

SUPPLEMENTARY MATERIAL TO
**Modeling the removal of Sunfix Red S3B from aqueous solution
by electrocoagulation process using artificial neural network**

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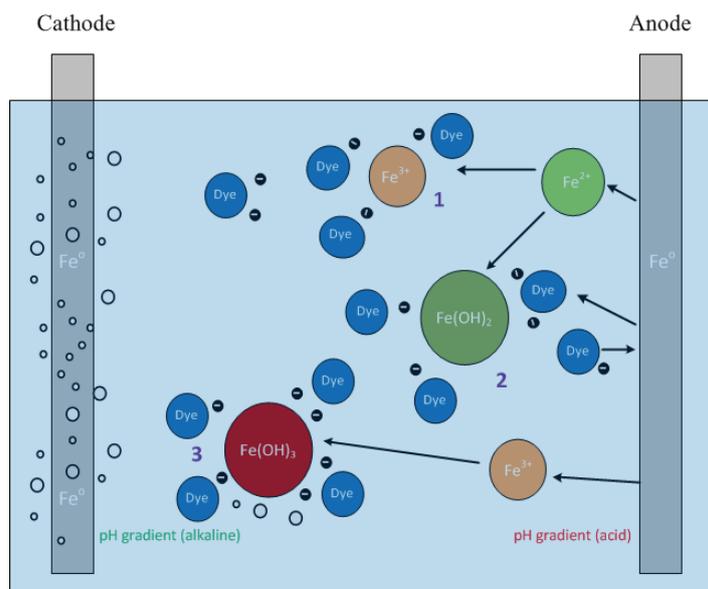


Fig. S-1. Schematics of dye removal mechanism of EC process with iron electrode; 1. precipitation; 2. adsorption; 3. flotation.⁷

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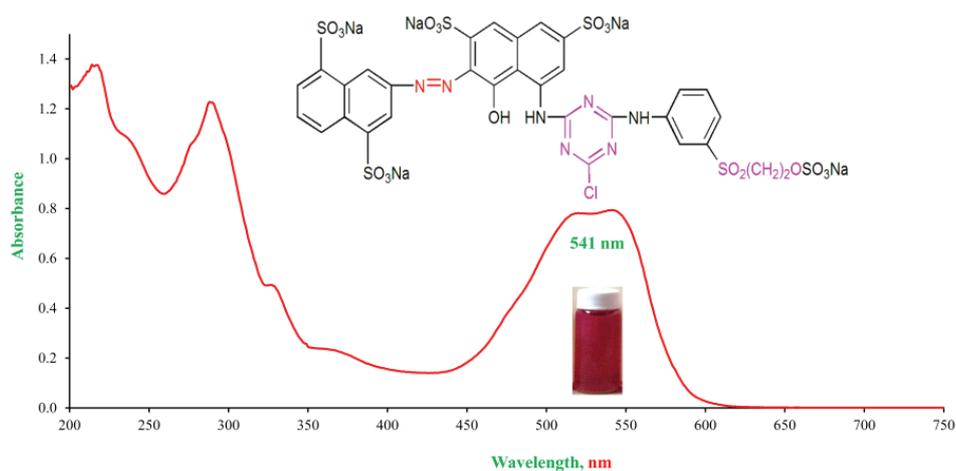


Fig. S-2. Chemical structure and UV-Visible spectral properties of Sunfix Red S3B.

TABLE S-I. Level of the variables applied to the fractional factorial design

Variable	High level (+)	Central level (0)	Low level (-)
Initial dye concentration, mg L ⁻¹	70	50	30
pH	11	7	3
Current density, A m ⁻²	108.3	86.6	65.0
Electrolysis time, min	7	5	3
Sulphate concentration, mg L ⁻¹	2000	1500	1000

TABLE S-II. Independent variables of the central composite design; initial dye concentration: 50 mg L⁻¹

Level of value	pH	Current density A m ⁻²	Electrolysis time min	Sulphate concentration mg L ⁻¹
-2	4	43.3	3	500
-1	6	65.0	4	1000
0	8	86.6	5	1500
1	10	108.3	6	2000
2	12	130.0	7	2500

TABLE S-III. Descriptive statistics of variables ($n = 86$) used in the construction of ANN

Variable	Minimum	Maximum	Mean	Standard deviation	Variance
Initial dye concentration, mg L ⁻¹	30	140	53.5	18.520	342.982
pH	3.13	12.04	8.6	2.624	6.887
Current density, A m ⁻²	43.3	130	81.1	18.245	332.873
Electrolysis time, min	2	8	4.7	1.252	1.568
Sulphate concentration, mg L ⁻¹	500	2500	1395.3	382.840	146566.347

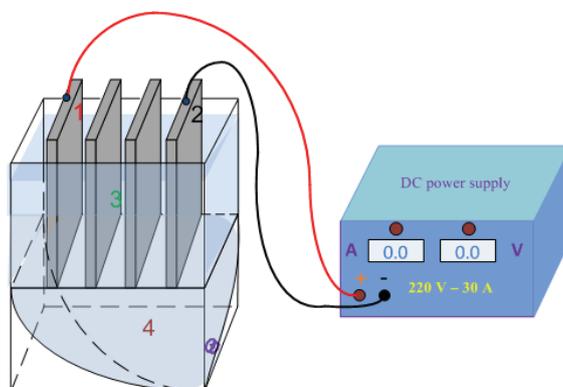


Fig. S-3. Bench scale of the electrocoagulator; 1. anode; 2. cathode; 3. electrocoagulation zone; 4. baffled settling zone.

TABLE S-IV. The effect of topology change on ANN's performance; total set includes training and validation sets

Number of neurons in hidden layer	Total set			Training set			Validation set			Test set		
	R^2	RMSE	MAPE	R^2	RMSE	MAPE	R^2	RMSE	MAPE	R^2	RMSE	MAPE
		%	%		%	%		%	%		%	%
1	0.670	13.977	20.090	0.713	13.025	19.046	0.465	17.078	24.005	0.564	16.312	19.035
2	0.676	13.843	19.864	0.735	12.550	17.804	0.450	17.879	27.590	0.648	14.655	17.318
3	0.695	13.431	19.023	0.752	11.979	17.068	0.504	17.853	26.354	0.586	15.889	19.964
4	0.775	11.532	15.686	0.821	10.304	14.085	0.601	15.285	21.688	0.836	9.998	15.340
5	0.816	10.427	14.970	0.831	10.216	14.718	0.750	11.184	15.914	0.815	10.630	15.071
6	0.829	10.072	13.599	0.845	9.429	12.878	0.764	12.186	16.304	0.903	7.680	14.573
7	0.836	9.844	13.776	0.838	9.940	14.037	0.827	9.478	12.795	0.879	8.602	18.439
8	0.825	10.166	14.797	0.842	9.340	12.394	0.778	12.797	23.805	0.846	9.679	17.307
9	0.825	10.186	13.675	0.852	9.451	13.046	0.706	12.564	16.036	0.772	11.786	33.068
10	0.822	10.262	14.414	0.861	9.095	12.506	0.667	13.782	21.567	0.687	13.820	20.985
11	0.846	9.542	14.256	0.891	8.131	12.495	0.653	13.587	20.859	0.702	13.472	24.473
12	0.837	9.813	12.931	0.890	7.987	11.135	0.659	14.771	19.668	0.804	10.945	167.790
13	0.848	9.483	12.292	0.904	7.661	10.543	0.592	14.392	18.850	0.162	22.606	97.741
14	0.850	9.429	12.559	0.909	7.411	9.800	0.587	14.709	22.907	0.555	16.475	27.604
15	0.828	10.099	14.785	0.905	7.442	9.573	0.555	16.635	34.330	0.712	13.255	18.268
16	0.827	10.125	12.635	0.902	7.680	9.788	0.517	16.303	23.312	0.498	17.491	21.808
17	0.844	9.608	11.265	0.941	5.822	7.364	0.527	17.645	25.896	0.380	19.438	25.275

TABLE S-V. Optimal network weights and biases for the ANN model of dye removal process using EC; HLN – Number of hidden layer neurons

HLN	Inputs to hidden					Hidden to outputs		
	I_1	I_2	I_3	I_4	I_5	O_1	O_2	Bias
	Dye con.	pH	Current density	Electrolysis time	Sulphate con.	Bias	Color removal	COD removal
H_1	0.050	0.715	-0.533	0.086	-0.301	0.597	0.903	-0.289
H_2	-0.666	0.219	-1.123	-0.440	-1.260	-0.403	-0.066	1.413

TABLE S-V. Continued

HLN	Inputs to hidden					Hidden to outputs				
	I_1	I_2	I_3	I_4	I_5	Bias	O_1	O_2	Bias	
	Dye con.	pH	Current density	Electrolysis time	Sulphate con.		Color removal	COD removal		
H_3	-0.529	1.498	-0.406	0.699	-1.371	-0.401	-0.652	-1.438	0.175	-0.432
H_4	0.261	0.141	-0.618	0.104	-0.798	-0.350	0.789	0.753		
H_5	0.793	1.282	-0.167	0.417	0.894	0.767	-0.263	1.499		
H_6	-0.359	0.677	1.872	1.581	0.065	0.196	1.519	0.251		
H_7	0.220	0.223	-0.872	-0.673	0.242	-0.166	0.514	-1.075		

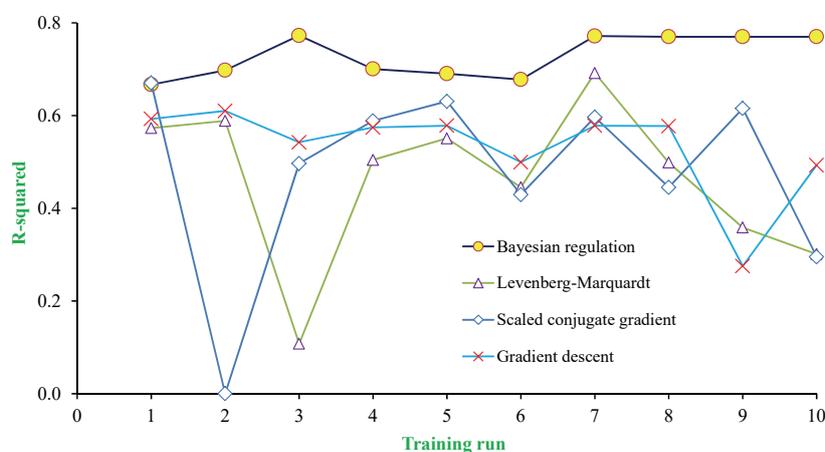


Fig. S-4. Comparison of determination coefficients (R^2) between four training algorithms with seven neurons in hidden layer.