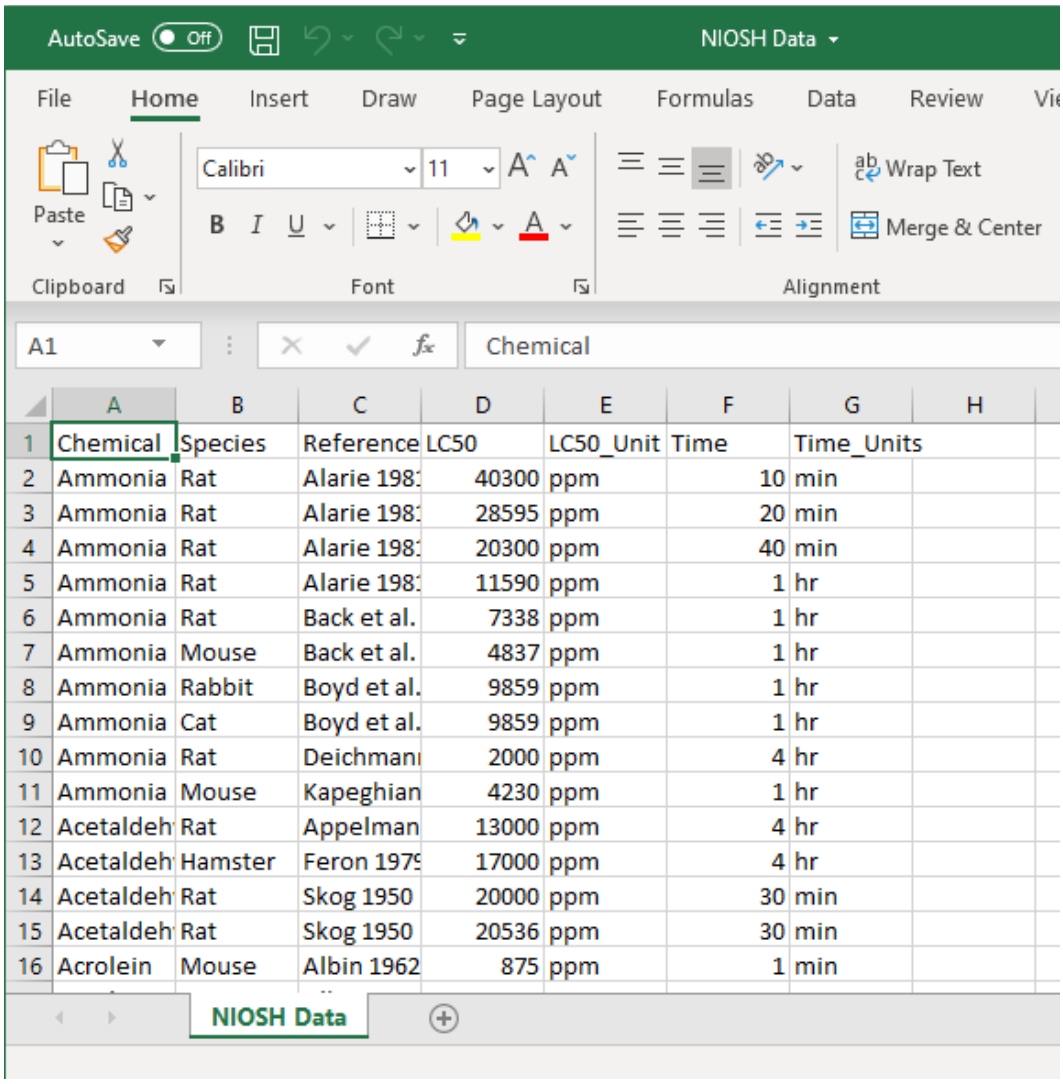
Worked Example - NIOSH Shiny App

For this demo walk through, we will give a tour of the app with screenshots in a step-by-step fashion to demonstrate of usage of the Shiny app, using an available .csv file containing empirical data from 31 chemicals.

Dataset

Please pay special attention to the format of the variables and make sure you input data, e.g. unit in the same way, and do not include extra space.



	A	B	C	D	E	F	G	H
1	Chemical	Species	Reference	LC50	LC50_Unit	Time	Time_Units	
2	Ammonia	Rat	Alarie 198	40300	ppm	10	min	
3	Ammonia	Rat	Alarie 198	28595	ppm	20	min	
4	Ammonia	Rat	Alarie 198	20300	ppm	40	min	
5	Ammonia	Rat	Alarie 198	11590	ppm	1	hr	
6	Ammonia	Rat	Back et al.	7338	ppm	1	hr	
7	Ammonia	Mouse	Back et al.	4837	ppm	1	hr	
8	Ammonia	Rabbit	Boyd et al.	9859	ppm	1	hr	
9	Ammonia	Cat	Boyd et al.	9859	ppm	1	hr	
10	Ammonia	Rat	Deichmani	2000	ppm	4	hr	
11	Ammonia	Mouse	Kapeghian	4230	ppm	1	hr	
12	Acetaldeh	Rat	Appelman	13000	ppm	4	hr	
13	Acetaldeh	Hamster	Feron 197	17000	ppm	4	hr	
14	Acetaldeh	Rat	Skog 1950	20000	ppm	30	min	
15	Acetaldeh	Rat	Skog 1950	20536	ppm	30	min	
16	Acrolein	Mouse	Albin 1962	875	ppm	1	min	

NIOSH Data

1. Home Tab

Before using the app, please carefully read the instructions listed in the Home Tab, as shown in the Figure 1. below.

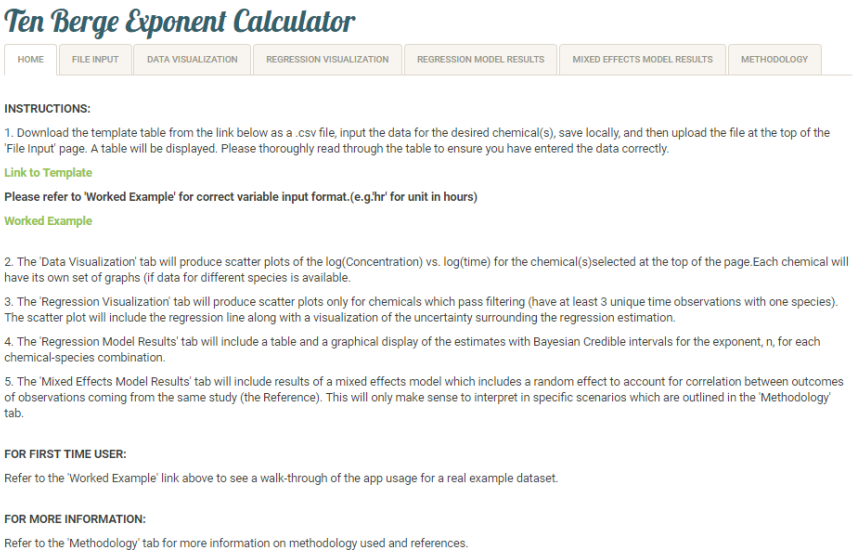


Figure 1. Home Tab

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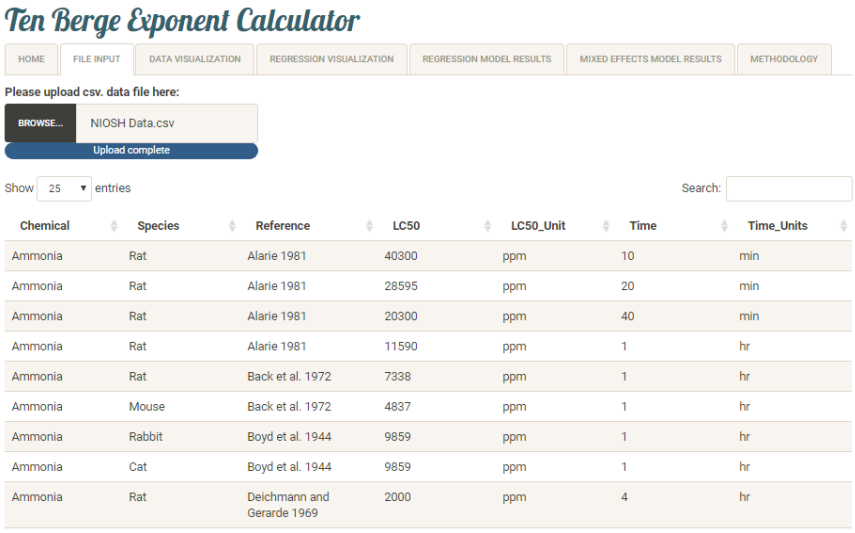
2. File Input Tab

Once the .csv file containing the raw data is ready, please click the “File Input” tab and “browse” to locate the .csv file and upload it; once uploaded, the raw data will be displayed as shown in Figure 2.



Chemical	Species	Reference	LC50	LC50_Unit	Time	Time_Units
Ammonia	Rat	Alarie 1981	40300	ppm	10	min
Ammonia	Rat	Alarie 1981	28595	ppm	20	min
Ammonia	Rat	Alarie 1981	20300	ppm	40	min
Ammonia	Rat	Alarie 1981	11590	ppm	1	hr
Ammonia	Rat	Back et al. 1972	7338	ppm	1	hr
Ammonia	Mouse	Back et al. 1972	4837	ppm	1	hr
Ammonia	Rabbit	Boyd et al. 1944	9859	ppm	1	hr
Ammonia	Cat	Boyd et al. 1944	9859	ppm	1	hr
Ammonia	Rat	Deichmann and Gerarde 1969	2000	ppm	4	hr

Figure 2. File Input Tab

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3. Data Visualization Tab

In this tab, click and select the chemicals of interest, if data for multiple species are available, multiple plots will be displayed in side-by-side scatterplots of log-transformed LC_{50} and exposure time, as shown in Figure 3. below. Points are color-coded by difference source of references. Selected chemicals can be removed from the visualization by simply removing them from the selection window.

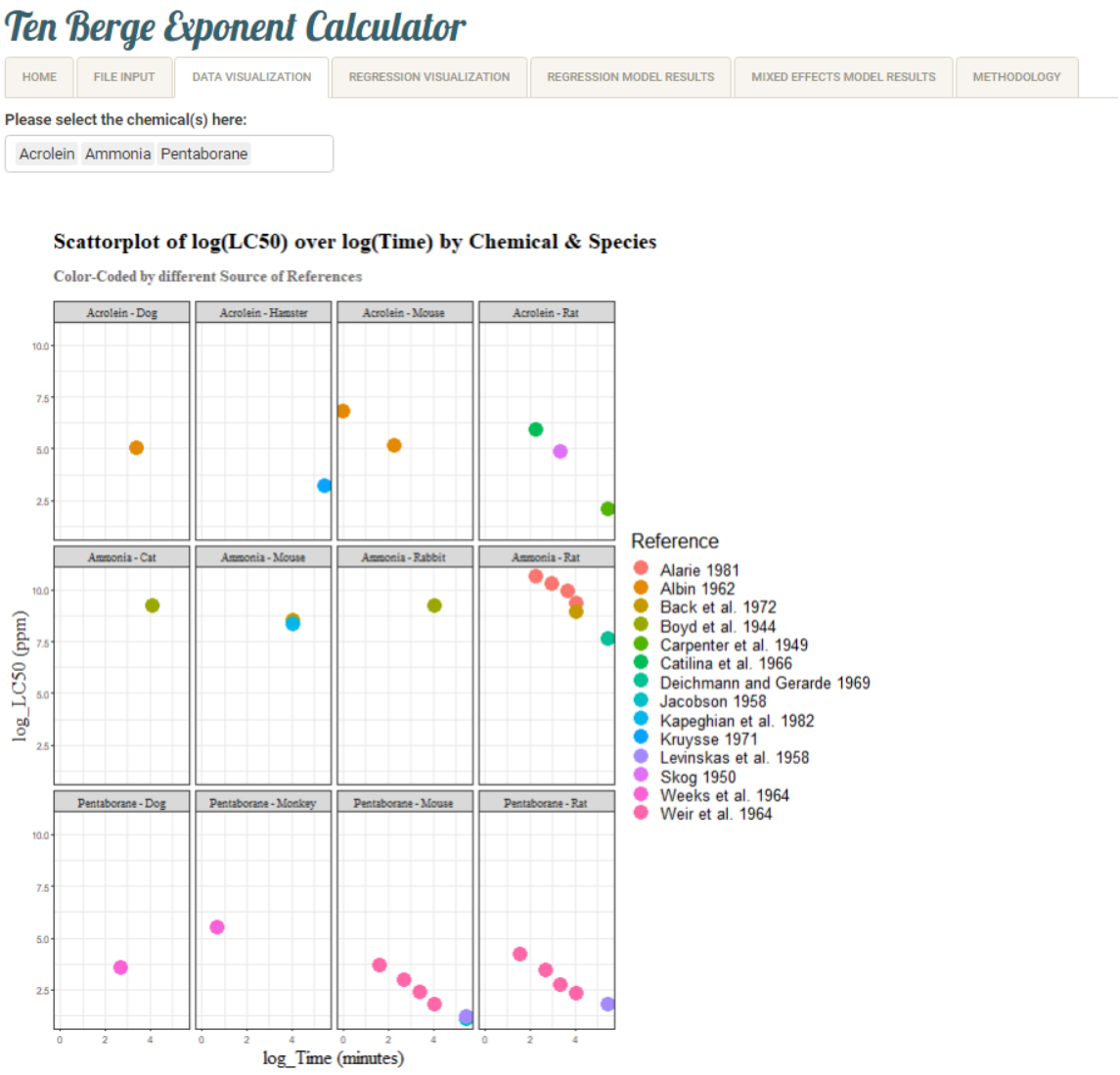


Figure 3. Data Visualization Tab

4. Regression Visualization Tab

Figure 4. displays the scatterplot of filtered log transformed LC_{50} and their according exposure time points, along with regression lines and additional standard error bands. In this demo, three chemicals are chosen; note that for "Pentaborane", enough data for two species (Mouse and Rat) are available, so two regression plots are drawn separately. In this plot, sources of studies are also color-coded.

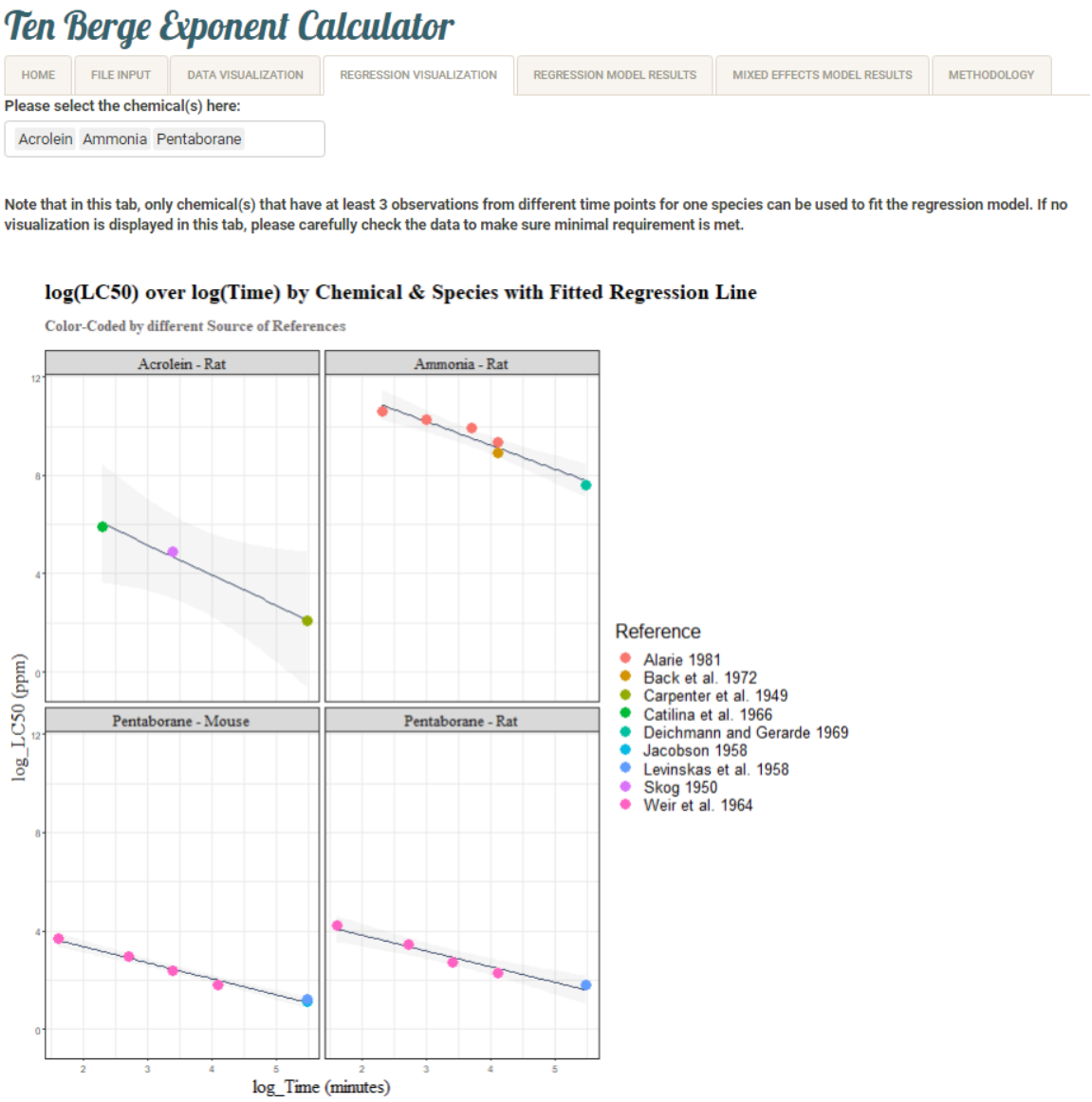
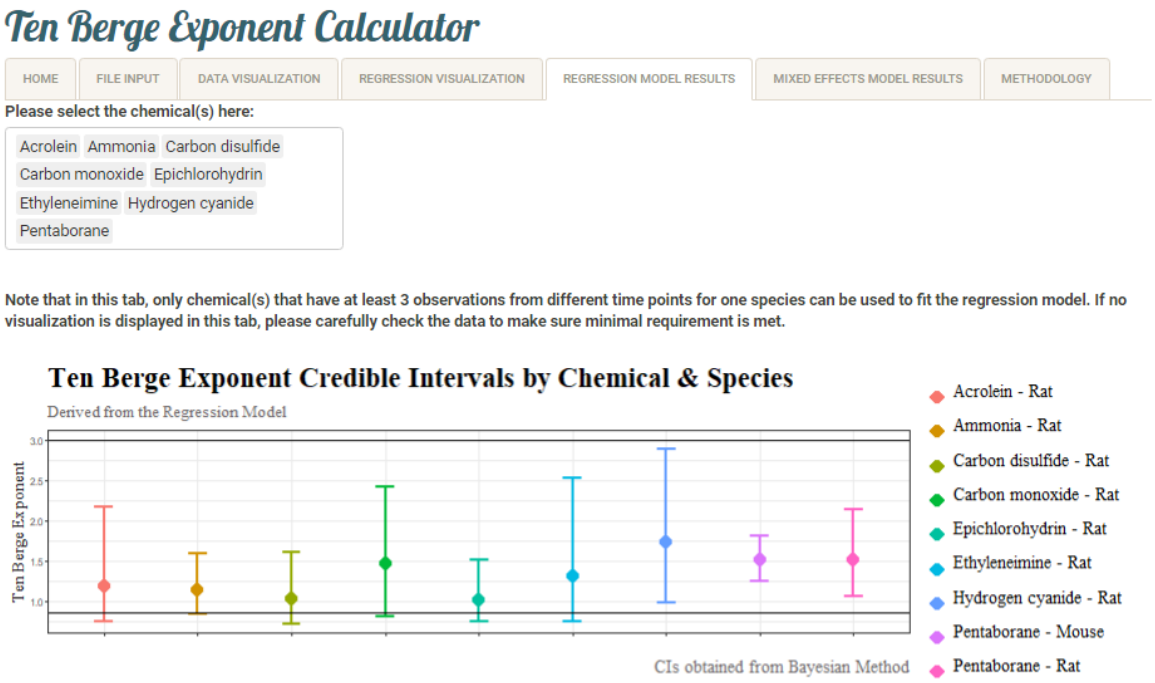


Figure 4. Regression Visualization Tab

5. Regression Model Results Tab

In Figure 5., a visualization of the ten Berge exponents is provided, in which the ten Berge exponent number n and its credible interval is displayed in vertical bars, with an additional indication that allows for identification of ten Berge exponents that fall out of the normal range (0.85 to 3.5). The lower section of the tab has the resulting table for the chemical-specific ten Berge n, as well as the lower and higher bounds of the estimated Credible Intervals for different chemicals using the Bayesian method.



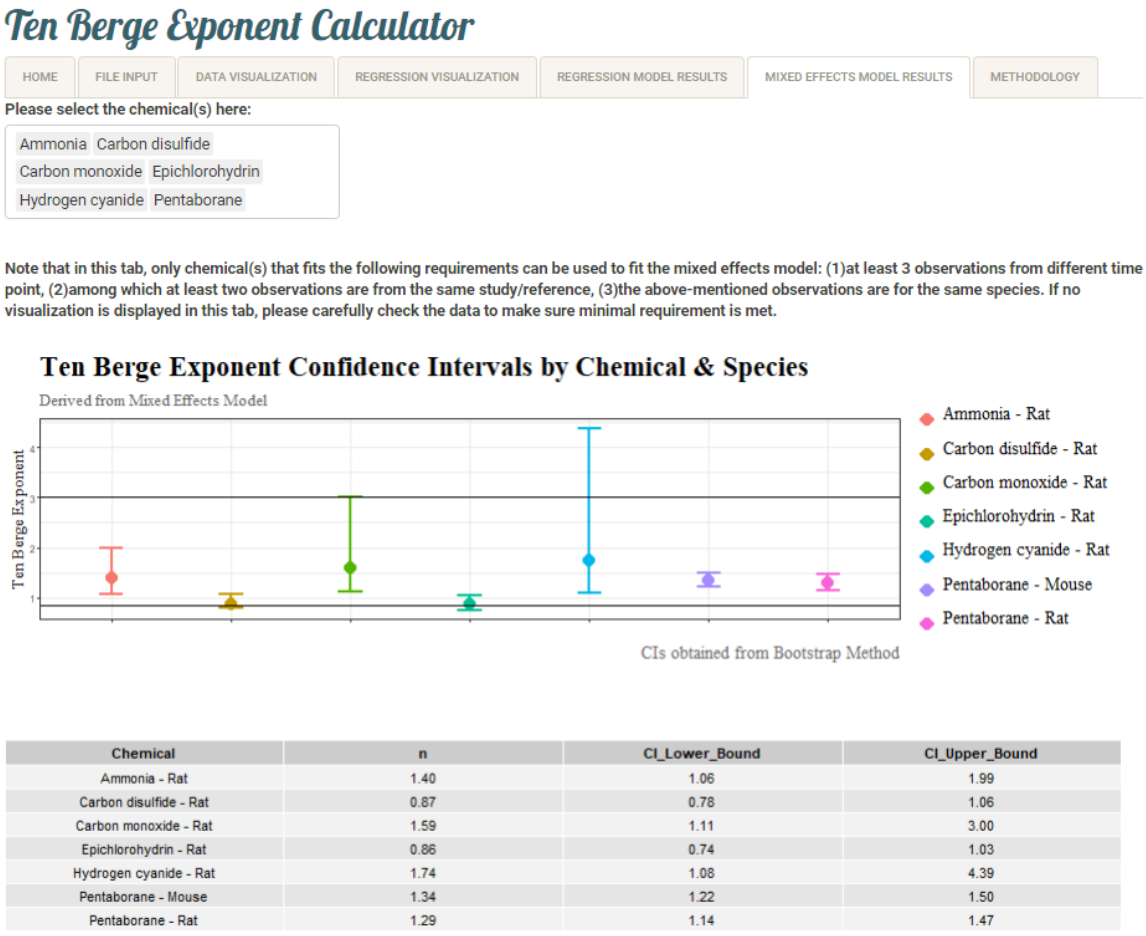
Chemical	n	CI_Lower_Bound	CI_Upper_Bound
Acrolein - Rat	1.18	0.74	2.17
Ammonia - Rat	1.13	0.83	1.58
Carbon disulfide - Rat	1.03	0.71	1.61
Carbon monoxide - Rat	1.46	0.81	2.41
Epichlorohydrin - Rat	1.01	0.75	1.51
Ethyleneimine - Rat	1.31	0.75	2.53
Hydrogen cyanide - Rat	1.73	0.98	2.88
Pentaborane - Mouse	1.51	1.24	1.80
Pentaborane - Rat	1.51	1.06	2.13

Figure 5. Regression Model Results Tab

6. Mixed Effects Model Results Tab

Similar to the previous tab for regression results, the Mixed Effects Model Results tab displays similar information, but the calculation scheme behind the results is from mixed effects models. Note that this method has a different data filtering criterion; therefore, the chemicals available for selecting in this tab may be different from those in the Regression Results Tab.

In this tab, the bootstrapping method described in the report of the Mixed Effects Model research group are used to obtain the confidence intervals.



Chemical	n	CI_Lower_Bound	CI_Upper_Bound
Ammonia - Rat	1.40	1.06	1.99
Carbon disulfide - Rat	0.87	0.78	1.06
Carbon monoxide - Rat	1.59	1.11	3.00
Epichlorohydrin - Rat	0.86	0.74	1.03
Hydrogen cyanide - Rat	1.74	1.08	4.39
Pentaborane - Mouse	1.34	1.22	1.50
Pentaborane - Rat	1.29	1.14	1.47

Figure 6. Mixed Effects Model Results Tab

The End.