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Supporting Information

Mechanistic Insight into Nanomolar Binding of Multivalent Neoglycopeptides to Wheat Germ Agglutinin

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chem_201600657_sm_miscellaneous_information.pdf

Supporting Information

S2

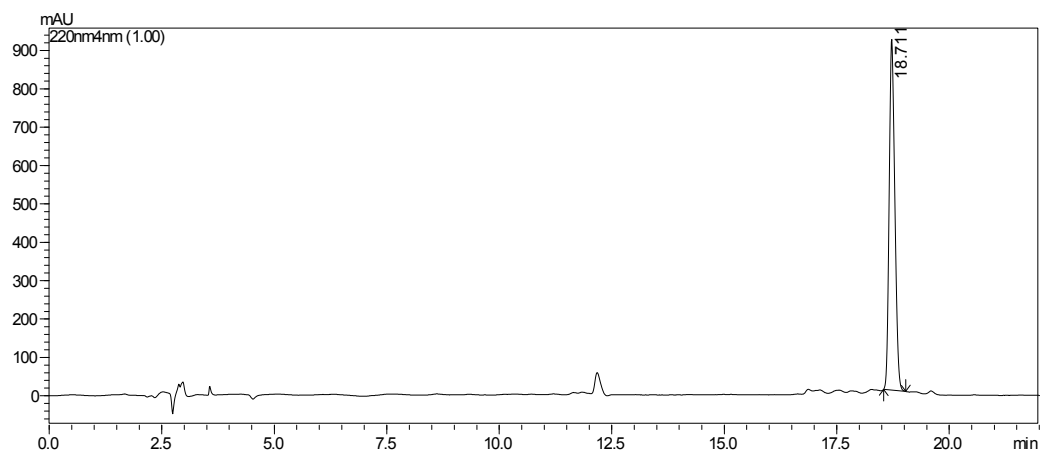**Content**

HPLC Profiles of Glycopeptides 1–10

Figure S1. HPLC profile of **1** (5-30% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
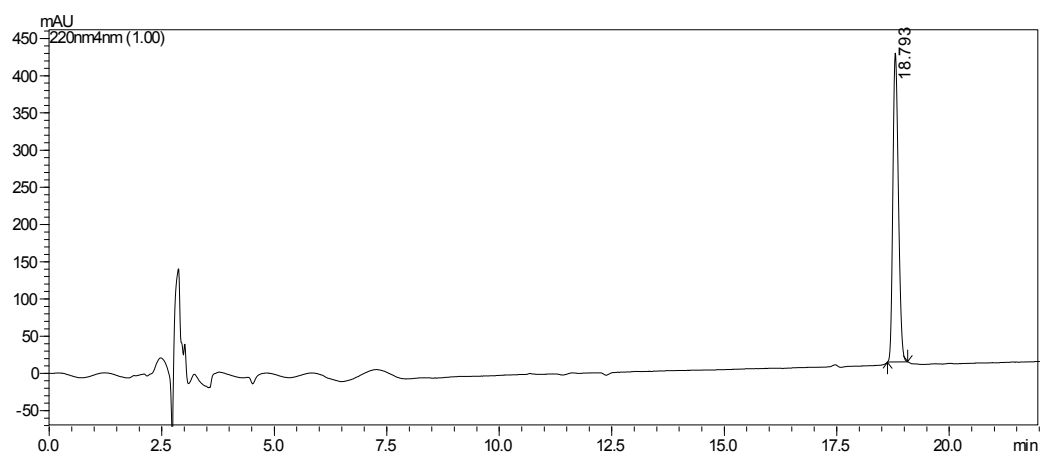

Figure S2. HPLC profile of **2** (5-30% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
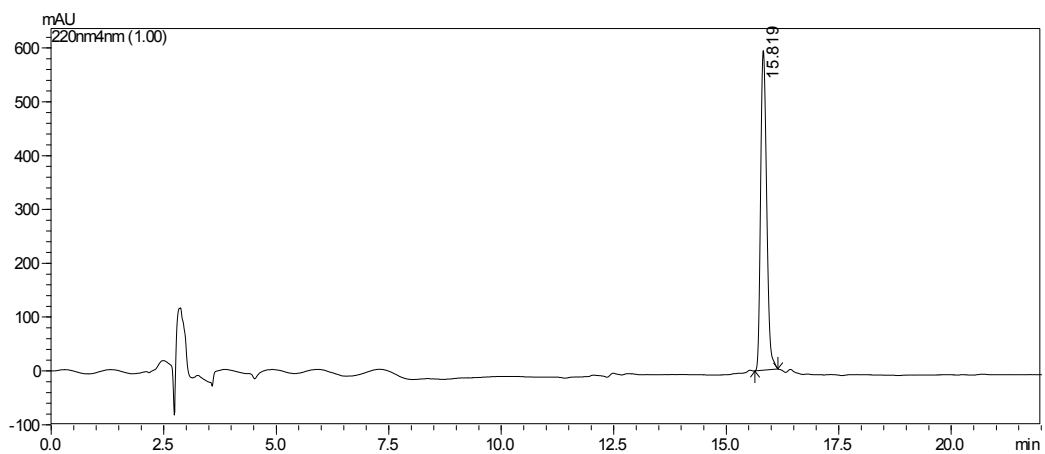
Figure S3 HPLC profile of **3** (5-20% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
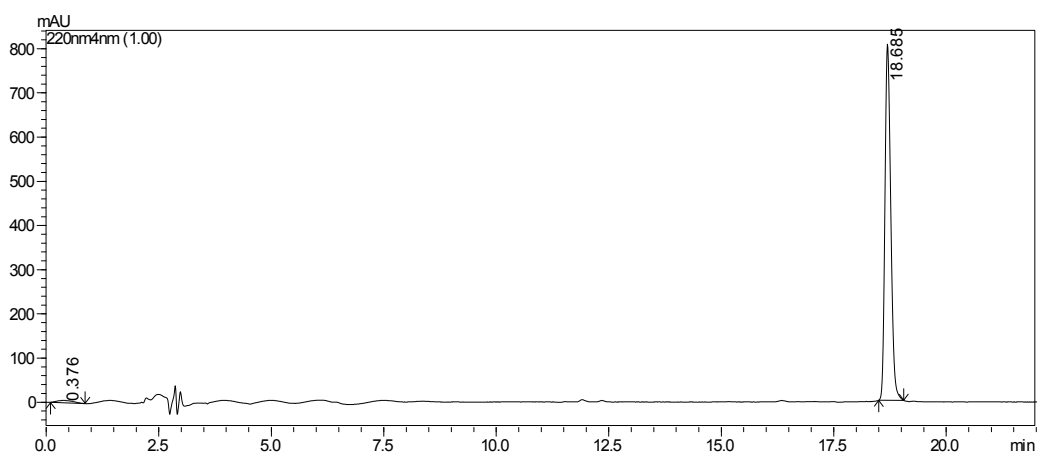

Figure S4. HPLC profile of **4** (5-30% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
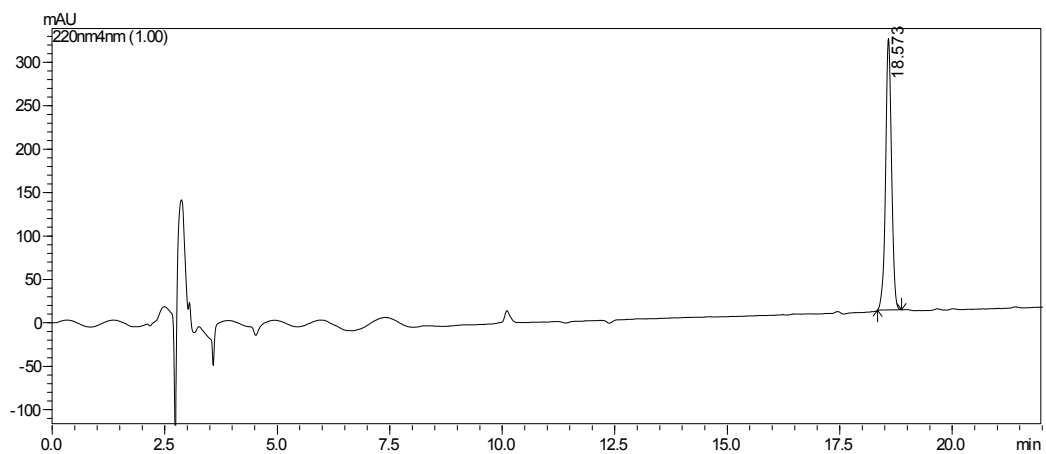
Figure S5. HPLC profile of **5** (5-30% MeCN in H$_2$O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
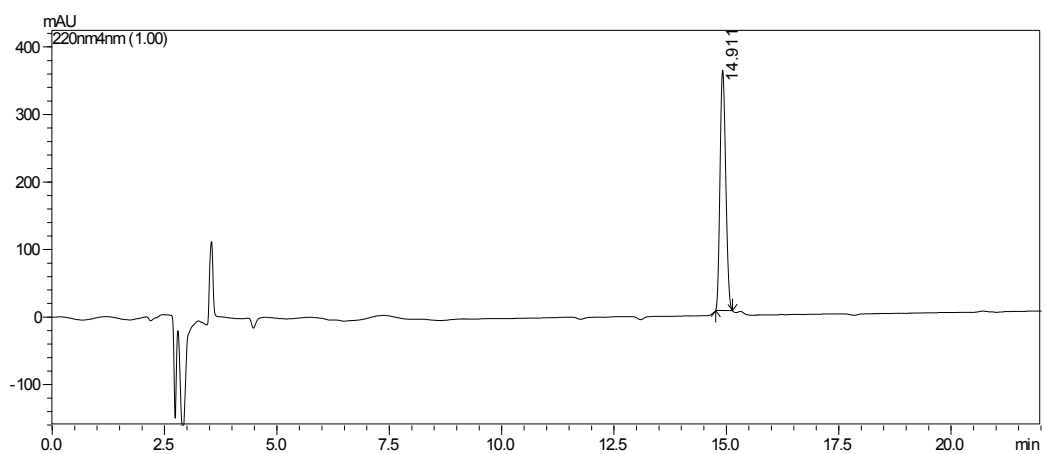

Figure S6. HPLC profile of **6** (5-20% MeCN in H$_2$O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
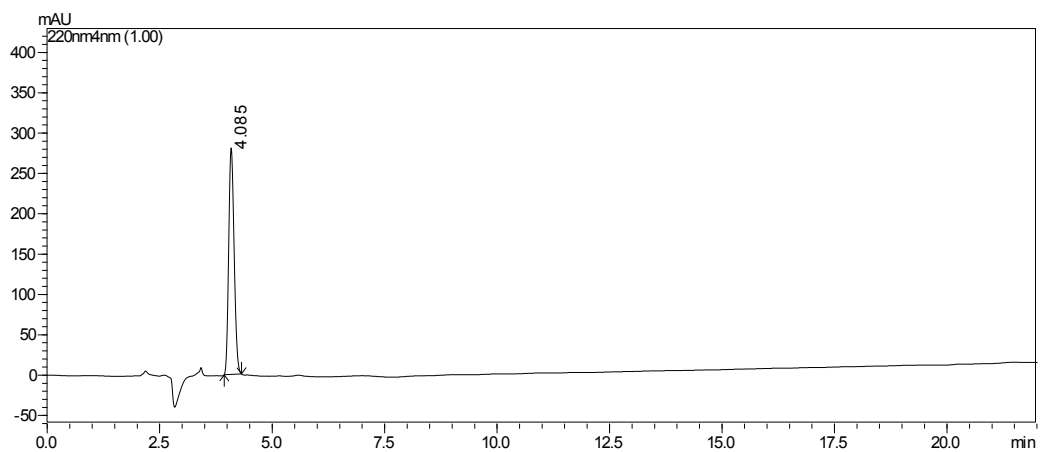
Figure S7. HPLC profile of **7** (5-10% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
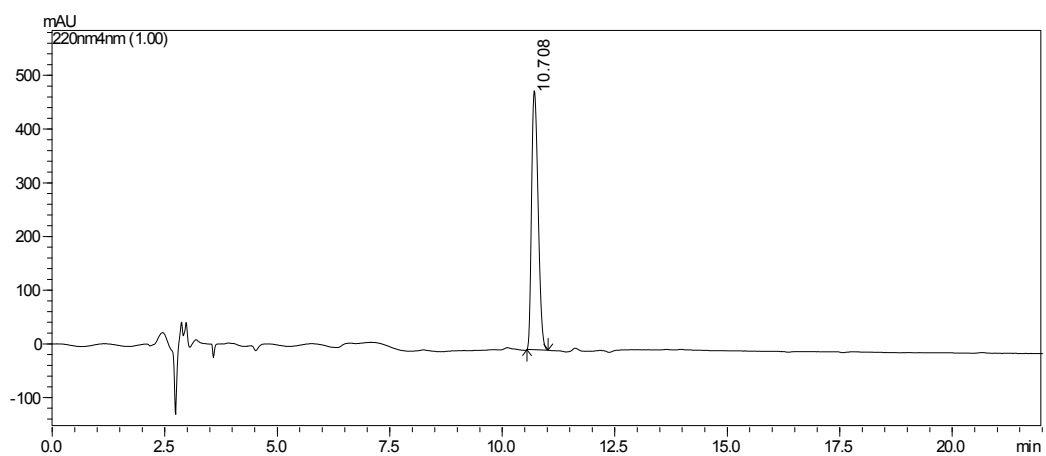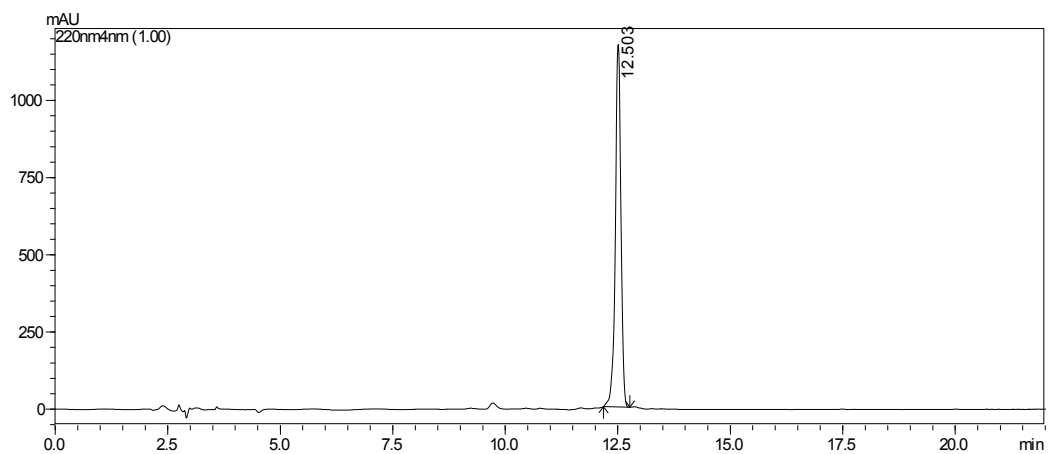

Figure S8. HPLC profile of **8** (5-20% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).

Figure S9. HPLC profile of **9** (5-30% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
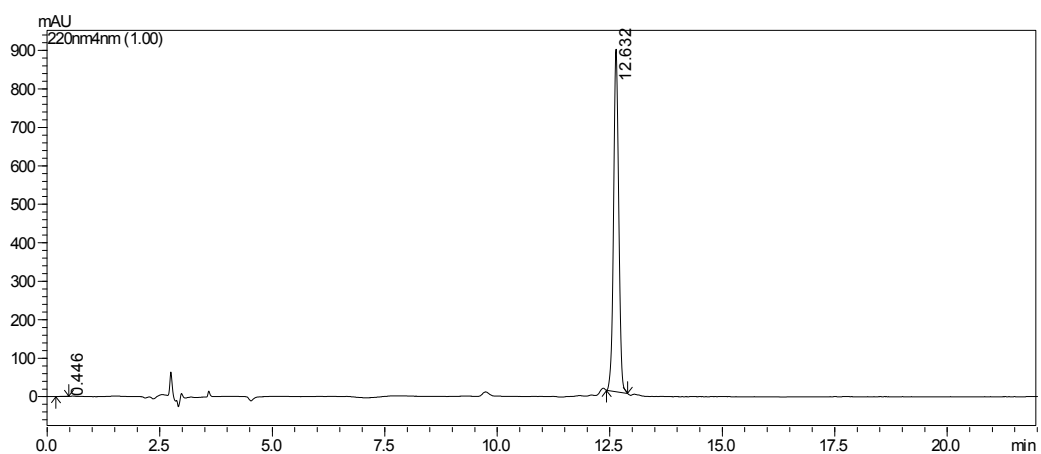

Figure S10. HPLC profile of **10** (5-30% MeCN in H_2O + 0.1% formic acid in 20 min, Macherey-Nagel EC 250/4 Nucleodur 100-5 C 18 ec).
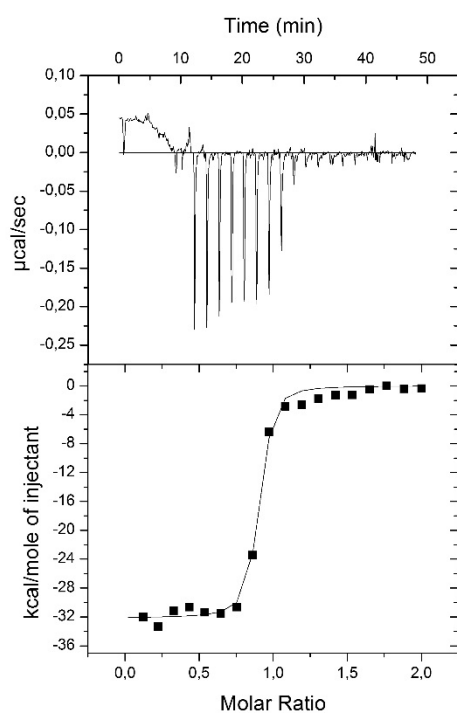
ITC Data of Glycopeptides 1–10

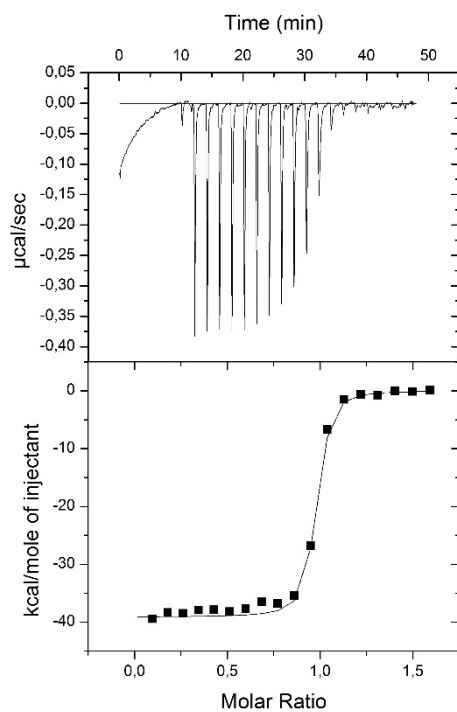**Figure S11.** ITC binding profile of **1**. [WGA] = 4 μM, [**1**] = 41 μM

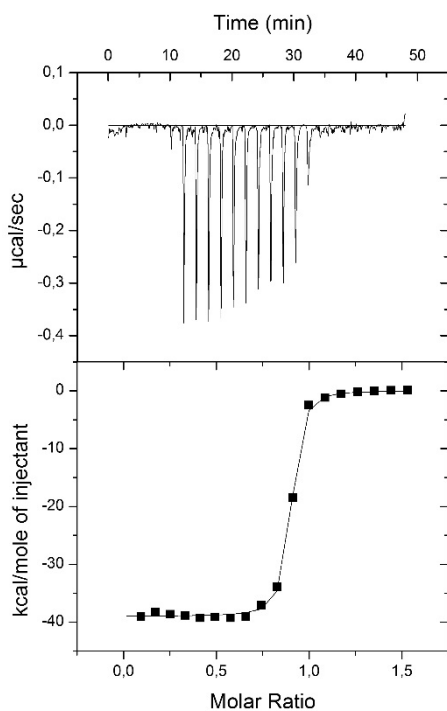**Figure S12.** ITC binding profile of **2**. [WGA] = 8 μM, [**2**] = 63 μM

Figure S13. ITC binding profile of **3**. [WGA] = 8 μM, [**3**] = 62 μM
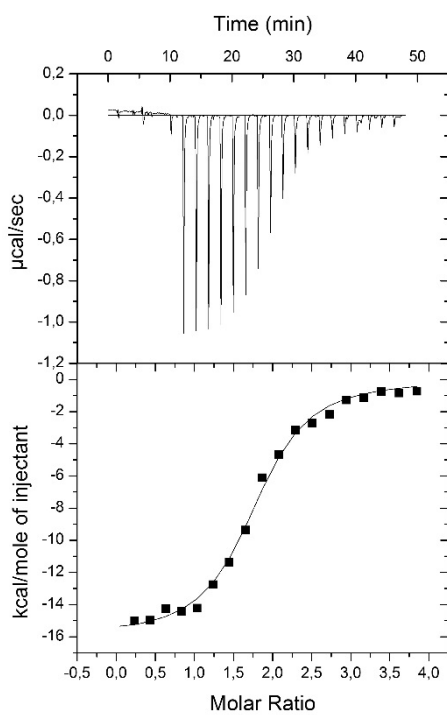
Figure S14. ITC binding profile of **4**. [WGA] = 20 μM, [**4**] = 390 μM
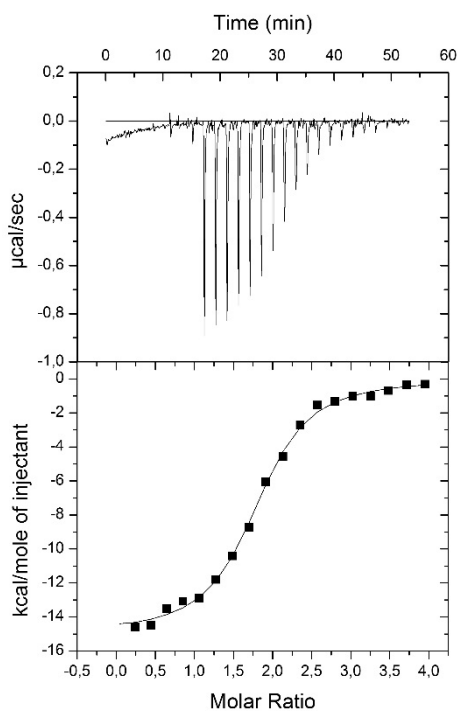
Figure S15. ITC binding profile of **5**. [WGA] = 18 µM, [**5**] = 378 µM
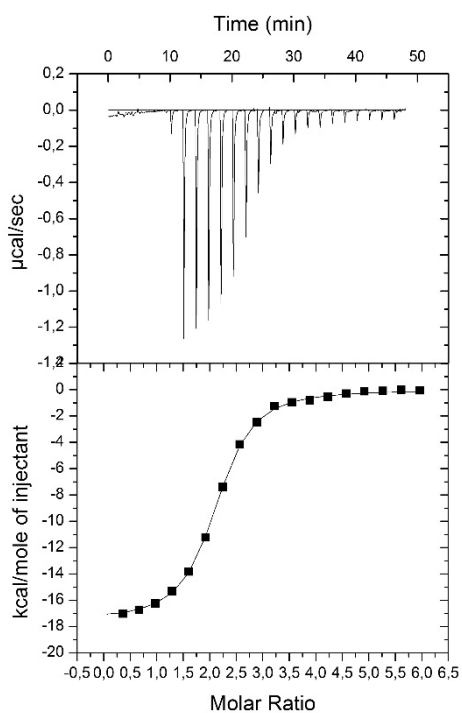
Figure S16. ITC binding profile of **6**. [WGA] = 14 µM, [**6**] = 430 µM
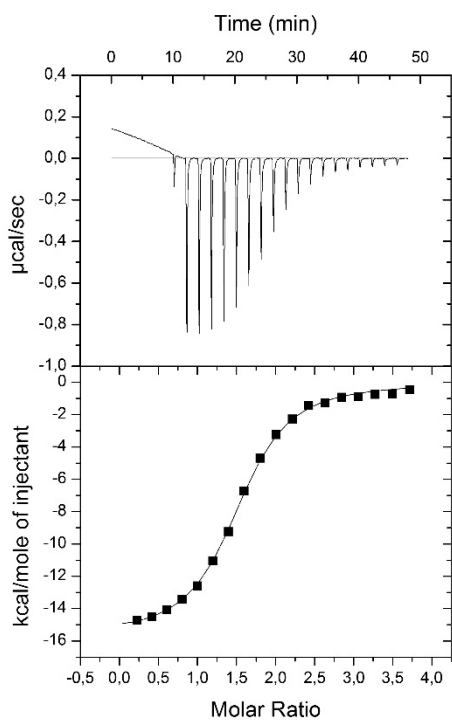
Figure S17. ITC binding profile of **7**. [WGA] = 19 µM, [**7**] = 365 µM
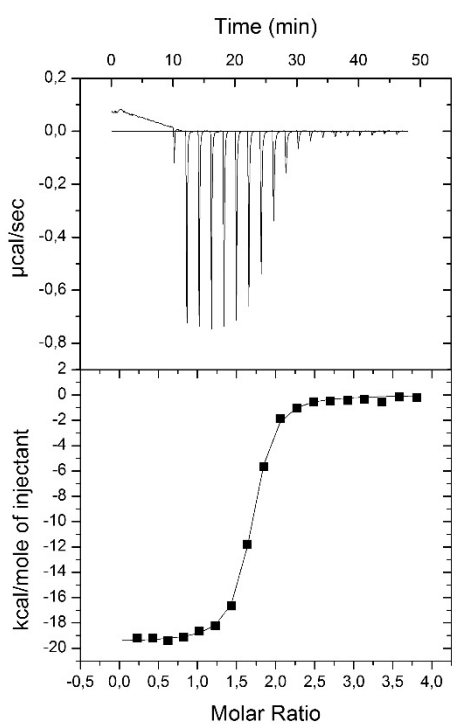
Figure S18. ITC binding profile of **8**. [WGA] = 11 µM, [**8**] = 226 µM
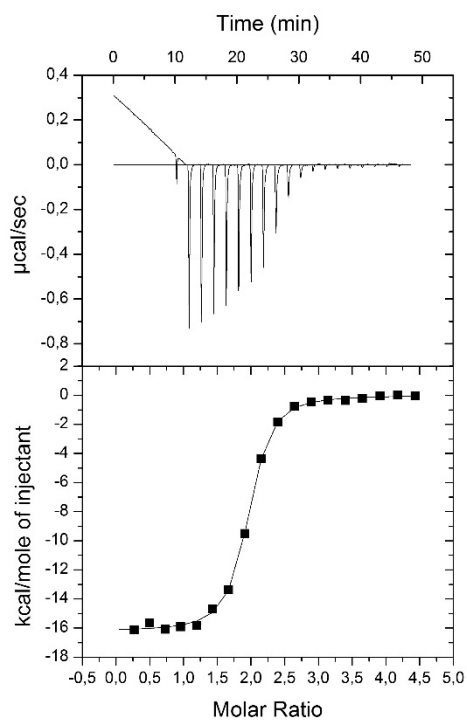
Figure S19. ITC binding profile of **9**. [WGA] = 11 μM, [**9**] = 226 μM
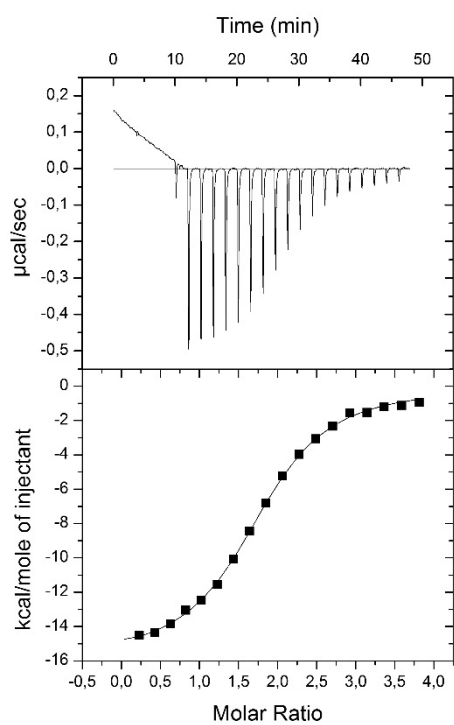
Figure S20. ITC binding profile of **10**. [WGA] = 11 μM, [**10**] = 216 μM

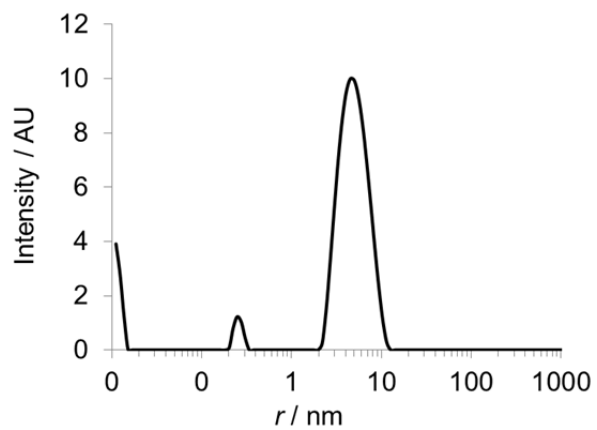**DLS Data Glycopeptides 1–10**

Figure S21. DLS intensity distribution of **1** incubated with WGA. [WGA] = 21 µM, [**1**] = 21 µM
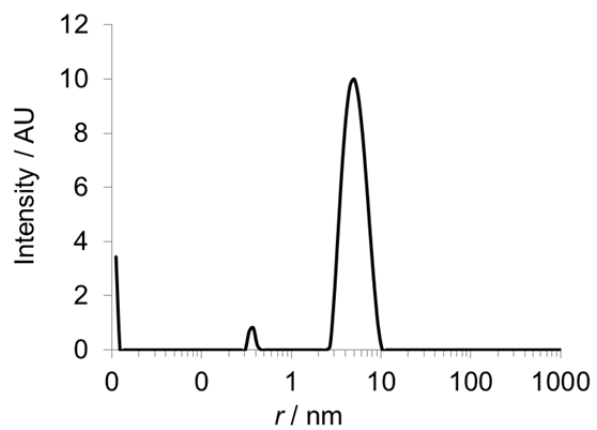

Figure S22. DLS intensity distribution of **2** incubated with WGA. [WGA] = 22 µM, [**2**] = 22 µM
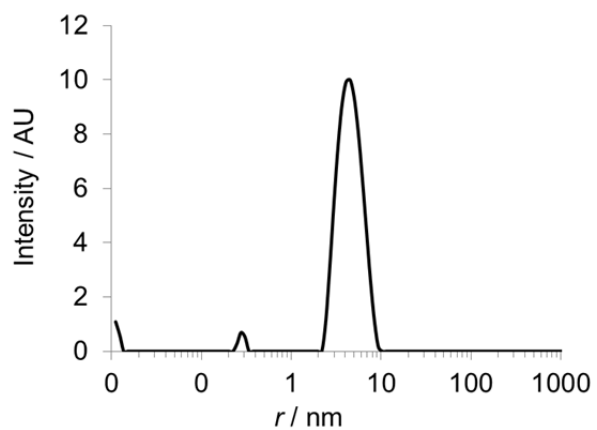
Figure S23. DLS intensity distribution of **3** incubated with WGA. [WGA] = 20 µM, [**3**] = 20 µM
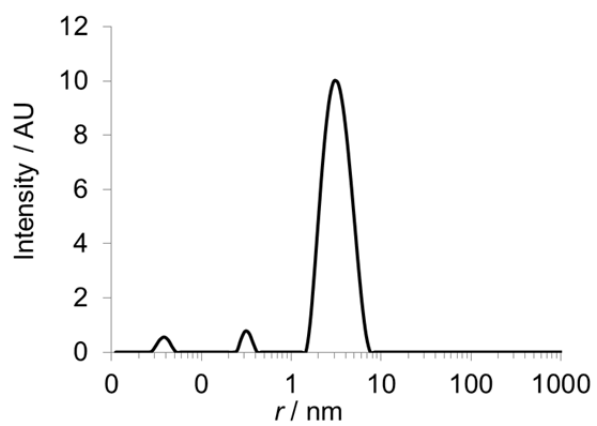

Figure S24. DLS intensity distribution of **4** incubated with WGA. [WGA] = 18 µM, [**4**] = 36 µM
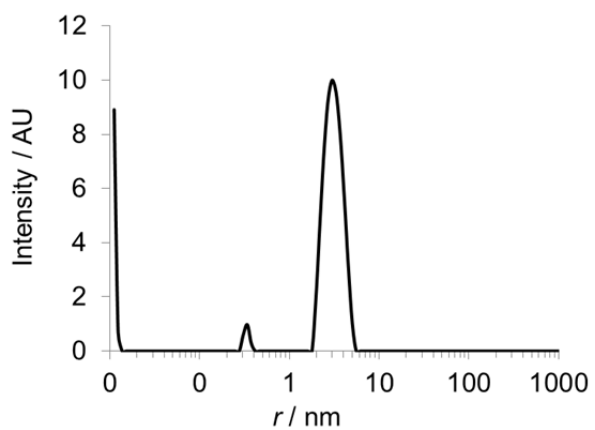
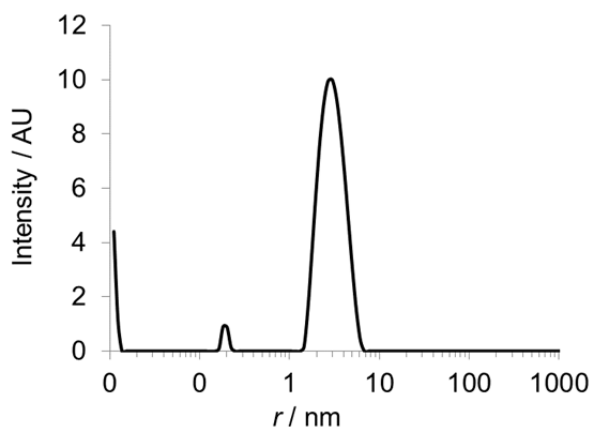**Figure S25.** DLS intensity distribution of **5** incubated with WGA. [WGA] = 21 µM, [**5**] = 41 µM

Figure S26. DLS intensity distribution of **6** incubated with WGA. [WGA] = 20 µM, [**6**] = 40 µM
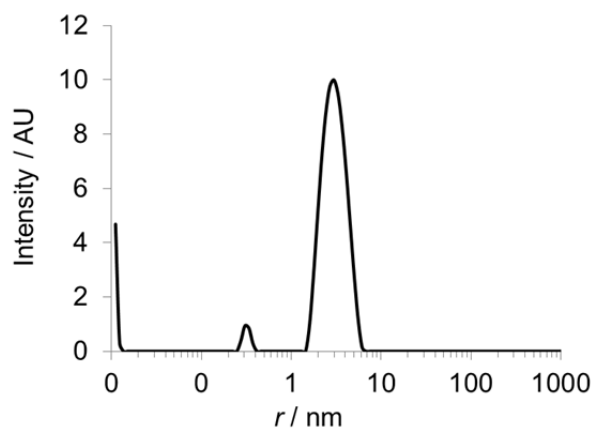
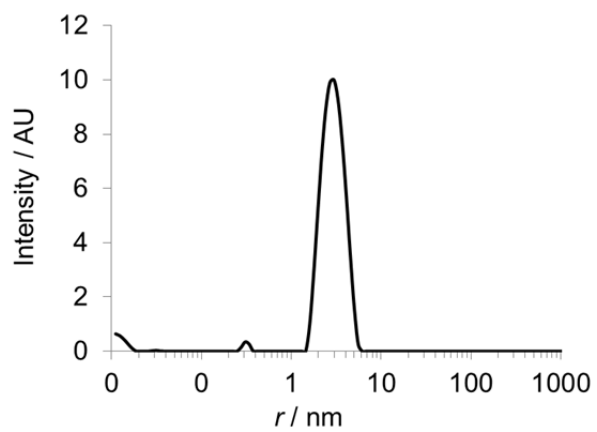**Figure S27.** DLS intensity distribution of **7** incubated with WGA. [WGA] = 22 µM, [**7**] = 43 µM

Figure S28. DLS intensity distribution of **8** incubated with WGA. [WGA] = 32 µM, [**8**] = 63 µM
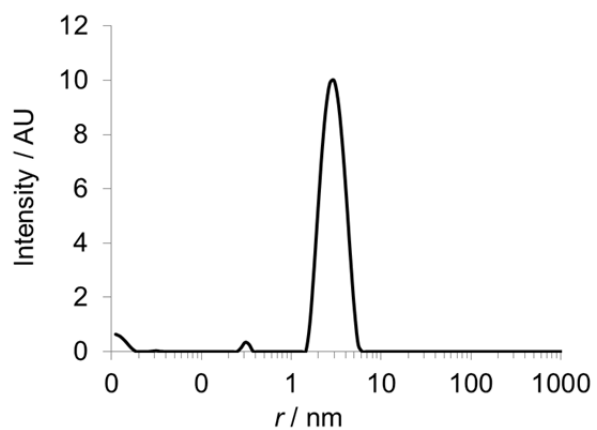
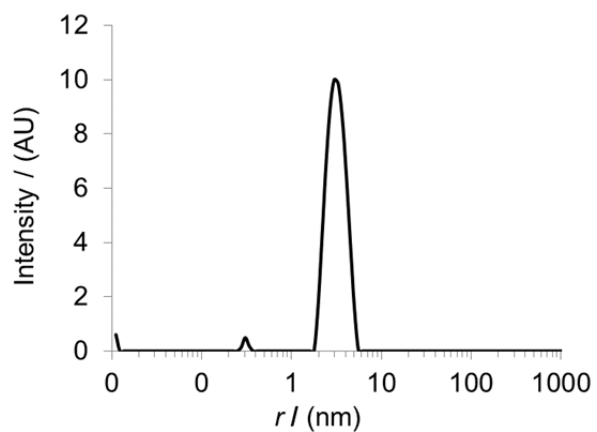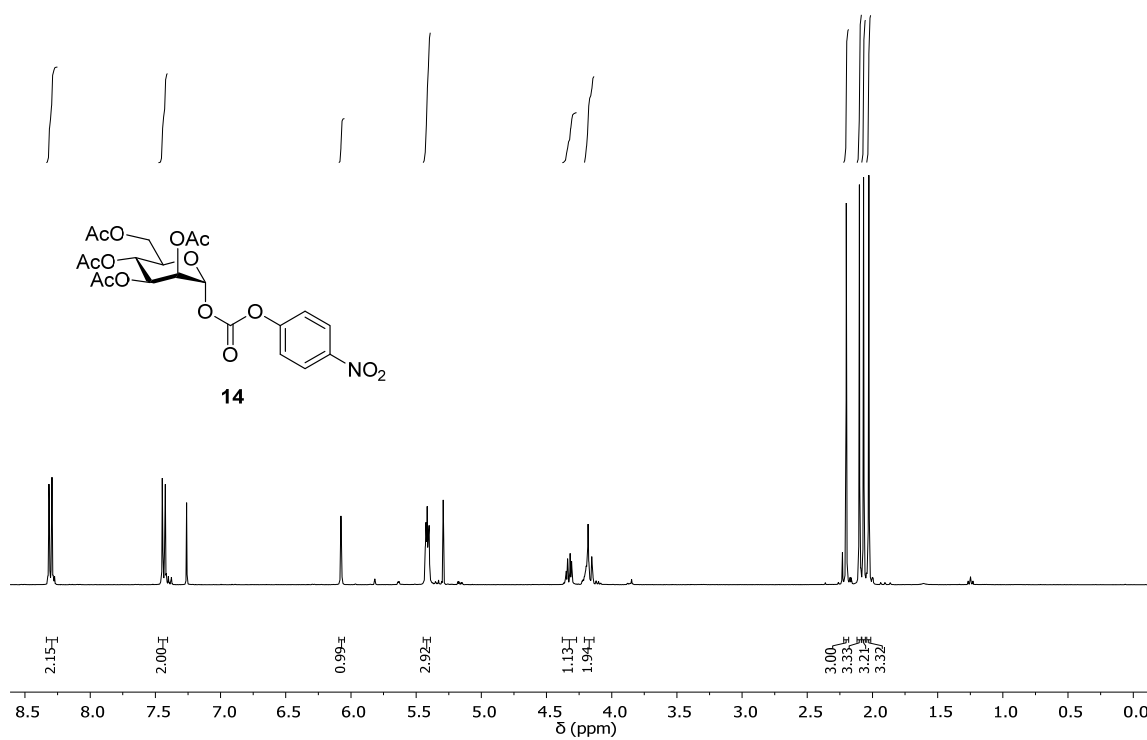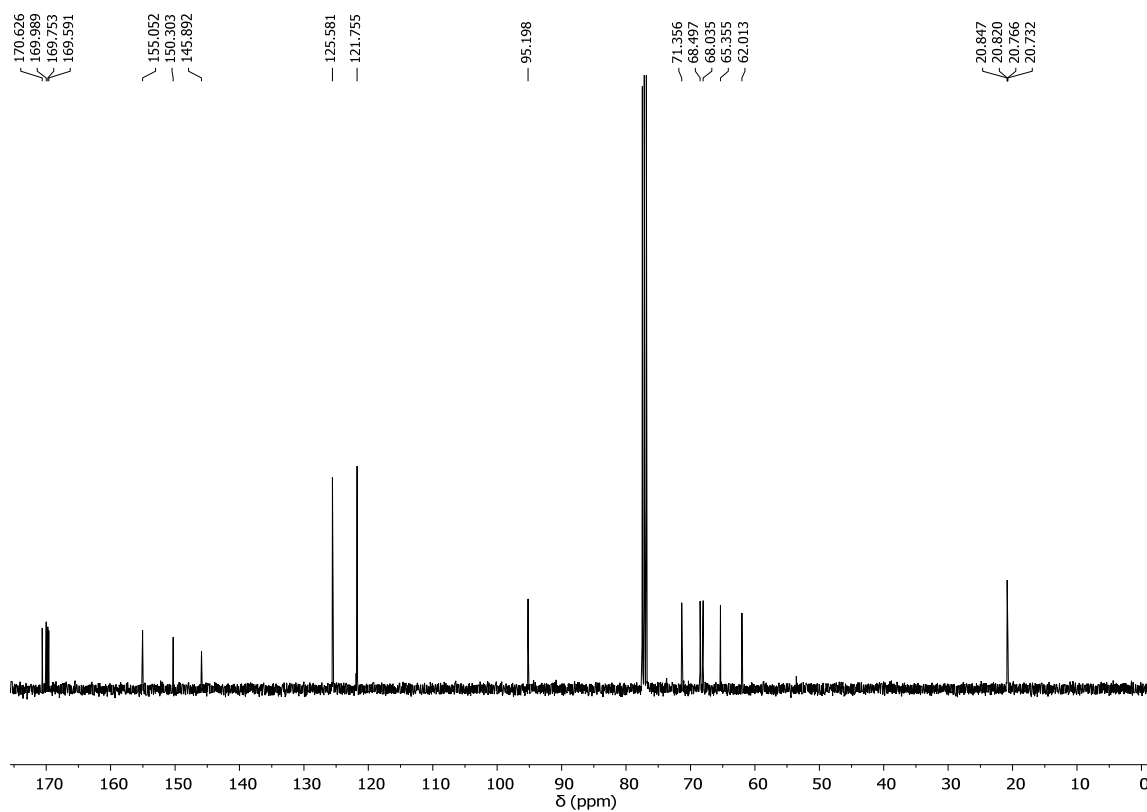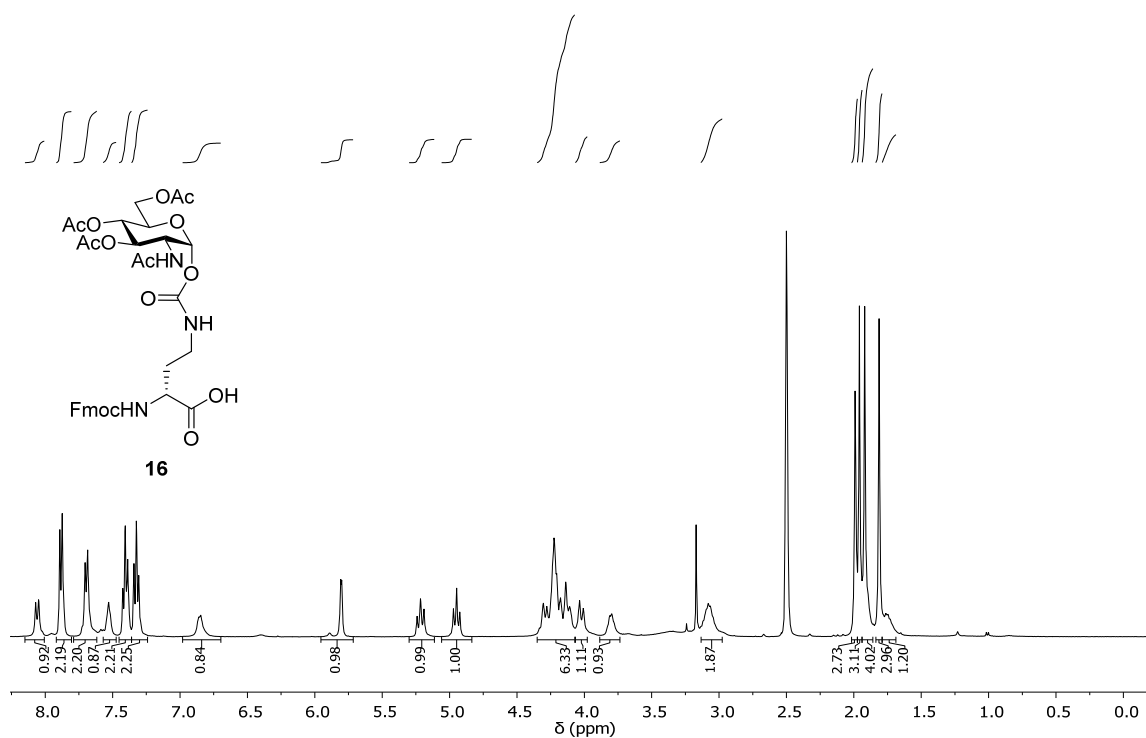**Figure S29.** DLS intensity distribution of **9** incubated with WGA. [WGA] = 32 µM, [**9**] = 63 µM

Figure S30. DLS intensity distribution of **10** incubated with WGA. [WGA] = 32 µM, [**9**] = 65 µM
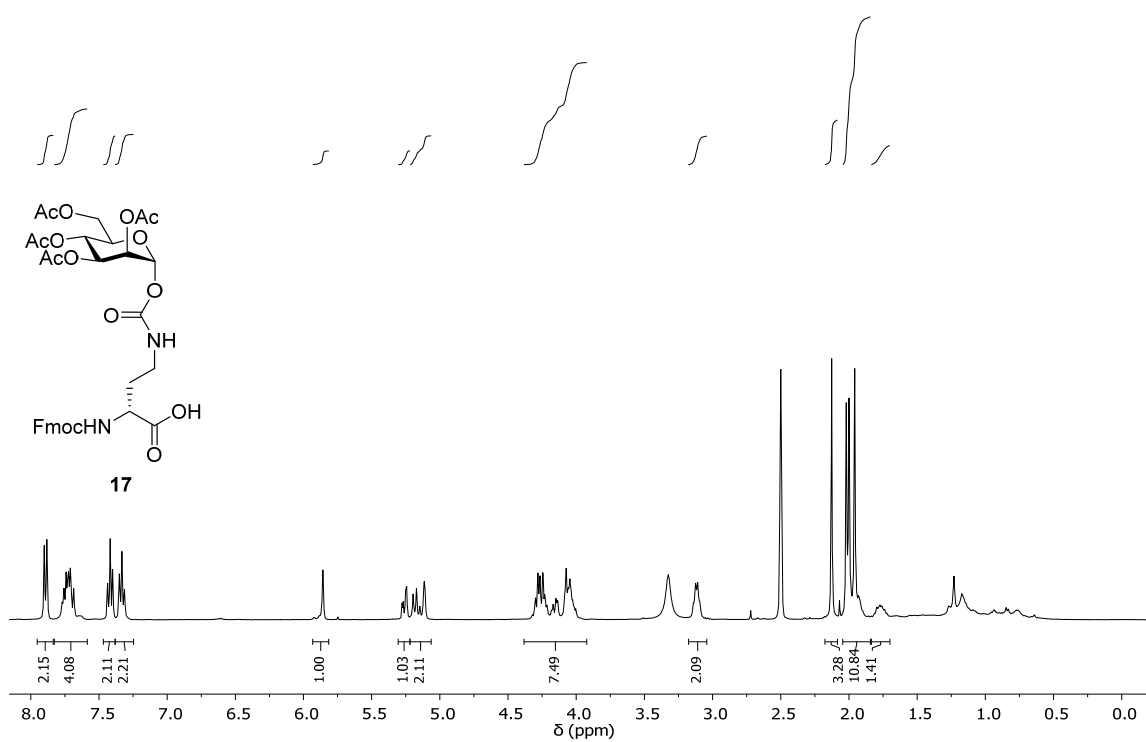
^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of **14**.
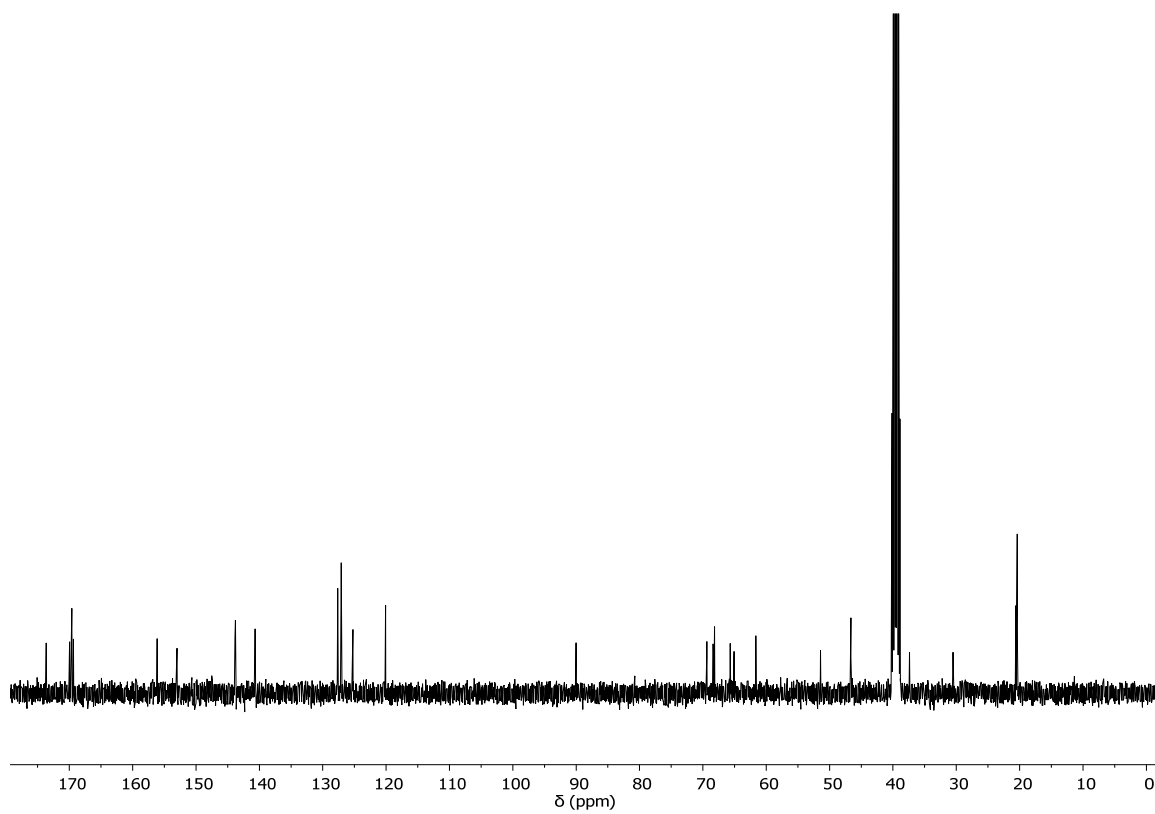

^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of **14**.

^{1}H NMR spectrum ([D$_6$]DMSO, 400 MHz) of **16**.
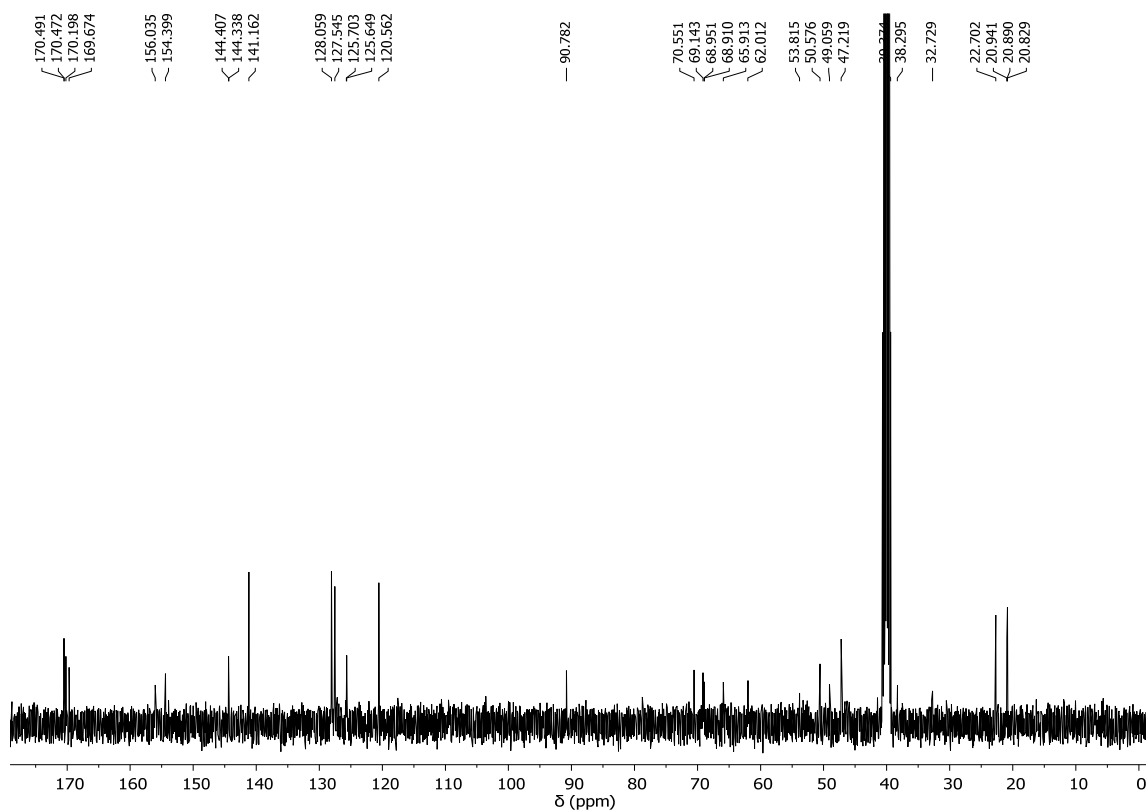
^{13}C NMR spectrum ([D$_6$]DMSO , 101 MHz) of **16**.

^{1}H NMR spectrum ([D$_6$]DMSO , 400 MHz) of **17**.

^{13}C NMR spectrum ([D$_6$]DMSO , 101 MHz) of **17**.