Electronic Supplementary Information

Triazole Linked *N*-acetylglucosamine Based Gelators for Crude Oil Separation and Dye Removal

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1. Organogel preparation

1.1. Gelation test:

5 mg gelator **5a** and measured amount of liquid were taken in a glass vial heated slowly to dissolve the gelator completely. Thereafter the mixture was allowed to cool down to room temperature and finally the vial was inversed. A system was considered as gel if it doesn't fell down on keeping vial upside down (Figure S1).

Figure S1. Gels of **5a** in different organic solvents (a) Benzene (b) Toluene (c) o-Xylene (d) m-xylene (e) p-xylene (f) mesitylene

1.2. Rheology data:

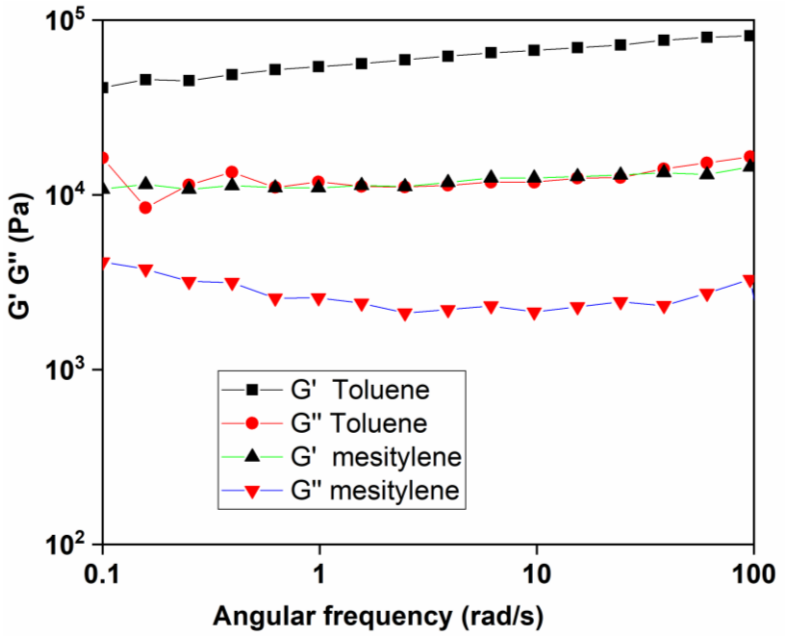


Figure S2: Frequency sweep experiment for toluene and mesitylene gel of **5a**.

2. VT ^{1}H NMR studies of compound 5b:

C-H proton of triazole ring in compound **5b** at 25 ºC resonate at δ 8.631 ppm whereas it gets gradually shifted upfield with increasing the temperature and at 70 ºC it appears at δ 8.754 ppm. This upfield shift (Δδ = 0.123 ppm) clearly indicates that, C-H proton of **5b** in triazole ring was participating in hydrogen bonding. The N-H proton of acetamido group was also got upfield shift with Δδ = 0.311 ppm suggesting it's involvement in hydrogen bonding which weaken with increases in temperature. The upfield shift for N-H protons clearly indicates that there was hydrogen bonding interactions along with π-π stacking responsible for the gel formation. Whereas methyl group of anomeric methoxya littleupfield shift (Δδ = 0.05 ppm) was observed, indicating methyl group may involve intramolecular hydrogen bond between C2-NH and anomeric methoxy group. Although gel formation is not affected with this intramolecular hydrogen bonding as it does affected by inter molecular hydrogen bonding.

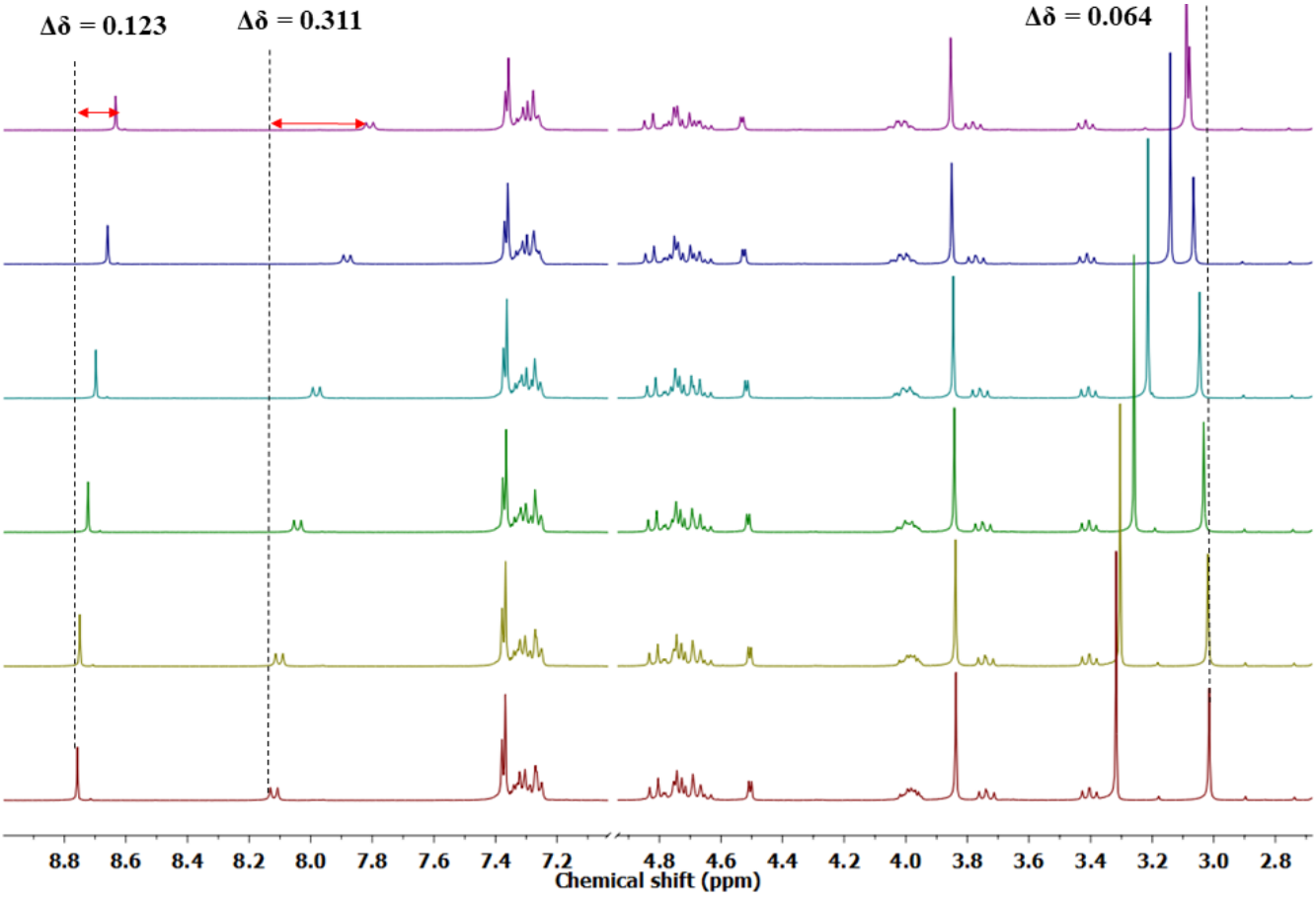


Figure S3. ^{1}H NMR spectra of compound **5b** at different temperature in DMSO-d_6

3. Recovery of diesel from gelator:

Thermo reversibility is an important property for gelator, which deals with fuel recovery from the gel. We tried to do the same with our gelator compound **5a** and obtained promising results shown in Figure S4. We performed an experiment in the laboratory to study thermos reversibility of gelator **5a**. In a glass bath, 5 mL of diesel is floating on 150 mL sodium chloride solution (mimicking sea water). Gelator **5a** was dissolved in ethyl acetate (0.3 mL), subsequently added on diesel layer. It instantly forms gel and within 15 min diesel completely turns into solid. It was removed through spatula (Figure S4 (b)). The solid was transferred to round bottom flask and, subsequently, using distillation technique gelator and crude oil was separated (Figure S4 (c)). We also performed the same experiment in small scale (0.5 mL diesel) and images are shown below are from the same experiment.

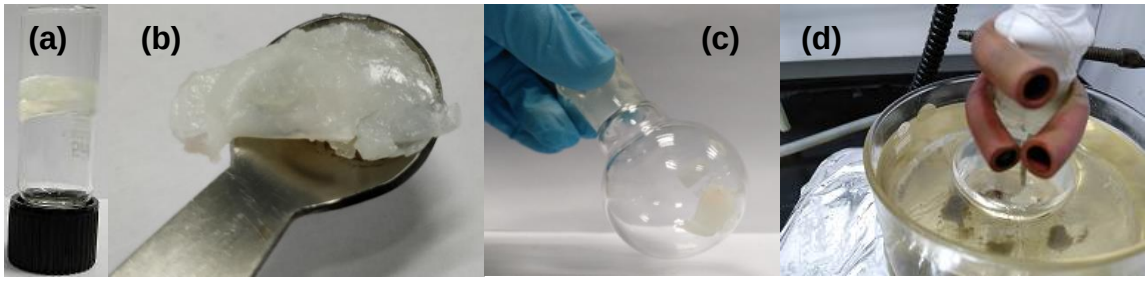


Figure S4: Thermo reversibility of gelator **5a** (a) 16 mg **5a** in ethyl acetate 0.5 mL of diesel: 2mL water (b) Scooped diesel gel (c) Disel gel transferred to rb flask for distillation (d) distillation of diesel and recovery of gelator.

5. Crude Oil Gelation:

Figure S5. Gelation with Erha crude oil at C.G.C (a) Compound **5a** (b) Compound **5b** (c) Compound **5f.**

Figure S6. Gelation with Kuwait export crude oil at C.G.C (a) Compound **5a** (b) Compound **5b** (c) Compound **5f.**

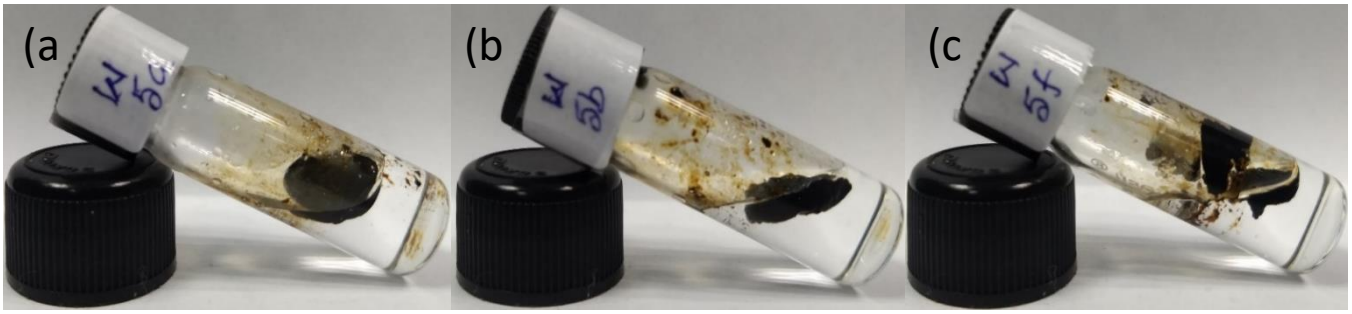


Figure S7. Gelation with WCS crude oil at C.G.C (a) Compound **5a** (b) Compound **5b** (c) Compound **5f.**

Table S1. Classification and composition of the three crude oils: Erha crude oil, Kuwait export, Western Canadian select (WCS).

Crude oil	**Erha Crude Oil**	**Kuwait export**	**WCS Crude Oil (WCS)**
API gravity	32.8°	31.4°	21°
Classification	light	medium	heavy
Sulphur content	0.21 %	2.5%	3.43%

6. Rheological experiments: These experiments were performed on an Anton paar MCR 702 modular compact rheometer using 25 mm size parallel plates. The distance between the

parallel plates was fixed at 0.8 mm and solvent trapping device was fixed above the plate to prevent the solvent evaporation. Frequency sweep experiment was measured from 0.1 to 600 rad/s at constant strain of 0.01%. Shear Stress experiment was done at constant frequency of 1 rad/s.

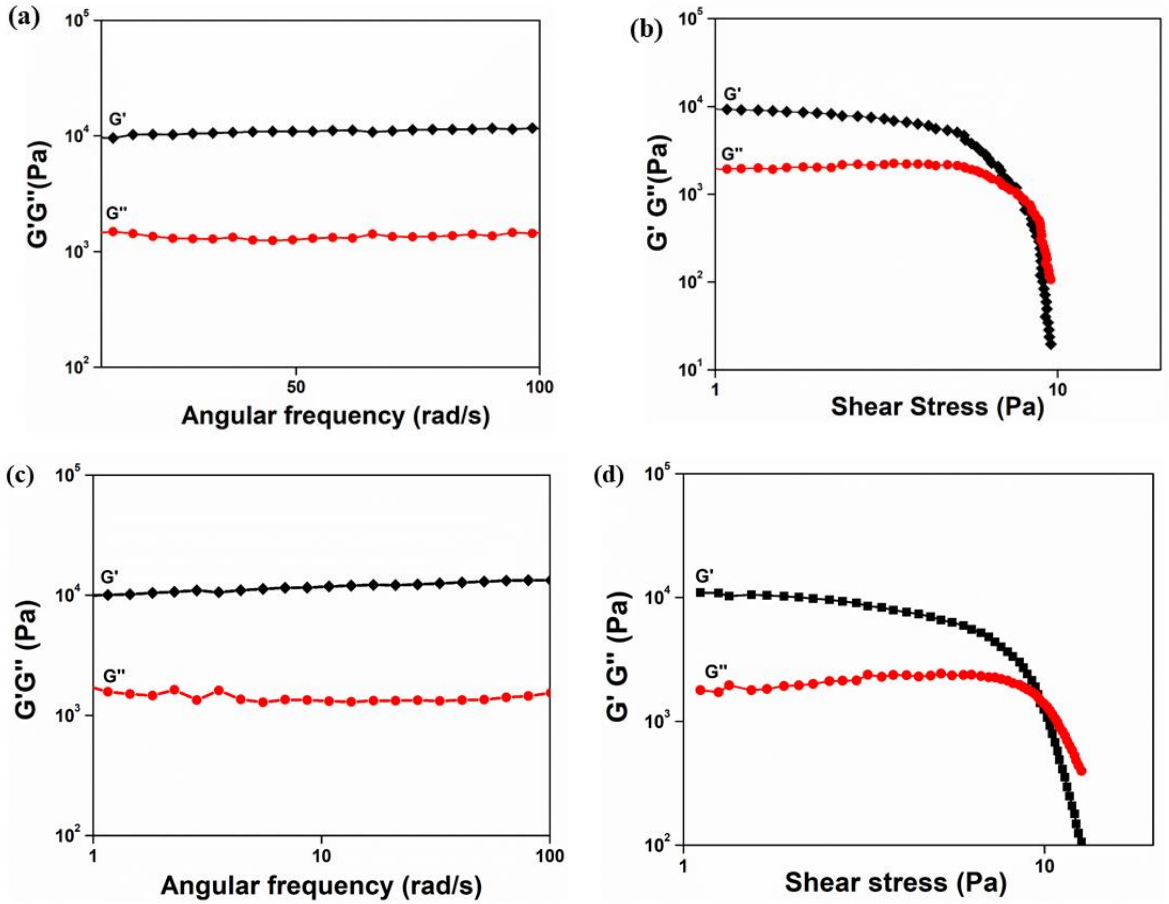


Figure S8. Rheology of Erha crude oil gels (a) frequency sweep of **5b** gel (b) Shear Stress of **5b** gel (c) frequency sweep of **5f** gel (d) Shear Stress of **5f** gel

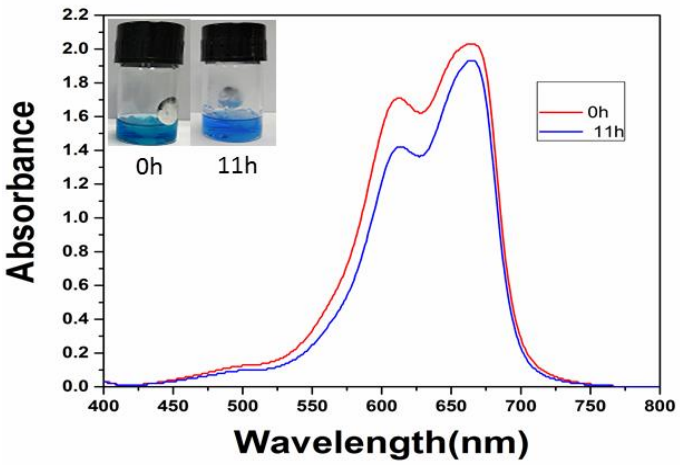
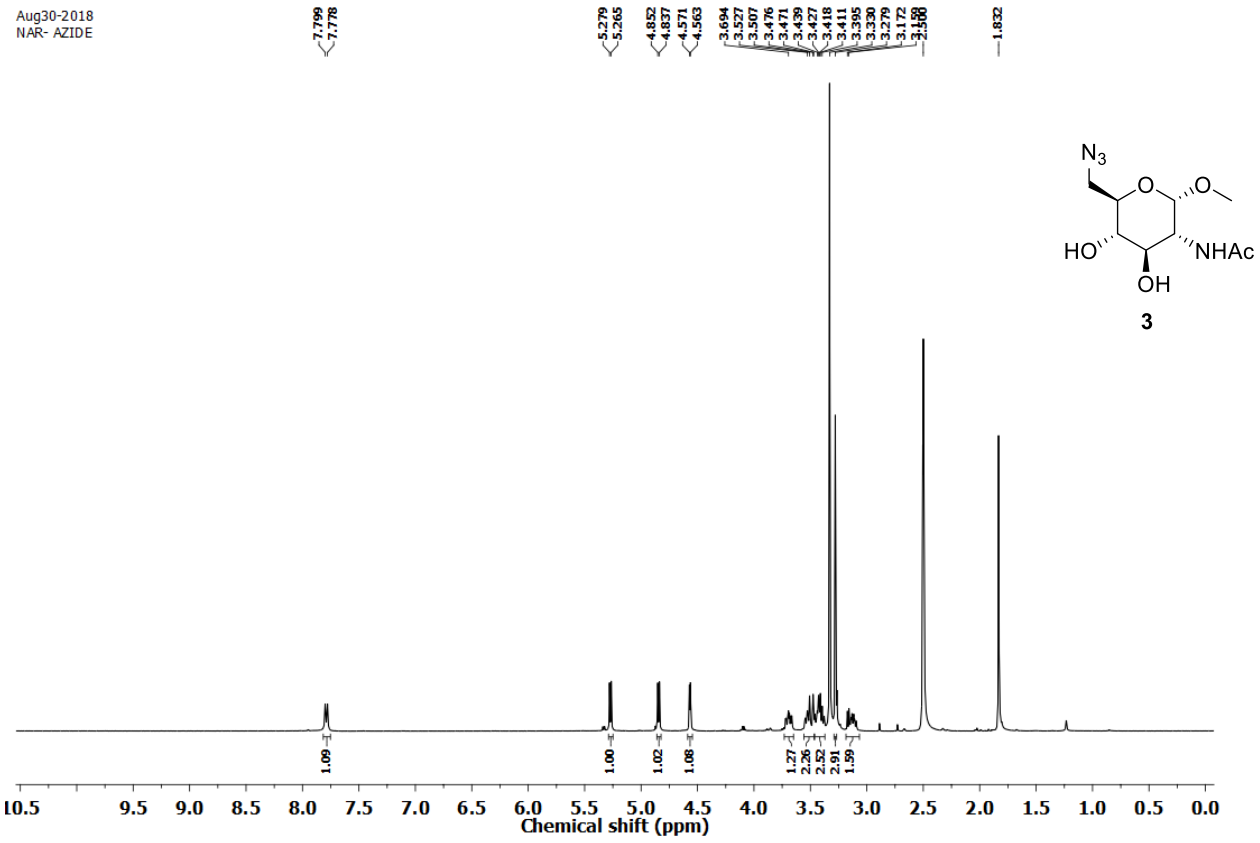
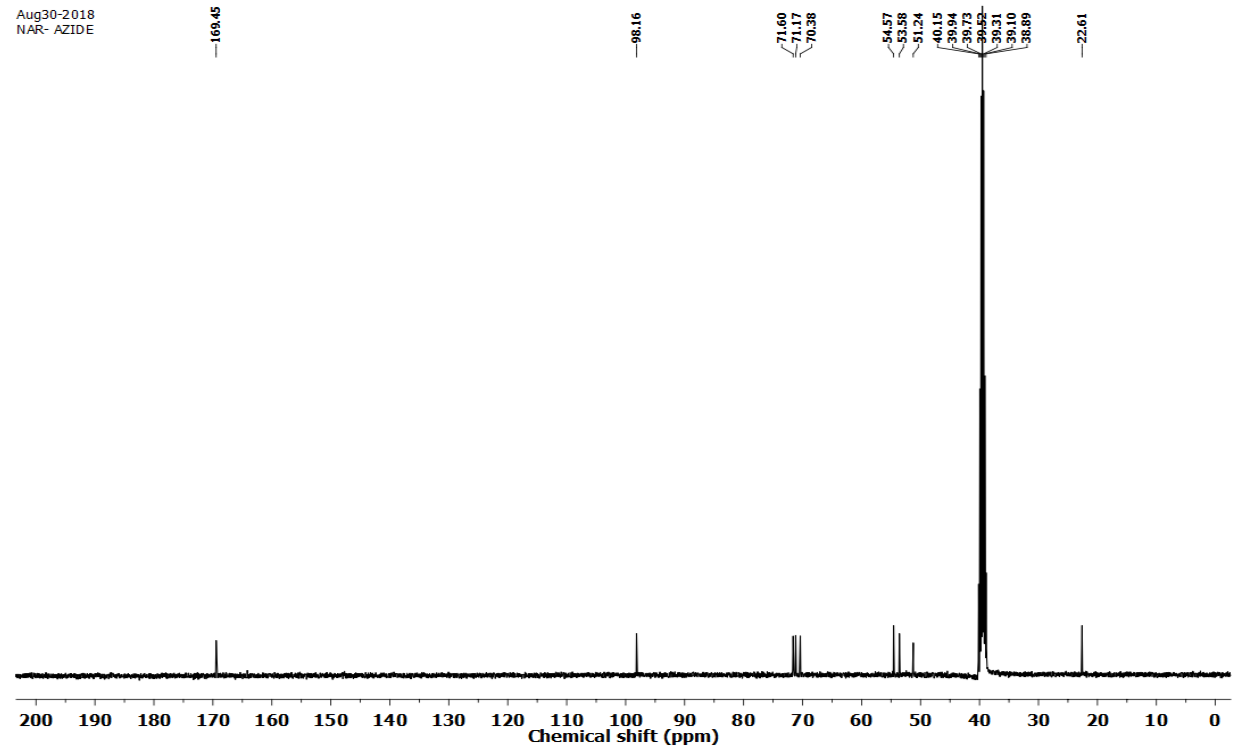


Figure S9. UV spectra for removal of dyes: methylene blue

Copies of ^{1}H and ^{13}C NMR spectra of all compounds.





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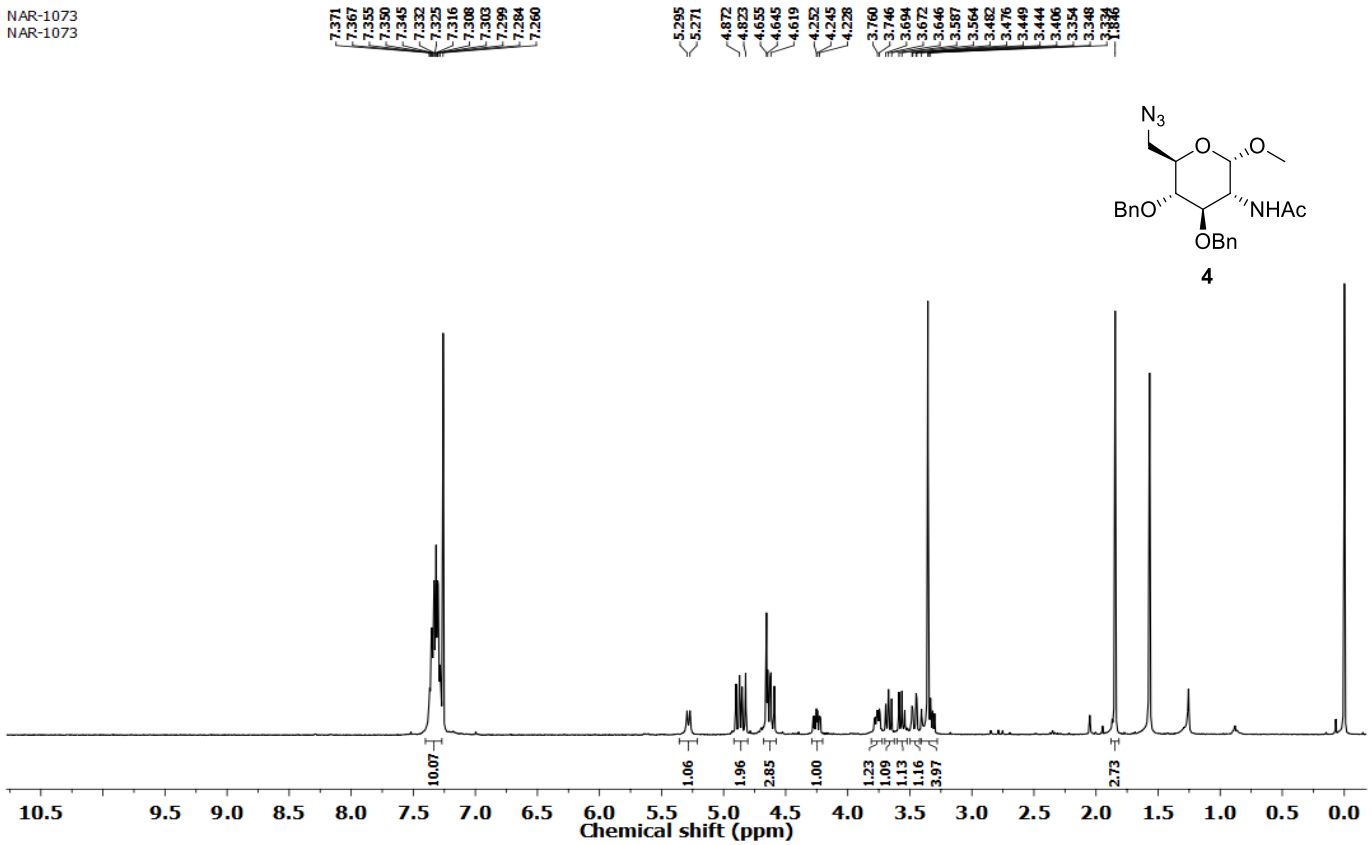
NAR-1073



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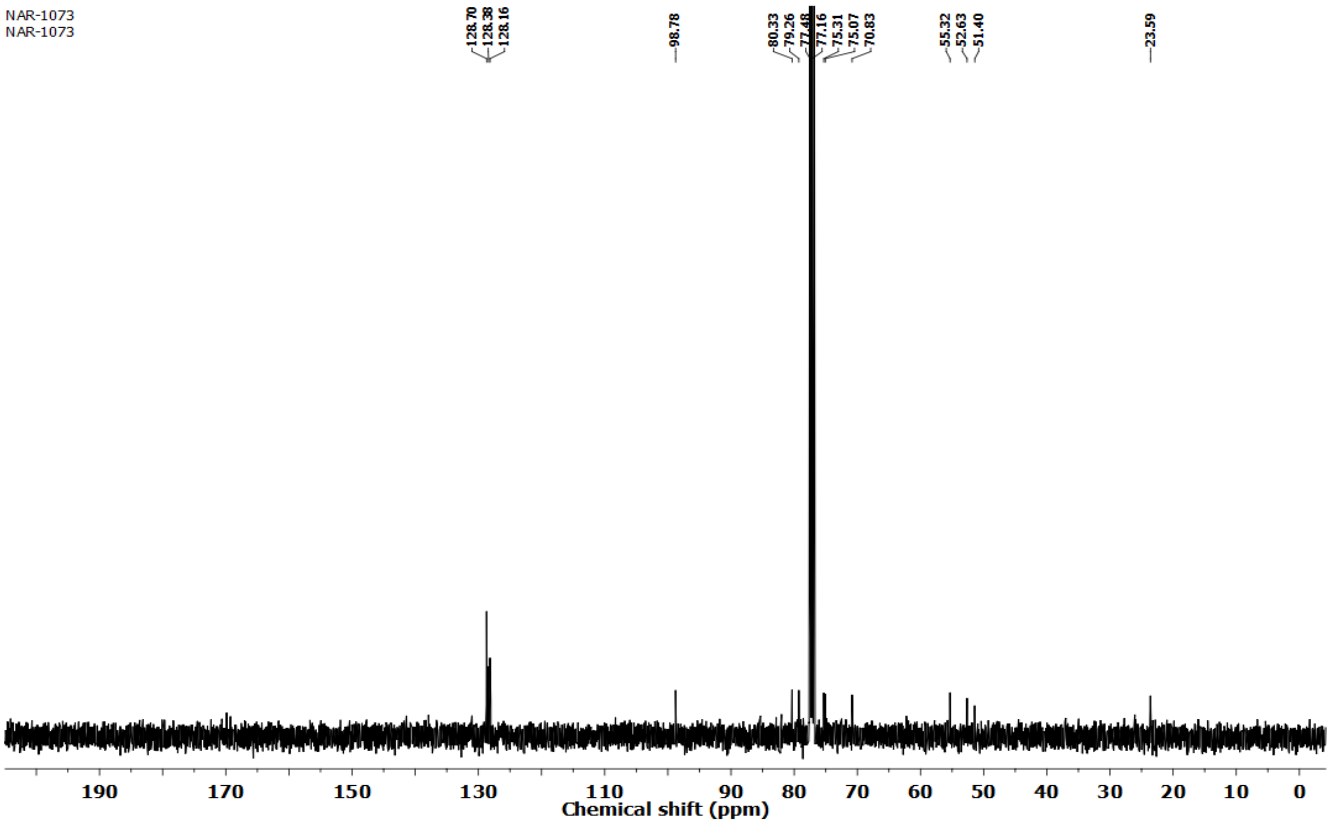

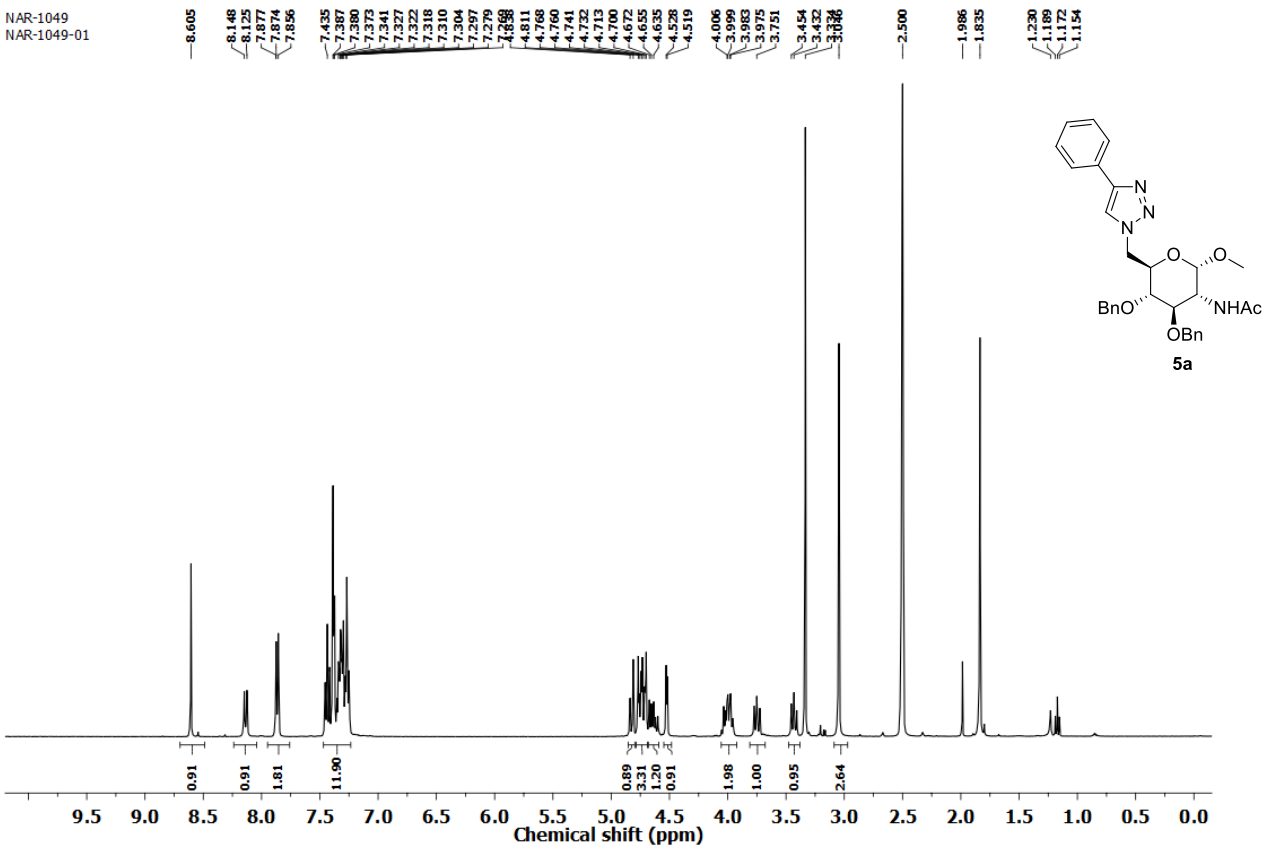
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0.91
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11.90
0.89
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1.20
0.91
1.98
1.00
0.95
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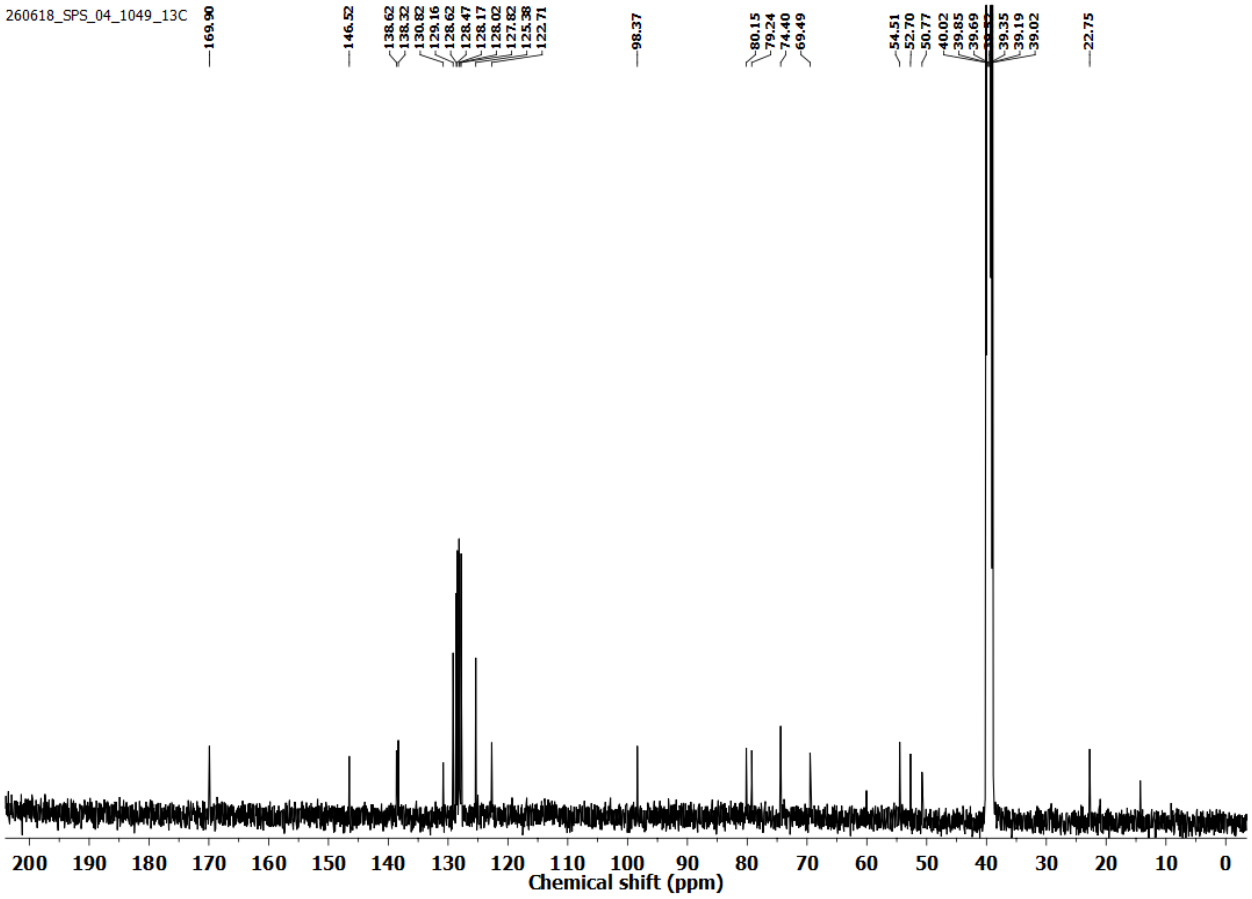
BnO
NHAc
OBn
5a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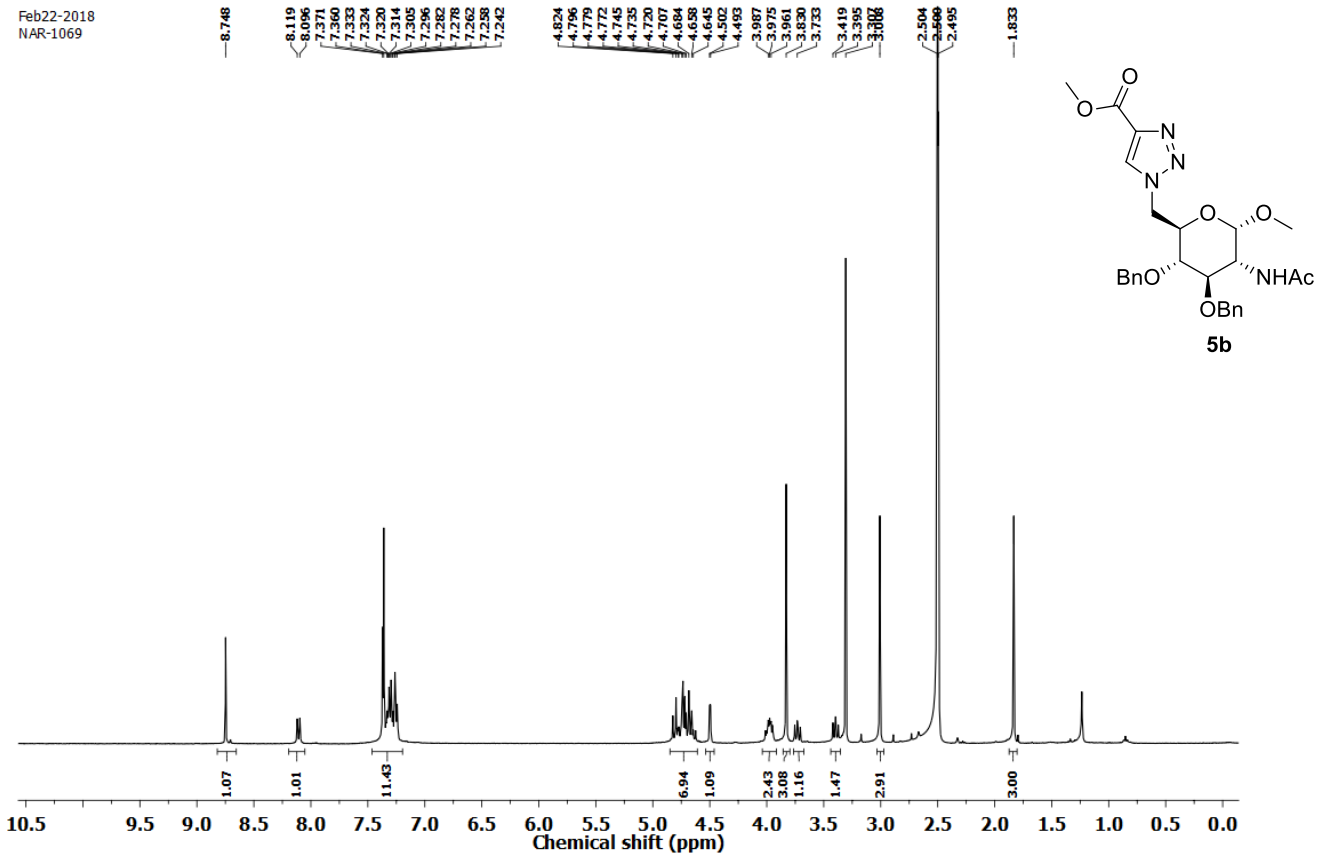
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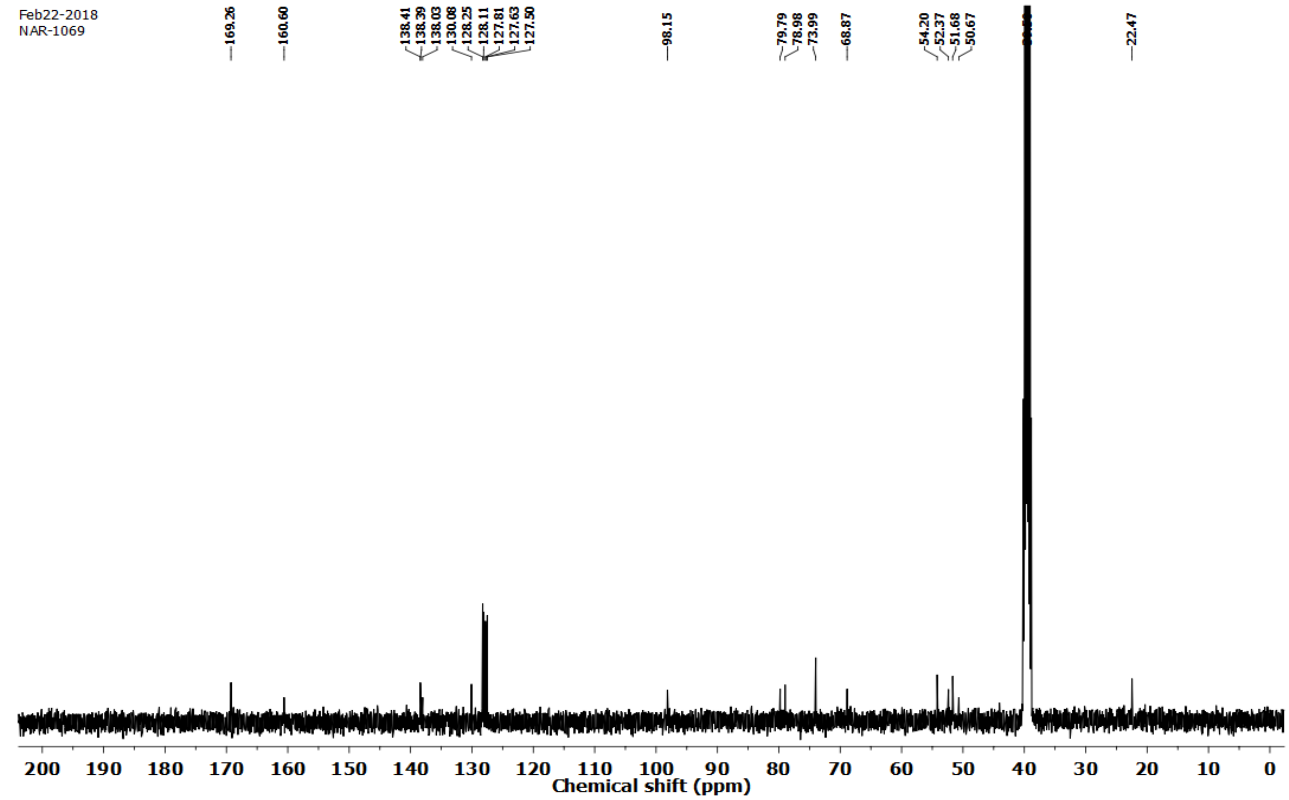
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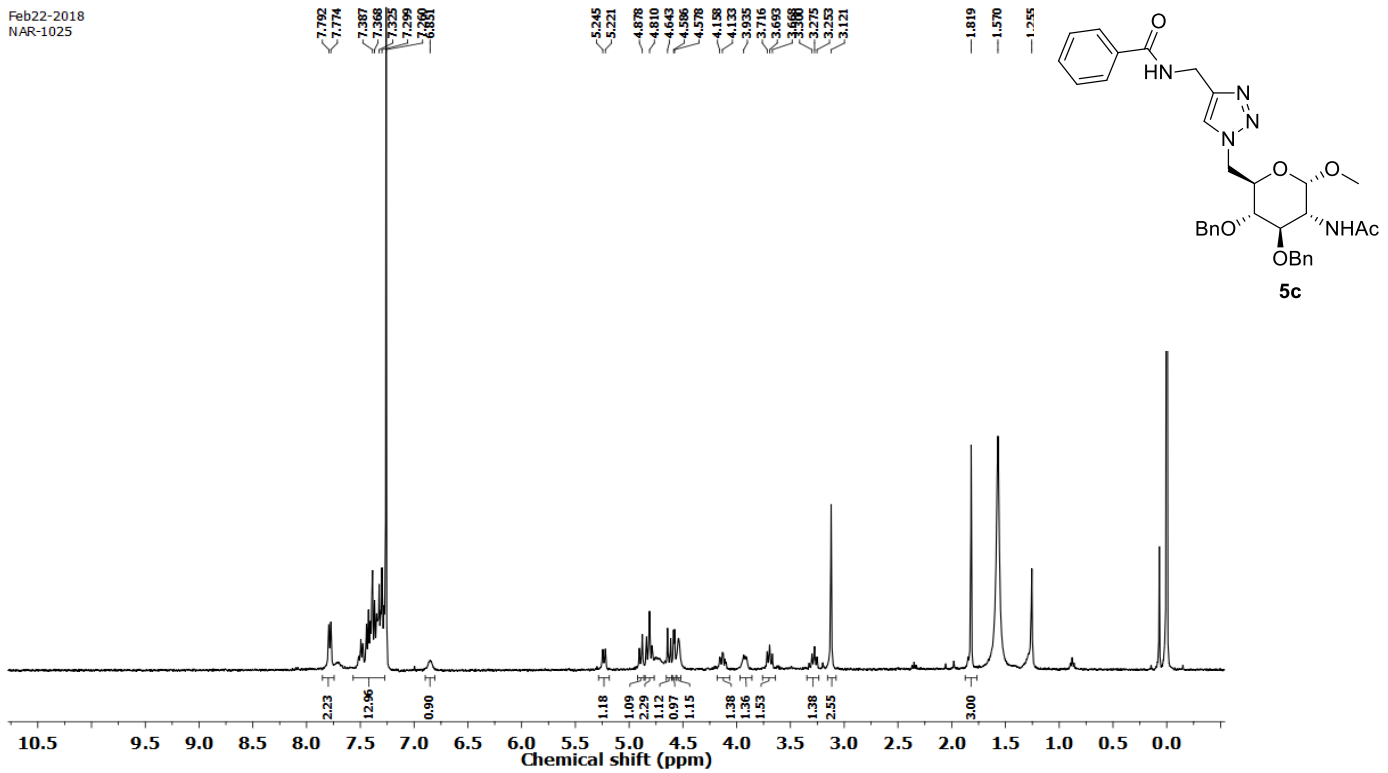
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1.12
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1.53
1.38
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2.5
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N
O
O
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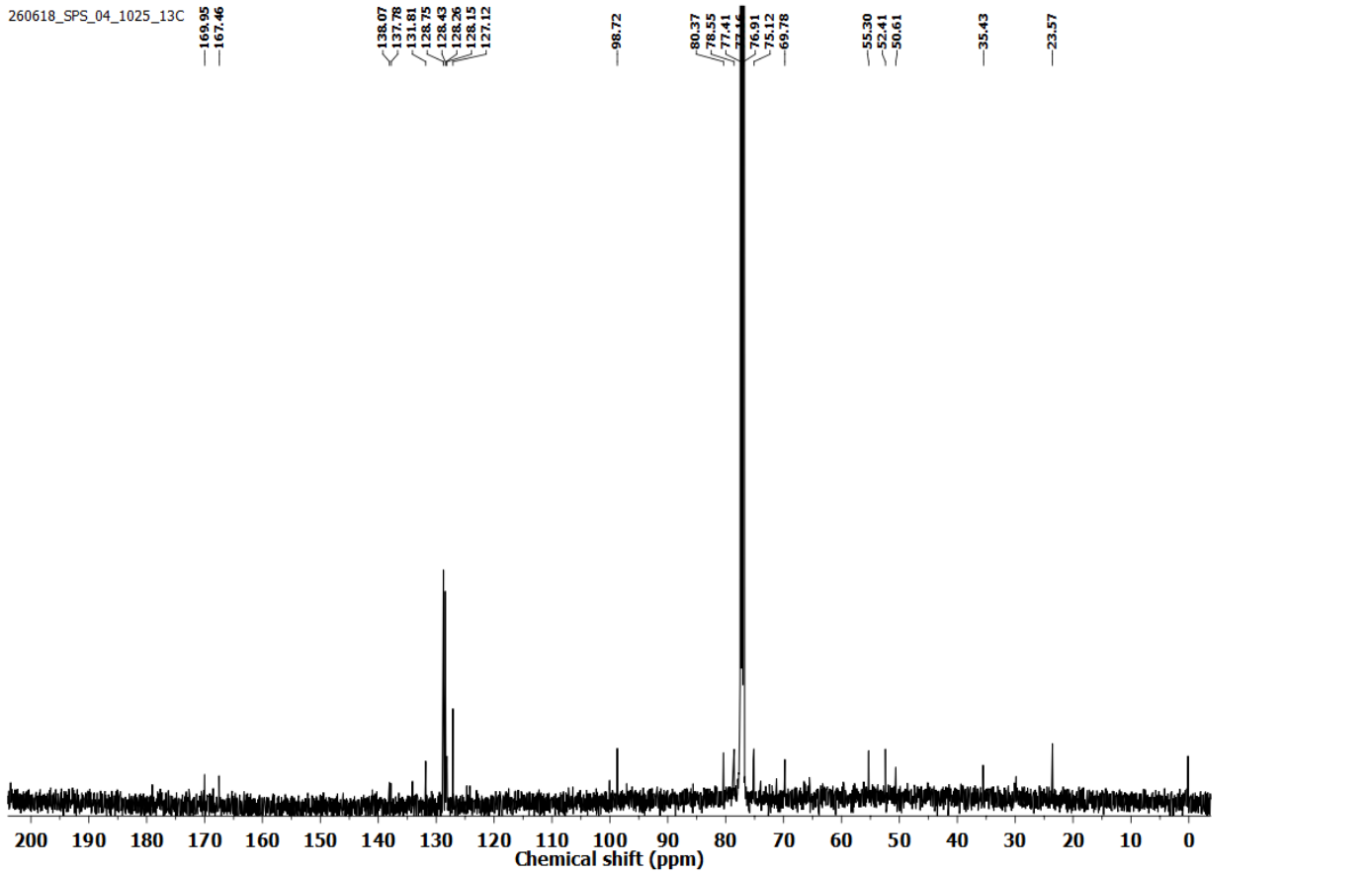
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180
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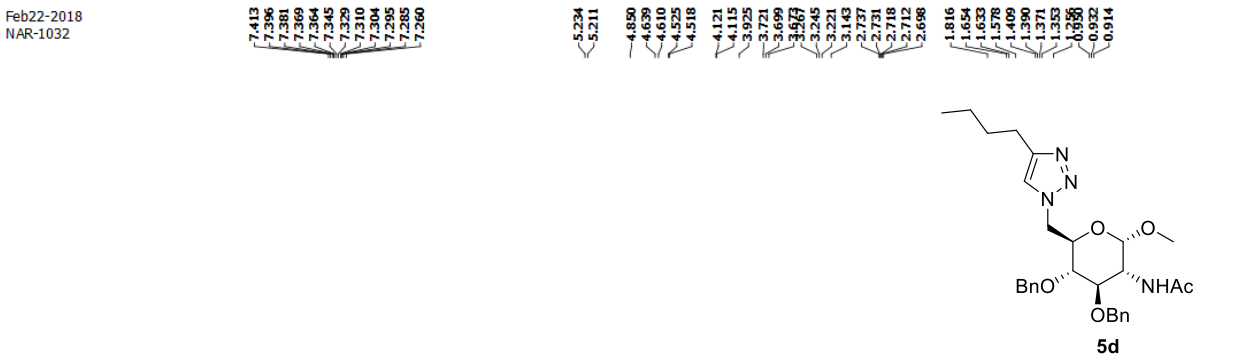

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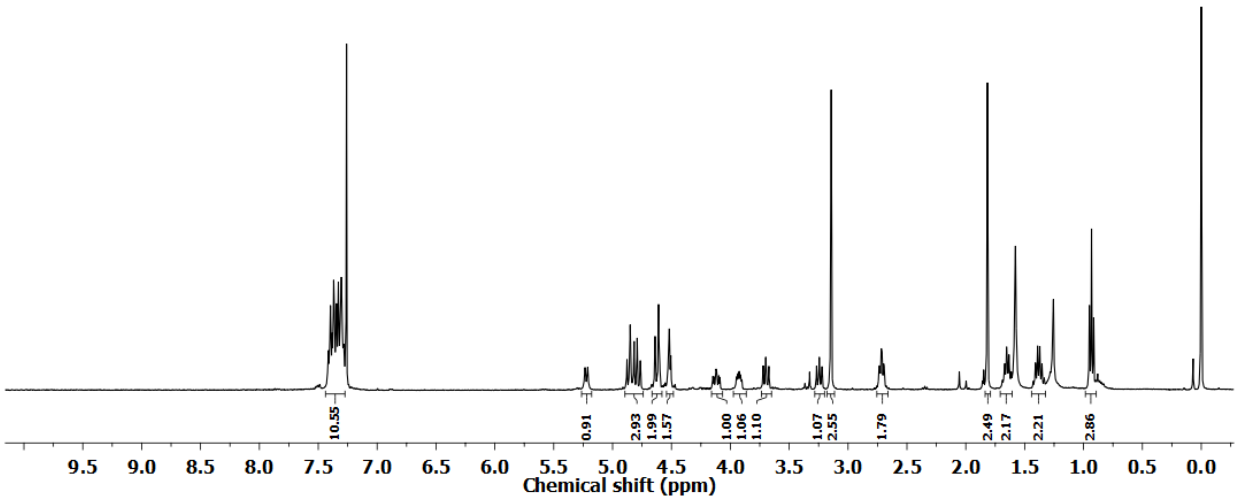

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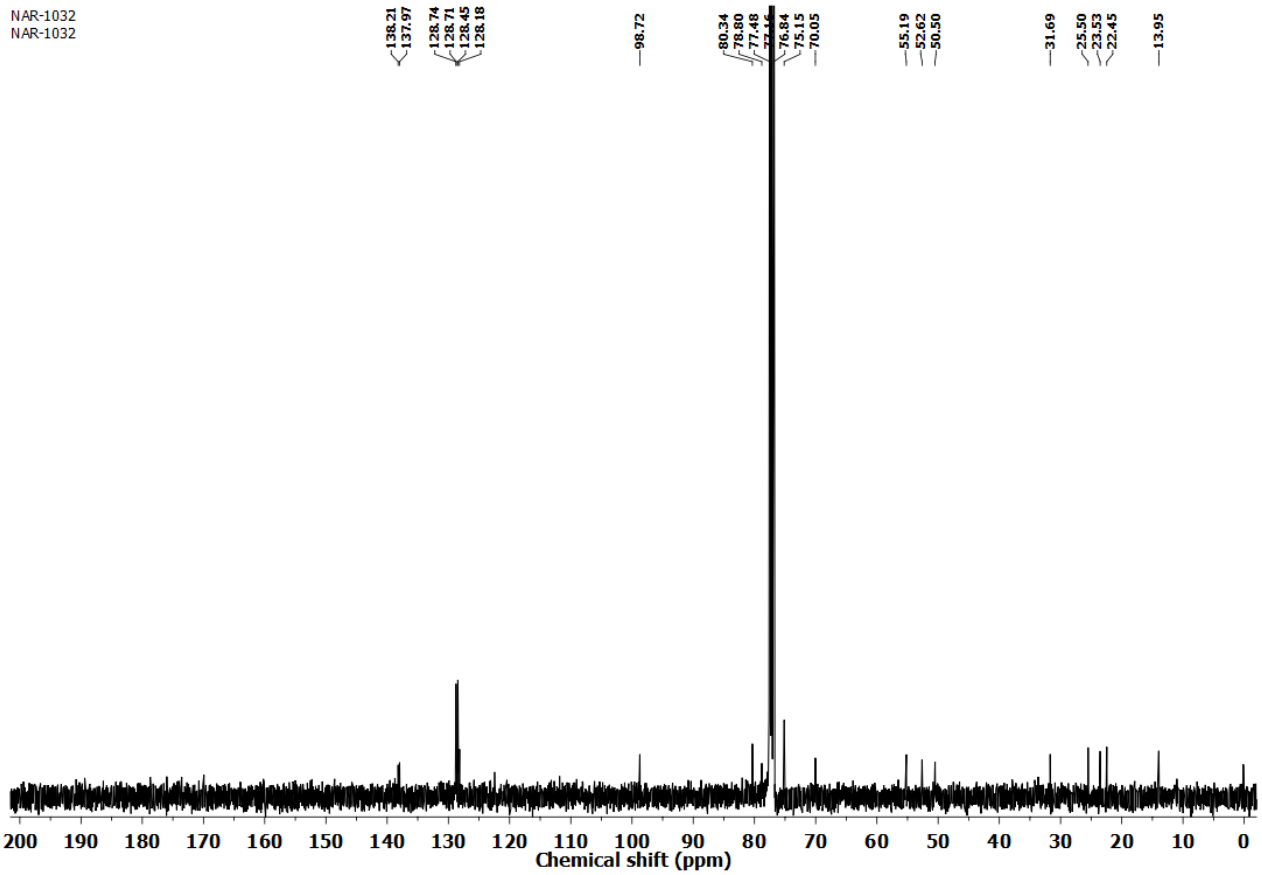

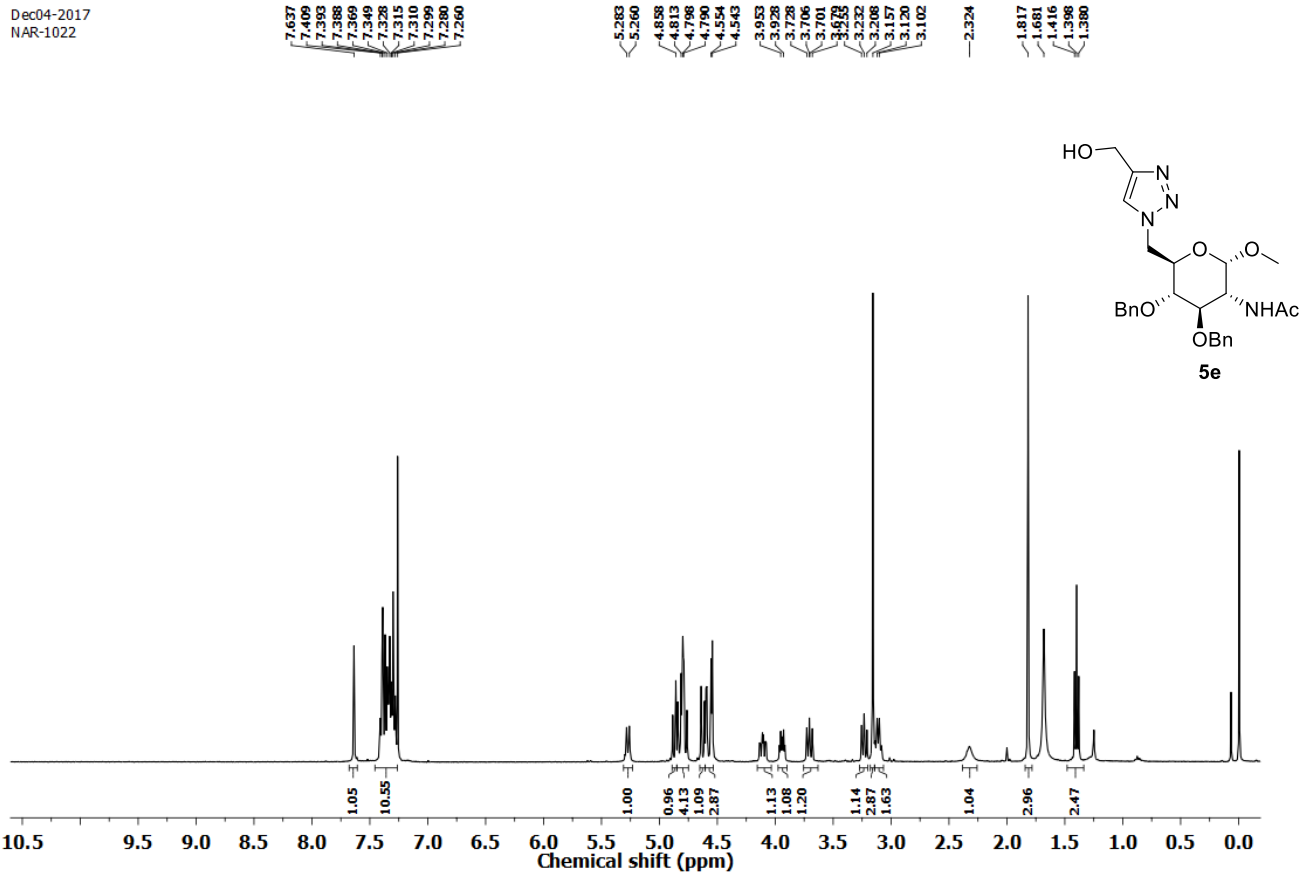
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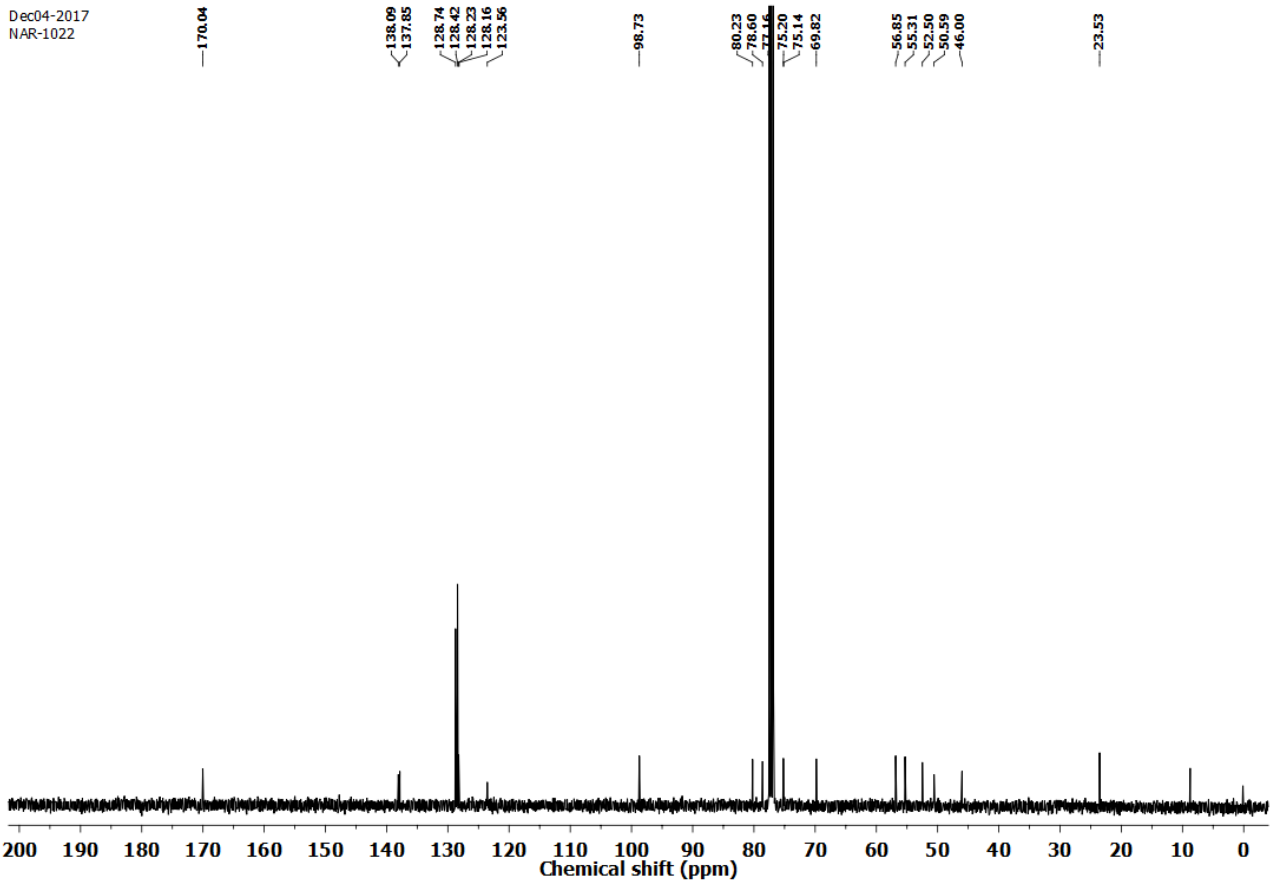
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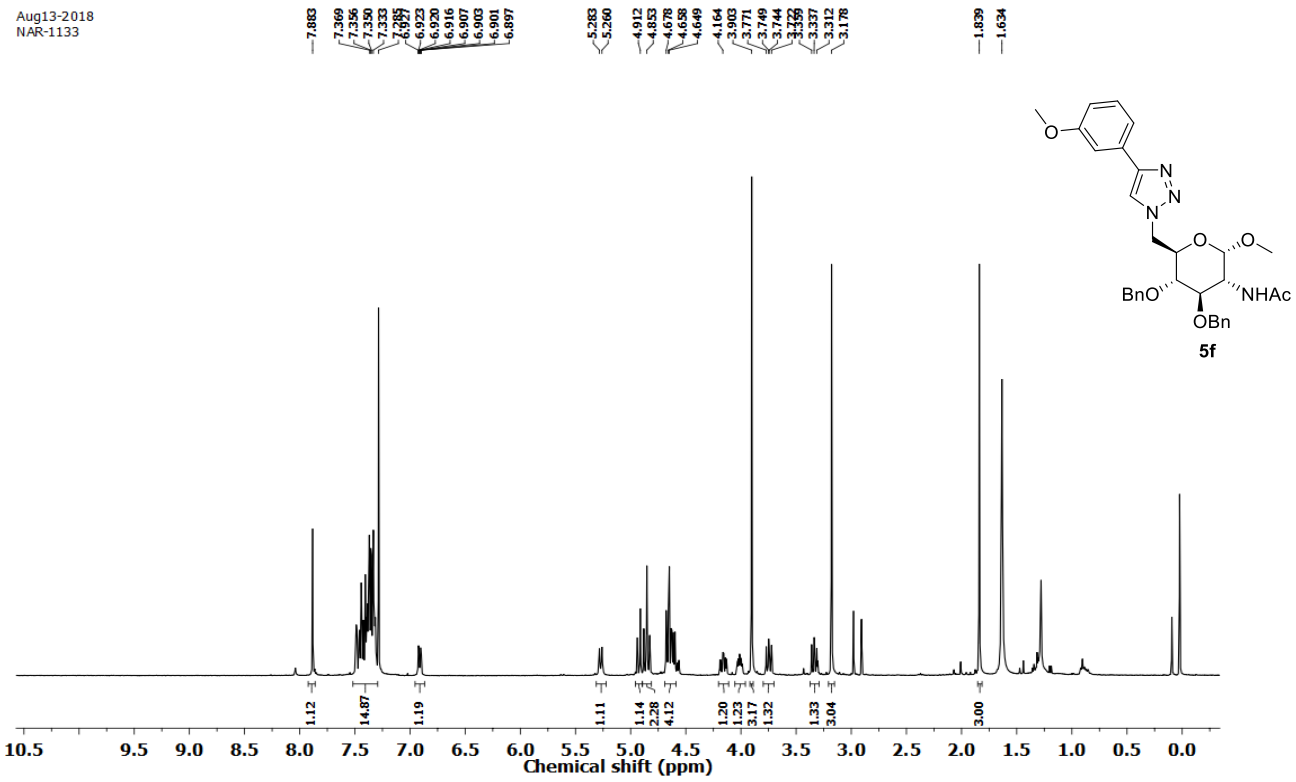
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N
O
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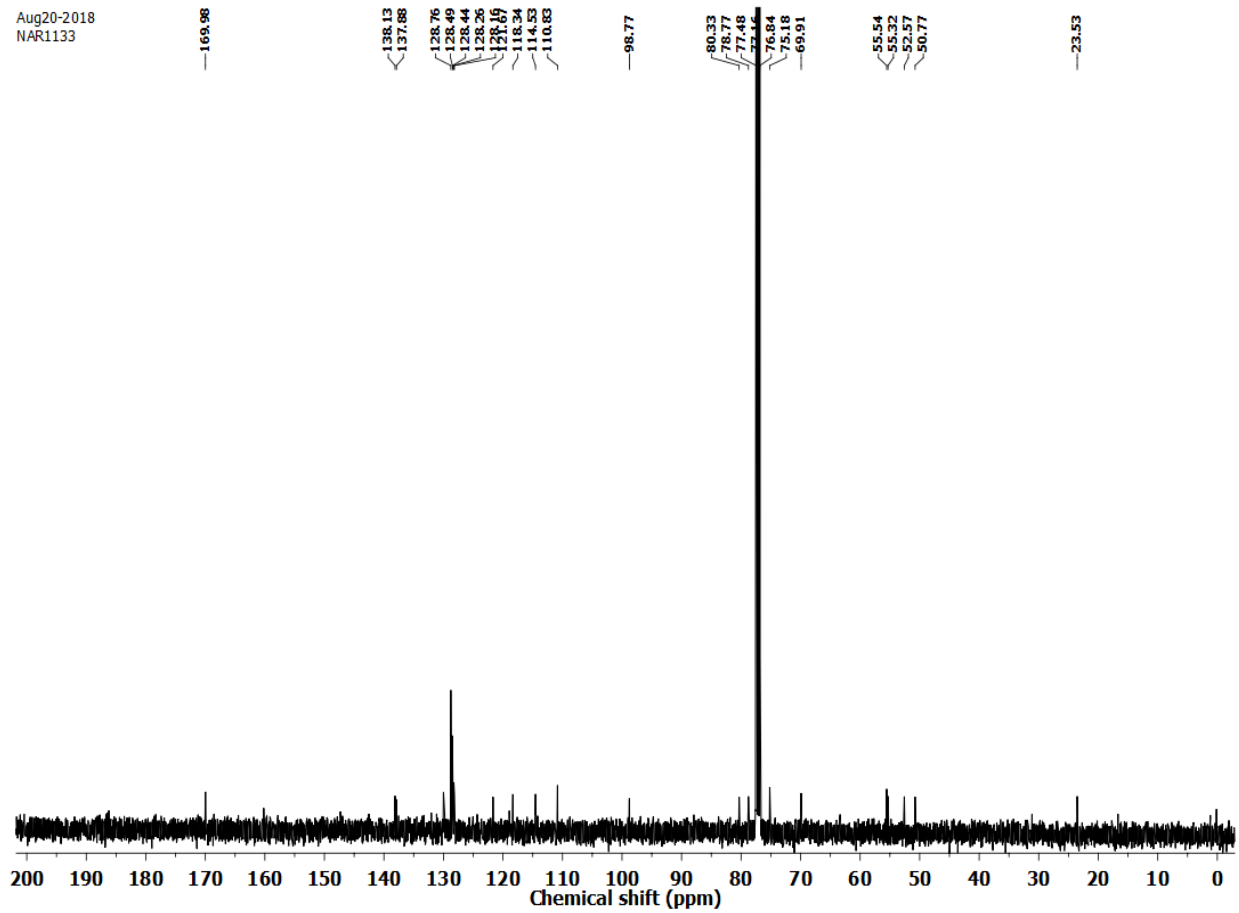
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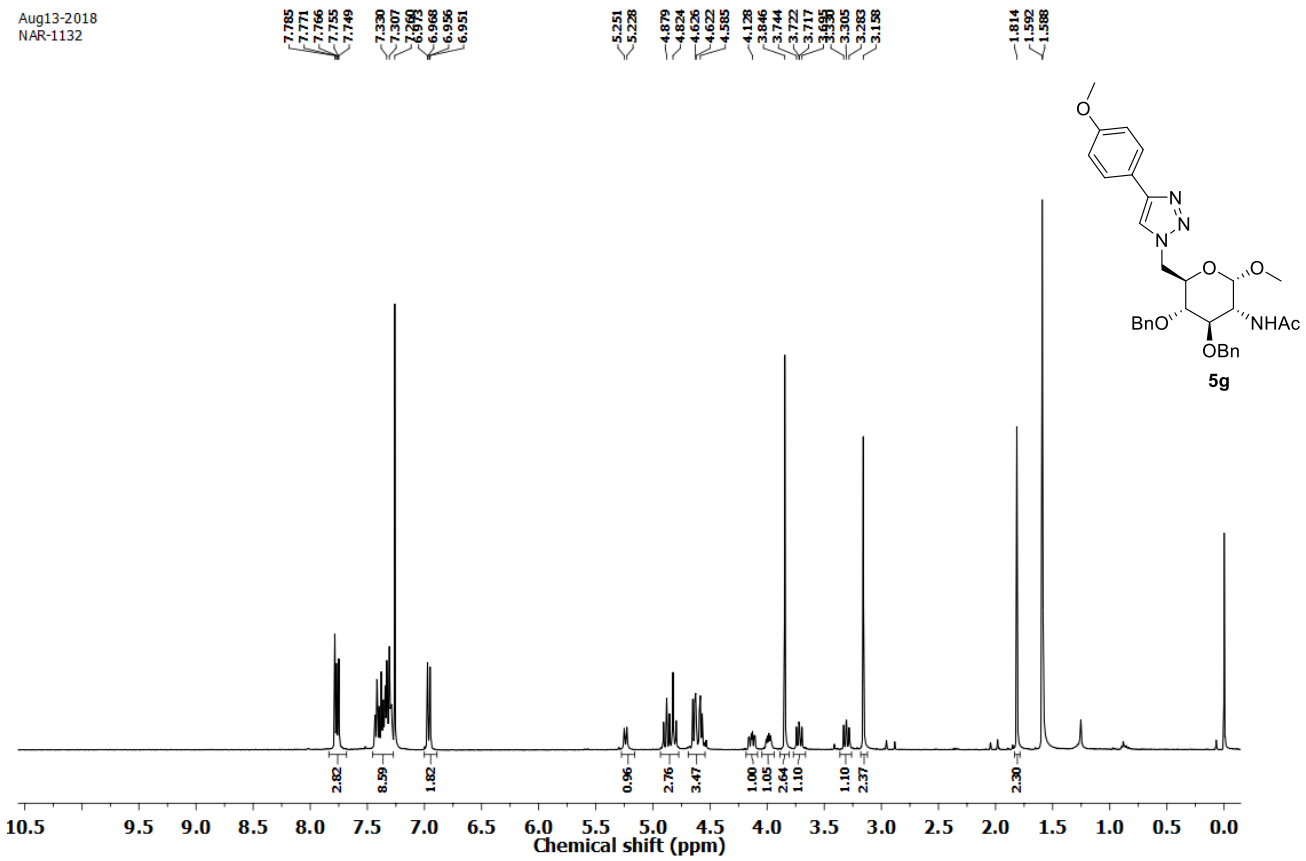
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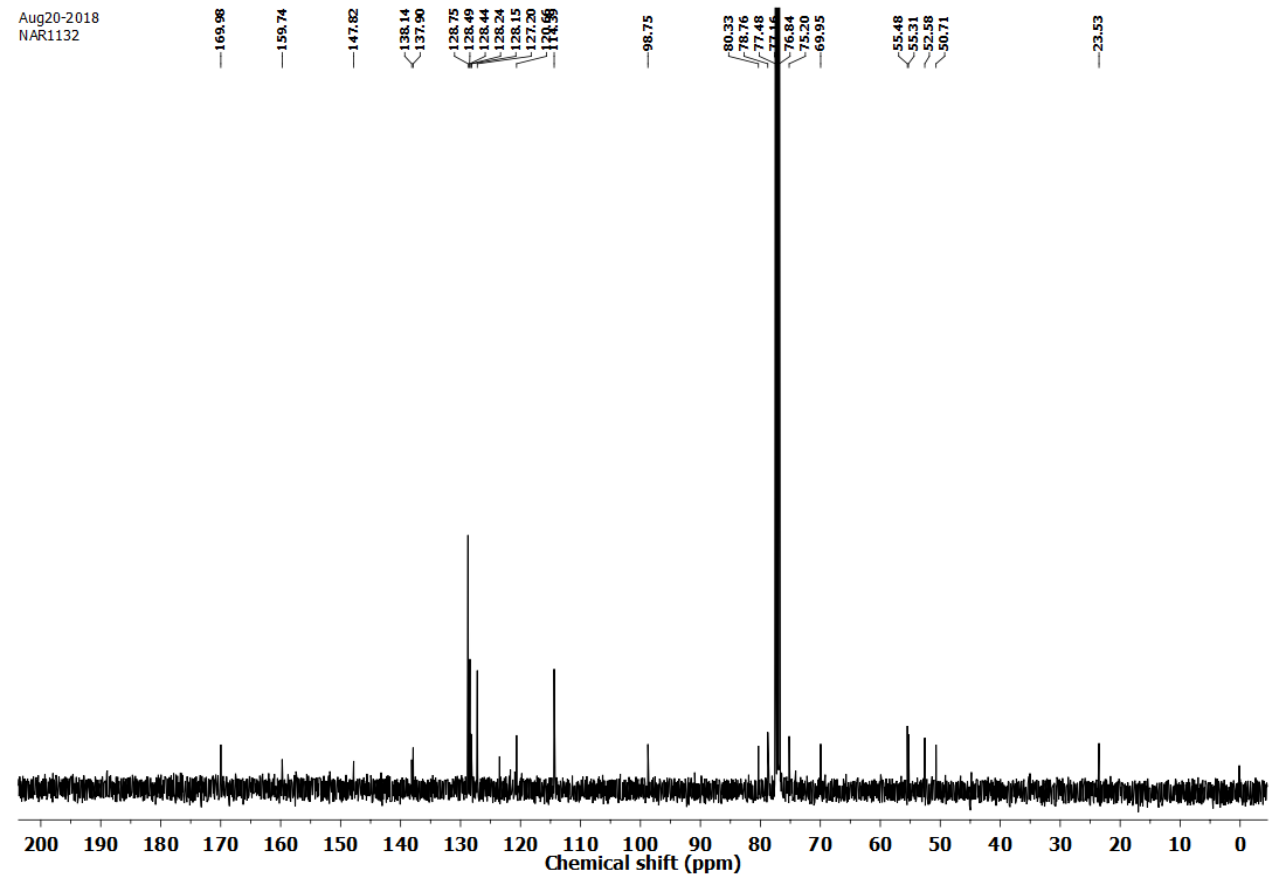
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10
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Chemical shift (ppm)