Supporting Information

for

Antimicrobial activity of a quaternized BODIPY

against *Staphylococcus* strains

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Photophysics and photochemistry

References

Checkcif files
X-Ray crystallography

Data for three compounds (for 3, 4, and 5) were obtained with Bruker APEX II QUAZAR three-circle diffractometer. Indexing was performed using APEX2 [1]. Data integration and reduction were carried out with SAINT. [2]. Absorption correction was performed by multi-scan method implemented in SADABS [3]. The structures were solved using the direct methods procedure in SHELXS-97 [4] and then refined by full-matrix least-squares refinements on $F^2$ using the SHELXL-97 [4]. All non-hydrogen atoms were refined anisotropically using all reflections with $I > 2\sigma(I)$. C-bound H atoms were positioned geometrically and refined using a riding mode. For 4, N-bound H atoms were located from the difference Fourier map and restrained to be 0.89 Å from N atom using DFIX and its position was constrained to refine on its parent N atom with $U_{\text{iso}}(H) = 1.2 U_{eq}(N)$. Crystallographic data and refinement details of 3, 4, and 5 are summarized in Table S1. Crystal structure validations and geometrical calculations were performed using Platon software [5]. Mercury software [6] was used for visualization of the cif files.

Table S1. Crystal data and refinement parameters for 3, 4, and 5.

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<th>4</th>
<th>5</th>
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<td>$\text{C}<em>{21}\text{H}</em>{26}\text{BF}_2\text{N}_3\text{O}$</td>
<td>$\text{C}<em>{23}\text{H}</em>{29}\text{BCl}_{2}\text{F}_2\text{IN}_3$</td>
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<td>b (Å)</td>
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<td>7.1238(5)</td>
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<td>90</td>
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<td>γ(°)</td>
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Crystal size (mm)
0.20 x 0.25 x 0.30 0.13 x 0.29 x 0.38 0.07 x 0.07 x 0.15

V (Å³)
1726.2(2) 1978.4(2) 1328.51(14)

Z
4 4 2

ρ_{caled} (g.cm⁻³)
1.421 1.293 1.485

μ (mm⁻¹)
0.107 0.093 1.436

F(000)
768 816 596

θ range for data collection (°)
1.35 - 25.03 1.56 - 25.04 2.18 - 25.00

h/k/l
-8,8/-9,9/-36,36 -19/19, -8/8, -20/20 -10/10, -11/11, -20/20

Reflections collected
25089 18188 30188

Independent reflections
3038 3510 4684

Absorption correction
Multi-scan Multi-scan Multi-scan

Data/restraints/parameters
3038 / 0 / 248 3510 / 2 / 265 4684 / 0 / 296

Goodness-of-fit on F² (S)
1.133 1.040 1.091

Final R indices [I > 2σ(I)]
R₁= 0.0405,  
wR₂= 0.1008
R₁= 0.0525,  
wR₂= 0.1449
R₁= 0.0852,  
wR₂= 0.2100

R indices (all data)
R₁= 0.0434,  
wR₂= 0.1023
R₁= 0.0700,  
wR₂= 0.1582
R₁= 0.1216,  
wR₂= 0.2288

Largest diff. peak and hole (e.Å⁻³)
0.186 and -0.231 0.318 and -0.240 1.795 and -1.450
Characterization spectra

Figure S1. ATR-IR spectrum of 3

Figure S2. MALDI-TOF-MS spectrum of 3 (matrix: DHB).
Figure S3. $^1$H NMR spectrum of 3 in DMSO-$d_6$

Figure S4. $^{13}$C NMR spectrum of 3 in DMSO-$d_6$
Figure S5. Crystal structure of compound 3. Displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown as small spheres of arbitrary radii. The red, grey, blue, pink, yellow, and white coloured atoms represent O, C, N, B, F, and H, respectively.
Figure S6. ATR-IR spectrum of 4.

Figure S7. ESI-MS spectrum of 4.
Figure S8. $^1$H NMR spectrum of 4 in DMSO-$d_6$

Figure S9. $^{13}$C NMR spectrum of 4 in DMSO-$d_6$
**Figure S10.** Crystal structure of compound 4 with EtOH solvate. Displacement ellipsoids are drawn at the 30% probability level. H-atoms are shown as small spheres of arbitrary radii. The red, grey, blue, pink, yellow, and white coloured atoms represent O, C, N, B, F, and H, respectively.

**Figure S11.** ATR-IR spectrum of 5.
Figure S12. HRMS spectrum of 5

Figure S13. MALDI-TOF-MS spectrum of 5 (no matrix)
Figure S14. $^1$H NMR spectrum of 5 in DMSO-$d_6$

Figure S15. $^{13}$C NMR spectrum of 5 in DMSO-$d_6$
Figure S16. Crystal structure of compound 5 with DCM solvate. Displacement ellipsoids are drawn at the 20% probability level. H-atoms are shown as small spheres of arbitrary radii. The grey, blue, pink, yellow, purple, green and white coloured atoms represent C, N, B, F, I, Cl and H, respectively.

Figure S17. Perspective view of crystal packing of compound 5, showing C-H⋯F, C-H⋯I interactions.
Photophysics and photochemistry

Figure S18. Left: Absorption spectra of 5 in DMSO at different four concentrations, Right: Absorbance vs concentration.

Figure S19. Left: Fluorescence excitation and emission spectra of 5 in DMSO (5 µM), Right: Fluorescence area integrate vs absorbance of 5 in DMSO and Rhodamine 6G in water at different three concentrations.
Figure S20. Fluorescence lifetime decay profile of 5 in DMSO.

Figure S21. 3D fluorescence emission spectra in DMSO (excitation ranges from 450 to 550 nm).
References

1. APEX2, version 2010.5-0, Bruker (2010), Bruker AXS Inc., Madison, WI.
2. SAINT, version 7.67A, Bruker (2009), Bruker AXS Inc., Madison, WI.
3. SADABS, version 2008/1, Bruker (2008), Bruker AXS Inc., Madison, WI.
checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.  CIF dictionary  Interpreting this report

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Bond precision:  C-C = 0.0027 Å  Wavelength=0.71073 Å

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Hall group: -P 2yn  -P 2yn

Moiety formula: C19 H18 B F2 N3 O2  ?

Sum formula: C19 H18 B F2 N3 O2  C19 H18 B F2 N3 O2

Mr: 369.17  369.17

Dx,g cm⁻³: 1.421  1.421

Z: 4  4

Mu (mm⁻¹): 0.107  0.107

F000: 768.0  768.0

F000’: 768.41

h,k,lmax: 8,9,36  8,9,36

Nref: 3045  3038

Tmin,Tmax: 0.968,0.979  0.880,0.980

Tmin’: 0.968

Correction method: MULTI-SCAN

Data completeness: 0.998  Theta(max) = 25.030°

R(reflections) = 0.0405(2815)  wR2(reflections) = 0.1023(3038)

S = 1.133  Npar = 248

The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.
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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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**PLATON version of 20/08/2014; check.def file version of 18/08/2014**
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No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0031 Å Wavelength=0.7107 Å

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Hall group -P 2yn -P 2yn
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Sum formula C21 H26 B F2 N3 O C21 H26 B F2 N3 O
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Dx,g cm\(^{-3}\) 1.293 1.293
Z 4 4
Mu (mm\(^{-1}\)) 0.093 0.093
F000 816.0 816.0
F000' 816.38
h,k,lmax 19,8,20 19,8,20
Nref 3515 3510
Tmin,Tmax 0.968,0.988 0.970,0.990
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Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.040

R(reflections)= 0.0525( 2624) wR2(reflections)= 0.1582( 3510)

S = 1.040 Npar= 265

The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level.
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No syntax errors found.  

[CIF dictionary]  [Interpreting this report]

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S = 1.091  Npar= 296

The following ALERTS were generated. Each ALERT has the format `test-name_ALERT_alert-type_alert-level.`

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