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DATASET

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

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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

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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:

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

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

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