Supplemental data

Optimized adsorption removal and capacity prediction of anionic pollutants using a hybrid strategy of machine learning algorithms

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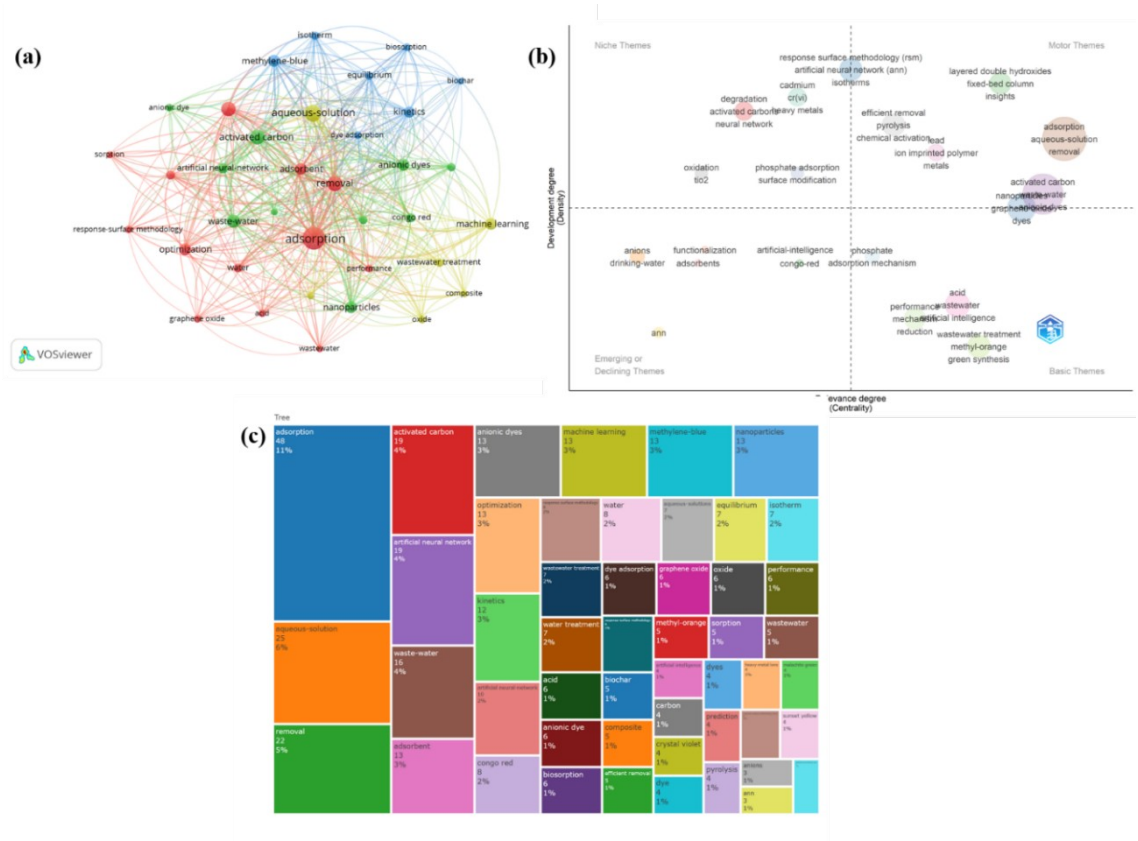

Figure S1. Thematic and keyword structure of machine learning-assisted adsorption research for wastewater treatment. (a) Keyword co-occurrence network illustrating conceptual relationships among major research terms, (b) Thematic map categorizing research themes based on centrality and development density, and (c) Keyword frequency treemap showing the relative prominence of dominant research terms

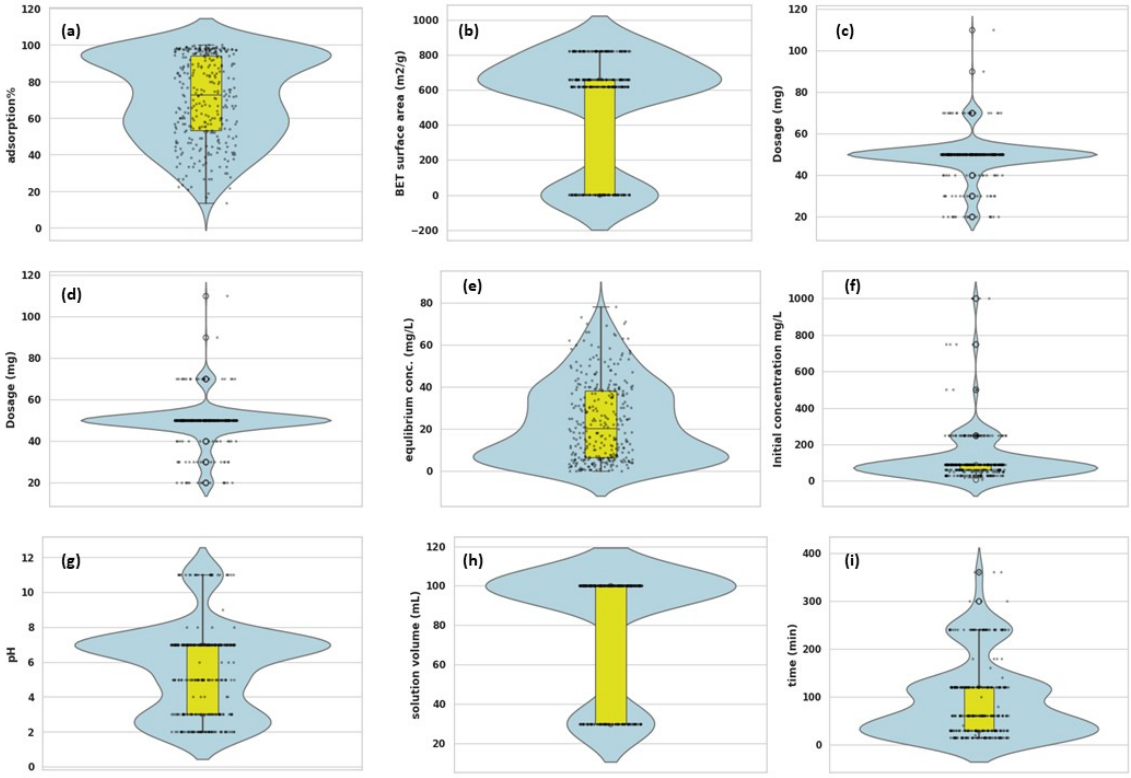

Figure S2. Distribution plots of selected variables for ML models training are presented in violin plots.

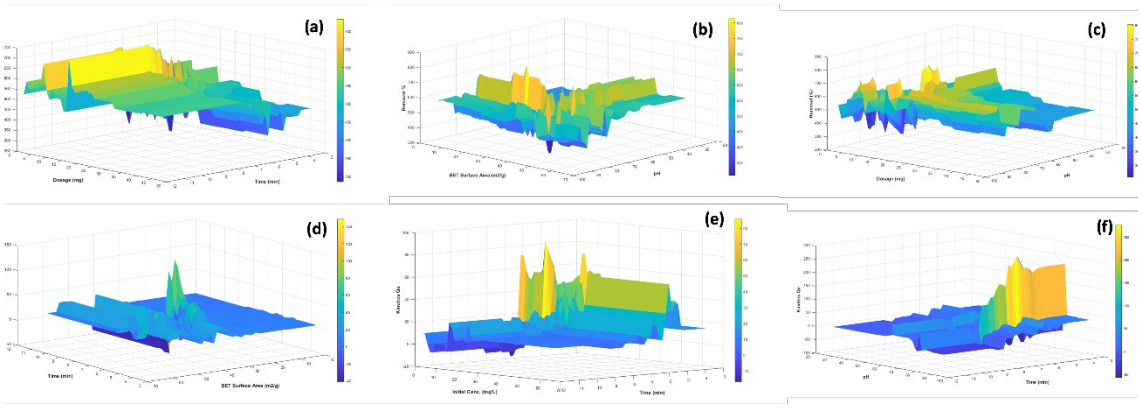

Figure S3. 3D PDPs of pollutants removal kinetics vs dependent experimental parameters.

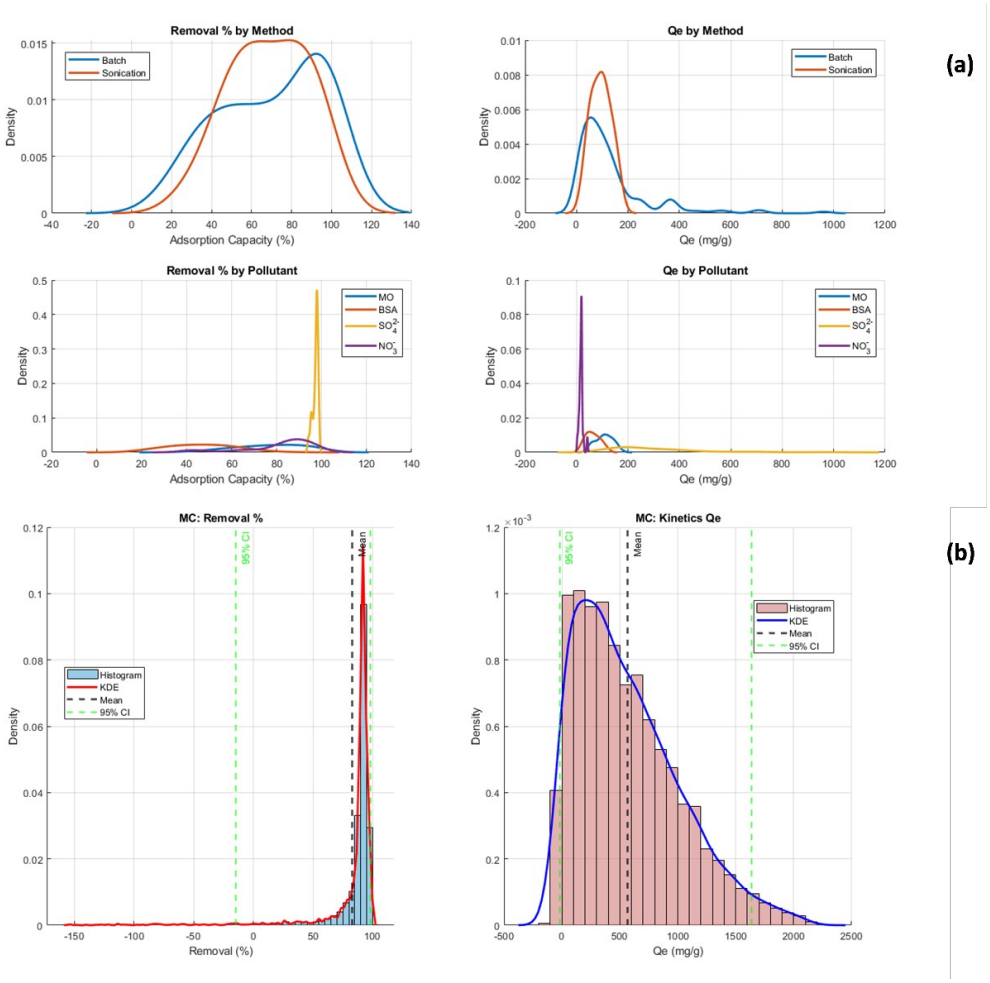

Figure S4. Kernel density plots of adsorption capacity and kinetics obtained by varying separation methods and pollutant type (a) and Monte Carlo simulations (n=1000) for quantification of prediction uncertainty of adsorption capacity and kinetics (b).

Table S1. Dataset used for training and testing applied ML models.

Method	Pollutant	Time	Equilibrium conc. (mg/L)	Adsorption %	Initial concentration mg/L	pH	temp (oC)	Dosage (mg)	solution volume (mL)	BET surface area (m^2/g)	Material	Kinetics Qe (mg/g)
Batch	MO	15	3.5	88.333	30	7	25	50	100	619	**PAC**	53.00
Batch	MO	30	2	93.333	30	7	25	50	100	619	**PAC**	56.00
Batch	MO	60	2	93.333	30	7	25	50	100	619	**PAC**	56.00
Batch	MO	120	2	93.333	30	7	25	50	100	619	**PAC**	56.00
Batch	MO	15	1	96.667	30	7	25	50	100	823	**TPAC**	58.00
Batch	MO	30	0.5	98.333	30	7	25	50	100	823	**TPAC**	59.00
Batch	MO	60	0.2	99.333	30	7	25	50	100	823	**TPAC**	59.60
Batch	MO	120	0.2	99.333	30	7	25	50	100	823	**TPAC**	59.60
Batch	MO	15	2.5	91.667	30	7	25	50	100	657	**CPAC**	55.00
Batch	MO	30	1	96.667	30	7	25	50	100	657	**CPAC**	58.00
Batch	MO	60	0.7	97.667	30	7	25	50	100	657	**CPAC**	58.60
Batch	MO	120	0.7	97.667	30	7	25	50	100	657	**CPAC**	58.60
Batch	MO	15	25	58.333	60	7	25	50	100	619	**PAC**	70.00
Batch	MO	30	18.5	69.167	60	7	25	50	100	619	**PAC**	83.00
Batch	MO	60	12.15	79.750	60	7	25	50	100	619	**PAC**	95.70

Batch	MO	120	12	80.000	60	7	25	50	100	619	**PAC**	96.00
Batch	MO	15	15.7	73.833	60	7	25	50	100	823	**TPAC**	88.60
Batch	MO	30	10	83.333	60	7	25	50	100	823	**TPAC**	100.00
Batch	MO	60	7	88.333	60	7	25	50	100	823	**TPAC**	106.00
Batch	MO	120	6.5	89.167	60	7	25	50	100	823	**TPAC**	107.00
Batch	MO	15	20.8	65.333	60	7	25	50	100	657	**CPAC**	78.40
Batch	MO	30	12.4	79.333	60	7	25	50	100	657	**CPAC**	95.20
Batch	MO	60	11	81.667	60	7	25	50	100	657	**CPAC**	98.00
Batch	MO	120	10.6	82.333	60	7	25	50	100	657	**CPAC**	98.80
Batch	MO	15	49.6	44.889	90	7	25	50	100	619	**PAC**	80.80
Batch	MO	30	41.5	53.889	90	7	25	50	100	619	**PAC**	97.00
Batch	MO	60	35.15	60.944	90	7	25	50	100	619	**PAC**	109.70
Batch	MO	120	35	61.111	90	7	25	50	100	619	**PAC**	110.00
Batch	MO	15	30.7	65.889	90	7	25	50	100	823	**TPAC**	118.60
Batch	MO	30	25.4	71.778	90	7	25	50	100	823	**TPAC**	129.20
Batch	MO	60	22	75.556	90	7	25	50	100	823	**TPAC**	136.00
Batch	MO	120	21	76.667	90	7	25	50	100	823	**TPAC**	138.00
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Batch	MO	120	37	58.889	90	11	25	50	100	619	**PAC**	106.00
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Batch	MO	30	26.5	70.556	90	11	25	50	100	823	**TPAC**	127.00
Batch	MO	60	25	72.222	90	11	25	50	100	823	**TPAC**	130.00
Batch	MO	120	24	73.333	90	11	25	50	100	823	**TPAC**	132.00
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Sonication	BSA	60	13	56.667	30	7	25	50	100	657	**CPAC**	34.00
Sonication	BSA	120	12	60.000	30	7	25	50	100	657	**CPAC**	36.00
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Sonication	BSA	120	24	60.000	60	7	25	50	100	619	**PAC**	72.00
Sonication	BSA	15	30	50.000	60	7	25	50	100	823	**TPAC**	60.00
Sonication	BSA	30	20	66.667	60	7	25	50	100	823	**TPAC**	80.00
Sonication	BSA	60	16	73.333	60	7	25	50	100	823	**TPAC**	88.00

Sonication	BSA	120	15	75.000	60	7	25	50	100	823	**TPAC**	90.00
Sonication	BSA	15	38	36.667	60	7	25	50	100	657	**CPAC**	44.00
Sonication	BSA	30	35	41.667	60	7	25	50	100	657	**CPAC**	50.00
Sonication	BSA	60	31	48.333	60	7	25	50	100	657	**CPAC**	58.00
Sonication	BSA	120	30	50.000	60	7	25	50	100	657	**CPAC**	60.00
Sonication	BSA	15	47	47.778	90	7	25	50	100	619	**PAC**	86.00
Sonication	BSA	30	46	48.889	90	7	25	50	100	619	**PAC**	88.00
Sonication	BSA	60	41	54.444	90	7	25	50	100	619	**PAC**	98.00
Sonication	BSA	120	40	55.556	90	7	25	50	100	619	**PAC**	100.00
Sonication	BSA	15	40	55.556	90	7	25	50	100	823	**TPAC**	100.00
Sonication	BSA	30	31	65.556	90	7	25	50	100	823	**TPAC**	118.00
Sonication	BSA	60	30	66.667	90	7	25	50	100	823	**TPAC**	120.00
Sonication	BSA	120	29.5	67.222	90	7	25	50	100	823	**TPAC**	121.00
Sonication	BSA	15	56	37.778	90	7	25	50	100	657	**CPAC**	68.00
Sonication	BSA	30	53	41.111	90	7	25	50	100	657	**CPAC**	74.00
Sonication	BSA	60	50	44.444	90	7	25	50	100	657	**CPAC**	80.00
Sonication	BSA	120	49	45.556	90	7	25	50	100	657	**CPAC**	82.00
Sonication	BSA	15	48	46.667	90	3	25	50	100	619	**PAC**	84.00
Sonication	BSA	30	47	47.778	90	3	25	50	100	619	**PAC**	86.00
Sonication	BSA	60	43	52.222	90	3	25	50	100	619	**PAC**	94.00
Sonication	BSA	120	41	54.444	90	3	25	50	100	619	**PAC**	98.00
Sonication	BSA	15	43	52.222	90	5	25	50	100	619	**PAC**	94.00
Sonication	BSA	30	41	54.444	90	5	25	50	100	619	**PAC**	98.00
Sonication	BSA	60	38	57.778	90	5	25	50	100	619	**PAC**	104.00
Sonication	BSA	120	36	60.000	90	5	25	50	100	619	**PAC**	108.00
Sonication	BSA	15	41	54.444	90	3	25	50	100	823	**TPAC**	98.00
Sonication	BSA	30	32.5	63.889	90	3	25	50	100	823	**TPAC**	115.00
Sonication	BSA	60	30	66.667	90	3	25	50	100	823	**TPAC**	120.00
Sonication	BSA	120	29.25	67.500	90	3	25	50	100	823	**TPAC**	121.50
Sonication	BSA	15	36	60.000	90	5	25	50	100	823	**TPAC**	108.00
Sonication	BSA	30	28	68.889	90	5	25	50	100	823	**TPAC**	124.00
Sonication	BSA	60	26	71.111	90	5	25	50	100	823	**TPAC**	128.00
Sonication	BSA	120	25	72.222	90	5	25	50	100	823	**TPAC**	130.00
Sonication	BSA	15	70	22.222	90	3	25	50	100	657	**CPAC**	40.00
Sonication	BSA	30	66	26.667	90	3	25	50	100	657	**CPAC**	48.00
Sonication	BSA	60	64.5	28.333	90	3	25	50	100	657	**CPAC**	51.00
Sonication	BSA	120	63	30.000	90	3	25	50	100	657	**CPAC**	54.00
Sonication	BSA	15	56	37.778	90	5	25	50	100	657	**CPAC**	68.00
Sonication	BSA	30	50	44.444	90	5	25	50	100	657	**CPAC**	80.00
Sonication	BSA	60	48	46.667	90	5	25	50	100	657	**CPAC**	84.00
Sonication	BSA	120	46	48.889	90	5	25	50	100	657	**CPAC**	88.00
Batch	SO4 -2	240	5.366	97.854	250	2	25	20	30	0.3255	**IECBs**	366.95
Batch	SO4 -2	240	29.9	94.020	500	2	25	20	30	0.3255	**IECBs**	705.15
Batch	SO4 -2	240	36.98	95.069	750	2	25	20	30	0.3255	**IECBs**	1069.53
Batch	SO4 -2	240	39.27	96.073	1000	2	25	20	30	0.3255	**IECBs**	1441.10
Batch	SO4 -2	240	5.494	97.802	250	2	25	30	30	0.3255	**IECBs**	244.51

Batch	SO4 -2	240	20.678	95.864	500	2	25	30	30	0.3255	**IECBs**	479.32
Batch	SO4 -2	240	36.56	95.125	750	2	25	30	30	0.3255	**IECBs**	713.44
Batch	SO4 -2	240	39.11	96.089	1000	2	25	30	30	0.3255	**IECBs**	960.89
Batch	SO4 -2	240	4.443	98.223	250	2	25	40	30	0.3255	**IECBs**	184.17
Batch	SO4 -2	240	21.27	95.746	500	2	25	40	30	0.3255	**IECBs**	359.05
Batch	SO4 -2	240	22.03	97.063	750	2	25	40	30	0.3255	**IECBs**	545.98
Batch	SO4 -2	240	26.33	97.367	1000	2	25	40	30	0.3255	**IECBs**	730.25
Batch	SO4 -2	240	3.705	98.518	250	2	25	50	30	0.3255	**IECBs**	147.78
Batch	SO4 -2	240	12.89	97.422	500	2	25	50	30	0.3255	**IECBs**	292.27
Batch	SO4 -2	240	24.48	96.736	750	2	25	50	30	0.3255	**IECBs**	435.31
Batch	SO4 -2	240	34.23	96.577	1000	2	25	50	30	0.3255	**IECBs**	579.46
Batch	SO4 -2	60	6.784	97.286	250	2	25	20	30	0.3255	**IECBs**	364.82
Batch	SO4 -2	120	5.921	97.632	250	2	25	20	30	0.3255	**IECBs**	366.12
Batch	SO4 -2	180	5.55	97.780	250	2	25	20	30	0.3255	**IECBs**	366.68
Batch	SO4 -2	240	5.366	97.854	250	2	25	20	30	0.3255	**IECBs**	366.95
Batch	SO4 -2	300	5.286	97.886	250	2	25	20	30	0.3255	**IECBs**	367.07
Batch	SO4 -2	360	5.276	97.890	250	2	25	20	30	0.3255	**IECBs**	367.09
Batch	SO4 -2	60	6.921	97.232	250	2	25	30	30	0.3255	**IECBs**	243.08
Batch	SO4 -2	120	6.105	97.558	250	2	25	30	30	0.3255	**IECBs**	243.90
Batch	SO4 -2	180	5.55	97.780	250	2	25	30	30	0.3255	**IECBs**	244.45
Batch	SO4 -2	240	5.024	97.990	250	2	25	30	30	0.3255	**IECBs**	244.98
Batch	SO4 -2	300	5.017	97.993	250	2	25	30	30	0.3255	**IECBs**	244.98
Batch	SO4 -2	360	4.968	98.013	250	2	25	30	30	0.3255	**IECBs**	245.03
Batch	SO4 -2	60	7.549	96.980	250	2	25	40	30	0.3255	**IECBs**	181.84
Batch	SO4 -2	120	6.676	97.330	250	2	25	40	30	0.3255	**IECBs**	182.49
Batch	SO4 -2	180	5.605	97.758	250	2	25	40	30	0.3255	**IECBs**	183.30
Batch	SO4 -2	240	4.443	98.223	250	2	25	40	30	0.3255	**IECBs**	184.17
Batch	SO4 -2	300	4.187	98.325	250	2	25	40	30	0.3255	**IECBs**	184.36
Batch	SO4 -2	360	4.145	98.342	250	2	25	40	30	0.3255	**IECBs**	184.39
Batch	SO4 -2	60	5.65	97.740	250	2	25	50	30	0.3255	**IECBs**	146.61
Batch	SO4 -2	120	4.25	98.300	250	2	25	50	30	0.3255	**IECBs**	147.45
Batch	SO4 -2	180	3.919	98.432	250	2	25	50	30	0.3255	**IECBs**	147.65
Batch	SO4 -2	240	3.305	98.678	250	2	25	50	30	0.3255	**IECBs**	148.02
Batch	SO4 -2	300	3.201	98.720	250	2	25	50	30	0.3255	**IECBs**	148.08
Batch	SO4 -2	360	3.209	98.716	250	2	25	50	30	0.3255	**IECBs**	148.07
Batch	SO4 -2	240	5.586	97.766	250	2	25	20	30	0.3255	**IECBs**	366.62
Batch	SO4 -2	240	4.968	98.013	250	2	25	30	30	0.3255	**IECBs**	245.03
Batch	SO4 -2	240	3.145	98.742	250	2	25	40	30	0.3255	**IECBs**	185.14
Batch	SO4 -2	240	2.119	99.152	250	2	25	50	30	0.3255	**IECBs**	148.73
Batch	SO4 -2	240	5.366	97.854	250	2	25	20	30	0.3255	**IECBs**	366.91
Batch	SO4 -2	240	6.862	97.255	250	4	25	20	30	0.3255	**IECBs**	364.71
Batch	SO4 -2	240	8.662	96.535	250	6	25	20	30	0.3255	**IECBs**	362.01
Batch	SO4 -2	240	11.343	95.463	250	8	25	20	30	0.3255	**IECBs**	357.99
Batch	SO4 -2	240	5.494	97.802	250	2	25	30	30	0.3255	**IECBs**	244.51
Batch	SO4 -2	240	6.37	97.452	250	4	25	30	30	0.3255	**IECBs**	243.63
Batch	SO4 -2	240	8.862	96.455	250	6	25	30	30	0.3255	**IECBs**	241.14

Batch	SO4 -2	240	11.847	95.261	250	8	25	30	30	0.3255	**IECBs**	238.15
Batch	SO4 -2	240	4.443	98.223	250	2	25	40	30	0.3255	**IECBs**	184.17
Batch	SO4 -2	240	6.056	97.578	250	4	25	40	30	0.3255	**IECBs**	182.96
Batch	SO4 -2	240	10.909	95.636	250	6	25	40	30	0.3255	**IECBs**	179.32
Batch	SO4 -2	240	14.221	94.312	250	8	25	40	30	0.3255	**IECBs**	176.83
Batch	SO4 -2	240	3.705	98.518	250	2	25	50	30	0.3255	**IECBs**	147.78
Batch	SO4 -2	240	4.96	98.016	250	4	25	50	30	0.3255	**IECBs**	147.02
Batch	SO4 -2	240	8.015	96.794	250	6	25	50	30	0.3255	**IECBs**	145.19
Batch	SO4 -2	240	12.11	95.156	250	8	25	50	30	0.3255	**IECBs**	142.73
Batch	NO3-	20	8.9	82.200	50	5	25	70	30	0.2304	**IECBs**	17.61
Batch	NO3-	40	8.23	83.540	50	5	25	70	30	0.2304	**IECBs**	17.90
Batch	NO3-	60	7.57	84.860	50	5	25	70	30	0.2304	**IECBs**	18.18
Batch	NO3-	80	6.24	87.520	50	5	25	70	30	0.2304	**IECBs**	18.75
Batch	NO3-	100	3.98	92.040	50	5	25	70	30	0.2304	**IECBs**	19.72
Batch	NO3-	120	2.99	94.020	50	5	25	70	30	0.2304	**IECBs**	20.15
Batch	NO3-	140	2.28	95.440	50	5	25	70	30	0.2304	**IECBs**	20.45
Batch	NO3-	160	2.09	95.820	50	5	25	70	30	0.2304	**IECBs**	20.53
Batch	NO3-	120	7.74	84.520	50	5	25	30	30	0.2304	**IECBs**	42.26
Batch	NO3-	120	5.42	89.160	50	5	25	50	30	0.2304	**IECBs**	26.75
Batch	NO3-	120	3.27	93.460	50	5	25	70	30	0.2304	**IECBs**	20.14
Batch	NO3-	120	7.58	84.840	50	5	25	90	30	0.2304	**IECBs**	14.14
Batch	NO3-	120	2.33	95.340	50	5	25	110	30	0.2304	**IECBs**	13.00
Batch	NO3-	120	28.13	43.740	50	3	25	70	30	0.2304	**IECBs**	9.37
Batch	NO3-	120	28.4	43.200	50	4	25	70	30	0.2304	**IECBs**	9.26
Batch	NO3-	120	3.98	92.040	50	5	25	70	30	0.2304	**IECBs**	19.72
Batch	NO3-	120	18.48	63.040	50	7	25	70	30	0.2304	**IECBs**	13.51
Batch	NO3-	120	17	66.000	50	9	25	70	30	0.2304	**IECBs**	10.51
Batch	NO3-	120	1.68	83.200	10	5	25	70	30	0.2304	**IECBs**	3.57
Batch	NO3-	120	2.39	88.050	20	5	25	70	30	0.2304	**IECBs**	7.55
Batch	NO3-	120	3.16	89.467	30	5	25	70	30	0.2304	**IECBs**	11.50
Batch	NO3-	120	4.12	89.700	40	5	25	70	30	0.2304	**IECBs**	15.38
Batch	NO3-	120	5.03	89.940	50	5	25	70	30	0.2304	**IECBs**	19.27
Batch	NO3-	120	15.03	74.950	60	5	25	70	30	0.2304	**IECBs**	19.27

Table S2. Tuned hyperparameters for optimization of utilized ML models.

ML Model	**Hyper Parameters**	**Set Value**
DT	Minimum Leaf Size	2
	Surrogate	Off
ELT	Minimum Leaf Size	20
	Numbers of Variables to Sample	8
	Method	Bag
	Numbers of Learning Cycles	278
	Learners	Template
GPR	Basic Function	None
	Kernel Function	Ardexponential
	Sigma	32.67
	Standardize	False
SVM	Kernel Function	Gaussian
	Kernel Scale	1.42×10^2
	Box Constraint	9.895×10^2
	Epsilon	11.66
	Standardize	True