**Supporting Information**

**Application of Cu-based metal-organic framework (Cu-BDC) as a sorbent for dispersive solid-phase extraction of gallic acid from orange juice samples using HPLC-UV method**

Ahmad Reza Bagheri, Mehrorang Ghaedi\*

Chemistry Department, Yasouj University, Yasouj 75918-74831, Iran.

\*Corresponding author. Tel/Fax: +98-741-2223048.  
E-mail addresses: m\_ghaedi@mail.yu.ac.ir (M. Ghaedi).

**Figures and Tables caption:**

Figure S1. The standardized main effect Pareto chart for extraction of gallic acid from orange juice samples.

Figure S2. The experimental data versus predicted data for extraction of gallic acid from orange juice samples.

Figure S3. Desirability function for extraction of gallic acid from orange juice samples. Dashed line indicated current values after optimization.

Figure S4. The reusability of prepared Cu-BDC.

Table S1. Experimental factors and levels in the central composite design for extraction of gallic acid from orange juice samples.

Table S2: Different isotherm models for determination of gallic acid by Cu-BDC.

Table S3: Different kinetic models for determination of gallic acid by Cu-BDC.

Figure S1. The standardized main effect Pareto chart for extraction of gallic acid from orange juice samples.

C:\Users\ahmad\Desktop\Pareto Chart of Standardized Effects.tif

Figure S2. The experimental data versus predicted data for extraction of gallic acid from orange juice samples.

C:\Users\ahmad\Desktop\Observed vs. Predicted Values.tif

Figure S3. Desirability function for extraction of gallic acid from orange juice samples. Dashed line indicated current values after optimization.

C:\Users\ahmad\Desktop\Profiles for Predicted Values and Desirability.tif

Figure S4. The reusability of prepared Cu-BDC.

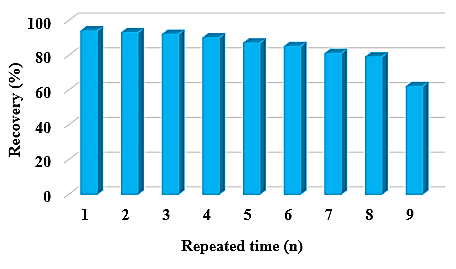


Table S1. Experimental factors and levels in the central composite design for extraction of gallic acid from orange juice samples.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Levels | | | | | | Code | Unit | Factors |
| α+ | High (+1) | Center (0) | | Low (-1) | α- |
| 35.0 | 30.0 | 25.0 | | 20.0 | 15.0 | A | mg | Sorbent dosage |
| 6.0 | 5.0 | 4.0 | | 3.0 | 2.0 | B | min | Ultrasonic time |
| 3.5 | 3.0 | 2.5 | | 2.0 | 1.5 | C | mL | Washing solvent volume |
| 3.5 | 3.0 | 2.5 | | 2.0 | 1.5 | D | mL | Eluent solvent volume |
| GA ER% | | | D | | C | B | A | Run |
| 52.00 | | | 2.5 | | 2.5 | 4.0 | 15.0 | 1 |
| 75.23 | | | 3.0 | | 2.0 | 5.0 | 20.0 | 2 |
| 96.20 | | | 2.0 | | 3.0 | 5.0 | 30.0 | 3 |
| 91.20 | | | 3.0 | | 3.0 | 3.0 | 30.0 | 4 |
| 84.85 | | | 3.0 | | 2.0 | 3.0 | 30.0 | 5 |
| 81.00 | | | 2.5 | | 2.5 | 4.0 | 25.0 | 6 |
| 80.00 | | | 2.0 | | 3.0 | 3.0 | 20.0 | 7 |
| 84.63 | | | 2.5 | | 2.5 | 4.0 | 25.0 | 8 |
| 97.14 | | | 3.5 | | 2.5 | 4.0 | 25.0 | 9 |
| 92.75 | | | 2.5 | | 3.5 | 4.0 | 25.0 | 10 |
| 87.62 | | | 2.0 | | 2.0 | 5.0 | 30.0 | 11 |
| 99.00 | | | 2.5 | | 2.5 | 4.0 | 35.0 | 12 |
| 75.00 | | | 1.5 | | 2.5 | 4.0 | 25.0 | 13 |
| 83.00 | | | 2.5 | | 2.5 | 4.0 | 25.0 | 14 |
| 86.32 | | | 2.5 | | 2.5 | 4.0 | 25.0 | 15 |
| 98.45 | | | 2.5 | | 2.5 | 6.0 | 25.0 | 16 |
| 82.64 | | | 2.5 | | 2.5 | 4.0 | 25.0 | 17 |
| 68.00 | | | 2.5 | | 2.5 | 2.0 | 25.0 | 18 |
| 70.00 | | | 2.0 | | 2.0 | 3.0 | 20.0 | 19 |
| 92.00 | | | 3.0 | | 3.0 | 5.0 | 20.0 | 20 |
| 72.00 | | | 2.5 | | 1.5 | 4.0 | 25.0 | 21 |

Table S2: Different isotherm models for determination of gallic acid by Cu-BDC.

|  |  |  |  |
| --- | --- | --- | --- |
| GA | Unit | Equation and parameters | Isotherm |
|  |  | Log qe = m Log Ce + log α | Freundlich |
|  |  | log qe vs. log Ce |
| 1.82 | - | m |
| 8.24 | L mg−1 | α |
| 0.8921 | - | R2 |
|  |  |  | Langmuir |
|  |  | Ce/qe = (1/Qm KL) + Ce/Qm |
|  |  | Ce/qe vs. Ce |
| 384.6 | mg g−1 | Q, Equilibrium |
| 300.00 | mg g−1 | Qm,cal |
| 0.666 | L mg−1 | KL |
| 0.029-0.230 |  | RL |
| 0.9965 | - | R2 |
|  |  |  | Temkin |
|  |  | qe = B1 ln KT + B1 lnCe |
|  |  | qe vs. log Ce |
| 76.51 | J mol-1 | B |
| 8.48 | L g−1 | KT |
| 0.9742 | - | R2 |
|  |  |  | Dubinin- Radushkevich |
|  |  | ln qe = ln Qs - βε2 |
|  |  | ln qe vs. ɛ2 |
| -7.0 | kJ mol-1 | β\*10-8 |
| 109.9 | mg g-1 | QS |
| 0.8000 | - | R2 |

Table S3: Different kinetic models for determination of gallic acid by Cu-BDC.

|  |  |  |  |
| --- | --- | --- | --- |
| GA | Unit | Equation and parameters | Kinetic |
|  |  | log(qe–qt) = log qe–( k1/2.303) t | Pseudo-first order |
|  |  | ln (qe–qt) vs. t |
| 0.67 | min-1 | K1 |
| 45.7 | mg g−1 | qe (calc) |
| 0.8629 | - | R2 |
|  |  | t/qt= 1 k2qe2 + t/qe | Pseudo-second order |
|  |  | t/qt vs. t |
| 0.009 | g mg-1 min-1 | K2 |
| 41.15 | mg g−1 | qe (calc) |
| 0.9921 | - | R2 |
|  |  | qt=Kdifft1/2+C | Intraparticle diffusion |
|  |  | qt VS. t1/2 |
| 9.9 | mg g-1 min-1/2 | Kdiff |
| 4.12 | mg g-1 | C |
| 0.93 |  | R2 |
|  |  | qt= 1/β Ln(αβ) + 1/β Ln (t) | Elovich |
| 0.109 | g mg-1 min-1 | β |
| 106938 | gmg | α |
| 0.90 |  | R2 |
| 38.23 |  | qe(exp) | Experimental |