Supplementary data

Reversible Non-Covalent Derivatisation of Carbon Nanotubes with Glycosides

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General

Thin-layer chromatography analyses were performed on pre-coated Merck silica gel plates (60F254) and visualized by with UV light. Melting points were determined on a Bibby Stuart Scientific SMP10 apparatus and are reported without correction. ^{1}H and ^{13}C NMR spectra were recorded on a Varian 400 MHz or 500 MHz spectrometer and chemical shifts are given in ppm (δ) using $CDCl_3$, CD_3OD or D_2O as internal standard. LC-MS analyses were performed on a Gilson reverse phase HPLC equipped with a Finnigan mass spectrometer ($MeCN/H_2O$ and 0.1% formic acid as mobile phase). Preparative HPLC was performed with a

Gilson 333 pump, a Gilson 231 XL sampling injector, a Gilson FC 204 fraction collector and a Gilson 118/119 UV/Vis detector. MeCN/H_2O (with 0.1% formic acid) was used as mobile phase and the chromatography was carried out with a YMC 150x20 mm C8 column. Centrifugation-assisted filtration was performed using an Eppendorf minispin centrifuge together with Vectaspin microvials equipped with a 0.45 μm polypropylene filter-membrane (Whatman Schleicher & Schuell). Raman spectra were recorded on a Renishaw Raman spectrometer using a 514 nm Argon laser, with a 50x lens and a laser power of 10 mW. IR spectra were recorded on a PerkinElmer Spectrum-100 FT-IR spectrometer with an ATR accessory. The samples were analyzed by placing neat samples directly on the ATR crystal. Fluorescence spectra were recorded on a Varian Cary Eclipse fluorescence spectrometer and UV spectra were recorded on a Varian Cary 3 Bio UV/Vis spectrometer.

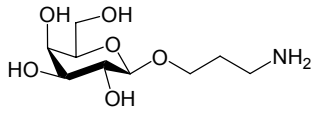
Acid-oxidized MWNTs (Shenzhen Nanotech Port, PRC, diameter range 10–30 nm) was prepared by literature procedure[1]. The reported special surface area for these MWNTs is 40-300 m^2/g.[2]

Preparation of acid-oxidized SWNTs

SWNTs (CNI HiPCO, lot p0332) (66 mg) was added to a 100 ml round bottomed flask together with HNO_3 (8M, 12.5 ml). The mixture was ultrasonicated for 10 minutes and then refluxed for 1 hour. The mixture was allowed to cool and the acidic solution was then separated from the SWNTs by centrifugation. The solid SWNT material was washed with aqueous KOH and with water and was then transferred to a vectaspin microvial equipped with a 0.45 μm polypropylene filter membrane. The SWNTs were washed with deionized water until the filtrate was neutral and the SWNTs was then dried in a vacuum oven at 160°C for 24 hours. The acid-oxidized SWNTs was analyzed by Raman and IR spectroscopy which

indicated a low degree of defects (see main text). The reported special surface areas for HiPCO SWNTs are 524-577 m^2/g.[3,4]

Synthesis of 3-Aminopropyl β-D-galactopyranoside **3**[5]



3-Aminopropyl β-D-galactopyranoside was prepared from penta-*O*-acetyl-β-D-galactopyranose in a three-step sequence:

1-Chloropropanol (1.1 mL, 11.3 mmol) and $BF_3{\cdot}Et_2O$ (1.8 mL, 11.3 mmol) were added to a solution of penta-*O*-acetyl-β-D-galactopyranose (2.20 g, 5.6 mmol) in dry CH_2Cl_2 (10 mL). After 2 hours stirring at room temperature, the reaction mixture was poured into ice-water (ca. 100 mL) and the crude product was extracted with CH_2Cl_2 (2 x 100 mL), washed with brine (50 mL), dried over $MgSO_4$ and concentrated. Flash chromatography (toluene → toluene/ethyl acetate, 5:1) gave 3-chloropropyl 2,3,4,6-tetra-*O*-acetyl-β-D-galactopyranoside (1.5 g, 3.5 mmol, 63 %). δ_H(400 MHz, $CDCl_3$, 25°C) 5.38 (1H , dd, J = 3.4 Hz, J = 0.9 Hz), 5.19 (1H, dd, J = 10.5 Hz, J = 7.9 Hz), 5.01 (1H, dd, J = 3.4, J = 10.5 Hz), 4.48 (1H, d, J = 7.9 Hz), 4.15 (2H, m), 3.94 (2 H, m), 3.60 (1H, m), 3.38 (2H, m), 2.15 (3H, s), 2.07 (2H, s), 2.05 (3H, s), 1.98 (3H, s), 1.86 (2H, s); δ_C(101 MHZ, $CDCl_3$, 25°C) 170.5, 170.2, 169.6, 101.7, 70.9, 70.8, 68.9, 66.5, 61.4, 41.5, 31.3, 20.9, 20.8.

3-Chloropropyl 2,3,4,6-tetra-*O*-acetyl-β-D-galactopyranoside (2.5 g, 5.9 mmol) and KI (1.95 g, 11.7 mmol), dissolved in DMF (15 mL), were stirred at 50°C for 30 min. NaN_3 (3.8 g, 59 mmol) was added and the reaction mixture kept under reflux (oil bath, 160°C) for 1 hour. The oil bath was removed. After additional 5 min, the still hot reaction mixture was poured on ice-

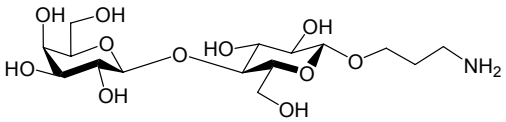
water (ca. 50 mL) and ethyl acetate (200 mL) was added. The organic phase was transferred into a separation funnel, washed with water (3 x 100 mL), dried over $MgSO_4$ and concentrated. Flash chromatography (toluene → toluene/ethyl acetate 5:1) gave 3-azidopropyl 2,3,4,6-tetra-*O*-acetyl-β-D-galactopyranoside (2.5 g, 5.9 mmol, quantitative). δ_H(400 MHz, $CDCl_3$, 25°C) 5.38 (1H, dd, *J* = 3.4 Hz, *J* = 0.9 Hz), 5.20 (1H, dd, *J* = 10.5 Hz, *J* = 7.9 Hz), 5.02 (1H, dd, *J* = 3.4 Hz, *J* = 10.5 Hz), 4.46 (1H, d, *J* = 7.9 Hz), 4.15 (2H, m), 3.96 (2H, m), 3.60 (1H, m), 3.38 (2H, m), 2.15 (3H, m), 2.04 (3H, s), 2.0 (3H, s), 1.98 (3H, s), 1.86 (2H, m); δ_C(101 MHZ, $CDCl_3$, 25°C) 170.5, 170.4, 170.3, 169.6, 101.5, 71.0, 70.8, 69.0, 67.1, 66.6, 61.4, 48.0, 29.1, 20.9, 20.8, 20.7.

3-Azidopropyl 2,3,4,6-tetra-*O*-acetyl-β-D-galactopyranoside (2.5 g, 5.9 mmol) was dissolved in methanol (50 mL) and some droplets sodium methoxide solution in methanol (1 M) were added (pH 8, wet pH-paper). The mixture was stirred at room temperature for 16 hours and then neutralized by gently stirring with some beads of ion exchange resin (Dowex 120 H^+). The resin was removed by filtration, washed with methanol and the filtrate concentrated under reduced pressure to give 3-azidopropyl β-D-galactopyranoside (1.2 g, 4.5 mmol, 75 %). δ_H(400 MHz, D_2O, 25°C) 4.37 (1H, d, *J* = 7.8 Hz), 4.11 – 4.03 (1H, m), 3.91 (1H, d, *J* = 3.4), 3.77 – 3.61 (5H, m), 3.49 (1H, dd, *J* = 10.2 Hz, 7.9 Hz), 3.45 (2H, t, *J* = 6.7 Hz), 1.88 (2H, m); δ_C(101 MHz, D_2O, 25°C) 103.0, 75.3, 72.9, 70.9, 68.8, 67.4, 61.1, 48.0, 28.5.

Pd/C (30 mg, 10 %) was added to a solution of 3-azidopropyl β-D-galactopyranoside (1.2 g, 4.5 mmol) in methanol (20 mL) and the mixture was stirred at room temperature under H_2 atmosphere (1 atm.) over night. The catalyst was removed by filtration using a filter sandwich (20 μm, 10 μm, 5 μm pore diameter). The filter residue was thoroughly washed with methanol and the combined methanolic solutions concentrated to give 3-Aminopropyl β-D-

galactopyranoside **3** (0.9 g, 3.8 mmol, 93%). δ_H(400 MHz, D_2O, 25°C): δ = 4.37 (1H, d, *J* = 7.8 Hz), 3.99-3.89 (2H, m), 3.76-3.61 (5H, m), 3.48 (1H, m), 3.23 (2H, t, *J* = 8.3 Hz) 2.73 (2H, m), 1.78 (2H, m); δ_C(101 MHz, D_2O, 25°C) 103.0, 75.3, 72.9, 70.9, 68.8, 68.4, 61.1, 37.7, 28.5.

Synthesis of 3-Aminopropyl β-D-galactopyranosyl-(1→4)-β-D-galactopyranoside **4**



3-Aminopropyl β-D-galactopyranosyl-(1→4)-β-D-galactopyranoside was synthesized from octa-*O*-acetyl-β-D-lactose as described above.

3-Chloropropyl hepta-O-acetyl-β-D-lactoside[6]

δ_H(400 MHz, $CDCl_3$, 25°C) 5.34 (1H, dd, *J* = 3.4 Hz, 1.0 Hz), 5.19 (1H, t, *J* = 9.3 Hz), 5.10 (1H, dd, *J* = 10.4 Hz, 7.9 Hz), 4.94 (1H, dd, *J* = 10.4 Hz, 3.4 Hz), 4.91 (1H, dd, *J* = 9.6 Hz, 7.9 Hz), 4.53 (3H, td, *J* = 7.6 Hz, 3.4 Hz), 4.17 – 4.02 (3H, m), 3.94 (1H, dt, *J* = 10.3 Hz, 5.3 Hz), 3.89 – 3.83 (1H, m), 3.78 (1H, t, *J* = 9.5 Hz), 3.72 (1H, ddd, *J* = 9.8 Hz, 8.2 Hz, 4.6 Hz), 3.64 – 3.54 (3H, m), 2.14 (3H, s), 2.11 (3H, s), 2.05 (3H, s), 2.04 (3H, s), 2.04 (6H, s), 1.96 (3H, s); δ_C(101 MHZ, $CDCl_3$, 25°C) 170.5, 170.5, 170.3, 170.2, 169.9, 169.8, 169.2, 101.2, 100.9, 76.4, 72.8, 72.8, 71.8, 71.1, 70.8, 69.3, 66.7, 66.5, 62.1, 61.0, 41.40, 32.4, 21.0, 20.9, 20.8, 20.8, 20.7.

3-Azidopropyl hepta-O-acetyl-β-D-lactoside[7]

δ_H(400 MHz, $CDCl_3$, 25°C) 5.31 (1H, dd, *J* = 3.4 Hz, 0.9 Hz), 5.16 (1H, t, *J* = 9.3 Hz), 5.07 (1H, dd, *J* = 10.4 Hz, 7.9 Hz), 4.92 (1H, dd, *J* = 10.4 Hz, 3.4 Hz), 4.85 (1H, dd, *J* = 9.6 Hz, 7.9 Hz), 4.45 (3H, t, *J* = 8.0 Hz), 4.14 – 4.00 (4H, m), 3.91 – 3.82 (2H, m), 3.76 (1H, t, *J* = 9.4

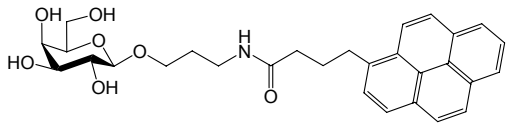
Hz), 3.61 – 3.49 (2H, m), 3.32 (2H, d, *J* = 3.4 Hz), 2.12 (3H, s), 2.09 (3H, s), 2.03 (7H, s), 2.01 (9H, s), 1.93 (3H, s), 1.79 (2H, d, *J* = 6.4 Hz); δ_C(101 MHZ, $CDCl_3$, 25°C) 170.4, 170.2, 170.1, 169.8, 169.7, 169.1, 101.1, 100.6, 76.3, 72.83, 72.8, 71.7, 71.1, 70.8, 69.2, 66.7, 66.5, 62.0, 60.9, 48.0, 29.0, 20.9, 20.9, 20.8, 20.7, 20.6.

3-Azidopropyl β-D-galactopyranosyl-(1→4)-β-D-galactopyranoside[8]

δ_H(400 MHz, D_2O, 25°C) 4.47 (1H, d, *J* = 8.0 Hz), 4.42 (1H, d, *J* = 7.8 Hz), 3.98-3.89 (2H, m), 3.79 - 3.43 (12H, m), 3.29 (2H, t, *J* = 8.6 Hz), 1.88 (2H, m); δ_C(101 MHZ, D_2O, 25°C) 103.1, 102.3, 78.5, 75.5, 74.9, 74.5, 73.0, 74.7, 71.1, 68.7, 67.5, 61.2, 60.2, 48.0, 28.4.

3-Aminopropyl β-D-galactopyranosyl-(1→4)-β-D-galactopyranoside **4** δ_H(400 MHz, D_2O, 25°C) 4.47 (1H, d, *J* = 8.1 Hz), 4.43 (1H, d, *J* = 7.8 Hz), 3.98 – 3.90 (2H, m), 3.77 – 3.62 (12H, m), 3.29 (2H, m), 1.77 (2H, m); δ_C(101 MHZ, D_2O, 25°C) 103.1, 102.2, 78.5, 75.5, 75.0, 74.6, 73.0, 72.7, 71.1, 68.7, 68.5, 61.2, 60.2, 37.7.

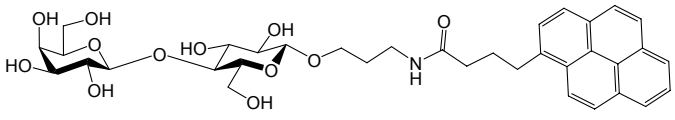
Synthesis of 3-[4'-(pyren-1-yl)butylamido]propyl β-D-galactopyranoside **1**



4-(1-pyrene)butyric acid (6.9 mg, 24 μmol) and 3-aminopropyl β-D-galactopyranoside **3** (5.2 mg, 22 μmol) were added to a 25 ml pear-shaped flask together with dry DMF (1 ml). The flask was cooled in an ice-bath and a solution of *N*,*N*′-Dicyclohexylcarbodiimide (DCC) (7.6 mg, 37 μmol) in dry DMF (1 ml) was added in portions. The mixture was stirred under nitrogen atmosphere for 10 minutes and 1-hydroxybenzotriazol (HOBt) (7.6 mg, 56 μmol) was then added to the cooled solution. The ice-bath was removed after 1 hour and the stirring

was continued for 12 hours. The solvent was then removed *in vacuo* and the residue dispersed in dichloromethane. Filtration of the dichloromethane dispersion through a 0.45 μm polypropylene filter membrane resulted in a sticky orange solid that was washed three times with dichloromethane (3 x 5 ml). The solid on the filter membrane was dissolved in methanol and purified by preparative HPLC (purified yield: 5.3 mg, 10.5 μmol, 48%). FT-IR (neat) ($\tilde{\nu}$ / cm^{-1}): 3316 (OH), 2926, 2873 (CH), 1676 (C=O), 1634 (C=O), 1458 (CH), 1432 (CH), 1377 (CH), 1203 (CO), 1181 (CO), 1132 (CO), 1075 (CO), 1030 (CO), 843, 801, 758, 722. δ_H(500 MHz, CD_3OD, 25°C) 8.36 (1H, d, J = 9.3 Hz), 8.19 (2H, m), 8.16 (1H, d, J = 9.3 Hz), 8.15 (1H, d, J = 7.7 Hz) 8.06 (1H, d, J = 8.9 Hz), 8.04 (1H, d, J = 8.9 Hz), 8,00 (1H, dd, J = 7.7 Hz) 7.92 (1H, d, J = 7.7 Hz), 4.24 (1H, d, J = 7.7 Hz), 3.92 (1H, dt, J = 5.9 Hz), 3.84 (1H, m), 3.64 (1H, m), 3.62 (1H, dt, J = 5.9 Hz), 3.39 (2H, m), 3.35 (1H, m), 3.33 (2H, m), 3.26 (1H, m), 3.25 (1H, m), 3.19 (1H, dd, J = 7.7, 9.0 Hz), 2.37 (2H, t, J = 7.4 Hz), 2.17 (2H, m), 1.80 (2H, m); δ_C(125 MHz, CD_3OD, 25°C) 178.8, 136.2, 131.7, 131.2, 131.1, 130.2, 128.8, 127.4, 127.3, 126.0, 125.1, 125, 124.8, 123.4, 104.0, 77.7, 77.6, 77.1, 74.8, 71.3, 68.1, 62.4, 35.7, 32.7, 29.2, 28.1. LC-MS (ESI+): *m/z:* 508 [M+H].

Synthesis of 3-[4'-(pyren-1-yl)butylamido]propyl β-D-galactopyranosyl-(1→4) β-D-glucopyranoside **2**



4-(1-pyrene)butyric acid (30 mg, 104 μmol) and 3-aminopropyl β-D-galactopyranosyl-(1→4) β-D-glucopyranoside **4** (37 mg, 92.5 μmol) were dissolved in dry DMF (1 ml) and added to a 25 ml pear-shaped flask. The flask was cooled to 0°C and a solution of *N*,*N*′-Dicyclohexylcarbodiimide (DCC) (33 mg, 160 μmol) in dry DMF (1 ml) was added to the

cooled mixture under nitrogen atmosphere. A solution of 1-hydroxybenzotriazol (HOBt) (40 mg, 294 μmol) in dry DMF (1 ml) was then added in portions to the cooled mixture. The mixture was then allowed to stir over night. The solvent was removed *in vacuo* and the residue was dispersed in dichloromethane. Filtration of the dichloromethane dispersion through a 0.45 μm polypropylene filter membrane resulted in an orange solid that was washed with dichloromethane (3 x 5 ml). The solid on the filter membrane was dissolved in methanol and purified by preparative HPLC to give the pure product as an almost colorless solid (purified yield: 37 mg, 55.5 μmol, 60%). M.p. 167-175 °C. FT-IR (neat) (ν/cm^{-1}): 3318 (OH), 2929, 2870 (CH), 1671 (C=O), 1631 (C=O), 1543 (C=O), 1435 (CH), 1378 (CH), 1324 (CO), 1200 (CO), 1136 (CO), 1062 (CO), 1022 (CO), 891 (CH), 837, 800, 721 (CH). δ_H(500 MHz, CD_3OD, 25°C) 8.35 (1H, d, J = 9.3 Hz), 8.19 (2H, m), 8.15 (1H, d, J = 9.3 Hz), 8.14 (1H, d, J = 7.7 Hz) 8.05 (1H, d, J = 8.9 Hz), 8.03 (1H, d, J = 8.9 Hz), 8,00 (1H, dd, J = 7.7 Hz) 7.91 (1H, d, J = 7.7 Hz), 4.32 (1H, d, J = 7.7 Hz), 4.27 (1H, d, J = 7.7 Hz), 3.92 (1H, dt, J = 12.0, 6.0 Hz), 3.86 (1H, dd, J = 12.0, 2.6 Hz), 3.81 (1H, dd, J = 3.2, 1.0 Hz), 3.79 (1H, dd, J = 12.0, 4.4 Hz), 3.77 (1H, dd, J = 11.4, 7.4 Hz), 3.69 (1H, dd, J = 11.4, 4.7 Hz), 3.60 (1H, dt, J = 12.0, 6.0 Hz), 3.56 (1H, ddd, J = 7.4, 4.7, 1.0 Hz), 3.54 (1H, dd, J = 9.7, 7.7 Hz), 3.53-3.50 (2H, m), 3.47 (1H, dd, J = 9.7, 3.2 Hz), 3.38 (2H, m), 3.37 (1H, m), 3.33 (2H, m), 3.25 (1H, m), 2.36 (2H, t, J = 7.3 Hz), 2.16 (2H, m), 1.80 (2H, m); δ_C(125 MHz, CD_3OD, 25°C) 178.8, 136.2, 131.7, 131.2, 131.1, 130.2, 128.8, 127.4, 127.3, 126.0, 125.1, 125, 124.8, 123.4, 104.8, 104, 80.5, 77.1, 76.9, 76.26, 76.23, 74.7, 74.6, 72.3, 70.1, 68.1, 62.2, 61.6, 35.7, 32.7, 29.2, 28.1. LC-MS (ESI+) *m/z:* 670 [M+H].

Preparation of SWNT/MWNT–pyreneglycoside assemblies. Acid-oxidized SWNT or MWNT was ultrasonicated in D_2O (1 ml) for 30 minutes. The resulting black dispersion was centrifuged and the dark supernatant was transferred to a 5 ml vial. Compound **1** or **2** was

added to the supernatant and the resulting mixture was ultrasonicated for 10 minutes prior to analysis.

Quantification of p-SWNT and p-SWNT-2 solutions

p-SWNT was sonicated in 1 ml H_2O together with compound **2** ($1{,}35 \cdot 10^{-6}$ mol) for 20 minutes. The formed heterogenous dispersion was left for sedimentation and the supernatant was collected and filtrated through a cotton-plug. The resulting visually non-scattering dispersion was analyzed by UV/Vis spectroscopy at 500 nm, and the absorbance was compared to a solution of only p-SWNT (prepared in the same exact way as above, but without compound **2**). The vial containing p-SWNT-**2** showed no signs of precipitation during a week, while the reference sample, containing only p-SWNT, partly precipitated during this period. The solubility of p-SWNT was determined to ~0.8 mg/ml H_2O while the solubility of p-SWNTs functionalized with **2** was determined to ~1 mg/ml H_2O.

Typical procedure for fluorescence titration. Purified CNTs (1 mg) was sonicated in H_2O for 30 minutes and the resulting black dispersion was filtrated through a cotton-plug. This yielded a non-scattering filtrate that was freeze-dried. The solid CNT material was weighted and then re-dispersed in H_2O. This yielded a non-scattering solution of CNTs of known concentration that was titrated with a solution of compound **2** in H_2O ($1.49 \cdot 10^{-4}$ M). The fluorescence emission of the CNT solution was continually monitored between each addition of **2,** and the solution was ultrasonicated for 1 minute between each addition.

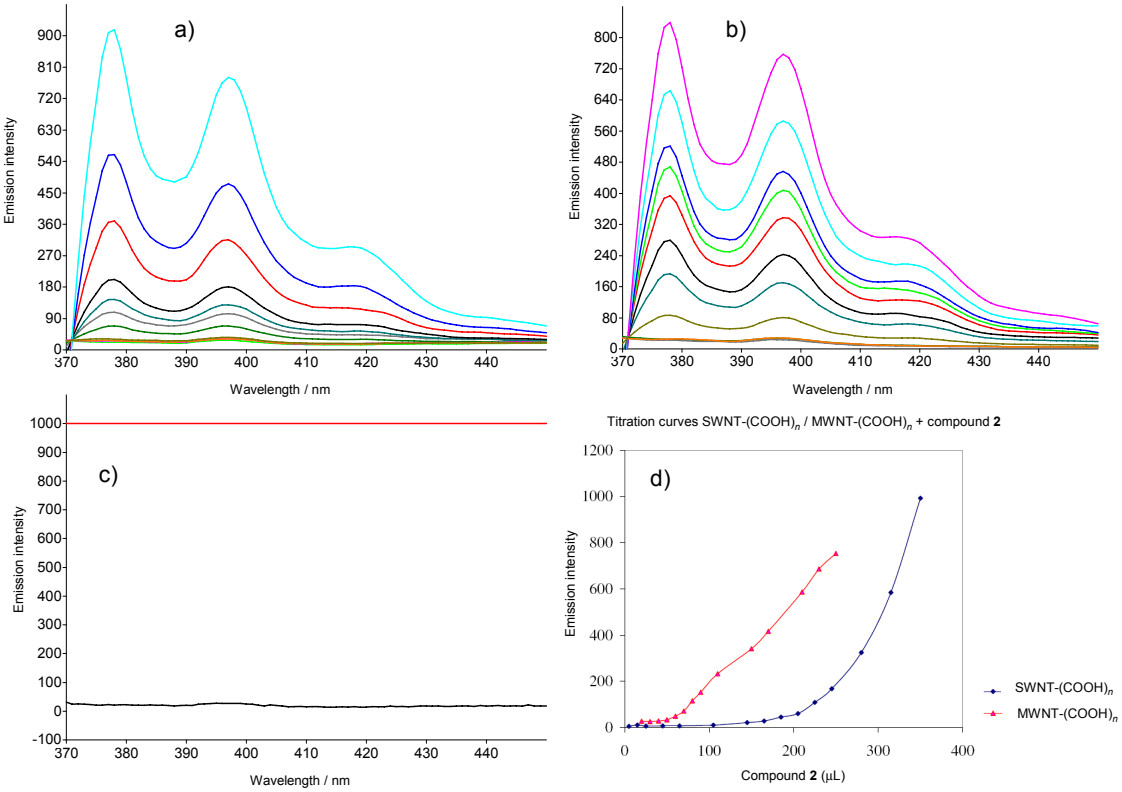


Figure S1. a): Fluorescence spectra of SWNT-**2** complex in H_2O (0.17 mg SWNTs / ml H_2O). The signal intensity increases with increased addition of compound (**2**). b): Corresponding fluorescence spectra of the MWNT-**2** complex in H_2O (0.60 mg MWNTs / ml H_2O) with addition of compound **2**. c) Fluorescence spectra of a $3 \cdot 10^{-6}$ M solution of **2** in H_2O before (red), and after (black) addition of 0.17 mg purified SWNT. The fluorescence signal intensity is above the scale before adding SWNTs. d): Titration curves derived from fluorescence titrations of aqueous solutions of purified CNTs with compound **2** ($c = 1.49 \cdot 10^{-4}$ M). (Blue): SWNT (0.17 mg/ml), (red): MWNT (0.60 mg/ml). The CNTs are saturated at a CNT mass ratio of 0.4 mg/mg SWNT and 0.04 mg/mg MWNT.

^{1}H NMR spectra of compounds 1-4

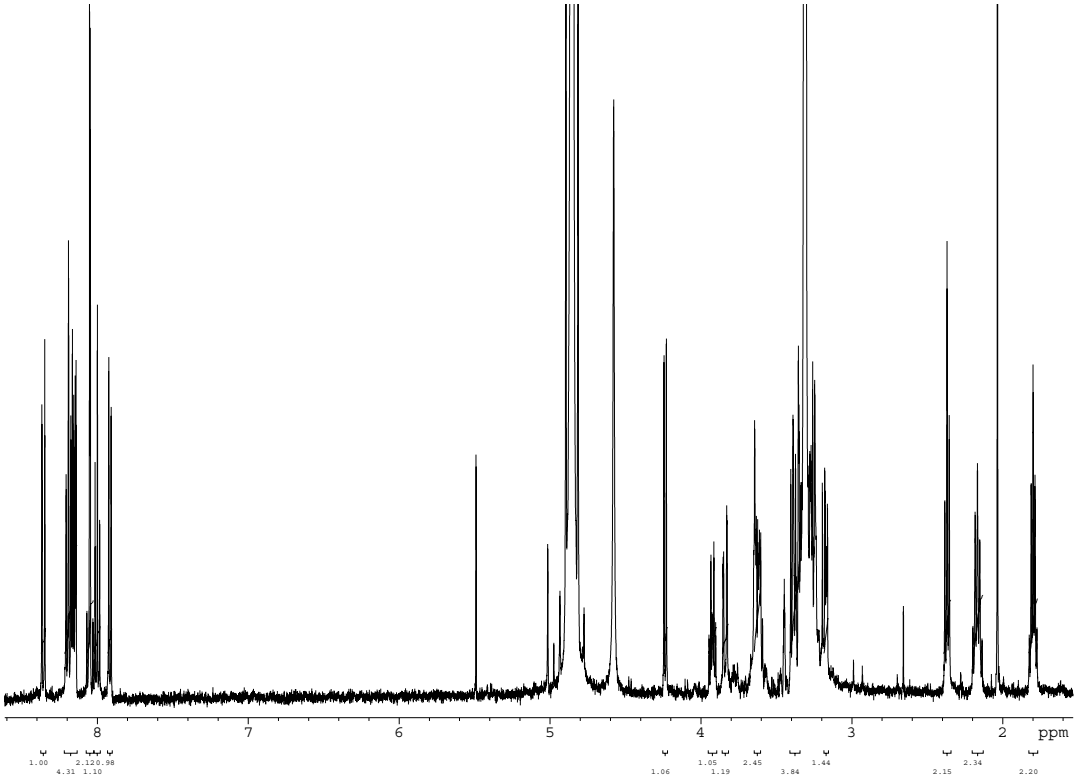


Figure S2. ^{1}H NMR of pyrene glycoside derivative **1** (500 MHz, CD_3OD, 25°C).

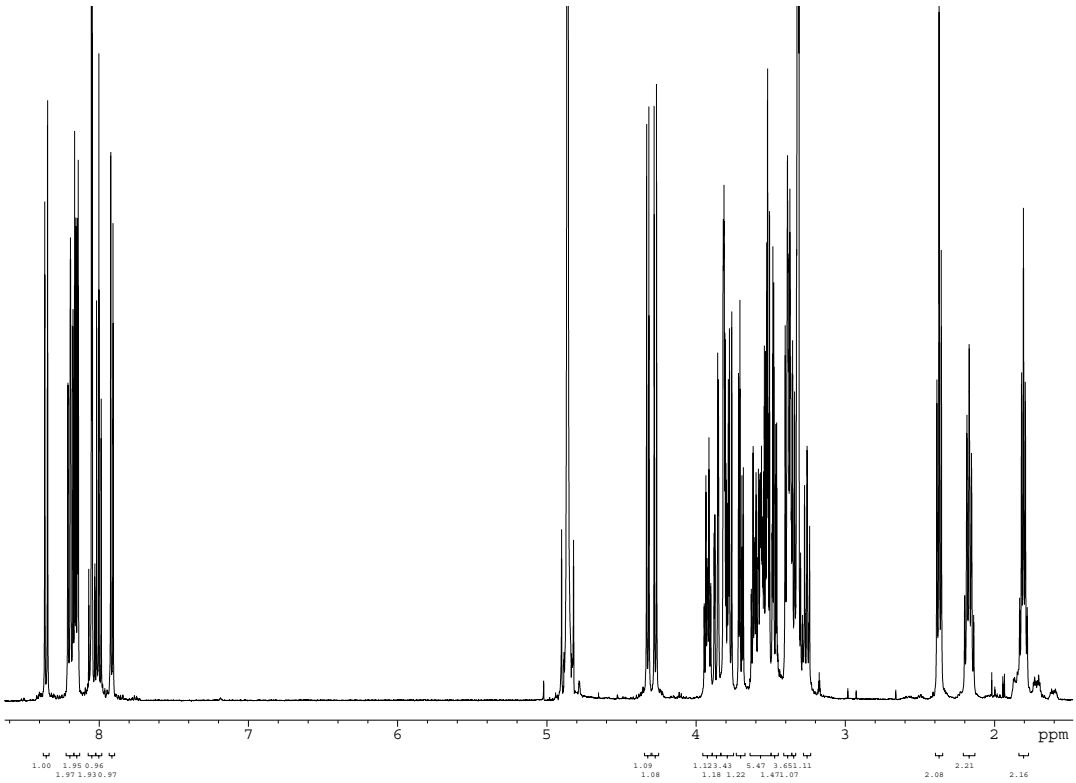


Figure S3. ^{1}H NMR of pyrene glycoside derivative **2** (500 MHz, CD_3OD, 25°C).

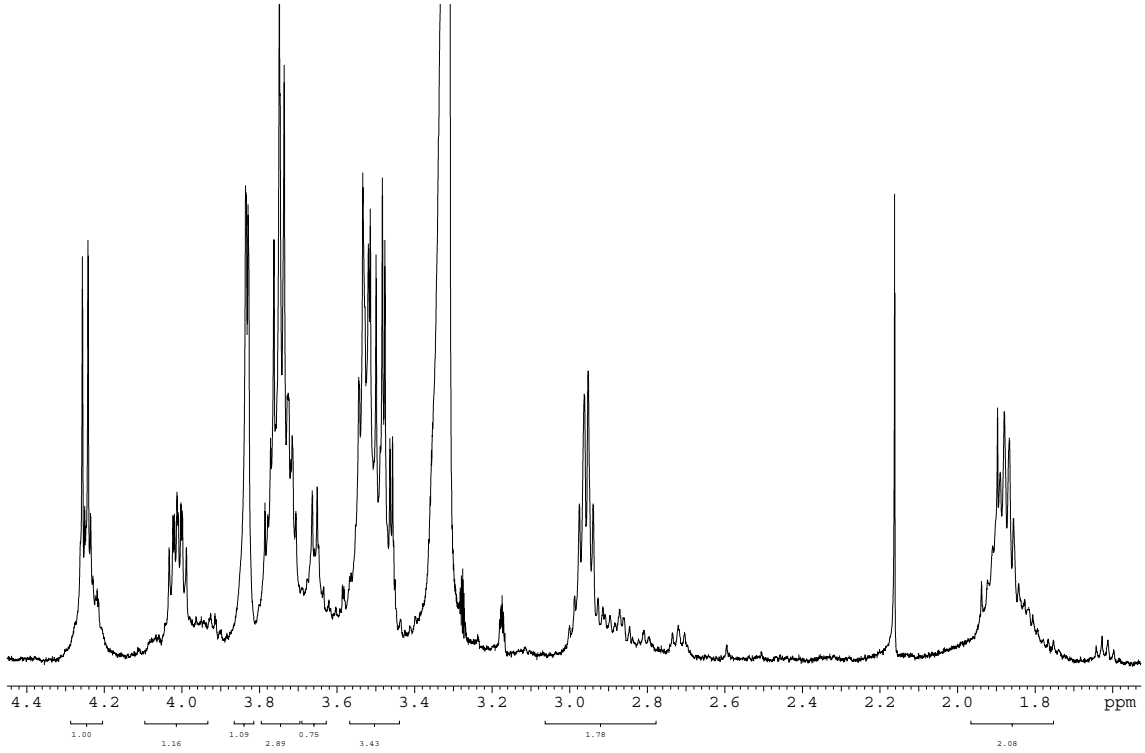


Figure S4. ^{1}H NMR of glycoside **3** (500 MHz, CD_3OD, 25°C).

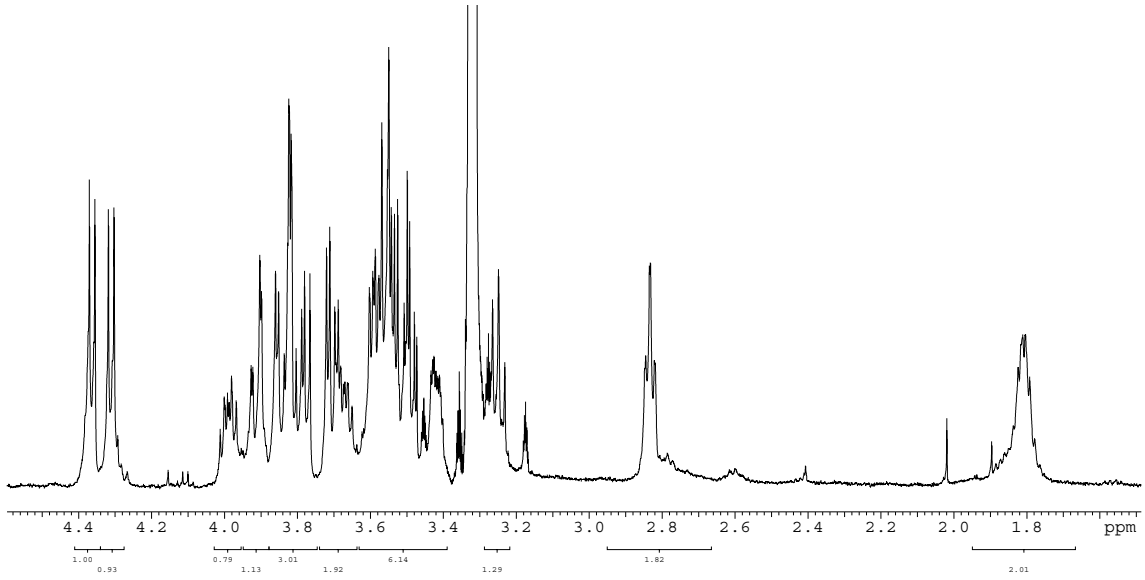
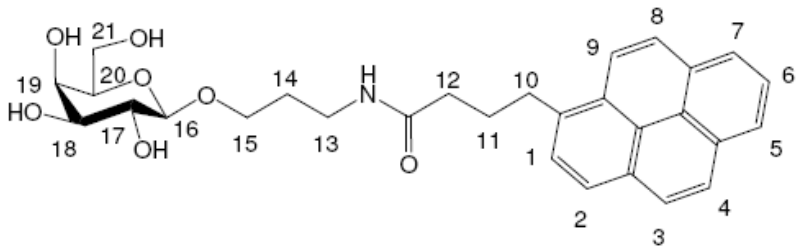


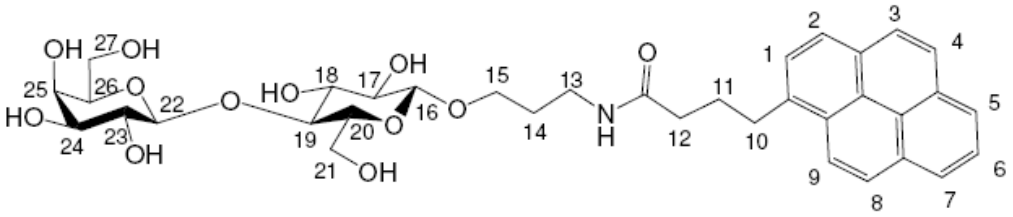
Figure S5. ^{1}H NMR of glycoside **4** (500 MHz, CD_3OD, 25°C).

NMR assignment of pyrene-glycoside 1 and 2



	^{1}H	Mult.	*J*	^{13}C
C=O				178.8
1	7.92	d	7.7 Hz	127.4
2	8.15	d	7.7 Hz	127.4
3	8.06	d	8.9 Hz	127.2
4	8.04	d	8.9 Hz	127.2
5	8.19	m		124.7
6	8.00	dd	7.7 Hz	126.0
7	8.19	m		124.7
8	8.16	d	9.3 Hz	124.9
9	8.36	d	9.3 Hz	123.4
10	3.39	m		32.7
11	2.17	m		28.1
12	2.37	t	7.4 Hz	35.7
13	3.33	m		77.1
14	1.80	m		29.2
15	3.92, 3.62	dt	6.0, 12.0 Hz	68.1
16	4.24	d	7.7 Hz	104.0
17	3.19	dd	7.7, 9.3 Hz	74.8
18	3.35	m		77.7
19	3.26	m		71.3
20	3.25	m		77.6
21	3.84, 3.64	m		62.4

Table 1. NMR assignment of compound **1** (assignment based on COSY, TOCSY, HSQC and HMBC experiments).



	^{1}H	Mult.	*J*	^{13}C
C=O				178.8
1	7.91	d	7.7 Hz	127.4
2	8.14	d	7.7 Hz	127.4
3	8.05	d	8.9 Hz	127.2
4	8.03	d	8.9 Hz	127.2
5	8.19	m		124.7
6	8.00	dd	7.7 Hz	126.0
7	8.19	m		124.7
8	8.15	d	9.3 Hz	124.9
9	8.35	d	9.3 Hz	123.4
10	3.38	m		32.7
11	2.16	m		28.1
12	2.36	t	7.4 Hz	35.7
13	3.33	m		77.1
14	1.80	m		29.2
15	3.92, 3.60	dt	12.0, 6.0 Hz	68.1
16	4.27	d	7.7 Hz	104.0
17	3.26	m		74.6
18	3.52	m		76.26
19	3.52	m		80.5
20	3.37	m		76.23
21a	3.86	dd	12.0, 2.6 Hz	61.6
21b	3.79	dd	12.0, 4.4 Hz	61.6
22	4.32	d	7.7 Hz	104.8
23	3.54	dd	9.7, 7.7 Hz	72.3
24	3.47	dd	9.7, 3.2 Hz	74.7
25	3.81	dd	3.2, 1.0 Hz	70.1
26	3.56	ddd	7.4, 4.7, 1.0 Hz	76.9
27a	3.77	dd	11.4, 7.4 Hz	62.2
27b	3.69	dd	11.4, 4.7 Hz	62.2

Table 2. NMR assignment of compound **2** (assignment based on COSY, TOCSY, HSQC and HMBC experiments).

IR spectra of compound 1 and 2

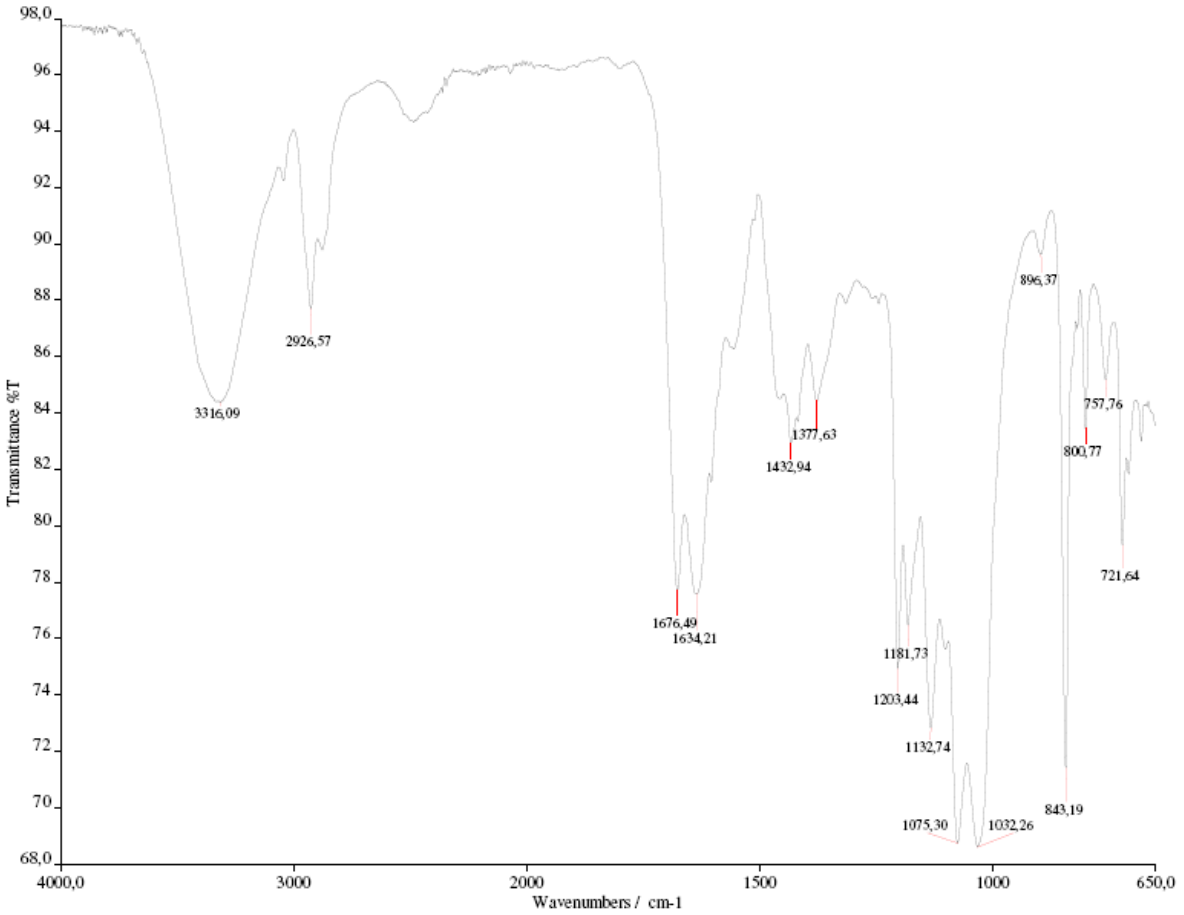


Figure S6. IR spectrum (neat) of compound **1** (3-[4'-(pyren-1-yl)butylamido]propyl β-D-galactopyranoside).

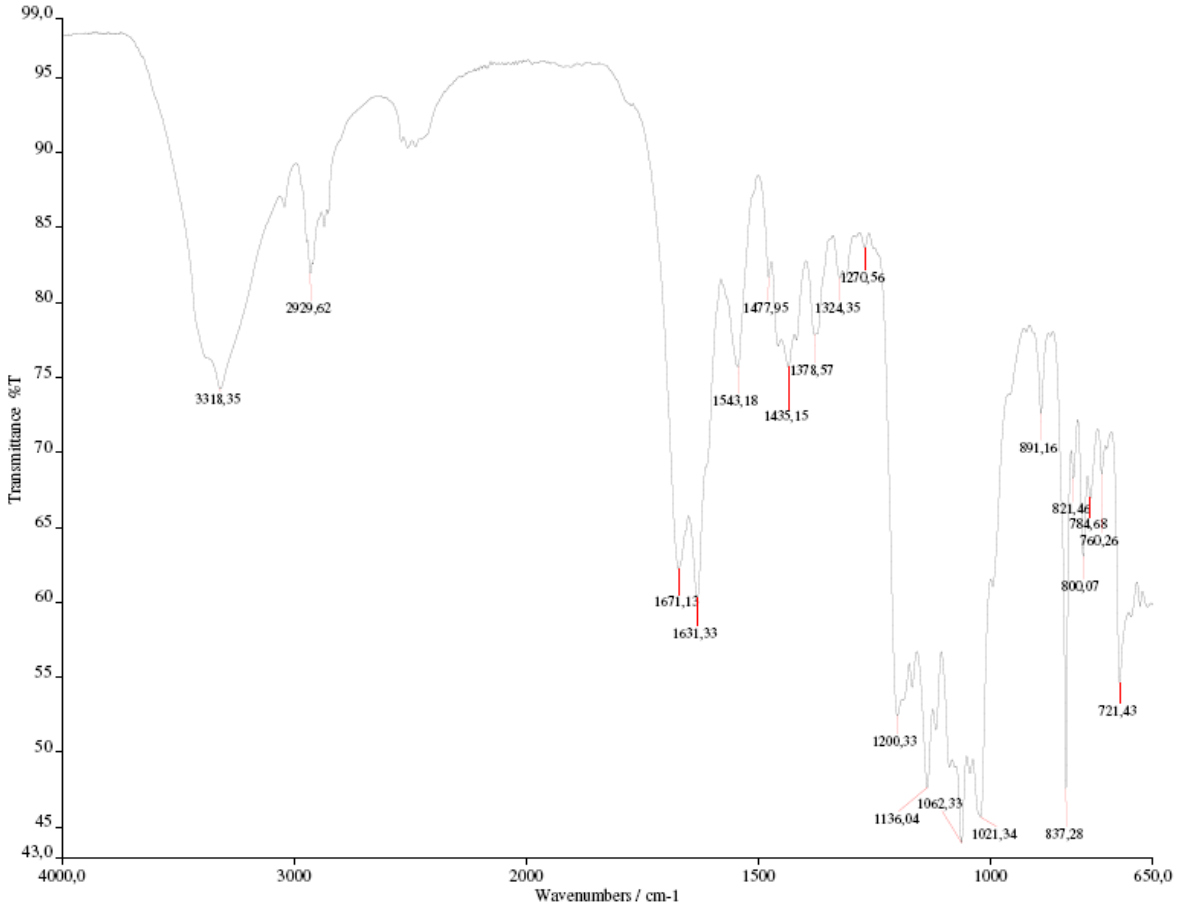


Figure S7. IR spectrum (neat) of compound **2** (3-[4'-(pyren-1-yl)butylamido]propyl β-D-galactopyranosyl-(1→4) β-D-glucopyranoside).

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