

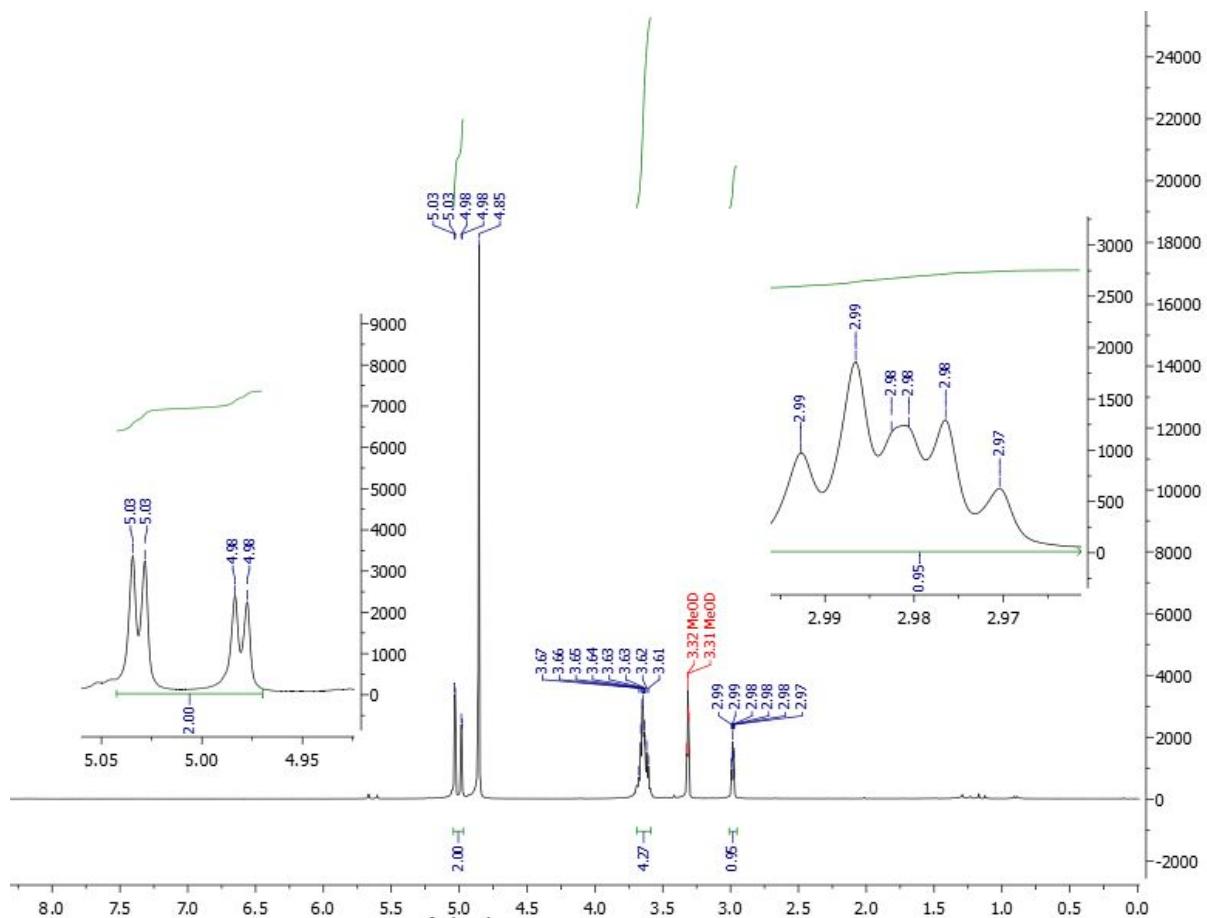
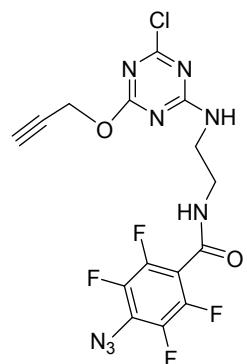
Supporting information

Unprecedented affinity-labelling of carbohydrate-binding proteins with *s*-triazinyl glycosides

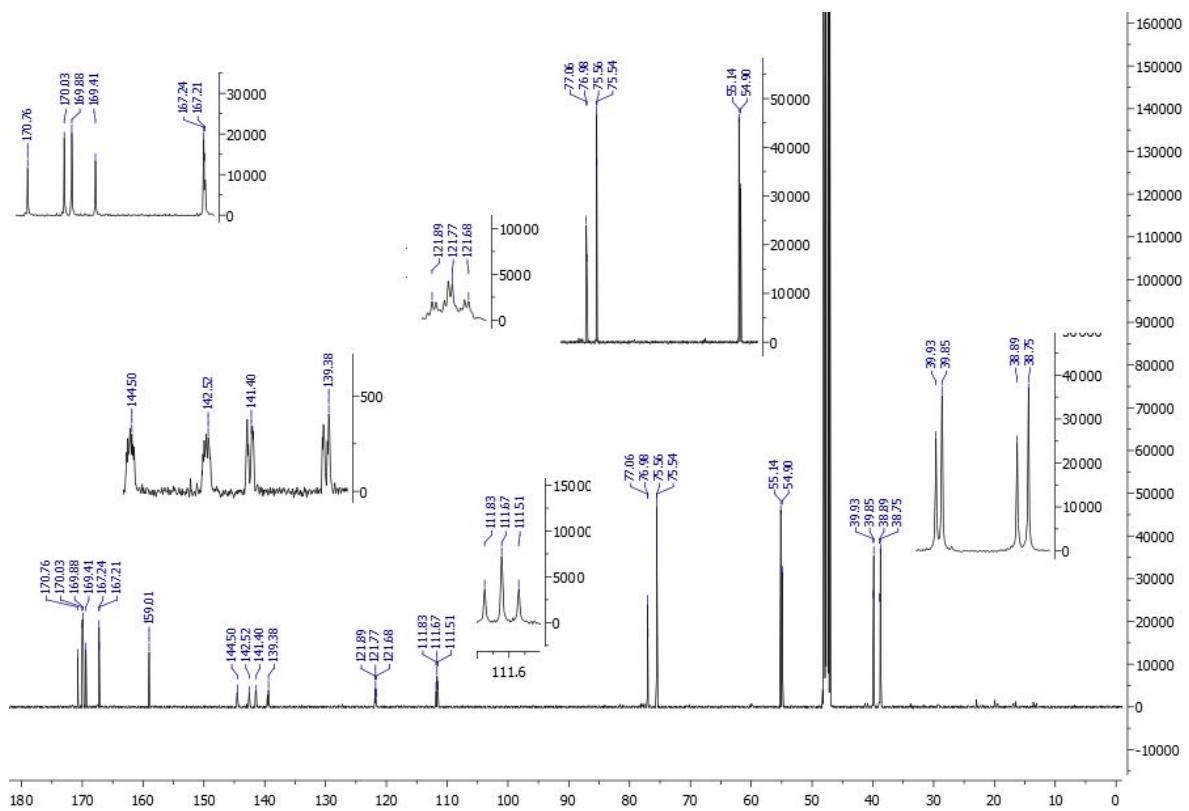
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Sébastien Fort¹

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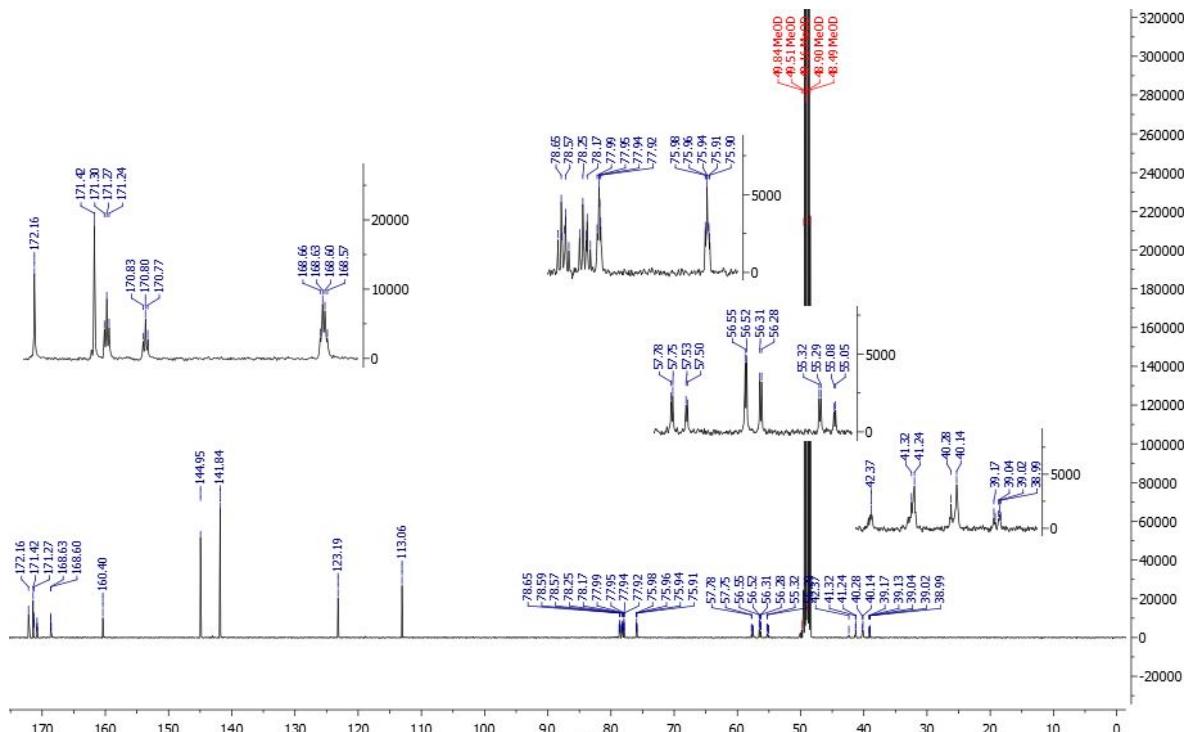
2-(*N*-(2-aminoethyl)-4-azido-tetrafluorobenzamide)-4-chloro-6-(prop-2-nyloxy)-1,3,5-triazine (2)



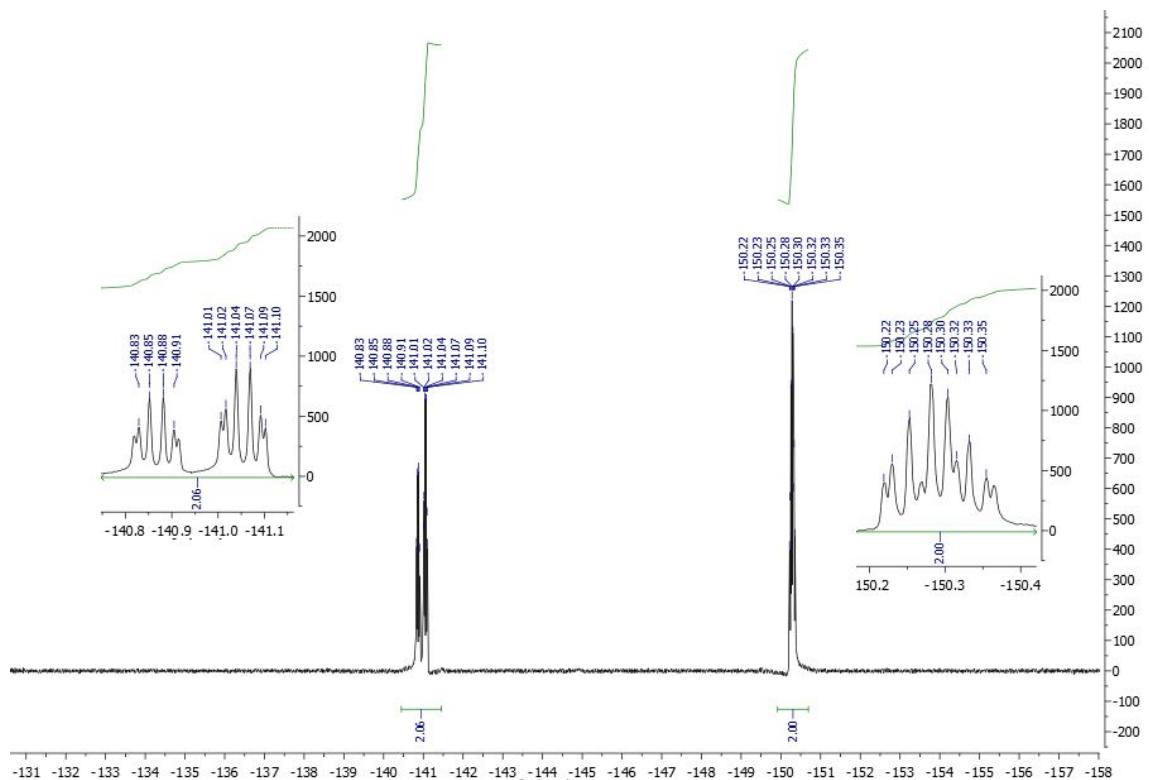
¹H NMR of 2-(*N*-(2-aminoethyl)-4-azido-tetrafluorobenzamide)-4-chloro-6-(prop-2-nyloxy)-1,3,5-triazine (2) (298 K, CD_3OD)



Proton decoupled ^{13}C NMR of 2-(*N*-(2-aminoethyl)-4-azido-tetrafluorobenzamide)-4-chloro-6-(prop-2-ynyoxy)-1,3,5-triazine (2) (298 K, CD_3OD)

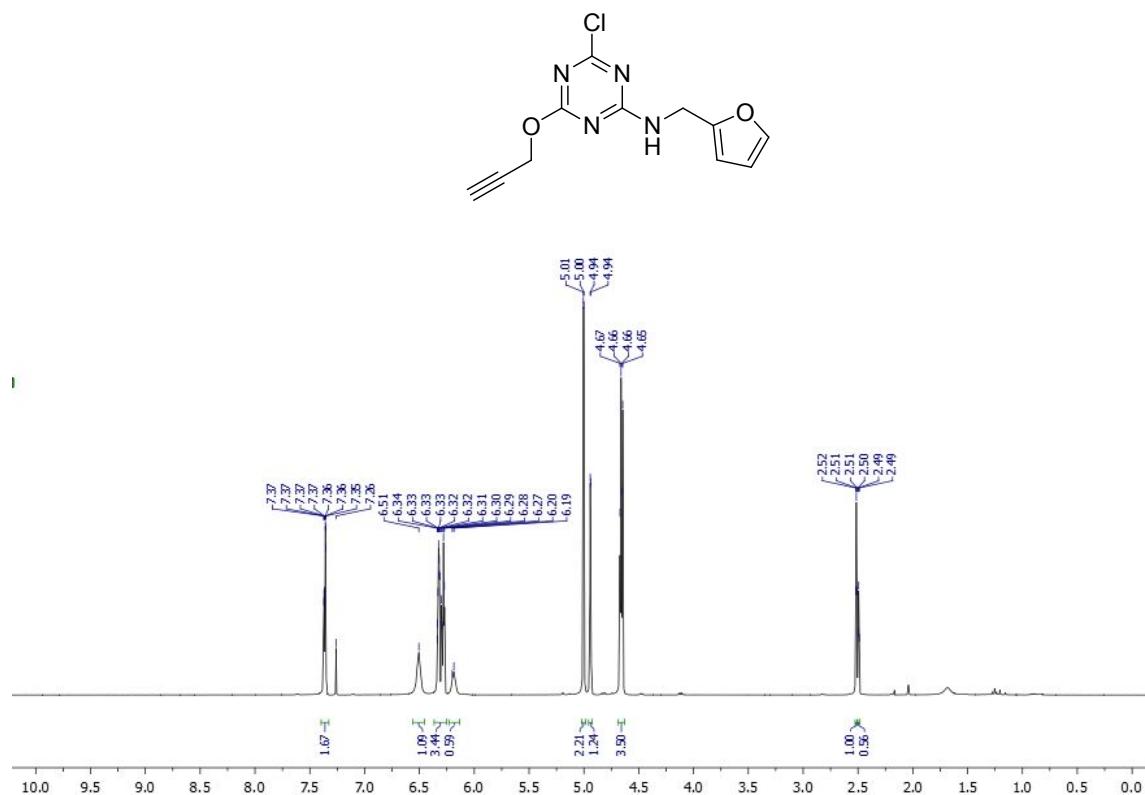


Fluorine decoupled ^{13}C NMR of 2-(*N*-(2-aminoethyl)-4-azido-tetrafluorobenzamide)-4-chloro-6-(prop-2-ynylloxy)-1,3,5-triazine (2) (298 K, CD_3OD)

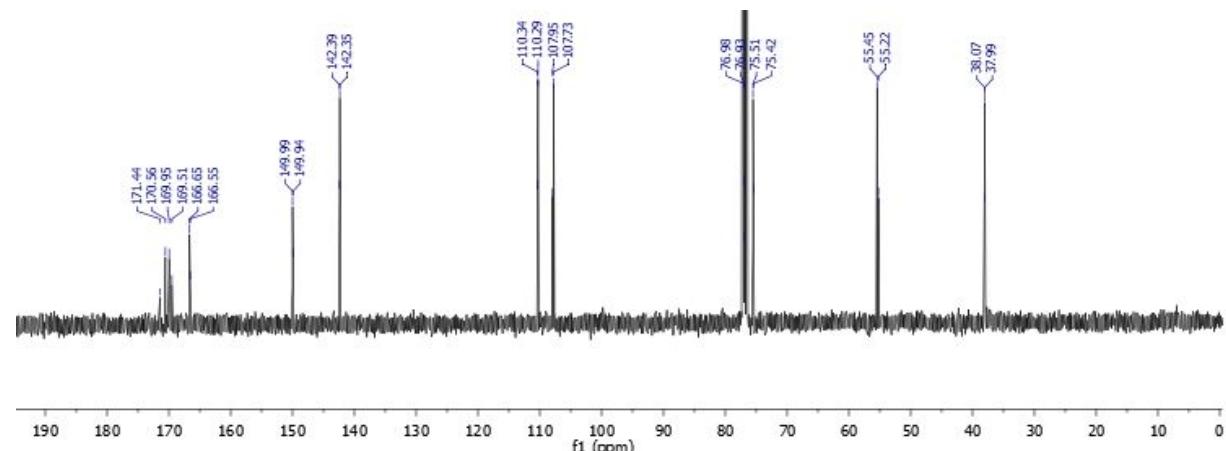


Proton decoupled ¹⁹F NMR of 2-(N-(2-aminoethyl)-4-azido-tetrafluorobenzamide)-4-chloro-6-(prop-2-ynyoxy)-1,3,5-triazine (2) (298 K, CD₃OD)

2-Chloro-4-(furan-2-ylmethylamino)-6-(prop-2-ynyoxy)-1,3,5-triazine (3)

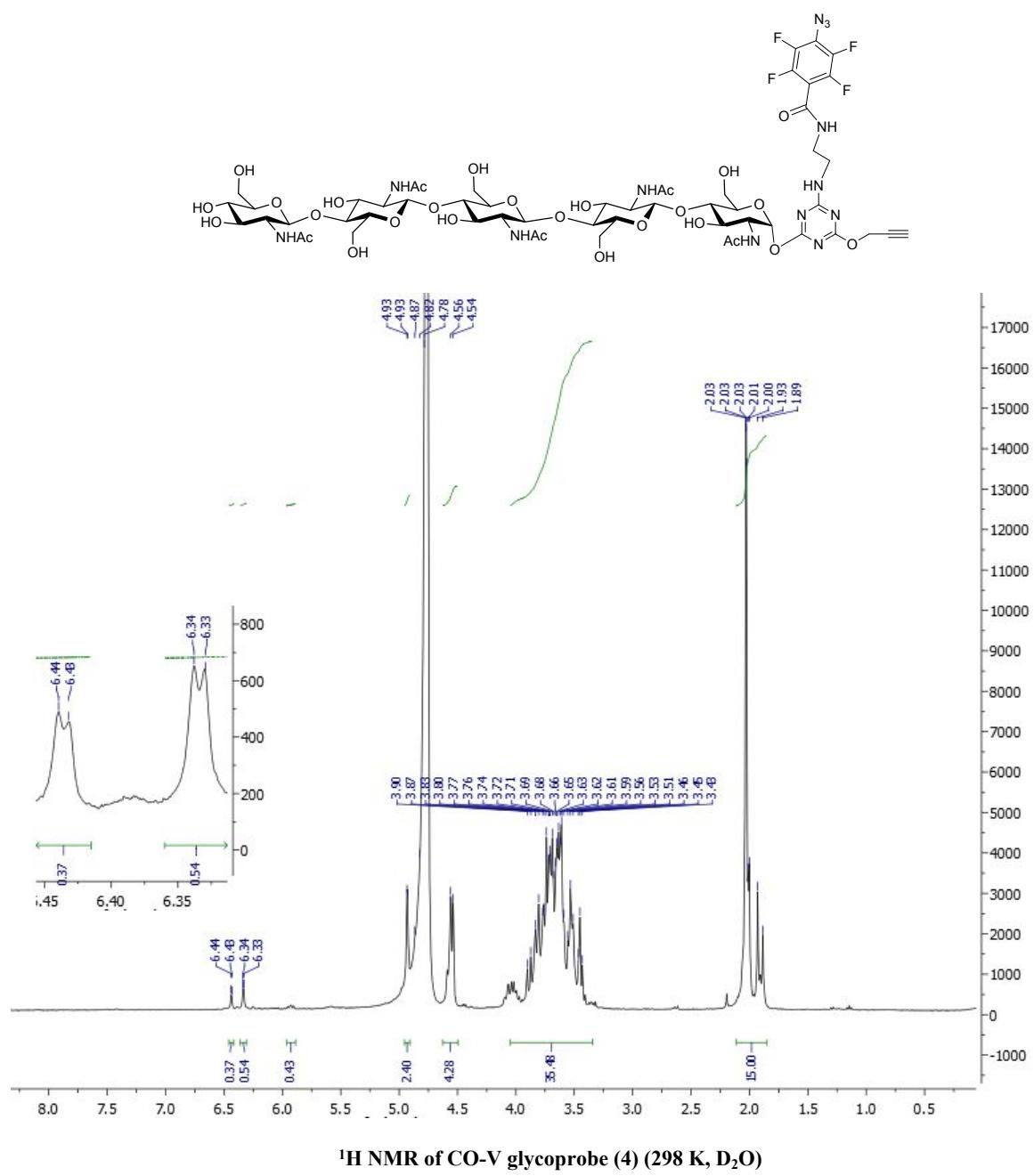


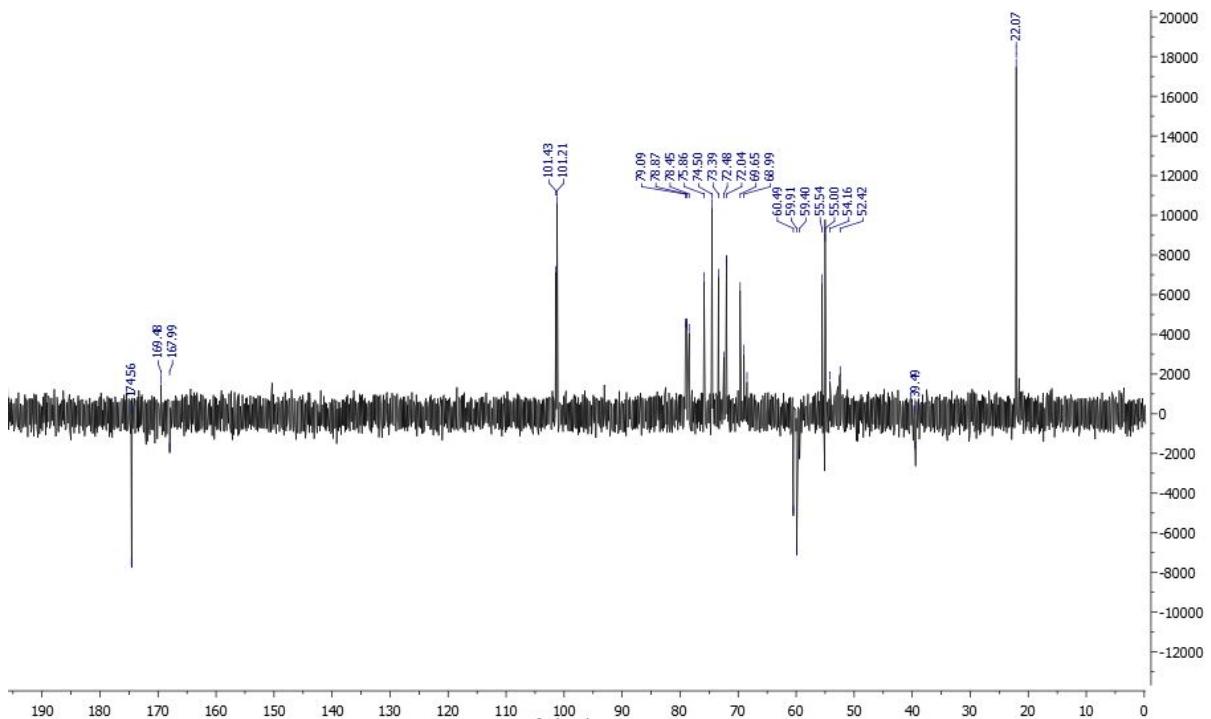
¹H NMR of 2-chloro-4-(furan-2-ylmethylamino)-6-(prop-2-ynyoxy)-1,3,5-triazine (3) (298 K, CDCl₃)



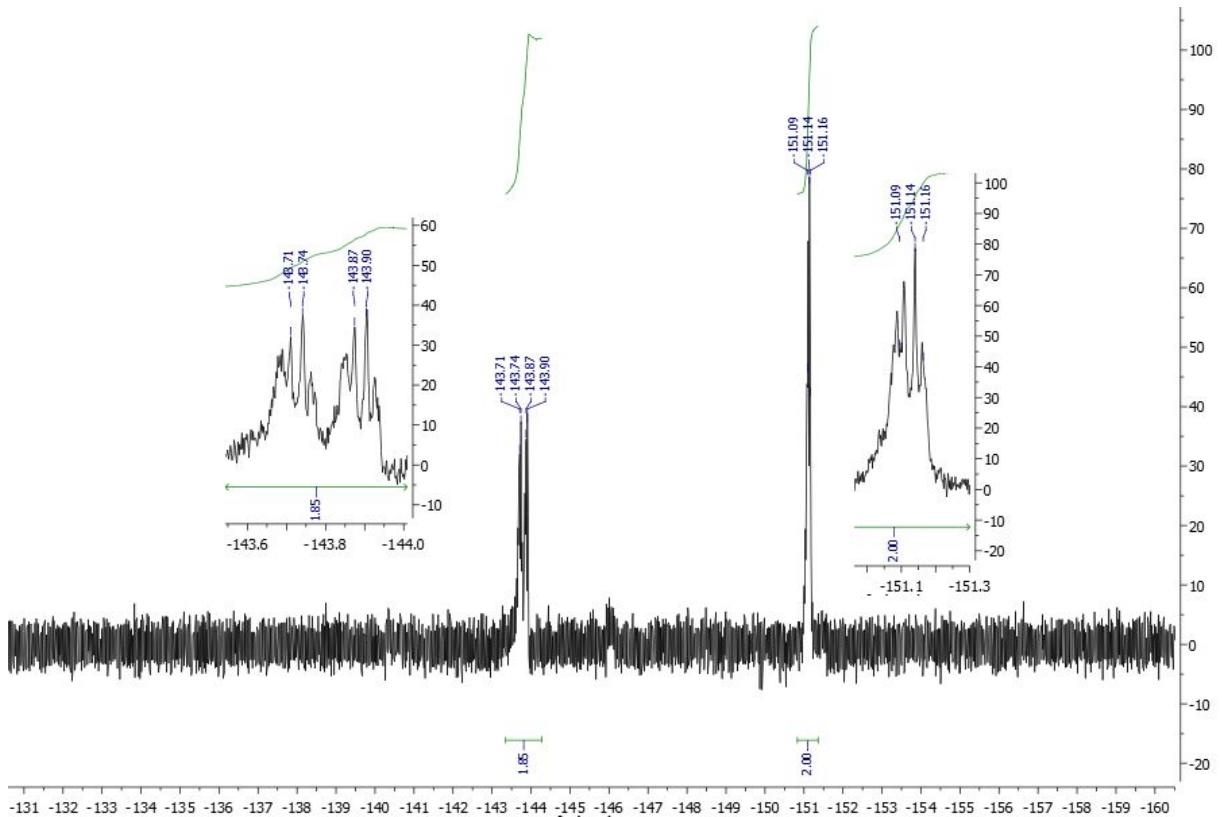
¹³C NMR of 2-chloro-4-(furan-2-ylmethylamino)-6-(prop-2-ynyoxy)-1,3,5-triazine (3) (298 K, CDCl₃)

CO-V glycoprobe (4)



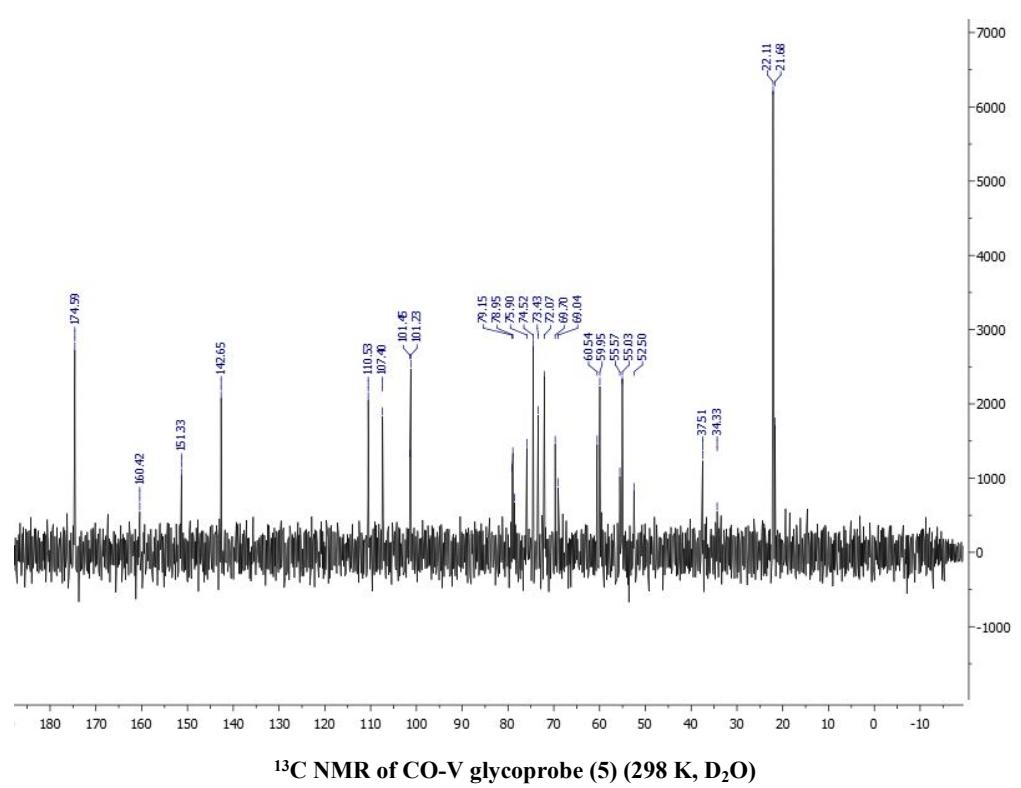
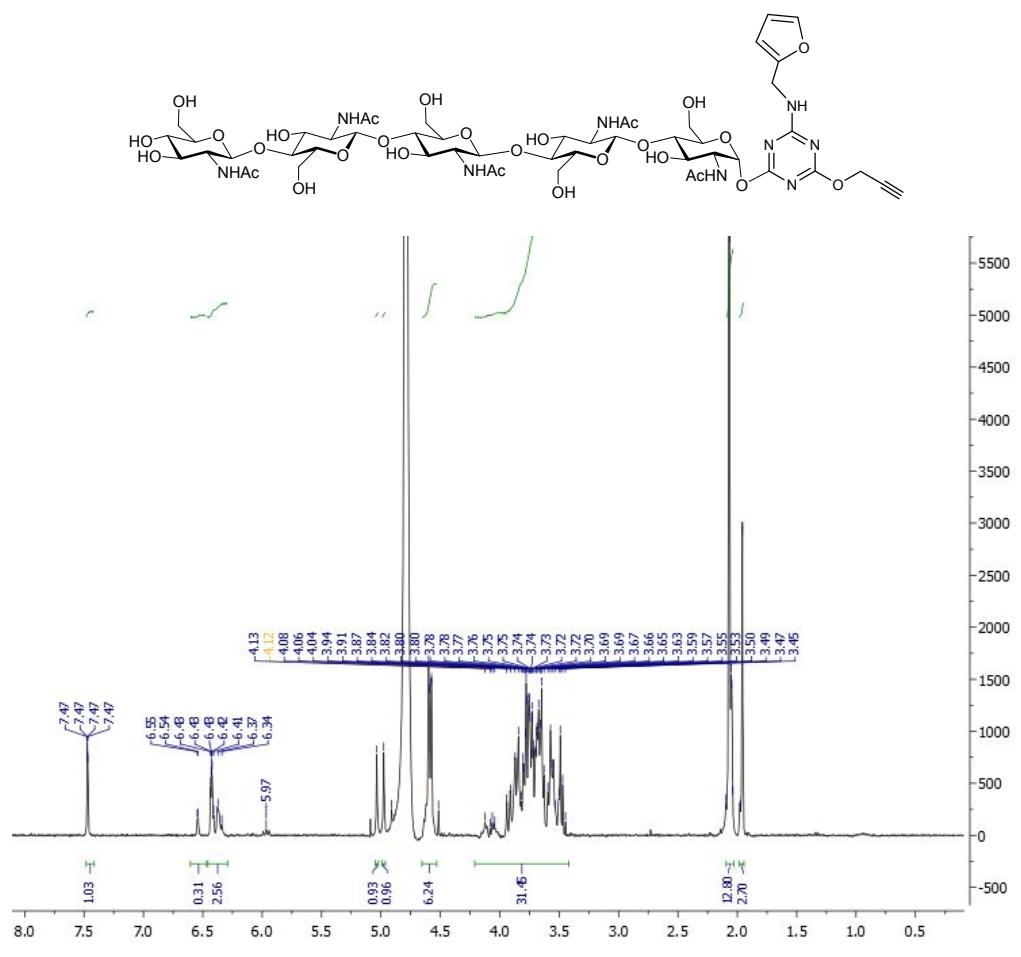


^{13}C (DEPTQ) NMR of CO-V glycoprobe (4) (298 K, D_2O)

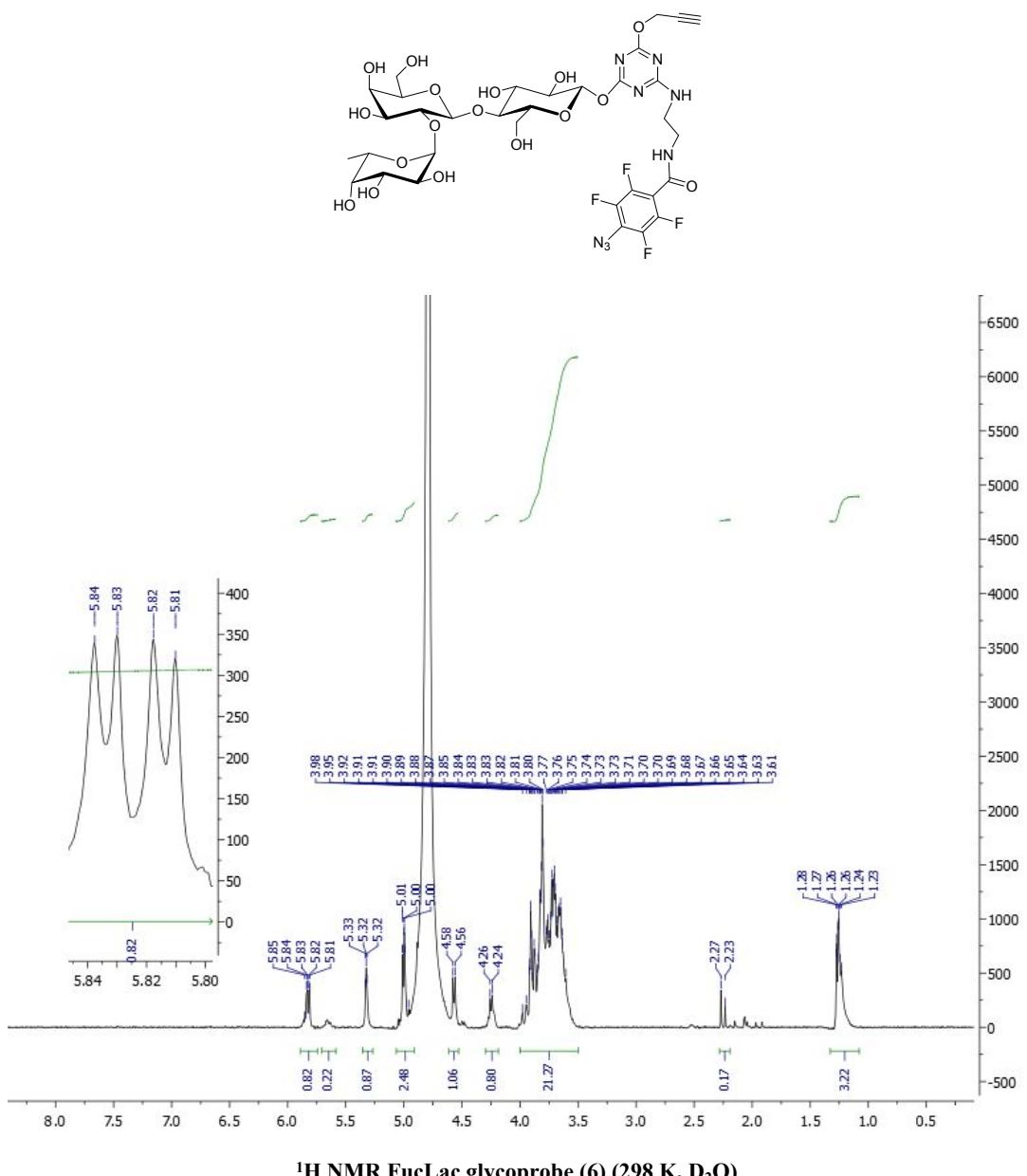


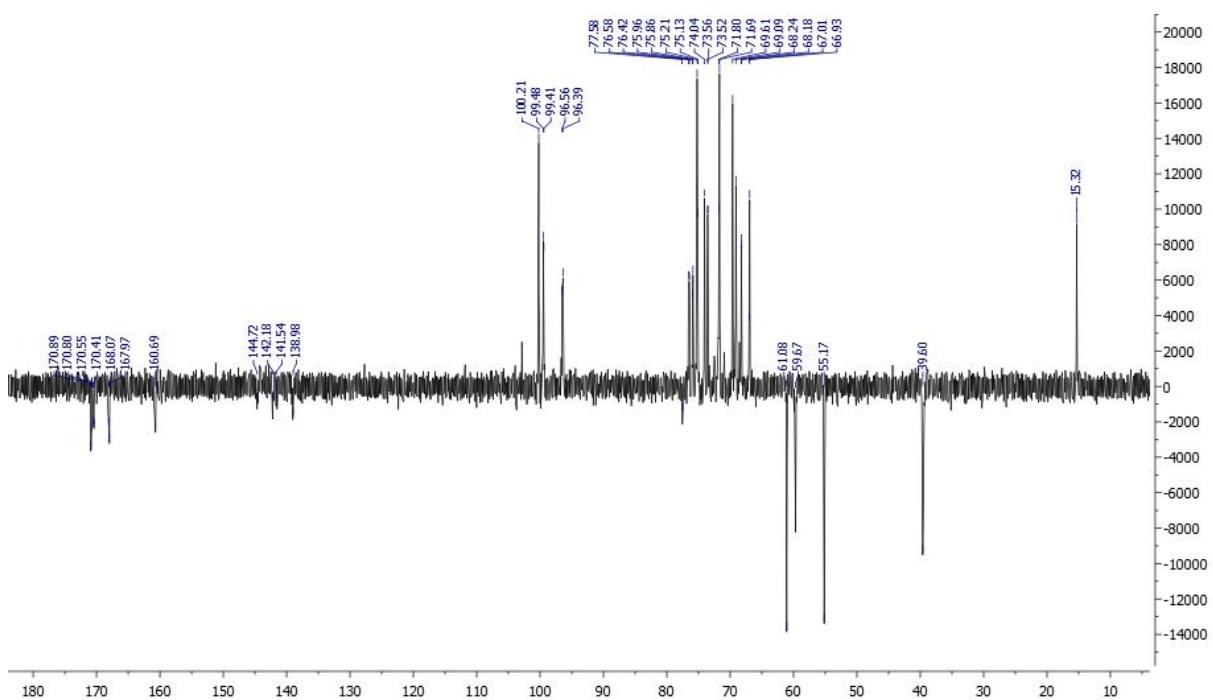
^{19}F NMR of CO-V glycoprobe (4) (298 K, D_2O)

CO-V glycoprobe (5)

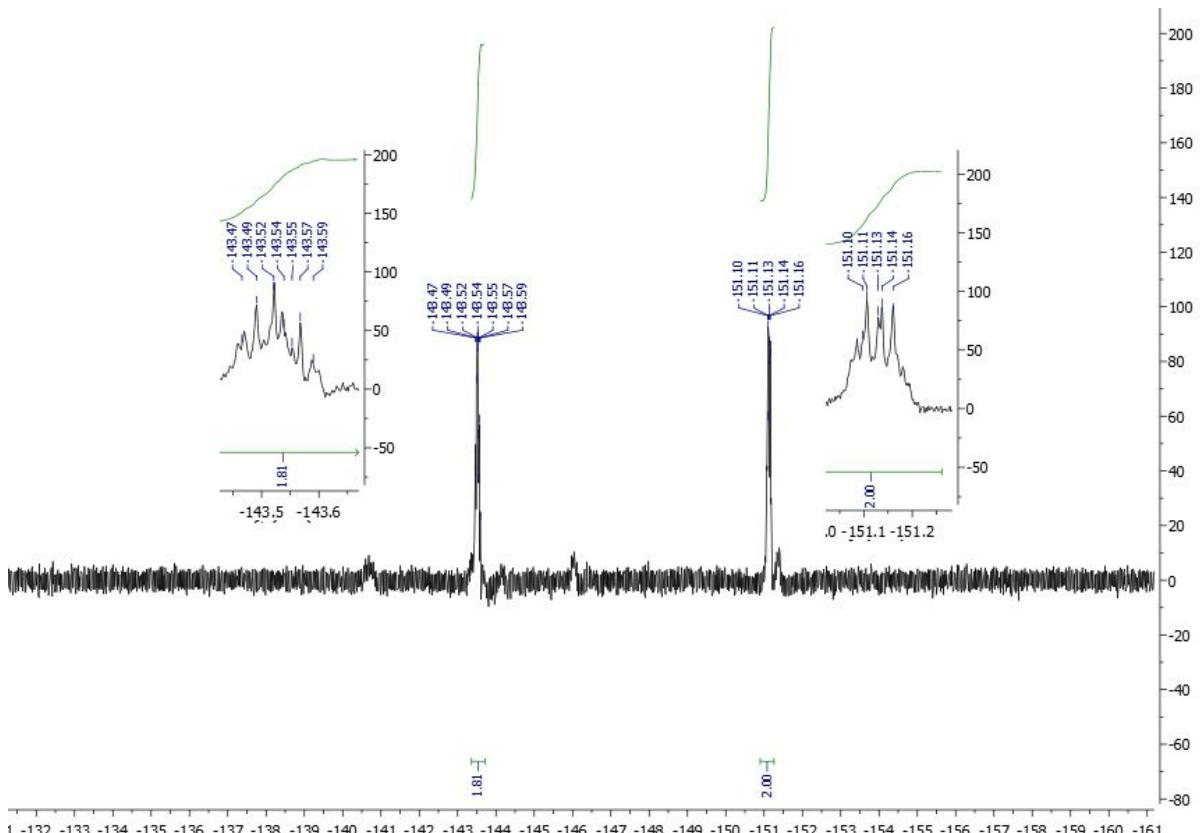


FucLac glycoprobe (6)



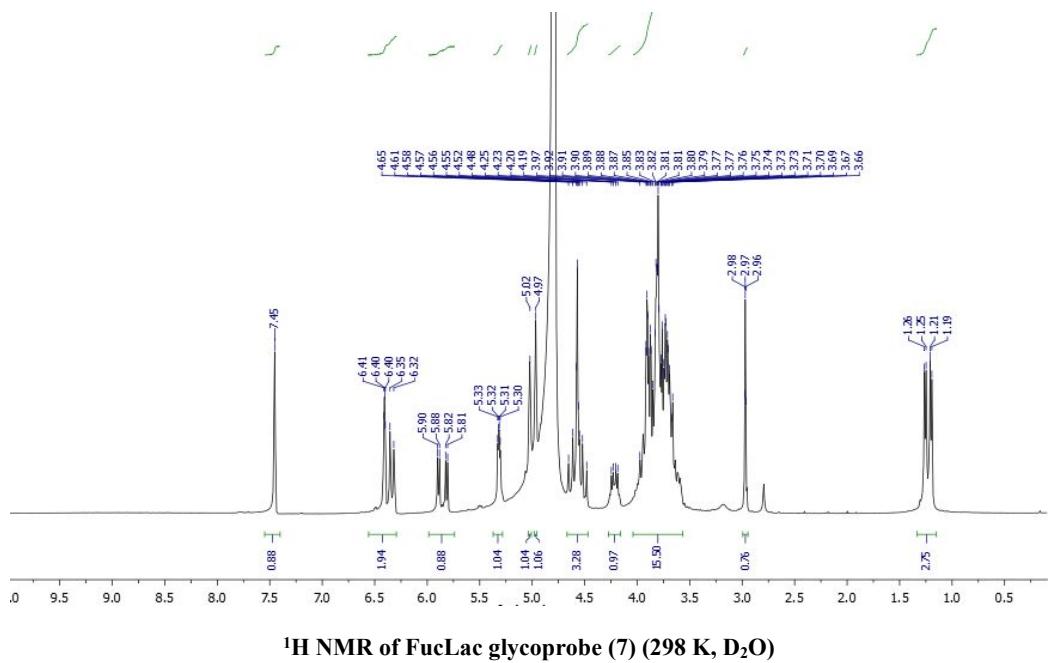
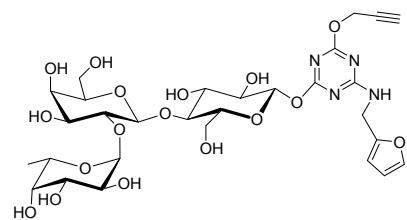


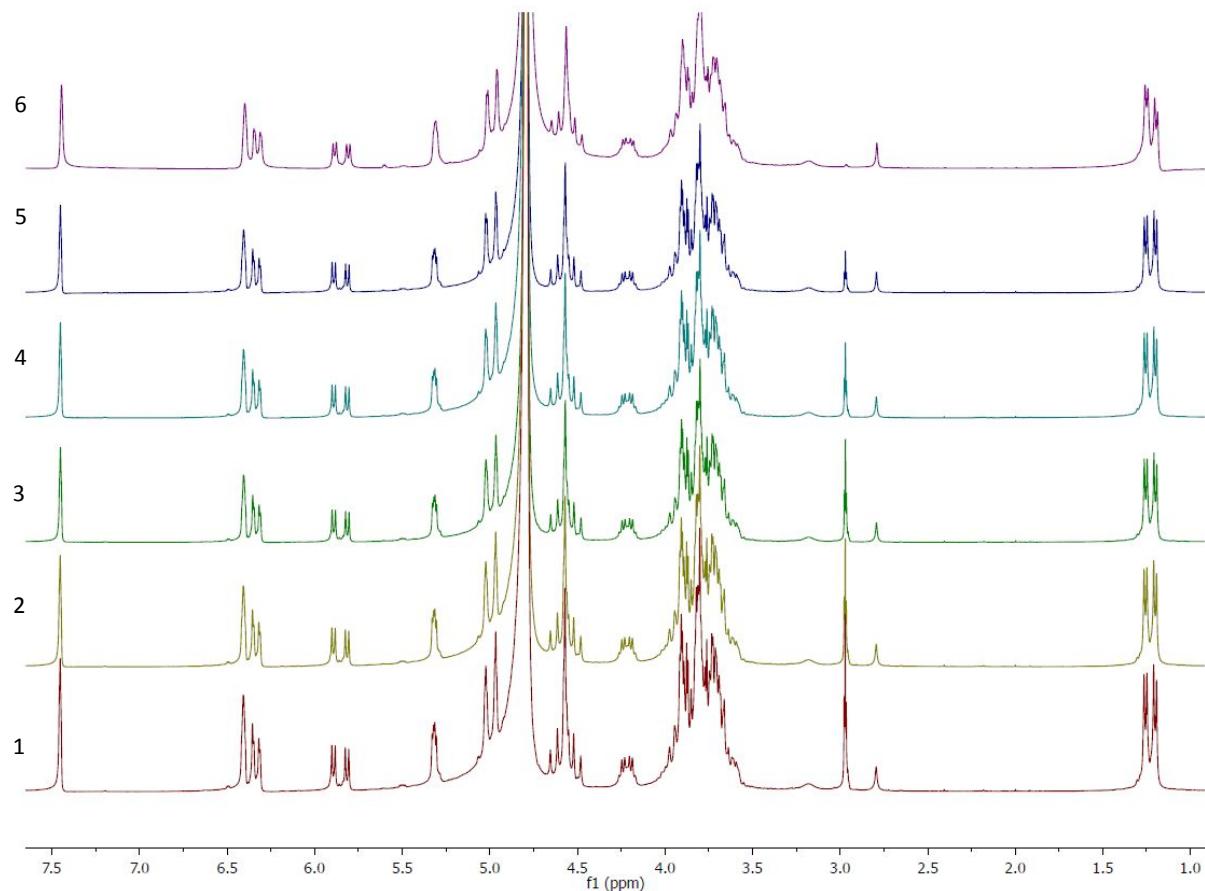
^{13}C NMR FucLac glycoprobe (6) (298 K, D_2O)



^2F NMR of FucLac glycoprobe (6) (298 K, D_2O)

FucLac glycoprobe (7)





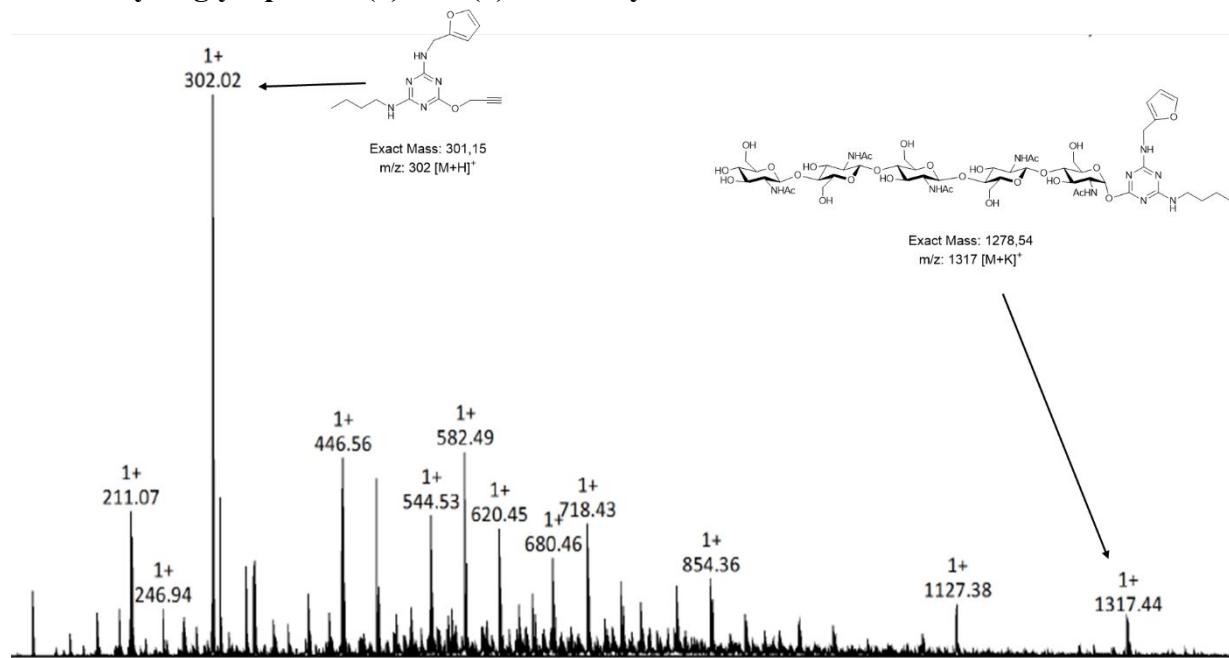
¹H NMR of glycoprobe (7) in D₂O (1) and in deuterated phosphate buffer (pH 7.0, 100 mM) over 48 hours (2-6 : 1, 2, 4, 8, 48h respectively).

WGA labelling by glycoprobe (5) in presence of excess of CO-V

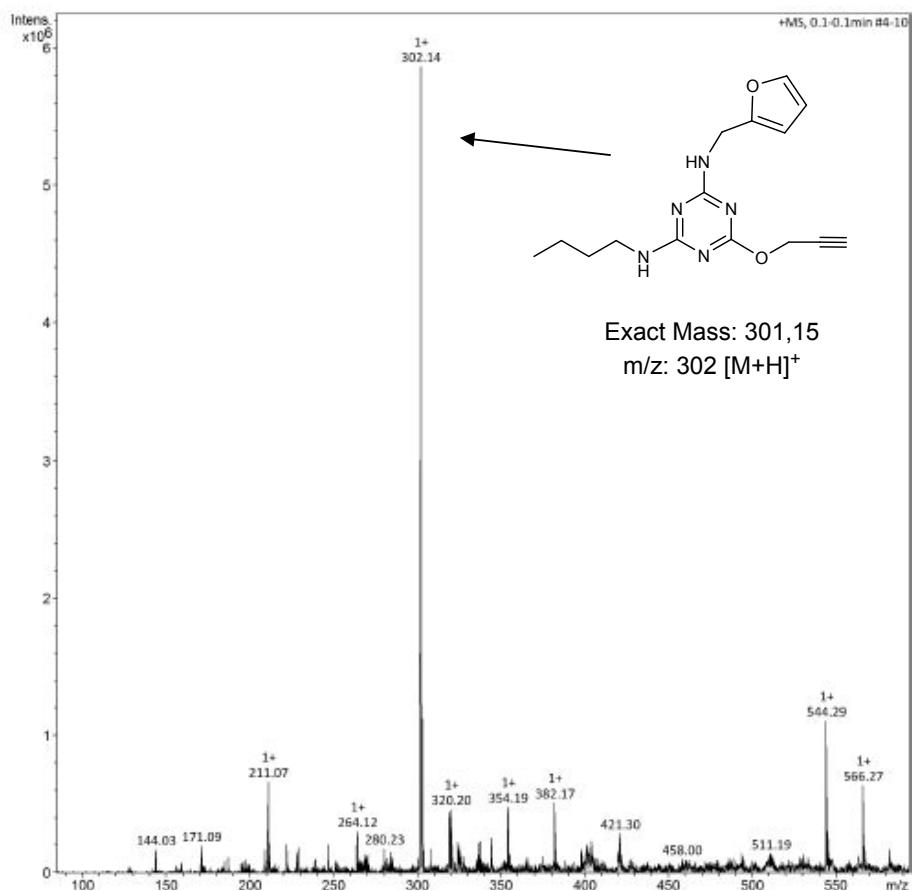


Glycoprobe **5** (5 µM) was incubated with WGA (0.1 mg/mL) in PBS buffer (60 mM, pH 7.2, 150 mM NaCl, 0.1 mM MnCl₂, 0.1 mM CaCl₂) in absence and in presence of **CO-V** (200 µM) and then labelled with FITC-N₃. After SDS-PAGE, WGA was detected by Coomassie blue staining (A) and by fluorescence detection (B)

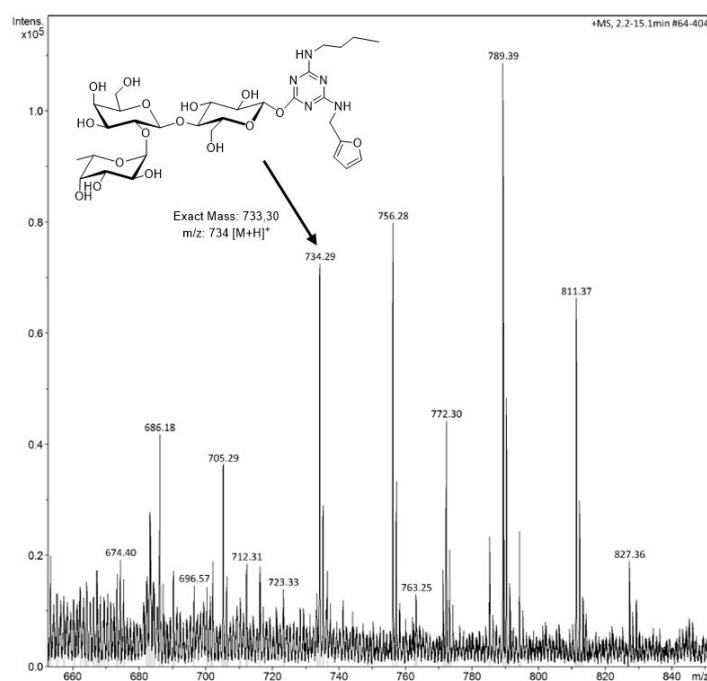
Reactivity of glycoprobes (**5**) and (**7**) with butylamine



ESI spectrum of the reaction mixture after 48 hours at RT of glycoprobe (**5**) in presence of 100 equivalents of butylamine in water



ESI spectrum of the reaction mixture after 48 hours at RT of glycoprobe (7) in presence of 100 equivalents of butylamine in water



ESI spectrum (zoom in between 650-850 m/z) of the reaction mixture after 48 hours at RT of glycoprobe (7) in presence of 100 equivalents of butylamine in water