

## Supporting Information for

### **Optimizing benefit-risk trade-off in nano-agrochemicals through explainable machine learning: Beyond concentration**

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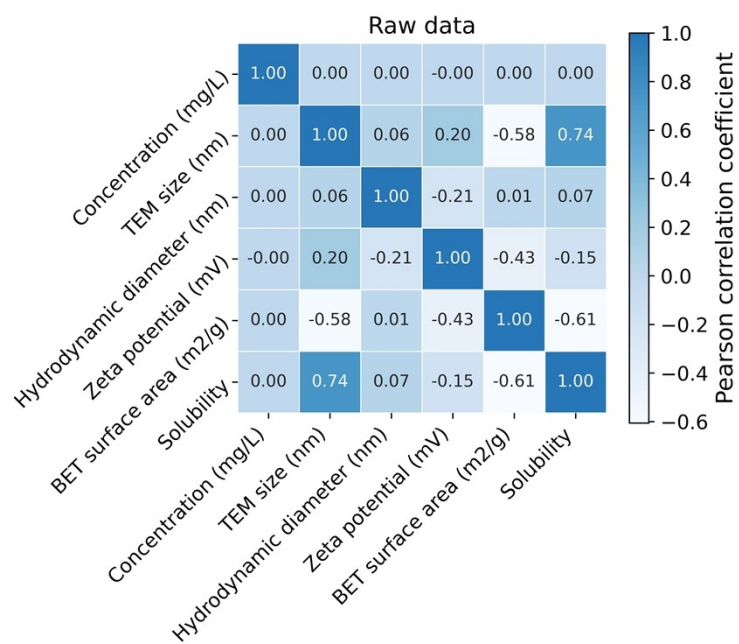
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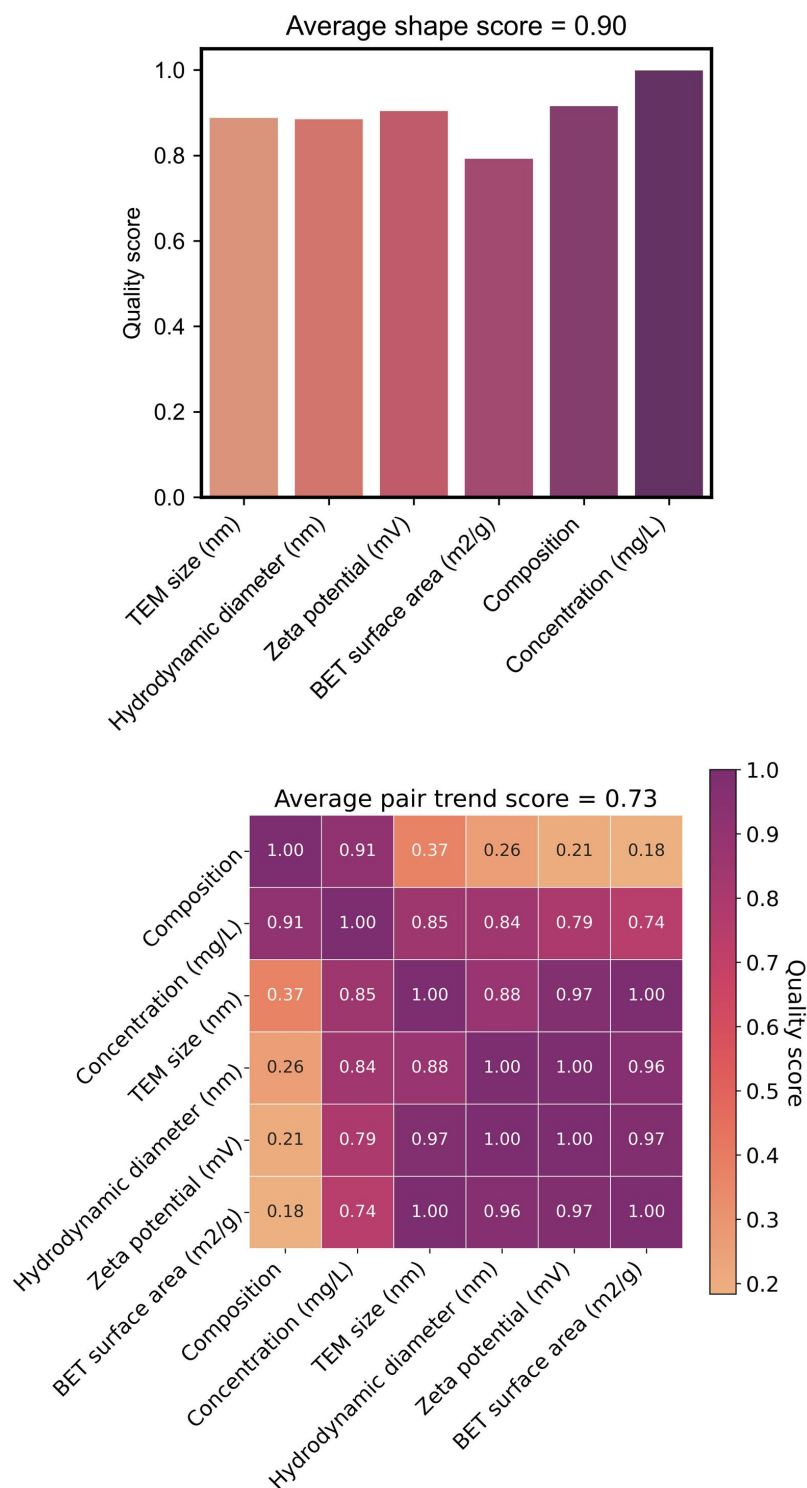
This information file includes:

- Figures S1-S12
- Tables S1-S10

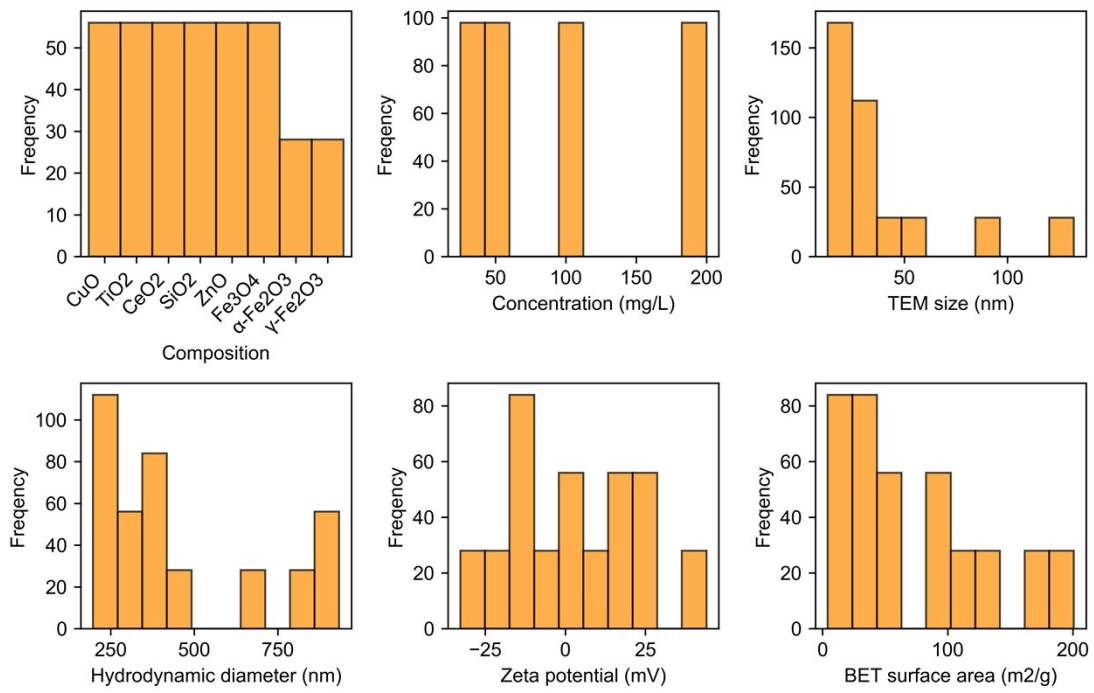
## Figures



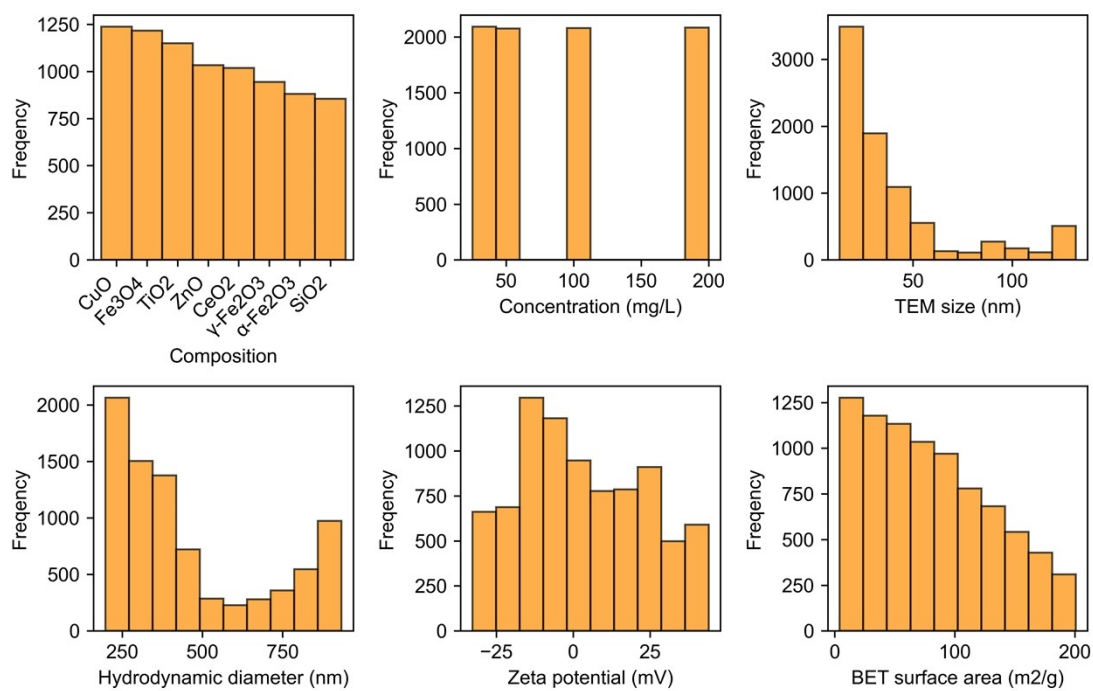
**Figure S1.** Person correlation coefficient of features in the collected datasets with solubility.



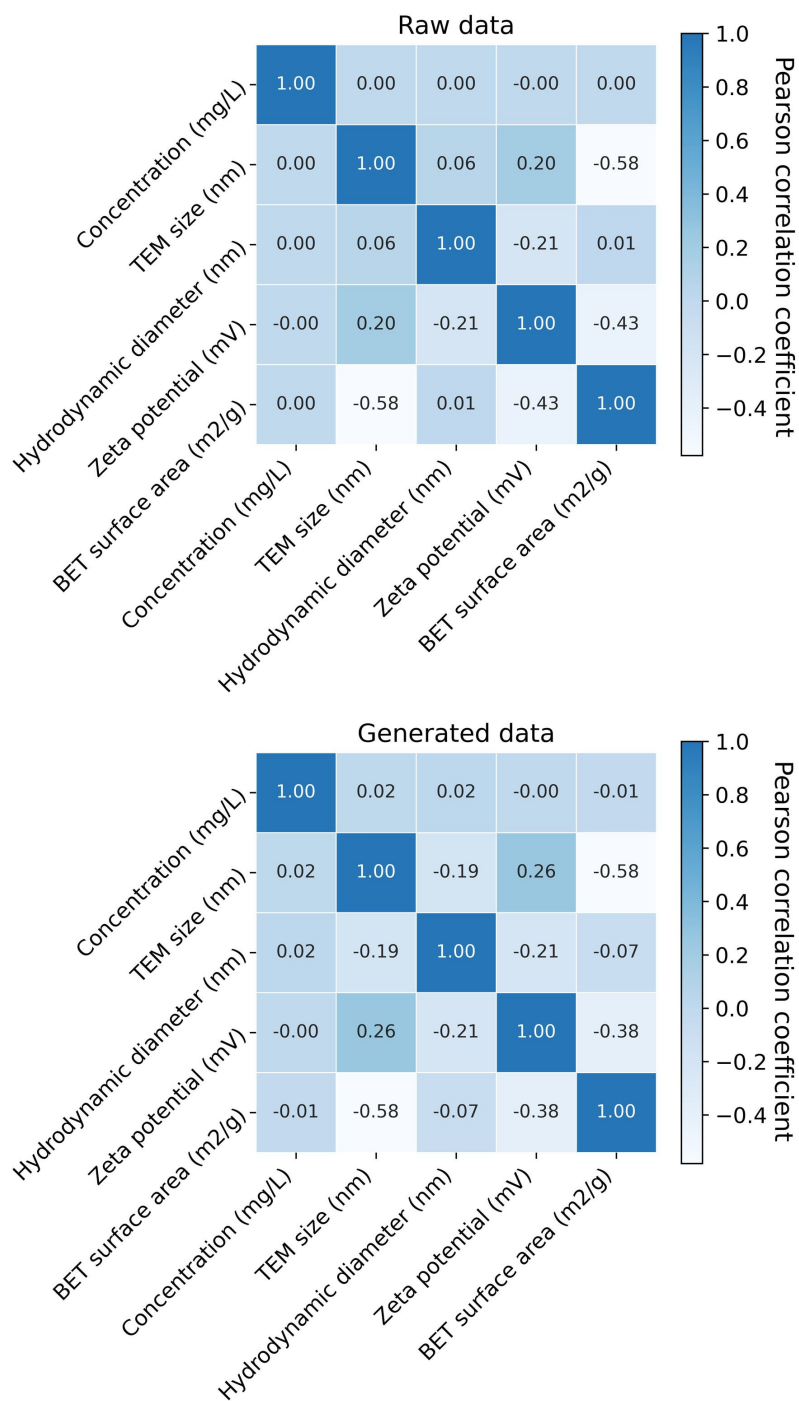
**Figure S2.** Average shape scores and pair trend scores for evaluating the data distribution and feature correlation of the generated data.



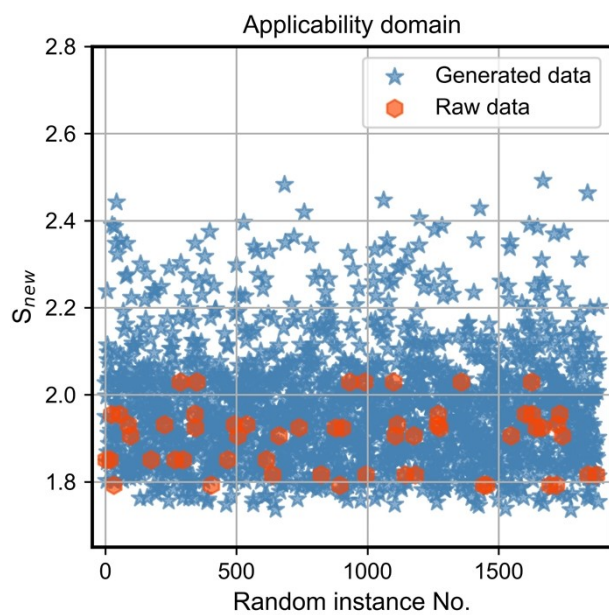
**Figure S3.** Data distribution of raw data used for machine learning.



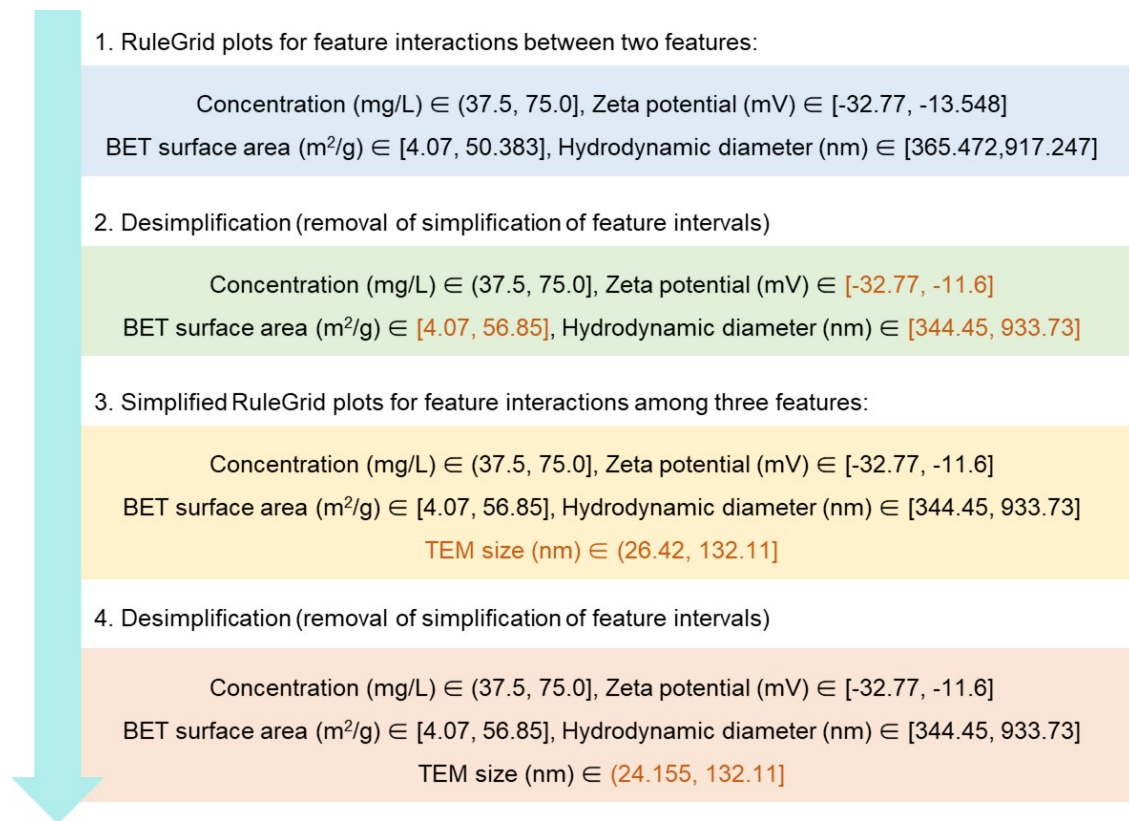
**Figure S4.** Data distribution of generated data used for MOO.



**Figure S5.** Feature correlation of the raw dataset and generated dataset.

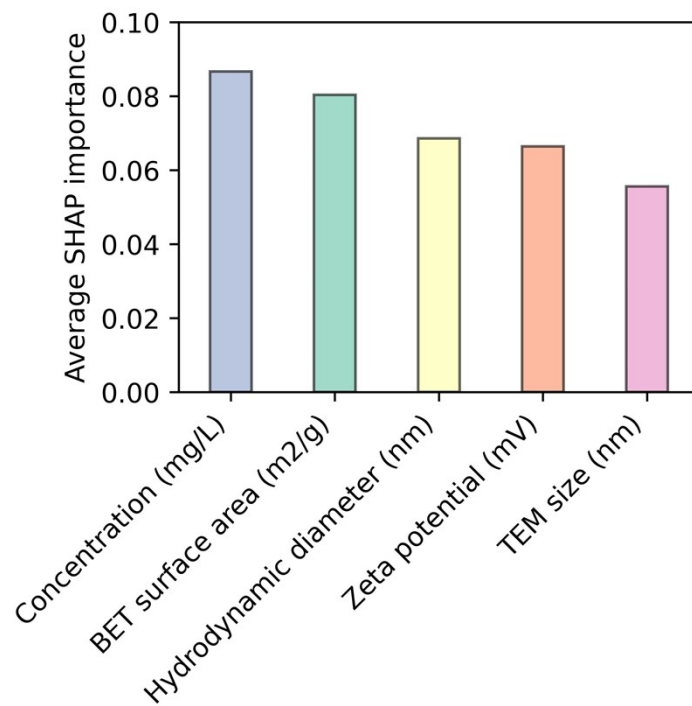


**Figure S6.** Applicability domain of the raw data and generated data (for instances that require the calculation of  $S_{new}$ ).

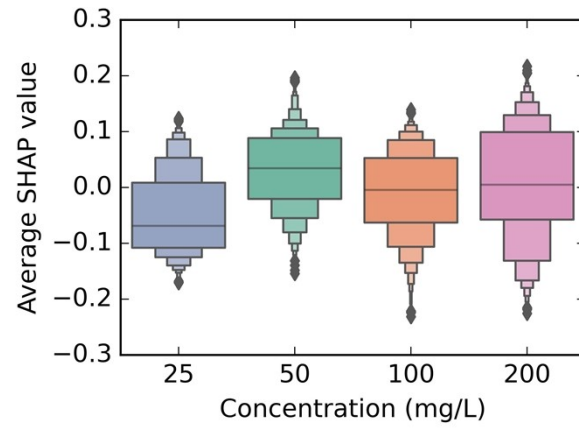


**Figure S7.** Selection workflow of feature intervals for maximum RDW and minimum RMC.

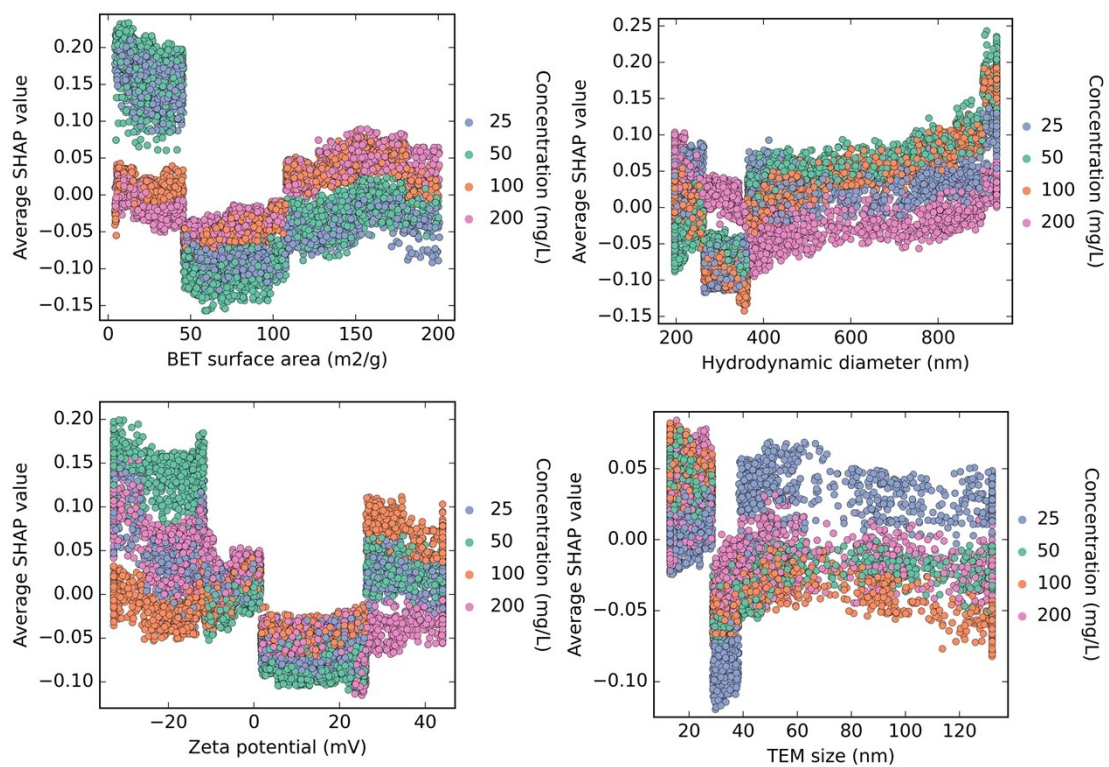




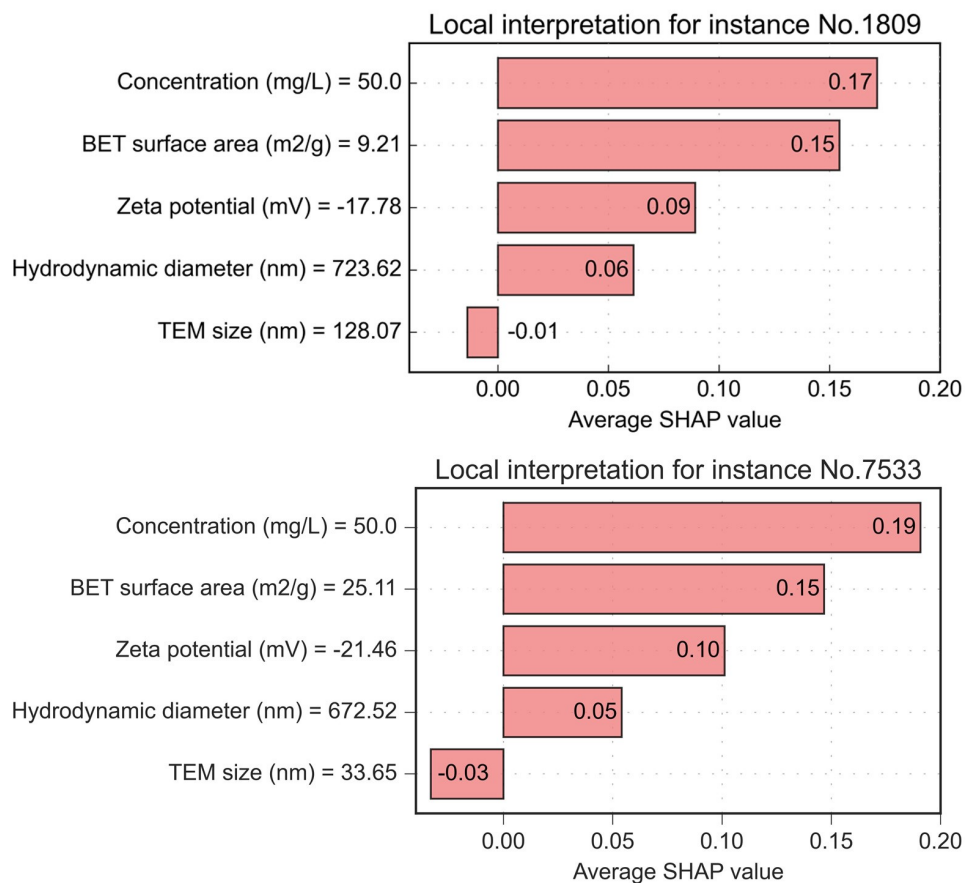
**Figure S8.** Average SHAP values for five features in the NPI prediction model.



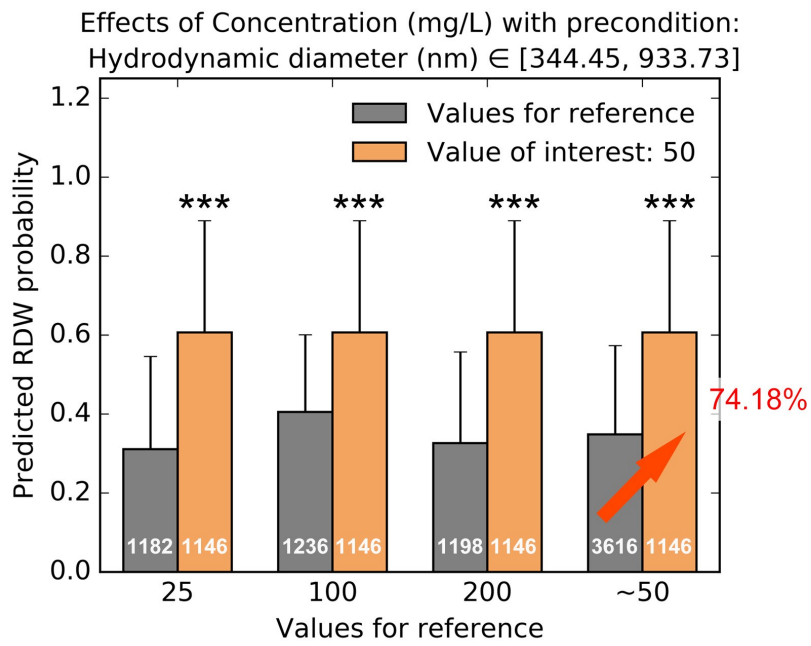
**Figure S9.** Letter-value plot for SHAP effects of concentration in the NPI prediction model.



**Figure S10.** SHAP plots for other four features in the NPI prediction model.



**Figure S11.** SHAP local interpretation for No. 1809 and No. 7533.



**Figure S12.** Independent effects of concentration and its combined effects with hydrodynamic diameter of [344.45, 933.73] nm.

## Tables

**Table S1.** The versions of the main software and packages used in this study.

<b>Software/packages</b>	<b>Version</b>
python	3.10.8
scikit-learn	1.2.0
shap	0.41.0
imodels	1.2.5
sdv	1.2.0

**Table S2.** The hyperparameters of the RuleFit models for RDW.

random state	max_rules	n_estimators	tree_generator	tree_size
1	30	300	RandomForestRegressor()	3
2	48	200	RandomForestRegressor()	3
3	38	300	GradientBoostingRegressor()	3
4	46	200	GradientBoostingRegressor()	4
5	42	200	GradientBoostingClassifier()	5
6	38	300	GradientBoostingClassifier()	3
7	42	200	GradientBoostingRegressor()	3
8	40	200	GradientBoostingClassifier()	3
9	52	700	RandomForestRegressor()	5
10	42	200	None	5

**Table S3.** The hyperparameters of the RuleFit models for RMC.

<b>random state</b>	<b>max_rules</b>	<b>n_estimators</b>	<b>tree_generator</b>	<b>tree_size</b>
1	26	100	None	3
2	30	100	RandomForestRegressor()	6
3	38	400	GradientBoostingRegressor()	5
4	32	500	RandomForestRegressor()	4
5	52	200	RandomForestRegressor()	3
6	34	300	GradientBoostingRegressor()	3
7	26	100	RandomForestRegressor()	4
8	38	100	None	3
9	30	100	GradientBoostingRegressor()	3
10	26	100	GradientBoostingRegressor()	5



**Table S4.** The rules generated by ten RuleFit models for RDW predictions (importance >0.1).

Rule	Coefficient	Support	Importance	Model
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 13.07	-4.5496	0.1488	1.6192	7
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and TEM size (nm) <= 24.155 and Zeta potential (mV) <= -14.585	-7.2962	0.0417	1.4580	2
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) <= 23.55	4.8211	0.1012	1.4540	2
Concentration (mg/L) <= 37.5 and Zeta potential (mV) <= 26.17 and Zeta potential (mV) > -13.03	3.8589	0.1667	1.4381	2
Concentration (mg/L) > 150.0 and TEM size (nm) <= 32.04 and Zeta potential (mV) > -9.325	-4.1698	0.0952	1.2240	5
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47	-2.5109	0.3571	1.2031	7
Concentration (mg/L) > 37.5 and Zeta potential (mV) > -13.03	-2.3405	0.5774	1.1562	8
Concentration (mg/L) <= 150.0 and Zeta potential (mV) > 26.17	3.6256	0.1131	1.1483	7
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 363.47	2.3560	0.3750	1.1406	8
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 263.34999	-2.8611	0.1786	1.0958	2
Concentration (mg/L) <= 75.0 and Zeta potential (mV) <= -11.6	3.0043	0.1548	1.0866	7
Concentration (mg/L) > 150.0 and TEM size (nm) > 19.155 and Hydrodynamic diameter (nm) <= 263.34999	-5.3958	0.0417	1.0782	2
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -11.6	3.9339	0.0714	1.0131	5
Concentration (mg/L) > 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) <= 23.25	2.6522	0.1607	0.9741	5
Concentration (mg/L) > 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) <= 26.17	2.5088	0.1667	0.9350	2
Concentration (mg/L) > 150.0 and Zeta potential (mV) <= -11.6	-3.7780	0.0655	0.9345	2
Concentration (mg/L) > 37.5 and Zeta potential (mV) <= 26.17 and Zeta potential (mV) > -13.03	-1.8709	0.4583	0.9322	2
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) <= 23.25	2.4483	0.1667	0.9124	8
Concentration (mg/L) > 37.5 and Hydrodynamic	2.7632	0.1190	0.8948	2

diameter (nm) > 276.06999 and BET surface area (m <sup>2</sup> /g) > 107.75				
Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -13.03	2.2546	0.1845	0.8746	2
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 363.47	1.7991	0.3750	0.8710	7
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999	3.6635	0.0595	0.8668	2
Concentration (mg/L) > 150.0 and TEM size (nm) <= 43.445 and Zeta potential (mV) <= -9.325	2.8875	0.0952	0.8476	6
Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > -11.6	-1.6831	0.5714	0.8329	8
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	3.2663	0.0655	0.8080	7
Concentration (mg/L) > 37.5 and TEM size (nm) > 13.07	1.7115	0.6845	0.7954	8
Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) <= 312.84999	1.6574	0.3036	0.7621	2
Concentration (mg/L) > 150.0 and TEM size (nm) <= 29.155	-2.1179	0.1488	0.7538	2
Concentration (mg/L) > 150.0 and TEM size (nm) > 29.155 and Hydrodynamic diameter (nm) <= 363.47	3.3315	0.0536	0.7501	3
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 736.38501	1.8589	0.1964	0.7385	2
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 543.41499 and BET surface area (m <sup>2</sup> /g) > 181.475	-5.4802	0.0179	0.7258	2
Concentration (mg/L) > 75.0 and Zeta potential (mV) > -4.945	1.6055	0.2857	0.7253	5
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -11.6	2.9223	0.0655	0.7229	3
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 276.06999 and Zeta potential (mV) <= 21.87	1.5546	0.3155	0.7224	2
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 415.67999	-2.5049	0.0893	0.7143	2
TEM size (nm) > 19.155 and BET surface area (m <sup>2</sup> /g) > 98.515	1.9673	0.1429	0.6884	7
Concentration (mg/L) > 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) <= 23.25	1.8686	0.1607	0.6863	10
BET surface area (m <sup>2</sup> /g) > 107.75	1.4815	0.2917	0.6734	7
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and Zeta potential (mV) >	3.6090	0.0357	0.6698	8

-13.03				
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) <= 26.17	-1.4680	0.2917	0.6672	2
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -11.6	2.4925	0.0714	0.6419	10
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Zeta potential (mV) <= -11.6	-2.5547	0.0655	0.6319	8
Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) > 415.67999	1.4459	0.2440	0.6211	2
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -11.6	2.4296	0.0655	0.6010	4
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 28.685	-2.5182	0.0595	0.5958	8
Concentration (mg/L) <= 37.5 and TEM size (nm) > 38.345 and BET surface area (m <sup>2</sup> /g) > 4.39	2.5809	0.0536	0.5811	3
Concentration (mg/L) <= 37.5 and Zeta potential (mV) <= -13.03	-2.3380	0.0655	0.5783	8
Concentration (mg/L) > 75.0 and BET surface area (m <sup>2</sup> /g) <= 27.46	-1.6669	0.1310	0.5623	5
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 344.45 and BET surface area (m <sup>2</sup> /g) <= 139.6	-1.7417	0.1131	0.5516	2
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > -4.945	-1.8111	0.1012	0.5462	5
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) <= 220.665	-4.1230	0.0179	0.5460	7
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 28.685	-2.3560	0.0536	0.5305	5
Hydrodynamic diameter (nm) > 312.84999 and Zeta potential (mV) <= 5.565 and Zeta potential (mV) > -25.835	-1.0726	0.4107	0.5277	2
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Zeta potential (mV) <= -11.6	-2.0465	0.0714	0.5270	7
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -11.6	2.0242	0.0714	0.5213	6
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) > 900.76498	3.0610	0.0298	0.5201	3
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and BET surface area (m <sup>2</sup> /g) <= 169.06499	2.9380	0.0298	0.4992	7

Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) > 23.25	-2.9258	0.0298	0.4972	8
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 263.34999	-1.2868	0.1786	0.4928	6
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) <= 23.55	-1.0959	0.2798	0.4919	8
Concentration (mg/L) > 150.0 and Zeta potential (mV) > -4.115 and BET surface area (m2/g) <= 27.46	2.1423	0.0536	0.4824	1
Concentration (mg/L) <= 150.0 and TEM size (nm) > 29.155 and Hydrodynamic diameter (nm) <= 363.47	-1.1969	0.2024	0.4809	1
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 900.76498	-3.1389	0.0238	0.4785	7
Concentration (mg/L) > 150.0 and BET surface area (m2/g) > 127.18999	2.0765	0.0536	0.4676	2
Hydrodynamic diameter (nm) > 263.34999 and BET surface area (m2/g) <= 139.6	-1.0166	0.7024	0.4648	3
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) > 220.665	1.1113	0.2202	0.4605	5
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 28.685	-1.9419	0.0595	0.4595	4
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 28.685	-1.8511	0.0655	0.4579	3
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 113.04 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > -7.22	-1.6251	0.0833	0.4492	10
Zeta potential (mV) > -25.835 and BET surface area (m2/g) > 45.705	-0.8934	0.5179	0.4464	2
BET surface area (m2/g) <= 4.39	1.7747	0.0655	0.4390	7
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 312.84999 and Zeta potential (mV) <= 19.25	-2.3516	0.0357	0.4364	2
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 390.5	0.9206	0.3214	0.4300	6
Concentration (mg/L) > 150.0 and TEM size (nm) <= 32.04 and Zeta potential (mV) > -9.325	-1.4174	0.1012	0.4275	10
Concentration (mg/L) > 75.0 and BET surface area (m2/g) <= 181.475	0.8462	0.4583	0.4216	3
Concentration (mg/L) > 37.5 and TEM size (nm) <= 113.04 and Hydrodynamic diameter (nm) > 344.45 and BET surface area (m2/g) <= 107.75	-0.9062	0.3036	0.4167	10
Concentration (mg/L) > 37.5 and Hydrodynamic	-0.9264	0.2738	0.4131	5

diameter (nm) <= 736.38501 and Hydrodynamic diameter (nm) > 344.45				
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 363.47	0.8463	0.3810	0.4110	1
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 13.07	3.0735	0.0179	0.4070	2
Concentration (mg/L) > 150.0 and TEM size (nm) <= 28.685 and Zeta potential (mV) <= -9.325	1.7116	0.0595	0.4050	3
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 33.23 and Zeta potential (mV) > -25.835	-1.1318	0.1488	0.4028	4
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 363.47 and Zeta potential (mV) <= 26.17	0.8431	0.3452	0.4009	2
BET surface area (m2/g) <= 107.75 and BET surface area (m2/g) > 45.705	-0.8646	0.3036	0.3975	6
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and Zeta potential (mV) > -25.835	-1.0807	0.1607	0.3969	1
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 415.67999	1.5306	0.0714	0.3942	2
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and BET surface area (m2/g) > 181.475	-2.5792	0.0238	0.3932	8
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 415.67999	-0.9867	0.1845	0.3827	2
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 363.47	0.8810	0.2500	0.3815	7
Concentration (mg/L) > 75.0 and BET surface area (m2/g) <= 181.475 and BET surface area (m2/g) > 92.805	1.0542	0.1548	0.3813	5
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 263.34999 and Zeta potential (mV) > 26.17	-2.4945	0.0238	0.3803	7
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 13.07	1.7827	0.0476	0.3797	8
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and Zeta potential (mV) > 0.865	2.2336	0.0298	0.3795	7
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345	-0.9387	0.2024	0.3771	8
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) <= 23.55	1.2977	0.0893	0.3700	8
Concentration (mg/L) > 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) <= 23.25	1.0180	0.1488	0.3623	9

Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 15.31	1.1990	0.1012	0.3616	3
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 900.76498	3.3250	0.0119	0.3606	8
Concentration (mg/L) > 150.0 and TEM size (nm) > 32.04 and Zeta potential (mV) > -25.835	1.0629	0.1310	0.3586	4
Concentration (mg/L) > 37.5 and TEM size (nm) <= 113.04 and Hydrodynamic diameter (nm) <= 344.45 and BET surface area (m <sup>2</sup> /g) <= 107.75	0.9441	0.1726	0.3568	10
Hydrodynamic diameter (nm) > 220.665 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 45.705	-0.7201	0.4286	0.3564	7
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 220.665	1.6662	0.0476	0.3548	8
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 220.665	2.0434	0.0298	0.3472	7
Concentration (mg/L) <= 150.0 and TEM size (nm) > 32.04	-0.7471	0.2976	0.3416	2
Concentration (mg/L) > 75.0 and TEM size (nm) <= 113.04 and Zeta potential (mV) <= -11.6	-0.9130	0.1667	0.3403	6
Concentration (mg/L) <= 150.0 and TEM size (nm) > 19.155 and Hydrodynamic diameter (nm) > 363.47 and Zeta potential (mV) <= 26.17	0.8948	0.1726	0.3382	2
Concentration (mg/L) <= 75.0 and Zeta potential (mV) <= -11.6	0.8994	0.1607	0.3303	8
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) <= 220.665	-2.4769	0.0179	0.3280	8
Concentration (mg/L) <= 75.0 and Zeta potential (mV) <= -13.03 and BET surface area (m <sup>2</sup> /g) <= 45.705	-1.6300	0.0417	0.3257	8
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 900.76498 and Hydrodynamic diameter (nm) > 344.45	0.9632	0.1310	0.3249	4
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 92.525 and Hydrodynamic diameter (nm) > 363.47	0.6892	0.3155	0.3203	4
Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 45.705	-0.6397	0.5179	0.3196	3
Concentration (mg/L) > 150.0 and TEM size (nm) <= 21.72 and TEM size (nm) > 14.68	1.3958	0.0536	0.3143	4
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -11.6	1.1319	0.0833	0.3128	9
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 29.155 and Zeta potential (mV) > 26.17	1.2638	0.0655	0.3126	7

Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) > 736.38501	1.0392	0.0952	0.3051	5
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -25.835	-1.5200	0.0417	0.3037	7
Concentration (mg/L) > 150.0 and TEM size (nm) <= 28.685 and Zeta potential (mV) > -9.325	-1.2174	0.0655	0.3011	3
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and BET surface area (m <sup>2</sup> /g) <= 169.06499	1.5056	0.0417	0.3009	3
BET surface area (m <sup>2</sup> /g) <= 127.18999 and BET surface area (m <sup>2</sup> /g) > 45.705	-0.6239	0.3631	0.3000	8
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Zeta potential (mV) > -4.945 and BET surface area (m <sup>2</sup> /g) > 33.53	1.0464	0.0893	0.2984	9
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	1.1118	0.0774	0.2971	4
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 363.47 and Zeta potential (mV) <= 5.565	0.6666	0.2619	0.2931	9
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 363.47	-0.8803	0.1250	0.2911	6
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 4.39	1.7044	0.0298	0.2896	8
Concentration (mg/L) > 150.0 and Zeta potential (mV) <= 35.27 and Zeta potential (mV) > 26.17	-1.8827	0.0238	0.2870	6
Concentration (mg/L) <= 75.0 and Zeta potential (mV) <= -16.015	1.1557	0.0655	0.2859	2
Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -9.325 and Zeta potential (mV) > -13.03	-0.9151	0.1071	0.2830	4
TEM size (nm) <= 32.04 and Zeta potential (mV) > -25.835	-0.5651	0.4583	0.2816	4
Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 45.705	-0.5568	0.5060	0.2784	5
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 73.455 and TEM size (nm) > 38.345	1.6047	0.0298	0.2727	6
Hydrodynamic diameter (nm) > 390.5	0.5422	0.4286	0.2683	6
Concentration (mg/L) <= 75.0 and TEM size (nm) <= 73.455 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.7769	0.1369	0.2670	6
Concentration (mg/L) > 37.5 and TEM size (nm) <= 38.345 and BET surface area (m <sup>2</sup> /g) > 107.75	0.7178	0.1607	0.2636	1
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 840.285	-1.2342	0.0476	0.2628	1

Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and TEM size (nm) > 14.68 and Zeta potential (mV) <= 26.17	-0.7045	0.1667	0.2626	9
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) > 363.47	0.5485	0.3512	0.2618	3
Concentration (mg/L) <= 75.0 and Zeta potential (mV) > -13.03 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.6441	0.2083	0.2616	9
Concentration (mg/L) > 150.0 and BET surface area (m <sup>2</sup> /g) <= 27.46	1.0361	0.0655	0.2563	6
Concentration (mg/L) <= 75.0 and Zeta potential (mV) > -13.03 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.6435	0.1964	0.2557	8
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > 5.565	1.0667	0.0595	0.2524	5
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and Zeta potential (mV) > -25.835	-0.6488	0.1845	0.2517	8
Concentration (mg/L) > 150.0 and TEM size (nm) > 38.345	1.0585	0.0595	0.2504	8
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 543.41499	-0.6318	0.1905	0.2481	2
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 363.47 and Zeta potential (mV) <= -10.655	1.0026	0.0655	0.2480	10
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and TEM size (nm) <= 47.84 and Zeta potential (mV) <= 35.27 and Zeta potential (mV) > -9.325	0.7641	0.1190	0.2474	10
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 840.285 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.5962	0.2143	0.2446	1
BET surface area (m <sup>2</sup> /g) > 127.18999	0.5873	0.2202	0.2434	8
TEM size (nm) <= 113.04 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > -11.6	-0.4862	0.5060	0.2431	6
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705 and BET surface area (m <sup>2</sup> /g) > 4.39	0.6210	0.1845	0.2409	4
Concentration (mg/L) <= 150.0 and Zeta potential (mV) <= 35.27 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.5692	0.2321	0.2403	10
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) <= 23.55	-0.5405	0.2679	0.2394	5
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 28.685	-1.1189	0.0476	0.2383	6
Concentration (mg/L) <= 37.5 and TEM size (nm) <=	-0.9480	0.0655	0.2345	7



38.345 and TEM size (nm) > 28.685				
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 27.46	0.6671	0.1429	0.2334	5
Concentration (mg/L) > 150.0 and TEM size (nm) <= 28.685 and Zeta potential (mV) > -9.325 and BET surface area (m <sup>2</sup> /g) > 27.46	-0.9050	0.0714	0.2331	9
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) > -4.945 and BET surface area (m <sup>2</sup> /g) <= 127.18999	0.5391	0.2440	0.2315	10
Concentration (mg/L) > 150.0 and TEM size (nm) > 29.155 and Hydrodynamic diameter (nm) <= 357.45	0.8969	0.0714	0.2310	9
Concentration (mg/L) <= 150.0 and Zeta potential (mV) <= 35.27 and Zeta potential (mV) > 26.17	0.8927	0.0714	0.2299	3
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Zeta potential (mV) > 35.27	1.7255	0.0179	0.2285	3
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 363.47 and Zeta potential (mV) > -25.835	-0.6756	0.1310	0.2279	10
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 276.06999 and Zeta potential (mV) > -25.835	1.0695	0.0476	0.2278	1
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 220.665	-0.4543	0.4702	0.2267	7
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and TEM size (nm) > 13.07 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 56.85	-0.9062	0.0655	0.2242	10
Concentration (mg/L) <= 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) <= 26.17	-0.4470	0.5357	0.2229	1
Concentration (mg/L) <= 37.5 and TEM size (nm) > 21.72 and Hydrodynamic diameter (nm) <= 263.34999	1.4604	0.0238	0.2227	4
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) <= 220.665	-1.4558	0.0238	0.2219	4
Concentration (mg/L) <= 75.0 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.5376	0.2143	0.2206	1
Hydrodynamic diameter (nm) > 344.45 and Zeta potential (mV) > -22.85	-0.4409	0.5238	0.2202	1
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	-0.5474	0.2024	0.2199	10
Concentration (mg/L) > 150.0 and TEM size (nm) <= 92.525 and Hydrodynamic diameter (nm) > 363.47	-0.7057	0.1071	0.2183	4
Concentration (mg/L) <= 150.0 and Zeta potential (mV) <= 35.27 and Zeta potential (mV) > 26.17	1.0901	0.0417	0.2178	4

Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 900.76498 and Hydrodynamic diameter (nm) > 363.47	0.7386	0.0952	0.2168	6
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 363.47	-0.6657	0.1190	0.2156	8
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > -9.325	-0.6064	0.1429	0.2122	9
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) <= 26.17	-0.4788	0.2679	0.2120	5
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) > -13.03	0.5492	0.1786	0.2104	5
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	-0.4985	0.2262	0.2086	4
Concentration (mg/L) > 37.5 and TEM size (nm) <= 38.345	0.4132	0.5179	0.2065	8
Concentration (mg/L) <= 150.0 and TEM size (nm) > 19.155 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	-0.4842	0.2024	0.1945	10
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m <sup>2</sup> /g) > 33.53	0.5362	0.1488	0.1908	5
Concentration (mg/L) > 37.5 and TEM size (nm) <= 73.455 and Hydrodynamic diameter (nm) <= 900.76498 and Hydrodynamic diameter (nm) > 344.45 and Zeta potential (mV) > -25.835	-0.4372	0.2500	0.1893	9
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47	-0.3820	0.4167	0.1883	3
Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 92.805	-0.4097	0.2917	0.1862	5
Concentration (mg/L) <= 75.0 and Zeta potential (mV) <= -25.835	1.2204	0.0238	0.1860	3
Concentration (mg/L) > 37.5 and Zeta potential (mV) <= -4.945 and Zeta potential (mV) > -13.03	-0.5098	0.1548	0.1844	5
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Zeta potential (mV) > 23.55	0.5564	0.1250	0.1840	8
Concentration (mg/L) > 75.0 and Zeta potential (mV) <= -4.945	-0.4195	0.2560	0.1831	6
Concentration (mg/L) > 37.5 and Zeta potential (mV) <= 35.27 and Zeta potential (mV) > -13.03	-0.3636	0.5298	0.1815	5

Concentration (mg/L) <= 150.0 and Zeta potential (mV) > 26.17	0.5464	0.1250	0.1807	8
TEM size (nm) <= 24.155 and TEM size (nm) > 13.07 and Zeta potential (mV) > -25.835	-0.3946	0.2976	0.1804	8
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 29.155 and Zeta potential (mV) > 26.17	0.7005	0.0714	0.1804	3
BET surface area (m2/g) <= 149.7 and BET surface area (m2/g) > 45.705	-0.3621	0.4345	0.1795	2
Concentration (mg/L) <= 150.0 and TEM size (nm) > 19.155 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	-0.4171	0.2381	0.1776	9
TEM size (nm) > 19.155 and BET surface area (m2/g) > 98.515	0.5305	0.1250	0.1754	1
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 543.41499 and Hydrodynamic diameter (nm) > 220.665 and Zeta potential (mV) <= 26.17	-0.5246	0.1250	0.1735	10
TEM size (nm) <= 24.155 and Zeta potential (mV) > -25.835	-0.3544	0.3750	0.1716	5
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and BET surface area (m2/g) > 169.06499	-1.1021	0.0238	0.1680	7
Concentration (mg/L) <= 37.5 and Zeta potential (mV) <= 35.27 and Zeta potential (mV) > -13.03	0.4350	0.1786	0.1666	5
Concentration (mg/L) > 37.5 and TEM size (nm) <= 73.455 and Zeta potential (mV) <= 26.17 and Zeta potential (mV) > -13.03	-0.3436	0.3690	0.1658	9
Concentration (mg/L) <= 75.0 and TEM size (nm) <= 24.155 and Zeta potential (mV) <= -14.585	0.6694	0.0655	0.1656	2
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 363.47 and BET surface area (m2/g) <= 73.47	-0.5469	0.1012	0.1649	4
BET surface area (m2/g) <= 181.475 and BET surface area (m2/g) > 92.805	-0.3643	0.2857	0.1646	7
Concentration (mg/L) > 37.5 and BET surface area (m2/g) <= 45.705	0.3447	0.3512	0.1645	6
Concentration (mg/L) <= 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) > 26.17	0.5415	0.1012	0.1633	1
Concentration (mg/L) > 150.0 and TEM size (nm) > 29.155 and Hydrodynamic diameter (nm) <= 344.45	0.5671	0.0893	0.1617	4
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 47.84 and Hydrodynamic diameter (nm) > 263.34999	-0.4606	0.1429	0.1612	9
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 363.47 and BET surface area (m2/g) >	-0.5159	0.1071	0.1596	4

5.01				
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 28.685 and TEM size (nm) > 19.155	0.6636	0.0595	0.1570	10
Zeta potential (mV) > -14.585 and BET surface area (m2/g) > 45.705	-0.3126	0.4345	0.1549	2
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 840.285	0.8300	0.0357	0.1540	2
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 113.04 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) > -4.945	-0.4893	0.1071	0.1513	9
Hydrodynamic diameter (nm) > 220.665 and Zeta potential (mV) > -25.835 and BET surface area (m2/g) > 45.705	-0.3022	0.4405	0.1500	5
TEM size (nm) <= 24.155 and Zeta potential (mV) > -25.835	-0.3126	0.3512	0.1492	6
Concentration (mg/L) <= 150.0 and Zeta potential (mV) <= -11.6	0.3611	0.2143	0.1482	2
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) > 263.34999 and Zeta potential (mV) <= -13.03	0.7971	0.0357	0.1479	4
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and Zeta potential (mV) > 0.865	0.8550	0.0298	0.1453	5
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 736.38501 and Zeta potential (mV) <= 19.25 and Zeta potential (mV) > -25.835	-0.3077	0.3155	0.1430	10
Hydrodynamic diameter (nm) <= 840.285 and BET surface area (m2/g) <= 15.31	0.3609	0.1905	0.1417	2
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	0.6250	0.0536	0.1407	5
Concentration (mg/L) <= 75.0 and Zeta potential (mV) > -11.6	-0.2908	0.3452	0.1383	6
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 38.345 and Hydrodynamic diameter (nm) > 263.34999	-0.3914	0.1429	0.1369	9
Concentration (mg/L) > 150.0 and TEM size (nm) <= 13.07	-1.0340	0.0179	0.1369	8
TEM size (nm) <= 33.23 and Zeta potential (mV) > -25.835	-0.2666	0.5893	0.1312	1
BET surface area (m2/g) <= 107.75 and BET surface area (m2/g) > 45.705	-0.2845	0.2798	0.1277	7
BET surface area (m2/g) <= 15.31	0.3235	0.1905	0.1270	2
Concentration (mg/L) <= 75.0 and TEM size (nm) >	0.3308	0.1726	0.1250	1

16.785 and Hydrodynamic diameter (nm) > 363.47				
Concentration (mg/L) <= 75.0 and Concentration (mg/L) > 37.5 and TEM size (nm) <= 38.345 and Zeta potential (mV) > -25.835	0.3310	0.1667	0.1234	1
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 415.67999 and Hydrodynamic diameter (nm) > 263.34999	0.4088	0.1012	0.1233	9
Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m2/g) > 73.47	0.2546	0.3512	0.1215	1
Concentration (mg/L) <= 150.0 and BET surface area (m2/g) <= 45.705 and BET surface area (m2/g) > 27.46	0.4117	0.0952	0.1208	6
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) <= 415.67999 and BET surface area (m2/g) <= 149.7 and BET surface area (m2/g) > 45.705	-0.4670	0.0714	0.1203	9
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 113.04 and TEM size (nm) > 38.345	0.5646	0.0476	0.1202	5
Hydrodynamic diameter (nm) > 900.76498	-0.4145	0.0833	0.1145	2
Concentration (mg/L) <= 37.5 and TEM size (nm) > 13.07 and Hydrodynamic diameter (nm) > 263.34999	-0.2889	0.1905	0.1134	8
Concentration (mg/L) <= 150.0 and Hydrodynamic diameter (nm) <= 363.47 and Hydrodynamic diameter (nm) > 263.34999	-0.2699	0.2143	0.1108	5
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and Zeta potential (mV) > -13.03	0.5537	0.0417	0.1106	10
TEM size (nm) <= 24.155 and Zeta potential (mV) > -25.835	-0.2318	0.3333	0.1093	4
Concentration (mg/L) <= 75.0 and Zeta potential (mV) > -11.6	-0.2279	0.3452	0.1083	7
Concentration (mg/L) > 150.0 and BET surface area (m2/g) <= 127.18999 and BET surface area (m2/g) > 31.38	-0.3304	0.1190	0.1070	10
Concentration (mg/L) > 75.0 and Zeta potential (mV) > -9.325 and BET surface area (m2/g) > 107.75	0.4275	0.0655	0.1057	4
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 28.685 and Zeta potential (mV) > -9.325	0.2544	0.2202	0.1054	3
Concentration (mg/L) > 150.0 and Zeta potential (mV) <= -25.835	0.6811	0.0238	0.1038	7
Concentration (mg/L) <= 150.0 and Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 331.87 and BET surface area (m2/g) <= 27.46	-0.6080	0.0298	0.1033	10
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 263.34999 and BET surface area	0.5059	0.0417	0.1011	10

(m <sup>2</sup> /g) <= 149.7				
Concentration (mg/L) > 75.0 and TEM size (nm) <= 16.785 and Zeta potential (mV) > -25.835	-0.3170	0.1131	0.1004	1
Hydrodynamic diameter (nm) <= 312.84999 and Hydrodynamic diameter (nm) > 276.06999	0.3514	0.0893	0.1002	2

**Table S5.** The rules generated by ten RuleFit models for RMC predictions (importance >0.1).

Rule	Coefficient	Support	Importance	Model
Concentration (mg/L) > 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) > -25.835	10.3069	0.1858	4.0091	5
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) > 45.705	7.7363	0.2920	3.5177	5
Concentration (mg/L) > 75.0 and TEM size (nm) > 14.68 and BET surface area (m <sup>2</sup> /g) <= 45.705	8.2850	0.2124	3.3886	5
Concentration (mg/L) <= 150.0 and TEM size (nm) > 14.68 and Zeta potential (mV) > -25.835	-6.4794	0.6018	3.1719	5
Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) > 840.285	-8.0683	0.1239	2.6582	5
Concentration (mg/L) <= 150.0 and TEM size (nm) > 21.72	5.2965	0.4956	2.6481	5
Concentration (mg/L) <= 150.0 and TEM size (nm) > 28.685 and BET surface area (m <sup>2</sup> /g) <= 27.46	-6.1359	0.1947	2.4296	5
Concentration (mg/L) > 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	4.7506	0.2301	1.9995	8
Concentration (mg/L) > 150.0 and BET surface area (m <sup>2</sup> /g) <= 92.805	-5.1862	0.1593	1.8979	5
Hydrodynamic diameter (nm) > 363.47 and Zeta potential (mV) <= 1.595	-3.9821	0.2832	1.7941	5
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 840.285	-3.9836	0.2035	1.6039	5
Concentration (mg/L) <= 37.5 and Zeta potential (mV) > 1.595	4.8770	0.1150	1.5561	5
Concentration (mg/L) > 75.0 and TEM size (nm) > 31.95 and Hydrodynamic diameter (nm) > 253.07999	3.9876	0.1770	1.5219	5
Concentration (mg/L) <= 150.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	-3.2607	0.3097	1.5077	9
Concentration (mg/L) > 150.0 and TEM size (nm) > 21.72	-4.0208	0.1593	1.4714	5
Concentration (mg/L) > 75.0 and BET surface area (m <sup>2</sup> /g) > 45.705	-2.9750	0.2832	1.3404	8
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	-2.9596	0.2124	1.2105	9
Concentration (mg/L) <= 150.0 and TEM size (nm) > 14.68 and BET surface area (m <sup>2</sup> /g) <= 45.705	-2.4872	0.3186	1.1589	5
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m <sup>2</sup> /g) > 45.705	2.4756	0.2478	1.0688	1
Concentration (mg/L) > 75.0 and TEM size (nm) >	2.4103	0.2301	1.0144	9

28.685 and Hydrodynamic diameter (nm) > 253.07999				
Hydrodynamic diameter (nm) > 900.76498	-3.8744	0.0708	0.9937	9
TEM size (nm) <= 47.235 and Hydrodynamic diameter (nm) <= 763.89999 and BET surface area (m2/g) > 5.01	2.0663	0.6549	0.9824	8
Concentration (mg/L) > 62.5 and BET surface area (m2/g) <= 5.01	3.6064	0.0796	0.9764	5
Concentration (mg/L) <= 75.0 and TEM size (nm) > 18.56 and Zeta potential (mV) <= -13.03	-3.6387	0.0708	0.9333	9
Concentration (mg/L) <= 75.0 and TEM size (nm) > 28.685 and BET surface area (m2/g) > 44.675	4.0941	0.0531	0.9180	9
Concentration (mg/L) > 75.0 and TEM size (nm) <= 28.685	-2.0351	0.2478	0.8786	9
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 253.07999 and BET surface area (m2/g) > 56.85	-2.2046	0.1858	0.8575	8
Concentration (mg/L) > 75.0 and Zeta potential (mV) <= -13.03	2.9025	0.0885	0.8243	9
Concentration (mg/L) > 150.0 and TEM size (nm) <= 27.04	-2.5799	0.1150	0.8232	5
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 253.07999	3.1716	0.0708	0.8135	5
Concentration (mg/L) > 75.0 and BET surface area (m2/g) <= 127.18999	-1.6454	0.3982	0.8055	5
Concentration (mg/L) <= 75.0 and TEM size (nm) > 28.685 and BET surface area (m2/g) > 44.675	3.1335	0.0708	0.8037	5
Concentration (mg/L) > 75.0 and BET surface area (m2/g) <= 56.85	1.7828	0.2566	0.7787	9
Concentration (mg/L) > 75.0 and TEM size (nm) > 113.04	3.7236	0.0442	0.7657	9
Concentration (mg/L) <= 75.0 and TEM size (nm) > 16.785 and BET surface area (m2/g) <= 45.705	-1.9001	0.2035	0.7650	7
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 840.285	7.7317	0.0088	0.7241	5
Concentration (mg/L) <= 150.0 and Zeta potential (mV) <= -9.325 and BET surface area (m2/g) <= 41.785	-2.1684	0.1239	0.7144	8
Zeta potential (mV) <= 1.595 and Zeta potential (mV) > -13.03	-1.5367	0.2920	0.6987	1
Concentration (mg/L) > 150.0 and TEM size (nm) > 24.155	-1.9778	0.1416	0.6895	9
Concentration (mg/L) > 150.0 and TEM size (nm) <= 31.95 and TEM size (nm) > 21.72	-2.8090	0.0619	0.6771	8
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 840.285 and BET surface area (m2/g) <= 45.705	-1.5091	0.2124	0.6172	6



Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m2/g) > 45.705	1.2226	0.5044	0.6113	8
Concentration (mg/L) > 150.0 and TEM size (nm) <= 28.685	-1.8578	0.1150	0.5928	5
Hydrodynamic diameter (nm) <= 276.06999	-1.2858	0.2832	0.5793	8
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 253.07999	-2.3650	0.0619	0.5701	5
Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m2/g) <= 45.705	-1.1484	0.4248	0.5677	8
Concentration (mg/L) > 37.5 and Hydrodynamic diameter (nm) > 415.67999	-1.2594	0.2743	0.5619	9
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 840.285 and BET surface area (m2/g) > 45.705	1.3170	0.2301	0.5543	6
Concentration (mg/L) <= 150.0 and TEM size (nm) > 14.68 and BET surface area (m2/g) > 45.705	1.1579	0.3451	0.5505	5
Concentration (mg/L) > 37.5 and BET surface area (m2/g) > 73.47	-1.1784	0.3097	0.5449	6
Concentration (mg/L) > 75.0 and Zeta potential (mV) <= -16.015	2.1975	0.0619	0.5297	5
Concentration (mg/L) > 150.0 and BET surface area (m2/g) <= 45.705	1.6598	0.1150	0.5296	9
Concentration (mg/L) > 37.5 and TEM size (nm) > 19.155 and Zeta potential (mV) <= 26.17	1.0645	0.4425	0.5287	8
Concentration (mg/L) > 37.5 and TEM size (nm) <= 16.785	-1.4074	0.1593	0.5150	1
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 220.665 and BET surface area (m2/g) <= 45.705	-1.2431	0.2124	0.5084	1
Concentration (mg/L) <= 75.0 and BET surface area (m2/g) <= 45.705	-1.2417	0.2124	0.5078	6
Concentration (mg/L) > 37.5 and Zeta potential (mV) <= 1.595 and Zeta potential (mV) > -13.03	-1.1867	0.2389	0.5061	10
Hydrodynamic diameter (nm) > 344.45 and Zeta potential (mV) <= 1.595	-1.0137	0.3628	0.4874	9
TEM size (nm) > 28.685 and BET surface area (m2/g) > 27.46	1.1160	0.2478	0.4818	8
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 840.285 and BET surface area (m2/g) <= 45.705	-1.1039	0.2301	0.4646	2
BET surface area (m2/g) <= 45.705	-0.9374	0.4248	0.4634	8
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m2/g) <= 149.7 and BET surface area (m2/g) > 56.85	1.3903	0.1239	0.4581	2

Concentration (mg/L) > 37.5 and TEM size (nm) <= 28.685 and Zeta potential (mV) > -25.835	-0.9840	0.3097	0.4550	3
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 220.665 and BET surface area (m <sup>2</sup> /g) <= 45.705	1.0955	0.2124	0.4481	3
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 253.07999	-1.9464	0.0531	0.4364	9
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) > 415.67999	1.4639	0.0973	0.4339	9
Concentration (mg/L) <= 150.0	-0.9533	0.7257	0.4253	8
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 13.07	4.4642	0.0088	0.4181	8
Concentration (mg/L) <= 75.0 and Zeta potential (mV) <= -11.7	-1.1638	0.1504	0.4161	1
Concentration (mg/L) <= 37.5 and TEM size (nm) > 13.07 and Hydrodynamic diameter (nm) > 253.07999	-1.0646	0.1858	0.4141	10
Concentration (mg/L) > 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	1.0003	0.2124	0.4091	6
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 56.85	-0.9542	0.2389	0.4069	3
Concentration (mg/L) > 62.5 and BET surface area (m <sup>2</sup> /g) <= 5.01	1.6772	0.0619	0.4043	1
Concentration (mg/L) > 75.0 and Zeta potential (mV) <= 26.17 and Zeta potential (mV) > 23.25	-1.9482	0.0442	0.4006	9
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.9788	0.2124	0.4003	3
Concentration (mg/L) <= 150.0 and TEM size (nm) > 21.72 and Hydrodynamic diameter (nm) <= 401.64999	-0.7930	0.3805	0.3850	8
Concentration (mg/L) > 37.5 and TEM size (nm) <= 24.475 and Hydrodynamic diameter (nm) > 415.67999	-1.0024	0.1593	0.3668	2
Concentration (mg/L) > 75.0 and TEM size (nm) > 24.155 and BET surface area (m <sup>2</sup> /g) <= 127.18999	0.8495	0.2478	0.3668	10
Concentration (mg/L) > 150.0 and BET surface area (m <sup>2</sup> /g) > 45.705	-1.0688	0.1327	0.3626	9
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.8777	0.2124	0.3590	10
Concentration (mg/L) <= 150.0 and Zeta potential (mV) > 26.17	1.0792	0.1062	0.3325	9
Concentration (mg/L) > 150.0 and TEM size (nm) > 37.02	1.1289	0.0885	0.3206	6
Zeta potential (mV) <= 1.595 and Zeta potential (mV) > -13.03 and BET surface area (m <sup>2</sup> /g) > 4.39	-0.7037	0.2920	0.3200	7
Zeta potential (mV) <= 1.595 and Zeta potential (mV) >	-0.6944	0.3009	0.3185	6

-13.03				
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 253.07999 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.7593	0.2124	0.3105	6
Concentration (mg/L) > 150.0 and TEM size (nm) <= 37.02	-0.7918	0.1858	0.3080	6
Concentration (mg/L) > 37.5 and TEM size (nm) <= 113.04 and Hydrodynamic diameter (nm) > 543.41499	-0.7852	0.1858	0.3054	4
Concentration (mg/L) <= 150.0 and Zeta potential (mV) <= 26.17	0.6365	0.6549	0.3026	5
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m <sup>2</sup> /g) > 45.705	0.6722	0.2566	0.2936	10
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 16.785	1.1231	0.0708	0.2881	1
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.6833	0.2124	0.2795	1
Concentration (mg/L) > 75.0 and BET surface area (m <sup>2</sup> /g) > 45.705	-0.6022	0.3097	0.2785	4
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 28.685	-0.5484	0.4159	0.2703	1
TEM size (nm) <= 73.455 and BET surface area (m <sup>2</sup> /g) <= 27.46	-0.7457	0.1504	0.2666	8
Concentration (mg/L) > 150.0 and Hydrodynamic diameter (nm) <= 415.67999 and Zeta potential (mV) <= 35.27 and BET surface area (m <sup>2</sup> /g) <= 181.475	0.8257	0.1062	0.2544	1
Concentration (mg/L) <= 150.0 and TEM size (nm) > 13.07	-0.5571	0.7257	0.2486	1
Concentration (mg/L) <= 150.0 and BET surface area (m <sup>2</sup> /g) <= 127.18999	0.5015	0.5929	0.2464	5
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.6017	0.2124	0.2461	1
Concentration (mg/L) <= 150.0 and BET surface area (m <sup>2</sup> /g) <= 15.31 and BET surface area (m <sup>2</sup> /g) > 5.01	-1.0179	0.0619	0.2454	6
Concentration (mg/L) > 37.5 and Zeta potential (mV) > -13.03 and BET surface area (m <sup>2</sup> /g) > 5.01	-0.4906	0.4602	0.2445	3
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.5898	0.2124	0.2412	10
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 253.07999 and BET surface area (m <sup>2</sup> /g) <= 5.01	0.9162	0.0708	0.2350	8
TEM size (nm) <= 28.685 and Zeta potential (mV) > -25.835	-0.4794	0.3982	0.2347	2

Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 291.38 and Zeta potential (mV) <= -11.7	0.7325	0.1150	0.2337	1
Concentration (mg/L) > 150.0 and Zeta potential (mV) > 5.565	0.7043	0.1239	0.2320	8
Concentration (mg/L) > 75.0 and TEM size (nm) <= 73.455 and Zeta potential (mV) > -25.835	-0.4692	0.3717	0.2267	10
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 220.665	0.4545	0.4513	0.2262	1
Concentration (mg/L) <= 75.0 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.5331	0.2301	0.2244	2
Concentration (mg/L) <= 37.5 and Hydrodynamic diameter (nm) <= 543.41499 and Zeta potential (mV) <= -16.015	-0.9633	0.0531	0.2160	1
Concentration (mg/L) > 75.0 and TEM size (nm) > 24.155 and BET surface area (m <sup>2</sup> /g) <= 56.85	0.5184	0.2124	0.2120	10
Concentration (mg/L) <= 150.0 and TEM size (nm) > 21.72 and Hydrodynamic diameter (nm) > 401.64999	0.7054	0.0973	0.2091	8
Concentration (mg/L) <= 37.5 and TEM size (nm) <= 24.155 and BET surface area (m <sup>2</sup> /g) <= 107.75	0.8489	0.0619	0.2046	3
Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) <= 26.17	0.4851	0.7699	0.2042	3
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.4987	0.2124	0.2040	4
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and BET surface area (m <sup>2</sup> /g) > 45.705	0.4770	0.2389	0.2034	7
Concentration (mg/L) > 75.0 and TEM size (nm) <= 24.155 and Zeta potential (mV) > -25.835	-0.5185	0.1858	0.2017	10
Concentration (mg/L) <= 75.0 and TEM size (nm) > 24.155 and BET surface area (m <sup>2</sup> /g) <= 48.595	-0.4905	0.2124	0.2006	10
Concentration (mg/L) > 75.0 and TEM size (nm) > 28.685 and Zeta potential (mV) <= 19.25	0.5912	0.1327	0.2006	2
Concentration (mg/L) <= 37.5 and TEM size (nm) > 16.785	-0.4937	0.2035	0.1988	1
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 45.705	0.4553	0.2124	0.1862	4
Concentration (mg/L) > 150.0 and TEM size (nm) <= 24.155	0.6026	0.1062	0.1857	9
Concentration (mg/L) > 62.5 and TEM size (nm) > 73.455	0.7039	0.0708	0.1805	8
Hydrodynamic diameter (nm) > 220.665 and Zeta	-0.3777	0.3451	0.1796	2

potential (mV) <= 5.565 and Zeta potential (mV) > -13.03				
TEM size (nm) <= 73.455 and TEM size (nm) > 28.685 and BET surface area (m <sup>2</sup> /g) > 27.46	0.4606	0.1858	0.1792	10
Zeta potential (mV) > -13.03	-0.4187	0.7699	0.1762	1
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 253.07999	-0.3545	0.4336	0.1757	3
Concentration (mg/L) <= 75.0 and TEM size (nm) > 73.455	-0.7480	0.0531	0.1677	8
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 900.76498 and Hydrodynamic diameter (nm) > 220.665 and BET surface area (m <sup>2</sup> /g) <= 45.705	-0.4086	0.2124	0.1671	4
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 253.07999 and BET surface area (m <sup>2</sup> /g) > 5.01	-0.3439	0.3717	0.1662	8
Concentration (mg/L) <= 75.0 and TEM size (nm) > 14.68 and Hydrodynamic diameter (nm) <= 543.41499 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 45.705	0.5023	0.1239	0.1655	7
BET surface area (m <sup>2</sup> /g) > 5.01	-0.4336	0.8496	0.1550	5
Zeta potential (mV) <= 26.17 and Zeta potential (mV) > 1.595	0.3259	0.3451	0.1549	9
Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) <= 26.17	0.3734	0.7876	0.1527	9
Concentration (mg/L) > 37.5 and TEM size (nm) <= 28.685 and Zeta potential (mV) > -14.585	-0.3405	0.2655	0.1504	10
Concentration (mg/L) > 75.0 and Hydrodynamic diameter (nm) > 253.07999 and BET surface area (m <sup>2</sup> /g) <= 45.705	0.3756	0.1947	0.1487	2
Concentration (mg/L) > 75.0 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 127.18999	-0.5740	0.0708	0.1472	3
Concentration (mg/L) > 150.0 and TEM size (nm) > 32.42	0.4746	0.1062	0.1462	10
Hydrodynamic diameter (nm) <= 900.76498 and Zeta potential (mV) <= 26.17	0.3529	0.7876	0.1443	6
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) <= 736.38501 and Zeta potential (mV) > -25.835 and BET surface area (m <sup>2</sup> /g) > 45.705	0.3915	0.1593	0.1433	2
Concentration (mg/L) > 75.0 and TEM size (nm) > 28.685 and Hydrodynamic diameter (nm) > 242.13499	0.3498	0.2124	0.1431	5
Concentration (mg/L) > 150.0 and BET surface area (m <sup>2</sup> /g) > 92.805	0.5276	0.0796	0.1428	5
Hydrodynamic diameter (nm) > 276.06999 and Zeta	0.4080	0.1416	0.1422	5

potential (mV) > 12.15				
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 220.665	-0.2834	0.4690	0.1414	10
Concentration (mg/L) > 75.0 and BET surface area (m2/g) <= 48.595	0.3390	0.2124	0.1387	1
Concentration (mg/L) <= 37.5 and TEM size (nm) > 13.07 and Hydrodynamic diameter (nm) <= 532.265 and Hydrodynamic diameter (nm) > 220.665	-0.3727	0.1593	0.1364	2
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 220.665 and BET surface area (m2/g) <= 56.85	-0.3139	0.2389	0.1339	3
Concentration (mg/L) <= 75.0 and TEM size (nm) > 14.68 and Zeta potential (mV) > -14.585 and BET surface area (m2/g) > 45.705	0.4037	0.1239	0.1330	7
Concentration (mg/L) > 75.0 and TEM size (nm) > 28.685 and BET surface area (m2/g) <= 44.675	0.3353	0.1947	0.1328	7
TEM size (nm) > 28.685 and BET surface area (m2/g) <= 27.46	-0.2937	0.2743	0.1310	8
Concentration (mg/L) > 75.0 and TEM size (nm) > 14.68	0.2651	0.4159	0.1306	10
Concentration (mg/L) > 75.0 and BET surface area (m2/g) <= 45.705	0.3255	0.1947	0.1289	2
Concentration (mg/L) <= 75.0 and TEM size (nm) > 24.155 and BET surface area (m2/g) <= 48.595	-0.3083	0.2124	0.1261	4
Concentration (mg/L) <= 75.0 and BET surface area (m2/g) > 73.47	0.2963	0.2124	0.1212	6
Zeta potential (mV) <= 5.565	-0.2419	0.5752	0.1196	8
Concentration (mg/L) <= 150.0 and TEM size (nm) <= 73.455 and BET surface area (m2/g) <= 27.46	-0.3448	0.1239	0.1136	10
Concentration (mg/L) > 37.5 and TEM size (nm) <= 16.785	-0.2923	0.1681	0.1093	7
Concentration (mg/L) > 150.0 and TEM size (nm) > 31.95	0.3497	0.1062	0.1077	7
Concentration (mg/L) <= 75.0 and Hydrodynamic diameter (nm) > 253.07999 and BET surface area (m2/g) <= 48.595	-0.2511	0.2301	0.1057	2
Concentration (mg/L) > 150.0 and Zeta potential (mV) <= 2.46 and BET surface area (m2/g) > 29.635	-0.4368	0.0619	0.1053	1
Concentration (mg/L) <= 75.0 and TEM size (nm) > 16.785 and BET surface area (m2/g) <= 45.705	-0.2467	0.2301	0.1038	2
Concentration (mg/L) > 75.0 and BET surface area (m2/g) > 45.705	-0.2290	0.2743	0.1022	6
Concentration (mg/L) > 75.0 and TEM size (nm) > 28.685 and Hydrodynamic diameter (nm) > 253.07999	0.2535	0.1947	0.1004	7

and BET surface area (m <sup>2</sup> /g) ≤ 44.675				
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**Table S6.** Simplified intervals in different RuleGrid plots for RDW prediction.

**Table S6.1.** Simplified intervals of the hydrodynamic diameter in the RuleGrid plot for interactions between concentration and hydrodynamic diameter.

<b>Raw interval</b>	<b>Simply interval</b>
[197, 220.665]	[197.0,220.665]
[197, 263.34999]	[197.0,263.35]
[197, 312.84999]	[197.0,312.85]
[197, 363.47]	[197.0,363.47]
[197, 543.41499]	[197.0,543.415]
[197, 736.38501]	[197.0,736.385]
(220.665, 933.73]	(220.665,933.73]
(263.34999, 363.47]	(263.35,363.47]
(263.34999, 415.67999]	(263.35,415.68]
(263.34999, 933.73]	(263.35,933.73]
(344.45, 736.38501]	(344.45,736.385]
(344.45, 900.76498]	(365.472,917.247]
(363.47, 900.76498]	(365.472,917.247]
(363.47, 933.73]	(365.472,917.247]
(390.5, 933.73]	(365.472,917.247]
(415.67999, 933.73]	(415.68,933.73]
(736.38501, 933.73]	(736.385,933.73]
(840.285, 933.73]	(840.285,933.73]
(900.76498, 933.73]	(900.765,933.73]

**Table S6.2.** Simplified intervals of the TEM size in the RuleGrid plot for interactions between concentration and TEM size.

<b>Raw interval</b>	<b>Simply interval</b>
[12.97, 13.07]	[12.97,13.07]
[12.97, 29.155]	[12.97,29.155]
[12.97, 38.345]	[13.02,38.345]
(13.07, 38.345]	(13.02,38.345]
(13.07, 132.11]	(13.07,132.11]
(14.68, 21.72]	(14.68,21.72]
(19.155, 28.685]	(19.155,28.685]
(28.685, 38.345]	(28.685,38.345]
(32.04, 132.11]	(32.04,132.11]
(38.345, 73.455]	(38.345,73.455]
(38.345, 113.04]	(38.345,113.04]



(38.345, 132.11]

(38.345,132.11]

**Table S6.3.** Simplified intervals of the zeta potential in the RuleGrid plot for interactions between concentration and zeta potential.

<b>Raw interval</b>	<b>Simply interval</b>
[-32.77, -25.835]	[-32.77,-25.835]
[-32.77, -16.015]	[-32.77,-13.548]
[-32.77, -13.03]	[-32.77,-13.548]
[-32.77, -11.6]	[-32.77,-13.548]
[-32.77, -4.945]	[-32.77,-4.945]
(-13.03, -9.325]	(-13.03,-9.325]
(-13.03, -4.945]	(-13.03,-4.945]
(-13.03, 26.17]	(-13.03,26.17]
(-13.03, 35.27]	(-13.03,35.27]
(-13.03, 44.07]	(-12.315,44.07]
(-11.6, 44.07]	(-12.315,44.07]
(-4.945, 44.07]	(-4.945,44.07]
(26.17, 35.27]	(26.17,35.27]
(26.17, 44.07]	(26.17,44.07]
(35.27, 44.07]	(35.27,44.07]

**Table S6.4.** Simplified intervals of the zeta potential in the RuleGrid plot for interactions among concentration, hydrodynamic diameter, and zeta potential.

<b>Raw interval</b>	<b>Simply interval</b>
[-32.77, -10.655]	[-32.77,-10.655]
[-32.77, 5.565]	[-32.77,5.565]
[-32.77, 21.87]	[-32.77,23.863]
[-32.77, 23.55]	[-32.77,23.863]
[-32.77, 26.17]	[-32.77,23.863]
(-25.835, 19.25]	(-25.835,19.25]

**Table S7.** Simplified intervals in different RuleGrid plots for RMC prediction.

**Table S7.1.** Simplified intervals of the BET surface area in the RuleGrid plot for interactions between concentration and BET surface area.

<b>Raw interval</b>	<b>Simply interval</b>
[4.07, 5.01]	[4.07,5.01]
[4.07, 45.705]	[4.07,50.383]
[4.07, 48.595]	[4.07,50.383]
[4.07, 56.85]	[4.07,50.383]
[4.07, 92.805]	[4.07,92.805]
[4.07, 127.18999]	[4.07,127.19]
(5.01, 15.31]	(5.01,15.31]
(45.705, 200.84]	(45.705,200.84]
(73.47, 200.84]	(73.47,200.84]
(92.805, 200.84]	(92.805,200.84]

**Table S7.2.** Simplified intervals of the TEM size in the RuleGrid plot for interactions between concentration and TEM size.

<b>Raw interval</b>	<b>Simply interval</b>
[12.97, 13.07]	[12.97,14.928]
[12.97, 16.785]	[12.97,14.928]
[12.97, 24.155]	[12.97,26.627]
[12.97, 27.04]	[12.97,26.627]
[12.97, 28.685]	[12.97,26.627]
[12.97, 37.02]	[12.97,37.02]
(13.07, 132.11]	(14.845,132.11]
(14.68, 132.11]	(14.845,132.11]
(16.785, 132.11]	(14.845,132.11]
(21.72, 132.11]	(22.938,132.11]
(21.72, 31.95]	(21.72,31.95]
(24.155, 132.11]	(22.938,132.11]
(31.95, 132.11]	(33.797,132.11]
(32.42, 132.11]	(33.797,132.11]
(37.02, 132.11]	(33.797,132.11]
(73.455, 132.11]	(73.455,132.11]
(113.04, 132.11]	(113.04,132.11]

**Table S7.3.** Simplified intervals of the zeta potential in the RuleGrid plot for interactions between concentration and zeta potential.

Raw interval	Simply interval
[-32.77, -16.015]	[-32.77,-13.582]
[-32.77, -13.03]	[-32.77,-13.582]
[-32.77, -11.7]	[-32.77,-13.582]
[-32.77, 26.17]	[-32.77,26.17]
(-13.03, 1.595]	(-13.03,1.595]
(1.595, 44.07]	(1.595,44.07]
(5.565, 44.07]	(5.565,44.07]
(23.25, 26.17]	(23.25,26.17]
(26.17, 44.07]	(26.17,44.07]

**Table S7.4.** Simplified intervals of the BET surface area in the RuleGrid plot for interactions among concentration, BET surface area, and TEM size.

Raw interval	Simply interval
[4.07, 27.46]	[4.07,27.46]
[4.07, 45.705]	[4.07,47.15]
[4.07, 48.595]	[4.07,47.15]
(44.675, 200.84]	(45.19,200.84]
(45.705, 200.84]	(45.19,200.84]

**Table S7.5.** Simplified intervals of the TEM size in the RuleGrid plot for interactions among concentration, BET surface area, and TEM size.

Raw interval	Simply interval
[12.97, 73.455]	[12.97,73.455]
(14.68, 132.11]	(15.732,132.11]
(16.785, 132.11]	(15.732,132.11]
(24.155, 132.11]	(26.42,132.11]
(28.685, 132.11]	(26.42,132.11]

**Table S7.6.** Simplified intervals of the zeta potential in the RuleGrid plot for interactions among concentration, TEM size, and zeta potential.

<b>Raw interval</b>	<b>Simply interval</b>
(14.68, 132.11]	(17.465,132.11]
(18.56, 132.11]	(17.465,132.11]
(19.155, 132.11]	(17.465,132.11]
[12.97, 28.685]	[12.97,28.685]

**Table S8.** The top ten solutions obtained by three weighted sum methods.

**Table S8.1.** Equal-weighted solutions.

<b>Instance No.</b>	1809	6095	2728	4934	7533	2727	786	5146	696	947
<b>Composition</b>	CuO	CuO	CeO2	CeO2	CeO2	CuO	$\alpha$ -Fe2O3	$\gamma$ -Fe2O3	ZnO	CeO2
<b>Concentration (mg/L)</b>	50	50	50	50	50	50	50	50	50	50
<b>TEM size (nm)</b>	128.07	122.52	126.49	100.22	33.65	27.42	34.84	34.5	112.77	121.53
<b>Hydrodynamic diameter (nm)</b>	723.62	377.07	380.08	364.51	672.52	777.1	448.64	389.66	545.25	679.01
<b>Zeta potential (mV)</b>	-17.78	-22.88	-18.01	-21.79	-21.46	-25.28	-18.71	-15.07	-14.39	-14.54
<b>BET surface area (m<sup>2</sup>/g)</b>	9.21	32.24	9.85	10.8	25.11	39.32	23.35	34.32	15.68	23.81
<b>RDW</b>	0.9835	0.9815	0.9801	0.9796	0.9768	0.9752	0.9768	0.9758	0.9731	0.9737
<b>RMC</b>	0.0026	0.0033	0.0026	0.0026	0.0020	0.0010	0.0030	0.0035	0.0021	0.0032
<b>Equal-weighted</b>	0.9905	0.9891	0.9888	0.9885	0.9874	0.9871	0.9869	0.9862	0.9855	0.9852

**Table S8.2.** RDW-first solutions.

<b>Instance No.</b>	1809	6095	2728	4934	7533	786	2727	5146	947	7640
<b>Composition</b>	CuO	CuO	CeO2	CeO2	CeO2	$\alpha$ -Fe2O3	CuO	$\gamma$ -Fe2O3	CeO2	$\alpha$ -Fe2O3
<b>Concentration (mg/L)</b>	50	50	50	50	50	50	50	50	50	50
<b>TEM size (nm)</b>	128.07	122.52	126.49	100.22	33.65	34.84	27.42	34.5	121.53	118.21
<b>Hydrodynamic diameter (nm)</b>	723.62	377.07	380.08	364.51	672.52	448.64	777.1	389.66	679.01	487.81
<b>Zeta potential (mV)</b>	-17.78	-22.88	-18.01	-21.79	-21.46	-18.71	-25.28	-15.07	-14.54	-14.42
<b>BET surface area (m<sup>2</sup>/g)</b>	9.21	32.24	9.85	10.8	25.11	23.35	39.32	34.32	23.81	20.91
<b>RDW</b>	0.9835	0.9815	0.9801	0.9796	0.9768	0.9768	0.9752	0.9758	0.9737	0.9737

<b>RMC</b>	0.0026	0.0033	0.0026	0.0026	0.0020	0.0030	0.0010	0.0035	0.0032	0.0032
<b>RDW-first</b>	0.9877	0.9861	0.9853	0.9849	0.9831	0.9828	0.9824	0.9820	0.9806	0.9806

**Table S8.3.** RMC-first solutions.

<b>Instance No.</b>	1809	2728	6095	4934	2727	7533	786	696	5146	947
<b>Composition</b>	CuO	CeO2	CuO	CeO2	CuO	CeO2	$\alpha$ -Fe2O3	ZnO	$\gamma$ -Fe2O3	CeO2
<b>Concentration (mg/L)</b>	50	50	50	50	50	50	50	50	50	50
<b>TEM size (nm)</b>	128.07	126.49	122.52	100.22	27.42	33.65	34.84	112.77	34.5	121.53
<b>Hydrodynamic diameter (nm)</b>	723.62	380.08	377.07	364.51	777.1	672.52	448.64	545.25	389.66	679.01
<b>Zeta potential (mV)</b>	-17.78	-18.01	-22.88	-21.79	-25.28	-21.46	-18.71	-14.39	-15.07	-14.54
<b>BET surface area (m2/g)</b>	9.21	9.85	32.24	10.8	39.32	25.11	23.35	15.68	34.32	23.81
<b>RDW</b>	0.9835	0.9801	0.9815	0.9796	0.9752	0.9768	0.9768	0.9731	0.9758	0.9737
<b>RMC</b>	0.0026	0.0026	0.0033	0.0026	0.0010	0.0020	0.0030	0.0021	0.0035	0.0032
<b>RMC-first</b>	0.9933	0.9922	0.9922	0.9921	0.9919	0.9916	0.9909	0.9904	0.9903	0.9898

**Table S9.** The 49 nanopriming candidates selected from RuleGrid plots.

No.	Composition	Concentration (mg/L)	TEM size (nm)	Hydrodynamic diameter (nm)	Zeta potential (mV)	BET surface area (m <sup>2</sup> /g)
582	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	25.36	490.65	-17.08	38.1
680	Fe <sub>3</sub> O <sub>4</sub>	50	28.78	852.38	-16.66	30.52
696	ZnO	50	112.77	545.25	-14.39	15.68
786	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	34.84	448.64	-18.71	23.35
848	ZnO	50	132.11	823.24	-21.38	37.91
919	Fe <sub>3</sub> O <sub>4</sub>	50	38.66	553.29	-17.31	43.3
947	CeO <sub>2</sub>	50	121.53	679.01	-14.54	23.81
1209	CeO <sub>2</sub>	50	94.51	361.4	-12.9	18.09
1330	TiO <sub>2</sub>	50	37.24	895.89	-15.38	18.05
1506	ZnO	50	70.58	886.6	-32.77	28.67
1526	CeO <sub>2</sub>	50	26.18	444.64	-11.78	38.17
1698	SiO <sub>2</sub>	50	47.84	914.24	-22.55	6.24
1799	CuO	50	121.62	739.5	-13.52	22.35
1809	CuO	50	128.07	723.62	-17.78	9.21
2075	SiO <sub>2</sub>	50	50.9	672.81	-18.8	27.82
2225	Fe <sub>3</sub> O <sub>4</sub>	50	26.55	888.02	-12.9	24.22
2271	Fe <sub>3</sub> O <sub>4</sub>	50	91.34	923.17	-11.82	16.59
2542	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	42.3	769.66	-26.02	15.4
2727	CuO	50	27.42	777.1	-25.28	39.32
2728	CeO <sub>2</sub>	50	126.49	380.08	-18.01	9.85
3103	CeO <sub>2</sub>	50	66.11	485.08	-13.46	29.89
3724	SiO <sub>2</sub>	50	55.88	933.73	-12.39	19.72
3763	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	54.25	801.01	-32.77	21.5
4077	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	62.09	933.73	-21.64	9.2
4141	SiO <sub>2</sub>	50	24.18	906.82	-12.75	12.26
4334	Fe <sub>3</sub> O <sub>4</sub>	50	45.05	844.64	-32.45	43.73
4683	Fe <sub>3</sub> O <sub>4</sub>	50	39.15	933.73	-21.51	32.93
4799	CeO <sub>2</sub>	50	41.86	907.43	-18.45	15.49
4934	CeO <sub>2</sub>	50	100.22	364.51	-21.79	10.8
5146	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	34.5	389.66	-15.07	34.32
5356	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	26.3	933.73	-29.12	23.79
5504	Fe <sub>3</sub> O <sub>4</sub>	50	42.01	895.99	-21.25	12.68
5690	Fe <sub>3</sub> O <sub>4</sub>	50	104.48	488.46	-20.5	33.2
5792	CeO <sub>2</sub>	50	41.35	767.13	-12.76	20.34
6008	Fe <sub>3</sub> O <sub>4</sub>	50	41.99	933.73	-20.16	12.8
6095	CuO	50	122.52	377.07	-22.88	32.24
6138	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	117.72	385.45	-19.49	24.04
6626	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	37.98	381.28	-11.48	26.98
6646	Fe <sub>3</sub> O <sub>4</sub>	50	26.09	933.73	-15.54	4.82
6769	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	124.88	595.9	-13.93	33.46

<b>6777</b>	TiO2	50	24.99	495.65	-12.49	19.16
<b>7234</b>	$\alpha$ -Fe2O3	50	44.36	363.84	-18.97	38.46
<b>7335</b>	TiO2	50	40.74	412.54	-11.35	25.01
<b>7528</b>	ZnO	50	36.72	749.7	-21.46	39.44
<b>7533</b>	CeO2	50	33.65	672.52	-21.46	25.11
<b>7640</b>	$\alpha$ -Fe2O3	50	118.21	487.81	-14.42	20.91
<b>7641</b>	SiO2	50	87.45	790.79	-32.77	8.53
<b>7658</b>	Fe3O4	50	36.16	933.73	-32.77	29.3
<b>8063</b>	SiO2	50	43.94	447.35	-15.38	24.05

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**Table S10.** The top 49 nanopriming candidates ranked by their highest sum SHAP

values.

No.	Composition	Concentration (mg/L)	TEM size (nm)	Hydrodynamic diameter (nm)	Zeta potential (mV)	BET surface area (m <sup>2</sup> /g)
267	ZnO	50	16.73	815.1	-15.45	34.23
332	ZnO	50	36.89	894.75	-23.03	45.65
582	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	25.36	490.65	-17.08	38.1
696	ZnO	50	112.77	545.25	-14.39	15.68
786	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	34.84	448.64	-18.71	23.35
848	ZnO	50	132.11	823.24	-21.38	37.91
947	CeO <sub>2</sub>	50	121.53	679.01	-14.54	23.81
1526	CeO <sub>2</sub>	50	26.18	444.64	-11.78	38.17
1698	SiO <sub>2</sub>	50	47.84	914.24	-22.55	6.24
1799	CuO	50	121.62	739.5	-13.52	22.35
1809	CuO	50	128.07	723.62	-17.78	9.21
2075	SiO <sub>2</sub>	50	50.9	672.81	-18.8	27.82
2260	CuO	25	72.19	257.99	33.44	13.49
2465	CuO	25	51.13	262.02	31.65	14.72
2542	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	42.3	769.66	-26.02	15.4
2717	TiO <sub>2</sub>	25	47.61	257.76	31.53	26.99
2727	CuO	50	27.42	777.1	-25.28	39.32
2728	CeO <sub>2</sub>	50	126.49	380.08	-18.01	9.85
3103	CeO <sub>2</sub>	50	66.11	485.08	-13.46	29.89
3398	CuO	25	66.57	197	29.97	25.38
3763	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	54.25	801.01	-32.77	21.5
3799	CuO	25	51.87	197	28.57	16.93
4077	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	62.09	933.73	-21.64	9.2
4141	SiO <sub>2</sub>	50	24.18	906.82	-12.75	12.26
4636	SiO <sub>2</sub>	50	21.82	730.53	-13.7	37.17
4934	CeO <sub>2</sub>	50	100.22	364.51	-21.79	10.8
5146	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	34.5	389.66	-15.07	34.32
5356	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	26.3	933.73	-29.12	23.79
5504	Fe <sub>3</sub> O <sub>4</sub>	50	42.01	895.99	-21.25	12.68
5690	Fe <sub>3</sub> O <sub>4</sub>	50	104.48	488.46	-20.5	33.2
5836	TiO <sub>2</sub>	50	57.89	752.1	-20.33	44.58
6008	Fe <sub>3</sub> O <sub>4</sub>	50	41.99	933.73	-20.16	12.8
6095	CuO	50	122.52	377.07	-22.88	32.24
6134	ZnO	50	12.97	933.73	-32.77	35.23
6138	$\gamma$ -Fe <sub>2</sub> O <sub>3</sub>	50	117.72	385.45	-19.49	24.04
6205	CeO <sub>2</sub>	50	19.22	933.73	-25.96	41.76
6446	SiO <sub>2</sub>	50	21.44	456.86	-22.02	37.62
6646	Fe <sub>3</sub> O <sub>4</sub>	50	26.09	933.73	-15.54	4.82

<b>6769</b>	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	124.88	595.9	-13.93	33.46
<b>6777</b>	TiO <sub>2</sub>	50	24.99	495.65	-12.49	19.16
<b>7234</b>	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	44.36	363.84	-18.97	38.46
<b>7357</b>	CeO <sub>2</sub>	50	21.96	933.73	-29.4	30.1
<b>7528</b>	ZnO	50	36.72	749.7	-21.46	39.44
<b>7533</b>	CeO <sub>2</sub>	50	33.65	672.52	-21.46	25.11
<b>7640</b>	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub>	50	118.21	487.81	-14.42	20.91
<b>7641</b>	SiO <sub>2</sub>	50	87.45	790.79	-32.77	8.53
<b>7968</b>	CuO	25	39.28	197	35.24	22.97
<b>8063</b>	SiO <sub>2</sub>	50	43.94	447.35	-15.38	24.05
<b>8130</b>	Fe <sub>3</sub> O <sub>4</sub>	50	14.41	783.91	-14.06	36.79

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