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Supporting Information

Synthesis of [60]Fullerene Hybrids Endowed with Steroids and Monosaccharides: Theoretical Underpinning as Promising anti-SARS-CoV-2 Agents

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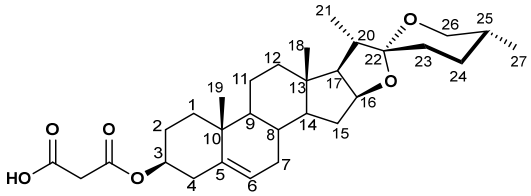
1. Synthesis and Characterization

1.1. Synthesis of mono-carboxylic malonates 2a and 2b

To a solution of the appropriate steroid diosgenin (**1a**) or cholesterol (**1b**) (4.82 mmol) in toluene (100 mL), Meldrum´s acid (1.04 g, 7.24 mmol) was added and the mixture was stirred under reflux. After 1 h the solvent was removed under reduced pressure. The crude product was purified by column chromatography on silica gel with *n*-hexane/ethyl acetate (1:1) as the eluent.

3-[((22R, 25R)-Spirost-5-en-3β-yl)oxy]-3-oxopropanoic acid (2a)



This compound was obtained from **1a**. The product was isolated as a yellow solid.

Yield: 2.4 g (4.79 mmol, 86%)

M.p.: 186-187 ºC

^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.38 (d, *J* = 5.2 Hz, 1H, H6), 4.70 (m, 1H, H3), 4.41 (m, 1H, H16), 3.48 (d, *J* = 9.4 Hz, 1H, H26), 3.41 (s, 2H, $OCCH_2CO$), 3.37 (t, *J* = 11.1 Hz, 1H, H26), 2.36 (m, 2H, H4), 1.98 (m, 2H, H1), 1.87 (m, 3H, H12, H20, H23), 1.78 (dd, *J* = 9.5, 6.0 Hz, 1H, H17), 1.74 (m, 1H, H2), 1.67 (m, 2H, H7), 1.62 (m, 3H, H8, H25, H24), 1.58 – 1.50 (m, 2H, H11, H12), 1.45 (m, 2H, H24, H11), 1.31 – 1.25 (m, 2H, H15), 1.18 (m, 1H, H2), 1.13-1.09 (m, 2H, H14, H23), 1.03 (s, 3H, H19), 0.99 - 0.95 (m, 4H, H9, H21), 0.79 (t, *J* = 3.2 Hz, 6H, H18, H27).

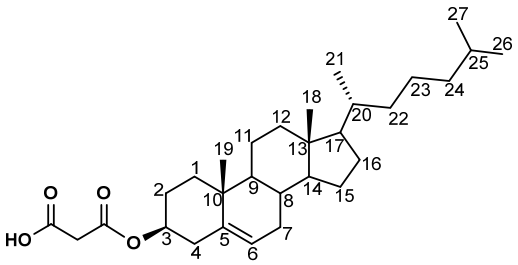
^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm):169.5 (C=O), 167.4 (C=O), 139.2 (C5), 123.0 (C6), 109.6 (C22), 81.0 (C16), 77.1 (C3), 67.0 (C26), 62.1 (C17), 56.5 (C14), 50.0 (C9), 41.7 (C20), 40.6 ($OCCH_2CO$), 40.4 (C13), 39.8 (C2), 37.9 (C4), 37.0 (C1), 36.8 (C10), 32.2 (C23), 31.9 (C15), 31.5 (C8), 31.4 (C7), 30.4 (C25), 28.9 (C24), 27.6 (C12), 20.9 (C11), 19.4 (C19), 17.3 (C27), 16.4 (C18), 14.6 (C21).

FTIR: ν 2946, 2904, 1733, 1454, 1155, 735 cm^{-1}.

MS (ESI): 499.0 $[M-H]^-$

Anal. Calcd for $C_{30}H_{44}O_6$: C 71.97, H 8.86; found C 72.01, H 8.89.

3-[(Cholest-5-en-3β-yl)oxy]-3-oxopropanoic acid (2b)



This compound was obtained from **1b**. The product was isolated as a white solid.

Yield: 1.89 g (4.01 mmol, 85%)

M.p.:165-166 ºC

^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.39 (d, *J* = 5.1 Hz, 1H, H6), 4.72 (m, 1H, H3), 3.42 (s, 2H, ($OCCH_2CO$), 2.36 (d, *J* = 7.9 Hz, 2H, H4), 2.02 (d, *J* = 3.5 Hz, 2H, H12), 2.01 – 1.98 (m, 1H, H7), 1.96 (t, *J* = 5.3 Hz, 1H, H7), 1.89 (m, 3H, H2, H1), 1.81 (m, 1H, H16), 1.62 (m, 1H, H2), 1.60 (m, 2H, H23), 1.56 (m, 1H, H25), 1.50 (m, 2H, H11), 1.44 (m,1H, H8), 1.37 (m, 1H, H20), 1.34 (m, 2H, H15, H22), 1.26 (d, *J* = 10.6 Hz, 1H, H16), 1.16 (d, *J* = 4.1 Hz, 1H, H24), 1.14 (t, *J* = 4.1 Hz, 2H, H15, H24), 1.09 (d, *J* = 9.1 Hz, 1H, H17), 1.02 (s, 3H, H19), 1.00 (m, 2H, H14, H22), 0.97 (d, *J* = 2.1 Hz, 1H, H9), 0.91 (d, *J* = 6.5 Hz, 3H, H21), 0.86 (dd, *J* = 6.7, 3.3 Hz, 6H, H26, H27), 0.67 (s, 3H, H18).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 169.9 (C=O), 167.5 (C=O), 139.2 (C5), 123.3 (C6), 76.3 (C3), 56.8 (C14), 56.2 (C17), 50.1 (C9), 42.4 (C13), 40.4 ($OCCH_2CO$), 39.8 (C24), 39.6 (C12), 37.9 (C4), 37.1 (C1), 36.7 (C10), 36.3 (C22), 35.9 (C20), 32.0 (C7), 32.0 (C8), 28.4 (C2), 28.1 (C25), 27.7 (C16), 24.4 (C15), 24.0 (C23), 23.0 (C26), 22.7 (C27), 21.2 (C11), 19.4 (C19), 18.8 (C21), 12.0 (C18).

FTIR: ν 3302, 2925, 2854, 1746, 1712, 1462, 1214, 1173, 736 cm^{-1}.

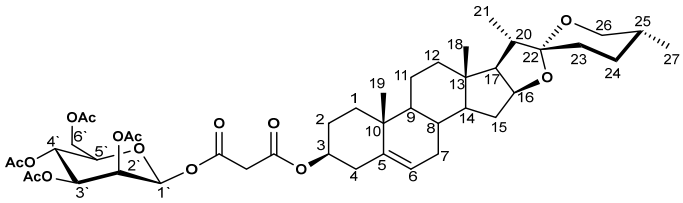
MS (ESI): 495.4 $[M+Na]^+$

Anal. Calcd for $C_{30}H_{48}O_4$: C 76.23, H 10.24; found: C 76.26, H 10.27.

1.2. Synthesis of steroid-sugar conjugates

Method A

(22R,25R)-spirost-5-en-3β-yl malonate-2',3',4',6'-tetra-O-acetyl-β-D-mannopyranoside (4a)



A solution of malonate **2a** (0.94 g, 1.87 mmol), **3a** (0.54 g, 1.10 mmol), 4 Å molecular sieves (0.5 g) in dry CH_2Cl_2 (10 mL) was stirred for 5 min. The solution was cooled to 0 °C and $BF_3 \cdot Et_2O$ (0.3 mL, 2.37 mmol) was added over 5 min over argon. The mixture was stirred for 1 h at room temperature and the reaction mixture was neutralized with Et_3N, filtered through celite, the solvent was removed and the residue was purified by column chromatography in silica gel with *n*-hexane/ethyl acetate (3:1) as the eluent. The product was isolated as a white solid;

Yield: 0.54 g (0.65 mmol, 60%)

M.p.: 90-91 ºC

^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 6.11 (d, *J* = 1.9 Hz, 1H, H1'), 5.40 (d, *J* = 9.3 Hz, 1H, H6), 5.33 (m, 2H, H3', H4'), 5.28 (d, *J* = 1.3 Hz, 1H, H2'), 4.68 (m, 1H, H3), 4.40 (m, 1H, H16), 4.29 (dd, *J* = 12.9, 5.4 Hz, 1H, H6'), 4.11 (m, 2H, H5', H6'), 3.45 (m, 3H, H26, $OCCH_2CO$), 3.37 (t, *J* = 11.0 Hz, 1H, H26), 2.37 (m, 2H, H4), 2.18 (s, 3H, CH_3), 2.09 (s, 3H, CH_3), 2.05 (s, 3H, CH_3), 2.00 (s, 3H, CH_3), 1.99 – 1.95 (m, 2H, H1), 1.92 – 1.84 (m, 3H, H12, H20, H23), 1.80 – 1.76 (m, 1H, H17), 1.73 (m, 1H, H2), 1.68 - 1.59 (m, 5H, H7, H8, H24, H25), 1.57 - 1.42 (m, 2H, H11, H24), 1.27 (m, 2H, H11, H12), 1.20 – 1.08 (m, 5H, H2, H14, H15, H23), 1.03 (s, 3H, H19), 0.97 (d, *J* = 7.0 Hz, 4H, H9, H21), 0.78 (m, 6H, H18, H27).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 170.8 (C=O) mannose, 167.0 (C=O) mannose, 169.8 (C=O) mannose, 169.7 (C=O) mannose, 165.3 (C=O), 164.1 (C=O), 139.4 (C5), 122.9 (C6), 109.4 (C22), 91.4 (C1'), 80.9 (C16), 75.9 (C3), 70.9 (C5'), 68.8 (C3'), 68.3 (C2'), 67.0 (C26), 65.5 (C4'), 62.2 (C17), 62.0 (C6'), 56.5 (C14), 50.0 (C9), 41.7 (C20), 41.7 ($OCCH_2CO$), 40.4 (C13), 39.8 (C2), 37.9 (C4), 37.0 (C1), 36.8 (C10), 32.2 (C23), 31.9 (C15), 31.5 (C7, C8), 30.4 (C25), 28.9 (C24), 27.7 (C12), 21.0 (C11), 20.9 (CH_3), 20.8 (CH_3), 20.8 (CH_3), 20.7 (CH_3), 19.4 (C19), 17.3 (C27), 16.4 (C18), 14.7 (C21).

FTIR: ν 2930, 2852, 1747, 1217, 736, 598 cm^{-1}.

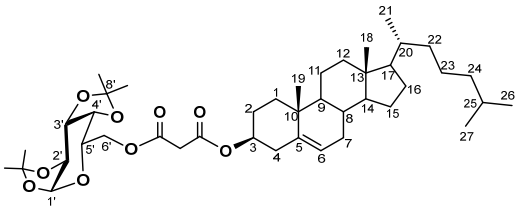
HRMS (MALDI-TOF) m/z: $[M+H]^+$ calcd for $C_{44}H_{63}O_{15}$: 831,4167; found 831,4197.

Anal. Calcd for $C_{44}H_{63}O_{15}$: C 63.60, H 7.52; found C 63.69, H 7.60.

Method B

To a stirred solution of the corresponding monosaccharide **3b** or **3c** (0.38 mmol) in dry CH_2Cl_2 (5 mL), was added the corresponding malonic acid (**2a** or **2b**) (0.5 mmol) followed by EDC·HCl (221 mg, 1.15 mmol). After stirring at 25 °C for 1 h the mixture was diluted with CH_2Cl_2 (5 mL). The solution mixture was washed with two 10 mL portions of water and saturated NaCl aqueous solution (15 mL). The organic layer was dried ($MgSO_4$) and filtered, and the solvent was removed under reduced pressure. The crude product was purified by column chromatography on silica gel with *n*-hexane/ethyl acetate (6:1) as the eluent.

6'-(Cholest-5-en-3β-y malonate)-1',2':3',4'-di-O- isopropylidene-α-D-galactopyranoside (4b)



This compound was obtained from the monosacharide **3b** and the steroidal acid **2b**. The product was isolated as a white solid.

Yield: 0.20 g (0.28 mmol, 71%). **M.p.**: 105-106 ºC.

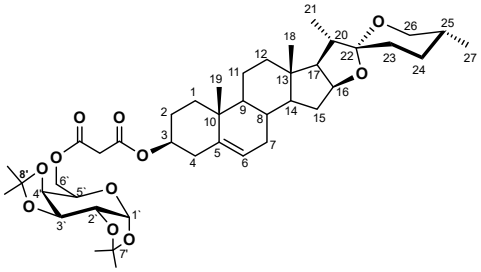
^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.53 (d, *J* = 5.0 Hz, 1H, H1′), 5.38 (d, *J* = 5.2 Hz, 1H, H6), 4.66 (m, 1H, H3), 4.62 (dd, *J* = 7.9, 2.5 Hz, 1H, H3′), 4.35 (d, *J* = 5.0 Hz, 1H, H6′), 4.33 (m, 1H, H2'), 4.27 (dd, *J* = 11.5, 7.5 Hz, 1H, H6′), 4.24 (dd, *J* = 7.8, 1.8 Hz, 1H, H4′), 4.04 (m, 1H, H5′), 3.40 (s, 2H, $OCCH_2CO$), 2.34 (dd, *J* = 12.7, 3.9 Hz, 2H, H4), 2.01 (m, 2H, H12), 1.95 (m, 1H, H7), 1.87 (d, *J* = 14.1 Hz, 1H, H2), 1.85 (t, *J* = 3.6 Hz, 1H, H1), 1.83 (m, 1H, H16), 1.60 (m, 3H, H2, H23), 1.52 (s, 3H, CH_3), 1.45 (s, 3H, CH_3), 1.44 (m, 4H, H7, H11, H25), 1.42 (d, *J* = 11.6 Hz, 1H, H8), 1.37 (m, 1H, H20), 1.33 (m, 7H, H22, 2 CH_3), 1.25 (m, 1H, H16), 1.14 (m, 4H, H1, H24, H25), 1.07 (m, 3H, H15, H17), 1.01 (s, 3H, H19), 0.99 (d, *J* = 8.2 Hz, 2H, H14, H22), 0.94 (m, 1H, H9), 0.91 (d, *J* = 6.5 Hz, 3H, H21), 0.86 (dd, *J* = 6.7, 3.2 Hz, 6H, H26, H27), 0.67 (s, 3H, H18).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 166.8 (C=O), 166.0 (C=O), 139.6 (C5), 123.0 (C6), 109.8 (C7′), 109.0 (C8′), 96.4 (C1′), 75.5 (C3), 71.1 (C4′), 70.8 (C3′), 70.5 (C2′), 65.9 (C5′), 64.4 (C6′), 56.9 (C14), 56.3 (C17), 50.1 (C9), 42.4 (C13), 41.9 ($OCCH_2CO$), 39.8 (C24), 39.7 (C12), 38.0 (C4), 37.0 (C1), 36.7 (C10), 36.3 (C22), 35.9 (C20), 32.0 (C7), 32.0 (C8), 28.4 (C2), 28.2 (C25), 27.7 (C16), 26.2 (CH_3), 26.1 (CH_3), 25.1 (CH_3), 24.6 (CH_3), 24.4 (C15), 24.0 (C23), 23.0 (C26), 22.7 (C27), 21.2 (C11), 19.4 (C19), 18.9 (C21), 12.0 (C18).

FTIR: ν 2931, 2856, 1735, 1463, 1377, 1071, 1007, 737 cm^{-1}.

MS (ESI): 737.5 $[M+Na]^+$. Anal. Calcd for $C_{42}H_{66}O_9$: C 70.56, H 9.30; found C 70.61, H 9.35.

6'-(22R,25R)-Spirost-5-en-3β-yl-malonate)-1',2':3',4'-di-O-isopropylidene-α-D-galacto-pyranoside (4c)



This compound was obtained from the monosacharide **3b** and the steroidal acid **2a**. The product was isolated as a white solid.

Yield: 0.22 g (0.30 mmol, 75%)

M.p.: 123-124 ºC

^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.53 (d, *J* = 4.9 Hz, 1H, H1'), 5.37 (dt, *J* = 5.4, 2.0 Hz, 1H, H6), 4.65 (m, 1H, H3), 4.62 (dd, *J* = 7.9, 2.6 Hz, 1H, H3'), 4.41 (m, 1H, H16), 4.37 – 4.30 (m, 2H, H2', H6'), 4.30 – 4.22 (m, 2H, H5', H6'), 4.04 (m, 1H, H4'), 3.47 (m, 1H, H26), 3.37 (t, *J*= 11.0 Hz, 1H, H26), 3.38 (s, 2H, $OCCH_2CO$), 2.35 (m, 2H, H4), 1.99 (m, 2H, H1), 1.87 (m, 4H, H12, H20, H23), 1.77 (m, 1H, H17), 1.73 (m, 1H, H2), 1.71 – 1.56 (m, 5H, H7, H8, H24, H25),1.56 – 1.52 (m, 1H, H11), 1.51 (s, 3H, CH_3), 1.49 – 1.45 (m, 1H, H11), 1.45 (s, 3H, CH_3), 1.34 (s, 3H, CH_3), 1.33 (s, 3H, CH_3), 1.32 – 1.23 (m, 1H, H7), 1.21 – 1.07 (m, 5H, H2, H14, H15, H23), 1.03 (s, 3H, H19), 0.97 (d, *J* = 7.0 Hz, 4H, H9, H21), 0.79 (d, *J* = 5.6 Hz, 6H, H18, H27).

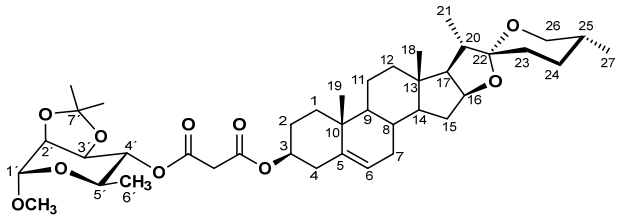
^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 166.8 (C=O), 165.9 (C=O), 139.6 (C5), 122.7 (C6), 109.8 (C22), 109.4 (C7'), 109.0 (C8'), 96.4 (C1'), 80.9 (C16), 75.3 (C3), 71.1 (C2'), 70.8 (C5'), 70.5 (C3'), 67 (C26), 65.9 (C4'), 64.4 (C6'), 62.2 (C17), 56.5 (C14), 50.0 (C9), 41.9 ($OCCH_2CO$), 41.7 (C20), 40.4 (C13), 39.8 (C2), 37.9 (C4), 37.0 (C23), 36.8 (C10), 32.2 (C1), 32.0 (C15), 31.5 (C7, C8), 30.4 (C25), 28.9 (C24), 27.7 (C12), 26.2 (CH_3), 26.1 (CH_3), 25.1(CH_3), 24.6 (CH_3), 20.9 (C11), 19.5 (C19), 17.3 (C27), 16.4 (C18), 14.7 (C21).

FTIR: ν = 2925, 2853, 1734, 1376, 1069, 896, 736 cm^{-1}.

HRMS (MALDI-TOF) m/z: $[M+H]^+$ Calcd for $C_{42}H_{63}O_{11}$: 743.4370; found 743.4394.

Anal. Calcd for $C_{42}H_{63}O_{11}$: C 67.90, H 8.41; found C 67.97, H 8.46.

Methyl-6'-((22R,25R)-spirost-5-en-3β-ylmalonate)-2',3'-O-isopropylidene-α-L-rhamnopyranoside (4d)



This compound was obtained from the monosacharide **3c** and the steroidal acid **2b**. The product was isolated as a white solid.

Yield: 0.19 g (0.28 mmol, 72%). **M.p.**: 77-78 ºC

^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.37 (m, 1H, H6), 4.89 (m, 2H, H1′, H4′), 4.65 (m, 1H, H3), 4.41(m, 1H, H16), 4.16 (dd, *J* = 7.8, 5.4 Hz, 1H, H2′), 4.13 (d, *J* = 5.5 Hz, 1H, H3′), 3.72 (m, 1H, H5′), 3.47 (m, 1H, H26), 3.43 – 3.26 (m, 4H, CH_3O, H26), 3.38 (s, 2H, $OCCH_2CO$), 2.34 (m, 2H, H4), 1.99 (m, 2H, H1), 1.87 (m, 4H, H12, H20, H23), 1.80 – 1.71 (m, 2H, H2, H17), 1.71 – 1.59 (m, 6H, H7, H8, H24, H25), 1.52 (s, 3H, CH_3), 1.48 – 1.38 (m, 2H, H11), 1.34 (s, 3H, CH_3), 1.28 (m, 2H, H15), 1.23 (d, *J* = 6.3 Hz, 3H, H6′), 1.21 – 1.11 (m, 2H, H2, H14), 1.10 (m, 1H, H23), 1.02 (s, 3H, H19), 0.97 (d, *J* = 6.8 Hz, 4H, H9, H21), 0.79 (d, *J* = 5.8 Hz, 6H, H18, H27).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 165.9 (2 C=O), 139.5 (C5), 122.8 (C6), 110.0 (C7′), 109.4 (C22), 98.1 (C1′), 80.9 (C16), 76.0 (C3′), 75.8 (C2′), 75.6 (C4′), 75.5 (C3), 67.0 (C26), 63.8 (C5′), 62.2 (C17), 56.5 (C14), 55.1 (CH_3-O), 50.0 (C9), 42.2 ($OCCH_2CO$), 41.7 (C20), 40.4 (C13), 39.8 (C2), 37.9 (C4), 37.0 (C23), 36.8 (C10), 32.2 (C1), 32.0 (C15), 31.5 (C7,C8), 30.4 (C25), 28.9 (C24), 27.9 (CH_3), 27.7 (C12), 26.5 (CH_3), 20.9 (C11), 19.4 (C19), 17.3 (C6'), 17.1 (C27), 16.4 (C18), 14.7 (C21).

FTIR: ν 2942, 1735, 1454, 1142, 1091, 982, 736 cm^{-1}. **MS** (ESI): 699.2 $[M-H]^-$.

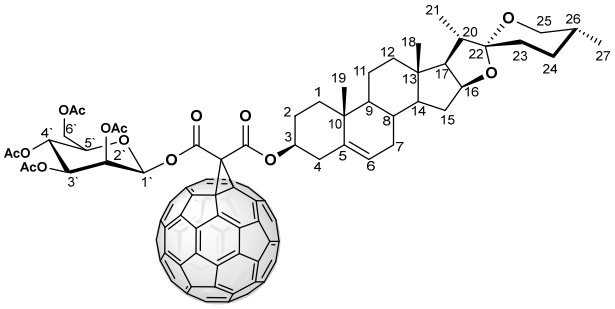
Anal. Calcd for $C_{40}H_{60}O_{10}$: C 68.54, H 8.63; found C 68.59, H 8.68.

1.3. Synthesis of Bingel–Hirsch hybrids

A solution of C_{60} (50 mg, 0.069 mmol) in toluene (100 mL) was prepared. The corresponding malonate (0.069 mmol), CBr_4 (0.12 mmol), and diazabicyclo[4.2.0]undec-7-ene (DBU; 0.19 mL, 1.35 mmol) were added in that order. The reaction mixture was then stirred at room temperature for 2 h. Water was added, and the residue was extracted with toluene. The combined extracts were dried ($MgSO_4$) and filtered, and the solvent was removed under reduced pressure. Purification of

the products was achieved by column chromatography on silica gel, first with CS_2 to elute unreacted C_{60} and finally with dichloromethane for the monoadduct.

61-(3β-O-Carbetoxy-(22R,25R)-spirost-5-en)-61-(2',3',4',6'-tetra-O-acetyl-β-D-mannopyranoside) methano[60]fullerene (5a)



This compound was prepared from **4a**.

Yield: 80 mg (0.05 mmol, 63%); brown solid.

HPLC: toluene/acetonitrile, flow rate 1 mL/min, t_R = 5.3 min.

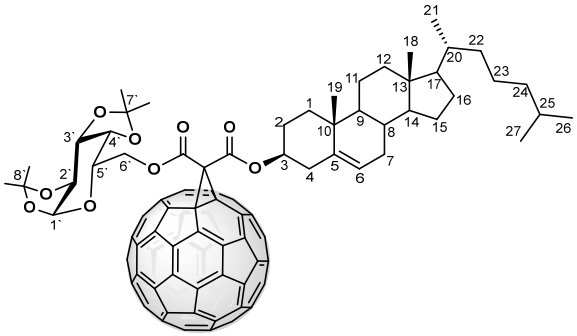
^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 6.05 (d, *J* = 8.3 Hz, 1H, H1'), 5.54 – 5.49 (m, 2H, H4', H6), 5.16 (m, 1H, H3'), 5.03 – 4.96 (m, 1H, H3), 4.42 (m, 1H, H16), 4.25 (m, 1H, H6'), 4.20 (m, 1H, H6'), 4.12 (m, 1H, H2'), 3.82 – 3.76 (m, 1H, H5'), 3.43 – 3.39 (m, 1H, H26), 3.38 (t, *J* = 5.0 Hz, 1H, H26), 2.61 –2.58 (m, 1H, H4), 2.54 –2.50 (m, 1H, H4), 2.21 (s, 3H, CH_3), 2.08 (s, 3H, CH_3), 2.02 (s, 3H, CH_3), 1.94 –1.92 (m, 4H, H1, H23), 1.95 (s, 3H, CH_3), 1.83 –1.76 (m, 1H, H20), 1.75 –1.72 (m, 1H, H17), 1.70 – 1.68 (m, 1H, H2), 1.61– 1.58 (m, 2H, H7), 1.55 (m, 4H, H8, H11, H24, H25), 1.37 (d, *J* = 6.7 Hz, 3H, H11, H12), 1.18 (s, 1H, H24), 1.16 – 1.12 (m, 4H, H2, H14, H15), 1.04 (s, 3H, H19), 1.01 – 0.94 (m, 1H, H9), 0.91 (d, *J* = 7.0 Hz, 3H, H21), 0.8 (m, 6H, H18, H27).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 171.2 (C=O) mannose, 170.4 (C=O) mannose, 170.1 (C=O) mannose, 170.0 (C=O) mannose, 162.2 (C=O), 162.0 (C=O), 145.4, 145.3, 145.2, 145.1, 144.7, 144.7, 143.9, 143.1, 143.0, 139.4 (C5), 123.1 (C6), 109.3 (C22), 93.8 (C1'), 80.8 (C16), 78.0 (C3), 71.4 (C5'), 70.2 (Csp^3 cyclopropane ring), 70.1 (Csp^3 cyclopropane ring), 69.9 (C3'), 68.7 (C2'), 67.4 (C26), 66.9 (C4'), 62.0 (C17), 61.0 (C6'), 52.4 (Csp^3 cyclopropane ring), 56.4 (C14), 49.9 (C9), 41.6 (C20), 40.3 (C13), 39.7 (C2), 37.7 (C4), 36.9 (C1), 36.8 (C10), 32.1 (C23), 31.8 (C15), 31.4 (C7), 30.3 (C8), 29.7 (C25), 28.8 (C24), 27.7 (C12), 20.9 (C11), 20.7 (2 CH_3), 20.6 (CH_3), 20.6 (CH_3), 19.4 (C19), 17.2 (C27), 16.3 (C18), 14.5 (C21).

FTIR: ν 2921, 2852, 1737, 1458, 1188, 1157, 800, 735 cm^{-1}.

HRMS (MALDI-TOF) m/z: $[M+H]^+$ Calcd for $C_{104}H_{61}O_{15}$: 1549.4010; found 1549.4014.

61-(3β-O-Carbetoxy-cholest-5-en)-61-(1',2':3',4'-di-O-isopropylidene-α-D-galactopyranoside) methano[60]fullerene (5b)



This compound was prepared from **4b**.

Yield: 77 mg (0.05 mmol, 65%); brown solid.

HPLC: toluene/acetonitrile, flow rate 1 mL/min, t_R = 5.2 min.

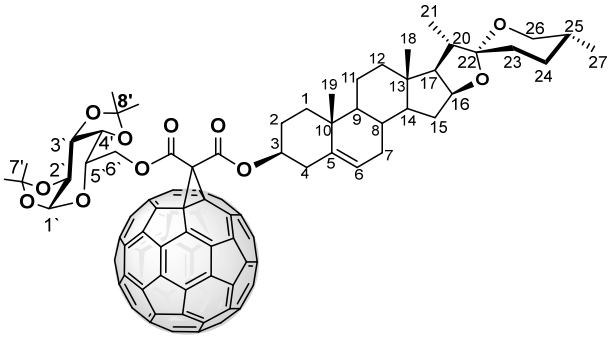
^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.57 (dd, *J* = 6.9, 5.0 Hz, 1H, H1'), 5.49 (m, 1H, H6), 5.00 (m, 1H, H3), 4.72 – 4.57 (m, 2H, H3', H6'), 4.38 – 4.31 (m, 2H, H2', H4'), 4.29 – 4.21 (m, 2H, H5', H6'), 2.58 (m, 2H, H4), 2.23 (m, 2H, H2), 2.03 (m, 3H, H7, H12), 1.96 (m, 1H, H1), 1.84 (m 2H, H16), 1.53 (s, 3H, CH_3), 1.50 (s, 3H, CH_3), 1.53 – 1.44 (m, 3H, H8, H11), 1.40 – 1.31 (m, 2H, H20, H22), 1.35 (s, 3H, CH_3), 1.33 (s, 3H, CH_3), 1.26 (m, 3H, H1, H24), 1.22 – 1.09 (m, 7H, H12, H15, H17, H23, H25), 1.08 (s, 3H, H19), 1.04 – 0.98 (m, 3H, H9, H14, H22), 0.92 (dd, *J* = 9.5, 6.5 Hz, 3H, H21), 0.88 – 0.85 (m, 6H, H26, H27), 0.69 (s, 3H, H18).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 163.7 (C=O), 163.0 (C=O), 145.4, 145.3, 145.3, 145.0, 144.8, 143.2, 143.1, 142.3, 142.1, 142.0, 141.0, 139.4 (C5), 123.5 (C6), 109.9 (C7') , 109.0 (C8'), 96.4 (C1'), 77.9 (C3), 71.8 (Csp^3 cyclopropane ring), 71.7 (Csp^3 cyclopropane ring), 71.0 (C4'), 70.8 (C3'), 70.5 (C2'), 65.9 (C5'), 65.7 (C6'), 56.8 (C14), 56.3 (C17), 52.4 (Csp^3 cyclopropane ring), 50.1 (C9), 42.5 (C13), 39.8 (C24), 39.6 (C12), 37.9 (C4), 37.1 (C1), 36.8 (C10), 36.3 (C22), 35.9 (C20), 32.1 (C7), 32.0 (C8), 28.4 (C2), 28.2 (C25), 27.8 (C16), 26.3 (CH_3), 26.2 (CH_3), 25.1 (CH_3), 24.7 (CH_3), 24.4 (C15), 24.0 (C23), 23.0 (C26), 22.7 (C27), 21.2 (C11), 19.5 (C19), 18.9 (C21), 12.0 (C18).

FTIR: ν 2923, 2853, 1745, 1492, 1239, 1074, 968, 745 cm^{-1}.

HRMS (MALDI-TOF) m/z: $[M]^{\bullet+}$ Calc. for $C_{102}H_{64}O_9$: 1432.4550; found 1432.4534.

61-(3β-O-Carbetoxy-(22*R*,25*R*)-spirost-5-en)-61-(1',2':3',4'-di-O-isopropylidene-α-D-galactopyranoside) methano[60]fullerene (5c)



This compound was prepared from **4c**.

Yield: 68 mg (0.05 mmol, 65%); brown solid.

HPLC: toluene/acetonitrile, flow rate 1 mL/min, t_R = 5.6 min.

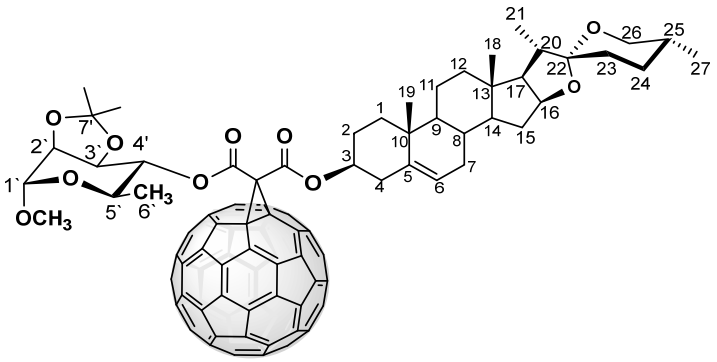
^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.57 (d, *J* = 5.0 Hz, 1H, H1'), 5.49 (d, *J* = 5.0 Hz, 1H, H6), 4.99 (m, 1H, H3), 4.73 – 4.57 (m, 3H, H3', H6'), 4.42 (m, 1H, H16), 4.35 (m, 2H, H2', H5'), 4.27 – 4.22 (m, 1H, H4'), 3.48 (dd, *J* = 11.9, 4.3 Hz, 1H, H26), 3.38 (t, *J* = 11.0 Hz, 1H, H26), 2.59 (m, 2H, H4), 2.11 (d, *J* = 12.0 Hz, 1H, H12), 2.02 (m, 2H, H1), 1.94 (m, 1H, H23), 1.91 – 1.83 (m, 2H, H12, H20), 1.85 – 1.73 (m, 2H, H2, H17), 1.69 (dd, *J* = 12.5, 3.8 Hz, 1H, H8), 1.68 – 1.55 (m, 3H, H7, H11), 1.53 (s, 3H, CH_3), 1.50 (s, 3H, CH_3), 1.45 (m, 2H, H24), 1.35 (s, 3H, CH_3), 1.33 (s, 3H, CH_3), 1.40 – 1.31 (m, 4H, H7, H15, H25), 1.26 – 1.20 (m, 2H, H2, H23), 1.14 (m, 1H, H14), 1.10 (s, 3H, H19), 1.03 (m, 1H, H9), 0.98 (d, *J* = 6.9 Hz, 3H, H21), 0.83 – 0.78 (m, 6H, H18, H27).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 163.7 (C=O), 163.0 (C=O), 145.4, 144.8, 144.0, 143.1, 142.3, 141.1, 139.4 (C5), 139.1, 129.2 , 128.4, 123.2 (C6), 109.9 (C22), 109.4 (C7'), 109.0 (C8'), 96.4 (C1'), 80.9 (C16), 77.9 (C3), 71.8 (Csp^3 cyclopropane ring), 71.7 (Csp^3 cyclopropane ring), 71.1 (C2'), 70.8 (C5'), 70.5 (C3'), 67.0 (C26), 65.9 (C6'), 65.8 (C4'), 62.2 (C17), 56.6 (C14), 52.4 (Csp^3 cyclopropane ring), 50.1 (C9), 41.8 (C20), 40.4 (C13), 39.9 (C2), 37.9 (C4), 37.1 (C23), 36.9 (C10), 32.2 (C1), 32.0 (C15), 31.5 (C7, C8), 30.4 (C25), 28.9 (C24), 27.8 (C12), 26.4 (CH_3), 26.2 (CH_3), 25.1 (CH_3), 24.7 (CH_3), 21.0 (C11), 19.6 (C19), 17.3 (C27), 16.5 (C18), 14.7 (C21).

FTIR: ν 2921, 2852, 1737, 1461, 1268, 1188, 748 cm-1.

HRMS (MALDI-TOF) m/z: $[M-H]^{\bullet-}$ Calc. for $C_{102}H_{59}O_{11}$: 1459.4057; found 1459.3912.

61-(3β-O-Carbetoxy-(22R,25R)-spirost-5-en)-61-[4'-(methyl-2',3'-O-isopropylidene-α-L-rhamnopyranoside)] methano[60]fullerene (5d)



This compound was prepared from **4d**.

Yield: 93 mg (0.07 mmol, 60%); brown solid.

HPLC: toluene/acetonitrile, flow rate 1 mL/min, t_R = 4.0 min.

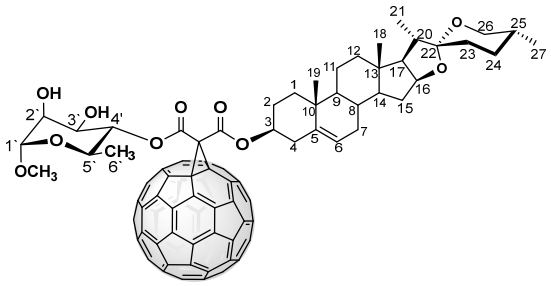
^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): .48 (d, *J* = 5.0 Hz, 1H, H6), 5.18 (dd, *J* = 10.2, 7.9 Hz, 1H, H4′), 5.01 (m, 1H, H3), 4.96 (s, 1H, H1′), 4.42 (m, 1H, H16), 4.33 (dd, *J* = 7.9, 5.3 Hz, 1H, H3′), 4.20 (d, *J* = 5.4 Hz, 1H, H2′), 3.93 (m , 1H, H5′), 3.48 (m, 1H, H26), 3.42 (s, 3H, CH_3O), 3.37 (m, 1H, H26), 2.63 (m, 2H, H4), 1.96 (m, 4H, H1, H12, H23), 1.87 (q, *J* = 6.4 Hz, 2H, H12, H20), 1.79 (dd, J = 8.6, 6.7 Hz, 1H, H17), 1.76 (m, 1H, H2), 1.69 - 1.59 (m, 3H, H7, H8, H25), 1.65 (s, 3H, CH_3), 1.56 (m, 2H, H11), 1.52 – 1.43 (m, 2H, H24), 1.37 (d, *J* = 2.6 Hz, 6H, H6′, CH_3), 1.31 (m, 3H, H7, H15), 1.22 (m, 2H, H2, H23), 1.15 (m, 1H, H14), 1.10 (s, 3H, H19), 1.03 (m, 1H, H9), 0.98 (d, *J* = 7.0 Hz, 3H, H21), 0.80 (m, 6H, H18, H27).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 162.9 (C=O), 162.8 (C=O), 145.5, 145.4, 145.0, 144.8, 144.0, 143.2, 143.1, 142.4, 142.3, 142.1, 142.0, 141.1, 139.8, 139.3 (C5), 123.2 (C6), 110.1 (C7'), 109.5 (C22), 98.3 (C1′), 80.9 (C16), 78.0 (C3), 78.0 (C4′), 76.2 (C2′), 75.5 (C3′), 71.7 (Csp3 cyclopropane ring), 71.6 (Csp3 cyclopropane ring), 67.0 (C26), 63.7 (C5′), 62.2 (C17), 56.5 (C14), 55.3 (H_3CO), 52.4 (Csp^3 cyclopropane ring), 50.0 (C9), 41.8 (C20), 40.4 (C13), 39.8 (C2), 37.7 (C4), 37.1 (C23), 37.0 (C10), 32.2 (C1), 32.0 (C15), 31.5 (C7, C8), 30.4 (25), 28.9 (C24), 28.1 (CH_3), 27.7 (C12), 26.8 (CH_3), 21.0 (C11), 19.6 (C19), 17.6 (C6′), 17.3 (C27), 16.5 (C18), 14.7 (C21).

FTIR: ν 2922, 2852, 1746, 1717, 1459, 1376, 1459, 1376, 980, 748 cm^{-1}.

HRMS (MALDI-TOF) m/z: $[M-H]^{\bullet-}$ Calc. for $C_{100}H_{57}O_{10}$: 1417.3951; found 1417.3925.

61-(3β-O-Carbetoxy-(22R,25R)-spirost-5-en)-61-[4'-(methyl-α-L-rhamnopyranoside)] methano[60]fullerene (6)



To a solution of hybrid **5d** (15 mg, 0.02 mmol) in $CHCl_3$ (3 mL) was added a 9:1 mixture of CF_3CO_2H/ H_2O (5 mL). The reaction mixture was stirred for 14 h at room temperature. Then it was neutralized with a aqueous saturated solution of Na_2CO_3 and the fullerene derivative was extracted with an three 30 mL portions of 7:3 mixture of $CHCl_3$/MeOH. The organic layer was dried over Na_2SO_4 and concentrated. The residue was precipitated by the addition of hexane affording a solid and filtered in vacuo. The solid was purified by column chromatography on silica gel with CS_2 and dichloromethane as eluents. **Yield**: 9 mg (0.007 mmol, 35%); brown solid.

HPLC: toluene/acetonitrile, flow rate 1 mL/min, t_R = 4.5 min.

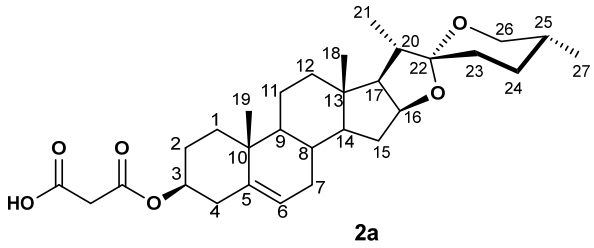
^{1}H NMR (700 MHz, $CDCl_3$, δ ppm): 5.48 (d, *J* = 5.1 Hz, 1H, H6), 5.25 (t, *J* = 9.6 Hz, 1H, H4′), 5.04 (m, 1H, H3), 4.78 (d, *J* = 1,5 Hz, 1H, H1′), 4.42 (m, H, H16), 4.11 (m, 1H, H3′), 4.06 (s, 1H, H2′), 3.97 (m, 1H, H5′), 3.48 (m, 1H, H26), 3.43 (s, 3H, CH_3O), 3.38 (t, *J* = 11.0 Hz, 1H, H26), 3.09 (d, *J* = 6.1 Hz, 1H, HO-3′), 2.59 (d, *J* = 7.1 Hz, 2H, H4), 2.50 (d, *J* = 4.0 Hz, 1H, HO-2′), 2.13 – 2.09 (m, 1H, H12), 2.07 – 1.94 (m, 3H, H1, H23), 1.91 – 1.83 (m, 2H, H12, H20), 1.78 (m, 2H, H2, H17), 1.71 – 1.58 (m, 4H, H7, H8, H25), 1.52 – 1.43 (m, 4H, H11, H24), 1.40 (d, *J* = 6.2 Hz, 3H, H6'), 1.25 (m, 4H, H2, H15, H23), 1.17 (m, 1H, H14), 1.09 (s, 3H, H19), 1.06 – 1.01 (m, 1H, H9), 0.98 (d, *J* = 7.0 Hz, 3H, H21), 0.79 (m, 6H, H18, H27).

^{13}C{1H} NMR (175 MHz, $CDCl_3$, δ ppm): 163.9 (C=O), 163.8 (C=O), 146.0, 145.3, 145.2, 144.9, 143.9, 143.4, 143.1, 142.9, 142.4, 141.3, 141.1, 140.7, 148.5, 148.5, 146.0, 145.8, 145.3, 144.8, 144.1, 143.9, 143.4, 142.9, 142.2, 141.1, 140.7, 139.0 (C5), 123.6 (C6), 109.5 (C22), 100.5 (C1'), 80.7 (C16), 78.6 (C4'), 78.6 (C3), 71.5 (Csp^3 cyclopropane ring), 71.5 (Csp^3 cyclopropane ring), 71.2 (C2'), 70.1 (C3'), 67.0 (C26), 65.4 (C5'), 62.2 (C17), 56.6 (C14), 55.4 (H_3C-O), 52.4 (Csp^3 cyclopropane ring), 50.1 (C9), 41.8 (C20), 40.42 (C13), 39.8 (C2), 38.0 (C4), 37.1 (C10), 37.0 (C23), 32.2 (C1), 32.0 (C15), 31.6 (C7), 31.6 (C8), 30.5 (C25), 28.9 (C24), 27.8 (C12), 21.0 (C11), 19.5 (C19), 18.0 (C6'), 17.3 (C27), 16.5 (C18), 14.7 (C21).

FTIR: ν 3567, 2924, 2853, 1743, 1461, 1372, 1177, 747 cm^{-1}.

HRMS (MALDI-TOF) m/z: $[M+H]^+$ Calc. for $C_{97}H_{55}O_{10}$: 1379.3795; found 1379.3746.

2. Spectra of 3-[((22*R*, 25*R*)-spirost-5-en-3β-yl)oxy]-3-oxopropanoic acid (2a):



2a

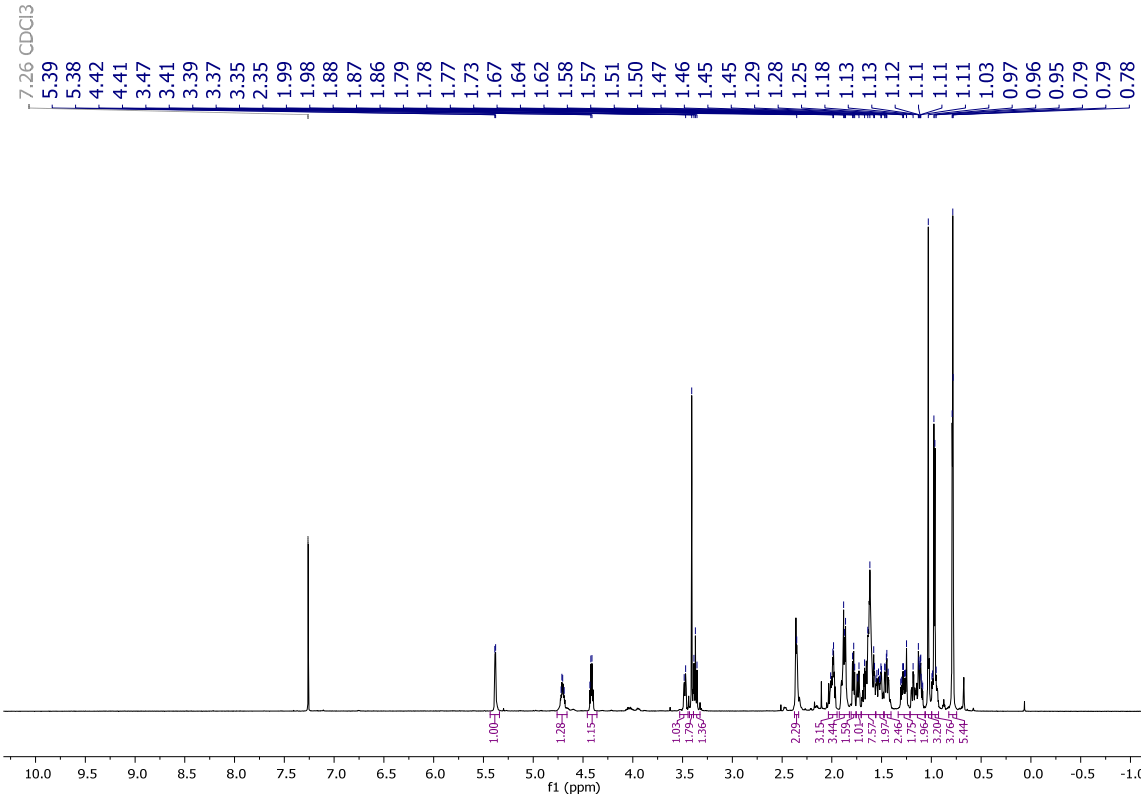


Figure S1. ^{1}H NMR spectrum of compound **2a**

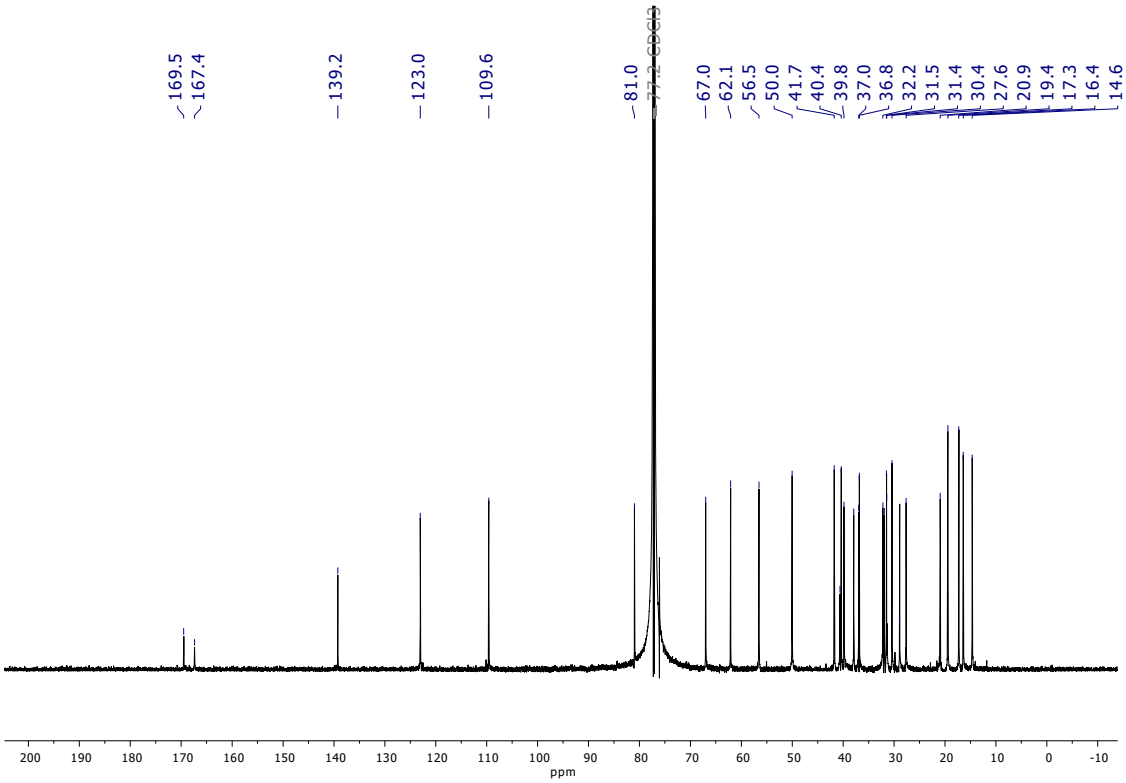


Figure S2. $^{13}C\{1H\}$ NMR spectrum of compound **2a**

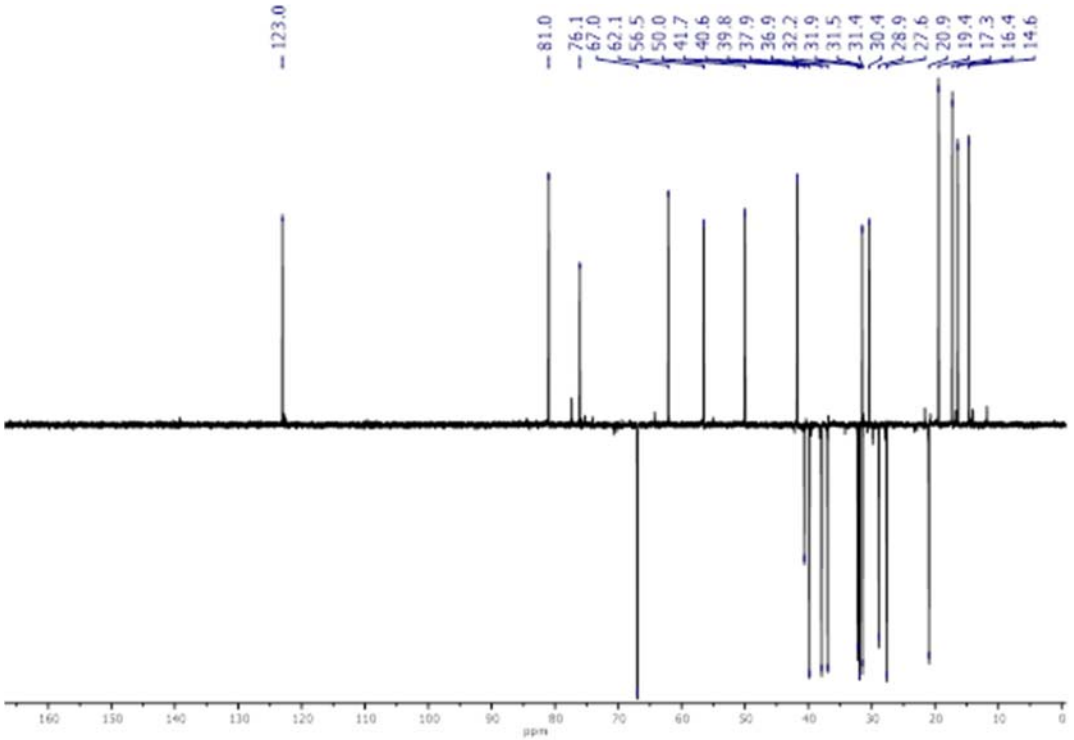


Figure S3. DEPT-135º spectrum of compound **2a**

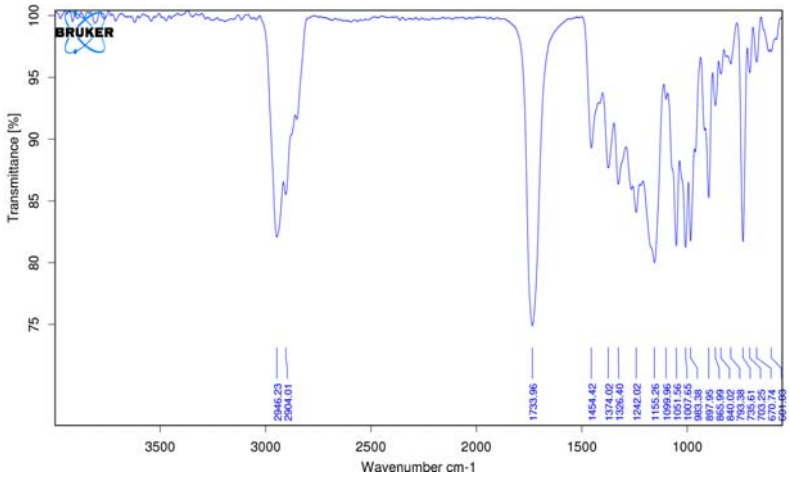


Figure S4. IR spectrum of compound **2a**

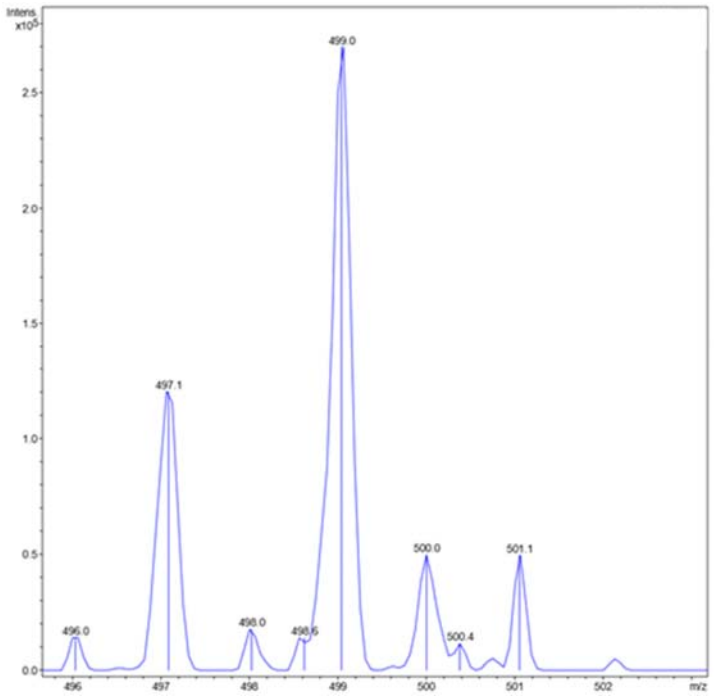


Figure S5. MS (ESI) of compound **2a**. m/z: 499.0 $[M+Na]^+$ for $C_{30}H_{44}NaO_6$

3. Spectra of 3-[(cholest-5-en-3β-yl)oxy]-3-oxopropanoic acid (2b)

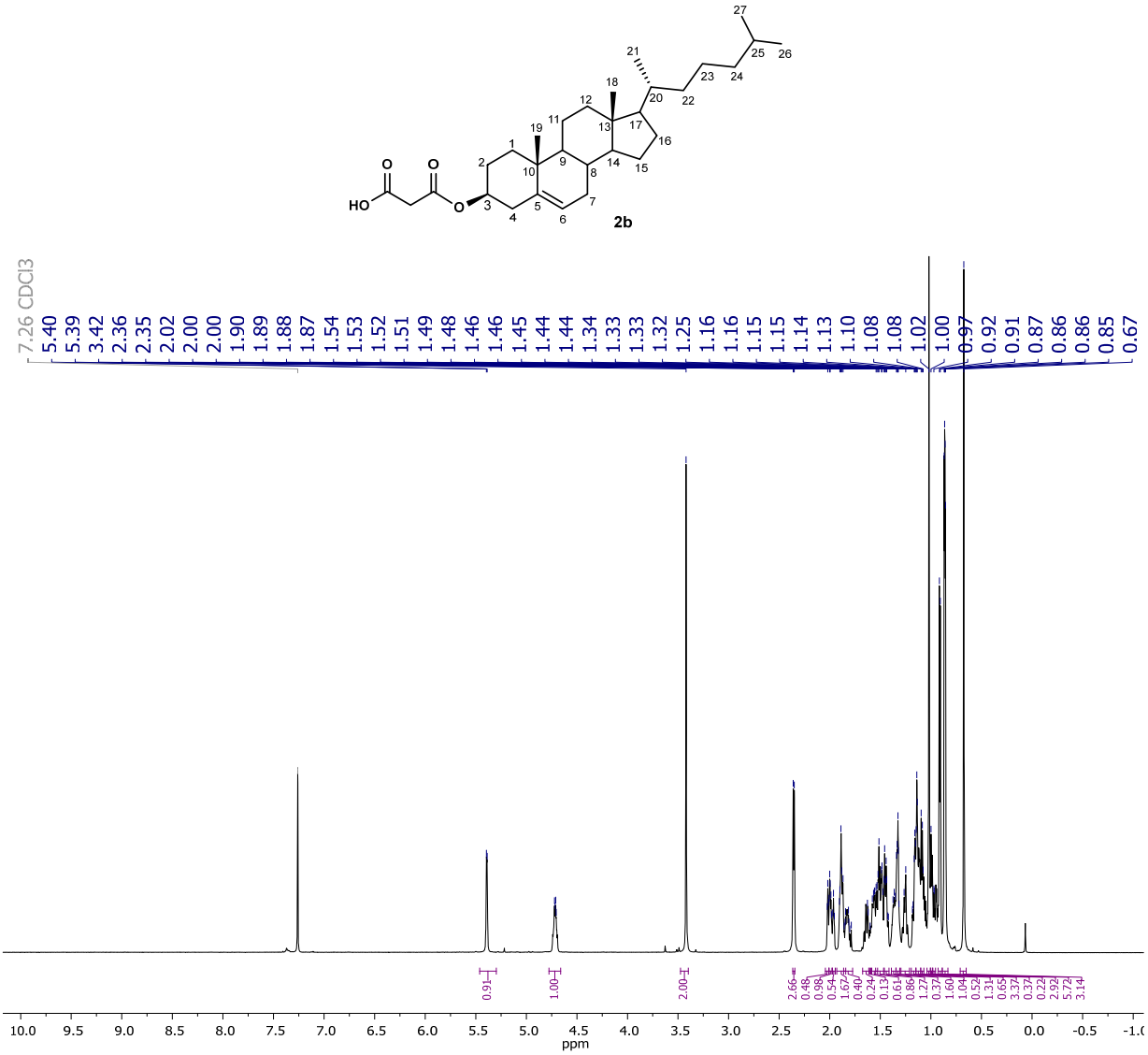


Figure S6. ^{1}H NMR spectrum of compound **2b**

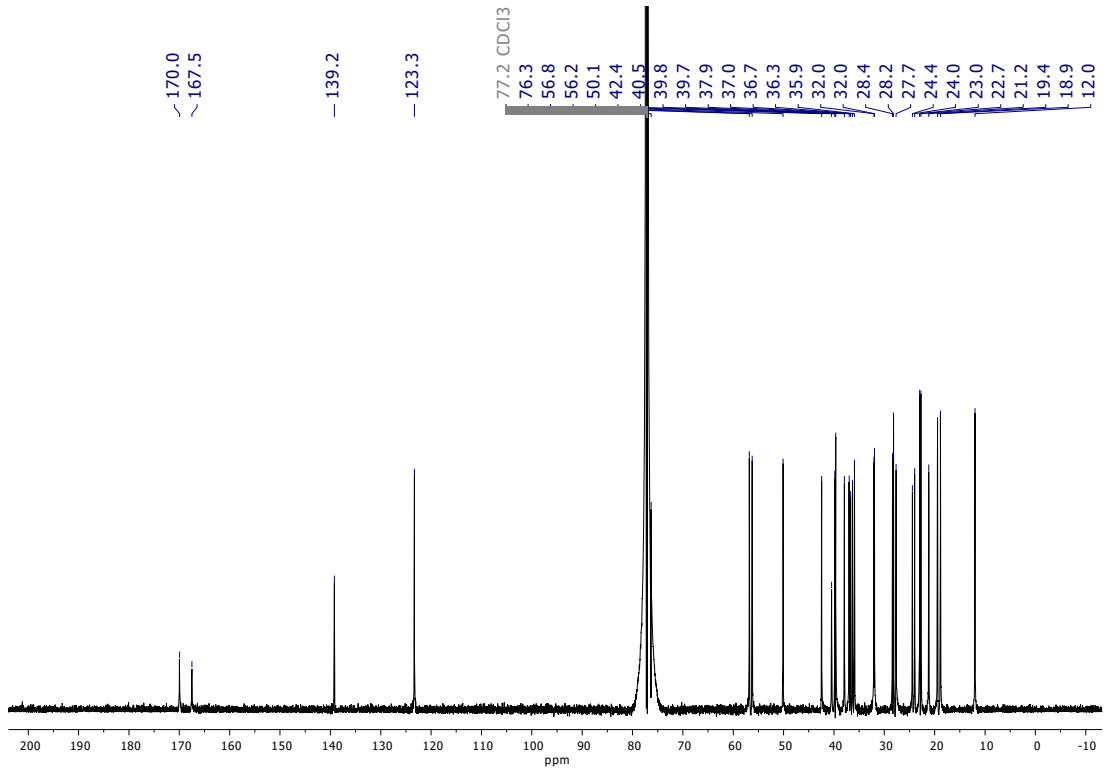


Figure S7. $^{13}C\{1H\}$ NMR spectrum of compound **2b**

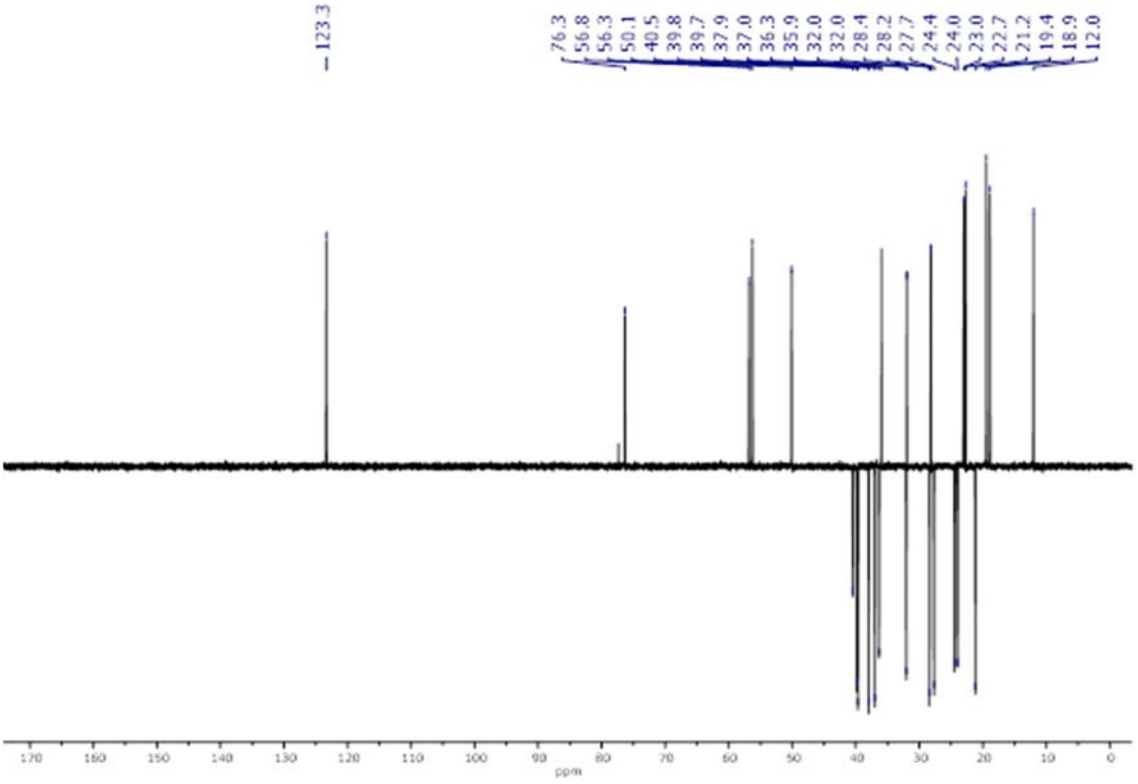


Figure S8. DEPT-135º spectrum of compound **2b**

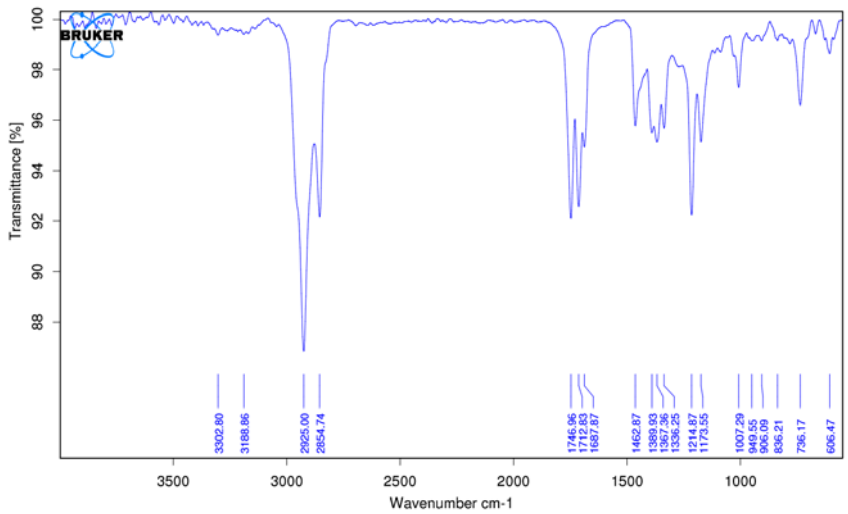


Figure S9. FTIR spectrum of compound **2b**

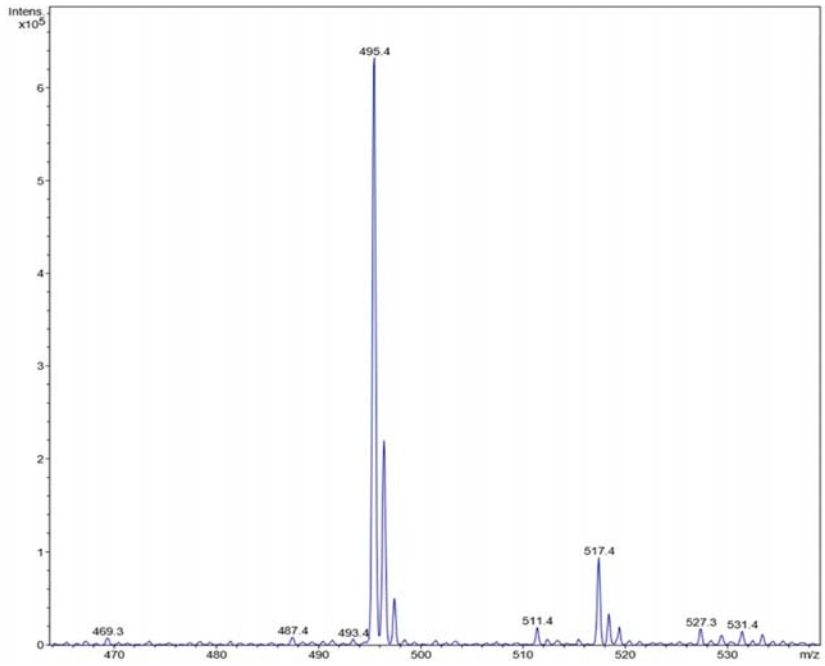


Figure S10. MS-ESI of compound **2b.** m/z =495.4 $[M+Na]^+$ for $C_{30}H_{48}NaO_4$

4. Spectra of (22*R*,25*R*)-spirost-5-en-3β-yl Malonate-2,3,4,6-tetra-*O*-acetyl-β-D-mannopyranoside (4a)

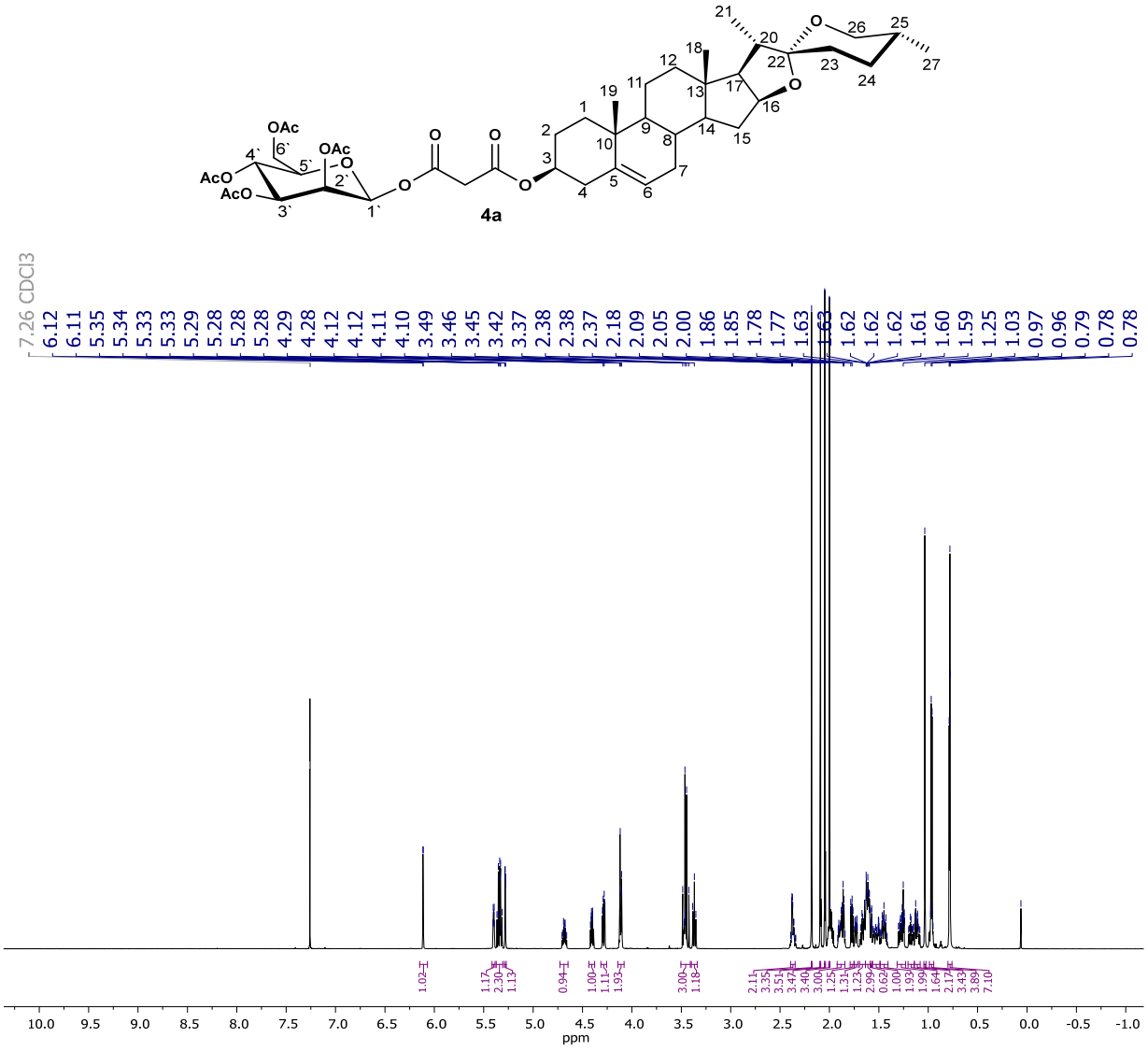


Figure S11. ^{1}H NMR spectrum of compound **4a**

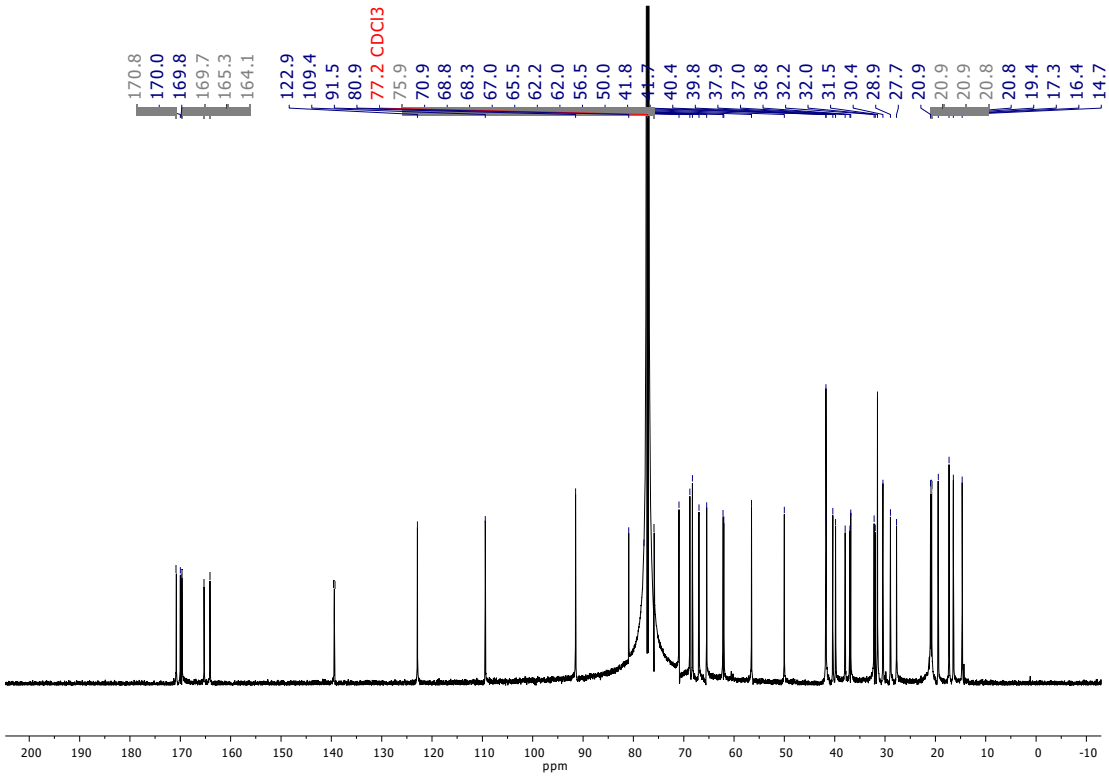


Figure S12. $^{13}C\{1H\}$ NMR spectrum of compound **4a**

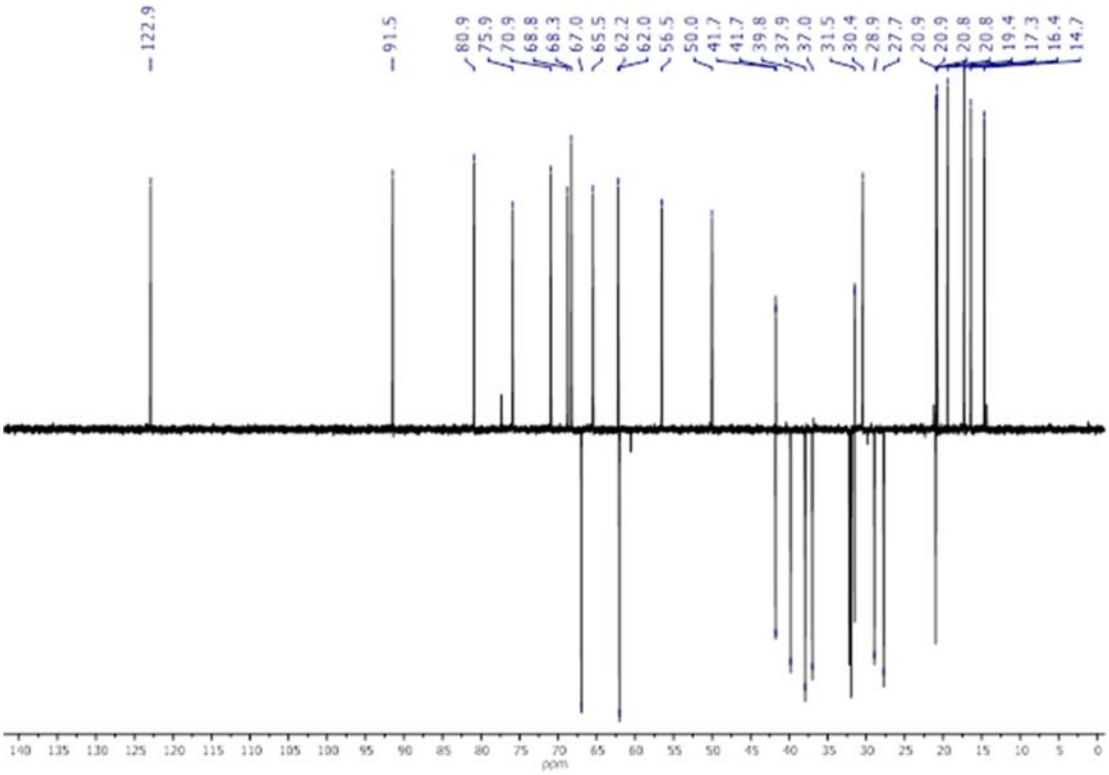


Figure S13. DEPT-135º spectrum of compound **4a**

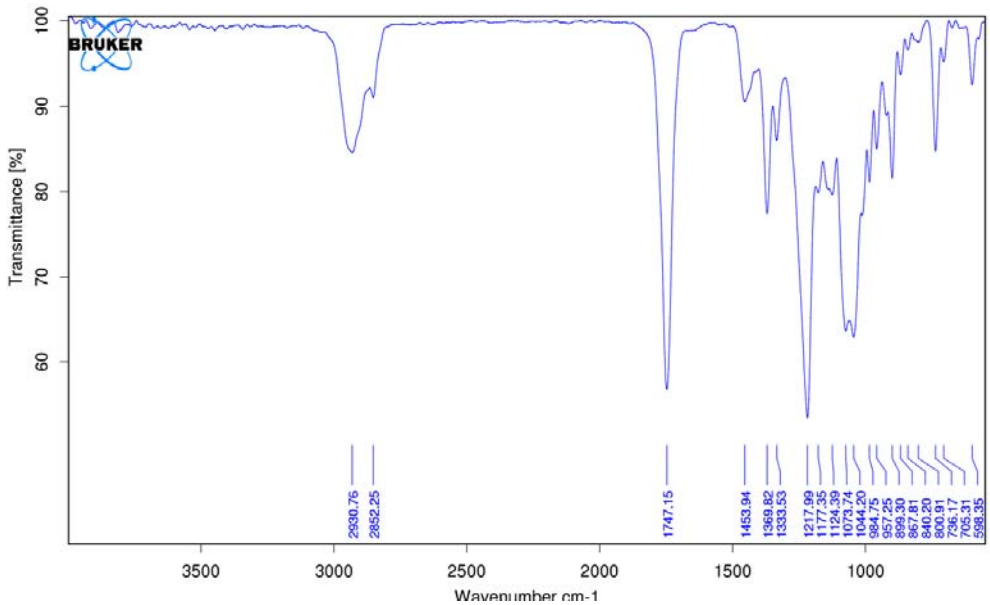


Figure S14. FTIR spectrum of compound **4a**

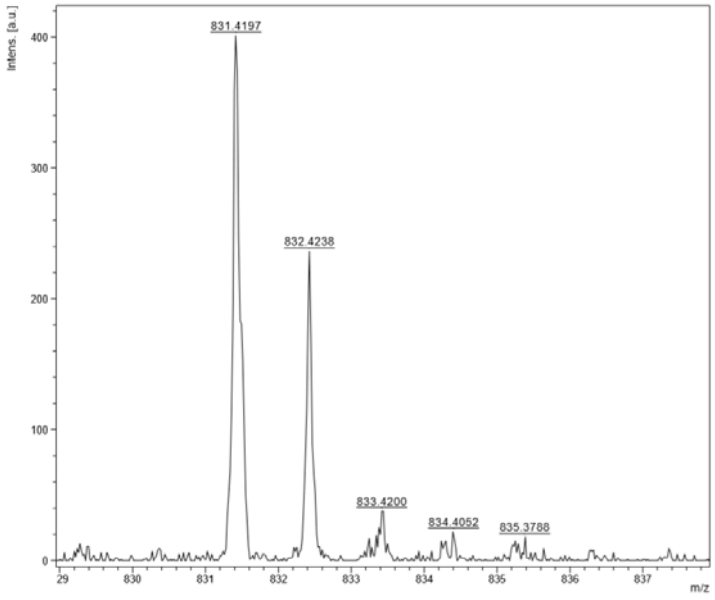


Figure S15. HRMS (MALDI-TOF) of compound **4a** showing the ionic pattern corresponding to $[M+H]^+$ 831.4197; calculated for $C_{44}H_{63}O_{15}$ 831.4167

5. Spectra of 6′-(Cholest-5-en-3β-ylmalonate)-1′,2′:3′,4′-di-*O*-isopropylidene-α-D-galactopyranoside (4b)

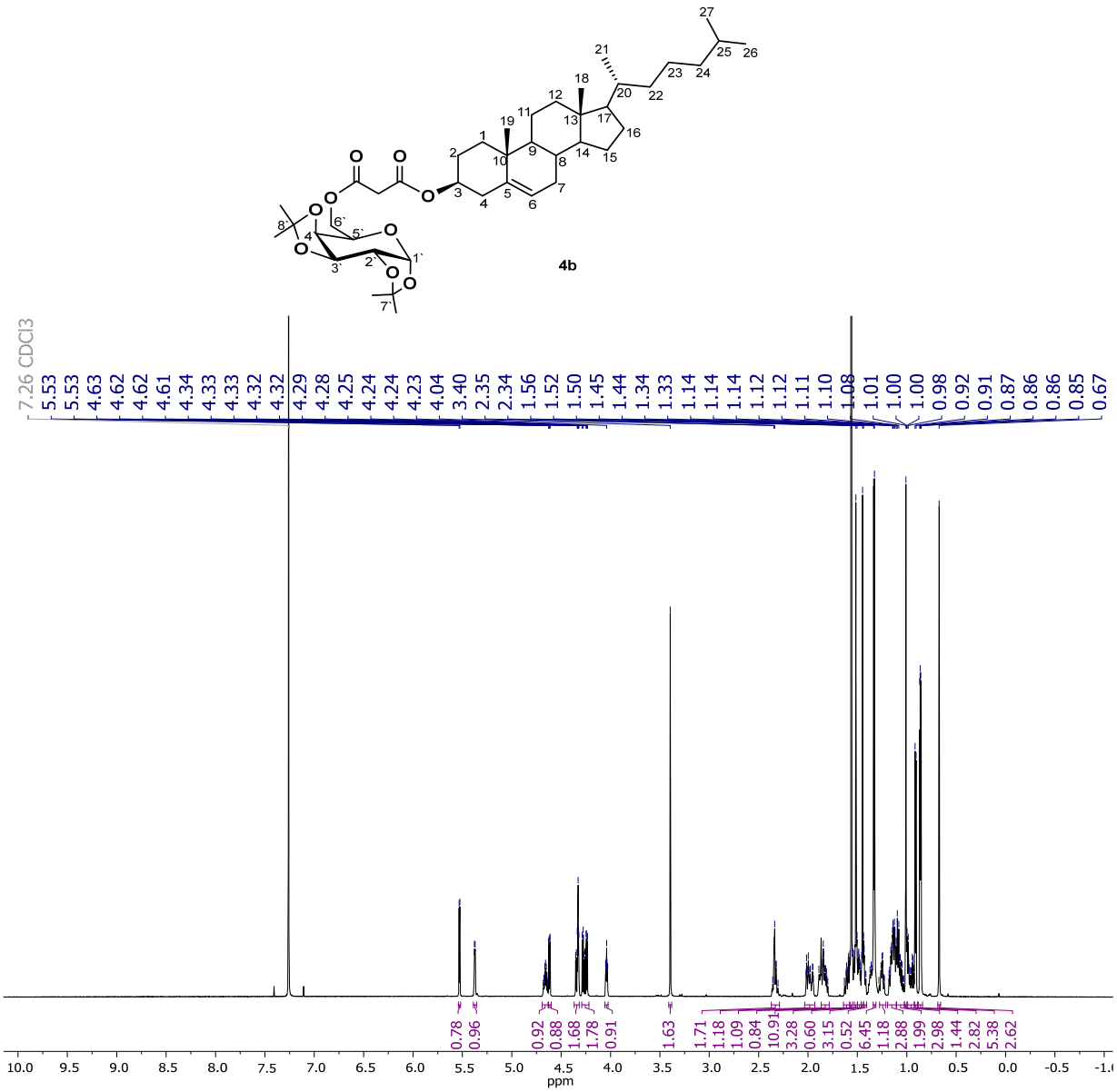


Figure S16. ^{1}H NMR spectrum of compound **4b**

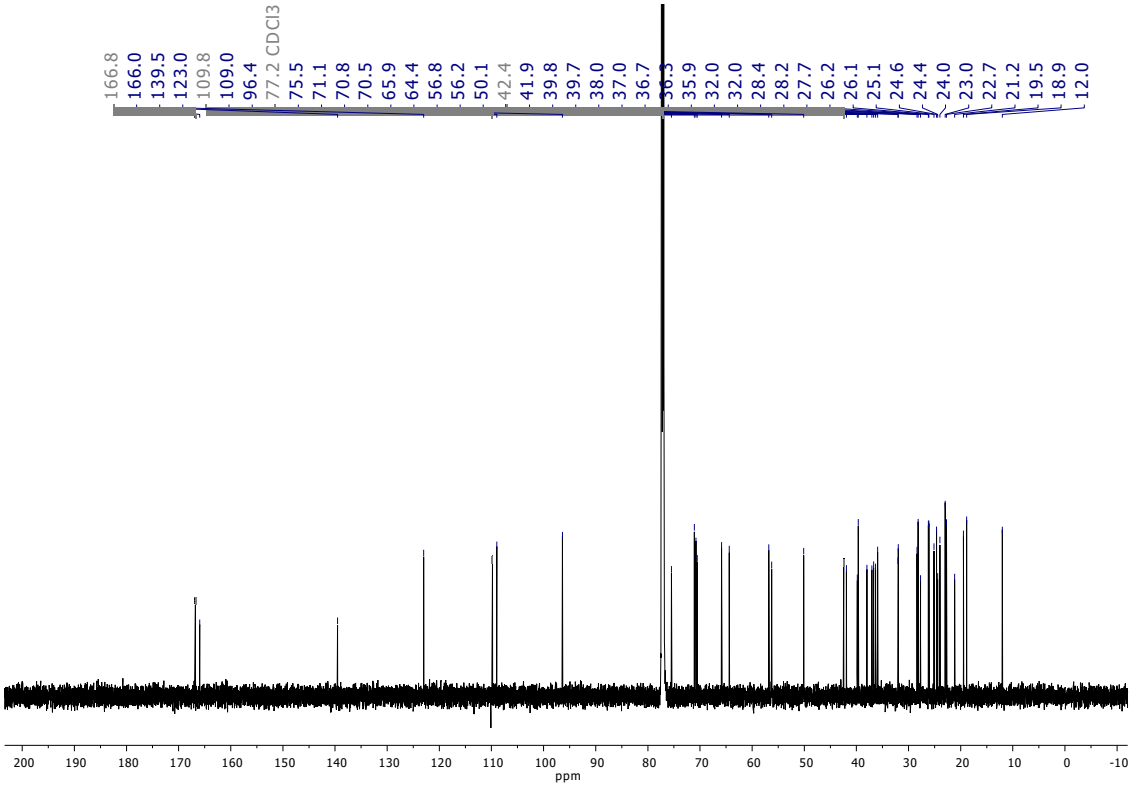


Figure S17. $^{13}C\{1H\}$ NMR spectrum of compound **4b**

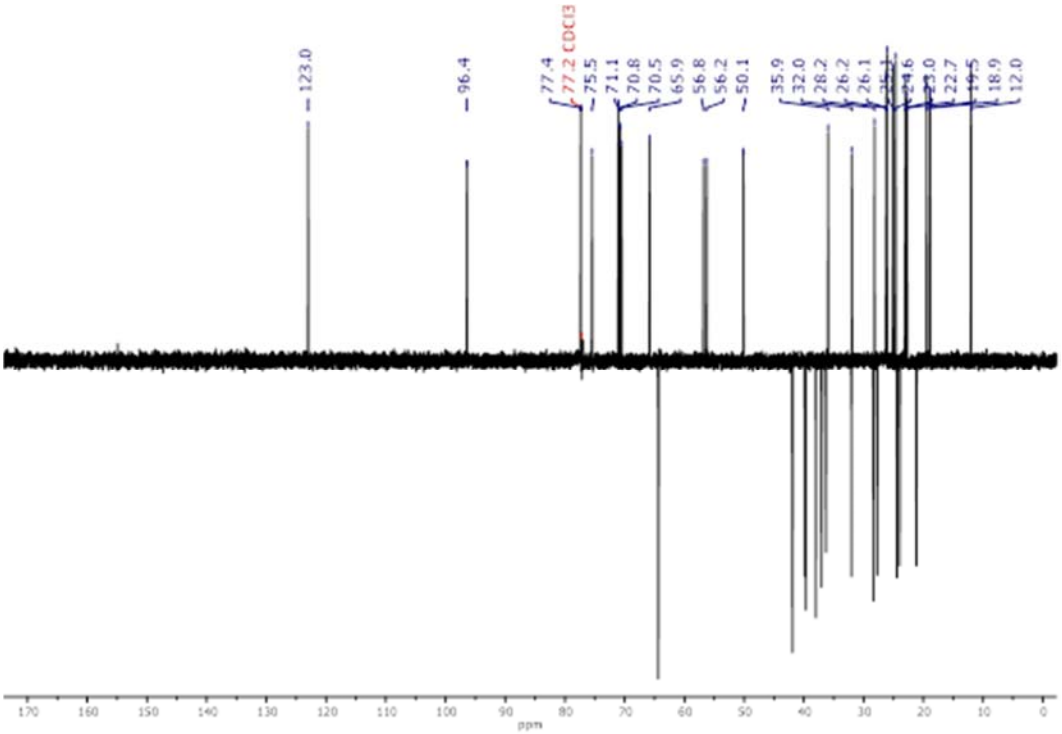


Figure S18. DEPT-135º spectrum of compound **4b**

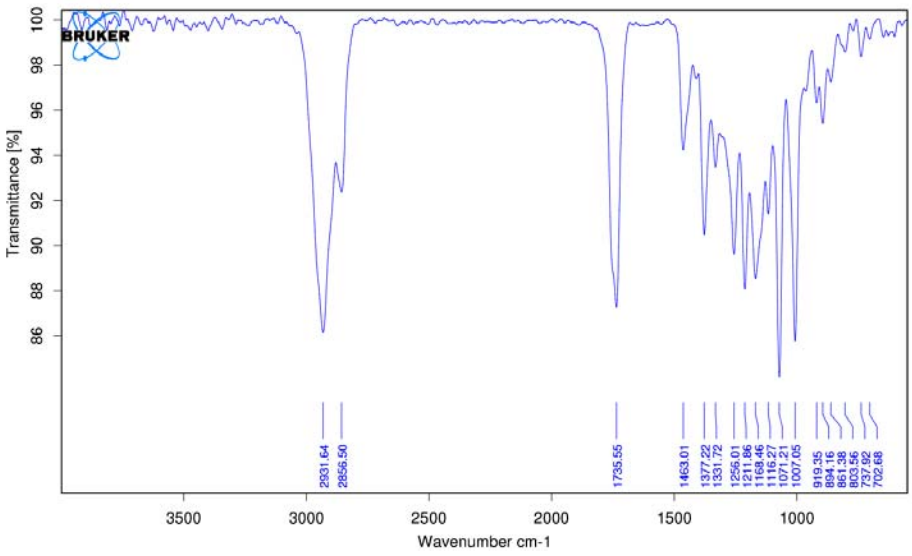


Figure S19. FTIR spectrum of compound **4b**

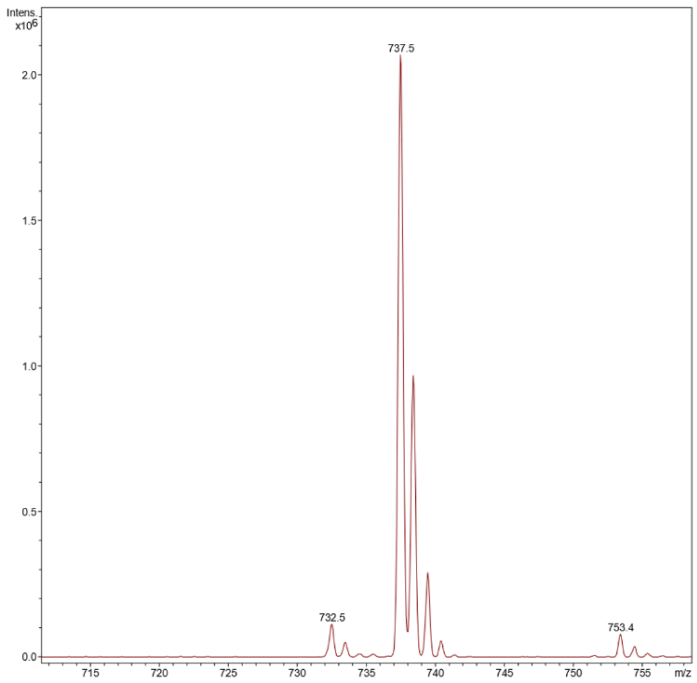


Figure S20. MS-ESI (MeOH) of compound **4b.** m/z =737.5 $[M+Na]^+$ for $C_{42}H_{66}NaO_9$

6. Spectra of 6′-(22*R*,25*R*)-spirost-5-en-3β-yl Malonate)-1′,2′:3′,4′-di-*O*-isopropylidene-α-D-galactopyranoside (4c)

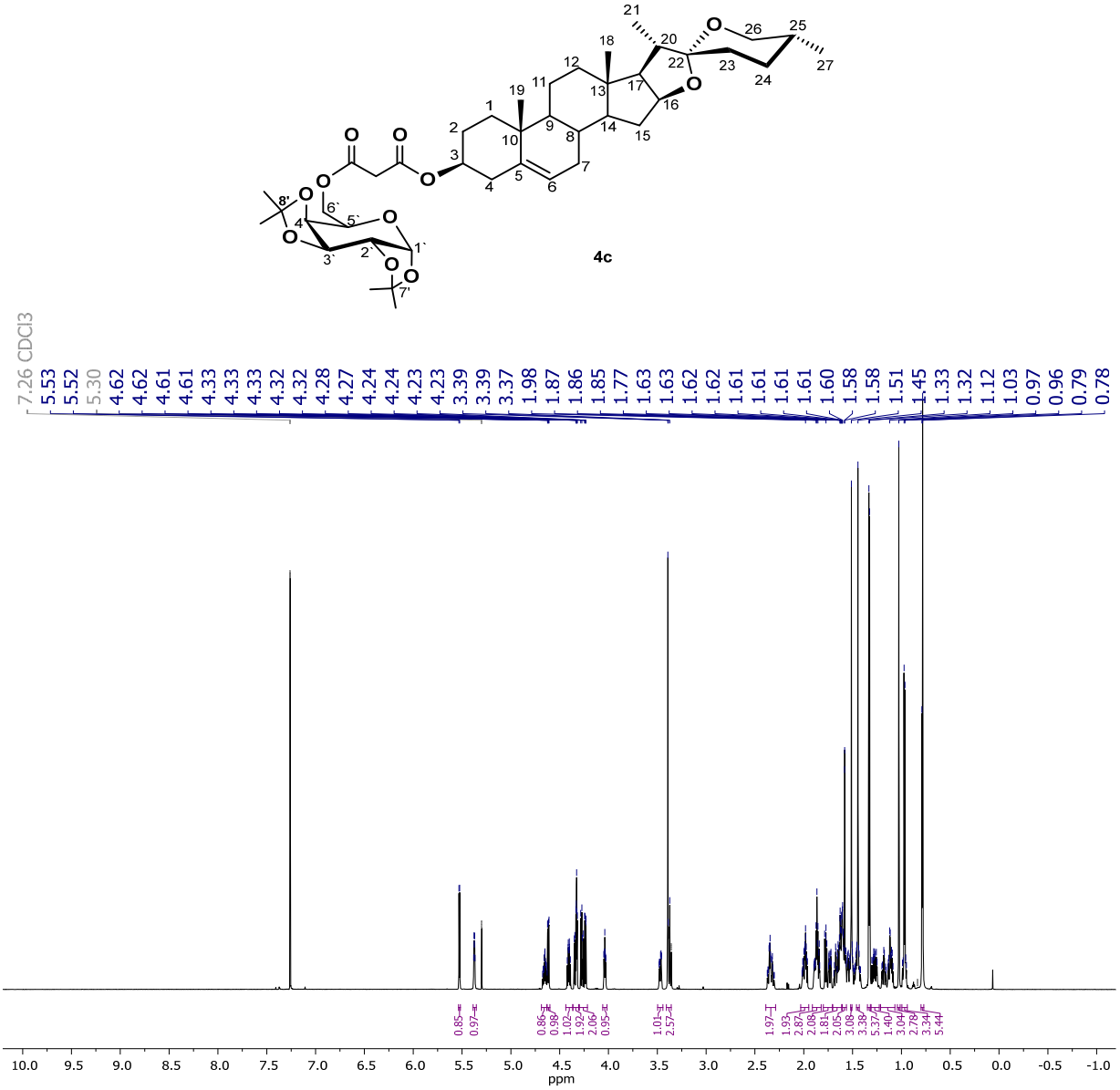


Figure S21. ^{1}H NMR spectrum of compound **4c**

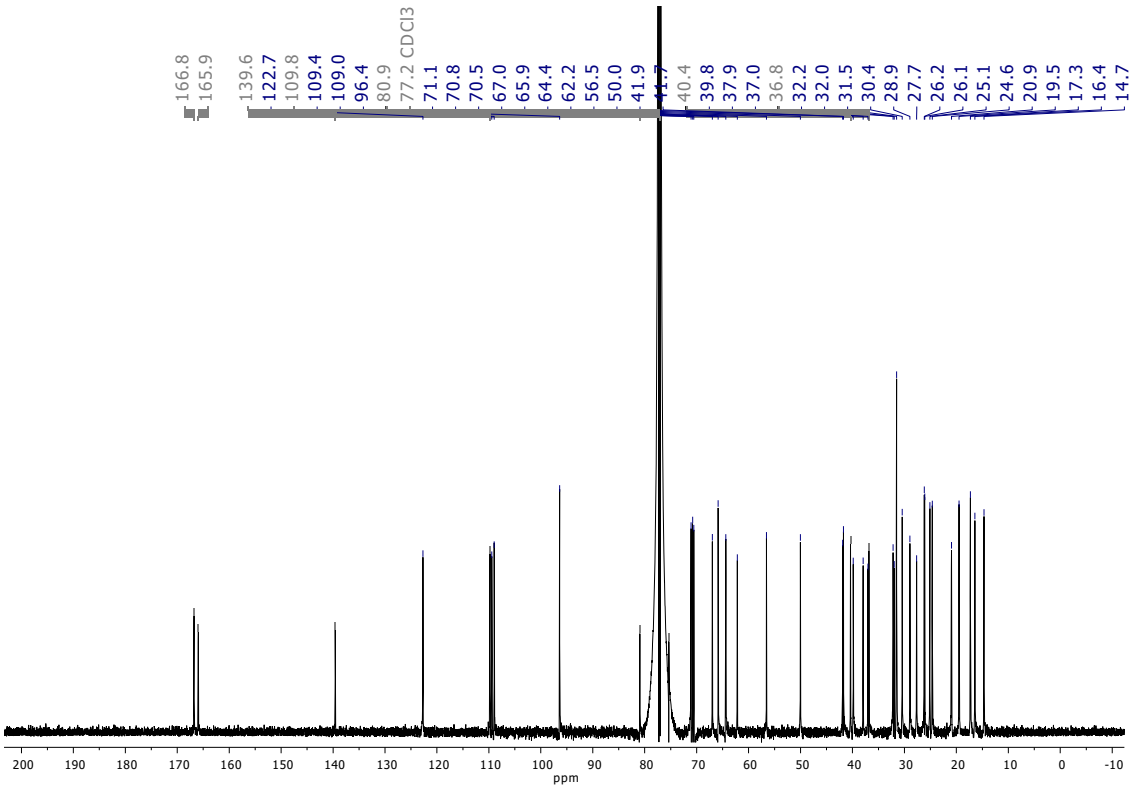


Figure S22 $^{13}C\{1H\}$ NMR spectrum of compound **4c**

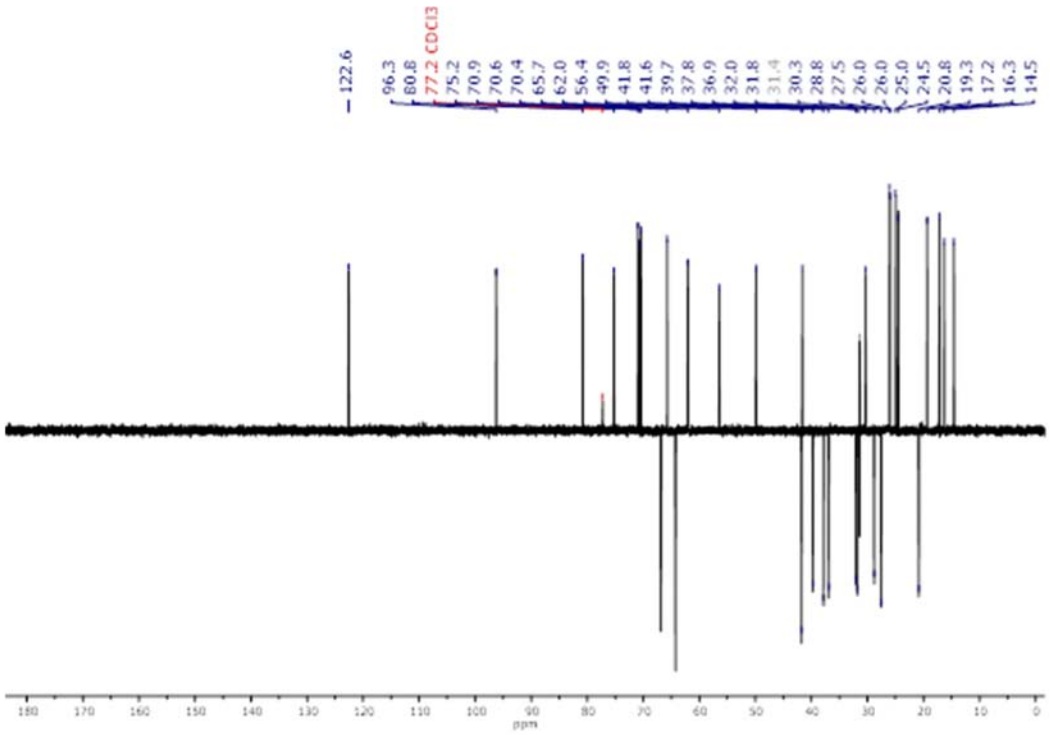


Figure S23. DEPT-135º spectrum of compound **4c**

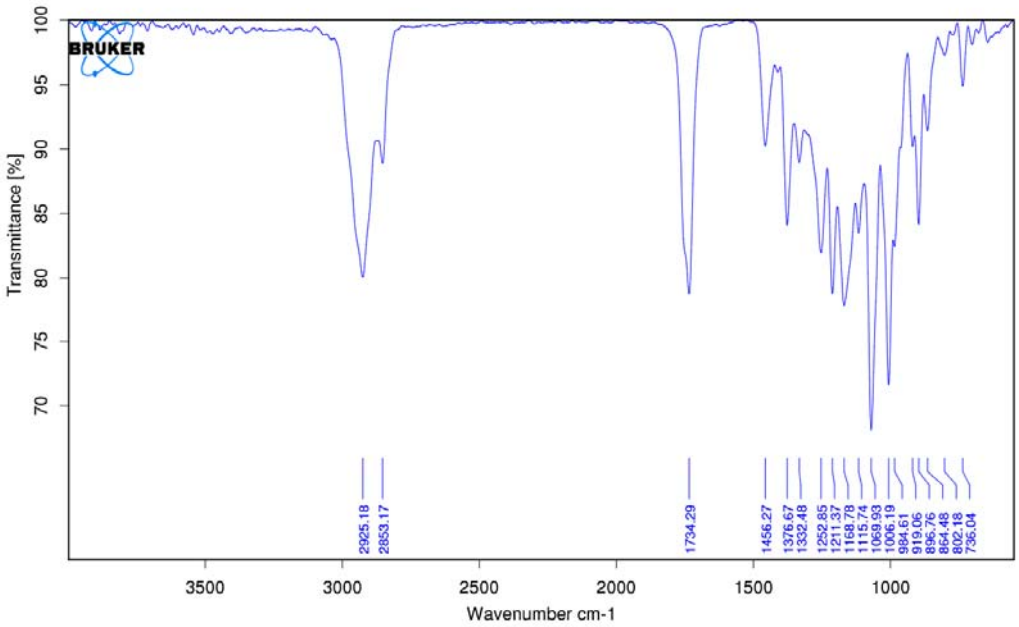


Figure S24. FTIR spectrum of compound **4c**

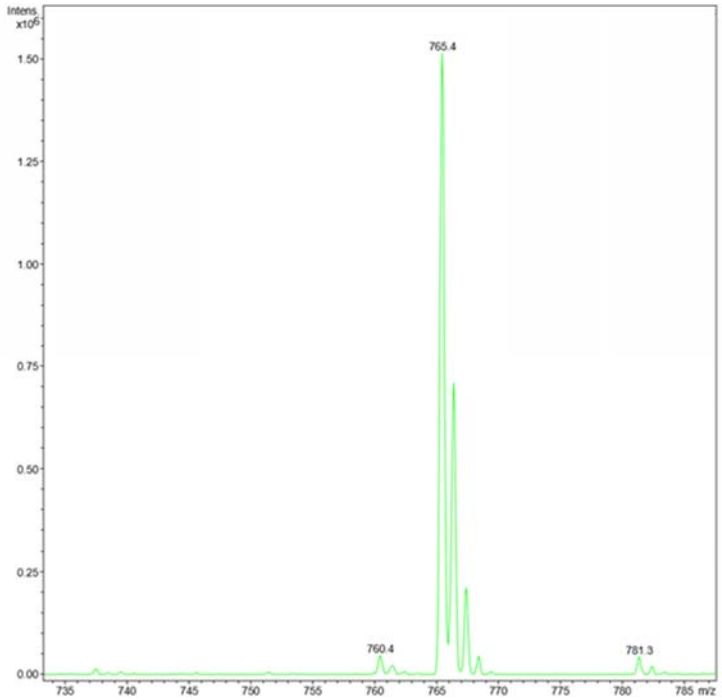
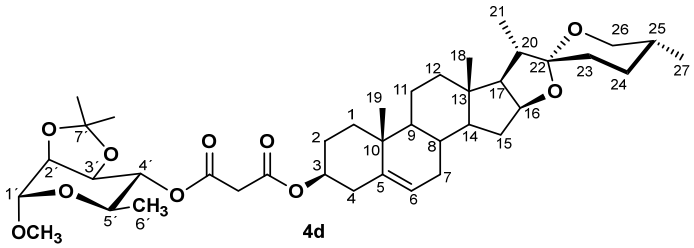


Figure S25. MS-ESI (MeOH) of compound **4c.** m/z =764.4 $[M+Na]^+$ for $C_{42}H_{62}NaO_{11}$

7. Spectra of methyl-6′-((22*R*,25*R*)-spirost-5-en-3β-yl malonate)-2′,3′-O-isopropylidene-α-L-rhamnopyranoside (4d)



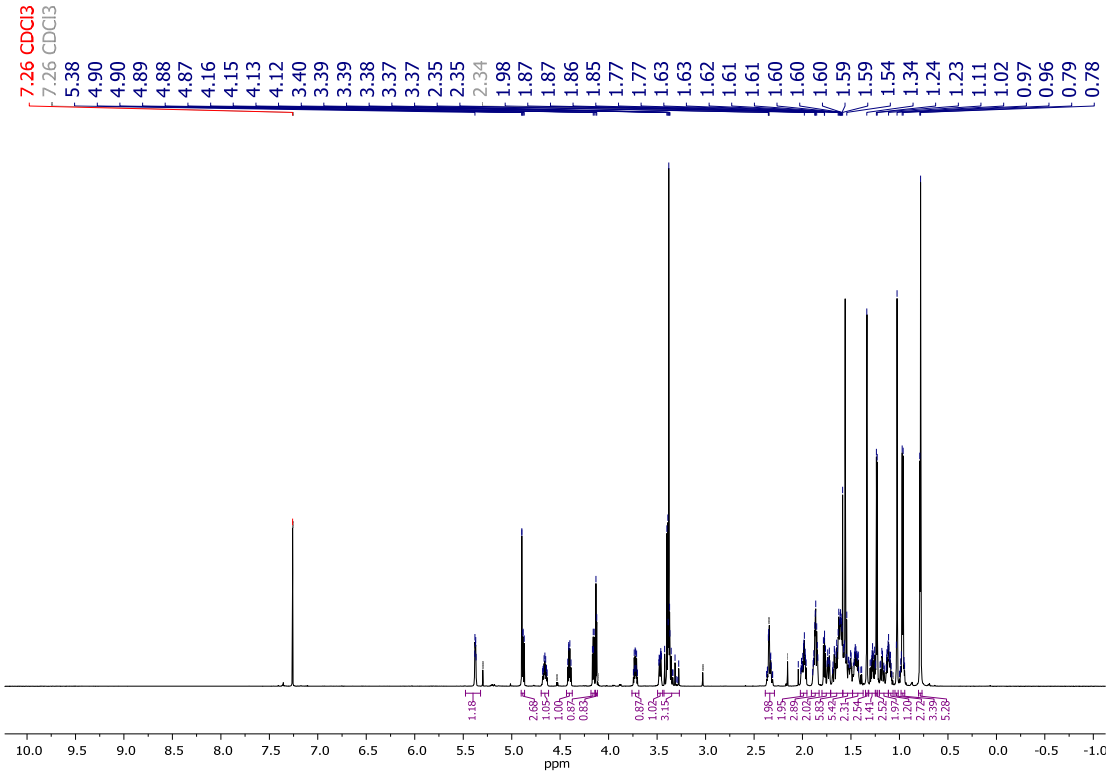


Figure S26. ^{1}H NMR spectrum of compound **4d**

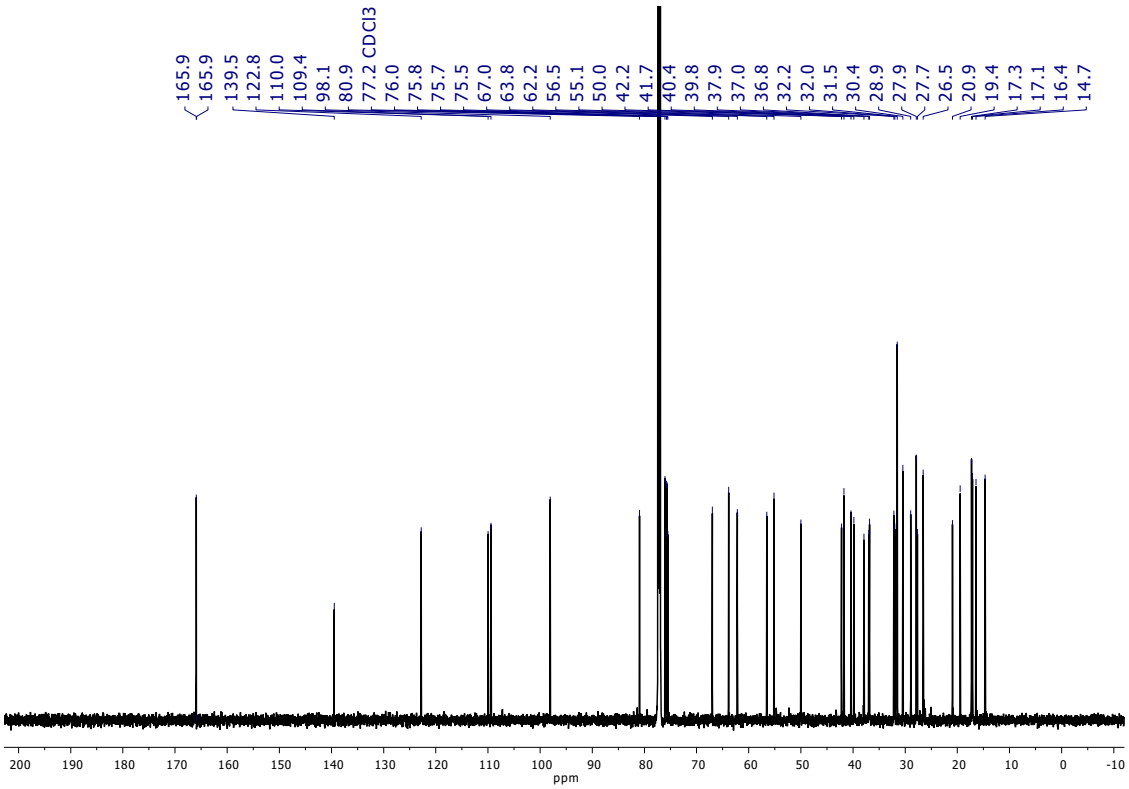


Figure S27. $^{13}C\{1H\}$ NMR spectrum of compound **4d**

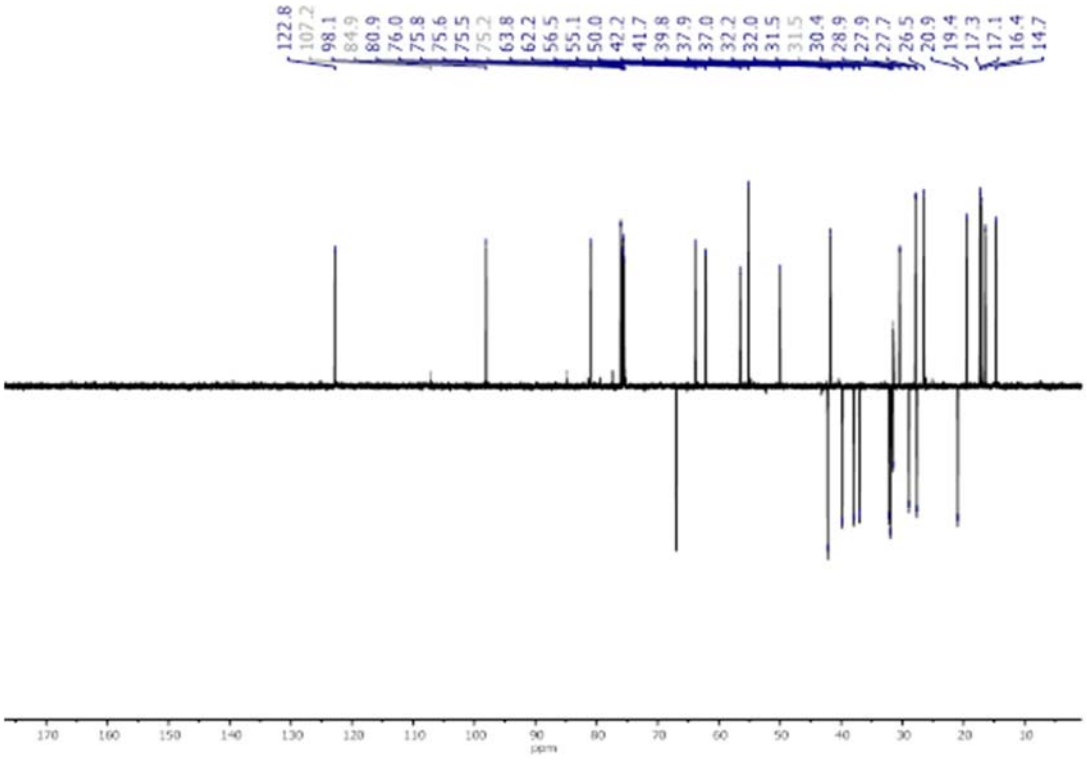


Figure S28. DEPT-135º spectrum of compound **4d**

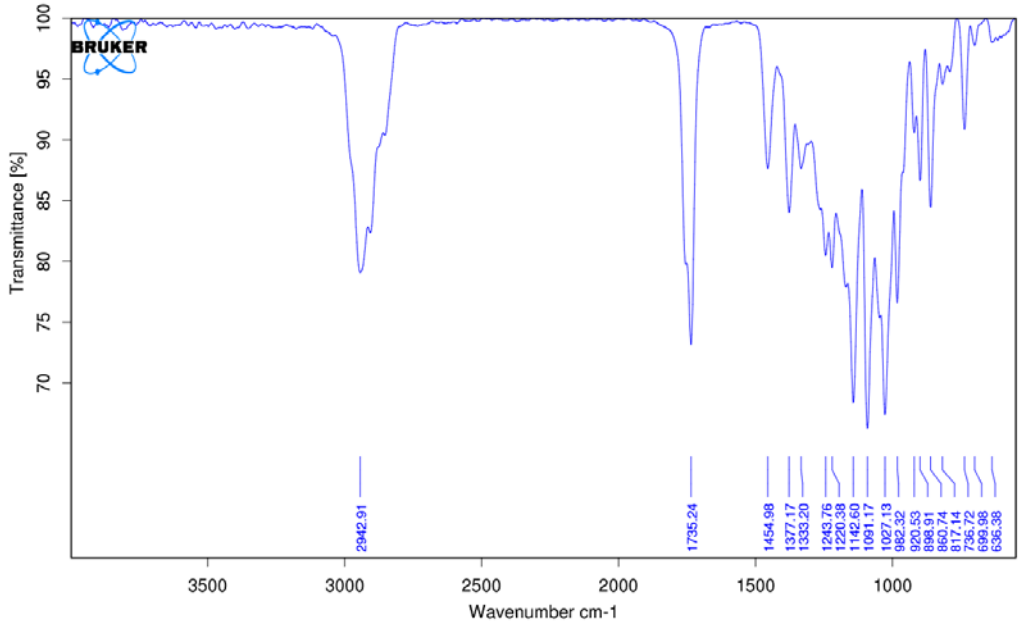


Figure S29. FTIR spectrum of compound **4d**

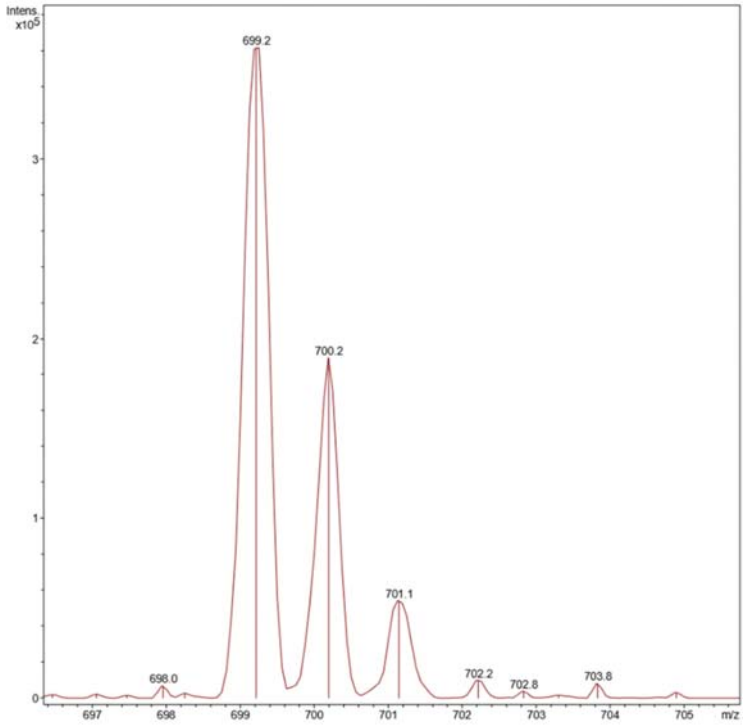
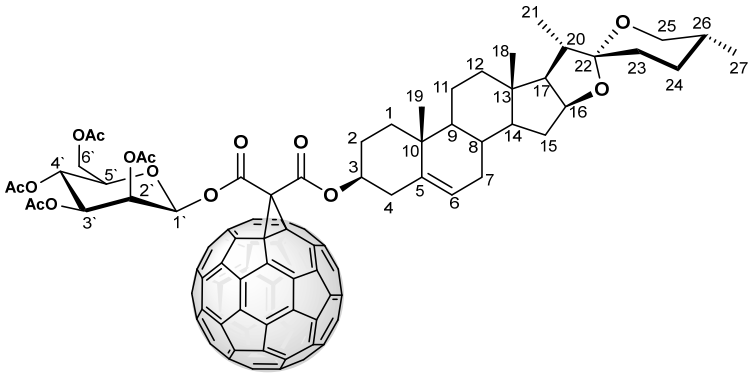


Figure S30. MS-ESI of compound **4d**

8. Spectra of 61-(3β-*O*-Carbetoxy-(22*R*,25*R*)-spirost-5-en)-61-(2′,3′,4′,6′-tetra-*O*-acetyl-β-D-mannopyranoside) methano[60]fullerene (5a)



5a

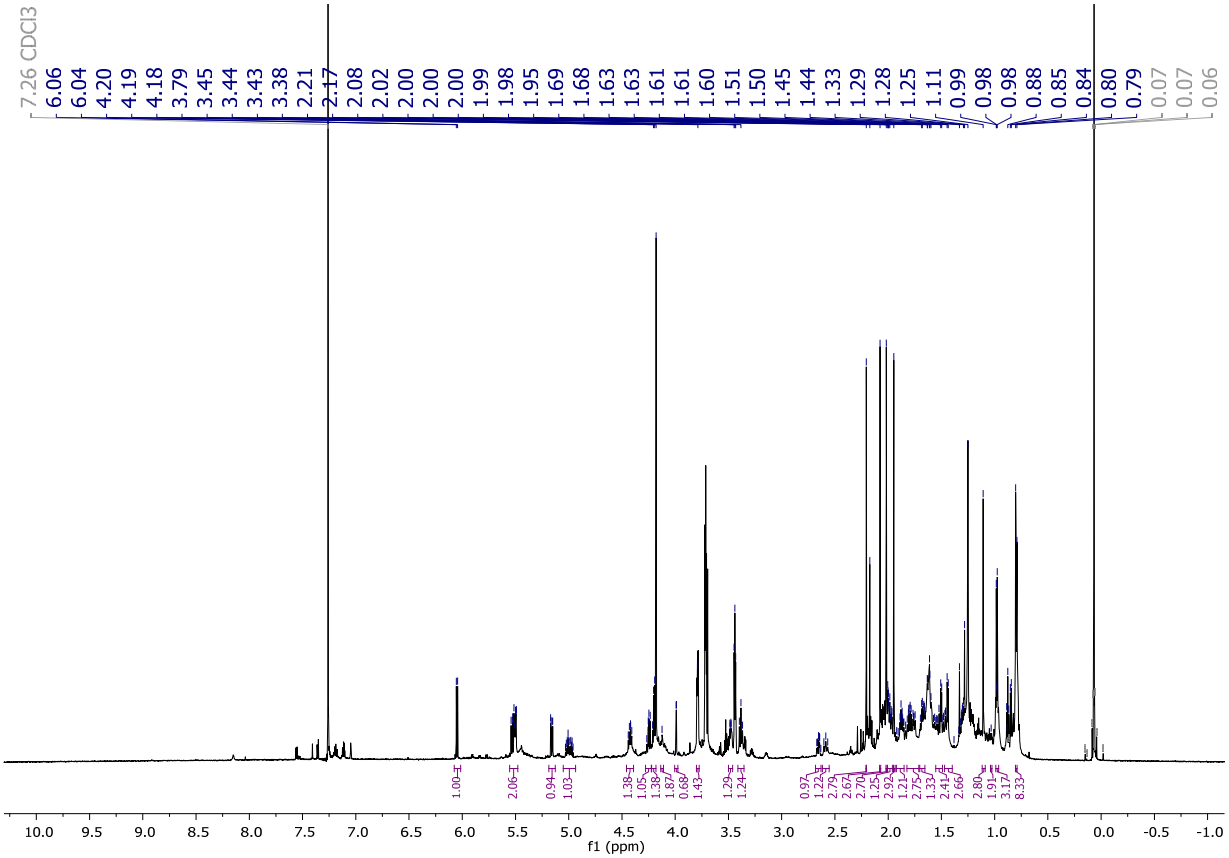


Figure S31. ^{1}H NMR spectrum of compound **5a**

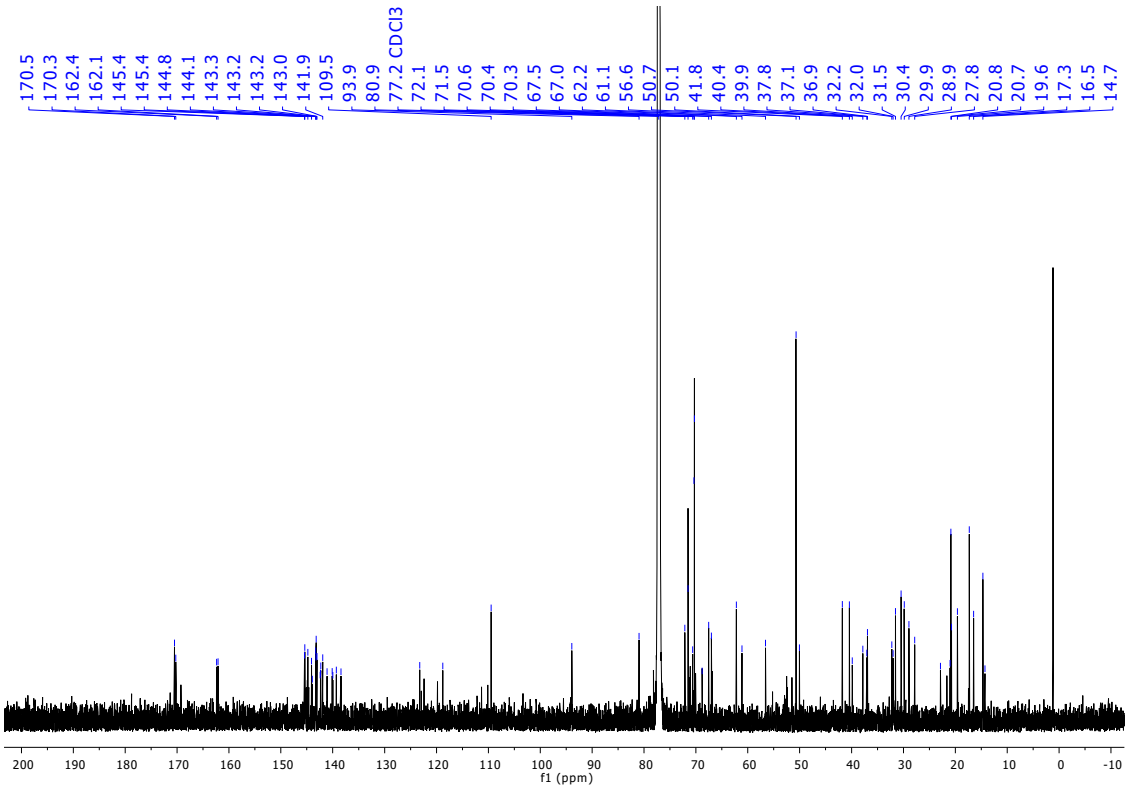


Figure S32. $^{13}C\{1H\}$ NMR spectrum of compound **5a**

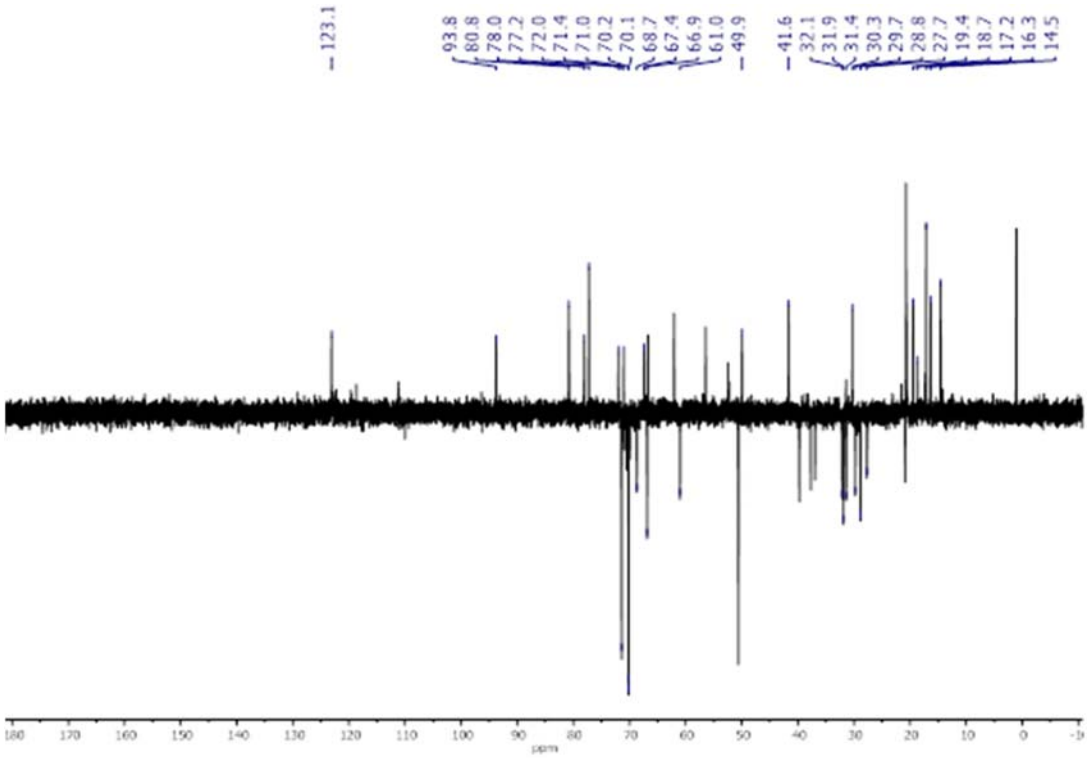


Figure S33. DEPT-135º spectrum of compound **5a**

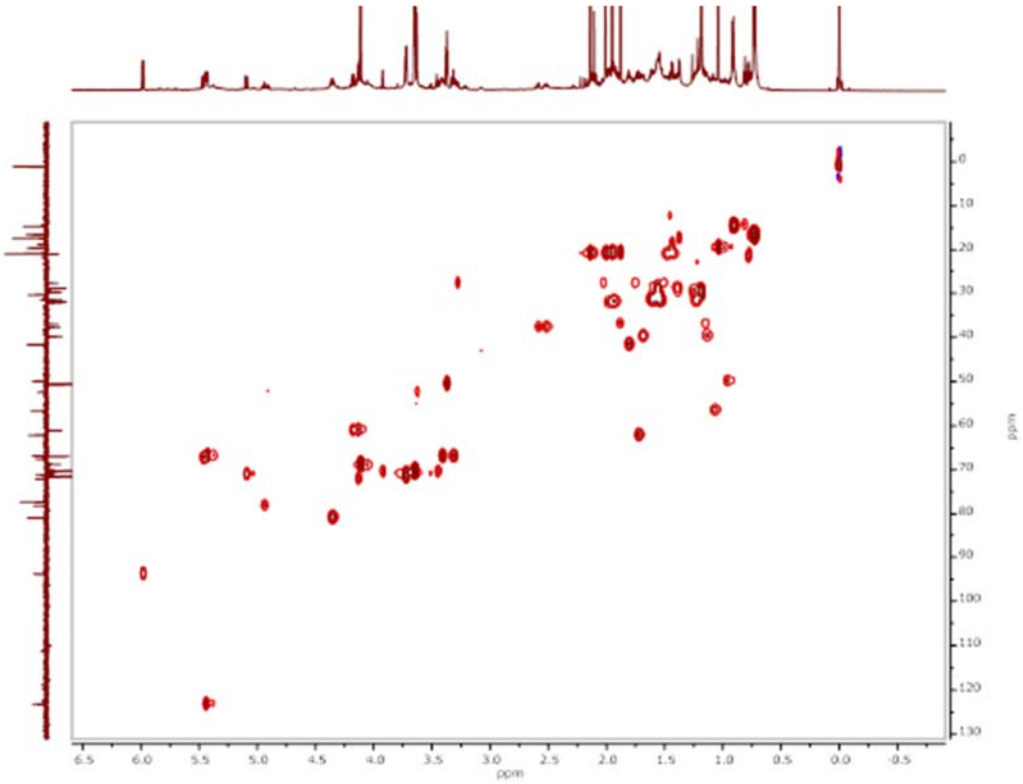


Figure S34. HSQC spectrum of compound **5a**

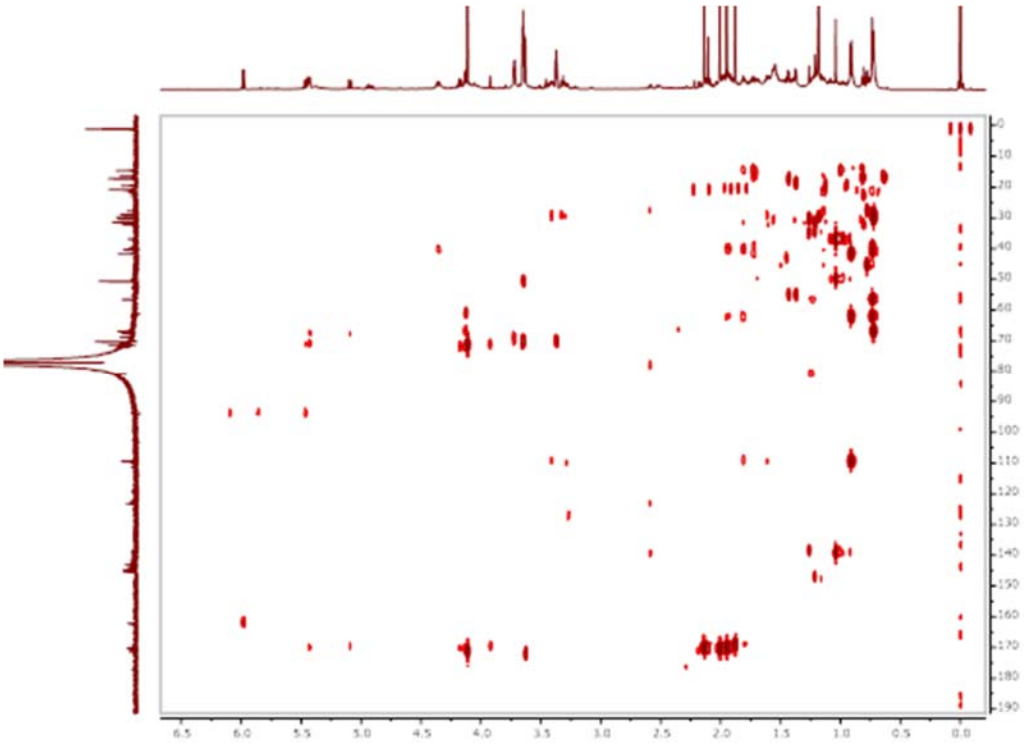


Figure S35. HMBC spectrum of compound **5a**

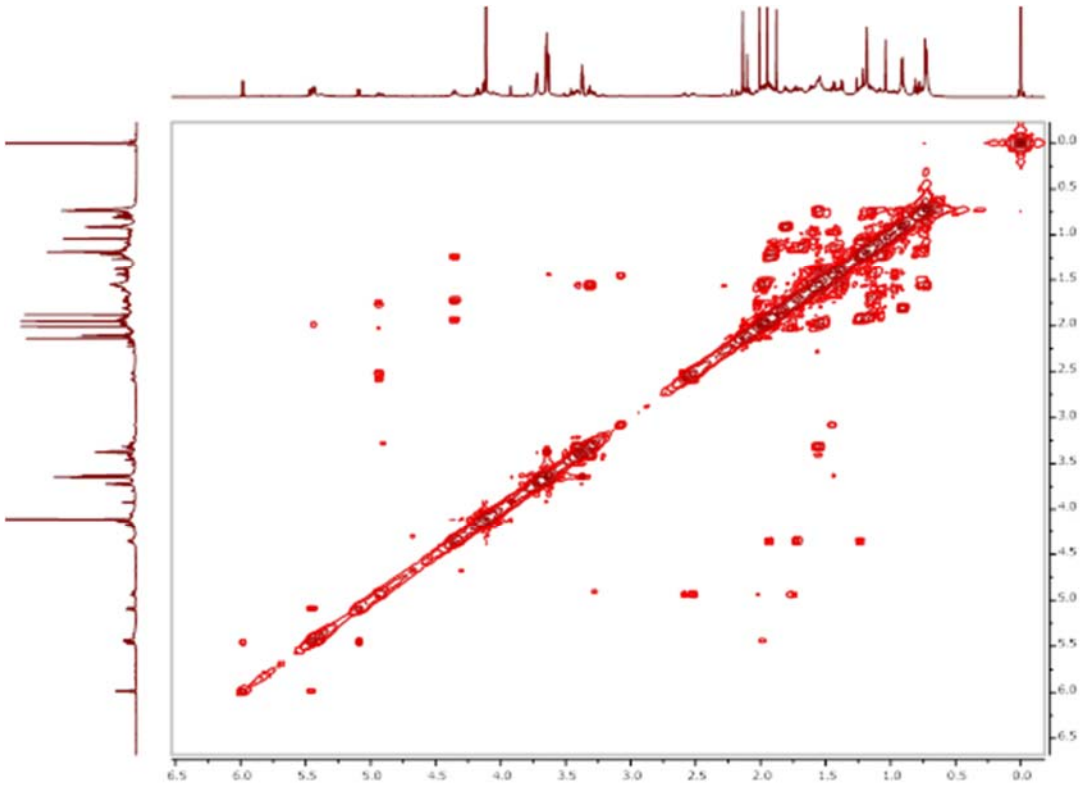


Figure S36. COSY spectrum of compound **5a**

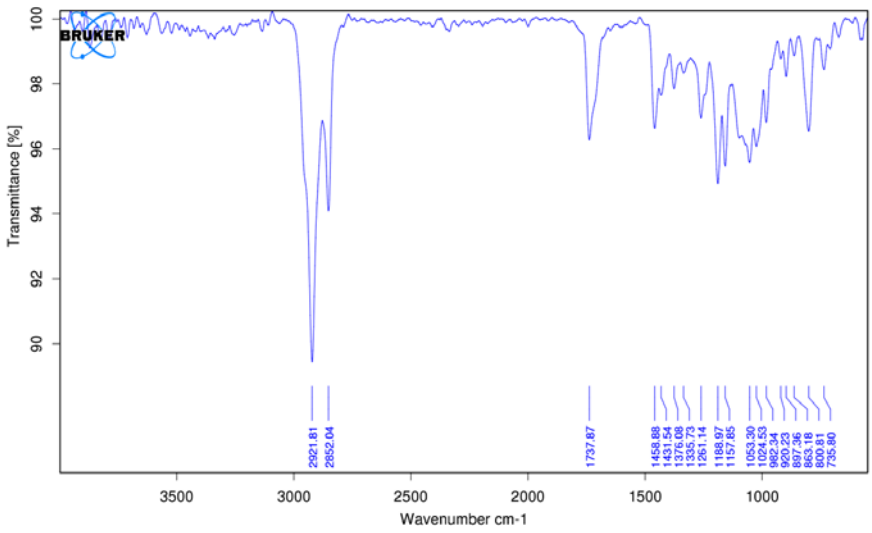


Figure S37. FTIR of compound **5a**

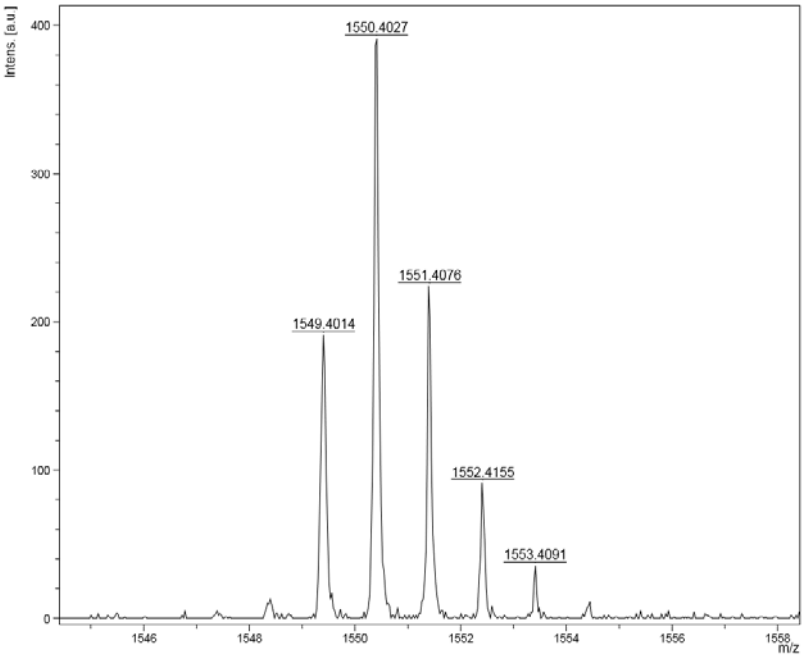
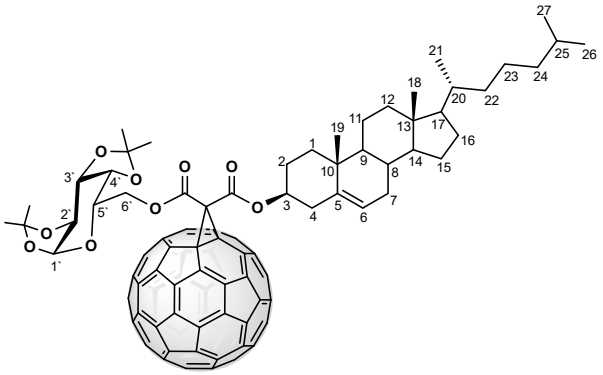


Figure S38. HRMS (MALDI-TOF) (Dithranol) of compound **5a** showing the ionic pattern corresponding to $[M+H]^+$ 1549.4014; calculated for $C_{104}H_{61}O_{15}$ 1549.4010.

9. Spectra of 61-(3β-*O*-Carbetoxycholest-5-en)-61-(1′,2′:3′,4′-di-*O*-isopropylidene-α-D-galactopyranoside) methano[60]fullerene (5b)



5b

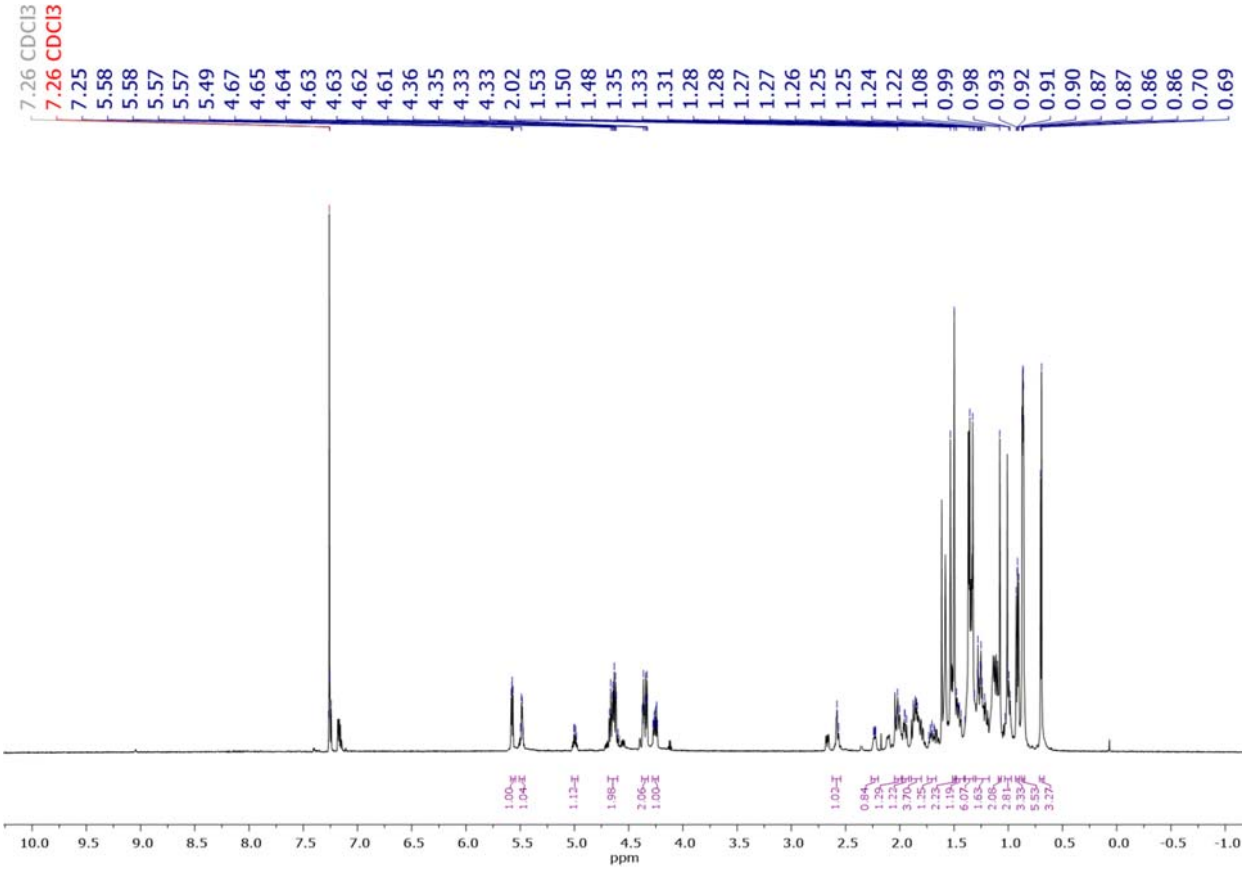


Figure S39. [1]H NMR spectrum of compound **5b**

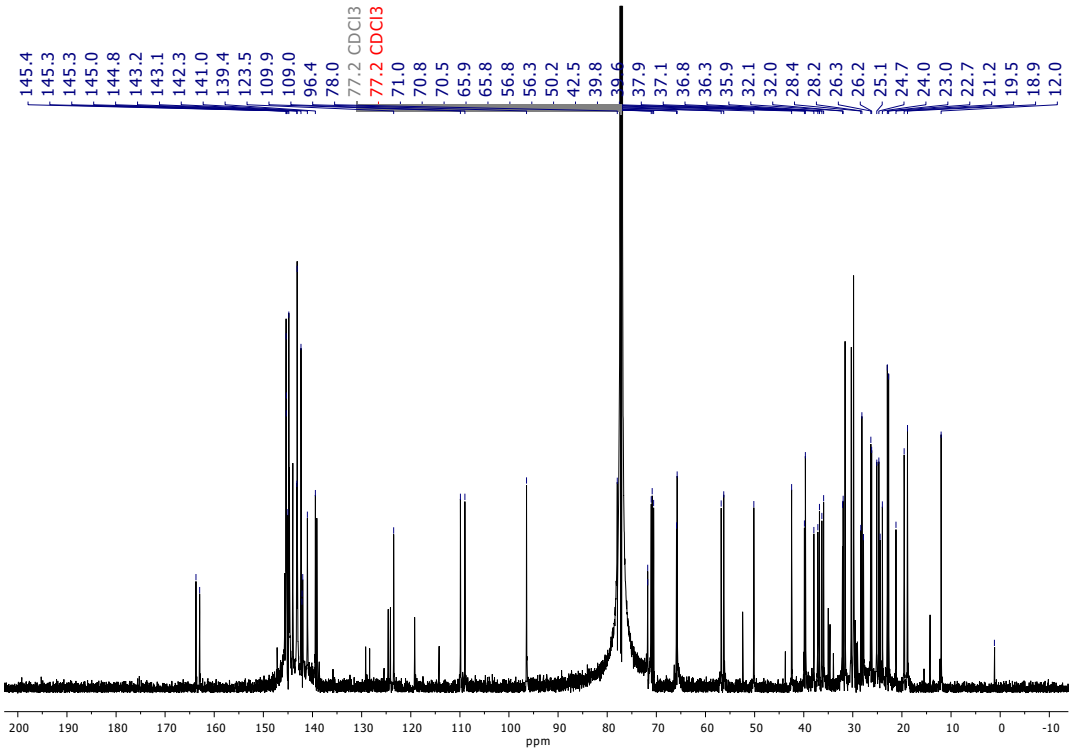


Figure S40. $^{13}C\{1H\}$ NMR spectrum of compound **5b**

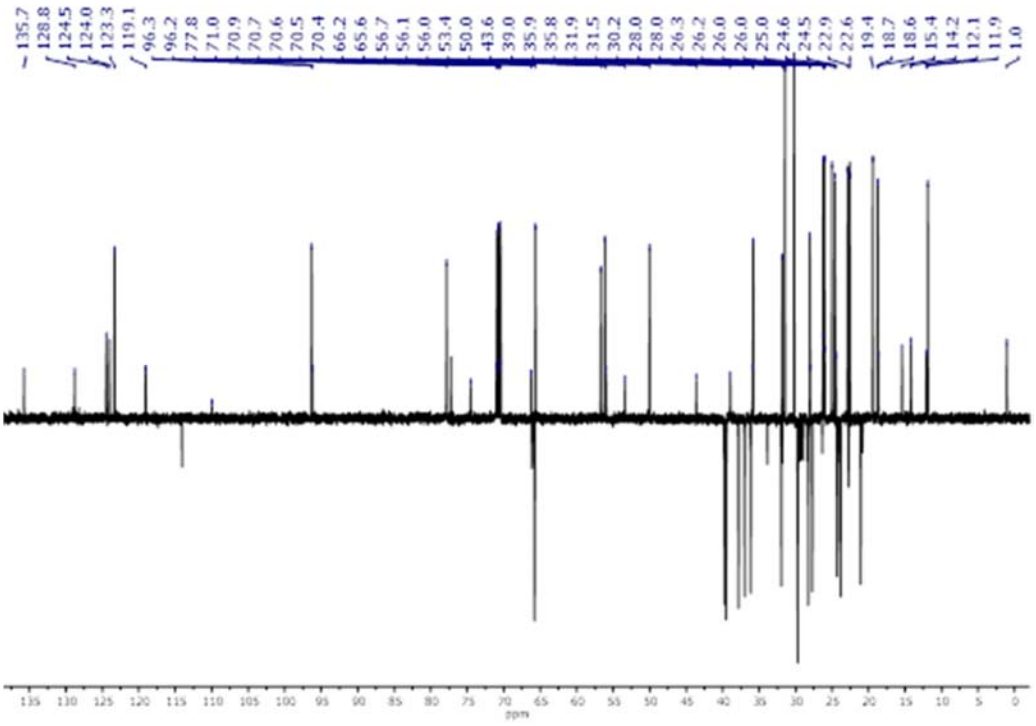


Figure S41. DEPT-135º spectrum of compound **5b**

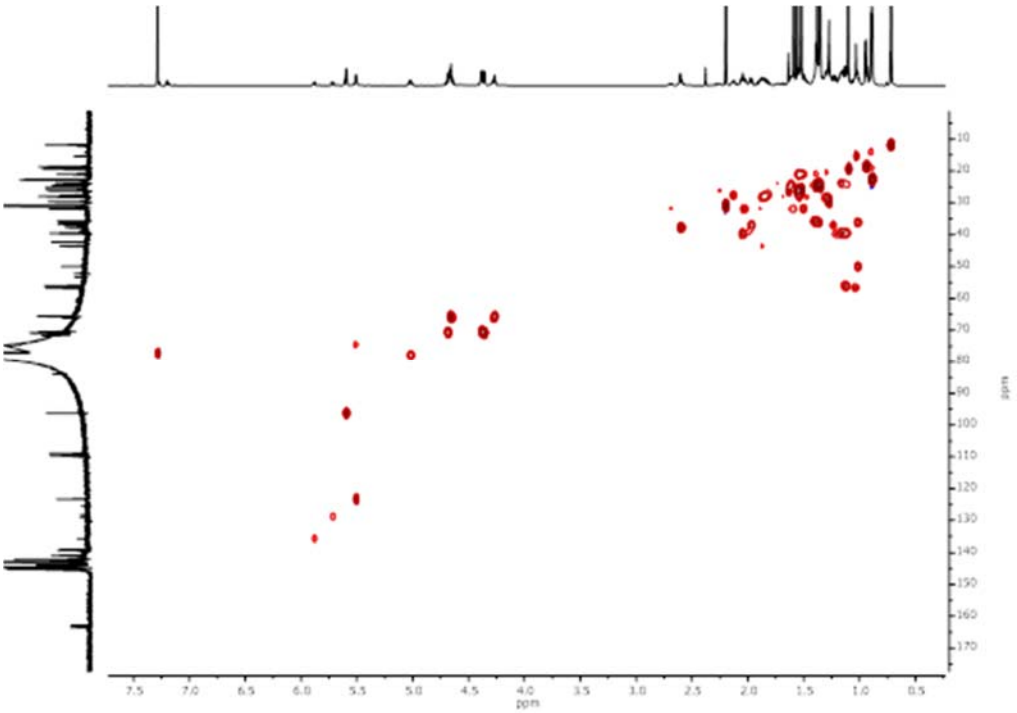


Figure S42. HSQC spectrum of compound **5b**

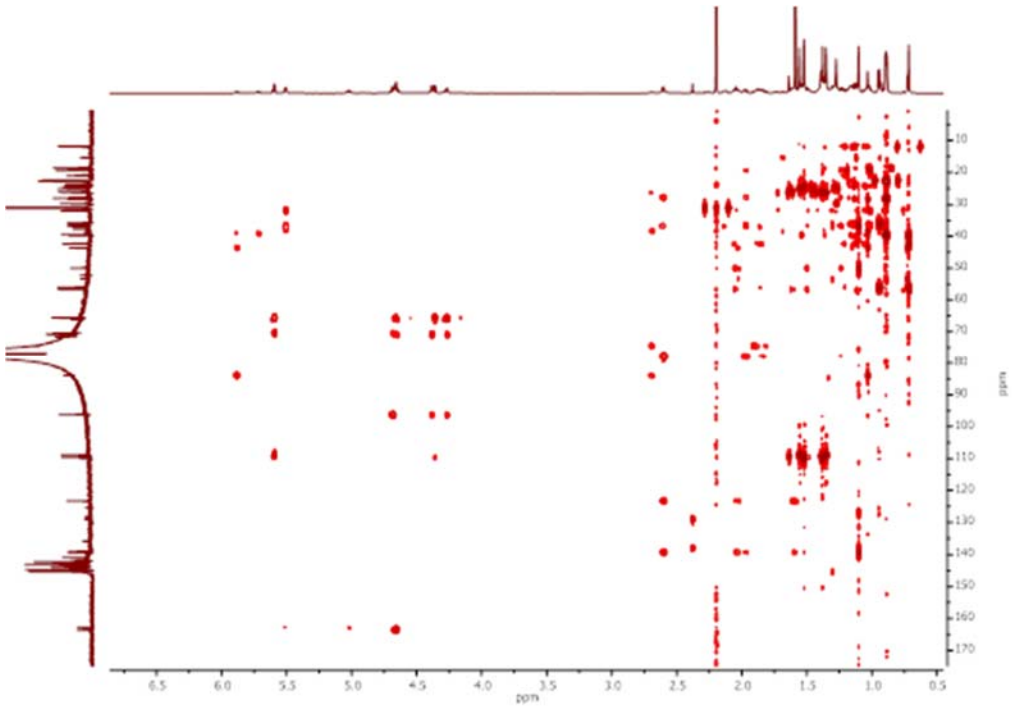


Figure S43. HMBC spectrum of compound **5b**

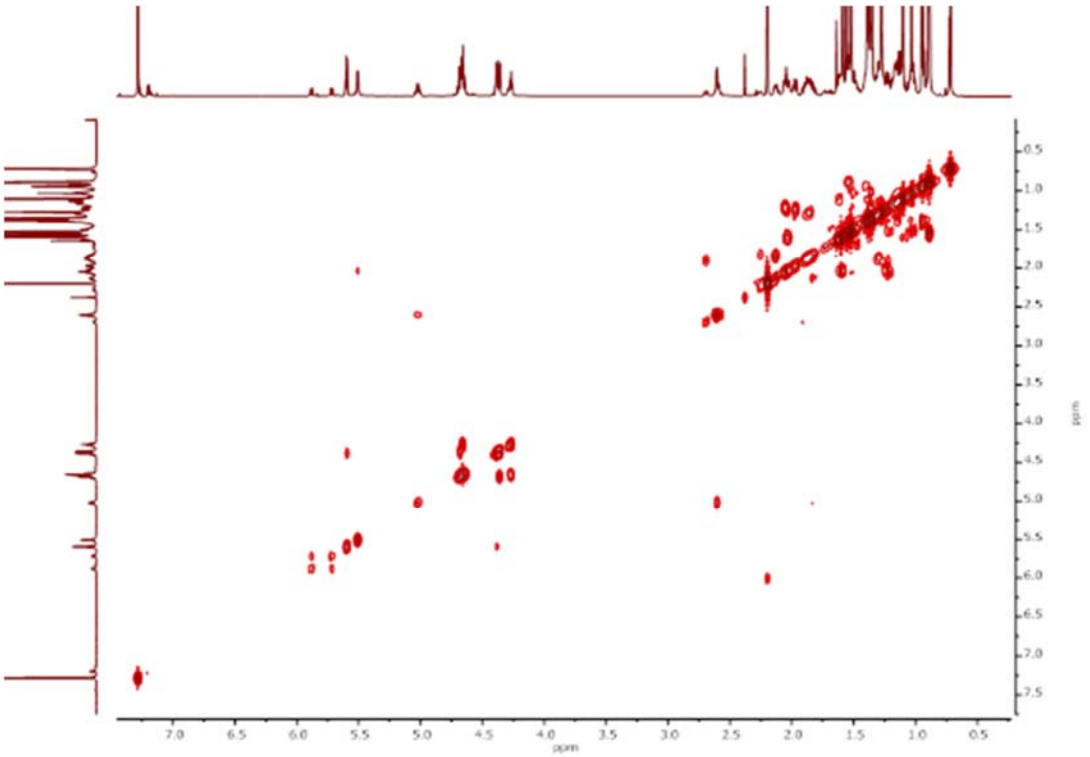


Figure S44. COSY spectrum of compound **5b**

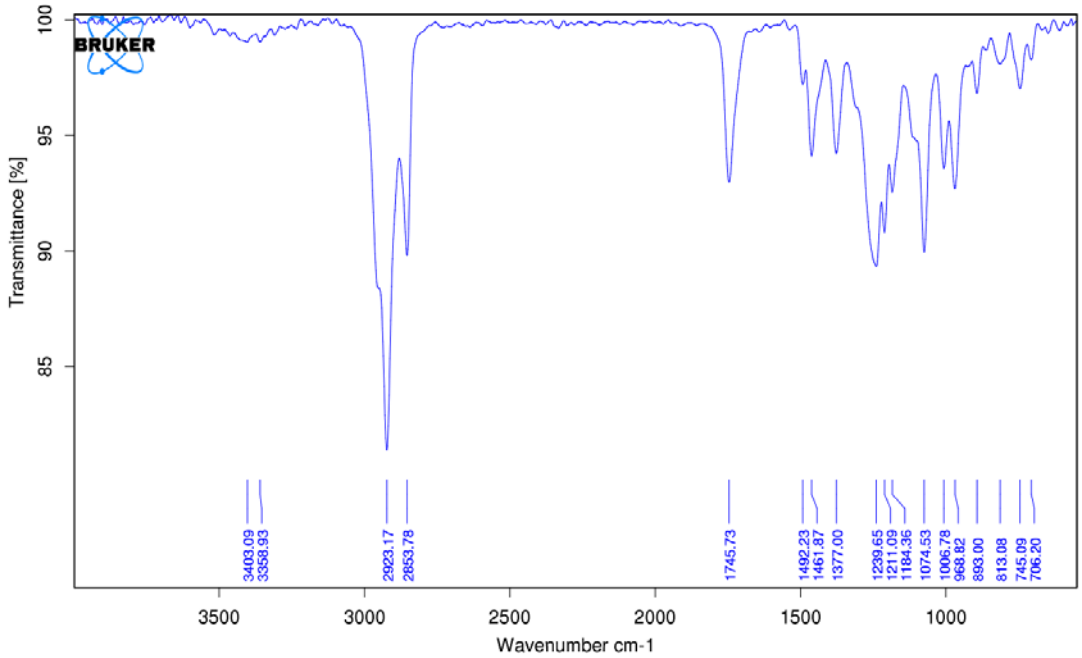


Figure S45. FTIR of compound **5b**

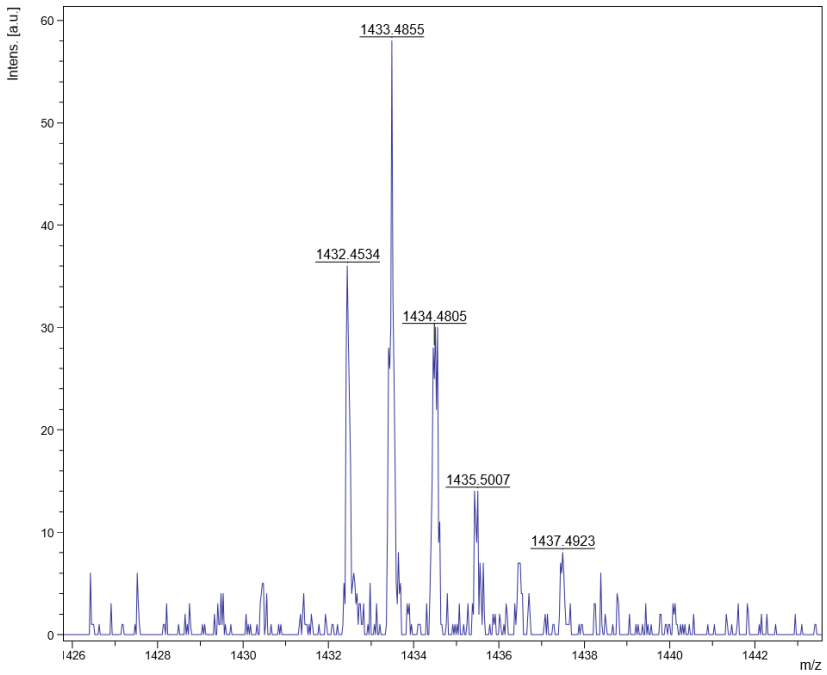


Figure S46. HRMS (MALDI-TOF) of compound **5b** showing the ionic pattern corresponding to $[M]^{\bullet+}$ 1432.4534; calculated for $C_{102}H_{64}O_9$ 1432.4550.

10. Spectra of 61-(3β-*O*-Carbetoxy-(22*R*,25*R*)-spirost-5-en)-61-(1′,2′:3′,4′-di-*O*-isopropylidene-α-D-galactopyranoside) methano[60]fullerene (5c)

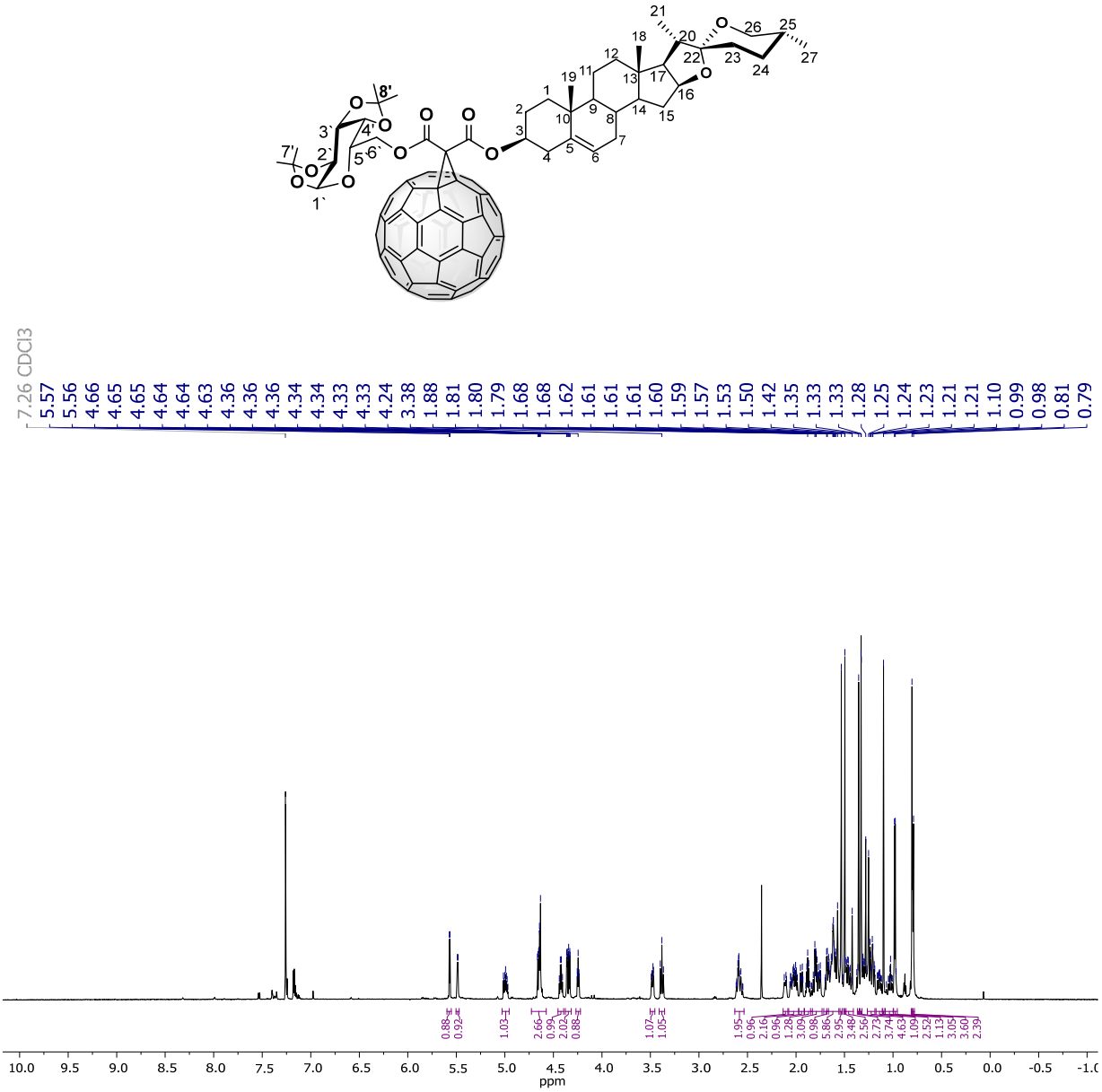


Figure S47. ^{1}H NMR spectrum of compound **5c**

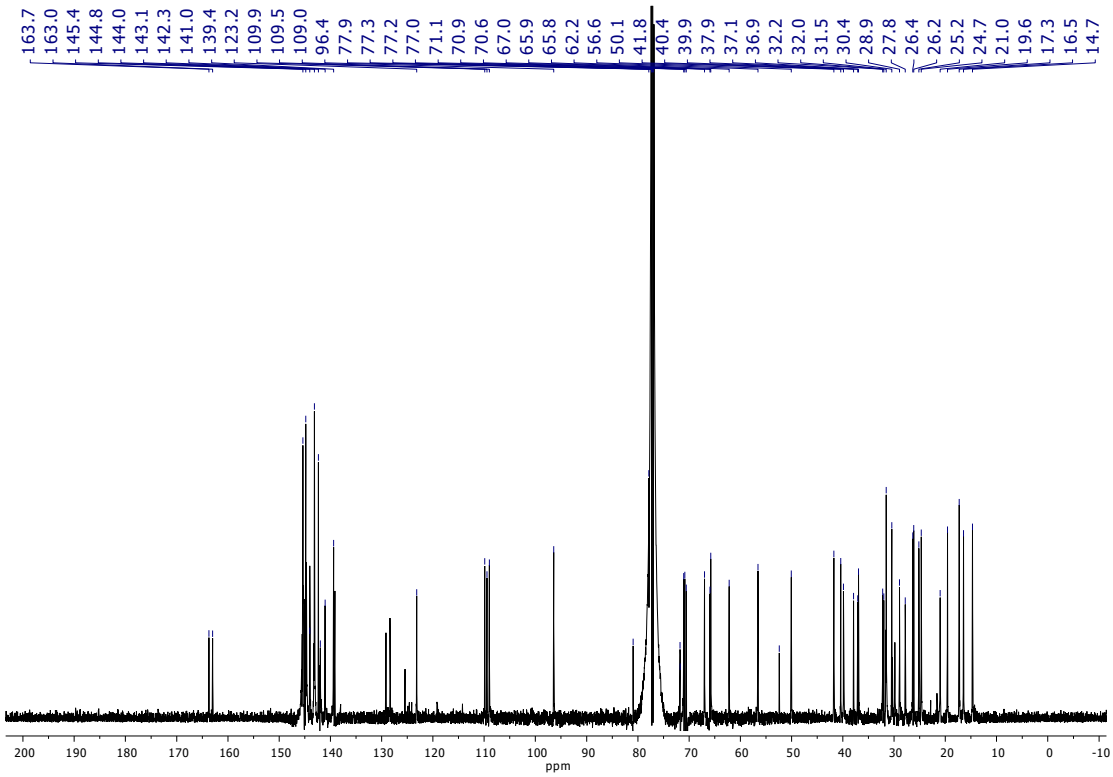


Figure S48. $^{13}C\{1H\}$ NMR spectrum of compound **5c**

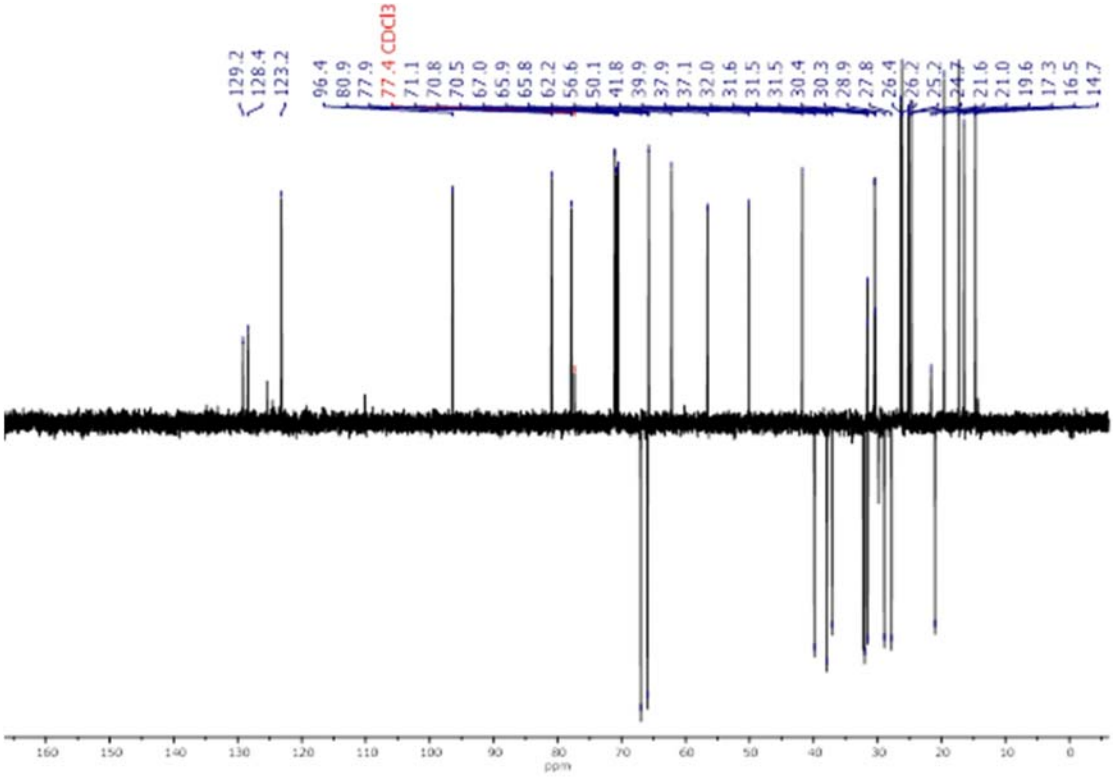


Figure S49. DEPT-135º spectrum of compound **5c**

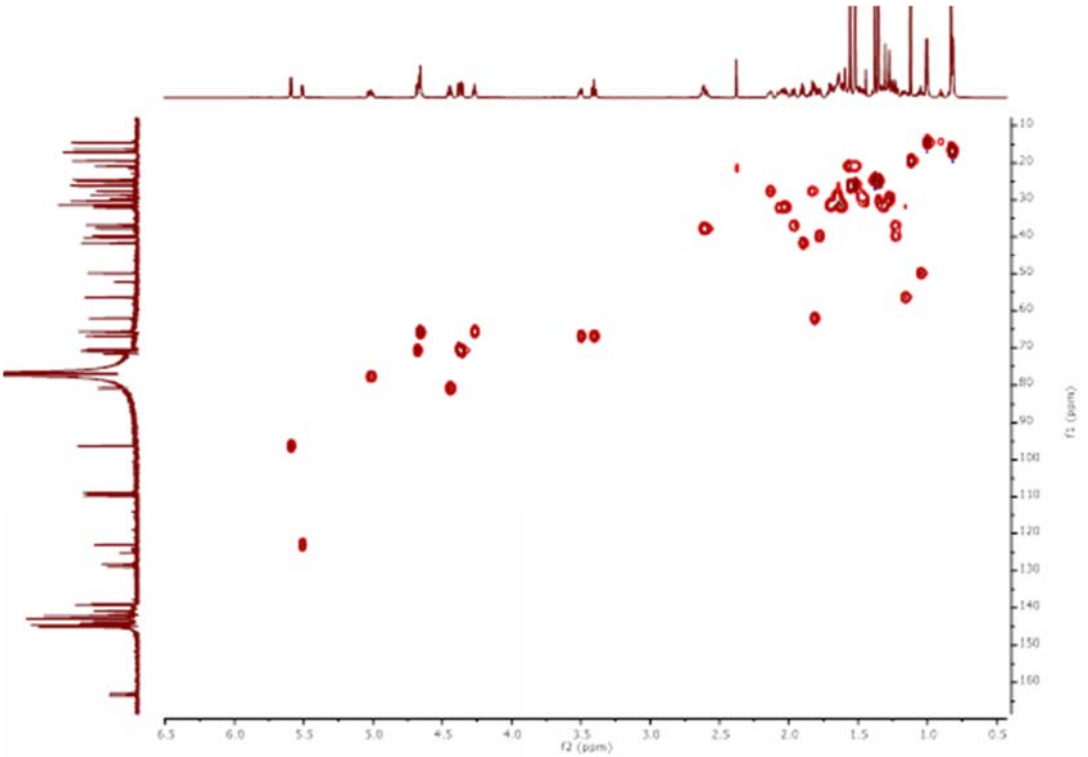


Figure S50. HSQC spectrum of compound **5c**

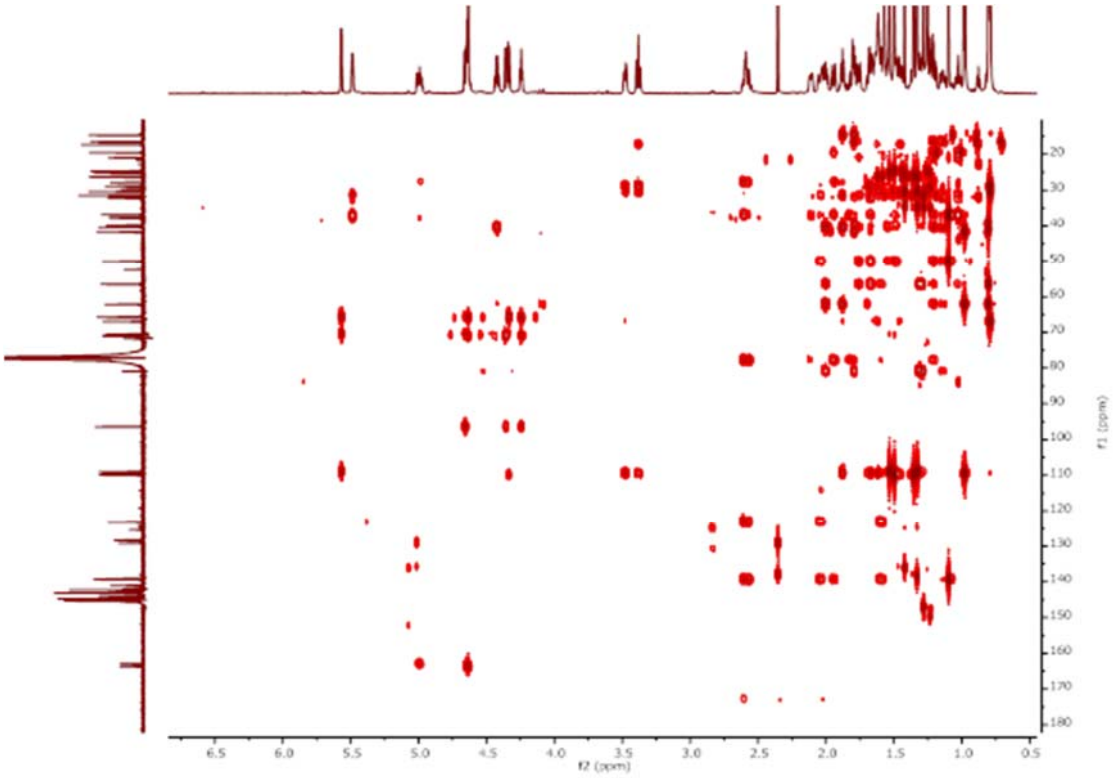


Figure S51. HMBC spectrum of compound **5c**

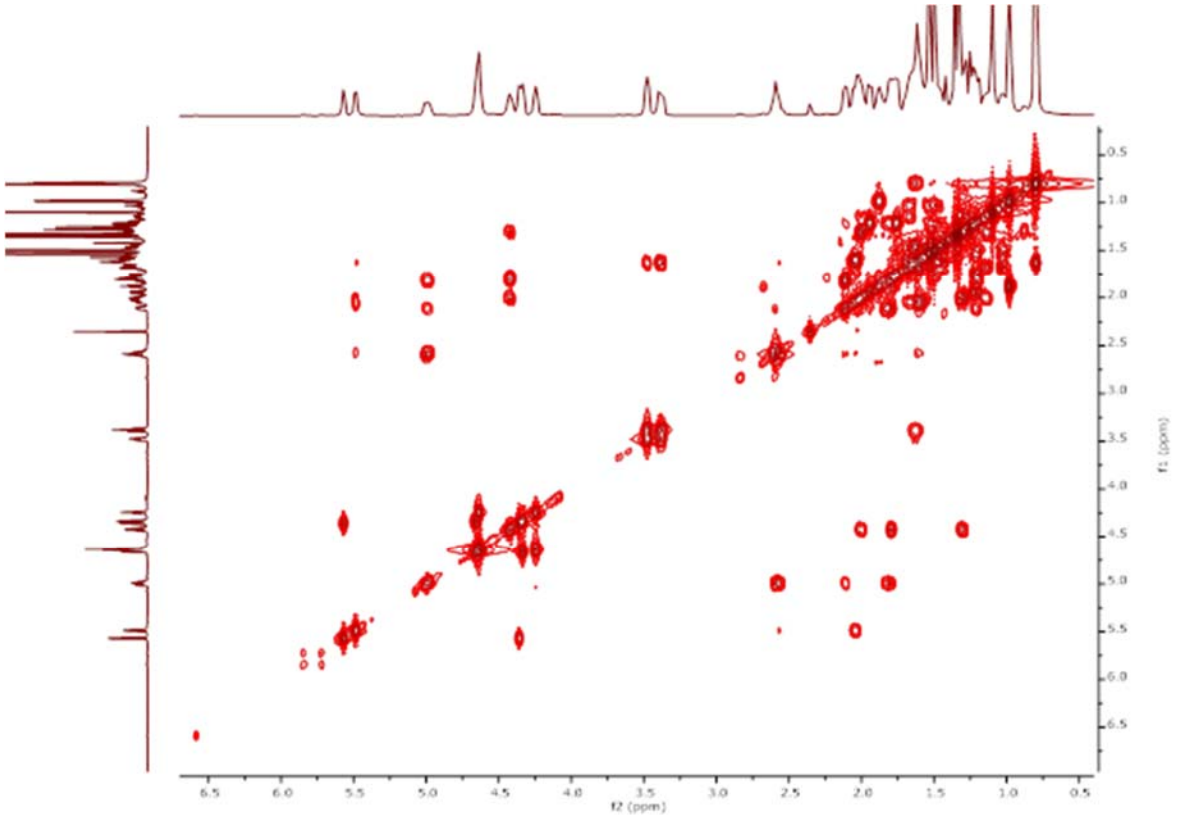


Figure S52. COSY spectrum of compound **5c**

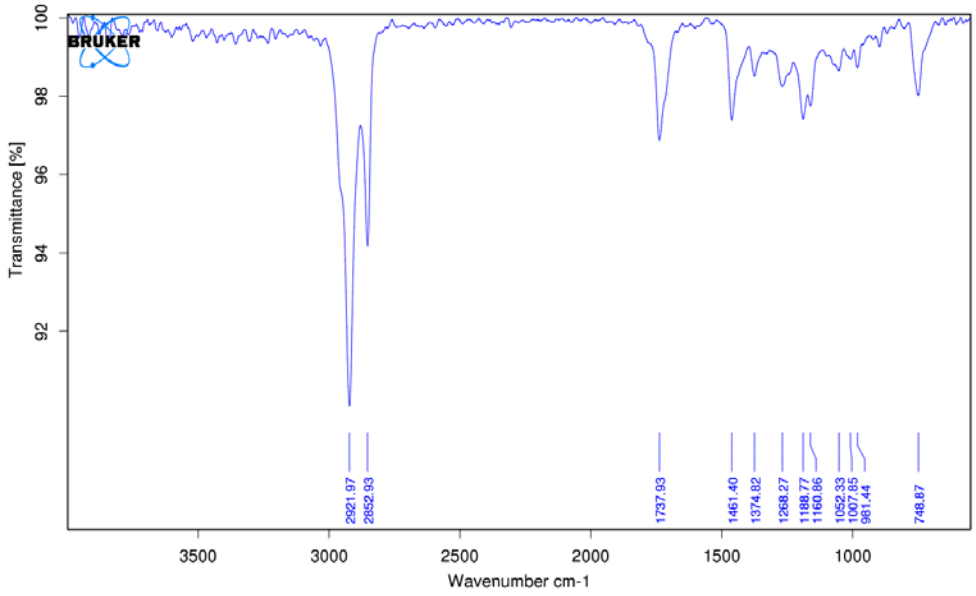


Figure S53. FTIR of compound **5c**

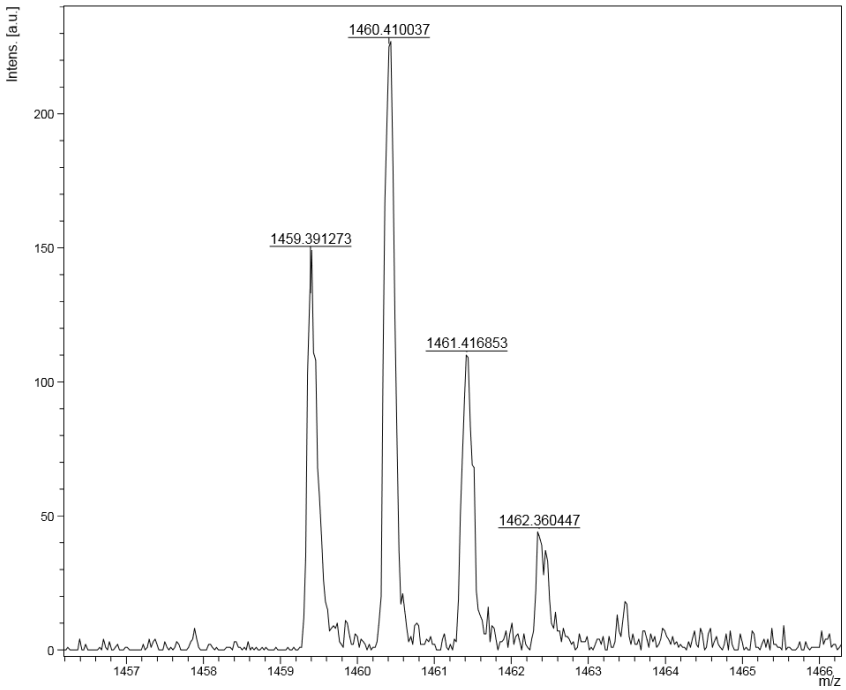


Figure S54. HRMS (MALDI-TOF) of compound **5c** showing the ionic pattern corresponding to $[M-H]^-$ 1459.3912; calculated for $C_{102}H_{59}O_{11}$ 1459.4057.

11. Spectra of 61-(3β-*O*-Carbetoxy-(22*R*,25*R*)-spirost-5-en)-61-[4′-(methyl-2,3-*O*-isopropylidene-α-L-rhamnopyranoside)] methano[60]fullerene (5d)

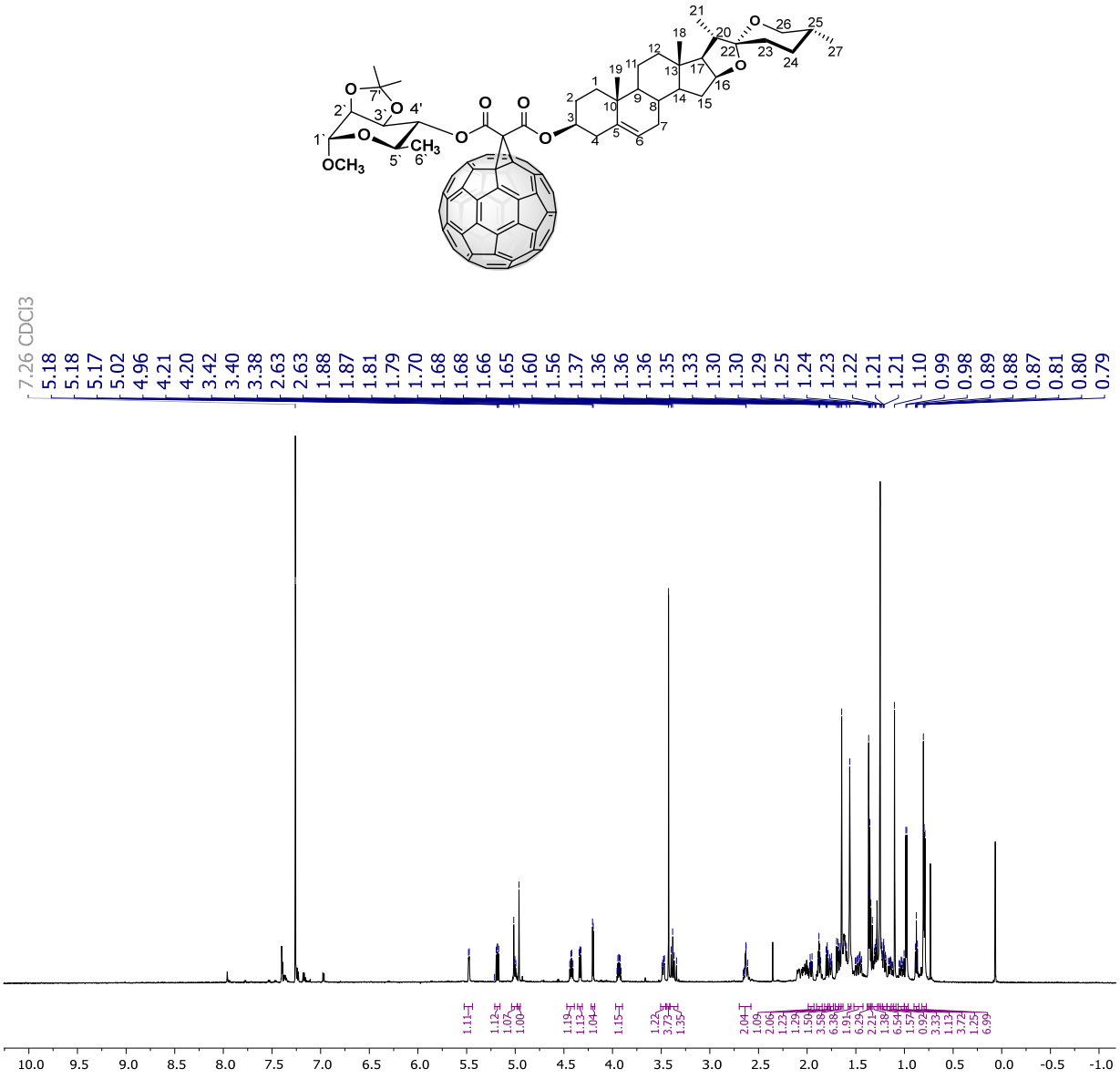


Figure S55. ^{1}H NMR spectrum of compound **5d**

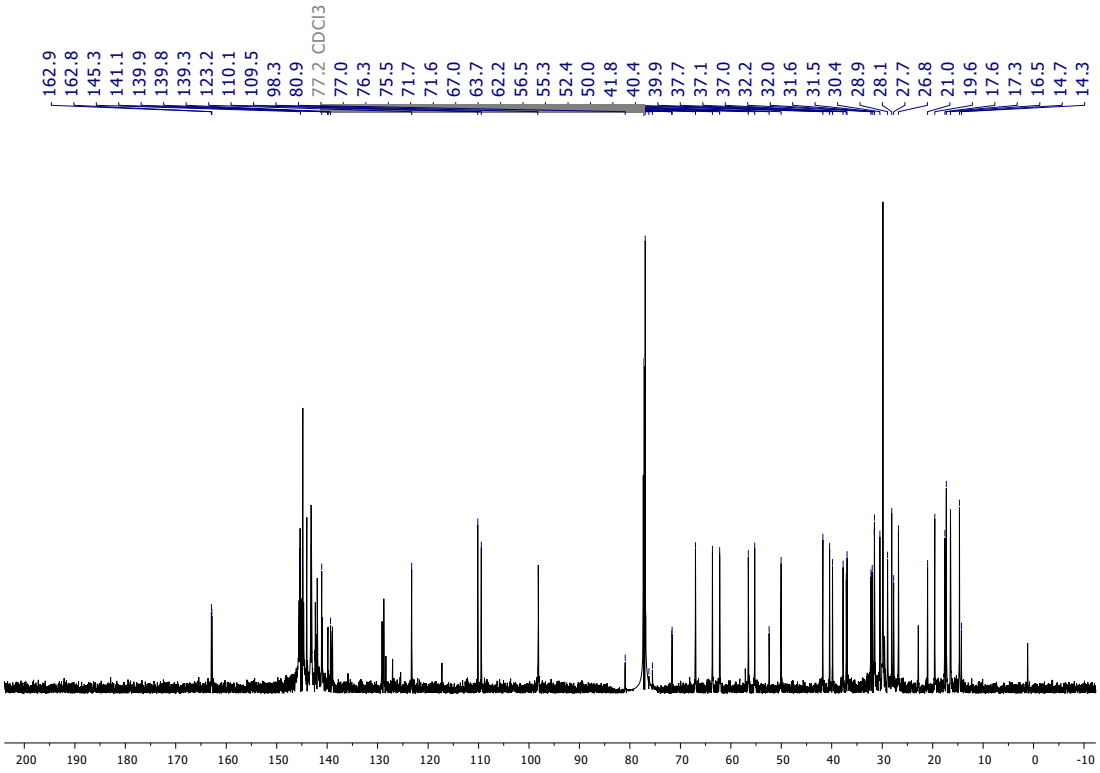


Figure S56. $^{13}C\{1H\}$ NMR spectrum of compound **5d**

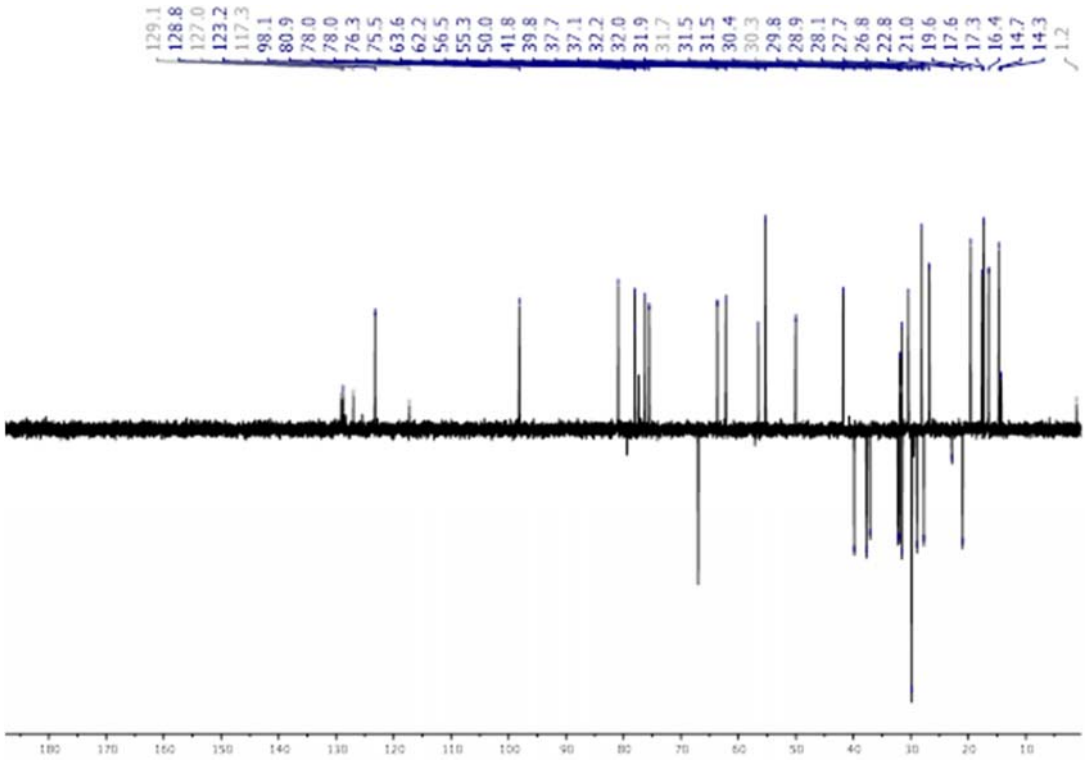


Figure S57. DEPT-135º spectrum of compound **5d**

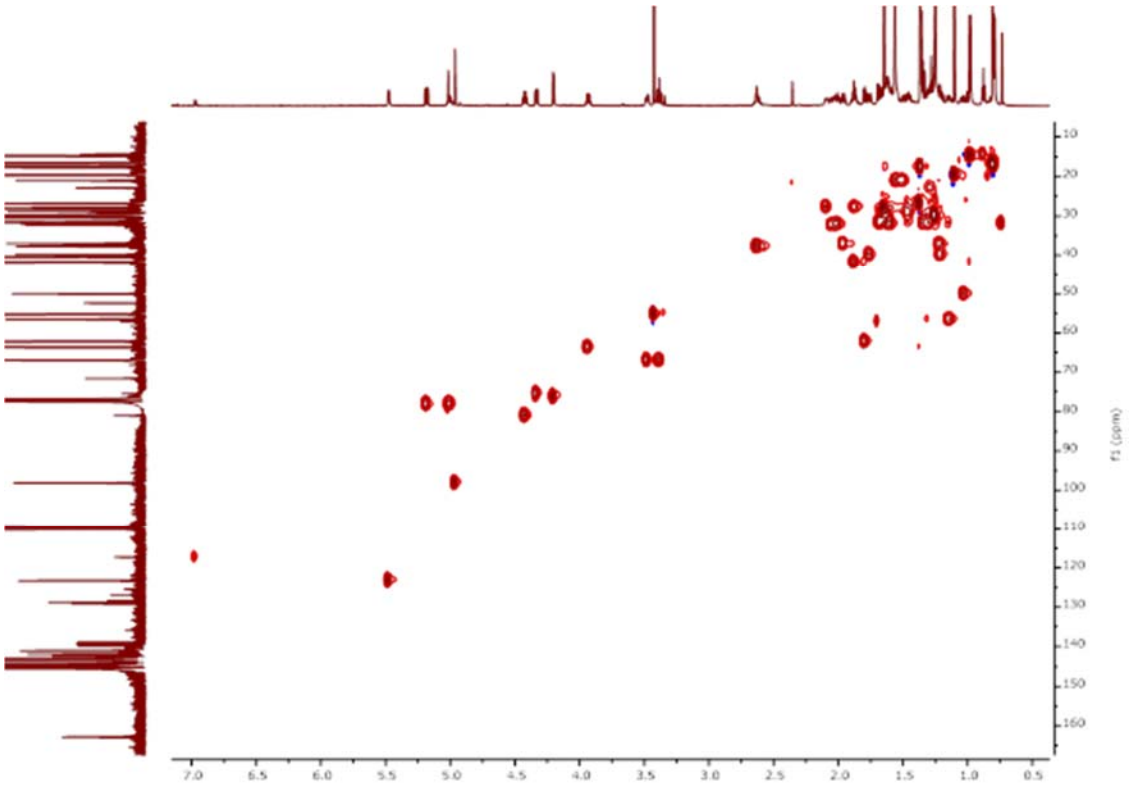


Figure S58. HSQC spectrum of compound **5d**

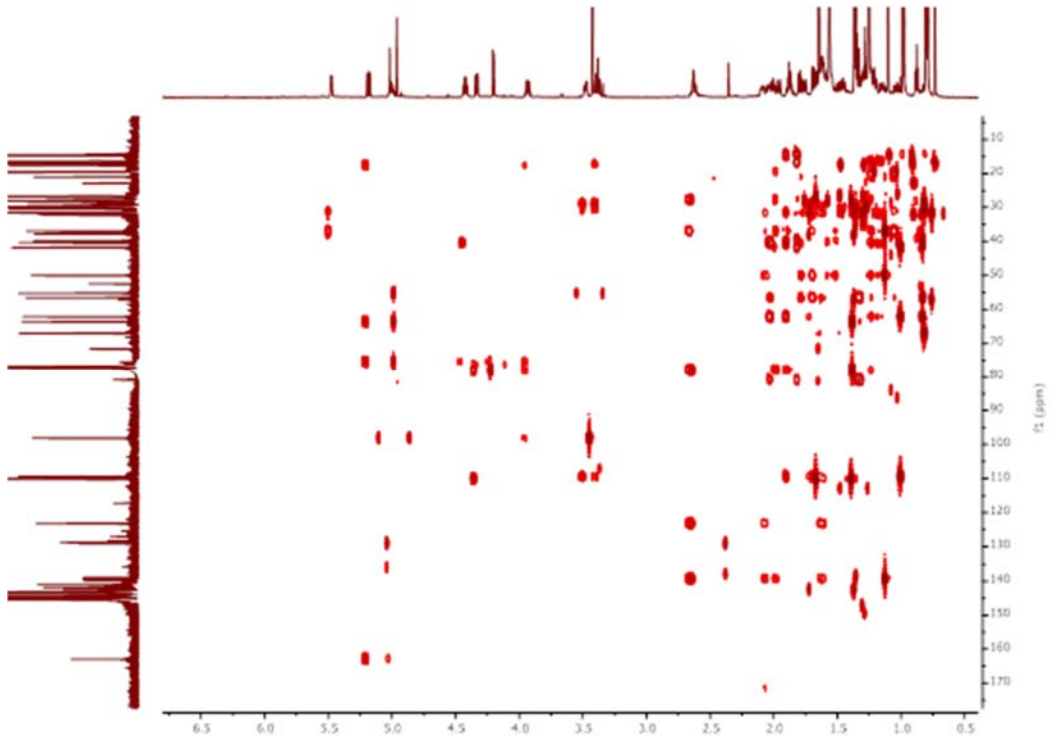


Figure S59. HMBC spectrum of compound **5d**

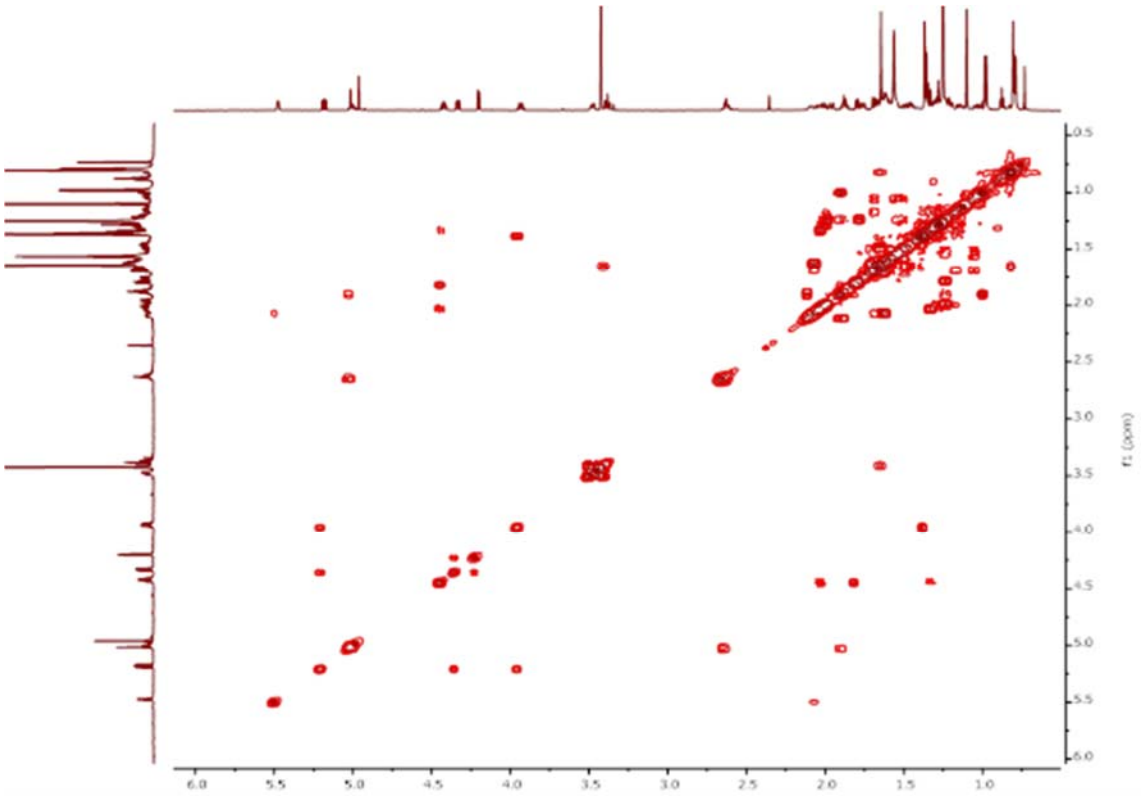


Figure S60. COSY spectrum of compound **5d**

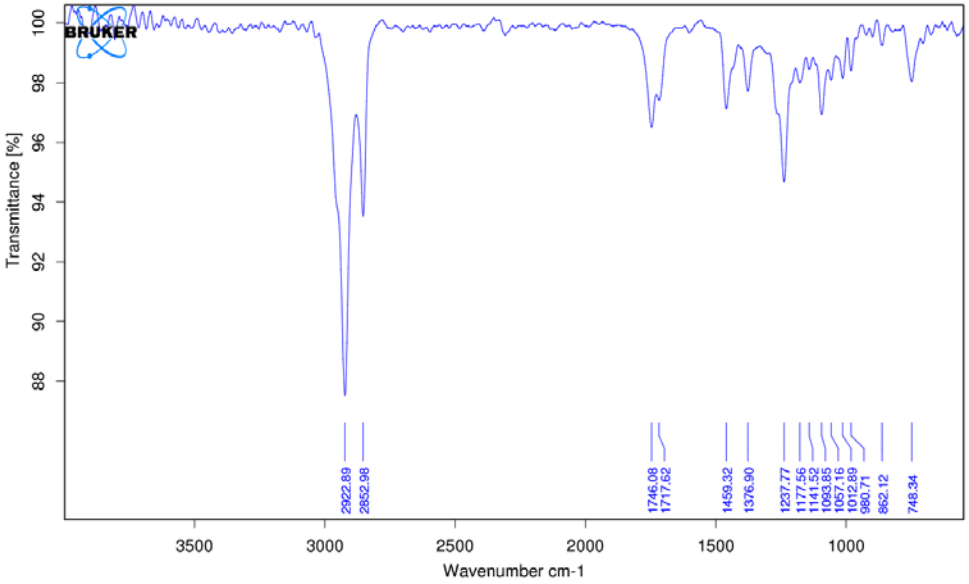


Figure S61. FTIR of compound **5d**

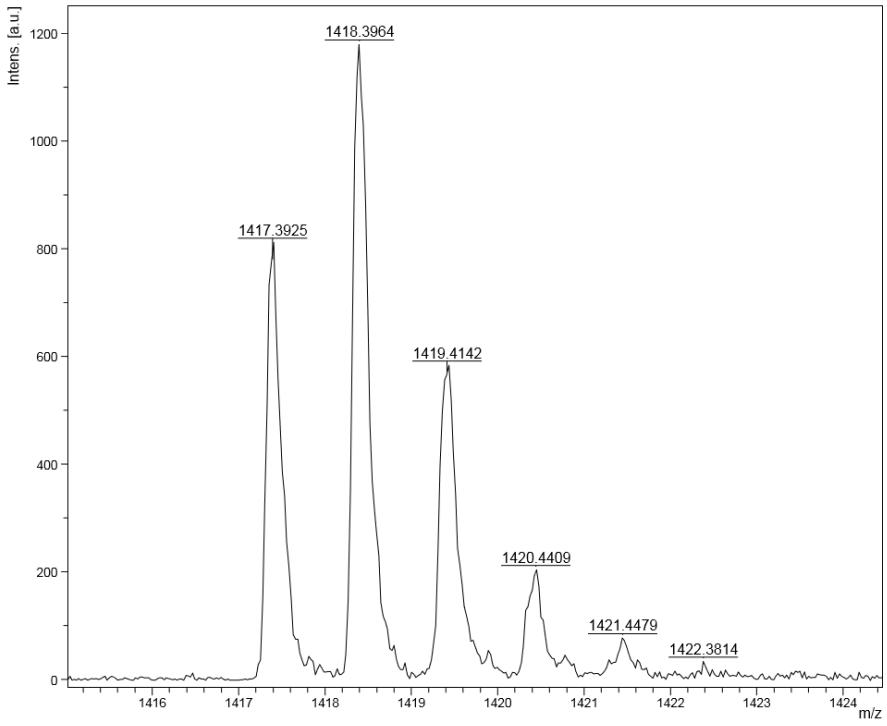


Figure S62. HRMS (MALDI-TOF) of compound **5d** showing the ionic pattern corresponding to $[M-H]^{\bullet-}$ 1417.3925; calculated for $C_{100}H_{59}O_{10}$ 1417.3951.

12. Spectra of 61-(3β-*O*-Carbetoxy-(22*R*,25*R*)-spirost-5-en)-61-[4′-(methyl-α-L-rhamnopyranoside)] methano[60]fullerene (6)

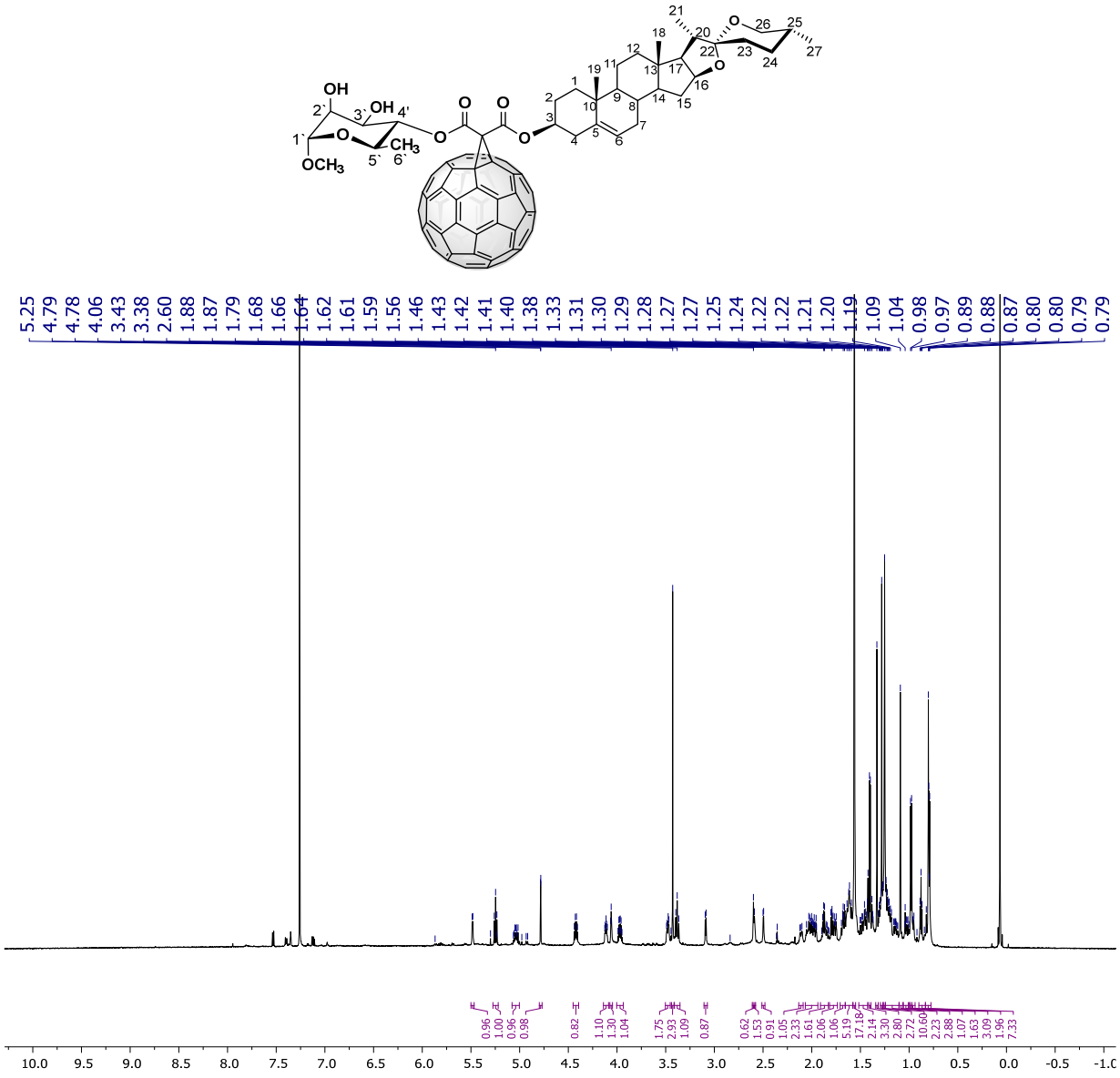


Figure S63. ^{1}H NMR spectrum of compound **6**

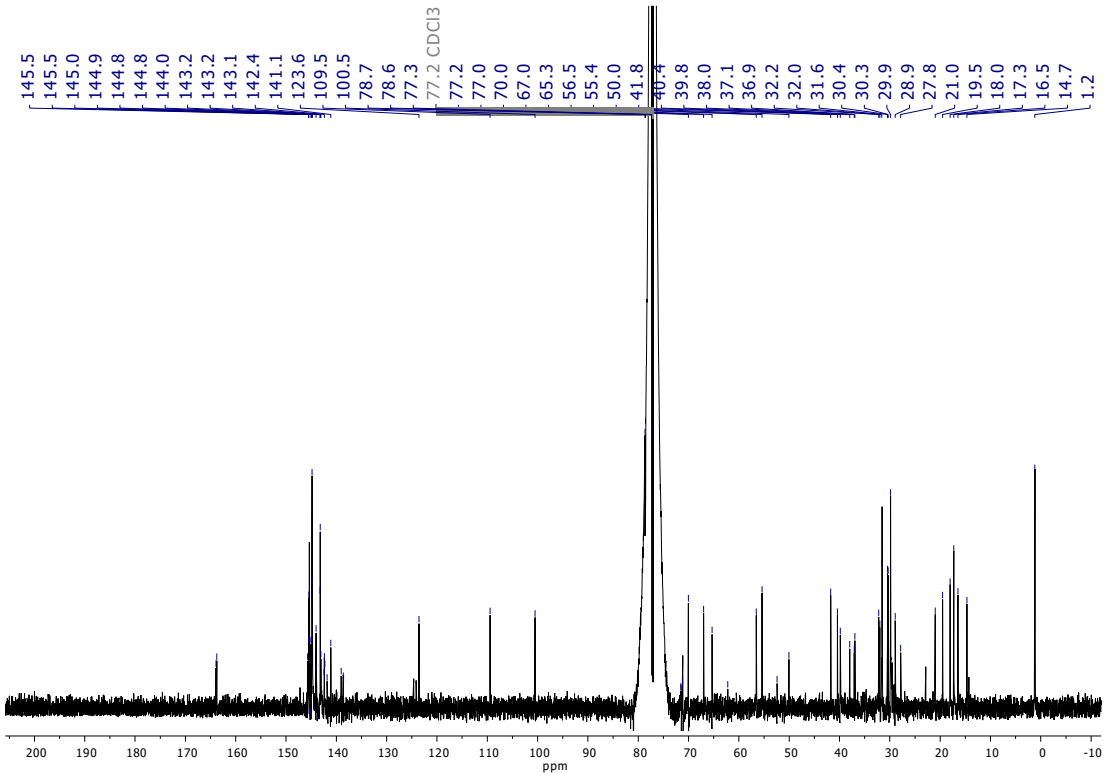


Figure S64. $^{13}C\{1H\}$ NMR spectrum of compound **6**

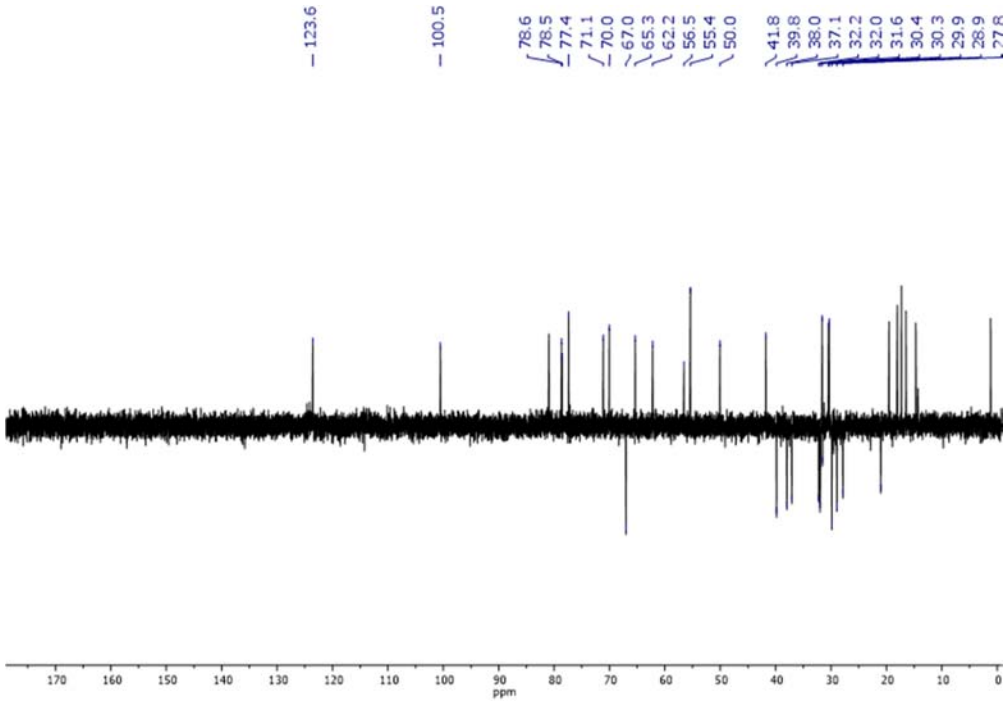


Figure S65. DEPT-135º spectrum of compound **6**

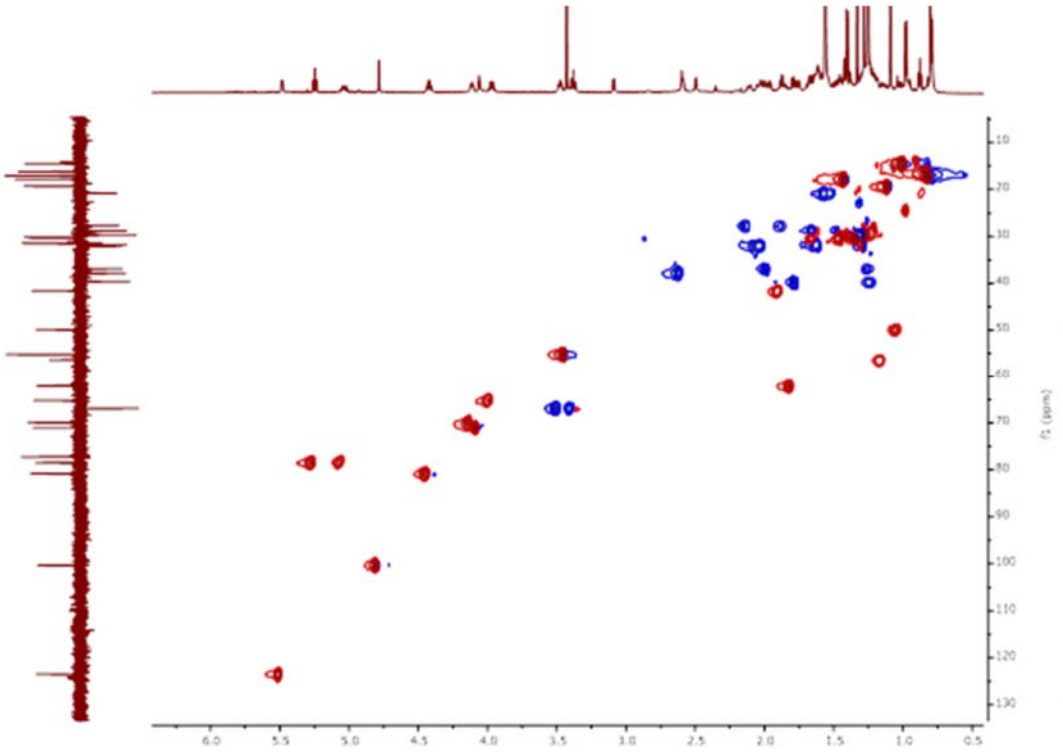


Figure S66. HSQC spectrum of compound **6**

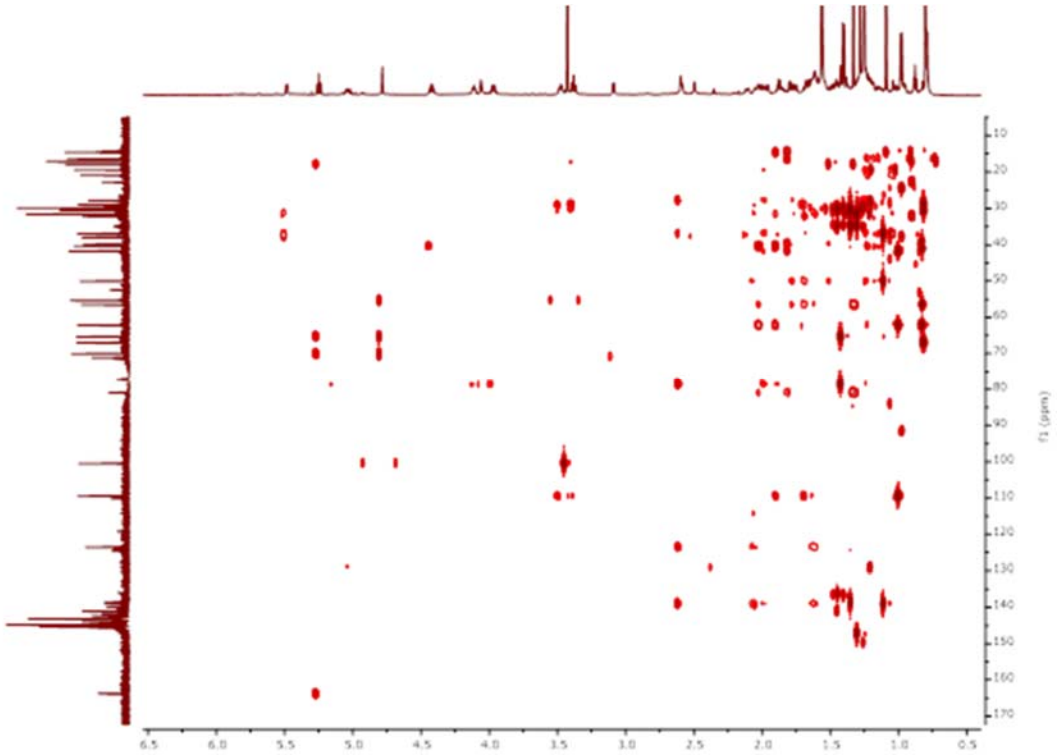


Figure S67. HMBC spectrum of compound **6**

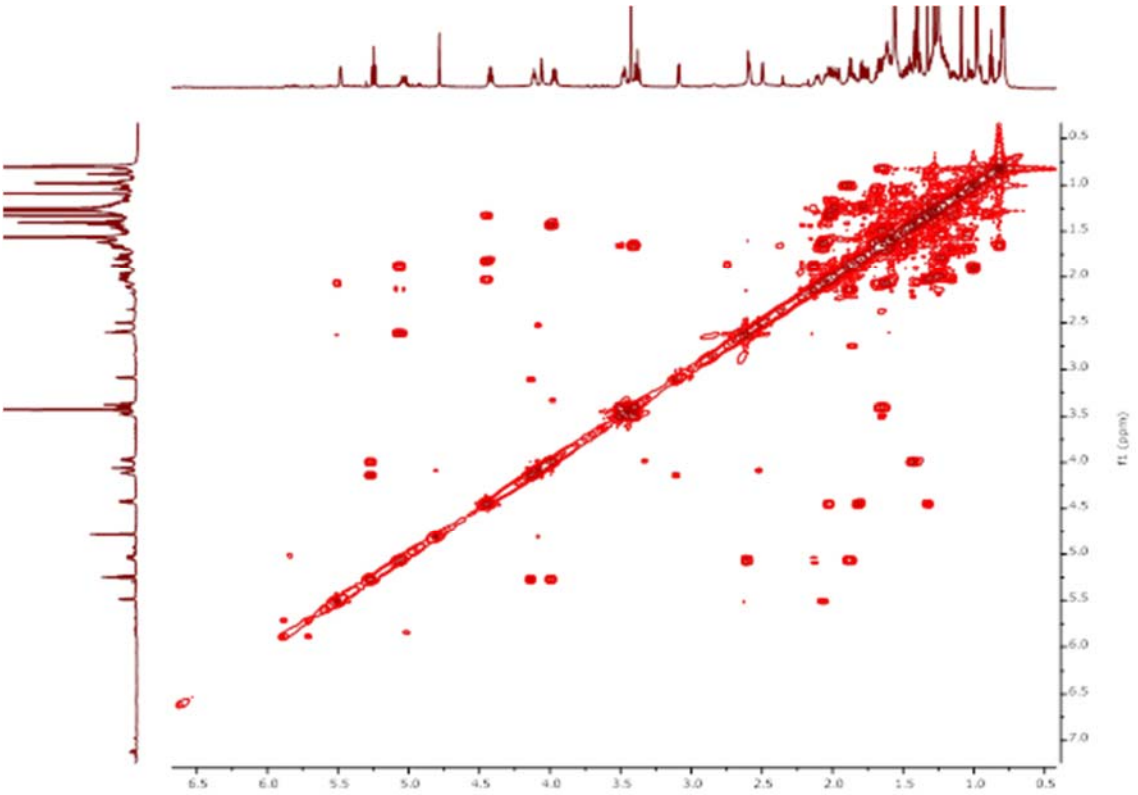


Figure S68. COSY spectrum of compound **6**

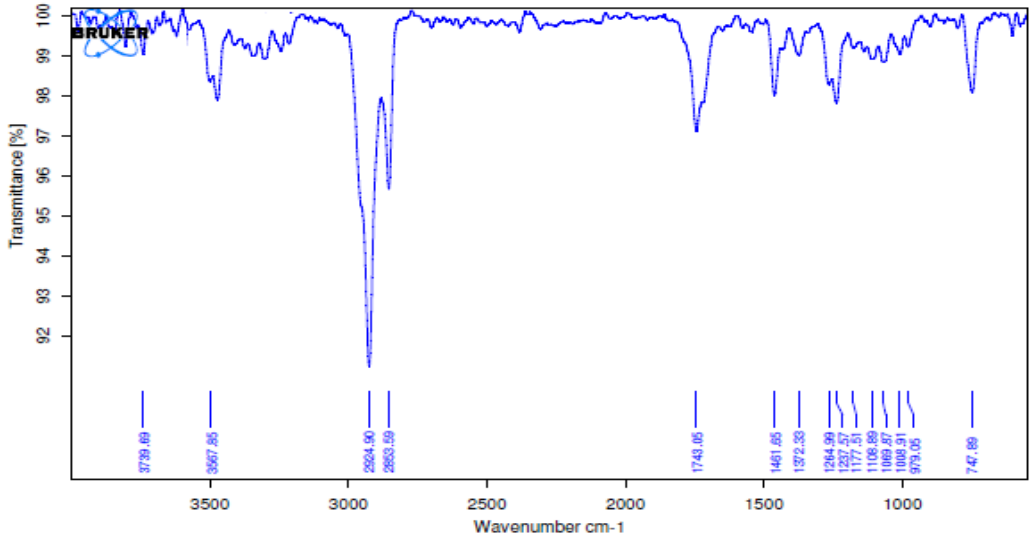


Figure S69. FTIR spectrum of compound **6**

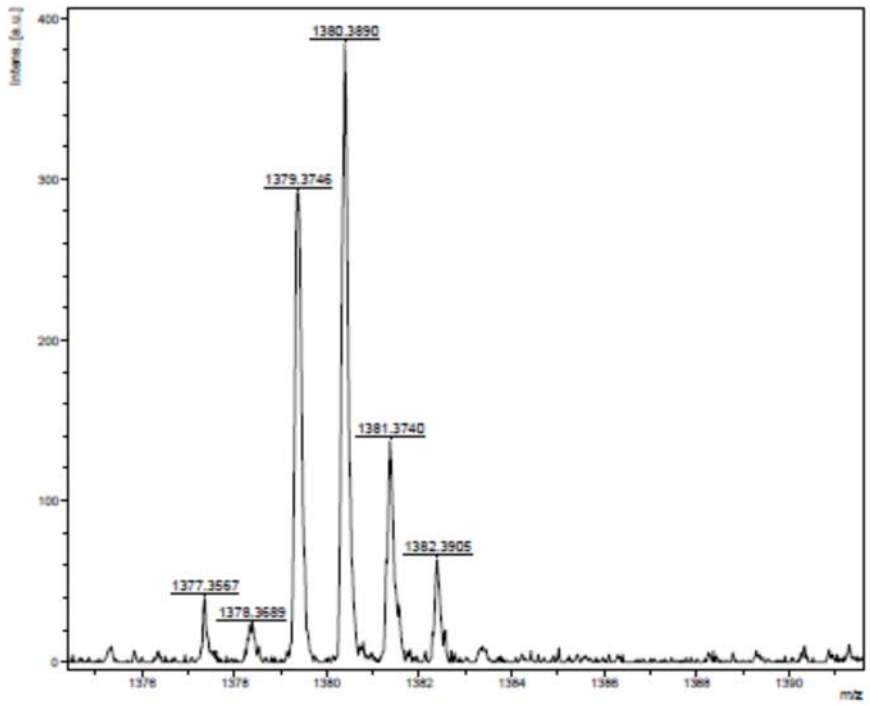


Figure S70. HRMS (MALDI-TOF) of compound **6** showing the ionic pattern corresponding to $[M+H]^+$ 1379.3746; calculated for $C_{97}H_{55}O_{10}$ 1379.3795.

13. UV-Vis spectra

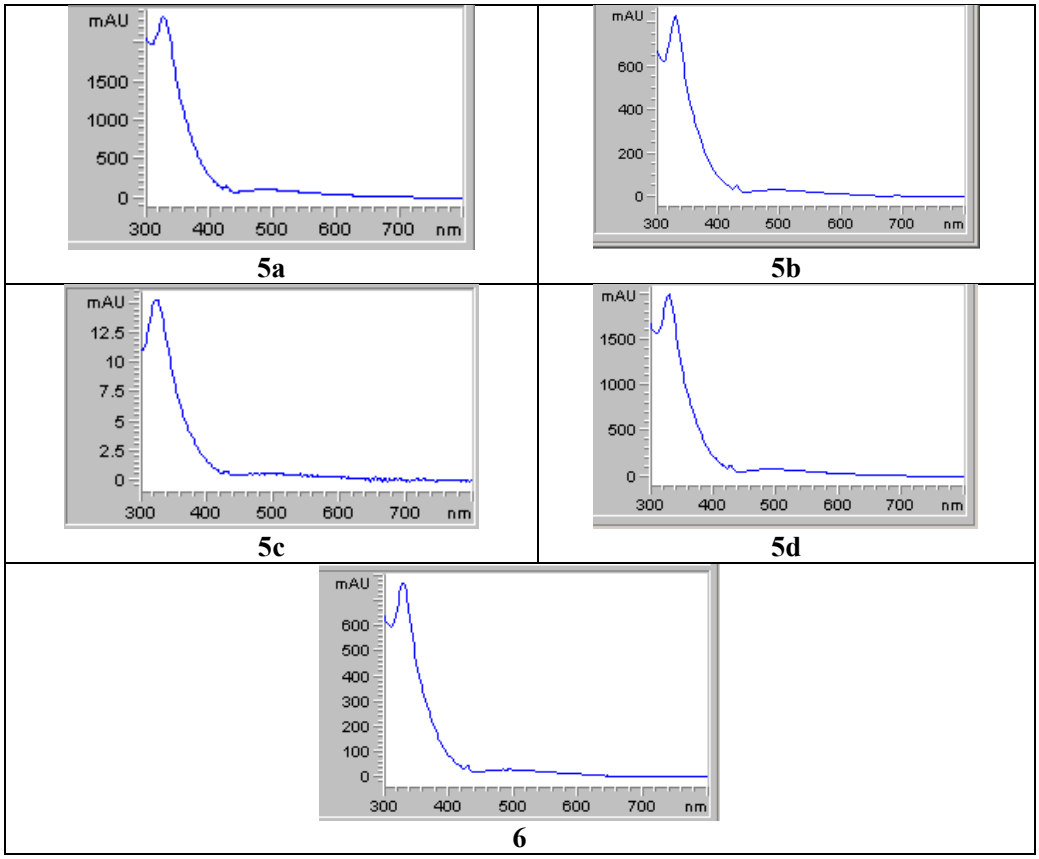
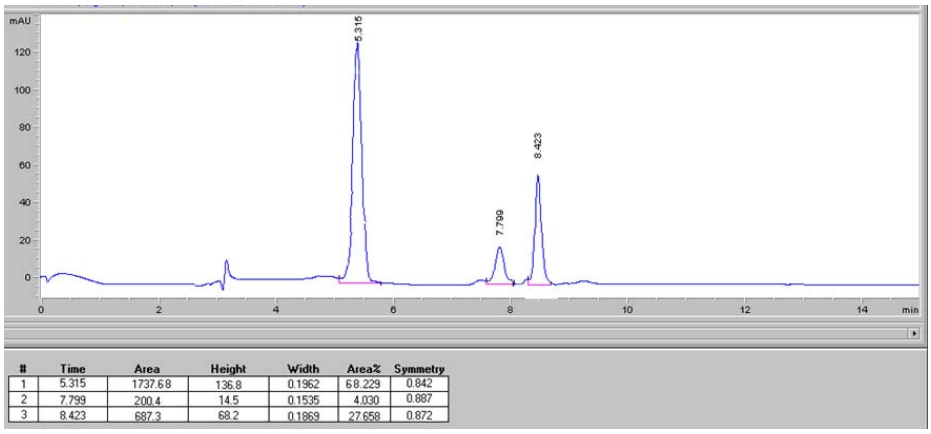


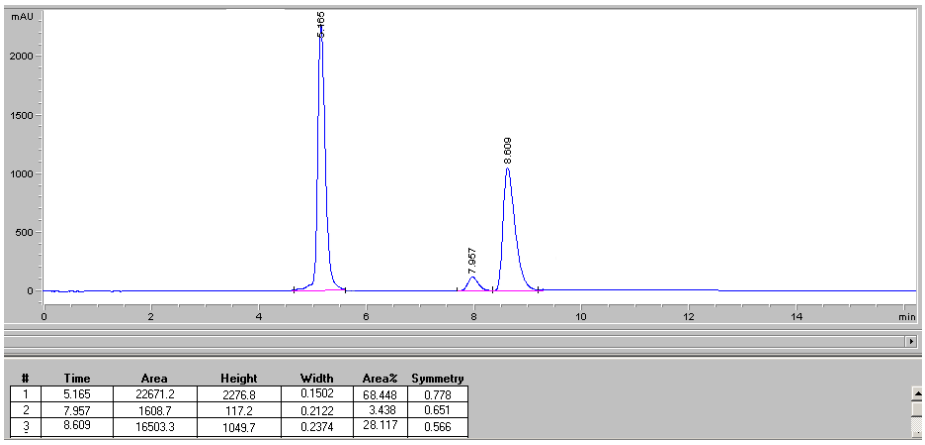
Figure S71. UV-vis spectra of monoadducts **5a-d** and **6**.

14. HPLC chromatograms



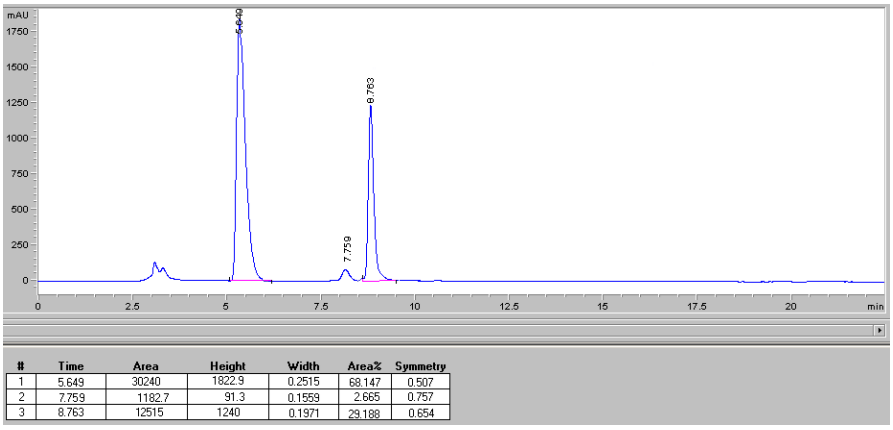
#	Time	Area	Height	Width	Area%	Symmetry
1	5.315	1737.68	136.8	0.1962	68.229	0.842
2	7.799	200.4	14.5	0.1535	4.030	0.887
3	8.423	687.3	68.2	0.1869	27.658	0.872

Figure S72. HPLC chromatogram of reaction mixture of **5a**: BuckyPrep, toluene/acetonitrile (9:1), flow rate 1 mL/min, t_R = 5.31 min.



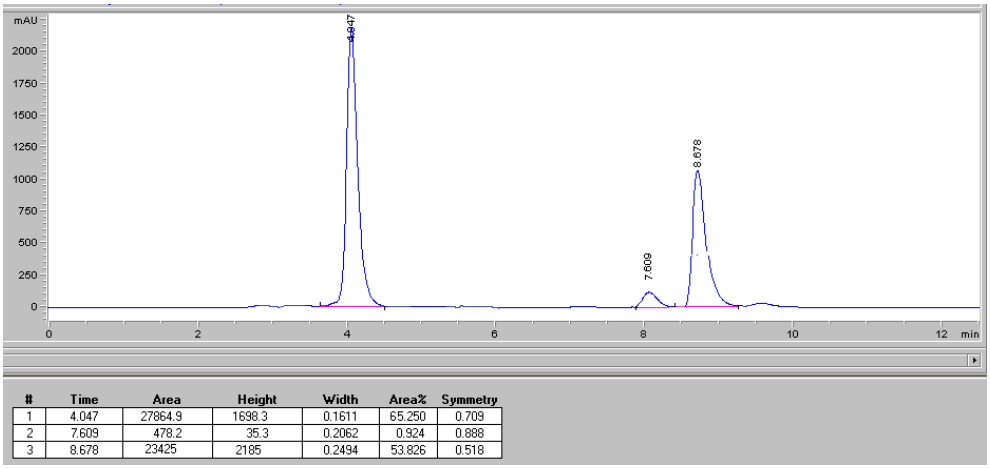
#	Time	Area	Height	Width	Area%	Symmetry
1	5.165	22671.2	2276.8	0.1502	68.448	0.778
2	7.957	1608.7	117.2	0.2122	3.438	0.651
3	8.609	16503.3	1049.7	0.2374	28.117	0.566

Figure S73. HPLC chromatogram of reaction mixture of **5b**: BuckyPrep, toluene/acetonitrile (9:1), flow rate 1 mL/min, t_R = 5.16 min.



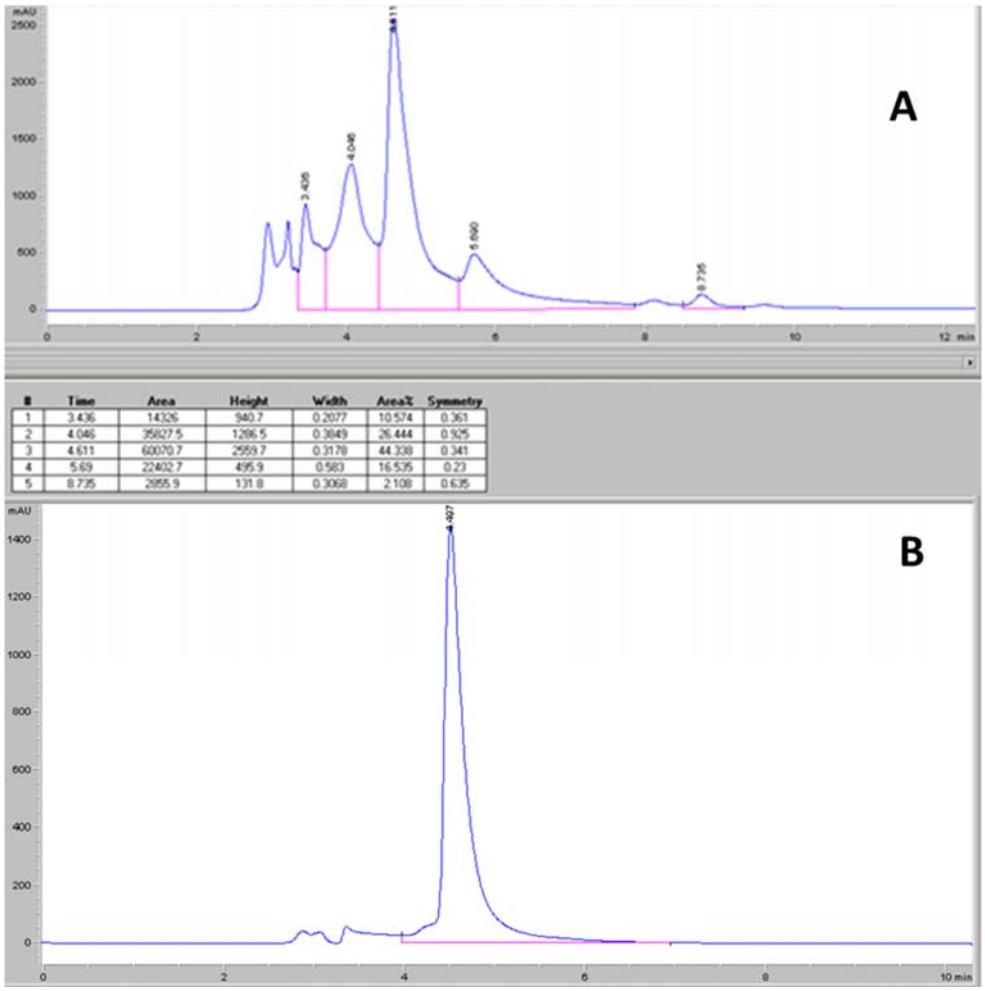
#	Time	Area	Height	Width	Area%	Symmetry
1	5.649	30240	1822.9	0.2515	68.147	0.507
2	7.759	1182.7	91.3	0.1559	2.665	0.757
3	8.763	12515	1240	0.1971	29.188	0.654

Figure S74. HPLC chromatogram of reaction mixture of **5c**: BuckyPrep, toluene/acetonitrile (9:1), flow rate 1 mL/min, t_R = 5.64 min.



#	Time	Area	Height	Width	Area%	Symmetry
1	4.047	27864.9	1698.3	0.1611	65.250	0.709
2	7.609	478.2	35.3	0.2062	0.924	0.888
3	8.678	23425	2185	0.2494	53.826	0.518

Figure S75. HPLC chromatogram of reaction mixture of **5d**: BuckyPrep, toluene/acetonitrile (9:1), flow rate 1 mL/min, t_R = 4.0 min.



#	Time	Area	Height	Width	Area%	Symmetry
1	3.436	14326	940.7	0.2077	10.574	0.361
2	4.046	35827.5	1286.5	0.3849	26.444	0.925
3	4.611	60070.7	2959.7	0.3178	44.338	0.341
4	5.69	22402.7	495.9	0.583	16.535	0.23
5	8.735	2855.9	131.8	0.3068	2.108	0.635

Figure S76. HPLC chromatogram of reaction mixture of **6**: BuckyPrep, toluene/acetonitrile (9:1), flow rate 1 mL/min, t_R = 4.5 min.

15. Cyclic Voltammetry

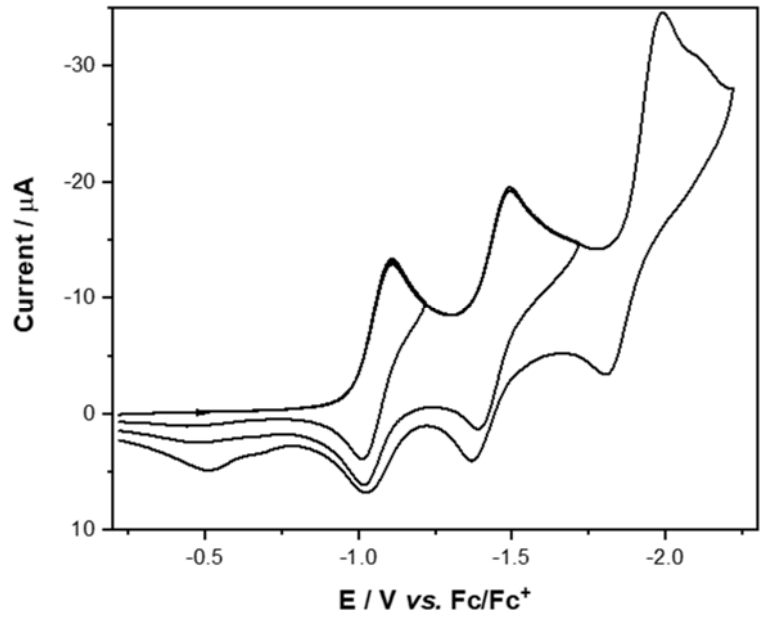


Figure S77. CV of **5b**

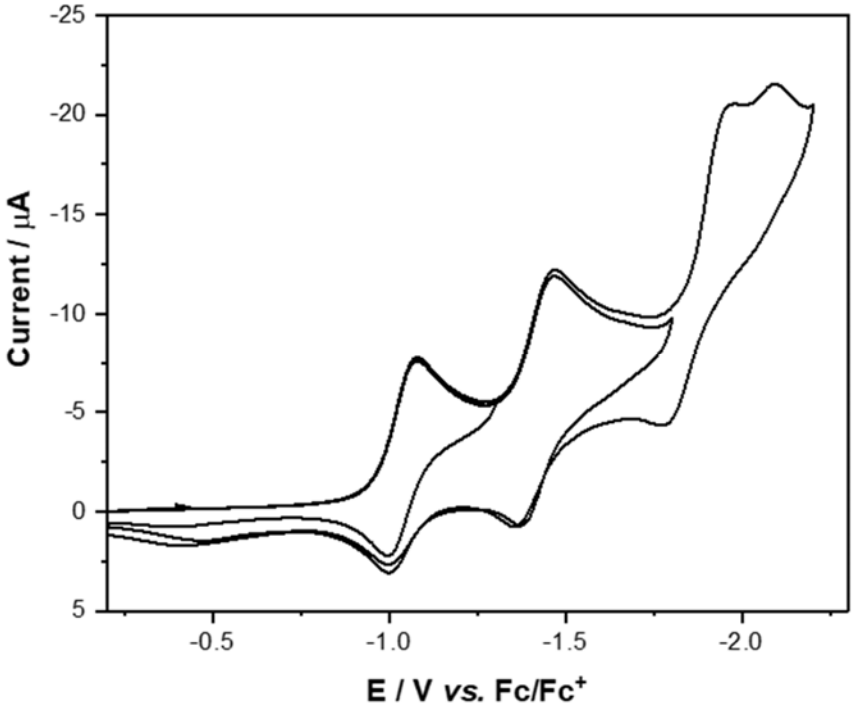


Figure S78. CV of **5b**

16. Thermogravimetric analysis

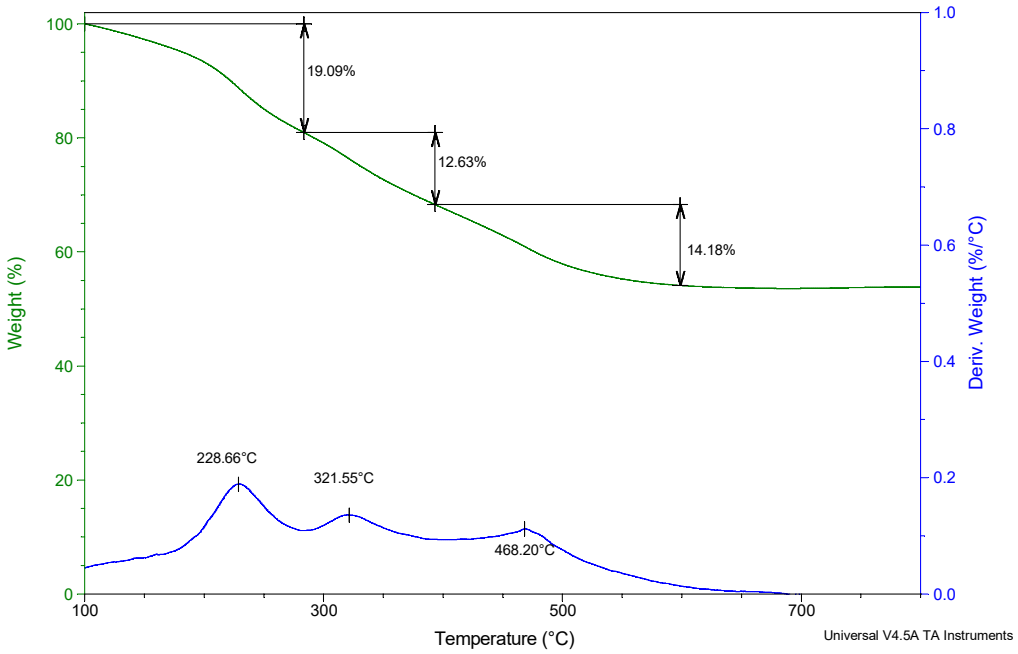


Figure S79. Thermogravimetric analysis and first derivative of **5a** under inert atmosphere.

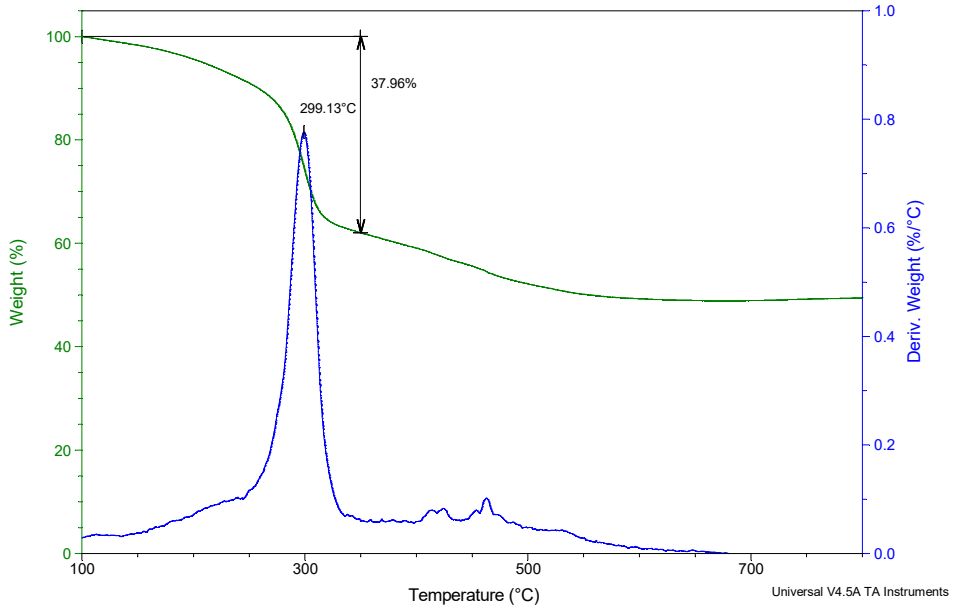


Figure S80. Thermogravimetric analysis and first derivative of **5a** under inert atmosphere.

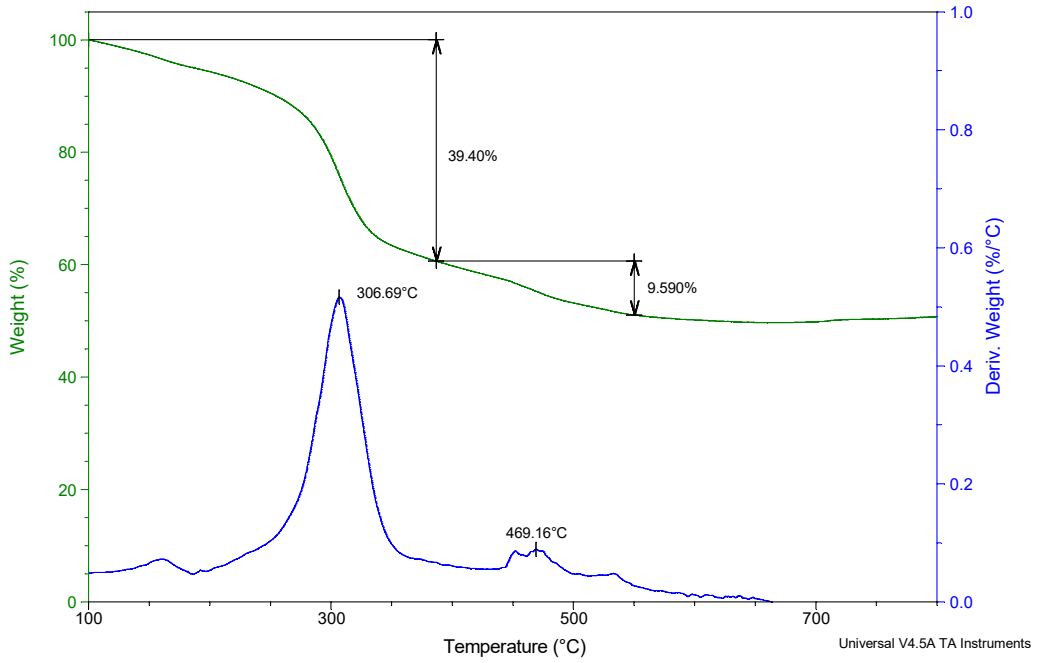


Figure S81. Thermogravimetric analysis and first derivative of **5c** under inert atmosphere.

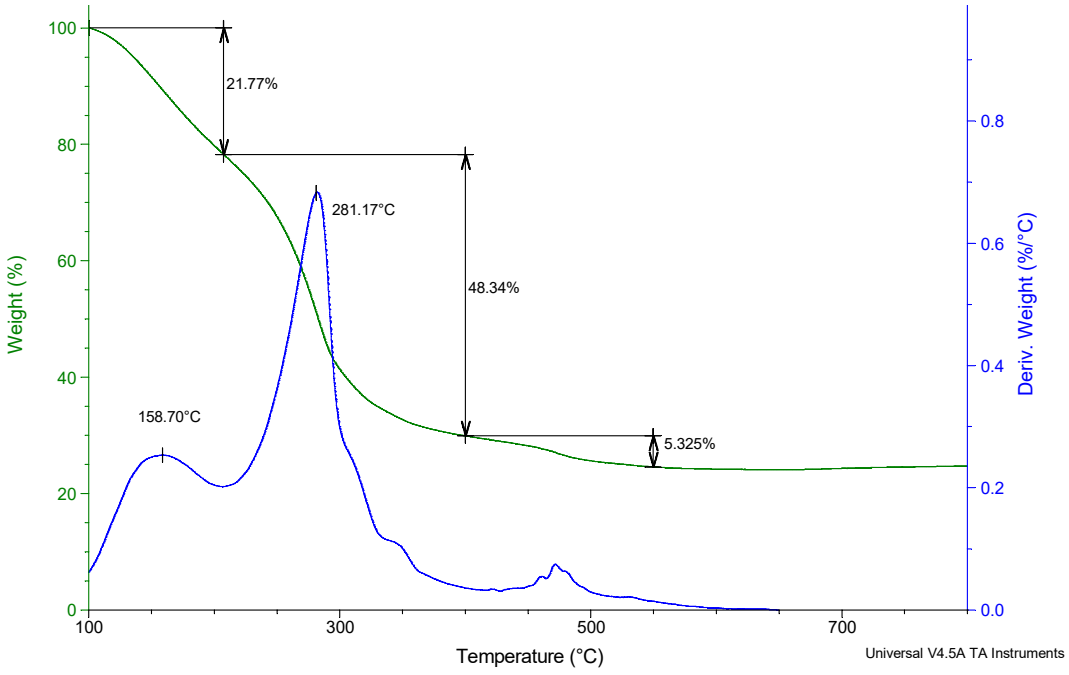


Figure S82. Thermogravimetric analysis and first derivative of **5d** under inert atmosphere.

17. Theoretical calculations

Table S1. XYZ of atom coordinates of compounds **5a** and **5b**.

5a				**5b**			
	X	y	Z		x	y	Z
O	2.64538194536266	2.00869842881952	0.14673830402573	O	1.072709	0.939458	-0.314831
C	1.72221844004539	2.11972775664860	-0.88296421082350	C	0.215973	1.620033	-1.240809
C	0.89388261631164	2.53726213737925	1.88629482911254	C	1.661783	2.870802	1.004780
C	2.22196612395256	1.84838653393091	1.52713908585548	C	0.978938	1.489318	1.006307
C	2.38873763177565	0.41982780752256	2.01689549824713	O	1.367967	3.593403	2.208997
C	0.51256935053021	2.98654233837659	-0.52474218742923	O	0.124368	4.548913	0.534705
C	-0.16673858277588	2.57057400140522	0.76282736809453	O	0.452694	1.094128	-2.509366
C	5.64965591977403	-1.32038310680444	-2.83973445972380	O	1.559902	3.109052	-2.386291
C	4.47772635137880	-1.76652695836158	-1.97111218761771	C	-0.454493	1.531395	1.563215
C	4.53939025343354	-1.14839356001698	-0.55729374428359	C	0.560186	3.115529	-1.363520
C	5.95807459993332	-0.78831829805029	-0.20523130507065	C	1.145873	3.790189	-0.124483
C	6.60166510609787	0.28336863605372	-1.08359849654311	O	-1.091562	0.252457	1.297194
C	6.02350339089977	0.13072747132391	-2.52799618433239	C	1.196468	2.071151	-3.301513
C	6.61387326333843	-1.42304696015524	0.78001108746533	C	2.463994	1.433509	-3.834909
C	8.05927498835846	-1.21381814297749	1.10847766474531	C	0.266675	2.592919	-4.394972
C	8.72378037052039	-0.06436110832084	0.33233345062342	C	0.628296	4.793396	1.854460
C	8.15293878483664	0.09335554230166	-1.09542470259718	C	-0.547158	4.956754	2.800481
C	10.25854078412037	-0.22367944445706	0.34218604053708	C	1.577337	5.992920	1.876069
C	11.02394182134888	0.88936894545611	-0.42698731998640	C	-1.251083	-3.045969	2.955345
C	10.41347666322821	1.01512442264898	-1.84367305681953	C	-1.568702	-2.015437	1.854142
C	8.89660408744992	1.22369535707639	-1.82818428024226	C	-1.119588	-0.642048	2.309191
C	10.80091168802894	-1.53153995916584	-0.27639874665119	O	-2.099804	-3.373315	3.752046
C	12.27241971015034	-1.24418372850308	-0.59149304376434	O	-0.802918	-0.410139	3.458478
C	12.46123719889912	0.30543088060892	-0.56243355023226	C	1.599471	-2.034639	1.844900
O	3.26093270694638	-1.26388142016684	-2.64849271685953	C	1.112199	-3.455466	2.103572
C	2.09112618480385	-1.76204388909095	-2.22061896852746	C	2.250014	-4.276836	2.776294
C	0.97394783744627	-0.93448455017812	-2.84118317024493	C	3.573721	-3.560801	2.655734
C	1.20547330962293	0.55142653844512	-2.62161473146107	C	3.642148	-2.189975	3.332210
O	1.29261703708042	0.77318277066487	-1.29011290483121	C	2.257631	-1.501279	3.117613
O	1.32197030227756	1.38349453549273	-3.49498317583762	C	4.563182	-4.035265	1.879919
O	1.94362069068943	-2.69144400736657	-1.45381850056094	C	5.855541	-3.325850	1.590444
C	10.97092346079497	2.24474866664298	0.28966863713987	C	6.067396	-2.094087	2.486184
C	6.19757162880183	1.67468595398958	-0.54011476738867	C	4.730218	-1.340653	2.626321
C	13.43149234349163	0.52506397194699	0.62084146998548	C	7.269419	-1.142848	2.113636
O	13.09308195722571	-1.77691525508705	0.47648298031160	C	6.860740	0.211712	1.435304
C	14.13586351468630	-0.84135643885333	0.72450524764846	C	5.664990	0.901450	2.161745
O	15.10619450846297	-0.87943256134320	-0.33421681224192	C	5.009344	0.033012	3.238340
C	14.77607079563599	-1.21105780527685	2.07496415177956	C	8.247676	-1.751284	1.087669

C	16.29780649319810	-1.03468924745063	2.03382380606869	C	7.713263	-1.303588	-0.296923
C	16.92872317151691	-1.93159354233512	0.94267071946846	C	6.578631	-0.277342	-0.024316
C	15.93387150189144	-2.04462527539873	-0.23447779281073	O	0.000748	-3.542067	3.072219
C	17.29354034355709	-3.32522298420062	1.46517850126227	C	3.906662	-2.333130	4.843246
C	14.37095781478009	1.72034559196333	0.49030535931264	C	8.056900	1.183545	1.449033
O	1.22326965035037	3.92163069726789	2.15474260360729	C	6.433793	0.737974	-1.178779
O	0.88290795478902	5.81611758938741	3.25731861508200	C	5.359305	1.813943	-0.956632
C	0.63263204522669	4.63800864055203	3.19255259074234	C	6.168442	-0.014758	-2.510799
C	-0.23832108557836	3.88270923404851	4.16823210984757	C	5.032308	-1.044548	-2.460285
O	-0.82767614799957	1.30382527330644	0.57213170995313	C	4.670959	-1.621067	-3.831826
O	-2.08090466340564	1.74297226424641	2.42110901960183	C	3.729125	-2.839367	-3.781790
C	-1.81612417312072	1.02687098002717	1.47193131660217	C	2.463394	-2.575930	-2.957460
C	-2.53820605280864	-0.23804732053244	1.10806510168609	C	3.362281	-3.294150	-5.200649
O	-0.44273224017440	2.98270774242526	-1.59446920495850	H	-0.835711	1.431522	-0.970900
O	0.69987648446807	4.72702537044566	-2.52337751494057	H	2.749567	2.717242	0.918942
C	-0.19699774262916	3.91602314868153	-2.58797820185457	H	1.561512	0.798327	1.632175
C	-1.15990810462882	3.73884133492667	-3.72528013147983	H	-0.428845	1.717832	2.643385
O	1.32815902266218	-0.44243030226859	1.56199099876373	H	-1.080490	2.285637	1.071334
O	2.62296339131101	-2.20182265843267	2.19408563100517	H	-0.335191	3.688401	-1.672588
C	1.58070783611333	-1.78220392580727	1.73226634987493	H	1.958420	4.450760	-0.476608
C	0.40810774395883	-2.61275927475124	1.29032984076979	H	3.058676	1.052451	-2.996037
H	2.25327089123596	2.55867217104113	-1.73816710903931	H	2.211772	0.600671	-4.505256
H	0.46189914167695	2.05103836331381	2.77111666984124	H	3.054046	2.173669	-4.393945
H	2.98733781605731	2.41814809707401	2.07853910244896	H	0.798223	3.315669	-5.030760
H	3.35980957755105	0.03091713835207	1.68234628359126	H	-0.083448	1.757022	-5.017139
H	2.39673370266511	0.42559494583758	3.12145449355076	H	-0.613965	3.084513	-3.958248
H	0.90514898982381	4.00677255419119	-0.38279250272954	H	-1.204590	4.079324	2.745049
H	-0.92378598724087	3.31698337372593	1.04659822225779	H	-0.183130	5.063451	3.831365
H	6.50426568175624	-1.98415464555854	-2.62783714945724	H	-1.126182	5.852650	2.534768
H	5.38708841886553	-1.45851466142981	-3.89990481694368	H	1.037893	6.911247	1.602637
H	4.38636568380015	-2.86071892946516	-1.92450187801893	H	1.999003	6.112448	2.883526
H	3.91287886364005	-0.23944185230787	-0.57655016243822	H	2.412541	5.851250	1.176020
H	4.10559220717155	-1.83132370829894	0.18433288038807	H	0.809155	-1.390619	1.446340
H	5.12280240984930	0.75921285510903	-2.63210141786983	H	2.344274	-2.095515	1.031119
H	6.74443228776705	0.51306698713793	-3.26472535560508	H	0.769181	-3.937115	1.175902
H	6.07569554429652	-2.18091583065055	1.36196808686135	H	2.305324	-5.286296	2.345509
H	8.59004934210001	-2.16351745058141	0.90443028556694	H	1.964251	-4.393405	3.834947
H	8.18858245678074	-1.04978478490800	2.19410169126340	H	1.588568	-1.695800	3.970808
H	8.49345439014424	0.87388703837816	0.87068011205695	H	2.389858	-0.409563	3.083875
H	8.34632015853414	-0.85303059455859	-1.64119756159780	H	4.417569	-5.001045	1.381125
H	10.58802515940607	-0.19310393636130	1.39927285535809	H	5.851973	-3.038434	0.521818
H	10.90741080726287	1.84932299202535	-2.37091296227013	H	6.692644	-4.036643	1.696655
H	10.64626389987968	0.10681449288562	-2.42652363923158	H	6.306481	-2.487578	3.491504

H	8.53613935685174	1.31702073204070	-2.86476855492568	H	4.338551	-1.165732	1.602147
H	8.66678087148688	2.18540473966929	-1.34050643912187	H	7.800694	-0.917349	3.053046
H	10.73137614140676	-2.39455225958081	0.39990152151011	H	6.000026	1.856995	2.598099
H	10.25523906333926	-1.79280129079315	-1.19706184092976	H	4.886175	1.154188	1.427219
H	12.60226072893681	-1.69209211370257	-1.54281148130994	H	5.667495	-0.077591	4.117922
H	12.93980130029796	0.66863613190925	-1.48637896965570	H	4.091397	0.526341	3.597338
H	11.39822645835767	2.18691460367237	1.30248849397277	H	9.258216	-1.351160	1.257364
H	11.52743445416772	3.01122687718695	-0.27321686837606	H	8.335774	-2.842963	1.176532
H	9.93691347316417	2.60656155157312	0.39766258255386	H	7.344589	-2.154180	-0.891706
H	5.10800012092421	1.73402797415822	-0.39212157222645	H	8.514630	-0.838320	-0.893695
H	6.67498164815488	1.88496734201388	0.42886947347929	H	5.621103	-0.824338	0.026148
H	6.47547131451887	2.47325088062232	-1.24530992460801	H	3.171206	-3.009084	5.305560
H	12.84378754958666	0.61377557952797	1.55137808457924	H	4.908962	-2.739047	5.045481
H	14.32215032308019	-0.60547091456813	2.87412562055912	H	3.820473	-1.356945	5.345692
H	14.51783064571950	-2.26075260412387	2.28850632094397	H	8.376059	1.385533	2.484142
H	16.73801008428039	-1.27008323867455	3.01646328634006	H	8.925903	0.800150	0.894640
H	16.53417503719323	0.01953184265064	1.82395008256792	H	7.775714	2.148217	0.996850
H	17.84763424412737	-1.43952693138951	0.58233224614798	H	7.403332	1.259742	-1.293361
H	15.28995396266124	-2.93579984884618	-0.10776272492864	H	5.259595	2.444239	-1.855090
H	16.45377795118463	-2.13626918360010	-1.19871771874418	H	5.608336	2.474596	-0.113868
H	16.41505375788605	-3.81957402025789	1.91240330106475	H	4.369113	1.373200	-0.755030
H	17.65997010110961	-3.97574216044208	0.65419395597797	H	5.942859	0.733800	-3.291286
H	18.08044708694039	-3.27024660880033	2.23350291793937	H	7.090127	-0.524518	-2.839833
H	15.01932873080904	1.81486642556801	1.37644203851370	H	5.321212	-1.879063	-1.795687
H	13.81111640546580	2.66073237722914	0.38752328085158	H	4.133563	-0.593288	-2.004983
H	15.01643926923306	1.59640983283602	-0.39049392059419	H	4.211927	-0.830313	-4.453925
H	-0.65029809838803	4.61188231975833	4.87354291290980	H	5.597583	-1.915920	-4.358391
H	-1.05441900846293	3.33680349904052	3.67109666703902	H	4.285402	-3.663131	-3.292043
H	0.35856933729680	3.14642954850116	4.73094341493849	H	1.801162	-3.456191	-2.971480
H	-3.00709946508182	-0.66120843201670	2.00371253731813	H	2.688175	-2.346540	-1.904478
H	-3.32639678608789	0.00160626411374	0.37728141005810	H	1.891528	-1.723399	-3.361179
H	-1.86100852536172	-0.95882131581533	0.63712659942087	H	2.757902	-4.214907	-5.184736
H	-1.32282449121916	4.70363938517649	-4.21945637329063	H	4.261034	-3.485789	-5.807893
H	-0.69183984348056	3.04966176221677	-4.44630820679065	H	2.769279	-2.517099	-5.713207
H	-2.10722621711814	3.29638834637648	-3.39441805530234	C	-4.463246	0.028779	-1.462198
H	0.68058398990027	-3.67191503246421	1.34124255462835	C	-3.848594	0.027079	-2.780233
H	-0.45463985458398	-2.41681089620509	1.94448034441308	C	-5.798495	-0.378219	-1.319176
H	0.13451239462749	-2.35849330951055	0.25813343960327	C	-4.583001	-0.375844	-3.902590
C	-2.66230669687653	-5.03031041540605	-2.56179847670108	C	-6.561585	-0.806491	-2.480680
C	-3.09503837707702	-3.81089317911854	-1.91555474157323	C	-5.965278	-0.807020	-3.749047
C	-1.37112642576746	-5.09911973158261	-3.11053225704093	C	-3.460385	-0.371502	-0.490577
C	-2.21471011429664	-2.71975165989142	-1.84768972938251	C	-2.461726	-0.380551	-2.630700
C	-3.79595295977114	-5.57904792258121	-3.28920475496436	C	-6.168513	-1.220759	-0.203100

C	-4.49839253636556	-3.59530458840603	-2.23509256903440	C	-2.210395	-0.630436	-1.225100
C	-0.86689225826881	-2.81385219742872	-2.35644559875495	C	-3.958867	-1.212870	-4.918063
C	-4.93229775278057	-4.69116225899719	-3.08718677092164	C	-7.407850	-1.920472	-2.075926
C	-0.46232515974095	-3.97331129325341	-3.00920019431576	C	-3.821293	-1.151685	0.604857
C	-1.16960384007360	-5.73431921830403	-4.40239052812840	C	-6.191492	-1.916310	-4.659977
C	-3.59829414564731	-6.18703341029561	-4.53595913694767	C	-5.186112	-1.617467	0.717660
C	-2.70742729006272	-1.37477474652215	-2.08786286092031	C	-7.165463	-2.176008	-0.664575
C	-4.97375216957086	-2.29802581257149	-2.46221865466356	C	-1.856794	-1.175246	-3.616409
C	-2.25839895553095	-6.27174758634041	-5.10003970398512	C	-2.620217	-1.604387	-4.776709
C	-4.06308045328145	-1.16528783941074	-2.38104526692643	C	-4.951249	-2.167319	-5.382593
C	-0.43904865263658	-1.45051247714972	-2.78337101585673	C	-7.623486	-2.992231	-2.953353
C	0.31327205996640	-3.90844178398122	-4.26081526976810	C	-1.351027	-1.652892	-0.838481
C	-5.82498491447238	-4.44480592432028	-4.13927514623686	C	-7.003729	-2.990108	-4.269374
C	-0.13562776615358	-4.99817759430052	-5.11135169399303	C	-2.925711	-2.198461	1.186761
C	-1.67143300681186	-0.61123619783033	-2.74274447423879	C	-0.999792	-2.267212	-3.215139
C	-4.52723277006028	-5.93658763742536	-5.62419406091039	C	-5.173282	-2.981659	1.215838
C	-5.90350096039993	-2.04105131347373	-3.55107486239740	C	-7.151374	-3.490136	-0.182908
C	-5.61970092704455	-5.08016933961880	-5.43052624640855	C	-1.567214	-2.466449	0.398352
C	-6.31911674930642	-3.09572142314671	-4.37538065681631	C	-0.782080	-2.509189	-1.849844
C	0.65614880637896	-2.68565031403320	-4.83144106456941	C	-2.224571	-2.969892	-5.094362
C	0.40516624462942	-1.37717566526075	-4.16284238378940	C	-4.571004	-3.483002	-5.685730
C	-2.36329026356151	-6.08497435322512	-6.53961960996576	C	-3.803767	-3.384549	1.414837
C	-4.42610288946389	-0.21222222196750	-3.40675150071425	C	-6.140713	-3.900184	0.779797
C	-0.23419184216092	-4.82880776967033	-6.50140638789759	C	-7.607211	-4.358710	-2.451419
C	-3.76357633758808	-5.87484394579661	-6.86410208065619	C	-6.605643	-4.354614	-4.581284
C	-2.01727476513541	0.27872201874731	-3.75522675489448	C	-1.218395	-3.379666	-4.126203
C	-5.56423971982999	-0.75032923543303	-4.13479130116291	C	-7.377349	-4.603059	-1.091146
C	-1.36884750827215	-5.37723346185407	-7.22719259033494	C	-3.182888	-3.891202	-5.537725
C	-3.41672555406036	0.48752445989669	-4.08779792531596	C	-5.413363	-4.596623	-5.275476
C	-5.98880378722438	-4.12624519593921	-6.46596950358855	C	-1.335716	-3.883112	-0.024488
C	-6.41888683976965	-2.89922139383200	-5.81276780158270	C	-6.977968	-5.199536	-3.457231
C	0.50076175253254	-2.49472725472818	-6.25572285534633	C	-0.765963	-3.872449	-1.352144
C	-0.15105394599238	-0.48678029796654	-5.22026019994815	C	-3.415704	-4.680776	1.094012
C	0.09272954378964	-3.54715735964373	-7.08785572386394	C	-5.745470	-5.257780	0.474610
C	-1.24835223167228	0.34077882853880	-5.01091367013769	C	-6.505808	-5.696633	-0.683983
C	-4.12243553378943	-4.95796243166425	-7.86203455714525	C	-1.201473	-4.694685	-3.645122
C	-5.65786210456267	-0.56529706341873	-5.52050364982191	C	-3.167010	-5.258215	-5.036065
C	0.00706248446980	-1.14932613029593	-6.49209535332411	C	-2.161788	-4.932915	0.363733
C	-5.25437119076115	-4.06600814536047	-7.65742686619904	C	-4.545419	-5.692921	-4.873334
C	-6.09615344282798	-1.65602613353913	-6.37396284634490	C	-0.964674	-4.947633	-2.231553
C	-1.74105239990838	-4.42715951301485	-8.26563162287618	C	-4.400154	-5.633885	0.618540
C	-3.52057597621077	0.68009466440338	-5.52528101849453	C	-6.140893	-6.252663	-3.064837
C	-0.83471254542287	-3.29312512939935	-8.18101415903736	C	-2.194449	-5.652541	-4.107059

C	-2.18448938853434	0.58695078817819	-6.09099498200012	C	-5.900092	-6.505587	-1.654648
C	-3.09234322652964	-4.22002794792992	-8.57509236937882	C	-4.900832	-6.504803	-3.786902
C	-4.61933188897147	0.16938585451586	-6.22823320935939	C	-2.394974	-6.040446	-0.547797
C	-4.92200188112697	-2.77631853396436	-8.24326002707189	C	-1.801305	-6.055461	-1.820328
C	-5.33281408665261	-1.59320314668792	-7.61354804650576	C	-3.774046	-6.473290	-0.390623
C	-0.87823541057988	-0.90207812711208	-7.55242952333944	C	-2.564700	-6.493901	-2.977395
C	-1.31085986071856	-1.99630771111303	-8.40846434726807	C	-4.508087	-6.904939	-1.502286
C	-1.99945114488550	-0.01194439529195	-7.34793530510044	C	-3.893618	-6.910255	-2.821832
C	-3.58694313973138	-2.87118450692260	-8.81158558786939				
C	-4.42426893729451	-0.46271818173486	-7.52521071098501				
C	-2.71199845337489	-1.77924745320717	-8.73170699773914				
C	-3.13808669754691	-0.55113935157876	-8.07430337909961				

Table S2. XYZ of atom coordinates of compounds **5c** and **5d**

5c				**5d**			
	X	y	z		X	y	z
O	0.125098	1.263058	-3.382847	H	3.90207577029696	3.35647318652662	1.76540961171945
C	-0.637484	2.445575	-3.085568	H	4.49038328281961	1.66139924732196	1.60112805111454
C	1.123166	1.058359	-1.169353	H	3.71445233665598	2.19914702963560	3.12791626619139
C	0.253247	0.383599	-2.258511	H	15.09716009849159	1.31413811062117	-0.24528373434300
O	0.948531	0.406171	0.094601	H	13.83786071726084	2.54720570912641	0.04387707153533
O	-0.111363	2.423539	0.263482	H	15.03205732388568	2.18577958613190	1.30551608884396
O	-0.611146	3.270622	-4.204441	H	18.28059299047240	-1.97372974455580	4.06071283553929
O	1.018960	4.002182	-2.737004	H	17.95055727156224	-3.25470960227960	2.87173891027579
C	-1.117709	-0.103219	-1.774392	H	16.66995861750647	-2.73121141235785	3.98675051572936
C	0.028200	3.289240	-1.992128	H	16.65959565565688	-2.39128651690595	0.48792283965006
C	0.741807	2.530160	-0.880411	H	15.49634824120471	-2.74241882494403	1.79345538646910
O	-0.948117	-1.445326	-1.244130	H	17.94714337552195	-0.93018383765443	1.84126152542219
C	0.524331	4.176968	-4.076405	H	16.53483937061306	0.79265846700093	2.46515396502285
C	1.625087	3.777439	-5.046630	H	16.74164762345694	0.04161471312882	4.05110444502345
C	0.000082	5.593103	-4.273763	H	14.60627717812251	-1.27700880529713	3.68231180202915
C	0.469069	1.384399	1.058993	H	14.30764280784294	0.46367770426536	3.61238308534720
C	-0.611988	0.754398	1.914417	H	12.87182182529445	1.06224379075338	1.86739261246592
C	1.650550	1.899964	1.884777	H	5.29938257809080	1.31434917263987	-0.63739363790897
O	0.609398	-3.976669	-0.290754	H	6.67012874064020	1.59908967406299	-1.73727534471579
C	-0.620781	-4.014495	-0.822241	H	6.87799215474815	1.77969337805259	0.02552834072398
C	-1.604045	-3.266758	0.075147	H	10.01747296946514	2.38804486982487	-0.10163904358862
C	-1.924089	-1.872828	-0.411599	H	11.62562153165132	2.53150510696175	-0.83310974339111

O	-0.946839	-4.537691	-1.866777	H	11.45238948070514	2.39553568732878	0.93575724401402
O	-2.888846	-1.216289	-0.078340	H	13.11552700488645	-0.05075962025386	-0.95469852324513
C	2.314539	-3.470152	-1.926092	H	12.78427340563999	-2.25720685654505	-0.11209017405065
C	1.713922	-4.571777	-1.065801	H	10.43028345684716	-2.26960893504683	0.18081383482940
C	2.741832	-5.089269	-0.049793	H	10.85158613710360	-2.18393367739780	1.90077767944085
C	3.890338	-4.128078	0.199981	H	8.83827409529373	1.30166988042367	-1.58376715032802
C	3.553288	-2.640767	0.223857	H	8.75866589196250	-0.10639962327936	-2.63661763225729
C	2.699531	-2.272485	-1.048167	H	10.85304870382045	-1.01318886856792	-1.66804821376657
C	5.128440	-4.601341	0.421298	H	11.11543917182610	0.60827542440351	-2.31259776833705
C	6.319584	-3.755643	0.756577	H	10.65339164787578	0.22507651220374	1.94575238471564
C	5.947352	-2.317485	1.144038	H	8.48257573515356	-1.60541036487945	-0.66802815880280
C	4.854800	-1.774354	0.203806	H	8.58011248107584	0.96339201325295	0.97422701891709
C	7.200111	-1.416752	1.200393	H	8.26189504422510	-0.32594807245608	2.93539852009485
C	6.904346	0.086934	1.471954	H	8.62891347526501	-1.84768080885331	2.14533699536715
C	5.829012	0.567477	0.467158	H	6.10593671668347	-1.58493033003510	2.55149395594093
C	4.564520	-0.292617	0.494288	H	6.98452936609715	-1.05578810237945	-2.71430346729010
C	8.062035	-1.392399	-0.080915	H	5.36347441332391	-0.47723580700408	-2.34513022331221
C	8.894416	-0.108849	0.011571	H	4.14614048581639	-1.61864734821264	1.29457412604468
C	8.247600	0.785480	1.114904	H	4.02559079262263	-0.43305875242620	-0.00856733621651
C	6.434838	0.346778	2.906952	H	4.28901671976555	-3.39500764447703	-0.27495447990874
C	2.713795	-2.370985	1.500226	H	5.50397570211541	-3.03450532314190	-2.52297173918655
C	9.335996	0.845350	2.210018	H	6.52541519391694	-3.01915514461062	-1.07626753019439
O	10.226171	-0.438579	0.479144	H	0.99988693122710	5.25723445833172	-0.37423387816287
C	10.619925	0.569063	1.403618	H	-0.53517141846995	5.72314397691501	0.41236761100996
O	10.934060	1.789555	0.713911	H	-0.36920699387727	5.85223933115326	-1.36341397583359
C	11.842923	0.036028	2.170785	H	-2.47130516315717	4.34640335089358	-1.59191406465919
C	12.855346	1.154372	2.444434	H	-2.59369770472984	4.09028084865715	0.17613609915882
C	13.360114	1.776944	1.119847	H	-2.42159058637489	2.69262403380611	-0.91071762297392
C	12.217384	1.712650	0.081864	H	3.13695187512087	3.02929018199617	-3.57111934216504
C	14.610358	1.074198	0.579665	H	4.15466034049305	3.25086711373454	-2.12422033464792
C	9.362511	2.126133	3.039728	H	2.44465719508141	3.79910448635656	-2.12924334276745
H	-1.689002	2.184310	-2.876133	H	2.32769114369914	3.31322981387958	0.10174369958160
H	2.178332	0.995183	-1.481528	H	0.35500731938662	1.04376195299603	0.62119322504885
H	0.788742	-0.493218	-2.652118	H	-0.69313034061251	1.28992902036142	-1.54580031700130
H	-1.565508	0.536797	-1.003483	H	1.08782575776260	1.48276053290220	-3.39240516042850
H	-1.798637	-0.167990	-2.637692	H	3.40023820091178	0.88337712806732	-2.44050423927910
H	-0.713068	3.972350	-1.532431	C	3.70532894040005	2.30184813677120	2.03498458621463

H	1.649207	3.111424	-0.635966	O	2.39911819098802	1.90258643763448	1.60510735587281
H	1.896096	2.729593	-4.867537	C	14.41864285732597	1.73735420411063	0.50858710496794
H	1.275312	3.888384	-6.082963	C	17.51697773477702	-2.37637541978943	3.37695113323082
H	2.507955	4.416317	-4.898464	C	16.10743838970394	-1.94520364686586	1.32687721849582
H	0.825286	6.315006	-4.195973	C	17.05962665787698	-1.31867914001771	2.36816395369477
H	-0.467649	5.689313	-5.264022	C	16.33739022698664	-0.12557217901018	3.03953302365596
H	-0.752471	5.824586	-3.506999	C	14.82424844620027	-0.36459030693350	3.10370984969117
H	-1.455600	0.424155	1.295400	O	15.23819485966179	-0.95848680604800	0.75899859210416
H	-0.202672	-0.114208	2.449373	C	14.22914589091807	-0.55345231157940	1.69703191780804
H	-0.978815	1.478609	2.655401	O	13.21294643858806	-1.54616885335287	1.79551665837519
H	1.311050	2.670298	2.592374	C	13.50385317332830	0.64731110732148	1.06075405514701
H	2.097310	1.069539	2.449284	C	6.38485859895222	1.18402023237978	-0.75705160994591
H	2.433689	2.327171	1.243338	C	11.05776321044215	2.03848221283831	-0.02789622729585
H	3.202584	-3.889050	-2.430615	O	2.53987833061398	-4.20309872507155	-1.55019975950005
H	1.600812	-3.166105	-2.707903	O	2.11740309586103	-0.62145667834382	-4.13285097218277
H	1.277791	-5.380876	-1.667308	O	1.11313350732856	-0.18647752321884	-2.13213798888389
H	2.209539	-5.313970	0.891038	C	1.58507506618532	-0.99218042205554	-3.10866831610350
H	3.148886	-6.047397	-0.407983	C	1.35782446198175	-2.44630348594819	-2.72518835252800
H	1.781601	-1.765084	-0.722635	C	2.47139754891553	-3.03826749032888	-1.88393322113188
H	3.260306	-1.552333	-1.666098	O	3.34135579905512	-2.06308302261884	-1.56171458199205
H	5.292790	-5.684843	0.363014	C	12.59464651773149	-0.04057756331719	0.01633685941886
H	7.009686	-3.746313	-0.109075	C	12.42068008639221	-1.48414213323793	0.58387058949330
H	6.895293	-4.225115	1.575726	C	10.93888905031129	-1.65623818292496	0.94104347925094
H	5.518007	-2.349751	2.163424	C	9.08318051463745	0.22831951906195	-1.63798673987735
H	5.248646	-1.845848	-0.830180	C	10.59834255335747	0.04968647097046	-1.51348965636914
H	7.837920	-1.790635	2.025454	C	11.15033137209020	0.51349513729770	-0.14334398213463
H	5.581907	1.620621	0.689719	C	10.36298545168003	-0.22366827997556	0.97582154738676
H	6.251740	0.562262	-0.553494	C	8.30297847606170	-0.51923348898132	-0.54105586276499
H	3.828700	0.099939	-0.225756	C	8.83044208510199	-0.10690742412886	0.85188271673128
H	4.083959	-0.204402	1.481812	C	8.13007060859200	-0.87320143990791	1.98347783227827
H	8.732681	-2.258319	-0.166446	C	6.67744714671664	-1.13579368218047	1.73018574839585
H	7.429409	-1.379784	-0.982814	C	6.21375498609169	-1.04431177521528	-1.92961828749909
H	8.982869	0.412439	-0.955101	C	6.75731176002665	-0.31447705749665	-0.65689054124111
H	8.063400	1.806935	0.744607	C	6.05258279808291	-0.91082263116304	0.56258396201634
H	7.189897	0.029531	3.641771	C	4.60960399186266	-1.29797156418118	0.35015759890078
H	6.231790	1.418096	3.068060	C	4.50133384485396	-2.41107255079637	-0.71320711633008
H	5.507603	-0.198926	3.138727	C	5.73721668341881	-2.46243307556303	-1.61170518716400

H	3.330616	-2.469273	2.407574	C	-0.09380774298640	5.25812087882495	-0.47982293044764
H	2.267362	-1.367585	1.468342	C	-2.11665656238524	3.73630653933157	-0.74888947570981
H	1.885838	-3.088259	1.581302	C	-0.59827607787864	3.83099356791868	-0.62129731636237
H	9.225635	-0.027275	2.878213	O	-0.18647259159309	3.04161189282354	0.52542458941754
H	11.509652	-0.443128	3.103970	O	0.04723929918800	3.24030594301786	-1.76626790499797
H	12.303474	-0.754384	1.555696	C	3.13718048503659	3.01919575934996	-2.47072416564640
H	13.705678	0.767757	3.029131	O	2.93852893310329	1.43122188439064	-0.56528355834624
H	12.377616	1.934261	3.057625	C	2.11003325828074	2.23999178854693	0.28920254550097
H	13.604884	2.835928	1.307633	C	0.61713239461915	1.95317242369231	0.06026747688044
H	12.278926	0.772656	-0.499576	C	0.24465685831125	1.86547693254796	-1.42599294661110
H	12.263051	2.552833	-0.626097	C	1.29765722839442	1.24526515135869	-2.33850895663451
H	14.430045	-0.006617	0.452248	C	2.73751353370149	1.62774122139385	-1.97540485364361
H	14.906292	1.477478	-0.402025	C	-2.47264019654417	-5.96988356540982	-0.87366429536002
H	15.463710	1.196579	1.264599	C	-2.78157995002981	-4.57448347036674	-0.65425357207575
H	10.156301	2.088084	3.802958	C	-1.23310422555540	-6.32205051637021	-1.43049461766510
H	8.408731	2.285330	3.563014	C	-1.83587851405585	-3.59744369189936	-1.00158526996953
H	9.556387	2.990387	2.389436	C	-3.68876862265807	-6.63629006686621	-1.31251610757149
C	-6.372331	-3.905982	2.785478	C	-4.19087190031634	-4.36550835232650	-0.95488088068630
C	-6.904287	-4.529730	3.986449	C	-0.53713178859606	-3.96373990863504	-1.52004505160632
C	-6.076265	-4.951671	1.831482	C	-4.75267464660739	-5.64377325336042	-1.36324196298305
C	-6.938020	-5.968823	3.768536	C	-0.25534845214576	-5.30342583057316	-1.76501974099447
C	-6.424096	-6.229975	2.433107	C	-1.16912532538552	-7.36471517408757	-2.44210418356941
C	-5.510179	-2.802630	2.886740	C	-3.62254845171217	-7.63953299515313	-2.28800428576530
C	-6.566045	-4.021560	5.247669	C	-2.27104178905679	-2.37276268670975	-1.65174899292539
C	-4.933497	-4.843133	1.023052	C	-4.60825202486077	-3.18390125195240	-1.57901763218548
C	-6.630074	-6.844321	4.818948	C	-2.33649963459374	-8.01500470760260	-2.85958038740203
C	-5.628355	-7.356574	2.195132	C	-3.63060223985811	-2.16546314608459	-1.93076421077740
C	-5.163402	-2.277009	4.197072	C	-0.07434118226944	-2.86359419572715	-2.41710084438260
C	-5.683740	-2.867859	5.354809	C	0.42030247866586	-5.72144108781413	-3.00483263960964
C	-4.082656	-3.676958	1.082809	C	-5.70826757080460	-5.69153396072732	-2.38720851318226
C	-4.347160	-2.692686	2.028533	C	-0.15253347956691	-6.98988184013315	-3.41202286063908
C	-6.251105	-4.928939	6.336988	C	-1.25327236453662	-1.96704098557156	-2.58923417352531
C	-6.281126	-6.314710	6.127304	C	-4.61502844407939	-7.69124102769694	-3.34751832312752
C	-4.107190	-6.012144	0.777944	C	-5.60170110035516	-3.23093774295684	-2.64033500699389
C	-4.450005	-7.247634	1.348168	C	-5.63859627032629	-6.73509656805264	-3.39762710167552
C	-5.801284	-8.015448	4.572091	C	-6.13995586579297	-4.46248283912990	-3.03793212548612
C	-5.309785	-8.266594	3.283882	C	0.79987898877532	-4.78848127588176	-3.96431231232339

C	-3.776466	-1.842332	4.155612	C	0.66603790423261	-3.31319016371027	-3.75902364755404
C	-3.261914	-2.091094	2.820823	C	-2.53973175504895	-8.30868934131533	-4.27190631884964
C	-4.830137	-3.060070	6.519294	C	-4.01537673338177	-1.58208786826778	-3.19740387500274
C	-2.695467	-4.097549	0.716318	C	-0.34396134786183	-7.28612518207235	-4.77027286109916
C	-5.177874	-4.334573	7.123223	C	-3.94543321132898	-8.10478433880167	-4.57407605590526
C	-2.730052	-5.591338	0.688499	C	-1.61879711679634	-1.42854834631578	-3.81841130087646
C	-5.238091	-7.158152	6.690627	C	-5.23426953812302	-2.23966032357941	-3.64204616196952
C	-4.941303	-8.208961	5.728783	C	-1.56072805159391	-7.95226105759487	-5.20883353025634
C	-3.410846	-8.087482	1.902669	C	-3.02325973433950	-1.23120505263524	-4.12778119208606
C	-3.937620	-8.718705	3.102445	C	-6.02817294391944	-6.15267089006965	-4.67328604978154
C	-2.959509	-2.017046	5.283709	C	-6.33614413053436	-4.74761294161935	-4.45010176958658
C	-3.493420	-2.640670	6.484580	C	0.54437375864413	-5.06867980559272	-5.35918683036860
C	-1.941825	-2.496856	2.650760	C	0.08225431889156	-2.78799553870068	-5.02902865808718
C	-1.517580	-3.455742	1.586826	C	0.01212742237553	-6.30186599524462	-5.76790267065251
C	-4.175648	-5.149122	7.668197	C	-0.94068479663194	-1.84726986197933	-5.05925130944279
C	-1.731810	-6.383495	1.247568	C	-4.32549450724607	-7.54771105545177	-5.80321109628182
C	-4.206175	-6.586777	7.446762	C	-5.42226253486774	-2.51779376492944	-5.00234010908745
C	-2.075891	-7.654159	1.861254	C	0.11061400849515	-3.84426658246755	-6.00991097452617
C	-3.620755	-8.645650	5.553978	C	-5.38443516810954	-6.55058383971388	-5.85218333843495
C	-3.110566	-8.902582	4.218459	C	-5.98523692751269	-3.79184539667726	-5.41365260677835
C	-1.597886	-2.473725	5.109765	C	-1.95462635631640	-7.37387324890139	-6.48499223633721
C	-1.118322	-2.732094	3.816464	C	-3.22309482361740	-1.52017848485913	-5.53930385831480
C	-2.452508	-3.485797	7.052322	C	-0.98002205325306	-6.35138151575872	-6.83177219858765
C	-2.787529	-4.717187	7.632336	C	-1.94039557646309	-1.90077023770592	-6.10979713776502
C	-0.647368	-5.784947	2.047045	C	-3.31100176389679	-7.17429359961262	-6.77592342594849
C	-0.598006	-4.413113	2.262218	C	-4.39986820284173	-2.14580630427716	-5.97009246668411
C	-2.835755	-7.043010	7.270928	C	-5.02329736657400	-5.55999386011455	-6.85498625806759
C	-1.219888	-7.848329	3.021687	C	-5.31585758244571	-4.20630361933389	-6.64004676049381
C	-2.547753	-8.051098	6.340153	C	-0.83619930195540	-3.89333408766307	-7.04433765565934
C	-1.723910	-8.462314	4.175372	C	-1.39534484004109	-5.17104478774897	-7.45906917568587
C	-1.277003	-3.381589	6.201887	C	-1.88584484708928	-2.89939243980371	-7.09512001387201
C	-0.292623	-3.902358	3.574583	C	-3.74332542919015	-5.94535227999740	-7.42682303975391
C	-1.958392	-5.888263	7.385993	C	-4.34007201410337	-3.18729566657593	-6.98596328698350
C	-0.342457	-6.694695	3.134780	C	-2.80266789423193	-4.96235188642467	-7.76325292975008
C	-1.374650	-7.942964	5.489835	C	-3.10561079969342	-3.55629254488132	-7.53708355907687
C	-0.479854	-4.508223	5.966114				
C	0.028624	-4.771469	4.628677				

C	-0.824107	-5.785836	6.569328				
C	0.002246	-6.200328	4.403740				
C	-0.526279	-6.833022	5.601322				

Table S3. XYZ of atom coordinates of compounds **6**

6			
	x	Y	z
C	8.660734	0.783101	0.537639
C	8.114757	-0.567298	1.085216
C	5.841391	-0.220894	-0.067303
C	6.578490	-0.620939	1.232476
C	6.132460	-1.995335	1.756163
C	4.678160	-2.282986	1.548486
C	3.595366	-0.205548	-1.296196
C	4.289062	-0.242296	0.106133
C	3.852207	-1.528803	0.806431
C	2.439125	-1.959856	0.508111
C	2.348916	-2.373389	-0.975960
C	3.355982	-1.614880	-1.842341
O	-1.585456	3.674716	-3.851024
O	-2.637192	1.222117	-4.150792
C	0.121143	1.673156	0.012534
O	-1.113410	3.444635	-0.976949
C	-2.298158	3.938209	-1.594251
C	-2.583015	3.256151	-2.931481
C	-2.560668	1.719419	-2.808893
C	-1.302355	1.281262	-2.059583
C	-1.155228	2.032427	-0.726198
H	-3.342619	5.601641	0.186243
H	-2.557222	4.235905	1.049679
H	-4.350739	4.317638	0.940305
H	12.506937	2.017707	0.424202
H	11.280983	2.680819	1.541473
H	12.692621	1.812904	2.181795
H	16.422432	-2.818529	1.513582

H	15.931231	-3.180876	-0.157662
H	14.816139	-3.519056	1.182962
H	14.285809	-1.169329	-1.393576
H	13.368259	-2.367542	-0.442822
H	15.778104	-0.704860	0.384344
H	14.441479	0.208956	2.052336
H	14.944282	-1.278703	2.867897
H	12.796838	-2.395477	2.095674
H	12.463356	-0.973551	3.091448
H	10.709380	0.303600	2.239468
H	3.883010	1.904031	0.374900
H	4.359234	1.059922	1.875957
H	2.732870	0.838677	1.203431
H	7.487768	2.111528	1.822716
H	8.942114	2.863281	1.141267
H	9.076684	1.699449	2.483687
H	10.460453	1.067935	-0.694748
H	10.370773	-1.238249	-1.290956
H	8.114127	-1.748257	-0.762517
H	8.845942	-2.609148	0.602484
H	6.095968	1.917937	0.169534
H	5.876792	1.422648	-1.506408
H	8.147488	0.418585	-1.550693
H	8.226780	2.126269	-1.112579
H	8.549372	-0.727170	2.091804
H	6.078587	-0.979702	-0.839534
H	6.298530	0.127541	1.996643
H	6.394232	-2.084368	2.826563
H	6.710537	-2.795503	1.256239
H	4.285615	-3.201830	2.000606
H	4.203401	0.383487	-1.999083
H	2.626421	0.315167	-1.221046
H	2.111887	-2.784043	1.156566
H	1.739385	-1.119461	0.662316
H	2.459220	-3.462092	-1.080378
H	2.990219	-1.596036	-2.880119
H	4.302641	-2.180908	-1.844284

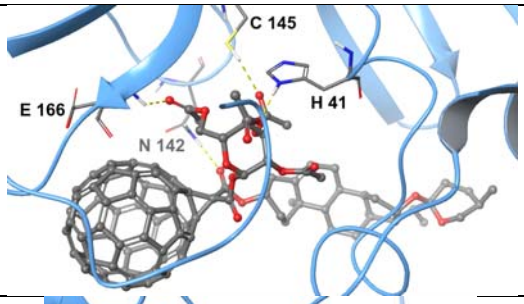
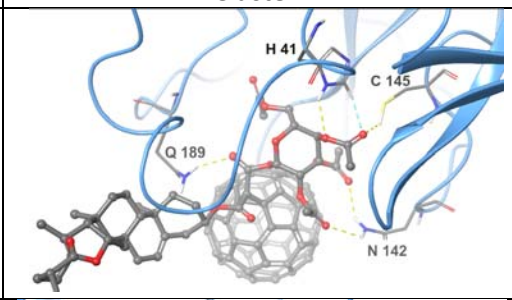
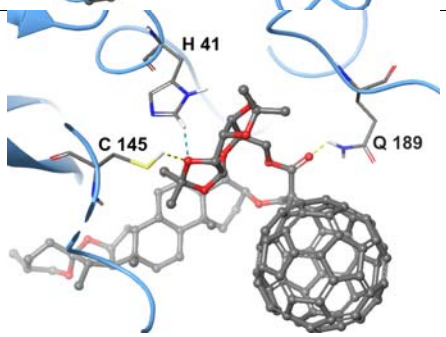
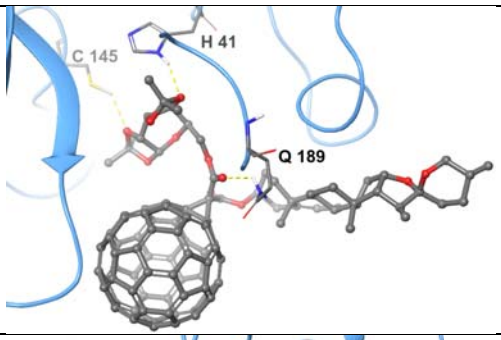
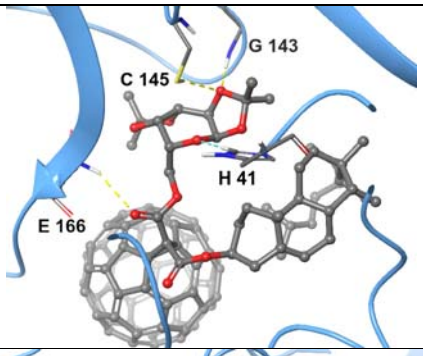
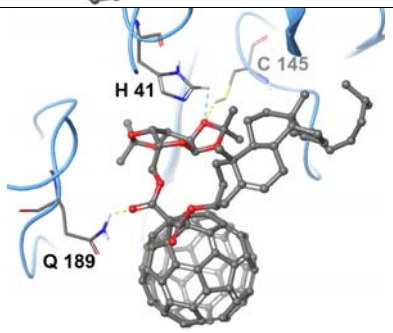
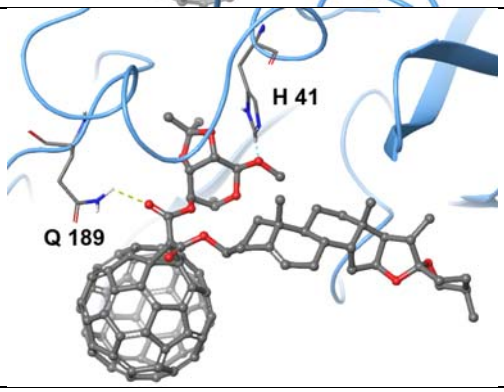
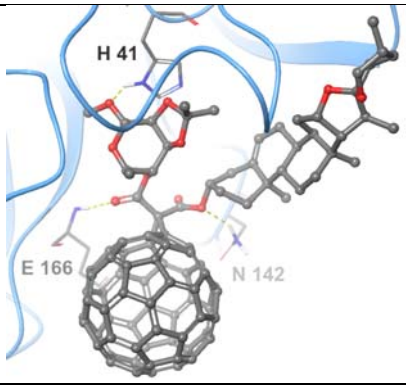
H	-1.689364	3.048251	-4.594764
H	-1.984425	0.496962	-4.245393
H	0.141474	0.597722	0.237645
H	0.182058	2.235347	0.954082
H	0.998492	1.929592	-0.600567
H	-2.085673	5.010304	-1.755711
H	-3.594971	3.560724	-3.262214
H	-3.440141	1.382393	-2.229201
H	-0.407284	1.418180	-2.686387
H	-2.039275	1.791328	-0.106827
C	-3.410864	4.520422	0.410956
O	-3.446178	3.752502	-0.793104
C	11.959734	1.835530	1.359577
C	15.572045	-2.805924	0.814379
C	13.874460	-1.384622	-0.397323
C	14.976599	-1.399934	0.685911
C	14.367812	-0.889093	2.013529
C	12.894872	-1.298175	2.132178
O	12.899527	-0.367115	-0.138514
C	12.062565	-0.718525	0.973947
O	11.116333	-1.711243	0.592610
C	11.193237	0.518845	1.270081
C	3.793899	0.962522	0.938624
C	8.537150	1.924563	1.551731
O	0.137919	-3.964016	-0.661041
O	-0.835541	-0.867339	-3.755533
O	-1.401293	-0.133533	-1.671132
C	-1.118583	-1.071300	-2.586830
C	-1.233211	-2.449481	-1.962447
C	0.029240	-2.927963	-1.283227
O	1.013484	-2.032540	-1.503190
C	10.128945	0.443860	0.150889
C	10.114072	-1.069077	-0.232405
C	8.732427	-1.619936	0.138864
C	6.367818	1.138909	-0.561421
C	7.886688	1.138739	-0.755728
C	-4.656604	-5.592111	1.019467

C	-4.943539	-4.175515	1.066813
C	-3.521706	-6.043228	0.327210
C	-4.081289	-3.276902	0.419133
C	-5.919399	-6.303219	0.895779
C	-6.385761	-3.998406	0.973595
C	-2.881192	-3.737507	-0.241314
C	-6.989974	-5.317758	0.866794
C	-2.625687	-5.102209	-0.317377
C	-3.609844	-7.232238	-0.504945
C	-6.001135	-7.447603	0.091516
C	-4.633883	-2.164362	-0.334735
C	-6.915626	-2.924628	0.248193
C	-4.821659	-7.924111	-0.618319
C	-6.023485	-1.985875	-0.414820
C	-2.586835	-2.799453	-1.364617
C	-2.156368	-5.716060	-1.571124
C	-8.100705	-5.512961	0.034707
C	-2.771617	-7.026180	-1.675419
C	-3.790956	-1.924005	-1.479772
C	-7.153738	-7.651862	-0.768190
C	-8.069361	-3.124828	-0.614681
C	-8.184081	-6.702048	-0.797680
C	-8.651258	-4.395645	-0.719939
C	-1.954150	-4.949759	-2.715112
C	-2.079190	-3.459994	-2.723362
C	-5.250730	-8.431882	-1.913518
C	-6.619146	-1.603817	-1.676937
C	-3.182620	-7.526727	-2.920696
C	-6.689780	-8.260727	-2.008021
C	-4.361762	-1.580797	-2.700617
C	-7.884997	-2.307447	-1.805413
C	-4.444856	-8.238539	-3.042958
C	-5.799952	-1.414357	-2.801435
C	-8.786658	-6.321667	-2.066426
C	-9.073894	-4.895841	-2.018307
C	-2.431581	-5.441380	-3.988371
C	-2.867317	-3.132128	-3.947830

C	-3.008669	-6.715739	-4.105111
C	-3.891992	-2.193211	-3.956469
C	-7.274289	-7.897250	-3.229311
C	-8.292557	-2.791768	-3.055695
C	-2.984541	-4.328887	-4.742061
C	-8.340115	-6.907039	-3.258207
C	-8.899077	-4.107264	-3.164168
C	-5.050977	-7.862773	-4.312137
C	-6.226135	-1.916935	-4.097481
C	-4.161144	-6.919501	-4.970865
C	-5.050279	-2.398550	-4.805363
C	-6.439454	-7.693641	-4.402853
C	-7.448764	-2.588185	-4.224806
C	-8.163218	-6.090723	-4.449763
C	-8.434949	-4.716299	-4.404104
C	-4.088211	-4.527179	-5.585589
C	-4.690533	-5.847194	-5.698504
C	-5.144903	-3.540377	-5.617121
C	-6.990232	-6.577175	-5.157763
C	-7.542365	-3.776880	-5.060290
C	-6.131567	-5.671142	-5.795341
C	-6.411781	-4.243166	-5.744227

19. Molecular docking calculations

Table S4. Representative conformations of fullerene derivatives bound to Mpro.

Ligand	Representative conformations	
	Cluster A	Cluster B
5a		
5b		
5c		
5d		

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