

洋金花种子的化学成分研究（I）

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摘要：目的 研究洋金花 *Datura metel* 种子的化学成分。方法 采用硅胶、ODS、Sephadex LH-20 及 HPLC 等色谱方法分离化合物，利用 NMR、MS 波谱学方法鉴定其结构。结果 从洋金花种子 95%乙醇回流提取物的醋酸乙酯部位分离得到 11 个化合物，分别鉴定为大麻酰胺 D（1）、大麻酰胺 E（2）、顺式-大麻酰胺 E（3）、大麻酰胺 F（4）、大麻酰胺 L（5）、大麻酰胺 G（6）、大海米菊酰胺 K（7）、莨菪内半缩醛（8）、曼陀罗醇酮（9）、N-trans-feruloyl tryptamine（10）、秦皮素（11）。结论 化合物 2、4 为首次从茄科植物中分离得到，1、3、5~7 为首次从该属中分离得到，8~11 位首次从该植物中分离得到。

关键词： 洋金花；大麻酰胺 E；大麻酰胺 F；曼陀罗醇酮；秦皮素

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Chemical constituents from seeds of *Datura metel* (I)

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Abstract: Objective To study the chemical constituents in the seeds of *Datura metel*. **Methods** The constituents were isolated and purified by silica gel, ODS, and Sephadex LH-20 column chromatographies as well as HPLC. Their chemical structures were elucidated on the basis of spectral data. **Results** The compounds were isolated from the EtOAc fraction of *D. metel* extract and identified as cannabisin D (1), cannabisin E (2), cis-cannabisin E (3), cannabisin F (4), cannabisin L (5), cannabisin G (6), grossamide K (7), hyoscyamilactol (8), daturaolone (9), N-trans-feruloyl tryptamine (10), and fraxetin (11), respectively. **Conclusion** Compounds 2 and 4 are firstly isolated from the plants in Solanaceae, compounds 1, 3, and 5~7 are firstly isolated from the plants in genus *Datura* L. and compounds 8~11 are isolated from this plant for the first time.

Key words: *Datura metel* L.; cannabisin E; cannabisin F; daturaolone; fraxetin

洋金花 *Datura metel* L. 为茄科 (Solanaceae) 曼陀罗属植物，又名曼陀罗花、风茄花和白曼陀罗。《中国药典》2010 年版记载其性温、味辛，有毒。其生理活性较强，具有平喘止咳、解痉镇痛之功效，主要用于哮喘咳嗽、脘腹冷痛、风湿痹痛和外科麻醉^[1]。在民间，洋金花种子也入药使用。但关于洋金花种子的各方面研究报道却很罕见，化学成分方面甚少。为了合理开发该药用资源，明确其药效物质基础，本实验对洋金花种子的化学成分进行了较系统的研究，从洋金花种子 95%乙醇提取物的醋酸乙酯部位中分离得到 11 个化合物，分别鉴定为大麻酰胺 D (cannabisin D, 1)、大麻酰胺 E (cannabisin

E, 2)、顺式-大麻酰胺 E (cis-cannabisin E, 3)、大麻酰胺 F (cannabisin F, 4)、大麻酰胺 L (cannabisin L, 5)、大麻酰胺 G (cannabisin G, 6)、大海米菊酰胺 K (grossamide K, 7)、莨菪内半缩醛 (hyoscyamilactol, 8)、曼陀罗醇酮 (daturaolone, 9)、N-trans-feruloyl tryptamine (10)、秦皮素 (fraxetin, 11)。化合物 2、4 为首次从茄科植物中分离得到，化合物 1、3、5~7 为首次从该属植物中分离得到，化合物 8~11 为首次从该植物中分离得到。

1 仪器与材料

Bruker—400 超导核磁共振光谱仪 (Bruker 公司); Acquity Ultra Performance LCTM 液质联用色谱

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仪; Delta 600—2487型制备HPLC(美国Water公司); 2695—2996型分析HPLC(美国Water公司); Waters C₁₈(250 mm×4.6 mm, 5 μm)分析型色谱柱; Waters C₁₈(250 mm×19 mm, 10 μm)制备型色谱柱; 柱色谱用硅胶为青岛海洋化工产品; 柱色谱反相ODS-AM(日本YMC公司); TLC用硅胶板(Silicagel60 F254)和RP₁₈反相板均为德国Merck公司产品; 所用试剂均为分析纯(北京化工厂)。

洋金花种子采收于黑龙江中医药大学药用植物园, 经黑龙江中医药大学药学院中药资源教研室王振月教授鉴定为茄科曼陀罗属植物洋金花 *Datura metel* L. 的种子。原植物标本(2010035)保存于黑龙江中医药大学中药化学教研室。

2 提取与分离

干燥粉碎的洋金花种子(30 kg)用95%乙醇回流提取3次,每次2.5 h,减压回收溶剂,得提取物1.38 kg。提取物与水混悬均匀,依次用石油醚、醋酸乙酯、水饱和正丁醇萃取。醋酸乙酯部分(100 g)经正相硅胶柱色谱,氯仿-甲醇系统梯度洗脱,得到6个部分。二氯甲烷-甲醇(10:1)洗脱部分经反复柱色谱硅胶,并结合ODS、制备型HPLC纯化得到化合物**1**(9 mg)、**2**(11 mg)、**3**(8 mg)、**4**(11 mg)、**5**(7 mg)、**6**(9 mg)、**7**(12 mg); 二氯甲烷-甲醇(30:1)洗脱部分,反复硅胶柱色谱并结合Sephadex LH-20色谱纯化得到化合物**8**(12 mg)、**9**(10 mg); 二氯甲烷-甲醇(7:1)洗脱部分经反复硅胶柱色谱并结合ODS、Sephadex LH-20纯化得到化合物**10**(300 mg)、**11**(9 mg)。

3 结构鉴定

化合物**1**: 不定形粉末(甲醇),分子式为C₃₆H₃₄N₂O₈, ESI-MS m/z: 625 [M+H]⁺. ¹H-NMR(400 MHz, CD₃OD) δ: 6.88 (1H, s, H-2), 6.51 (1H, s, H-5), 7.20 (1H, s, H-7), 6.69 (1H, d, J = 1.9 Hz, H-2'), 6.77 (2H, d, J = 8.2 Hz, H-5'), 6.40 (1H, dd, J = 1.9, 8.2 Hz, H-6'), 4.33 (1H, d, J = 8.2 Hz, H-7'), 3.68 (1H, d, J = 4.1 Hz, H-8'), 6.97 (2H, d, J = 8.5 Hz, H-2'', 6''), 6.63 (2H, d, J = 8.5 Hz, H-3'', 5''), 3.35 (2H, m, H-α''), 2.69 (2H, m, H-β''), 6.81 (2H, d, J = 8.5 Hz, H-2'', 6''), 6.63 (2H, d, J = 8.5 Hz, H-3'', 5''), 3.22 (2H, m, H-α''), 2.46 (2H, m, H-β''), 3.89 (3H, s, 3-OCH₃), 3.74 (3H, s, 3'-OCH₃); ¹³C-NMR(100 MHz, CD₃OD) δ: 124.9 (C-1), 113.2 (C-2), 148.2 (C-3), 148.9 (C-4), 117.2 (C-5), 132.6 (C-6), 134.7

(C-7), 127.6 (C-8), 170.4 (C-9), 135.9 (C-1'), 112.5 (C-2'), 149.6 (C-3'), 149.3 (C-4'), 116.0 (C-5'), 121.4 (C-6'), 47.6 (C-7'), 51.0 (C-8'), 174.6 (C-9'), 131.4 (C-1''), 130.8 (C-2'', 6''), 116.2 (C-3'', 5''), 156.9 (C-4''), 42.7 (C-α''), 35.7 (C-β''), 131.2 (C-1'''), 130.7 (C-2''', 6'''), 116.2 (C-3''', 5'''), 156.8 (C-4'''), 42.4 (C-α'''), 35.5 (C-β'''), 56.6 (3-OCH₃), 56.3 (3'-OCH₃)。以上数据与文献报道基本一致^[2], 故鉴定化合物**1**为大麻酰胺D。

化合物**2**: 不定形粉末(甲醇),分子式为C₃₆H₃₈N₂O₉, ESI-MS m/z: 643 [M+H]⁺. ¹H-NMR(400 MHz, CD₃OD) δ: 7.06 (1H, s, H-2), 6.77 (1H, d, J = 8.1 Hz, H-5), 6.84 (1H, dd, J = 1.6, 8.1 Hz, H-6), 4.76 (1H, d, J = 4.2 Hz, H-7), 5.10 (1H, d, J = 4.2 Hz, H-8), 7.14 (1H, d, J = 1.6 Hz, H-2'), 6.95 (1H, d, J = 8.2 Hz, H-5'), 7.00 (1H, d, J = 8.4 Hz, H-6'), 7.43 (1H, d, J = 15.7 Hz, H-7'), 6.46 (1H, d, J = 15.7 Hz, H-8'), 7.30 (2H, d, J = 8.5 Hz, H-2'', 6''), 6.71 (2H, dd, J = 3.3, 8.5 Hz, H-3'', 5''), 3.15 (2H, m, H-α''), 2.52 (2H, m, H-β''), 6.71 (2H, dd, J = 3.3, 8.5 Hz, H-2''', 6''), 6.61 (2H, d, J = 8.5 Hz, H-3''', 5''), 3.22 (2H, t, J = 7.3 Hz, H-α'''), 2.73 (2H, t, J = 7.3 Hz, H-β'''), 3.62 (3H, s, 3-OCH₃), 3.83 (3H, s, 3'-OCH₃); ¹³C-NMR(100 MHz, CD₃OD) δ: 132.3 (C-1), 112.3 (C-2), 148.7 (C-3), 147.5 (C-4), 115.5 (C-5), 121.7 (C-6), 75.3 (C-7), 86.4 (C-8), 171.4 (C-9), 131.5 (C-1'), 112.6 (C-2'), 151.5 (C-3'), 150.4 (C-4'), 118.2 (C-5'), 122.7 (C-6'), 141.4 (C-7'), 120.8 (C-8'), 168.8 (C-9'), 130.9 (C-1''), 130.8 (C-2'', 6''), 116.3 (C-3'', 5''), 156.9 (C-4''), 41.7 (C-α''), 35.5 (C-β''), 131.3 (C-1'''), 130.8 (C-2''', 6''), 116.4 (C-3''', 5''), 156.8 (C-4'''), 42.6 (C-α'''), 35.8 (C-β'''), 56.4 (3-OCH₃), 56.5 (3'-OCH₃)。以上数据与文献报道基本一致^[2], 故鉴定化合物**2**为大麻酰胺E。

化合物**3**: 不定形粉末(甲醇),分子式为C₃₆H₃₈N₂O₉, ESI-MS m/z: 643 [M+H]⁺. ¹H-NMR(400 MHz, CD₃OD) δ: 7.09 (1H, d, J = 1.9 Hz, H-2), 6.77 (1H, d, J = 8.2 Hz, H-5), 6.88 (1H, dd, J = 1.9, 8.2 Hz, H-6), 5.14 (1H, d, J = 3.5 Hz, H-7), 5.10 (1H, d, J = 3.5 Hz, H-8), 7.10 (1H, d, J = 1.7 Hz, H-2'), 6.37 (1H, d, J = 8.4 Hz, H-5'), 6.92 (1H, dd, J = 1.7, 8.4 Hz, H-6'), 7.40 (1H, d, J = 15.7 Hz, H-7'), 6.44 (1H, d, J = 15.7 Hz, H-8'), 7.04 (2H, d, J = 8.5 Hz,

H-2'', 6''), 6.71 (2H, d, $J = 8.5$ Hz, H-3'', 5''), 2.73 (2H, t, $J = 7.3$ Hz H-7''), 3.45 (2H, t, $J = 7.3$ Hz, H-8''), 6.88 (2H, d, $J = 8.4$ Hz, H-2'', 6''), 6.61 (2H, d, $J = 8.4$ Hz, H-3'', 5''), 2.58 (2H, m H-7''), 3.40 (1H, m, H-8''), 3.32 (1H, m, H-8''), 3.79 (3H, s, 3-OCH₃), 3.76 (3H, s, 3'-OCH₃); ¹³C-NMR (100 MHz, CD₃OD) δ : 133.4 (C-1), 111.7 (C-2), 149.0 (C-3), 147.3 (C-4), 116.0 (C-5), 120.6 (C-6), 75.1 (C-7), 87 (C-8), 171.6 (C-9), 131.5 (C-1'), 112.2 (C-2'), 151.4 (C-3'), 150.2 (C-4'), 117.8 (C-5'), 122.4 (C-6'), 141.2 (C-7'), 120.8 (C-8'), 168.8 (C-9'), 131.0 (C-1''), 130.8 (C-2'', 6''), 116.3 (C-3'', 5''), 156.9 (C-4''), 35.5 (C-7''), 42.1 (C-8''), 131.3 (C-1''), 130.8 (C-2'', 6''), 116.4 (C-3'', 5''), 156.8 (C-4''), 35.8 (C-7''), 42.6 (C-8''), 56.4 (3-OCH₃), 56.4 (3'-OCH₃)。以上数据与文献报道基本一致^[3], 故鉴定化合物 3 为顺式-大麻酰胺 E。

化合物 4: 不定形粉末(甲醇), 分子式为 C₃₆H₃₆N₂O₉, ESI-MS m/z : 625 [M+H]⁺。¹H-NMR (400 MHz, CD₃OD) δ : 7.18 (1H, d, $J = 1.5$ Hz, H-2), 6.68 (1H, d, $J = 8.4$ Hz, H-5), 6.96 (1H, dd, $J = 1.5$, 8.4 Hz, H-6), 7.24 (1H, s, H-7), 7.24 (1H, s, H-2'), 6.71 (1H, d, $J = 8.4$ Hz, H-5'), 7.03 (1H, d, $J = 8.4$ Hz, H-6'), 7.44 (1H, d, $J = 15.7$ Hz, H-7'), 6.48 (1H, d, $J = 15.7$ Hz, H-8'), 7.03 (2H, d, $J = 8.4$ Hz, H-2'', 6''), 6.58 (2H, d, $J = 8.4$ Hz, H-3'', 5''), 3.43 (2H, t, $J = 6.8$ Hz, H- α'''), 2.60 (2H, t, $J = 6.8$ Hz, H- β'''), 6.80 (2H, d, $J = 8.4$ Hz, H-2'', 6''), 6.71 (2H, d, $J = 8.4$ Hz, H-3'', 5''), 3.45 (2H, t, $J = 7.3$ Hz, H- α'''), 2.73 (2H, t, $J = 7.3$ Hz, H- β'''), 3.61 (3H, s, 3-OCH₃), 3.83 (3H, s, 3'-OCH₃); ¹³C-NMR (100 MHz, CD₃OD) δ : 125.5 (C-1), 112.5 (C-2), 148.9 (C-3), 147.5 (C-4), 115.2 (C-5), 121.0 (C-6), 125.5 (C-7), 141.4 (C-8), 168.8 (C-9), 131.8 (C-1'), 113.7 (C-2'), 150.4 (C-3'), 149.5 (C-4'), 116.3 (C-5'), 126.4 (C-6'), 141.2 (C-7'), 122.4 (C-8'), 165.5 (C-9'), 130.9 (C-1''), 130.7 (C-2'', 6''), 116.4 (C-3'', 5''), 156.9 (C-4''), 42.3 (C- α''), 35.6 (C- β''), 131.3 (C-1''), 130.7 (C-2'', 6''), 116.3 (C-3'', 5''), 156.8 (C-4''), 42.6 (C- α''), 35.8 (C- β''), 56.1 (3-OCH₃), 56.4 (3'-OCH₃)。以上数据与文献报道基本一致^[4], 故鉴定化合物 4 为大麻酰胺 F。

化合物 5: 不定形粉末(甲醇), 分子式为 C₃₆H₃₄N₂O₁₀, ESI-MS m/z : 654 [M+H]⁺。¹H-NMR (400 MHz, CD₃OD) δ : 6.98 (1H, d, $J = 5.1$ Hz, H-2),

6.86 (1H, d, $J = 5.2$ Hz, H-5), 6.88 (1H, d, $J = 5.2$ Hz, H-6), 7.57 (1H, d, $J = 1.8$ Hz, H-2'), 6.96 (1H, dd, $J = 1.8$, 8.3 Hz, H-5'), 7.45 (1H, dd, $J = 1.8$, 8.3 Hz, H-6'), 6.77 (2H, d, $J = 8.5$ Hz, H-2'', 6''), 6.64 (2H, d, $J = 4.6$ Hz, H-3'', 5''), 2.44 (2H, t, $J = 6.5$ Hz, H-7''), 3.25 (2H, t, $J = 6.5$ Hz, H-8''), 6.83 (2H, d, $J = 8.5$ Hz, H-2'', 6''), 6.62 (2H, d, $J = 4.7$ Hz, H-3'', 5''), 2.67 (1H, m, H-7''), 2.33 (1H, m, H-7''), 3.18 (1H, m, H-8''), 3.35 (1H, m, H-8''), 3.91 (3H, s, 3-OCH₃), 3.82 (3H, s, 3'-OCH₃); ¹³C-NMR (100 MHz, CD₃OD) δ : 129.6 (C-1), 110.2 (C-2), 149.5 (C-3), 148.8 (C-4), 116.0 (C-5), 116.8 (C-6), 91.7 (C-7), 140.6 (C-8), 161.7 (C-9), 128.0 (C-1'), 111.9 (C-2'), 149.6 (C-3'), 154.9 (C-4'), 119.9 (C-5'), 127.0 (C-6'), 191.2 (C-7'), 150.8 (C-8'), 167.3 (C-9'), 130.8 (C-1''), 130.6 (C-2'', 6''), 116.4 (C-3'', 5''), 157.0 (C-4''), 35.2 (C-7''), 41.9 (C-8''), 130.5 (C-1''), 130.5 (C-2'', 6''), 116.2 (C-3'', 5''), 157.0 (C-4''), 34.7 (C-7''), 42.5 (C-8''), 56.5 (3-OCH₃), 56.5 (3'-OCH₃)。以上数据与文献报道基本一致^[3], 故鉴定化合物 5 为大麻酰胺 L。

化合物 6: 白色不定形粉末(甲醇), 分子式为 C₃₆H₃₆N₂O₈, ESI-MS m/z : 624 [M+H]⁺。¹H-NMR (400 MHz, CD₃OD) δ : 7.16 (1H, d, $J = 5.1$ Hz, H-2, 2'), 6.78 (1H, d, $J = 5.2$ Hz, H-5, 5'), 7.02 (2H, d, $J = 5.2$ Hz, H-6, 6'), 7.84 (2H, s, H-9, 9'), 6.78 (4H, dd, $J = 2.8$, 8.4 Hz, H-2'', 6'', 2'', 6''), 6.61 (4H, dd, $J = 1.8$, 6.6 Hz, H-3'', 5'', 3'', 5''), 3.17 (2H, m, H- β'' , β'''), 3.40 (2H, m, H- α'' , α'''), 2.44 (2H, m, H- β'' , β'''), 2.34 (2H, m, H- β'' , β'''), 3.72 (6H, s, OCH₃-3, 3'); ¹³C-NMR (100 MHz, CD₃OD) δ : 128.0 (C-1, 1'), 113.5 (C-2, 2'), 149.1 (C-3, 3'), 150.0 (C-4, 4'), 116.5 (C-5, 5'), 126.3 (C-6, 6'), 167.9 (C-7, 7'), 127.2 (C-8, 8'), 142.2 (C-9, 9'), 131.1 (C-1'', 1''), 130.6 (C-2'', 6'', 2'', 6''), 116.3 (C-3'', 5'', 3'', 5''), 156.8 (C-4', 4''), 41.9 (C- α'' , α'''), 35.5 (C- β'' , β'''), 56.3 (3, 3'-OCH₃)。以上数据与文献报道基本一致^[2], 故鉴定化合物 6 为大麻酰胺 G。

化合物 7: 不定形粉末(甲醇), 分子式为 C₂₈H₂₉NO₇, ESI-MS m/z : 492 [M+H]⁺。¹H-NMR (400 MHz, CD₃OD) δ : 5.55 (1H, d, $J = 6.4$ Hz, H-2), 3.52 (1H, q, $J = 6.4$ Hz, H-3), 7.14 (1H, s, H-4), 7.07 (1H, d, $J = 1.2$ Hz, H-6), 6.94 (1H, d, $J = 1.8$ Hz, H-2'), 6.76 (1H, d, $J = 8.2$ Hz, H-5'), 6.82 (1H, dd, $J =$

1.8, 8.2 Hz, H-6'), 3.82 (2H, m, H-1"), 7.46 (1H, d, $J = 15.7$ Hz, H-1''), 6.42 (1H, d, $J = 15.7$ Hz, H-2'''), 3.45 (2H, t, $J = 7.3$ Hz, H-1''''), 2.74 (2H, t, $J = 7.3$ Hz, H-2'''''), 7.04 (2H, d, $J = 8.5$ Hz, H-2'''''', 6'''''), 6.71 (2H, d, $J = 8.5$ Hz, H-3'''''', 5'''''); ^{13}C -NMR (100 MHz, CD₃OD) δ : 88.7 (C-2), 54.9 (C-3), 118.5 (C-4), 130.3 (C-5), 113.3 (C-6), 145.8 (C-7), 151.3 (C-8), 130.9 (C-9), 134.2 (C-1'), 110.6 (C-2'), 149.2 (C-3'), 147.7 (C-4'), 116.2 (C-5'), 119.8 (C-6'), 64.7 (C-1''), 142.0 (C-1''), 119.8 (C-2''), 42.6 (C-1'''), 35.8 (C-2''''), 130.9 (C-1'''''), 130.7 (C-2''''', 6'''''), 116.3 (C-3''''', 5'''''), 157.0 (C-4'''''), 56.8 (7-OCH₃), 56.4 (3'-OCH₃), 169.1 (-CONH-)。以上数据与文献报道基本一致^[5], 故鉴定化合物 7 为大海米菊酰胺 K。

化合物 8: 白色不定形粉末(甲醇), 分子式为 C₂₈H₄₀O₆, ESI-MS m/z : 495 [M+Na]⁺。 ^{13}C -NMR (100 MHz, CD₃OD) δ : 203.3 (C-1), 129.0 (C-2), 139.6 (C-3), 36.7 (C-4), 73.3 (C-5), 56.3 (C-6), 57.3 (C-7), 35.7 (C-8), 35.5 (C-9), 51.0 (C-10), 21.9 (C-11), 39.9 (C-12), 43.4 (C-13), 51.3 (C-14), 23.5 (C-15), 27.2 (C-16), 52.4 (C-17), 12.1 (C-18), 14.7 (C-19), 39.1 (C-20), 12.6 (C-21), 65.0 (C-22), 29.3 (C-23), 63.8 (C-24), 65.3 (C-25), 91.8 (C-26), 16.6 (C-27), 19.0 (C-28)。以上数据与文献报道基本一致^[6], 故鉴定化合物 8 为莨菪内半缩醛。

化合物 9: 无色针状结晶(甲醇), 分子式为 C₃₀H₄₀O₂, ESI-MS m/z : 441 [M+H]⁺。 ^{13}C -NMR (100 MHz, CD₃OD) δ : 42.0 (C-1), 34.8 (C-2), 215.6 (C-3), 49.3 (C-4), 56.9 (C-5), 34.9 (C-6), 68.2 (C-7), 39.6 (C-8), 36.8 (C-9), 24.0 (C-10), 21.9 (C-11), 122.5 (C-12), 144.7 (C-13), 42.6 (C-14), 26.5 (C-15), 27.2 (C-16), 32.8 (C-17), 47.6 (C-18), 47.0 (C-19), 31.2 (C-20), 34.9 (C-21), 37.4 (C-22), 24.2 (C-23), 25.9 (C-24), 16.5 (C-25), 18.6 (C-26), 26.3 (C-27), 28.6 (C-28), 33.5 (C-29), 23.8 (C-30)。以上数据与文献报道基本一致^[7], 故鉴定化合物 9 为曼陀罗醇酮。

化合物 10: 白色针状结晶(甲醇), 分子式为 C₁₈H₁₉NO₄, ESI-MS m/z : 314 [M+H]⁺。 ^{13}C -NMR

(100 MHz, CD₃OD) δ : 128.3 (C-1), 111.5 (C-2), 149.3 (C-3), 149.8 (C-4), 116.5 (C-5), 118.8 (C-6), 142.0 (C-7), 123.2 (C-8), 169.2 (C-9), 131.3 (C-1'), 130.7 (C-2', 6'), 116.3 (C-3', 5'), 156.9 (C-4'), 35.8 (C-7'), 42.6 (C-8')⁵, 56.4 (3-OCH₃)。以上数据与文献报道基本一致^[8], 故鉴定化合物 10 为 N-trans-feruloyl tryptamine。

化合物 11: 白色片状结晶(甲醇), 分子式为 C₁₀H₈O₅, ESI-MS m/z : 209 [M+H]⁺。 ^{13}C -NMR (100 MHz, CD₃OD) δ : 163.7 (C-2), 112.7 (C-3), 146.8 (C-4), 101.0 (C-5), 147.1 (C-6), 140.7 (C-7), 134.1 (C-8), 140.6 (C-9), 112.2 (C-10)。以上数据与文献报道基本一致^[9], 故鉴定化合物 11 为秦皮素。

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