

AgroChemical Libraries

The term “agrichemical” (or “agrochemical”) usually refers to a broad range of pesticides, including insecticides, herbicides, fungicides and nematicides. It may also include synthetic fertilizers, hormones and other chemical growth agents.

Several libraries of agrochemical-like compounds were created by assessing physicochemical properties and structural features of the Life Chemicals HTS Compound Collection. At the first stage the following restrictions were applied:

- $250 < MW < 500$
- $0.3 < ClogP < 4.5$
- $HBD \leq 2$
- $HBA < 10$
- $RotB < 11$

Then, compounds were picked out by similarity search (Tanimoto method with 80 % cut-off) against the reference set of known agrochemical compounds (www.pesticideinfo.org). In addition, a substructure search was also applied. Substructural cores of each class of agrochemical compounds (fungicides, insecticides, herbicides, microbiocides) were selected from the literature [1–18] and on-line databases. Selection of compounds that belong to the corresponding chemical classes was performed with SYBYL-X and MDL ISIS software packages.

Presented below is a list of agrochemical-like compound sets designed by Life Chemicals and as well as corresponding chemical classes they comprise:

Insecticides (1,800 in-stock compounds)

- Alkyl phthalates
- Chloronicotinyl compounds
- Diacylhydrazines
- N-Methyl carbamates
- Organochlorine compounds (oligochlorinated)
- Organophosphorus compounds
- Pheromones
- Chlorinated pyrazoles

Microbiocides (1,900 in-stock compounds)

- Chlorinated phenols
- Hydantoins
- Isothiazolones
- Phenols
- Quaternary ammonium compounds

Herbicides (7,700 in-stock compounds)

- 2,6-Dinitroanilines
- Imidazolinones
- Dinitrophenols
- Sulfonylurea
- Benzoic acids, chlorine substituted
- Benzoyl urea, chlorine substituted
- Bipyridilium compounds
- Chlorophenoxy acids/esters
- Chloropyridinyls
- Cyclohexenones
- Thiocarbamates
- Triazines
- Uracils
- *N*-phenyl, *N'*-alkyl substituted ureas
- *N*-alkyl, *N'*-thiadiazole substituted ureas
- Bis-carbamates

Fungicides (1,000 in-stock compounds)

- Azoles
- Benzimidazoles
- Dicarboxamides
- Chlorinated benzenes

References

1. C. Lamberth, S. Jeanmart, T. Luksch, A. Plant, Current challenges and trends in the discovery of agrochemicals, *Science*, 2013, Vol. 341, pp. 742–746.
2. O. Ort, in *Modern Crop Protection Compounds*, W. Krämer, U. Schirmer, P. Jeschke, M. Witschel, Eds. (Wiley-VCH, Weinheim, Germany, 2012), pp. 50–88.
3. M. A. Hanagan, R. J. Pasteris, R. Shapiro, Y. Henry, B. Klyashchitsky, paper presented at the 242nd American Chemical Society (ACS) National Meeting, Denver, CO, 28 August to 1 September 2011, abstr. no. AGRO-79.
4. T. Pitterna et al., *Bioorg. Med. Chem.* 17, 4085–4095 (2009).
5. A. Plant, *Agrow Silver Jubilee Issue*, XI–XV (2010).
6. R. M. Hollingworth, in *Agrochemical Discovery*, D. R. Baker, N. K. Umetsu, Eds. (American Chemical Society, Washington, DC, 2001), pp. 238–255.
7. C. L. Cantrell, F. E. Dayan, S. O. Duke, *J. Nat. Prod.* 75, 1231–1242 (2012).
8. F. E. Dayan, C. L. Cantrell, S. O. Duke, *Bioorg. Med. Chem.* 17, 4022–4034 (2009).
9. C. Lamberth, *Nachr. Chem.* 55, 130–134 (2007).
10. S. D. Lindell, L. C. Pattenden, J. Shannon, *Bioorg. Med. Chem.* 17, 4035–4046 (2009).
11. L. Zirngibl, *Antifungal Azoles* (Wiley-VCH, Weinheim, Germany, 1998).
12. K.-J. Schleifer, in *Pesticide Chemistry*, H. Ohkawa, H. Miyagawa, P. W. Lee, Eds. (Wiley-VCH, Weinheim, Germany, 2007), pp. 77–88.
13. C. M. Tice, *Pest Manag. Sci.* 57, 3–16 (2001).
14. C. M. Tice, *Pest Manag. Sci.* 58, 219–233 (2002).
15. C. Lamberth, J. Dinges, in *Bioactive Heterocyclic Compound Classes - Agrochemicals*, C. Lamberth, J. Dinges, Eds. (Wiley-VCH, Weinheim, Germany, 2012), pp. 3–20.
16. P. Jeschke, in *Modern Methods in Crop Protection Research*, P. Jeschke, W. Krämer, U. Schirmer, M. Witschel, Eds. (Wiley-VCH, Weinheim, Germany, 2012), pp. 73–128.G.
17. Theodoridis, in *Fluorine and the Environment – Agrochemicals, Archaeology, Green Chemistry and Water*, A. Tressaud, Ed. (Elsevier, Amsterdam, 2006), pp. 121–175.
18. M. López-Ramos, F. Perruccio, *J. Chem. Inf. Model.* 50, 801–814 (2010).