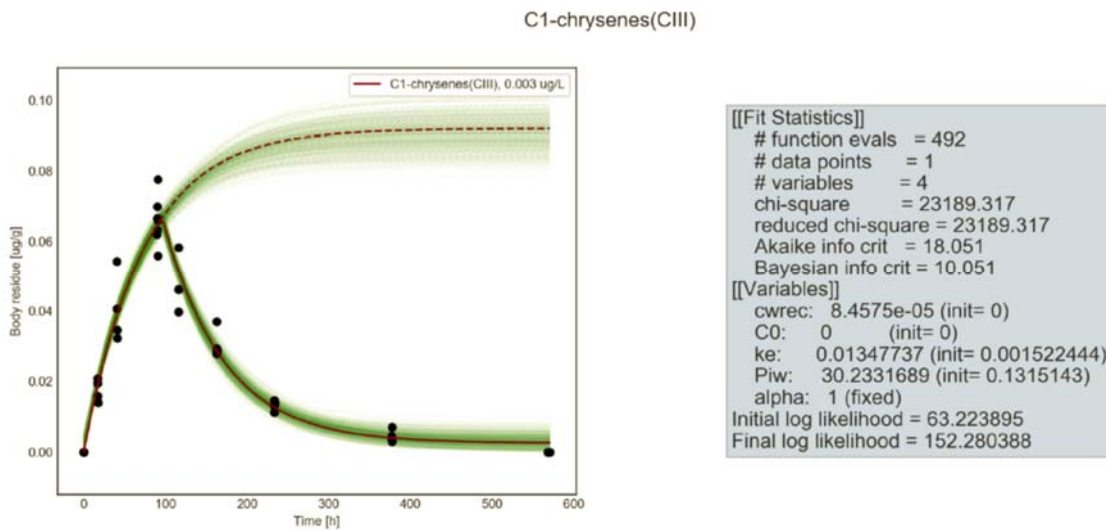


Text section 7: Model fits for all components including MCMC uncertainty estimates

In this section we have includes all model fits for all components in both stages. The figures show the body residue data points (black dots; $\mu\text{g/g}$) with fitted models (red solid line) for all components for CIIIs and CVs. The dashed red line indicates the forecasted uptake curve assuming continued exposure. The figures include samples from the MCMC posterior plotted in the data space, indicating the uncertainty of the parameters from the fitted model (green lines). The number in the figure panel gives the exposure concentration ($\mu\text{g/L}$).

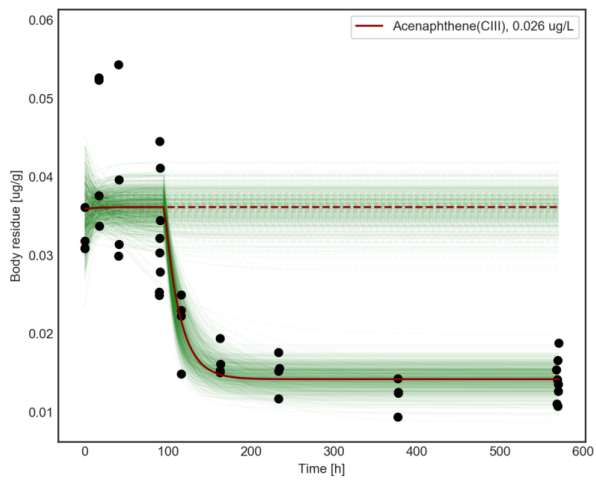
The panel on the right contains information of the model fit statistics and the estimated variables, provided by the lmfit package.¹ including values of the likelihood function before and after the optimization.

Example figure:



1. Matthew. N.; Stensitzki. T. LMFIT: non-linear least-square minimization and curve-fitting for Python. Astrophysics Source Code Library 2016.

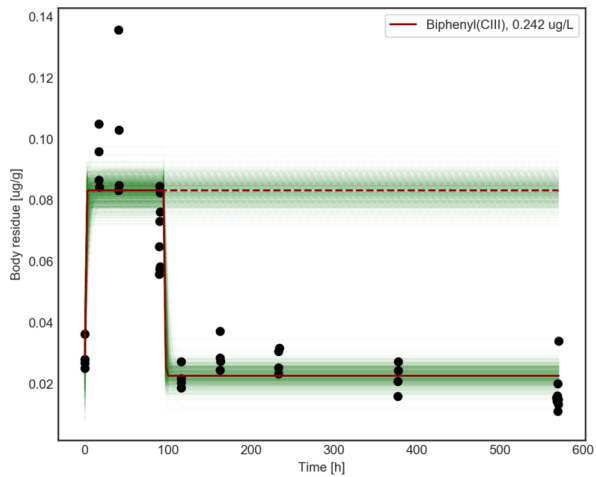
Acenaphthene(CIII)



```

[[Fit Statistics]]
# function evals = 800
# data points = 1
# variables = 4
chi-square = 19817.404
reduced chi-square = 19817.404
Akaike info crit = 17.894
Bayesian info crit = 9.894
[[Variables]]
cwrec: 0.01027502 (init= 0)
C0: 0.03594036 (init= 0)
ke: 0.05413393 (init= 0.2353063)
Piw: 1.38387006 (init= 0.0004168319)
alpha: 1 (fixed)
Initial log likelihood = 74.586275
Final log likelihood = 140.774302
    
```

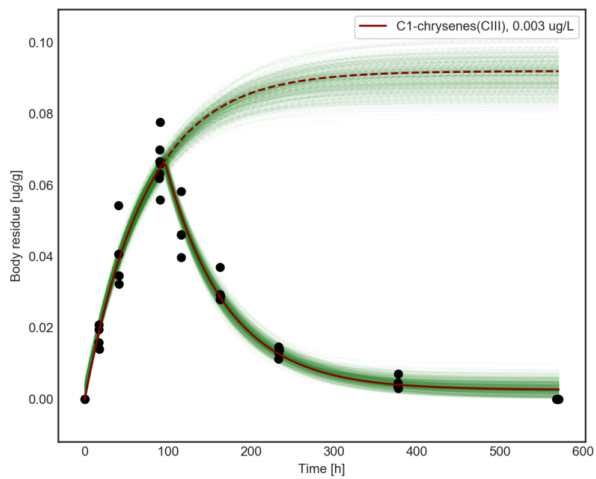
Biphenyl(CIII)



```

[[Fit Statistics]]
# function evals = 747
# data points = 1
# variables = 4
chi-square = 11580.168
reduced chi-square = 11580.168
Akaike info crit = 17.357
Bayesian info crit = 9.357
[[Variables]]
cwrec: 0.06601162 (init= 0)
C0: 0.02909707 (init= 0)
ke: 1.97447764 (init= 0.2274014)
Piw: 0.34364042 (init= 0.0004465755)
alpha: 1 (fixed)
Initial log likelihood = 44.236996
Final log likelihood = 107.611191
    
```

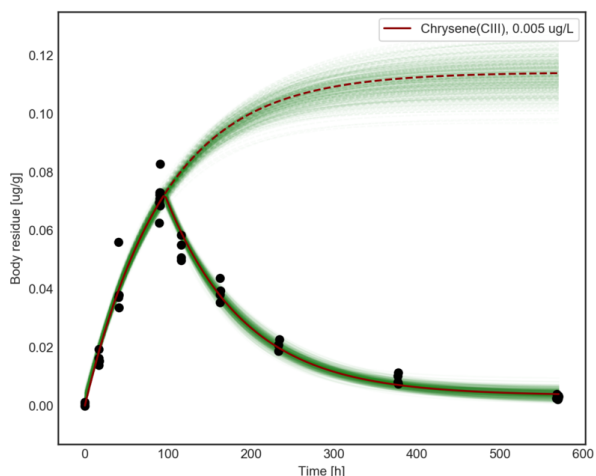
C1-chrysenes(CIII)



```

[[Fit Statistics]]
# function evals = 492
# data points = 1
# variables = 4
chi-square = 23189.317
reduced chi-square = 23189.317
Akaike info crit = 18.051
Bayesian info crit = 10.051
[[Variables]]
cwrec: 8.4575e-05 (init= 0)
C0: 0 (init= 0)
ke: 0.01347737 (init= 0.001522444)
Piw: 30.2331689 (init= 0.1315143)
alpha: 1 (fixed)
Initial log likelihood = 63.223895
Final log likelihood = 152.280388
    
```

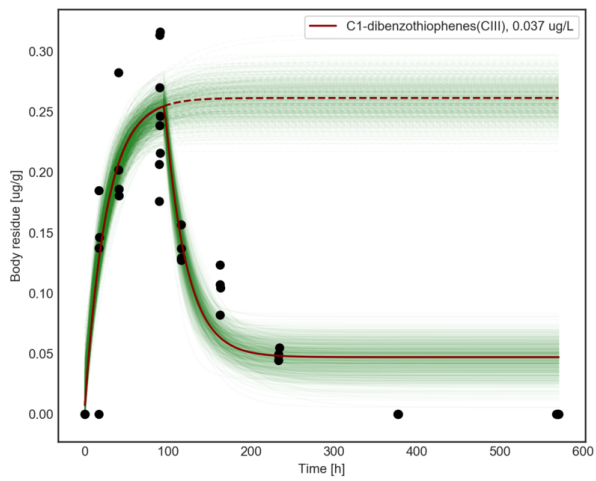
Chrysene(CIII)



```

[[Fit Statistics]]
# function evals = 486
# data points = 1
# variables = 4
chi-square = 23909.850
reduced chi-square = 23909.850
Akaike info crit = 18.082
Bayesian info crit = 10.082
[[Variables]]
cwrec: 0.00015867 (init= 0)
C0: 0 (init= 0)
ke: 0.01047206 (init= 0.005479931)
Piw: 21.8691361 (init= 0.03622275)
alpha: 1 (fixed)
Initial log likelihood = 58.796869
Final log likelihood = 154.628102
    
```

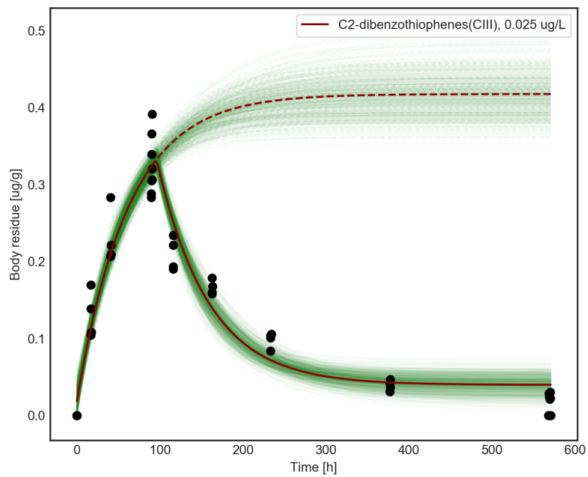
C1-dibenzothiophenes(CIII)



```

[[Fit Statistics]]
# function evals = 403
# data points = 1
# variables = 4
chi-square = 4505.451
reduced chi-square = 4505.451
Akaike info crit = 16.413
Bayesian info crit = 8.413
[[Variables]]
cwrec: 0.00675980 (init= 0)
C0: 0.00743944 (init= 0)
ke: 0.03814042 (init= 0.04949)
Piw: 6.98254562 (init= 0.00362313)
alpha: 1 (fixed)
Initial log likelihood = 2.283956
Final log likelihood = 67.122654
    
```

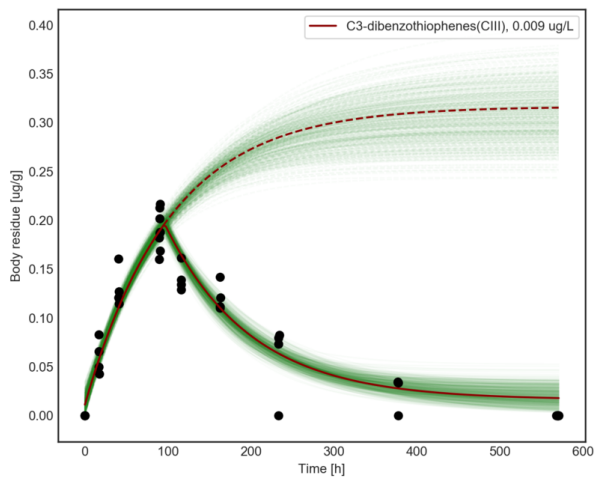
C2-dibenzothiophenes(CIII)



```

[[Fit Statistics]]
# function evals = 358
# data points = 1
# variables = 4
chi-square = 5150.754
reduced chi-square = 5150.754
Akaike info crit = 16.547
Bayesian info crit = 8.547
[[Variables]]
cwrec: 0.00240327 (init= 0)
C0: 0.01919162 (init= 0)
ke: 0.01609197 (init= 0.01236359)
Piw: 16.6149644 (init= 0.01581234)
alpha: 1 (fixed)
Initial log likelihood = -8.594111
Final log likelihood = 71.768754
    
```

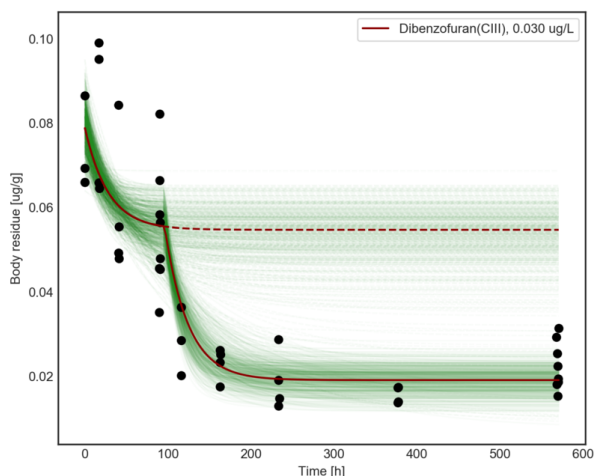
C3-dibenzothiophenes(CIII)



```

[[Fit Statistics]]
# function evals = 415
# data points = 1
# variables = 4
chi-square = 8870.153
reduced chi-square = 8870.153
Akaike info crit = 17.090
Bayesian info crit = 9.090
[[Variables]]
cwrec: 0.00047253 (init= 0)
C0: 0.01132992 (init= 0)
ke: 0.00971877 (init= 0.007361609)
Piw: 34.5019902 (init= 0.02685254)
alpha: 1 (fixed)
Initial log likelihood = 13.662650
Final log likelihood = 94.181490
    
```

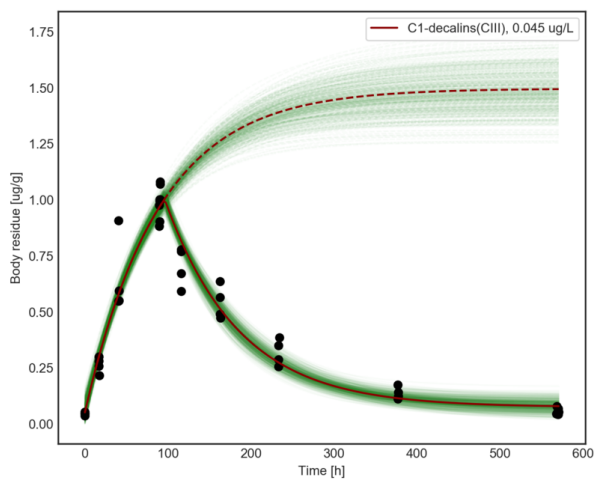
Dibenzofuran(CIII)



```

[[Fit Statistics]]
# function evals = 594
# data points = 1
# variables = 4
chi-square = 13086.373
reduced chi-square = 13086.373
Akaike info crit = 17.479
Bayesian info crit = 9.479
[[Variables]]
cwrec: 0.01043315 (init= 0)
C0: 0.07888186 (init= 0)
ke: 0.03554564 (init= 0.1609331)
Piw: 1.83169325 (init= 0.000811855)
alpha: 1 (fixed)
Initial log likelihood = 50.288533
Final log likelihood = 114.395684
    
```

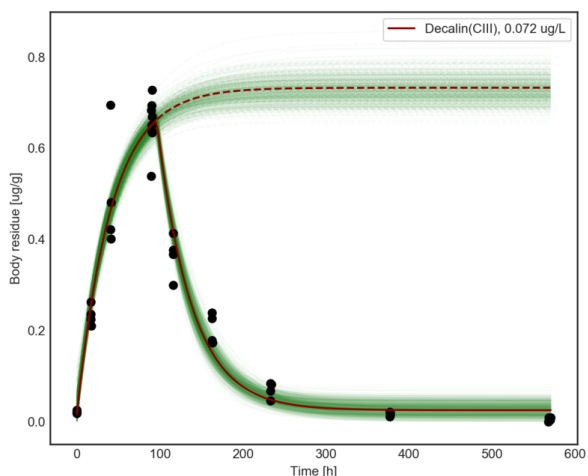
C1-decalins(CIII)



```

[[Fit Statistics]]
# function evals = 530
# data points = 1
# variables = 4
chi-square = 789.393
reduced chi-square = 789.393
Akaike info crit = 14.671
Bayesian info crit = 6.671
[[Variables]]
cwrec: 0.00229210 (init= 0)
C0: 0.05236046 (init= 0)
ke: 0.01120256 (init= 0.08120081)
Piw: 33.1031896 (init= 0.002037851)
alpha: 1 (fixed)
Initial log likelihood = -57.555076
Final log likelihood = 28.096139
    
```

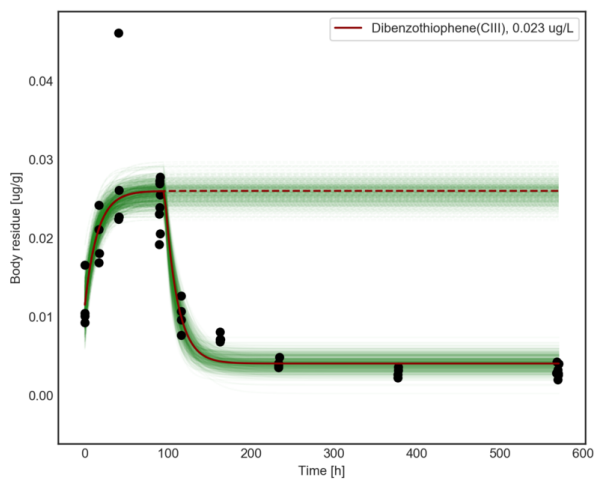
Decalin(CIII)



```

[[Fit Statistics]]
# function evals = 388
# data points = 1
# variables = 4
chi-square = 2118.801
reduced chi-square = 2118.801
Akaike info crit = 15.659
Bayesian info crit = 7.659
[[Variables]]
cwrec: 0.00245549 (init= 0)
C0: 0.01704923 (init= 0)
ke: 0.02414104 (init= 0.1633471)
Piw: 10.2107487 (init= 0.0007933966)
alpha: 1 (fixed)
Initial log likelihood = -37.329717
Final log likelihood = 46.030433
    
```

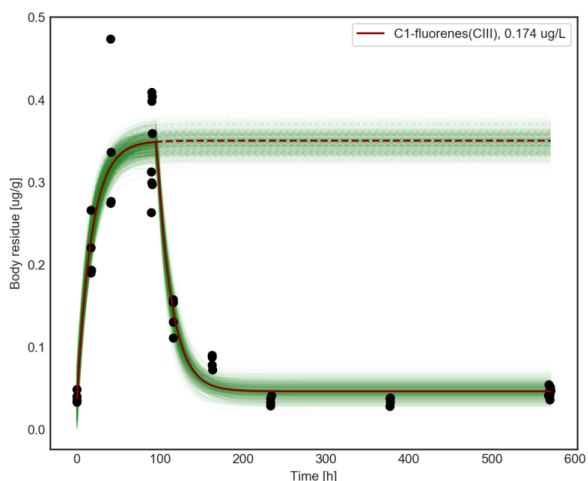
Dibenzothiophene(CIII)



```

[[Fit Statistics]]
# function evals = 484
# data points = 1
# variables = 4
chi-square = 25590.170
reduced chi-square = 25590.170
Akaike info crit = 18.150
Bayesian info crit = 10.150
[[Variables]]
cwrec: 0.00358138 (init= 0)
C0: 0.01153677 (init= 0)
ke: 0.06541306 (init= 0.1013422)
Piw: 1.13466011 (init= 0.001546098)
alpha: 1 (fixed)
Initial log likelihood = 97.932104
Final log likelihood = 159.969280
    
```

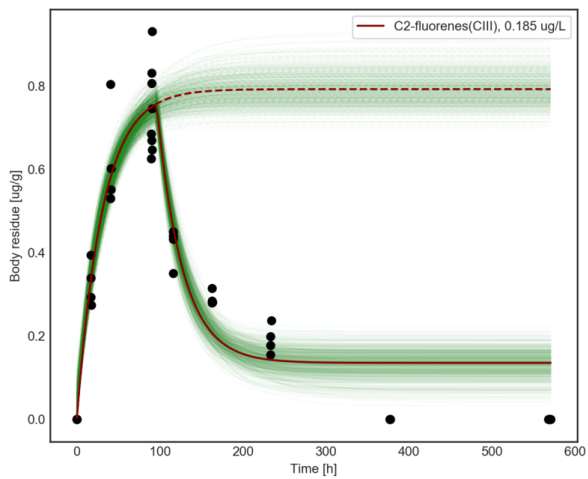
C1-fluorenes(CIII)



```

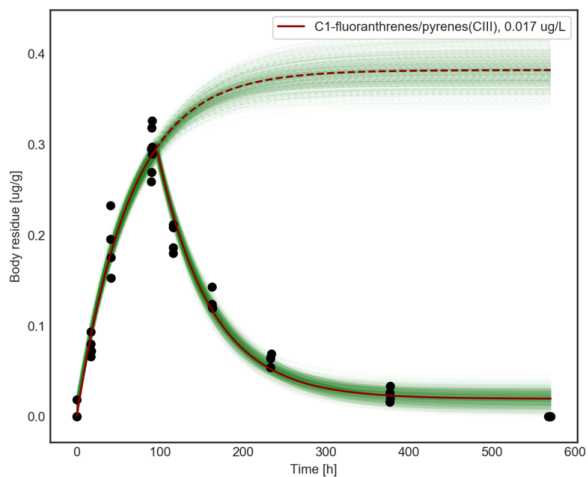
[[Fit Statistics]]
# function evals = 426
# data points = 1
# variables = 4
chi-square = 3724.047
reduced chi-square = 3724.047
Akaike info crit = 16.223
Bayesian info crit = 8.223
[[Variables]]
cwrec: 0.02306579 (init= 0)
C0: 0.03743909 (init= 0)
ke: 0.05629993 (init= 0.03936483)
Piw: 2.01744118 (init= 0.004667222)
alpha: 1 (fixed)
Initial log likelihood = -12.687314
Final log likelihood = 61.024967
    
```

C2-fluorenes(CIII)



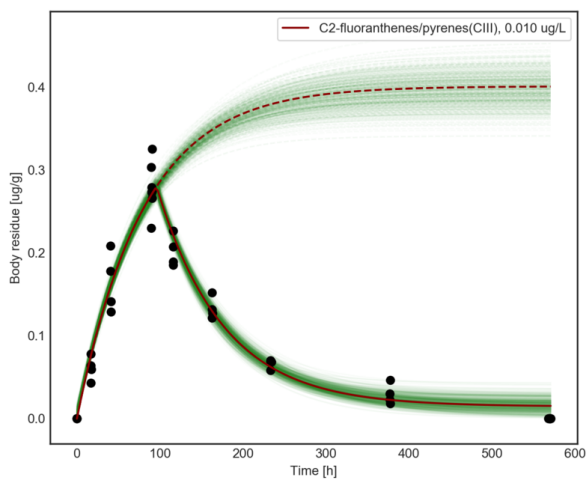
```
[[Fit Statistics]]
# function evals = 545
# data points = 1
# variables = 4
chi-square = 912.040
reduced chi-square = 912.040
Akaike info crit = 14.816
Bayesian info crit = 6.816
[[Variables]]
cwrec: 0.03157444 (init= 0)
C0: 0.00355133 (init= 0)
ke: 0.03238090 (init= 0.02402561)
Piw: 4.29248346 (init= 0.007925416)
alpha: 1 (fixed)
Initial log likelihood = -44.874993
Final log likelihood = 30.200001
```

C1-fluoranthrenes/pyrenes(CIII)



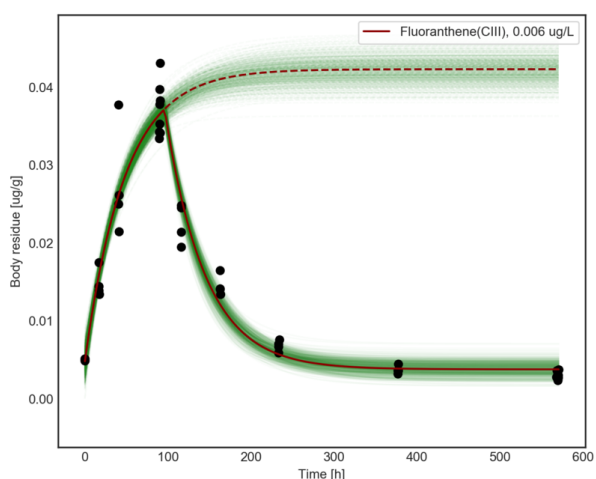
```
[[Fit Statistics]]
# function evals = 389
# data points = 1
# variables = 4
chi-square = 8670.950
reduced chi-square = 8670.950
Akaike info crit = 17.068
Bayesian info crit = 9.068
[[Variables]]
cwrec: 0.00087297 (init= 0)
C0: 0.00122597 (init= 0)
ke: 0.01552873 (init= 0.007530275)
Piw: 22.6549222 (init= 0.02624132)
alpha: 1 (fixed)
Initial log likelihood = -2.197130
Final log likelihood = 93.117939
```

C2-fluoranthrenes/pyrenes(CIII)



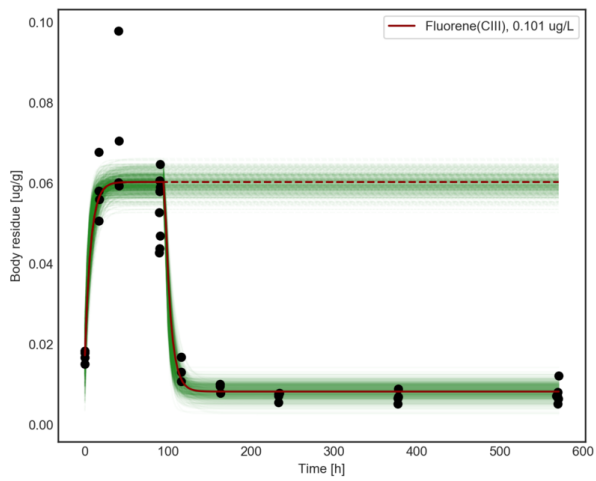
```
[[Fit Statistics]]
# function evals = 381
# data points = 1
# variables = 4
chi-square = 8355.241
reduced chi-square = 8355.241
Akaike info crit = 17.031
Bayesian info crit = 9.031
[[Variables]]
cwrec: 0.00035975 (init= 0)
C0: 0 (init= 0)
ke: 0.01248916 (init= 0.003719245)
Piw: 41.0440151 (init= 0.05357692)
alpha: 1 (fixed)
Initial log likelihood = -0.185095
Final log likelihood = 91.407007
```

Fluoranthene(CIII)



```
[[Fit Statistics]]
# function evals = 441
# data points = 1
# variables = 4
chi-square = 30487.497
reduced chi-square = 30487.497
Akaike info crit = 18.325
Bayesian info crit = 10.325
[[Variables]]
cwrec: 0.00057959 (init= 0)
C0: 0.00484023 (init= 0)
ke: 0.02075134 (init= 0.02299837)
Piw: 6.57038733 (init= 0.008298885)
alpha: 1 (fixed)
Initial log likelihood = 87.865624
Final log likelihood = 174.606691
```

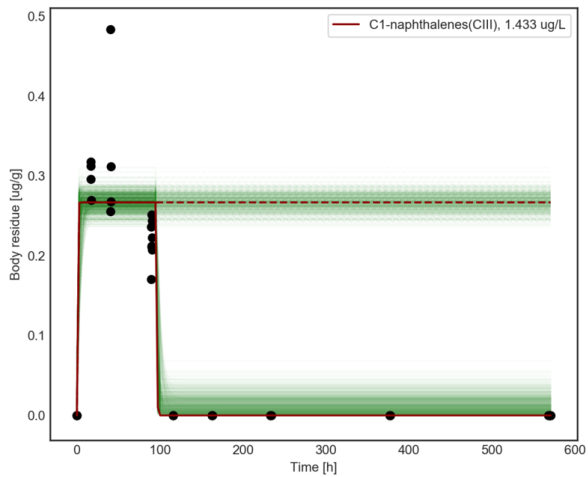
Fluorene(CIII)



```

[[Fit Statistics]]
# function evals = 600
# data points = 1
# variables = 4
chi-square = 16970.555
reduced chi-square = 16970.555
Akaike info crit = 17.739
Bayesian info crit = 9.739
[[Variables]]
cwrec: 0.01394790 (init= 0)
C0: 0.01730241 (init= 0)
ke: 0.14139573 (init= 0.1682223)
Piw: 0.59595922 (init= 0.0007577306)
alpha: 1 (fixed)
Initial log likelihood = 61.154501
Final log likelihood = 130.271083
    
```

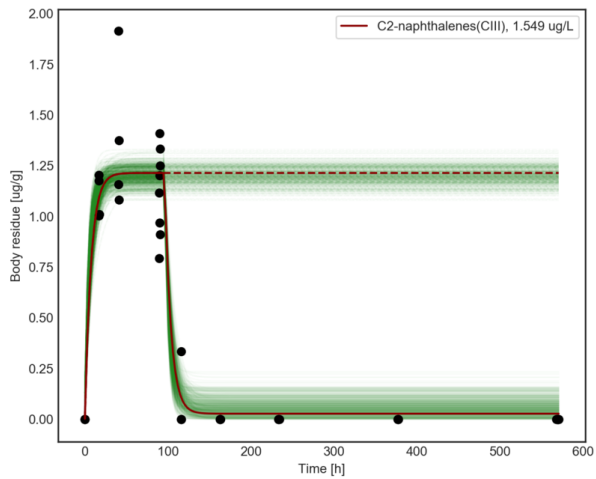
C1-naphthalenes(CIII)



```

[[Fit Statistics]]
# function evals = 620
# data points = 1
# variables = 4
chi-square = 3171.551
reduced chi-square = 3171.551
Akaike info crit = 16.062
Bayesian info crit = 8.062
[[Variables]]
cwrec: 7.3606e-09 (init= 0)
C0: 4.4464e-10 (init= 0)
ke: 2.14175725 (init= 0.2484319)
Piw: 0.18636089 (init= 0.0003716051)
alpha: 1 (fixed)
Initial log likelihood = -4.250427
Final log likelihood = 56.316529
    
```

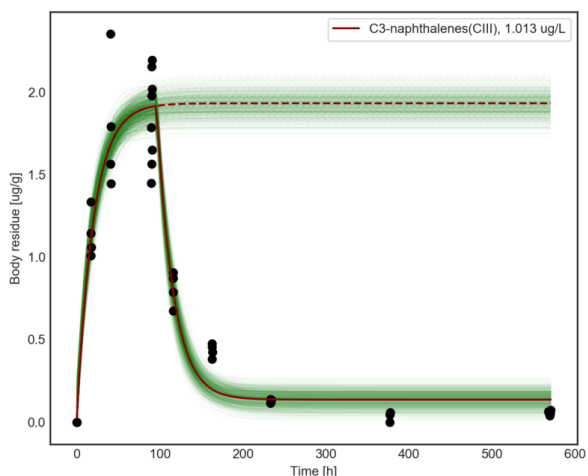
C2-naphthalenes(CIII)



```

[[Fit Statistics]]
# function evals = 572
# data points = 1
# variables = 4
chi-square = 0.636
reduced chi-square = 0.636
Akaike info crit = 7.547
Bayesian info crit = -0.453
[[Variables]]
cwrec: 0.03525350 (init= 0)
C0: 0.00193441 (init= 0)
ke: 0.13495807 (init= 0.1248276)
Piw: 0.78394536 (init= 0.001173064)
alpha: 1 (fixed)
Initial log likelihood = -69.363400
Final log likelihood = -0.797227
    
```

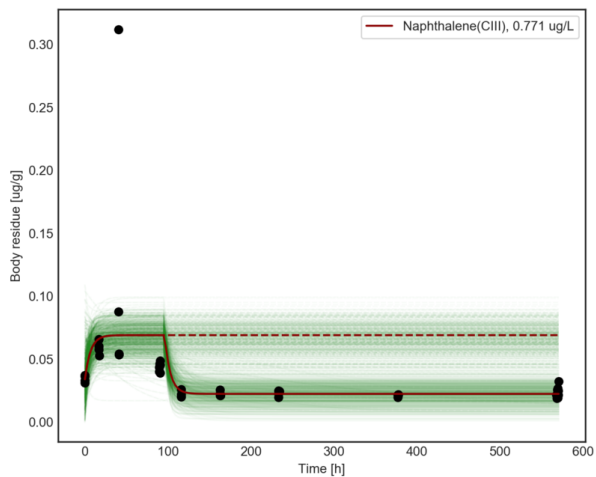
C3-naphthalenes(CIII)



```

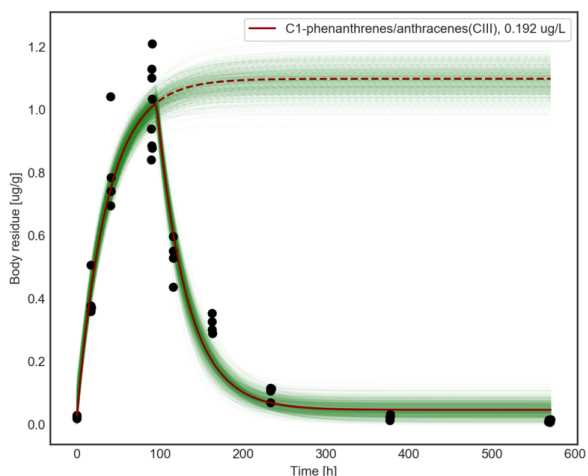
[[Fit Statistics]]
# function evals = 536
# data points = 1
# variables = 4
chi-square = 85.015
reduced chi-square = 85.015
Akaike info crit = 12.443
Bayesian info crit = 4.443
[[Variables]]
cwrec: 0.07092686 (init= 0)
C0: 0.02472611 (init= 0)
ke: 0.04990323 (init= 0.05480856)
Piw: 1.90953372 (init= 0.003229221)
alpha: 1 (fixed)
Initial log likelihood = -86.007267
Final log likelihood = -9.220372
    
```

Naphthalene(CIII)



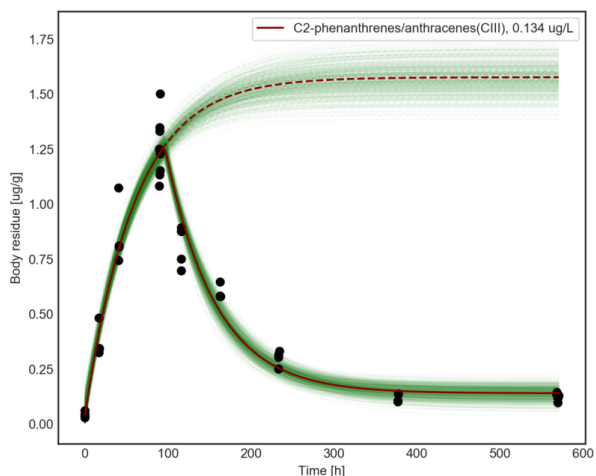
```
[[Fit Statistics]]
# function evals = 488
# data points = 1
# variables = 4
chi-square = 3587.367
reduced chi-square = 3587.367
Akaike info crit = 16.185
Bayesian info crit = 8.185
[[Variables]]
cwrec: 0.25051413 (init= 0)
C0: 0.03397416 (init= 0)
ke: 0.14752148 (init= 0.3602759)
Piw: 0.08956692 (init= 0.0001181614)
alpha: 1 (fixed)
Initial log likelihood = 40.673114
Final log likelihood = 59.894635
```

C1-phenanthrenes/anthracenes(CIII)



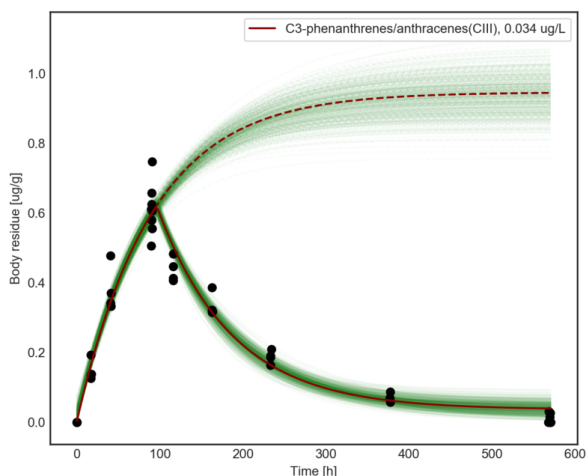
```
[[Fit Statistics]]
# function evals = 476
# data points = 1
# variables = 4
chi-square = 534.126
reduced chi-square = 534.126
Akaike info crit = 14.281
Bayesian info crit = 6.281
[[Variables]]
cwrec: 0.00815823 (init= 0)
C0: 0.02880339 (init= 0)
ke: 0.02748385 (init= 0.02737316)
Piw: 5.70775443 (init= 0.006902871)
alpha: 1 (fixed)
Initial log likelihood = -56.640149
Final log likelihood = 23.111157
```

C2-phenanthrenes/anthracenes(CIII)



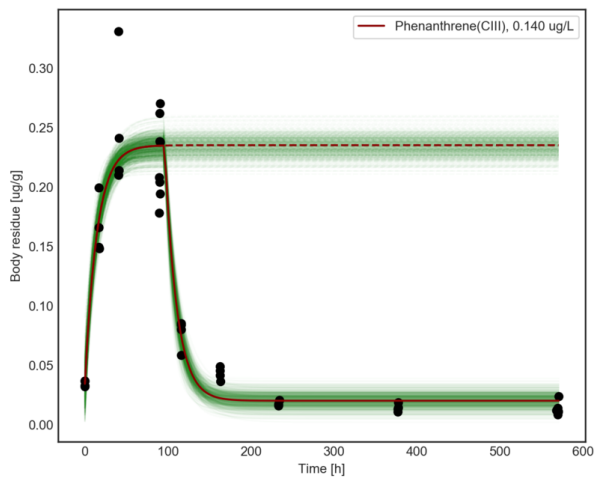
```
[[Fit Statistics]]
# function evals = 421
# data points = 1
# variables = 4
chi-square = 396.866
reduced chi-square = 396.866
Akaike info crit = 13.984
Bayesian info crit = 5.984
[[Variables]]
cwrec: 0.01193905 (init= 0)
C0: 0.03988842 (init= 0)
ke: 0.01660429 (init= 0.01208956)
Piw: 11.7810173 (init= 0.01618063)
alpha: 1 (fixed)
Initial log likelihood = -66.867451
Final log likelihood = 19.921508
```

C3-phenanthrenes/anthracenes(CIII)



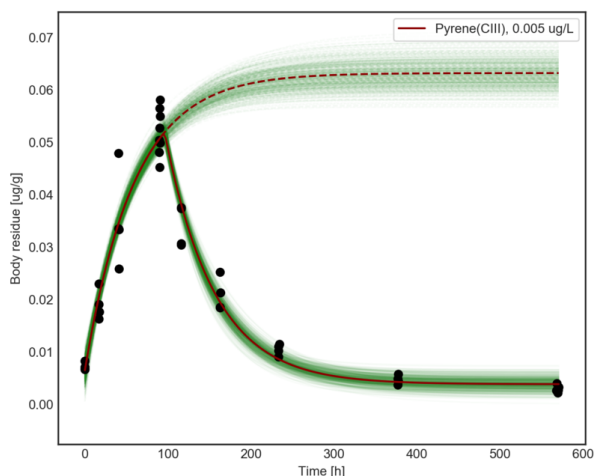
```
[[Fit Statistics]]
# function evals = 442
# data points = 1
# variables = 4
chi-square = 2730.771
reduced chi-square = 2730.771
Akaike info crit = 15.912
Bayesian info crit = 7.912
[[Variables]]
cwrec: 0.00130334 (init= 0)
C0: 0.00404947 (init= 0)
ke: 0.01107723 (init= 0.004074891)
Piw: 28.0885683 (init= 0.04886281)
alpha: 1 (fixed)
Initial log likelihood = -35.778478
Final log likelihood = 52.256781
```

Phenanthrene(CIII)



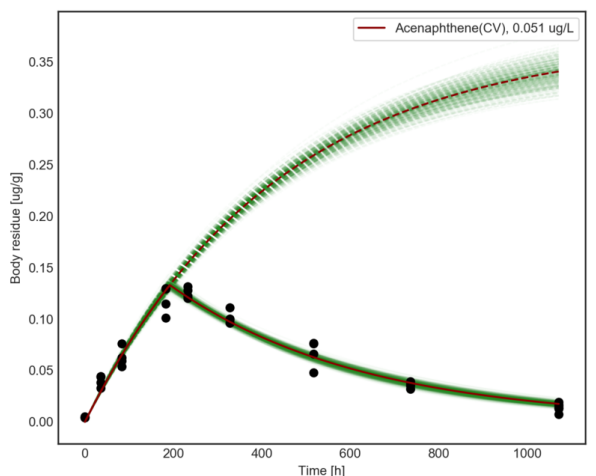
```
[[Fit Statistics]]
# function evals = 433
# data points = 1
# variables = 4
chi-square = 6455.731
reduced chi-square = 6455.731
Akaike info crit = 16.773
Bayesian info crit = 8.773
[[Variables]]
cwrec: 0.01199434 (init= 0)
C0: 0.03447191 (init= 0)
ke: 0.06858442 (init= 0.09254176)
Piw: 1.68595879 (init= 0.001734634)
alpha: 1 (fixed)
Initial log likelihood = 4.404864
Final log likelihood = 80.347562
```

Pyrene(CIII)



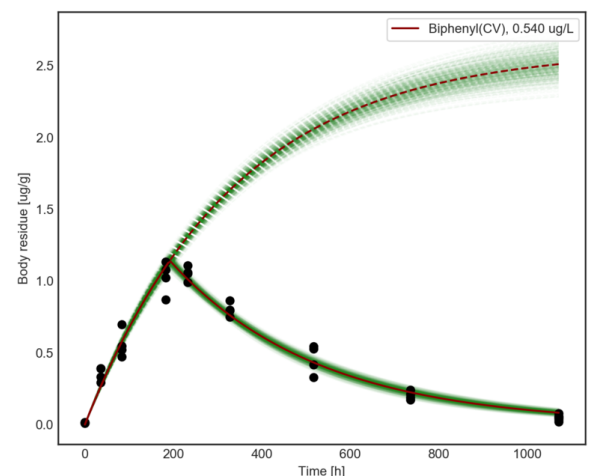
```
[[Fit Statistics]]
# function evals = 433
# data points = 1
# variables = 4
chi-square = 26347.572
reduced chi-square = 26347.572
Akaike info crit = 18.179
Bayesian info crit = 10.179
[[Variables]]
cwrec: 0.00030621 (init= 0)
C0: 0.00650768 (init= 0)
ke: 0.01680253 (init= 0.02509609)
Piw: 12.5568850 (init= 0.007568756)
alpha: 1 (fixed)
Initial log likelihood = 73.336327
Final log likelihood = 162.319352
```

Acenaphthene(CV)



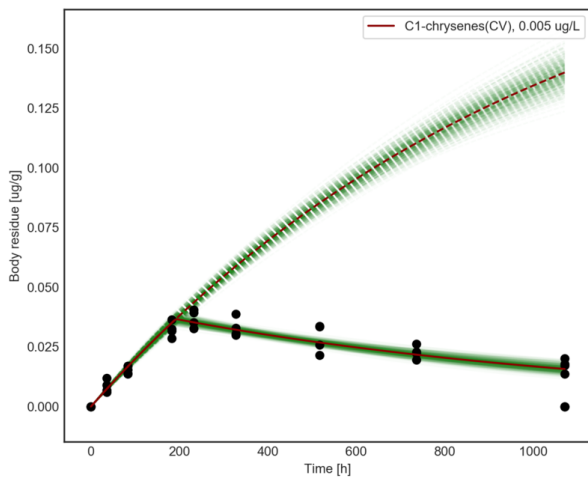
```
[[Fit Statistics]]
# function evals = 178
# data points = 1
# variables = 2
chi-square = 13587.272
reduced chi-square = 13587.272
Akaike info crit = 13.517
Bayesian info crit = 9.517
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00230511 (init= 0.007457141)
Piw: 7.29492007 (init= 0.004159319)
alpha: 1 (fixed)
Initial log likelihood = 31.273567
Final log likelihood = 116.564455
```

Biphenyl(CV)



```
[[Fit Statistics]]
# function evals = 174
# data points = 1
# variables = 2
chi-square = 1022.721
reduced chi-square = 1022.721
Akaike info crit = 10.930
Bayesian info crit = 6.930
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00298728 (init= 0.007205586)
Piw: 4.85125523 (init= 0.004456755)
alpha: 1 (fixed)
Initial log likelihood = -52.893327
Final log likelihood = 31.980008
```

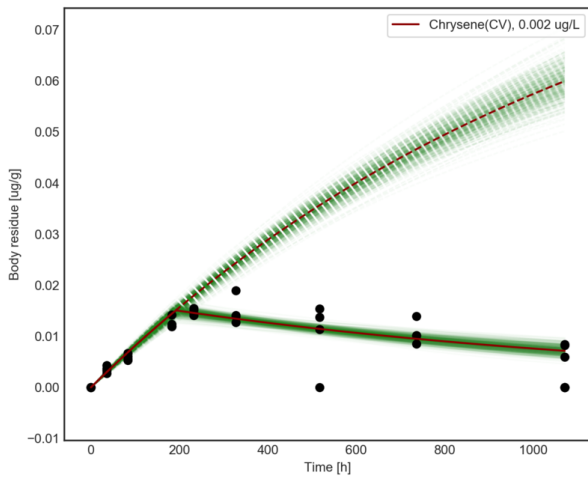

C1-chrysenes(CV)



```

[[Fit Statistics]]
# function evals = 190
# data points = 1
# variables = 2
chi-square = 21718.586
reduced chi-square = 21718.586
Akaike info crit = 13.986
Bayesian info crit = 9.986
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00096148 (init= 4.814425e-05)
Piw: 46.1257185 (init= 1.315134)
alpha: 1 (fixed)
Initial log likelihood = 76.355525
Final log likelihood = 147.372271
    
```

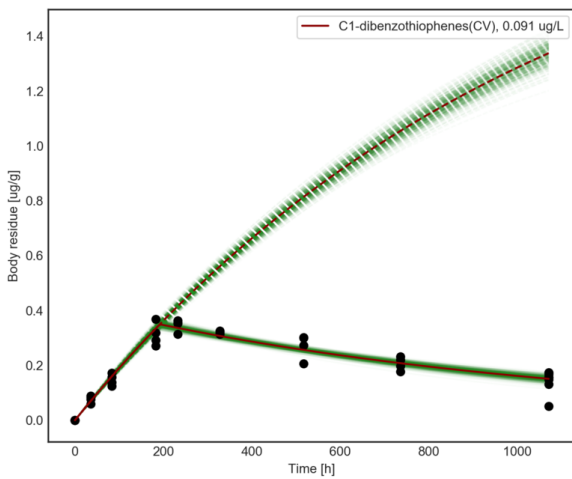
Chrysene(CV)



```

[[Fit Statistics]]
# function evals = 204
# data points = 1
# variables = 2
chi-square = 29036.546
reduced chi-square = 29036.546
Akaike info crit = 14.276
Bayesian info crit = 10.276
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00084713 (init= 0.0001732949)
Piw: 48.7156324 (init= 0.3622185)
alpha: 1 (fixed)
Initial log likelihood = 111.313573
Final log likelihood = 170.401131
    
```

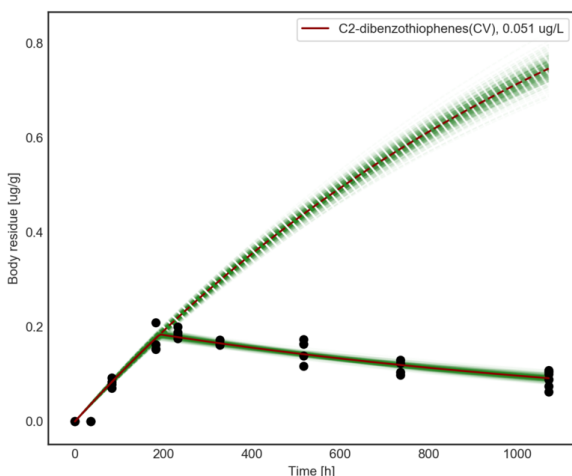
C1-dibenzothiophenes(CV)



```

[[Fit Statistics]]
# function evals = 175
# data points = 1
# variables = 2
chi-square = 4702.365
reduced chi-square = 4702.365
Akaike info crit = 12.456
Bayesian info crit = 8.456
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00095436 (init= 0.0015654)
Piw: 22.9823547 (init= 0.0362223)
alpha: 1 (fixed)
Initial log likelihood = -14.310823
Final log likelihood = 68.573789
    
```

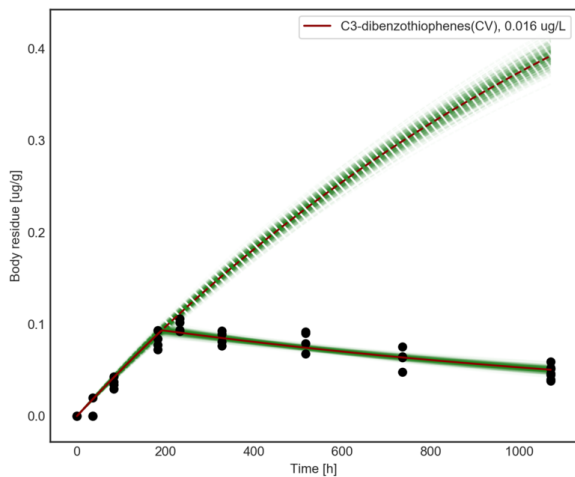
C2-dibenzothiophenes(CV)



```

[[Fit Statistics]]
# function evals = 182
# data points = 1
# variables = 2
chi-square = 8748.160
reduced chi-square = 8748.160
Akaike info crit = 13.077
Bayesian info crit = 9.077
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00079398 (init= 0.0003909934)
Piw: 25.4441323 (init= 0.1581144)
alpha: 1 (fixed)
Initial log likelihood = 10.168842
Final log likelihood = 93.531599
    
```

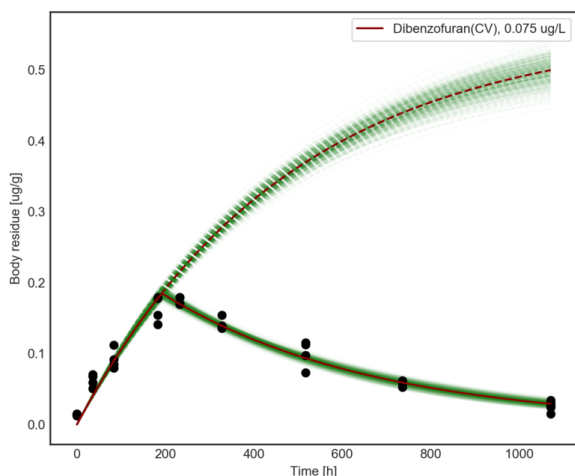
C3-dibenzothiophenes(CV)



```

[[Fit Statistics]]
# function evals = 172
# data points = 1
# variables = 2
chi-square = 13720.681
reduced chi-square = 13720.681
Akaike info crit = 13.527
Bayesian info crit = 9.527
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00070088 (init= 0.0002328023)
Piw: 46.7857766 (init= 0.2685164)
alpha: 1 (fixed)
Initial log likelihood = 36.325055
Final log likelihood = 117.135311
    
```

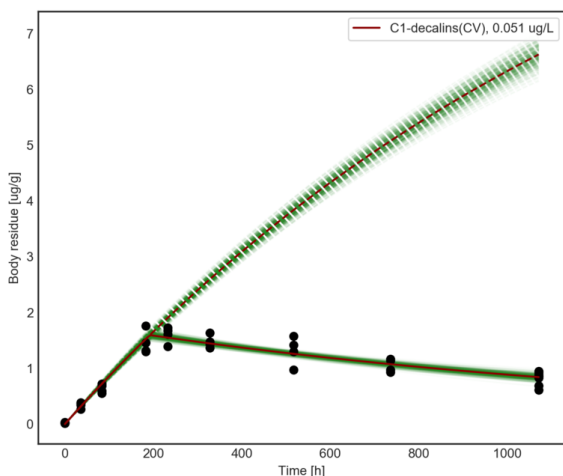
Dibenzofuran(CV)



```

[[Fit Statistics]]
# function evals = 165
# data points = 1
# variables = 2
chi-square = 9582.327
reduced chi-square = 9582.327
Akaike info crit = 13.168
Bayesian info crit = 9.168
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00209633 (init= 0.005094801)
Piw: 7.48592958 (init= 0.00810955)
alpha: 1 (fixed)
Initial log likelihood = 17.289620
Final log likelihood = 97.889361
    
```

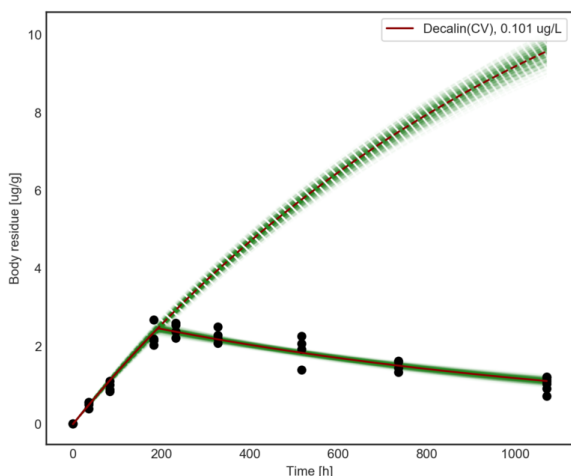
C1-decalins(CV)



```

[[Fit Statistics]]
# function evals = 201
# data points = 1
# variables = 2
chi-square = 56.911
reduced chi-square = 56.911
Akaike info crit = 8.041
Bayesian info crit = 4.041
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00072744 (init= 0.00256893)
Piw: 238.154419 (init= 0.02036951)
alpha: 1 (fixed)
Initial log likelihood = -77.022176
Final log likelihood = 7.543954
    
```

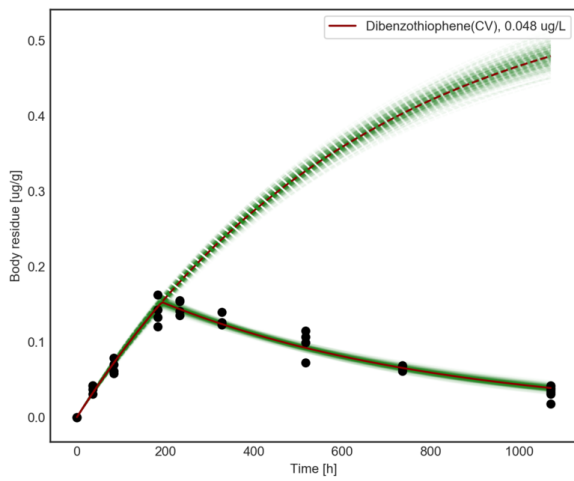
Decalin(CV)



```

[[Fit Statistics]]
# function evals = 204
# data points = 1
# variables = 2
chi-square = 41.860
reduced chi-square = 41.860
Akaike info crit = 7.734
Bayesian info crit = 3.734
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00090769 (init= 0.005171354)
Piw: 152.901379 (init= 0.007924966)
alpha: 1 (fixed)
Initial log likelihood = -92.801761
Final log likelihood = -6.469910
    
```

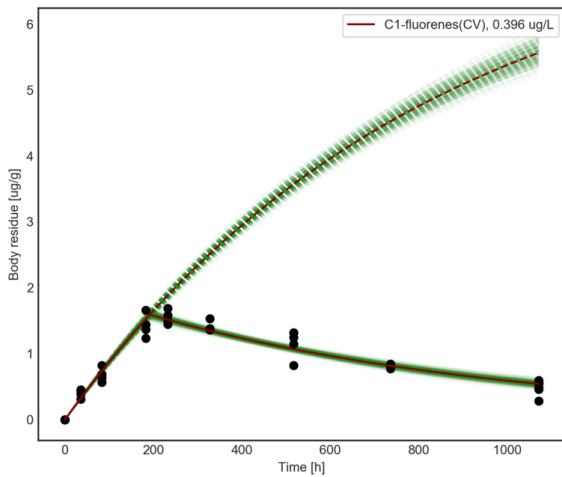
Dibenzothiophene(CV)



```

[[Fit Statistics]]
# function evals = 164
# data points = 1
# variables = 2
chi-square = 12118.568
reduced chi-square = 12118.568
Akaike info crit = 13.402
Bayesian info crit = 9.402
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00155884 (init= 0.003206588)
Piw: 12.2750491 (init= 0.01545198)
alpha: 1 (fixed)
Initial log likelihood = 22.778883
Final log likelihood = 110.084369
    
```

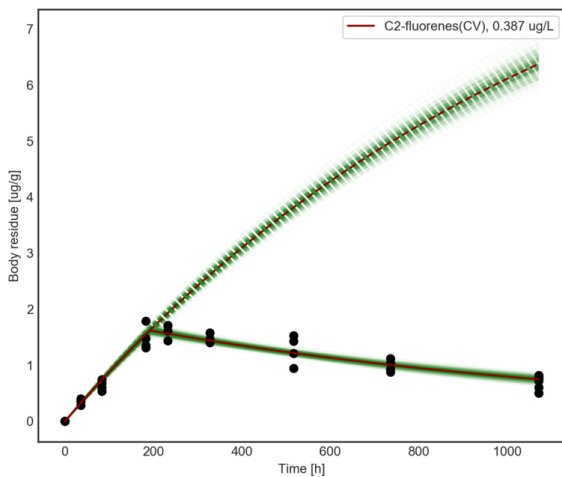
C1-fluorenes(CV)



```

[[Fit Statistics]]
# function evals = 181
# data points = 1
# variables = 2
chi-square = 160.317
reduced chi-square = 160.317
Akaike info crit = 9.077
Bayesian info crit = 5.077
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00122286 (init= 0.001245065)
Piw: 19.2514596 (init= 0.04666322)
alpha: 1 (fixed)
Initial log likelihood = -72.995346
Final log likelihood = 12.661626
    
```

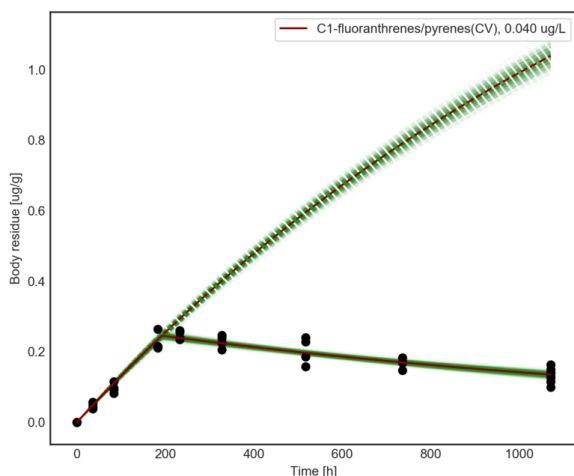
C2-fluorenes(CV)



```

[[Fit Statistics]]
# function evals = 170
# data points = 1
# variables = 2
chi-square = 71.931
reduced chi-square = 71.931
Akaike info crit = 8.276
Bayesian info crit = 4.276
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00087739 (init= 0.0007598428)
Piw: 27.0297879 (init= 0.07924516)
alpha: 1 (fixed)
Initial log likelihood = -76.253960
Final log likelihood = 8.481244
    
```

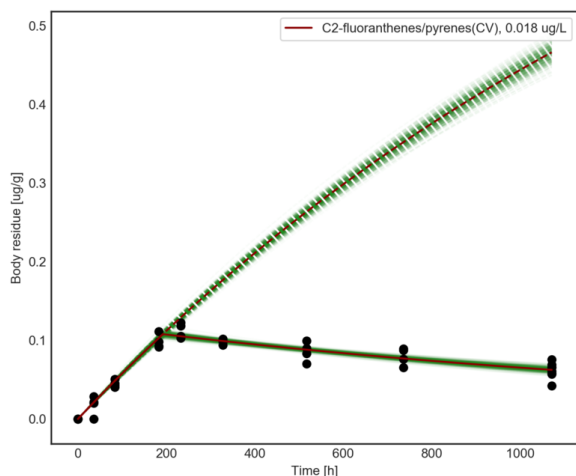
C1-fluoranthrenes/pyrenes(CV)



```

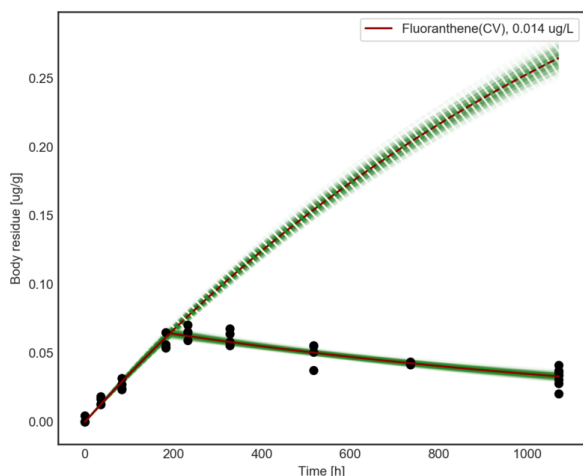
[[Fit Statistics]]
# function evals = 196
# data points = 1
# variables = 2
chi-square = 7406.441
reduced chi-square = 7406.441
Akaike info crit = 12.910
Bayesian info crit = 8.910
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00067896 (init= 0.0002381364)
Piw: 50.4905785 (init= 0.2624042)
alpha: 1 (fixed)
Initial log likelihood = -2.526026
Final log likelihood = 86.060683
    
```

C2-fluoranthenes/pyrenes(CV)



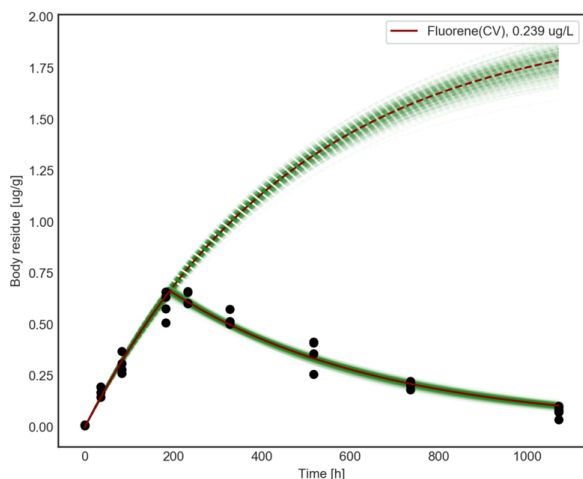
```
[[Fit Statistics]]
# function evals = 202
# data points = 1
# variables = 2
chi-square = 14007.916
reduced chi-square = 14007.916
Akaike info crit = 13.547
Bayesian info crit = 9.547
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00062126 (init= 0.0001176148)
Piw: 52.5964461 (init= 0.5357602)
alpha: 1 (fixed)
Initial log likelihood = 29.881137
Final log likelihood = 118.355042
```

Fluoranthene(CV)



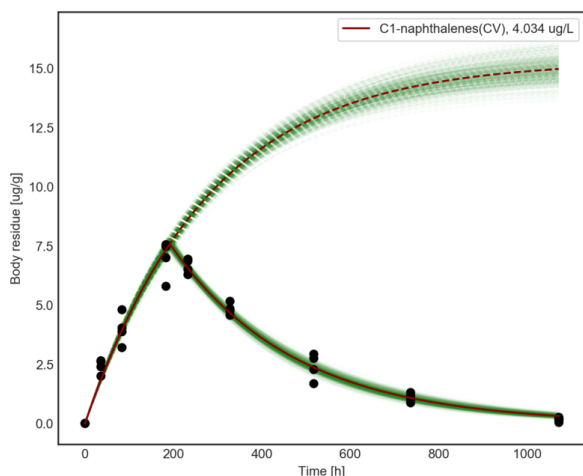
```
[[Fit Statistics]]
# function evals = 177
# data points = 1
# variables = 2
chi-square = 19006.572
reduced chi-square = 19006.572
Akaike info crit = 13.853
Bayesian info crit = 9.853
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00075628 (init= 0.0007273513)
Piw: 35.0945925 (init= 0.08297985)
alpha: 1 (fixed)
Initial log likelihood = 51.733134
Final log likelihood = 137.864326
```

Fluorene(CV)



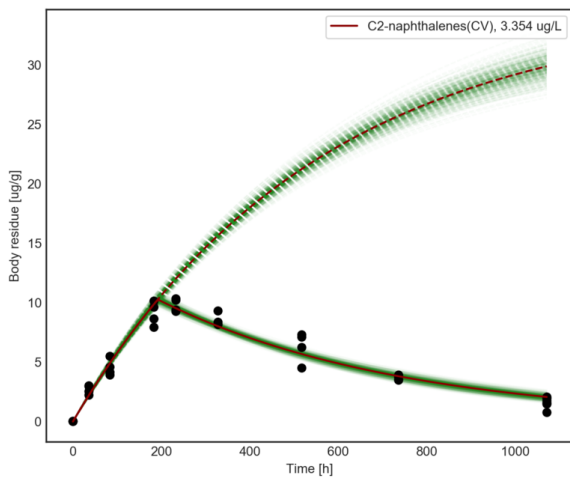
```
[[Fit Statistics]]
# function evals = 177
# data points = 1
# variables = 2
chi-square = 2743.280
reduced chi-square = 2743.280
Akaike info crit = 11.917
Bayesian info crit = 7.917
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00210795 (init= 0.005325982)
Piw: 8.37055781 (init= 0.007568306)
alpha: 1 (fixed)
Initial log likelihood = -33.697652
Final log likelihood = 52.376335
```

C1-naphthalenes(CV)



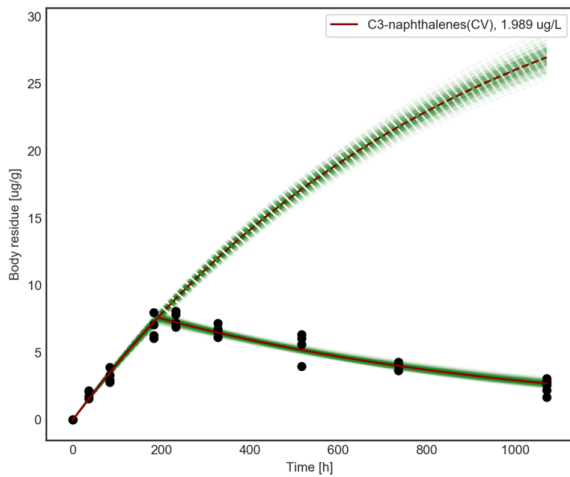
```
[[Fit Statistics]]
# function evals = 174
# data points = 1
# variables = 2
chi-square = 1608.328
reduced chi-square = 1608.328
Akaike info crit = 11.383
Bayesian info crit = 7.383
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00356843 (init= 0.007875178)
Piw: 3.79664853 (init= 0.003707051)
alpha: 1 (fixed)
Initial log likelihood = -127.479455
Final log likelihood = -40.103969
```

C2-naphthalenes(CV)



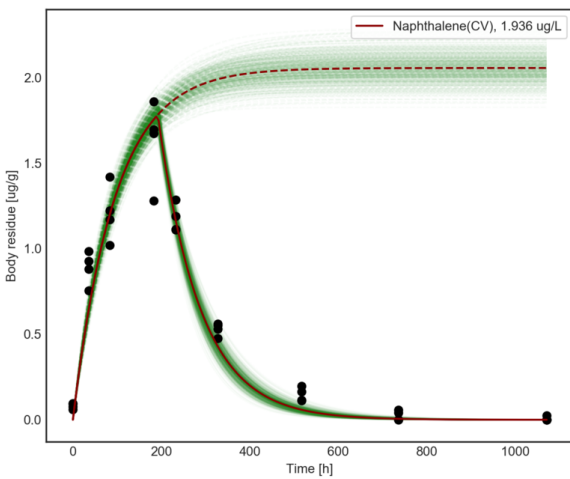
```
[[Fit Statistics]]
# function evals = 184
# data points = 1
# variables = 2
chi-square = 3673.403
reduced chi-square = 3673.403
Akaike info crit = 12.209
Bayesian info crit = 8.209
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00181806 (init= 0.003950426)
Piw: 10.3917458 (init= 0.01172164)
alpha: 1 (fixed)
Initial log likelihood = -144.370097
Final log likelihood = -60.608606
```

C3-naphthalenes(CV)



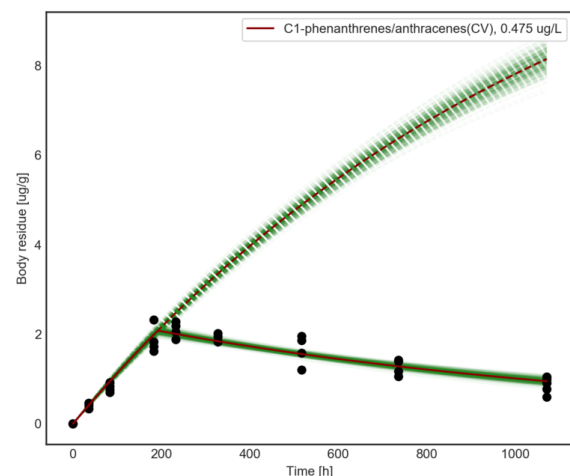
```
[[Fit Statistics]]
# function evals = 177
# data points = 1
# variables = 2
chi-square = 2498.268
reduced chi-square = 2498.268
Akaike info crit = 11.823
Bayesian info crit = 7.823
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00117637 (init= 0.001733682)
Piw: 18.9297837 (init= 0.03228321)
alpha: 1 (fixed)
Initial log likelihood = -135.825304
Final log likelihood = -49.982675
```

Naphthalene(CV)



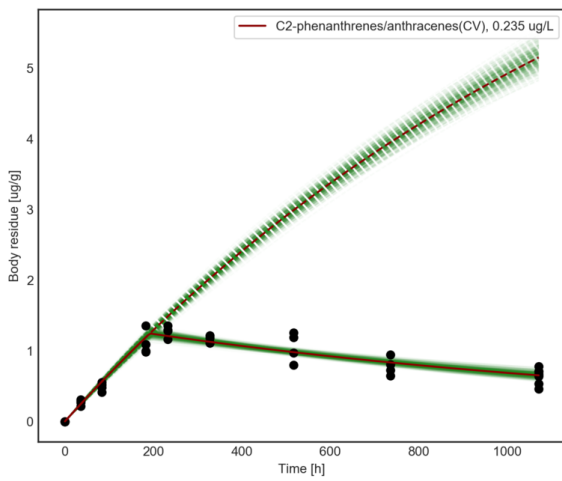
```
[[Fit Statistics]]
# function evals = 193
# data points = 1
# variables = 2
chi-square = 40.011
reduced chi-square = 40.011
Akaike info crit = 7.689
Bayesian info crit = 3.689
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.01050903 (init= 0.01148037)
Piw: 1.06177769 (init= 0.001172614)
alpha: 1 (fixed)
Initial log likelihood = -65.623658
Final log likelihood = 6.325410
```

C1-phenanthrenes/anthracenes(CV)



```
[[Fit Statistics]]
# function evals = 175
# data points = 1
# variables = 2
chi-square = 21.883
reduced chi-square = 21.883
Akaike info crit = 7.086
Bayesian info crit = 3.086
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00088936 (init= 0.0008657281)
Piw: 27.9337652 (init= 0.06901971)
alpha: 1 (fixed)
Initial log likelihood = -86.180181
Final log likelihood = -4.677908
```

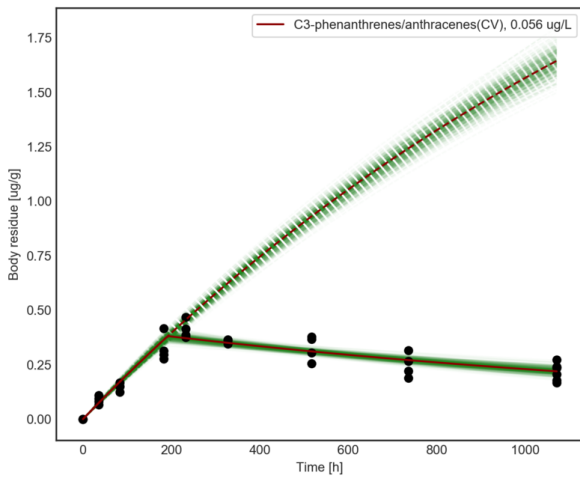
C2-phenanthrenes/anthracenes(CV)



```

[[Fit Statistics]]
# function evals = 183
# data points = 1
# variables = 2
chi-square = 210.721
reduced chi-square = 210.721
Akaike info crit = 9.351
Bayesian info crit = 5.351
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00073611 (init= 0.0003823269)
Piw: 40.1884924 (init= 0.1617973)
alpha: 1 (fixed)
Initial log likelihood = -67.009098
Final log likelihood = 14.516226
    
```

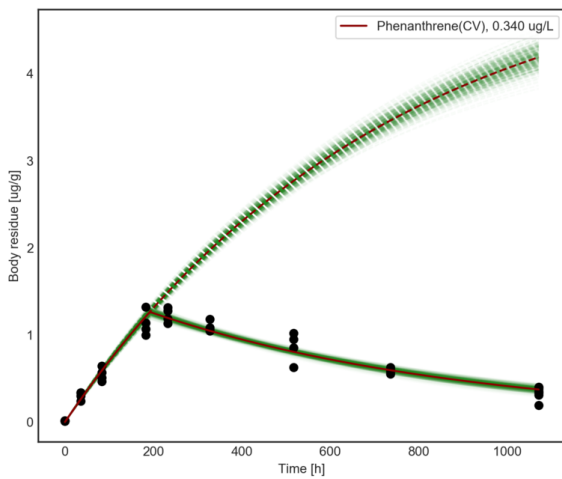
C3-phenanthrenes/anthracenes(CV)



```

[[Fit Statistics]]
# function evals = 189
# data points = 1
# variables = 2
chi-square = 2990.199
reduced chi-square = 2990.199
Akaike info crit = 12.003
Bayesian info crit = 8.003
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00062721 (init= 0.0001288618)
Piw: 59.8996888 (init= 0.4886191)
alpha: 1 (fixed)
Initial log likelihood = -20.848526
Final log likelihood = 54.682708
    
```

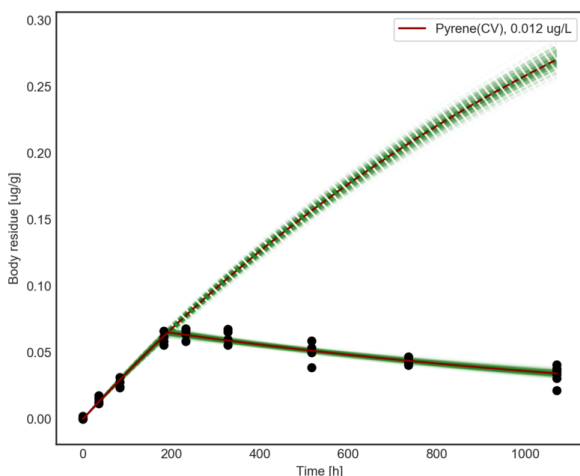
Phenanthrene(CV)



```

[[Fit Statistics]]
# function evals = 182
# data points = 1
# variables = 2
chi-square = 550.875
reduced chi-square = 550.875
Akaike info crit = 10.312
Bayesian info crit = 6.312
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00138399 (init= 0.002927946)
Piw: 15.9292046 (init= 0.01733734)
alpha: 1 (fixed)
Initial log likelihood = -62.749314
Final log likelihood = 23.470725
    
```

Pyrene(CV)



```

[[Fit Statistics]]
# function evals = 180
# data points = 1
# variables = 2
chi-square = 20017.140
reduced chi-square = 20017.140
Akaike info crit = 13.904
Bayesian info crit = 9.904
[[Variables]]
cwrec: 0 (fixed)
C0: 0 (fixed)
ke: 0.00073011 (init= 0.0007937026)
Piw: 41.7817468 (init= 0.07567856)
alpha: 1 (fixed)
Initial log likelihood = 51.037836
Final log likelihood = 141.481943
    
```