

# **ENVIRONMENTAL ORGANIC CHEMISTRY**

## **CHEM 331**

**Where do organic contaminants go?**

**How long will they remain?**

**What happens to them?**

Science News - August 3, 2005

**Brominated flame retardant impairs male hormones**

**Pharmaceuticals, Hormones, and  
Other Organic Wastewater  
Contaminants in U.S. Streams,  
1999-2000: A National  
Reconnaissance**

Science News - August 31, 2005

**Bird droppings move POPs in the Arctic**

Science News - April 6, 2005

**When chlorine + antimicrobials = unintended  
consequences**

Science News - June 8, 2005

**Environmental toxins permanently alter genetics**

**Transformation of Acetaminophen by  
Chlorination Produces the Toxicants  
1,4-Benzoquinone and  
N-Acetyl-p-benzoquinone Imine**

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WILLIAM A. MACCREHAN  
*Analytical Chemistry Division, National Institute of  
Standards and Technology, Mailstop 8392,  
Gaithersburg, Maryland 20899-8392*

Science News - August 4, 2005

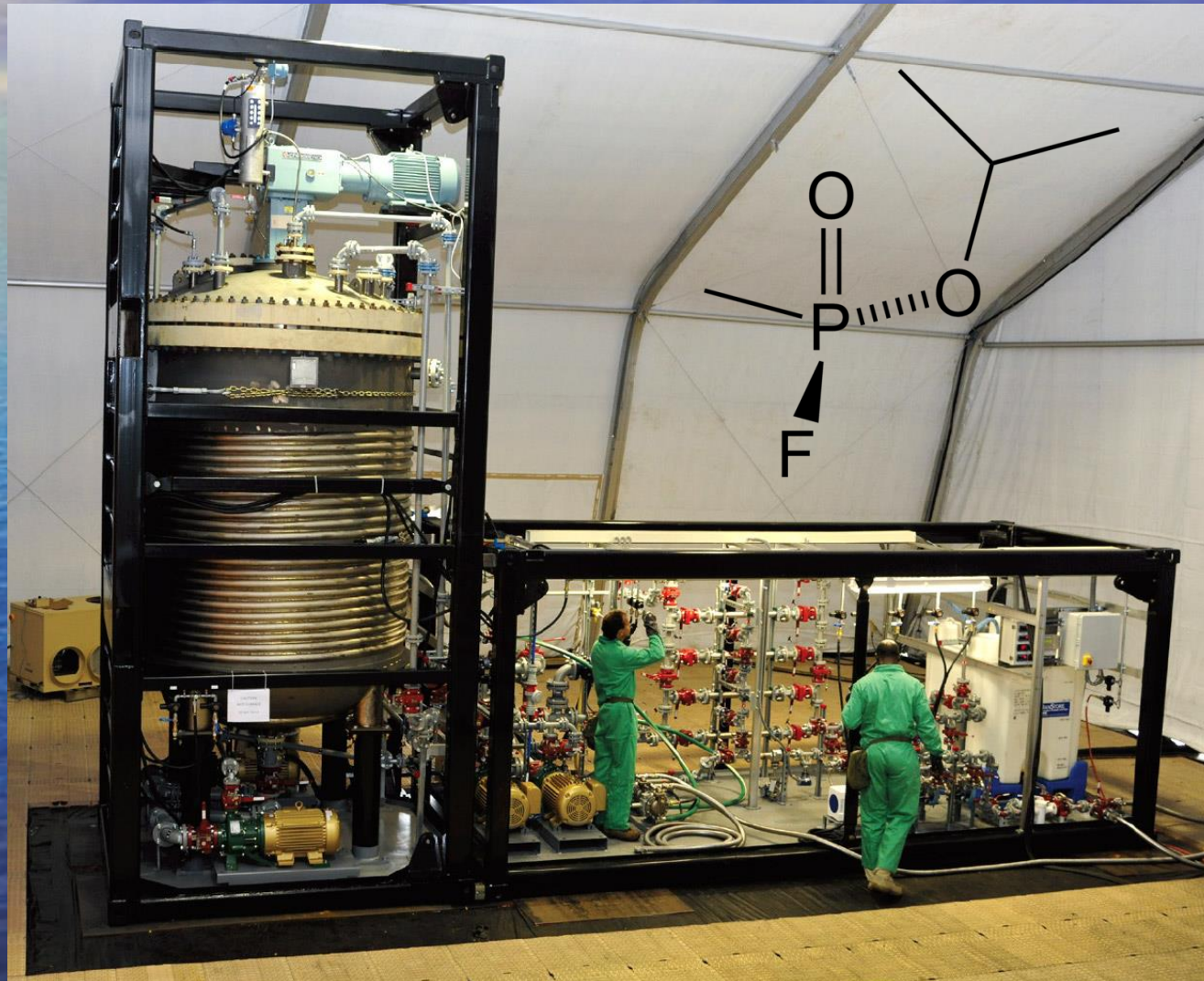
**Grizzly bears, salmon, and contaminant transport**

Science News - October 26, 2005

**Household pesticides are poisoning city creeks**

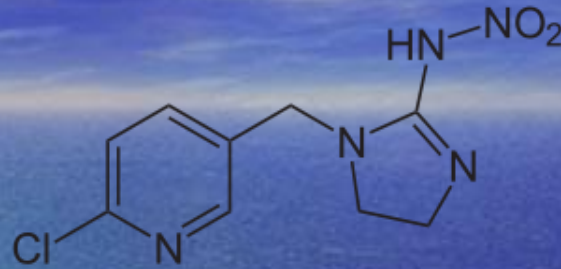
**Although safer for humans, pyrethroid insecticides pose  
unforeseen dangers to the environment.**

# Portable 'hydrolyzer' lab to guzzle Syria's sarin stockpile



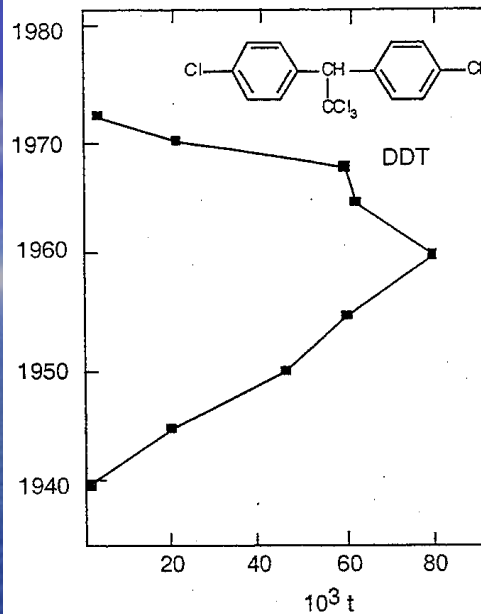
D. MacKenzie, New Scientist, October 11, 2013

# Neonicotinoids Implicated in Bee Colony Collapse Banned by EU

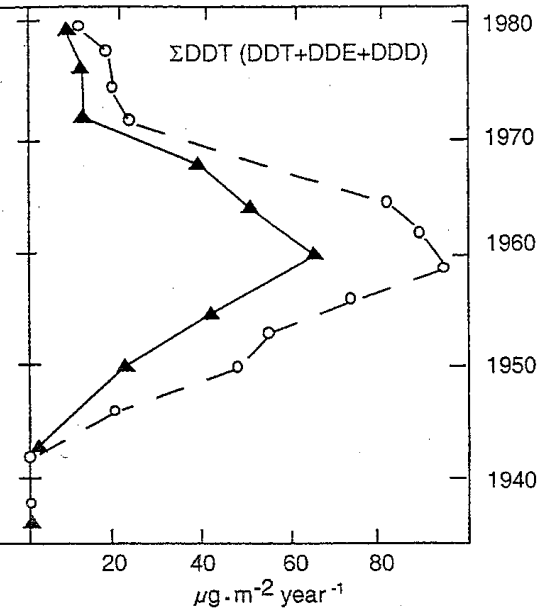


# DDT and PCBs

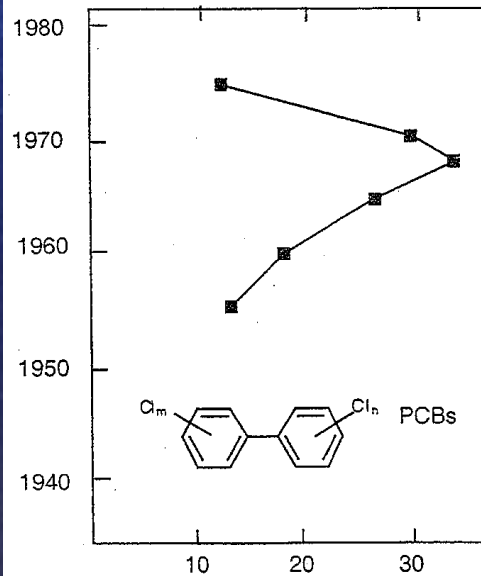
DDT production in the United States



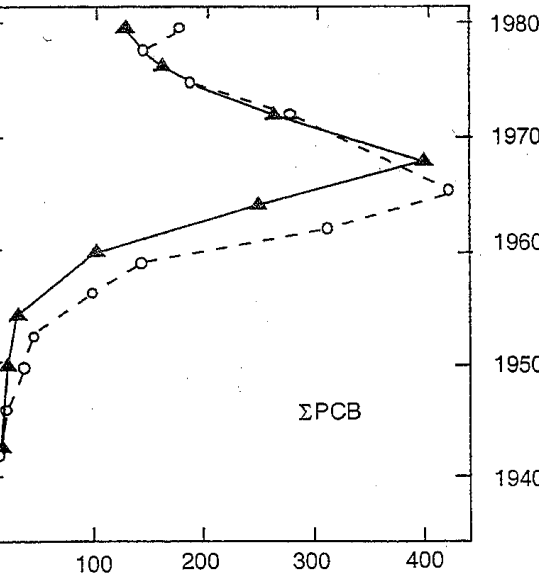
Accumulation rate in the sediments of Lake Ontario (data from 2 different sediment cores)



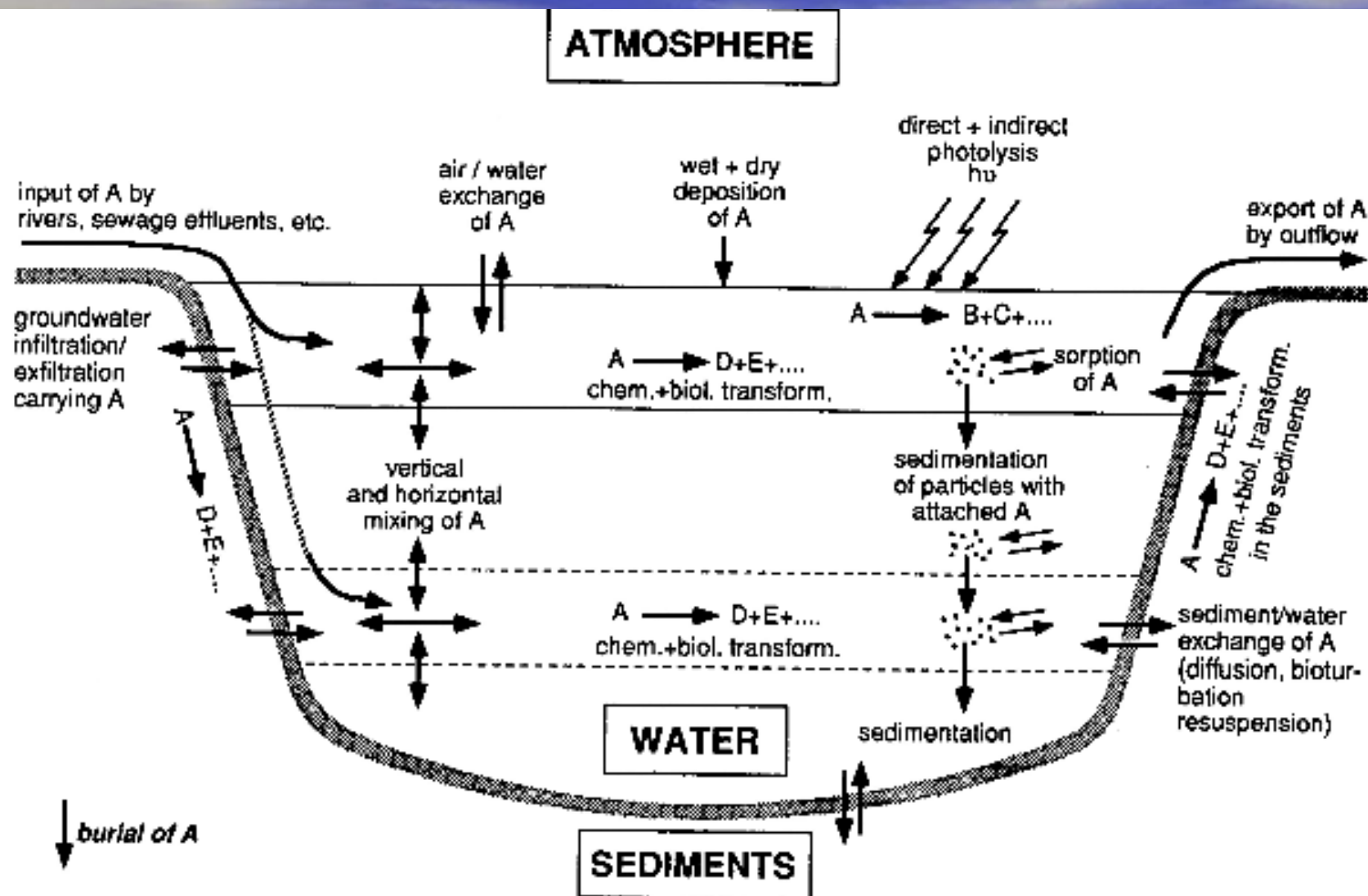
PCB sales in the United States



Accumulation rate in the sediments of Lake Ontario (data from 2 different sediment cores)



# Distribution and Fate in the Environment



**Figure 1.3** Processes that determine the distribution, residence time, and sinks of an anthropogenic organic compound in a lake.

# PHYSICAL PROCESSES

- Partitioning (Equilibrium Constants)
  - air-water,  $K_{aw}$  (aka  $K_H$ )
  - octanol-water,  $K_{ow}$
  - organic matter-water,  $K_{om}$  (and  $K_d$ )
- Vapour Pressure,  $P^0$
- Water Solubility,  $C_w^{sat}$

Depend on Physical Properties of Molecules

Inter and Intra Molecular Forces

Functional Groups and Substituents:

STRUCTURE – ACTIVITY RELATIONSHIPS

# CHEMICAL PROCESSES

- Nucleophilic Substitution (eg. Nu=H<sub>2</sub>O, Hydrolysis)
- Acid/base
- Oxidation
- Reduction
- Photochemistry

Functional groups: affect chemical products

Substituents: affect thermodynamics and kinetics

**STRUCTURE – REACTIVITY RELATIONSHIPS**



# Factors that Affect Thermodynamics and Kinetics of Organic Reactions

- Quantifying Steric and Electronic Effects

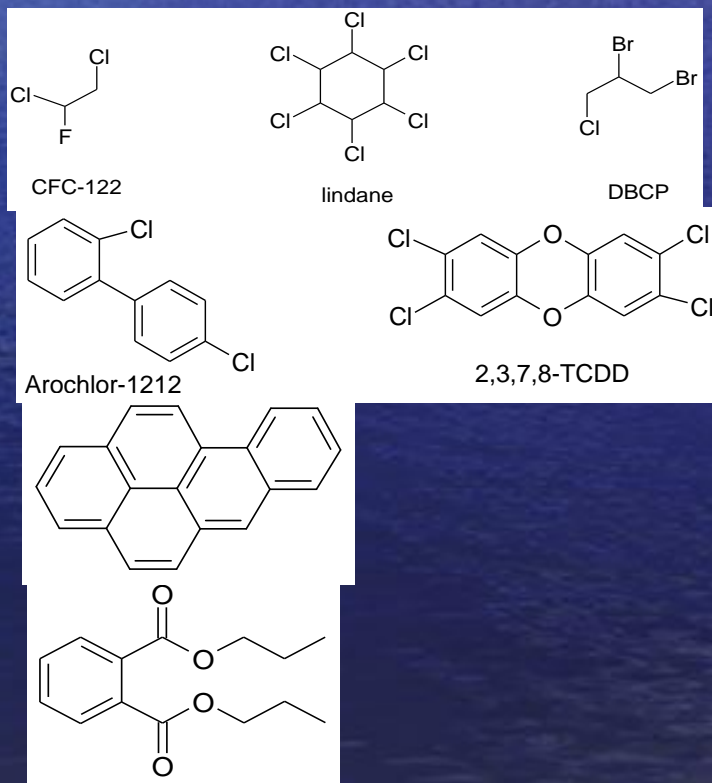
## REACTION MECHANISMS

$S_N1$ ,  $S_N2$ , E1, E2,  $E_{cb}1$ ,

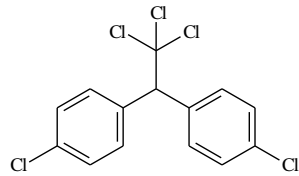
EAS, NAS, A1, A2, B1, B2

# CLASSES of ENVIRONMENTALLY RELEVANT ORGANIC MOLECULES

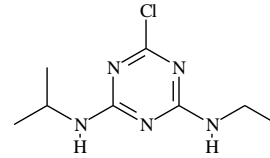
Class	Examples
Haloalkanes	CFC's, lindane
Haloaromatics	PCB's, dioxins
PAHs	benzo[a]pyrene
Phthalates	dipropyl phthalate



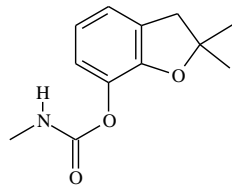
# Examples of Common Insecticides



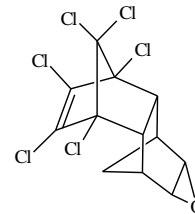
DDT



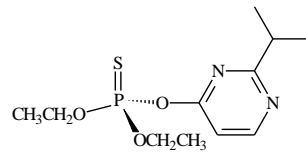
Atrazine



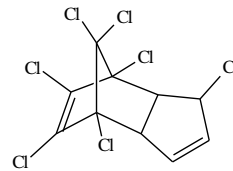
Carbofuran



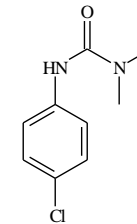
Dieldrin



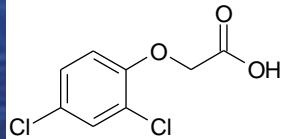
Diazinon



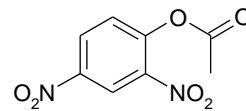
Heptachlor



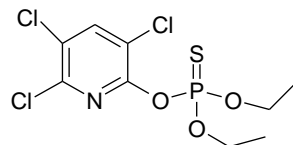
Monuron



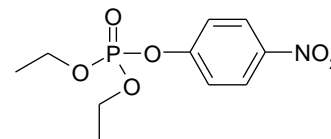
2,4-D



2,4-Dinitrophenylacetate



Chlorpyrifos



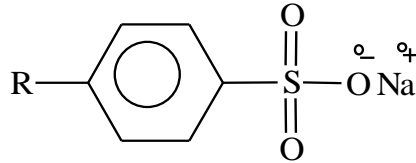
Parathion

# Examples of Common Surfactants



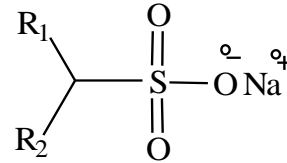
R = C<sub>10</sub> to C<sub>16</sub>

Soaps



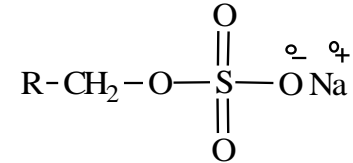
R = C<sub>10</sub> to C<sub>13</sub>

Linear alkylbenzene sulfonates (LAS)



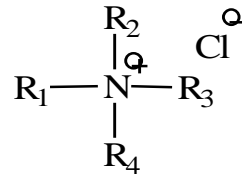
R<sub>1</sub>, R<sub>2</sub> = C<sub>1</sub> to C<sub>7</sub>

Secondary alkylsulfonates (SAS)



R = C<sub>11</sub> to C<sub>17</sub>

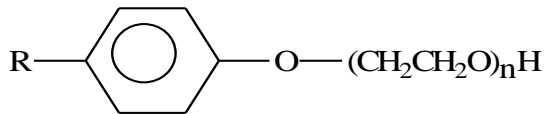
Fatty alcohol sulfates (alkyl sulfates, FAS)



R<sub>1</sub> = R<sub>2</sub> = C<sub>1</sub>

R<sub>3</sub> = R<sub>4</sub> = C<sub>16</sub> to C<sub>18</sub>

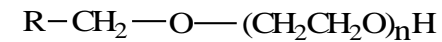
Quaternary ammonium chloride (QAC)



R = C<sub>8</sub> to C<sub>12</sub>

n = 5 to 10

Alkylphenol polyethyleneglycol (APEO)



R = C<sub>8</sub> to C<sub>17</sub> n = 3 to 10

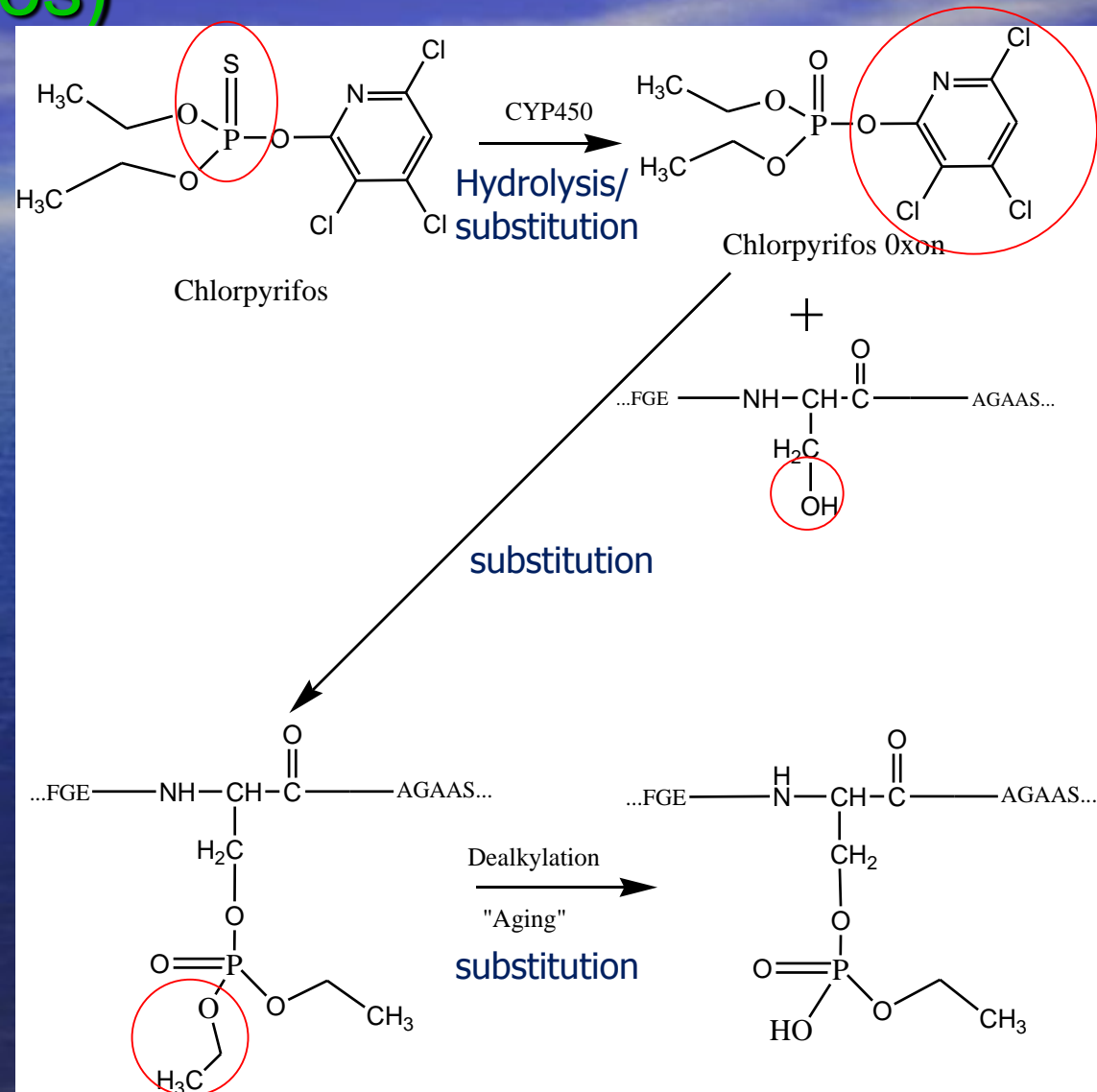
Fatty alcohol polyethyleneglycol ethers (FAEO)

# Toxicological Mechanism – Organophosphate pesticide (Chlorpyrifos)

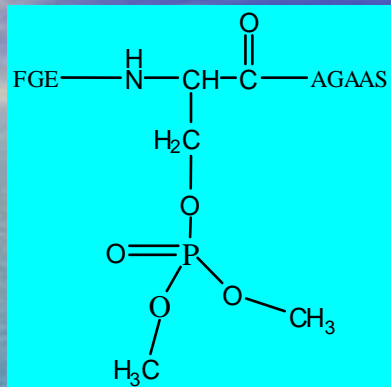
Metabolism →

Adduct formation →

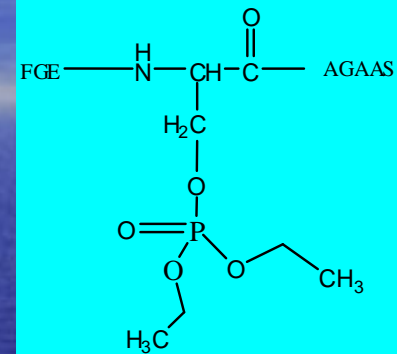
'Aging' →



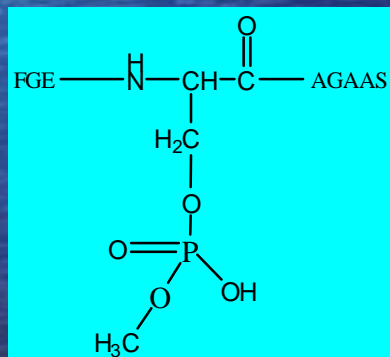
# Chemical Structures of OP Adducts



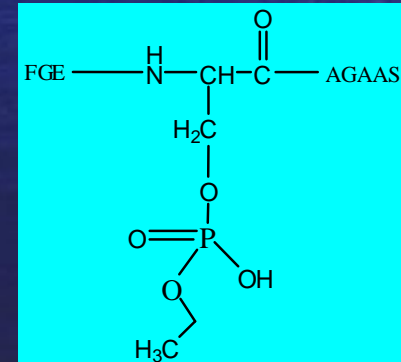
Dimethyl adduct



Diethyl adduct



Aged methyl adduct



Aged ethyl adduct

# Poster Assignment 2018

Perfluorooctanoic Acids

Naphthenic Acids

Triazine pesticides

Nonyl phenols

Chlorinated alkanes/alkenes

N-nitrosoamines

Neonictinoids

Phthalates

Parabens

Benzophenone sunscreens

Polychlorinated biphenyls

Polychlorinated dibenzodioxins/furans

Organophosphate esters

Carbamate pesticides

**Transport and  
Fate of Emerging  
Class of  
Environmental  
Contaminants**