Supporting Information

for

Antimicrobial activity of a quaternized BODIPY against *Staphylococcus* strains

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Content

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 Uiso(H) = 1.2Ueq(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**.

Crystal parameters	**3**	**4**	**5**
CCDC	979889	979886	979888
Empirical Formula	$C_{19}H_{18}BF_2N_3O_2$	$C_{21}H_{26}BF_2N_3O$	$C_{23}H_{29}BCl_2F_2IN_3$
Formula weight (g.mol^{-1})	369.17	385.26	594.10
Temperature (K)	120(2)	120(2)	150(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic

Space group	$P2_1/n$	$P2_1/n$	P-1
***a* (Å)**	6.8808(5)	16.4780(12)	8.5150(5)
***b* (Å)**	8.3233(6)	7.1238(5)	9.7941(6)
***c* (Å)**	30.274(2)	17.2258(12)	17.2071(10)
α(°)	90	90	76.580(3)
β(°)	95.360(3)	101.934(4)	76.491(3)
γ(°)	90	90	75.658(4)
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* (Å^3)**	1726.2(2)	1978.4(2)	1328.51(14)
Z	4	4	2
ρ_{calcd} (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 F^2 (S)	1.133	1.040	1.091
Final R indices [$I > 2\sigma(I)$]	R_1= 0.0405, wR_2= 0.1008	R_1= 0.0525, wR_2= 0.1449	R_1= 0.0852, wR_2= 0.2100
R indices (all data)	R_1= 0.0434, wR_2= 0.1023	R_1= 0.0700, wR_2= 0.1582	R_1= 0.1216, wR_2= 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

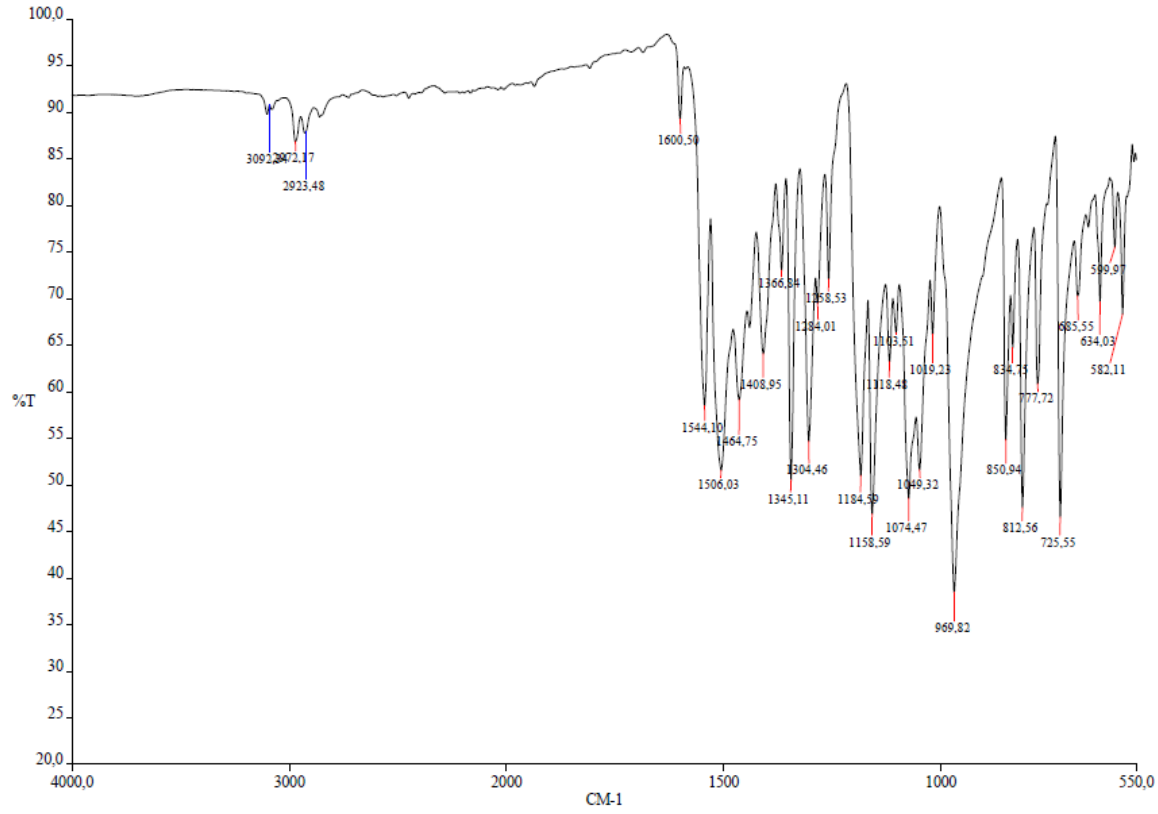

Figure S1. ATR-IR spectrum of **3**

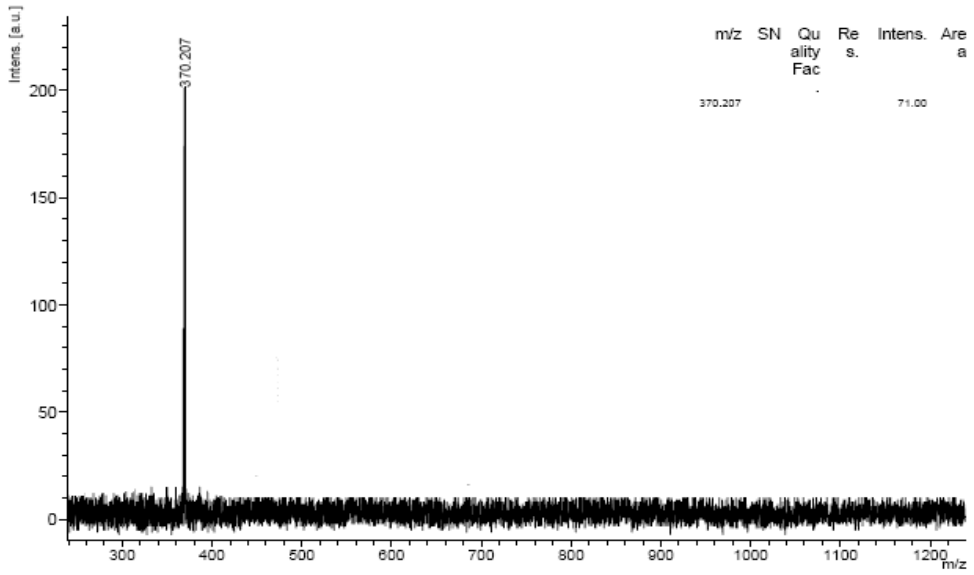

Figure S2. MALDI-TOF-MS spectrum of **3** (matrix: DHB).

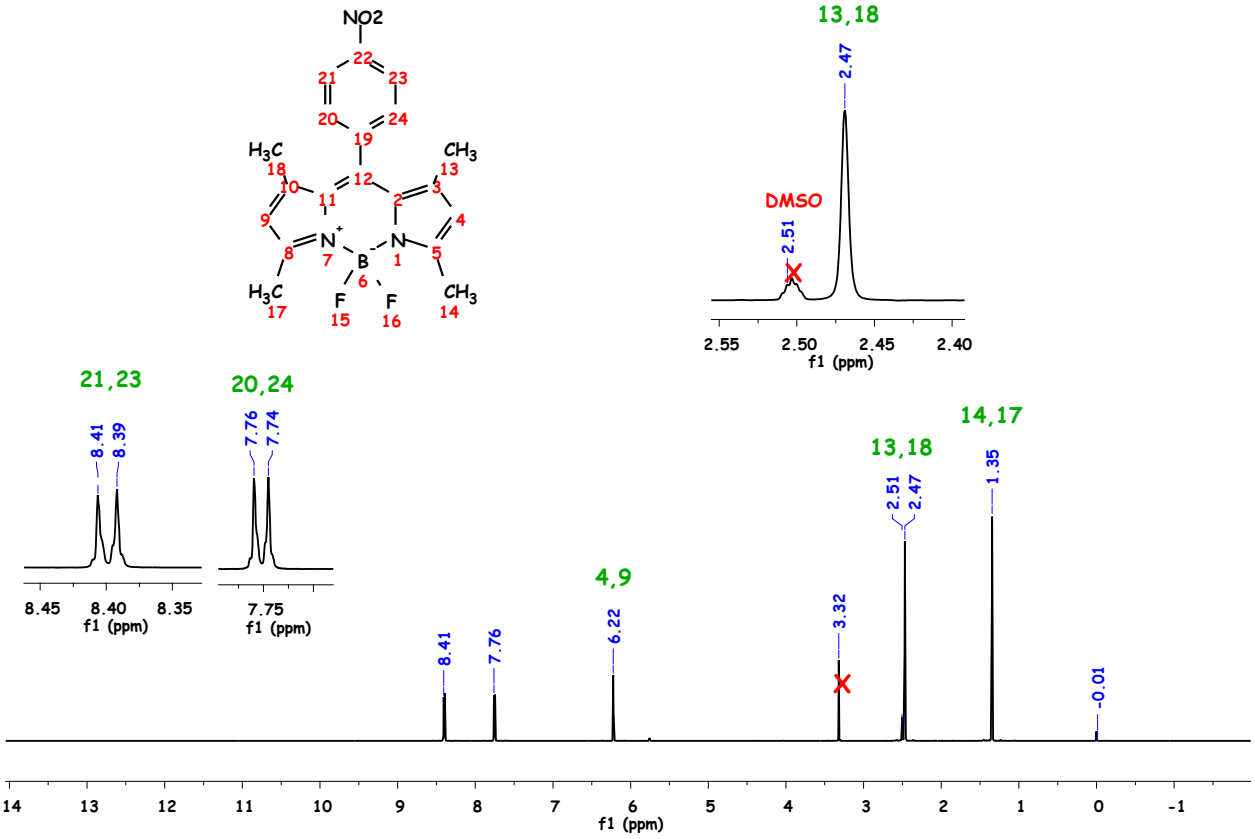

Figure S3. ^{1}H NMR spectrum of **3** in DMSO-d_6

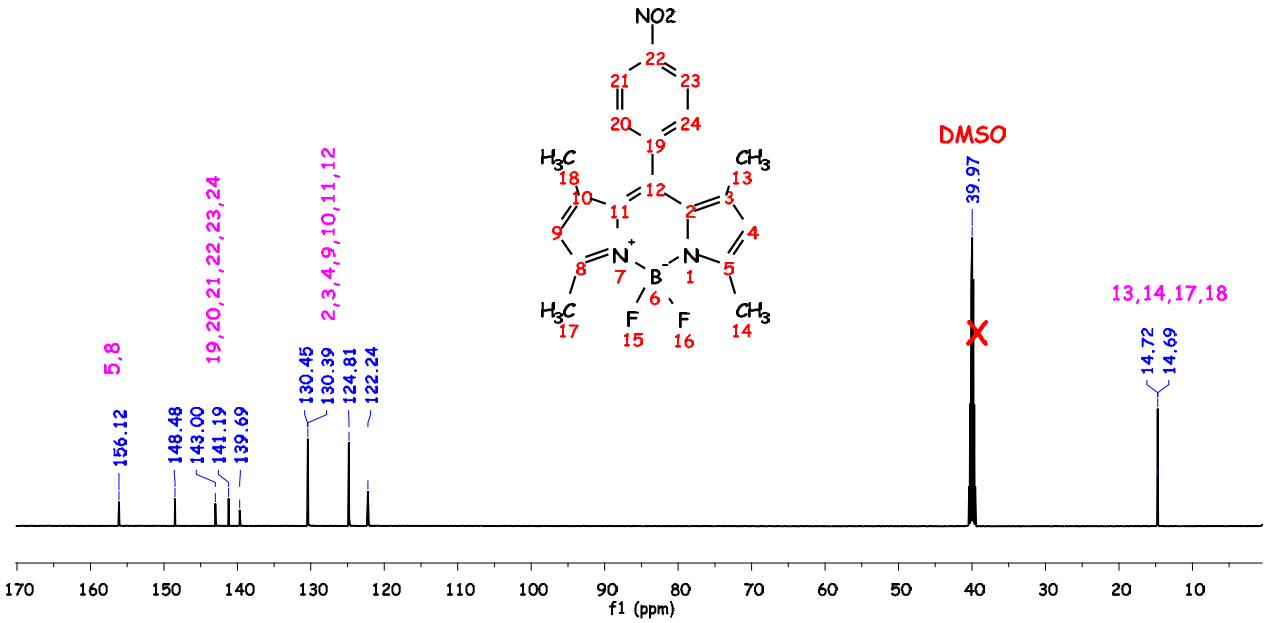

Figure S4. ^{13}C NMR spectrum of **3** in DMSO-d_6

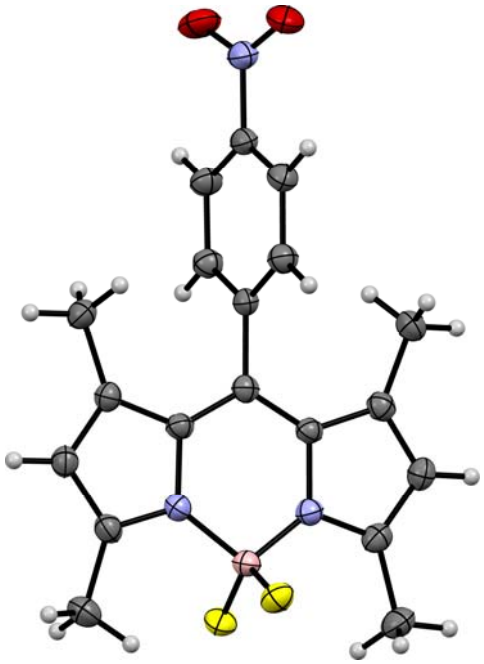

Figure S5. Crystal structure of compound **3**. Displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown as small spheres of arbitrary radii. The red, grey, blue, pink, yellow, and white coloured atoms represent O, C, N, B, F, and H, respectively.

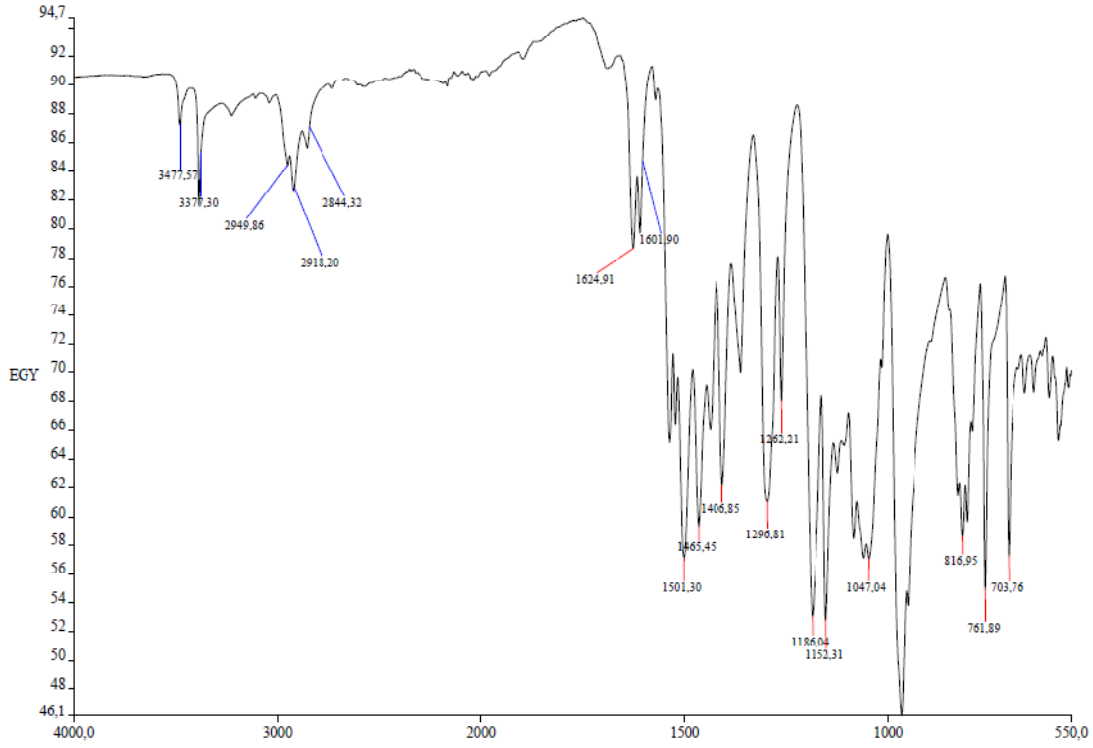

Figure S6. ATR-IR spectrum of **4.**

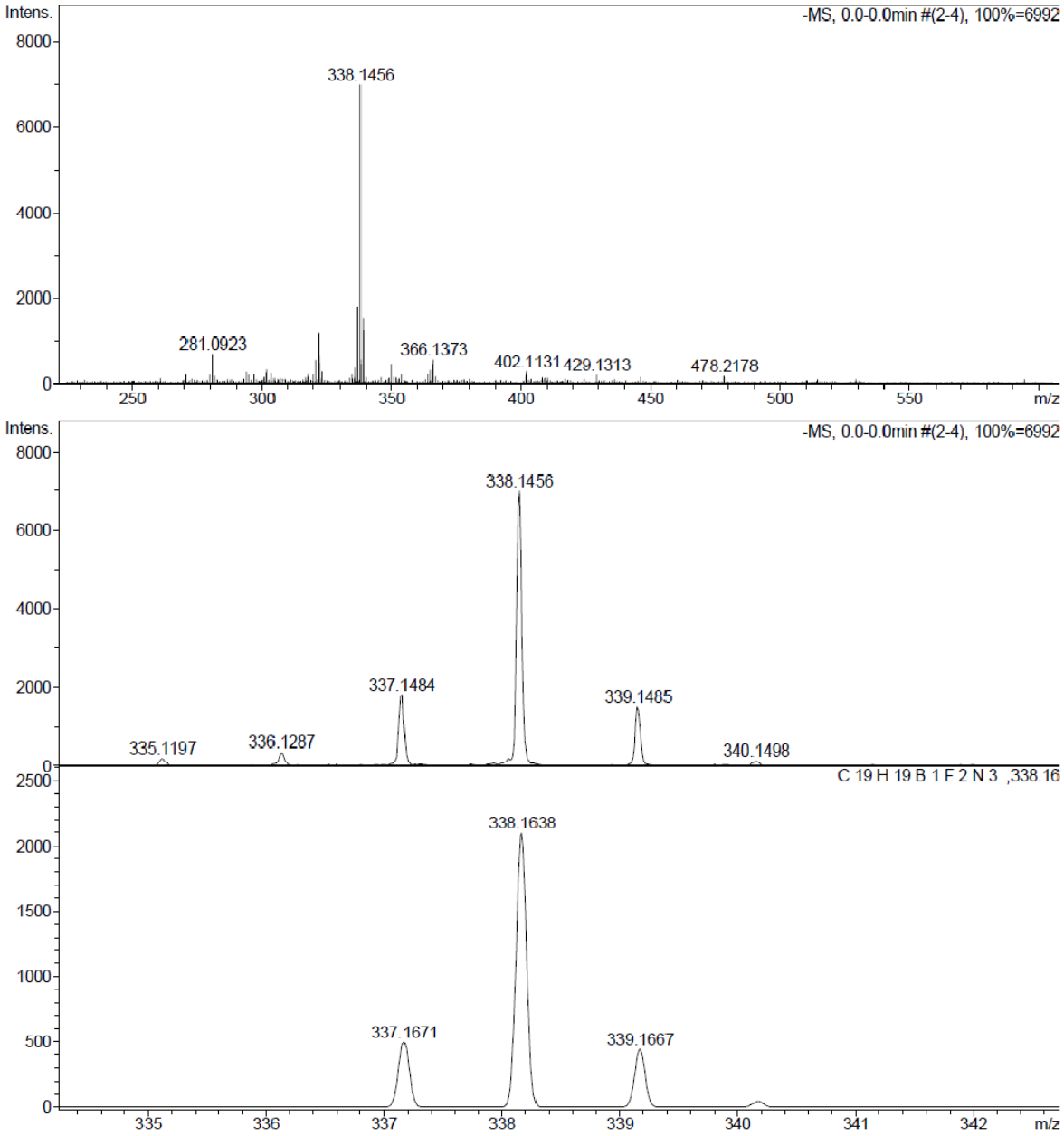

Figure S7. ESI-MS spectrum of **4.**

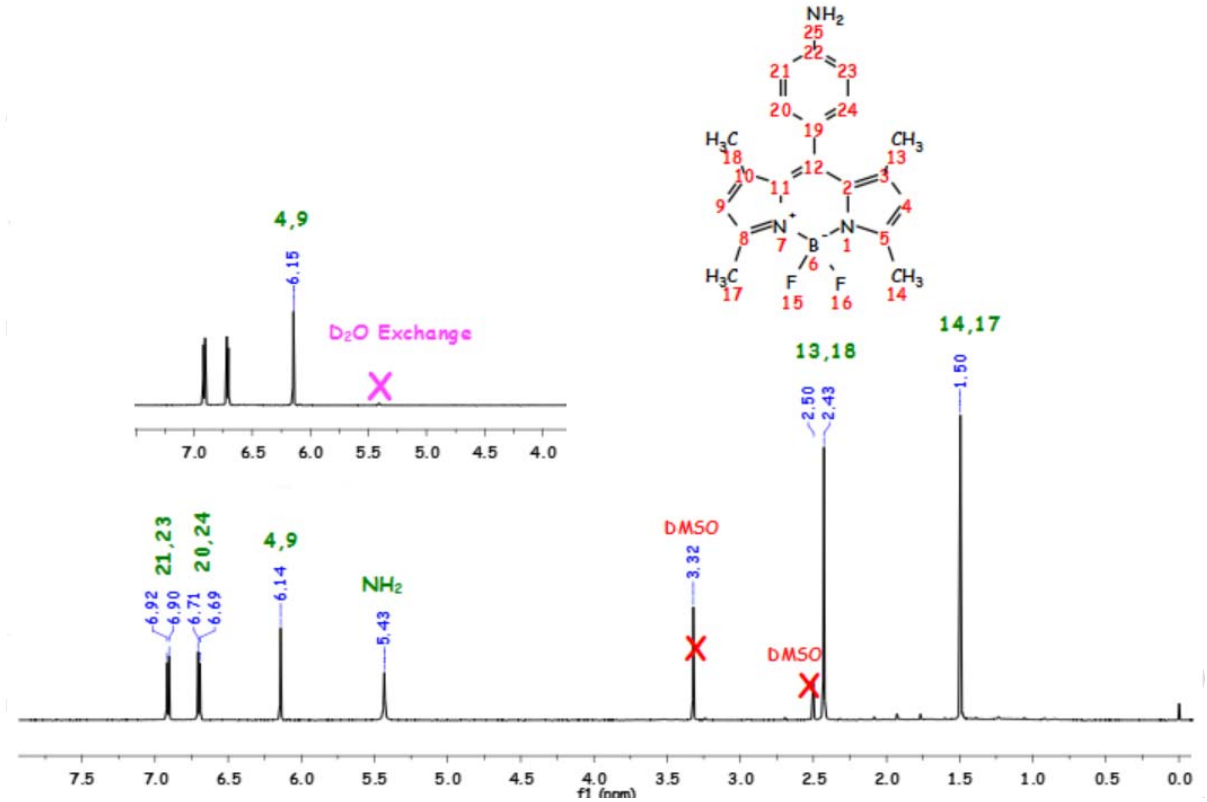

Figure S8. ^{1}H NMR spectrum of **4** in DMSO-d_6

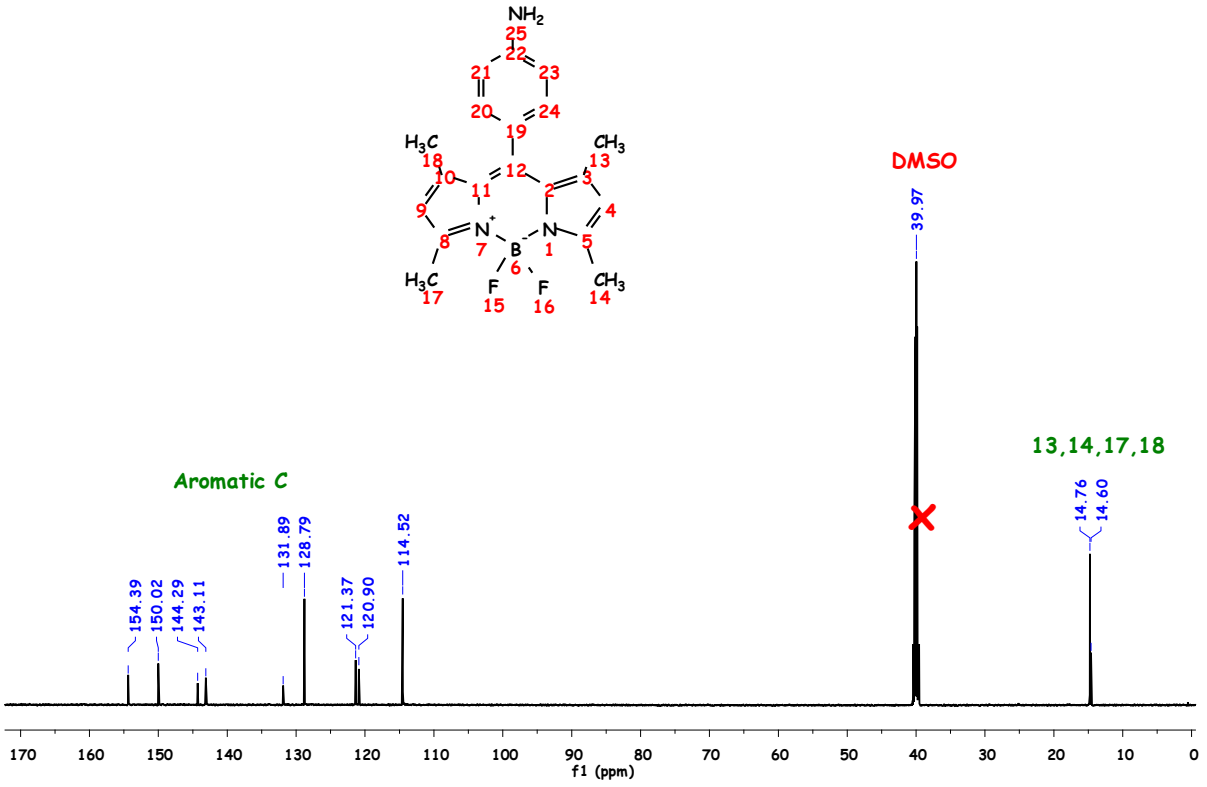

Figure S9. ^{13}C NMR spectrum of **4** in DMSO-d_6

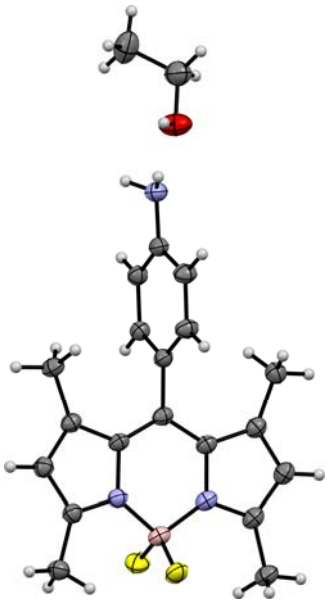

Figure S10. Crystal structure of compound **4** with EtOH solvate. Displacement ellipsoids are drawn at the 30% probability level. H-atoms are shown as small spheres of arbitrary radii. The red, grey, blue, pink, yellow, and white coloured atoms represent O, C, N, B, F, and H, respectively.

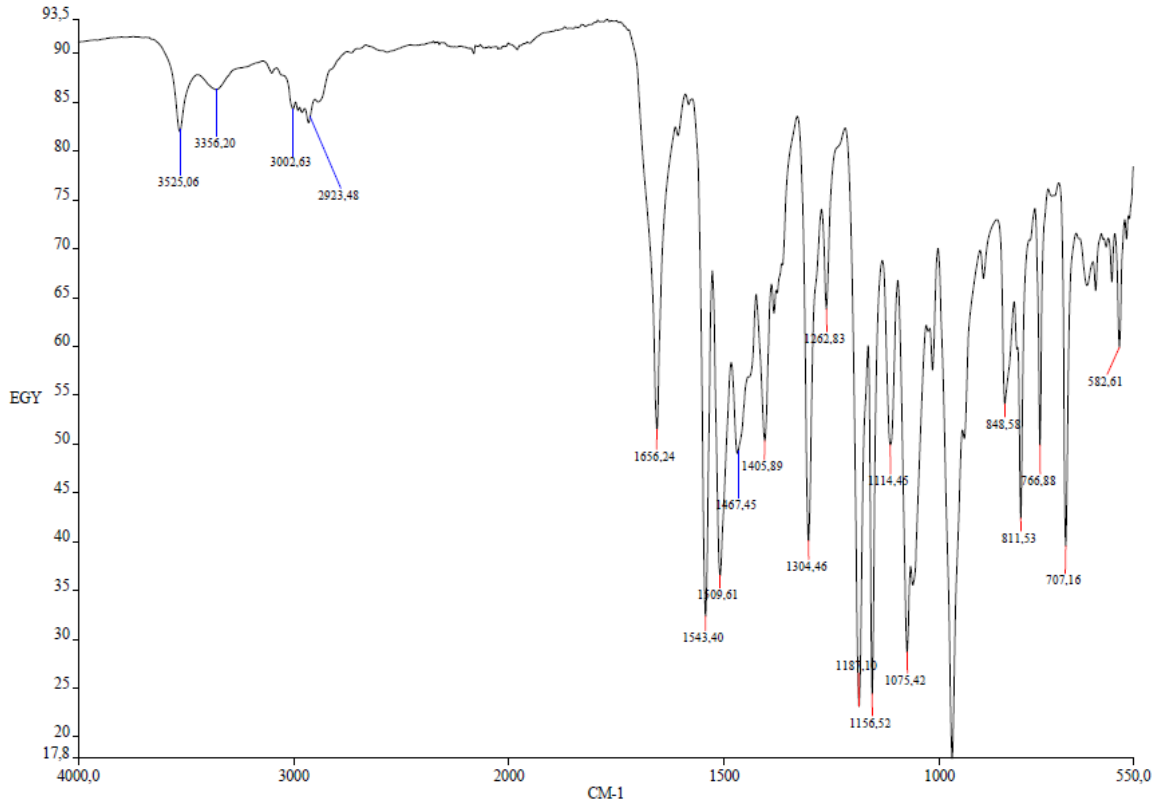

Figure S11. ATR-IR spectrum of **5.**

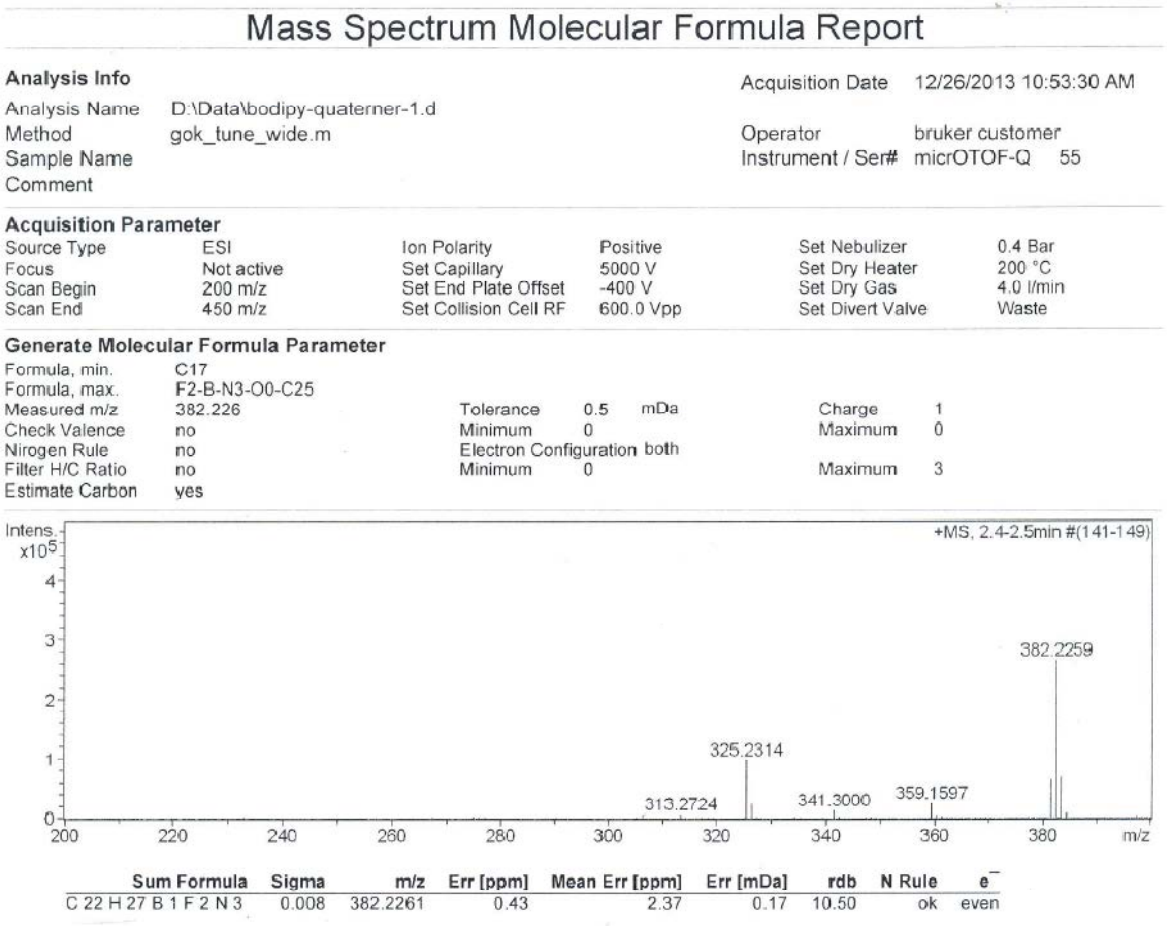

Figure S12. HRMS spectrum of **5**

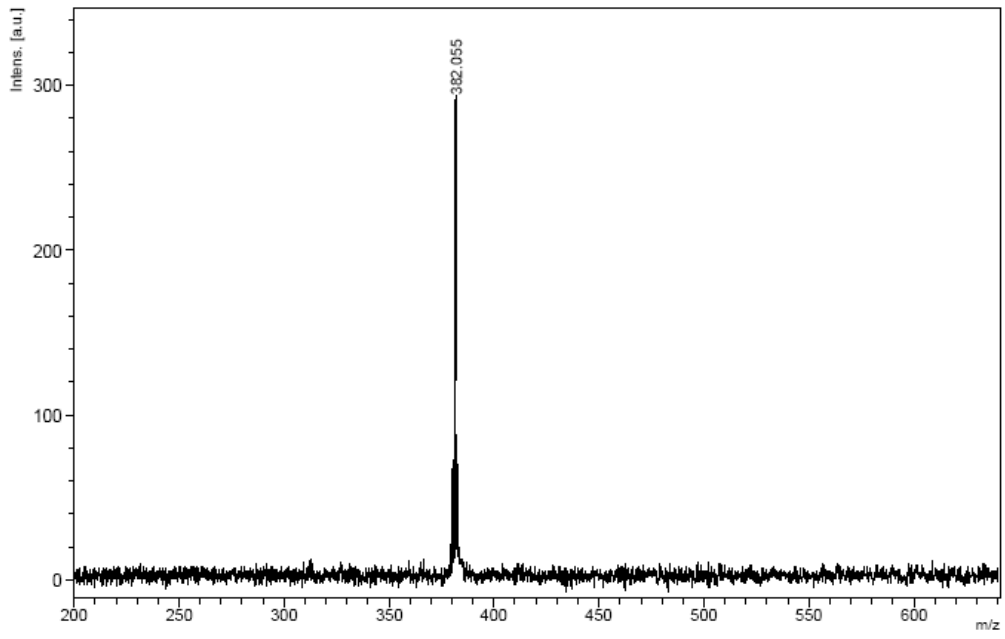

Figure S13. MALDI-TOF-MS spectrum of **5** (no matrix)

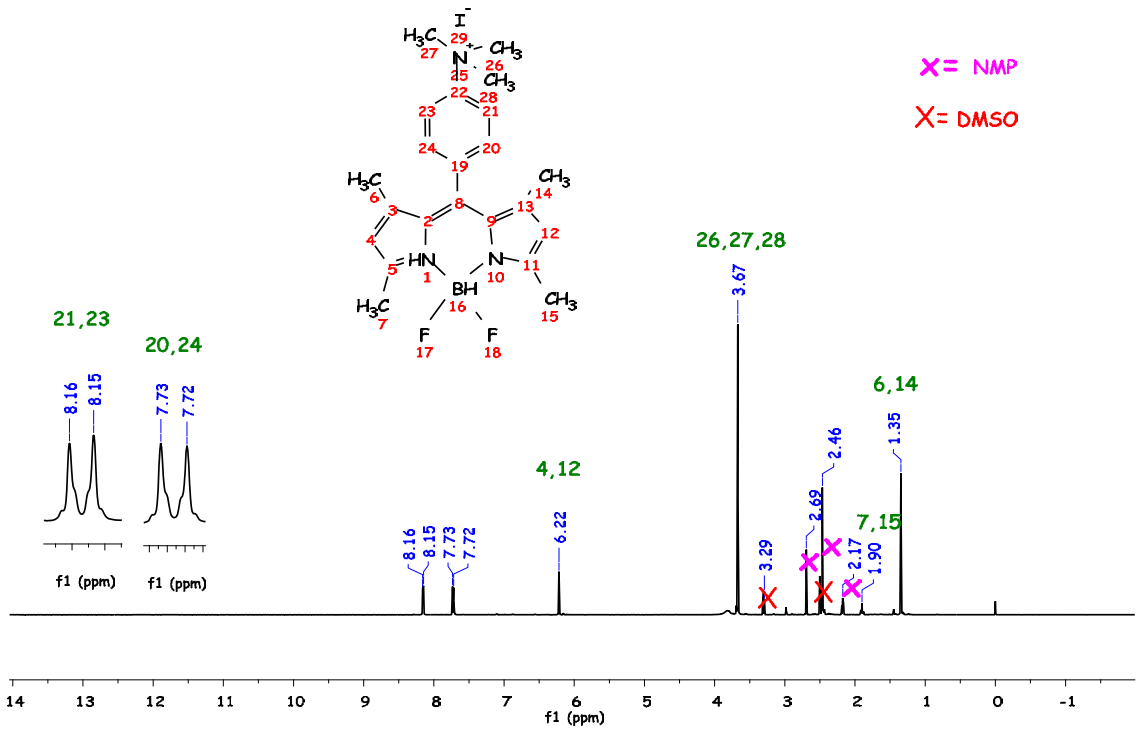

Figure S14. ^{1}H NMR spectrum of **5** in DMSO-d_6

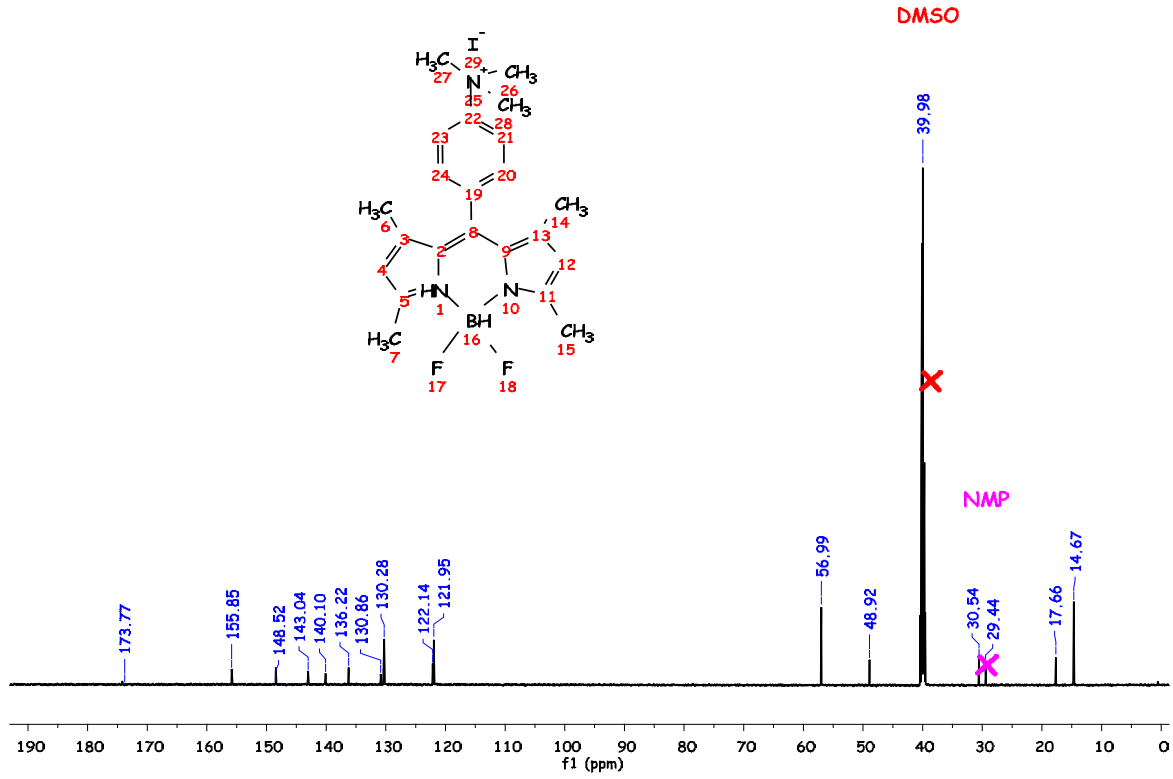

Figure S15. ^{13}C NMR spectrum of **5** in DMSO-d_6

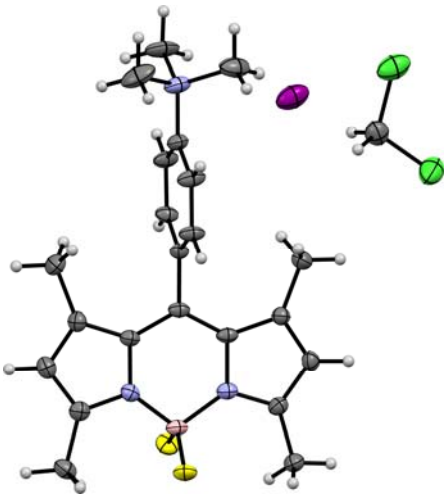

Figure S16. Crystal structure of compound **5** with DCM solvate. Displacement ellipsoids are drawn at the 20% probability level. H-atoms are shown as small spheres of arbitrary radii. The grey, blue, pink, yellow, purple, green and white coloured atoms represent C, N, B, F, I, Cl and H, respectively.

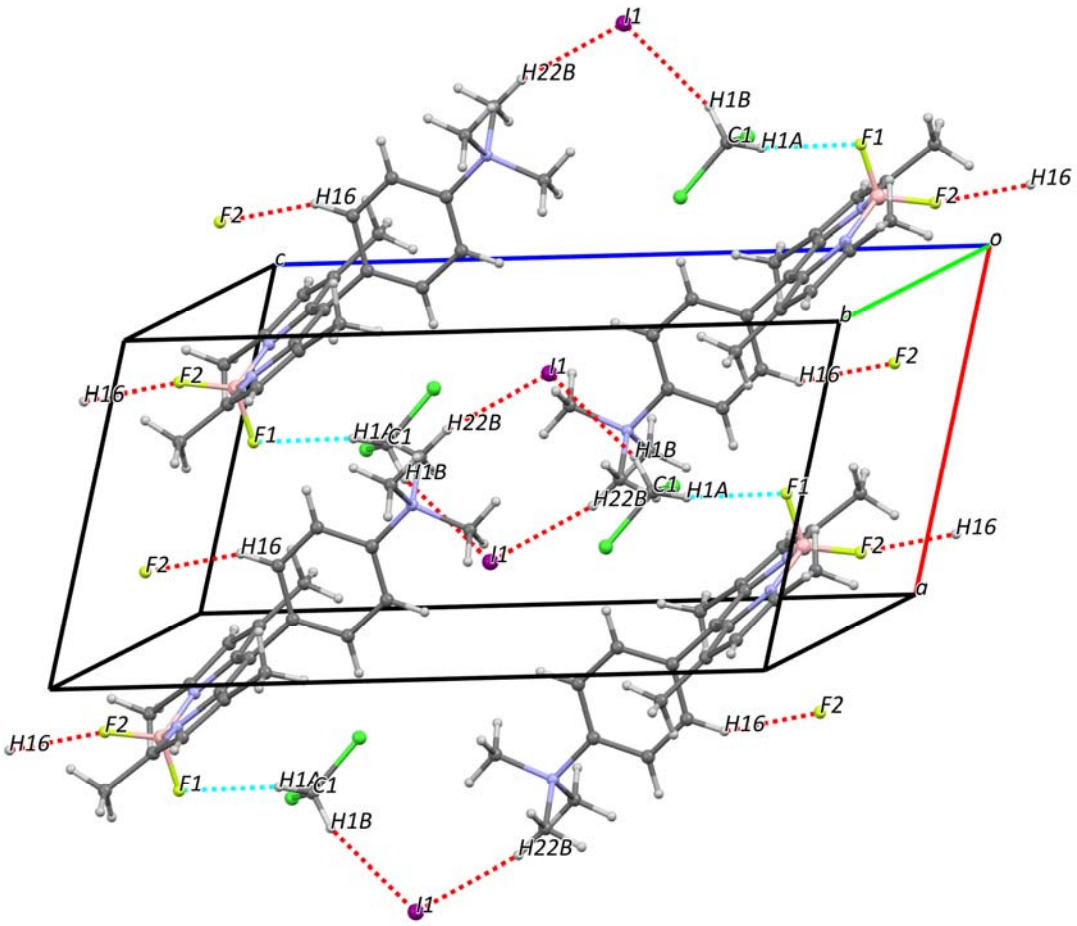

Figure S17. Perspective view of crystal packing of compound **5**, showing C-H···F, C-H···I interactions.

Photophysics and photochemistry

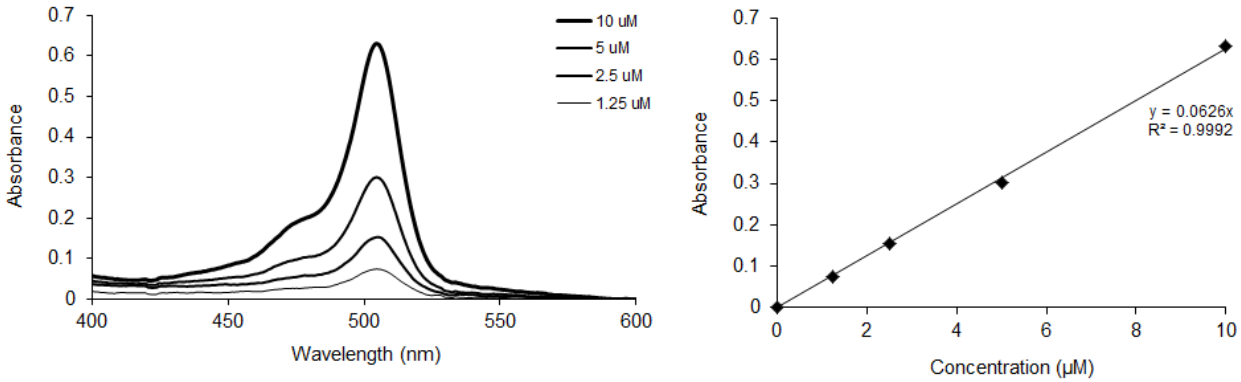

Figure S18. Left: Absorption spectra of **5** in DMSO at different four concentrations, Right: Absorbance *vs* concentration.

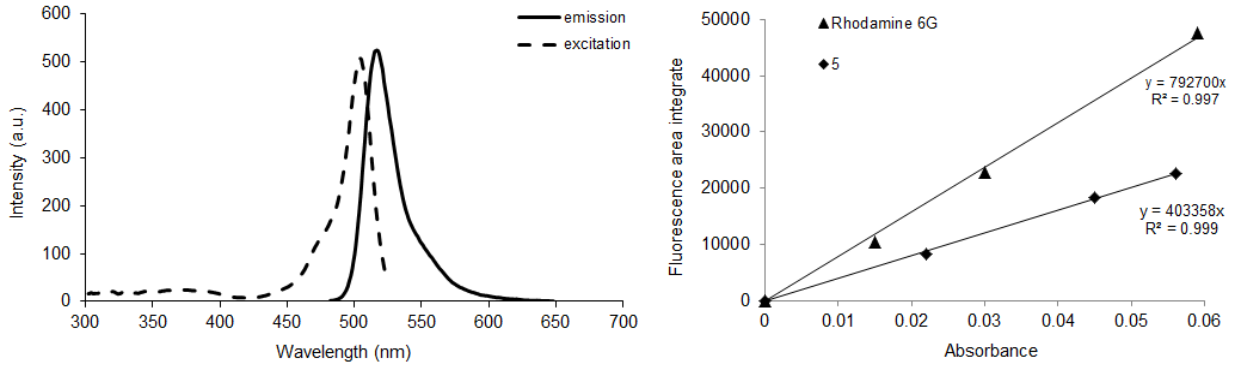

Figure S19. Left: Fluorescence excitation and emission spectra of **5** in DMSO (5 μM), Right: Fluorescence area integrate *vs* absorbance of **5** in DMSO and Rhodamine 6G in water at different three concentrations.

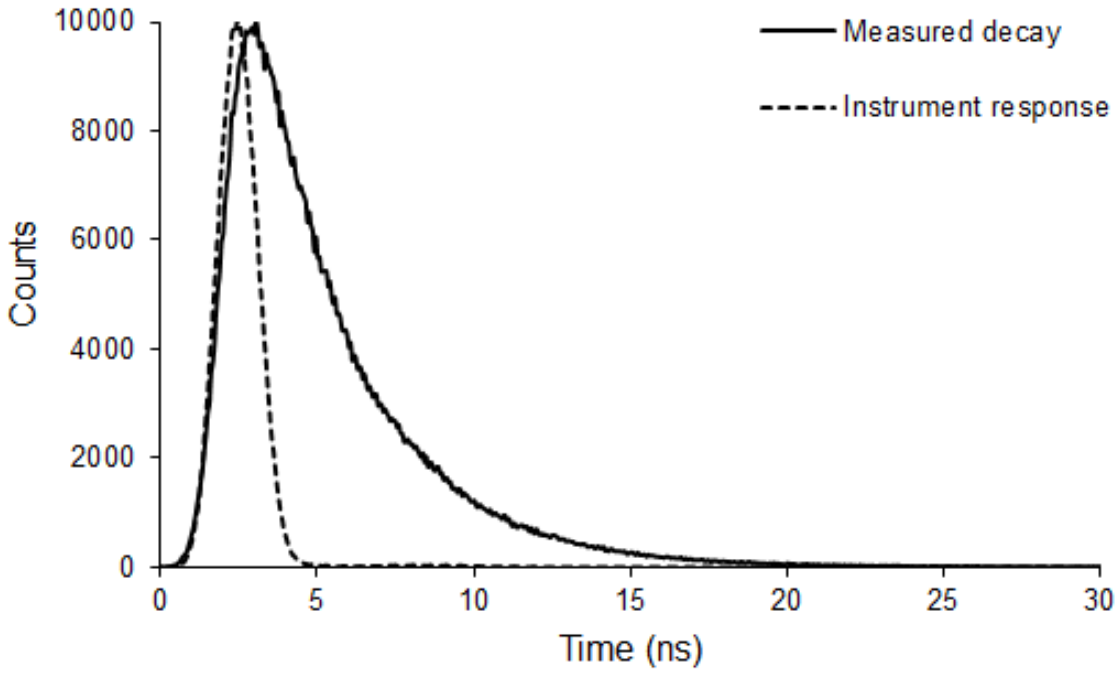

Figure S20. Fluorescence lifetime decay profile of **5** in DMSO.

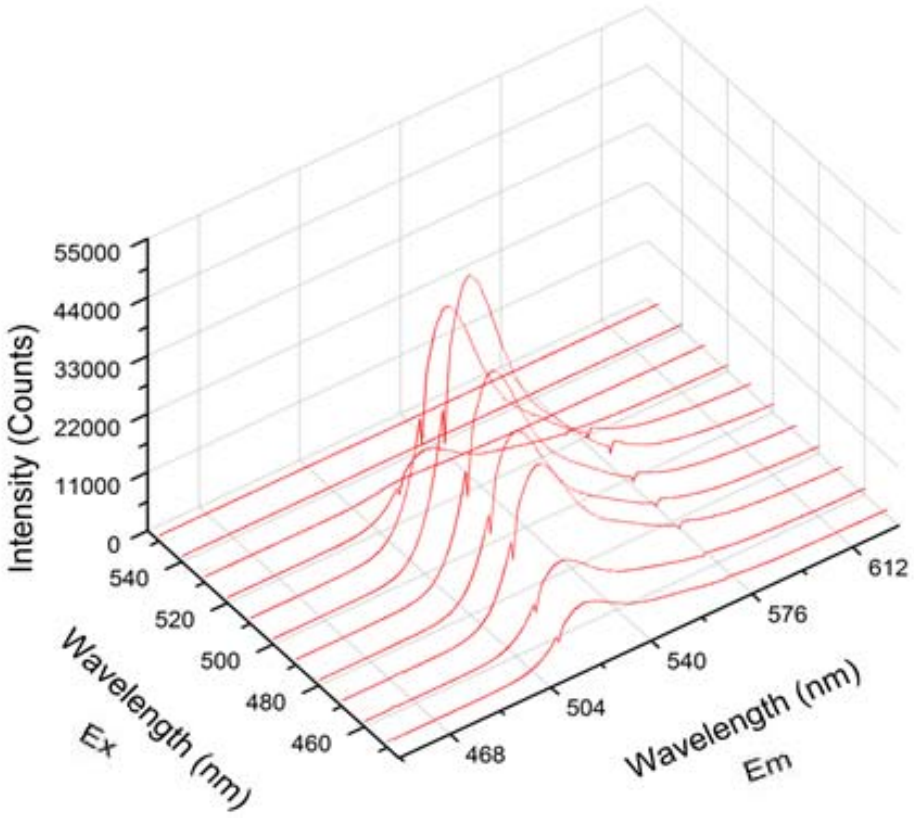

Figure S21. 3D fluorescence emission spectra in DMSO (excitation ranges from 450 to 550 nm).

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.
4. G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112-122.
5. A. L. Spek, *Acta Cryst*. 2009, **D65**, 148-155.
6. C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Cryst*., 2006, **39**, 453-457.

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

Datablock: I

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

Cell:            a=6.8808(5)     b=8.3233(6)         c=30.274(2)
                 alpha=90        beta=95.360(3)      gamma=90
Temperature:     120 K
```

	Calculated	Reported
Volume	1726.2(2)	1726.2(2)
Space group	P 21/n	P 1 21/n 1
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	

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Correction method= MULTI-SCAN

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S = 1.133                 Npar= 248
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Click on the hyperlinks for more details of the test.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

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

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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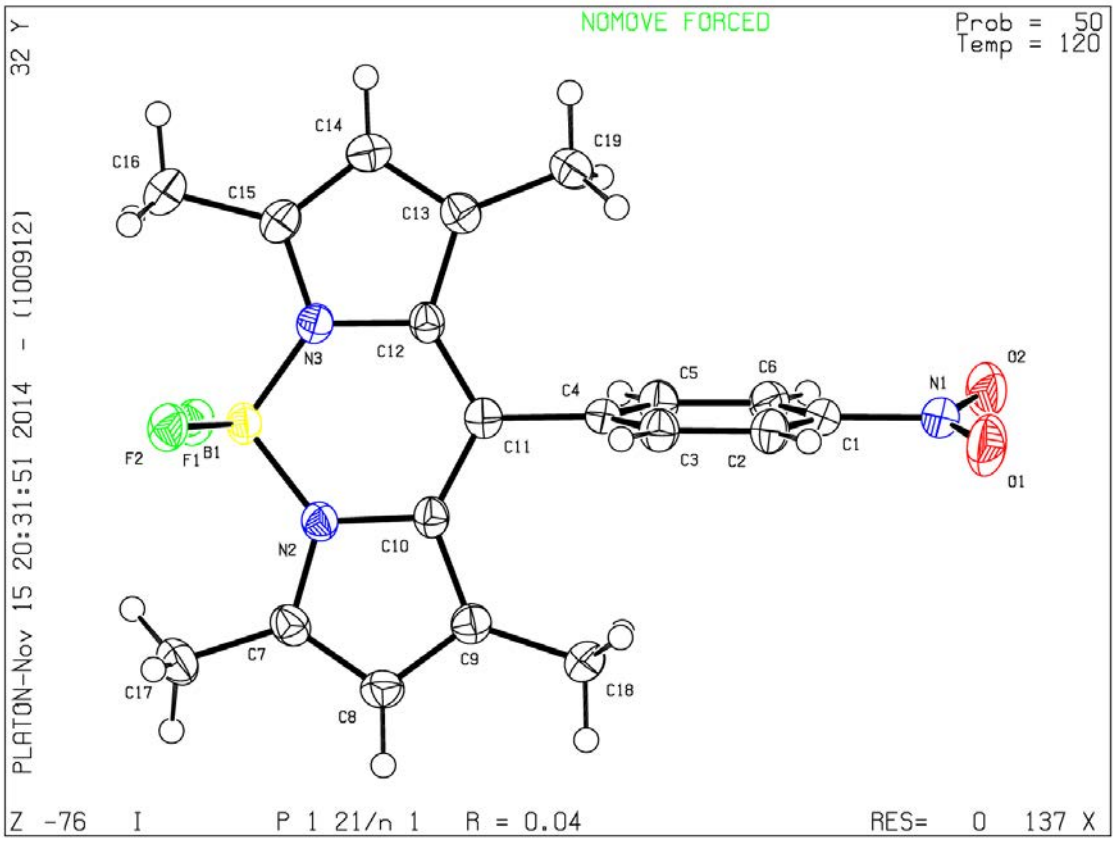
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock I - ellipsoid plot



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

Datablock: I

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=16.4780(12) b=7.1238(5) c=17.2258(12)
alpha=90 beta=101.934(4) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	1978.4(2)	1978.4(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C19 H20 B F2 N3, C2 H6 O	C19 H20 B F2 N3, C2 H6 O
Sum formula	C21 H26 B F2 N3 O	C21 H26 B F2 N3 O
Mr	385.26	385.26
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
Tmin’	0.965	

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
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Click on the hyperlinks for more details of the test.

Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         1 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         2 Note
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```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   0 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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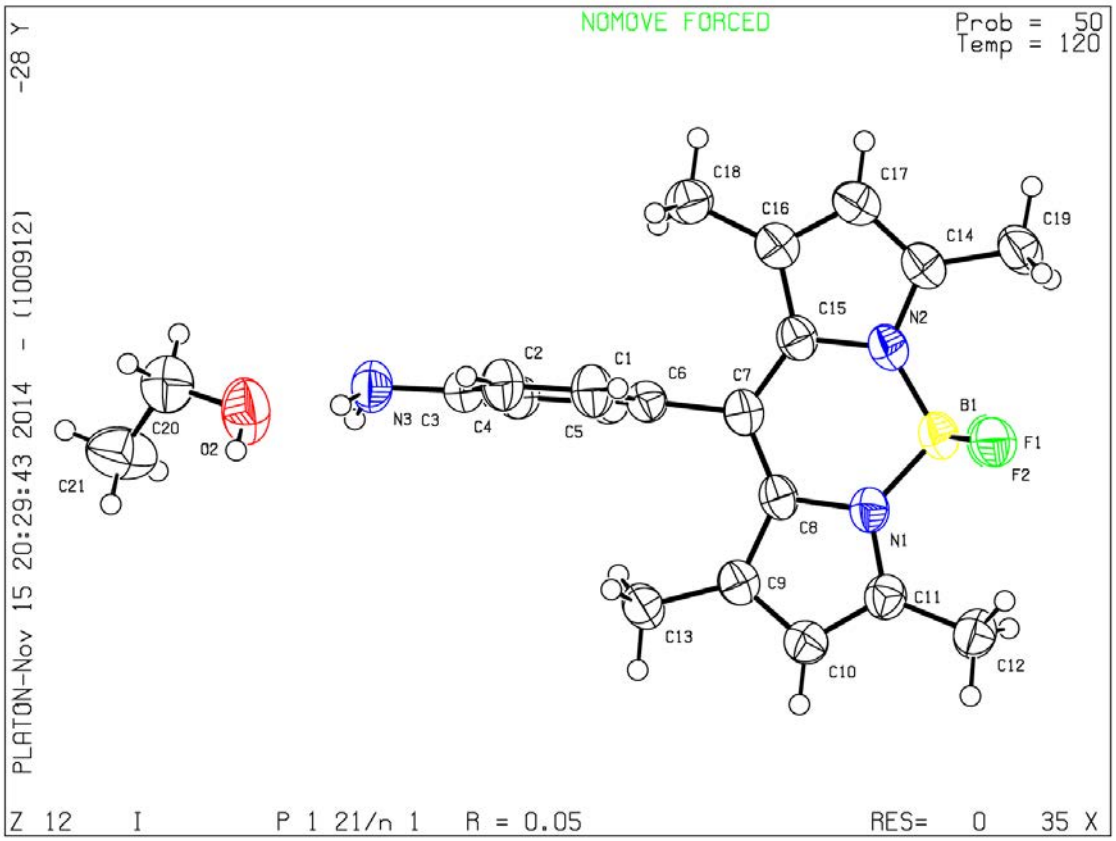
PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock I - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0113 A Wavelength=0.71073

Cell: a=8.5150(5) b=9.7941(6) c=17.2071(10)
alpha=76.580(3) beta=76.491(3) gamma=75.658(4)
Temperature: 150 K

	Calculated	Reported
Volume	1328.51(14)	1328.51(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H27 B F2 N3, C H2 Cl2, I	C22 H27 B F2 N3, C H2 Cl2, I
Sum formula	C23 H29 B Cl2 F2 I N3	C23 H29 B Cl2 F2 I N3
Mr	594.10	594.10
Dx,g cm-3	1.485	1.485
Z	2	2
Mu (mm-1)	1.436	1.436
F000	596.0	596.0
F000’	595.85	
h,k,lmax	10,11,20	10,11,20
Nref	4688	4684
Tmin,Tmax	0.886,0.904	0.720,0.910
Tmin’	0.806	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0852(3021) wR2(reflections)= 0.2288(4684)

S = 1.091 Npar= 296

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.

Alert level C

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N3 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          C1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0113 Ang.
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       6.10 Why ?
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .         16 A**3
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock I - ellipsoid plot