**Efficient analysis of small molecules via laser desorption/ionization time-of-flight mass spectrometry (LDI–TOF MS) using gold nanoshells with nanogaps**

Noori Kim 1,+, Yoon-Hee Kim 1,+, Jin Yoo 1, Seung-min Park 2, Bong-Hyun Jun 1,\*, and Woon-Seok Yeo 1,\*

a Department of Bioscience and Biotechnology, Konkuk University, Seoul 05029, Republic of Korea

b Department of Urology, Stanford University School of Medicine, Stanford, 94305, United States

+ N. Kim and Y.-H. Kim contributed equally to this work.

\* Corresponding authors.

*E-mail addresses:* bjun@konkuk.ac.kr (B.-H. Jun), wsyeo@konkuk.ac.kr (W.-S. Yeo)

**차트이(가) 표시된 사진

자동 생성된 설명**

**Figure S1**. Absorption spectra of SiO2@Au NGS prepared with different concentration of gold precursor (0, 0.5, 1.0, 1.5, and 2.0 mM Au3+).

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**Figure S2**. Signal variation of cellobiose. The spectra were obtained from 25 different sample spots using SiO2@Au NGS2.0. The solution of cellobiose (100 μΜ) was serial diluted with SiO2@Au NGS2.0 to become 100 pmole in 1 μL on the target plate.

**Table S1.** Detailed peak assignments for mass spectra in Fig. 2.

a. Serine

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | **0** | **0.5** | **1.0** | **1.5** | **2.0** |
| [M+H]+  (intens.) | |  |  |  | 105.947  (103.99) | 105.960  (228.63) |
| [M+Na]+  (intens.) | |  | 127.953  (77.15) | 127.960  (135.46) | 127.953  (137.66) | 127.970  (540.94) |
| [M+K]+ (intens.) | |  | 143.940  (31.20) | 143.951  (50.62) | 143.941  (46.75) | 143.95  (151.88) |

b. Mannitol

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | **0** | **0.5** | **1.0** | **1.5** | **2.0** |
| [M+H]+  (intens.) | |  |  |  |  |  |
| [M+Na]+  (intens.) | |  |  | 205.138  (153.56) | 205.126  (90.21) | 205.083  (2259.55) |
| [M+K]+ (intens.) | |  |  |  | 221.112  (42.29) | 221.056  (1003.41) |

c. quercetin

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | **0** | **0.5** | **1.0** | **1.5** | **2.0** |
| [M+H]+  (intens.) | | 303.178  (7849.84) | 303.086  (4640.69) | 303.097  (1378.87) | 303.096  (2187.50) | 303.104  (2442.22) |
| [M+Na]+  (intens.) | | 325.112  (108.22) | 325.050  (277.99) | 325.064  (280.27) | 325.059  (248.51) | 325.064  (245.79) |
| [M+K]+ (intens.) | | 341.118  (408.70) | 341.050  (176.34) | 341.064  (5157.73) | 341.061  (1175.17) | 341.074  (1389.15) |

d. penta(ethylene glycol)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | **0** | **0.5** | **1.0** | **1.5** | **2.0** |
| [M+H]+  (intens.) | |  |  |  |  |  |
| [M+Na]+  (intens.) | |  | 261.393  (66.88) | 261.303  (1613.38) | 261.337  (889.41) | 261.345  (9112.91) |
| [M+K]+ (intens.) | |  | 277.386  (38.49) | 277.397  (889.03) | 277.326  (429.51) | 277.327  (4166.70) |

**Table S2.** Detailed peak assignments for mass spectra in Fig. 3.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Analyte** | | **[M+H]+** | **[M+Na]+** | **[M+K]+** |
| Amino Acid | Aspartic acid | 133.924  (493.68) | 155.915  (893.81) | 171.895  (499.65) |
| Glutamic acid | 147.982  (2064.82) | 169.973  (149.77) | 185.955  (55.46) |
| Glutamine | 146.975  (69.8) | 168.969  (330.7) | 184.950  (193.1) |
| Oligo Ethylene  Glycol, | Tri(ethylene glycol) | 151.058  (316.71) | 173.200  (3822.80) | 189.189  (1550.37) |
| tetra(ethylene glycol) |  | 217.316  (4850.78) | 233.303  (1439.47) |
| Sugar | Mannitol |  | 205.083  (2259.55) | 221.056  (1003.41) |
| Galactose |  | 203.079  (2580.23) | 219.211  (133.95) |
| Flavonoid | Quercetin | 303.096  (2187.50) | 325.059  (248.51) | 341.061  (1175.17) |
| kaempferol | 287.092  (17905.57) | 309.046  (3220.18) | 325.083  (7918.13) |

**Table S3.** Detailed peak assignments for mass spectra in Fig. 4.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Mixed analyte** | | **[M+H]+** | **[M+Na]+** | **[M+K]+** |
| Mixed Amino Acid | Glutamine |  | 169.044  (76.85) | 185.039  (79.78) |
| Histidine | 156.054  (117.43) | 178.063  (257.97) | 194.047  (140.88) |
| Arginine | 175.116  (416.62) |  |  |
| Mixed Oligo Ethylene Glycol | Tri(ethylene glycol) |  | 173.097  (805.15) | 189.082  (176.55) |
| Tetra(ethylene glycol) |  | 217.172  (2641.89) | 233.154  (660.77) |
| Penta(ethylene glycol) |  | 261.236  (3291.96) | 277.211  (992.08) |
| Mixed  Sugar | Galactose | 180.830  (81.30) | 202.982  (345.46 | 218.965  (28.02) |
| Mannitol |  | 205.007  (805.28) | 220.985  (100.91) |
| Cellobiose |  | 365.068  (1289.41) |  |
| Mixed  Small molecules | Tryptophan |  | 226.998  (151.15) |  |
| Quercetin |  | 302.994  (719.32) | 340.942  (344.31) |
| Cellobiose |  | 365.049  (2182.82) |  |