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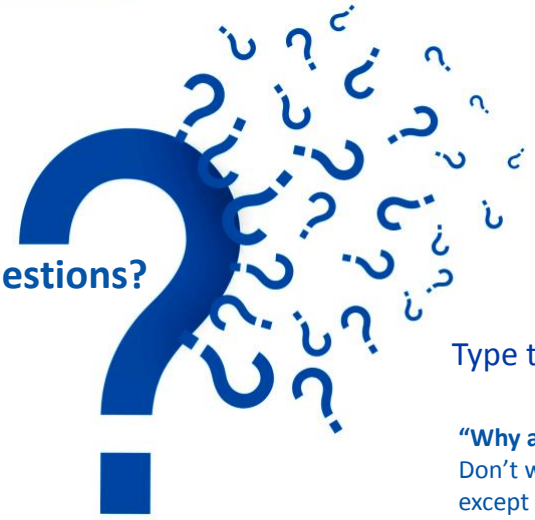

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"It provided the opportunity to discover and learn more about CRO. A nice informative presentation and pleasant way to spend an afternoon."

Fan of the Week

Elena Baboi

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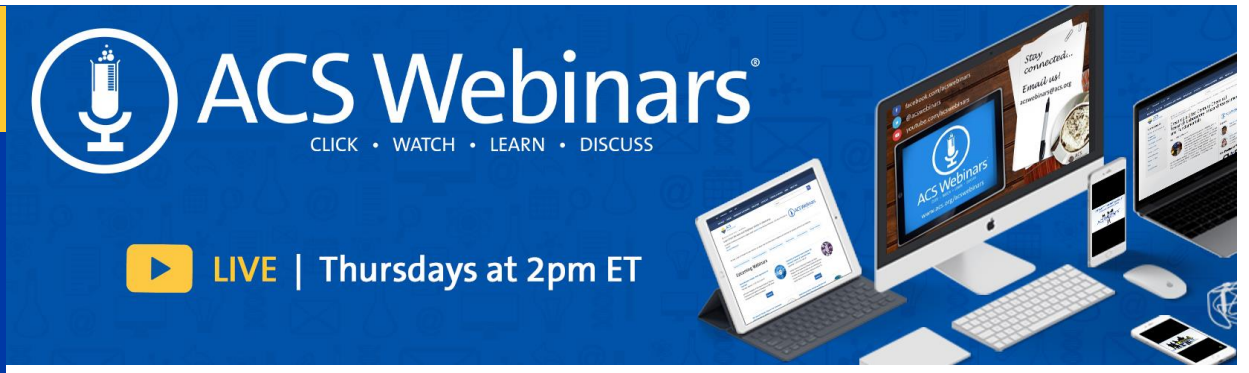

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2018 Winners: AstraZeneca, DuPont, Pfizer, SeattleGenetics

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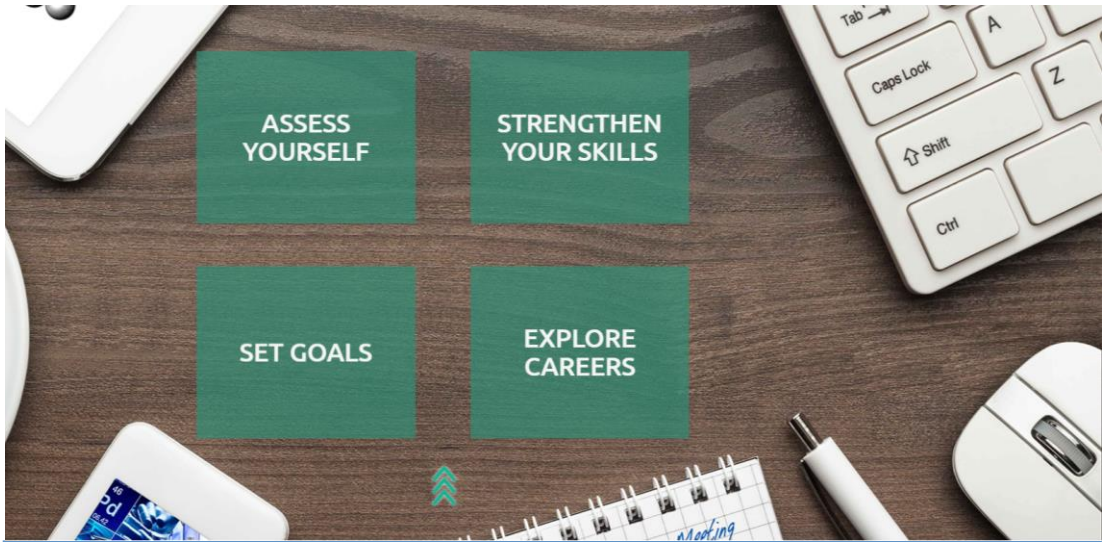
An individual development planning tool for you!



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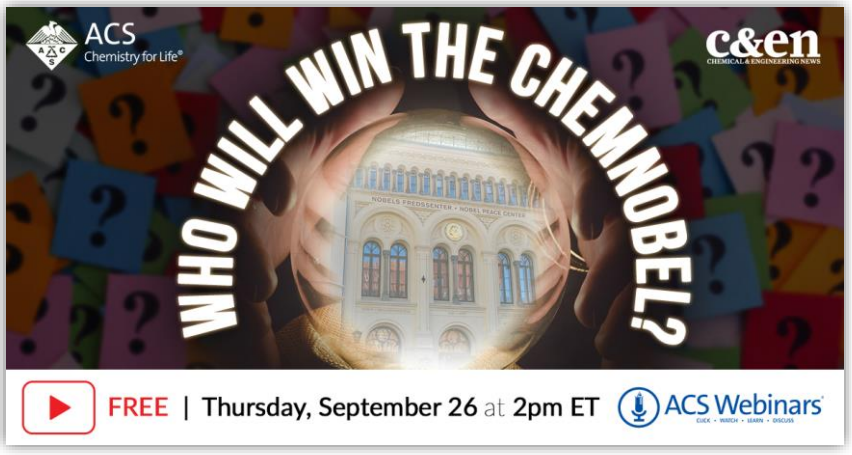

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Upcoming ACS Webinar!

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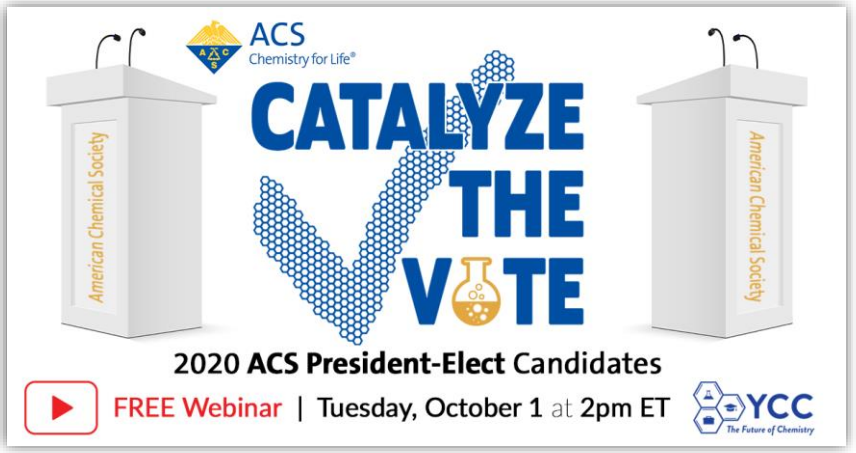

https://www.acs.org/content/acs/en/acs-webinars/popular-chemistry/catalyze-the-vote-2020.html

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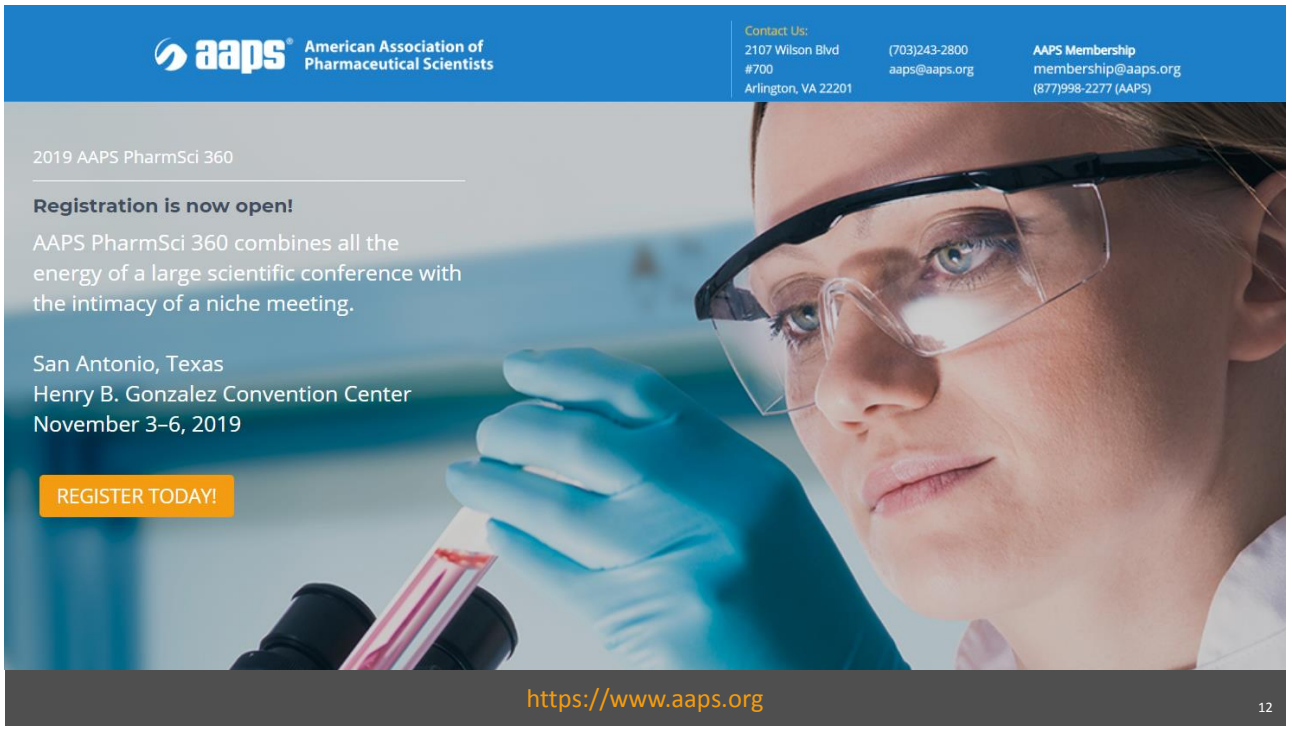

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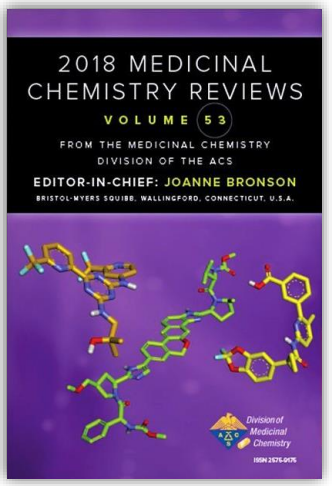

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Jan 31	**How to Succeed in Drug Discovery: Insight from Medicinal Chemists** (1.5 hrs.) John Lowe III - JL3 Pharm Mark Murcko - Relay Therapeutics Ann Weber - Kallyope William Greenlee - MedChem Discovery Consulting
Feb 28	**Cosolvent Molecular Dynamics: Mapping Protein Surfaces to Discover Allosteric Sites** Heather Carlson - University of Michigan Rommie Amaro - UC San Diego
Mar 28	**Women at the Interface of Computational Chemistry and Drug Discovery** (1.5 hrs) Zoe Cournia - Biomedical Research Foundation and *JCIM* Kate Holloway - Gfree Bio Yvonne C. Martin - Previously of Abbott Laboratories Shana Posy - Bristol-Myers Squibb
Apr 18	**Effective Exploration of Chemical Space in Hit-Finding** Hanneke Jansen - Novartis Institutes for BioMedical Research Zoe Cournia - Biomedical Research Foundation and *JCIM*
May 30	**Widening the Therapeutic Window: Kinetic Selectivity and Target Vulnerability** Peter Tonge - Stony Brook University and *ACS Infectious Diseases* Stewart Fisher - C4 Therapeutics
Jun 27	**Precision Control of CRISPR-Cas9** Amit Choudhary - Broad Institute of Harvard and MIT Venkat Krishnamurthy - AstraZeneca
Aug 8	**Transformation of Recombinant Cells to FDA Approved Products: Clinical Development to Marketplace** (New Date) Rodney Ho - University of Washington Venkat Krishnamurthy - AstraZeneca
Aug 22	**The Evolving Outsourcing Landscape in Pharma R&D: Pros and Cons of Different Models** Bart DeCorte - MercachemSyncom Allen Reitz - Fox Chase Chemical Diversity Center
Sep 19	**Thinking Outside the Pillbox: Lead Generation and Optimization in Crop Protection Research** Fides Benfatti - Syngenta
Oct 24	**Treating Diabetes: Designing the Once-Weekly and Oral GLP-1 Semaglutide** Jesper Lau - Novo Nordisk A/S
Nov 28	**Prodrugs** Jarkko Rautio - University of Eastern Finland

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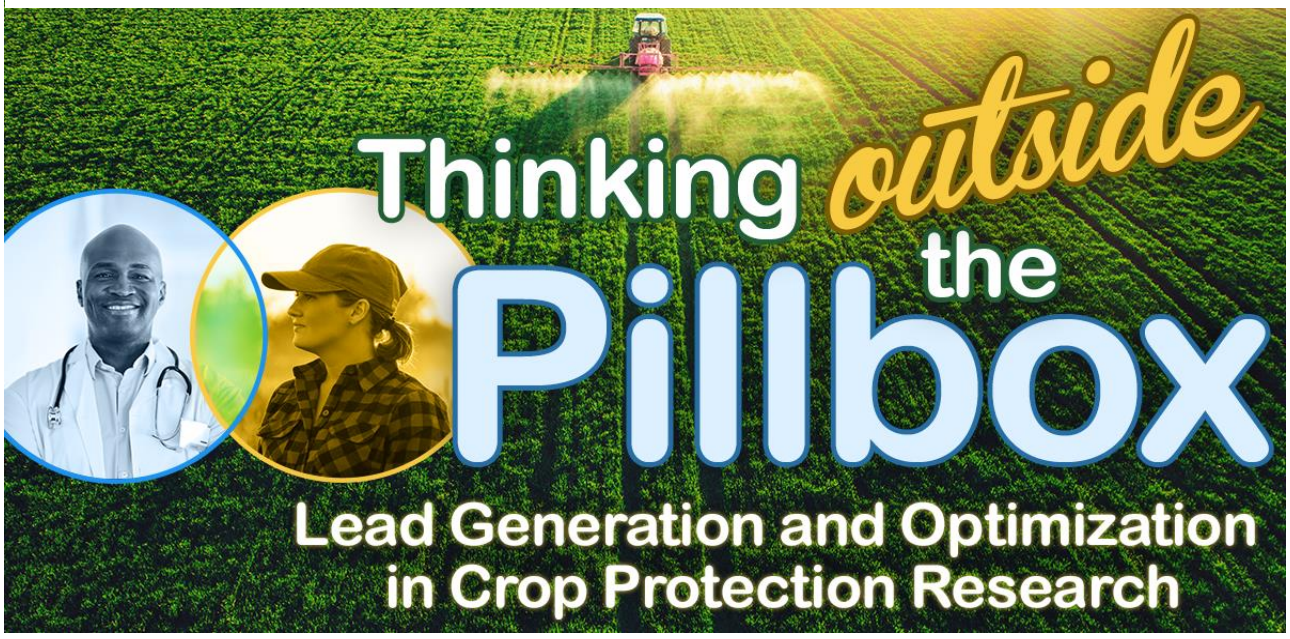

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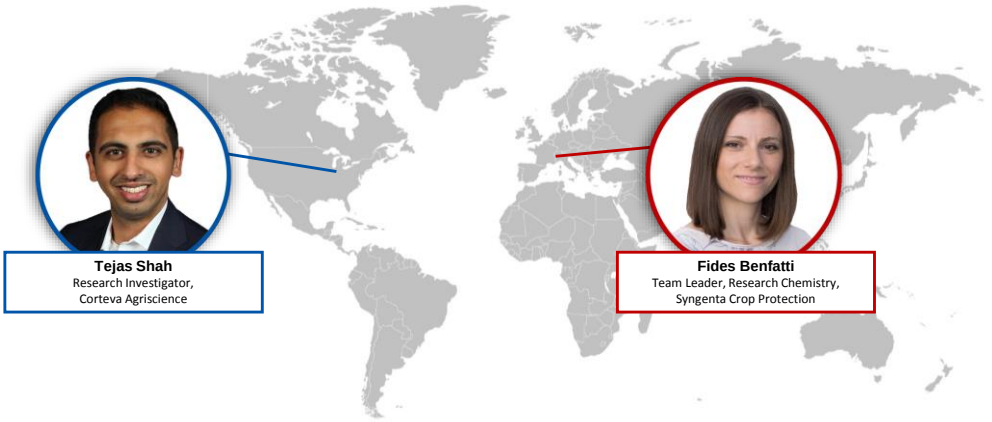
Thinking Outside the Pillbox: Lead Generation and Optimization in Crop Protection Research



Tejas Shah
Research Investigator,
Corteva Agriscience

Fides Benfatti
Team Leader, Research Chemistry,
Syngenta Crop Protection

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Thinking Outside the Pillbox: Lead Generation and Optimization in Crop Protection Research

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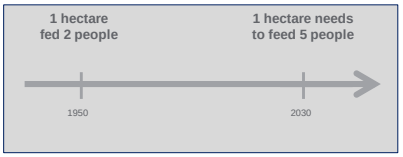
Fides Benfatti
Senior Team Leader Chemical Research

Syngenta Crop Protection
fides.benfatti@syngenta.com

Classification: PUBLIC

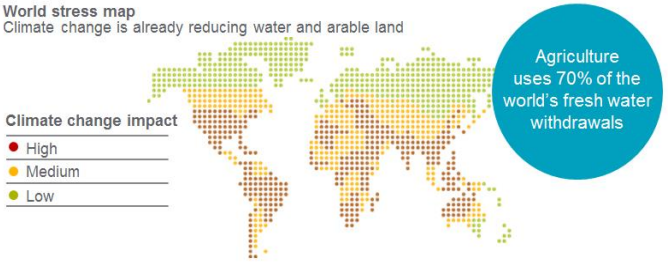
Why do we need new Crop Protection products?

- Growing more with less



Source: UNEP, Cline, Syngenta

- Climate change



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Why do we need new Crop Protection products?

- Resistance development and shifting pest populations

Source: www.plantmanagementnetwork.org

- Changing regulatory landscape

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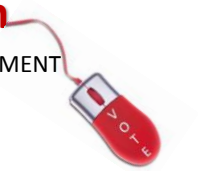
Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



Approximately how much was lost in billons (USD) **to plant diseases and infestations from 2005 to 2015?**

- 1 billion
- 3.5 billion
- 5 billion
- 7 billion
- 9.5 billion

** If your answer differs greatly from the choices above tell us in the chat!*

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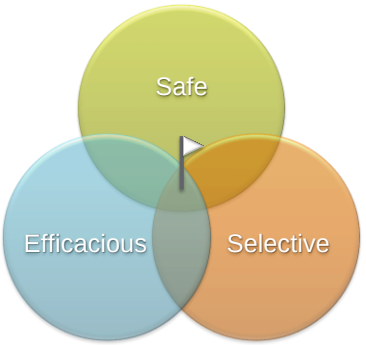
How are crop protection products discovered and optimized

Outline

- Discovery of insecticidal spiroindolines
- Bioavailability-guided design of new aphicides
- Modern crop protection products targeting ion channels



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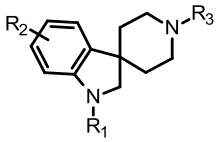
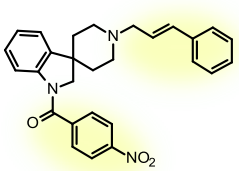
Discovery of insecticidal spiroindolines



Spiro[indoline-3,4'-piperidine]



Insecticidal Hit!

- Screening of a chemical library (obtained from Oxford Asymmetry, now Evotec)

- Insecticidal hit compound identified by high throughput screening
- Activity on *Drosophila melanogaster*, *Plutella xylostella* and *Heliothis virescens* at 1000 ppm
- Only compounds possessing a cinnamyl group displayed insecticidal activity

Hughes, D. J.; Worthington, P. A.; Russell, C. A.; Clarke, E. D.; Peace, J. E.; Ashton, M. R.; Coulter, T. S.; Roberts, R. S.; Molleyres, L.-P.; Cederbaum, F.; Cassayre, J.; Maienfisch, P. **WO2003106457**

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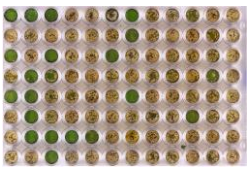
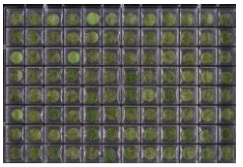
Agrochemical research: screening cascade

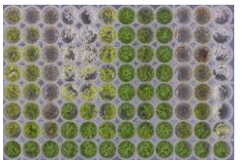
- *In vivo* on-target test from day 1



Insecticide HTS



Fungicide HTS



Herbicide HTS

- Increase in tests size parallel to project stage (HTS >>> field)

Micro Profiling Screens

Profiling Screens

Field Trials

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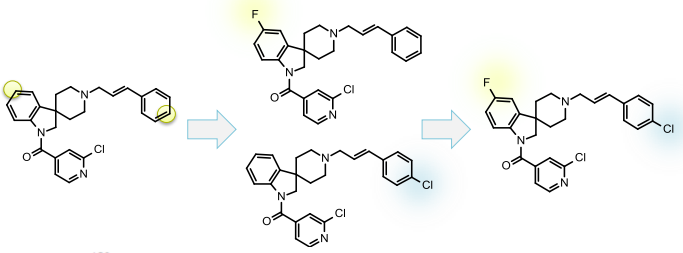
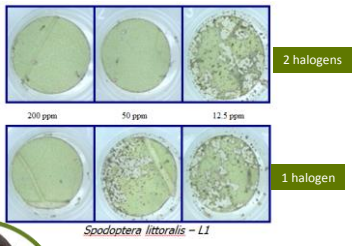
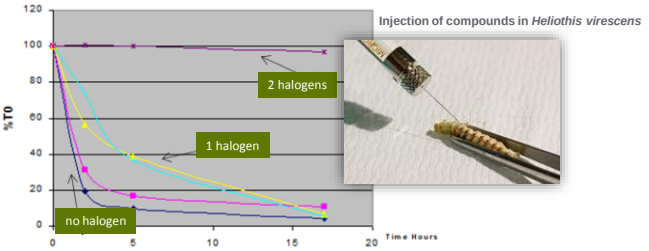
Discovery of insecticidal spiroindolines: Hit-to-Lead Optimization

Block metabolically weak positions
→ improved potency
→ cumulative effect







Hughes, D. J.; Worthington, P. A.; Russell, C. A.; Clarke, E. D.; Peace, J. E.; Ashton, M. R.; Coulter, T. S.; Roberts, R. S.; Molleyres, L.-P.; Cederbaum, F.; Cassayre, J.; Maienfisch, P. **WO2003106457**

Sluder A.; Shah, S.; Cassayre, J.; Clover R.; Maienfisch, P.; Molleyres, L.-P. et al *PLoS One* **2012**, *7*(5), e34712

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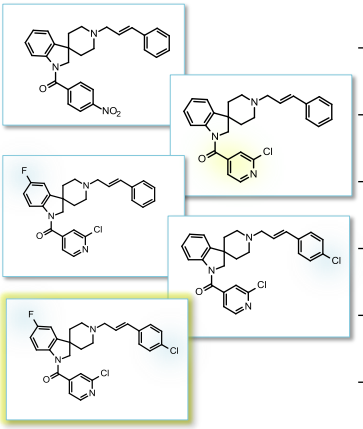
Discovery of insecticidal spiroindolines: Hit-to-Lead Optimization

- Cumulative effect observed cross lepidopteran target species
- Lead shows promising activity at low dose



Spodoptera littoralis L1	Heliothis virescens L1	Plutella xylostella L2
> 500	> 500	>500
200	200	200
200	50	200
50	≤12	<50
12	0.8	3

Primary screening [EC80-100 in ppm (mg/L)]

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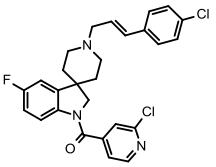
Properties and insecticidal activity of spiroindoline lead



Spiroindoline Lead

Melting Point (M.p.)	168-170°C
Aqueous solubility	5 ppm@pH 6.5
Log P	5.94
pKa	7.88
Photostability T_{50} 114 mins	
Rat acute toxicity	MLD_{50} > 200 mg/Kg

Lepidopteran control (activity given as effective concentration EC_{80} in ppm (mg / L)

effective concentration EC_{80} in ppm (mg / L)	*Spodoptera littoralis L1*	*Heliothis virescens L1*	*Plutella xylostella L3*	*Cydia pomonella L1*
Spiroindoline 6b	**12**	**0.8**	**6**	**3**
Spinosad	0.8	0.8	0. 2	12
Indoxacarb	3	3	3	12

Check

Spinosad 10 g / hl*

Spirodindoline 8 g / hl*

Diamondback moth, *Plutella xylostella*, on cabbage

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Symptomology – insights into the mode of action

- Exploiting genetic model systems – *C. elegans* and *Drosophila*

Decades of academic work linking phenotype (visible effects) to genetic disfunction

- Comparing chemical symptoms to genetic phenotypes identifies candidate target proteins e.g. Spiroindolines

For a recent extensive analysis of *C. elegans* behavorial phenotype:

A database of *Caenorhabditis elegans* behavioral phenotypes, E. Yemini *et al* *Nature Methods*, **2013**, *10*, 877-879

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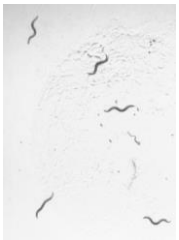
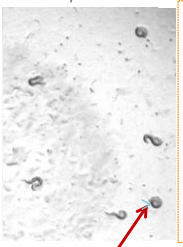
Symptomology in *C. elegans*

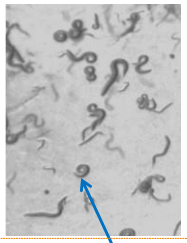
- Spiroindolines induces characteristic symptoms in *C. elegans*

C. elegans untreated



+ spiroindoline





Genetic mutation in acetylcholine signalling discovered in 1993

(Alfonso *et al.* The Caenorhabditis elegans unc-17 gene: a putative vesicular acetylcholine transporter. Science, **1993**, *261*, 617-9.)

Photo: Syngenta

Symptom resembles **phenotype**

Hypothesis: Spiroindolines affect cholinergic signaling

PLoS ONE **2012**, *7*, e34712.

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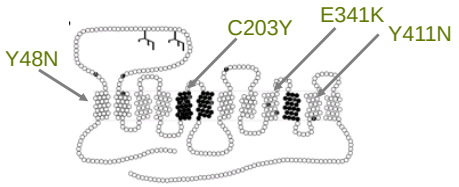
Confirming the hypothesis

- Forward genetics used to identify mutant strains resistant to SPIRO

C. elegans (Lots) → + Mutagen (EMS) → +SPIRO (No Growth Dose) → Resistant *C. elegans*

EMS= Ethane methyl sulfonate



Locate resistance mutations using genetic mapping and sequencing

- Resistance mutations locate to **vesicular acetylcholine transporter** (VAChT)
- Binding of spiroindoline to VAChT can now be confirmed using standard biochemical approaches *in vitro*

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Bioavailability-guided design of new aphicides

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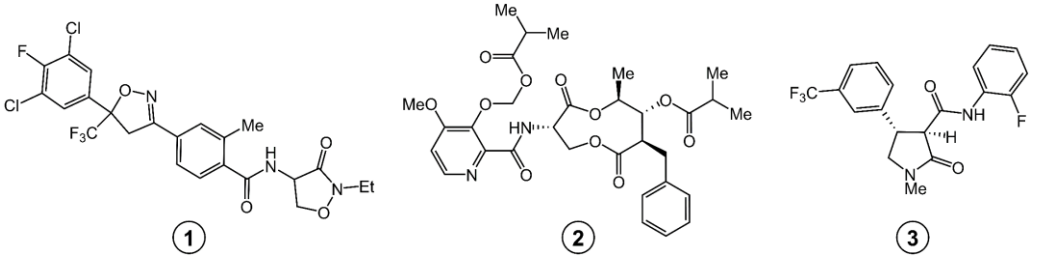
Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Which of these molecules is an or are agrochemical(s)?

(Select all that apply)



** If your answer differs greatly from the choices above tell us in the chat!*

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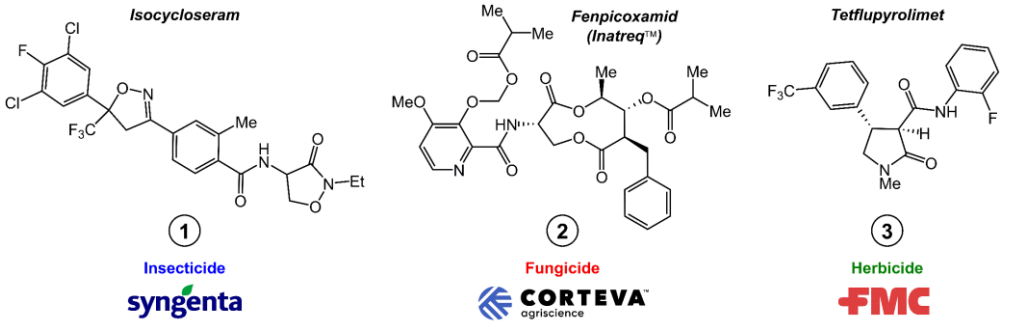
Audience Survey Question

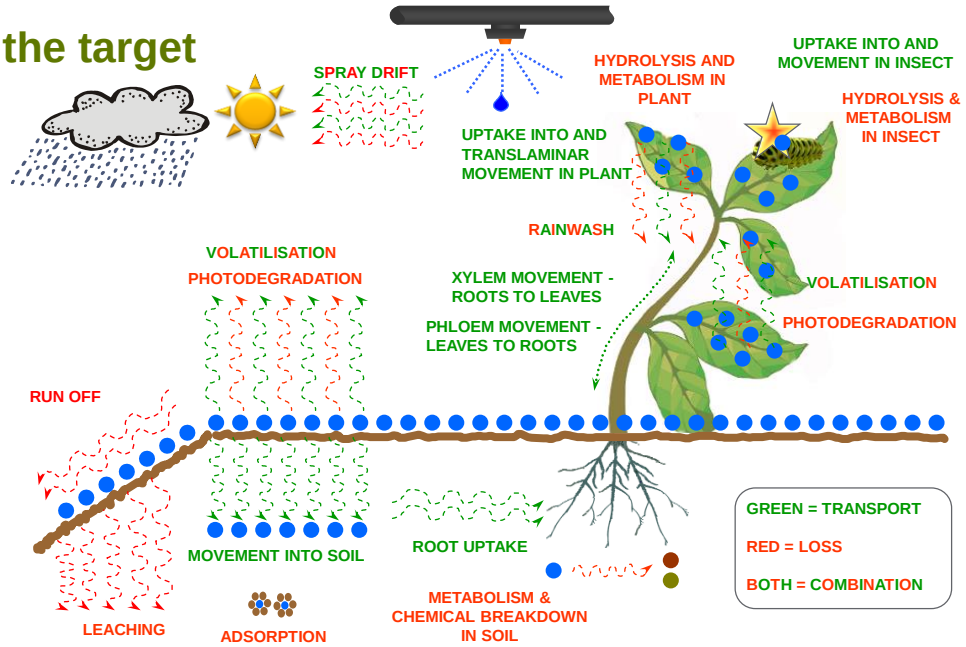
ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Which of these molecules is an or are agrochemical(s)?



** If your answer differs greatly from the choices above tell us in the chat!*

How to reach the target



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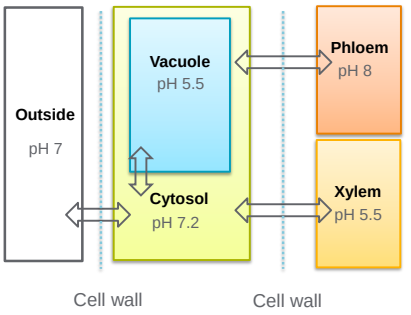
Influence of physical chemical properties on the uptake into plants



The **logP** and **pka** of agrochemicals dictate their distribution in plants

- Weak acids with intermediate lipophilicity get trapped in phloem
- Basic molecules get trapped in vacuoles
- Caveat: carrier proteins, channels can provide active transport

Trapp S. 2009 in J. Devillers, Ed.: Ecotoxicology Modeling. Springer, Dordrecht
Buchholz, A.; O'Sullivan, A. C.; Trapp, S. In *Discovery and Synthesis of Crop Protection Products*; American Chemical Society: 2015; Vol. 1204, p 93.

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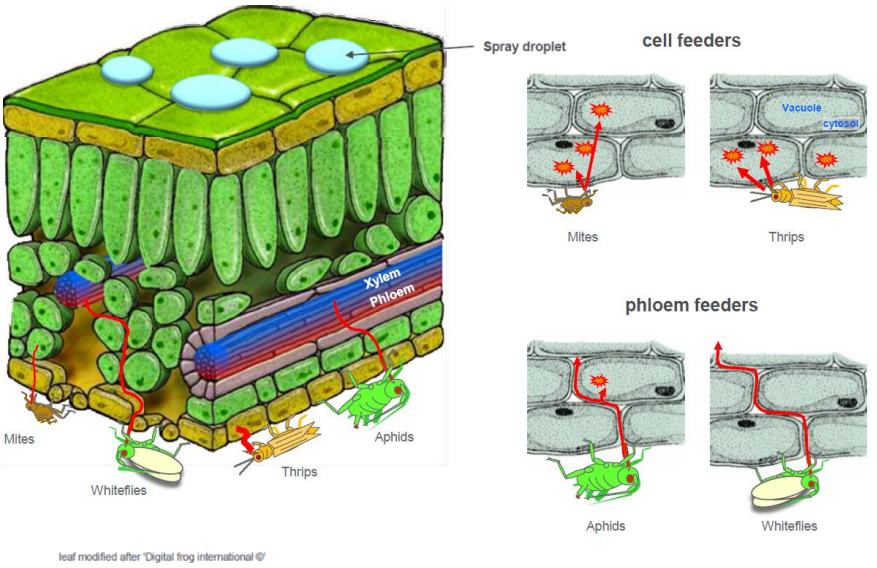
Feeding behaviour of insect pests



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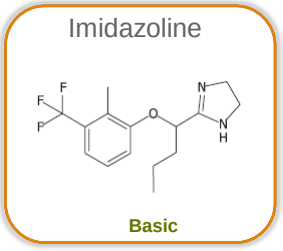
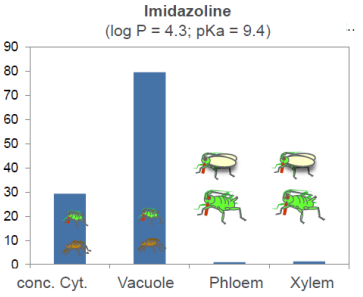
Which compound won't be efficacious for aphids control?





Remember:

- Aphids are phloem and xylem feeders
- Weak acids get trapped in phloem
- Basic molecules get trapped in vacuoles (i.e. cells)

Buchholz, A., Trapp, S., Pest Manag. Sci. (2016); 72: 929–939

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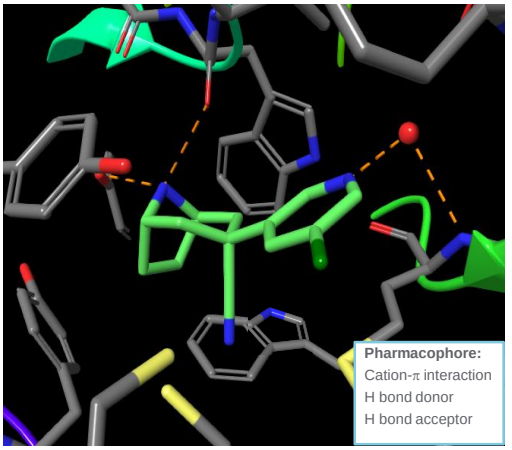
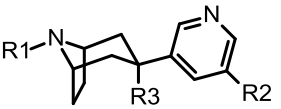
nAChR agonists for aphids control



AChBP co-crystal structure with lead



Our target
- Low lipophilicity (logP < 2.5)
- ✓ Low molecular volume
- Non-basic

Proc. Brighton Crop Protection Conf: Pest and Diseases **2002**, *1*, 145 – 152.

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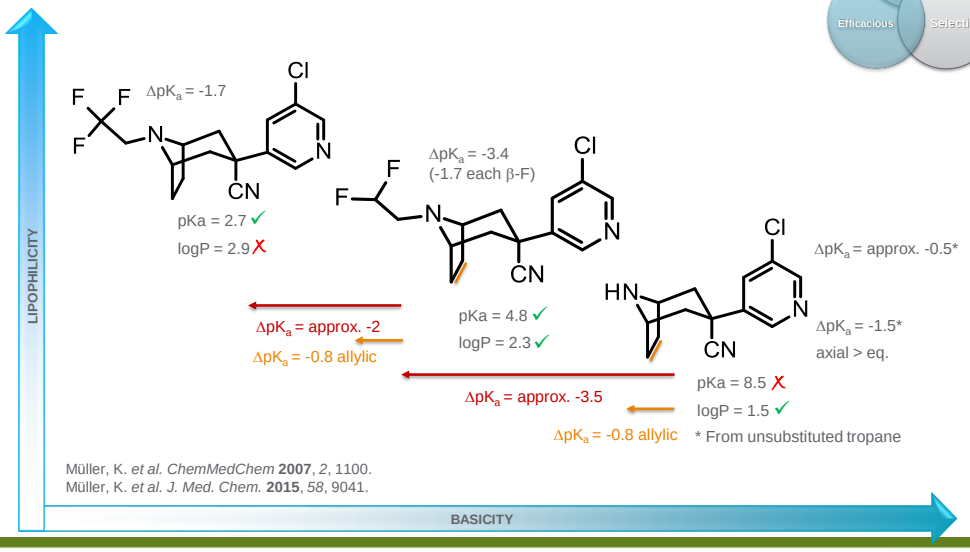
Tuning physicochemical properties



Müller, K. *et al. ChemMedChem* **2007**, *2*, 1100.
Müller, K. *et al. J. Med. Chem.* **2015**, *58*, 9041.

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Modern crop protection products targeting ion channels

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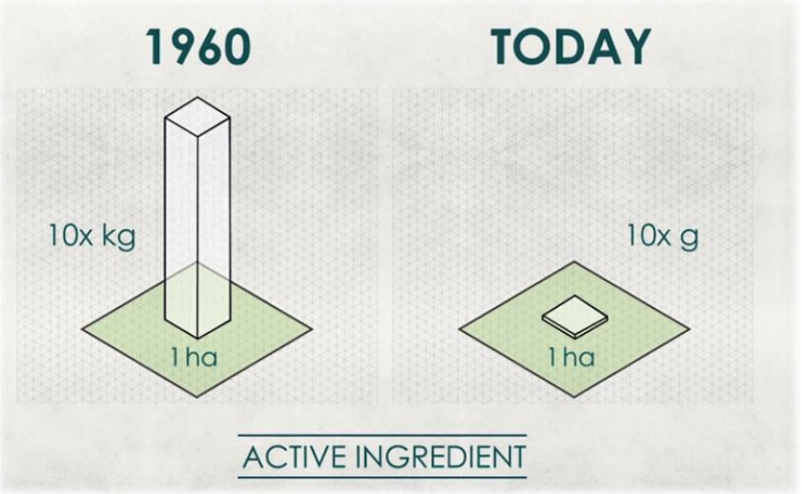
Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

The crop science in the 1960's used 10 Kgs of active ingredient per hectare to protect crops (1 hectare is almost 2.5 acres). **How much active ingredient is used today in comparison?**

- 1 kilogram
- 500 grams
- 100 grams
- 10 grams
- 1 gram

** If your answer differs greatly from the choices above tell us in the chat!*



https://croplife.org/crop-protection/innovation-in-crop-protection-products/

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Product Safety – Who is being protected?

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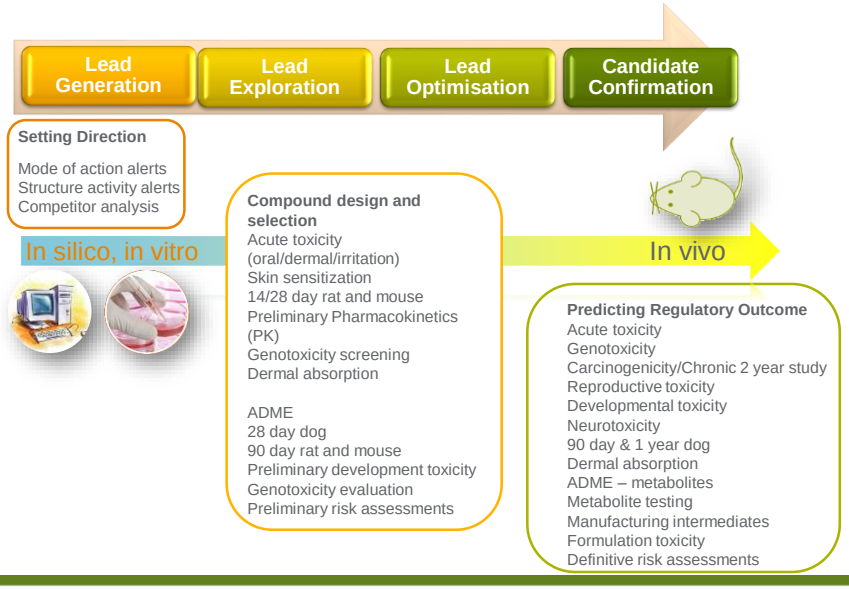
Product safety: studies per stage



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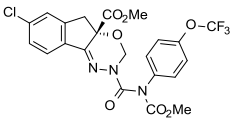
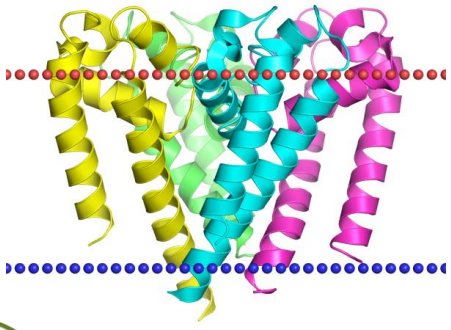
Efficacious, safe and selective: Indoxacarb





Spodoptera litura (Oriental leafworm moth) feeding on a cabbage leaf

- Indoxacarb (DuPont) is an insecticide that exerts its mode of action by targeting the Voltage-gated Sodium channel
- It is active against Lepidoptera (moths)

Channels **2008**, *2*, 100.
Bioorg. Med. Chem. Lett. **2014**, *24*, 3690.
J. Med. Chem. **2015**, *58*, 7093–7118

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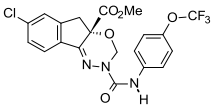
Mammalian safety of Indoxacarb

Differential binding

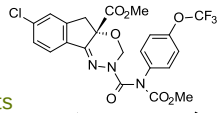


DCJW Active ingredient

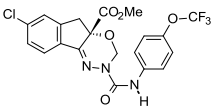
IC_{50} = **1000** nM on rat Na_V 1.4
IC_{50} = **25** nM on Bg Na_V 1-1a
(Bg = Blattella Germanica)

Pestic. Biochem. Physiol. **2010**, *97*, 87.

Selective metabolism

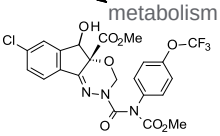


In insects
Hydrolases



DCJW

In higher animals
Oxydative metabolism



+ other metabolites

Crop Protection **2000**, *19*, 537.
Indoxacarb, *JMPR* Evaluation report 2005.

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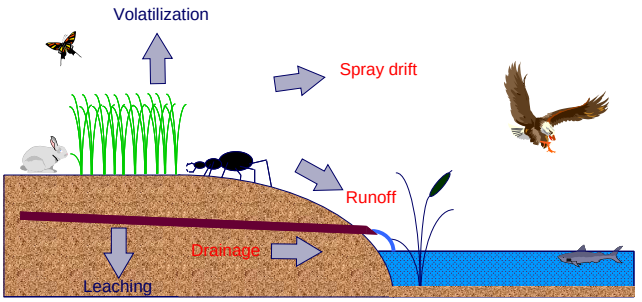
Environmental Safety – What is being protected?

- **Groundwater** – Drinking water (human exposure), irrigation water, the aquifer itself as an entity
- **Surface Water** – Drinking water, irrigation water, aquatic organisms (fish and aquatic plants)
- **Soil** – Persistence in soil, topsoil erosion, carry-over into follow on crops
- **Non target insects, plants and the organisms**
  - Bees, beneficial insects, worms, off target plant species, birds, field dwelling mammals
- **Air** – long range transport, atmospheric degradation, vapour movement



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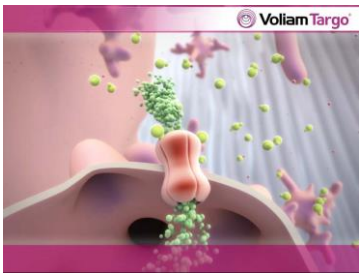
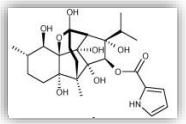
Efficacious, safe and selective: Anthranilic amides

Anthranilic amides bind to the insect ryanodine receptor in muscle cells



Intrinsic target-based selectivity:
Insect vs. Mammal

	EC50 (nM)
Cockroach	36
Fruit Fly	48
Mouse	14'000
Rat	> 100'000



Ryanodine (plant metabolite)

VOLIAM TARGO | Untreated

Active in the field at rates as low as **5 g/ha**!
(typical rate for organophosphates = **1 Kg/ha**)

Crop: Cauliflower
Source: Taiwan, Syngenta trials 2007

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Pest Manage. Sci. **2013**, *69*, 7.; *Invert. Neurosci.* **2008**, *8*, 107-19; *Biochemistry*, **2009**, *48*, 10342

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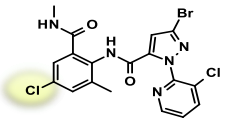
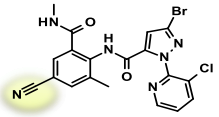
Modulation of soil persistance



Chlorantraniliprole (DuPont)

M.p. (°C) 208-210
logP 2.76
pKa (acid) 10.8

Water solubility (mg/l, 20-25 °C) 1.0
Water DT50 10 d (pH 9, 25 °C)
Soil DT50 < 2–12 mo



Cyantraniliprole (DuPont/Syngenta)

M.p. (°C) 224
logP 1.94
pKa (acid) 8.8

Water solubility (mg/l, 20-25 °C) 14.24
Water DT50 < 1 d (pH 9, 25 °C)
Soil DT50 average 32 d

Improved plant mobility
Increased spectrum of insect control (aphids and leafhoppers)

(Data from BCPC Pesticide Manual)

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Classification: PUBLIC

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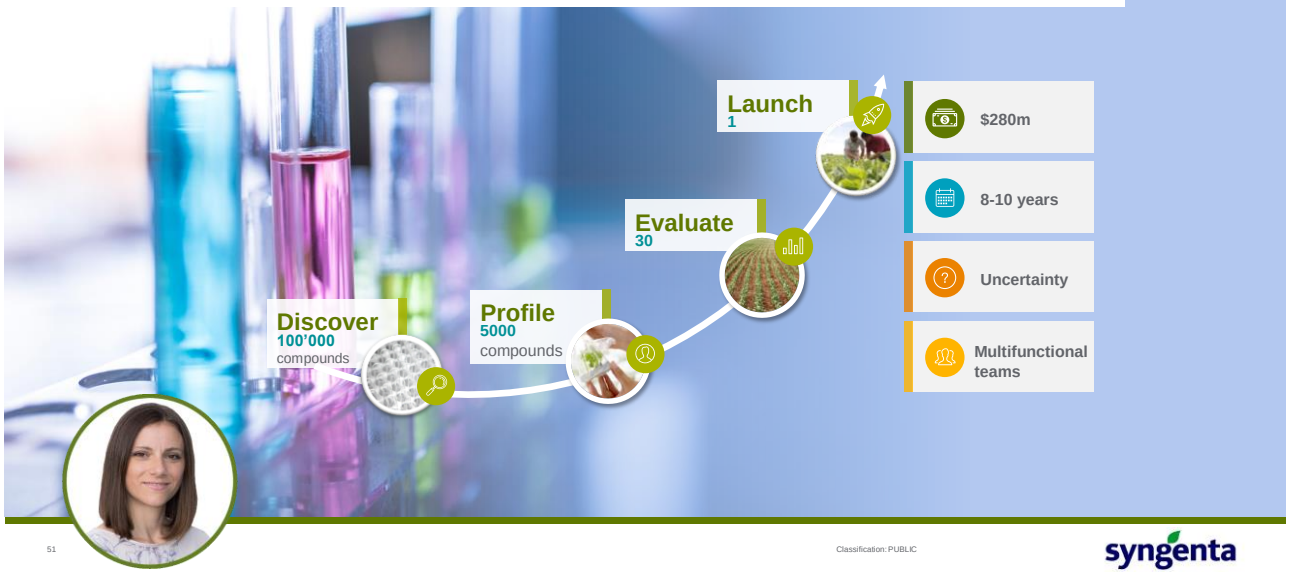
CP Research & Development



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Liz Hirst
Penny Cutler
Janet Phillips

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Ann Sluder**
Sheetal Shah
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***C. elegans* biology**
Anthony Flemming and team

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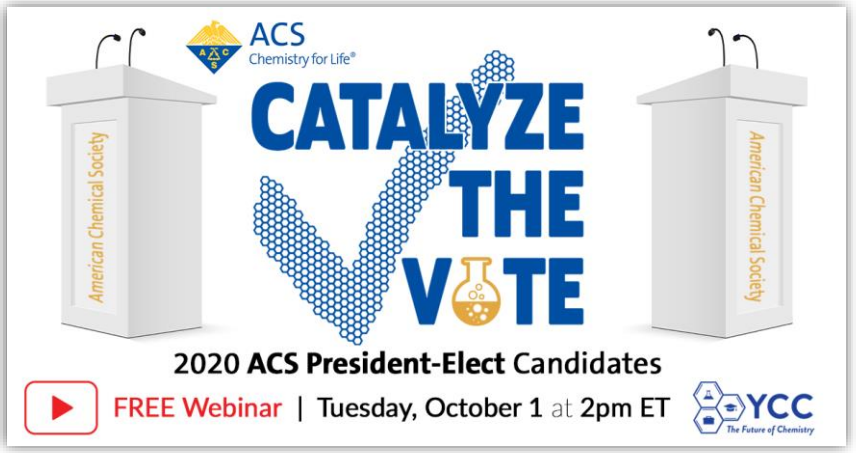

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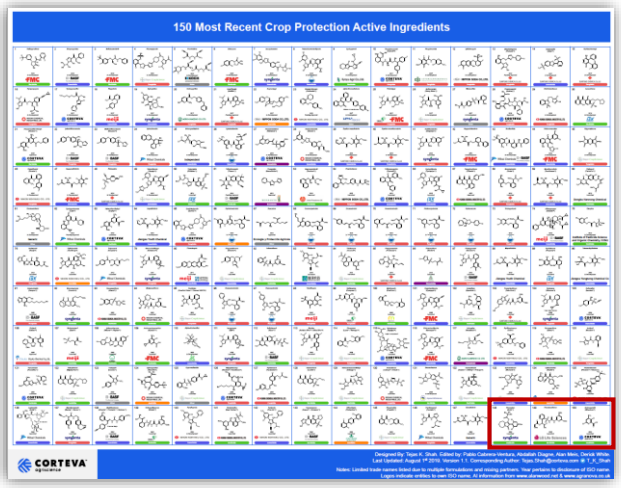
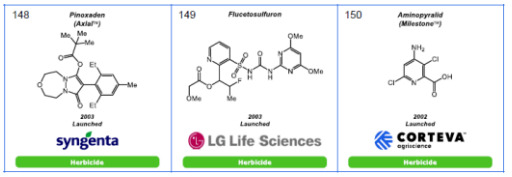
Webinar Additional Resource!

150 Most Recent Crop Protection Active Ingredients





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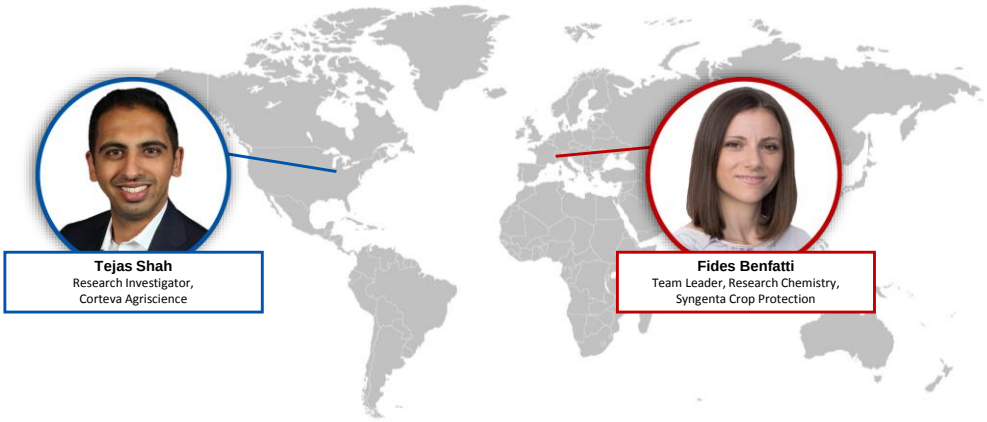

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Research Investigator,
Corteva Agriscience

Fides Benfatti
Team Leader, Research Chemistry,
Syngenta Crop Protection

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1. Drug Discovery Series #1 - Current Drug Discovery and Development Process
(DDS #1) Watch this overview of the drug discovery and development process to learn the stages and challenges in every step.
2. Primer in Drug Target Classes
(DDS #2) Listen in on a discussion on the big four druggable families and the difference between small molecule and biotherapeutic targets.
3. Key Concepts in Identifying Drug Leads
(DDS #3) Discover how drug-likeness is a deceiving concept, explore the Rule of Five, and show how lessons from the past may guide the present.
4. Lead Optimization - Building Efficacy & Safety
(DDS #4) Learn strategies on how to effectively optimize small molecule hits and rapidly assess your findings.
5. Tips for Filing IND and Starting your Clinical Trials
(DDS #5) What do you need to know when filing for Investigational New Drug submissions to the United States Food and Drug Administration?
6. The Role of Chemistry in Clinical Trials: The Big Expense & Lessons Learned
(DDS #6) Learn how the properties of the candidate impact decisions in the discovery process.
7. Pharmacoeconomics and IP Strategies in Drug Development
(DDS #7) Review the basic principles of Pharmacoeconomics in drug development strategies as well as its role in determining health insurance coverage of drug products.
8. Future of Drug Discovery - Challenges, Risks and Rewards
(DDS #8) Explore how how risks and challenges will be dealt with in the future and the key skill sets required of future medicinal chemists.

2015

1. Designing Better Drug Candidates
(January) Learn various factors that can be used to improve candidate quality from Dr. Paul Leeson.
2. Strategies to Improve Solubility of Drug Candidates
(February) Learn a number of different strategies for improving drug solubility through structural modification.
3. Fragment-Based Drug Design Strategies
(March) Finding the right drug target is becoming increasingly difficult. Learn how focusing on the smaller picture can have big results.
4. Screening Strategies
(April) Learn the pros and cons of different screening strategies.
5. Avoiding PAINS (pan-assay interference compounds)
(May) Jonathan Baell shares some tips on how to avoid the dead ends of drug discovery.
6. Accelerating CNS Positron Emission Tomography (PET) Ligand Discovery
(June) Jon Lee Zheng as he laysout a set of preferred parameters for which has yielded successful PET ligands and reduced resources and timelines.
7. X-ray Crystallography in Drug Discovery
(July) Jon Mason and Mike Congreve describe what protein-ligand X-ray data can do for you.
8. Choices and Trends in Solid Dosage Form Selection
(August) Discover the pros and cons of the different solid state forms and what to consider when selecting.
9. Delivery Options to Support Dose Escalation in Preclinical Toxicology and Pharmacodynamic Activity Studies
(September) Gain an understanding of acceptable drug delivery approaches to support preclinical dose escalation.
10. Pharmacokinetic Considerations in Drug Design and Development
Learn about key pharmacokinetic concepts including clearance, volume of distribution, half life and protein binding.
11. Prodrugs in Drug Discovery
(November) John Higgins shares the utility of prodrugs, their general properties and prerequisites for optimal performance.

2016

I - Time: The Fourth Dimension in Drug Discovery
1. The Importance of Drug-Target Kinetics in Drug Design
Robert Copeland - Epizyme, Inc
Dan Erlanson - Carmot Therapeutics
2. Long-Acting Injectable Medications: Strategies and Mechanistic Considerations
Jules Remenar - Alkermes
Annette Bak - Merck
3. Modified Release Formulations for Solubility Starved Compounds
Mengwei Hu - Merck
John Morrison - BMS
4. *The Medicinal Chemist of Tomorrow (Special Topic)*
Joel Barrish - Achillion
Ravi Nargund - Merck
Maly Schmid - Tech Coast Angels

II - Beyond Traditional Small Molecules
5. Design of Deliverable Macrocycles
Scott Lokey - UC Santa Cruz
Nicholas Meanwell - BMS
6. Dreaming Big and Thinking Small: Applying Medicinal Chemistry Strategy to Antibody-Drug-Conjugates
L. Nathan Tumey - Pfizer
Peter Senter - Seattle Genetics
7. Nucleic Acids Therapeutics: Making Sense of Antisense Oligonucleotides
Punit Seth - Ionis
Richard Olson - BMS
8. Crystallography as a Drug Design and Delivery Tool (Special Topic)
Robert Wenslow - Crystal Pharmatech
Vincent Stoll - Abbvie
Andrew Brunskill - Merck

III - Pharmacology Revisited
9. Dealing with Reactive Drug Metabolites in Drug Discovery: Can We Predict Toxicities of Drug Candidates that form Reactive Metabolites?
Deepak Dalvie - Pfizer
Frederick Peter Guengerich - Vanderbilt University
10. Rational Design of Small Molecules Targeting RNA
Matt Disney - Scripps Ri Florida
Amanda Garner - University of Michigan
11. Cell Penetrating Peptides to Improve Cellular Drug Uptake
Dehua Pei - The Ohio State University
Scott Hart - Bristol-Myers Squibb

2017

I - Fighting Cancer
4. Fighting Cancer: Targeting CNS Malignancy with Kinase Inhibitors
Timothy P. Heffron - Genentech
Mark Witman - Bristol-Myers Squibb
2. Fighting Cancer: Epigenetic targets for Oncology
Stuart Conway - Oxford
Sharan Bagal - AstraZeneca
3. Fighting Cancer: Allostery and Targeting Cancer Cell Metabolism
Stefan Gross - Agios
Scott Edmundson - AstraZeneca

Special Broadcast
4. Cystic Fibrosis: Discovery of CFTR Modulators
Peter Grootenhuis - Vertex
Nick Meanwell - Bristol-Myers Squibb

II - Anti-Infectives
5. Anti-Infectives: Rational Approaches to the Design and Optimization
Jason Sello - Brown University
Courtney Aldrich - University of Minnesota
6. Tuberculosis: An Introduction for Medicinal Chemists
Carl Nathan - Weill Cornell Medicine
Christopher Boyce - Merck
7. Viral Hepatitis: The Search for a Cure
Mike Sofia - Arbutus Biopharma
Stephen Mason - CaroGen Corporation

Special Broadcast
8. Spinal Muscular Atrophy
Kevin Hodgetts - Harvard Medical School
Alyson Weidmann - ACS Publications

III - Immunology
9. Psoriasis: Treatment and Novel Approaches
Frank Narjes - AstraZeneca
John Morrison - Bristol-Myers Squibb
10. Lupus: Treatment and Novel Approaches
Laurence Menard - Bristol-Myers Squibb
Mary Struthers - Bristol-Myers Squibb

2018

1. Jan 25 — A New Strategy in Drug Discovery: Protac-Induced Protein Degradation
Ian Churcher - BenevolentBio
Aaron Balog - Bristol-Myers Squibb
2. Feb 22 — Women in Drug Discovery and Development: How to Succeed as a Female in Academia and Industry
Annette Bak - AstraZeneca
Donna Huryn - University of Pittsburgh
Erika Araujo - Bristol-Myers Squibb
Nurulain Zaveri - Astraea Therapeutics
3. Mar 29 — A Nanomedicine Overview for mRNA Delivery: Innovative Methods Using Lipid Nanoparticles
Marianna Yanez Arteta - AstraZeneca
Dennis Luenig - Genentech
4. Apr 26 — Nanomaterials for Fighting Antibiotic-Resistant Bacteria
Vincent Rotello - University of Massachusetts at Amherst
Christopher England - American Chemical Society
5. May 31 — Advanced Nano-Delivery Systems: Facilitating Tumor Delivery and Mitigating Resistance
Mansoor Amiji - Northeastern University
Venkat Krishnamurthy - AstraZeneca
6. Jun 28 — Pitfalls and Promise of Central Nervous System Drug Discovery
Valentin Gribkoff - Yale University
Nicholas Meanwell - Bristol-Myers Squibb
7. Jul 26 — How to Optimize Central Nervous System Therapeutics: Med Chem Strategies, Tactics, and Workflows
Craig Lindsley - Vanderbilt Center for Neuroscience Drug Discovery
Amy Newman - Intramural Research Program, NIH
8. Sept 20 — A Novel Strategy for the Treatment of Chronic Pain: Antagonising PAR2 with a Monoclonal Antibody
Pete Thornton - AstraZeneca
Nurulain Zaveri - Astraea Therapeutics
9. Oct 18 — How to Predict Human CNS PK/PD: Preclinical Experiments and Advanced Mathematical Modelling
Elizabeth de Lange - Leiden Academic Center for Drug Research
Alexander Tropsha - University of North Carolina
10. Nov 29 — Human Exosomes: An Ideal Vehicle for Delivery of Therapeutic RNAs to Cells and Organs
Hadi Valadi - University of Gothenburg
Alexander Kapustin - AstraZeneca

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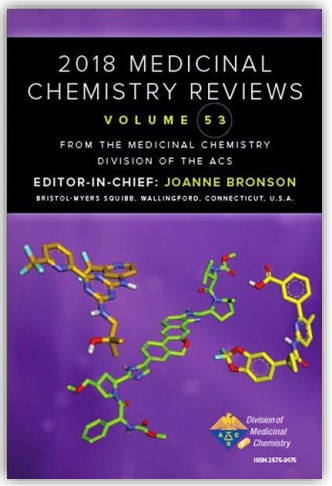

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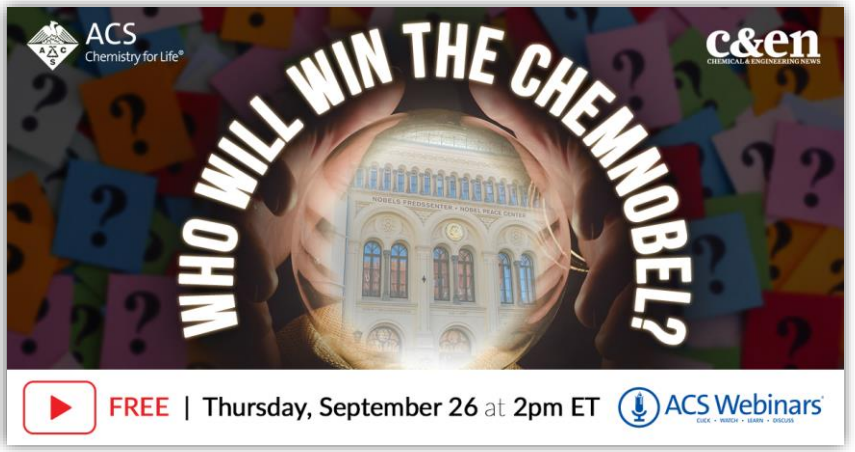

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