Systemic Investigation on Quinoxaline Derivatization of Sialic Acids and Their Quantitation Applicability using High Performance Liquid Chromatography

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Supporting Information

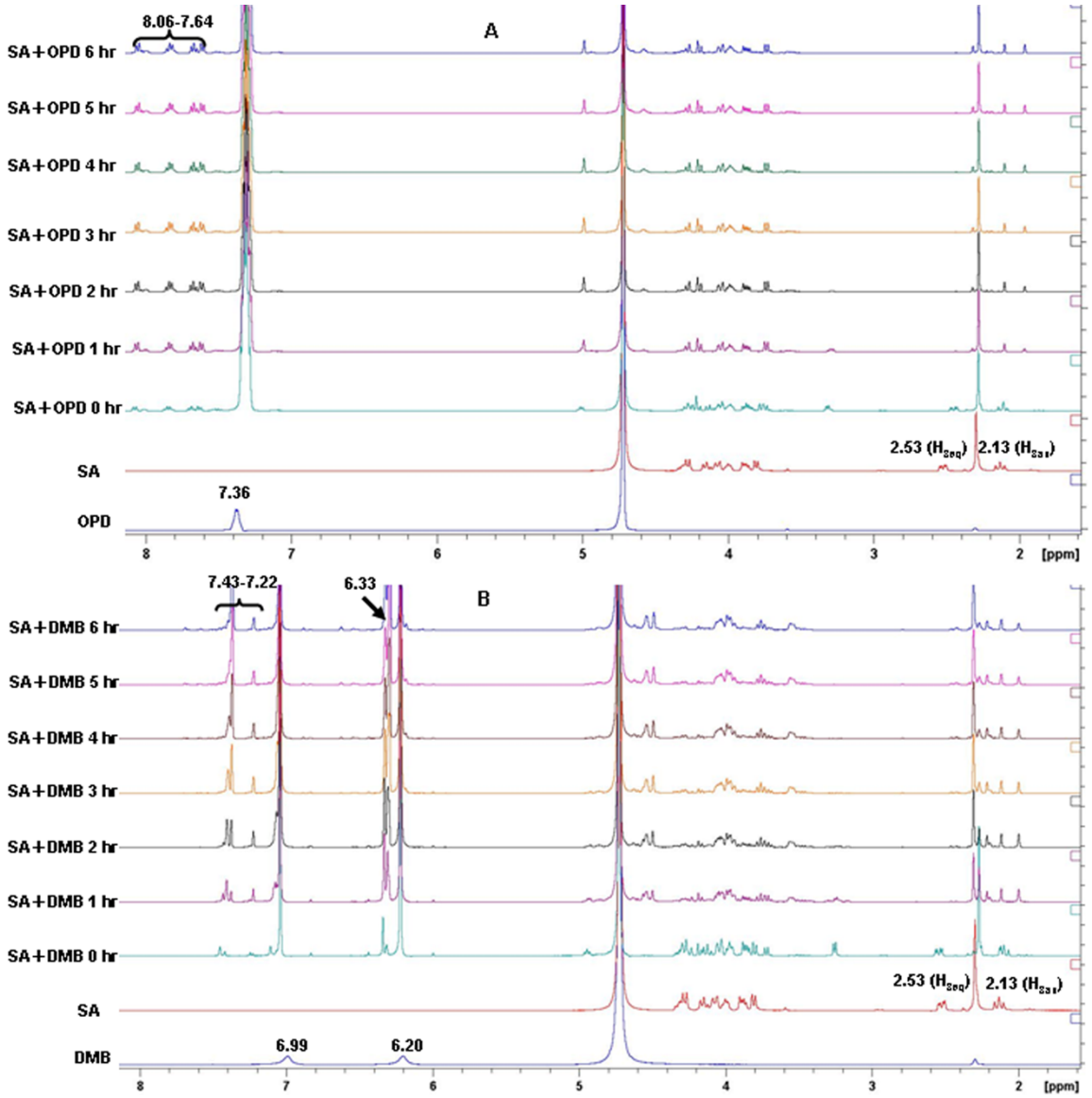

Fig. S1 ^{1}H-NMR kinetic spectra of Neu5Ac (SA) derivatization with OPD (**A**) and DMB (**B**) at 60 ^{o}C from 0 to 6 hr. (in D_2O).

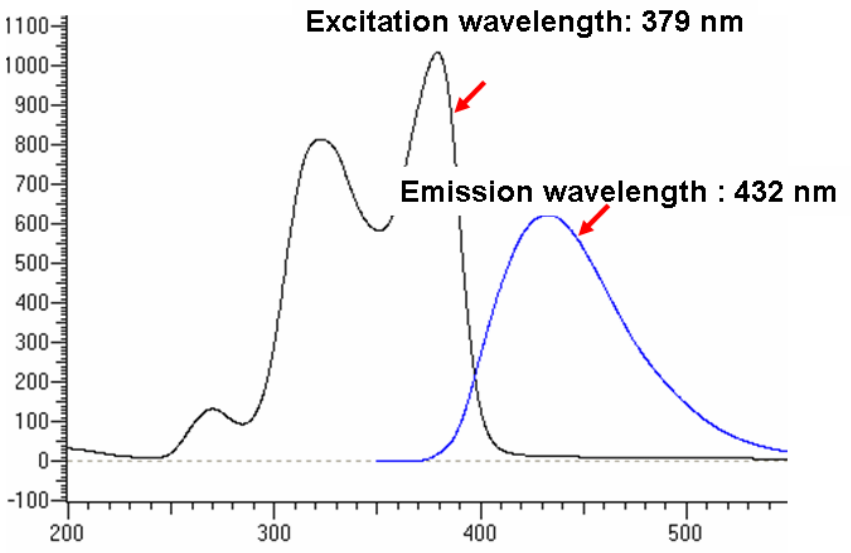

Fig. S2 Fluorescent spectrum of Neu5Ac-DMBA derivative.

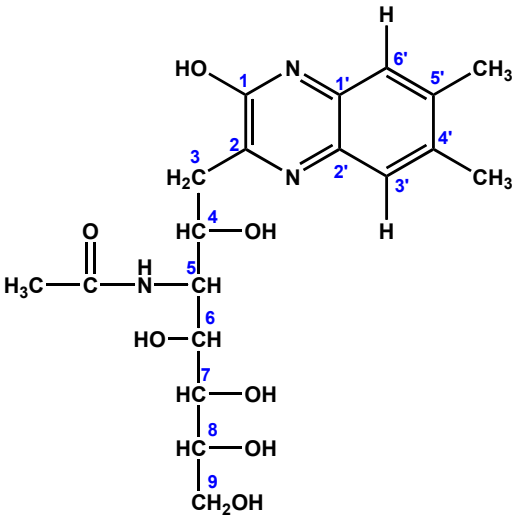

Fig. S3 The structure of compound Neu5Ac-DMBA: The standard Neu5Ac 50 mg was dissolved in 10 mL water, and mixed with 108 mg DMBA together with 0.8 mL acetic acid. The react solution was heated at 60 ℃ for 1 hr, and then using the lyophilizer (Labconco Corporation, Kansas, Missouri, USA) to dry the sample. The crud product (130 mg) was subjected to silica gel column (10 g), gradient eluted by $CHCl_3$: MeOH (15:1~1:1, v/v) to give the compound **1** (Neu5Ac-DMBA, 27 mg, 51.9%).

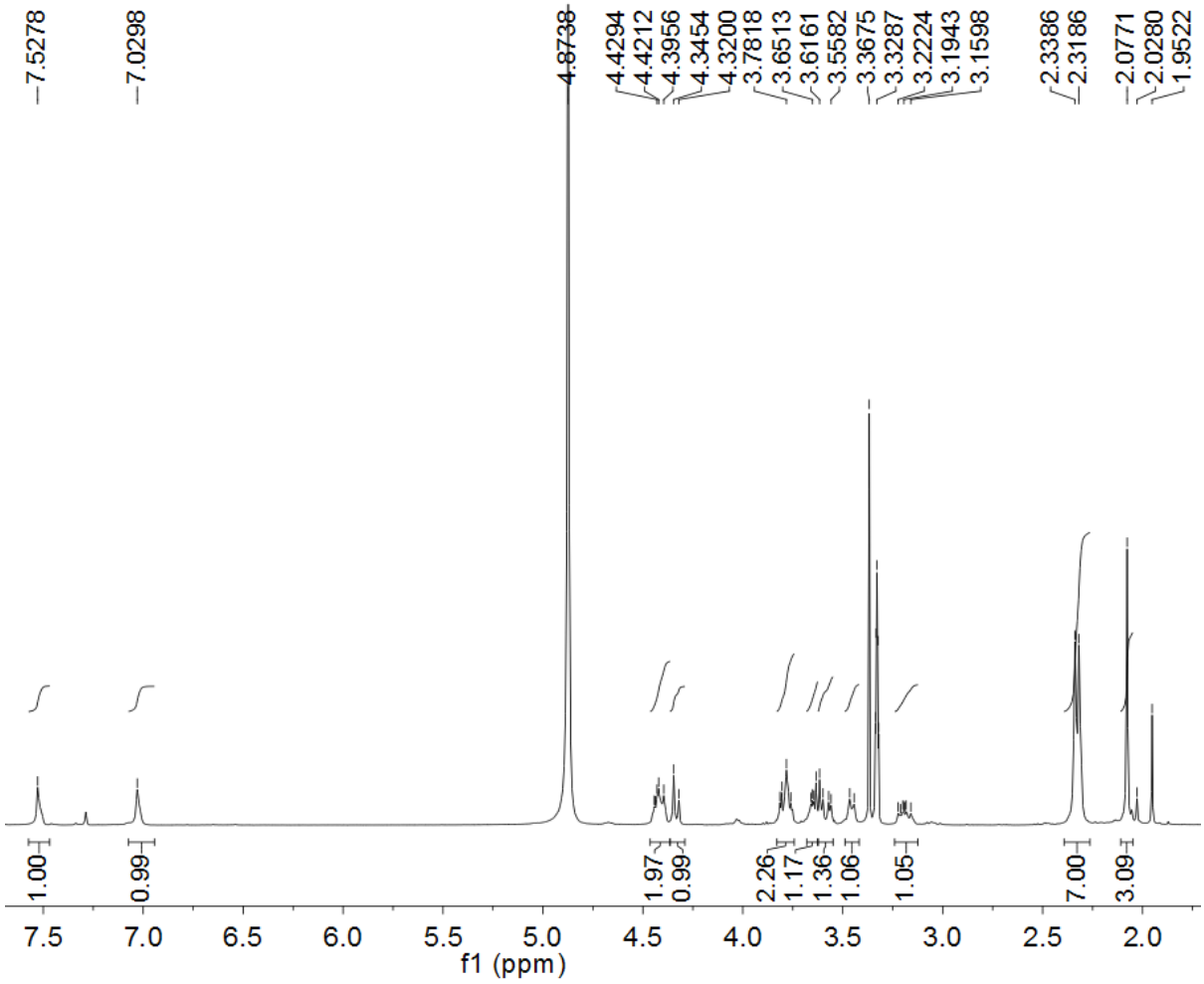

Fig. S4 ^{1}H-NMR spectrum of Neu5Ac-DMBA derivative (in CD_3OD)

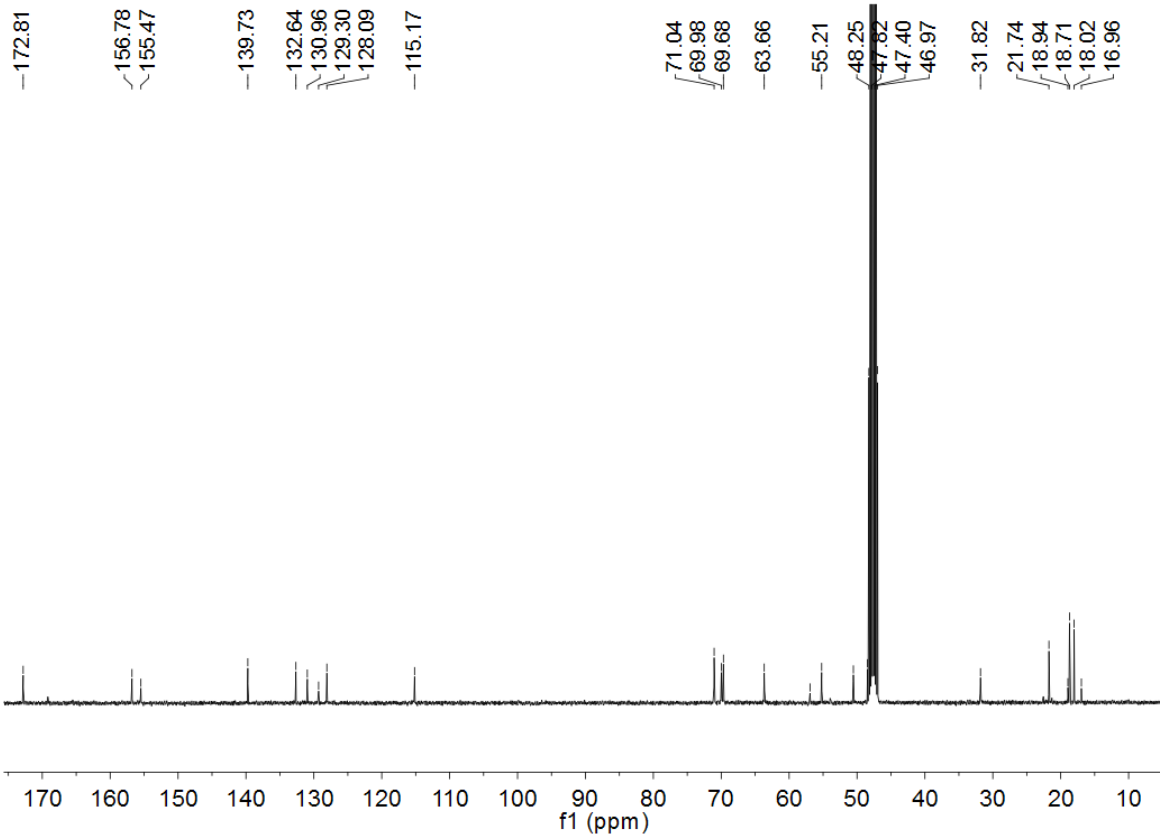

Fig. S5 ^{13}C-NMR spectrum of Neu5Ac-DMBA derivative (in CD_3OD)

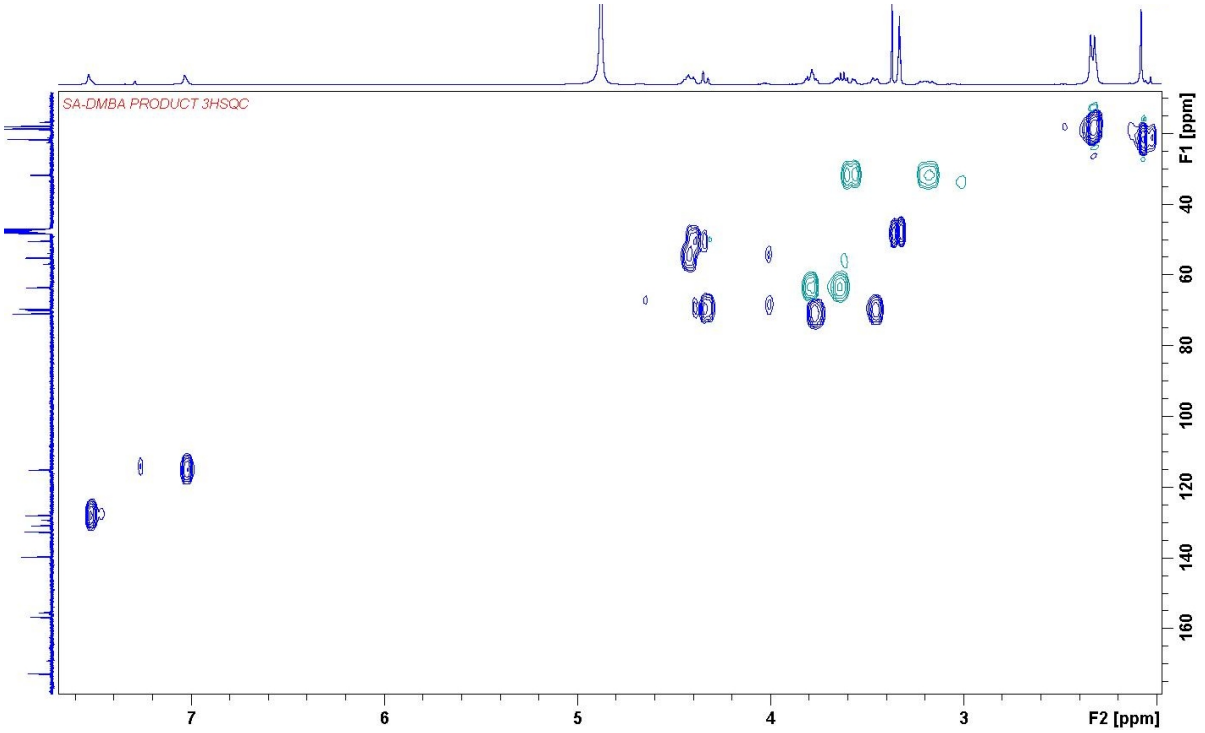

Fig. S6 HSQC spectrum of Neu5Ac-DMBA derivative (in CD_3OD)

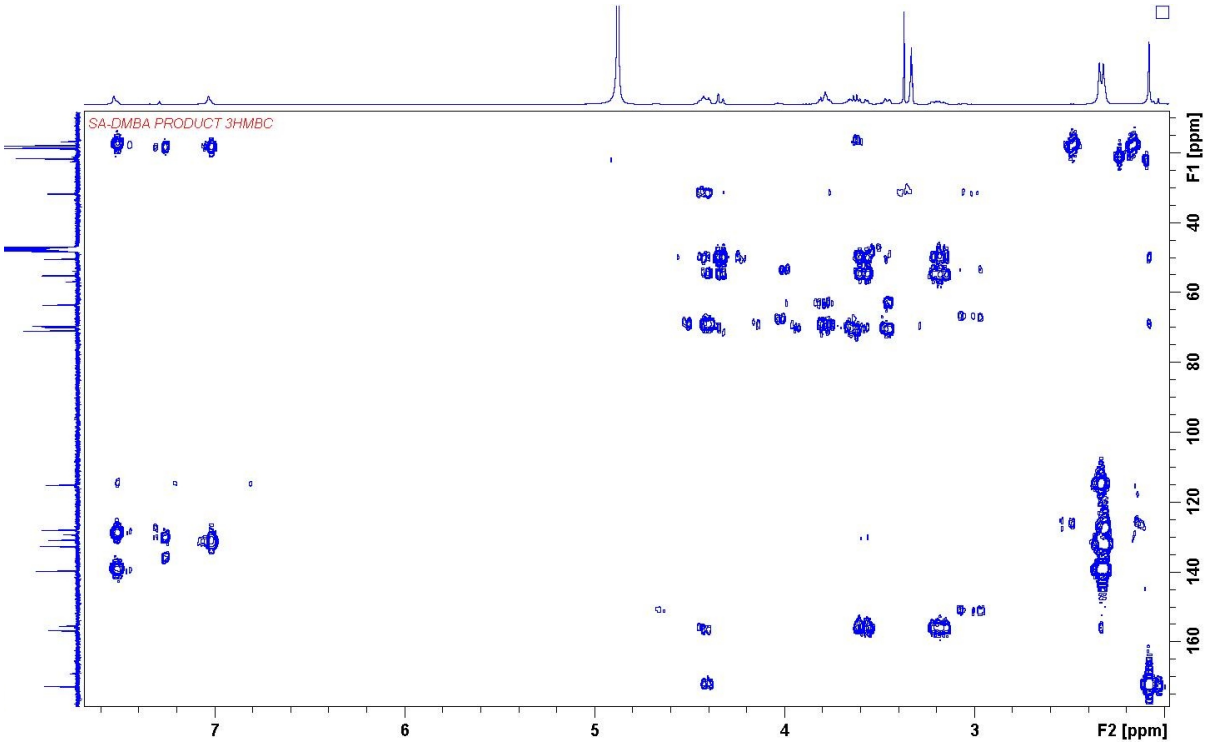

Fig. S7 HMBC spectrum of Neu5Ac-DMBA derivative (in CD_3OD)

Table S1 The NMR (in CD_3OD, 400 MHz) data of Neu5Ac-DMBA derivative

Position	^{1}H-NMR (*J*, Hz)	^{13}C-NMR	^{1}H-^{1}H COSY	HMBC
1	-	155.5		
2	-	156.8		
3	3.20 (1H, m), 3.57 (1H, br.d, 4.9)	31.8	H-4	C-2,4,5
4	4.42 (1H, m)	55.2	H-3,5	C-2,3,5
5	4.40 (1H, m)	50.5	H-4,6	C-4,6,7, C=O
6	4.34 (1H, br.d, 10.2)	69.7	H-5,7	C-5,7,8
7	3.45 (1H, br.d, 8.7)	69.9	H-6,8	C-5,6,8,9
8	3.76 (1H, m)	71.0	H-7,9	C-6,7, 9
9	3.66 (1H, m), 3.80 (1H, m)	63.6	H-8	C-7, 8
1′	-	131.0		
2′	-	129.3		
3′	7.53 (1H, s)	128.1	-	C-2′, 4′, 5′
4′	-	132.6	-	
5′	-	139.7	-	
6′	7.03 (1H, s)	115.2	-	C-1′, 4′, 5′
4′-CH_3	2.32 (3H, s)	18.0	-	C-3′, 4′, 5′
5′-CH_3	2.34 (3H, s)	18.7	-	C-4′, 5′, 6′
5-NHCOCH_3	2.07 (3H, s)	21.3	-	C=O
5-NH$CO$$CH_3$	-	172.8	-	-