Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Comparison of Biokinetic Models for Non-dissolvable Engineered Nanomaterials in Freshwater Aquatic Organisms

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Supporting Information

1 Calculation of measures for goodness-of-fit

For each nonlinear regression, we calculated the following measures for goodness-of-fit.

Adjusted R squared (adjusted R^2) determines the extent of the variance of the dependent variable, which can be explained by the independent variable. It can compensate for possible bias due to different number of parameters:

$$R_{adj}^2 = 1 - \frac{n-1}{n-p} * (1 - R^2) \tag{1}$$

where n = sample size and p = number of parameters, and R^2 using the most general definition:[1,2]

$$R^2 = 1 - \frac{RSS}{TSS} = 1 - \frac{\sum(\gamma - \hat{\gamma})^2}{\sum(\gamma - \bar{\gamma})^2} \tag{2}$$

where RSS = residual sum-of-squares, TSS = total sum-of-squares, γ = response values, $\hat{\gamma}$ = fitted values and $\bar{\gamma}$ = the mean of response values.

The Akaike Information Criterion (AIC) is a measure that is widely accepted for measuring the validity within a cohort of nonlinear models and frequently used for model selection.[3–5] The smaller the value is, the better the model fits:

$$AIC = 2p - 2\ln(L) \tag{3}$$

where p = number of parameters and $\ln(L)$ = maximum log-likelihood of the estimated model. $\ln(L)$ in the case of a nonlinear fit with normally distributed errors is calculated by

$$\ln(L) = 0.5 * \left(-N * \left(\ln 2\pi + 1 - \ln N + \ln \sum_{i=1}^{n} {x_i}^2\right)\right) \tag{4}$$

where $x_1, \dots, x_n$ = the residuals form the nonlinear least-squares fit and N = their number.

It has been suggested that when the sample size is small, especially when the ratio of sample (n) and number of parameters (p) is less than 40, a bias-corrected AIC (AICc) should be used.[6] The models for comparison do not need to be nested:

$$AICc = AIC + \frac{2p(p+1)}{n-p-1} \tag{5}$$

where n = sample size and p = number of parameters. It is important to note that AIC or AICc is only a comparator between models, but not an indication of the quality of the fit itself.[7]

In order to obtain values for the validity of a fit, we used Akaike weights which calculate the weight of evidence for each model within a cohort of models in question:[8,9]

$$w_i(AIC) = \frac{\exp\left\{-\frac{1}{2}\Delta_i(AIC)\right\}}{\sum_{k=1}^{K}\exp\left\{-\frac{1}{2}\Delta_k(AIC)\right\}} \tag{6}$$

where *i*, *k* = model numbers, $\Delta_i(AIC)$ = the difference in AIC of each model in comparison the model with the lowest AIC, subsequently normalized to their sum (denominator). Here, we used the bias-corrected AICc for calculating the Akaike weights. To interpret Akaike weight, for example, w_i of 0.8 for a model implies that it has an 80% chance of being the best among the considered models.

2 Model comparison

Table S1: Summary of the non-linear regression results predictions for five models for each dataset. C_w = water concentration (mg/L), GO = graphene oxide, k_u = uptake rate; k_e = elimination rate; SF = storage fraction, C_{sat} = body burden at saturated state, K_M = Michaelis-Menten constant.

Dataset number	Organisms	Material	Exposure type	C_w^{*} mg/L	Depuration with feeding	Model	k_u^{**} L/kg/h	k_e 1/h	SF	C_{sat} mg/kg	K_M h	Adjusted R^2	AICc	$\Delta(\mathrm{AIC})$	Akaike weights	Visually cover by 95% confidence bands	Reference
1	*S. obliquus*	C_{60}	aqueous	2	No	Model 1	1697	1.861	-	-	-	0.928	115.0	2.6	0.13	No	[10]
1	*S. obliquus*	C_{60}	aqueous	2	No	Model 2	1884	2.080	0.068	-	-	0.926	118.3	6.0	0.02	Yes	[10]
1	*S. obliquus*	C_{60}	aqueous	2	No	Model 3	2316	2.713	0.002	-	-	0.953	113.8	1.5	0.23	Yes	[10]
1	*S. obliquus*	C_{60}	aqueous	2	No	Model 4	1697	1.831	-	-	-	0.928	115.0	2.6	0.13	No	[10]
1	*S. obliquus*	C_{60}	aqueous	2	No	Model 5	-	2.386	-	2026	0.555	0.944	112.3	0.0	0.48	No	[10]
2	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	33380	0.637	-	-	-	0.977	539.6	0.0	0.37	Yes	[11]
2	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	33682	0.644	0.012	-	-	0.977	541.6	2.0	0.13	Yes	[11]
2	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	33874	0.653	0.001	-	-	0.977	541.6	2.0	0.13	Yes	[11]
2	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	33380	0.624	-	-	-	0.977	539.6	0.0	0.37	Yes	[11]
2	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	0.906	-	61554	1.428	0.971	549.3	9.7	0.00	Yes	[11]
3	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	14157	0.420	-	-	-	0.924	547.1	2.4	0.17	Yes	[11]
3	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	14197	0.421	0.005	-	-	0.921	549.7	5.0	0.05	Yes	[11]
3	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	14330	0.429	0.001	-	-	0.922	549.5	4.8	0.05	Yes	[11]
3	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	14157	0.407	-	-	-	0.924	547.1	2.4	0.17	Yes	[11]
3	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	0.729	-	43659	2.861	0.932	544.7	0.0	0.56	Yes	[11]
4	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	24998	0.305	-	-	-	0.953	585.6	7.7	0.02	Yes	[11]
4	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	24998	0.305	0.000	-	-	0.951	588.2	10.3	0.01	Yes	[11]
4	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	25028	0.306	0.000	-	-	0.950	588.3	10.4	0.01	Yes	[11]
4	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	24998	0.292	-	-	-	0.953	585.7	7.8	0.02	Yes	[11]
4	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	0.480	-	107190	3.987	0.964	577.9	0.0	0.95	Yes	[11]
5	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	59546	0.789	-	-	-	0.966	580.8	0.0	0.39	Yes	[11]
5	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	59637	0.790	0.002	-	-	0.964	583.3	2.5	0.11	Yes	[11]
5	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	59658	0.701	0.000	-	-	0.966	583.4	2.6	0.10	Yes	[11]
5	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	59546	0.776	-	-	-	0.966	580.8	0.0	0.38	Yes	[11]
5	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	1.389	-	88405	1.177	0.963	587.0	6.2	0.02	Yes	[11]
6	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	29201	0.741	-	-	-	0.978	521.2	0.0	0.31	Yes	[11]
6	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	29635	0.755	0.020	-	-	0.978	522.4	1.2	0.16	Yes	[11]
6	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	29953	0.772	0.001	-	-	0.978	521.9	0.7	0.21	Yes	[11]
6	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	29201	0.729	-	-	-	0.978	521.2	0.0	0.30	Yes	[11]
6	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	1.090	-	45772	1.191	0.975	527.1	5.9	0.02	Yes	[11]
7	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	13197	0.463	-	-	-	0.921	539.2	24.9	0.00	Yes	[11]
7	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	13204	0.464	0.001	-	-	0.920	541.3	27.0	0.00	Yes	[11]
7	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	13524	0.484	0.002	-	-	0.920	541.4	27.1	0.00	Yes	[11]
7	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	13197	0.451	-	-	-	0.921	539.2	24.9	0.00	Yes	[11]
7	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	1.026	-	39163	3.109	0.965	514.3	0.0	1.00	Yes	[11]

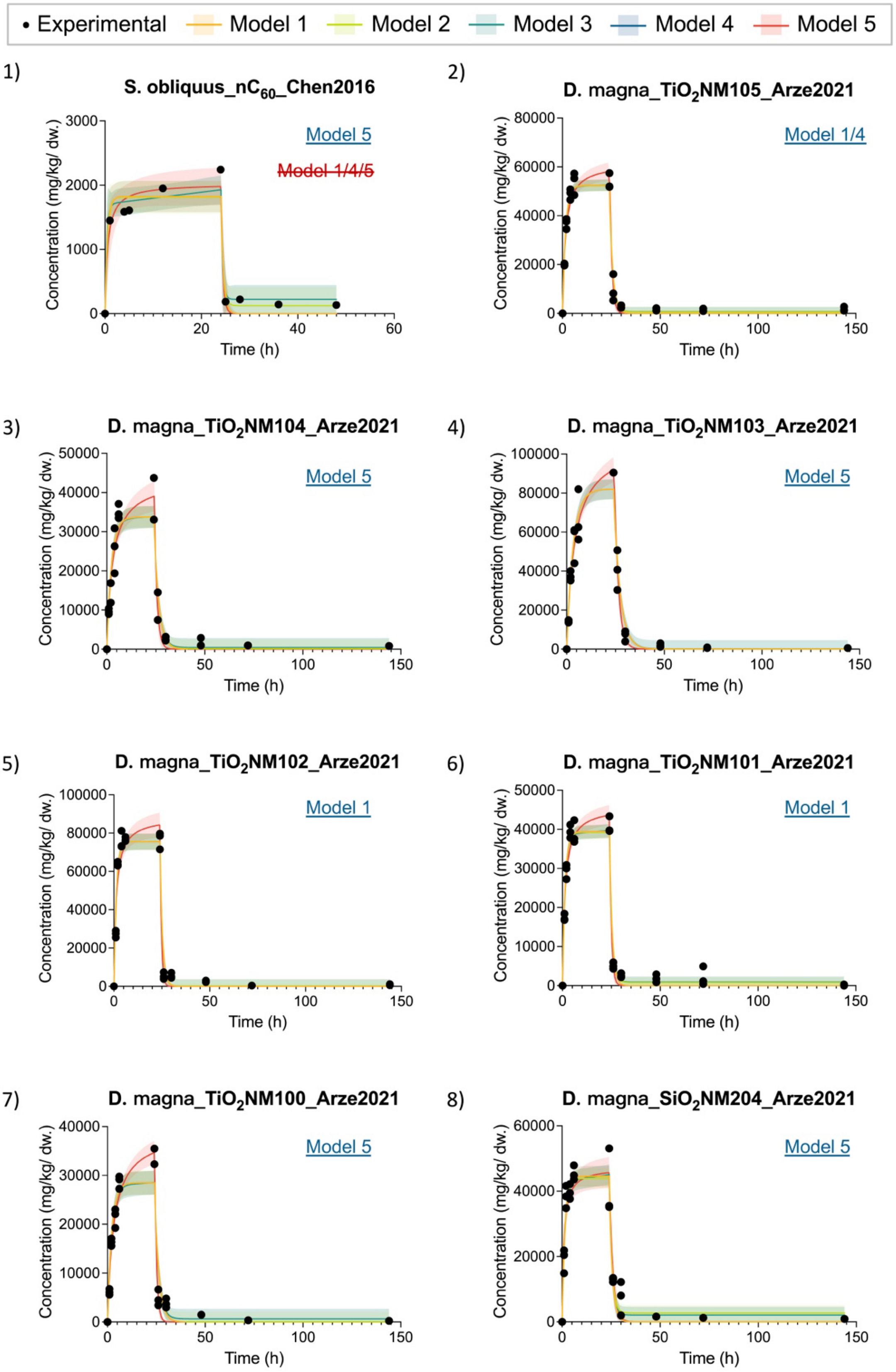
8	*D. magna*	SiO_2	aqueous	1	Yes	Model 1	11698	0.676	-	-	-	0.846	529.1	18.3	0.00	Yes	11
8	*D. magna*	SiO_2	aqueous	1	Yes	Model 2	12718	0.750	0.094	-	-	0.862	527.0	16.2	0.00	Yes	11
8	*D. magna*	SiO_2	aqueous	1	Yes	Model 3	14134	0.900	0.007	-	-	0.886	520.7	9.9	0.01	Yes	11
8	*D. magna*	SiO_2	aqueous	1	Yes	Model 4	11699	0.663	-	-	-	0.840	529.5	18.7	0.00	Yes	11
8	*D. magna*	SiO_2	aqueous	1	Yes	Model 5	-	0.072	-	22387	1.951	0.915	510.8	0.0	0.99	Yes	11
9	*D. magna*	SiO_2	aqueous	1	Yes	Model 1	29596	0.664	-	-	-	0.936	560.7	2.4	0.15	Yes	11
9	*D. magna*	SiO_2	aqueous	1	Yes	Model 2	31408	0.715	0.062	-	-	0.943	558.3	0.0	0.51	Yes	11
9	*D. magna*	SiO_2	aqueous	1	Yes	Model 3	31398	0.729	0.003	-	-	0.940	560.4	2.1	0.18	Yes	11
9	*D. magna*	SiO_2	aqueous	1	Yes	Model 4	29596	0.651	-	-	-	0.936	560.8	2.5	0.15	Yes	11
9	*D. magna*	SiO_2	aqueous	1	Yes	Model 5	-	0.587	-	47362	0.872	0.920	569.7	11.4	0.00	Yes	11
10	*D. magna*	TiO_2	aqueous	1	Yes	Model 1	52	0.026	-	-	-	0.858	99.5	0.0	0.31	Yes	12
10	*D. magna*	TiO_2	aqueous	1	Yes	Model 2	59	0.038	0.168	-	-	0.852	104.3	4.9	0.03	Yes	12
10	*D. magna*	TiO_2	aqueous	1	Yes	Model 3	55	0.035	0.085	-	-	0.841	105.0	5.6	0.02	Yes	12
10	*D. magna*	TiO_2	aqueous	1	Yes	Model 4	52	0.014	-	-	-	0.858	99.5	0.0	0.31	Yes	12
10	*D. magna*	TiO_2	aqueous	1	Yes	Model 5	-	0.020	-	1225	12.010	0.909	99.4	0.0	0.32	Yes	12
11	*D. magna*	TiO_2	aqueous	1	No	Model 1	3557	0.014	-	-	-	0.413	197.9	33.0	0.00	No	12
11	*D. magna*	TiO_2	aqueous	1	No	Model 2	10591	0.156	0.685	-	-	0.777	192.7	27.8	0.00	Yes	12
11	*D. magna*	TiO_2	aqueous	1	No	Model 3	Unstable	0.928	0.075	-	-	-	-	-	-	No	12
11	*D. magna*	TiO_2	aqueous	1	No	Model 4	3557	0.001	-	-	-	0.413	197.9	33.0	0.00	No	12
11	*D. magna*	TiO_2	aqueous	1	No	Model 5	-	0.008	-	70541	3.674	0.986	164.9	0.0	1.00	Yes	12
12	*D. magna*	TiO_2	aqueous	0.1	No	Model 1	3894	0.039	-	-	-	0.483	148.3	15.6	0.00	Yes	12
12	*D. magna*	TiO_2	aqueous	0.1	No	Model 2	6738	0.106	0.325	-	-	0.665	149.9	17.2	0.00	Yes	12
12	*D. magna*	TiO_2	aqueous	0.1	No	Model 3	5356	0.088	0.117	-	-	0.505	152.3	19.6	0.00	Yes	12
12	*D. magna*	TiO_2	aqueous	0.1	No	Model 4	3894	0.026	-	-	-	0.483	148.3	15.6	0.00	Yes	12
12	*D. magna*	TiO_2	aqueous	0.1	No	Model 5	-	0.020	-	5310	2.589	0.930	132.7	0.0	1.00	Yes	12
13	*D. magna*	C_{60}	dietary	15.02	No	Model 1	129	0.219	-	-	-	-0.107	194.1	21.2	0.00	No	10
13	*D. magna*	C_{60}	dietary	15.02	No	Model 2	332	0.635	0.455	-	-	0.848	172.9	0.0	0.90	Yes	10
13	*D. magna*	C_{60}	dietary	15.02	No	Model 3	348	0.832	0.014	-	-	0.783	177.2	4.3	0.10	Yes	10
13	*D. magna*	C_{60}	dietary	15.02	No	Model 4	129	0.207	-	-	-	-0.107	194.1	21.2	0.00	No	10
13	*D. magna*	C_{60}	dietary	15.02	No	Model 5	-	0.042	-	8046	0.761	0.320	192.2	19.3	0.00	No	10
14	*D. magna*	Graphene	aqueous	0.25	Yes	Model 1	19164	0.915	-	-	-	0.798	133.9	16.2	0.00	No	13
14	*D. magna*	Graphene	aqueous	0.25	Yes	Model 2	19164	0.915	0.000	-	-	0.758	139.2	21.5	0.00	Yes	13
14	*D. magna*	Graphene	aqueous	0.25	Yes	Model 3	20492	1.008	0.002	-	-	0.762	139.0	21.3	0.00	Yes	13
14	*D. magna*	Graphene	aqueous	0.25	Yes	Model 4	19164	0.902	-	-	-	0.798	133.9	16.2	0.00	No	13
14	*D. magna*	Graphene	aqueous	0.25	Yes	Model 5	-	2.780	-	7988.00	3.595	0.984	117.7	0.0	1.00	No	13
15	*D. magna*	Graphene	aqueous	0.1	Yes	Model 1	14934	0.539	-	-	-	0.541	130.0	10.8	0.00	No	13
15	*D. magna*	Graphene	aqueous	0.1	Yes	Model 2	15491	0.562	0.031	-	-	0.537	137.0	17.8	0.00	Yes	13
15	*D. magna*	Graphene	aqueous	0.1	Yes	Model 3	22133	0.892	0.007	-	-	0.541	136.5	17.3	0.00	Yes	13
15	*D. magna*	Graphene	aqueous	0.1	Yes	Model 4	14934	0.527	-	-	-	0.636	130.0	10.8	0.00	No	13
15	*D. magna*	Graphene	aqueous	0.1	Yes	Model 5	-	2.713	-	5414	7.848	0.936	119.2	0.0	0.99	No	13
16	*D. magna*	Graphene	aqueous	0.05	Yes	Model 1	23789	0.875	-	-	-	0.655	113.5	4.4	0.09	No	13
16	*D. magna*	Graphene	aqueous	0.05	Yes	Model 2	26368	0.983	0.107	-	-	0.614	118.1	9.0	0.01	Yes	13
16	*D. magna*	Graphene	aqueous	0.05	Yes	Model 3	34902	1.477	0.007	-	-	0.692	116.1	7.0	0.02	Yes	13
16	*D. magna*	Graphene	aqueous	0.05	Yes	Model 4	23789	0.862	-	-	-	0.655	113.5	4.4	0.09	No	13
16	*D. magna*	Graphene	aqueous	0.05	Yes	Model 5	-	2.707	-	2325	5.276	0.902	109.1	0.0	0.79	No	13
17	*D. magna*	Graphene	aqueous	0.25	Yes	Model 1	2729	0.063	-	-	-	0.822	132.0	10.9	0.00	Yes	13
17	*D. magna*	Graphene	aqueous	0.25	Yes	Model 2	4335	0.128	0.373	-	-	0.897	130.7	9.6	0.01	Yes	13
17	*D. magna*	Graphene	aqueous	0.25	Yes	Model 3	4088	0.162	0.125	-	-	0.858	133.6	12.5	0.00	Yes	13
17	*D. magna*	Graphene	aqueous	0.25	Yes	Model 4	2729	0.051	-	-	-	0.822	132.0	10.9	0.00	Yes	13
17	*D. magna*	Graphene	aqueous	0.25	Yes	Model 5	-	0.042	-	8423	4.056	0.975	121.1	0.0	0.98	Yes	13
18	*D. magna*	Graphene	aqueous	0.1	Yes	Model 1	2531	0.043	-	-	-	0.532	129.0	8.4	0.01	Yes	13
18	*D. magna*	Graphene	aqueous	0.1	Yes	Model 2	6967	0.196	0.623	-	-	0.901	120.6	0.0	0.79	Yes	13

18	*D. magna*	Graphene	aqueous	0.1	Yes	Model 3	9444	0.490	0.100	-	-	0.861	123.6	3.0	0.18	Yes	13
18	*D. magna*	Graphene	aqueous	0.1	Yes	Model 4	2531	0.030	-	-	-	0.532	129.0	8.4	0.01	Yes	13
18	*D. magna*	Graphene	aqueous	0.1	Yes	Model 5	-	0.034	-	5414	7.848	0.801	131.0	10.4	0.00	No	13
19	*D. magna*	Graphene	aqueous	0.05	Yes	Model 1	2144	0.014	-	-	-	0.749	112.3	12.3	0.00	No	13
19	*D. magna*	Graphene	aqueous	0.05	Yes	Model 2	6068	0.146	0.886	-	-	0.960	102.8	2.8	0.19	Yes	13
19	*D. magna*	Graphene	aqueous	0.05	Yes	Model 3	12629	1.015	0.118	-	-	0.907	107.0	7.0	0.02	Yes	13
19	*D. magna*	Graphene	aqueous	0.05	Yes	Model 4	2144	0.001	-	-	-	0.749	113.7	13.7	0.00	No	13
19	*D. magna*	Graphene	aqueous	0.05	Yes	Model 5	-	0.004	-	2357	5.431	0.970	100.0	0.0	0.78	Yes	13
20	*D. magna*	GO	aqueous	10	No	Model 1	1519	0.104	-	-	-	0.891	142.0	0.0	0.48	Yes	14
20	*D. magna*	GO	aqueous	10	No	Model 2	1795	0.134	0.143	-	-	0.884	147.7	5.6	0.03	Yes	14
20	*D. magna*	GO	aqueous	10	No	Model 3	1616	0.120	0.025	-	-	0.860	149.0	6.9	0.01	Yes	14
20	*D. magna*	GO	aqueous	10	No	Model 4	1519	0.091	-	-	-	0.891	142.0	0.0	0.48	Yes	14
20	*D. magna*	GO	aqueous	10	No	Model 5	-	0.077	-	12598	2.138	0.950	151.7	9.7	0.00	Yes	14
21	*D. magna*	GO	aqueous	5	No	Model 1	2915	0.117	-	-	-	0.972	131.7	0.0	0.49	Yes	14
21	*D. magna*	GO	aqueous	5	No	Model 2	2956	0.119	0.013	-	-	0.962	138.9	7.2	0.01	Yes	14
21	*D. magna*	GO	aqueous	5	No	Model 3	2830	0.109	0.000	-	-	0.954	150.3	18.6	0.00	Yes	14
21	*D. magna*	GO	aqueous	5	No	Model 4	2915	0.104	-	-	-	0.972	131.7	0.0	0.49	Yes	14
21	*D. magna*	GO	aqueous	5	No	Model 5	-	0.103	-	131492	4.742	0.975	146.0	14.3	0.00	Yes	14
22	*D. magna*	C_{60}	aqueous	2	No	Model 1	26318	1.285	-	-	-	0.867	201.3	0.9	0.26	No	14
22	*D. magna*	C_{60}	aqueous	2	No	Model 2	27275	1.335	0.041	-	-	0.852	205.4	5.0	0.03	Yes	15
22	*D. magna*	C_{60}	aqueous	2	No	Model 3	28675	1.437	0.001	-	-	0.855	205.1	4.7	0.04	Yes	15
22	*D. magna*	C_{60}	aqueous	2	No	Model 4	26318	1.273	-	-	-	0.867	201.3	0.9	0.26	No	15
22	*D. magna*	C_{60}	aqueous	2	No	Model 5	-	2.170	-	47683	1.243	0.919	200.4	0.0	0.40	No	15
23	*D. magna*	C_{60}	aqueous	0.2	No	Model 1	79505	1.140	-	-	-	0.736	152.0	6.7	0.03	No	15
23	*D. magna*	C_{60}	aqueous	0.2	No	Model 2	100939	1.469	0.233	-	-	0.842	151.0	5.7	0.05	Yes	15
23	*D. magna*	C_{60}	aqueous	0.2	No	Model 3	127725	2.081	0.003	-	-	0.916	145.3	0.0	0.89	Yes	15
23	*D. magna*	C_{60}	aqueous	0.2	No	Model 4	79505	1.140	-	-	-	0.735	152.0	6.8	0.03	No	15
23	*D. magna*	C_{60}	aqueous	0.2	No	Model 5	-	1.516	-	15702	1.020	0.745	184.4	39.1	0.00	No	15
24	*D. magna*	C_{60}	aqueous	2	No	Model 1	1826	0.035	-	-	-	0.858	185.4	2.6	0.16	No	15
24	*D. magna*	C_{60}	aqueous	2	No	Model 2	3673	0.111	0.320	-	-	0.882	186.8	4.0	0.08	Yes	16
24	*D. magna*	C_{60}	aqueous	2	No	Model 3	3166	0.120	0.124	-	-	0.857	188.7	5.9	0.03	Yes	16
24	*D. magna*	C_{60}	aqueous	2	No	Model 4	1826	0.022	-	-	-	0.858	185.4	2.6	0.16	No	16
24	*D. magna*	C_{60}	aqueous	2	No	Model 5	-	0.033	-	75288	6.062	0.937	182.8	0.0	0.58	Yes	16
25	*D. magna*	Au	aqueous	0.05	No	Model 1	18709	0.145	-	-	-	0.273	169.8	0.0	0.48	No	17
25	*D. magna*	Au	aqueous	0.05	No	Model 2	18709	0.145	0.000	-	-	0.152	175.8	6.0	0.02	No	17
25	*D. magna*	Au	aqueous	0.05	No	Model 3	18714	0.145	0.000	-	-	0.152	175.8	6.0	0.02	No	17
25	*D. magna*	Au	aqueous	0.05	No	Model 4	18709	0.132	-	-	-	0.273	169.8	0.0	0.48	No	17
25	*D. magna*	Au	aqueous	0.05	No	Model 5	-		-	-	-	-	-	-	-	No	17
26	*D. magna*	Au	aqueous	0.4	Yes	Model 1	13364	0.399	-	-	-	0.800	205.6	25.0	0.00	No	17
26	*D. magna*	Au	aqueous	0.4	Yes	Model 2	13364	0.399	0.000	-	-	0.850	210.0	29.4	0.00	No	17
26	*D. magna*	Au	aqueous	0.4	Yes	Model 3	13764	0.419	0.002	-	-	0.866	207.2	26.6	0.00	No	17
26	*D. magna*	Au	aqueous	0.4	Yes	Model 4	13364	0.386	-	-	-	0.822	201.9	21.3	0.00	No	17
26	*D. magna*	Au	aqueous	0.4	Yes	Model 5	-	3.895	-	83356	44.710	0.992	180.6	0.0	1.00	Yes	17
27	*D. magna*	Au	aqueous	0.4	No	Model 1	18897	0.285	-	-	-	0.760	220.2	53.0	0.00	No	17
27	*D. magna*	Au	aqueous	0.4	No	Model 2	18897	0.285	0.000	-	-	0.820	224.5	57.3	0.00	No	17
27	*D. magna*	Au	aqueous	0.4	No	Model 3	18897	0.285	0.000	-	-	0.820	212.4	45.2	0.00	No	17
27	*D. magna*	Au	aqueous	0.4	No	Model 4	18897	0.273	-	-	-	0.760	212.6	45.4	0.00	No	17
27	*D. magna*	Au	aqueous	0.4	No	Model 5	-	1.257	-	287755	109.600	0.999	167.2	0.0	1.00	Yes	17
28	*D. rerio*	TiO_2	dietary	61086	Yes	Model 1	0.0003	0.041	-	-	-	0.827	103.4	0.0	0.35	Yes	18
28	*D. rerio*	TiO_2	dietary	61086	Yes	Model 2	0.0003	0.041	0.000	-	-	0.803	107.0	3.6	0.06	Yes	18
28	*D. rerio*	TiO_2	dietary	61086	Yes	Model 3	0.0003	0.054	0.006	-	-	0.816	106.3	2.9	0.08	Yes	18
28	*D. rerio*	TiO_2	dietary	61086	Yes	Model 4	0.0003	0.040	-	-	-	0.846	103.4	0.0	0.35	Yes	18

28	*D. rerio*	TiO_2	dietary	61086	Yes	Model 5	-	0.057	-	517.70	40.090	0.860	104.9	1.5	0.16	Yes	18
29	*D. rerio*	TiO_2	dietary	4520	Yes	Model 1	0.0012	0.055	-	-	-	0.923	62.3	0.0	0.35	Yes	18
29	*D. rerio*	TiO_2	dietary	4520	Yes	Model 2	0.0014	0.061	0.060	-	-	0.919	65.8	3.5	0.06	Yes	18
29	*D. rerio*	TiO_2	dietary	4520	Yes	Model 3	0.0015	0.072	0.004	-	-	0.930	64.2	1.8	0.14	Yes	18
29	*D. rerio*	TiO_2	dietary	4520	Yes	Model 4	0.0012	0.053	-	-	-	0.923	62.3	0.0	0.35	Yes	18
29	*D. rerio*	TiO_2	dietary	4520	Yes	Model 5	-	0.050	-	108.80	9.715	0.925	64.9	2.6	0.10	Yes	18
30	*D. rerio*	TiO_2	aqueous	0.55	Yes	Model 1	1.54	0.009	-	-	-	0.855	63.9	1.6	0.21	Yes	18
30	*D. rerio*	TiO_2	aqueous	0.55	Yes	Model 2	1.54	0.009	0.000	-	-	0.834	69.2	6.8	0.02	Yes	18
30	*D. rerio*	TiO_2	aqueous	0.55	Yes	Model 3	1.52	0.009	0.000	-	-	0.832	69.3	7.0	0.01	Yes	18
30	*D. rerio*	TiO_2	aqueous	0.55	Yes	Model 4	1.54	0.008	-	-	-	0.855	63.2	0.8	0.30	Yes	18
30	*D. rerio*	TiO_2	aqueous	0.55	Yes	Model 5	-	0.013	-	234	410.900	0.911	62.3	0.0	0.46	Yes	18
31	*D. rerio*	TiO_2	aqueous	0.06	Yes	Model 1	0.29	0.009	-	-	-	0.106	-15.8	1.3	0.13	Yes	18
31	*D. rerio*	TiO_2	aqueous	0.06	Yes	Model 2	0.60	0.023	0.498	-	-	0.432	-17.0	0.1	0.24	Yes	18
31	*D. rerio*	TiO_2	aqueous	0.06	Yes	Model 3	0.62	0.033	0.058	-	-	0.345	-17.1	0.0	0.25	Yes	18
31	*D. rerio*	TiO_2	aqueous	0.06	Yes	Model 4	0.29	0.008	-	-	-	0.106	-15.8	1.3	0.13	Yes	18
31	*D. rerio*	TiO_2	aqueous	0.06	Yes	Model 5	-	0.006	-	1.69	29.250	0.434	-17.0	0.1	0.24	Yes	18
32	*D. rerio*	CNTs	aqueous	0.2	Yes	Model 1	6.97	0.023	-	-	-	0.433	425.6	9.5	0.01	Yes	15
32	*D. rerio*	CNTs	aqueous	0.2	Yes	Model 2	6.97	0.023	0.000	-	-	0.418	426.3	10.2	0.01	Yes	15
32	*D. rerio*	CNTs	aqueous	0.2	Yes	Model 3	6.97	0.023	0.000	-	-	0.418	426.3	10.2	0.01	Yes	15
32	*D. rerio*	CNTs	aqueous	0.2	Yes	Model 4	6.97	0.022	-	-	-	0.433	425.6	9.5	0.01	Yes	15
32	*D. rerio*	CNTs	aqueous	0.2	Yes	Model 5	-	0.301	-	902	343.300	0.644	416.1	0.0	0.97	Yes	15
33	*D. rerio*	C_{60}	aqueous	1	Yes	Model 1	129.72	0.082	-	-	-	0.306	155.6	0.0	0.40	Yes	15
33	*D. rerio*	C_{60}	aqueous	1	Yes	Model 2	149.95	0.096	0.120	-	-	0.250	158.6	3.0	0.09	Yes	15
33	*D. rerio*	C_{60}	aqueous	1	Yes	Model 3	104.00	0.057	0.000	-	-	0.178	160.7	5.1	0.03	Yes	15
33	*D. rerio*	C_{60}	aqueous	1	Yes	Model 4	129.72	0.080	-	-	-	0.306	155.6	0.0	0.40	Yes	15
33	*D. rerio*	C_{60}	aqueous	1	Yes	Model 5	-	0.081	-	323.80	5.213	0.229	159.1	3.5	0.07	Yes	15
34	*D. rerio*	C_{60}	aqueous	2	Yes	Model 1	12.87	0.077	-	-	-	0.105	169.5	0.0	0.35	Yes	15
34	*D. rerio*	C_{60}	aqueous	2	Yes	Model 2	14.47	0.088	0.112	-	-	0.027	172.6	3.1	0.07	Yes	15
34	*D. rerio*	C_{60}	aqueous	2	Yes	Model 3	12.87	0.080	0.000	-	-	0.023	170.7	1.2	0.19	Yes	15
34	*D. rerio*	C_{60}	aqueous	2	Yes	Model 4	12.87	0.075	-	-	-	0.104	169.5	0.0	0.35	Yes	15
34	*D. rerio*	C_{60}	aqueous	2	Yes	Model 5	-	0.033	-	351.10	6.610	0.004	173.6	4.1	0.04	Yes	15

[*] For dietary exposure, units for food concentration (C_f) are in mg/kg.

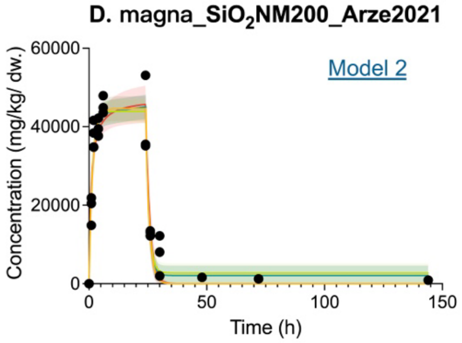
[**] For dietary exposure, units for k_u are in mg/kg/h.



• Experimental
Model 1
Model 2
Model 3
Model 4
Model 5
1)
S. obliquus_nC$_{60}$_Chen2016
Model 5
~~Model 1/4/5~~
Concentration (mg/kg/ dw.)
3000
2000
1000
0
0
20
40
60
Time (h)
2)
D. magna_TiO$_2$NM105_Arze2021
Model 1/4
Concentration (mg/kg/ dw.)
80000
60000
40000
20000
0
0
50
100
150
Time (h)
3)
D. magna_TiO$_2$NM104_Arze2021
Model 5
Concentration (mg/kg/ dw.)
50000
40000
30000
20000
10000
0
0
50
100
150
Time (h)
4)
D. magna_TiO$_2$NM103_Arze2021
Model 5
Concentration (mg/kg/ dw.)
100000
80000
60000
40000
20000
0
0
50
100
150
Time (h)
5)
D. magna_TiO$_2$NM102_Arze2021
Model 1
Concentration (mg/kg/ dw.)
100000
80000
60000
40000
20000
0
0
50
100
150
Time (h)
6)
D. magna_TiO$_2$NM101_Arze2021
Model 1
Concentration (mg/kg/ dw.)
50000
40000
30000
20000
10000
0
0
50
100
150
Time (h)
7)
D. magna_TiO$_2$NM100_Arze2021
Model 5
Concentration (mg/kg/ dw.)
40000
30000
20000
10000
0
0
50
100
150
Time (h)
8)
D. magna_SiO$_2$NM204_Arze2021
Model 5
Concentration (mg/kg/ dw.)
60000
40000
20000
0
0
50
100
150
Time (h)

• Experimental — Model 1 — Model 2 — Model 3 — Model 4 — Model 5

9)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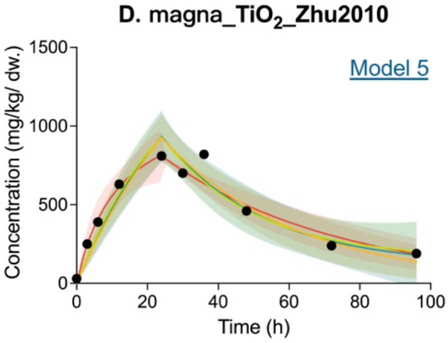
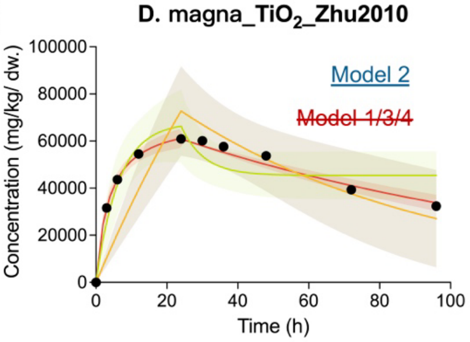

D. magna_TiO$_2$_Zhu2010

11)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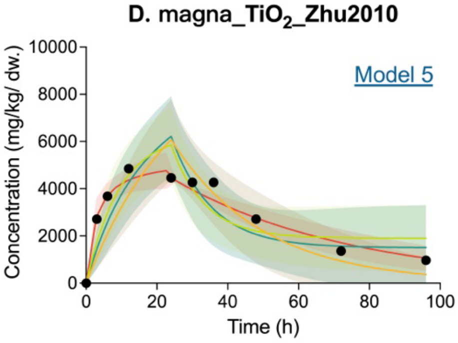
12)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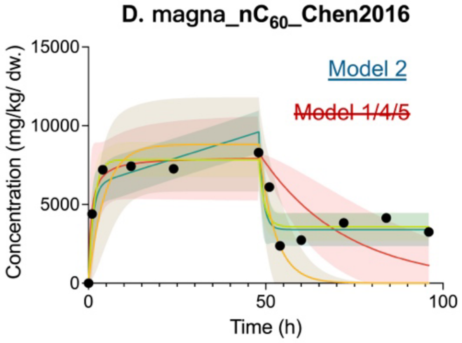
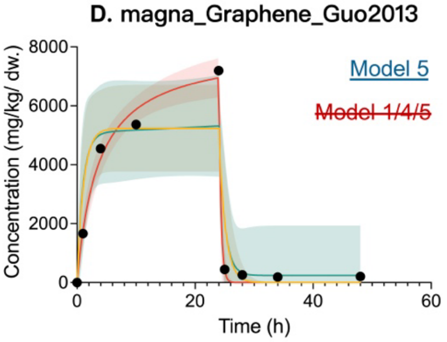
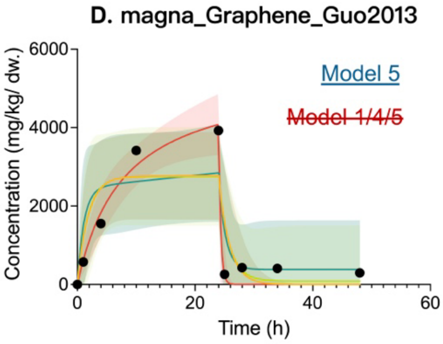

D. magna_nC$_{60}$_Chen2016

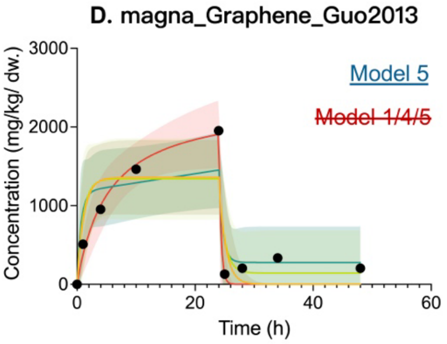
14)


D. magna_Graphene_Guo2013

15)


D. magna_Graphene_Guo2013

16)


D. magna_Graphene_Guo2013

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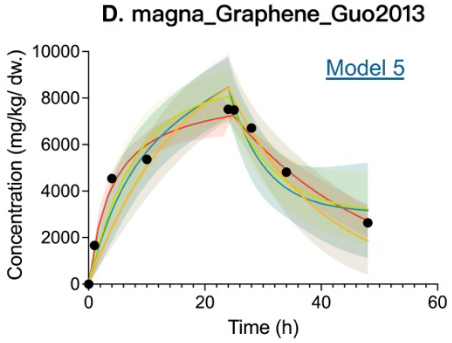

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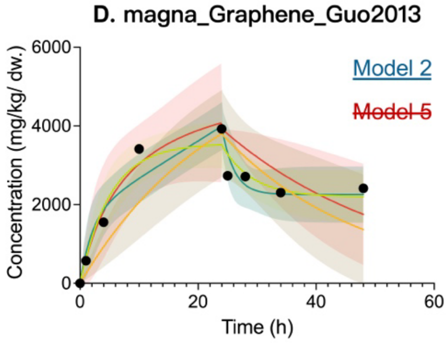

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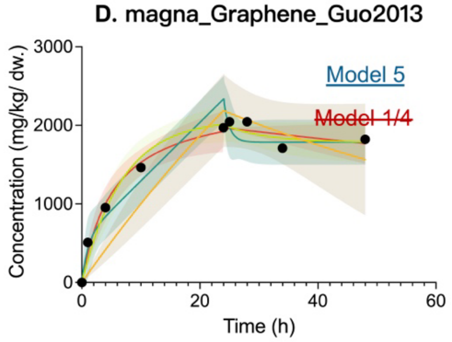

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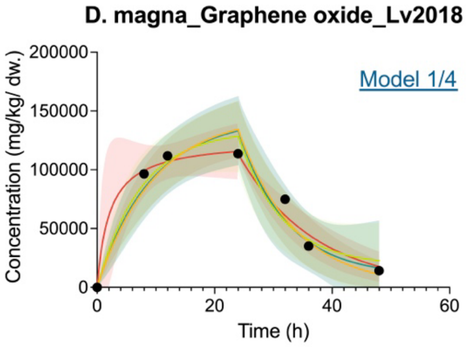

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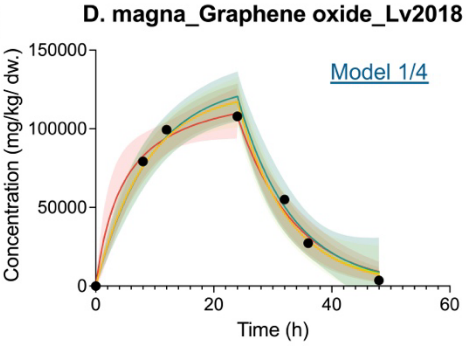

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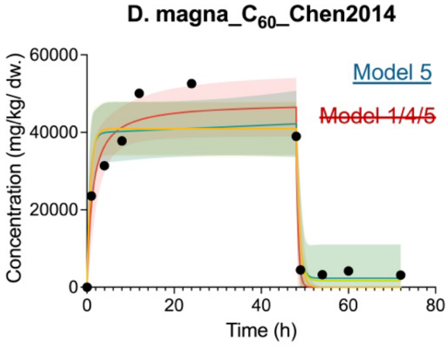

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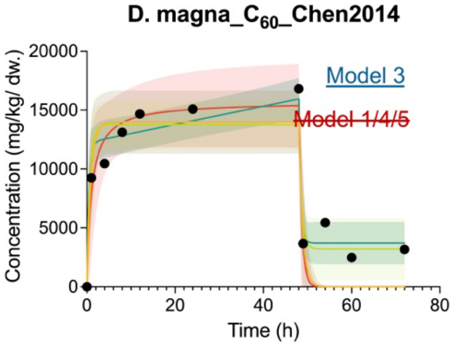

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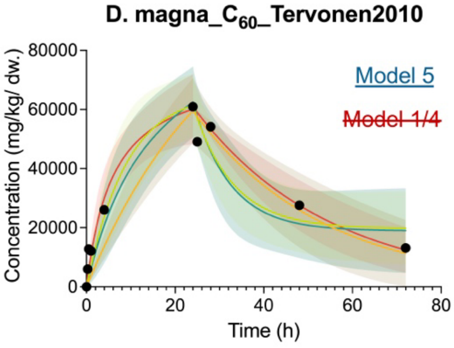

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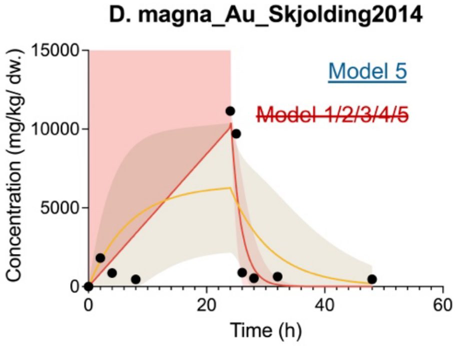

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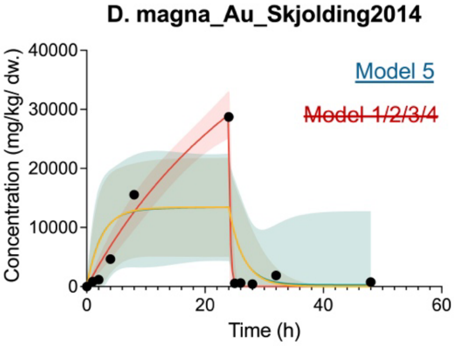

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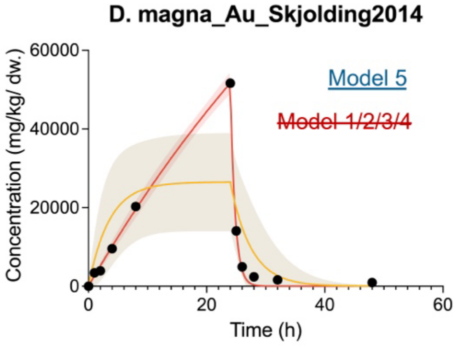

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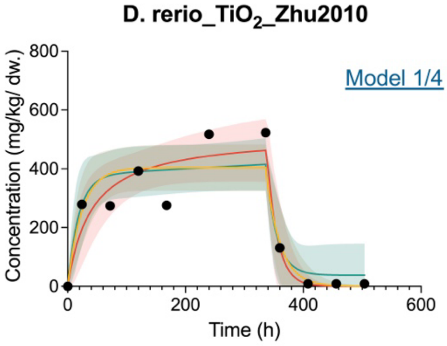

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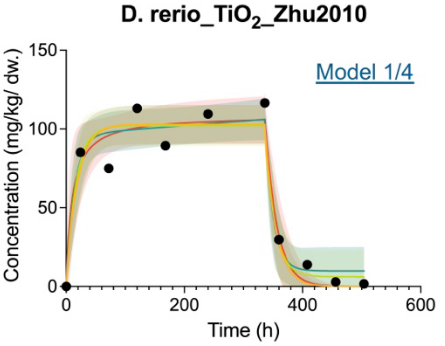

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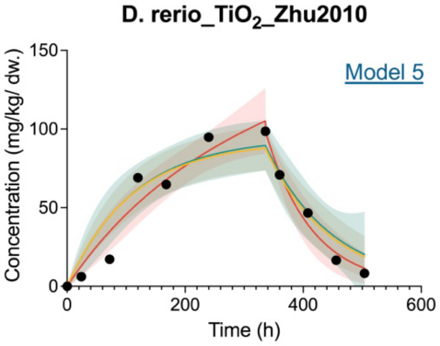

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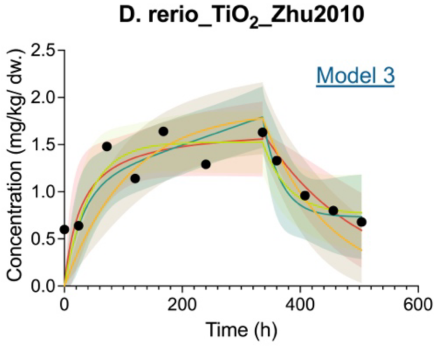

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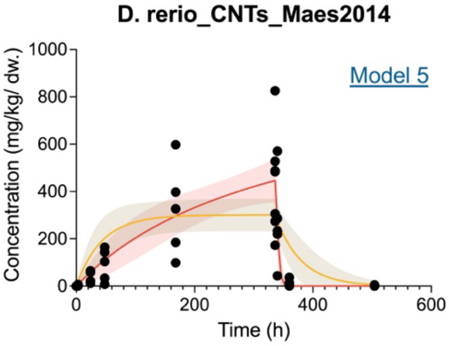

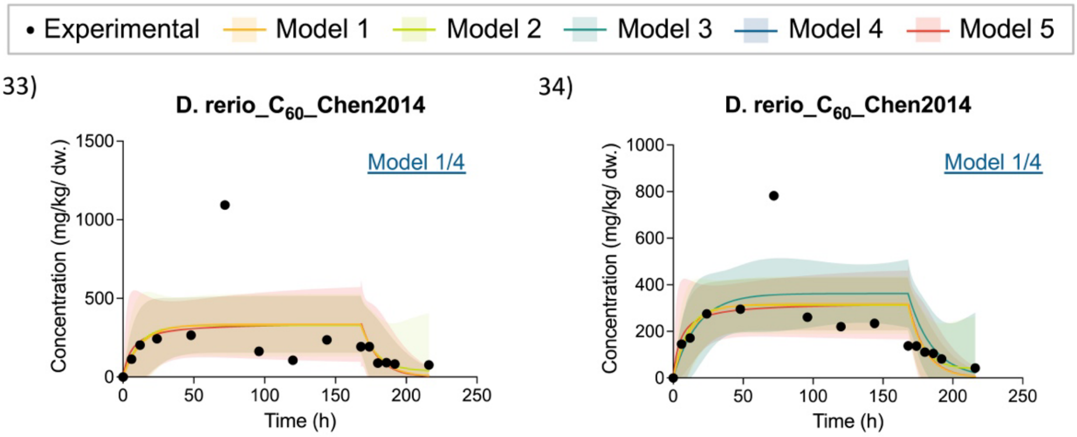

Figure S1: Predicted organism body burden during uptake and elimination of ENMs with 95% confidence bands from five models in comparison with the experimental data for all datasets. The model with an underline in blue is the model with the lowest AICc score. The model with a strikethrough in red is excluded for further statistical analysis based on a visual inspection with reference to the 95% confidence bands.

3 References

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