

## SUPPLEMENTARY INFORMATION

### Oligosaccharides based antibacterial drug conjugates

Von der Naturwissenschaftlichen Fakultät der  
Gottfried Wilhelm Leibniz Universität Hannover  
zur Erlangung des Grades

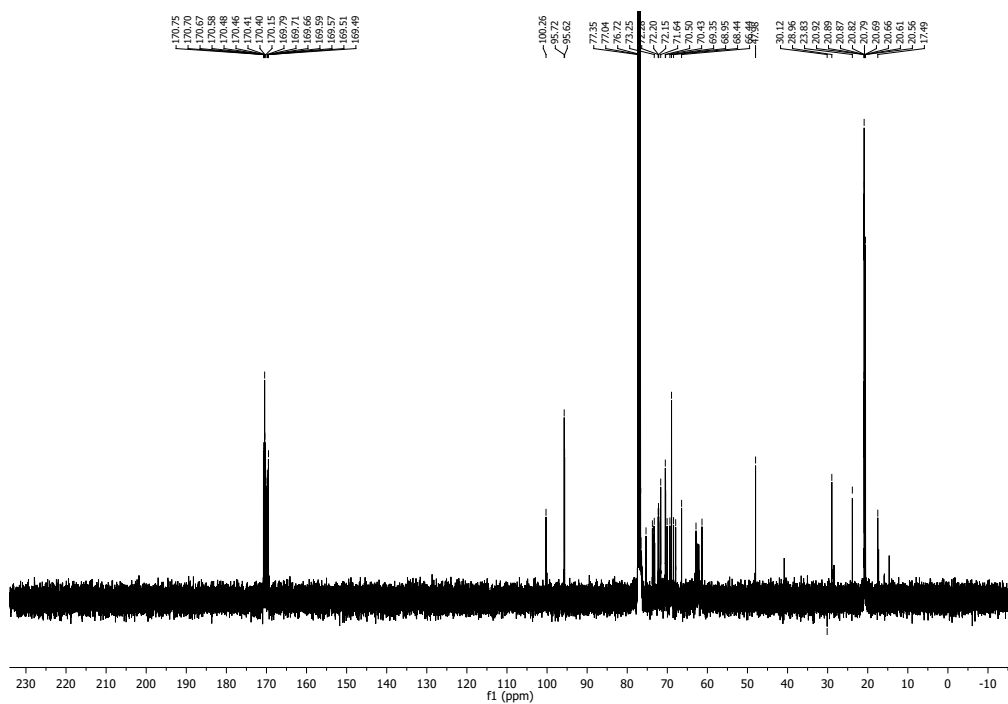
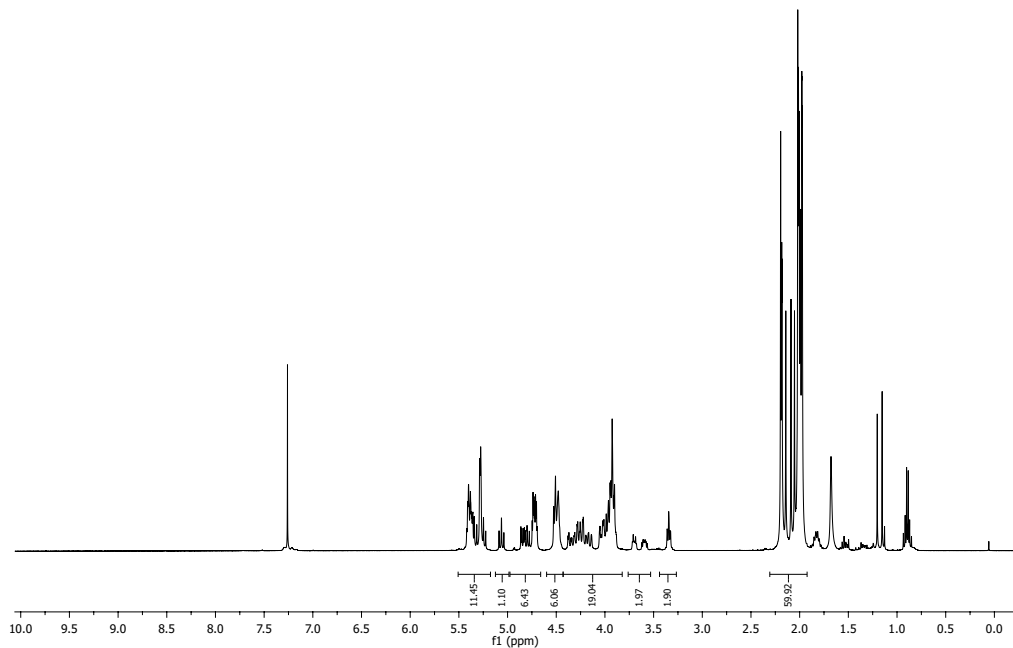
Doktorin der Naturwissenschaften (Dr. rer. nat)

genehmigte Dissertation  
von

Steffi Kruba Stephen, M.Sc. (Indien)

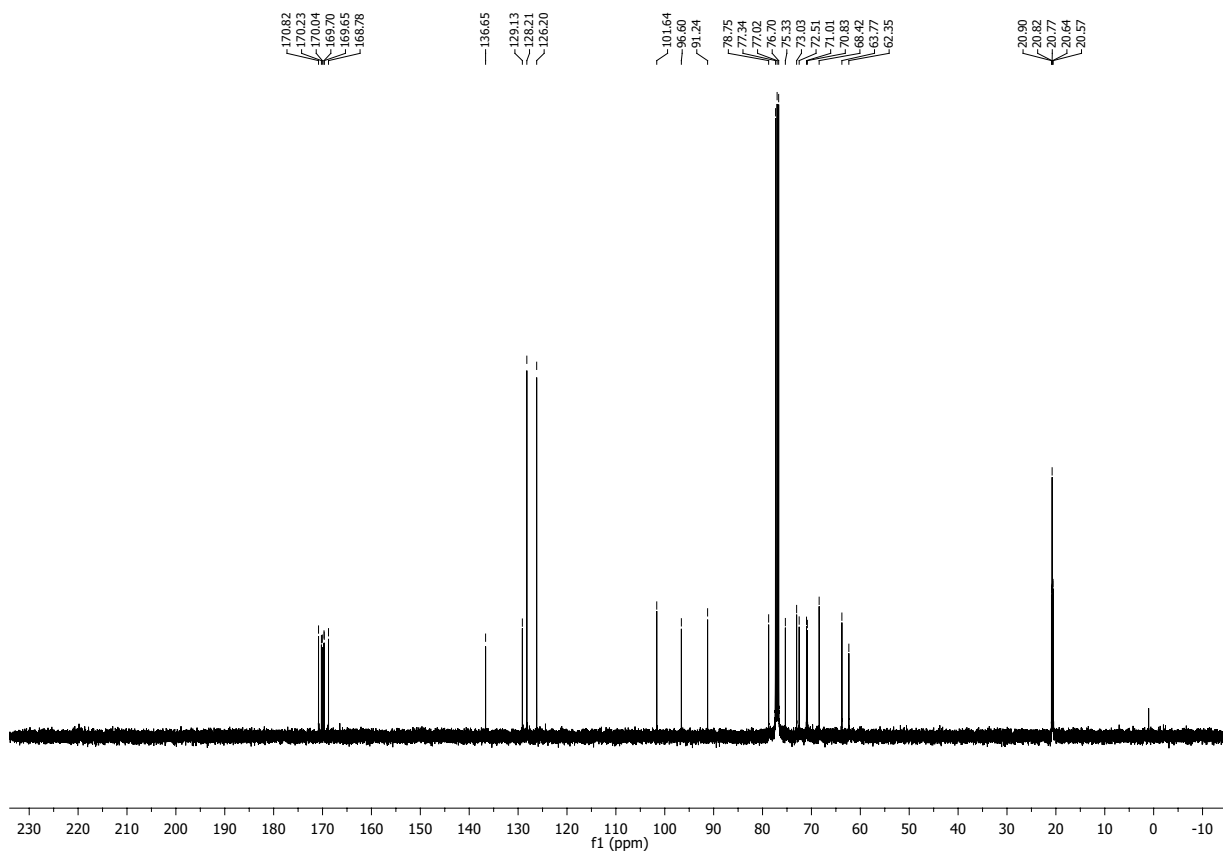
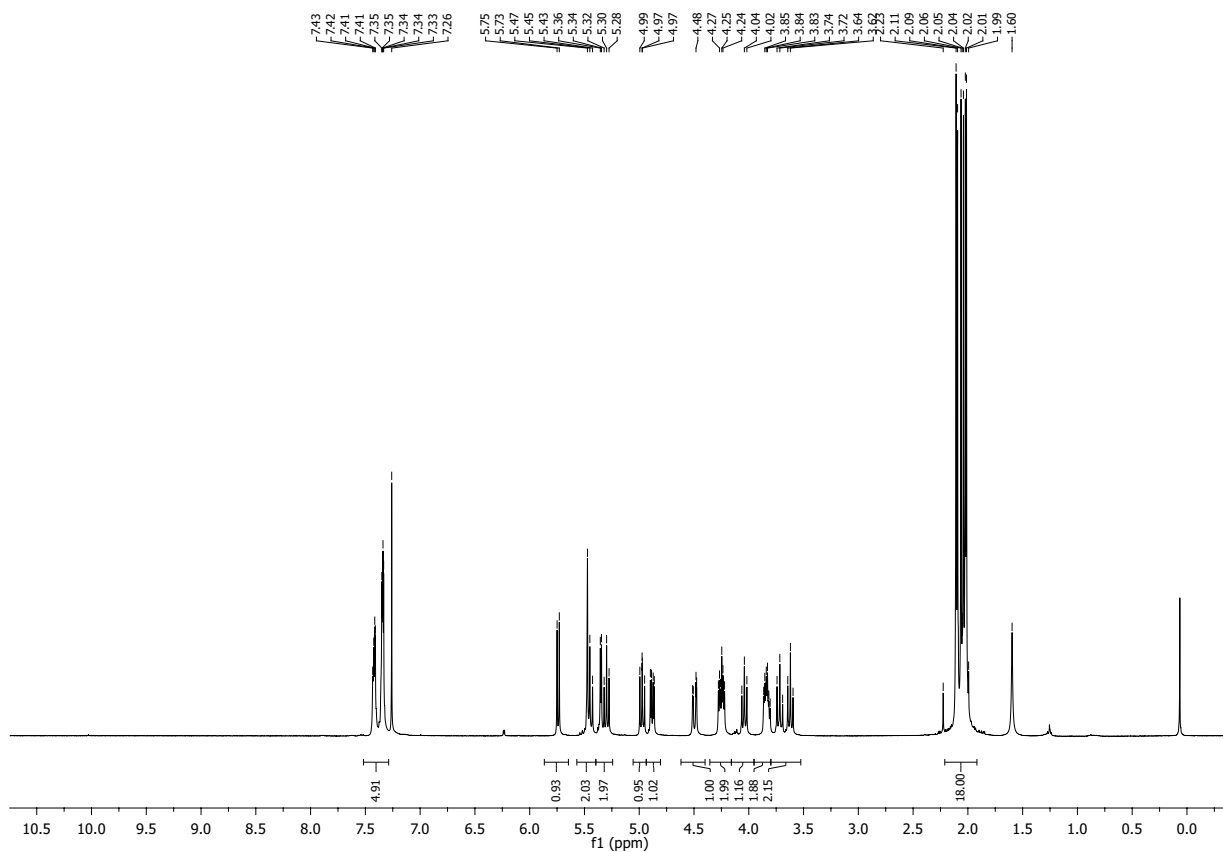
2021

$\beta$ -D-Glucopyranose,2,3,4,6-tetra-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2,3,6-tri-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2,3,6-tri-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2,3,6-tri-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2,3,6-tri-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2,3,6-triacetate-1-(3'-bromopropyl),**2**

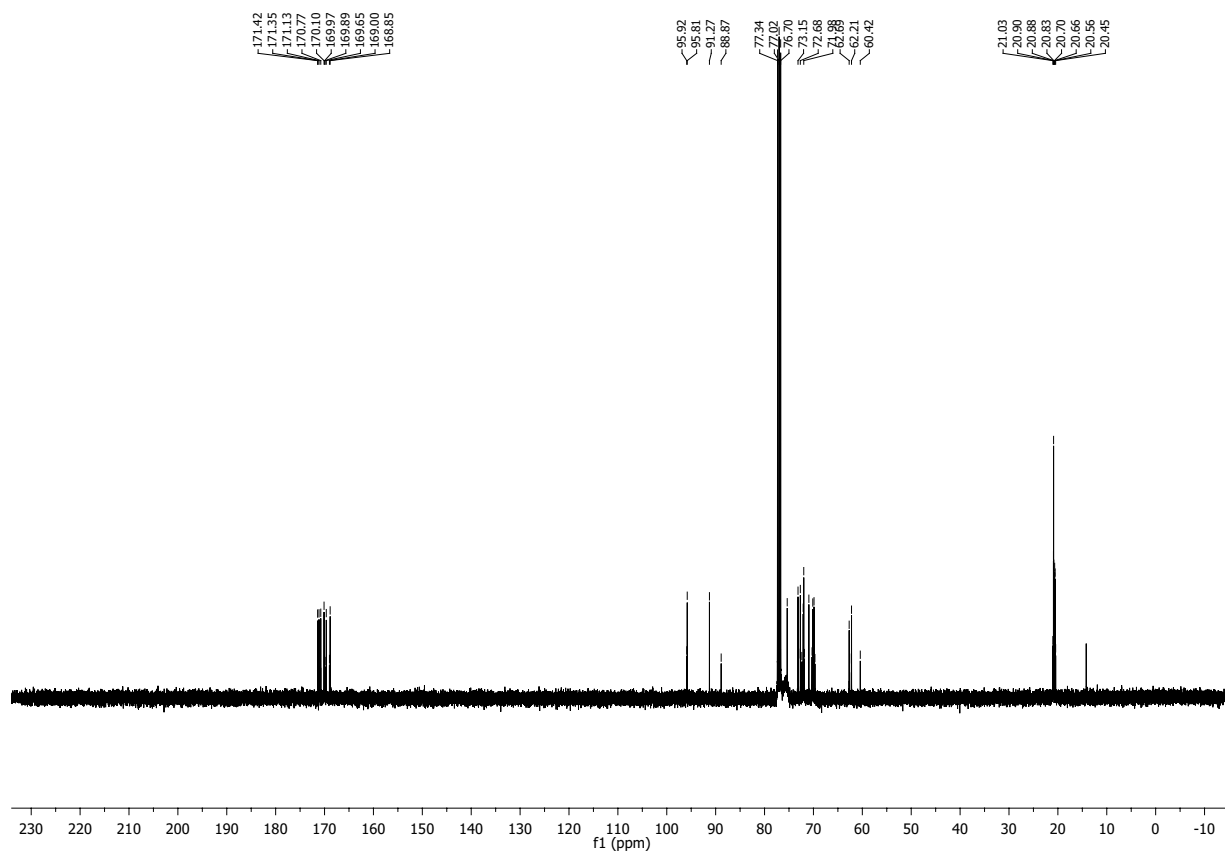
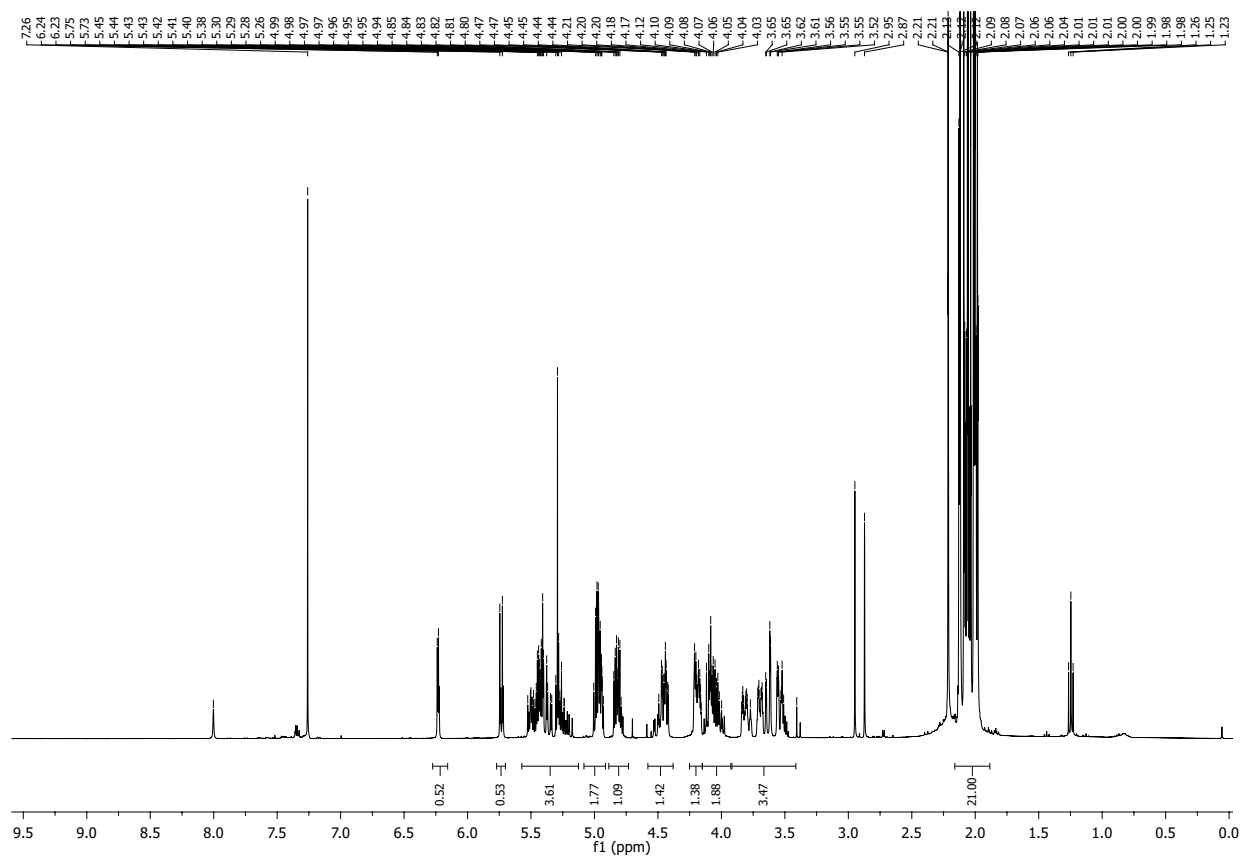




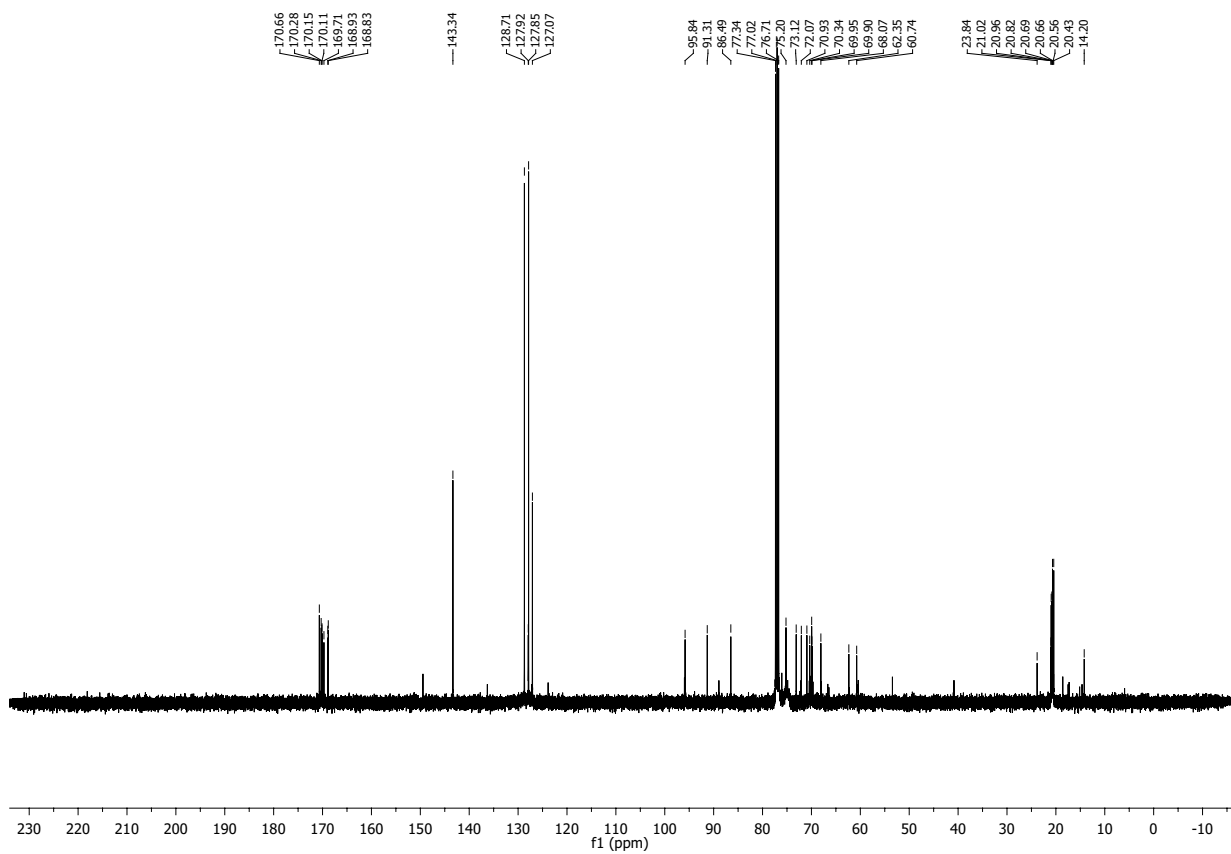
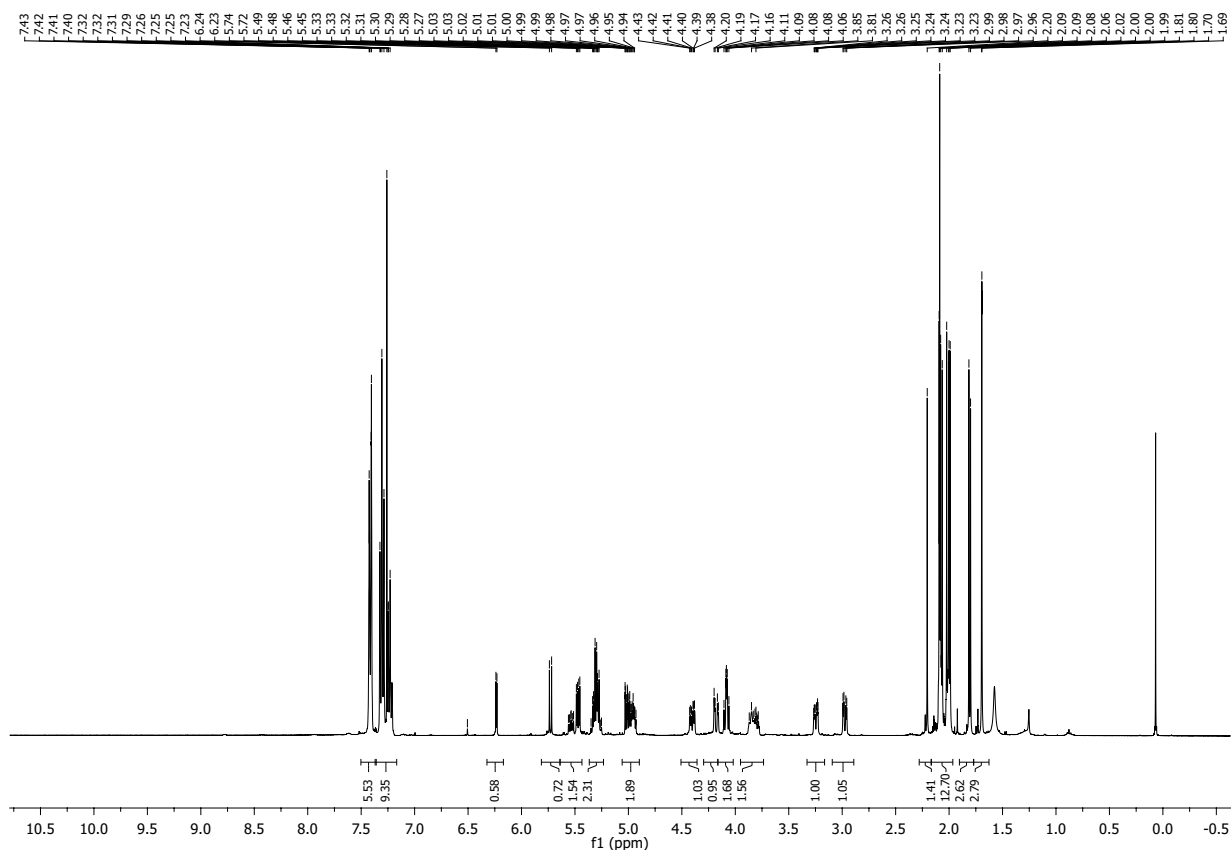
1,2,3,6,2',3'-hexa-O-acetyl-4',6'-O-benzylidene-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **6**



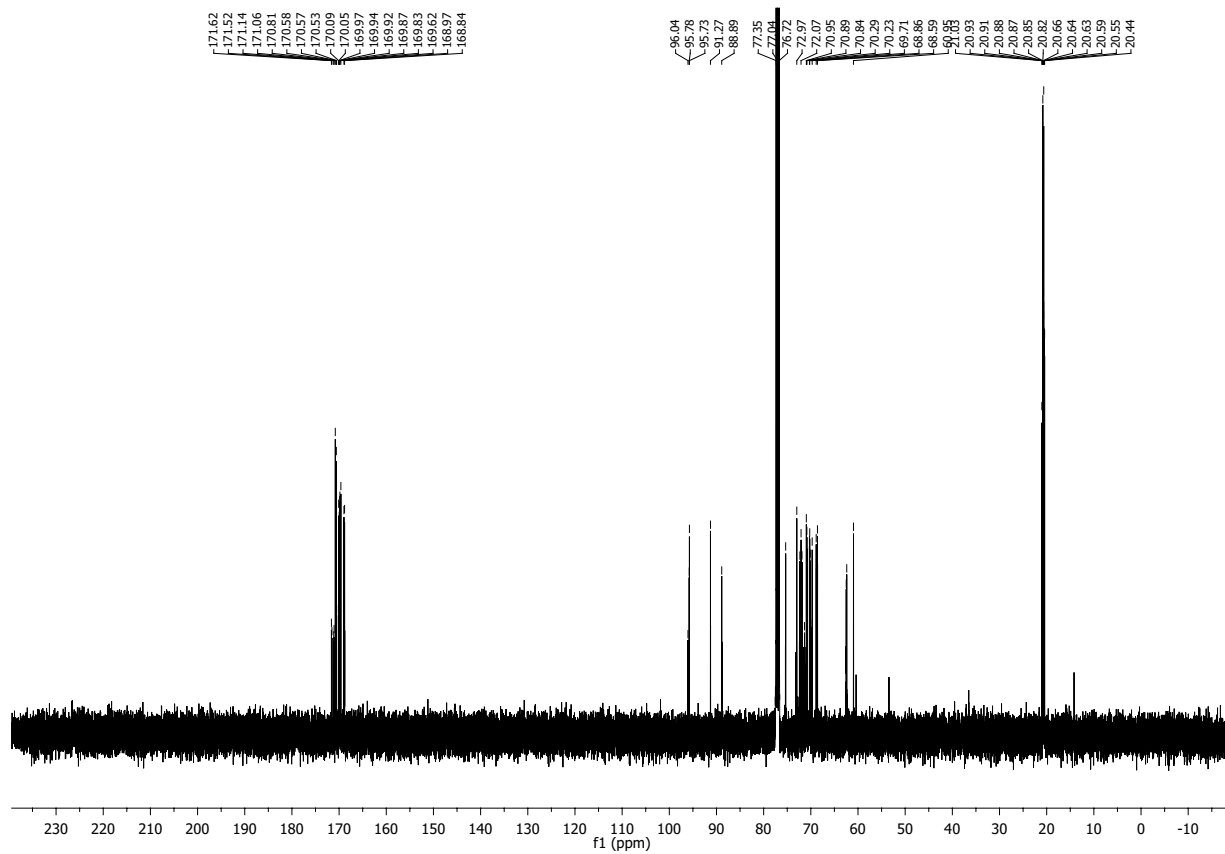
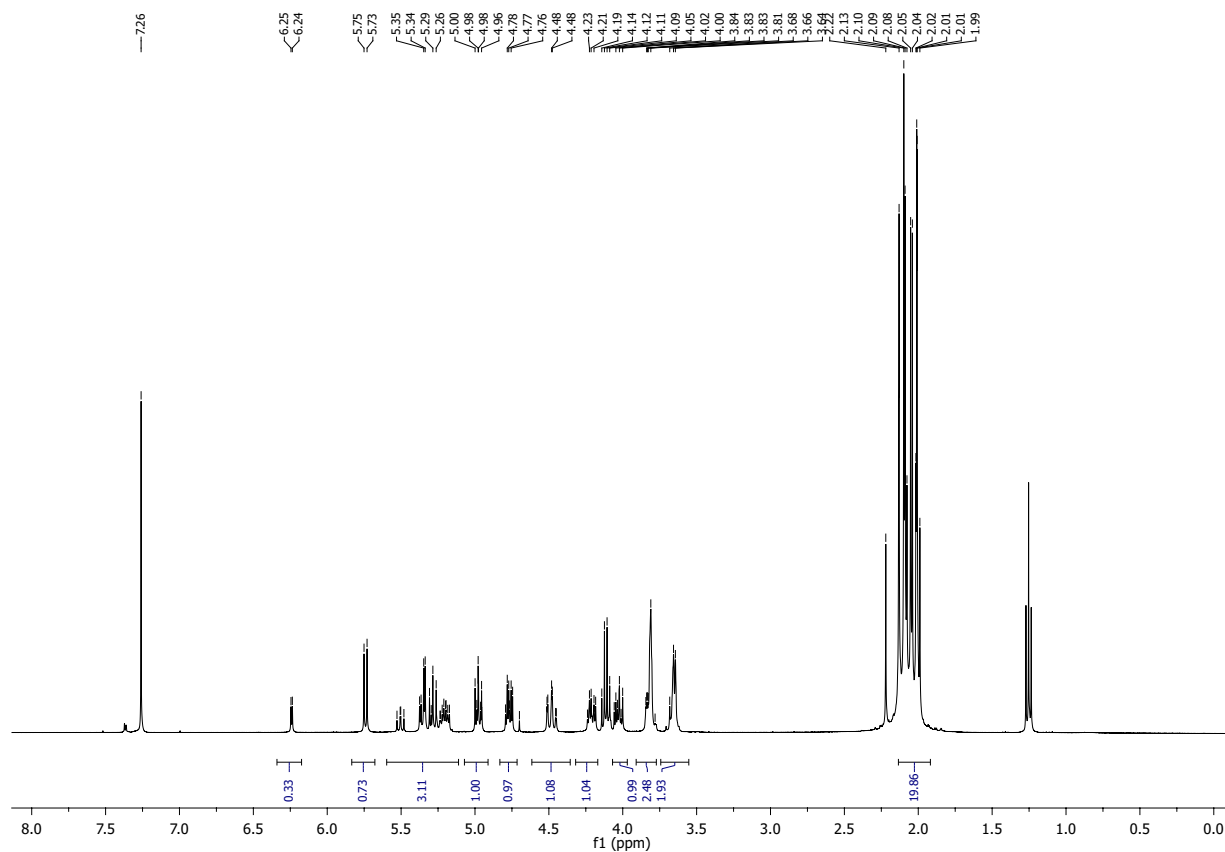
1,2,3,6,2',3'-hexa-O-acetyl-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **7**



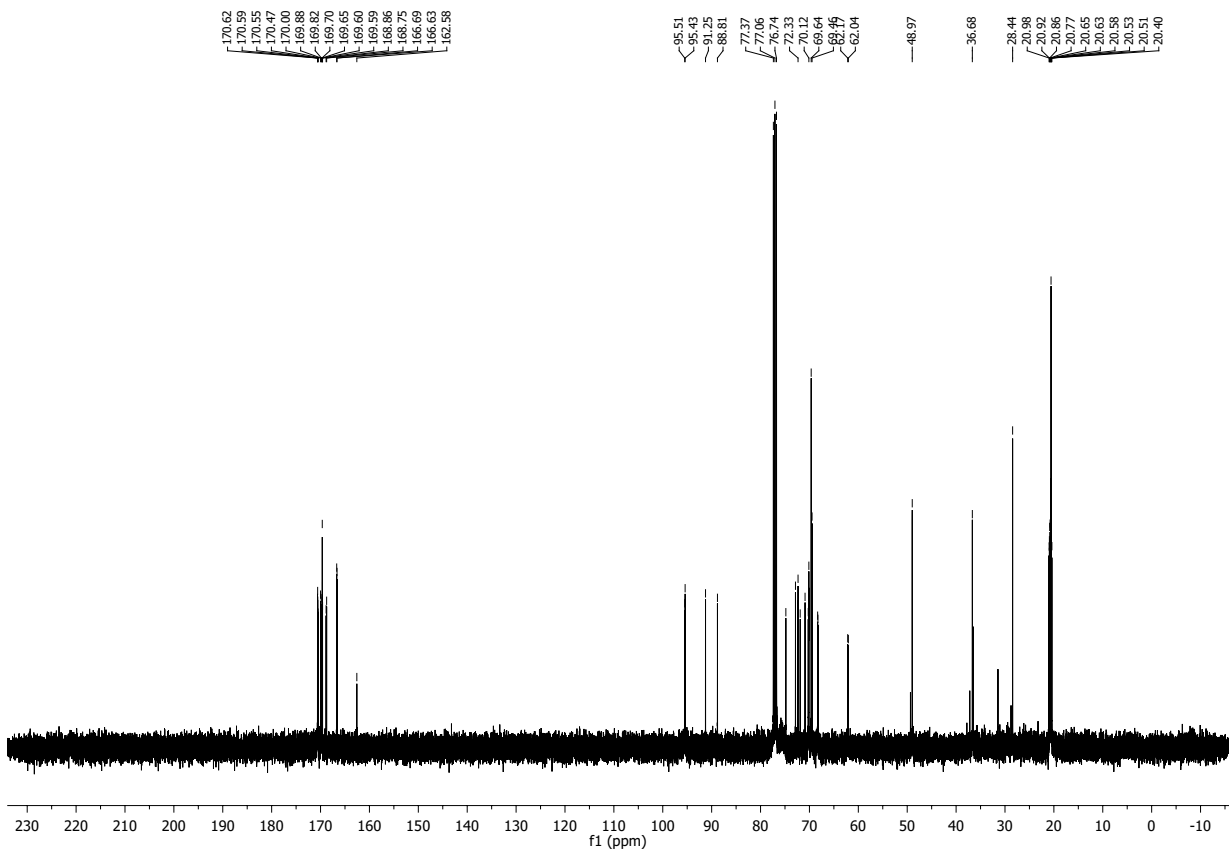
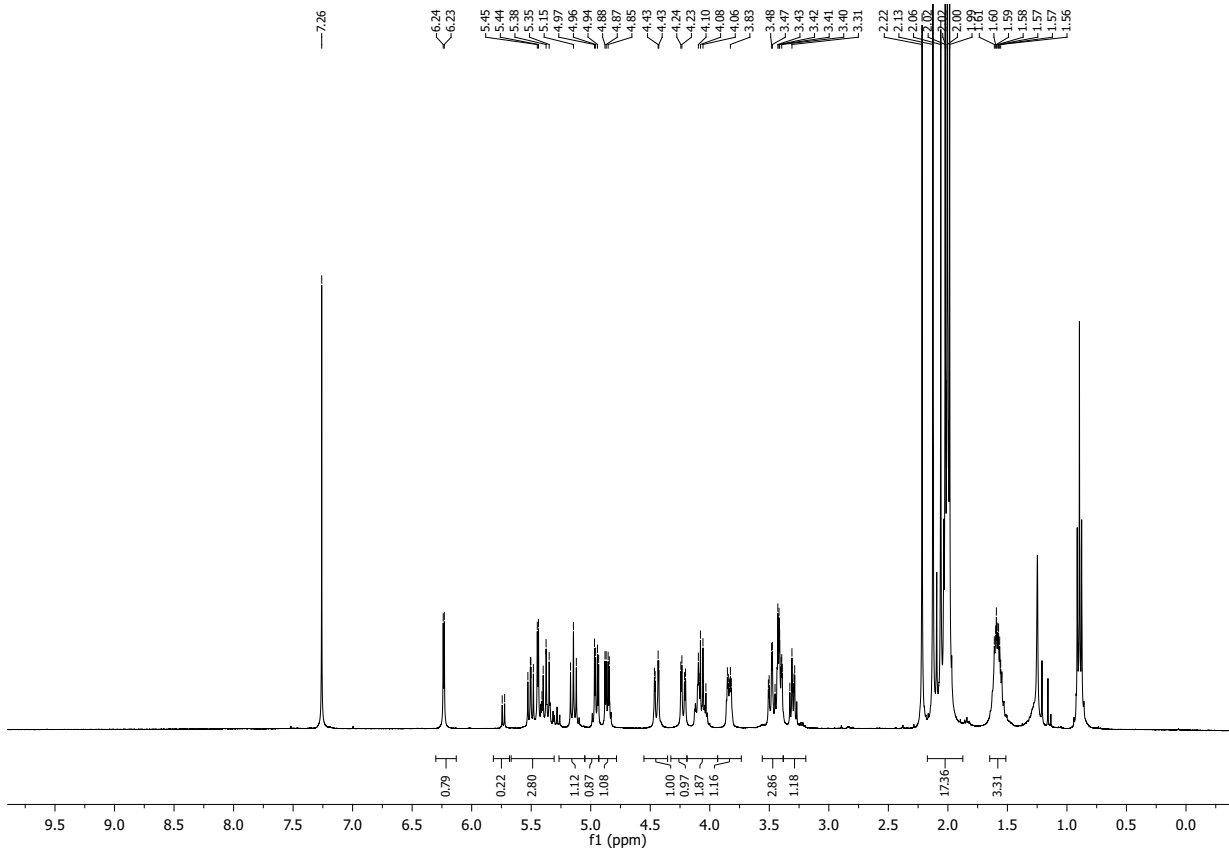
1,2,3,6,2',3'-hexa-O-acetyl-6'-O-trityl-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **8**



1,2,3,6,2',3',4'-hepta-O-acetyl-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **9**

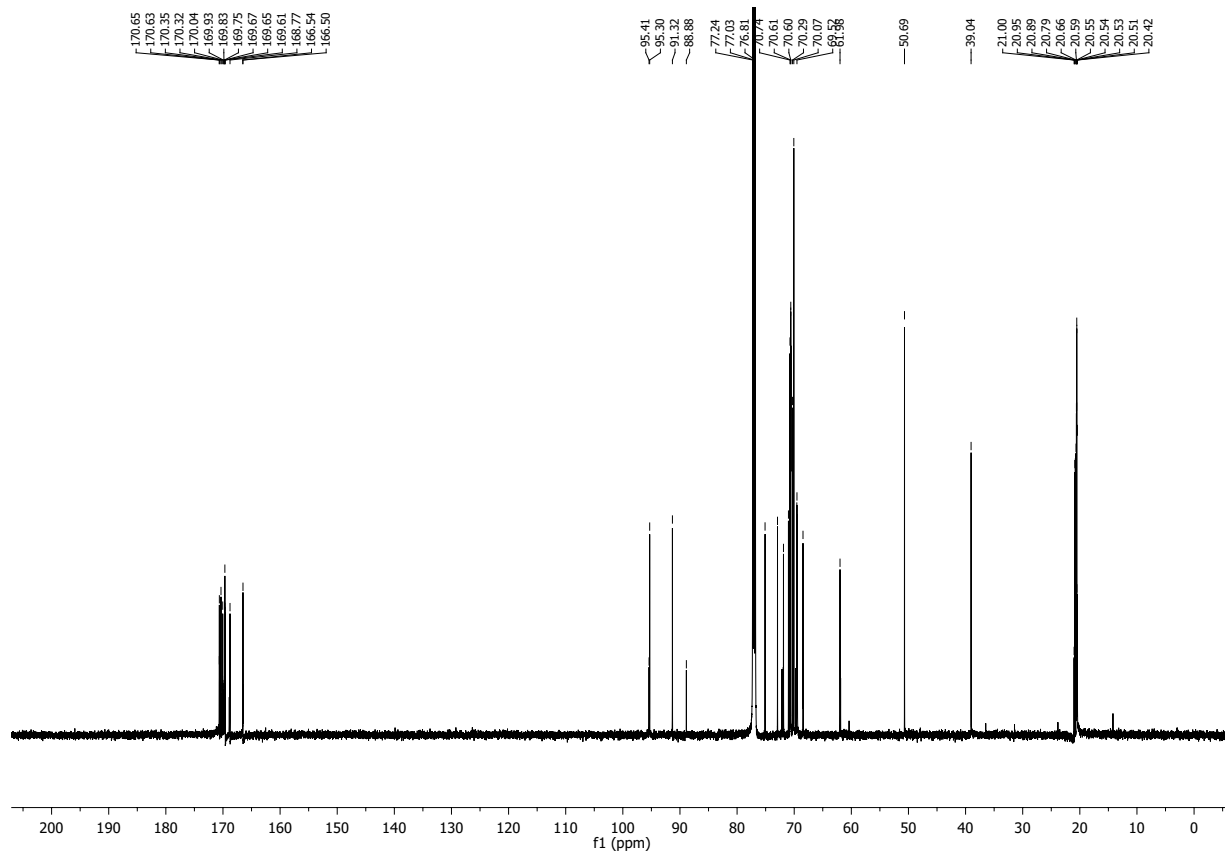
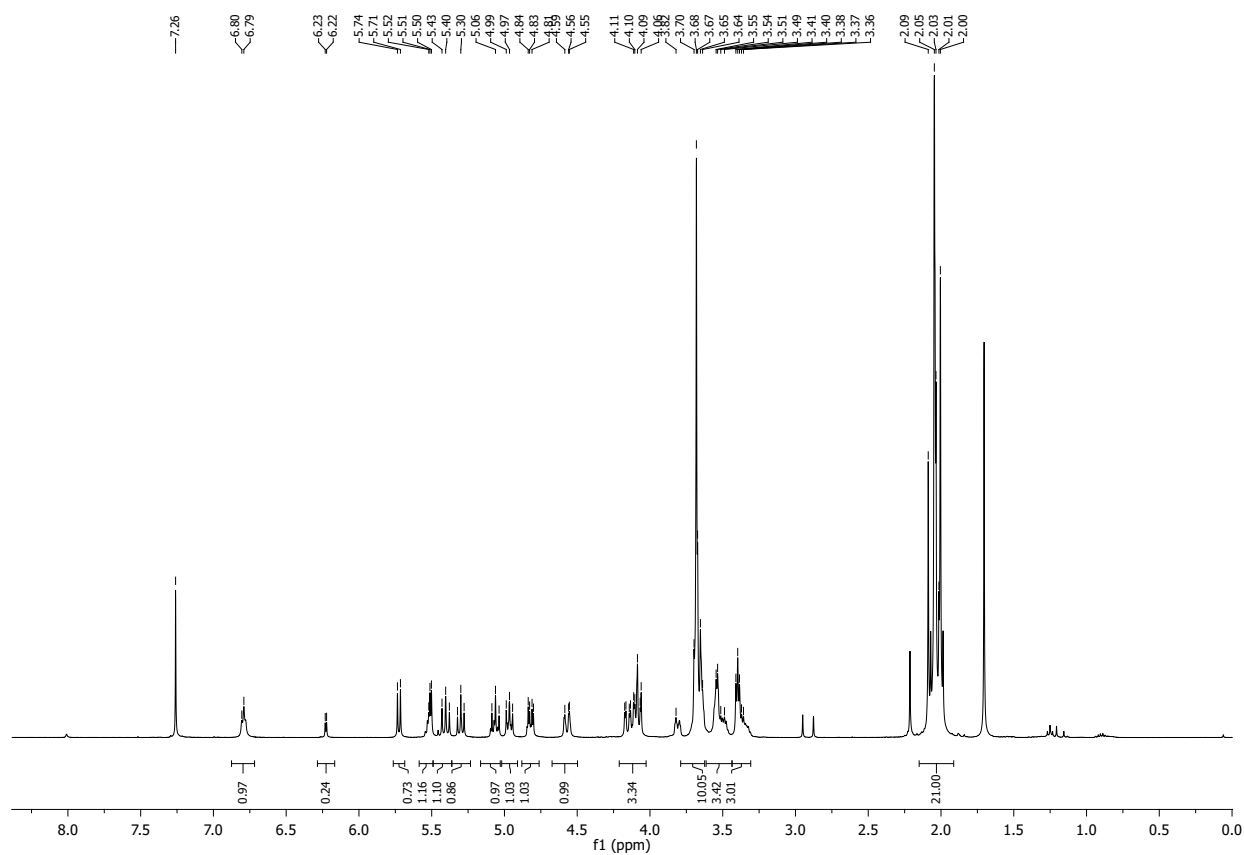


1,2,3,6,2',3',4'-hepta-O-acetyl-6'-O-((3-azidopropyl)carbamoyl)4-O-( $\alpha$ -D-glucopyranuronosyl)- $\beta$ -D-glucopyranose, **12**

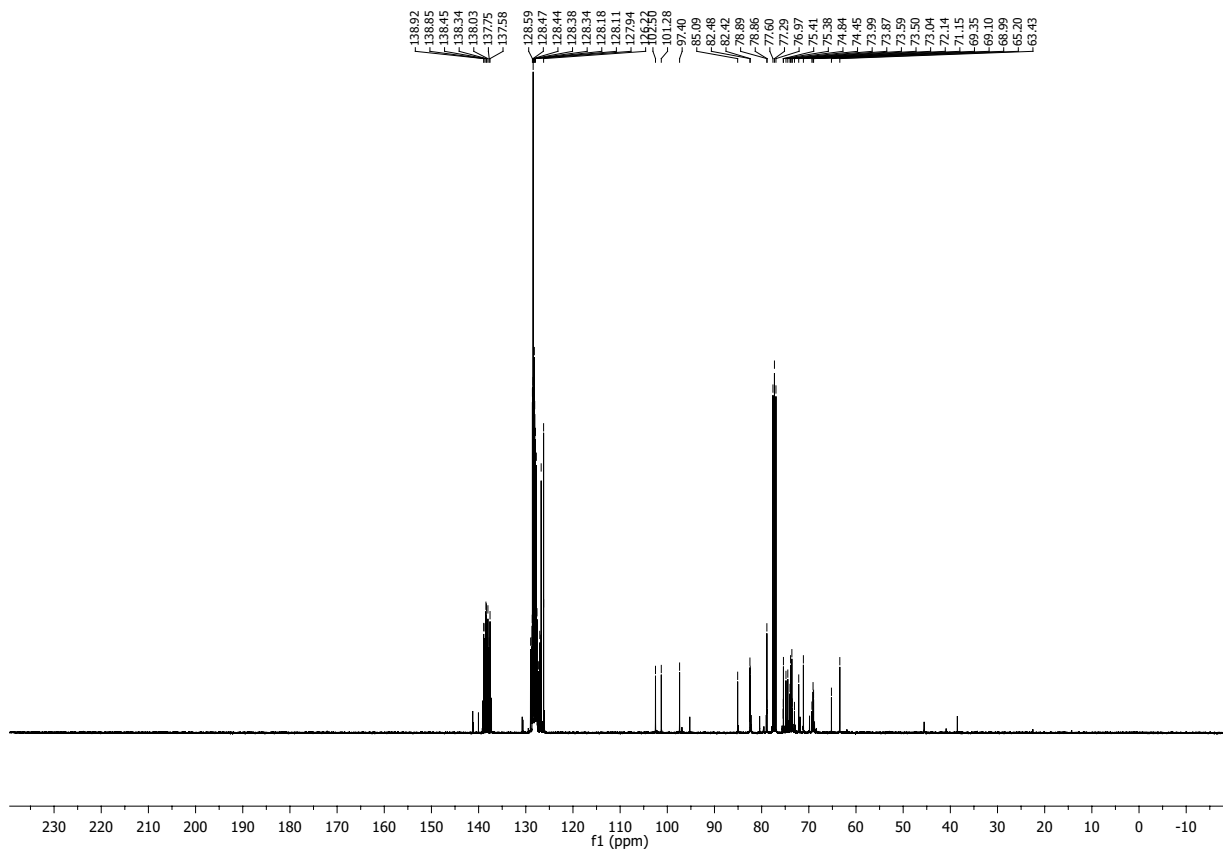
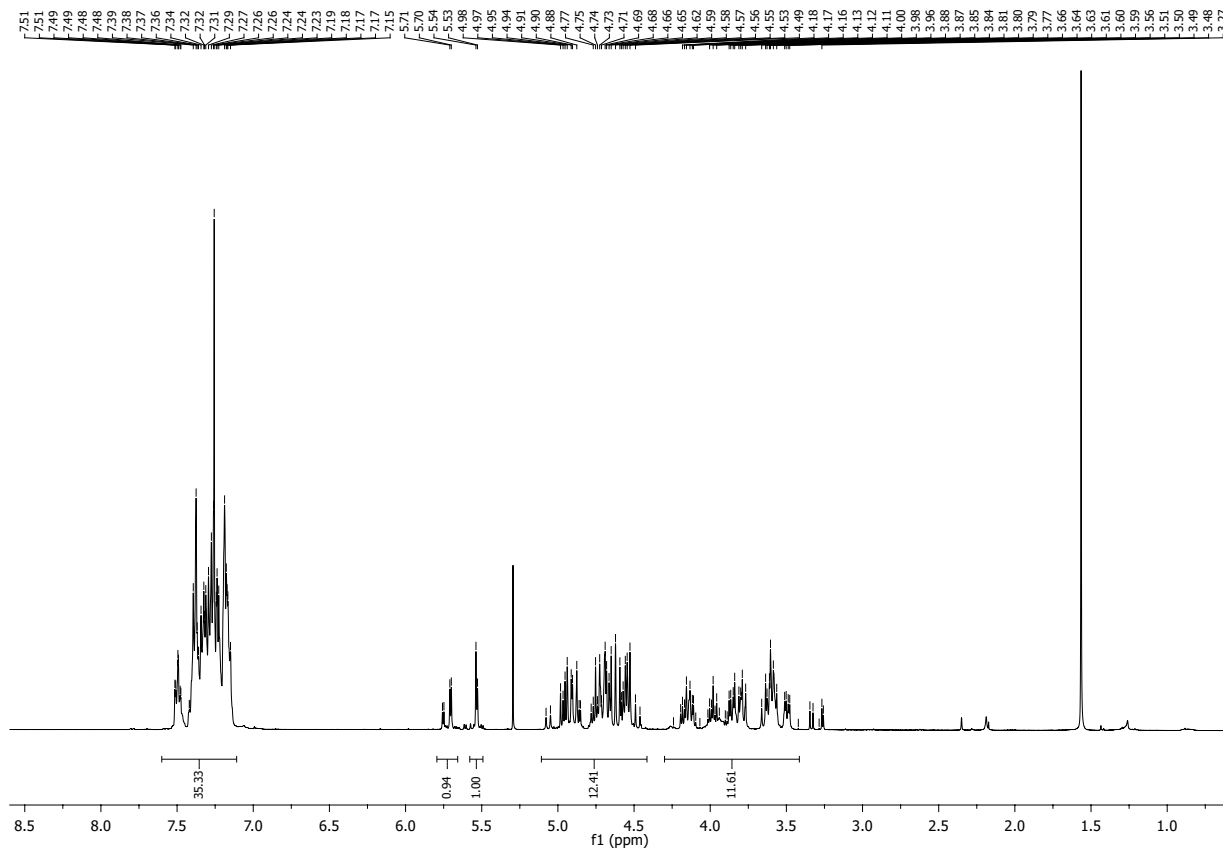




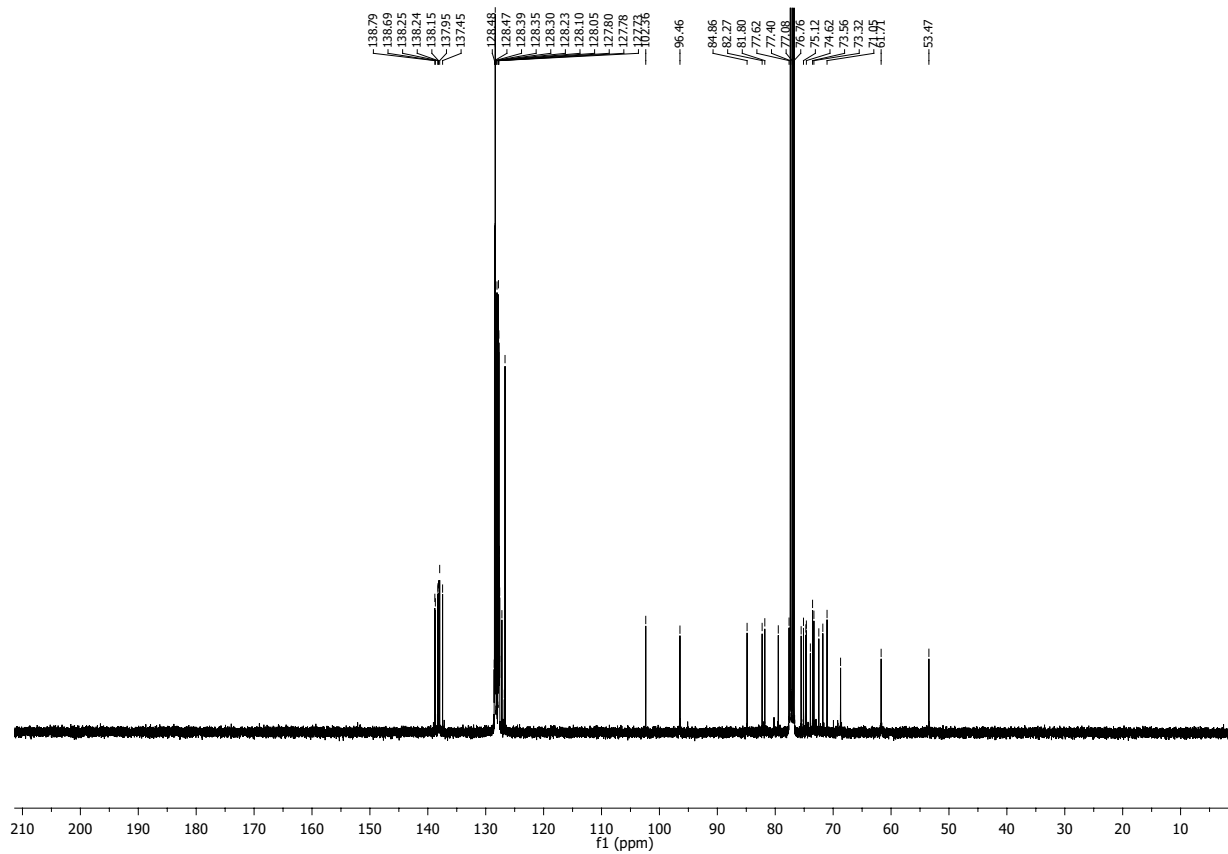
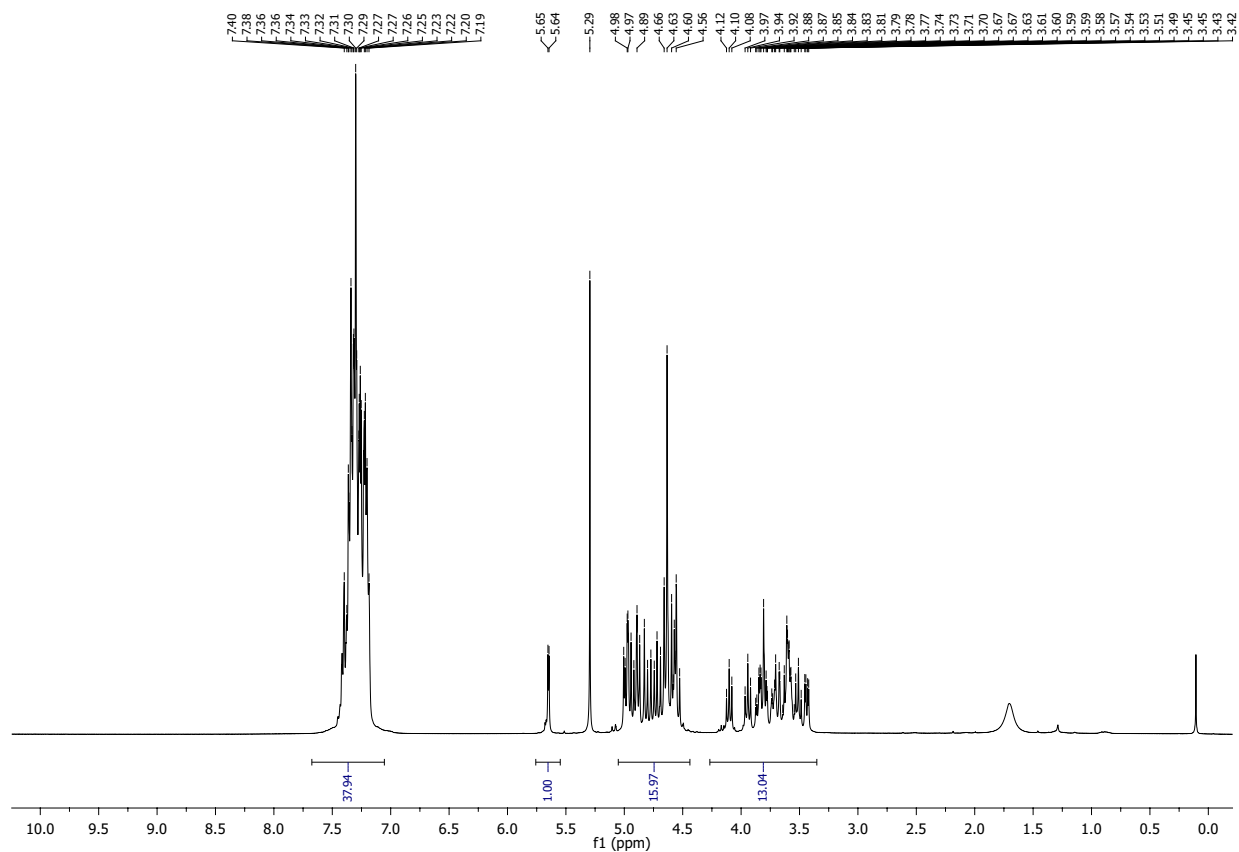
1,2,3,6,2',3',4'-hepta-O-acetyl-6'-((2-(2-azidoethoxy)ethyl)carbamoyl)-4-O-( $\alpha$ -D-glucopyranuronosyl)- $\beta$ -D-glucopyranose, **13**



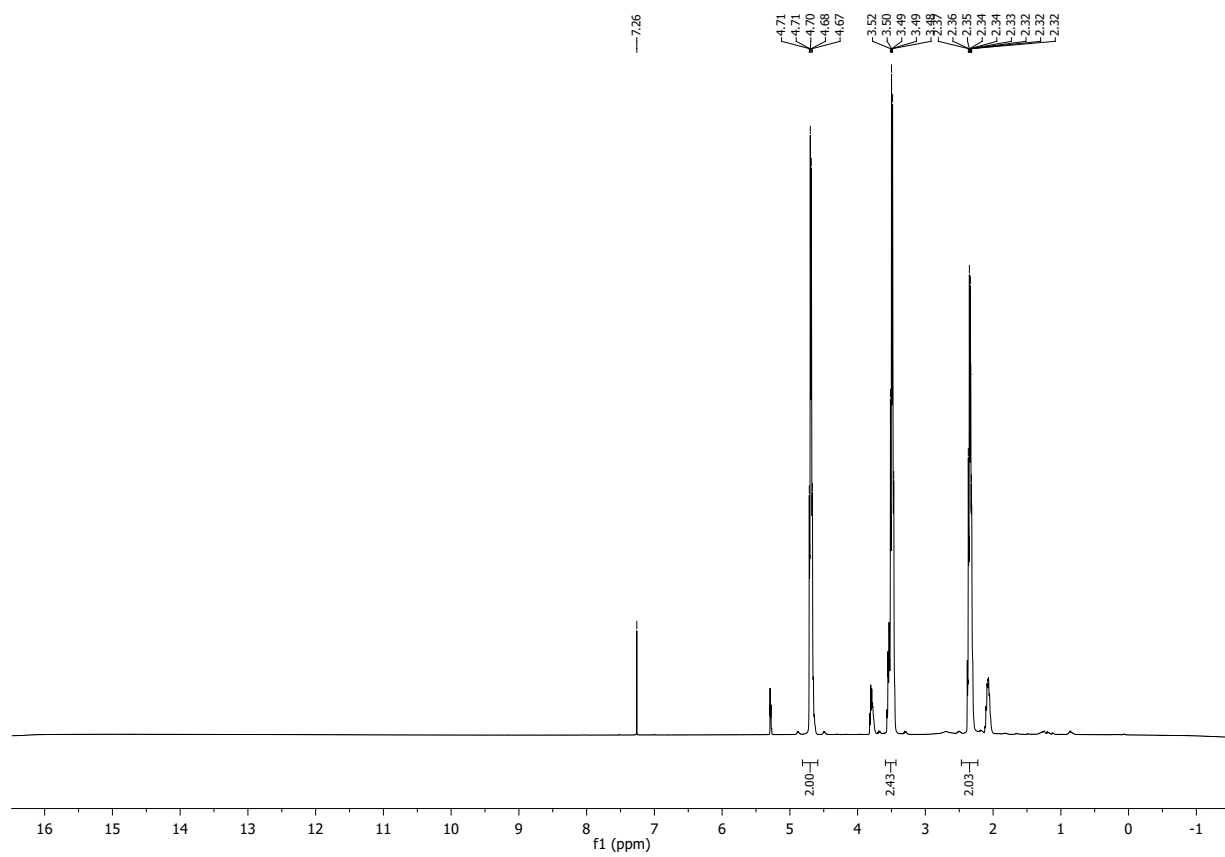
1,2,3,6,2',3'-hexa-O-benzyl-4',6'-O-benzylidene-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **16**



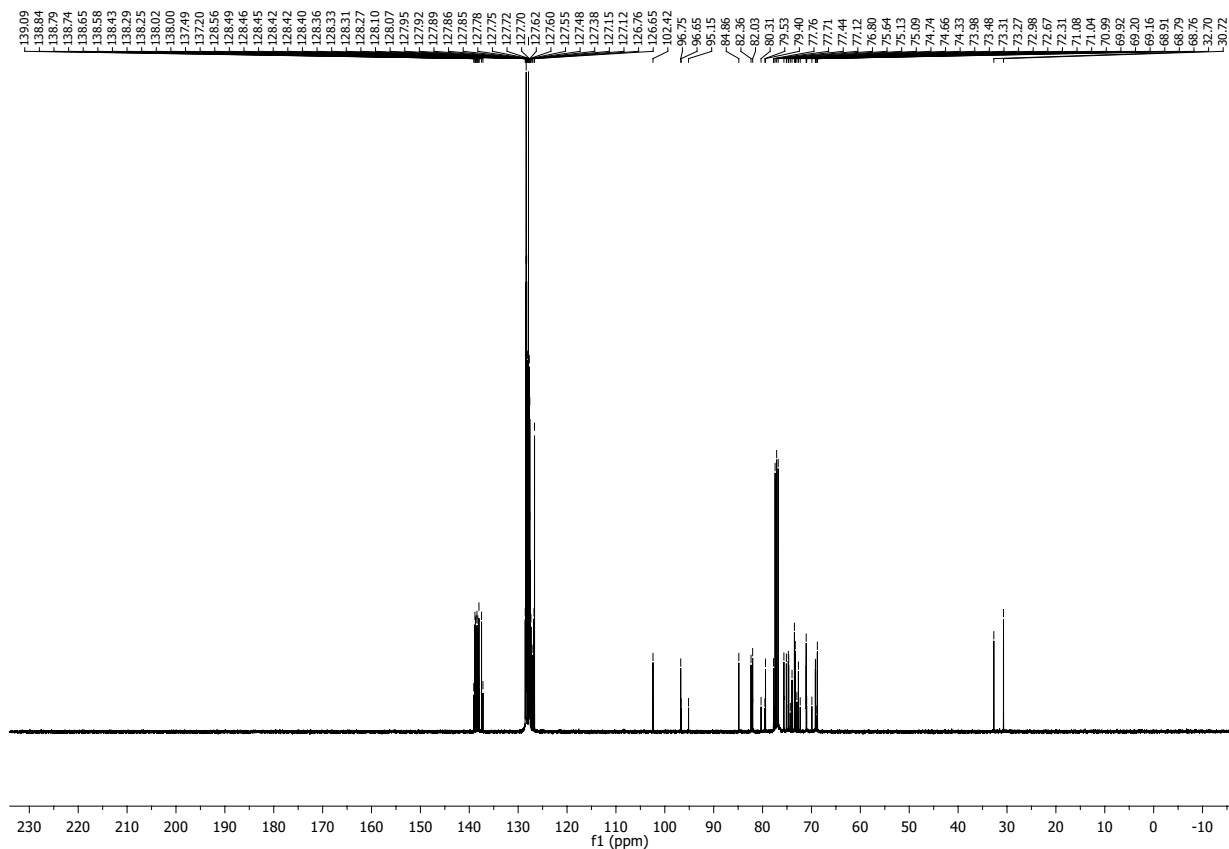
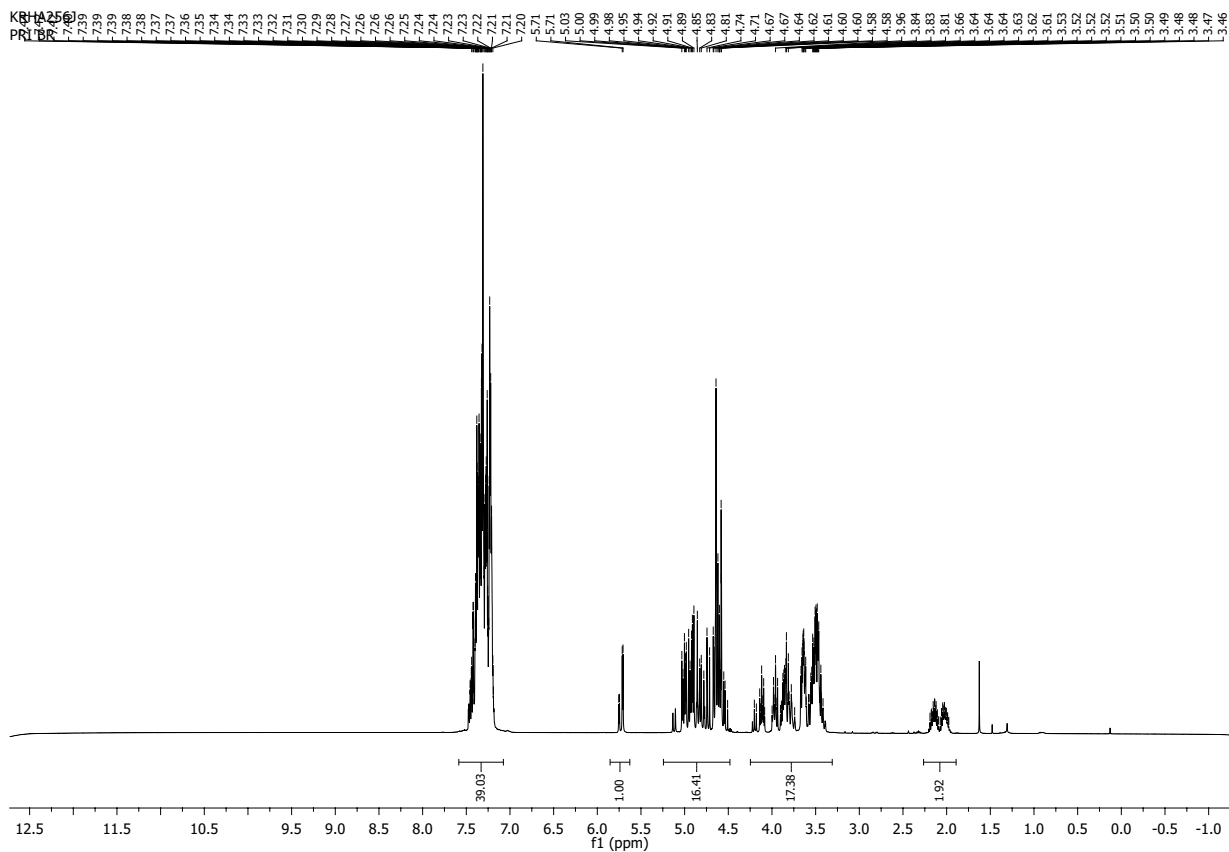
1,2,3,6,2',3',4'-hepta-O-benzyl-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **17**



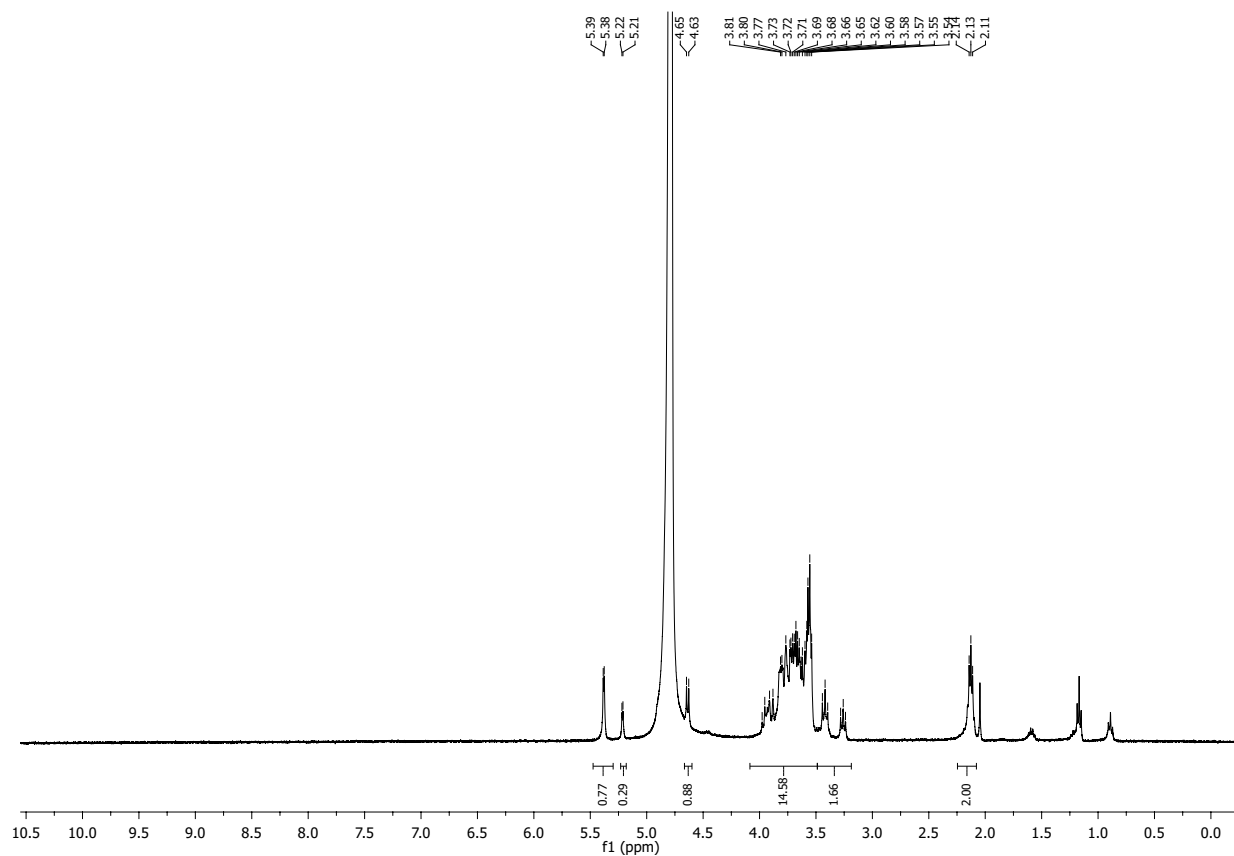
3-bromopropyl trifluoromethanesulfonate, **21**



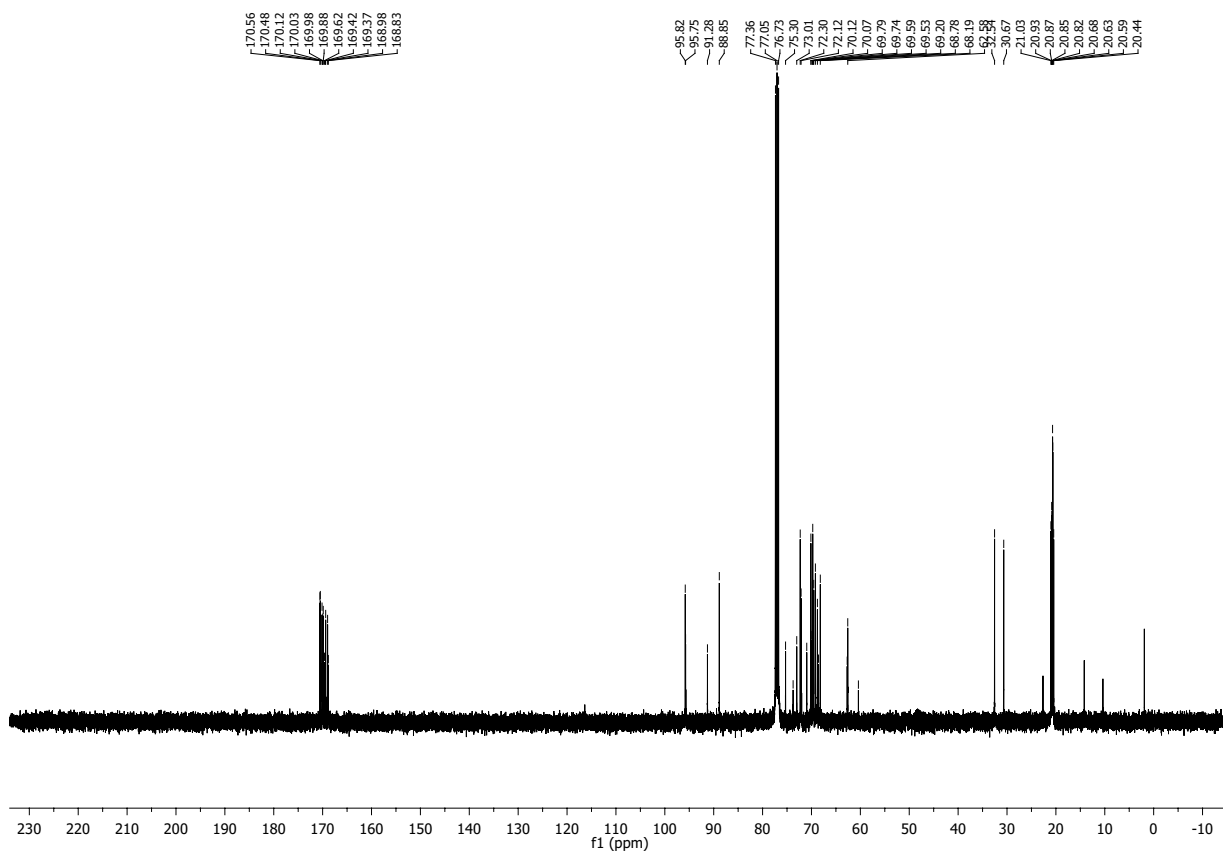
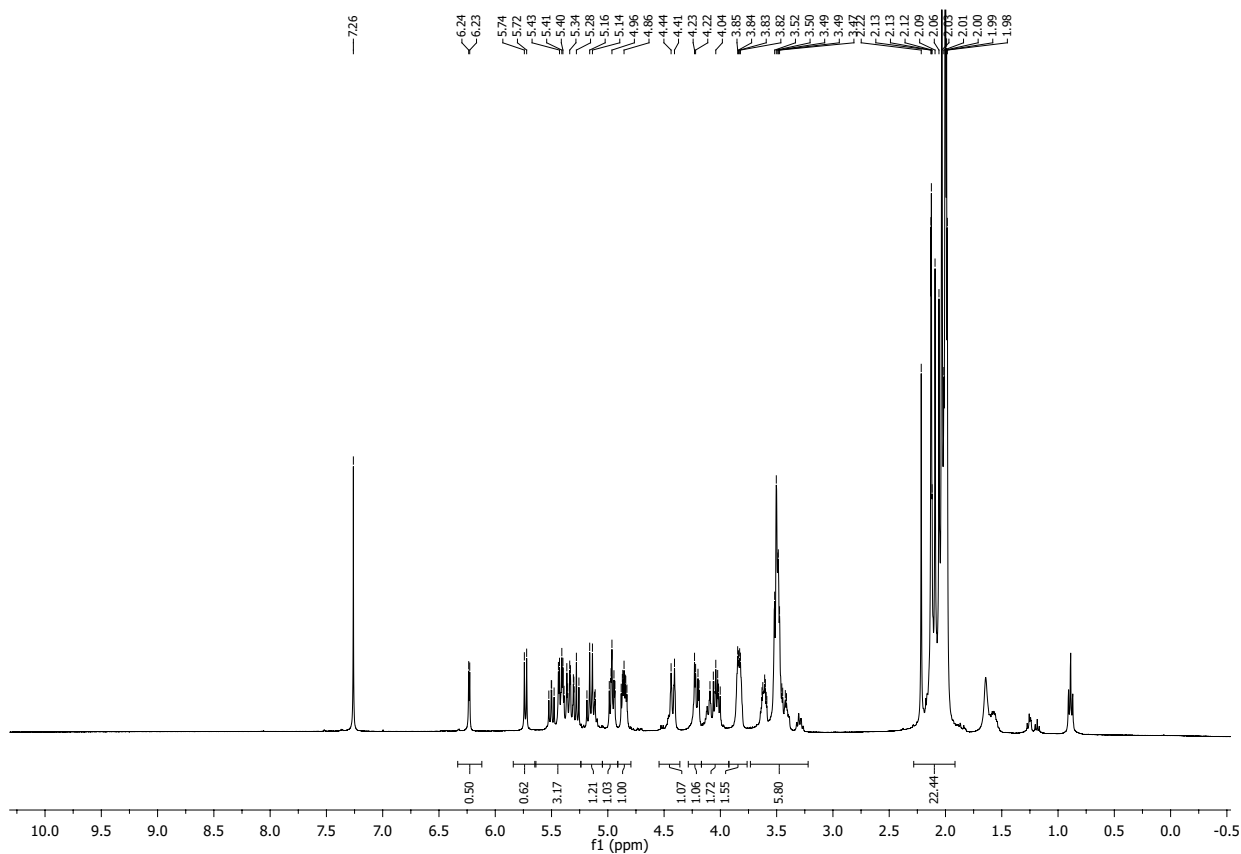
1,2,3,6,2',3',4'-hepta-O-benzyl-6'-O-(3-bromopropyl)-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **19**



6'-O-(3-bromopropyl)-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **24**



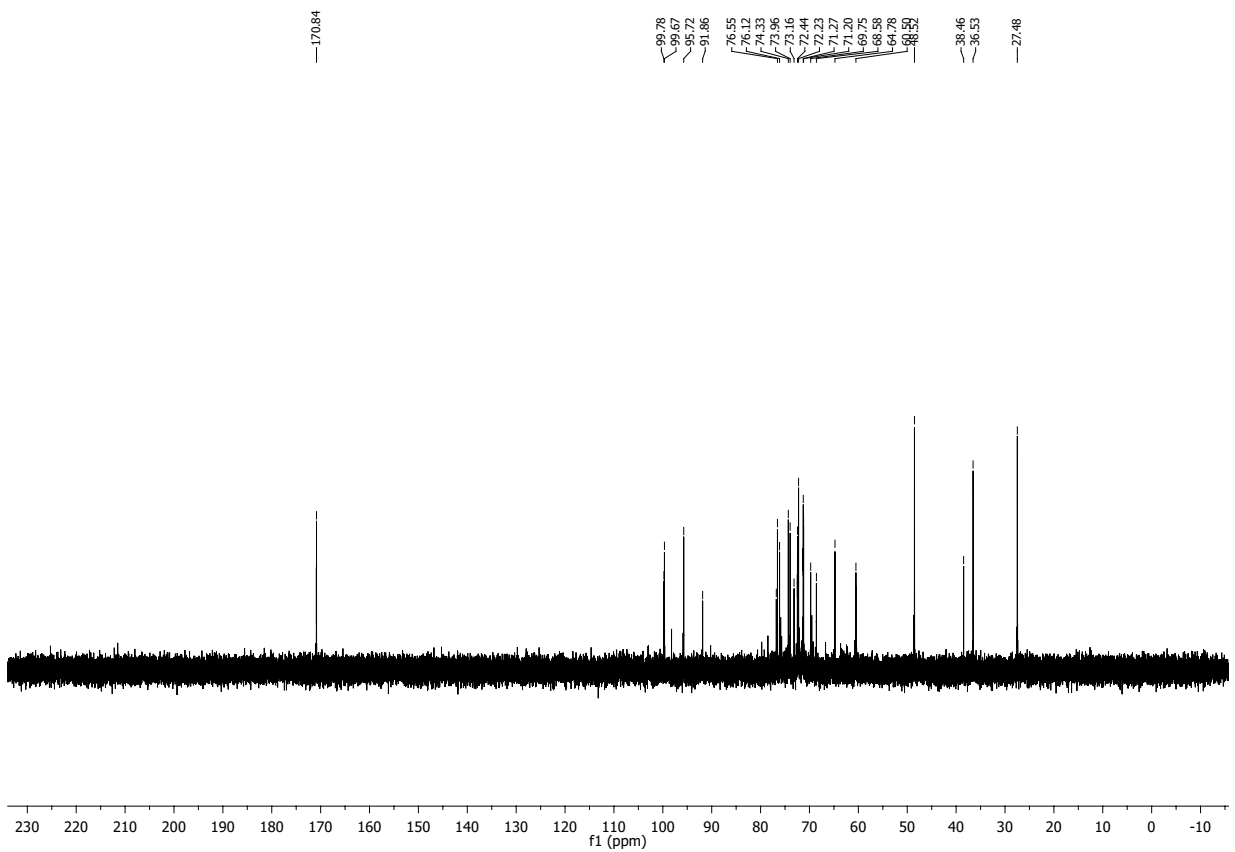
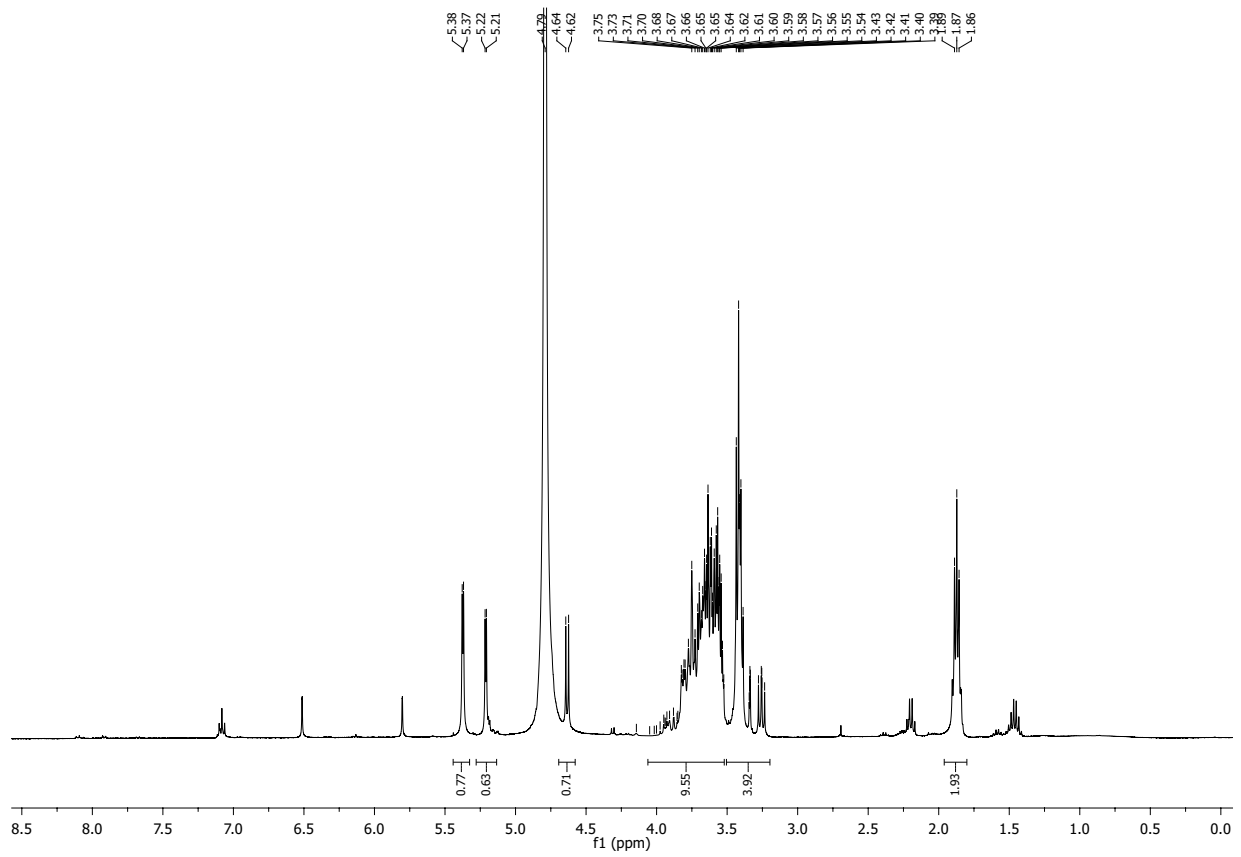
1,2,3,6,2',3',4'-hepta-O-acetyl-6'-O-(3-bromopropyl)-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **14**



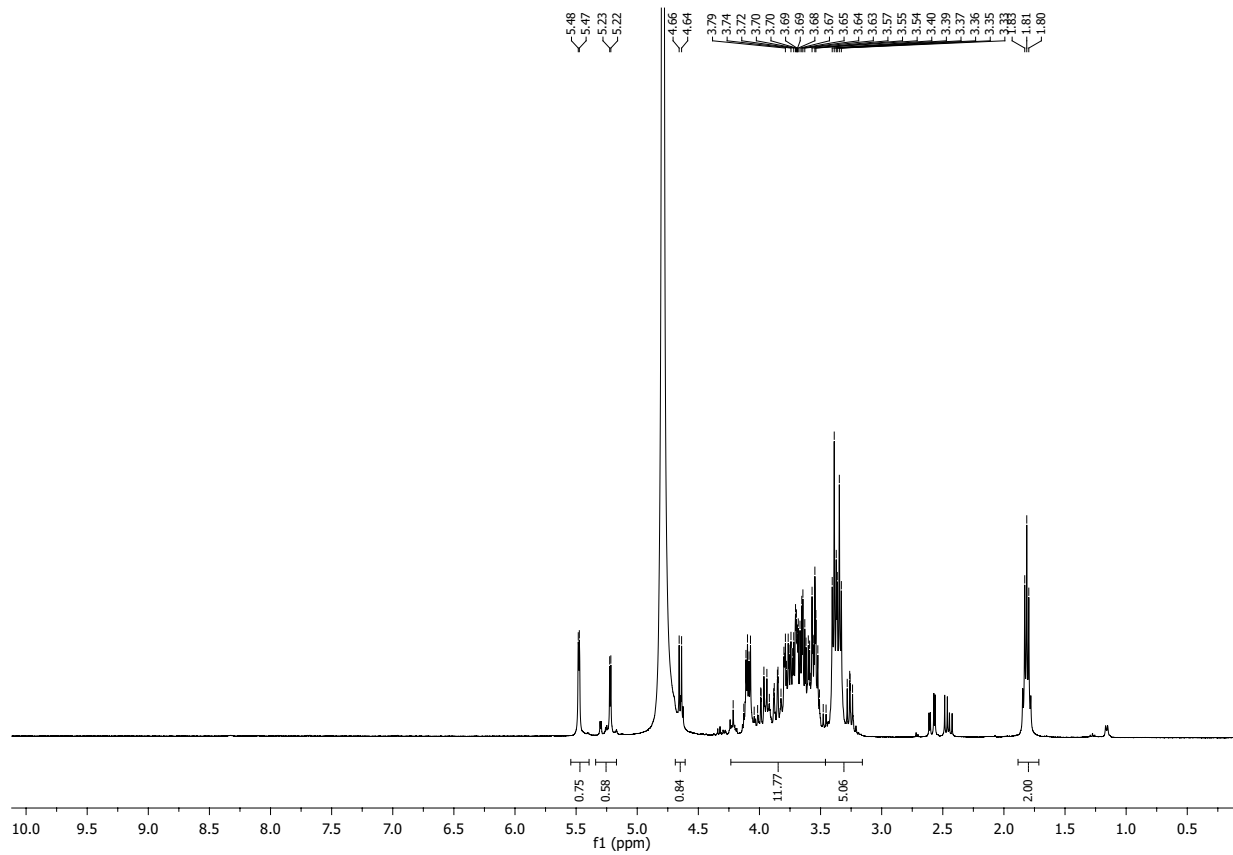




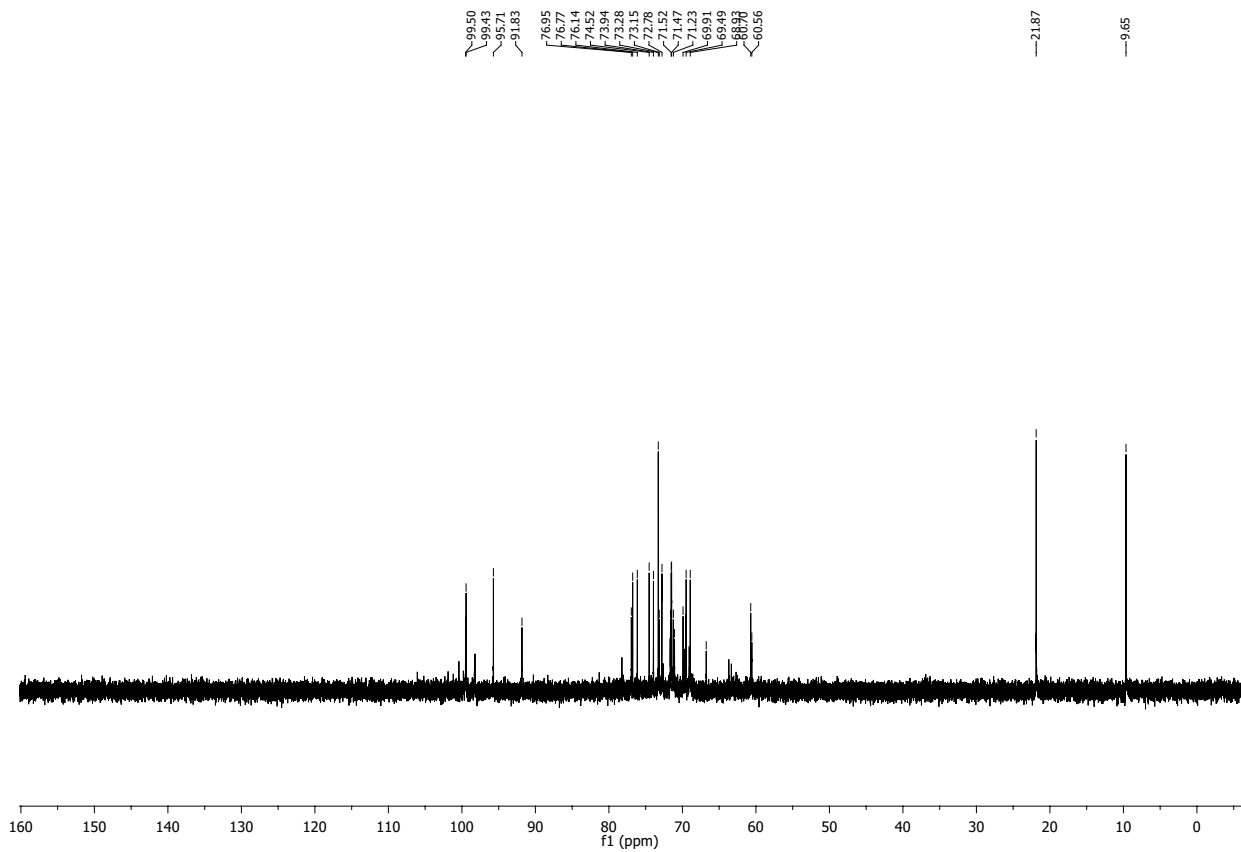
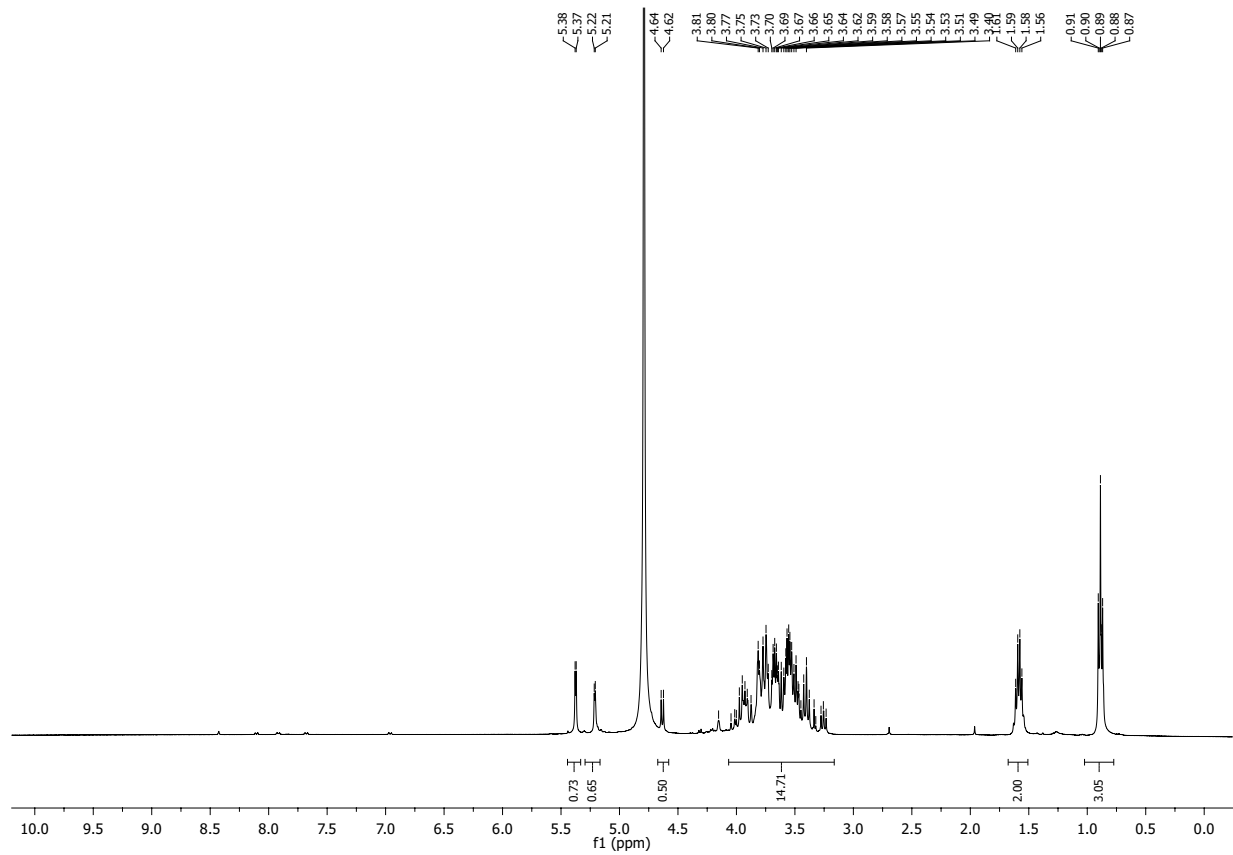
6'-O-((3-azidopropyl)carbamoyl)4-O-( $\alpha$ -D-glucopyranuronosyl)- $\beta$ -D-glucopyranose, BOT\_41



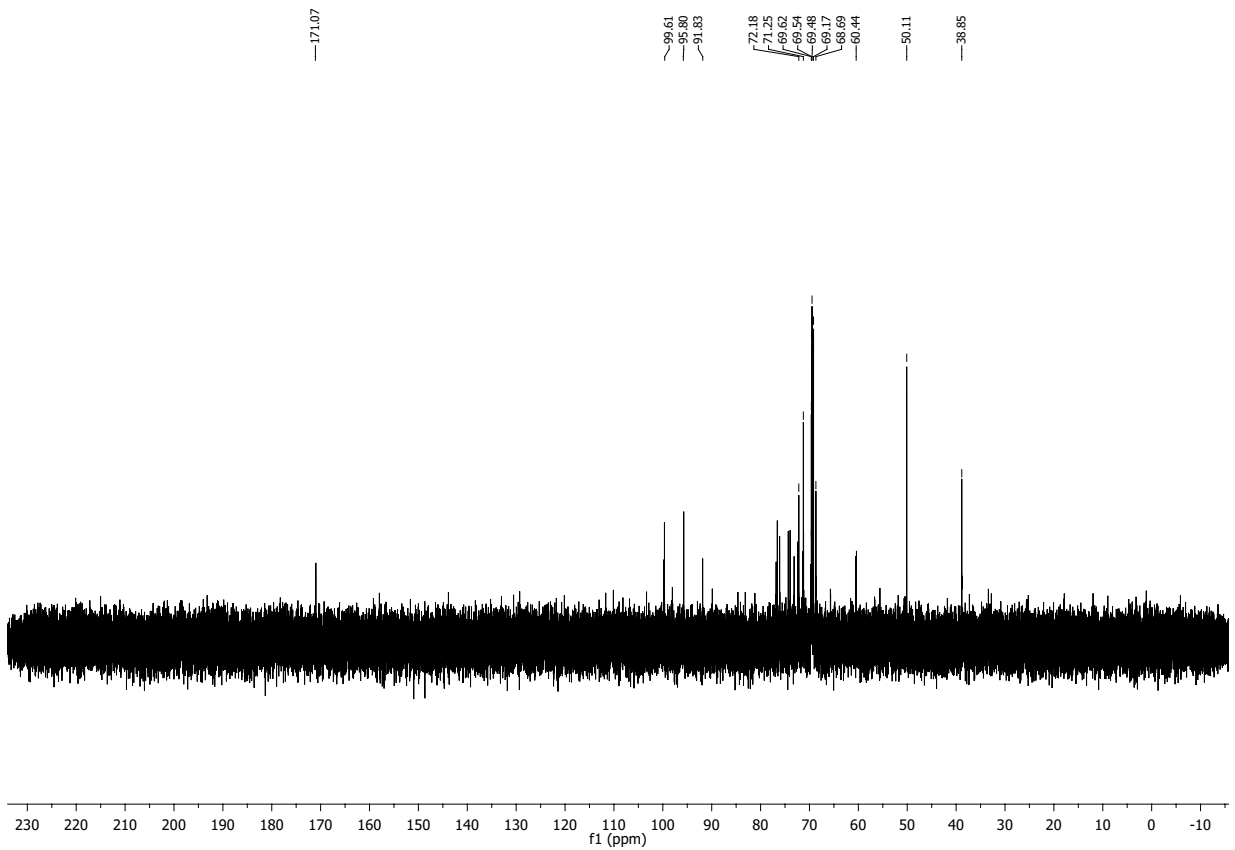
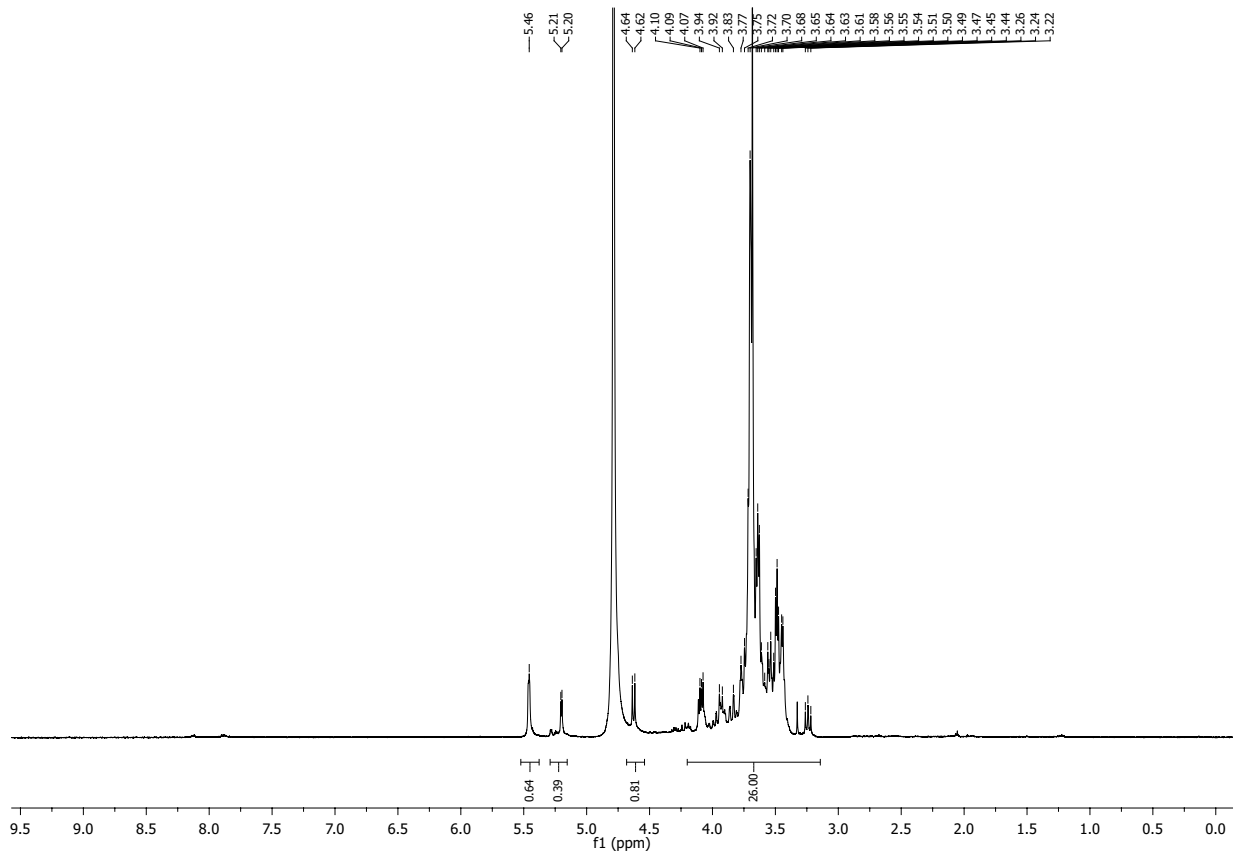
6'-O-(3-azidopropyl)-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, BOT\_42



6'-O-propyl-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, BOT\_43

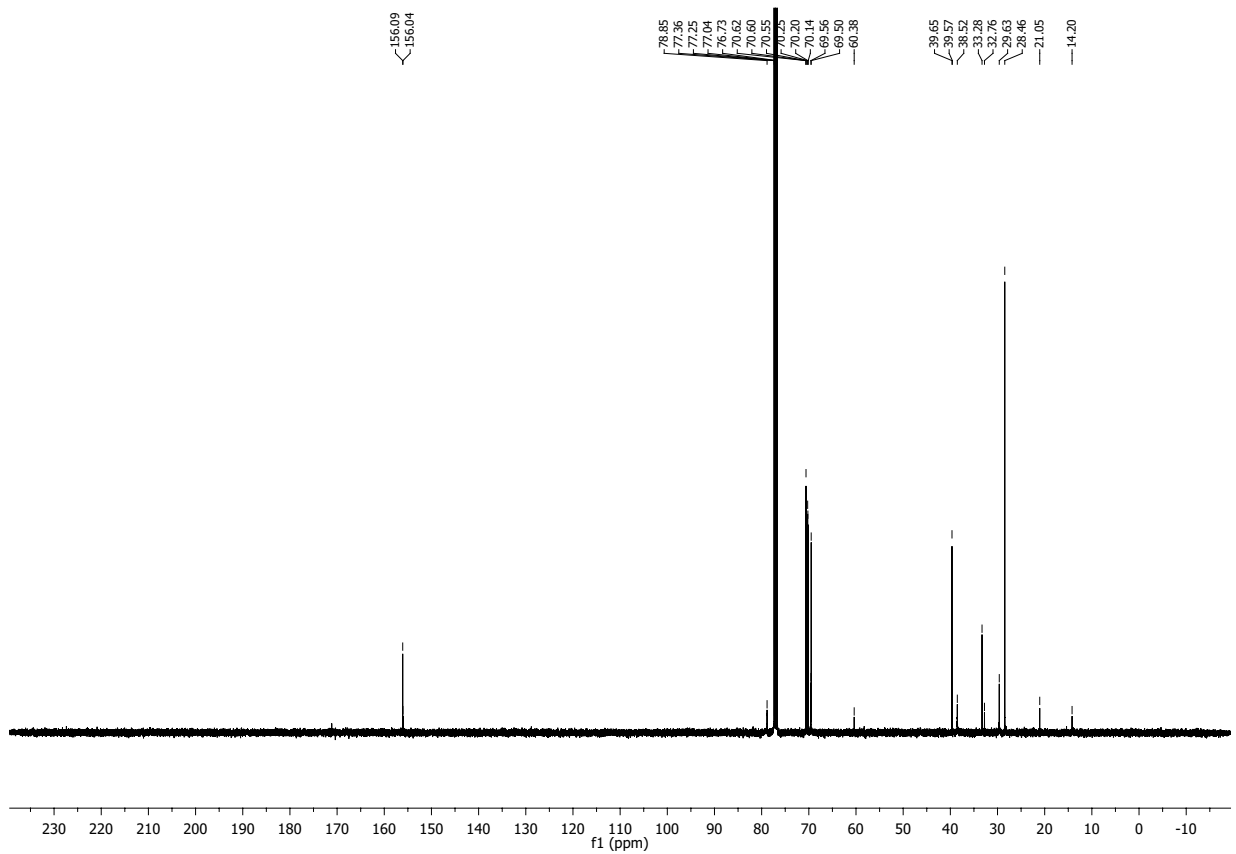
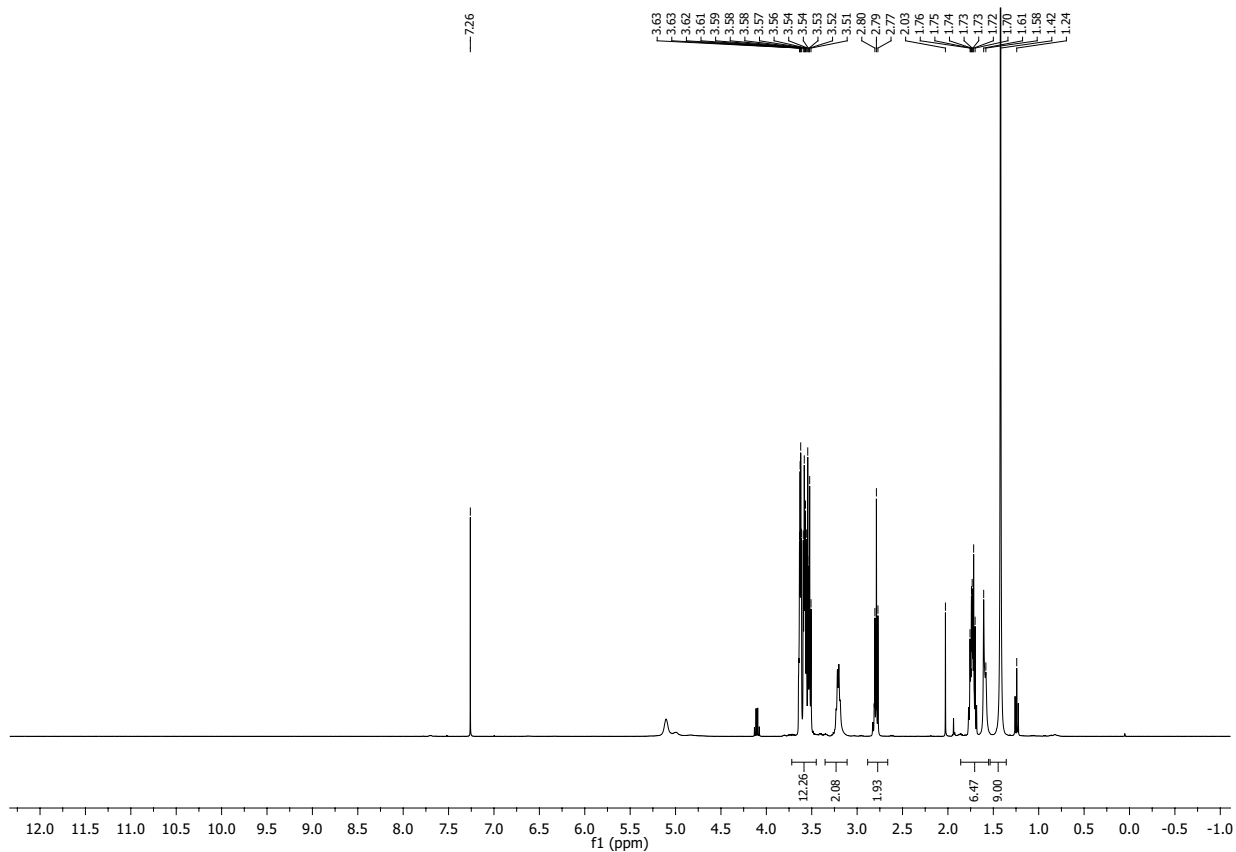


6'-((2-(2-azidoethoxy)ethyl)carbamoyl)-4-O-( $\alpha$ -D-glucopyranuronosyl)- $\beta$ -D-glucopyranose, BOT\_49



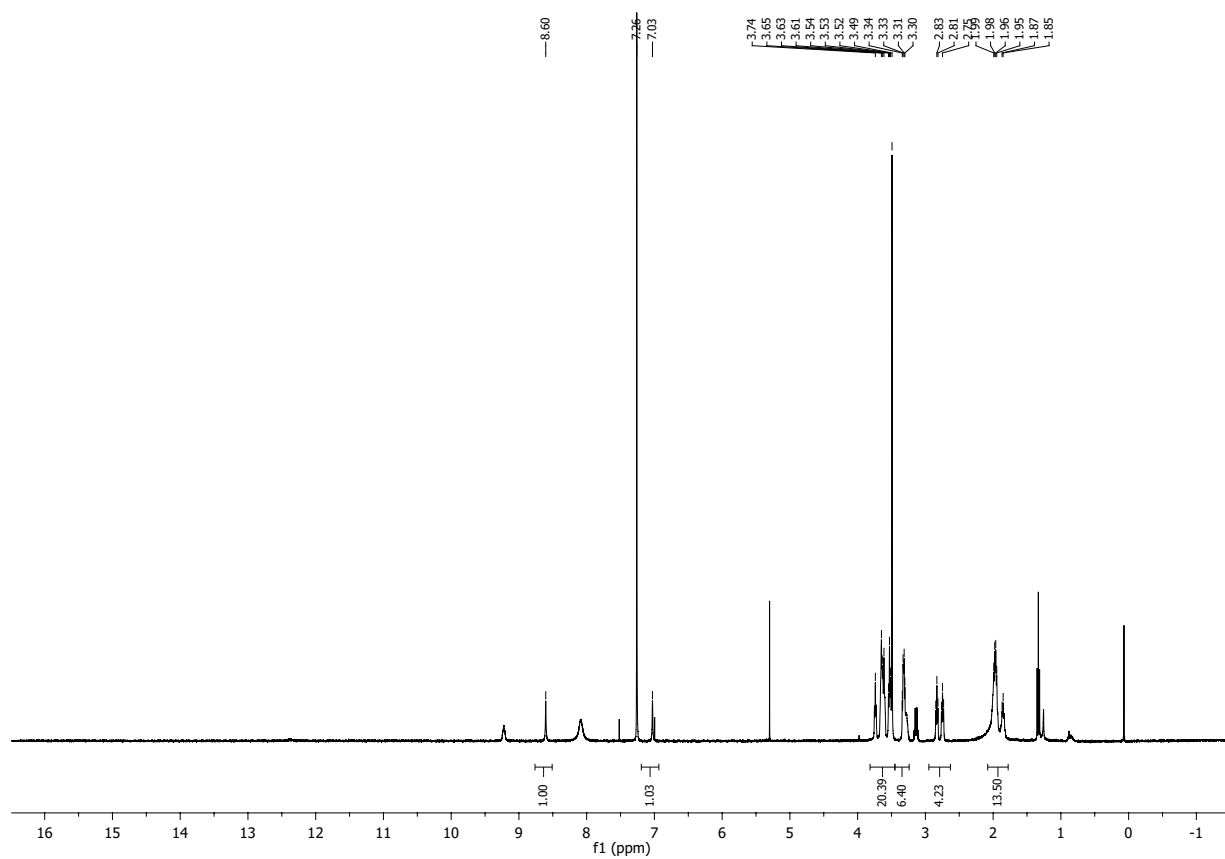


*tert*-butyl (3-(3-aminopropoxy)propyl)carbamate, **28**



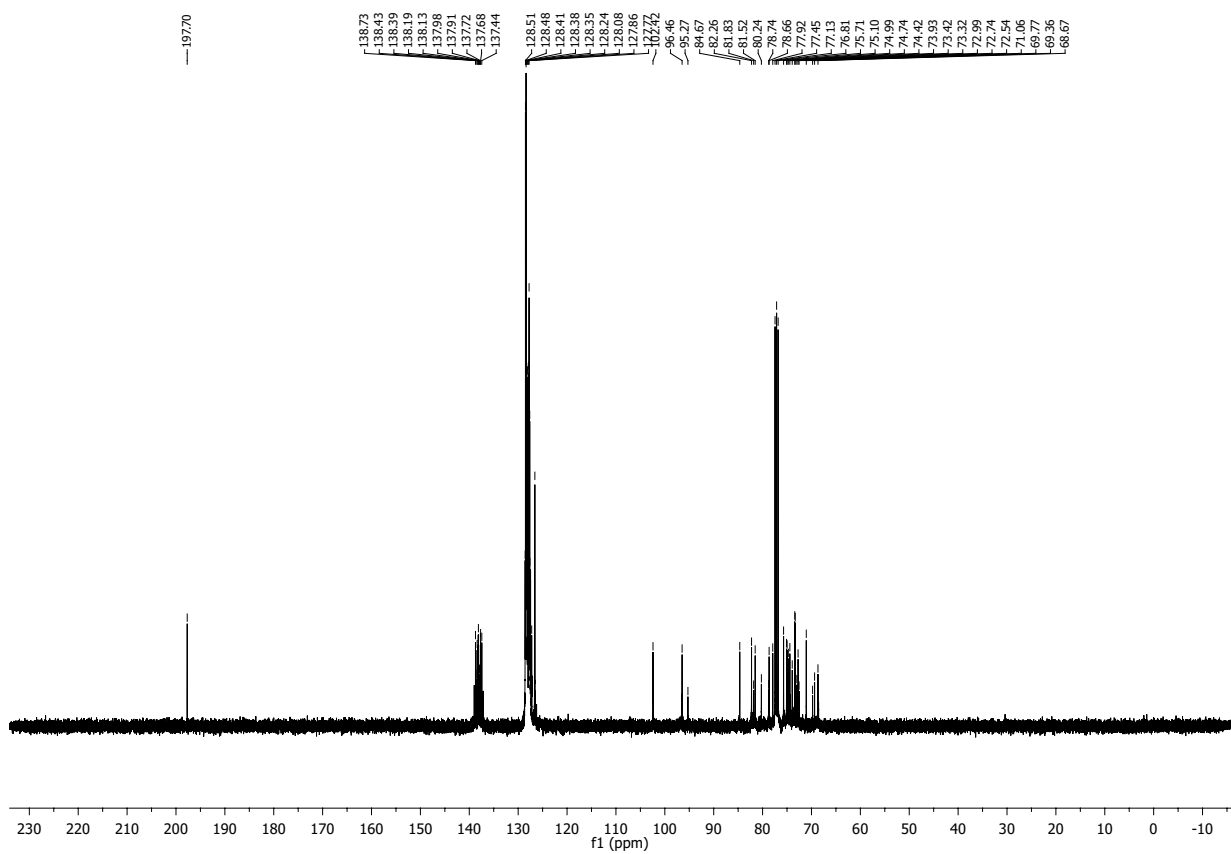
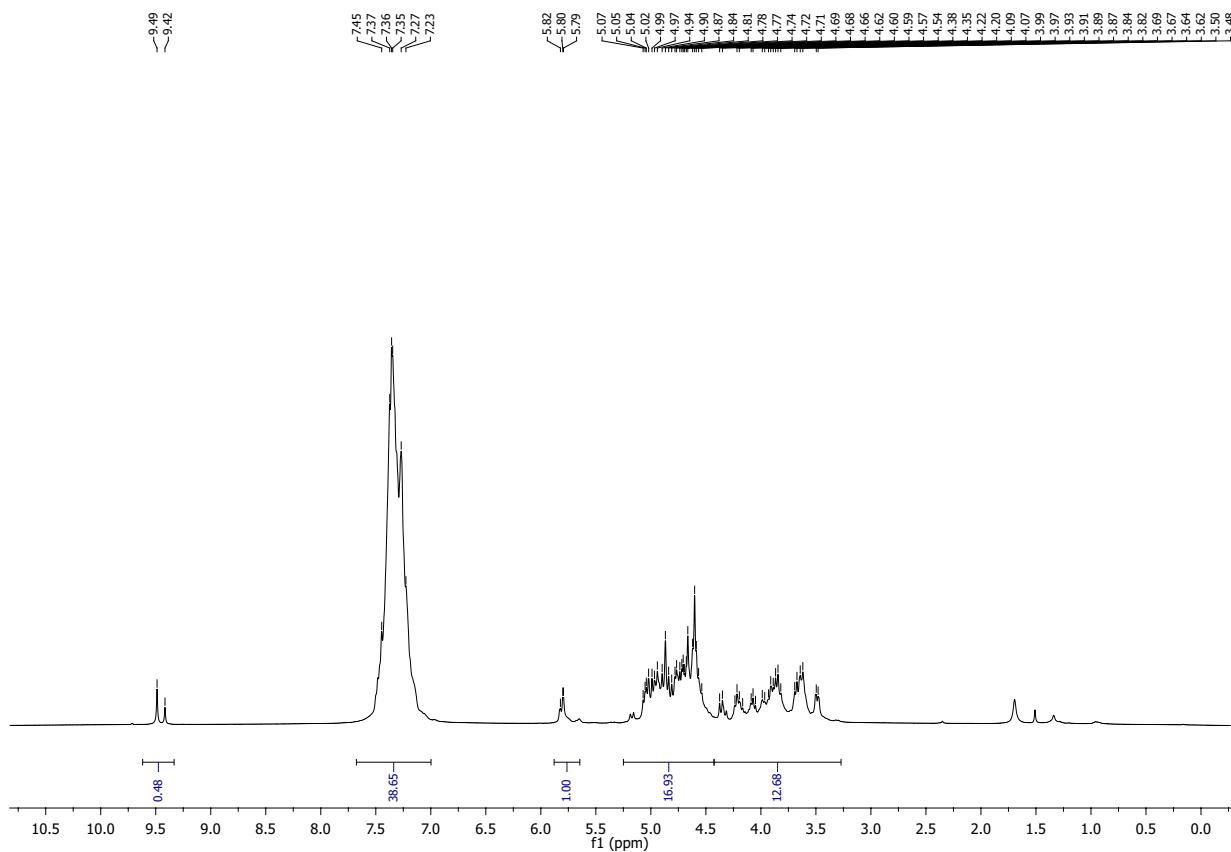


N-(3-(2-(2-(3-aminopropoxy)ethoxy)ethoxy)propyl)-11-oxo-2,3,6,7-tetrahydro-1H,5H,11H-pyrano[2,3-f]pyrido[3,2,1-ij]quinoline-10-carboxamide, **31**

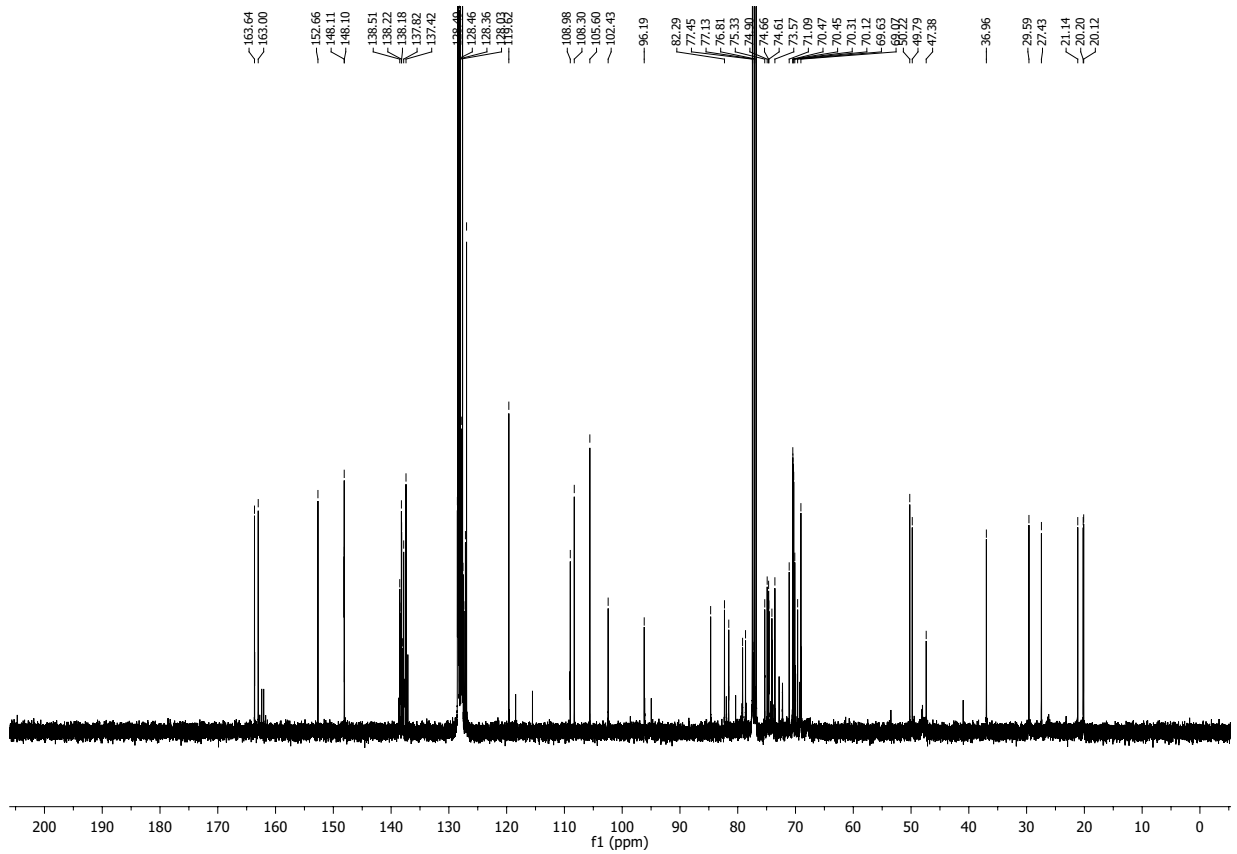
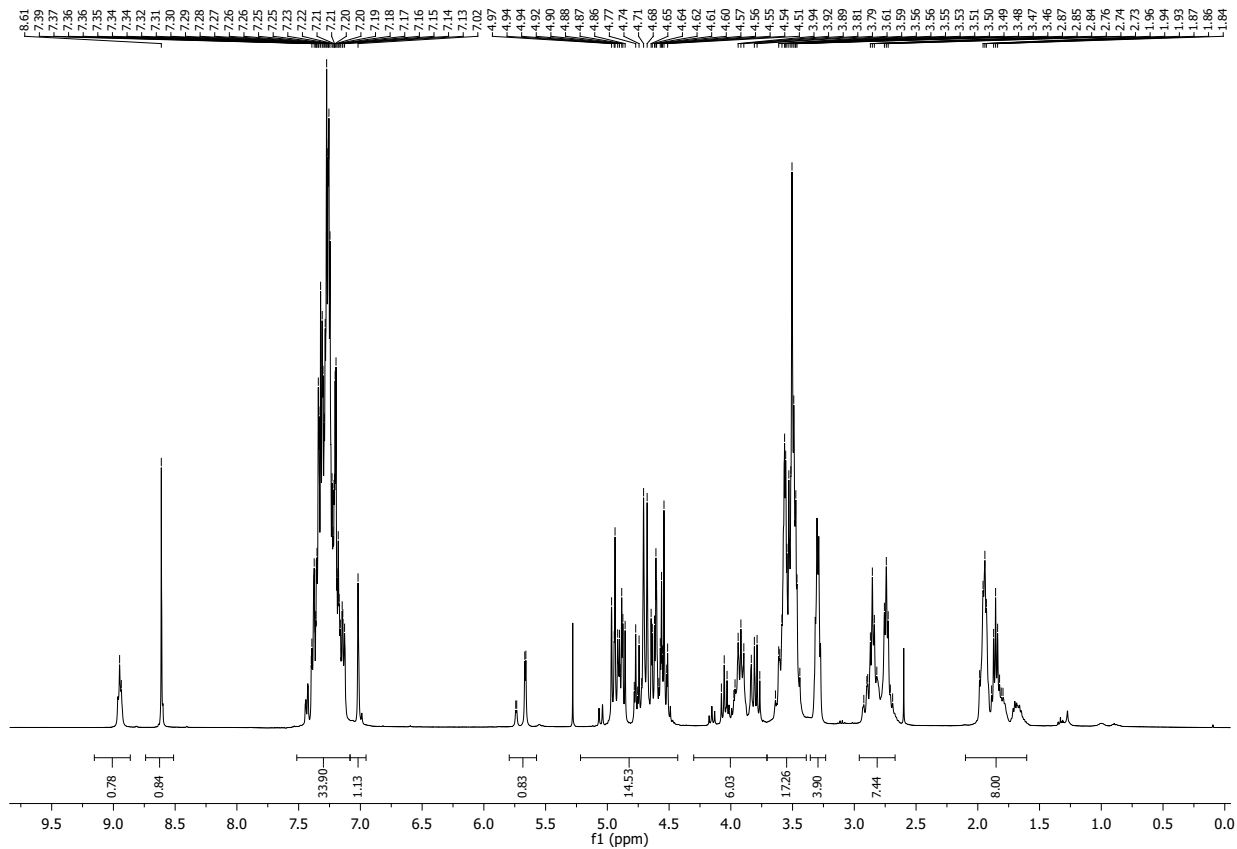




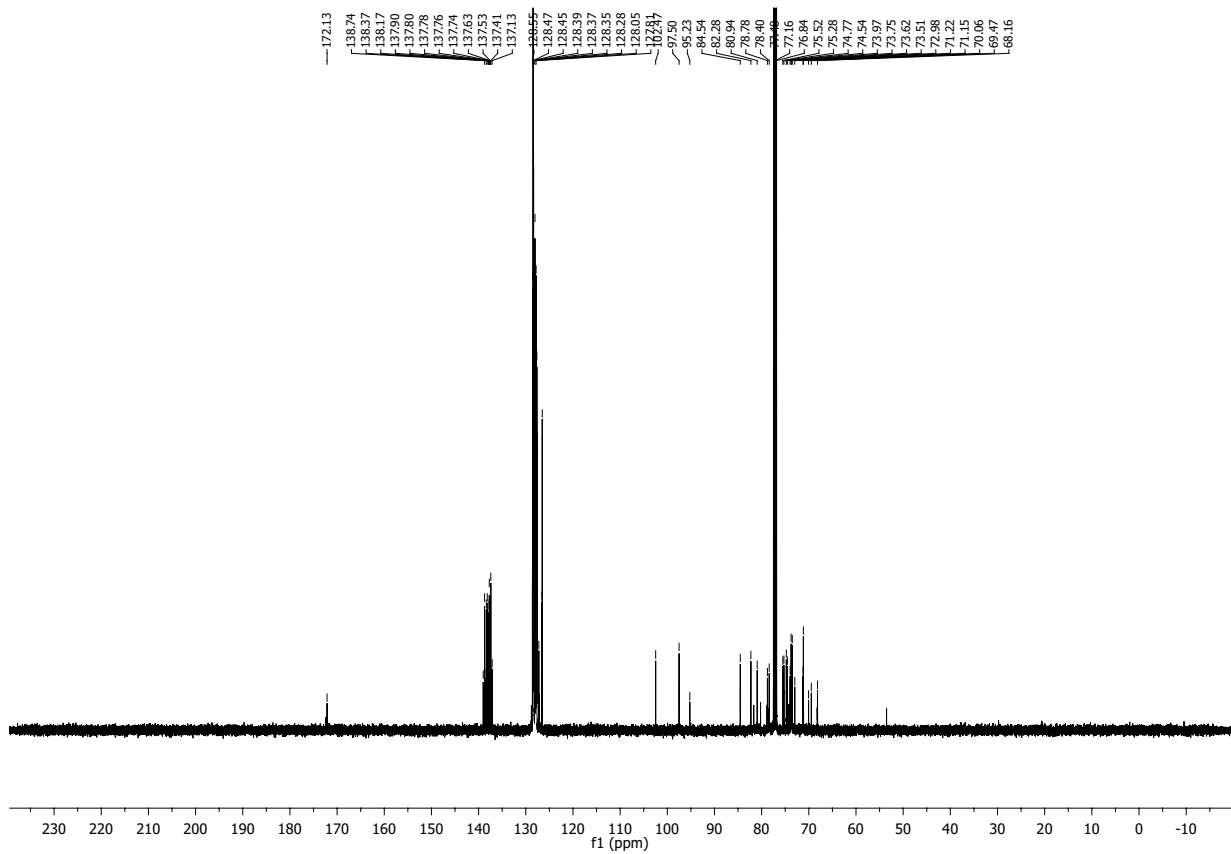
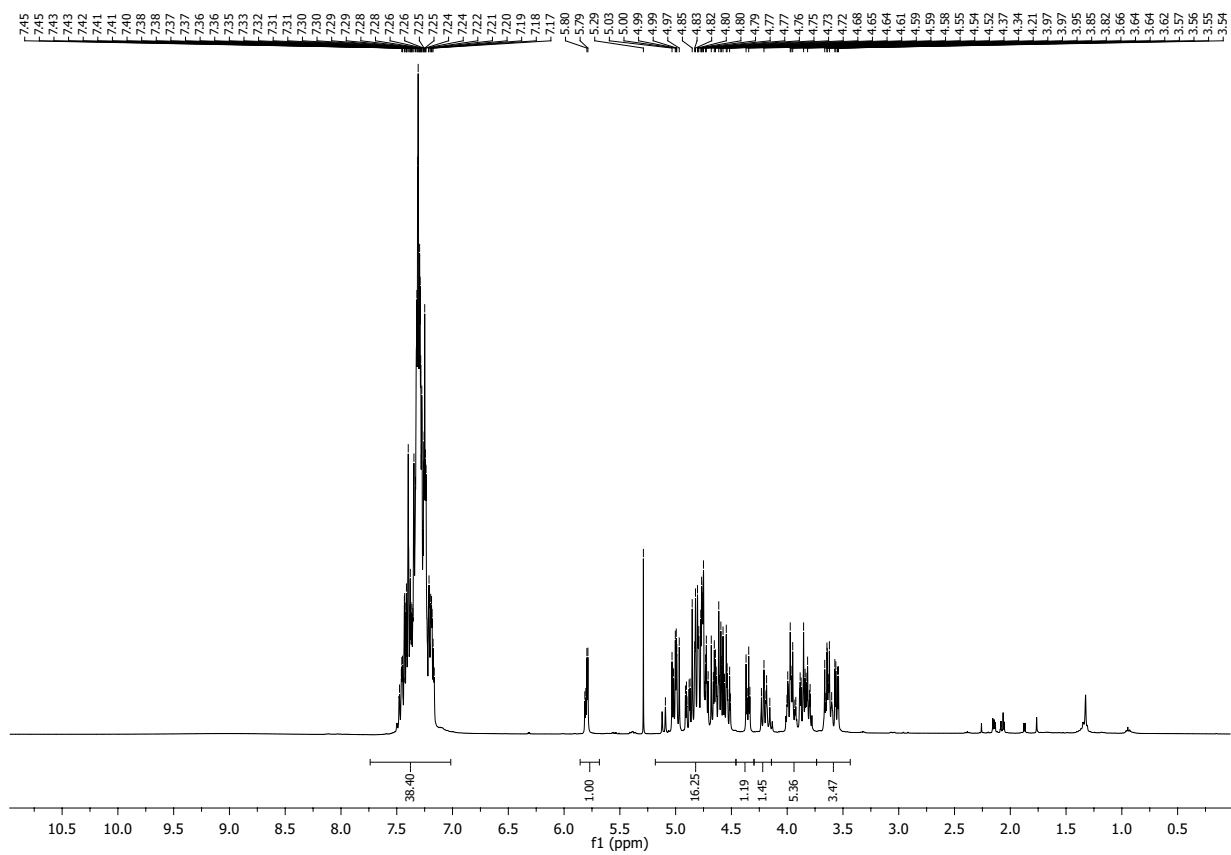
1,2,3,6,2',3',4'-hepta-O-acetyl-4-O-( $\alpha$ -D-1,5-glucohexodialdo)- $\beta$ -D-glucopyranose, **36**



Benzylated BOT.15, 35

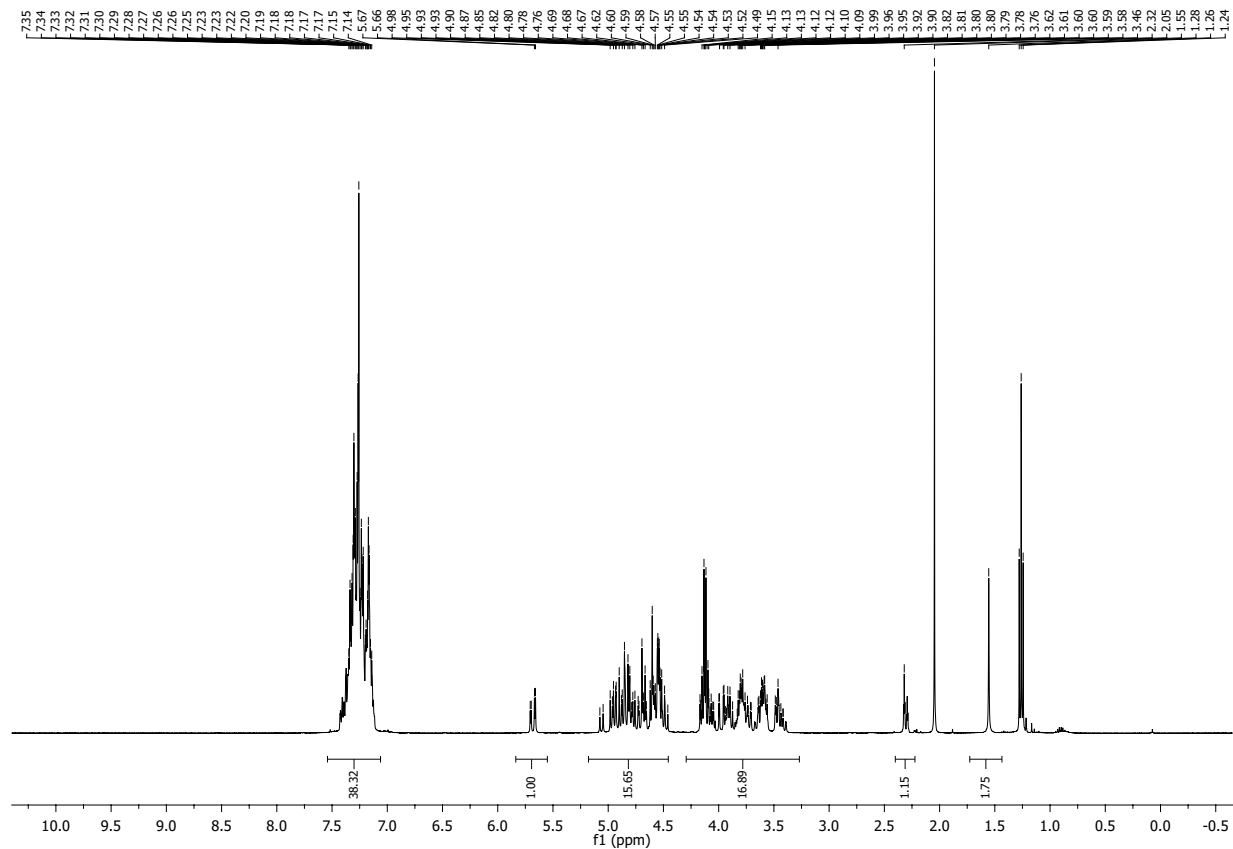


1,2,3,6,2',3',4'-hepta-O-benzyl-4-O-( $\alpha$ -D-glucopyranuronosyl)- $\beta$ -D-glucopyranose, **38**

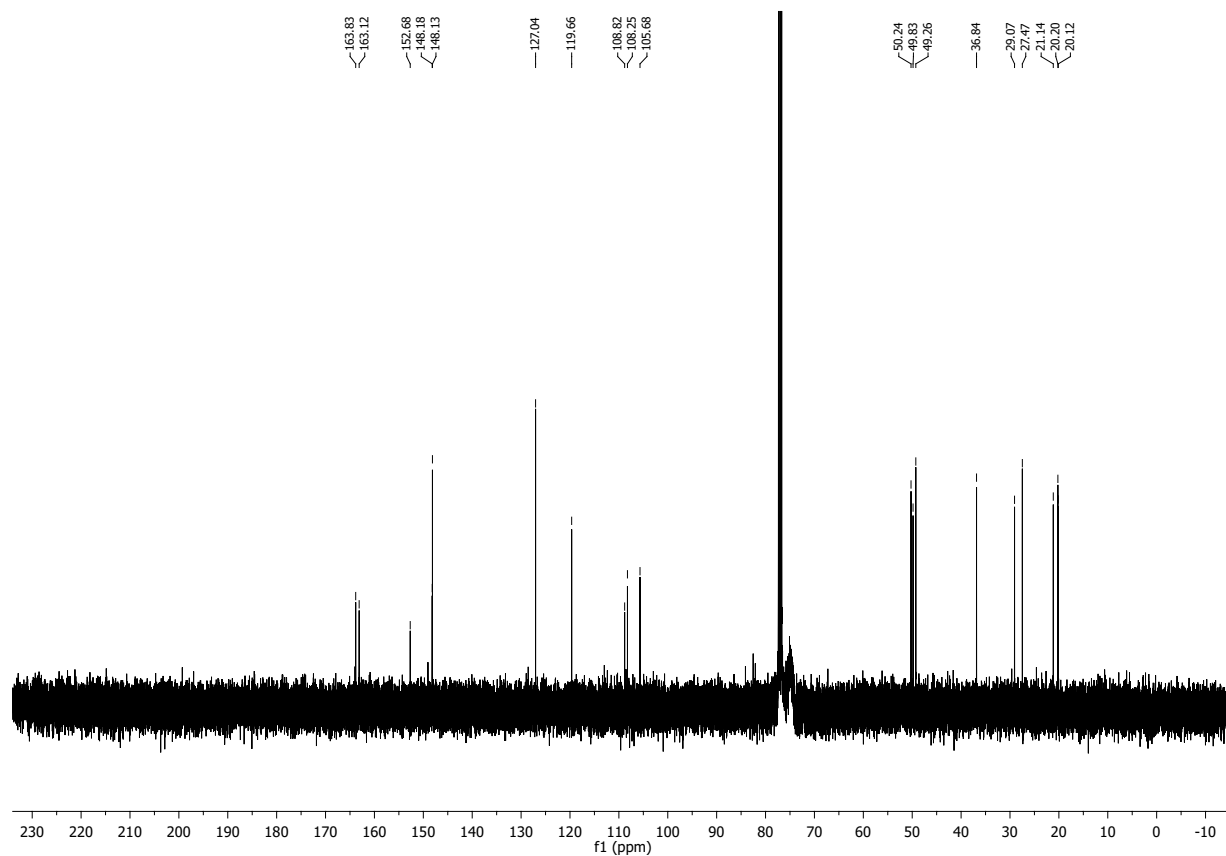
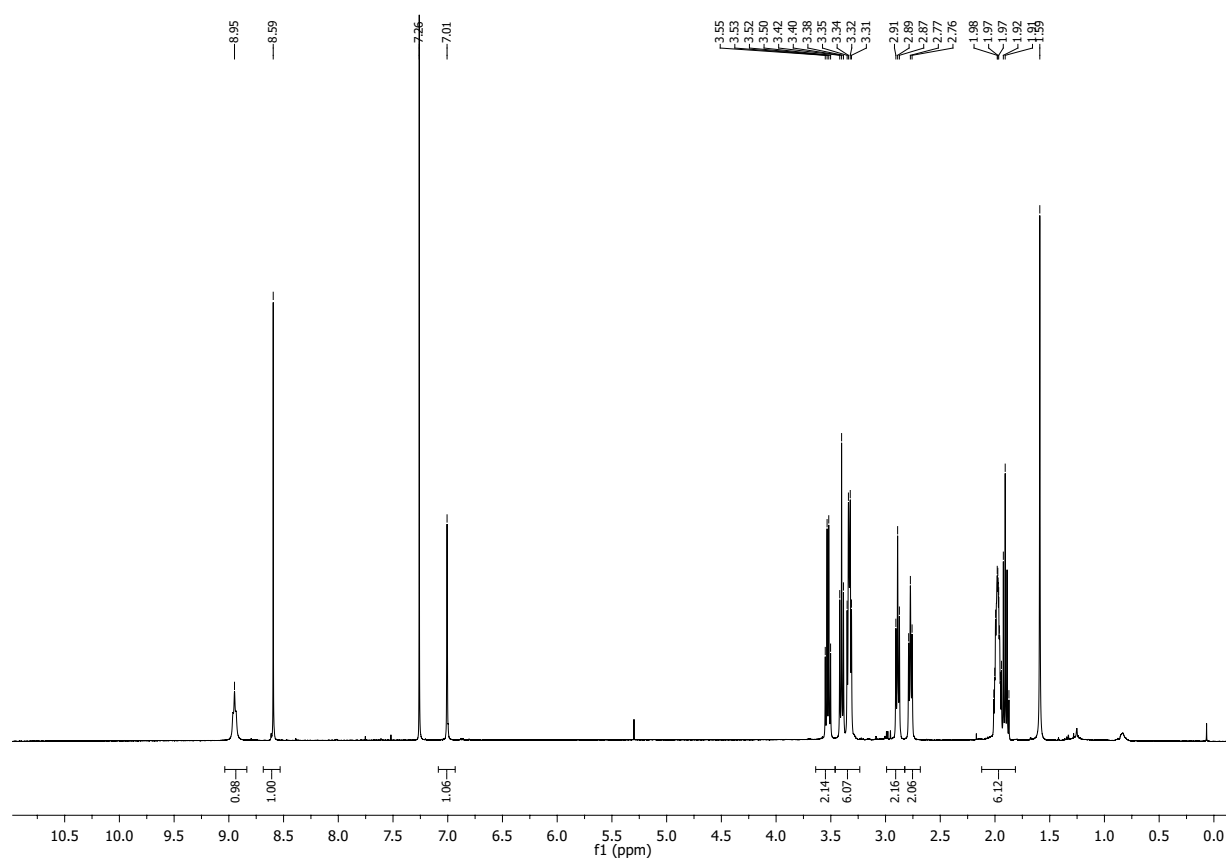




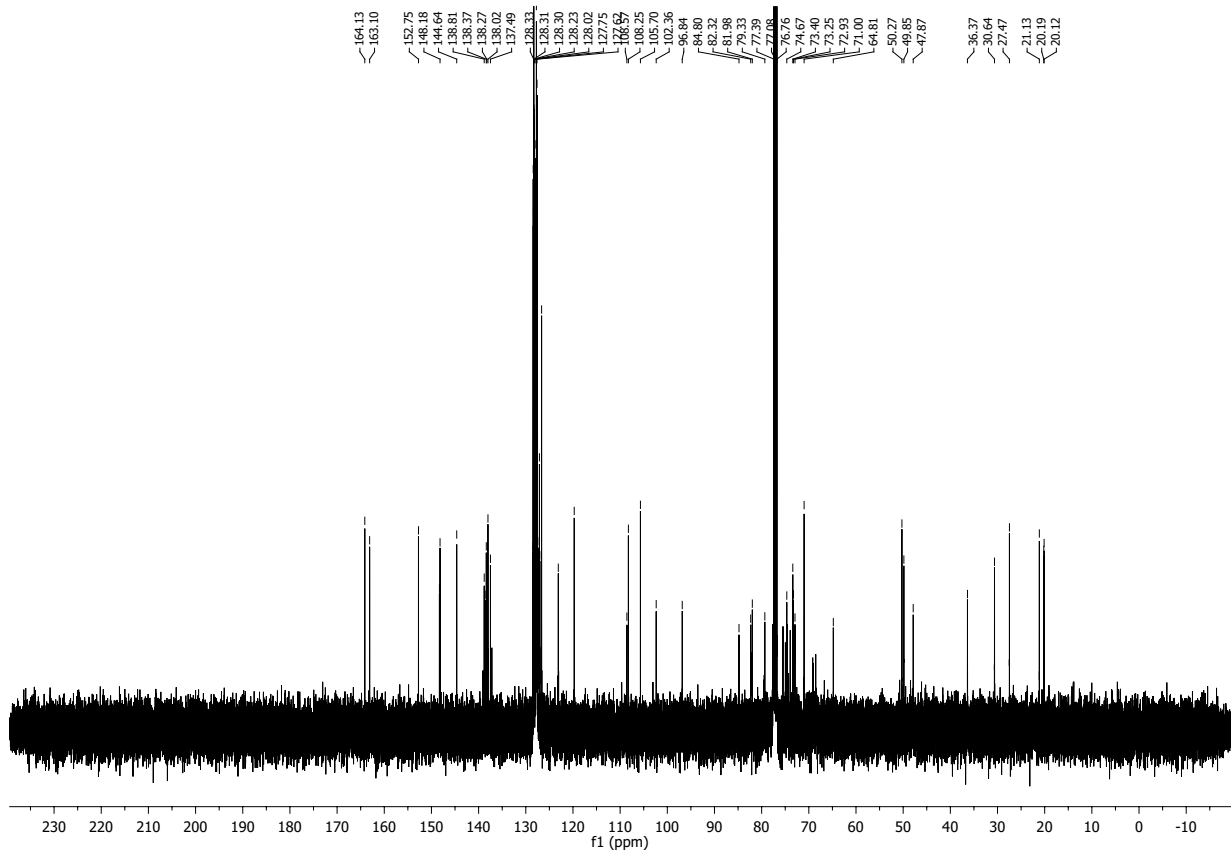
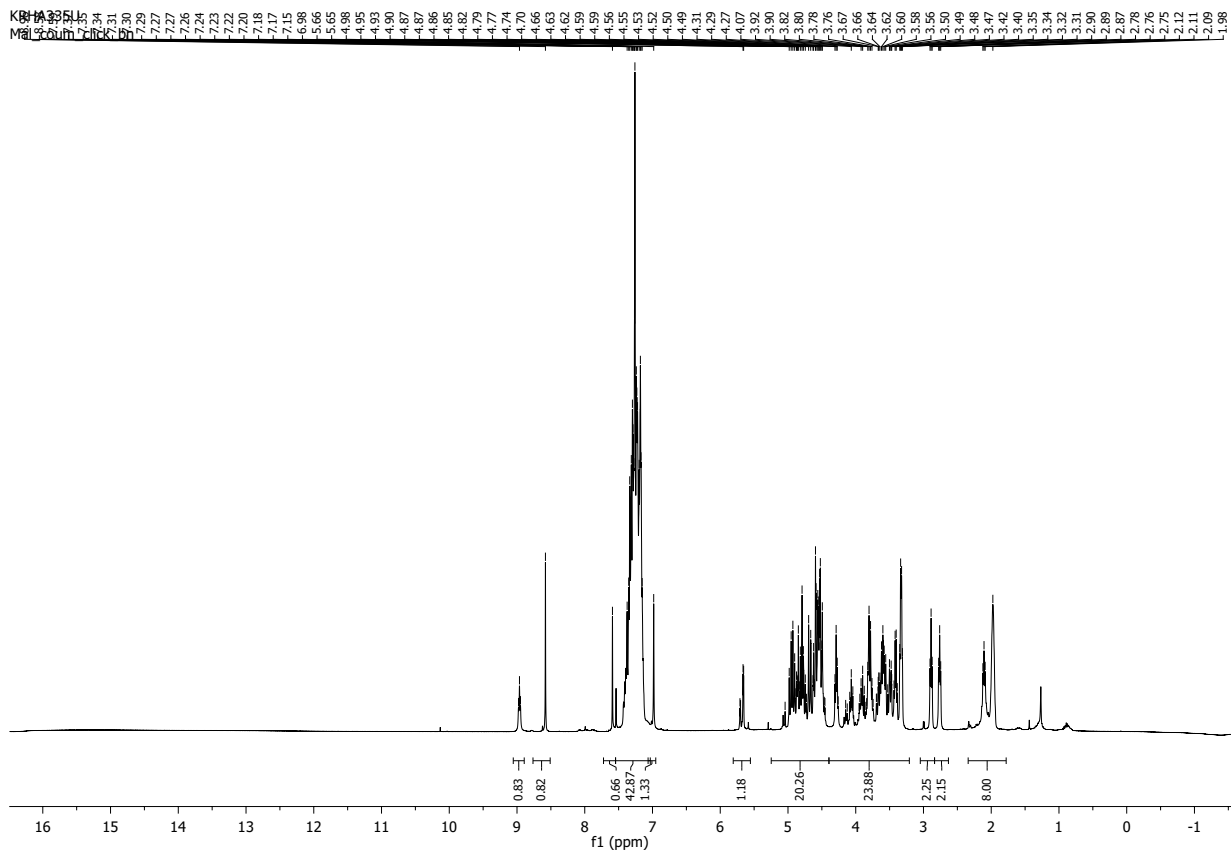
1,2,3,6,2',3'-hexa-O-benzyl-6'-O-propargyl-4-O-( $\alpha$ -D-glucopyranosyl)- $\beta$ -D-glucopyranose, **39**



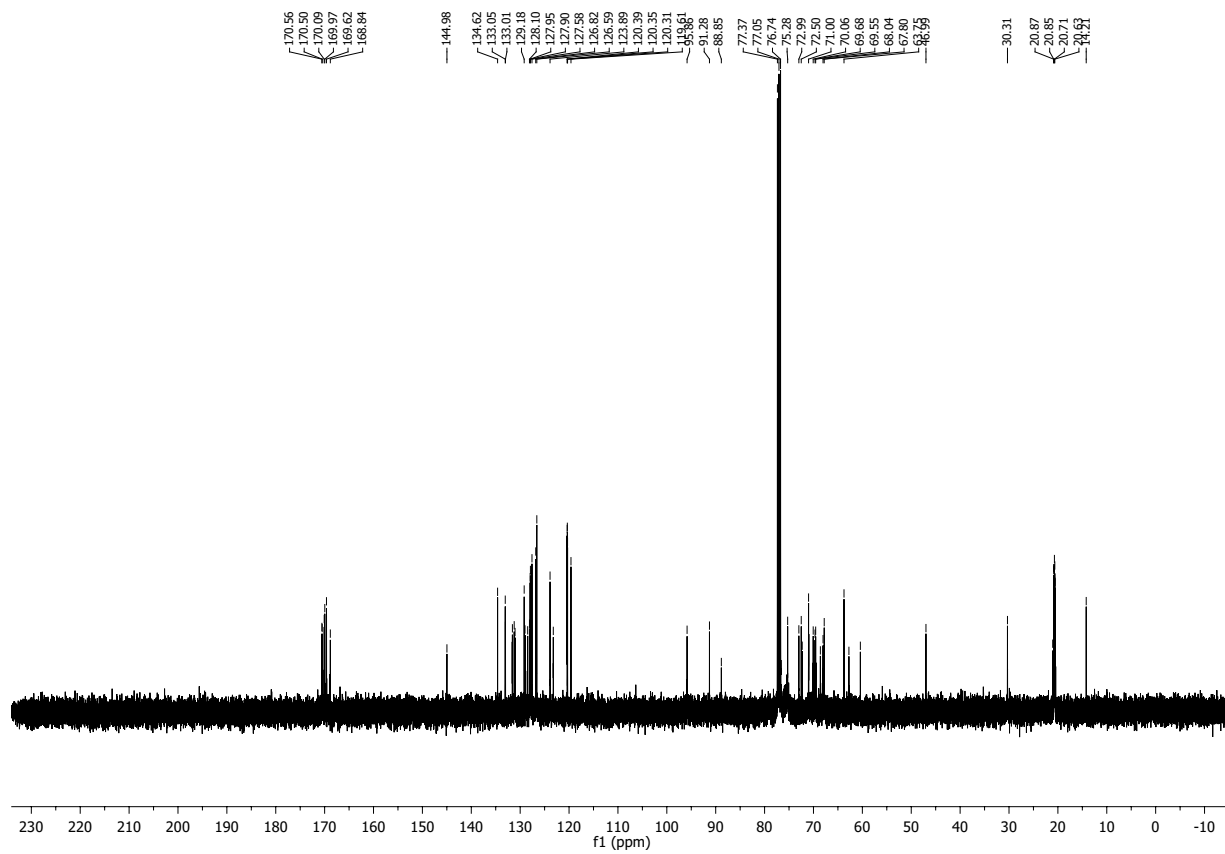
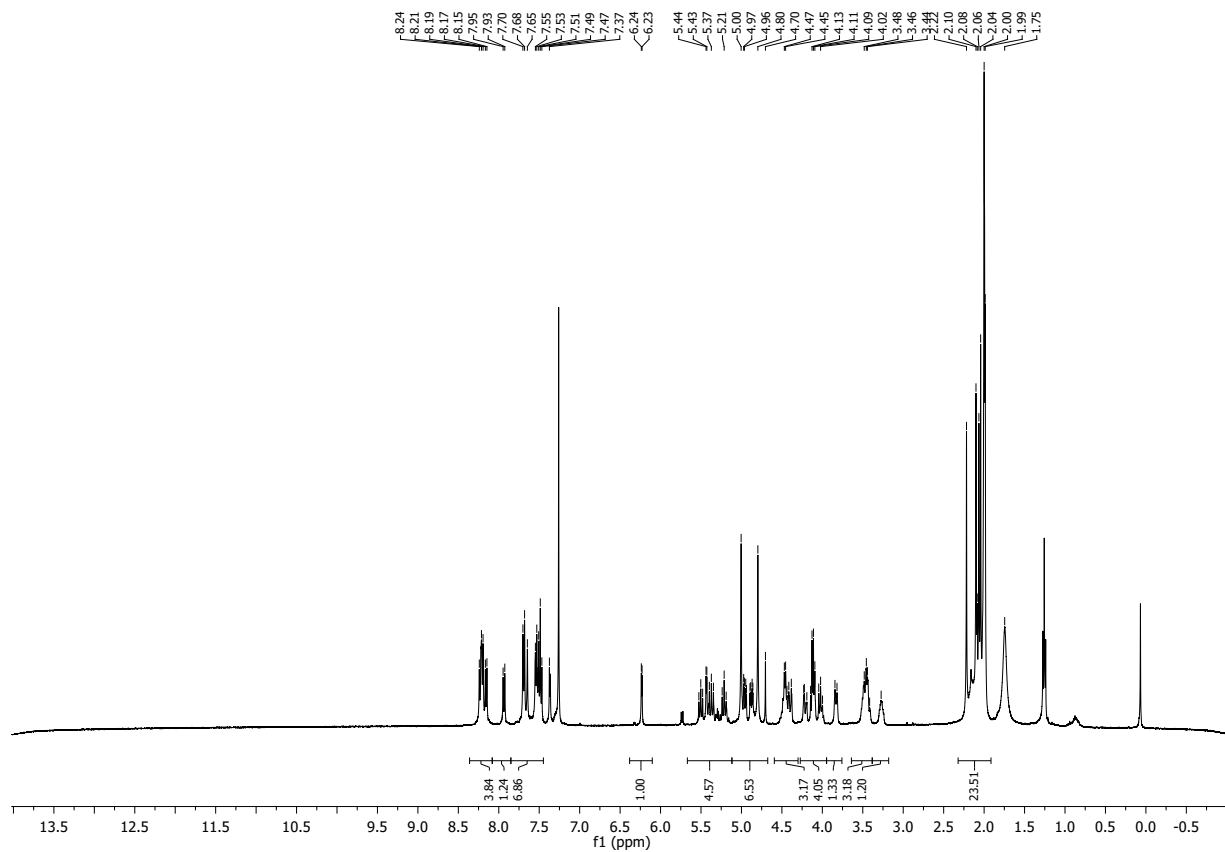
N-(3-azidopropyl)-11-oxo-2,3,6,7-tetrahydro-1H,5H,11H-pyrano[2,3-f]pyrido[3,2,1-ij]quinoline-10-carboxamide, 40



Benzylated BOT.18, 41

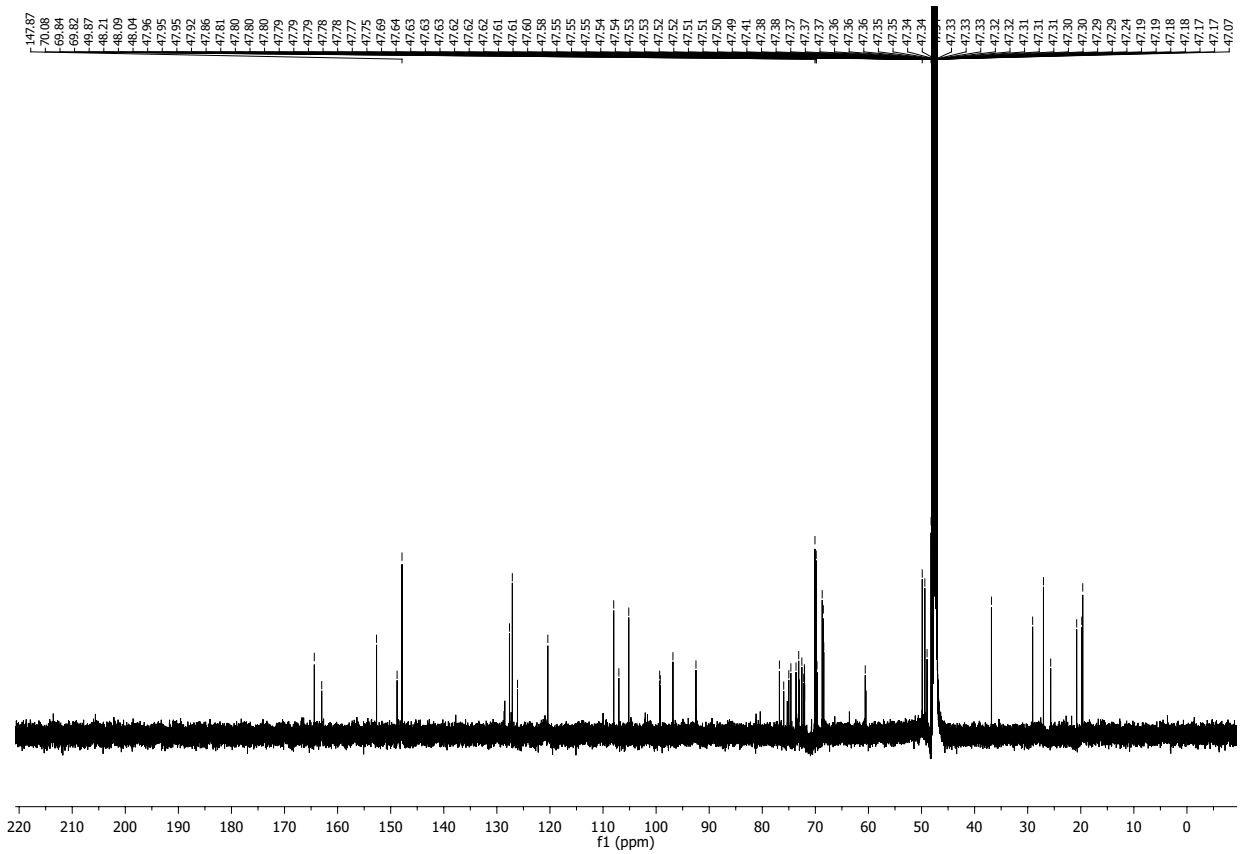
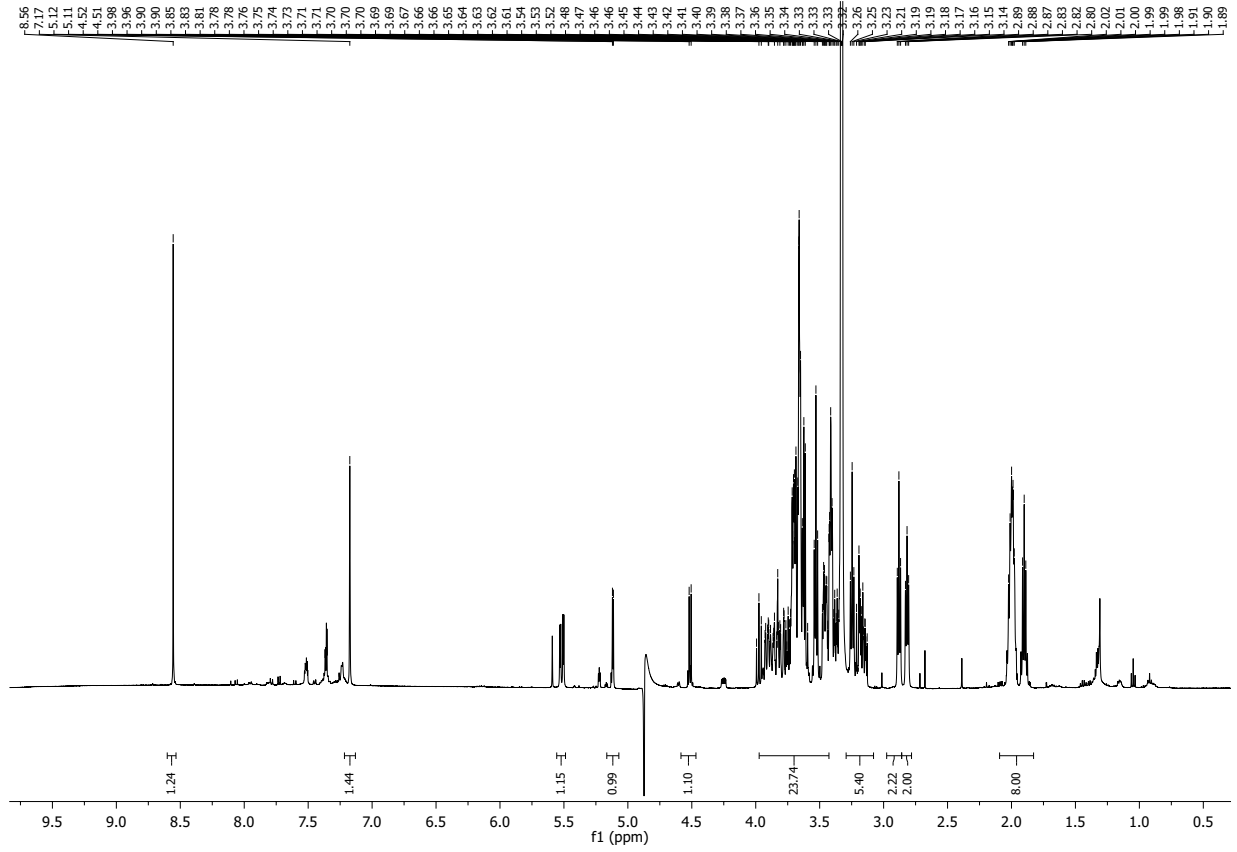


Acetylated BOT\_47, 44

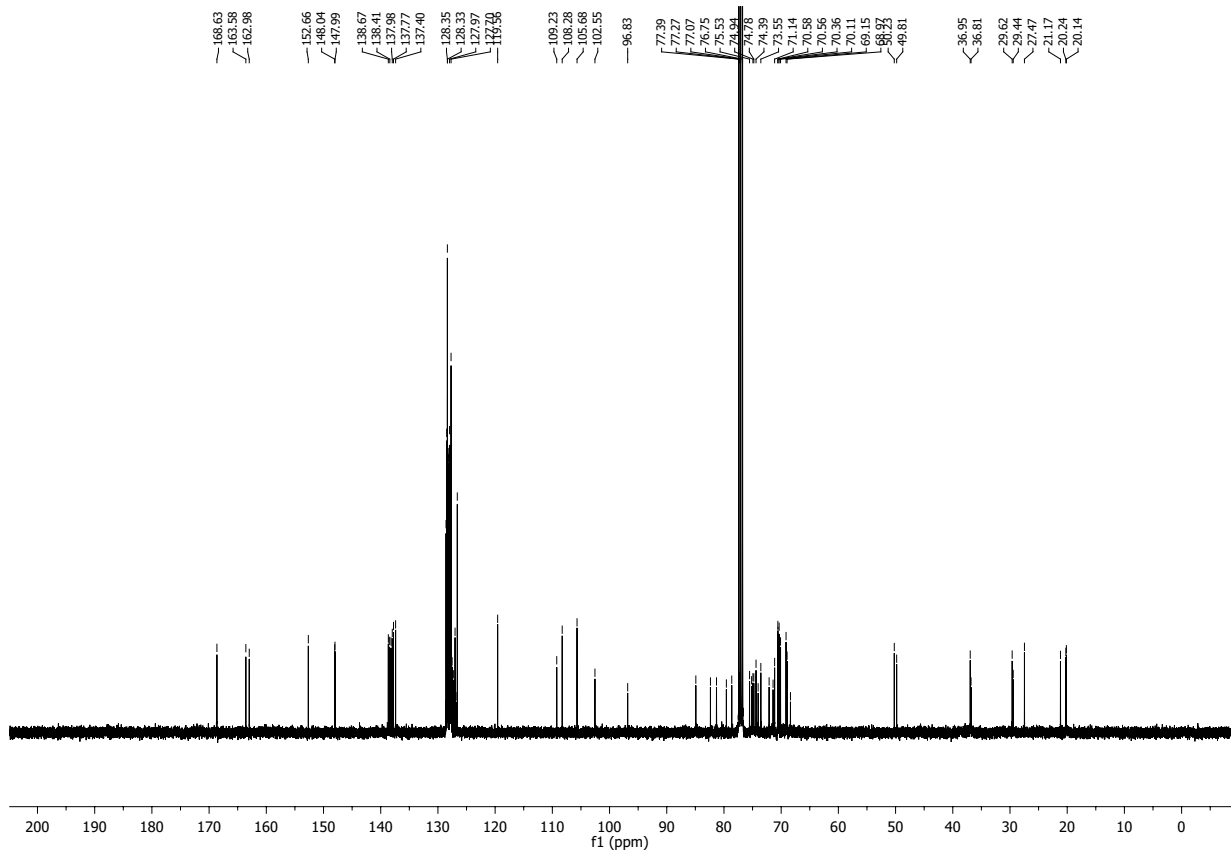
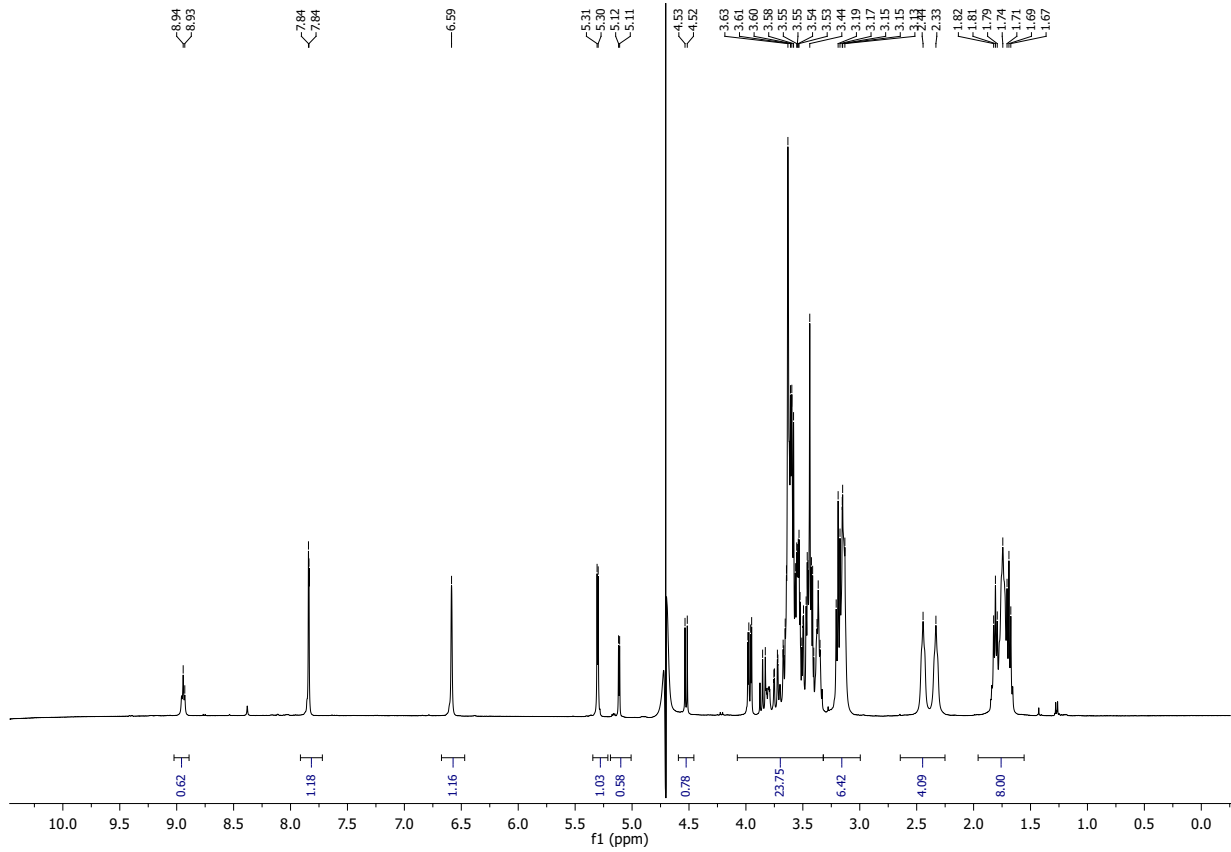




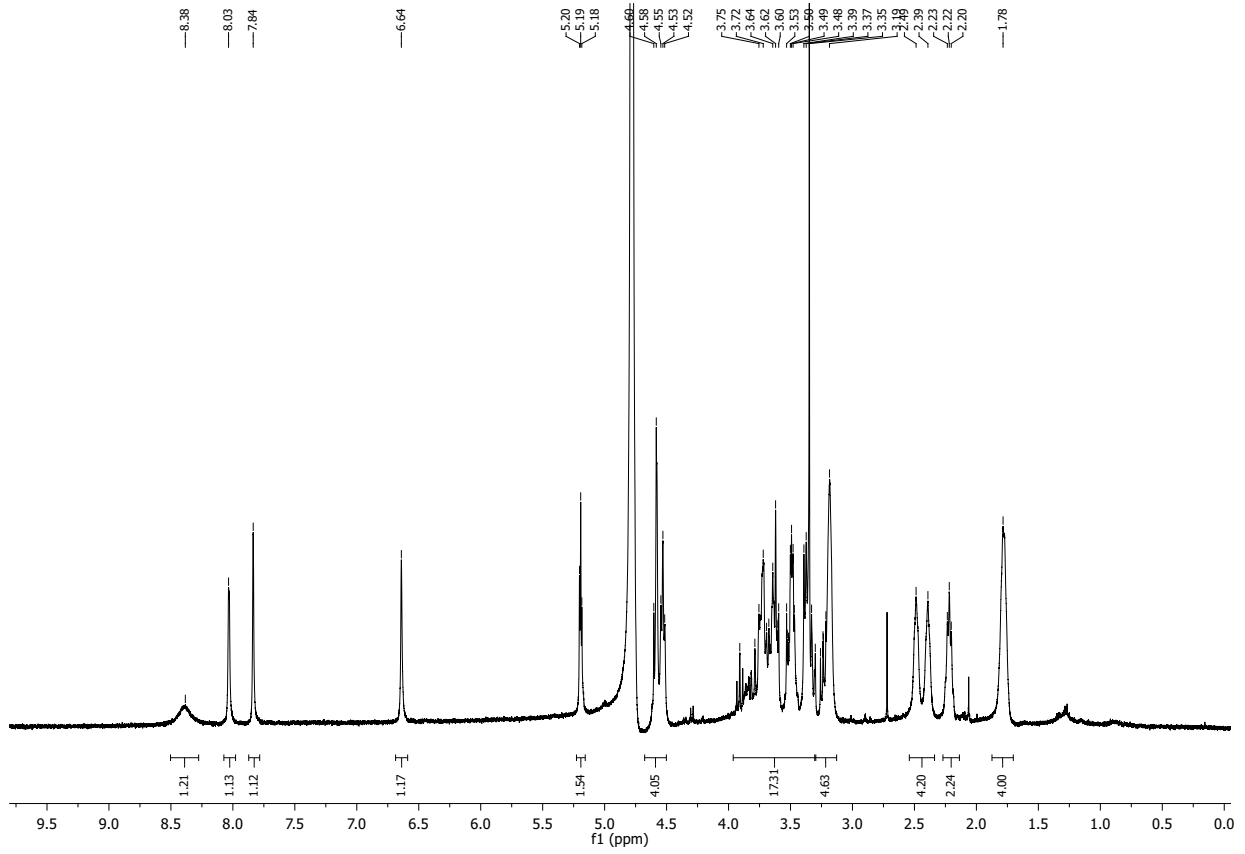
Maltose-PEG-Coumarin 343 conjugate, BOT\_15



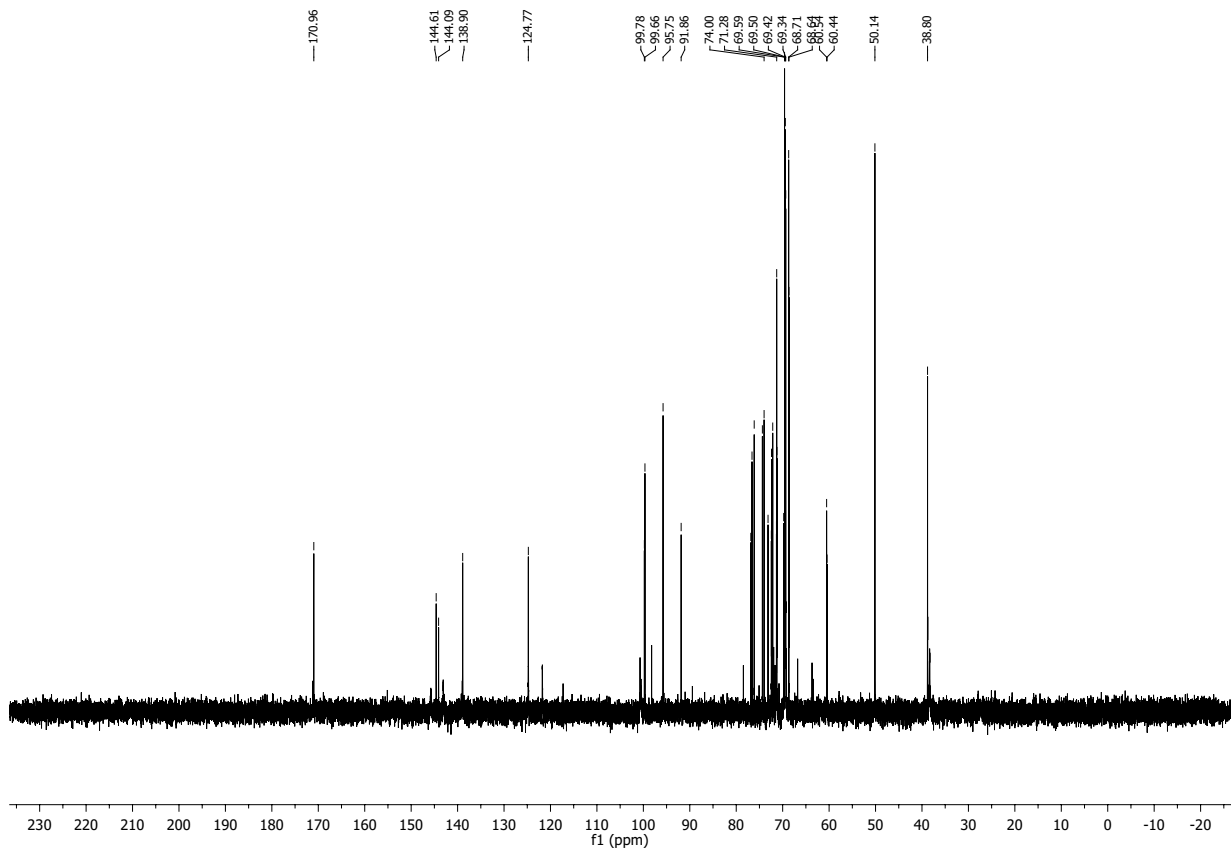
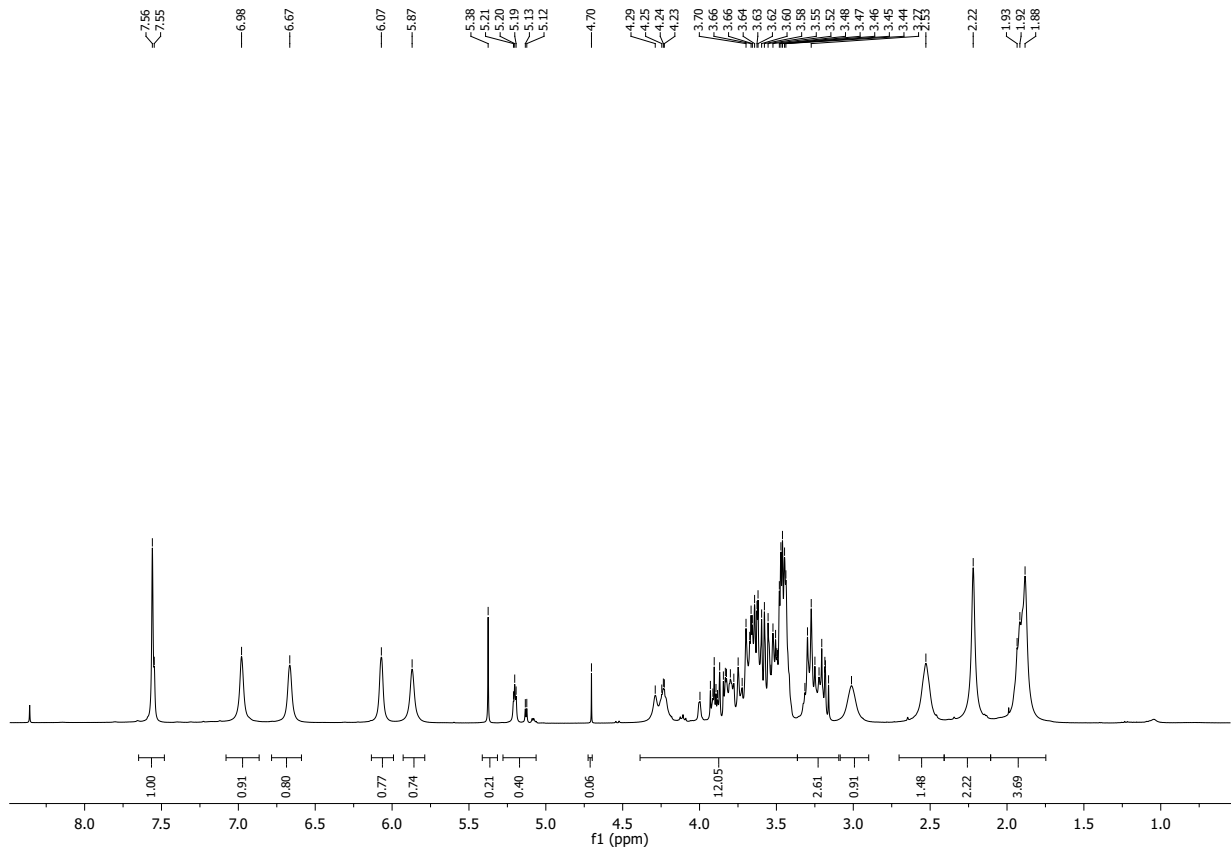
Maltose PEG coumarin 343 conjugate, BOT\_16



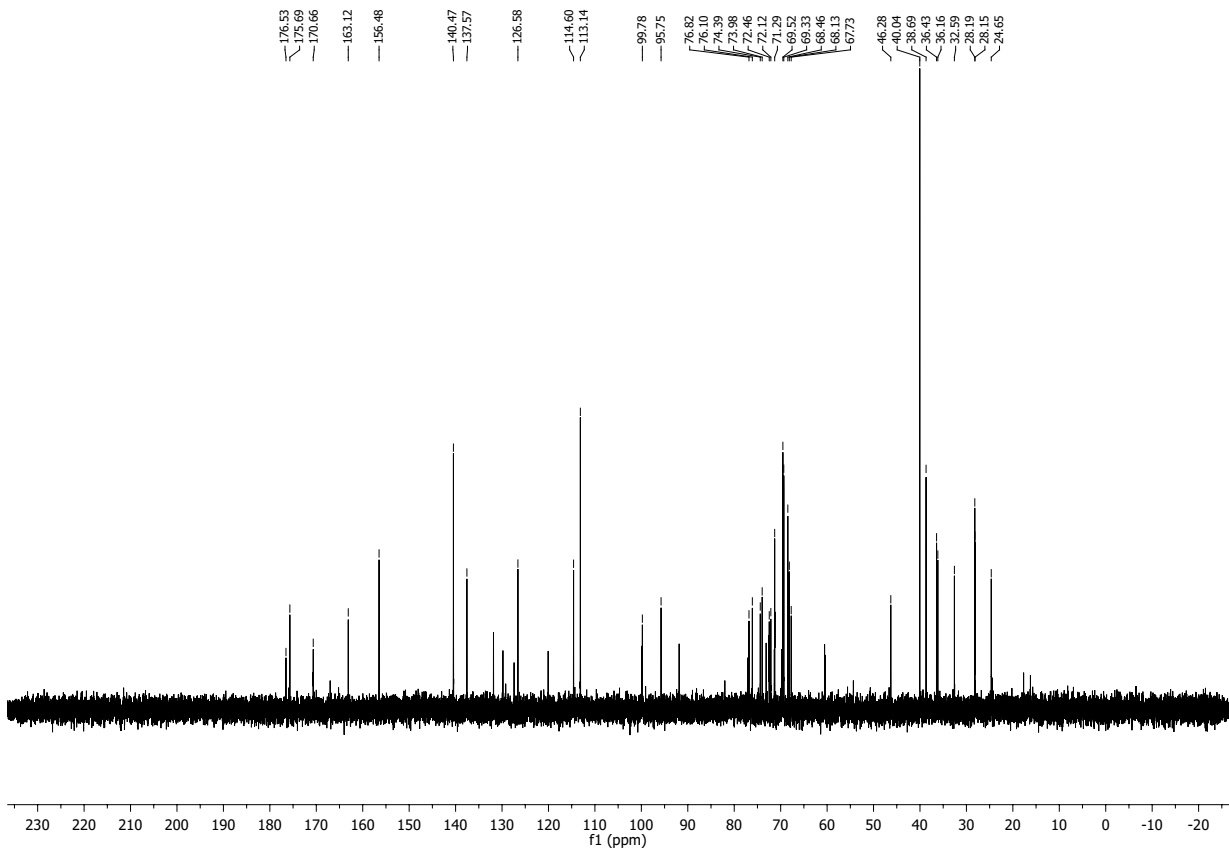
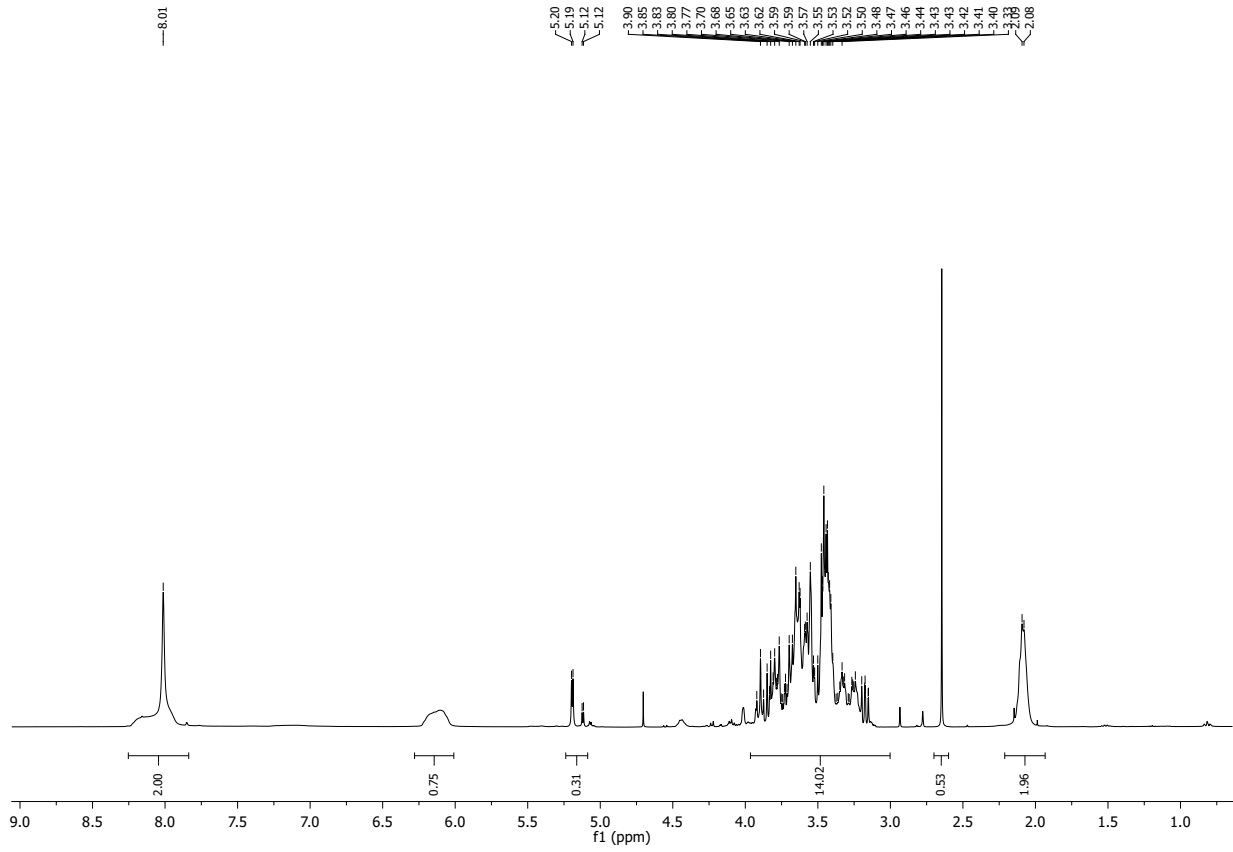
Maltose triazole coumarin conjugate, BOT\_18



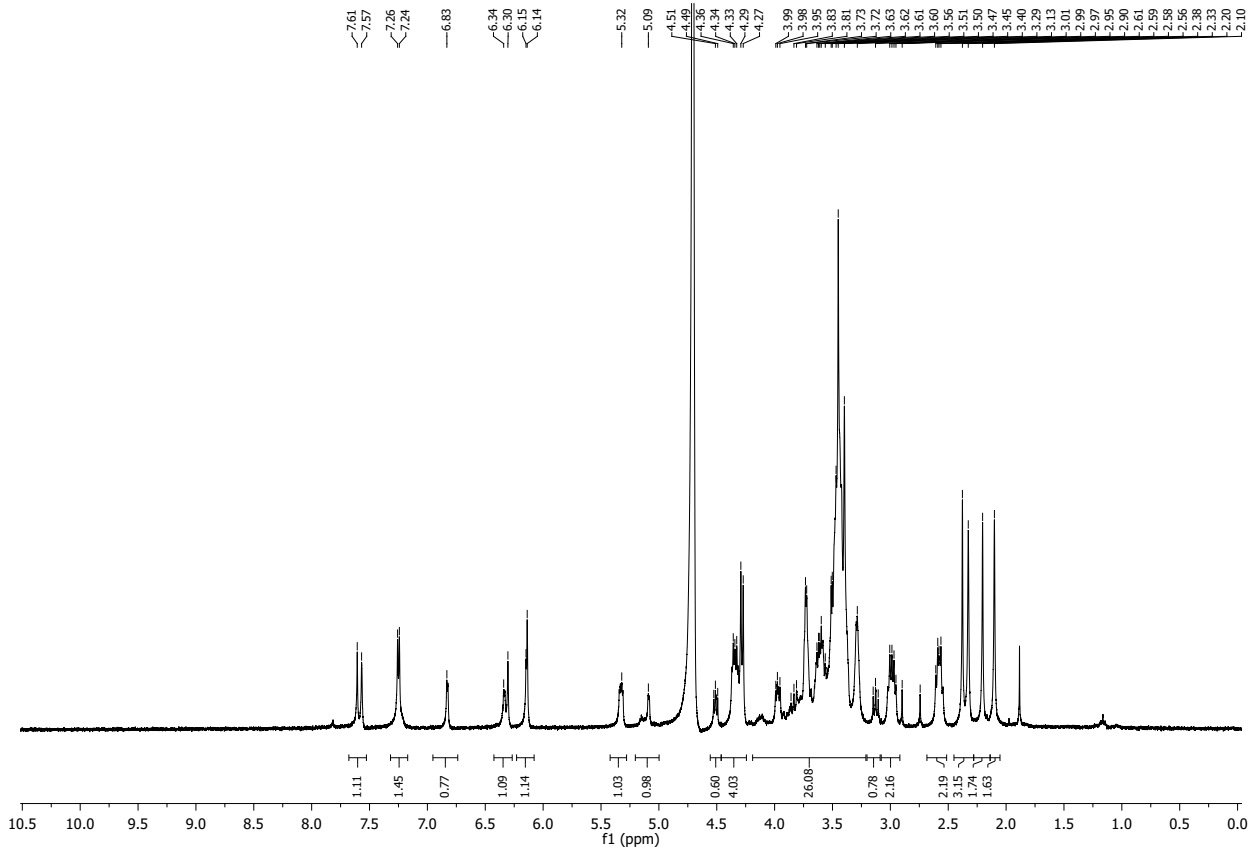
Maltose triazole BODIPY conjugate, **BOT\_44**



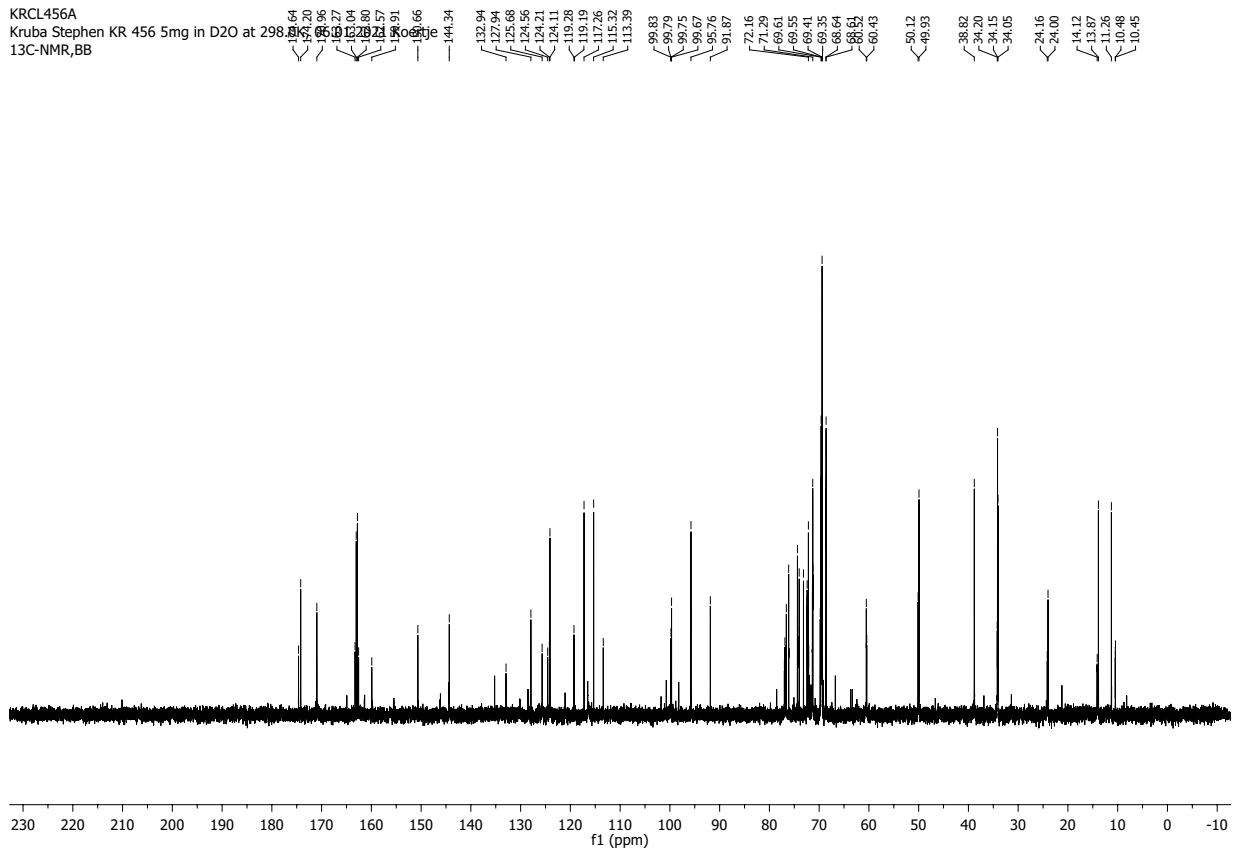
Maltose triazole NBD conjugate, BOT\_45



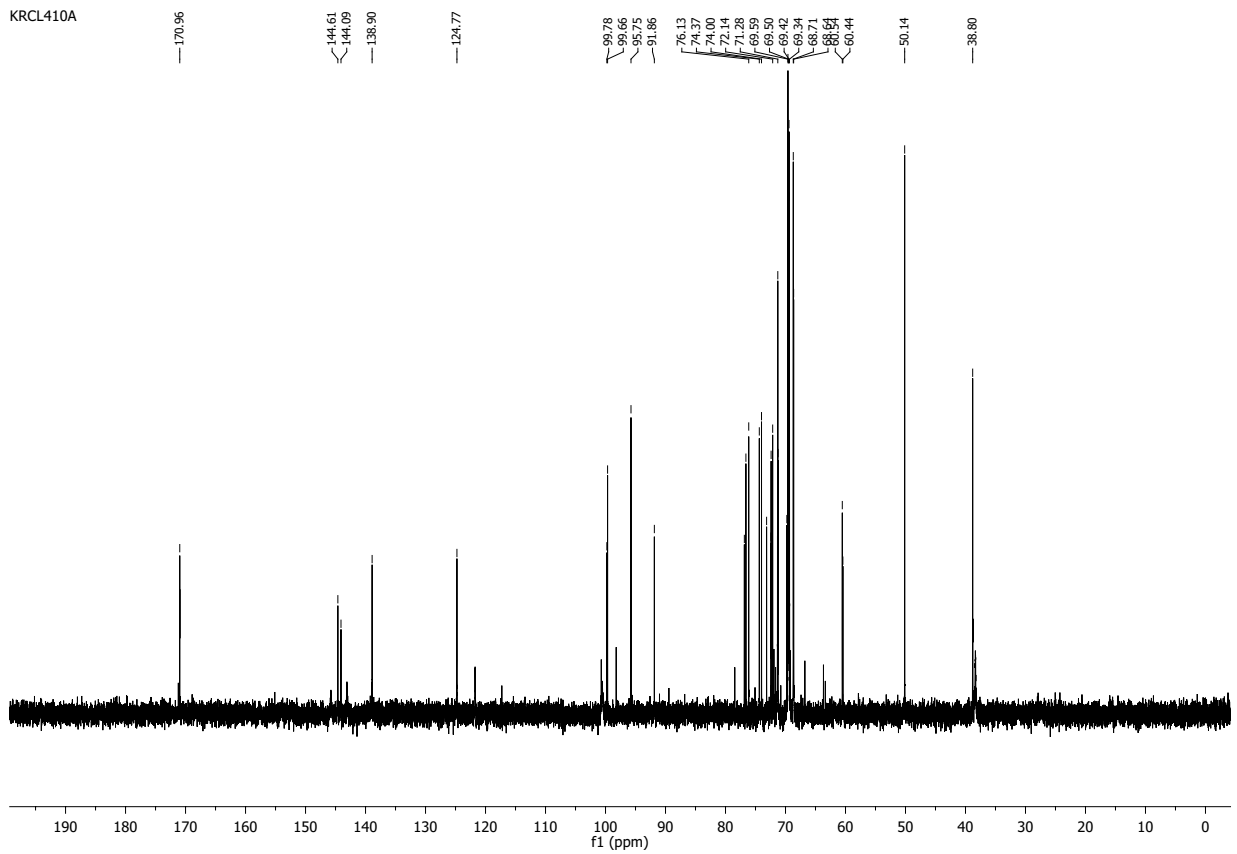
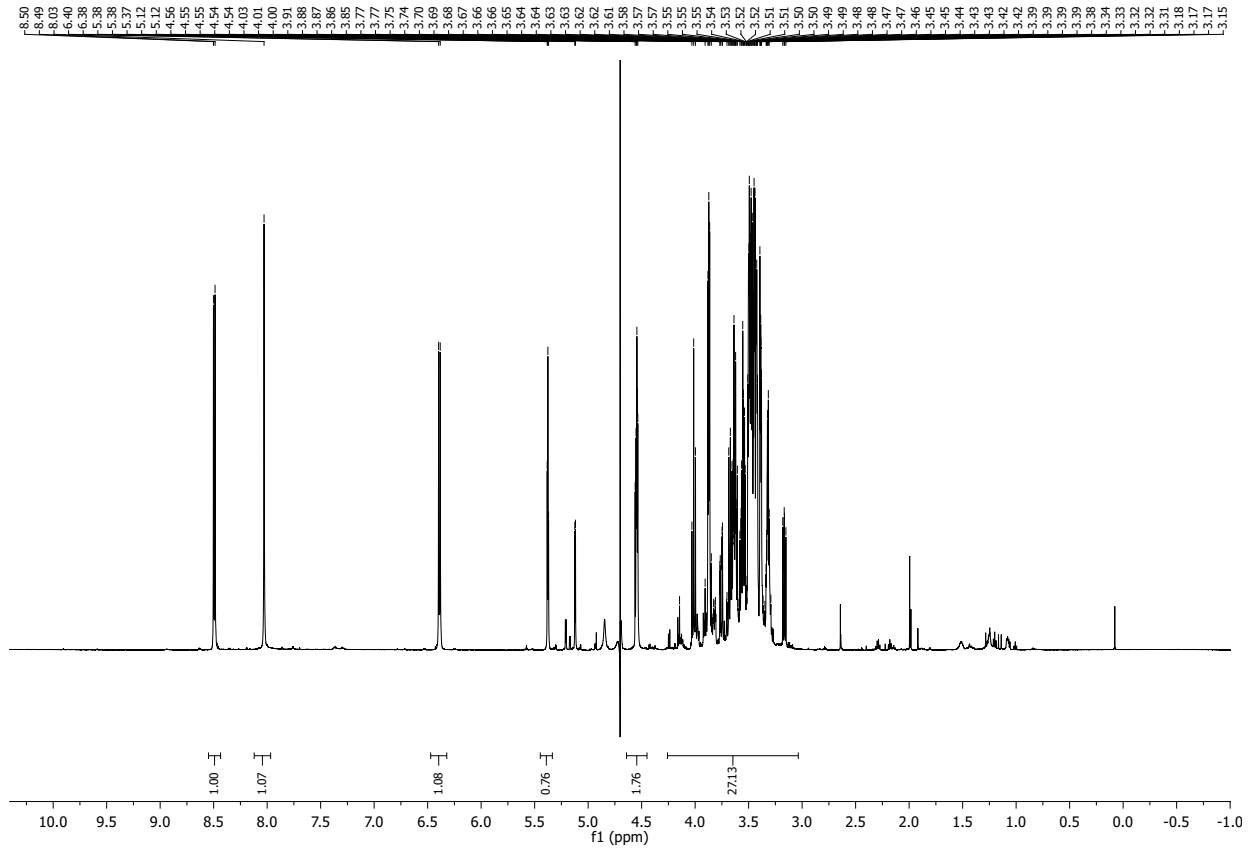
Maltose PEG BODIPY conjugate, BOT\_48



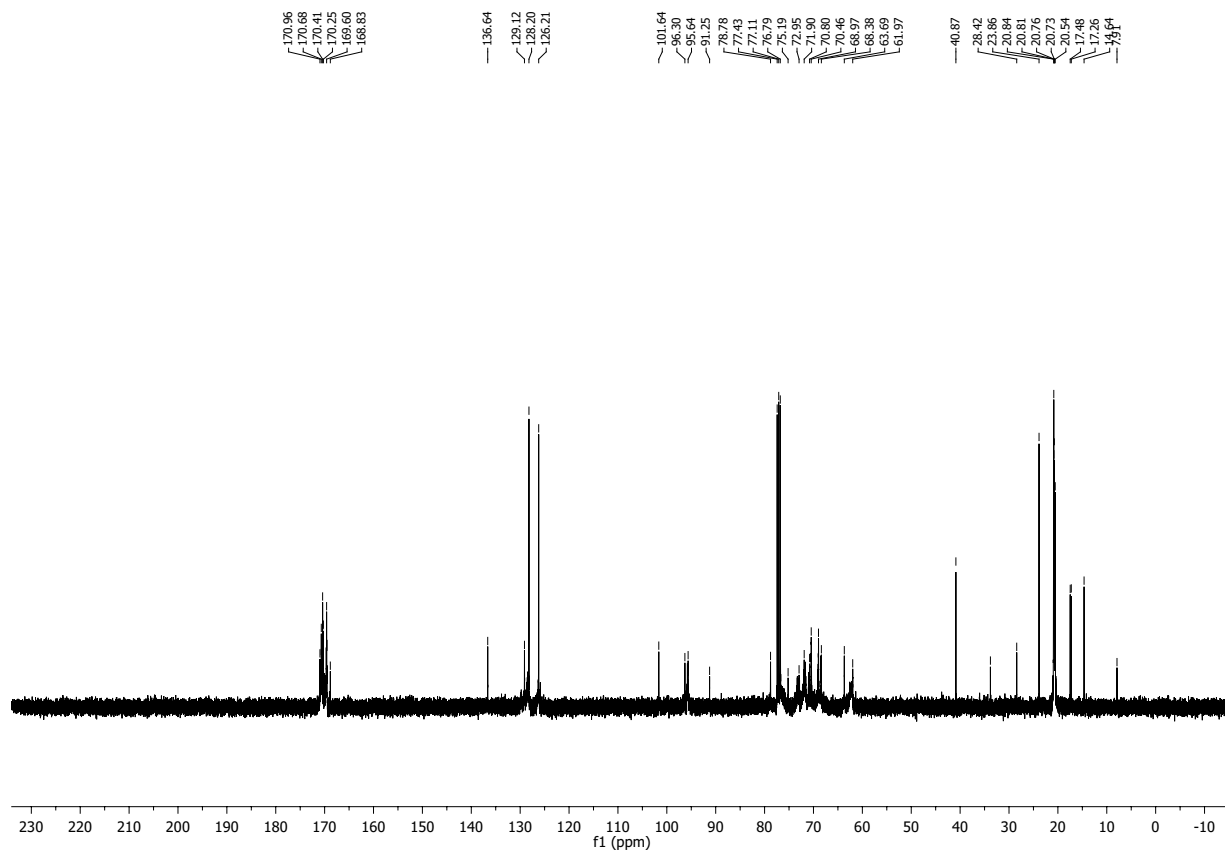
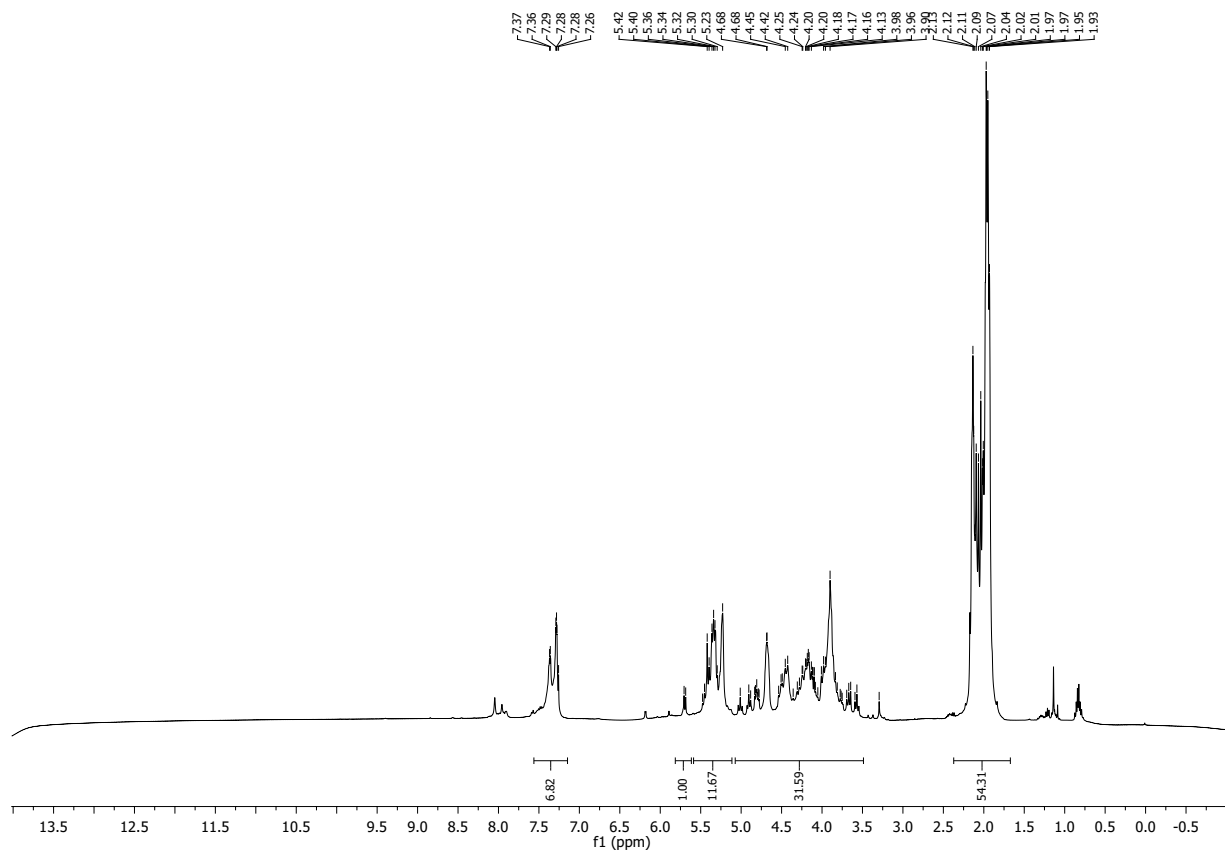
KRCL456A  
 Kruba Stephen KR 456 5mg in D2O at 298.15K  
 13C-NMR, BB



Maltose PEG NBD conjugate, BOT\_50

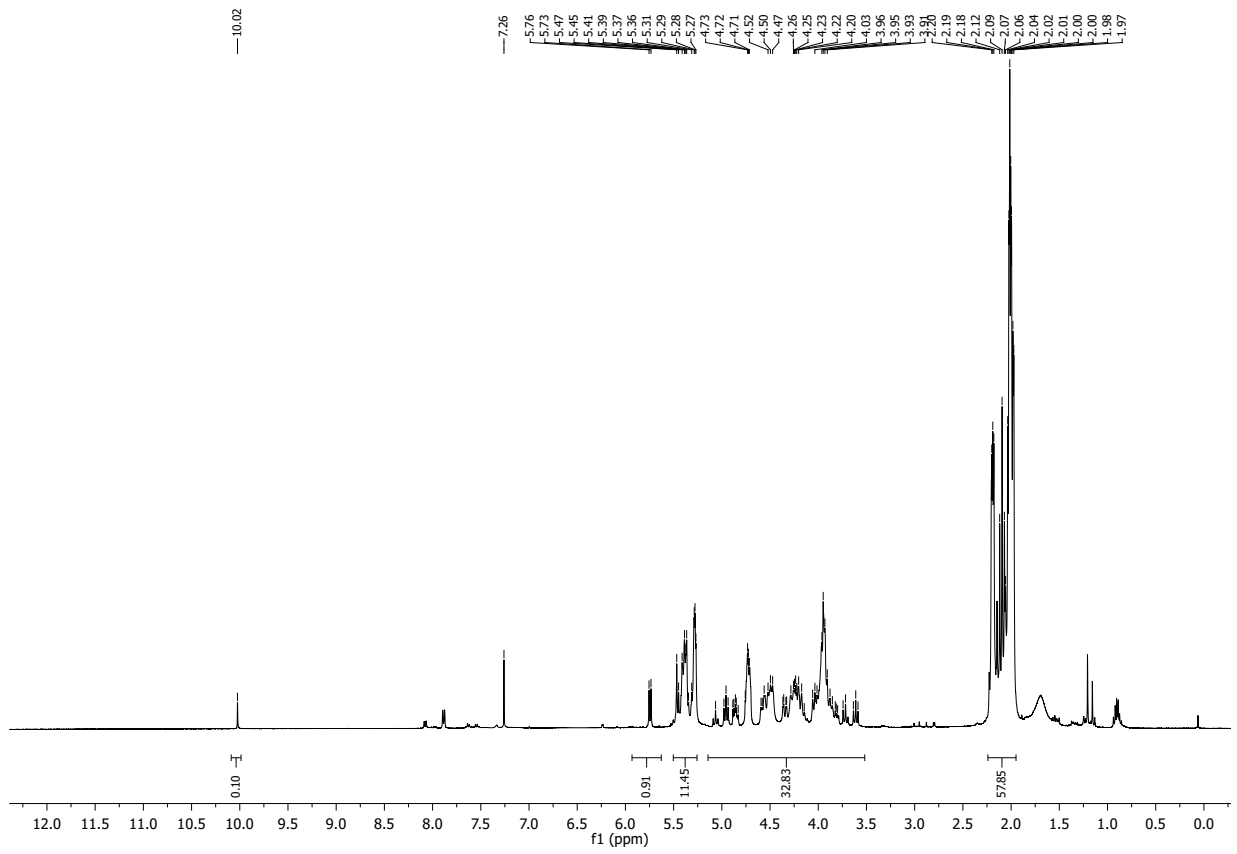


Acetylated maltohexose benzylidene acetal, **50**

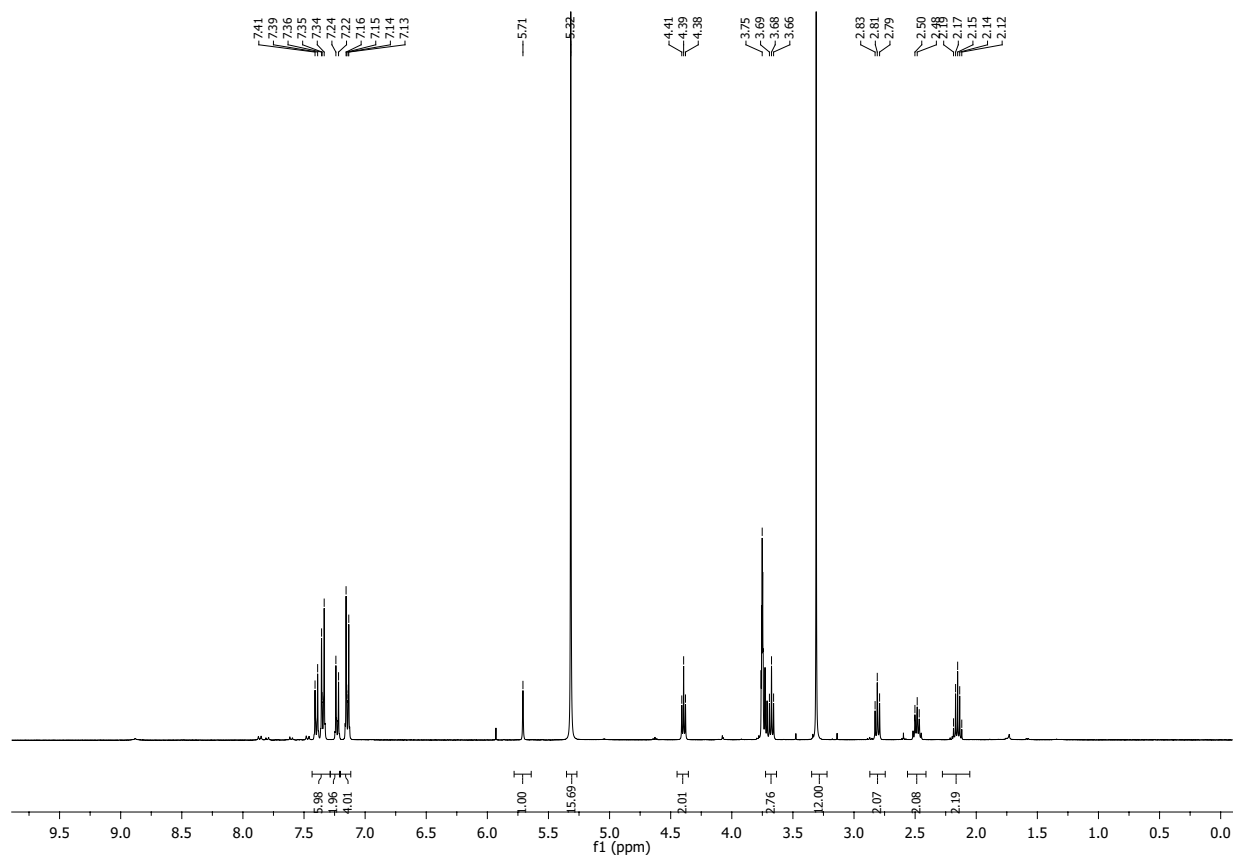




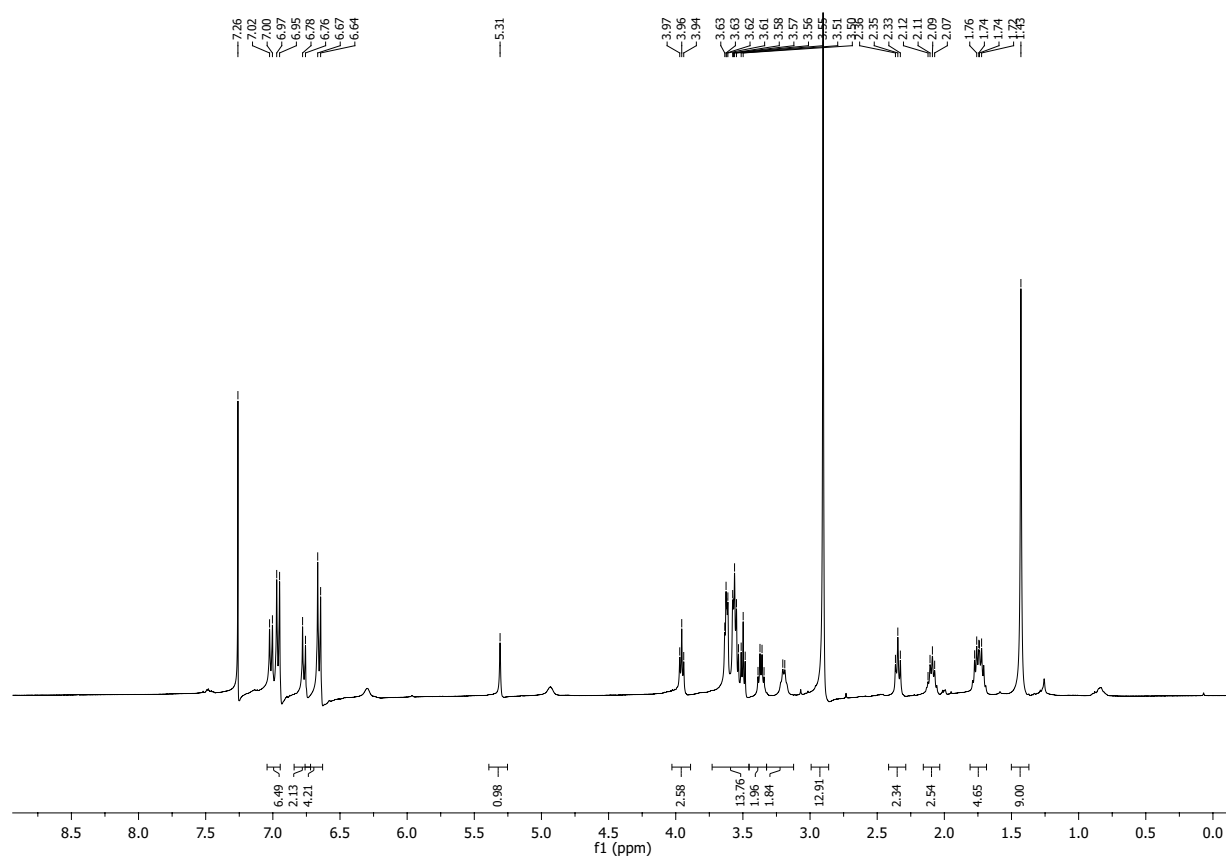
Maltohexose primary carboxylic acid, 47



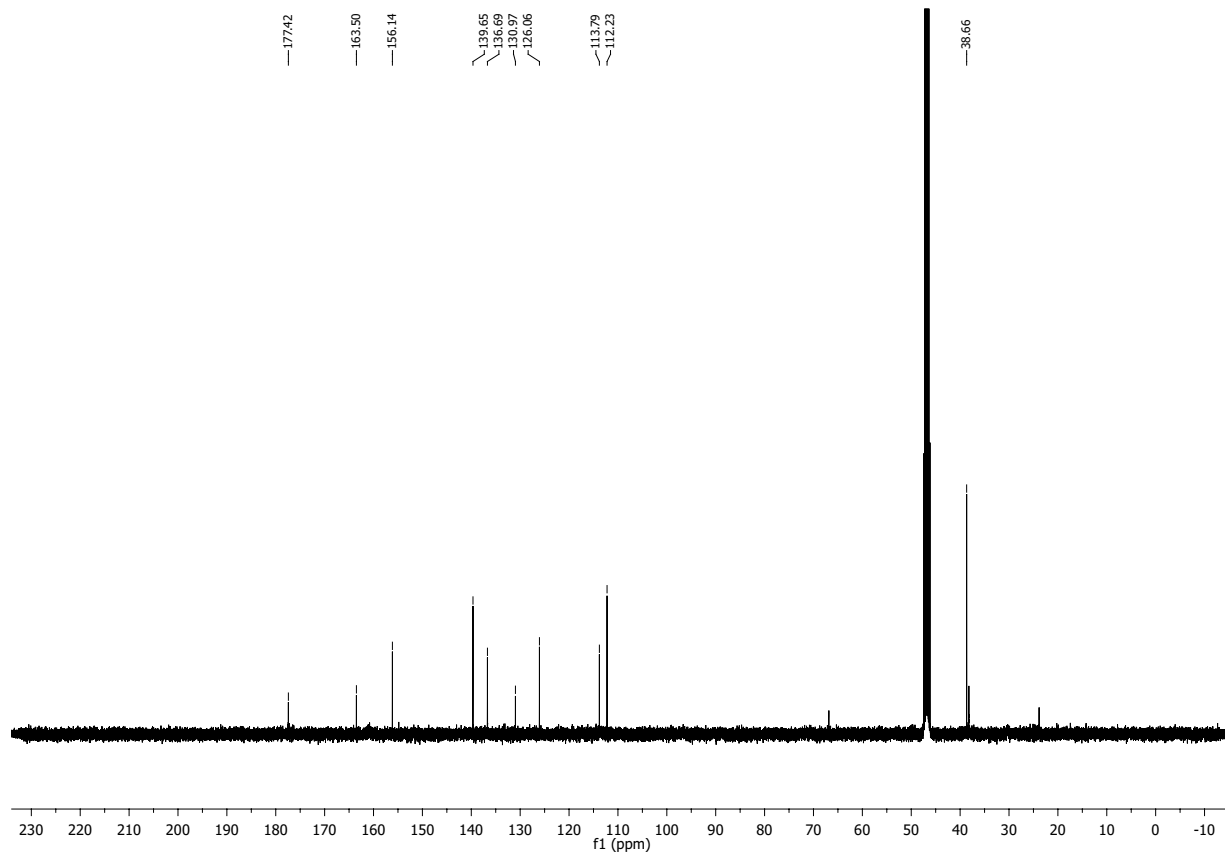
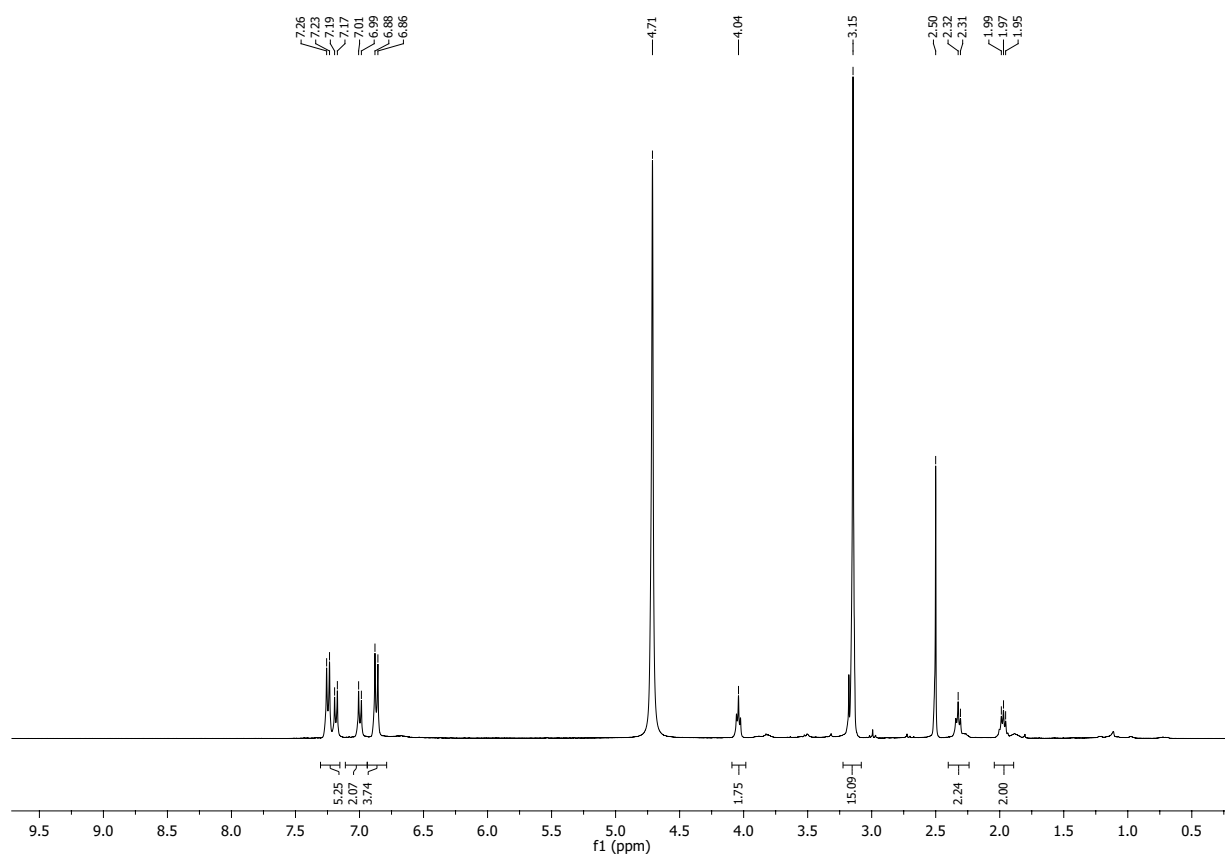
N-(3-azidopropyl)-4-(4-(bis(4-(dimethylamino)phenyl)methyl)phenoxy)butanamide, **56**



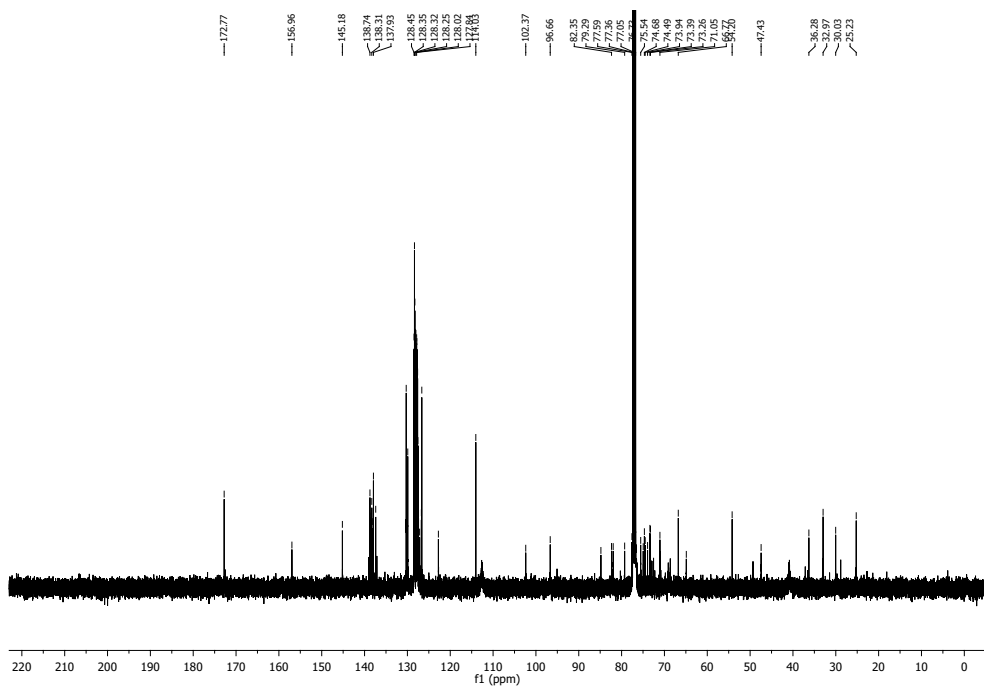
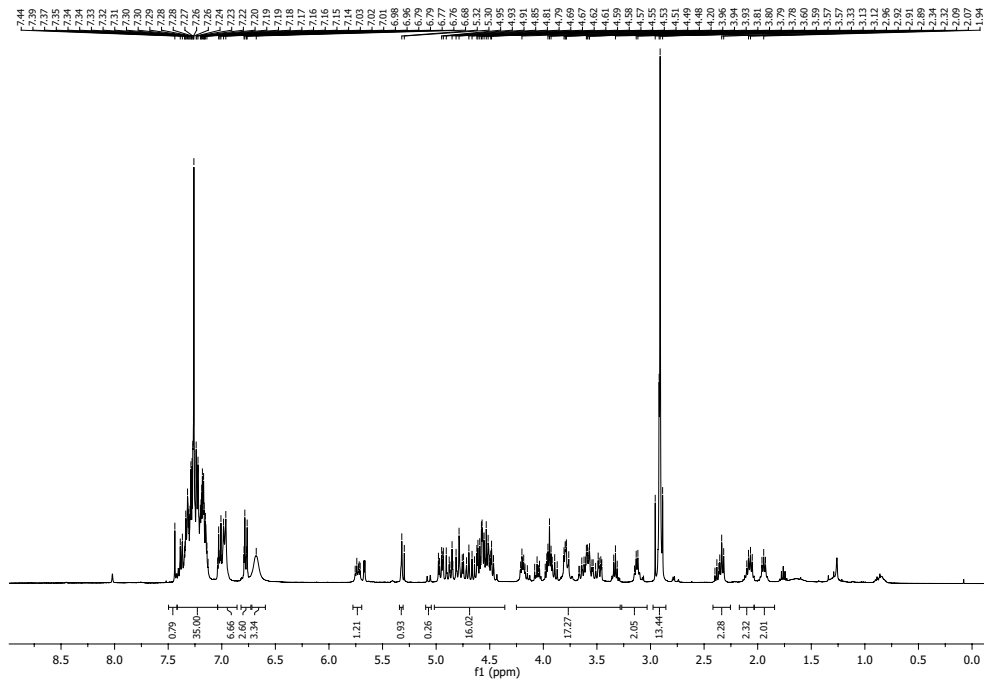
*tert*-butyl (3-(3-(4-(4-(bis(4-(dimethylamino)phenyl)methyl) phenoxy)butanamido)propoxy)propyl)carbamate, **58**



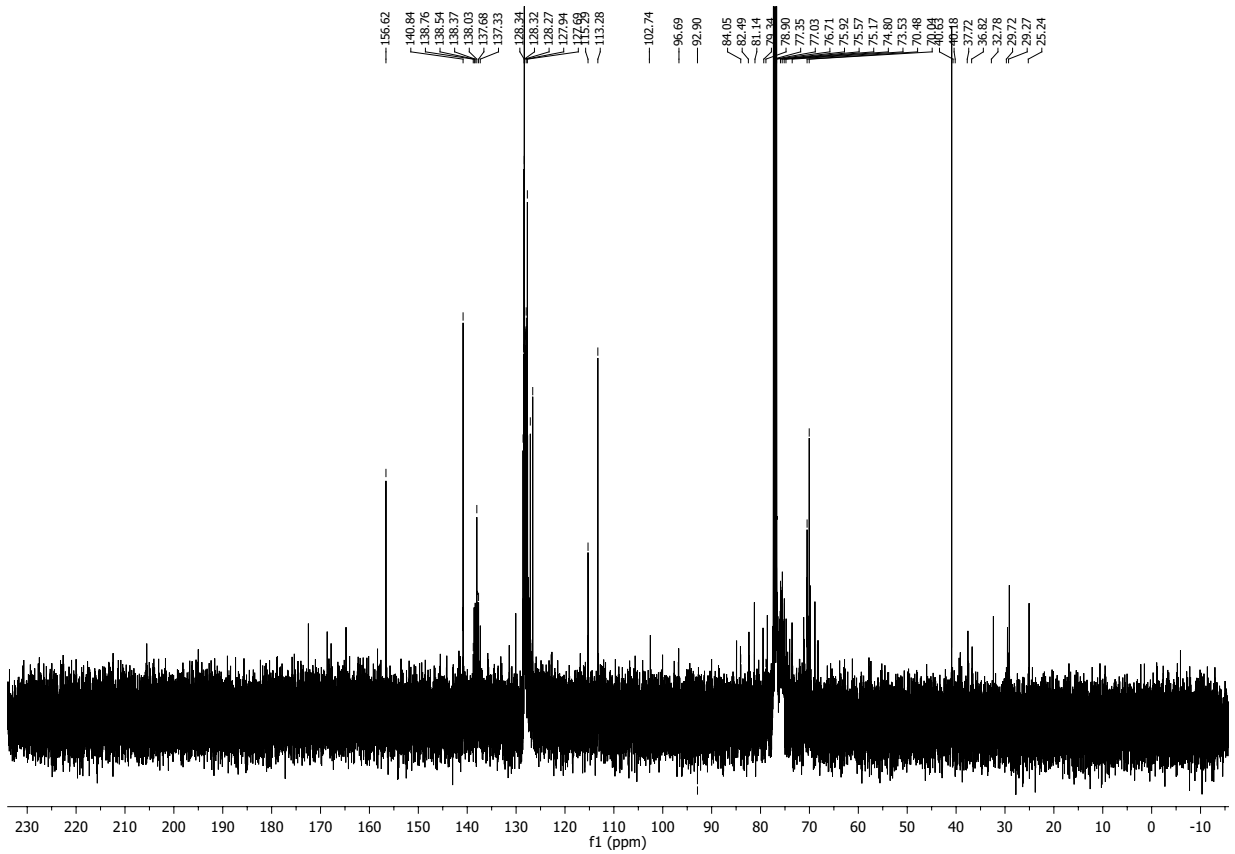
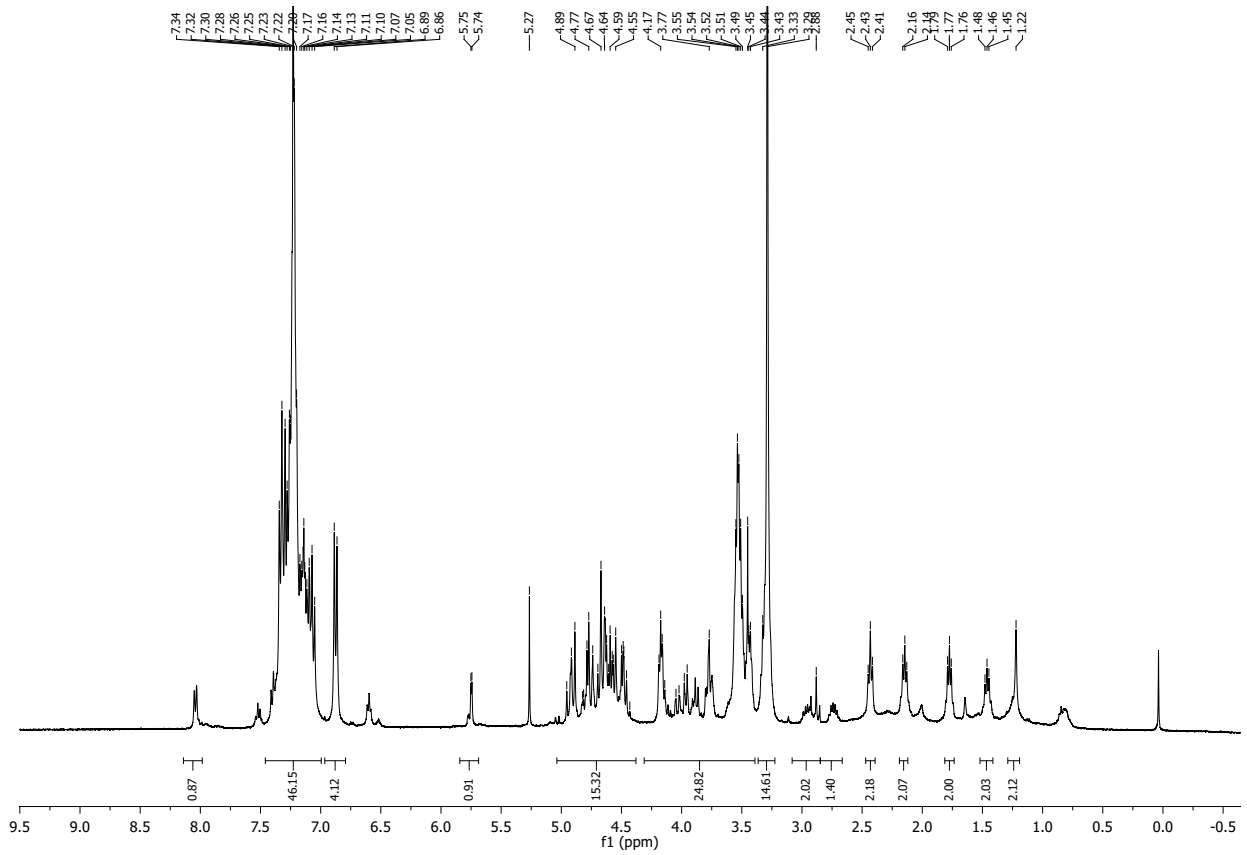
N-(4-((4-(3-carboxypropoxy)phenyl)(4-(dimethylamino)phenyl)methylene)cyclohexa-2,5-dien-1-ylidene)-N-methylmethanaminium, **60**



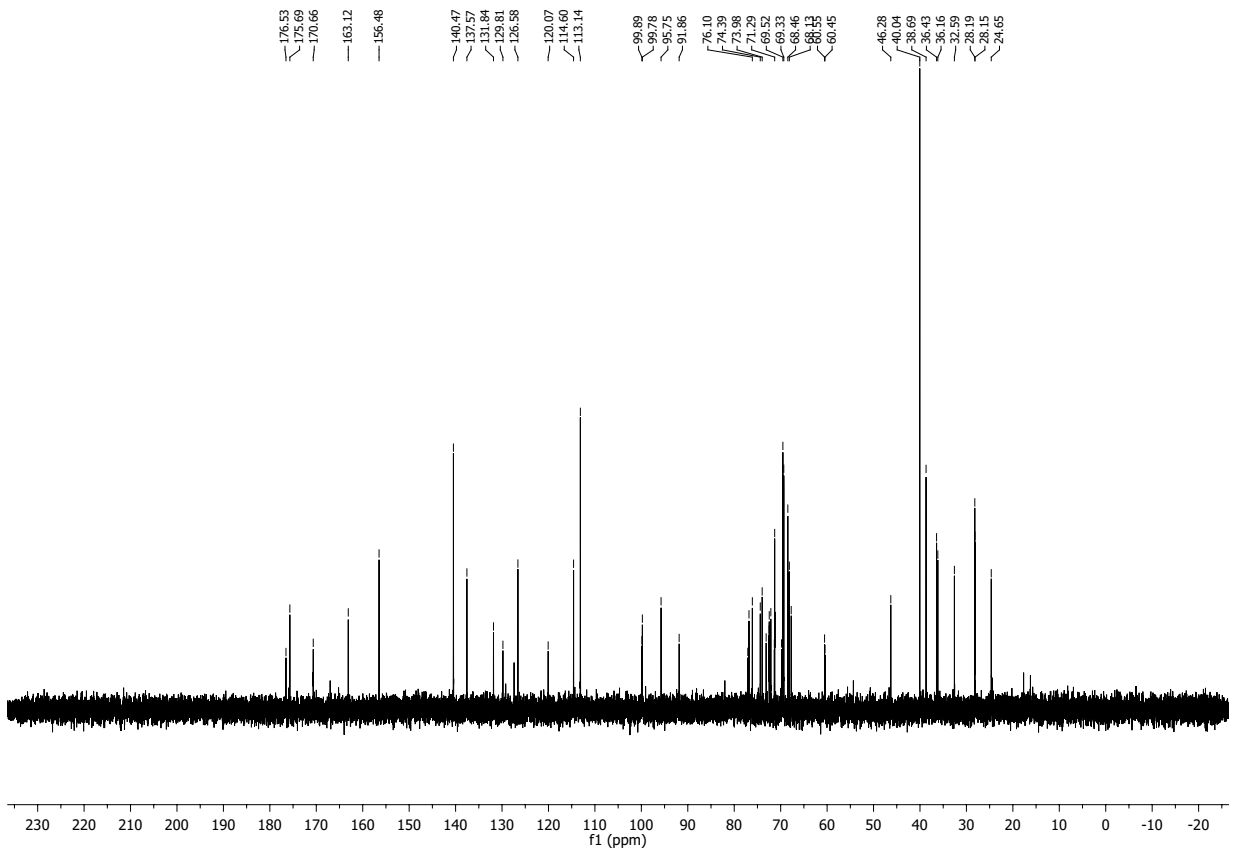
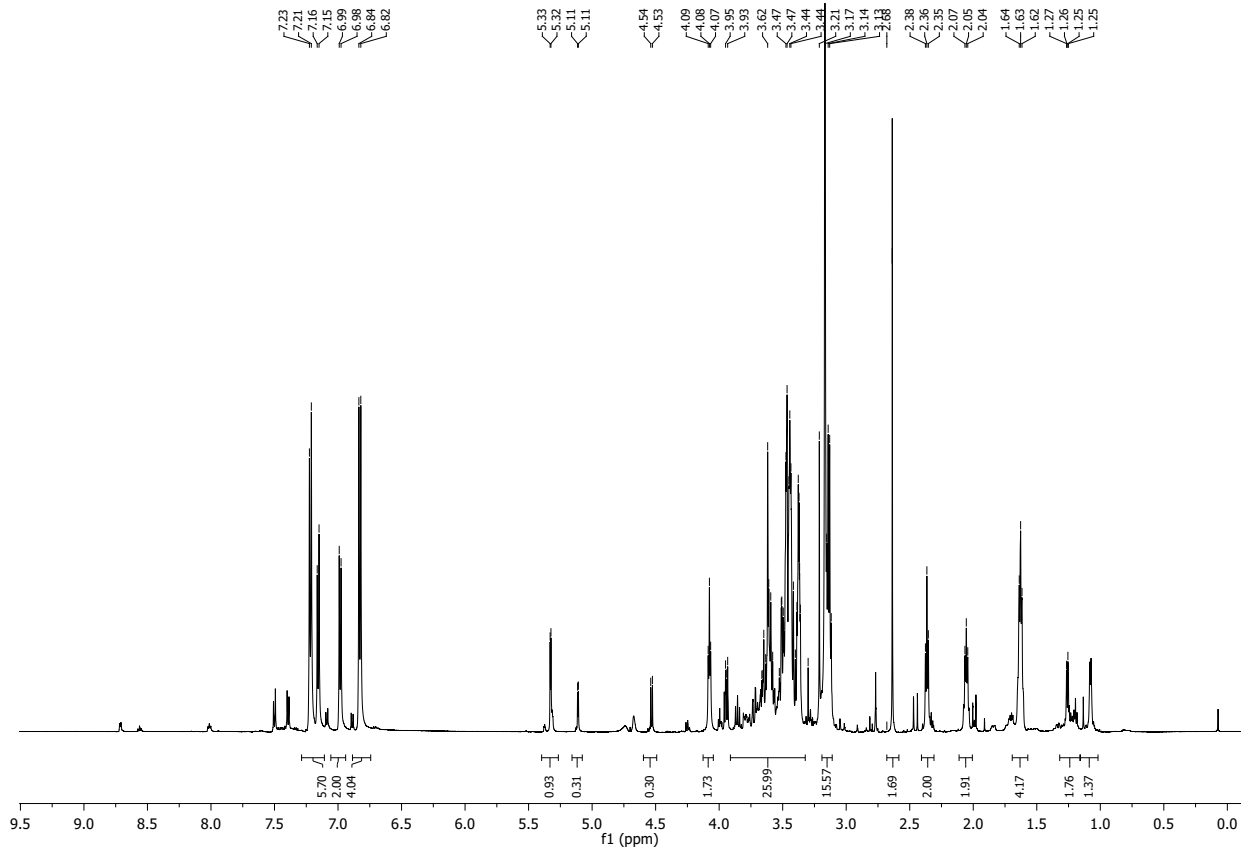
Benzylated BOT\_17, 61



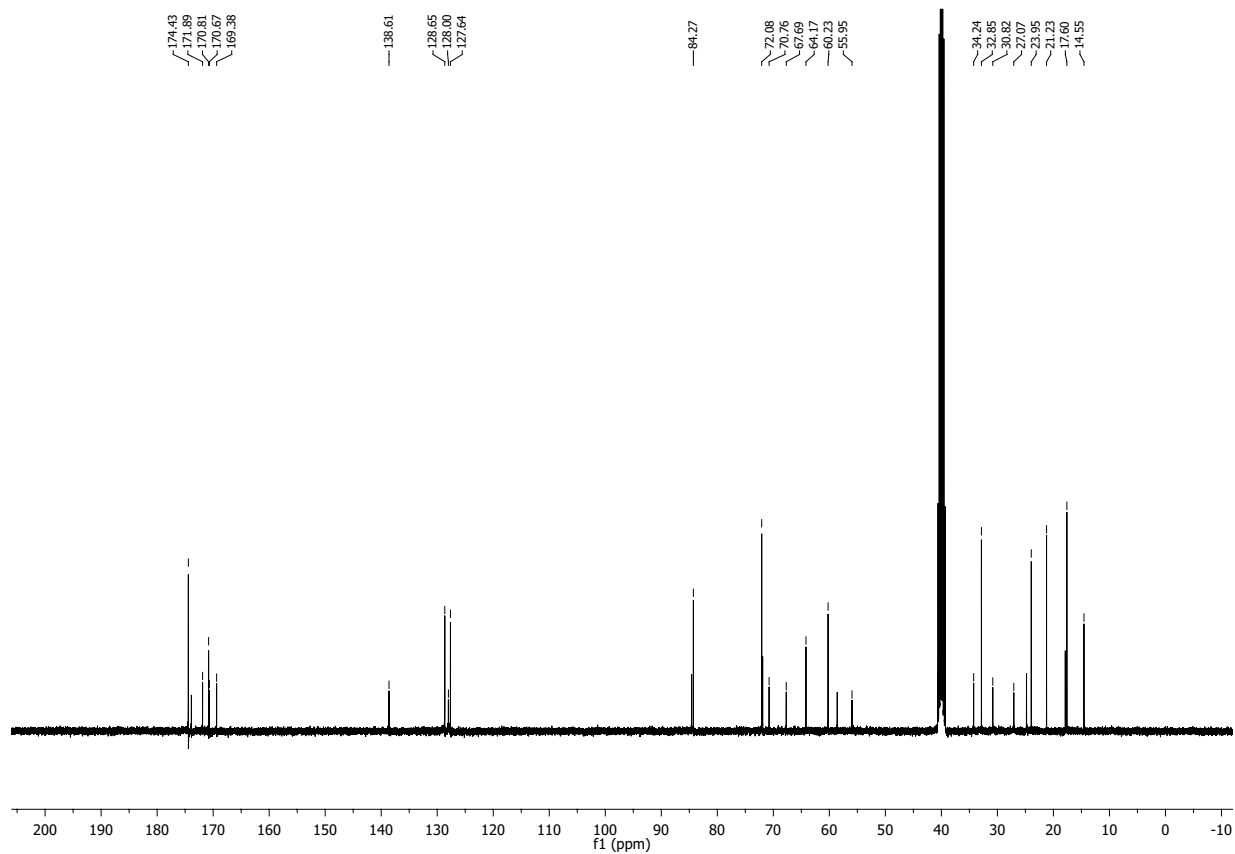
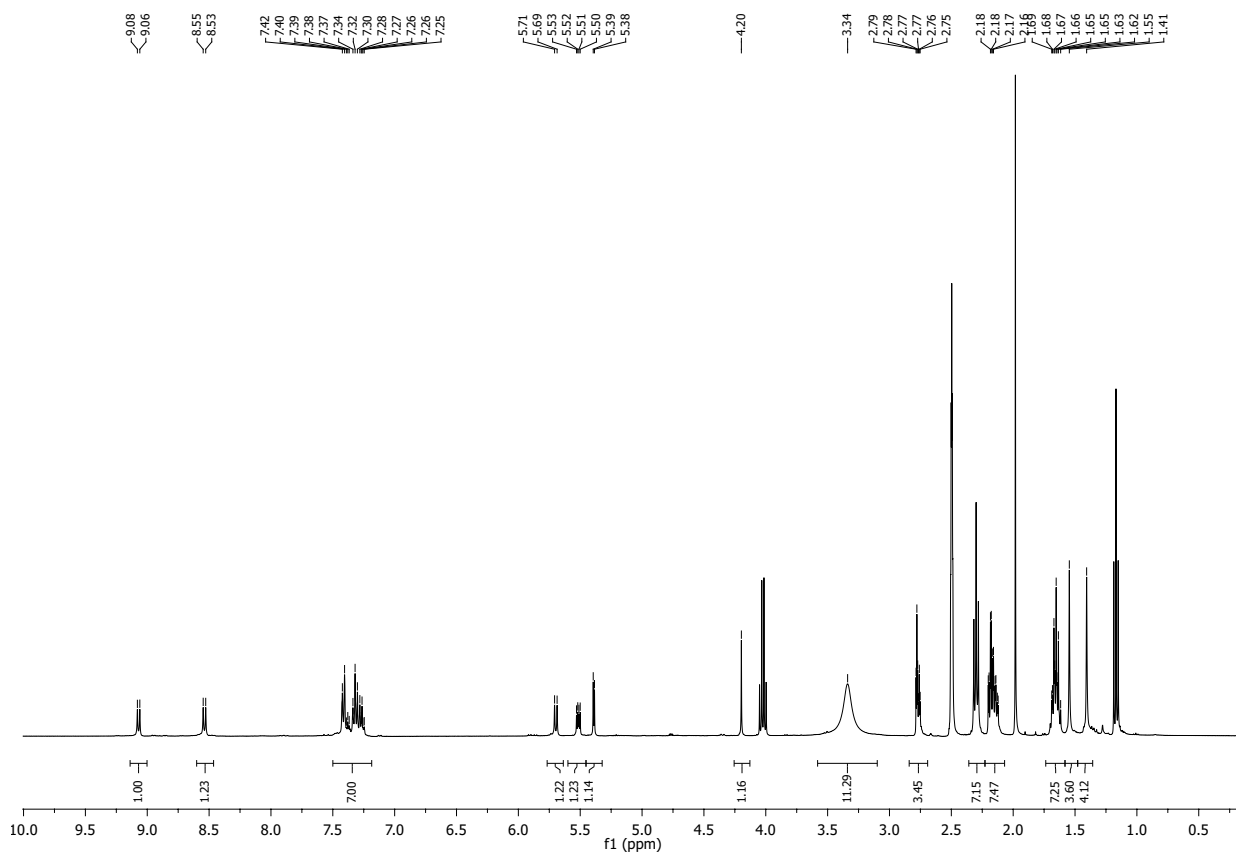
Benzylated BOT.52, 64



Maltose PEG MG conjugate, BOT\_52

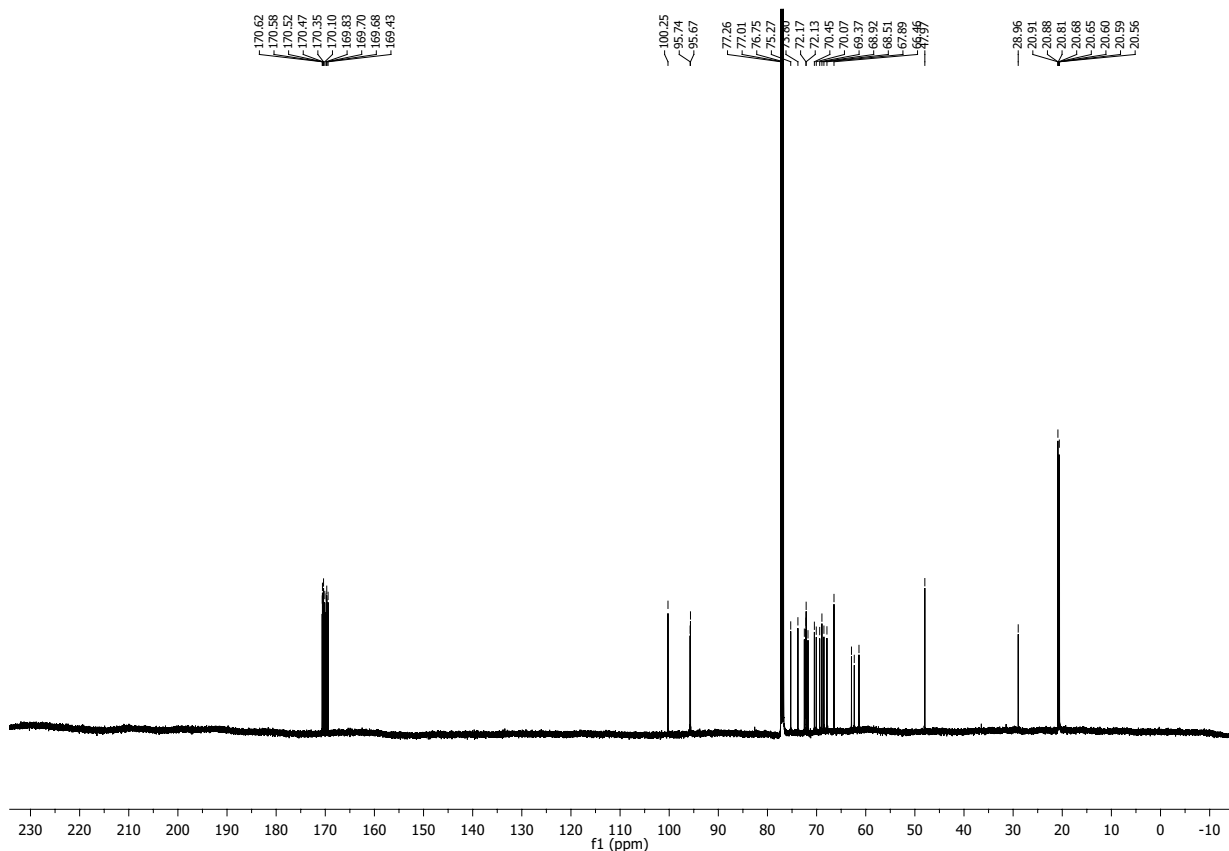
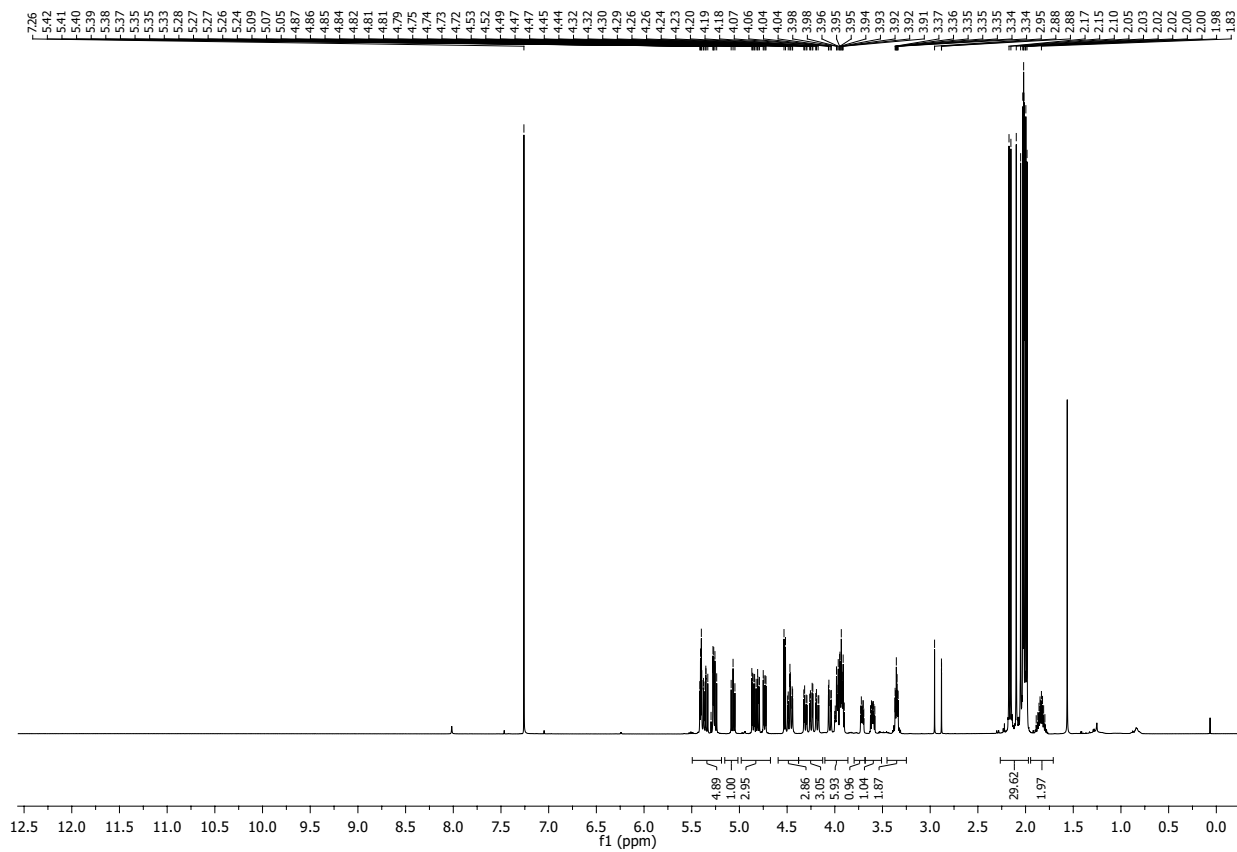


(2S,5R,6R)-6-((R)-2-(hex-5-ynamido)-2-phenylacetamido)-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid,  
68

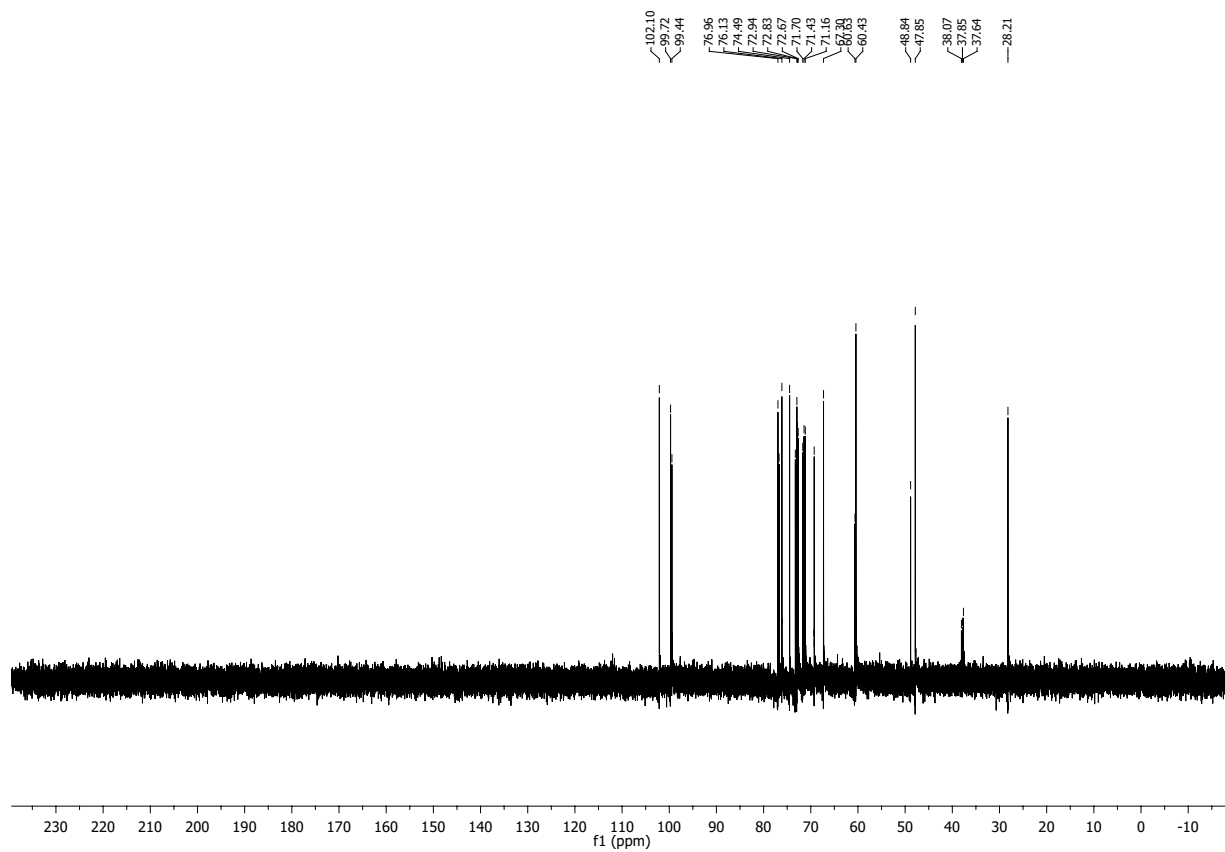
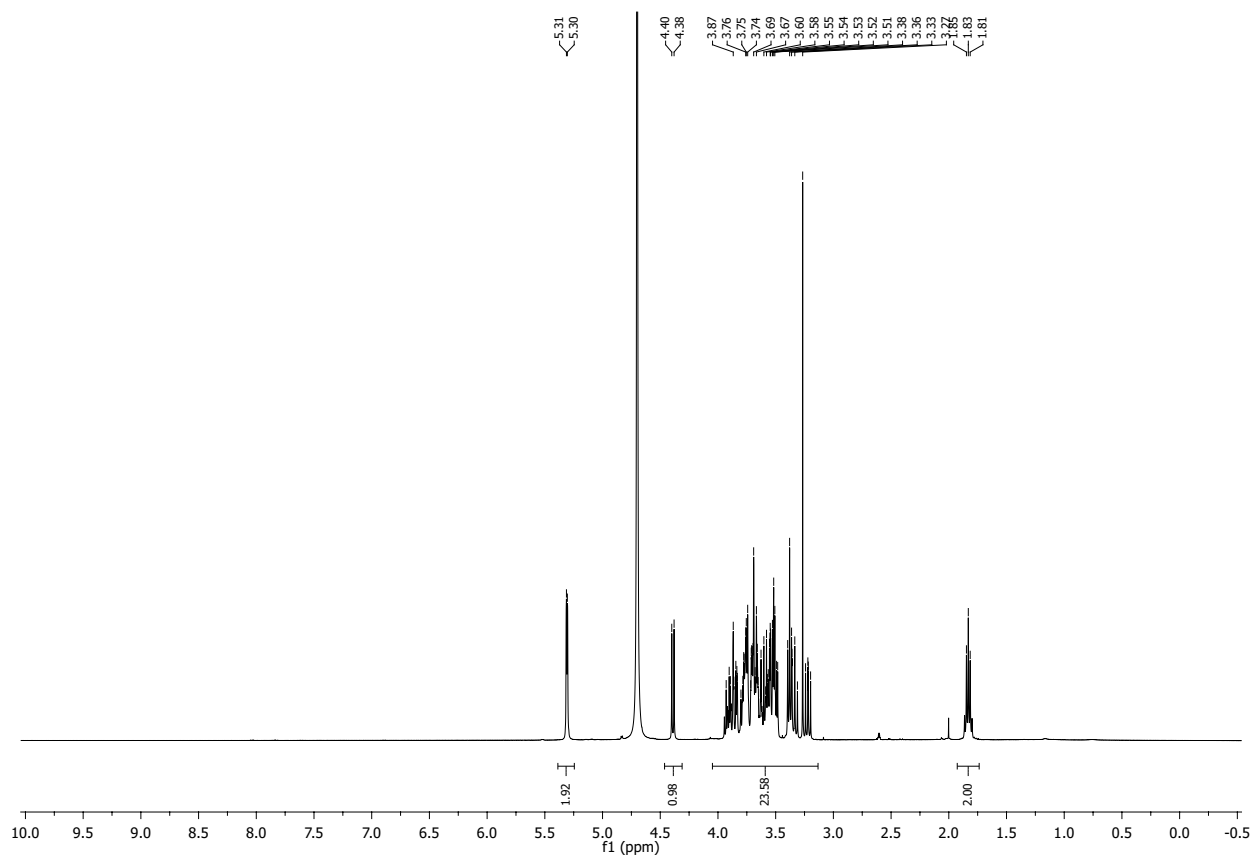




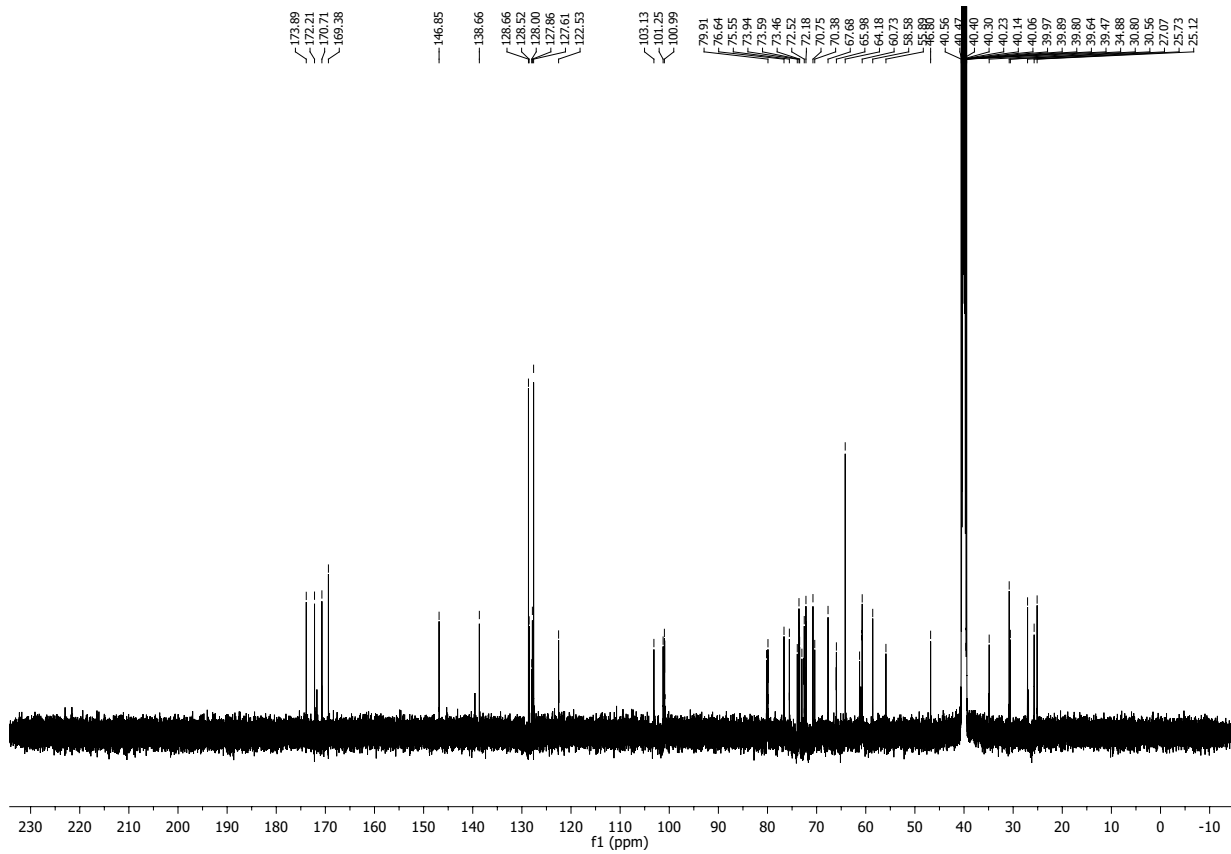
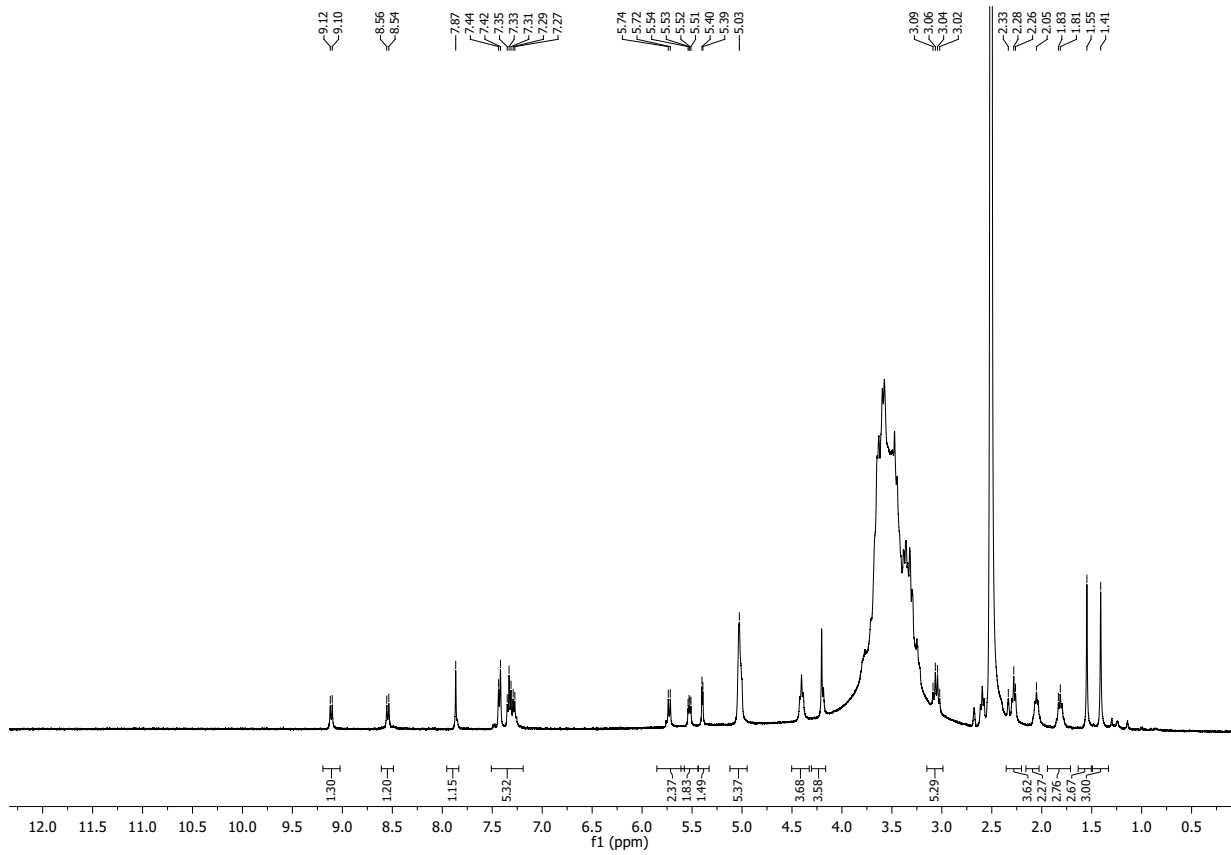
$\beta$ -D-glucopyranose,2,3,4,6-tetra-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2,3,6-tri-O-acetyl- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-2,3,6-triacetate 1-(3'-azidopropyl),  
**71**



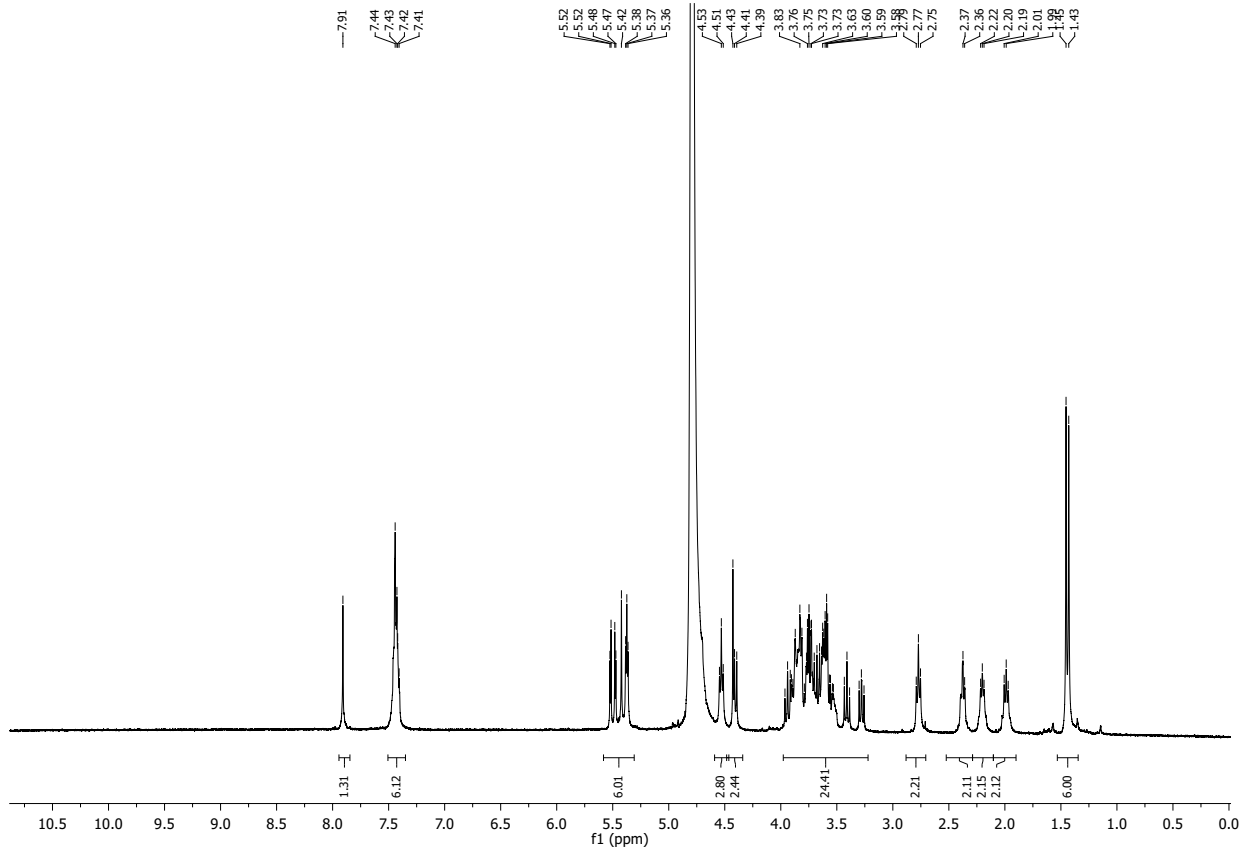
$\beta$ -D-glucopyranose- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-1-(3'-azidopropyl), **72**



Maltohexose-Ampicillin conjugate, BOT\_54



Maltotriose-ampicillin conjugate, BOT\_55



Maltose ampicillin conjugate, BOT\_56

