# Example CCL Universe Data Set: Progress and Recommendations

Presentation to NDWAC CCL Work Group
Washington, DC

July 15, 2003

# Review Example CCL Universe Data Set/Analysis

- Purpose/Intent of Example CCL Universe Data Set
- Development of the Data Set
- Findings
- What insights do we have about this data set?
  - Availability
  - Quality
  - Other
- Will this data set be sufficient to test the proposed “gate” screening?
- What can we say about the use of this data set for attribute/scoring and classification?

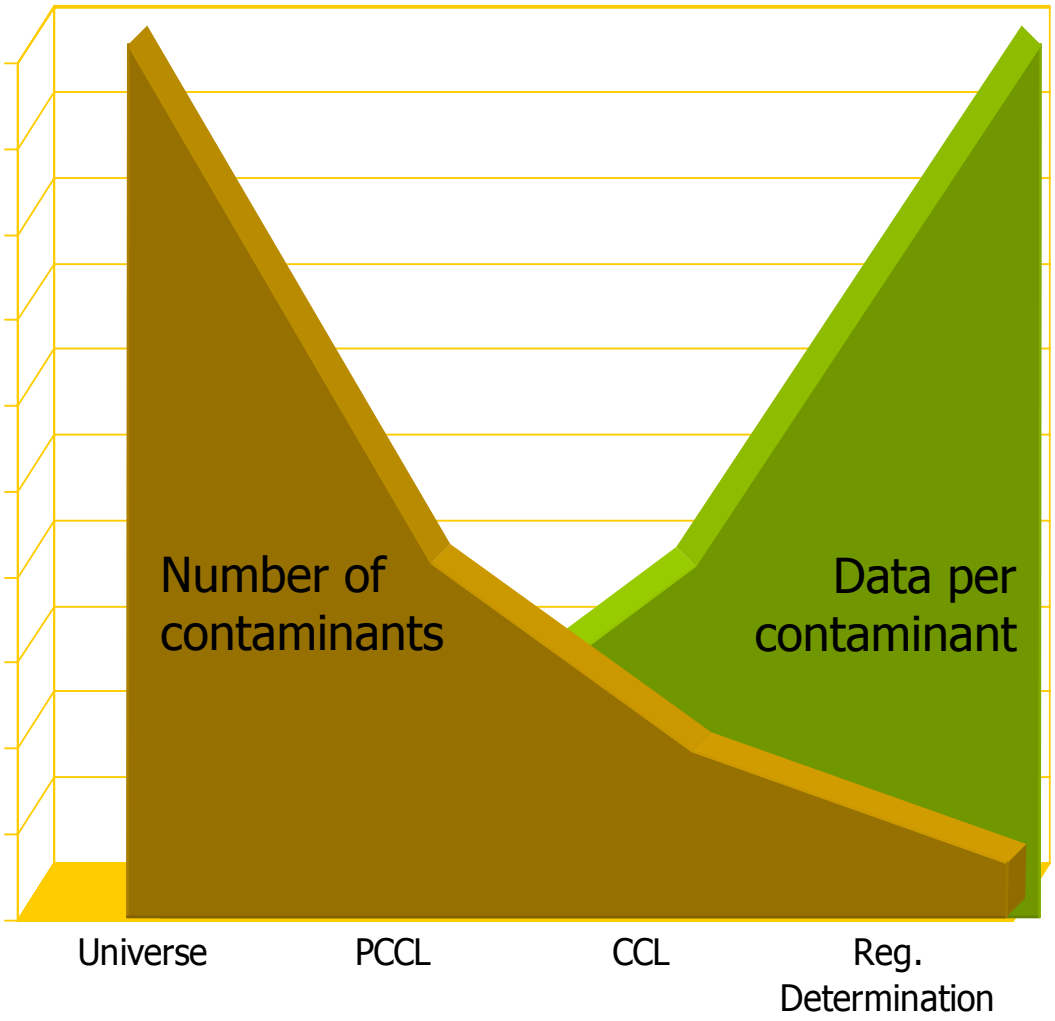
# Overview: Purpose

- The NRC has recommended a CCL process requiring data for the following steps:
  - identify the "universe" of potential drinking water contaminants;
  - select a Preliminary CCL from the "universe" by a screening process;
  - develop a training set of compounds to train a prototype algorithm to prioritize drinking water contaminants;
  - apply a prototype algorithm to classify the PCCL into a CCL; and
  - conduct an expert review of the algorithm results.

# Overview: Purpose of the Example CCL Universe Data Set

- Gather some data to support NDWAC's process
- Test the proposed approaches:
  - Building the CCL Universe
  - "Gates" screening approach
  - Attribute Scoring
  - Use of a prototype algorithm to classify the PCCL into a CCL
- Gain insights about available data on contaminants, identify data elements, issues and gaps.

# Overview: Structure




As the process moves from "universe" to CCL,

the data requirements of each contaminant will grow,

while the pool of contaminants will shrink.

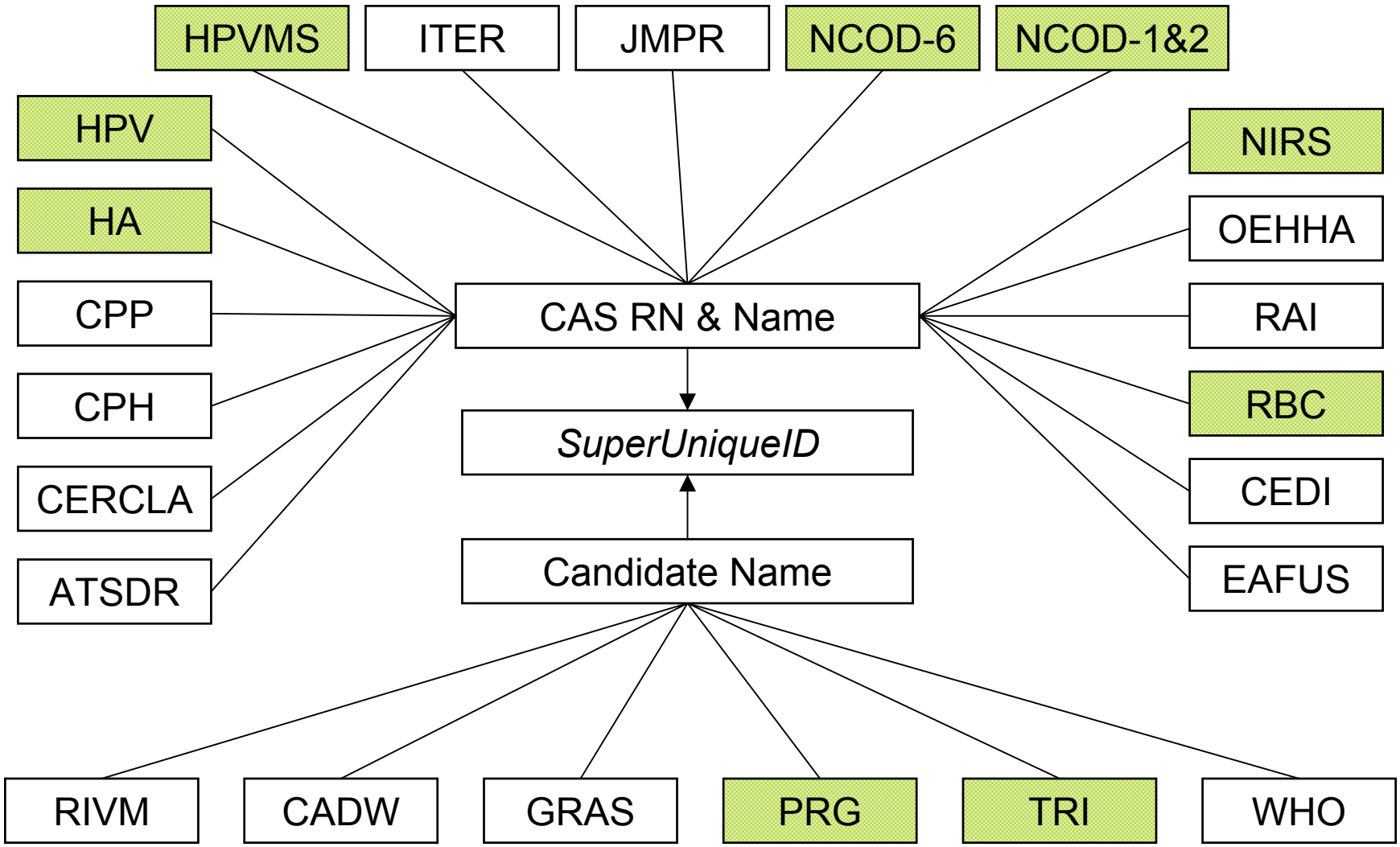
# Data Retrieval

- Began with list of more than 200 data sources
- Chose 23 sources based on the following criteria:
  - high-quality data
  - easily accessible electronically
  - contained information relevant to building the CCL Universe (i.e., occurrence data, etc.)
- Downloaded tables from 23 sources
  - a total of 87 tables
- All tables formatted as Microsoft Excel files
- Performed QA/QC review on Excel files to ensure accurate reproduction of data from original source

# Linking Data

- To link data across tables, contaminants need a unique identifier
- Unique identifier was first assigned to a CAS number
- If the CAS number was not listed or available, a unique identifying number was assigned to the contaminant by name
- A table was created to list each contaminant with its corresponding identifier
- Not a perfect process

# Data Sources



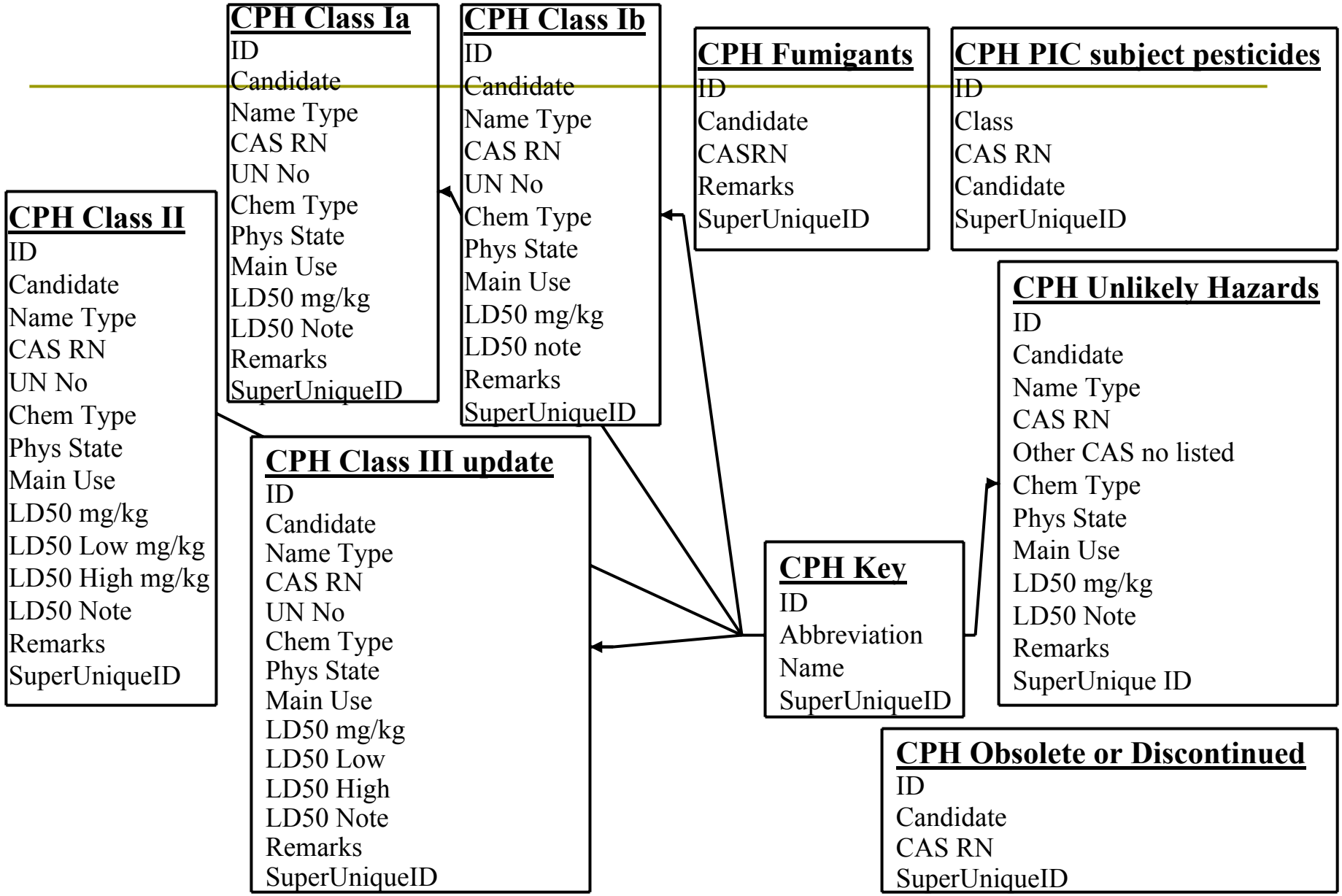
# Classifying Data Sources

- The 23 data sources were classified according to the type(s) of data and/or information available in each
  - First it was determined what data elements were in each data sources
  - Then the data elements were classified, and the data sources were classified according to what kinds of data elements were available in the source
  - Data sources could be classified into one or more categories: HE Data, HE Info, Occ Data, Occ Info, or No Data or Info

# Types of Data and/or Information in the Data Sources

| Example Data Set Sources With | | | | |
|---|---|---|---|---|
| **HE Data** | **HE Info** | **Occ Data** | **Occ Info** | **No Data or Info** |
| ATSDR MRLs | ATSDR MRLs | NIRS | CADW | ATSDR CERCLA |
| CADW | CADW | NCOD Round 1 and 2 | PRGs | HPV |
| CPH | CEDI | NCOD Six Year Review | RAIS | HPV Master Summary Table |
| CPP | HA | | RBCs | GRAS |
| HA | ITER | | TRI | EAFUS |
| ITER | OEHHA | | | |
| WHO | PRGs | | | |
| OEHHA | RBCs | | | |
| PRGs | RIVM | | | |
| RBCs | | | | |
| RIVM | | | | |
| WHO | | | | |
| CEDI | | | | |
| JMPR | | | | |

# The World Health Organization (WHO): Classification of Pesticides by Hazard (CPH)



# Classifying Data Elements

| Type of Data | NRC 2001 definition | NDWAC CCL CP Workgroups draft definition |
|---|---|---|
| measurements in natural waters | demonstrated occurrence | occurrence data |
| other information about contaminant occurrence | potential occurrence | occurrence information |
| health effects measurements from toxicological studies that relate to exposures via drinking water | demonstrated health effects | health effects data |
| other information about adverse health effects | potential health effects | health effects information |

# Data Mapping

- All data elements (848 total) were mapped to 5 categories:
  - Health Effects Data (108)
  - Occurrence Data (49)
  - Health Effects Information (67)
  - Occurrence Information (69)
  - Other (555)
- Classification of data elements to these categories allows summarizing the candidates by each of the screening 'gates'

# Data Set Findings: Overview

- Overview
  - 1,500 records (out of 30,000, or 5 percent) had a chemical name but no CAS RN
    - Assigned CAS RN to 721 (~50 percent) of these
  - 11,000 records had multiple chemical names assigned a single CAS RN
  - 108 records had multiple CAS RNs assigned to one chemical name

# Example CCL Universe Data Set Summary Statistics

| Database Subset | Data Sources | Chemicals | Data Elements | |
|---|---|---|---|---|
| | | Contaminants | Available Data or Info Only[1] | Total (data, info, other) |
| Entire Example Data Set | 23 | 10,360 | 293 | 848 |
| All Chemicals with Health Effects Data or Information AND Occurrence Data or Information | 18 | 774 | 293 | 848 |
| Chemicals with Health Effects Data AND Occurrence Data | 16 | 62 | 157 | <848 |

# Data Set Summary Statistics Compared With CCL

| Database Subset | Data Sources | Contaminants | Chemicals | |
|---|---|---|---|---|
| | | | Out of 262 on Draft CCL | Out of 50 on Final CCL |
| Entire Example Data Set | 23 | 10,360 | 244 | 45 |
| All Chemicals with Health Effects Data or Information AND Occurrence Data or Information | 18 | 774 | 188 | 40 |
| Chemicals with Health Effects data AND Occurrence data | 16 | 62 | 35 | 18 |

# Screening Gates

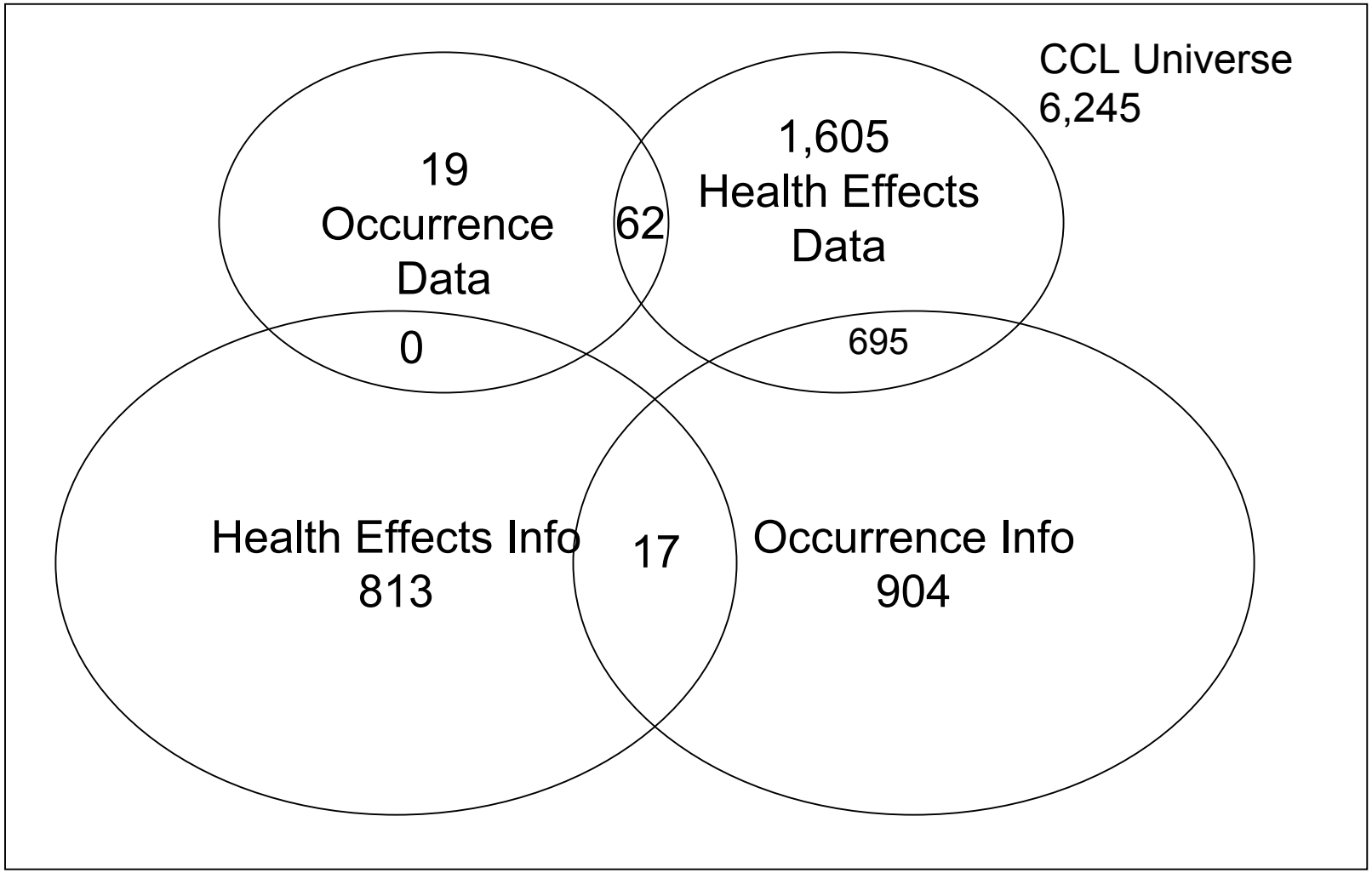
- "Gates" will be used to screen contaminants from the Universe to the PCCL based on varying criteria:
  - Gate 1: Contaminants have Health Effects Data and Occurrence Data
  - Gate 2: Contaminants have Health Effects Information and Occurrence Data
  - Gate 3: Contaminants have Health Effects Data and Occurrence Information
  - Gate 4: Contaminants have Health Effects Information and Occurrence Information
  - Gate 5: Expert Judgement

# Number of Chemicals with Data/Information

- Number of chemicals in various categories related to data/information elements in the Example CCL Universe Data Set

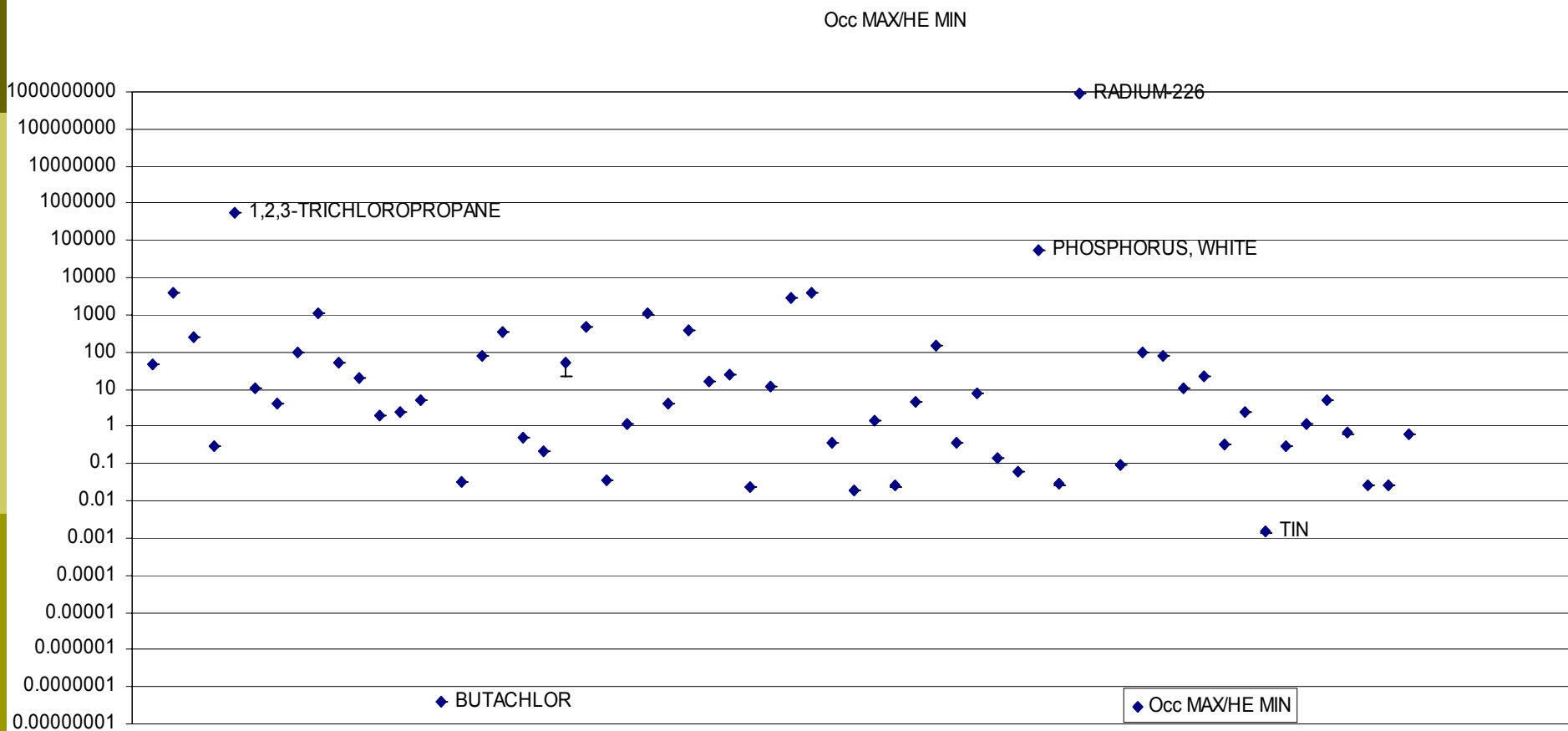
| Category or Criteria of Data/Information Available; Gate Screening Criteria | Number of Chemicals in Example Data Set Meeting the Criteria | Percentage of Chemicals in Example Data Set Meeting the Criteria |
|---|---|---|
| Health Effects DATA AND Occurrence DATA; **Gate 1** | 62 | 0.6% |
| Health Effects Information AND Occurrence DATA; **Gate 2** | 0 | 0.0% |
| Health Effects DATA AND Occurrence Information; **Gate 3** | 695 | 6.7% |
| Health Effects Information AND Occurrence Information; **Gate 4** | 17 | 0.2% |
| Subtotal of Candidates Through Gates 1-4: | 774 | 7.5% |

# The Example CCL Data Set and the NRC'S Venn Diagram



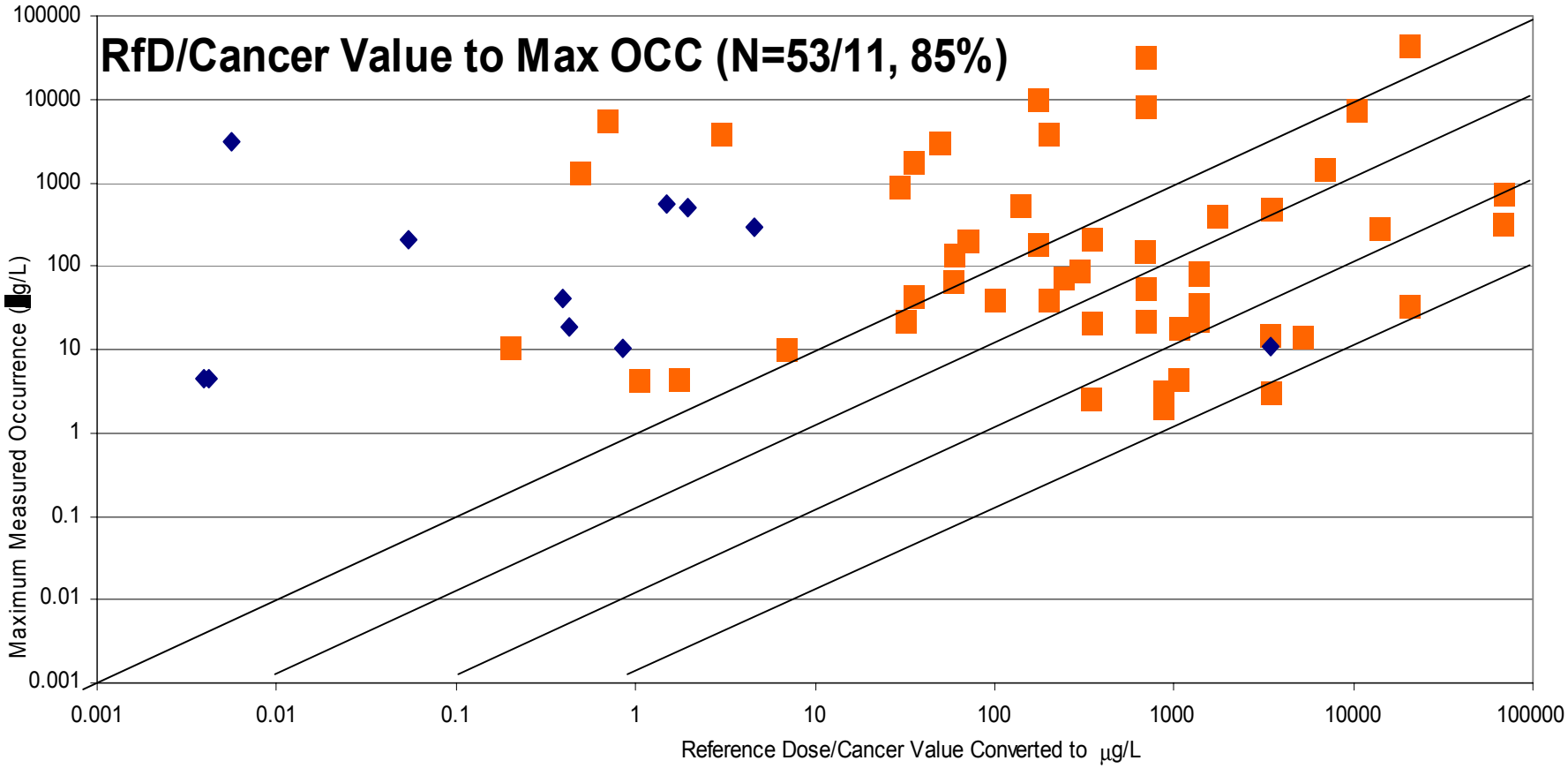
# Quantitative “GATE 1” Screening Results

# Ratio of Maximum Occurrence to Minimum Health Effect Level




- **Most GATE 1 chemical occurrence is within two orders of magnitude (1 to 100) of lowest health effect level with exceptions noted.**

# Ratio of Max Occurrence to Reference Dose: screen out ~ 60% of Gate 1 if 1:1



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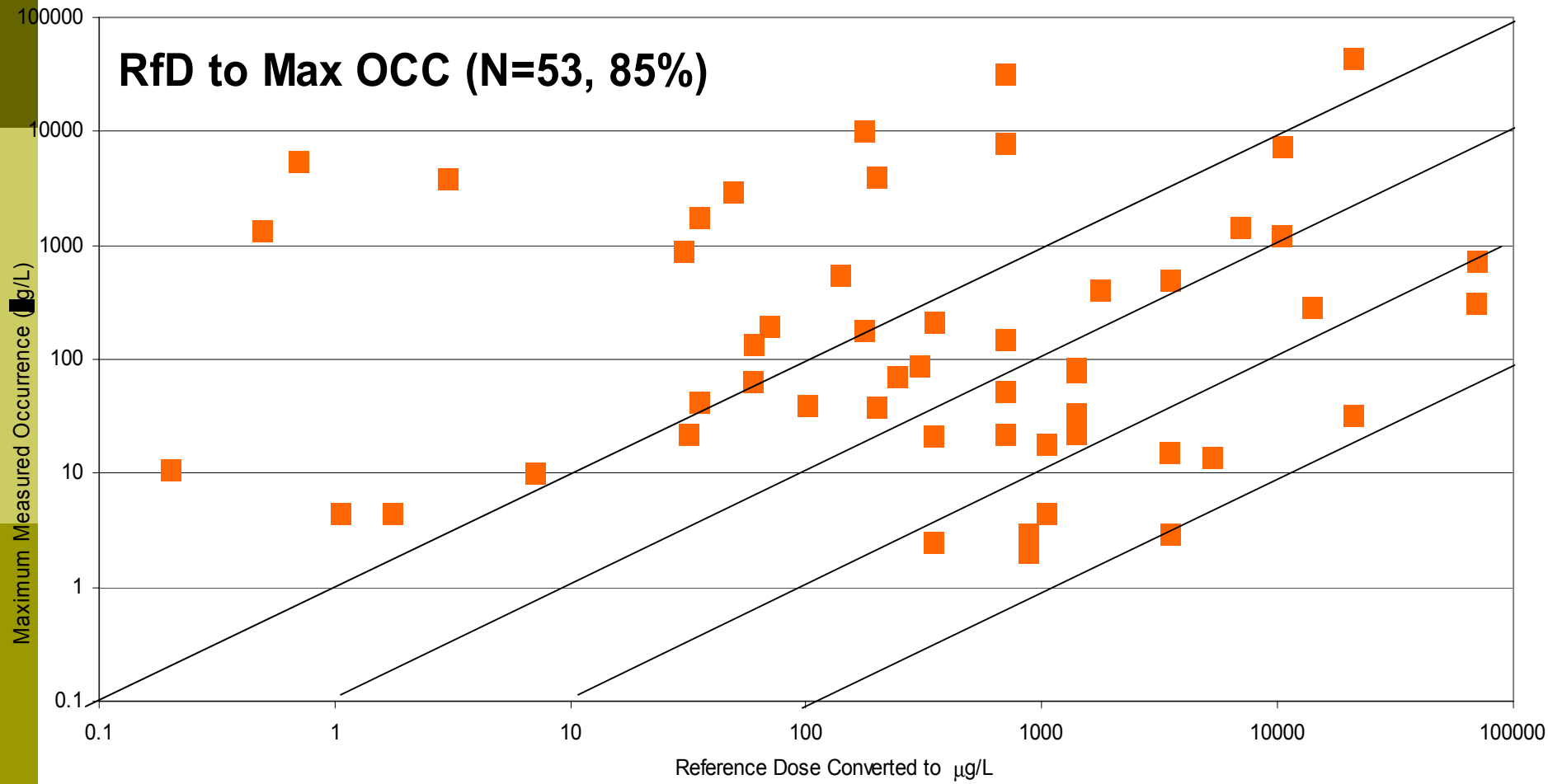
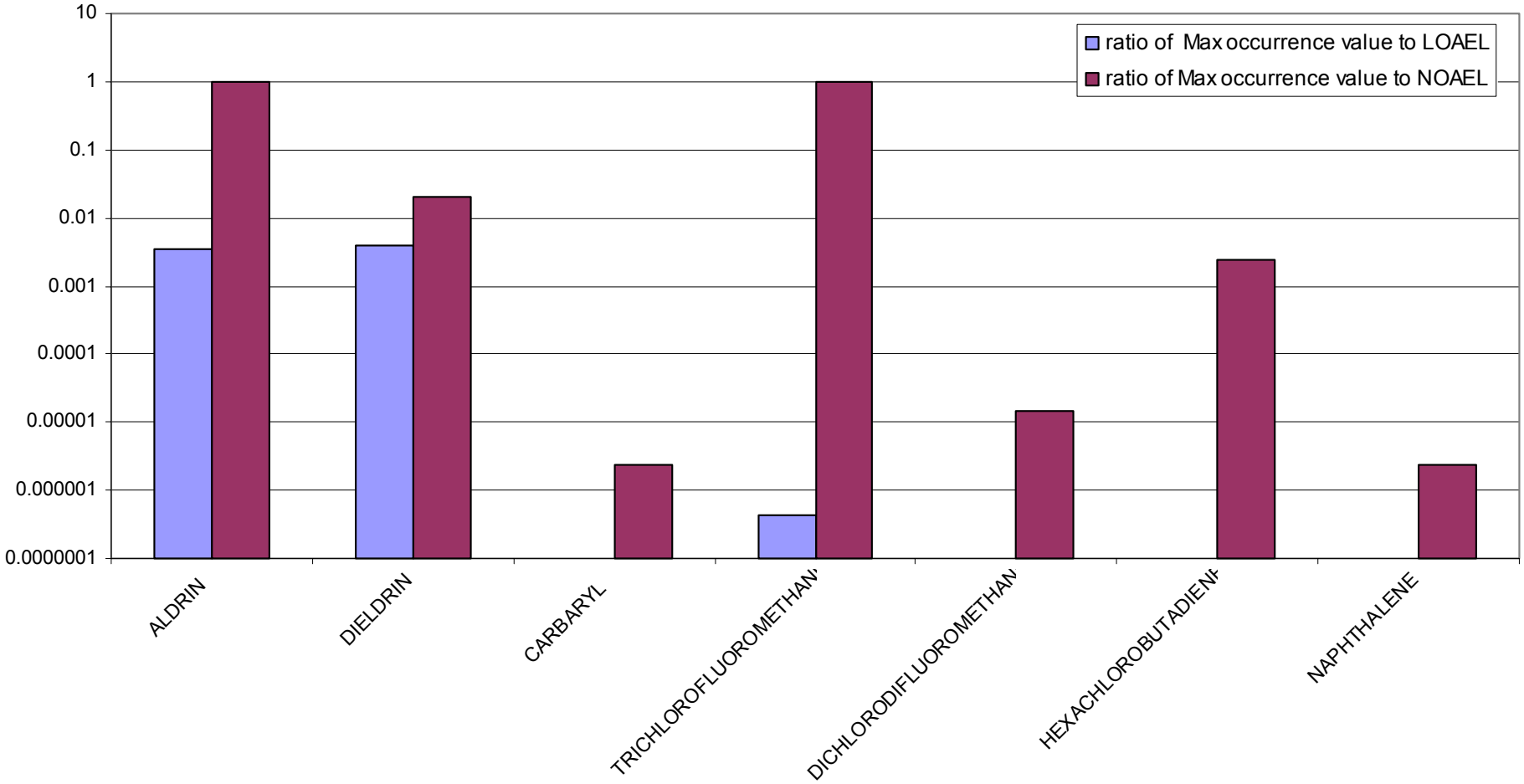
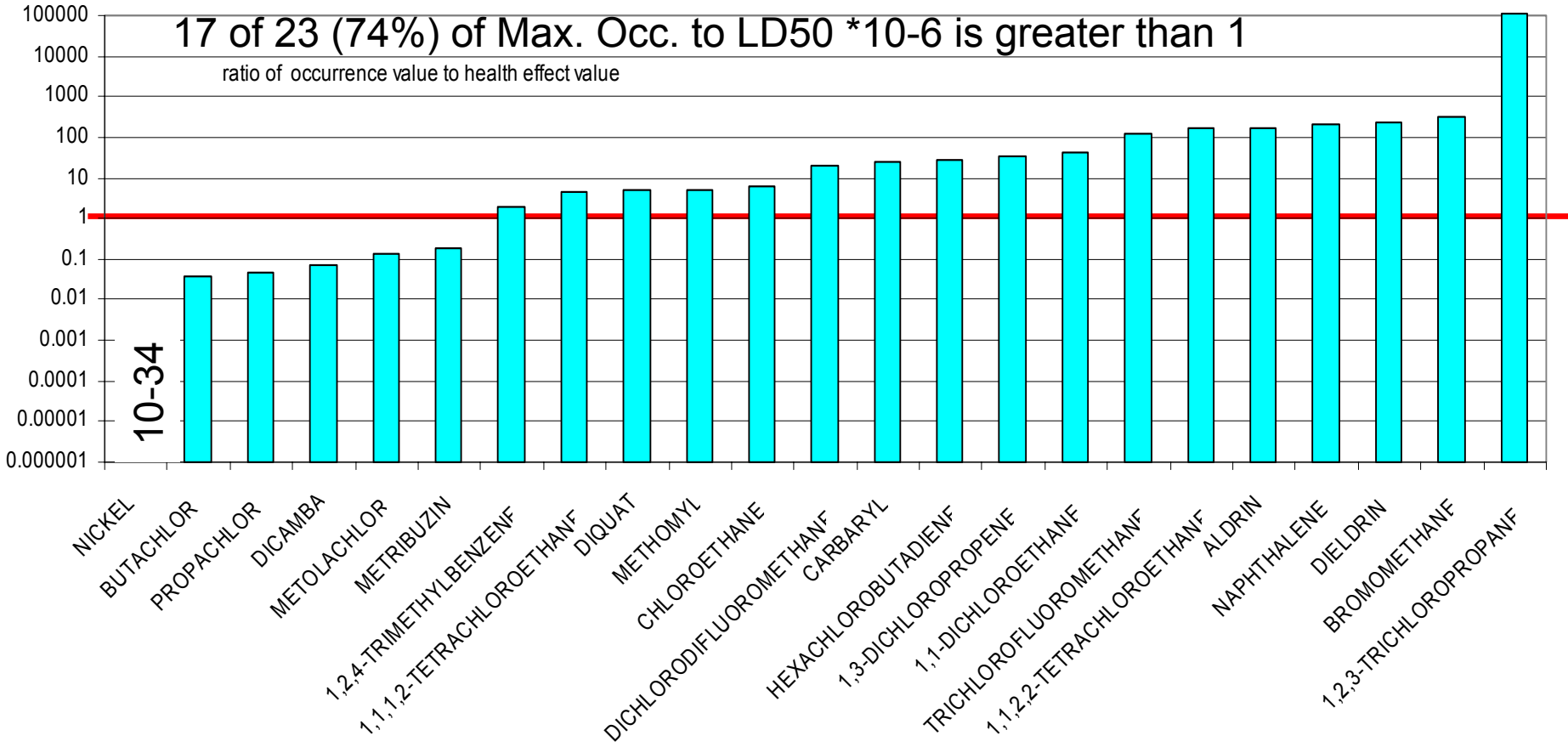


# Max. Occurrence to NOAEL/LOAEL



# Ratio of Max Occ to LD50(*10-6)



# Summary of Gate 1 Quantitative Screening

| Gate 1 Screening Criteria Ratio (Occ:HE) | Max Occurrence/ Lowest HE | Max Occurrence/ Lowest RfD | Max Occurrence/Highest NOAEL/ Lowest LOAEL | Max Occurrence/ Lowest LD50 |
|---|---|---|---|---|
| 1:1 or greater | 65% | 42% | 0% | 74% |
| 1:0.1 | 81% | 64% | 0% | 83% |
| 1:0.01 | 97% | 83% | 14% | 96% |
| 1:0.001 | 98% | 98% | 43% | 96% |
| 1:0.0001 | 98% | 100% | 86% | 96% |
| >1:0.00001 | 100% | 100% | 100% | 100% |
| **N** | 62 | 53 | 7 | 23 |

# Insights

- Data Availability is better for health effects than for water occurrence. Lack of contaminants for Gate 2 an indicator that water occurrence data may be a limiting factor
- Used high quality sources – few additional sources will be of similar quality – need data quality measures for additional sources

# Relationships among Data Sources:

- Use of prioritized lists informative for screening, but may want background data for attribute scoring (iterative process)
- E.g. ATSDR data sources
  - HazDat Data
  - CERCLA Priority List
  - Toxicity Profiles
  - Minimal Risk Levels
- Another Example: ITER
  - Derived endpoints e.g. Reference Dose
  - Can get background data from RAIS, EPA, etc.
  - ITER useful for screening, may want additional data for attribute scoring

# How Representative are the 23?

- 10% of reviewed data sources included
- 10,360 contaminants (~10% of anticipated CCL Universe)
- 750 (about 7.5%) get through “qualitative” “gate” screening
- 90% of CCL 1998 chemicals included
- 80% of CCL 1998 through “qualitative” “gates” (40 of 50)

# Is the Example Data Set Adequate for Screening?

- Sufficient data are available for screening
- Gate 1 screening demonstrates adequacy for decision making
  - Qualitative screening is simple, and effective for this example
  - With larger numbers ( e.g. Actual CCL Universe), quantitative screening may be needed to limit size of PCCL
  - Other gates probably require a quantitative screening
- Would increase representativeness to include additional occurrence data (e.g. NAWQA, NREC) in Example CCL Data Set

- RECOMMENDATION:
  - **Use Qualitative Screening for NDWAC Example PCCL**
  - **Add more Occurrence Data sources**

# Findings and Recommendations

- Using tabular sources maximizes the number of elements for screening
- Have many derived health effect endpoints and redundancies
- Have included national drinking water surveys
- Could identify additional Gate 1 contaminants with other natural water surveys (e.g. NAWQA)
- Additional data sources would be helpful for attributes scoring

# What can we say about the use of this data set for attribute/scoring and classification?

- Additional sources may provide needed elements and perhaps should be added to data set
- Additional elements may be helpful for attribute scoring.
  - For example, critical effect information to score severity from derived “potency” endpoints may not be available.
- Additional sources may require manual manipulation and judgment for use in PCCL to CCL
  - E.g., additional occurrence data is in raw data format, so statistics must be calculated