

Electronic Supplementary Information

for

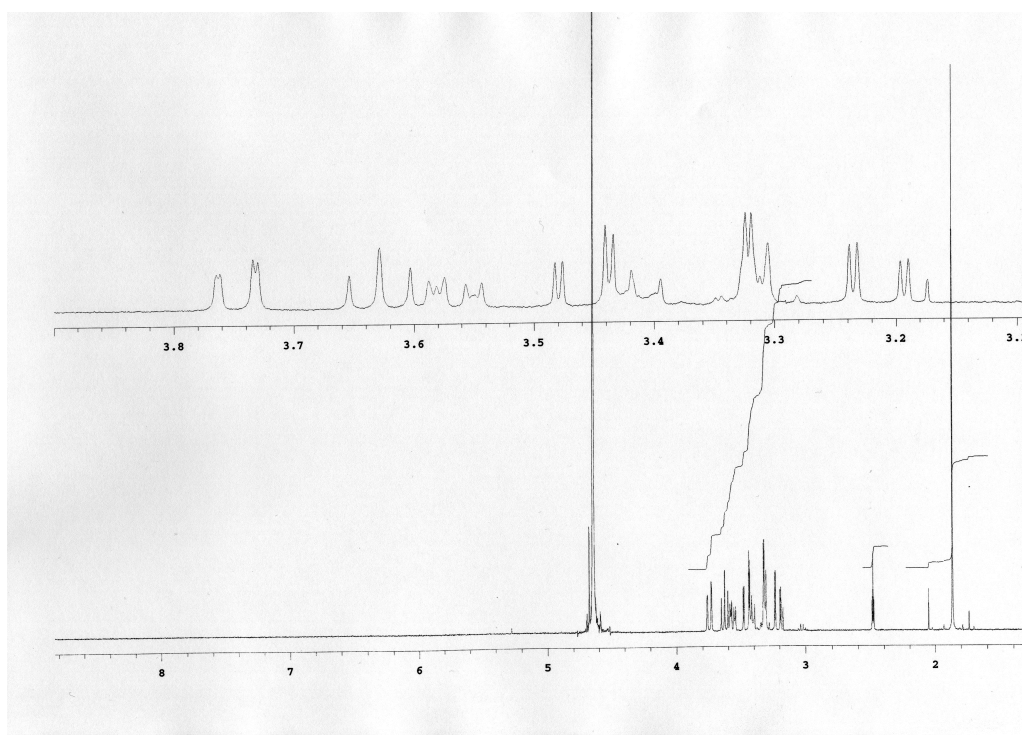
Tetravalent glycopeptide with nanomolar affinity to wheat germ agglutinin

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Anne Imberty and Olivier Renaudet

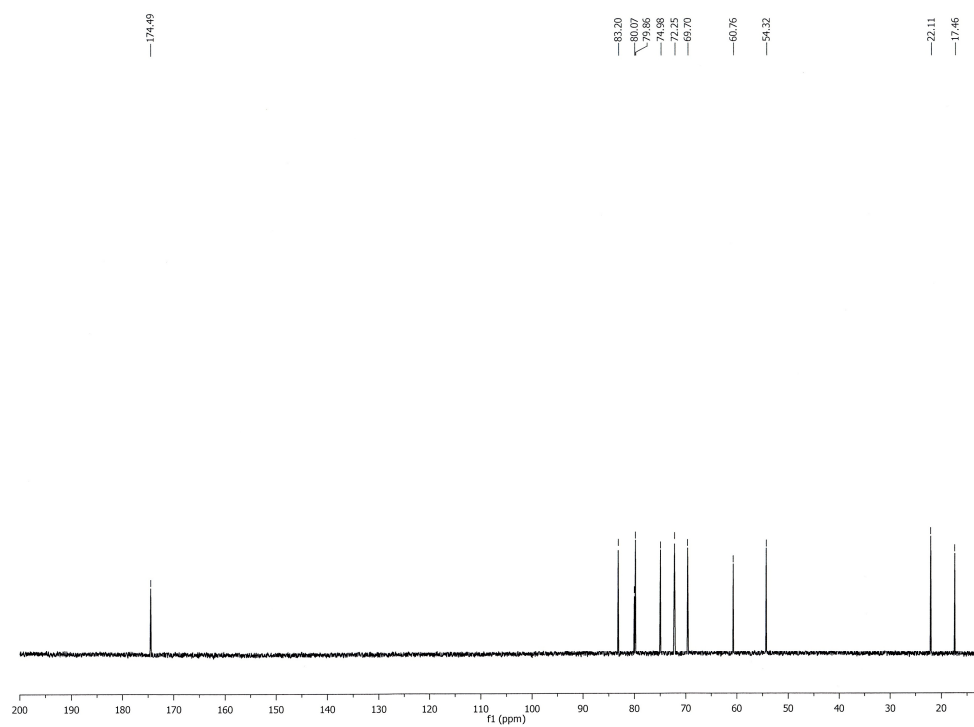
¹ H and ¹³ C NMR spectrum of 9	S2
¹ H and ¹³ C NMR spectrum of 2-acetamido-3,4,6-tri-O-acetyl-2-deoxy-β-D-glucopyranosyl-N-hydroxyphthalimide	S3
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- S2 -

^1H NMR spectrum of **9** (400 MHz, CDCl_3).

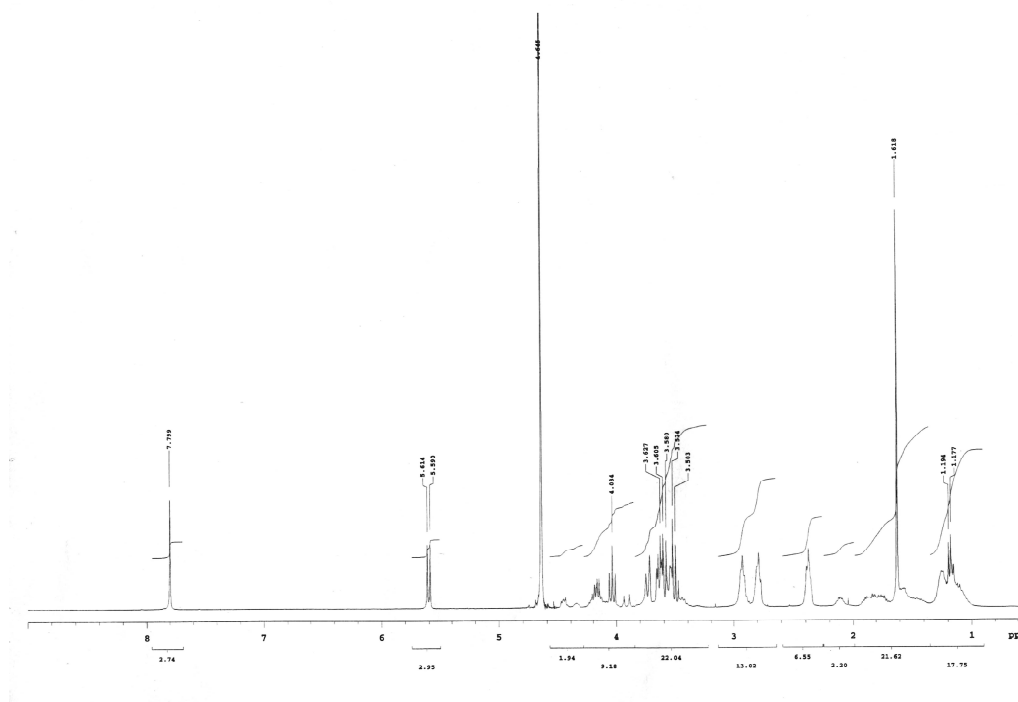


^{13}C NMR spectrum of **9** (100 MHz, CDCl_3).

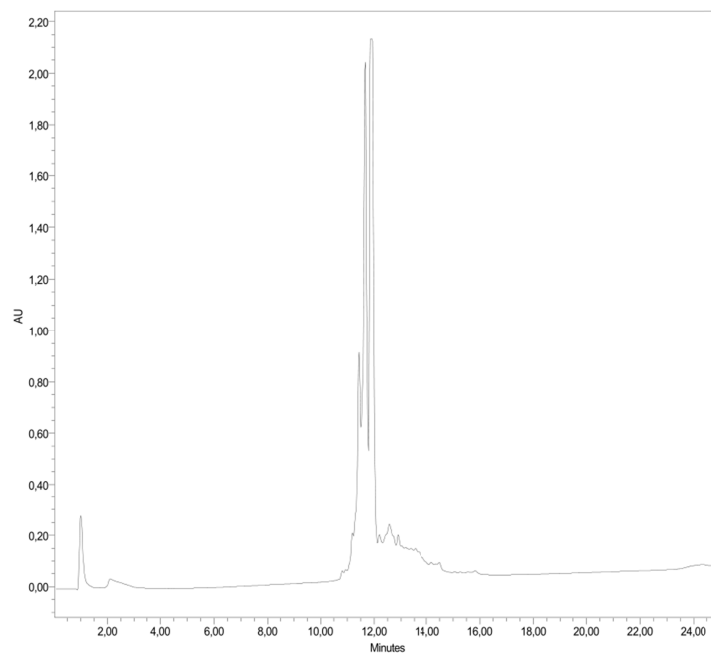


- S4 -

^1H NMR spectrum of **12** (400 MHz, D_2O).

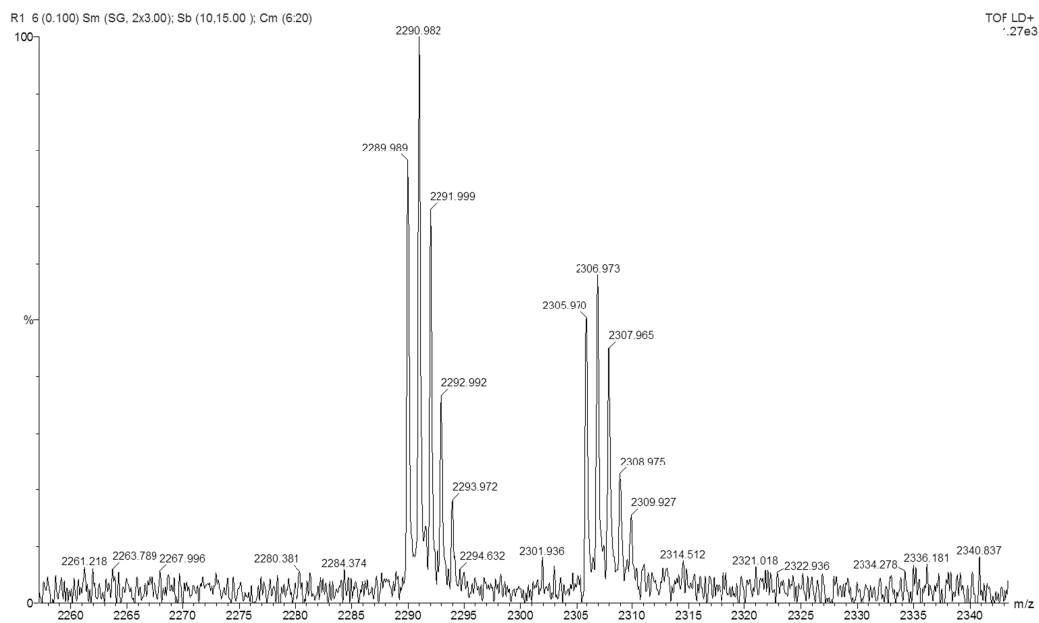


Crude RP-HPLC profile (5 to 100% B in 20 min, $\lambda = 214$ nm) of **12**.

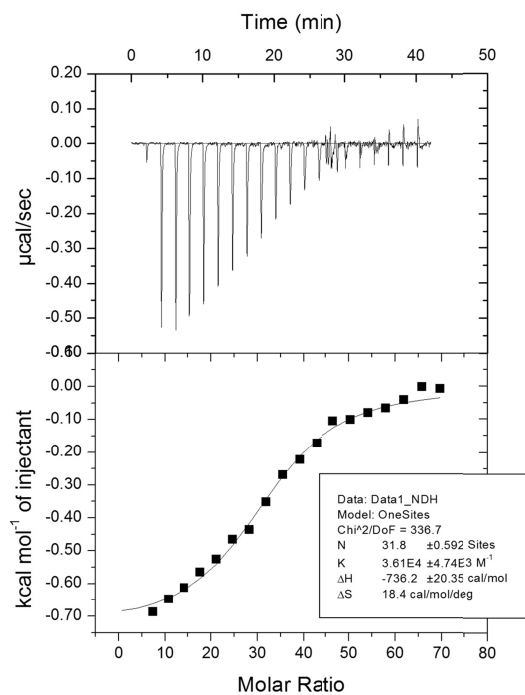


- S5 -

MALDI-TOF MS of **12**: m/z calcd. for $C_{96}H_{150}NaN_3O_{34}$ ($M + Na$)⁺ 2290.08, found 2289.99.

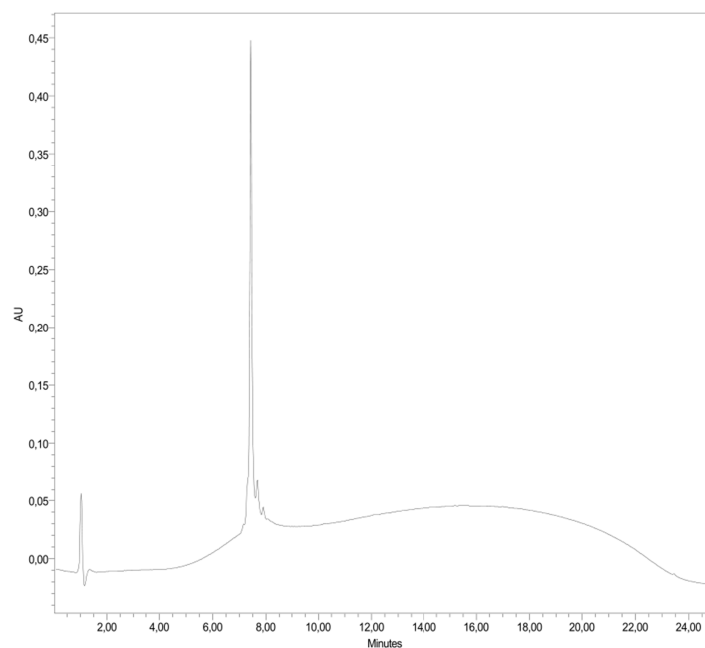


ITC data of **12** (ITC 200).

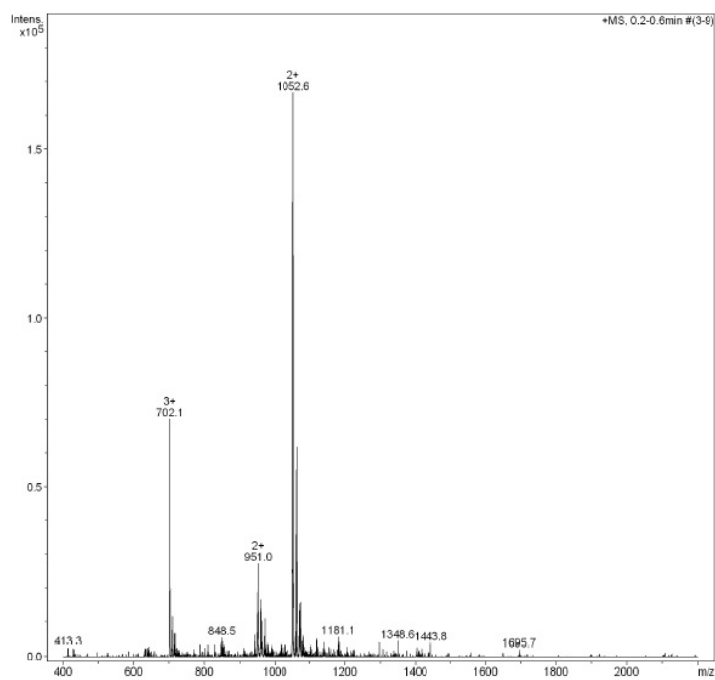


- S6 -

Crude RP-HPLC profile (5 to 100% B in 20 min, $\lambda = 214$ nm) of **13**.

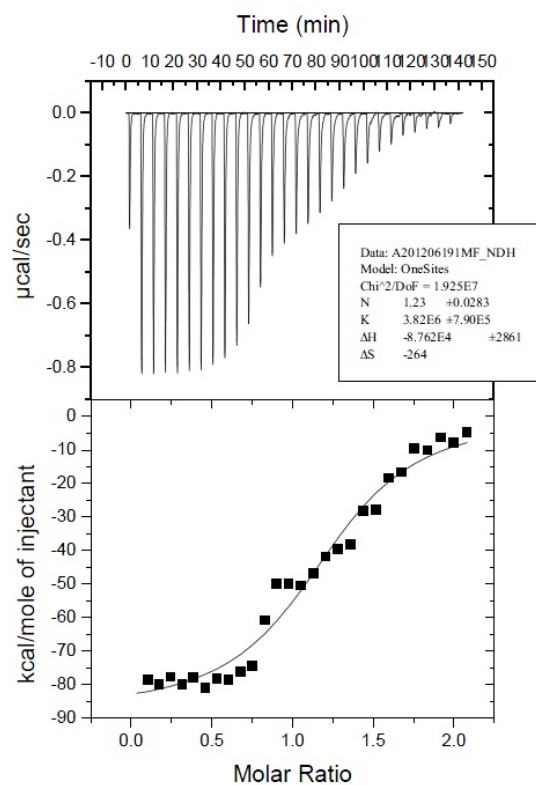


ESI MS spectrum of **13**: m/z calcd. for $C_{88}H_{145}N_{30}O_{34}$ ($M + H$)⁺ 2105.3, found 2105.1.



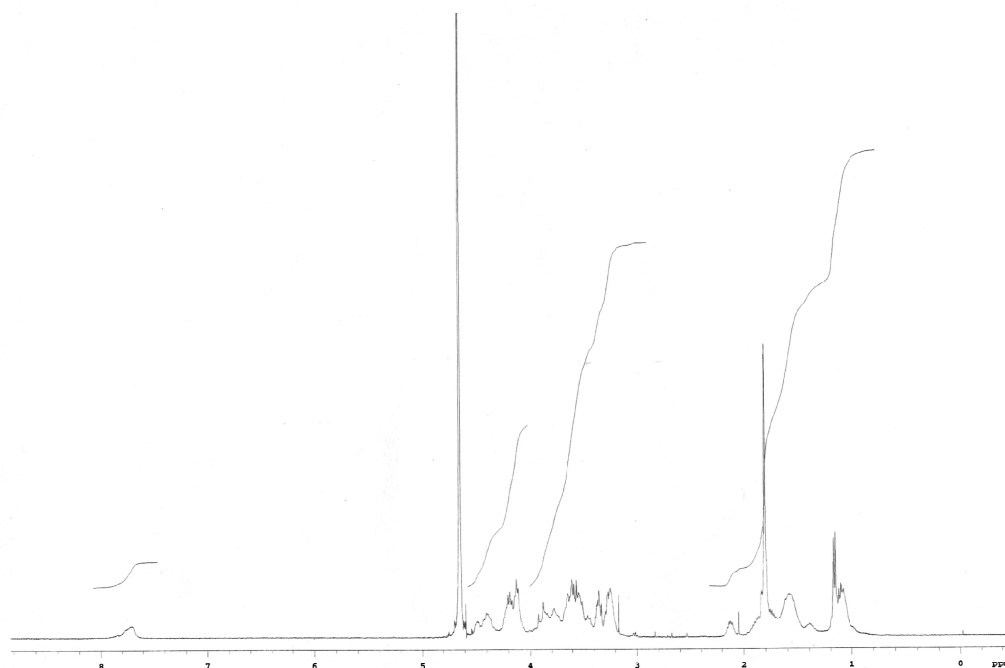
- S7 -

ITC data of **13** (VP-ITC).

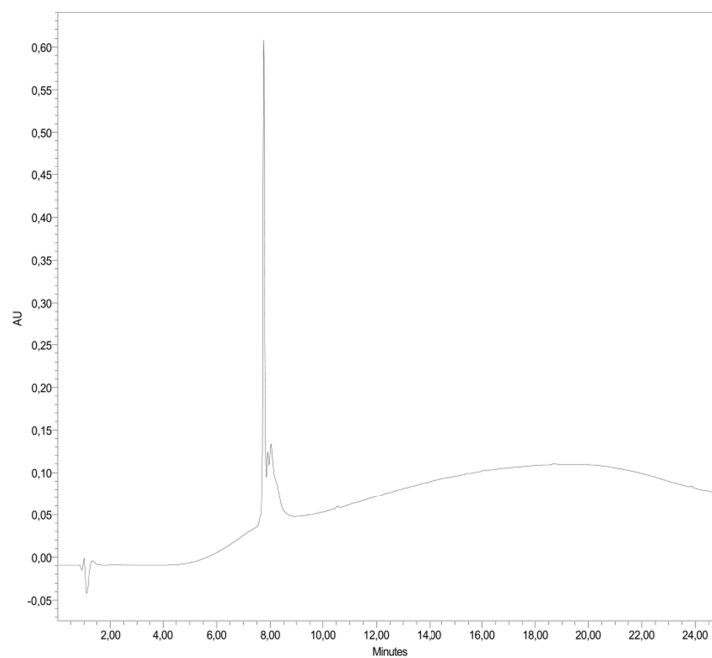


- S8 -

^1H NMR of **14** (D_2O , 400 MHz).

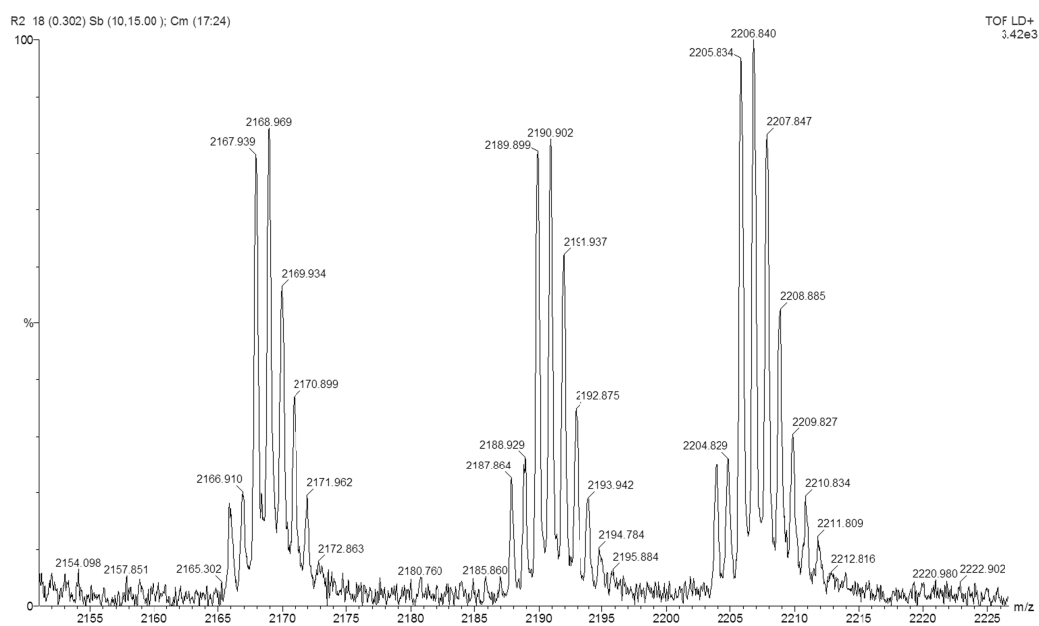


HPLC profile (5 to 100% B in 20 min, $\lambda = 214$ nm) of **14**.

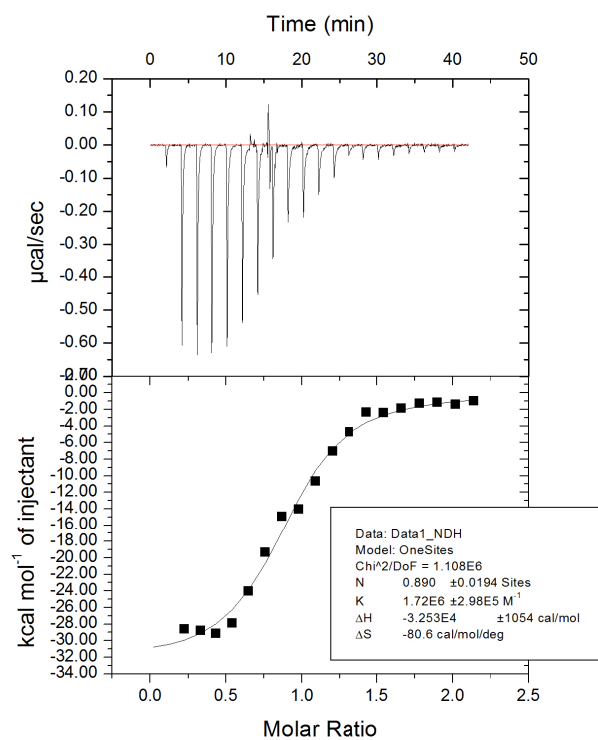


- S9 -

MALDI-TOF MS of **14**: calcd. for $C_{88}H_{138}N_{26}NaO_{30}S_4 (M + Na)^+$ 2189.88, found 2189.90.

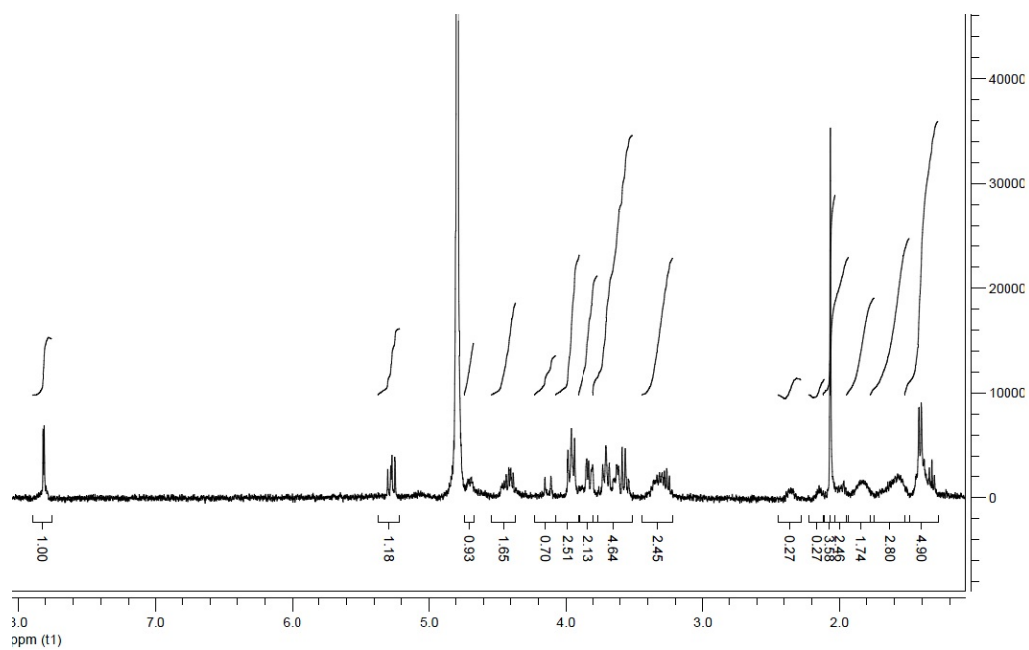


ITC data of **14** (ITC 200).

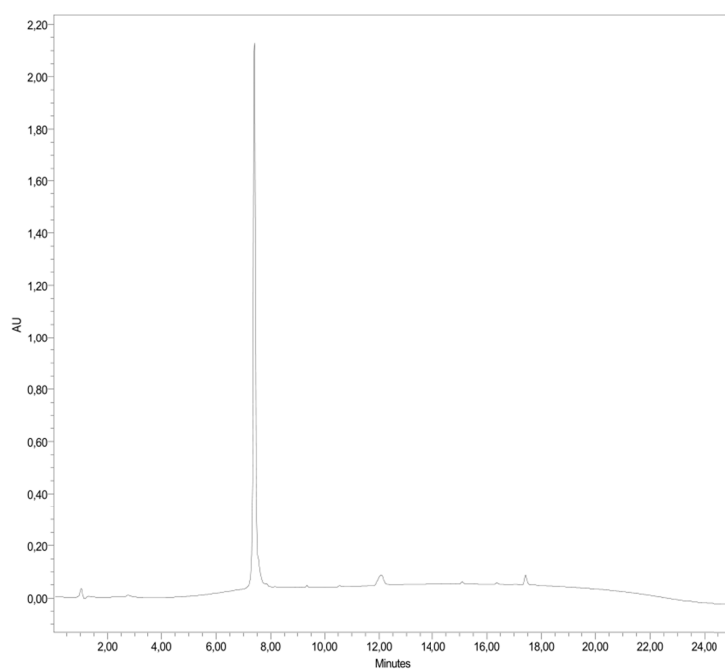


- S10 -

^1H NMR spectrum of **15** (D_2O , 400 MHz)

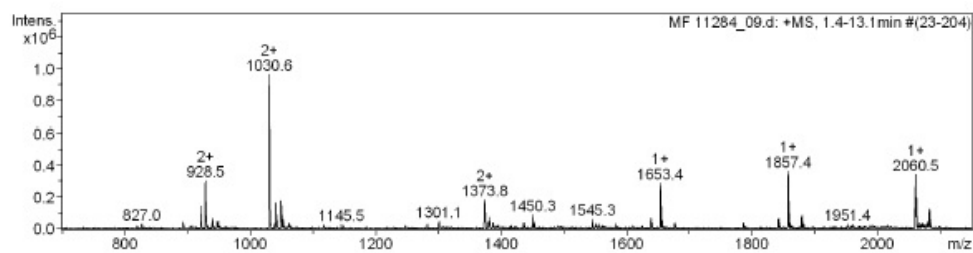


HPLC profile of **15** (5 to 100% B in 20 min, $\lambda = 214$ nm)

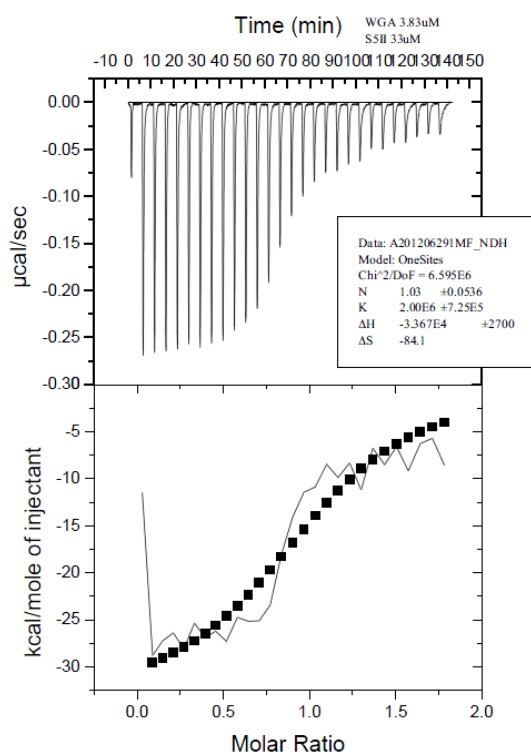


- S11 -

ESI MS of **15**: m/z calcd. for $C_{84}H_{135}N_{22}O_{38} (M + H)^+$ 2060.1, found 2060.3.

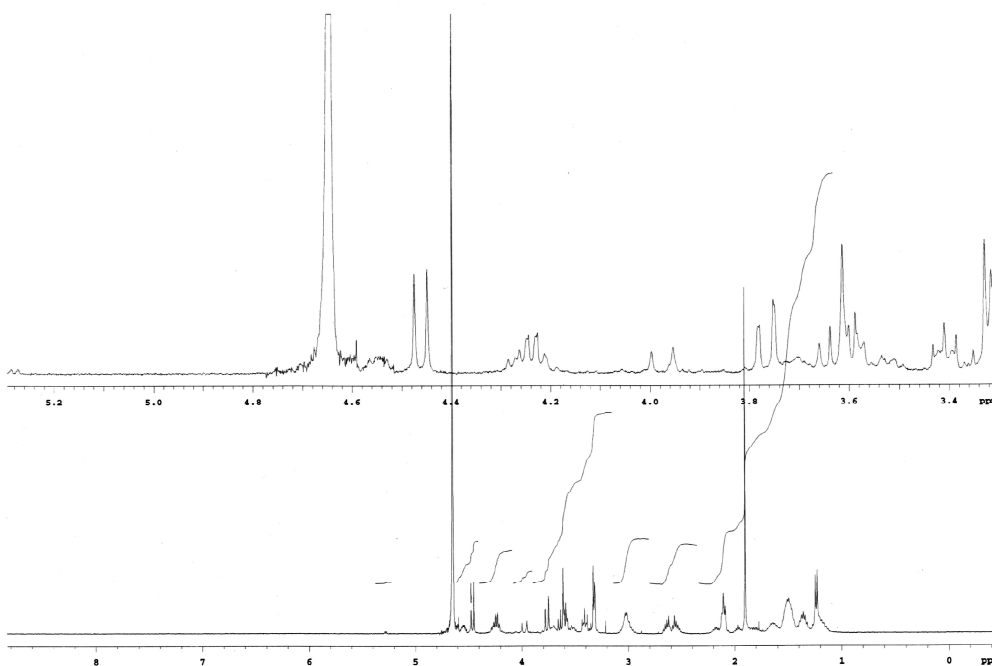


ITC data of **15** (VP-ITC).

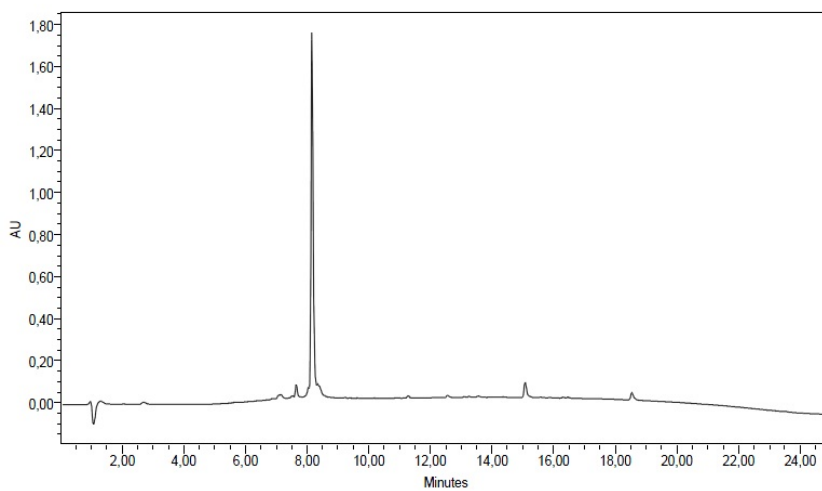


- S12 -

^1H NMR spectrum of **16** (400 MHz, D_2O).

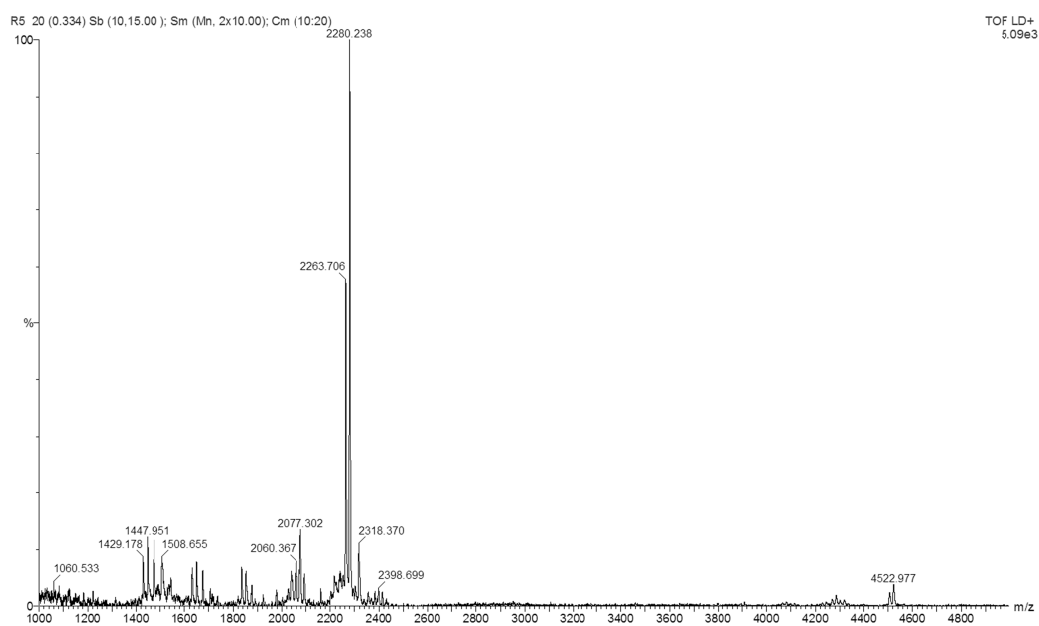


HPLC profile of **16** (5 to 100% B in 20 min, $\lambda = 214$ nm).

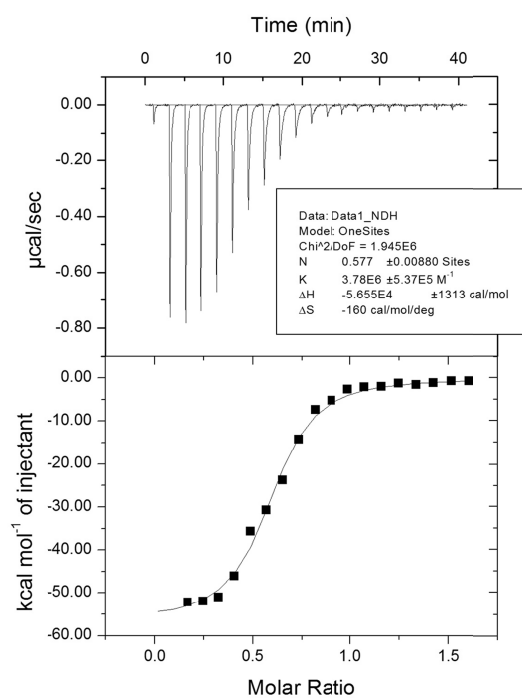


- S13 -

MALDI-TOF MS of **16**: m/z calcd. for $C_{96}H_{162}N_{18}NaO_{34}S_4 (M + Na)^+$ 2263.70, found 2263.71.

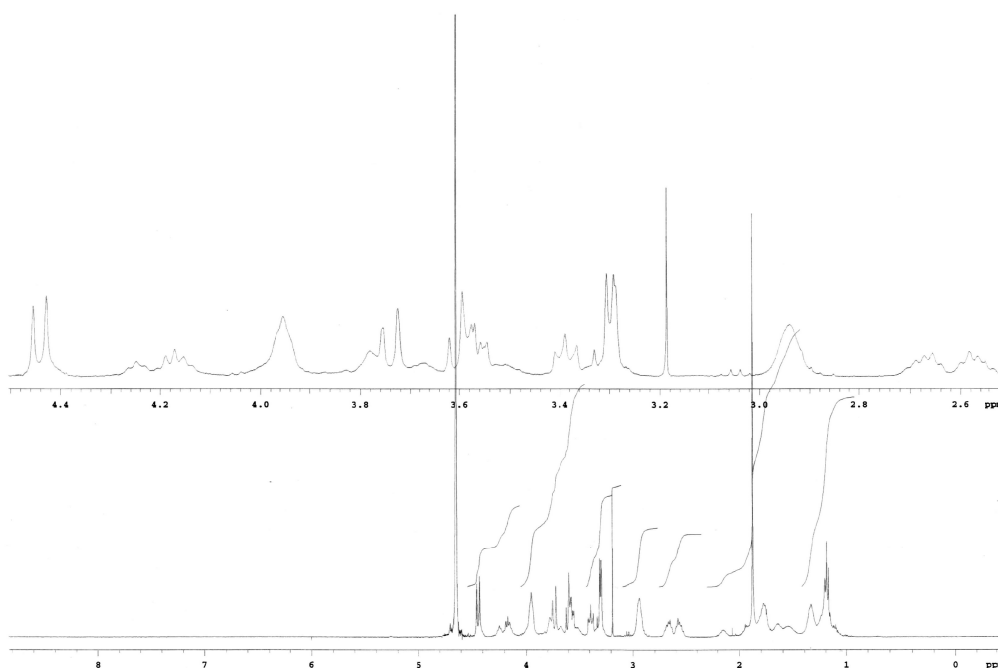


ITC data of **16** (ITC 200).

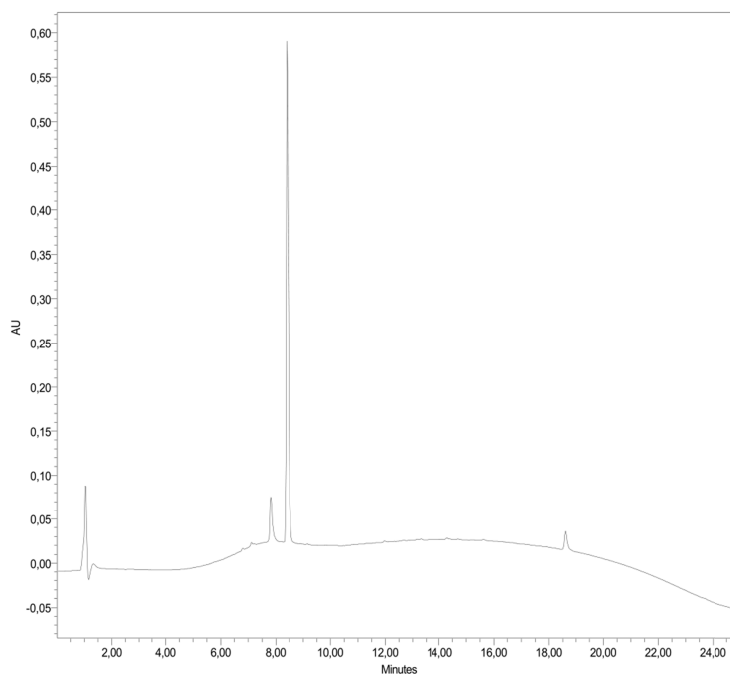


- S14 -

^1H NMR spectrum of **17** (D_2O , 400MHz).

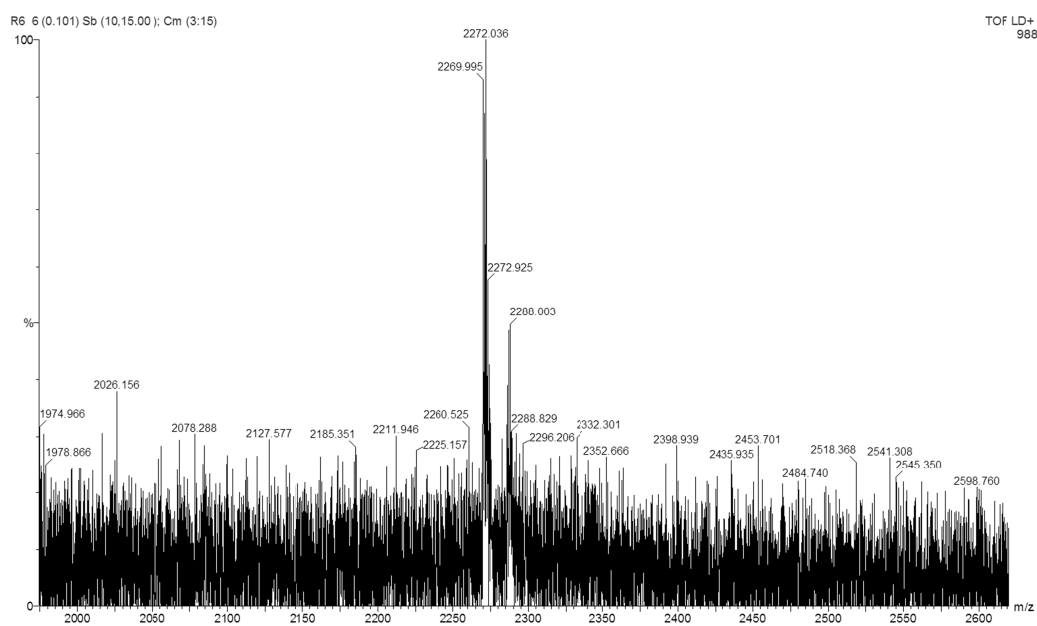


HPLC profile of **17** (5 to 100% B in 20 min, $\lambda = 214$ nm).

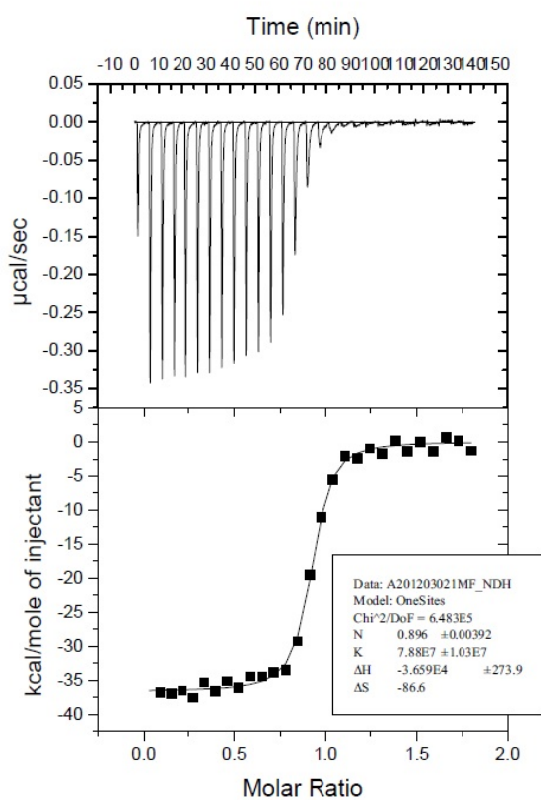


- S15 -

MALDI-TOF MS of **17**: m/z calcd. for $C_{92}H_{154}N_{18}NaO_{38}S_4 (M + Na)^+$ 2269.94, found 2269.99.

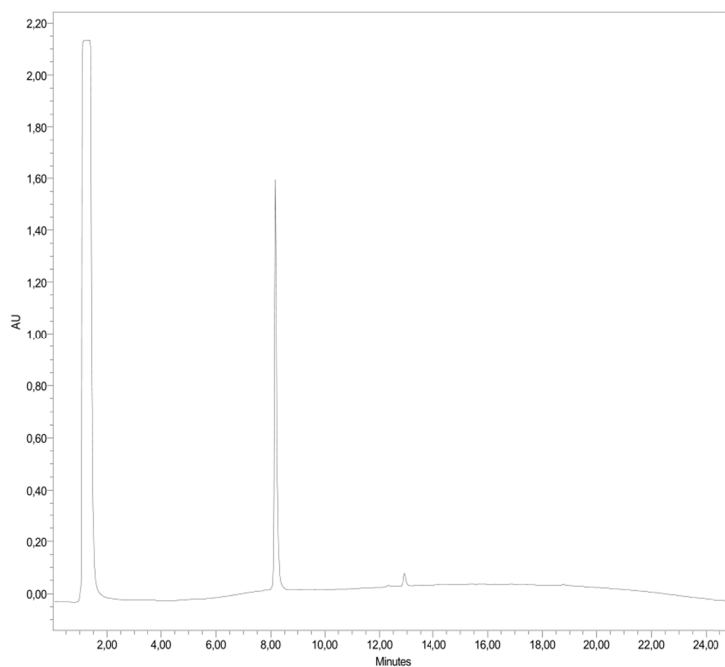


ITC data of **17** (VP-ITC).

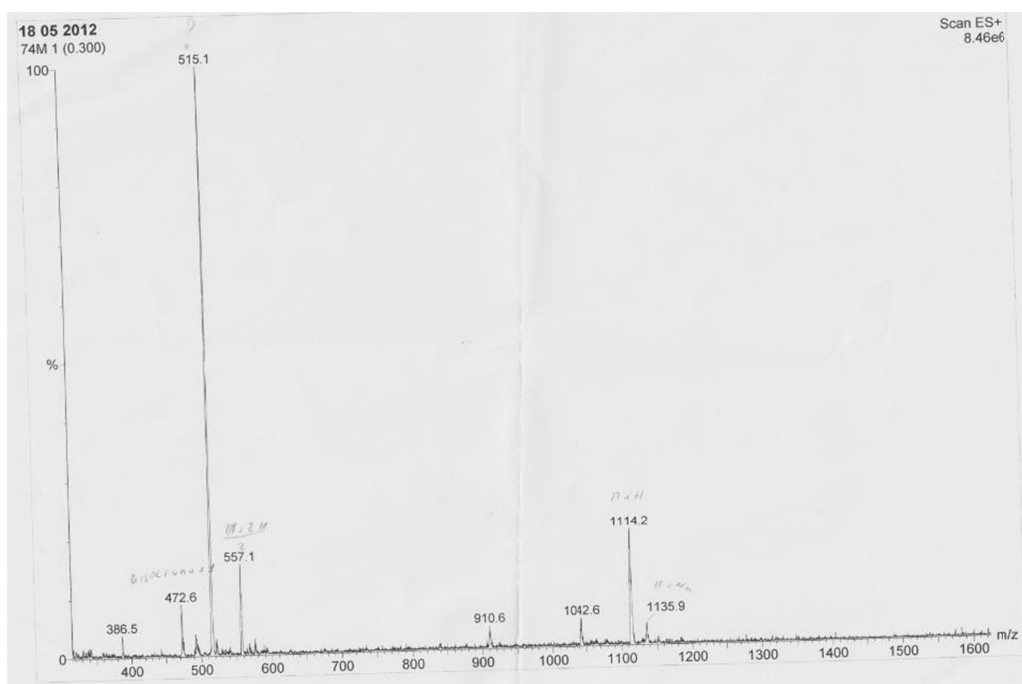


- S16 -

HPLC profile of **19** (5 to 100% B in 20 min, $\lambda = 214$ nm).

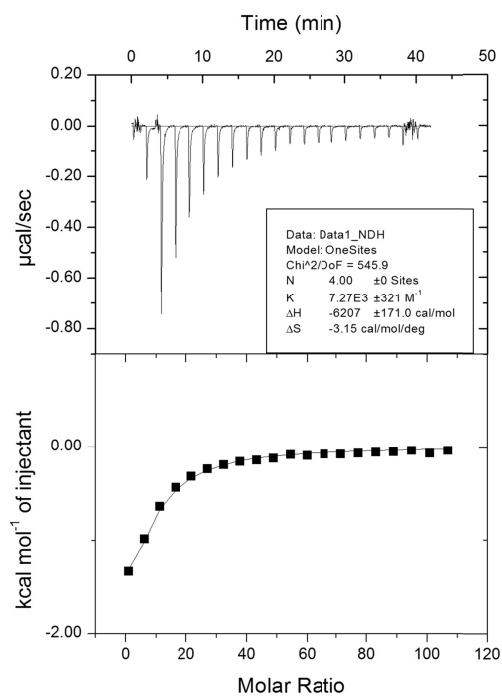


ESI MS of **19**: m/z calcd. for $C_{48}H_{79}N_{12}O_{16}S$ ($M + H$)⁺ 1113.7, found 1113.2.



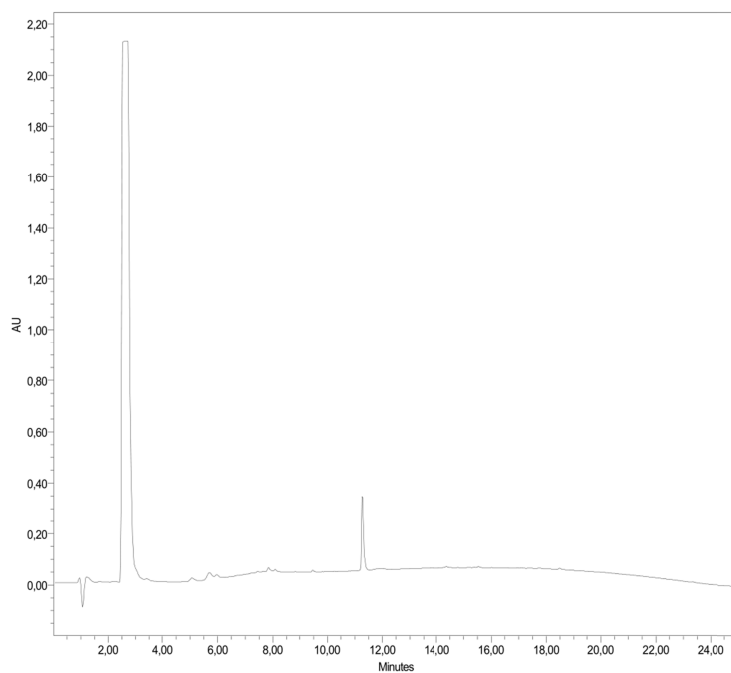
- S17 -

ITC data of **19** (VP-ITC).

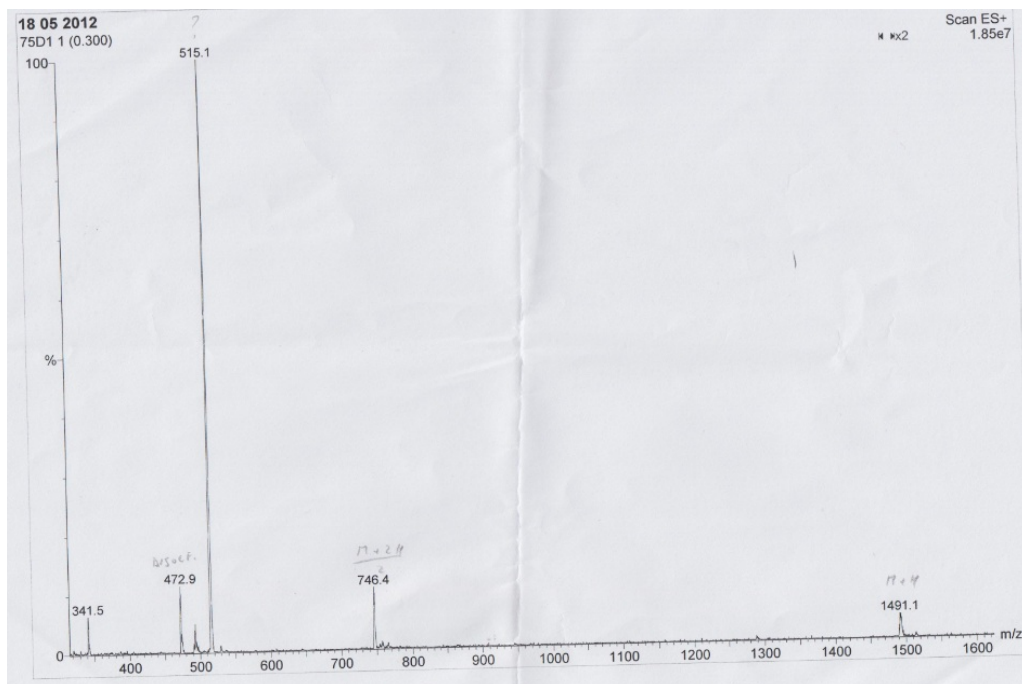


- S18 -

HPLC profile of **21** (5 to 100% B in 20 min, $\lambda = 214$ nm)

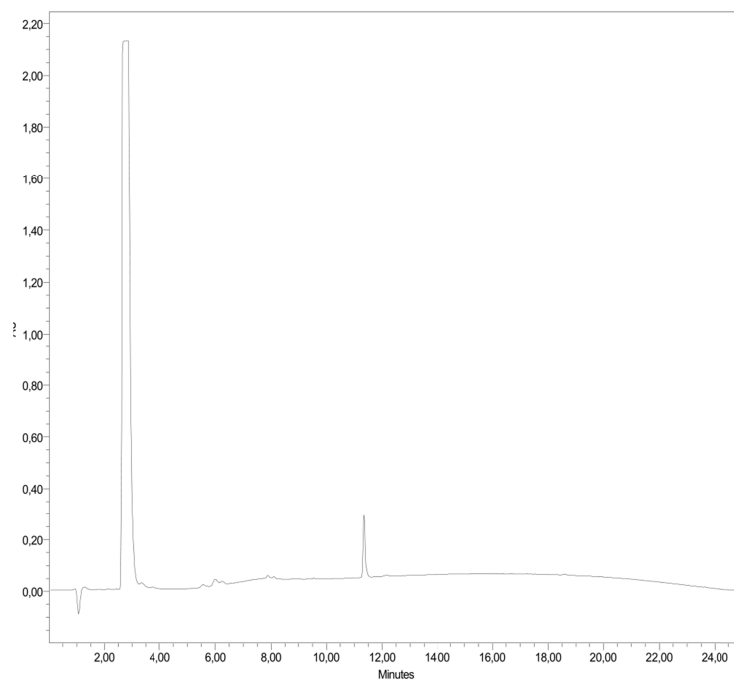


ESI MS of **21**: m/z calcd. for $C_{64}H_{107}N_{14}O_{22}S_4$ ($M + H$)⁺ 1491.4, found m/z 1491.1.

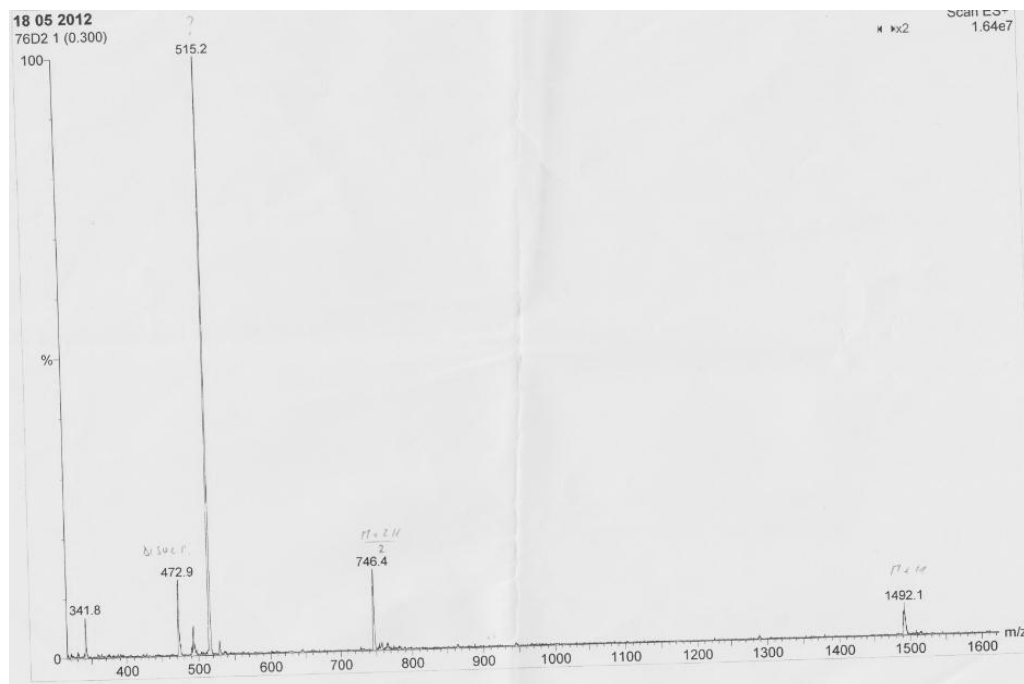


- S19 -

HPLC profile of **23** (5 to 100% B in 20 min, $\lambda = 214$ nm).

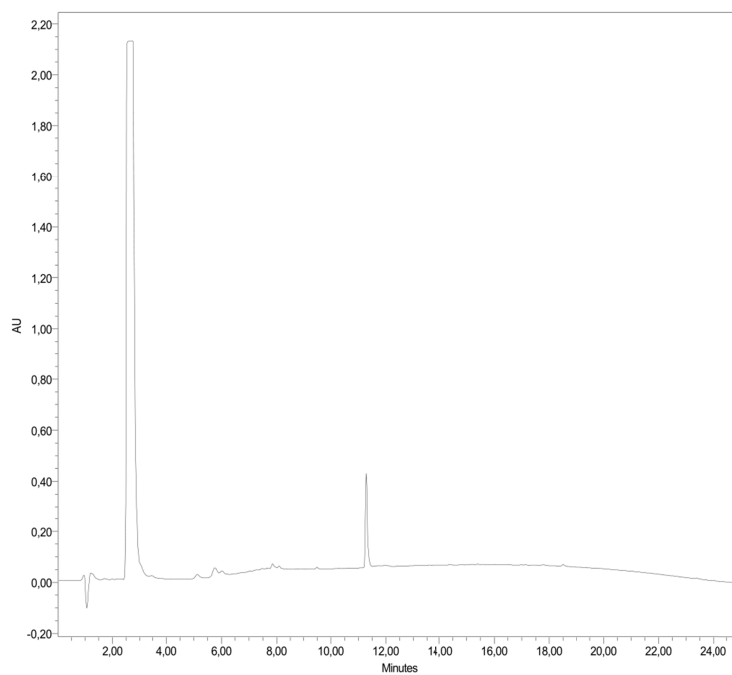


ESI MS of **23**: m/z calcd. for $C_{64}H_{107}N_{14}O_{22}S_4$ ($M + H$)⁺ 1491.4, found m/z 1492.0.

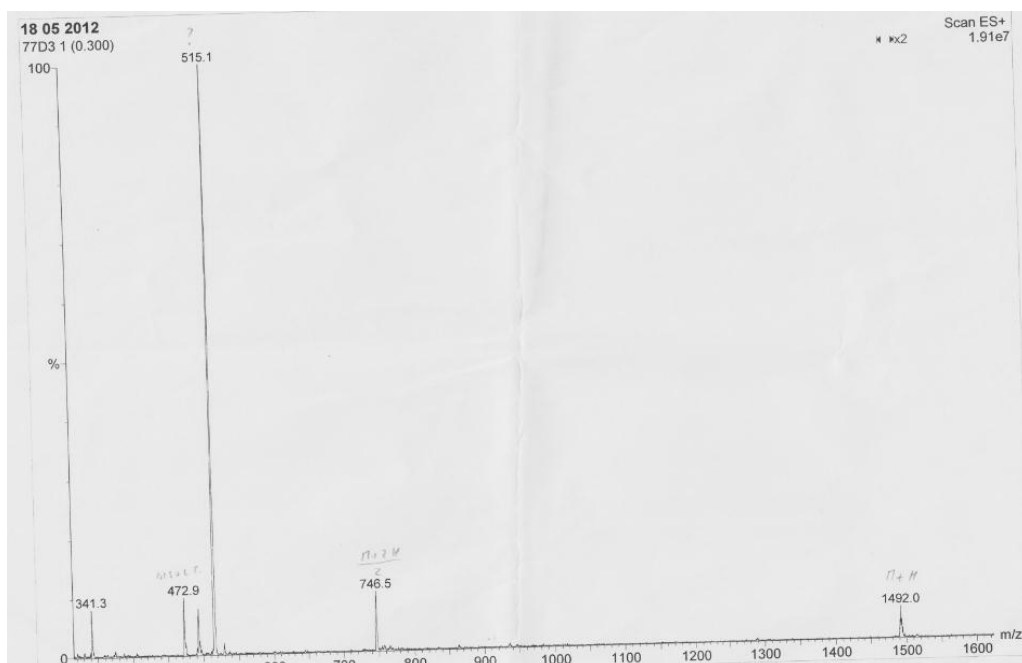


- S20 -

HPLC profile of **25** (5 to 100% B in 20 min, $\lambda = 214$ nm).

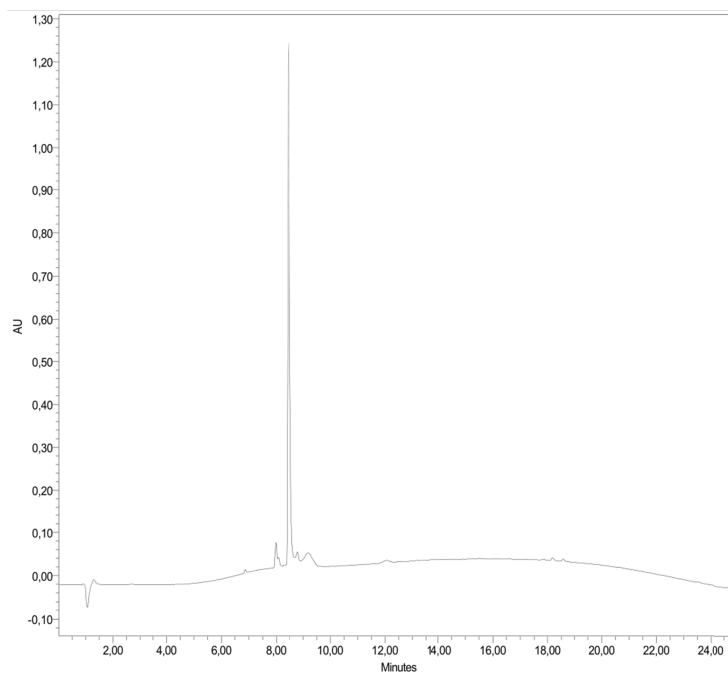


ESI MS of **25**: m/z calcd. for $C_{64}H_{107}N_{14}O_{22}S_4$ ($M + H$)⁺ 1491.4, found m/z 1492.0.

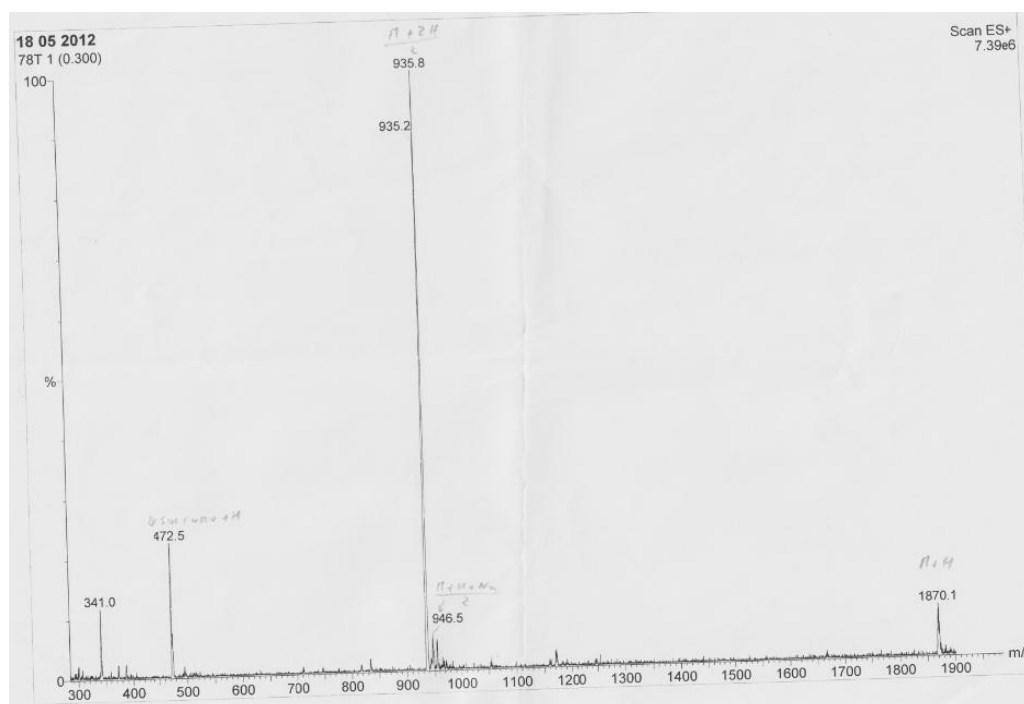


- S21 -

HPLC profile of **27** (5 to 100% B in 20 min, $\lambda = 214$ nm).

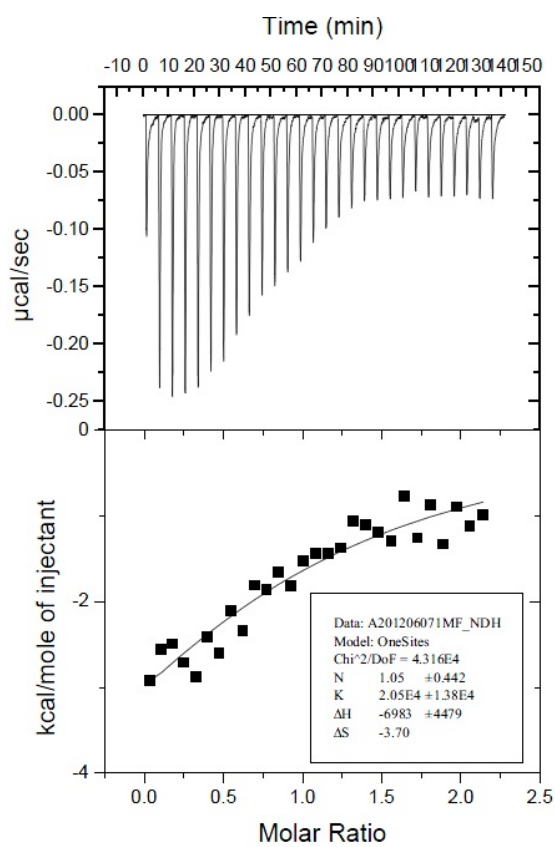


ESI MS of **27**: m/z calcd. for $C_{80}H_{135}N_{16}O_{28}S_3$ ($M + H$)⁺ 1870.3, found 1870.1.



- S22 -

ITC data of **27** (VP-ITC).



- S23 -

ITC data of GlcNAc (VP-ITC).

