Supplementary Material (ESI) for Soft Matter

Supporting Information for the Manuscript Entitled

Self-assembled carbohydrate-based micelles for lectin targeting

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1. Summary of the Spherical Copolymer Micelle Model developed by Pedersen and Gerstenberg (*Macromolecules*, 1996, *13*, 1063).

The Spherical Copolymer Micelle Model describes the scattering for micelles as consisting of a homogeneous spherical core having corona chains that follow Gaussian statistics attached to the core surface as depicted in Figure S1.

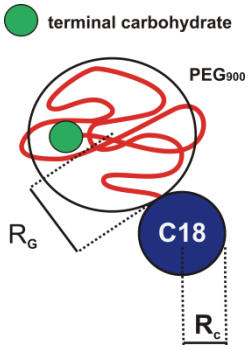


Figure S1. Schematic representation for the micellar form factor analysis according to the spherical copolymer micelle model. It considers a spherical core of radius R_c and Gaussian chains with radius of gyration R_G attached to the core.

The micellar form factor $P_{mic}(q)$ involves four terms: self-correlation of the core, self-correlation of the chains, cross term between core and chains and the cross term between different chains:

$$P_{mic}(q) = N_{agg}^2 \beta_{core}^2 F_{core}(q, R_c) + N_{agg} \beta_{chain}^2 F_{chain}(q, R_G) + N_{agg}(N_{agg} - 1)\beta_{chain}^2 S_{chain-chain}(q) + 2N_{agg}^2 \beta_{chain} \beta_{core} S_{core-chain}(q) \quad (1)$$

N_{agg} is the number of aggregation of the micelles and β_{core} and β_{chain} accounts for the excess scattering length density of the core-forming (C_{18}) and corona-forming block (PEG).

$F_{core}(q,R_c)$ is the self-correlation of a spherical core with radius R_c and it is given by the form factor amplitude of a sphere with a smoothly decaying scattering density at the surface:

$$F_{core}(q,R_c) = [\Phi(q,R_c)]^2 = \left[3\frac{\sin(qR_c) - qR_c\cos(qR_c)}{(qR_c)^3}\right]^2 \quad (2)$$

The chains self-term is described by the Debye function:

$$F_{chain}(q,R_G) = \frac{2[\exp(-q^2R_G^2) - 1 + q^2R_G^2]}{(q^2R_G^2)^2} \quad (3)$$

wherein, R_G is the radius of gyration of the Gaussian chains anchored to the core. The core-chain term is given by:

$$S_{core-chain}(q) = \psi(q,R_G)\Phi(q,R_c)\frac{\sin[q(R_c + dR_G)]}{q(R_c + dR_G)} \quad (4)$$

the function $\psi(q,R_G)$ is:

$$\psi(q,R_G) = \frac{1 - \exp(-q^2R_G^2)}{q^2R_G^2} \quad (5)$$

and $d \sim 1$ should be used in order to mimic the nonpenetration of the corona chains into the core, which is physically impossible. If $d \sim 1$, the starting point of the Gaussian chains is displaced to a value $R` \sim R_c + R_G$ away from the center of the particle.

The chain-chain term is given by:

$$S_{chain-chain}(q) = \psi^2(q,R_G)\left[\frac{\sin[q(R_c + dR_G)]}{q(R_c + dR_G)}\right]^2 \quad (6)$$

The value of β_{chain} for PEG_{900} as calculated in the following way:

$$\beta_{chain} = NV_{PEG}(\sigma_{PEG} - \sigma_{solvent}) \quad (7)$$

where N is the degree of polymerization of the polymer segment (N = 19), V_{PEG} is the volume of one PEG monomer unit, σ_{PEG} is the scattering length density of the polymer segment and $\sigma_{solvent}$ is the scattering length density of the solvent (water). The volume occupied by a single monomer unit V_{PEG} was determined by taking into account the homopolymer density (d_{PEG}) as:

$$V_{PEG} = \frac{M_{PEG}}{d_{PEG} N_A} \tag{8}$$

and the values of the scattering length densities of the solvent and monomer unit was calculated using the average chemical composition of each component and its mass density (d_x) as:

$$\sigma_x = \frac{b_e d_x N_A}{M_x} \sum_i n_i z_i \tag{9}$$

where x accounts for H_2O or PEG, N_A is the Avogadro's number, and n_i accounts for the number of atoms i in each component and z_i is the atomic number of the atom i ($n_i z_i$ is the number of electrons in each unit). Finally, b_e is the Thomson scattering length (the scattering length of an electron - $b_e = 2.817 \times 10^{-13}$ cm). All the parameters thus calculated are given in Table S1

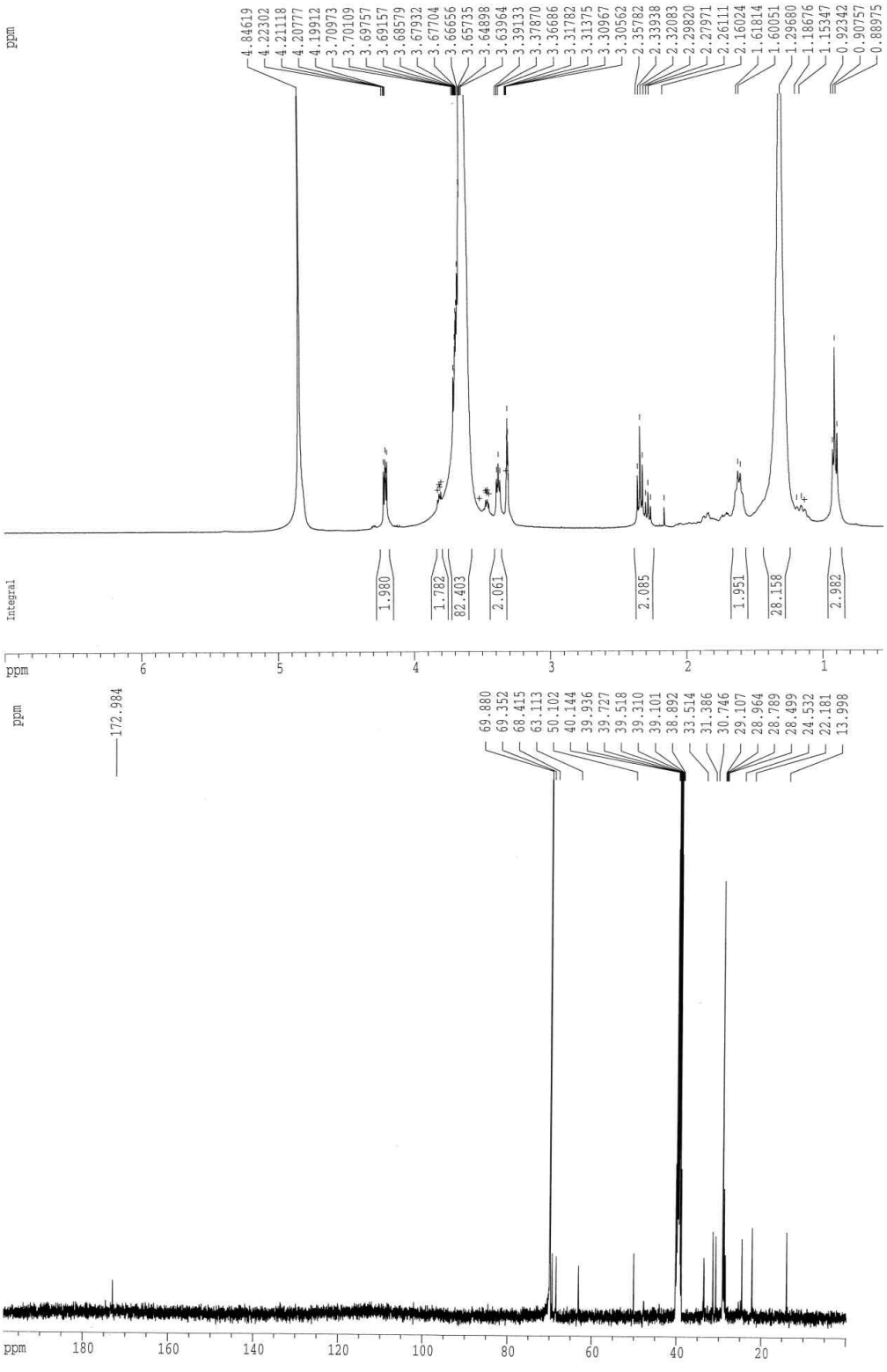
Table S1. Parameters used to determine β_{chain}

	d[a] (g/cm^3)	V (10^{-23} cm^3)	M (g/mol)	chemical composition	$\Sigma n_i z_i$	σ (10^{10} cm^{-2})
PEG	1.08	6.76	44.0	C_2H_4O	24	9.99
H_2O	1.00	2.99	18.0	H_2O	10	9.42

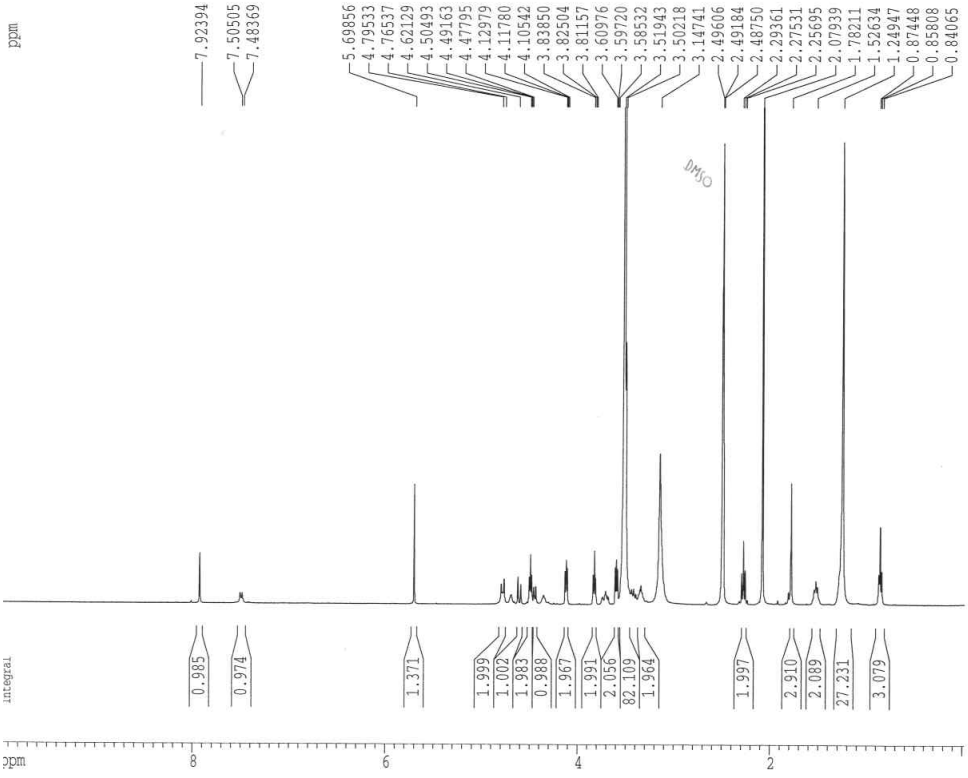
[a] values taken from reference 1.08 g/cm^3 (PEG) and g/cm^3 (H_20) from Kell Mortensen Polym. *Adv. Technol.* **2001**, 12, 2-22

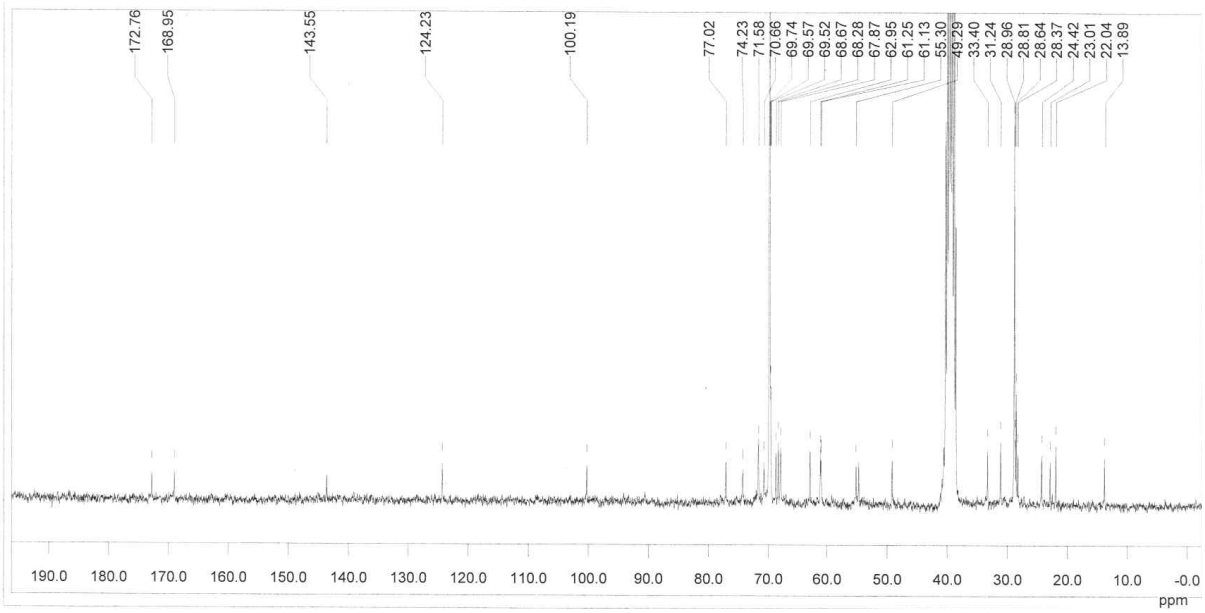
2. NMR Data

NMR spectra of Azide-PEG 900-stearate (3)



NMR spectra of *N*-acetyl-β-D-glucosaminyl-PEG 900-stearate conjugate (4)





NMR spectra of β-Lactosyl-PEG 900-stearate conjugate (5)