BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Towards the preparation of synthetic outer membrane vesicle models with micromolar affinity to wheat germ agglutinin using a dialkyl thioglycoside

Dimitri Fayolle, Nathalie Berthet, Bastien Doumeche, Olivier Renaudet, Peter Strazewski and Michele Fiore

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Additional Figures S1–S6 and spectra of synthesized glycolipids and starting materials

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3. Spectra of synthesized glycolipids S8

1. Supporting Information Figures S1–S6

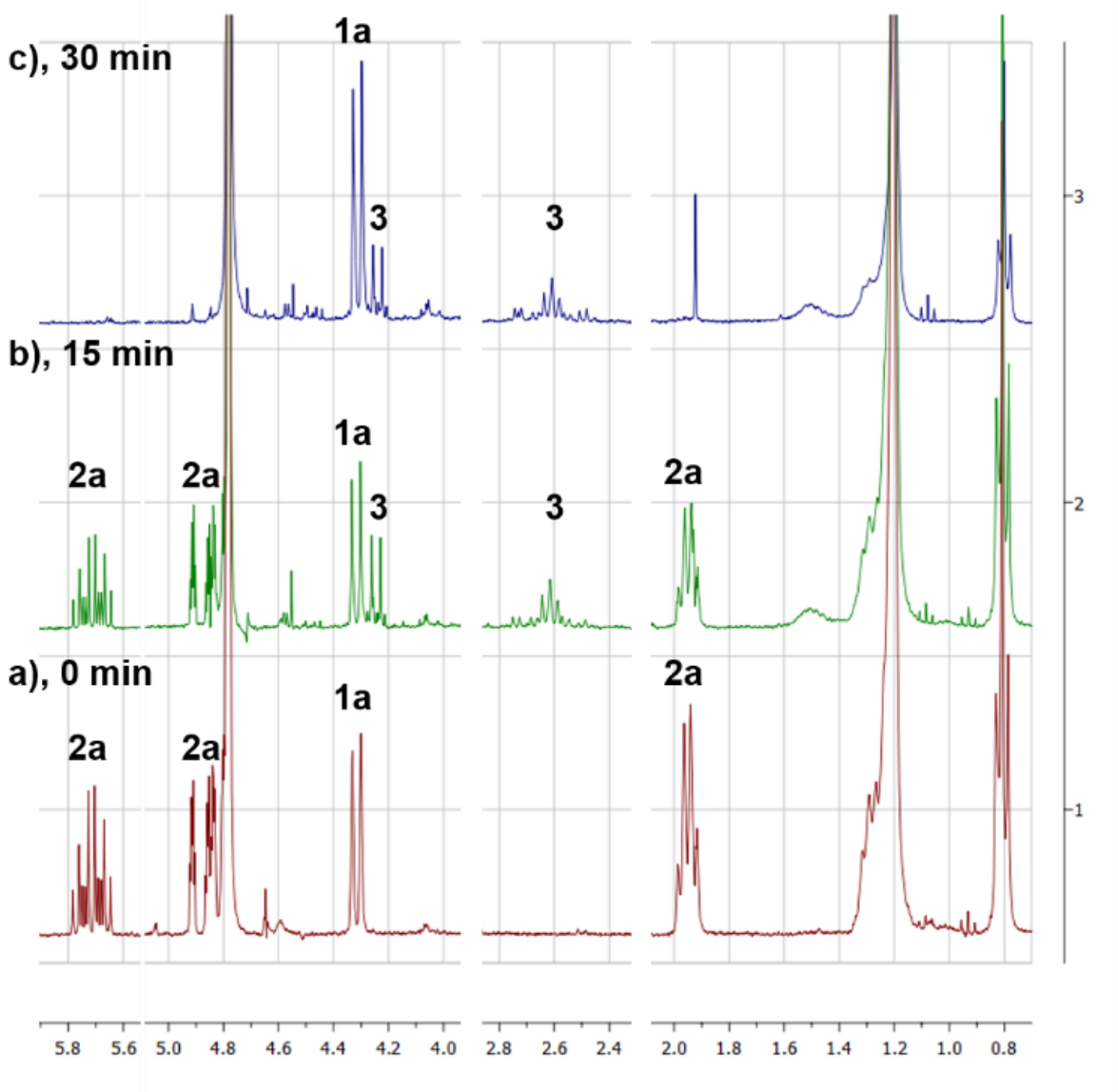


Figure S1. Periodic ^{1}H NMR (300 MHz, CD_3OD) monitoring of the formation of product **3** under TEC conditions.

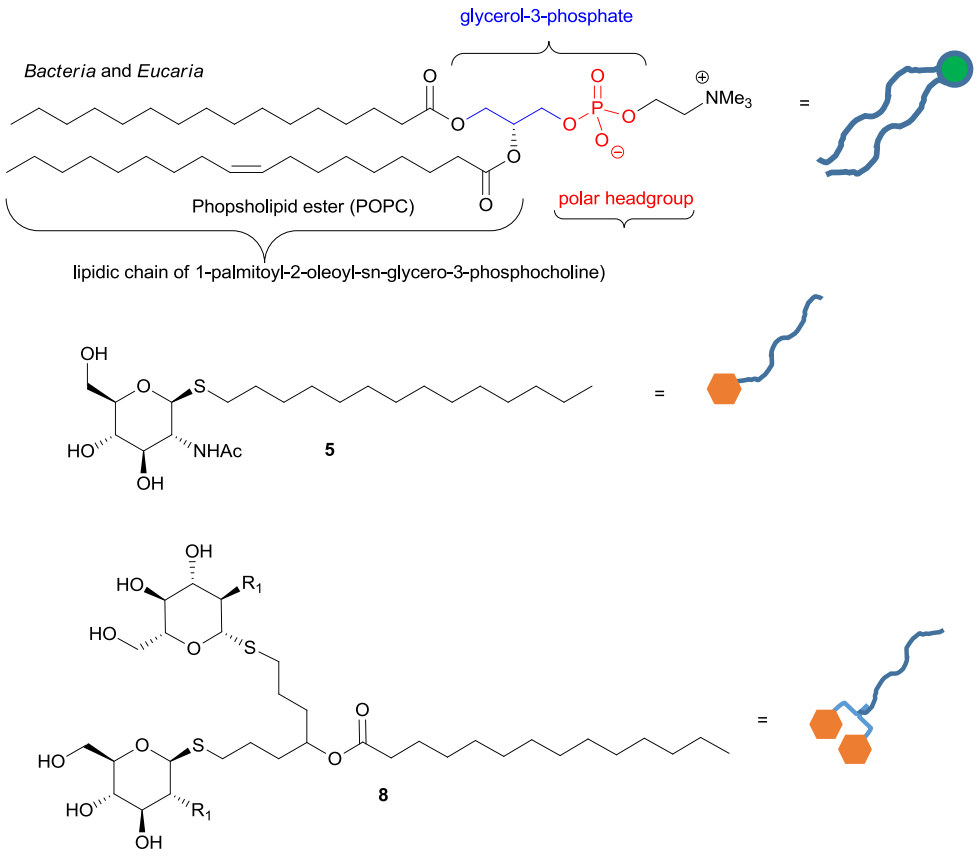


Figure S2. Graphical representation of the amphiphiles used in this research.

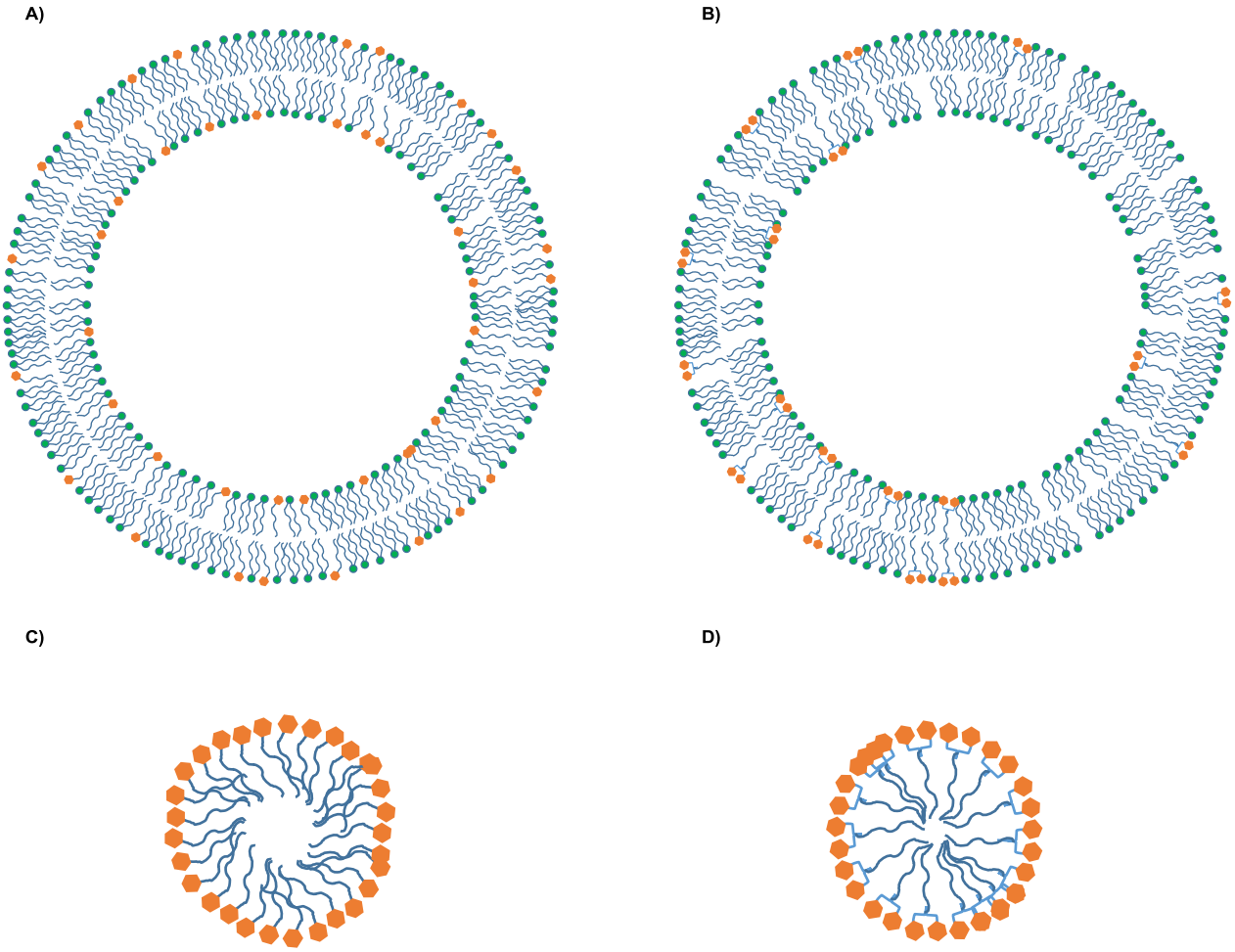


Figure S3. Graphical representation (not in scale) of the giant vesicles (A and B) and of the micelles (C and D) obtained by hydration of a thin film of POPC, **5** and **8** or suspending **5** or **8** in PBS buffer at pH 7.4.

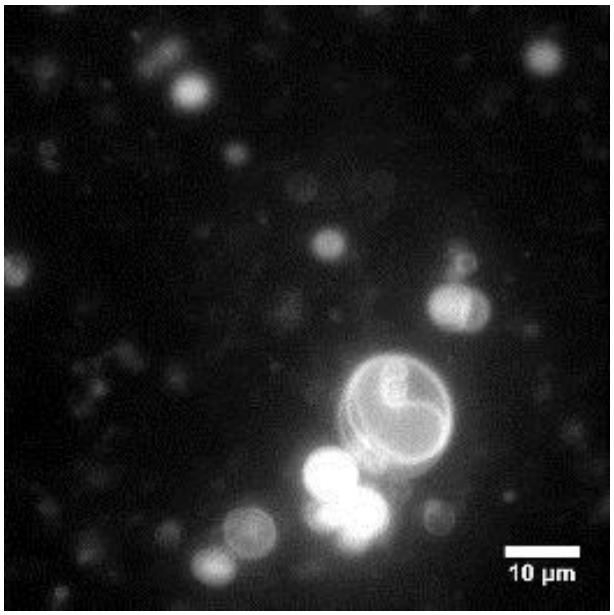


Figure S4. Picture of multilamellar GVs obtained by hydrating pure POPC in PBS buffer at pH 7.4. The sample was stained with Nile Red® (1 mM in DMSO, 1 µL, $\lambda_{[excit]}$ = 561 nm) before the microscopic observation. This structure is very similar to that observed by Holst et al., (Reference 1, page B5) and to that reported in Figure 3 of the present article.

2. Additional docking experiments figures

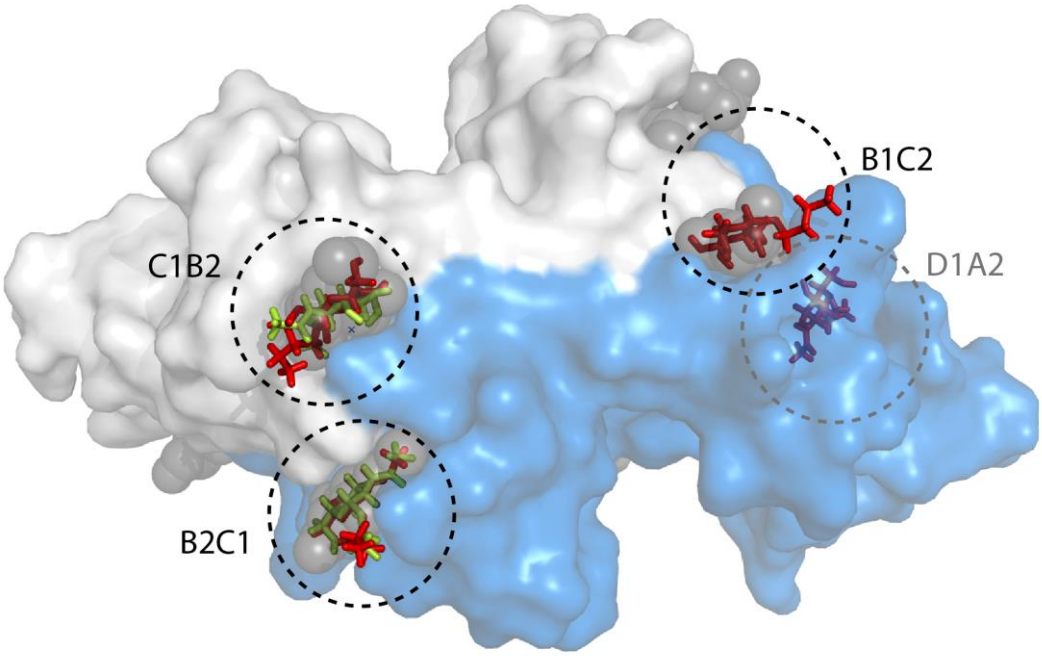


Figure S5: Main poses obtained for docking of **$5C_2$** (green) and **$5C_4$** (red) on 2UVO. GlcNAc are positioned as transparent grey spheres. Ligands are principally recovered on primary binding sites (C1B2, B2C1 and B1C2) and less frequently on the secondary binding site D1A2.

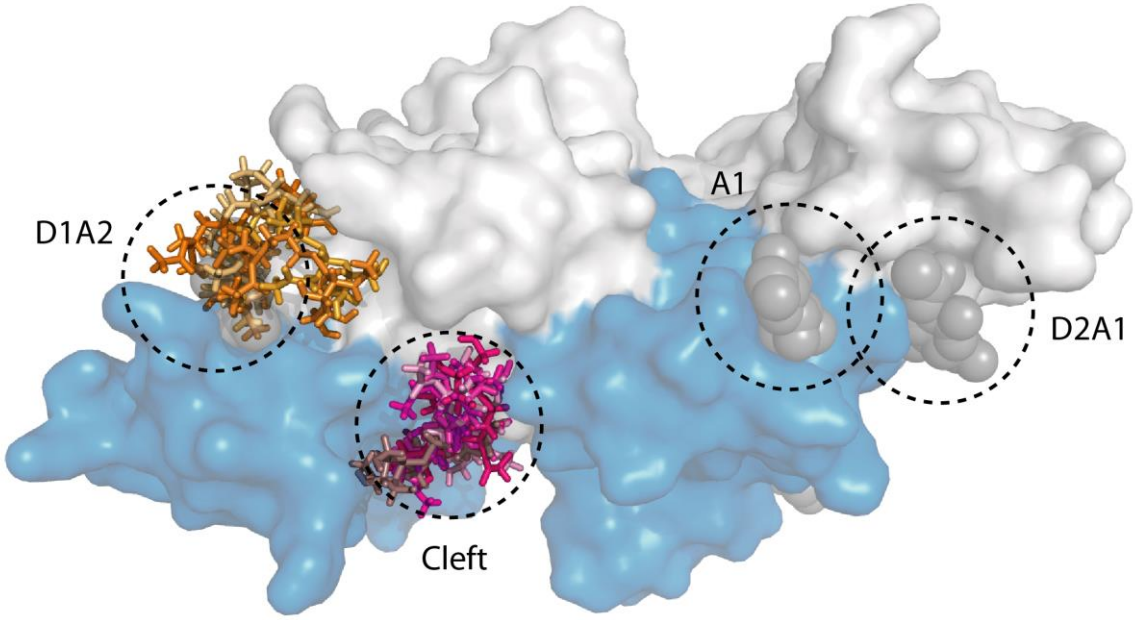
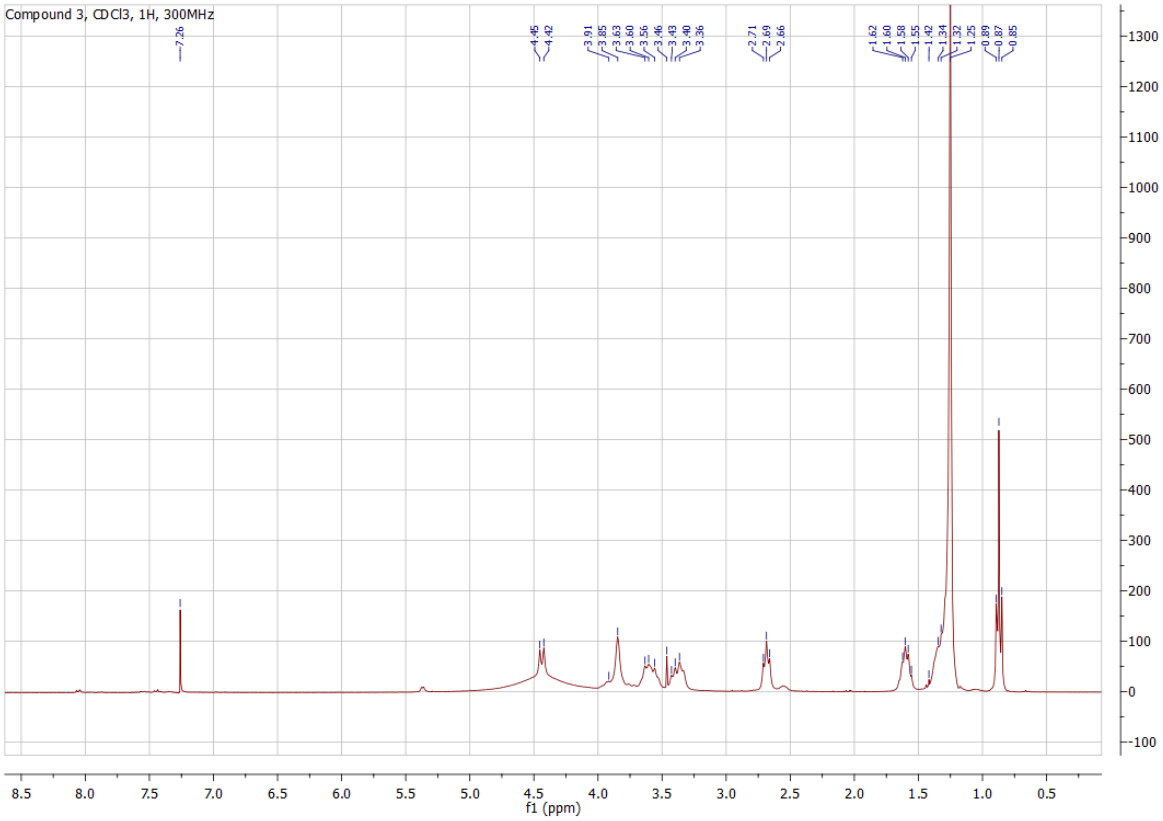
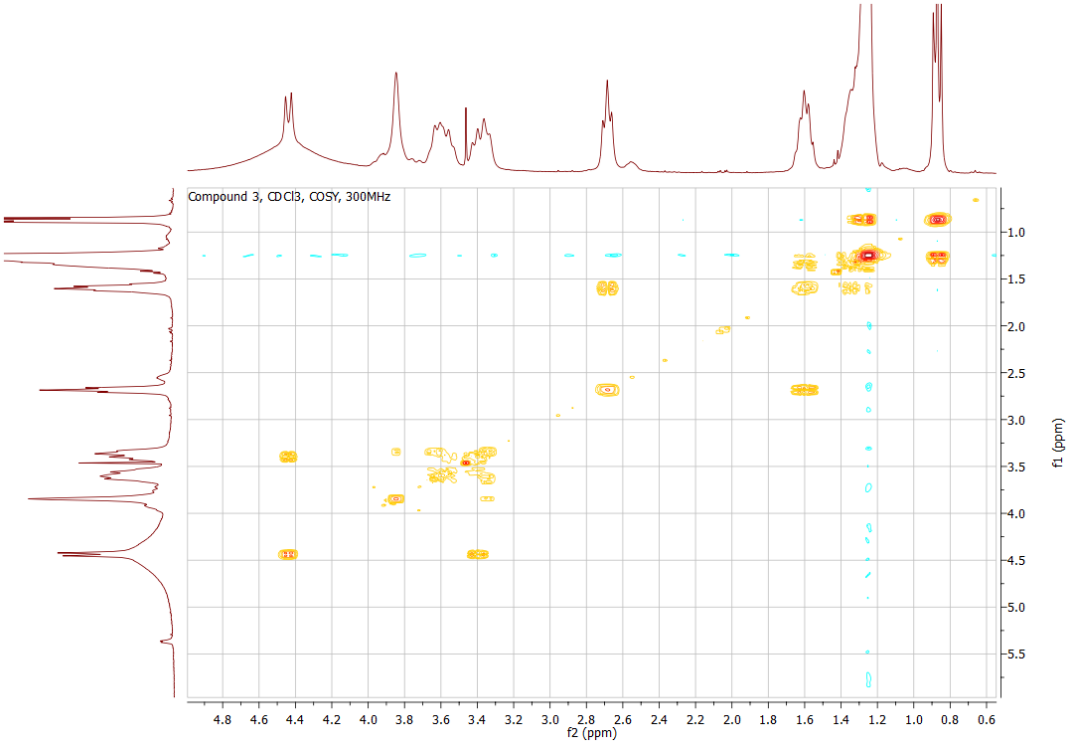


Figure S6: Main poses obtained for docking of **8C$_2$** on 2UVO. GlcNAc are positioned as transparent grey spheres. Positions found on the D1A2 are shown as orange sticks while the position found in the cleft between the two WGA monomers are in pink-purple sticks.

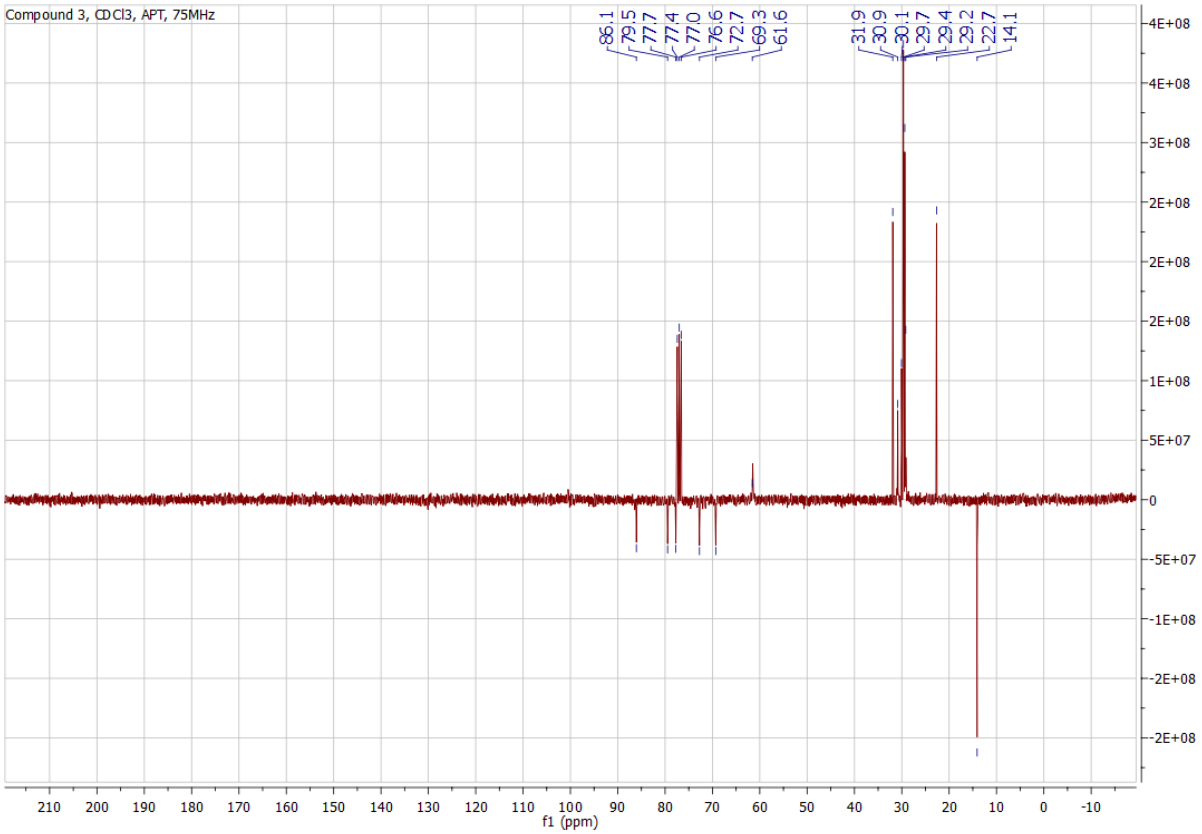
3. Spectra of synthesized glycolipids



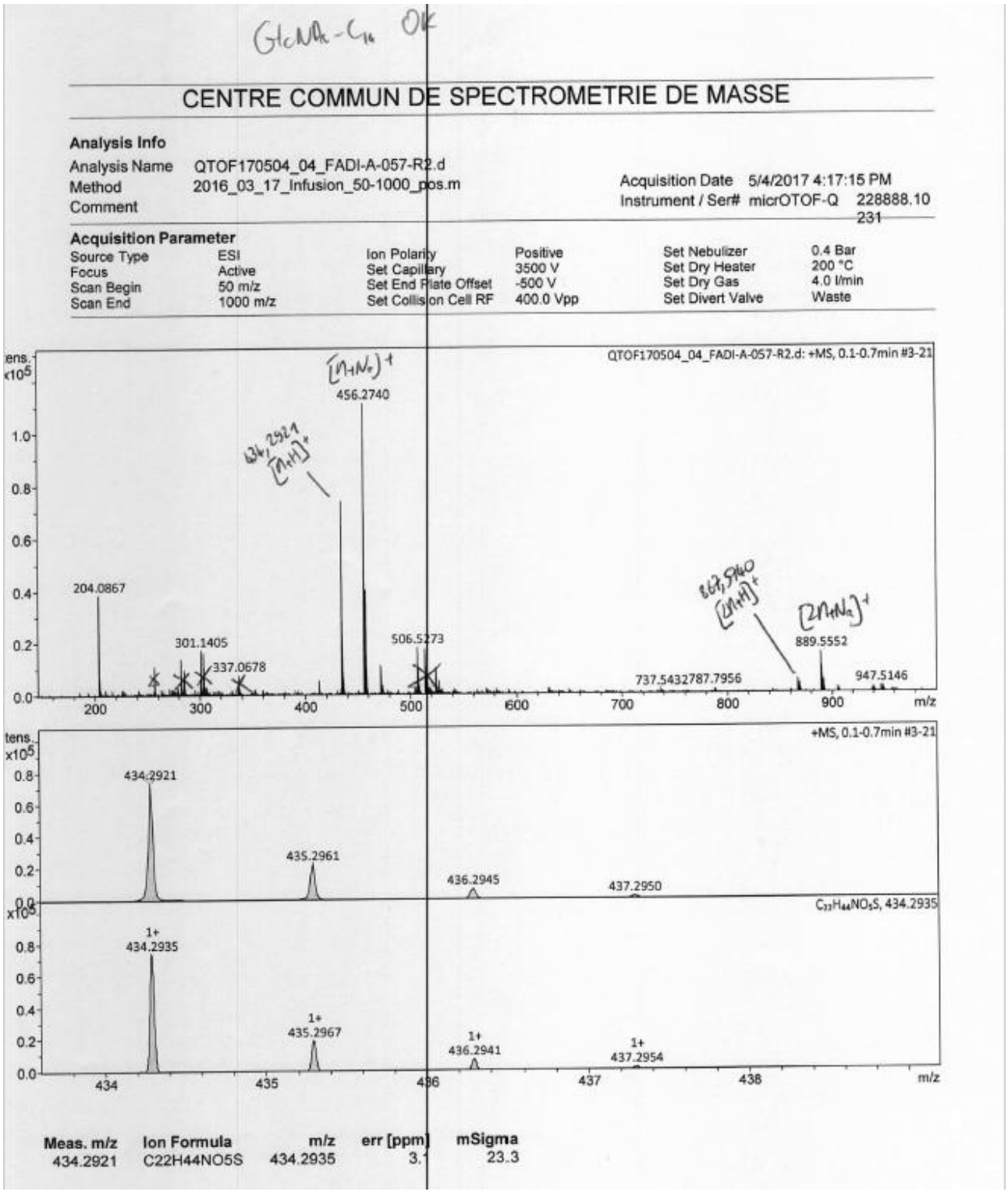
^{1}H NMR (300 MHz, $CDCl_3$) of compound 3



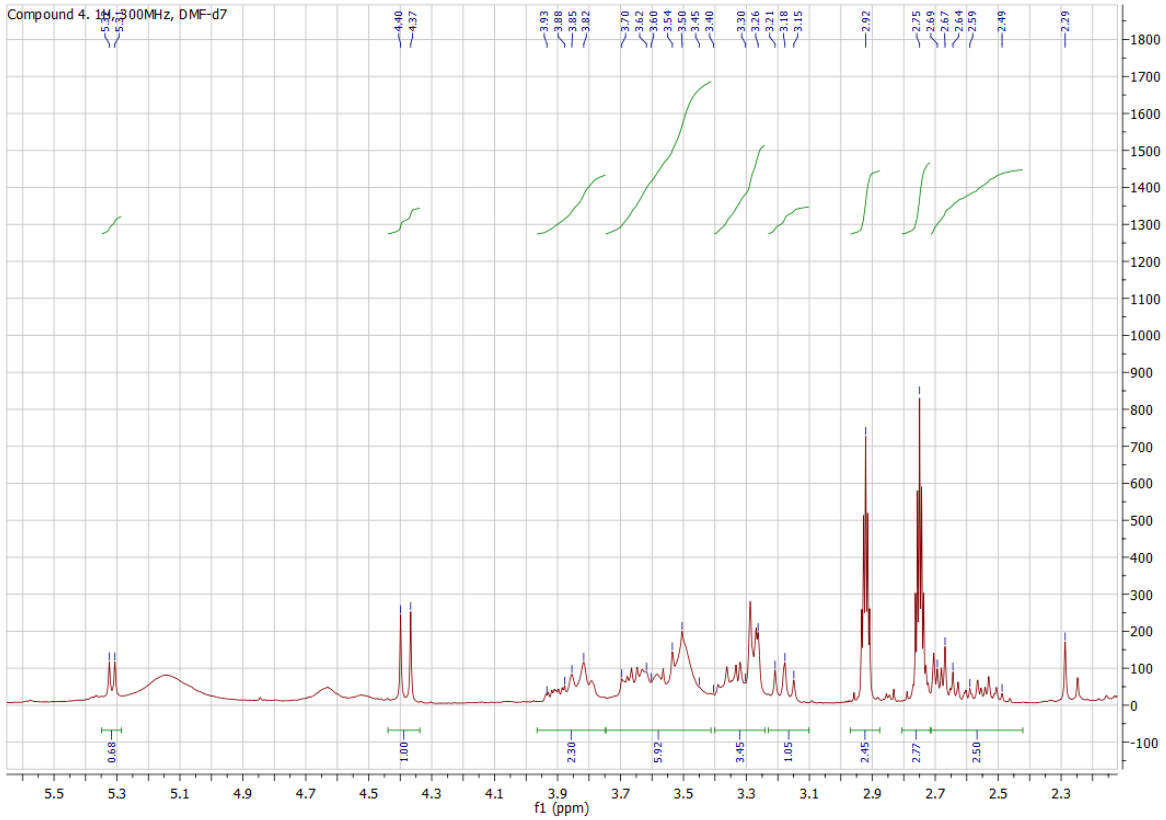
COSY (300 MHz, $CDCl_3$) of compound 3



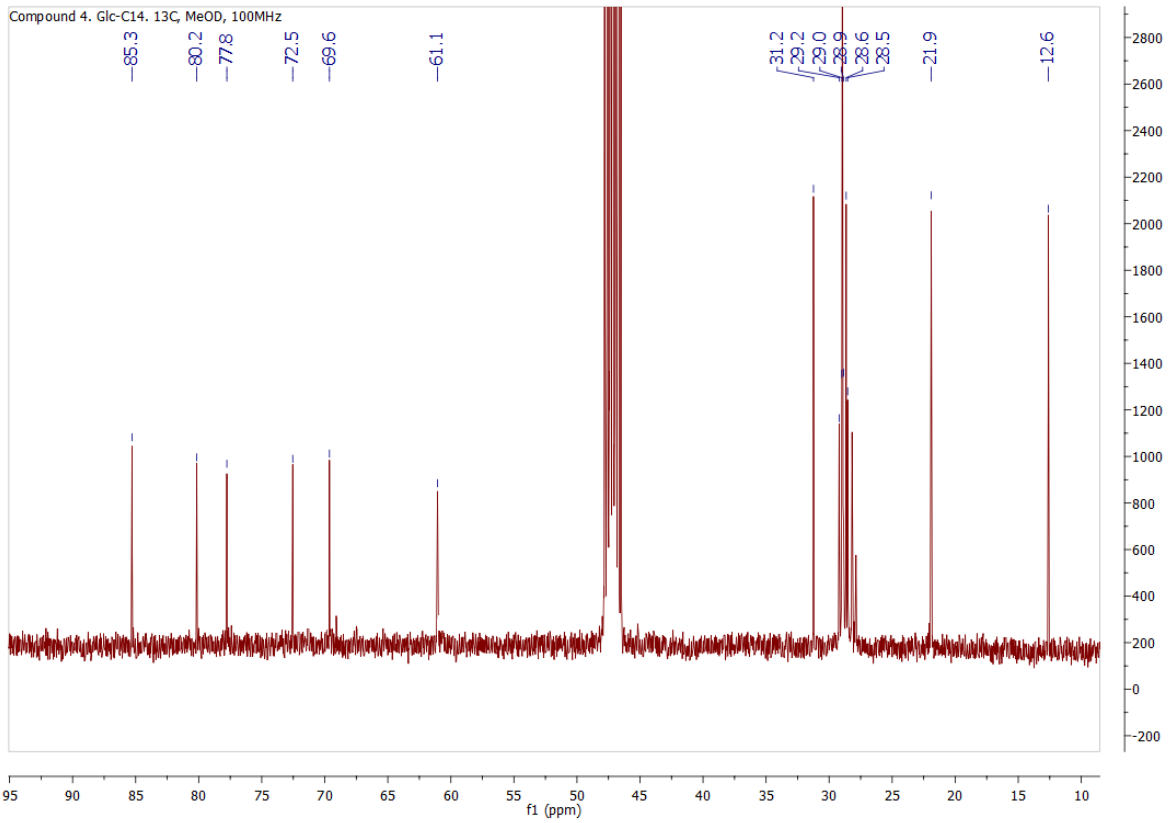
^{13}C APT (75 MHz, $CDCl_3$) of compound 3



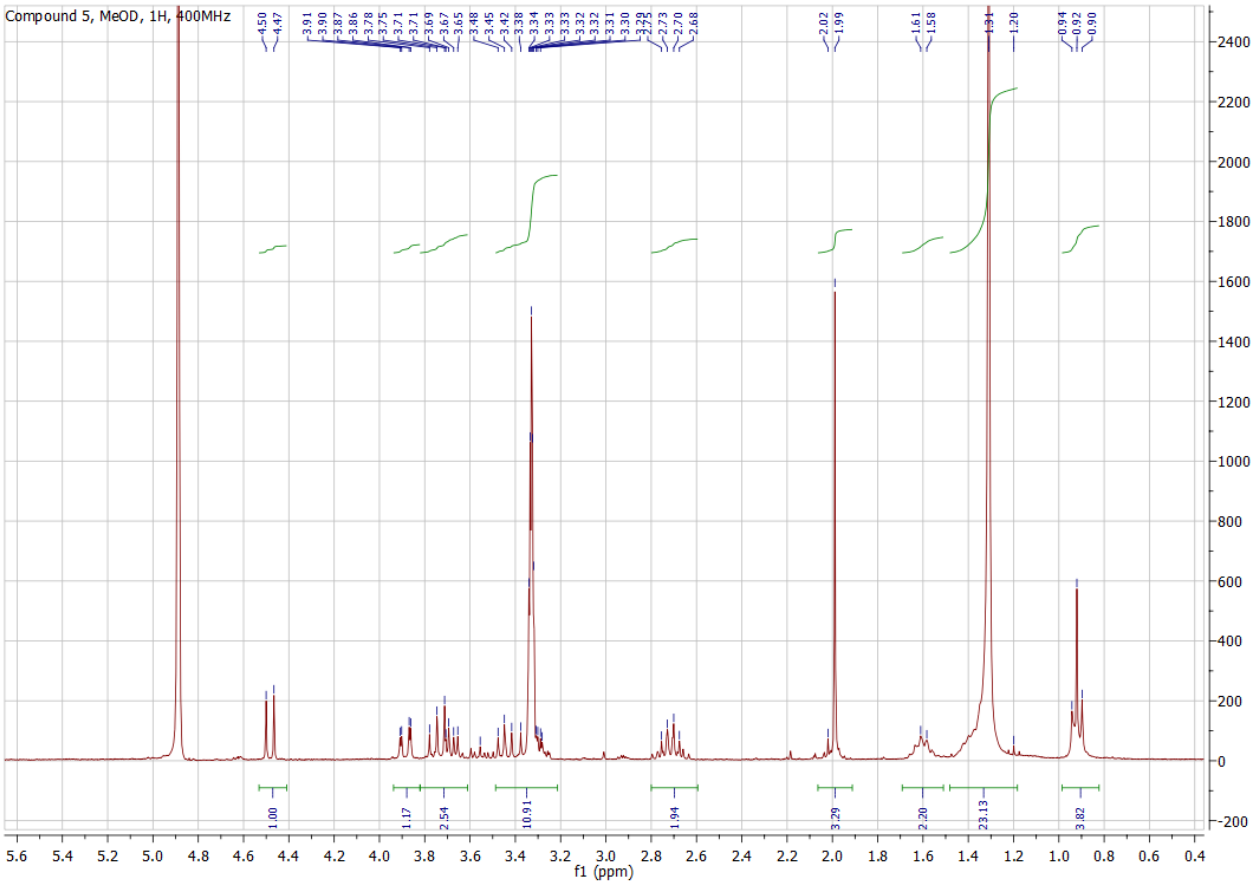
HRMS of compound 3



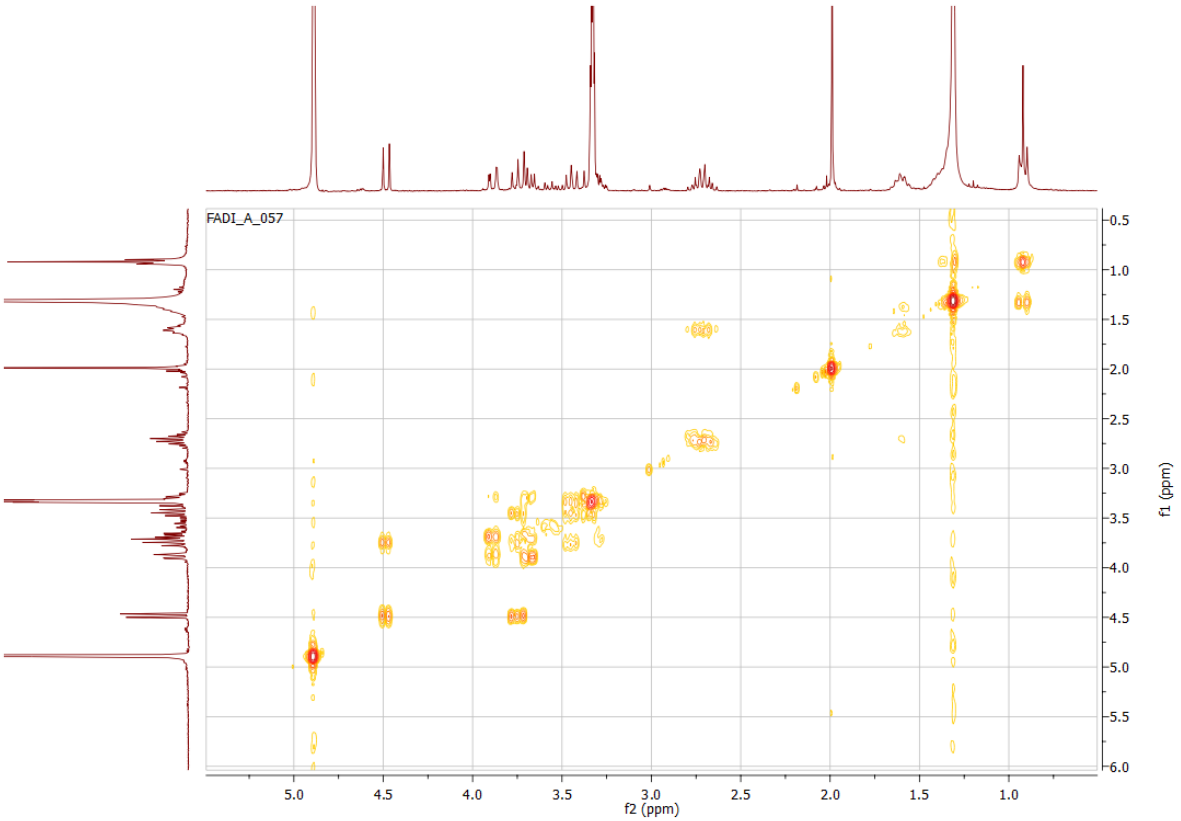
^{1}H NMR (300 MHz, DMF-d_7) of compound 4



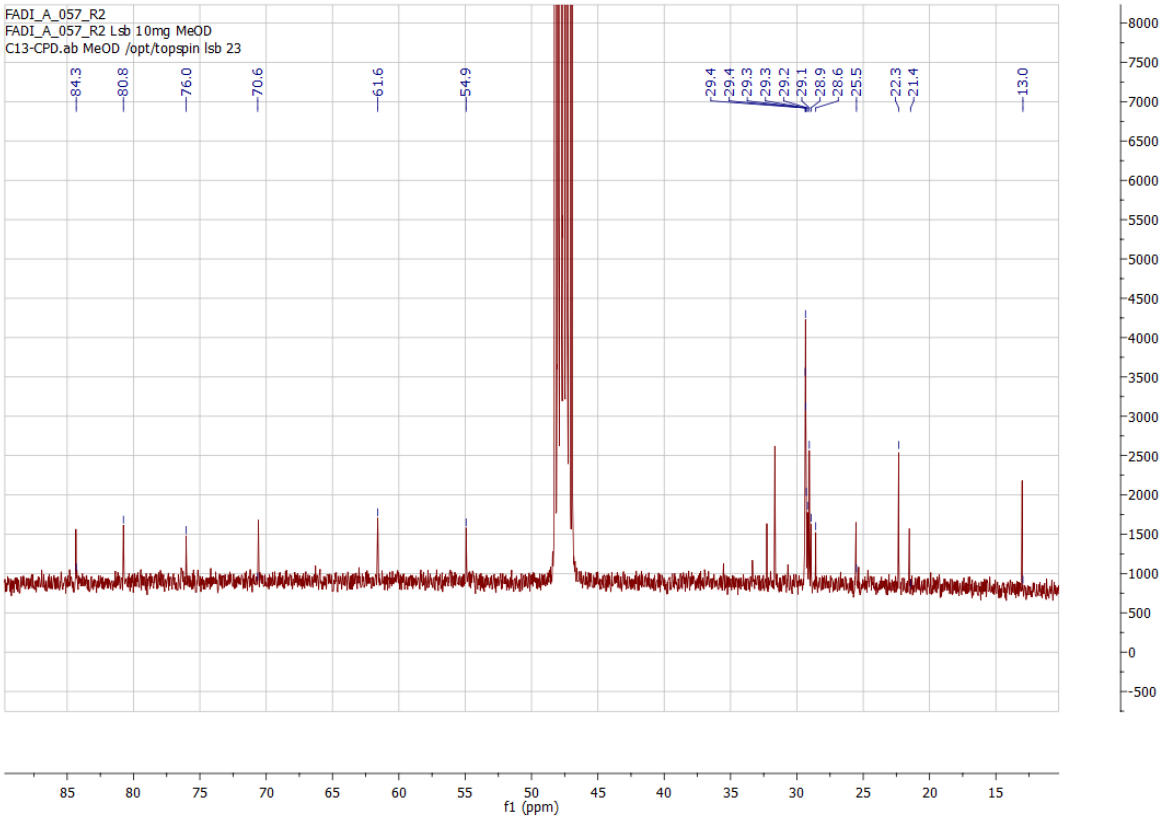
^{13}C NMR (75 MHz, CD_3OD) of compound 4



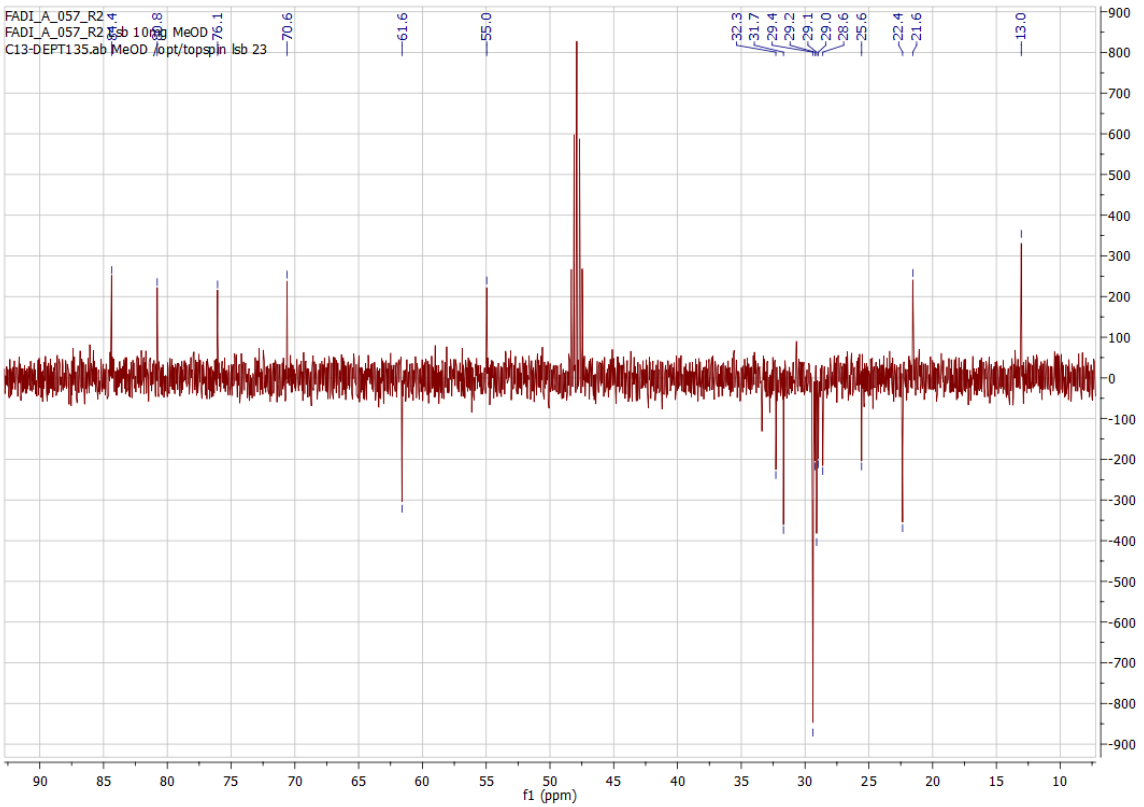
^{1}H NMR (400 MHz, CD_3OD) of compound 5



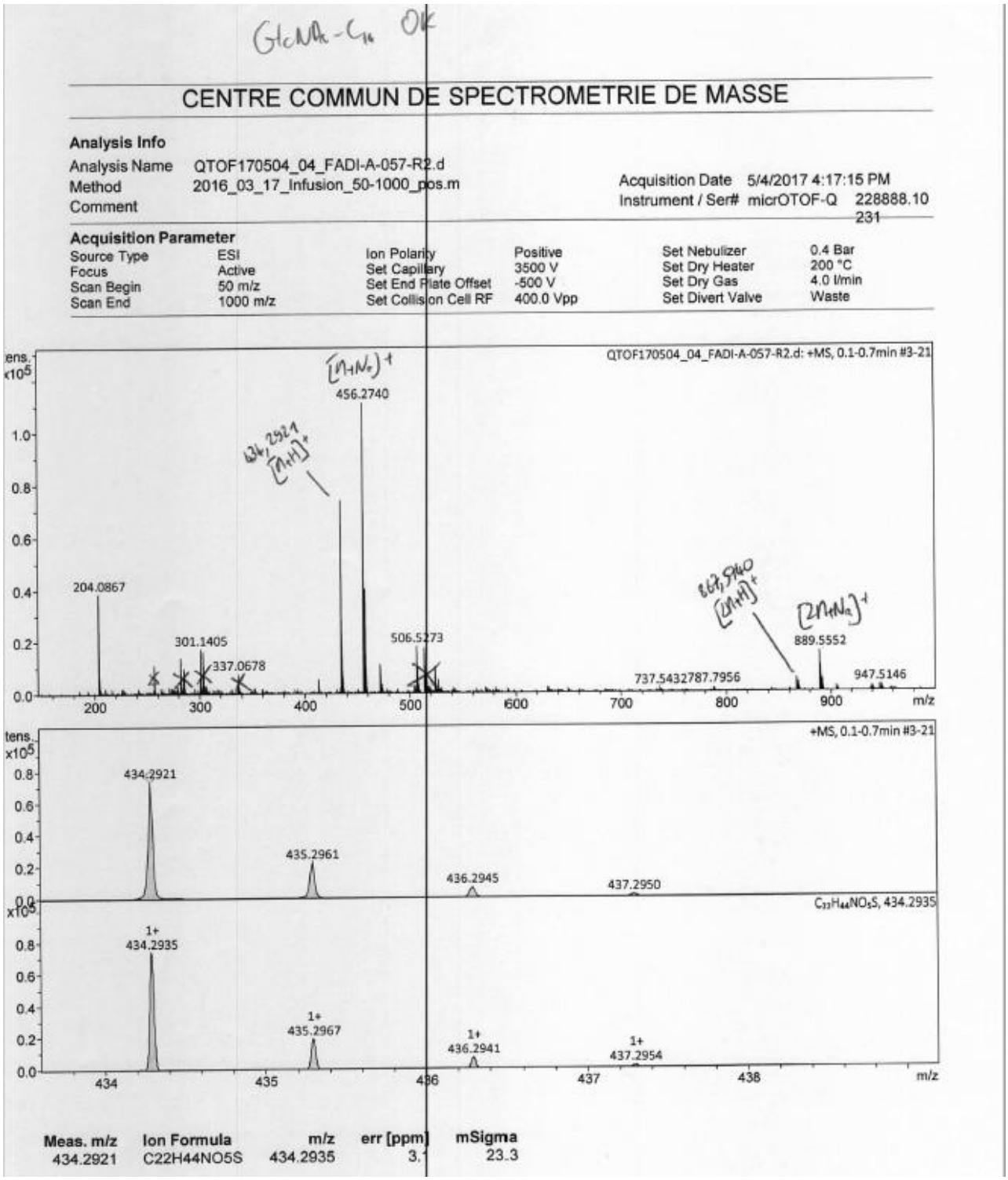
COSY (400 MHz, CD_3OD) of compound 5



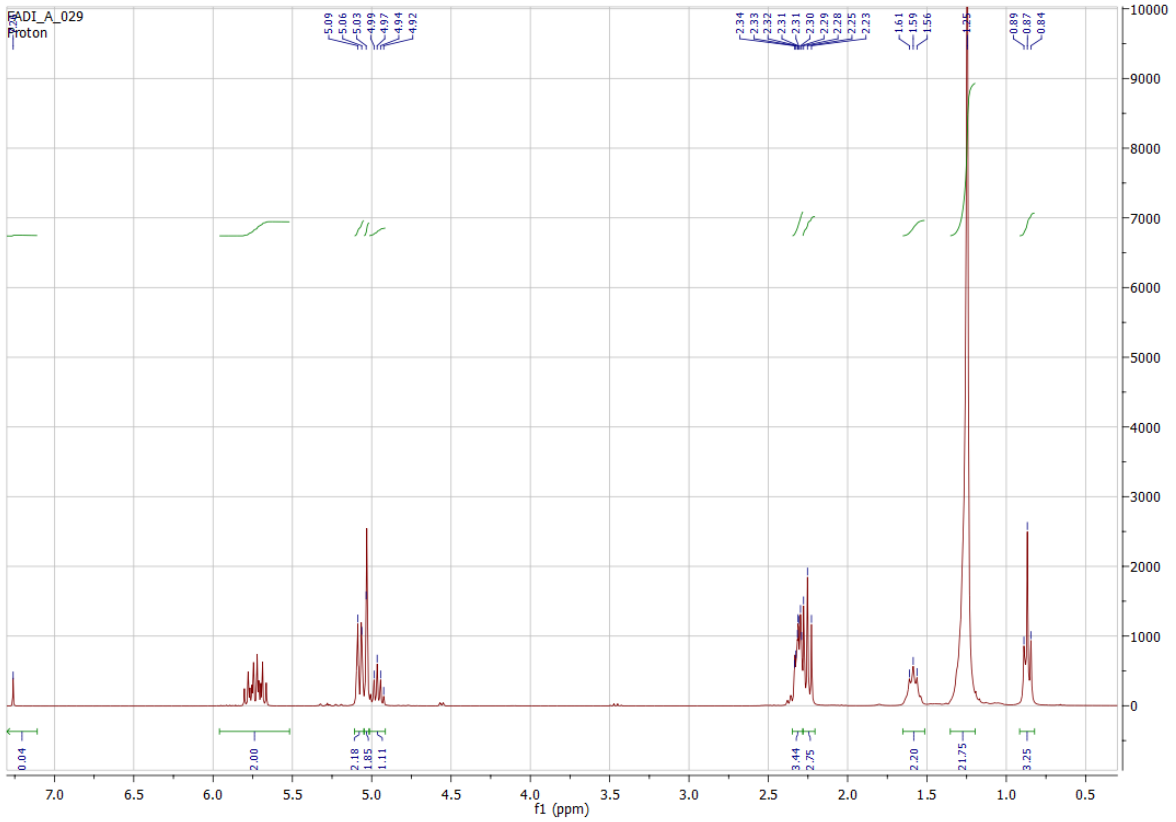
^{13}C NMR (100 MHz, CD_3OD) of compound 5



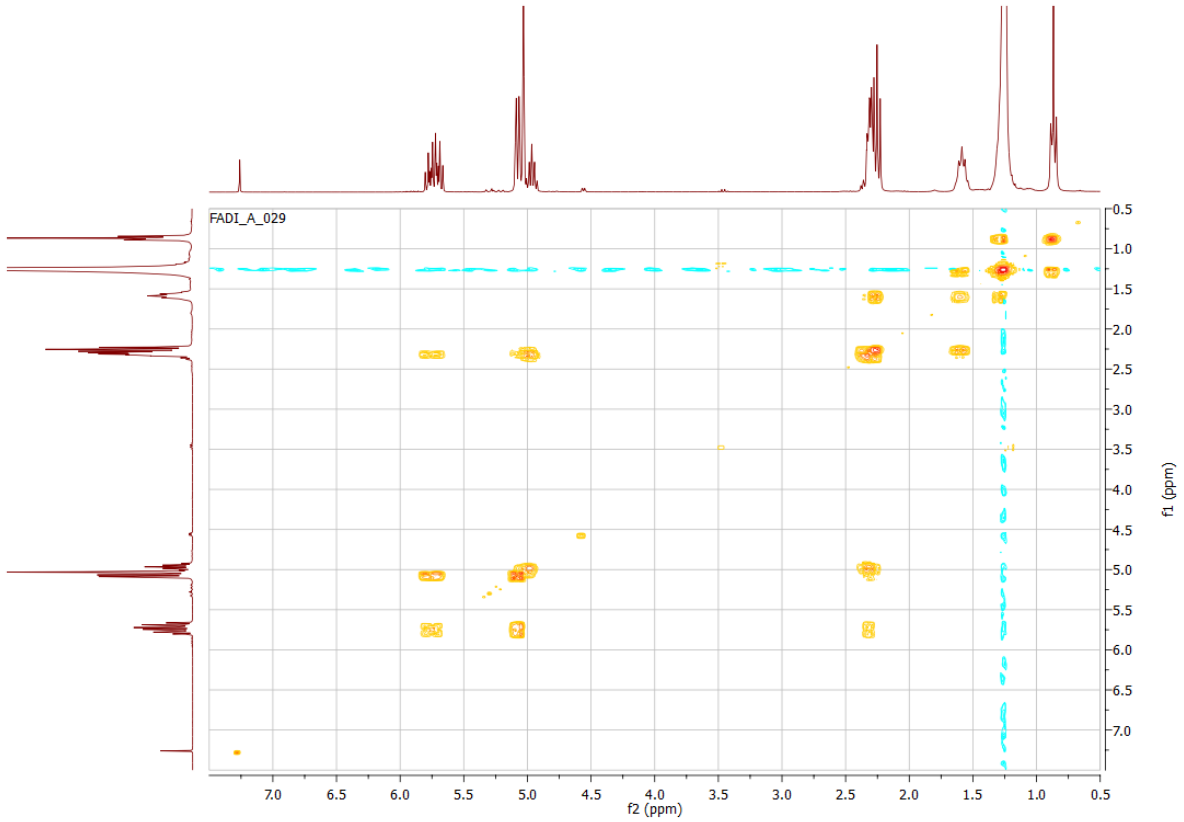
DEPT (100 MHz, CD_3OD) of compound 5



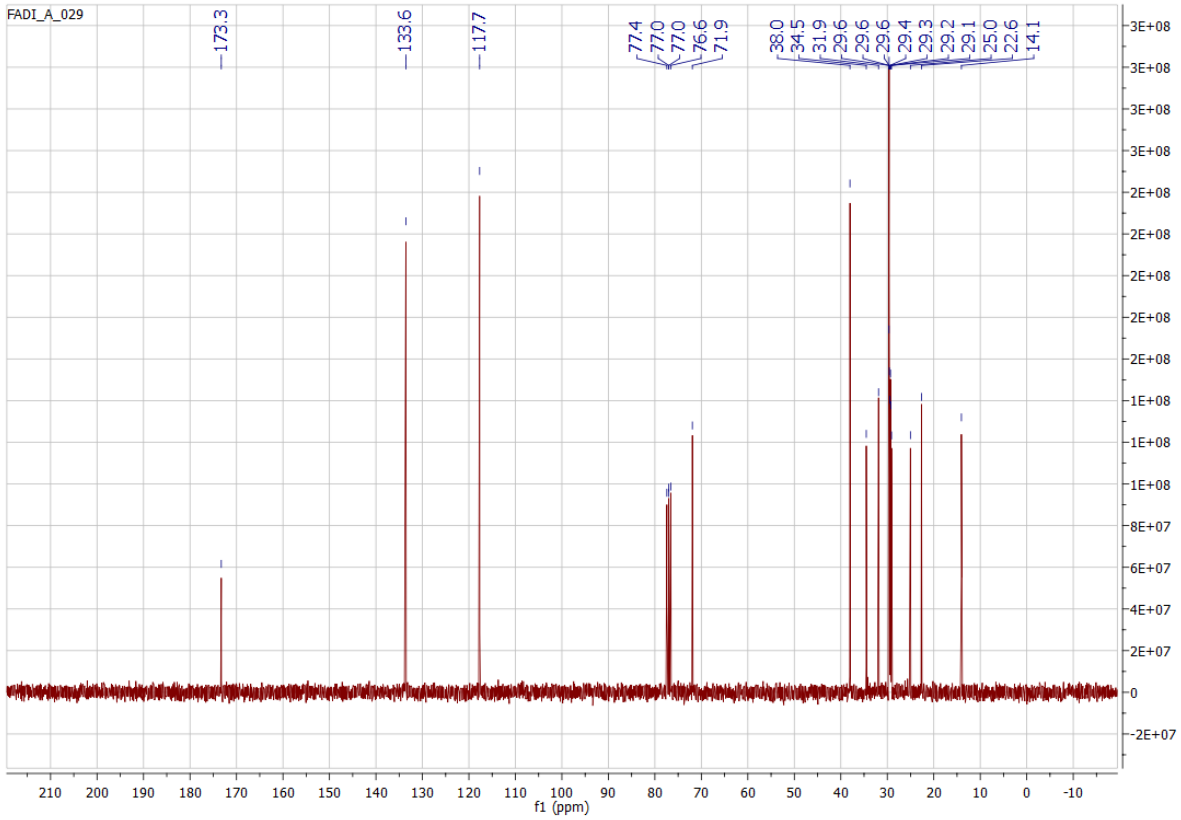
HRMS of compound 5



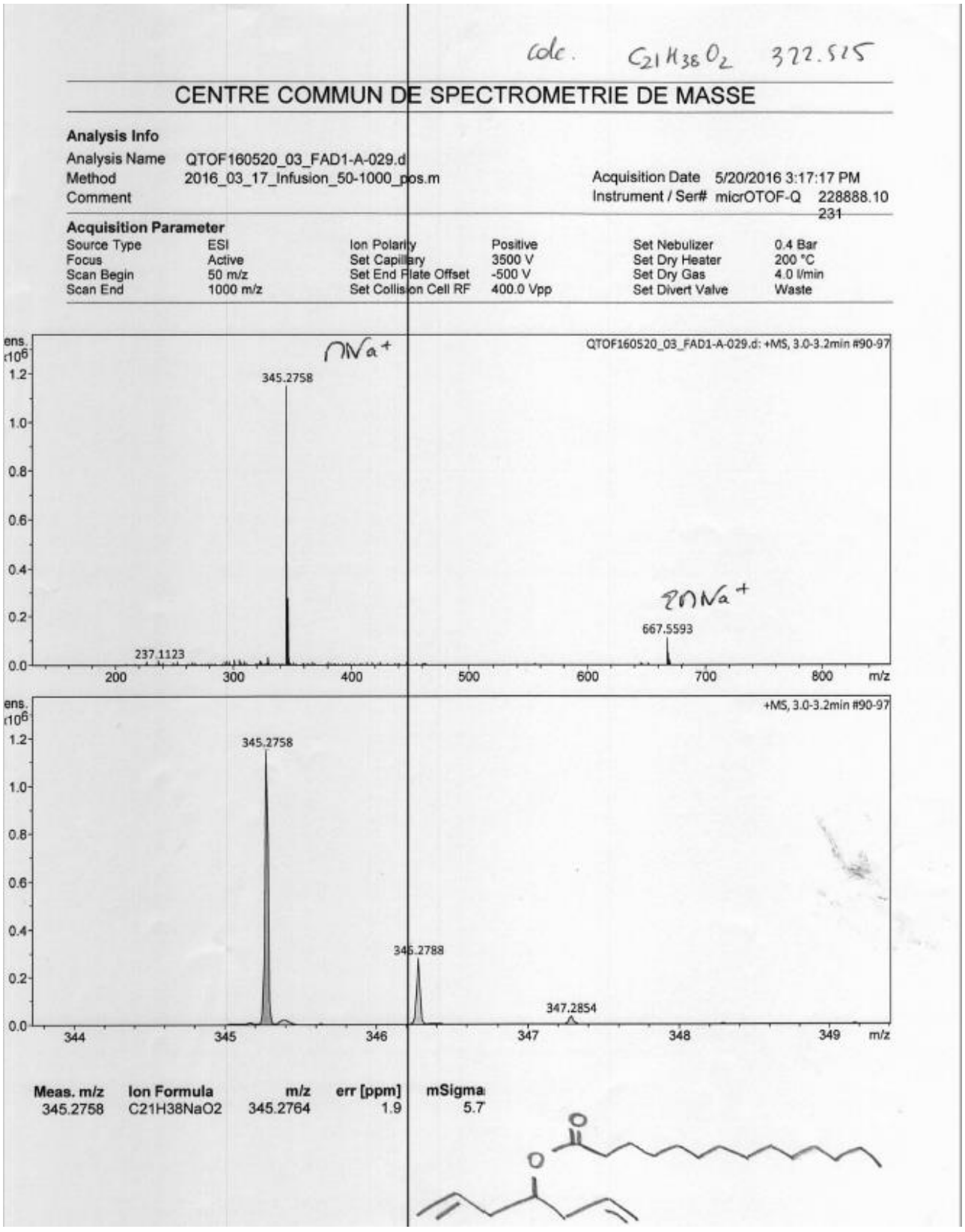
^{1}H NMR (300 MHz, $CDCl_3$) of compound 6



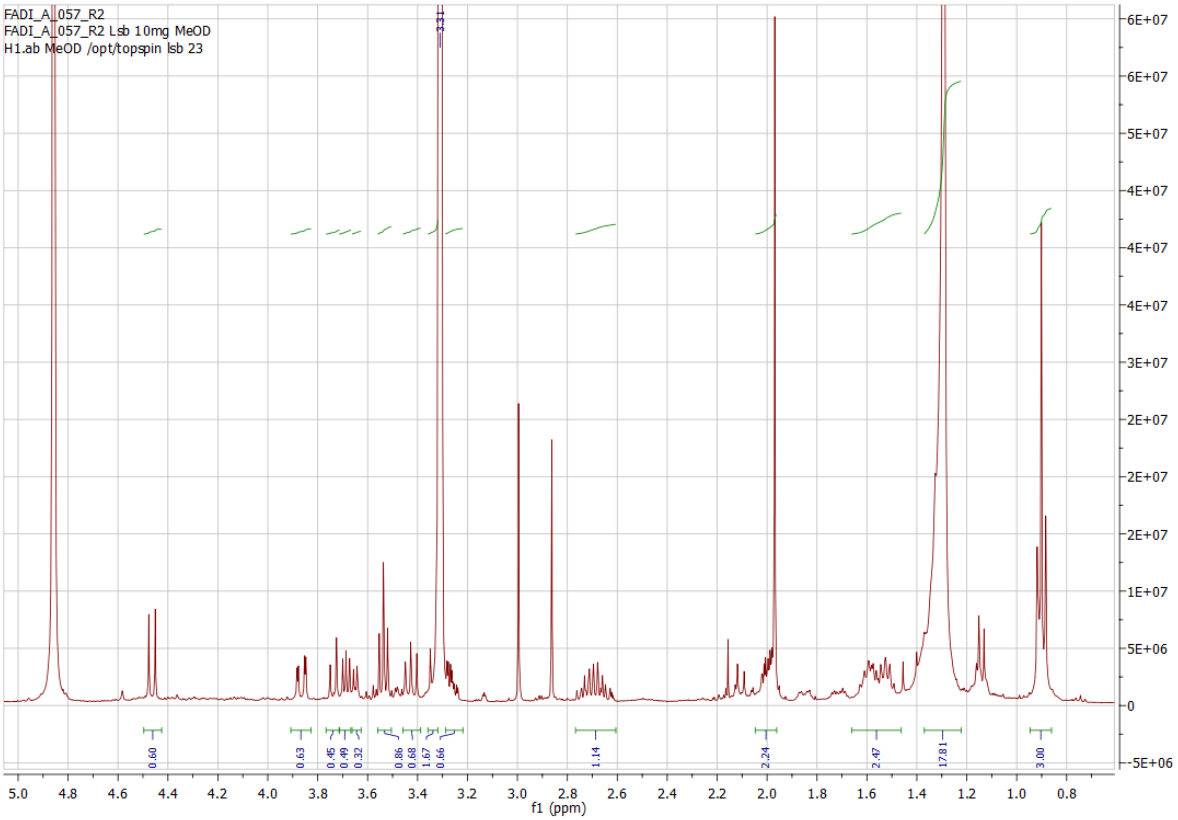
COSY (300 MHz, $CDCl_3$) of compound 6



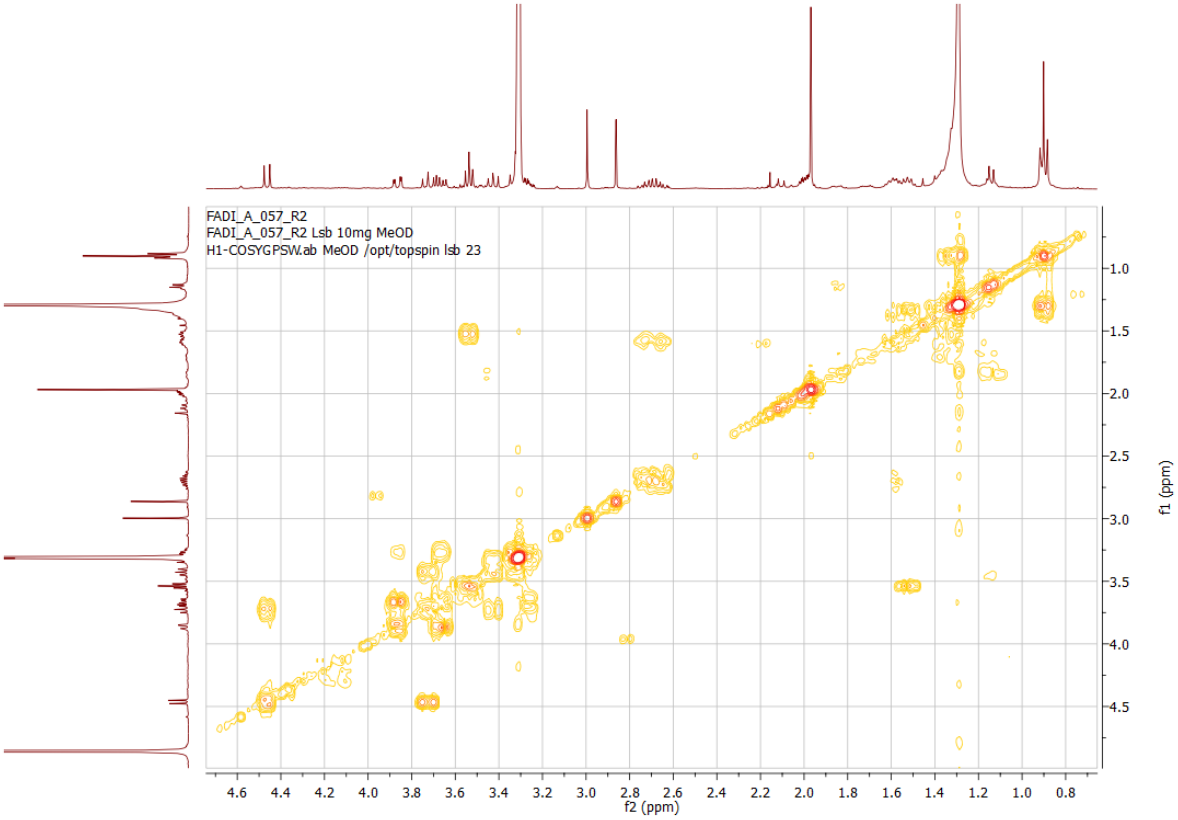
^{13}C NMR (75 MHz, $CDCl_3$) of compound 6



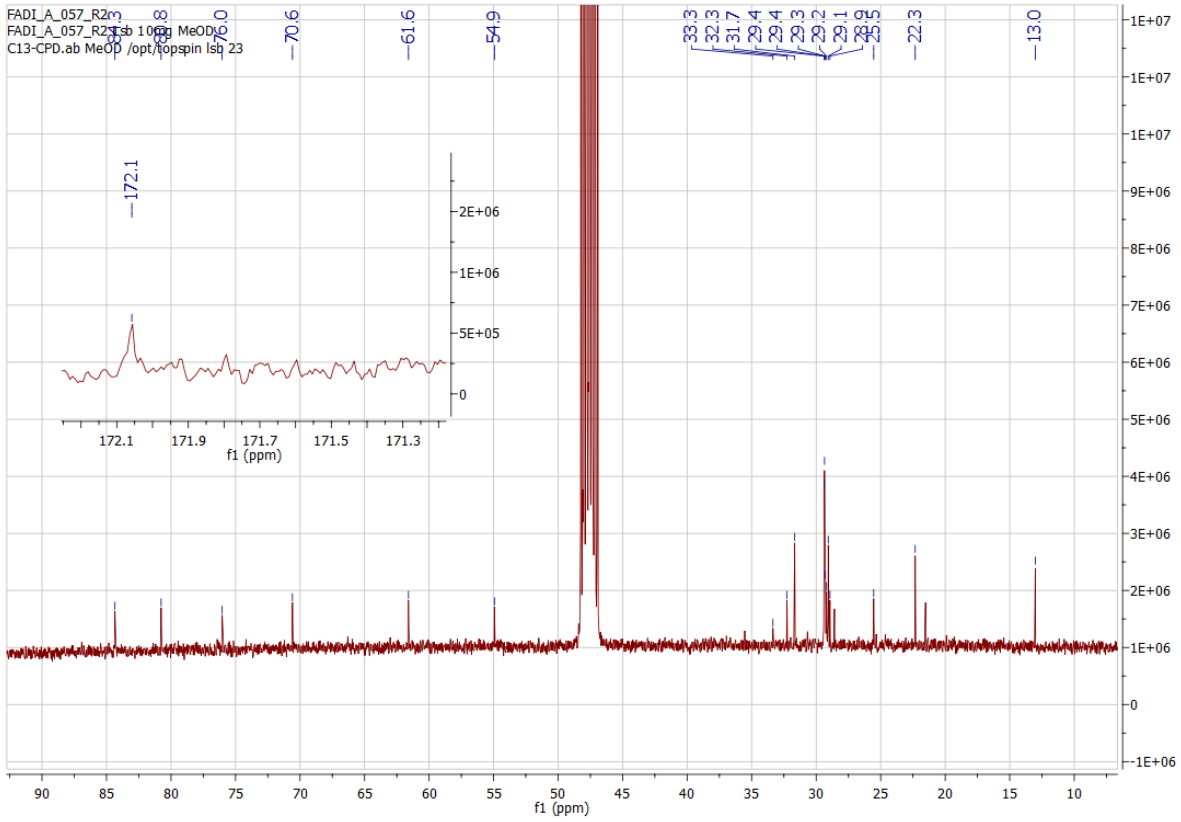
HRMS of compound 6



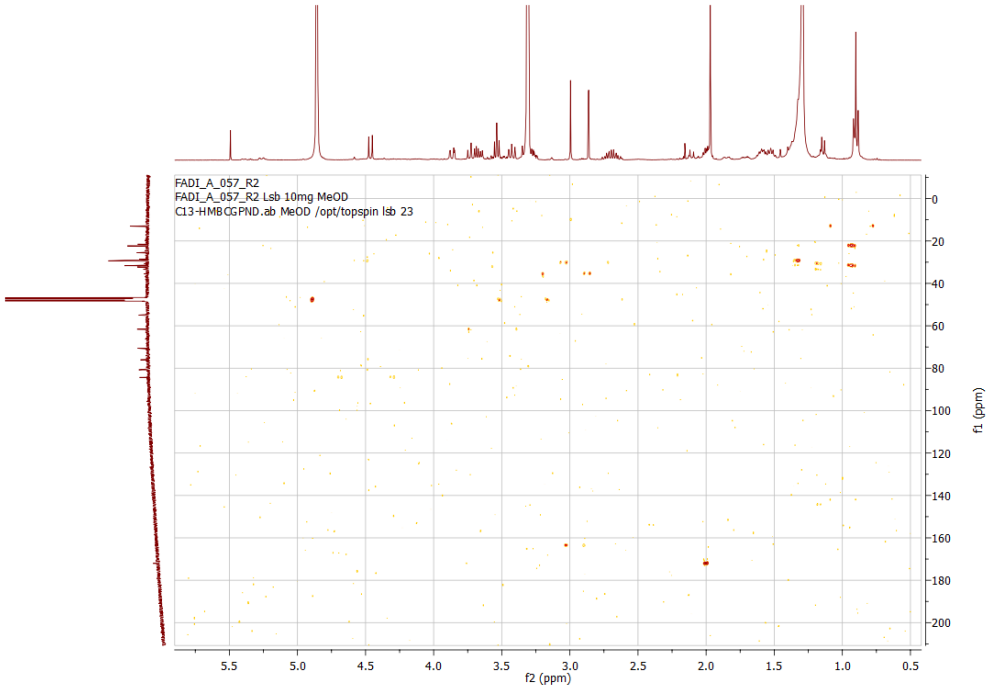
^{1}H NMR (400 MHz, CD_3OD) of compound 7



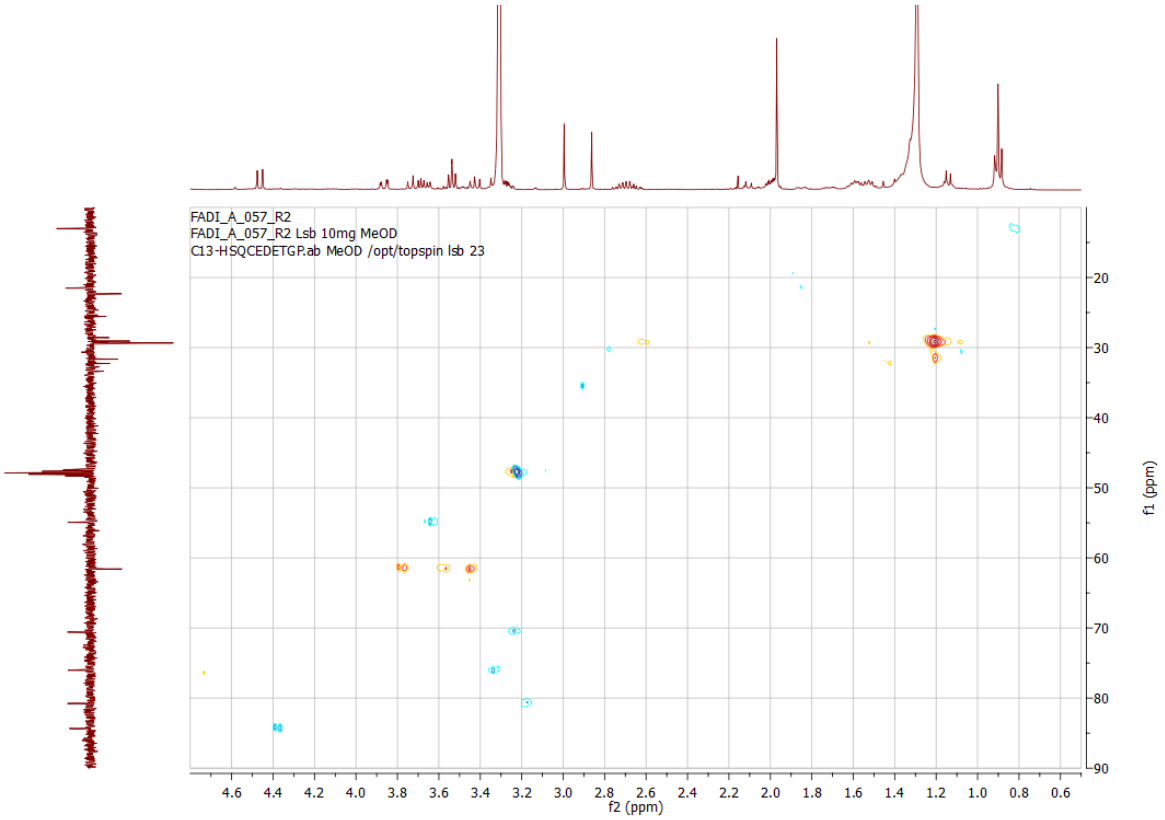
COSY (400 MHz, CD_3OD) of compound 7



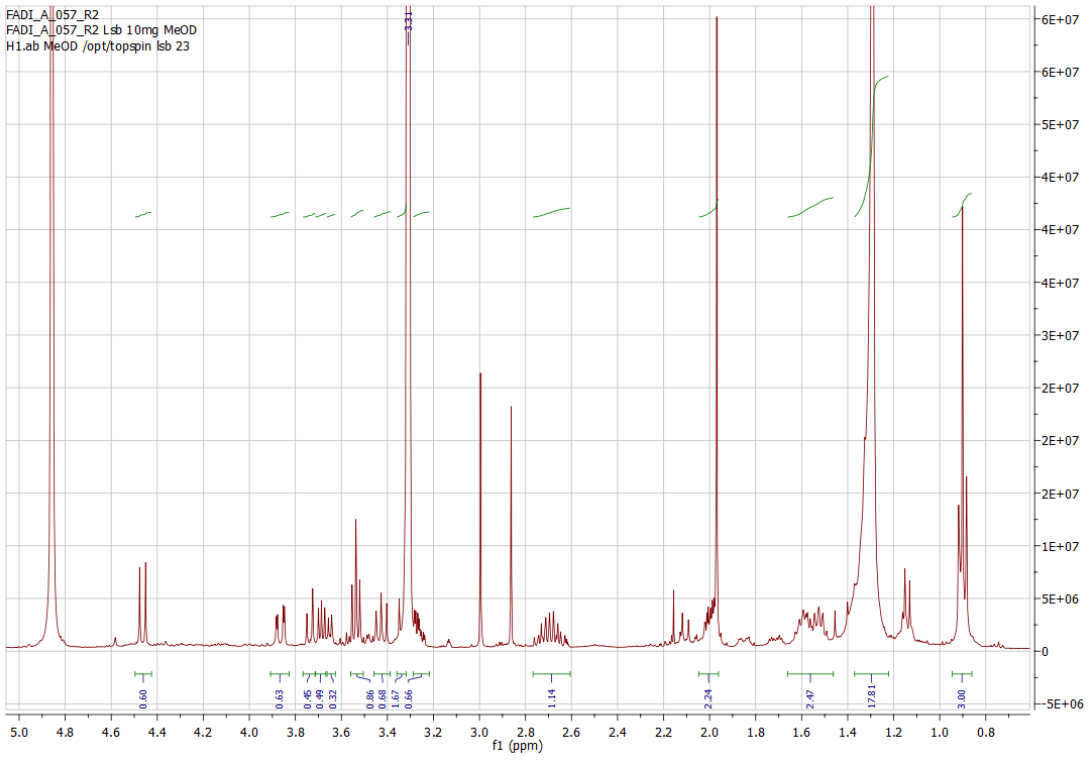
^{13}C NMR (100 MHz, $CDCl_3$) of compound 7



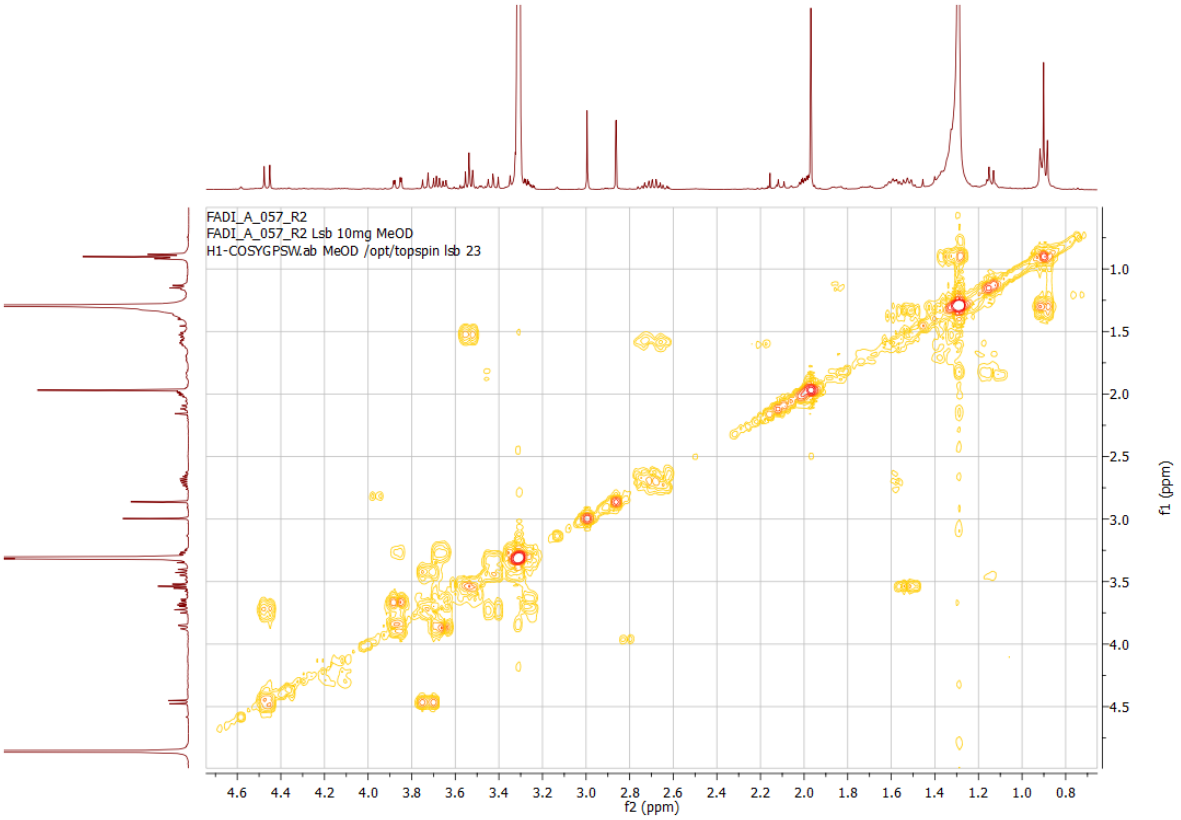
HMBC ($CDCl_3$) of compound 7



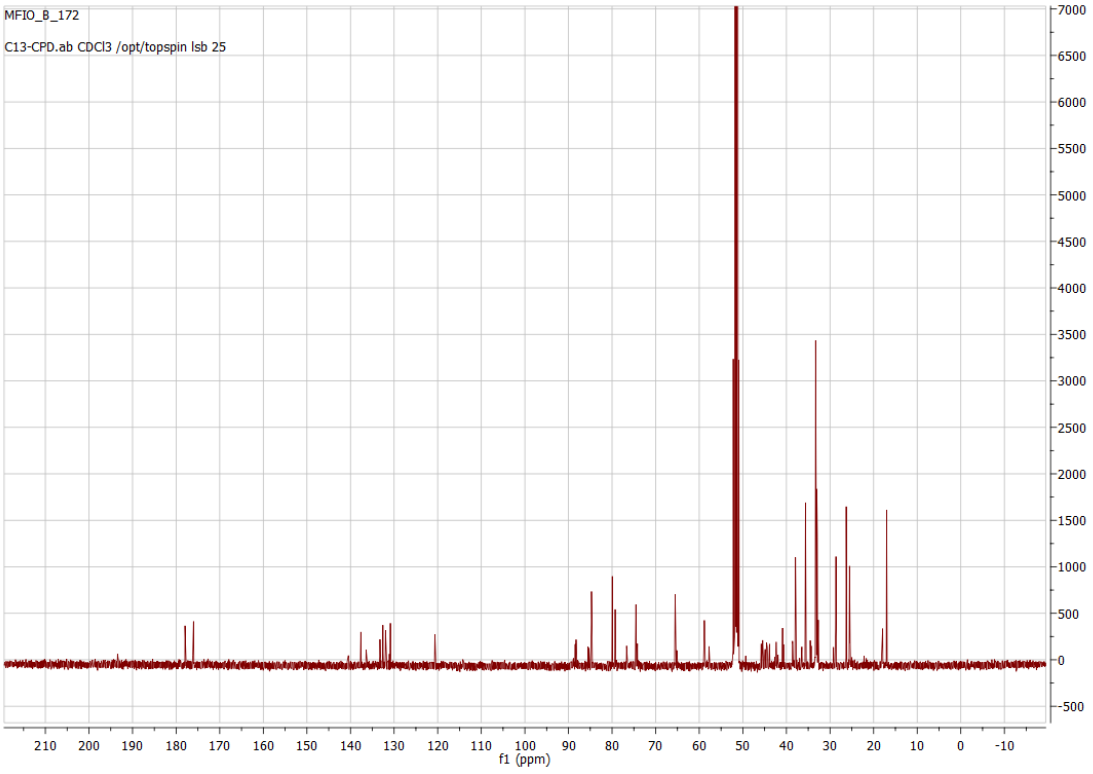
HSQC ($CDCl_3$) of compound 7



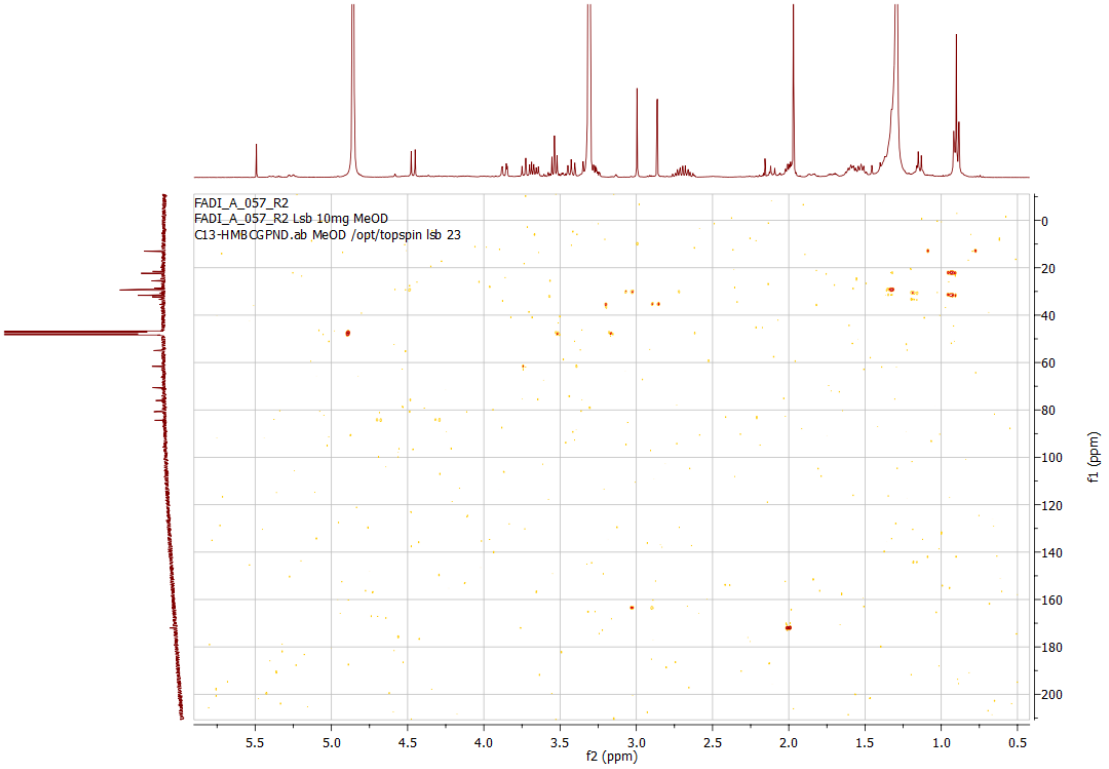
^{1}H NMR (400 MHz, CD_3OD) of compound 8



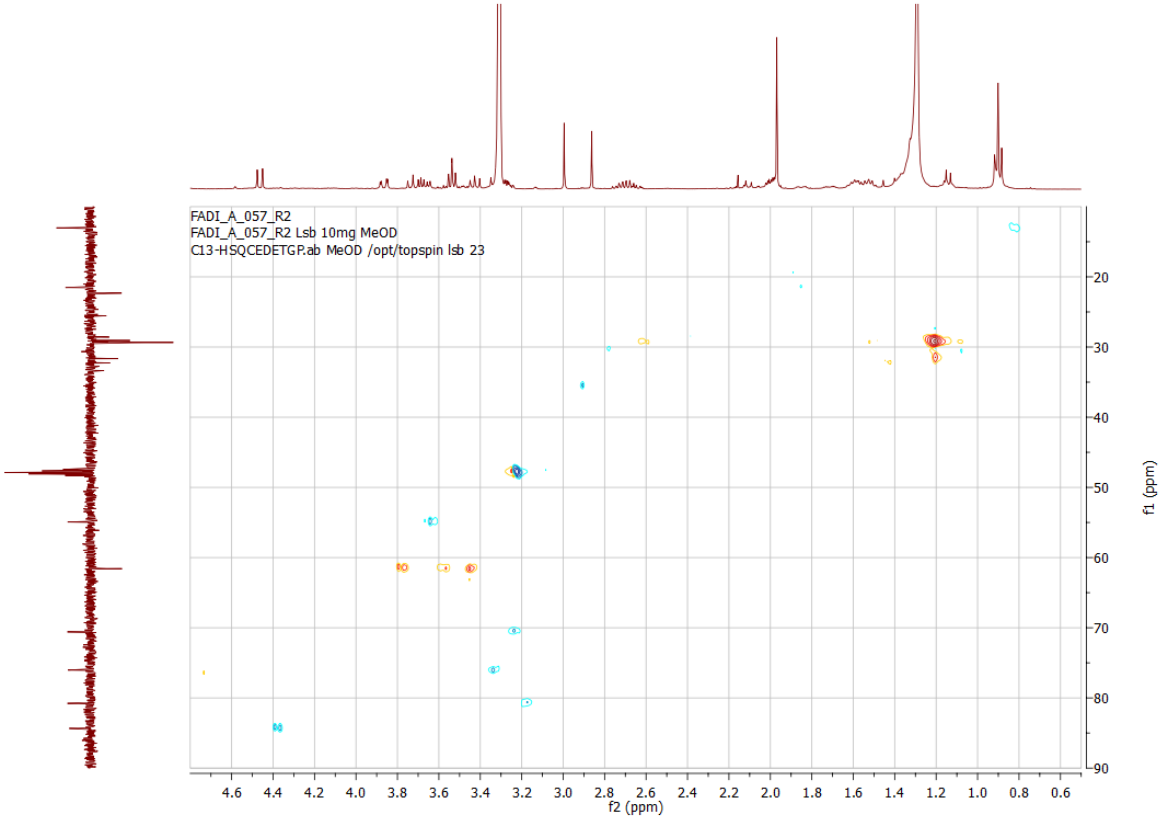
COSY (400 MHz, CD_3OD) of compound 8



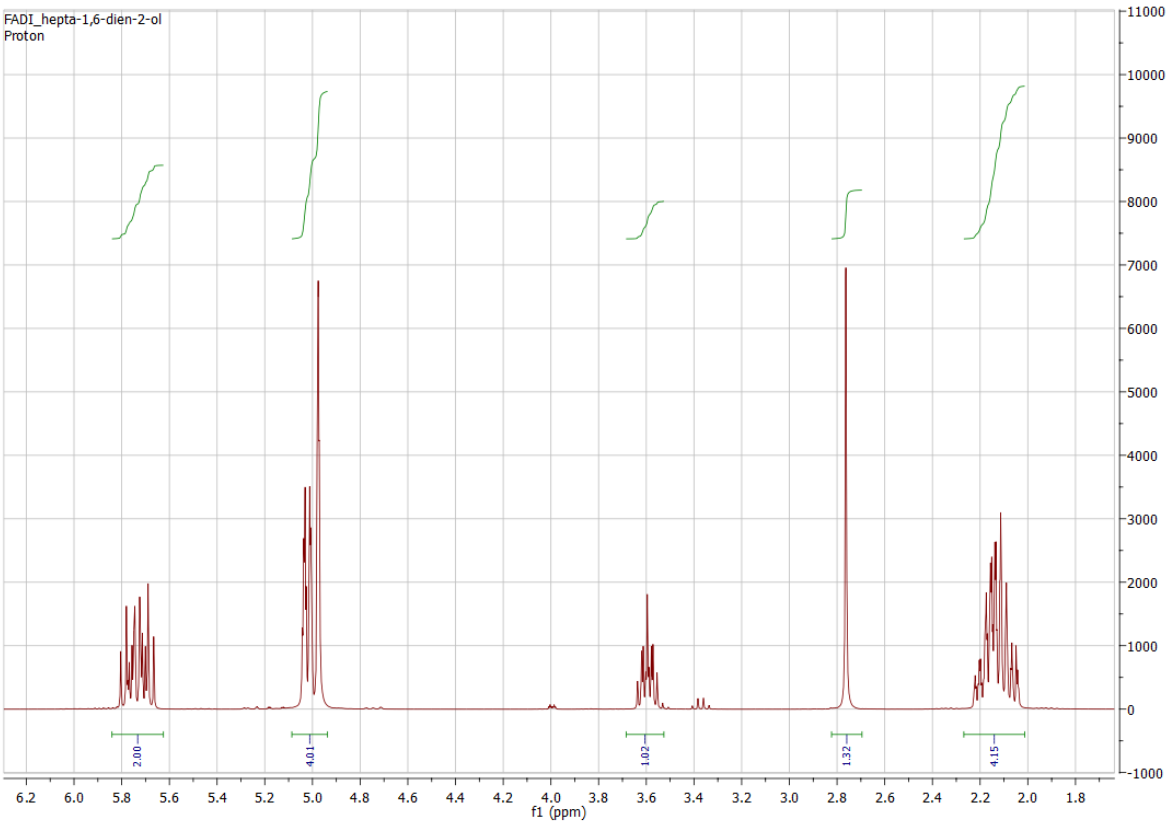
^{13}C NMR (100 MHz, $CDCl_3$) of compound 8



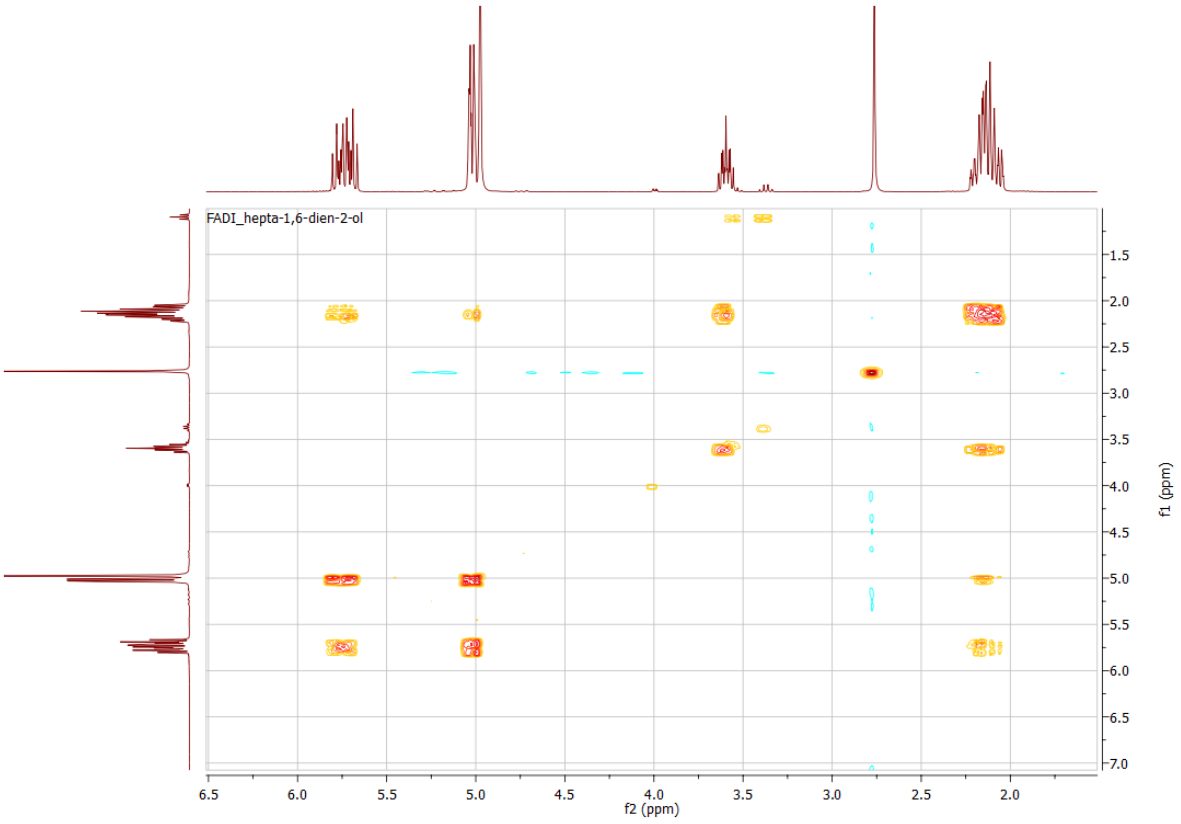
HMBC (CD_3OD) of compound 8



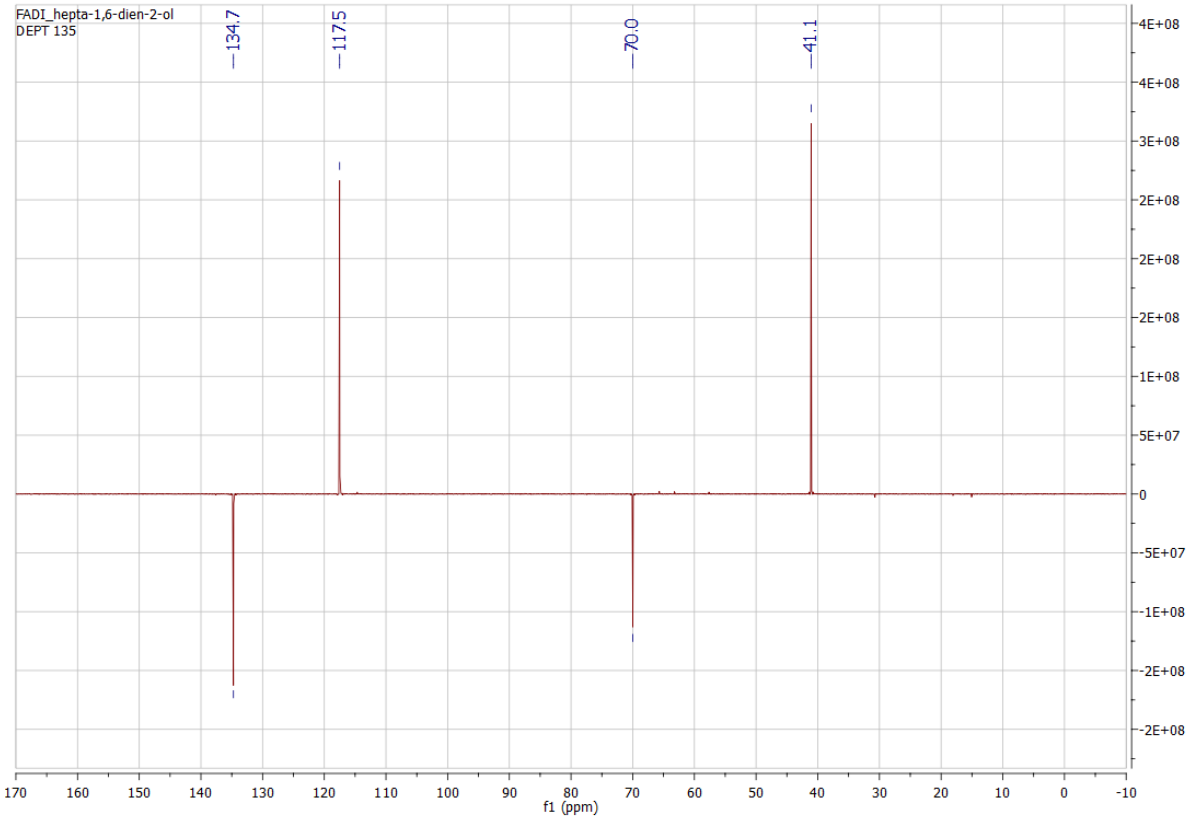
HSQC (CD_3OD) of compound 8



^{1}H NMR (300 MHz, $CDCl_3$) of compound 9



COSY (300 MHz, $CDCl_3$) of compound 9



DEPT (75 MHz, $CDCl_3$) of compound 9