

Agrochemical Library 2009 Generation (ChemDiv, Inc.)

The new agrochemical collection consists of *nearly 20,000 compounds* selected specifically to promote new discoveries impacting a wide range of agricultural benefits. We have considered many factors, which are elaborated below.

Due to the intense and widespread attention being given to the undesirable side-effects of some commercial agrochemical products such as residual contamination, resistance, ecosystem impairments, and waste generation, the discovery of new, **natural and semi-synthetic agrochemicals** that are biologically safe will prove to be significant and profitable. Natural substances and analogues are available for virtually every aspect of plant biology and the ChemDiv collection is an excellent place to start or embellish your cutting-edge research program.

A plethora of **fungicidal compounds** exist covering a broad range of chemotypes. The ChemDiv collection serves to expand IP potential and to expedite the discovery of improved properties, especially specificity.

Prominent **cholinesterase inhibitors** are malathion (an organophosphorous) and bendiocarb (a carbamate) used extensively as **insecticides** with low mammalian toxicity. The search continues for greater selectivity and also molluscicidal and acaricidal activities.

Neonicotinoids, such as **imidacloprid**, are **nicotinic acetylcholine receptor (nAChR) agonists** with potent insecticidal activity. Recently, imidacloprid (Advantage) and related nicotinoids have begun replacing organophosphorus and methylcarbamate compounds as insecticides to control insect pests on major crops. Nicotinoids act with remarkable effectiveness against insects while being safe for mammals; they are quickly degraded and do not persist in the environment.

Insect **GABA gated-chloride channels** are targets of several classes of chemicals with insecticidal activity including dieldrin, picrotoxin and BIDN (3, 3-bis(trifluoromethyl)-bicyclo [2,2,1]-heptane-2, 2-dicarbonitrile).

Research has shown that agonists of **muscarinic receptor** could induce stomatal opening, while the antagonists (eg. atropine) could block stomatal opening induced by acetylcholine. The evidence that mAChR localizes in the guard cells provides a new possible signal transduction pathway in acetylcholine-mediated stomata movement.

Selamectin is the active ingredient in Revolution, a topical insecticide and antihelminthic used on dogs and cats. Selamectin works by replacing glutamate which normally interacts with receptors that open **chloride channels** at muscle synapses found in parasites.

Non-selective **cation channels** are ubiquitous in plant membranes and may function in nutrient uptake, signaling and intra-plant transport. Plants possess **NMDA-like receptors**, generically referred to as **glutamate receptors (GLRs)**. Agonists and antagonists of animal glutamate receptors function to modulate expression of plant genes and as plant growth regulators. These agonists and antagonists structurally do not resemble glutamate. Thus, their actions in plants likely are due to their specific interaction with one or more plant glutamate receptors, rather than to general effects on glutamate-utilizing enzymes.

A recent patent describes a **plant growth promoter** comprising as an active ingredient a phenylglycine which is relatively easily available and low in cost. The ChemDiv Agro library contains dozens of **arylglycine** derivatives.

The **organophosphorus** insecticides are a very important group of compounds that vary tremendously in chemical structure and chemical properties. Most exist as phosphates, phosphonates, phosphorothionates, phosphorodithioates, phosphoramidothioates, etc. Our collection includes hundreds of such compounds including **aminophosphonic acids**.

Please find below the statistical data for the current generation of ChemDiv's Agro Library.

Library	Size	Unique Heterocycles	Diversity Coefficient	Screens	Property Range
Agro	18,862 compounds	998	0.758	5,663	177 < MW < 659; 406 on average 0 < HBA < 13; 5 on average 0 < HBD < 9; 1 on average 0 < Rotatable Bonds < 16; 7 on average -12.0 < logD (pH 7.4) < 10.0; 3.1 on average -8.7 < log of solubility in water (pH 7.4) < 10.9; -2.9 on average