Fucosylated Chondroitin Sulfates from the Body Wall of the Sea Cucumber *Holothuria forskali*. Conformation, Selectin Binding and Biological Activity.

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Supplemental material

Figure 1S: Dihedral angles during the course of MD simulation of the [→3)GalNAcβ4,6S(1→4)[Fucα2,4S (1→3)]GlcAβ(1→3)]$_4$ dodecasaccharide.

Figure 2S: Dihedral angles during the course of MD simulation of the [→3)GalNAcβ4,6S(1→4) [Fucα3,4S(1→3)]GlcAβ(1→3)]$_4$ dodecasaccharide.

Figure 3S: Dihedral angles of the sulfate groups during the course of MD simulation of fCS dodecasaccharides.

Table 1S. Dihedral angles of glycosidic linkages of fCS, CS and Le^x.

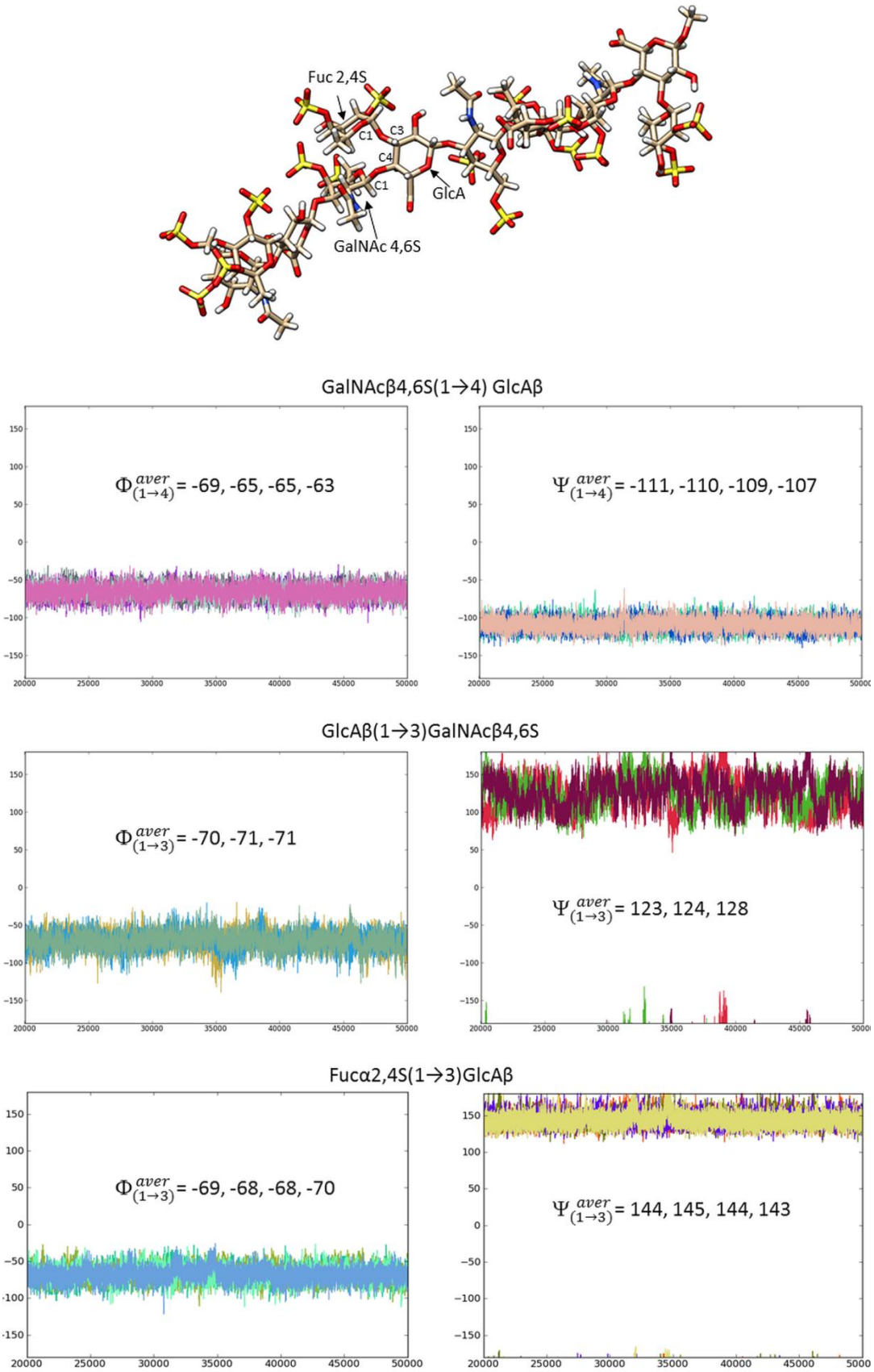

Figure 1S: Dihedral angles of the last 30,000 frames (30ns) of the MD simulation of the [→3)GalNAcβ4,6S(1→4)[Fucα2,4S(1→3)]GlcAβ(1→3)]$_4$ dodecasaccharide (closest to the average MD derive structure at the top) with GalNAc being the non-reducing residue. The average angles are given for the glycosidic bonds starting the non-reducing end. IUPAC definitions for the glycosidic $\Phi_{1\rightarrow X}$= O_5-C_1-O-C'$_X$ and $\Psi_{1\rightarrow X}$= C_1-O-C_X-C'$_{(X+1)}$ angles were used.

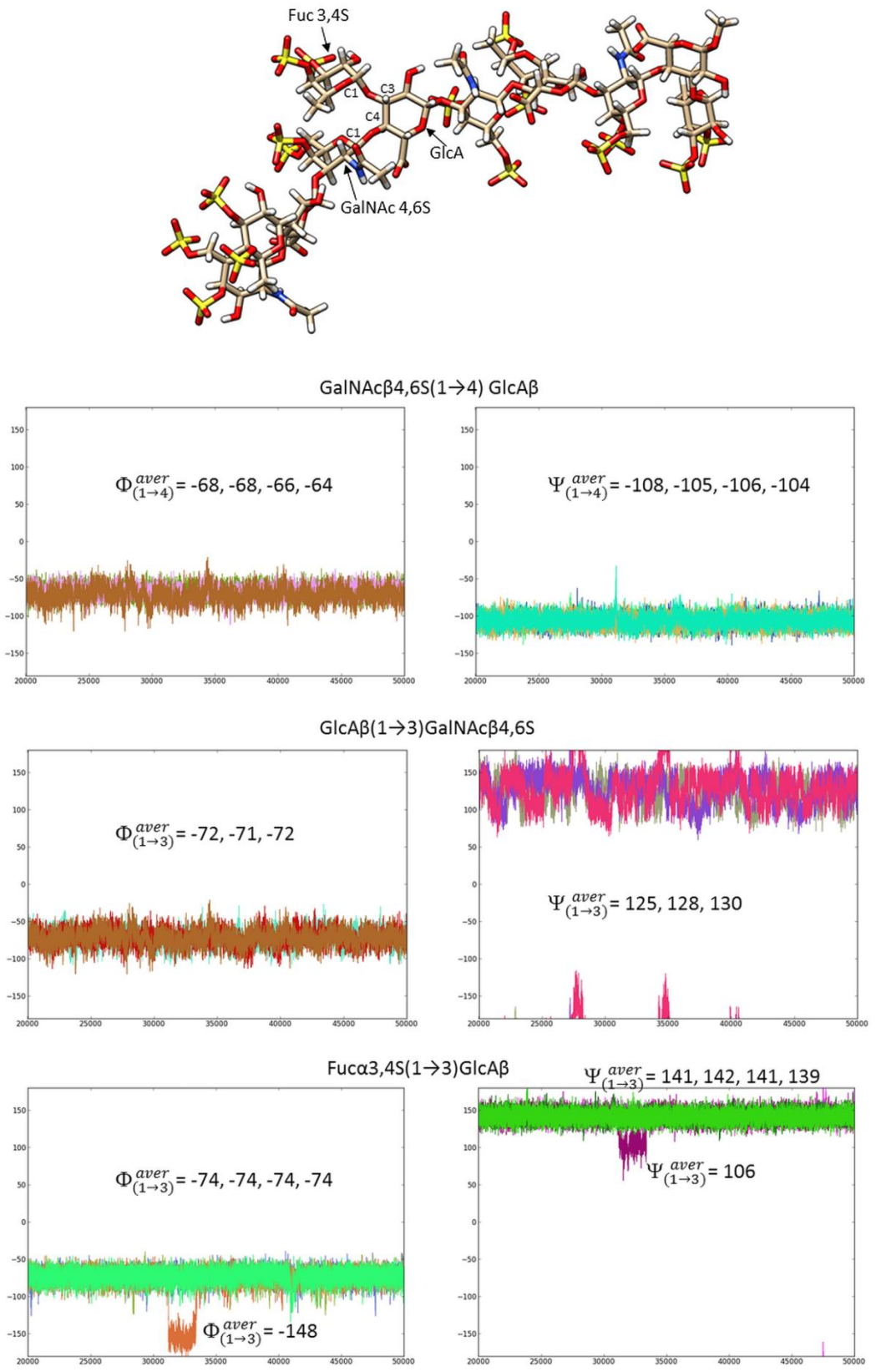

Figure 2S: Dihedral angles of the last 30,000 frames (30ns) of the MD simulation of the [→3)GalNAcβ4,6S(1→4) [Fucα3,4S(1→3)]GlcAβ(1→3)]$_4$ dodecasaccharide (closest to the average MD derive structure at the top) with GalNAc being the non-reducing residue. The average angles are given for the glycosidic bonds starting the non-reducing end. IUPAC definitions for the glycosidic $\Phi_{1\rightarrow X}$= O_5-C_1-O-C'$_X$ and $\Psi_{1\rightarrow X}$= C_1-O-C_X-C'$_{(X+1)}$ angles were used.

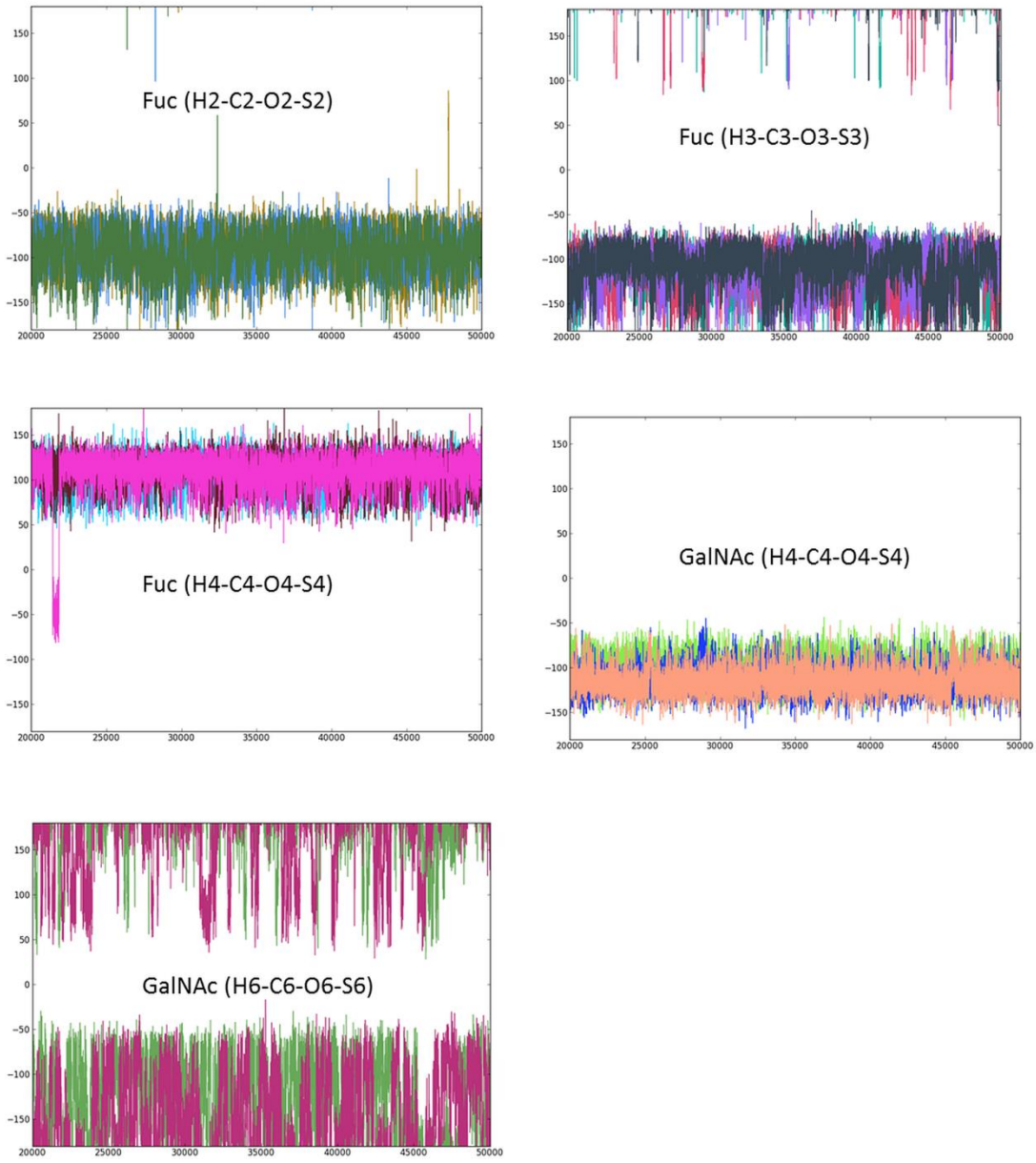

Figure 3S: Dihedral angles of the sulfate groups over the last 30,000 frames (30ns) of the MD simulation of the fCS dodecasaccharides. Only C6-sulfates show considerable rotational freedom.

Table 1S. Dihedral angles of glycosidic linkages of fCS, CS and Le^x

Structure	dp[a]	Dihedral angle	β(1→4)	β(1→3)	α(1→3)
MD	8	Φ	**-66**[b]	**-71**[c]	**-69**[d]
		Ψ	**-107**[b]	**126**[c]	**144**[d]
CS-ol	5	Φ	-67[e]	-61[f]	-
		Ψ	-124[e]	109[f]	-
de4S-CS	6	Φ	-73[g]	-72[h]	-
		Ψ	-117[g]	108[h]	-
X-ray CS fibre	4	Φ	-98	-80	-
		Ψ	-174	107	-
X-ray chondroitinase B CS complex	4	Φ	-69	-86[i]	-
		Ψ	-108	103[i]	-
[j]Le^x	2	Φ	-66	-	-73
		Ψ	-105	-	149
[k]X-ray Le^x	2	Φ	-76	-	-75
		Ψ	-106	-	139

[a] degree of depolymerisation of the main chain

[b] this work, average over 4 linkages of fCS-**I** (Fuc 3,4) and fCS-**II** (Fuc 3,4) dodecasaccharide

[c] this work, average over 3 linkages of fCS-**I** (Fuc 3,4) and fCS-**II** (Fuc 3,4) dodecasaccharide

[d] this work, average over 4 linkages of fCS-**II** (Fuc 3,4) dodecasaccharide

[e] reduced pentasaccharide, average over 2 linkages (ref. 59)

[f] reduced pentasaccharide, the inner linkage linkages (ref. 59)

[g] average over 2 linkages (ref. 60)

[h] average over 3 linkages (ref. 60)

[I] average of 2 linkages (ref. 62)

[j] RDC based structure (ref. 58)

[k] average over two similar conformations (ref. 53)