"Click-made" biaryl-linker improving efficiency in protein labelling for the membrane target protein of a bioactive compound

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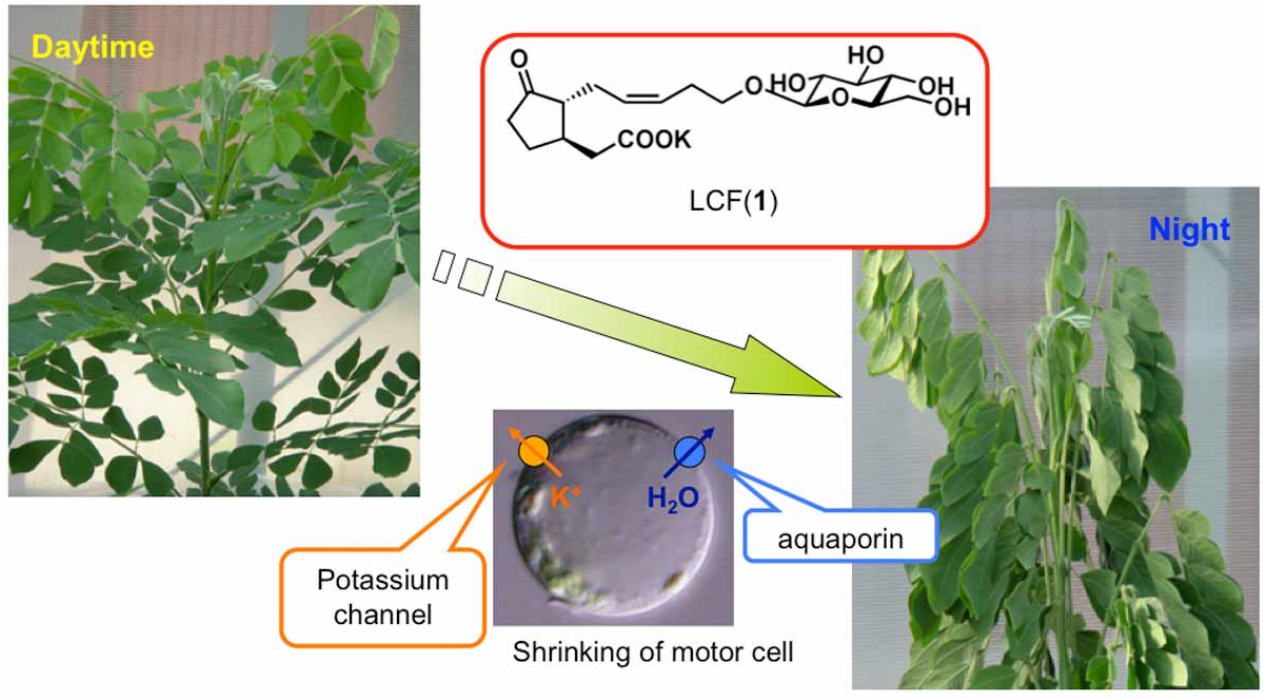


Figure S1. Nyctinastic movement of *Samanea saman*.

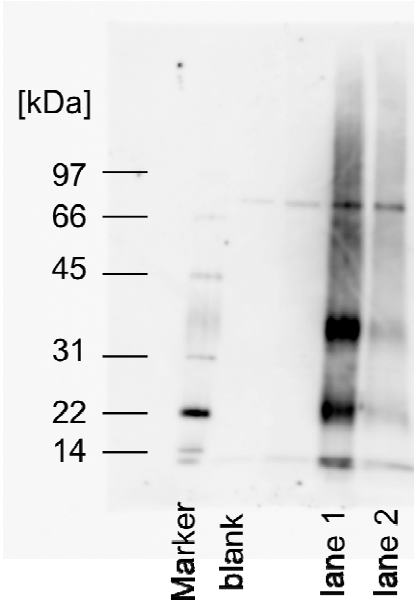


Figure S2. Competitive inhibition on the binding of 6 with excess amount of 1. lane 1: membrane fraction treated with **6** (1×10^{-5} M), lane 2: membrane fraction treated with **6** (1×10^{-5} M) and **1** (1×10^{-3} M)

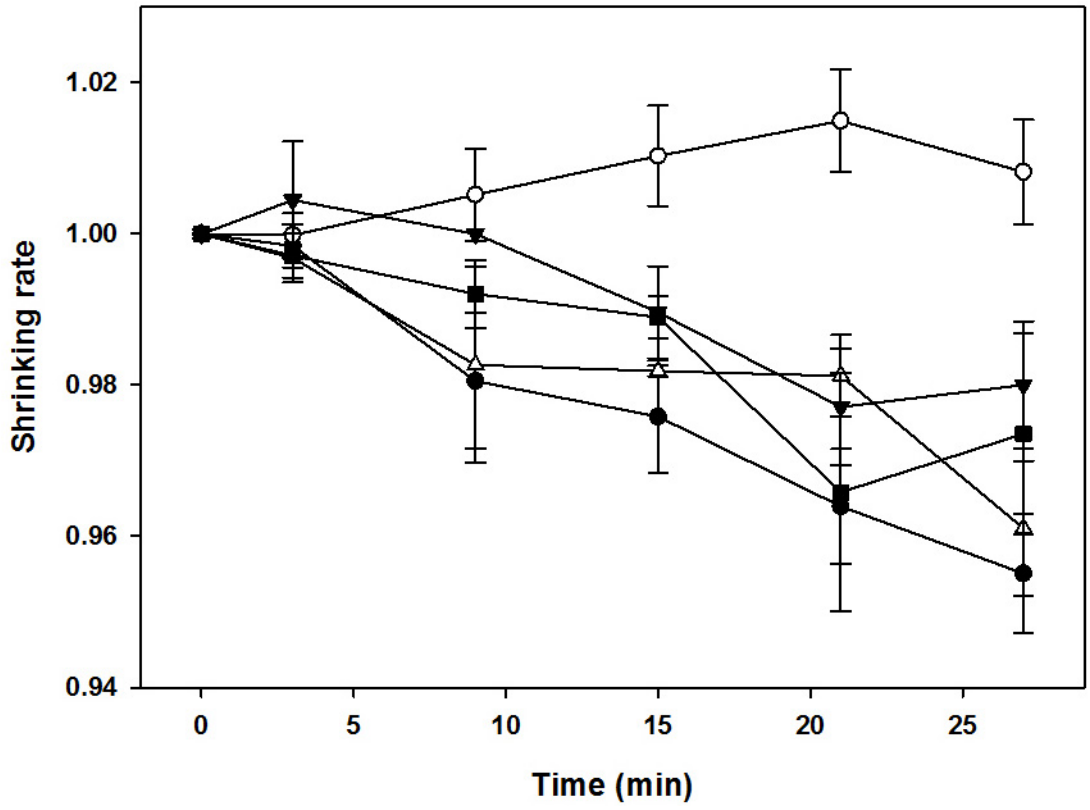
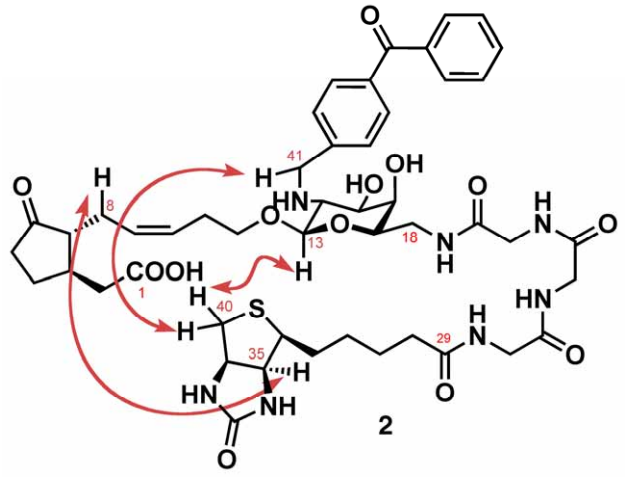


Figure S3. Motor cell-shrinking assay using **1** (□; n = 9), **2** (□; n = 3), **4** (□; n = 3), **6** (□; n = 3), and blank (○; buffer, n = 10) (average ±standard error). Each sample was added at 6 min at a final concentration of 1×10^{-5} M with 0.1% DMSO. The cell-shrinking activities were assessed by the shrinking rate at 27 min, which is ca. 20 min after addition of compounds because each probes were incubated with protoplasts for 20 min in MTJG labeling experiments.



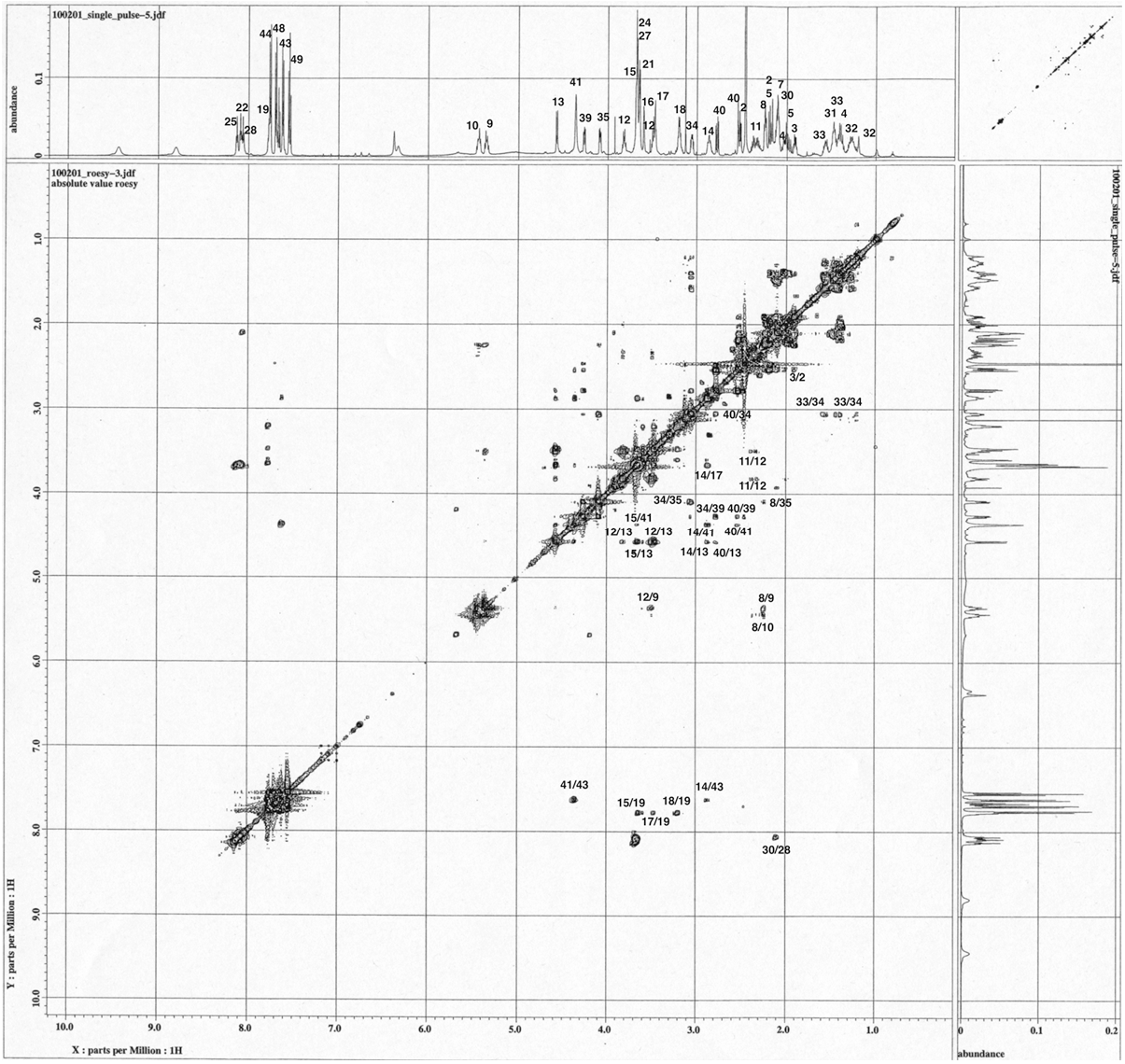


Figure S4. Important ROE correlations and ROESY spectrum of probe 2.

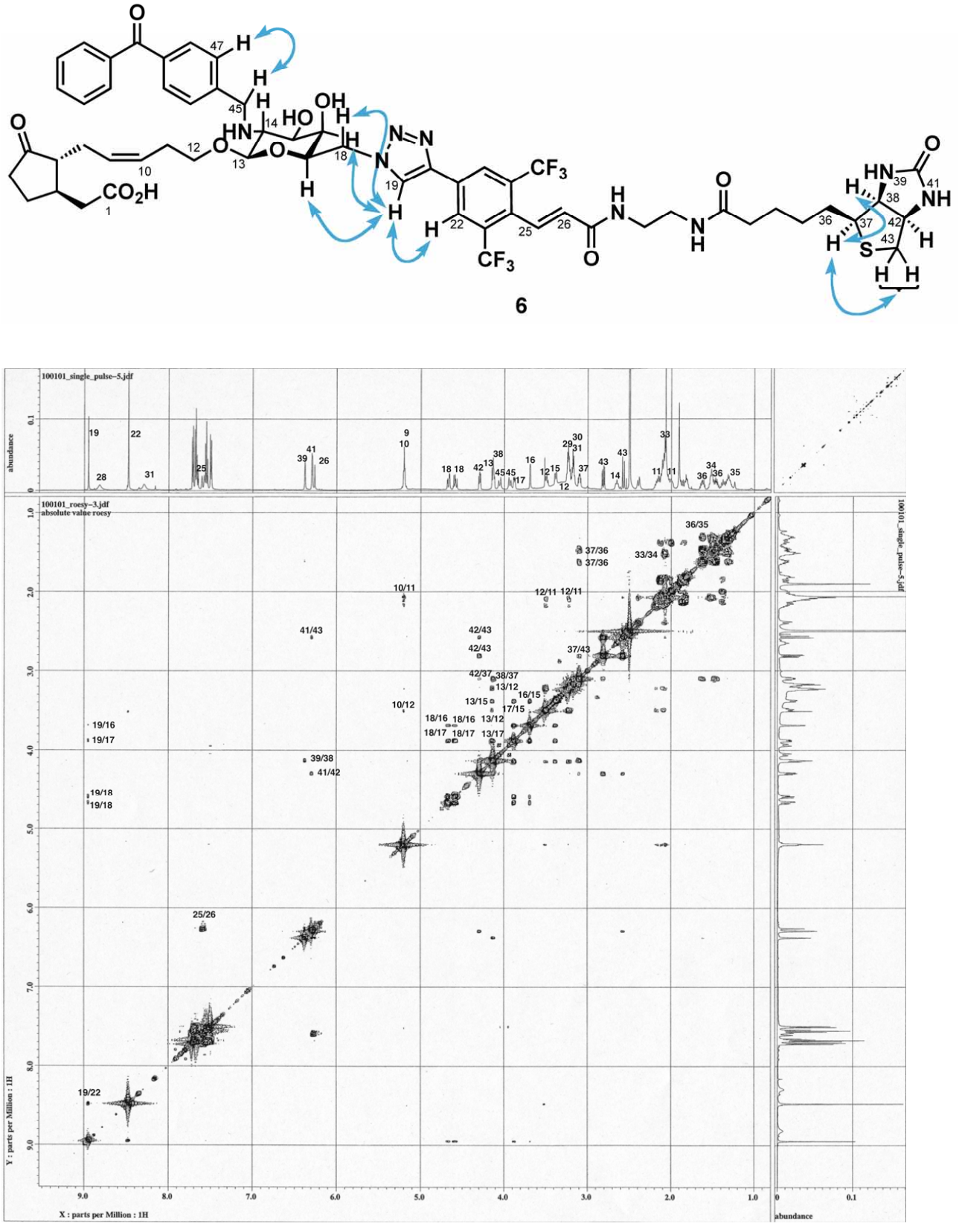


Figure S5. Important ROE correlations and ROESY spectrum of BArL probe 6.

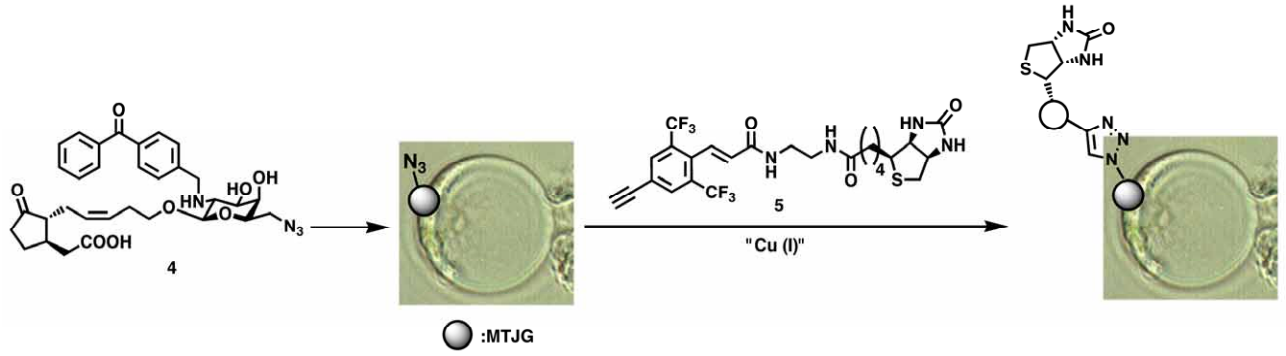


Figure S6. Schematic representation of stepwise biotinylation using 4 and 5.

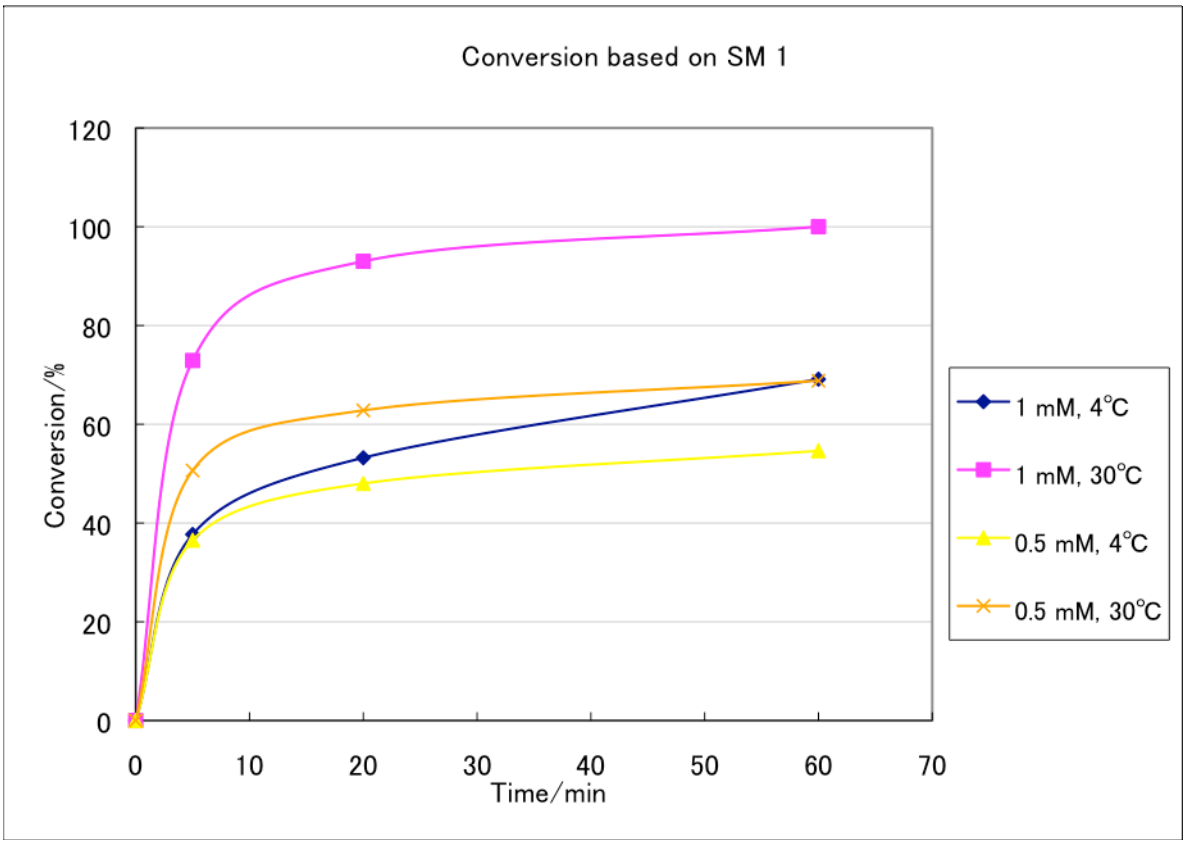


Figure S7. In vitro examination of CuAAC conditions using **4** and **5**: CuAAC reactions were carried out using **4** (1×10^{-4} M) and **5** (1×10^{-4} M) with $CuSO_4 \cdot 5H_2O$ (1 mM or 0.5 mM), **10** (1 mM or 0.5 mM), and ascorbic acid (1 mM or 0.5 mM) in 25 mM HEPES-KOH (pH 7)-2%DMSO. The conversion of **4** into **6** was compared between at 4 °C and at 30 °C. The reaction mixture was analyzed at 5 min, 20 min, and 60 min using Agilent UHPLC HP1290 (Agilent Co., Ltd.) under following conditions; Column: Eclipse plus C18 RRHD (Agilent Co., Ltd.) 1.8 mm (ϕ 2.0 × 50 mm), solvent: 30% CH_3CNaq. containing 0.1% HCOOH, detection: 280 nm. Conversion (%) = [1 - (peak area of **4** at X min)/ (peak area of **4** at 0 min)] × 100. Conversion (%) reached to plateau around 30 min at both temperatures, and strongly affected by the concentration of Cu (I) at 30 °C. Then CuAAC was carried out under mild condition for living cell using 0.5 mM Cu (I) at 4 °C, or under hard condition using 1 mM Cu (I) at 30 °C.

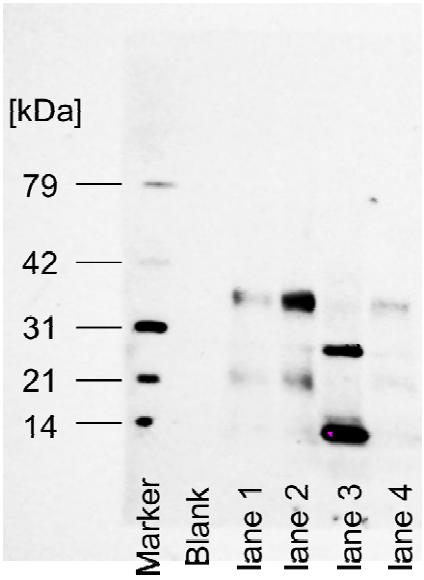


Figure S8. SDS-PAGE on chemiluminescence detection of MTJG by using 6, 11, 12, and 13. lane 1: membrane fraction treated with **6** (1×10^{-4} M), lane 2: membrane fraction treated with **11** (1×10^{-4} M), lane 3: membrane fraction treated with **12** (1×10^{-4} M), lane 4: membrane fraction treated with **13** (1×10^{-4} M).

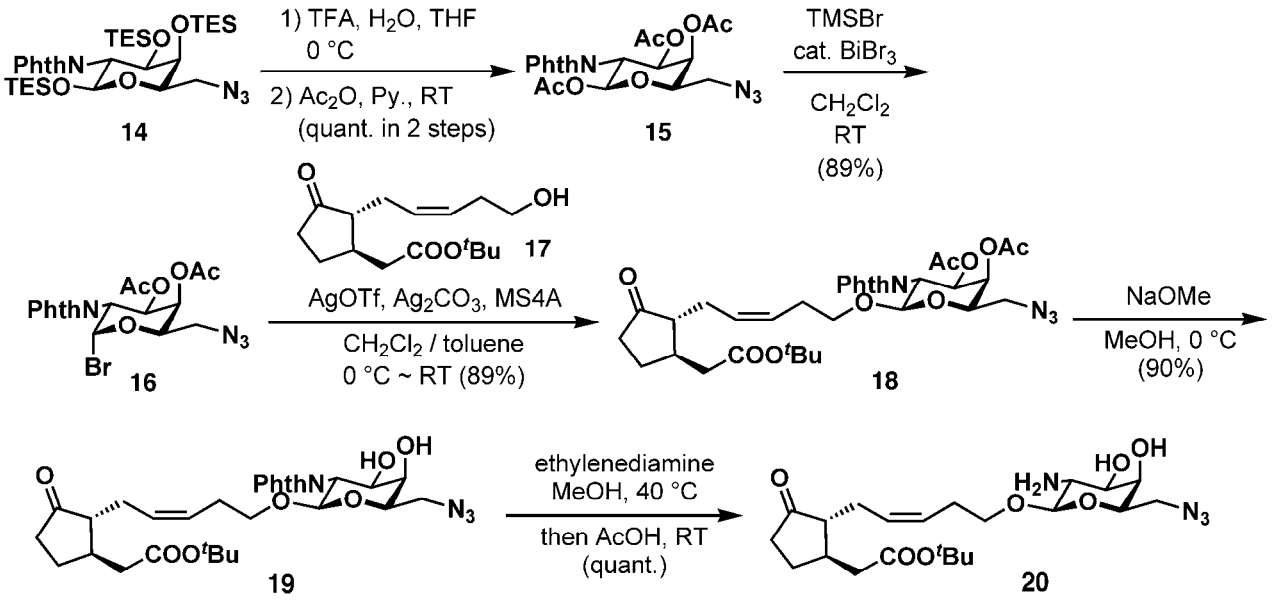
As shown in Figure S8, the band pattern depended on the nature of reactive functionalities in probes. Then, 28 kDa and 13 kDa bands in lane 3 of Figure S8 can be attributed to the nonspecific binding proteins which were trapped by reactive functionalities; The SH-rich protein will be trapped more easily by IA probe **12**, etc. However, 22-kDa in lane 1 and 2 appeared at random, and no constant repeatability was observed. And this band disappeared in competitive inhibition exam in Figure S2 along with MTJG. Thus, we considered that this band would be a degradation product of MTJG, and appears in SDS-PAGE when our treatment of living cell was not appropriate.

Materials and Methods.

Unless otherwise stated, reactions were performed in flame-dried glassware under an argon or nitrogen atmosphere using dry solvents. Solvents were dried over an activated molecular sieves under argon. All the starting materials were purchased from commercial sources and used as received, unless otherwise stated. Liquids and solutions were transferred via syringe or positive-pressure cannula. Brine solutions refer to saturated aqueous sodium chloride solutions. Thin-layer chromatography (TLC) was performed using silica gel 60 F_{254} precoated plates (0.25 mm) and visualized by UV fluorescence quenching, anisaldehyde, or $H_3(PMo_{12}O_{40})$ staining. Silica gel 60N (particle size 63–210 μm) was used for column chromatography. HPLC purifications were carried out using PU-2089 with UV-2075 detector (Jasco Ltd.) equipped with Cosmosil 5C18AR (ϕ20×250 mm, Nakalai. Tesque Ltd.) at a flow rate of 4.0 mL/min. ^{1}H and ^{13}C NMR spectra were recorded on Lambda 400, Alpha 500, and Alpha 600 spectrometers (Jeol Ltd.) using TMS in $CDCl_3$, CD_2HOD in CD_3OD (^{1}H; 3.33 ppm, ^{13}C; 49.8 ppm) as internal standards at various temperatures. Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm) (integration, multiplicity, coupling constant (Hz)). Multiplicity and qualifier abbreviations are as follows: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, br = broad. IR spectra were recorded on FT/IR-410 spectrometer (Jasco Co., Ltd.) and are reported in frequency of absorption (cm^{-1}). LR and HR MS were recorded on an ESI-mode by using Esquire 4000 and APEX-III spectrometer (Bruker Daltonics Ltd.), DART-mode by using Jeol JMS-T100LC Accu TOF (Jeol Ltd.), and EI-mode by using Jeol JMS-700 (Jeol Ltd.). LC-MS analyses were carried out using Esquire 4000 (Bruker Daltonics Ltd.) with PU-980 and UV-970 HPLC system (Jasco Ltd.) equipped with LG-980-02 gradient unit (Jasco Ltd.) using an ODS-HG3 column (ϕ2.0×150 mm, Nomura Chemical Ltd.). Optical rotation was recorded on a DIP-360 spectrometer using 100-mm cell.

Experimental Procedures

Scheme S1. Synthesis of amine intermediate 20



Compound **15**

To a solution of **14**[1] (763.0 mg, 1.13 mmol) in THF (4 mL) and H_2O (1 mL) was added TFA (5 mL) at 0 ˚C. After being stirred for 2.5 hrs at 0 ˚C, the reaction mixture was concentrated *in vacuo*. To the residue were added pyridine (5 mL) and Ac_2O (5 mL) at 0 ˚C. After being stirred for further 4 h at RT, the reaction mixture was concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc=2/1-1/1) gave **15** (533.8 mg, 1.13 mmol, quant.) as a colorless viscous oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 5.6 Hz, 3.2 Hz, 2 H), 7.77 (dd, *J* = 5.6 Hz, 3.2 Hz, 2 H), 6.47 (d, *J* = 8.8 Hz, 1 H), 5.93 (dd, *J* = 11.2 Hz, 3.2 Hz, 1 H), 5.50 (dd, *J* = 3.2 Hz, 0.8 Hz, 1 H), 4.68 (dd, *J* = 11.2 Hz, 8.8 Hz, 1 H), 4.15 (ddd, *J* = 7.2 Hz, 5.2 Hz, 0.8 Hz, 1 H), 3.58 (dd, *J* = 12.8 Hz, 7.2 Hz, 1 H), 3.27 (dd, *J* = 12.8 Hz, 5.2 Hz, 1 H), 2.24 (s, 3 H), 2.01 (s, 3 H), 1.86 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 170.0, 169.5, 168.6, 134.4, 123.7, 123.6, 90.1, 73.1, 67.6, 67.1, 50.2, 50.1, 20.7, 20.4; IR (film) 3028, 2957, 2941, 2106, 1752, 1719, 1388, 1337, 1216, 1127, 1110, 1068, 1048, 1015, 950, 756, 722, 667, 629, 601, 530, 461, 409 cm^{-1}; $[\alpha]_D^{16}$ +15.6 (*c* 1.00, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{20}H_{20}N_4O_9Na$ 483.1128, found 483.1150.

Compound **16**

To a solution of **15** (2.6 g, 5.65 mmol) and $BiBr_3$ (126.8 mg, 0.28 mmol) in anhydrous CH_2Cl_2 (56 ml) was added TMSBr[2)] (2.9 ml, 22.4 mmol) at 0 ˚C under N_2 atmosphere. After being stirred for 12 hrs at RT, the reaction mixture was diluted with $CHCl_3$, quenched with sat. aq. $NaHCO_3$ at 0 ˚C, and extracted with $CHCl_3$. The combined organic layer was washed with brine, filtered, dried over Na_2SO_4, and concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc=10/1-5/1-3/1-2/1) gave bromide **16** (2.43 g, 5.05 mmol, 89%) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (br, 2 H), 7.77 (dd, *J* = 5.6 Hz, 3.2 Hz, 2 H), 6.70 (d, *J* = 3.6 Hz, 1 H), 6.51 (dd, *J* = 12.0 Hz, 3.2 Hz, 1 H), 5.69 (d, *J* = 2.8 Hz, 1 H), 4.84 (dd, *J* = 12.0 Hz, 3.6 Hz, 1 H), 4.51 (dd, *J* = 7.2 Hz, 4.8 Hz, 1 H), 3.54 (dd, *J* = 13.2 Hz, 7.6 Hz, 1 H), 3.34 (dd, *J* = 13.2 Hz, 4.8 Hz, 1 H), 2.19 (s, 3 H), 1.91 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 169.0, 134.5, 123.9, 123.5, 88.4, 72.6, 67.1, 65.6, 52.7, 50.1, 20.6, 20.5; IR (film) 3022, 2935, 2921, 2106, 1754, 1723, 1612, 1469, 1434, 1386, 1233, 1167, 1123, 1103, 1075, 1008, 946, 912, 888, 858, 823, 758, 718, 671, 649, 624, 606, 575, 546, 531, 515, 479, 460, 442, 419, 411 cm^{-1}; $[\alpha]_D^{16}$ +87.7 (*c* 1.00, $CHCl_3$); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{20}H_{17}BrN_4O_7Na$ 503.0178, found 503.0200.

Compound **18**

To a suspension of **16** (303.1 mg, 0.63 mmol), **17** (87.7 mg, 0.31 mmol), Ag_2CO_3 (209.6 mg, 0.76 mmol) and MS4A (883 mg) in anhydrous CH_2Cl_2 (3.1 mL) was slowly added AgOTf (96.5 mg, 0.38 mmol) in anhydrous toluene (3.1 mL) at 0 ˚C under N_2 atmosphere.[3)] After being stirred for 15 min at RT, the reaction mixture was diluted with $CHCl_3$ and filtered through a pad of Celite. The filtrate was successively washed with sat. aq. $NaHCO_3$, brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica gel column chromatography (toluene/acetone=50/1-20/1-10/1) gave **18** (189.5 mg, 0.28 mmol, 89%) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (br, 2 H), 7.76 (dd, *J* = 5.6 Hz, 3.2 Hz, 2 H), 5.78 (dd, *J* = 11.6 Hz, 3.2 Hz, 1 H), 5.43 (d, *J* = 2.8 Hz, 1 H), 5.35 (d, *J* = 8.4 Hz, 1 H), 5.17 (dt, *J* = 10.8 Hz, 7.6 Hz, 1 H), 5.03 (dt, *J* = 10.8 Hz, 7.6 Hz, 1 H), 4.54 (dd, *J* = 11.6 Hz, 8.4 Hz, 1 H), 4.44 (dd, *J* = 8.4 Hz, 4.4 Hz, 1 H), 3.93 (dt, *J* = 9.6 Hz, 6.4 Hz, 1 H), 3.61 (dd, *J* = 12.8 Hz, 8.4 Hz, 1 H), 3.45 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.16 (dd, *J* = 12.8 Hz, 4.4 Hz, 1 H), 2.50 (dd, *J* = 18.8 Hz, 8.0 Hz, 1 H),

2.35-2.00 (m, 13 H), 1.86 (s, 3 H), 1.77 (dt, *J* = 9.2 Hz, 5.2 Hz, 1 H), 1.45 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 218.8, 171.4, 170.3 (2C), 169.7, 134.3, 131.4, 127.9, 127.3, 123.4, 98.6, 80.6, 73.0, 69.5, 68.0, 67.7, 53.8, 51.3, 50.7, 40.2, 38.0, 37.6, 28.1, 27.5, 27.0, 25.3, 20.7, 20.5; IR (film) 3008, 2976, 2935, 2102, 1751, 1718, 1615, 1469, 1430, 1389, 1368, 1336, 1237, 1153, 1126, 1069, 1015, 950, 914, 797, 760, 722, 702, 681, 669, 647, 629, 606, 557, 531, 517, 467, 457, 442, 425, 418 cm^{-1}; $[\alpha]_D^{18}$ -35.1 (*c* 1.00, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{34}H_{42}N_4O_{11}Na$ 705.2758, found 705.2737.

Compound **19**

To a solution of **18** (99.7 mg, 0.12 mmol) in MeOH (2.4 mL) was added NaOMe (6.3 mg, 0.12 mmol) at 0 ˚C under N_2 atmosphere. After being stirred for 2 hrs at 0 ˚C, the reaction mixture was neutralized by Amberlite IR120B, filtered, and concentrated *in vacuo*. Purification by silica gel column chromatography ($CHCl_3$/MeOH=1/0-100/1-50/1-20/1) gave **19** (63.3 mg, 0.11mmol, 90%) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 5.6 Hz, 3.2 Hz, 2H), 7.72 (dd, *J* = 5.6 Hz, 3.2 Hz, 2 H), 5.22-5.16 (m, 2 H), 5.09 (dt, *J* = 10.8 Hz, 7.6 Hz, 1 H), 4.40 (dd, *J* = 10.8 Hz, 3.2 Hz, 1 H), 4.28 (dd, *J* = 10.8 Hz, 8.4 Hz, 1 H), 3.96 (d, *J* = 3.2 Hz, 1 H), 3.89-3.83 (m, 2 H), 3.76 (dd, *J* = 12.8 Hz, 8.0 Hz, 1 H), 3.45 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.36 (dd, *J* = 12.8 Hz, 4.4 Hz, 1 H), 2.53 (dd, *J* = 18.8 Hz, 8.0 Hz, 1 H), 2.35-2.02 (m, 10 H), 1.77 (dt, *J* = 5.6 Hz, 4.8 Hz, 1 H), 1.44 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 219.3, 171.6, 168.6, 134.1, 131.7, 127.8, 127.5, 123.4, 98.6, 80.7, 74.2, 69.3, 69.1, 68.5, 54.3, 53.9, 51.1, 40.3, 38.1, 37.6, 28.1, 27.6, 26.9, 25.3; IR (film) 3462, 3012, 2976, 2934, 2888, 2101, 1774, 1713, 1614, 1469, 1456, 1390, 1368, 1335, 1280, 1257, 1197, 1152, 1115, 1072, 988, 950, 925, 883, 847, 794, 755, 722, 702, 666, 640, 605, 585, 553, 531, 496, 483, 471, 454, 441, 423, 411 cm^{-1}; $[\alpha]_D^{22}$ -51.5 (*c* 0.50, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{30}H_{38}N_4O_9Na$ 621.2537, found 621.2537.

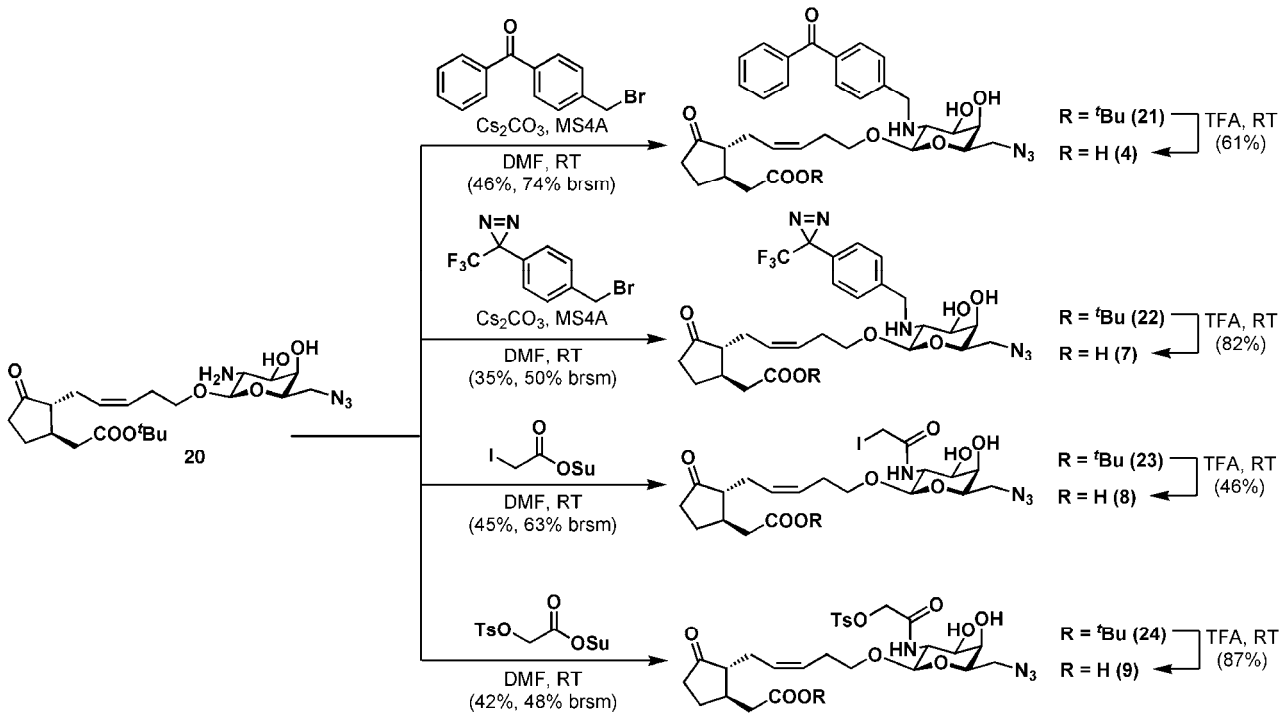
Compound **20**

0.8 M Ethylenediamine in MeOH (0.7 mL) was added to **19** (21.6 mg, 36 mmol) at RT under N_2 atmosphere. After being stirred for 22 h at 40 ˚C, the reaction mixture was cooled to 0 ˚C, and quenched with AcOH (0.1 mL). After additional one-hour-stirring at RT, the mixture was diluted

with EtOAc, absolute $NaHCO_3$ aq., and then extracted with EtOAc. The combined organic layer was washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Resulting **20** (18.5 mg, quant.) obtained as a yellow viscous oil, was immediately subjected to further reactions without purification.

^{1}H NMR (400 MHz, CD_3OD) δ 5.53-5.40 (m, 2H), 4.49 (d, J = 8.4 Hz, 1 H), 3.90 (dt, J = 9.6, 6.8 Hz, 1 H), 3,75-3.59 (m, 5 H), 3.25 (dd, J = 12.4, 3.6 Hz, 1 H), 3.08 (dd, J = 10.8, 8.4 Hz, 1 H), 2.60 (dd, J = 18.8, 8.4 Hz, 1 H), 2.49-2.04 (m, 9 H), 1.99-1.95 (m, 1 H), 1.61-1.48 (m, 1 H), 1.46 (s, 9 H); HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{22}H_{37}N_4O_7$ 469.2662, found 469.2690.

Scheme S2. Syntheses of amine units 4, 7-9.



Compound **21**

To a suspension of **20** (19.6 mg, 23 mmol) and MS4A (98 mg) in anhydrous DMF (0.5 mL) was added Cs_2CO_3 [4] (11.3 mg, 35 mmol) at RT under N_2 atmosphere. After being stirred for 30 min at RT, 4-(bromomethyl)benzophenone (7 mg, 26 mmol) was added to the reaction mixture. After being stirred for further 19 h at RT in the dark, the reaction mixture was filtered through a pad of

Celite, quenched with AcOH (5 drops), and concentrated *in vacuo*. Purification by preparative TLC ($CHCl_3$/MeOH=20/1) gave **21** (7.0 mg, 11 mmol, 46%, 74% brsm) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 7.77-7.43 (m, 4H), 7.66-7.61 (m, 1 H), 7.55-7.50 (m, 4 H), 5.53 (dt, *J* = 10.8 Hz, 7.2 Hz, 1 H), 5.42 (dt, *J* = 10.8 Hz, 7.6 Hz, 1 H), 4.37 (d, *J* = 8.0 Hz, 1 H), 4.20 (d, *J* = 14.0 Hz, 1 H), 4.06 (d, *J* = 14.0 Hz, 1 H), 3.97 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.69-3.61 (m, 3 H), 3.57 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.49 (dd, *J* = 10.8 Hz, 3.2 Hz, 1 H), 3.20 (dd, *J* = 11.6 Hz, 2.0 Hz, 1 H), 2.81 (dd, *J* = 10.4 Hz, 8.0 Hz, 1 H), 2.58 (dd, *J* = 18.8 Hz, 8.4 Hz, 1 H), 2.48-2.12 (m, 8 H), 2.08-1.99 (m, 1 H), 1.96-1.92 (m, 1 H), 1.51-1.44 (m, 1 H), 1.42 (s, 9 H); ^{13}C NMR (100 MHz, CD_3OD) δ 221.4, 198.3, 173.4, 146.4, 138.9, 137.5, 133.7, 131.4, 131.0, 129.7, 129.5, 129.4, 129.1, 105.7, 81.8, 75.9, 73.4, 70.1, 70.0, 60.0, 55.1, 53.6, 52.6, 41.2, 39.4, 38.5, 29.1, 28.4, 28.0, 26.4; IR (film) 3430, 3060, 3009, 2975, 2930, 2874, 2099, 1728, 1656, 1606, 1577, 1473, 1447, 1412, 1392, 1367, 1317, 1279, 1153, 1119, 1079, 1057, 1029, 939, 925, 884, 846, 756, 703, 667, 644 cm^{-1}; $[\alpha]_D^{18}$ -27.7 (*c* 1.00, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{36}H_{46}N_4O_8Na$ 685.3213, found 685.3195.

Compound **4**

Compound **21** (3.8 mg, 5.7 mmol) was treated by TFA (0.3 mL) at RT under N_2 atmosphere. After being stirred for 30 min at RT in the dark, the reaction mixture was concentrated *in vacuo*. Purification by HPLC (60% MeOH aq. containing 0.1% TFA, UV 280 nm) gave **4** (2.1 mg, 3.5 mmol, 61%) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 7.86 (d, *J* = 7.6 Hz, 2 H), 7.78 (d, *J* = 8.4 Hz, 2 H), 7.69-7.65 (m, 3 H), 7.54 (dd, *J* = 8.0 Hz, 8.0 Hz, 2 H), 5.56-5.44 (m, 2 H), 4.76 (d, *J* = 8.4 Hz, 1 H), 4.55 (d, *J* = 13.2 Hz, 1 H), 4.51 (d, *J* = 13.2 Hz, 1 H), 3.99 (dt, *J* = 9.2 Hz, 6.8 Hz, 1 H), 3.87 (dd, *J* = 11.2 Hz, 2.0 Hz, 1 H), 3.80 (d, *J* = 2.8 Hz, 1 H), 3.77 (dd, *J* = 8.8 Hz, 4.0 Hz, 1 H), 3.70-3.63 (m, 3 H), 3.27-3.21 (m, 2 H), 2.65 (dd, J = 19.6 Hz, 8.4 Hz, 1 H), 2.57-2.16 (m, 8 H), 2.08-1.93 (m, 1 H), 1.56-1.46 (m, 1 H); ^{13}C NMR (100 MHz, CD_3OD) δ 221.2, 197.3, 175.7, 139.6, 138.2, 136.4, 133.9, 131.4, 131.3, 130.8, 129.44, 129.41, 128.6, 100.1, 76.1, 70.28, 70.25, 69.8, 59.6, 55.1, 52.2, 51.3, 39.7, 39.2, 38.7, 28.9, 28.2, 26.4; IR (film) 3347, 3018, 2961, 2933, 2890, 2657, 2102, 1731, 1667, 1611, 1599, 1508, 1447, 1417, 1374, 1320, 1281, 1201, 1142, 1078, 1061, 1024, 940, 926, 884, 839, 798, 756, 722, 704, 666, 642, 628, 603, 556, 545, 517, 475 cm^{-1}; $[\alpha]_D^{24}$ -21.9 (*c* 0.15, MeOH); HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{32}H_{39}N_4O_8$ 607.2768, found 607.2764.

Compound **22**

To a suspension of **20** (18.6 mg, 39 mmol) and MS4A (93 mg) in anhydrous DMF (0.8 mL) was added Cs_2CO_3 (19.1 mg, 59 mmol) at RT under N_2 atmosphere. After being stirred for 30 min at RT, 4-(bromomethyl)trifluoromethyldiazirine (12 mg, 43 mmol) in anhydrous DMF (0.1 mL) was added. After being stirred for 12 h at RT in the dark, the reaction mixture was quenched with AcOH (4 drops), filtered through a pad of Celite, and concentrated *in vacuo*. Purification by silica gel column chromatography ($CHCl_3$/MeOH=1/0-100/1-80/1-60/1-10/1-5/1) gave **22** (9.1 mg, 14 mmol, 35%, 50% brsm) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 7.47 (d, *J* = 8.4 Hz, 2 H), 7.22 (d, *J* = 8.4 Hz, 2 H), 5.55-5.31 (m, 2 H), 4.37 (d, *J* = 8.4 Hz, 1 H), 4.13 (d, *J* = 13.6 Hz, 1 H), 4.00 (d, *J* = 13.6 Hz, 1 H), 3.95 (dt, *J* = 9.2 Hz, 6.8 Hz, 1 H), 3.68-3.60 (m, 3 H), 3.56 (dt, *J* = 9.2 Hz, 6.8 Hz, 1 H), 3.47 (dd, *J* = 10.4 Hz, 3.2 Hz, 1 H), 3.19 (dd, *J* = 11.2 Hz, 2.0 Hz, 1 H), 2.76 (dd, *J* = 11.2 Hz, 8.0 Hz, 1 H), 2.58 (dd, *J* = 18.8 Hz, 8.4 Hz, 1 H), 2.48-2.13 (m, 8 H), 2.10-2.00 (m, 1 H), 1.96-1.92 (m, 1 H)1.53-1.46 (m, 1 H), 1.44 (s, 9 H); ^{13}C NMR (100 MHz, CD_3OD) δ 221.4, 173.4, 143.0, 129.3, 129.14, 129.11 (q, *J* = 273 Hz), 129.0, 128.85, 128.78, 105.4, 81.8, 75.9, 75.8, 73.2, 70.1, 70.0, 59.8, 55.1, 53.2, 52.5, 41.2, 39.4, 38.5, 29.0, 28.4, 28.0, 26.4; IR (film) 3358, 3011, 2977, 2932, 2886, 2099, 1732, 1614, 1541, 1522, 1457, 1408, 1393, 1368, 1342, 1233, 1182, 1153, 1119, 1074, 1054, 1028, 938, 884, 844, 812, 759, 645, 616, 577, 550 cm^{-1}; $[\alpha]_D^{16}$ -32.4 (*c* 1.00, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{31}H_{41}F_3N_6O_7Na$ 689.2887, found 689.2893.

Compound **7**

Compound **22** (5.1 mg, 7.7 mmol) was treated by TFA (0.2 mL) at RT. After being stirred for 1 h at RT in the dark, the mixture was concentrated *in vacuo*. Purification by HPLC (38% MeCN aq. containing 0.1% TFA, UV 227 nm) gave **7** (3.8 mg, 6.2 mmol, 82%) as a pale yellow viscous oil.

^{1}H NMR (500 MHz, CD_3OD) δ 7.62 (d, *J* = 8.0 Hz, 2 H), 7.35 (d, *J* = 8.0 Hz, 2 H), 5.53-5.45 (m, 2 H), 4.74 (d, *J* = 8.0 Hz, 1 H), 4.47 (d, *J* = 13.5 Hz, 1 H), 4.44 (d, *J* = 13.5 Hz, 1 H), 3.97 (dt, *J* = 9.5 Hz, 6.5 Hz, 1 H), 3.84 (ddd, *J* = 11.0 Hz, 4.5 Hz, 3.0 Hz, 1 H), 3.78 (d, *J* = 3.0 Hz, 1 H), 3.75 (dd, *J* = 8.5 Hz, 4.0 Hz, 1 H), 3.67-3.62 (m, 2H), 3.24 (dd, *J* = 13.0 Hz, 4.0 Hz, 1 H), 3.15 (dd, *J* = 11.0 Hz, 8.0 Hz, 1 H), 2.65 (dd, *J* = 14.5 Hz, 3.5 Hz, 1 H), 2.56-2.17 (m, 8 H), 2.09-1.99 (m, 2 H), 1.57-1.48 (m, 1 H); ^{13}C NMR (125 MHz, CD_3OD) δ 221.7, 176.0, 134.3, 132.3, 131.4, 129.6, 128.8, 128.3, 123.5 (q, *J* = 273 Hz), 100.3, 76.2, 70.3, 69.8, 59.5, 55.1, 52.2, 51.1, 41.8, 39.7, 39.1, 38.6, 36.2, 28.9, 28.2, 26.4; IR (film) 3334, 3022, 2954, 2925, 2856, 2103, 1729, 1672, 1614, 1436, 1347, 1231, 1189, 1152, 1080, 1058, 940, 883, 839, 816, 799, 758, 722, 641, 631, 603, 548, 416

cm^{-1}; $[\alpha]_D^{23}$ -17.0 (*c* 0.50, MeOH); HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{27}H_{34}F_3N_6O_7$ 611.2441, found 611.2457.

Compound **23**

To a solution of **20** (4 mg, 8.8 mmol) in DMF (0.2 mL) was added iodoacetyl succinimide activated ester (4 mg, 13 mmol) at 0 ˚C under N_2 atmosphere. After being stirred for 3.5 h at RT, the reaction mixture was quenched with AcOH (2 drops), concentrated *in vacuo*. Partial purification by preparative TLC ($CHCl_3$/MeOH=10/1) gave crude IA. Resultant crude IA was dissolved in EtOAc, washed with H_2O and brine, dried over Na_2SO_4, filtered, concentrated in vacuo. Pure **23** (2.5 mg, 3.9 mmol, 45%, 74% brsm) was obtained as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 5.54-5.37 (m, 2 H), 4.45 (d, *J* = 8.4 Hz, 1 H), 3.88-3.83 (m, 2 H), 3.76-3.63 (m, 5 H), 3.51 (dt, *J* = 9.6, 6.8 Hz, 1 H), 3.26 (m, 1 H), 2.61 (d, *J* = 18.8, 8.4 Hz, 1 H), 2.41-2.04 (m, 10 H), 1.98-1.94 (m, 1 H), 1.64-1.49 (m, 1 H), 1.46 (s, 9 H); ^{13}C NMR (100 MHz, CD_3OD) δ 221.6, 173.5, 171.8, 129.0, 102.7, 81.8, 75.8, 72.7, 72.5, 70.2, 55.1, 54.6, 52.5, 43.5, 41.2, 39.5, 38.6, 29.0, 28.4, 28.0, 26.5, -1.50; IR (film) 3448, 3297, 3074, 3007, 2970, 2929, 2874, 2100, 1729, 1648, 1615, 1555, 1466, 1437, 1409, 1392, 1368, 1336, 1257, 1154, 1131, 1078, 1021, 984, 924, 886, 757, 667, 650, 612, 596, 572, 563, 418 cm^{-1}; $[\alpha]_D^{16}$ -32.4 (*c* 1.00, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{24}H_{37}IN_4O_8Na$ 659.1554, found 659.1547.

Compound **8**

Compound **23** (2.5 mg, 3.9 mmol) was treated by TFA (0.1 ml) at RT. After being stirred for 5 min at RT, the mixture was concentrated *in vacuo*. Purification by HPLC (55% MeOH aq. containing 0.1% TFA, UV 210 nm) gave **8** (1 mg, 1.7 mmol, 44%) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 5.53-5.37 (m, 2 H), 4.46 (d, *J* = 8.4 Hz, 1 H), 3.87-3.82 (m, 2 H), 3.75-3.71 (m, 3 H), 3.69-3.63 (m, 3 H), 3.52 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.24 (dd, *J* = 16.4 Hz, 8.0 Hz, 1 H), 2.67 (dd, *J* = 19.6 Hz, 8.4 Hz, 1 H), 2.41-2.18 (m, 8 H), 2.14-2.04 (m, 1 H), 2.00-1.95 (m, 1 H), 1.58-1.48 (m, 1 H); ^{13}C NMR (100 MHz, CD_3OD) δ 221.8, 176.0, 171.8, 129.0, 102.7, 75.8, 72.7, 70.2, 55.1, 54.7, 52.5, 39.7, 39.3, 38.6, 29.0, 28.1, 26.5, -1.58; IR (film) 3329, 3298, 3082, 3.11, 2957, 2925, 2856, 2102, 1731, 1664, 1555, 1408, 1366, 1274, 1201, 1168, 1126, 1069, 925, 882, 799, 755, 722, 666, 648, 624, 596, 553 cm^{-1}; $[\alpha]_D^{16}$ -49.6 (*c* 0.20, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{20}H_{29}IN_4O_8Na$ 603.0928, found 603.0927.

Compound **24**

To a solution of **20** (19.0 mg, 39 mmol) in DMF (0.8 mL) was added tosyloxyacetyl succinimide activated ester (15.2 mg, 46 mmol) at 0 ˚C under N_2 atmosphere. After being stirred for 2 h at RT, the reaction mixture was quenched with AcOH (3 drops), and concentrated *in vacuo*. The residue was partially purified by silica gel column chromatography ($CHCl_3$/MeOH=1/0, 100/1, 80/1, 60/1, 10/1, and 5/1). The obtained crude was dissolved in EtOAc, washed with H_2O and brine, dried over Na_2SO_4, concentrated *in vacuo*. Pure **24** (11.1 mg, 16 mmol, 42%, 48% brsm) was obtained as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 7.85 (d, *J* = 8.0 Hz, 2 H), 7.47 (d, *J* = 8.0 Hz, 2 H), 5.45-5.31 (m, 2 H), 4.48 (d, *J* = 8.4 Hz, 1 H), 4.43 (s, 2 H), 3.95 (dd, *J* = 10.4 Hz, 8.4 Hz, 1 H), 3.85 (dt, *J* = 9.6 Hz, 6.4 Hz, 1 H), 3.73 (d, *J* = 3.2 Hz, 1 H), 3.69 (dd, *J* = 10.4 Hz, 3.2 Hz, 1 H), 3.67-3.63 (m 2 H), 3.46 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.26-3.20 (m, 1 H), 2.60 (dd, *J* = 18.8 Hz, 8.4 Hz, 1 H), 2.46 (s, 3 H), 2.33-2.03 (m, 9 H), 1.96-1.91 (m, 1 H), 1.57-1.47 (m, 1 H), 1.45 (s, 9 H); ^{13}C NMR (100 MHz, CD_3OD) δ 221.7, 173.5, 168.3, 147.1, 133.5, 131.3, 129.3, 129.0, 128.9, 102.5, 81.8, 75.8, 72.3, 70.15, 70.12, 68.1, 55.0, 54.1, 52.5, 41.2, 39.5, 38.6, 28.8, 28.4, 28.0, 26.4, 21.7; IR (film) 3347, 3093, 3006, 2977, 2931, 2896, 2100, 1730, 1670, 1598, 1553, 1495, 1437, 1405, 1368, 1292, 1257, 1213, 1191, 1177, 1154, 1119, 1096, 1041, 965, 925, 883, 840, 817, 761, 704, 666, 555, 445, 434, 424, 413 cm^{-1}; $[\alpha]_D^{20}$ -30.2 (*c* 1.00, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{31}H_{44}N_4O_{11}SNa$ 703.2625, found 703.2614.

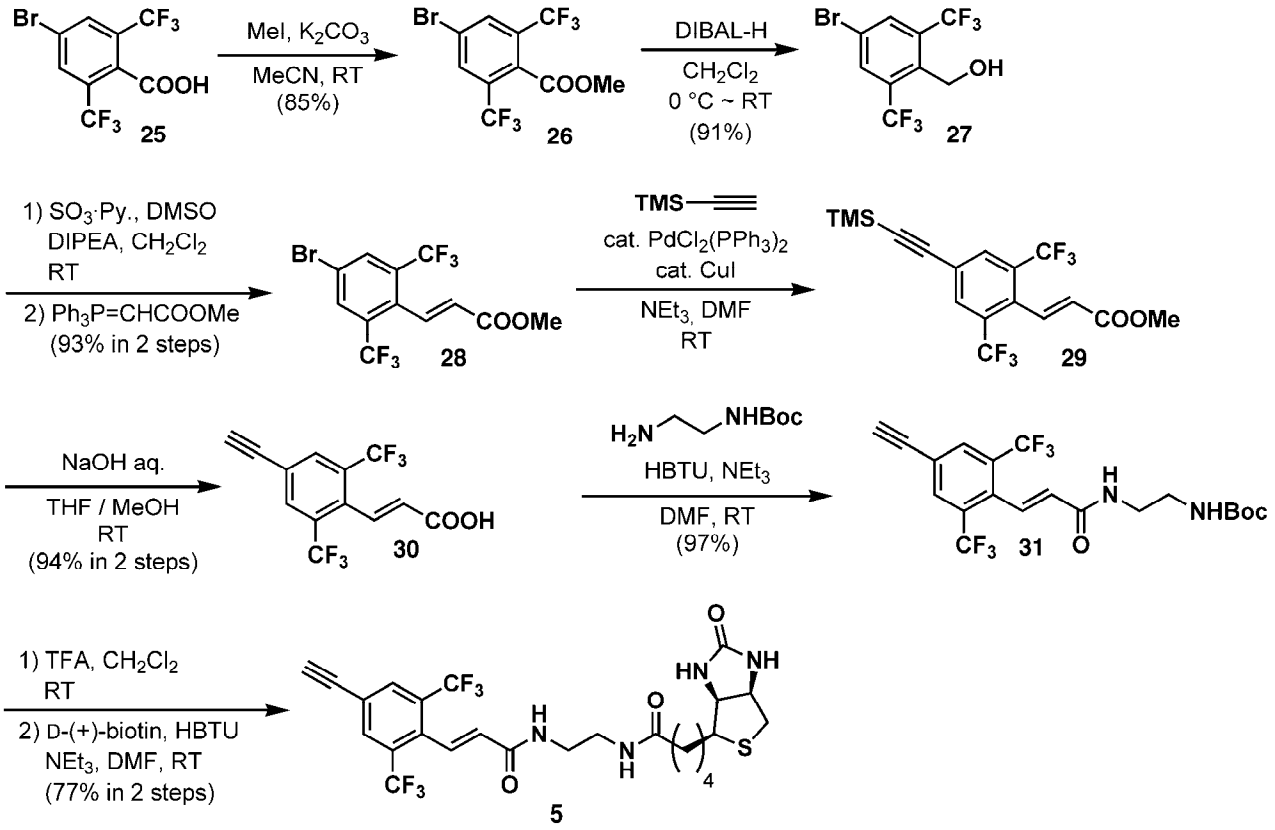
Compound **9**

Compound **24** (6.0 mg, 8.8 mmol) was treated by TFA (0.2 mL) at RT. After being stirred for 5 min at RT, the mixture was concentrated *in vacuo*. Purification by HPLC (36% MeCN aq. containing 0.1% TFA, UV 230 nm) gave **9** (4.8 mg, 7.7 mmol, 87%) as a pale yellow viscous oil.

^{1}H NMR (400 MHz, CD_3OD) δ 7.85 (d, *J* = 8.4 Hz, 2 H), 7.47 (d, *J* = 8.4 Hz, 2 H), 5.44-5.30 (m, 2 H), 4.48 (d, *J* = 8.4 Hz, 1 H), 4.43 (s, 2 H), 3.94 (dd, *J* = 10.4 Hz, 8.4 Hz, 1 H), 3.84 (dt, *J* = 9.6 Hz, 6.4 Hz, 1 H), 3.73 (d, *J* = 3.2 Hz, 1 H), 3.70 (dd, *J* = 10.8 Hz, 3.2 Hz, 1 H), 3.66-3.62 (m 2 H), 3.46 (dt, *J* = 9.6 Hz, 6.8 Hz, 1 H), 3.26-3.20 (m, 1 H), 2.66 (dd, *J* = 19.6 Hz, 8.4 Hz, 1 H), 2.46 (s, 3 H), 2.38-2.20 (m, 8 H), 2.13-2.04 (m, 1 H), 1.99-1.93 (m, 1 H), 1.57-1.47 (m, 1 H); ^{13}C NMR (125

MHz, CD_3OD) δ 221.8, 176.1, 168.3, 147.1, 133.6, 131.3, 129.3, 129.1, 129.0, 102.5, 75.8, 72.3, 70.2, 70.1, 68.1, 55.1, 54.2, 52.5, 39.7, 39.2, 38.6, 28.8, 28.2, 26.4, 21.7; IR (film) 3329, 3.98, 3017, 2929, 2101, 1733, 1671, 1598, 1556, 1437, 1406, 1368, 1282, 1191, 1177, 1119, 1095, 1059, 967, 840, 816, 769, 724, 666, 592, 554 cm^{-1}; $[\alpha]_D^{20}$ -34.4 (*c* 0.40, MeOH); HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd for $C_{27}H_{36}N_4O_{11}SNa$ 647.1999, found 647.1996.

Scheme S3. Synthesis of alkyne unit 5



Compound **26**

To a solution of 4-bromo-2,6-bis(trifluoromethyl) benzoic acid [5] (2.65 g, 7.86 mmol) in acetonitrile (30 mL) were added iodomethane (2.40 mL, 39.3 mmol) and K_2CO_3 (2.71 g, 19.6 mmol) at RT under N_2 atmosphere. After being stirred for 6 h at RT, the reaction mixture was quenched with sat. aq. $Na_2S_2O_3$, diluted with EtOAc, washed with water and brine, dried over Na_2SO_4, filtered,

concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc) gave **26** (2.35 g, 6.69 mmol, 85%) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 2H), 3.96 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) d 164.7, 133.0 (q, *J* = 4.8 Hz), 130.7 (q, *J* = 34 Hz), 130.1, 124.1, 121.9 (q, *J* = 275 Hz), 53.5; IR (film) 3090, 2960, 1754, 1596, 1579, 1456, 1436, 1336, 1291, 1265, 1198, 1146, 1110, 1064, 956, 893, 842, 793, 756, 714, 684 cm^{-1}; mp 66 °C; HRMS (DART, positive) [$(M+H)^+$] calcd for $C_{10}H_6BrF_6O_2$ 350.9455, found 350.9477.

Compound **27**

To a solution of **26** (2.35 g, 6.69 mmol) in anhydrous CH_2Cl_2 (20 mL) was added a solution of DIBALH (ca. 1.0 M in *n*-hexane, 20 mL, 20 mmol) at 0 °C under N_2 atmosphere. After being stirred for 3 h at RT, the reaction mixture was quenched with MeOH and then with sat. aq. Na^+/K^+ tartrate at 0 °C, diluted with EtOAc, and stirred at RT until the layers were separated. Resultant mixture was extracted with EtOAc, washed with H_2O and brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc) gave **27** (1.97 g, 6.10 mmol, 91%) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_{3,}$) δ 8.04 (s, 2H), 4.87 (d, *J* = 5.6 Hz, 2H), 1.95 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) d 136.3 (m), 133.2 (q, *J* = 31.5 Hz), 133.2 (qd, *J* = 6.1, 0.9 Hz), 122.9 (q, *J* = 275.2 Hz), 122.6, 56.7 (m); IR (film) 3639, 3375, 3096, 3946, 1808, 1589, 1457, 1425, 1334, 1297, 1267, 1246, 1181, 1137, 1077, 1023, 980, 895, 846, 828, 791, 739, 684 cm^{-1}; HRMS (EI, positive) [M^+] calcd for $C_9H_5BrF_6O$ 321.9428, found 321.9424.

Compound **28**

To a solution of **27** (1.97 g, 6.10 mmol) in anhydrous DMSO (30 mL) and anhydrous CH_2Cl_2 (10 mL) were added ^{i}Pr$_2$NEt (6.20 mL, 36.6 mmol) and SO_3·pyridine complex (2.91 g, 18.3 mmol) at RT under N_2 atmosphere. After being stirred for 5 h at RT, the reaction mixture was diluted with Et_2O, washed with sat. aq. NH_4Cl and brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Resultant crude aldehyde was subjected to the next reaction without further purification. To a solution of this crude aldehyde in anhydrous CH_2Cl_2 (30 mL) was added methyl

triphenylphosphoranilidene acetate ($Ph_3P{=}CHCO_2Me$) (5.10 g, 15.3 mmol). After being stirred for 11 h at RT, the reaction mixture was directly filtered through a pad of silica gel and concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexaneEtOAc) gave **28** (2.14 g, 5.67 mmol, 93% in 2 steps) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 2H), 7.78 (d, *J* = 16.0 Hz, 1H), 6.09 (d, *J* = 16.0 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.2, 136.5, 133.3 (m), 132.6 (qd, *J* = 6.0, 0.9 Hz), 132.0 (q, *J* = 31.0 Hz), 128.0 (m), 122.3, 122.2 (q, *J* = 274.7 Hz), 52.1; IR (film) 3087, 3000, 2954, 2361, 2355, 2342, 1733, 1654, 1574, 1462, 1438, 1337, 1288, 1261, 1174, 1137, 1037, 1009, 978, 938, 895, 838, 793, 683 cm^{-1}; mp 69 °C; HRMS (DART) [$(M+H)^+$] calcd for $C_{12}H_8BrF_6O_2$ 376.9612, found 376.9603.

Compound **30**

To a solution of **28** (77.7 mg, 0.205 mmol) in anhydrous DMF (1.0 mL) were added TMS acetylene (0.043 mL, 0.31 mmol), Et_3N (0.086 mL, 0.62 mmol), CuI (11.7 mg, 0.0615 mmol), and $PdCl_2(PPh_3)_2$ (14.4 mg, 0.0205 mmol) at RT under N_2 atmosphere. After being stirred for 1 h at RT, the reaction mixture was diluted with Et_2O, washed with H_2O and brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc) gave alkyne **29** (85.4 mg) as a pale yellow oil, which was subjected to the next reaction without further purification.

To a solution of crude **29** (85.4 mg) in THF (1.0 mL) and MeOH (0.5 mL) was added 2 M aqueous NaOH (0.5 mL) at RT under N_2 atmosphere. After being stirred for 5 h at RT, additional portion of 2 M aqueous NaOH (0.5 mL) was added. After being stirred for further 2 h, the reaction mixture was neutralized with 1 M HCl aq., extracted with EtOAc. The organic layer was washed with H_2O and brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc) gave **30** (59.6 mg, 0.19 mmol, 94% in 2 steps) as a pale yellow powder.

29: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 2H), 7.85 (m, 1H), 6.08 (d, J = 16.0 Hz, 1H), 3.83 (s, 3H), 0.27 (s, 9H).

30: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 2H), 7.96 (m, 1H), 6.12 (d, *J* = 16.0 Hz, 1H), 3.30 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 139.3, 133.8, 132.7 (q, *J* = 5.2 Hz, 2C), 130.8 (q, *J* =

31.0 Hz, 2C), 127.4 (m, 1C), 123.6, 122.6 (q, J = 274.3 Hz, 2C), 81.4, 80.3; IR (film) 3310, 3284, 3260, 3000, 2707, 2598, 1702, 1650, 1568, 1466, 1421, 1356, 1289, 1267, 1224, 1197, 1168, 1143, 978, 950, 915, 883, 843, 762, 723, 685 cm^{-1}; HRMS (DART, positive) [$(M+H)^+$] calcd for $C_{13}H_7F_6O_2$ 309.0350, found 309.0332

Compound **31**

To a solution of **30** (151.6 mg, 0.50 mmol) and monoBoc-ethyleneamine [6] (96.1 mg, 0.60 mmol) in anhydrous DMF (2.5 mL) were added Et_3N (0.14 mL, 1.0 mmol), HBTU (322.4 mg, 0.85 mmol) at RT under N_2 atmosphere. After being stirred for 12 h at RT, the reaction mixture was diluted with EtOAc, washed with H_2O and brine, dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (*n*-hexane/EtOAc) gave **31** (205.2 mg, 0.46 mmol, 91%) as a white powder.

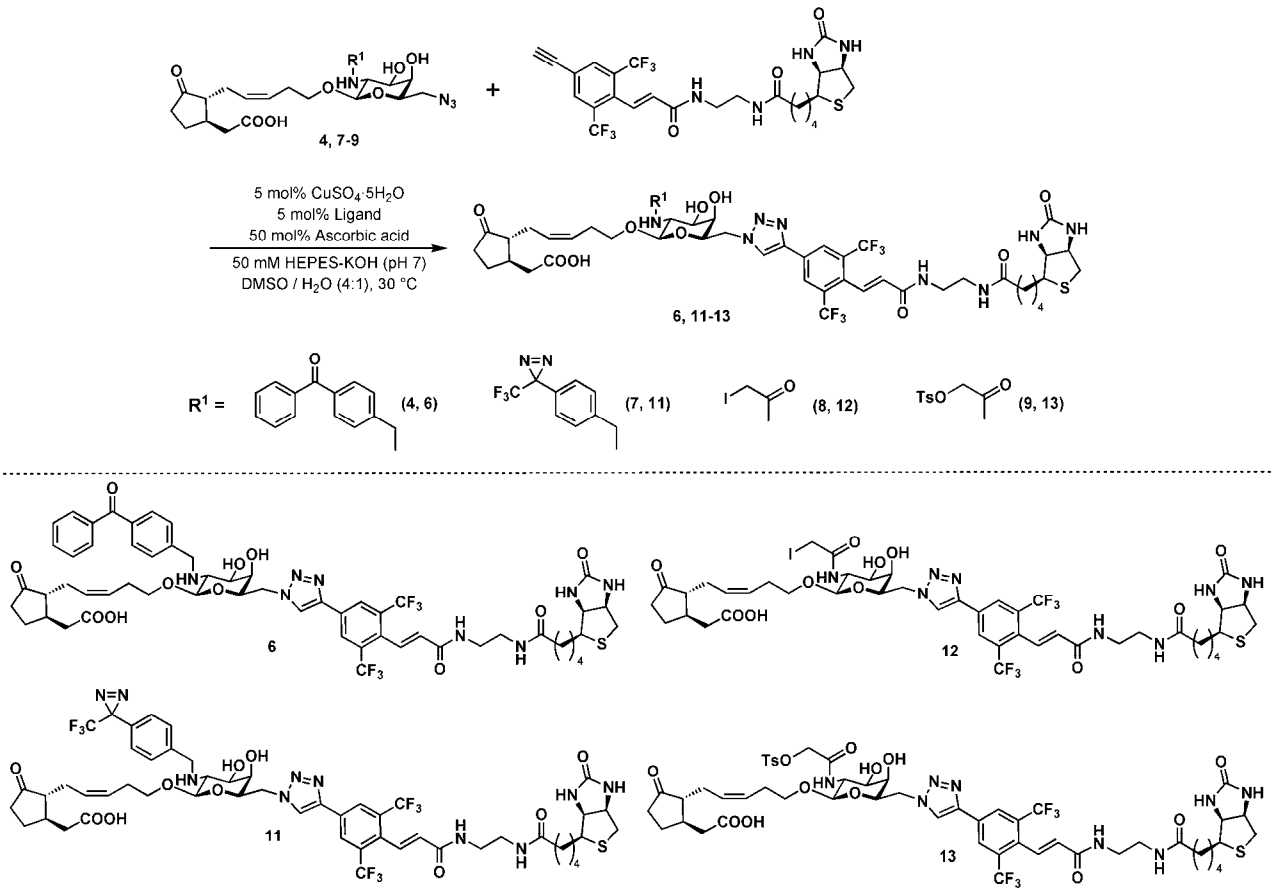
^1H NMR (500 MHz, $CDCl_3$) δ 7.96 (s, 2H), 7.74 (d, J = 16.0 Hz, 1H), 6.74 (brs, 1H), 6.03 (d, J = 16.0 Hz, 1H), 5.01 (brs, 1H), 3.50-3.47 (m, 2H), 3.37-3.35 (m, 2H), 3.28 (s, 1H), 1.42 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 157.3, 135.4, 132.9, 132.6 (q, J = 5.2 Hz), 130.9 (q, J = 30.7 Hz), 130.3, 122.8, 122.7 (q, J = 274.7 Hz), 81.0, 80.5, 79.9, 41.7, 39.8, 28.2; IR (film) 3305, 3095, 2982, 2936, 2487, 1678, 1628, 1561, 1528, 1465, 1432, 1362, 1290, 1256, 1171, 1127, 973, 908, 687 cm^{-1}; HRMS (ESI, positive) [$(M+Na)^+$] calcd for $C_{20}H_{20}F_6N_2O_3Na$ 473.1276, found 473.1297.

Compound **5**

To a solution of alkyne (127.0 mg, 0.282 mmol) in CH_2Cl_2 (3.0 mL) was added trifluoroacetic acid (1.5 mL). After being stirred at room temperature for 30 min, the reaction mixture was directly concentrated *in vacuo*. Resultant crude amine was subjected to the next reaction without further purification. To a solution of above crude amine in DMF (5.0 mL) were added Et_3N (0.1 mL, 0.71 mmol), D-(+)-biotin (75.7 mg, 0.31 mmol), and HBTU (117.6 mg, 0.31 mmol). After being stirred for 3 h at RT, the reaction mixture was concentrated under reduced pressure. Purification by silica gel column chromatography ($CHCl_3$/MeOH=1/0-15/85) followed by recrystallization gave **5** (124.3 mg, 77% in 2 steps) as a white powder: IR (film) 3419, 3287, 2927, 2255, 2125, 1698, 1636, 1564, 1466, 1428, 1360, 1291, 1247, 1172, 1128, 1026, 1003, 907, 825, 764 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$-CD_3OD = 1:1v/v) δ 7.99 (s, 2H), 7.71 (d, J = 16.0 Hz, 1H), 6.13 (d, J = 16.0 Hz, 1H), 4.48

(dd, J = 8.0, 4.0 Hz, 1H), 4.29 (dd, J = 8.0, 4.4 Hz, 1H), 3.62 (s, 1H), 3.45-3.37 (m, 2H), 3.37-3.30 (m, 2H), 3.16 (m, 1H), 2.89 (dd, J = 12.8, 5.2 Hz, 1H), 2.70 (d, J = 12.8 Hz, 1H), 2.19 (ddd, J = 7.6, 7.6, 1.6 Hz, 2H), 1.75-1.55 (m, 4H), 1.48-1.38 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$-CD_3OD = 1:1v/v) δ 175.8, 166.1, 165.2, 135.8, 133.7, 133.3 (q, J = 5.4 Hz), 131.5 (q, J = 30.6 Hz), 124.1, 123.5 (q, J = 273.8 Hz), 82.4, 80.8, 62.7, 60.9, 56.3, 40.7, 40.0, 39.6, 36.3, 29.1, 28.8, 26.1; HRMS (DART, positive) [$(M+H)^+$] calcd for $C_{25}H_{27}F_6N_4O_3S$ 577.1708, found 577.1723.

Scheme S4. Syntheses of biaryl probes 6, 11-13.



Compounds **6**,**11-13**

To a solution of **4**, **7**, **8**, or **9** (1.0 eq.) and **5** (1.2 eq.) in DMSO/250 mM HEPES buffer (pH 7) (4:1) were added $CuSO_4$·$5H_2O$-triazole ligand **10** [7] complex (5 mol%) and ascorbic acid [8] (50 mol%). After 1-h incubation at 30 ˚C, the reaction mixture was cooled to RT, and then purified by HPLC.

Compound **6**

Purification by HPLC (38% MeCN aq. containing 0.1% TFA, detection: UV 280 nm) gave **6** (85%) as a pale yellow solid.

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.45 (br, 1 H), 8.95 (s, 1 H), 8.86 (br, 1 H), 8.47 (s, 2 H), 8.35 (t, J = 5.5 Hz, 1 H), 7.86 (t, J = 5.5 Hz, 1 H), 7.79 (d, J = 8.5 Hz, 2 H), 7.72 (d, J = 8.5 Hz, 2 H), 7.69 (d, J = 8.0 Hz, 1 H), 7.66-7.62 (m, 3 H), 7.59-7.56 (m, 3 H), 6.38 (br, 1 H), 6.20 (d, J = 16.0 Hz, 1 H), 5.32-5.24 (m, 2 H), 4.70 (dd, J = 14.0 Hz, 3.5 Hz, 1 H), 4.61-4.55 (m, 2 H), 4.39 (s, 2 H), 4.29 (dd, J = 7.5 Hz, 5.0 Hz, 1 H), 4.12 (dd, J = 7.5 Hz, 4.5 Hz, 1 H), 4.04 (dd, J = 9.5 Hz, 3.5 Hz, 1 H), 3.79-3.76 (m, 2 H), 3.56 (dt, J = 9.5 Hz, 7.0 Hz, 1 H), 3.39 (dt, J = 9.5 Hz, 7.0 Hz, 1 H), 3.25-3.21 (m, 2 H), 3.17-3.13 (m, 2 H), 3.11-3.07 (m, 1 H), 2.98 (t, J = 8.5 Hz, 1 H), 2.80 (dd, J = 12.0 Hz, 5.0 Hz, 1 H), 2.57 (d, J = 12.5 Hz, 1 H), 2.53 (s, 1 H), 2.45 (d, J = 4.0 Hz, 1 H), 2.31-2.26 (m, 1 H), 2.23-1.90 (m, 10 H), 1.85-1.81 (m, 1 H), 1.65-1.58 (m, 1 H), 1.54-1.22 (m, 7 H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 218.3, 195.3, 173.3, 172.2, 163.3, 162.6, 158.3, 158.0, 143.2, 137.4, 136.7, 135.8, 133.7, 132.9, 131.5, 131.2, 130.9, 130.4, 129.8 (q, J = 31 Hz), 129.7, 129.5, 128.6, 128.1, 127.1, 125.7 (m), 124.5, 123.1 (q, J = 274 Hz), 98.9, 73.0, 69.7, 68.9, 68.5, 67.4, 61.0, 59.2, 57.3, 55.3, 53.0, 50.5, 49.7, 38.3, 38.1, 37.2, 37.1, 35.2, 28.1, 28.0, 27.1, 26.5, 25.1, 24.8; IR (film) 3284, 3084, 3008, 2930, 2874, 1672, 1555, 1461, 1434, 1372, 1319, 1293, 1201, 1177, 1131, 1092, 1052, 1026, 954, 926, 836, 799, 739, 719, 705, 685, 638 cm^{-1}; $[\alpha]_D^{21}$ +20.7 (*c* 0.40, DMSO); HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{57}H_{65}F_6N_8O_{11}S$ 1183.4398, found 1183.4399.

Compound **11**

Purification by HPLC (38% MeCN aq. containing 0.1% TFA, detection: UV 280 nm) gave **11** (87%) as a pale yellow solid.

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.43 (br, 1 H), 8.93 (s, 1 H), 8.82 (br, 1 H), 8.46 (s, 2 H), 8.36 (t, J = 5.0 Hz, 1 H), 7.96 (br, 1 H), 7.87 (t, J = 5.0 Hz, 1 H), 7.62-7.59 (m, 3 H), 7.36 (d, J = 8.0 Hz, 1 H), 7.25 (br, 1 H), 6.38 (br, 1 H), 6.20 (d, J = 16.0 Hz, 1 H), 5.30-5.23 (m, 2 H), 4.69 (dd, J = 14.0 Hz, 3.0 Hz, 1 H), 4.58-4.53 (m, 2 H). 4.32-4.28 (m, 3 H), 4.12 (dd, J = 7.5 Hz, 4.5 Hz, 1 H), 4.04-4.00 (m, 1 H), 3.77-3.73 (m, 2 H), 3.55-3.50 (m, 1 H), 3.35 (dt, J = 9.5 Hz, 7.0 Hz, 1 H), 3.25-3.21 (m, 2 H), 3.17-3.13 (m, 2 H), 3.11-3.07 (m, 1 H), 2.90 (t, J = 5.0 Hz, 1 H), 2.80 (dd, J = 12.0 Hz, 5.0 Hz, 1 H), 2.57 (d, J = 12.5 Hz, 1 H), 2.46 (d, J = 3.5 Hz, 1 H), 2.28-1.90 (m, 11 H),

1.86-1.82 (m, 1 H), 1.75-1.58 (m, 1 H), 1.54-1.25 (m, 7 H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 218.3, 173.3, 172.3, 171.4, 163.3, 162.6, 158.2, 157.9, 143.2, 133.7, 131.5, 131.3, 131.2, 130.9, 129.9 (q, J = 30 Hz), 128.2, 128.1, 127.0, 126.7, 125.7 (m), 124.4, 123.1 (q, J = 275 Hz), 122.9, 98.9, 73.0, 69.7, 68.9, 68.5, 67.4, 61.0, 59.2, 57.2, 55.3, 53.0, 50.5, 49.4, 38.3, 38.1, 37.2, 36.4, 35.2, 28.1, 28.0, 27.1, 26.5, 25.1, 24.8, 22.4; IR (film) 3281, 3085, 3021, 2925, 2862, 1673, 1557, 1461, 1435, 1335, 1293, 1184, 1132, 1052, 1025, 954, 939, 837, 799, 721, 685 cm^{-1}; $[\alpha]_D^{23}$ +11.4 (*c* 0.50, DMSO); HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{52}H_{60}F_9N_{10}O_{10}S$ 1187.4071, found 1187.4086.

Compound **12**

Purification by HPLC (38% MeCN aq. containing 0.1% TFA, detection: UV 280 nm) gave **12** (72%) as a pale yellow viscous oil.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.92 (s, 1 H), 8.43 (s, 2 H), 8.30 (t, J = 5.0 Hz, 1 H), 8.00 (d, J = 9.0 Hz, 1 H), 7.82 (t, J = 5.0 Hz, 1 H), 7.56 (d, J = 16.0 Hz, 1 H), 6.34 (br, 1 H), 6.16 (d, J = 16.0 Hz, 1 H), 5.25-5.15 (m, 2 H), 4.62 (dd, J = 14.0 Hz, 4.0 Hz, 1 H), 4.56 (dd, J = 14.0 Hz, 9.0 Hz, 1 H), 4.26-4.23 (m, 2 H), 4.08 (dd, J = 8.5 Hz, 4.0 Hz, 1 H), 3.87 (dd, J = 8.5 Hz, 4.0 Hz, 1 H), 3.68-3.61 (m, 2 H), 3.59 (d, J = 9.5 Hz, 1 H), 3.56 (d, J = 9.5 Hz, 1 H), 3.51 (dd, J = 10.5 Hz, 2.5 Hz, 1 H), 3.46 (s, 1 H), 3.43 (dt, J = 9.5 Hz, 7.0 Hz, 1 H), 3.23-3.17 (m, 3 H), 3.13-3.09 (m, 2 H), 3.07-3.03 (m, 1 H), 2.77 (dd, J = 12.5 Hz, 5.0 Hz, 1 H), 2.52 (d, J = 12.5 Hz, 1 H), 2.41 (d, J = 3.5 Hz, 1 H), 2.21-1.90 (m, 10 H), 1.79-1.75 (m, 1 H), 1.61-1.54 (m, 1 H), 1.50-1.22 (m, 7 H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 218.3, 173.3, 172.2, 167.5, 163.3, 162.6, 143.1, 133.6, 131.6, 131.2, 130.8, 129.6 (q, J = 31 Hz), 127.7, 127.0, 125.7 (m), 124.3, 123.1 (q, J = 274 Hz), 101.0, 72.7, 70.6, 69.7, 68.0, 67.8, 61.0, 59.1, 55.3, 52.9, 52.3, 50.8, 38.3, 38.1, 37.3, 37.1, 35.1, 28.1, 27.9, 27.3, 25.1, 24.8, 1.34; HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{45}H_{56}F_6IN_8O_{11}S$ 1157.2738, found 1157.2744.

Compound **13**

Purification by HPLC (40% MeCN aq. containing 0.1% TFA, detection: UV 280 nm) gave **13** (73%) as a white solid.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.95 (s, 1 H), 8.47 (s, 2 H), 8.34 (t, J = 5.5 Hz), 7.88-7.85 (m, 2 H), 7.81 (d, J = 8.5 Hz, 2 H), 7.60 (d, J = 16.5 Hz, 1 H), 7.47 (d, J = 8.5 Hz, 2 H), 6.38 (br, 1 H), 6.20 (d, J = 16.0 Hz, 1 H), 5.19-5.13 (m, 2 H), 4.66 (dd, J = 14.0, 4.0 Hz, 1 H), 4.59 (dd, J = 14.0, 9.0 Hz, 1 H), 4.35 (s, 2 H), 4.30-4.27 (m, 2 H), 4.12 (dd, J = 7.5, 4.5 Hz, 1 H), 3.88 (dd, J = 9.0, 4.5 Hz, 1 H), 3.77 (dd, J = 18.5, 9.0 Hz, 1 H), 3.68 (d, J = 3.0 Hz, 1 H), 3.57 (dd, J = 10.5, 3.0 Hz, 1 H), 3.50 (s, 1 H), 3.42 (dt, J = 10.0, 6.5 Hz, 1 H), 3.25-3.13 (m, 5 H), 3.11-3.07 (m, 1 H), 2.80 (dd, J = 12.5, 5.0 Hz, 1 H), 2.56 (d, J = 12.5 Hz, 1 H), 2.53 (s, 1 H), 2.46 (dd, J = 15.5, 4.0 Hz, 1 H), 2.40 (s, 3 H), 2.21-1.94 (m, 12 H), 1.81-1.77 (m, 1 H), 1.65-1.58 (m, 1 H), 1.54-1.22 (m, 7 H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 218.3, 173.3, 172.2, 164.3, 163.3, 162.6, 145.2, 143.1, 136.7, 133.6, 131.8, 131.6, 131.2, 130.8, 130.1, 129.8 (q, J = 30 Hz), 127.73, 127.66, 127.0, 125.6 (m), 124.4, 123.1 (q, J = 275 Hz), 100.8, 72.8, 70.3, 69.7, 67.9, 67.7, 67.0, 61.0, 59.2, 55.3, 52.9, 51.9, 50.8, 38.3, 38.1, 37.2, 37.1, 35.2, 28.1, 28.0, 27.2, 26.5, 25.1, 24.8, 21.0; IR (film) 3293, 3083, 2931, 2861, 1735, 1702, 1683, 1667, 1636, 1550, 1463, 1436, 1367, 1322, 1296, 1242, 1173, 1125, 1049, 969, 822, 686, 667, 552 cm^{-1}; $[\alpha]_D^{24}$ +11.0 (*c* 0.40, DMSO); HRMS (ESI, positive) *m/z* $[M+H]^+$ calcd for $C_{52}H_{63}F_6N_8O_{14}S_2$ 1201.3809, found 1201.3790.

ROESY experiment on probes 2 and 6

ROESY experiment was carried out on a Jeol ECA-600 spectometer (Jeol Ltd.). Probe **2** (6.6 mg) and BArL probe **6** (10 mg) was dissolved in 0.5 mL of DMSO-d_6 (99.9%D), respectively. The ROESY experiment was carried out at 35 °C with mixing time of 0.25 sec.

Cross-link formation between BArL probes and protoplast and analysis of biotinylated proteins

Samanea saman grown as previously described[4] was used in all experiments. The tertiary pulvini were collected from compound leaves on the 3rd or 4th branch from the shoot apex. Motor cell protoplasts were prepared according to the previously reported method.[4] To a suspension of protoplasts {about 1 × 10^4 protoplasts in 0.1 mL wash solution [25 mM HEPES (pH 7.0), 0.5 M sorbitol, and one tablet of Complete^{TM} (Roche Co., Ltd.)/500 mL]} was added a) **6** or **11** (1 × 10^{-4} M) or b) **12** or **13** (1× 10^{-4} M) and the mixture was incubated for 5 min at 0 °C in the dark. After cross-linking by a) irradiation with UV light (365 nm, irradiated from ca. 1 cm above the surface,

As one handy UV lamp LUV-16 [AS ONE, Co., Ltd]) for 20 min at 4 °C, or b) allowing to stand for 20 min or 60 min at 4 °C, the cross-linked protoplasts were sedimented by centrifugation (110 × *g*, 5 min, 4 °C) and the supernatant was decanted. The extraction buffer (0.6 mL) was added to this sediment (0.1 mL) and the mixture was homogenized using a glass rod. Centrifuging the lysate twice (1st: 3,000 × *g*, 15 min, 4 °C, Kokusan H-9R with A_N rotor [Kokusan Co. Ltd.]; 2nd: 100,000 × *g*, 1 h, 4 °C, Beckman Coulter Optima TLX [Beckman Coulter Inc.]) gave a crude membrane fraction pellet. The content of total protein in this fraction was *ca*. 0.6 mg based on the Bradford method with BSA as standard. Membrane ATPase activity was determined to be *ca.* 0.2 mmol/mg protein·min by Sandstrom's method.[9] The crude membrane fractions were suspended in 10 mL of extraction buffer. Electrophoresis buffer (0.3 M Tris-Cl, 10% SDS, 30% glycerol, 9.3% DTT, pH 6.8) was added to the membrane fraction and the solution was heated at 95 °C for 5 min. The reaction mixture was analyzed by SDS-PAGE (Ready Gel J 7.5-15% polyacrylamide gels, Bio-Rad Laboratories, Inc.) with a molecular weight marker (biotinylated SDS-PAGE standard, high-range, Bio-Rad Laboratories, Inc.). After western blotting using Hybond-P PVDF membrane (GE Healthcare UK, Ltd.), protein bands were detected by chemiluminescence using an ECL Advance western blotting detection kit (GE Healthcare UK, Ltd.) with an LAS-4000 Bioimager (Fuji Film Co., Ltd.). The intensity of chemiluminescence was recorded with an LAS-4000 Bioimager (Fuji Film Co., Ltd.) and analyzed using MultiGauge software (Fuji Film Co., Ltd.).

Stepwise labeling

Labeling reaction by probe **4** using living cells was carried out as described above. The labeled protoplasts were suspended in 97 µL ligation buffer (25 mM HEPES (pH 8.0), 0.5 M sorbitol), and was added alkyne unit **5** (1.0×10^{-8} mol in 1µL DMSO), and $CuSO_4$ and ligand **10** ($CuSO_4$ (5.0×10^{-8} mol) in 1 µL DMSO), and ascorbic acid (5.0×10^{-8} mol in 1µL ligation buffer). After this suspension was incubated for 30 min at 4 °C, the protoplasts were sedimented by centrifugation (110 × *g*, 5 min, 4 °C) and the supernatant was decanted. After homogenizing the protoplasts, the membrane fraction was analyzed by SDS-PAGE and chemiluminescence detection as described above.

Motor cell-shrinking assay

The tertiary pulvini of *S. saman* were collected from compound leaves on the 2nd or 3rd branch from the short apex. These pulvini were separated into extensor (adaxial) part and flexor (abaxial) part with a sharp razor blade under stereomicroscope. Protoplasts were prepared from extensor part according to the previously reported method.[1] The isolated protoplasts were suspended in the wash solution (0.57 M sorbitol, 10 mM KCl, 1 mM $CaCl_2$, 20 mM MES-Tris pH 5.5) and centrifuged at 110 x *g* for 5 min. This procedure was repeated twice. Resulting pellet containing protoplasts was suspended in a small amount of the wash solution.

The freshly prepared protoplasts in 450 μL wash solution were added to a glass bottom petri dish (ϕ 35 mm x 12 mm), and the dish was placed on the sample stage of an inverted microscope (IX-71, Olympus, Tokyo, Japan). The protoplasts were monitored with continuous irradiation of the light (50 μmol m^{-2} s^{-1}) passed through a green filter (43IF550-W45, Olympus, Tokyo, Japan).

After the protoplasts were incubated for 6 min on the microscope stage, a 50 μL wash solution including each probe ($1x10^{-4}$ M with 1% DMSO) was added and the solution was covered with cover glass. The status of protoplasts was recorded with timelapse photography (3-min intervals) for 27 min by using a digital camera (DP 72, Olympus, Tokyo, Japan) and analyzed by Bio-imaging analysis software (Lumina Vision, Mitani Co., Tokyo, Japan). The diameter for each magnified photoimage of protoplast were measured precisely by Photoshop software (Adobe systems, USA). For the volume analysis, protoplasts were selected only with regard to roundness and clarity of the margin.

Computational Methods

Conformation searching were carried out using MMFF molecular mechanics model implemented in Mac Spartan Pro Ver 1.0.4.[10] The conformers within 10 kcal/mol from the lowest energy were chosen from 1200 calculated conformers using Monte-Carlo method (technique), which randomly sample conformational space, and were calculated with geometric optimizations using the B3LYP/6-31G* method and basis set implemented in the Gaussian 03 program.[11] 5*d* functions were used for the *d* orbital. Calculations were performed without assuming symmetry.

Optimized structures with B3LYP/6-31G* of compound **2**

E^{rel}=0.0 kcal/mol (Figure 1b)

0,1¥C,0.0828818618,-0.5657337083,0.7294895747¥C,-0.1111909842,-0.2644871616,2.2141230246¥H,0.8726849635,-0.280414402,2.6972671766¥C,-1.0160257632,-1.2212689945,2.9856203584¥C,-0.9243986544,-0.8214994554,4.4641691591¥H,0.0888439975,-1.0470338592,4.81367894¥O,-1.8046458712,-1.593006826,5.2669630752¥H,-2.6450793222,-1.6280450693,4.7736939946¥C,-1.232329794,0.6877715603,4.6698244104¥C,-0.4985990656,1.5883367114,3.6462545281¥H,0.5760495143,1.6398953329,3.8563638613¥O,-0.9276920614,2.923557128,3.640796527¥C,-2.2667178698,3.1836548045,3.1630256414¥H,-2.3375153472,2.8663123684,2.1170048602¥C,-2.5425823964,4.6838912933,3.2720944434¥H,-1.8297775453,5.2173045754,2.6255746036¥C,-2.4571704298,5.2298843698,4.6744180598¥C,-3.4433830711,5.7764559788,5.3966670869¥C,-4.8859027049,5.9673249363,5.0100822045¥H,-5.0660262462,7.0201277582,4.7467217304¥C,-5.8792299244,5.6323061443,6.1363210837¥H,-5.5507854972,6.1550277219,7.0532902401¥C,-7.2802165768,6.2006112681,5.8415199776¥C,-8.3350408049,5.2441804086,6.400311145¥H,-9.1008206039,5.7876724234,6.9625398865¥H,-8.840443252,4.7773234858,5.5430071853¥C,-7.5323364379,4.215008812,7.2068555787¥H,-8.009072665,3.2304389016,7.251559917¥H,-7.4069491581,4.5624714454,8.2417520829¥C,-6.1489172396,4.1541504118,6.5099299228¥H,-6.251089877,3.5696266744,5.5856894954¥C,-5.0823555989,3.4670229063,7.377072489¥C,-4.0081935507,2.732813642,6.5892309404¥O,-4.2472720286,2.1132382105,5.5605123688¥O,-2.8157972856,2.787402238,7.1701540568¥H,-2.1400150041,2.2120580132,6.6619472991¥H,-5.5675338816,2.6926798602,7.9900814829¥H,-4.6137078705,4.1659302816,8.0772810359¥O,-7.5018734883,7.2340716997,5.2481488016¥H,-5.140633351,5.381167486,4.1197414564¥H,-3.1860818944,6.1402126025,6.3929843949¥H,-1.4747031567,5.1593945008,5.1388595488¥H,-3.5334244461,4.859735096,2.8397030413¥H,-2.9940476704,2.6330827062,3.7646588087¥O,-0.6785969182,1.0519415495,2.3295684342¥H,-2.3100743135,0.8104757955,4.5137023404¥N,-0.9888074167,1.0794447054,6.0799059188¥H,-1.3195541476,0.2824258152,6.6305115846¥C,0.4339181251,1.3300415212,6.4404484668¥C,0.6277289447,1.2863100798,7.9405796327¥C,0.0754348577,2.271115842,8.7717100954¥C,0.2684811314,2.2280874298,10.1512947189¥C,1.0144717639,1.1921883998,10.7362569434¥C,1.5430705299,0.1912380836,9.9074634216¥C,1.3609946376,0.2456538269,8.529084004¥H,1.7901225412,-0.5291108704,7.8979918687¥H,2.0938293623,-0.6240463019,10.3652594629¥C,1.2068120492,1.0482517756,12.2177984831¥O,1.3538358097,-0.0682311877,12.7039799749¥C,1.2245288,2.255412051,13.1095863917¥C,0.8724032695,2.0757670915,14.4574533697¥C,0.9151965841,3.1445592146,15.3477693064¥C,1.3360958704,4.4042659821,14.9090542846¥C,1.7131394282,4.5878263809,13.5776643327¥C,1.6527536701,3.521178649,12.6793803372¥H,1.9642697596,3.6669084194,11.6501010954¥H,2.0582709155,5.5605362954,13.2378021411¥H,1.3760350308,5.237733709,15.6053992428¥H,0.6276868518,2.9976688573,16.3853195483¥H,0.5703756311,1.0860403511,14.7843588479¥H,-0.1832916464,2.9915107105,10.7764299882¥H,-0.5215116832,3.0693067496,8.3404578044¥H,0.7120760253,2.3153283727,6.0520591622¥H,1.1099504284,0.6035392538,5.967923485¥O,-2.3685210213,-1.1737730121,2.5296707235¥H,-2.5548989387,-0.2358732981,2.3452050011¥H,-0.6918184326,-2.2612443476,2.8718461072¥N,1.1197422894,0.2750817868,0.1289705681¥C,2.4584022875,0.2495697522,0.3947642393¥O,3.1846847376,1.1986760998,0.1013634615¥C,3.071223559,-1.0284968064,1.0048231401¥H,3.5513955974,-1.5767417966,0.1864905188¥H,2.3290506828,-1.684810518,1.4582678034¥N,4.0722201392,-0.7094147077,2.0023382316¥C,3.7333812105,-0.452143528,3.2956309879¥O,2.6249243844,-0.6982253034,3.7773548339¥C,4.8442094383,0.2191098875,4.1171104932¥H,5.7727581574,-0.3552294013,4.0483132595¥H,4.5122662392,0.2613705478,5.1549665407¥N,5.1056587912,1.5731865918,3.6424832546¥C,5.881505553,1.7762333

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43,6.030669277,1.0902596931¥H,0.5379106153,5.0706527075,1.29623232¥H,0
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51539093,3.7181192588¥N,1.2908129116,4.9202473912,3.8321784232¥H,0.520
4694847,4.2683997538,3.6987568803¥C,2.5425465245,4.4792422447,4.149081
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,4.2085690355¥C,2.6260510819,6.8382659572,4.1557287602¥H,2.5703451033,
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56551,4.7228608826¥H,0.4531836433,6.7530397155,4.4267763209¥H,2.336155
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22¥H,7.0374914921,3.4403842618,1.8723693526¥H,5.6154653688,3.929120223
7,2.8025125485¥H,4.4579911381,2.3053209684,3.9476862575¥H,4.9772932779
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0. 4252149

E^{rel}=0.3 kcal/mol

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2,0.4361309651¥C,2.8470914447,0.7320556738,2.1250799041¥C,1.4473907575
,0.682731589,1.4852117816¥H,1.2356517157,1.6740161555,1.0557168982¥O,0
.5752943865,0.3961360281,2.5714732169¥H,-0.3657541337,0.5347499936,2.3
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699702007,-0.5565294664¥H,2.5991705522,0.534927983,-1.1839195531¥O,2.5
414741674,-1.5200186681,-1.3430162439¥C,3.4494986223,-1.5236165636,-2.
4591125058¥H,3.0879375065,-0.8169831932,-3.2147269379¥C,3.5090244125,-
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9,-1.3289845608¥C,2.714760638,-5.1261982498,-0.8138239421¥H,1.94736169
51,-4.9148514489,-1.5661537573¥C,2.3255242881,-4.3360244442,0.46119546
95¥H,2.3336694854,-3.2759750113,0.1737383777¥C,0.8919742374,-4.6485157
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,3.8251825372¥H,2.0603179293,-3.2730452351,3.1069385508¥C,3.1947252382
,-4.5179982776,1.7313562106¥H,3.5887329084,-5.5437998474,1.7622539926¥
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,2.9528125077¥O,5.23432479,-4.5970673154,3.8000446373¥O,6.2863275051,-
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87,-1.1940040297,-1.3908806055¥C,-2.5091024387,-0.1068334914,-2.015868
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3158754,-1.3912414349¥C,-4.0612428757,-2.0962625213,-0.8269975407¥C,-2
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-0.3355770517¥H,-4.6575361949,-2.8657767238,-0.3456225161¥C,-6.1485069
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6969¥H,-9.9283504755,-4.4697151265,-1.8751184692¥H,-7.6634963013,-4.83
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.1656330979,-2.2527474612¥O,3.0352557593,-0.380969033,2.9881833686¥H,2
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4155572¥N,6.3773934434,0.6700683191,0.5687278783¥C,6.706369722,1.63785
34584,-0.3325504894¥O,7.3868138983,1.4056492023,-1.3284183729¥C,6.2535
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6668¥H,5.4716351726,3.1882154287,0.6790616455¥N,5.7496620574,3.6510461
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1987¥H,-0.6449341455,4.6653147429,-0.0456692774¥H,-0.8038788016,2.9028
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22955828,4.7171215402,-1.5081086445¥C,-3.2886800801,4.0431554707,0.488
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1222016¥C,-3.1599063009,1.0328521764,2.1381431613¥O,-2.0577516498,0.60
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E^{rel}=0.5 kcal/mol

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.7537538813,-1.1612219084,2.9450812764¥C,-0.7477041081,-1.0355103419,4
.4764100351¥H,0.2674010891,-1.2369046742,4.8413936583¥O,-1.5828336425,
-2.0159600704,5.0703684119¥H,-2.3875903421,-2.0402855149,4.5196856825¥
C,-1.1923287528,0.3803035974,4.9247154891¥C,-0.3717864927,1.4580465584

,4.1796408974¥H,0.6899200093,1.3908563448,4.4511644137¥O,-0.7339918003
,2.7770741917,4.4445751545¥C,-2.0134873213,3.2160804603,3.9398577972¥H
,-1.9838677155,3.2086996777,2.844200257¥C,-2.2707519962,4.6367375891,4
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E^{rel}=6.7 kcal/mol

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E^{rel}=8.5 kcal/mol

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1.8562433

E^{rel}=10.3 kcal/mol

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,3.9793579705¥C,-1.8849530017,0.5438357323,3.0273716202¥C,-0.604478156
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,-2.4383698789,0.8014232545¥H,0.1973194355,-3.0506773403,0.7659835366¥
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,3.7614996373,-4.9118512494,0.1917879454¥C,4.214586666,-3.9074518553,-
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E^{rel}=11.1 kcal/mol

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,-1.8759958118,3.8329670313¥H,-2.0400939358,-2.7826474735,3.9116064806
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58,-1.1753537,1.548134

Optimized structures with B3LYP/6-31G* of compound **6**

E^{rel}=0.0 kcal/mol

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,-0.7291449929,3.0542495432¥H,0.412643788,-0.8635481137,3.6646964738¥C
,-1.6750501324,-1.4728808782,3.75343214¥C,-2.7366511999,-0.4628305737,
4.2142571873¥H,-2.3351612565,0.1636507704,5.0161946794¥O,-3.8572822601
,-1.1418334143,4.7522433437¥H,-3.9991371665,-1.9098445153,4.1687305182
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,2.5317208344¥H,-1.9216793256,2.2252325466,2.9332892214¥O,-1.920079067
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63¥F,2.5353728955,-8.8870542658,0.1727819786¥H,1.9798438142,-6.7784562
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6,-0.2258127,0.7462332

E^{rel}=5.0 kcal/mol (Figure 1b)

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C,-1.5076695169,-1.3249445162,1.5907557332¥C,-2.5214141149,-0.86650657
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7502,-1.9405540642,3.0008762658¥H,-3.528438255,-2.4218918681,2.1656015
981¥C,-3.3164463992,0.3279932402,2.0893159292¥C,-2.3480256906,1.503154
7545,1.8696719034¥H,-2.3593459566,2.145799491,2.7580126185¥O,-2.767389
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74¥H,-2.6332896502,4.1427187129,1.540316482¥C,-2.6600323195,4.20604218
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,-4.7929237298¥O,-1.899305221,3.497953534,-4.5181613262¥O,-3.550102099
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4¥H,-4.9525263308,4.5286272553,-5.0056060267¥H,-4.4805250664,4.1110488
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67,-4.7258257311¥F,3.8150186832,-5.4035246696,-6.4120449886¥F,2.928282
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5,-2.1389957

E^{rel}=5.7 kcal/mol

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3¥H,-4.7674885432,2.9420049217,2.2375014742¥C,-4.7022388948,3.94027098
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,5.0875694821,0.6396341691¥O,-1.2770770508,3.966506844,-1.0768503573¥H
,-2.1122617016,3.4971964456,-1.2982090211¥H,-3.2433359168,5.6573404236
,-0.6000220299¥H,-3.4248497282,4.2933739559,0.4926587406¥O,-5.15642466
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E^{rel}=8.3 kcal/mol

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E^{rel}=9.4 kcal/mol

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E^{rel}=9.9 kcal/mol

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E^{rel}=10.4 kcal/mol

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10. Mac Spartan Pro Ver 1.0.4 were released from Wavefunction, Inc., 18401, Von Karman Avenue, Suite 370, Irvine, CA 92612 U.S.A.

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