

**Table S1**

Design matrix and responses for FFD.

| Run | Block | Variables for FFD |                    |                                      |                                |  |   | Responses            |                     |
|-----|-------|-------------------|--------------------|--------------------------------------|--------------------------------|--|---|----------------------|---------------------|
|     |       | pH                | APDC amount (%w/v) | Chelating Treatment Temperature (°C) | Chelating Treatment Time (min) | Sample Flow Rate (mL.min <sup>-1</sup> ) | Elution Flow Rate (mL.min <sup>-1</sup> ) | Peak Area of Cr(III) | Peak Area of Cr(VI) |
| 1   | 1     | 0                 | 0                  | 0                                    | 0                              | 0  | 0   | 598.4                | 572.3               |
| 2   | 1     | -1                | -1                 | -1                                   | -1                             | -1                                       | -1  | 571.5                | 263.9               |
| 3   | 1     | +1                | +1                 | -1                                   | +1                             | +1                                       | -1  | 572.1                | 584.2               |
| 4   | 1     | -1                | -1                 | +1                                   | -1                             | -1                                       | -1  | 552.3                | 280.7               |
| 5   | 1     | +1                | +1                 | +1                                   | -1                             | +1                                       | +1  | 514.0                | 347.6               |
| 6   | 1     | -1                | -1                 | -1                                   | -1                             | +1                                       | +1  | 480.1                | 204.6               |
| 7   | 1     | +1                | +1                 | -1                                   | -1                             | -1                                       | -1  | 582.3                | 335.1               |
| 8   | 1     | -1                | -1                 | +1                                   | -1                             | +1                                       | +1  | 474.6                | 220.6               |
| 9   | 1     | +1                | -1                 | +1                                   | +1                             | +1                                       | -1  | 615.2                | 613.5               |
| 10  | 1     | 0                 | 0                  | 0                                    | 0                              | 0  | 0   | 582.3                | 560.5               |
| 11  | 1     | -1                | +1                 | +1                                   | +1                             | -1                                       | +1  | 526.9                | 517.9               |
| 12  | 1     | 0                 | 0                  | 0                                    | 0                              | 0  | 0   | 560.8                | 548.6               |
| 13  | 1     | +1                | -1                 | +1                                   | +1                             | -1                                       | +1  | 512.4                | 515.0               |
| 14  | 1     | -1                | +1                 | +1                                   | -1                             | -1                                       | -1  | 571.5                | 414.1               |
| 15  | 1     | +1                | -1                 | -1                                   | +1                             | -1                                       | +1  | 517.8                | 430.0               |
| 16  | 1     | -1                | -1                 | -1                                   | +1                             | +1                                       | -1  | 560.8                | 530.8               |
| 17  | 1     | +1                | +1                 | +1                                   | +1                             | +1                                       | -1  | 624.1                | 685.9               |
| 18  | 1     | -1                | +1                 | -1                                   | +1                             | -1                                       | +1  | 490.9                | 530.8               |
| 19  | 1     | +1                | +1                 | -1                                   | -1                             | +1                                       | +1  | 501.6                | 305.4               |
| 20  | 2     | -1                | +1                 | +1                                   | -1                             | -1                                       | +1  | 507.0                | 346.9               |
| 21  | 2     | +1                | +1                 | +1                                   | -1                             | +1                                       | -1  | 587.6                | 424.0               |
| 22  | 2     | 0                 | 0                  | 0                                    | 0                              | 0  | 0   | 566.1                | 584.2               |
| 23  | 2     | -1                | -1                 | -1                                   | +1                             | +1                                       | +1  | 521.7                | 435.7               |
| 24  | 2     | +1                | -1                 | +1                                   | +1                             | -1                                       | -1  | 614.5                | 596.1               |
| 25  | 2     | -1                | -1                 | +1                                   | -1                             | +1                                       | -1  | 566.2                | 275.8               |
| 26  | 2     | +1                | +1                 | +1                                   | +1                             | +1                                       | +1  | 520.5                | 602.0               |
| 27  | 2     | -1                | +1                 | -1                                   | -1                             | +1                                       | -1  | 582.1                | 337.6               |
| 28  | 2     | 0                 | 0                  | 0                                    | 0                              | 0  | 0   | 544.6                | 566.4               |
| 29  | 2     | +1                | +1                 | -1                                   | -1                             | -1                                       | +1  | 513.1                | 319.3               |
| 30  | 2     | -1                | -1                 | +1                                   | +1                             | +1                                       | +1  | 514.0                | 513.0               |
| 31  | 2     | +1                | -1                 | -1                                   | -1                             | -1                                       | +1  | 467.4                | 212.8               |
| 32  | 2     | -1                | +1                 | -1                                   | +1                             | -1                                       | -1  | 570.9                | 578.1               |
| 33  | 2     | +1                | +1                 | -1                                   | +1                             | +1                                       | +1  | 498.2                | 529.3               |
| 34  | 2     | -1                | -1                 | +1                                   | -1                             | -1                                       | +1  | 474.8                | 216.5               |
| 35  | 2     | +1                | -1                 | -1                                   | -1                             | +1                                       | -1  | 565.2                | 264.7               |
| 36  | 2     | -1                | -1                 | -1                                   | +1                             | -1                                       | -1  | 566.7                | 536.4               |
| 37  | 2     | 0                 | 0                  | 0                                    | 0                              | 0  | 0   | 571.5                | 590.1               |
| 38  | 2     | +1                | +1                 | +1                                   | +1                             | -1                                       | -1  | 625.2                | 679.1               |

**Table S2**

Analysis of variance (ANOVA) for FFD.

| Factor                                      | Peak Area of Cr(III) |                 |                 |          |                   | Peak Area of Cr(VI) |    |         |         |                   |
|---|----------------------|-----------------|-----------------|----------|-------------------|---------------------|----|---------|---------|-------------------|
|   | SS <sup>a</sup>      | df <sup>b</sup> | MS <sup>c</sup> | F-Value  | p-Value           | SS                  | df | MS      | F-Value | p-Value           |
| Blocks                                      | 565.5                | 1               | 565.5           | 0.0792   | 0.7822            | 27.2                | 1  | 27.2    | 0.0681  | 0.7977            |
| A-pH  | 178.1                | 1               | 178.1           | 0.0250   | 0.8766            | 179.2               | 1  | 179.2   | 0.4482  | 0.5134            |
| B-APDC amount (%w/v)                        | 63673.0              | 1               | 63673.0         | 8.9207   | <b>0.0092</b>     | 1417.7              | 1  | 1417.7  | 3.5456  | 0.0792            |
| C-Chelating Temperature (°C)                | 22565.9              | 1               | 22565.9         | 3.1615   | 0.0957            | 1778.7              | 1  | 1778.7  | 4.4483  | 0.0521            |
| D-Chelating Time (min)                      | 527317.0             | 1               | 527317.0        | 73.8778  | <b>&lt;0.0001</b> | 3624.5              | 1  | 3624.5  | 9.0647  | <b>0.0088</b>     |
| E-Sample Flow Rate (mL.min <sup>-1</sup> )  | 326.1                | 1               | 326.1           | 0.0457   | 0.8336            | 33.4                | 1  | 33.4    | 0.0835  | 0.7765            |
| F-Elution Flow Rate (mL.min <sup>-1</sup> ) | 41517.2              | 1               | 41517.2         | 5.8166   | <b>0.0291</b>     | 52264.8             | 1  | 52264.8 | 130.71  | <b>&lt;0.0001</b> |
| AB  | 11.4                 | 1               | 11.4            | 0.0016   | 0.9686            | 1188.5              | 1  | 1188.5  | 2.9725  | 0.1052            |
| AC  | 0.3                  | 1               | 0.3             | 0.00005  | 0.9946            | 569.6               | 1  | 569.6   | 1.4245  | 0.2512            |
| AD  | 1957.5               | 1               | 1957.5          | 0.2742   | 0.6081            | 106.8               | 1  | 106.8   | 0.2671  | 0.6128            |
| AE  | 499.6                | 1               | 499.6           | 0.0699   | 0.7950            | 44.6                | 1  | 44.6    | 0.1115  | 0.7431            |
| AF  | 1654.4               | 1               | 1654.4          | 0.2318   | 0.6371            | 104.5               | 1  | 104.5   | 0.2612  | 0.6167            |
| BC  | 663.4                | 1               | 663.4           | 0.0929   | 0.7647            | 271.3               | 1  | 271.3   | 0.6785  | 0.4231            |
| BD  | 3912.8               | 1               | 3912.8          | 0.5482   | 0.4705            | 1269.3              | 1  | 1269.3  | 3.1745  | 0.0951            |
| BE  | 238.5                | 1               | 238.5           | 0.0334   | 0.8574            | 2.00                | 1  | 2.00    | 0.0050  | 0.9445            |
| BF  | 173.9                | 1               | 173.9           | 0.0244   | 0.8781            | 1.14                | 1  | 1.14    | 0.0029  | 0.9580            |
| CD  | 2527.3               | 1               | 2527.3          | 0.3541   | 0.5607            | 2262.7              | 1  | 2262.7  | 5.6588  | <b>0.0311</b>     |
| CE  | 530.9                | 1               | 530.9           | 0.0744   | 0.7888            | 28.6                | 1  | 28.6    | 0.0715  | 0.7928            |
| CF  | 1605.8               | 1               | 1605.8          | 0.2250   | 0.6421            | 541.5               | 1  | 541.5   | 1.3543  | 0.2627            |
| DE  | 449.5                | 1               | 449.5           | 0.0630   | 0.8053            | 29.4                | 1  | 29.4    | 0.0736  | 0.7898            |
| DF  | 2969.4               | 1               | 2969.4          | 0.4160   | 0.5287            | 0.05                | 1  | 0.05    | 0.0001  | 0.9915            |
| EF  | 40.2                 | 1               | 40.2            | 0.0056   | 0.9411            | 0.39                | 1  | 0.39    | 0.0010  | 0.9753            |
| Curvature                                   | 104573.8             | 1               | 104573.8        | 587.6068 | <b>&lt;0.0001</b> | 3970.1              | 1  | 3970.1  | 27.410  | <b>&lt;0.0001</b> |
| Residual                                    | 2491.5               | 14              | 177.9657        |          |                   | 2027.7              | 14 | 144.8   |         |                   |
| LOF   | 1905.3               | 10              | 190.5289        | 1.300    | 0.4308            | 910.6               | 10 | 91.1    | 0.3260  | 0.9314            |
| Pure Error                                  | 586.2309             | 4               | 146.5577        |          |                   | 1117.1              | 4  | 279.3   |         |                   |
| Total SS                                    | 780442.9             | 37              |                 |          |                   | 71743.6             | 37 |         |         |                   |

<sup>a</sup> Sum of Square<sup>b</sup> Degree of Freedom<sup>c</sup> Mean Square

**Table S3**

Design matrix and responses for CCD.

| Run | Block | Variables for CCD  |                                      |                                |   | Responses           |                      |
|-----|-------|--------------------|--------------------------------------|--------------------------------|---|---------------------|----------------------|
|     |       | APDC amount (%w/v) | Chelating Treatment Temperature (°C) | Chelating Treatment Time (min) | Elution Flow Rate (mL min <sup>-1</sup> ) | Peak Area of Cr(VI) | Peak Area of Cr(III) |
| 1   | 1     | 0                  | 0                                    | 0                              | 0   | 591.1               | 569.9                |
| 2   | 1     | -1                 | +1                                   | -1                             | -1  | 563.1               | 584.5                |
| 3   | 1     | +1                 | +1                                   | +1                             | -1  | 609.7               | 656.3                |
| 4   | 1     | -1                 | -1                                   | +1                             | -1  | 570.9               | 559.7                |
| 5   | 1     | +1                 | +1                                   | -1                             | +1  | 511.9               | 345.4                |
| 6   | 1     | -1                 | +1                                   | +1                             | +1  | 527.3               | 496.2                |
| 7   | 1     | +1                 | -1                                   | -1                             | -1  | 581.8               | 383.2                |
| 8   | 1     | 0                  | 0                                    | 0                              | 0   | 561.6               | 544.1                |
| 9   | 1     | -1                 | -1                                   | -1                             | +1  | 479.2               | 222.0                |
| 10  | 1     | 0                  | 0                                    | 0                              | 0   | 583.3               | 564.5                |
| 11  | 1     | +1                 | -1                                   | +1                             | +1  | 517.8               | 534.9                |
| 12  | 1     | 0                  | 0                                    | 0                              | 0   | 562.8               | 584.5                |
| 13  | 2     | -1                 | -1                                   | +1                             | +1  | 502.5               | 500.9                |
| 14  | 2     | +1                 | +1                                   | +1                             | +1  | 536.7               | 559.9                |
| 15  | 2     | +1                 | -1                                   | -1                             | +1  | 505.6               | 330.5                |
| 16  | 2     | 0                  | 0                                    | 0                              | 0   | 578.7               | 560.2                |
| 17  | 2     | +1                 | +1                                   | -1                             | -1  | 580.2               | 395.6                |
| 18  | 2     | -1                 | +1                                   | -1                             | +1  | 474.6               | 212.5                |
| 19  | 2     | +1                 | -1                                   | +1                             | -1  | 570.9               | 641.8                |
| 20  | 2     | 0                  | 0                                    | 0                              | 0   | 572.4               | 582.9                |
| 21  | 2     | 0                  | 0                                    | 0                              | 0   | 586.4               | 586.6                |
| 22  | 2     | -1                 | +1                                   | +1                             | -1  | 598.9               | 570.5                |
| 23  | 2     | 0                  | 0                                    | 0                              | 0   | 564.7               | 564.3                |
| 24  | 2     | -1                 | -1                                   | -1                             | -1  | 558.5               | 275.7                |
| 25  | 3     | 0                  | +2                                   | 0                              | 0   | 558.5               | 540.9                |
| 26  | 3     | +2                 | 0                                    | 0                              | 0   | 574.0               | 619.2                |
| 27  | 3     | 0                  | 0                                    | -2                             | 0   | 482.3               | 127.7                |
| 28  | 3     | 0                  | 0                                    | +2                             | 0   | 542.9               | 668.1                |
| 29  | 3     | 0                  | 0                                    | 0                              | 0   | 573.4               | 558.9                |
| 30  | 3     | 0                  | -2                                   | 0                              | 0   | 524.8               | 231.9                |
| 31  | 3     | -2                 | 0                                    | 0                              | 0   | 525.8               | 370.8                |
| 32  | 3     | 0                  | 0                                    | 0                              | 0   | 588.0               | 584.5                |
| 33  | 3     | 0                  | 0                                    | 0                              | 0   | 571.8               | 592.2                |
| 34  | 3     | 0                  | 0                                    | 0                              | -2  | 614.4               | 660.7                |
| 35  | 3     | 0                  | 0                                    | 0                              | 0   | 562.6               | 564.3                |
| 36  | 3     | 0                  | 0                                    | 0                              | +2  | 483.9               | 505.1                |

**Table S4**

Analysis of variance (ANOVA) for CCD.

| Factor                                      | Peak Area of Cr(III) |    |          |          |         | Peak Area of Cr(VI) |    |         |          |         |
|---|----------------------|----|----------|----------|---------|---------------------|----|---------|----------|---------|
|   | SS                   | df | MS       | F-Value  | p-Value | SS                  | df | MS      | F-Value  | p-Value |
| Blocks                                      | 122.6                | 2  | 61.3     | 0.267    | 0.7686  | 140.2               | 2  | 70.1    | 0.8599   | 0.4390  |
| Model                                       | 79455.6              | 14 | 56751.29 | 247.033  | <0.0001 | 48769.7             | 14 | 3483.6  | 42.72    | <0.0001 |
| A-APDC amount (%w/v)                        | 64045.3              | 1  | 64045.3  | 278.783  | <0.0001 | 2320.2              | 1  | 2320.2  | 28.4558  | <0.0001 |
| B-Chelating Temperature (°C)                | 589.9                | 1  | 589.9    | 2.568    | 0.1256  | 1388.3              | 1  | 1388.3  | 17.0260  | 0.0006  |
| C-Chelating Time (min)                      | 418497.9             | 1  | 418497.9 | 1821.682 | <0.0001 | 3773.0              | 1  | 3773.0  | 46.2726  | <0.0001 |
| D-Elution Flow Rate (mL.min <sup>-1</sup> ) | 30721.6              | 1  | 30721.6  | 133.728  | <0.0001 | 29354.9             | 1  | 29354.9 | 360.0162 | <0.0001 |
| AB  | 387.4                | 1  | 387.4    | 1.686    | 0.2096  | 6.0                 | 1  | 6.0     | 0.0734   | 0.7893  |
| AC  | 2803.0               | 1  | 2803.0   | 12.201   | 0.0024  | 293.3               | 1  | 293.3   | 3.5976   | 0.0732  |
| AD  | 261.4                | 1  | 261.4    | 1.138    | 0.2995  | 86.2                | 1  | 86.2    | 1.0567   | 0.3169  |
| BC  | 83.8                 | 1  | 83.8     | 0.365    | 0.5531  | 699.5               | 1  | 699.5   | 8.5790   | 0.0086  |
| BD  | 0.7                  | 1  | 0.7      | 0.003    | 0.9565  | 38.1                | 1  | 38.1    | 0.4677   | 0.5023  |
| CD  | 982.3                | 1  | 982.3    | 4.276    | 0.0525  | 133.0               | 1  | 133.0   | 1.6318   | 0.2168  |
| A <sup>2</sup>                              | 10964.7              | 1  | 10964.7  | 47.728   | <0.0001 | 936.1               | 1  | 936.1   | 11.4810  | 0.0031  |
| B <sup>2</sup>                              | 206218.1             | 1  | 206218.1 | 897.648  | <0.0001 | 1793.6              | 1  | 1793.6  | 21.9968  | 0.0002  |
| C <sup>2</sup>                              | 58573.7              | 1  | 58573.7  | 254.966  | <0.0001 | 6943.0              | 1  | 6943.0  | 85.1507  | <0.0001 |
| D <sup>2</sup>                              | 388.0                | 1  | 388.0    | 1.689    | 0.2093  | 1004.6              | 1  | 1004.6  | 12.3205  | 0.0023  |
| Residual                                    | 4364.87              | 19 | 229.73   |          |         | 1549.21             | 19 | 81.54   |          |         |
| LOF   | 2244.37              | 10 | 224.44   | 0.95     | 0.5336  | 306.43              | 10 | 30.64   | 0.2200   | 0.9862  |
| Pure Error                                  | 2120.50              | 9  | 235.61   |          |         | 1242.78             | 9  | 138.09  |          |         |
| Total SS                                    | 799005.1             | 35 |          |          |         | 50459.2             | 35 |         |          |         |

**Model statistics**

|                                | Peak Area of Cr(III) | Peak Area of Cr(VI) |
|--------------------------------|----------------------|---------------------|
| R <sup>2</sup>                 | 0.9931               | 0.9640              |
| R <sup>2</sup> <sub>adj</sub>  | 0.9906               | 0.9483              |
| R <sup>2</sup> <sub>pred</sub> | 0.9796               | 0.9227              |

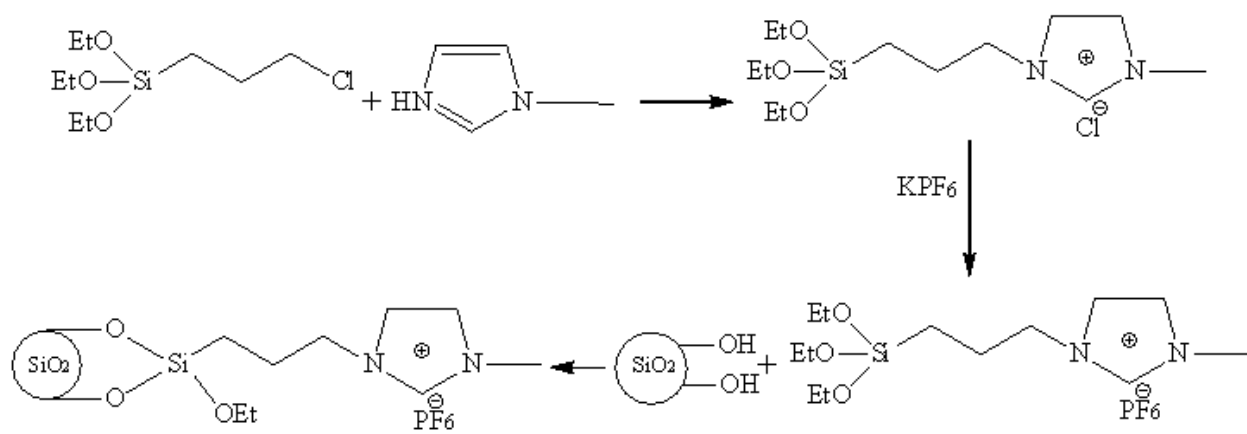
### Figure captions

**Fig. S1.** Schematic diagram for synthesis of N-methylimidazolium–hexafluorophosphate functionalized silica.

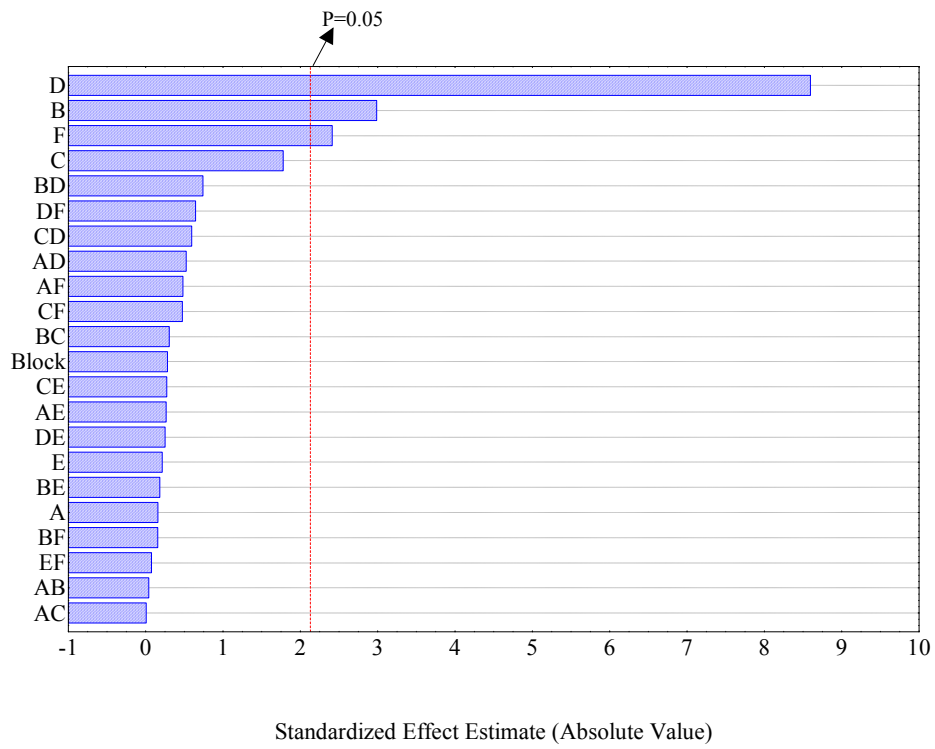
**Fig. S2.** Pareto chart of standardized effects of the main parameters on peak area of Cr(III) (a) and Cr(VI) (b). The vertical dashed line indicated the level of significance at  $p = 0.05$ .

**Fig. S3.** Normal probability plot of studentized residuals for the refined quadratic models of Cr(III) (a) and Cr(VI) (b).

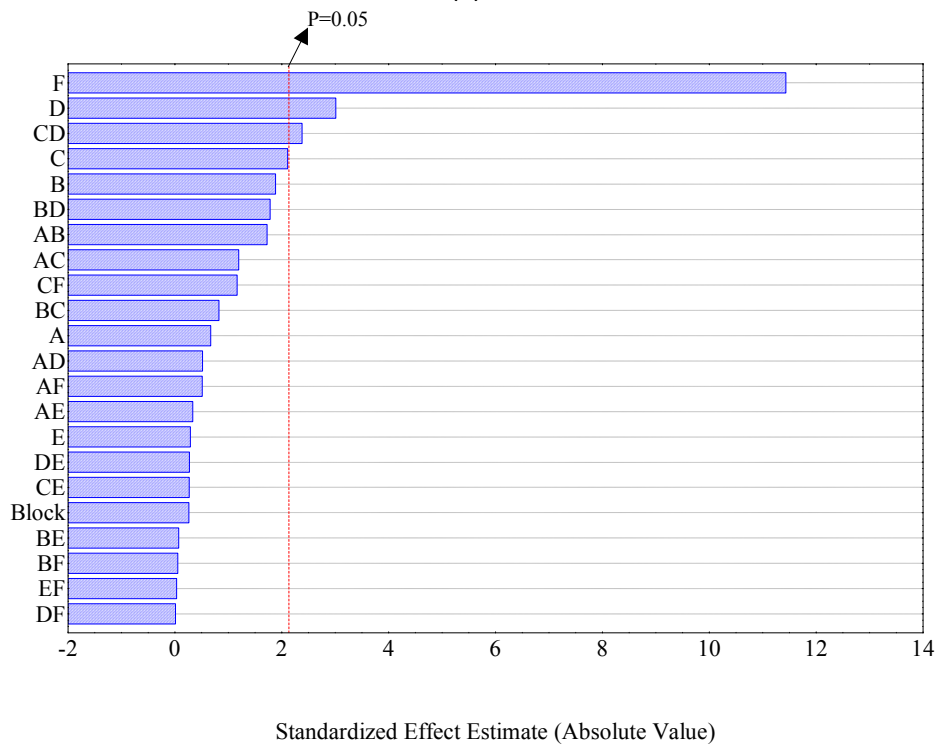
**Fig. S4.** 3-D graphical representation of the peak area of (A) Cr(III) and (B) Cr(VI) complexes with APDC: (a) APDC concentration–chelation treatment temperature, (b) APDC concentration–chelation treatment time, (c) APDC concentration–elution flow rate, (d) chelation treatment temperature–chelation treatment time, (e) chelation treatment temperature–elution flow rate, and (f) chelation treatment time– elution flow rate.



**Figure S1**

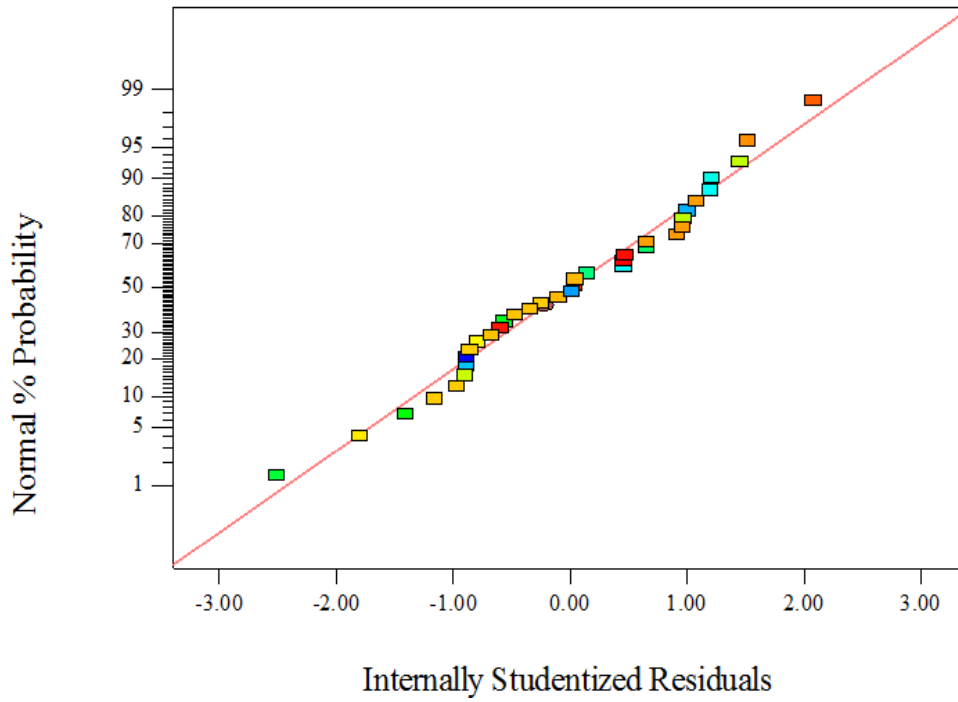


(a)

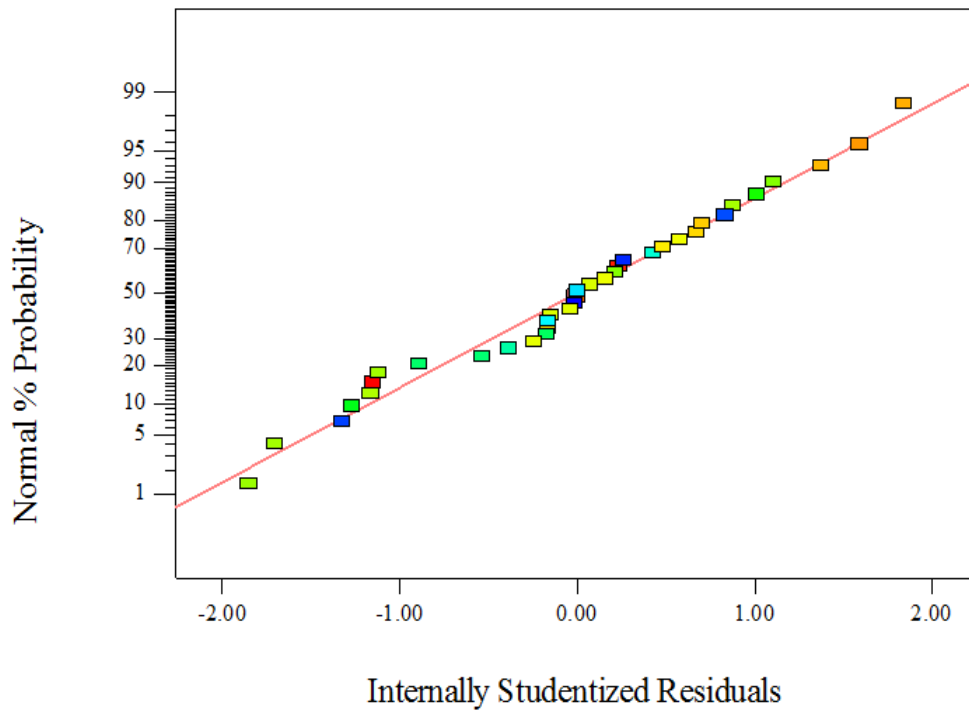


(b)

**Figure S2**



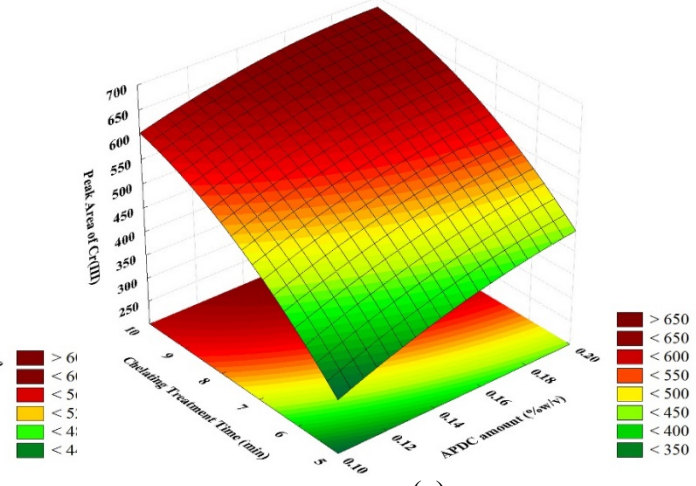
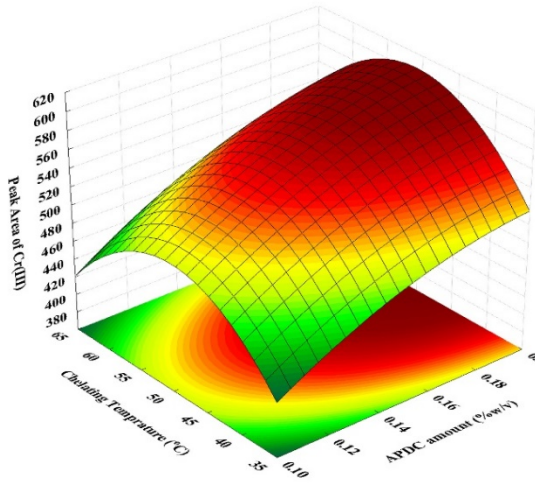
(a)



(b)

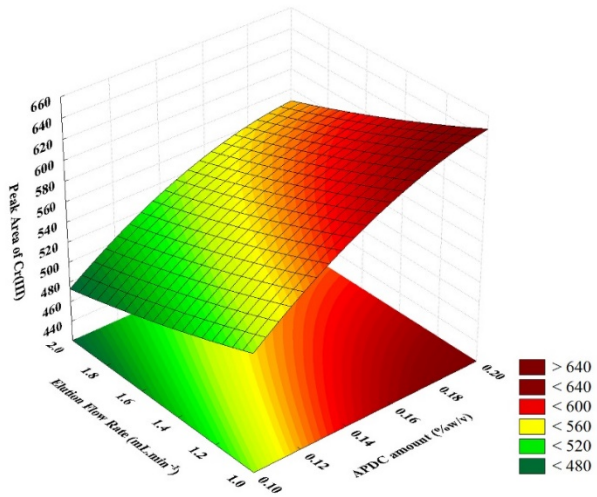
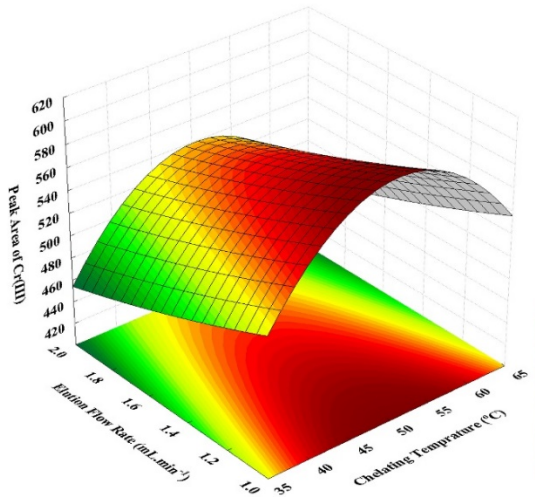
Figure S3





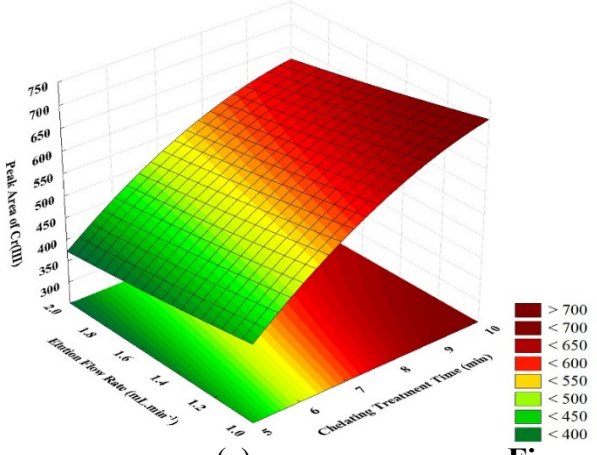
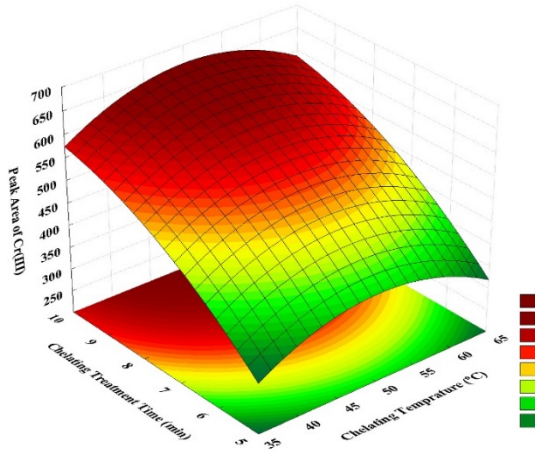
(b)

(a)



(d)

(c)

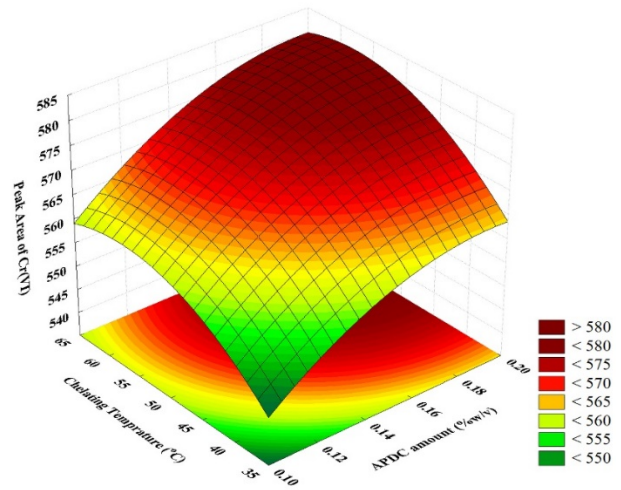


S4A

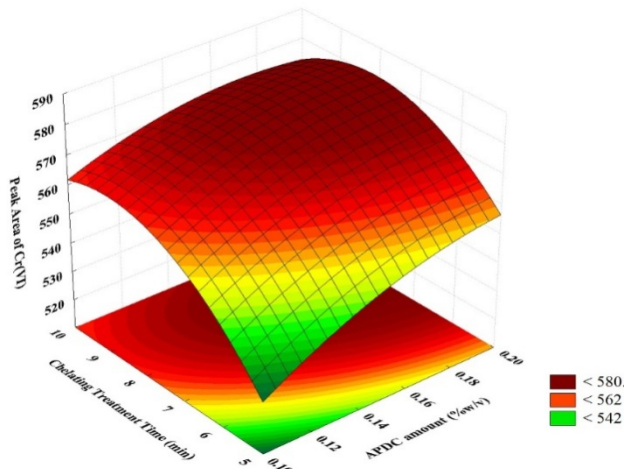
(f)

(e)

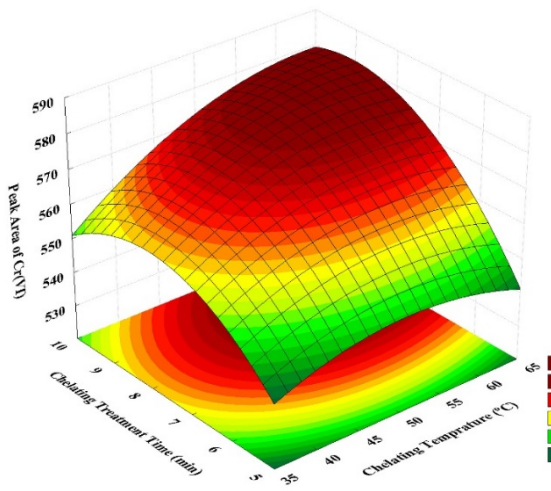
Figure



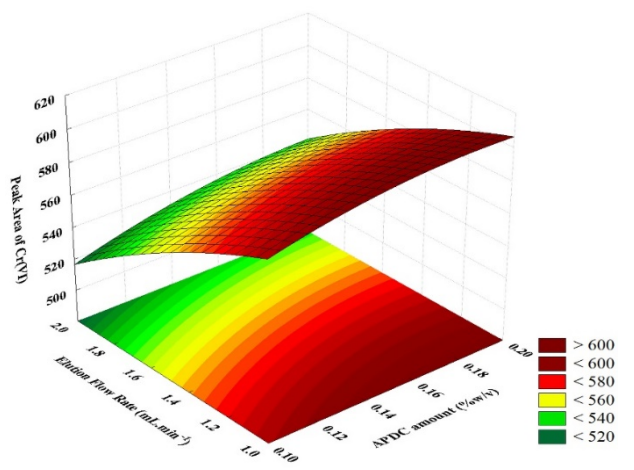
(b)



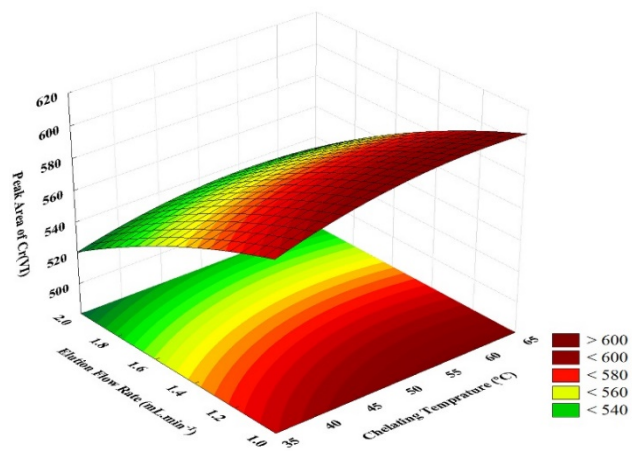
(a)



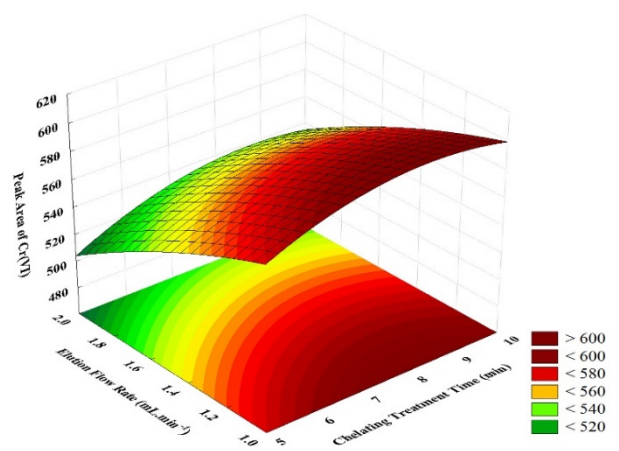
(c)



(d)



(f)



(e)

Figure S4B