Electronic Supporting Information

Disilanylene-bridged BODIPY-based D-σ-A architectures: a novel promising series of NLO chromophores

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1. Experimental Details

All reagents were obtained from commercial suppliers and used without further purification unless otherwise indicated. All air and moisture-sensitive reactions were carried out under nitrogen atmosphere in oven-dried glassware. Glassware was dried in an oven at 120 °C and cooled under a stream of inert gas before use. Tetrahydrofuran were distilled over sodium. $^1$H NMR and $^{13}$C NMR spectra were recorded on a Bruker DRX400 spectrometer and DRX500 spectrometer, and referenced to the residual proton signals of deuterated solvents. HR-MS were recorded on a Bruker Daltonics microTOF-Q II spectrometer. All the solvents employed for the spectroscopic measurements were of UV spectroscopic grade (Aldrich).

X-ray structure determination

The X-ray diffraction data were collected on a Bruker Smart Apex CCD diffractometer with graphite monochromated Mo Kα radiation ($\lambda = 0.71073$ Å) using the $\omega$-2θ scan mode. The structure was solved by direct methods and refined on $F^2$ by full-matrix least-squares methods using SHELX-2000. All calculations and molecular graphics were carried out on a computer using the SHELX-2000 program package and Diamond 3.2. CCDC 1839779 (1a) and 1839780 (1c) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

1a: C$_{28}$H$_{33}$BF$_2$N$_2$Si$_2$, A red block-like crystal of the approximate dimensions 0.26×0.09×0.39 mm$^3$ was measured. Triclinic, C2/c, $a = 21.64(2)$ Å, $b = 8.223(6)$ Å, $c = 32.26(3)$ Å, $\alpha = 90^\circ$, $\beta = 97.40(2)^\circ$, $\gamma = 90^\circ$ V = 5693(9) Å$^3$, Z = 8, F(000) = 2128, $\rho = 1.173$ Mgm$^{-3}$, $R_1 = 0.0886$, $wR_2 = 0.2346$, GOF = 1.015, residual electron density between 0.382 and -0.345 eÅ$^{-3}$

1c: C$_{30}$H$_{38}$BF$_2$N$_3$Si$_2$, A red block-like crystal of the approximate dimensions 0.13×0.14×0.16 mm$^3$ was measured. Triclinic, P-1, $a = 11.115(5)$ Å, $b = 11.547(5)$ Å, $c = 13.669(7)$ Å, $\alpha = 69.556(8)^\circ$, $\beta = 82.496(8)^\circ$, $\gamma = 79.484(9)^\circ$ V = 1612.0(13) Å$^3$, Z = 2, F(000) = 580, $\rho = 1.124$ Mgm$^{-3}$, $R_1 = 0.0651$, $wR_2 = 0.2115$, GOF = 1.072, residual electron density between 0.877 and -0.513 eÅ$^{-3}$
Spectroscopic measurements

UV-visible absorption spectra were recorded on a Shimadzu 1800 spectrophotometer. Fluorescence spectra and the fluorescence lifetimes of the samples were determined with a Horiba Jobin Yvon Fluorolog-3 spectrofluorimeter. The goodness of the fit of the single exponential decays were judged using the chi-squared ($\chi^2$) and the autocorrelation function $C(j)$ values. Low residuals ($\chi^2 < 1.2$) were consistently observed. Absorption and emission measurements were carried out in 1×1 cm quartz cuvettes. For all measurements, the temperature was kept constant at (298±2) K. Dilute solutions with absorbance of less than 0.05 at the excitation wavelength were used for the measurement of fluorescence quantum yields. Fluorescein was used as the standard ($\Phi_F = 0.86$ in 0.1mol/L NaOH). The quantum yield, $\Phi$, was calculated using equation

$$\Phi_{\text{sample}} = \Phi_{\text{std}} \left[ \frac{I_{\text{sample}}}{I_{\text{std}}} \right] \left[ \frac{A_{\text{std}}}{A_{\text{sample}}} \right] \left[ \frac{n_{\text{sample}}}{n_{\text{std}}} \right]^2$$

(1)

where the sample and std subscripts denote the sample and standard, respectively, $I$ is the integrated emission intensity, $A$ stands for the absorbance, and $n$ is refractive index.

When the fluorescence decays were monoexponential, the rate constants of radiative ($k_r$) and nonradiative ($k_{nr}$) deactivation were calculated from the measured fluorescence quantum yield ($\Phi_F$) and fluorescence lifetime ($\tau$) according to equations (2) and (3):

$$k_r = \frac{\Phi_F}{\tau}$$

(2)

$$k_{nr} = \frac{(1-\Phi_F)}{\tau}$$

(3)

DFT calculations

The G09W software package was used to carry out a DFT geometry optimization using the CAM-B3LYP functional with 6-31G(d) basis sets. UV-visible were calculated by using the time-dependent density functional theory (TD-DFT) approach with the CAM-B3LYP functional and 6-31G(d) basis sets. The calculations were made both in the gas phase and in toluene using the polarizable continuum model (PCM).
Non-linear optical properties

The Z-scan method with a femtosecond laser pulse and a Ti:95 sapphire system was used to measure nonlinear absorption property. The nonlinear absorption data are fitted using the following equations:

\[ T(z,s=1) = \sum_{m=0}^{\infty} \left[-q_0(z)\right]^{m} \quad \text{for} \quad |q_0| < 1 \quad (4) \]

\[ q_0(z) = \frac{\beta I_0 L_{eff}}{1 + \chi^2} \quad (5) \]

\[ \sigma = \frac{h \gamma \beta}{N_A d \times 10^{-3}} \quad (6) \]

In equations (4) and (5), \( \beta \) is second-order nonlinear coefficient of the solution, \( I_0 \) is the intensity of laser beam at focus \( (z = 0) \), \( L_{eff} = [1-\exp(-\alpha_0 L)]/\alpha_0 \) is the effective length with \( \alpha_0 \) the linear absorption coefficient, \( L \) is the sample length, \( l \) is the wavelength of the beam, \( z \) is the sample position, and \( z_0 = \pi \omega_0^2/\lambda \) is the diffraction length of the beam with \( \omega_0 \) the spot size at focus. Where in equation (6), \( \sigma \) is molecular 2PA cross-section, \( h \) is the Planck’s constant, \( \gamma \) is the frequency of incident laser, \( N_A \) is the Avogadro constant, and \( d \) is the concentration of the sample. According to equations (4) and (5), the 2PA coefficient \( \beta \) (in units of cm/GW) can be deduced, then bring \( \beta \) into equation (6), 2PA cross section \( \sigma \) could be calculated.

The effective third-order NLO susceptibility \( \chi^{(3)} \) can be deduced using the following equations:

\[ R_{e} \chi^{(3)} = 10^{-4} n_0^2 \varepsilon_0 c^2 \gamma / \pi \quad (7) \]

\[ I_{m} \chi^{(3)} = 10^{-2} n_0^2 \varepsilon_0 c^2 \beta \lambda / 4\pi^2 \quad (8) \]

\[ \chi^{(3)} = \sqrt{(R_{e} \chi^{(3)})^2 + (I_{m} \chi^{(3)})^2} \quad (9) \]

In equations (7-9), \( \varepsilon_0 \) is the vacuum permittivity, \( c \) is the speed of light in vacuum and \( n_0 \) is the linear refractive index of the solvent. The third-order nonlinear refractive index \( \Delta n \) can be deduced from the equation: \( \Delta T_{pv} = 0.406(1 - S)^{0.25} I \Delta \phi I, \Delta \phi = K L_{eff} \gamma I_0 \). \( \Delta T_{pv} \) is the difference between the peak and the valley of the normalized transmission, and \( S \) is the linear ratio of transmitted beam through the aperture.
2 Synthesis and characterization

2.1 General synthesis of 1-(4-R-phenyl)-1,1,2,2-tetramethyldisilane

Under an argon atmosphere, phenylmagnesium bromide (100 mmol) in THF (100 mL) was added slowly to a solution of 1,1,2,2-tetramethyl-1,2-dichlorodisilane (10.2 mL, 110 mmol) in THF (50 mL) at −78 °C over 2 h, then the reaction mixture was warmed to room temperature. The mixture was cooled to 0 °C, and LiAlH₄ (3.795 g, 100 mmol) was added. The reaction mixture was warmed to room temperature and stirred overnight. The mixture was quenched with water very slowly and the aqueous layer was extracted three times with diethyl ether. The combined organic layer was washed with brine and dried over sodium sulfate. The solvent was purified by chromatography over silica gel (EA/hexane 1:100) to provide disilane in range of yields of 34-68% as a colorless oil.

1-phenyl-1,1,2,2-tetramethyldisilane: Yield 56%. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.49 (dd, J = 6.3, 3.2 Hz, 2 H), 7.35 (dd, J = 4.9, 1.9 Hz, 3 H), 3.75 (s, 1 H), 0.39 (s, 6 H), 0.14 (d, J = 4.5 Hz, 6 H).

1-(4-methoxyphenyl)-1,1,2,2-tetramethyldisilane: Yield 57%. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.45 – 7.38 (m, 2 H), 6.96 – 6.89 (m, 2 H), 3.82 (s, 3 H), 3.74 (dd, J = 9.0 Hz, 4.5 Hz, 1 H), 0.36 (s, 6 H), 0.14 (d, J = 3.9 Hz, 6 H).

1-(4-N,N-dimethylphenyl)-1,1,2,2-tetramethyldisilane: Yield 68%. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, J = 8.7 Hz, 2 H), 6.77 (d, J = 8.2 Hz, 2 H), 3.75 (dd, J = 9.0, 4.5 Hz, 1 H), 2.98 (s, 6 H), 0.37 (m, 6 H), 0.12 (d, J = 4 Hz, 6 H).

1-(4-trifluoromethylphenyl)-1,1,2,2-tetramethyldisilane: Yield 34%. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.59 (s, 4 H), 3.75 (m, 1 H), 0.40 (s, 6 H), 0.14 (d, J = 4.5 Hz, 6 H).
2.2 General synthesis of D(A)-Si-Si-BODIPY

Under an argon atmosphere, N, N-diisopropylethylamine (0.076 mL, 0.46 mmol) and 1-phenyl-1,1,2,2-tetramethyldisilane (45 mg, 0.23 mmol) were added to a solution of 2-iodo-meso-Mes-BODIPY (100 mg, 0.23 mmol) and bis(tri-tert-butylphosphine) palladium(0) (1.2 mg, 0.0023 mmol, 1% mol) in mesitylene (3 mL) at 0 °C. The mixture was stirred for 2 d at 0 °C. The reaction mixture was purified by column chromatography to afford 1a (24 mg, 21%) and recrystallized from CH\textsubscript{2}Cl\textsubscript{2}/Hexane. \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) \textdelta 7.87 (s, 1 H), 7.76 (s, 1 H), 7.33 (dd, \textit{J} = 6.7, 2.8 Hz, 2 H), 7.27 (d, \textit{J} = 1.9 Hz, 2 H), 7.24 (s, 1 H), 6.96 (s, 2 H), 6.63 (d, \textit{J} = 4.0 Hz, 1 H), 6.50 (s, 1 H), 6.45 (d, \textit{J} = 2.5 Hz, 1 H), 2.39 (s, 3 H), 2.07 (s, 6 H), 0.31 (s, 6 H), 0.24 (s, 6 H). \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}) \textdelta 149.70, 146.64, 143.58, 138.86, 138.47, 137.25, 136.88, 136.45, 135.41, 133.81, 129.94, 128.75, 128.32, 127.95, 118.50, 21.31, 20.14, -3.44, -4.03. HRMS-ESI: m/z: calcld \([C_{28}H_{33}BF_2N_2Si_2]^+\) m/z = 525.2141, found m/z = 525.2165.

Compounds 1b, 1c and 1d were obtained as red solid by using a similar procedure to that for 1a in yield of 18, 23 and 7%, respectively.

1b: \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) \textdelta 7.87 (s, 1 H), 7.77 (s, 1 H), 7.26 (s, 1 H), 7.24 (s, 1 H), 6.96 (s, 2 H), 6.83 (d, \textit{J} = 8.5 Hz, 2 H), 6.63 (d, \textit{J} = 3.7 Hz, 1 H), 6.55 (s, 1 H), 6.45 (d, \textit{J} = 2.4 Hz, 1 H), 3.80 (s, 3 H), 2.38 (s, 3 H), 2.07 (s, 6 H), 0.28 (s, 6 H), 0.23 (s, 6 H). \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}) \textdelta 160.31, 149.80, 148.18, 143.51, 138.86, 138.47, 136.89, 136.45, 135.18, 129.95, 128.32, 127.95, 118.48, 117.17, 113.84, 55.12, 21.31, 20.14, -3.45, -3.79. HRMS-ESI: m/z: calcld \([C_{29}H_{35}BF_2N_2Si_2+Na]^+\) m/z = 555.2247, found m/z = 555.2266.

1c \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) \textdelta 7.87 (d, \textit{J} = 4.9 Hz, 1 H), 7.78 (s, 1 H), 7.21 (d, \textit{J} = 7.8 Hz, 2 H), 6.96 (s, 2 H), 6.70 (s, 2 H), 6.61 (s, 2 H), 6.44 (s, 1 H), 2.96 (s, 6 H), 2.38 (s, 3 H), 2.09 (s, 6 H), 0.26(s, 6 H), 0.23(s, 6 H). \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}) \textdelta 150.12, 146.43, 143.23, 138.79, 137.36, 137.03, 136.49, 135.33, 134.92, 134.28, 130.03, 129.67, 128.31, 118.27, 112.41, 40.41, 21.30,
20.14, -3.39, -3.71. HRMS-ESI: m/z: calcd [C$_{30}$H$_{38}$BF$_2$N$_2$Si$_2$ +H]$^+$ m/z = 546.2744, found m/z = 546.2733.

1d  $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.90 (s, 1 H), 7.80 (s, 1 H), 7.49 (d, $J$ = 7.9 Hz, 2 H), 7.42 (d, $J$ = 7.9 Hz, 2 H), 6.96 (s, 2 H), 6.66 (d, $J$ = 4.1 Hz, 1 H), 6.47 (s, 2 H), 2.38 (s, 3 H), 2.05 (s, 6 H), 0.33 (s, 6 H), 0.25 (s, 6 H). HRMS-ESI: m/z: calcd [C$_{29}$H$_{32}$BF$_5$N$_2$Si$_2$Na]$^+$ m/z=593.2015, found m/z=593.2029. calcd [C$_{29}$H$_{32}$BF$_4$N$_2$Si$_2$-F]$^+$ m/z=551.2133, found m/z=551.2033.

2.3 General synthesis of D-Si-Si-BODIPY-Si-Si-D

Under an argon atmosphere, N,N-diisopropylethylamine (0.12 mL, 0.72 mmol) and 1-phenyl-1,1,2,2-tetramethyldisilane (70.0 mg, 0.36 mmol) were added to a solution of 2,6-diiodo-meso-Mes-BODIPY (100 mg, 0.18 mmol) and bis(tri-tert-butylphosphine) palladium (0) (1.8 mg, 0.0036 mmol, 2 mol%) in mesitylene (3 mL) at 0 °C. The mixture was stirred for 2 d at 0 °C. The reaction mixture was purified by column chromatography to afford 2a with yield of 13% and recrystallized from CH$_2$Cl$_2$/Hexane. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.73 (s, 2 H), 7.33 (dd, $J$ = 4.4, 3.0 Hz, 4 H), 7.27 (d, $J$ = 1.7 Hz, 4 H), 7.24 (d, $J$ = 1.3 Hz, 2 H), 6.97 (s, 2 H), 6.45 (s, 2 H), 2.41 (s, 3 H), 2.04 (s, 6 H), 0.30 (s, 12 H), 0.23 (s, 12 H).$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 148.96, 145.46, 138.72, 138.54, 137.41, 137.17, 136.51, 136.44, 133.83, 130.03, 128.73, 128.34, 127.94, 21.35, 20.17, -3.42, -4.02. HRMS-ESI: calcd [C$_{38}$H$_{43}$BF$_2$N$_2$Si$_4$Na]$^+$ m/z=717.2932, found m/z=717.2944.

Compounds 2b and 2c were obtained as red solid by using a similar procedure to that for 2a in yield of 12 and 10 %, respectively.  

2b  $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.73 (s, 2 H), 7.25 (m, 2 H), 7.23 (s, 2 H), 6.96 (s, 2 H), 6.83 (d, $J$ = 8.5 Hz, 4 H), 6.50 (s, 2 H), 3.80 (s, 6 H), 2.40 (s, 3 H), 2.04 (s, 6 H), 0.27 (s, 12 H), 0.22 (s, 12 H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.14, 148.85, 144.95, 138.72, 136.99, 136.29, 135.05, 129.89, 128.88, 128.71, 128.18, 113.68, 99.96, 55.26, 21.42, 20.0
4, -3.57, -3.90. HRMS-ESI: calcd \([C_{40}H_{53}BF_2N_2O_2Si_4+Na]^+\) m/z=777.3143, found m/z=777.3155.

2c \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.73 (s, 2 H), 7.21 (d, \(J = 8.2\) Hz, 4 H), 6.96 (s, 2 H), 6.69 (s, 4 H), 6.56 (s, 2 H), 2.96 (s, 12 H), 2.39 (s, 3 H), 2.07 (s, 6 H), 0.26 (s, 12 H), 0.22 (s, 12 H). \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 152.06, 145.83, 139.14, 138.58, 137.73, 136.40, 134.90, 134.11, 131.57, 129.48, 128.43, 127.04, 29.84, 21.31, 20.18, -3.50, -3.79. HRMS-ESI: calcd \([C_{42}H_{59}BF_2N_4Si_4+H]^+\) m/z=781.3956, found m/z=781.3969.

2.4 Synthesis of A-Si-Si-BODIPY-Si-Si-A:

We have tried to optimize the reaction condition of 1-(4-trifluoromethylphenyl)-1,1,2,2-tetramethyldisilane and 2,6-diiodo-\textit{meso}-Mes-BODIPY by change of reaction temperature, catalyst, kind of solvent et al., the desired chromophore was not detected by Maldi-TOF mass, only 2-iodo-6-(4-trifluoromethylphenyl)dimethylsilyl-BODIPY was isolated with yield of 8%, due to the cleavage of Si-Si bond, which was markedly facilitated by electron-withdrawal in the substituent. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.95 (s, 1 H), 7.82 (s, 1 H), 7.59 (s, 4 H), 6.97 (s, 2 H), 6.83 (s, 1 H), 6.78 (s, 1 H), 2.37 (s, 3 H), 2.09 (s, 6 H), 0.49 (s, 6 H). \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 150.81, 147.56, 146.79, 144.05, 142.35, 139.45, 138.27, 137.42, 136.65, 136.36, 135.30, 134.25, 130.34, 129.27, 128.54, 124.66, 21.30, 20.25, -2.00. HRMS-ESI: calcd \([C_{27}H_{25}BF_5N_2Si+Na]^+\) m/z=661.0743. found m/z=661.0755.
3 Optical spectra

Figure S1. Emission spectra of 1a-1d in kind of solvents with different polarity.
Table S1. Photophysical properties of the D(A)-Si-Si-BODIPY 1a-1d in kind of solvents with different polarity and MesBDP in toluene.

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Figure S2. Emission spectra of 2a-2b in kind of solvents with different polarity.

Table S2. Photophysical properties of the D-Si-Si-BODIPY-Si-Si-D 2a-2c in kind of solvents with different polarity.

<table>
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<tr>
<th>Solvent</th>
<th>λ_{abs} [a] [nm]</th>
<th>ε_{abs} [b] [cm⁻¹]</th>
<th>λ_{em} [b] [nm]</th>
<th>Δv_{em-abs} [c] [cm⁻¹]</th>
<th>Φ_F [d]</th>
<th>τ_f [e] [ns]</th>
<th>k_r [f] [10^8 s⁻¹]</th>
<th>k_{nr} [g] [10^8 s⁻¹]</th>
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**Figure S3.** Open-aperture Z-scan data for 1a-1d and 2a-2c in toluene at 100 μM.
Figure S4. Normalized close-aperture Z-scan spectra for 1a-1c and 2a-2c in toluene at 100 μM.
4 Crystallographic structures

Figure S5. X-ray crystal structures of 1a (left) and 1c (right). The thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms are omitted for clarity in both views.

5 DFT calculations

Figure S6. Optimised structure of 1c and 2c in the twisted and parallel conformations. Calculations were performed at CAM-B3LYP/6-31G(d) level.
Table S3. SCF energies in Hartrees for the folded, extended conformations of 1c and 2c in the gas phase and toluene with the polarisable continuum model (PCM) by using the CAM-B3LYP functional with 6-31G(d) basis sets.

The Folded optimised structure of 1c and 2c is more stable than the extended structure, being in consistent with the X-ray structure.

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<th>Conformation</th>
<th>E/ Hartrees</th>
<th>Environment</th>
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<td>Extended 1c</td>
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<td>gas phase</td>
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<td>Extended 2c</td>
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<td>gas phase</td>
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</tr>
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<td>Extended 1c</td>
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<tr>
<td>Extended 2c</td>
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Figure S7. Frontier MOs and their energy levels of MesBDP and all the chromophores. Calculations were performed at CAM-B3LYP/6-31G(d) level in toluene with the polarisable continuum model (PCM).

Table S4. Calculated electronic excitations energies, oscillator strengths and the related wave functions for MesBDP, 1a-1d and 2a-2c in toluene calculated with the polarisable continuum model (PCM) by using the CAM-B3LYP functional with 6-31G(d) basis sets

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<thead>
<tr>
<th>State[a]</th>
<th>Energy (eV)</th>
<th>λ (nm)</th>
<th>f[b]</th>
<th>Orbitals (coefficient) [c]</th>
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<td>1c</td>
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[a] Excited state. [b] Oscillator strength. [c] MOs involved in the transitions; H and L denote the HOMO and LUMO of the system, respectively.
6 References


7 $^1$H NMR Spectra and HR-MS Spectra

Compound 1a
Compound 1b

Acquisition Parameter
Source Type    ESI    Ion Polarity  Positive    Set Nebulizer  0.2 Bar
Focus           Active Set Capillary  4000 V    Set Dry Heater  180 °C
Scan Begin     50 m/z     Set End Plate Offset -500 V    Set Dry Gas    2.0 l/min
Scan End         800 m/z   Set Collision Cell RF 120.0 Vpp Set Divert Valve Waste

Intens.
540  550  560  570  580  590
Meas. m/z   # Formula  Score  m/z   err [mDa]  err [ppm]  mSigma  rdb  e⁻  Conf  N-Rule
555.2266  1   C₂₉H₃₅BF₂NaOSi₂  100.00  555.2247  -1.9  -3.4  30.6  14.5  even  ok

[M+Na]^+  555.2266

[M+K]^+  571.2126
Compound 1c

**Acquisition Parameter**
- Source Type: ESI
- Focus: Active
- Scan Begin: 50 m/z
- Scan End: 800 m/z
- Ion Polarity: Positive
- Set Capillary: 4000 V
- Set End Plate Offset: -500 V
- Set Collision Cell RF: 120.0 Vpp
- Set Dry Heater: 180 °C
- Set Dry Gas: 2.0 l/min
- Set Nebulizer: 0.2 Bar
- Set Divert Valve: Waste

**MS Scan**
- **[M+H]^+**
- Meas. m/z: 546.2733
- Score: 100.00
- m/z: 546.2744
- err [mDa]: 1.1
- err [ppm]: 2.0
- mSigma: 29.6
- ndb: 14.5
- e− Conf: even
- N-Rule: ok

**Chemical Structure**

```
N \equiv \equiv N
  \equiv \equiv F
  \equiv \equiv Si
  \equiv \equiv N
```

**NMR Spectrum**

- f1 (ppm)
  - 9.0
  - 8.5
  - 8.0
  - 7.5
  - 7.0
  - 6.5
  - 6.0
  - 5.5
  - 5.0
  - 4.5
  - 4.0
  - 3.5
  - 3.0
  - 2.5
  - 2.0
  - 1.5
  - 1.0
  - 0.5
  - 0.0
  - 0.5
Compound 1d

Acquisition Parameter

Source Type: ESI  
Ion Polarity: Positive  
Set Nebulizer: 0.4 Bar  
Set Dry Gas: 4.0 l/min

Focus: Active  
Set Capillary: 4000 V  
Set Dry Heater: 200 °C

Scan Begin: 50 m/z  
Set End Plate Offset: -500 V  
Set Divert Valve: Waste

Scan End: 600 m/z  
Set Collision Cell RF: 1200.0 Vpp  
Set Delivery: Waste

[M+Na]^+  
551.2033

593.2029  C 29 H 32 B F 5 N 2 Na Si 2  100.00  593.2015 -1.4 -2.3 54.2 14.5 even  ok
Compound 2a
Compound 2b

Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\DataTOF-LUH-170426-zzh-SI_3_01.d
Method: tune_100-1000-170426.m
Sample Name: 
Comment: 

Acquisition Date: 4/26/2017 2:10:19 PM
Operator: Jiang
Instrument / Sen#: microTOF-Q II 10324

Acquisition Parameter
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Focus: Active
Set Capillary: 4500 V
Set End Plate Offset: -500 V
Scan Begin: 100 m/z
Set Dry Heater: 250 °C
Scan End: 1000 m/z
Set Dry Gas: 2.6 l/min
Set Collision Cell RF: 1200 Vpp
Set Divert Valve: Source

Intens.
4000
3000
2000
1000
0
7.20 7.40 7.60 7.80 8.00 8.20 8.40 8.60 8.80
m/z

[M+Na]^+
777.3155
793.3105

Mass, m/z # Formula Score m/z err [mDa] err [ppm] mSigma ret eConf N-Rule
777.3155 1 C40 H53 B2 F2 N2 O2 S1 4 100.00 777.3145 -1.0 -1.2 26.5 16.5 even ok
2-Iodo-6-(4-trifluoromethylphenyl)dimethylsilyl-BODIPY