

Supporting Information
For
**Development of a Tri-Functional Nanoprobe for Background-Free SERS Detection of
Sialic Acid on the Cell Surface**

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Table of Contents

1. Sensitivity of AgNCs towards reporter 6	S1
Table S1. Listed spatial resolution of SERS based sialic acid detection methods	S1
References	S2
2. NMR Spectra	S3
¹ H NMR spectrum of compound 1 (500 MHz, MeOD).....	S3
¹³ C NMR spectrum of compound 1 (125 MHz, MeOD)	S3
¹ H NMR spectrum of compound 2 (500 MHz, MeOD).....	S4
¹³ C NMR spectrum of compound 2 (125 MHz, MeOD)	S4
¹ H NMR spectrum of compound 3 (500 MHz, MeOD).....	S5
¹³ C NMR spectrum of compound 3 (125 MHz, MeOD)	S5
¹ H NMR spectrum of compound 4 (500 MHz, MeOD).....	S6
¹³ C NMR spectrum of compound 4 (125 MHz, MeOD)	S6
¹ H NMR spectrum of compound 5 (500 MHz, MeOD).....	S7
¹³ C NMR spectrum of compound 5 (125 MHz, MeOD)	S7
¹ H NMR spectrum of compound 6 (500 MHz, MeOD).....	S8
¹³ C NMR spectrum of compound 6 (125 MHz, MeOD)	S8
¹ H- ¹³ C 2D HMQC NMR spectrum of 6 (500/125 MHz, MeOD).....	S9
¹ H- ¹³ C 2D HMBC NMR spectrum of 6 (500/125 MHz, MeOD)	S9
¹ H- ¹ H 2D COSY NMR spectrum of 6 (500/125 MHz, MeOD)	S10
High Resolution Mass Spectra of compound 6	S10

1. Sensitivity of AgNCs towards reporter 6

AgNCs (1 μ L) were reacted with 10 μ L of solution of reporter **6** in EtOH with different concentration (100 μ M, 10 μ M, 1 μ M, 100 nM, and 10 nM). Then, the solution was dropped on defined area of silicon wafer, and dried under ambient atmosphere before Raman measurements. The line in Figure S1 was generated between SERS intensity vs. moles of reporter **6**.

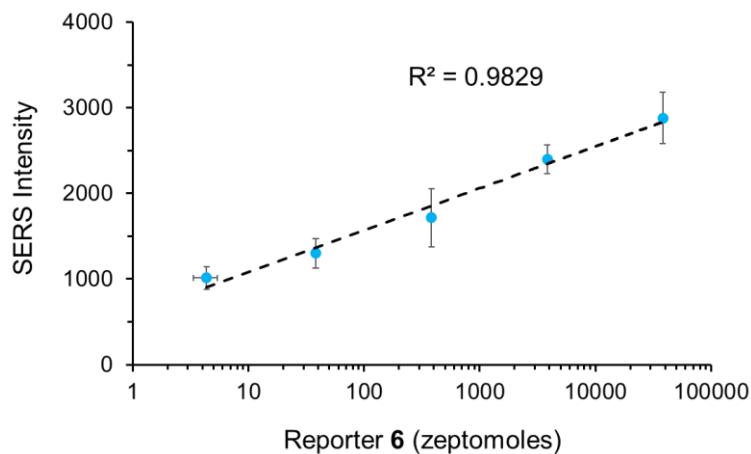


Figure S1. Sensitivity of AgNCs towards reporter **6**.

Table S1. Listed spatial resolution of SERS based sialic acid detection methods

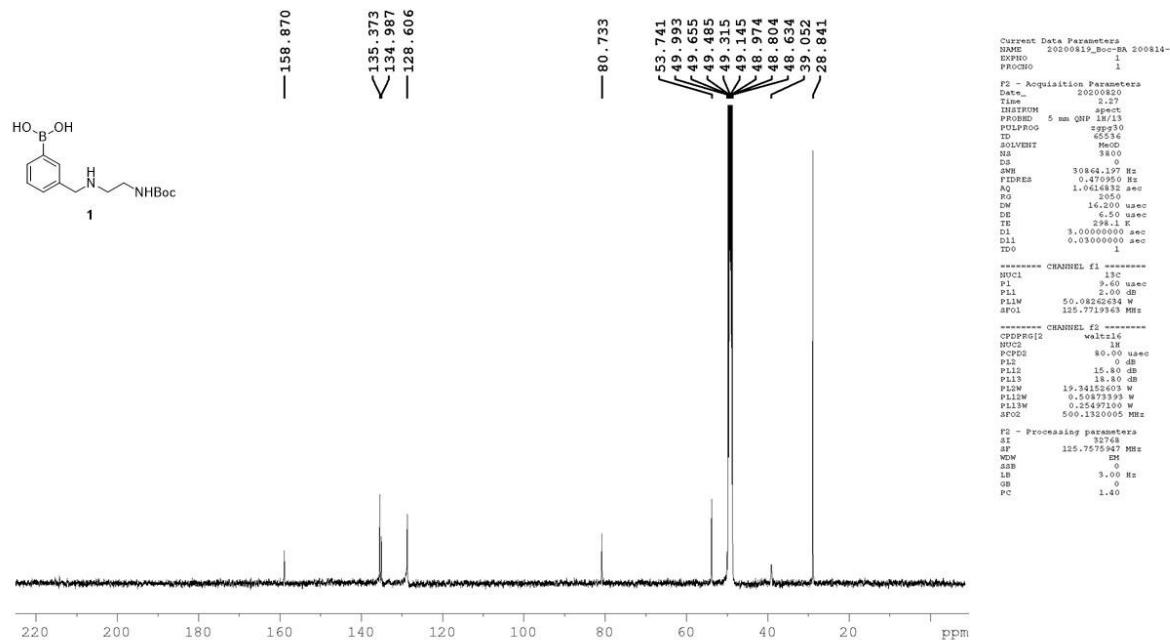
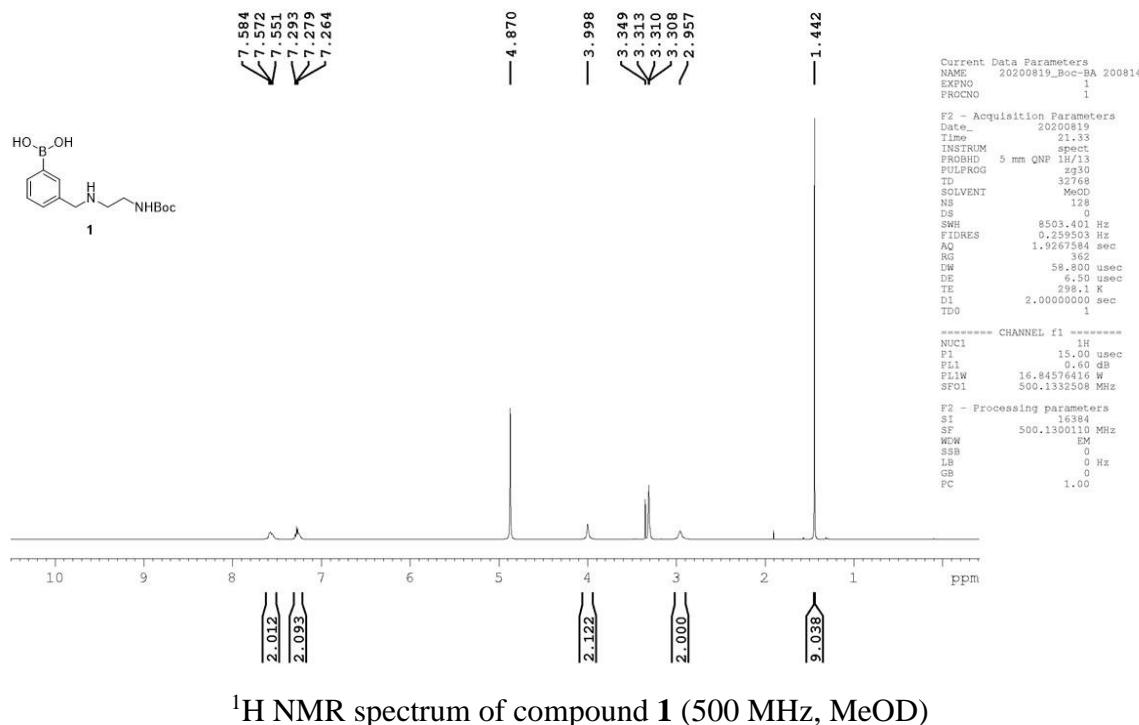
Reference	Spatial resolution ^a	Type of cell image performed
This work	382 nm	SERS mapping image
Ref. [1]	309 nm	Dark field image
Ref. [2]	858 nm	Dark field image
Ref. [3]	-	SERS mapping image

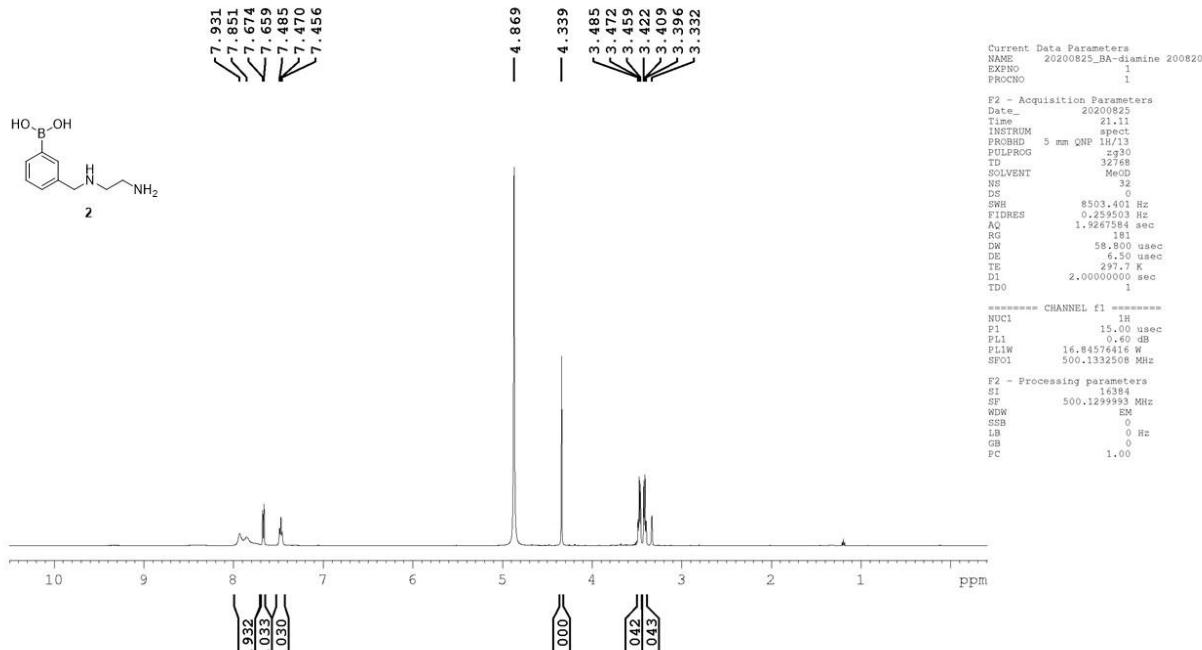
^aSpatial resolution was calculated by formula: $(0.61 \times \lambda)/\text{N.A.}$;
N.A. = Numerical aperture.

References

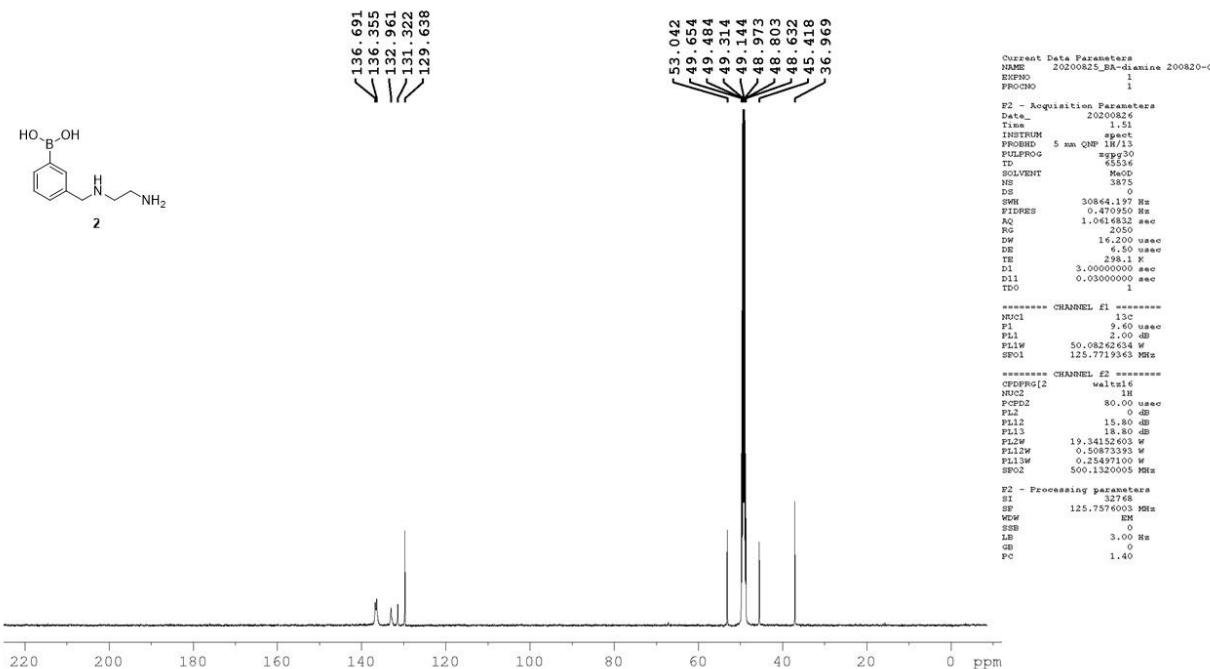
1. Gong, T.; Cui, Y.; Goh, D.; Voon, K.K.; Shum, P.P.; Humbert, G.; Auguste, J.-L.; Dinh, X.-Q.; Yong, K.-T.; Olivo, M. Highly sensitive SERS detection and quantification of sialic acid on single cell using photonic-crystal fiber with gold nanoparticles. *Biosensors and Bioelectronics* **2015**, *64*, 227-233.
2. Deng, R.; Yue, J.; Qu, H.; Liang, L.; Sun, D.; Zhang, J.; Liang, C.; Xu, W.; Xu, S. Glucose-bridged silver nanoparticle assemblies for highly sensitive molecular recognition of sialic acid on cancer cells via surface-enhanced Raman scattering spectroscopy. *Talanta* **2018**, *179*, 200-206.
3. He, X.-N.; Wang, Y.-N.; Wang, Y.; Xu, Z.-R. Accurate quantitative detection of cell surface sialic acids with a background-free SERS probe. *Talanta* **2020**, *209*, 120579.

2. NMR Spectra

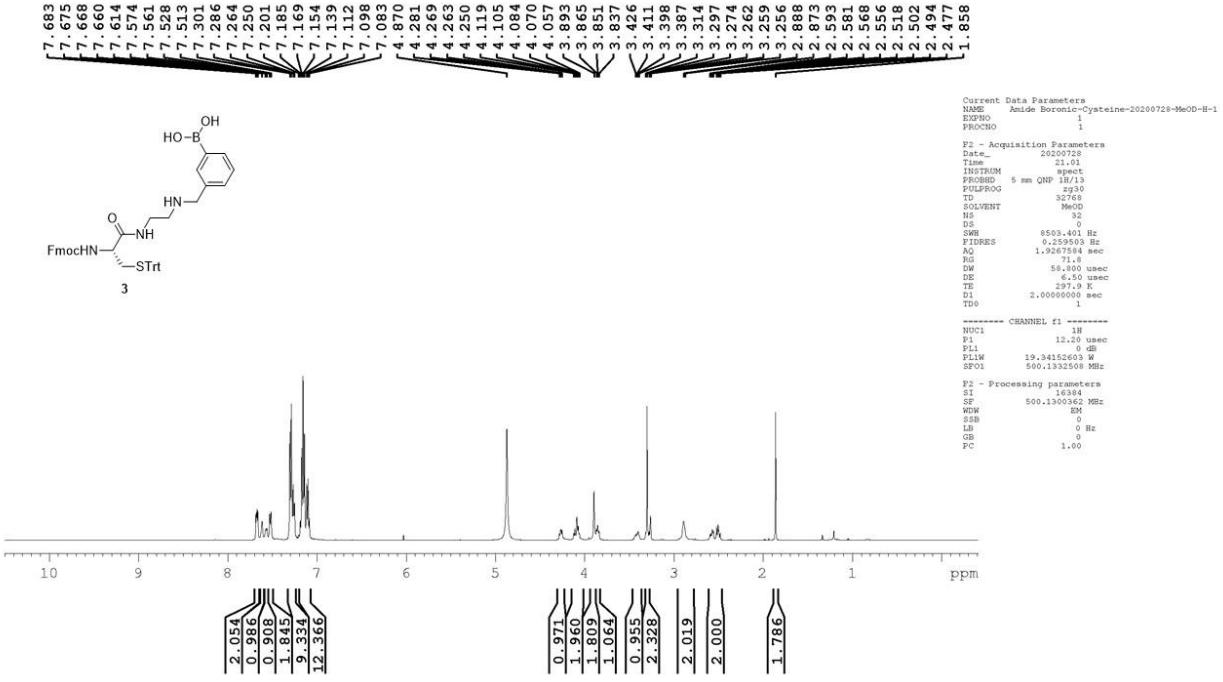




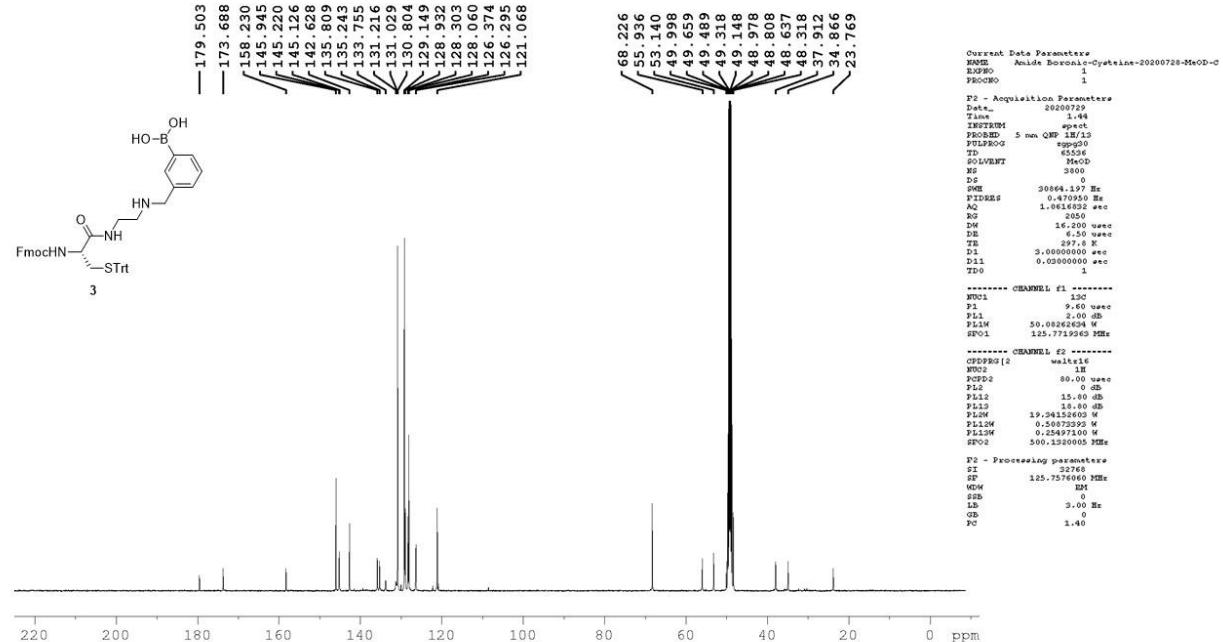
^1H NMR spectrum of compound 2 (500 MHz, MeOD)



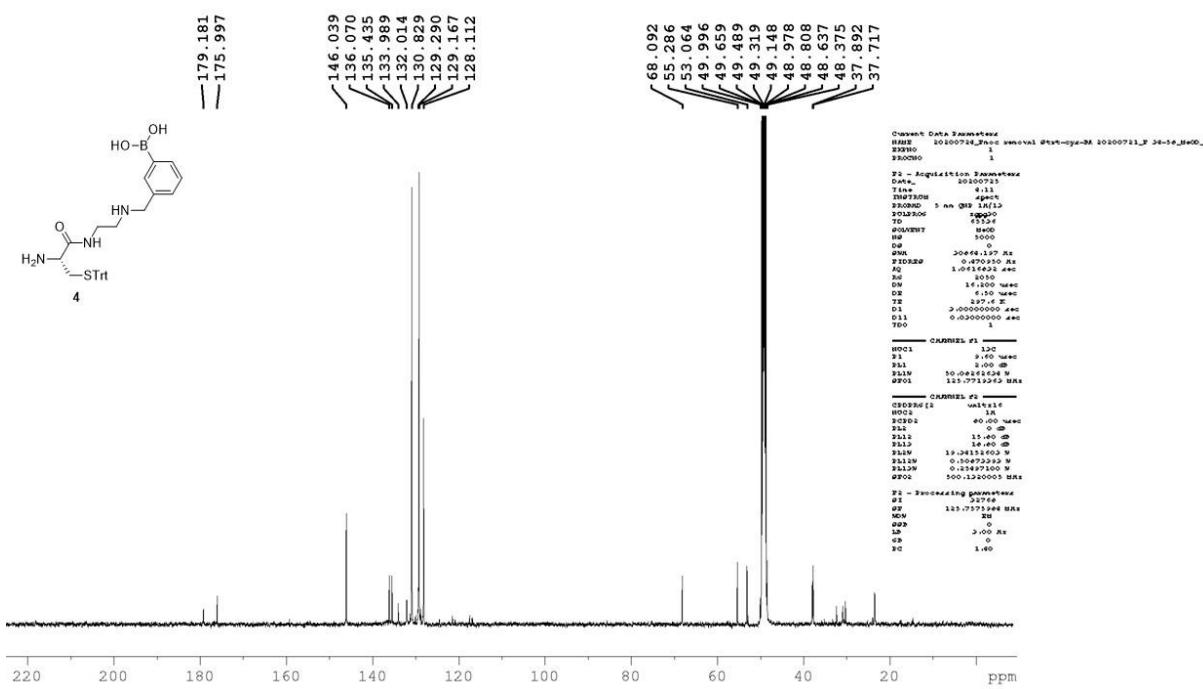
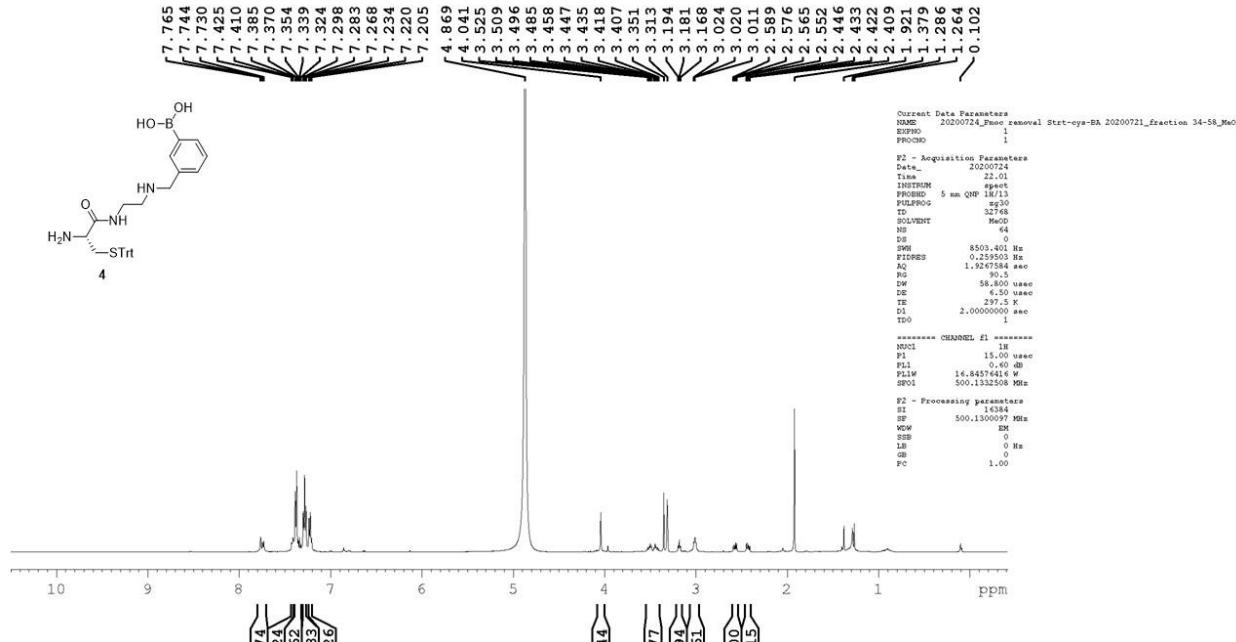
^{13}C NMR spectrum of compound 2 (125 MHz, MeOD)

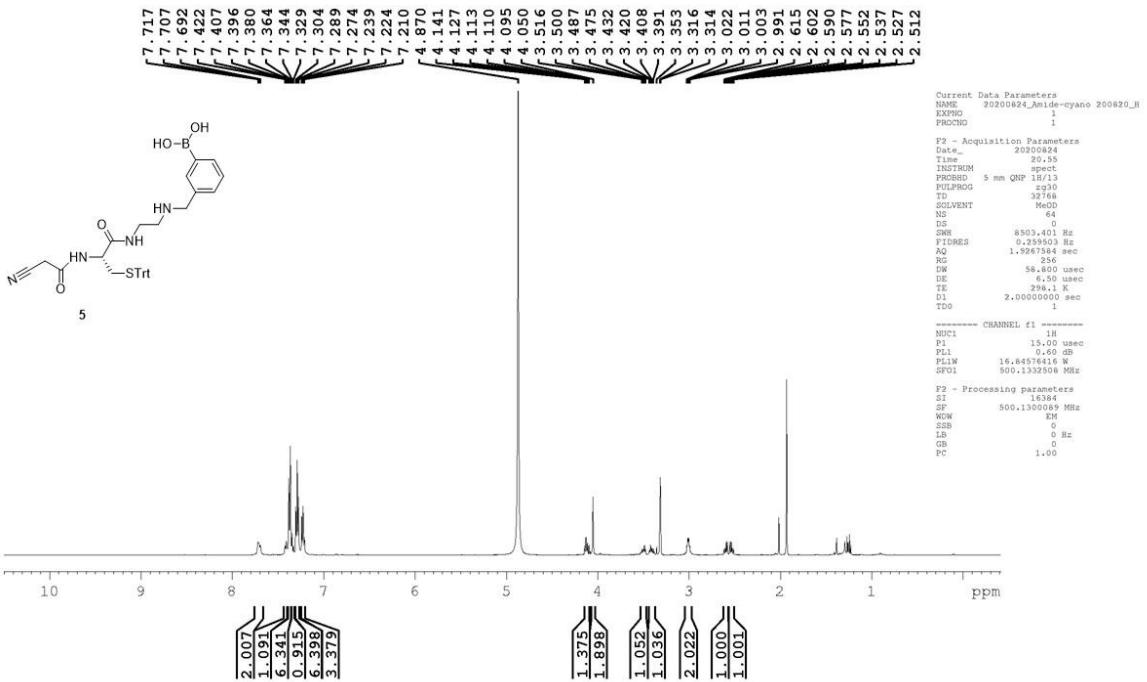


^1H NMR spectrum of compound **3** (500 MHz, MeOD)

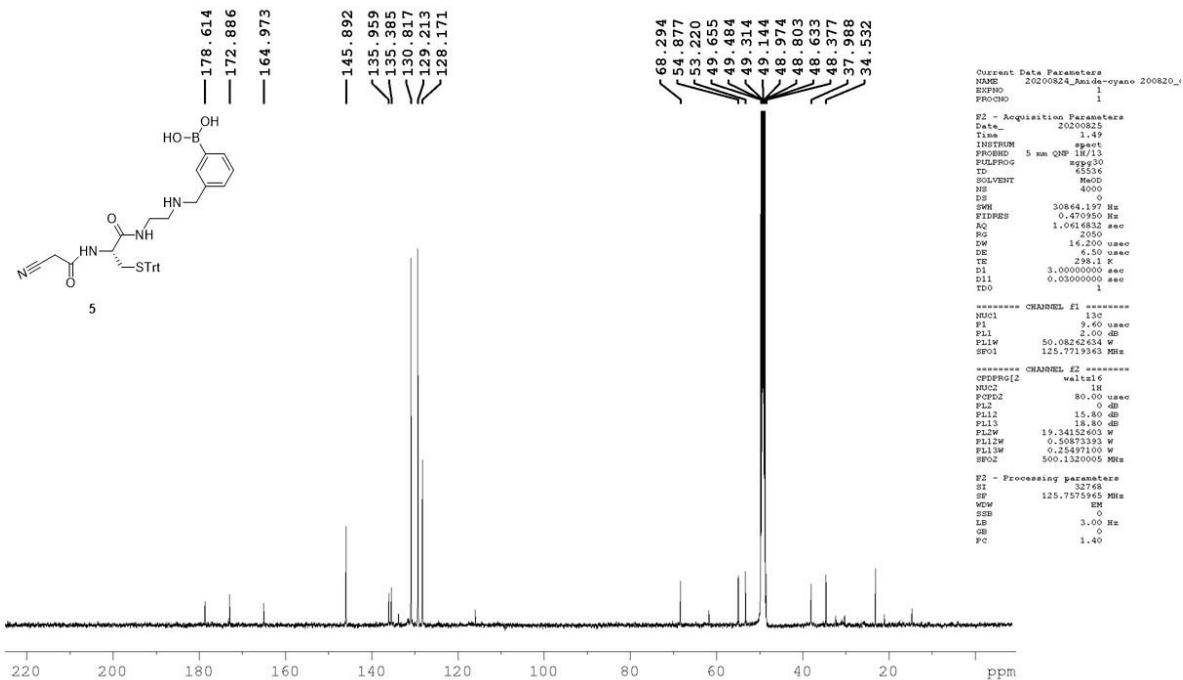


^{13}C NMR spectrum of compound **3** (125 MHz, MeOD)

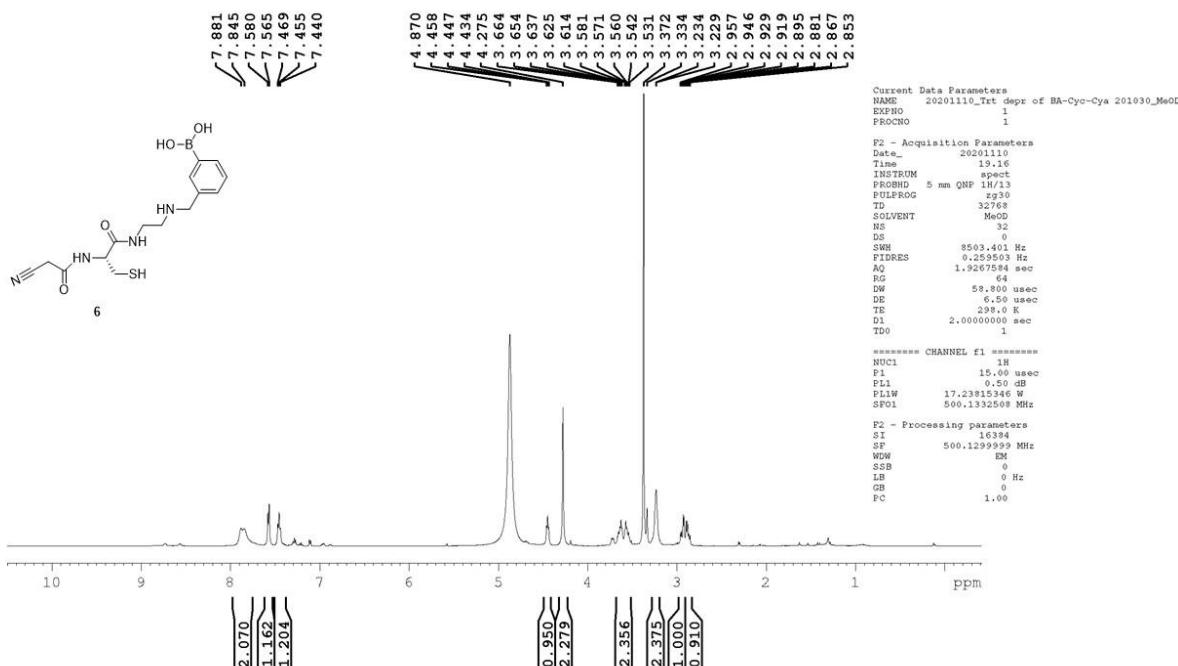




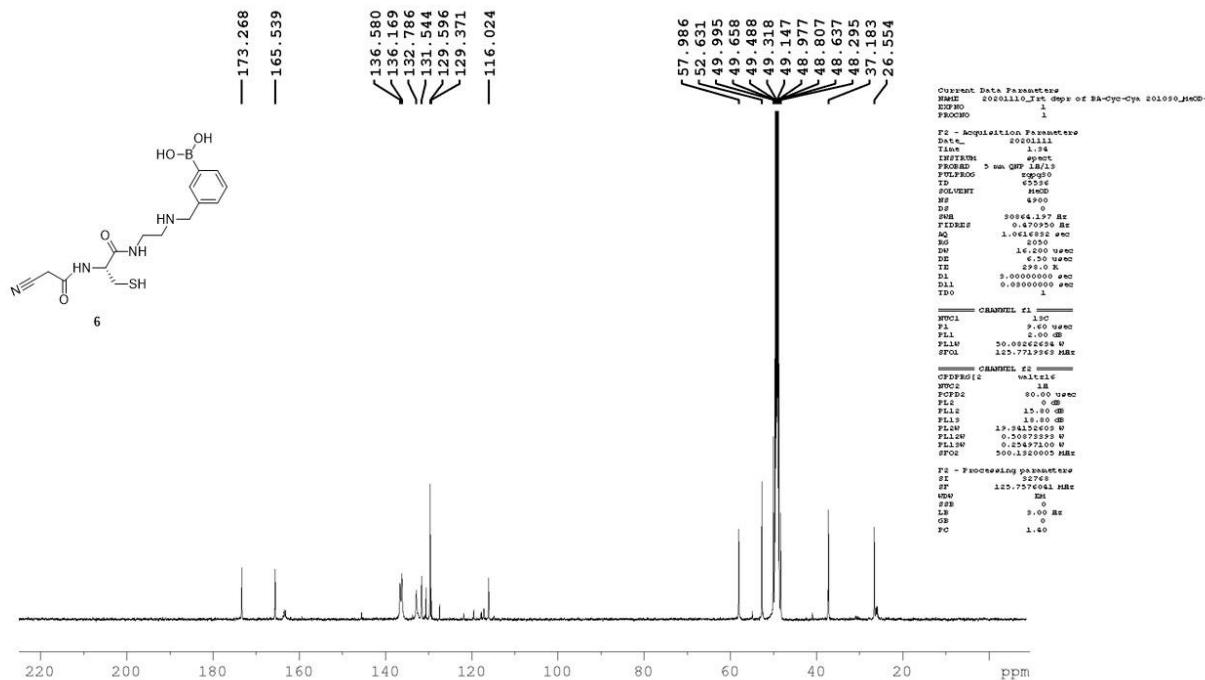
¹H NMR spectrum of compound **5** (500 MHz, MeOD)



¹³C NMR spectrum of compound **5** (125 MHz, MeOD)

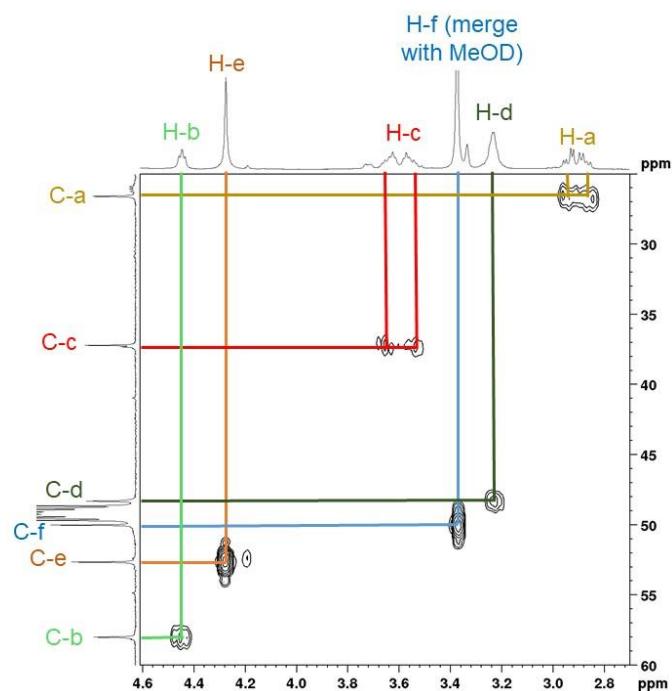
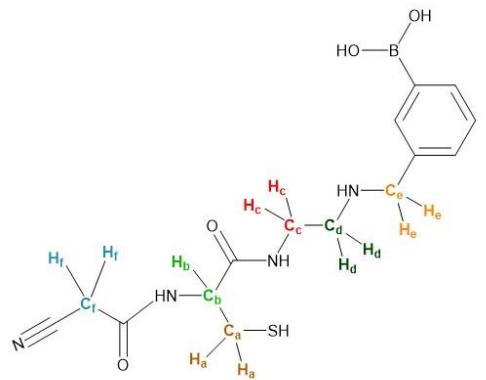


¹H NMR spectrum of compound **6** (500 MHz, MeOD)



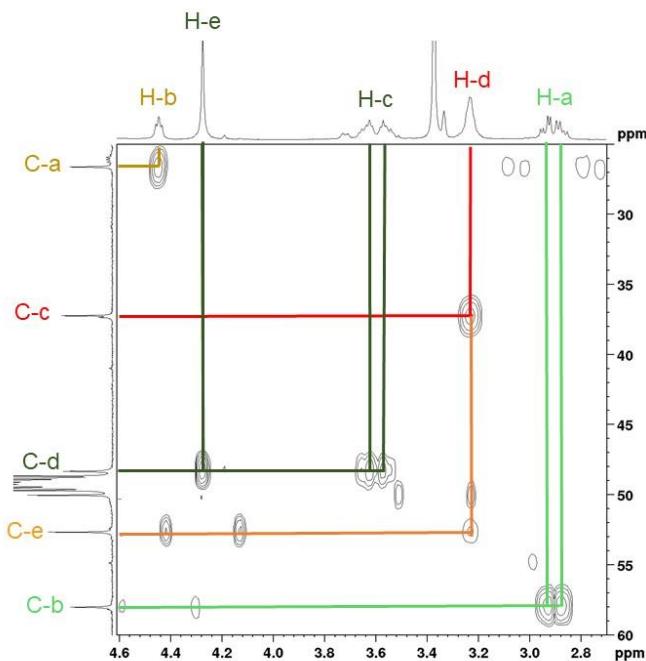
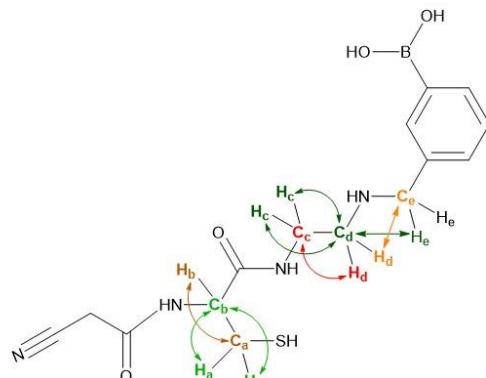
¹³C NMR spectrum of compound **6** (125 MHz, MeOD)

^1H - ^{13}C HMQC correlations of 6



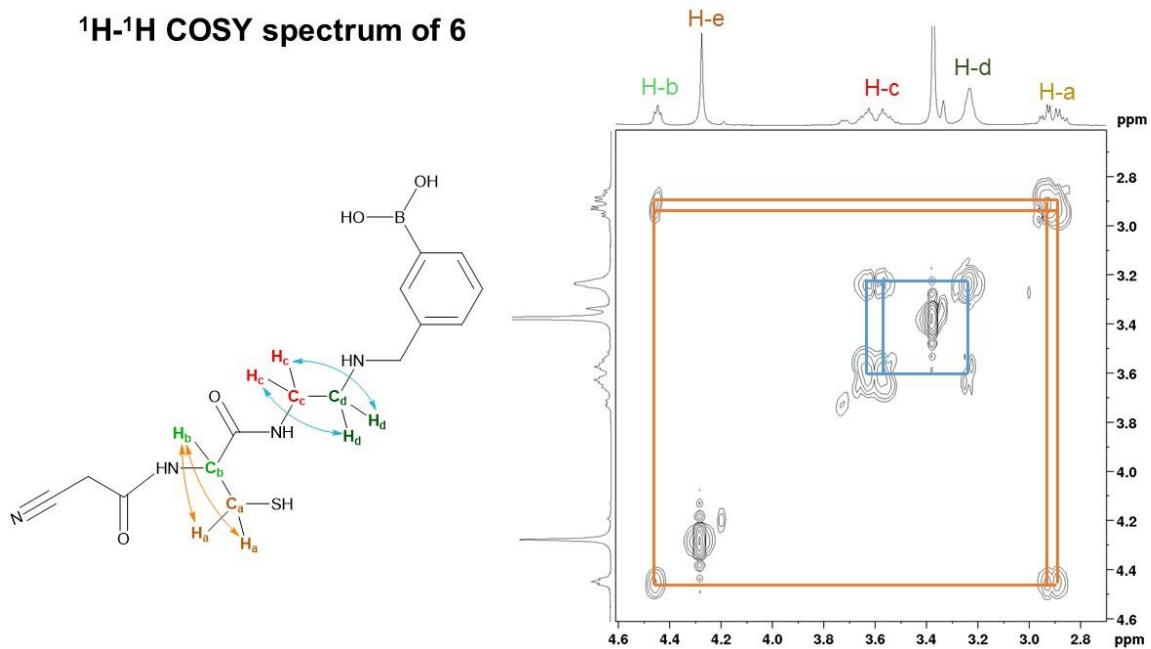
^1H - ^{13}C 2D HMQC NMR spectrum of **6** (500/125 MHz, MeOD)

^1H - ^{13}C HMBC correlations of 6

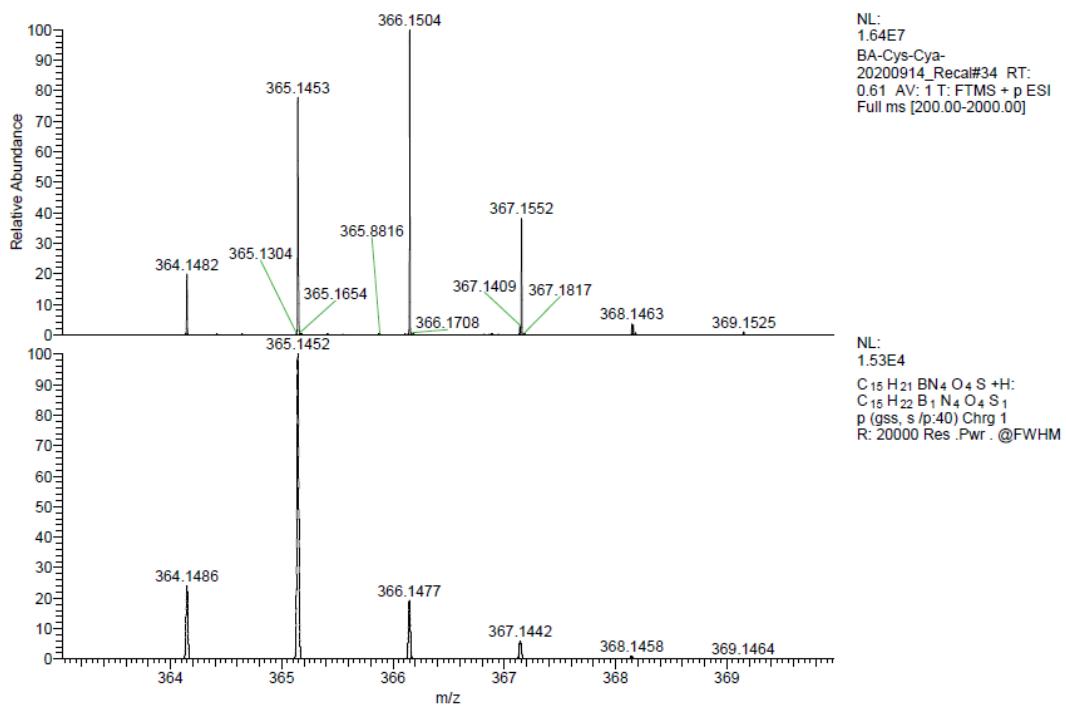


^1H - ^{13}C 2D HMBC NMR spectrum of **6** (500/125 MHz, MeOD)

¹H-¹H COSY spectrum of 6



¹H-¹H 2D COSY NMR spectrum of 6 (500/125 MHz, MeOD)



High Resolution Mass Spectra of compound 6