EPA IRIS Assessment Database Web Scrape for Use in Risk Assessment Fact Sheets - Revision 1

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Abstract

Web scraping is an increasingly common practice for collecting data from the web via a programming or scripting language. In this work, a web scrape of the Environmental Protection Agency's (EPA) Integrated Risk Information System (IRIS) assessments database of chemicals is performed for updating risk assessment fact sheets. All data from the IRIS assessments is successfully scraped and stored into a Comma Separated Values (CSV) file for ease of access and viewing. The CSV file of the collected data and the Python scripts used to perform the web scrape and clean the data is publicly available on the author's GitHub. An updated web scrape was performed on November 27, 2021. Two chemicals (tert-Butyl Alcohol (tBA) and Ethyl Tertiary Butyl Ether (ETBE)) have been updated, and the new scrape is stored in the CSV file "EPA_IRIS_Assessments_clean-2021-11-27.csv" The updated CSV file is located on the author's GitHub within the Rev_1 directory (as well as the web scrape and data comparison Python scripts).

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1 Introduction

Web scraping is the process of extracting data from a website. Generally, the process of web scraping is done via the aid of a programming/scripting language. In particular, this work uses Python with the popular package

BeautifulSoup to perform a web scrape of the Environmental Protection Agency's (EPA) online database of Integrated Risk Information System (IRIS) assessments.

At the request of Dr. Margaret MacDonell of Argonne National Laboratory (ANL), I was asked to perform a web scrape of the EPA's online, publicly-available dataset of chemicals that have IRIS assessments for the purpose of updating risk assessment fact sheets.

Motivation for the web scrape request is due to each IRIS assessment chemical containing a link to its respective information. Unfortunately, the fact that each chemical in the IRIS assessment database has an individual link makes manually accessing each chemical's key information inconvenient due to load times and page layout. To improve convenience and speed of accessing the IRIS assessment data, the web scrape performed in this work aims to agglomerate all of the key data for each chemical into one, single table to be viewed as a spreadsheet via MS Excel or similar software.

Before jumping in and scraping data from the webpage(s), a preliminary examination of what an IRIS assessment involves helps identify what important information is desired.

Part of the EPA's mission is to "protect human health and the environment" [1]. The EPA's IRIS Program aims to aid in achieving this goal by identifying and characterizing possible health hazards of chemicals found within the environment. IRIS assessments are performed for individual chemicals, a group of related chemicals, or a complex mixture of chemicals, and contain toxicity information that is used by many domestic and world-wide health agencies and organizations. IRIS assessments include the following toxicity values and information (see Basic Information about the Integrated Risk Information System [1] for definitions): Reference Concentration (RfC), Reference Dose (RfD), cancer descriptors, Oral Slope Factor (OSF), and Inhalation Unit Risk (IUR). Therefore, the main goal of this work is to collect all toxicity and assessment information for each chemical assessed in the IRIS assessments database into a single spreadsheet with chemical names listed as rows and toxicity information listed as columns. Sometimes there exist multiple toxicity values and/or descriptors for certain chemicals; this is reflected in the resulting tables by repeating the chemical name along with the respective toxicity information collected (e.g. some chemicals in the IRIS assessment database have multiple RfC and/or RfD values and are therefore listed over multiple rows with their differing values to reflect this fact).

An updated web scrape was performed on November 27, 2021. There has been no increase or decrease in rows relative to the original web scrape, however, rows 114 and 115 (both rows refer to the chemical tert-Butyl Alcohol (tBA)) have changed; rows 320 and 321 (both rows refer to the chemical Ethyl Tertiary Butyl Ether (ETBE)) have also changed. Both chemicals have been updated and stored in a CSV file named "EPA_IRIS_Assessments_clean-2021-11-27.csv". The updated CSV file is available on the author's GitHub and can be found within the directory Rev_1. The Python script for the web scrape and the Python script for the comparison of files are also available on the author's github and are also located within the directory Rev_1.

2 Methodology

The Python programming language has a very useful package for web scraping called BeautifulSoup whose documentation is found here: BeautifulSoup Documentation [2].

To make use of the BeautifulSoup Python package, we first examine the EPA's IRIS assessment HTML page layout as well as the HTML page layout of some individual chemicals in order to get a sense of what relevant patterns and HTML tags exist in the html page contents [3] (see Figure 1). The IRIS Assessments main page contains a table listing the chemicals in the EPA's IRIS assessments database. Each chemical name contains a hyperlink to its respective assessment page (see Figure 2).

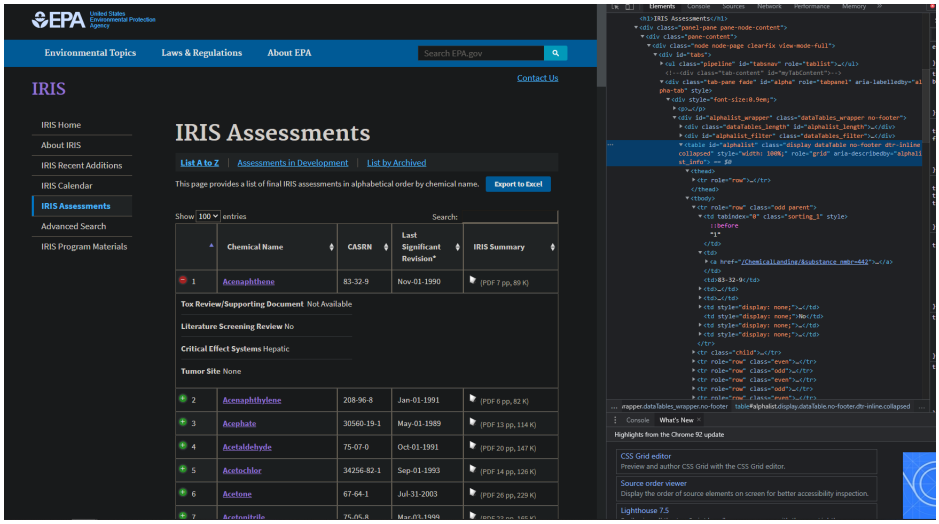

Figure 1:
IRIS Assessments main page with sample HTML layout.

The general process is as follows. Each chemical assessment page contains two main sections: "Noncancer Assessment" and "Cancer Assessment" (Note: some chemicals have no assessments of one or both sections, but the Python script accounts for this). To breakdown the process of obtaining all relevant data, the web scrape is performed with the following procedure: (1) Scrape the main table of the IRIS Assessments main page (see Figure 1). (2) Access the link to each chemical assessment and scrape the data from the "Noncancer Assessment" section (see Figure 2). (3) Access the link to each chemical assessment and scrape the data from the "Cancer Assessment" section (see Figure 2). Note: The "Cancer Assessment" scrape is achieved in a two-stage web scrape: one scrape for Weight of Evidence (WOE) data, and one scrape for oral and inhalation data. (4) Merge each table obtained from each of the web scrapes mentioned in (1), (2), and (3). (5) Clean the data by columns for readability in MS Excel (or similar software). (6) Finally, drop all identical, duplicate rows (if

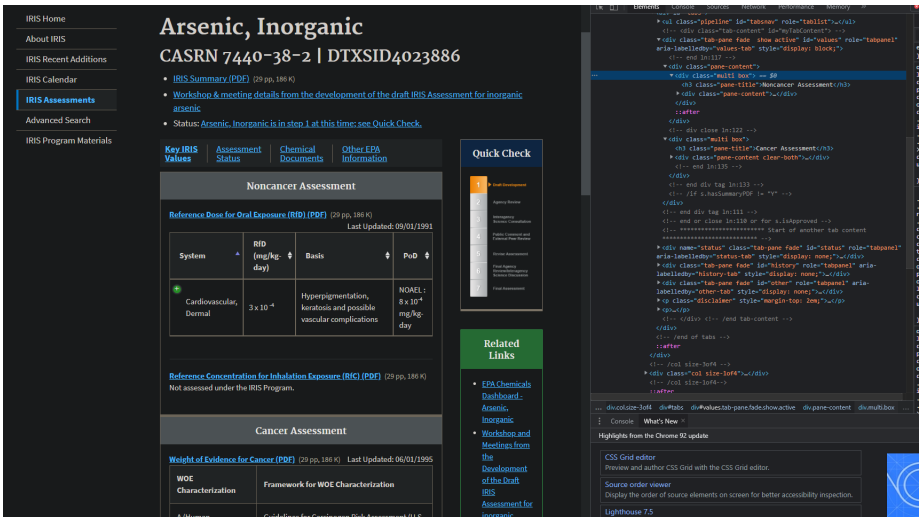

Figure 2:
Arsenic, Inorganic assessment page accessed through Arsenic, Inorganic's link with sample HTML layout.

any).

The details of how each of the above steps are carried out is not the subject of this work, but, for those who are interested, and for purposes of being thorough, the web scrape and data cleaning scripts are both available as two separate Jupyter notebooks which are available on the author's GitHub here: EPA IRIS Assessments Web Scrape. The Python script that performs the raw web scrape can be accessed directly here, and the Python script that performs the data cleaning (after running the web scrape) can be accessed directly here. Both Python scripts store the resulting data tables as CSV files (both CSV files are also on the author's GitHub).

3 Results

The final table obtained from web scraping and merging contains 693 rows with 571 unique chemical names along with 28 columns. As was mentioned earlier, repeated rows result when a single chemical has additional assessment information for the same column(s) such as multiple RfC and/or RfD values. This means that some chemical names are repeated with different column information for at least *one* column. To view and/or download the entire data table see the author's GitHub: EPA IRIS Assessments clean data table.

See Figure 3 for snapshots of the resulting tables for each web scrape performed: initial web scrape of IRIS Assessments main table (3a); noncancer assessment data (3b); cancer assessment data for WOE character-

ization, framework for WOE characterization, and basis (3c); and cancer assessments regarding oral and inhalation data (3d).

See Figure 4 for a snapshot of the table that results from performing each scrape, and then merging them all into a single table. Since the table has a total of 28 columns, it is too long to capture in a single screenshot. See Figure 4a for the first five rows and first 16 columns of the table and Figure 4b for the first five rows and last 12 columns of the table.

Lastly, see Figure 5 for the table that results after the data cleaning process (cleaning the data in the table from Figure 4). Again, the table is too long for a single screenshot. See Figure 5a for the first five rows and first 16 columns of the cleaned data table and Figure 5b for the first five rows and last 12 columns of the cleaned data table.

	CHEMICAL NAME	CASRN	LAST SIGNIFICANT REVISION*	IRIS SUMMARY	TOX REVIEW/SUPPORTING DOCUMENT	LITERATURE SCREENING REVIEW	CRITICAL EFFECT SYSTEMS	TUMOR SITE	PESTICIDE	ARCHIVE
0	Acenaphthene	83-32-9	19901101 Nov-01-1990	(PDF 7 pp, 89 K)	Not Available	No	Hepatic	None		
1	Acenaphthylene	208-96-8	19910101 Jan-01-1991	(PDF 6 pp, 82 K)	Not Available	No	None	None		
2	Acephate	30560-19-1	19890501 May-01-1989	(PDF 13 pp, 114 K)	Not Available	Yes	Nervous	Hepatic	pesticide	archive
3	Acetaldehyde	75-07-0	19911001 Oct-01-1991	(PDF 20 pp, 147 K)	Not Available	No	Nervous ...	Respiratory		
4	Acetochlor	34256-82-1	19930901 Sep-01-1993	(PDF 14 pp, 126 K)	Not Available	Yes	Hematologic ...	None	pesticide	

(a)

	CHEMICAL NAME	NONCANCER ASSESSMENT TYPE	SYSTEM (RfD)	RfD (mg/kg-day)	BASIS (RfD)	PoD (RfD)	COMPOSITE UF (RfD)	CONFIDENCE (RfD)	SYSTEM (RfC)	RfC (mg/m^3)	Basis (RfC)	PoD (RfC)	COMPOSITE UF (RfC)	CONFIDENCE (RfC)
0	Acenaphthene	Oral	Hepatic	6 x 10 -2	Hepatotoxicity	NOAEL : 1.75 x 102 mg/kg-day	3000	Low	NaN	NaN	NaN	NaN	NaN	NaN
1	Acenaphthylene	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
2	Acephate	Oral	Nervous	4 x 10 -3	Inhibition of brain ChE	LEL : 1.2 x 10-1 mg/kg-day	30	High	NaN	NaN	NaN	NaN	NaN	NaN
3	Acetaldehyde	Inhalation	NaN	NaN	NaN	NaN	NaN	NaN	Nervous; Respiratory	9 x 10 -3	Degeneration of olfactory epithelium	NOAEL (HEC): 8.7 mg/m3	1000	Low
4	Acetochlor	Oral	Nervous; Reproductive; Hepatic; Urinary; Hemat...	2 x 10 -2	Salivation; increased ALT and ornithine carbam...	NOAEL : 2 mg/kg-day	100	High	NaN	NaN	NaN	NaN	NaN	NaN

(b)

	CHEMICAL NAME	WOE CHARACTERIZATION	FRAMEWORK FOR WOE CHARACTERIZATION	WOE BASIS
0	Acenaphthene	NaN	NaN	NaN
1	Acenaphthylene	D (Not classifiable as to human carcinogenicity)	Guidelines for Carcinogen Risk Assessment (U.S...	Based on no human data and inadequate data fro...
2	Acephate	C (Possible human carcinogen)	Guidelines for Carcinogen Risk Assessment (U.S...	The classification is based on increased incid...
3	Acetaldehyde	B2 (Probable human carcinogen - based on suffi...	Guidelines for Carcinogen Risk Assessment (U.S...	Based on increased incidence of nasal tumors i...
4	Acetochlor	NaN	NaN	NaN

(c)

	CHEMICAL NAME	QUANT. EST. OF CARC. RISK FROM ORAL EXPOSURE	QUANT. EST. OF CARC. RISK FROM INHALATION EXPOSURE
0	Acenaphthene	NaN	NaN
1	Acenaphthylene	NaN	NaN
2	Acephate	Oral Slope Factor:\n 8.7\n ...	NaN
3	Acetaldehyde	NaN	Inhalation Unit Risk:\n 2.2\n ...
4	Acetochlor	NaN	NaN

(d)

Figure 3: Snapshots of the resulting data tables from each web scrape described in the Methodology section. Each data table shows the first five rows with *all* of its columns. 3a: Initial web scrape of IRIS Assessments main page; 3b: Web scrape of "Noncancer Assessments" section of each chemical assessment; 3c: Web scrape of "Cancer Assessment" section of WOE table and basis for WOE characterization; 3d: Web scrape of "Cancer Assessment" section of oral and inhalation assessment data.

	CHEMICAL NAME	CASRN	LAST SIGNIFICANT REVISION*	IRIS SUMMARY	TOX REVIEW/SUPPORTING DOCUMENT	LITERATURE SCREENING REVIEW	CRITICAL EFFECT SYSTEMS	TUMOR SITE	PESTICIDE	ARCHIVE	NONCANCER ASSESSMENT TYPE	SYSTEM (RfD)	RfD (mg/kg-day)	BASIS (RfD)	PoD (RfD)	COMPOSITE UF (RfD)
0	Acenaphthene	83-32-9	19901101 Nov-01-1990	(PDF 7 pp, 89 K)	Not Available	No	Hepatic	None			Oral	Hepatic	6 x 10 -2	Hepatotoxicity	NOAEL : 1.75 x 102 mg/kg-day	3000
1	Acenaphthene	83-32-9	19901101 Nov-01-1990	(PDF 7 pp, 89 K)	Not Available	No	Hepatic	None			Oral	Hepatic	6 x 10 -2	Hepatotoxicity	NOAEL : 1.75 x 102 mg/kg-day	3000
2	Acenaphthylene	208-96-8	19910101 Jan-01-1991	(PDF 6 pp, 82 K)	Not Available	No	None	None			NaN	NaN	NaN	NaN	NaN	NaN
3	Acephate	30560-19-1	19890501 May-01-1989	(PDF 13 pp, 114 K)	Not Available	Yes	Nervous	Hepatic	pesticide	archive	Oral	Nervous	4 x 10 -3	Inhibition of brain ChE	LEL : 1.2 x 10-1 mg/kg-day	30
4	Acetaldehyde	75-07-0	19911001 Oct-01-1991	(PDF 20 pp, 147 K)	Not Available	No	Nervous ...	Respiratory			Inhalation	NaN	NaN	NaN	NaN	NaN

(a)

CONFIDENCE (RfD)	SYSTEM (RfC)	RfC (mg/m^3)	Basis (RfC)	PoD (RfC)	COMPOSITE UF (RfC)	CONFIDENCE (RfC)	WOE CHARACTERIZATION	FRAMEWORK FOR WOE CHARACTERIZATION	WOE BASIS	QUANT. EST. OF CARC. RISK FROM ORAL EXPOSURE	QUANT. EST. OF CARC. RISK FROM INHALATION EXPOSURE
Low	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
Low	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
NaN	NaN	NaN	NaN	NaN	NaN	NaN	D (Not classifiable as to human carcinogenicity)	Guidelines for Carcinogen Risk Assessment (U.S...	Based on no human data and inadequate data fro...	NaN	NaN
High	NaN	NaN	NaN	NaN	NaN	NaN	C (Possible human carcinogen)	Guidelines for Carcinogen Risk Assessment (U.S...	The classification is based on increased incid...	Oral Slope Factor:\n 8.7\n ...	NaN
NaN	Nervous; Respiratory	9 x 10 -3	Degeneration of olfactory epithelium	NOAEL (HEC): 8.7 mg/m3	1000	Low	B2 (Probable human carcinogen - based on suffi...	Guidelines for Carcinogen Risk Assessment (U.S...	Based on increased incidence of nasal tumors i...	NaN	Inhalation Unit Risk:\n 2.2\n ...

(b)

Figure 4: Resulting table from merging each of the tables from the individual web scrapes mentioned in the Methodology section without any data cleaning (raw web scrape, merged into one table). The table spans a total of 28 columns. 4a: First five rows and first 16 columns of resulting table. 4b: First five rows and last 12 columns of resulting table.

	CHEMICAL NAME	CASRN	LAST SIGNIFICANT REVISION	IRIS SUMMARY	TOX REVIEW/SUPPORTING DOCUMENT	LITERATURE SCREENING REVIEW	CRITICAL EFFECT SYSTEMS	TUMOR SITE	PESTICIDE	ARCHIVE	NONCANCER ASSESSMENT TYPE	SYSTEM (RfD)	RfD (mg/kg-day)	BASIS (RfD)	PoD (RfD)
0	Acenaphthene	83-32-9	Nov-01-1990	(PDF 7 pp, 89 K)	Not Available	No	Hepatic	None	NaN	NaN	Oral	Hepatic	6 x 10 -2	Hepatotoxicity	NOAEL: 1.75 x 102 mg/kg-day
2	Acenaphthylene	208-96-8	Jan-01-1991	(PDF 6 pp, 82 K)	Not Available	No	None	None	NaN	NaN	NaN	NaN	NaN	NaN	NaN
3	Acephate	30560-19-1	May-01-1989	(PDF 13 pp, 114 K)	Not Available	Yes	Nervous	Hepatic	pesticide	archive	Oral	Nervous	4 x 10 -3	Inhibition of brain ChE	LEL: 1.2 x 10-1 mg/kg-day
4	Acetaldehyde	75-07-0	Oct-01-1991	(PDF 20 pp, 147 K)	Not Available	No	Nervous; Respiratory	Respiratory	NaN	NaN	Inhalation	NaN	NaN	NaN	NaN
5	Acetochlor	34256-82-1	Sep-01-1993	(PDF 14 pp, 126 K)	Not Available	Yes	Hematologic; Hepatic; Nervous; Reproductive; U...	None	pesticide	NaN	Oral	Nervous; Reproductive; Hepatic; Urinary; Hemat...	2 x 10 -2	Salivation; increased ALT and ornithine carbam...	NOAEL: 2 mg/kg-day

(a)

COMPOSITE UF (RfD)	CONFIDENCE (RfD)	SYSTEM (RfC)	RfC (mg/m^3)	BASIS (RfC)	PoD (RfC)	COMPOSITE UF (RfC)	CONFIDENCE (RfC)	WOE CHARACTERIZATION	FRAMEWORK FOR WOE CHARACTERIZATION	WOE BASIS	QUANT. EST. OF CARC. RISK FROM ORAL EXPOSURE	QUANT. EST. OF CARC. RISK FROM INHALATION EXPOSURE
3000	Low	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	D (Not classifiable as to human carcinogenicity)	Guidelines for Carcinogen Risk Assessment (U.S...	Based on no human data and inadequate data fro...	NaN	NaN
30	High	NaN	NaN	NaN	NaN	NaN	NaN	C (Possible human carcinogen)	Guidelines for Carcinogen Risk Assessment (U.S...	The classification is based on increased incid...	Oral Slope Factor: 8.7 x 10-3 per mg/kg-day\nD...	NaN
NaN	NaN	Nervous; Respiratory	9 x 10 -3	Degeneration of olfactory epithelium	NOAEL (HEC): 8.7 mg/m3	1000	Low	B2 (Probable human carcinogen - based on suffi...	Guidelines for Carcinogen Risk Assessment (U.S...	Based on increased incidence of nasal tumors i...	NaN	Inhalation Unit Risk: 2.2 x 10-6 per µg/m3\nEx...
100	High	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN

(b)

Figure 5: Resulting table after cleaning the data from the merged table from Figure 4. The table again spans a total of 28 columns. 4a: First five rows and first 16 columns of resulting table. 4b: First five rows and last 12 columns of resulting table.

4 Discussion

The main item to discuss is data verification. The immediate question that comes to mind is: is the final data table obtained from the web scrape and merge correct?

To answer this question, we first note that the IRIS Assessments chemical database consists of 571 unique chemicals which can be quickly verified using the numbering at the left of the table on the IRIS Assessments webpage [3]. Checking the number of *unique* chemicals in the final resulting data table saved to the CSV also contains 571 *unique* chemicals. Therefore, it is reasonable to assume that each chemical from the original source appears at least one time. Furthermore, checking several rows of the data table with several chemical assessments from the original source have matching values. In particular, there are matching values for the first five rows of the data table; Arsenic, Inorganic also checks out; as well as Xylenes and Zinc and Compounds, both of which contain multiple rows due to multiple, differing assessment information.

5 Conclusion

Although the arguments regarding data correctness in the Discussions section does not provide a complete and thorough verification the data scraped and merged, it is reasonable to conclude that the final data table obtained contains all the necessary information from the IRIS Assessments database. Of course, for full-proof verification one would need to go through each and every chemical assessment and verify the data matches that which was collected. But naturally, this was precisely the process we were trying to avoid in the first place.

6 References

[1] U.S. Environmental Protection Agency. Basic information about the integrated risk information system. https://www.epa.gov/iris/basic-information-about-integrated-risk-information-system. Accessed: 2021-08-16.

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