ESI for New Journal of Chemistry

## **Supplementary Information**

# Novel styrylpyrazole-glucosides and their dioxolo-bridged doppelgangers: synthesis and cytotoxicity

Ana R. F. Carreira, <sup>a</sup> David M. Pereira, <sup>b</sup> Paula B. Andrade, <sup>b</sup> Patrícia Valentão, <sup>b</sup> Artur M. S. Silva, <sup>a</sup> Susana Santos Braga,<sup>\*a</sup> Vera L. M. Silva <sup>\*a</sup>

 <sup>a</sup> Chemistry Department, QOPNA and LAQV-REQUIMTE, University of Aveiro, 3810-193 Aveiro, Portugal
<sup>b</sup> REQUIMTE/LAQV, Laboratório de Farmacognosia, Departamento de Química, Faculdade de Farmácia, Universidade do Porto, R. Jorge Viterbo Ferreira, nº 228, 4050-313 Porto, Portugal

Emails: <a href="mailto:sbraga@ua.pt">sbraga@ua.pt</a> and <a href="mailto:verasilva@ua.pt">verasilva@ua.pt</a>

#### **Table of Contents:**

1. NMR spectra	<b>S3</b>
Figure S1. <sup>1</sup> H NMR spectrum of compound 1d (CDCl <sub>3</sub> , 300.13 MHz)	<b>S</b> 3
Figure S2. <sup>13</sup> C NMR spectrum of compound 1d (CDCl <sub>3</sub> , 75.47 MHz)	<b>S</b> 3
<b>Figure S3.</b> <sup>1</sup> H NMR spectrum of compound <b>2a</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	<b>S</b> 4
Figure S4. <sup>13</sup> C NMR spectrum of compound 2a [(CD <sub>3</sub> ) <sub>2</sub> CO, 125.77 MHz]	<b>S</b> 4
<b>Figure S5.</b> <sup>1</sup> H NMR spectrum of compound <b>2b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 300.13 MHz]	S5
Figure S6. <sup>13</sup> C NMR spectrum of compound <b>2b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	S5
<b>Figure S7.</b> <sup>1</sup> H NMR spectrum of compound <b>2c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	<b>S</b> 6
Figure S8. <sup>13</sup> C NMR spectrum of compound 2c [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	<b>S</b> 6
Figure S9. <sup>1</sup> H NMR spectrum of the mixture of $(E)$ - and $(Z)$ -isomers of compound 2d	
[(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	<b>S</b> 7
Figure S10. <sup>13</sup> C NMR spectrum of the mixture of ( $E$ )- and ( $Z$ )-isomers of compound 2d	
[(CD <sub>3</sub> ) <sub>2</sub> CO, 125.77 MHz]	S7
Figure S11. <sup>1</sup> H NMR spectrum of compound <b>3a</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	<b>S</b> 8
Figure S12. <sup>13</sup> C NMR spectrum of compound 3a [(CD <sub>3</sub> ) <sub>2</sub> CO, 125.77 MHz]	<b>S</b> 8
<b>Figure S13.</b> <sup>1</sup> H NMR spectrum of compound <b>3b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 300.13 MHz]	<b>S</b> 9
Figure S14. <sup>13</sup> C NMR spectrum of compound <b>3b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	<b>S</b> 9
<b>Figure S15.</b> <sup>1</sup> H NMR spectrum of compound <b>3c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	S10

<b>Figure S16.</b> <sup>13</sup> C NMR spectrum of compound <b>3c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	<b>S</b> 10
Figure S17. <sup>1</sup> H NMR spectrum of the mixture of $(E)$ - and $(Z)$ -isomers of compound 3d	
[(CD <sub>3</sub> ) <sub>2</sub> CO, 300.13 MHz]	<b>S</b> 11
<b>Figure S18.</b> <sup>1</sup> H NMR spectrum of compound <b>4a</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	<b>S</b> 11
<b>Figure S19.</b> <sup>13</sup> C NMR spectrum of compound <b>4a</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	S12
<b>Figure S20.</b> <sup>1</sup> H NMR spectrum of compound <b>4b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	S12
<b>Figure S21.</b> <sup>13</sup> C NMR spectrum of compound <b>4b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	<b>S</b> 13
<b>Figure S22.</b> <sup>1</sup> H NMR spectrum of compound <b>4c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	<b>S</b> 13
<b>Figure S23.</b> <sup>13</sup> C NMR spectrum of compound <b>4c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	S14
Figure S24. <sup>1</sup> H NMR spectrum of the mixture of $(E)$ - and $(Z)$ -isomers of compound 4d	
[CD <sub>3</sub> ) <sub>2</sub> CO, 300.13 MHz]	S14
<b>Figure S25.</b> <sup>1</sup> H NMR spectrum of compound <b>5b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	S15
<b>Figure S26.</b> <sup>13</sup> C NMR spectrum of compound <b>5b</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	S15
<b>Figure S27.</b> <sup>1</sup> H NMR spectrum of compound <b>5c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 500.16 MHz]	S16
<b>Figure S28.</b> <sup>13</sup> C NMR spectrum of compound <b>5c</b> [(CD <sub>3</sub> ) <sub>2</sub> CO, 75.47 MHz]	<b>S</b> 16

### ESI for New Journal of Chemistry

#### 1. NMR spectra



Figure S1. <sup>1</sup>H NMR spectrum of compound 1d (CDCl<sub>3</sub>, 300.13 MHz).



Figure S2. <sup>13</sup>C NMR spectrum of compound 1d (CDCl<sub>3</sub>, 75.47 MHz).



Figure S3. <sup>1</sup>H NMR spectrum of compound 2a [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S4. <sup>13</sup>C NMR spectrum of compound 2a [(CD<sub>3</sub>)<sub>2</sub>CO, 125.77 MHz].



Figure S5. <sup>1</sup>H NMR spectrum of compound 2b [(CD<sub>3</sub>)<sub>2</sub>CO, 300.13 MHz].



Figure S6. <sup>13</sup>C NMR spectrum of compound 2b [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



Figure S7. <sup>1</sup>H NMR spectrum of compound 2c [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S8. <sup>13</sup>C NMR spectrum of compound 2c [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



Figure S9. <sup>1</sup>H NMR spectrum of the mixture of (*E*)- and (*Z*)-isomers of compound 2d  $[(CD_3)_2CO, 500.16 \text{ MHz}].$ 



Figure S10. <sup>13</sup>C NMR spectrum of the mixture of (*E*)- and (*Z*)-isomers of compound 2d  $[(CD_3)_2CO, 125.77 \text{ MHz}].$ 



Figure S11. <sup>1</sup>H NMR spectrum of compound **3a** [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S12. <sup>13</sup>C NMR spectrum of compound 3a [(CD<sub>3</sub>)<sub>2</sub>CO, 125.77 MHz].



Figure S13. <sup>1</sup>H NMR spectrum of compound 3b [(CD<sub>3</sub>)<sub>2</sub>CO, 300.13 MHz].



Figure S14. <sup>13</sup>C NMR spectrum of compound 3b [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



Figure S15. <sup>1</sup>H NMR spectrum of compound 3c [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S16. <sup>13</sup>C NMR spectrum of compound 3c [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



**Figure S17.** <sup>1</sup>H NMR spectrum of the mixture of (*E*)- and (*Z*)-isomers of compound **3d**  $[(CD_3)_2CO, 300.13 \text{ MHz}].$ 



Figure S18. <sup>1</sup>H NMR spectrum of compound 4a [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S19. <sup>13</sup>C NMR spectrum of compound 4a [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



Figure S20. <sup>1</sup>H NMR spectrum of compound 4b [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S21. <sup>13</sup>C NMR spectrum of compound 4b [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



Figure S22. <sup>1</sup>H NMR spectrum of compound 4c [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S23. <sup>13</sup>C NMR spectrum of compound 4c [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



**Figure S24.** <sup>1</sup>H NMR spectrum of the mixture of (*E*)- and (*Z*)-isomers of compound **4d**  $[(CD_3)_2CO, 300.13 \text{ MHz}].$ 



Figure S25. <sup>1</sup>H NMR spectrum of compound 5b [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S26. <sup>13</sup>C NMR spectrum of compound 5b [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].



Figure S27. <sup>1</sup>H NMR spectrum of compound 5c [(CD<sub>3</sub>)<sub>2</sub>CO, 500.16 MHz].



Figure S28. <sup>13</sup>C NMR spectrum of compound 5c [(CD<sub>3</sub>)<sub>2</sub>CO, 75.47 MHz].