Electronic supplementary information for

New Securinega alkaloids with anti-HIV activity from *Fluegga virosa*

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bMcGill University Aids Centre, The Lady Davis Institute for Medical Research, Jewish General Hospital, 3755 Cote Ste-Catherine Road, Montreal, Quebec H3T 1E2, Canada

Table S1. NMR data comparison of alkaloid 3 with virosecurinine and fluggenine A in CDCl3.

Figure S1a. Key 2D NMR correlations for alkaloids 5–8.
Figure S1b. CD spectra for alkaloids 1, 2 and 4–9.

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Figure S2. 13C NMR spectrum for flueggenine E (1) in CDCl3.
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Figure S10. 1H NMR spectrum for flueggenine F (2) in CDCl3.
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Figure S21. 1H–1H COSY spectrum for flueggenine G (3) in CDCl3.

† Equal contribution. ∗Corresponding author. Tel.: 86-21-50806718; E-mail: jmyue@simm.ac.cn
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Figure S81. (+)-HRESIMS spectrum for flueggenine H (9).
Table S1. NMR data comparison of alkaloid 3 with virosecurinine and fluggenine A in CDCl₃.

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<sup>c</sup> Interchangeable assignments.
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Figure S9. (+)-HRESIMS spectrum for flueggenine E (1).

**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
266 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 6-80  H: 2-120  N: 0-3  O: 0-20

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Figure S10. $^1$H NMR spectrum for flueggenine F (2) in CDCl$_3$. 
Figure S11. $^{13}$C NMR spectrum for flueggenine F (2) in CDCl$_3$. 
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Figure S27. HREIMS spectrum for flueggenine G (3).

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Figure S28. $^1$H NMR spectrum for flueggenine H (4) in CDCl$_3$ (5% CD$_3$OD).
Figure S29. $^{13}$C NMR spectrum for flueggenine H (4) in CDCl$_3$ (5% CD$_3$OD).
Figure S30. $^1\text{H}^-^1\text{H}$ COSY spectrum for flueggenine H (4) in CDCl$_3$ (5% CD$_3$OD).
Figure S31. HSQC spectrum for flueggenine H (4) in CDCl$_3$ (5% CD$_3$OD).
Figure S32. HMBC spectrum for flueggenine H (4) in CDCl₃ (5% CD₃OD).
Figure S33. ROESY spectrum for flueggenine H (4) in CDCl$_3$ (5% CD$_3$OD).
Figure S34. IR spectrum for fluegenine H (4).
Figure S35. (+)-ESIMS spectrum for flueggenine H (4).
Figure S36. (+)-HRESIMS spectrum for flueggenine H (4).
Figure S37. $^1$H NMR spectrum for flueggenine I (5) in CDCl$_3$. 
Figure S38. $^{13}$C NMR spectrum for flueggenine I (5) in CDC$_3$. 
Figure S39. $^1$H–$^1$H COSY spectrum for flueggenine I (5) in CDCl$_3$. 
Figure S40. HSQC spectrum for flueggenine I (5) CDCl₃.
Figure S41. HMBC spectrum for flueggenine I (5) in CDCl$_3$. 
Figure S42. ROESY spectrum for flueggenine I (5) in CDCl₃.
Figure S43. IR spectrum for flueggenine I (5).
Figure S44. (+)-ESIMS spectrum for flueggenine I (5).
Figure S45. (+)-HRESIMS spectrum for flueggenine I (5).

Elemental Composition Report

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
403 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
- C: 5-80
- H: 2-120
- N: 0-4
- O: 0-20

LCT PXE KE324

G4el_0927 27 (0.583) AM2 (Ar,10000,0.00,1.00), ABS, Cm (11.27)

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Figure S46. $^1$H NMR spectrum for fluevirosine E (6) in CDCl$_3$. 
Figure S47. $^{13}$C NMR spectrum for fluggenine E (6) in CDCl$_3$. 
Figure S48. $^1$H–$^1$H COSY spectrum for flueggenine E (6) in CDCl$_3$. 
Figure S49. HSQC spectrum for flueggenine E (6) CDCl₃.
Figure S50. HMBC spectrum for flueggenine E (6) in CDCl₃.
Figure S51. ROESY spectrum for flueggenine E (6) in CDCl₃.
Figure S52. IR spectrum for flueggenine E (6).
Figure S53. (+)-ESIMS spectrum for flueggenine E (6).
Figure S54. (+)-HRESIMS spectrum for flueggenine E (6).

### Elemental Composition Report

**Single Mass Analysis**

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

793 formula(s) evaluated with 3 results within limits (up to 50 closest results for each mass)

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G4giB  LCT PXE KE324  13-Sep-2013  15:18:06
G4giB_0913 27 (0.555) AM2 (Av,10000.0,0.0,0.0,1.00); ABSS; Cm (26:42)  1:TOF MS ES+

| 1.71×10⁴ |

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Figure S55. $^1$H NMR spectrum for fluevirosine F (7) in CDCl$_3$. 
Figure S56. $^{13}$C NMR spectrum for flueggenine F (7) in CDCl$_3$. 
Figure S57. $^1$H–$^1$H COSY spectrum for flueggenine F (7) in CDCl$_3$. 
Figure S58. HSQC spectrum for flueggenine F (7) CDCl₃.
Figure S59. HMBC spectrum for flueggenine F (7) in CDCl₃.
Figure S60. ROESY spectrum for flueggenine F (7) in CDCl₃.
Figure S61. IR spectrum for flueggenine F (7).
Figure S62. (+)-ESIMS spectrum for fluegenine F (7).
Figure S63. (+)-HRESIMS spectrum for flueggenine F (7).
Figure S64. $^1$H NMR spectrum for fluevirosine G (8) in CDCl$_3$. 
Figure S65. $^{13}$C NMR spectrum for flueggenine G (8) in CDCl$_3$. 
Figure S66. $^1$H−$^1$H COSY spectrum for flueggenine G (8) in CDCl$_3$. 
Figure S67. HSQC spectrum for fluegenine G (8) CDCl₃.
Figure S68. HMBC spectrum for fluegenine G (8) in CDCl₃.
Figure S69. ROESY spectrum for flueggenine G (8) in CDCl₃.
Figure S70. IR spectrum for flueggenine G (8).
Figure S71. (+)-ESIMS spectrum for flueggenine G (8).
Figure S72. (+)-HRESIMS spectrum for flueggenine G (8).

### Elemental Composition Report

**Single Mass Analysis**

- **Tolerance:** 5.0 PPM / DBE: min = -1.5, max = 50.0
- **Element prediction:** Off
- **Number of isotope peaks used for i-FIT:** 3

**Monoisotopic Mass, Even Electron Ions**

626 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

**Elements Used:**
- C: 5-80
- H: 2-120
- N: 0-4
- O: 0-20

**Calc. Mass**

- **m/z:** 610.2931
- **PEM:** 610.2927
- **DBE:** -0.7
- **i-FIT:** 89.9
- **i-FIT (Norm):** 1.5
- **Formula:** C36 H40 N3 O6

**Calc. Mass**

- **m/z:** 610.2932
- **PEM:** 610.2928
- **DBE:** -1.2
- **i-FIT:** 96.7
- **i-FIT (Norm):** 6.8
- **Formula:** C33 H48 N O17

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Figure S73. $^1$H NMR spectrum for fluvirosine H (9) in CDCl$_3$. 
Figure S74. $^{13}$C NMR spectrum for flueggenine H (9) in CDCl$_3$. 
Figure S75. $^1$H–$^1$H COSY spectrum for fluegenine H (9) in CDCl$_3$. 
Figure S76. HSQC spectrum for flueggenine H (9) CDCl₃.
Figure S77. HMBC spectrum for flueggenine H (9) in CDCl$_3$. 

![HMBC Spectrum](image)
Figure S78. ROESY spectrum for flueggenine H (9) in CDCl₃.
Figure S79. IR spectrum for fluggenine H (9).
Figure S80. (+)-ESIMS spectrum for flueggenine H (9).
Figure S81. (−)-HRESIMS spectrum for flueggenine H (9).
Figure S82. $^1$H NMR spectrum for fluevirosine I (10) in CDCl$_3$. 
Figure S83. $^{13}$C NMR spectrum for flueggenine I (10) in CDCl$_3$. 
Figure S84. $^1$H–$^1$H COSY spectrum for flueggenine I (10) in CDCl$_3$. 
Figure S85. HSQC spectrum for flueggenine I (10) CDCl₃.
Figure S86. HMBC spectrum for flueggenine I (10) in CDCl$_3$. 
Figure S87. ROESY spectrum for flueggenine I (10) in CDCl₃.
Figure S88. IR spectrum for flueggenine I (10).
Figure S89. (+)-ESIMS spectrum for flueggoine 1 (10).
Figure S90. (+)-HRESIMS spectrum for flueggenine I (10).