

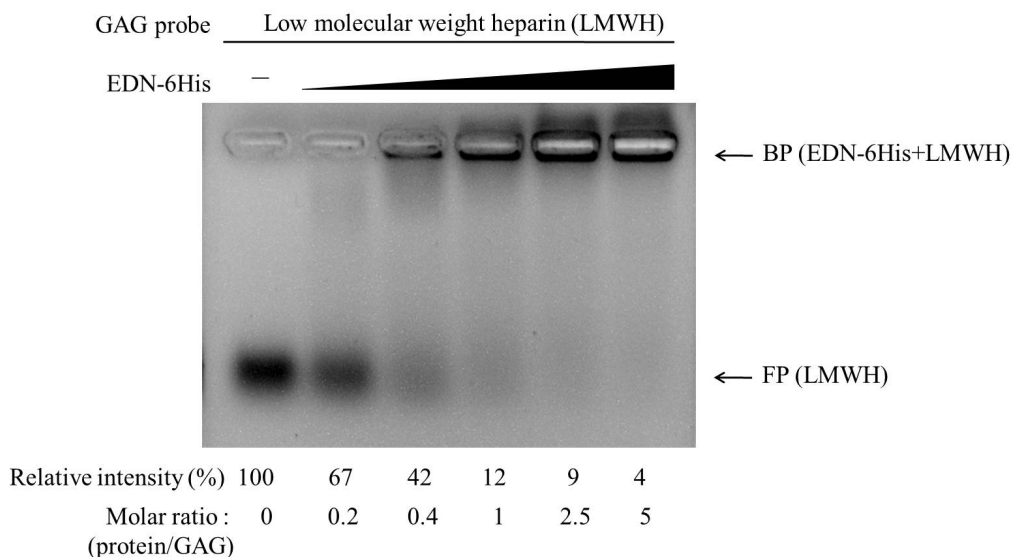
Supplementary Information

Table S1. Predicted interaction between wild type EDN and heparin hexasaccharide

Residue	Atom/group	Type of interaction	Residue	Atom/group
Lys ¹	α -NH ₃ ⁺	H-bond/Ionic	IDS6	Oxygen of 2- <i>O</i> -sulfate
Trp ⁷	C-4	vDW	SGN5	Oxygen of <i>N</i> -sulfate
	C-5	vDW	SGN5	C-1
Trp ¹⁰	N-1	H-bond	SGN5	Oxygen of 3-OH
Gln ¹⁴	Amide NH ₂	vDW	IDS4	Oxygen of 2- <i>O</i> -sulfate
	Amide NH ₂	vDW	SGN5	Nitrogen, hydrogen, and oxygen of <i>N</i> -sulfonyl group
His ¹⁵	Hydrogen of τ -nitrogen	H-bond	SGN5	Oxygen of <i>N</i> -sulfonyl group
	C-2	vDW	IDS4	Oxygen of 2- <i>O</i> -sulfate
Gln ³⁴	Carbon of side-chain amide group	vDW	IDS6	Ring oxygen
Arg ³⁶	δ - and ω -Nitrogen	H-bond/Ionic	IDS6	Oxygen of C-6 carboxyl group
	ω -Nitrogen	Ionic	SGN1	Oxygen of <i>N</i> -Sulfonyl group
	C-5	vDW	SGN1	Oxygen of <i>N</i> -Sulfonyl group
Lys ³⁸	ϵ -NH ₃ ⁺ group	Ionic	SGN1	Oxygen of <i>N</i> -Sulfonyl group
	Hydrogen of ϵ -NH ₃ ⁺ group	vDW	SGN1	Oxygen of C3-OH group
Asn ³⁹	Hydrogen of side-chain amide group	vDW	SGN1	Oxygen of sulfonyl group
Gln ⁴⁰	C-3	vDW	IDS2	C-1
	C-4	vDW	IDS2	C-1 and oxygen of 2- <i>O</i> -sulfonyl group
	Nitrogen of side-chain amide group	vDW	IDS2	C-1, C-5, and C-6
	Nitrogen of side-chain amide group	H-bond	IDS2	Ring oxygen
His ¹²⁹	C-5	vDW	IDS4	C-4
	C-5	vDW	SGN5	C-1
Leu ¹³⁰	C-1	vDW	IDS4	Hydrogen of C-3-OH
	Backbone carbonyl oxygen	H-bond	IDS4	C-3-OH
Arg ¹³²	ω -Nitrogen	Ionic	SGN3	<i>N</i> -sulfate
	ω -Nitrogen	Ionic	IDS2	2- <i>O</i> -sulfate

H-bond, hydrogen bond; vDW, van der Waals force; SGN, 6-*O*-sulfated, *N*-sulfated glucosamine; IDS, 2-*O*-sulfated iduronic acid.

Figure S1. Binding activity of recombinant EDN-6His to low molecular weight heparin (LMWH). FACE was carried out by incubating 2-aminoacridone (AMAC)-labeled LMWH (0.33 nmol) with or without increasing concentrations of proteins in PBS at 25 °C for 15 min, and the reaction products were separated on a 1% agarose gel. The reacted probe and protein were shown above the gel, and the numbers below the gel indicated the relative intensity (%) of free probe and the molar ratio of protein to LMWH. FP, free probe; BP, bound probe.



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