatriphosphinane 2,4,6-trioxide
<b>Synonyms:</b>	Propylphosphonic anhydride n-Propylphosphonic cyclic anhydride 1-Propanephosphonic acid cyclic anhydride, 50% in ethyl acetate 1-Propanephosphonic acid cyclic anhydride

### Chemical Structure



### Commercial Applications & Industrial Uses

Used in: paper industry, pharmaceutical industry, plastics and synthetic resin industries, and peptide synthesis.

Used as flame retardant and paper making auxiliaries.

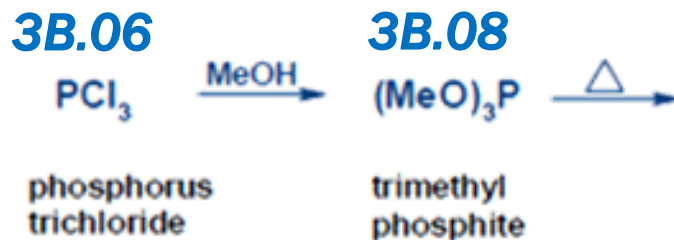
**Precursors?**





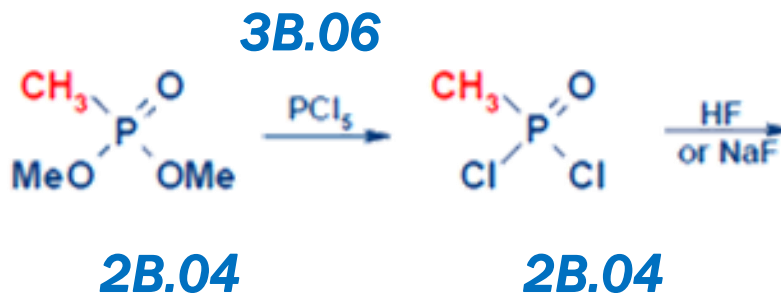
# Chemical Warfare Agents and Precursors

## Schedule 3



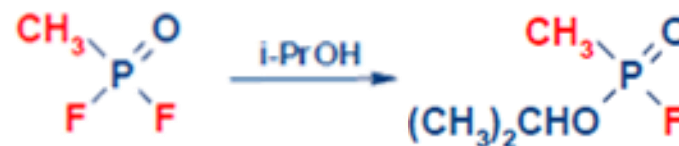
*“Chemical weapon” (historical or potential)*  
*Key precursor to S1 or S2(A)*  
*Produced in large commercial quantities*

## Schedule 2



*Potential chemical weapon;*  
*Final stage or key precursor to S1 or S2(A)*  
*Not produced in large commercial quantities*

## Schedule 1



**1B.09**

**Sarin (1A.01)**  
**chemical warfare agent**

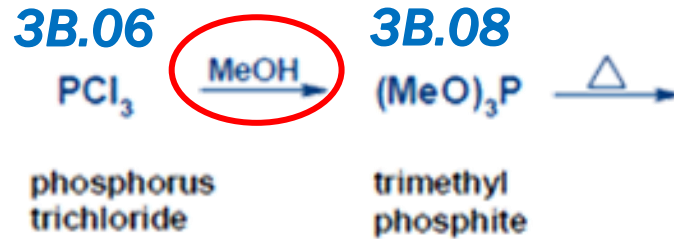
*“Chemical weapon” (historical or potential)*  
*Closely related chemical structure to S1(A)*  
*Comparable properties to S1(A)*  
*Final stage precursor to S1(A)*  
*No (or limited) non-prohibited uses*



OPCW

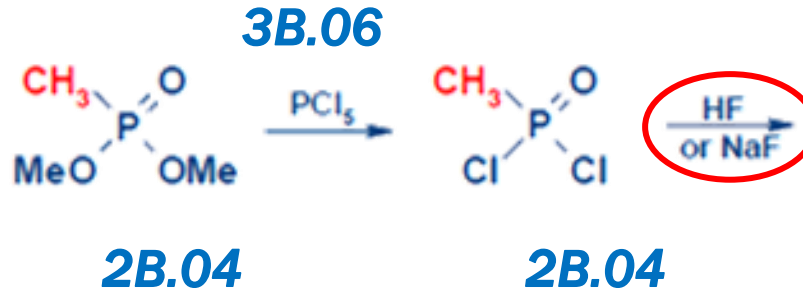
# Chemical Warfare Agents and Precursors

## Schedule 3



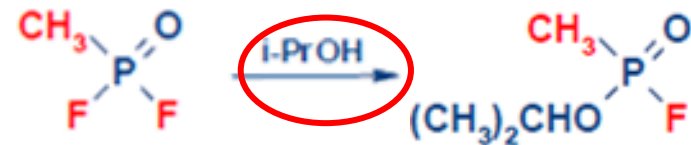
*"Chemical weapon" (historical or potential)  
 Key precursor to S1 or S2(A)  
 Produced in large commercial quantities*

## Schedule 2



*Potential chemical weapon;  
 Final stage or key precursor to S1 or S2(A)  
 Not produced in large commercial quantities*

## Schedule 1



*"Chemical weapon" (historical or potential)  
 Closely related chemical structure to S1(A)  
 Comparable properties to S1(A)  
 Final stage precursor to S1(A)  
 No (or limited) non-prohibited uses*

**Sarin (1A.01)  
 chemical warfare agent**



# Chemical Warfare Agents and Precursors

**MeOH (methanol), *i*-PrOH (iso-propyl alcohol), HF (hydrogen fluoride), and NaF (sodium fluoride) are unscheduled “precursors” (*they are not considered “key” precursors*)**



**If making sarin for prohibited uses, under Article II, these chemicals would be classed as:**  
**“unscheduled chemical weapons”**



OPCW

# How Many Chemicals are Contained within the Schedules?

**B. SCHEDULES OF CHEMICALS**

The following Schedules list toxic chemicals and their precursors. For the purpose of implementing this Convention, these Schedules identify chemicals for the application of verification measures according to the provisions of the Verification Annex. Pursuant to Article II, subparagraph 1 (a), these Schedules do not constitute a definition of chemical weapons.

(Whenever reference is made to groups of dialkylated chemicals, followed by a list of alkyl groups in parentheses, all chemicals possible by all possible combinations of alkyl groups listed in the parentheses are considered as listed in the respective Schedule as long as they are not explicitly exempted. A chemical marked "\*" on Schedule 2, part A, is subject to special thresholds for declaration and verification, as specified in Part VII of the Verification Annex.)

Schedule 1	(CAS registry number)
<b>A. Toxic chemicals:</b>	
(1) O-Alkyl ( $\leq C_{10}$ , incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates	
e.g. Sarin: O-Isopropyl methylphosphonofluoridate	(107-44-8)
Soman: O-Pinacolyl methylphosphonofluoridate	(96-64-0)
(2) O-Alkyl ( $\leq C_{10}$ , incl. cycloalkyl) N,N-dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidocyanidates	
e.g. Tabun: O-Ethyl N,N-dimethyl phosphoramidocyanidate	(77-81-6)
(3) O-Alkyl (H or $\leq C_{10}$ , incl. cycloalkyl) S-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonothiolates and corresponding alkylated or protonated salts	
e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate	(50782-69-9)
(4) Sulfur mustards:	
2-Chloroethylchloromethylsulfide	(2625-76-5)
Mustard gas: Bis(2-chloroethyl)sulfide	(505-60-2)
Bis(2-chloroethylthio)methane	(63869-13-6)
Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane	(3563-36-8)
1,3-Bis(2-chloroethylthio)-n-propane	(63905-10-2)
1,4-Bis(2-chloroethylthio)-n-butane	(142868-93-7)
1,5-Bis(2-chloroethylthio)-n-pentane	(142868-94-8)
Bis(2-chloroethylthiomethyl)ether	(63918-90-1)
O-Mustard: Bis(2-chloroethylthioethyl)ether	(63918-89-8)

(5) Lewisties:	
Lewistate 1: 2-Chlorovinylchloroarsine	(541-25-3)
Lewistate 2: Bis(2-chlorovinyl)chloroarsine	(40334-69-8)
Lewistate 3: Tris(2-chlorovinyl)arsine	(40334-70-1)
(6) Nitrogen mustard:	
HN1: Bis(2-chloroethyl)ethylamine	(538-07-8)
HN2: Bis(2-chloroethyl)methylamine	(51-75-2)
HN3: Tris(2-chloroethyl)amine	(555-77-1)
(7) Saxitoxin	(35523-89-8)
(8) Ricin	(9009-86-3)
<b>B. Precursors:</b>	
(9) Alkyl (Me, Et, n-Pr or i-Pr) phosphonyldifluorides	
e.g. DF: Methylphosphonyldifluoride	(676-99-3)
(10) O-Alkyl (H or $\leq C_{10}$ , incl. cycloalkyl) O-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonites and corresponding alkylated or protonated salts	
e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite	(57856-11-8)
(11) Chlorosarin: O-Isopropyl methylphosphonochloridate	(1445-76-7)
(12) Chlorosoman: O-Pinacolyl methylphosphonochloridate	(7040-57-5)

Schedule 2	
<b>A. Toxic chemicals:</b>	
(1) Amton: O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate and corresponding alkylated or protonated salts	(78-53-5)
(2) PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene	(382-21-8)
(3) BZ: 3-Quinuclidinyl benzilate (*)	(6581-06-2)
<b>B. Precursors:</b>	
(4) 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.	
e.g. Methylphosphonyl dichloride	(676-97-1)
Dimethyl methylphosphonate	(756-79-6)
Exemption: Fonofos: O-Ethyl S-phenyl ethylphosphonodithiothionate	(944-22-9)
(5) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides	
(6) Dialkyl (Me, Et, n-Pr or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates	
(7) Arsenic trichloride	(7784-34-1)
(8) 2,2-Diphenyl-2-hydroxyacetic acid	(76-93-7)
(9) Quinuclidin-3-ol	(1619-34-7)
(10) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts	
(11) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-ols and corresponding protonated salts	
Exemptions: N,N-Dimethylaminoethanol and corresponding protonated salts	(108-01-0)
N,N-Diethylaminoethanol and corresponding protonated salts	(100-37-8)
(12) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-thiols and corresponding protonated salts	
(13) Thioglycol: Bis(2-hydroxyethyl)sulfide	(111-48-8)
(14) Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol	(464-07-3)

Schedule 3	
<b>A. Toxic chemicals:</b>	
(1) Phosgene: Carbonyl dichloride	(75-44-5)
(2) Cynogen chloride	(506-77-4)
(3) Hydrogen cyanide	(74-90-8)
(4) Chloropicrin: Trichloronitromethane	(76-06-2)
<b>B. Precursors:</b>	
(5) Phosphorus oxychloride	(10025-87-3)
(6) Phosphorus trichloride	(7719-12-2)
(7) Phosphorus pentachloride	(10026-13-8)
(8) Trimethyl phosphite	(121-45-9)
(9) Triethyl phosphite	(122-52-1)
(10) Dimethyl phosphite	(868-85-9)
(11) Diethyl phosphite	(762-04-9)
(12) Sulfur monochloride	(10025-67-9)
(13) Sulfur dichloride	(10545-99-0)
(14) Thionyl chloride	(7719-09-7)
(15) Ethyldiethanolamine	(139-87-7)
(16) Methyl-diethanolamine	(105-59-9)
(17) Triethanolamine	(102-71-6)



# How Many Chemicals are Contained within the Schedules?

**Chemical Abstracts  
Service (CAS)  
Registry Numbers**

**B. SCHEDULES OF CHEMICALS**

The following Schedules list toxic chemicals and their precursors. For the purpose of implementing this Convention, these Schedules identify chemicals for the application of verification measures according to the provisions of the Verification Annex. Pursuant to Article II, subparagraph 1 (a), these Schedules do not constitute a definition of chemical weapons.

(Whenever reference is made to groups of dialkylated chemicals, followed by a list of alkyl groups in parentheses, all chemicals possible by all possible combinations of alkyl groups listed in the parentheses are considered as listed in the respective Schedule as long as they are not explicitly exempted. A chemical marked "\*" on Schedule 2, part A, is subject to special thresholds for declaration and verification, as specified in Part VII of the Verification Annex.)

**Schedule 1** (CAS registry number)

**A. Toxic chemicals:**

(1) O-Alkyl ( $\leq C_{10}$ , incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates  
 e.g. Sarin: O-Isopropyl methylphosphonofluoridate (107-44-8)  
 Soman: O-Pinacolyl methylphosphonofluoridate (96-64-0)

(2) O-Alkyl ( $\leq C_{10}$ , incl. cycloalkyl) N,N-dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidocyanidates  
 e.g. Tabun: O-Ethyl N,N-dimethyl phosphoramidocyanidate (77-81-6)

(3) O-Alkyl (H or  $\leq C_{10}$ , incl. cycloalkyl) S-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonothiolates and corresponding alkylated or protonated salts  
 e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (50782-69-9)

(4) Sulfur mustards:  
 2-Chloroethylchloromethylsulfide (2625-76-5)  
 Mustard gas: Bis(2-chloroethyl)sulfide (505-60-2)  
 Bis(2-chloroethylthio)methane (63869-13-6)  
 Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane (3563-36-8)  
 1,3-Bis(2-chloroethylthio)-n-propane (63905-10-2)  
 1,4-Bis(2-chloroethylthio)-n-butane (142868-93-7)  
 1,5-Bis(2-chloroethylthio)-n-pentane (142868-94-8)  
 Bis(2-chloroethylthio)methyl ether (63918-90-1)  
 O-Mustard: Bis(2-chloroethylthio)ethyl ether (63918-89-8)

**descriptions/formulas**

(5) Lewisites:  
 Lewisite 1: 2-Chlorovinylchloroarsine (541-25-3)  
 Lewisite 2: Bis(2-chlorovinyl)chloroarsine (40334-69-8)  
 Lewisite 3: Tris(2-chlorovinyl)arsine (40334-70-1)

(6) Nitrogen mustard:  
 HN1: Bis(2-chloroethyl)ethylamine (538-07-8)  
 HN2: Bis(2-chloroethyl)methylamine (51-75-2)  
 HN3: Tris(2-chloroethyl)amine (555-77-1)

(7) Saxitoxin (35523-89-8)

(8) Ricin (9009-86-3)

**B. Precursors:**

(9) O-Alkyl (Me, Et, n-Pr or i-Pr) phosphonyldifluorides  
 e.g. DF: Methylphosphonyldifluoride (676-99-3)

(10) O-Alkyl (H or  $\leq C_{10}$ , incl. cycloalkyl) O-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonites and corresponding alkylated or protonated salts  
 e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite (57856-11-8)

(11) Chlorosarin: O-Isopropyl methylphosphonochloridate (1445-76-7)

(12) Chlorosoman: O-Pinacolyl methylphosphonochloridate (7040-57-5)

**Schedule 2**

**A. Toxic chemicals:**

(1) Amion: O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate and corresponding alkylated or protonated salts (78-53-5)

(2) PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene (382-21-8)

(3) BZ: 3-Quinuclidinyl benzilate (\*) (6581-06-2)

**B. Precursors:**

(4) 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.  
 e.g. Methylphosphonyl dichloride (676-97-1)  
 Dimethyl methylphosphonate (756-79-6)  
 Exemption: Fonofos: O-Ethyl S-phenyl ethylphosphonodithiothionate (944-22-9)

(5) NN-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides

(6) Dialkyl (Me, Et, n-Pr or i-Pr) NN-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates

(7) Arsenic trichloride (7782-38-4)

(8) 2,2-Diphenyl-2-hydroxyacetic acid (10545-99-0)

(9) Quinuclidin-3-ol (7719-09-7)

(10) NN-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidates and corresponding alkylated or protonated salts (139-87-7)

(11) NN-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidates and corresponding alkylated or protonated salts (105-59-9)

(12) N-Ethyl N-(2-dimethylaminoethyl) methanamine (102-71-6)

**Specific chemicals**

**Schedule 3**

**A. Toxic chemicals:**

(1) Phosgene: Carbonyl dichloride (75-44-5)

(2) Cyanogen chloride (506-77-4)

(3) Hydrogen cyanide (74-90-8)

(4) Chloropicrin: Trichloronitromethane (76-06-2)

**B. Precursors:**

(5) Phosphorus oxychloride

(6) Phosphorus trichloride

(7) Phosphorus pentachloride

(8) Trimethyl phosphite

(9) ...

**53 specific chemicals are listed by chemical name, CAS number and/or uniquely defined chemical formula (3 are exemptions to the Schedule they would otherwise fall under)**



# Scheduled Chemicals under the Chemical Weapons Convention (CWC)

## Schedule 1

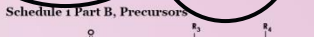
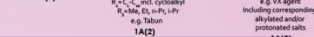
### Guidelines for Schedule 1

The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

- It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1 and is capable of being produced in large quantities for purposes not prohibited under this Convention because one or more of the following conditions are met:
  - It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1 and is capable of being produced in large quantities for purposes not prohibited under this Convention because one or more of the following conditions are met:
    - It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;
    - It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;
    - It has little or no use for purposes not prohibited under this Convention.
- It has little or no use for purposes not prohibited under this Convention.

## 3 Groups of compounds (15 compounds in total)

### Schedule 1 Part A, Toxic Chemicals



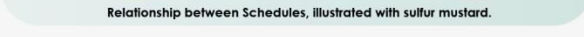
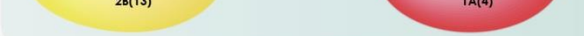
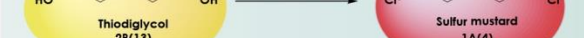
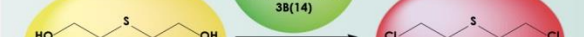
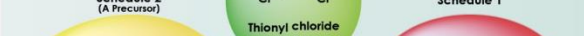
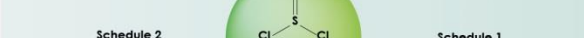
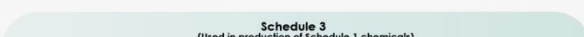
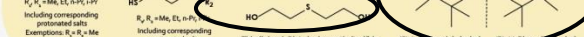
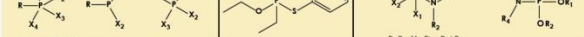
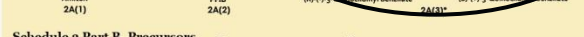
## Schedule 2

### Guidelines for Schedule 2

The following criteria shall be taken into account in considering whether a chemical or precursor should be included in Schedule 2:

- It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity that could enable it to be used as a chemical weapon;
- It may be used as a precursor in one of the chemical reactions in its final stage of formation of a chemical listed in Schedule 1 or Schedule 2, part A;
- It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 2, part A;
- It is not produced in large commercial quantities for purposes not prohibited under this Convention.

### Schedule 2 Part A, Toxic Chemicals



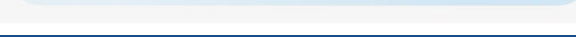
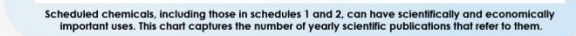
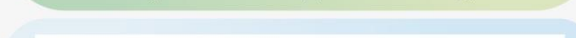
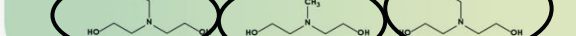
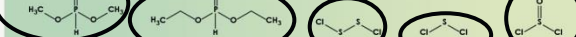
## Schedule 3

### 26 Single chemical substances

The following criteria shall be taken into account in considering whether a chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

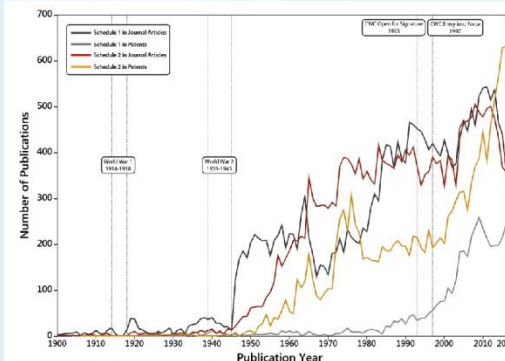
- It has been produced, stockpiled or used as a chemical weapon;
- It poses a risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity that might enable it to be used as a chemical weapon;
- It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;
- It is not produced in large commercial quantities for purposes not prohibited under this Convention.

### Schedule 3 Part A, Toxic Chemicals



ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons



Scheduled chemicals, including those in schedules 1 and 2, can have scientifically and economically important uses. This chart captures the number of yearly scientific publications that refer to them.



# Scheduled Chemicals under the Chemical Weapons Convention (CWC)

## Schedule 1

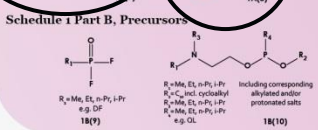
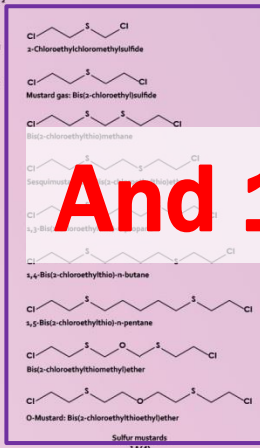
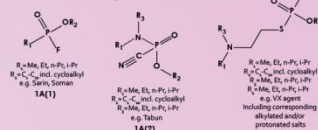
### Guidelines for Schedule 1

The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

**3 Groups of compounds (15 compounds in total)**

- It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1 or to other toxic chemicals listed in Schedule 2, part A, such that it could be used as a chemical weapon because of the one or more of the following conditions are met:
  - It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1 or to other toxic chemicals listed in Schedule 2, part A, such that it could be used as a chemical weapon because of the one or more of the following conditions are met:
  - It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;
  - It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;
- It has little or no use for purposes not prohibited under this Convention.

#### Schedule 1 Part A. Toxic Chemicals

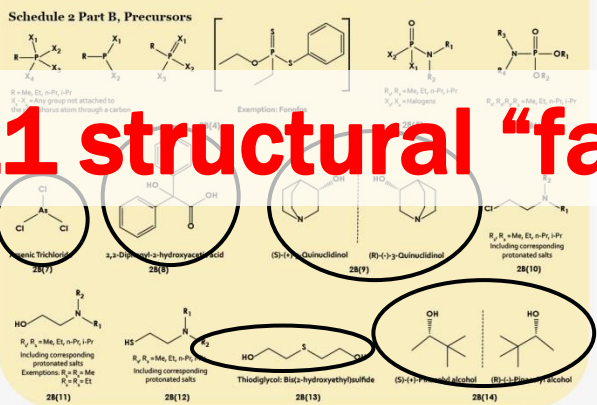
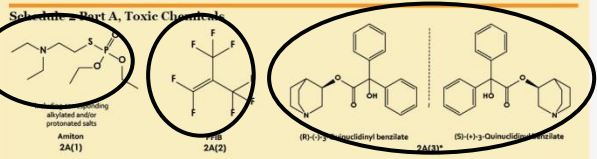


## Schedule 2

### Guidelines for Schedule 2

The following criteria shall be taken into account in considering whether a chemical or precursor should be included in Schedule 2:

- It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity that it could enable it to be used as a chemical weapon;
- It may be used as a precursor in one of the chemical reactions in a final stage of formation of a chemical listed in Schedule 1 or Schedule 2, part A;
- It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 2, part A;
- It is not produced in large commercial quantities for purposes not prohibited under this Convention.



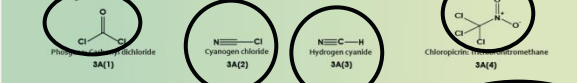
## Schedule 3

### 26 Single chemical substances

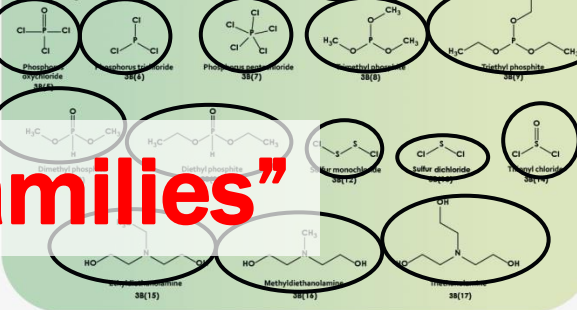
### 3 Single chemical substances

### Show here as stereoisomers

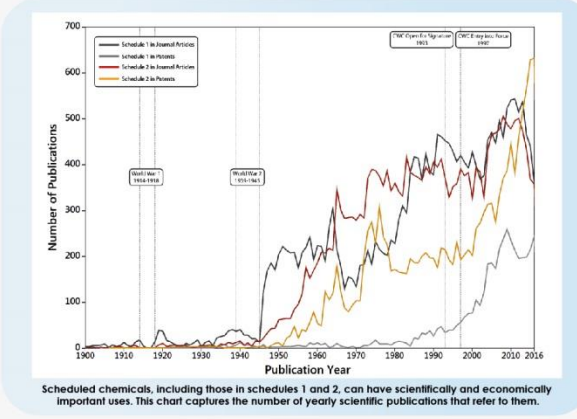
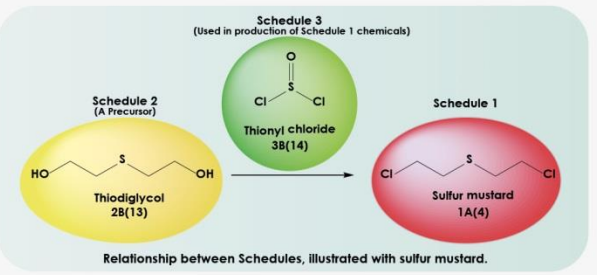
#### Schedule 3 Part A. Toxic Chemicals



#### Schedule 3 Part B. Precursors



**And 11 structural "families"**

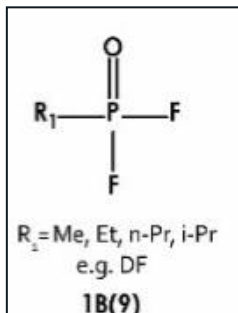


ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

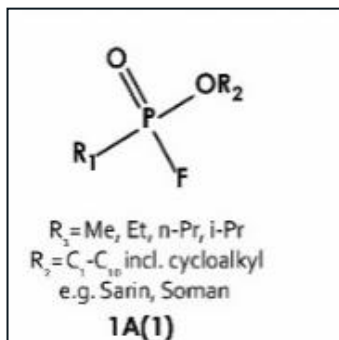
Working Together for a World Free of Chemical Weapons



# Families of Chemicals?



## ■ 1B.09: Four members



## ■ 1A.01

- $R_1$  has four possible structures
- *What about  $R_2$ ?*

$R_2 = \text{C}_1$  (-CH<sub>3</sub>), 1 structure X 4 = **4 1A.01 chemicals**

$R_2 = \text{C}_2$  (-CH<sub>2</sub>CH<sub>3</sub>), 1 structure X 4 = **4 1A.01 chemicals**

$R_2 = \text{C}_3$  (-CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> or -CH(CH<sub>3</sub>)<sub>2</sub> or  $\Delta$ ), 3 structures X 4 = **12 1A.01 chemicals**

■

■

$R_2 = \text{C}_6$

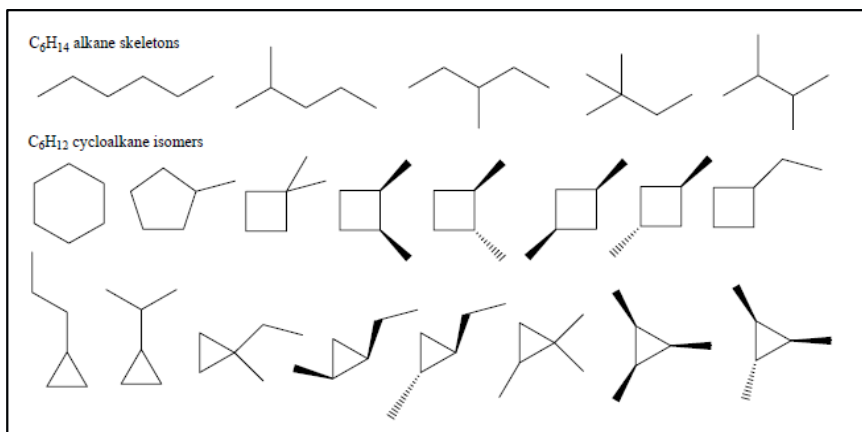
21 structures

83 ways of attachment

**332 1A.01 chemicals**

*Includes soman, cyclosarin*

With one variable R group from C1 to C10 for 1A.01, 1A.02 and 1A.03: > 1.3 million possible chemicals in these three Schedules

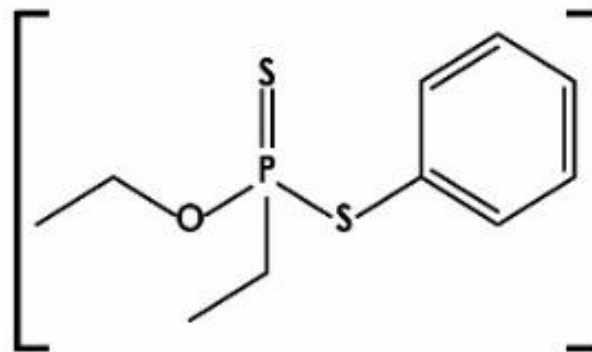
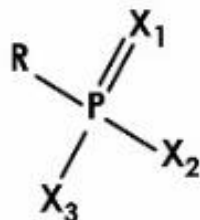
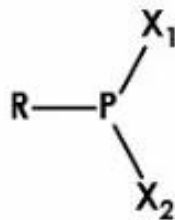
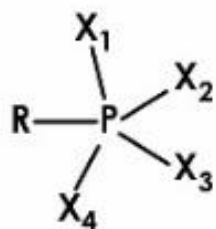


*Includes sarin*





# Families of Chemicals?



R = Me, Et, n Pr, i Pr

X<sub>1</sub> - X<sub>4</sub> = Any group not attached to the phosphorus atom through a carbon.

Exemption: Fonofos

2B(4)



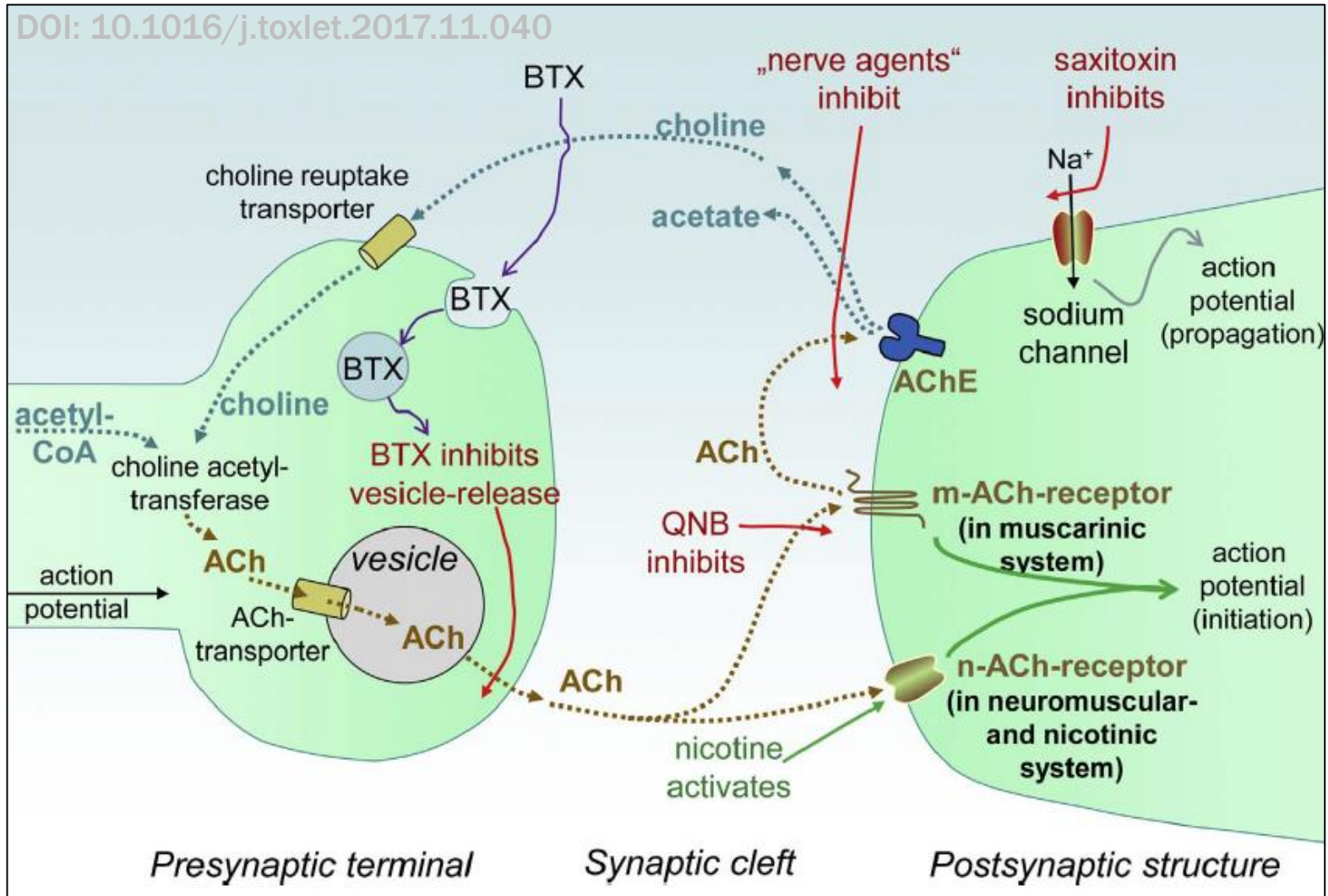
OPCW



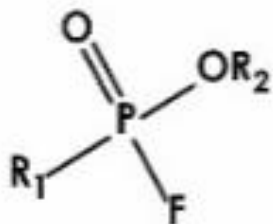
**2B.04 is the Largest Family on the Schedules**  
**(unlimited possibilities with one exemption)**

# Is that all a bit too complicated?

DOI: 10.1016/j.toxlet.2017.11.040



# Is that all a bit too complicated?



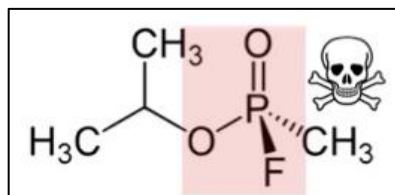
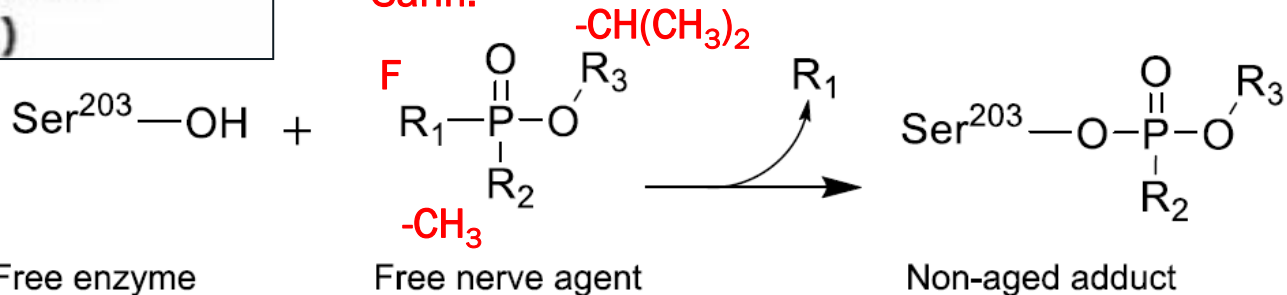
R<sub>1</sub> = Me, Et, n-Pr, i-Pr  
R<sub>2</sub> = C<sub>1</sub>-C<sub>10</sub>, incl. cycloalkyl  
e.g. Sarin, Soman

1A(1)

## Why stop at C<sub>10</sub>?

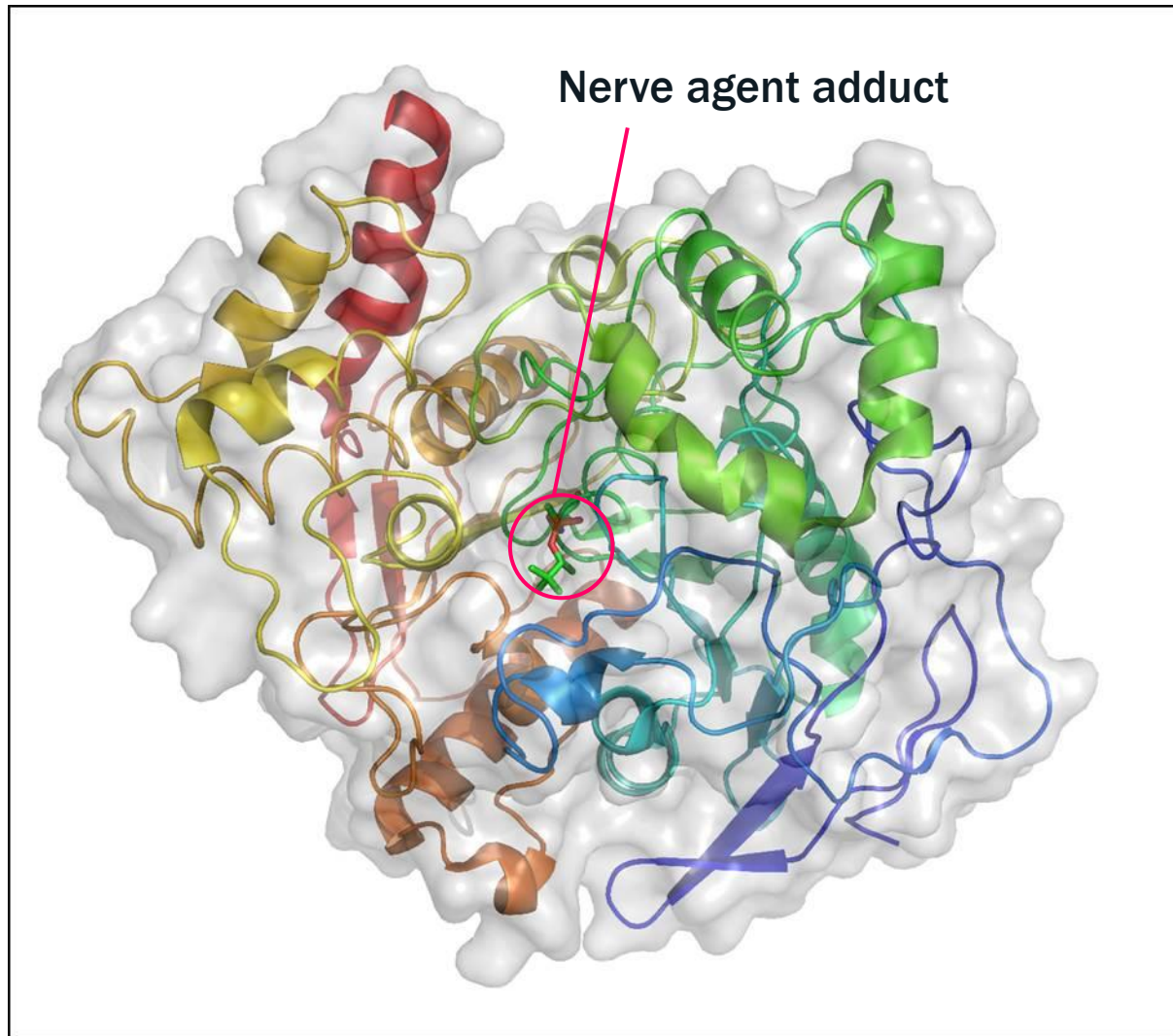
DOI: 10.1021/acschemneuro.8b00148

Sarin:

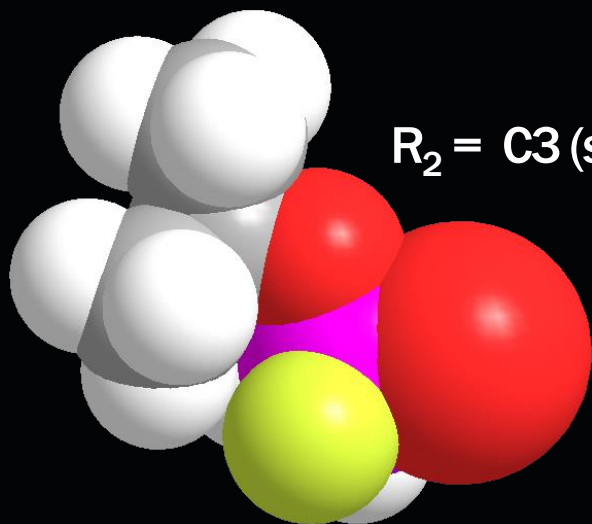


OPCW

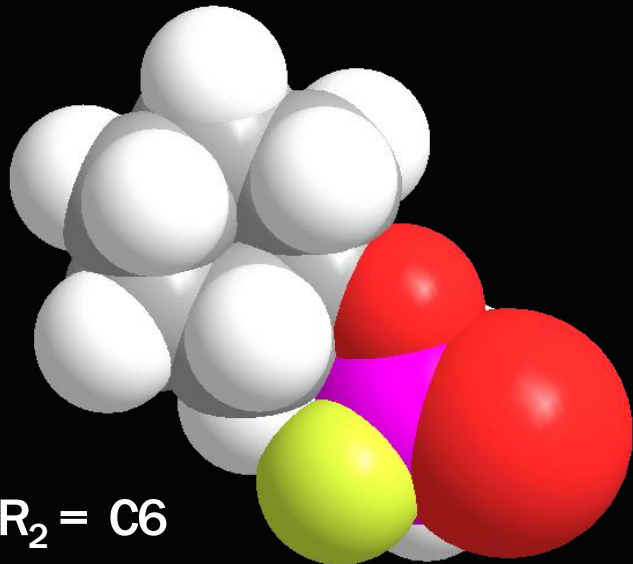
# Is that all a bit too complicated?



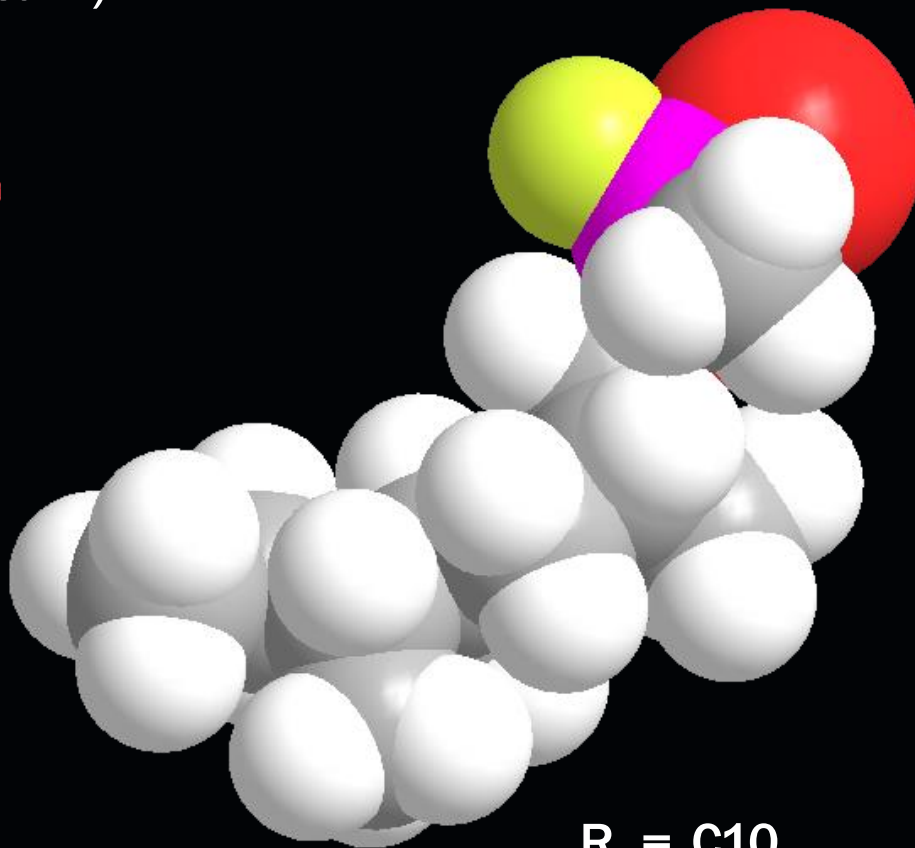
# A Matter of Size



$R_2 = C3$  (sarin)



$R_2 = C6$

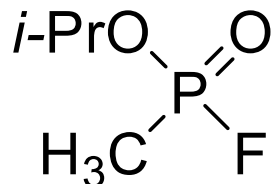


$R_2 = C10$

Families also help to mitigate issues of “designer” compounds being exempt from monitoring and control



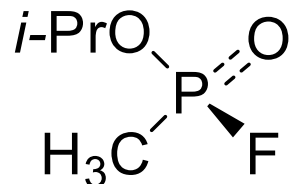
# Are Individual Chemicals any Less Complicated?



Sarin

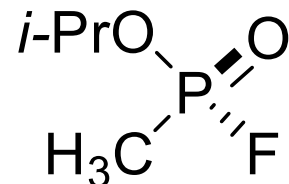
CAS 107-44-8

Schedule 1.A.01



(*R*)-(-)-Sarin

CAS 6171-94-4



(*S*)-(+)-Sarin

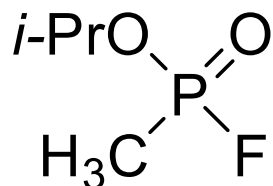
CAS 6171-93-3



OPCW



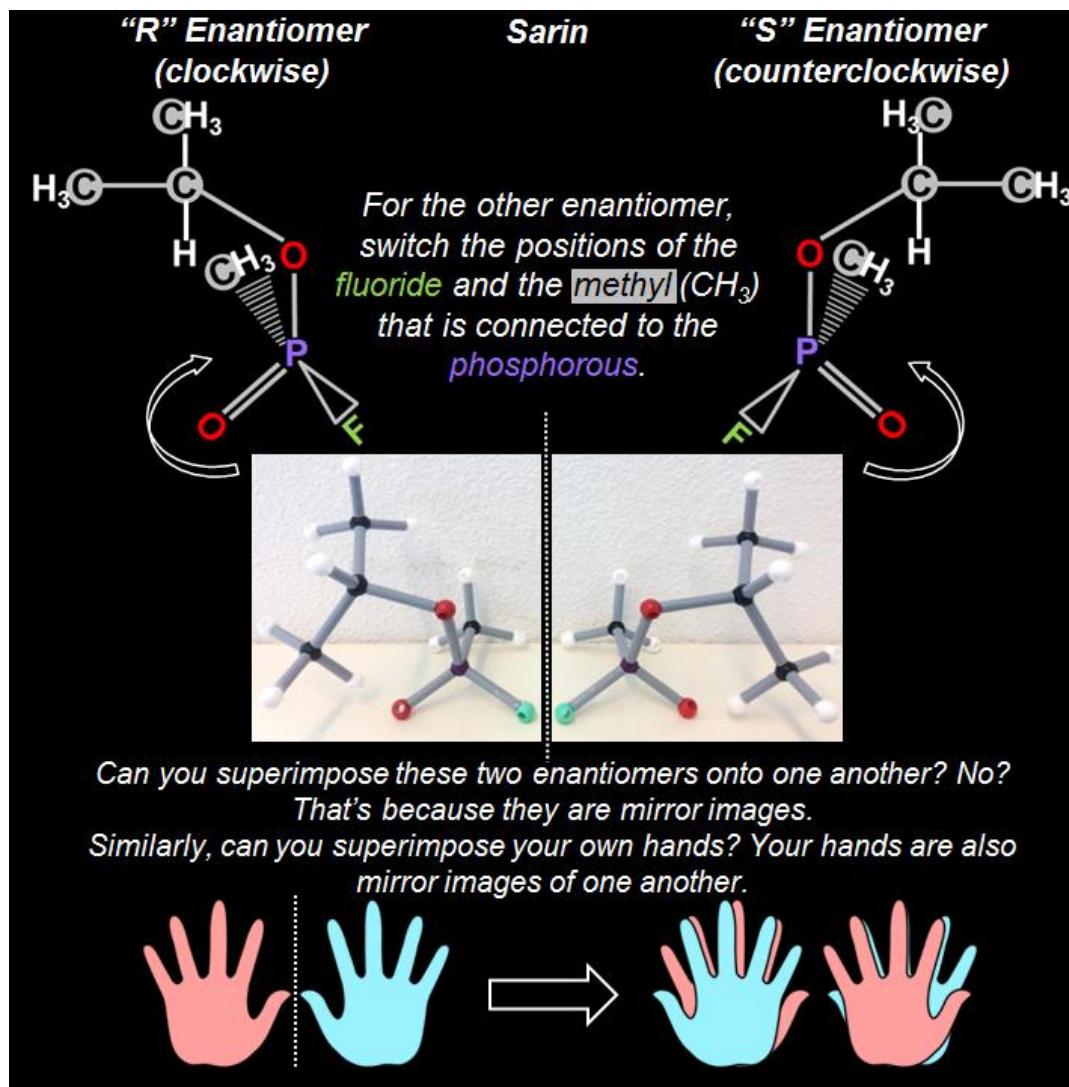
# Are Individual Chemicals any Less Complicated?



Sarin

CAS 107-44-8

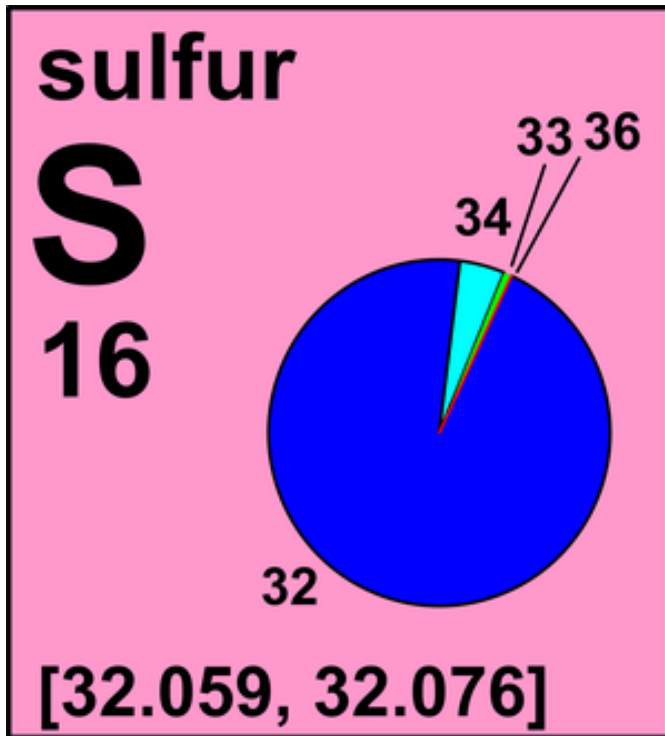
Schedule 1.A.01



OPCW

**Stereoisomers should still fall under the Schedule of the parent compound (SAB Recommendation)**

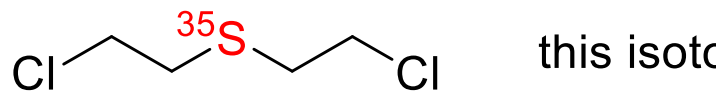
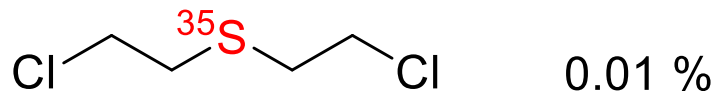
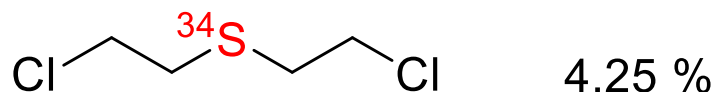
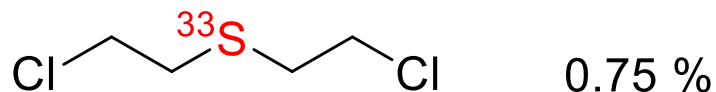
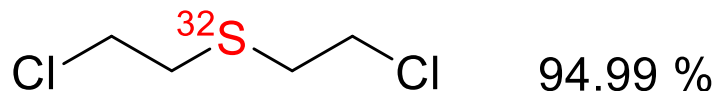
# ISOTOPES



**16 protons**  
**+**  
**16, 17, 18 or 19 neutrons**  
**=**  
**4 isotopes (<sup>32</sup>S, <sup>33</sup>S, <sup>34</sup>S, <sup>35</sup>S)**

# ISOTOPES

**Isotopically labeled chemicals should still fall under the Schedule of the parent compound (SAB Recommendation)**



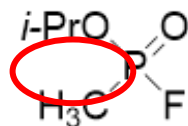
this isotopically labelled form has CAS 6755-76-6

sulfur mustard: bis(2-chloroethyl)sulfide  
as listed within Schedule 1.A.04 under  
CAS 505-60-2

# ISOTOPES

**Just to complicate things more:**

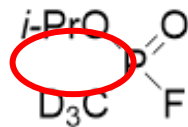
Hydrogen isotopes are written in chemical structures as: H ( $^1\text{H}$ ), D ( $^2\text{H}$ ) or T ( $^3\text{H}$ )



sarin

Schedule 1.A.01

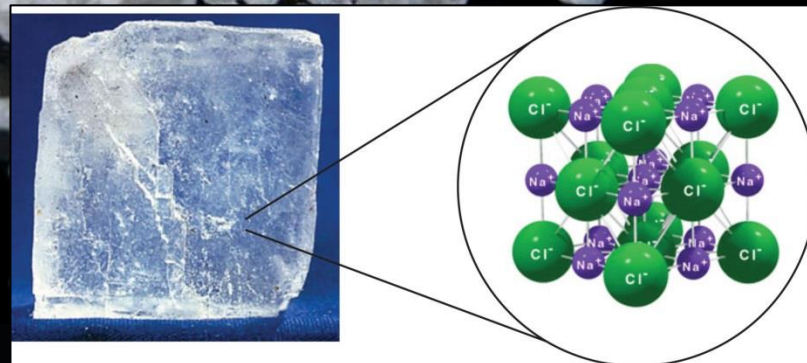
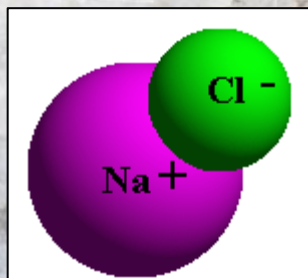
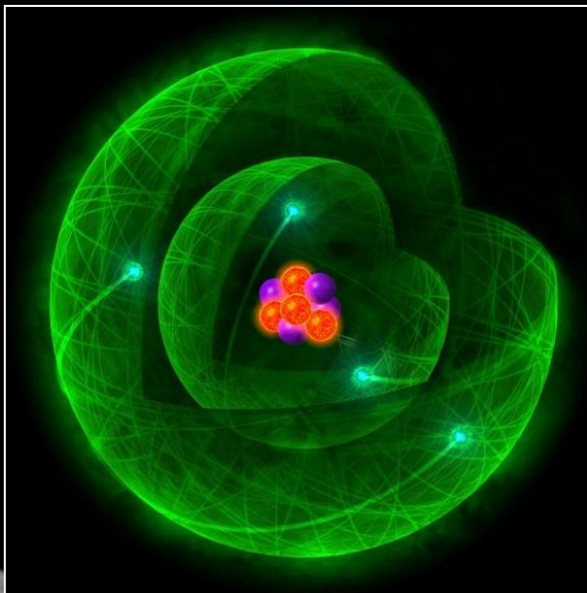
CAS 107-44-8



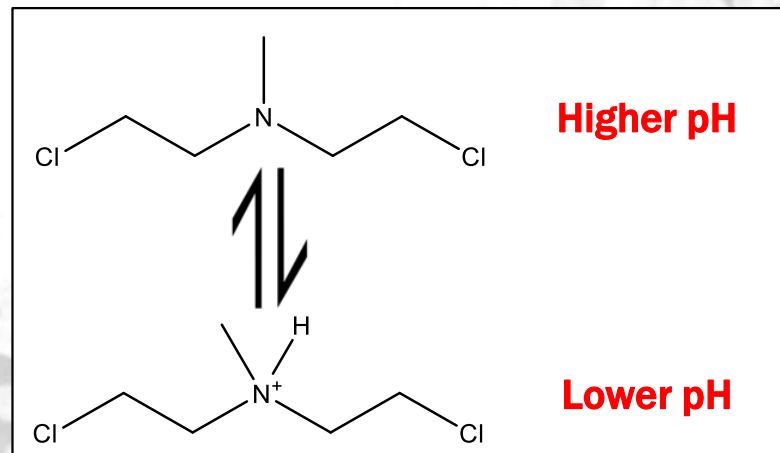
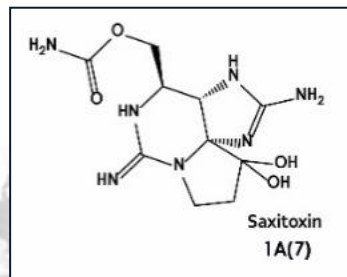
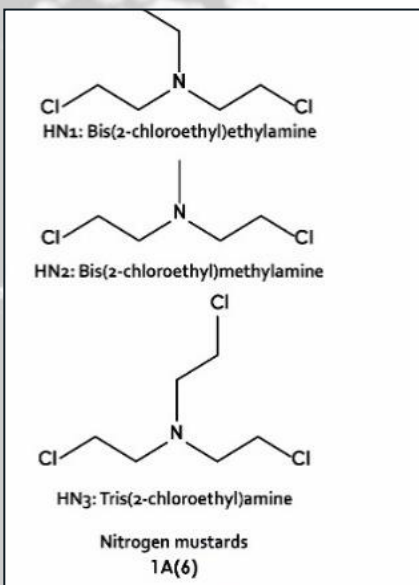
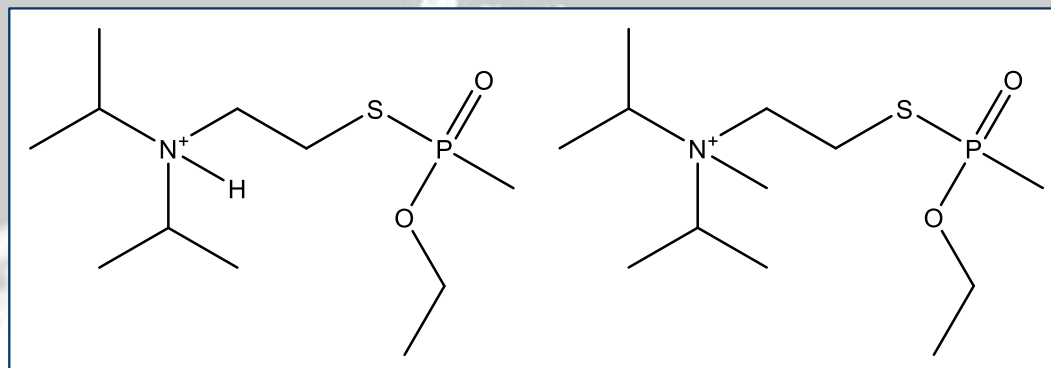
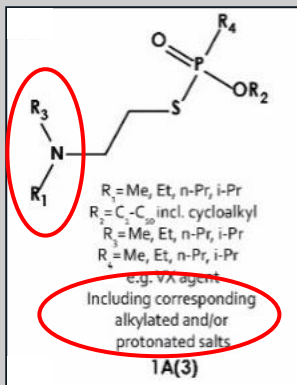
sarin-*d*<sub>3</sub>

CAS 104801-08-3

# Salts?

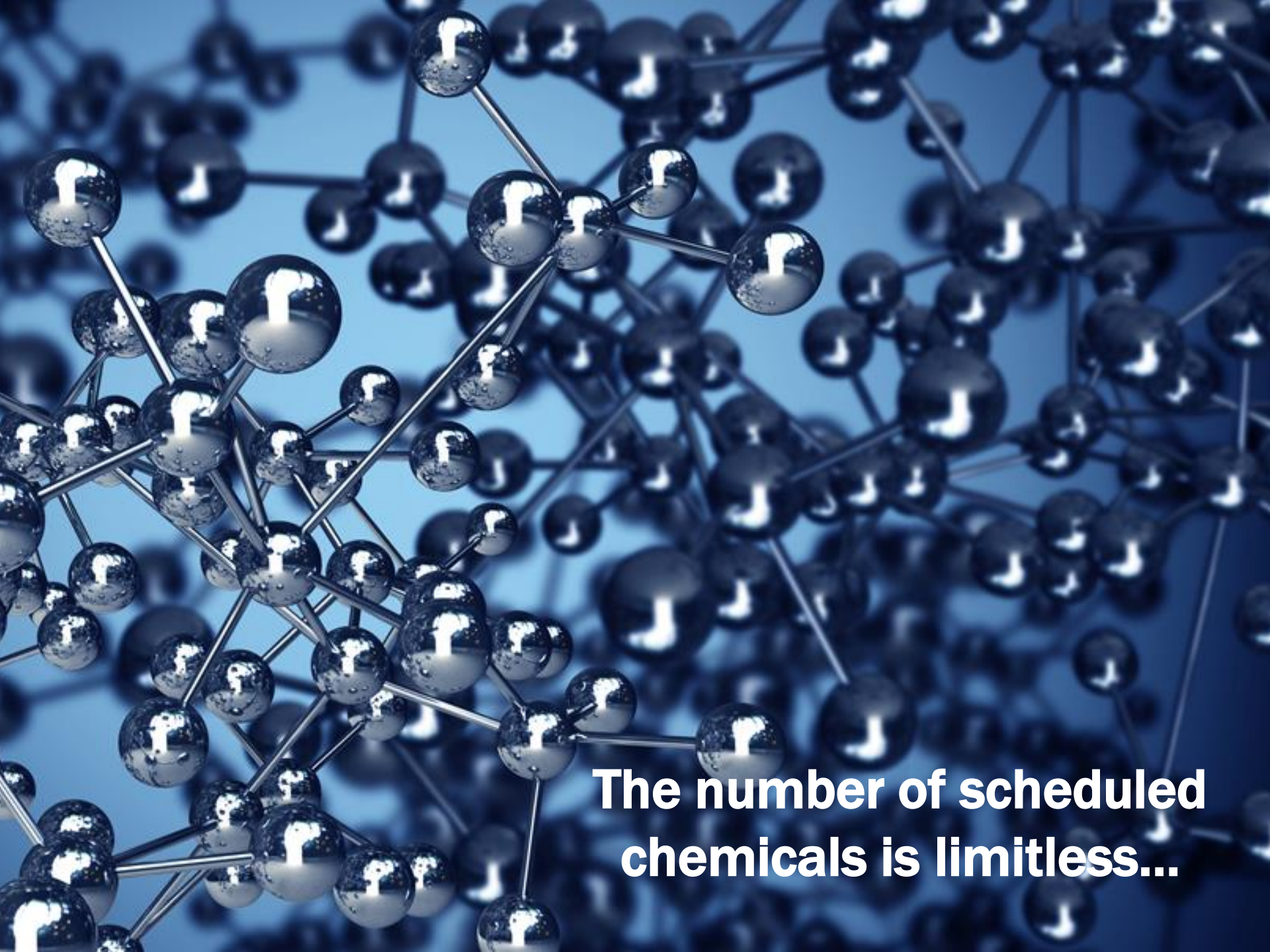


# Why Does This Matter?



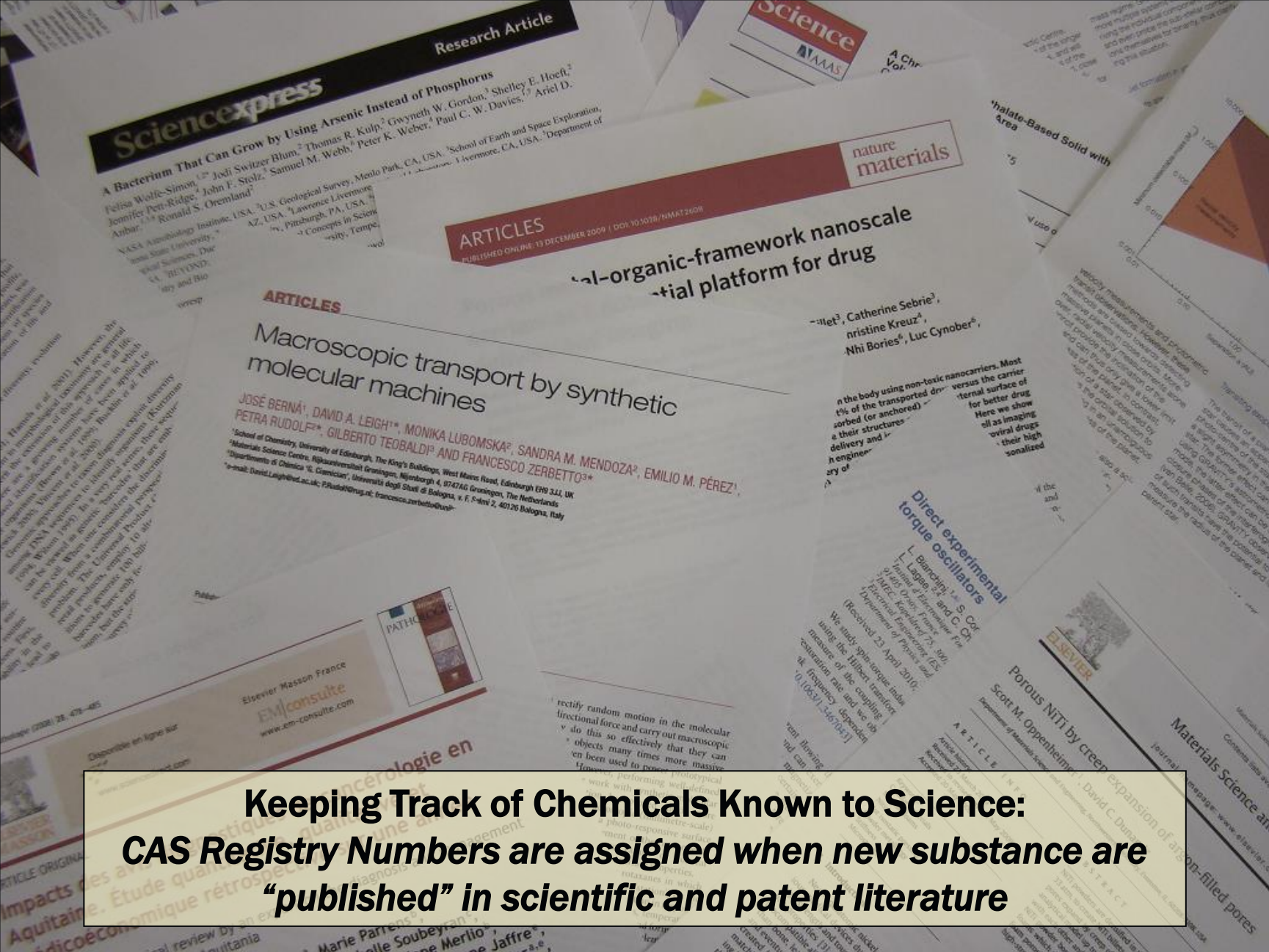
**Are salts of 1A.04 and 1A.07 chemicals scheduled?**

**Should salts of scheduled chemicals not specified on the schedules be scheduled?**



**The number of scheduled  
chemicals is limitless...**

**Keeping Track of Chemicals Known to Science:  
CAS Registry Numbers are assigned when new substance are  
“published” in scientific and patent literature**







## Scheduled Chemicals Database

### Login

Email:

Password:

Login

[New user?](#) | [Forgot your password?](#)



[Search chemicals](#)

[Send a comment](#)

**~32,000 CAS numbers assigned  
to scheduled chemicals**

## Chemicals

Ordered by Schedule and by CAS Registry Number or Key

**Chemical name:** 1-Isobutyl-3-methylbutyl isopropylphosphonofluoridate

Schedule: IA01

**CAS RN:**

HS code: 2931.39

Key: (108-82-7)-11A1

Molecular formula: C<sub>12</sub>H<sub>26</sub>FO<sub>2</sub>P

CAS Index Name: Phosphonofluoric acid, 1-methylethyl-, 1-isobutyl-3-methylbutyl ester

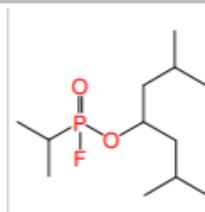
**IUPAC name:** 1-Isobutyl-3-methylbutyl isopropylphosphonofluoridate

Synonyms: Phosphonofluoric acid, 1-methylethyl-, 2,6-dimethylhept-4-yl ester

O-1-Isobutyl-3-methylbutyl isopropylphosphonofluoridate

2,6-Dimethylheptan-4-yl 1-methylethylphosphonofluoridate

2,6-Dimethylhept-4-yl 1-methylethylphosphonofluoridate



**Chemical name:** 1-Isobutyl-3-methylbutyl propylphosphonofluoridate

Schedule: IA01

**CAS RN:**

HS code: 2931.39

Key: (108-82-7)-P1A1

Molecular formula: C<sub>12</sub>H<sub>26</sub>FO<sub>2</sub>P

CAS Index Name: Phosphonofluoric acid, propyl-, 1-isobutyl-3-methylbutyl ester

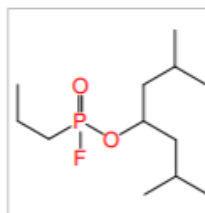
**IUPAC name:** 1-Isobutyl-3-methylbutyl propylphosphonofluoridate

Synonyms: Phosphonofluoric acid, propyl-, 2,6-dimethylhept-4-yl ester

O-1-Isobutyl-3-methylbutyl propylphosphonofluoridate

2,6-Dimethylheptan-4-yl propylphosphonofluoridate

2,6-Dimethylhept-4-yl propylphosphonofluoridate



**Chemical name:** Cyclohexyl methyl-d3-phosphonofluoridate

Schedule: IA01

**CAS RN:**

HS code: 2845.90

Key: (108-93-0)-M1A1(D3)

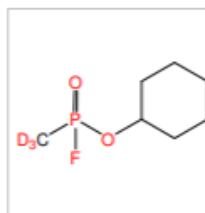
Molecular formula: C<sub>7</sub>H<sub>11</sub>D<sub>3</sub>FO<sub>2</sub>P

CAS Index Name: Phosphonofluoric acid, methyl-d3-, cyclohexyl ester

**IUPAC name:** Cyclohexyl methyl-d3-phosphonofluoridate

Synonyms: O-Cyclohexyl trideuteriomethylphosphonofluoridate

O-Cyclohexyl methyl-d3-phosphonofluoridate



**Not all scheduled chemicals that have been declared have CAS numbers**

Handbook on Chemicals 2017 Revised version 1

[www.opcw.org/our-work/non-proliferation/declarations-adviser/handbook-on-chemicals/](http://www.opcw.org/our-work/non-proliferation/declarations-adviser/handbook-on-chemicals/)

# What About Chemicals Not on Schedules?

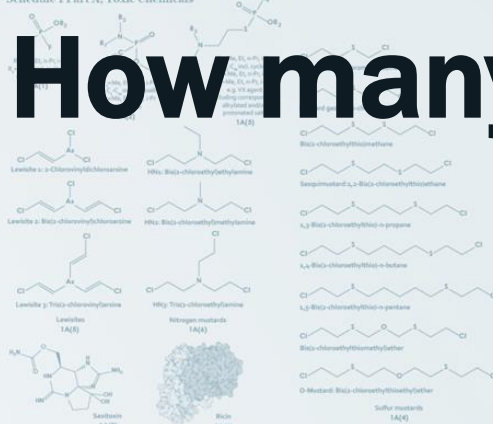
## Schedule 1

### Guidelines for Schedule 1

The following criteria shall be taken into account in considering whether a toxic chemical or precursor shall be included in Schedule 1:

- (a) It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article I;
- (b) It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:
  - (i) It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparable properties;
  - (ii) It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon; it may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;
  - (c) It has little or no use for purposes not prohibited under this Convention.

#### Schedule 1 Part A, Toxic Chemicals



#### Schedule 1 Part B, Precursors



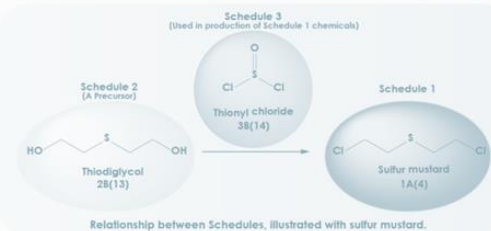
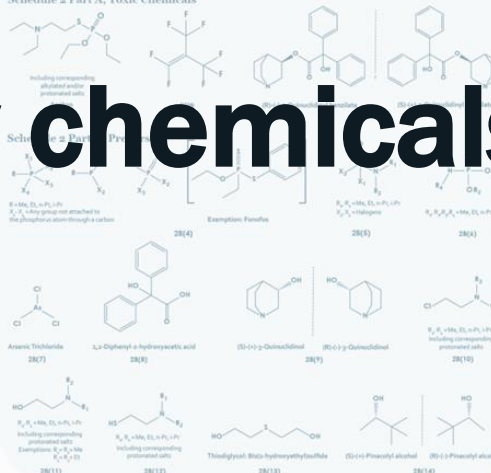
## Schedule 2

### Guidelines for Schedule 2

The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:

- (a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;
- (b) 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;
- (c) It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;
- (d) It is not produced in large commercial quantities for purposes not prohibited under this Convention.

#### Schedule 2 Part A, Toxic Chemicals



## Schedule 3

### Guidelines for Schedule 3

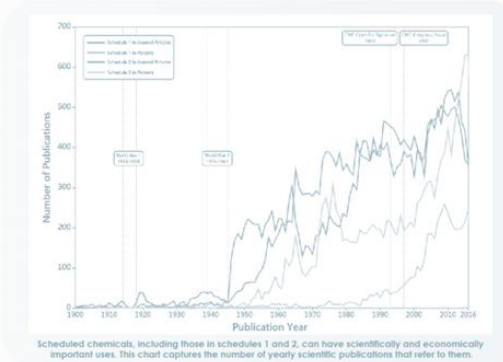
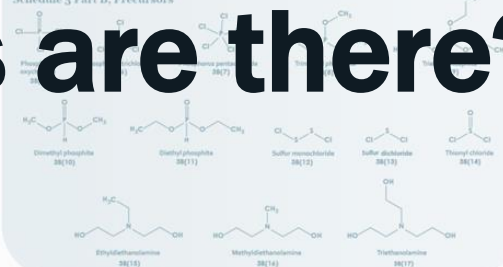
The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

- (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;
- (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.

#### Schedule 3 Part A, Toxic Chemicals



#### Schedule 3 Part B, Precursors



Scheduled chemicals, including those in schedules 1 and 2, can have scientifically and economically important uses. This chart captures the number of yearly scientific publications that refer to them.



ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

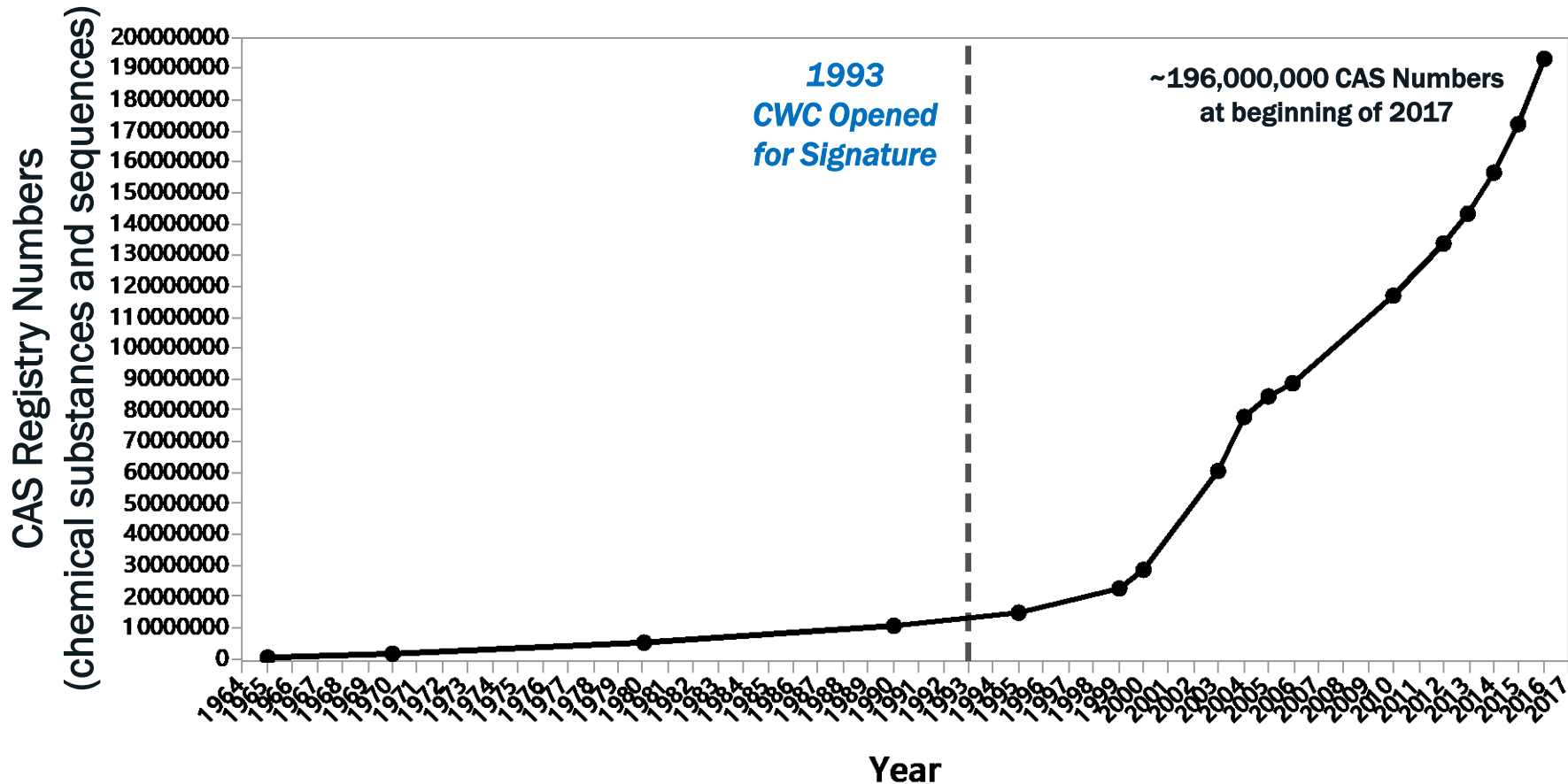
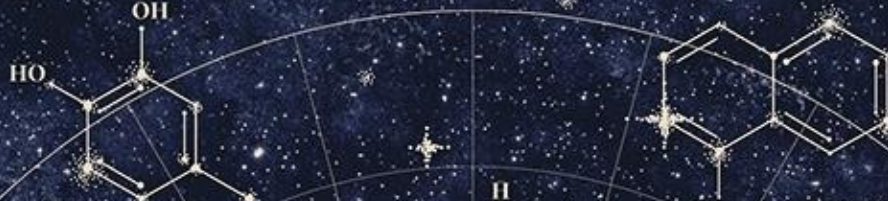
[@opcw](#)
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*More Possible Chemicals  
than Atoms in the Universe!*



SCANNING SPACE...

**> 209 million CAS Numbers as of July 2018...**  
**> 142 million are organic/inorganic chemical substances**  
**> 13 million new CAS numbers in past 18 months...**

# What About Chemicals Not on Schedules?

## Which unscheduled chemicals matter?

### Definition of a Toxic Chemical

Any chemical which through its chemical action on life processes can cause death, temporary incapacitation or permanent harm to humans or animals. ***This includes all such chemicals, regardless of their origin or of their method of production***, and regardless of whether they are produced in facilities, in munitions or elsewhere

Chemical Weapons Convention Article II, Paragraph 2



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OPCW

# Riot Control Agents

Fauzia Nurul Izzati, Jonathan E. Forman and Christopher M. Timperley

Riot control agents cannot be scheduled...


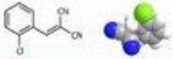
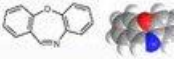


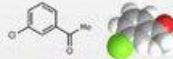
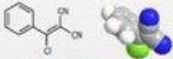


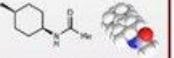
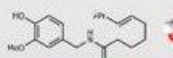


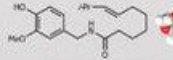
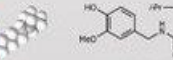

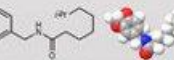
## What is the definition of a Riot Control Agent (RCA)?

From paragraph 7, Article II of the Chemical Weapons Convention:

"Any chemical not listed in a Schedule, which can produce rapidly in humans sensory irritation or disabling physical effects which disappear within a short time following termination of exposure."

## What are Riot Control Agents?

Chemicals that meet the criteria of an RCA include the following:

 <b>2-Chloroacetophenone (CN)</b> Synonyms: Mace, CAE, KM CB (10% CN, 45% benzoxon, 40% carbon-tetrachloride), CWC (30% CN, 70% chlorobenzonitrile), and CS (23% CN, 38.4% chlorobenzonitrile, 38.4% chlorobenzonitrile). Physical states: White solid with odour of apple blossom Melting Point 54-56 °C; Boiling Point 245 °C	 <b>2-Chlorobenzylidene malonitrile (CS)</b> Synonyms: 2-Chlorobenzylidene malonitrile, $\alpha$ -chlorobenzylidene malonitrile, R62 CS (green), CS1 (5% CS, 5% silica aerosol), CS2 (CS and silica aerosol), CSX (1 g CS, 99 g <i>o</i> - <i>n</i> -acetyl phosphates); CS dissolved in methyl ethyl ketone is used in spray devices. Physical states: White solid with pungent property odour Melting Point 93-95 °C; Boiling Point 310-315 °C, dec	 <b>Dibenz(b,f)(1,4)oxazepine (CB)</b> Synonyms: CB Physical states: Yellow stable powder Melting Point 72 °C; Boiling Point 335 °C	 <b>2'-Chloroacetophenone</b> Synonyms: $\alpha$ -chloroacetophenone Physical states: Colourless liquid Boiling Point 220 °C	 <b>4-Nonanoylmorpholine</b> Synonyms: MPA, MPK, patergonic acid morpholide Physical states: Liquid Boiling Point 310 °C
 <b>3'-Chloroacetophenone</b> Synonyms: <i>m</i> -chloroacetophenone Physical states: Colourless liquid Boiling Point 228 °C	 <b><math>\alpha</math>-Chlorobenzylidene malonitrile</b> Synonyms: none Physical states: White solid Melting Point 48-70 °C; Boiling Point 138 °C @ 1 mmHg	 <b>N,N'-Bis(isopropyl)ethylene diamine</b> Synonyms: Diamine Physical states: Volatile tan-colored solid Melting Point 48-50 °C	 <b>N,N'-Bis(tert-butyl)ethylene diamine</b> Synonyms: none Physical states: White solid Melting Point 39-43 °C	 <b>Cis-4-Acetylamino cyclohexylmethane</b> Synonyms: none Physical states: White solid Melting Point 112 °C
 <b>8-Methyl-N-vanillyl-trans-6-nonenamide</b> Synonyms: C, capesin, Maltin, Zacin Physical states: White solid Melting Point 62-65 °C; Boiling Point 210-220 °C at 0.1 mmHg	 <b>8-Methyl-N-vanillylnonanamide</b> Synonyms: Dihydrocapsaicin, DHC Physical states: White solid Physical data unavailable	 <b>N-Vanillylnonanamide</b> Synonyms: N-(4-hydroxy-3-methoxy-benzyl)nonanamide, nonivamide, pseudo-capsaicin, patergonic acid vanillylamide, PAVA Physical states: White solid with stinging odour Melting Point 53 °C		
 <b>N-Vanillyl-9-methyldec-7-ED-enamide</b> Synonyms: homocapsaicin Physical states: Lipophilic colourless odourless crystalline or waxy solid	 <b>N-Vanillyl-9-methyldecaneamide</b> Synonyms: homodihydrocapsaicin Physical states: Lipophilic colourless odourless crystalline or waxy solid	 <b>N-Vanillyl-7-methyloctanamide</b> Synonyms: nor(dihydro)capsaicin Physical states: Lipophilic colourless odourless crystalline or waxy solid	 <b>Oleoresin capaicin (OC)</b> This is a mixture containing $\geq$ 8% capsaicin, capsinin, dihydrocapsaicin, and non(dihydro)capsaicin dissolved in an organic solvent.	

## How do Riot Control Agents work?

RCAs produce irritation through binding to TRP (Transient Receptor Potential) receptors. This activates some of the same biochemical pathways that are triggered by eating horseradish or hot peppers.

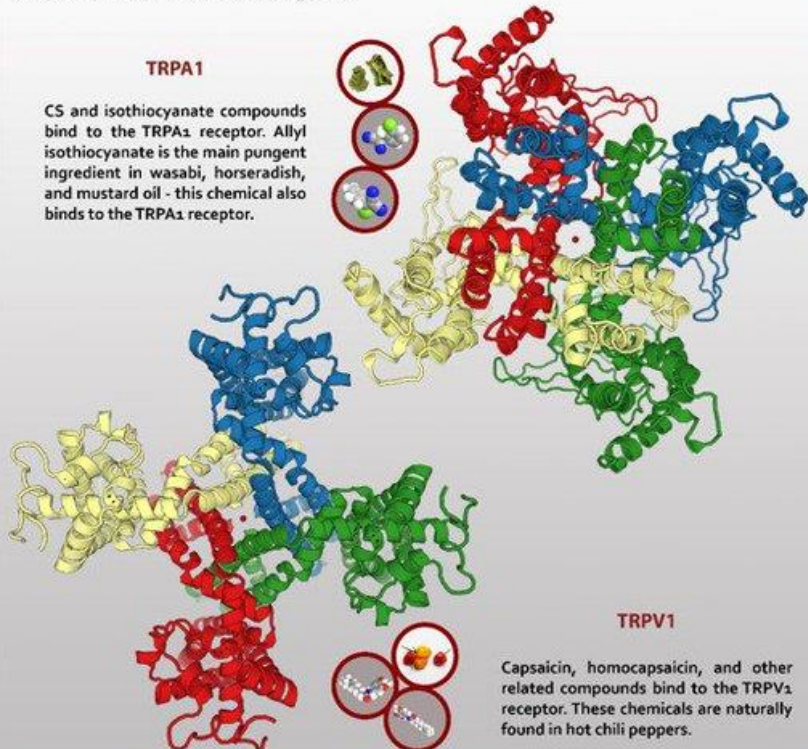
## What are TRP Receptors?

TRP receptors are a family of ion channel receptors mainly located on cell membranes of multicellular organisms. TRP receptors are classified into seven subfamilies: TRPC (canonical or classical), TRPV (vanilloid), TRPM (melastatin), TRPA (ANKTM1 homologues), TRPP (polycystin), TRPML (mucolipin), and TRPN (NOMP-C homologues).

TRP receptor functions are diverse; the receptors serve as versatile sensors that allow individual cells and entire organisms to detect changes in their environment. This includes experiencing changes in temperature, touch, taste and other stimuli (including pain).

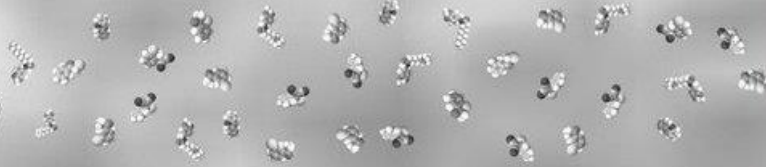
**TRPA1**

CS and isothiocyanate compounds bind to the TRPA1 receptor. Allyl isothiocyanate is the main pungent ingredient in wasabi, horseradish, and mustard oil - this chemical also binds to the TRPA1 receptor.



**TRPV1**

Capsaicin, homocapsaicin, and other related compounds bind to the TRPV1 receptor. These chemicals are naturally found in hot chili peppers.



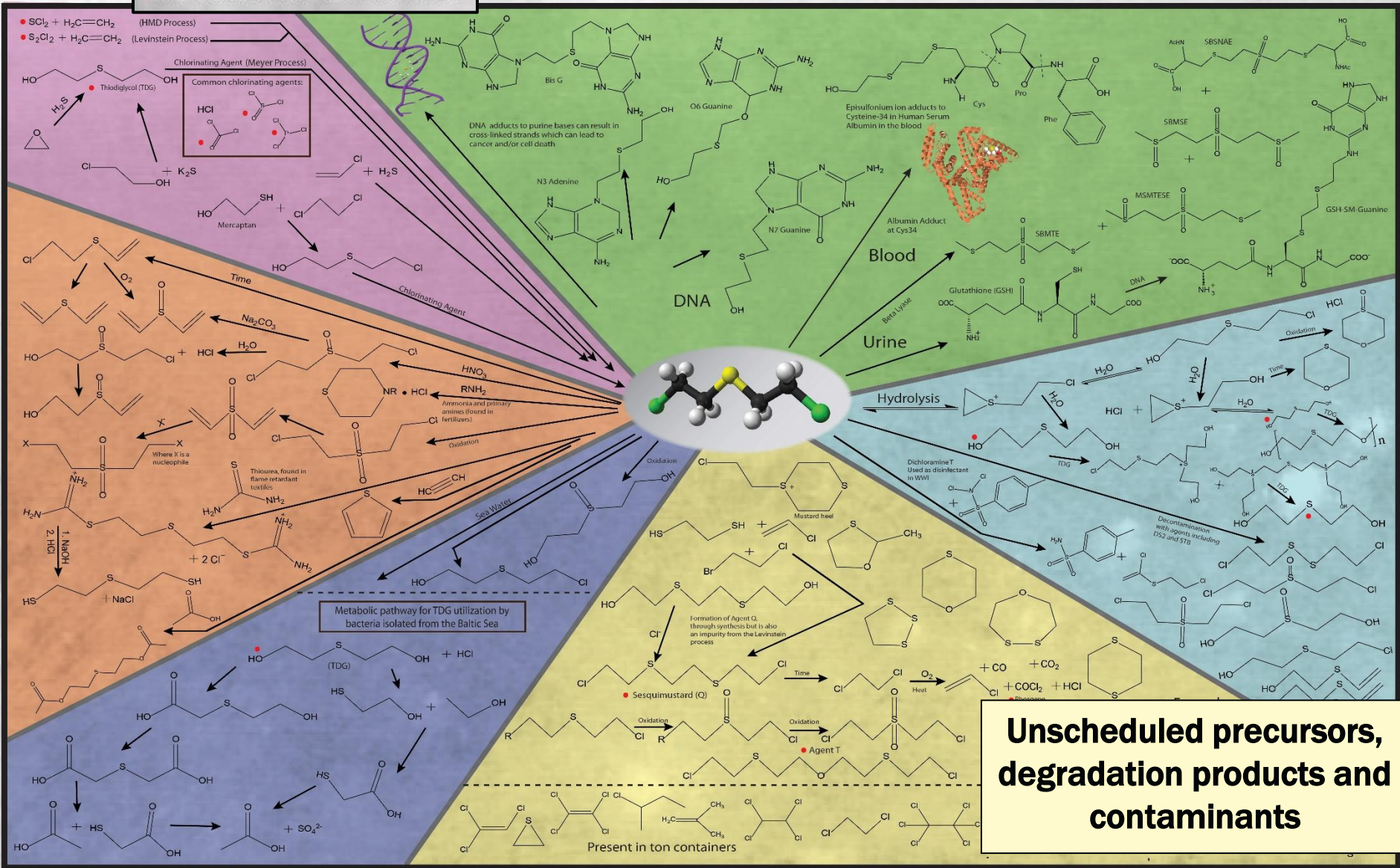


# Degradation and Environmental Fate of Sulfur Mustard

Darcy van Eerten

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## Scheduled Chemical



**Unscheduled precursors, degradation products and contaminants**



# Toxic Industrial Chemicals

TICs listed by hazard index

High	Medium	Low
Ammonia (CAS# 7664-41-7)	Acetone cyanohydrin (CAS# 75-86-5)	Allyl isothiocyanate (CAS# 57-06-7)
Arsine (CAS# 7784-42-1)	Acrolein (CAS# 107-02-8)	Arsenic trichloride (CAS# 7784-34-1)
Boron trichloride (CAS#10294-34-5)	Acrylonitrile (CAS# 107-13-1)	Bromine (CAS# 7726-95-6)
Boron trifluoride (CAS#7637-07-2)	Allyl alcohol (CAS# 107-18-6)	Bromine chloride (CAS# 13863-41-7)
Carbon disulfide (CAS# 75-15-0)	Allylamine (CAS# 107-11-9)	Bromine pentafluoride (CAS# 7789-30-2)
Chlorine (CAS# 7782-50-5)	Allyl chlorocarbonate (CAS# 2937-50-0)	Bromine trifluoride (CAS# 7787-71-5)
Diborane (CAS# 19287-45-7)	Boron tribromide (CAS# 10294-33-4)	Carbonyl fluoride (CAS# 353-50-4)
Ethylene oxide (CAS# 75-21-8)	Carbon monoxide (CAS# 630-08-0)	Chlorine pentafluoride (CAS# 13637-63-3)
Fluorine (CAS# 7782-41-4)	Carbonyl sulfide (CAS# 463-58-1)	Chlorine trifluoride (CAS# 7790-91-2)
Formaldehyde (CAS# 50-00-0)	Chloroacetone (CAS# 78-95-5)	Chloroacetaldehyde (CAS# 107-20-0)
Hydrogen bromide (CAS# 10035-10-6)	Chloroacetonitrile (CAS# 7790-94-5)	Chloroacetyl chloride (CAS# 79-04-9)
Hydrogen chloride (CAS# 7647-01-0)	Chlorosulfonic acid (CAS# 7790-94-5)	Crotonaldehyde (CAS# 123-73-9)
Hydrogen cyanide (CAS#74-90-8)	Diketene (CAS# 674-82-8)	Cyanogen chloride (CAS# 506-77-4)
Hydrogen fluoride (CAS# 7664-39-3)	1,2-Dimethylhydrazine (CAS# 540-73-8)	Dimethyl sulfate (CAS# 77-78-1)
Hydrogen sulfide (CAS# 7783-0604)	Ethylene dibromide (CAS# 106-93-4)	Diphenylmethane-4,4'-diisocyanate (CAS# 101-68-8)
Nitric acid, fuming (CAS# 7697-37-2)	Hydrogen selenide (CAS# 7783-07-5)	Ethyl chloroformate (CAS# 541-41-3)
Phosgene (CAS# 75-44-5)	Methanesulfonyl chloride (CAS# 124-63-0)	Ethyl chlorothioformate (CAS# 2941-64-2)

⋮

Some are  
scheduled

⋮

⋮

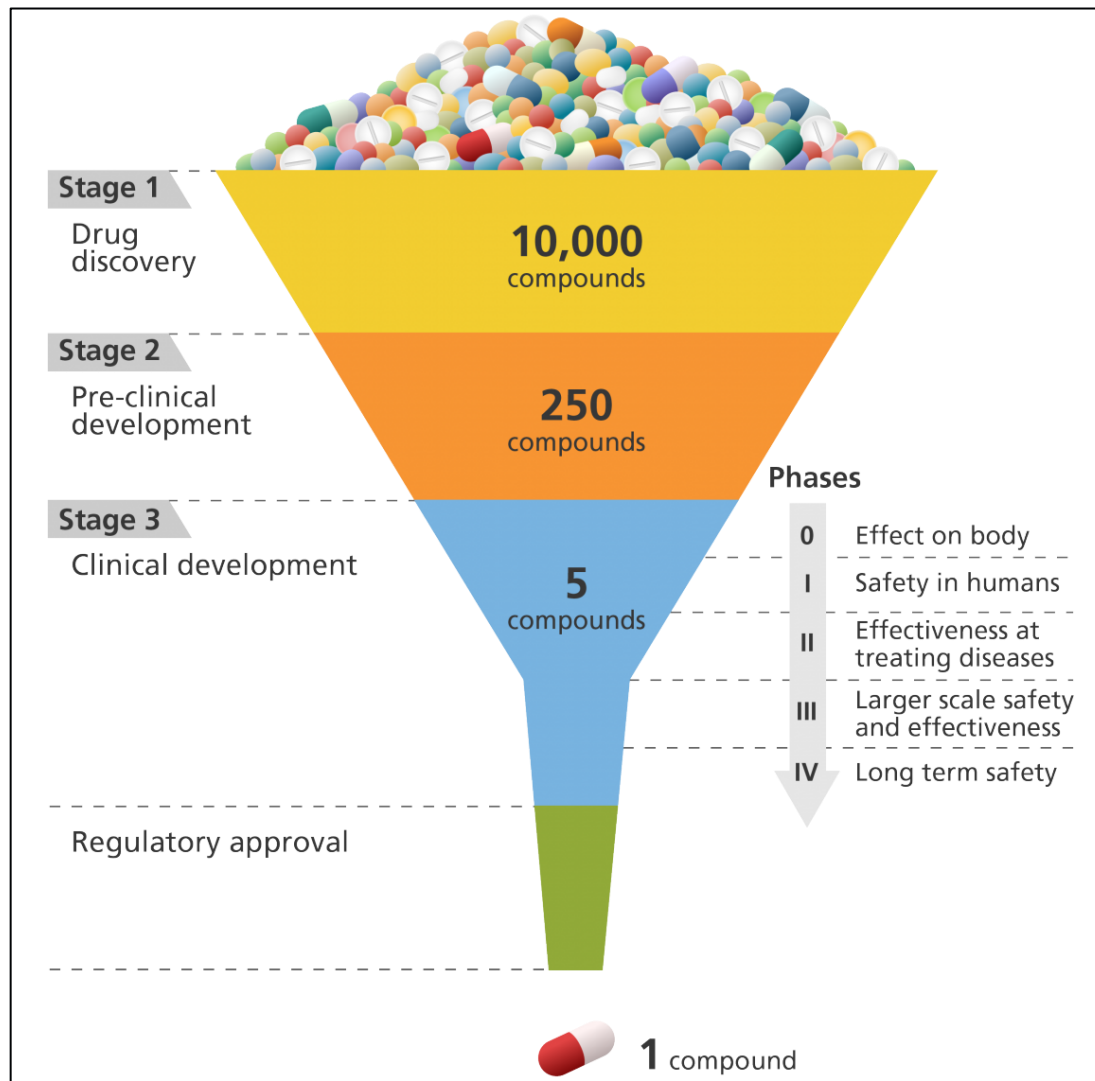
	n-Octyl mercaptan (CAS# 111-88-6)	Tetraethyl lead (CAS# 78-00-2)
	Titanium tetrachloride (CAS# 7550-45-0)	Tetraethyl pyrophosphate (CAS# 107-49-3)
	Trichloroacetyl chloride (CAS# 76-02-8)	Tetramethyl lead (CAS# 75-74-1)
	Trifluoroacetyl chloride (CAS# 354-32-5)	Toluene 2,4-diisocyanate (CAS# 584-84-9)
		Toluene 2,6-diisocyanate (CAS# 91-08-7)

<https://www.osha.gov/SLTC/emergencypreparedness/guides/chemical.html>

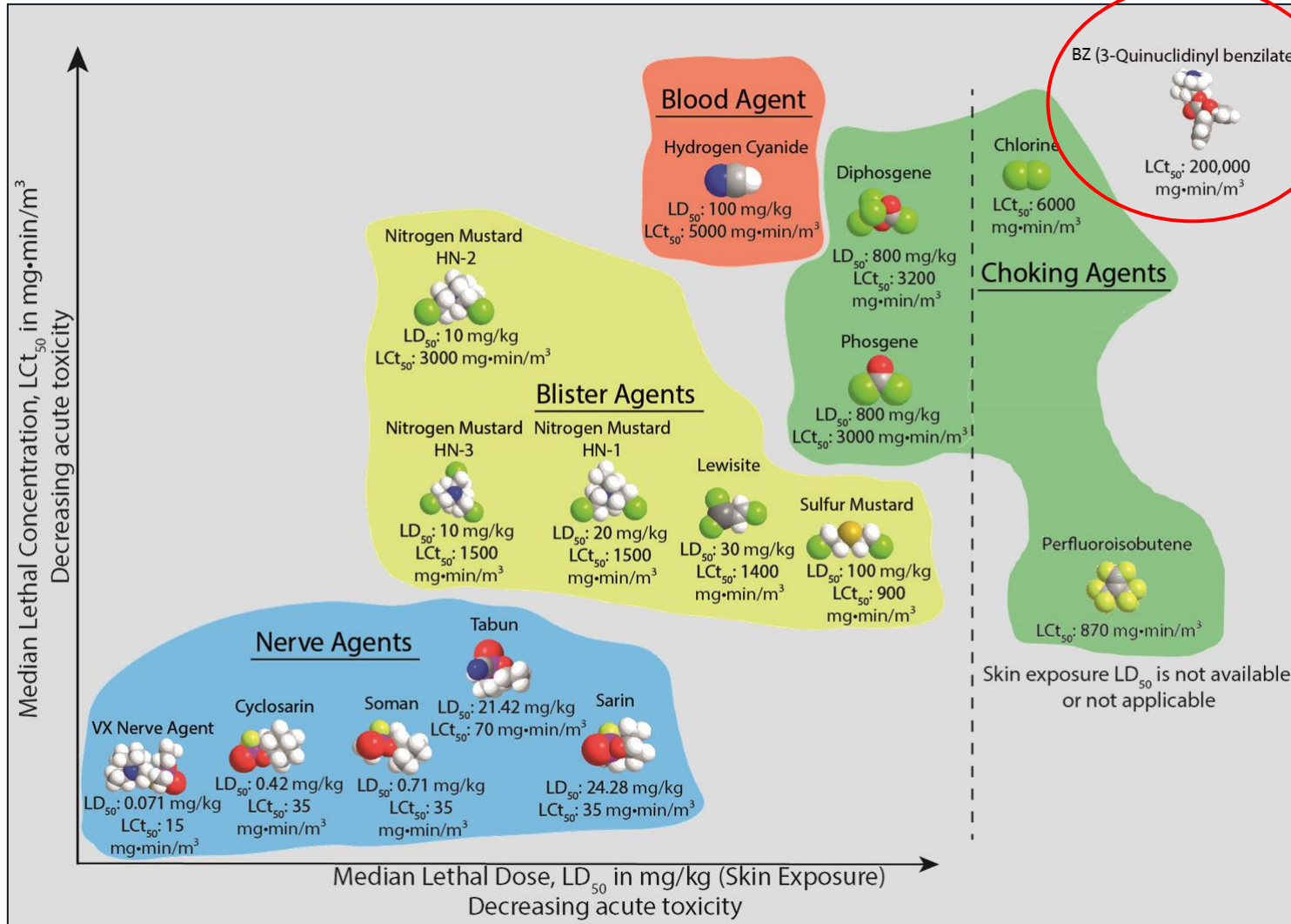


OPCW

# Central Nervous System-Acting Chemicals

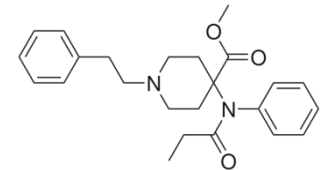


# Relative Toxicity?



Can be lower than other CW

Can also be very high!

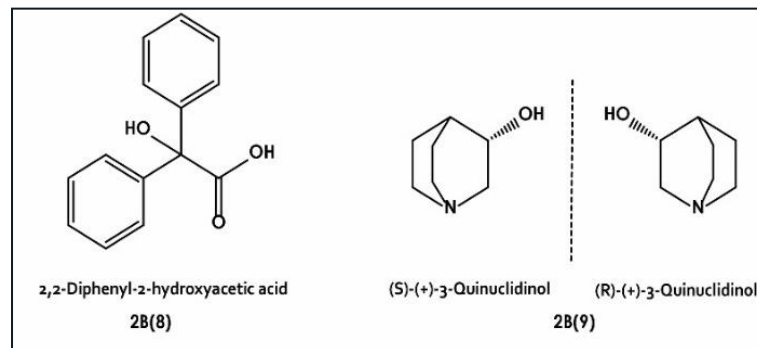
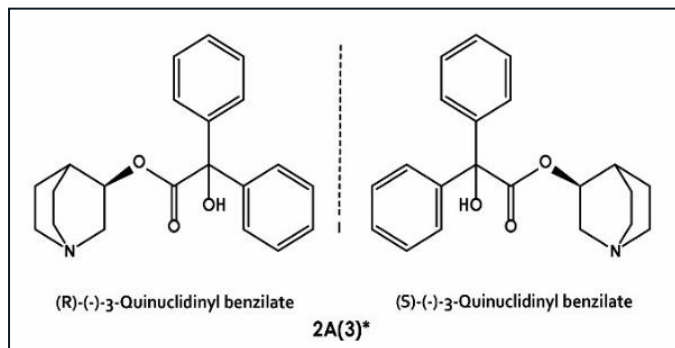


e.g. Carfentanil



OPCW

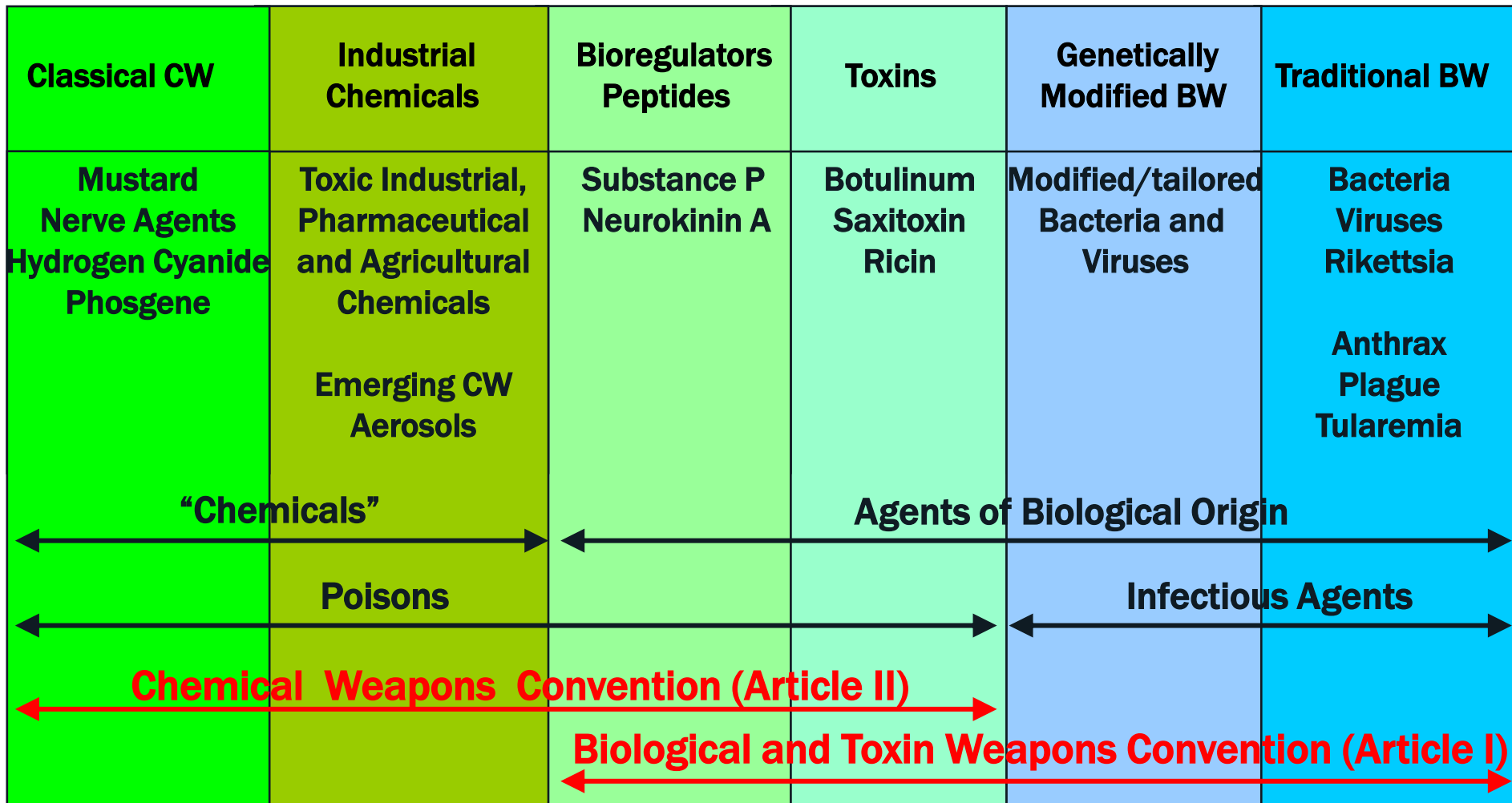
# A scheduled CNS-acting chemical and its precursors



**These precursors are not as widely used for pharmaceuticals as in the past**  
***thanks to new and improved chemistry!***



# Chemical – Biological Threat Spectrum



Adopted from Graham S Pearson, ASA Newsletter, 90-1, February 1990 and Robert Mathews at TWG on Convergence. 1<sup>st</sup> Meeting 2011



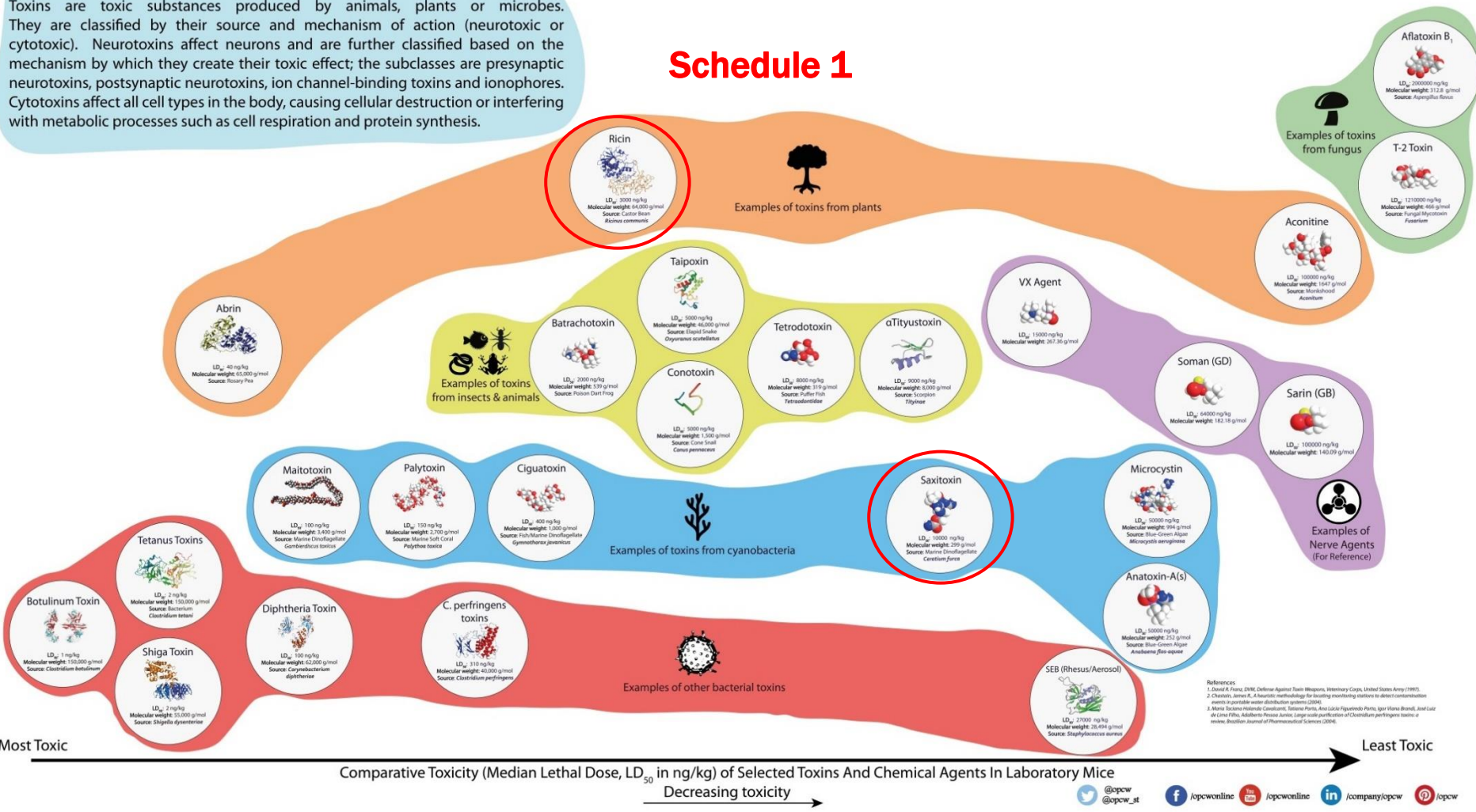
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# Toxins

## What are Toxins?

Toxins are toxic substances produced by animals, plants or microbes. They are classified by their source and mechanism of action (neurotoxic or cytotoxic). Neurotoxins affect neurons and are further classified based on the mechanism by which they create their toxic effect; the subclasses are presynaptic neurotoxins, postsynaptic neurotoxins, ion channel-binding toxins and ionophores. Cytotoxins affect all cell types in the body, causing cellular destruction or interfering with metabolic processes such as cell respiration and protein synthesis.

## Schedule 1



References:  
 1. David F. Franz, DVM, Defense Against Twin Weapons, Veterinary Corps, United States Army (1995).  
 2. Chavakis, Armin, et al. A neuronal membrane for locating monitoring stations to detect contamination events in portable water distribution systems (2006).  
 3. Maria Do Carmo Pinheiro Cavalcanti, Simone Porto, Ana Lucia Figueiredo Porto, Igor Mano Brandi, and Luiz de Cleyr Filho, Antibiotic Pseudo-Antibiotic, Large scale purification of Clostridium perfringens toxin: a review, Brazilian Journal of Pharmaceutical Sciences (2006).

# Toxins

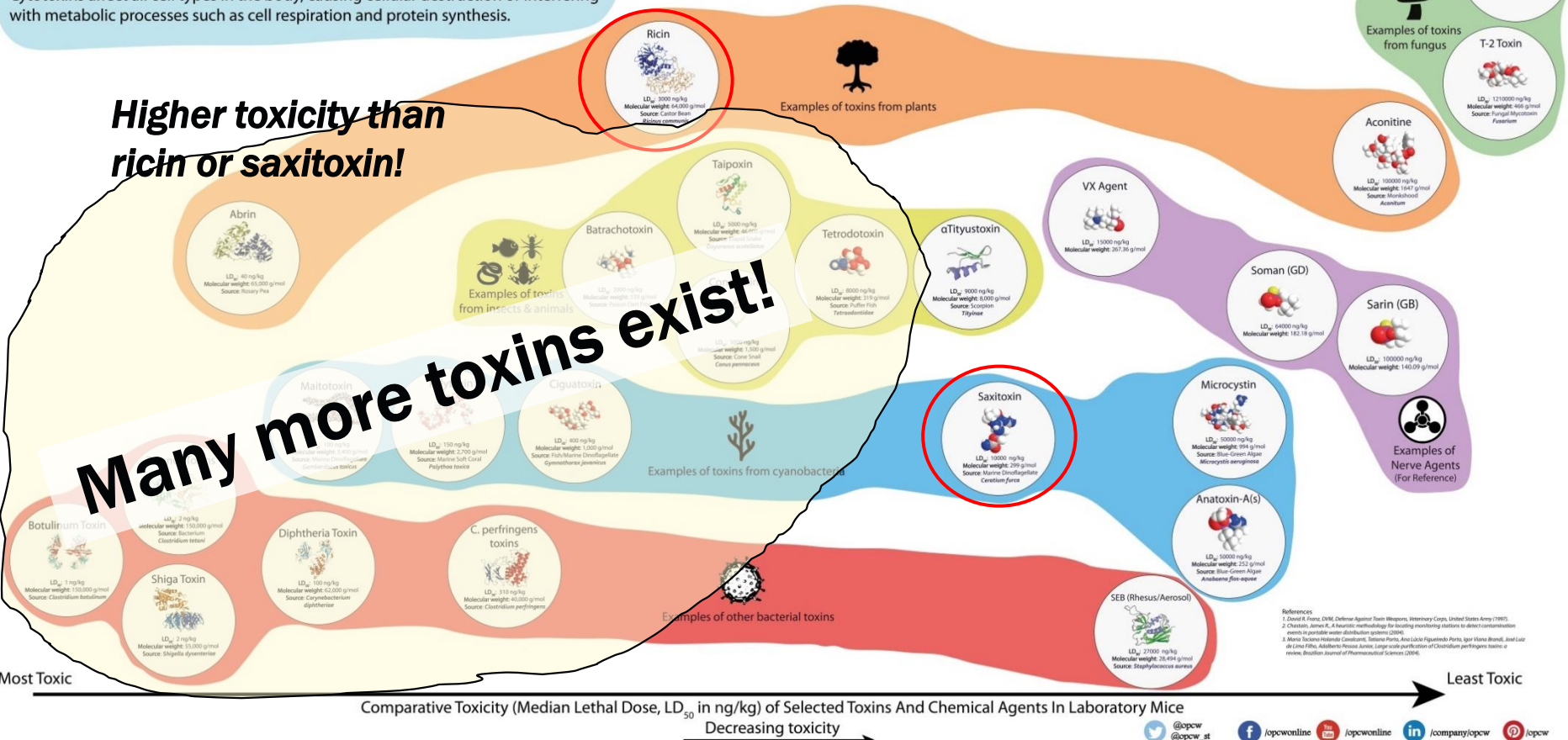
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## Schedule 1

Higher toxicity than ricin or saxitoxin!

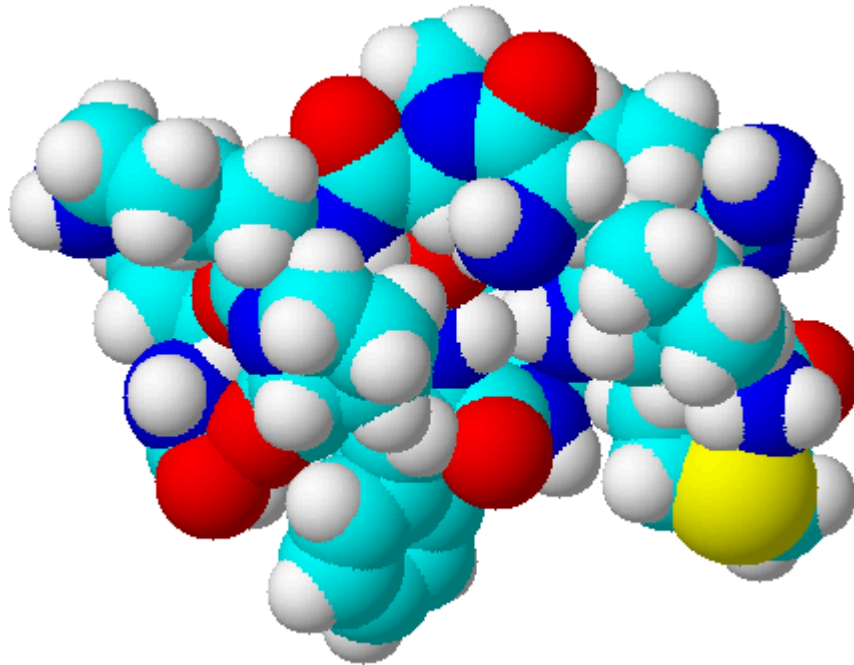
Many more toxins exist!



References:  
 1. David F. Francis, DVM, Defense Against Toxic Weapons, Veterinary Corps, United States Army (1995).  
 2. Chavakis, Jörn, et al. A neural methodology for locating monitoring stations to detect contamination events in portable water distribution systems (2006).  
 3. Maria Inês de Almeida Cavalcanti, Simone Porto, Ana Lúcia Figueiredo Porto, Igor Mano Brandi, and Luiz de Cássio Filho, Antibiotic Pseudo-Antibiotic, Large scale purification of Clostridium perfringens toxin a review. Brazilian Journal of Pharmaceutical Sciences (2006).

# Bioregulators

- Endogenous molecules that regulate life processes...

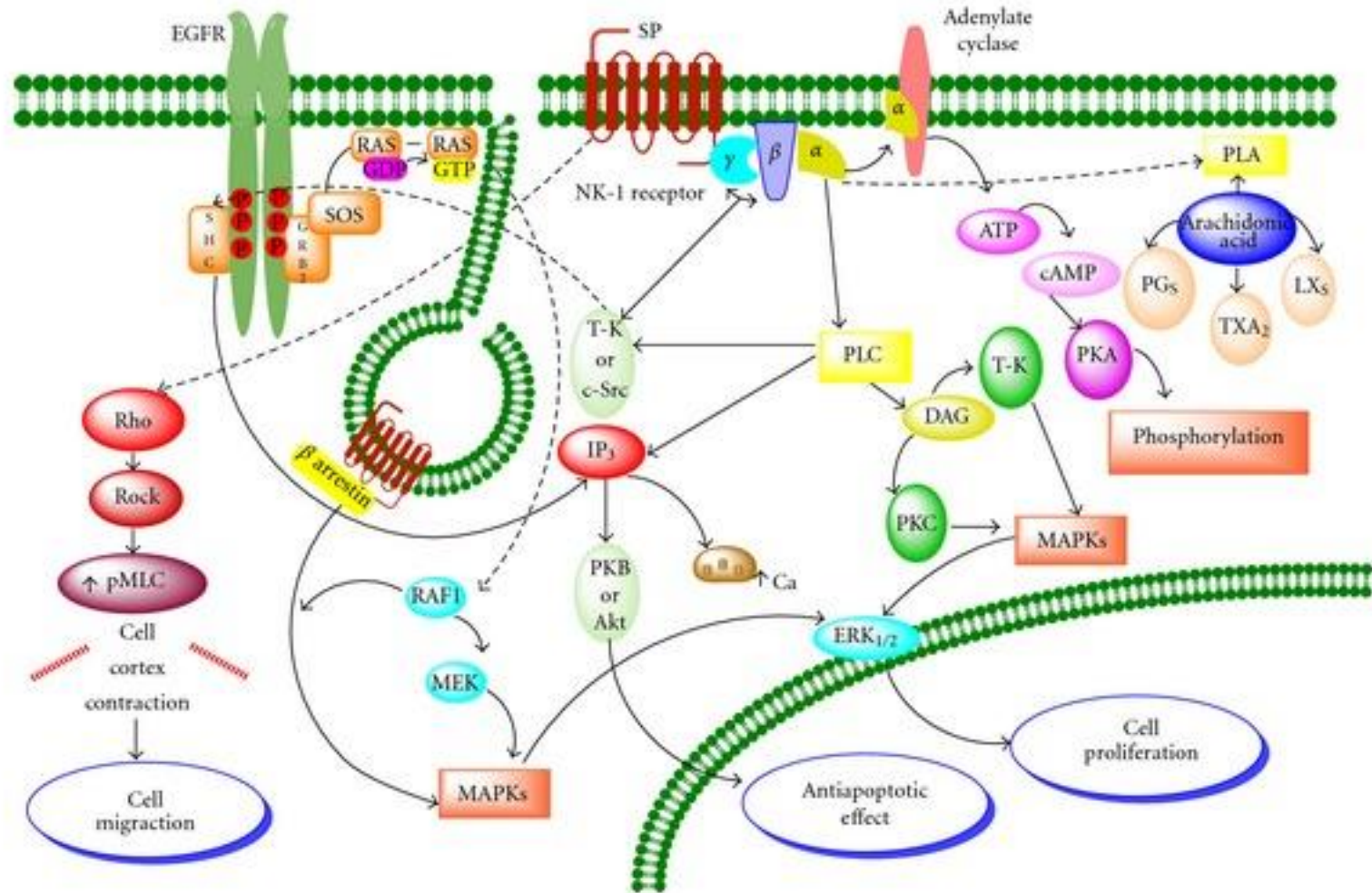


*Substance P (pain modulation)*





# Bioregulators



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**SAB does not view advances in research on bioregulators as posing a risk at present**

# Unscheduled Chemicals that Pose a Risk to the Convention?



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# Recent Advice from the Scientific Advisory Board

S/1621/2018  
Annex  
page 2

Annex

## DIRECTOR-GENERAL'S REQUEST TO THE SCIENTIFIC ADVISORY BOARD TO PROVIDE ADVICE ON NEW TYPES OF NERVE AGENTS

1. Recent events involving the use of nerve agents against individuals in Malaysia and Great Britain and Northern Ireland have drawn considerable attention, including in the scientific community. While the Malaysia ill-known V-series nerve agent, the incident in the United Kingdom involved a highly toxic nerve agent with a structure that has appeared in the past but has never been declared under the Chemical Weapons Convention. In the United Kingdom incident, no information has been published in the scientific literature.

Many types of nerve agents have been developed as weapons since the Second World War. The United Kingdom has included organophosphorus structures that would fall under the Convention's Annex on Chemicals, as well as related structures that would not belong to any of the current schedules. The incident from the United Kingdom is not included in the result of the incident in the United Kingdom, articles are now appearing in society membership publications<sup>2</sup> and journals<sup>3</sup> speculating on the implications of the chemical used and other related chemicals that have been developed as nerve agents. These publications have broad implications for the development of new types of toxic chemicals to the Convention and the re-emergence of chemical weapons, a clear, factual basis for future discussions. Information is necessary as background for the States Parties of possible measures to address the potential threat posed by these chemicals.

of the report of the Scientific Advisory Board at its Sixteenth Session (1) [www.opcw.org/fileadmin/OPCW/SAB/en/sab-16-01\\_e.pdf](http://www.opcw.org/fileadmin/OPCW/SAB/en/sab-16-01_e.pdf) (2) *In Association for the Advancement of Science*; R. Stone, *Science*, 2018, *vol.* 324, *no.* 6053; <http://www.sciencemag.org/news/2018/03/uk-attack-shines-light-on-developed-soviet-scientists>. (b) American Chemical Society; M. Peplow, *ACS*, 2018, *vol.* 12, *no.* 3; <https://cen.acs.org/articles/96/i12/Nerve-agent-attack-on-spy-used>. (c) The Royal Society of Chemistry; E. Stoye, *Chemistry World*, [www.chemistryworld.com/news/newsroom-news/uk-nerve-agent-linked-to-attack](http://www.chemistryworld.com/news/newsroom-news/uk-nerve-agent-linked-to-attack) (d) The University of Melbourne; G. Braiberg, *Parasit. Immunol.*, *2018*, *vol.* 48, *no.* 1; <http://onlinelibrary.wiley.com/doi/abs/10.1002/cit.201870202>. (e) German *Chem. Unserer Zeit*, 2018, *vol.* 52, *no.* 71; <https://doi.org/10.1002/cit.201870202>. (f) H. Machado, M. Mitchell, *ACS Chem. Neurosci.*, 2018, Just Accepted <https://doi.org/10.1021/acschemneuro.8b00148>.



OPCW

Technical Secretariat

S/1621/2018  
2 May 2018  
ENGLISH only

### NOTE BY THE DIRECTOR-GENERAL

#### REQUEST FOR INFORMATION FROM STATES PARTIES ON NEW TYPES OF NERVE AGENTS

1. In view of the findings of the March 2018 technical assistance visit requested by the United Kingdom of Great Britain and Northern Ireland (TAV/02/18),<sup>1</sup> the Director-General has tasked the Scientific Advisory Board (SAB) with providing advice on toxic chemicals that have been identified as, or are suspected of being, new types of nerve agents. The SAB is currently working on this request and intends to issue a report and brief States Parties before the Eighty-Eighth Session of the Executive Council. The full text of the request is contained in the Annex to this Note.
2. The Director-General requests States Parties in a position to do so to make available, by the end of May 2018, any information that could assist the SAB in its work.
3. States Parties possessing relevant information that can be provided to the SAB are requested to contact the SAB Secretary ([scitech@opcw.org](mailto:scitech@opcw.org)).

Annex: Director-General's Request to the Scientific Advisory Board to Provide Advice on New Types of Nerve Agents

<sup>1</sup> S/1612/2018, dated 12 April 2018.



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# Scheduled Chemicals under the Chemical Weapons Convention (CWC)

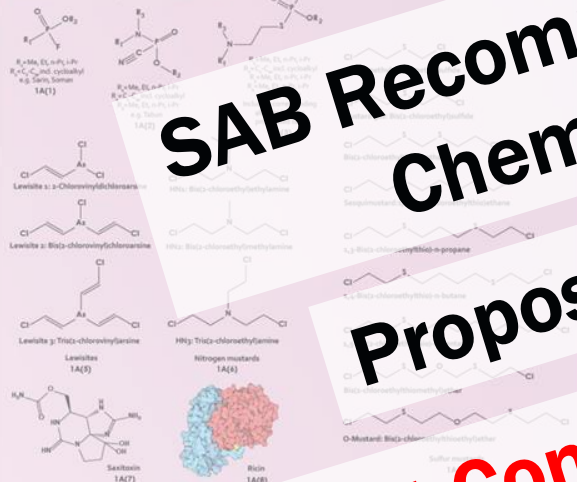
## Schedule 1

### Guidelines for Schedule 1

The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

- (a) It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- (b) It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:
  - (i) It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparable properties;
  - (ii) It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;
  - (iii) It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;
- (c) It has little or no use for purposes not prohibited under this Convention.

### Schedule 1 Part A, Toxic Chemicals



### Schedule 1 Part B, Precursors



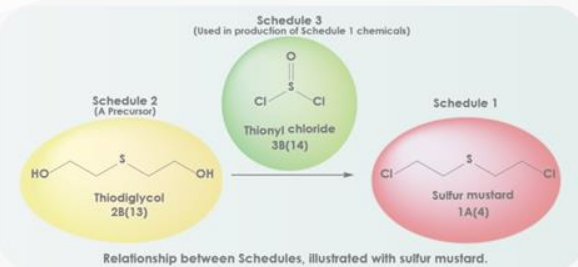
## Schedule 2

### Guidelines for Schedule 2

The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:

- (a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;
- (b) 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;
- (c) It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;
- (d) It is not produced in large commercial quantities for purposes not prohibited under this Convention.

### Schedule 2 Part A, Toxic Chemicals



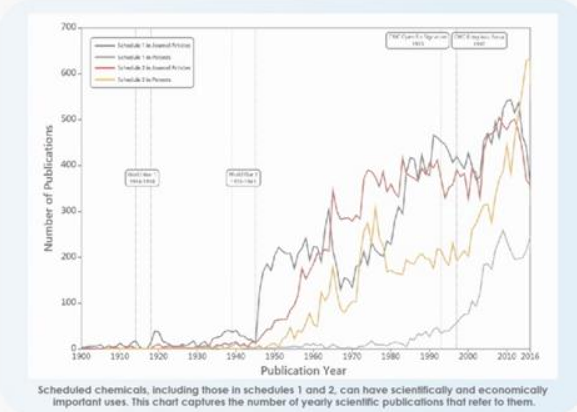
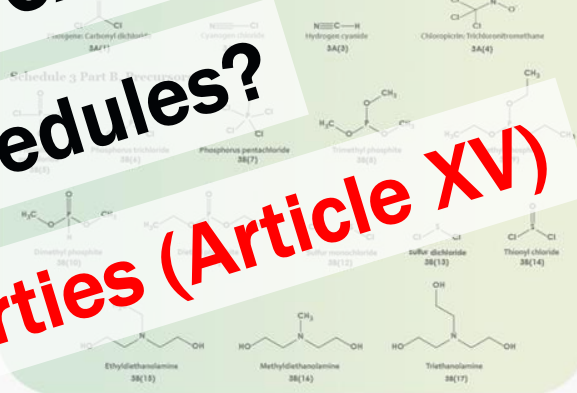
## Schedule 3

### Guidelines for Schedule 3

The following criteria shall be 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 in large commercial quantities for purposes not prohibited under this Convention;
- (b) It poses otherwise a high risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;
- (c) It poses a significant 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.

### Schedule 3 Part B, Precursors



**SAB Recommendations on Unscheduled Chemicals: Detection! OCAD! Proposals to Change Schedules? Must Come From States Parties (Article XV)**



# Scientific Advisory Board from January to July 2018



Scientific Advisory Board 2018



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Organisation for the Prohibition of Chemical Weapons



Summary of the First Meeting of the Scientific Advisory Board's Temporary Working Group on Investigative Science and Technology  
*(SAB-27/WP.1, dated 26 February 2018)*



Report of the Scientific Advisory Board at its Twenty-Seventh Session  
*(SAB-27/1, dated 23 March 2018)*



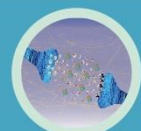
Director-General's Response to the Report of the Twenty-Seventh Session of the Scientific Advisory Board  
*(EC-88/DG.5, dated 9 May 2018)*



Report of the Scientific Advisory Board on Developments in Science and Technology for the Fourth Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention  
*(RC-4/DG.1, dated 30 April 2018)*



Response by the Director-General to the report of the Scientific Advisory Board on Developments in Science and Technology for the Fourth Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention  
*(RC-4/DG.2, dated 1 June 2018)*



Response To The Director-General's Request To Provide Advice On New Types Of Nerve Agents  
*(SAB-28/1, dated 3 July 2018)*





# OPCW

منظمة حظر الأسلحة الكيميائية

禁止化学武器组织

Organisation for the Prohibition of Chemical Weapons

Organisation pour l'Interdiction des Armes Chimiques

Организация по запрещению химического оружия

Organización para la Prohibición de las Armas Químicas