Priority Ranking of HPV Chemicals Based On Production, Persistence, & Chemical Properties

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BACKGROUND

- 70,000 to 100,000 chemicals currently in U.S. commerce; ~1,000 new chemicals are introduced every year;
- 2865 HPV Chemicals (>10^6 lbs/y, excl. polymers, H_2SO_4, etc.)
- 1749 HPVs if obvious mixtures are excluded (e.g., “petrol. distillates”)
- Need for science-based strategy for ranking compounds.

USGS Interest

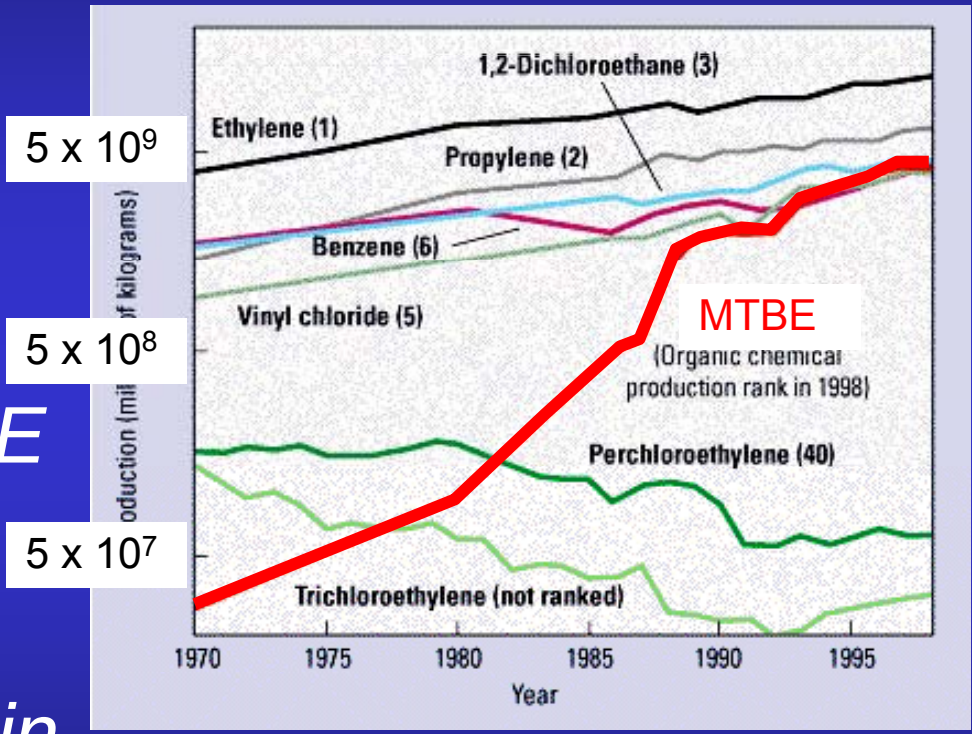
USGS “NAWQA” Program* (Natl. Water-Qual. Assessment) seeks comprehensive understanding of contaminant levels in natural waters of the US (e.g., VOCs, pesticides, PAHs, metals, etc.).

**Design of the National Water-Quality Assessment Program: Occurrence and Distribution of Water-Quality Conditions*; U.S. Geological Survey Circular 1112.

A Cautionary Tale - MTBE

- *1973 – commercial production begins in Italy for use as an octane enhancer*

  (isobutylene + methanol = MTBE)
- *1979 –EPA allows ARCO to use up to 7% by volume MTBE as an octane enhancer*
- *1990 – Federal Law passed requiring 2.7% by wt. oxygen in certain "CO non-attainment" areas*



Johnson, Pankow, Bender, Price, Zogorski ES&T (2000)

MTBE Properties of Interest

physical properties…

- volatile
- very soluble in water (50,000 mg/L)
- soluble in precipation from atmosphere

degradation…

- atmos. reaction with OH• radical – slow
- chemical hydrolysis – slow
- biodegradation – slow

→ MTBE *can get into water and remain there:*

detected in 7% of national aquifer samples taken by USGS in NAWQA program

see : http://pubs.usgs.gov/circ/circ1292/pdf/circular1292.pdf

Goal

to help avoid scenarios like that experienced with:

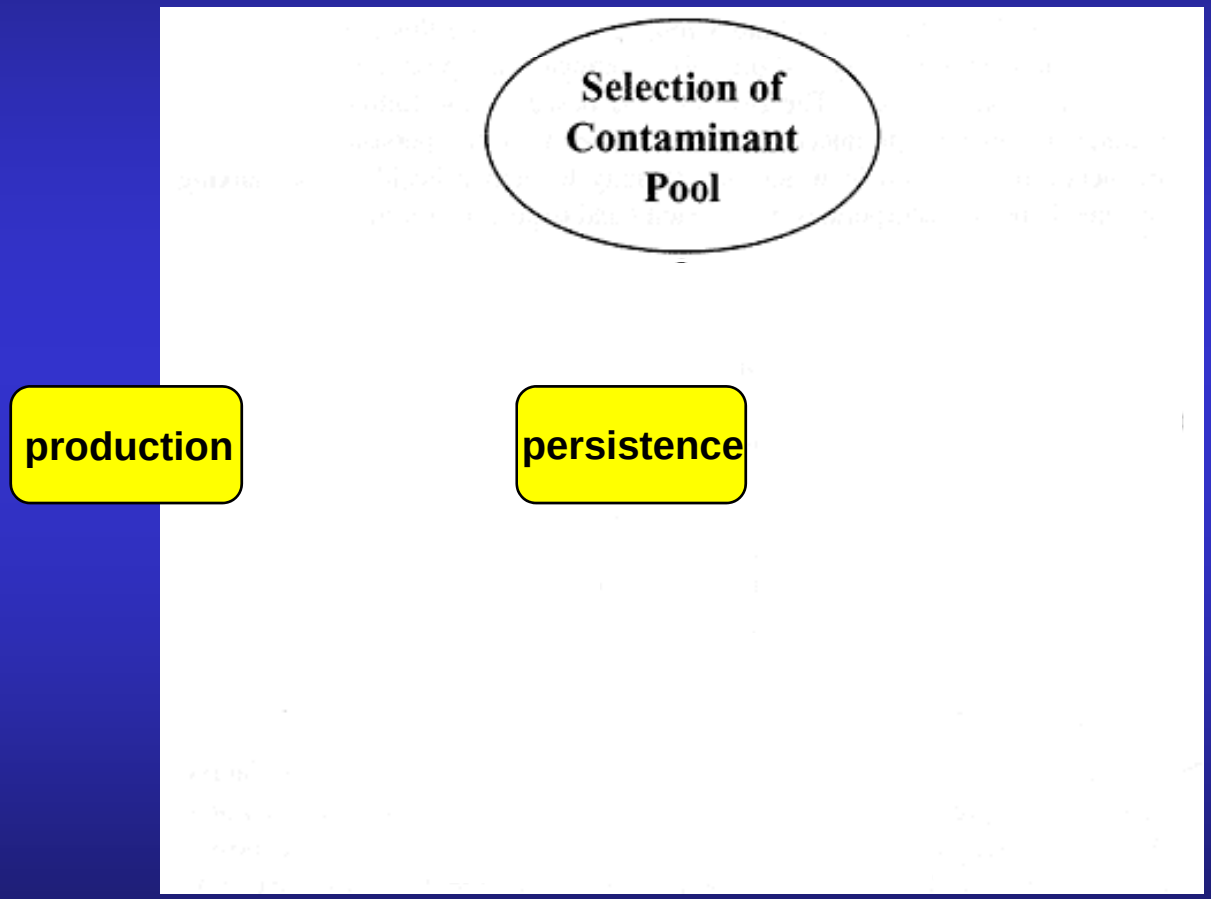
MTBE (persistent & water soluble)
PCBs (persistent & lipid soluble)
etc.

develop a simple flexible user-friendly tool for prioritization rankings of the HPV chemical list

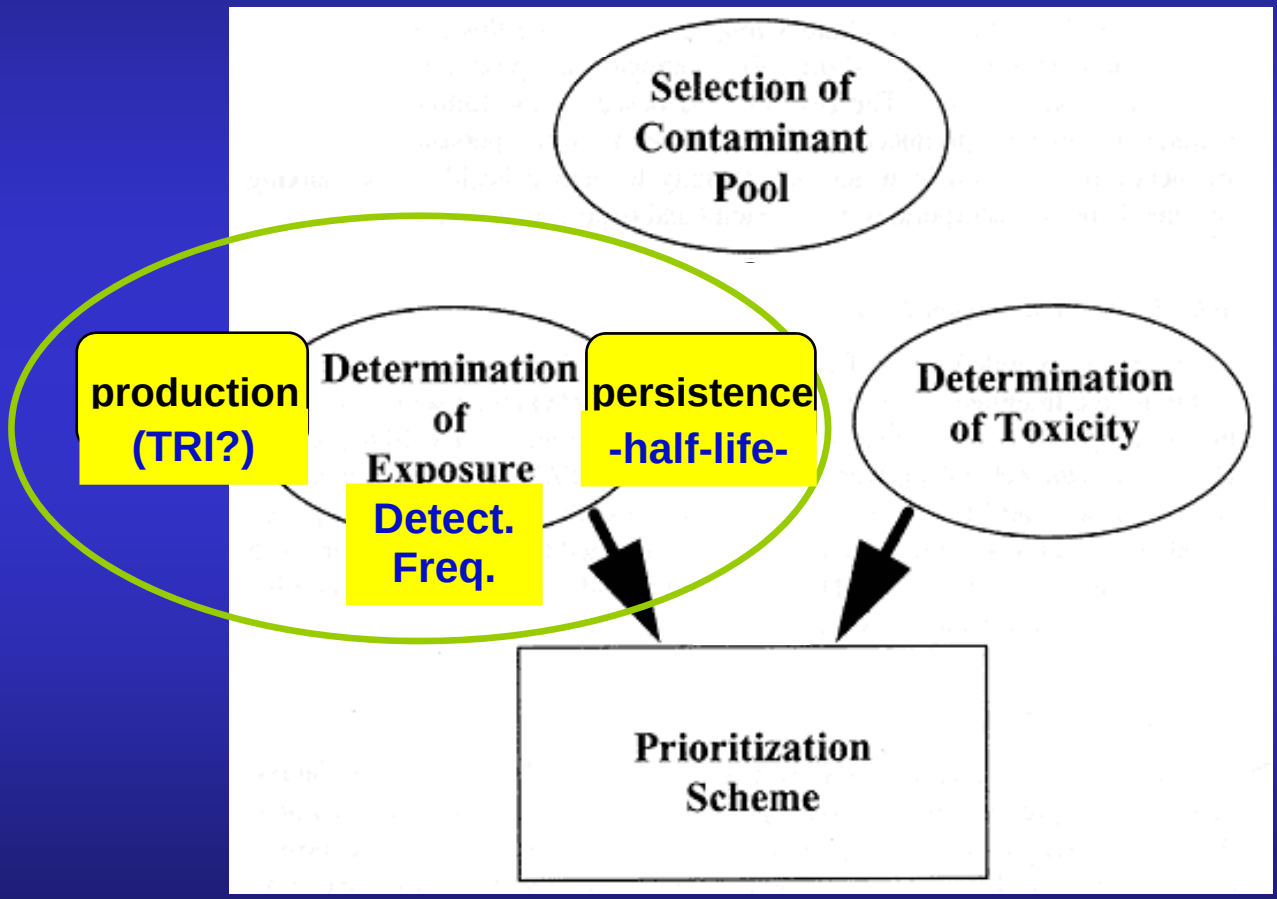
"Chemical Prioritization System (CPS) Calculator"

Logic Elements of One Type of Prioritization Scheme

(Nat. Res. Council: Setting Priorities for Drinking Water Contaminants)



paradigm of EPA's Waste Minimization Prioritization Tool.1


Selection of Contaminant Pool
production (TRI?)
Determination of Exposure
persistence -half-life-
Detect. Freq.
Determination of Toxicity
Prioritization Scheme

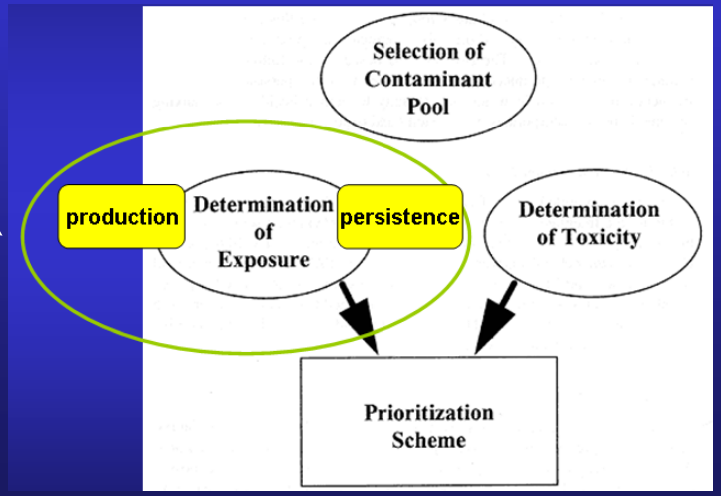
Regression: NatI. USGS Data for 36 Compounds:

log [Detect. Freq.] =

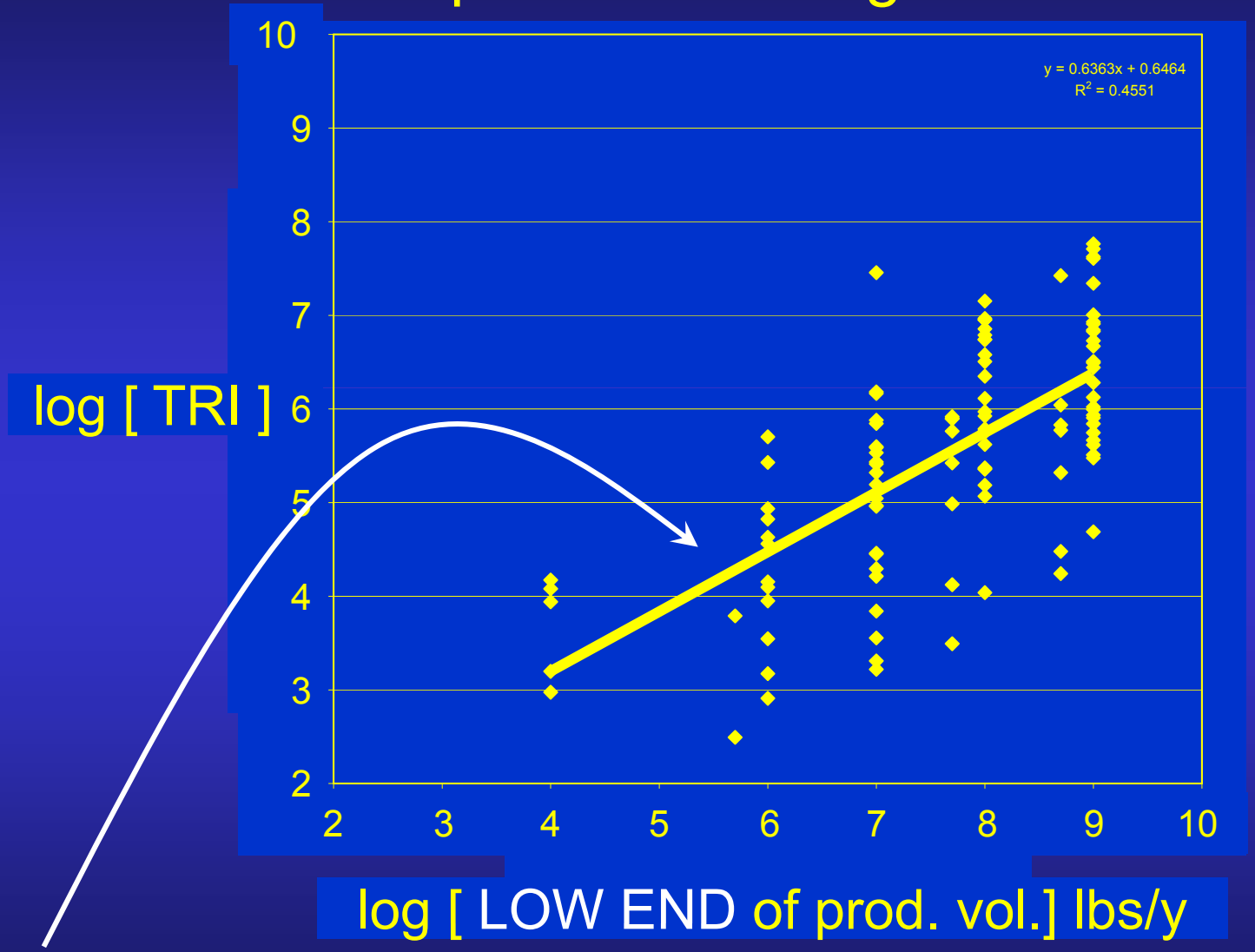
0.51 log [TRI] + 0.57 log [half life] - 4.72

(r = 0.41, p = 0.00064)

✓ environ. exposure can be related to release & half-life



But, TRI Data Not Available for Most HPV Chemicals…
Use production range data?



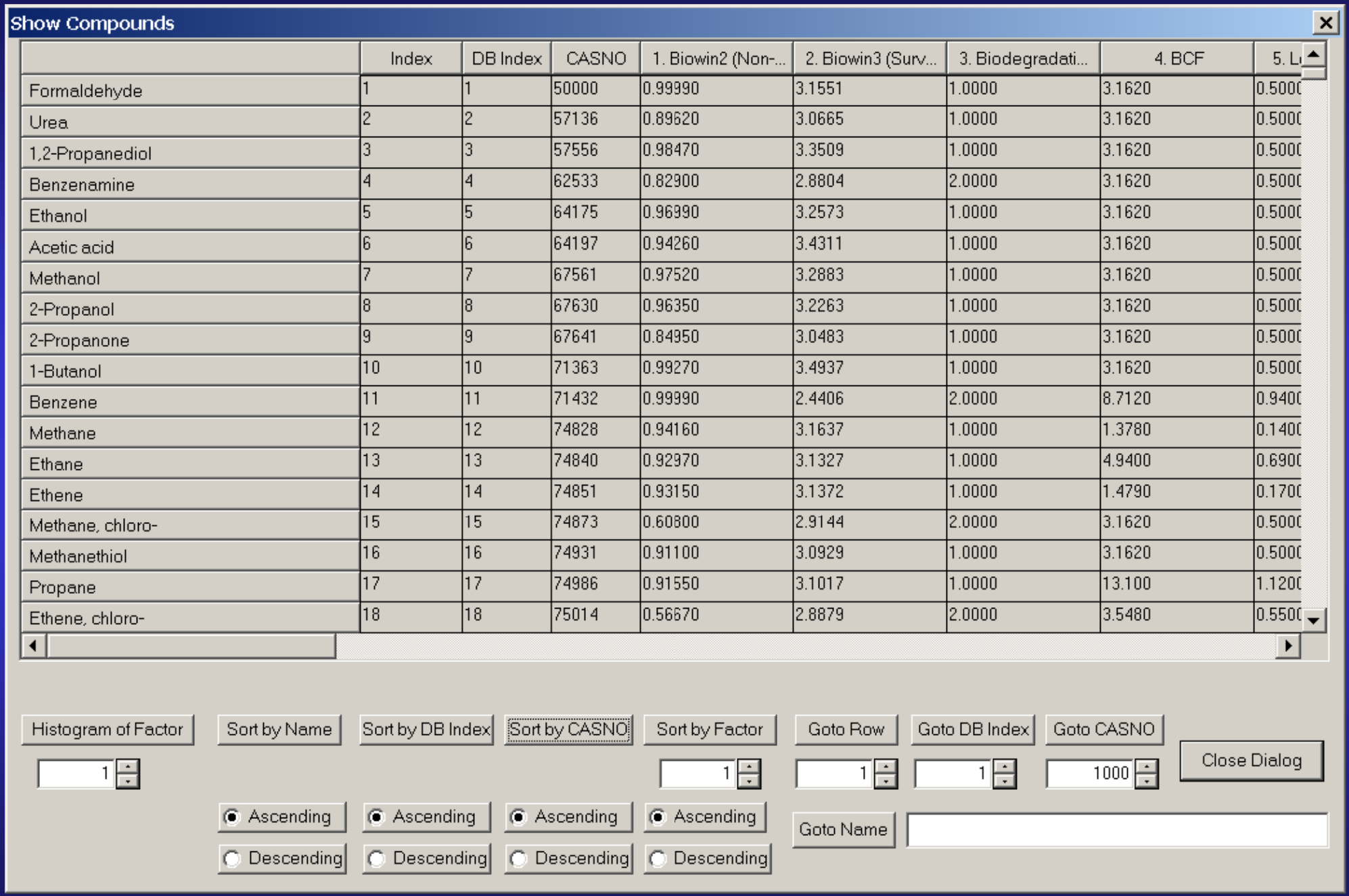
log [TRI] = 0.64 log [low end of prod. volume] + 0.65 r^2 = 0.455 p < 0.001

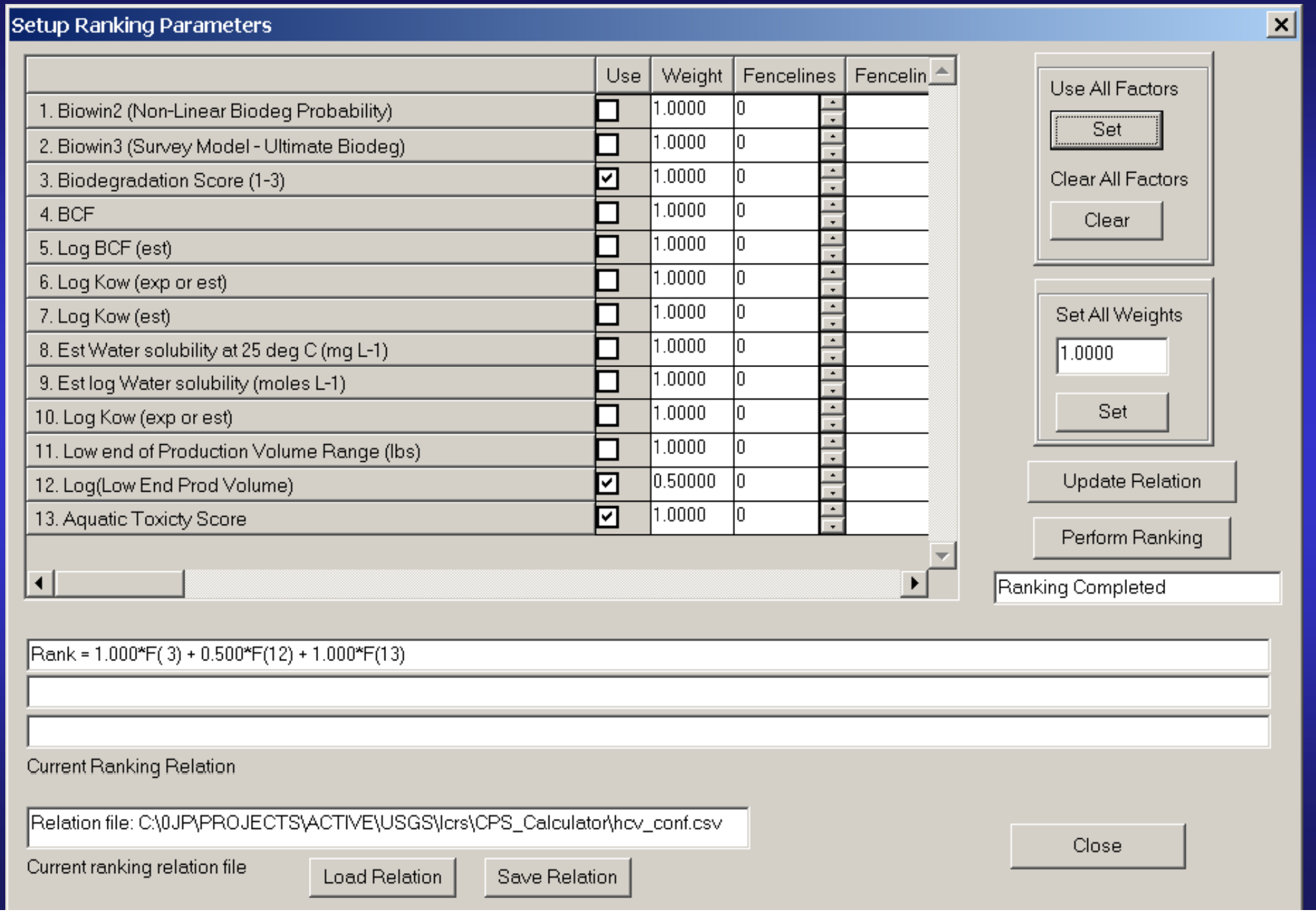
CPS Calculator

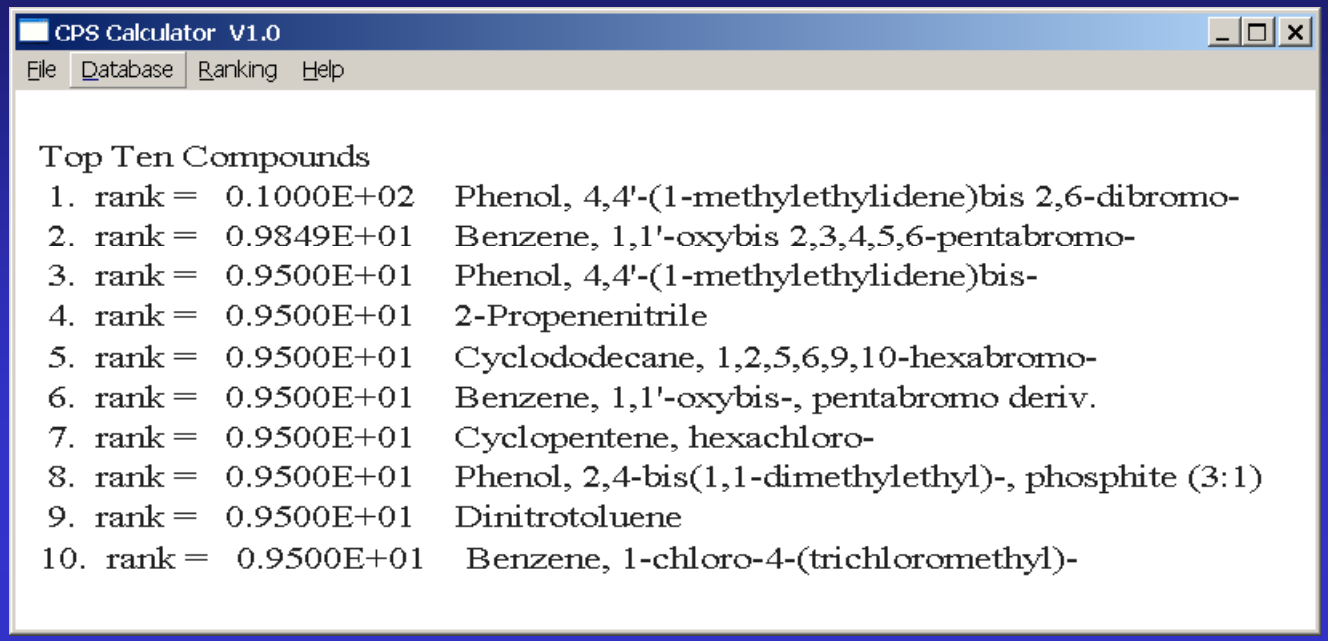
1689 compounds

Conducts rankings based on user-chosen relations involving:

- log (low end of HPV production volume)
- BIOWIN degradability
- log Bioconcentration factor (log BCF)
- log K_{ow}
- log water solubility
- aquatic toxicity score (ECOSAR-based)
- ….

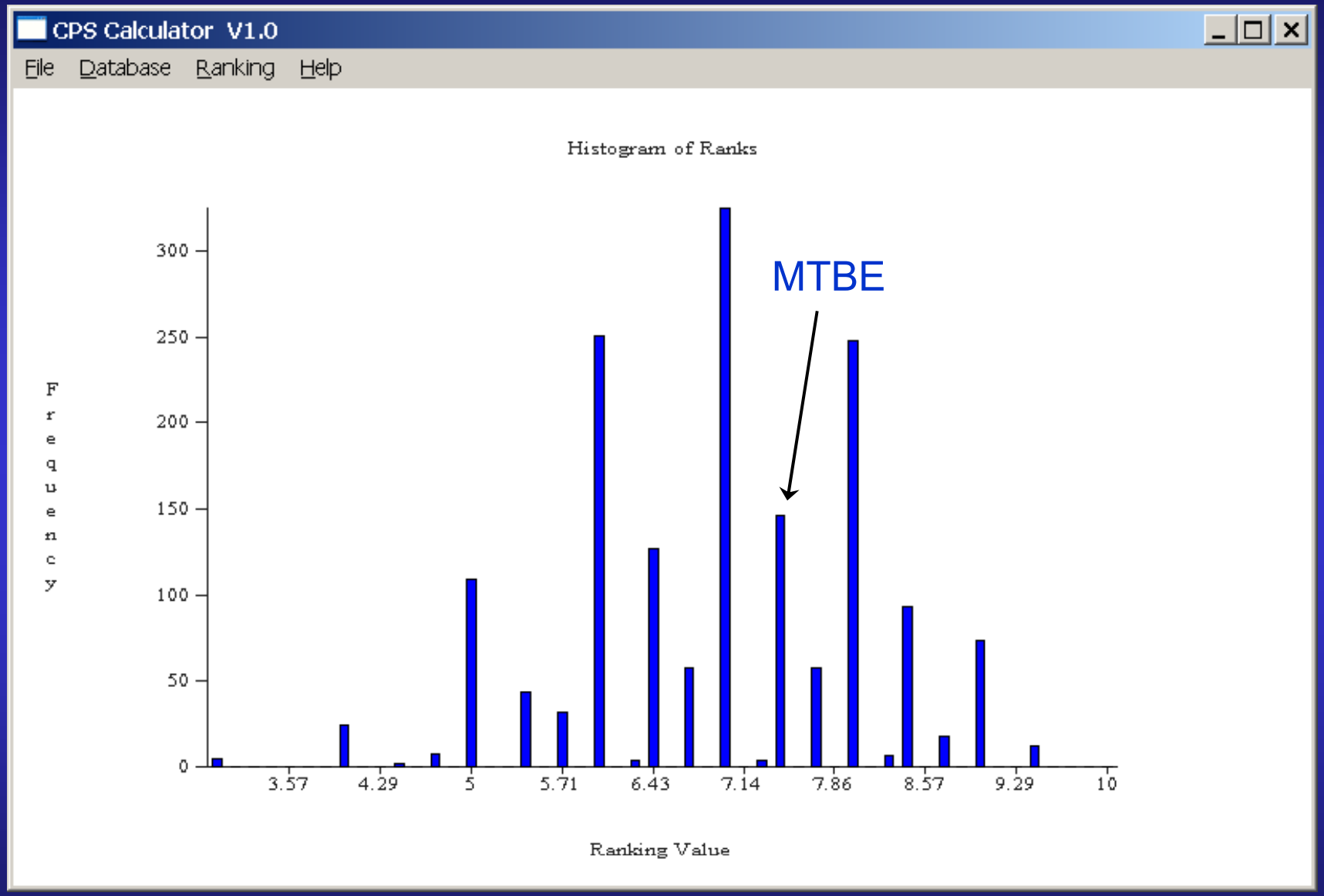

Show Compounds
Index
DB Index
CASNO
1. Biowin2 (Non-...
2. Biowin3 (Surv...
3. Biodegradati...
4. BCF
5. L
Formaldehyde 1 1 50000 0.99990 3.1551 1.0000 3.1620 0.5000
Urea 2 2 57136 0.89620 3.0665 1.0000 3.1620 0.5000
1,2-Propanediol 3 3 57556 0.98470 3.3509 1.0000 3.1620 0.5000
Benzenamine 4 4 62533 0.82900 2.8804 2.0000 3.1620 0.5000
Ethanol 5 5 64175 0.96990 3.2573 1.0000 3.1620 0.5000
Acetic acid 6 6 64197 0.94260 3.4311 1.0000 3.1620 0.5000
Methanol 7 7 67561 0.97520 3.2883 1.0000 3.1620 0.5000
2-Propanol 8 8 67630 0.96350 3.2263 1.0000 3.1620 0.5000
2-Propanone 9 9 67641 0.84950 3.0483 1.0000 3.1620 0.5000
1-Butanol 10 10 71363 0.99270 3.4937 1.0000 3.1620 0.5000
Benzene 11 11 71432 0.99990 2.4406 2.0000 8.7120 0.9400
Methane 12 12 74828 0.94160 3.1637 1.0000 1.3780 0.1400
Ethane 13 13 74840 0.92970 3.1327 1.0000 4.9400 0.6900
Ethene 14 14 74851 0.93150 3.1372 1.0000 1.4790 0.1700
Methane, chloro- 15 15 74873 0.60800 2.9144 2.0000 3.1620 0.5000
Methanethiol 16 16 74931 0.91100 3.0929 1.0000 3.1620 0.5000
Propane 17 17 74986 0.91550 3.1017 1.0000 13.100 1.1200
Ethene, chloro- 18 18 75014 0.56670 2.8879 2.0000 3.5480 0.5500
Histogram of Factor
1
Sort by Name
Sort by DB Index
Sort by CASNO
Sort by Factor
1
Goto Row
1
Goto DB Index
1
Goto CASNO
1000
Close Dialog
Ascending
Descending
Ascending
Descending
Ascending
Descending
Ascending
Descending
Goto Name


Setup Ranking Parameters
Use
Weight
Fencelines
Fencelin
1. Biowin2 (Non-Linear Biodeg Probability) 1.0000 0
2. Biowin3 (Survey Model - Ultimate Biodeg) 1.0000 0
3. Biodegradation Score (1-3) 1.0000 0
4. BCF 1.0000 0
5. Log BCF (est) 1.0000 0
6. Log Kow (exp or est) 1.0000 0
7. Log Kow (est) 1.0000 0
8. Est Water solubility at 25 deg C (mg L-1) 1.0000 0
9. Est log Water solubility (moles L-1) 1.0000 0
10. Log Kow (exp or est) 1.0000 0
11. Low end of Production Volume Range (lbs) 1.0000 0
12. Log(Low End Prod Volume) 0.50000 0
13. Aquatic Toxicty Score 1.0000 0
Use All Factors
Set
Clear All Factors
Clear
Set All Weights
1.0000
Set
Update Relation
Perform Ranking
Ranking Completed
Rank = 1.000*F(3) + 0.500*F(12) + 1.000*F(13)
Current Ranking Relation
Relation file: C:\0JP\PROJECTS\ACTIVE\USGS\lcrs\CPS_Calculator\hcv_conf.csv
Current ranking relation file
Load Relation
Save Relation
Close



rank = biodeg score (1 to 3)
+ 0.5 log (low end of production volume)
+ aquatic tox score (1 to 3)

MTBE is ranked 554 out of 1689


CPS Calculator V1.0
File
Database
Ranking
Help
Histogram of Ranks
MTBE
Frequency
300
250
200
150
100
50
0
3.57
4.29
5
5.71
6.43
7.14
7.86
8.57
9.29
10
Ranking Value

Conclusions

- for HPV chemicals, need more extensive TRI data, or actual production data (rather than ranges)
- simple ranking tools are needed for HPV chemicals

  → "CPS Calculator" will be one such tool

  flexible

  user-friendly

  will allow use of any parameters of interest