Supporting information

Importance of topology for glycoclusters binding to *Pseudomonas aeruginosa* and *Burkholderia ambifaria* bacterial lectins

Caroline Ligeour, Lucie Dupin, Anthony Angeli, Gérard Vergoten, Sébastien Vidal, Albert Meyer, Eliane Souteyrand, Jean-Jacques Vasseur, Yann Chevolot and François Morvan

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Table S1. HPLC retention time (Rt) and MALDI-TOF mass spectrometry data for glycoclusters.

Glycoclusters	Sequence	Rt (min)[a]	MALDI-TOF MS[b]	
			m/z calc.	*m/z* exp.
G1a	3	13.99	7116.22	7117.87
G1b	3	15.49	7116.22	7115.60
G1c	4	14.82	7116.22	7116.09
G2a	4	13.95	7296.38	7296.91
G2b	2	15.56	7296.38	7295.40
G2c	2	14.88	7296.38	7295.70
G3a	1	13.63	7954.82	7954.15
G3b	1	13.56	8255.08	8255.32
G3c	1	13.04	10287.03	10287.83
F1a	3	14.35	7017.25	7017.66
F1b	3	16.31	7017.25	7018.39
F1c	4	15.22	7017.25	7018.91
F2a	4	14.48	7197.41	7198.35
F2b	2	15.85	7197.41	7196.50
F3c	2	15.30	7197.41	7198.14
F3a	1	15.69	7789.88	7790.87
F3b	1	15.98	8090.14	8089.61
F3c	1	16.17	9957.15	9956.71

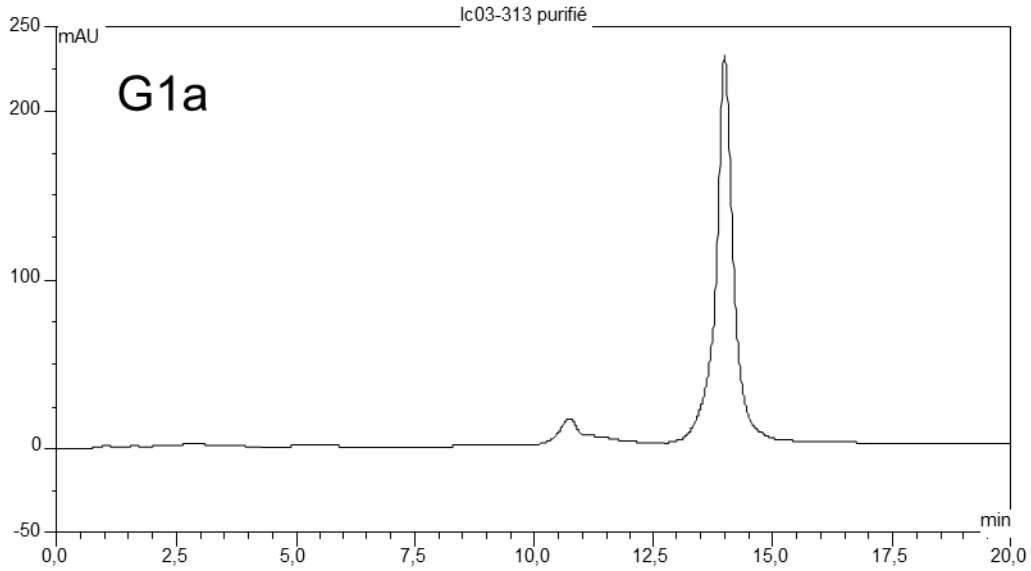
#	Sequence
1	5'-CTG CCT CTG GGC TCA-3'
2	5'-GCT CTC CAC TGC TGG-3'
3	5'-GCT TGG TGC CTC CAC-3'
4	5'-TGC CAC CTC GCT TGG-3'

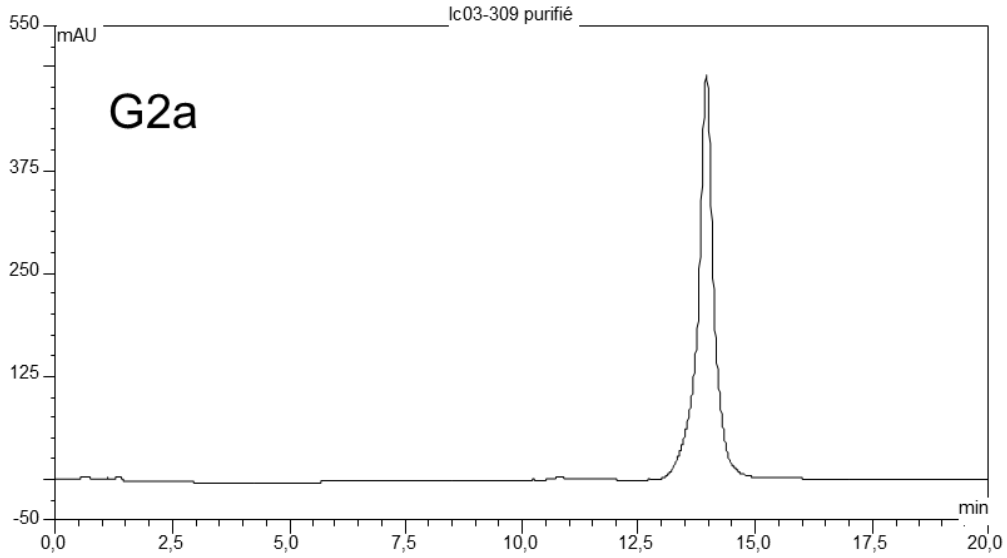
[a]Linear gradient from 0 to 32% of acetonitrile in 50 mM TEAAc buffer, pH 7.0 in 20 min. [b]HPA matrix with 10% ammonium citrate.

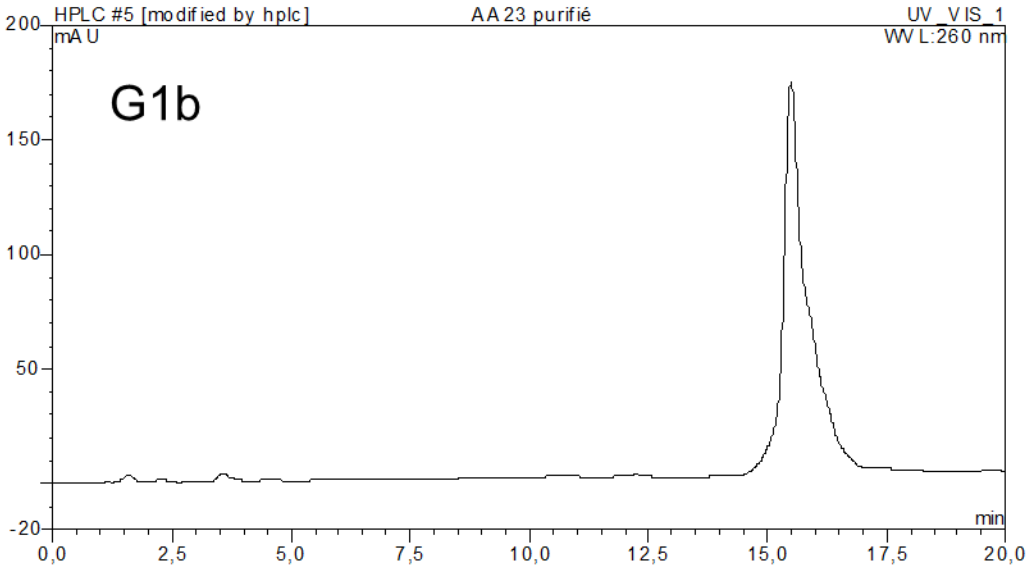
Table S2: K_d values and coefficient of determination (r^2) of the DNA-glycoclusters towards LecA, LecB or BambL determined by DNA Directed Immobilization glycoarray.

Glycoclusters		LecA		LecB		BambL	
		K_d (nM)	r^2	K_d (nM)	r^2	K_d (nM)	r^2
G1a	riboPro	66	0.998	/	/	/	/
G2a	riboEG_2M	54	0.998	/	/	/	/
G1b	araPro	64	0.998	/	/	/	/
G2b	araEG_2M	62	0.995	/	/	/	/
G1c	xyloPro	54	0.995	/	/	/	/
G2c	xyloEG_2M	49	0.996	/	/	/	/
G3a	mannipro	66	0.998	/	/	/	/
G3b	manniEG_2M	78	0.998	/	/	/	/
G3c	manni2	50	0.999	/	/	/	/
F1a	riboPro	/	/	56	0.987	20.1	0.997
F2a	riboEG_2M	/	/	73	0.987	21.2	0.993
F1b	araPro	/	/	81	0.937	25.1	0.996
F2b	araEG_2M	/	/	76	0.993	29.6	0.997
F1c	xyloPro	/	/	62	0.988	20.5	0.998
F2c	xyloEG_2M	/	/	93	0.967	26.5	0.999
F3a	manniPro	/	/	91	0.986	22.8	0.998
F3b	manniEG_2M	/	/	95	0.986	18.2	0.997
F3c	manni2	/	/	84	0.972	13.8	0.997

HPLC profiles of purified oligonucleotide-glycoclusters



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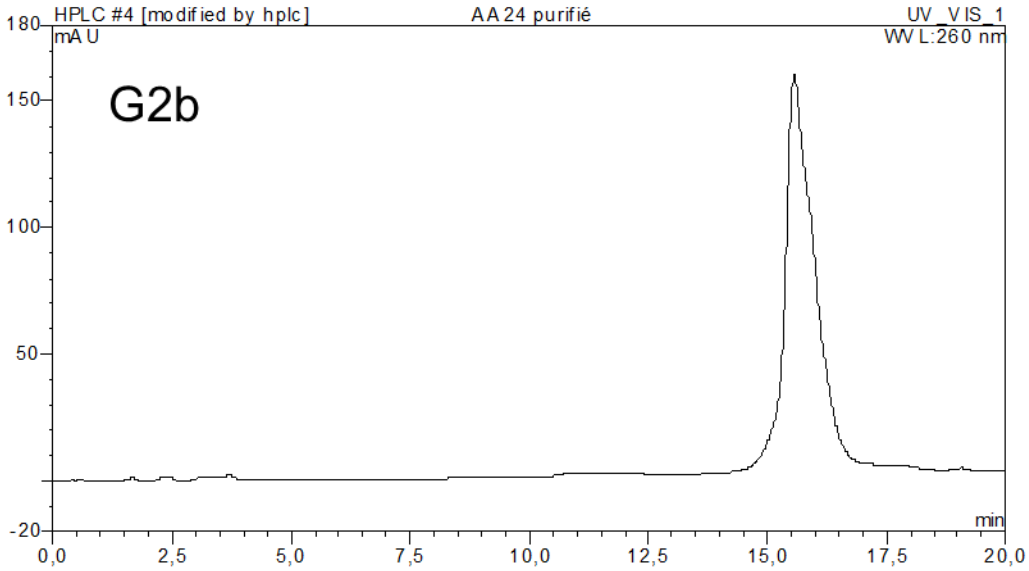
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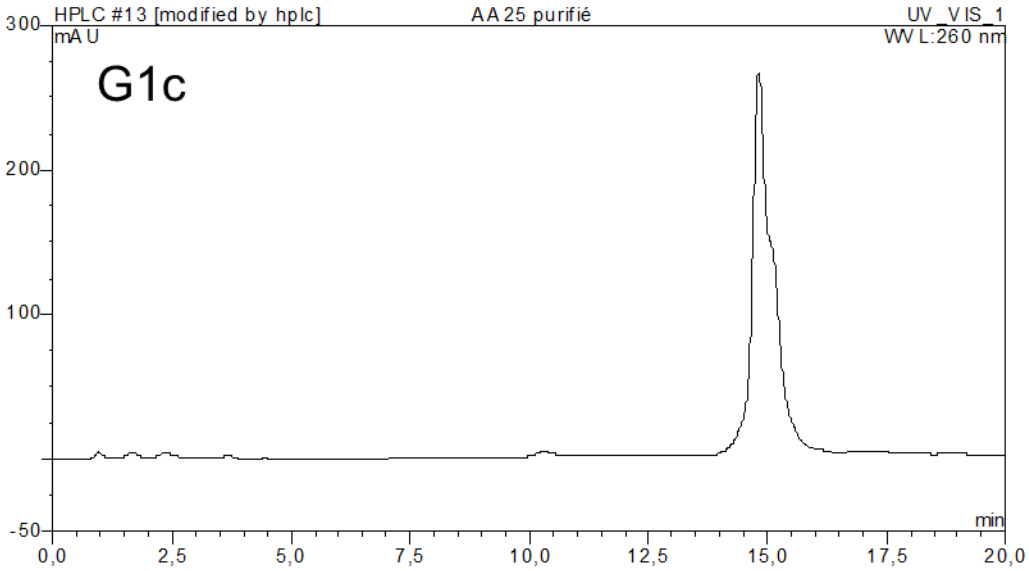
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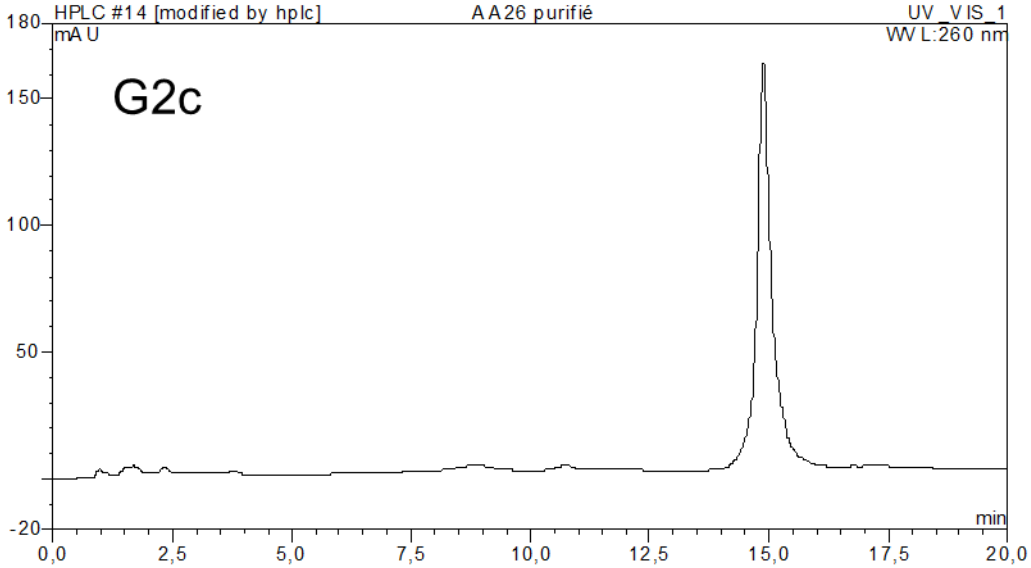
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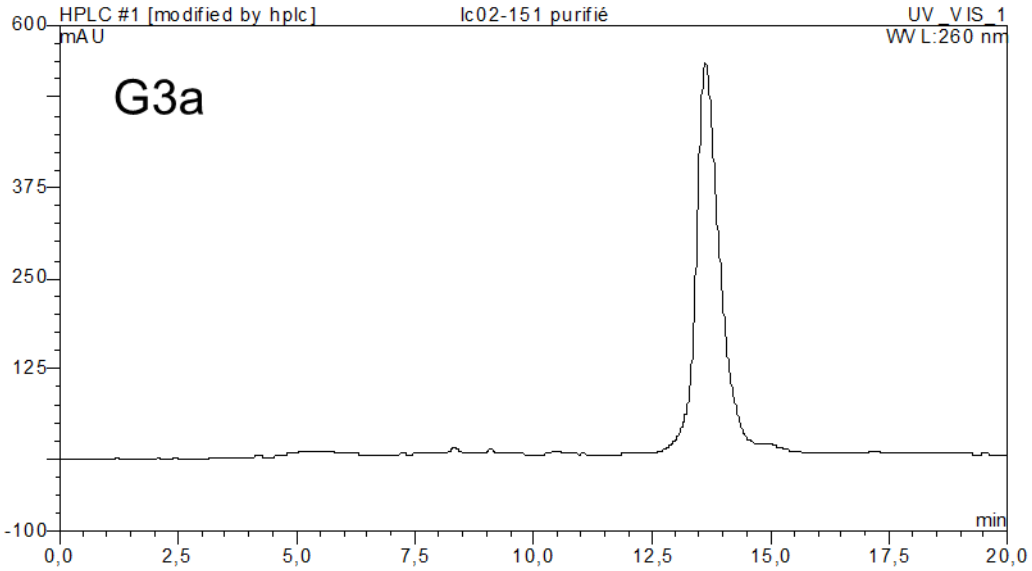
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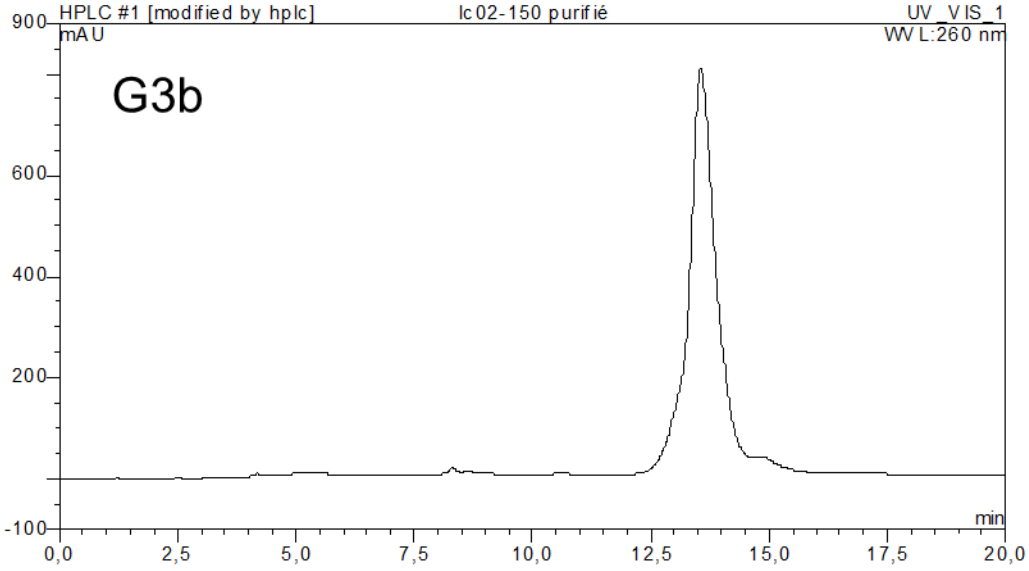
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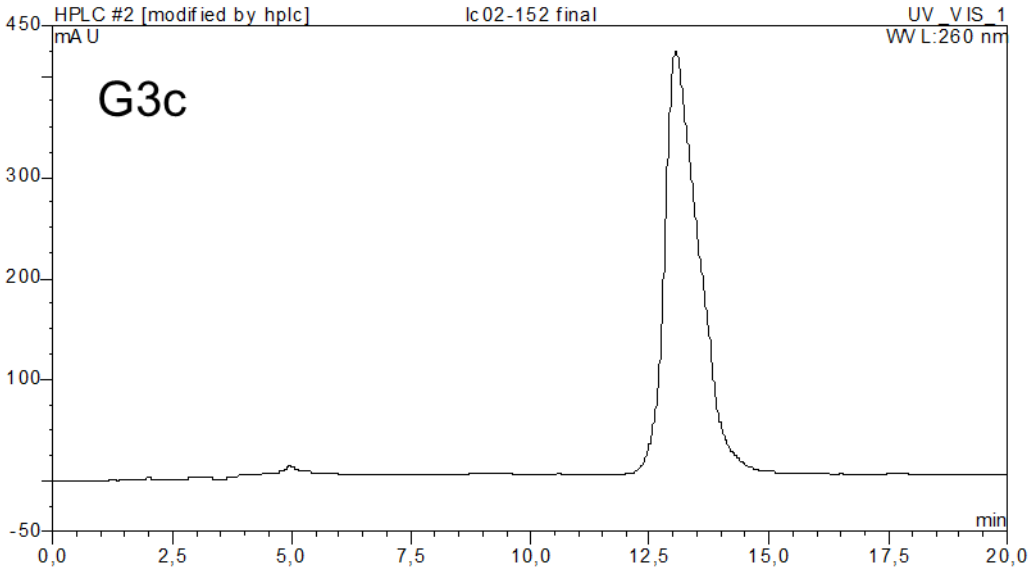
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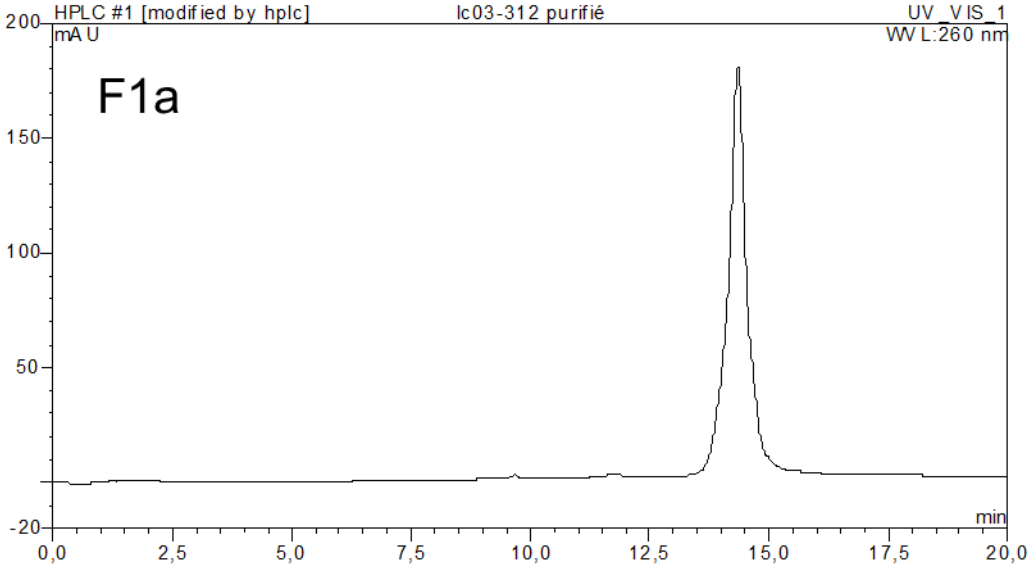
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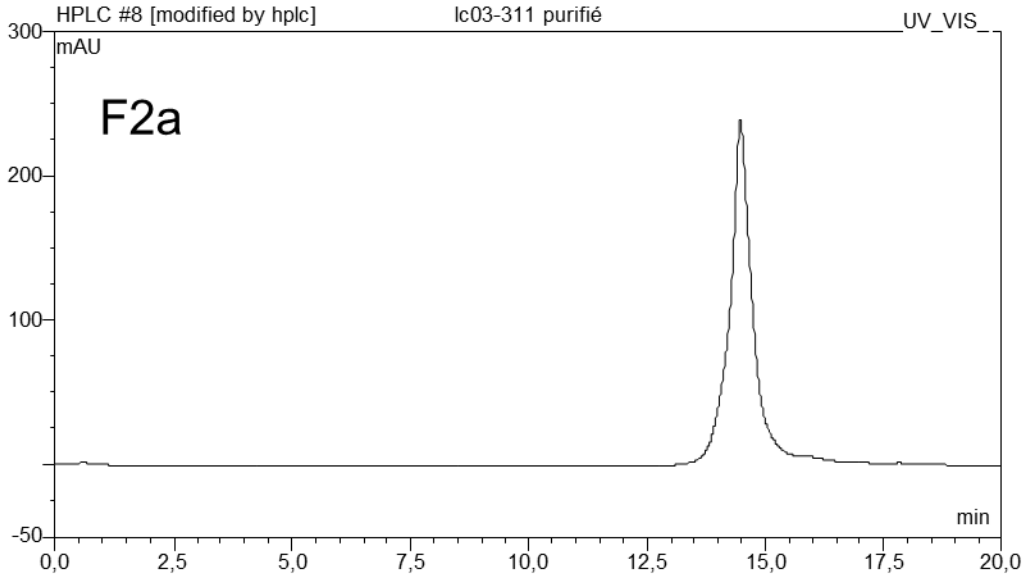
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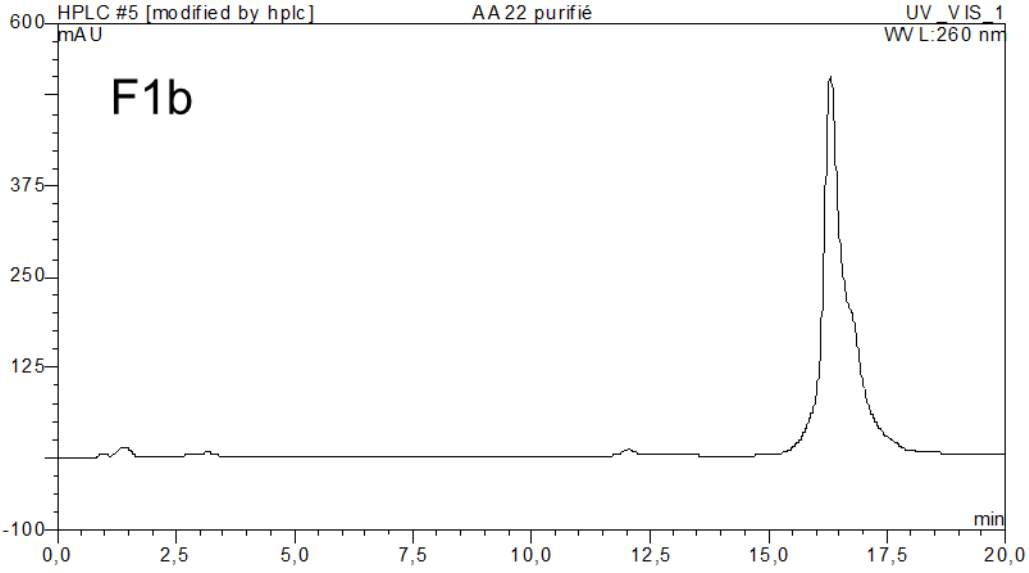
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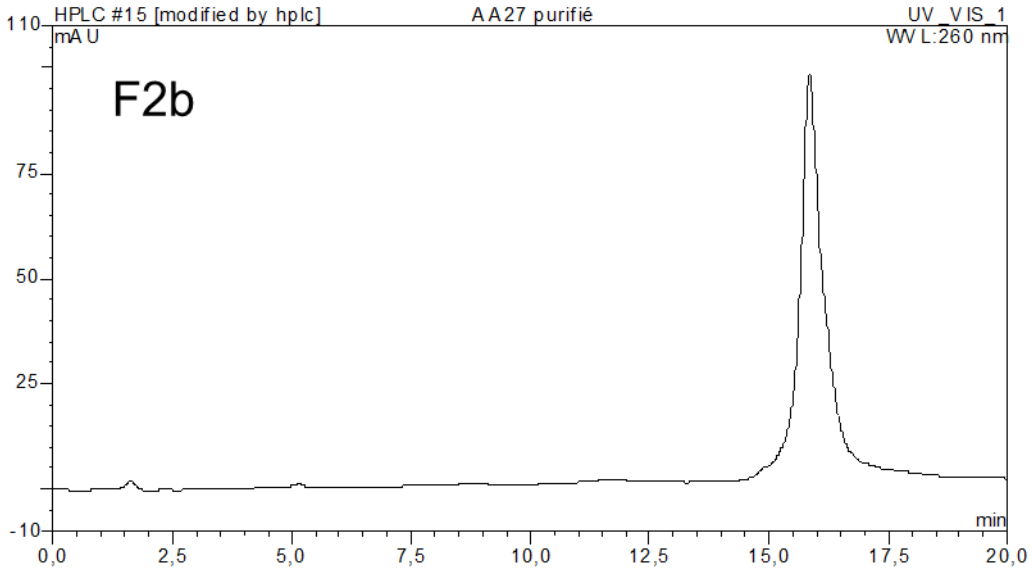
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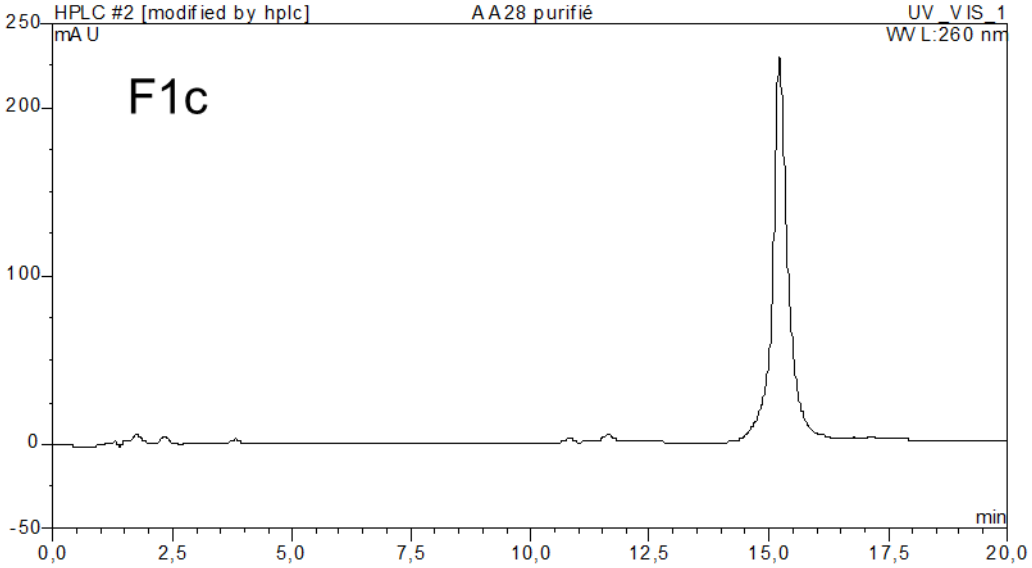
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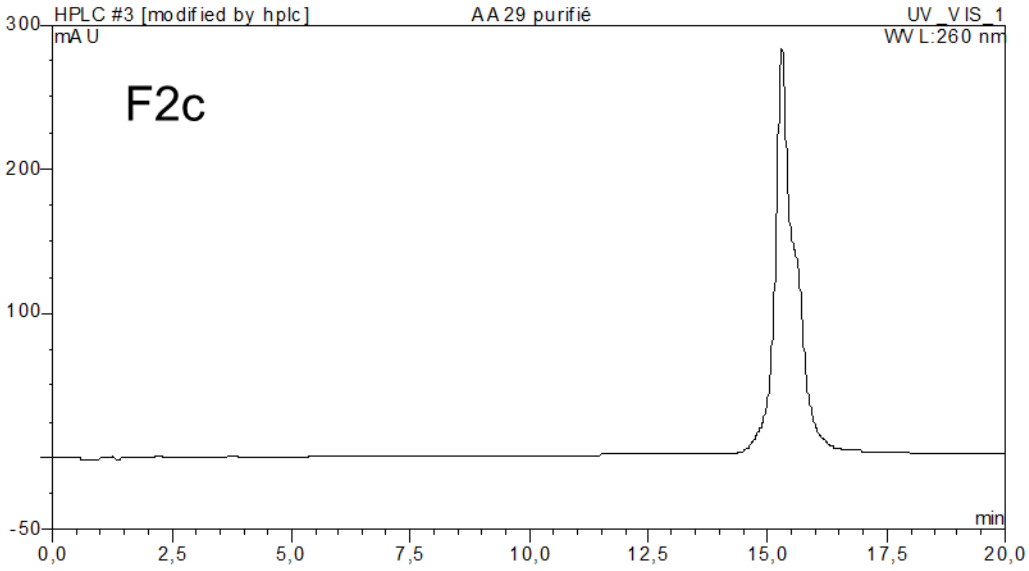
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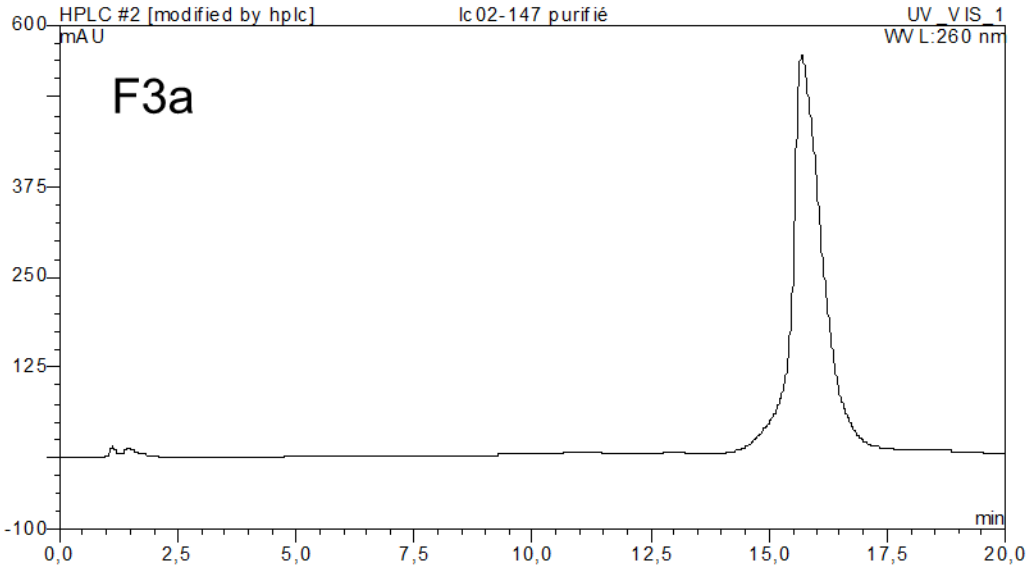
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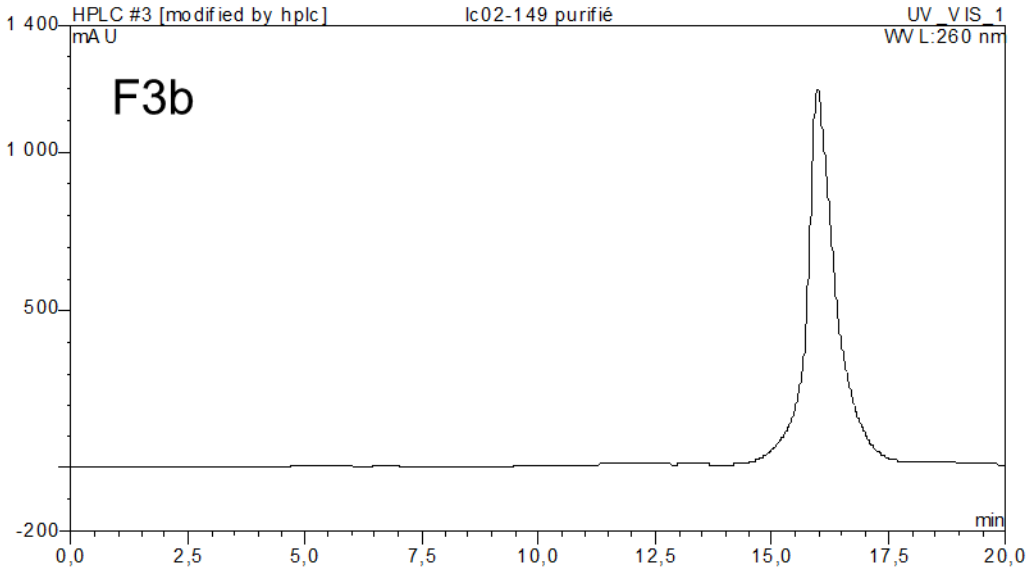
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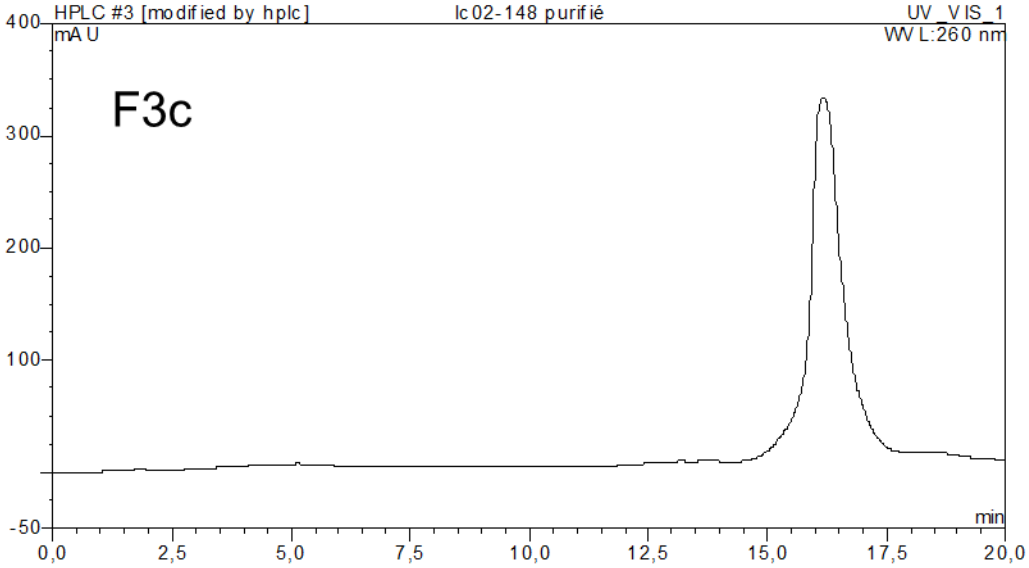
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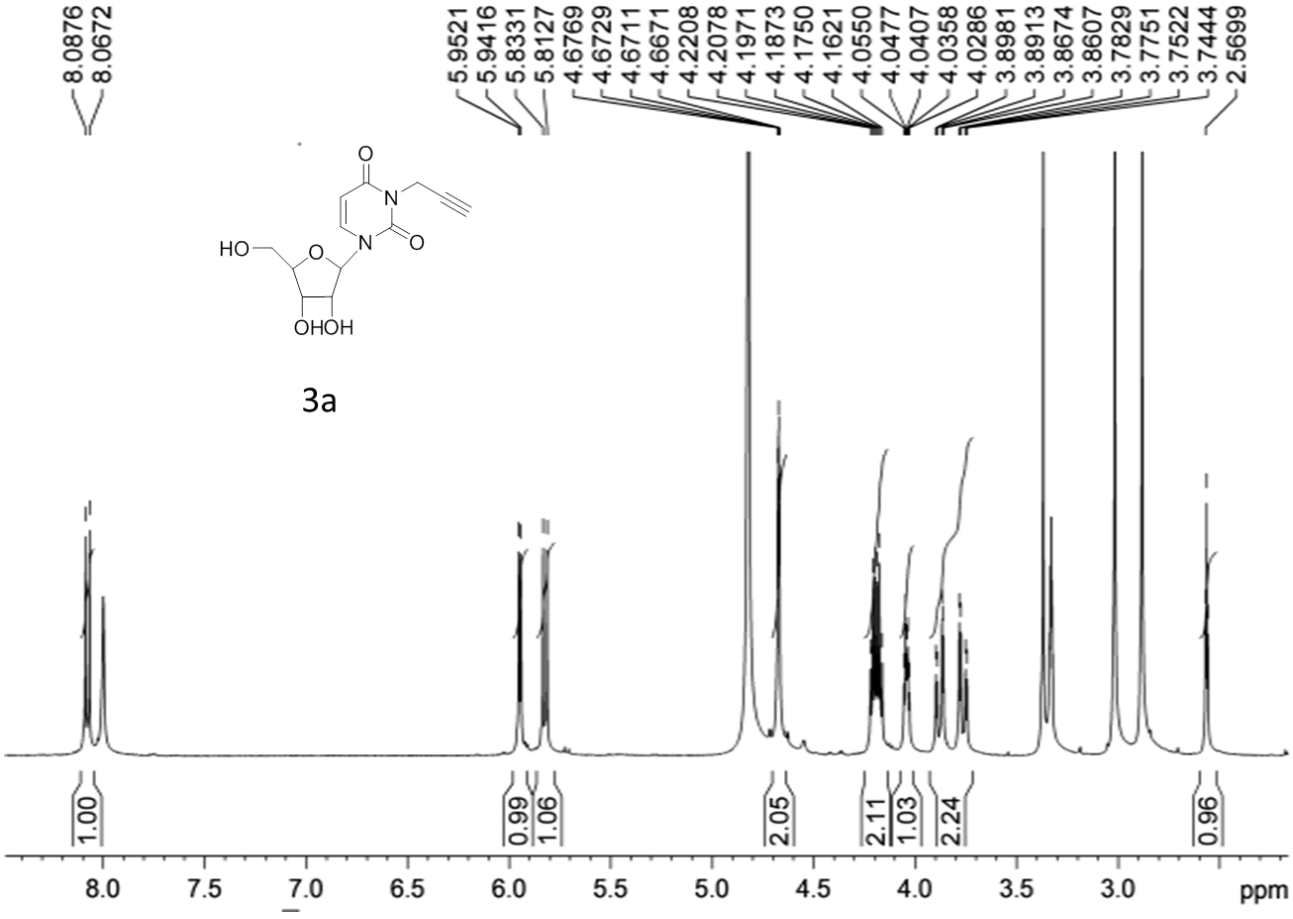
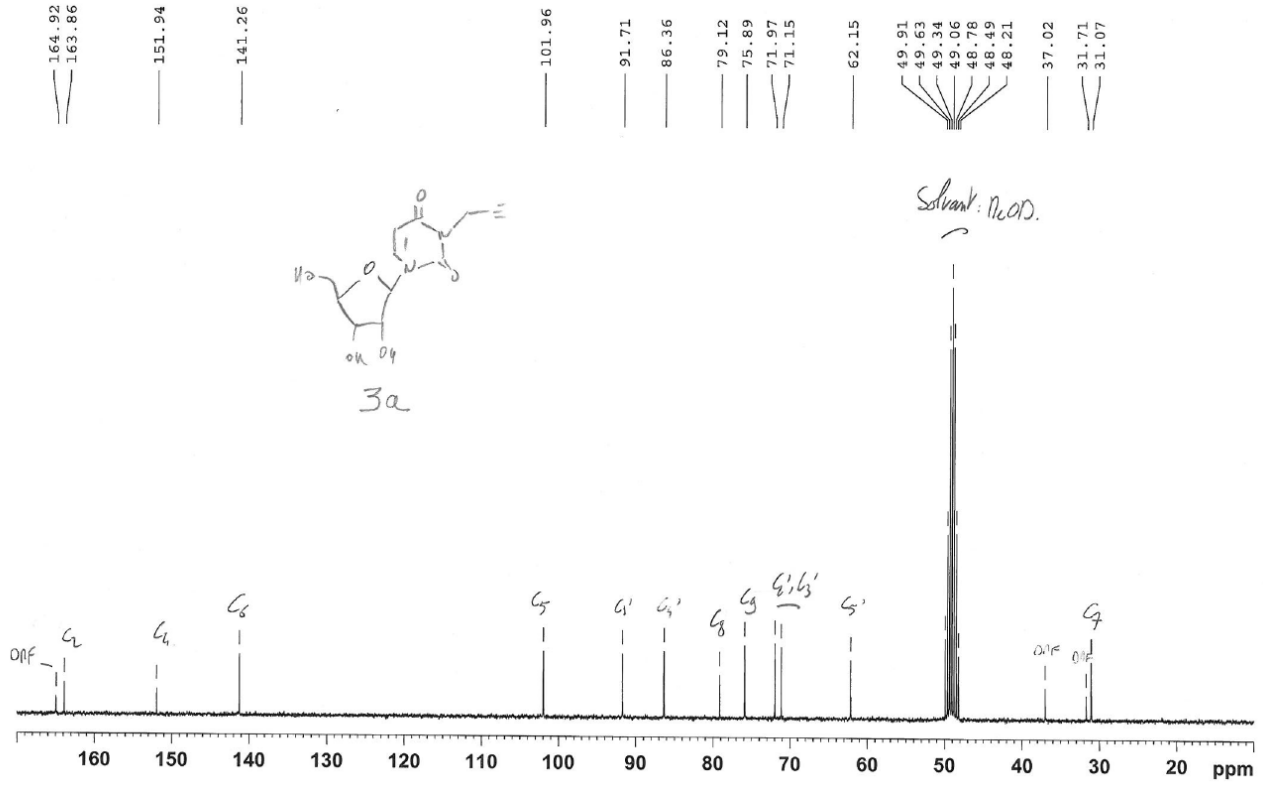
^{1}H NMR of compound **3a**



^{13}C NMR of compound **3a**



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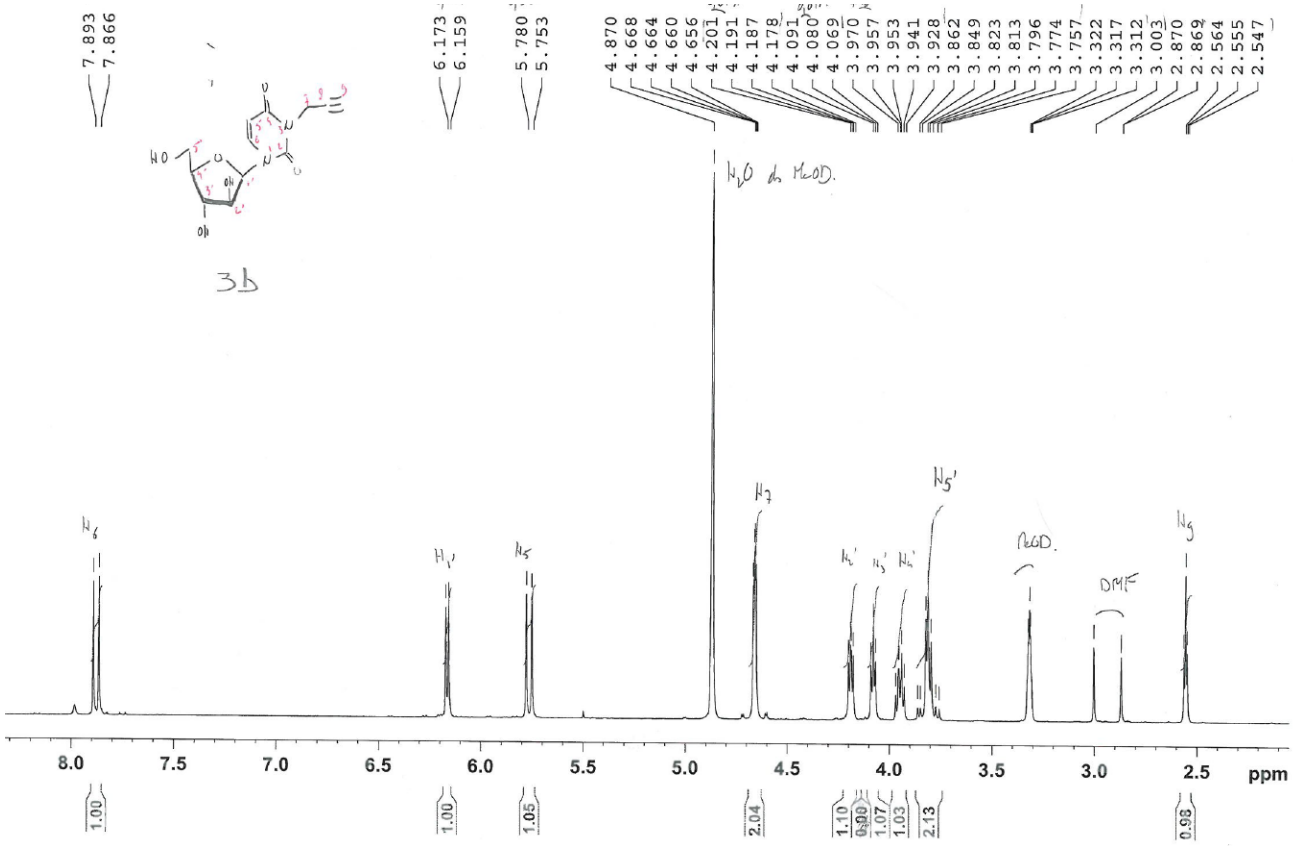

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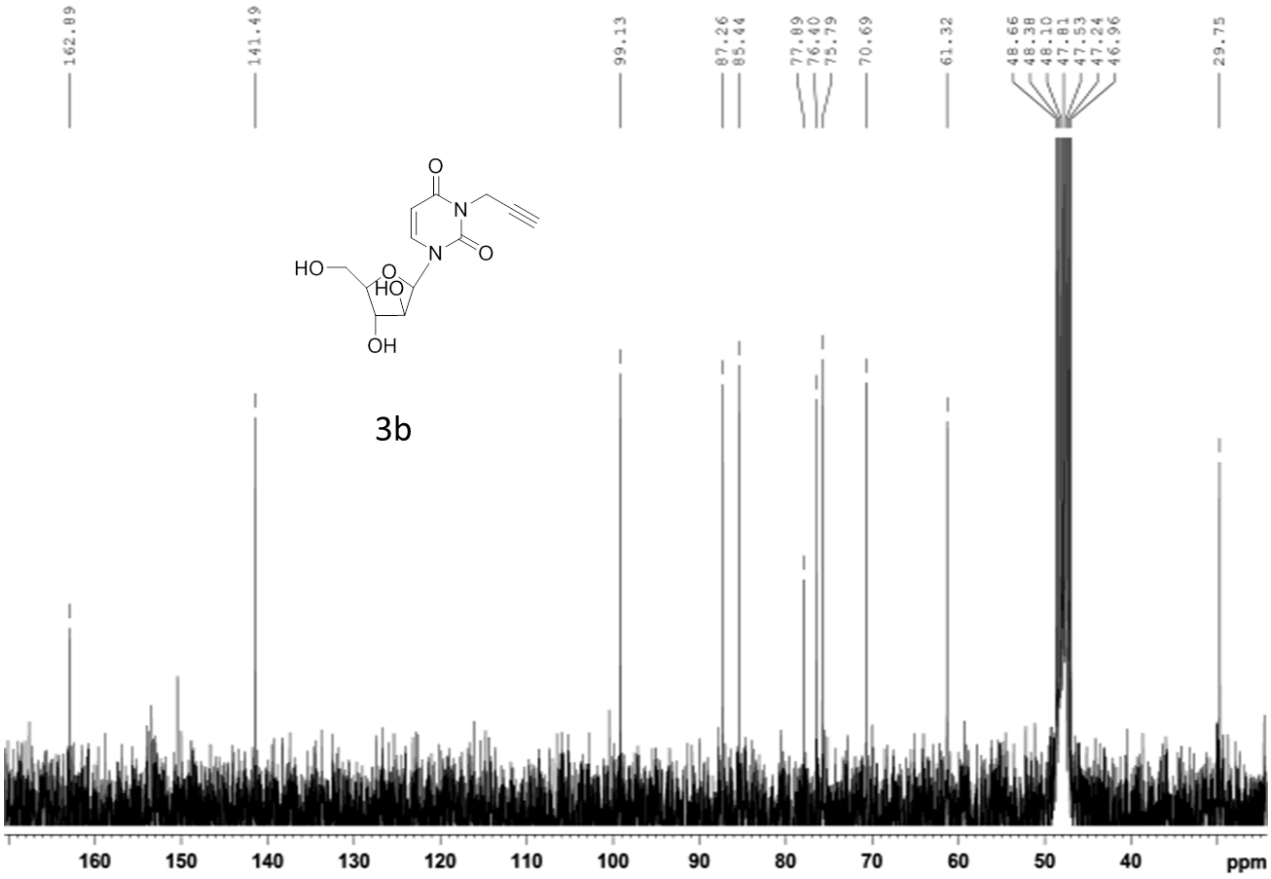
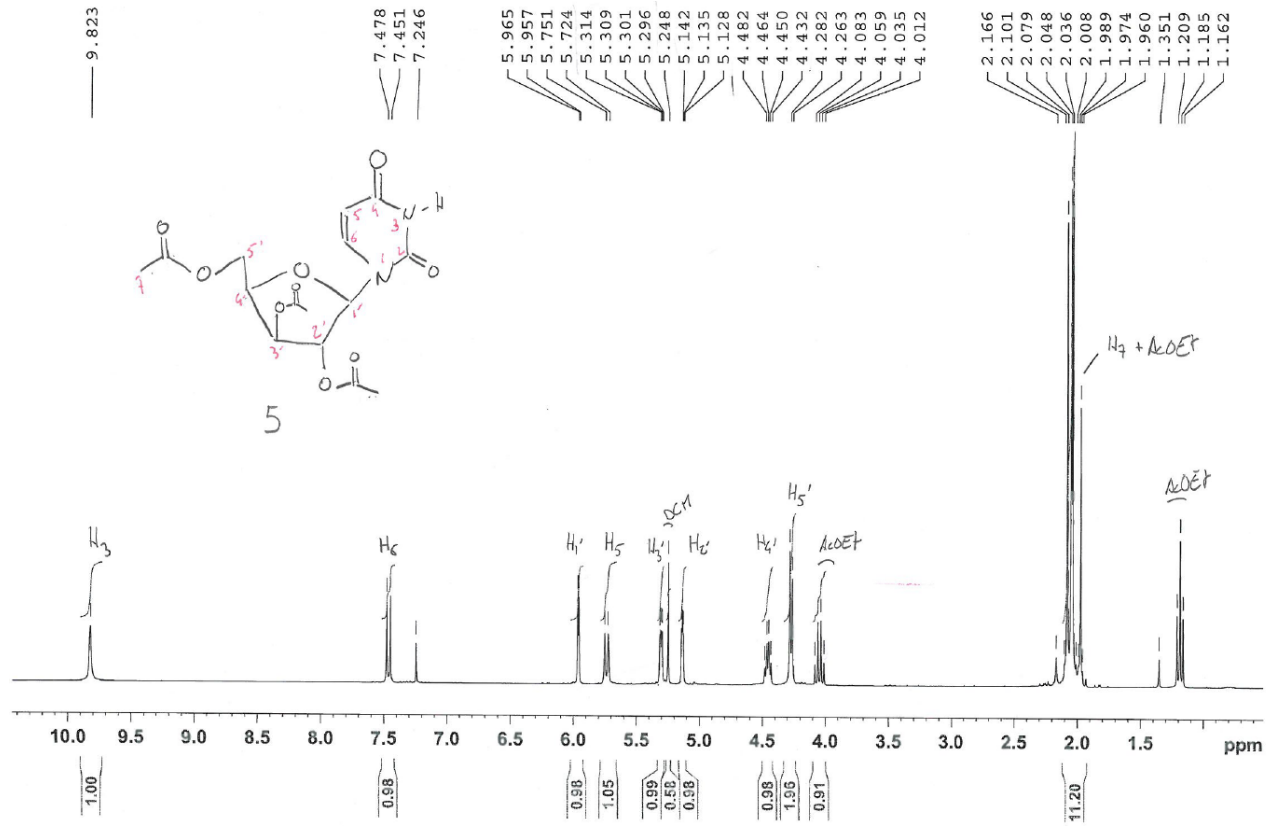


^{1}H NMR of compound **5**



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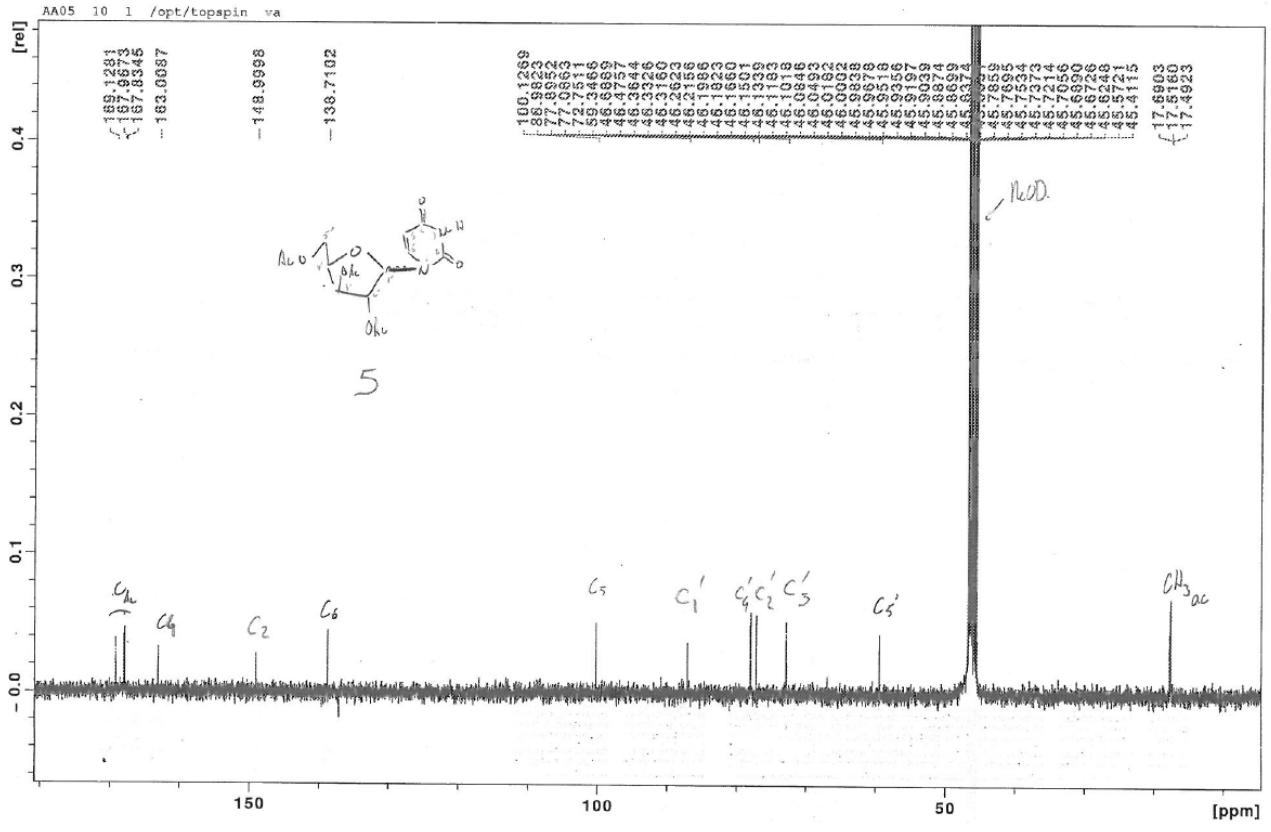
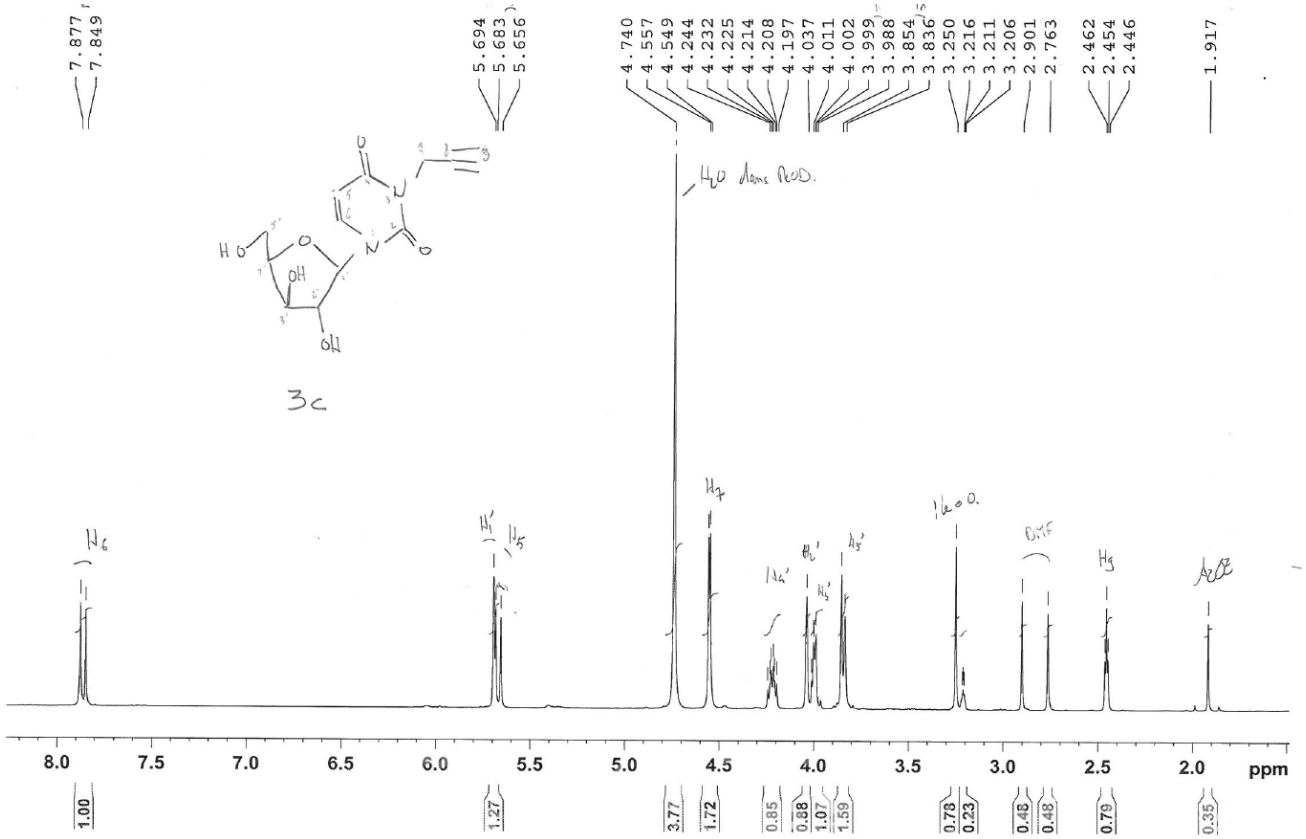
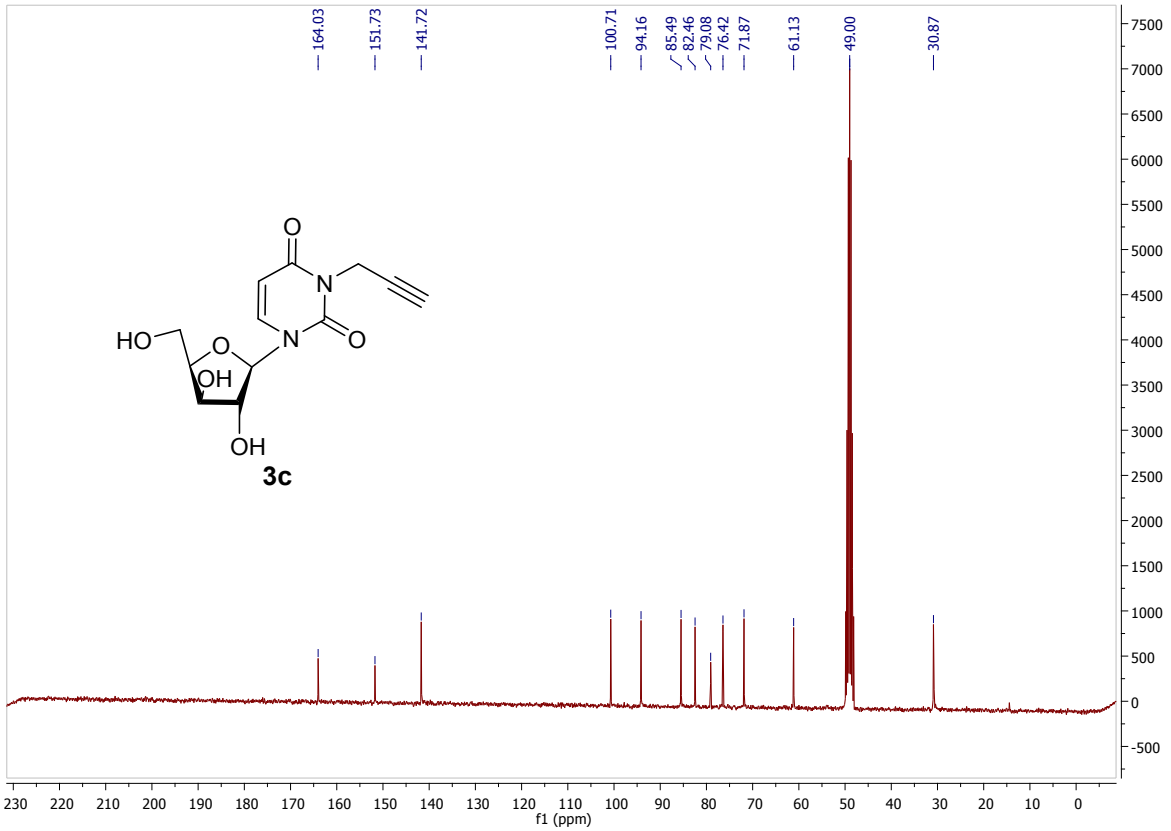


^{1}H NMR of compound **3c**



^{13}C NMR of compound **3c**



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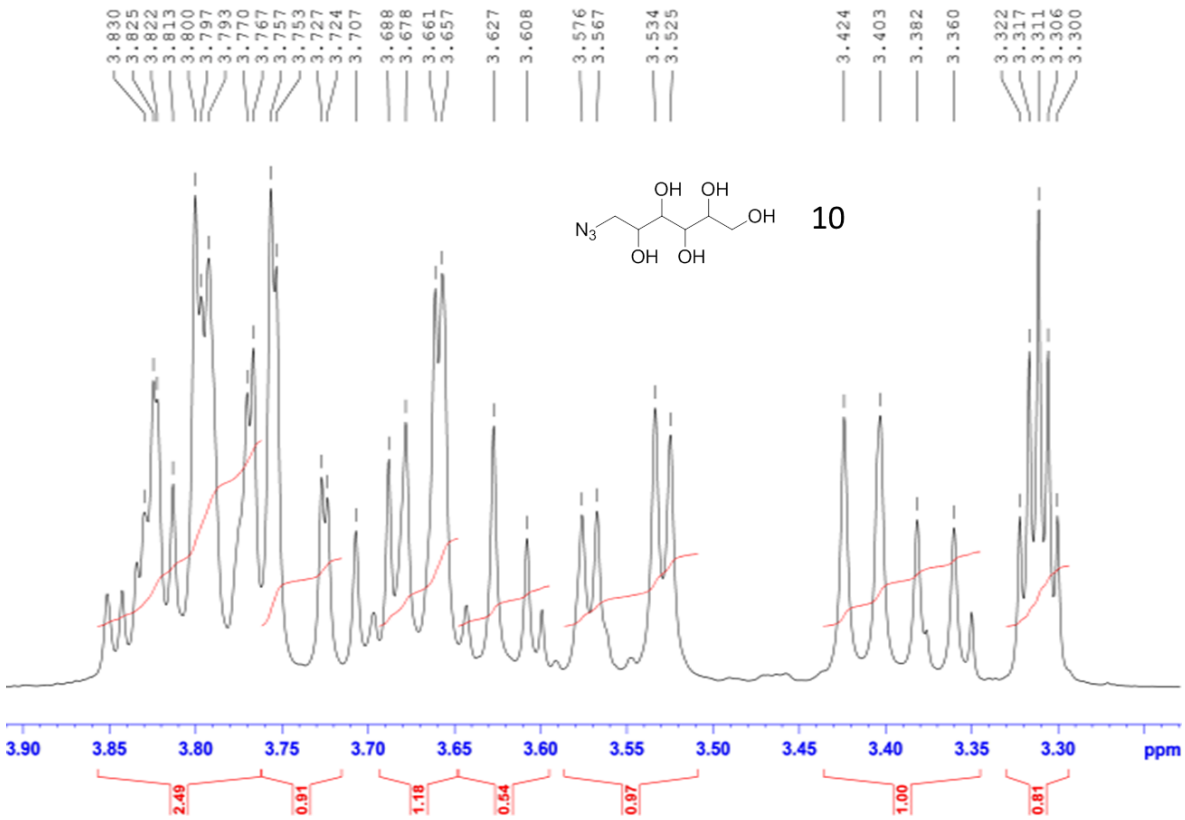

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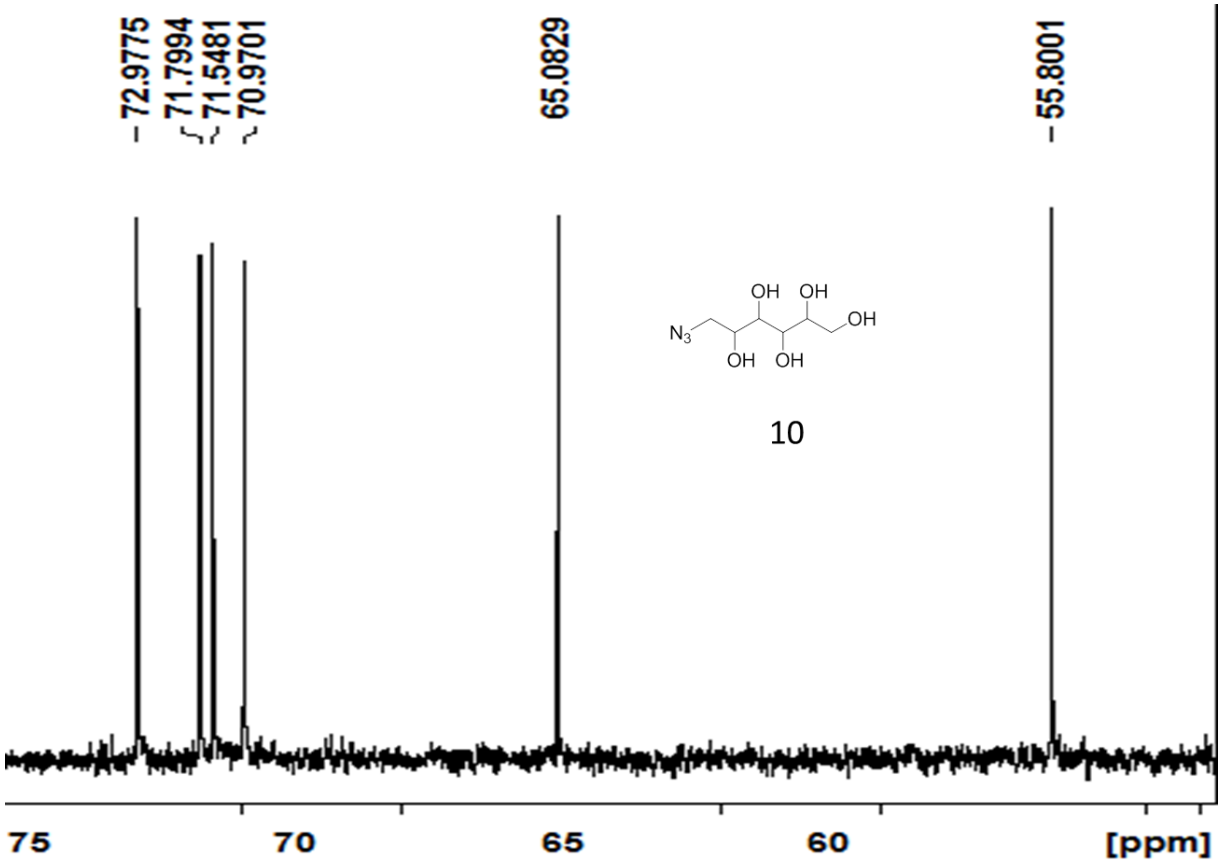

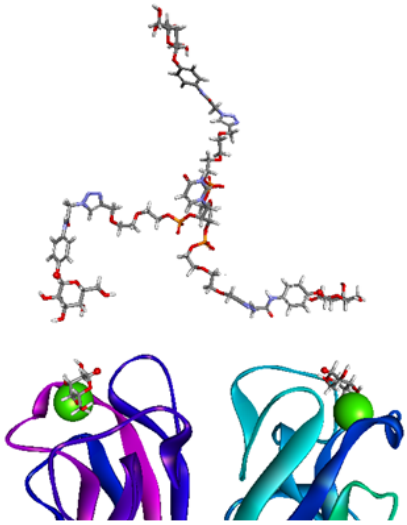

Figure S1. LecA + **G2b**

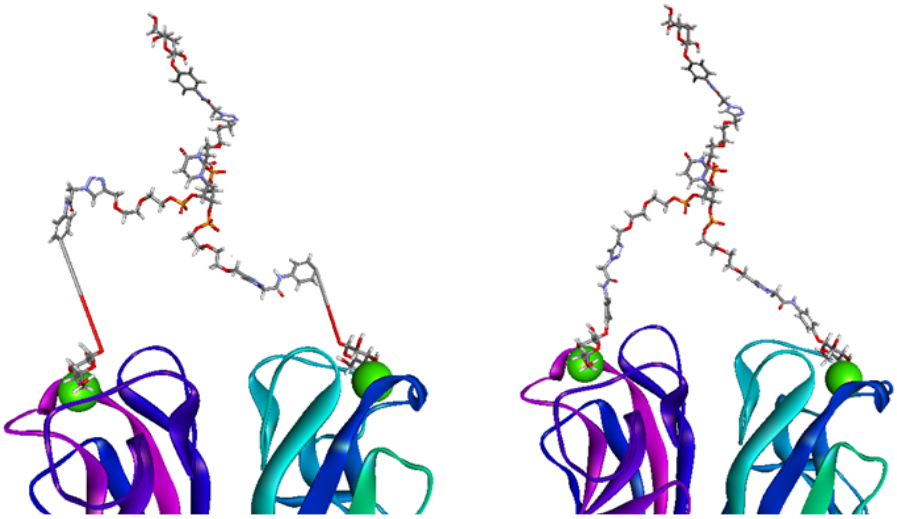

Figure S2. LecA with galactoses on C2 and C3 of **G2b** in the CDR left) before and right) after optimization

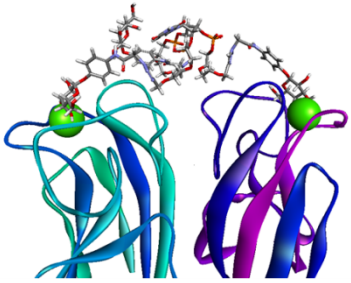

Figure S3 Final docking of **G2b** with LecA

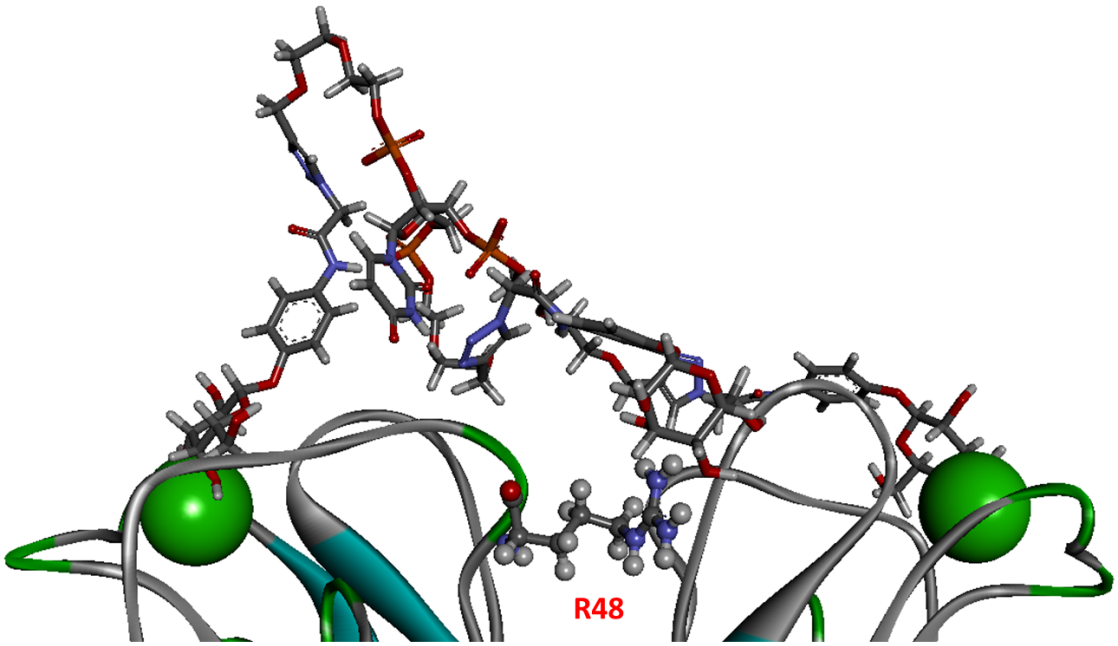

Figure S4a LecA in complex with **G2a**

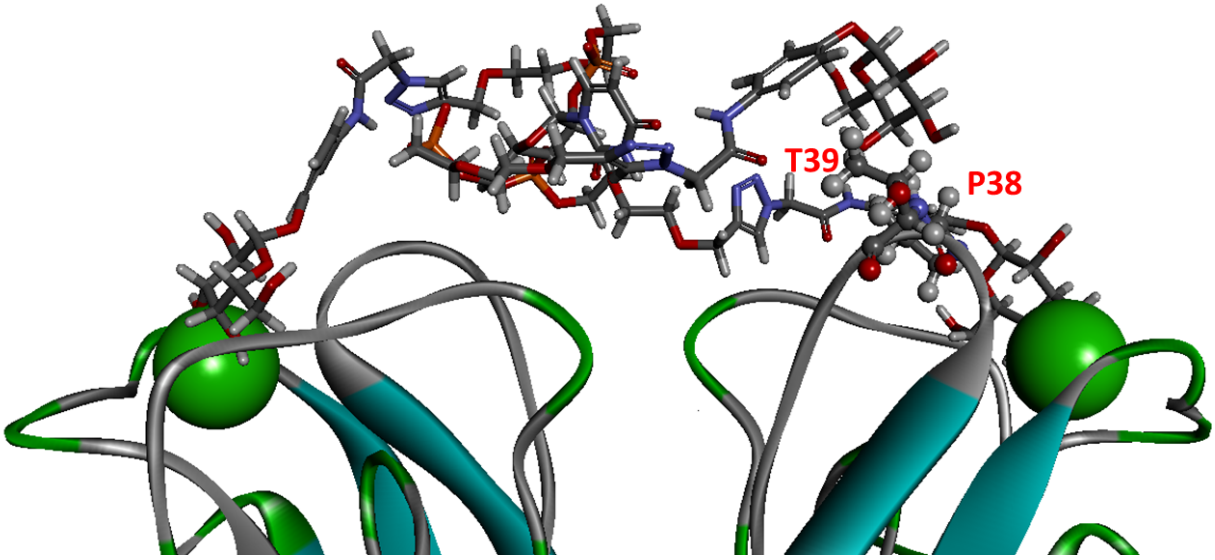

Figure S4b LecA in complex with **G2c**

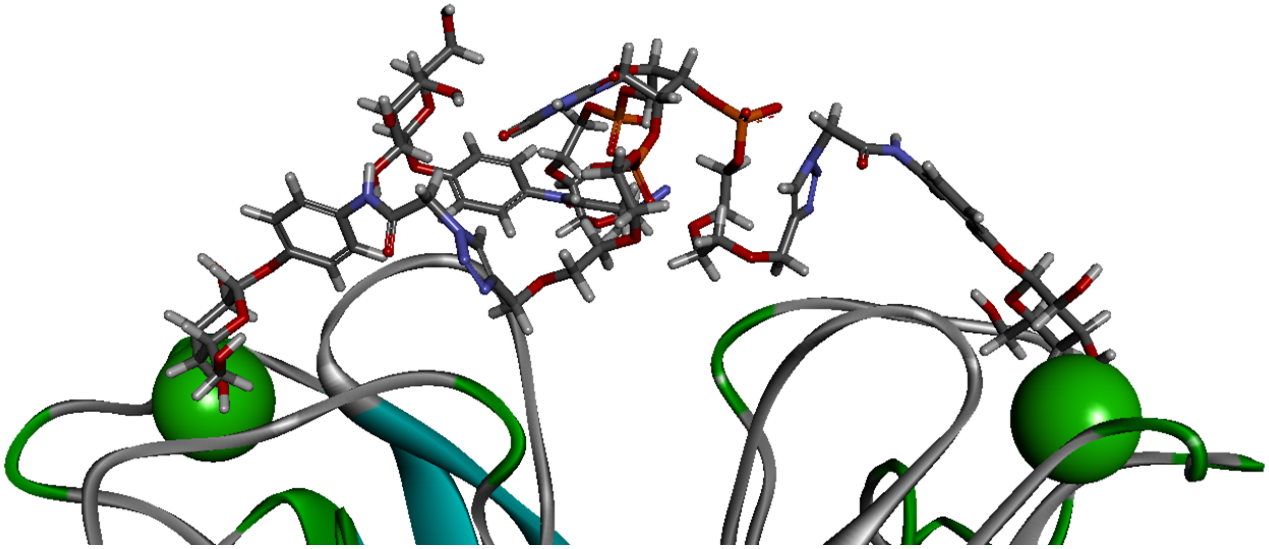

Figure S4c LecA in complex with **G2b**

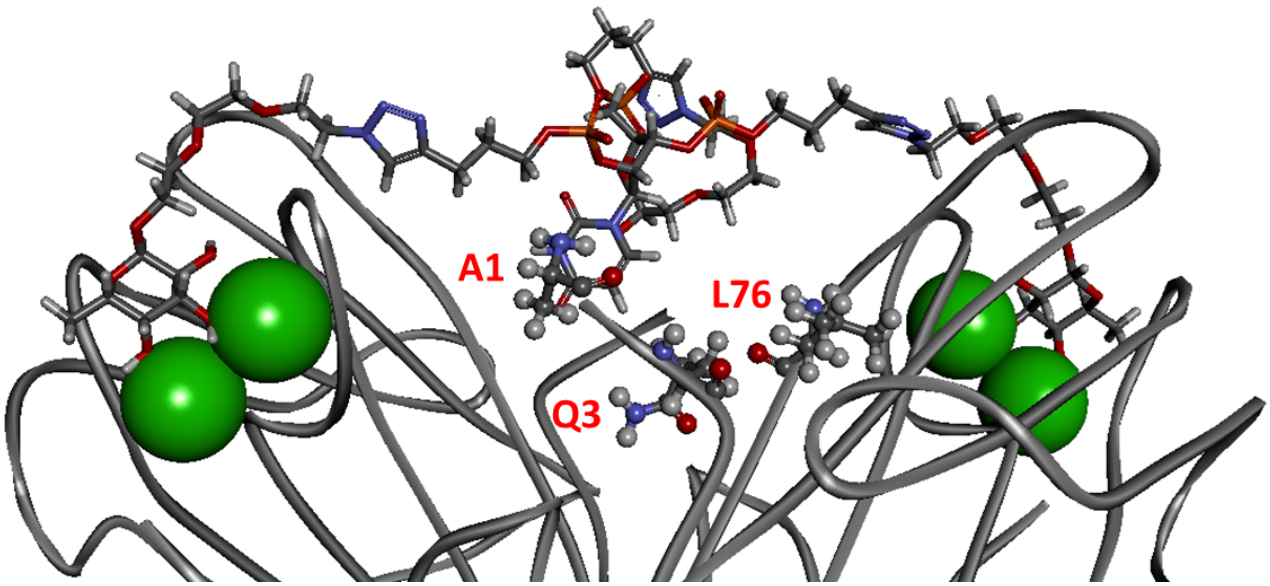

Figure S5a. LecB in complex with **F1a**

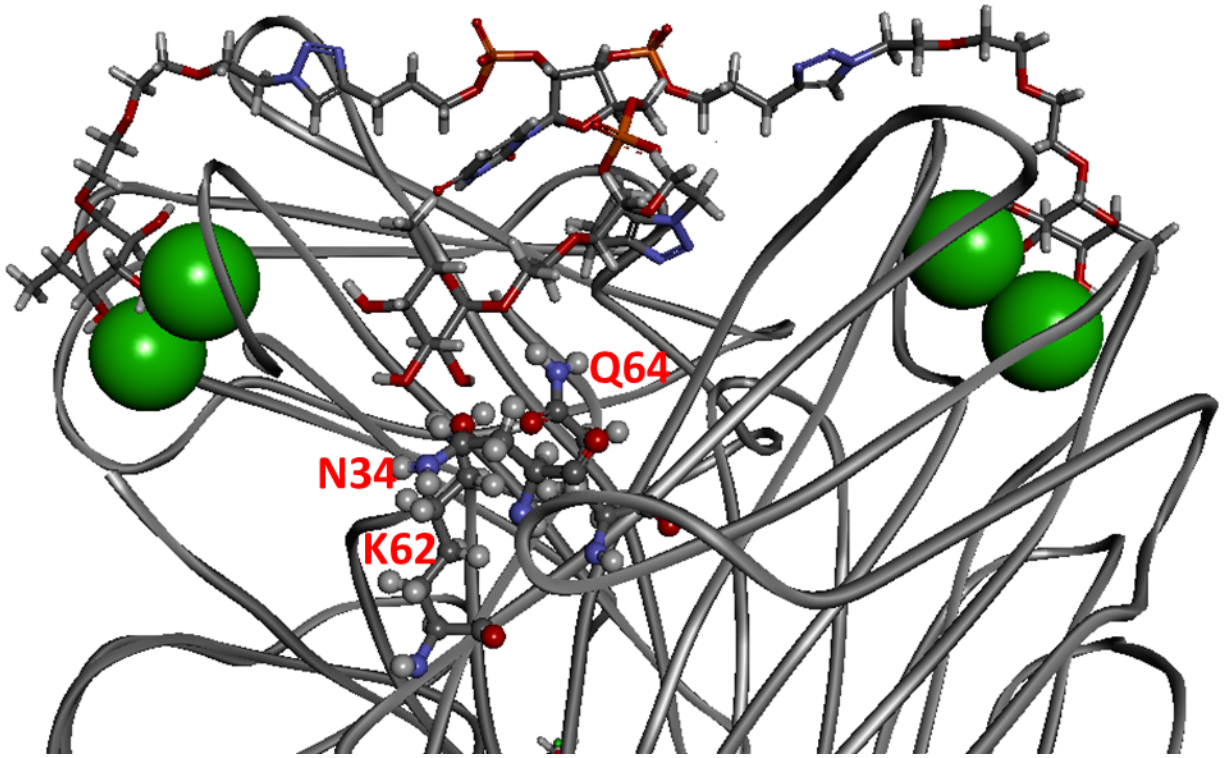

Figure S5b. LecB in complex with **F1c**

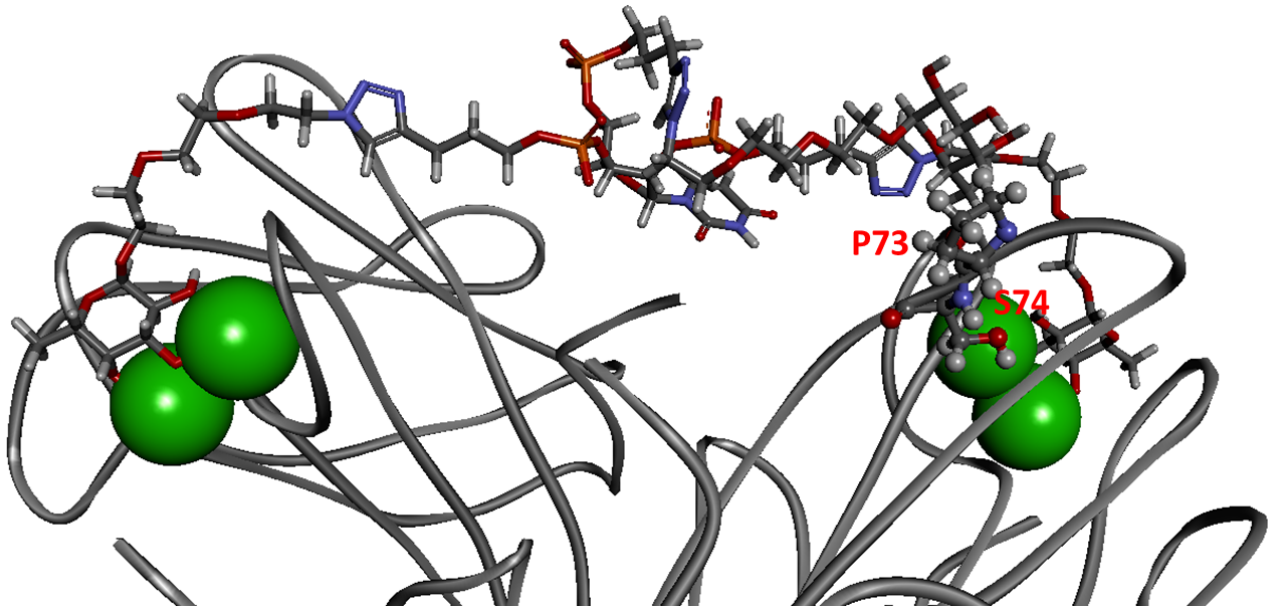

Figure S5c. LecB in complex with **F1b**