Adsorption potential of polymer metal oxide composites for crystal violet and basic fuchsin: Isotherm, kinetics, and thermodynamic studies

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Supplementary file

Figures

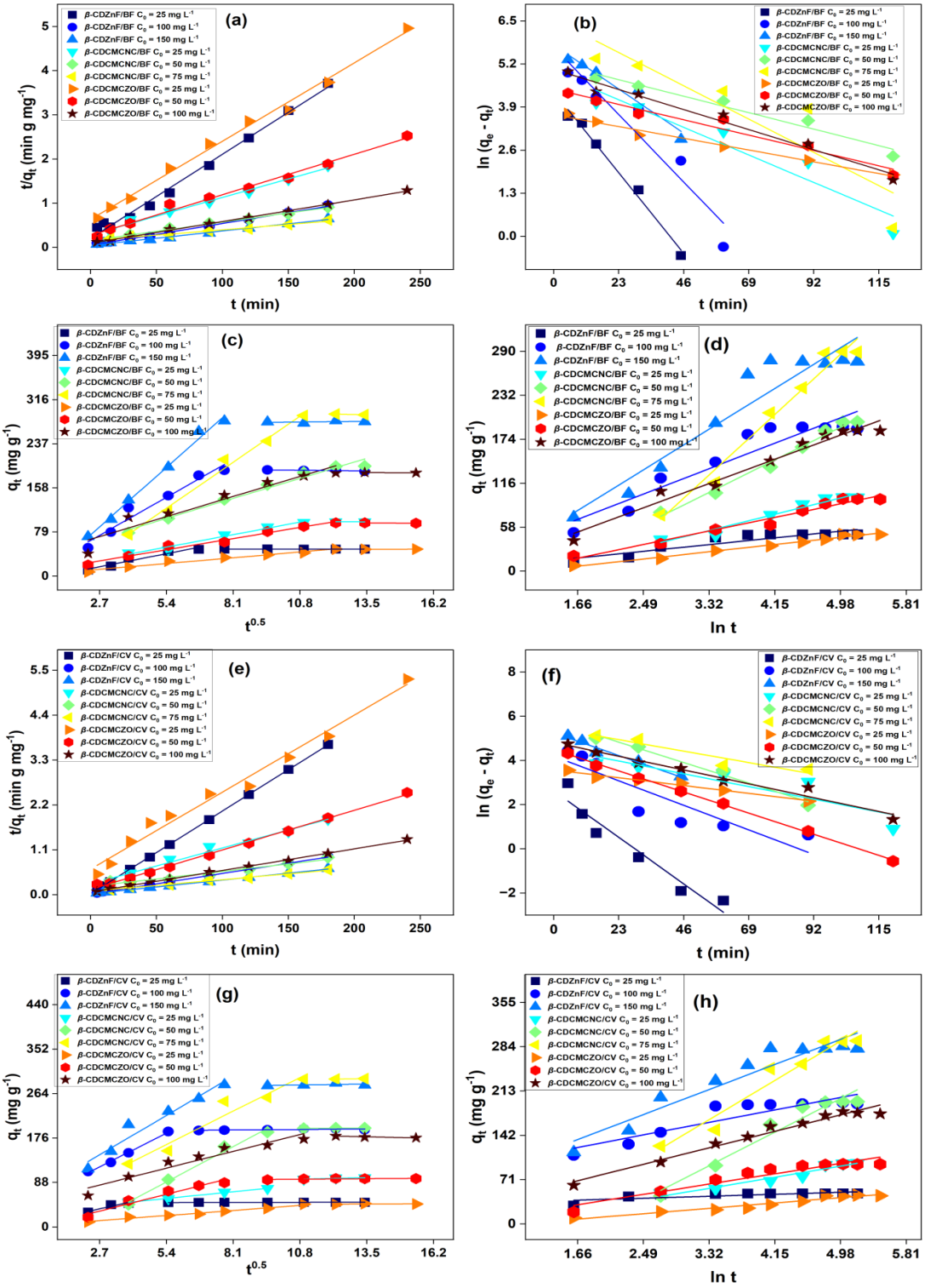

Fig S1. Linear fitting plots for the adsorption of BF and CV (a-h)

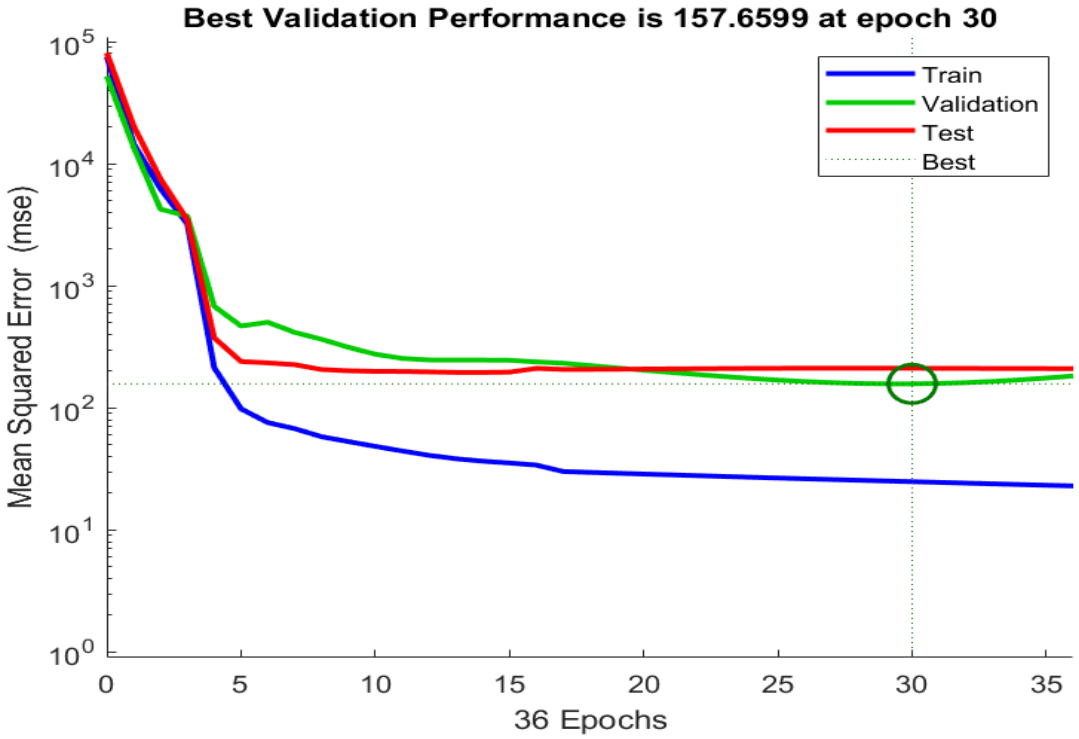

Fig S2. Performance plot of the ANNs trained for the adsorption of BF using LM algorithm

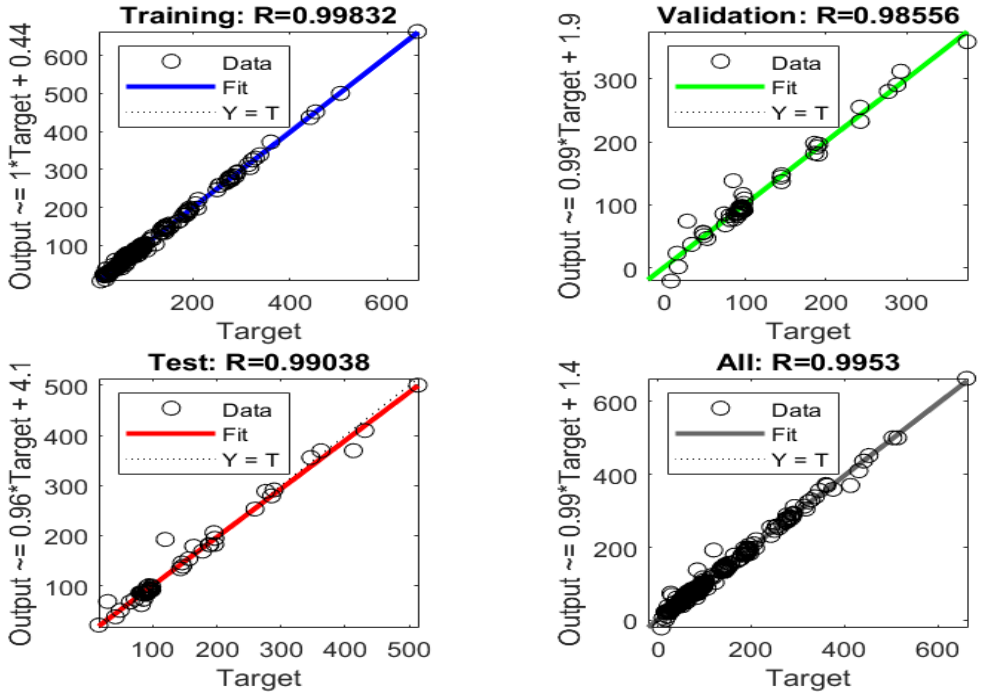

Fig S3. Regression plot of the ANNs trained for the adsorption of BF using LM algorithm

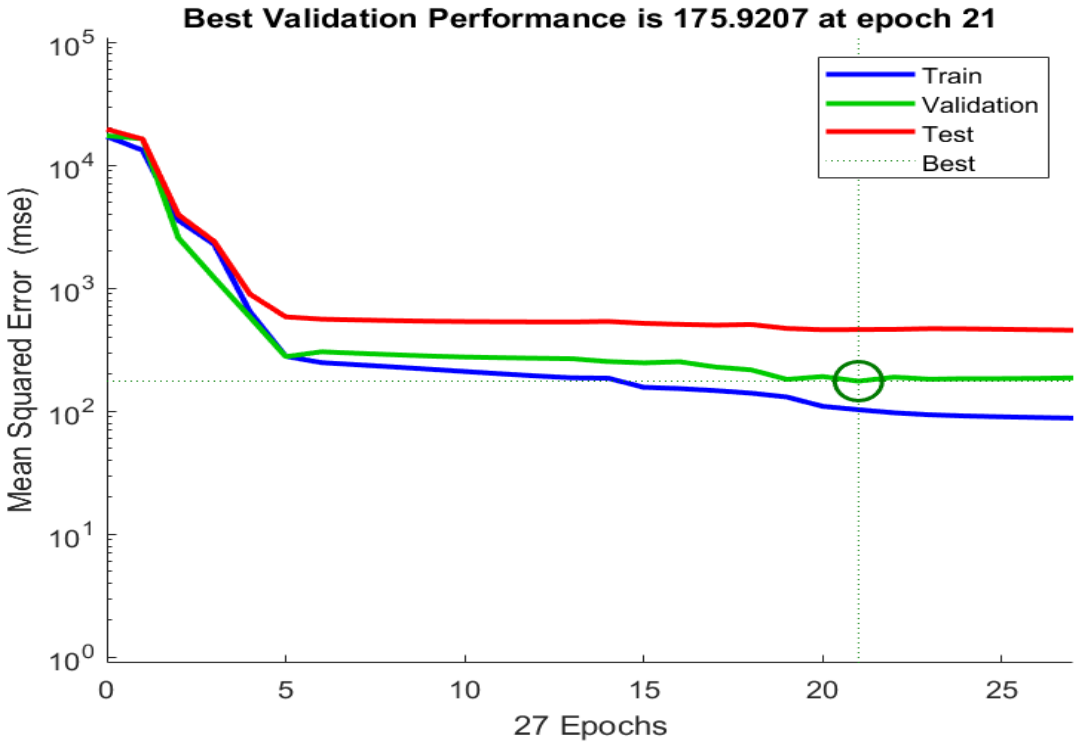

Fig S4. Performance plot of the ANNs trained for the adsorption of CV using LM algorithm

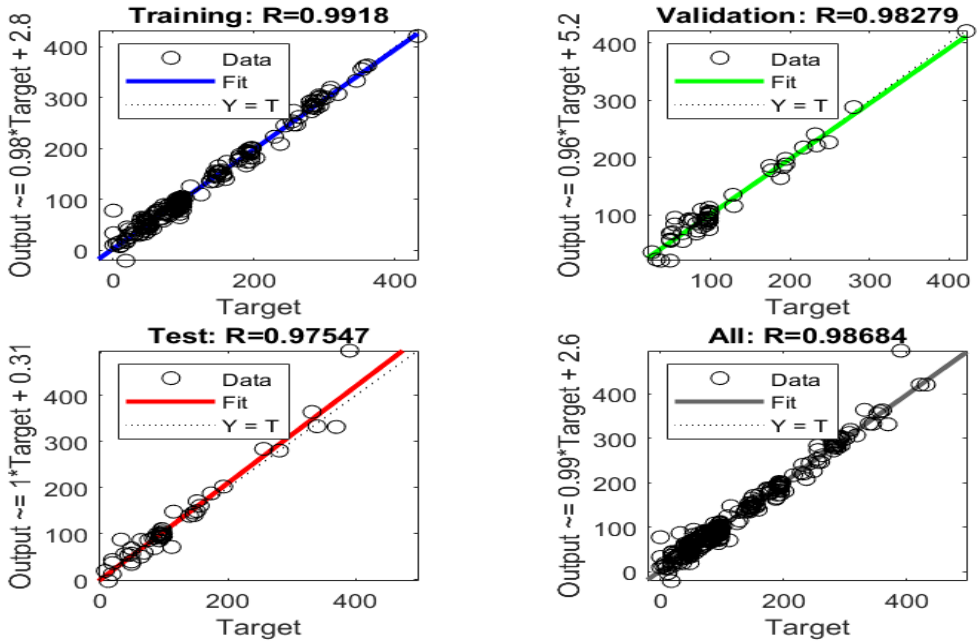

Fig S5. Regerssion plot of the ANNs trained for the adsorption of CV using LM algorithm

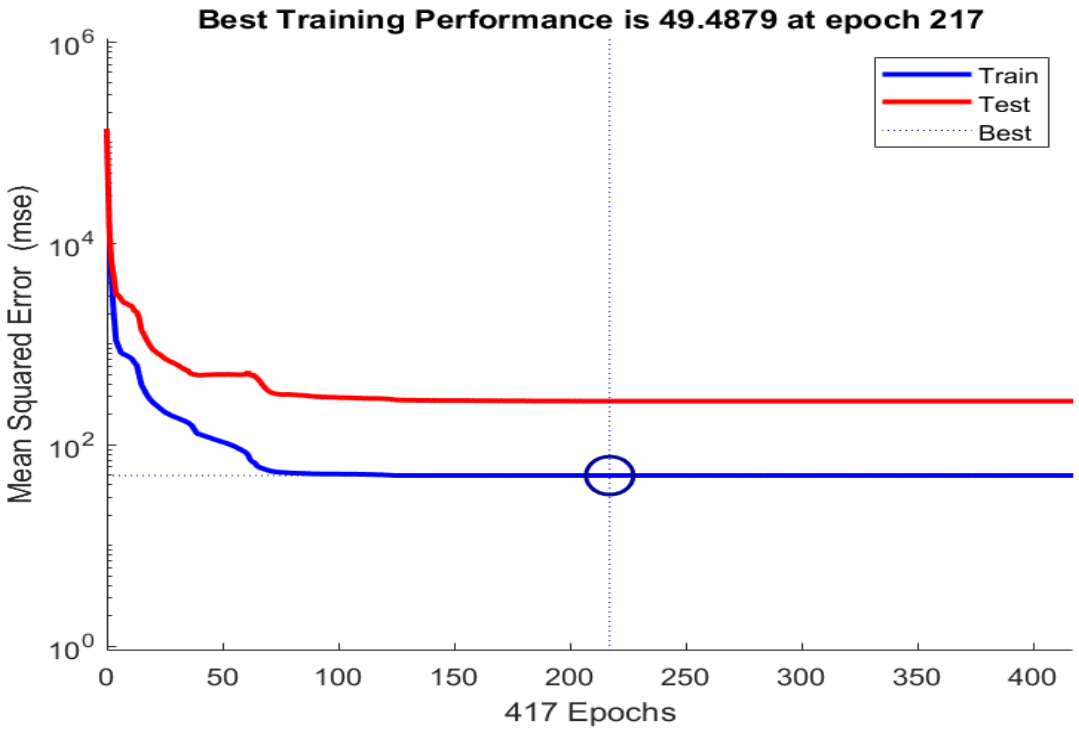

Fig S6. Performance plot of the ANNs trained for the adsorption of BF using BF algorithm

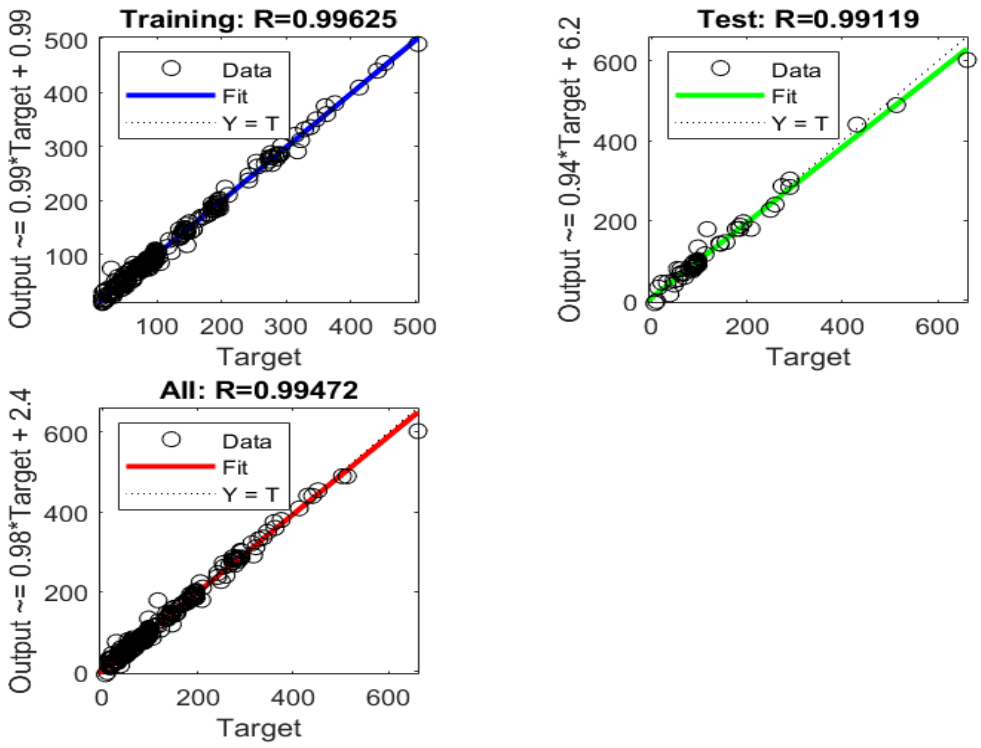

Fig S7. Regerssion plot of the ANNs trained for the adsorption of BF using BR algorithm

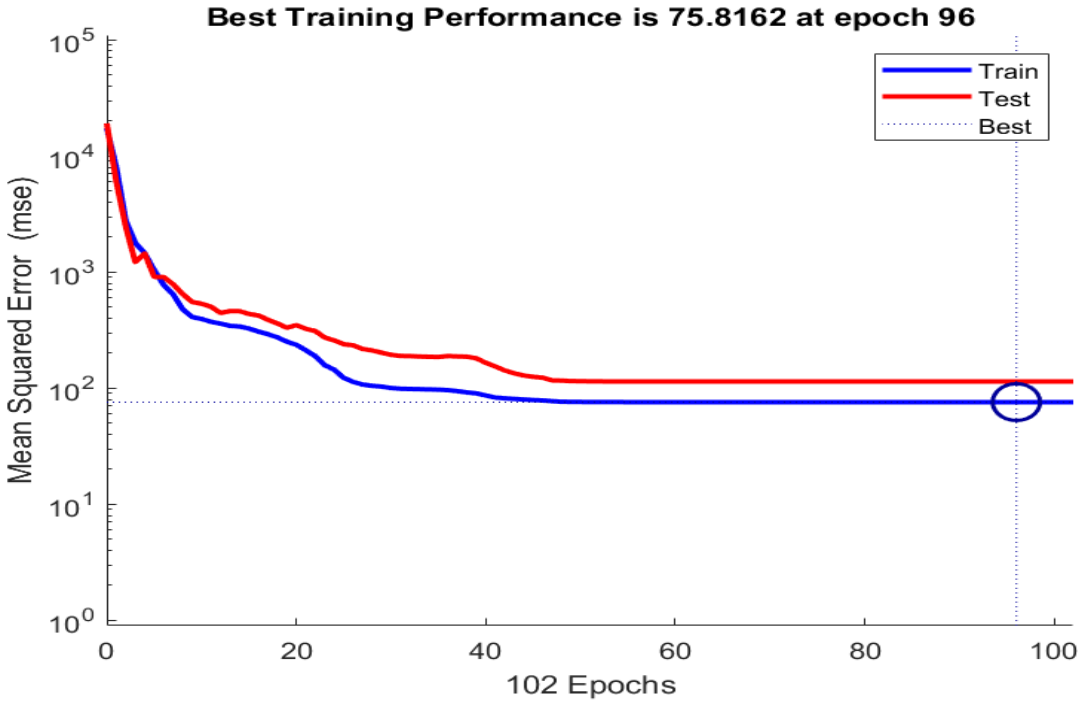

Fig S8. Performance plot of the ANNs trained for the adsorption of CV using BR algorithm

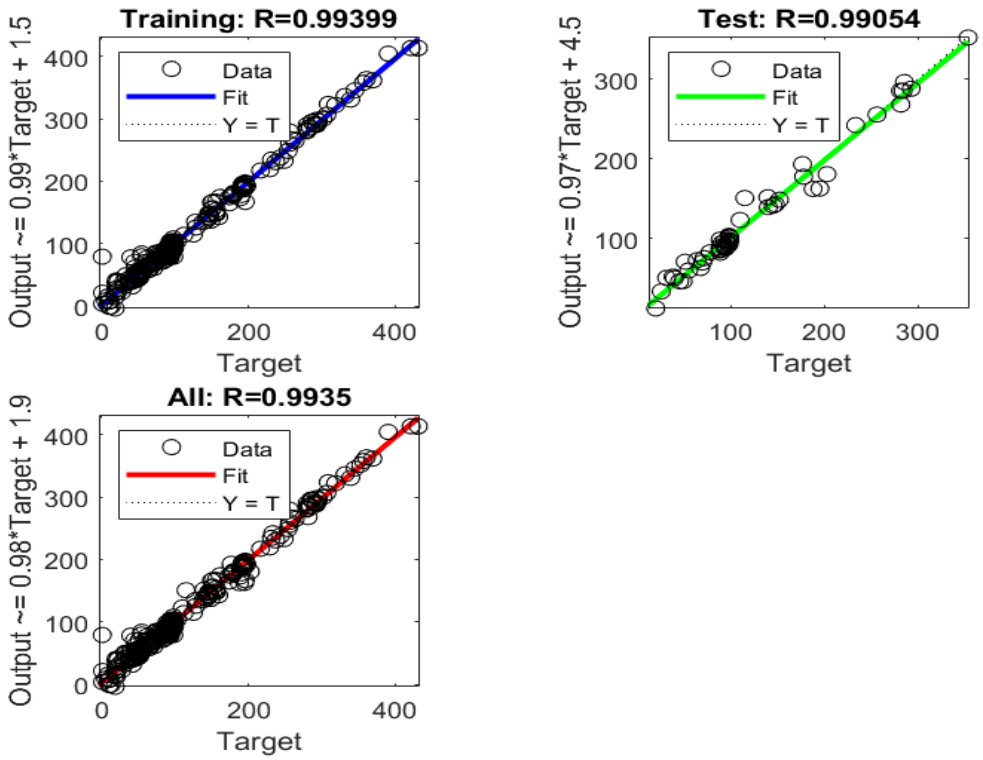

Fig S9. Regression plot of the ANNs trained for the adsorption of CV using BR algorithm

Tables

Table S1: Adsorption kinetics fitting data for the adsorption of BF onto *β*-CDZnF

Model	Type	Parameter	BF concentration (mg L^{-1})		
			25	**100**	**150**
PFO	Non linear	$q_{e,1}$ (mg g^{-1})	49.3±1.1	190±3	280±5
		k_1 (min^{-1})	(6.16±0.56)E-02	(5.88±0.4)E-02	(4.66±0.32)E-02
		R^2	0.975	0.984	0.986
	Linear	$q_{e,1}$ (mg g^{-1})	78.1±11.8	302±107	322±62
		k_1 (min^{-1})	(2.44±0.15)E-01	0.204±0.030	0.133±0.019
		R^2	0.889	0.921	0.941
PSO	Non linear	$q_{e,2}$ (mg g^{-1})	55.6±2.9	214±8	323±14
		k_2 (g mg^{-1} min^{-1})	(1.39±0.39)E-03	(3.53±0.65)E-04	(1.76±0.36)E-04
		R^2	0.919	0.960	0.959
	Linear	$q_{e,2}$ (mg g^{-1})	52.5±1.62	204±5	307±8
		k_2 (g mg^{-1} min^{-1})	(1.77±0.38)E-03	(4.56±0.77)E-04	(2.22±0.33)E-04
		R^2	0.992	0.996	0.994
Elovich	Non linear	α (mg g^{-1} min^{-1})	9.99±6.52	38.6±19.1	35.8±15.0
		β (g mg^{-1})	(9.36±1.98)E-02	(2.44±0.39)E-02	(1.48±0.24)E-02
		R^2	0.813	0.882	0.900
	Linear	α (mg g^{-1} min^{-1})	10.4±4.86	41.7±15.9	42.5±14.9
		β (g mg^{-1})	(9.38±1.30)E-02	(2.48±0.27)E-02	(1.55±0.15)E-02
		R^2	0.828	0.892	0.911
IPD	Non linear	k_i (mg g^{-1} $min^{-0.5}$)	2.90±0.78	11.3±2.5	18.5±3.58
		C (mg g^{-1})	17.8±6.5	67.4±20.8	75.8±30
		R^2	0.634	0.723	0.769
	Linear-point 1	$k_{i,1}$ (mg g^{-1} $min^{-0.5}$)	8.67±1.29	25.2±2.8	39.4±1.77
		C (mg g^{-1})	-6.5±5.93	5.20±14.6	-18.0±9.26
		R^2	0.937	0.956	0.992
	Linear Point 2	$k_{i,2}$ (mg g^{-1} $min^{-0.5}$)	(-2.93±0.92)E-02	-0.472±0.418	0.417±0.757
		C (mg g^{-1})	48.8±0.10	195±4.86	272±9
		R^2	0.773	0.389	0.132

Table S2. Adsorption kinetics fitting data for the adsorption of BF onto *β*-CDCMCNC

Model	Type	Parameter	BF concentration (mg L^{-1})		
			25	**50**	**75**
PFO	Non linear	$q_{e,1}$ (mg g^{-1})	98.8±3.9	196±8	312±10
		k_1 (min^{-1})	(2.54±0.35)E-02	(2.41±0.34)E-02	(1.76±0.16)E-02
		R^2	0.955	0.953	0.990
	Linear	$q_{e,1}$ (mg g^{-1})	141±51	186±31	702±410
		k_1 (min^{-1})	(8.32±1.41)E-02	(4.97±0.56)E-02	(1.01±0.27)E-01
		R^2	0.920	0.963	0.818
PSO	Non linear	$q_{e,2}$ (mg g^{-1})	120±7	240±10	416±30
		k_2 (g mg^{-1} min^{-1})	(2.29±0.55)E-04	(1.08±0.19)E-04	(3.69±0.94)E-05
		R^2	0.964	0.981	0.981
	Linear	$q_{e,2}$ (mg g^{-1})	119±5	241±8	415±26
		k_2 (g mg^{-1} min^{-1})	(2.44±0.31)E-04	(1.08±0.10)E-04	(3.63±0.35)E-05
		R^2	0.989	0.994	0.979
Elovich	Non linear	α (mg g^{-1} min^{-1})	5.49±1.49	9.93±1.24	7.89±1.78
		β (g mg^{-1})	(3.46±0.45)E-02	(1.70±0.11)E-02	(8.11±1.35)E-03
		R^2	0.960	0.991	0.967
	Linear	α (mg g^{-1} min^{-1})	7.45±2.49	13.9±2.75	13.0±3.42
		β (g mg^{-1})	(3.87±0.33)E-02	(1.93±0.09)E-02	(1.04±0.07)E-02
		R^2	0.958	0.987	0.988
IPD	Non linear	k_i (mg g^{-1} $min^{-0.5}$)	6.56±0.82	13.3±0.93	23.9±1.0
		C (mg g^{-1})	18.3±7.9	31.8±8.9	1E-14
		R^2	0.927	0.976	0.936
	Linear-point 1	$k_{i,1}$ (mg g^{-1} $min^{-0.5}$)	8.31±0.70	13.3±0.93	30.6±1.8
		C (mg g^{-1})	7.17±5.57	31.8±8.9	-43.4±14.4
		R^2	0.979	0.976	0.990
	Linear Point 2	$k_{i,2}$ (mg g^{-1} $min^{-0.5}$)	-0.110	13.3±0.93	-1.04
		C (mg g^{-1})	98.8	31.8±8.92	303
		R^2	~1	0.976	~1

Table S3. Adsorption kinetics fitting data for the adsorption of BF onto *β*-CDCMCZO

Model	Type	Parameter	BF concentration (mg L^{-1})		
			25	**50**	**100**
PFO	Non linear	$q_{e,1}$ (mg g^{-1})	47.3±1.7	94.0±4.0	179±6
		k_1 (min^{-1})	(2.40±0.31)E-02	(2.51±0.40)E-02	(4.03±0.64)E-02
		R^2	0.969	0.947	0.936
	Linear	$q_{e,1}$ (mg g^{-1})	39.2±2.6	85.2±11	154±20
		k_1 (min^{-1})	(3.55±0.23)E-02	(4.64±0.46)E-02	(6.06±0.48)E-02
		R^2	0.983	0.963	0.976
PSO	Non linear	$q_{e,2}$ (mg g^{-1})	56.6±1.9	111±5	203±6
		k_2 (g mg^{-1} min^{-1})	(4.83±0.74)E-04	(2.74±0.60)E-04	(2.62±0.46)E-04
		R^2	0.988	0.971	0.974
	Linear	$q_{e,2}$ (mg g^{-1})	56.4±1.54	109±4	203±4
		k_2 (g mg^{-1} min^{-1})	(5.00±0.41)E-04	(3.00±0.41)E-04	(2.60±0.28)E-04
		R^2	0.994	0.990	0.998
Elovich	Non linear	α (mg g^{-1} min^{-1})	2.48±0.43	5.95±1.33	23.6±7.2
		β (g mg^{-1})	(7.42±0.59)E-02	(4.00±0.38)E-02	(2.48±0.25)E-02
		R^2	0.985	0.975	0.961
	Linear	α (mg g^{-1} min^{-1})	3.91±0.69	9.15±2.26	28.1±7.0
		β (g mg^{-1})	(8.75±0.38)E-02	(4.63±0.29)E-02	(2.60±0.16)E-02
		R^2	0.986	0.970	0.969
IPD	Non linear	k_i (mg g^{-1} $min^{-0.5}$)	3.16±0.33	6.01±0.65	10.3±1.6
		C (mg g^{-1})	5.98±3.26	15.7±6.42	52.5±15.9
		R^2	0.930	0.925	0.856
	Linear-point 1	$k_{i,1}$ (mg g^{-1} $min^{-0.5}$)	3.83±0.29	7.40±0.46	13.3±1.7
		C (mg g^{-1})	2.05±2.37	7.40±3.81	34.8±14.2
		R^2	0.972	0.977	0.922
	Linear Point 2	$k_{i,2}$ (mg g^{-1} $min^{-0.5}$)	0.104	-0.318	-0.216
		C (mg g^{-1})	46.8	99.8	189
		R^2	~1	~1	~1

Table S4. Adsorption kinetics fitting data for the adsorption of CV onto *β*-CDZnF

Model	Type	Parameter	CV concentration ($mg\ L^{-1}$)		
			25	**100**	**150**
PFO	Non linear	$q_{e,1}$ ($mg\ g^{-1}$)	48.3 ±0.35	192±4	276±6
		k_1 (min^{-1})	(17.3±0.69)E-02	0.124±0.012	(8.26±0.77)E-02
		R^2	0.983	0.918	0.956
	Linear	$q_{e,1}$ ($mg\ g^{-1}$)	13.8±4.7	66.6±25.5	190±20
		k_1 (min^{-1})	(2.11±0.29)E-01	0.112±0.024	(1.02±0.10)E-01
		R^2	0.931	0.811	0.970
PSO	Non linear	$q_{e,2}$ ($mg\ g^{-1}$)	50.7±0.56	204±4	303±6
		k_2 ($g\ mg^{-1}\ min^{-1}$)	(6.26±0.60)E-03	(1.02±0.14)E-03	(3.84±0.41)E-04
		R^2	0.970	0.950	0.980
	Linear	$q_{e,2}$ ($mg\ g^{-1}$)	49.3±0.23	198±1.77	297±4
		k_2 ($g\ mg^{-1}\ min^{-1}$)	(1.58±0.40)E-02	(1.49±0.29)E-03	(4.58±0.59)E-04
		R^2	0.999	0.999	0.999
Elovich	Non linear	α ($mg\ g^{-1}\ min^{-1}$)	1926±3302	745±752	146±72
		β ($g\ mg^{-1}$)	(2.17±0.42)E-01	(4.15±0.67)E-02	(2.06±0.25)E-02
		R^2	0.771	0.833	0.912
	Linear	α ($mg\ g^{-1}\ min^{-1}$)	16137±11132	744±343	151±52
		β ($g\ mg^{-1}$)	(2.62±0.60)E-01	(4.15±0.57)E-02	(2.07±0.20)E-02
		R^2	0.583	0.813	0.915
IPD	Non linear	k_i ($mg\ g^{-1}\ min^{-0.5}$)	1.23±0.38	6.60±1.73	13.6±2.8
		C ($mg\ g^{-1}$)	35.9±3.2	123±14	133±23
		R^2	0.564	0.646	0.756
	Linear-point 1	$k_{i,1}$ ($mg\ g^{-1}\ min^{-0.5}$)	10.9±3.3	24.7±1.2	28.9±3.36
		C ($mg\ g^{-1}$)	6.44±10.5	52.7±4.48	64.9±17.6
		R^2	0.914	0.996	0.948
	Linear Point 2	$k_{i,2}$ ($mg\ g^{-1}\ min^{-0.5}$)	(6.28±2.54)E-02	0.373±0.195	0.620±0.839
		C ($mg\ g^{-1}$)	48.1±0.25	189±2	274±10
		R^2	0.550	0.477	0.214

Table S5. Adsorption kinetics fitting data for the adsorption of CV onto *β*-CDCMCNC

Model	Type	Parameter	CV concentration (mg L^{-1})		
			25	**50**	**75**
PFO	Non linear	$q_{e,1}$ (mg g^{-1})	92.8±5.9	207±7	294±10
		k_1 (min^{-1})	(3.13±0.77)E-02	(2.18±0.25)E-02	(2.85±0.36)E-02
		R^2	0.798	0.980	0.959
	Linear	$q_{e,1}$ (mg g^{-1})	94.4±38.8	318±63	236±58
		k_1 (min^{-1})	(5.76±1.66)E-02	(9.30±0.90)E-02	(5.21±1.15)E-02
		R^2	0.801	0.982	0.912
PSO	Non linear	$q_{e,2}$ (mg g^{-1})	109±8	268±25	355±18
		k_2 (g mg^{-1} min^{-1})	(3.57±1.23)E-04	(7.52±2.67)E-05	(8.89±2.08)E-05
		R^2	0.894	0.954	0.963
	Linear	$q_{e,2}$ (mg g^{-1})	114±7	272±25	350±14
		k_2 (g mg^{-1} min^{-1})	(2.88±0.52)E-04	(6.53±1.05)E-05	(9.46±1.25)E-05
		R^2	0.981	0.953	0.991
Elovich	Non linear	α (mg g^{-1} min^{-1})	8.89±3.05	6.97±2.62	19.5±6.3
		β (g mg^{-1})	(4.35±0.57)E-02	(1.34±0.32)E-02	(1.22±0.18)E-02
		R^2	0.946	0.922	0.947
	Linear	α (mg g^{-1} min^{-1})	11.2±4.3	9.90±3.59	24.9±8.9
		β (g mg^{-1})	(4.67±0.47)E-02	(1.54±0.14)E-02	(1.32±0.12)E-02
		R^2	0.941	0.949	0.950
IPD	Non linear	k_i (mg g^{-1} $min^{-0.5}$)	5.60±0.46	15.9±2.9	19.0±2.88
		C (mg g^{-1})	26.4±4.44	9.56±27.7	65.6±27.7
		R^2	0.967	0.859	0.897
	Linear-point 1	$k_{i,1}$ (mg g^{-1} $min^{-0.5}$)	4.93±0.18	25.9±2.18	24.6±3.32
		C (mg g^{-1})	29.7±1.23	-50.9±15.2	30.3±26.4
		R^2	0.997	0.986	0.948
	Linear Point 2	$k_{i,2}$ (mg g^{-1} $min^{-0.5}$)	1.24±0.42	0.361±0.178	0.862
		C (mg g^{-1})	81.2±5.1	191±2	282
		R^2	0.899	0.804	~1

Table S6. Adsorption kinetics fitting data for the adsorption of CV onto *β*-CDCMCZO

Model	Type	Parameter	CV concentration (mg L^{-1})		
			25	**50**	**100**
PFO	Non linear	$q_{e,1}$ (mg g^{-1})	45.8±2.3	95.0±0.8	171±5
		k_1 (min^{-1})	(2.21±0.36)E-02	(4.75±0.18)E-02	(5.23±0.74)E-02
		R^2	0.926	0.996	0.919
	Linear	$q_{e,1}$ (mg g^{-1})	35.7±2.0	88.3±3.83	124±17
		k_1 (min^{-1})	(3.55±0.26)E-02	(9.56±0.16)E-02	(6.27±0.51)E-02
		R^2	0.978	0.999	0.968
PSO	Non linear	$q_{e,2}$ (mg g^{-1})	54.4±3.40	106±2	189±4
		k_2 (g mg^{-1} min^{-1})	(4.83±1.28)E-04	(6.02±0.76)E-04	(4.10±0.45)E-04
		R^2	0.948	0.984	0.983
	Linear	$q_{e,2}$ (mg g^{-1})	53.0±2.30	103±2	189±2
		k_2 (g mg^{-1} min^{-1})	(5.65±0.78)E-04	(7.03±0.95)E-04	(4.19±0.47)E-04
		R^2	0.984	0.997	0.998
Elovich	Non linear	α (mg g^{-1} min^{-1})	2.61±0.65	17.0±8.1	49.4±14.2
		β (g mg^{-1})	(8.12±0.91)E-02	(4.98±0.73)E-02	(3.10±0.24)E-02
		R^2	0.960	0.902	0.966
	Linear	α (mg g^{-1} min^{-1})	4.24±1.25	17.8±6.47	53.6±12.5
		β (g mg^{-1})	(9.69±0.74)E-02	(5.01±0.48)E-02	(3.15±0.19)E-02
		R^2	0.948	0.916	0.969
IPD	Non linear	k_i (mg g^{-1} $min^{-0.5}$)	2.88±0.28	4.96±1.11	8.27±1.34
		C (mg g^{-1})	7.49±2.75	35.3±10.7	73.1±12.9
		R^2	0.927	0.713	0.827
	Linear-point 1	$k_{i,1}$ (mg g^{-1} $min^{-0.5}$)	3.71±0.25	12.3±1.6	12.3±1.56
		C (mg g^{-1})	2.60±1.83	-1.63±8.87	49.7±11.2
		R^2	0.977	0.952	0.926
	Linear Point 2	$k_{i,2}$ (mg g^{-1} $min^{-0.5}$)	0.171±0.520	0.381±0.171	-1.07±0.40
		C (mg g^{-1})	43.1±7.2	90.4±2.1	193±5
		R^2	0.0973	0.622	0.880

Equations:

$q_t = q_{e1}[1 - e^{-k_1 t}]$ PFO non-linear……....(S1)

$q_t = \frac{q_{e2}^2 k_2 t}{k_2 q_{e2} t+1}$ PSO non-linear……(S2)

$q_t = \frac{1}{\beta}\ln(1 + \alpha\beta t)$ Elovich non-linear.....(S3)

$\log(q_e - q_t) = \log q_{e,1} - \frac{k_1 t}{2.303}$ PFO linear……....(S4)

$\frac{t}{q_t} = \frac{1}{K_2\, q_{e,2}^2} + \frac{t}{q_{e,2}}$ PSO linear……(S5)

$q_t = \frac{1}{\beta}\ln(\alpha.\beta) + \frac{1}{\beta}\ln t$ Elovich linear.....(S6)

$q_t = k_p\sqrt{t} + C$ IPD linear.....(S7)

Where k_1 is PFO constant (min^{-1}); C is associated with boundary layer thickness (mg g^{-1}); k_2 (g mg^{-1} min^{-1}) is PSO constant; $q_{e,1}$ (mg g^{-1}) is q_e obtained using PFO; k_p (mg g^{-1} $min^{-0.5}$) is constant corresponding to the IPD; β & α are constants associated with Elovich constants; β is related to the activation energy and surface coverage during chemisorptions (g mg^{-1}); α is the initial adsorption rate (mg g^{-1} min^{-1}); $q_{e,2}$ (mg g^{-1}) is q_e obtained using PSO.

$q_e = \frac{q_m K_L C_e}{1+K_L Ce}$ Langmuir..... (S8)

$q_e = K_F C_e^{\,1/n_F}$ Freundlich.....(S9)

$q_e = B\ ln\ (A_T C_e)$ Temkin..... (S10)

$q_e = \frac{q_m K_g {C_e}^{n_L}}{1+K_L {C_e}^{n_L}}$ Liu.....(S11)

Eq. S8 to S9 are non-linear forms. Where K_F (mg g^{-1} (mg $L^{-1})^{-1/n}$) and n_F are Freundlich constant/exponent, q_m (mg g^{-1}) stands for maximum adsorption capacity, R is the Universal gas constant (8.314 J mol^{-1} K^{-1}) K_L (L mg^{-1}) and K_g (L mg^{-1}) are Langmuir and Liu constants, respectively, n_L is Liu constant/exponent, B is Temkin constant (RT/b_T), A_T (L g^{-1})is equilibrium binding constant belonging to Temkin model.

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