Supporting Information for

New Insight into the Application of GFP Chromophore Inspired Derivatives: a F^- Fluorescent Chemodosimeter

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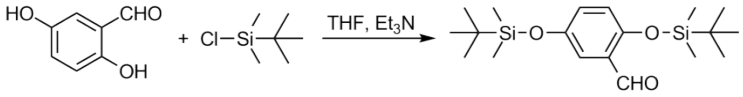
Table of Contents

General Methods

N,N-dimethylformamide (DMF) and other chemical reagents for synthesis and analysis are analytical grade, obtained from commercial suppliers, and used without further purification unless specified. DMF was initially dried by distillation over CaH_2 before use. All the anionic compounds such as $[Bu_4N]F$, $[Bu_4N]Cl$, $[Bu_4N]Br$, $[Bu_4N]I$, $[Bu_4N]HSO_4$, $[Bu_4N]NO_3$, $[Bu_4N]ClO_4$, $[Bu_4N]AcO$ and $[Bu_4N]H_2PO_4$ were purchase from Energy Chemical Co.. ^1H NMR and ^{13}C NMR were acquired in $CDCl_3$ on BRUKER AVANCE 500 spectrometer using TMS as an internal standard. Mass spectrum was obtained on HP 5989 mass spectrometer.

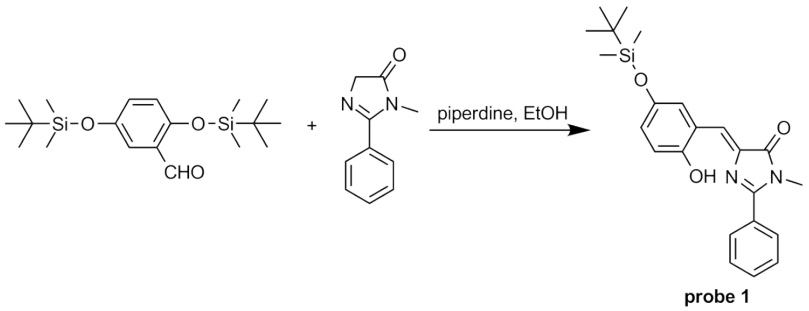
Synthesis

Synthesis of 2,5-bis(tert-butyldimethylsilyloxy)benzaldehyde



A solution of 2,5-dihydroxybenzaldehyde (0.69 g, 5.0 mmol) in CH_2Cl_2 (10 mL) was added to a mixture of tert-butyldimethylsilyl chloride (3.00 g, 20.0 mmol) and Et_3N (2.77 mL, 20.0 mmol) in CH_2Cl_2 (20 mL) at 0oC. At same temperature the reaction solution was stirred for 2 h, then poured into sat.NH_4Cl, extracted with CH_2Cl_2 and dried ($MgSO_4$). After concentrated, the residue was purified by silica gel column chromatography to get the 2,5-bis(tert-butyldimethylsilyloxy)benzaldehyde (0.75 g, 41.8%) as a colorless oil.[1] δ_H (400 MHz, $CDCl_3$) 10.31 (1 H, s), 7.16 (1 H, s), 6.89 (1 H, d, J 6.5), 6.68 (1 H, d, J 8.8), 0.93 (9 H, s), 0.89 (9 H, s), 0.16 (6 H, s), 0.10 (6 H, s).

Synthesis of compound 1

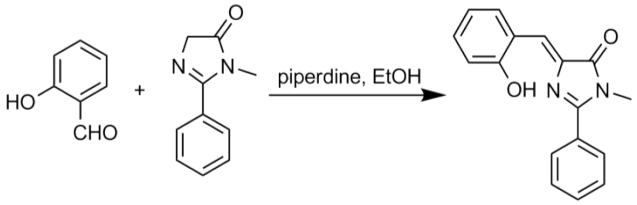


probe 1

A solution of 2,5-bis(tert-butyldimethylsilyloxy)benzaldehyde (0.36 g, 1.0 mmol), 1-methyl-2-phenyl-1H-imidazol-5(4H)-one (0.17 g, 1.0mmol) and 2-3 drops piperdine in 6 ml ethanol in 25 ml round-bottom flask was stirred at 80°C for 4h. When the reaction is completed, the mixture

was cooled. After evaporation of the solvent, the oily residue was purified by column chromatography to afford chemosensor 1 (0.13 g, 31.8%) as a orange solid.2 δ_H (400 MHz, CDCl3) 13.60 (1 H, s), 7.81 (2 H, d, J 8.0), 7.62-7.51 (3 H, m), 7.23 (1 H, s), 6.92 – 6.80 (3 H, m), 3.45 (3 H, s), 0.99 (9 H, s), 0.19 (6 H, s); δc (101 MHz, CDCl3) 169.34, 167.91, 156.15, 152.47, 146.90, 132.39, 131.11, 130.36, 128.10, 127.38, 126.68, 126.16, 124.57, 123.43, 118.9, 28.36, 25.08, 24.66 , 23.5, 17.14, -5.52; MS calculated for C23H28N2O3Si 408.1869, found 408.1870.

4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one



4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one was synthesized using same method as compound **1**. The product was pilfered and dried to afford 4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one as a yellow solid, yield 81 %; δ_H (400 MHz, DMSO) 11.64 (1 H, s), 8.37 (1 H, d, J 7.7), 7.93 (2 H, d, J 7.4), 7.72–7.56 (3 H, m), 7.47 (1 H, s), 7.31 (1 H, t, J 7.6), 6.91 (2 H, t, J 8.6), 3.30 (3 H, s); δ_C (101 MHz, DMSO) 170.21, 161.19, 158.38, 136.55, 134.31, 133.36, 132.24, 129.40, 129.06, 124.36, 121.08, 119.99, 117.19, 29.26; Mass spectrum: calculated for C17H14N2O2 278.1055, found 278.1058.

Fluorometric Analysis

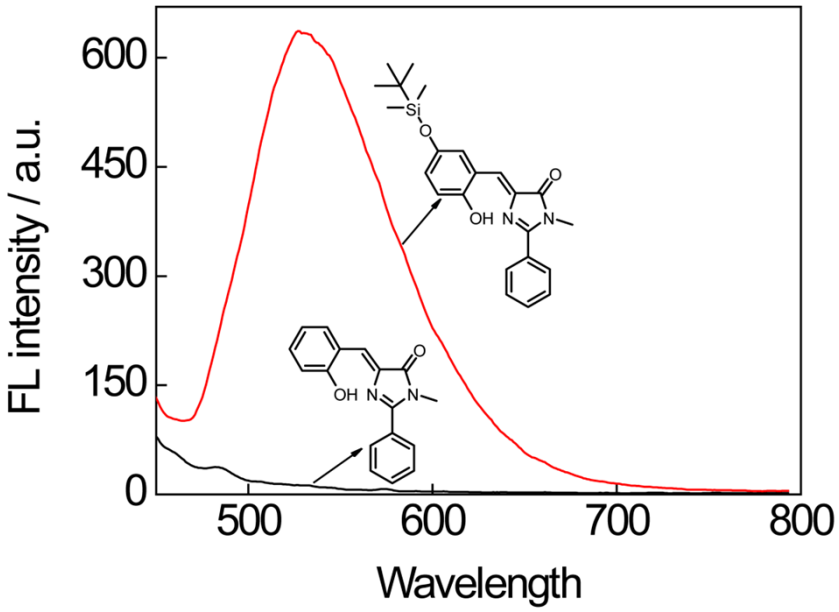


Figure S1. Fluorescence spectra of compound 1 (5 μM) and 4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one (5 μM) in DMF at λex = 420 nm.

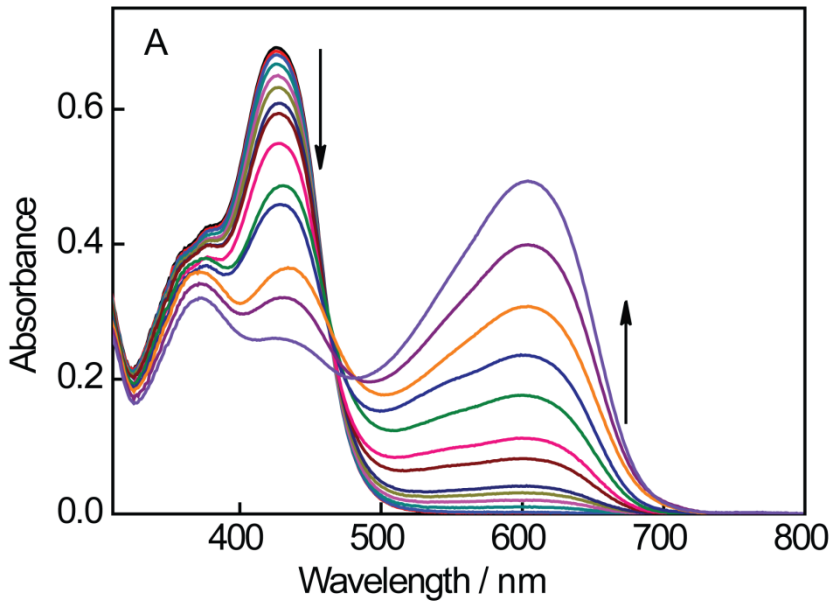


Figure S2. A: UV-vis absorption spectra changes of compound **1** (50 μM) in the presence of F^- concentrations (0, 5, 10, 20, 30, 40, 50, 75, 100, 150, 200, 300, 600 μM) in DMF.

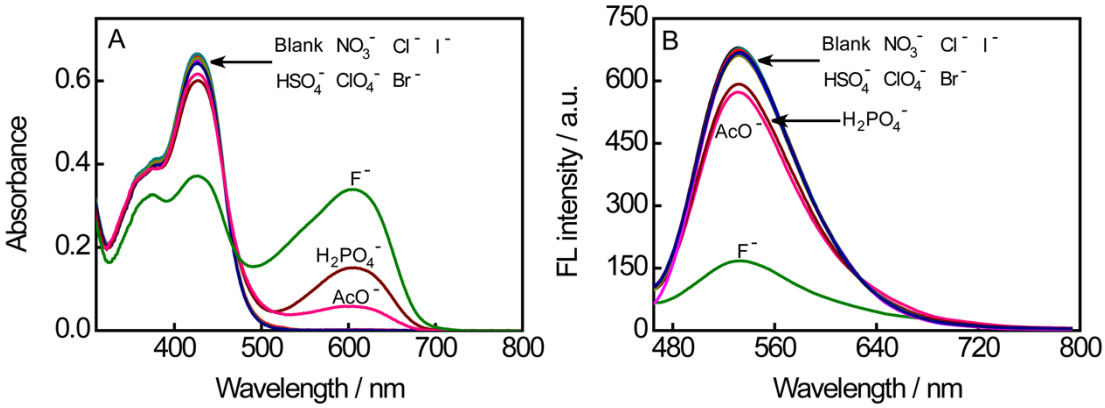


Figure. S3 A: UV-vis absorption spectral changes of compound **1** (50 μM) after treatment with 8.0 equivalents of Cl^-、Br^-、I^-、NO_3^-、ClO_4^-、HSO_4^- 、$H_2PO_4^-$、AcO^- and F^- as tetrabutyl-ammonium salt in DMF; B: Fluorescence changes of coumpound **1** (5 μM) after treatment with 64.0 equivalents of Cl^-、Br^-、I^-、NO_3^-、ClO_4^-、HSO_4^-、$H_2PO_4^-$、AcO^- and F^- as tetrabutyl-ammonium salt in DMF at λex = 420nm.

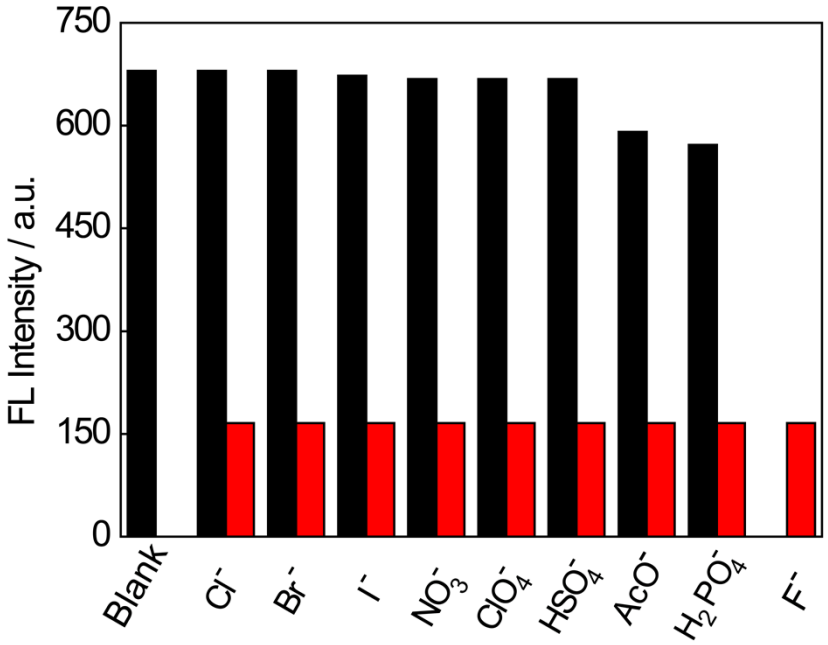


Figure. S4 Fluorescence responses of competitive experiment of compound **1** (5 μM) with common anions in DMF at λex = 420nm. Black bars represent the fluorescence

responses of blank and a single anion including 64.0 equivalents of Cl^-、 Br^-、I^-、NO_3^-、ClO_4^-、HSO_4^-、$H_2PO_4^-$、AcO^- and F^- as tetrabutyl-ammonium salt; red bars represent the subsequent addition of F^- to the mixture solution. All data is the fluorescent intensity at 532 nm.

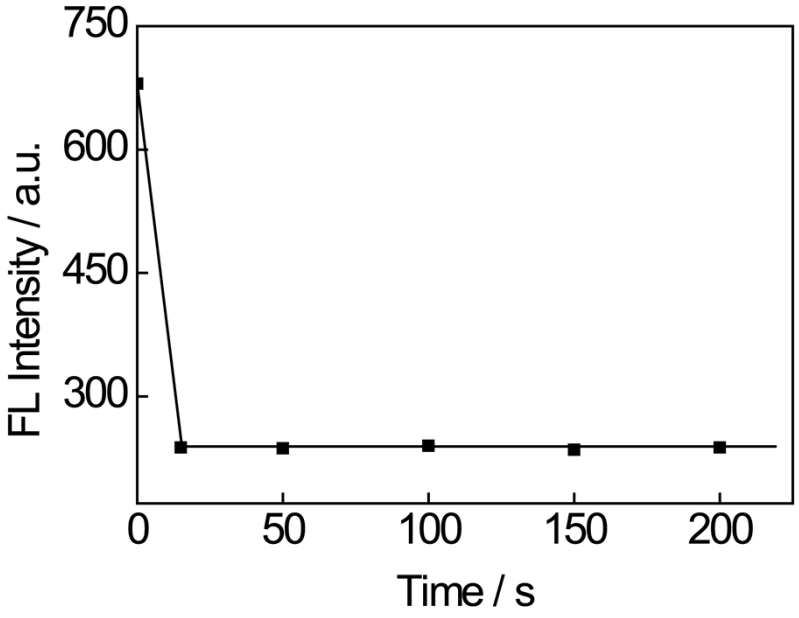


Figure. S5 Effect of reaction time on the fluorescence intensity of compound **1** (5 μM) with 36.0 equivalents of F^- in DMF at λex = 420nm. All data is the fluorescent intensity at 532 nm.

NMR and MS spectra

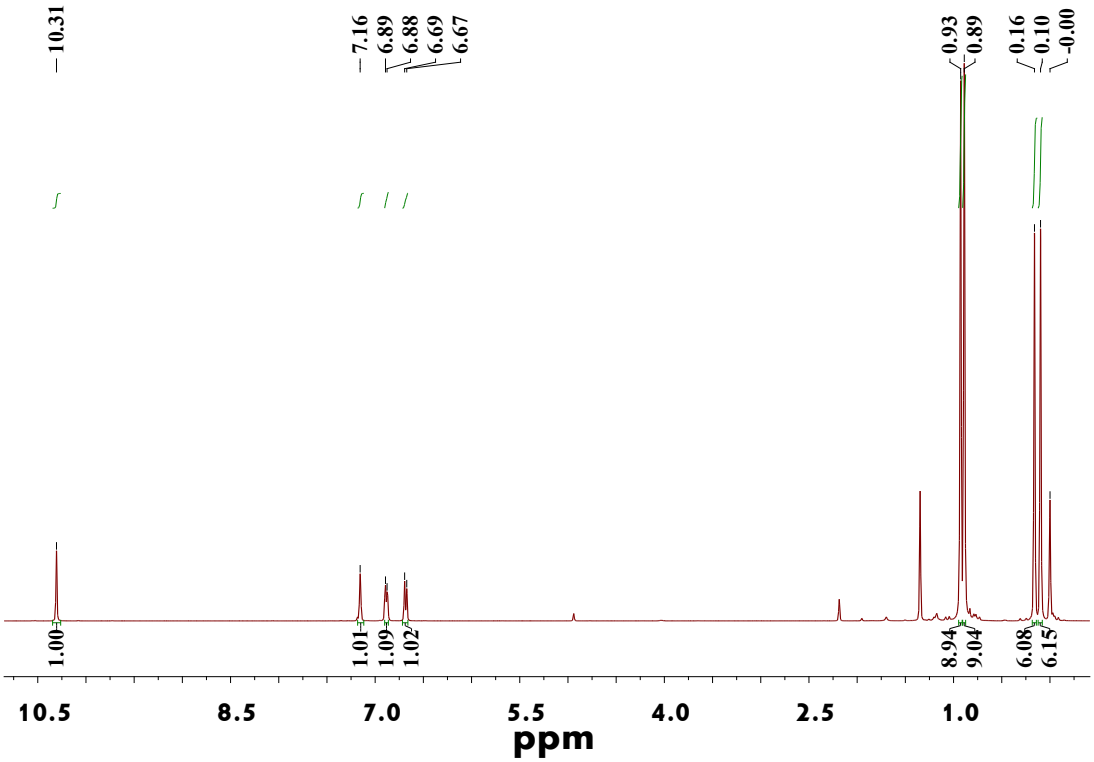


Figure S5. ^{1}H NMR spectrum of 2,5-bis(tert-butyldimethylsilyloxy)benzaldehyde in $CDCl_3$

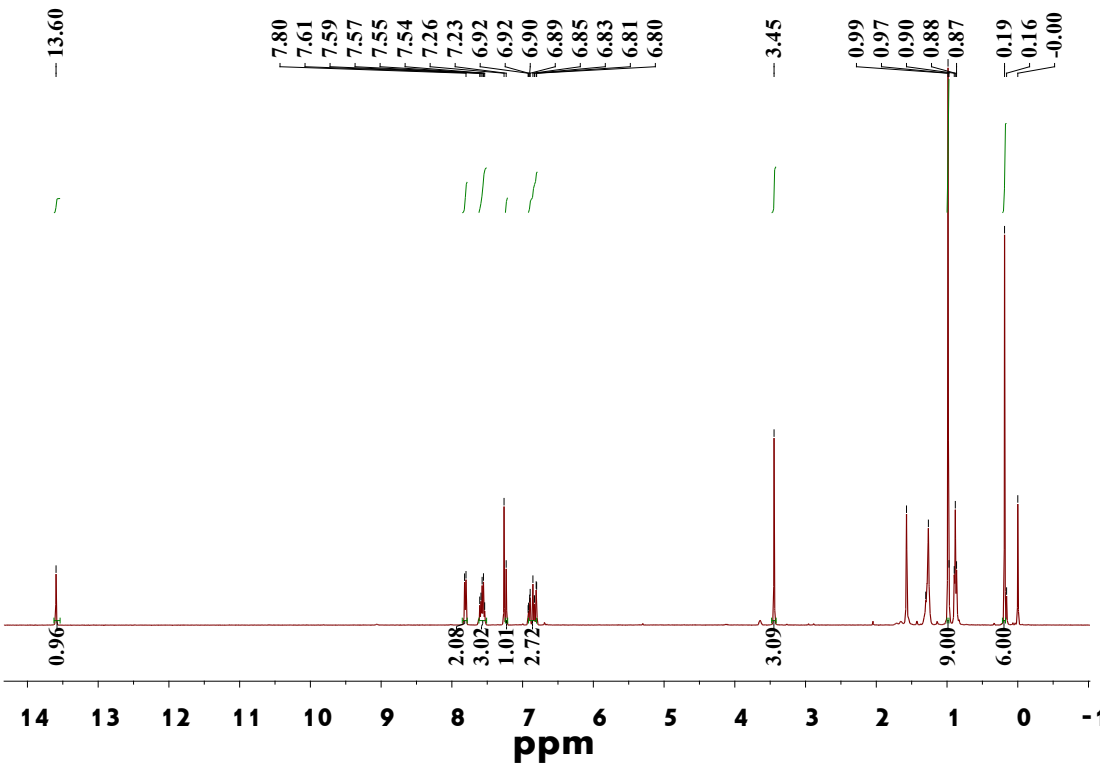


Figure S6. ^{1}H NMR spectrum of compound **1** in $CDCl_3$

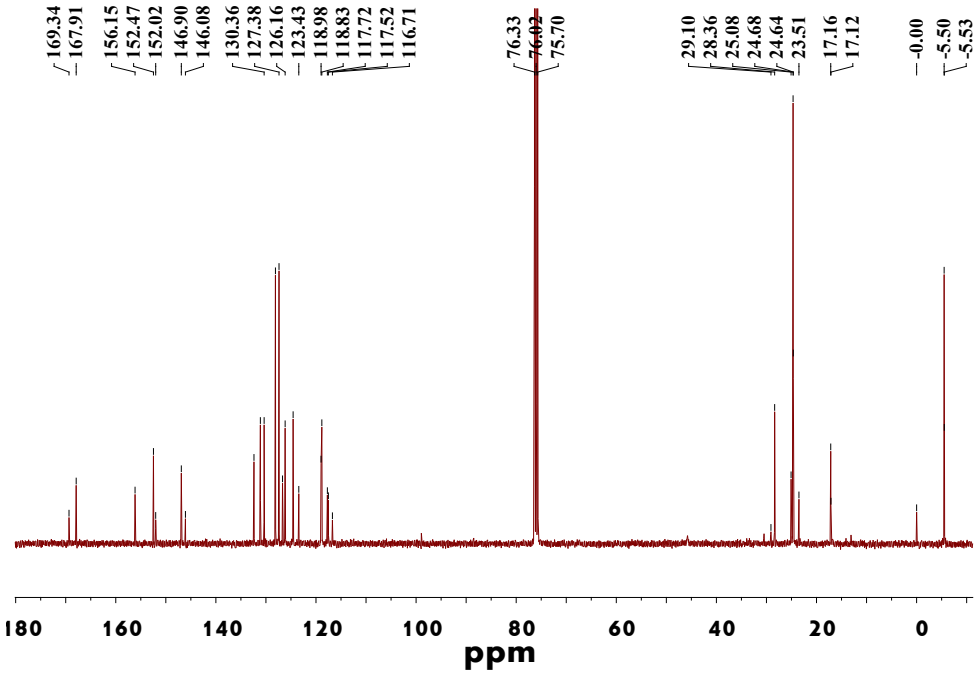


Figure S7. ^{13}C NMR spectrum of compound **1** in $CDCl_3$

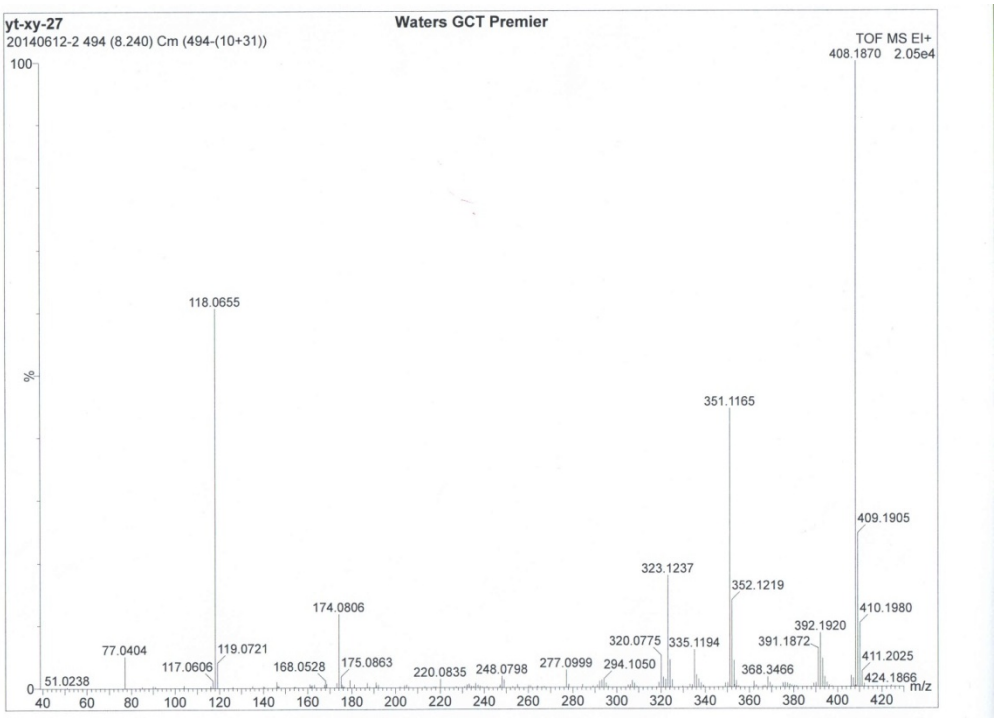


Figure S8. MS spectrum of compound **1** in $CDCl_3$

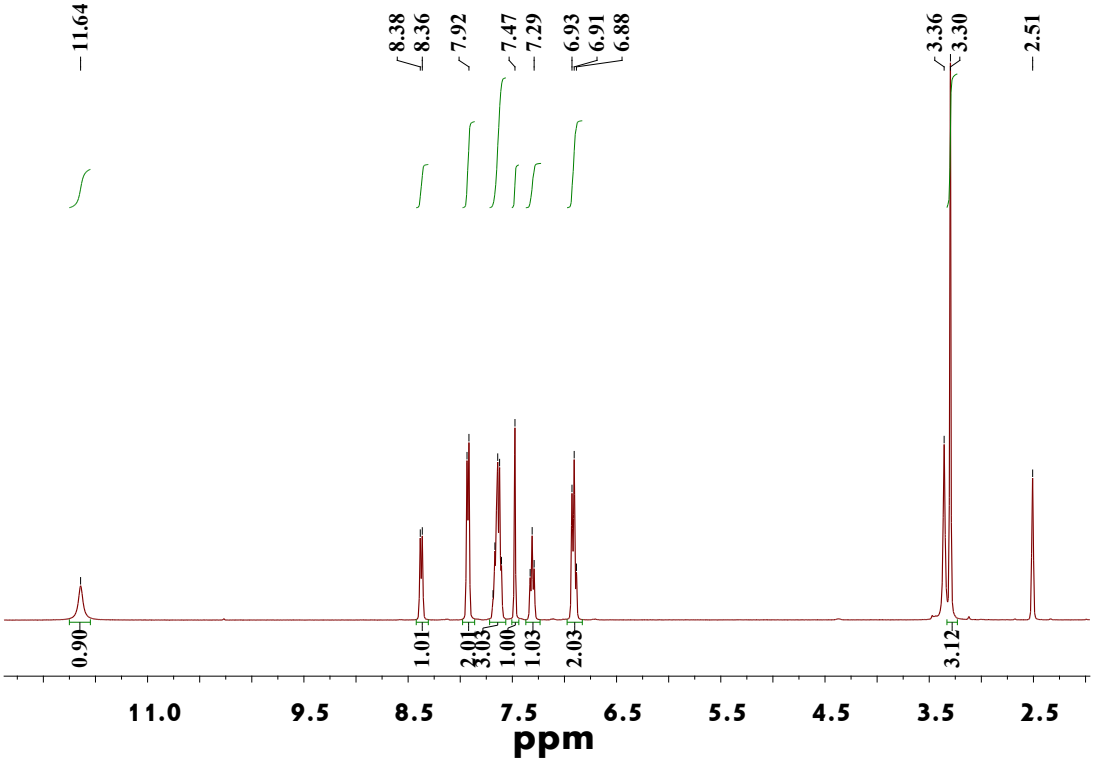


Figure S9. ^1H NMR spectrum of 4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one in $CDCl_3$

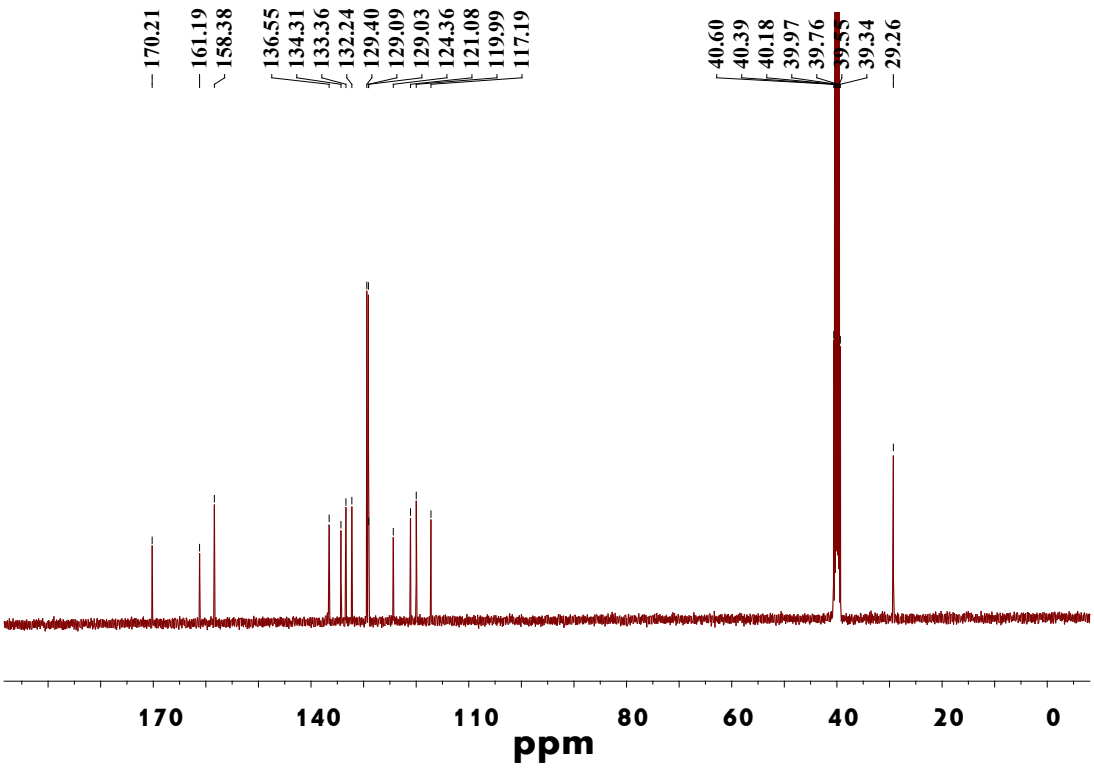


Figure S10. ^{13}C NMR spectrum of 4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one in $CDCl_3$

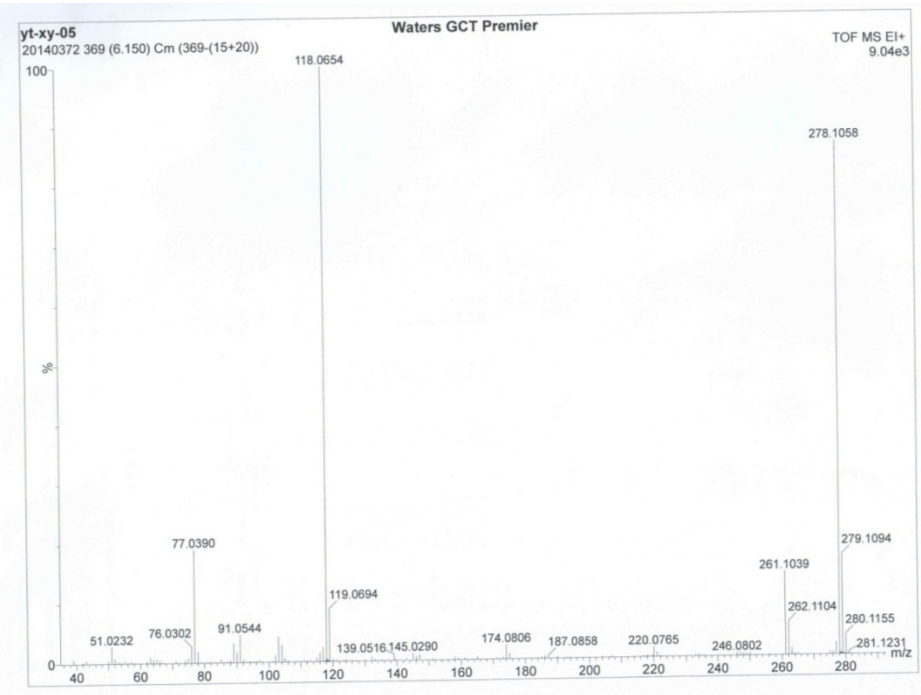


Figure S11. MS spectrum of 4-(2-hydroxybenzylidene)-1-methyl-2-phenyl-1H-imidazol-5(4H)-one in $CDCl_3$

References

1. A. Kojima, T. Takemoto, M. Sodeoka and M. Shibasaki, *J. Org. Chem.*, 1996, **61**, 4876-4877.
2. Y. Li, L. Shi, L. X. Qin, L. L. Qu, C. Jing, M. Lan, T. D. James and Y. T. Long, *Chem. Commun.*, 2011, **47**, 4361-4363.

Single Crystal Data

Table 1. Crystal data and structure refinement for compound 1.

Identification code	cd214277	
Empirical formula	C23 H28 N2 O3 Si	
Formula weight	408.56	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 32.516(6) Å	α= 90°.
	b = 10.7386(19) Å	β= 113.348(4)°.
	c = 13.927(3) Å	γ = 90°.
Volume	4464.7(14) $Å^3$	
Z	8	
Density (calculated)	1.216 Mg/m^3	
Absorption coefficient	0.131 mm^{-1}	
F(000)	1744	
Crystal size	0.211 x 0.175 x 0.087 mm^3	
Theta range for data collection	2.015 to 25.499°.	
Index ranges	-36<=h<=39, -9<=k<=13, -16<=l<=16	

Reflections collected	12754
Independent reflections	4151 [R(int) = 0.0598]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6221
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4151 / 79 / 340
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0800, wR2 = 0.2120
R indices (all data)	R1 = 0.1349, wR2 = 0.2523
Largest diff. peak and hole	0.689 and -0.383 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	-607(1)	5065(3)	3280(2)	67(1)
N(2)	126(1)	5426(3)	3792(2)	66(1)
O(1)	-615(1)	2915(3)	3411(2)	92(1)
O(2)	995(1)	5484(3)	4380(2)	90(1)
O(3)	1701(1)	729(3)	4905(3)	118(1)
C(1)	-271(1)	5931(3)	3469(2)	63(1)
C(2)	-414(1)	3888(4)	3485(3)	71(1)
C(3)	67(1)	4144(3)	3805(3)	66(1)
C(4)	378(1)	3242(3)	4038(3)	73(1)
C(5)	856(1)	3237(4)	4337(3)	73(1)
C(6)	1061(2)	2056(4)	4488(3)	84(1)
C(7)	1509(2)	1905(5)	4781(4)	95(1)
C(8)	1775(2)	2942(5)	4907(4)	102(1)
C(9)	1589(2)	4112(5)	4775(4)	95(1)
C(10)	1133(1)	4282(4)	4497(3)	77(1)
C(11)	-342(1)	7275(3)	3323(3)	64(1)
C(12)	-15(1)	8073(3)	3953(3)	76(1)
C(13)	-65(2)	9339(4)	3823(4)	86(1)
C(14)	-442(2)	9832(4)	3062(4)	89(1)
C(15)	-770(2)	9052(4)	2418(3)	87(1)
C(16)	-723(1)	7775(4)	2540(3)	76(1)
C(17)	-1081(1)	5241(4)	3044(3)	82(1)

Si(1)	1742(1)	-438(3)	5657(2)	115(1)
C(18)	1900(5)	-1942(12)	5087(12)	123(4)
C(19)	1180(3)	-942(15)	5548(11)	106(4)
C(20)	2104(4)	-67(12)	7003(10)	150(4)
C(21)	2087(5)	-1147(14)	7707(9)	181(5)
C(23)	2598(4)	94(16)	6986(11)	160(5)
C(22)	1865(8)	1040(20)	7310(20)	171(11)
Si(1')	2002(1)	205(4)	6223(4)	98(1)
C(18')	1956(9)	1220(20)	7200(20)	86(5)
C(19')	2581(6)	-60(20)	6280(16)	136(6)
C(20')	1737(5)	-1335(14)	6127(11)	121(4)
C(21')	1948(8)	-2076(19)	7149(15)	184(8)
C(22')	1992(11)	-1900(40)	5500(20)	226(18)
C(23')	1238(8)	-1120(30)	5970(20)	186(15)

Table 3. Bond lengths [Å] and angles [°] for compound 1.

N(1)-C(1)	1.380(4)
N(1)-C(2)	1.391(4)
N(1)-C(17)	1.454(5)
N(2)-C(1)	1.303(4)
N(2)-C(3)	1.391(4)
O(1)-C(2)	1.216(4)
O(2)-C(10)	1.355(5)
O(2)-H(2)	0.837(19)
O(3)-C(7)	1.389(5)
O(3)-Si(1)	1.605(4)
O(3)-Si(1')	1.795(6)
C(1)-C(11)	1.463(5)
C(2)-C(3)	1.471(5)
C(3)-C(4)	1.343(5)
C(4)-C(5)	1.443(6)
C(4)-H(4)	0.9300
C(5)-C(10)	1.400(5)
C(5)-C(6)	1.409(5)
C(6)-C(7)	1.359(6)
C(6)-H(6)	0.9300
C(7)-C(8)	1.377(7)

C(8)-C(9)	1.375(6)
C(8)-H(8)	0.9300
C(9)-C(10)	1.388(6)
C(9)-H(9)	0.9300
C(11)-C(12)	1.378(5)
C(11)-C(16)	1.393(5)
C(12)-C(13)	1.373(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.369(6)
C(13)-H(13)	0.9300
C(14)-C(15)	1.374(6)
C(14)-H(14)	0.9300
C(15)-C(16)	1.382(5)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
Si(1)-C(20)	1.819(13)
Si(1)-C(19)	1.854(12)
Si(1)-C(18)	1.957(10)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-C(21)	1.534(13)
C(20)-C(22)	1.569(17)
C(20)-C(23)	1.627(13)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600

C(22)-H(22C)	0.9600
Si(1')-C(18')	1.79(2)
Si(1')-C(20')	1.844(15)
Si(1')-C(19')	1.874(17)
C(18')-H(18D)	0.9600
C(18')-H(18E)	0.9600
C(18')-H(18F)	0.9600
C(19')-H(19D)	0.9600
C(19')-H(19E)	0.9600
C(19')-H(19F)	0.9600
C(20')-C(21')	1.535(15)
C(20')-C(22')	1.545(18)
C(20')-C(23')	1.566(18)
C(21')-H(21D)	0.9600
C(21')-H(21E)	0.9600
C(21')-H(21F)	0.9600
C(22')-H(22D)	0.9600
C(22')-H(22E)	0.9600
C(22')-H(22F)	0.9600
C(23')-H(23D)	0.9600
C(23')-H(23E)	0.9600
C(23')-H(23F)	0.9600

C(1)-N(1)-C(2)	108.3(3)
C(1)-N(1)-C(17)	130.1(3)
C(2)-N(1)-C(17)	121.2(3)
C(1)-N(2)-C(3)	107.1(3)
C(10)-O(2)-H(2)	112(3)
C(7)-O(3)-Si(1)	135.2(3)
C(7)-O(3)-Si(1')	116.7(3)
N(2)-C(1)-N(1)	112.7(3)
N(2)-C(1)-C(11)	122.7(3)
N(1)-C(1)-C(11)	124.6(3)
O(1)-C(2)-N(1)	125.4(4)
O(1)-C(2)-C(3)	131.2(4)
N(1)-C(2)-C(3)	103.4(3)
C(4)-C(3)-N(2)	128.5(4)
C(4)-C(3)-C(2)	123.0(3)

N(2)-C(3)-C(2)	108.5(3)
C(3)-C(4)-C(5)	134.0(4)
C(3)-C(4)-H(4)	113.0
C(5)-C(4)-H(4)	113.0
C(10)-C(5)-C(6)	117.5(4)
C(10)-C(5)-C(4)	126.5(3)
C(6)-C(5)-C(4)	116.0(4)
C(7)-C(6)-C(5)	122.7(4)
C(7)-C(6)-H(6)	118.7
C(5)-C(6)-H(6)	118.7
C(6)-C(7)-C(8)	119.1(4)
C(6)-C(7)-O(3)	121.4(5)
C(8)-C(7)-O(3)	119.5(5)
C(9)-C(8)-C(7)	120.0(5)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	121.5(4)
C(8)-C(9)-H(9)	119.2
C(10)-C(9)-H(9)	119.2
O(2)-C(10)-C(9)	115.1(4)
O(2)-C(10)-C(5)	125.7(4)
C(9)-C(10)-C(5)	119.1(4)
C(12)-C(11)-C(16)	118.8(3)
C(12)-C(11)-C(1)	119.0(3)
C(16)-C(11)-C(1)	122.2(3)
C(13)-C(12)-C(11)	120.7(4)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(14)-C(13)-C(12)	120.5(4)
C(14)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(13)-C(14)-C(15)	119.6(4)
C(13)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
C(14)-C(15)-C(16)	120.4(4)
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(15)-C(16)-C(11)	120.0(4)

C(15)-C(16)-H(16)	120.0
C(11)-C(16)-H(16)	120.0
N(1)-C(17)-H(17A)	109.5
N(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(3)-Si(1)-C(20)	110.7(5)
O(3)-Si(1)-C(19)	110.5(5)
C(20)-Si(1)-C(19)	111.3(6)
O(3)-Si(1)-C(18)	110.3(6)
C(20)-Si(1)-C(18)	115.6(6)
C(19)-Si(1)-C(18)	97.8(7)
Si(1)-C(18)-H(18A)	109.5
Si(1)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
Si(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
Si(1)-C(19)-H(19A)	109.5
Si(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(22)	104.6(15)
C(21)-C(20)-C(23)	112.1(11)
C(22)-C(20)-C(23)	121.5(14)
C(21)-C(20)-Si(1)	108.7(9)
C(22)-C(20)-Si(1)	105.0(12)
C(23)-C(20)-Si(1)	104.4(9)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(18')-Si(1')-O(3)	114.2(9)
C(18')-Si(1')-C(20')	114.9(11)
O(3)-Si(1')-C(20')	99.0(5)
C(18')-Si(1')-C(19')	116.4(11)
O(3)-Si(1')-C(19')	102.9(7)
C(20')-Si(1')-C(19')	107.4(9)
Si(1')-C(18')-H(18D)	109.5
Si(1')-C(18')-H(18E)	109.5
H(18D)-C(18')-H(18E)	109.5
Si(1')-C(18')-H(18F)	109.5
H(18D)-C(18')-H(18F)	109.5
H(18E)-C(18')-H(18F)	109.5
Si(1')-C(19')-H(19D)	109.5
Si(1')-C(19')-H(19E)	109.5
H(19D)-C(19')-H(19E)	109.5
Si(1')-C(19')-H(19F)	109.5
H(19D)-C(19')-H(19F)	109.5
H(19E)-C(19')-H(19F)	109.5
C(21')-C(20')-C(22')	100.3(19)
C(21')-C(20')-C(23')	105.4(17)
C(22')-C(20')-C(23')	137(2)
C(21')-C(20')-Si(1')	112.0(11)
C(22')-C(20')-Si(1')	93.1(18)
C(23')-C(20')-Si(1')	107.8(16)
C(20')-C(21')-H(21D)	109.4
C(20')-C(21')-H(21E)	109.6

H(21D)-C(21')-H(21E)	109.5
C(20')-C(21')-H(21F)	109.5
H(21D)-C(21')-H(21F)	109.5
H(21E)-C(21')-H(21F)	109.5
C(20')-C(22')-H(22D)	109.5
C(20')-C(22')-H(22E)	109.5
H(22D)-C(22')-H(22E)	109.5
C(20')-C(22')-H(22F)	109.5
H(22D)-C(22')-H(22F)	109.5
H(22E)-C(22')-H(22F)	109.5
C(20')-C(23')-H(23D)	109.5
C(20')-C(23')-H(23E)	109.5
H(23D)-C(23')-H(23E)	109.5
C(20')-C(23')-H(23F)	109.5
H(23D)-C(23')-H(23F)	109.5
H(23E)-C(23')-H(23F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	70(2)	63(2)	65(2)	4(1)	23(1)	4(2)
N(2)	77(2)	63(2)	58(2)	1(1)	26(1)	5(2)
O(1)	97(2)	65(2)	107(2)	5(2)	32(2)	-8(2)
O(2)	82(2)	73(2)	112(2)	4(2)	37(2)	4(2)
O(3)	124(3)	101(2)	142(3)	42(2)	68(2)	49(2)
C(1)	74(2)	62(2)	51(2)	-1(2)	22(2)	0(2)
C(2)	86(3)	63(2)	62(2)	1(2)	27(2)	1(2)
C(3)	80(2)	58(2)	57(2)	2(2)	23(2)	5(2)
C(4)	87(3)	62(2)	65(2)	3(2)	24(2)	5(2)
C(5)	84(3)	73(3)	60(2)	8(2)	28(2)	12(2)
C(6)	93(3)	76(3)	84(3)	14(2)	35(2)	18(2)
C(7)	102(4)	92(3)	95(3)	25(3)	43(3)	30(3)
C(8)	86(3)	111(4)	110(4)	17(3)	41(3)	21(3)
C(9)	86(3)	94(3)	104(3)	15(3)	39(2)	9(3)
C(10)	87(3)	74(3)	71(2)	8(2)	32(2)	12(2)

C(11)	74(2)	58(2)	62(2)	-3(2)	31(2)	1(2)
C(12)	85(3)	71(3)	72(2)	-1(2)	31(2)	-5(2)
C(13)	97(3)	68(3)	98(3)	-8(2)	42(3)	-12(2)
C(14)	105(3)	59(2)	120(4)	-3(2)	62(3)	0(2)
C(15)	90(3)	73(3)	100(3)	11(2)	41(2)	18(2)
C(16)	81(3)	65(2)	79(3)	-1(2)	29(2)	4(2)
C(17)	79(3)	85(3)	85(3)	1(2)	35(2)	-2(2)
Si(1)	112(2)	91(2)	120(2)	28(2)	21(2)	8(1)
C(18)	123(8)	96(7)	132(8)	-41(6)	31(6)	40(6)
C(19)	67(5)	130(8)	108(7)	13(7)	22(4)	-21(5)
C(20)	158(8)	161(8)	131(7)	31(7)	57(6)	19(6)
C(21)	209(12)	195(12)	120(8)	52(8)	45(8)	16(10)
C(23)	71(6)	206(11)	186(12)	-1(11)	33(8)	7(6)
C(22)	179(18)	240(20)	126(12)	1(13)	91(11)	55(16)
Si(1')	83(2)	93(2)	114(3)	12(2)	33(2)	0(2)
C(18')	94(9)	91(9)	72(9)	-24(7)	33(8)	-3(7)
C(19')	86(9)	167(13)	172(14)	-4(12)	68(10)	-16(8)
C(20')	100(7)	118(8)	140(8)	37(7)	42(6)	-1(6)
C(21')	214(15)	141(12)	160(14)	73(11)	36(11)	-34(11)
C(22')	190(20)	250(20)	250(30)	15(16)	91(18)	60(16)
C(23')	146(18)	200(20)	230(20)	24(17)	91(16)	-24(13)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for compound 1.

	x	y	z	U(eq)
H(4)	258	2448	3997	88
H(6)	882	1352	4383	101
H(8)	2081	2851	5082	122
H(9)	1773	4805	4875	114
H(12)	243	7750	4472	91
H(13)	159	9866	4255	104
H(14)	-475	10691	2983	107
H(15)	-1025	9384	1896	104
H(16)	-946	7251	2100	91
H(17A)	-1121	5996	3364	124

H(17B)	-1190	4549	3311	124
H(17C)	-1244	5293	2300	124
H(18A)	1702	-2033	4365	184
H(18B)	1873	-2655	5473	184
H(18C)	2203	-1876	5142	184
H(19A)	981	-992	4823	159
H(19B)	1065	-351	5896	159
H(19C)	1202	-1746	5867	159
H(21A)	2187	-861	8417	271
H(21B)	2278	-1808	7667	271
H(21C)	1785	-1447	7479	271
H(23A)	2804	389	7655	240
H(23B)	2584	684	6455	240
H(23C)	2699	-695	6838	240
H(22A)	1565	801	7196	257
H(22B)	1856	1753	6885	257
H(22C)	2027	1245	8033	257
H(18D)	2045	2043	7103	129
H(18E)	2147	919	7881	129
H(18F)	1652	1227	7138	129
H(19D)	2770	623	6635	205
H(19E)	2570	-124	5583	205
H(19F)	2699	-820	6652	205
H(21D)	1846	-1743	7656	276
H(21E)	2268	-2015	7411	276
H(21F)	1860	-2934	7020	276
H(22D)	2176	-2575	5890	338
H(22E)	2176	-1273	5381	338
H(22F)	1780	-2205	4842	338
H(23D)	1216	-1106	6635	278
H(23E)	1055	-1780	5549	278
H(23F)	1136	-337	5619	278
H(2)	719(7)	5540(40)	4220(30)	96(16)

Table 6. Torsion angles [°] for compound 1.

C(3)-N(2)-C(1)-N(1)	1.7(4)
C(3)-N(2)-C(1)-C(11)	-178.0(3)

C(2)-N(1)-C(1)-N(2)	-0.8(4)
C(17)-N(1)-C(1)-N(2)	171.3(3)
C(2)-N(1)-C(1)-C(11)	178.8(3)
C(17)-N(1)-C(1)-C(11)	-9.1(5)
C(1)-N(1)-C(2)-O(1)	179.0(4)
C(17)-N(1)-C(2)-O(1)	6.0(6)
C(1)-N(1)-C(2)-C(3)	-0.4(4)
C(17)-N(1)-C(2)-C(3)	-173.3(3)
C(1)-N(2)-C(3)-C(4)	176.8(4)
C(1)-N(2)-C(3)-C(2)	-1.9(4)
O(1)-C(2)-C(3)-C(4)	3.3(6)
N(1)-C(2)-C(3)-C(4)	-177.4(3)
O(1)-C(2)-C(3)-N(2)	-177.9(4)
N(1)-C(2)-C(3)-N(2)	1.4(4)
N(2)-C(3)-C(4)-C(5)	-0.4(7)
C(2)-C(3)-C(4)-C(5)	178.0(4)
C(3)-C(4)-C(5)-C(10)	2.3(7)
C(3)-C(4)-C(5)-C(6)	-178.3(4)
C(10)-C(5)-C(6)-C(7)	0.2(6)
C(4)-C(5)-C(6)-C(7)	-179.3(4)
C(5)-C(6)-C(7)-C(8)	-2.0(7)
C(5)-C(6)-C(7)-O(3)	-178.8(4)
Si(1)-O(3)-C(7)-C(6)	-62.5(7)
Si(1')-O(3)-C(7)-C(6)	-105.0(5)
Si(1)-O(3)-C(7)-C(8)	120.7(5)
Si(1')-O(3)-C(7)-C(8)	78.2(5)
C(6)-C(7)-C(8)-C(9)	2.4(7)
O(3)-C(7)-C(8)-C(9)	179.3(4)
C(7)-C(8)-C(9)-C(10)	-1.1(7)
C(8)-C(9)-C(10)-O(2)	-179.1(4)
C(8)-C(9)-C(10)-C(5)	-0.7(7)
C(6)-C(5)-C(10)-O(2)	179.3(4)
C(4)-C(5)-C(10)-O(2)	-1.3(6)
C(6)-C(5)-C(10)-C(9)	1.2(6)
C(4)-C(5)-C(10)-C(9)	-179.4(4)
N(2)-C(1)-C(11)-C(12)	-30.9(5)
N(1)-C(1)-C(11)-C(12)	149.5(3)
N(2)-C(1)-C(11)-C(16)	146.4(4)

N(1)-C(1)-C(11)-C(16)	-33.2(5)
C(16)-C(11)-C(12)-C(13)	0.9(6)
C(1)-C(11)-C(12)-C(13)	178.4(4)
C(11)-C(12)-C(13)-C(14)	0.0(6)
C(12)-C(13)-C(14)-C(15)	-0.7(7)
C(13)-C(14)-C(15)-C(16)	0.6(7)
C(14)-C(15)-C(16)-C(11)	0.3(6)
C(12)-C(11)-C(16)-C(15)	-1.0(6)
C(1)-C(11)-C(16)-C(15)	-178.4(4)
C(7)-O(3)-Si(1)-C(20)	-68.0(7)
Si(1')-O(3)-Si(1)-C(20)	8.0(5)
C(7)-O(3)-Si(1)-C(19)	55.8(8)
Si(1')-O(3)-Si(1)-C(19)	131.7(6)
C(7)-O(3)-Si(1)-C(18)	162.7(7)
Si(1')-O(3)-Si(1)-C(18)	-121.3(6)
O(3)-Si(1)-C(20)-C(21)	173.2(8)
C(19)-Si(1)-C(20)-C(21)	49.9(11)
C(18)-Si(1)-C(20)-C(21)	-60.5(11)
O(3)-Si(1)-C(20)-C(22)	61.7(12)
C(19)-Si(1)-C(20)-C(22)	-61.6(13)
C(18)-Si(1)-C(20)-C(22)	-171.9(13)
O(3)-Si(1)-C(20)-C(23)	-67.1(9)
C(19)-Si(1)-C(20)-C(23)	169.6(9)
C(18)-Si(1)-C(20)-C(23)	59.3(11)
C(7)-O(3)-Si(1')-C(18')	7.0(11)
Si(1)-O(3)-Si(1')-C(18')	-123.1(10)
C(7)-O(3)-Si(1')-C(20')	129.6(6)
Si(1)-O(3)-Si(1')-C(20')	-0.5(5)
C(7)-O(3)-Si(1')-C(19')	-120.1(8)
Si(1)-O(3)-Si(1')-C(19')	109.8(8)
C(18')-Si(1')-C(20')-C(21')	-61.1(18)
O(3)-Si(1')-C(20')-C(21')	176.8(14)
C(19')-Si(1')-C(20')-C(21')	70.1(16)
C(18')-Si(1')-C(20')-C(22')	-163.5(16)
O(3)-Si(1')-C(20')-C(22')	74.4(14)
C(19')-Si(1')-C(20')-C(22')	-32.3(16)
C(18')-Si(1')-C(20')-C(23')	54.3(18)
O(3)-Si(1')-C(20')-C(23')	-67.8(15)

C(19')-Si(1')-C(20')-C(23') -174.5(15)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for compound 1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)
O(2)-H(2)...N(2)	0.837(19)	1.78(2)	2.614(4)	171(4)

Symmetry transformations used to generate equivalent atoms: