Design, synthesis and biological evaluation of new carbohydrate-based coumarin derivatives as selective carbonic anhydrase IX inhibitors via “click” reaction

Naying Chu [1,2,†], Yitong Wang [3,†], Hao Jia [1], Jie Han [1], Xiaoyi Wang [1] and Zhuang Hou [3,*]

[1] *Department of Pharmacy, The First People’s Hospital of Shangqiu, Suiyang District, 292 Kaixuan Road, Shangqiu 476000, China;*

[2] *China-Japan Research Institute of Medical and Pharmaceutical Sciences, Shenyang Pharmaceutical University, 103 Wenhua Road, Shenyang 110016, China*

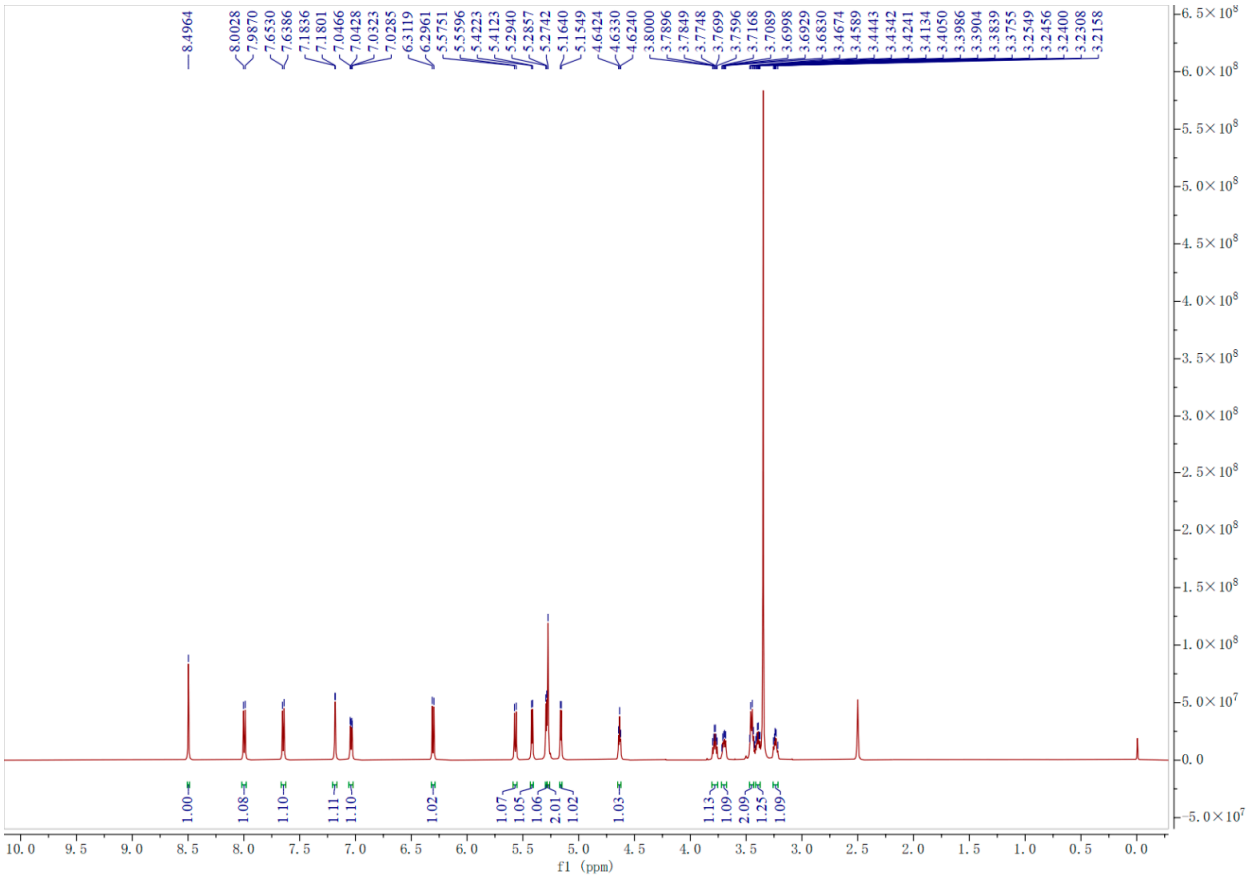
[3] *Key Laboratory of Structure-Based Drugs Design and Discovery (Ministry of Education), Shenyang Pharmaceutical University, Shenyang 110016, China*

***** *Correspondence: houzhuang8@sina.com*

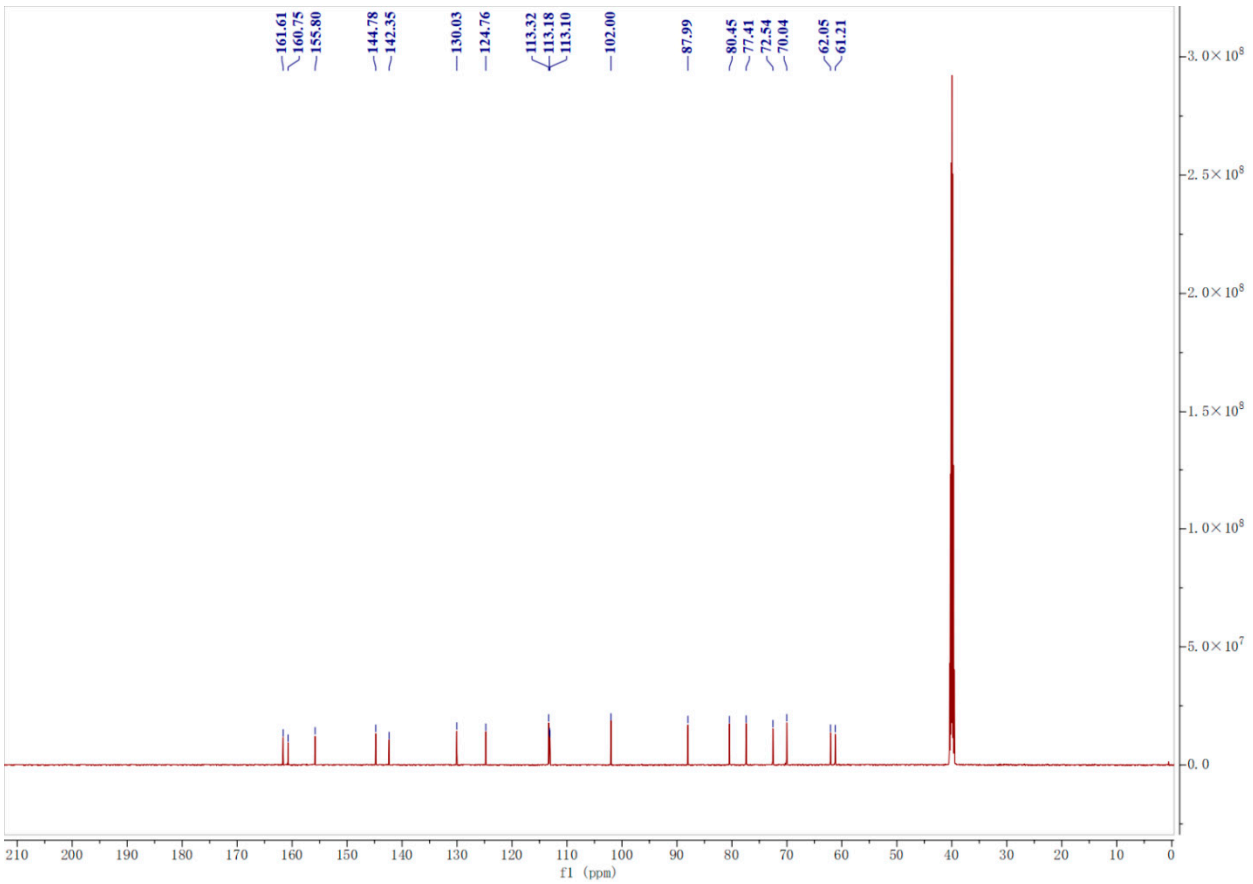
† These authors contributed equally to this work.

The ^{1}H and ^{13}C NMR spectra were recorded at 600 MHz and 150 MHz on a Bruker ARX 600 MHz spectrometer using $(CD_3)_2SO$ as solvents with TMS as the internal standard. The NMR spectra were analyzed and interpreted using MestReNova. The solvent peaks were 2.5 ppm and 40 ppm in the ^{1}H and ^{13}C NMR spectra, respectively.

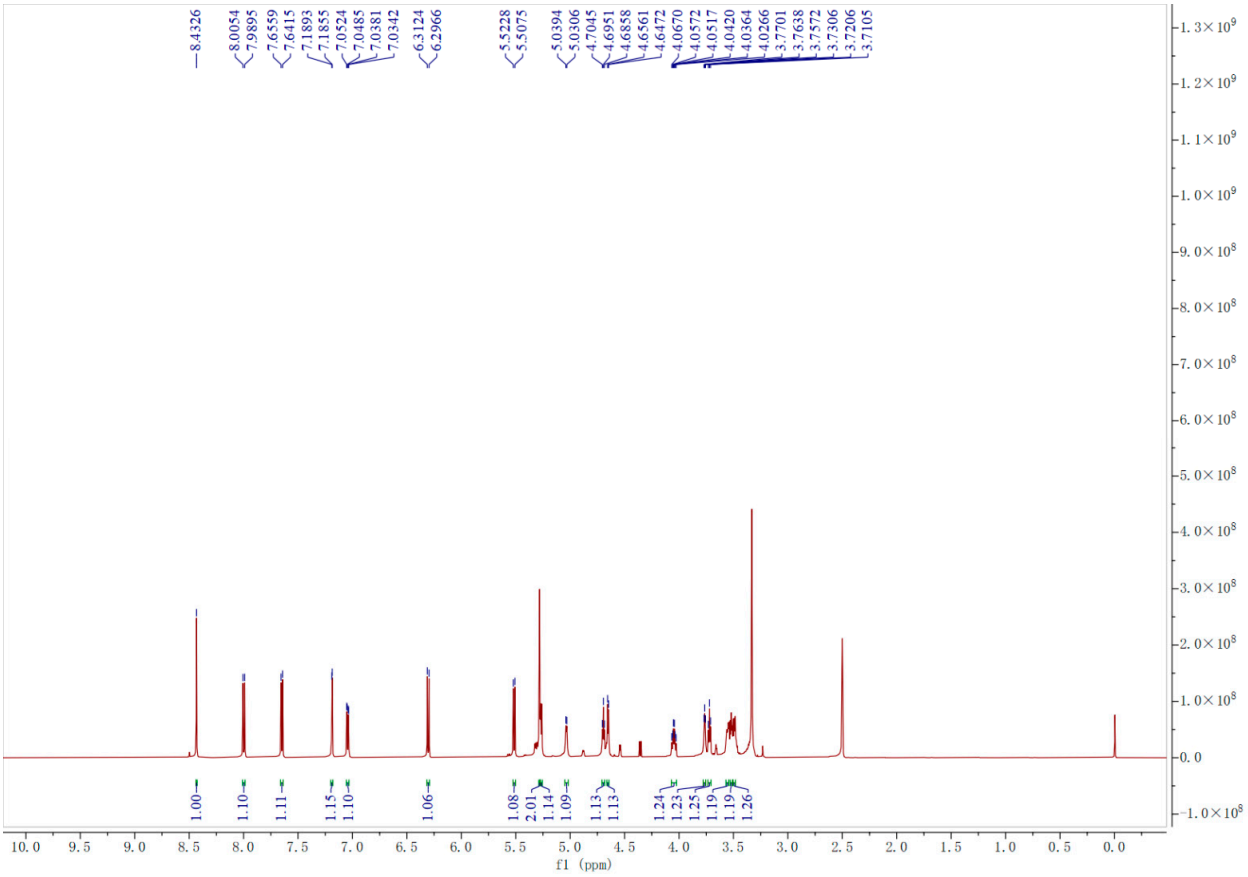
*Figures S1. The [1]H-NMR spectrum of 7- [(1-β-D-glucopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10a**)*



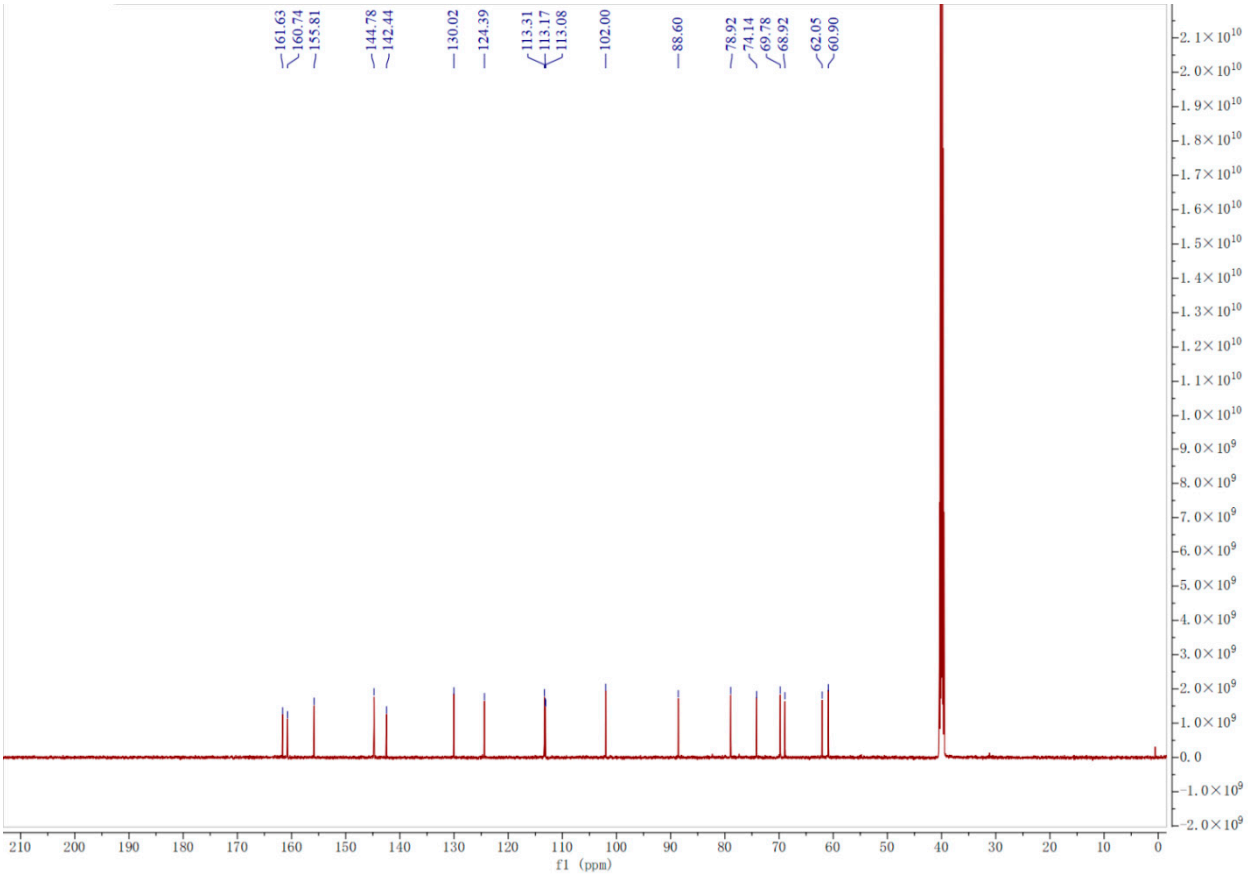
*Figures S2. The [13]C-NMR spectrum of 7- [(1-β-D-glucopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10a**)*



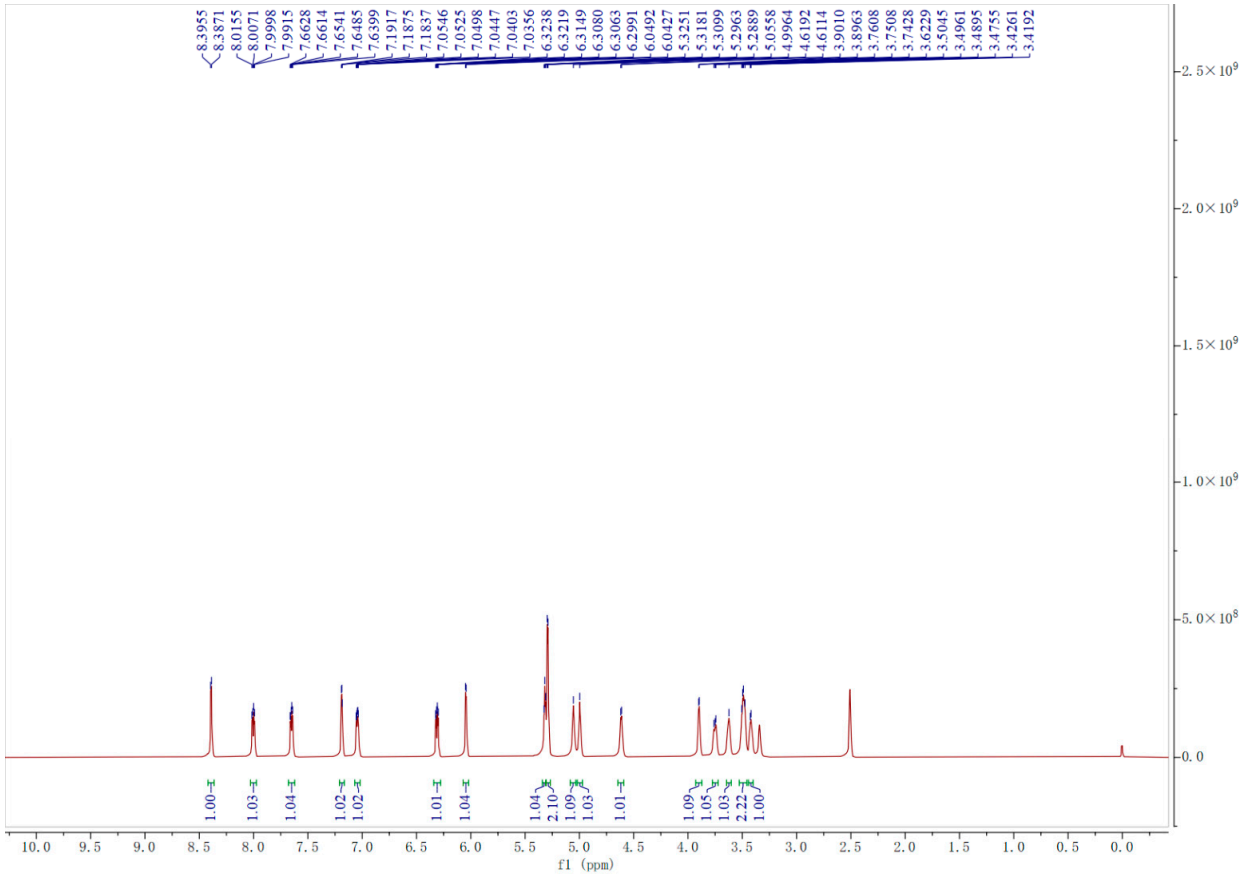
*Figures S3. The [1]H-NMR spectrum of 7- [(1-β-D-galactopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10b**)*



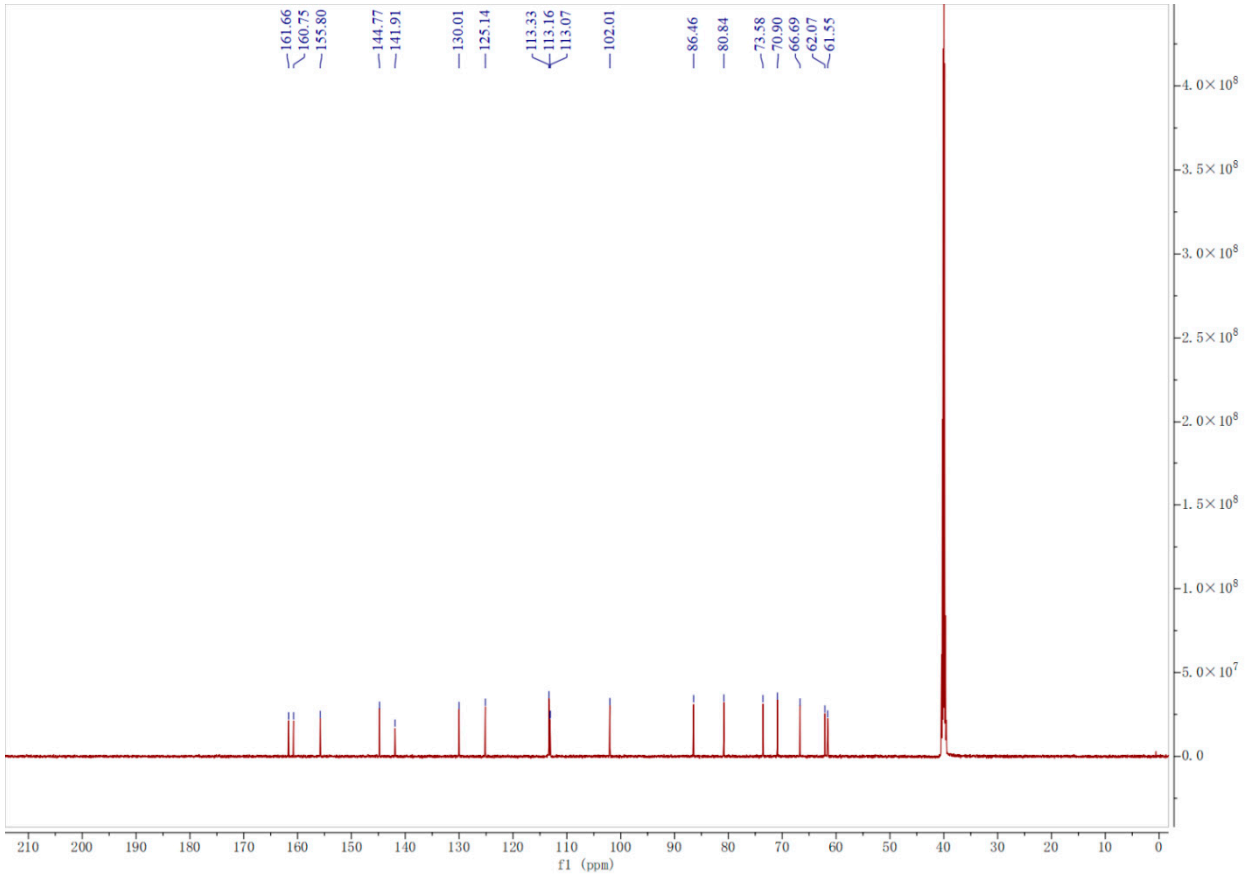
*Figures S4. The [13]C-NMR spectrum of 7- [(1-β-D-galactopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10b**)*



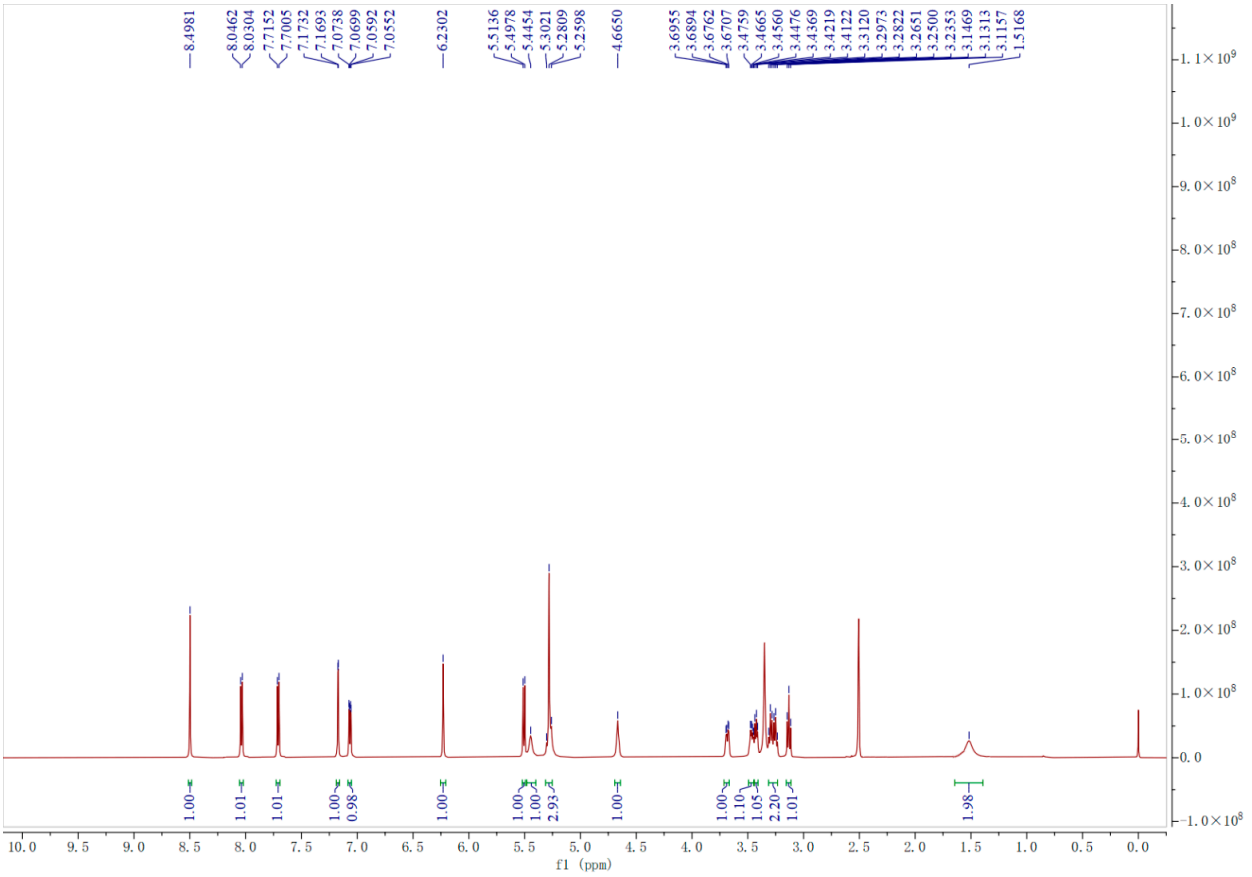
Figures S5. The [1]H-NMR spectrum of 7- [(1-β-D-mannopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10c**)



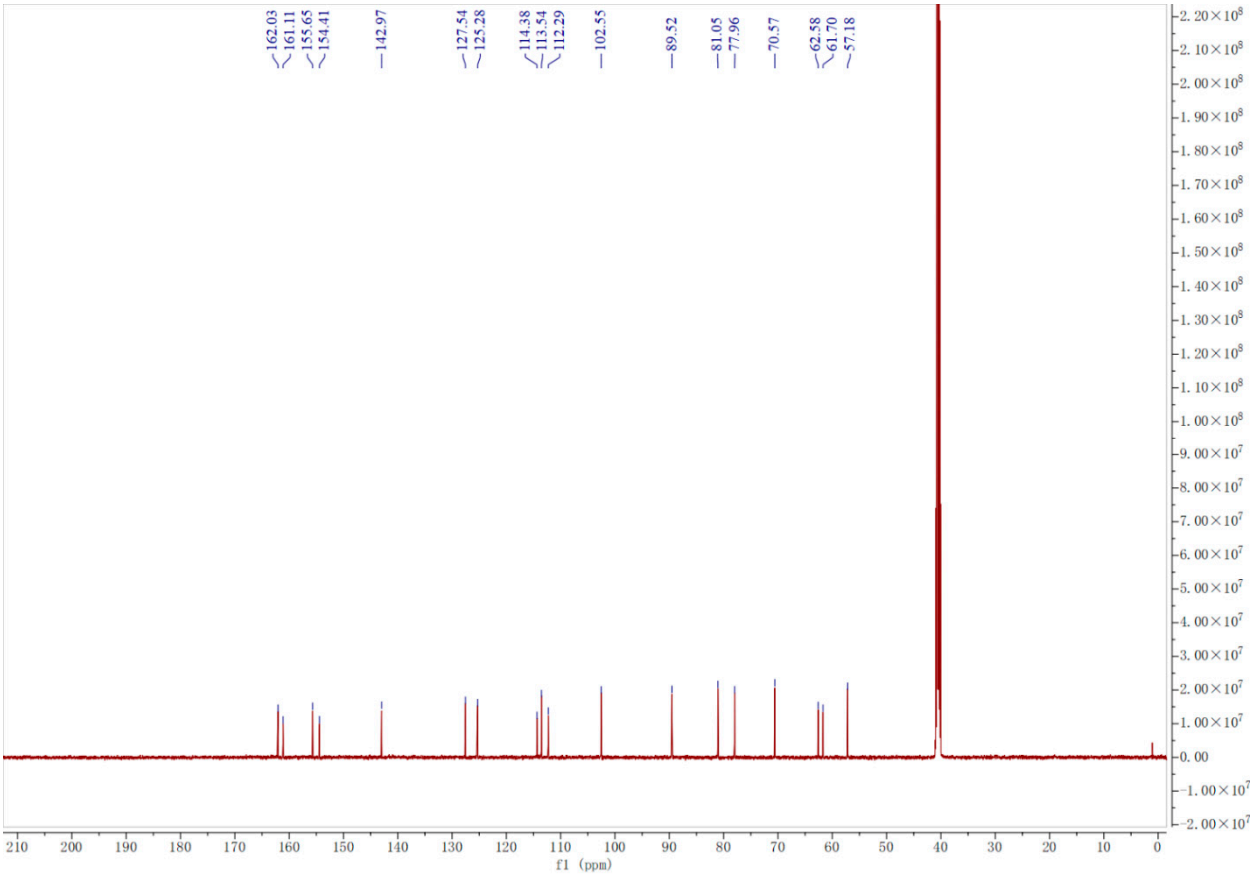
Figures S6. The [13]C-NMR spectrum of 7- [(1-β-D-mannopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10c**)



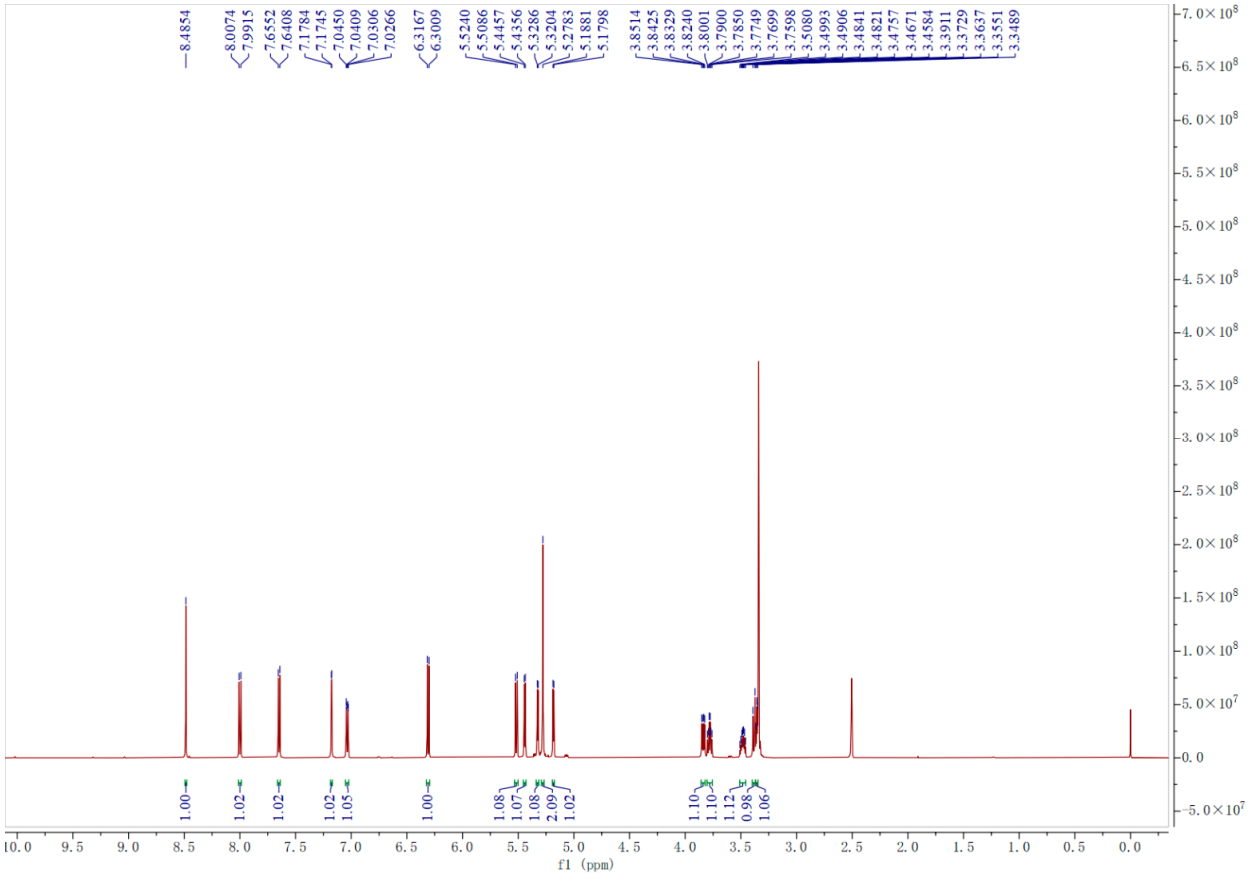
Figures S7. The [1]H-NMR spectrum of 7- [(1-β-D-glucosaminogly-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10d**)



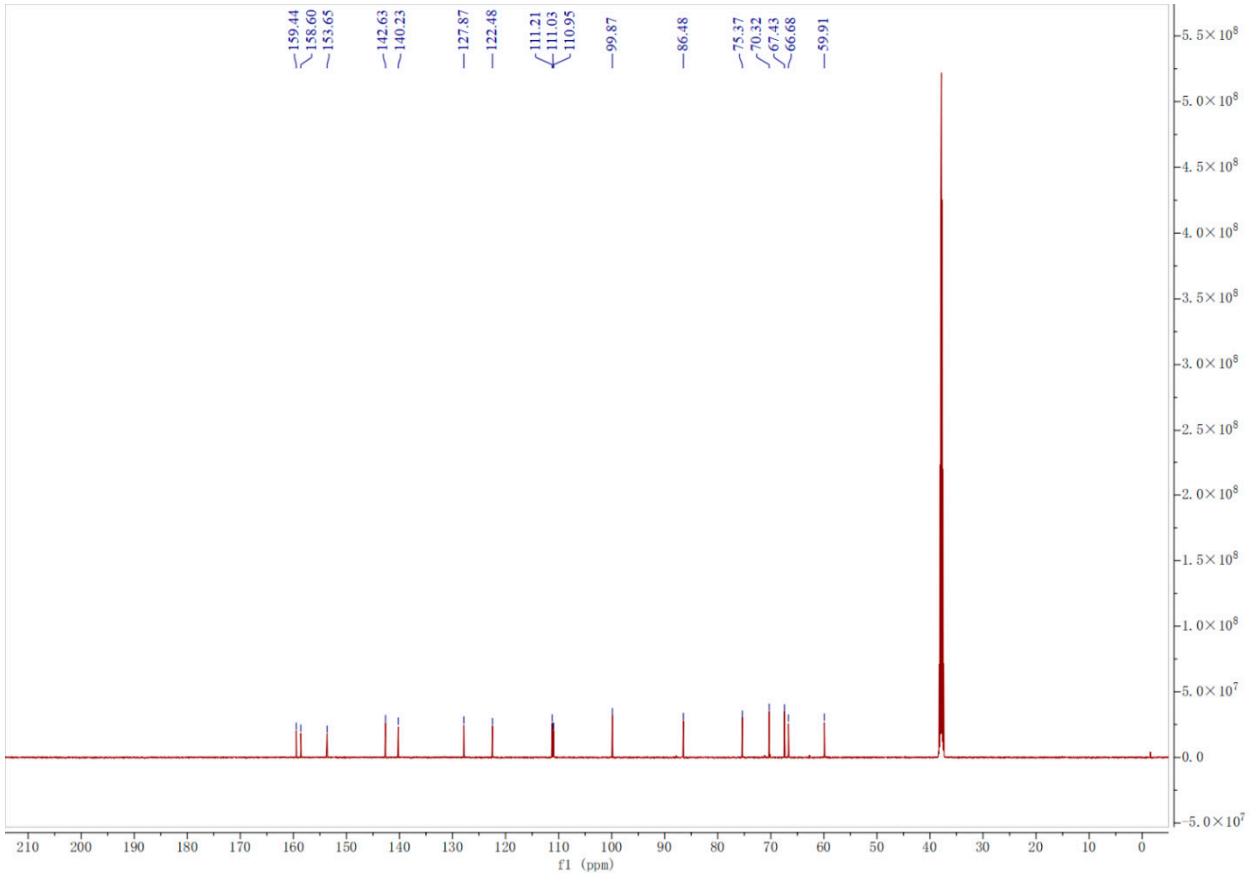
Figures S8. The [13]C -NMR spectrum of 7- [(1-β-D-glucosaminogly-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10d**)



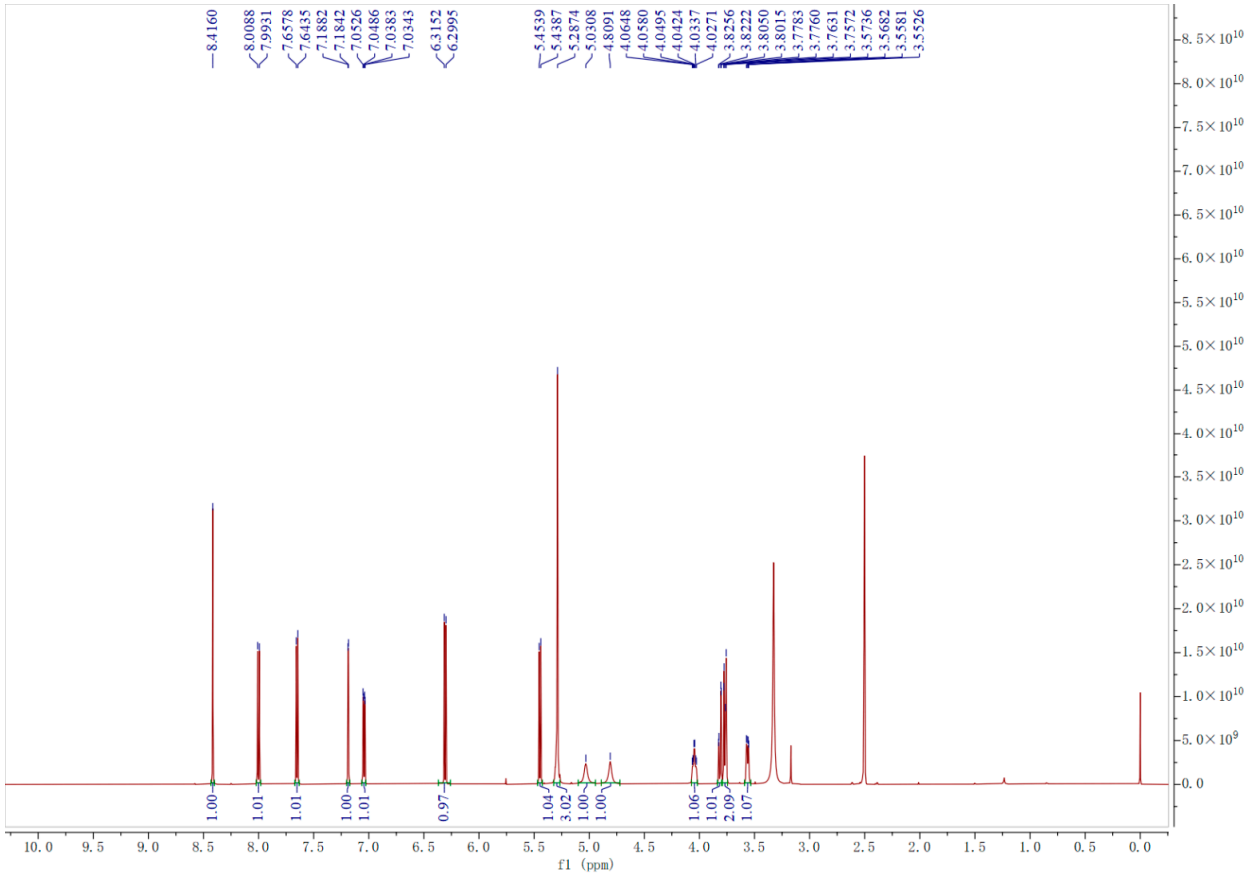
Figures S9. The [1]H-NMR spectrum of 7- [(1-β-D-xylopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10e**)



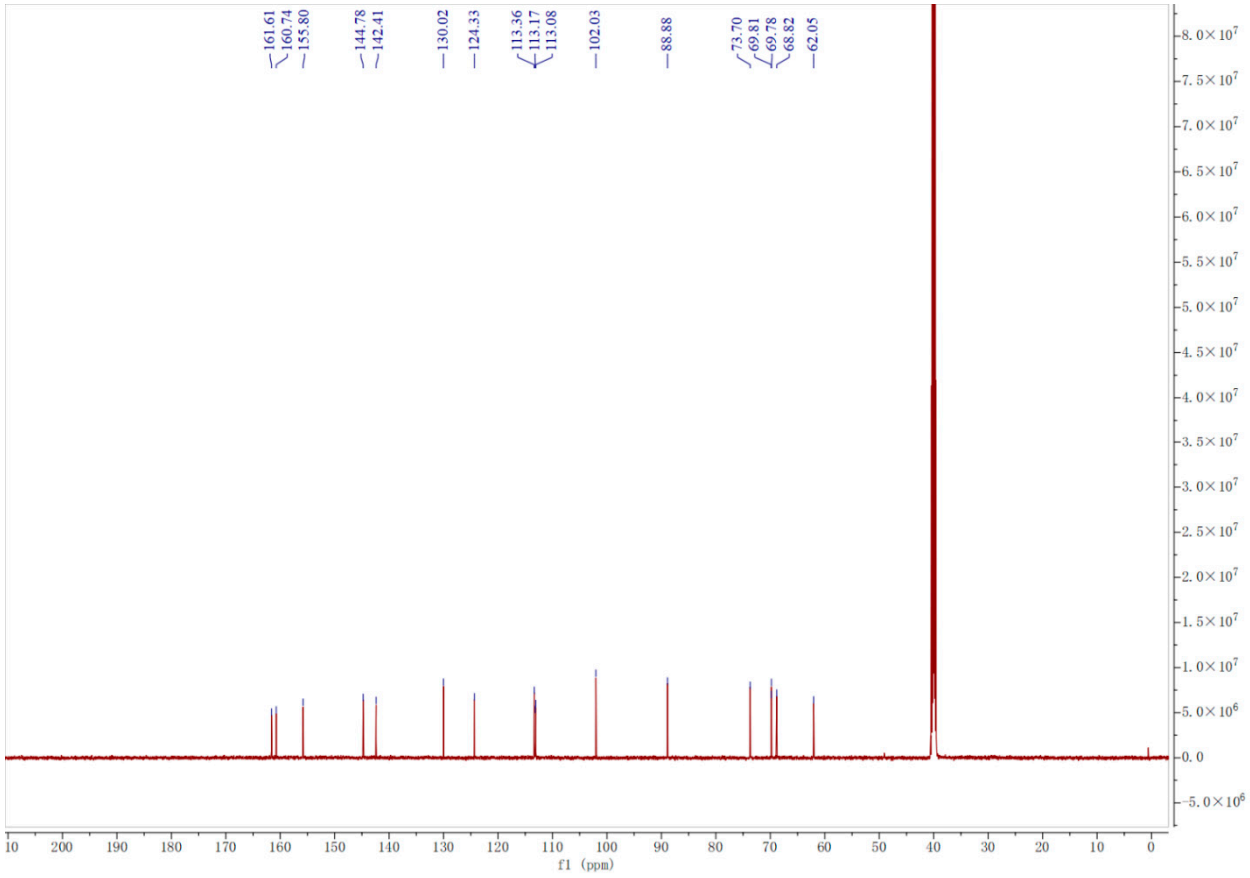
Figures S10. The [13]C-NMR spectrum of 7- [(1-β-D-xylopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10e**)



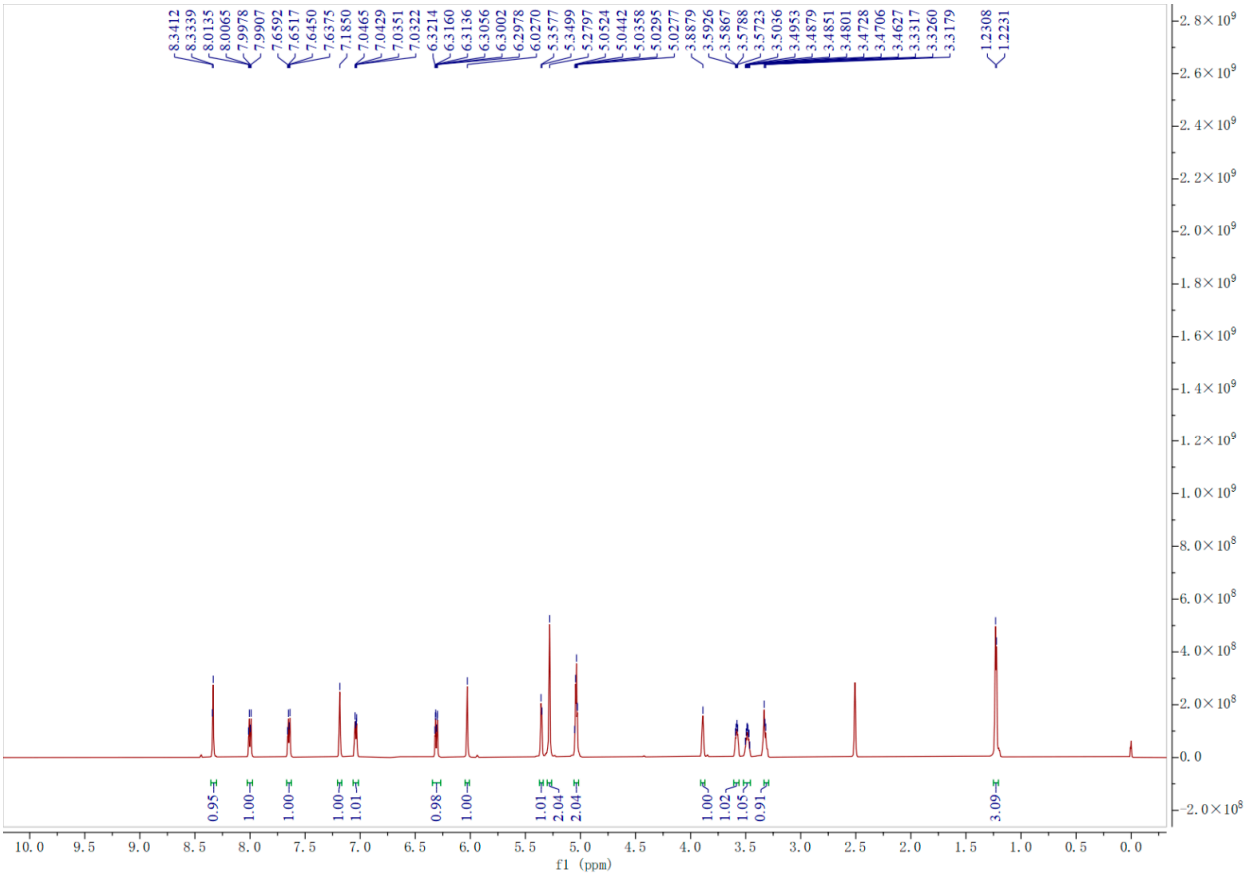
Figures S11. The [1]H-NMR spectrum of 7- [(1-β-L-arabinopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10f**)



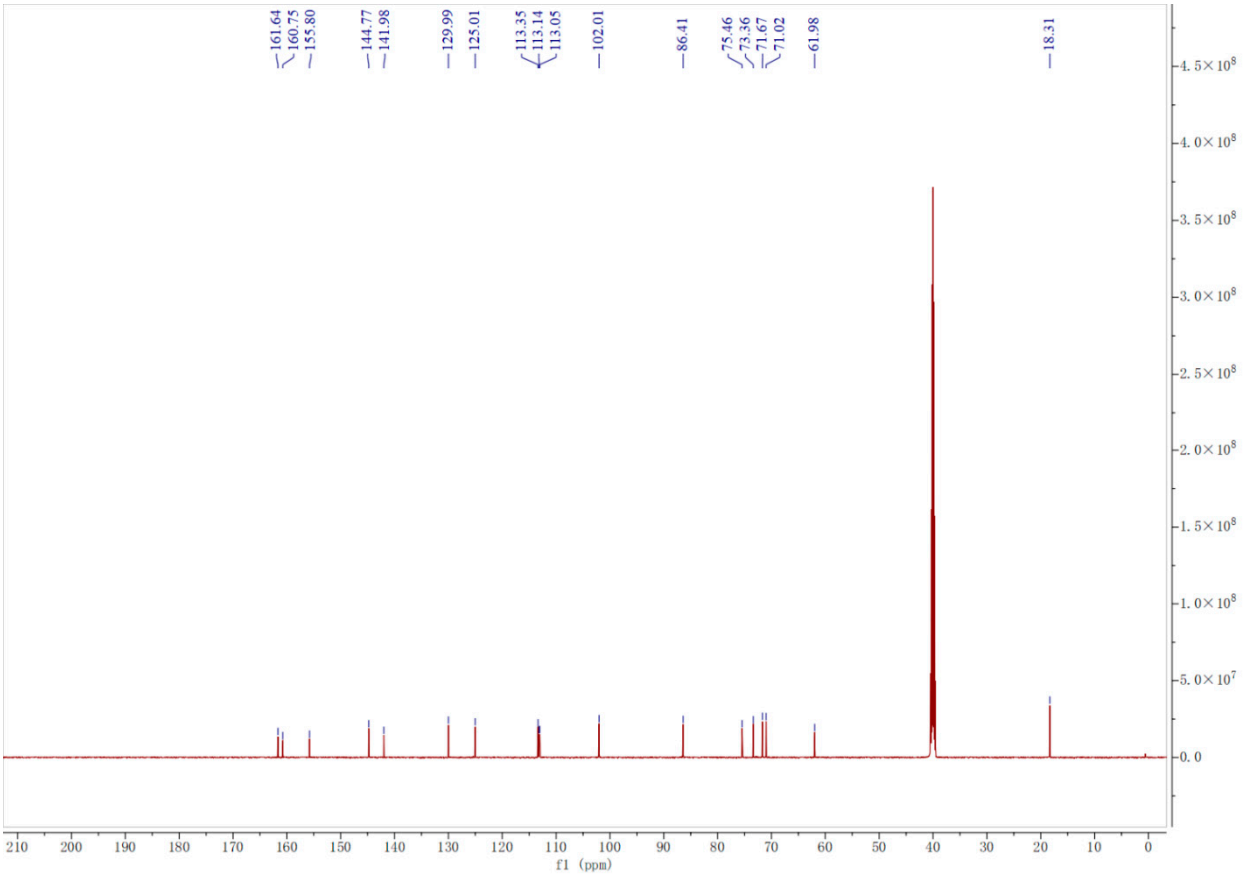
Figures S12. The [13]C-NMR spectrum of 7- [(1-β-L-arabinopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10f**)



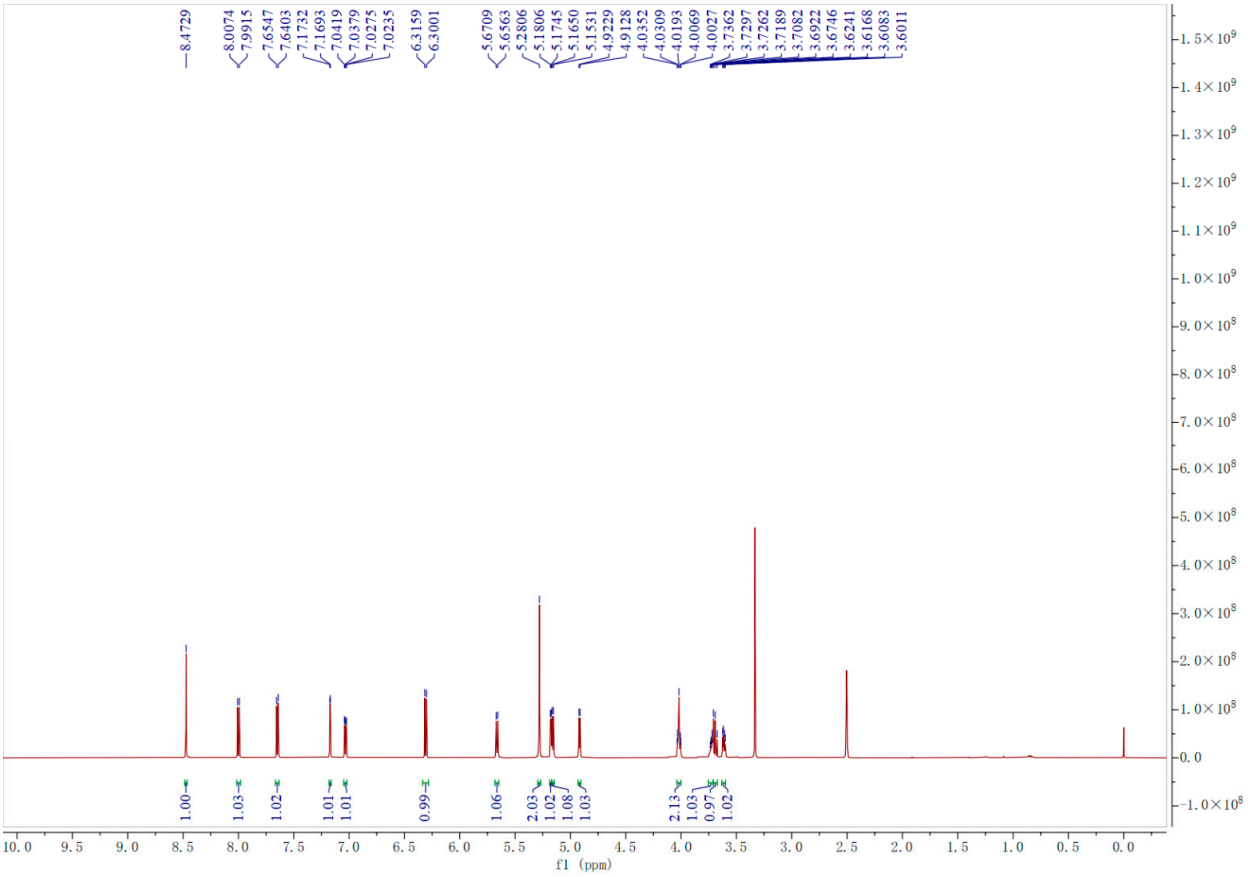
Figures S13. The [1]H-NMR spectrum of 7- [(1-β-L-rhamnosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10g**)



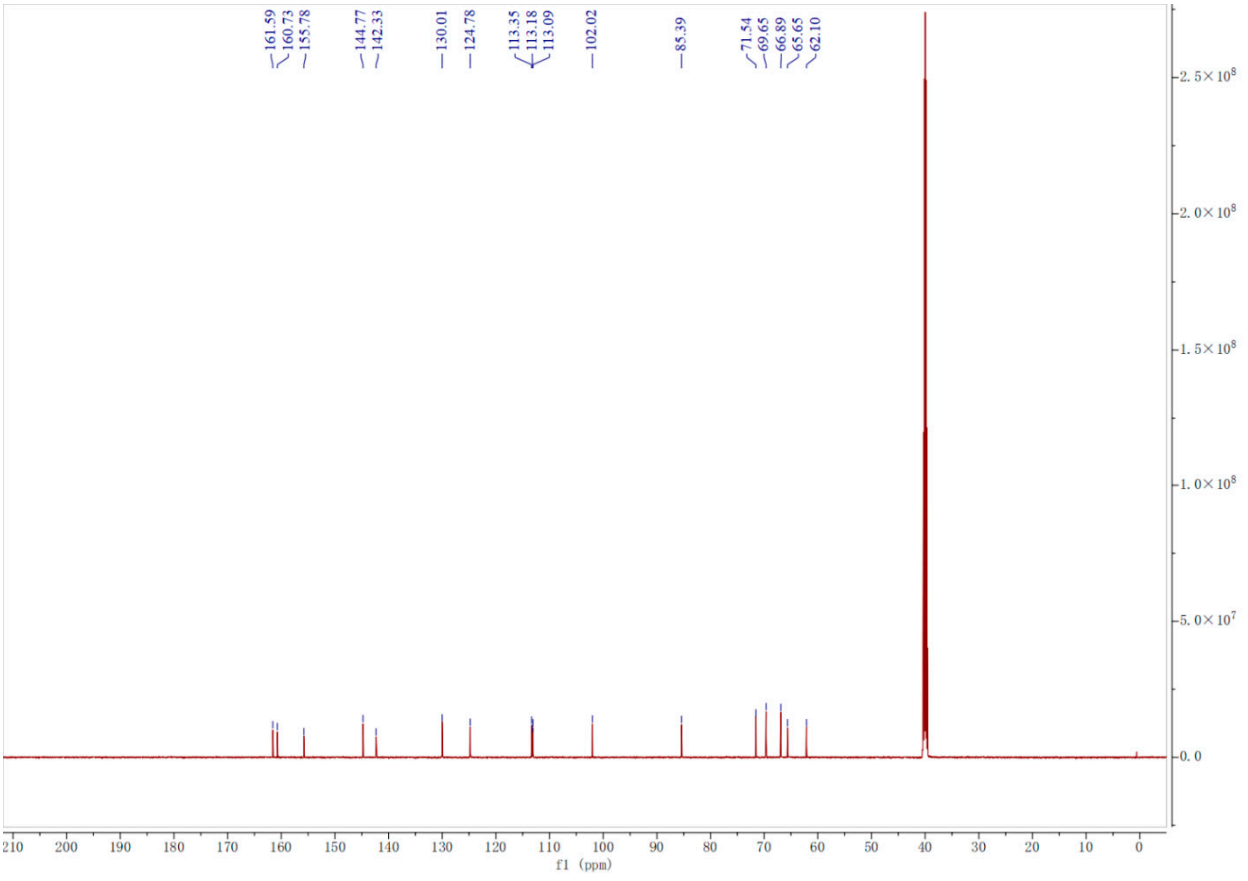
Figures S14. The [13]C-NMR spectrum of 7- [(1-β-L-rhamnosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10g**)



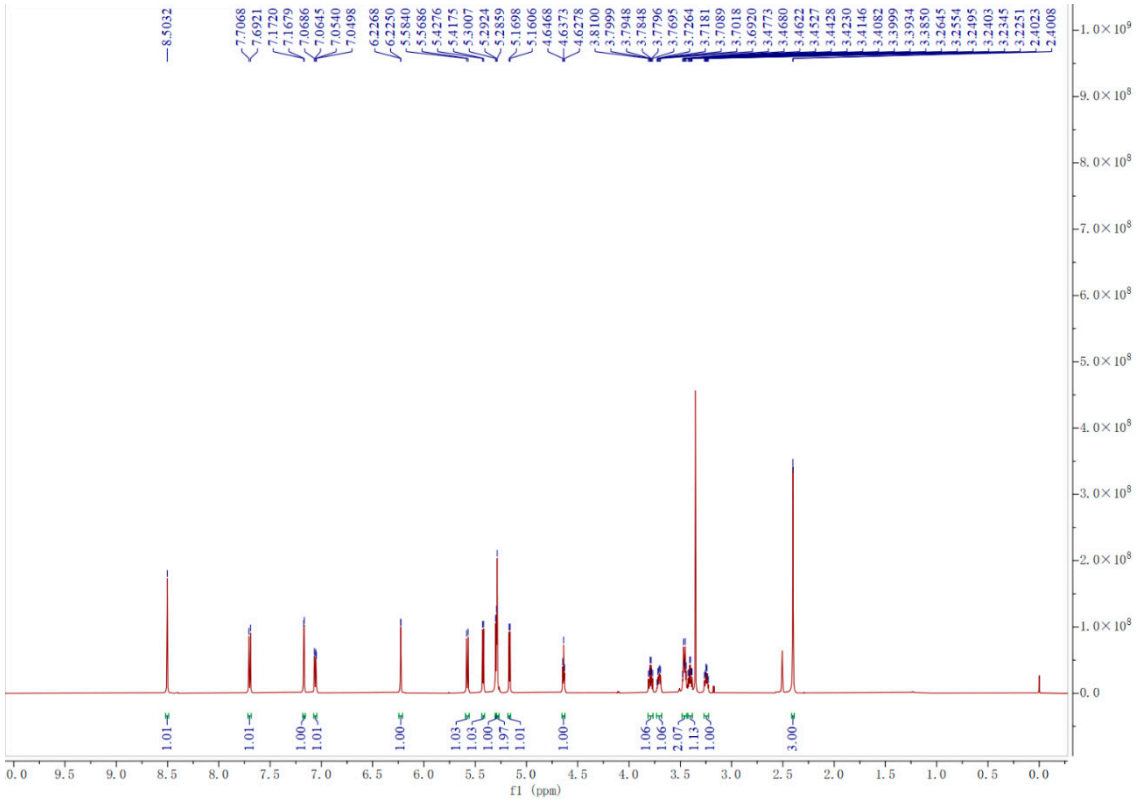
Figures S15. The [1]H-NMR spectrum of 7- [(1-β-D-ribofuranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10h**)



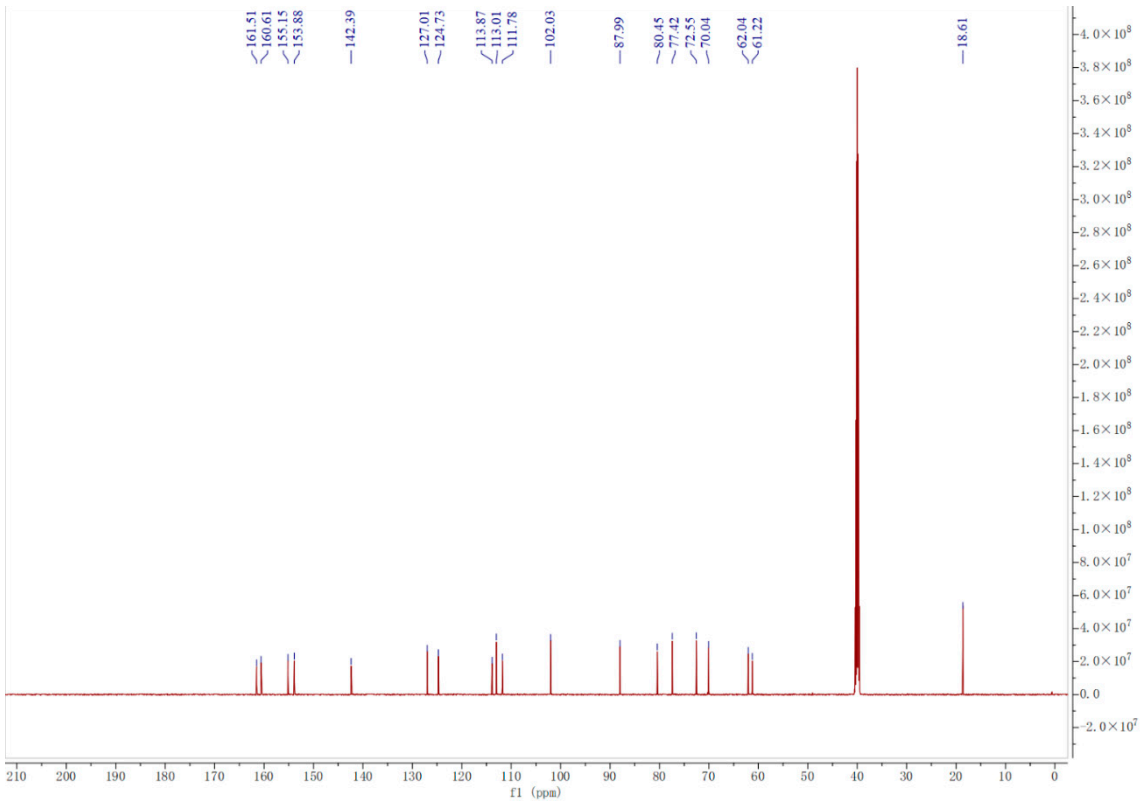
Figures S16. The [13]C-NMR spectrum of 7- [(1-β-D-ribofuranosyl-1H-1,2,3-triazol-4-yl) methoxy]-2H-chromen-2-one (**10h**)



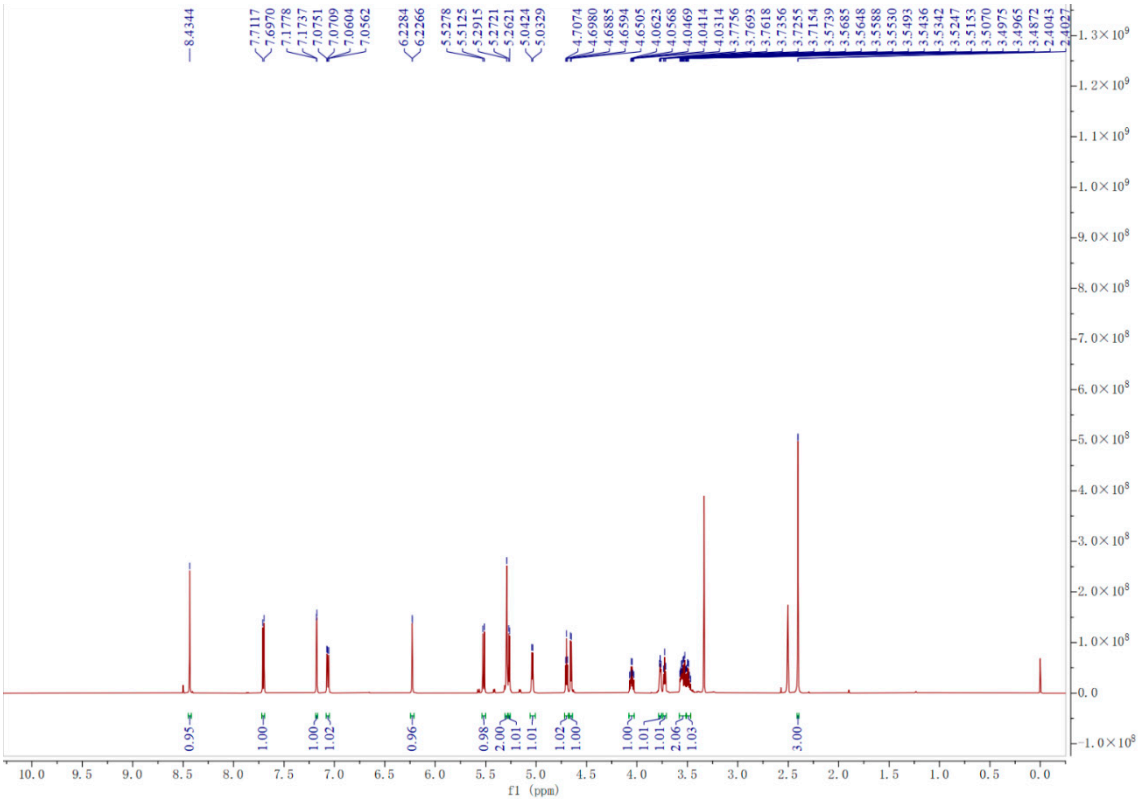
Figures S17. The [1]H-NMR spectrum of 7- [(1-β-D-glucopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10i**)



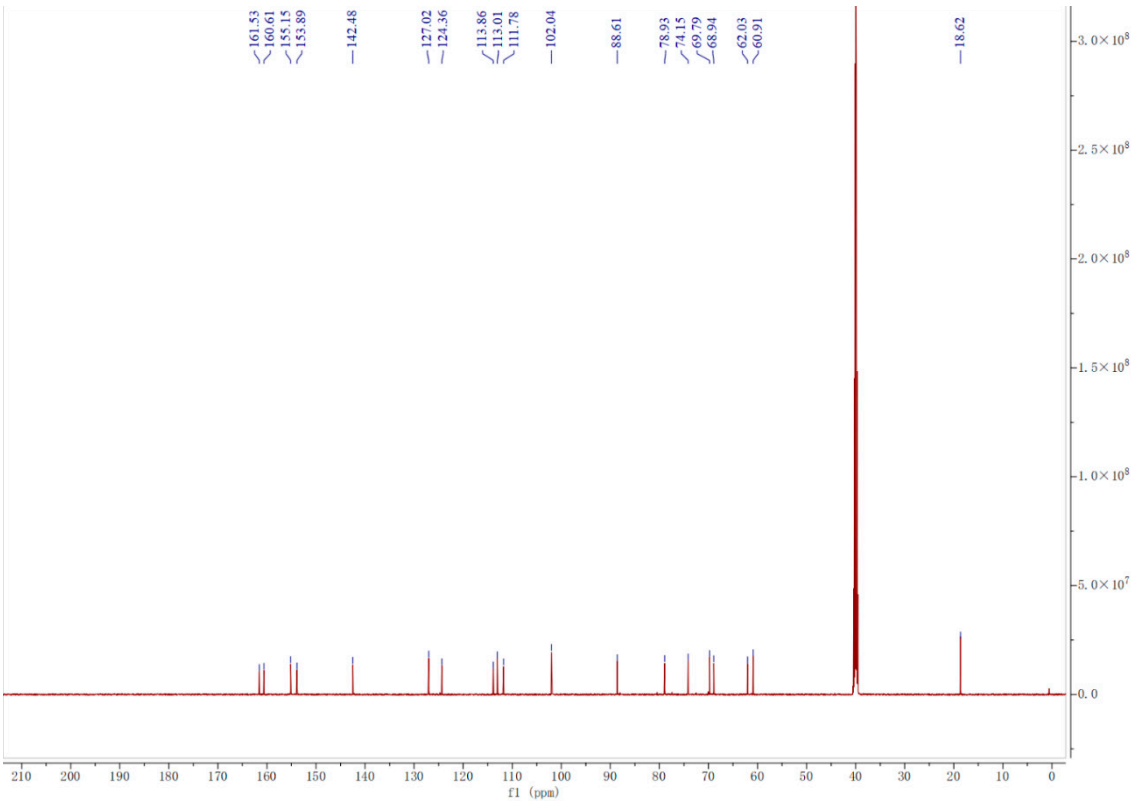
Figures S18. The [13]C-NMR spectrum of 7- [(1-β-D-glucopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10i**)



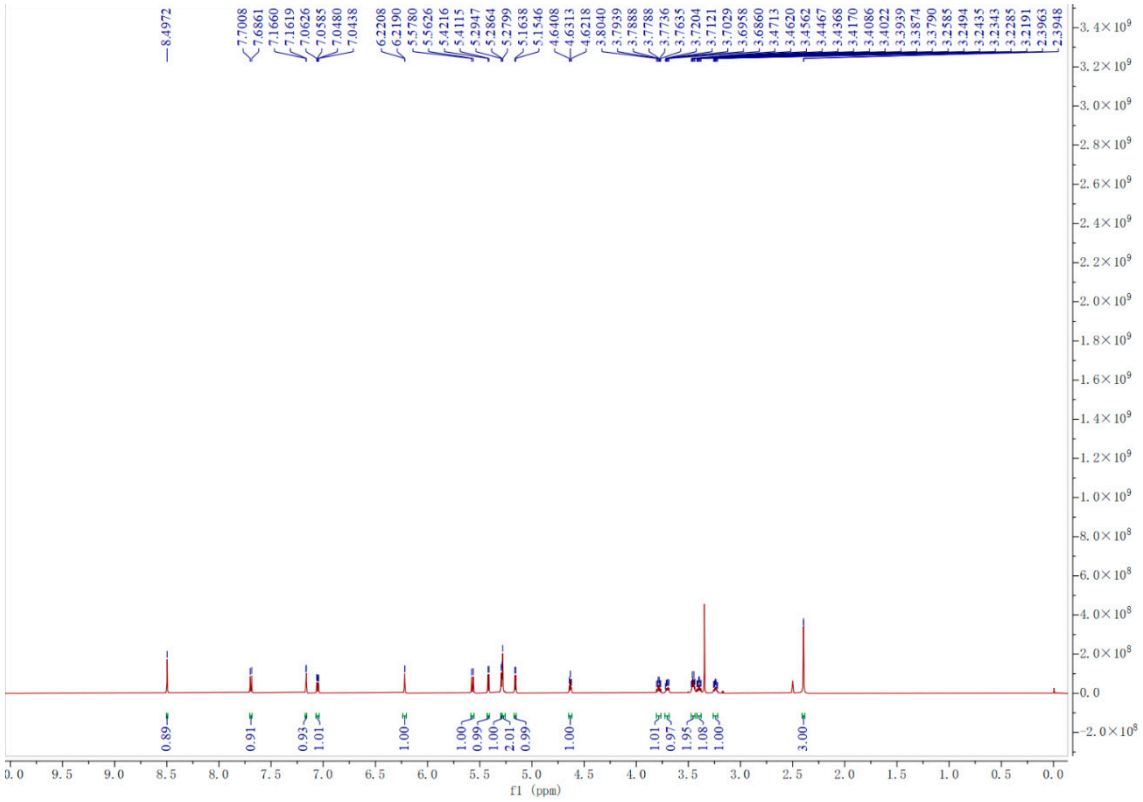
Figures S19. The [1]H-NMR spectrum of 7- [(1-β-D-galactopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10j**)



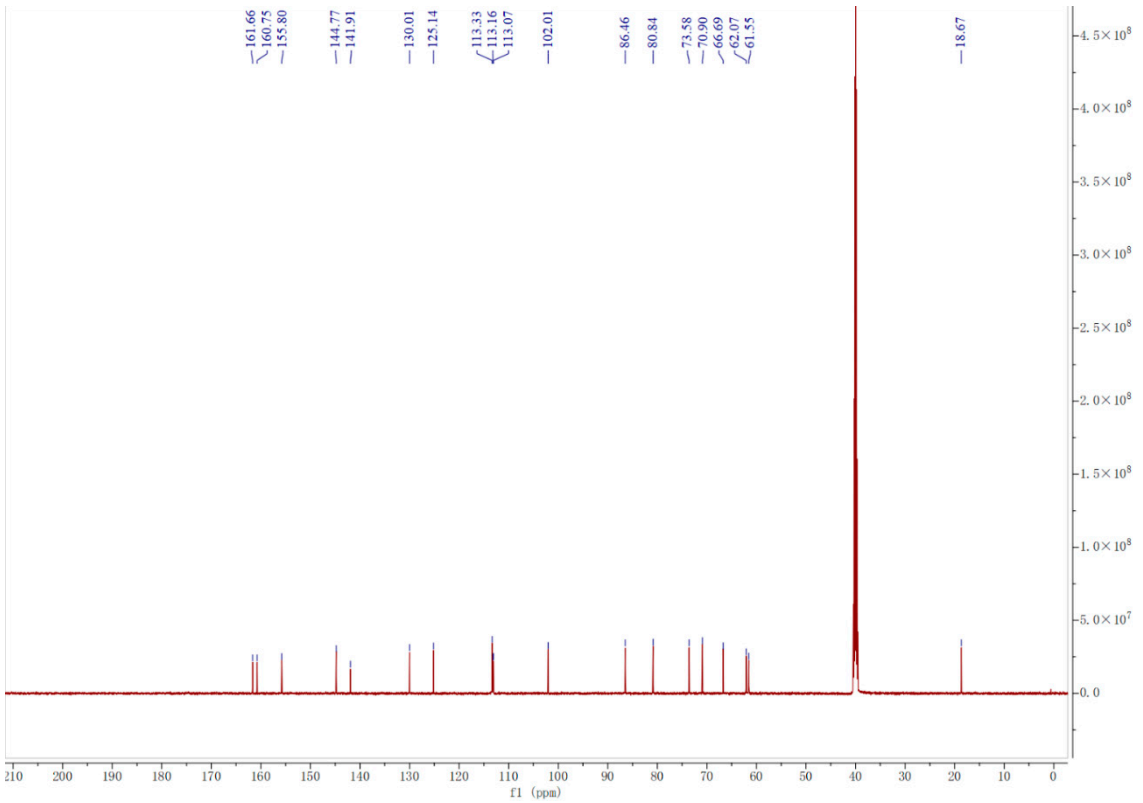
Figures S20. The [13]C-NMR spectrum of 7- [(1-β-D-galactopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10j**)



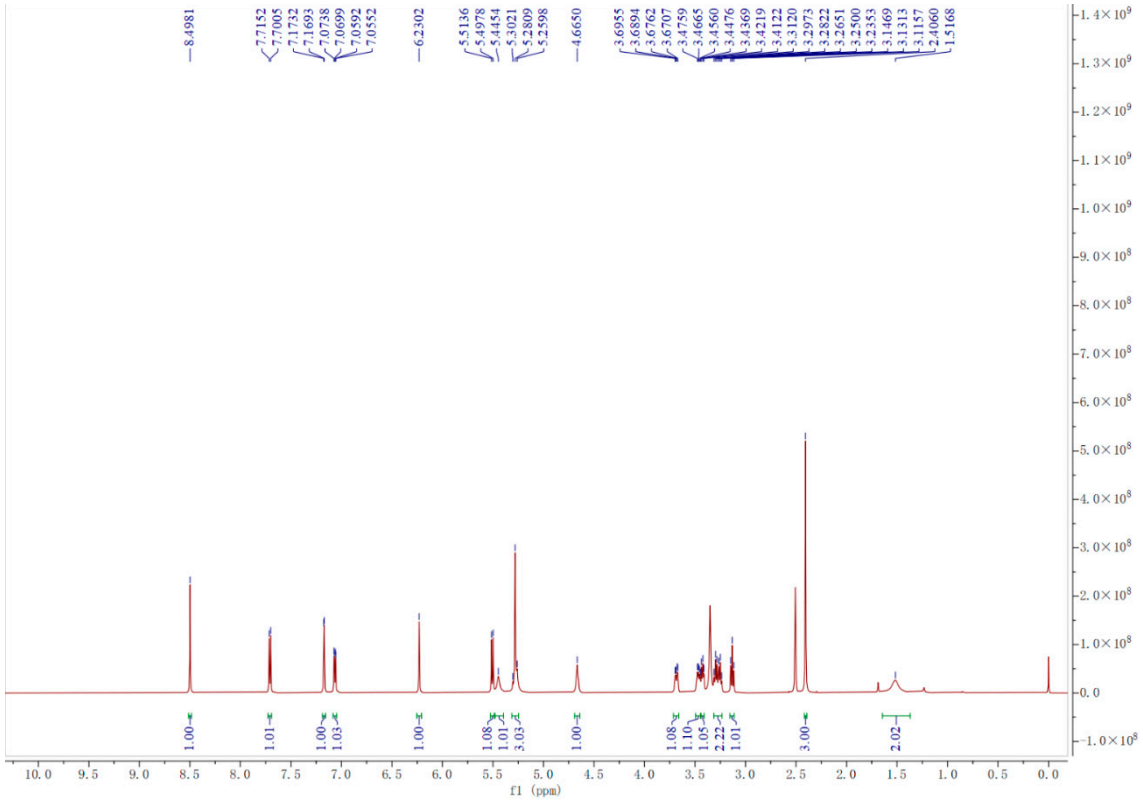
Figures S21. The [1]H-NMR spectrum of 7- [(1-β-D-mannopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10k**)



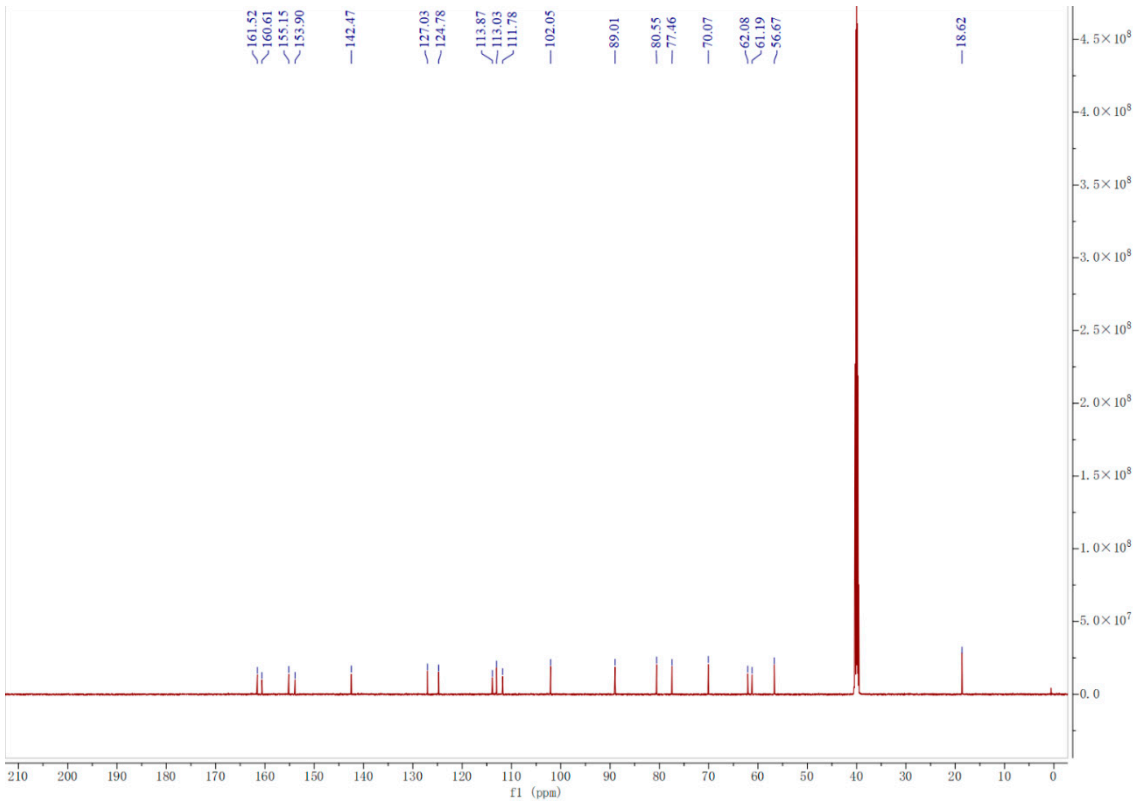
Figures S22. The [13]C-NMR spectrum of 7- [(1-β-D-mannopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10k**)



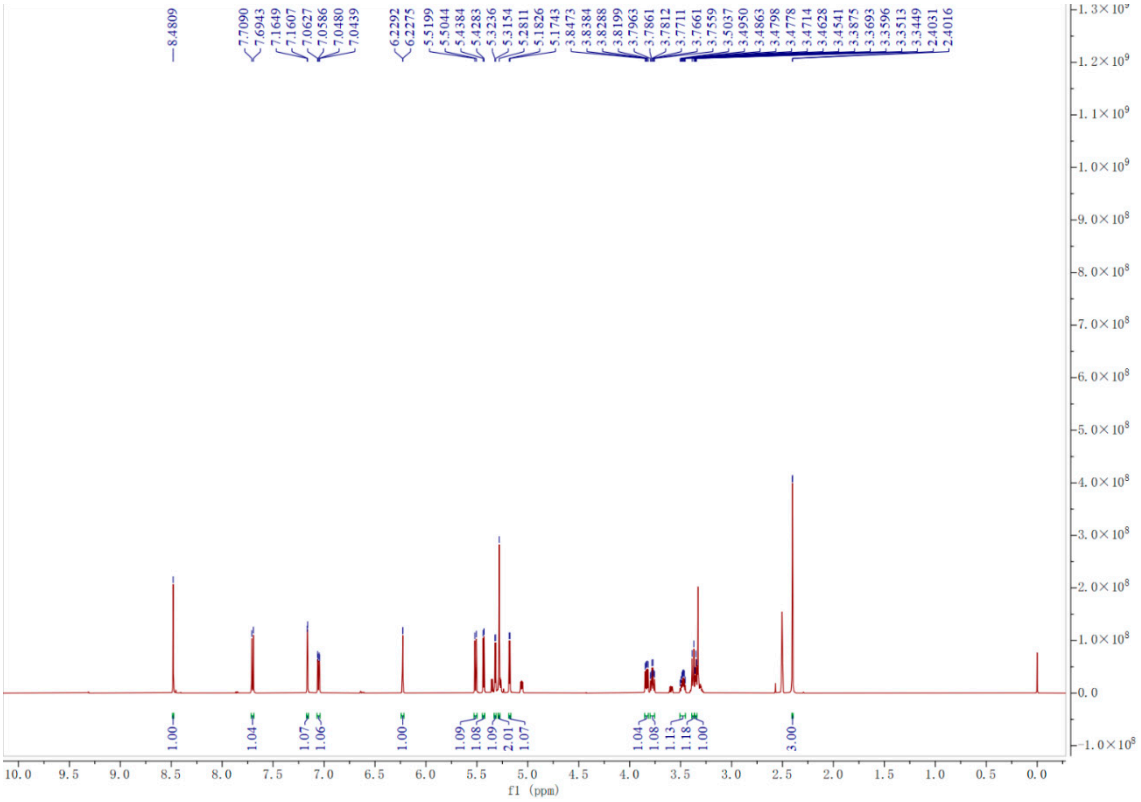
Figures S23. The [1]H-NMR spectrum of 7- [(1-β-D-glucosaminogly-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10l**)



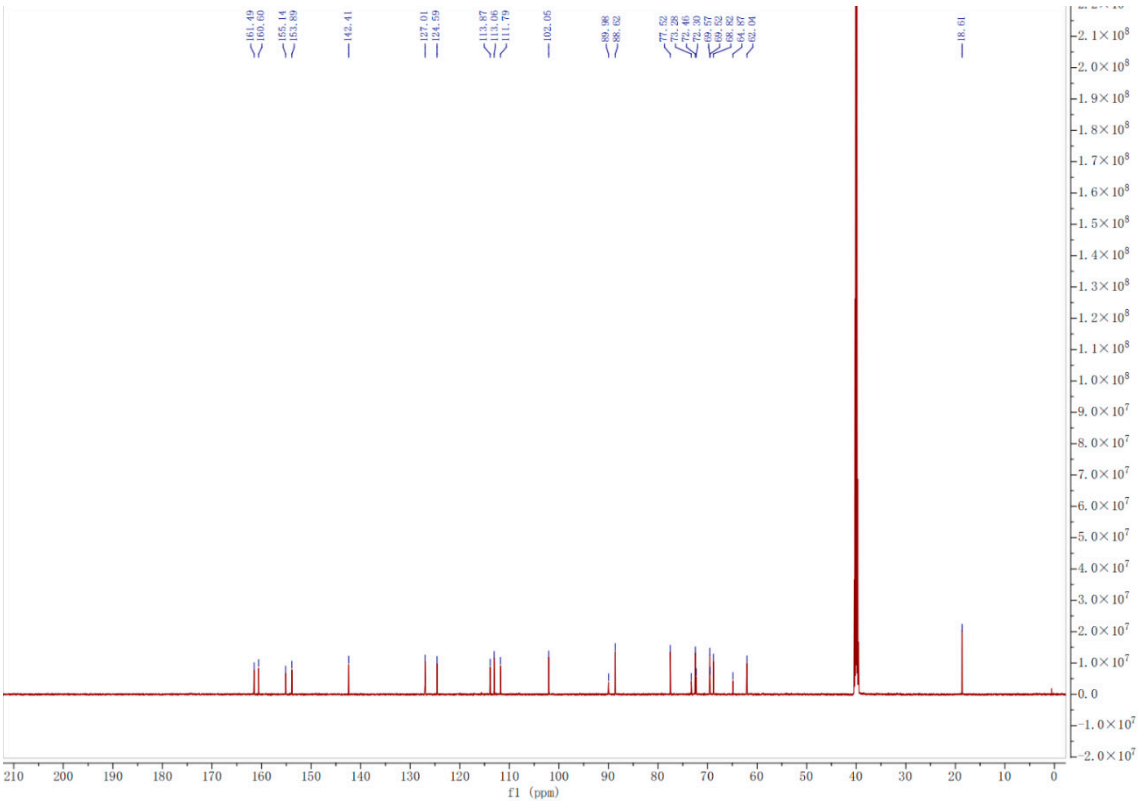
Figures S24. The [13]C-NMR spectrum of 7- [(1-β-D-glucosaminogly-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10l**)



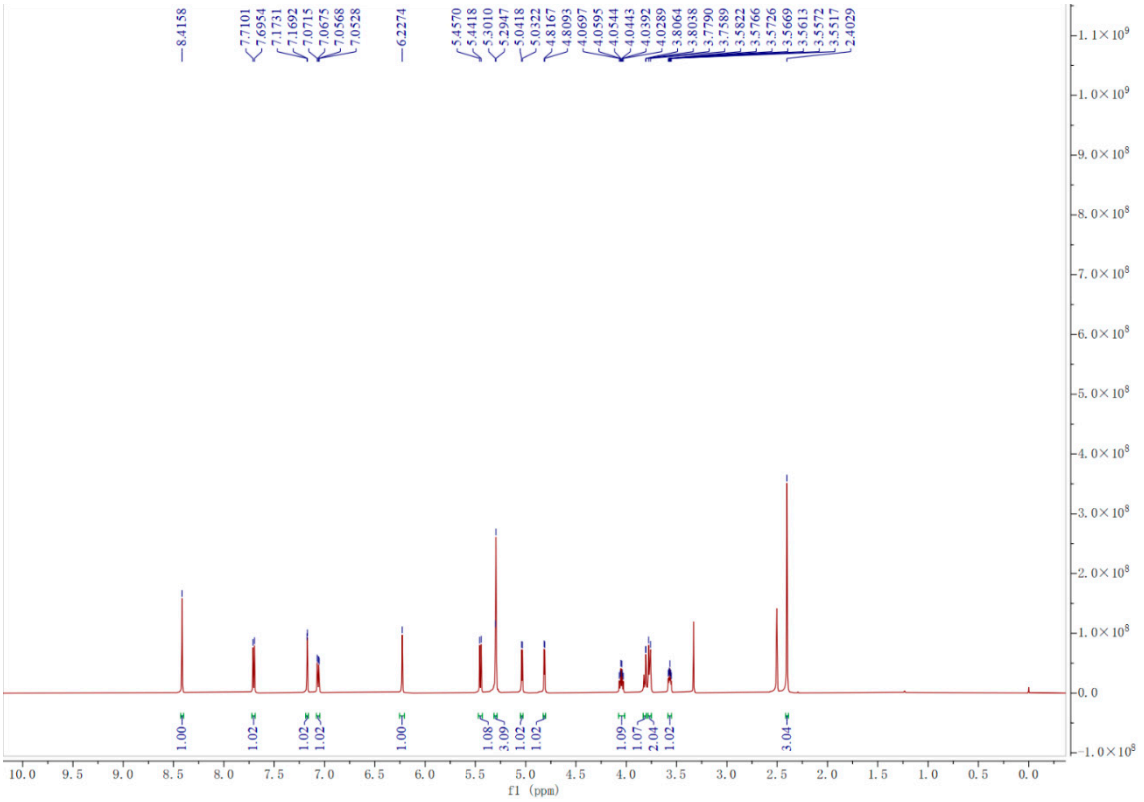
Figures S25. The [1]H-NMR spectrum of 7- [(1-β-D-xylopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10m**)



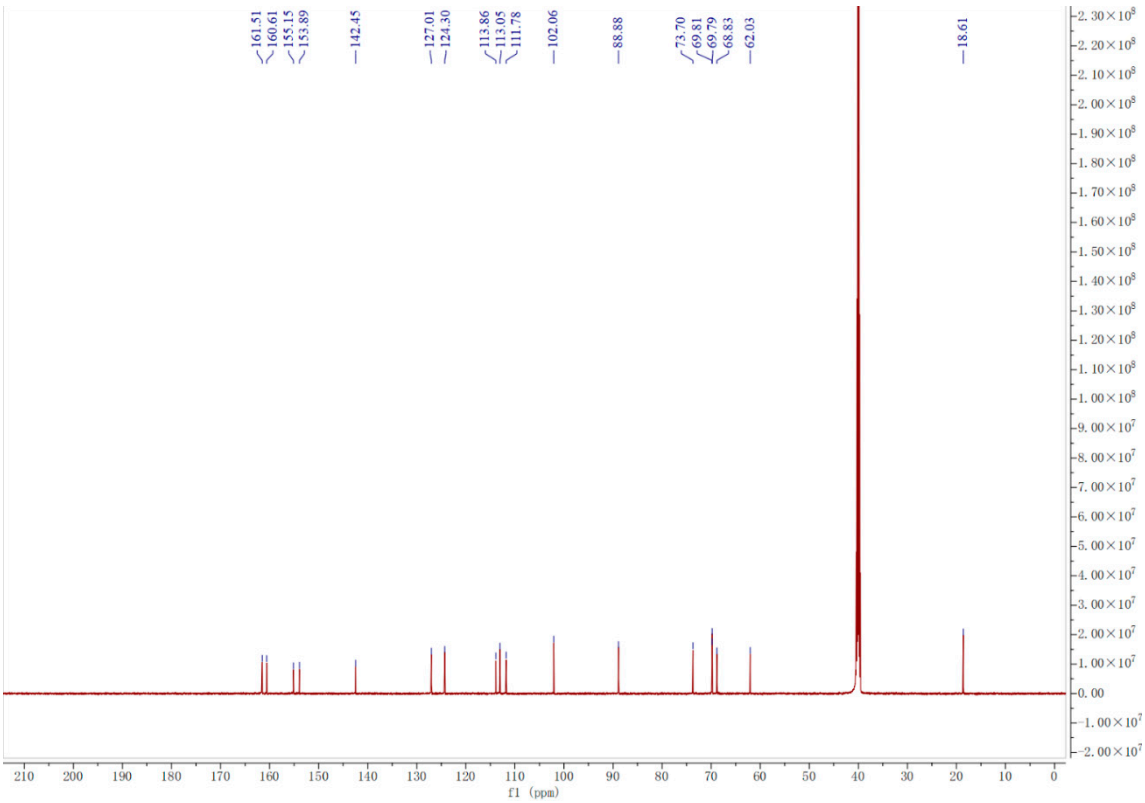
Figures S26. The [13]C-NMR spectrum of 7- [(1-β-D-xylopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10m**)



Figures S27. The [1]H-NMR spectrum of 7- [(1-β-L-arabinopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10n**)

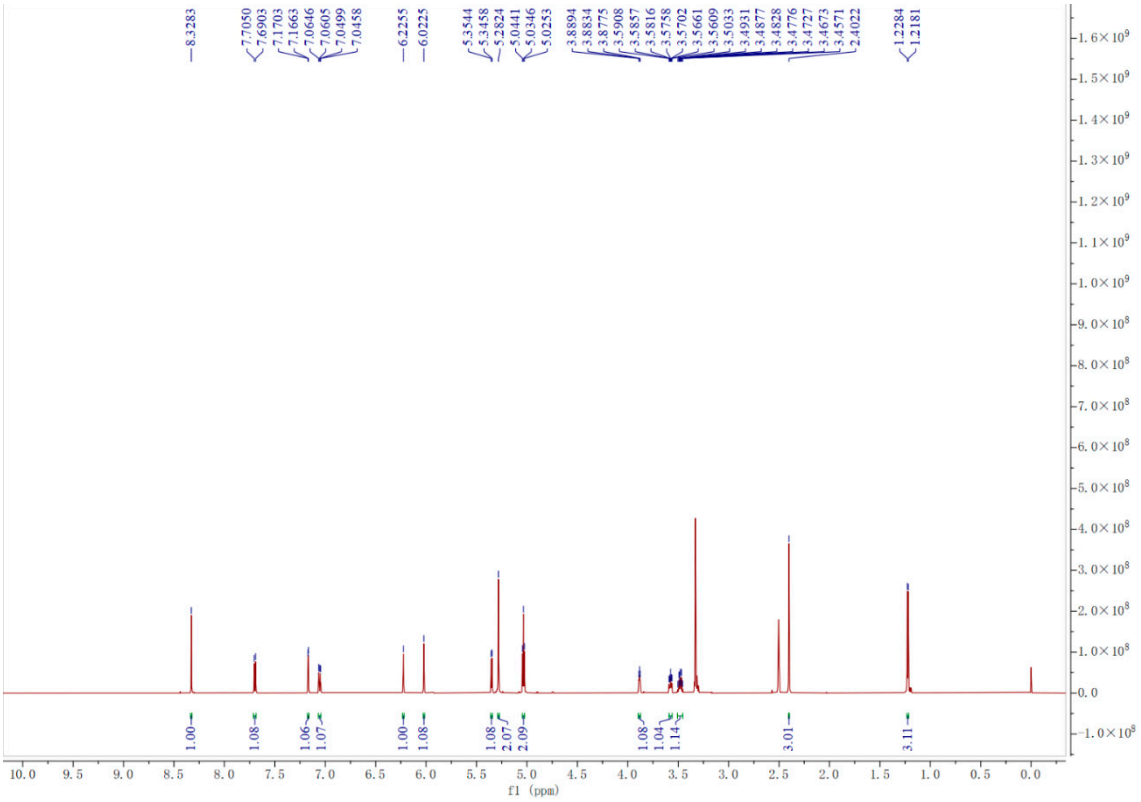


Figures S28. The [13]C-NMR spectrum of 7- [(1-β-L-arabinopyranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one (**10n**)



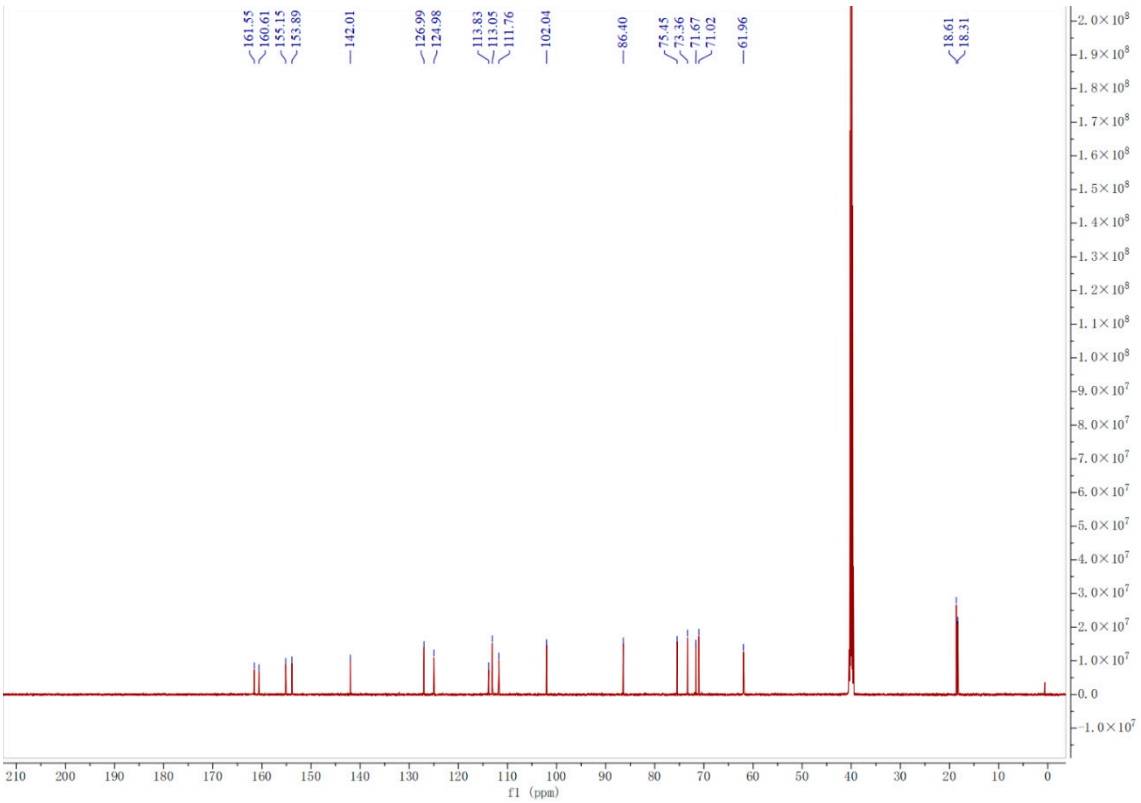
Figures S29. The [1]H-NMR spectrum of 7- [(1-β-L-rhamnosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one

(10o)



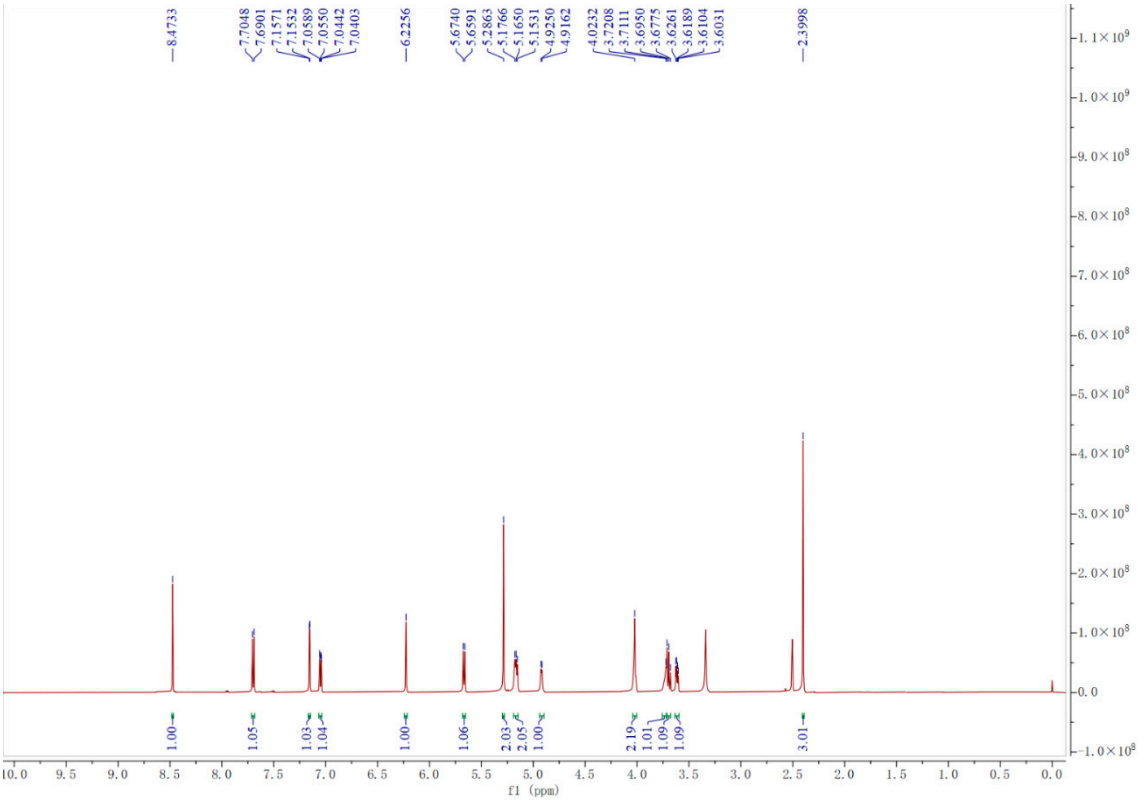
Figures S30. The [13]C-NMR spectrum of 7- [(1-β-L-rhamnosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one

(10o)



Figures S31. The [1]H-NMR spectrum of 7- [(1-β-D-ribofuranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one

(10p)



Figures S32. The [13]C-NMR spectrum of 7- [(1-β-D-ribofuranosyl-1H-1,2,3-triazol-4-yl) methoxy]-4-methyl-2H-chromen-2-one

(10p)