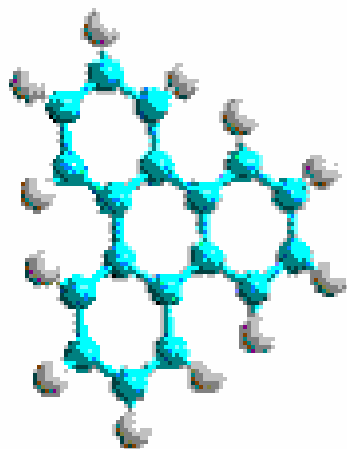


Analog Identification Methodology (AIM)

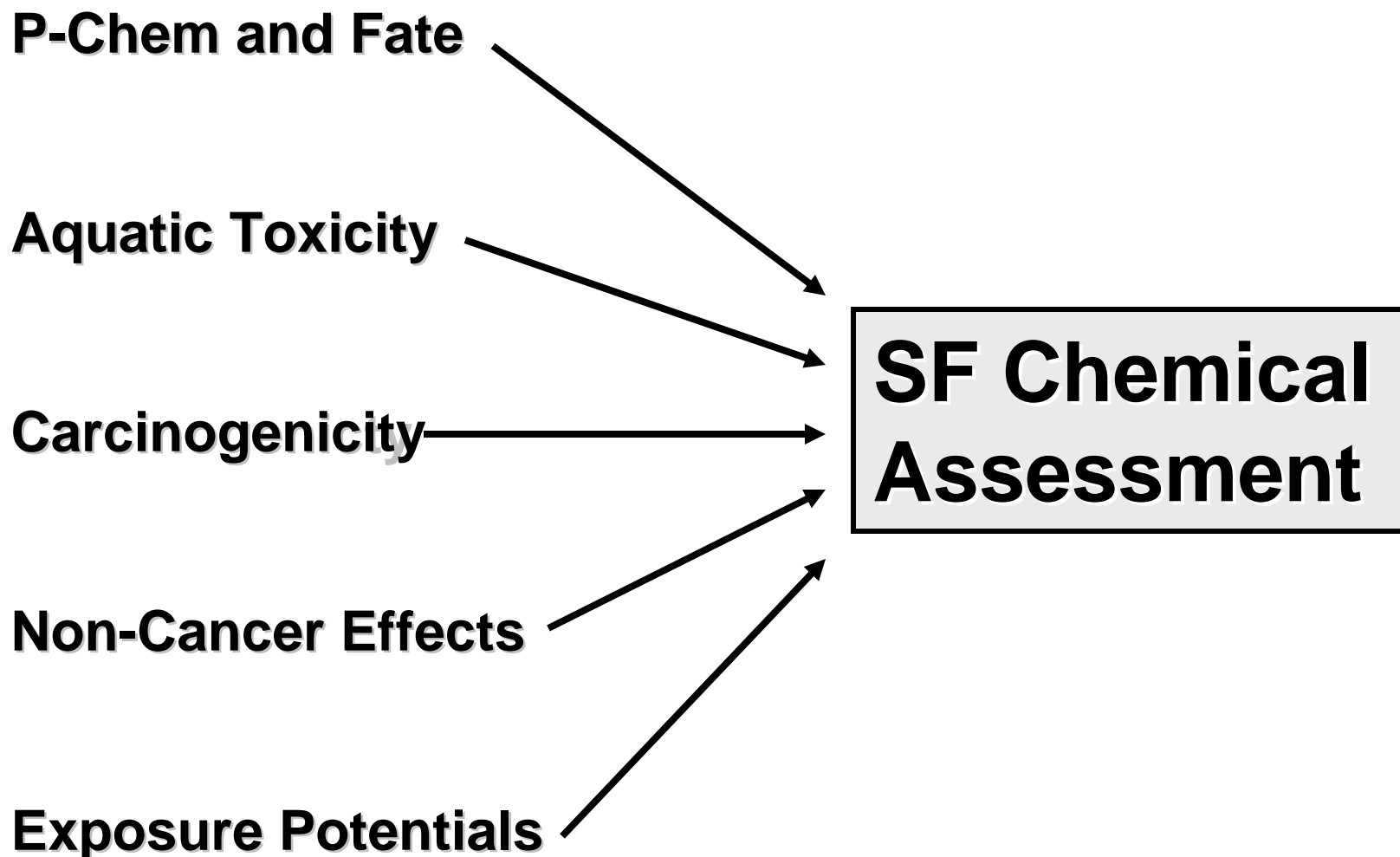


**Analog
Identification
Methodology**

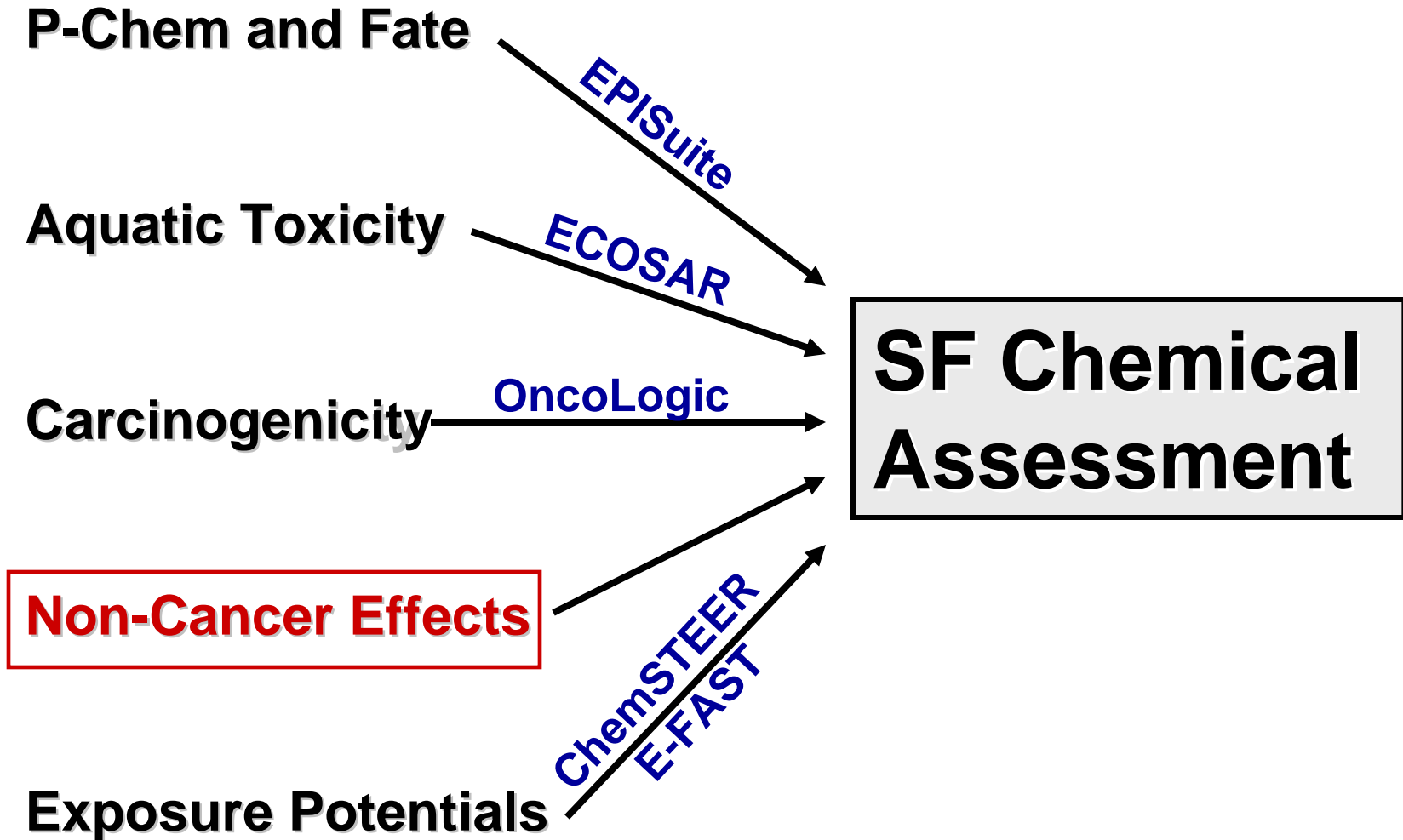
Sustainable Futures Initiative

- + OPPT's Sustainable Futures Initiative encourages companies to screen chemicals at R&D for potential hazards and risks using OPPT's predictive models and methods**
- + Promotes the design of safer chemicals and the use of safer chemical alternatives**

Sustainable Futures Chemical Assessment



Sustainable Futures Chemical Assessment



Non-Cancer Hazard Effects Screening Protocol

Identify experimental data on chemical of interest

Determine appropriate analog(s)

Identify experimental data on analog(s)

**Assign a hazard concern level for chemical
of interest using analog data**

Non-Cancer Hazard Effects Screening Protocol

Identify experimental data on chemical of interest

✓ Determine appropriate analog(s)

Analog
Identification
Methodology

✓ Identify experimental data on analog(s)

Analog
Identification
Methodology

Assign a hazard concern level for chemical of interest using analog data

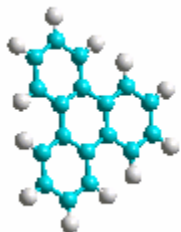
AIM Methodology

- ✚ The AIM database contains 31,031 potential analogs with publicly available toxicity data
- ✚ Experimental data sources Indexed
 - On-Line Databases
TSCATS, HSDB, IRIS
 - U.S. Government Documents
NTP, ATSDR, HPV Challenge Program
 - Other Sources
DSSTox, RTECS, IUCLID, AEGLS
- ✚ Uses a chemical fragment-based approach with 645 individual chemical fragments to identify potential analogs.

AIM Methodology (cont.)

- ✚ Uses a “three-pass” methodology to identify analogs:
 - Pass 1- Analogs are selected when a match of 645 possible chemical fragments occurs. If less than 7 analogs are identified, then:
 - Pass 2 - Analogs are selected when a match of 200 fragments occur and allows alkyl substitutions. If less than 7 analogs are identified again, then:
 - Pass 3 - Allows halogens (chlorine, bromine, or iodine) substitutions.
- ✚ Results from first pass (search) are displayed in numerical order by CAS RN, followed by results from second, then third passes. First analog displayed may not be the closest analog with data.

Opening Screen of Internet Based Model



Analog Identification Methodology

The Analog Identification Methodology (AIM) was designed to help identify publicly available, experimental toxicity data on closely related chemical structures

The AIM database contains 31,031 chemicals

Experimental Data Sources Indexed

On-Line Databases

[TSCATS](#)

[HSDB](#)

[IRIS](#)

U.S. Government Documents

[NTP](#)

[ATSDR](#)

[HPV Challenge Program](#)

Other Sources

[DSSTox](#)

[RTECS](#)

[IUCLID](#)

[AEGLS](#)

There are three ways to run AIM

1) Quick Search by SMILES notation

Submit SMILES Notation

2) Draw your compound

Draw your structure



3) CAS Registry number Search

Submit

[About the AIM Methodology](#)

Running AIM by Entering SMILES

The Analog Identification Methodology (AIM) was designed to help identify publicly available, experimental toxicity data on closely related chemical structures.

The AIM database contains 31,031 chemicals

Experimental Data Sources Indexed

On-Line Databases

[TSCATS](#)

[HSDB](#)

[IRIS](#)

U.S. Government Documents

[NTP](#)

[ATSDR](#)

[HPV Challenge Program](#)


Other Sources

[DSSTox](#)

[RTECS](#)

[IUCLID](#)

[AEGLS](#)

| There are three ways to run AIM | |
|---|--|
| 1) Quick Search by SMILES notation | <input type="text" value="O=C(C=C)OCCCCCCCCC(C)C"/> <input type="button" value="Submit SMILES Notation"/> |
| 2) Draw your compound | Draw your structure  |
| 3) CAS Registry number Search | <input type="text"/> <input type="button" value="Submit"/> |

Isodecyl acrylate SMILES Entered

Running AIM by Using Integrated Draw Program

Home Submit Structure

Select Erase Clear Undo Redo Clean Fit

More...

+

-

H

C

O

N

P

S

Cl

I

More

Add

Isodecyl acrylate
CAS 1330-61-6
Drawn and Entered



This drawing applet is part of ChemS³

Running AIM by Entering CAS RN

The Analog Identification Methodology (AIM) was designed to help identify publicly available, experimental toxicity data on closely related chemical structures.

The AIM database contains 31,031 chemicals

Experimental Data Sources Indexed

On-Line Databases

[TSCATS](#)

[HSDB](#)

[IRIS](#)

U.S. Government Documents

[NTP](#)

[ATSDR](#)

[HPV Challenge Program](#)


Other Sources

[DSSTox](#)

[RTECS](#)

[IUCLID](#)

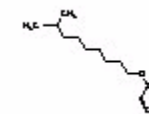
[AEGLS](#)

| There are three ways to run AIM | |
|------------------------------------|--|
| 1) Quick Search by SMILES notation | <input type="text"/> Submit SMILES Notation |
| 2) Draw your compound | Draw your structure  |
| 3) CAS Registry number Search | <input type="text" value="1330-61-6"/> Submit |

Isodecyl acrylate CAS 1330-61-6 Entered

Results

Found 12 Analogs for:



First 6 analogs found for Isodecyl acrylate, #1 is the same chemical

| ISODECYL ACRYLATE [CAS No. 1330-61-6] | | | |
|---------------------------------------|---|---------------------------|---------------|
| <p><u>Analog # 1</u></p> | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | | | <u>RTECS</u> |

| 2-PROPENOIC ACID, 1-METHYL-1,3-PROPANEDIYL ESTER [CAS No. 19485-03-1] | | | |
|---|---|---------------------------|---------------|
| <p><u>Analog # 4</u></p> | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | <u>TSCATS</u> | | <u>RTECS</u> |

| 1,3-BUTYLENEDIMETHACRYLATE [CAS No. 1189-08-8] | | | |
|--|---|---------------------------|---------------|
| <p><u>Analog # 2</u></p> | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | <u>TSCATS</u> | | <u>RTECS</u> |

| 2-ETHYLHEXYL 2-METHYL-2-PROPENOATE [CAS No. 688-84-6] | | | |
|---|---|---------------------------|---------------|
| <p><u>Analog # 5</u></p> | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | <u>TSCATS</u> | | <u>RTECS</u> |

| ISODECYL METHACRYLATE [CAS No. 29964-84-9] | | | |
|--|---|---------------------------|-------------------------------|
| <p><u>Analog # 3</u></p> | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | <u>TSCATS</u> | | <u>RTECS</u> <u>IUCLID</u> |

| [CAS No. 1322-13-0] | | | |
|--------------------------|---|---------------------------|---------------|
| <p><u>Analog # 6</u></p> | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | | | <u>RTECS</u> |

Search for Analogs to Butyl Acrylate CAS RN 141-32-2

The Analog Identification Methodology (AIM) was designed to help identify publicly available, experimental toxicity data on closely related chemical structures.

Butyl acrylate CAS 141-32-2 Entered

The AIM database contains 31,031 chemicals

Experimental Data Sources Indexed

On-Line Databases


[TSCATS](#)
[HSDB](#)
[IRIS](#)

U.S. Government Documents

[NTP](#)
[ATSDR](#)
[HPV Challenge Program](#)

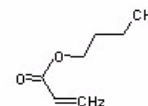
Other Sources

[DSSTox](#)
[RTECS](#)
[IUCLID](#)
[AEGLS](#)

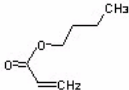
| There are three ways to run AIM | |
|------------------------------------|---|
| 1) Quick Search by SMILES notation | <input type="text"/> <input type="submit" value="Submit SMILES Notation"/> |
| 2) Draw your compound | Draw your structure  |
| 3) CAS Registry number Search | <input type="text" value="141-32-2"/> <input type="submit" value="Submit"/> |

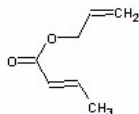
Results

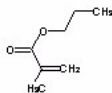
Found 12 Analogs for:

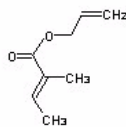


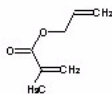
Analogs found for butyl acrylate, #1 is the same chemical

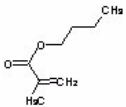
| BUTYL ACRYLATE [CAS No. 141-32-2] | | | |
|--|---|---------------------------|-----------------|
| <p><u>Analog # 1</u></p>  | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | TSCATS HSDB | | RTECS IUCLID |

| 2-BUTENOIC ACID, 2-PROPENYL ESTER [CAS No. 20474-93-5] | | | |
|--|---|---------------------------|---------------|
| <p><u>Analog # 4</u></p>  | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | | | RTECS |

| N-PROPYL METHACRYLATE [CAS No. 2210-28-8] | | | |
|---|---|---------------------------|---------------|
| <p><u>Analog # 2</u></p>  | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | TSCATS | | RTECS |

| 2-BUTENOIC ACID, 2-METHYL-, 2-PROPENYL ESTER, (E)- [CAS No. 7493-71-2] | | | |
|---|---|---------------------------|---------------|
| <p><u>Analog # 5</u></p>  | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | | | RTECS |

| ALLYL METHACRYLATE [CAS No. 96-05-9] | | | |
|--|---|---------------------------|---------------------------|
| <p><u>Analog # 3</u></p>  | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | TSCATS | | RTECS DSSTox Minnow |

| METHACRYLIC ACID, N-BUTYL ESTER [CAS No. 97-88-1] | | | |
|--|---|---------------------------|-----------------|
| <p><u>Analog # 6</u></p>  | Toxicity Data Available for this Compound | | |
| | On-Line Databases | U.S. Government Documents | Other Sources |
| | TSCATS HSDB | | RTECS IUCLID |

Analogue Identification Methodology

Currently Soliciting Beta Test Participants

- ✦ Internet-based, easy to use model
- ✦ Operates on password-protected site
- ✦ For information on AIM or Sustainable Futures contact:

Bill Waugh
202-564-7657
waugh.bill@epa.gov

OR

Kelly Mayo-Bean
202-564-7662
mayo.kelly@epa.gov

- ✦ To become a participant in the AIM beta test and to set-up access to the website, please contact:

Jim Santory, 412-751-8958, jsantory@cermonline.com