

# Supplementary Information

## Synthesis and *in vitro* Evaluation of Novel Galactosyl-triazolo-benzenesulfonamides Against *Trypanosoma cruzi*

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4-azidobenzenesulfonamide (**30**)<sup>1-3</sup>

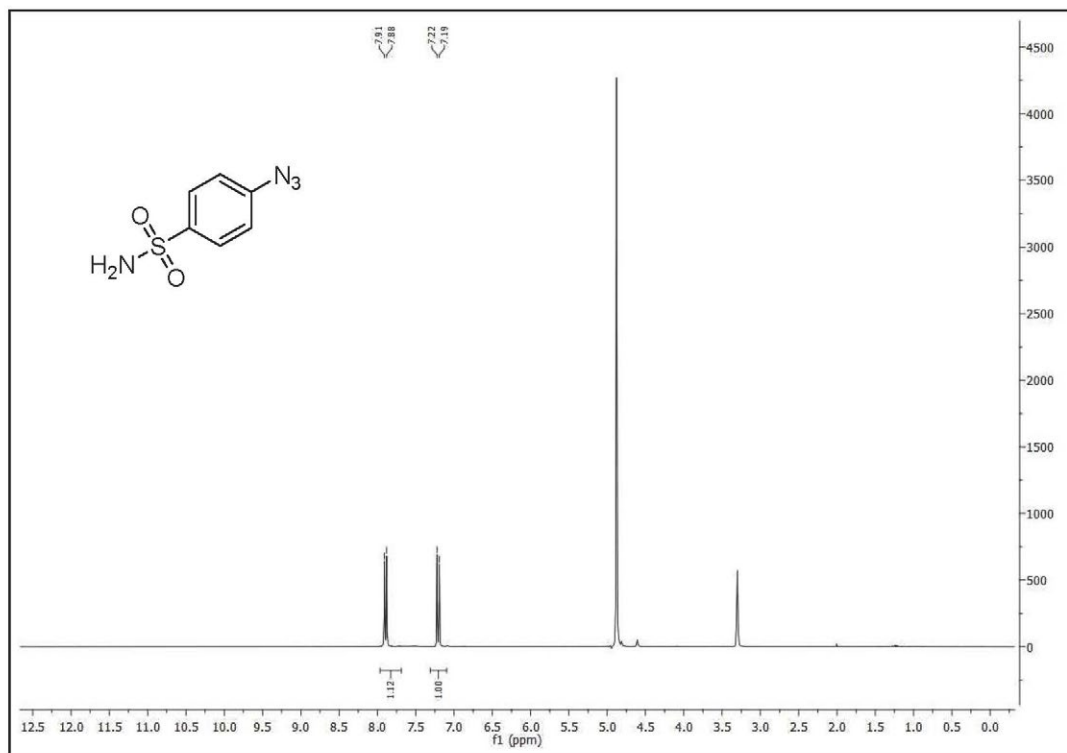


Figure S1. <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound **30**.

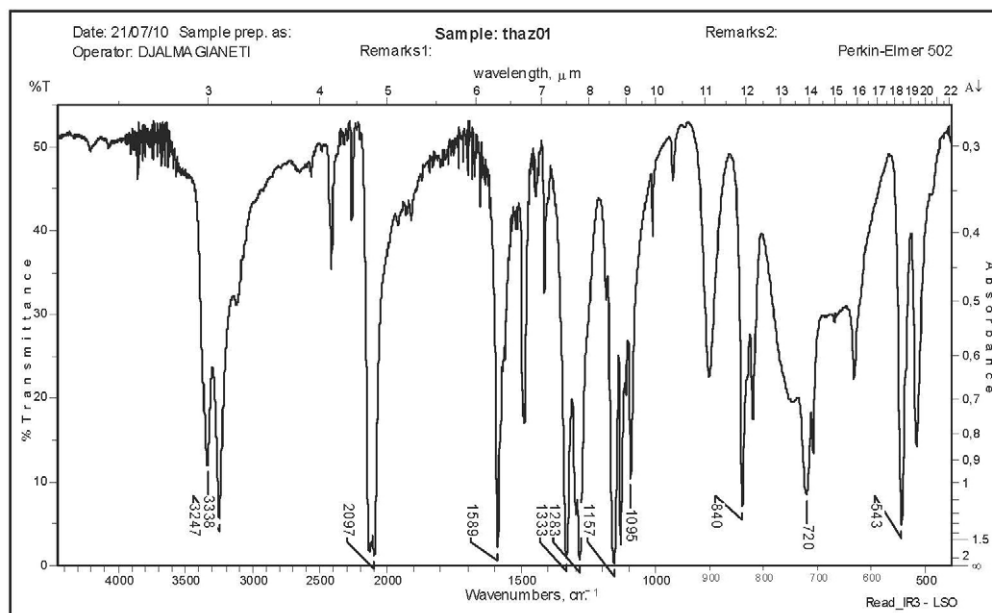


Figure S2. FT-IR (KBr) of compound **30**.

*N*-[(4-azidophenyl)sulfonyl]acetamide (**31**)<sup>1-3</sup>

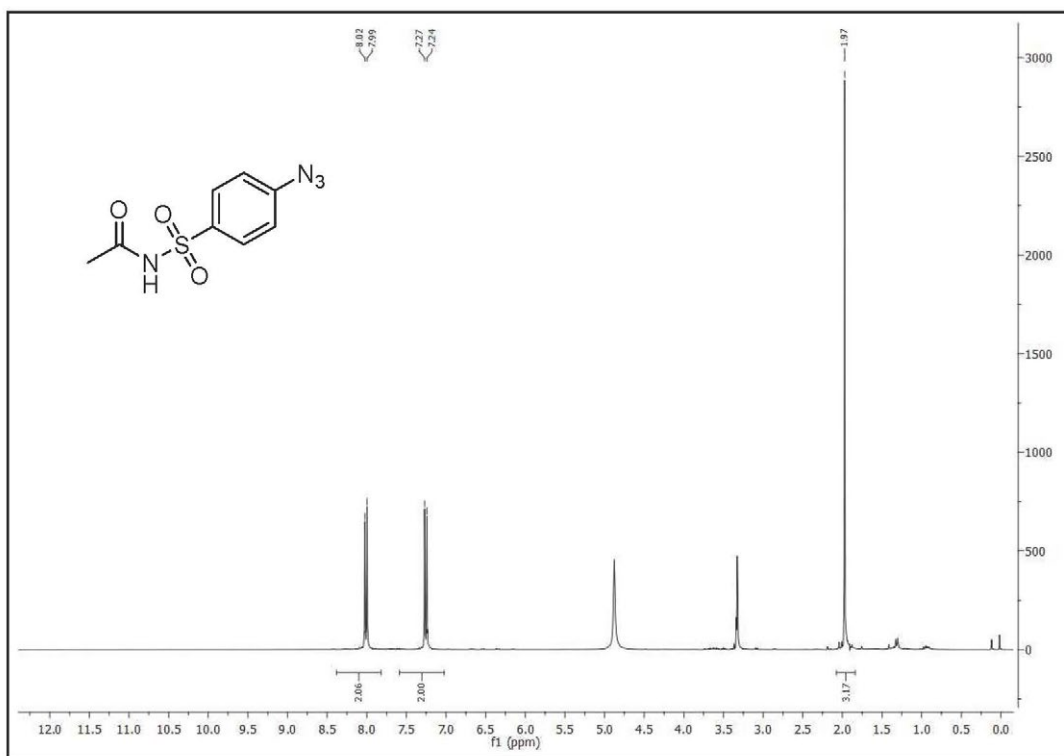
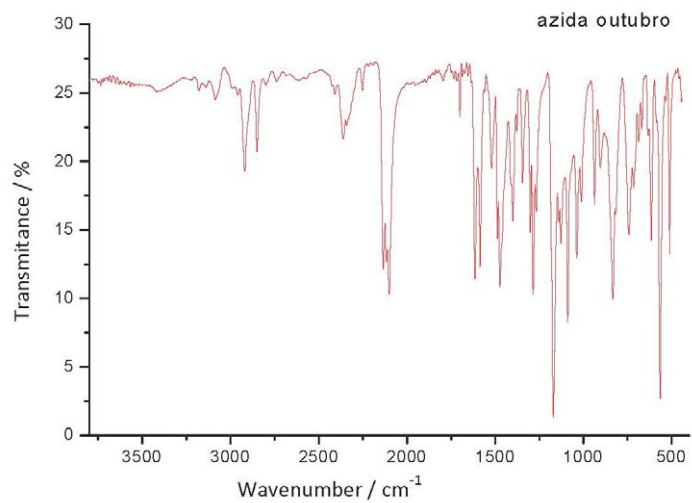
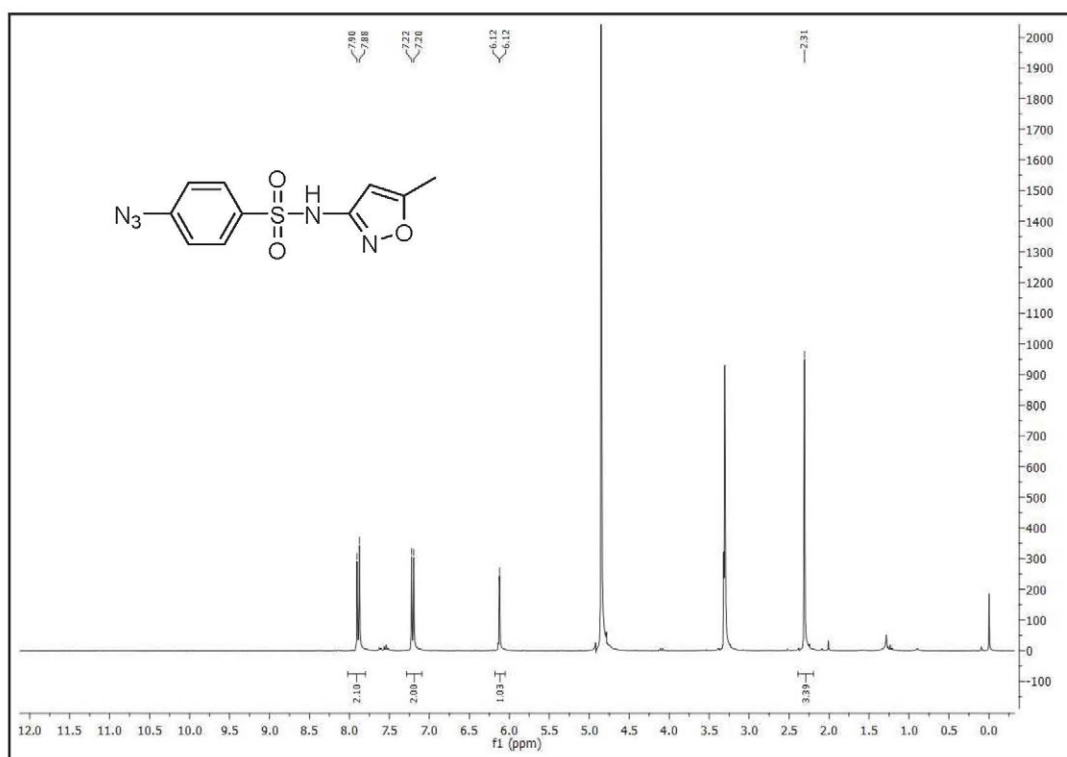


Figure S3. <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound **31**.



**Figure S4.** FT-IR (KBr) of compound **31**.

4-azido-*N*-(5-methylisoxazol-3-yl)benzenesulfonamide (**32**)<sup>1-3</sup>



**Figure S5.** <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound **32**.

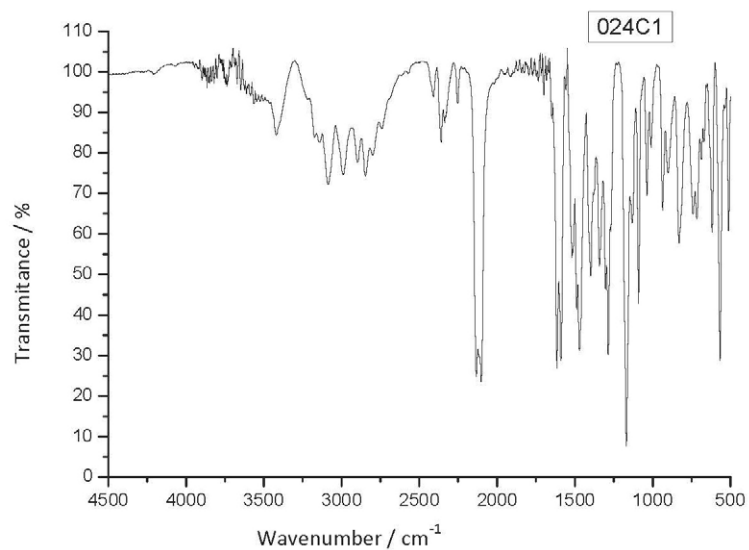


Figure S6. FT-IR (KBr) of compound **32**.

4-azido-*N*-(4-methylpyrimidin-2-yl)benzenesulfonamide (**33**)<sup>1-3</sup>

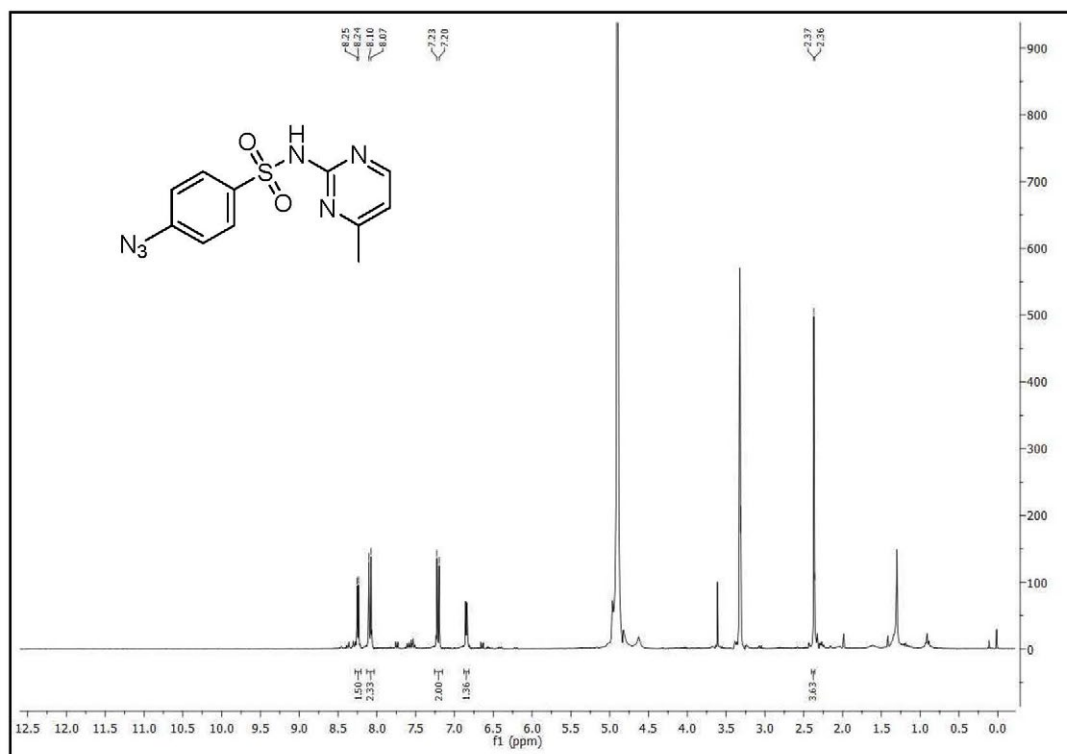
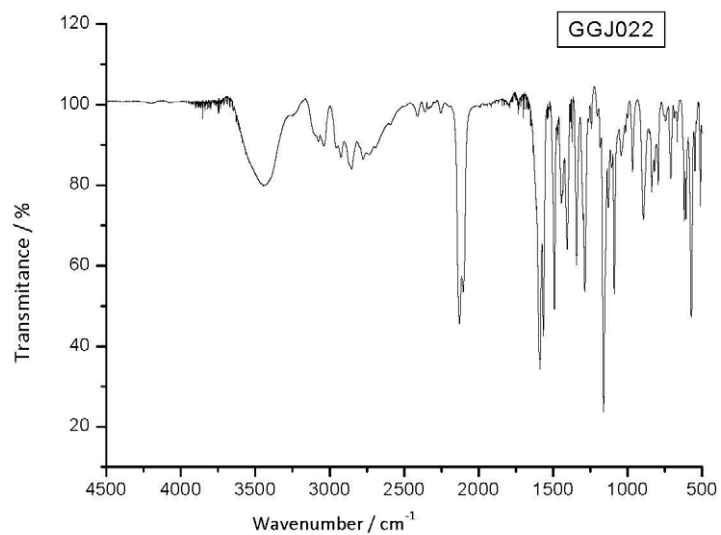
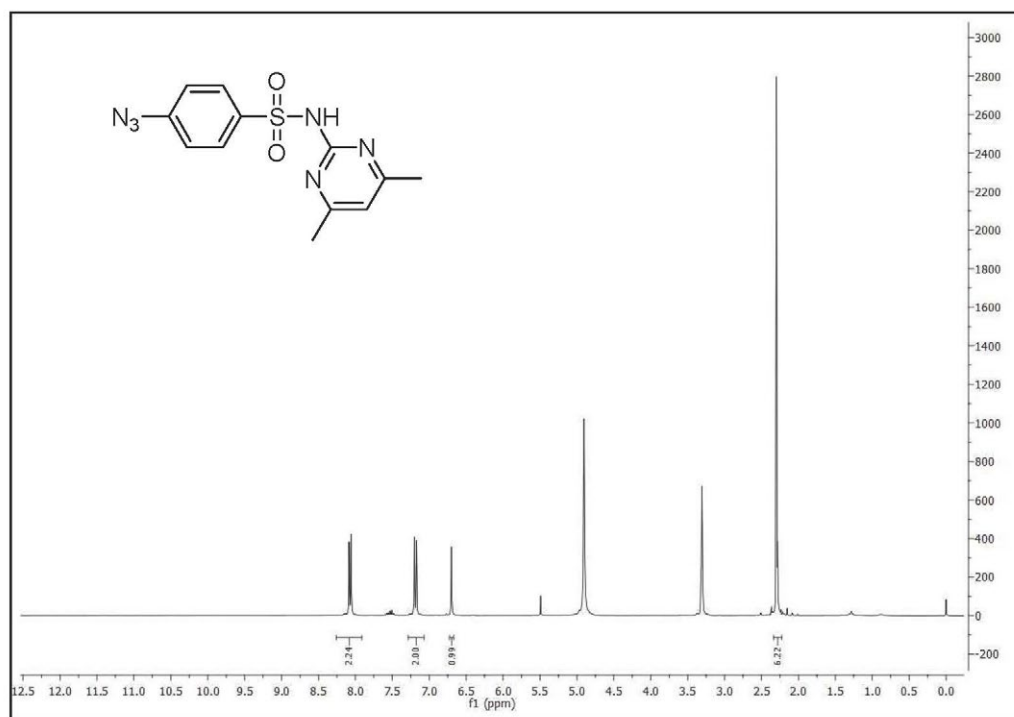


Figure S7. <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound **33**.



**Figure S8.** FT-IR (KBr) of compound **33**.

4-azido-*N*-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide (**34**)<sup>1-3</sup>



**Figure S9.** <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound **34**.

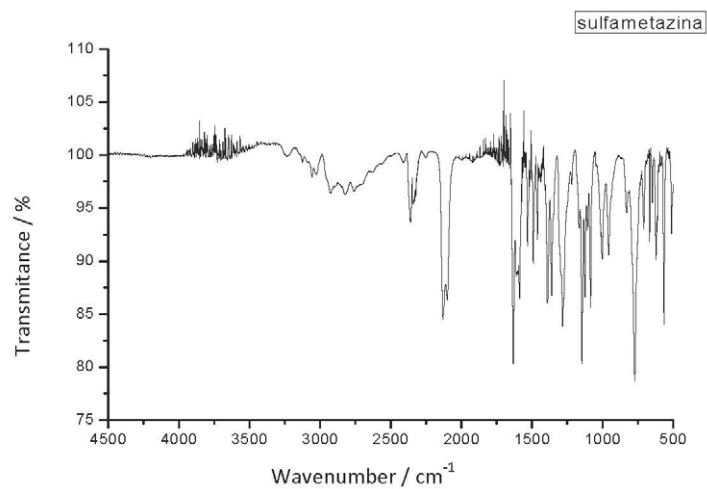


Figure S10. IR (KBr) of compound 34.

4-azido-*N*-(2,6-dimethoxypyrimidin-4-yl)benzenesulfonamide (**35**)<sup>1-3</sup>

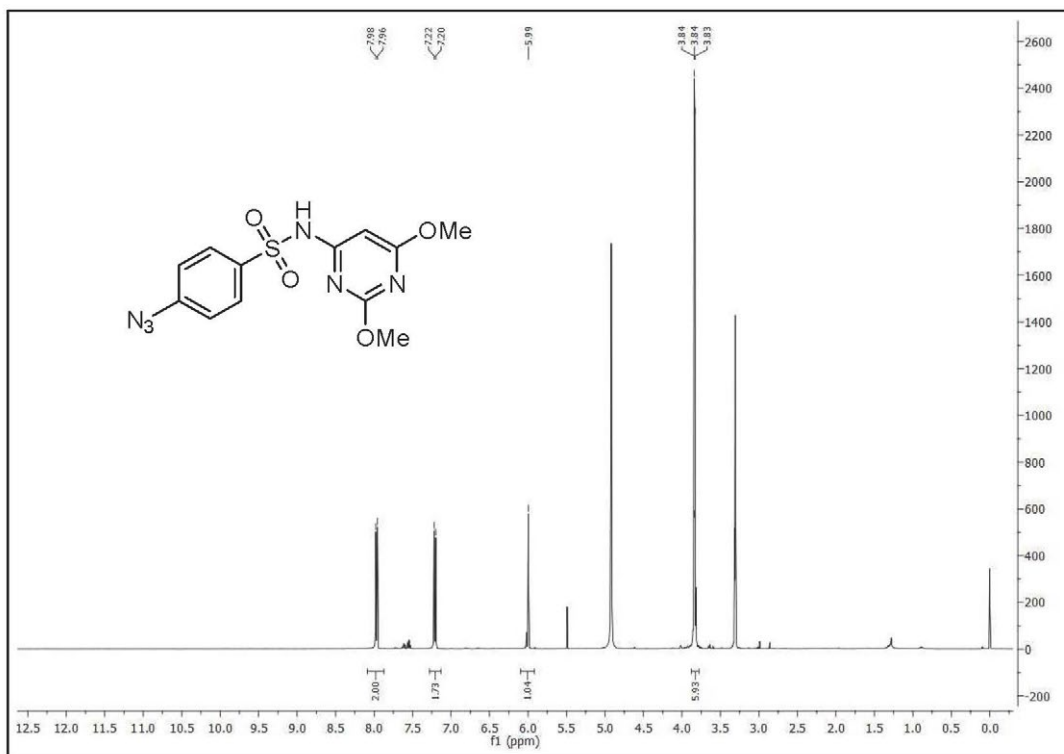


Figure S11. <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound 35.

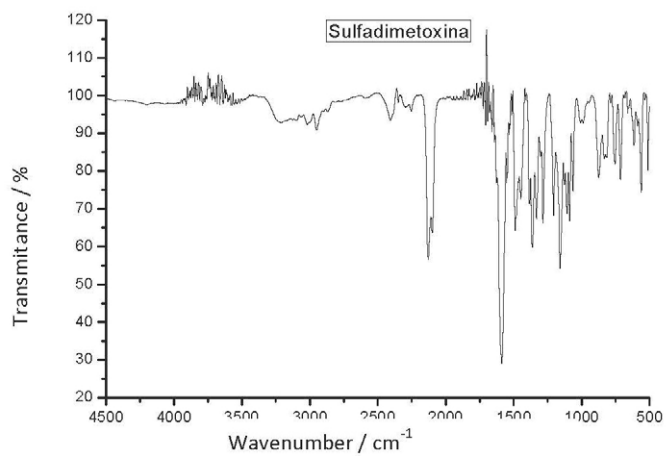


Figure S12. FT-IR (KBr) of compound 35.

4-azido-*N*-pyridin-2-yl-benzenesulfonamide (**36**)<sup>1-3</sup>

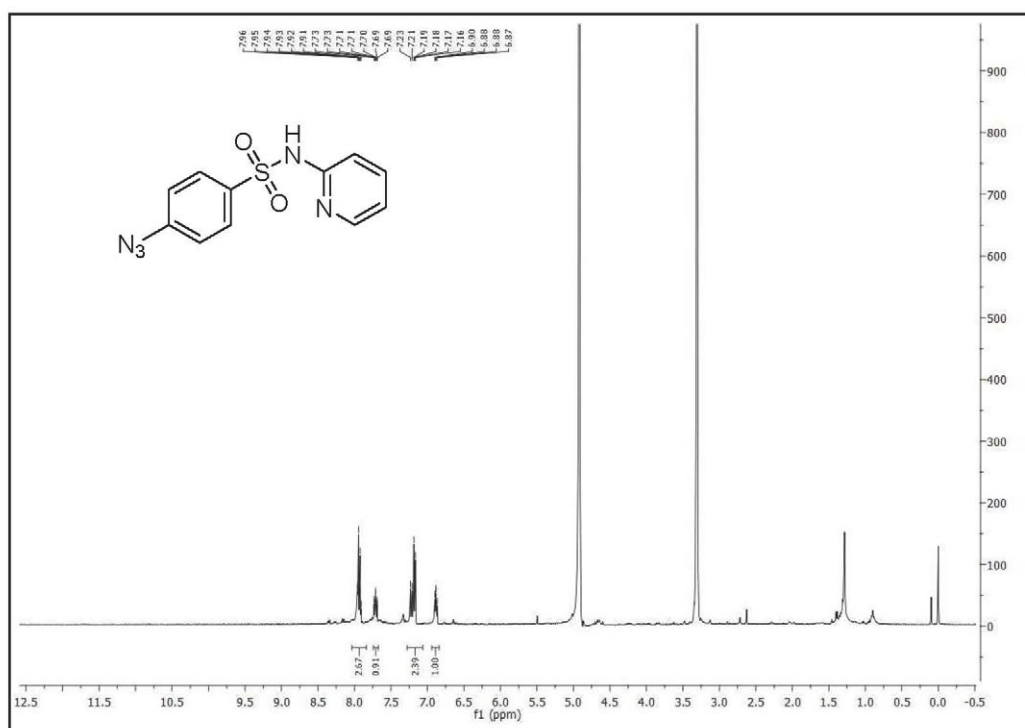
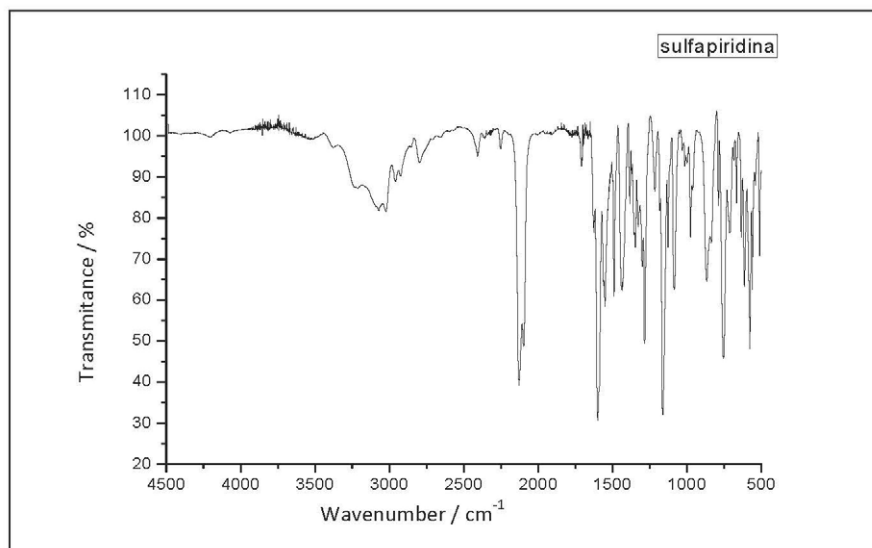
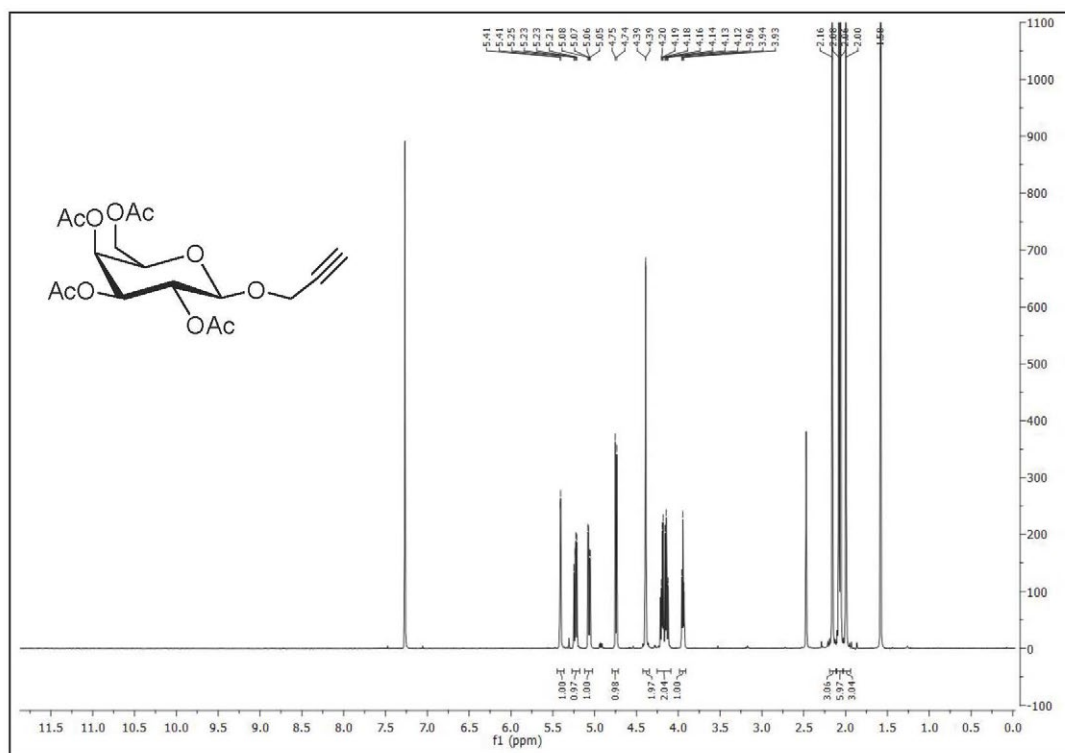


Figure S13. <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound 36.

**Figure S14.** FT-IR (KBr) spectrum of compound **36**.2-propynyl 2,3,4,6-tetra-*O*-acetyl- $\beta$ -D-galactopyranoside (**15**)<sup>4</sup>**Figure S15.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of compound **15**.



4-{4-[(2',3',4',6'-tetra-*O*-acetyl- $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3 triazol-1-yl}benzenesulfonamide (**37**)<sup>5,6</sup>

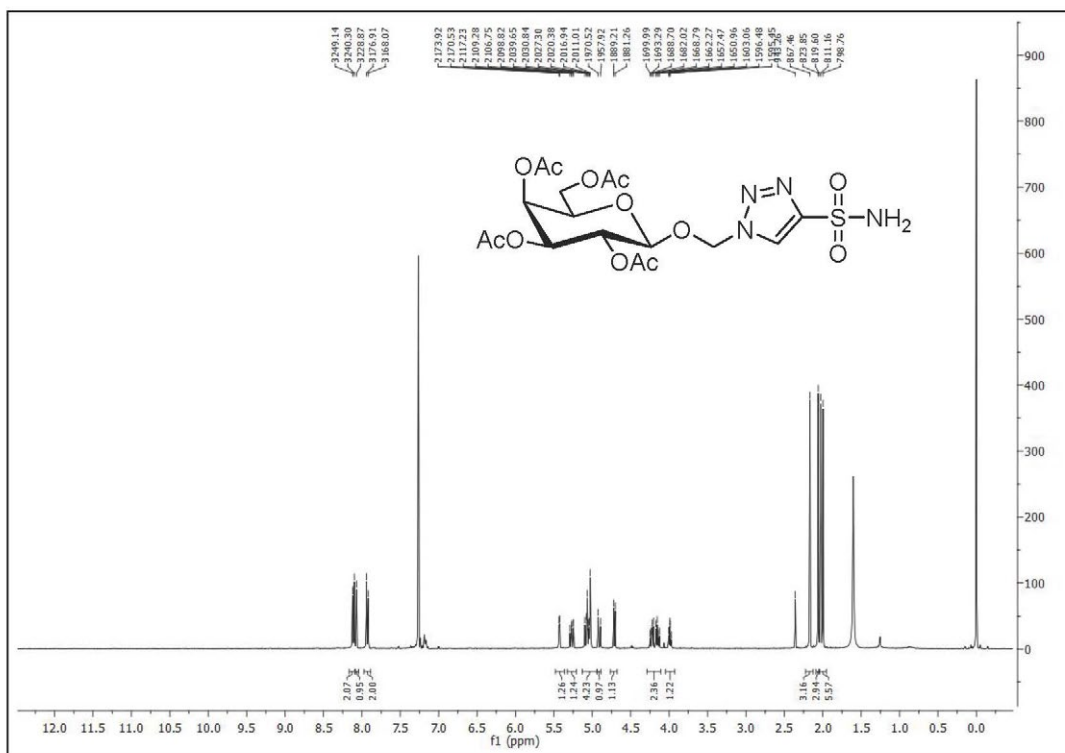


Figure S16. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of compound 37.

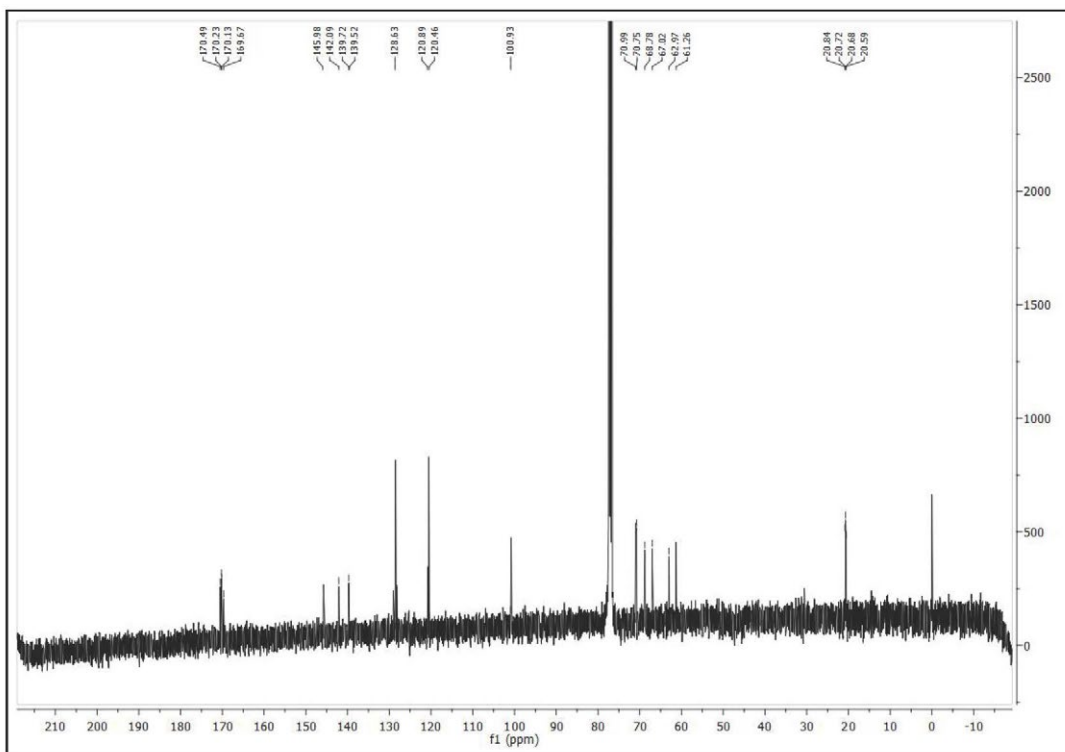


Figure S17. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) spectrum of compound 37.

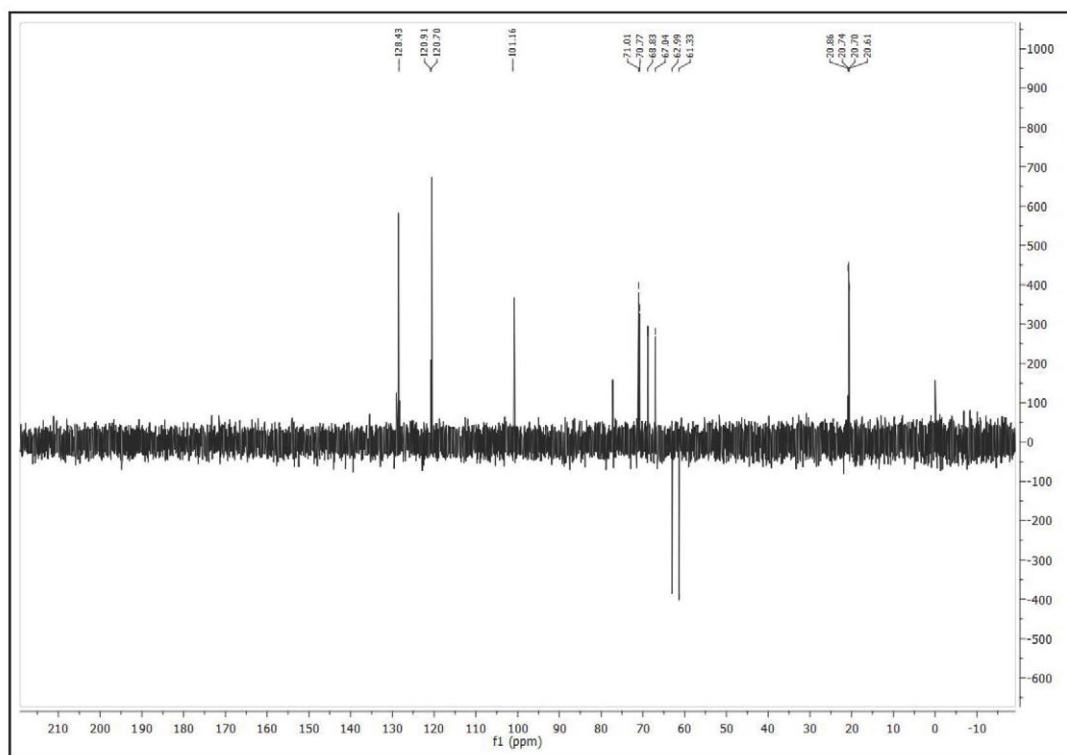


Figure S18. <sup>13</sup>C NMR DEPT (75 MHz, CDCl<sub>3</sub>) spectrum of compound 37.

4-[4-[(β-D-galactopyranosyl)-oxymethyl]-1-H-1,2,3-triazol-1-yl]benzenesulfonamide (**8**)<sup>6</sup>

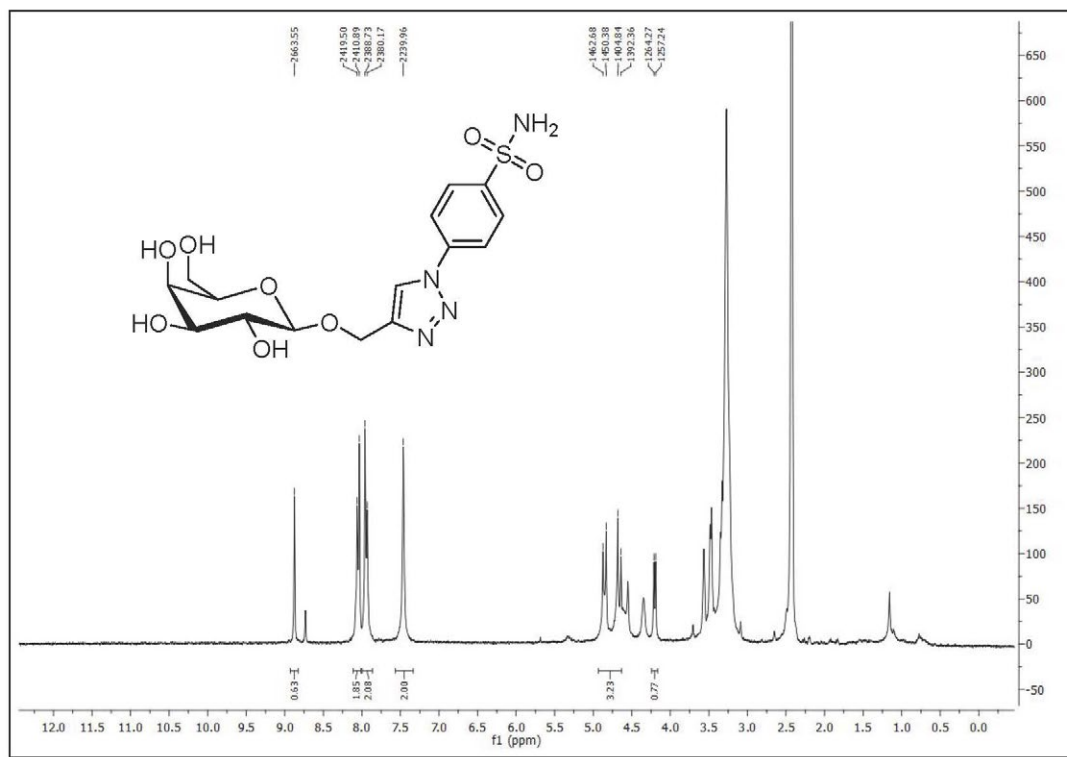
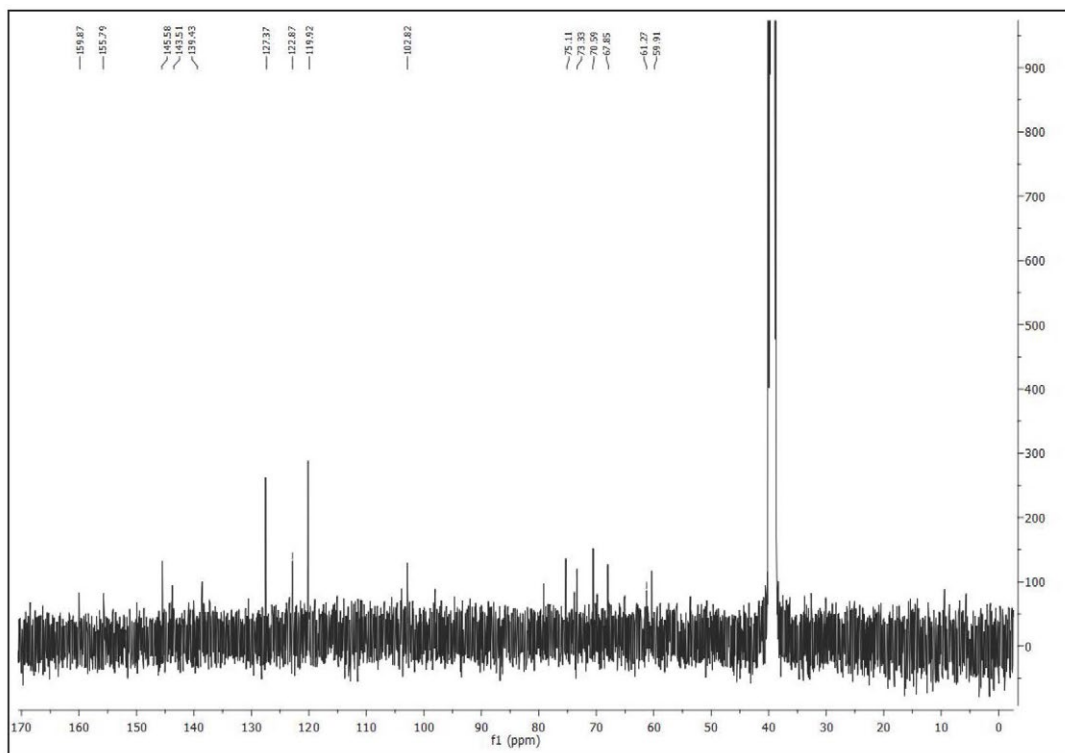
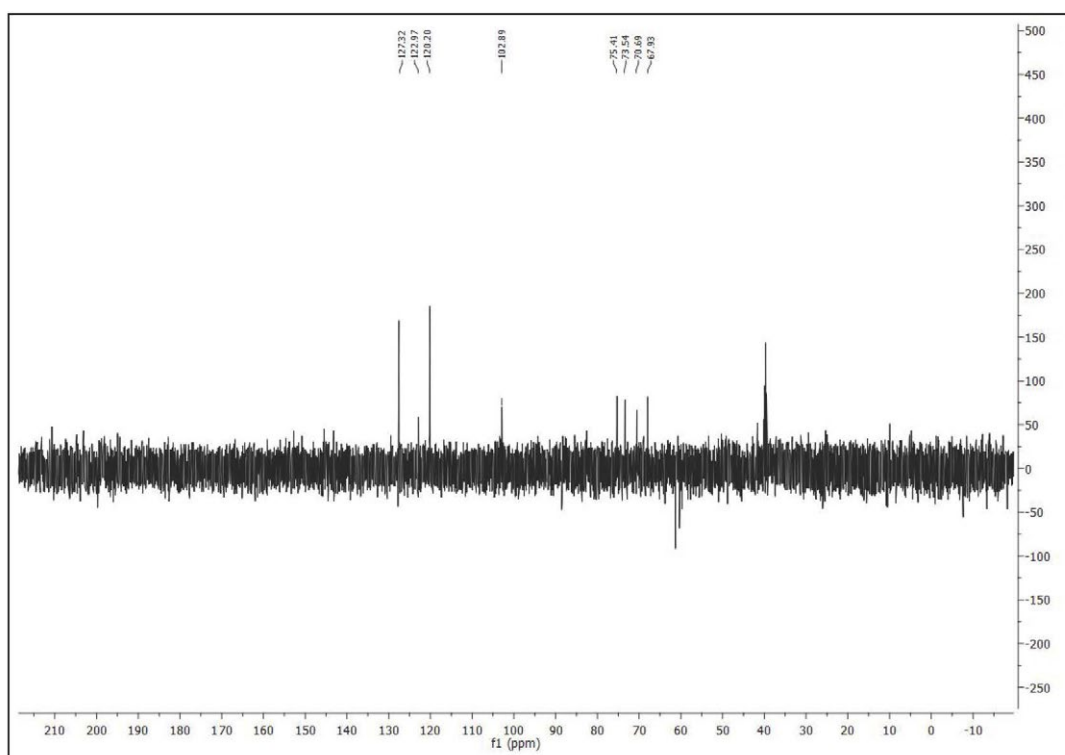


Figure S19. <sup>1</sup>H NMR (300 MHz, DMSO) spectrum of compound 8.



**Figure S20.**  $^{13}\text{C}$  NMR (75 MHz, DMSO) spectrum of compound **8**.



**Figure S21.**  $^{13}\text{C}$  NMR DEPT (75 MHz, DMSO) spectrum of compound **8**.

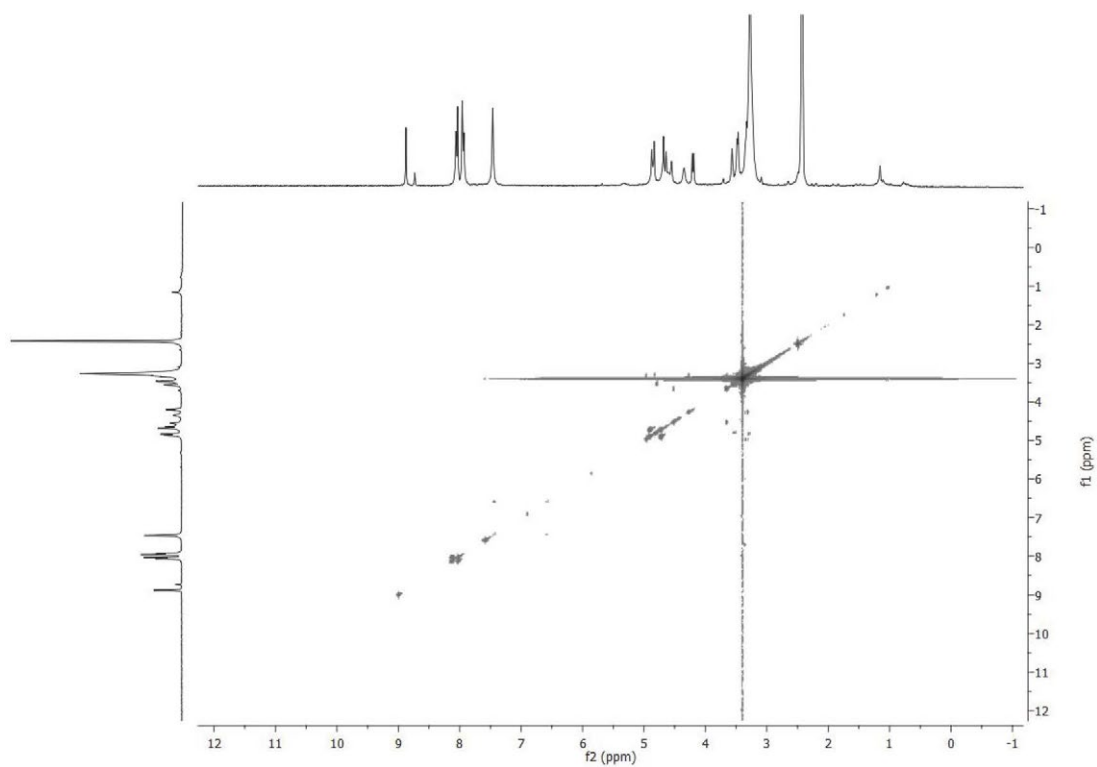


Figure S22. Bi-dimensional (COSY) spectrum of compound **8**.

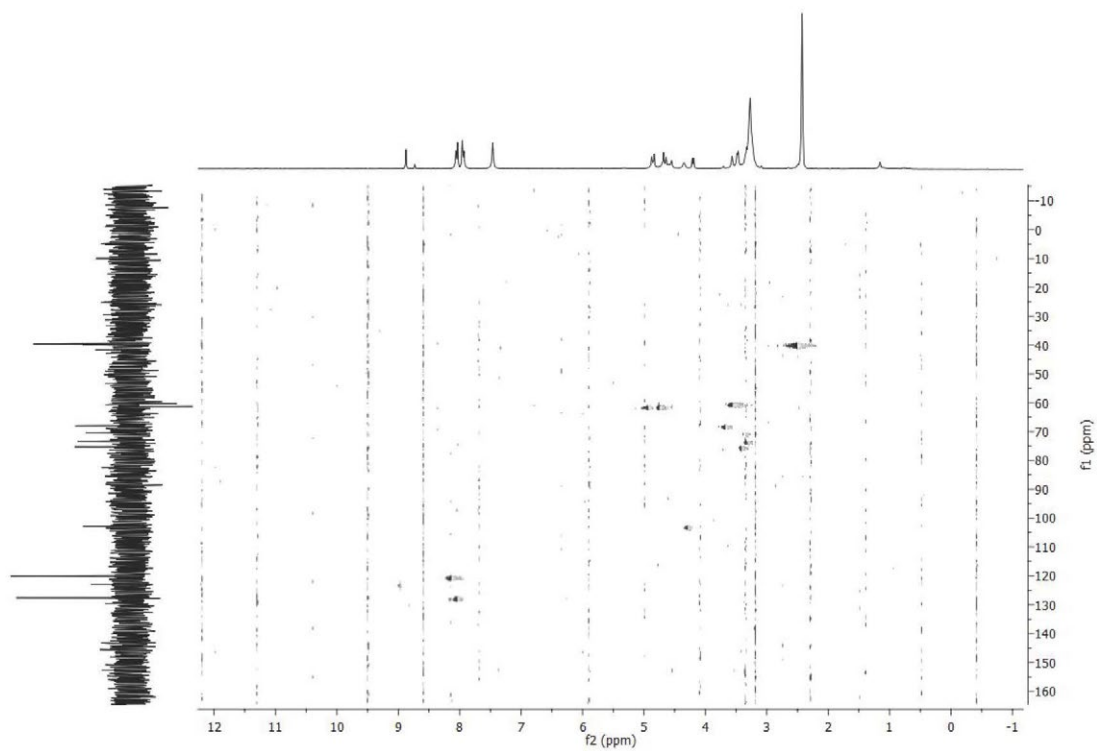
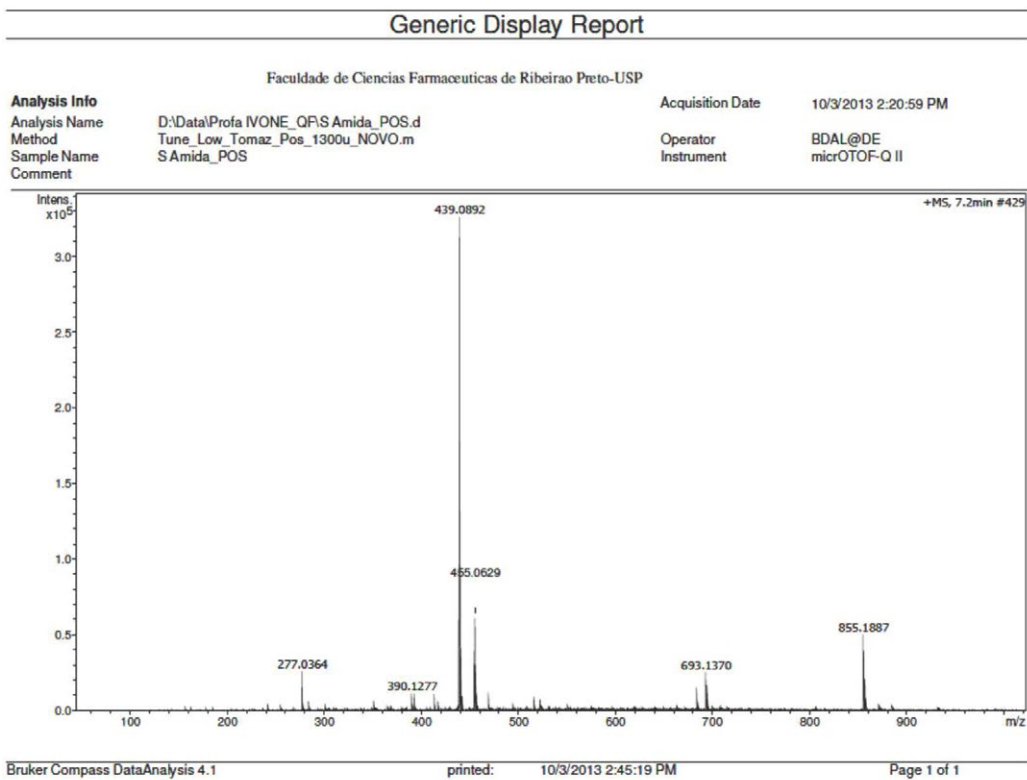
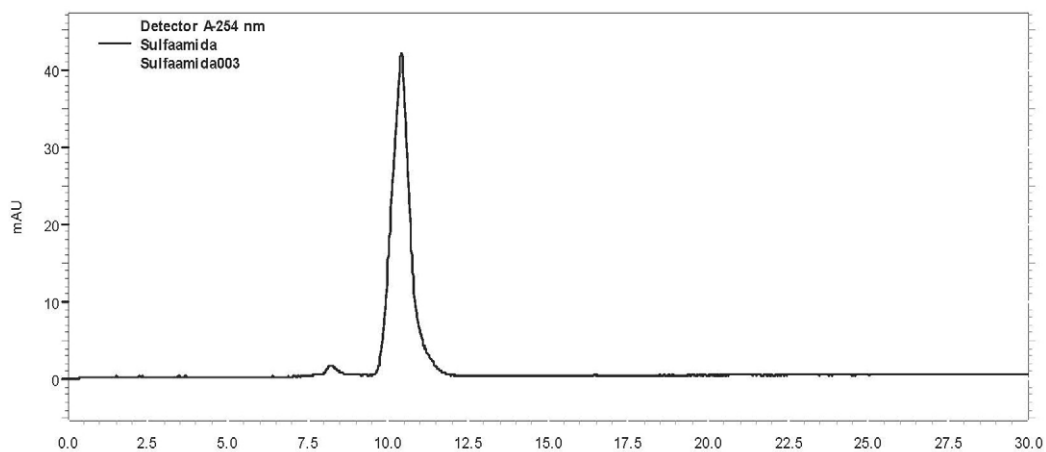


Figure S23. Bi-dimensional (HMQC) spectrum of compound **8**.



**Figure S24.** Mass spectrum (ESI-MS) of compound **8**.



**Figure S25.** HPLC chromatogram of compound **8**. Flow 0.9 mL min<sup>-1</sup>; mobile phase 40% MeOH, 60% H<sub>2</sub>O, TFA 0.1%; temp 24.5 °C.

4-{4-[(2',3',4',6'-Tetra-*O*-acetyl- $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3 triazol-1-yl}-*N*[(phenyl)sulfonyl]acetamide (**38**)<sup>5</sup>

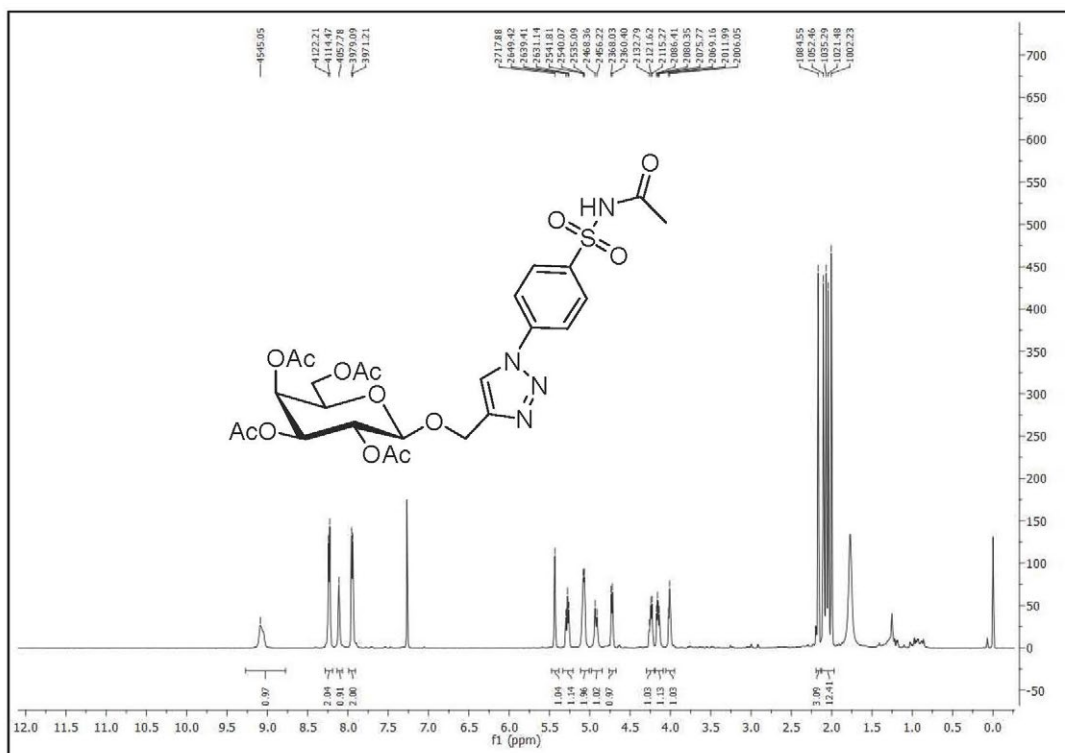


Figure S26.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of compound **38**.

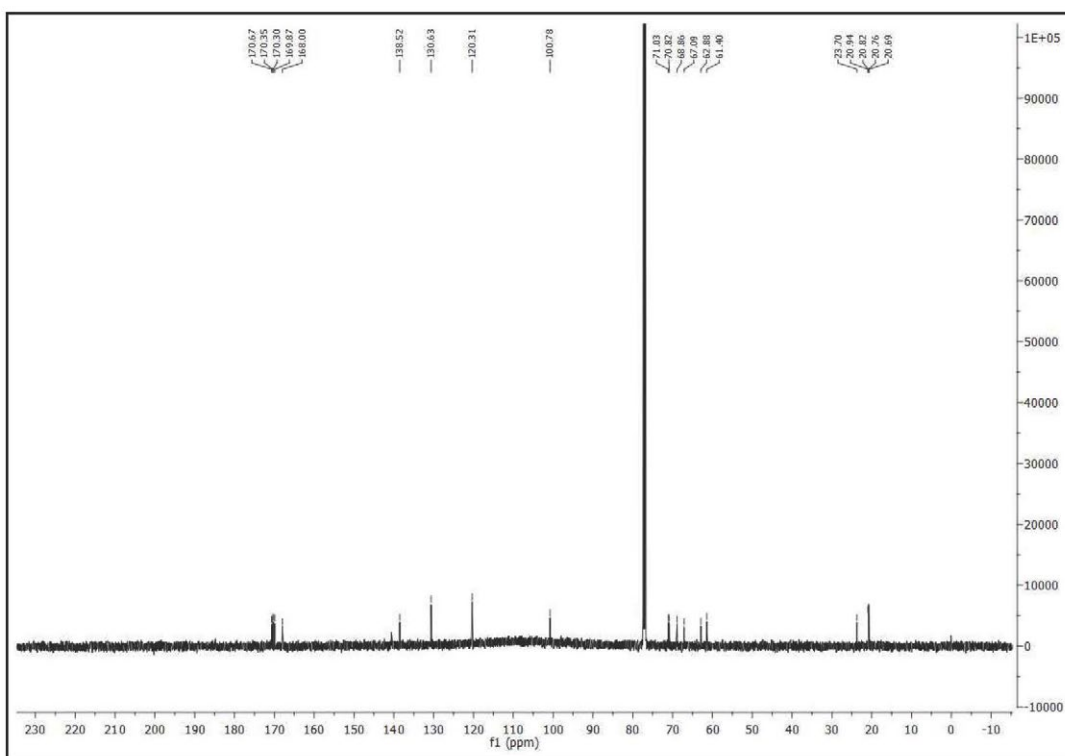
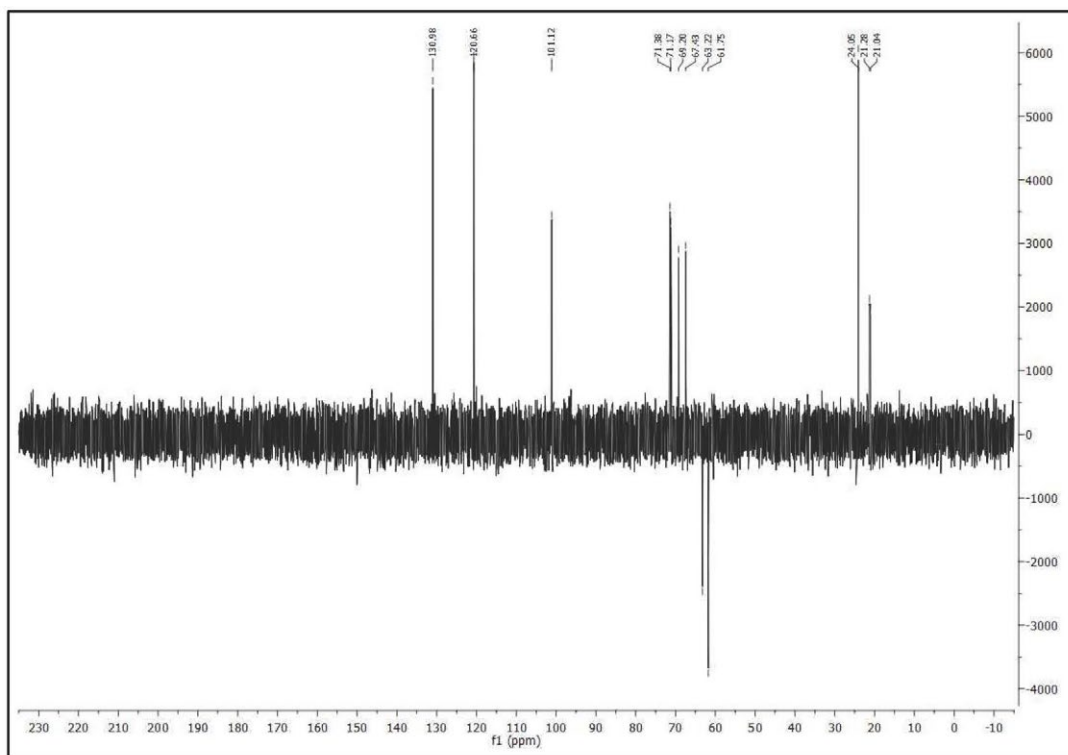
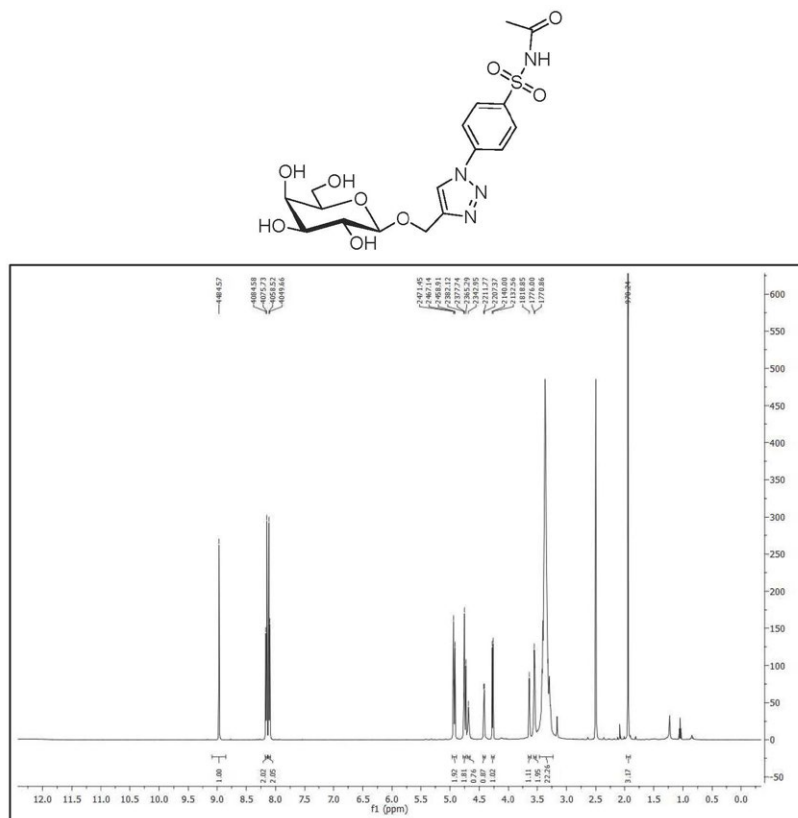


Figure S27.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of compound **38**.



**Figure S28.**  $^{13}\text{C}$  NMR DEPT (75 MHz,  $\text{CDCl}_3$ ) spectrum of compound **38**.

4-{4-[( $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3-triazol-1-yl]-*N*-(phenyl sulfonyl) acetamide (**9**)



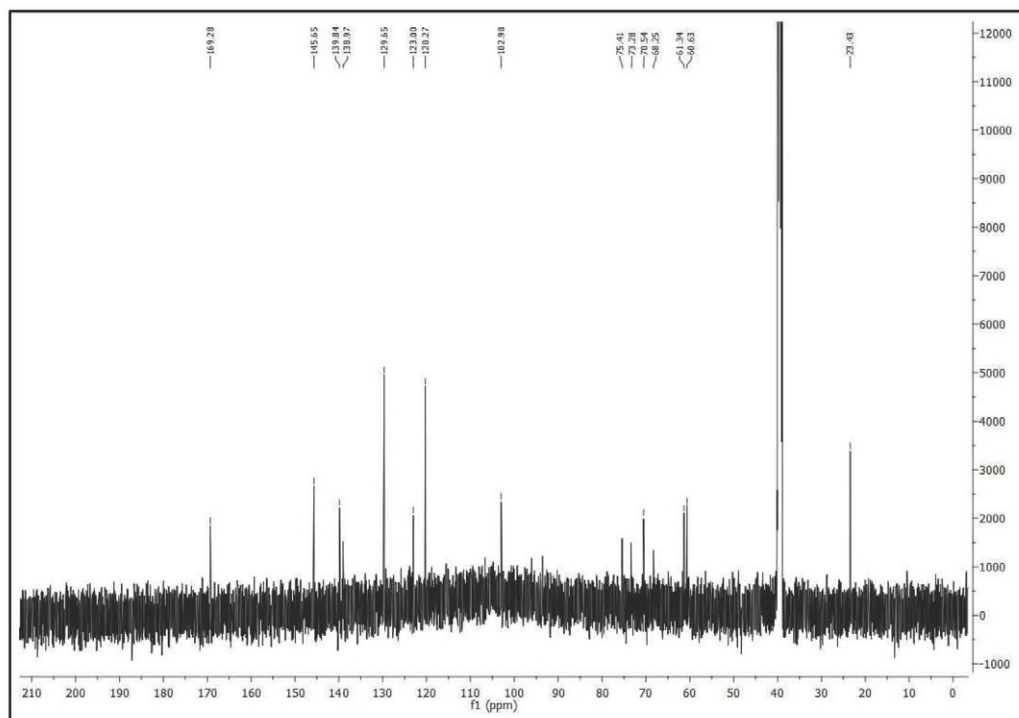


Figure S30.  $^{13}\text{C}$  NMR (75 MHz, DMSO) spectrum of compound **9**.

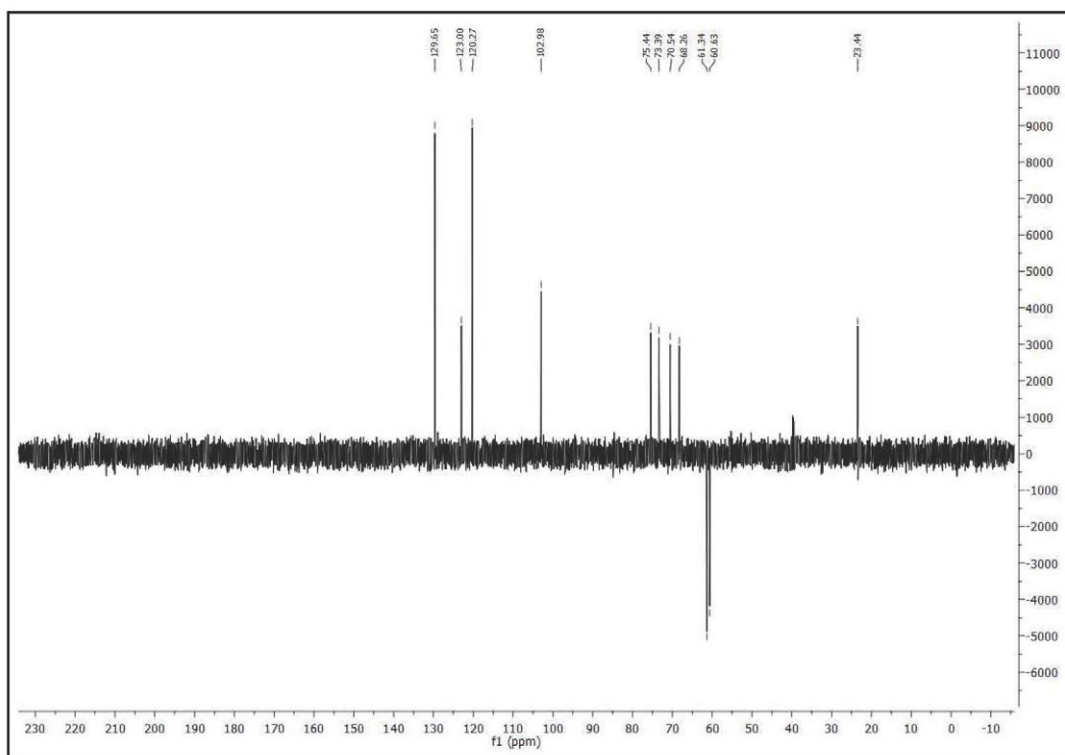
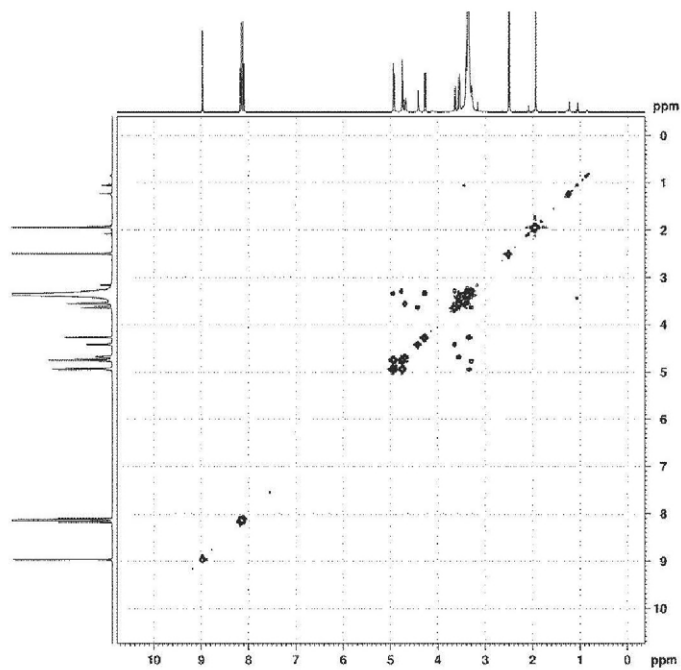
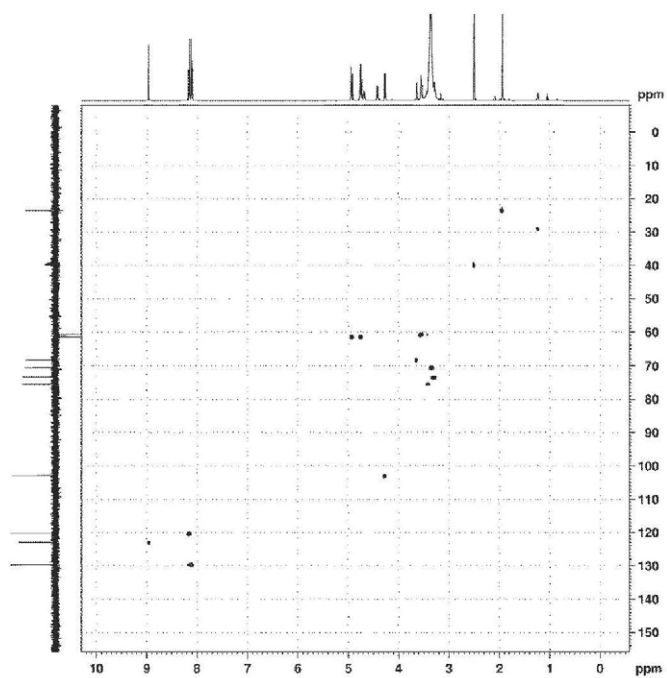


Figure S31.  $^{13}\text{C}$  NMR DEPT (75 MHz, DMSO) spectrum of compound **9**.

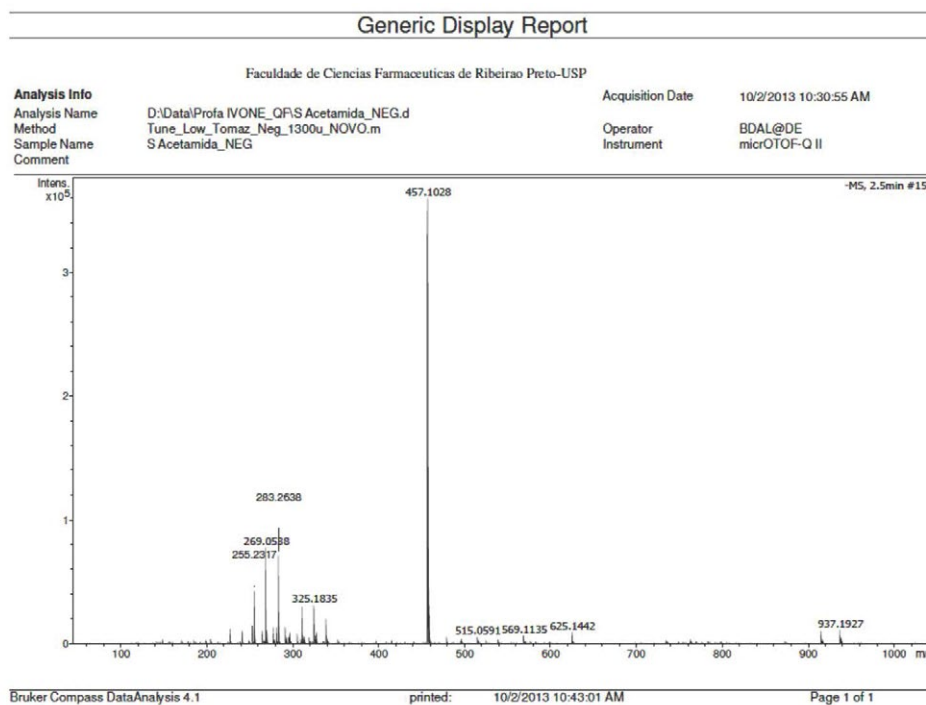




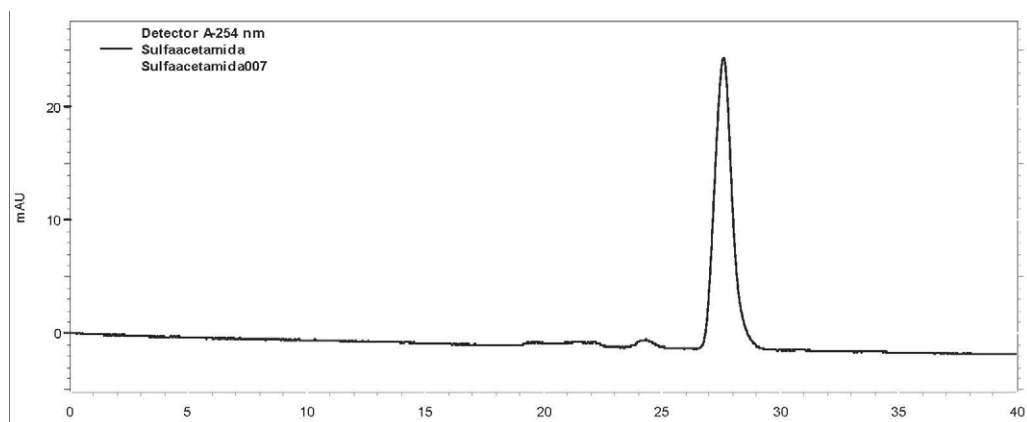
**Figure S32.** Bi-dimensional (COSY) spectrum of compound **9**.



**Figure S33.** Bi-dimensional (HMQC) spectrum of compound **9**.



**Figure S34.** Mass spectrum (ESI-MS) of compound **9**.



**Figure S35.** HPLC chromatogram of compound **9**. Flow 0.9 mL min<sup>-1</sup>; mobile phase 40% MeOH, 60% H<sub>2</sub>O, TFA 0.1%; temp. 24.5 °C.

4-{4-[(2',3',4',6'-Tetra-*O*-acetyl- $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3 triazol-1-yl)-*N*-(5-methylisoxazol-3-yl) benzenesulfonamide (**39**)<sup>5</sup>

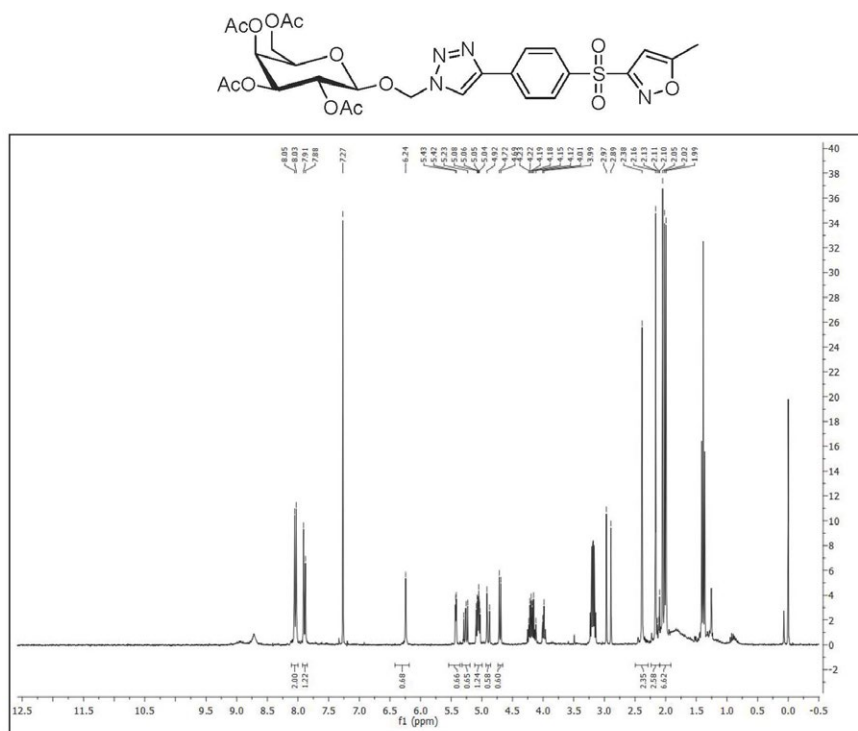


Figure S36. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of compound **39**.

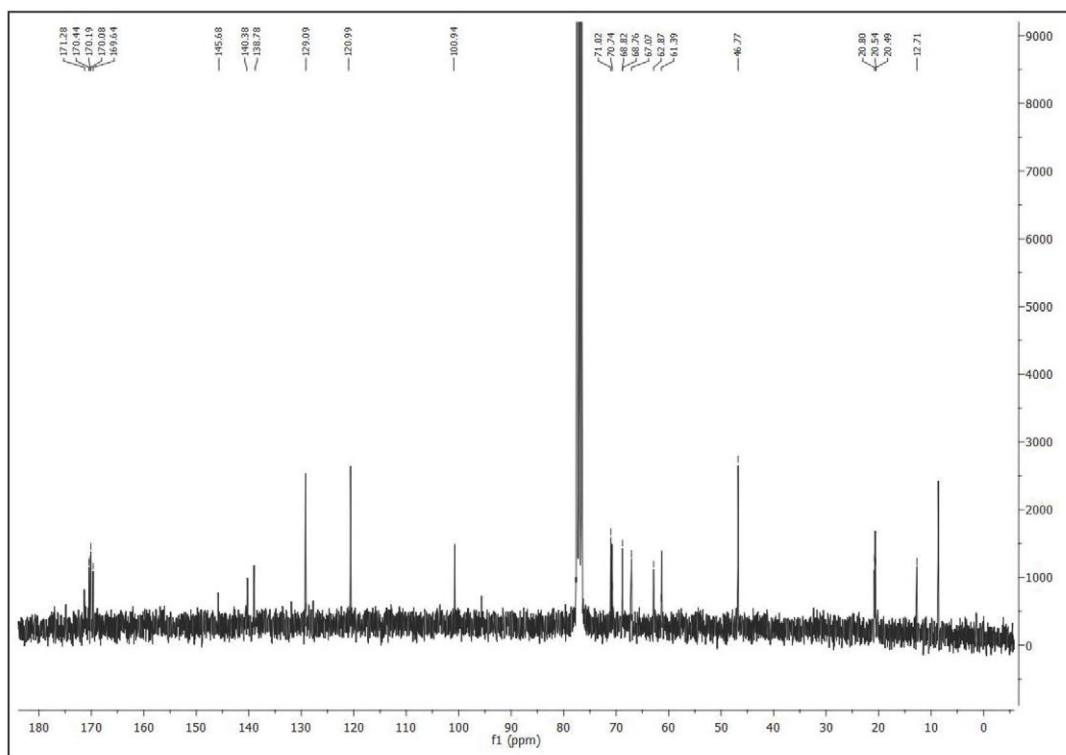


Figure S37. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) spectrum of compound **39**.

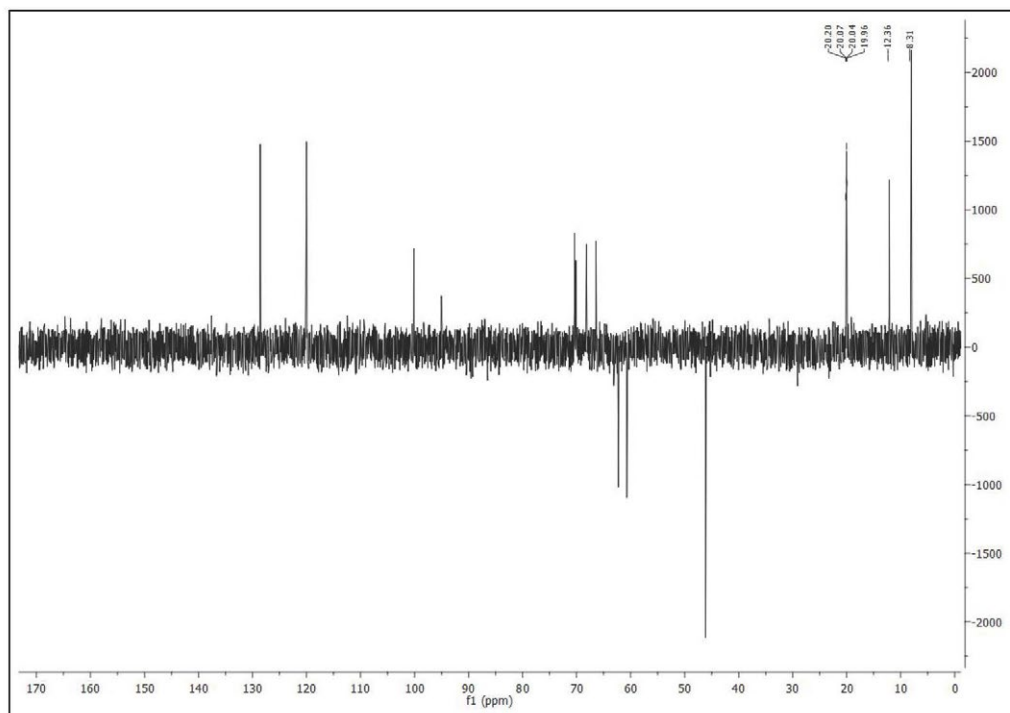


Figure S38.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of compound **39**.

4-{4-[( $\beta$ -D-galactopyranosyl)-oxymethyl]-1-H-1,2,3-triazol-1-yl}-N-(5-methyl isoxazol-3-yl)benzenesulfonamide (**10**)

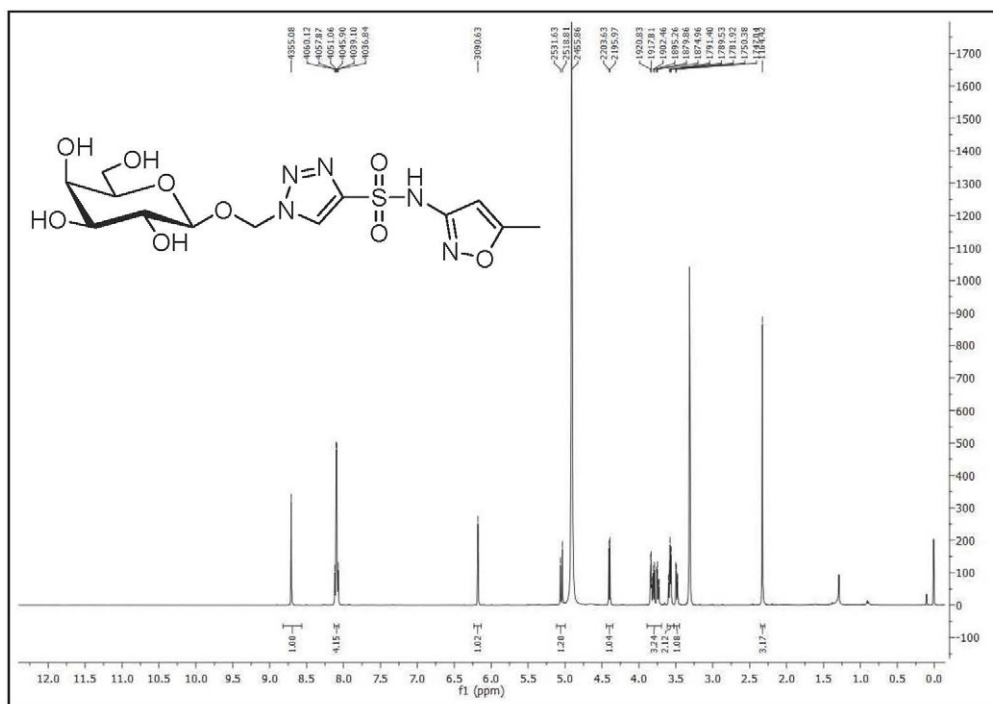


Figure S39.  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **10**.

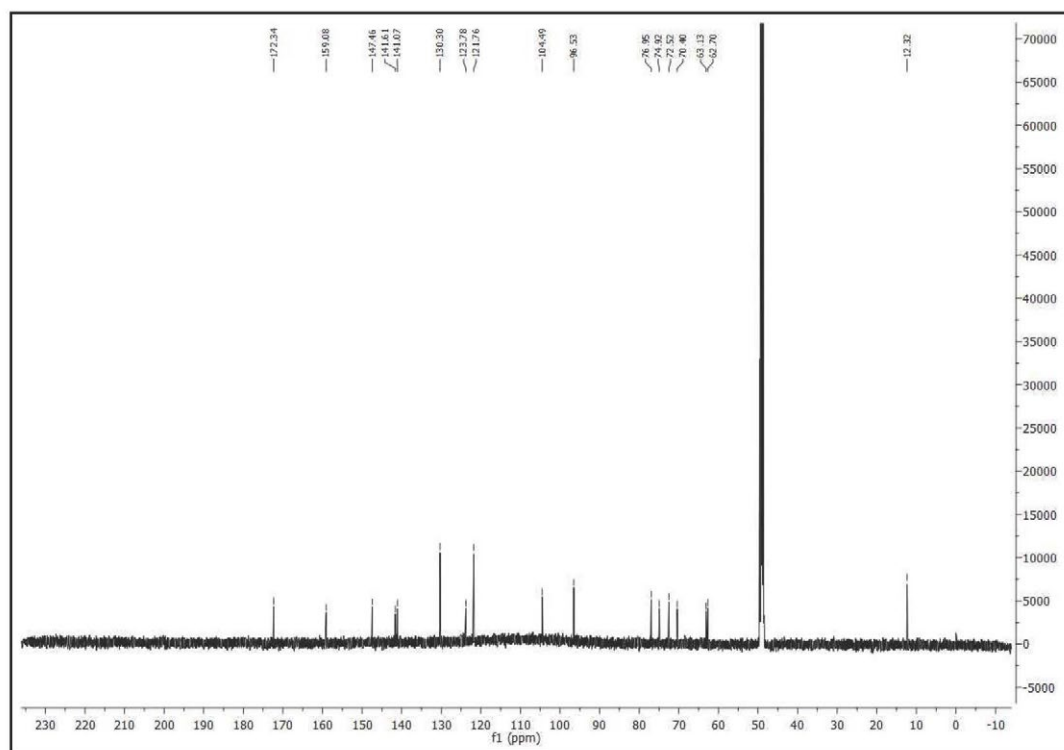


Figure S40.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 10.

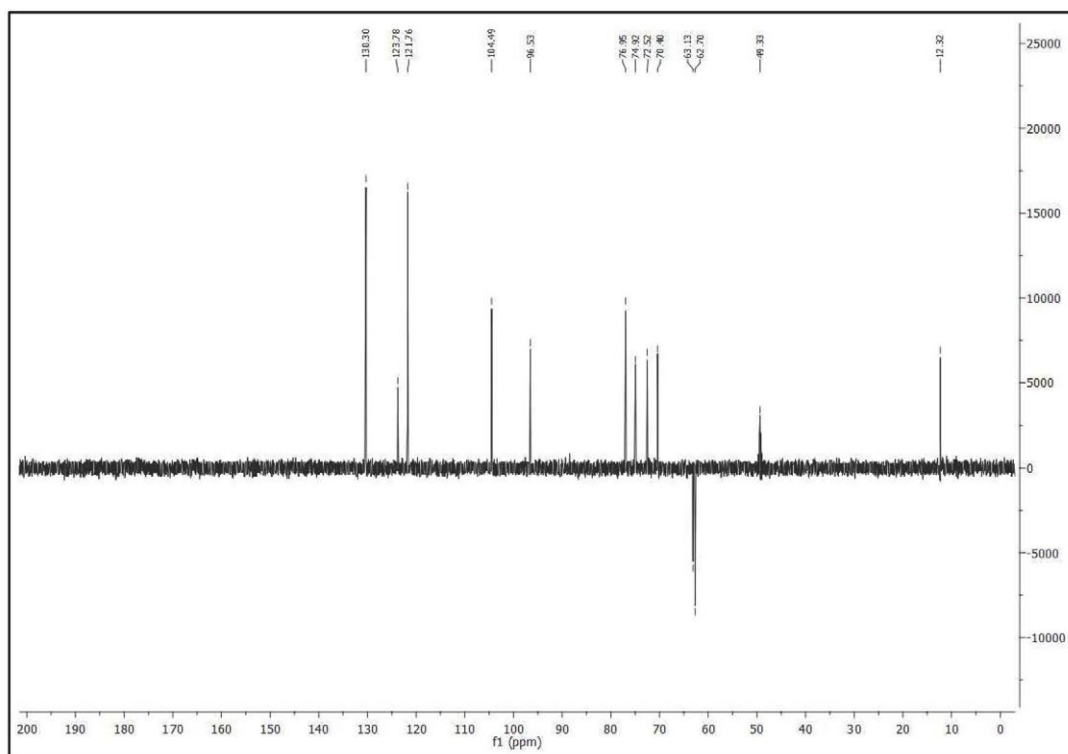


Figure S41.  $^{13}\text{C}$  NMR DEPT (75 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 10.

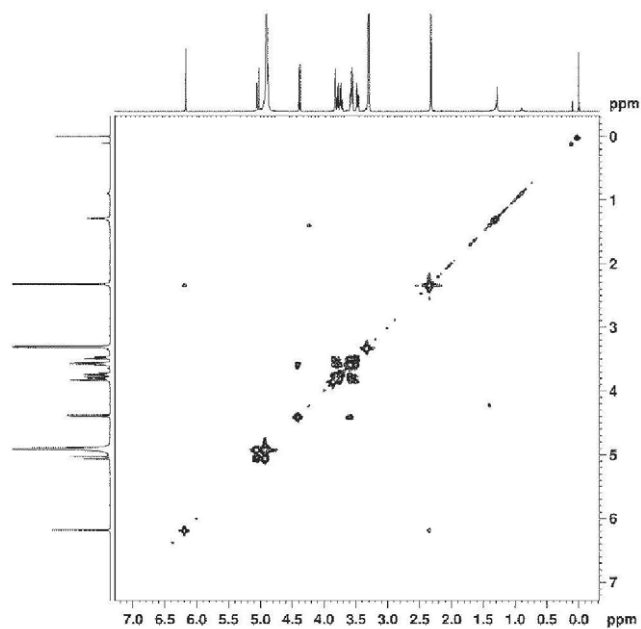


Figure S42. Bi-dimensional (COSY) spectrum of compound 10.

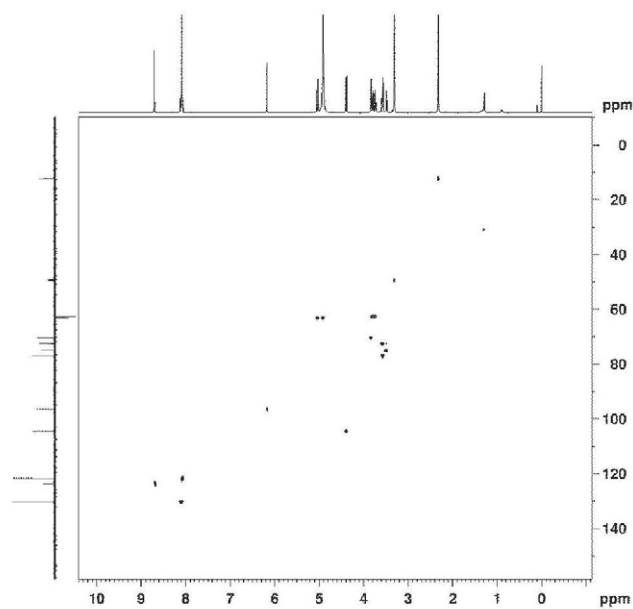
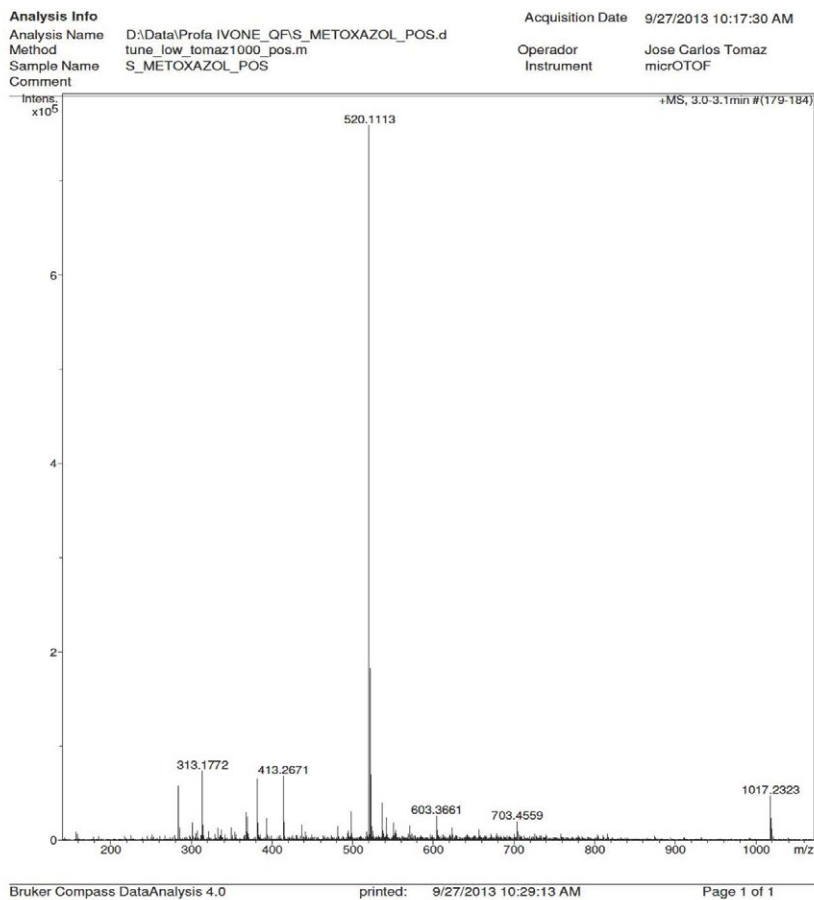
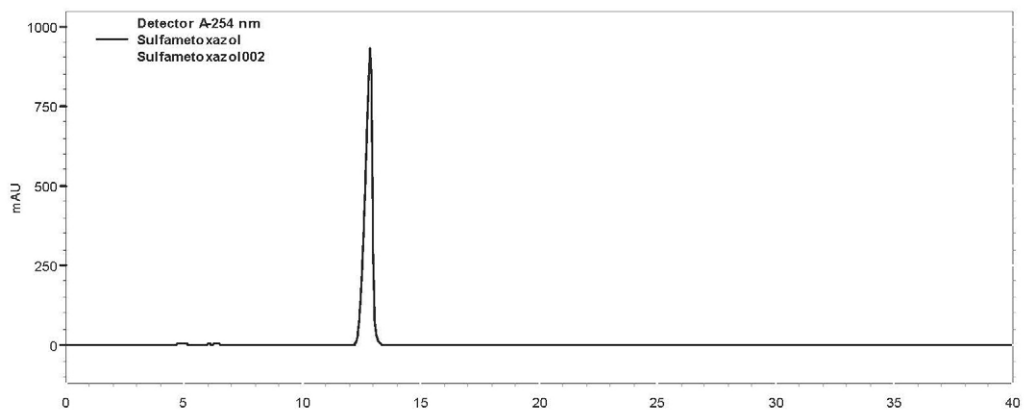


Figure S43. Mass Spectrum (ESI-MS) of compound 10.



**Figure S44.** Mass spectrum (ESI-MS) of compound **10**.



**Figure S45.** HPLC chromatogram of compound **10**. Flow  $0.9 \text{ mL min}^{-1}$ ; mobile phase 40% MeOH, 60%  $\text{H}_2\text{O}$ , TFA 0.1%; temp.  $24.5^\circ\text{C}$ .

4-{4-[(2',3',4',6'-Tetra-*O*-acetyl- $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3 triazol-1-yl}-*N*-(4-methylpyrimidin-2-yl) benzenesulfonamide (**40**)<sup>5</sup>

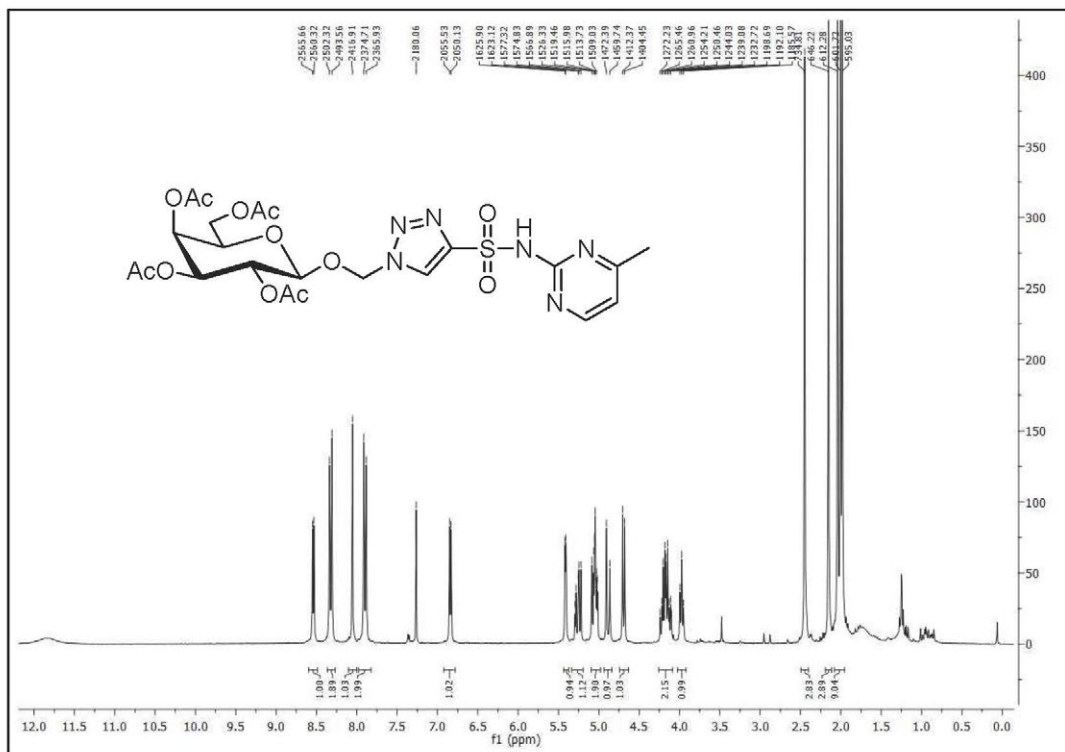
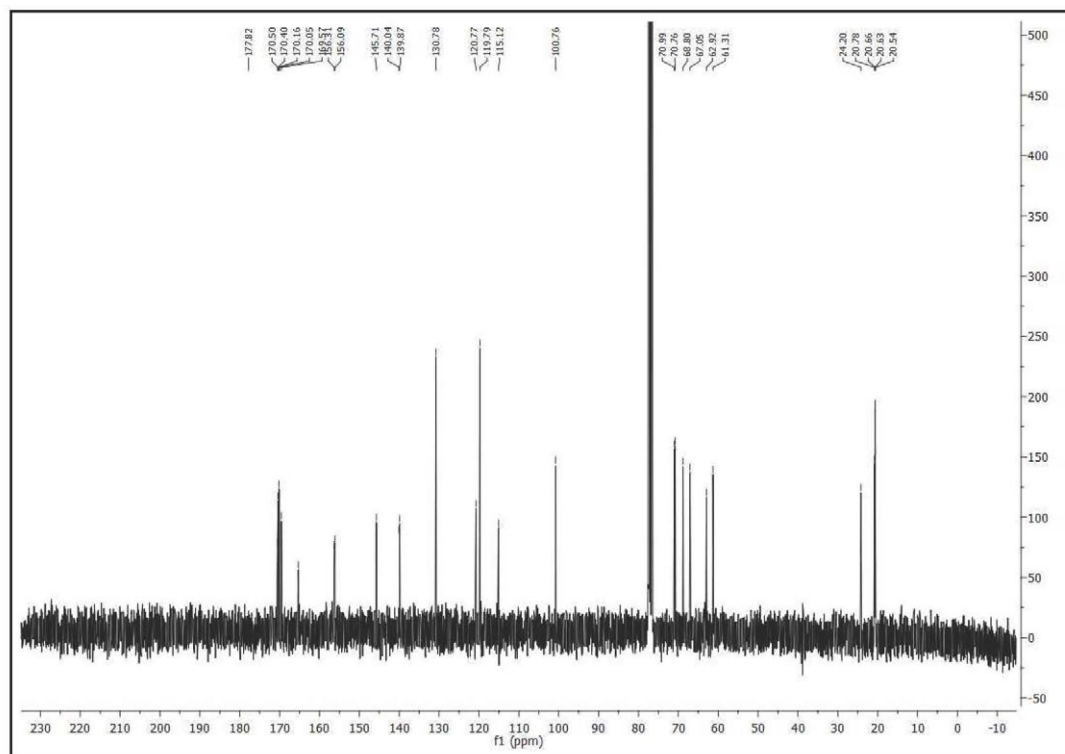


Figure S46. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of compound **40**.





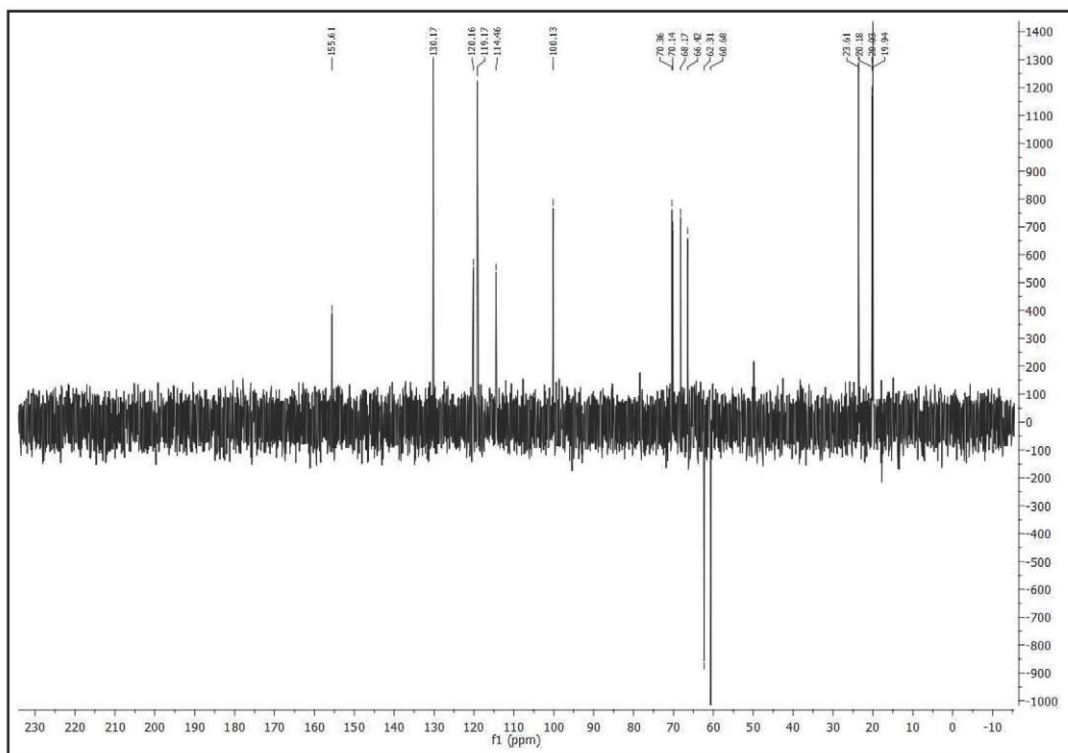


Figure S48.  $^{13}\text{C}$  NMR DEPT (75 MHz,  $\text{CDCl}_3$ ) spectrum of compound **40**.

4-{4-[( $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3-triazol-1-yl}-*N*-(4-methyl pyrimidin-2-yl)benzenesulfonamide (**11**)

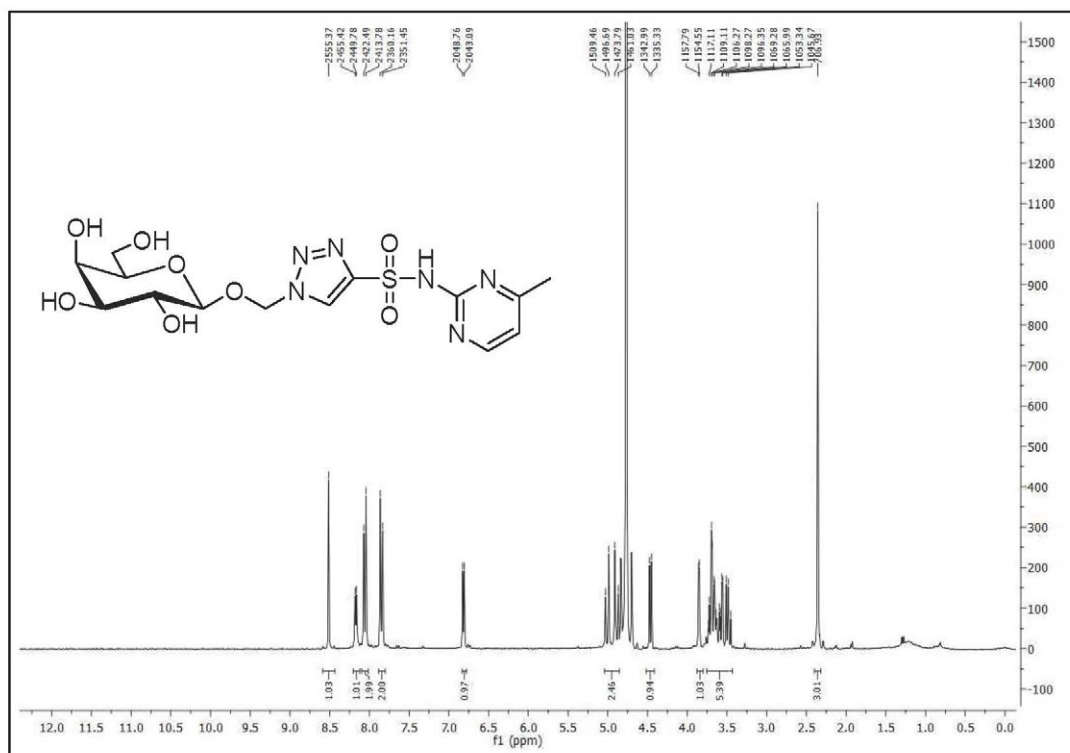


Figure S49.  $^1\text{H}$  NMR (300 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound **11**.

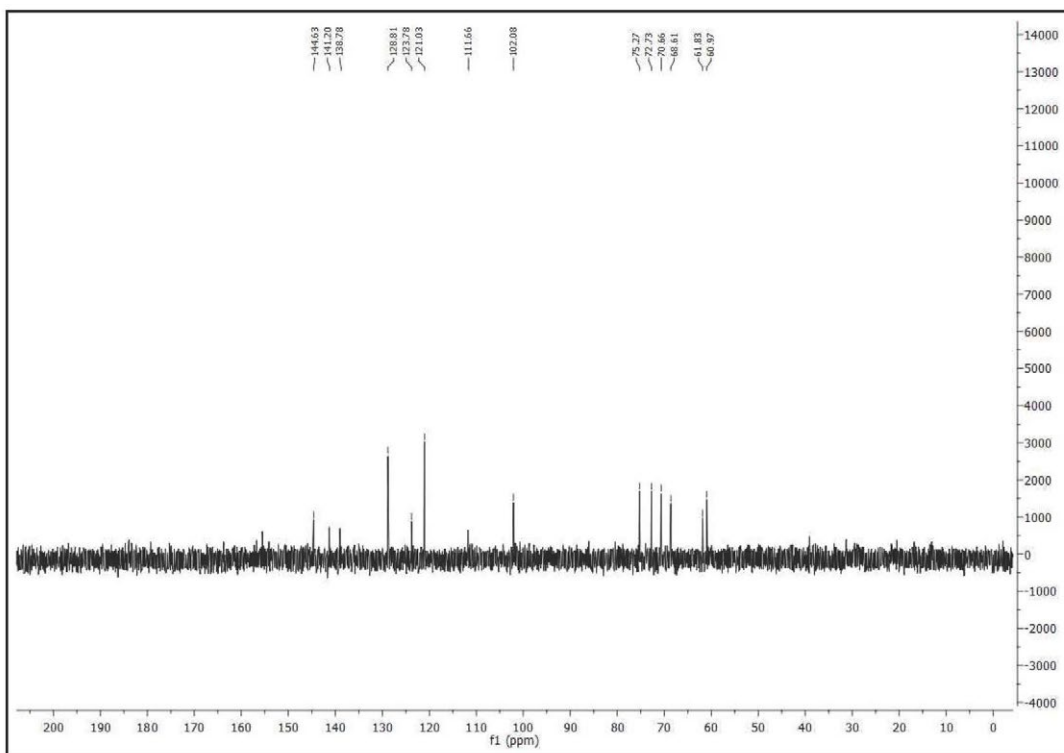


Figure S50. <sup>13</sup>C NMR (75 MHz, D<sub>2</sub>O) spectrum of compound 11.

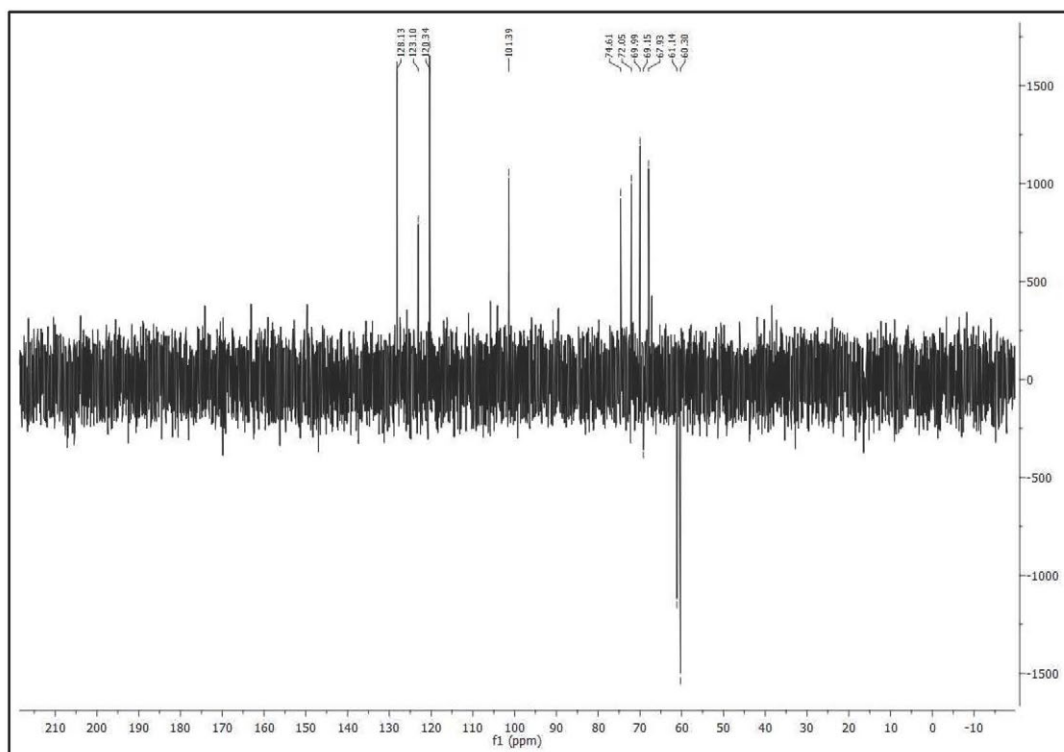


Figure S51. <sup>13</sup>C NMR DEPT (75 MHz, D<sub>2</sub>O) spectrum of compound 11.

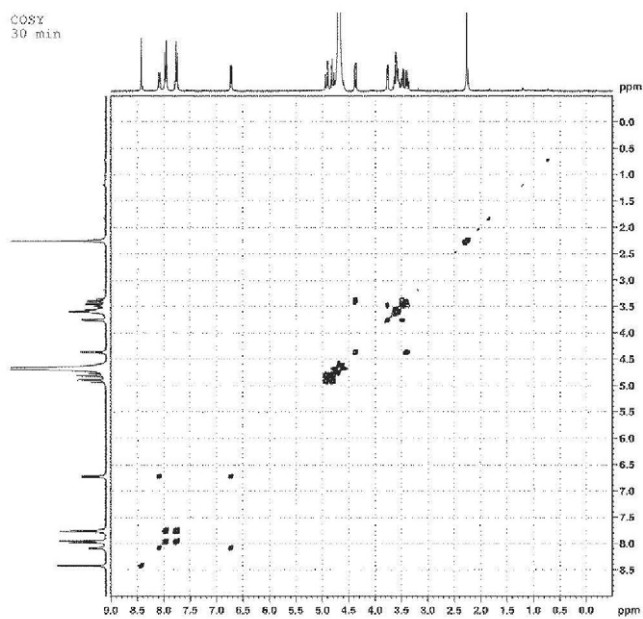


Figure S52. Bi-dimensional (COSY) spectrum of compound **11**.

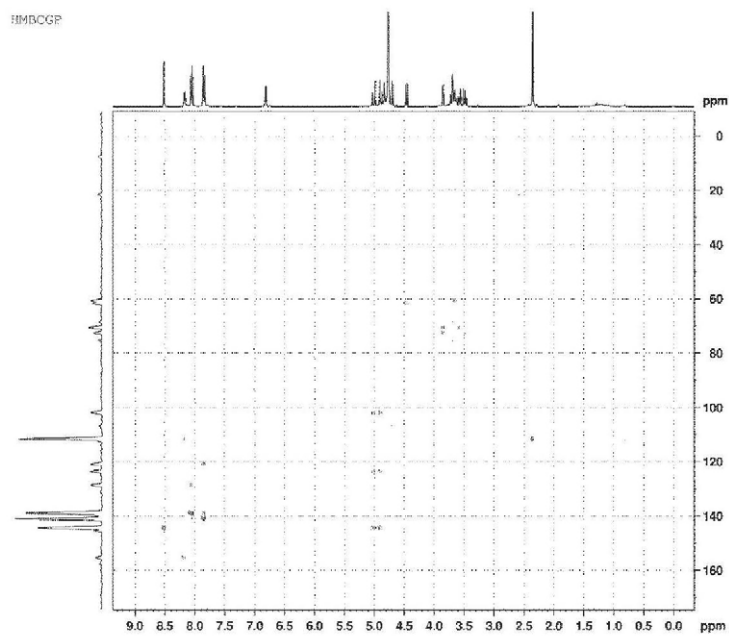
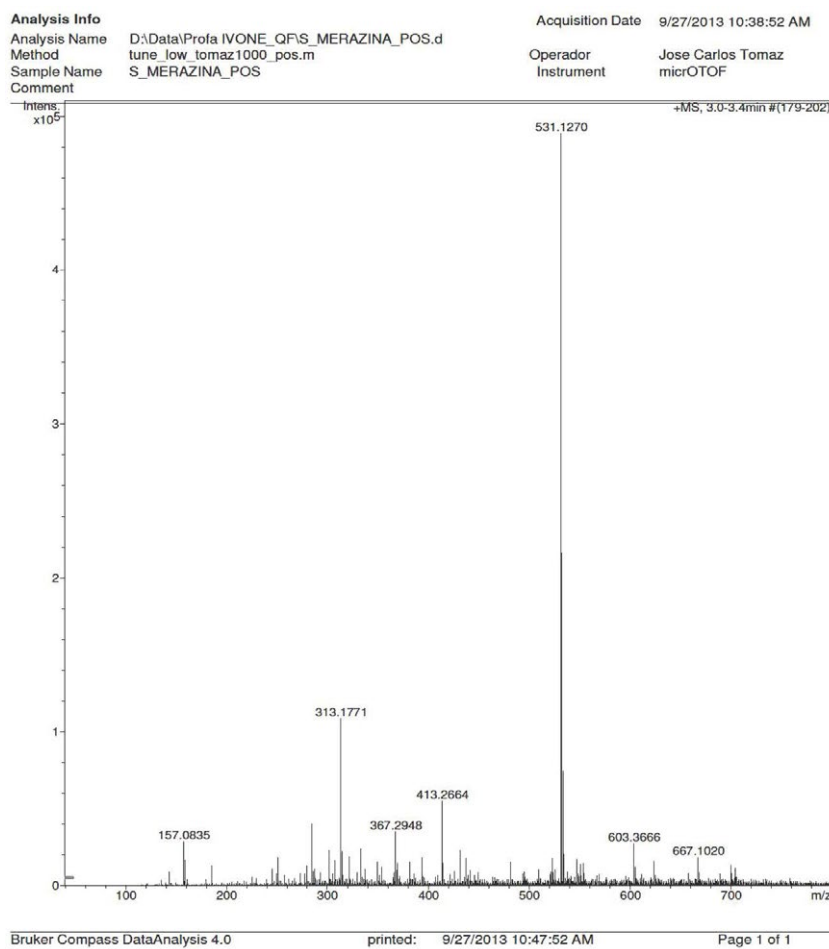
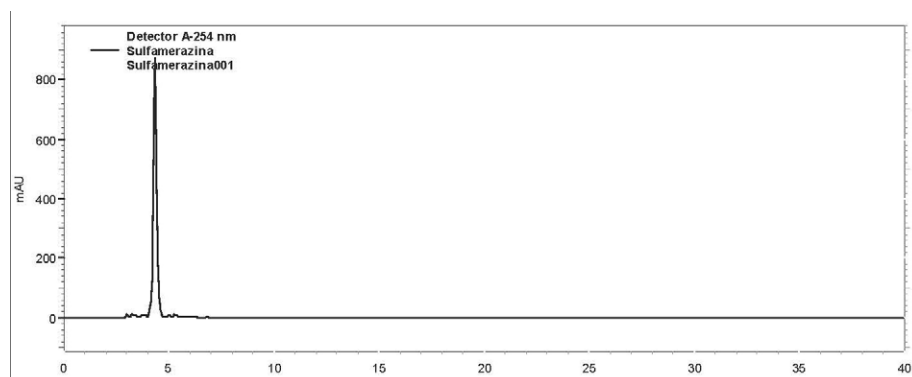


Figure 53. Bi-dimensional (HMQC) spectrum of compound **11**.



**Figure S54.** Mass spectrum (ESI-MS) of compound **11**.



**Figure S55.** HPLC chromatogram of compound **11**. Flow 0.9 mL min<sup>-1</sup>; mobile phase 40% MeOH, 60% H<sub>2</sub>O, TFA 0.1%; temp. 24.5 °C.

4-{4-[(2',3',4',6'-tetra-*O*-acetyl- $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3 triazol-1-yl}-*N*-(4,6-dimethylpyrimidin-2-yl) benzenesulfonamide (**41**)<sup>5</sup>

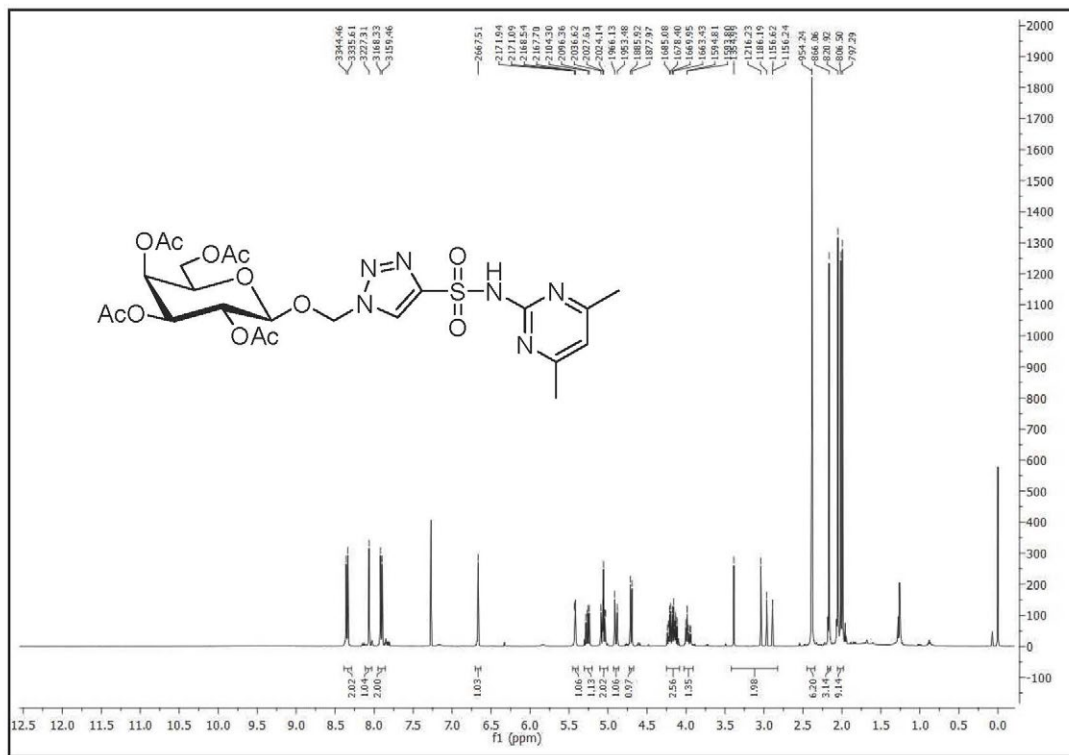


Figure S56. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **41**.

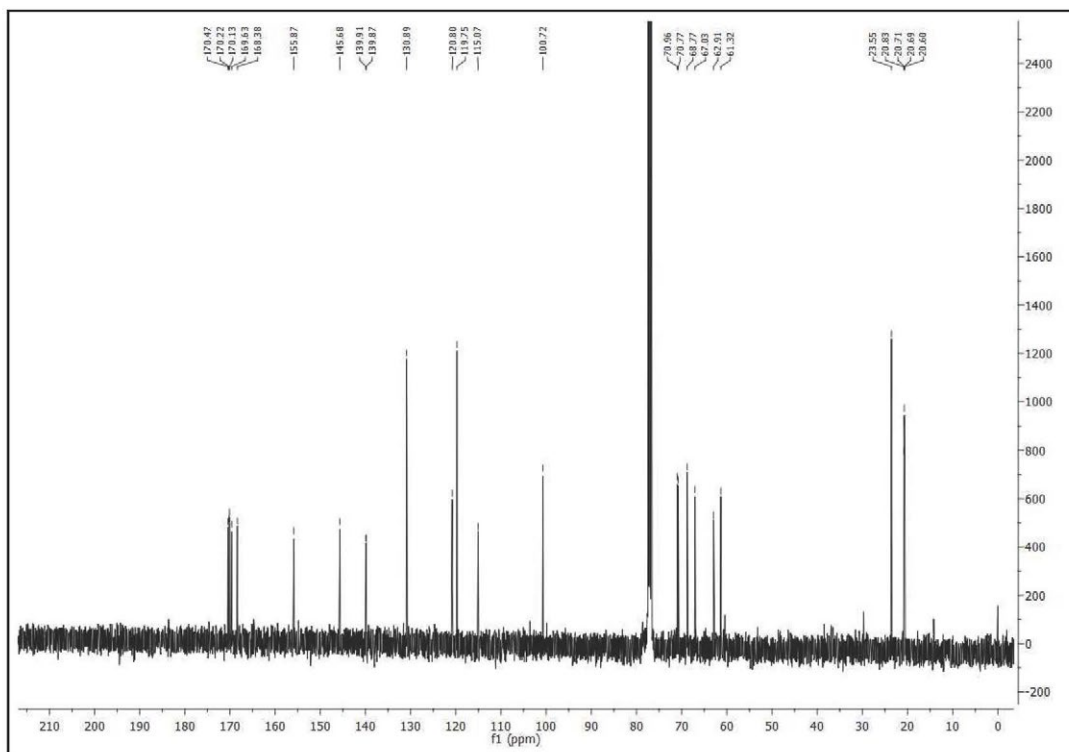


Figure S57. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound **41**.

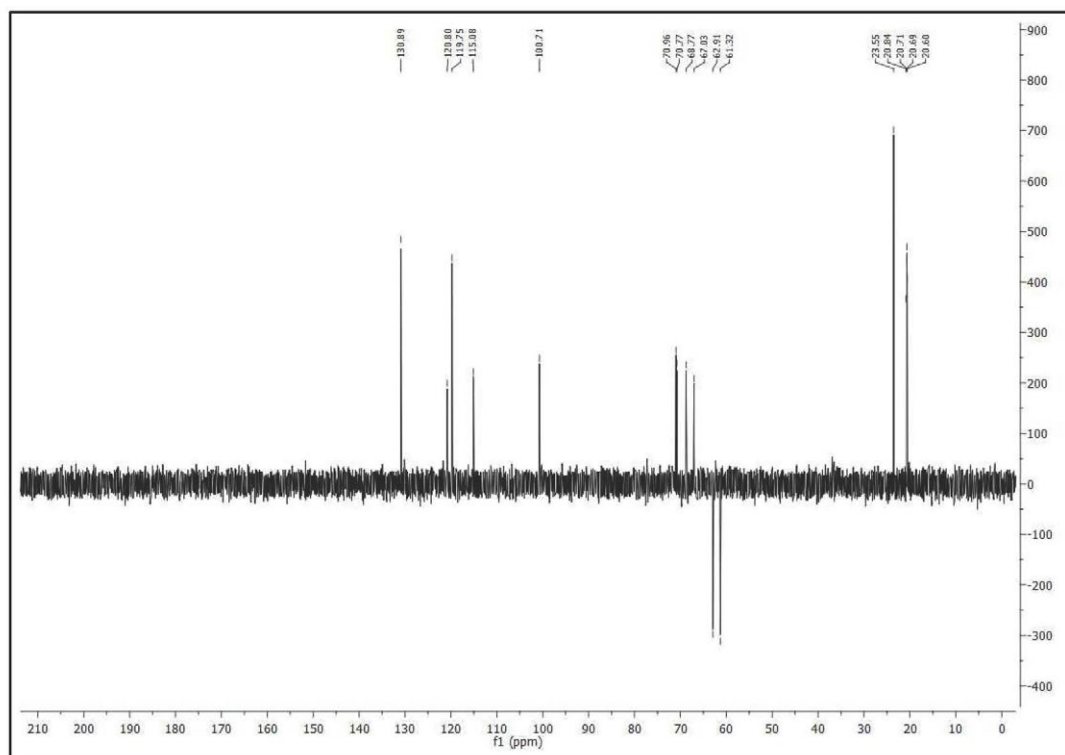


Figure S58. <sup>13</sup>C NMR DEPT (100 MHz, CDCl<sub>3</sub>) spectrum of compound 41.

4-{4-[(β-D-galactopyranosyl)-oxymethyl]-1-H-1,2,3-triazol-1-yl}-N-(4,6-dimethyl pyrimidin-2-yl) benzenesulfonamide (**12**)

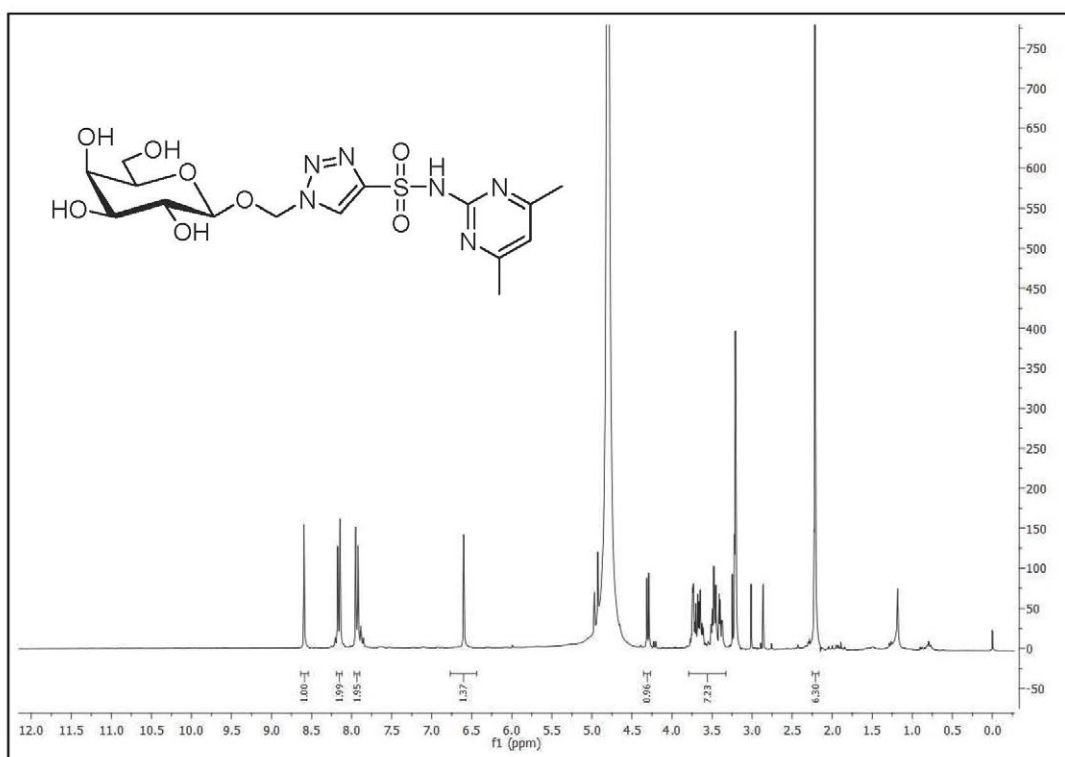


Figure S59. <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD) spectrum of compound 12.

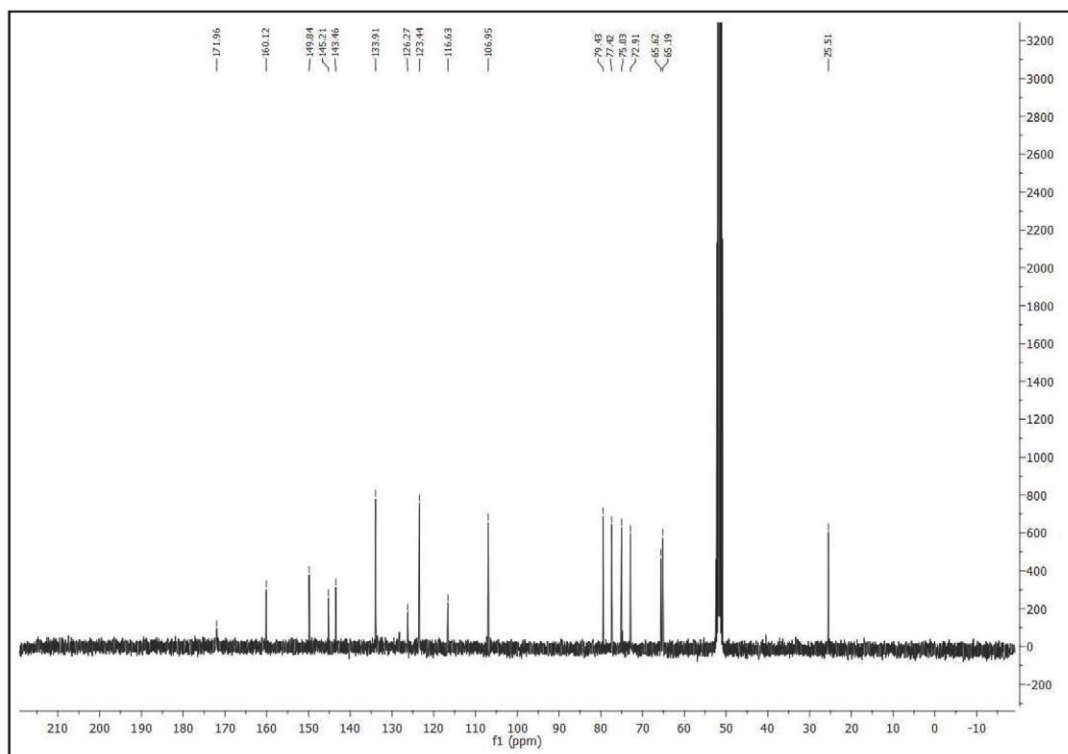


Figure S60.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 12.

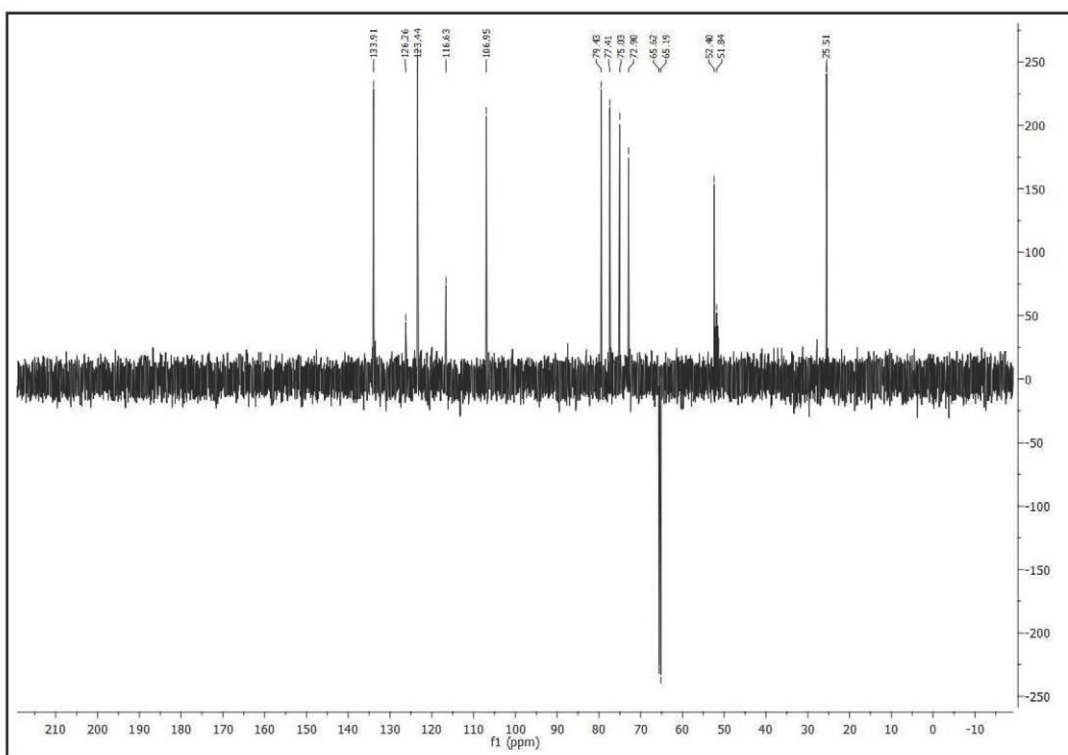


Figure S61.  $^{13}\text{C}$  NMR DEPT (75 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 12.

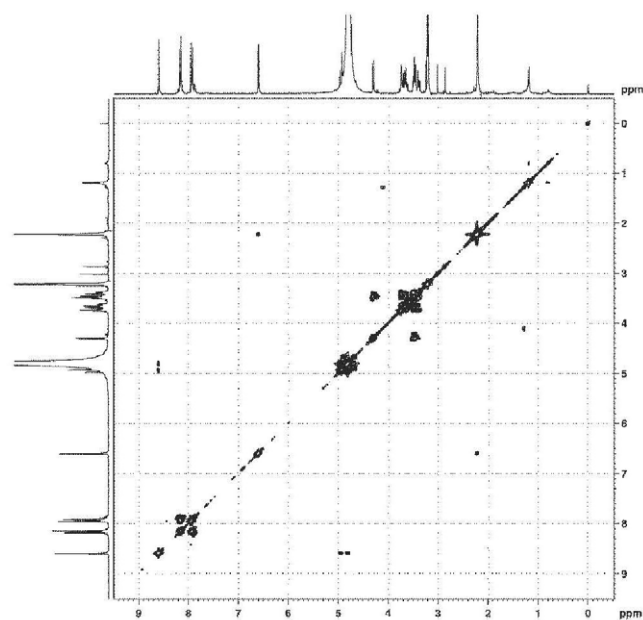


Figure S62. Bi-dimensional (COSY) spectrum of compound 12.

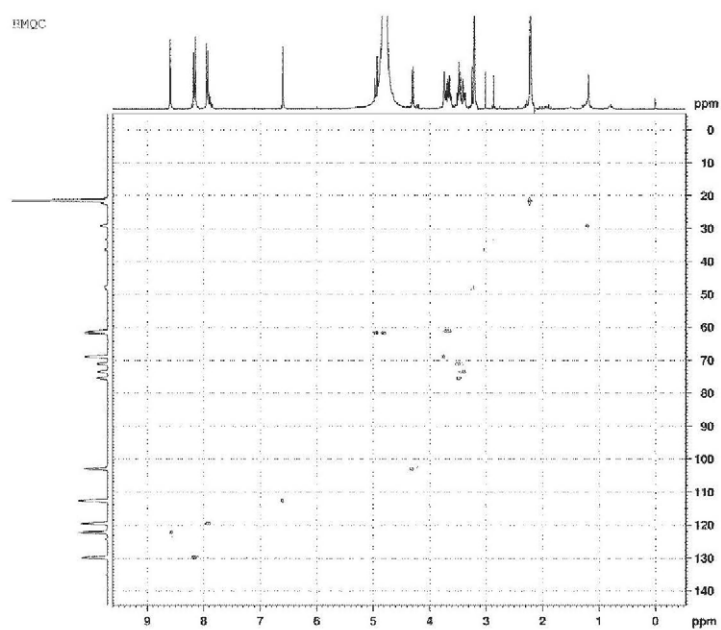
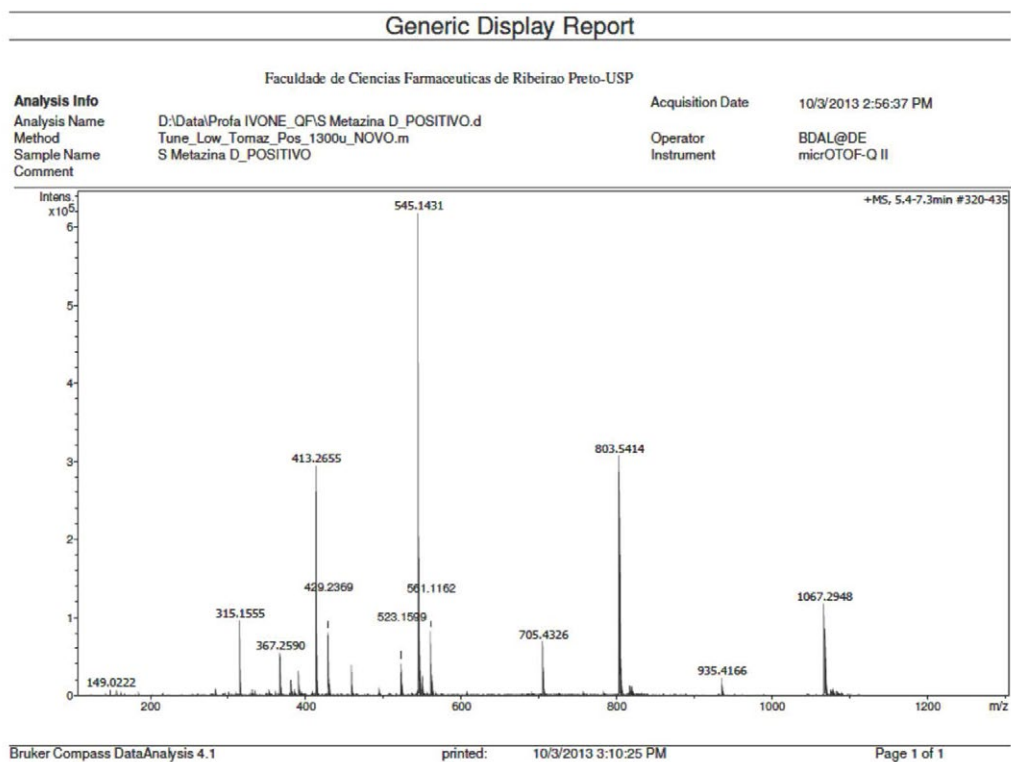
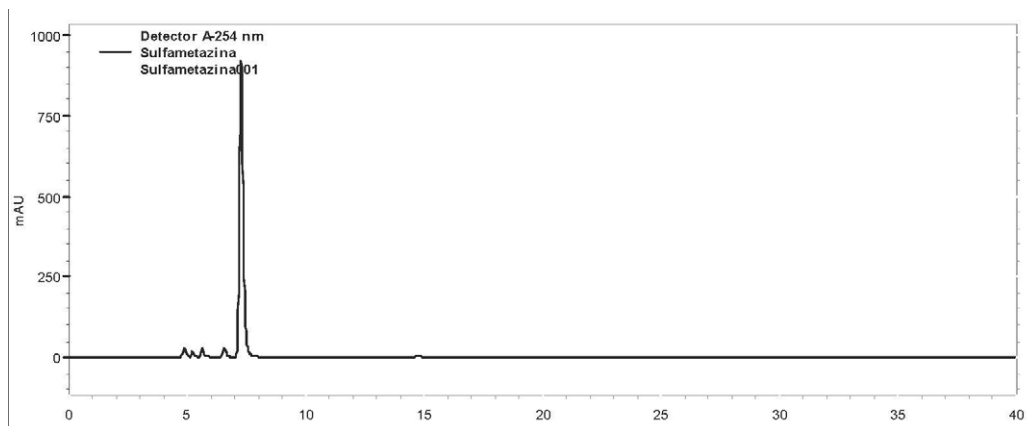


Figure S63. Bi-dimensional (HMQC) spectrum of compound 12.





**Figure S64.** Mass spectrum (ESI-MS) of compound **12**.



**Figure S65.** HPLC chromatogram of compound **12**. Flow  $0.9 \text{ mL min}^{-1}$ ; mobile phase 40% MeOH, 60% H<sub>2</sub>O, TFA 0.1%; temp. 24.5 °C.

4-{4-[(2',3',4',6'-tetra-*O*-acetyl- $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3-triazol-1-yl}-*N*-(2,6-dimethoxypyrimidin-4-yl) benzenesulfonamide (**42**)<sup>5</sup>

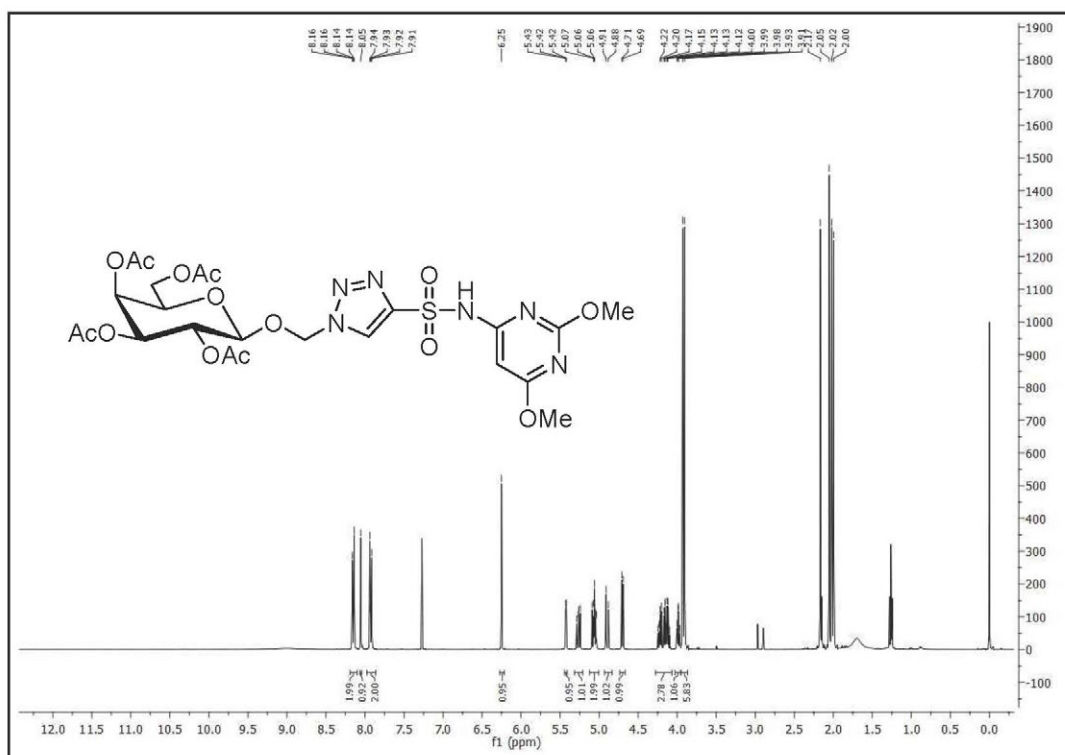


Figure S66. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **42**.

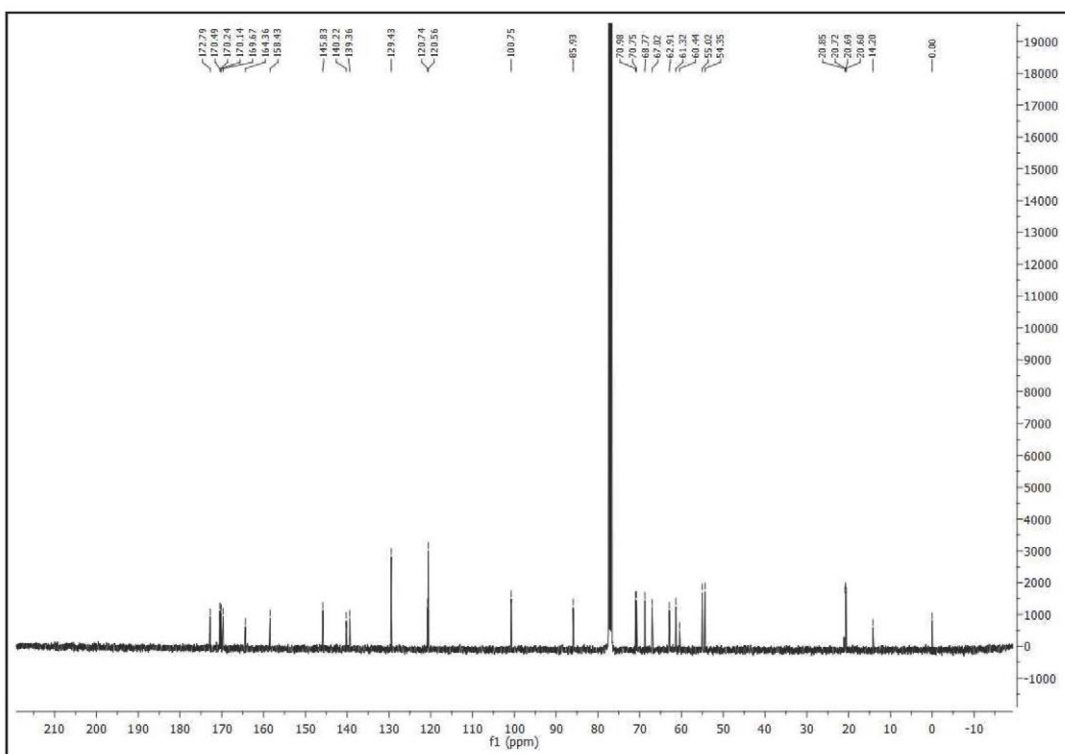
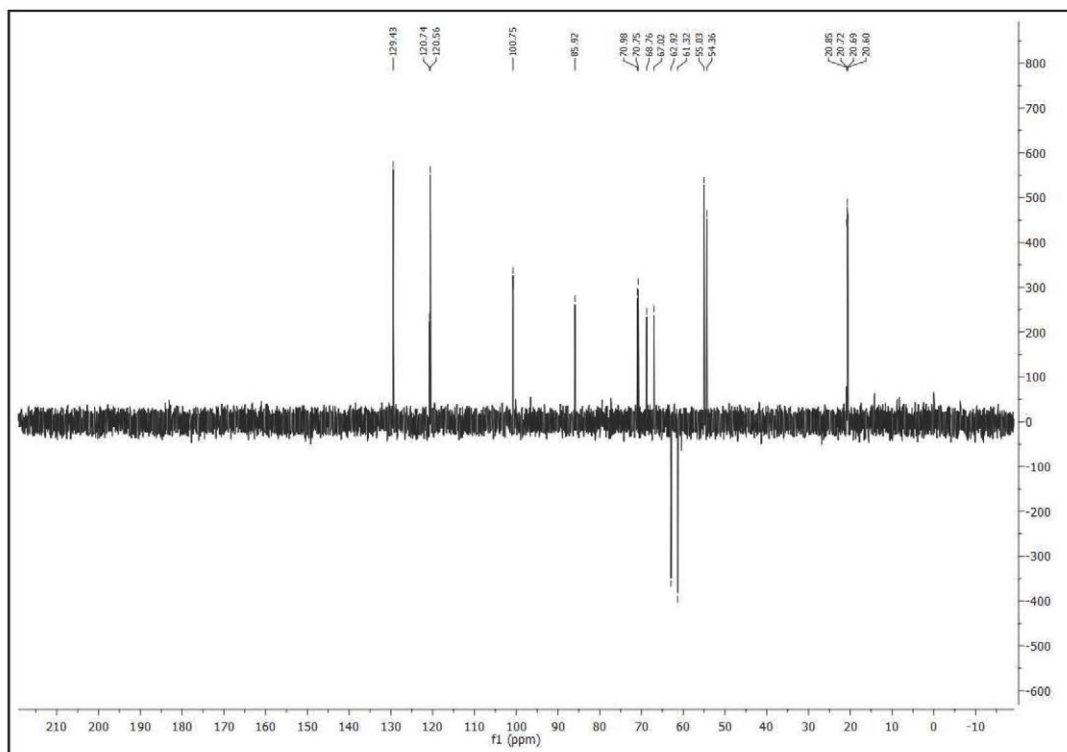
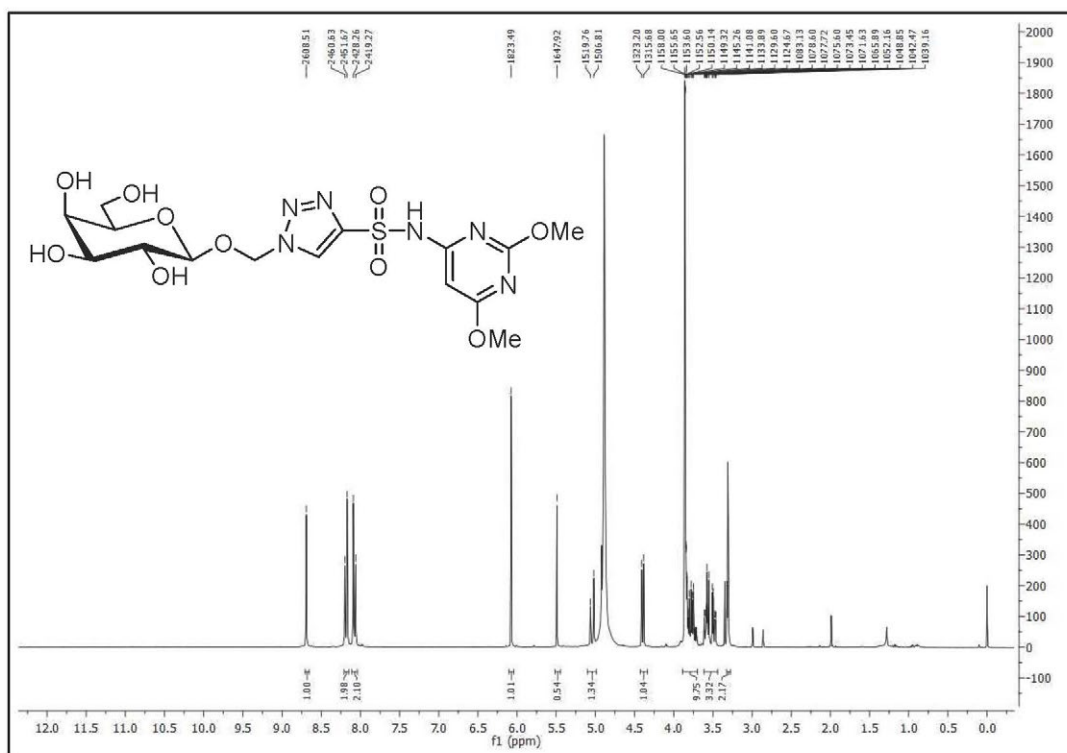


Figure S67. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound **42**.



**Figure S68.**  $^{13}\text{C}$  NMR DEPT (100 MHz,  $\text{CDCl}_3$ ) spectrum of compound **42**.

4-{4-[( $\beta$ -D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3-triazol-1-yl]-*N*-(2,6-dimethoxy pyrimidin-4-yl)benzenesulfonamide (**13**)



**Figure S69.**  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **13**.

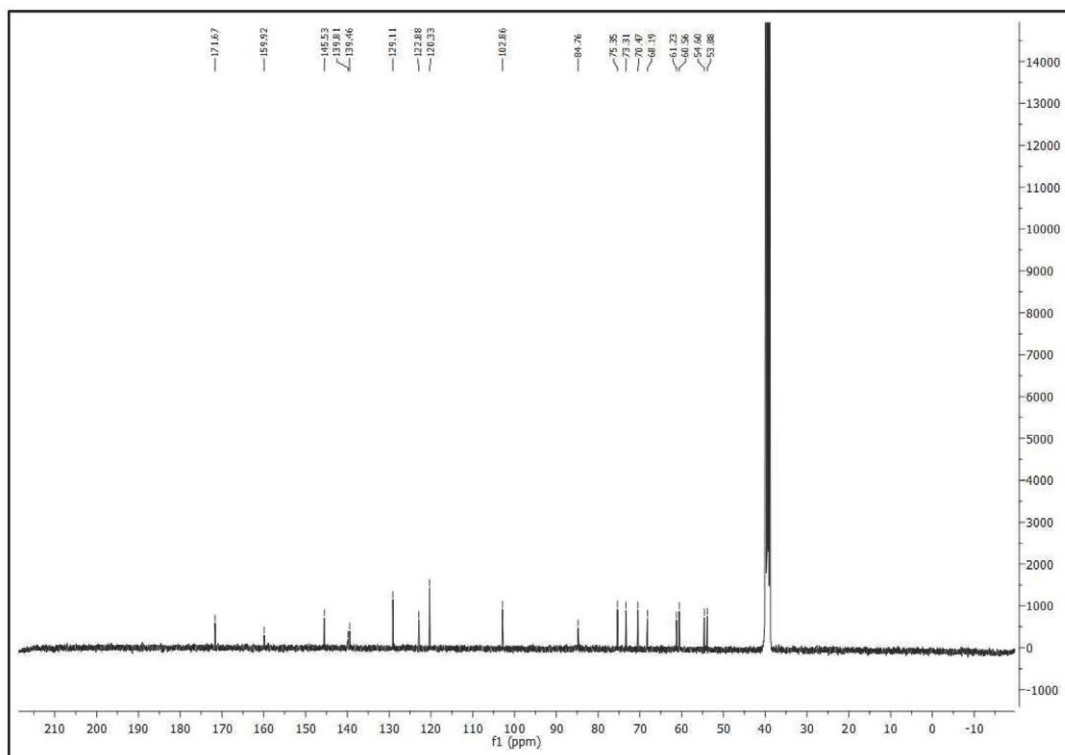


Figure S70. <sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>OD) spectrum of compound 13.

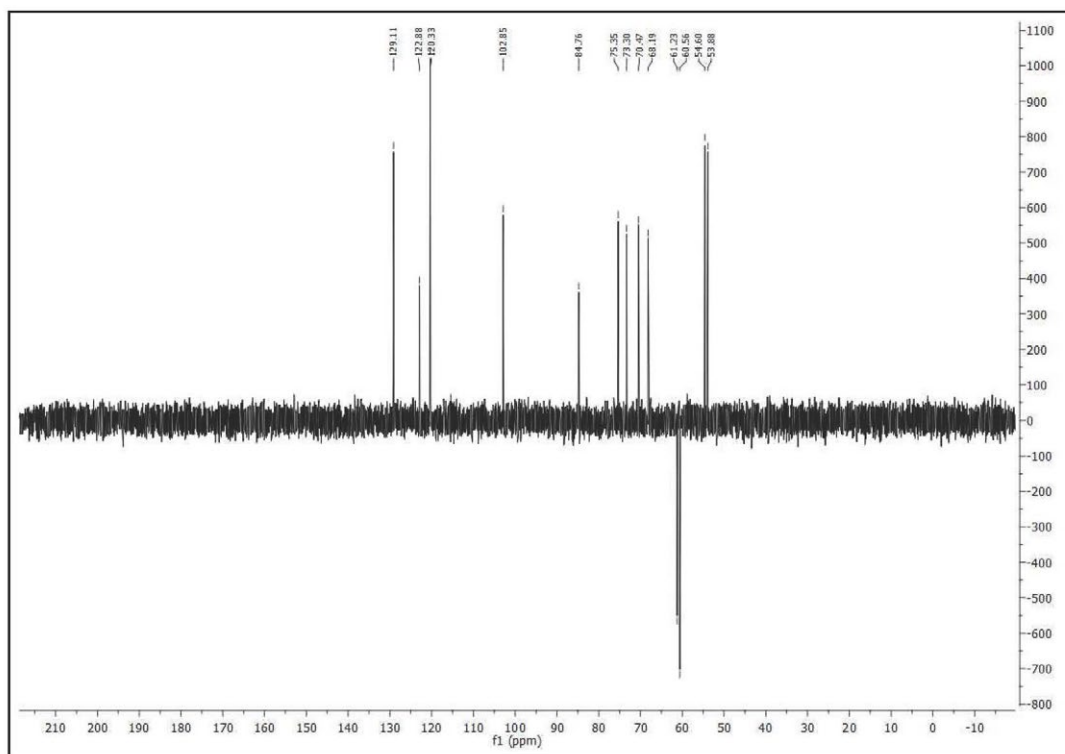
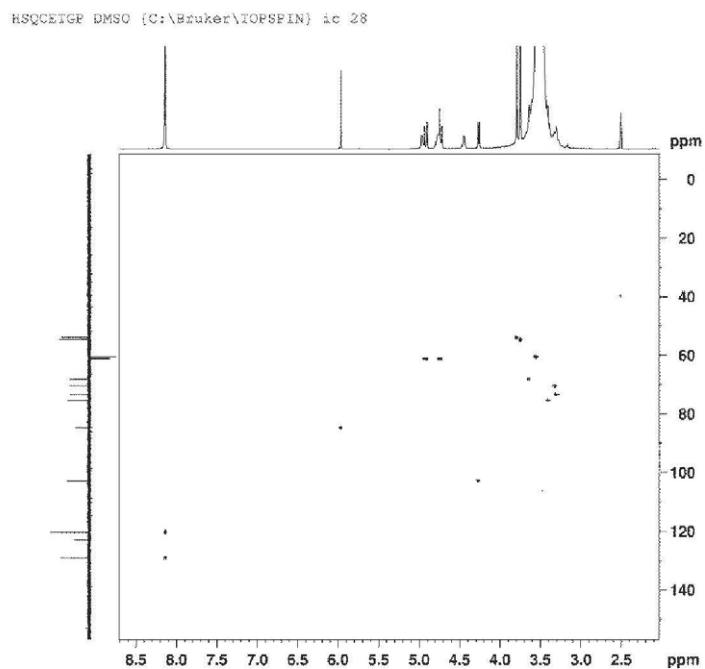
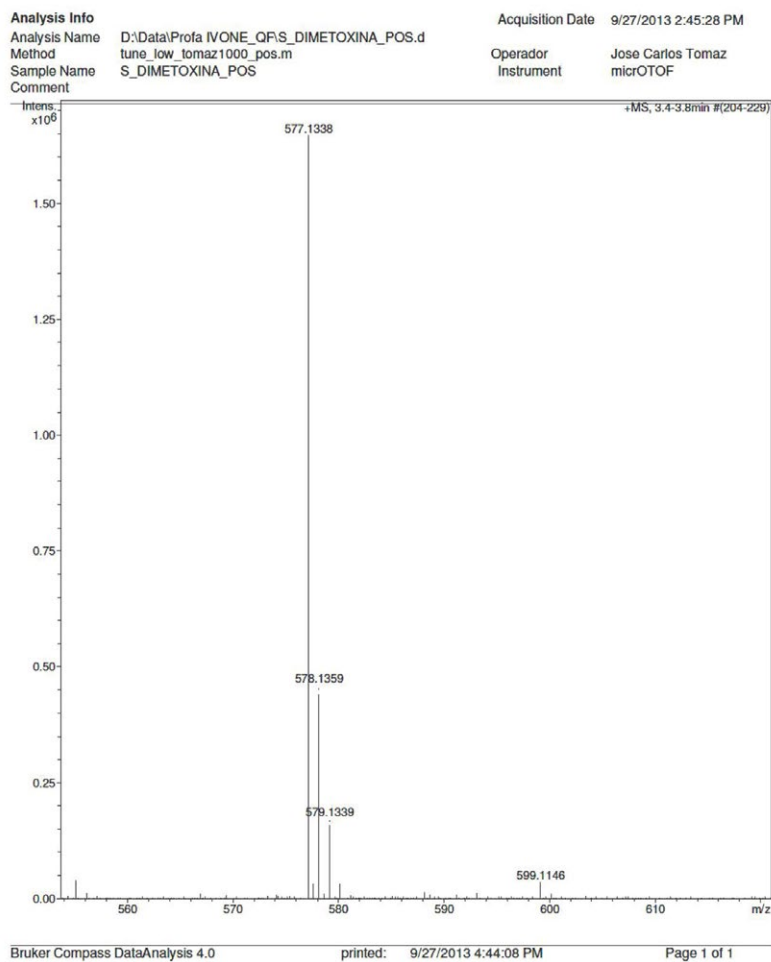


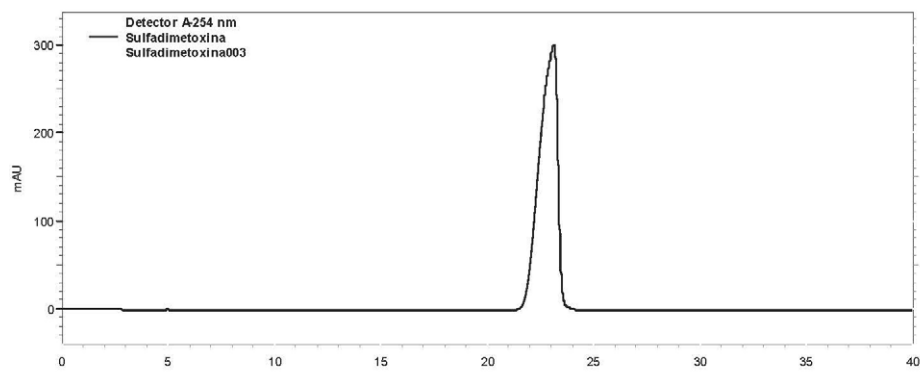
Figure S71. <sup>13</sup>C NMR DEPT(75 MHz, CD<sub>3</sub>OD) spectrum of compound 13.



**Figure S72.** Bi-dimensional spectrum (HMOC) of compound **13**.

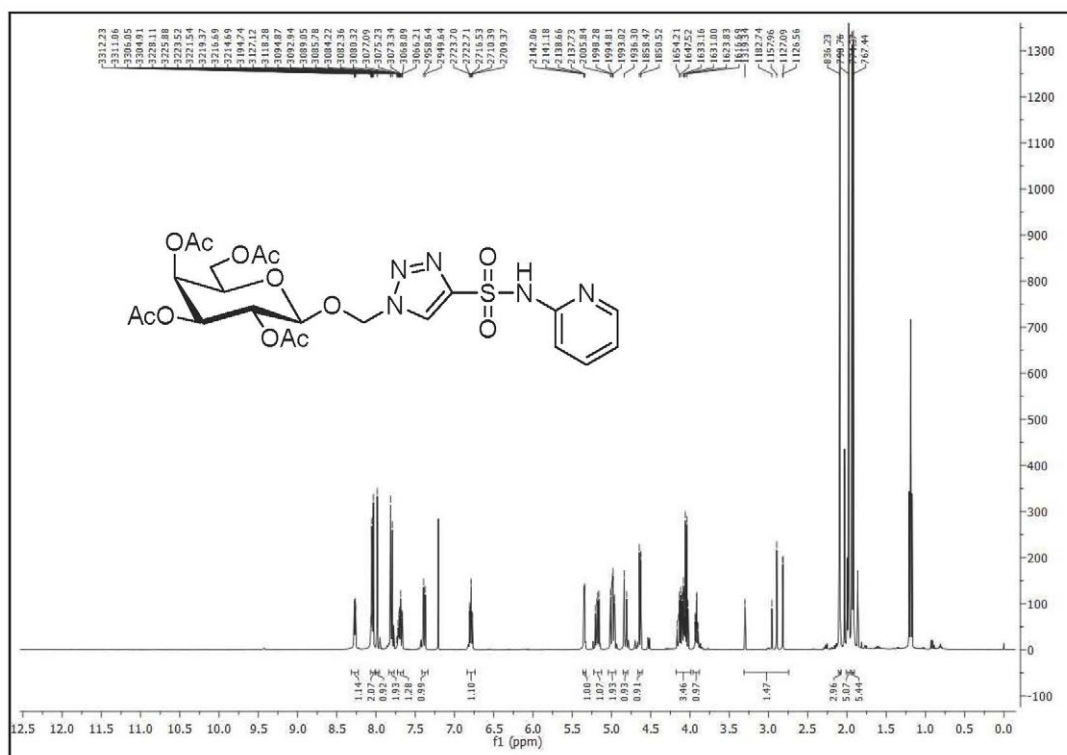


**Figure S73.** Mass spectrum (ESI-MS) of compound **13**.



**Figure S74.** HPLC chromatogram of compound **13**. Flow 0.9 mL min<sup>-1</sup>; mobile phase 40% MeOH, 60% H<sub>2</sub>O, TFA 0.1%; temp. 24.5 °C.

4-{4-[(2',3',4',6'-Tetra-*O*-acetyl-β-D-galactopyranosyl)-oxymethyl]-1-*H*-1,2,3 triazol-1-yl}benzenesulfa-*ortho*-pyridine (**43**)<sup>5</sup>



**Figure S75.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **43**.

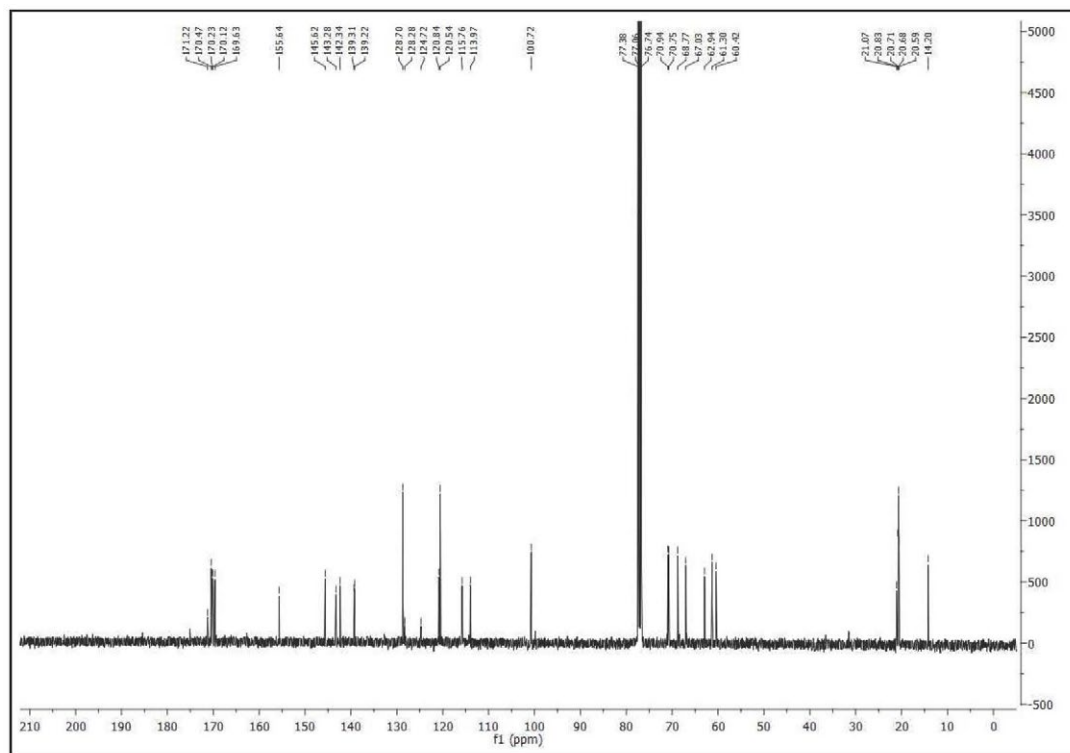


Figure S76.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of compound 43.

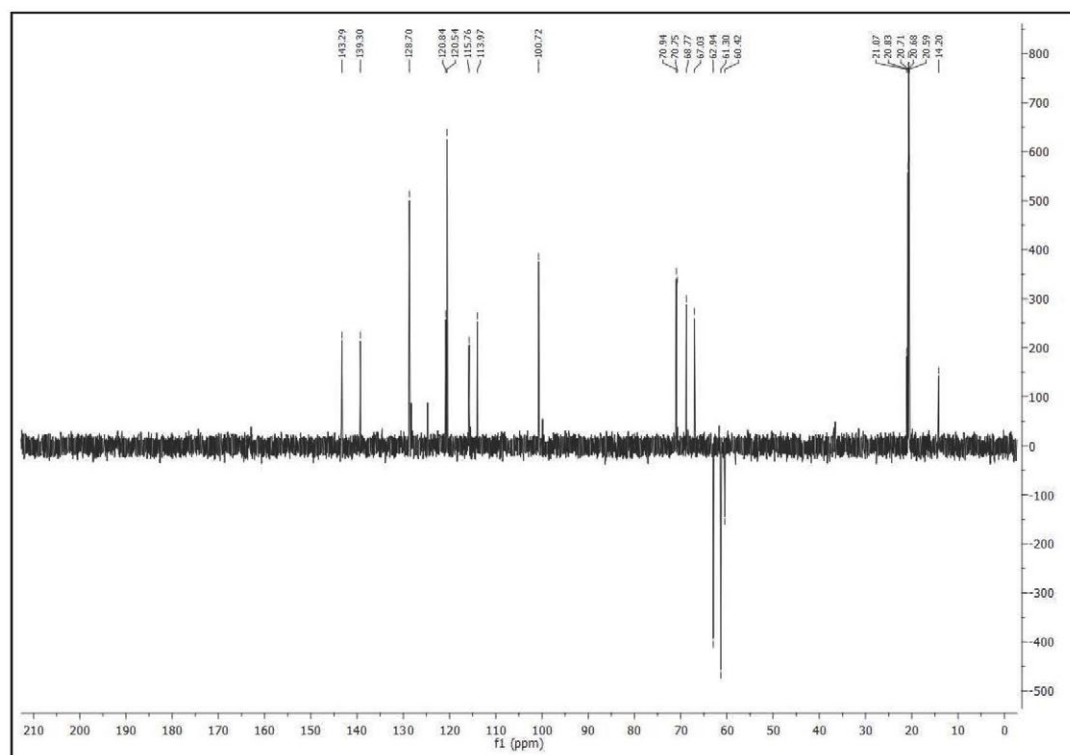
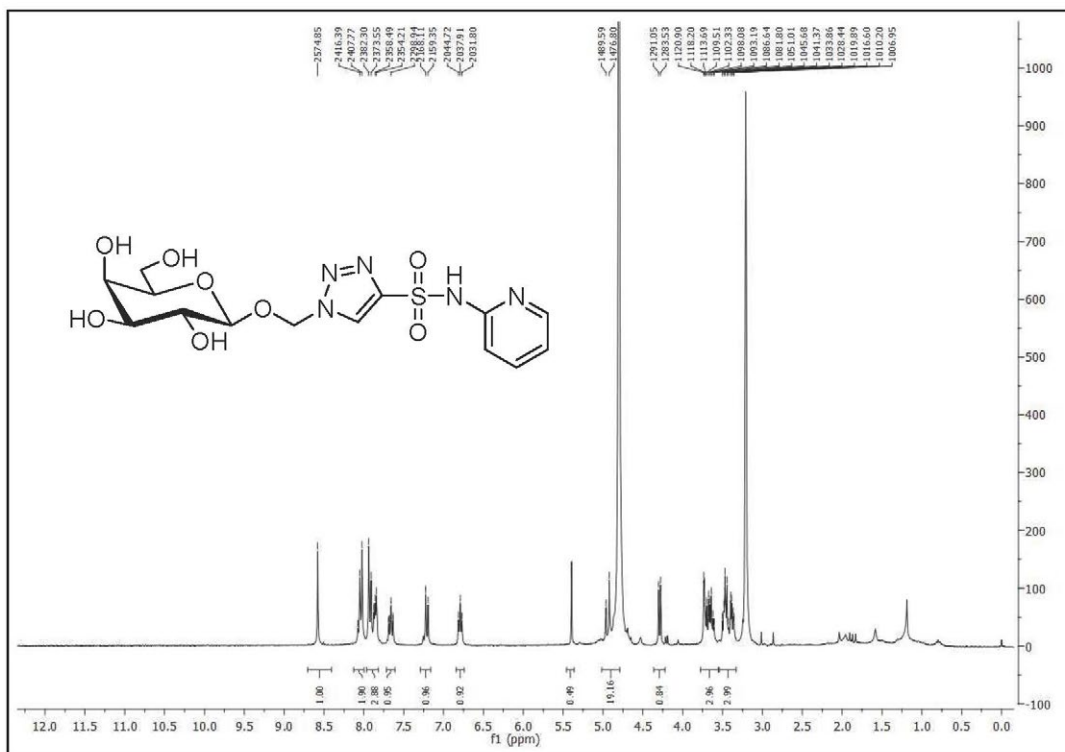
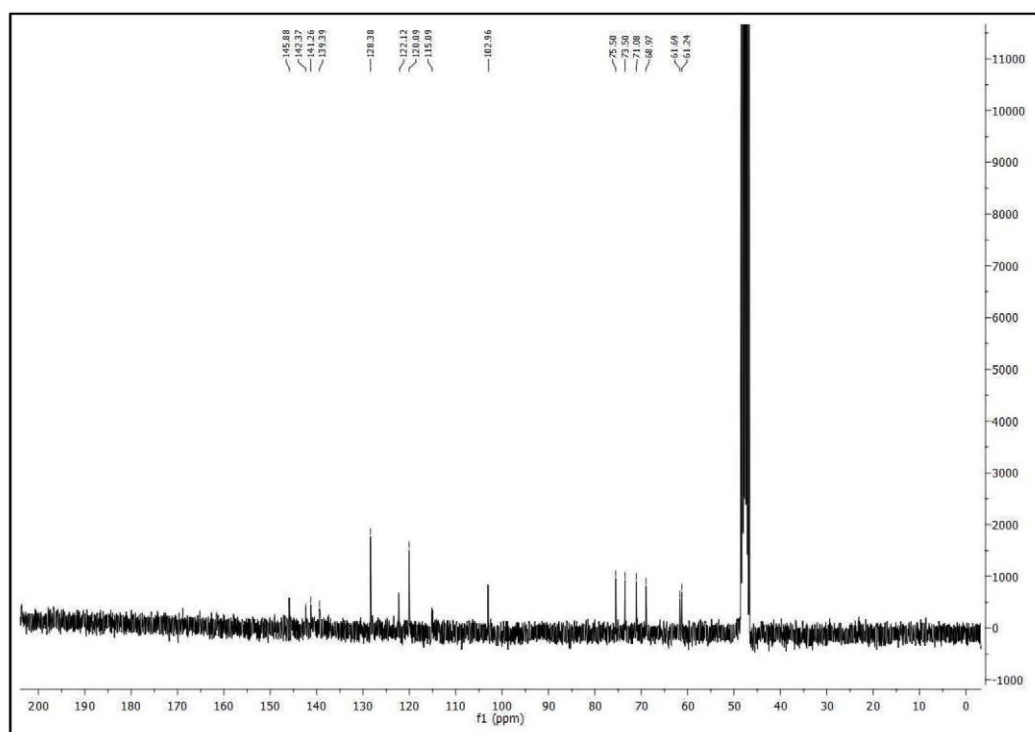


Figure S77.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of compound 43.

4-{4-[( $\beta$ -D-galactopyranosyl)-oxymethyl]-1-H-1,2,3-triazol-1-yl}benzenesulfa-*ortho*-pyridine (**14**)**Figure S78.**  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **14**.**Figure S79.**  $^{13}\text{C}$  NMR (75 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **14**.



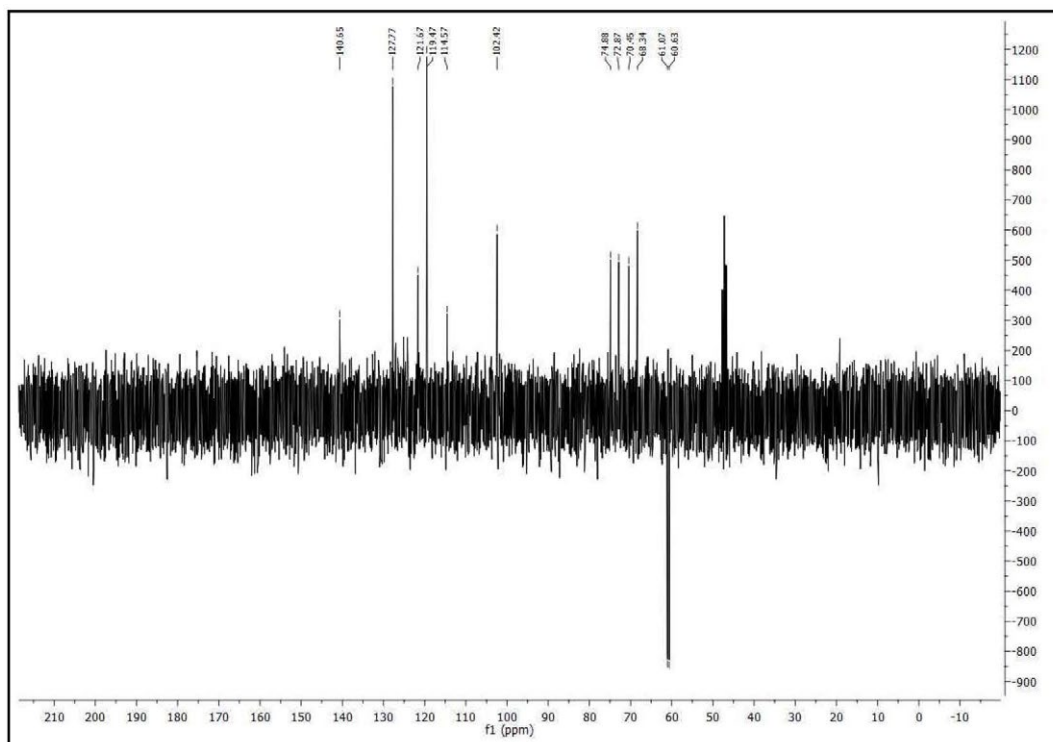


Figure S80.  $^{13}\text{C}$  NMR DEPT (75 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 14.

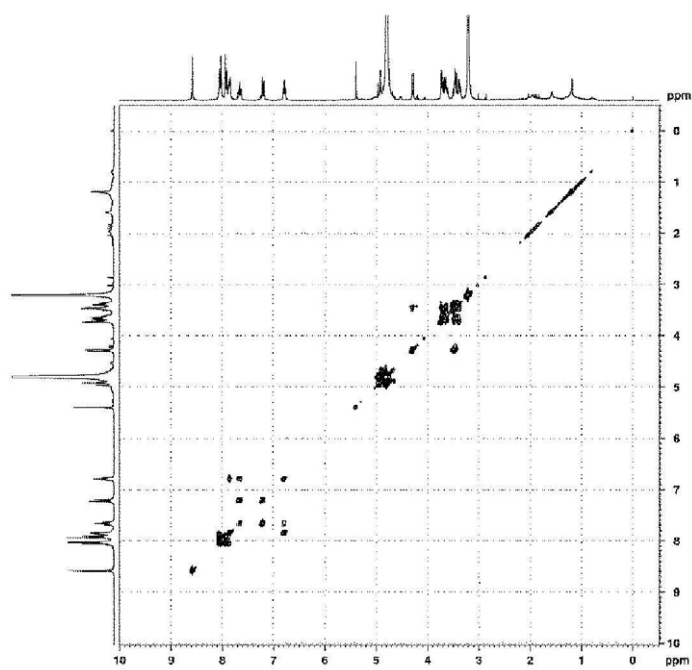


Figure S81. Bi-dimensional spectrum (COSY) of compound 14.

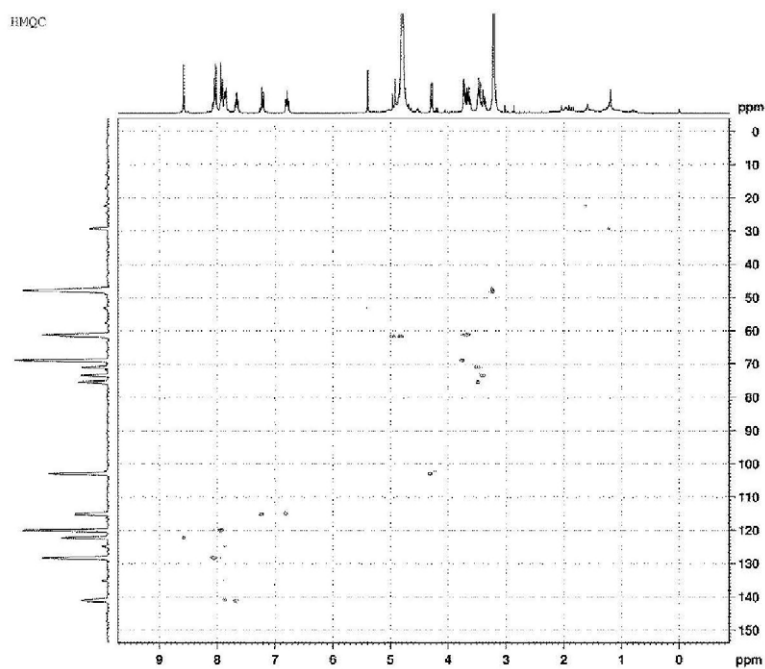


Figure S82. Bi-dimensional spectrum (HMQC) of compound 14.

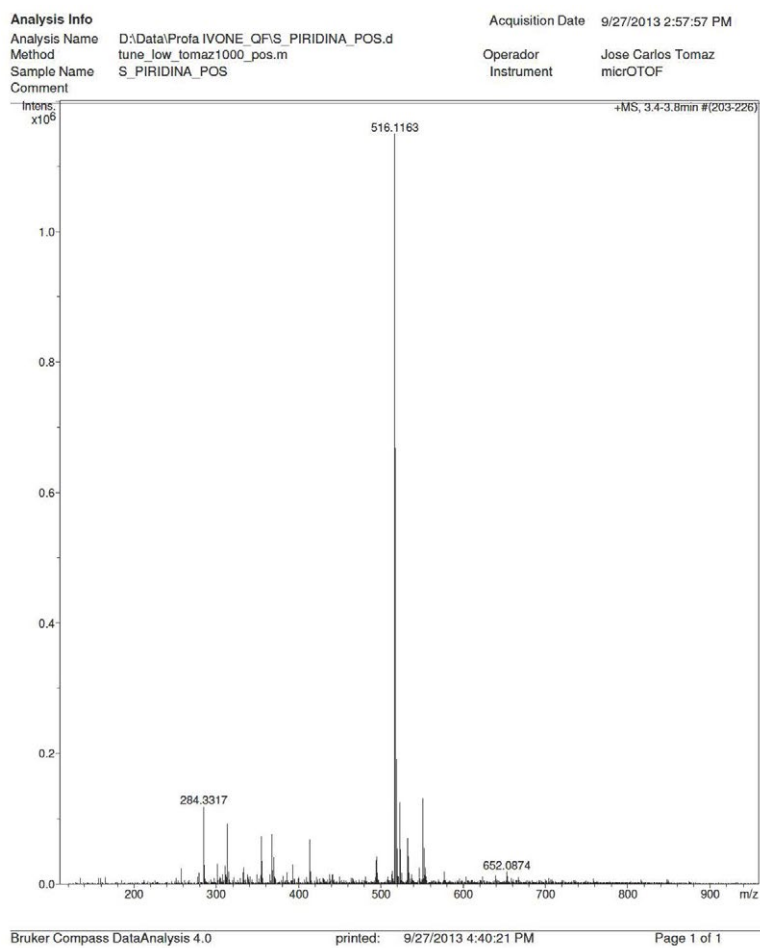
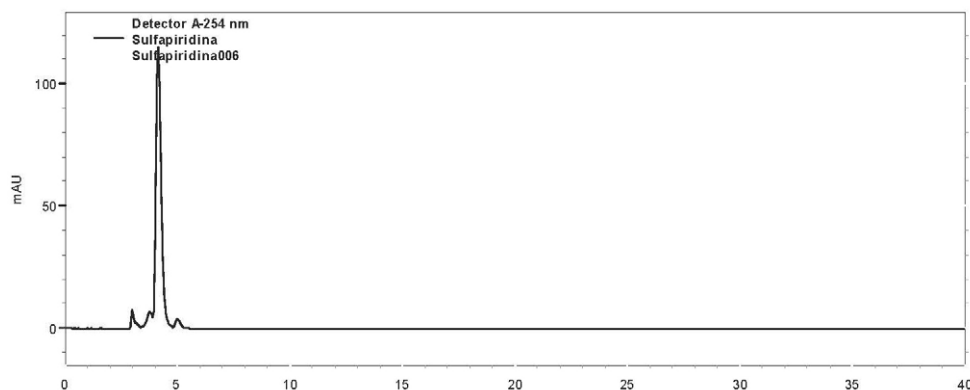


Figure S83. Mass spectrum (ESI-MS) of compound 14.



**Figure S84.** HPLC chromatogram of compound **14**. Flow 0.9 mL min<sup>-1</sup>; mobile phase 40% MeOH, 60% H<sub>2</sub>O, TFA 0.1%; temp. 24.5 °C.

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