

# Package: extractox (via r-universe)

December 19, 2024

**Title** Extract Tox Info from Various Databases

**Version** 0.1.9001

**Description** Extract toxicological and chemical information from databases maintained by scientific agencies and resources, including the Comparative Toxicogenomics Database <<https://ctdbase.org/>>, the Integrated Chemical Environment <<https://ice.ntp.niehs.nih.gov/>>, the Integrated Risk Information System <<https://cfpub.epa.gov/ncea/iris/>>, the CompTox Chemicals Dashboard Resource Hub <<https://www.epa.gov/comptox-tools/comptox-chemicals-dashboard-resource-hub>>, and PubChem <<https://pubchem.ncbi.nlm.nih.gov/>>.

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**URL** <https://github.com/clau6i0/extractox>,  
<https://clau6i0.github.io/extractox/>

**BugReports** <https://github.com/clau6i0/extractox/issues>

**Depends** R (>= 4.1)

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**Repository** <https://clau6i0.r-universe.dev>

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---

extr\_casrn\_from\_cid    *Retrieve CASRN for PubChem CIDs*

---

### Description

This function retrieves the CASRN for a given set of PubChem Compound Identifiers (CID). It queries PubChem through the webchem package and extracts the CASRN from the depositor-supplied synonyms.

### Usage

```
extr_casrn_from_cid(pubchem_id, verbose = TRUE)
```

### Arguments

**pubchem\_id**    A numeric vector of PubChem CIDs. These are unique identifiers for chemical compounds in the PubChem database.

**verbose**        A logical value indicating whether to print detailed messages. Default is TRUE.

### Value

A data frame containing the CID, CASRN, and IUPAC name of the compound. The returned data frame includes three columns:

**CID**    The PubChem Compound Identifier.

**cas\_rn**    The corresponding CASRN of the compound.

**IUPACName**    The IUPAC name of the compound.

### See Also

[PubChem](#)

## Examples

```
# Example with formaldehyde and aflatoxin
cids <- c(712, 14434) # CID for formaldehyde and aflatoxin B1
extr_casrn_from_cid(cids)
```

---

extr\_chem\_info

*Query Chemical Information from IUPAC Names*

---

## Description

This function takes a vector of IUPAC names and queries the PubChem database (using the webchem package) to obtain the corresponding CASRN and CID for each compound. It reshapes the resulting data, ensuring that each compound has a unique row with the CID, CASRN, and additional chemical properties.

## Usage

```
extr_chem_info(IUPAC_names, stop_on_warning = FALSE, verbose = TRUE)
```

## Arguments

**IUPAC\_names** A character vector of IUPAC names. These are standardized names of chemical compounds that will be used to search in the PubChem database.

**stop\_on\_warning** Logical. If set to TRUE, the function will stop and throw an error if any substances are not found in PubChem. Defaults to FALSE, in which case a warning is issued.

**verbose** A logical value indicating whether to print detailed messages. Default is TRUE.

## Value

A data frame with information on the queried compounds, including:

**iupac\_name** The IUPAC name of the compound.

**cid** The PubChem Compound Identifier (CID).

**isomeric\_smiles** The SMILES string (Simplified Molecular Input Line Entry System).

## Examples

```
# Example with formaldehyde and aflatoxin
extr_chem_info(IUPAC_names = c("Formaldehyde", "Aflatoxin B1"))
```

---

 extr\_comptox

*Download and Extract Data from CompTox Chemistry Dashboard*


---

## Description

This function interacts with the CompTox Chemistry Dashboard to download and extract a wide range of chemical data based on user-defined search criteria. It allows for flexible input types and supports downloading various chemical properties, identifiers, and predictive data. It was inspired by the ECOTOXr::websearch\_comptox function.

## Usage

```
extr_comptox(
  ids,
  download_items = c("CASRN", "INCHIKEY", "IUPAC_NAME", "SMILES", "INCHI_STRING",
    "MS_READY_SMILES", "QSAR_READY_SMILES", "MOLECULAR_FORMULA", "AVERAGE_MASS",
    "MONOISOTOPIC_MASS", "QC_LEVEL", "SAFETY_DATA", "EXPOCAST", "DATA_SOURCES",
    "TOXVAL_DATA", "NUMBER_OF_PUBMED_ARTICLES", "PUBCHEM_DATA_SOURCES", "CPDAT_COUNT",
    "IRIS_LINK", "PPRTV_LINK", "WIKIPEDIA_ARTICLE", "QC_NOTES", "ABSTRACT_SHIFTER",
    "TOXPRINT_FINGERPRINT", "ACTOR_REPORT", "SYNONYM_IDENTIFIER", "RELATED_RELATIONSHIP",
    "ASSOCIATED_TOXCAST_ASSAYS", "TOXVAL_DETAILS",
    "CHEMICAL_PROPERTIES_DETAILS",
    "BIOCONCENTRATION_FACTOR_TEST_PRED", "BOILING_POINT_DEGC_TEST_PRED",
    "48HR_DAPHNIA_LC50_MOL/L_TEST_PRED", "DENSITY_G/CM^3_TEST_PRED", "DEVTOX_TEST_PRED",
    "96HR_FATHEAD_MINNOW_MOL/L_TEST_PRED", "FLASH_POINT_DEGC_TEST_PRED",
    "MELTING_POINT_DEGC_TEST_PRED", "AMES_MUTAGENICITY_TEST_PRED",
    "ORAL_RAT_LD50_MOL/KG_TEST_PRED", "SURFACE_TENSION_DYN/CM_TEST_PRED",
    "THERMAL_CONDUCTIVITY_MW/(M*K)_TEST_PRED",
    "TETRAHYMENA_PYRIFORMIS_IGC50_MOL/L_TEST_PRED", "VISCOSITY_CP_CP_TEST_PRED",

    "VAPOR_PRESSURE_MMHG_TEST_PRED", "WATER_SOLUBILITY_MOL/L_TEST_PRED",
    "ATMOSPHERIC_HYDROXYLATION_RATE_(AOH)_CM3/MOLECULE*SEC_OPERA_PRED",
    "BIOCONCENTRATION_FACTOR_OPERA_PRED",
    "BIODEGRADATION_HALF_LIFE_DAYS_DAYS_OPERA_PRED", "BOILING_POINT_DEGC_OPERA_PRED",
    "HENRYS_LAW_ATM-M3/MOLE_OPERA_PRED", "OPERA_KM_DAYS_OPERA_PRED",
    "OCTANOL_AIR_PARTITION_COEFF_LOGKOA_OPERA_PRED",
    "SOIL_ADSORPTION_COEFFICIENT_KOC_L/KG_OPERA_PRED",
    "OCTANOL_WATER_PARTITION_LOGP_OPERA_PRED", "MELTING_POINT_DEGC_OPERA_PRED",

    "OPERA_PKAA_OPERA_PRED", "OPERA_PKAB_OPERA_PRED", "VAPOR_PRESSURE_MMHG_OPERA_PRED",
    "WATER_SOLUBILITY_MOL/L_OPERA_PRED",
    "EXPOCAST_MEDIAN_EXPOSURE_PREDICTION_MG/KG-BW/DAY", "NHANES",
    "TOXCAST_NUMBER_OF_ASSAYS/TOTAL", "TOXCAST_PERCENT_ACTIVE"),
  mass_error = 0,
  verify_ssl = FALSE,
  verbose = TRUE,
  ...
)
```

)

**Arguments**

- ids** A character vector containing the items to be searched within the CompTox Chemistry Dashboard. These can be chemical names, CAS Registry Numbers (CASRN), InChIKeys, or DSSTox substance identifiers (DTXSID).
- download\_items** A character vector of items to be downloaded. This includes a comprehensive set of chemical properties, identifiers, predictive data, and other relevant information. By Default, it download all the info
- CASRN** The Chemical Abstracts Service Registry Number, a unique numerical identifier for chemical substances.
- INCHIKEY** The hashed version of the full International Chemical Identifier (InChI) string.
- IUPAC\_NAME** The International Union of Pure and Applied Chemistry (IUPAC) name of the chemical.
- SMILES** The Simplified Molecular Input Line Entry System (SMILES) representation of the chemical structure.
- INCHI\_STRING** The full International Chemical Identifier (InChI) string.
- MS\_READY\_SMILES** The SMILES representation of the chemical structure, prepared for mass spectrometry analysis.
- QSAR\_READY\_SMILES** The SMILES representation of the chemical structure, prepared for quantitative structure-activity relationship (QSAR) modeling.
- MOLECULAR\_FORMULA** The chemical formula representing the number and type of atoms in a molecule.
- AVERAGE\_MASS** The average mass of the molecule, calculated based on the isotopic distribution of the elements.
- MONOISOTOPIC\_MASS** The mass of the molecule calculated using the most abundant isotope of each element.
- QC\_LEVEL** The quality control level of the data.
- SAFETY\_DATA** Safety information related to the chemical.
- EXPOCAST** Exposure predictions from the EPA's ExpoCast program.
- DATA\_SOURCES** Sources of the data provided.
- TOXVAL\_DATA** Toxicological values related to the chemical.
- NUMBER\_OF\_PUBMED\_ARTICLES** The number of articles related to the chemical in PubMed.
- PUBCHEM\_DATA\_SOURCES** Sources of data from PubChem.
- CPDAT\_COUNT** The number of entries in the Chemical and Product Categories Database (CPDat).
- IRIS\_LINK** Link to the EPA's Integrated Risk Information System (IRIS) entry for the chemical.
- PPRTV\_LINK** Link to the EPA's Provisional Peer-Reviewed Toxicity Values (PPRTV) entry for the chemical.
- WIKIPEDIA\_ARTICLE** Link to the Wikipedia article for the chemical.

**QC\_NOTES** Notes related to the quality control of the data.

**ABSTRACT\_SHIFTER** Information related to the abstract shifter.

**TOXPRINT\_FINGERPRINT** The ToxPrint chemoinformatics fingerprint of the chemical.

**ACTOR\_REPORT** The Aggregated Computational Toxicology Resource (ACTOR) report for the chemical.

**SYNONYM\_IDENTIFIER** Identifiers for synonyms of the chemical.

**RELATED\_RELATIONSHIP** Information on related chemicals.

**ASSOCIATED\_TOXCAST\_ASSAYS** Assays associated with the chemical in the ToxCast database.

**TOXVAL\_DETAILS** Details of toxicological values.

**CHEMICAL\_PROPERTIES\_DETAILS** Details of the chemical properties.

**BIOCONCENTRATION\_FACTOR\_TEST\_PRED** Predicted bioconcentration factor from tests.

**BOILING\_POINT\_DEGC\_TEST\_PRED** Predicted boiling point in degrees Celsius from tests.

**48HR\_DAPHNIA\_LC50\_MOL/L\_TEST\_PRED** Predicted 48-hour LC50 for Daphnia in mol/L from tests.

**DENSITY\_G/CM^3\_TEST\_PRED** Predicted density in g/cm<sup>3</sup> from tests.

**DEVTOX\_TEST\_PRED** Predicted developmental toxicity from tests.

**96HR\_FATHEAD\_MINNOW\_MOL/L\_TEST\_PRED** Predicted 96-hour LC50 for fathead minnow in mol/L from tests.

**FLASH\_POINT\_DEGC\_TEST\_PRED** Predicted flash point in degrees Celsius from tests.

**MELTING\_POINT\_DEGC\_TEST\_PRED** Predicted melting point in degrees Celsius from tests.

**AMES\_MUTAGENICITY\_TEST\_PRED** Predicted Ames mutagenicity from tests.

**ORAL\_RAT\_LD50\_MOL/KG\_TEST\_PRED** Predicted oral LD50 for rats in mol/kg from tests.

**SURFACE\_TENSION\_DYN/CM\_TEST\_PRED** Predicted surface tension in dyn/cm from tests.

**THERMAL\_CONDUCTIVITY\_MW\_MxK\_TEST\_PRED** Predicted thermal conductivity in mW/m×K from tests.

**TETRAHYMENA\_PYRIFORMIS\_IGC50\_MOL/L\_TEST\_PRED** Predicted IGC50 for Tetrahymena pyriformis in mol/L from tests.

**VISCOSITY\_CP\_CP\_TEST\_PRED** Predicted viscosity in cP from tests.

**VAPOR\_PRESSURE\_MMHG\_TEST\_PRED** Predicted vapor pressure in mmHg from tests.

**WATER\_SOLUBILITY\_MOL/L\_TEST\_PRED** Predicted water solubility in mol/L from tests.

**ATMOSPHERIC\_HYDROXYLATION\_RATE\_(AOH)\_CM3/MOLECULE\*SEC\_OPERA\_PRED** Predicted atmospheric hydroxylation rate in cm<sup>3</sup>/molecule\*sec from OPERA.

**BIOCONCENTRATION\_FACTOR\_OPERA\_PRED** Predicted bioconcentration factor from OPERA.

	<b>BIODEGRADATION_HALF_LIFE_DAYS_DAYS_OPERA_PRED</b> Predicted biodegradation half-life in days from OPERA.
	<b>BOILING_POINT_DEGC_OPERA_PRED</b> Predicted boiling point in degrees Celsius from OPERA.
	<b>HENRYS_LAW_ATM-M3/MOLE_OPERA_PRED</b> Predicted Henry's law constant in atm-m <sup>3</sup> /mole from OPERA.
	<b>OPERA_KM_DAYS_OPERA_PRED</b> Predicted Km in days from OPERA.
	<b>OCTANOL_AIR_PARTITION_COEFF_LOGKOA_OPERA_PRED</b> Predicted octanol-air partition coefficient (log Koa) from OPERA.
	<b>SOIL_ADSORPTION_COEFFICIENT_KOC_L/KG_OPERA_PRED</b> Predicted soil adsorption coefficient (Koc) in L/kg from OPERA.
	<b>OCTANOL_WATER_PARTITION_LOGP_OPERA_PRED</b> Predicted octanol-water partition coefficient (log P) from OPERA.
	<b>MELTING_POINT_DEGC_OPERA_PRED</b> Predicted melting point in degrees Celsius from OPERA.
	<b>OPERA_PKAA_OPERA_PRED</b> Predicted pKa (acidic) from OPERA.
	<b>OPERA_PKAB_OPERA_PRED</b> Predicted pKa (basic) from OPERA.
	<b>VAPOR_PRESSURE_MMHG_OPERA_PRED</b> Predicted vapor pressure in mmHg from OPERA.
	<b>WATER_SOLUBILITY_MOL/L_OPERA_PRED</b> Predicted water solubility in mol/L from OPERA.
	<b>EXPOCAST_MEDIAN_EXPOSURE_PREDICTION_MG/KG-BW/DAY</b> Predicted median exposure from ExpoCast in mg/kg-bw/day.
	<b>NHANES</b> National Health and Nutrition Examination Survey data.
	<b>TOXCAST_NUMBER_OF_ASSAYS/TOTAL</b> Number of assays in ToxCast.
	<b>TOXCAST_PERCENT_ACTIVE</b> Percentage of active assays in ToxCast.
mass_error	Numeric value indicating the mass error tolerance for searches involving mass data. Default is 0.
verify_ssl	Logical value indicating whether SSL certificates should be verified. Default is FALSE. Note that this argument is not used on linux OS.
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.
...	Additional arguments passed to <code>httr2::req_options()</code> . Note that this argument is not used on linux OS.

### Details

Please note that this function, which pulls data from EPA servers, may encounter issues on some Linux systems. This is because those servers do not accept secure legacy renegotiation. On Linux systems, the current function depends on `curl` and `OpenSSL`, which have known problems with unsafe legacy renegotiation in newer versions. One workaround is to downgrade to `curl v7.78.0` and `OpenSSL v1.1.1`. However, please be aware that using these older versions might introduce potential security vulnerabilities. Refer to [this gist](#) for instructions on how to downgrade `curl` and `OpenSSL` on Ubuntu.

### Value

A cleaned data frame containing the requested data from CompTox.

## See Also

[CompTox Chemicals Dashboard Resource Hub](#)

## Examples

```
# Example usage of the function:
extr_comptox(ids = c("Aspirin", "50-00-0"))
```

---

extr\_ctd

*Extract Data from the CTD API*

---

## Description

This function queries the Comparative Toxicogenomics Database API to retrieve data related to chemicals, diseases, genes, or other categories.

## Usage

```
extr_ctd(
  input_terms,
  category = "chem",
  report_type = "genes_curated",
  input_term_search_type = "directAssociations",
  action_types = NULL,
  ontology = NULL,
  verify_ssl = FALSE,
  verbose = TRUE,
  ...
)
```

## Arguments

input_terms	A character vector of input terms such as CAS numbers or IUPAC names.
category	A string specifying the category of data to query. Valid options are "all", "chem", "disease", "gene", "go", "pathway", "reference", and "taxon". Default is "chem".
report_type	A string specifying the type of report to return. Default is "genes_curated". Valid options include: <b>"cgixns"</b> Curated chemical-gene interactions. Requires at least one <code>action_types</code> parameter. <b>"chems"</b> All chemical associations. <b>"chems_curated"</b> Curated chemical associations. <b>"chems_inferred"</b> Inferred chemical associations. <b>"genes"</b> All gene associations. <b>"genes_curated"</b> Curated gene associations.



	" <b>genes_inferred</b> " Inferred gene associations.
	" <b>diseases</b> " All disease associations.
	" <b>diseases_curated</b> " Curated disease associations.
	" <b>diseases_inferred</b> " Inferred disease associations.
	" <b>pathways_curated</b> " Curated pathway associations.
	" <b>pathways_inferred</b> " Inferred pathway associations.
	" <b>pathways_enriched</b> " Enriched pathway associations.
	" <b>phenotypes_curated</b> " Curated phenotype associations.
	" <b>phenotypes_inferred</b> " Inferred phenotype associations.
	" <b>go</b> " All Gene Ontology (GO) associations. Requires at least one ontology parameter.
	" <b>go_enriched</b> " Enriched GO associations. Requires at least one ontology parameter.
input_term_search_type	A string specifying the search method to use. Options are "hierarchicalAssociations" or "directAssociations". Default is "directAssociations".
action_types	An optional character vector specifying one or more interaction types for filtering results. Default is "ANY". Other acceptable inputs are "abundance", "activity", "binding", "cotreatment", "expression", "folding", "localization", "metabolic processing"...See <a href="https://ctdbase.org/tools/batchQuery.go">https://ctdbase.org/tools/batchQuery.go</a> for a full list.
ontology	An optional character vector specifying one or more ontologies for filtering GO reports. Default NULL.
verify_ssl	Boolean to control of SSL should be verified or not.
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.
...	Any other arguments to be supplied to req_option and thus to libcurl.

**Value**

A data frame containing the queried data in CSV format.

**References**

- Davis, A. P., Grondin, C. J., Johnson, R. J., Sciaky, D., McMorran, R., Wieggers, T. C., & Mattingly, C. J. (2019). The Comparative Toxicogenomics Database: update 2019. *Nucleic acids research*, 47(D1), D948–D954. doi:10.1093/nar/gky868

**See Also**

[Comparative Toxicogenomics Database](#)

**Examples**

```
input_terms <- c("50-00-0", "64-17-5", "methanal", "ethanol")
dat <- extr_ctd(
  input_terms = input_terms,
  category = "chem",
  report_type = "genes_curated",
```

```
input_term_search_type = "directAssociations",
action_types = "ANY",
ontology = c("go_bp", "go_cc")
)
str(dat)

# Get expression data
dat2 <- extr_ctd(
  input_terms = input_terms,
  report_type = "cgixns",
  category = "chem",
  action_types = "expression"
)

str(dat2)
```

---

extr\_ice

*Extract Data from NTP ICE Database*

---

## Description

The `extr_ice` function sends a POST request to the ICE API to search for information based on specified chemical IDs and assays.

## Usage

```
extr_ice(casrn, assays = NULL, verify_ssl = FALSE, verbose = TRUE, ...)
```

## Arguments

<code>casrn</code>	A character vector specifying the CASRNs for the search.
<code>assays</code>	A character vector specifying the assays to include in the search. Default is <code>NULL</code> , meaning all assays are included. If you don't know the exact assay name, you can use the <code>extr_ice_assay_names()</code> function to search for assay names that match a pattern you're interested in.
<code>verify_ssl</code>	Boolean to control of SSL should be verified or not.
<code>verbose</code>	A logical value indicating whether to print detailed messages. Default is <code>TRUE</code> .
<code>...</code>	Any other arguments to be supplied to <code>req_option</code> and thus to <code>libcurl</code> .

## Value

A data frame containing the extracted data from the ICE API.

## See Also

[extr\\_ice\\_assay\\_names](#), [NTP ICE database](#)

**Examples**

```
extr_ice(c("50-00-0"))
```

---

extr\_ice\_assay\_names     *Extract Assay Names from the ICE Database*

---

**Description**

This function allows users to search for assay names in the ICE database using a regular expression. If no search pattern is provided (regex = NULL), it returns all available assay names.

**Usage**

```
extr_ice_assay_names(regex = NULL)
```

**Arguments**

regex                    A character string containing the regular expression to search for, or NULL to retrieve all assay names.

**Value**

A character vector of matching assay names.

**Examples**

```
extr_ice_assay_names("OPERA")
extr_ice_assay_names(NULL)
extr_ice_assay_names("Vivo")
```

---

extr\_iris                    *Extract Data from EPA IRIS Database*

---

**Description**

The `extr_iris` function sends a request to the EPA IRIS database to search for information based on a specified keywords and cancer types. It retrieves and parses the HTML content from the response. Note that if keywords is not provide all dataset are retrieved.

**Usage**

```
extr_iris(
  casrn = NULL,
  cancer_types = c("non_cancer", "cancer"),
  verbose = TRUE
)
```

**Arguments**

casrn	A vector CASRN for the search.
cancer_types	A character vector specifying the types of cancer to include in the search. Must be either "non_cancer" or "cancer".
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.

**Value**

A data frame containing the extracted data.

**See Also**

[EPA IRIS database](#)

**Examples**

```
extr_iris(c("1332-21-4", "50-00-0"))
```

---

extr_monograph	<i>Retrieve WHO IARC Monograph Information</i>
----------------	--

---

**Description**

This function retrieves information regarding Monographs from the World Health Organization (WHO) International Agency for Research on Cancer (IARC) based on CAS Registry Number or Name of the chemical.

**Usage**

```
extr_monograph(ids, search_type = "casrn", verbose = TRUE)
```

**Arguments**

ids	A character vector of IDs to search for.
search_type	A character string specifying the type of search to perform. Valid options are "cas_rn" (CAS Registry Number) and "name" (name of the chemical). If search_type is "casrn", the function filters by the CAS Registry Number. If search_type is "name", the function performs a partial match search for the chemical name.
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.

**Value**

A data frame containing the relevant information from the WHO IARC, including Monograph volume, volume\_publication\_year, evaluation\_year, and additional\_information where the chemical was described.

**See Also**

<https://monographs.iarc.who.int/list-of-classifications/>

**Examples**

```
{
  dat <- extr_monograph(search_type = "casrn", ids = c("105-74-8", "120-58-1"))
  str(dat)

  # Example usage for name search
  dat2 <- extr_monograph(search_type = "name", ids = c("Aloe", "Schistosoma", "Styrene"))
  str(dat2)
}
```

---

extr_pubchem_fema	<i>Extract FEMA from PubChem</i>
-------------------	----------------------------------

---

**Description**

This function retrieves FEMA (Flavor and Extract Manufacturers Association) flavor profile information for a list of CAS Registry Numbers (CASRN) from the PubChem database using the webchem package. It applies the function `extr_fema_pubchem_` to each CASRN in the input vector and combines the results into a single data frame.

**Usage**

```
extr_pubchem_fema(casrn, verbose = TRUE)
```

**Arguments**

casrn	A vector of CAS Registry Numbers (CASRN) as atomic vectors.
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.

**Value**

A data frame containing the FEMA flavor profile information for each CASRN. If no information is found for a particular CASRN, the output will include a row indicating this.

**See Also**

[PubChem](#)

**Examples**

```
extr_pubchem_fema(c("83-67-0", "1490-04-6"))
```

---

extr\_pubchem\_ghs      *Extract GHS Codes from PubChem*

---

### Description

This function extracts GHS (Globally Harmonized System) codes from PubChem. It relies on the webchem package to interact with PubChem.

### Usage

```
extr_pubchem_ghs(casrn, verbose = TRUE)
```

### Arguments

casrn                  Character vector of CAS Registry Numbers (CASRN).  
verbose                A logical value indicating whether to print detailed messages. Default is TRUE.

### Value

A dataframe containing GHS information.

### See Also

[PubChem](#)

### Examples

```
extr_pubchem_ghs(casrn = c("50-00-0", "64-17-5"))
```

---

extr\_tetramer      *Extract Tetramer Data from the CTD API*

---

### Description

This function queries the Comparative Toxicogenomics Database API to retrieve tetramer data based on chemicals, diseases, genes, or other categories.

## Usage

```
extr_tetramer(  
  chem,  
  disease = "",  
  gene = "",  
  go = "",  
  input_term_search_type = "directAssociations",  
  qt_match_type = "equals",  
  verify_ssl = FALSE,  
  verbose = TRUE,  
  ...  
)
```

## Arguments

chem	A string indicating the chemical identifiers such as CAS number or IUPAC name of the chemical.
disease	A string indicating a disease term. Default is an empty string.
gene	A string indicating a gene symbol. Default is an empty string.
go	A string indicating a Gene Ontology term. Default is an empty string.
input_term_search_type	A string specifying the search method to use. Options are "hierarchicalAssociations" or "directAssociations". Default is "directAssociations".
qt_match_type	A string specifying the query type match method. Options are "equals" or "contains". Default is "equals".
verify_ssl	Boolean to control if SSL should be verified or not. Default is FALSE.
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.
...	Any other arguments to be supplied to req_option and thus to libcurl.

## Value

A data frame containing the queried tetramer data in CSV format.

## References

- Comparative Toxicogenomics Database: <http://ctdbase.org>
- Davis, A. P., Grondin, C. J., Johnson, R. J., Sciaky, D., McMorran, R., Wiegiers, T. C., & Mattingly, C. J. (2019). The Comparative Toxicogenomics Database: update 2019. *Nucleic acids research*, 47(D1), D948–D954. doi:10.1093/nar/gky868
- Davis, A. P., Wiegiers, T. C., Wiegiers, J., Wyatt, B., Johnson, R. J., Sciaky, D., Barkalow, F., Strong, M., Planchart, A., & Mattingly, C. J. (2023). CTD tetramers: A new online tool that computationally links curated chemicals, genes, phenotypes, and diseases to inform molecular mechanisms for environmental health. *Toxicological Sciences*, 195(2), 155–168. doi:10.1093/toxsci/kfad069

**See Also**

[Comparative Toxicogenomics Database](#)

**Examples**

```
tetramer_data <- extr_tetramer(  
  chem = c("50-00-0", "ethanol"),  
  disease = "",  
  gene = "",  
  go = "",  
  input_term_search_type = "directAssociations",  
  qt_match_type = "equals"  
)  
str(tetramer_data)
```

---

extr\_tox

*Extract Toxicological Information from Multiple Databases*

---

**Description**

This wrapper function retrieves toxicological information for specified chemicals by calling several external functions to query multiple databases, including PubChem, the Integrated Chemical Environment (ICE), CompTox Chemicals Dashboard, and the Integrated Risk Information System (IRIS).

**Usage**

```
extr_tox(casrn, verbose = TRUE)
```

**Arguments**

casrn	A character vector of CAS Registry Numbers (CASRN) representing the chemicals of interest.
verbose	A logical value indicating whether to print detailed messages. Default is TRUE.

**Details**

Specifically, this function:

- Calls [extr\\_monograph](#) to return monographs informations from WHO IARC.
- Calls [extr\\_pubchem\\_ghs](#) to retrieve GHS classification data from PubChem.
- Calls [extr\\_ice](#) to gather assay data from the ICE database.
- Calls [extr\\_iris](#) to retrieve risk assessment information from the IRIS database.
- Calls [extr\\_comptox](#) to retrieve data from the CompTox Chemicals Dashboard.



**Value**

A list of data frames containing toxicological information retrieved from each database:

**who\_iarc\_monographs** Lists if any, the WHO IARC monographs related to that chemical.

**ghs\_dat** Toxicity data from PubChem's Globally Harmonized System (GHS) classification.

**ice\_dat** Assay data from the Integrated Chemical Environment (ICE) database.

**iris** Risk assessment data from the IRIS database.

**iris** Risk assessment data from the IRIS database.

**comptox\_list** List of dataframe with toxicity information from the CompTox Chemicals Dashboard.

**Examples**

```
extr_tox(casrn = c("100-00-5", "107-02-8"))
```

---

```
write_dataframes_to_excel
```

*Write Dataframes to Excel*

---

**Description**

This function creates an Excel file with each dataframe in a list as a separate sheet.

**Usage**

```
write_dataframes_to_excel(df_list, filename)
```

**Arguments**

**df\_list** A named list of dataframes to write to the Excel file.

**filename** The name of the Excel file to create.

**Value**

No return value. The function prints a message indicating the completion of the Excel file writing.

**Examples**

```
tox_dat <- extr_tox("50-00-0")
temp_file <- tempfile(fileext = ".xlsx")
write_dataframes_to_excel(tox_dat, filename = temp_file)
```

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