ECOCYCLES
Scientific journal of the European Ecocycles Society

2017

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.).

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	fluazolate	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
diethatyl-ethyl	MCPA	sethoxydim
diflufenican	MCPB	sulcotrione
diflufenzopyr	mecoprop	sulfentrazone
dimefuron	mesosulfuron-methyl	tefuryltrione
dimethachlor	mesotrione	tembotrione
dimethenamid	metamifop	tepraloxydim

14

terbacil
thiencarbazone-methyl
topramezone

tralkoxydim
trifloxysulfuron
trifluralin

tritosulfuron
vernolate

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

acibenzolar-Ss-methyl
ametoctradin
amisulbrom
azoxystrobin
benalaxyl
benalaxyl-M
benomyl
benthiavalicarb-isopropyl
benzovindiflupyr
bitertanol
bixafen
boscalid
bromuconazole
bupirimate
carbendazim
carboxin
chlorothalonil
cyazofamid
cyflufenamid
cymoxanil
cyproconazole
cyprodinil
dichlobenzthiazox
dichlofluanid
diclobutrazol
diclocymet
difenoconazole
diflumetorim
dimethomorph
dimoxystrobin
diniconazole
dinocap
dithianon
dodemorph
epoxiconazole
ethaboxam
famoxadone
fenamidone
fenarimol
fenhexamid
fenoxasulfone

fenpiclonil
fenpropimorph
fenpyrazamine
fluazinam
fludioxonil
flumorph
fluopicolide
fluopyram
fluoxastrobin
fluquinconazole
flusilazole
flutriafol
fluxapyroxad
folpet
fuberidazole
furametpyr
hexaconazole
hymexazol
imazalil
ipconazole
iprodione
iprovalicarb
isofetamid
isoprothiolane
isopyrazam
isotianil
kresoxim-methyl
mandestrobin
mandipropamid
meptyldinocap
metalaxyl
metalaxyl-m
metconazole
metrafenone
myclobutanil
nabam
nuarimol
orysastrobin
oxadixyl
oxathiapiprolin
oxycarboxin

penconazole
pencycuron
penflufen
penthiopyrad
picoxystrobin
prochloraz
procymidone
propiconazole
proquinazid
prothioconazole
pydiflumetofen
pyraclostrobin
pyribencarb
pyrifenox
pyrimethanil
pyriofenone
quinomethionat
quinoxyfen
sedaxane
silthiofam
spiroxamine
tebuconazole
tetraconazole
thiabendazole
thifluzamide
thiophanate-methyl
TMTD
tolylfluanid
tralopyril
triadimefon
triadimenol
triazoxide
tridemorph
trifloxistrobin
triflumizole
triforine
triticonazole
valifenalate
vinclozolin
ziram
zoxamide

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

acephate
acetamiprid
acrinathrin
aldicarb

alpha-cypermethrin
amidoflumet
amitraz

azinphos-methyl
bendiocarb
benfuracarb

15

bensultap
beta-cyfluthrin
beta-cypermethrin
bifenazate
bifenthrin
bioallethrin
bioresmethrin
buprofezin
butoxycarboxim
carbaryl
carbofuran
carbosulfan
cartap
chlorantraniliprole
chlorfluazuron
chlorpyrifos
chlorpyrifos-methyl
chromafenozide
clofentezin
clothianidin
cyantraniliprole
cyenopyrafen
cyhexatin
cypermethrin
cyromazine-fix
DDT
deltamethrin
diafenthiuron
diazinone
dichlorvos
diflovidazin
diflubenzuron
dimefluthrin
dimethoate
dinotefuran
dioxacarb
DNOC
endosulfan
esfenvalerate
ethiprole
etofenprox

etoxazole
etrimfos
fenazaquin
fenitrothion
fenoxycarb
fenpropathrin
fenpyroximate
fenthion
fenvalerate
fipronil
flonicamid
flubendiamide
flucycloxuron
flufenerim
flufenoxuron
formothion
halofenozide
heptenophos
hexaflumuron
hexythioazox
imidacloprid
indoxacarb
lambda-cyhalothrin
lindane
lufenuron
malathion
metaflumizone
methamidophos
methidathion
methiocarb
methomyl
methoxyfenozide
metofluthrin
nereistoxin
nicarbazin
nicotine
nitenpyram
noviflumuron
oxamyl
oxydemeton-methyl
paraoxon

parathion
parathion-methyl
permethrin
phenthoate
phorate
phosalone
phosmet
phosmethylan
phosphamidon
phosthiazat
pirimicarb
pirimiphos-methyl
profluthrin
propargite
pymetrozine
pyrazophos
pyrethrin-i
pyridaben
pyridafenthion
pyrifluquinazon
pyriproxyfen
quinalphos
spirotetramat
sulfotep
tebufenozide
tebufenpyrad
teflubenzuron
tefluthrin
tepp
terbuphos
tetradyfon
tetramethrin
thiacloprid
thiamethoxam
thiocylam
triazamate
triazophos
triflumuron
zeta-cypermethrin

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

AD-67
benoxacor
bpcms
cloquintocet-mexyl
cumyluron
cyometrinil
cyprosulfamide
daimuron
dichlormid

dicyclonon
dietholate
dimepiperate
fenclorazole-ethyl
fenclorim
flurazole
fluxofenim
furilazole
isoxaben

isoxadifen-ethyl
jiecaowan (also known as MG-191)
mefenpyr-diethyl
mephenate
methoxyphenone
naphthalic-anhydride
oxabetrinil

16