Table of Contents

S1. MATERIALS, INSTRUMENTATION, TECHNIQUES AND METHODS

S1.1. Synthesis

All synthetic procedures were carried out at room temperature under a nitrogen atmosphere and all reagents and solvents were used as received from commercial suppliers, unless otherwise stated. Dried solvents were collected from an LC Technologies SP-1 solvent purifier. Glassware used for reactions was dried overnight in an oven at 110 °C and flushed with nitrogen before use. $BF_3.OEt_2$ and BCl_3 were added to Schlenk flasks using Hamilton gas-tight syringes.

S1.2. Purification

For column chromatography the silica used was either Chem-Supply brand, silica gel 60 Å 0.04-0.06 mm (230-400 mesh ASTM) or Davisil brand, LC60A 0.04 - 0.06 mm. Alumina used was activated basic and activated neutral, Brockmann Grade I, 58 Å (ECP). Reactions were monitored using TLC carried out on Kiesgel 60 silica and the spots were visualised using UV light. The deactivated silica gel used was 20% water deactivated silica gel. This was prepared by dropwise addition of water (20 mL) into 80 g of silica gel with continuous agitation. The mixture was then rotated on a rotavap for a couple of hours and left to stand overnight before using it. HPLC methods were established on a Thermo Scientific Dionex UltiMate 3000 UHPLC$^+$ using a Thermo Fisher scientific Hypersil GOLD reversed-phase HPLC column (5 µm, 250 x 4.6 mm) at a flow rate of 0.5 mL/min. For purification and collection, an Agilent Eclipse XDB-C18 (5 µm, 9.4 x 250 mm) column was used at a flow rate of 2 mL/min with detection at 250 and 500 nm.

S1.3. Characterisation

NMR spectroscopy: carried out at 25 ^oC and the residual solvent peaks were used as internal standards. All 1D (^1H, $^{13}C\{^1H\}$ and $^{11}B\{^1H\}$) and 2D NMR (^1H-^1H COSY, ^1H-^1H NOESY, ^1H-^1H TOCSY, ^1H-^{13}C HSQC, HSQC-DEPT, ^1H-^{13}C HMBC, ^1H-^{11}B HMBC) spectra were obtained on a Bruker Avance III 400 MHz NMR spectrometers. $^{11}B\{^1H\}$ NMR spectrum was externally referenced to $BF_3.Et_2O$ (δ = 0.00 ppm). Assignments of signals in NMR spectra were made on the basis of chemical shift position, the integral values in ^1H NMR spectra, and by the use of above-mentioned 2D spectra.

Mass spectrometry: HRMS analysis was performed on a Bruker Daltronics MicrOTOF-QII instrument using direct infusion (ESI).

X-ray crystallography: X-ray diffraction analysis of single crystals of **3, 3Ra, 3Rd, and 4** were performed on a Rigaku Oxford Diffraction XtaLAB-Synergy-S single-crystal diffractometer with a PILATUS 200K hybrid pixel array detector using Cu Kα radiation (Table S4.1). The data were processed with the SHELX2018/3[9] and Olex2[10] software packages. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were inserted at calculated positions and refined with a riding model or without restrictions. Mercury 2020.1.1[11] was used to visualize the molecular structures. CCDC 2040727, 2040728, 2040729, and 2040727 contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

UV-vis and fluorescence spectroscopy: UV-vis spectra were recorded on a Shimadzu UV-3600 Plus instrument using 1 cm quartz cuvettes and CH_2Cl_2 as the solvent. Fluorescence spectra were recorded in CH_2Cl_2 using a JASCO spectrofluorometer FP-8600. The absolute fluorescence quantum yield data was obtained using the Edinburgh FLS980 fluorescence spectrometer. All samples were excited at 480 nm.

FTIR spectroscopy: FTIR spectra were collected on a Bruker Vertex 70 Fourier Transform spectrometer between 4000 and 300 cm^{-1}.

S1.4. Computational methods

DFT optimised geometries of all sugar-O-BODIPY conjugates were calculated using the B3LYP functional[1–3] and 6-31G(d) basis set using Gaussian,[4] unless otherwise stated. The input structures for optimisations were generated using the Avogadro program.[5] In some cases, TD-DFT calculations were also performed on the DFT optimised geometry using the CAM-B3LYP functional[6] and 6-31G(d) basis set to find out the orbitals involved in the absorption and the spatial overlap in the electron densities of these orbitals.

S2. TABLES OF DATA

Table S2.1. Summary of characterised sugar-O-BODIPY conjugates**.**

Conjugate number[a]	BODIPY binding site(s)	Anomeric ring form of sugar	Yield (%)
3Ga	(1,2)(3)(5,6)	α-D-glucofuranose	64
4Ga	(1,2)(3)(5,6)	α-D-glucofuranose	2
4Gb	(1,2)(3,5)	α-D-glucofuranose	23
4Gc	(1,2)(3,4)	α-D-glucoseptanose	34
4Gd	(1,2)	α-D-glucofuranose	3
3Xa	(1,2)(3,5)	α-D-xylofuranose	38
3Xb	(1,2)(3)	α-D-xylofuranose	6
3Xc	(1,2)	α-D-xylopyranose	17
3Xd	(1,2)	α-D-xylofuranose	9
4Xa	(1,2)(3,5)	α-D-xylofuranose	34
4Xb	(1,2)	α-D-xylopyranose	9
4Xc	(1,2)	α-D-xylofuranose	6
3Ra	(1,5)(2,3)	β-D-ribofuranose	17
3Rb	(1,2)(3,4)	α-D-ribopyranose	13
3Rc	(1,2)	α-D-ribopyranose	12
3Rd	(2,3)	β-D-ribofuranose	53
4Ra	(1,5)(2,3)	β-D-ribofuranose	9
4Rb	(1,2)	α-D-ribopyranose	4
4Rc	(2,3)	β-D-ribofuranose	51[b]
4Rc’	(2,3)	α-D-ribopyranose	7[b]
4Rd	(1,2)	α-D-ribofuranose	23

[a] G = glucose, X = xylose, R = ribose; [b] Inseparable conjugates, proportions determined by integration ratios of BODIPY α-proton peaks in the ^{1}H NMR spectrum.

Table S2.2. Selected atom distances (Å) between BODIPY-α-protons and sugar protons for **3Ra** X-ray crystal structure and DFT optimised geometries

BODIPY proton	Sugar proton	XRD	6-31G	6-31G (d)	6-31G +(d,p)	6-311G ++(d,p)
α1	1	2.77725(4)	2.81446	2.79225	2.78862	2.80647
α1	4	2.88847(4)	2.80558	2.90288	2.95978	2.95969
α1’	2	3.74894(4)	3.39627	3.35001	3.35713	3.35863
α1’	3	3.41380(5)	3.33017	3.21077	3.18680	3.18638
α2	1	3.57908(6)	3.40848	3.45316	3.47444	3.46996
α2	4	3.59586(4)	3.70535	3.73745	3.79607	3.79070
α2’	2	2.78766(5)	2.63182	2.51562	2.50741	2.53394
α2’	3	4.19191(6)	4.13 607	4.16193	4.21391	4.22668

Table S2.3. Selected atom distances (Å) between BODIPY-α-protons and sugar protons for **3Rd** X-ray crystal structure and DFT optimised geometries

BODIPY proton	Sugar proton	XRD	6-31G	6-31G (d)	6-31G +(d,p)	6-311G ++(d,p)
α1	1	3.20990(6)	2.97483	2.99567	2.84518	2.84790
α1	4	2.75225(8)	2.52350	2.54103	2.75767	2.77552
α1'	2	3.29342(8)	3.16383	3.07241	3.21979	3.19846
α1'	3	3.41643(6)	3.67385	3.63978	3.39953	3.43072

Table S2.4. Comparison of **3Ra** and **3Rd** O-B-O bond angels (°) from the X-ray crystal structures and DFT optimised geometries using various DFT basis sets.

Conjugate number	XRD	6-31G	6-31G (d)	6-31G +(d,p)	6-311G ++(d,p)
3Ra-BI	106.68	105.345	107.45	107.04	107.02
3Ra-BII	116.34	115.04	117.19	116.95	116.93
3Rd	107.10	105.02	107.12	106.83	106.82

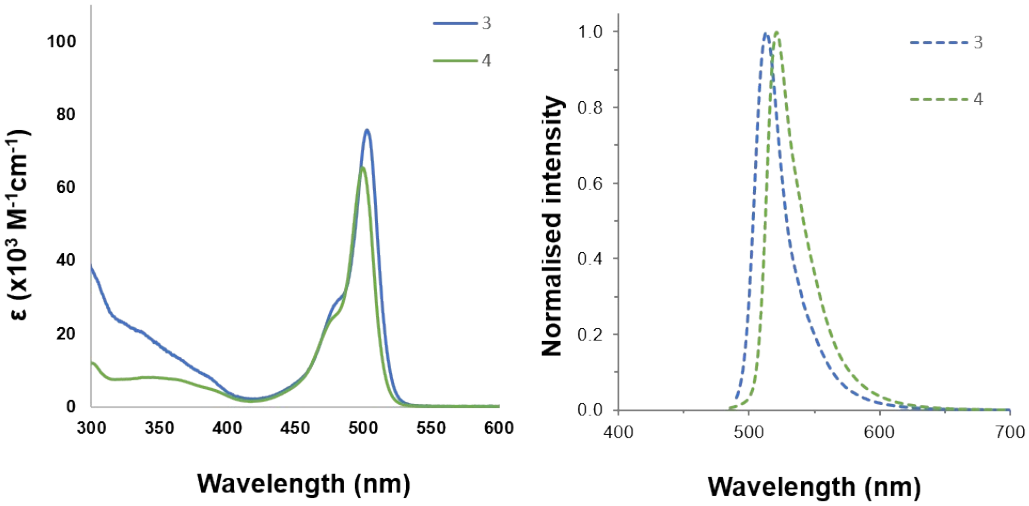
Table S2.5. Dihedral angle comparisons for **3Xc/3Xd, 4Xb/4Xc, 4Rb/4Rd**.

Conjugate number	O-C-C-O
3Xc	30.453
3Xd	-23.880
4Xb	-15.095
4Xc	-24.132
4Rb	-29.506
4Rd	-24.892

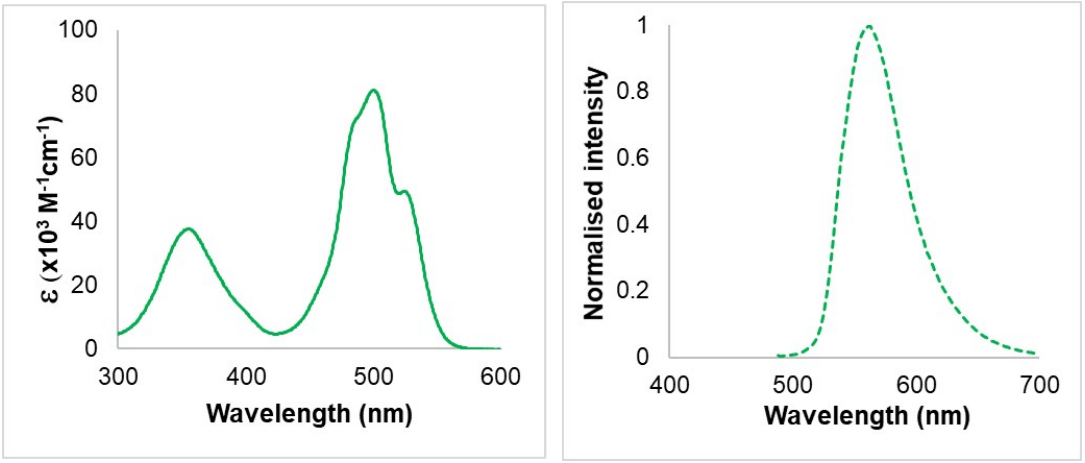
S3. UV-VIS AND EMISSION SPECTROSCOPY

For emission spectra of all the compounds: Excitation occurred at 480 nm.

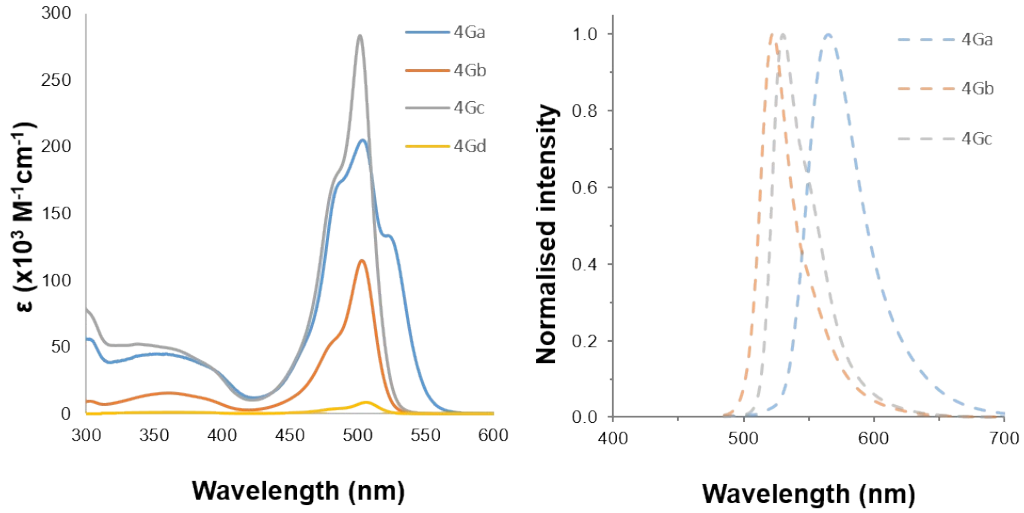
S3.1. O-BODIPYs 3 and 4:



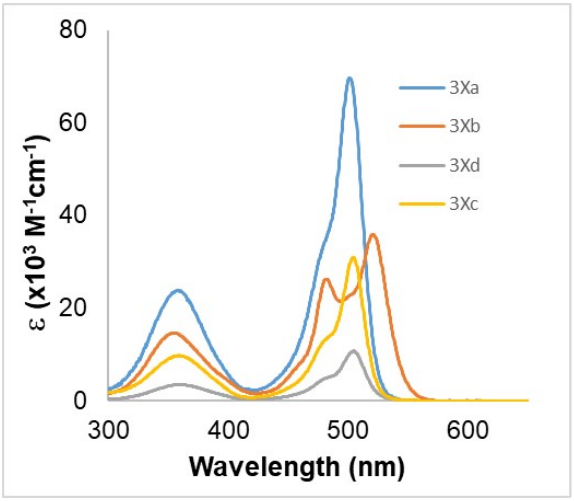
S3.2. O-BODIPY 3 Glucose conjugate

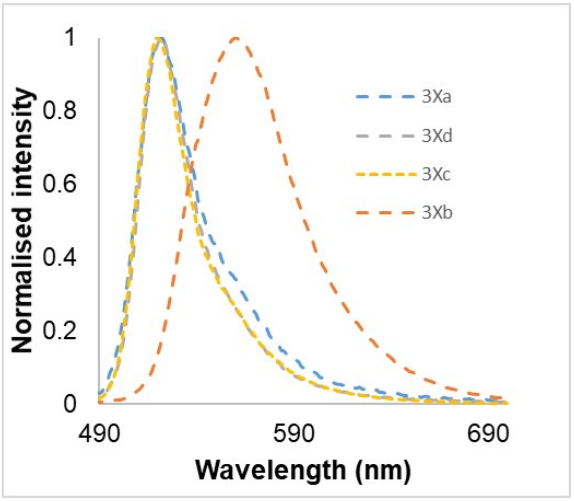


S3.3. O-BODIPY 4 Glucose conjugates

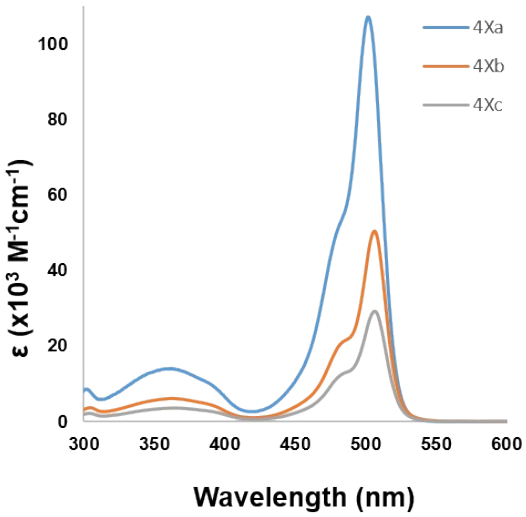


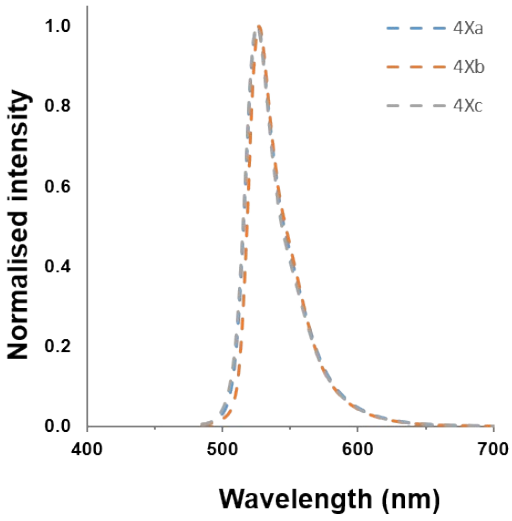
S3.4. O-BODIPY 3 Xylose conjugates



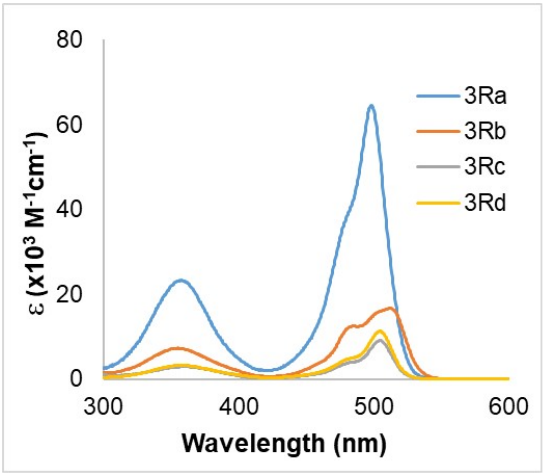


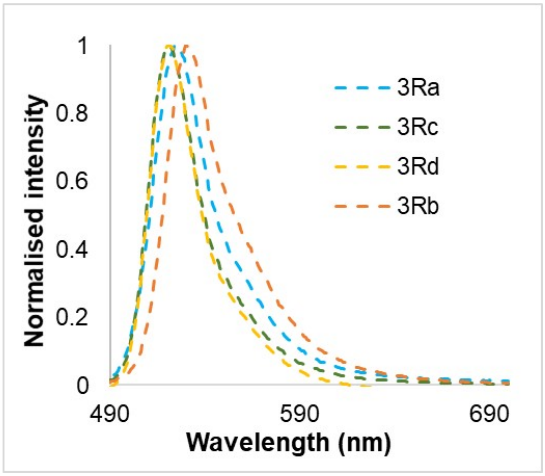
S3.5. O-BODIPY 4 Xylose conjugates



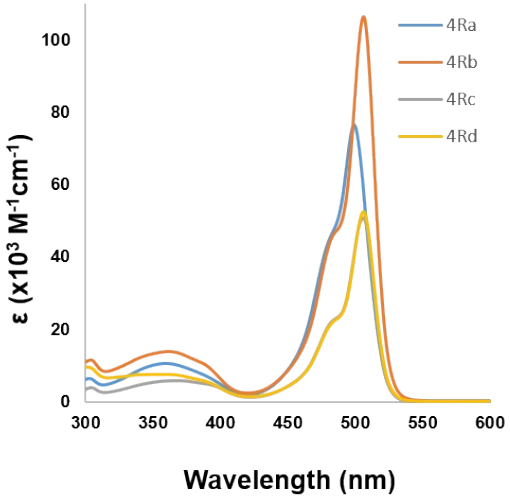


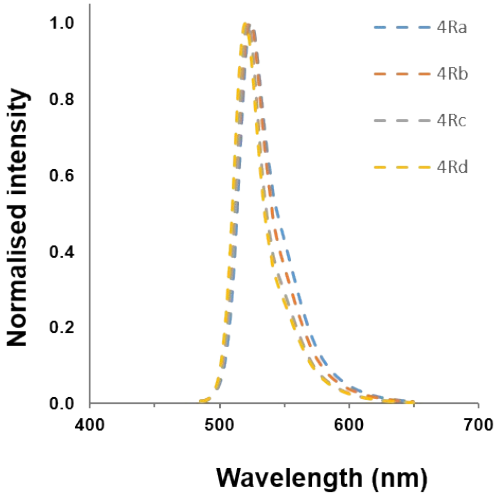
S3.6. O-BODIPY 3 Ribose conjugates





S3.7. O-BODIPY 4 Ribose conjugates





S4. SYNTHETIC PROCEDURES AND CHARACTERISATION DATA

S4.1. Synthesis of F-BODIPYs 1 and 2

Prepared as described in the literature.[7,8]

S4.2. Synthesis of O-BODIPYs 3 and 4

F-BODIPY (1 equiv) was dissolved in anhydrous CH_2Cl_2 under a nitrogen atmosphere. BCl_3 (3 equiv) was added dropwise and the mixture allowed to stir for 60 minutes. Solvent was removed *in vacuo* leaving a dark red solid. $NaOCH_3$ (5 equiv) dissolved in anhydrous MeOH was added to the flask. Stirring continued for a further 60 minutes before the reaction was quenched with saturated aqueous $NaHCO_3$ solution. The organic layer was washed three times with water, then dried over anhydrous Na_2SO_4. Column chromatography (SiO_2, MeCN/CH_2Cl_2 1:1 v/v) was used to isolate O-BODIPY from the crude mixture eluting as the main orange band.

3 orange oil (quantitative yield): **UV-vis** λ_{max} (CH_2Cl_2)/nm 499.5 (ε/M^{-1} cm^{-1} 44909), **Emission** λ_{em} CH_2Cl_2/nm 517 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.045.; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 2.47 (s, 3H, p-CH_3), 3.09 (s, 6H,O-CH_3), 6.53 (dd, *J* = 4.5, 2.0 Hz, 2H, β), 6.93 (dd, *J* = 4.5, 1.5 Hz, 2H, γ), 7.34-7.32 (m, 2H, m), 7.52-7.49 (m, 2H, o), 7.87 (br t, *J* = 1.4 Hz, 2H, α); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 21.59 (p-CH_3), 50.02 (O-CH3), 117.90 (Cβ), 129.14 (Cm), 130.35 (Co), 130.79, 137.73 (Cγ), 135.96, 141.00, 144.11 (Cα), 147.31; **^{11}B NMR (128 MHz, $CDCl_3$)** δ 2.27 (br s); **FT-IR (ATR)** 1/λ (cm^{-1}) 3093.52, 3027.94 (C-H aromatic), 2964.30, 2937.30, 2817.72, 2815.79 (Alkyl C-H), 1606.54 (C=N), 1567.97, 1540.33 (C=N, C-C in aromatic), 1253.60 (C-O), 1199.60 (C-N), **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{18}H_{19}BN_2O_2Na$, 329.1435; found, 329.1429.

4 orange oil (88% yield): **UV-vis** λ_{max} (CH_2Cl_2)/nm 500.0 (ε/M^{-1} cm^{-1} 65272), **Emission** λ_{em} CH_2Cl_2/nm 521 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.88.; **^{1}H NMR (400 MHz, $CDCl_3$)** *δ* = 7.82 (bs, 1H, Hα), 6.92 (s, 2H, *m*-CH), 6.60 (bd, *J* = 4.0 Hz, 2H, Hγ), 6.42 (dd, *J* = 4.0, 2.0 Hz, 2H, Hβ), 3.02 (s, 6H, OCH_3), 2.33 (s, 3H, *p*-CH_3), 2.07 (s, 6H, *o*-CH_3); **^{13}C NMR (100 MHz, $CDCl_3$)** *δ* = 146.96, 144.34 (Cα), 138.50, 136.40, 136.10, 130.35, 128.71 (Cγ), 128.06 (*m*-CH), 118.02 (Cβ), 49.87 (OCH_3), 21.11 (*p*-CH_3), 19.75 (*o*-CH_3); **^{11}B NMR (128 MHz, $CDCl_3$)** *δ* = 2.46 (bs); **FT-IR (ATR)** 1/λ (cm^{-1}) 3108.94 (C-H aromatic),

2948.87, 2918.01, 2810.01 (Alkyl C-H), 1567.97, 1539.04 (C=N, C-C in aromatic), 1253.60 (C-O), 1199.60 (C-N); **HRMS (ESI):** *m/z* $[M+Na]^+$ calcd for $C_{20}H_{23}BN_2NaO_2$, 357.1748; found 357.1745;

S4.3. General procedure for the synthesis of sugar-O-BODIPY conjugates

Solid sugar (1 equiv) was added to a flask containing O-BODIPY (1 equiv) dissolved in anhydrous MeCN. A catalytic amount of PTSA dissolved in anhydrous MeCN was added dropwise to the solution. The reaction mixture was left to stir at RT until TLC showed no further change. The reaction was quenched with saturated aqueous $NaHCO_3$ solution and CH_2Cl_2 added to induce phase separation. The organic layer containing the products was washed with water three times and then dried over anhydrous Na_2SO_4. The conjugates were isolated and purified by various chromatography techniques.

S4.4. Synthesis of glucose-O-BODIPY conjugate 3Ga

Glucose (28 mg, 0.156 mmol) was added to a flask containing **3** (49 mg, 0.156 mmol) dissolved in anhydrous MeCN (5 mL). PTSA (7 mol %) dissolved in anhydrous MeCN was then added to the reaction mixture changing the colour from orange to bright red. After 10 minutes of stirring, the reaction mixture was quenched by adding a saturated aqueous $NaHCO_3$ solution, which resulted in precipitation of the product. CH_2Cl_2 was added to induce phase separation, dissolving the precipitates and forming an orange-pink organic layer. The organic layer containing the products was washed with water three times and then dried over anhydrous Na_2SO_4. Flash chromatography on basic alumina using CH_2Cl_2/MeCN (100:5) afforded **3Ga.**

3Ga orange-pink film (20.0 mg, 64%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 501 (ε/M^{-1} cm^{-1} 81159), **Emission** λ_{em} CH_2Cl_2/nm 562 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.15; **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.17 (br t, *J* = 1.4 Hz, 1H), 8.07 (br t, *J* = 1.4 Hz, 1H), 7.99 (br t, ^{3}*J* = 1.4 Hz, 1H), 7.95 (br t, *J* = 1.4 Hz, 2H), 7.85 (br t, *J* = 1.4 Hz, 1H), 7.49-7.46 (m, 6H), 7.32-7.30 (m, 6H), 6.89-6.86 (m, 3H), 6.85 (t, *J* = 1.4 Hz, 1H), 6.84 (t, *J* = 1.4 Hz, 1H), 6.79 (dd, *J* = 4.1 Hz, *J* = 1.4 Hz, 1H), 6.53 (dd, *J* = 4.1, 2.0 Hz, 1H), 6.47 (dd, *J* = 4.1, 2.0 Hz, 1H), 6.41 (dd, *J* = 4.1, 2.0 Hz, 1H), 6.18 (dd, *J* = 4.1, 2.0 Hz, 1H), 6.16 (dd, *J* = 4.1, 2.0 Hz, 1H), 6.06 (dd, *J* = 4.1, 2.0 Hz, 1H), 5.47 (d,*J* = 3.8 Hz, 1H, H1), 4.60-4.59 (m, 1H, H5), 4.59-4.58 (m, 1H, H3), 4.55 (d, *J* = 3.9 Hz, 1H, H2), 4.55-4.54 (m, 1H, H4), 4.41-4.37 (m, 1H, H6), 4.25-4.22 (m, 1H, H6), 3.45 (s, 3H, -OCH_3), 2.44 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.69, 147.61, 146.71, 146.54, 146.44, 145.65, 146.19, 143.77, 140.70, 140.63, 135.69, 135.55, 135.42, 135.29, 135.18, 131.73, 131.70, 131.16, 130.74, 130.67, 130.60, 130.55, 130.47, 130.40, 130.15, 129.00, 128.96, 118.75, 118.47, 118.41, 117.83, 117.63, 117.72, 105.34 (C1), 82.55 (C2), 81.36 (C3), 80.08 (C5), 78.65 (C4), 68.41 (C6), 55.18 (-OCH_3), 21.47; **^{11}B NMR (128**

MHz, $CDCl_3$) δ 5.43 (br s), 5.03 (br s); **FT-IR (ATR)** 1/λ (cm^{-1}) 3101.23 (C-H aromatic); 2887.15, 2860.15 (Alkyl C-H); 1606.54 (C=N); 1556.40, 1533.25 (C=N, C-C in aromatic); 1253.60 (C-O); 1141.75, 1103.17 (C-N, C-O); **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{55}H_{49}B_3N_6O_7Na$, 961.3858; found, 961.3826.

S4.5. Synthesis of glucose-O-BODIPY conjugates 4Ga-d

Glucose (53.9 mg, 0.299 mmol) was added to a flask containing **4** (100 mg, 0.299 mmol) dissolved in anhydrous MeCN (5mL). PTSA (7 mol %) dissolved in anhydrous MeCN was then added to the solution changing the colour from orange to brick red. The reaction mixture was left to stir at RT for 90 minutes. The reaction was quenched with aqueous saturated aqueous $NaHCO_3$ solution and CH_2Cl_2 was added to induce phase separation. The organic layer containing the products was washed with water three times and then dried over anhydrous Na_2SO_4. The desired conjugates were isolated via column chromatography. Chromatography of the crude residue on basic alumina using CH_2Cl_2 eluted **4Ga** as the first orange band. Transitioning the eluent from CH_2Cl_2 to MeCN eluted **4Gb** and **4Gc** together as the second yellow band and **4Gd** eluted in the third yellow band when the H_2O/MeCN solvent ratio reached 1:4. Column chromatography of the second fraction with deactivated silica gel eluted **4Gb** when the MeCN/CH_2Cl_2 gradient reached a ratio of 1:9 (v/v) and **4Gc** eluted when the ratio reached 1:4. Column chromatography of the third fraction on neutral alumina using acetonitrile/H_2O (9:1) afforded **4Gd** as the first band. **4Gb, 4Gc** and **4Gd** were further purified by HPLC for molar absorbance and fluorescence measurements. The samples were dissolved in AR MeCN and loaded onto the HPLC column that was pre-eluted with 70:30 MeCN:H_2O. A 70:30 to 90:10 MeCN:H_2O gradient was set with a 1% increase in MeCN per minute. The column continued at 90:10 MeCN:H_2O for 10minutes then a 90:10 to 70:30 MeCN:H_2O gradient was set with a 1% decrease in MeCN per minute. The **4Gd** peak was collected at t_R = 7.09 min, **4Gc** at t_R = 19.07 min and **4Gb** at t_R = 21.56 min. The solvent was removed and the samples dried under high vacuum before analysis.

4Ga orange-pink film (1.6 mg, 2%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 503 (ε/M^{-1} cm^{-1} 203 300), **Emission** λ_{em} CH_2Cl_2/nm 565 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.75; **^{1}H NMR (400 MHz, $CDCl_3$)** *δ* = 8.25 (bs, 1H), 8.05 (bs, 1H), 8.01 (s, 1H), 7.94 (s, 2H), 7.82 (s, 1H), 6.96-6.91 (m, 6H), 6.64 (dd, *J* = 4.1, 1.0 Hz, 1H), 6.60-6.58 (m, 2H), 6.54 (dd, *J* = 4.0, 1.0 Hz, 1H), 6.49 (dd, *J* = 4.0, 1.0 Hz, 1H), 6.46 (dd, *J* =4.0, 1.5 Hz, 1H), 6.42 (dd, *J* = 4.0, 1.5 Hz, 1H), 6.40-6.37 (m, 2H), 6.06 (dd, *J* = 4.5,2.0 Hz, 1H), 5.95 (dd, *J* = 4.0,1.5 Hz, 1H), 5.89 (dd, *J* = 4.0, 1.5 Hz, 1H), 5.51 (d, *J* = 3.7 Hz, 1H, H1), 4.65 (dd, *J* = 8.0, 6.4 Hz, 1H, H4), 4.61 (ddd, *J* = 6.3, 6.0, 5.8 Hz, 1H, H5), 4.47 (dd, *J* = 8.0, 1.0 Hz, 1H,

H3), 4.42 (dd, *J* = 3.7, 1.0 Hz, 1H, H2), 4.40-4.33 (m, 2H, H6), 2.35 (s, 9H), 2.21 (s, 3H), 2.18 (s, 3H), 2.12 (s, 3H), 2.10 (s, 3H), 2.08 (s, 3H), 2.07 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** *δ* = 148.17, 147.51, 147.13, 146.33, 146.02, 145.77, 144.12, 143.88, 143.42, 138.40, 138.35, 136.67, 136.59, 136.52, 136.48, 136.40, 136.29, 135.98, 135.83, 135.50, 135.42, 135.37, 130.49, 129.77, 129.29, 129.14, 129.05, 128.90, 128.68, 128.11, 128.03, 127.79, 127.48, 118.94, 118.51, 118.39, 117.96, 117.70, 117.66, 105.63 (C1), 82.67 (C2), 80.25 (C3), 78.86 (C5), 78.05 (C4), 66.98 (C6), 55.31 (OCH_3), 21.15, 20.10, 19.93; **^{11}B NMR (128 MHz, $CDCl_3$)** *δ* = 5.43 (bs); **FT-IR (ATR)** 1/λ (cm^{-1}) 2918.01, 2856.29 (Alkyl C-H); 1612.33 (C=N); 1554.47, 1540.97 (C=N, C-C in aromatic); 1253.60 (C-O); 1143.67, 1112.81, 1099.31 (C-N, C-O); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{61}H_{61}B_3N_6NaO_7$:1045.4800; found 1045.4808.

4Gb red film (25.2 mg, 23%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 502 (ε/M^{-1} cm^{-1} 286800), **Emission** λ_{em} CH_2Cl_2/nm 530 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.91; **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.01 (s, 1H), 7.99 (s, 1H), 7.78 (s, 1H), 7.66 (s, 1H), 6.94 (s, 4H), 6.67 (dd, *J* = 4.0, 1.0 Hz, 1H), 6.66-6.63 (m, 2H), 6.61 (dd, *J* = 4.0, 1.0 Hz, 1H), 6.47 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.44 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.40-6.38 (m, 2H), 6.32 (d, *J* = 3.0 Hz, 1H, H1), 4.80 (d, *J* = 3.5 Hz, 1H, H2), 4.77 (dd, *J* = 6.0, 4.0 Hz, 1H, H4), 4.55 (d, *J*=4.0 Hz, 1H, H3), 4.10-4.04 (m, 1H, H5), 3.97 (dd, *J* = 11.0, 3.5 Hz, 1H, H6), 3.83 (dd, *J* = 11.0, 6.0 Hz, 1H, H6), 2.36 (s, 3H), 2.35 (s, 3H), 2.11 (s, 3H), 2.11 (s, 3H), 2.10 (s, 3H), 2.07 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.20, 147.16, 145.80, 144.92, 144.20, 143.94, 138.65, 138.58, 136.50, 136.45, 136.41, 135.90, 135.64, 135.55, 130.47, 130.22, 130.04, 129.93, 129.70, 129.65, 128.09, 118.65, 118.32, 118.11, 117.75, 106.13 (C1), 85.94 (C2), 80.15 (C4), 76.44 (C3), 72.32 (C5), 65.69 (C6), 21.16, 20.09, 20.04, 20.01; **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.7 (bs), 1.44 (bs); **FT-IR (ATR)** 1/λ (cm^{-1}) 3398.21 (O-H); 2921.87 (Alkyl C-H); 1612.40 (C=N); 1542.90 (C=N, C-C in aromatic); 1253.60 (C-O); 1149.46, 1137.89, 1097.38 (C-N, C-O); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{42}H_{42}B_2N_4NaO_6$: 743.3205; found 743.3196.

4Gc red film (36.8 mg, 34%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 503 (ε/M^{-1} cm^{-1} 117200), **Emission** λ_{em} CH_2Cl_2/nm 522 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.75; **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.26 (s, 1H), 8.12 (s, 1H), 7.85 (s, 1H), 7.70 (s, 1H), 6.94-6.89 (m, 4H), 6.63-6.59 (m, 3H), 6.53 (dd, *J* = 4.0, 1.4 Hz, 1H), 6.45-6.41 (m, 3H, H2), 6.34 (dd, *J* = 4.0, 2.0 Hz, 1H), 5.40 (d, *J* = 3.7 Hz, 1H, H1), 4.89 (dd, *J* = 9.5, 7.5 Hz, 1H), 4.55 (dd, *J* = 7.5, 3.7 Hz, 1H, H2), 4.43 (d, *J* = 14.0 Hz, 1H, H6), 4.26-4.21 (m, 2H, H4,5), 3.81 (dd, *J* = 14.0, 2.0 Hz, 1H, H6), 2.33 (s, 3H), 2.32 (s, 3H), 2.11 (s, 3H), 2.07 (s, 3H), 2.01 (s, 3H), 1.99 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.91, 146.94, 146.47, 145.84, 144.67, 144.12, 138.56, 138.44, 136.44, 136.29, 136.31, 135.88, 135.61, 135.26, 130.29, 130.18, 129.84, 129.57 128.93, 128.10, 128.02, 118.99, 118.55, 118.06, 117.51, 106.56 (C1), 83.54 (C2), 78.54 (C4), 77.18 (C3), 70.94 (C5,6), 21.14, 20.05, 19.93, 19.85; **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.74 (bs), 4.88 (bs); **FT-IR (ATR)**

1/λ (cm^{-1}) 3355.81 (O-H); 2952.73, 2931.51, 2844.72 (Alkyl C-H); 1608.47 (C=N); 1542.90 (C=N, C-C in aromatic); 1257.46 (C-O); 1149.46, 1118.60, 1099.31 (C-N, C-O); **HRMS (ESI+):** *m/z*: $[M+Na]^+$ calcd for $C_{42}H_{42}B_2N_4NaO_6$: 743.3205; found 743.3196.

4Gd red film (4.2 mg, 3%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 506 (ε/M^{-1} cm^{-1} 8184), **Emission** λ_{em} CH_2Cl_2/nm 530 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.91; **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.85 (s, 1H), 7.68 (s, 1H), 6.93 (s, 2H), 6.66-6.61 (m, 2H), 6.44-6.40 (m, 2H), 6.20 (bs, 1H, H1), 4.67 (d, *J* = 3.5 Hz, 1H, H2), 4.49 (d, *J* = 3.0 Hz, 1H, H3), 4.43 (dd, *J* = 6.5, 3.0 Hz, 1H, H4), 4.22-4.16 (m, 1H, H5), 3.95 (dd, *J* = 11.5, 3.5 Hz, 1H, H6), 3.86 (dd, *J* = 11.5, 5.5 Hz, 1H, H6), 2.35 (s, 3H), 2.12 (s, 3H), 2.05 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.51, 144.93, 144.35, 138.76, 136.40, 135.94, 135.70, 130.62, 130.11, 129.90, 128.17, 128.13, 118.52, 118.46, 105.35 (C1), 85.38 (C2), 79.90 (C4), 76.44 (C3), 71.16 (C5), 63.98 (C6), 21.16, 20.12, 19.98; **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.62 (bs); **HRMS (ESI+):** *m/z*: $[M+Na]^+$ calcd for $C_{24}H_{27}BN_2NaO_6$: 473.1859; found 473.1845; **HRMS (ESI+):** *m/z* $[M+Na]^+$ 473.1845, calculated 473.1859 for $C_{24}H_{27}BN_2NaO_6$.

S4.6. Synthesis of xylose-O-BODIPY conjugates 3Xa-d

Xylose (28 mg, 0.189 mmol) was added to a flask containing **3** (55 mg, 0.177 mmol) dissolved in anhydrous MeCN (5 mL). PTSA (5 mol %) dissolved in anhydrous MeCN was then added to the reaction mixture changing the colour from orange to dark red. After 1h 45 min, the reaction mixture was quenched by adding a saturated aqueous $NaHCO_3$ solution and CH_2Cl_2 was added to induce phase separation. The organic layer containing the products was washed with water (3x) and then dried over anhydrous Na_2SO_4. Flash chromatography on silica-gel column chromatography using a mixture of CH_2Cl_2/MeCN as the eluent was performed to isolate the conjugates. The most non-polar band corresponding to **3Xa** was eluted using CH_2Cl_2/MeCN (5:1). **3Xb** and **3Xc** were eluted together and further isolated on a deactivated silica-gel column using CH_2Cl_2/MeCN (5:3). **3Xd** was isolated by carefully eluting with CH_2Cl_2/MeCN (1:1).

3Xa orange film (19.5 mg, 38%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 501.5 (ε/M^{-1} cm^{-1} 69688), **Emission** λ_{em} CH_2Cl_2/nm 522 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.07 (br t, *J* = 1.5 Hz, 1H), 8.03 (br t, *J* = 1.5 Hz, 1H), 7.81 (br t, *J* = 1.5 Hz, 1 H), 7.71 (br t, *J* = 1.5 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 4H), 7.30 (dd, *J* = 8.0, 4.7 Hz, 4H), 6.92-6.88 (m, 4H), 6.53-6.50 (m, 2H), 6.48-6.46 (m, 2H), 6.37 (d, *J* = 2.9 Hz, 1H, H1), 4.81-4.79 (m,

1H, H4), 4.71 (d, *J* = 3.2 Hz, 1H, H2), 4.63 (d, *J* = 3.1 Hz, 1H, H3), 4.35 (dd, *J* = 12.7, 4.2 Hz, 1H, H5), 4.24 (dd, *J* = 12.7, 2.7 Hz, 1H, H5), 2.46 (s, 3H), 2.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.32, 147.00, 145.22, 144.82, 143.83, 142.99, 141.03, 140.73, 135.54, 135.25, 135.02, 131.80, 131.62, 131.33, 131.23, 130.62, 130.57, 130.32, 129.08, 128.97, 118.20, 118.13, 118.06, 117.58, 106.14 (C1), 86.00 (C2), 76.36 (C3/4), 61.44 (C5), 21.45. **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.79 (br s), 0.47 (br s). **HRMS (ESI) *m/z*:** $[M+H]^+$ calcd. for $C_{37}H_{33}B_2N_4O_5$, 635.2644; found, 635.2644. $[M+Na]^+$ calcd. for $C_{37}H_{32}B_2N_4O_5Na$, 657.2463; found, 657.2454.

3Xb red-pink film (3.2 mg, 6%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 521 (ε/M^{-1} cm^{-1} 35954), **Emission** λ_{em} CH_2Cl_2/nm 561 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.12 (br t, *J* = 1.4 Hz, 1H), 8.03 (br t, *J* = 1.4 Hz, 1H), 7.96 (br t, *J* = 1.4 Hz, 1H), 7.95 (br t, *J* = 1.4 Hz, 1H), 7.45-7.43 (m, 4H), 7.32-7.28 (m, 4H), 6.89 (dd, *J* = 4.3, 0.9 Hz, 1H), 6.86 (dd, *J* = 4.3, 0.9 Hz, 1H), 6.84 (dd, *J* = 4.3, 0.9 Hz, 1H), 6.78 (dd, *J* = 4.3, 0.9 Hz, 1H), 6.51-6.48 (m, 2H), 6.16 (dd, *J* = 4.3, 1.8 Hz, 1H), 6.04 (dd, *J* = 4.3, 1.7 Hz, 1H), 5.45 (d, *J* = 3.3 Hz, 1H, H1), 4.47 - 4.42 (m, 2H, H3/H4), 4.20 (d, *J* = 3.5 Hz, 1 H, H2), 3.94 (dd, *J* = 11.7, 2.2 Hz, 1H, H5), 3.71 (dd, *J* = 11.7, 2.1 Hz,1H, H5), 3.51 (s, 3H, -OCH_3), 2.46 (s, 3H), 2.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 146.61, 146.25, 145.65, 145.33, 144.23, 142.60, 139.82, 139.68, 134.38, 134.30, 134.10, 130.58, 130.51, 129.92, 129.80, 129.52, 129.48, 128.02, 127.97, 117.70, 117.27, 117.05, 116.87, 104.39 (C1), 80.59 (C2), overlap with $CDCl_3$ (C3/4), 61.62 (C5), 54.15 (-OCH_3), 20.43. **^{11}B NMR (128 MHz, $CDCl_3$):** δ = 5.55 (br s), 4.77 (br s). **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{38}H_{36}B_2N_4O_6Na$, 689.2726; found, 689.2696.

3Xc red film (10.9 mg, 17%)**: UV-vis** λ_{max} (CH_2Cl_2)/nm 504.5 (ε/M^{-1} cm^{-1} 30962), **Emission** λ_{em} CH_2Cl_2/nm 520 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.49 (s, 1H), 7.72 (s, 1H), 7.45 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 6.92 (ddd, *J* = 11.0, 4.3, 1.1 Hz, 2H), 6.46 (dd, *J* = 4.2, 1.9 Hz), 6.45 (dd, *J* = 4.2, 1.9 Hz, 1H), 5.46 (br s, 1H, H1), 4.24 (s, 1H, H3), 4.06 (s, 1H, H2), 4.03 (s, 1H, H5), 3.93-3.90 (m, 1H, H5), 3.58-3.50 (m, 2H, H4,-OH4), 2.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.52, 147.32, 143.46, 141.24, 135.76, 135.19, 132.43, 131.31, 131.27, 130.72, 129.23, 119.21, 117.99, 96.37 (C1), overlaps with $CDCl_3$ (C2), 69.06 (C4), 68.88 (C3), 64.24 (C5), 21.58. **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 4.91 (br s). **FT-IR (ATR)** 1/λ (cm^{-1}) 3400-3300 broad (O-H); 3107.02 (C-H aromatic); 2962.37, 2914.15, 2858.22 (Alkyl C-H); 1608.47 (C=N); 1569.90, 1537.11 (C=N, C-C in aromatic); 1257.46 (C-O); 1107.03, 1068.46 (C-N, C-O); **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{21}H_{21}BN_2O_5Na$, 415.1439; found, 415.1438.

3Xd red film (5.7 mg, 9%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 505 (ε/M^{-1} cm^{-1} 10713), **Emission** λ_{em} CH_2Cl_2/nm 523 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.88 (s, 1H). 7.70

(s, 1H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.30 - 7.28 (m, 2H), 6.93-6.90 (m, 2H), 6.47-6.50 (m, 2H), 6.23 (br s, 1H, H1), 4.61 (d, *J* = 3.3 Hz, 1H, H2), 4.52 (q, *J* = 3.1 Hz,1H, H4), 4.41 (d, *J* = 3.1 Hz, 1H, H3), 4.19 (dd, *J* = 12.3, 3.9 Hz, 1H, H5), 4.08 (dd, *J* = 12.3, 2.8 Hz, 1H, H5), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.51, 144.35, 143.84, 141.18, 135.52, 135.25, 131.93, 131.47, 131.20, 130.59, 129.12, 118.31, 118.14, 105.57 (C1), 85.64 (C2), 78.99 (C4), 78.58 (C3), 61.96 (C5), 21.47. **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.64 (br s). **FT-IR (ATR)** 1/λ (cm^{-1}) 3400-3300 broad (O-H); 3101.23 (C-H aromatic); 2960.44, 2921.87, 2856.29 (Alkyl C-H); 1606.54 (C=N); 1558.33, 1539.04 (C=N, C-C in aromatic); 1255.53 (C-O); 1149.46, 1101.24, 1068.46, 1016.38 (C-N, C-O); **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{21}H_{21}BN_2O_5Na$, 415.1439; found, 415.1438.

S4.7. Synthesis of xylose-O-BODIPY conjugates 4Xa-c

Xylose (24.8 mg, 0.160 mmol) was added to a flask containing **4** (53.6 mg, 0.160 mmol) dissolved in anhydrous MeCN. PTSA (5 mol %) dissolved in anhydrous MeCN was added dropwise to the solution. The reaction mixture was left to stir at RT for 35 minutes. The reaction was quenched with saturated aqueous $NaHCO_3$ solution and CH_2Cl_2 added to induce phase separation. The organic layer containing the products was washed with water three times and then dried over anhydrous Na_2SO_4. The desired conjugates were isolated via column chromatography. Chromatography of the crude residue on deactivated silica gel using MeCN/CH_2Cl_2 (1:19) eluted **4Xa** as the first fluorescent orange band. Transitioning the eluent MeCN/CH_2Cl_2 (1:4) afforded 4Xb as the second yellow band and MeCN afforded **4Xc** as the third yellow band. **4Xa**, **4Xb** and **4Xc** were further purified by HPLC for molar absorbance and fluorescence measurements. The samples were dissolved in AR MeCN and loaded onto the HPLC column that was pre-eluted with 70:30 MeCN:H_2O. The column ran at 70:30 MeCN:H_2O for 15 minutes then a 70:30 to 90:10 MeCN:H_2O gradient was set with a 2% increase in MeCN per minute, followed by a 90:10 to 70:30 MeCN:H_2O gradient set to a 2% decrease in MeCN per minute. The column was then run at 70:30 MeCN:H_2O for 5 minutes. The **4Xa** peak was collected at t_R = 27.7 min, **4Xb** at t_R = 8.3 min and **4Xc** at t_R = 7.6 min. The solvent was removed and the samples dried under high vacuum before analysis.

4Xa orange film (18.8 mg, 34%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 503 (ε/M^{-1} cm^{-1} 107226), **Emission** λ_{em} CH_2Cl_2/nm 526 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.79; **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.03 (s, 1H), 8.01 (s, 1H), 7.80 (s, 1H), 7.71 (s, 1H), 6.94 (s, 4H), 6.66-6.63 (m, 2H), 6.63-6.61 (m, 2H), 6.45 (dd, *J* = 4.8, 2.4 Hz, 2H), 6.40 (dd, *J* = 4.5, 1.9 Hz,

2H), 6.37 (bs, 1H, H1), 4.84 (m, 1H, H4), 4.79 (d, *J* = 3.5 Hz, 1H, H2), 4.68 (d, *J* = 3.5 Hz, 1H, H3), 4.33 (dd, *J* = 12.3, 5.0 Hz, 1H, H5), 4.18 (dd, *J* = 12.3, 3.5 Hz, 1H, H5), 2.35 (s, 3H), 2.14 (s, 3H), 2.11 (s, 3H), 2.10 (s, 3H), 2.07 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.25, 146.95, 145.34, 145.30, 144.35, 143.42, 138.63, 138.46, 136.62, 136.45, 136.41, 135.89, 135.65, 135.53, 135.42, 130.39, 130.36, 130.03, 129.82, 129.00, 128.13, 128.04, 118.36, 118.33, 118.11, 117.65, 106.09 (C1), 86.13 (C2), 77.06 (C4), 76.46 (C3), 61.41 (C5), 21.14, 20.15, 20.10, 20.01; **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.78 (bs), 0.68 (bs); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{41}H_{40}B_2N_4NaO_5$: 713.3090; found 713.3091.

4Xb orange film (6.1 mg, 9%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 506 (ε/M^{-1} cm^{-1} 50481), **Emission** λ_{em} CH_2Cl_2/nm 527 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.46 (s, 1H), 7.70 (s, 1H), 6.93 (s, 2H), 6.65 (dd, *J* = 4.0, 1.0 Hz, 1H), 6.63 (dd, *J* = 4.1, 1.1 Hz, 1H), 6.44 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.38 (dd, *J* = 3.9, 2.0 Hz, 1H), 5.45 (bs, 1H, H1), 4.26-4.21 (m, 1H, H3), 4.08 (dd, *J* = 2.8, 1.2 Hz, 1H, H2), 4.03 (dd, *J* = 12.3, 1.4 Hz, 1H, H5), 3.90 (dd, *J* = 12.3, 1.4 Hz, 1H, H5), 3.63 (bd, *J* = 9.9 Hz, 1H, OH4), 3.58 (d, *J* = 9.9 Hz, 1H, H4), 2.34 (s, 3H), 2.13 (s, 3H), 2.04 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.95, 147.09, 143.83, 138.69, 136.38, 136.04, 135.45, 130.89, 129.89, 129.69, 128.13, 128.09, 119.25, 118.05, 96.31 (C1), 77.64 (C2), 68.95 (C4), 68.73 (C3), 64.16 (C5), 21.13, 20.15, 19.95; **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 4.94 (bs); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{23}H_{25}BN_2NaO_5$: 443.1751; found 443.1753.

4Xc orange film (4.2 mg, 6%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 506 (ε/M^{-1} cm^{-1} 29378), **Emission** λ_{em} CH_2Cl_2/nm 526 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.82; **^{1}H NMR (400 MHz, $CDCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.85 (s, 1H), 7.69 (s, 1H), 6.93 (s, 2H), 6.65-6.62 (m, 2H), 6.43-6.40 (m, 2H), 6.23 (bs, 1H, H1), 4.66 (d, *J* = 3.5 Hz, 1H, H2), 4.52 (dd, *J* = 6.9, 3.3 Hz, 1H, H4), 4.46 (bd, *J* = 3.3 Hz, 1H, H3), 4.19 (dd, *J* = 12.2, 4.1 Hz, 1H, H5), 3.63 (dd, *J* = 12.2, 2.4 Hz, 1H, H5), 3.77 (bs, 1H, OH3), 2.35 (s, 3H), 2.12 (s, 3H), 2.05 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.51, 144.81, 144.41, 138.75, 136.40, 135.92, 135.73, 130.55, 130.13, 129.90, 128.17, 128.12, 118.54, 118.32, 105.49 (C1), 85.93 (C2), 79.04 (C4), 78.64 (C3), 61.96 (C5), 21.16, 20.14, 19.98; **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.51, 144.81, 144.41, 138.75, 136.40, 135.92, 135.73, 130.55, 130.13, 129.90, 128.17, 128.12, 118.54, 118.32, 105.49 (C1), 85.93 (C2), 79.04 (C4), 78.64 (C3), 61.96 (C5), 21.16, 20.14, 19.98; **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.67 (bs); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{23}H_{25}BN_2NaO_5$: 443.1751; found 443.1758.

S4.8. Synthesis of ribose-O-BODIPY conjugates 3Ra-d

Ribose (28 mg, 0.189 mmol) was added to a flask containing **3** (55 mg, 0.177 mmol) dissolved in anhydrous MeCN (5 mL). PTSA (5 mol %) dissolved in anhydrous MeCN was then added to the reaction mixture changing the colour from orange to dark red. After 1h 45 min, the reaction mixture was quenched by adding a saturated aqueous $NaHCO_3$ solution and CH_2Cl_2 was added to induce phase separation. The organic layer containing the products was washed with water (3x) and then dried over anhydrous Na_2SO_4. Flash chromatography on silica-gel column chromatography using a mixture of CH_2Cl_2/MeCN as the eluent was performed to isolate the conjugates. The most non-polar band corresponding to **3Ra** was eluted using CH_2Cl_2/MeCN (5:1) and further purified by column chromatography on basic alumina. **3Rb** and **3Rc** were eluted together and further isolated on a deactivated silica-gel column using CH_2Cl_2/MeCN (100:3). **3Rd** was isolated by carefully eluting with CH_2Cl_2/MeCN (1:1). The samples used for the quantum yield measurements were collected from HPLC using a semi-preparative C18 reverse-phase silica column. For conjugate **3Ra**, an isocratic method with 95 % MeCN in water was used where the compound was eluted at t_R = 13.0 min. While, for conjugate **8,** 90 % MeCN in water was used to elute the conjugate at t_R = 6.6 min. The solvent was removed, and the samples dried under high vacuum before analysis

3Ra red solid (8.6 mg, 17 %): **UV-vis** λ_{max} (CH_2Cl_2)/nm 498.5 (ε/M^{-1} cm^{-1} 64578), **Emission** λ_{em} CH_2Cl_2/nm 524 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.030; **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.36 (br t, *J* = 1.5 Hz, 2H), 7.99 (br t, *J* = 1.5 Hz, 1H), 7.81 (br t, *J* = 1.5 Hz, 1H), 7.48-7.45 (m, 4H), 7.32-7.29 (m, 4H), 6.96-6.95 (m, 1H), 6.93-6.90 (m, 2H), 6.88-6.87 (m, 1H), 6.54-6.52 (m, 1H), 6.51-6.48 (m, 3H), 5.71 (br s, 1H, H1), 5.17-5.14 (m, 2H, H2/3), 4.60-4.59 (m, 1H, H4), 3.67-3.64 (m, 1H, H5), 3.51 (dd, *J* = 12.6 Hz, 1.5 Hz, 1H, H5), 2.46 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 147.08, 146.89, 146.71, 146.05, 143.75, 143.68, 140.83, 140.68, 135.77, 135.23, 135.05, 130.98, 131.61, 131.55, 131.26, 130.65, 130.55, 129.03, 128.97, 118.56, 117.81, 117.53, 116.82, 107.99 (C1), 90.40 (C4), 88.66 (C2), 83.60 (C3), 64.18 (C5), 21.43. **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.90 (br s), 2.30 (br s). **FT-IR (ATR)** 1/λ (cm^{-1}) 3107.02 (C-H aromatic); 2929.58, 2850.51 (Alkyl C-H); 1606.54 (C=N); 1567.97 (C=N, C-C in aromatic); 1255.53 (C-O); 1135.96 (C-N, C-O); **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{37}H_{32}B_2N_4O_5Na$, 657.2463; found, 657.2458.

3Rb orange film (4.3 mg, 8%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 512.5 (ε/M^{-1} cm^{-1} 16681), **Emission** λ_{em} CH_2Cl_2/nm 530 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.53 (br t, *J* = 1.5 Hz, 1H), 8.34 (br t, *J* = 1.5 Hz, 1H), 7.80 (br t, *J* = 1.5 Hz, 1H), 7.74 (br t, *J* = 1.5 Hz, 1H), 7.44 - 7.40 (m, 4H), 7.30-7.27 (m, 4H), 6.89-6.86 (m, 2H), 6.83-6.82 (m, 2H), 6.45-6.43 (m, 2H), 6.31-6.30 (m, 1H), 6.20-6.18 (m, 1H), 5.65 (d, *J* = 4.5 Hz, 1H, H1), 4.76-4.72 (m, 1H, H3), 4.60-4.56 (m, 2H, H2/4), 4.28 (dd, *J* = 12.4, 4.7 Hz, 1H, H5), 3.95 (dd, *J* = 12.4, 5.1 Hz, 1H, H5), 2.45 (s, 3H), 2.44 (s, 3H). **^{13}C NMR (100**

MHz, $CDCl_3$) δ = 147.68, 146.17, 145.85, 145.33, 142.76, 142.36, 139.81, 139.58, 134.73, 134.36, 134.15, 130.63, 130.50, 130.48, 130.43, 129.78, 129.54, 129.51, 129.02, 128.00, 127.91, 117.22, 117.12, 116.68, 116.37, 98.02 (C1), 72.95 (C3), 71.88 (C4), 69.89 (C2), 64.52 (C5), 20.41. **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.29 and 5.37 (br s). **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{37}H_{32}B_2N_4O_5Na$, 657.2463; found, 657.2454.

3Rc orange film (7.9 mg, 13%)**: UV-vis** λ_{max} (CH_2Cl_2)/nm 504.5 (ε/M^{-1} cm^{-1} 9062.7), **Emission** λ_{em} CH_2Cl_2/nm 521 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.49 (br s, 1H), 7.73 (br s, 1H), 7.46-7.44 (m, 2H), 7.32-7.30 (m, 2H), 6.94-6.92 (dd, *J* = 7.9, 1.2 Hz, 1H), 6.92-6.90 (dd, *J* = 7.9 Hz, 1.0 Hz, 1H), 6.53-6.51 (dd, *J* = 4.2,1.9 Hz, 1H), 6.48 - 6.46 (dd, *J* = 4.2, 1.9 Hz, 1H), 5.35 (d, *J* = 4.4 Hz, 1H, H1), 4.38-4.36 (m, 1H, H2), 4.15 (dd, *J* = 12.8, 2.4 Hz, 1H, OH5), 3.83-3.79 (m, 2H, H3/4), 3.58 (d, *J* = 12.8 Hz, 1H, H5), 3.36 (d, *J* = 9.9 Hz, -OH3/4), 2.91 (d, *J* = 10.2 Hz, 1H, OH3/4), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 146.23, 142.58, 140.14, 134.62, 134.12, 131.24, 130.26, 130.13, 129.57, 128.09, 118.05, 116.93, 97.0 (C1), 76.52 (C2), 68.28 (C3/4), 67.32(C3/4), 65.03 (C5), 20.44. **^{11}B NMR (128 MHz, $CDCl_3$)** δ = 5.12 (br s). **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{21}H_{21}BN_2O_5Na$, 415.1439; found, 415.1441.

3Rd red-pink solid (33.3 mg, 53%)**: UV-vis** λ_{max} (CH_2Cl_2)/nm 504.5 (ε/M^{-1} cm^{-1} 11268), **Emission** λ_{em} CH_2Cl_2/nm 521 (λ_{ex} = 480 nm), **Φ** (CH_2Cl_2) = 0.047; **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.07 (br t, *J* = 1.5 Hz, 1H), 7.70 (br t, *J* = 1.5 Hz, 1H), 7.44-7.42 (m, 2H), 7.30-7.28 (m, 2H), 6.90-6.86 (m, 2H), 6.47 - 6.46 (m, 2H), 5.49 (s, 1H, H1), 5.04 (d, *J* = 6.0 Hz, 1H, H3), 4.77 (d, *J* = 6.0 Hz, 1H, H2), 4.59 (br s, 1H, -OH1), 4.49-4.48 (m, 1H, H4), 3.77 (br s, 2H, H5), 3.55 (br s, 1H, OH5), 2.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 147.15, 145.33, 143.77, 140.99, 135.63, 135.18, 131.66, 131.26, 130.99, 130.51, 129.04, 118.46, 118.00, 104.93 (C1), 90.46 (C4), 87.08 (C2), 81.20 (C3), 64.03 (C5), 21.43. **^{11}B NMR (128 MHz, $CDCl_3$):** δ = 5.75 (br s). **FT-IR (ATR)** 1/λ (cm^{-1}) 3400-3300 (O-H); 3114.73 (C-H aromatic); 2925.73 (Alkyl C-H); 1569.90, 1539.04 (C=N, C-C in aromatic); 1257.46 (C-O); 1147.53 (C-N, C-O); **HRMS (ESI) *m/z*:** $[M+Na]^+$ calcd. for $C_{21}H_{21}BN_2O_5Na$, 415.1439; found, 415.1428.

S4.9. Synthesis of ribose-O-BODIPY conjugates 4Ra-d

Ribose (31.7 mg, 0.211 mmol) was added to a flask containing **4** (62.8 mg, 0.188 mmol) dissolved in anhydrous MeCN. PTSA (5 mol %) dissolved in anhydrous MeCN was added dropwise to the solution. The reaction mixture was left to stir at RT for 60 minutes. The reaction was quenched with saturated aqueous $NaHCO_3$ solution and

CH_2Cl_2 added to induce phase separation. The organic layer containing the products was washed with water three times and then dried over anhydrous Na_2SO_4. Chromatography of the crude residue on deactivated silica gel using CH_2Cl_2 eluted **4Ra** as the first fluorescent orange band. Transitioning the eluent to CH_2Cl_2/MeCN (0.1:30) eluted **4Rb** as the second yellow band then **4Rc** and **4Rd** eluted together as the third yellow band with CH_2Cl_2/MeCN (1:20). Column chromatography of the third fraction with deactivated silica gel and EtOAc:*n*-hexane (1:1) eluted **4Rc** as the first yellow band and **4Rd** as the second yellow band.

4Ra: red-pink film (11.2 mg, 9%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 500 (ε/M^{-1} cm^{-1} 76587), **Emission** λ_{em} CH_2Cl_2/nm 524 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.32 (s, 1H), 8.32 (s, 1H), 7.98 (s, 1H), 7.77 (s, 1H), 6.94 (s, 4H), 6.68 (dd, *J* = 4.4, 1.1 Hz, 1H), 6.66-6.63 (m, 2H), 6.60 (dd, *J* = 4.4, 1.5 Hz, 1H), 6.47 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.45-6.41 (m, 3H), 5.77 (bs, 1H, H1), 5.21-5.16 (m, 1H, H2,3), 4.61 (bs, 1H, H4), 3.66 (d, *J* = 12.6 Hz, 1H, H5), 3.46 (dd, *J* = 12.6, 1.5 Hz, 1H, H5), 2.36 (s, 6H), 2.14 (s, 3H), 2.13 (s, 3H), 2.10 (s, 3H), 2.03 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$** δ 147.25, 146.79, 146.70, 146.50, 144.06, 143.98, 138.53, 138.47, 136.61, 136.50, 136.45, 136.31, 136.03, 135.56, 135.44, 135.27, 130.36, 130.26, 130.22, 130.01, 129.73, 129.28, 128.08, 128.01, 118.73, 118.07, 117.68, 116.85, 108.04 (C1), 90.38 (C4), 88.72 (C2), 83.62 (C3), 64.14 (C5), 21.17, 20.12, 20.04, 19.96, 19.88; **^{11}B NMR (128 MHz, $CDCl_3$)** δ 5.92 (bs), 2.44 (bs); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{41}H_{40}B_2N_4NaO_5$: 713.3091; found 713.3101.

4Rb red film (2.8 mg, 4%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 506 (ε/M^{-1} cm^{-1} 106314), **Emission** λ_{em} CH_2Cl_2/nm 524 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.46 (s, 1H), 7.70 (s, 1H), 6.95 (s, 1H), 6.93 (s, 1H), 6.66 (dd, *J* = 4.5, 1.5 Hz, 1H), 6.63 (dd, *J* = 4.5, 1.5 Hz, 1H), 6.45 (dd, *J* = 4.5, 2.0 Hz, 1H), 6.40 (dd, *J* = 4.5, 2.0 Hz, 1H), 5.35 (s, 1H, H1), 4.40-4.36 (m, 1H, H2), 4.16 (dd, *J* = 12.9, 2.4 Hz, 1H, H5), 3.88-3.80 (m, 2H, H3,4), 3.59 (d, *J* = 12.9 Hz, 1H, H5), 2.35 (s, 3H), 2.16 (s, 3H), 2.05 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.78, 147.23, 144.09, 138.75, 136.48, 136.40, 135.59, 130.90, 128.16, 119.23, 118.14, 98.14 (C1), 77.60 (C2), 69.32 (C4), 68.42 (C3), 66.07 (C5), 21.16, 20.23, 19.99; **^{11}B NMR (128 MHz, $CDCl_3$)** δ 5.16 (bs); **HRMS (ESI+):** *m/z*: [*M*+Na]$^+$ calcd for $C_{23}H_{25}BN_2NaO_5$: 443.1753; found 443.1748.

4Rc red film (40.3 mg, 51%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 506 (ε/M^{-1} cm^{-1} 50741), **Emission** λ_{em} CH_2Cl_2/nm 522 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.07 (s, 1H), 7.70 (s, 1H), 6.92 (s, 2H), 6.63 (dd, *J* = 4.5, 1.5 Hz, 1H), 6.60 (dd, *J* = 4.5, 1.5 Hz, 1H), 6.43-6.39 (m, 2H), 5.54 (s, 1H, H1), 5.07 (d, *J* = 6.0 Hz, 1H, H2), 4.81 (d, *J* = 6.0 Hz, 1H, H3), 4.54-5.50 (m, 1H, H4), 3.80 (d, *J* = 2.8 Hz, 2H, H5), 2.34 (s, 3H), 2.09 (s, 6H); **^{13}C NMR (100 MHz, $CDCl_3$** δ 147.06, 145.84 144.28, 138.64, 136.41, 136.02,

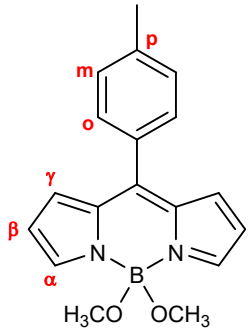
135.60, 130.34, 130.07, 129.88, 129.68, 128.11, 118.81, 118.27, 104.97 (C1), 90.48 (C4), 87.20 (C3), 81.32 (C2), 64.14 (C1), 21.15, 20.05; **^{11}B NMR (128 MHz, $CDCl_3$):** δ 5.80 (bs); **FT-IR (ATR)** 1/λ (cm^{-1}) 3400-3300 broad (O-H); 2916.08 (Alkyl C-H); 1610.40 (C=N); 1552.54 (C=N, C-C in aromatic); 1255.53 (C-O); 1166.82. 1141.74 (C-N, C-O); **HRMS (ESI+):** *m/z*: $[M+Na]^+$ calcd for $C_{23}H_{25}BN_2NaO_5$: 443.1753; found 443.1748.

4Rc' (5.8 mg, 7%): **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.18 (s, 1H), 7.75 (s, 1H), 6.94 (s, 2H), 6.67 (dd, *J* = 4.5, 1.4 Hz, 1H), 6.64 (dd, *J* = 4.5, 1.4 Hz, 1H), 6.44 (dd, *J* = 4.0, 2.0 Hz, 2H), 5.50 (dd, *J* = 9.2, 4.0 Hz, 1H, H1), 4.89 (dd, *J* = 6.5, 2.5 Hz, 1H, H3), 4.83-4.81 (m, 1H, H2), 4.30-4.26 (m, 1H, H4), 3.85-3.81 (m, 1H, H5), 3.74-3.70 (m, 1H, H5), 2.35 (s, 3H), 2.13 (s, 3H), 2.07 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.13, 145.96 144.38, 138.73, 136.50, 136.11, 135.69, 130.42, 130.16, 129.75, 128.20, 118.77, 118.35, 98.02 (C1), 84.40 (C4), 80.28 (C3), 79.51 (C2), 63.38 (C5), 21.25, 20.20; **^{11}B NMR (128 MHz, $CDCl_3$)** δ 5.99 (bs); **HRMS (ESI+):** *m/z*: $[M+Na]^+$ calcd for $C_{23}H_{25}BN_2NaO_5$: 443.1753; found 443.1748.

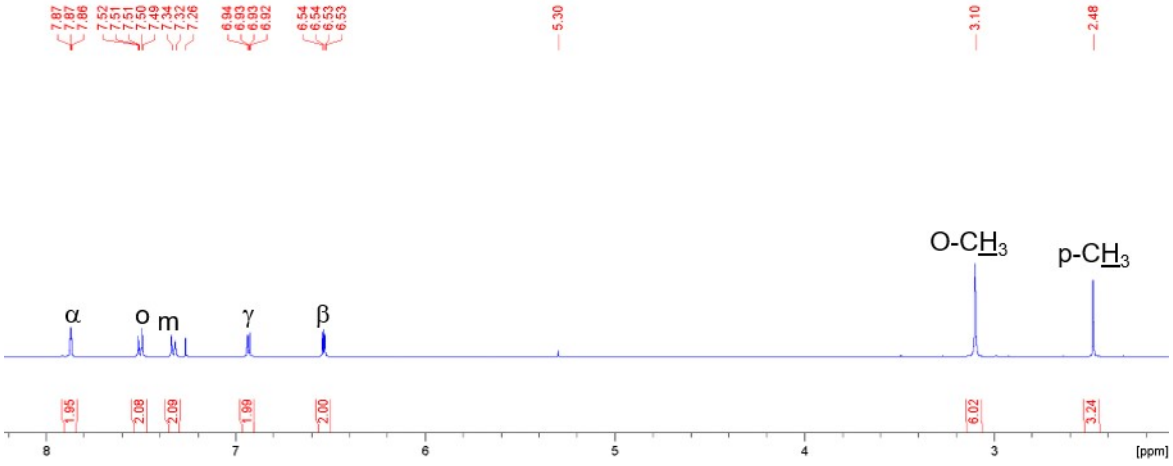
4Rd red film (16.7 mg, 23%): **UV-vis** λ_{max} (CH_2Cl_2)/nm 506 (ε/M^{-1} cm^{-1} 52607), **Emission** λ_{em} CH_2Cl_2/nm 520 (λ_{ex} = 480 nm); **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 87.98 (s, 1H), 7.68 (s, 1H), 6.94 (s, 2H), 6.68 (dd, *J* = 7.0, 1.0 Hz, 1H), 6.66 (dd, *J* = 7.0, 1.5 Hz, 1H), 6.46-6.42 (m, 2H), 6.06 (bs, 1H, H1), 4.75-4.71 (m, 1H, H2), 4.18-4.12 (m, 1H, H4), 4.12-4.05 (m, 1H, H3), 4.01 (d, *J* = 12.1 Hz, 1H, H5), 3.85-4.76 (m, 1H, H5), 2.35 (s, 3H), 2.14 (s, 3H), 2.09 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 147.69, 145.00 144.30, 138.83, 136.35, 136.05, 135.71, 130.78, 130.19, 129.82, 128.21, 128.16, 118.50, 104.59 (C1), 82.60 (C4), 78.89 (C2), 71.61 (C3), 62.44 (C5), 21.16, 20.11, 20.00; **^{11}B NMR (128 MHz, $CDCl_3$):** δ = 5.72 (bs); **FT-IR (ATR)** 1/λ (cm^{-1}) 2958.51, 2919.94, 2852.44 (Alkyl C-H); 1560.26 (C=N, C-C in aromatic); 1257.46 (C-O); 1066.53 (C-N, C-O); **HRMS (ESI+):** *m/z*: $[M+Na]^+$ calcd for $C_{23}H_{25}BN_2NaO_5$: 443.1753; found 443.1752.

S5. NMR SPECTRA

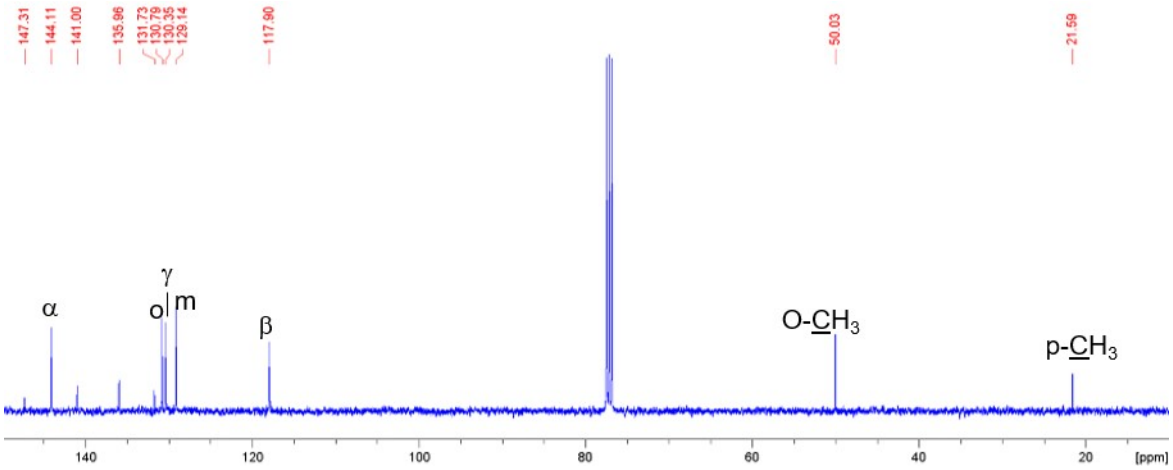
S5.1 O-BODIPY 3: meso-tolyl-O-BODIPY



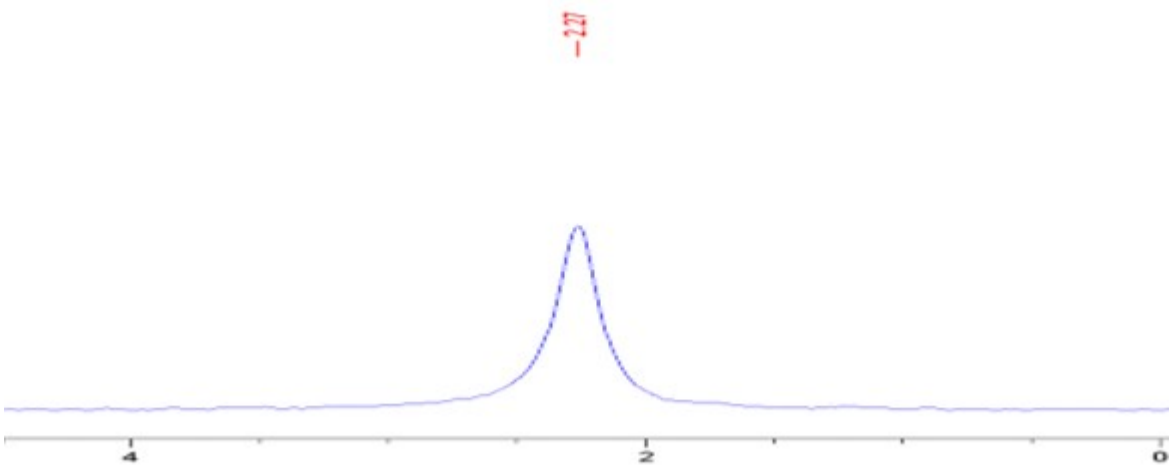
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3



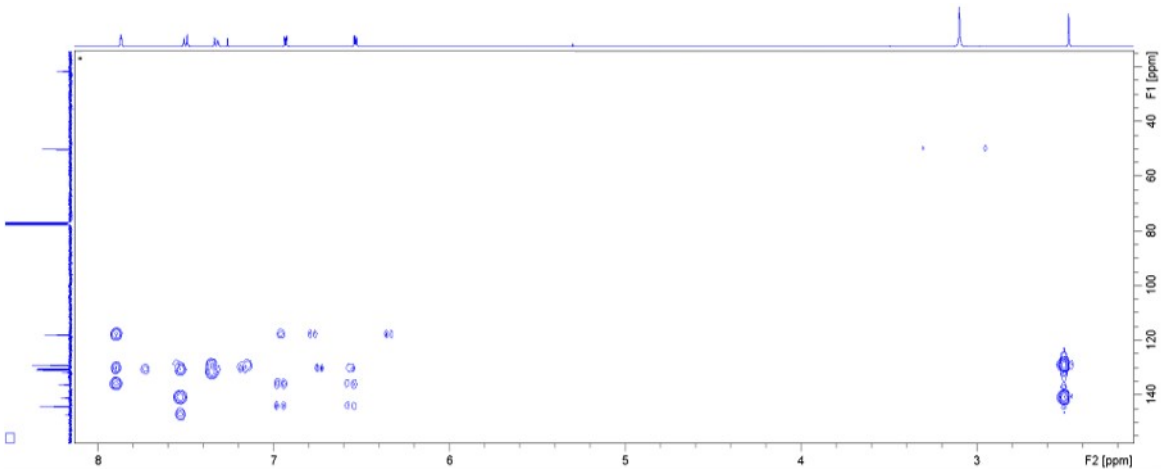
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3



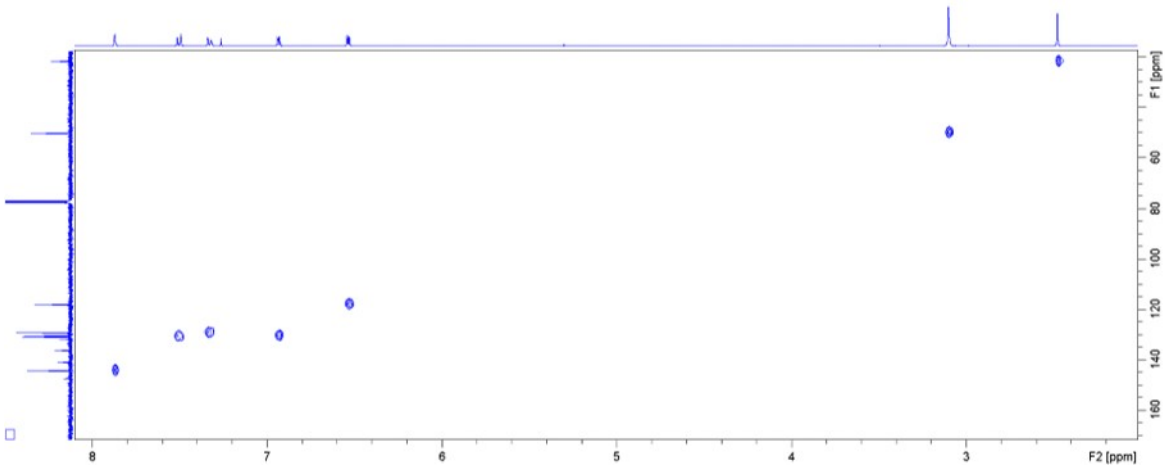
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3



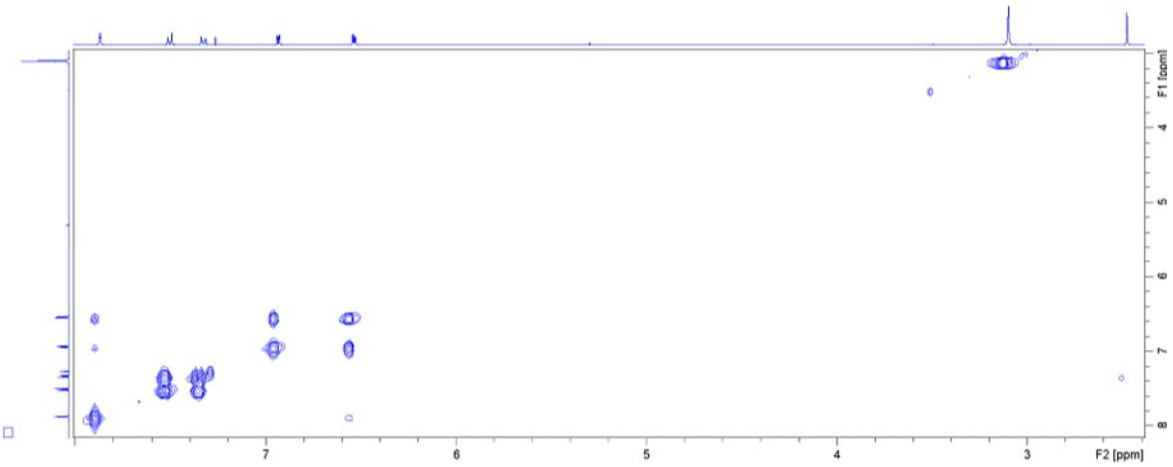
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3



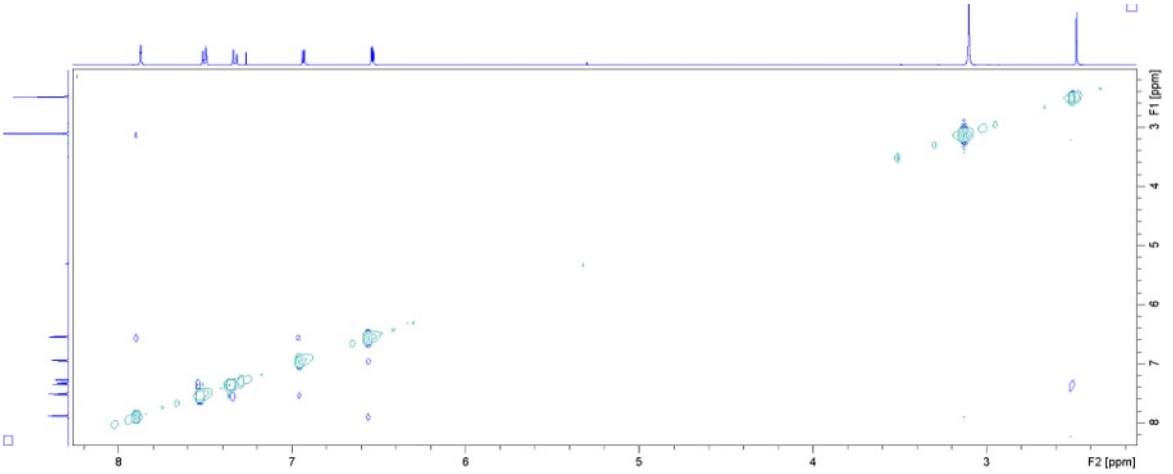
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3



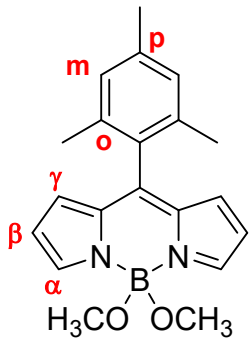
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3



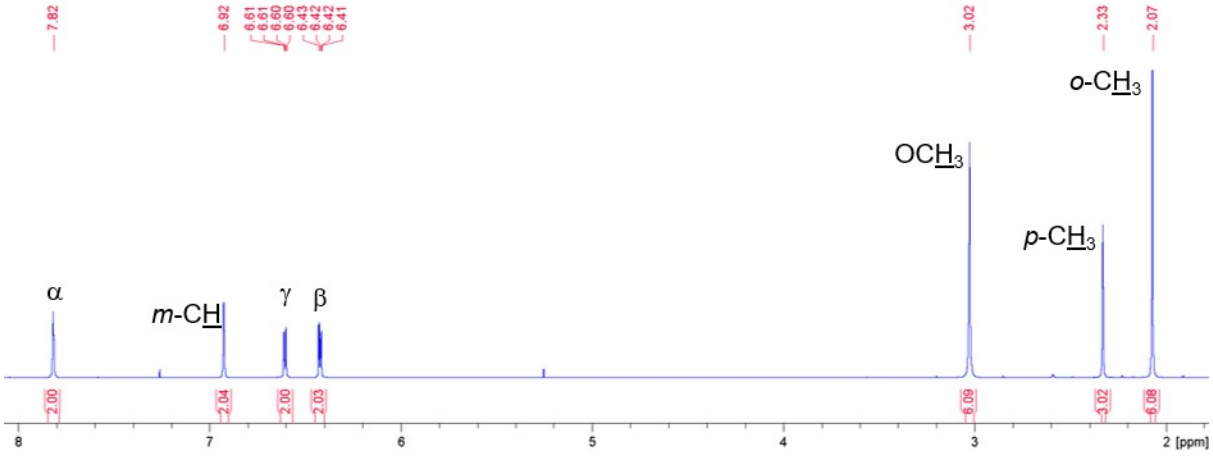
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3



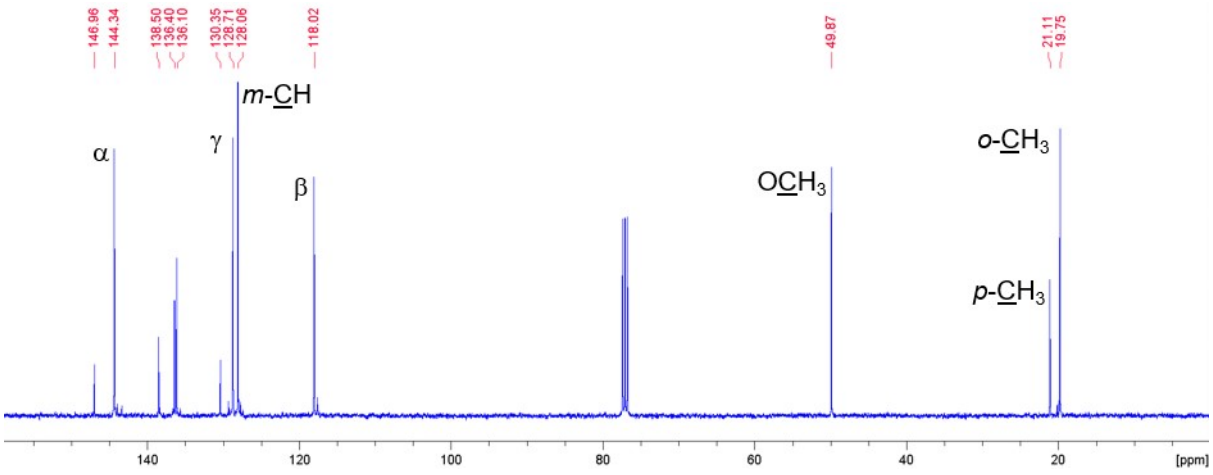
S5.2 O-BODIPY 4: meso-mestiyl-O-BODIPY



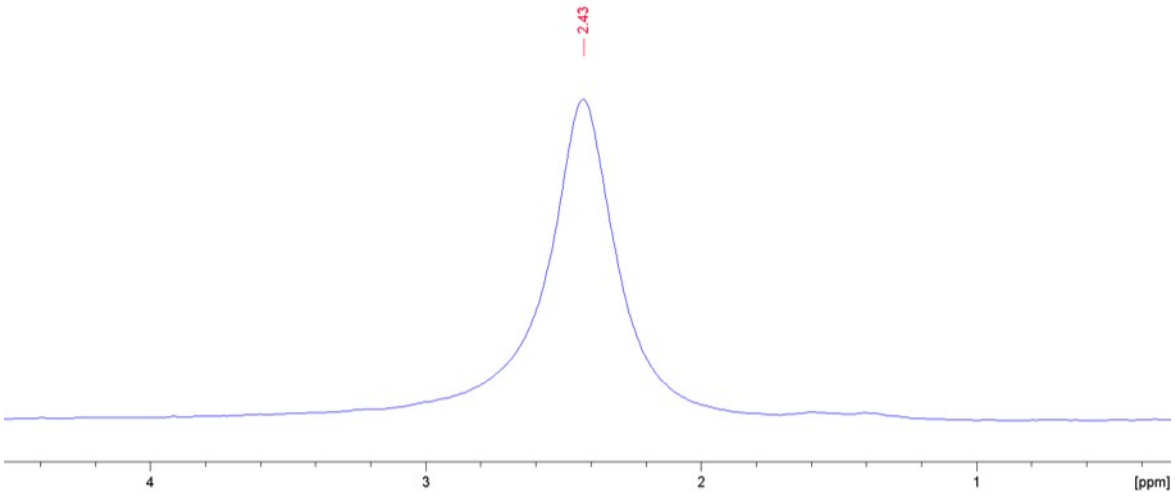
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4



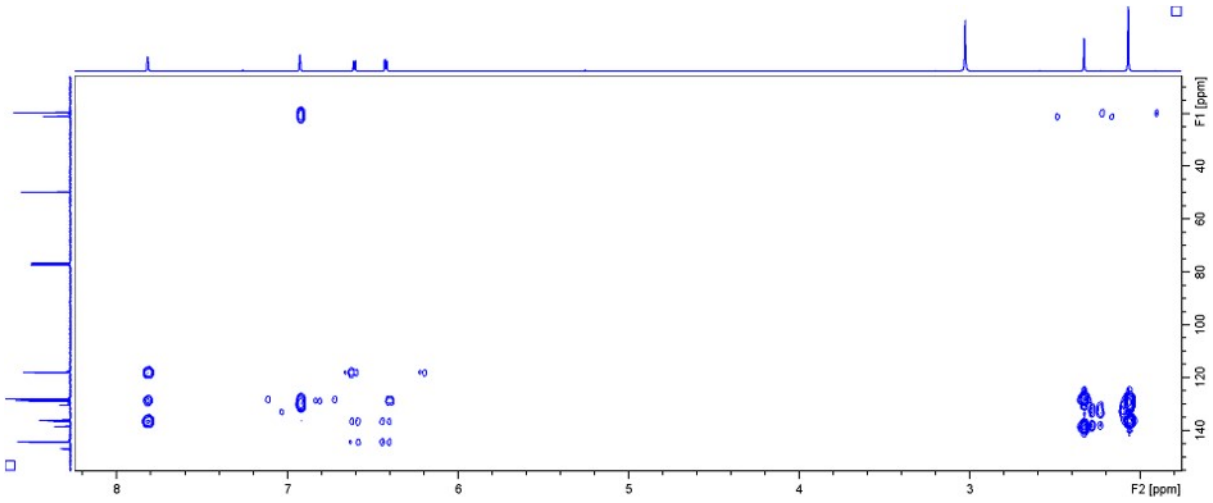
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4



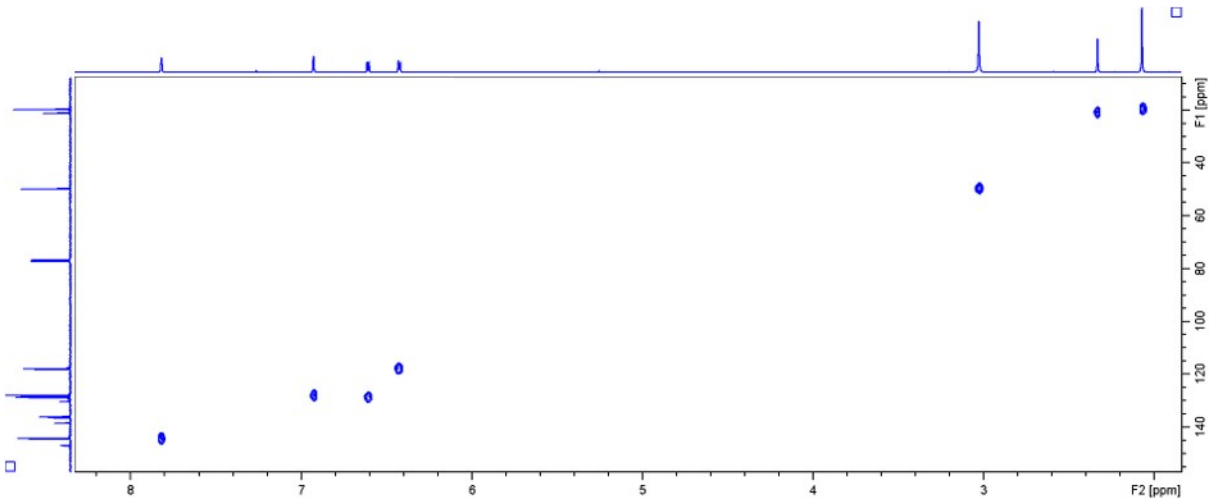
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4



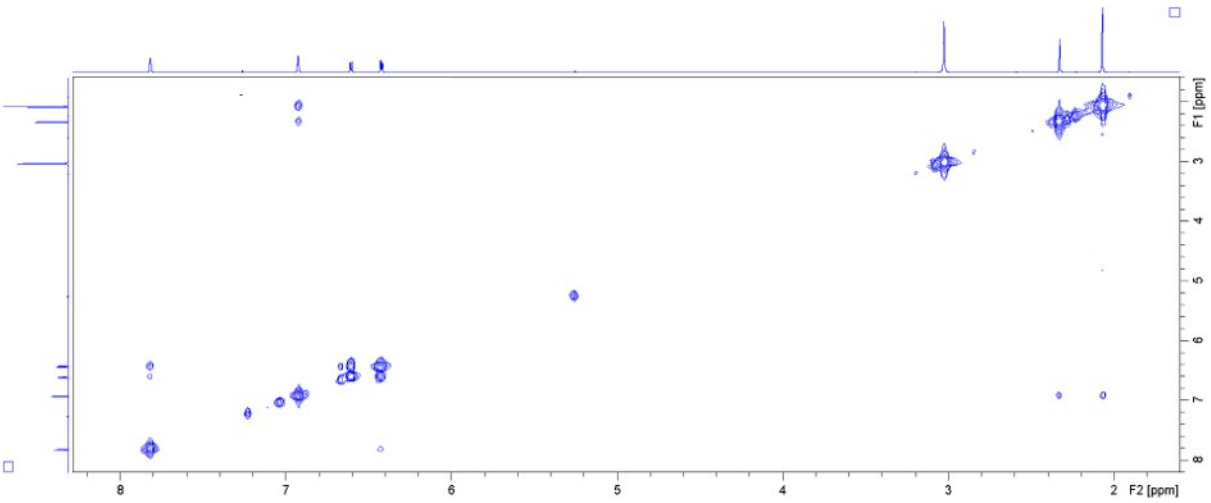
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4



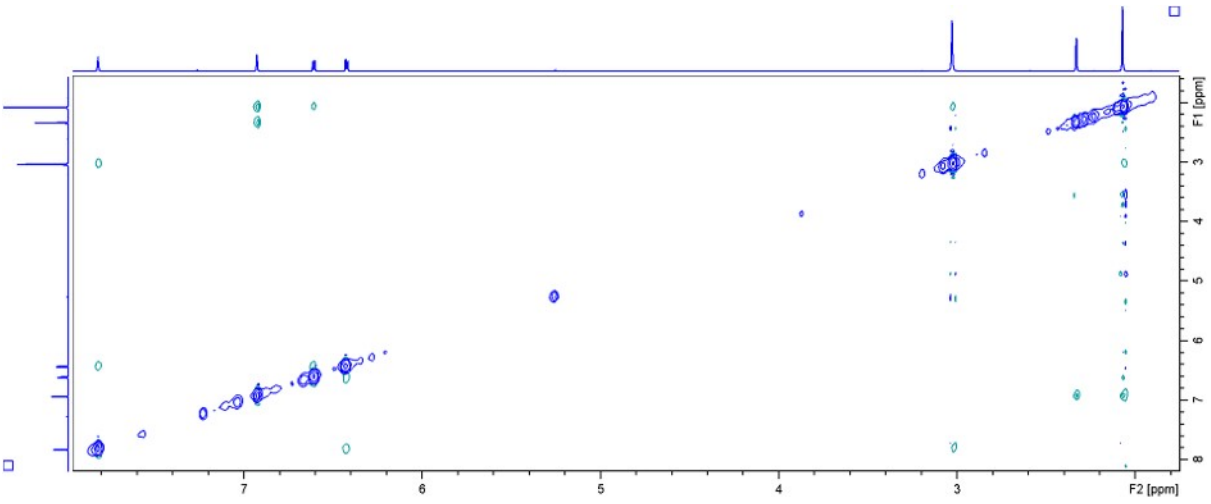
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4


F1 [ppm]
40
60
80
100
120
140
8
7
6
5
4
3
F2 [ppm]

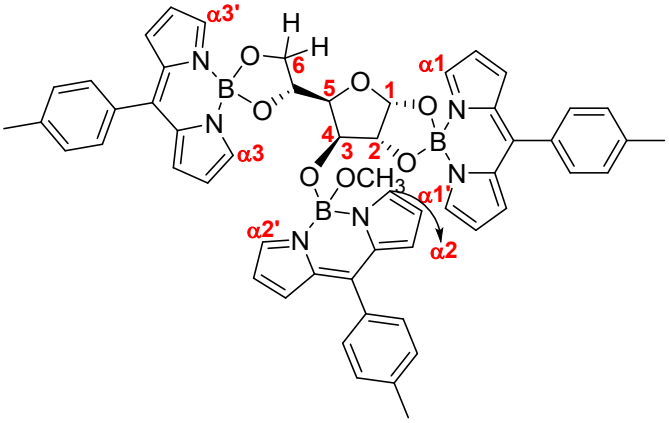
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4



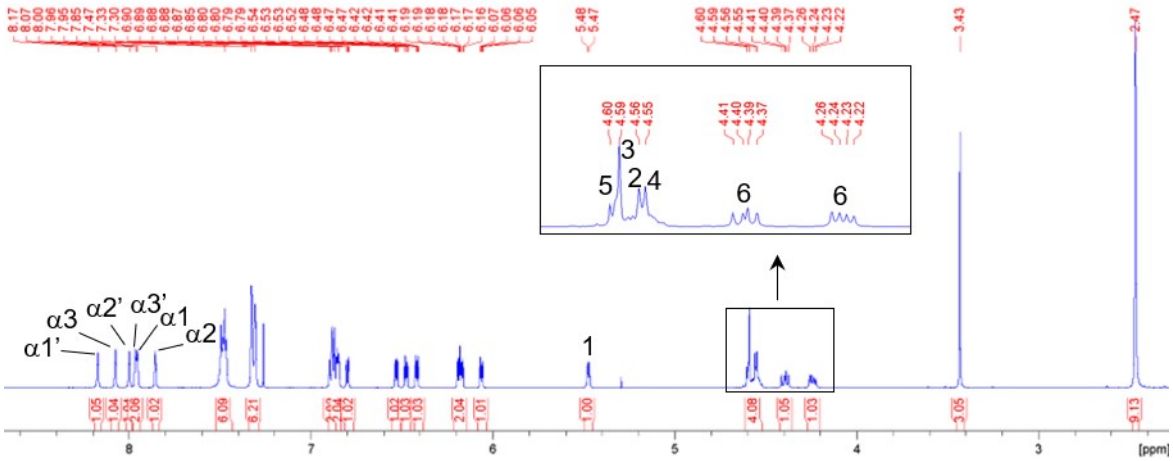
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4



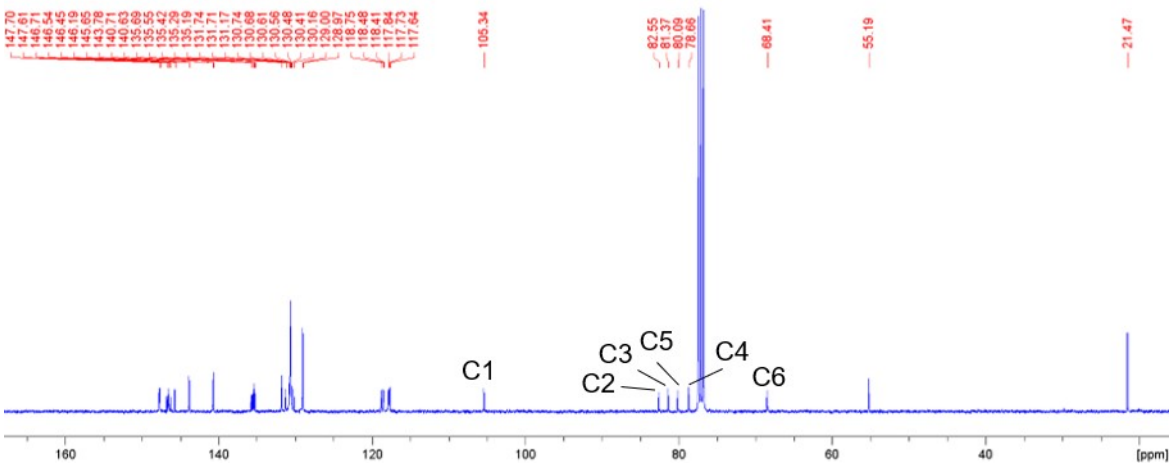
S5.3 Conjugate 3Ga: α-Glucofuranose-(1,2)(3)(5,6)-O-BODIPY(OMe)



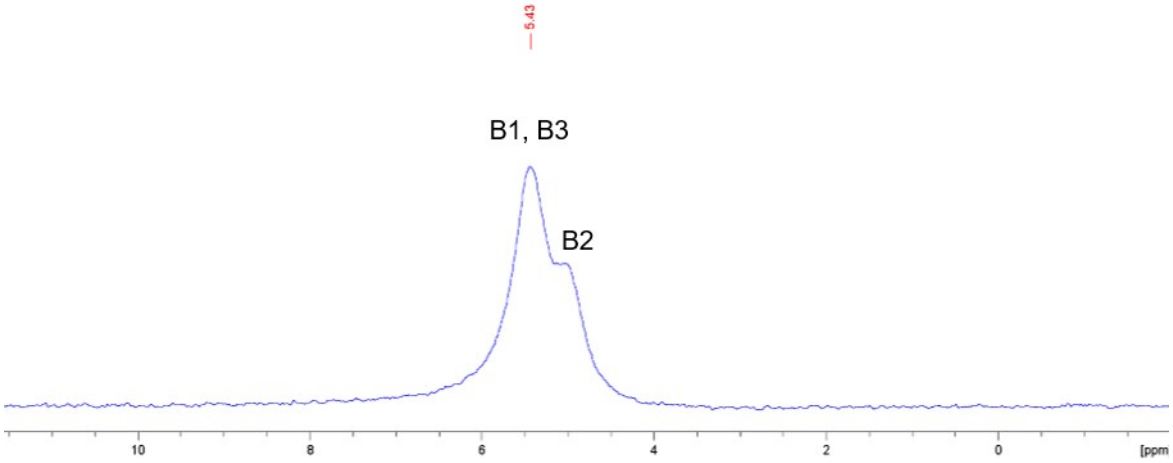
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Ga



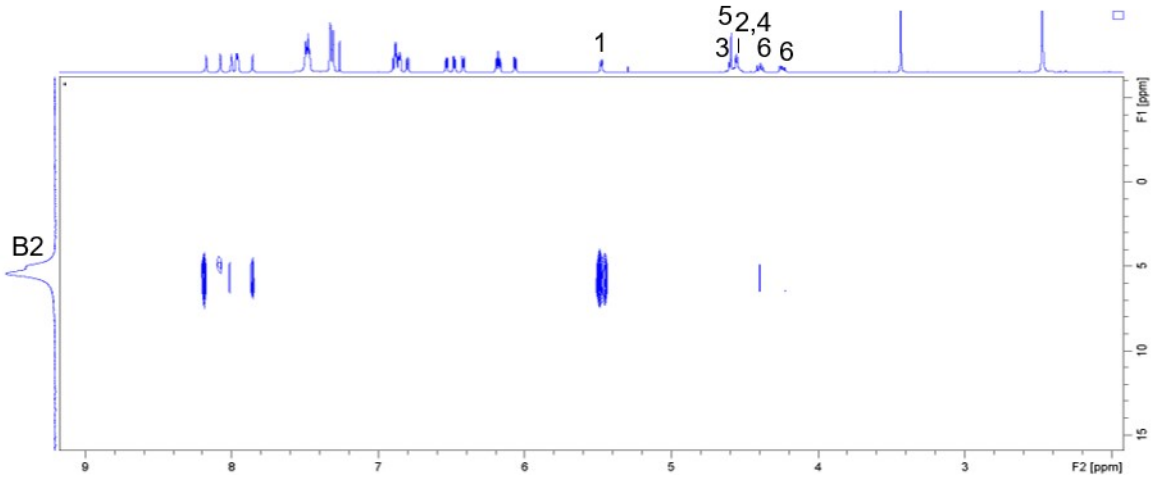
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Ga



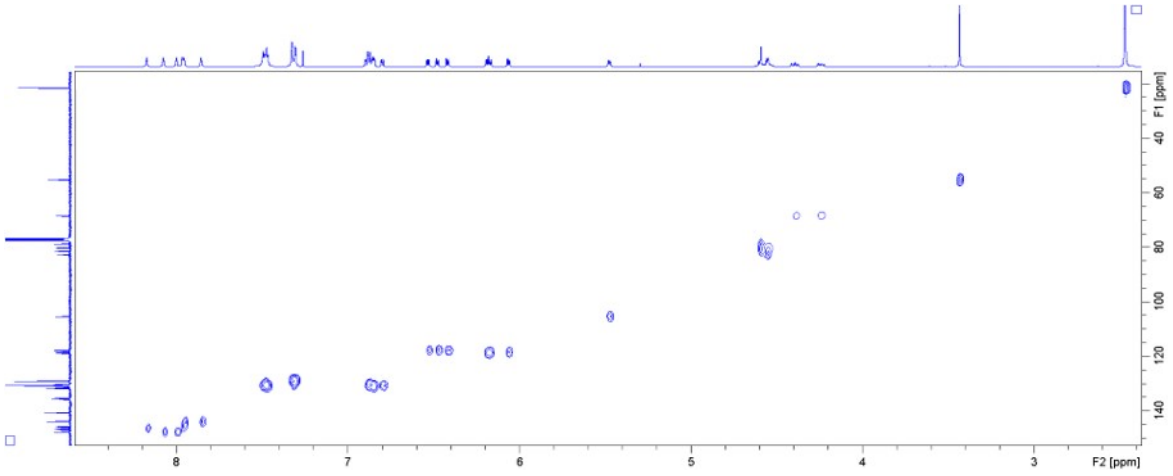
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Ga



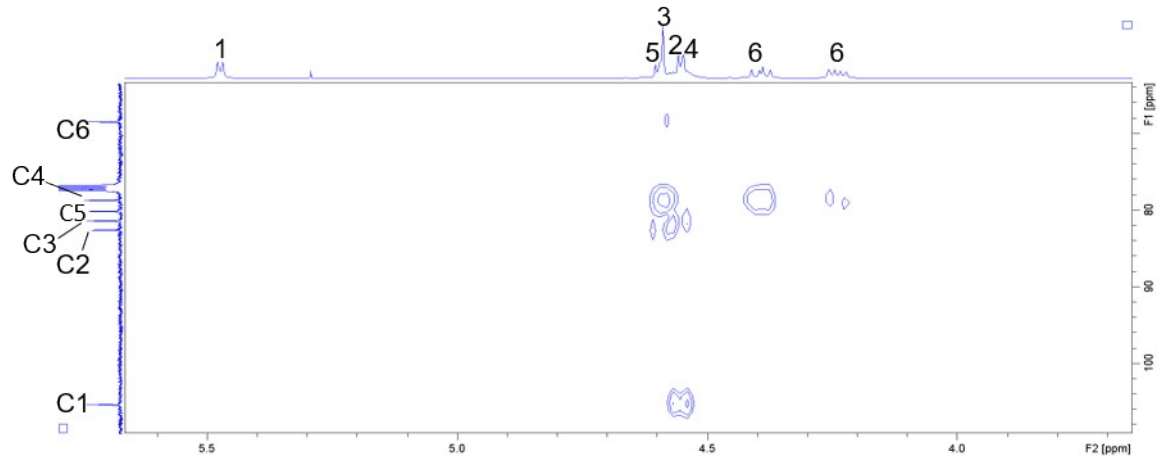
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Ga



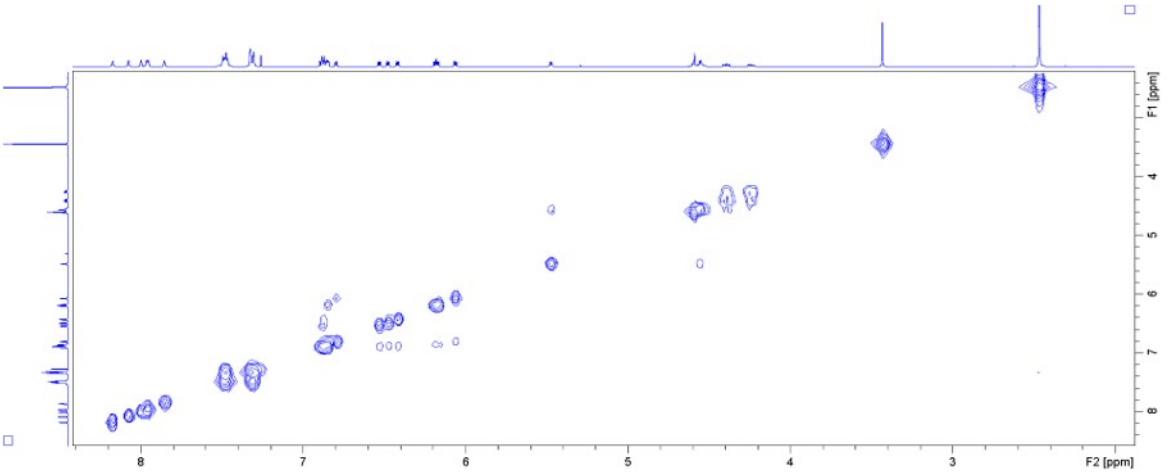
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Ga



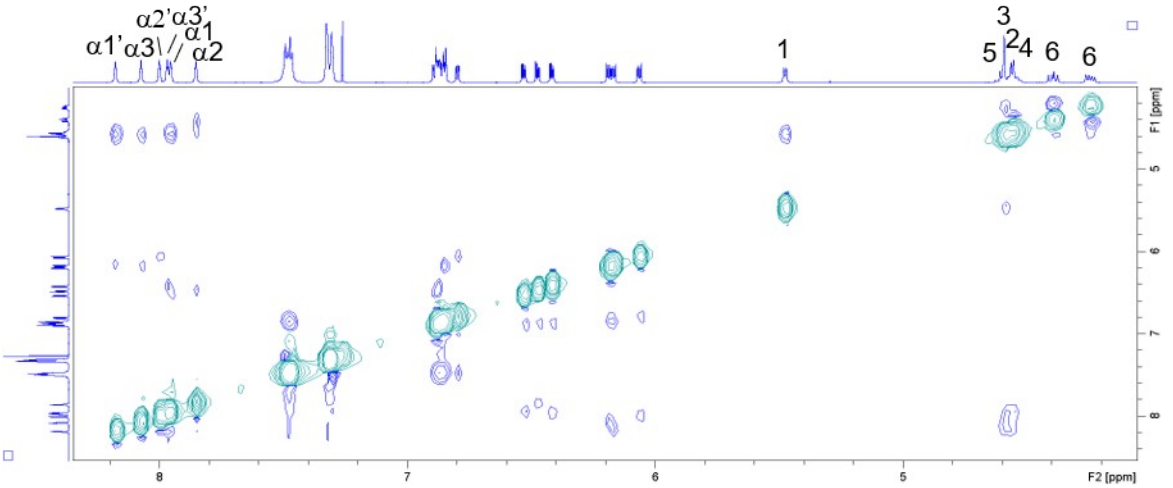
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Ga



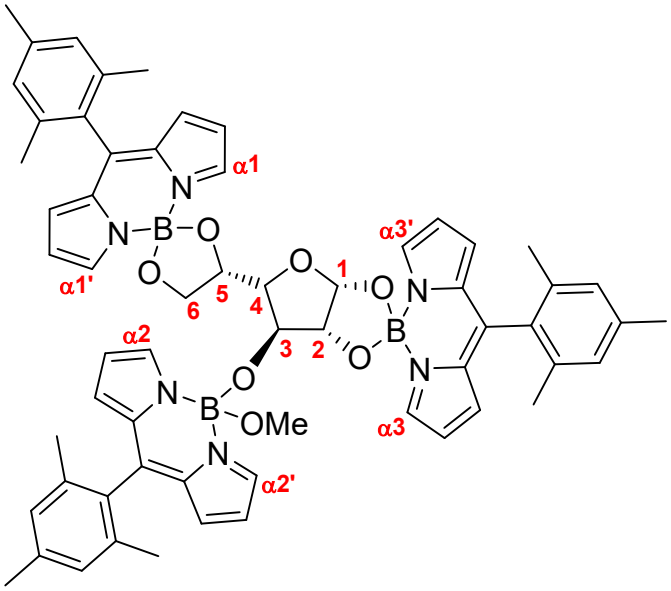
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Ga



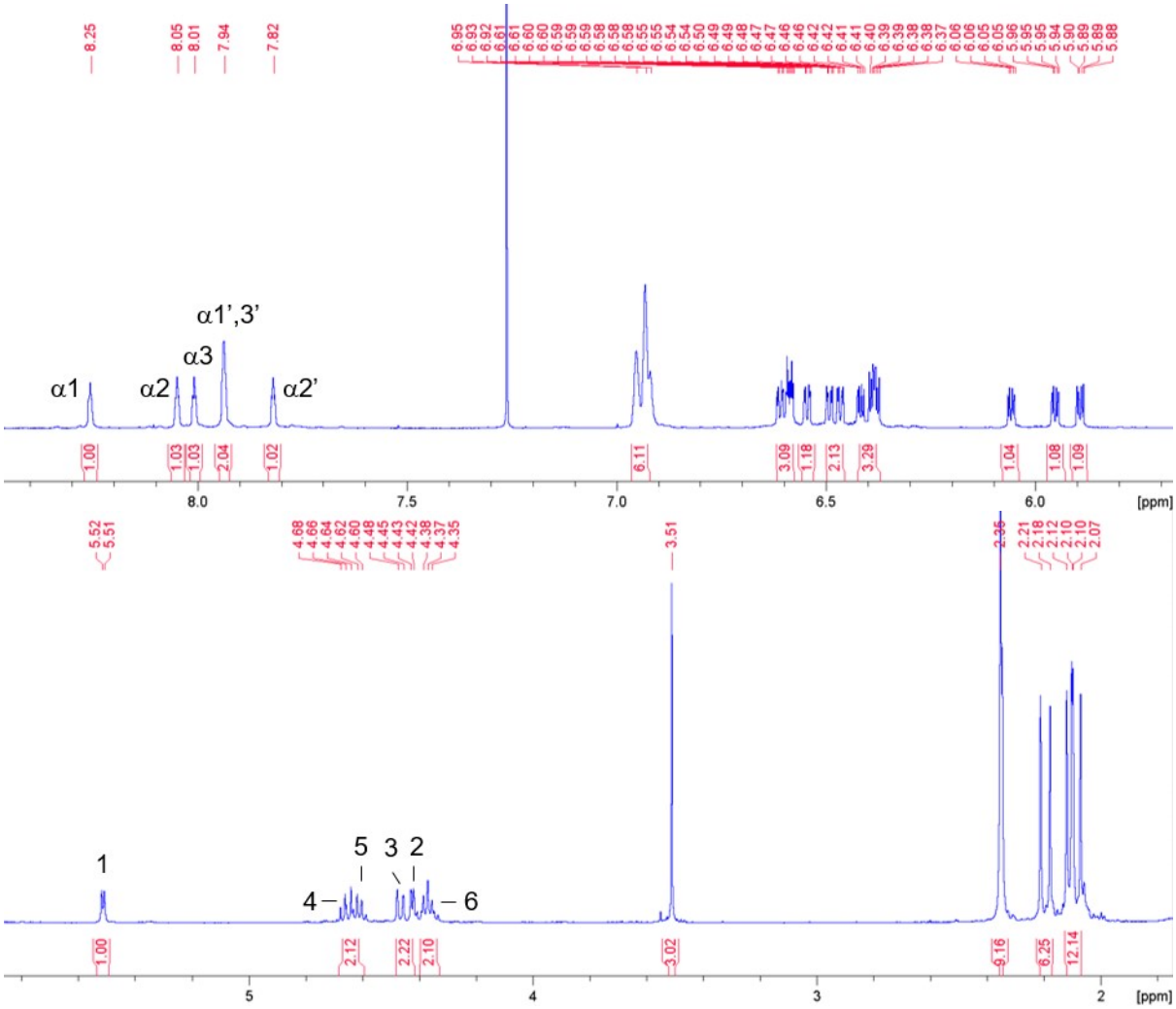
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Ga



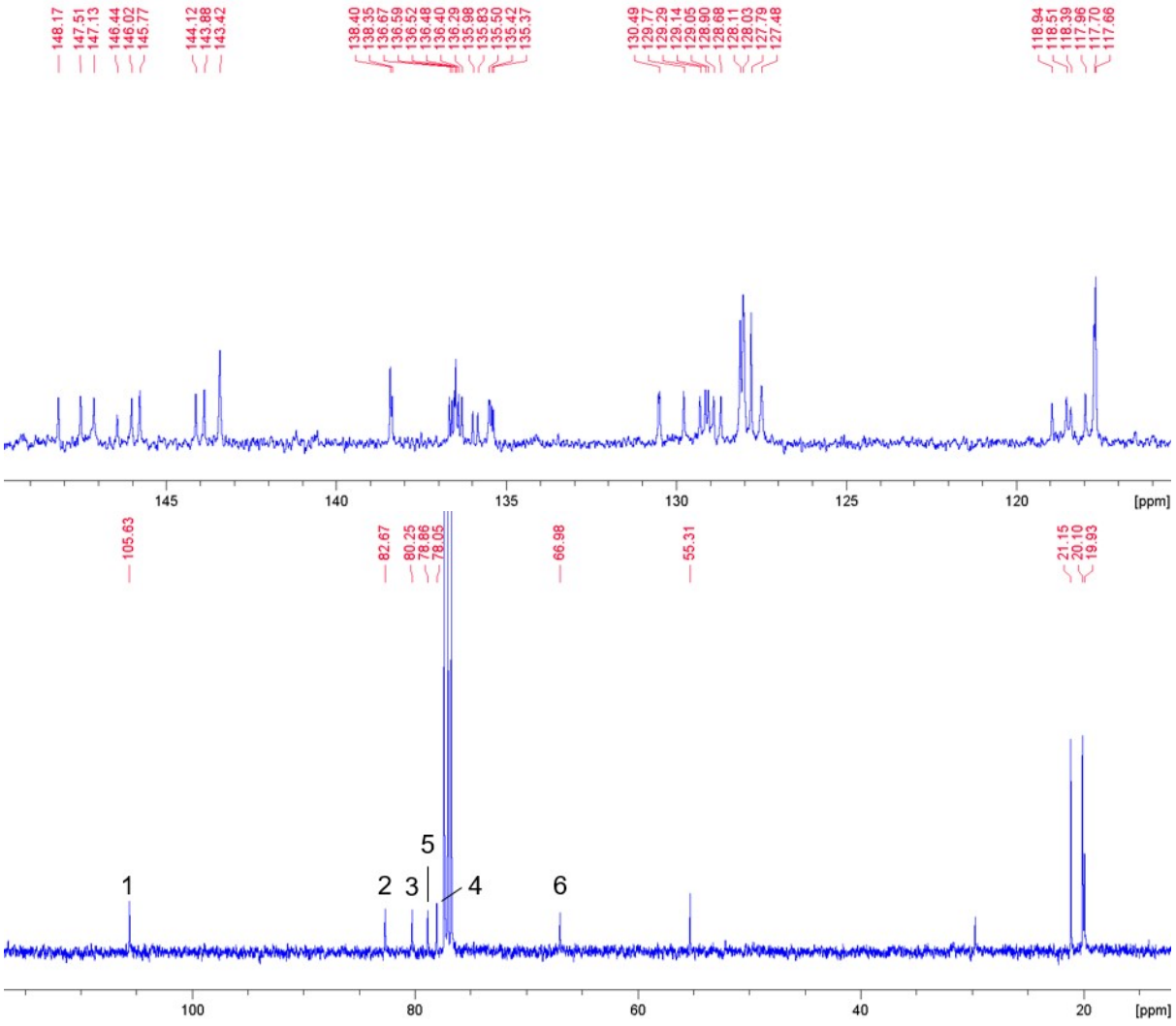
S5.4 Conjugate 4Ga: α-Glucofuranose-(1,2)(3)(5,6)-O-BODIPY(OMe)



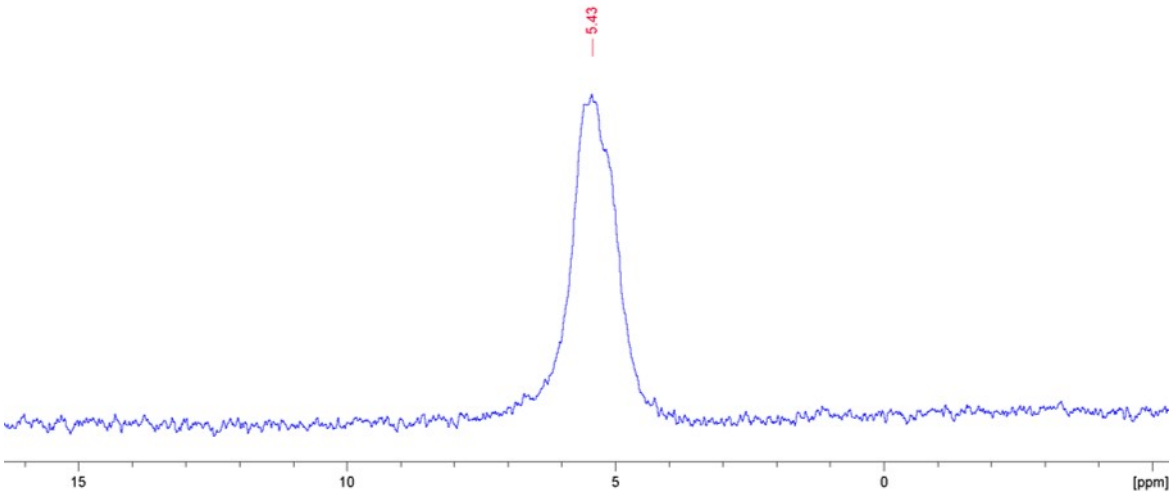
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Ga



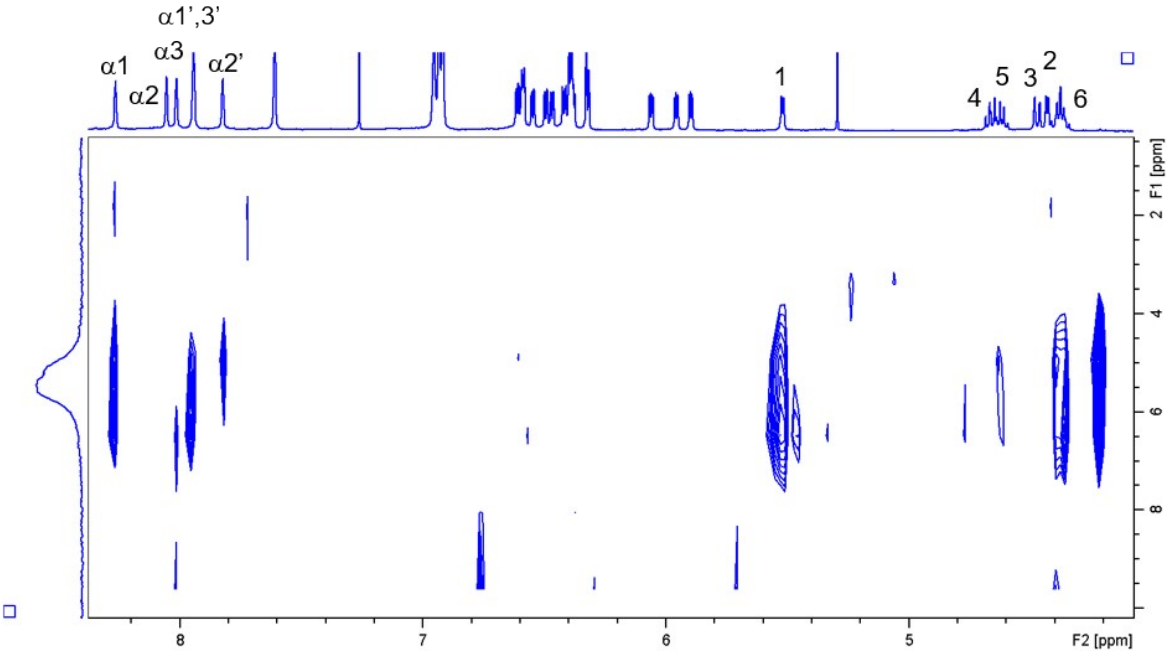
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Ga



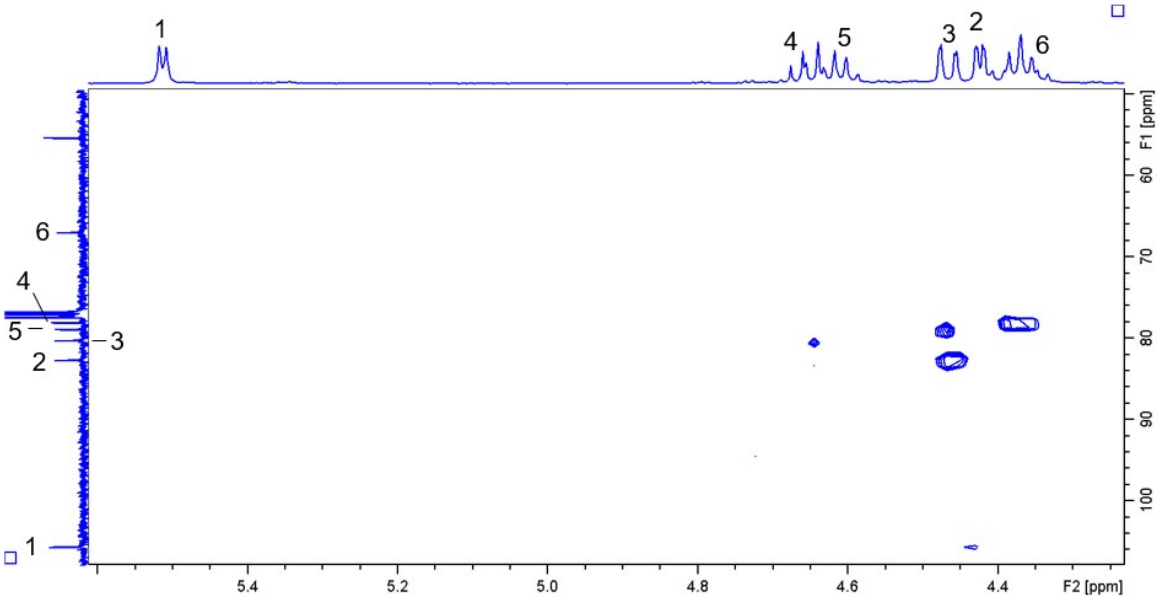
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Ga



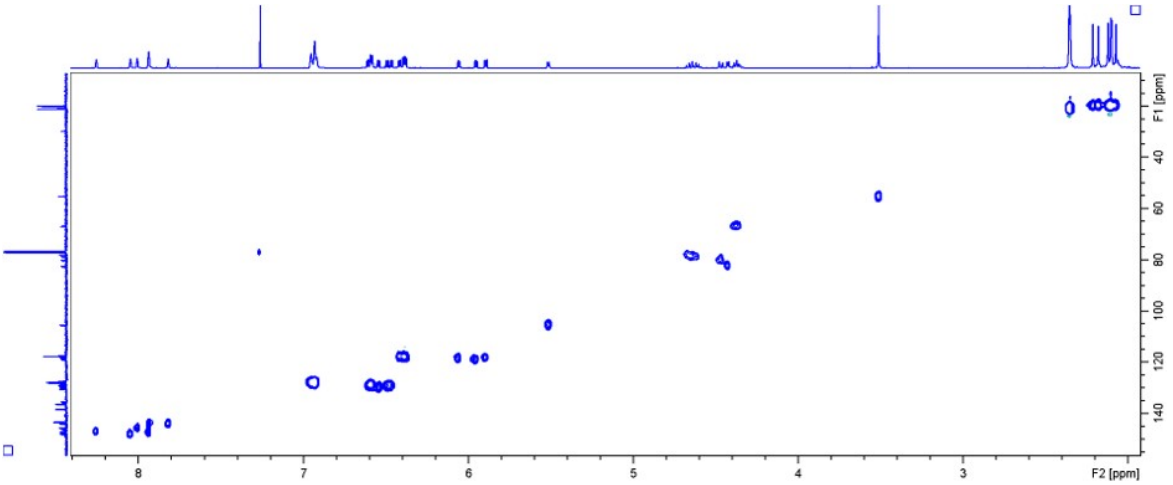
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 4Ga



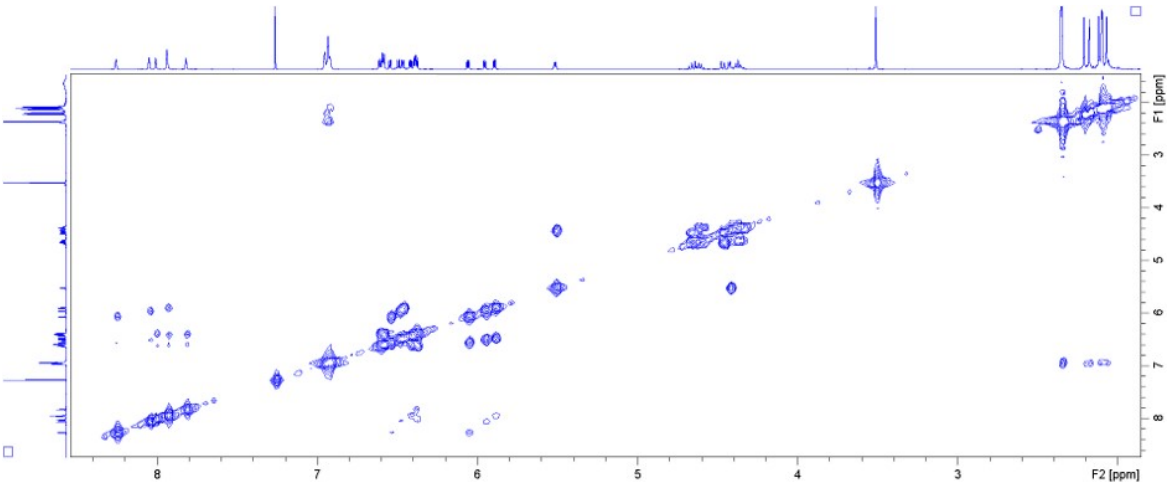
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Ga



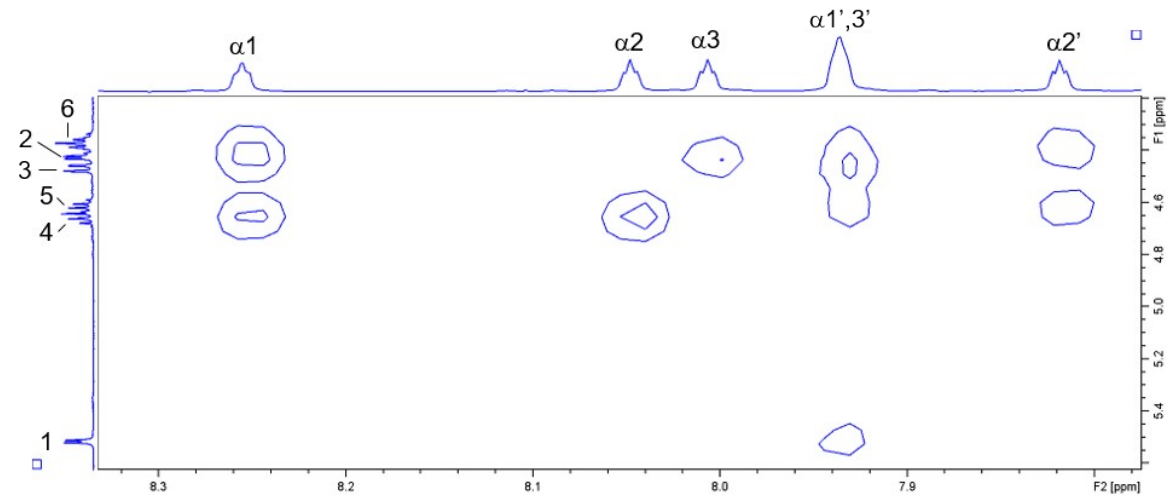
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Ga



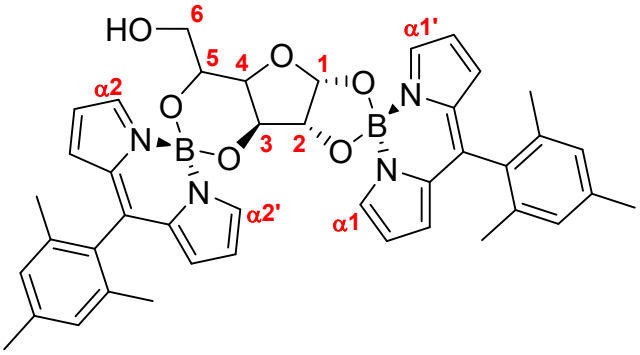
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Ga



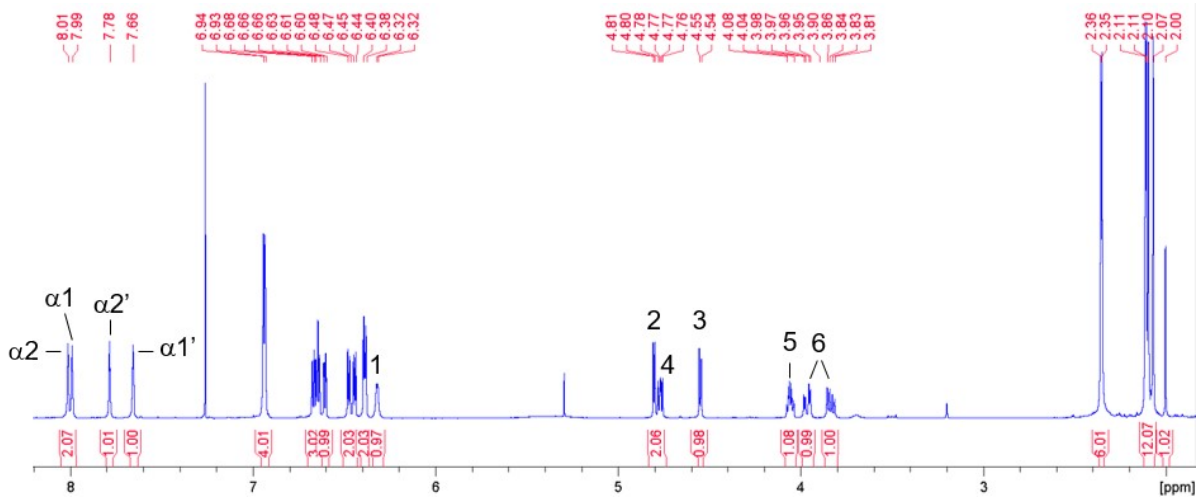
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Ga



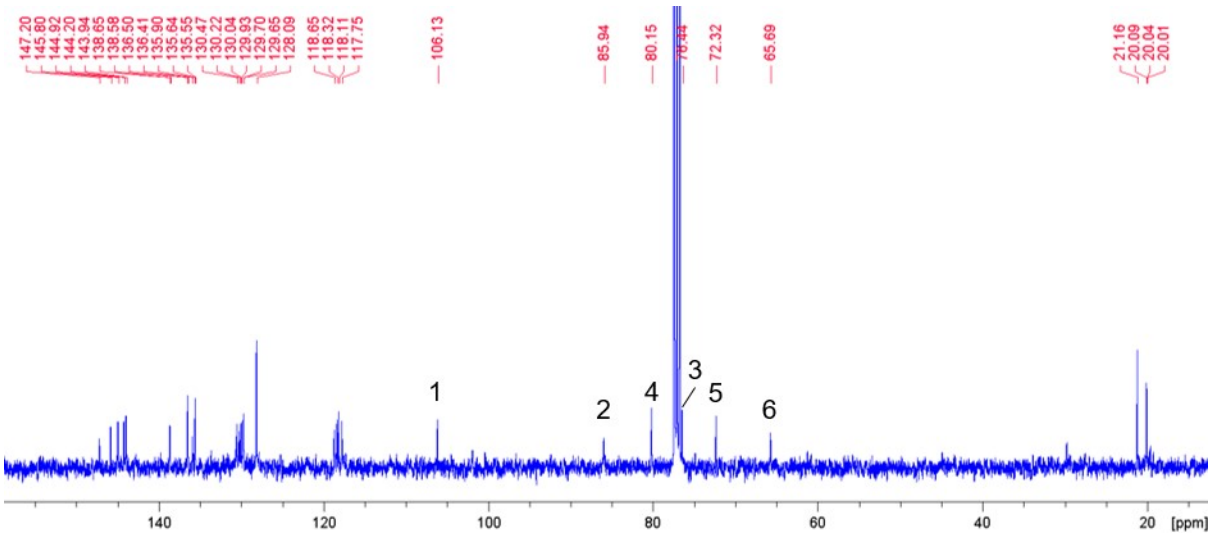
S5.5 Conjugate 4Gb: α-Glucofuranose-(1,2)(3,5)-O-BODIPY



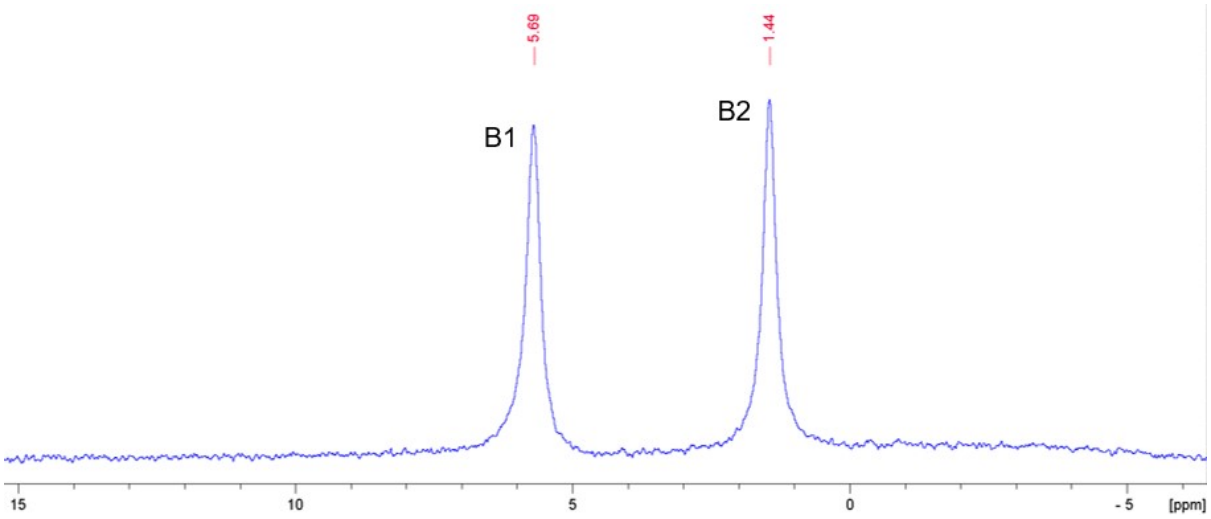
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Gb



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Gb


147.20
145.80
144.92
144.20
143.94
138.65
138.58
136.50
136.41
135.90
135.64
135.55
130.47
130.22
130.04
129.93
129.70
129.65
128.09
118.65
118.32
118.11
117.75
106.13
85.94
80.15
72.32
65.69
21.16
20.09
20.04
20.01
1
2
3
4
5
6
140
120
100
80
60
40
20
[ppm]

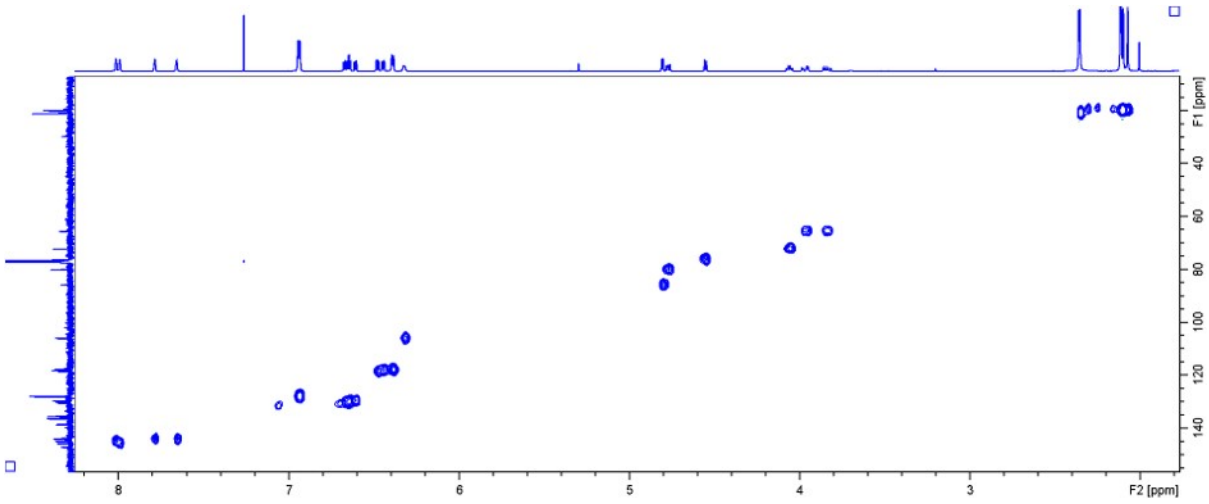
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Gb



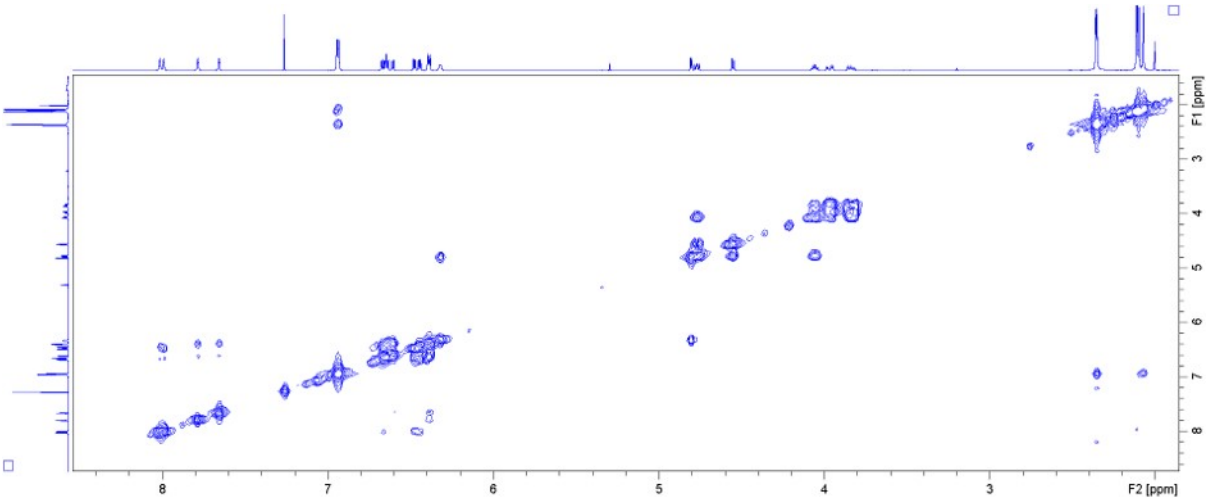
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 4Gb

^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Gb

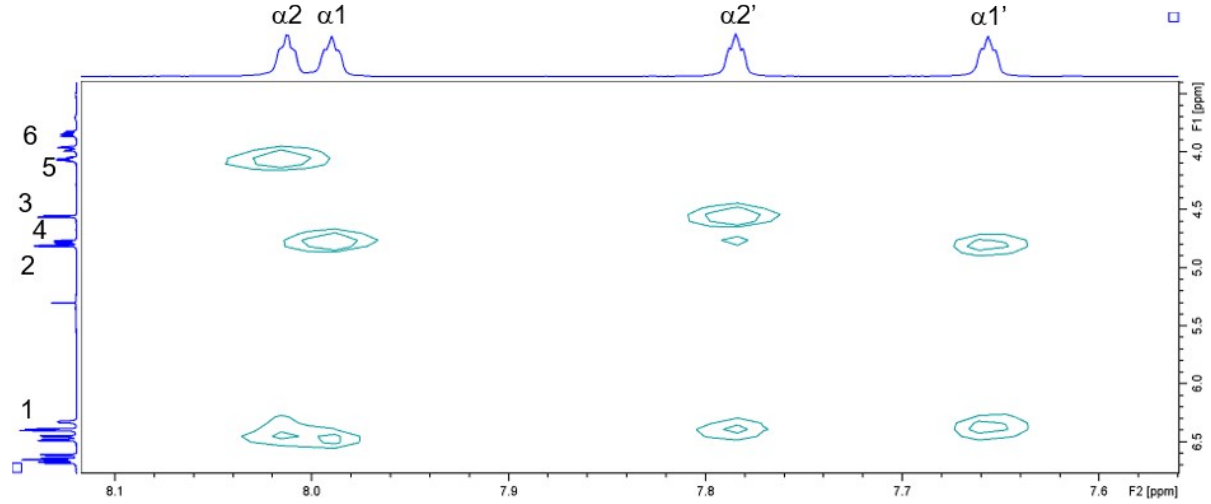
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Gb



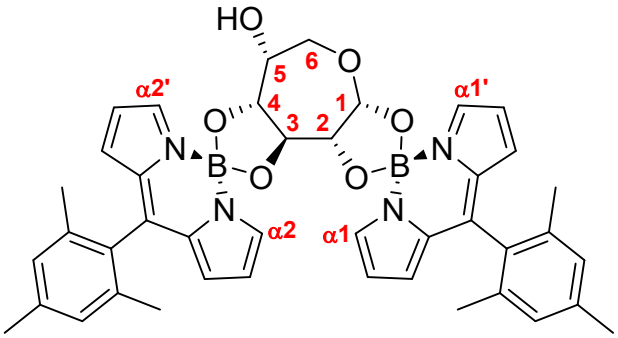
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Gb



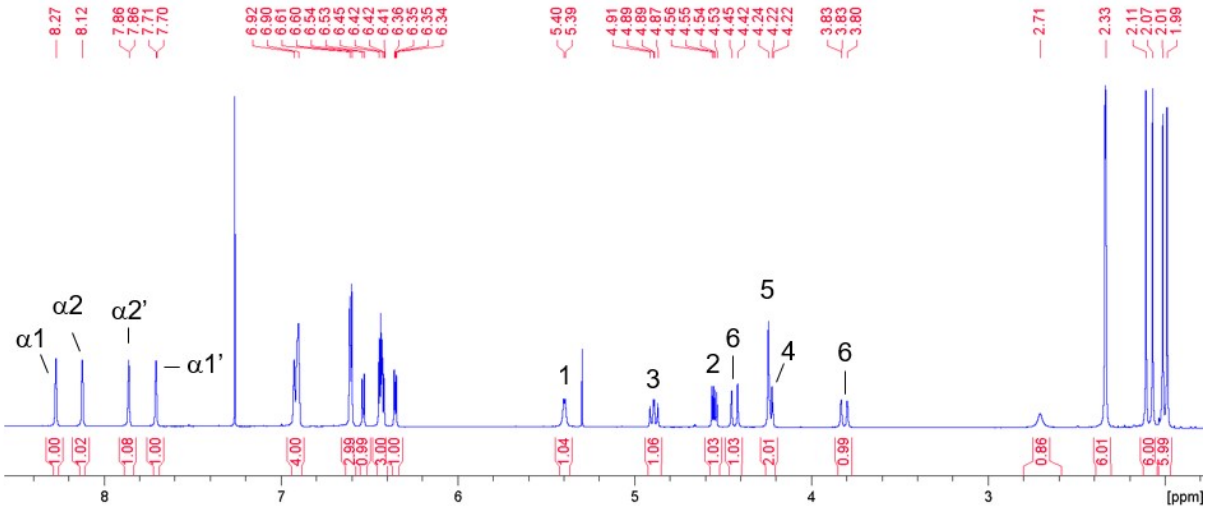
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Gb



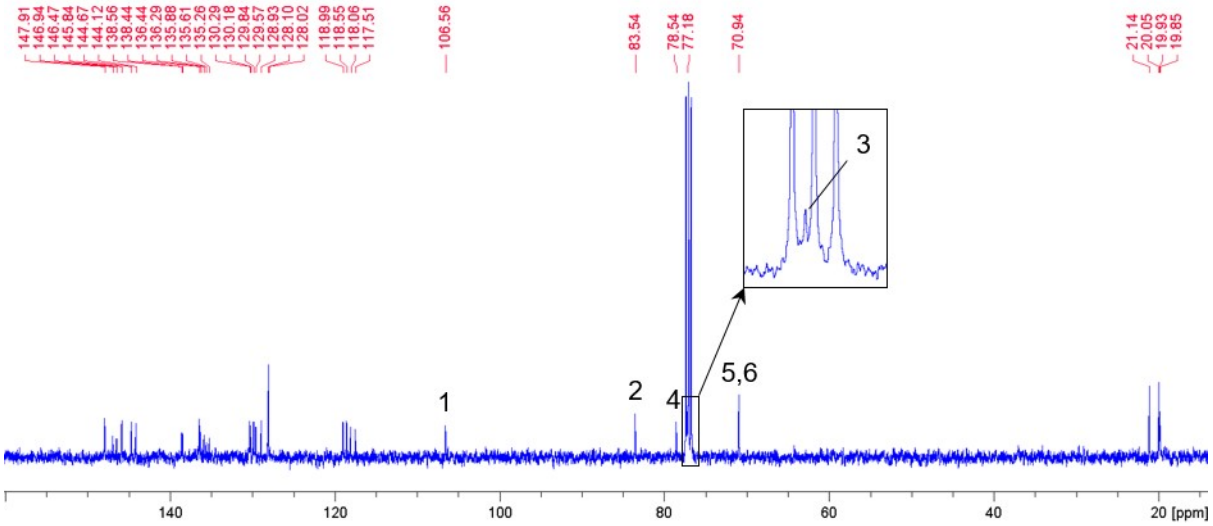
S5.6 Conjugate 4Gc: α-Glucoseptanose-(1,2)(3,4)-O-BODIPY



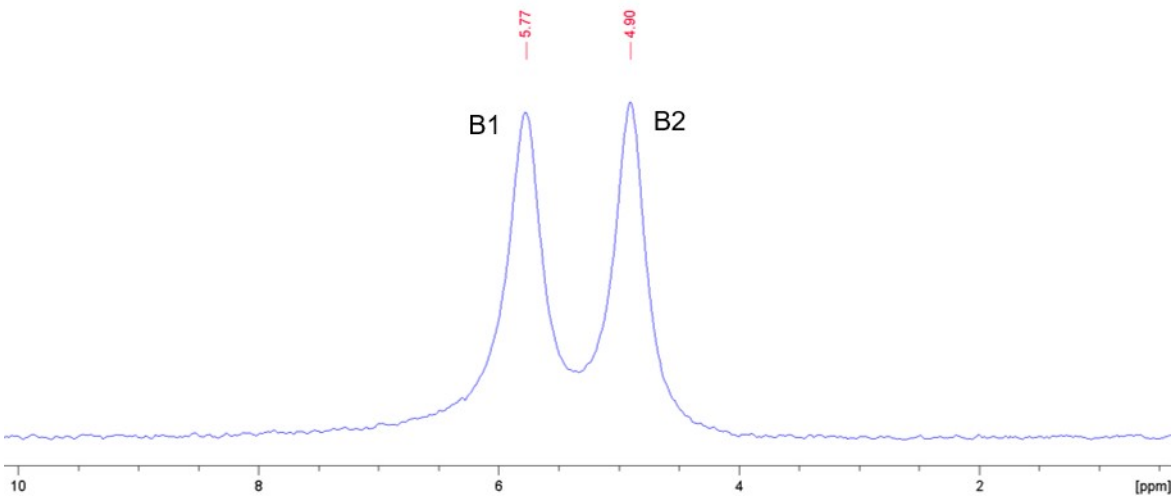
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Gc



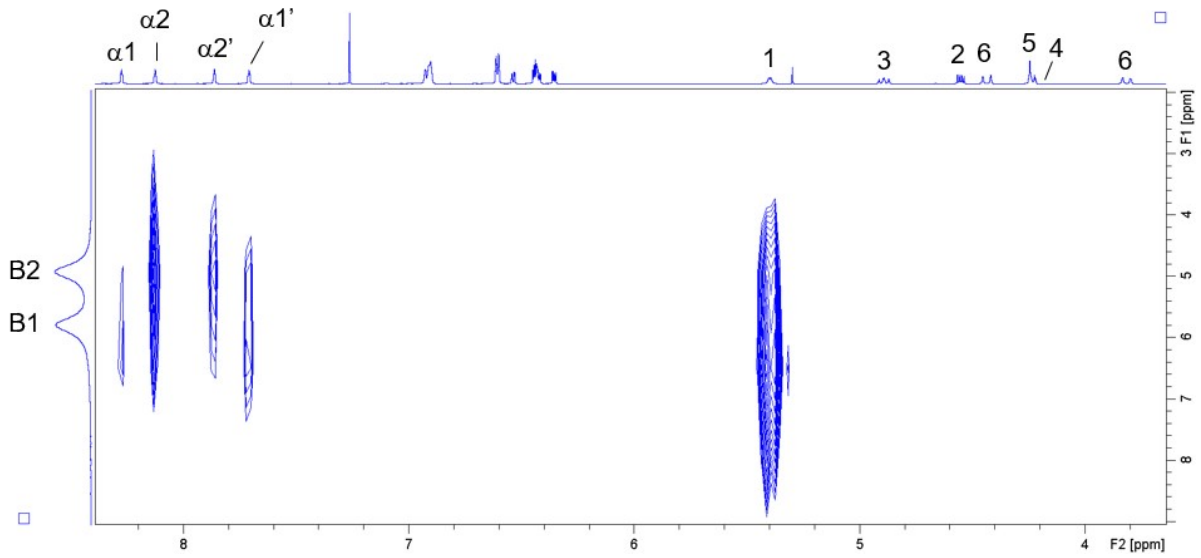
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Gc



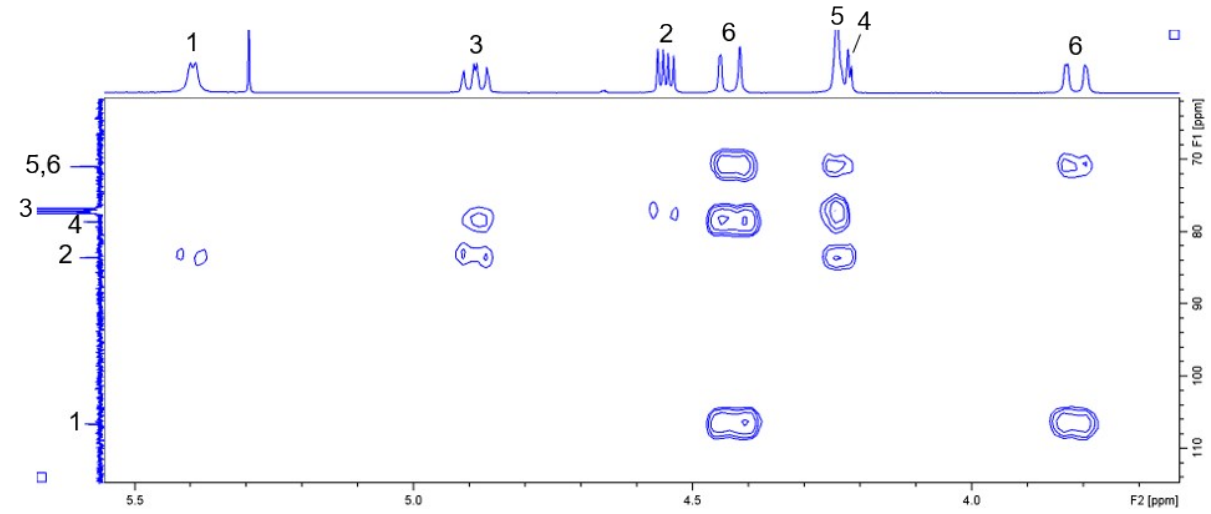
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Gc



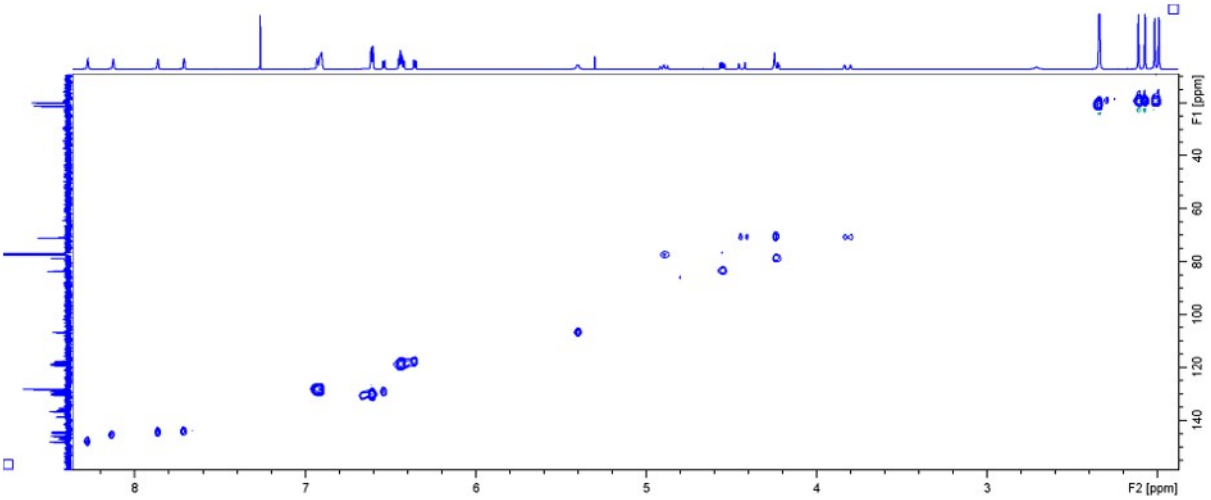
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 4Gc



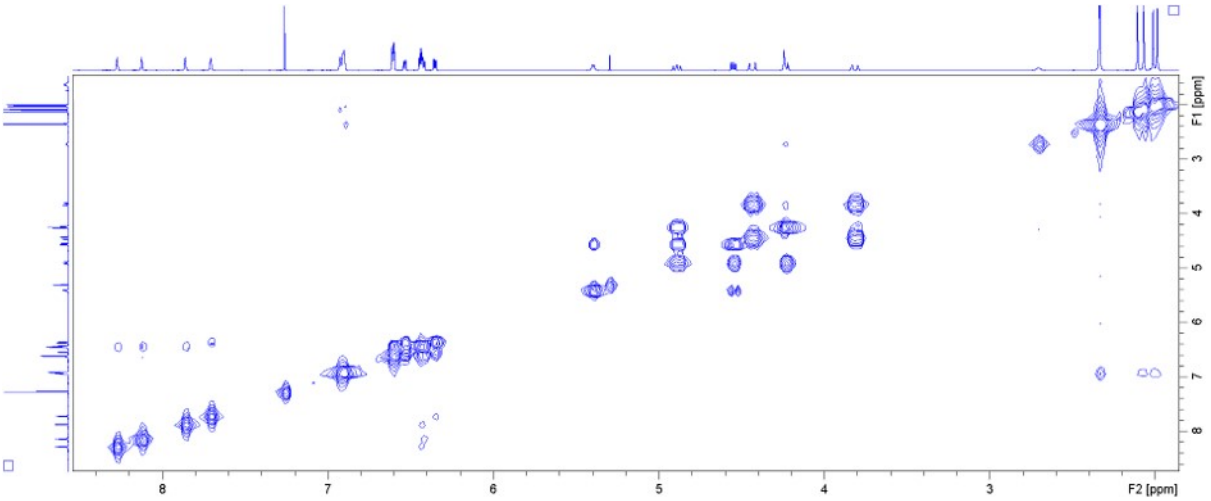
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Gc



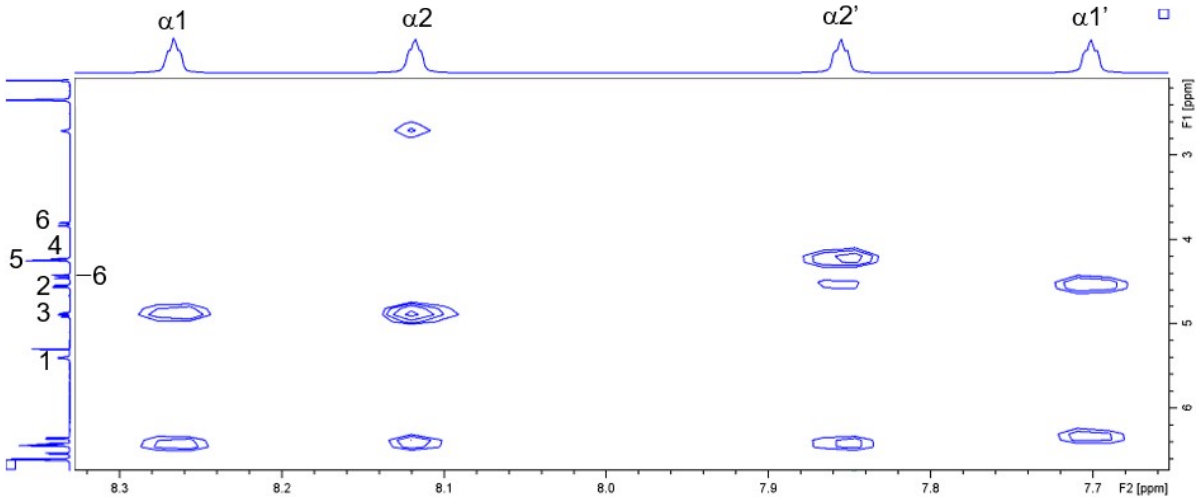
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Gc



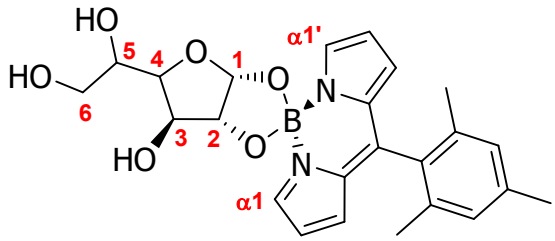
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Gc



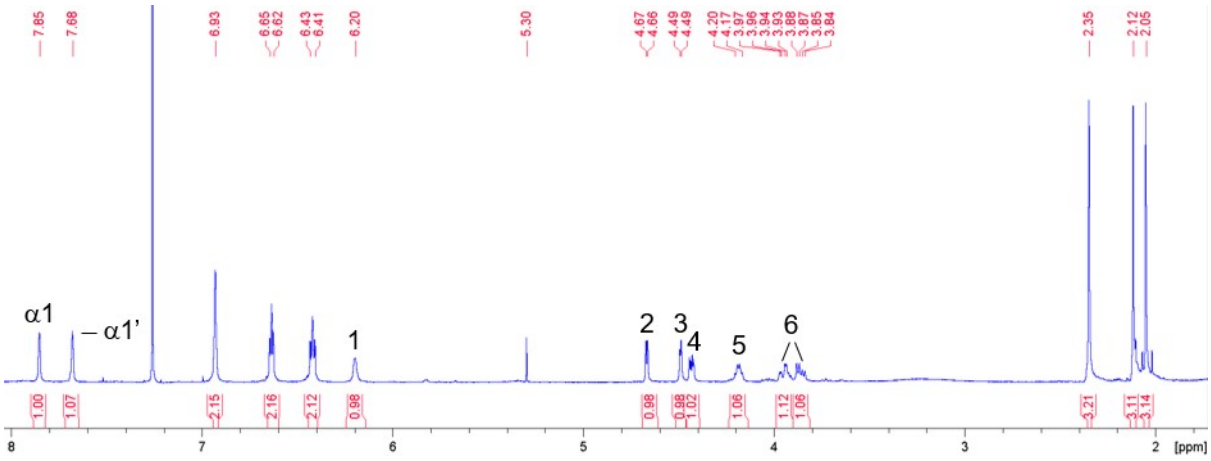
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Gc



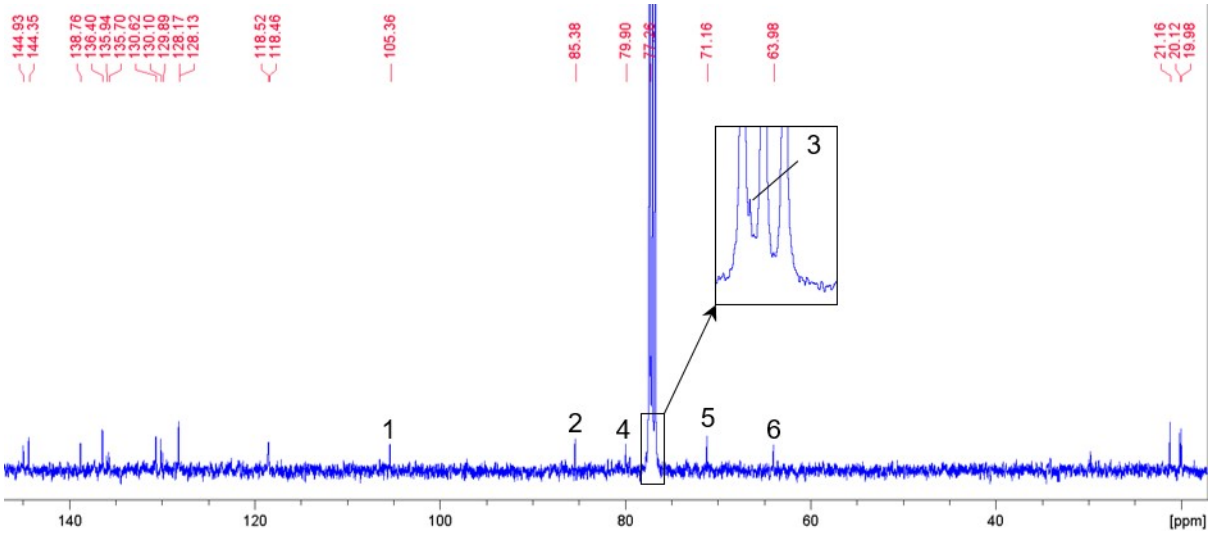
S5.7 Conjugate 4Gd: α-Glucofuranose-(1,2)-O-BODIPY



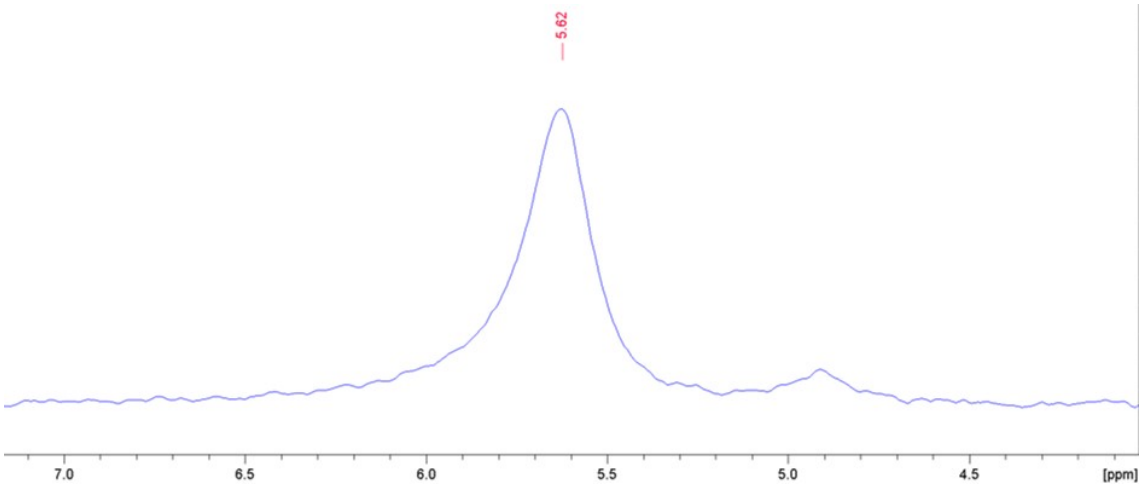
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Gd



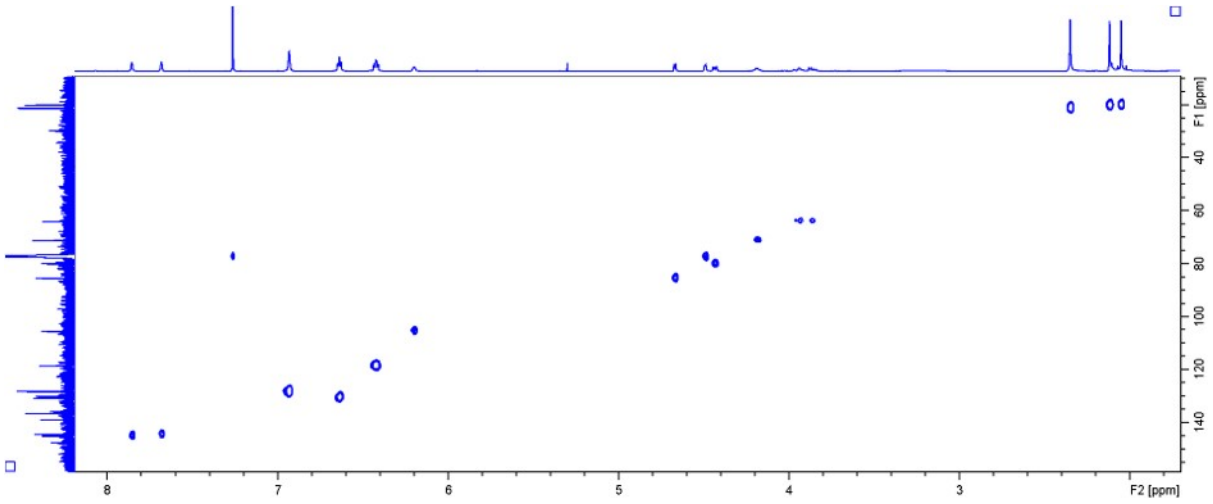
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Gd



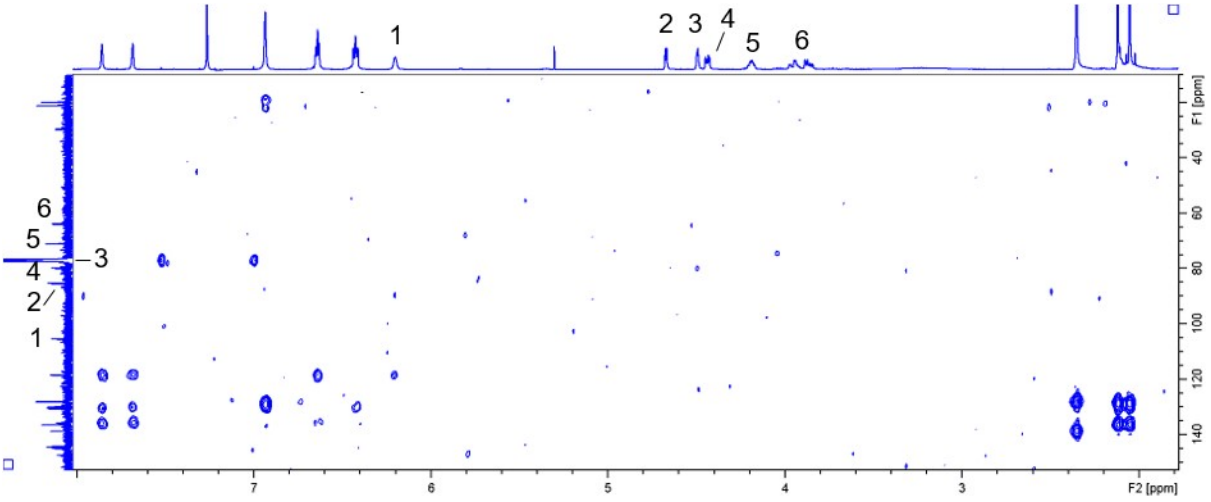
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Gd



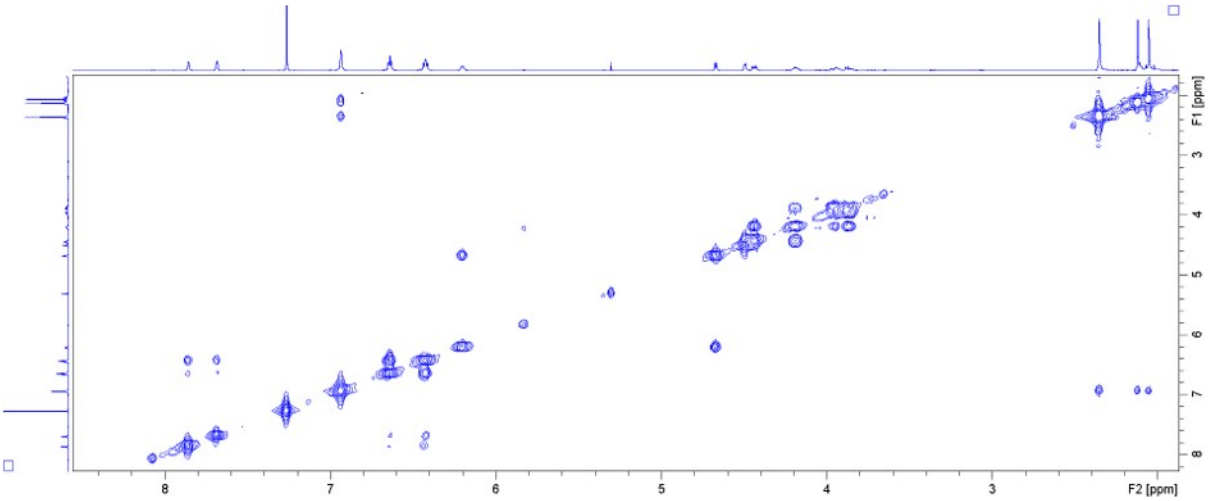
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Gd



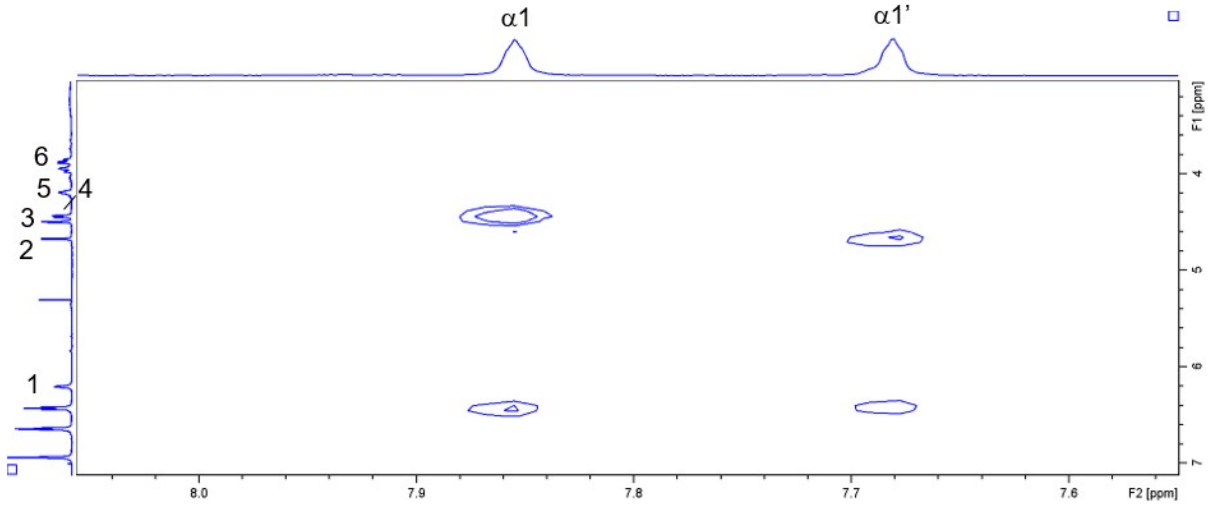
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Gd


1
2 3 4
5
6
6
5
4
2
1
3
7
6
5
4
3
F2 [ppm]
F1 [ppm]
40
60
80
100
120
140

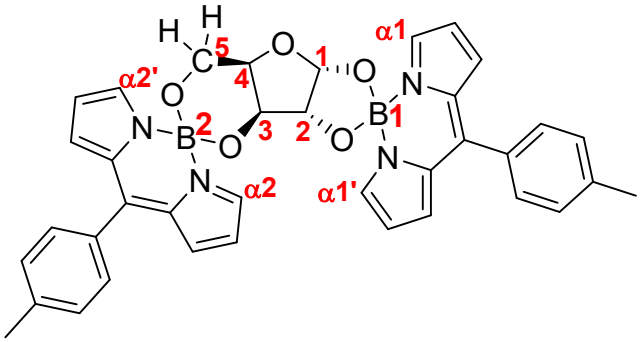
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Gd



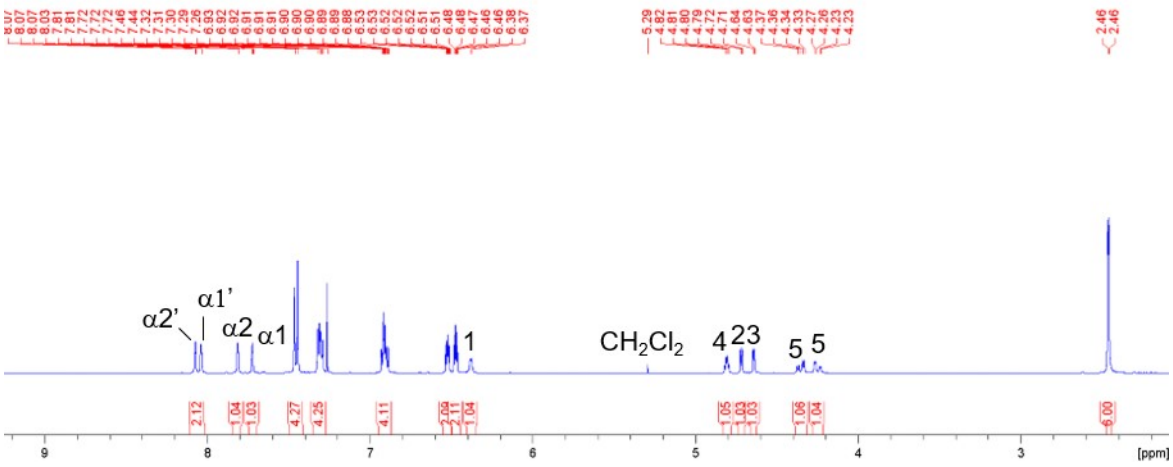
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Gd



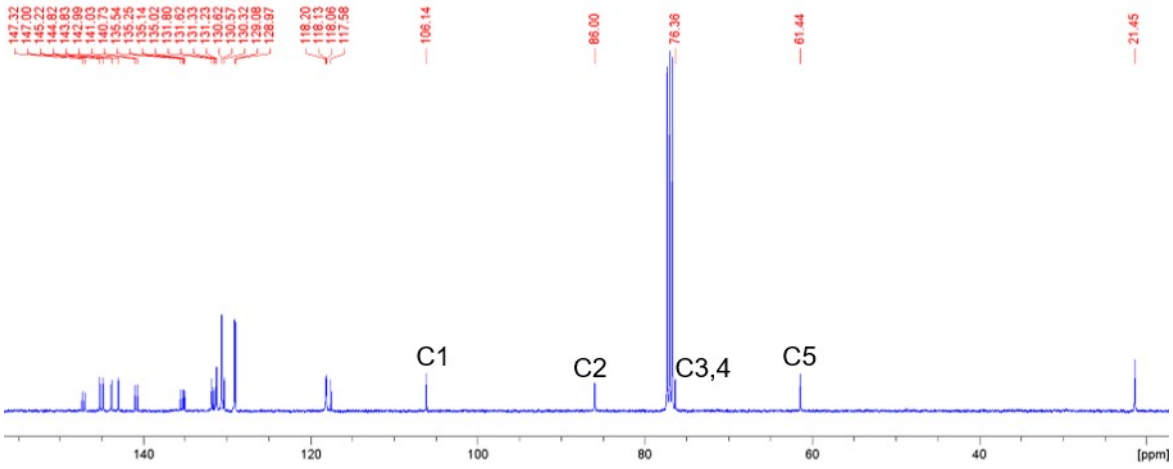
S5.8 Conjugate 3Xa: α-Xylofuranose-(1,2)(3,5)-O-BODIPY



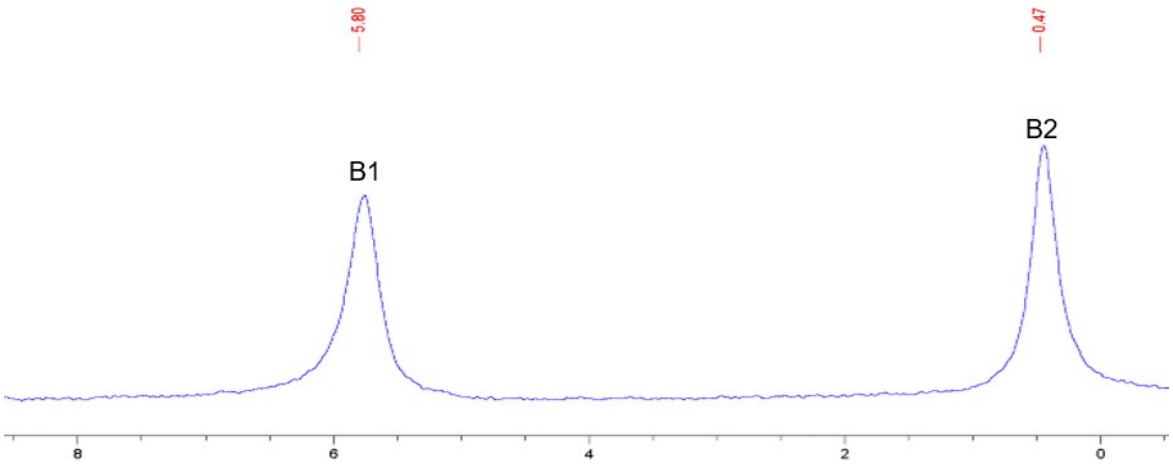
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Xa



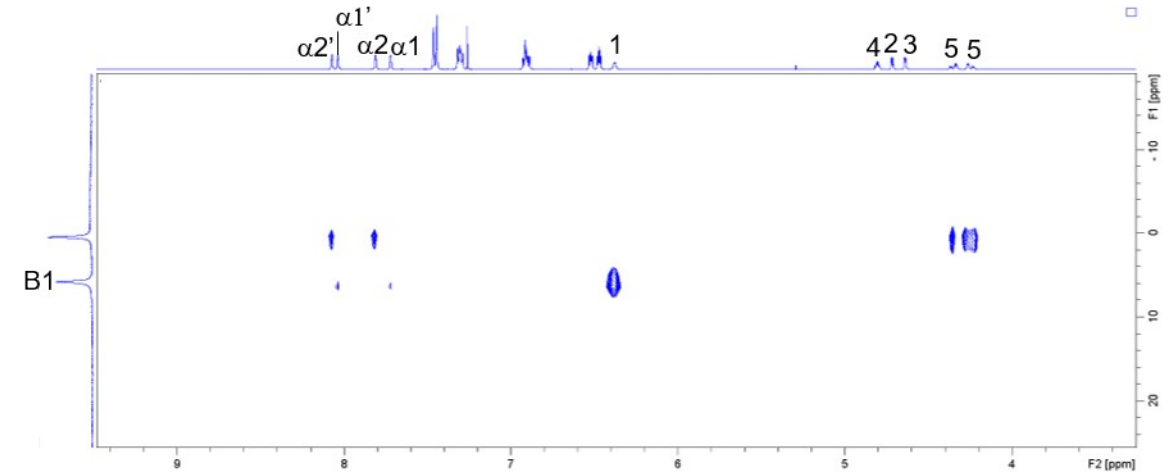
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Xa



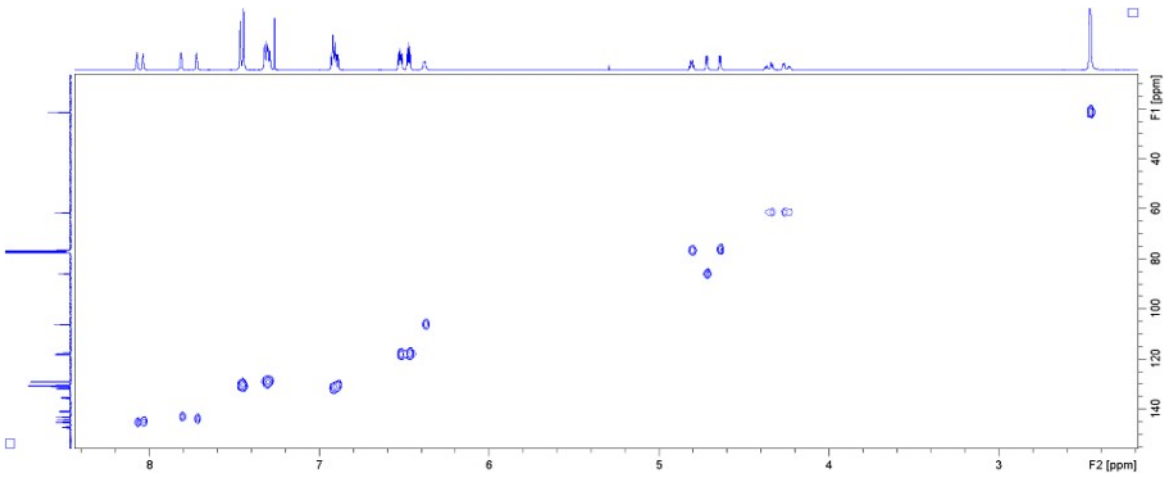
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Xa



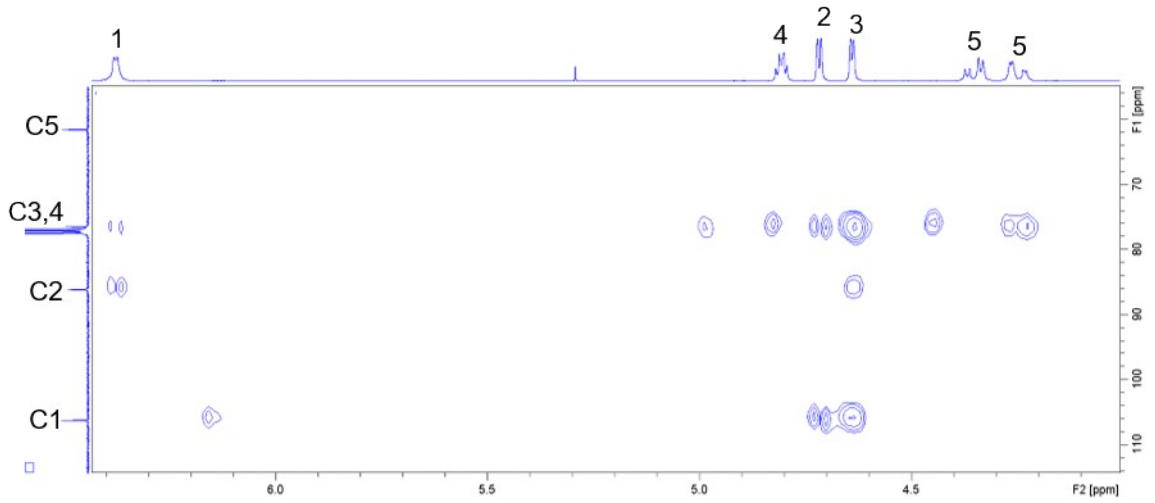
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Xa



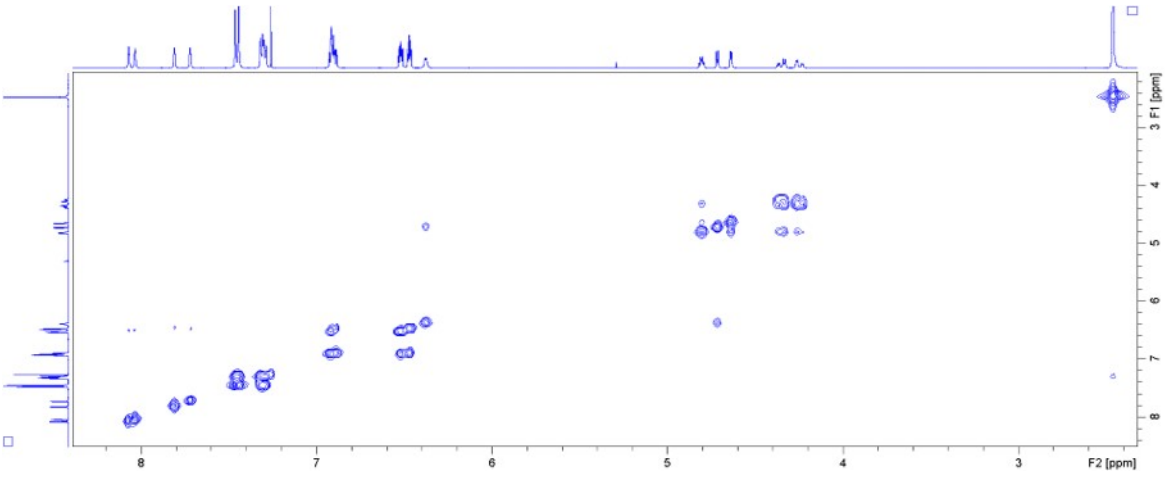
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Xa



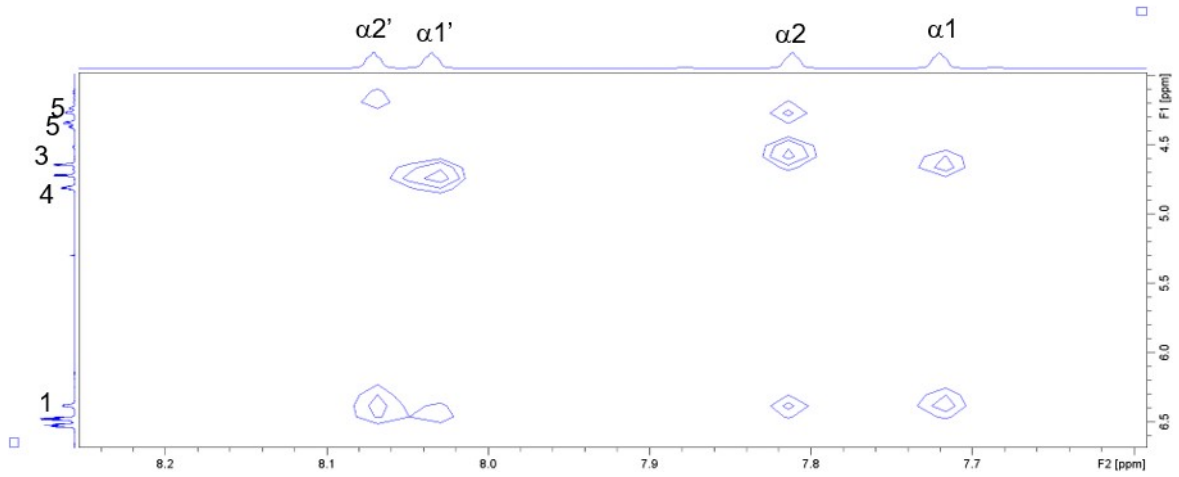
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Xa



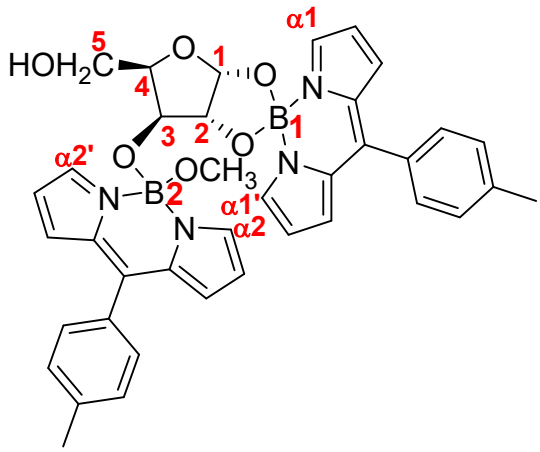
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Xa



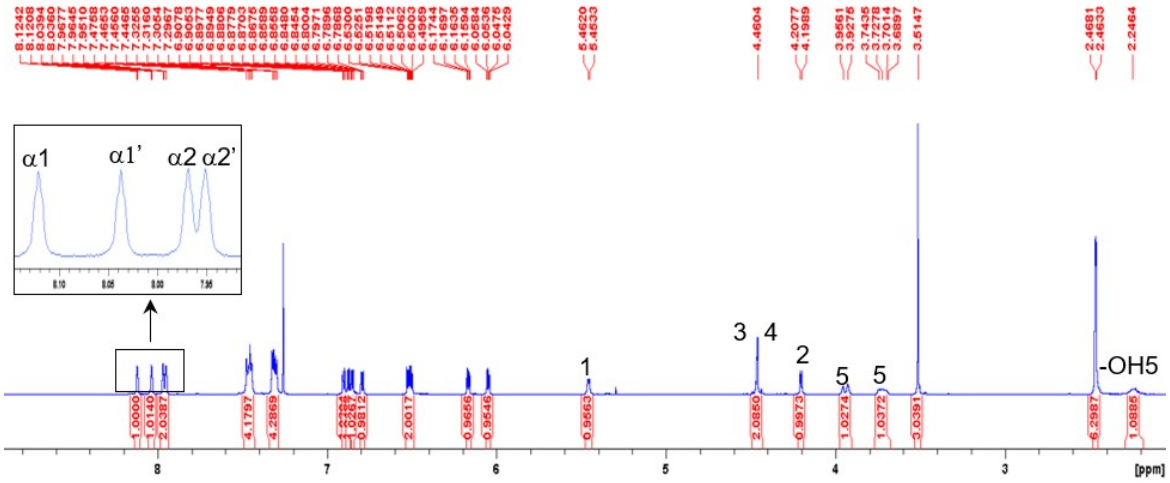
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Xa



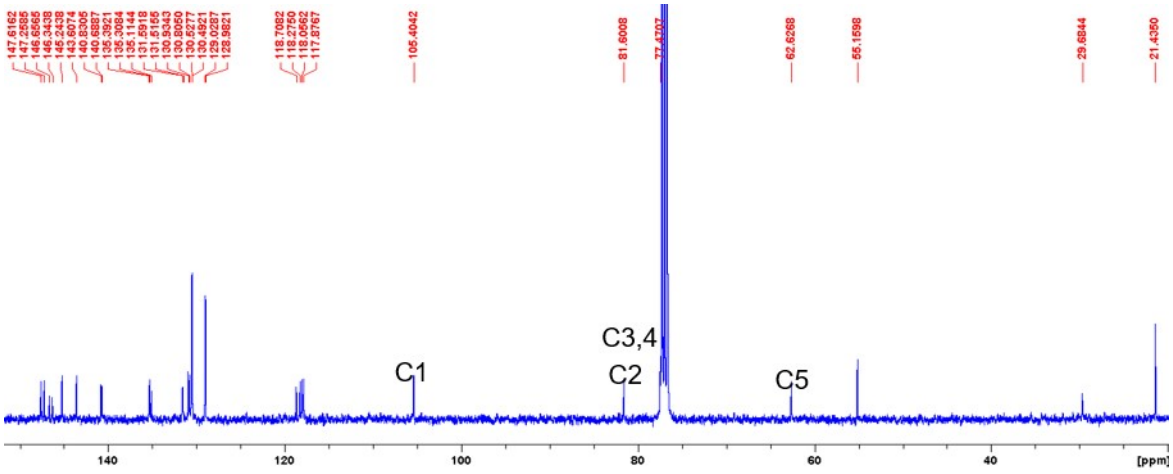
S5.9 Conjugate 3Xb: α-Xylofuranose-(1,2)(3)(4)-O-BODIPY(OMe)



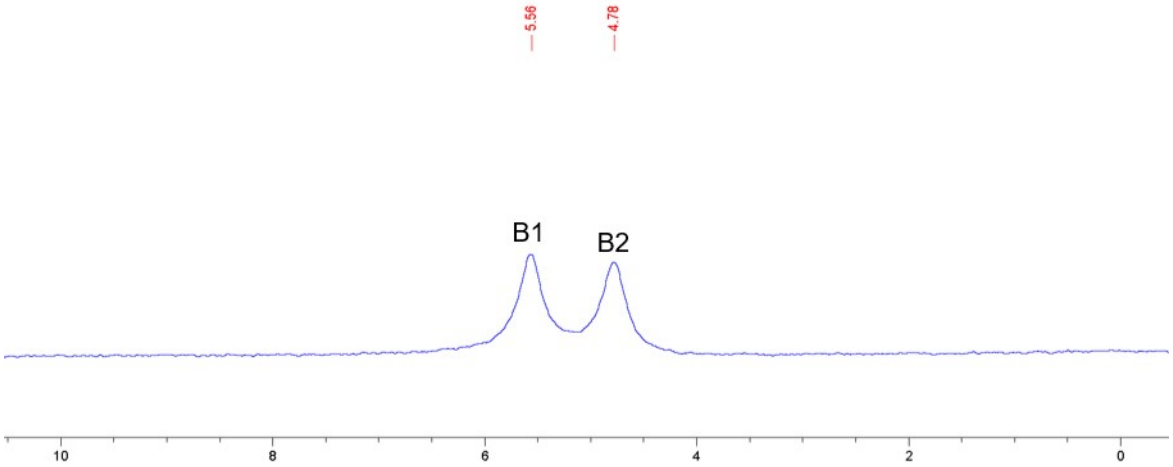
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Xb



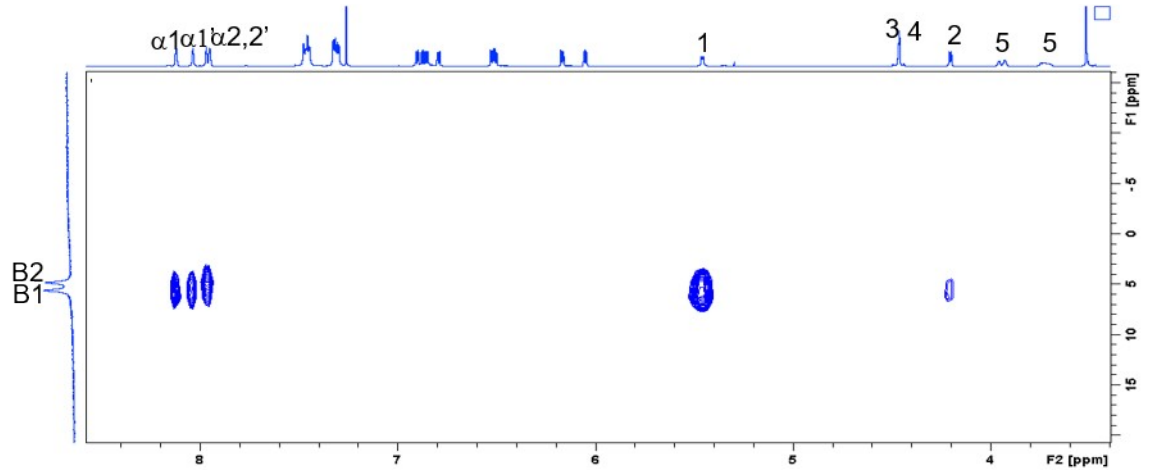
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Xb



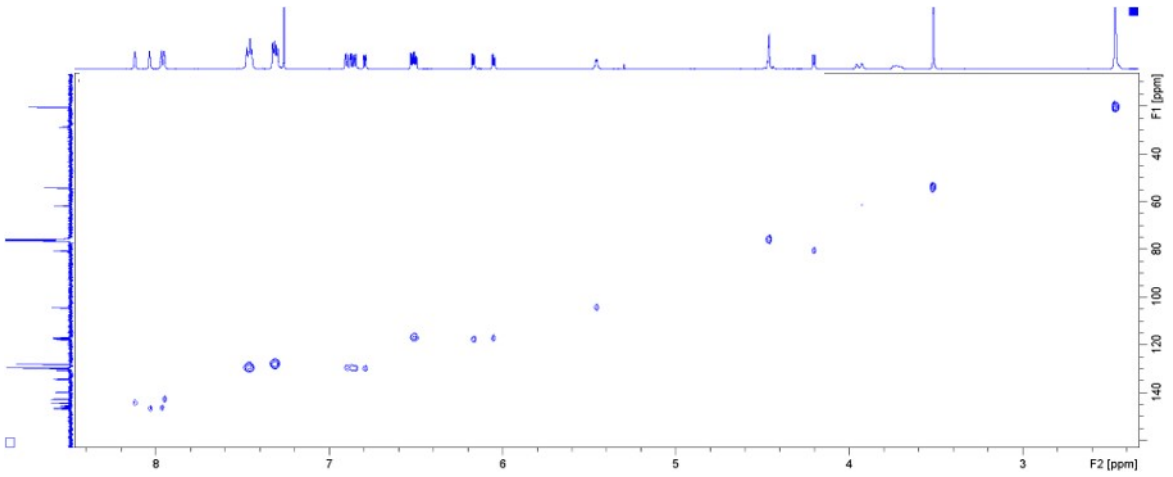
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Xb



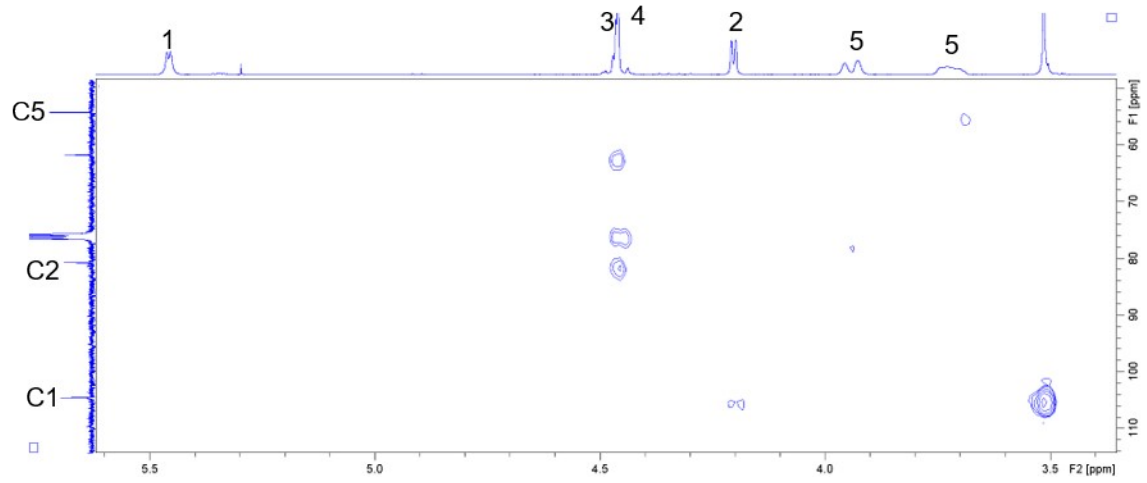
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Xb



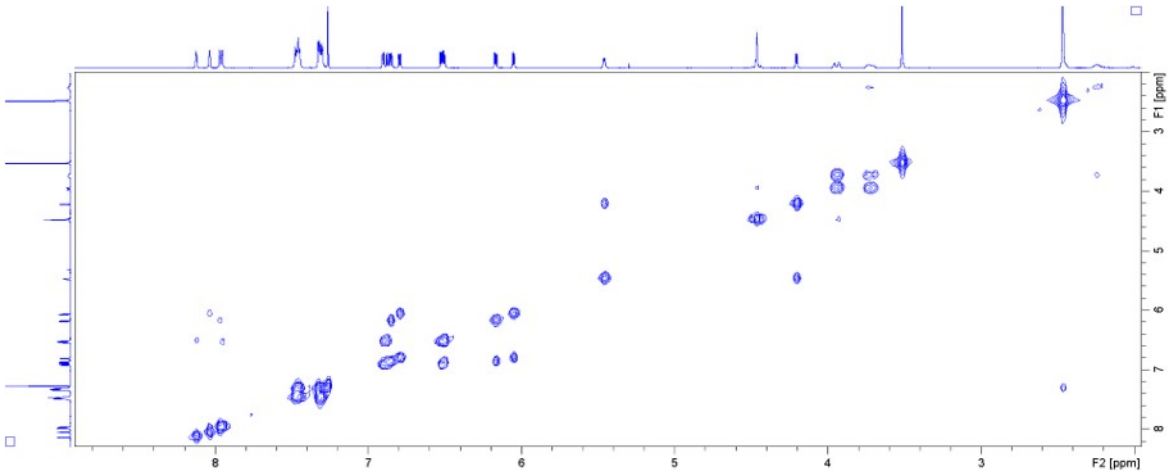
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Xb



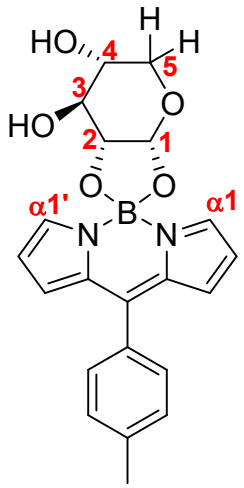
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Xb



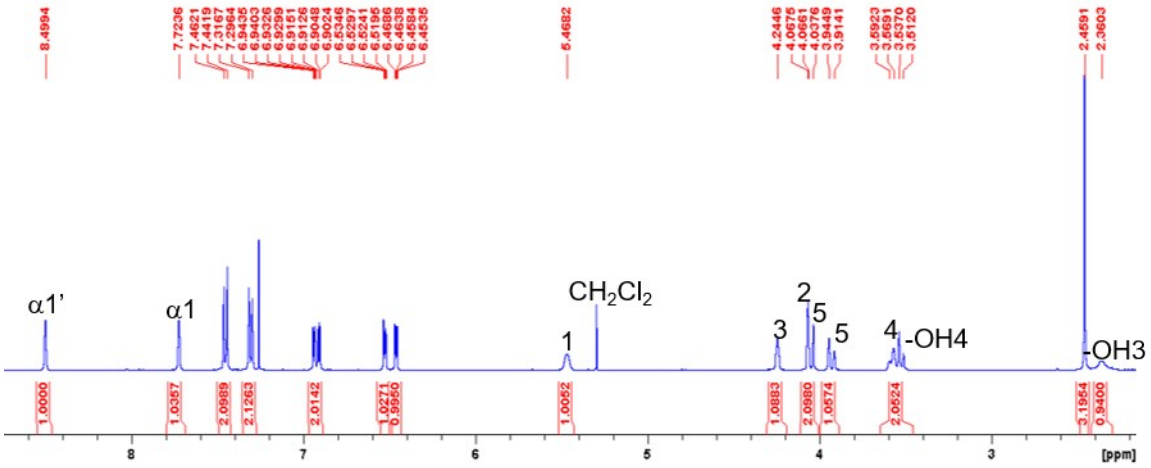
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Xb



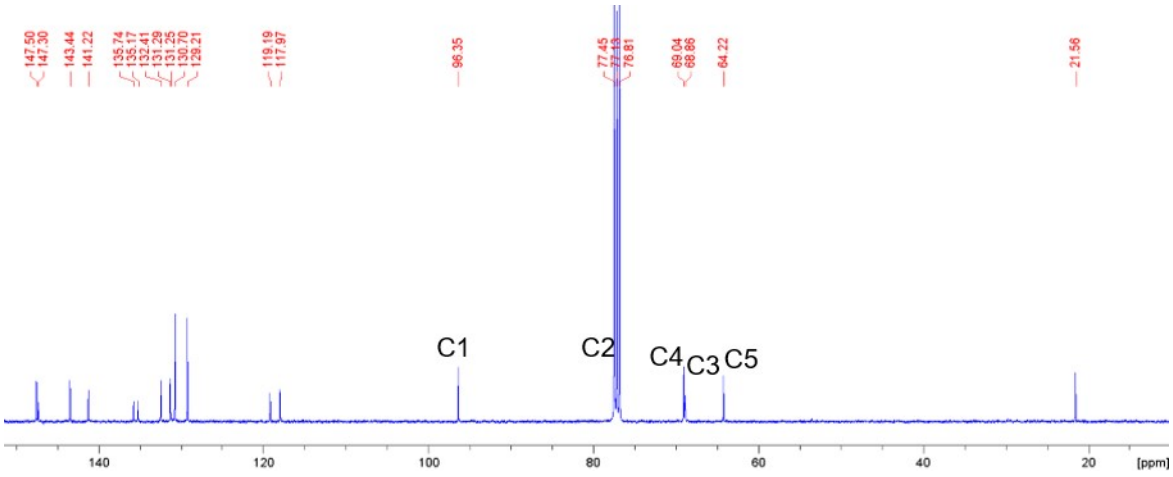
S5.10 Conjugate 3Xc: α-Xylopyranose-(1,2)-O-BODIPY



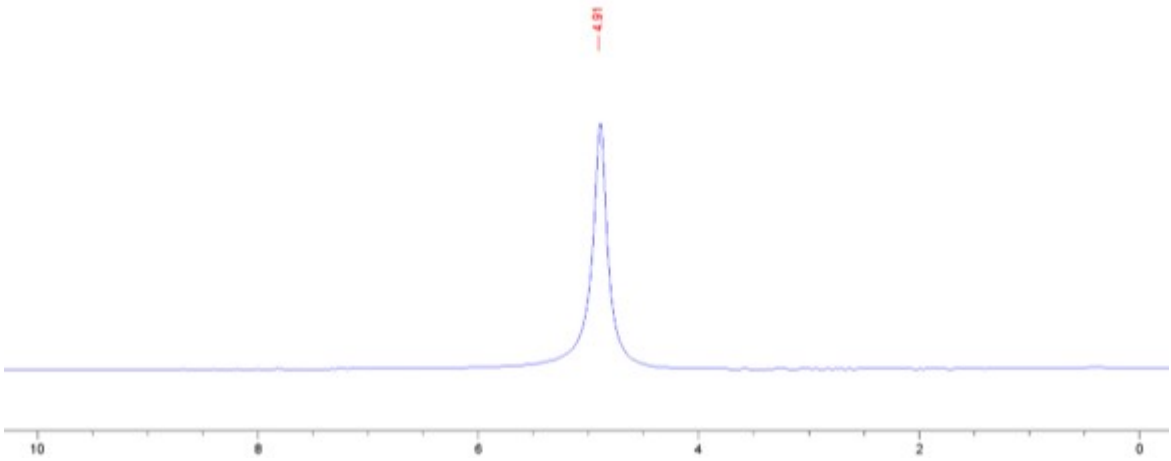
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Xc



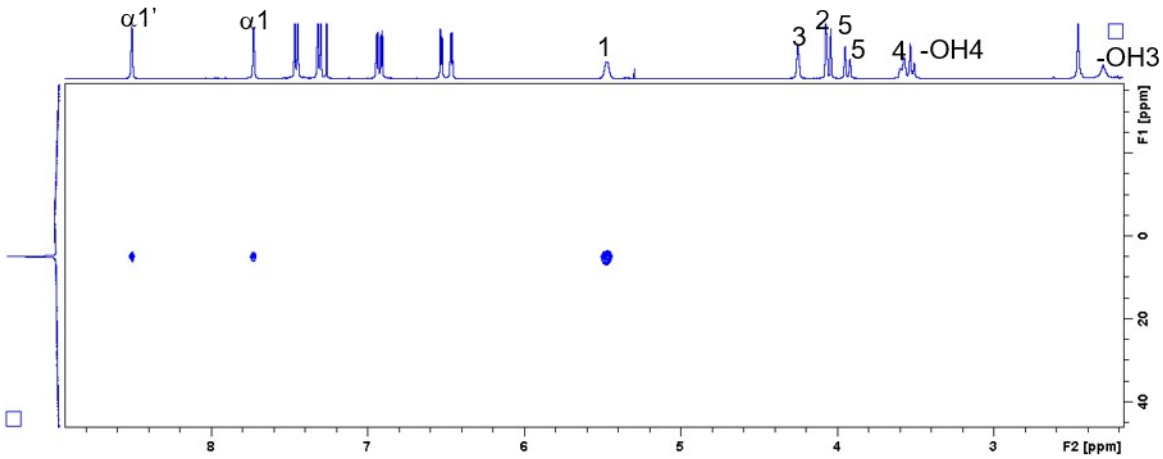
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Xc



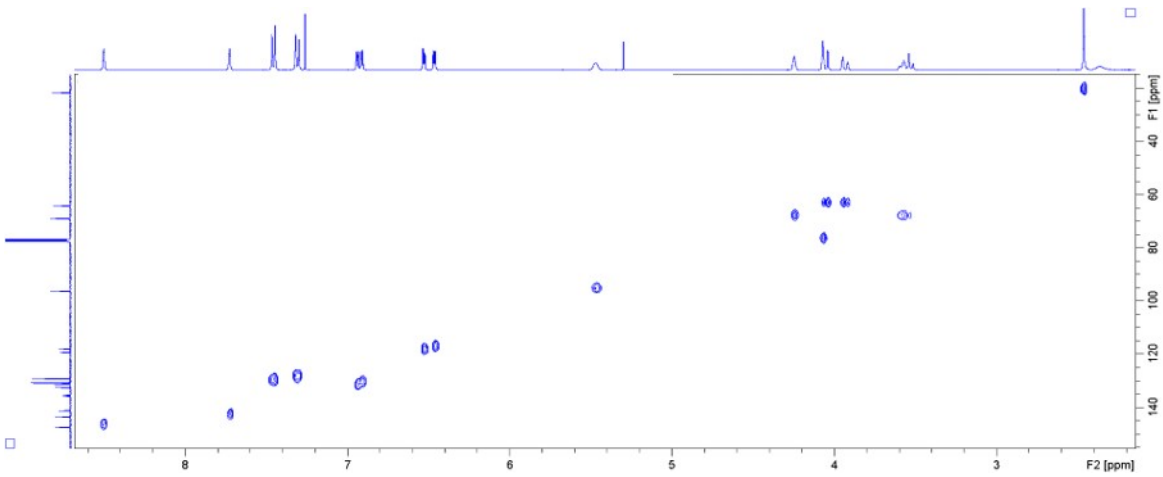
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Xc



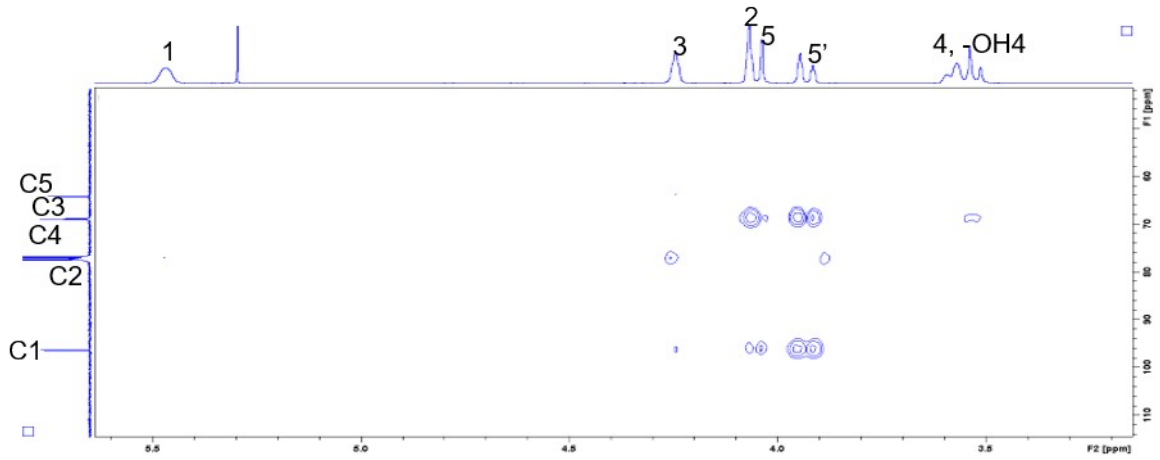
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Xc



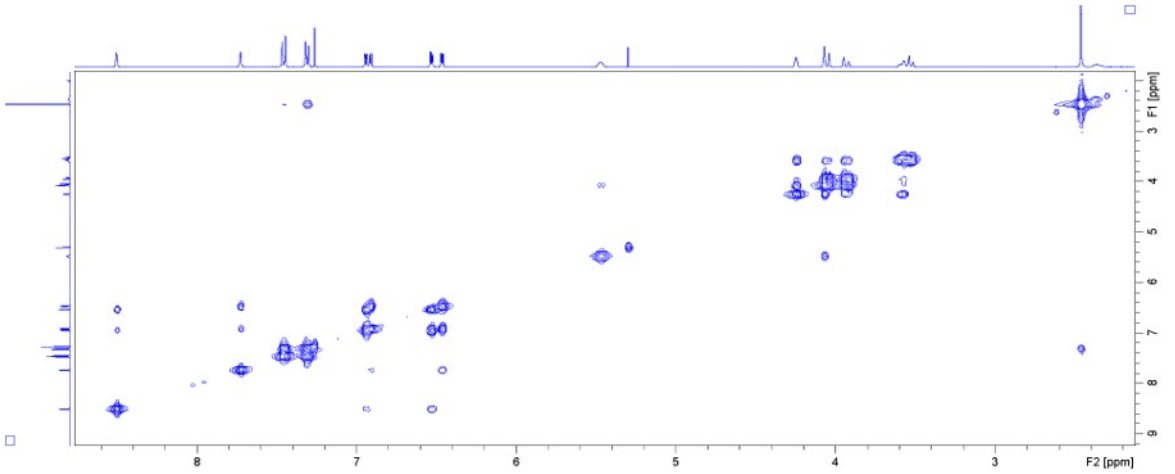
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Xc



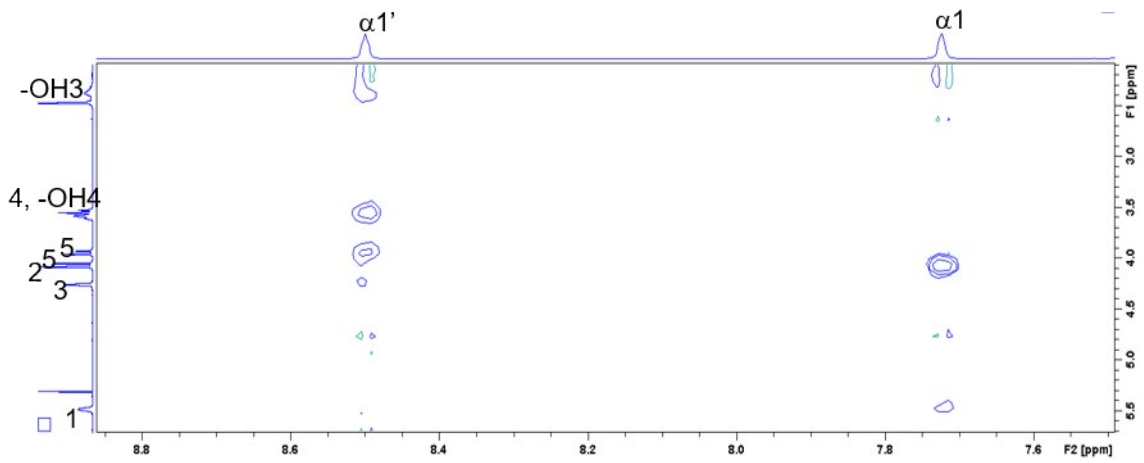
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Xc



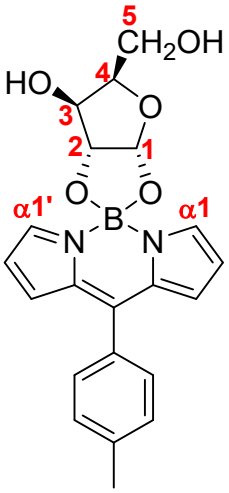
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Xc



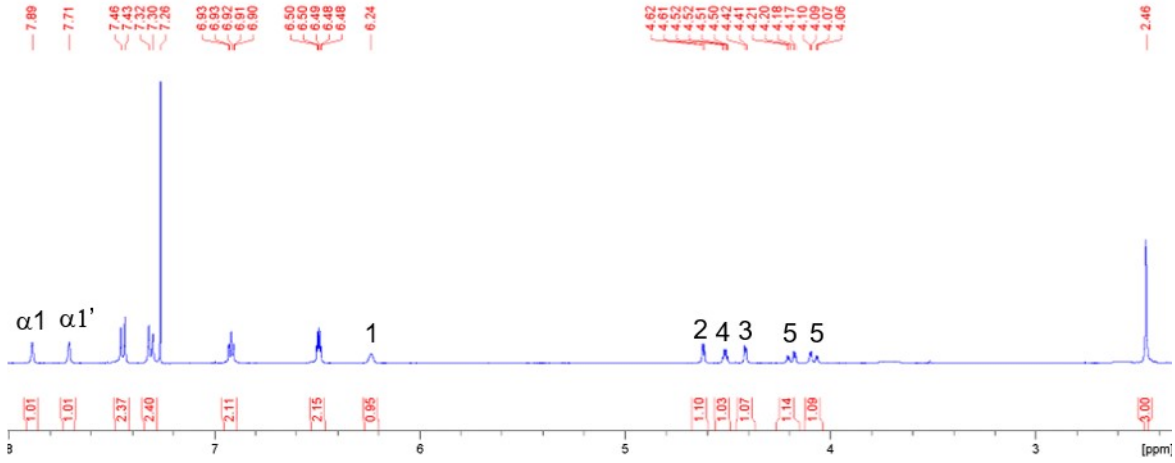
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Xc



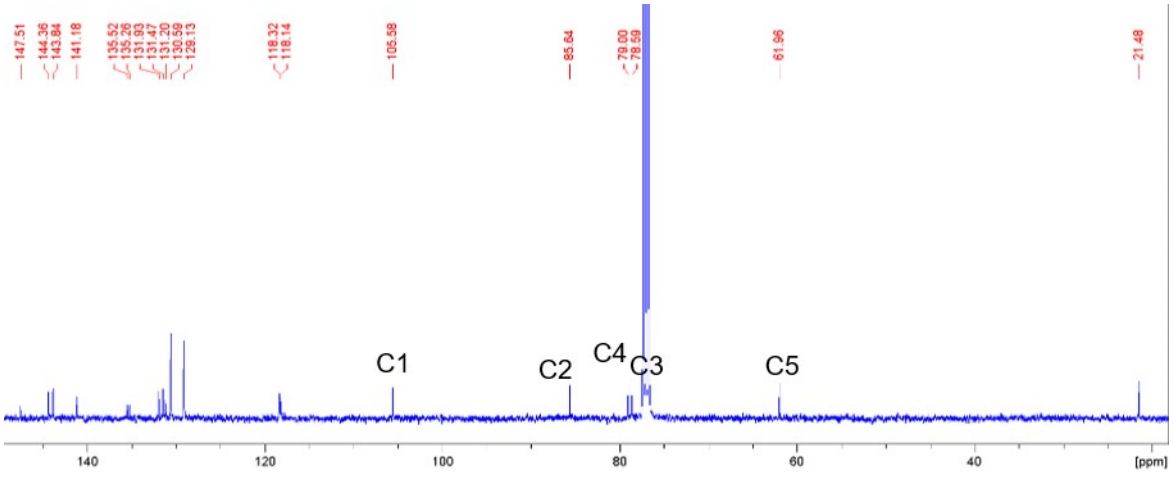
S5.11 Conjugate 3Xd: α-Xylofuranose-(1,2)-O-BODIPY



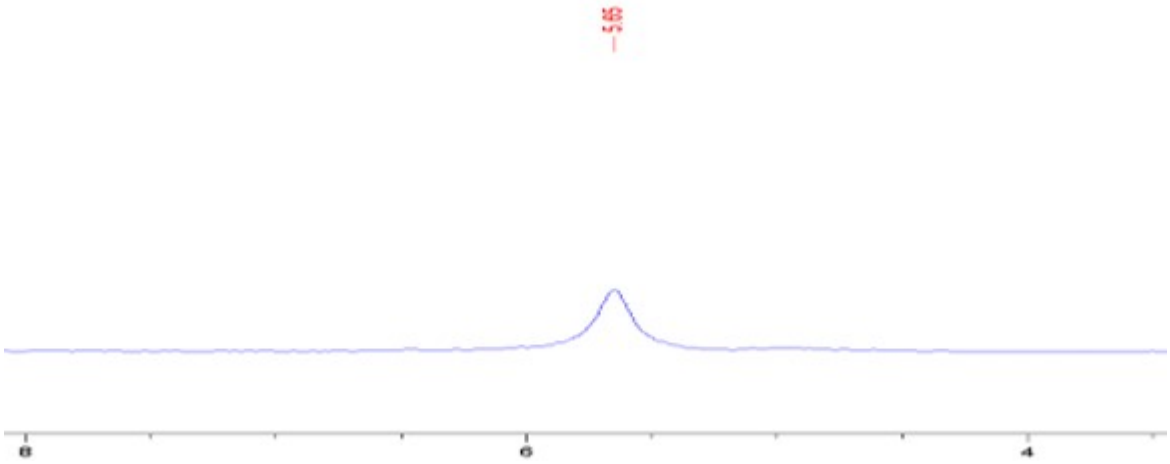
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Xd



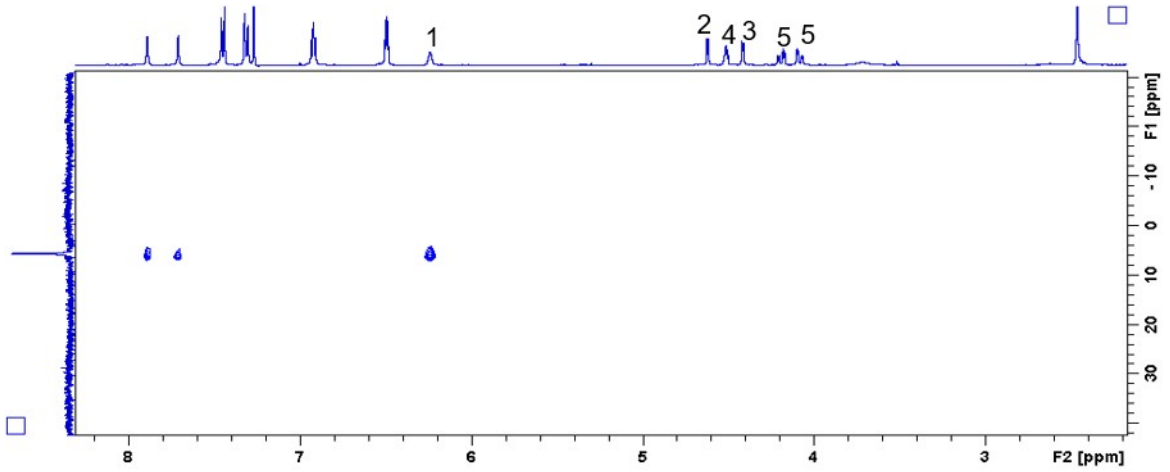
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Xd



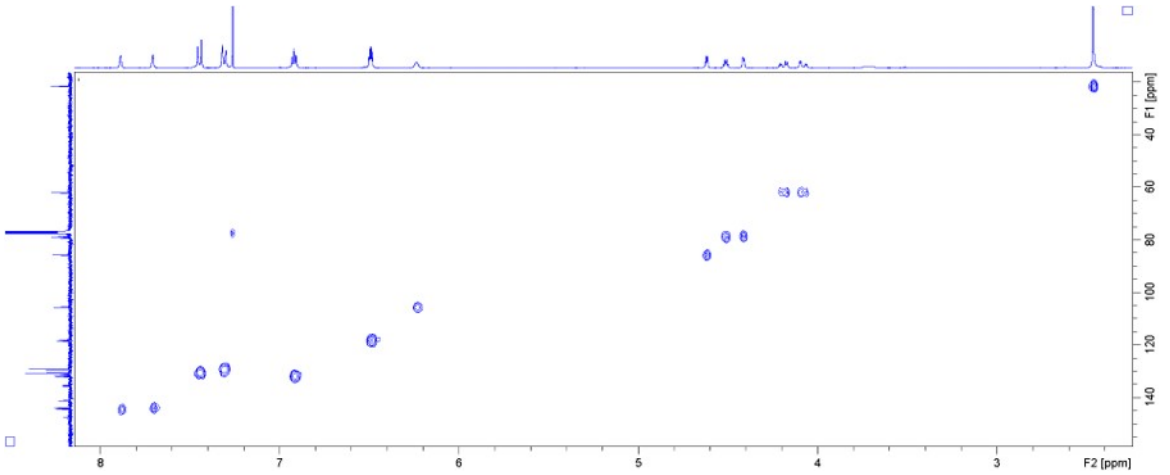
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Xd



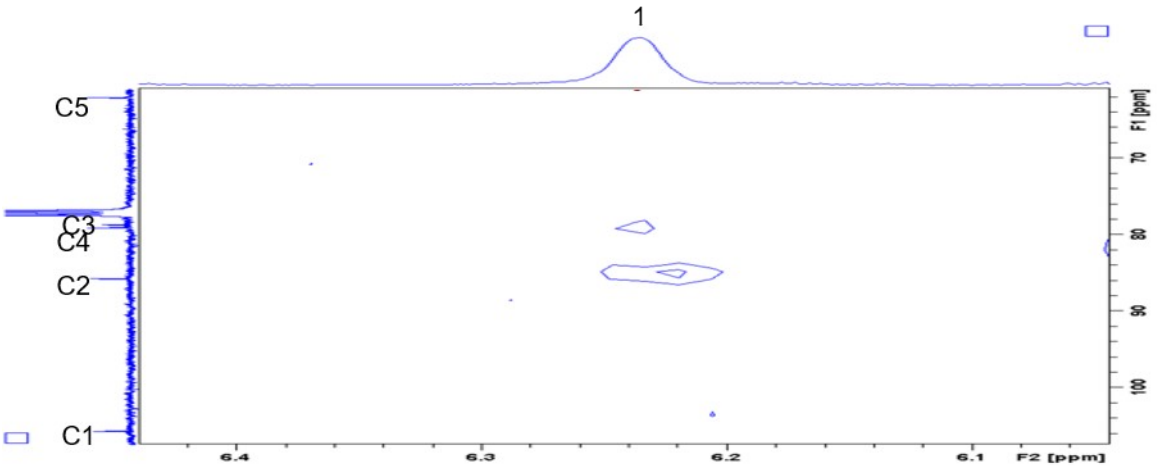
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Xd



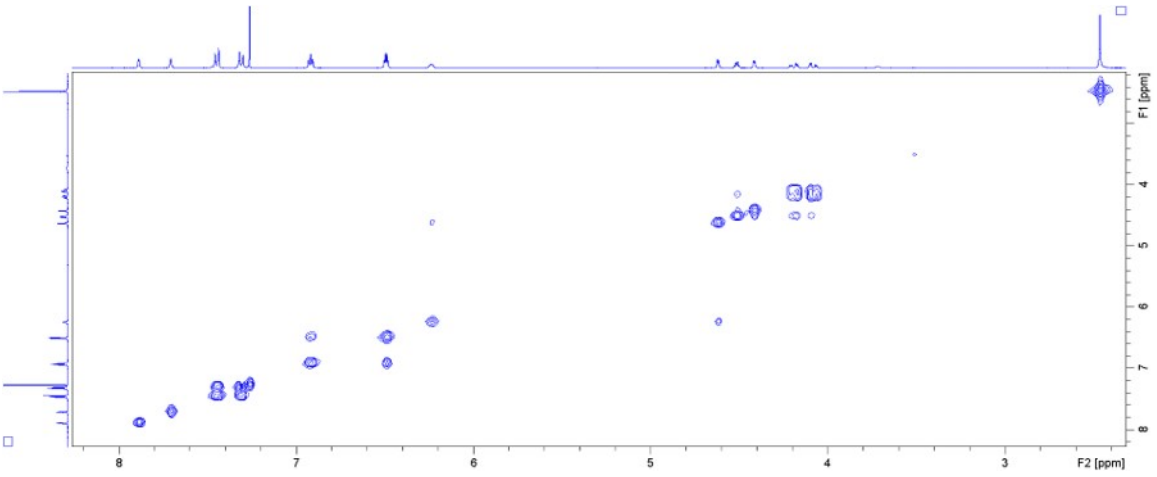
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Xd



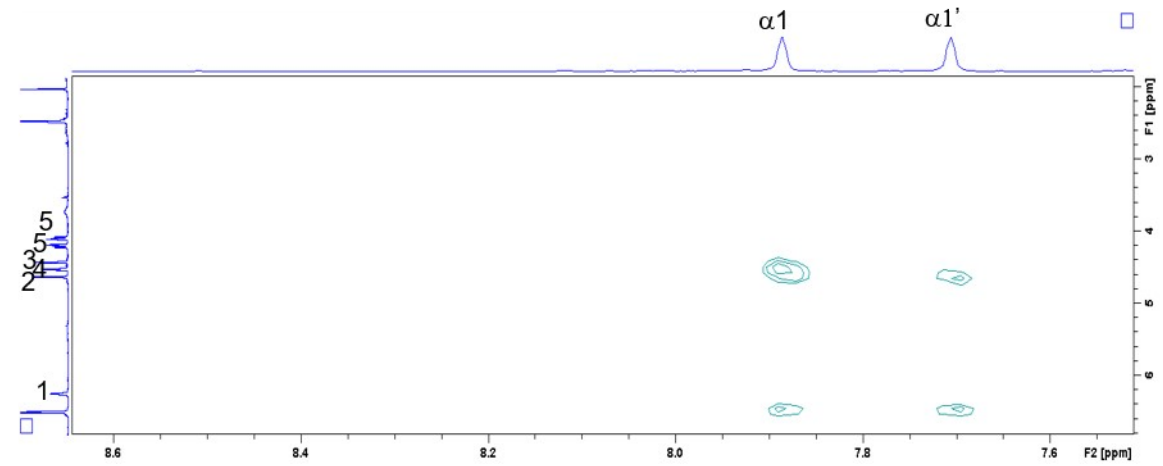
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Xd



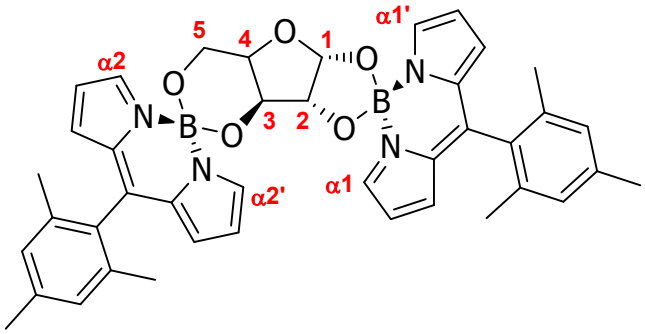
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Xd



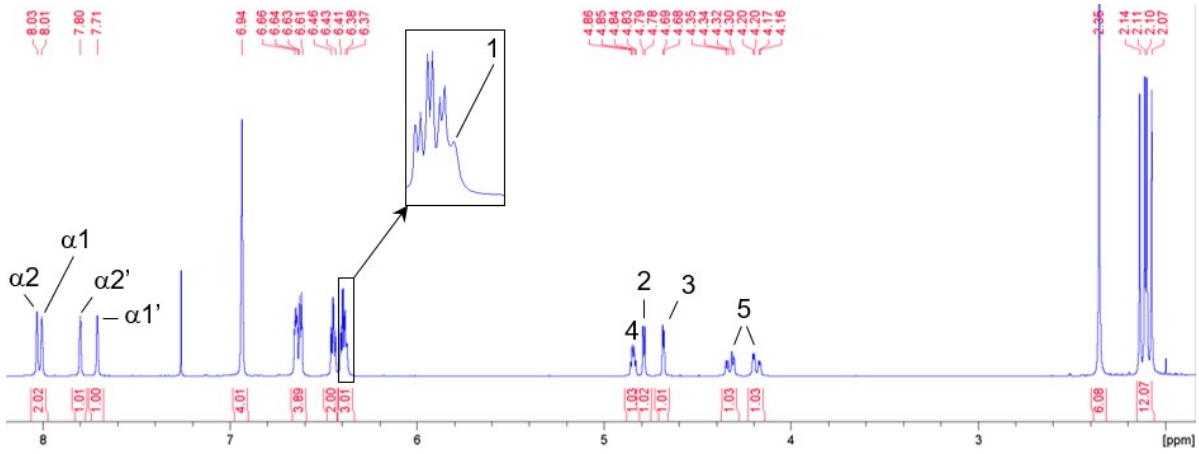
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Xd



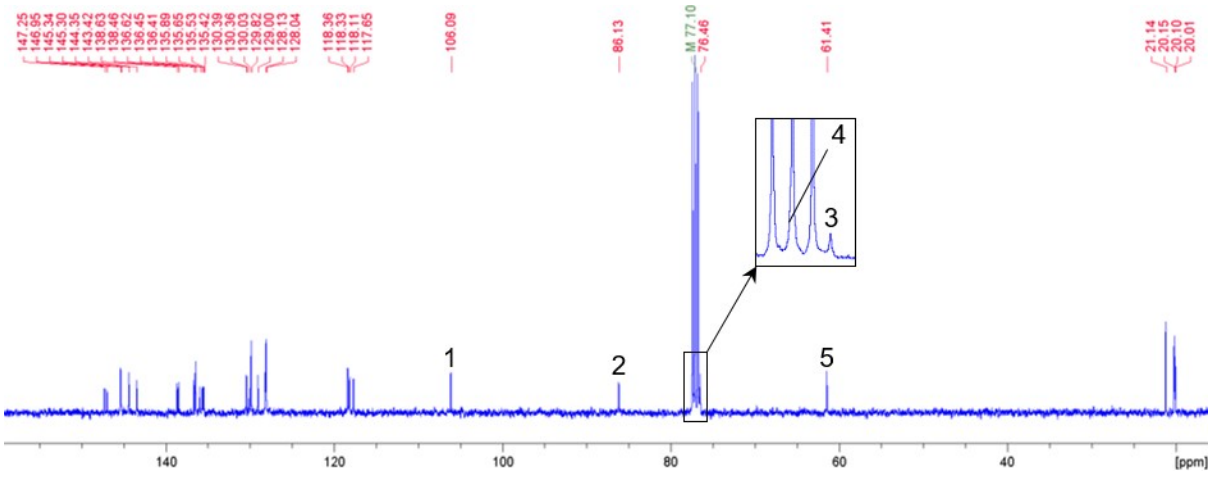
S5.12 Conjugate 4Xa: α-Xylofuranose-(1,2)(3,5)-O-BODIPY



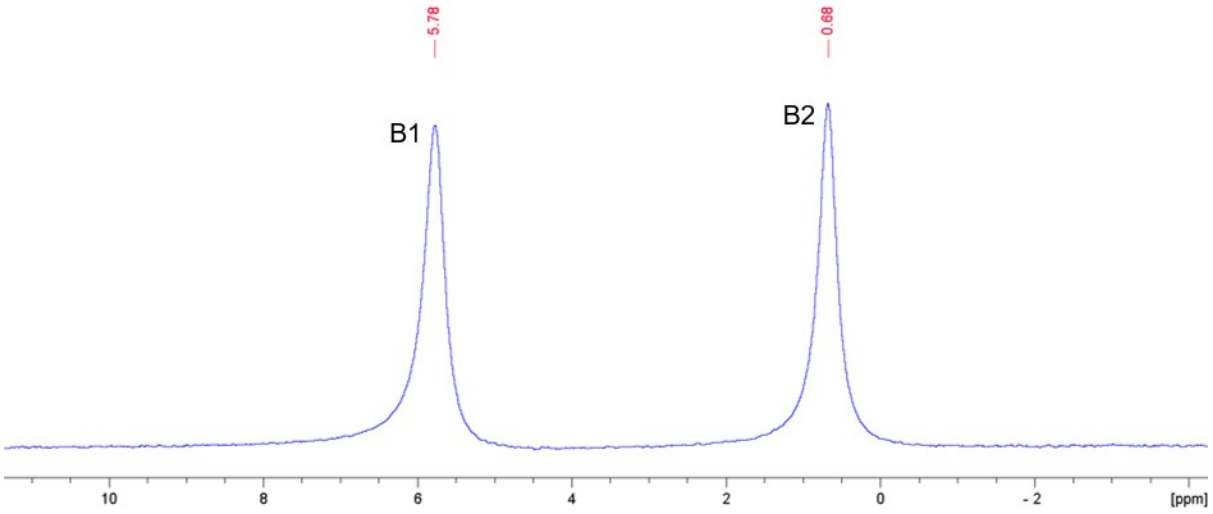
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Xa



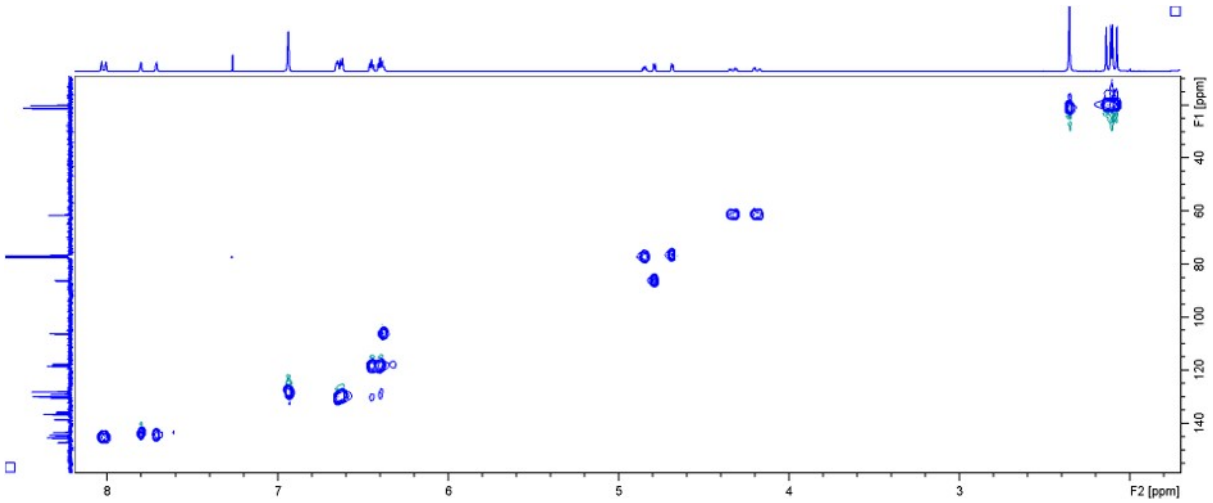
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Xa



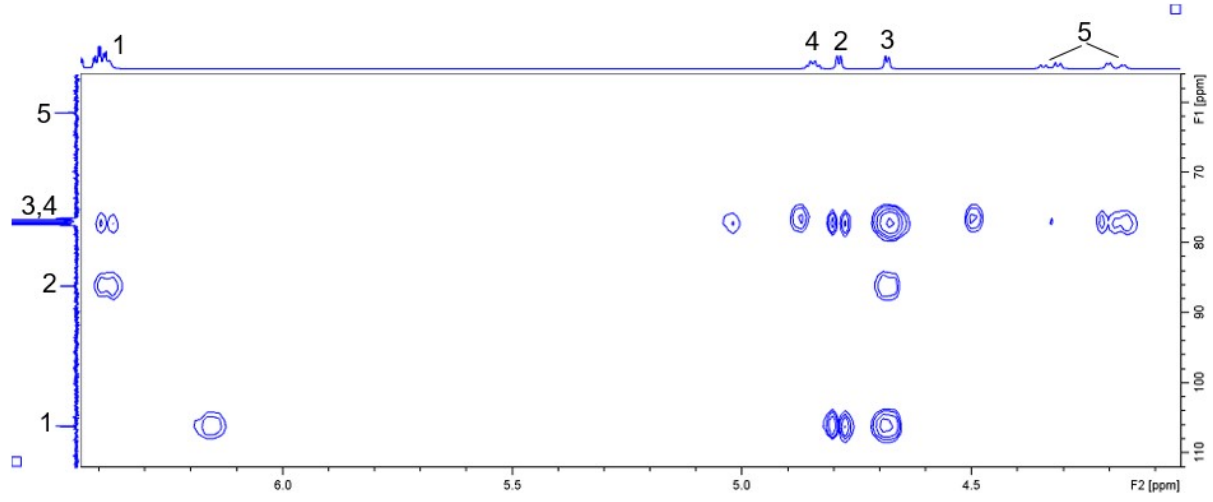
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Xa



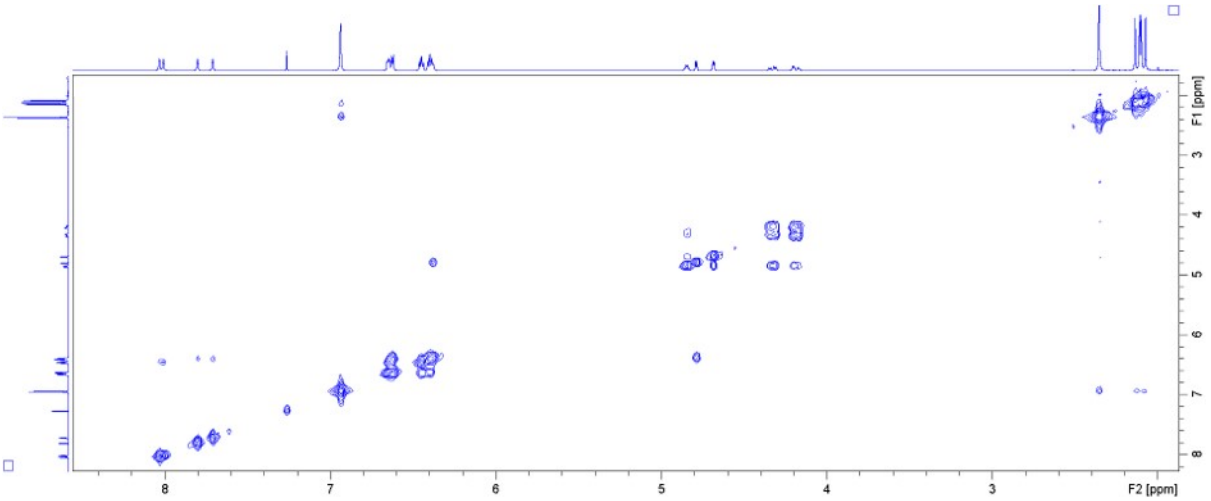
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Xa



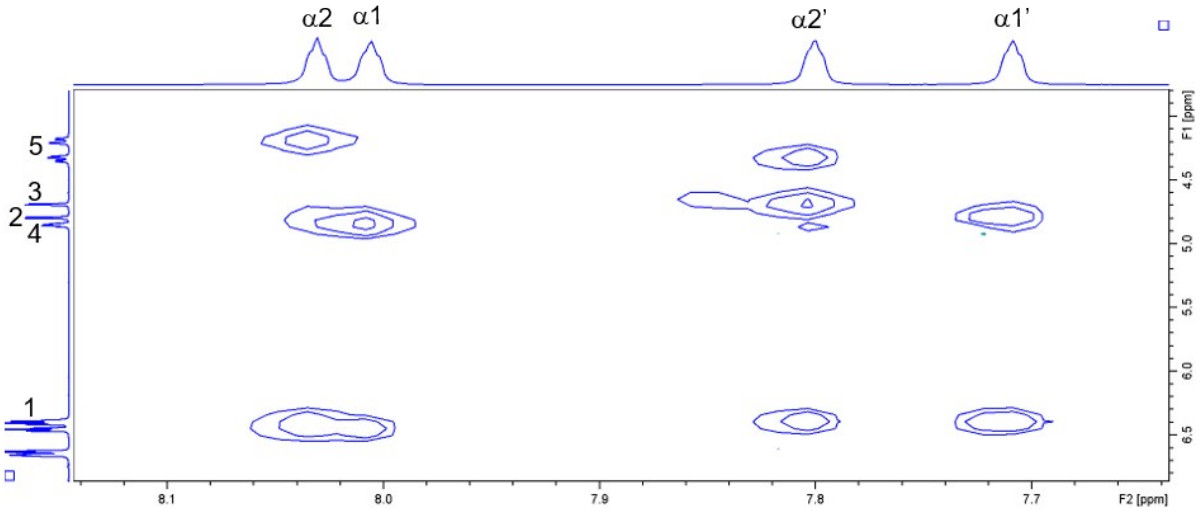
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Xa



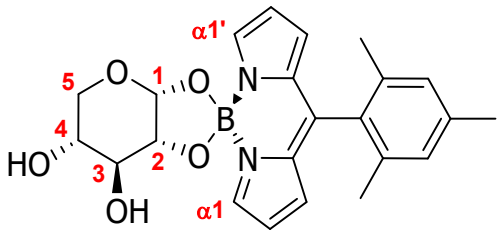
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Xa



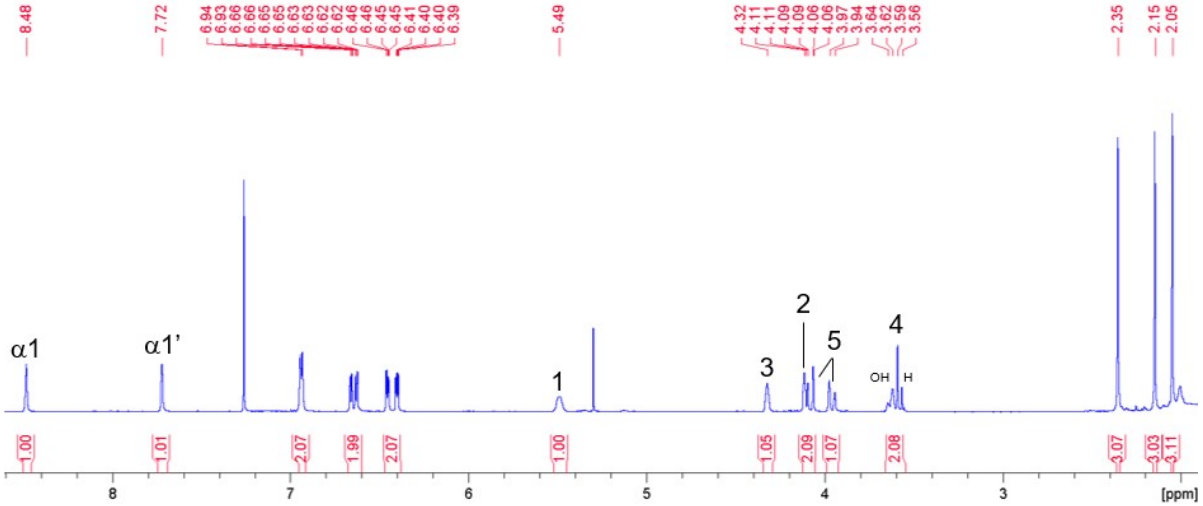
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Xa



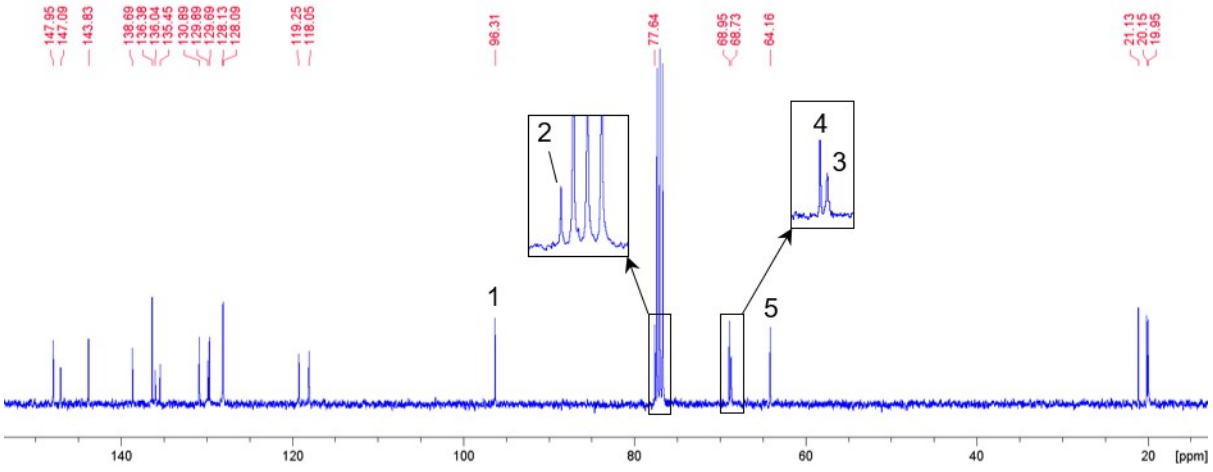
S5.13 Conjugate 4Xb: α-Xylopyranose-(1,2)-O-BODIPY



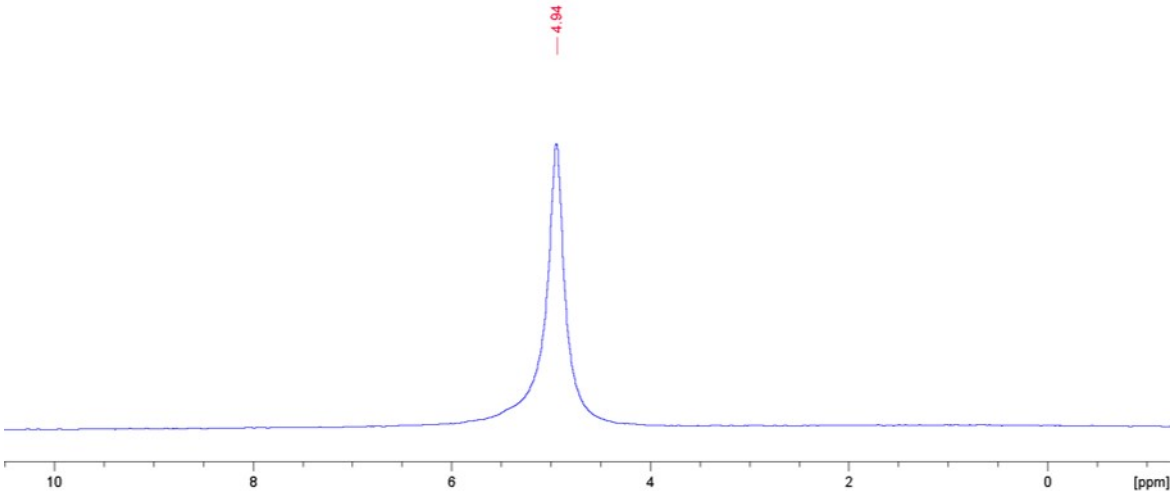
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Xb



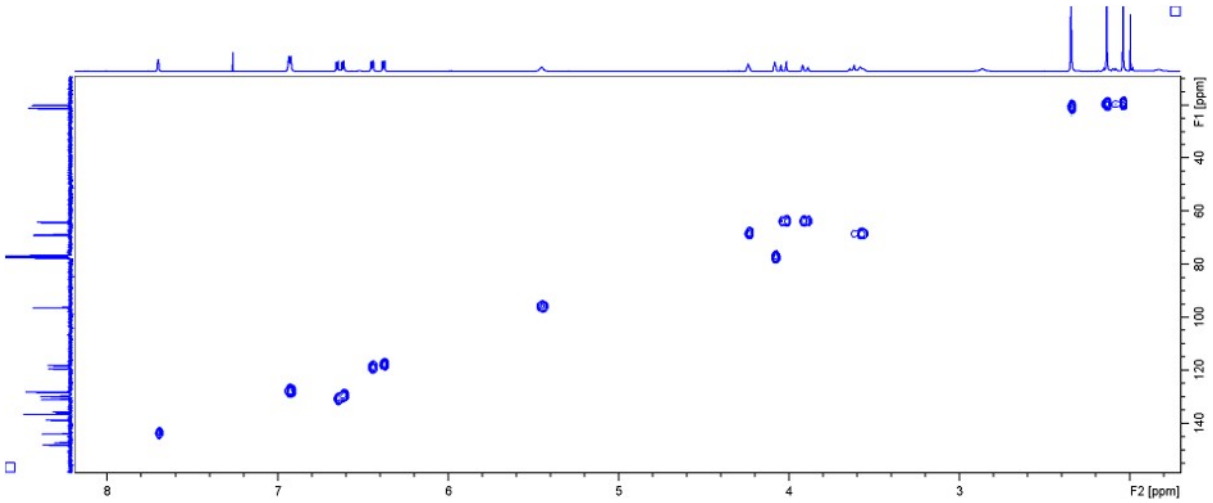
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Xb



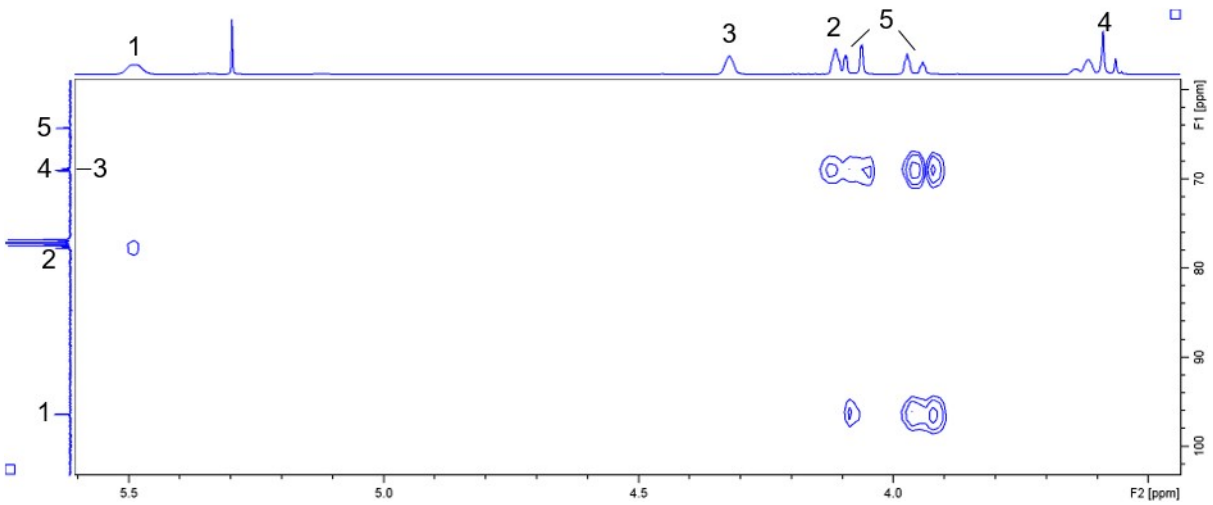
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Xb



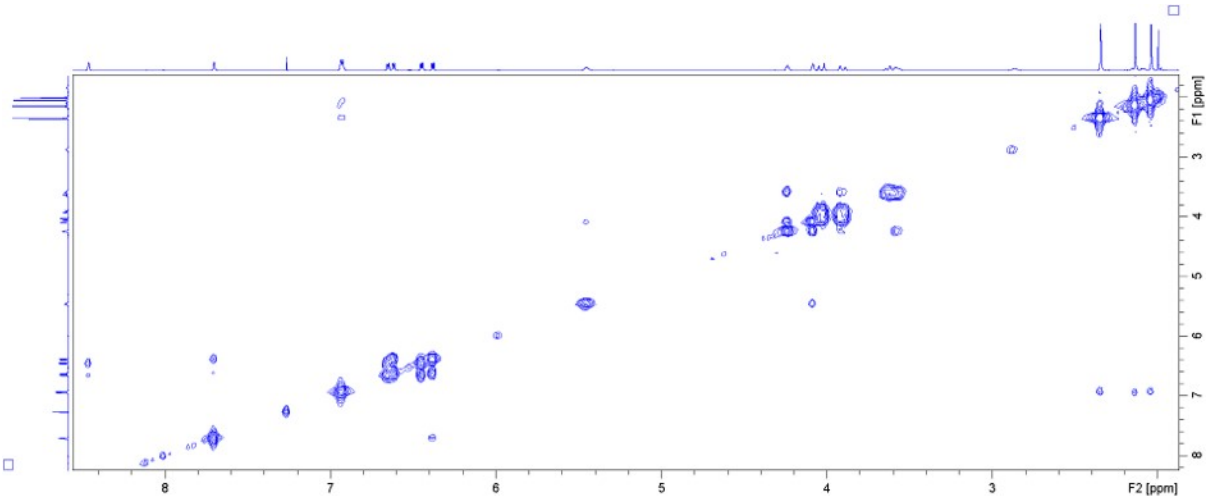
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Xb



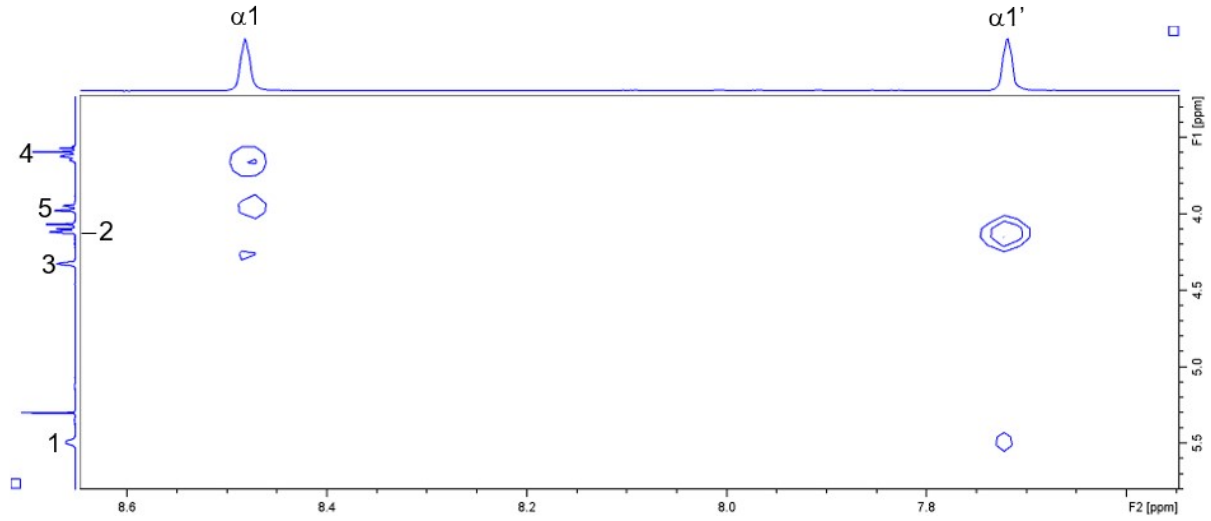
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Xb



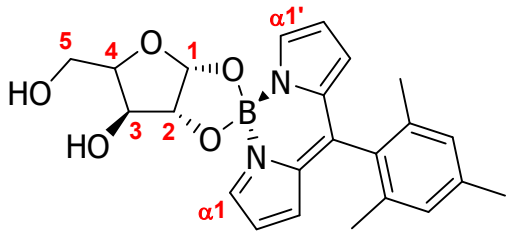
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Xb



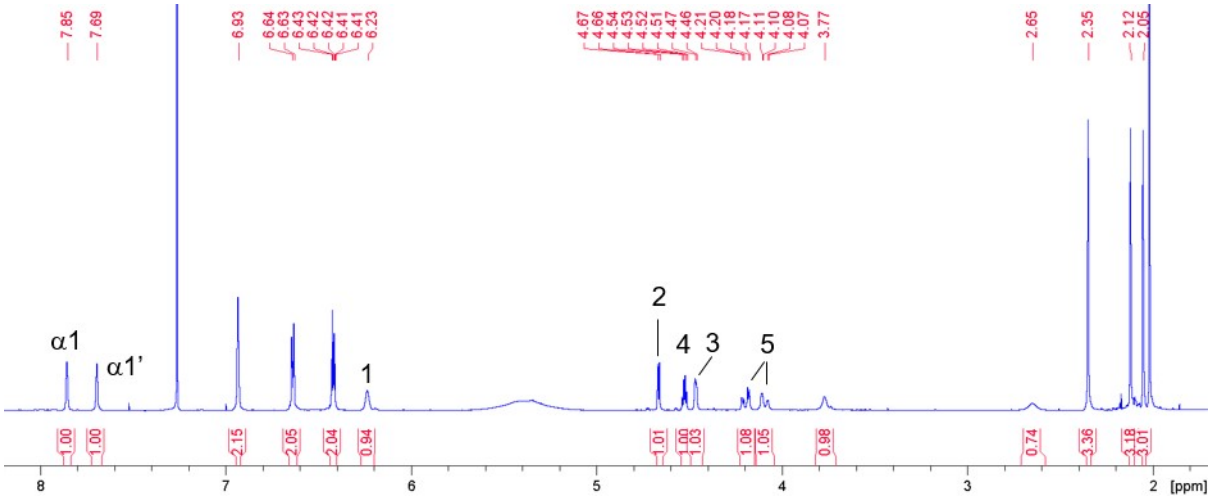
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Xb



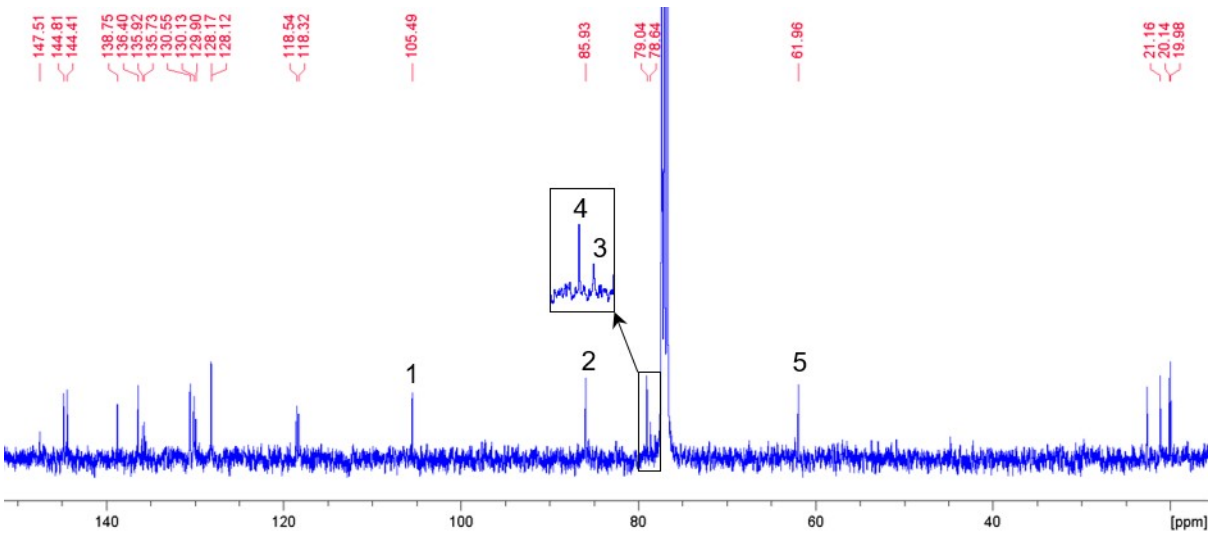
S5.14 Conjugate 4Xc: α-Xylofuranose-(1,2)-O-BODIPY



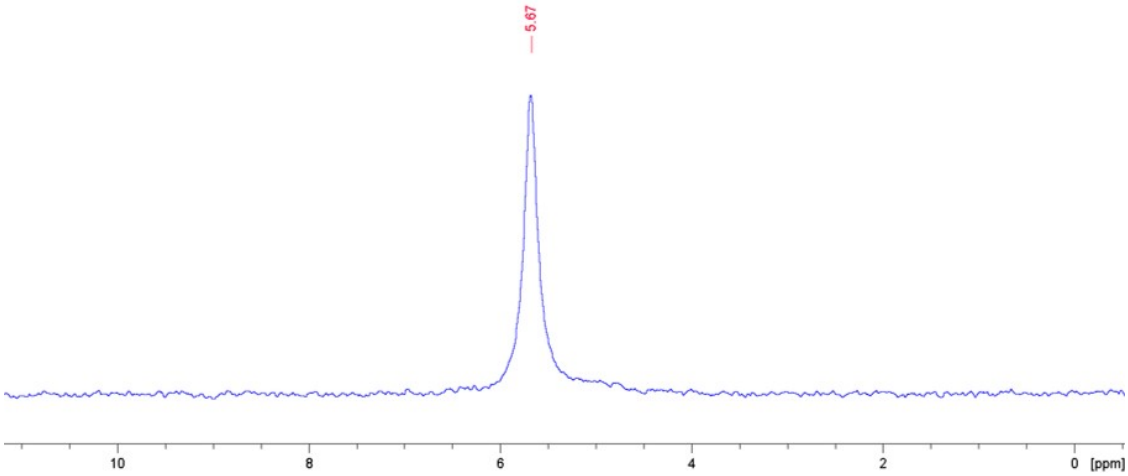
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Xc



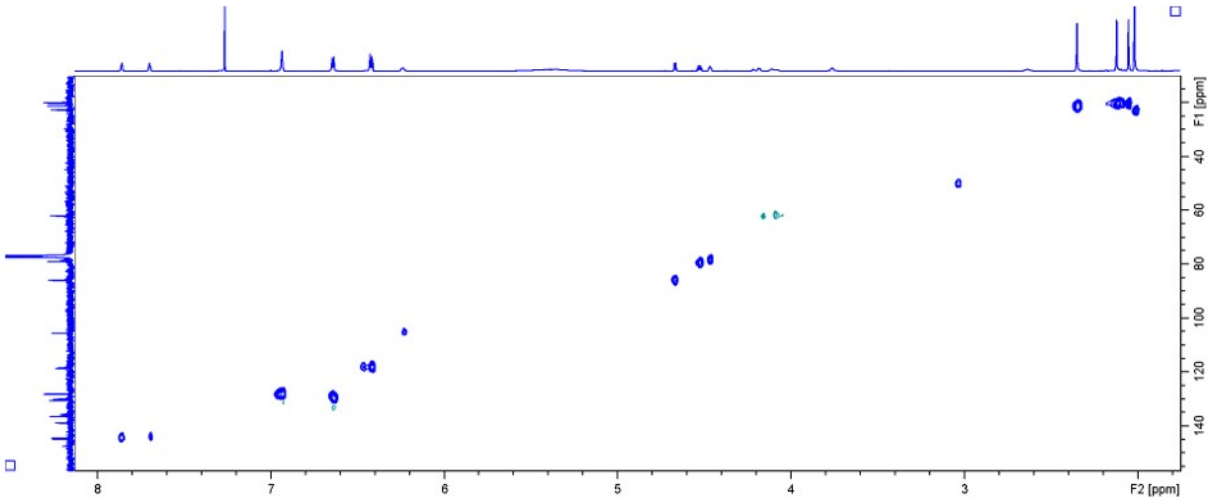
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Xc



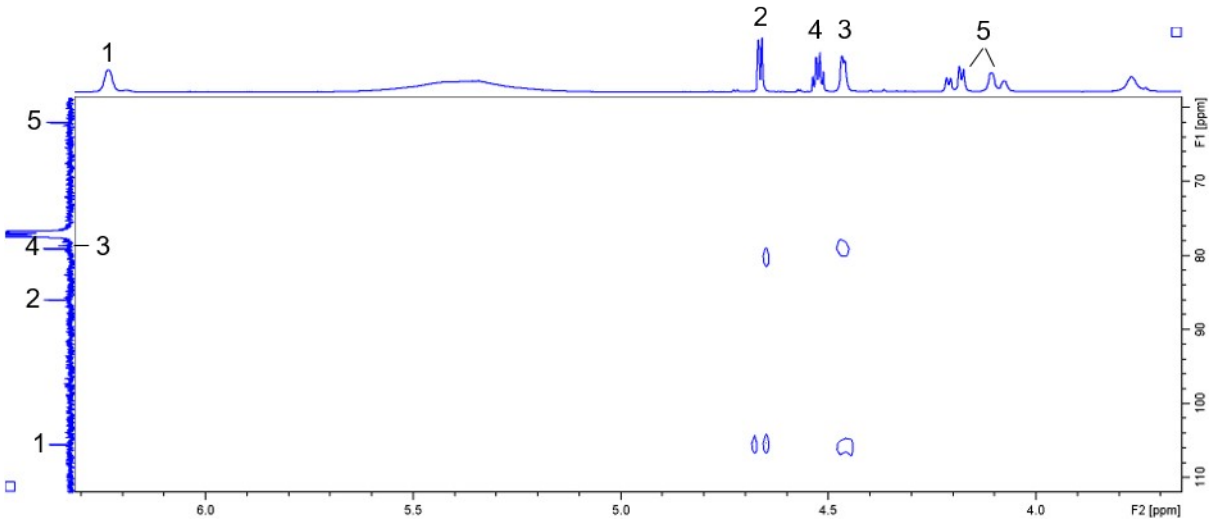
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Xc



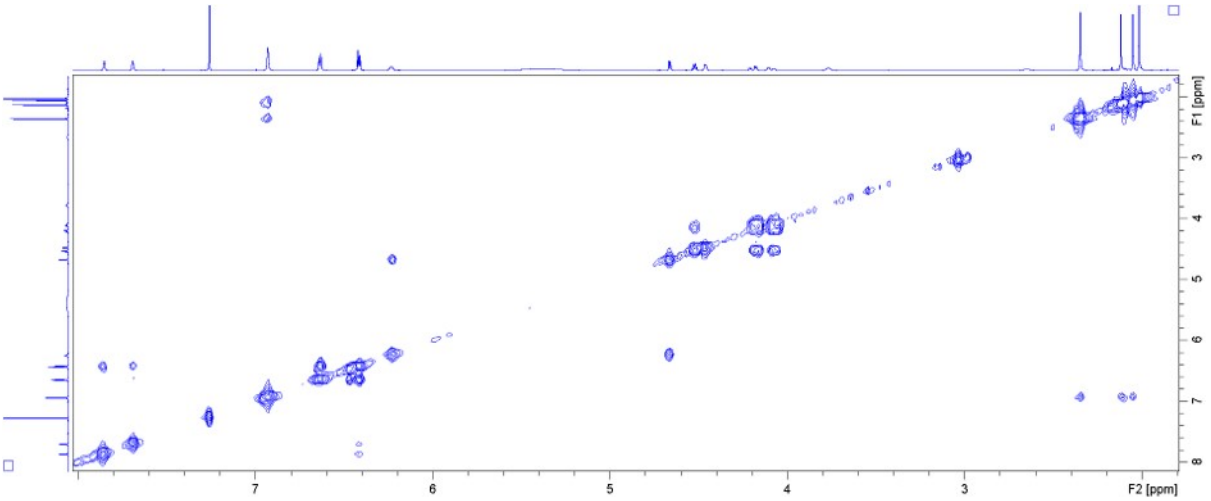
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Xc



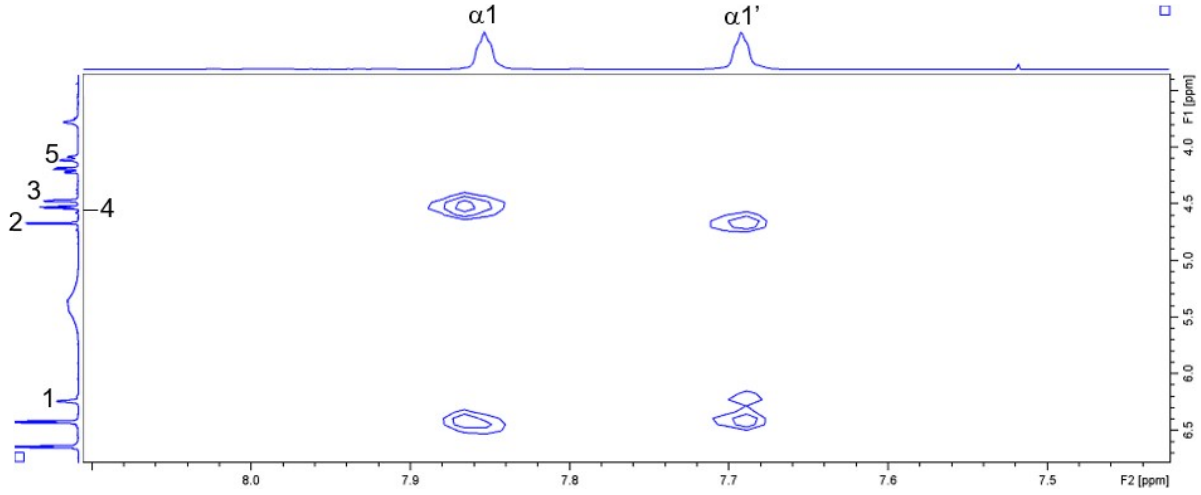
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Xc



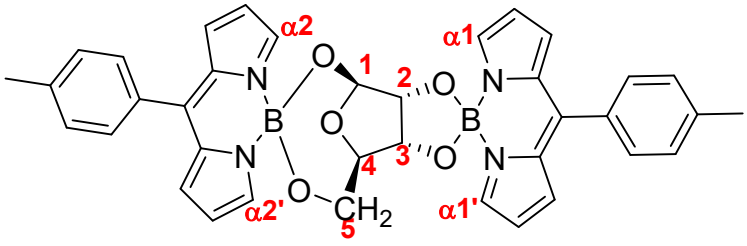
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Xc



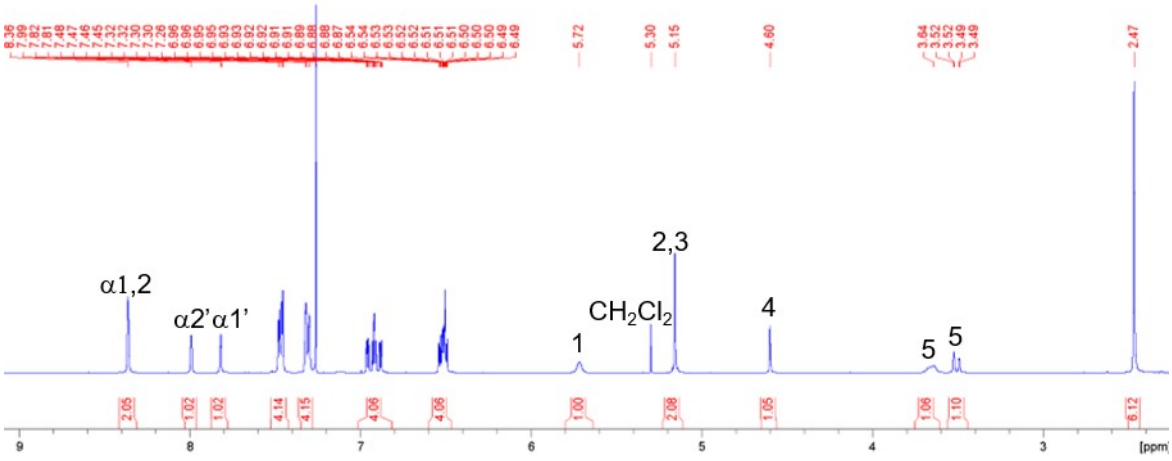
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Xc



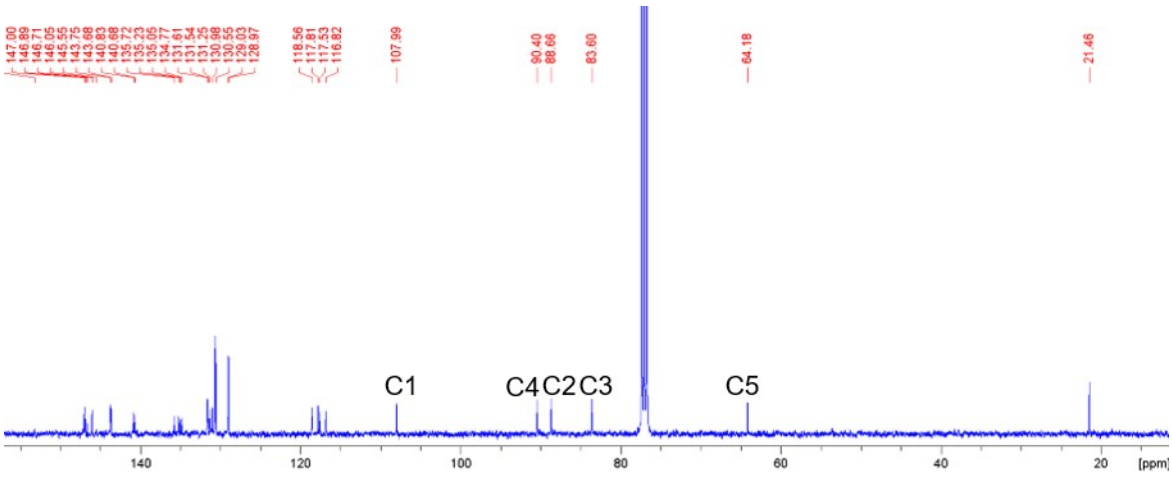
S5.15 Conjugate 3Ra: β-Ribofuranose-(1,5)(2,3)-O-BODIPY



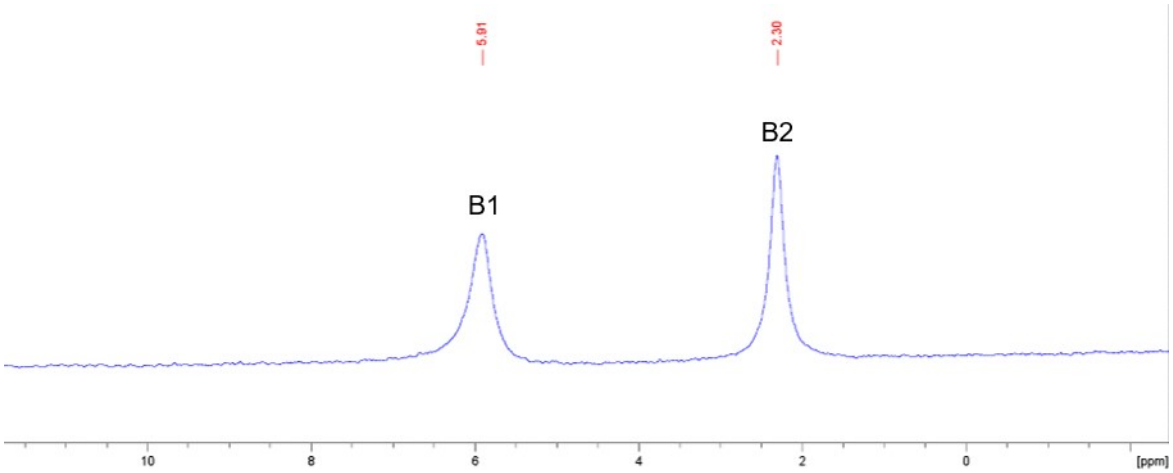
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Ra



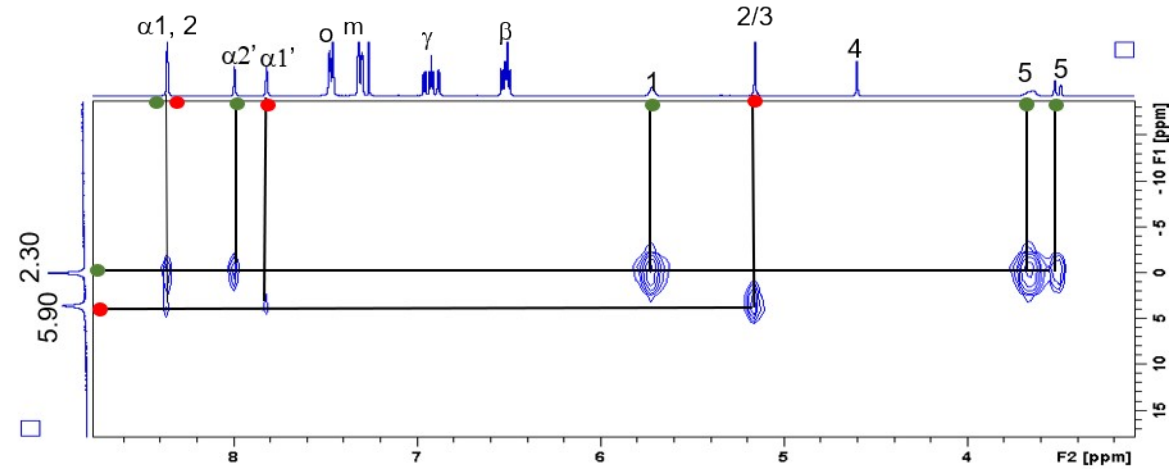
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Ra



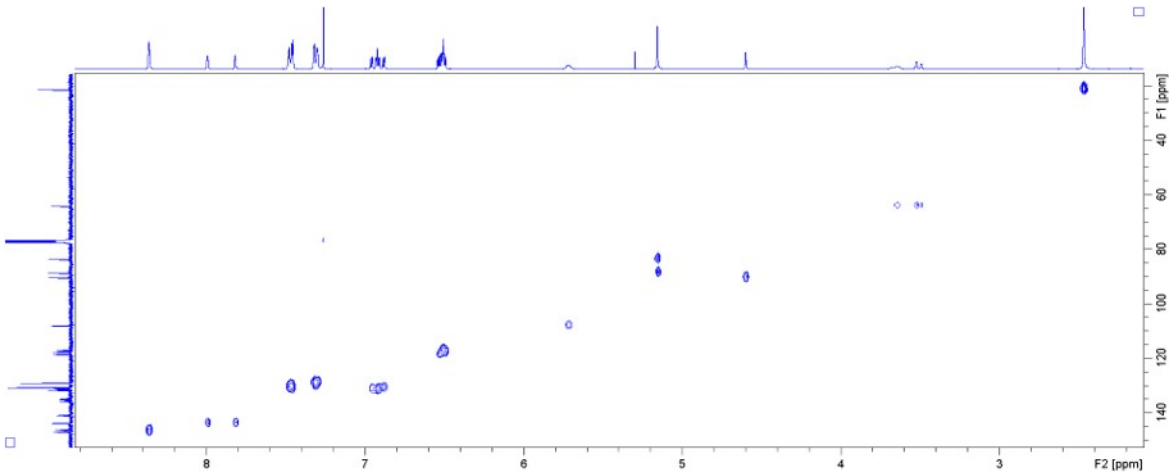
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Ra



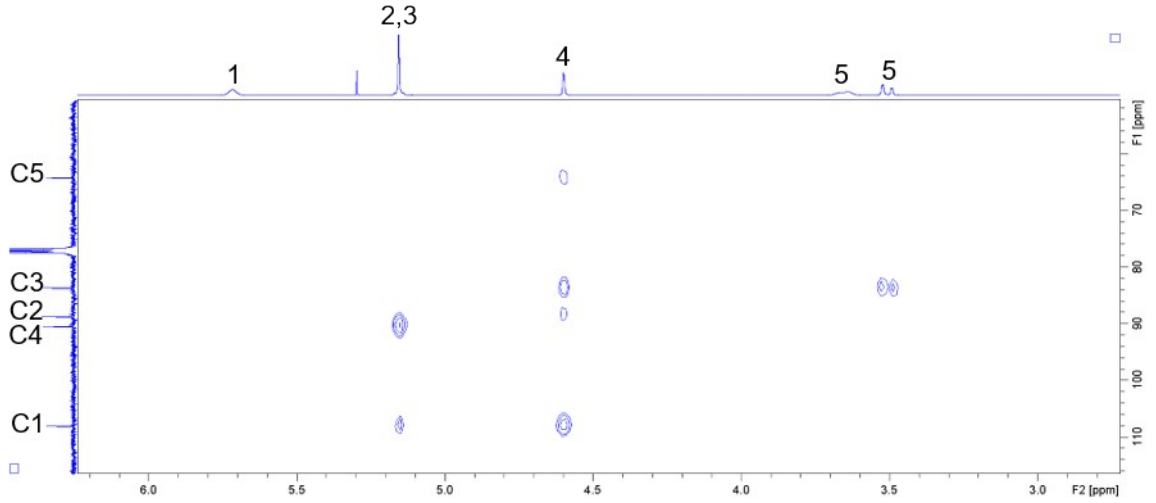
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Ra



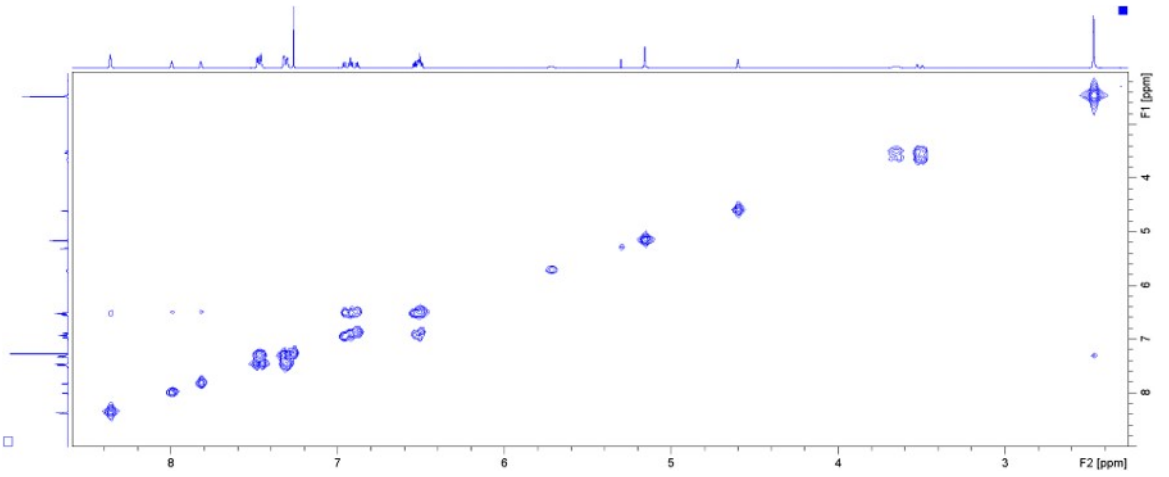
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Ra



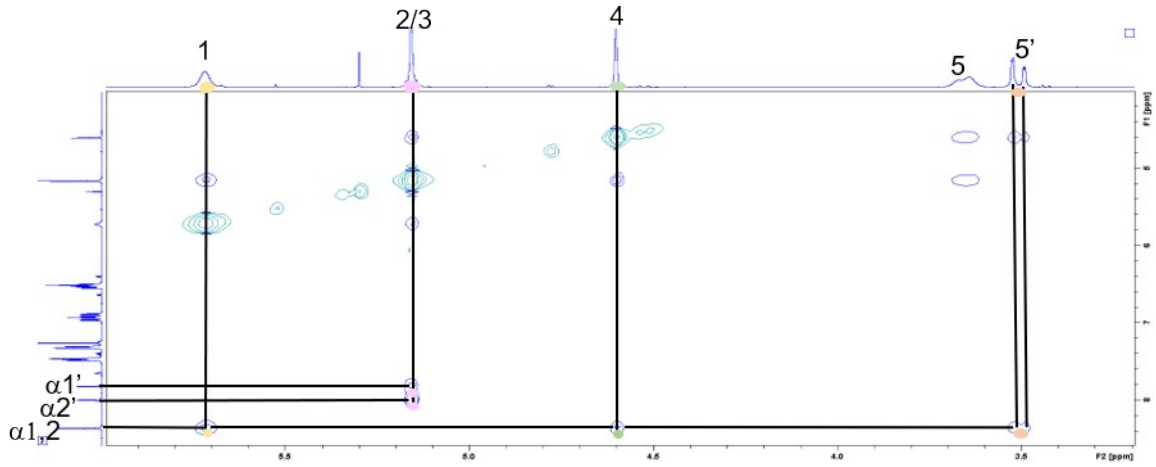
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Ra



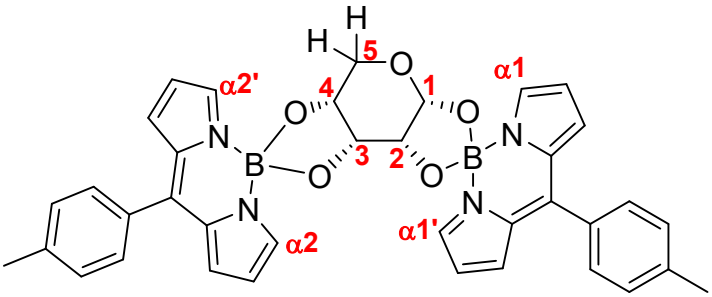
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Ra



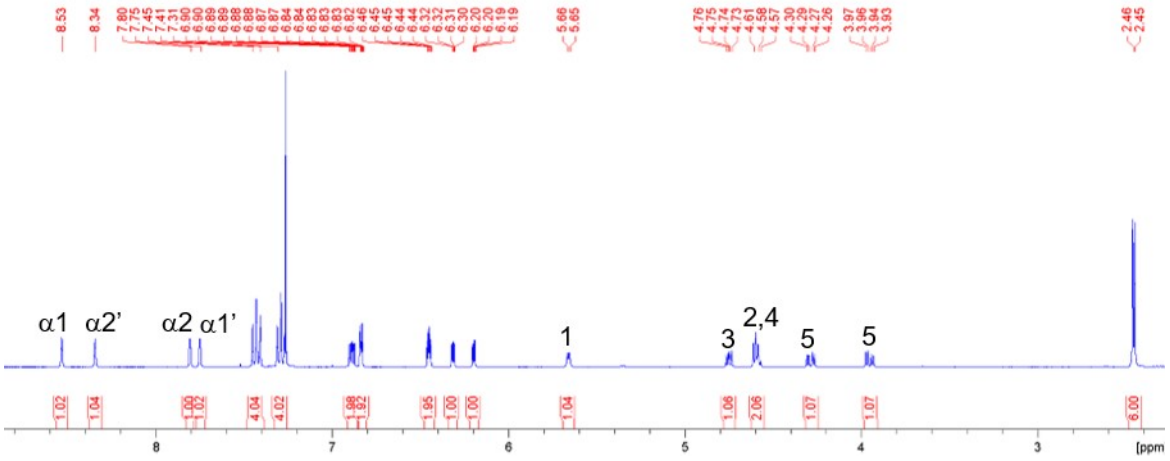
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Ra



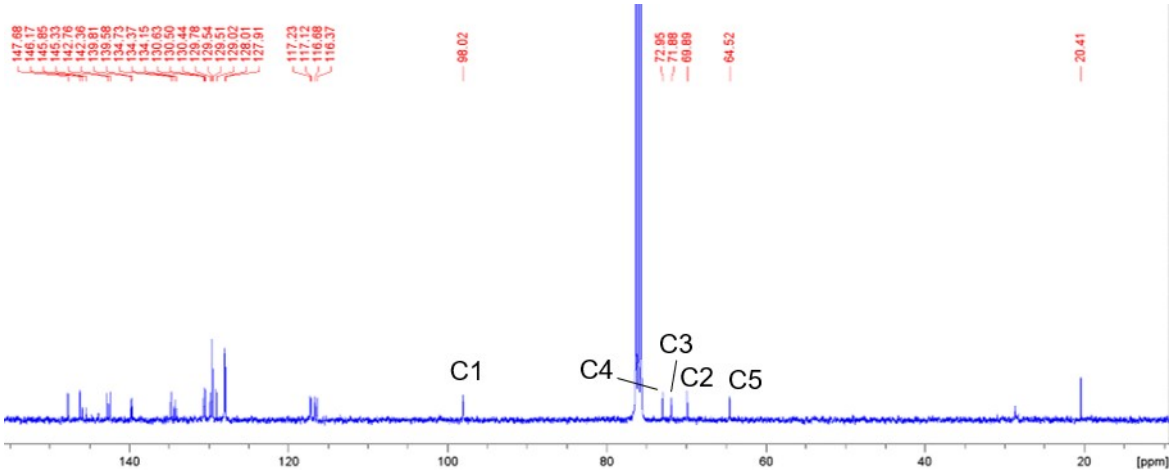
S5.16 Conjugate 3Rb: α-Ribopyranose-(1,2)(3,4)-O-BODIPY



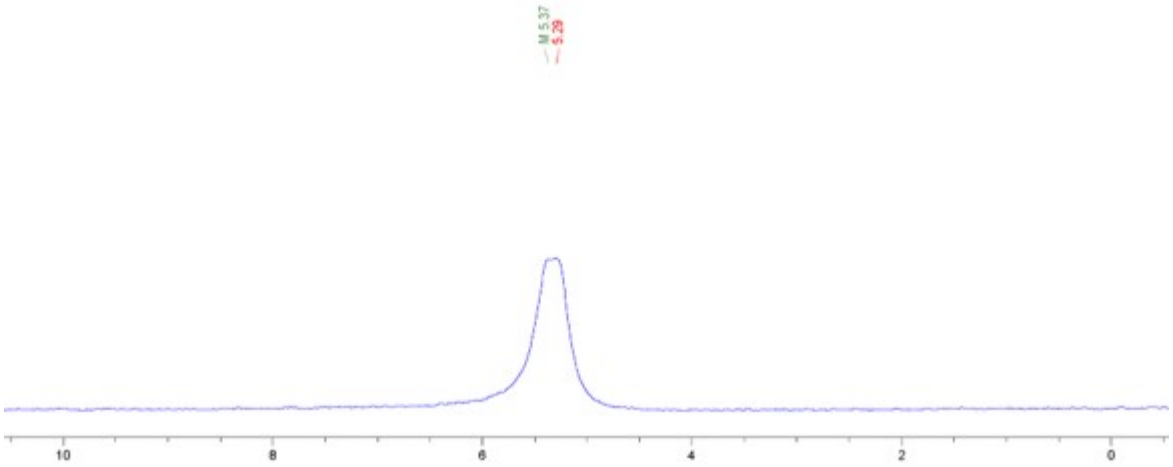
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Rb



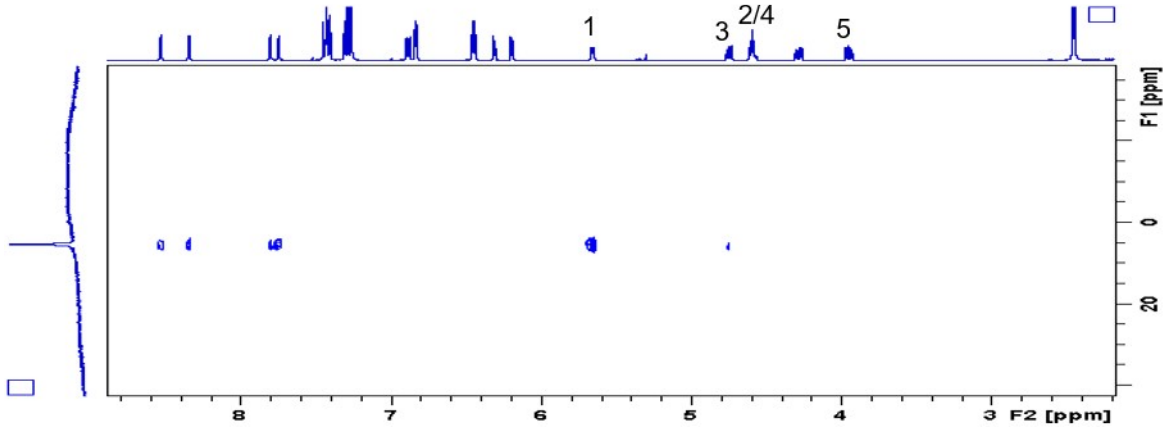
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Rb



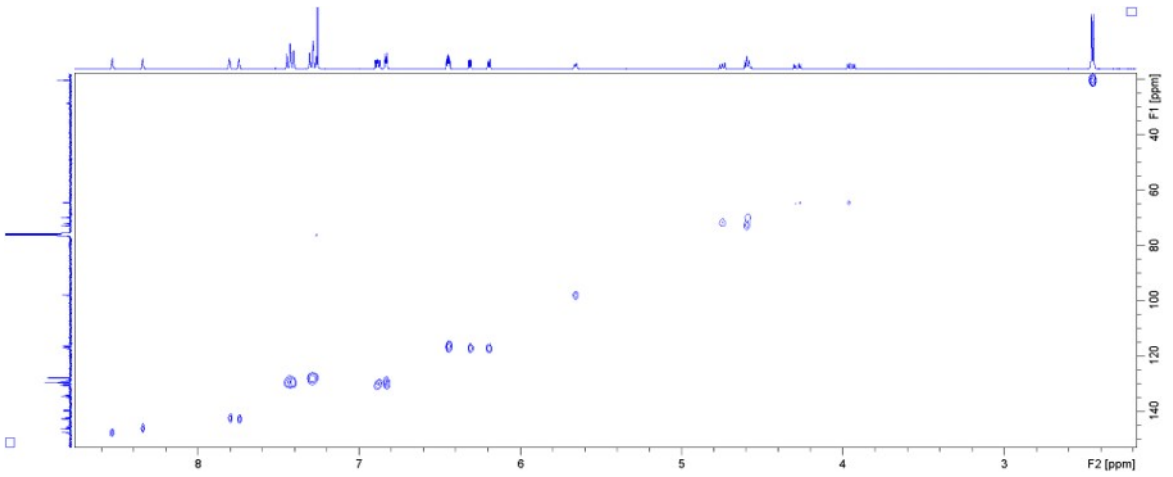
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Rb



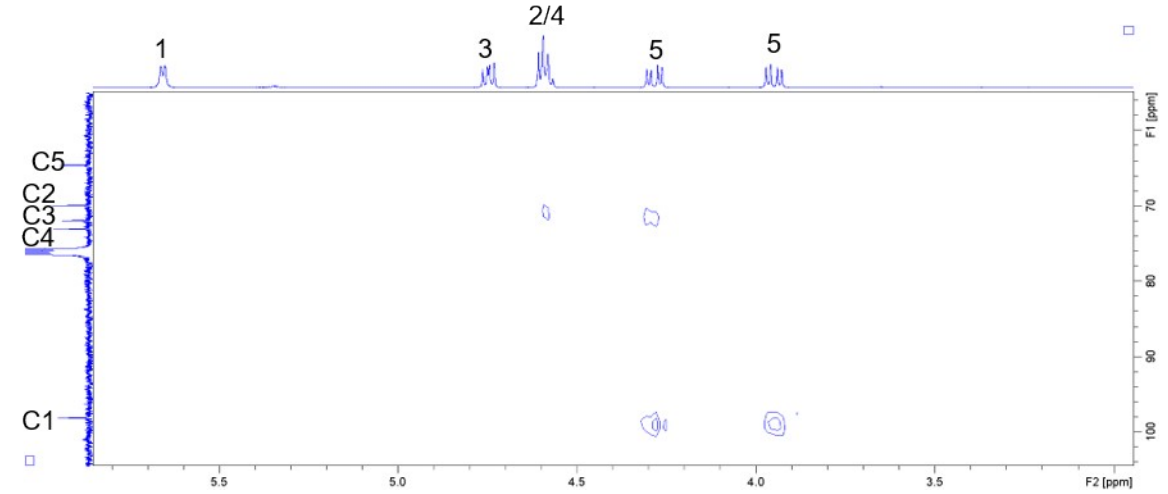
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Rb



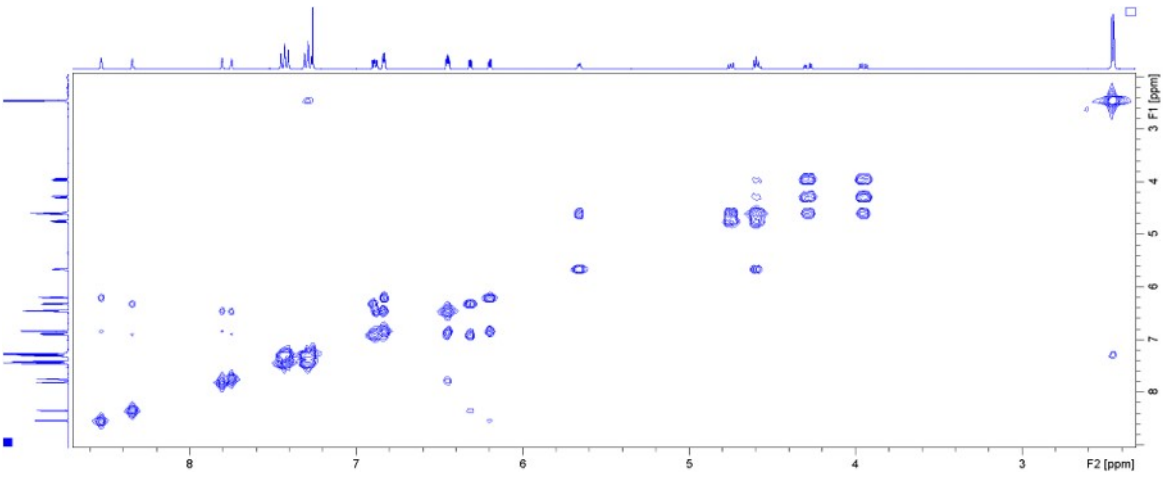
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Rb



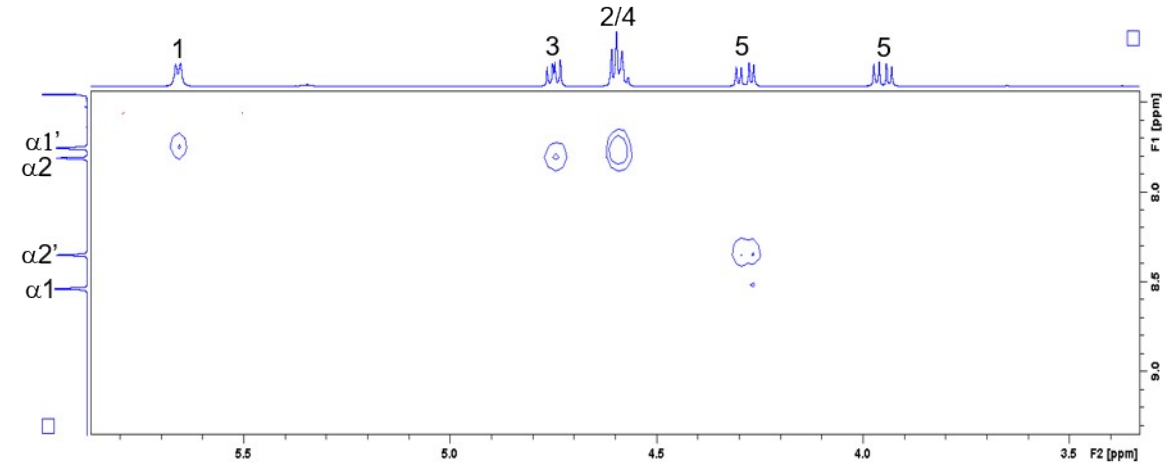
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Rb



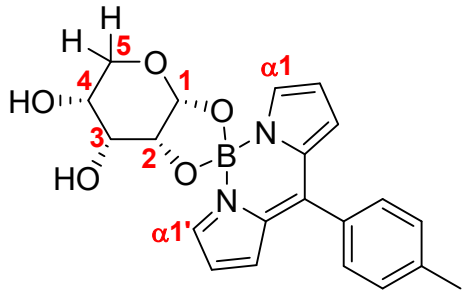
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Rb



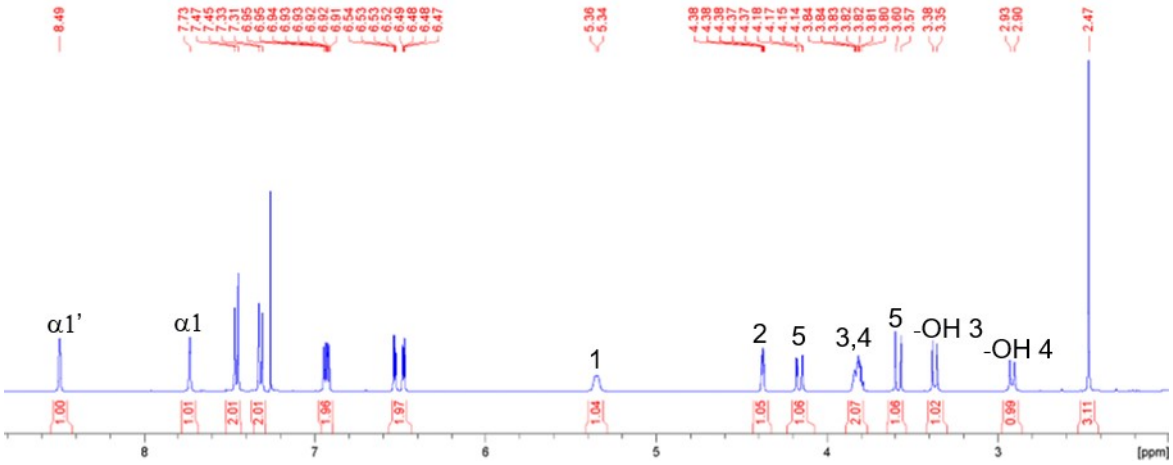
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Rb



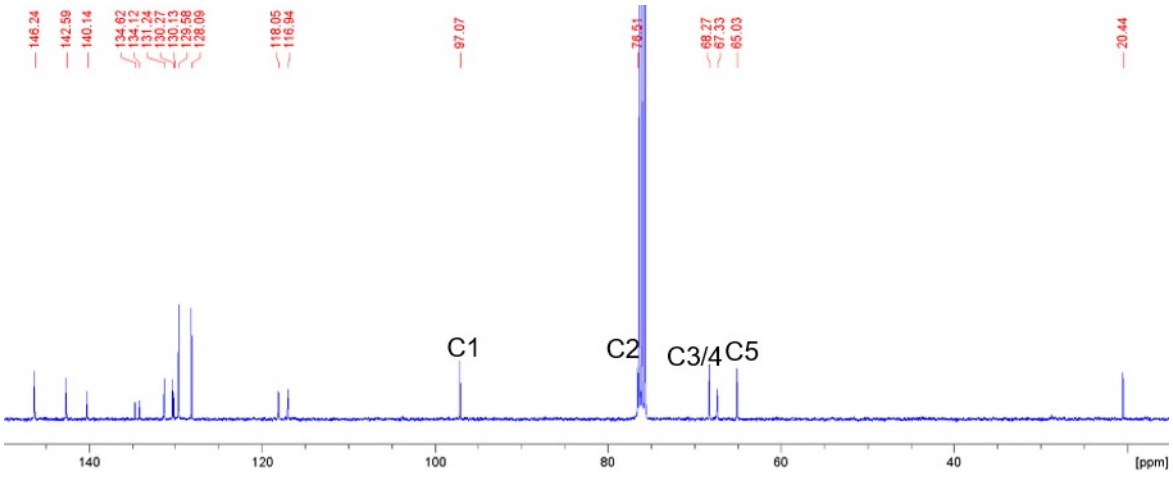
S5.17 Conjugate 3Rc: α-Ribopyranose-(1,2)-O-BODIPY



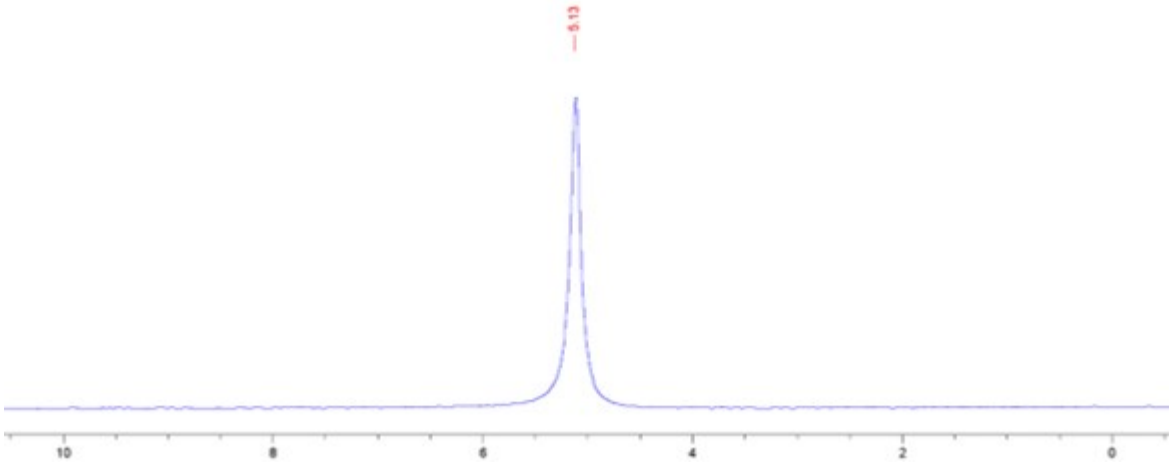
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Rc



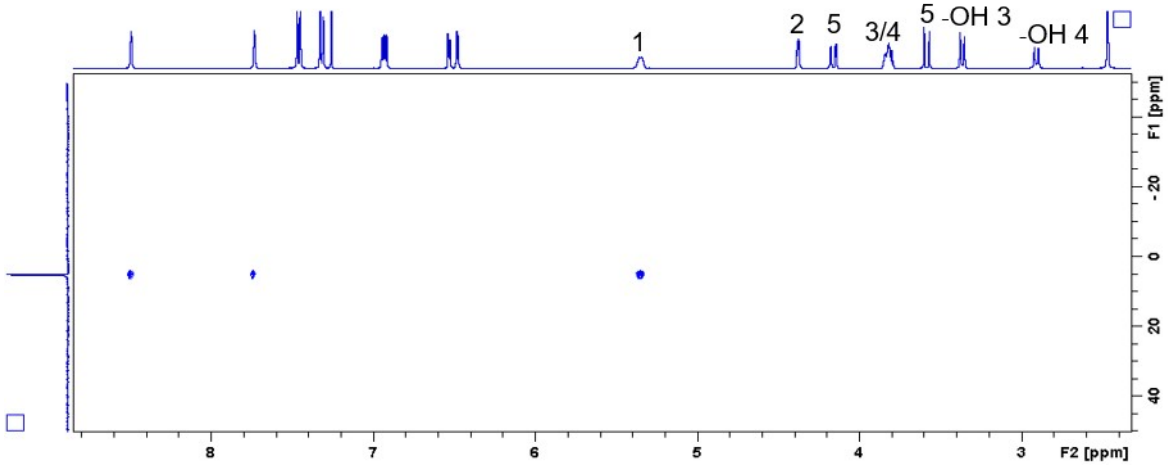
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Rc



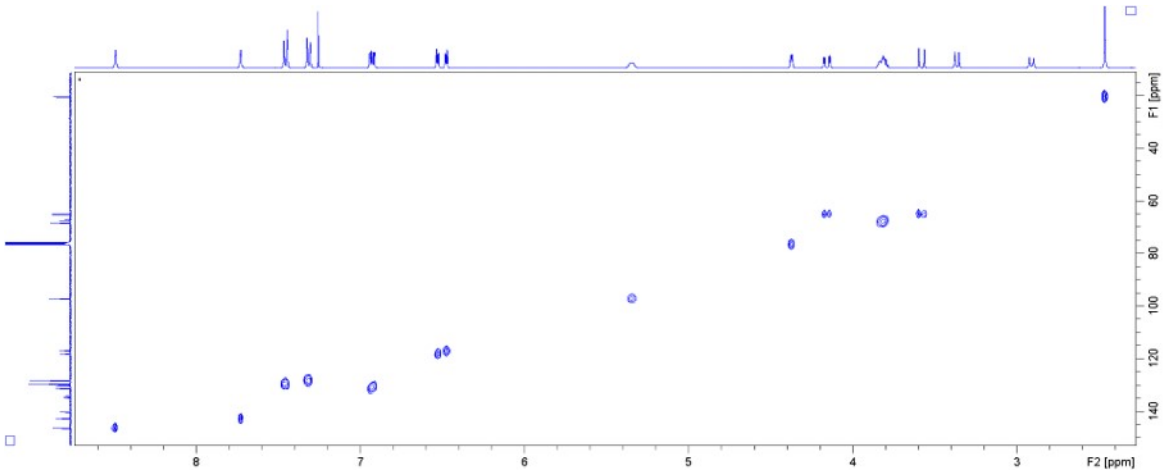
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Rc



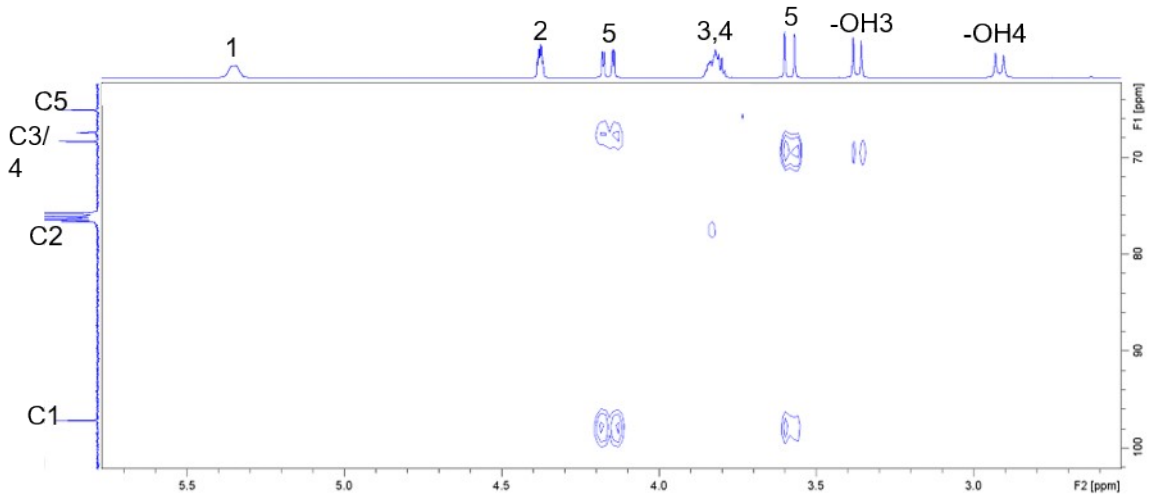
^{1}H-^{11}B HMBC NMR ($CDCl_3$) spectrum of 3Rc



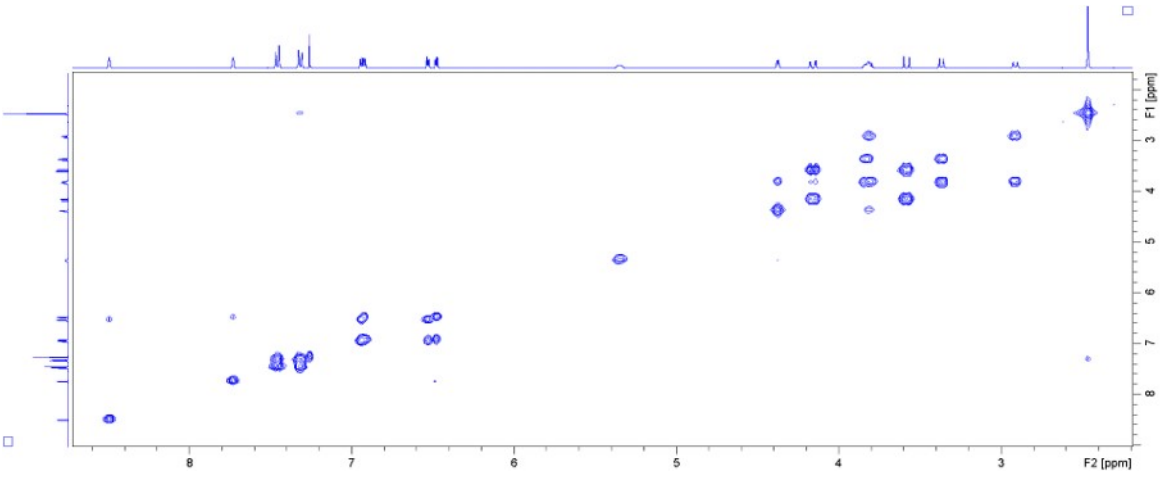
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Rc



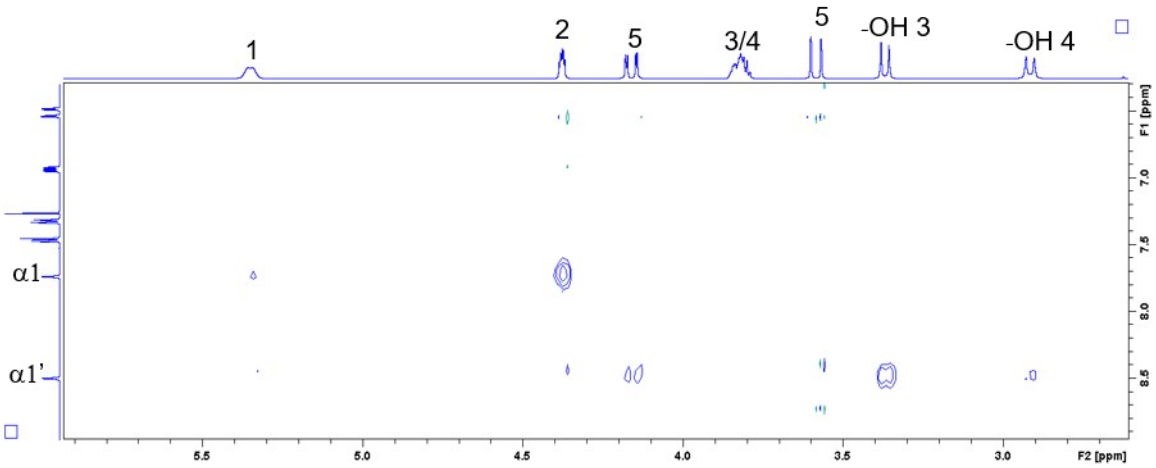
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Rc



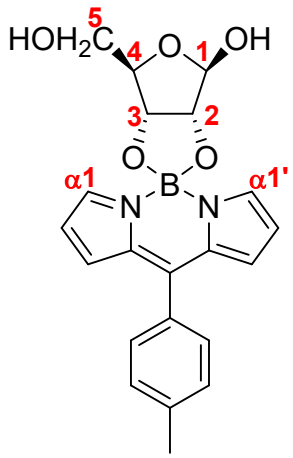
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Rc



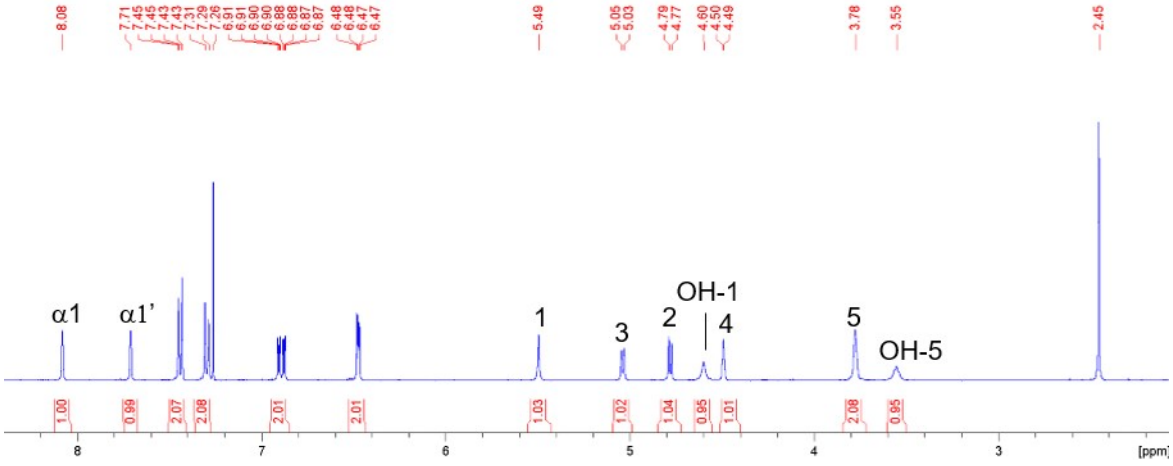
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Rc



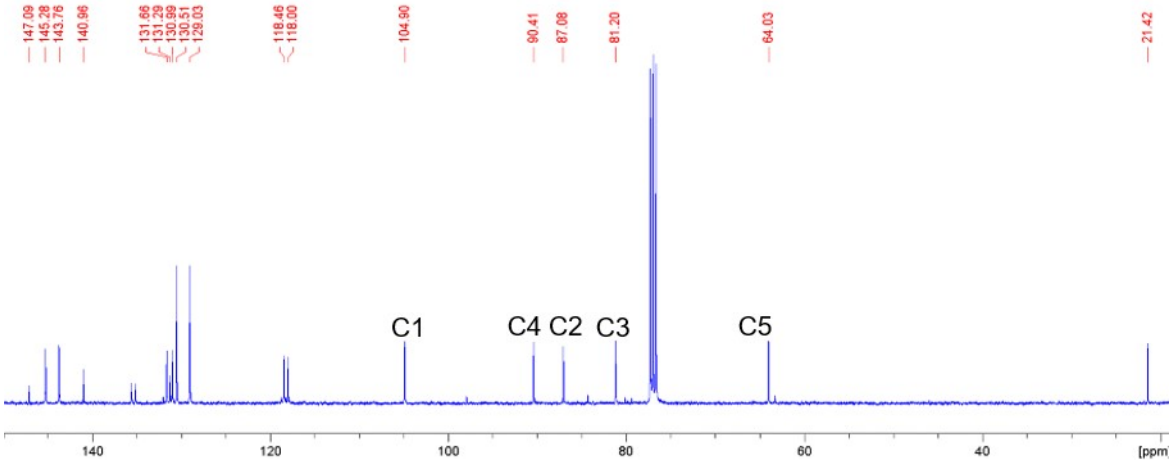
S5.18 Conjugate 3Rd: β-Ribofuranose-(2,3)-O-BODIPY



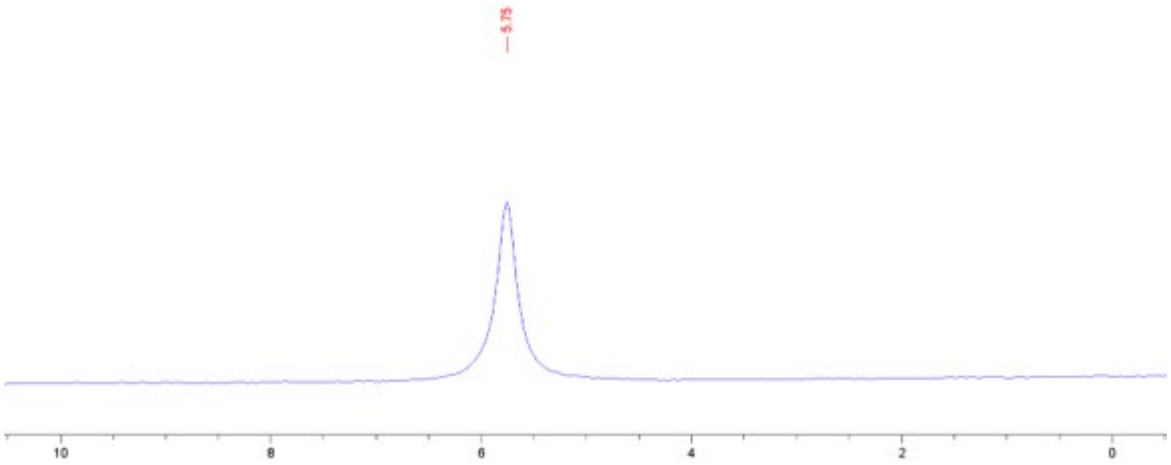
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3Rd



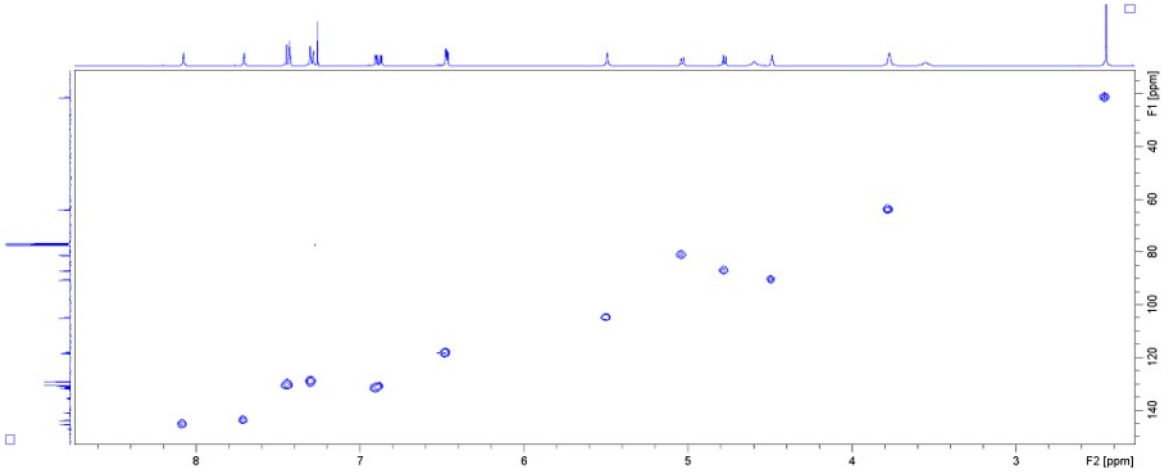
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 3Rd



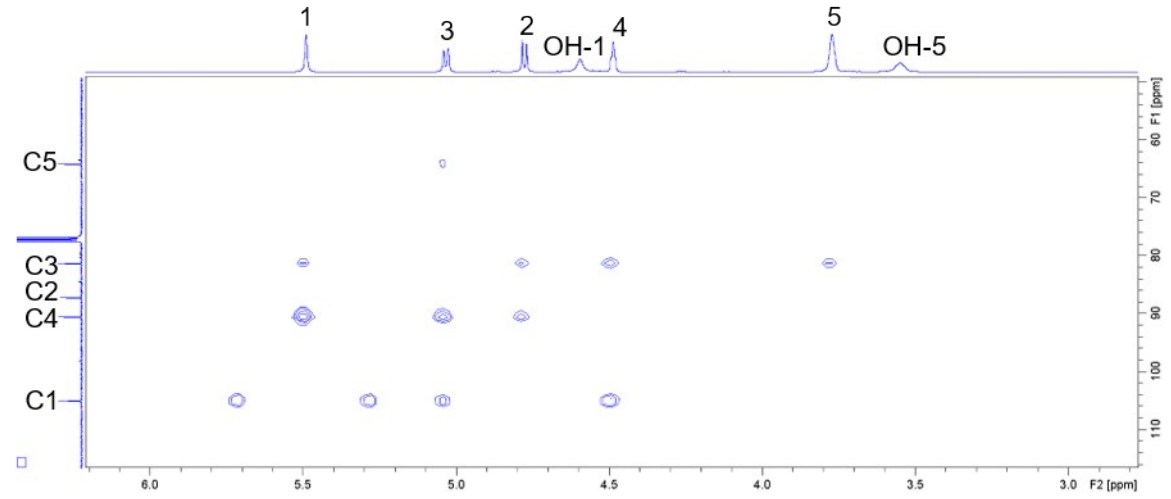
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 3Rd



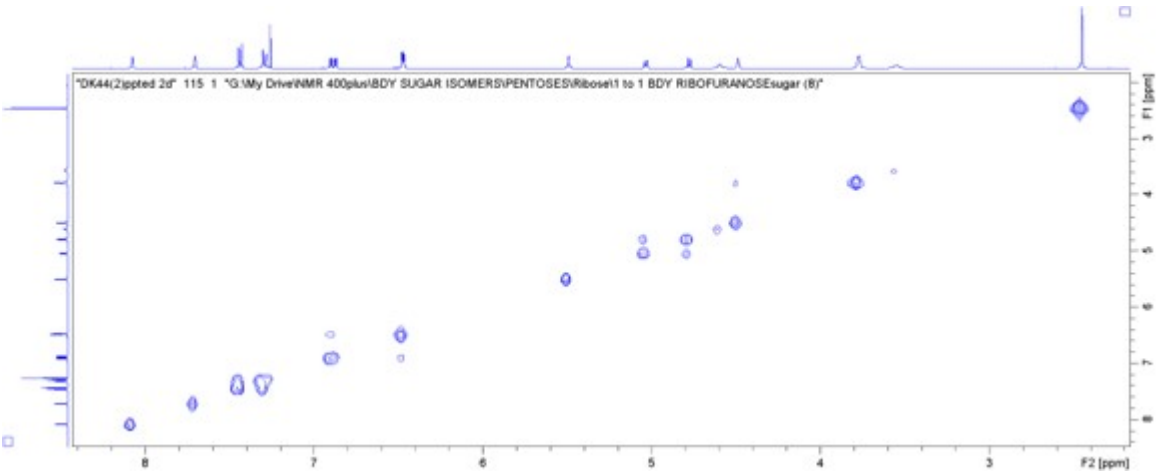
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 3Rd



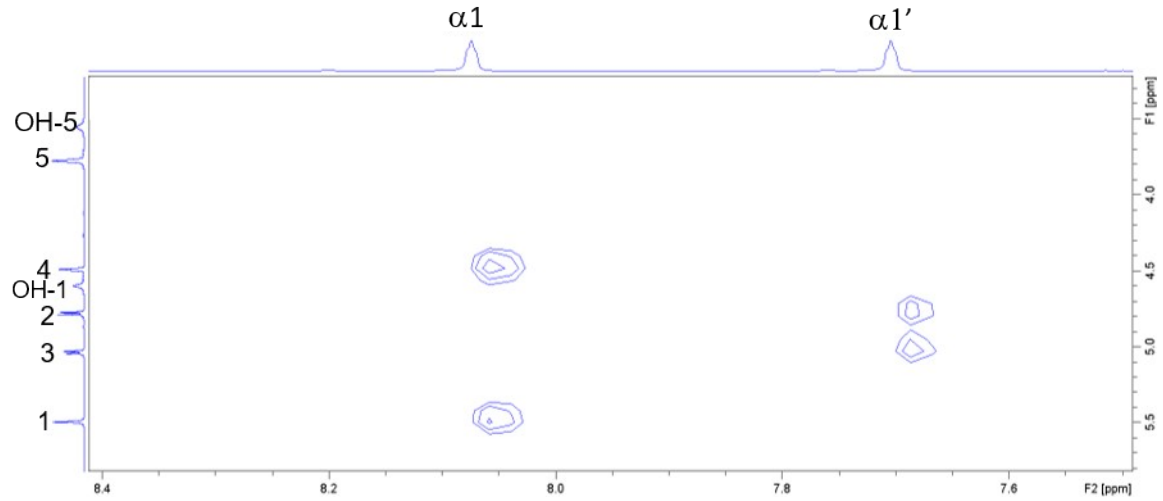
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 3Rd



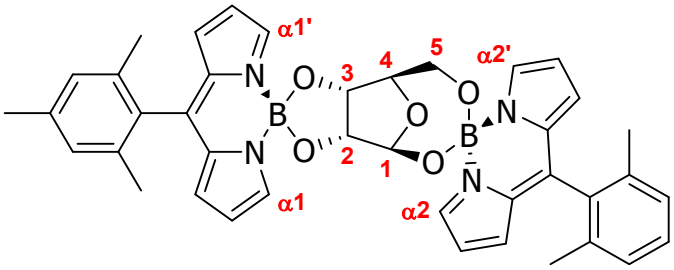
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 3Rd



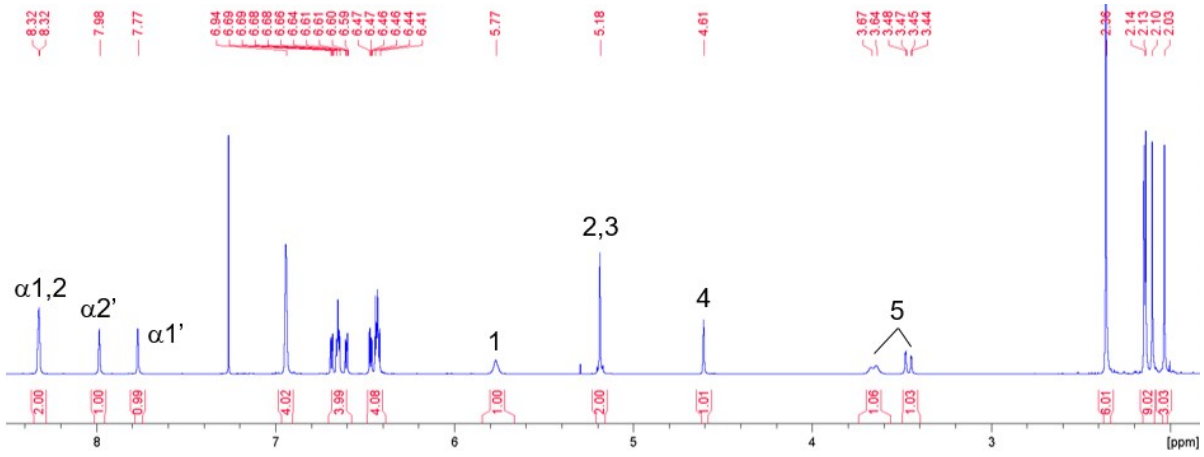
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 3Rd



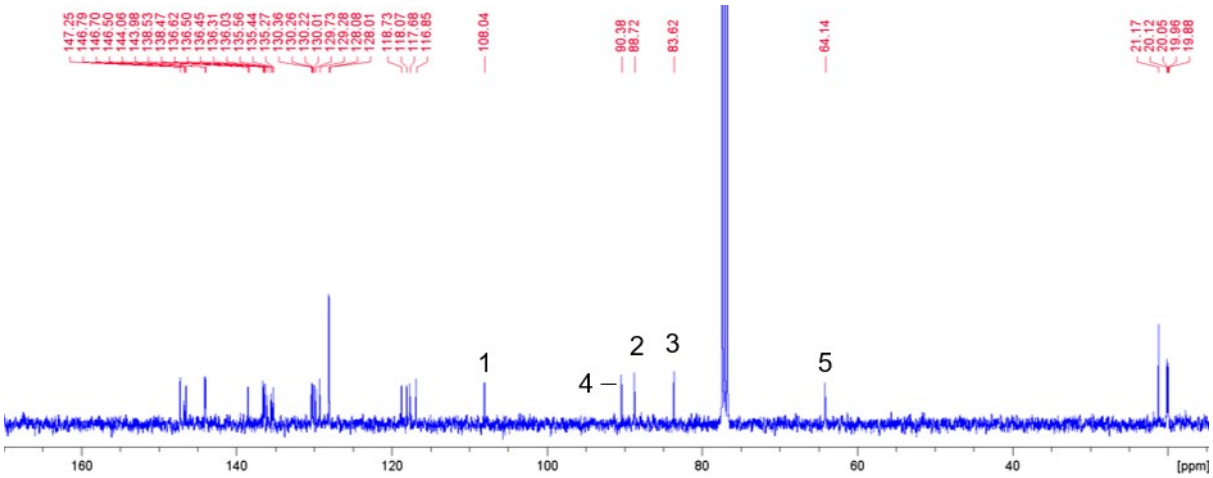
S5.19 Conjugate 4Ra: β-Ribofuranose-(1,5)(2,3)-O-BODIPY



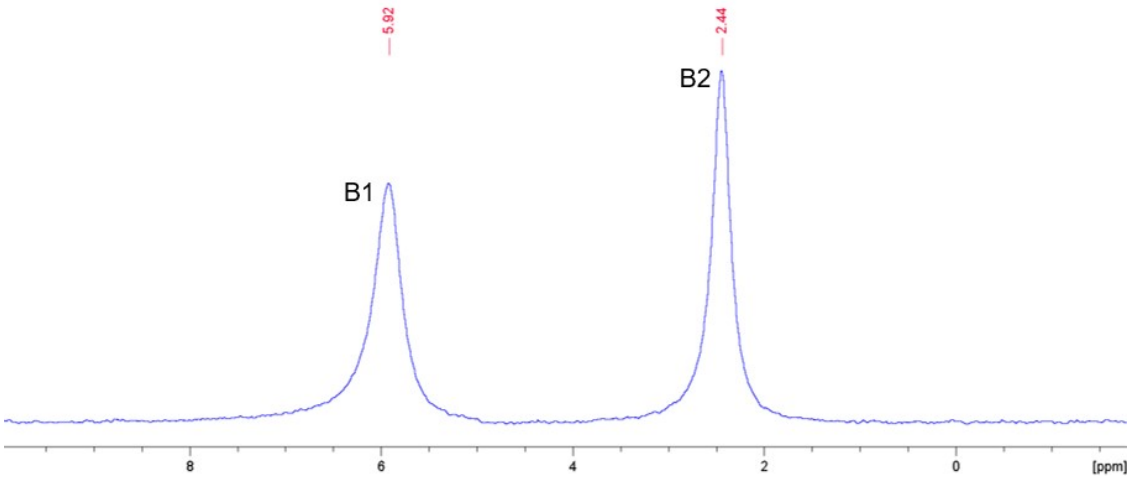
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Ra



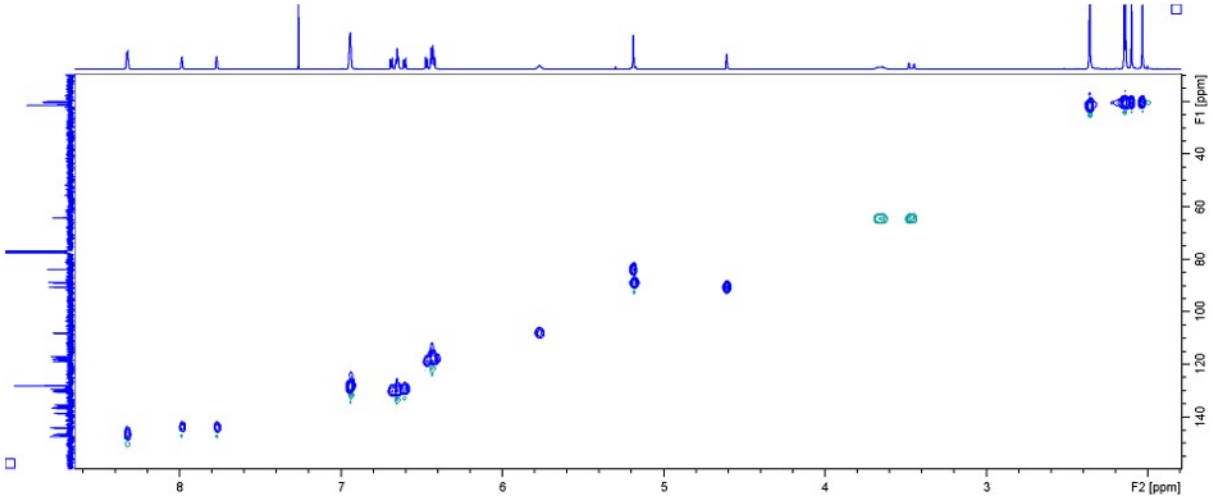
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Ra



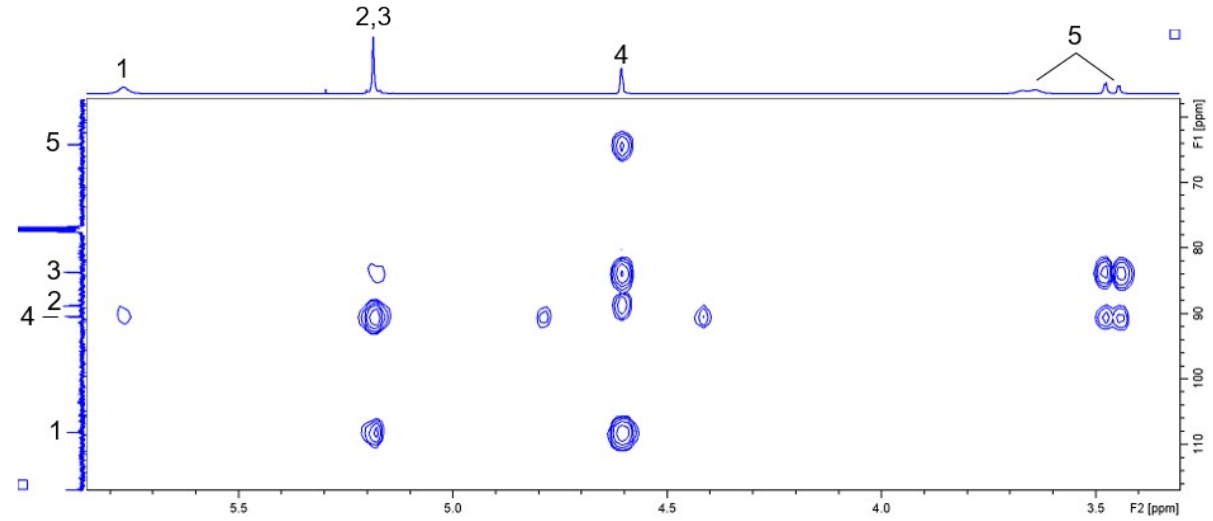
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Ra



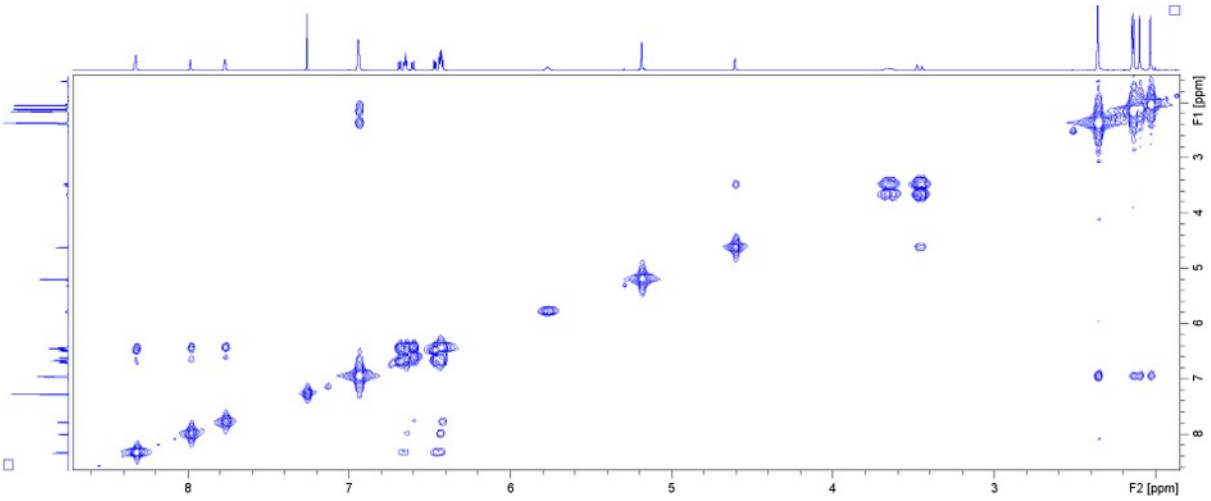
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Ra



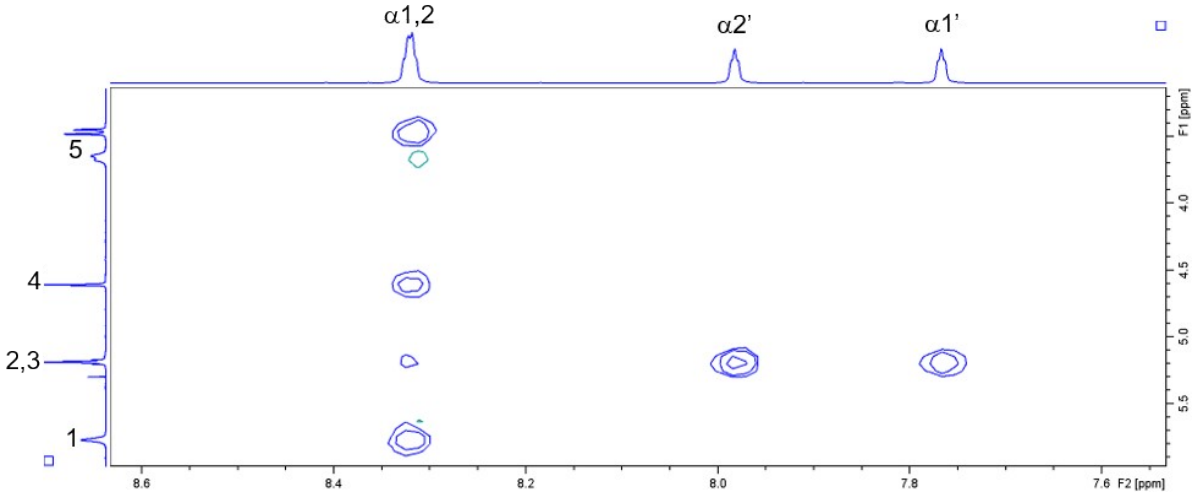
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Ra



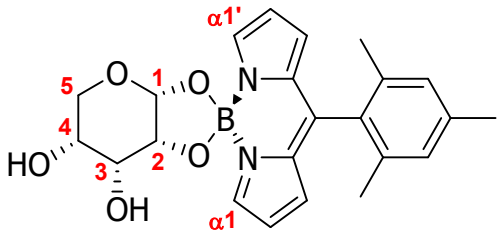
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Ra



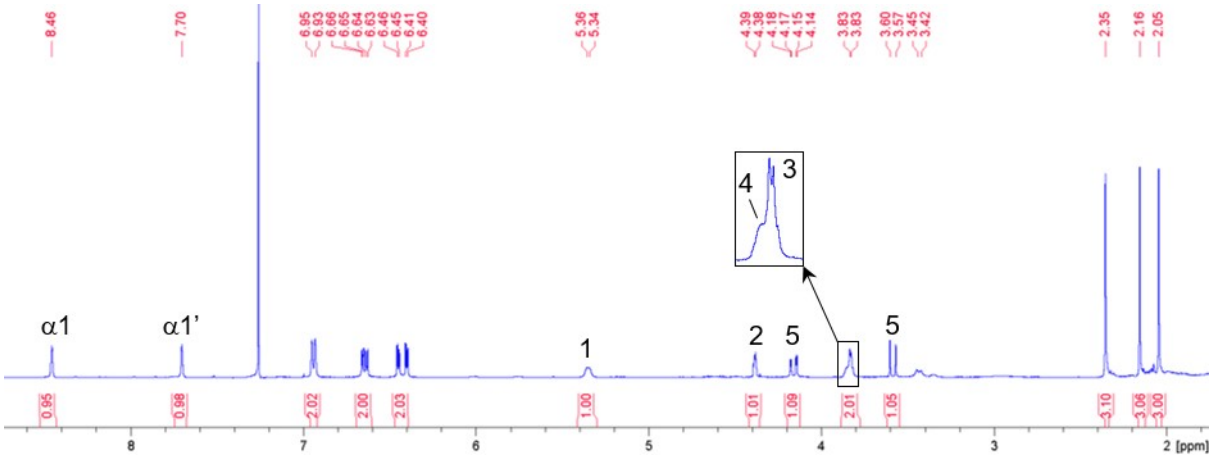
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Ra



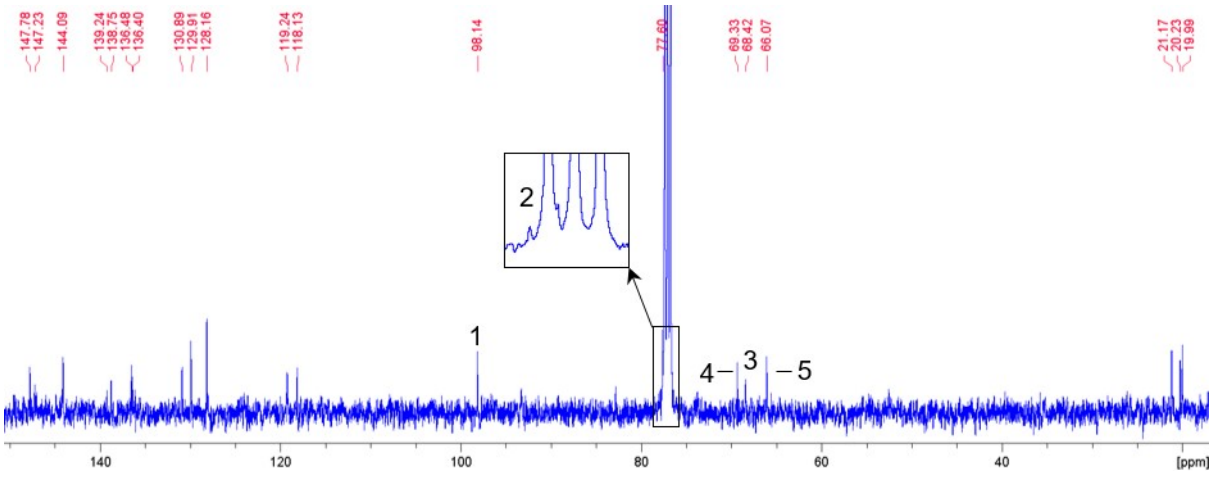
S5.20 Conjugate 4Rb: α-Ribopyranose-(1,2)-O-BODIPY



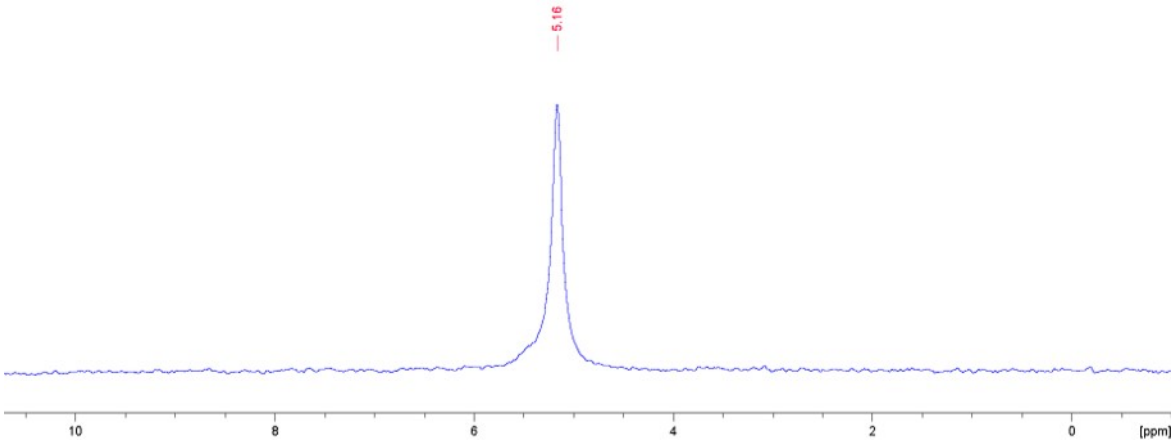
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Rb



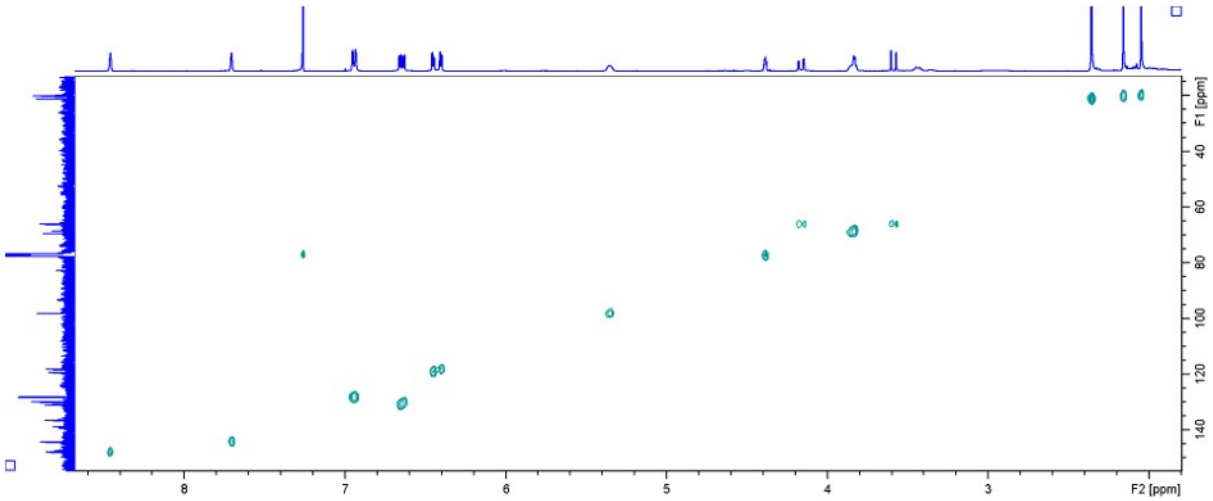
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Rb



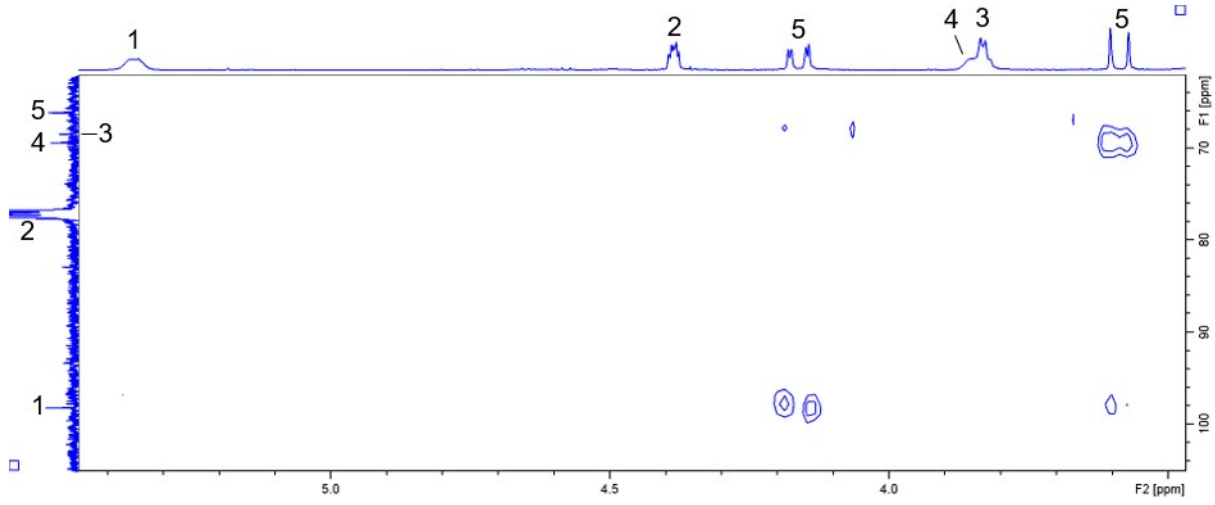
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Rb



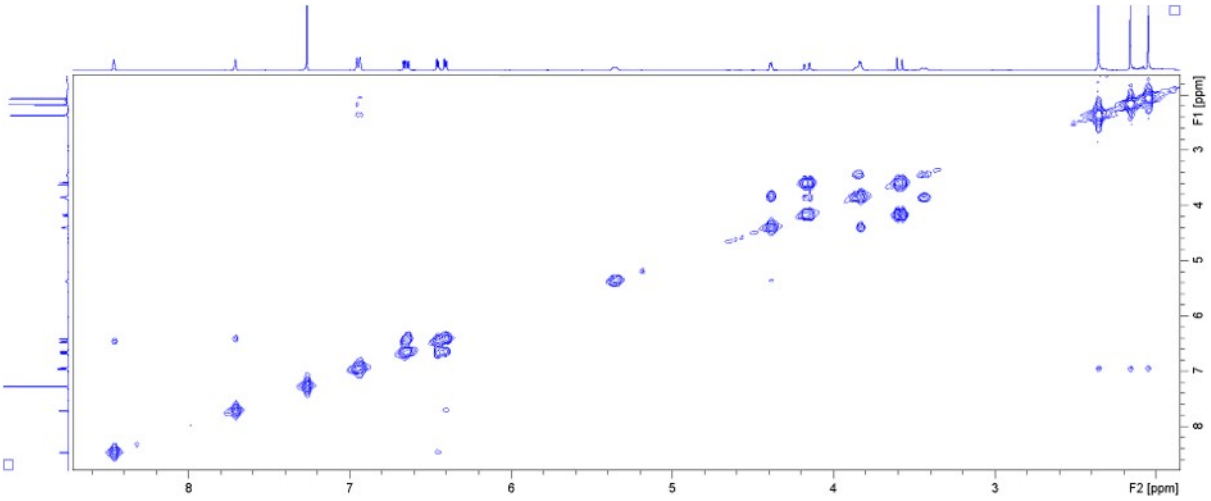
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Rb



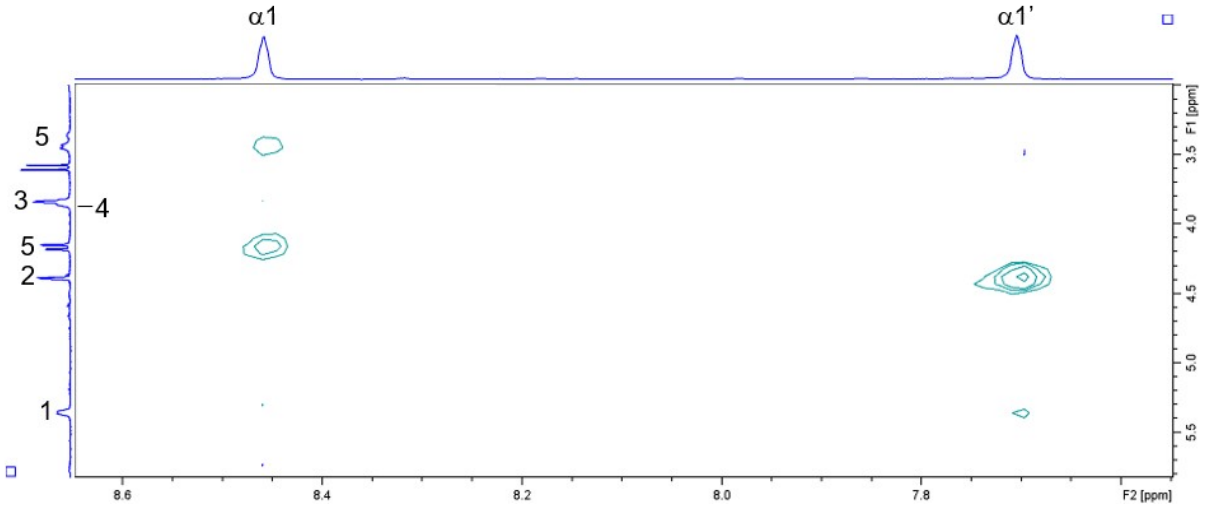
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Rb



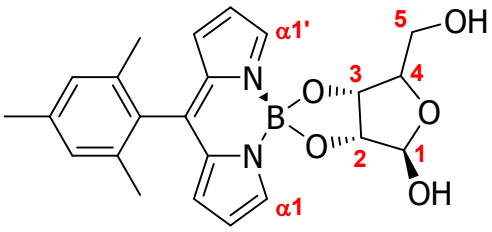
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Rb



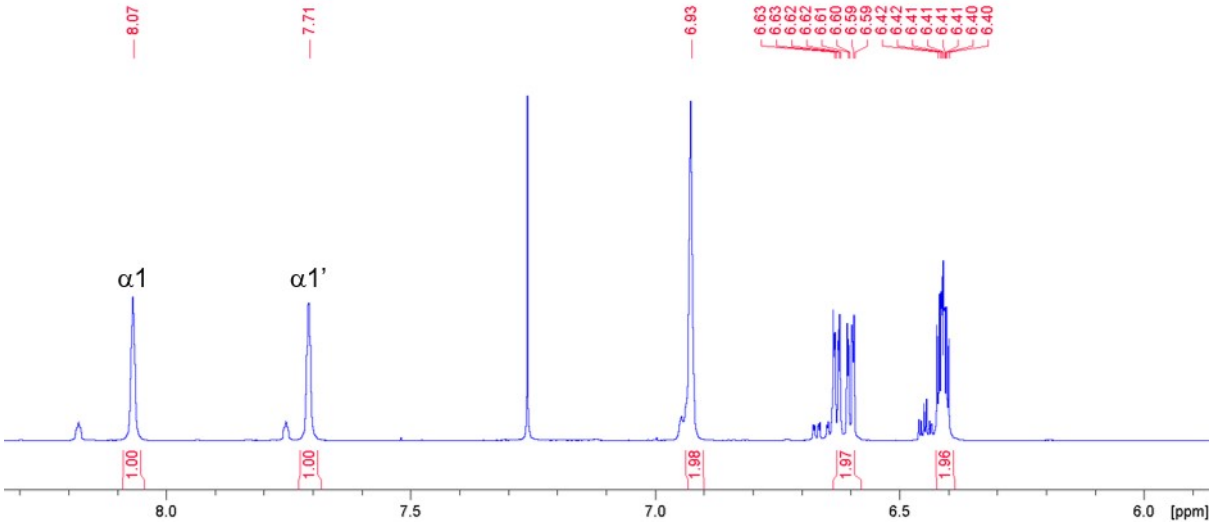
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Rb

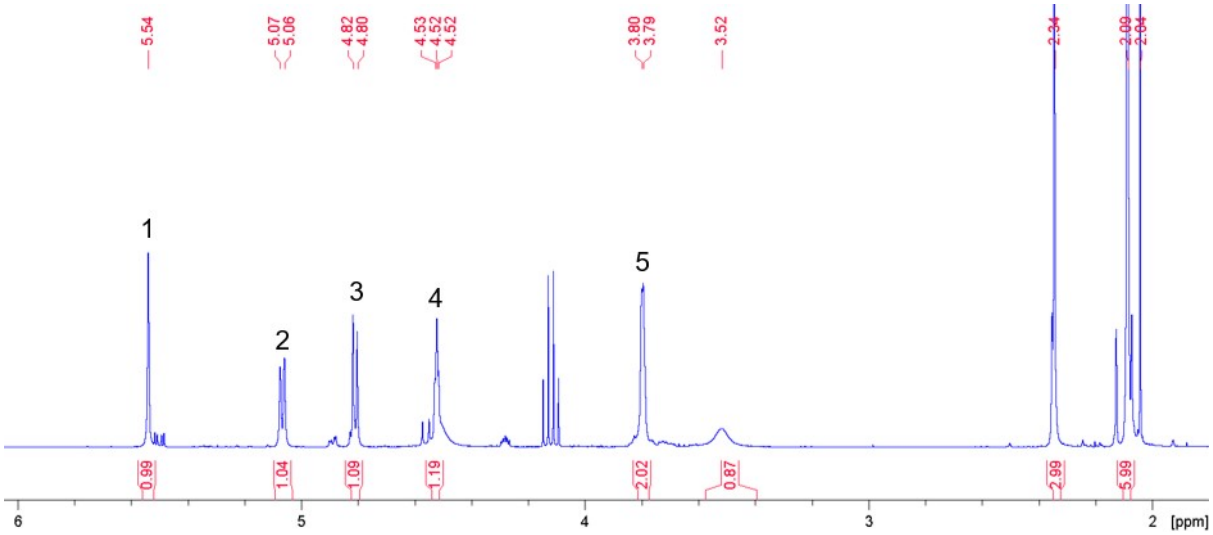


S5.21 Conjugate 4Rc: β-Ribofuranose-(2,3)-O-BODIPY

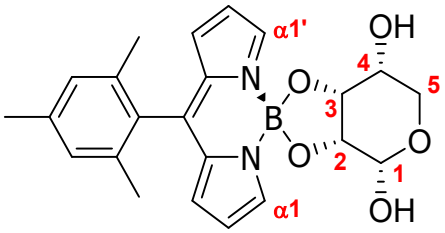


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Rc

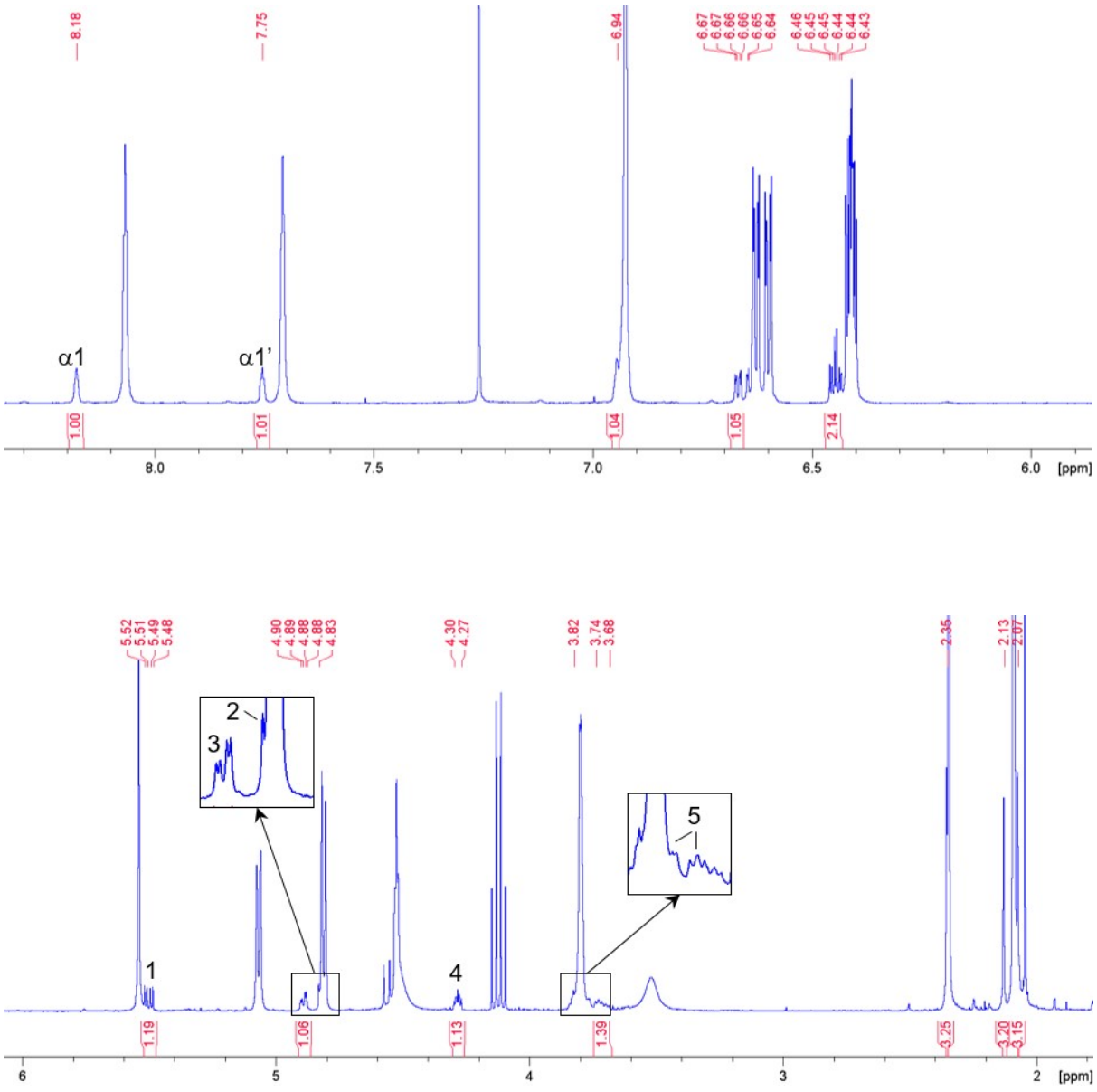




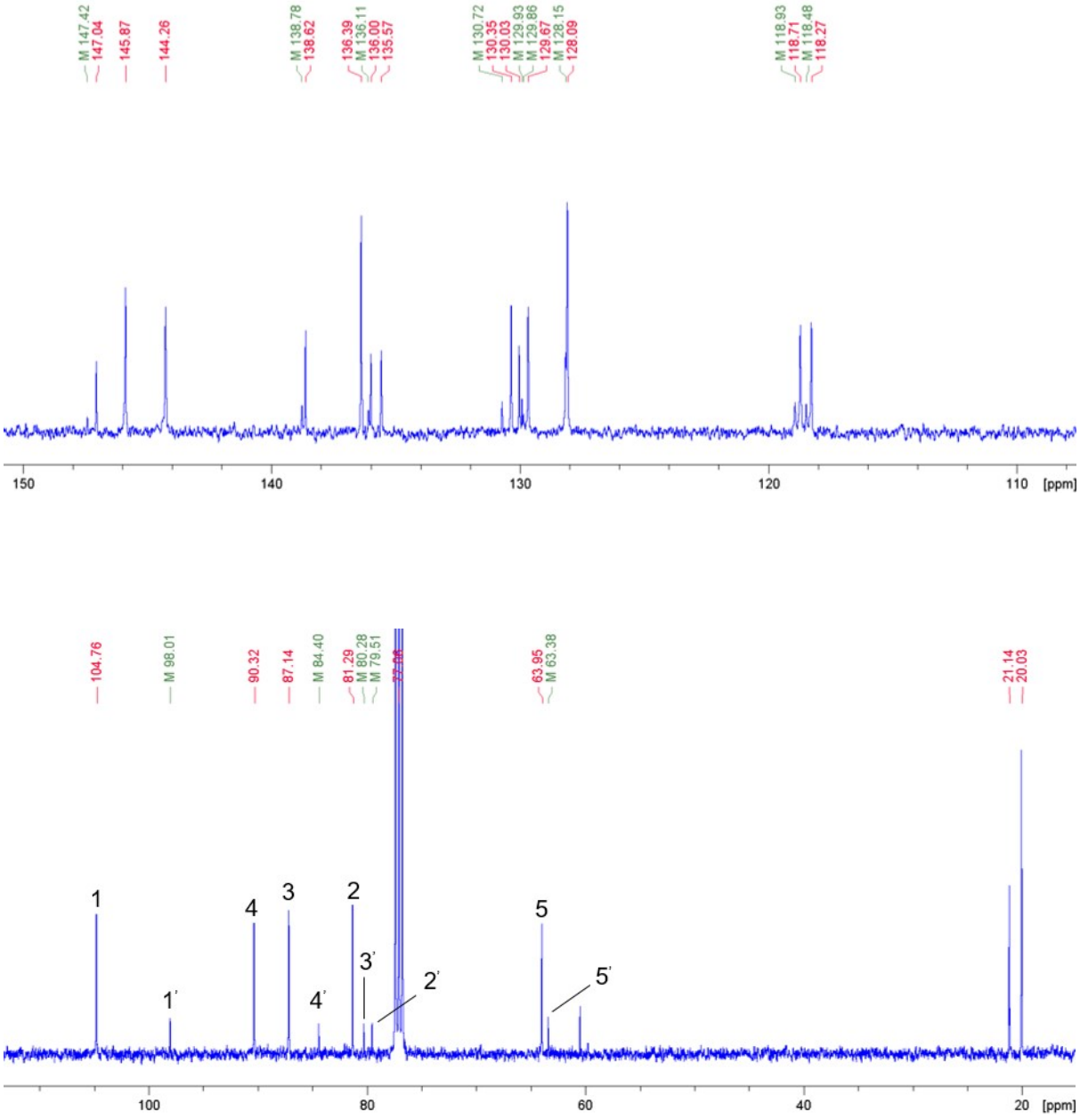
S5.22 Conjugate 4Rc': α-Ribopyranose-(2,3)-O-BODIPY



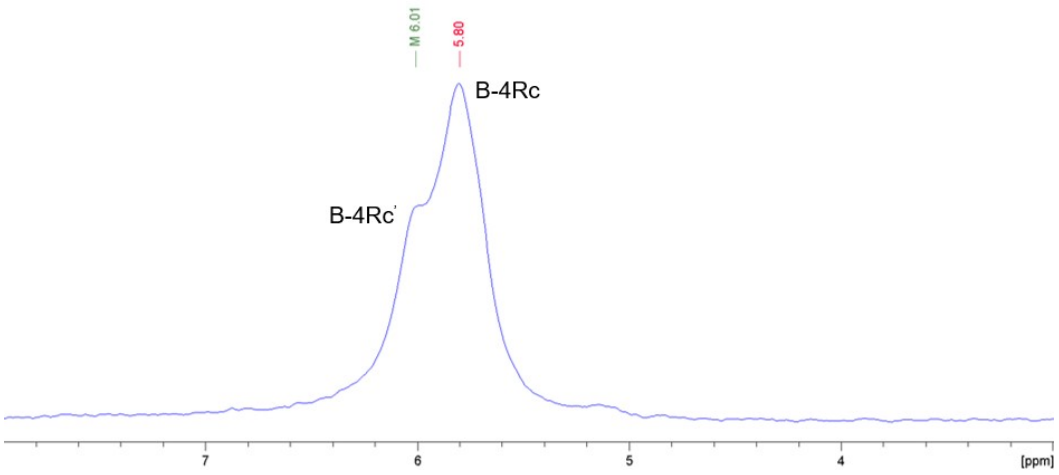
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Rc'



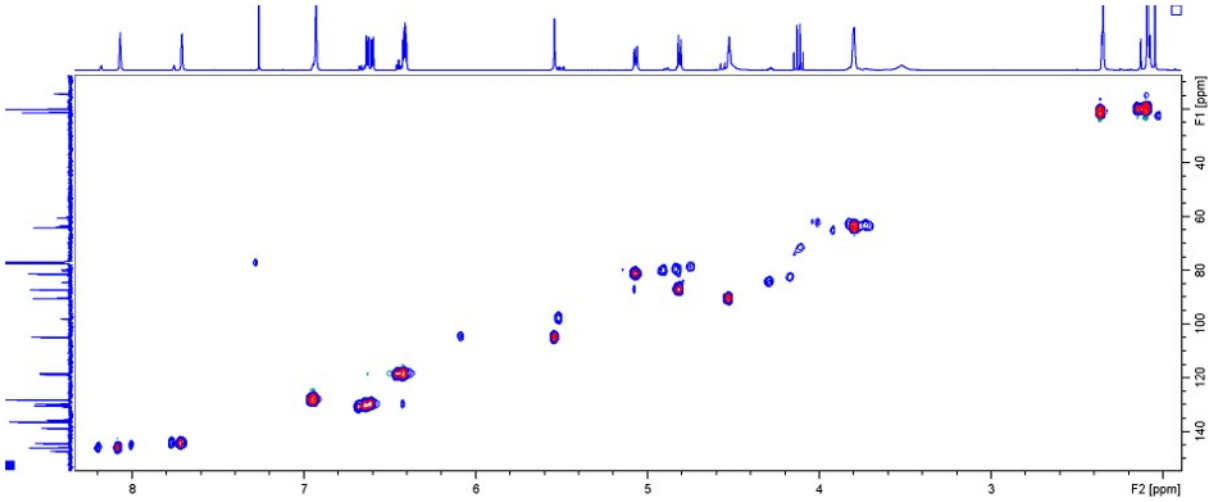
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Rc (red) and 4Rc' (green)



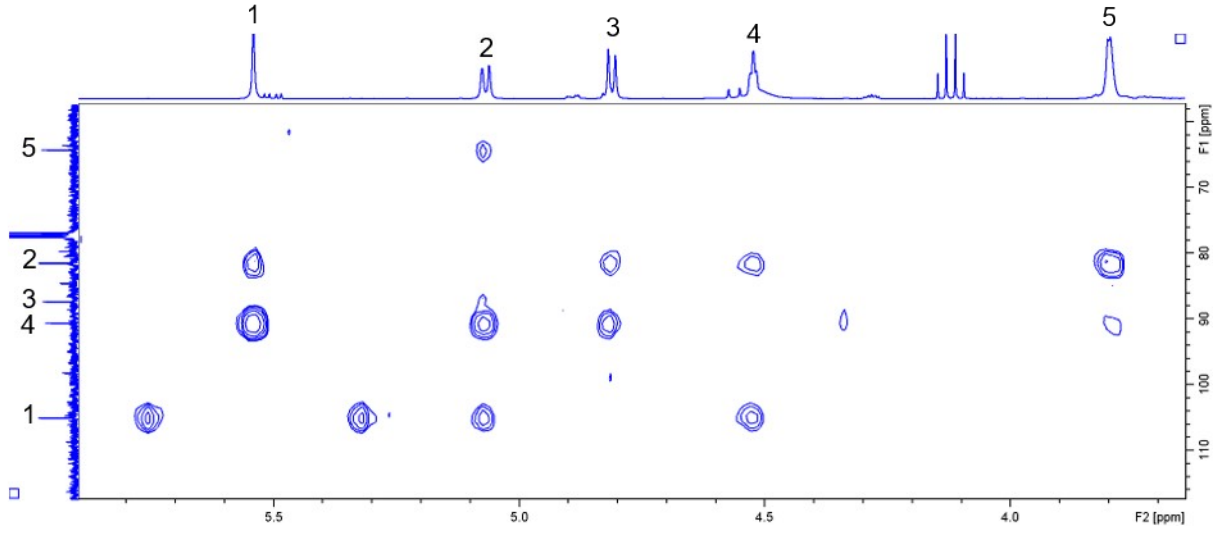
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Rc



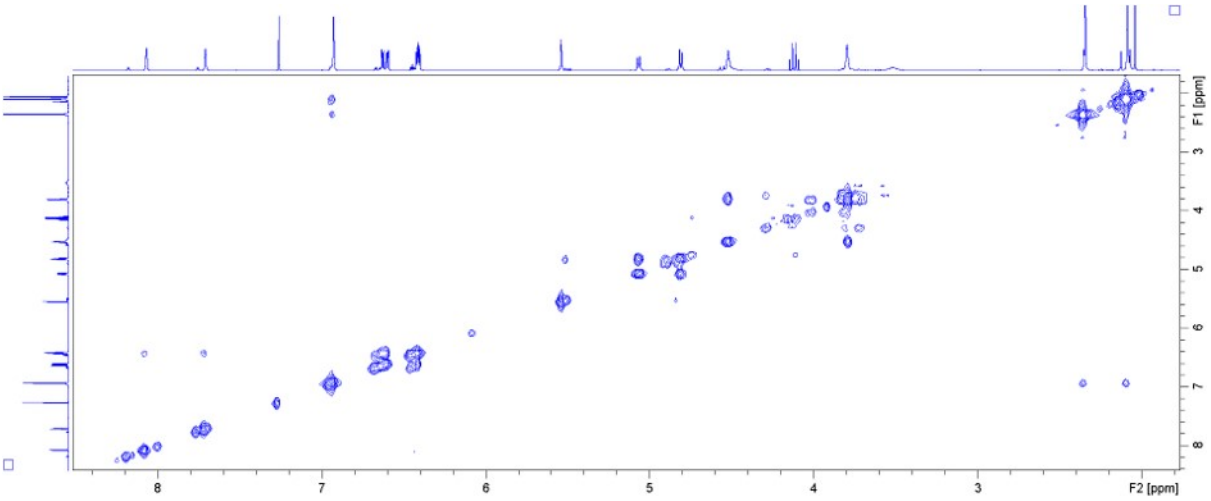
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Rc



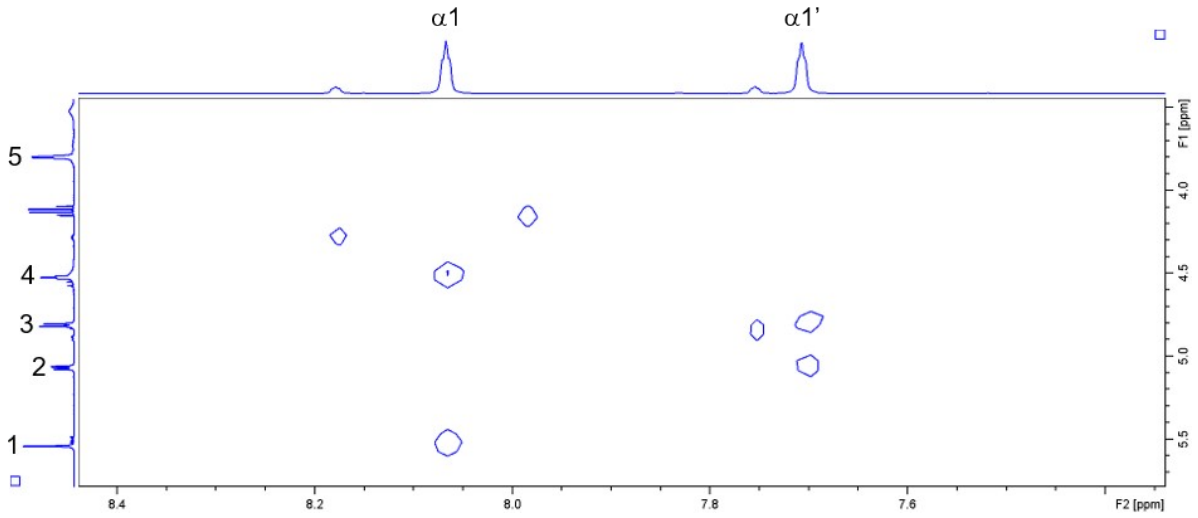
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Rc



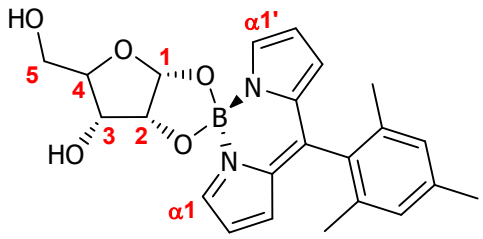
^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Rc



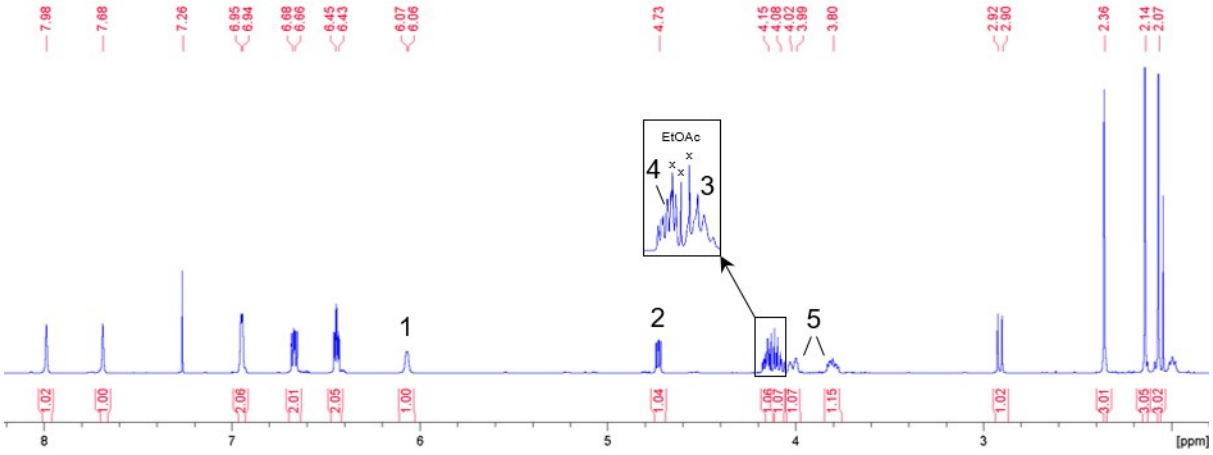
^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Rc



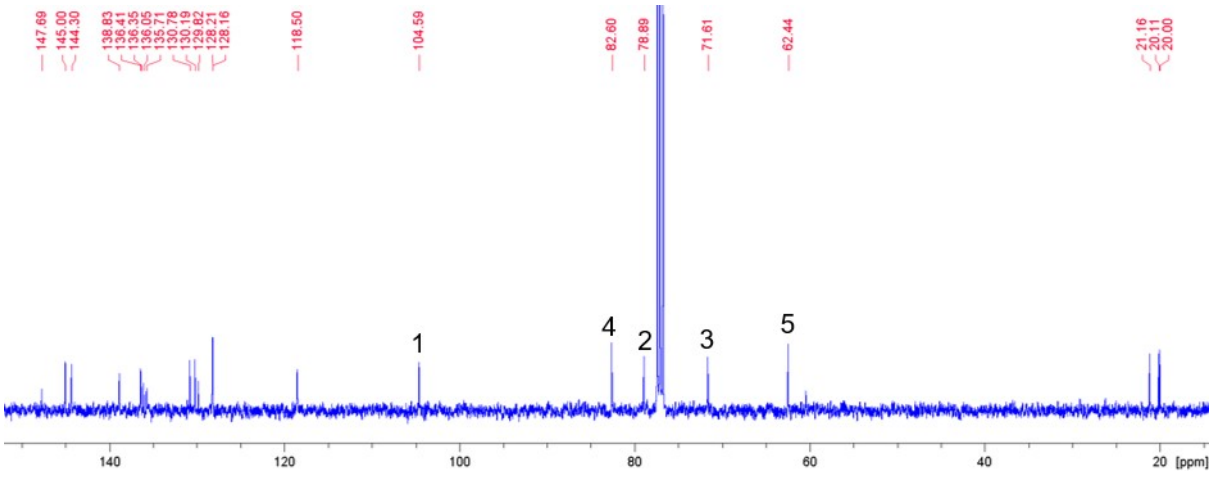
S5.23 Conjugate 4Rd: α-Ribofuranose-(1,2)-O-BODIPY



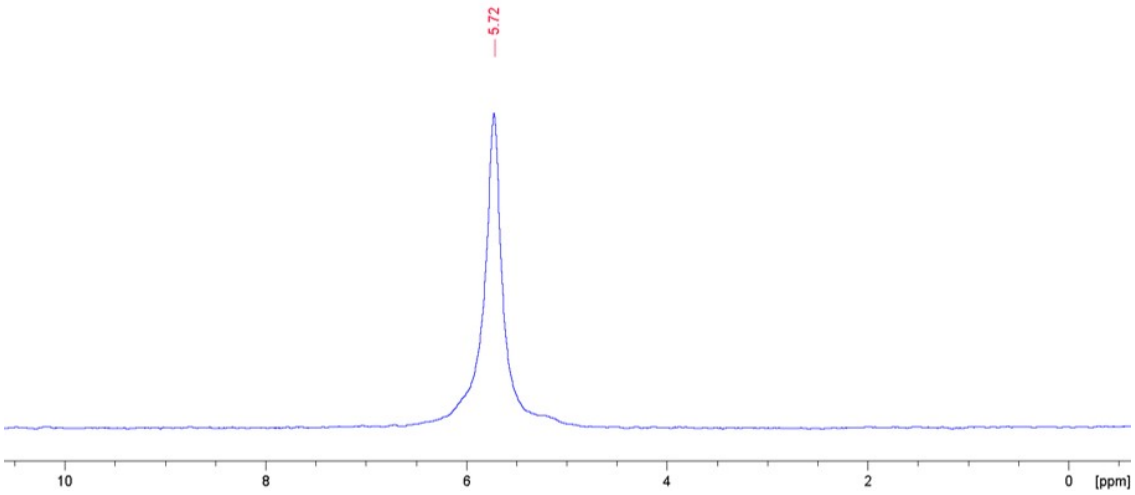
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4Rd



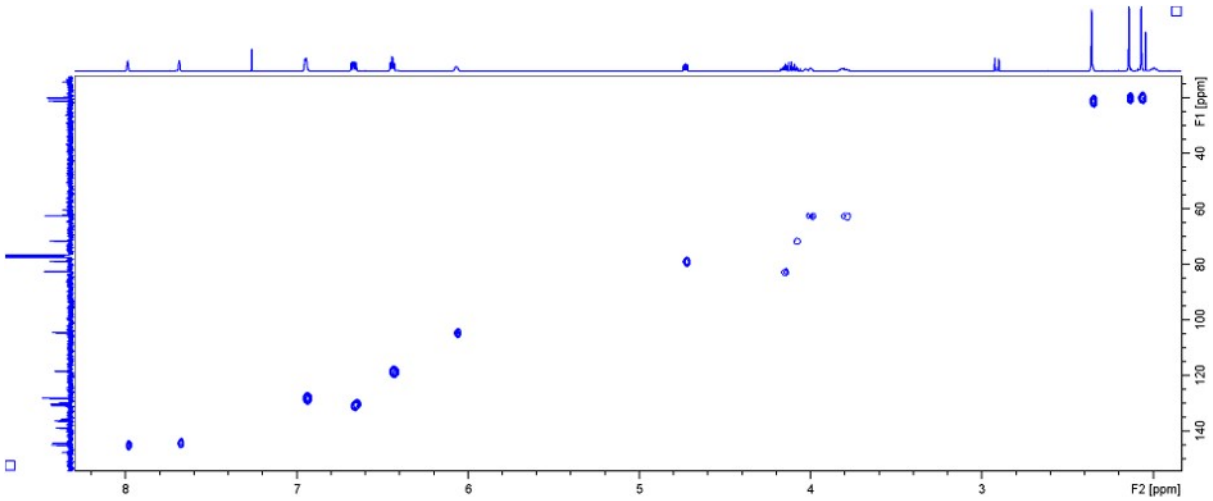
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4Rd



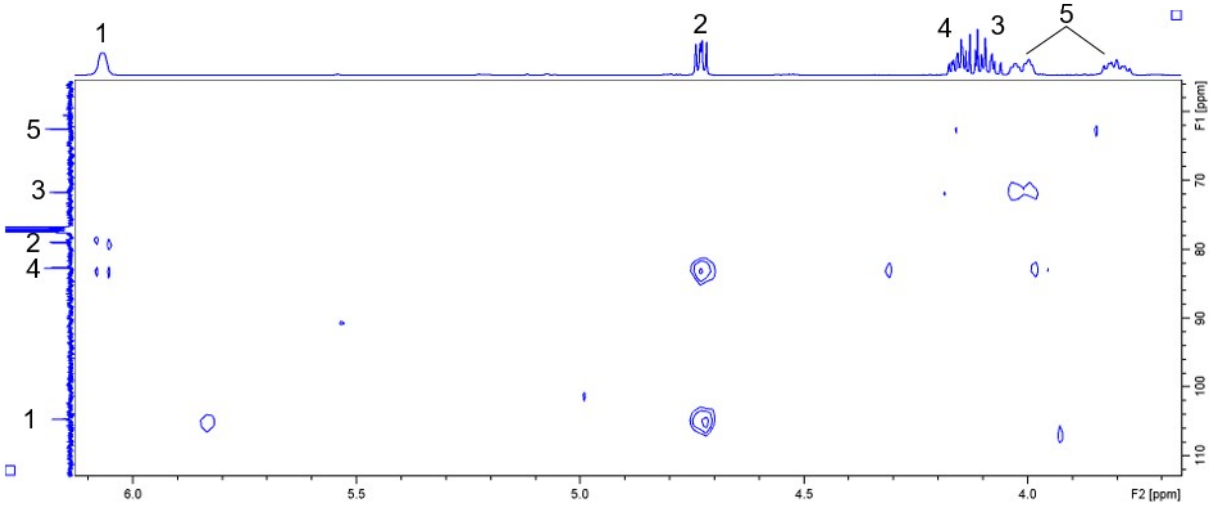
^{11}B NMR (128 MHz, $CDCl_3$) spectrum of 4Rd



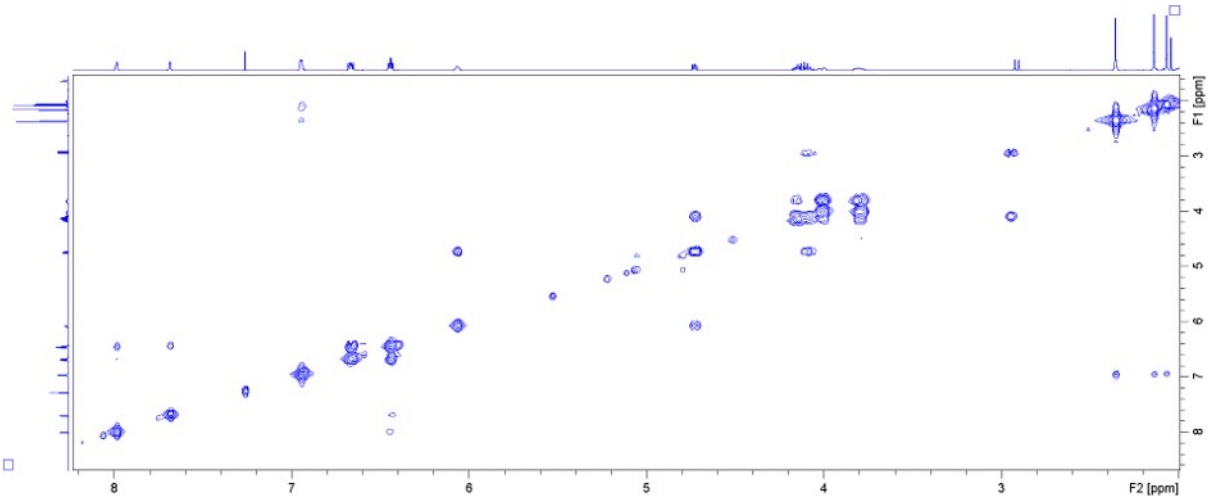
^{1}H-^{13}C HSQC NMR ($CDCl_3$) spectrum of 4Rd



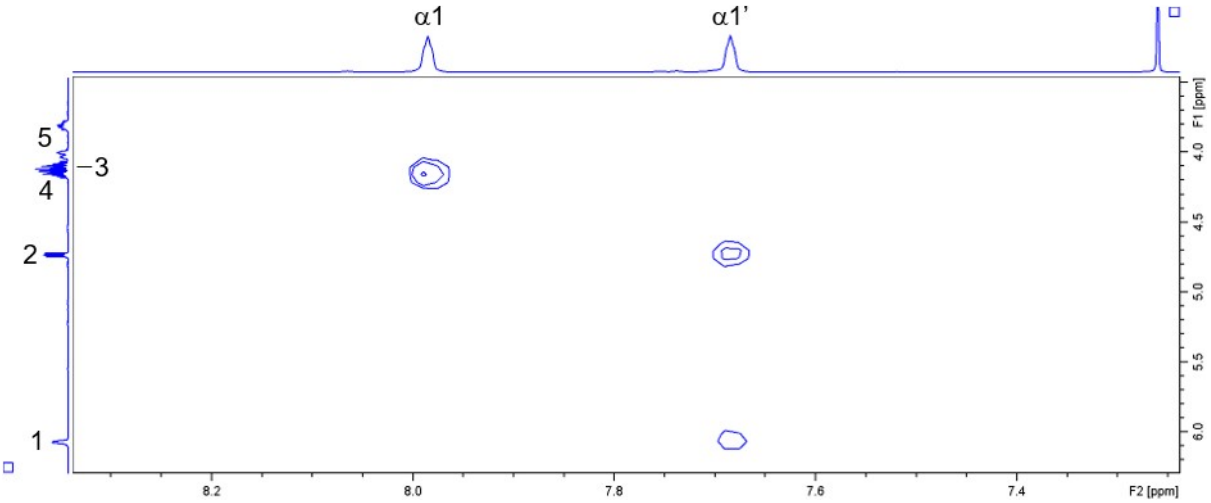
^{1}H-^{13}C HMBC NMR ($CDCl_3$) spectrum of 4Rd



^{1}H-^{1}H COSY NMR ($CDCl_3$) spectrum of 4Rd



^{1}H-^{1}H NOESY NMR ($CDCl_3$) spectrum of 4Rd



S6 XRD data tables for compounds 3, 3Ra, 3Rd, 4: **3**: Crystals were grown by the slow evaporation of a CH_2Cl_2:n-hexane solution in the dark at room temperature, **3Ra** and **3Rd**: Crystals were grown by the slow evaporation of a CH_2Cl_2:MeCN solution in the dark at room temperature, **4**: Crystals were grown by the slow evaporation of a CH_2Cl_2 solution in the dark at 3 °C.

	3	**3Ra**	**3Rd**	**4**
CCDC	2040727	2040728	2040729	2040730
Formula	$C_{18}H_{19}BN_2O_2$	$C_{37}H_{32}B2N_4O5 \cdot 2/3\ C_2H_3N \cdot 0.2\ CH_2Cl_2$	$C_{21}H_{21}BN_2O5$	$C_{20}H_{23}BN_2O_2$
Formula weight (g mol^{-1})	306.16	679.30	392.21	334.21
Temperature/K	100.0(1)	100.0(9)	105(8)	100.0(1)
Crystal system	monoclinic	orthorhombic	orthorhombic	orthorhombic
Space group	*C*2/*c*	$P2_12_12_1$	$P2_12_12_1$	*Pbca*
Unit cell dimensions	*a* = 13.6344(2)Å *b* = 9.5665(1) Å *c* = 23.8456(3) Å *β* = 97.092(1)°	*a* = 11.0231(2) Å *b* = 11.6298(2) Å *c* = 26.1050(5)Å	*a* = 6.6897(2) Å *b* = 6.8564(2) Å *c* = 39.6011(11) Å	*a* = 11.8127(2) Å *b* = 8.2716(1) Å *c* = 38.1140(6) Å
Volume (Å^3)	3086.47(7)	3346.6(1)	1816.39(9)	3724.12(10)
Z	8	4	4	8
Density $_{calcd}$ (g cm^{-3})	1.318	1.348	1.434	1.192
μ (mm^{-1})	0.681	1.011	0.839	0.603
***F*(000)**	1296.0	1421.0	824.0	1424.0
Crystal size/mm^3	0.15 x 0.12 x 0.1	0.083 x 0.072 x 0.041	0.2 x 0.16 x 0.1	0.15 x 0.12 x 0.11
2Θ range (deg)	11.328 to 136.496	11.568 to 136.472	13.104 to 135.474	11.934 to 136.498
***h* range**	-16 to 16	-13 to 13	-7 to 8	-12 to 14
***k* range**	-11 to 11	-14 to 14	-6 to 8	-9 to 9
***l* range**	-28 to 28	-31 to 31	-47 to 41	-45 to 45
Reflections collected / Independent reflections	18118 / 2826	27509 / 6115	9362 / 3280	18535 / 3395
***R*$_{int}$/*R*$_{sigma}$**	R_{int} = 0.0289, R_{sigma} = 0.0181	R_{int} = 0.0543, R_{sigma} = 0.0400	R_{int} = 0.0335, R_{sigma} = 0.0376	R_{int} = 0.0302, R_{sigma} = 0.0240
Restraints / parameters	0/212	1/487	0/272	0/232
Goodness-of-fit	1.063	1.036	1.039	1.038
Final *R* indexes [*I* > 2σ (*I*)]	R_1 = 0.0320, wR_2 = 0.0811	R_1 = 0.0381, wR_2 = 0.0975	R_1 = 0.0322, wR_2 = 0.0761	R_1 = 0.0365, wR_2 = 0.0937
***R* indices (all data)**	R_1 = 0.0336, wR_2 = 0.00824	R_1 = 0.0407, wR_2 = 0.0995	R_1 = 0.0358, wR_2 = 0.0780	R_1 = 0.0406, wR_2 = 0.0966
Largest diff. peak/hole eÅ^{-3}	0.26/-0.19	0.28/-0.17	0.20/-0.17	0.27/-0.19
Flack parameter	-	-0.01(4)	0.04(10)	-

1 P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, Ab Initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields, *J. Phys. Chem.*, 1994, **98**, 11623–11627.

2 A. D. Becke, Density-functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys.*, 1993, **98**, 5648–5652.

3 C. Lee, W. Yang and R. G. Parr, Local softness and chemical reactivity in the molecules CO, SCN- and H_2CO, *Phys. Rev. B*, 1988, **37**, 785–789.

4 M. J. Frisch, G. W. Trucks, H. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson and others, Gaussian 09, Revision D. 01, Gaussian, Inc., Wallingford CT, 2013 Search PubMed;(b) AD Becke, *J. Chem. Phys*, 1993, **98**, 785–789.

5 M. D. Hanwell, D. Curtis, D. Lonie, T. Vandermeersch, E. Zurek and G. Hutchison, Avogadro: an open-source molecular builder and visualization tool, *J. Cheminfo.*, 2012, 4, 17.

6 T. Yanai, D. P. Tew and N. C. Handy, A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP), *Chem. Phys. Lett.*, 2004, **393**, 51–57.

7 T. Rohand, E. Dolusic, T. H. Ngo, W. Maes and W. Dehaen, Efficient synthesis of aryldipyrromethanes in water and their application in the synthesis of corroles and dipyrromethenes, *Arkivoc*, 2007, **10**, 307–

324.

8 B. R. Groves, S. M. Crawford, T. Lundrigan, C. F. Matta, S. Sowlati-Hashjin and A. Thompson, Synthesis and characterisation of the unsubstituted dipyrrin and 4,4-dichloro-4-bora-3a,4a-diaza-s-indacene: Improved synthesis and functionalisation of the simplest BODIPY framework, *Chem. Commun.*, 2013, **49**, 816–818.

9 Sheldrick, G. Crystal structure refinement with SHELXL. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **2015,** *71*, 3-8.

10 Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **2009,** *42*, 339-341.

11 Macrae, C. F.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Shields, G. P.; Taylor, R.; Towler, M.; van de Streek, J. Mercury: visualization and analysis of crystal structures. *J. Appl. Crystallogr.* **2006,** *39*, 453-457.