Alternativní metody testování toxicity – *in silico*, Praha 2008

Pallas for Windows

CompuDrug International, 115 Morgan Drive, Sedona, Arizona

HAZARDEXPERT SYSTEM (METABOLEXPERT SYSTEM log P)

Státní zdravotní ústav, Praha

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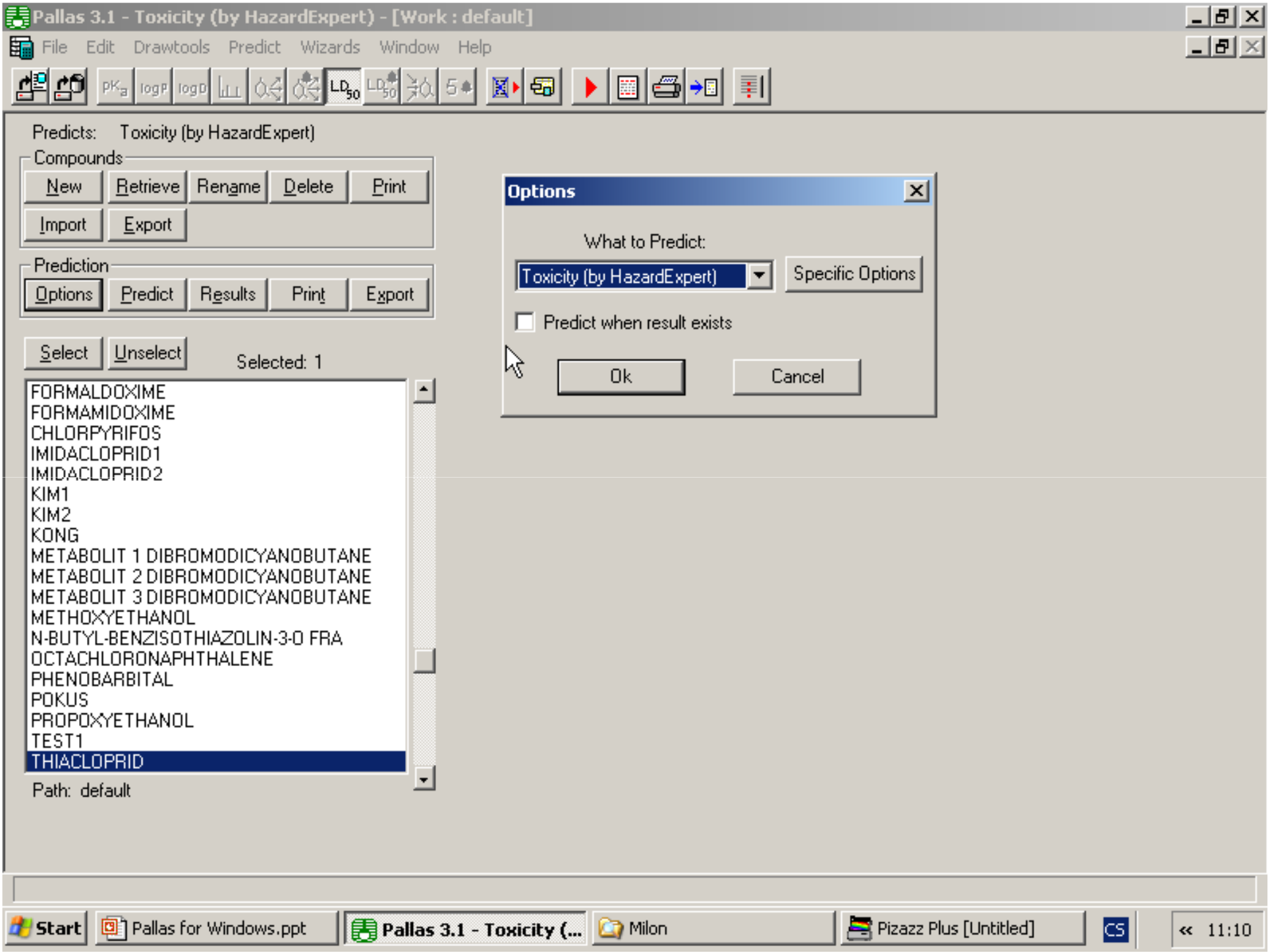
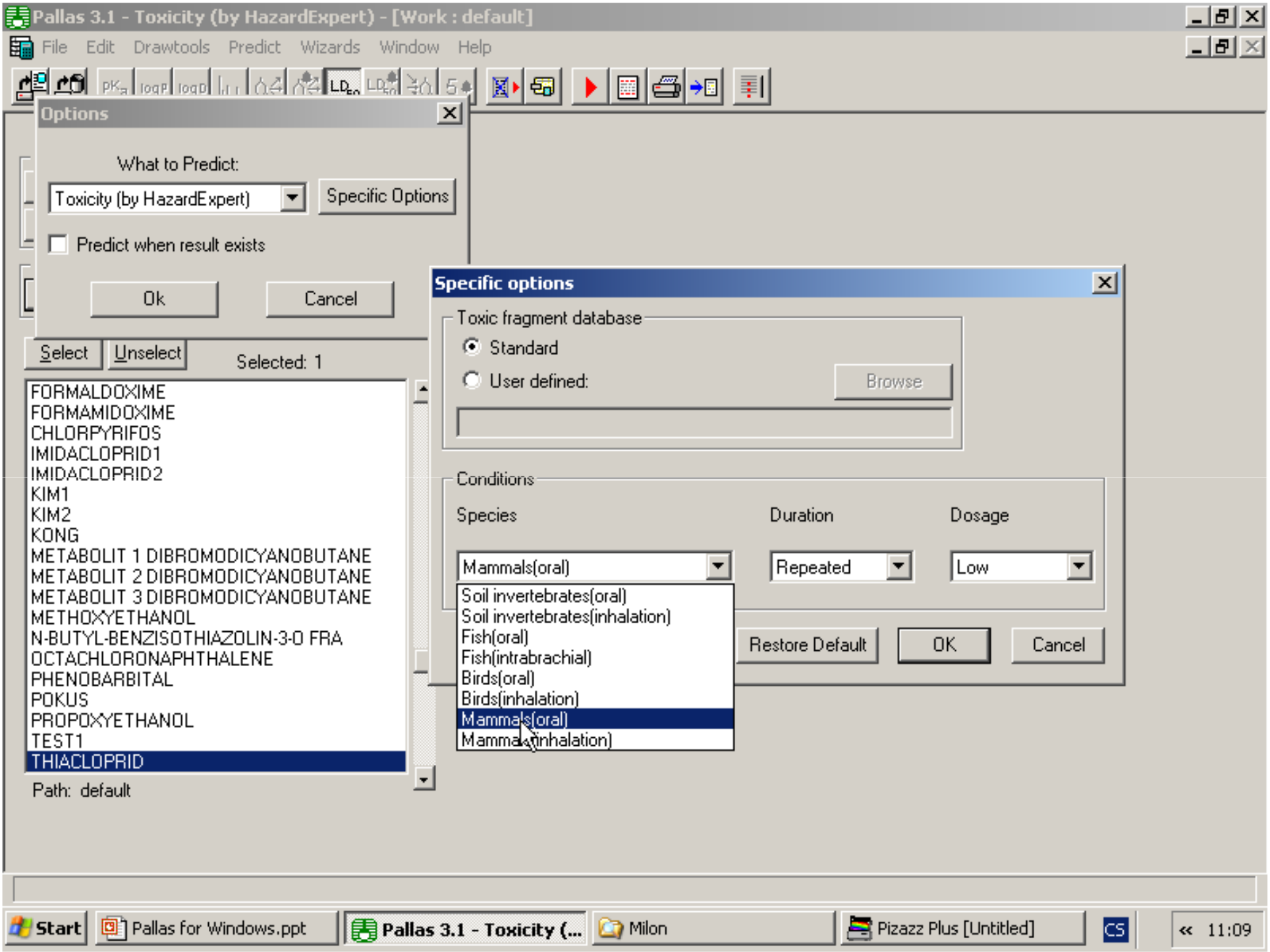
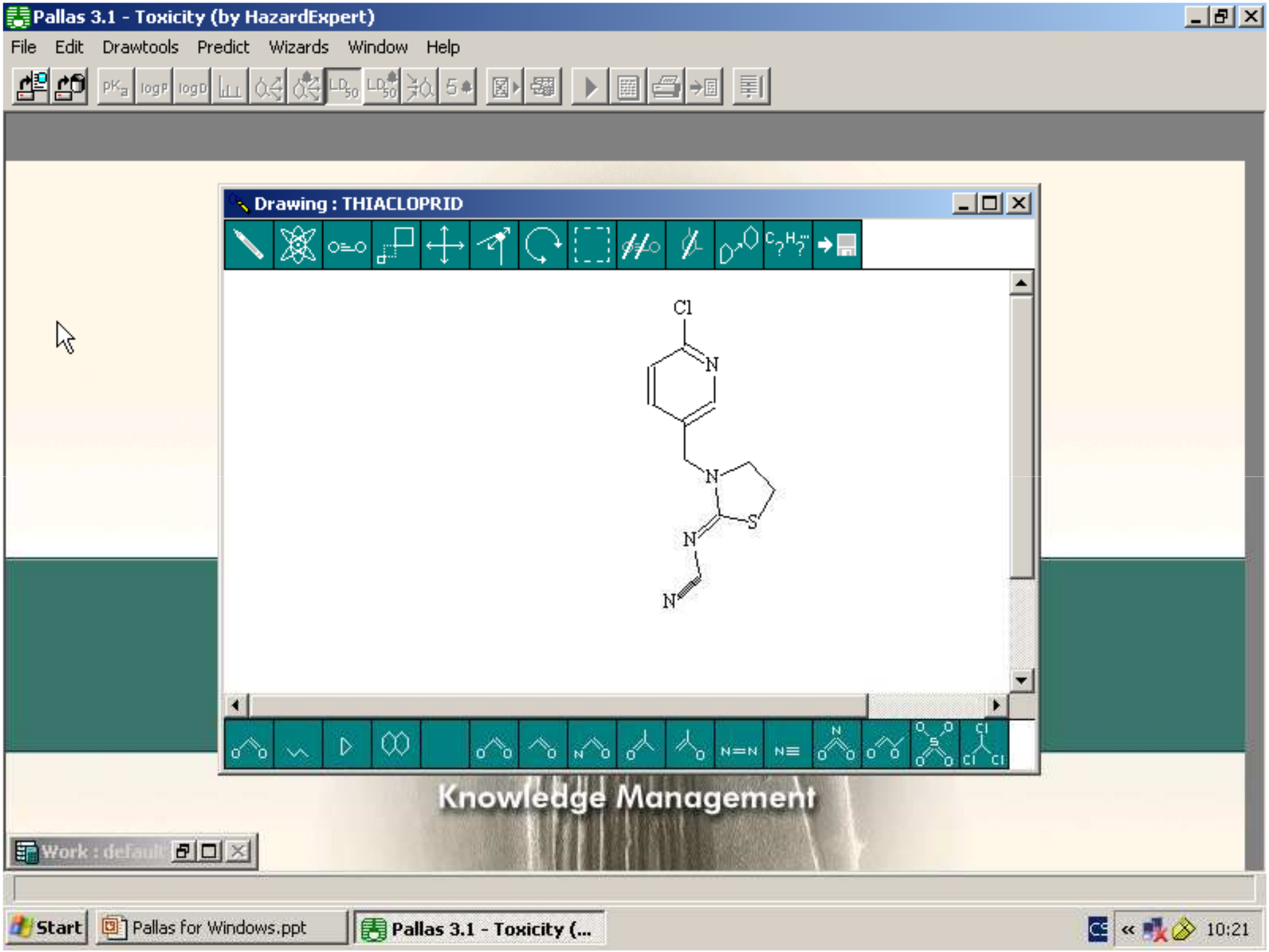
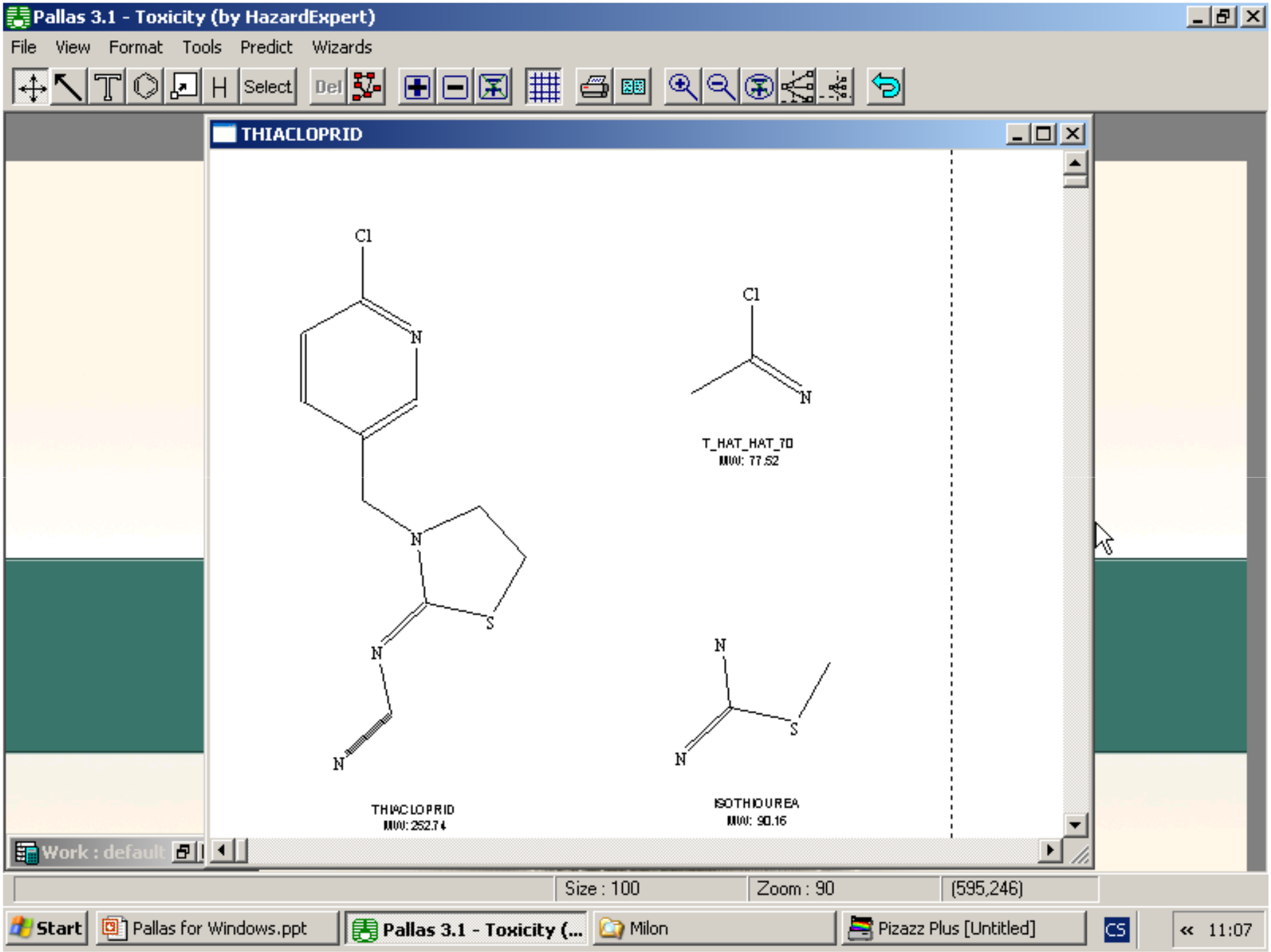
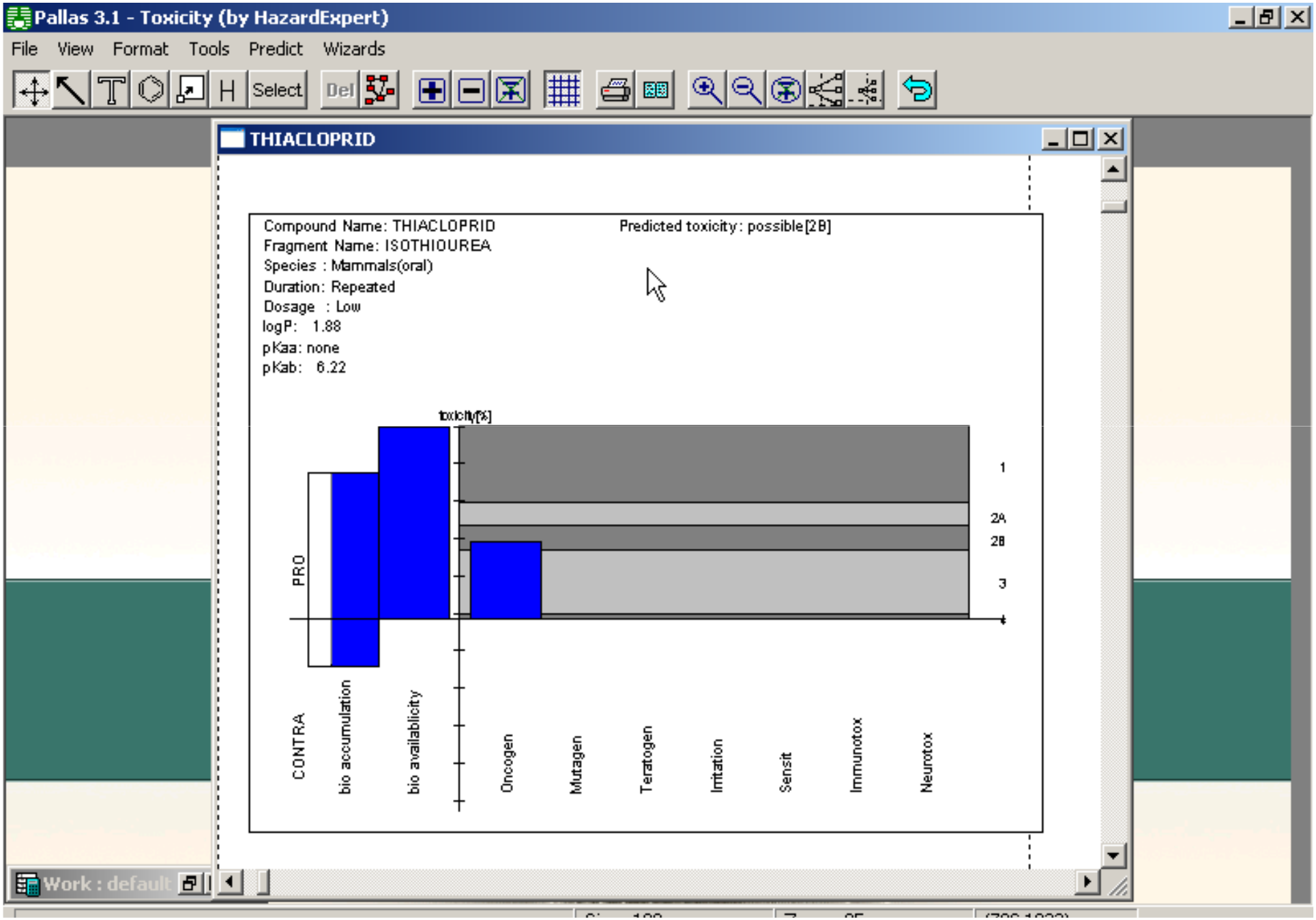
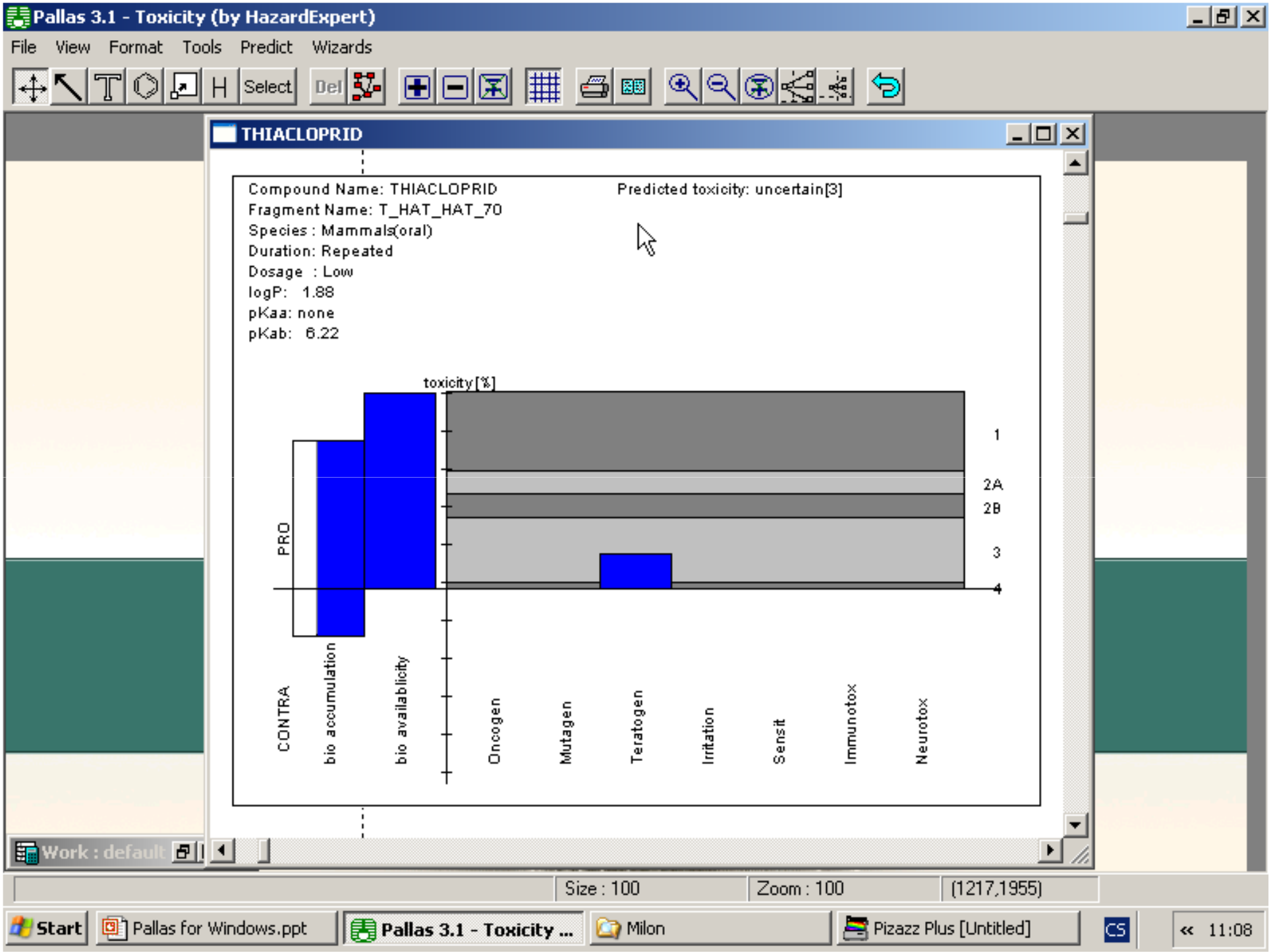

Pallas 3.1 - Toxicity (by HazardExpert) - [Work : default]
File Edit Drawtools Predict Wizards Window Help
Predicts: Toxicity (by HazardExpert)
Compounds
New Retrieve Rename Delete Print
Import Export
Prediction
Options Predict Results Print Export
Select Unselect
Selected: 1
FORMALDOXIME
FORMAMIDOXIME
CHLORPYRIFOS
IMIDACLOPRID1
IMIDACLOPRID2
KIM1
KIM2
KONG
METABOLIT 1 DIBROMODICYANOBUTANE
METABOLIT 2 DIBROMODICYANOBUTANE
METABOLIT 3 DIBROMODICYANOBUTANE
METHOXYETHANOL
N-BUTYL-BENZISOTHIAZOLIN-3-O FRA
OCTACHLORONAPHTHALENE
PHENOBARBITAL
POKUS
PROPOXYETHANOL
TEST1
THIACLOPRID
Path: default
Options
What to Predict:
Toxicity (by HazardExpert)
Specific Options
Predict when result exists
Ok
Cancel
Start
Pallas for Windows.ppt
Pallas 3.1 - Toxicity (...
Milon
Pizazz Plus [Untitled]
CS
« 11:10


Pallas 3.1 - Toxicity (by HazardExpert) - [Work : default]
File Edit Drawtools Predict Wizards Window Help
Options
What to Predict:
Toxicity (by HazardExpert)
Specific Options
Predict when result exists
Ok
Cancel
Select
Unselect
Selected: 1
FORMALDOXIME
FORMAMIDOXIME
CHLORPYRIFOS
IMIDACLOPRID1
IMIDACLOPRID2
KIM1
KIM2
KONG
METABOLIT 1 DIBROMODICYANOBUTANE
METABOLIT 2 DIBROMODICYANOBUTANE
METABOLIT 3 DIBROMODICYANOBUTANE
METHOXYETHANOL
N-BUTYL-BENZISOTHIAZOLIN-3-O FRA
OCTACHLORONAPHTHALENE
PHENOBARBITAL
POKUS
PROPOXYETHANOL
TEST1
THIACLOPRID
Path: default
Specific options
Toxic fragment database
Standard
User defined:
Browse
Conditions
Species
Duration
Dosage
Mammals(oral)
Repeated
Low
Soil invertebrates(oral)
Soil invertebrates(inhalation)
Fish(oral)
Fish(intrabrachial)
Birds(oral)
Birds(inhalation)
Mammals(oral)
Mammals(inhalation)
Restore Default
OK
Cancel
Start
Pallas for Windows.ppt
Pallas 3.1 - Toxicity (...
Milon
Pizazz Plus [Untitled]
CS
« 11:09


Pallas 3.1 - Toxicity (by HazardExpert)
File Edit Drawtools Predict Wizards Window Help
Drawing : THIACLOPRID
Cl
N
N
S
N
N
Knowledge Management
Work : default
Start
Pallas for Windows.ppt
Pallas 3.1 - Toxicity (...
10:21


Pallas 3.1 - Toxicity (by HazardExpert)
File View Format Tools Predict Wizards
H Select Del
THIACLOPRID
Cl
N
N
N
S
N
N
THIACLOPRID
MW: 252.74
Cl
N
T_HAT_HAT_70
MW: 77.52
N
N
S
ISOTHIOUREA
MW: 90.16
Work : default
Size : 100
Zoom : 90
(595,246)
Start
Pallas for Windows.ppt
Pallas 3.1 - Toxicity (...
Milon
Pizazz Plus [Untitled]
CS
« 11:07


Pallas 3.1 - Toxicity (by HazardExpert)
File View Format Tools Predict Wizards
Select Del H
THIACLOPRID
Compound Name: THIACLOPRID
Fragment Name: ISOTHIOUREA
Species : Mammals(oral)
Duration: Repeated
Dosage : Low
logP: 1.88
pKaa: none
pKab: 6.22
Predicted toxicity: possible[2B]
toxicity[%]
PRO
1
2A
2B
3
CONTRA
bio accumulation
bio availability
Oncogen
Mutagen
Teratogen
Irritation
Sensit
Immunotox
Neurotox
Work : default


Pallas 3.1 - Toxicity (by HazardExpert)
File View Format Tools Predict Wizards
Select Del H
THIACLOPRID
Compound Name: THIACLOPRID
Fragment Name: T_HAT_HAT_70
Species : Mammals(oral)
Duration: Repeated
Dosage : Low
logP: 1.88
pKaa: none
pKab: 6.22
Predicted toxicity: uncertain[3]
toxicity [%]
1
2A
2B
3
4
PRO
CONTRA
bio accumulation
bio availablicity
Oncogen
Mutagen
Teratogen
Irritation
Sensit
Immunotox
Neurotox
Work : default
Size : 100
Zoom : 100
(1217,1955)
Start
Pallas for Windows.ppt
Pallas 3.1 - Toxicity ...
Milon
Pizazz Plus [Untitled]
CS
« 11:08

Jiný příklad viz skripta (2) str.68

Pavel Dubský: Ukázka užití predikčního modelu.