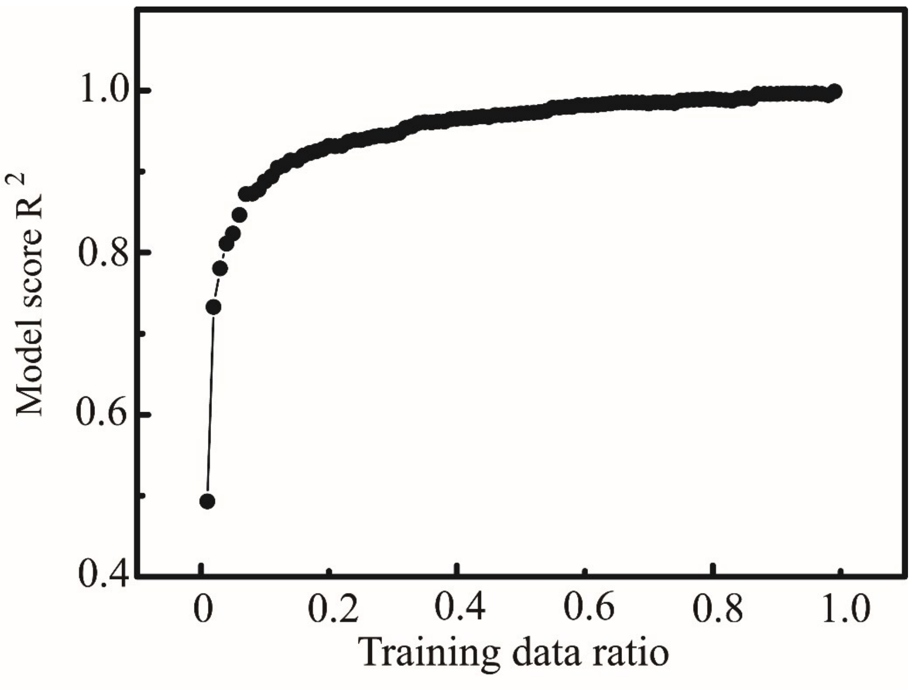
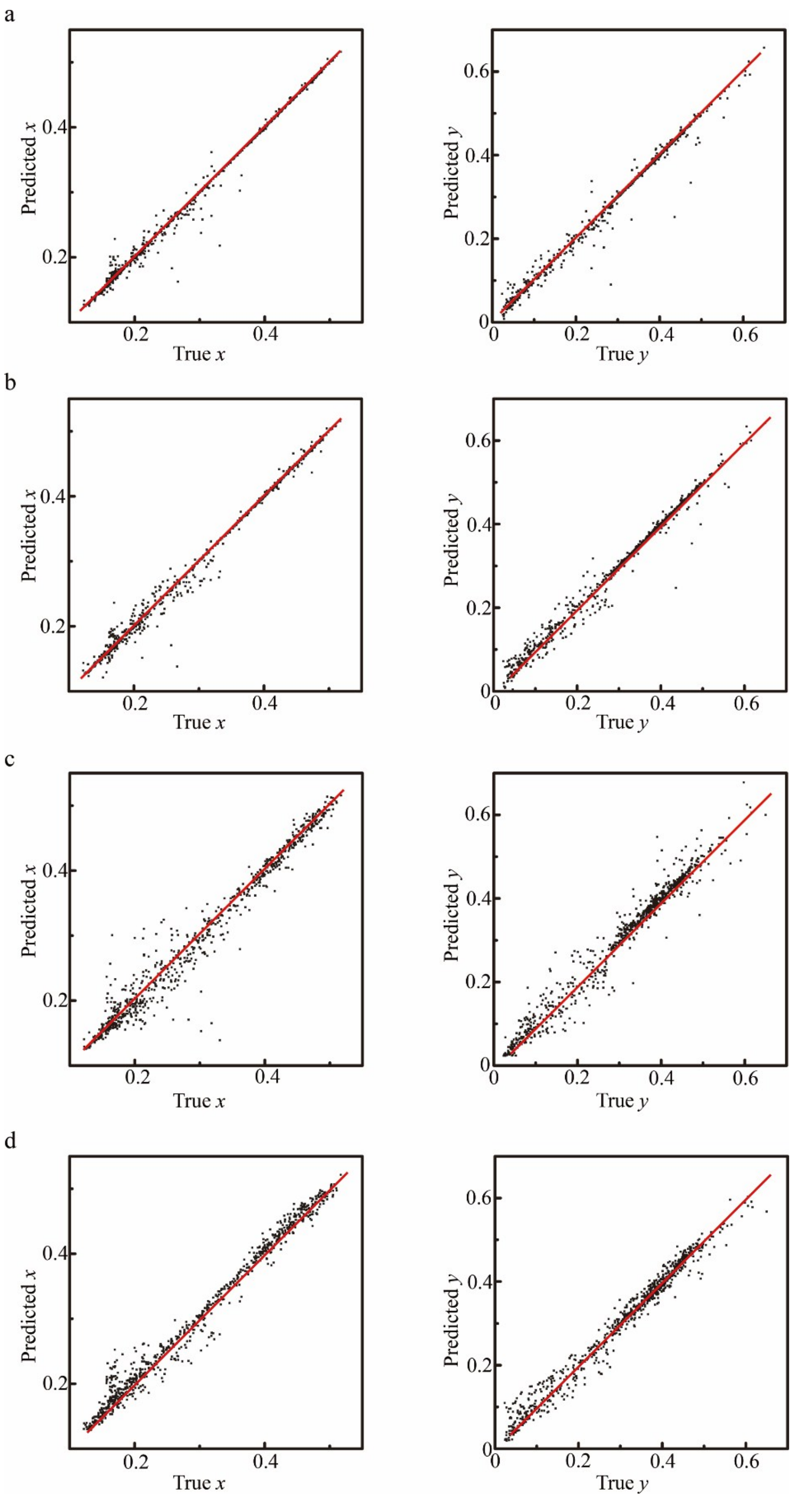
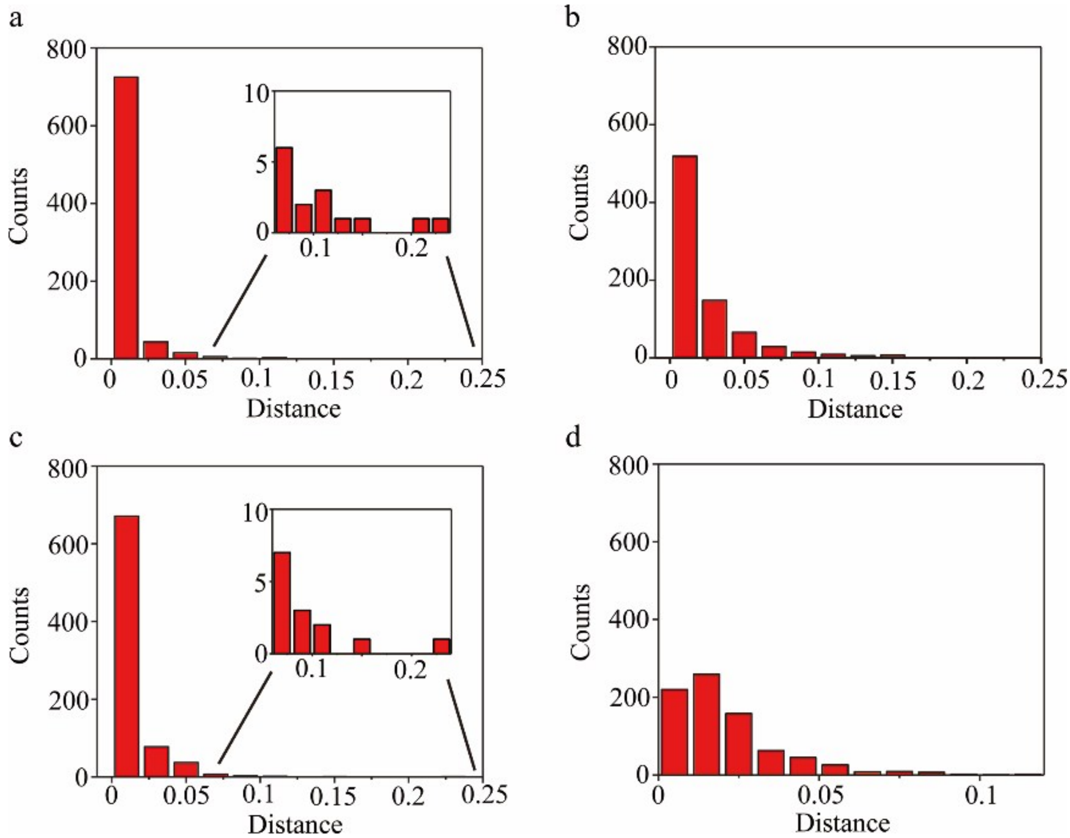


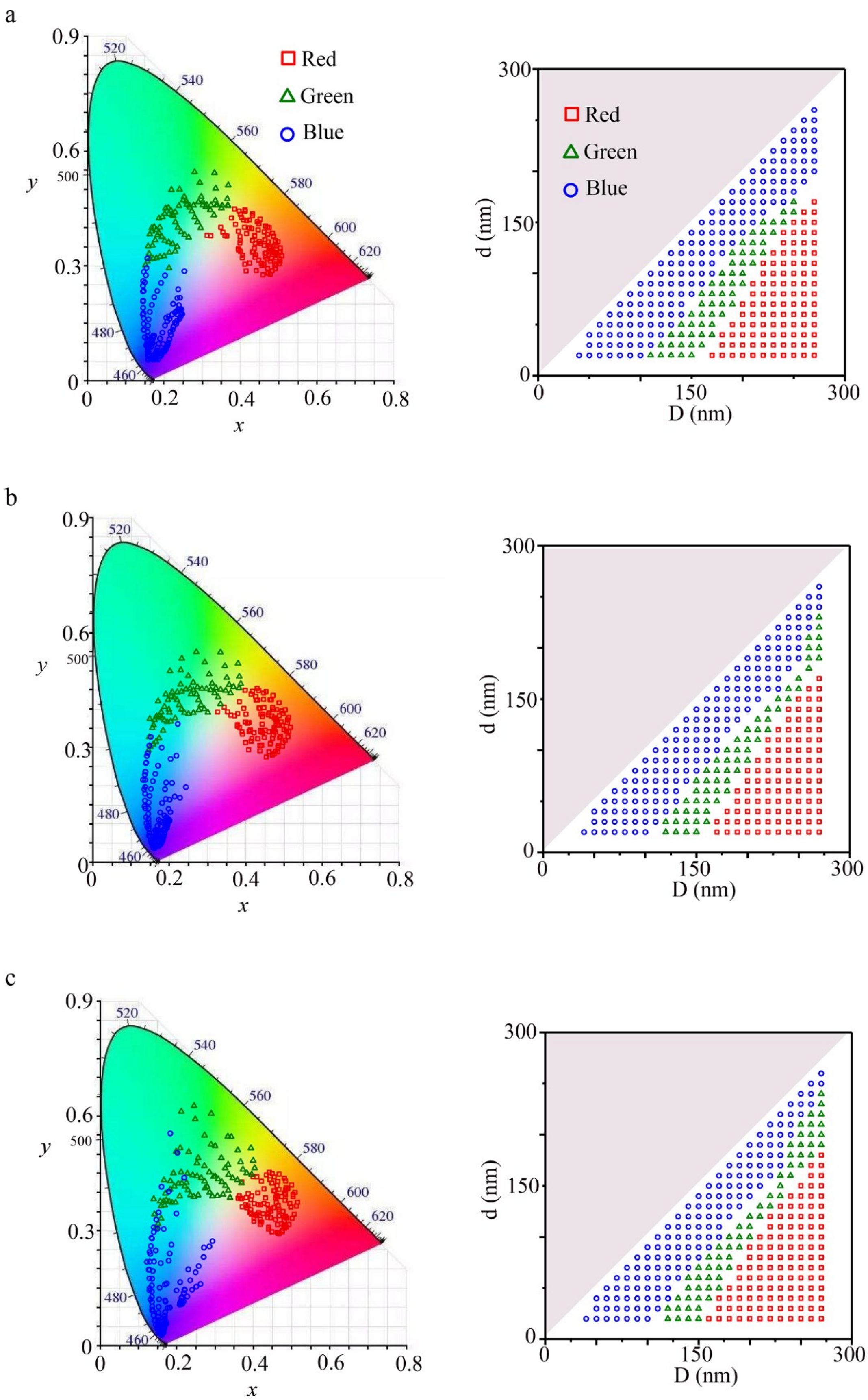
Supplementary Figure 1 | Test performance on different training dataset ratio. The test percentage of training data set is from 1% to 99%. Each training data set is used to train the ML model and record the model score, which is coefficient of determination (R^2). The test score R^2 exceeds 95% on the training data radio of 30%.



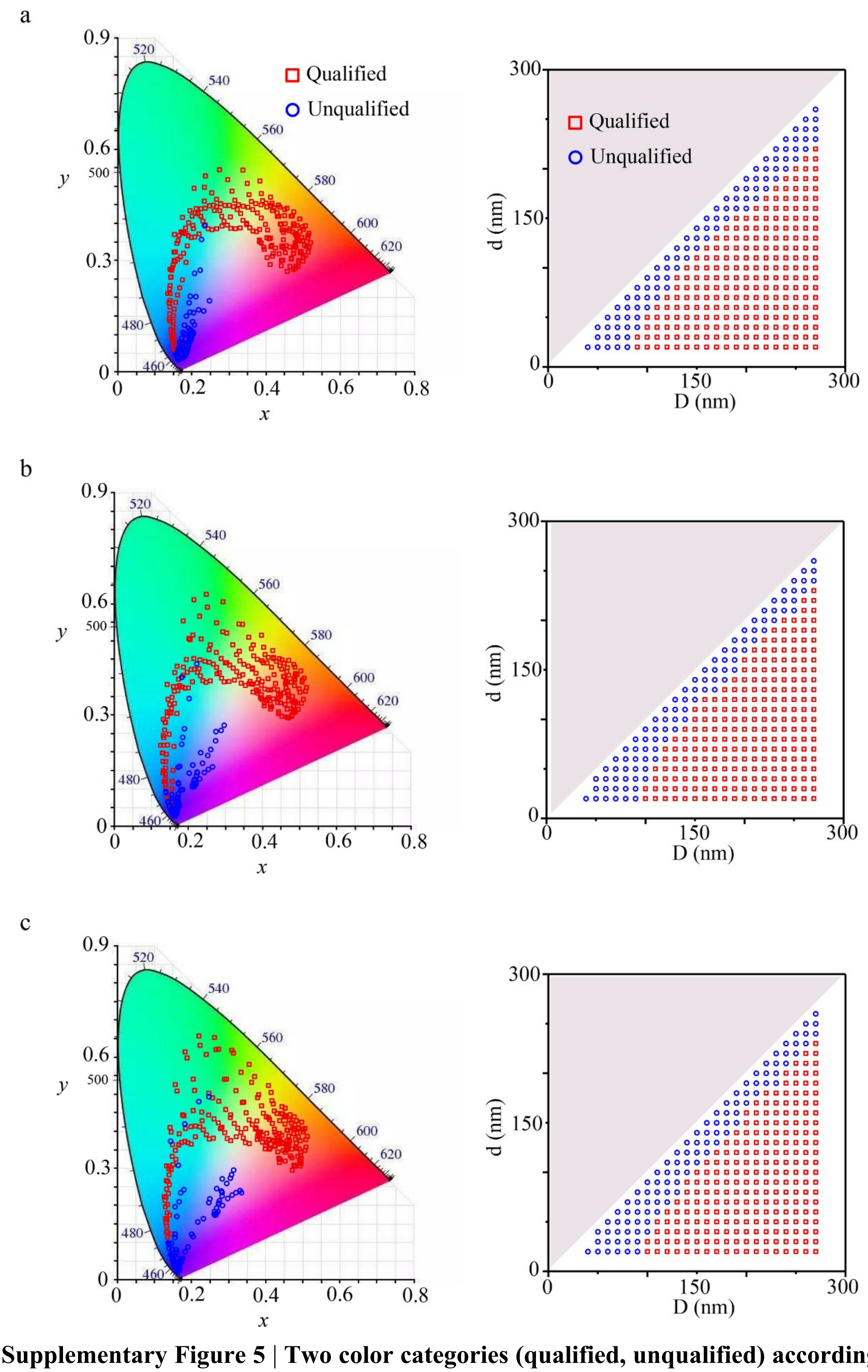
Supplementary Figure 2 | Scatter plots of the true coordinates (*x*, *y*) and the predicted coordinates (*x*, *y*) in CIE 1931 color space. a KRR, **b** DTR, **c** GPR and **d** MLPR.



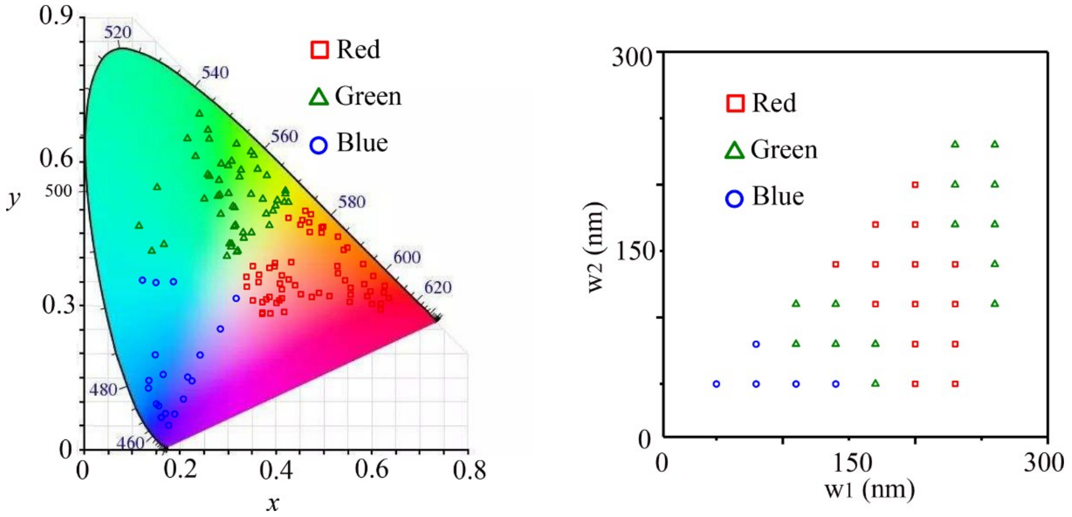
Supplementary Figure 3 | The counts of regular residual of the forward KRR model according to the distance between true coordinates and predicted coordinates. **a** KRR, **b** DTR, **c** GPR and **d** MLPR.



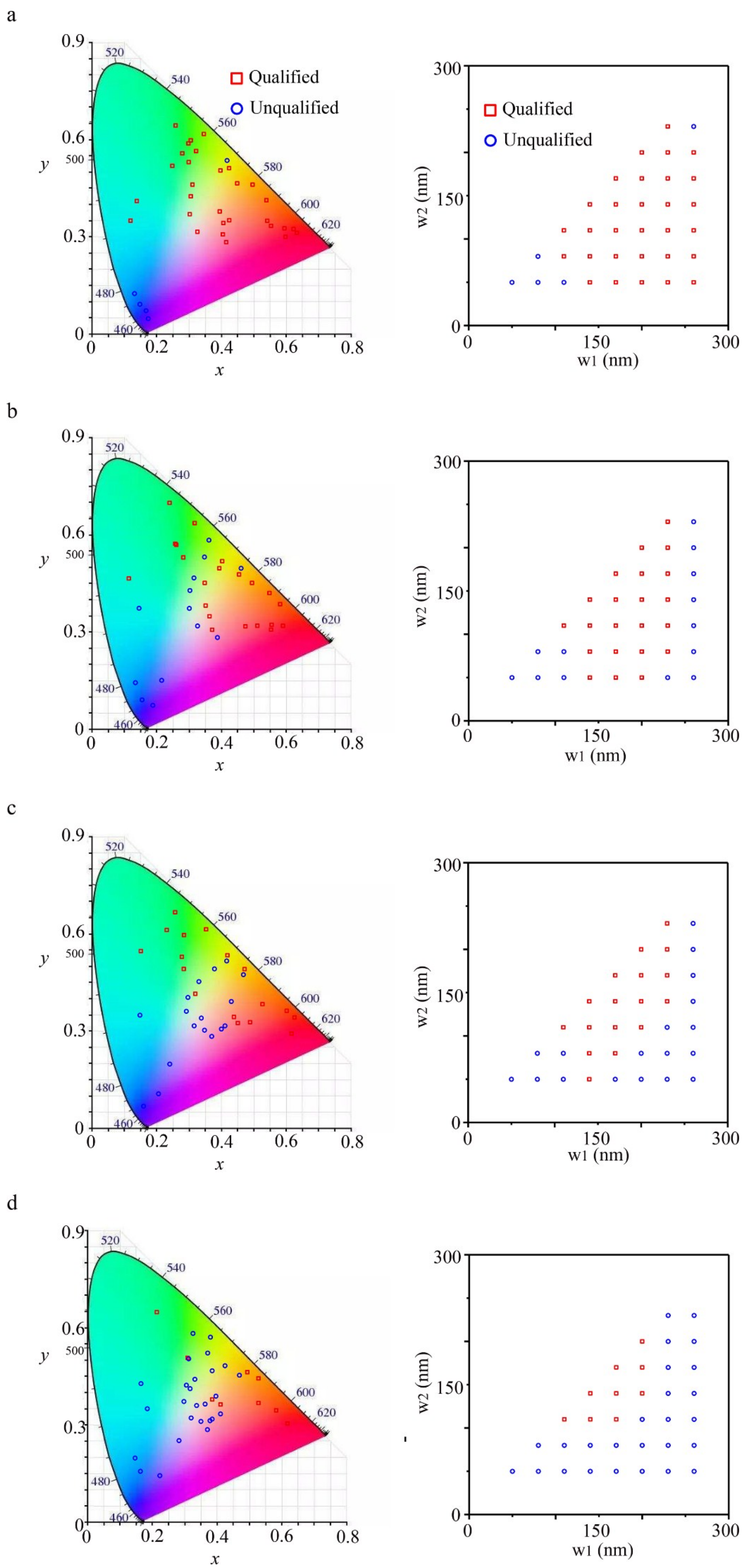
Supplementary Figure 4 | Three color categories (red, green, blue) in CIE 1931 color space and *D-d* plane for **a** g=40 nm. **b** g=60 nm. **c** g=80 nm.



Supplementary Figure 5 | Two color categories (qualified, unqualified) according to reflection peak intensity in CIE 1931 color space and *D*-*d* plane for **a** *g*=60 nm. **b** *g*=80 nm. **c** *g*=100 nm.



Supplementary Figure 6 | Three color categories (red, green, blue) in CIE 1931 color space and w_1-w_2 plane for g=30 nm.


a
b
c
d
Qualified
Unqualified
520
540
560
580
600
620
500
480
460
x
y
0
0.2
0.4
0.6
0.8
0.3
0.9
w1 (nm)
w2 (nm)
150
300

Supplementary Figure 7 | Two color categories (qualified, unqualified) according to reflection peak intensity in CIE 1931 color space and w1-w2 plane for **a** g=30 nm. **b** g=60 nm. **c** g=90 nm. **d** g=120 nm. As g increases, the interaction between adjacent resonators becomes weaker, leading to the decrease of reflection intensity.

ML model	R^2	T (s)	Advantage	Disadvantage
KRR	0.989	1.6	nonlinear relationship, regularization	-------------------
DTR	0.962	0.06	fast, no prior information	overfitting, can't handle complex nonlinear
GPR	0.988	69.9	kernel, probabilistic	not sparse
MLPR	0.979	3.1	complex nonlinear relationship	large amount of data

Supplementary Table 1 | The learning performances of four ML models. We execute one hundred times cross-validations and calculate the mean R^2 and T.

g (nm)	MA
10	0.983
20	0.993
30	0.987
40	0.974
50	0.977
60	0.98
70	0.977
80	0.971
90	0.961
100	0.968
110	0.974
120	0.932

Supplementary Table 2 | The mean accuracy (MA) of the classification results for different *g* group.

Desired color (x, y)	Predefined d, g (nm)	Final D, d, g (nm)	Color (x, y)
(0.5,0.35)	60, 60	226, 40, 60	(0.492,0.365)
	100, 60	229, 90, 60	(0.496,0.393)
	120, 60	229.15, 60	(0.474,0.377)
(0.3,0.55)	60, 60	124, 11, 60	(0.265,0.566)
	100, 60	128, 10, 60	(0.289,0.573)
	120, 60	121.10, 60	(0.243,0.557)
(0.15,0.15)	60, 60	124, 40, 60	(0.134,0.149)
	100, 60	229, 90, 60	(0.139,0.145)
	120, 60	229.15, 60	(0.141,0.139)

Supplementary Table 3 | Inverse design result with different predefined geometry parameters. The reinforcement learning (RL) algorithm find different geometries with different predefined geometry parameters, which generate similar colors with the desired ones. The results show high stability under different predefined geometry parameters.