Supplementary Material for

JSFit: a method for the fitting and prediction of J- and S-shaped concentration-response curves

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Supplementary Material includes the following: The observed effects (three replications) of ionic liquid ([epy]Cl) of different concentrations against *Vibrio Qinghaiensis* sp.-Q67 at different times (Table S1). Original forms of five biphasic models with their corresponding interpretation of each parameter (Table S2). Model coefficients and GoFs of training set models and the effects predicted by the training set models at four concentrations (Table S3). Outliers analysis of observed effect on the basis of confidence intervals relative error (Table S4).The concentration-response curves of [epy]Cl against *Vibrio Qinghaiensis* sp.-Q67 at different exposure times of 0.25, 2, 4, 6, 8, 10, and 12 h. (Fig. S1). The concentration-response relationships of ionic liquid ([epy]Cl) against *Vibrio Qinghaiensis* sp.-Q67 (Fig. S2). Fitting CRCs of different category data of different types of chemicals against Q67 (Fig. S3). The goodness-of-fit parameters, R^2_{adj} (a), RMSE (b), and AIC (c), of two models (M5 and model 4) in five different times (Fig. S4).

Table S1 The observed effects (three replications) of ionic liquid ([epy]Cl) of different concentrations against *Vibrio Qinghaiensis* sp.-Q67 at different times

Concentration (mol/L)	Time (h)						
	0.25	2	4	6	8	10	12
0.0005816	-0.009	0.007	0.038	0.051	0.044	0.019	-0.010
	-0.044	-0.066	-0.043	-0.042	-0.066	-0.088	-0.081
	-0.062	-0.085	-0.102	-0.103	-0.200	-0.192	-0.078
0.0008143	-0.015	-0.019	-0.008	-0.004	-0.013	-0.035	-0.051
	-0.005	-0.030	-0.008	-0.015	-0.035	-0.062	-0.082
	-0.055	-0.032	-0.037	-0.025	-0.007	-0.042	-0.040
0.001241	0.052	-0.015	-0.024	-0.029	-0.042	-0.058	-0.074
	0.058	-0.047	-0.032	-0.057	-0.071	-0.086	-0.099
	0.035	-0.025	-0.044	-0.047	-0.027	-0.062	-0.122
0.001784	0.103	0.006	-0.029	-0.045	-0.070	-0.086	-0.096
	0.133	0.023	0.003	-0.002	-0.030	-0.053	-0.084
	0.085	-0.029	-0.078	-0.091	-0.088	-0.125	-0.138
0.002637	0.178	-0.018	-0.090	-0.120	-0.151	-0.176	-0.191
	0.186	-0.048	-0.139	-0.179	-0.215	-0.236	-0.237
	0.159	-0.006	-0.079	-0.098	-0.111	-0.152	-0.146
0.003878	0.282	0.001	-0.159	-0.201	-0.279	-0.315	-0.344
	0.290	0.027	-0.137	-0.181	-0.249	-0.282	-0.306
	0.267	0.033	-0.114	-0.156	-0.175	-0.263	-0.291
0.005816	0.435	0.204	0.036	-0.070	-0.130	-0.185	-0.232
	0.441	0.193	0.066	-0.041	-0.096	-0.147	-0.208
	0.380	0.173	0.062	-0.002	-0.043	-0.116	-0.208
0.008531	0.589	0.456	0.451	0.264	0.185	0.059	-0.074
	0.588	0.431	0.451	0.268	0.227	0.078	-0.034
	0.544	0.369	0.416	0.297	0.214	0.098	-0.019
0.01241	0.723	0.600	0.704	0.634	0.526	0.424	0.295
	0.720	0.595	0.713	0.655	0.567	0.488	0.380
	0.674	0.523	0.684	0.635	0.566	0.472	0.334
0.01784	0.772	0.673	0.804	0.817	0.788	0.693	0.588
	0.772	0.677	0.810	0.819	0.789	0.687	0.580
	0.741	0.613	0.795	0.824	0.800	0.735	0.608
0.02637	0.801	0.690	0.846	0.887	0.909	0.897	0.856
	0.800	0.718	0.857	0.892	0.913	0.903	0.867
	0.779	0.683	0.849	0.896	0.921	0.919	0.893
0.03878	0.849	0.798	0.906	0.934	0.965	0.981	0.978
	0.844	0.805	0.907	0.935	0.965	0.982	0.983
	0.828	0.775	0.898	0.930	0.958	0.973	0.976

Table S2 Original forms of five biphasic models with their corresponding interpretation of each parameter

model	Original form	Parameters
M1	$y=\dfrac{k+\gamma x}{1+e^{bg}x^{b}}+d$	k: untreated control d: expected response at infinite concentration γ :the initial rate of increase at low concentration b: the way in which response decreases with concentration g: no simple interpretation
M2	$y=1-\dfrac{k(1+\gamma x)}{1+(1+2\gamma EC_{50})\cdot(x/EC_{50})^{b}}$	k: untreated control γ :the initial rate of increase at low concentration b: no simple interpretation *EC50*: concentration causing
M3	$y=C+\dfrac{d-c+\gamma\exp(-1/x^{\alpha})}{1+\exp(b[\ln(x)-\ln(e)])}$	d: untreated control C: expected response at infinite concentration γ :the initial rate of increase at low concentration α : the rate of the hormetic effect manifests itself b: the steepness of the curve after the maximum hormetic effect e: the lower bound on the EC50 level
M4	$y=\dfrac{\min-\alpha+(\omega-\min/(1+(\varepsilon_{Up}/x)^{\beta_{Up}}))}{1+(x/\varepsilon_{Dn})^{\beta_{Dn}}}+\alpha$	α : untreated control ω : expected response at infinite concentration min: the minimum effect that would be approached by the downslope ε_{Dn}: the concentration at the midpoint of the rising slope absence of the upslope β_{Up}: the steepness of the rising (positive) slope ε_{Up}: the concentration at the midpoint of the falling slope β_{Dn}: the steepness of the falling (negative) slope
M5	$y=\min+(\alpha-\min/(1+10^{(x-\varepsilon_{Dn})\beta_{Dn}}))+(\omega-\min/(1+10^{(\varepsilon_{Up}-x)\beta_{Up}}))$	α : untreated control ω : expected response at infinite concentration min: the minimum effect that would be approached by the downslope in the absence of the upslope β_{Up}: the steepness of the rising (positive) slope ε_{Up}: the concentration at the midpoint of the rising slope β_{Dn}: the steepness of the falling (negative) slope ε_{Dn}: the concentration at the midpoint of the falling slope

Table S3 Model coefficients and GoFs of training set models and the effects predicted by the training set models (HM6) at four concentrations

Time	Model coefficients and GoF of training set model								Predicted Effects and predictive determination coefficient [a]				
/h	E_m	EC_{mid1}	H_1	E_{max}	EC_{mid2}	H_2	RMSE	R^2	Pred.1	Pred.2	Pred.3	Pred.4	q^2_{ext}
12	-23.675	5.295E-03	2.634	1.461	1.950E-04	0.745	0.0397	0.9978	-0.0357	-0.2337	0.0310	0.8165	0.9884
10	-1.658	4.673E-03	2.398	1.091	5.646E-03	1.663	0.0592	0.9954	-0.0232	-0.2134	0.1375	0.8804	0.9940
8	-3.197	9.318E-03	2.172	1.014	4.701E-03	3.409	0.0510	0.9966	-0.0159	-0.1626	0.2377	0.9081	0.9989
6	-1.191	6.952E-03	2.111	0.962	5.768E-03	3.620	0.0238	0.9992	-0.0127	-0.1229	0.3284	0.8997	0.9954
4	-0.460	6.645E-03	1.636	0.957	5.875E-03	37.961	0.0223	0.9993	-0.0144	-0.0832	0.5747	0.8661	0.9676
4*	-0.793	7.093E-03	1.972	0.937	5.663E-03	5.107	0.0243	0.9990	-0.0110	-0.0947	0.6798	0.8709	0.9988

[a]: The concentrations corresponding to four predictive effects, Pred. 1, Pred. 2, Pred. 3 and Pred. 4, are 0.0008143, 0.002637, 0.008531 (0.01241 for 4 h*), and 0.02637 mol/L, respectively.

Table S4 Outliers analysis of observed effect on the basis of confidence intervals relative error [a]

model (Threshol)	time (h)	concentration (mol/L)	observed effect	predicted effect	predicted effect range	RE_{CI}	outlier	p_{out}
HM6 (1.635)	10	0.0005816	-0.192	-0.024	[-0.129 0.081]	1.595	0	0
	8	0.0005816	-0.200	-0.006	[-0.091 0.079]	2.277	1	0.028
	6	0.0005816	0.051	-0.005	[-0.055 0.049]	-1.146	0	0.028
	6	0.0005816	-0.103	-0.005	[-0.055 0.049]	1.970	1	
	6	0.001784	-0.002	-0.067	[-0.117 -0.018]	-1.305	0	
	4	0.0005816	-0.102	-0.007	[-0.102 -0.007]	1.984	1	0.028
	4	0.001784	0.003	-0.054	[-0.102 -0.007]	-1.212	0	
HM7-1 (1.692)	10	0.0005816	-0.192	-0.068	[-0.123 -0.013]	2.250	1	0.028
	10	0.0005816	0.019	-0.068	[-0.123 -0.013]	-1.599	0	
	8	0.0005816	-0.200	-0.046	[-0.092 -0.001]	3.393	1	0.056
	8	0.0005816	0.044	-0.046	[-0.092 -0.001]	-1.982	1	
	6	0.0005816	0.051	-0.028	[-0.059 0.003]	-2.567	1	0.056
	6	0.0005816	-0.103	-0.028	[-0.059 0.003]	2.421	1	
	6	0.001784	-0.002	-0.049	[-0.080 -0.019]	-1.524	0	
	6	0.001784	-0.092	-0.049	[-0.080 -0.019]	1.369	0	
	6	0.002637	-0.179	-0.132	[-0.166 -0.098]	1.371	0	
	4	0.0005816	0.038	-0.033	[-0.064 -0.001]	-2.269	1	0.056
	4	0.0005816	-0.102	-0.033	[-0.064 -0.001]	2.231	1	
	4	0.001784	0.003	-0.045	[-0.077 -0.014]	-1.556	0	
	4	0.002637	-0.140	-0.096	[-0.129 -0.065]	1.401	0	
HM7-2 (1.692)	10	0.0005816	-0.192	-0.068	[-0.123 -0.013]	2.257	1	0.028
	10	0.0005816	0.019	-0.068	[-0.123 -0.013]	-1.597	0	
	8	0.0005816	-0.200	-0.046	[-0.091 -0.001]	3.392	1	0.056
	8	0.0005816	0.043	-0.046	[-0.091 -0.001]	-1.975	1	
	6	0.0005816	0.051	-0.028	[-0.059 0.003]	-2.569	1	0.056
	6	0.0005816	-0.103	-0.028	[-0.059 0.003]	2.423	1	
	6	0.001784	-0.002	-0.049	[-0.080 -0.018]	-1.525	0	
	6	0.001784	-0.091	-0.049	[-0.080 -0.018]	1.370	0	
	6	0.002637	-0.179	-0.131	[-0.166 -0.098]	1.376	0	
	4	0.0005816	0.038	-0.024	[-0.059 0.010]	-1.800	1	0.056
	4	0.0005816	-0.102	-0.024	[-0.059 0.010]	2.237	1	
	4	0.001784	0.003	-0.048	[-0.082 -0.013]	-1.456	0	
	4	0.002637	-0.139	-0.094	[-0.129 -0.060]	1.299	0	
HM5 (1.556)	10	0.0005816	-0.192	-0.019	[-0.133 0.095]	1.513	0	0
	8	0.0005816	-0.200	-0.009	[-0.095 0.077]	2.218	1	0.028
	6	0.0005816	0.051	-0.013	[-0.076 0.049]	-1.032	0	0.028
	6	0.0005816	-0.103	-0.013	[-0.076 0.049]	1.432	0	
	6	0.001784	-0.179	-0.074	[-0.137 -0.012]	1.660	1	
	4	0.0005816	-0.102	-0.002	[-0.084 0.081]	1.213	0	0

[a]: RE_{CI} refers to confidence intervals relative error, which is used to measure deviation degree of observed effect. p_{out} is outliers ratio of observed effect at the corresponding time.

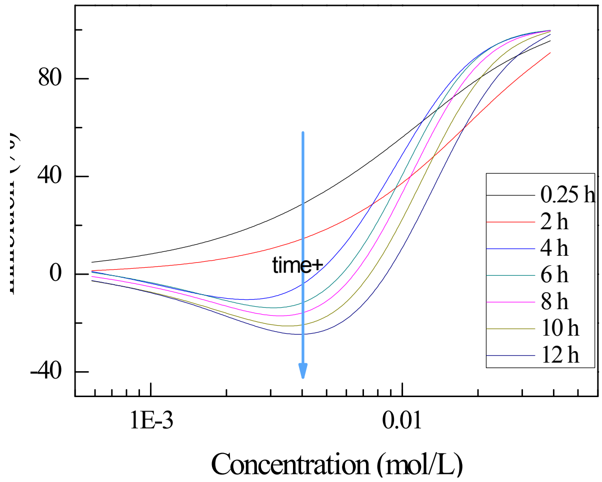


Fig. S1 The concentration-response curves of [epy]Cl against *Vibrio Qinghaiensis* sp.-Q67 at different exposure times of 0.25, 2, 4, 6, 8, 10, and 12 h. At a concentration of 0.004 mol/L, the effect decreases with time.

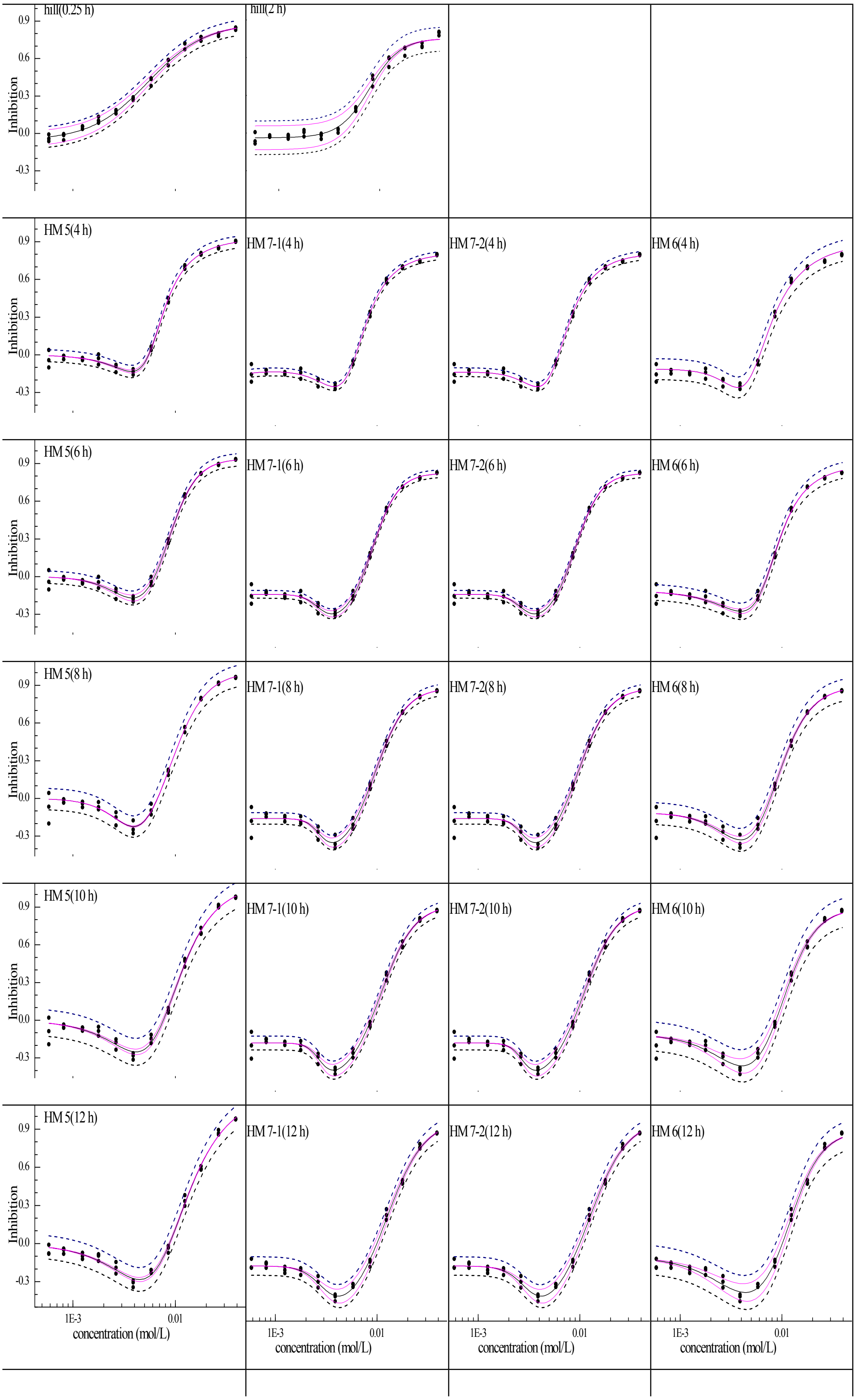
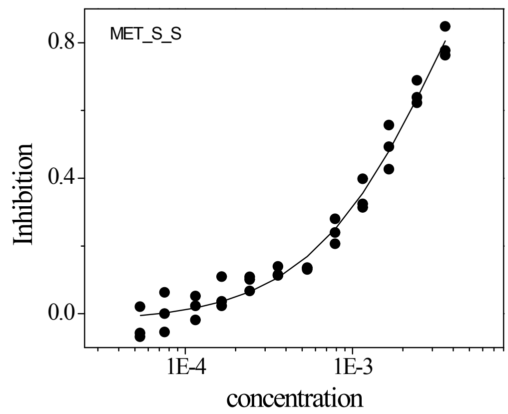
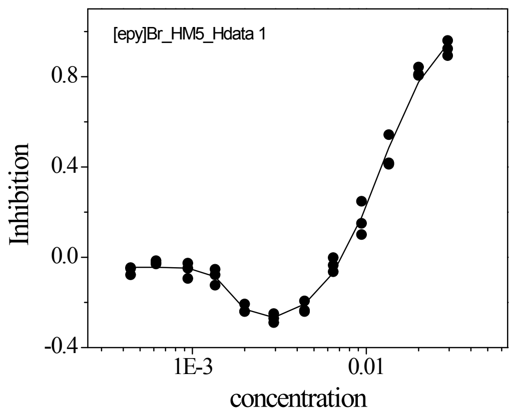


Fig. S2 The concentration-response relationships of ionic liquid ([epy]Cl) against *Vibrio Qinghaiensis* sp.-Q67 where "----" is the OCIs, "—" the FCIs, "—" the fitting CRCs, "ഗ" the experimental scatters, “hill(T)” represents S-shaped CRC at the time of T (T=0.25 or 2) h, and “Y(T)” represents J-shape CRC at the time T (T=4, 6, 8, 10, or 12) *h* by the model Y.



(A)



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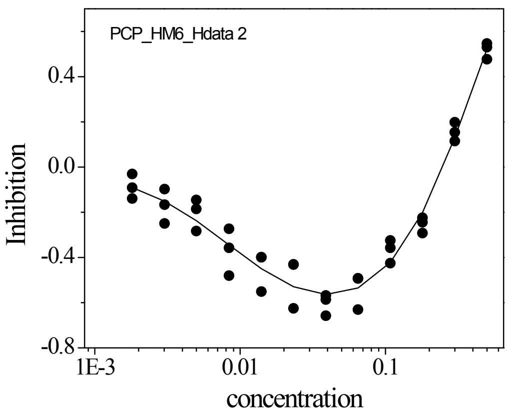

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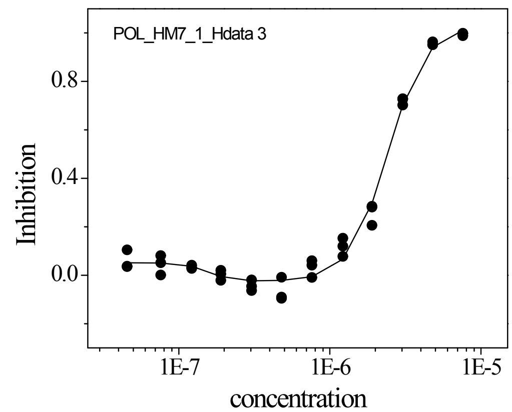
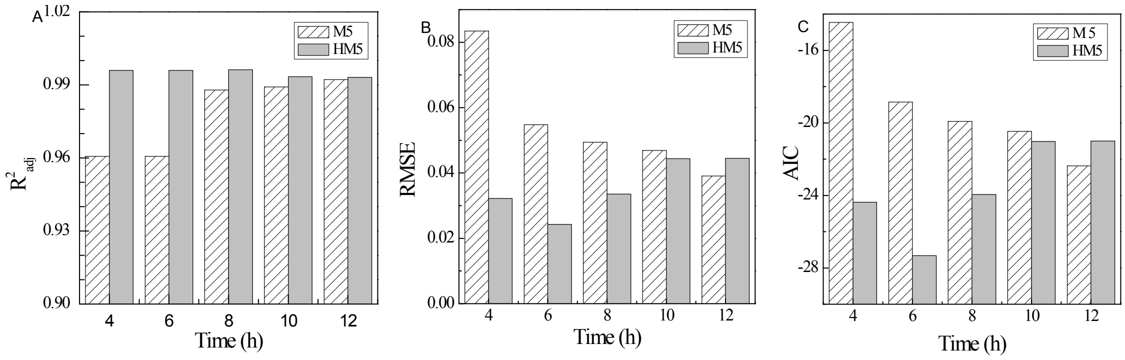


(D)

Fig. S3 Fitting CRCs of different category data of different types of chemicals against Q67. “X_Y_Z” represents CRC of “Z” (Z=S, Hdata 1, Hdata 2 or Hdata 3) category data of chemical “X” with molder “Y” (Y=S, HM5, HM6 or HM7_1).



(a) (b) (c)

Fig. S4 The goodness-of-fit parameters, R^2_{adj} (a), R MSE (b), and AIC (c), of two models (M5 and HM5) in five different times.