**Supporting Information**

**Targeted metabolomics analysis of nucleosides and identification of biomarkers for colorectal adenomas and colorectal cancer**

Weifang Zheng1#\*, Mingwei Wang2#, Xiaoyin Chai3, Fuzhen Pan1, Meihui Xu1, Yingchen Wang1, Liuhao Lan3, Feiran Hu1, Zhe Zhang3, Zhu Chen1

1Lanxi Hospital of Traditional Chinese Medicine, Jinhua, China.

2College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, China.

3Lanxi Red Cross Hospital, Jinhua, China.

#These authors contributed equally.

\*Corresponding author:

Weifang Zheng, zhengweifang1972@163.com

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**Fig. S1.** Identification of m3U, Gm, m1G and m2G in human serum. Representative MRM chromatograms of m3U, Gm, m1G, and m2G (A) in a serum sample, and (B) standard.

**Table S1.** The basic information of individuals recruited.

|  |  |  |  |
| --- | --- | --- | --- |
| **Group** | **Healthy control** | **Colorectal cancer** | **Colorectal adenoma** |
| Number of cases | 51 | 37 | 55 |
| Age (year) | 65.6± 2.4 | 66.0± 6.0 | 65.2± 7.7 |
| Gender(Male/Female) | 37/16 | 23/16 | 37/20 |

**Table S2.** The optimized MRM parameters applied to the analysis of nucleosides and their isotope labelled internal standards.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound** | **MRM****ion transition (*m/z*)** | **CE (V)** | **DP (V)** | **EP (V)** | **CXP (V)** |
| m1A | 282.1→150.0 | 25 | 55 | 10 | 10 |
| [D3]m1A | 285.1→153.0 | 25 | 50 | 10 | 10 |
| m6A | 282.1→150.0 | 25 | 55 | 10 | 10 |
| [D3]m6A | 285.1→153.0 | 25 | 50 | 10 | 10 |
| m3U | 259.1→127.0 | 16 | 45 | 7 | 10 |
| m5U | 259.1→127.0 | 16 | 40 | 9 | 9 |
| [13C5]m5U | 264.1→127.0 | 20 | 45 | 8 | 10 |
| Um | 259.1→113.0 | 18 | 45 | 6 | 16 |
| [D3]Um | 262.1→113.0 | 12 | 40 | 8 | 9 |
| m1G | 298.1→166.0 | 20 | 55 | 7 | 14 |
| m2G | 298.1→166.0 | 22 | 55 | 6 | 13 |
| Gm | 298.1→152.0 | 16 | 50 | 7 | 12 |
| [D6]m2,2G | 318.1→186.0 | 30 | 60 | 10 | 14 |
| Cm | 258.1→112.0 | 16 | 45 | 10 | 8 |
| [D3]Cm | 261.1→112.0 | 18 | 40 | 10 | 8 |

*CE* collision energy, *DP* declustering potential, *EP* entrance potential, *CXP* collision cell exit potential

**Table S3.** The mean concentrations of A, m1A, m6A, U, m3U, m5U, Um, Cm, m2G, m1G and Gm in serum from patients with colorectal cancer, patients with colorectal adenoma and healthy controls.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **healthy controls** | **colorectal adenoma** | **colorectal cancer** |
| A | 0.66 | 0.46 | 0.39 |
| m1A | 64.70 | 77.32 | 105.85 |
| m6A | 16.62 | 21.43 | 40.09 |
| m5U | 225.57 | 210.47 | 206.68 |
| m3U | 29.23 | 28.80 | 51.31 |
| U | 4803.45 | 4634.80 | 4377.36 |
| Um | 31.17 | 24.17 | 10.72 |
| m2G | 14.04 | 13.85 | 9.67 |
| m1G | 25.87 | 24.66 | 25.06 |
| Gm | 14.80 | 13.18 | 11.09 |
| Cm | 25.69 | 26.89 | 24.75 |

**Fig. S1.** Identification of m3U, Gm, m1G and m2G in human serum. Representative MRM chromatograms of m3U, Gm, m1G, and m2G (A) in a serum sample, and (B) standard.