

Investigation of Glycofullerene Dynamics by NMR Spectroscopy

*Olof Engström,¹ Antonio Muñoz,² Beatriz M. Illescas,² Nazario Martín,² Renato Ribeiro-Viana,³
Javier Rojo,³ and Göran Widmalm^{1*}*

1. Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University,
S-106 91 Stockholm, Sweden.
2. Departamento de Química Orgánica, Facultad de Química, Universidad Complutense,
E-28040 Madrid, Spain.
3. Glycosystems Laboratory, Instituto de Investigaciones Químicas (IIQ), CSIC – Universidad de Sevilla,
Av. Américo Vespucio 49, E-41092 Seville, Spain.

*Corresponding author. Email: goran.widmalm@su.se

Electronic Supplementary Information

CONTENTS:

Figure S1	S2
Table S1	S3

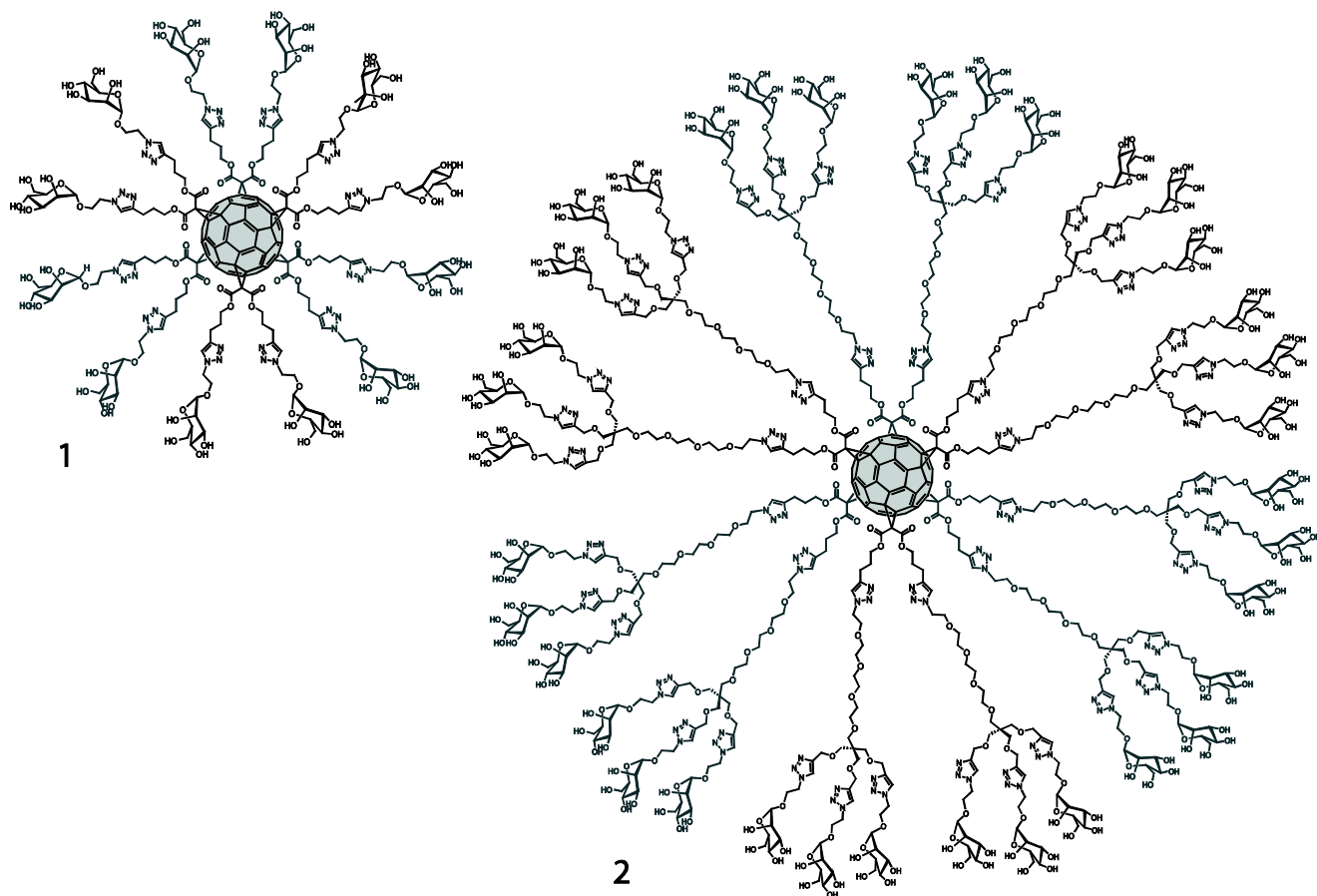


Figure S1. Schematic representation of compounds **1** and **2**.

Table S1. ^{13}C NMR relaxation parameters measured for endocyclic carbon atoms in the mannosyl unit of **1** and **2** (Expt. refers to the number of experiments carried out).

Glycofullerene 1							
	Field	Expt.	C1	C2	C3	C4	C5
NOE	11.75 T	3	1.76 $\pm$ 0.04	1.65 $\pm$ 0.03	1.62 $\pm$ 0.02	1.64 $\pm$ 0.05	1.64 $\pm$ 0.04
	14.09 T	4	1.76 $\pm$ 0.15	1.73 $\pm$ 0.04	1.60 $\pm$ 0.09	1.70 $\pm$ 0.07	1.57 $\pm$ 0.00
	16.44 T	3	1.70 $\pm$ 0.08	1.67 $\pm$ 0.09	1.57 $\pm$ 0.08	1.60 $\pm$ 0.05	1.61 $\pm$ 0.02
R_1	11.75 T	3	2.73 $\pm$ 0.07	2.91 $\pm$ 0.04	2.88 $\pm$ 0.12	2.71 $\pm$ 0.08	2.79 $\pm$ 0.08
	14.09 T	3	2.00 $\pm$ 0.21	1.97 $\pm$ 0.11	2.05 $\pm$ 0.07	2.00 $\pm$ 0.06	2.05 $\pm$ 0.10
	16.44 T	3	2.03 $\pm$ 0.04	2.06 $\pm$ 0.06	2.01 $\pm$ 0.05	2.03 $\pm$ 0.06	2.02 $\pm$ 0.05
R_2	11.75 T	2	11.22 $\pm$ 0.75	11.60 $\pm$ 1.73	12.57 $\pm$ 0.51	8.97 $\pm$ 0.32	9.73 $\pm$ 1.19
	16.44 T	4	8.88 $\pm$ 0.42	9.82 $\pm$ 0.23	10.96 $\pm$ 0.56	10.62 $\pm$ 0.25	11.33 $\pm$ 0.85

Glycofullerene 2							
	Field	Expt	C1	C2	C3	C4	C5
NOE	11.75 T	3	1.85 $\pm$ 0.02	1.85 $\pm$ 0.05	1.81 $\pm$ 0.01	1.78 $\pm$ 0.07	1.81 $\pm$ 0.05
	14.09 T	3	1.97 $\pm$ 0.05	1.86 $\pm$ 0.01	1.80 $\pm$ 0.05	1.88 $\pm$ 0.02	1.89 $\pm$ 0.01
	16.44 T	3	1.95 $\pm$ 0.04	1.82 $\pm$ 0.03	1.80 $\pm$ 0.02	1.83 $\pm$ 0.01	1.82 $\pm$ 0.04
R_1	11.75 T	5	2.60 $\pm$ 0.12	2.94 $\pm$ 0.40	3.03 $\pm$ 0.41	2.85 $\pm$ 0.37	2.87 $\pm$ 0.31
	14.09 T	4	2.40 $\pm$ 0.00	2.37 $\pm$ 0.07	2.49 $\pm$ 0.07	2.35 $\pm$ 0.04	2.39 $\pm$ 0.06
	16.44 T	3	2.02 $\pm$ 0.02	2.11 $\pm$ 0.06	2.15 $\pm$ 0.02	2.09 $\pm$ 0.02	2.10 $\pm$ 0.02
R_2	11.75 T	3	4.39 $\pm$ 0.35	5.34 $\pm$ 0.14	5.39 $\pm$ 0.20	4.75 $\pm$ 0.46	5.22 $\pm$ 0.52
	16.44 T	4	4.38 $\pm$ 0.16	4.99 $\pm$ 0.26	5.48 $\pm$ 0.33	4.74 $\pm$ 0.09	4.95 $\pm$ 0.11