

的直链状的 α -(1 $\rightarrow$ 6)结合的葡聚糖 细脚拟青霉多糖 I 的生理活性正在研究之中。

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大蒜有机硫化合物的研究

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摘要:目的 对大蒜 *Allium sativum* 的有机硫化合物进行了研究 方法 利用硅胶柱层析、硅胶薄层层析、高效液相色谱进行分离, 根据化合物的光谱数据鉴定其结构。结果 从大蒜环己烷提取物中分得 9 个化合物, 分别鉴定为 Z-1, 6, 11-三烯-4, 5, 9-三硫杂十二烷-9-氧化物 (Z-ajoene, I), E-1, 6, 11-三烯-4, 5, 9-三硫杂十二烷-9-氧化物 (E-ajoene, II), Z-1, 6, 11-三烯-4, 5, 9-三硫杂十二烷-9, 9-二氧化物 (III), E-1, 6, 11-三烯-4, 5, 9-三硫杂十二烷-9, 9-二氧化物 (IV), E-1, 7, 11-三烯-4, 5, 9-三硫杂十二烷-9, 9-二氧化物 (V), Z-4, 9-二烯-2, 3, 7-三硫杂癸烷-7-氧化物 (VI), 2-乙烯基-4H-1, 3-二硫杂苯 (VII), 3-乙烯基-6H-1, 2-二硫杂苯-2-氧化物 (VIII), 2-乙烯基-4H-1, 3-二硫杂苯-3-氧化物 (IX)。结论 化合物 V, VI, VIII, IX 为新化合物。

关键词: 大蒜; 有机硫化合物; E-1, 7, 11-三烯-4, 5, 9-三硫杂十二烷-9, 9-二氧化物; Z-4, 9-二烯-2, 3, 7-三硫杂癸烷-7-氧化物; 3-乙烯基-6H-1, 2-二硫杂苯-2-氧化物; 2-乙烯基-4H-1, 3-二硫杂苯-3-氧化物

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Studies on organosulfur compounds in *Allium sativum*

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Abstract **Object** To study the organosulfur compounds in garlic (*Allium sativum* L.). **Methods** Compounds were separated by silica gel column chromatography, TLC, and HPLC. Their structures were elucidated by spectroscopic analysis. **Results** Nine compounds were isolated from the cyclohexane extracts. They were identified as Z-1, 6, 11-triene-4, 5, 9-trithiadodeca-9-oxide (Z-ajoene) (I), E-1, 6, 11-triene-4, 5, 9-trithiadodeca-9-oxide (E-ajoene) (II), Z-1, 6, 11-triene-4, 5, 9-trithiadodeca-9, 9-dioxide (III), E-1, 6, 11-triene-4, 5, 9-trithiadodeca-9, 9-dioxide (IV), E-1, 7, 11-triene-4, 5, 9-trithiadodeca-9, 9-dioxide (V), Z-4, 9-diene-2, 3, 7-trithiadeca-7-oxide (VI), 2-vinyl-4H-1, 3-dithiin (VII), 3-vinyl-6H-1, 2-dithiin-2-oxide (VIII), 2-vinyl-4H-1, 3-dithiin-3-oxide (IX). **Conclusion** Compounds V, VI, VIII, and IX were new.

Key words *Allium sativum* L.; organosulfur compounds; E-1, 7, 11-triene-4, 5, 9-trithiadodeca-9, 9-dioxide; Z-4, 9-diene-2, 3, 7-trithiadeca-7-oxide; 3-vinyl-6H-1, 2-dithiin-2-oxide; 2-vinyl-4H-1, 3-dithiin-3-oxide

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大蒜系百合科植物 *Allium sativum* L. 的鳞茎, 作为民间药物具有杀菌、抗真菌、抗原虫、抗肿瘤、降血压、抗动脉粥样硬化等作用^[1-3]。大蒜破碎后, 其所含的蒜氨酸 (alliin) 在蒜酶 (allinase) 的作用下迅速生成蒜辣素 (allicin), 蒜辣素在室温下不稳定, 易转化为阿霍烯类 (ajoenes) 及乙烯基二硫杂苯类 (vinylidithiins) 等有机硫化物^[2]。阿霍烯具有抗血小板聚集及抗肿瘤等活性^[2-5]。我们对大蒜环己烷提取物的有机硫化物进行了系统的研究, 分离得到 9 个化合物, 经光谱解析, 确定了它们的结构, 其中 V, VI, VIII, IX 为新化合物。

化合物 V: 浅黄色油状液体。FAB-MS 给出分子离子峰为 250[M⁺], 结合 ¹H NMR 和 ¹³C NMR 推出分子式为 C₆H₄S₃O₂。IR 光谱中 1 315, 1 124 cm⁻¹ 的吸收峰表明分子中存在亚砷, 2 290, 1 630, 931 cm⁻¹ 的吸收峰表明分子中有端乙烯基。¹H NMR 显示 2 个连硫的亚甲基质子, δ 3.34 (2H, d, J = 7.2 Hz), 3.42 (2H, d, J = 7.8 Hz), 1 个连砷的亚甲基质子, δ 3.74 (2H, d, J = 7.5 Hz), 1 个连砷的双键烯质子, δ 6.38 (1H, d, J = 14.7 Hz, EO₂SCH=CH), 6.84 (1H, d, t, J = 14.7, 7.8 Hz), 2 个端乙烯基质子, δ 5.23 (1H, d, J = 17.1 Hz), 5.19 (1H, d, J = 10.2 Hz), 5.42 (1H, d, J = 18.3 Hz), 5.47 (1H, d, J = 10.5 Hz), 可推测此化合物的基本结构为阿霍烯类结构。从它们的偶合情况及偶合常数看, δ: 6.38 应为 8 位质子信号, 其偶合常数 J = 14.7 Hz, 显然是与邻位质子发生偶合且为反式, 7 位质子发生了双重偶合。一偶合常数为 14.7 Hz (与 8 位质子偶合), 一偶合常数为 7.8 Hz (与 6 位质子偶合), 故此双键与砷直接相连, 受此 ππ 共轭效应影响, 7 位 H 及 7 位 C 向低场位移, 8 位 H 及 8 位 C 向高场位移, 综上所述推断此化合物的结构为 E-1, 7, 11-三烯-4, 5, 9-三硫杂十二烷-9, 9-二氧化物。其 ¹³C NMR, APT, ¹H-¹H COSY, ¹H-¹³C COSY 亦确证了它的结构及 C¹³H 归属。

化合物 VI: 无色油状液体。FAB-MS 给出分子离子峰为 209[M⁺], 结合 ¹H NMR 及 ¹³C NMR 推出分子式为 C₇H₂S₃O₂。IR 光谱中 1 043 cm⁻¹ 吸收峰表明分子中存在亚砷, 3 082, 1 633, 930 cm⁻¹ 吸收峰表明分子中存在端乙烯基。¹H NMR 显示 1 个连硫的甲基质子, δ 2.47 (3H, s), 2 个连亚砷的亚甲基质子, δ 3.47 (1H, dd, J = 13.4, 7.3 Hz), 3.55 (1H, dd, J = 13.4, 6.6 Hz), 3.61 (1H, dd, J = 13.5, 8.5 Hz), 3.68 (1H, dd, J = 13.5, 7.9 Hz), 1 个连硫的烯

质子, δ 6.64 (1H, d, J = 9.3 Hz, Z SSCH=CH), 1 个端乙烯基质子, δ 5.44 (1H, d, J = 16.5 Hz), 5.48 (1H, d, J = 9.9 Hz), 综上所述推断此化合物的结构为 Z-4, 9-二烯-2, 3, 7-三硫杂癸烷-7-氧化物。其 ¹³C NMR, APT, ¹H-¹H COSY, ¹H-¹³C COSY 亦确证了它的结构及 C¹³H 归属。

化合物 VIII: 无色油状液体。EI-MS 给出分子离子峰为 160[M⁺], 结合 ¹H NMR 和 ¹³C NMR 推出分子式为 C₆H₆S₂O。IR 光谱中 1 057 cm⁻¹ 吸收峰表明分子中存在亚砷, 3 087, 1 611, 865 cm⁻¹ 吸收峰表明分子中存在端乙烯基。¹H NMR 显示 1 个连硫的亚甲基质子, δ 3.42 (2H, m), 1 个连亚砷的次甲基质子, δ 4.60 (1H, d, J = 7.8 Hz), 1 个环内双键烯质子, δ 5.78 (1H, m), 6.31 (1H, d, J = 10.2 Hz), 1 个端乙烯基质子, δ 5.59 (1H, d, J = 16.5 Hz), 5.52 (1H, d, J = 9.6 Hz), 可推测此化合物的基本结构为乙烯基二硫杂苯类结构。¹H-¹H COSY 中显示 H-3 与 H-7, H-4 与 H-5, H-5 与 H-6 相关, ¹H-¹H NOESY 中显示 H-3 与 H-7, H-3 与 H-4, H-4 与 H-5, H-5 与 H-6 有 NOE 效应, 因 H-3 与 H-4 二平面间的夹角为 90 度, 故 H-3 与 H-4 间不发生偶合^[6]。综上所述推断此化合物的结构为 3-乙烯基-6H-1, 2-二硫杂苯-2-氧化物, 其 ¹³C NMR, APT, ¹H-¹³C COSY 亦确证了它的结构及 C¹³H 归属。

化合物 IX: 无色油状液体。EI-MS 给出分子离子峰为 160[M⁺], 结合 ¹H NMR 和 ¹³C NMR 推出分子式为 C₆H₆S₂O。IR 光谱中 1 050 cm⁻¹ 吸收峰表明分子中存在亚砷, 2 921, 1 609, 935 cm⁻¹ 吸收峰表明分子中有端乙烯基。¹H NMR 显示 1 个连亚砷的亚甲基质子, δ 3.41 (1H, dd, J = 17.6, 4.3 Hz), 3.51 (1H, dd, J = 17.6, 4.7 Hz), 1 个与亚砷及硫相连的次甲基质子, δ 4.52 (1H, d, J = 7.2 Hz), 1 个与硫相连的环内双键烯质子, δ 5.73 (1H, ddd, J = 10.2, 4.7, 4.3 Hz), 6.19 (1H, d, J = 10.2 Hz), 1 个端乙烯基质子, δ 5.59 (1H, d, J = 16.8 Hz), 5.64 (1H, d, J = 9.9 Hz), 6.04 (1H, ddd, J = 16.8, 9.9, 7.2 Hz), 可推测此化合物的基本结构为乙烯基二硫杂苯类结构。从它们的偶合情况及偶合常数看, δ: 6.19 应为 6 位质子信号, 其偶合常数 J = 10.2 Hz, 显然是与邻位质子发生偶合, 5 位质子发生了叁重偶合, 一偶合常数为 10.2 Hz (与 6 位质子偶合), 另二偶合常数为 4.7, 4.3 Hz (与 4 位质子偶合), δ: 4.52 应为 2 位质子信号, 其偶合常数 J = 7.2 Hz, 显然是与邻位质子发生偶合, 7 位质子也发生了叁重偶合, 一偶合

常数 7.2 Hz(与 2 位质子偶合),另二偶合常数为 16.8, 9.9 Hz(与 8 位质子偶合), $^1\text{H}-^1\text{HCO SY}$ 中显示 H-2 与 H-7 相关, H-2 与 H-8 有远程偶合, H-4 与 H-5 相关, H-4 与 H-6 有远程偶合。综上所述推断此化合物的结构为 2-乙烯基-4H-1,3-二硫杂苯-3-氧化物,其 $^{13}\text{C NMR}$, APT, $^1\text{H}-^{13}\text{C COSY}$ 亦确证了它的结构及 C H 归属。化合物 V, VI, VIII, IX 的结构见图 1

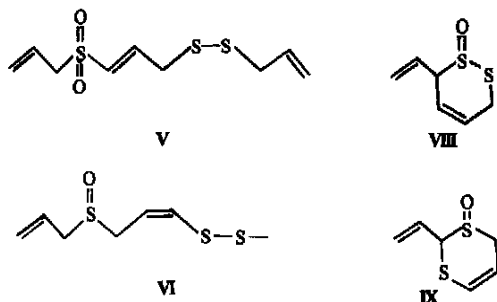


图 1 化合物 V, VI, VIII 和 IX 的化学结构式

1 仪器和材料

红外光谱用 Perkin-Elmer 983 型红外光谱仪测定;直接涂片;核磁共振用 Varian-VXR 300 测定;质谱用 VG 20-253 型和 MS-50 型质谱仪测定;高效液相色谱用 Varian 2510 泵, 2550 检测器, KYGW C₁₈ 10 μ m, 15 mm $\times$ 150 mm 柱;层析用硅胶由青岛海洋化工厂生产。

2 提取和分离

大蒜 5.0 kg 粉碎后用 6 倍量甲醇浸渍提取 3 次,提取液减压浓缩,加等量水稀释,用乙醚萃取 ($\times$ 2 500 mL),乙醚提取液经无水硫酸钠脱水后减压浓缩,残留物配成 10% 甲醇溶液室温放置 4 d 过滤,滤液减压浓缩得 16 g 油状物,将其分散于 50% 甲醇中 (1 600 mL),用环己烷萃取 ($\times$ 500 mL),环己烷提取液经无水硫酸钠脱水,减压浓缩得 9 g 环己烷提取物,将其经硅胶柱层析,以环己烷-乙酸乙酯系统进行梯度洗脱,所得组分经薄层析制备,再经高效液相制备分离,分别得到化合物: I (570 mg), II (10 mg), III (3 mg), IV (4 mg), V (3 mg), VI (4 mg), VII (390 mg), VIII (20 mg), IX (5 mg)

3 鉴定

化合物 I: 无色油状液体 FAB-MS m/z 235 [$M+1$] $^+$ 。IR $_{\max}$ cm^{-1} : 3 082, 1 632, 1 040 (S, 亚砷), 990 ^1H 和 ^{13}C 数据与文献^[2]报道 Z-1,6,11-三烯-4,5,9-三硫杂十二烷-9-氧化物 (Z-ajoene) 一致。

化合物 II: 无色油状液体 FAB-MS m/z 235 [$M+1$] $^+$ 。IR $_{\max}$ cm^{-1} : 3 080, 1 635, 1 042 (S, 亚

砷), ^1H 和 ^{13}C 数据与文献^[2]报道 E-1,6,11-三烯-4,5,9-三硫杂十二烷-9-氧化物 (E-ajoene) 一致。

化合物 III: 无色油状液体 FAB-MS m/z 250 [M] $^+$ 。IR $_{\max}$ cm^{-1} : 2 919, 2 851, 1 312 (S, 砷), 1 120 (S, 砷), 927 ^1H 和 ^{13}C 数据与文献^[2]报道 Z-1,6,11-三烯-4,5,9-三硫杂十二烷-9,9-二氧化物一致。

化合物 IV: 无色油状液体 FAB-MS m/z 250 [M] $^+$ 。IR $_{\max}$ cm^{-1} : 2 923, 1 632, 1 313 (S, 砷), 1 121 (S, 砷), 937 ^1H 和 ^{13}C 数据与文献^[2]报道 E-1,6,11-三烯-4,5,9-三硫杂十二烷-9,9-二氧化物一致。

化合物 V: 浅黄色油状液体 FAB-MS m/z 250 [M] $^+$ 。IR $_{\max}$ cm^{-1} : 2 290, 1 630, 1 315 (S, 砷), 1 124 (S, 砷), 931 $^1\text{H NMR}$ (CDCl_3) δ 3.34 (2H, d, J = 7.2 Hz, H-3), 3.42 (2H, d, J = 7.8 Hz, H-6), 3.74 (2H, d, J = 7.5 Hz, H-10), 6.38 (1H, d, J = 14.7 Hz, H-8, EO_2 $\text{SCH}=\text{CH}$), 5.81 (1H, m, H-2), 6.84 (1H, d, t, J = 14.7, 7.8 Hz, H-3), 5.84 (2H, m, H-11), 5.23 (1H, d, J = 17.1 Hz, H-1), 5.19 (1H, d, J = 10.2 Hz, H-1), 5.42 (1H, d, J = 18.3 Hz, H-12), 5.47 (1H, d, J = 10.5 Hz, H-12)。 $^{13}\text{C NMR}$ (CDCl_3) δ 38.67 (C-6), 42.39 (C-3), 59.68 (C-10), 119.22 (C-1), 124.45 (C-11), 124.86 (C-12), 129.41 (C-8), 132.74 (C-2), 143.12 (C-7) 根据以上数据推断化合物 V 的结构为 E-1,7,11-三烯-4,5,9-三硫杂十二烷-9,9-二氧化物。

化合物 VI: 无色油状液体 FAB-MS m/z 209 [$M+1$] $^+$ 。IR $_{\max}$ cm^{-1} : 3 082, 1 633, 1 043 (S, 亚砷), 930 $^1\text{H NMR}$ (CDCl_3) δ 2.47 (3H, s, H-1), 3.47 (1H, dd, J = 13.4, 7.3 Hz, H-8), 3.55 (1H, dd, J = 13.4, 6.6 Hz, H-8), 3.61 (1H, dd, J = 13.5, 8.5 Hz, H-6), 3.68 (1H, dd, J = 13.5, 7.9 Hz, H-6), 6.64 (1H, d, J = 9.3 Hz, H-4, $\text{SSCH}=\text{CH}$), 5.82 (1H, m, H-5), 5.92 (1H, m, H-9), 5.44 (1H, d, J = 16.5 Hz, H-10), 5.48 (1H, d, J = 9.9 Hz, H-10), $^{13}\text{C NMR}$ (CDCl_3) δ 23.20 (C-1), 49.52 (C-6), 54.81 (C-8), 118.43 (C-5), 123.69 (C-10), 125.48 (C-9), 137.68 (C-4) 根据以上数据推断化合物 VI 的结构为 Z-4,9-二烯-2,3,7-三硫杂癸烷-7-氧化物。

化合物 VII: 无色油状液体 $^{13}\text{C NMR}$ 数据见表 1, $^1\text{H NMR}$ 数据与文献^[7]报道 2-乙烯基-4H-1,3-二硫杂苯一致。

化合物 VIII: 无色油状液体 FAB-MS m/z 160

表 1 化合物Ⅶ~Ⅸ的 ¹³ CNMR数据 (CDCl ₃)			
碳位	Ⅶ	Ⅷ	Ⅸ
2	45.28		57.81
3		60.88	
4	25.15	121.07	45.52
5	117.07	113.48	114.39
6	121.97	44.30	120.86
7	133.99	128.79	126.28
8	118.44	123.40	123.65

[M]⁺ (25), 112(35), 111(33), 97(34), 85(42), 79(100), 74(85). IR_{max} cm⁻¹: 3 087, 1 611, 1 057(S, 亚砷), 865⁻¹HNMR(CDCl₃) δ 3.42(2H, m, H-6), 4.60(1H, d, J= 7.8 Hz, H-3), 6.31(1H, d, J= 10.2 Hz, H-4), 5.78(1H, m, H-5), 5.80(1H, m, H-7), 5.52(1H, d, J= 9.6 Hz, H-8), 5.59(1H, d, J= 16.5 Hz, H-8) ¹³CNMR数据见表 1 根据以上数据推断化合物Ⅷ的结构为 3-乙烯基-6H-1, 2-二硫杂苯-2-氧化物。

化合物Ⅸ: 无色油状液体 FAB-MS m/z 160 [M]⁺ (33), 112(34), 111(30), 97(35), 85(47), 79(100), 71(94). IR_{max} cm⁻¹: 2 921, 1 609, 1 050(S, 亚砷), 935⁻¹HNMR(CDCl₃) δ 3.41(1H, d, d, J= 17.6, 4.3 Hz, H-4), 3.51(1H, d, d, J= 17.6, 4.7 Hz, H-4), 4.52(1H, d, J= 7.2 Hz, H-2), 5.73(1H,

d, d, d, J= 10.2, 4.7, 4.3 Hz, H-5), 6.19(1H, d, J= 10.2 Hz, H-6), 5.59(1H, d, J= 16.8 Hz, H-8), 5.64(1H, d, J= 9.9 Hz, H-8), 6.04(1H, ddd, J= 16.8, 9.9, 7.2 Hz, H-7). ¹³CNMR数据见表 1 根据以上数据推断化合物Ⅸ的结构为 2-乙烯基-4H-1, 3-二硫杂苯-3-氧化物

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Flavonoids isolated from *Pogostemon cablin*

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Abstract **Object** To isolate and identify the chemical constituents of *Pogostemon cablin* (Blanco) Benth. for the purpose to screen new natural antifungal drugs. **Methods** The compounds were isolated by chromatography. Their chemical structures were elucidated with UV, IR, MS, NMR (¹H, ¹³C, DEPT) spectroscopy. The antifungal activities of the four isolated compounds were examined *in vitro* by media dilution method. **Results** With antifungal guided fractionation, eight flavonoids were isolated from the alcoholic extract of the whole plant. Their structures were elucidated as 5-hydroxy-7, 3', 4'-trimethoxyflavanone (I), 5-hydroxy-7, 4'-dimethoxyflavanone (II), 3, 5, -dihydroxy-7, 4'-dimethoxyflavone (III), 5-hydroxy-3, 7, 4'-trimethoxyflavone (IV), 5-hydroxy-3, 7, 3', 4'-tetramethoxyflavone (V), 5, 4'-dihydroxy-3, 7, 3'-trimethoxyflavone (VI), 5, 4'-dihydroxy-7-methoxyflavone (VII), and 3, 5, 7, 3', 4'-pentahydroxyflavone (VIII) on the basis of spectroscopic data. The antifungal activities of compounds I, III, V, VI were examined *in vitro*. **Conclusion** All the flavonoids, except V and VI were isolated from

this plant for the first time. The four examined compounds exhibited certain antifungal activities against six strains of fungi *in vitro*.

Key words *Pogostemon cablin* (Blanco) Benth.; flavonoids; antifungal activity

广藿香中的黄酮类化合物

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摘要:目的 对广藿香全草进行研究以筛选天然抗真菌新药。方法 用色谱技术进行分离,通过 IR, UV, MS, NMR(¹H, ¹³C, DEPT)分析以及与标准品对照的方法鉴定化合物的结构。利用培养基药物浓度稀释法进行体外抗菌实验。结果 利用抗菌活性追踪,从广藿香中分离得到 8个黄酮类化合物,鉴定为: 5-羟基-3', 7, 4'-三甲氧基二氢黄酮(I); 5-羟基-7, 4'-二甲氧基二氢黄酮(II); 3, 5-二羟基-7, 4'-二甲氧基黄酮(III); 5-羟基-7, 3, 4'-三甲氧基黄酮(IV); 5-羟基-3, 7, 3', 4'-四甲氧基黄酮(V); 5, 4'-二羟基-3, 7, 3'-三甲氧基黄酮(VI); 5, 4'-二羟基-7-甲氧基黄酮(VII)和 3, 5, 7, 3', 4'-五羟基黄酮(VIII)。并对化合物I, III, V, VI进行了体外抗真菌活性研究。结论 除V和VI外,均为首次从该植物中分离得到。受测的 4个黄酮类化合物具有抗真菌活性。

关键词: 广藿香;黄酮类;抗真菌活性

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Pogostemon cablin (Blanco) Benth. (广藿香)

is widespread in southern China. The plant has been used as Chinese herbal medicine to remove dampness, relieve summer-heat, exterior syndrome, stop vomiting and stimulate the appetite. The essential oil of *P. cablin* collected by steam distillation was found to exhibit significant antifungal and antibacterial activities *in vitro* (MIC = 0.08~1.0 mg/L)^[1]. Its alcoholic extract also showed some antifungal activities (MIC < 2 mg/L). Bioassay-guided fractionation of this active extract has led to the isolation and characterization of eight flavonoids as 5-hydroxy-7, 3', 4'-trimethoxyflavanone (I)^[2], 5-hydroxy-7, 4'-dimethoxyflavanone (II)^[3], 3, 5, -dihydroxy-7, 4'-dimethoxyflavone (III)^[4], 5-hydroxy-3, 7, 4'-trimethoxyflavone (IV)^[5], 5-hydroxy-3, 7, 3', 4'-tetramethoxyflavone (V)^[6], 5, 4'-dihydroxy-3, 7, 3'-trimethoxyflavone (VI)^[6], 5, 4'-dihydroxy-7-methoxyflavone (VII)^[7], and 3, 5, 7, 3', 4'-pentahydroxyflavone (VIII)^[8]. We report herein on the structural elucidation of the isolated compounds and preliminary screening of the antifungal activities of compounds I, III, V, and VI.

Results and discussion

Compound I was crystalized from acetone as colorless needles. The IR spectrum showed absorptions typical of carbonyl groups, and benzene ring, and the UV spectrum was typical of a flavonoid. The ¹H NMR spectrum showed the presence of three methoxy groups (δ 3.81, 3.90 and 3.92), and a downfield signal (δ 12.01) due to a hydrogenbonded hydroxy group at 5 position. The aromatic protons of meta-coupled doublets (J = 2.5 Hz) at δ 6.06 and 6.08 corresponded to 6, 8 protons of ring A, three more aromatic protons at δ 6.90, 6.98 and 6.99 showed the presence of a para-substituted aromatic ring. The ¹³C NMR spectrum showed signals of four oxygenated aromatic carbons (δ 164.2, 168.0, 149.3 and 149.6) and one carbonyl carbon (δ 195.9). These assignment were further confirmed by the DEPT spectrum which indicated the presence of one methylene, three methoxy, and six methylidene. And with the positive-ion FABMS showed a quasimolecular peak $[M+H]^+$ at 331, the molecular formula was determined as C₁₈H₁₈O₆. All these data supported that the structure of flavanone I is 5-hydroxy-7,

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