



DATASET

Editable chemical structure files (sk2 and MDL mol) of pesticide active ingredients

Tamas Komives

Plant Protection Institute, Centre for Agricultural Research, Hungarian Academy of Sciences, Herman Otto 15, 1022 Budapest, Hungary and Faculty of Agricultural Sciences and Rural Development, Eszterhazy Karoly University, 3200 Gyongyos, Hungary

E-mail: komives.tamas@agrar.mta.hu

Abstract – This Dataset contains a long list of online, freely available sk2 and MDL mol files of a number of pesticide active ingredients for use by anyone interested (students, teachers, researchers, etc.).

Keywords – sk2, MDL mol, editable files, molecular editor, molecular modeling, pesticides, pesticide active ingredients

Received: November 28, 2016

Accepted: December 10, 2016

I have lived much of my life among molecules. They are good company.

George Wald

Introduction

During my professional career I drew a great number of molecules, just as so many of my colleagues (students, teachers, researchers, etc.) interested in chemistry did (and do today). I showed those molecules on my lectures, at conferences, in papers, book chapters, and patent applications. My intention with making available many of the molecules I drew in editable formats is to save time and energy for anyone interested in pesticide chemistry, biochemistry, environmental behavior, etc. and wish to draw the molecules in their own way.

Freely available chemical software ChemSketch 12.0 ([Advanced Chemistry Development](#), Inc., Toronto, Ontario, Canada, 2015) and [Arguslab](#) (developed by Mark Thompson) were used to create the sk2 and MDL mol chemical structure files listed in Tables 1-4.

The molecule files (sk2 and MDL mol) are freely downloadable from the website of this open access journal (<http://ecocycles.eu/pesticides>). My only request is that, if you use these files, please refer to this paper in your presentation, publication, lecture, etc. the following way:

Komives, T. (2017) Editable chemical structure files (sk2 and MDL mol) of pesticide active ingredients. *Ecocycles* 3(1) 13-16.
DOI: 10.19040/ecocycles.v3i1.64

There are different kinds of free and commercially available software for drawing and editing molecules: for a brief overview I suggest to consult the Wikipedia webpage “Molecule editor” (2016). Most molecule editor software accept sk2 and MDL mol files: these formats describe single molecular structures, which may contain disjoint fragments.

To download a molecule’s sk2 or MDL mol file please visit the website <http://ecocycles.eu/pesticides>, and click on the links beside the active ingredients in the Tables. Please note that, for technical reasons, the files are zipped.

Of course, users are free to modify the molecules for any purpose they like: the possibilities are almost endless (change the format, the atoms, the bonds, the stereochemistry, etc.).

And, to my regret, yes, there may be mistakes in the structures. If you find one (two, three, a lot), please let me know: I will modify the structure(s) as quick as I can.

For crosschecking the chemical structures and also for specific information on individual pesticide active ingredients I strongly recommend the reader to consult the excellent and comprehensive website entitled “Compendium of Pesticide Common Names” (Wood, 2016).

References

Molecule editor [WWW Document], 2016. Wikipedia. URL: <https://en.wikipedia.org/w/index.php?title=Molecule-editor&oldid=741260967> (accessed 11.8.16).

Wood, A., 2016. Compendium of Pesticide Common Names [WWW Document]. URL: <http://www.alanwood.net/pesticides/> (accessed 11.25.16).

Supplementary material

Table 1. List of herbicide active ingredients of which the MDL mol and sk2 files can be downloaded from [HERE](#)

2,4D	dimethenamid-P	metamitron
acetochlor	diuron	metazachlor
acifluorfen	EPTC	metazosulfuron
alachlor	ethalfluralin	methabenzthiazuron
amicarbazone	ethoxyfen	metobromuron
amidosulfuron	ethoxysulfuron	metolachlor
aminocyclopyrachlor	fenoxasulfone	metolachlor-S
aminopyralid	fentrazamide	metosulam
atrazine	flazasulfuron	metoxuron
beflubutamid	florasulam	metribuzin
bencarbazone	fluzolate	molinate
benfluralin	flucarbazone	monolinuron
benthiocarb	flucetosulfuron	naptalam
benzobicyclon	flufenpyr-ethyl	norflurazon
bialafos	flumetralin	orthosulfamuron
bicyclopyrone	flumetsulam	oxadiargyl
bifenox	flumiclorac-pentyl	oxadiazon
bromoxynil	flumioxazin	oxaziclomefone
butachlor	flupyrsulfuron-methyl	oxyfluorfen
butafenacil	flurochloridone	paraquat
butylate	fluthiacet-methyl	pendimethalin
carfentrazone	fomesafen	penoxsulam
CDAA	halauxifen-methyl	pentoxazone
chlorbromuron	haloxyfop-methyl	pethoxamid
chloridazon	haloxyfop-P	phenmedipham
chloroxuron	hexazinone	picolinafen
chlorsulfuron	imazamethabenz-methyl	pinoxaden
chlortoluron	imazamox	propachlor
cinidon-ethyl	imazapyr	propanil
clethodim	imazaquin	propoxycarbazone
clomazone	imazethapyr	pyraflufen-ethyl
cyanazine	indaziflam	pyrasulfotole
cyclanilide	ioxynil	pyribenzoxim
cycloate	isopropalin	pyridate
cycloxydim	isoproturon	pyriftalid
desmedipham	isoxaben	pyrimisulfan
dicamba	isoxaflutole	pyroxasulfone
dichlobenil	lenacil	pyroxsulam
diclofop-methyl	linuron	saflufenacil
diethyl-ethyl	MCPA	sethoxydim
diflufenican	MCPB	sulcotrione
diflufenzopyr	mecoprop	sulfentrazone
dimefuron	mesosulfuron-methyl	tefuryltrione
dimethachlor	mesotrione	tembotrione
dimethenamid	metamifop	tepraloxymid

terbacil	tralkoxydim	tritosulfuron
thiencarbazone-methyl	trifloxysulfuron	vernolate
topramezone	trifluralin	

Table 2. List of fungicide active ingredients of which the MDL mol and sk2 files can be downloaded from [HERE](#)

acibenzolar-Ss-methyl	fenpiclonil	penconazole
ametotradin	fenpropimorph	pencycuron
amisulbrom	fenpyrazamine	penflufen
azoxystrobin	fluazinam	penthiopyrad
benalaxyl	fludioxonil	picoxystrobin
benalaxyl-M	flumorph	prochloraz
benomyl	fluopicolide	procymidone
benthiavalicarb-isopropyl	fluopyram	propiconazole
benzovindiflupyr	fluoxastrobin	proquinazid
bitertanol	fluquinconazole	prothioconazole
bixafen	flusilazole	pydiflumetofen
boscalid	flutriafol	pyraclostrobin
bromuconazole	fluxapyroxad	pyribencarb
bupirimate	folpet	pyrifenox
carbendazim	fuberidazole	pyrimethanil
carboxin	furametpyr	pyriofenone
chlorothalonil	hexaconazole	quinomethionat
cyazofamid	hymexazol	quinoxifen
cyflufenamid	imazalil	sedaxane
cymoxanil	ipconazole	silthiofam
cyproconazole	iprodione	spiroxamine
cyprodinil	iprovalicarb	tebuconazole
dichlobenzthiazox	isofetamid	tetraconazole
dichlofluanid	isoprothiolane	thiabendazole
diclobutrazol	isopyrazam	thifluzamide
diclocymet	isotianil	thiophanate-methyl
difenoconazole	kresoxim-methyl	TMTD
diflumetorim	mandestrobim	tolyfluanid
dimethomorph	mandipropamid	tralopyril
dimoxystrobin	meptyldinocap	triadimefon
diniconazole	metalaxyl	triadimenol
dinocap	metalaxyl-m	triazoxide
dithianon	metconazole	tridemorph
dodemorph	metrafenone	trifloxistrobin
epoxiconazole	myclobutanil	triflumizole
ethaboxam	nabam	triforine
famoxadone	nuarimol	triticonazole
fenamidone	orysastrobin	valifenalate
fenarimol	oxadixyl	vinclozolin
fenhexamid	oxathiapiprolin	ziram
fenoxasulfone	oxycarboxin	zoxamide

Table 3. List of insecticide and acaricide active ingredients of which the MDL mol and sk2 files can be downloaded from [HERE](#)

acephate	alpha-cypermethrin	azinphos-methyl
acetamiprid	amidoflumet	bendiocarb
acrinathrin	amitraz	benfuracarb
aldicarb		

bensultap	etoxazole	parathion
beta-cyfluthrin	etrifos	parathion-methyl
beta-cypermethrin	fenazaquin	permethrin
bifenazate	fenitrothion	phenthoate
bifenthrin	fenoxy carb	phorate
bioallethrin	fenpropathrin	phosalone
bioresmethrin	fenpyroximate	phosmet
buprofezin	fenthion	phosmethylan
butoxycarboxim	fenvalerate	phosphamidon
carbaryl	fipronil	phosthiazat
carbofuran	flonicamid	pirimicarb
carbosulfan	flubendiamide	pirimiphos-methyl
cartap	flucycloxuron	profluthrin
chlordaniliprole	flufenerim	propargite
chlorfluazuron	flufenoxuron	pymetrozine
chlorpyrifos	formothion	pyrazophos
chlorpyrifos-methyl	halofenozide	pyrethrin-i
chromafenozide	heptenophos	pyridaben
clofentezin	hexaflumuron	pyridafenthion
clothianidin	hexythioazox	pyrifluquinazon
cyantraniliprole	imidacloprid	pyriproxyfen
cyenopyrafen	indoxacarb	quinalphos
cyhexatin	lambda-cyhalothrin	spirotetramat
cypermethrin	lindane	sulfotep
cyromazine-fix	lufenuron	tebufenozide
DDT	malathion	tebufenpyrad
deltamethrin	metaflumizone	teflubenzuron
diafenthiuron	methamidophos	tefluthrin
diazinone	methidathion	tepp
dichlorvos	methiocarb	terbuphos
diflovidazin	methomyl	tetradifon
diflubenzuron	methoxyfenozide	tetramethrin
dimefluthrin	metofluthrin	thiacloprid
dimethoate	neriestoxin	thiamethoxam
dinotefuran	nicarbazin	thiocylam
dioxacarb	nicotine	triazamate
DNOC	nitenpyram	triazophos
endosulfan	noviflumuron	triflumuron
esfenvalerate	oxamyl	zeta-cypermethrin
ethiprole	oxydemeton-methyl	
etofenprox	paraoxon	

Table 4. List of herbicide safener active ingredients of which the MDL mol and sk2 files can be downloaded from [HERE](#)

AD-67	dicyclonon	isoxadifen-ethyl
benoxacor	dietholate	jiecaowan (also known as MG-191)
bpcms	dimepiperate	mefenpyr-diethyl
cloquintocet-mexyl	fenclorazole-ethyl	mephenate
cumyluron	fenclorim	methoxyphenone
cyometrinil	flurazole	naphthalic-anhydride
cyprosulfamide	fluxofenim	oxabtrinil
daimuron	furilazole	
dichlormid	isoxaben	