Supporting information

Accurate identification of degraded products of Aflatoxin B₁ under UV Irradiation based on UPLC-Q-TOF-MS/MS and NMR analysis

Yan-Duo Wang¹, Cheng-Gang Song², Jian Yang³, Tao Zhou⁴, Yu-Yang Zhao³, Jian-Chun Qin², Lan-Ping Guo³, Gang Ding¹

¹Key Laboratory of Bioactive Substances and Resources Utilization of Chinese Herbal Medicine, Ministry of Education, Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100193, People’s Republic of China.
²College of Plant Sciences, Jilin University, Changchun, Jilin 130062, People’s Republic of China.
³State Key Laboratory Breeding Base of Dao-di Herbs, National Resource Center for Chinese Materia Medica, China Academy of Chinese Medical Sciences, Beijing 100700, People’s Republic of China.
⁴Guizhou University of Traditional Chinese Medicine, Guiyang, Guizhou 550025, People’s Republic of China.

†These authors have contributed equally to this work and share the first authorship.
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**Table S1** Mass accuracy measurement of 10 degraded products of aflatoxin B₁ in methanol solvent, using UPLC-Q-TOF-MS/MS.

| Retention time (min) | Experimental mass (m/z) | Theoretical mass (m/z) | Elemental composition | Error mDa | Error ppm | DBE | Scores (%) |
|----------------------|-------------------------|------------------------|----------------------|-----------|-----------|-----|------------|
| 4.47                 | 361.0912                | 361.0923               | C₁₈H₁₇O₈             | -1.1      | -3.0      | 11  | 100        |
| 4.70                 | 345.0960                | 345.0974               | C₁₈H₁₇O₇             | -1.4      | -4.1      | 11  | 98.74      |
| 4.82                 | 361.0905                | 361.0923               | C₁₈H₁₇O₈             | -1.8      | -5.0      | 11  | 99.29      |
| 4.93                 | 359.1118                | 359.1131               | C₁₉H₁₉O₇             | -1.3      | -3.6      | 11  | 97.72      |
| 5.40                 | 345.0963                | 345.0974               | C₁₈H₁₇O₇             | -1.1      | -3.2      | 11  | 99.70      |
| 5.84                 | 345.0971                | 345.0974               | C₁₈H₁₉O₇             | 0.3       | 0.9       | 11  | 100        |
| 5.99                 | 345.0963                | 345.0974               | C₁₈H₁₇O₇             | -1.1      | -3.2      | 11  | 86.77      |
| 6.41                 | 391.1380                | 391.1393               | C₂₀H₂₁O₈             | -1.3      | -3.3      | 10  | 99.18      |
| 7.08                 | 359.1127                | 359.1131               | C₁₉H₁₉O₇             | -0.4      | -0.9      | 11  | 100        |
| 7.30                 | 359.1121                | 359.1131               | C₁₉H₁₉O₇             | -1.0      | -2.8      | 11  | 98.97      |

**Table S2** Mass accuracy measurement of 7 degraded products of aflatoxin B₁ in acetone solvent, using UPLC-Q-TOF-MS/MS.

| Retention time (min) | Experimental mass (m/z) | Theoretical mass (m/z) | Elemental composition | Error mDa | Error ppm | DBE | Scores (%) |
|----------------------|-------------------------|------------------------|----------------------|-----------|-----------|-----|------------|
| 3.48                 | 347.0758                | 347.0767               | C₁₇H₁₅O₈             | 0.9       | 2.6       | 11  | 99.13      |
| 4.06                 | 331.0805                | 331.0818               | C₁₇H₁₅O₇             | 1.3       | 3.9       | 11  | 54.98      |
| 4.18                 | 331.0801                | 331.0818               | C₁₇H₁₅O₇             | 1.7       | 5.1       | 11  | 79.61      |
| 4.34                 | 371.1112                | 371.1131               | C₂₀H₂₁O₈             | 1.9       | 5.1       | 12  | 98.58      |
| 4.86                 | 401.1224                | 401.1236               | C₂₀H₂₁O₇             | 1.2       | 3.0       | 12  | 100        |
| 5.63                 | 371.1121                | 371.1131               | C₂₀H₂₁O₇             | 1.0       | 2.7       | 12  | 99.33      |
| 6.53                 | 401.1221                | 401.1236               | C₂₁H₂₁O₈             | 1.5       | 3.7       | 12  | 100        |
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$m/z \ 361, \ t_R = 4.47 \ min$

$1: \ TOF \ MS \ ES^+ \ 361.0912 \ 2.87e5$

$m/z \ 361, \ t_R = 4.82 \ min$

$1: \ TOF \ MS \ ES^+ \ 361.0905 \ 1.12e6$
Figure S4 Analysis of degraded products structures based on HR-ESI and MS/MS data at m/z 359, t_R = 4.94 min, 7.08 min and 7.30 min.
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$m/z$ 371, $t_R = 5.63$ min

$1: \text{TOF MS ES}^+$

7.70e3

273.0743

271.0581

259.0582

257.0785

256.1534

269.0783

261.0754

264.1920

261.1521

264.1920

261.1521

278.1734

274.0793

275.0527

$5.25e6$

371.1121

289.0694

285.0749

313.0696

290.0731

353.1009

345.0953

320.1839

369.0960

372.1147

373.1172

$1: \text{TOF MS ES}^+$

371.1121

5.25e6
Figure S9 Analysis of degraded products structures based on HR-ESI and MS/MS data at $m/z$ 401, $t_R = 4.86$ min and 6.54 min.
$m/z$ 401, $t_R = 4.86$ min

$1: \text{TOF MS ES}^+$

$1.50e4$

$283.0601$

$275.0545$

$287.0538$

$289.0704$

$290.0706$

$369.0967$

$m/z$ 401, $t_R = 6.54$ min

$1: \text{TOF MS ES}^+$

$9.87e3$

$283.0588$

$285.0743$

$287.0546$

$289.0699$

$297.0749$

$313.0699$

$315.0851$

$343.0803$

$351.0854$

$361.0912$

$370.0998$

$389.1223$

$401.1224$

$402.1258$

$m/z$ 401, $t_R = 6.54$ min

$2.80e5$

$283.0586$

$289.0699$

$315.0837$

$319.0736$

$327.0850$

$343.0803$

$351.0854$

$370.0992$

$376.1106$

$401.1221$

$402.1256$
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