Creating a Database of Amphibian Dermal Exposure Data

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Introduction

The purpose of this script is to combine the data sets from Van Meter et al. (2014, 2015, 2016, 2018, 2019), Glinski et al. (2018a, b, 2019, 2020), and Henson-Ramsey (2008) to create a collated database of amphibian dermal exposure data.

Manuscript	Data Set (Original Source Link)	Data Set (Repo Link)	Additional Data Sets
Van Meter et al. 2014	good data.csv	vm2014 data.csv	
Van Meter et al. 2015	good data.csv	vm2014 data.csv	
Van Meter et al. 2016	RDATA.csv	$vm2016$ _data.csv	
Van Meter et al. 2018	rvm2018.csv	rvm2018.csv	
Van Meter et al. 2019	rvm2019.csv	rvm2019.csv	
Glinski et al. 2018a	dehydration3.csv	dag2016_data_dehydration	1.CSV
(dehydration)		0 = = v	
Glinski et al. 2018b	exposure experiment.csv	dag2016 data metabolites	4merge.csv
(metabolites)		0	_ 0
Glinski et al. 2019	exposure mixtures3.csv	dag2018 data biomarkers.	csviomarker.csv
(biomarkers)	• —	0 = =	(dag biomarker2.csv)
Glinski et al. 2020	Water_soil.csv	dag2019 dermal routes.cs	v Dermal_routes_weights.csv
(dermal routes)	<u> </u>		(weights)
Henson-Ramsey 2008	HensonRamseyetal2008 data	a.phdf2008 data.csv	,
v	_	-	

Computational environment

This repository can be found at: https://github.com/puruckertom/amphib_dermal_collation

If you are on a Mac and get xquartz complaints (knitr), install from: https://www.xquartz.org/

Data from Relevant Studies

Henson-Ramsey 2008

Henson-Ramsey 2008 tested the biological impact of exposure to malathion for tiger salamanders ($Ambystoma\ tigrinum$). Tiger salamanders were exposed to contaminated soils with 50 ug/cm² or 100 ug/cm² malathion and through ingestion of an earthworm exposed to contaminated soils with 200 ug/cm² malathion. For each exposure, the malathion application rate was sprayed onto the approximately 1200g of soil in the 1060cm² polyethylene cages.

Tissue concentrations were assessed for five treatment groups: unexposed, exposed to 50 ug/cm² contaminated soil for 1 day, exposed to 50 ug/cm² for 2 days, exposed to 50 ug/cm² contaminated soil for 2 days and fed a contaminated worm on the first exposure day, and exposed to 100 ug/cm² contaminated soil for 2 days and fed a contaminated worm on the first exposure day.

Data Set Dimensions, Column Names, and Summary:

```
## [1]
       9 12
##
    [1] "chemical"
                            "species"
                                               "tissue_conc_ugg" "sample_id"
##
    [5] "body_weight_g"
                            "formulation"
                                               "soil_type"
                                                                   "application"
    [9] "app_rate_g_cm2"
##
                            "exp duration"
                                               "soil conc ugg"
                                                                   "source"
##
      chemical
                           species
                                             tissue_conc_ugg
                                                               sample_id
                                                     :0.050
                                                              Length:9
##
    Length:9
                        Length:9
    Class : character
                                             1st Qu.:0.350
                                                              Class : character
##
                        Class : character
##
    Mode
          :character
                        Mode
                              :character
                                             Median :1.420
                                                              Mode
                                                                     :character
##
                                                     :1.186
                                             Mean
##
                                             3rd Qu.:1.470
##
                                             Max.
                                                     :3.730
##
    body_weight_g
                     formulation
                                     soil_type
                                                     application
##
           :20.89
                     Mode:logical
                                     Mode:logical
                                                     Length:9
                                                      Class : character
##
    1st Qu.:44.15
                     NA's:9
                                     NA's:9
##
    Median :46.26
                                                      Mode
                                                            :character
##
    Mean
           :43.73
##
    3rd Qu.:48.93
##
            :50.92
    Max.
                      exp_duration soil_conc_ugg
##
    app_rate_g_cm2
                                                        source
##
            :5e-05
                     Min.
                             :24
                                    Mode:logical
                                                    Length:9
    Min.
                                    NA's:9
##
    1st Qu.:5e-05
                     1st Qu.:24
                                                    Class : character
##
    Median:5e-05
                     Median:48
                                                    Mode
                                                           :character
##
    Mean
            :5e-05
                     Mean
                             :40
    3rd Qu.:5e-05
##
                     3rd Qu.:48
##
    Max.
            :5e-05
                     Max.
                             :48
```

Van Meter et al. 2014 and Van Meter et al. 2015

Van Meter et al. 2014 performed exposures for 5 pesticide active ingredients (imidacloprid, pendimethalin, atrazine, fipronil, tridimefon) and 7 species (Southern leopard frog (*Lithobates sphenocephala*), Fowler's toad (*Anaxyrus fowleri*), gray treefrog (*Hyla versicolor*), Northern cricket frog (*Acris crepitans*), Eastern narrowmouth toad (*Gastrophryne carolinensis*), barking treefrog (*Hyla gratiosa*), and green treefrog (*Hyla cinerea*)). Whole body tissue concentrations were measured after an 8 hour exposure period to contaminated soil. Pesticides were applied at the maximum legally allowable application rates scaled down to the area of a 10-gallon aquarium (1225 cm²).

Van Meter et al. 2015 contrasted two pesticide exposure scenarios: direct exposure through aerial overspray and indirect exposure through soil. These scenarios tested the same 5 pesticide active ingredients and two of the species (barking treefrog (*Hyla gratiosa*) and green treefrog (*Hyla cinerea*)). Pesticides were applied at the maxium legally allowable application rates scaled down to the size of a 10-gallon aquarium, with the exception of pedimethalin which was applied at 30% of the permitted application rate. This was due to pedimethalin's insolubility in the limited solvent and the water volumes used in this study.

For our purposes, the Van Meter et al. 2015 essentially adds the aerial overspray exposures to the Van Meter et al. 2014 data set.

Note: this file does include metabolites into the total for the parents

Data Set Dimensions, Column Names, and Summary:

```
## [1] 474 23
```

```
[1] "Species"
                        "Sample"
                                        "Chemical"
                                                         "Instrument"
##
##
   [5] "good"
                        "Application"
                                        "app_rate_g_cm2"
                                                         "TissueConc"
##
   [9] "SoilConc"
                        "logKow"
                                        "BCF"
                                                         "bodyweight"
## [13] "initialweight"
                        "Solat20C_mgL"
                                        "Solat20C_gL"
                                                         "molmass gmol"
## [17] "Density_gcm3"
                        "AppFactor"
                                        "SA_cm2"
                                                         "VapPrs_mPa"
## [21] "Koc gmL"
                        "HalfLife day"
                                        "HabFac"
##
     Species
                         Sample
                                          Chemical
                                                           Instrument
   Length: 474
                      Length:474
                                        Length: 474
                                                           Length: 474
##
##
   Class :character
                      Class : character
                                        Class : character
                                                           Class : character
                     Mode :character
                                        Mode : character
                                                          Mode :character
   Mode :character
##
##
##
##
##
        good
               Application
                                 app_rate_g_cm2
                                                   TissueConc
   Min. :1
               Length: 474
                                 Min. :0e+00
                                                 Min. : 0.007484
##
   1st Qu.:1
##
               Class : character
                                 1st Qu.:0e+00
                                                 1st Qu.: 0.246753
##
   Median :1
               Mode :character
                                 Median :0e+00
                                                 Median: 0.575811
   Mean :1
                                 Mean :1e-05
                                                 Mean : 1.908242
   3rd Qu.:1
                                 3rd Qu.:2e-05
                                                 3rd Qu.: 1.743142
##
##
   Max. :1
                                 Max.
                                        :2e-05
                                                 Max. :23.441298
##
                                 NA's
                                        :151
##
      SoilConc
                         logKow
                                          BCF
                                                         bodyweight
   Min. : 0.00625
                      Min. :0.570
                                     Min. : 0.0018
                                                       Min. :0.5004
##
   1st Qu.: 0.20866
                      1st Qu.:2.500
                                     1st Qu.: 0.0755
                                                       1st Qu.:1.3162
##
   Median : 3.49248
                      Median :3.110
                                     Median : 0.2069
                                                       Median :1.8550
   Mean : 7.22468
                      Mean :3.142
                                     Mean : 11.3804
                                                       Mean :1.8658
   3rd Qu.:10.06719
                      3rd Qu.:4.000
                                     3rd Qu.: 1.0828
                                                       3rd Qu.:2.3489
##
##
   Max.
         :81.71115
                      Max. :5.180
                                     Max. :396.8461
                                                       Max. :3.9931
##
                     Solat20C_mgL
##
   initialweight
                                     Solat20C_gL
                                                       molmass_gmol
         :0.5004
                                                      Min. :215.7
##
   Min.
                    Min. : 0.30
                                    Min. :0.00030
##
   1st Qu.:1.6614
                    1st Qu.: 3.78
                                    1st Qu.:0.00378
                                                      1st Qu.:215.7
   Median :2.1766
                    Median : 30.00
                                    Median :0.03000
                                                      Median :291.7
   Mean :2.2307
                    Mean :123.20
                                    Mean :0.12320
                                                      Mean :299.5
##
   3rd Qu.:2.7601
                    3rd Qu.:260.00
                                    3rd Qu.:0.26000
                                                      3rd Qu.:291.7
##
##
   Max. :5.5480
                    Max. :510.00
                                    Max. :0.51000
                                                      Max. :437.1
##
##
    Density_gcm3
                    AppFactor
                                        SA_cm2
                                                       VapPrs_mPa
                                    Min. : 0.7915
##
   Min. :1.170
                   Min. : 850
                                                      Min. :0.00020
   1st Qu.:1.187
                   1st Qu.: 47011
                                    1st Qu.: 1.5393
                                                      1st Qu.:0.00037
   Median :1.220
                   Median: 143055
                                    Median: 1.7866
                                                      Median :0.02000
   Mean :1.288
                   Mean : 291904
                                    Mean : 3.0232
                                                      Mean :0.34774
##
##
   3rd Qu.:1.480
                   3rd Qu.: 348598
                                    3rd Qu.: 2.0882
                                                      3rd Qu.:0.04000
##
   Max. :1.543
                   Max. :4490329
                                    Max. :23.3326
                                                      Max.
                                                            :4.00000
##
                   NA's
                         :151
      Koc\_gmL
                                       HabFac
##
                    HalfLife_day
##
   Min. : 122
                   Min. : 26.00
                                    Length: 474
                                    Class : character
##
   1st Qu.: 122
                    1st Qu.: 26.00
##
   Median :
              520
                    Median : 80.00
                                    Mode : character
   Mean : 20406
                    Mean : 70.85
##
##
   3rd Qu.:
              825
                    3rd Qu.: 84.00
   Max. :243000
                    Max. :125.00
##
```

##

Van Meter et al. 2016

Van Meter et al. 2016 considered bioconcentration of 5 current-use pesticides (imidacloprid, atrazine, triadimefon, fipronil, and pedimethalin) in American toads ($Bufo\ americanus$) across soil types. Toads were exposed to one of two soil types with significantly different organic matter content ($14.1\% = high\ organic\ matter$, $3.1\% = low\ organic\ matter$). Whole body tissue concentrations were measured after an 8 hour exposure period to contaminated soil. Pesticides were applied at the maximum legally allowable application rates scaled down to the area of six $0.94\ L$ Pyrex glass bowls each with a 15 cm diameter.

Note: this file does include metabolites into the total for the parents

Data Set Dimensions, Column Names, and Summary:

```
## [1] 264
            11
##
    [1]
        "Day"
                        "Row"
                                       "Column"
                                                       "Pesticide"
                                                                      "SoilType"
##
    [6]
        "BodyBurden"
                        "Soil"
                                       "Weight"
                                                       "Total"
                                                                      "Formulation"
##
   [11] "Parent"
##
                                          Column
                                                             Pesticide
                           Row
         Day
                                       Length: 264
##
    Min.
            :0.000
                     Min.
                             :1.000
                                                            Length: 264
##
    1st Qu.:2.000
                     1st Qu.:2.000
                                       Class : character
                                                            Class : character
##
    Median :2.000
                     Median :4.000
                                       Mode
                                             :character
                                                            Mode
                                                                  :character
##
    Mean
            :2.326
                     Mean
                              :4.023
##
    3rd Qu.:3.000
                     3rd Qu.:6.000
            :3.000
                             :7.000
##
    Max.
                     Max.
##
      SoilType
                           BodyBurden
                                                  Soil
                                                                      Weight
##
    Length:264
                                 :-0.0378
                                             Min.
                                                    :-0.10518
                                                                 Min.
                                                                         : 6.964
##
                         1st Qu.: 0.0486
                                             1st Qu.: 0.02086
                                                                 1st Qu.:10.524
    Class : character
##
    Mode : character
                         Median: 0.1099
                                             Median: 1.49572
                                                                 Median :11.740
##
                                 : 0.4955
                                                    : 6.02720
                                                                         :12.044
                        Mean
                                             Mean
                                                                 Mean
##
                         3rd Qu.: 0.3650
                                             3rd Qu.: 8.64289
                                                                  3rd Qu.:13.440
##
                        Max.
                                 : 6.8744
                                             Max.
                                                    :39.57404
                                                                 Max.
                                                                          :23.340
##
        Total
                        Formulation
                                              Parent
##
            :0.0000
    Min.
                      Min.
                              :0.0000
                                         Min.
                                                 :0.0000
##
    1st Qu.:0.0000
                       1st Qu.:0.0000
                                         1st Qu.:0.0000
##
    Median :0.0000
                      Median :0.0000
                                         Median :1.0000
##
    Mean
            :0.3636
                      Mean
                              :0.4091
                                         Mean
                                                 :0.5909
                                         3rd Qu.:1.0000
##
    3rd Qu.:1.0000
                       3rd Qu.:1.0000
##
    Max.
            :1.0000
                      Max.
                               :1.0000
                                         Max.
                                                 :1.0000
```

Van Meter et al. 2018 (Multiple Pesticides Study)

Van Meter et al. 2018 evaluated risks to amphibians after exposure to a single pesticide and pesticide mixtures. The five pesticides studied were three herbicides (atrazine, metolachlor, and 2,4-D), one insecticide (malathion), and one fungicide (propiconazole). Juvenile green frogs (*Lithobates clamitans*) were exposed to contaminated soils for 8 hours and metabolic analysis of amphibian livers was conducted to measure the effects. Pesticides were applied at the maximum legally allowable application rates individually and in mixtures of two or three pesticides within an herbicide or mixed pesticide group, scaled down to the area of six 0.94 L Pyrex glass bowls each with a 15 cm diameter.

Two data sets were generated from this study, one containing data for exposure to herbicides (single and mixed) and the other containing data for exposure to mixed pesticide treatments (herbicides, insecticide, fungicide).

Herbicide Data Set Data Set Dimensions, Column Names, and Summary:

```
## [1] 126 12

## [1] "Group" "ATZ" "D" "ME" "AppRate" "Weight"

## [7] "SA" "Media" "Pesticide" "Conc" "soil" "sample_id"
```

```
##
                                                   D
                                                                      ME
                              ATZ
       Group
##
    Length: 126
                         Min.
                                :-1.0000
                                            Min.
                                                    :-1.0000
                                                                Min.
                                                                        :-1.0000
##
    Class : character
                         1st Qu.:-1.0000
                                            1st Qu.:-1.0000
                                                                1st Qu.:-1.0000
                        Median: 1.0000
                                            Median: 1.0000
                                                                Median: 1.0000
##
    Mode :character
                                                    : 0.1429
##
                        Mean
                                : 0.1429
                                            Mean
                                                                Mean
                                                                        : 0.1429
                         3rd Qu.: 1.0000
                                            3rd Qu.: 1.0000
##
                                                                3rd Qu.: 1.0000
                                : 1.0000
##
                                                    : 1.0000
                                                                        : 1.0000
                         Max.
                                            Max.
                                                                Max.
       AppRate
##
                          Weight
                                              SA
                                                            Media
                             :0.9634
                                                :1.107
                                                         Length: 126
##
    Min.
            :14.30
                     Min.
                                        Min.
##
    1st Qu.:23.60
                     1st Qu.:1.6929
                                        1st Qu.:1.534
                                                         Class : character
    Median :37.90
                     Median :2.0637
                                        Median :1.720
                                                         Mode
##
                                                                :character
##
            :39.31
                             :2.0892
                                                :1.715
    Mean
                     Mean
                                        Mean
##
    3rd Qu.:54.50
                     3rd Qu.:2.4927
                                        3rd Qu.:1.919
##
    Max.
            :68.80
                     Max.
                             :3.6843
                                        Max.
                                                :2.406
##
     Pesticide
                              Conc
                                                   soil
                                                                  sample_id
    Length: 126
                                : 0.00000
                                                     : 0.0000
                                                                 Length: 126
##
                        Min.
                                             Min.
##
    Class : character
                         1st Qu.: 0.00000
                                             1st Qu.: 0.0000
                                                                 Class : character
                        Median: 0.06614
                                             Median: 0.3629
                                                                 Mode :character
##
    Mode : character
##
                                : 5.87233
                                                     :10.7665
                        Mean
                                             Mean
##
                         3rd Qu.: 4.96882
                                             3rd Qu.:24.5367
##
                                :72.62672
                                                     :76.0357
                         Max.
                                             Max.
```

Mixed Pesticide Data Set Data Set Dimensions, Column Names, and Summary:

[1] 72 11

```
"PROP"
##
    [1] "Group"
                      "ATZ"
                                   "MA"
                                                             "Pesticide" "Media"
    [7] "Conc"
                      "Weight"
                                   "SA"
                                                "soil"
##
                                                             "sample_id"
##
                                                                     PROP
       Group
                              ATZ
                                                   MΑ
##
    Length:72
                                :-1.0000
                                                    :-1.0000
                                                                        :-1.0000
                                                                Min.
                         1st Qu.:-1.0000
                                            1st Qu.:-1.0000
                                                                1st Qu.:-1.0000
##
    Class : character
##
    Mode :character
                         Median : 1.0000
                                            Median : 1.0000
                                                                Median: 1.0000
##
                         Mean
                                : 0.3333
                                            Mean
                                                    : 0.3333
                                                                Mean
                                                                        : 0.3333
##
                         3rd Qu.: 1.0000
                                            3rd Qu.: 1.0000
                                                                3rd Qu.: 1.0000
##
                                : 1.0000
                                                    : 1.0000
                                                                        : 1.0000
                         Max.
                                            Max.
                                                                Max.
##
     Pesticide
                            Media
                                                   Conc
                                                                      Weight
##
    Length:72
                         Length:72
                                                     : 0.00054
                                                                          :1.188
                                             Min.
                                                                  Min.
##
    Class : character
                         Class : character
                                             1st Qu.: 0.32504
                                                                  1st Qu.:1.786
##
    Mode
          :character
                               :character
                                             Median : 1.33986
                                                                  Median :2.014
                         Mode
                                                     : 6.38788
##
                                             Mean
                                                                  Mean
                                                                          :2.203
##
                                             3rd Qu.: 6.65664
                                                                  3rd Qu.:2.455
##
                                             Max.
                                                     :71.52122
                                                                  Max.
                                                                          :4.014
##
          SA
                           soil
                                          sample id
##
    Min.
            :1.447
                     Min.
                             : 0.7354
                                         Length:72
    1st Qu.:1.833
                     1st Qu.: 2.2633
##
                                         Class : character
##
    Median :1.965
                     Median:10.5771
                                         Mode : character
##
    Mean
            :2.047
                     Mean
                             : 9.3745
                     3rd Qu.:13.9342
##
    3rd Qu.:2.203
##
    Max.
            :2.929
                     Max.
                             :25.7013
```

The herbicide and mixed pesticide data sets were cleaned prior and joined into a merged data set (referred to as Van Meter et al. 2018 Multiple Pesticides Study in subsequent steps). The single and mixed-pesticide treatments that were retained in the merged data set include atrazine, propiconazole, 2,4-D, malathion, and metolachlor. Original columns from the herbicide and mixed pesticide data sets were altered for standardization. These standardized columns will be used in future data cleaning steps in order to merge all data sets.

Merged Data Set Data Set Dimensions, Column Names, and Summary:

```
"body_weight_g"
                                               "chemical"
                                                                  "tissue_conc_ugg"
##
    [1] "app_rate_g_cm2"
    [5] "sample_id"
                                               "application"
                            "source"
                                                                  "exp_duration"
    [9] "formulation"
                                               "soil_type"
                                                                  "species"
##
                            "soil_conc_ugg"
##
    app_rate_g_cm2
                         body_weight_g
                                             chemical
                                                                tissue_conc_ugg
           :2.600e-06
                                 :0.9634
                                           Length: 137
                                                                      : 0.00054
##
    Min.
                         Min.
                                                               Min.
##
    1st Qu.:1.430e-05
                         1st Qu.:1.7623
                                           Class : character
                                                               1st Qu.: 0.27576
##
    Median :2.360e-05
                         Median :2.0136
                                           Mode :character
                                                               Median: 1.41009
##
    Mean
           :2.004e-05
                         Mean
                                 :2.1086
                                                               Mean
                                                                       : 7.36154
    3rd Qu.:2.590e-05
                                                                3rd Qu.: 9.95084
##
                         3rd Qu.:2.3395
##
    Max.
           :3.090e-05
                         Max.
                                 :4.0141
                                                               Max.
                                                                       :72.62672
##
     sample_id
                           source
                                            application
                                                                  exp_duration
   Length: 137
                                            Length: 137
                                                                        :8
##
                        Length: 137
                                                                 Min.
    Class : character
                        Class : character
                                            Class : character
                                                                 1st Qu.:8
    Mode :character
                        Mode :character
                                                                 Median:8
##
                                            Mode :character
##
                                                                 Mean
                                                                        :8
##
                                                                 3rd Qu.:8
##
                                                                 Max.
                                                                        :8
##
     formulation soil_conc_ugg
                                     soil_type
                                                       species
           :0
                  Min.
                         : 0.1639
                                                     Length: 137
##
    Min.
                                     Mode:logical
##
    1st Qu.:0
                  1st Qu.: 1.7763
                                     NA's:137
                                                     Class : character
                  Median :12.5989
##
    Median :0
                                                     Mode
                                                          :character
                         :14.1337
##
    Mean
           :0
                  Mean
##
    3rd Qu.:0
                  3rd Qu.:23.3872
                         :76.0357
##
    Max.
           :0
                  Max.
```

Van Meter et al. 2019

[1] 96 12

[1] 137

Van Meter et al. 2019 looked at joint exposure of two common herbicides (atrazine, alachlor) and a fertilizer (urea) while quantifying juvenile corticosterone stress levels, acetylcholinesterase (AChE) activity, and pesticide bioaccumulation in Southern leopard frogs. Single agrochemical or tank mixtures were applied to terrestrial microcosms, and then individual juveniles were added to microcosms for an 8-h exposure.

Data Set Dimensions, Column Names, and Summary:

```
"application"
                                               "body_weight_g"
                                                                  "chemical"
##
    [1] "app_rate_g_cm2"
    [5] "exp_duration"
                            "formulation"
                                               "sample_id"
                                                                  "soil_conc_ugg"
##
                            "source"
                                               "species"
##
    [9] "soil_type"
                                                                  "tissue_conc_ugg"
##
    app_rate_g_cm2
                        application
                                            body_weight_g
                                                                 chemical
           :2.36e-05
                        Length:96
                                            Min. : 1.398
                                                               Length:96
##
    Min.
##
    1st Qu.:2.36e-05
                        Class : character
                                            1st Qu.: 2.084
                                                               Class : character
    Median :2.92e-05
                                            Median : 2.550
##
                        Mode :character
                                                              Mode : character
##
    Mean
           :2.92e-05
                                            Mean
                                                   : 2.986
                                            3rd Qu.: 3.126
##
    3rd Qu.:3.48e-05
##
           :3.48e-05
                                            Max.
                                                    :20.235
    Max.
##
     exp duration formulation sample id
                                                     soil conc ugg
                                Length:96
##
   Min.
           :8
                          :0
                                                     Mode:logical
                  \mathtt{Min}.
##
    1st Qu.:8
                   1st Qu.:0
                                 Class : character
                                                     NA's:96
##
    Median:8
                  Median :0
                                Mode :character
                   Mean
##
   Mean
           :8
                          :0
```

```
##
    3rd Qu.:8
                   3rd Qu.:0
##
    Max.
           :8
                   Max.
                           :0
##
     soil_type
                                               species
                                                                  tissue_conc_ugg
                            source
                                             Length:96
                                                                         :0.08123
##
    Length:96
                        Length:96
                                                                  1st Qu.:0.40279
##
    Class : character
                        Class : character
                                             Class : character
                                                                  Median: 0.94646
##
          :character
                        Mode
                               :character
                                             Mode
                                                   :character
                                                                         :1.28035
##
                                                                  Mean
##
                                                                  3rd Qu.:1.43585
##
                                                                  Max.
                                                                         :6.61248
```

Van Meter et al. 2021

Van Meter et al. 2021

Data Set Dimensions, Column Names, and Summary:

```
## [1] 96 12
```

```
"chemical"
##
    [1] "app_rate_g_cm2"
                            "application"
                                               "body_weight_g"
##
                            "formulation"
                                               "sample_id"
                                                                  "soil_conc_ugg"
    [5] "exp_duration"
                            "source"
                                               "species"
##
    [9] "soil_type"
                                                                  "tissue_conc_ugg"
                        application
                                                                chemical
##
    app_rate_g_cm2
                                            body_weight_g
##
    Min.
           :2.36e-05
                        Length:48
                                            Min.
                                                    :2.091
                                                             Length:48
##
    1st Qu.:2.36e-05
                        Class : character
                                            1st Qu.:3.313
                                                             Class : character
##
    Median :2.92e-05
                        Mode :character
                                            Median :3.791
                                                             Mode : character
           :2.92e-05
                                                    :3.795
##
    Mean
                                            Mean
##
    3rd Qu.:3.48e-05
                                            3rd Qu.:4.342
##
           :3.48e-05
                                            Max.
                                                    :5.589
##
     exp_duration formulation sample_id
                                                     soil_conc_ugg
##
           :8
                   Min.
                          :0
                                 Length:48
                                                     Min.
                                                            : 3.705
    Min.
    1st Qu.:8
                   1st Qu.:0
                                                     1st Qu.: 7.427
##
                                 Class : character
##
    Median:8
                   Median:0
                                 Mode :character
                                                     Median :11.115
                   Mean
                          :0
                                                             :11.525
##
    Mean
           :8
                                                     Mean
##
    3rd Qu.:8
                   3rd Qu.:0
                                                     3rd Qu.:12.994
##
    Max.
           :8
                   Max.
                          :0
                                                     Max.
                                                             :25.873
                                              species
                                                                 tissue_conc_ugg
##
     soil_type
                           source
##
                                                                        : 0.2155
    Length:48
                        Length:48
                                            Length: 48
                                                                 Min.
                                                                 1st Qu.: 1.1327
##
    Class : character
                        Class : character
                                            Class : character
                                                                 Median : 1.9263
##
    Mode :character
                        Mode : character
                                            Mode :character
##
                                                                 Mean
                                                                        : 3.2363
                                                                 3rd Qu.: 3.9569
##
##
                                                                 Max.
                                                                        :13.9376
```

Glinski et al. 2018a (Dehydration)

Glinski et al. 2018a studied how amphibian hydration status influences uptake of pesticides through dermal exposure. Amphibians (Southern leopard frogs (*Lithobates sphenocephala*) and Fowler's toads (*Anaxyrus fowleri*)) were dehyrated for periods of 0, 2, 4, 6, 8, or 10 hours prior to exposure to pesticide-contaminated soils. Pesticides studied included atrazine, triadimefon, metolachlor, chlorothalonil, and imidacloprid. Soil and whole-body homogenates were measured after an 8 hour exposure period. Pesticides were applied at the maximum legally allowable application rates scaled down to the area of six 0.94 L Pyrex glass bowls each with a 15 cm diameter.

Note: this file does not combine daughters with parents

Note: this file has body burdens and soil concentrations as separate rows

Data Set Dimensions, column Names, and Summary:

[1] 1494 8

```
## [1] "time"
                             "analyte" "matrix"
                                                                        "ID"
                  "parent"
                                                  "species" "conc"
## [8] "weight"
##
         time
                     parent
                                         analyte
                                                              matrix
           : 0
                  Length: 1494
                                      Length: 1494
                                                           Length: 1494
##
    Min.
    1st Qu.: 2
                                      Class :character
                  Class :character
##
                                                           Class : character
##
    Median: 5
                  Mode
                        :character
                                      Mode :character
                                                           Mode :character
    Mean
           : 5
##
##
    3rd Qu.: 8
##
    Max.
           :10
      species
##
                                                   ID
                                                                       weight
                              conc
                                              Length: 1494
    Length: 1494
                                   0.00000
##
                        Min.
                                :
                                                                  Min.
                                                                          :0.6821
##
    Class : character
                        1st Qu.:
                                   0.02215
                                              Class : character
                                                                   1st Qu.:1.6108
                                   0.08482
##
    Mode : character
                        Median :
                                              Mode :character
                                                                   Median :3.0890
##
                                   6.17646
                                                                          :3.0810
                        Mean
                                                                  Mean
##
                        3rd Qu.:
                                   2.60007
                                                                   3rd Qu.:4.3124
##
                                :238.15019
                        Max.
                                                                  Max.
                                                                          :7.2481
```

Glinski et al. 2018b (Metabolites)

Glinski et al. 2018b assessed the potential metabolic activation of pesticides (atrazine, triadimefon, fopronil) in amphibians. This data set (1) contains in vitro and in vivo metabolic rate constants derived from toad (Anaxyrus terrestris) livers during experiments measuring the depletion of pesticides and the formation of their metabolites. Pesticides were applied at the maximum legally allowable application rates scaled down to the area of a 10-gallon aquarium (1225 cm²).

Metabolites Data Set (1) Data Set Dimensions, Column Names, and Summary:

```
## [1] 352
## [1] "time"
                    "parent"
                                 "analyte"
                                                                        "replicate"
                                              "matrix"
                                                           "conc"
##
         time
                        parent
                                            analyte
                                                                  matrix
           : 0.00
                     Length: 352
                                          Length:352
                                                              Length:352
##
    Min.
    1st Qu.: 2.00
                                          Class : character
                                                              Class : character
##
                     Class : character
    Median :12.00
##
                     Mode
                           :character
                                          Mode
                                               :character
                                                              Mode
                                                                    :character
           :16.41
##
    Mean
##
    3rd Qu.:24.00
##
    Max.
           :48.00
##
         conc
                           replicate
##
           :-0.01244
                        Min.
                                :1.00
##
    1st Qu.: 0.01292
                        1st Qu.:1.75
##
    Median: 0.08373
                        Median:2.50
##
    Mean
           : 2.12963
                        Mean
                                :2.50
##
    3rd Qu.: 0.97824
                         3rd Qu.:3.25
            :32.47385
##
    Max.
                        Max.
                                :4.00
```

The *in vitro* derived constants were assessed for their precitability by exposing Fowler's toads (*Anaxyrus fowleri*) to contaminated soils at maximum application rate for 2, 4, 12, and 48 hours. This data set (merged) contains the data from the Fowler's toad experiment along with the tissue concentrations from data set 1; this data set (merged) is used in subsequent steps.

Metabolites Data Set (merged) Data Set Dimensions, Column Names, and Summary:

[1] 60 12

```
"tissue_conc_ugg" "sample_id"
##
    [1] "exp_duration"
                           "chemical"
##
    [5] "soil type"
                           "app_rate_g_cm2"
                                              "soil conc ugg"
                                                                  "body weight g"
##
    [9] "formulation"
                           "species"
                                              "application"
                                                                  "source"
##
     exp_duration
                     chemical
                                       tissue_conc_ugg
                                                           sample_id
##
           : 2
                                              :0.08328
                                                          Length:60
    Min.
                   Length:60
                                       Min.
    1st Qu.: 4
##
                   Class :character
                                       1st Qu.:0.33733
                                                          Class : character
    Median:12
                  Mode :character
                                       Median :0.86010
                                                          Mode :character
##
##
    Mean
          :18
                                       Mean
                                             :1.42634
                                       3rd Qu.:1.88383
##
    3rd Qu.:24
    Max.
           :48
                                       Max.
                                              :7.62649
##
                                         soil_conc_ugg
##
    soil_type
                    app_rate_g_cm2
                                                            body_weight_g
                                                : 0.2858
##
    Mode:logical
                   Min.
                           :1.100e-06
                                         Min.
                                                            Min.
                                                                    :0.1879
##
    NA's:60
                    1st Qu.:1.100e-06
                                         1st Qu.: 0.9041
                                                            1st Qu.:0.5925
                   Median :2.700e-06
                                         Median: 4.8333
                                                            Median : 0.7144
##
                           :9.237e-06
##
                   Mean
                                         Mean
                                               : 9.1511
                                                            Mean
                                                                    :0.7350
##
                    3rd Qu.:2.290e-05
                                         3rd Qu.:18.0554
                                                            3rd Qu.:0.8782
##
                           :2.290e-05
                                                 :32.4738
                                                                    :1.4909
                                         Max.
                                                            Max.
                                                             source
##
     formulation
                    species
                                      application
##
    Min.
           :0
                 Length:60
                                      Length:60
                                                          Length:60
##
    1st Qu.:0
                                      Class : character
                                                          Class : character
                  Class : character
##
    Median:0
                 Mode :character
                                      Mode :character
                                                          Mode : character
##
           :0
    Mean
##
    3rd Qu.:0
##
    Max.
           :0
```

Glinski et al. 2019 (Biomarkers)

Glinski et al. 2019 exposed Southern leopard frogs (*Lithobates sphenocephala*) to either the maximum or 1/10th maximum pesticide application rate to single, double, or triple pesticide mixtures of bifenthrin, metolachlor, and triadime-fon to consider the typical co-application of pesticides during agricultural growing seasons. Tissue concentrations and metabolomic profiling of amphibian livers were studied after an 8 hour exposure period to pesticide-contaminated soil. Pesticides application rates were scaled down to the area of eight 0.94 L Pyrex glass bowls each with a 15 cm diameter.

Data Set Dimensions, Column Names, and Summary:

```
## [1] 192
             9
## [1] "group"
                                     "tdt"
                                                    "bif"
                                                                   "frog.weight"
  [6] "sample_id"
                      "pesticide"
                                                    "conc"
                                     "rate"
##
                                                 tdt
                                                                    bif
       group
                             met
                                                                      :-1.0000
##
    Length: 192
                        Min.
                                :-1.0000
                                           Min.
                                                   :-1.0000
                                                               Min.
##
    Class : character
                        1st Qu.:-1.0000
                                           1st Qu.:-1.0000
                                                               1st Qu.:-1.0000
##
    Mode :character
                        Median : 1.0000
                                           Median : 1.0000
                                                               Median : 1.0000
##
                               : 0.3333
                                                   : 0.3333
                                                                     : 0.3333
                        Mean
                                           Mean
                                                               Mean
##
                        3rd Qu.: 1.0000
                                           3rd Qu.: 1.0000
                                                               3rd Qu.: 1.0000
##
                        Max.
                                : 1.0000
                                           Max.
                                                   : 1.0000
                                                               Max.
                                                                      : 1.0000
##
     frog.weight
                      sample_id
                                          pesticide
                                                                  rate
##
    Min.
           :1.012
                     Length: 192
                                         Length: 192
                                                             Length: 192
    1st Qu.:2.745
##
                     Class :character
                                         Class : character
                                                              Class : character
##
    Median :3.142
                     Mode : character
                                         Mode :character
                                                             Mode :character
##
    Mean
           :3.299
##
    3rd Qu.:3.789
##
           :6.739
##
         conc
##
           : 0.001061
##
    1st Qu.: 0.069055
```

Median : 0.212920 ## Mean : 0.801643 ## 3rd Qu.: 0.521471 ## Max. :19.879783

[1] 192

Glinski et al. 2020 (Dermal Routes)

5

Glinski et al. 2020 assessed dermal uptake in amphibians from exposure to three pesticides (bifenthrin, chlorpyrifos, trifloxystrobin). Pesiticide body burdens and hepatic metabolome for Leopard frogs were measured for two routes of uptake: uptake from contaminated soils versus uptake from contaminated surface water. Pesticides were applied at 1 ppm, scaled down to the area of eight 0.94 L Pyrex glass bowls each with a 15 cm diameter.

Data Set Dimensions, Column Names, and Summary:

```
## [1] "Sample.ID"
                        "Analyte"
                                         "Media"
                                                           "Matrix"
## [5] "Concentration"
##
     Sample.ID
                          Analyte
                                                Media
                                                                    Matrix
##
    Length: 192
                        Length: 192
                                            Length: 192
                                                                 Length: 192
##
    Class : character
                        Class : character
                                            Class : character
                                                                 Class : character
##
    Mode :character
                        Mode :character
                                            Mode :character
                                                                 Mode :character
##
##
##
##
    Concentration
##
           :0.00000
##
    1st Qu.:0.01036
    Median :0.15326
##
           :0.33962
##
    Mean
##
    3rd Qu.:0.44162
           :3.40759
##
    Max.
```

Application Rates

The table below concisely displays the pesticide applications rates (ug/cm²) used in each relevant study as well as the variables used to compute the application rates.

pesticide	app_rate_ug_cm2	applied_mL	container	area cm2	total area cm2	density_g_cm3	pesticide
Van Meter et al. 2014/2		applied_IIIL	container	area_cm2	total_area_cmz	density_g_cms	pesticide_
		75 MeOH	101	1007	1005	1 1000	90.1
atrazine	22.9000	75 MeOH	10-gal aquarium	1225	1225 1225	1.1900	28.1
fipronil	1.1000		10-gal aquarium	1225		1.5515	1.3
imidacloprid	5.7000	75 MeOH	10-gal aquarium	1225	1225	1.6000	7.0
pendimethalin	19.8000	75 MeOH	10-gal aquarium	1225	1225	1.1700	24.3
triadimefon	2.7000	75 MeOH	10-gal aquarium	1225	1225	1.2200	3.3
Van Meter et al. 2016	22.000			Lagratio	1050		
atrazine	22.9000	75 MeOH	.94 L bowl	225*6	1350	1.1900	30.9
fipronil	1.1000	75 MeOH	.94 L bowl	225*6	1350	1.5515	1.5
imidacloprid	5.7000	75 MeOH	.94 L bowl	225*6	1350	1.6000	7.7
pendimethalin	69.8000	75 MeOH	.94 L bowl	225*6	1350	1.1700	94.2
triadimefon	2.7000	75 MeOH	.94 L bowl	225*6	1350	1.2200	3.6
Van Meter et al. 2018							
atrazine	23.6000	50 MeOH	.94 L bowl	225*6	1350	1.1900	31.9
2,4-D	14.3000	50 MeOH	.94 L bowl	225*6	1350	1.5000	19.3
metolachlor	30.9000	50 MeOH	.94 L bowl	225*6	1350	1.1000	41.7
malathion	25.9000	50 MeOH	.94 L bowl	225*6	1350	1.2300	35.0
propiconazole	2.6000	50 MeOH	.94 L bowl	225*6	1350	1.3000	3.5
Van Meter et al. 2019							
alachlor	34.8000	75 MeOH	.94 L bowl	225*6	1350	1.1300	47.0
atrazine	23.6000	75 MeOH	.94 L bowl	225*6	1350	1.1900	31.9
Van Meter et al. 2021							
alachlor	34.8000	75 MeOH	.94 L bowl	225*6	1350	1.1300	47.0
atrazine	23.6000	75 MeOH	.94 L bowl	225*10	1354	1.1900	31.9
Henson-Ramsey et al. 2	008						
malathion	50.0000	NA	cage	1060	NA	1.2300	NA
Glinski et al. 2018a							
atrazine	23.9500	75 MeOH	.94 L bowl	225*6	1350	1.1900	32.3
chlorothalonil	44.3000	75 MeOH	.94 L bowl	225*6	1350	1.8000	59.8
imidacloprid	5.3900	75 MeOH	.94 L bowl	225*6	1350	1.6000	7.3
metolachlor	31.0100	75 MeOH	.94 L bowl	225*6	1350	1.1000	41.9
triadimefon	2.9100	75 MeOH	.94 L bowl	225*6	1350	1.2200	3.9
Glinski et al. 2018b							
atrazine	22.9000	75 MeOH	10-gal aquarium	1225	1225	1.1900	28.1
fipronil	1.1000	75 MeOH	10-gal aquarium	1225	1225	1.5515	1.3
triadimefon	2.7000	75 MeOH	10-gal aquarium	1225	1225	1.2200	3.3
Glinski et al. 2019	<u> </u>			1	1	1	<u> </u>
bifenthrin (max)	3.4500	75 MeOH	.94 L bowl	225*8	1800	1.3000	6.2
metolachlor (max)	30.6200	75 MeOH	.94 L bowl	225*8	1800	1.1000	55.1
triadimefon (max)	2.8700	75 MeOH	.94 L bowl	225*8	1800	1.2200	5.2
$\frac{\text{bifenthrin } (1/10 \text{ max})}{\text{bifenthrin } (1/10 \text{ max})}$	0.3450	75 MeOH	.94 L bowl	225*8	1800	1.3000	0.6
metolachlor (1/10 max)	3.0620	75 MeOH	.94 L bowl	225*8	1800	1.1000	5.5
$\frac{\text{triadime fon } (1/10 \text{ max})}{\text{triadime fon } (1/10 \text{ max})}$	0.2870	75 MeOH	.94 L bowl	225*8	1800	1.2200	0.5
Glinski et al. 2020							
bifenthrin	0.2889	400ml of 1ppm pesticide in water	.94 L bowl	225*8	1800	1.3000	50ml/bow
chlorpyrifos	0.3111	400ml of 1ppm pesticide in water	.94 L bowl	225*8	1800	1.4000	50ml/bow
trifloxystrobin	0.3022	400ml of 1ppm pesticide in water	.94 L bowl	225*8	1800	1.3600	50ml/bow
ышохувиовш	0.3022	400mi of Thbin besucide in water	.54 L DOWI	440 0	1000	1.5000	nom /

Cleaning and Merging the Data Sets

Each data set was cleaned for merging. This consisted of dropping unneeded columns and standardizing column names of retained columns. Four columns were added to all data sets (soil type, formulation, exposure duration, and research study source).

Once each data set was cleaned, a local copy was saved and the data set was merged with the previously cleaned data sets.

The process of cleaning and merging each data set is briefly described below.

Van Meter et al. 2014/2015

Metabolites and parents that do not include metabolites were dropped from the data set. This includes atrazine, deisopropyl atrazine, desethyl atrazine, fipronil, fipronil-sulfone, triadimenol.

```
# drop metabolites and parents that do not include metabolites
vm2015_chem_drop <- c("Atrazine", "Deisopropyl Atrazine", "Desethyl Atrazine", "Fipronil", "Fipronil-Sulfone", "Tr
chem_vector_drop <- which(vm2015$Chemical %in% vm2015_chem_drop)
vm2015_subset1 <- vm2015[-chem_vector_drop,]
vm2015_subset2 <- droplevels(vm2015_subset1)</pre>
```

There were 278 observations with these chemicals. After dropping the 278 observations from the initial 474, the updated dimensions are:

```
## [1] 196 23
```

There were 15 unneeded columns dropped and 4 added for standarization.

```
# drop unneeded columns for merging
all_cols <- colnames(vm2015_subset2)
drop_cols <- c("Instrument", "good", "logKow", "BCF", "initialweight", "Solat20C_mgL", "Solat20C_gL", "molmass_gmo
    "AppFactor", "SA_cm2", "VapPrs_mPa", "Koc_gmL", "HalfLife_day", "HabFac")
vm2015_subset3 <- vm2015_subset2[, !(names(vm2015_subset2) %in% drop_cols)]</pre>
colnames(vm2015_subset3)
## [1] "Species"
                         "Sample"
                                           "Chemical"
                                                              "Application"
## [5] "app_rate_g_cm2" "TissueConc"
                                           "SoilConc"
                                                              "bodyweight"
# add columns
soil_type <- c(rep("PLE", nrow(vm2015_subset3)))</pre>
formulation <- (rep(0, nrow(vm2015_subset3)))</pre>
exp_duration <- (rep(8, nrow(vm2015_subset3)))</pre>
source <- c(rep("rvm2015", nrow(vm2015_subset3)))</pre>
vm2015_subset4 <- cbind(vm2015_subset3, formulation, soil_type, exp_duration, source)</pre>
# standardize column names
colnames(vm2015 subset4)
                          "Sample"
                                            "Chemical"
                                                               "Application"
##
    [1] "Species"
    [5] "app_rate_g_cm2" "TissueConc"
                                            "SoilConc"
                                                              "bodyweight"
                          "soil type"
                                                              "source"
    [9] "formulation"
                                            "exp duration"
```

```
colnames(vm2015_subset4)[which(colnames(vm2015_subset4) == "Species")] <- "species"</pre>
colnames(vm2015 subset4)[which(colnames(vm2015 subset4) == "Chemical")] <- "chemical"
colnames(vm2015_subset4)[which(colnames(vm2015_subset4) == "Application")] <- "application"
colnames(vm2015 subset4) [which(colnames(vm2015 subset4) == "TissueConc")] <- "tissue conc ugg"
colnames(vm2015_subset4)[which(colnames(vm2015_subset4) == "SoilConc")] <- "soil_conc_ugg"
colnames(vm2015_subset4)[which(colnames(vm2015_subset4) == "bodyweight")] <- "body_weight_g"
colnames(vm2015 subset4)
##
   [1] "species"
                          "sample_id"
                                             "chemical"
                                                               "application"
##
   [5] "app_rate_g_cm2"
                          "tissue_conc_ugg" "soil_conc_ugg"
                                                               "body_weight_g"
   [9] "formulation"
                          "soil_type"
                                             "exp_duration"
                                                               "source"
# reorder vm2015 alphabetically
vm2015_merge <- vm2015_subset4[, order(names(vm2015_subset4))]</pre>
# write a local copy
vm2015_merge_filename <- paste(amphibdir_data_out, "vm2015_merge.csv", sep = "")
write.csv(vm2015_merge, file = vm2015_merge_filename)
```

colnames(vm2015_subset4)[which(colnames(vm2015_subset4) == "Sample")] <- "sample_id"

The data set's dimensions are:

```
## [1] 196 12
```

Van Meter et al. 2016

From the initial 11 columns, 4 columns were dropped and consolidated into 1, and 4 columns were added.

```
# add sample_id
vm2016$sample_id <- paste(vm2016$Day, vm2016$Row, vm2016$Column, sep = "_")
vm2016_subset2 <- subset(vm2016, select = c(-Day, -Row, -Column, -Total))
# add additional columns
species <- c(rep("American toad", nrow(vm2016_subset2)))
application <- c(rep("Indirect", nrow(vm2016_subset2)))
exp_duration <- (rep(8, nrow(vm2016_subset2)))
source <- c(rep("rvm2016", nrow(vm2016_subset2)))
vm2016_subset3 <- cbind(vm2016_subset2, species, application, exp_duration, source)</pre>
```

Application rates for several pesticides were inserted. There were 108 observations with decay products that were not sprayed; these observations were dropped so as to only include the parents in the cleaned data set. There were 60 observations with atrazine, fipronil, or triadimefon that were dropped because they do not include metabolites in total.

```
# assign values to application rate unique(vm2016_subset3$Pesticide)
vm2016_subset3$app_rate_g_cm2[vm2016_subset3$Pesticide == "ATZTOT"] <- 2.29e-05
vm2016_subset3$app_rate_g_cm2[vm2016_subset3$Pesticide == "Imid"] <- 5.7e-06
vm2016_subset3$app_rate_g_cm2[vm2016_subset3$Pesticide == "FipTOT"] <- 1.1e-06
vm2016_subset3$app_rate_g_cm2[vm2016_subset3$Pesticide == "TNDTOT"] <- 2.7e-06
vm2016_subset3$app_rate_g_cm2[vm2016_subset3$Pesticide == "Pendi"] <- 6.98e-05
# drop decay products that were not sprayed, keeping only parents
rows_to_drop <- which(vm2016_subset3$Parent == 0)
vm2016_subset4 <- vm2016_subset3[-rows_to_drop, ]
# drop ATZ, Fip, TDN since do not include metabolites in total
chems_to_drop <- c("ATZ", "Fip", "TDN")
vm2016_subset5 <- vm2016_subset4[!(vm2016_subset4$Pesticide %in% chems_to_drop), ]
# drop parent field
drop_cols <- c("Parent")
vm2016_subset6 <- vm2016_subset5[, !(names(vm2016_subset5) %in% drop_cols)]</pre>
```

Several column names were standardized and all columns were ordered for ease of merging with the combined data set.

```
# standardize column names
colnames(vm2016_subset6)
##
    [1] "Pesticide"
                          "SoilType"
                                            "BodyBurden"
                                                              "Soil"
##
    [5] "Weight"
                          "Formulation"
                                            "sample_id"
                                                              "species"
                                            "source"
    [9] "application"
                          "exp_duration"
                                                              "app_rate_g_cm2"
colnames(vm2016_subset6)[which(colnames(vm2016_subset6) == "Pesticide")] <- "chemical"
colnames(vm2016_subset6)[which(colnames(vm2016_subset6) == "SoilType")] <- "soil_type"
colnames(vm2016_subset6)[which(colnames(vm2016_subset6) == "BodyBurden")] <- "tissue_conc_ugg"
colnames(vm2016_subset6) [which(colnames(vm2016_subset6) == "Soil")] <- "soil_conc_ugg"</pre>
colnames(vm2016_subset6)[which(colnames(vm2016_subset6) == "Weight")] <- "body_weight_g"</pre>
colnames(vm2016_subset6)[which(colnames(vm2016_subset6) == "Formulation")] <- "formulation"
# alter chemical name
vm2016 subset6$chemical <- as.character(vm2016 subset6$chemical)</pre>
vm2016_subset6$chemical[vm2016_subset6$chemical == "Imid"] <- "imidacloprid"</pre>
# reorder columns alphabetically to help with merge
colnames(vm2016 subset6)
                                              "tissue_conc_ugg" "soil_conc_ugg"
    [1] "chemical"
                           "soil type"
##
    [5] "body_weight_g"
                           "formulation"
                                              "sample_id"
                                                                 "species"
                                              "source"
   [9] "application"
                           "exp_duration"
                                                                 "app_rate_g_cm2"
vm2016_merge <- vm2016_subset6[, order(names(vm2016_subset6))]</pre>
colnames(vm2016_merge)
                           "application"
                                                                 "chemical"
##
    [1] "app_rate_g_cm2"
                                              "body_weight_g"
##
    [5] "exp_duration"
                           "formulation"
                                              "sample_id"
                                                                 "soil_conc_ugg"
   [9] "soil_type"
                           "source"
                                              "species"
                                                                 "tissue_conc_ugg"
# write a local copy
vm2016_merge_filename <- paste(amphibdir_data_out, "vm2016_merge.csv", sep = "")</pre>
write.csv(vm2016_merge, file = vm2016_merge_filename)
The updated dimensions are:
```

```
## [1] 96 12
```

The Van Meter et al. 2014/2015 and Van Meter et al. 2016 data sets were combined.

The combined data set's updated dimensions are:

```
## [1] 292 12
```

Glinski et al. 2018a (Dehydration)

The metabolite products were dropped from the data set; 600 rows from the initial 1494 rows were retained.

```
# drop metabolite products
parent_keepers <- which(as.vector(dag2016_dehy0$parent) == as.vector(dag2016_dehy0$analyte))
dag2016_dehy1 <- dag2016_dehy0[parent_keepers, ]</pre>
```

Several column names were altered for standarization across the data set, and 7 columns were added for standarization.

```
\textit{## time is length of dehydration colnames} (\textit{dag2016\_dehy1}) [\textit{which} (\textit{colnames} (\textit{dag2016\_dehy1}) == 'time')] <-'exp\_duration' == 'time') | <-'exp\_duration' == 'time' == 'time' | <-'exp\_duration' == 'time' == 'time'
```

```
# standardize column names
colnames(dag2016_dehy1)[which(colnames(dag2016_dehy1) == "analyte")] <- "chemical"
colnames(dag2016_dehy1)[which(colnames(dag2016_dehy1) == "conc")] <- "tissue_conc_ugg"
colnames(dag2016_dehy1)[which(colnames(dag2016_dehy1) == "ID")] <- "sample_id"
colnames(dag2016_dehy1)[which(colnames(dag2016_dehy1) == "weight")] <- "body_weight_g"

# add additional columns
exp_duration <- c(rep(8, nrow(dag2016_dehy1)))
soil_type <- c(rep("PLE", nrow(dag2016_dehy1)))
application <- c(rep("Indirect", nrow(dag2016_dehy1)))
formulation <- (rep(0, nrow(dag2016_dehy1)))
app_rate_g_cm2 <- (rep(0, nrow(dag2016_dehy1)))
soil_conc_ugg <- (rep(0, nrow(dag2016_dehy1)))
source <- c(rep("dag_dehydration", nrow(dag2016_dehy1)))
dag2016_dehy2 <- cbind(dag2016_dehy1, formulation, soil_type, application, app_rate_g_cm2, exp_duration, soil_conc_</pre>
```

The updated dimensions are:

```
## [1] 600 15
```

Multiple soil concentration observations were given the same ID. Until a many-to-one merge of soil concentrations could be executed, 300 rows were temporarily dropped. There were also 3 columns dropped.

```
# drop the soil until we can do a many-to-one merge of soil concentrations drop decay products that were not spray
# only parents
rows_to_drop <- which(dag2016_dehy2$matrix == "soil")
dag2016_dehy3 <- dag2016_dehy2[-rows_to_drop, ]
# parent, time and matrix columns delete
drop_cols <- c("parent", "time", "matrix")
dag2016_dehy4 <- dag2016_dehy3[, !(names(dag2016_dehy3) %in% drop_cols)]</pre>
```

The updated dimensions are:

```
## [1] 300 12
```

The application rate values were inserted, the temporarily dropped soil concentrations were updated to the current data set, and the species names were standardized.

```
# fill in application rates unique(dag2016_dehy4$chemical)
update_atrazine <- which(dag2016_dehy4$chemical == "atrazine")
dag2016_dehy4$app_rate_g_cm2[update_atrazine] <- 2.395e-05  # atrazine g/cm2
update_chloro <- which(dag2016_dehy4$chemical == "chloro+d")
dag2016_dehy4$app_rate_g_cm2[update_chloro] <- 4.43e-05  # chloro g/cm2
update_metol <- which(dag2016_dehy4$chemical == "metol")
dag2016_dehy4$app_rate_g_cm2[update_metol] <- 3.101e-05  # metol g/cm2
update_tdn <- which(dag2016_dehy4$chemical == "tdn")
dag2016_dehy4$app_rate_g_cm2[update_tdn] <- 2.91e-06  # tdn g/cm2
update_imid <- which(dag2016_dehy4$chemical == "imid")
dag2016_dehy4$app_rate_g_cm2[update_imid] <- 5.39e-06  # imid g/cm2

# add back in soil concentrations (in already-made soil_conc_ugg column)
dag2016_soil <- dag2016_dehy2[rows_to_drop, ]
dag2016_dehy4$soil_conc_ugg <- dag2016_soil$tissue_conc_ugg</pre>
```

```
# rename species names, according to standardized names
dag2016_dehy4$species <- as.character(dag2016_dehy4$species)
dag2016_dehy4$species[dag2016_dehy4$species == "LF"] <- "Leopard frog"
dag2016_dehy4$species[dag2016_dehy4$species == "BA"] <- "Fowlers toad"
dag2016_dehy4$species <- as.factor(dag2016_dehy4$species)</pre>
```

The dimensions are:

```
## [1] 300 12
```

The Glinkski et al. 2018a (Dehydration) was combined with the previously merged data sets.

The combined data set's updated dimensions are:

```
## [1] 592 12
```

Henson-Ramsey 2008

The Henson-Ramsey 2008 data set did not require any additional data cleaning. It was combined with the previously merged data sets.

The combined data set's updated dimensions are:

```
## [1] 601 12
```

Glinski et al. 2018b (Metabolites)

Apart from standardizing the species name, the Glinski et al. 2018b (Metabolites) data set did not require any additional data cleaning. It was combined with the previously merged data sets.

```
# rename species names, according to standardized names
dag2016_metabolite_merge$species <- as.character(dag2016_metabolite_merge$species)
dag2016_metabolite_merge$species[dag2016_metabolite_merge$species == "Anaxyrus_fowleri"] <- "Fowlers toad"
dag2016_metabolite_merge$species <- as.factor(dag2016_metabolite_merge$species)</pre>
```

The combined data set's updated dimensions are:

```
## [1] 661 12
```

Glinski et al. 2019 (Biomarkers)

Five columns were dropped from the original biomarkers data set and the names of two columns were standardized.

```
# drop columns
drop_cols <- c("met", "tdt", "bif", "rate", "group")
dag_biomarker_subset <- dag_biomarker[, !(names(dag_biomarker) %in% drop_cols)]

# standardize column names
colnames(dag_biomarker_subset)[which(colnames(dag_biomarker_subset) == "conc")] <- "tissue_conc_ugg"
colnames(dag_biomarker_subset)[which(colnames(dag_biomarker_subset) == "frog.weight")] <- "body_weight_g"</pre>
```

The updated column names and dimensions are:

```
## [1] "body_weight_g" "sample_id" "pesticide" "tissue_conc_ugg"
```

[1] 136 15

The application rates and soil concentrations were not included in the original biomarkers data set. Both are included in the following data set:

Data Set Dimensions, Column Names, and Summary:

```
[1] "frog.weight"
                                         "Met"
                                                         "TDN"
                                                                          "TDL"
##
                         "SAMPLE"
##
    [6] "BIF"
                         "soil.weight"
                                         "Met.soil"
                                                         "TDN.soil"
                                                                          "TDL.soil"
## [11] "BIF.soil"
                         "Rate"
                                         "app.rate.met"
                                                         "app.rate.tdn" "app.rate.bif"
                         SAMPLE
                                                                   TDN
##
     frog.weight
                                               Met
##
    Min.
            :1.012
                     Length: 136
                                          Min.
                                                  : 0.0000
                                                             Min.
                                                                     :0.0000
##
    1st Qu.:2.749
                     Class : character
                                          1st Qu.: 0.0000
                                                              1st Qu.:0.00000
    Median :3.164
                           :character
                                          Median : 0.0000
##
                     Mode
                                                              Median :0.00000
##
            :3.302
                                                 : 0.9123
                                                                     :0.06927
    Mean
                                          Mean
                                                             Mean
##
    3rd Qu.:3.762
                                          3rd Qu.: 0.4298
                                                              3rd Qu.:0.07447
##
    Max.
            :6.784
                                          Max.
                                                  :19.8798
                                                             Max.
                                                                     :0.55921
##
         TDL
                             BIF
                                           soil.weight
                                                                Met.soil
##
            :0.00000
                               :0.0000
                                                  : 4.476
                                                                    :0.000
    Min.
                       Min.
                                          Min.
                                                            Min.
##
    1st Qu.:0.00000
                       1st Qu.:0.0000
                                          1st Qu.: 6.731
                                                            1st Qu.:0.000
    Median :0.00000
                       Median :0.0000
                                          Median : 7.772
##
                                                            Median : 0.000
                                          Mean
##
    Mean
            :0.02259
                       Mean
                               :0.1276
                                                  : 8.043
                                                            Mean
                                                                    :1.605
##
    3rd\ Qu.:0.01770
                       3rd Qu.:0.1299
                                          3rd Qu.: 9.050
                                                            3rd Qu.:2.265
##
            :0.30815
                                                  :13.571
                                                                    :6.758
                       Max.
                               :1.0271
                                                            Max.
##
       TDN.soil
                          TDL.soil
                                              BIF.soil
                                                                  Rate
##
            :0.0000
                              :0.000000
                                                   :0.0000
                                                             Length: 136
    Min.
                      Min.
                                           Min.
##
    1st Qu.:0.0000
                      1st Qu.:0.000000
                                           1st Qu.:0.0000
                                                              Class : character
##
    Median :0.0000
                      Median :0.000000
                                           Median :0.0000
                                                              Mode : character
##
    Mean
            :0.7168
                      Mean
                              :0.010160
                                           Mean
                                                   :0.7417
##
    3rd Qu.:0.5312
                      3rd Qu.:0.007463
                                           3rd Qu.:1.1472
##
    Max.
            :3.6300
                      Max.
                              :0.061563
                                           Max.
                                                   :5.2658
                                          app.rate.bif
##
     app.rate.met
                       app.rate.tdn
##
           : 0.000
                              :0.0000
                                                 :0.0000
                      Min.
                                         Min.
##
    1st Qu.: 0.000
                      1st Qu.:0.0000
                                         1st Qu.:0.0000
##
    Median : 0.000
                      Median : 0.0000
                                         Median : 0.0000
##
            :14.263
                              :1.3389
    Mean
                      Mean
                                         Mean
                                                :1.6070
##
    3rd Qu.: 5.511
                      3rd Qu.:0.5173
                                         3rd Qu.:0.6209
            :55.106
                              :5.1730
                                                 :6.2090
##
    Max.
                      Max.
                                         Max.
```

The application rates were converted from mg to g/cm^2 .

```
dag_biomarker2_update <- replace.value(dag_biomarker2, "app.rate.met", from = 55.106, to = 3.062e-05, verbose = TR dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.met", from = 5.5106, to = 3.062e-06, verbose dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.tdn", from = 5.173, to = 2.87e-06, verbose dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.tdn", from = 0.5173, to = 2.87e-07, verbose dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.bif", from = 6.209, to = 3.45e-06, verbose dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update <- replace.value(dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", from = 0.6209, to = 3.45e-07, verbose dag_biomarker2_update, "app.rate.bif", fro
```

A one-to-one merge was conducted based on the unique sample id for each measured pesticide (either bifenthrin, metolachlor, or triadimefon) to join the original biomarkers data set and the data set containing the application rates and soil concentrations. Vectors containing the application rates and soil concentrations were joined to the original data set.

```
# bif extraction
dag_biomarker_subset_bif <- dag_biomarker_subset[dag_biomarker_subset$pesticide == "bif", ]
dag_biomarker2_subset_bif <- dag_biomarker2_update[dag_biomarker2_update$BIF != 0, ]
dag_biomarker_bif_merge <- merge(x = dag_biomarker_subset_bif, y = dag_biomarker2_subset_bif, by.x = "sample_id", '
    all.x = TRUE)
# met extraction
dag_biomarker_subset_met <- dag_biomarker_subset[dag_biomarker_subset$pesticide == "met", ]</pre>
dag_biomarker2_subset_met <- dag_biomarker2_update[dag_biomarker2_update$Met != 0, ]
dag_biomarker_met_merge <- merge(x = dag_biomarker_subset_met, y = dag_biomarker2_subset_met, by.x = "sample_id",
    all.x = TRUE)
# tdt extraction
dag_biomarker_subset_tdt <- dag_biomarker_subset[dag_biomarker_subset$pesticide == "tdt", ]
dag_biomarker2_subset_tdt <- dag_biomarker2_update[dag_biomarker2_update$TDN != 0, ]
dag_biomarker_tdt_merge <- merge(x = dag_biomarker_subset_tdt, y = dag_biomarker2_subset_tdt, by.x = "sample_id", i
    all.x = TRUE)
\# combine bif, met, and tdt
app_bind_bmt <- c(dag_biomarker_bif_merge[, "app.rate.bif"], dag_biomarker_met_merge[, "app.rate.met"], dag_biomar
soil_bind_bmt <- c(dag_biomarker_bif_merge[, "BIF.soil"], dag_biomarker_met_merge[, "Met.soil"], dag_biomarker_tdt
# join app and soil vectors to data set
dag_biomarker_subset2 <- dag_biomarker_subset[order(dag_biomarker_subset[, 3]), ]
rownames(dag_biomarker_subset2) <- seq(length = nrow(dag_biomarker_subset2))</pre>
dag_biomarker_subset3 <- cbind(dag_biomarker_subset2, app_bind_bmt, soil_bind_bmt)</pre>
# standardize column names
colnames(dag_biomarker_subset3)[which(colnames(dag_biomarker_subset3) == "app_bind_bmt")] <- "app_rate_g_cm2"
colnames(dag_biomarker_subset3)[which(colnames(dag_biomarker_subset3) == "soil_bind_bmt")] <- "soil_conc_ugg"
The updated column names and dimensions are:
## [1] "body_weight_g"
                          "sample_id"
                                            "pesticide"
                                                               "tissue_conc_ugg"
## [5] "app_rate_g_cm2"
                          "soil_conc_ugg"
## [1] 192
New columns were created for standarization, the columns were ordered alphabetically, and a local copy was stored.
# create new columns
application <- c(rep("soil", nrow(dag_biomarker_subset3)))</pre>
exp_duration <- c(rep(8, nrow(dag_biomarker_subset3)))</pre>
formulation <- c(rep(0, nrow(dag_biomarker_subset3)))</pre>
soil_type <- c(rep(NA, nrow(dag_biomarker_subset3)))</pre>
source <- c(rep("dag_biomarker", nrow(dag_biomarker_subset3)))</pre>
```

dag_biomarker_subset4 <- cbind(dag_biomarker_subset3, application, exp_duration, formulation, soil_type, source, s

species <- c(rep("Leopard frog", nrow(dag_biomarker_subset3)))</pre>

combine columns

```
# standardize pesticide column
dag_biomarker_subset4$pesticide <- as.character(dag_biomarker_subset4$pesticide)
dag_biomarker_subset4$pesticide[dag_biomarker_subset4$pesticide == "bif"] <- "Bifenthrin"
dag_biomarker_subset4$pesticide[dag_biomarker_subset4$pesticide == "met"] <- "Metolachlor"
dag_biomarker_subset4$pesticide[dag_biomarker_subset4$pesticide == "tdt"] <- "Triadimefon"

colnames(dag_biomarker_subset4)[which(colnames(dag_biomarker_subset4) == "pesticide")] <- "chemical"

# unite function for sample id and chemical
dag_biomarker_subset5 <- unite(data = dag_biomarker_subset4, col = "sample_id", "sample_id", "chemical", sep = " "

# order columns in abc for merge
dag_biomarker_merge <- dag_biomarker_subset5[, order(names(dag_biomarker_subset5))]</pre>
```

The updated column names and dimensions are:

```
## [1] "app_rate_g_cm2" "application" "body_weight_g" "chemical"
## [5] "exp_duration" "formulation" "sample_id" "soil_conc_ugg"
## [9] "soil_type" "source" "species" "tissue_conc_ugg"
## [1] 192 12
```

The Glinski et al. 2019 (Biomarkers) was combined with the previously merged data sets.

The combined data set's updated dimensions are:

```
## [1] 853 12
```

Van Meter et al. 2018 (Multiple Pesticides Study)

The Van Meter et al. 2018 (Multiple Pesticides Study) data set did not require any additional data cleaning. It was combined with the previously merged data sets.

The combined data set's updated dimensions are:

```
## [1] 990 12
```

Glinski et al. 2020 (Dermal Routes)

The dermal routes data set did not include the body weights for the measured amphibians. These weights were included in a separate data set:

Data Set Dimensions, Column Names, and Summary:

```
## [1] 48 2
## [1] "Weight_g" "Sample"
##
                        Sample
       Weight_g
         :0.9555
                     Length:48
##
   1st Qu.:1.4204
                     Class :character
##
   Median :1.7817
                     Mode :character
##
##
   Mean
          :1.7784
##
   3rd Qu.:2.1319
          :2.8197
##
   Max.
```

A one-to-many merge was employed to merge the dermal routes data set and the weights data set based on the Sample ID. Only rows where the Matrix is "Amphibian" have a body weight; all other rows are NA.

```
# merge (one-to-many) dermal routes data with weights data, based on Sample ID
dermal_routes_subset2 <- dermal_routes[order(dermal_routes$Sample.ID), ]
weights_2 <- weights[order(weights$Sample), ]
dermal_routes_subset3 <- merge(dermal_routes_subset2, weights_2, by.x = "Sample.ID", by.y = "Sample", all.x = TRUE</pre>
```

The updated dimensions are:

```
## [1] 192 6
```

The soil concentrations, where the Media and Matrix are both "Soil," was subset from the data set to be used later in the data cleaning process. These soil concentrations (currently listed in the "Concentration" column) will be used for the soil conc ugg column in the cleaned data set.

```
# subset soil to be used later for soil concentration column (will use 'Concentration' column)
soil_subset <- dermal_routes_subset2[dermal_routes_subset2$Media == "Soil", ]
soil_subset2 <- soil_subset[soil_subset$Matrix == "Soil", ]</pre>
```

The dimensions of this soil subset are:

```
## [1] 48 5
```

Referring back to the main dermal routes data set: we are only interested in the pesticide exposures on amphibians while in soil. These rows were subset.

```
# want Media == soil because interested in dermal exposure in soil
dermal_routes_subset4 <- dermal_routes_subset3[dermal_routes_subset3$Media == "Soil", ]
# sum(dermal_routes_subset3$Media == 'Soil') # == 96 dim(dermal_routes_subset4) # == 96 x 6

# want Matrix == Amphibian because interested in amphib exposure
dermal_routes_subset5 <- dermal_routes_subset4[dermal_routes_subset4$Matrix == "Amphibian", ]
# sum(dermal_routes_subset4$Matrix == 'Amphibian') # == 48 dim(dermal_routes_subset5) # == 48 x 6</pre>
```

The updated dimensions are:

```
## [1] 48 6
```

The soil concentrations were appended to the main dermal routes data set.

```
# add in soil concentration column, previously subset order by Sample.ID, then by Analyte name to match up rows fo
# sets
dermal_routes_subset6 <- dermal_routes_subset5[order(dermal_routes_subset5[, 1], dermal_routes_subset5[, 2]), ]
soil_subset3 <- soil_subset2[order(soil_subset2[, 1], soil_subset2[, 2]), ]
# dim(dermal_routes_subset6) # == 48 x 6 dim(soil_subset3) # == 48 x 5
dermal_routes_subset7 <- cbind(dermal_routes_subset6, soil_subset3$Concentration)</pre>
```

The updated dimensions are:

```
## [1] 48 7
```

The metabolites were dropped from the data set. Additionally, several new columns were created for standardization, existing columns were standardized according to the naming conventions of the collated data set, and unneeded columns were dropped. Columns were ordered alphabetically for ease of merging.

```
# drop metabolites
rows_to_drop <- c("4-OH", "CPO", "TFSa")</pre>
dermal_routes_subset8 <- dermal_routes_subset7[!(dermal_routes_subset7$Analyte %in% rows_to_drop), ]
# create new columns
app_rate_g_cm2 <- c(rep(NA, nrow(dermal_routes_subset8)))</pre>
application <- c(rep("soil", nrow(dermal_routes_subset8)))</pre>
exp_duration <- c(rep(8, nrow(dermal_routes_subset8)))</pre>
formulation <- c(rep(0, nrow(dermal_routes_subset8)))</pre>
soil_type <- c(rep("OLS", nrow(dermal_routes_subset8)))</pre>
source <- c(rep("dag_dermal_routes", nrow(dermal_routes_subset8)))</pre>
species <- c(rep("Leopard frog", nrow(dermal_routes_subset8)))</pre>
# alter existing column names
colnames(dermal_routes_subset8)
## [1] "Sample.ID"
                                     "Analyte"
## [3] "Media"
                                     "Matrix"
                                     "Weight_g"
## [5] "Concentration"
## [7] "soil_subset3$Concentration"
colnames(dermal_routes_subset8) [which(colnames(dermal_routes_subset8) == "Analyte")] <- "chemical"</pre>
colnames(dermal_routes_subset8) [which(colnames(dermal_routes_subset8) == "Sample.ID")] <- "sample_id"
colnames(dermal_routes_subset8)[which(colnames(dermal_routes_subset8) == "Concentration")] <- "tissue_conc_ugg"
colnames(dermal_routes_subset8)[which(colnames(dermal_routes_subset8) == "soil_subset3$Concentration")] <- "soil_collames"
colnames(dermal_routes_subset8)[which(colnames(dermal_routes_subset8) == "Weight_g")] <- "body_weight_g"
# combine columns
dermal_routes_subset9 <- cbind(dermal_routes_subset8, app_rate_g_cm2, application, exp_duration, formulation, soil
names(dermal_routes_subset9)
   [1] "sample_id"
                           "chemical"
                                              "Media"
                                                                 "Matrix"
##
##
    [5] "tissue_conc_ugg" "body_weight_g"
                                              "soil_conc_ugg"
                                                                "app_rate_g_cm2"
   [9] "application"
                           "exp_duration"
                                              "formulation"
                                                                "soil_type"
##
## [13] "source"
                           "species"
# drop columns
cols_to_drop <- c("Matrix", "Media")</pre>
dermal_routes_subset10 <- dermal_routes_subset9[, !(names(dermal_routes_subset9) %in% cols_to_drop)]
# insert application rates
dermal_routes_subset10$chemical <- as.character(dermal_routes_subset10$chemical)
unique(dermal_routes_subset10$chemical)
## [1] "BIF" "CPF" "TFS"
dermal_routes_subset10$app_rate_g_cm2[dermal_routes_subset10$chemical == "BIF"] <- 2.8889e-07 #bifenthrin g/cm2
dermal_routes_subset10$app_rate_g_cm2[dermal_routes_subset10$chemical == "CPF"] <- 3.1111e-07 #chlorpyrifos g/cm2
dermal_routes_subset10$app_rate_g_cm2[dermal_routes_subset10$chemical == "TFS"] <- 3.0222e-07 #trifloxystrobin g/
summary(dermal_routes_subset10$app_rate_g_cm2)
                                              3rd Qu.
        Min.
               1st Qu.
                          Median
                                       Mean
```

2.889e-07 2.889e-07 3.022e-07 3.007e-07 3.111e-07 3.111e-07

```
# order columns in abc for merge
dermal_routes_merge <- dermal_routes_subset10[, order(names(dermal_routes_subset10))]</pre>
```

The updated column names and dimensions are:

```
## [1] 24 12

## [1] "app_rate_g_cm2" "application" "body_weight_g" "chemical"

## [5] "exp_duration" "formulation" "sample_id" "soil_conc_ugg"

## [9] "soil_type" "source" "species" "tissue_conc_ugg"
```

A local copy was saved, and the data set was combined with the collated data set.

The combined data set's updated dimensions are:

```
## [1] 1014   12
```

Final Product

##

##

Min. 1st Qu.

0.1125 2.0326

Median

Minor alterations were made to the final collated data set to standardize names of the application types and chemicals.

```
amphib_dermal_collated <- combined_data6
colnames(amphib_dermal_collated)
   [1] "app_rate_g_cm2"
                          "application"
                                            "body weight g"
                                                              "chemical"
##
   [5] "exp_duration"
                          "formulation"
                                            "sample_id"
                                                              "soil_conc_ugg"
   [9] "soil_type"
                          "source"
                                            "species"
                                                              "tissue_conc_ugg"
# check to see if everything ok
summary(amphib_dermal_collated$app_rate_g_cm2)
##
               1st Qu.
                          Median
                                      Mean
                                             3rd Qu.
## 2.870e-07 2.790e-06 5.700e-06 1.616e-05 2.395e-05 6.980e-05
summary(amphib_dermal_collated$body_weight_g)
##
      Min. 1st Qu. Median
                              Mean 3rd Qu.
                                              Max.
   0.1879 1.3043 2.1247 3.3800 3.0412 50.9200
summary(amphib_dermal_collated$exp_duration)
                              Mean 3rd Qu.
##
     Min. 1st Qu. Median
                                              Max.
##
     2.000
            8.000
                   8.000
                             8.876
                                     8.000 48.000
summary(amphib_dermal_collated$soil_conc_ugg) # 206 NAs
```

Max.

Mean 3rd Qu.

5.5791 13.9733 16.7043 238.1502

NA's

9

[1] 1014 12

Variable Summaries

app_rate_g_cm2 application body_weight_g chemical

```
Min. : 0.1879
## Min. :2.870e-07
                      indirect :396
                                                       triadimefon:223
##
   1st Qu.:2.790e-06
                      overspray: 45
                                      1st Qu.: 1.3043
                                                       atrazine :191
##
   Median :5.700e-06
                      soil :573
                                      Median : 2.1247
                                                       metolachlor :154
   Mean :1.616e-05
                                      Mean : 3.3800
                                                       imidacloprid: 78
   3rd Qu.:2.395e-05
                                      3rd Qu.: 3.0412
                                                       bifenthrin: 72
##
                                                       fipronil : 71
   Max. :6.980e-05
                                      Max. :50.9200
##
##
                                                       (Other)
                                                                  :225
##
   exp\_duration
                    formulation
                                      sample_id
                                                       soil_conc_ugg
        : 2.000
                          :0.00000
                                     Length: 1014
                                                       Min. : 0.1125
##
   Min.
                   Min.
##
   1st Qu.: 8.000
                   1st Qu.:0.00000
                                     Class : character
                                                       1st Qu.: 2.0326
   Median : 8.000
                   Median :0.00000
##
                                     Mode :character
                                                       Median: 5.5791
   Mean : 8.876
                   Mean :0.03582
                                                       Mean : 13.9733
##
   3rd Qu.: 8.000
                   3rd Qu.:0.00000
                                                       3rd Qu.: 16.7043
##
   Max. :48.000
                   Max.
                          :1.00000
                                                       Max. :238.1502
##
                   NA's :9
                                                       NA's
                                                              :9
##
   soil_type
                                                          tissue_conc_ugg
                        source
                                         species
##
   Length: 1014
                     Length: 1014
                                       Length: 1014
                                                          Min. : 0.00054
##
   Class :character Class :character
                                       Class :character
                                                         1st Qu.: 0.16908
   Mode :character Mode :character
                                       Mode :character
                                                         Median: 0.52573
##
                                                          Mean : 2.51415
##
                                                          3rd Qu.: 2.06812
##
                                                          Max. :72.62672
##
```

Session Information

[25] grid_4.0.2

```
## R version 4.0.2 (2020-06-22)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## Running under: Windows 10 x64 (build 18363)
##
## Matrix products: default
##
## locale:
## [1] LC_COLLATE=English_United States.1252
## [2] LC CTYPE=English United States.1252
## [3] LC_MONETARY=English_United States.1252
## [4] LC_NUMERIC=C
## [5] LC_TIME=English_United States.1252
## attached base packages:
                                               datasets methods
## [1] stats
                 graphics grDevices utils
                                                                   base
##
## other attached packages:
##
   [1] tinytex_0.32
                         formatR_1.11
                                          anchors_3.0-8
                                                           MASS_7.3-51.6
   [5] rgenoud_5.8-3.0 stringr_1.4.0
##
                                          tidyr_1.1.2
                                                            dplyr_1.0.5
   [9] knitr_1.31
                         kableExtra_1.3.4 reshape2_1.4.4
                                                           gridExtra_2.3
## [13] ggplot2_3.3.3
##
## loaded via a namespace (and not attached):
                                                              plyr_1.8.6
## [1] Rcpp 1.0.6
                          pillar 1.6.0
                                            compiler 4.0.2
## [5] tools_4.0.2
                          digest_0.6.27
                                            viridisLite_0.3.0 evaluate_0.14
  [9] lifecycle_1.0.0
##
                          tibble_3.1.1
                                            gtable_0.3.0
                                                              pkgconfig_2.0.3
## [13] rlang_0.4.10
                          rstudioapi_0.13
                                            DBI_1.1.1
                                                              yaml_2.2.1
                          xm12_1.3.2
## [17] xfun_0.24
                                            httr_1.4.2
                                                              withr_2.4.1
                                                              webshot_0.5.2
## [21] systemfonts_1.0.2 generics_0.1.0
                                            vctrs_0.3.7
```

glue_1.4.1

tidyselect_1.1.0 svglite_2.0.0

##	[29] R6_2.5.0	fansi_0.4.2	rmarkdown_2.6	purrr_0.3.4
##	[33] magrittr_2.0.1	scales_1.1.1	ellipsis_0.3.1	htmltools_0.5.1.1
##	[37] rvest_0.3.6	assertthat_0.2.1	colorspace_1.4-1	utf8_1.2.1
##	[41] stringi_1.5.3	munsell_0.5.0	crayon_1.4.1	