# Minimalistic bis-triarylpyridinium cations: effective antimicrobials

# against bacterial and fungal pathogens

Ana M. López-Fernández,<sup>a</sup> Jean C. Neto<sup>a</sup>, Rosa de Llanos,<sup>\*b</sup> Juan F. Miravet,<sup>a</sup> Francisco Galindo<sup>\*a</sup>

(a) Departamento de Química Inorgánica y Orgánica, Universitat Jaume I, Av. V. Sos Baynat s/n, 12071, Castellón, Spain. E-mail: <u>francisco.galindo@uji.es</u>

(b) Unidad Predepartamental de Medicina, Universitat Jaume I, Av. V. Sos Baynat s/n, 12071, Castellón, Spain. E-mail: <u>dellanos@uji.es</u>

### **Table of Contents**

Spectroscopic data of compounds	2
Determination of MICs for all the studied compounds	30

#### Spectroscopic data of compounds

2,4,6-triphenylpyrylium tetrafluoroborate (4a)



**Figure S1.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of the precursor 2,4,6-triphenylpyrylium tetrafluoroborate (4a).



**Figure S2.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>) spectra of the precursor 2,4,6-triphenylpyrylium tetrafluoroborate (4a).

4-(4-bromophenyl)-2,6-diphenylpyrylium tetrafluoroborate (4b)



**Figure S3.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of the precursor *4-(4-bromophenyl)-2,6diphenylpyrylium tetrafluoroborate* (**4***b*).



**Figure S4.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>) spectra of the precursor *4-(4-bromophenyl)-2,6diphenylpyrylium tetrafluoroborate* (*4b*).



**Figure S5.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of the precursor 2,6-*bis*(4-*bromophenyl*)-4*phenylpyrylium tetrafluoroborate* (4c).



**Figure S6.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>) spectra of the precursor 2,6-*bis*(4-*bromophenyl*)-4-*phenylpyrylium tetrafluoroborate* (**4***c*).



**Figure S7.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of the precursor 2,4,6-*tris*(4-*bromophenyl*)*pyrylium tetrafluoroborate* (*4d*).



**Figure S8.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>) spectra of the precursor 2,4,6-tris(4-bromophenyl)pyrylium tetrafluoroborate (4d).

### **Compound 1a**



Figure S9. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 1a.



Figure S10. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 1a.



Figure S11. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 1a.



Figure S12. HRMS spectra of compound 1a.

### **Compound 1b**



Figure S13. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 1b.



Figure S14. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 1b.



Figure S15. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 1b.



Figure S16. HRMS spectra of compound 1b.

### **Compound 1c**



Figure S17. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 1c.



Figure S18. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 1c.



**Figure S19.** <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound **1c**.



Figure S20. HRMS spectra of compound 1c.

## Compound 1d



Figure S21. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 1d.



Figure S22. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 1d.



Figure S23. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 1d.



Figure S24. HRMS spectra of compound 1d.

### **Compound 2a**



Figure S25. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 2a.



Figure S26. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 2a.



Figure S27. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 2a.



Figure S28. HRMS spectra of compound 2a.

### **Compound 2b**



Figure S29. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 2b.



Figure S30. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 2b.



Figure S31. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 2b.



### **Compound 2c**



Figure S33. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 2c.



Figure S34. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 2c.



Figure S35. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 2c.





**Figure S37.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of compound **2d**.



Figure S38. <sup>13</sup>C NMR (DMSO-d<sub>6</sub>) spectra of compound 2d.



**Figure S39.** <sup>1</sup>H COSY NMR (DMSO-d<sub>6</sub>) spectra of compound **2d**.



Figure S40. HRMS spectra of compound 2d.

### **Compound 3a**



Figure S41. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 3a.



Figure S42. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 3a.



Figure S43. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 3a.



Figure S44. HRMS spectra of compound 3a.

### Compound 3b



Figure S45. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 3b.



Figure S46. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 3b.



Figure S47. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 3b.



Figure S48. HRMS spectra of compound 3b.

### Compound 3c



Figure S49. <sup>1</sup>H NMR (CDCl<sub>3</sub>) spectra of compound 3c.



Figure S50. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 3c.



**Figure S51.** <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound **3c**.



Figure S52. HRMS spectra of compound 3c.



Figure S54. <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra of compound 3d.



Figure S55. <sup>1</sup>H COSY NMR (CDCl<sub>3</sub>) spectra of compound 3d.



Figure S56. HRMS spectra of compound 3d.



Figure S57. Determination of MICs for all the studied compounds.