Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## Stereoselective innovative synthesis and biological evaluation of new real carba analogues of minimal epitope Manα(1,2)Man as DC-SIGN inhibitors

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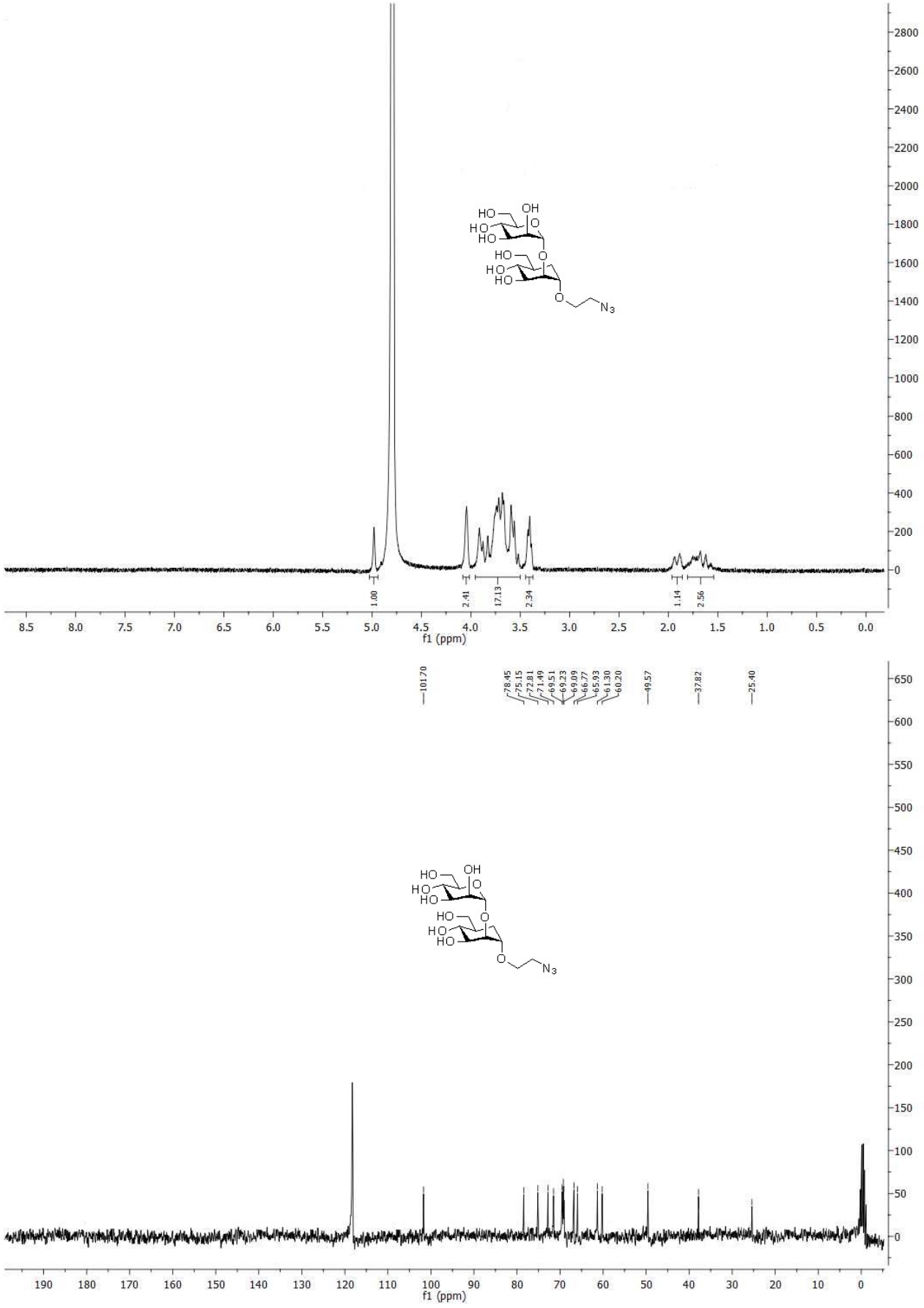



**Figure S1.** $^{1}$H NMR and $^{13}$C NMR of compound **4**.

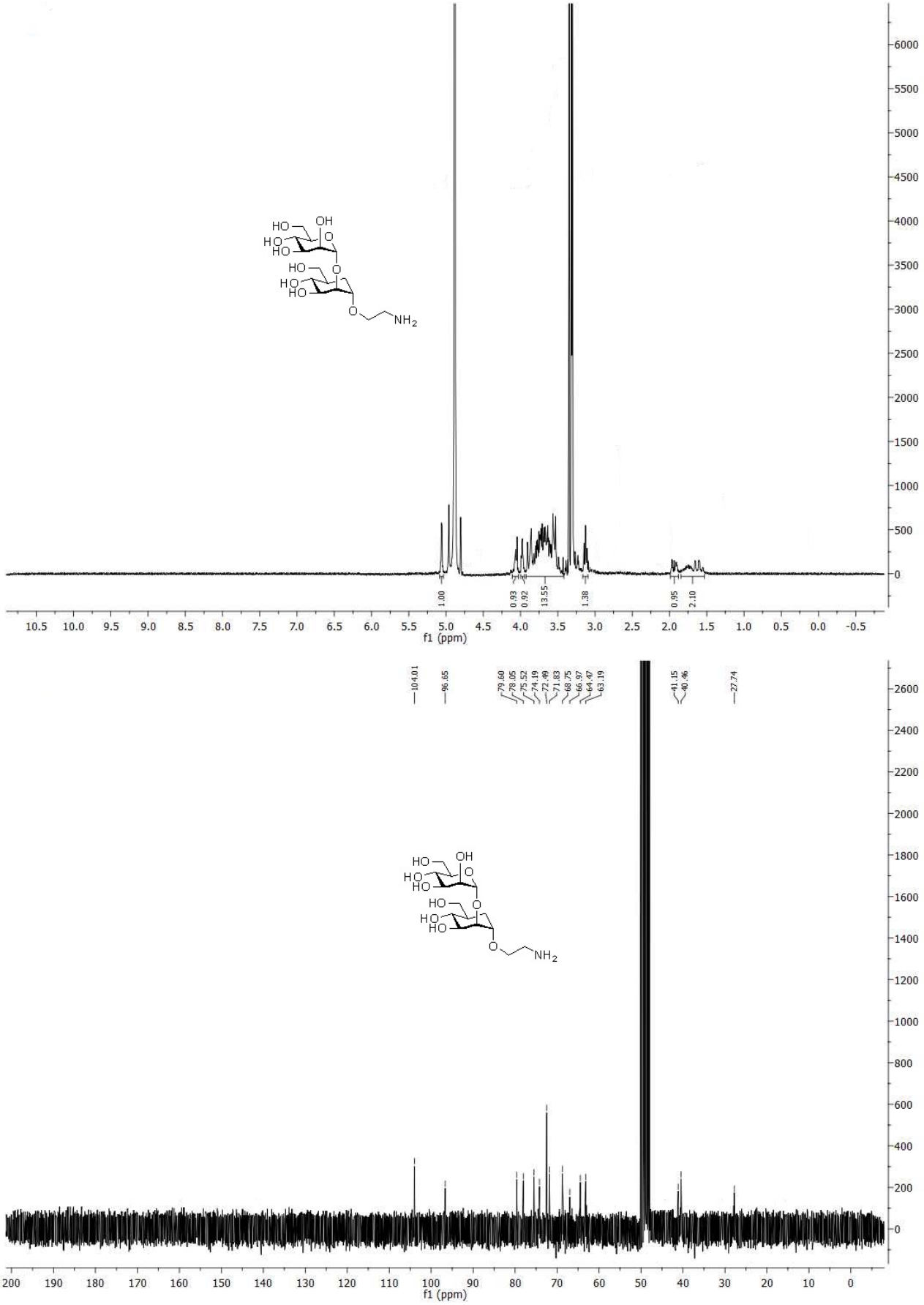



**Figure S2.** $^{1}$H NMR and $^{13}$C NMR of compound **5**.

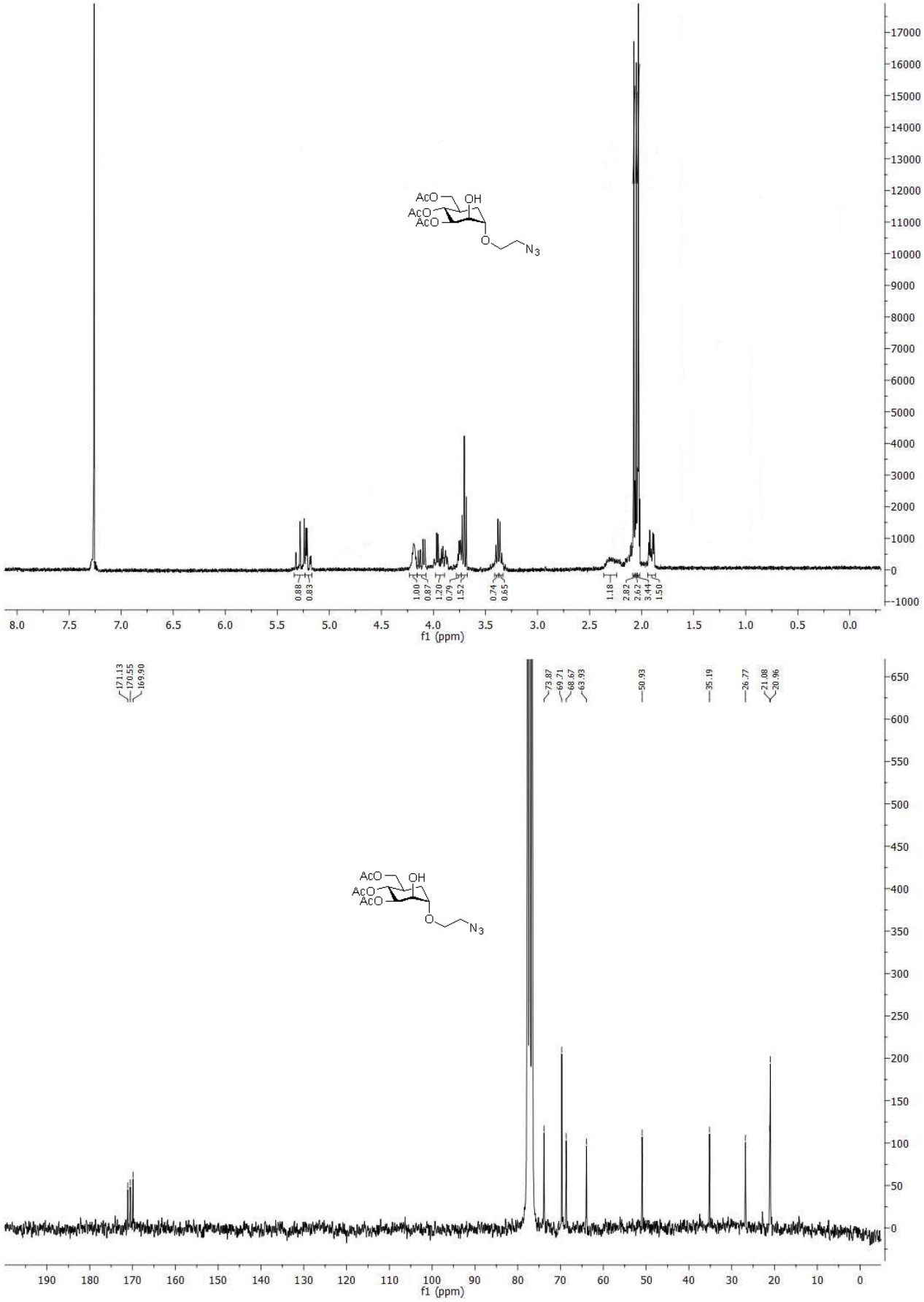



**Figure S3.** $^{1}$H NMR and $^{13}$C NMR of compound **15**.

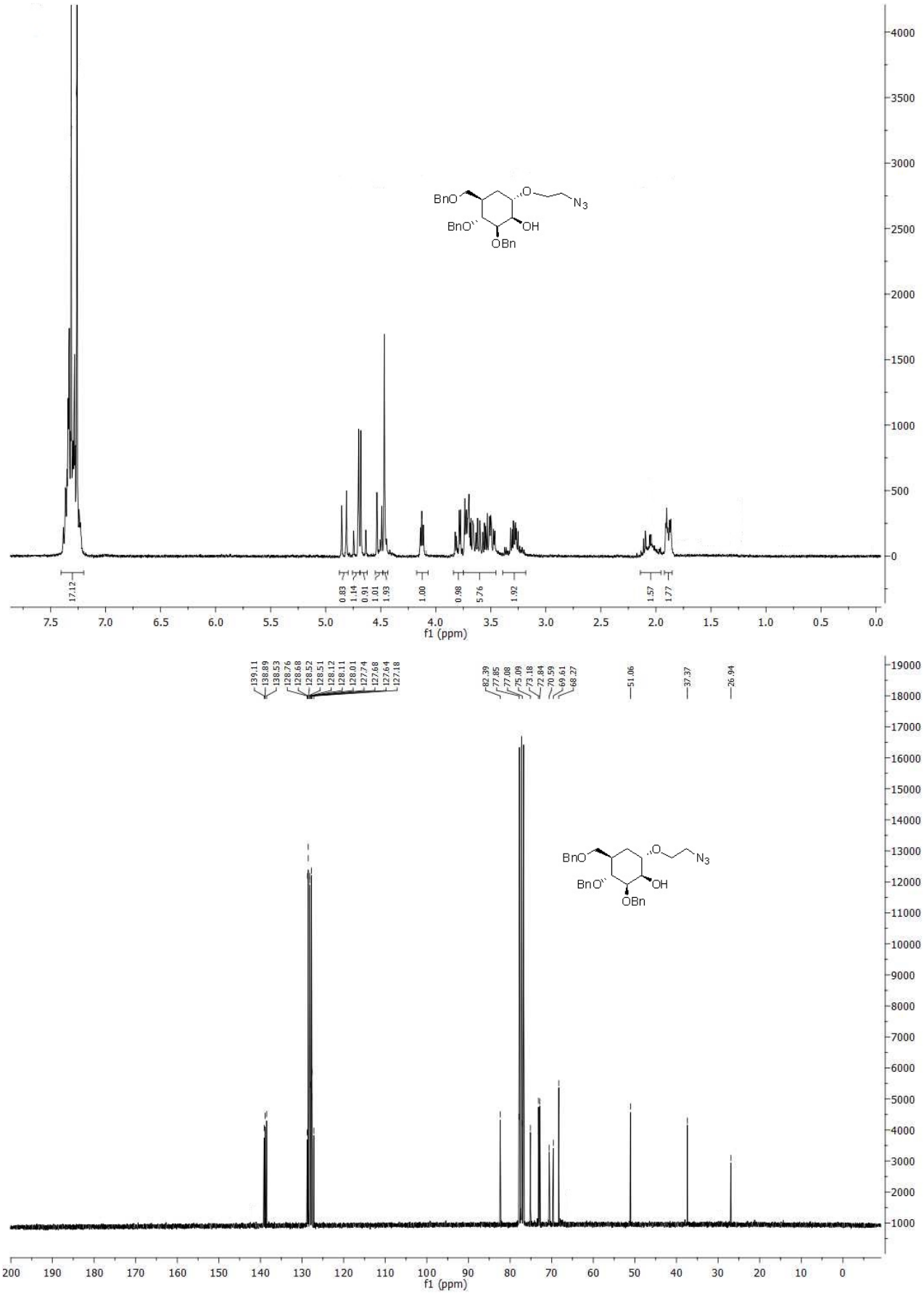



**Figure S4.** $^{1}$H NMR and $^{13}$C NMR of compound **16**.

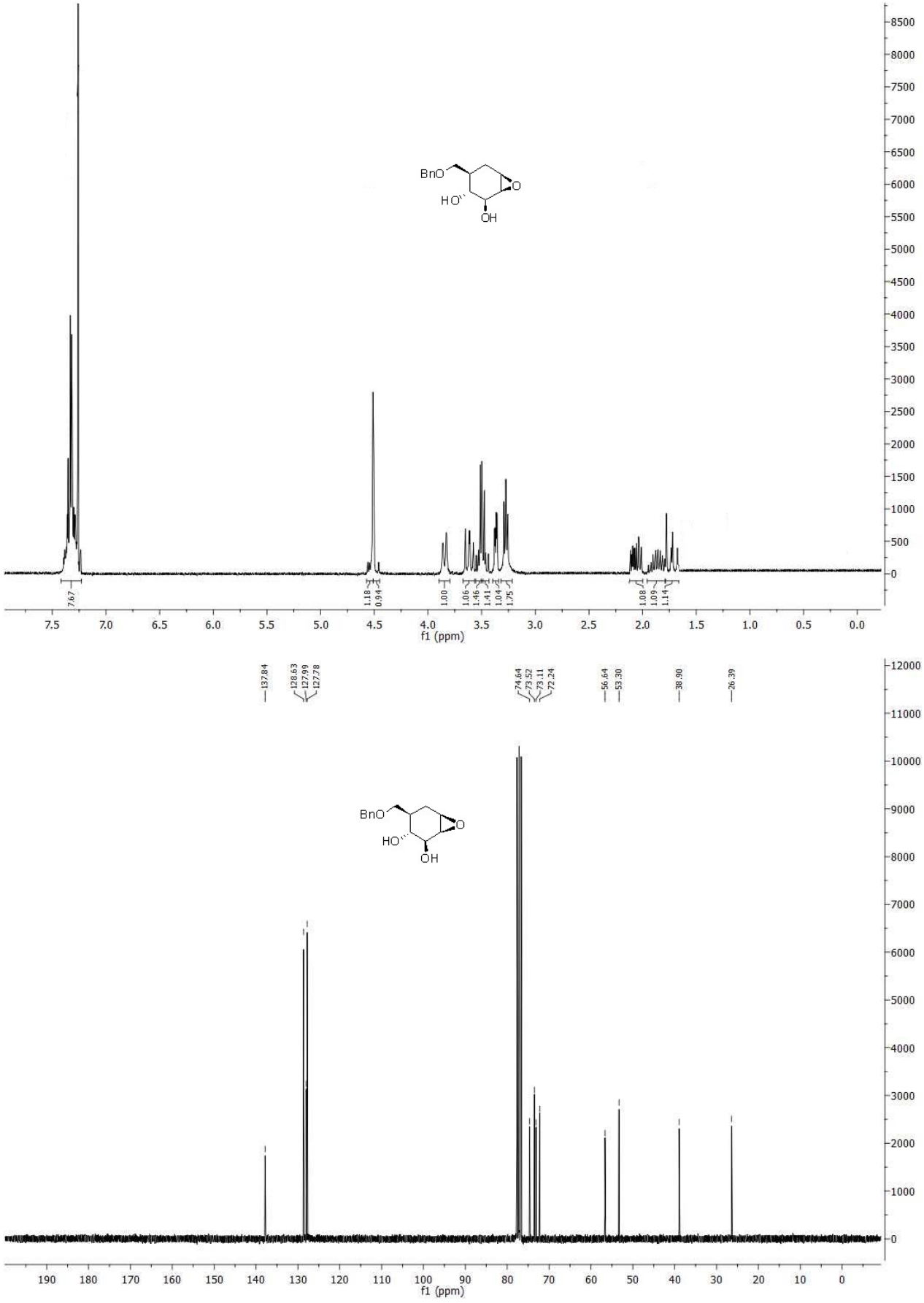



**Figure S5.** $^{1}$H NMR and $^{13}$C NMR of compound **11**.

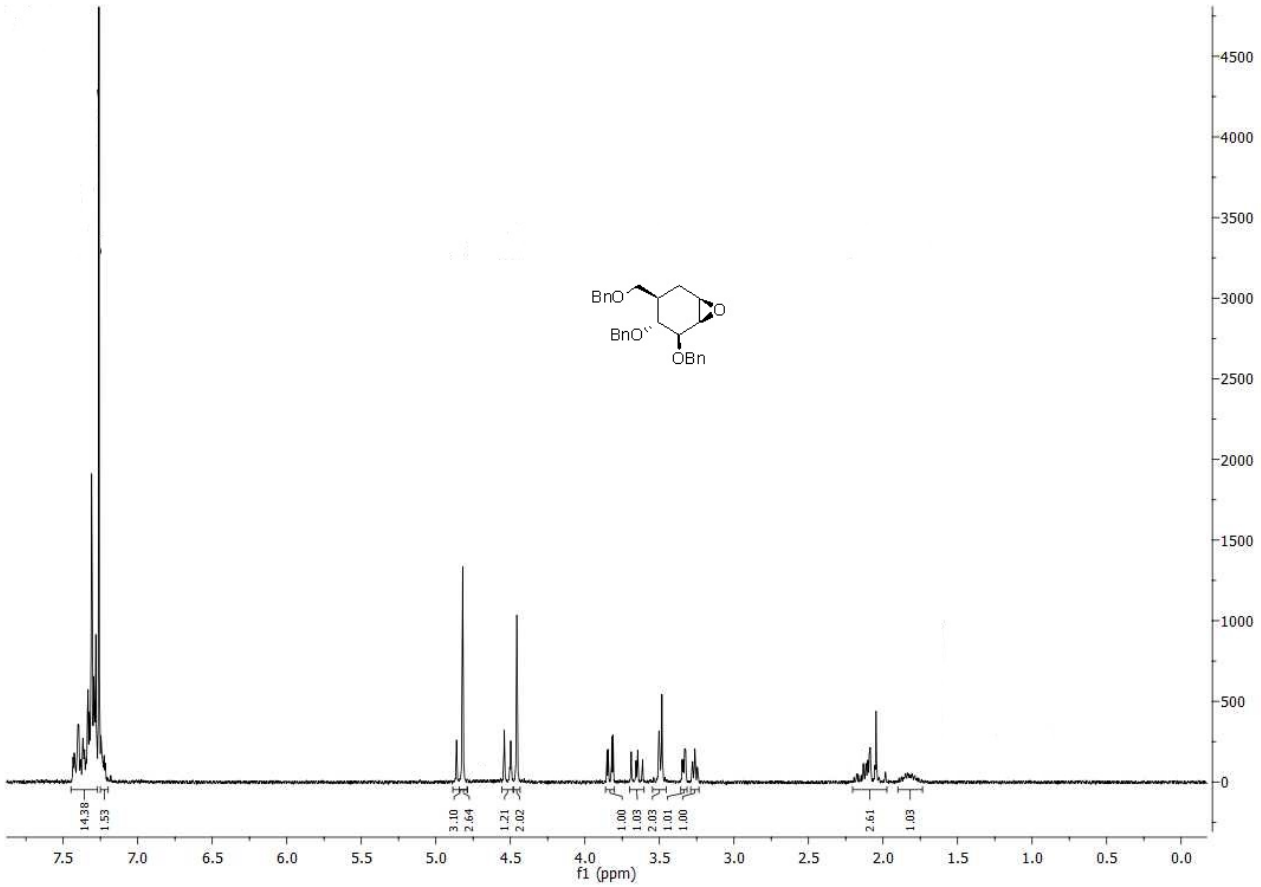



**Figure S6.** $^{1}$H NMR of compound **14**.

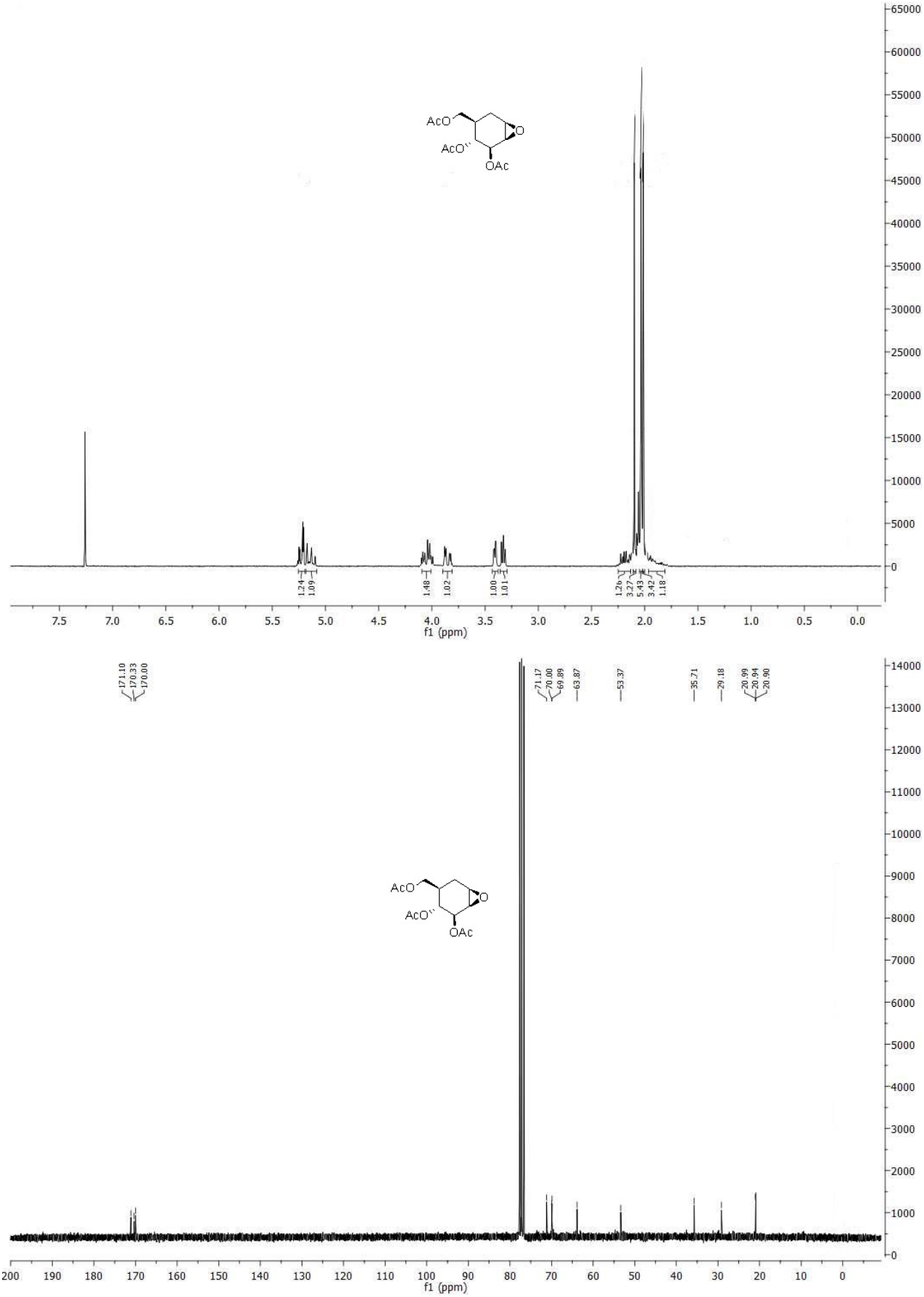



**Figure S7.** $^{1}$H NMR and $^{13}$C NMR of compound **13**.

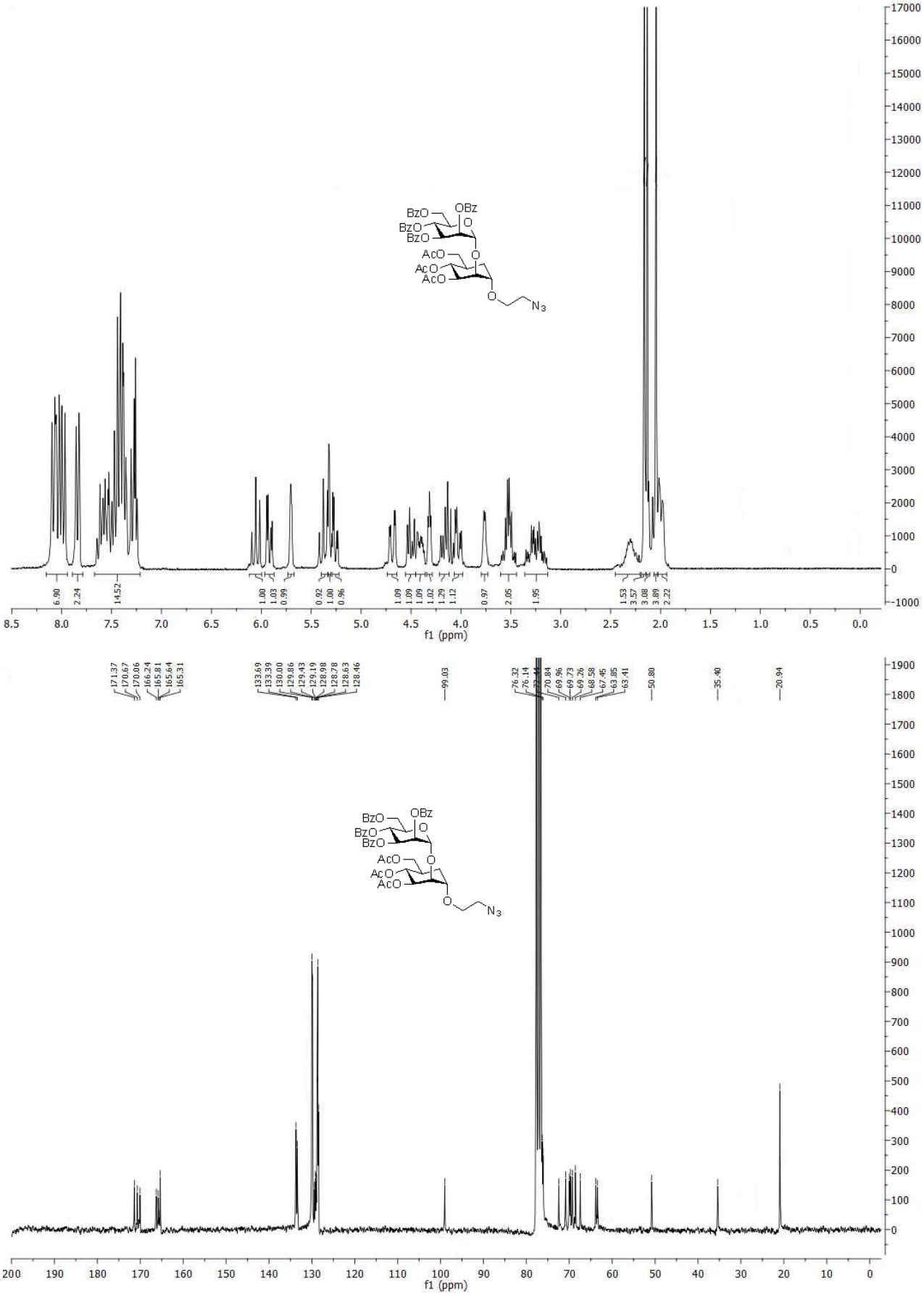



**Figure S8.** $^{1}$H NMR and $^{13}$C NMR of compound **17**.

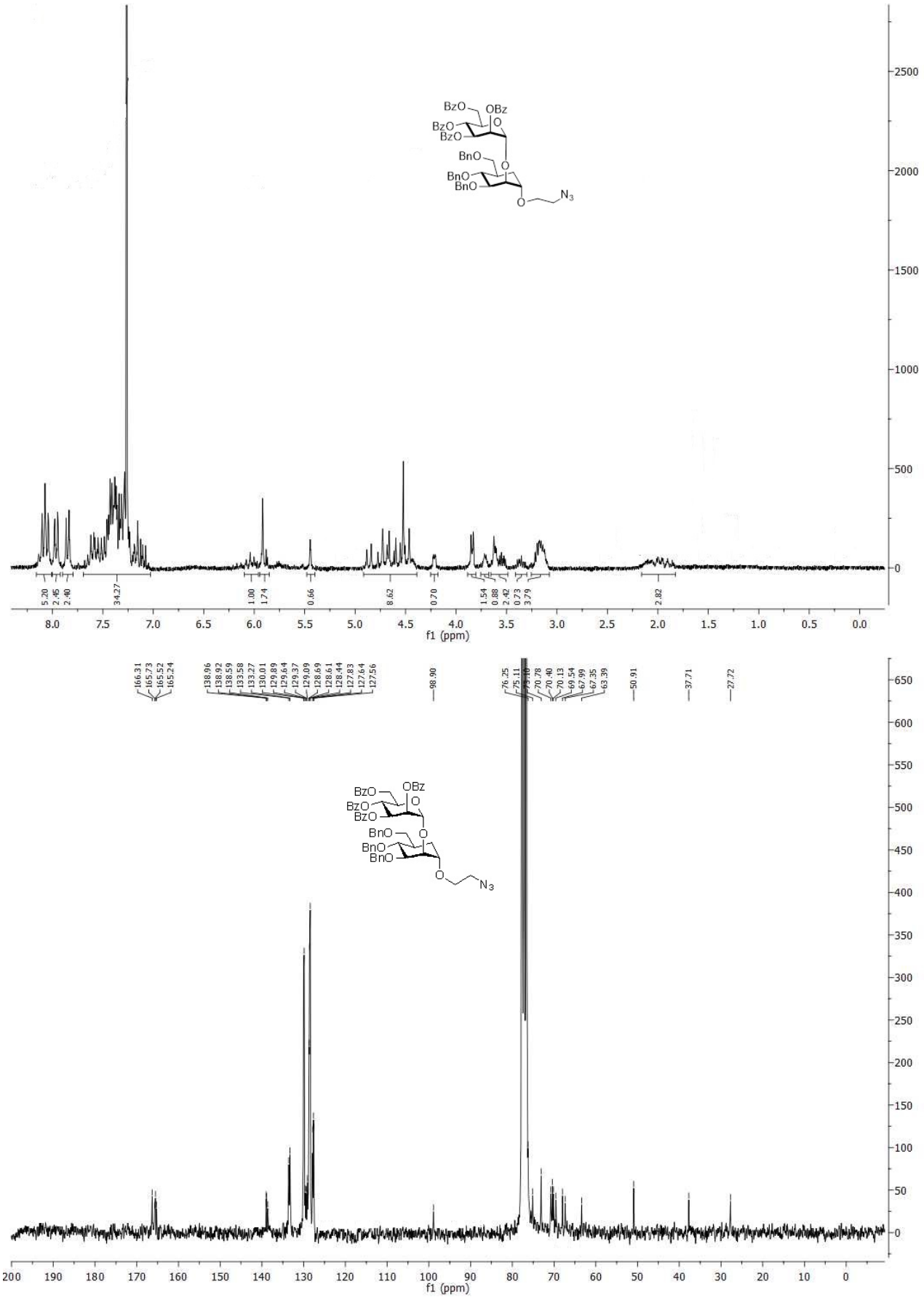



**Figure S9.** $^{1}$H NMR and $^{13}$C NMR of compound **18**.

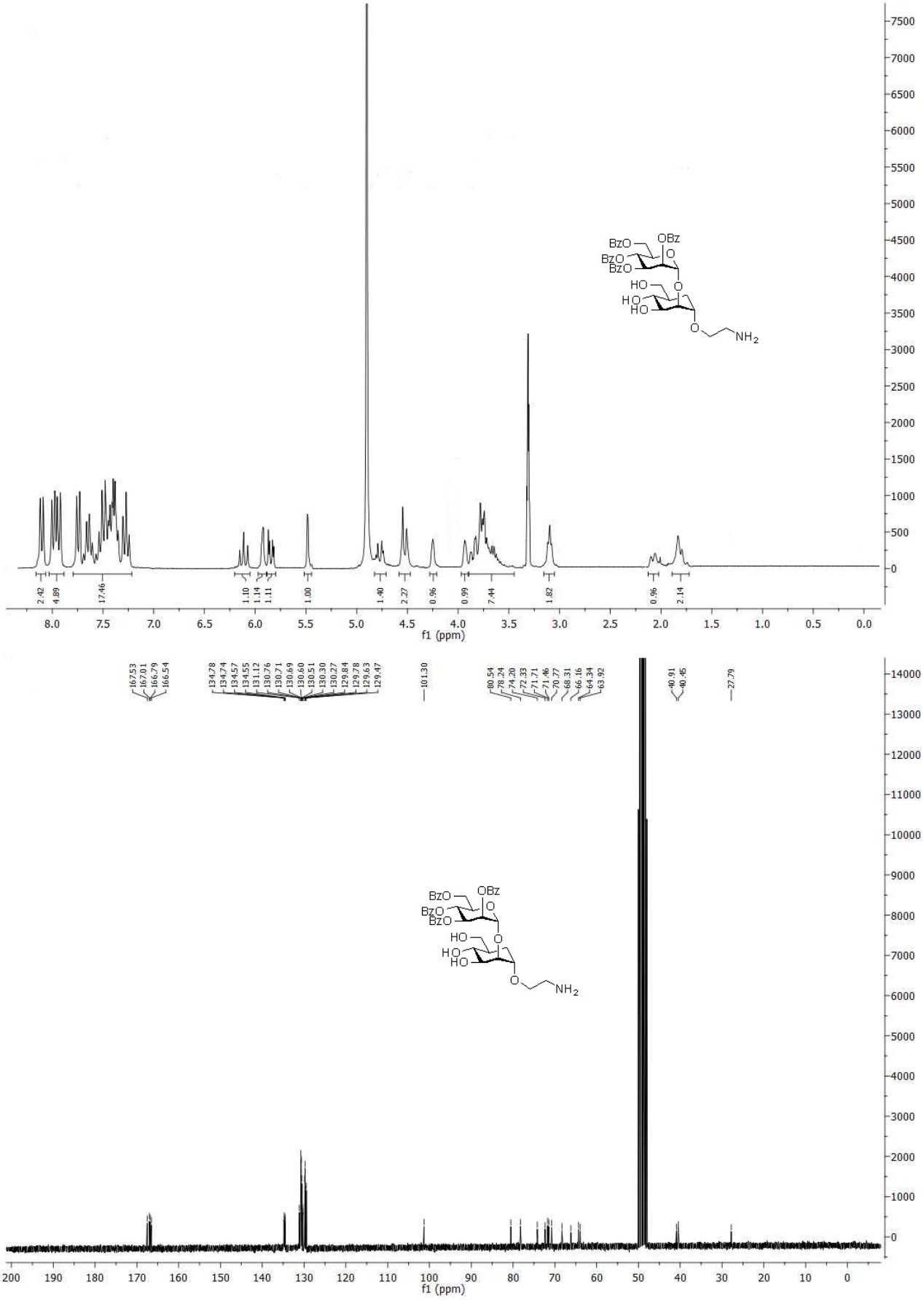
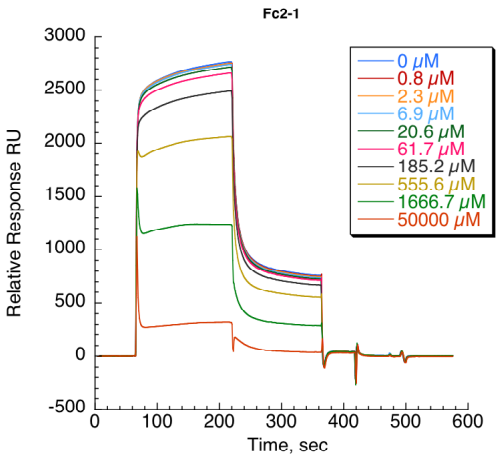



**Figure S10.** $^{1}$H NMR and $^{13}$C NMR of compound **19**.

## Sensorgrams and inhibition curves

### Compound 5

Fc2-1




4 parameter equation

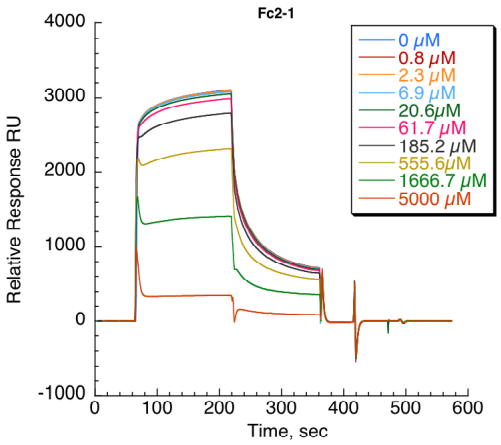
$IC_{50}$= 1420$\mu$M ( $X^2$=0.04)

| Conc uM | % DC-SIGN activity | Req |
|---|---|---|
| | | |
| 0.0 | 100.0 | 2760.0 |
| 0.8 | 99.6 | 2750.0 |
| 2.3 | 99.6 | 2750.0 |
| 6.9 | 99.3 | 2740.0 |
| 20.6 | 98.2 | 2710.0 |
| 61.7 | 96.4 | 2660.0 |
| 185.2 | 90.2 | 2490.0 |
| 555.6 | 74.6 | 2060.0 |
| 1666.7 | 44.9 | 1240.0 |
| 5000.0 | 11.6 | 320.0 |

**Figure S11.** Sensorgram of compound **5**.

**Compound 4**

Fc2-1




4 parameter equation

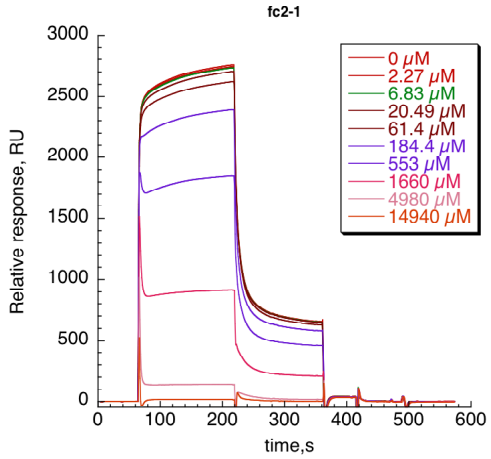
$IC_{50}$= 1430$\mu$M ( $X^2$=0.08)

| Conc uM | % DC-SIGN activity | Req |
|---|---|---|
| | | |
| 0.0 | 100.0 | 3110.0 |
| 0.8 | 99.7 | 3100.0 |
| 2.3 | 99.7 | 3100.0 |
| 6.9 | 99.0 | 3080.0 |
| 20.6 | 98.1 | 3050.0 |
| 61.7 | 96.1 | 2990.0 |
| 185.2 | 89.7 | 2790.0 |
| 555.6 | 74.6 | 2320.0 |
| 1666.7 | 45.0 | 1400.0 |
| 5000.0 | 11.4 | 353.0 |

**Figure S12.** Sensorgram of compound **4**.

**Manα1,2-Man (2)**

Fc2-1

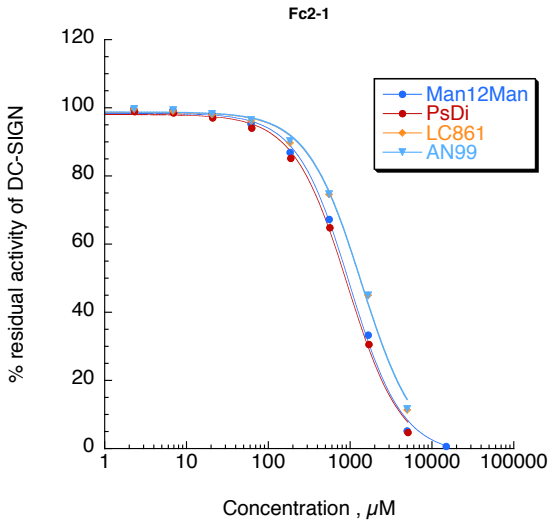


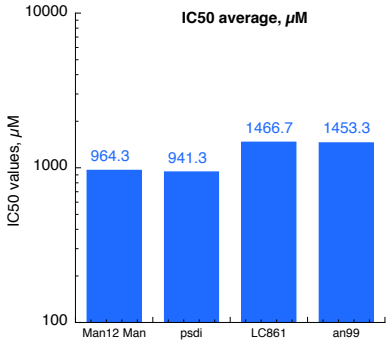

4 parameter equation

$IC_{50}$= 949$\mu$M ( $X^2$=3.2)

| Conc | % DC-SIGN activity | Req |
|---|---|---|
| 0.0 | 100.0 | 2750.0 |
| 2.3 | 99.6 | 2740.0 |
| 6.8 | 99.3 | 2730.0 |
| 20.5 | 98.2 | 2700.0 |
| 61.4 | 95.3 | 2620.0 |
| 184.4 | 86.9 | 2390.0 |
| 553.0 | 67.3 | 1850.0 |
| 1660.0 | 33.3 | 916.0 |
| 4980.0 | 5.2 | 142.0 |
| 14940.0 | 0.6 | 17.2 |

**Figure S13.** Sensorgram of minimal epitope **Mana(1,2)Man (2)**.




## $IC_{50}$ values

| | IC50 μM | | | | |
|---|---|---|---|---|---|
| | Fc2-1 | Fc3-1 | Fc4-1 | IC50 average, μM | ±SD |
| Manα(1,2) Man | 949 | 966 | 978 | 964 | 14.6 |
| Psdi (compound **3**) | 918 | 953 | 953 | 941 | 20.2 |
| LC861 (compound **4**) | 1430 | 1480 | 1490 | 1467 | 32.1 |
| an99 (compound **5**) | 1420 | 1460 | 1480 | 1453 | 30.6 |

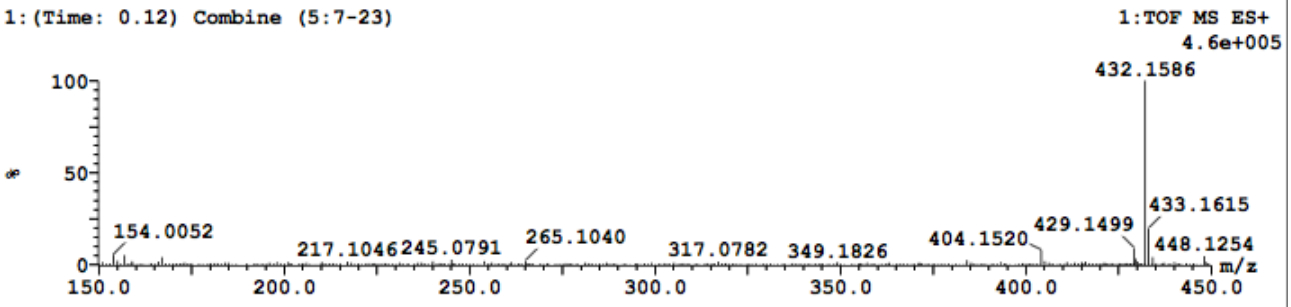
Amount of immobilized BSA-Man: Fc2-1 1664 RU; Fc3-1 1376 RU; Fc4-1 1847 RU

**Figure S14.** Inhibition curves of **Mana(1,2)Man (2),** compound **3,** compound **4** and compound **5**.

**ICMG - Plateau de Spectrometrie de Masse - Elemental Composition** Page 1
HRMS - ESI/QTOF - Waters Xevo G2-S QTof

**File LC861 Description 5 10e-5 M ds ACN/eau**

| Target Mass | Mass Found | Error PPM | Compound |
|---|---|---|---|
| 432.1594 | 432.16 | -1.9 | Found |




| Mass | PPM | i-FIT (norm) | Formula | Calc. Mass |
|---|---|---|---|---|
| 432.1586 | -1.9 | 0.1 | C15 H27 N3 O10 Na | 432.1594 |
| 432.1586 | -1.2 | 2.1 | C14 H28 N2 O13 | 432.1591 |
| 432.1586 | 4.4 | 6.3 | C12 H29 N2 O13 Na | 432.1567 |
| 432.1586 | 3.0 | 11.4 | C26 H24 O6 | 432.1573 |
| 432.1586 | 0.0 | 12.4 | C27 H20 N4 O2 | 432.1586 |
| 432.1586 | 2.3 | 12.5 | C27 H23 N O3 Na | 432.1576 |
| 432.1586 | -3.2 | 14.5 | C29 H22 N O3 | 432.1600 |
| 432.1586 | -3.7 | 15.6 | C30 H21 N2 Na | 432.1602 |

**Figure S15.** HRMS of compound **4.**

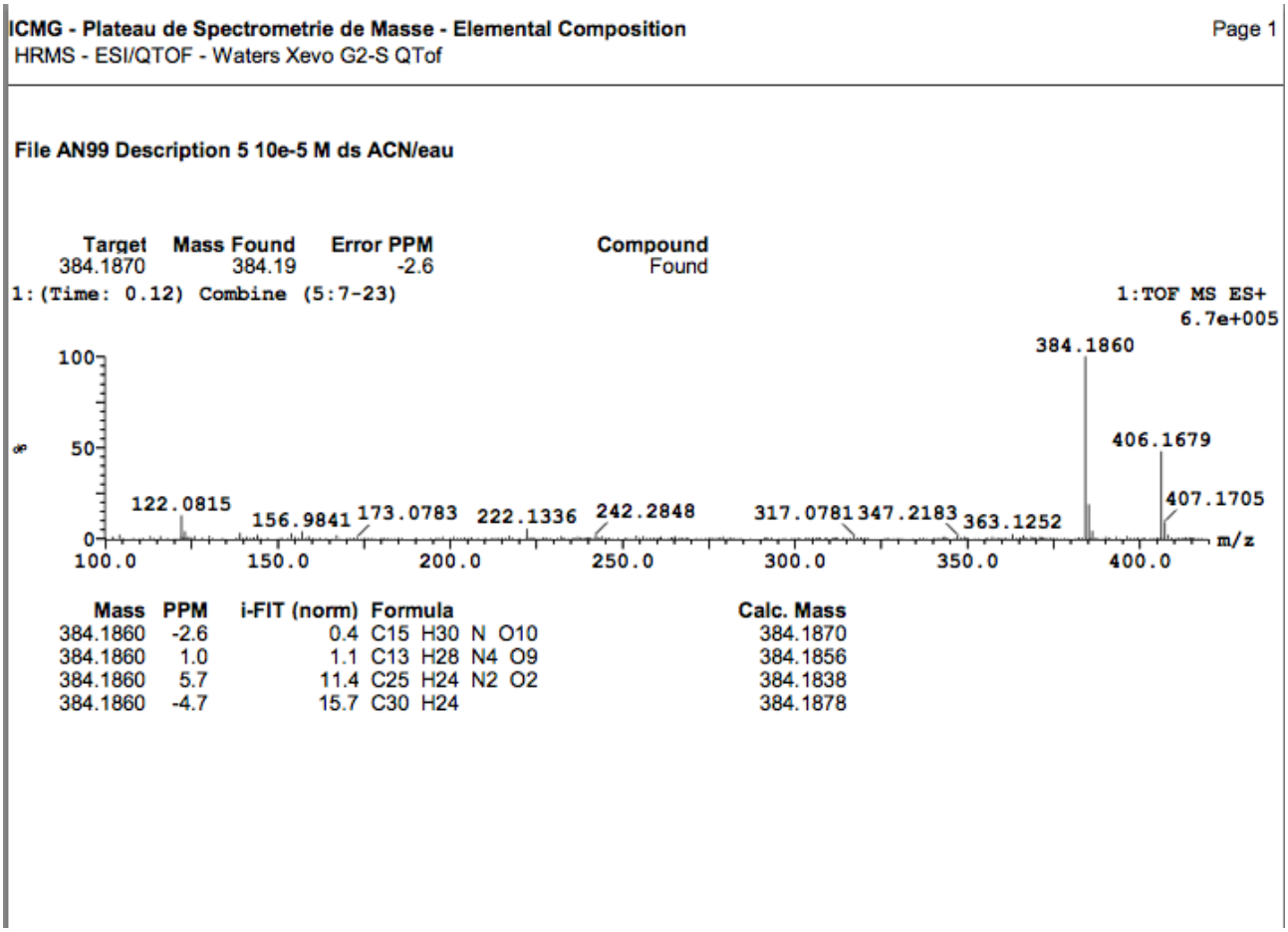



**Figure S16.** HRMS of compound **5.**