

Supporting information

Synthesis of Novel Types of Polyester Glycodendrimers as potential inhibitors of Urinary Tract Infections

Jean-d'Amour K. Twibanire,^{a,b,*} Nawal K. Paul, and T. Bruce Grindley^{a,*}

^aDepartment of Chemistry, Dalhousie University, Halifax, N.S. B3H 4J3, Canada

^bCanAm Bioresearch Inc., Winnipeg, MB R3T 0P4, Canada

*Corresponding Author

Email(s): twibanire@dal.ca (J.K.T.), bruce.grindley@dal.ca (T.B.G.)

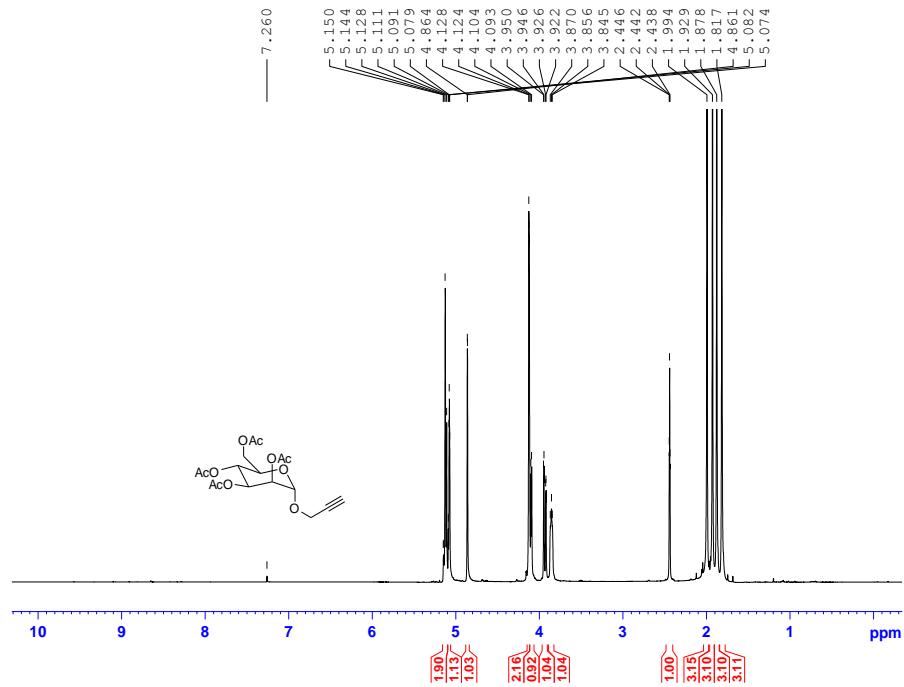
Table of Contents

Title	Page
500.13 MHz ^1H NMR spectrum of 2-propynyl 2,3,4,6-tetra- O -acetyl- α -D-mannopyranoside (6) in chloroform- d	S5
125.7 MHz ^{13}C NMR spectrum of 2-propynyl 2,3,4,6-tetra- O -acetyl- α -D-mannopyranoside (6) in chloroform- d	S6
300.15 MHz ^1H NMR spectrum of 2-propynyl α -D-mannopyranoside (7) in methanol- d_4	S6
75.5 MHz ^{13}C NMR spectrum of 2-propynyl α -D-mannopyranoside (7) in methanol- d_4	S7
500.13 MHz ^1H NMR spectrum of 6-azidohexyl 2,3,4,6-tetra- O -acetyl- α -D-mannopyranoside (9) in chloroform- d	S8
125.7 MHz ^{13}C NMR spectrum of 6-azidohexyl 2,3,4,6-tetra- O -acetyl- α -D-mannopyranoside (9) in chloroform- d	S9
500.13 MHz ^1H NMR spectrum of 6-azidohexyl α -D-mannopyranoside (10) in methanol- d	S9
125.7 MHz ^{13}C NMR spectrum of 6-azidohexyl α -D-mannopyranoside (10) in methanol- d	S10
500.13 MHz ^1H NMR spectrum of methyl and benzyl-protected hydroquinone-cored first generation dendrimer (15) in chloroform- d	S11
125.7 MHz ^{13}C NMR spectrum of methyl and benzyl-protected hydroquinone-cored first generation dendrimer (15) in chloroform- d	S12
500.13 MHz ^1H NMR spectrum of bis(2-(3-hydroxy-2,2-bis-(methoxymethyl)-propanoyloxy)ethoxy)benzene (16) in acetone- d_6	S12
125.7 MHz ^{13}C NMR spectrum of bis(2-(3-hydroxy-2,2-bis-(methoxymethyl)-propanoyloxy)-ethoxy)benzene (16) in acetone- d_6	S13
300.15 MHz ^1H NMR spectrum of azide-functionalized divalent first generation dendrimer (17) in chloroform- d	S13
75.5 MHz ^{13}C NMR spectrum of azide-functionalized divalent first generation dendrimer (17) in chloroform- d	S14
500.13 MHz ^1H NMR spectrum of benzyl-functionalized divalent dendrimer (18) in chloroform- d	S15
125.7 MHz ^{13}C NMR spectrum of benzyl-functionalized divalent dendrimer (18) in chloroform- d	S16
500.13 MHz ^1H NMR spectrum of hydroxyl-terminated divalent dendrimer (19) in methanol- d_4	S16
125.7 MHz ^{13}C NMR spectrum of hydroxyl-terminated divalent dendrimer (19) in methanol- d_4	S17
300.15 MHz ^1H NMR spectrum of azide-functionalized divalent dendrimer (20) in chloroform- d	S18
75.5 ^{13}C NMR spectrum of azide-functionalized divalent dendrimer (20) in chloroform- d	S19
500.13 MHz ^1H NMR spectrum of benzylidene-protected hydroquinone-cored third generation dendrimer (23) in chloroform- d	S19
125.7 MHz ^{13}C NMR spectrum of benzylidene-protected hydroquinone-cored third generation dendrimer (23) in chloroform- d	S20
500.13 MHz ^1H NMR spectrum of third generation dendrimer (24) in DMSO- d_6	S21
125.7 MHz ^{13}C NMR spectrum of third generation dendrimer (24) in DMSO- d_6	S22

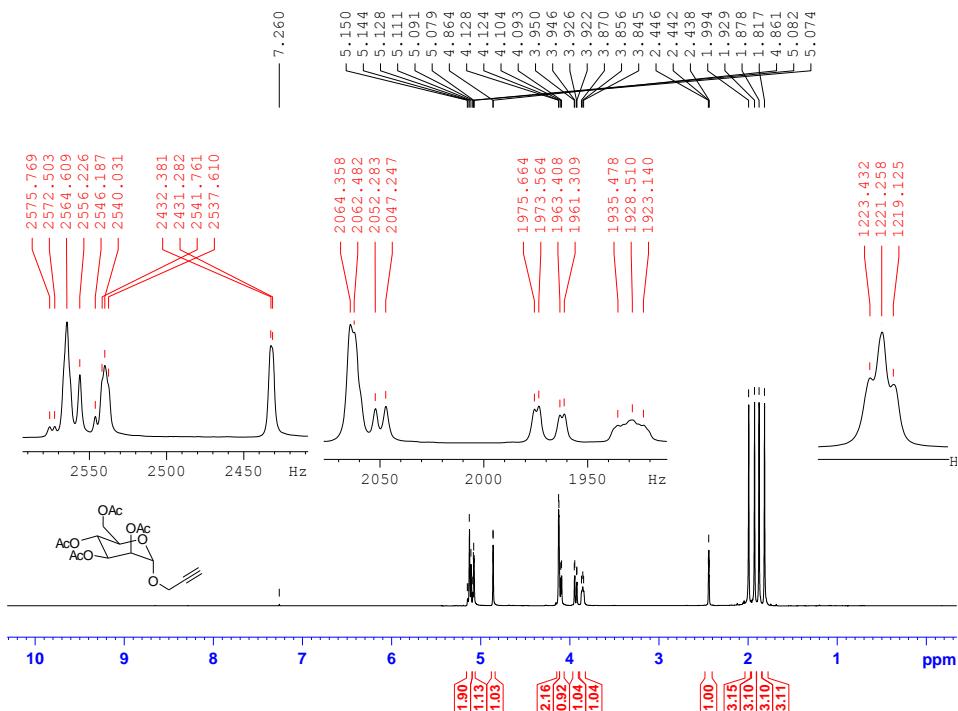
500.13 MHz ^1H NMR spectrum of azide-functionalized hydroquinone-cored third generation dendrimer (25) in chloroform- <i>d</i>	S23
125.7 MHz ^{13}C NMR spectrum of azide-functionalized hydroquinone-cored third generation dendrimer (25) in chloroform- <i>d</i>	S24
500.13 MHz ^1H NMR spectrum of extended divalent α -D-mannopyranoside-terminated dendrimer (27) in methanol- <i>d</i> ₄	S25
125.7 MHz ^{13}C NMR spectrum of extended divalent α -D-mannopyranoside-terminated dendrimer (27) in methanol- <i>d</i> ₄	S26
500.13 MHz ^1H NMR spectrum of third generation dendrimer bearing 16 mannose residues (28) in water- <i>d</i> ₂	S27
125.7 MHz ^{13}C NMR spectrum of third generation dendrimer bearing 16 mannose residues (28) in water- <i>d</i> ₂	S27
500.13 MHz ^1H NMR spectrum of bis(2-(2-propynyloxy)ethoxy)benzene (29) in chloroform- <i>d</i>	S28
125.7 MHz ^{13}C NMR spectrum of bis(2-(2-propynyloxy)ethoxy)benzene (29) in chloroform- <i>d</i>	S28
500.13 MHz ^1H NMR spectrum of divalent α -D-mannopyranoside-terminated dendrimer with a hexyl linker (30) in DMSO- <i>d</i> ₆ / methanol- <i>d</i> ₄	S29
125.7 MHz ^{13}C NMR spectrum of divalent α -D-mannopyranoside-terminated dendrimer with a hexyl linker (30) in DMSO- <i>d</i> ₆ / methanol- <i>d</i> ₄	S30
500.13 MHz ^1H NMR spectrum of 2,2'-bis-(2-propynyloxymethyl)propanoic acid (31) in chloroform- <i>d</i>	S31
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis-(2-propynyloxymethyl)propanoic acid (31) in chloroform- <i>d</i>	S32
500.13 MHz ^1H NMR spectrum of 2,2'-bis-(2-propynyloxymethyl)propanoyl anhydride (32) in chloroform- <i>d</i>	S32
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis-(2-propynyloxymethyl)propanoyl anhydride (32) in chloroform- <i>d</i>	S33
500.13 MHz ^1H NMR spectrum of 1,4-bis-2-(2,2'-bis-(2-propynyloxy)methyl)propanoyloxy)-ethoxy (33) in chloroform- <i>d</i>	S34
125.7 MHz ^{13}C NMR spectrum of 1,4-bis-2-(2,2'-bis-(2-propynyloxy)methyl)propanoyloxy)-ethoxy (33) in chloroform- <i>d</i>	S35
500.13 MHz ^1H NMR spectrum of tetramannoside polyester dendrimer (34) in dimethyl sulfoxide- <i>d</i> ₆	S36
125.7 MHz ^{13}C DeptQ spectrum of tetramannoside polyester dendrimer (34) in dimethyl sulfoxide- <i>d</i> ₆	S38
500.13 MHz ^1H NMR spectrum of 2-(p-toluenesulfonyl)ethyl 2,2'-bis(2,2'-bis-(2-propynyl-oxymethyl)propanoyloxy)methyl)propanoate (36) in chloroform- <i>d</i>	S39
125.7 MHz ^{13}C NMR spectrum of 2-(p-toluenesulfonyl)ethyl 2,2'-bis(2,2'-bis-(2-propynyl-oxymethyl)propanoyloxy)methyl)propanoate (36) in chloroform- <i>d</i>	S41
500.13 MHz ^1H NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynyloxymethyl)propanoyloxy)methyl)-propanoic acid (37) in chloroform- <i>d</i>	S42
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynyloxymethyl)propanoyloxy)methyl)-propanoic acid (37) in chloroform- <i>d</i>	S44
500.13 MHz ^1H NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynyloxymethyl)propanoyloxy)methyl)-propanoic anhydride (38) in chloroform- <i>d</i>	S45

125.7 MHz ^{13}C NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynylloxymethyl)propanoyloxymethyl)-propanoic anhydride (38) in chloroform- <i>d</i>	S47
500.13 MHz ^1H NMR spectrum of octapropargylated polyester dendrimer (39) in chloroform- <i>d</i>	S48
125.7 MHz ^{13}C NMR spectrum of octapropargylated polyester dendrimer (39) in chloroform- <i>d</i>	S50
500.13 MHz ^1H NMR spectrum of octavalent mannose-terminated polyester dendrimer (40) in water- <i>d</i> ₂	S51
125.7 MHz ^{13}C NMR spectrum of octavalent mannose-terminated polyester dendrimer (40) in water- <i>d</i> ₂	S52
125.7 MHz ^{13}C DEPT Q NMR spectrum of octavalent mannose-terminated polyester dendrimer (40) in water- <i>d</i> ₂	S54

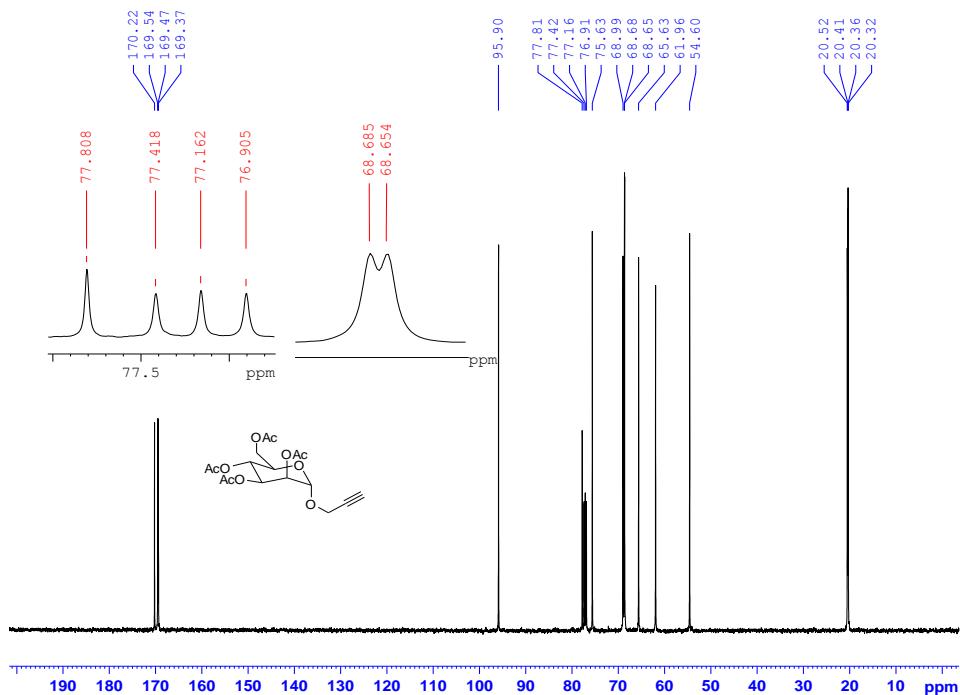
500.13 MHz ^1H NMR spectrum of 2-propynyl 2,3,4,6-tetra-O-acetyl- α -D-mannopyranoside (6) in chloroform- d



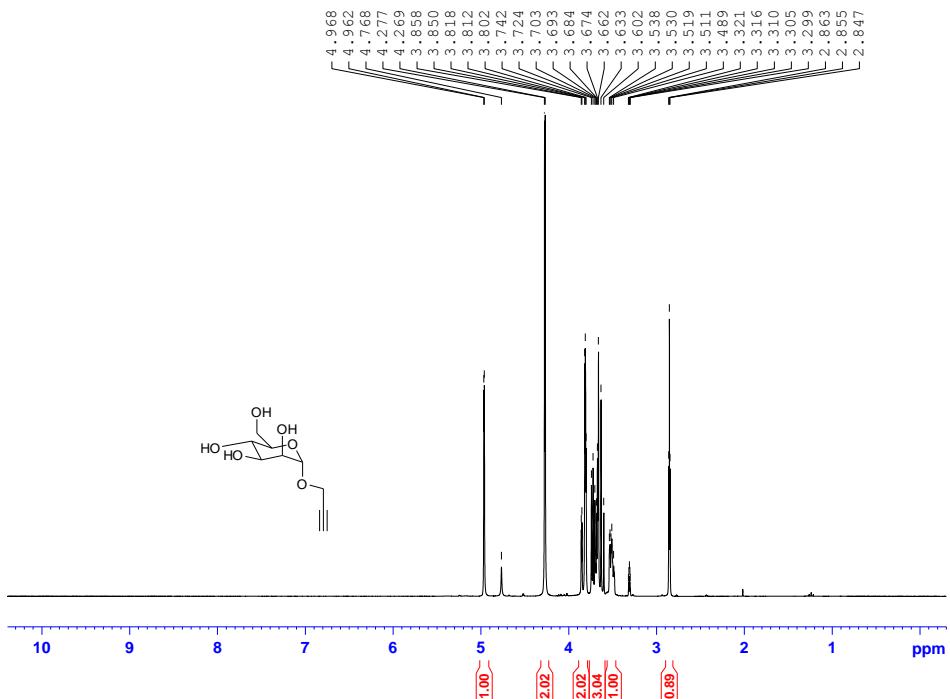
Expansions of parts of the 500.13 MHz ^1H NMR spectrum of 2-propynyl 2,3,4,6-tetra-O-acetyl- α -D-mannopyranoside (6) in chloroform- d



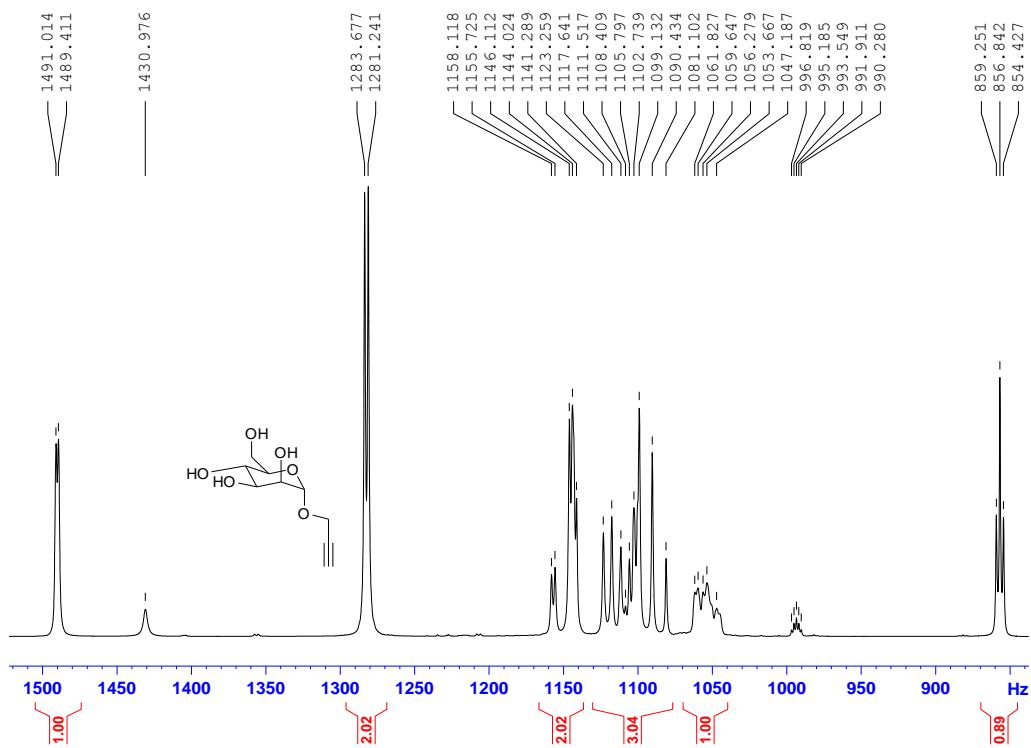
125.7 MHz ^{13}C NMR spectrum of 2-propynyl 2,3,4,6-tetra-*O*-acetyl- α -D-mannopyranoside (6) in chloroform-*d*



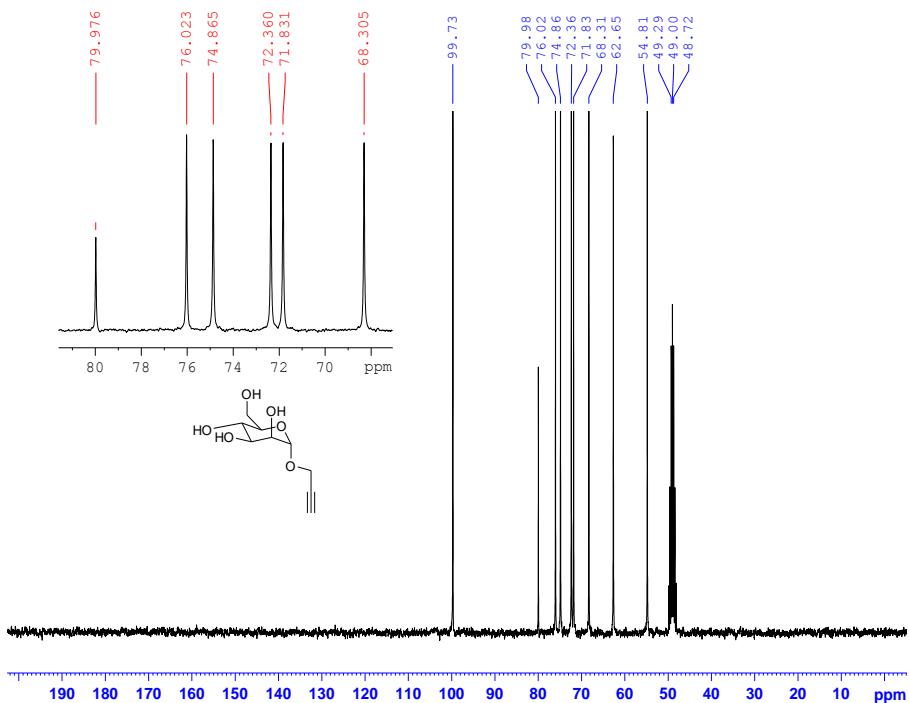
300.15 MHz ^1H NMR spectrum of 2-propynyl α -D-mannopyranoside (7) in methanol-*d*₄



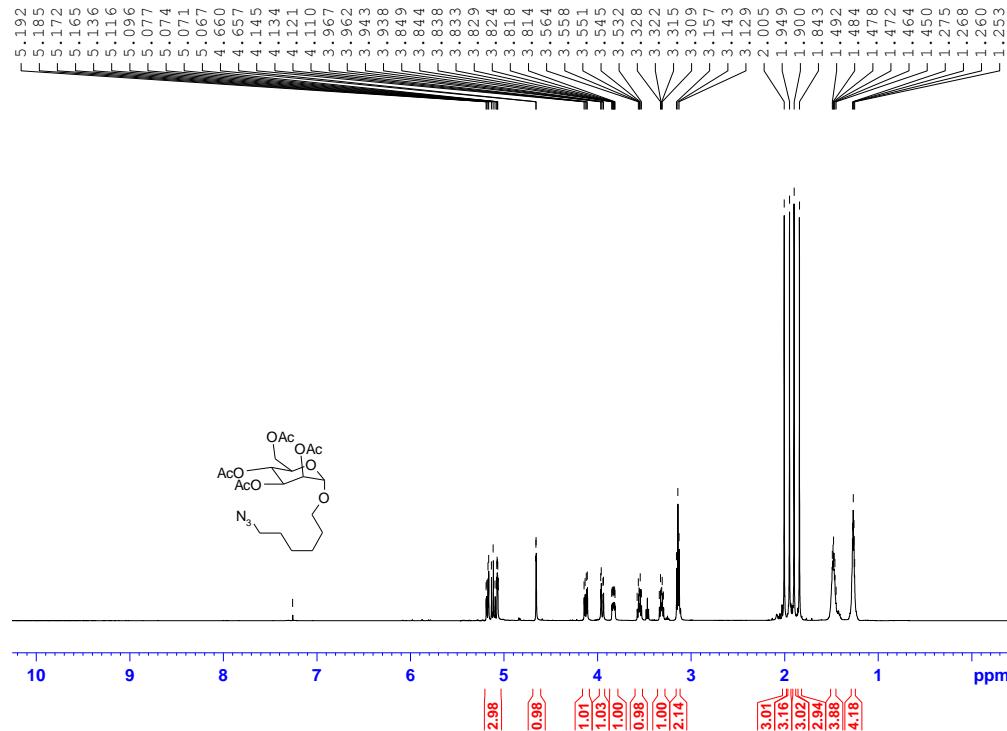
Expansions of part of the 300.15 MHz ^1H NMR spectrum of 2-propynyl α -D-mannopyranoside (7) in methanol- d_4



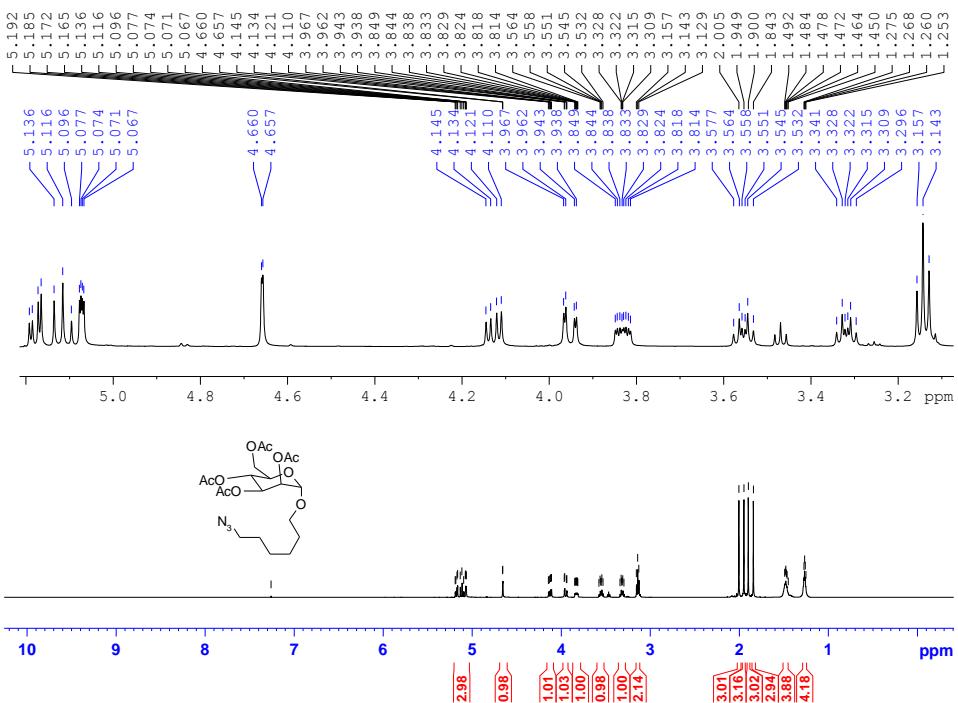
75.5 MHz ^{13}C NMR spectrum of 2-propynyl α -D-mannopyranoside (7) in methanol- d_4



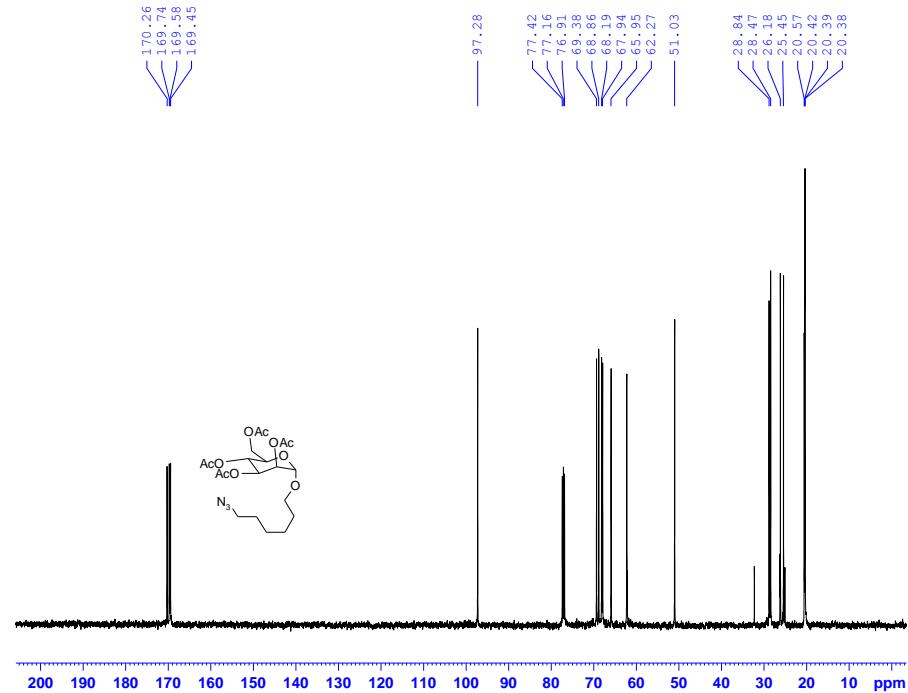
500.13 MHz ^1H NMR spectrum of 6-azidohexyl 2,3,4,6-tetra-*O*-acetyl- α -D-mannopyranoside (9**) in chloroform-*d***



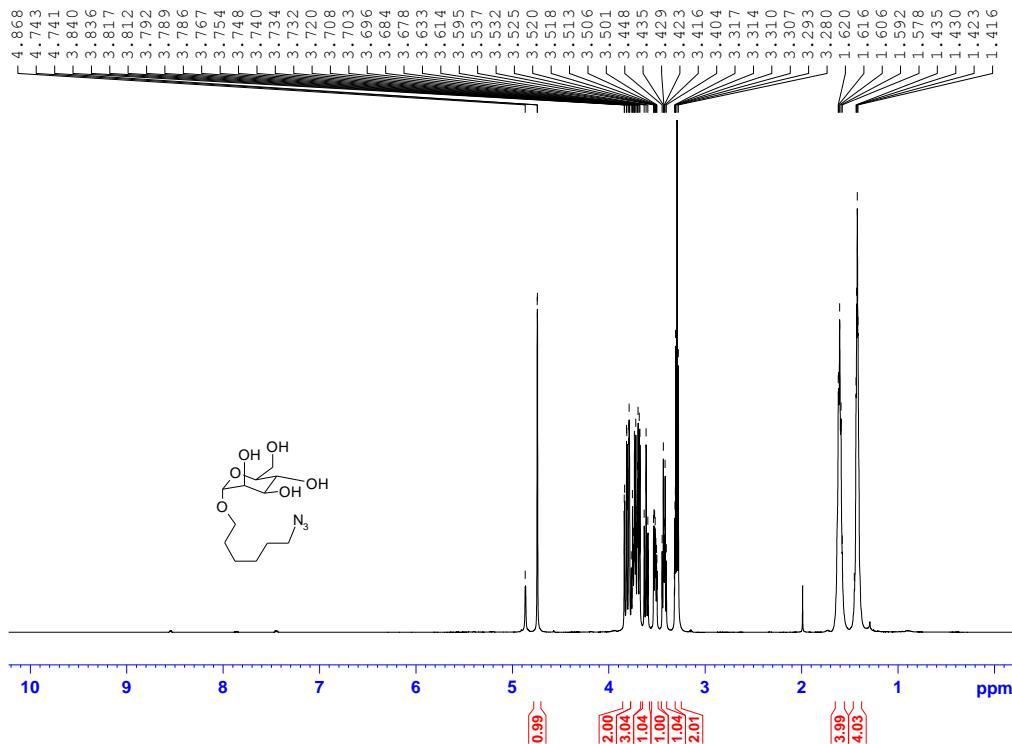
Expansions of part of the 500.13 MHz ^1H NMR spectrum of 6-azidohexyl 2,3,4,6-tetra-*O*-acetyl- α -D-mannopyranoside (9**) in chloroform-*d***



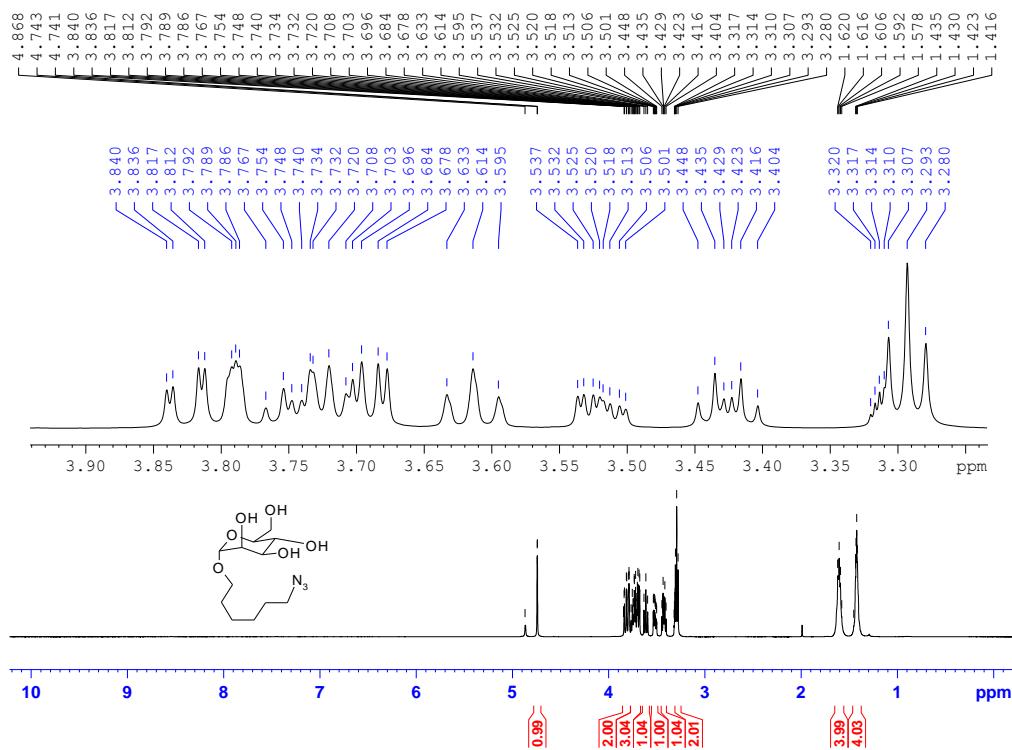
125.7 MHz ^{13}C NMR spectrum of 6-azidohexyl 2,3,4,6-tetra-O-acetyl- α -D-mannopyranoside (9**) in chloroform-d**



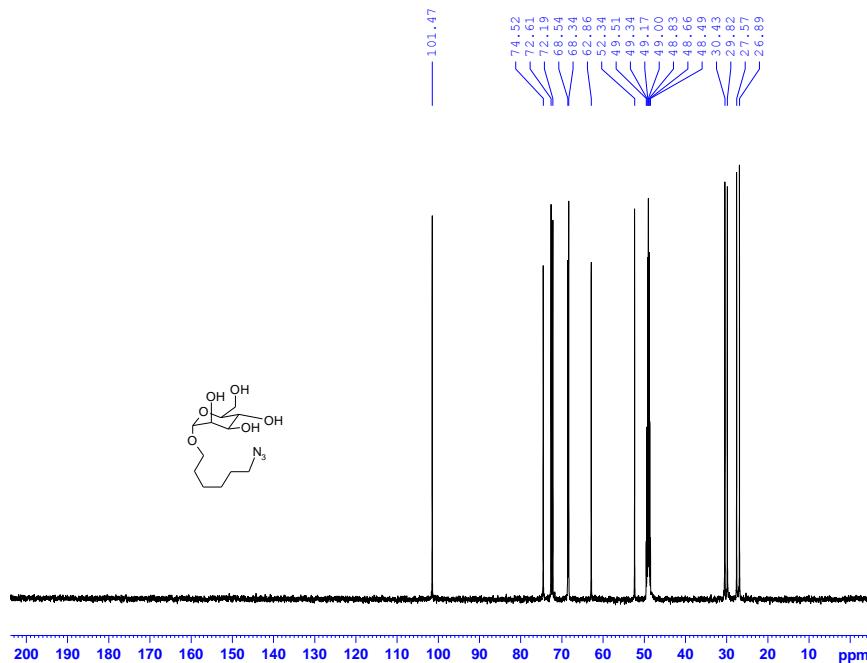
500.13 MHz ^1H NMR spectrum of 6-azidohexyl α -D-mannopyranoside (10**) in methanol-d**



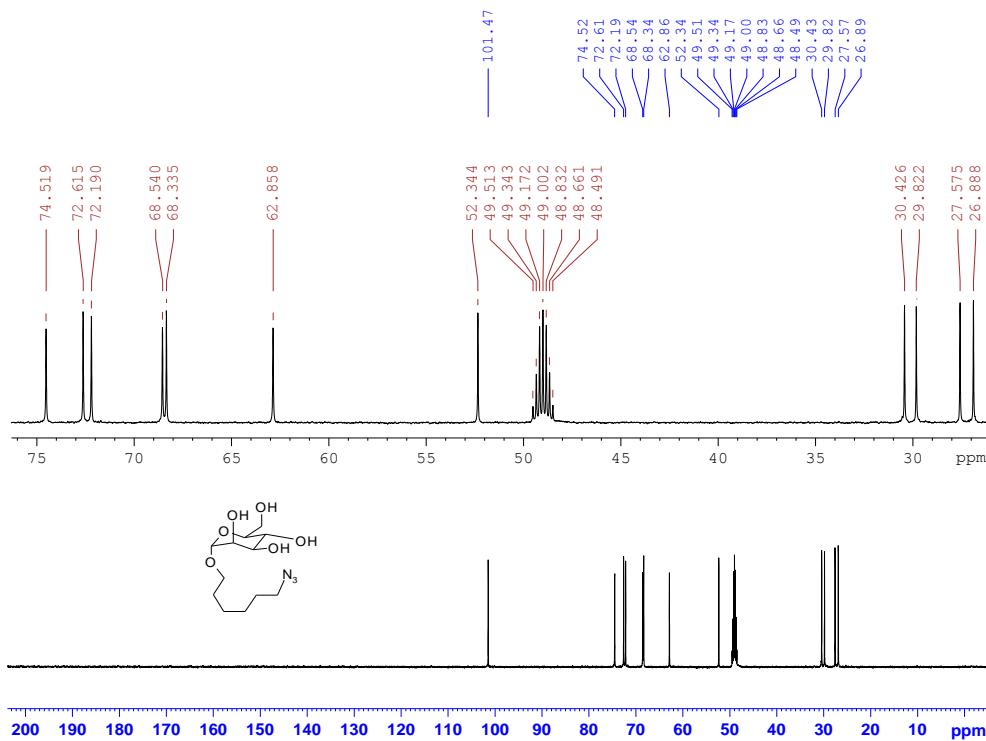
Expansion of part of the 500.13 MHz ^1H NMR spectrum of 6-azidohexyl α -D-mannopyranoside (10) in methanol-d₄



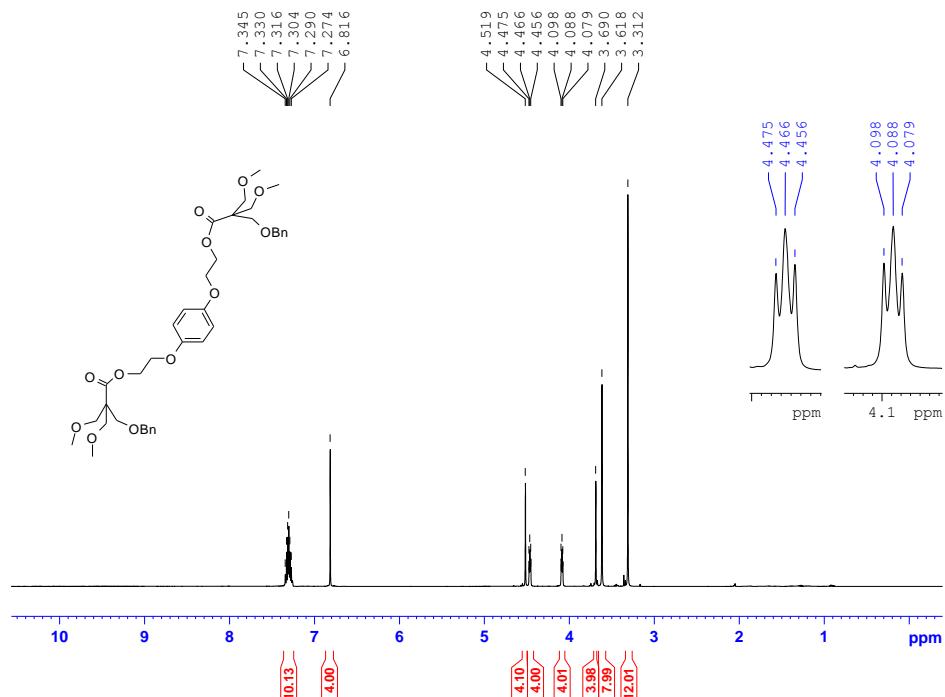
125.7 MHz ^{13}C NMR spectrum of 6-azidohexyl α -D-mannopyranoside (10) in methanol-d₄



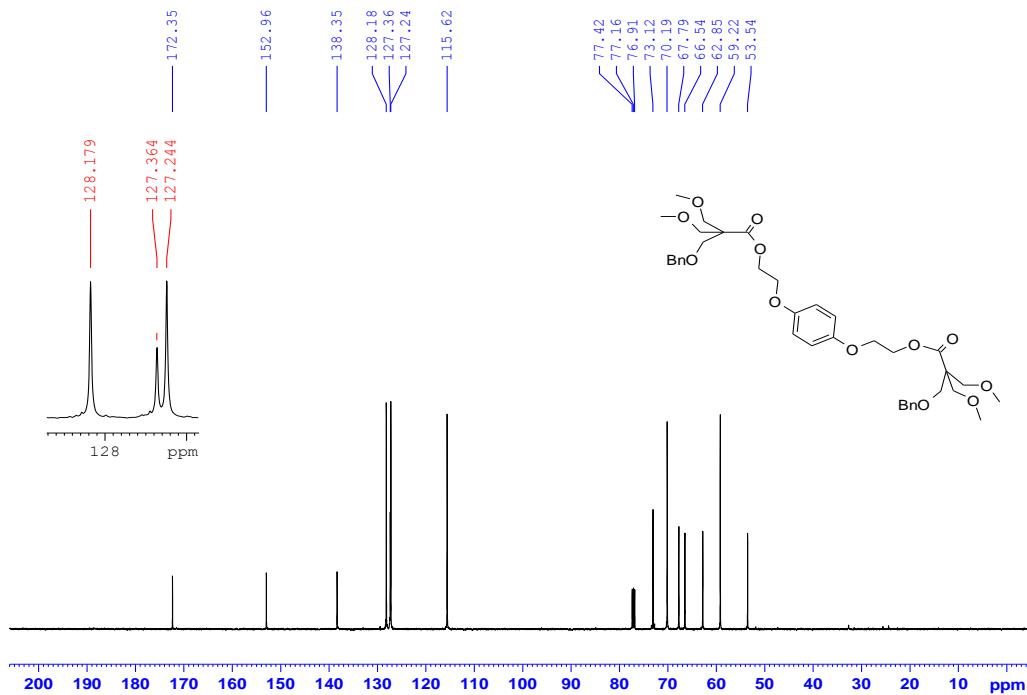
Expansion of part of the 125.7 MHz ^{13}C NMR spectrum of 6-azidohexyl α -D-mannopyranoside (10**) in methanol-*d***



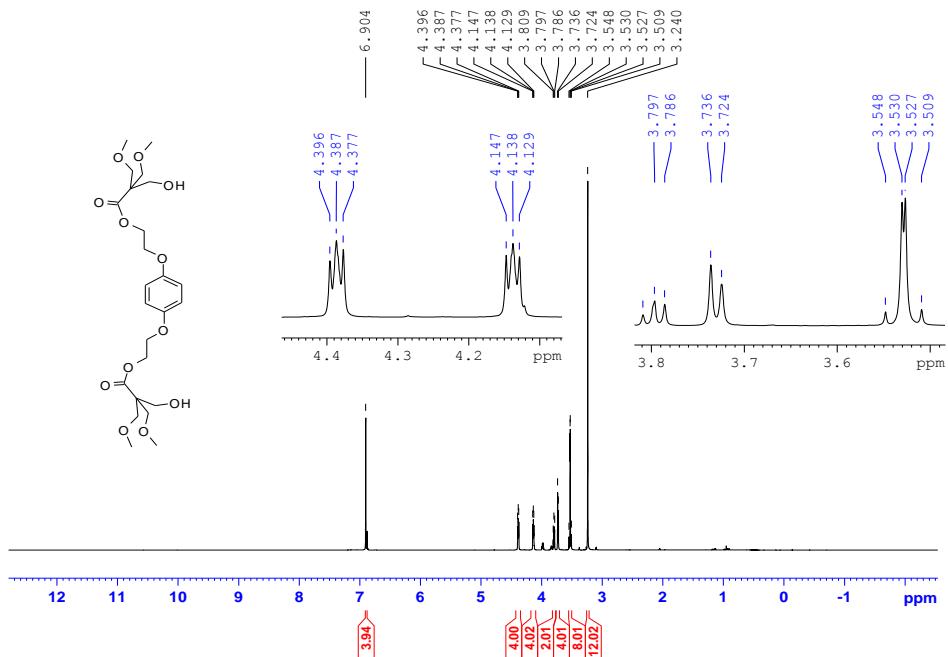
500.13 MHz ^1H NMR spectrum of methyl and benzyl-protected hydroquinone-cored first generation dendrimer (15**) in chloroform-*d***



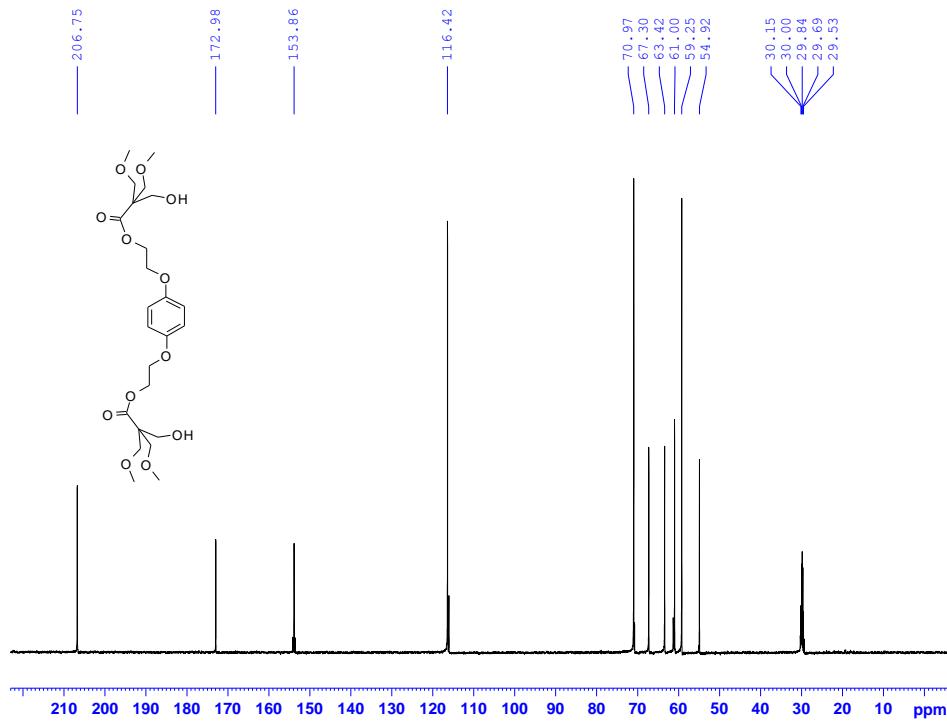
125.7 MHz ^{13}C NMR spectrum of methyl and benzyl-protected hydroquinone-cored first generation dendrimer (15**) in chloroform-*d***



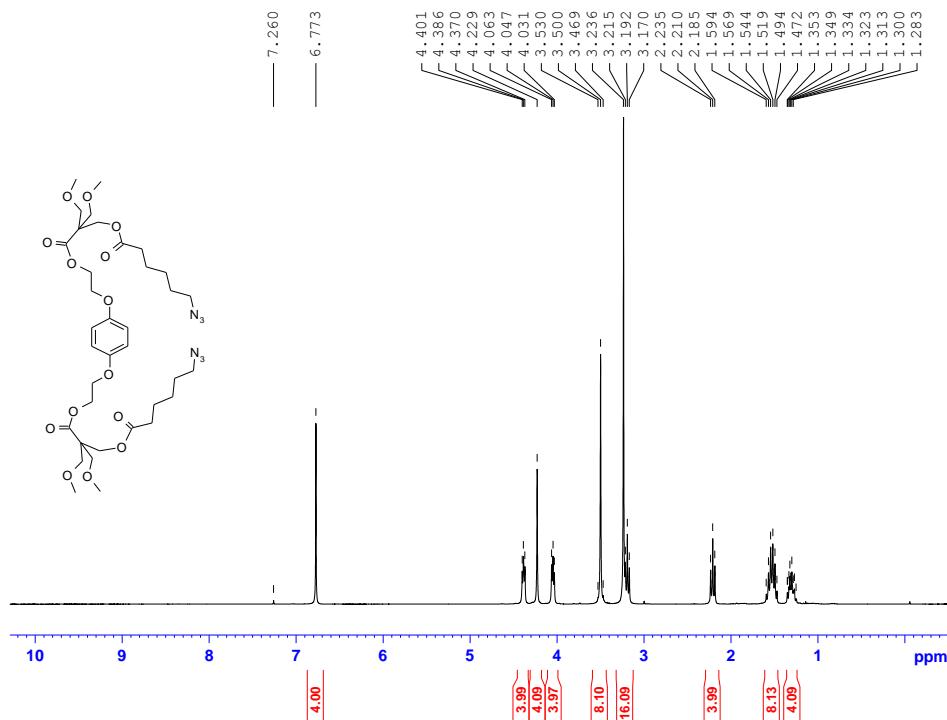
500.13 MHz ^1H NMR spectrum of hydroquinone-cored first generation dendrimer (16**) in acetone-*d*₆**



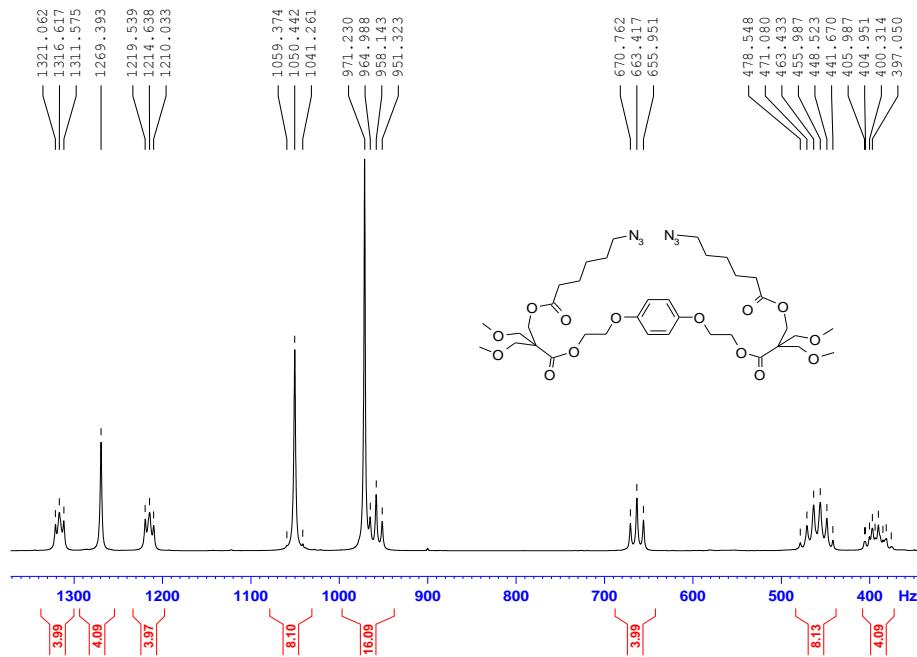
500.13 MHz ^1H NMR spectrum of bis(2-(3-hydroxy-2,2-bis-(methoxymethyl)propanoyloxy)-ethoxy)benzene (16) in acetone- d_6



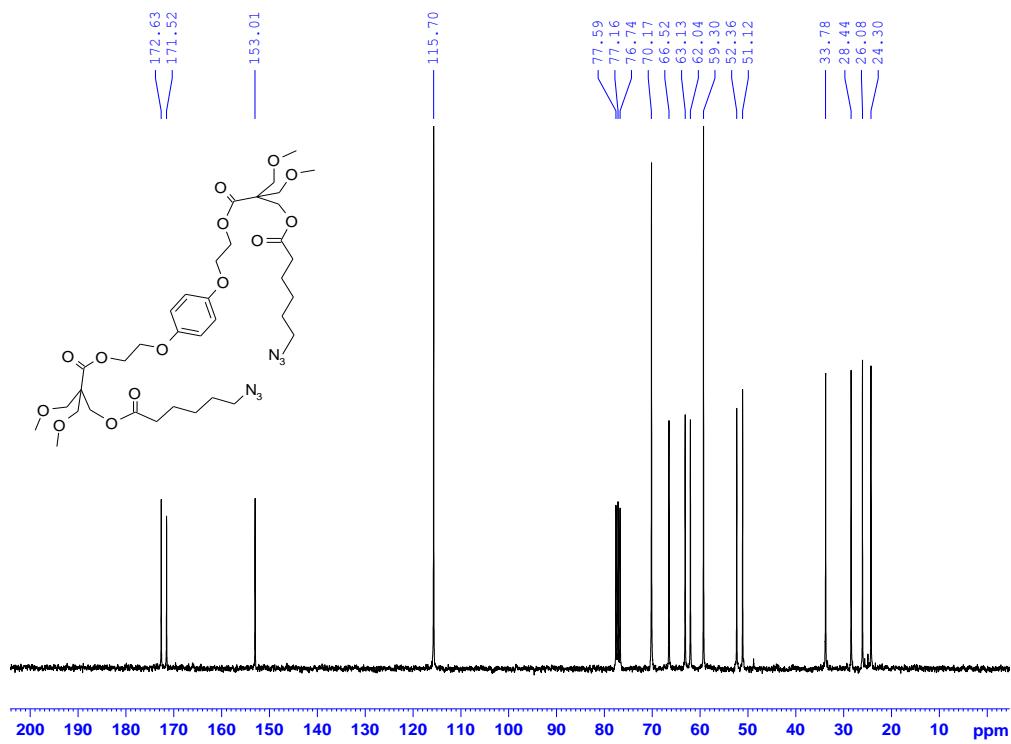
300.15 MHz ^1H NMR spectrum of azide-functionalized divalent first generation dendrimer (17) in chloroform- d



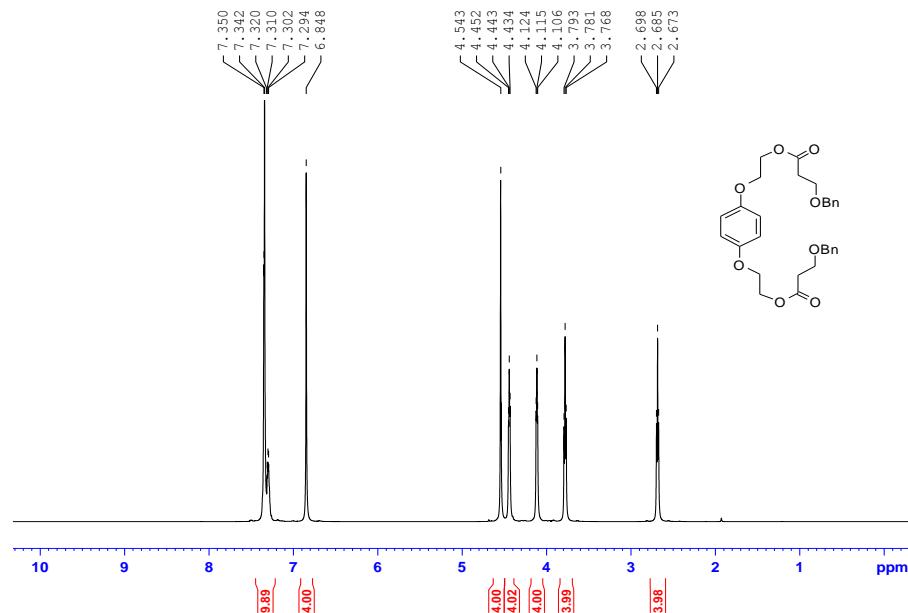
Expansion of part of the 300.15 MHz ^1H NMR spectrum of azide-functionalized divalent first generation dendrimer (17) in chloroform- d



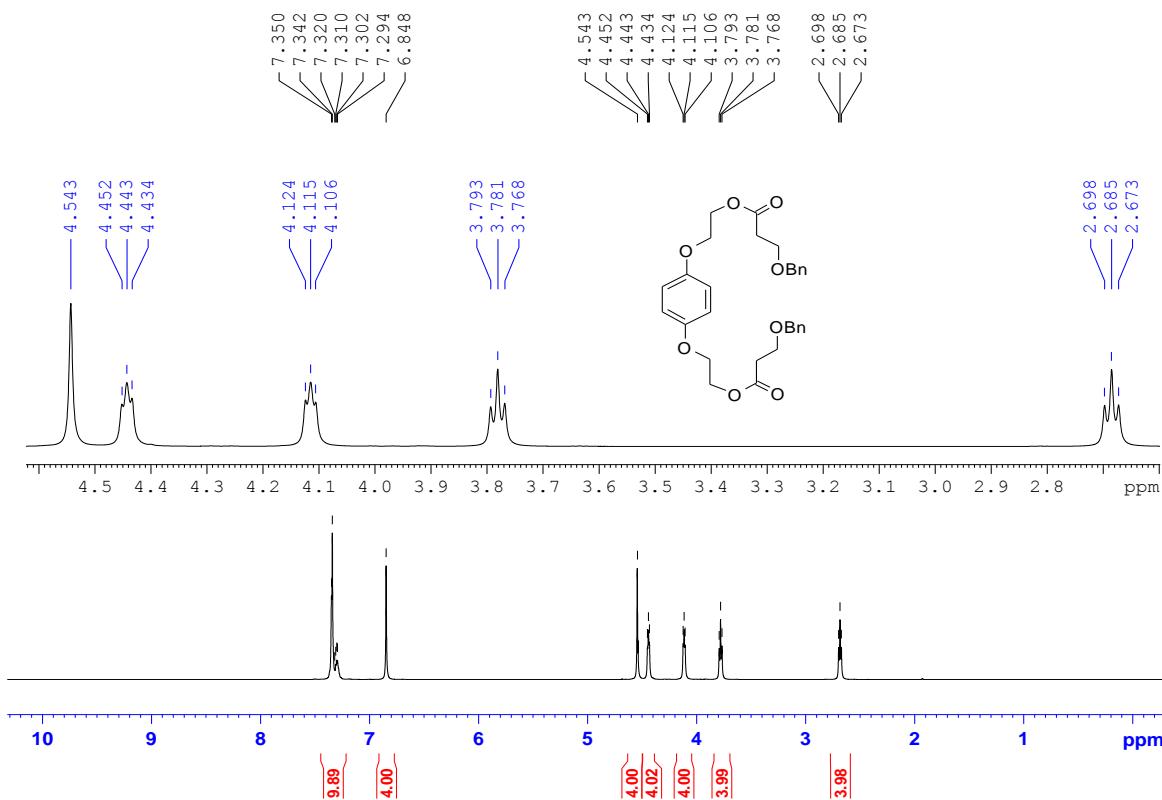
75.5 MHz ^{13}C NMR spectrum of azide-functionalized divalent first generation dendrimer (17) in chloroform- d



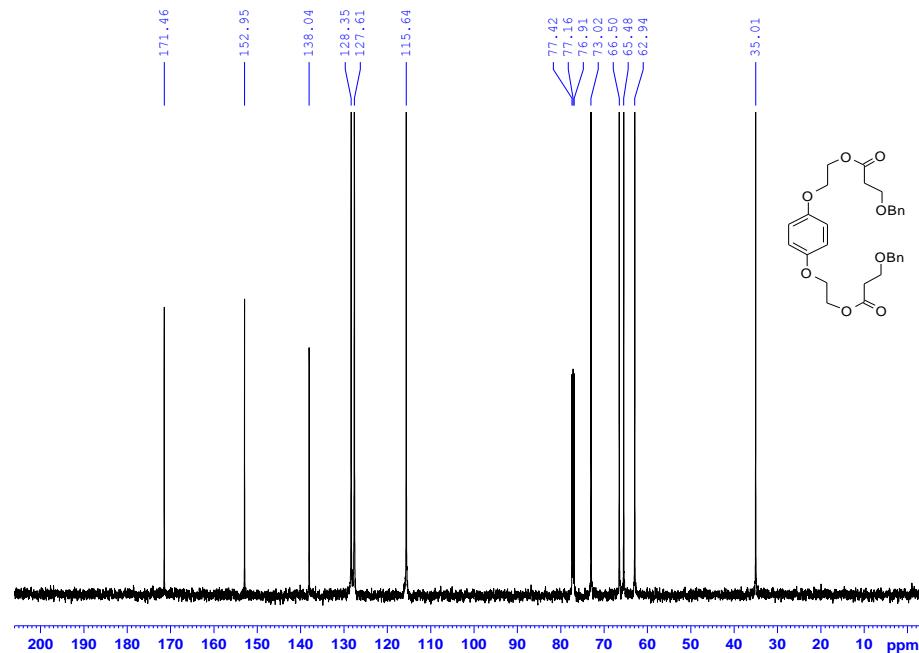
500.13 MHz ^1H NMR spectrum of benzyl-functionalized divalent dendrimer (18**) in chloroform-d**



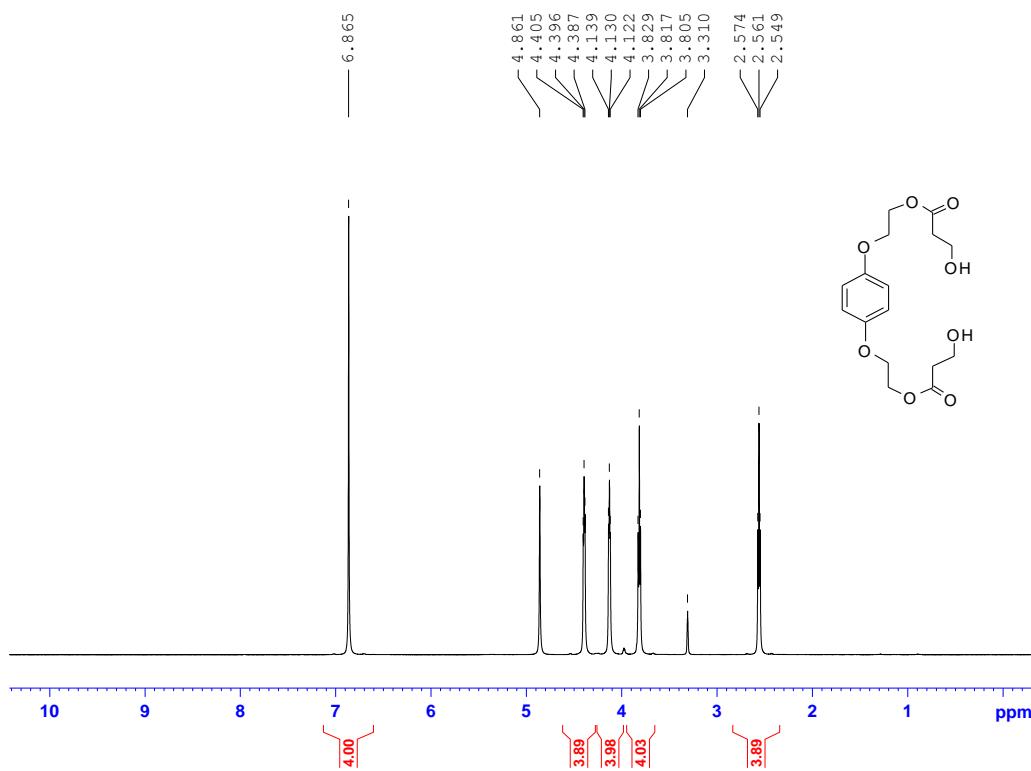
Expansion of part of the 500.13 MHz ^1H NMR spectrum of benzyl-functionalized divalent dendrimer (18**) in chloroform-d**



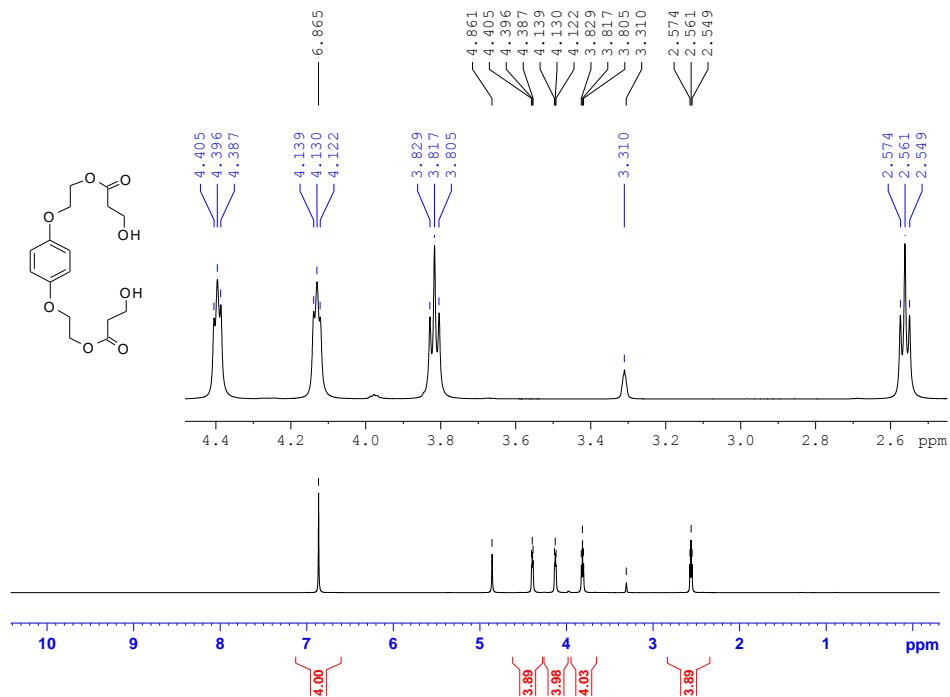
125.7 MHz ^{13}C NMR spectrum of benzyl-functionalized divalent dendrimer (18**) in chloroform- d**



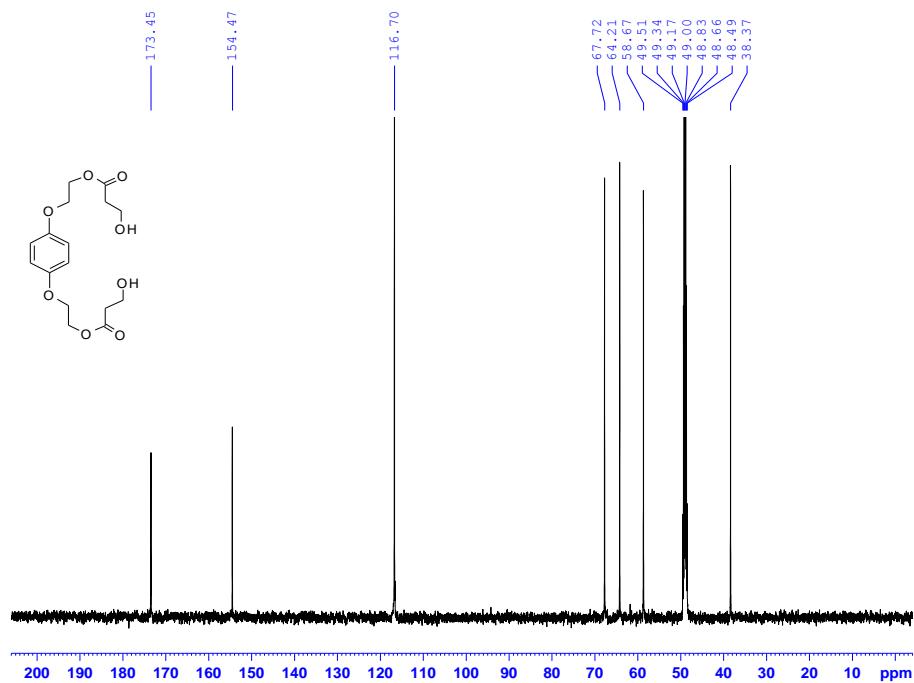
500.13 MHz ^1H NMR spectrum of hydroxyl-terminated divalent dendrimer (19**) in methanol- d_4**



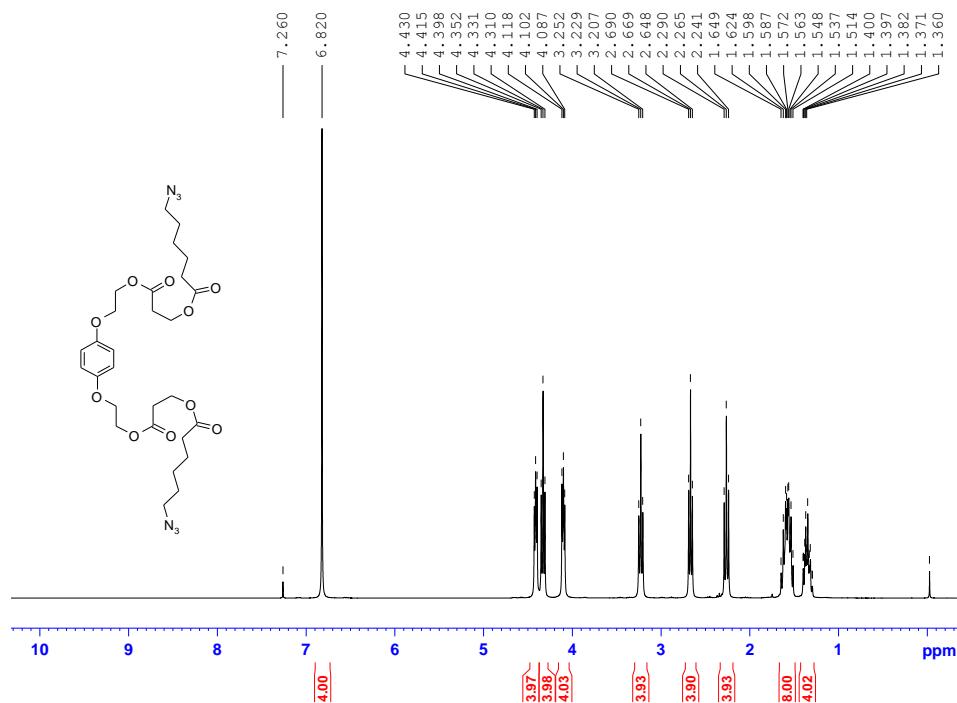
Expansion of part of the 500.13 MHz ^1H NMR spectrum of hydroxyl-terminated divalent dendrimer (19**) in methanol- d_4**



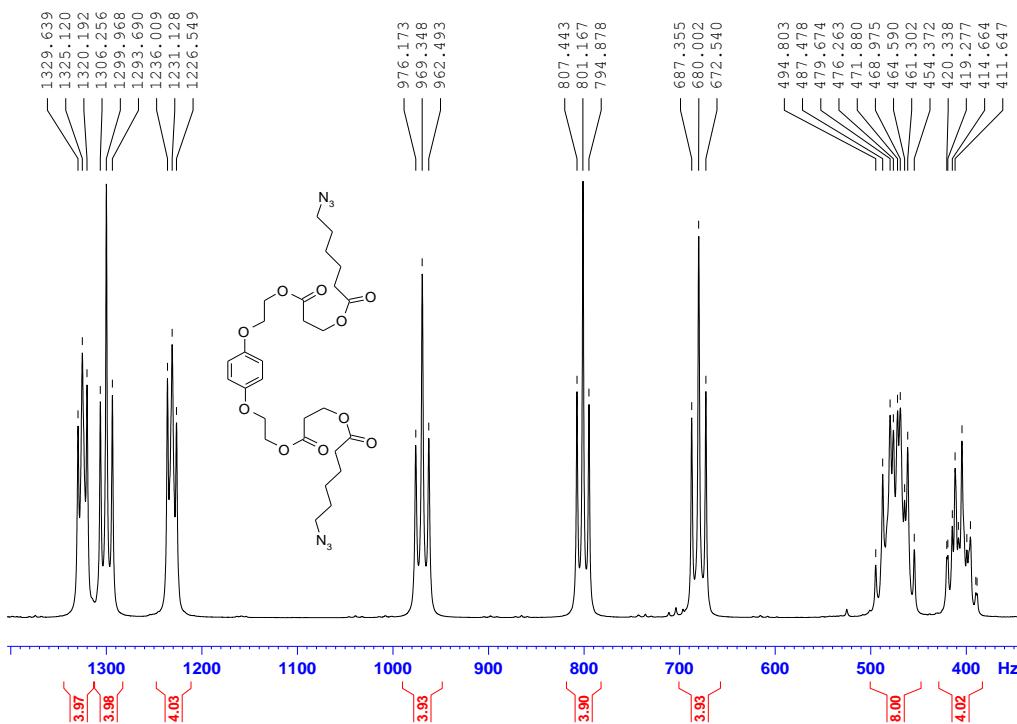
125.7 MHz ^{13}C NMR spectrum of hydroxyl-terminated divalent dendrimer (19**) in methanol- d_4**



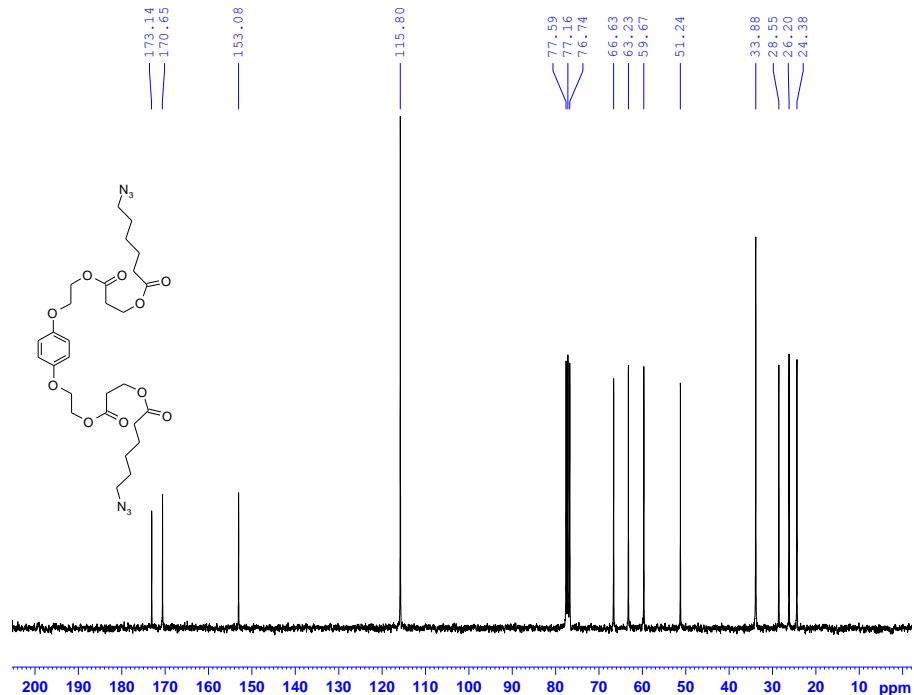
300.15 MHz ^1H NMR spectrum of azide-functionalized divalent dendrimer (20**) in chloroform-*d***



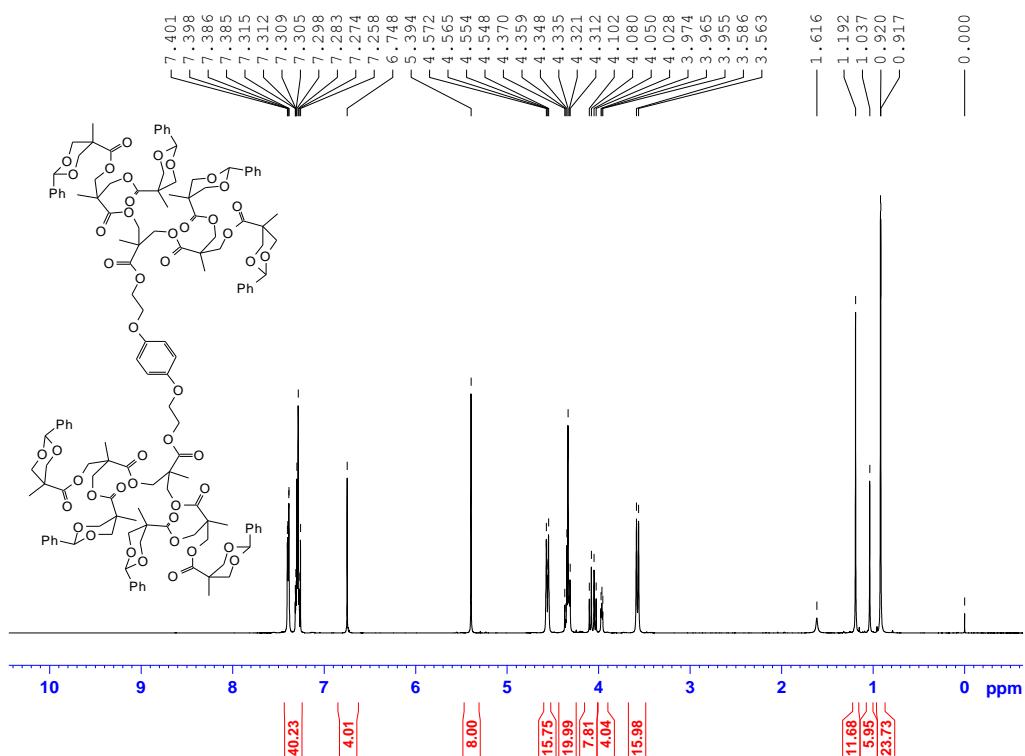
Expansion of part of the 300.15 MHz ^1H NMR spectrum of azide-functionalized divalent dendrimer (20**) in chloroform-*d***



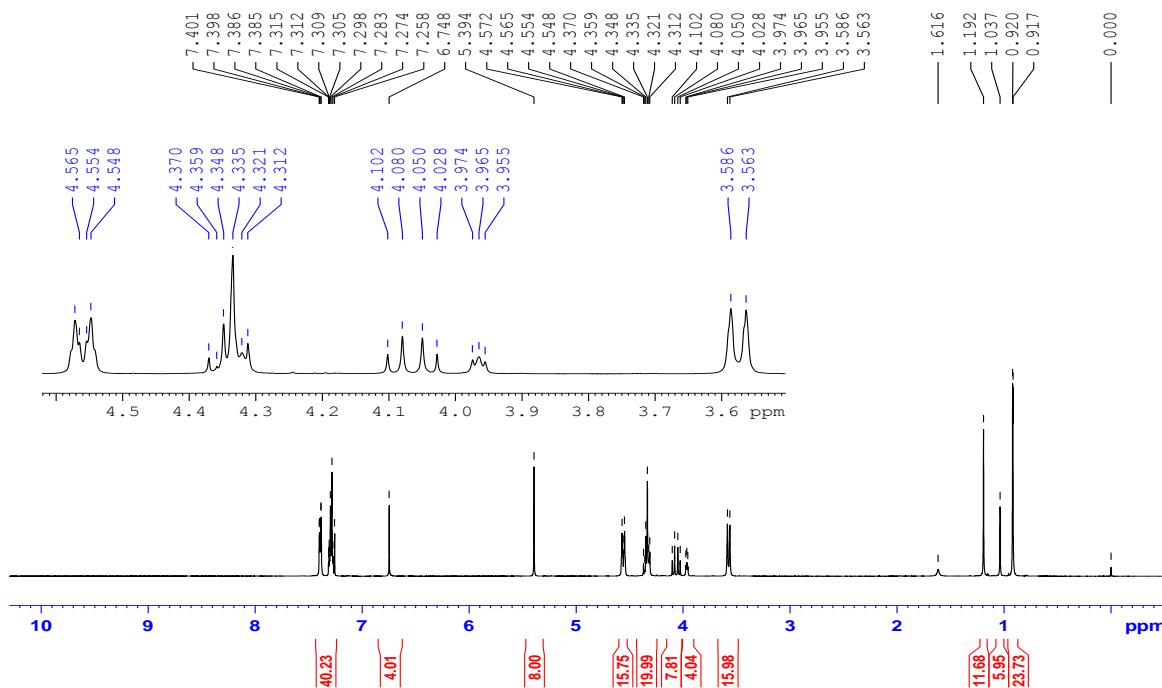
75.5 ^{13}C NMR spectrum of azide-functionalized divalent dendrimer (20) in chloroform- d



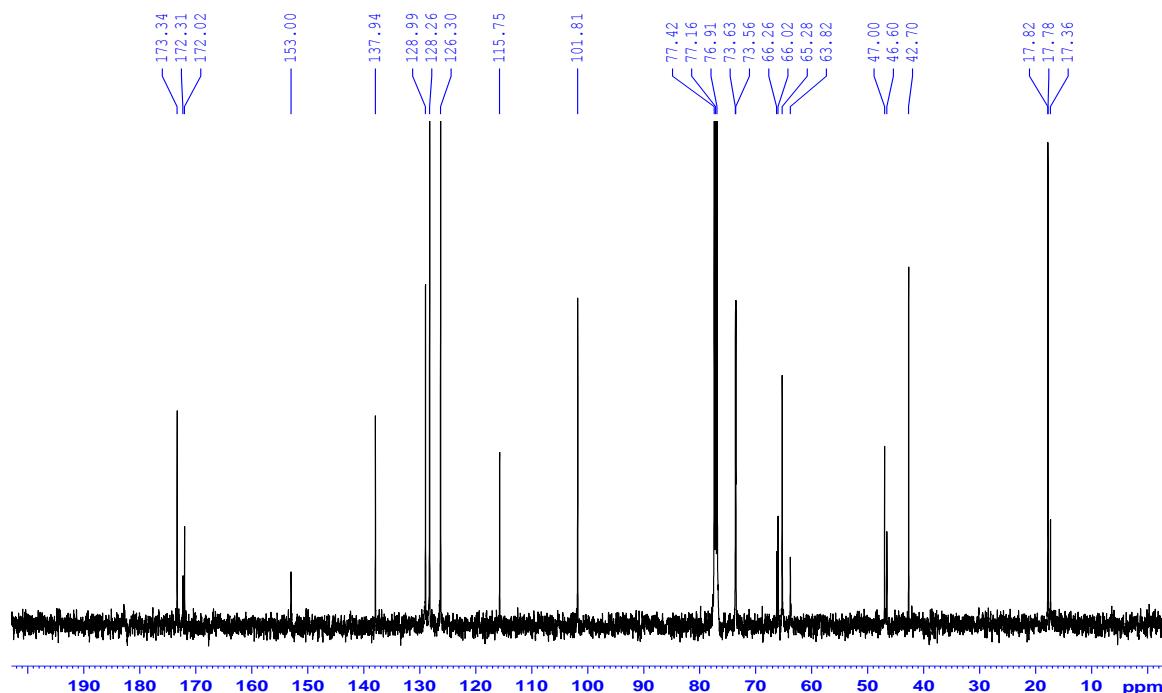
500.13 MHz ^1H NMR spectrum of benzylidene-protected hydroquinone-cored third generation dendrimer (23) in chloroform- d



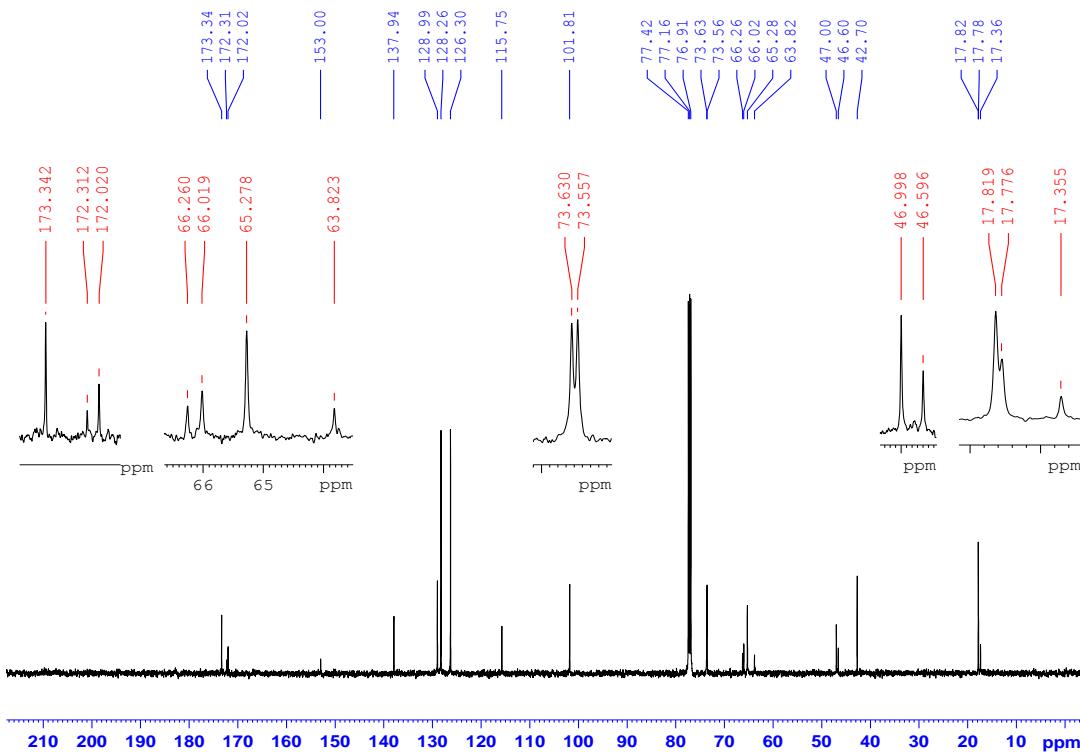
Expansion of part of the 500.13 MHz ^1H NMR spectrum of benzylidene-protected hydroquinone-cored third generation dendrimer (23) in chloroform-*d*



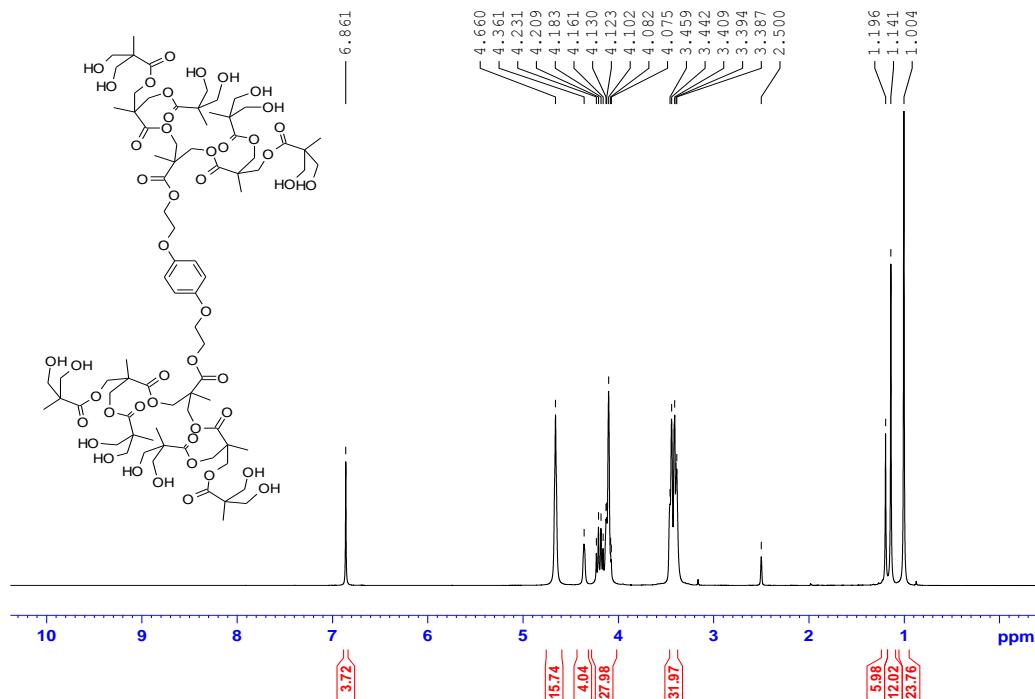
125.7 MHz ^{13}C NMR spectrum of benzylidene-protected hydroquinone-cored third generation dendrimer (23) in chloroform-*d*



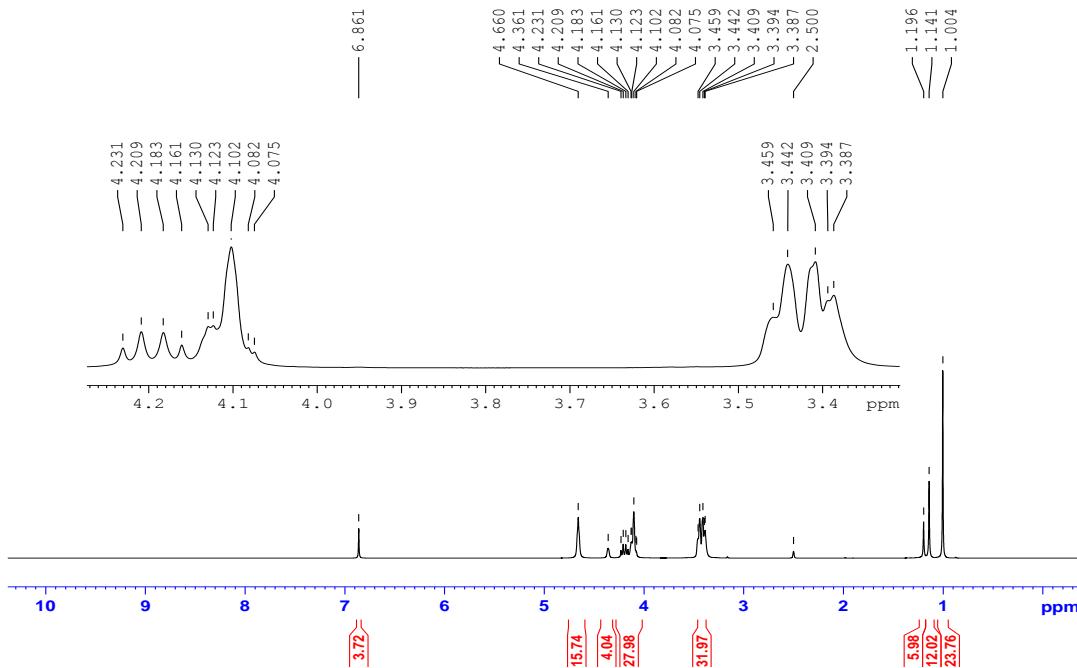
Expansions of parts of the 125.7 MHz ^{13}C NMR spectrum of benzylidene-protected hydroquinone-cored third generation dendrimer (23) in chloroform-*d*



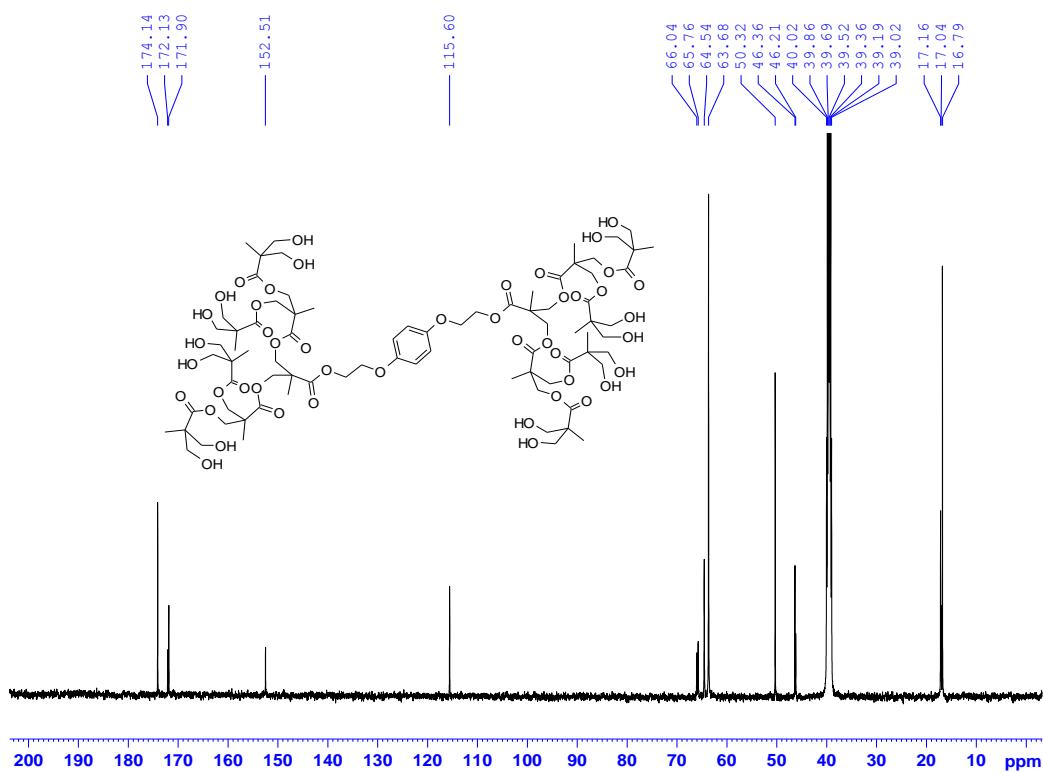
500.13 MHz ^1H NMR spectrum of third generation dendrimer (24) in DMSO-*d*₆



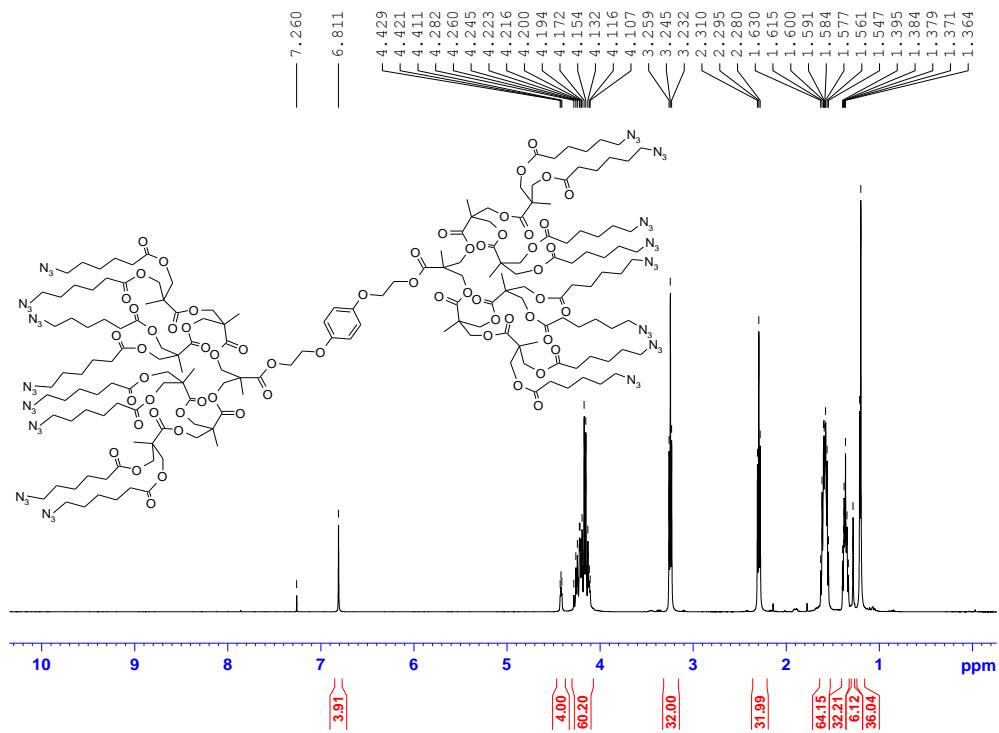
Expansion of part of the 500.13 MHz ^1H NMR spectrum of third generation dendrimer (24) in DMSO- d_6



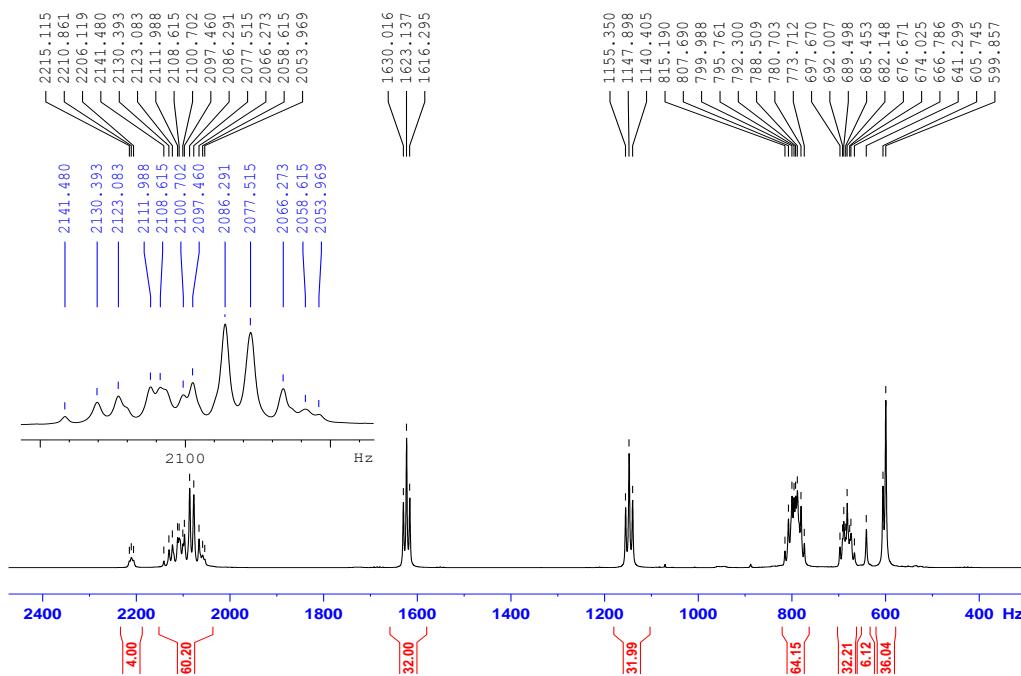
125.7 MHz ^{13}C NMR spectrum of third generation dendrimer (24) in DMSO- d_6



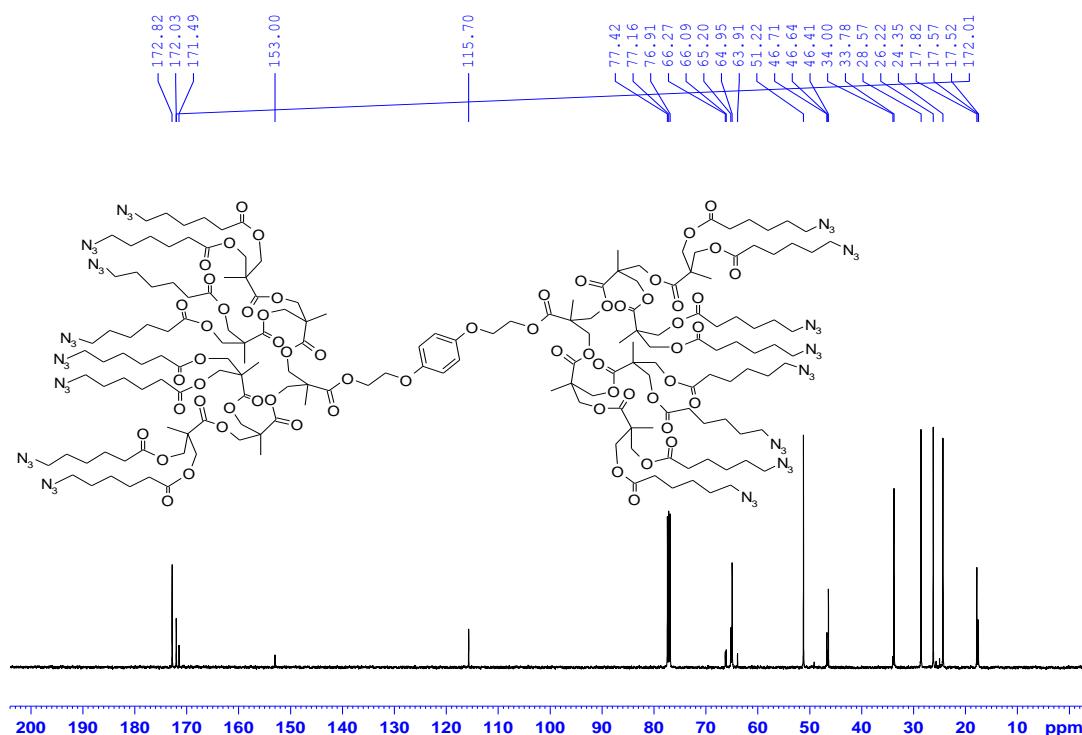
500.13 MHz ^1H NMR spectrum of azide-functionalized hydroquinone-cored third generation dendrimer (25**) in chloroform-*d***



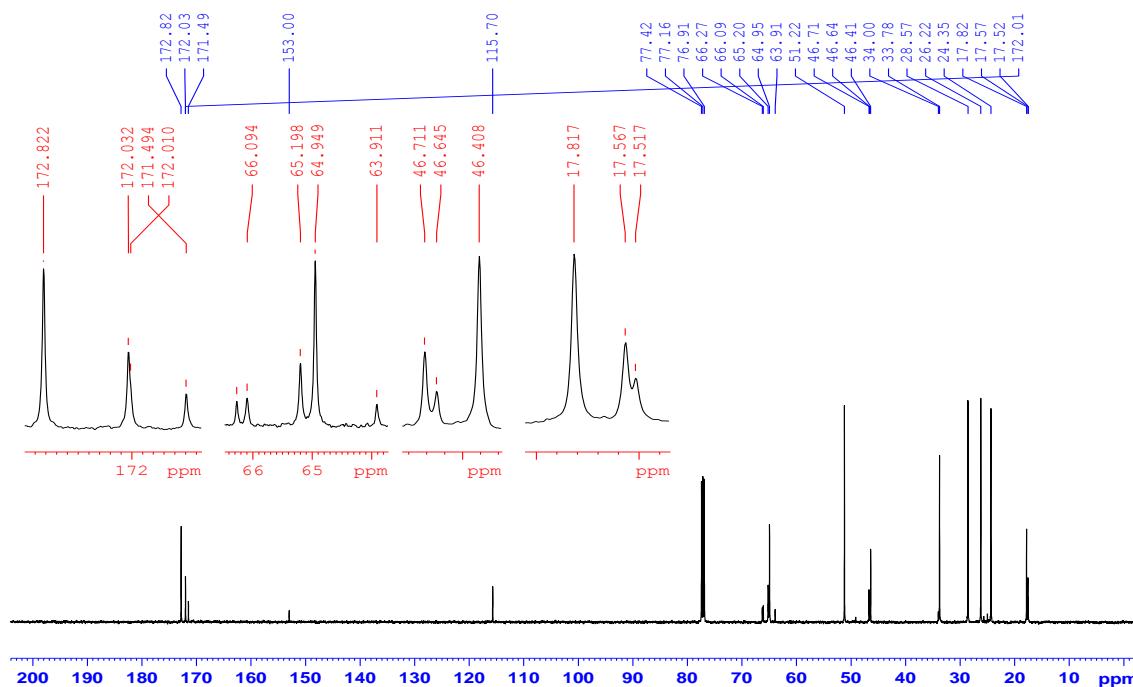
Expansions of parts of the 500.13 MHz ^1H NMR spectrum of azide-functionalized hydroquinone-cored third generation dendrimer (25**) in chloroform-*d***



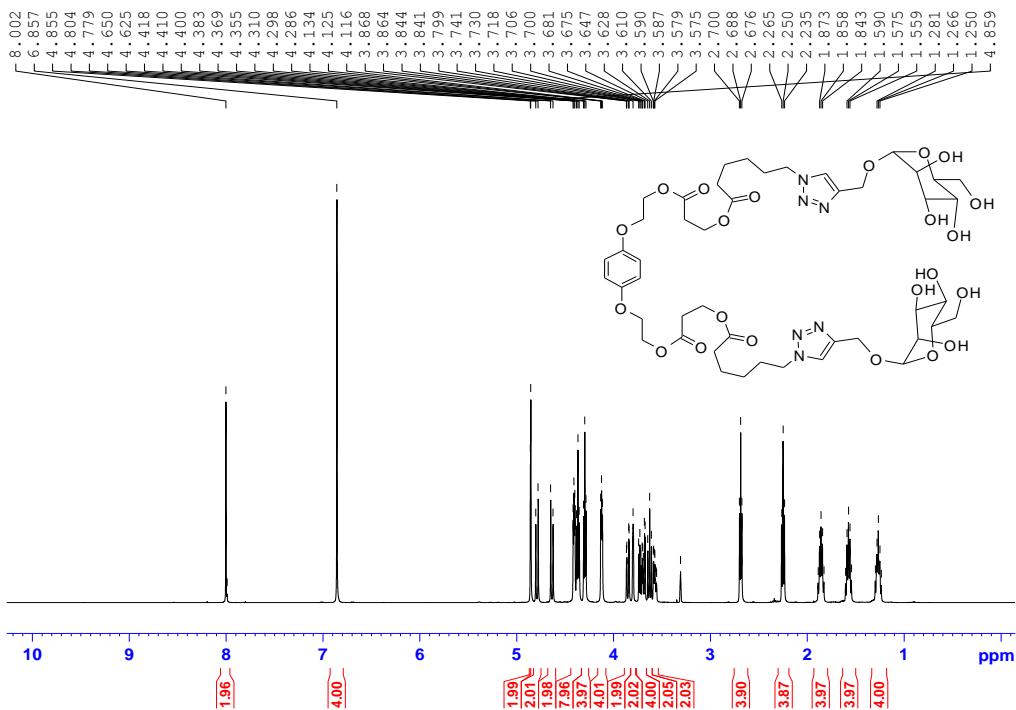
125.7 MHz ^{13}C NMR spectrum of azide-functionalized hydroquinone-cored third generation dendrimer (25) in chloroform-*d*



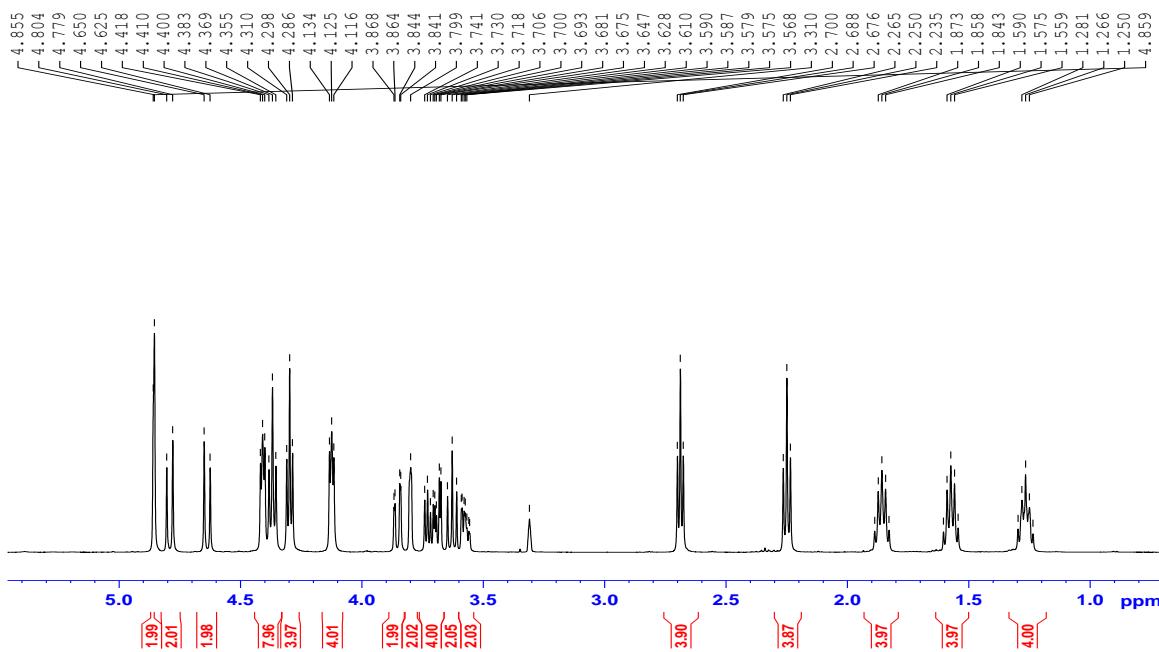
Expansions of the 125.7 MHz ^{13}C NMR spectrum of azide-functionalized hydroquinone-cored third generation dendrimer (25) in chloroform-*d*



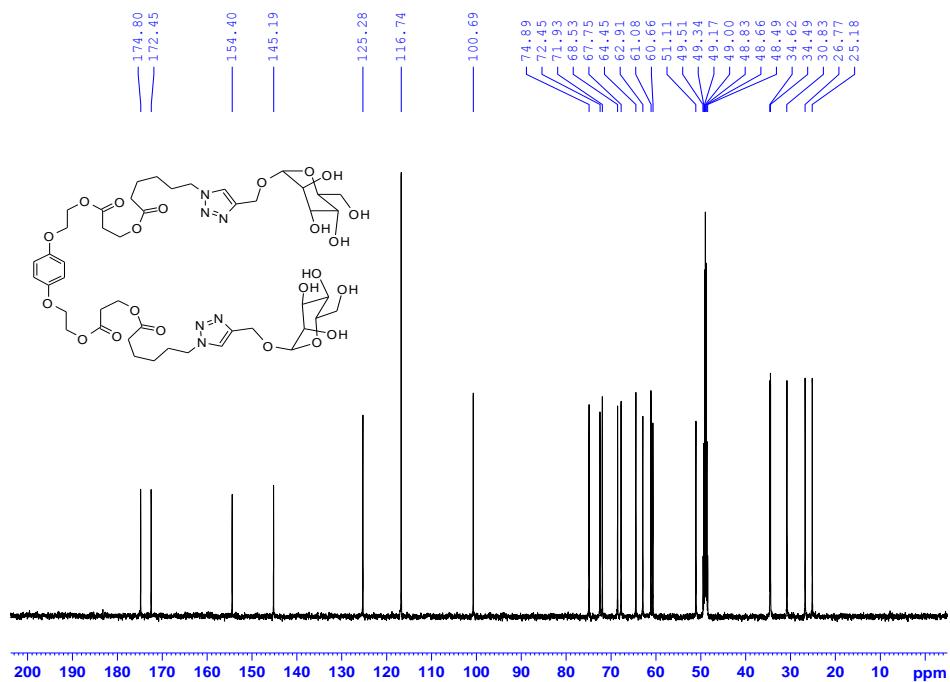
500.13 MHz ^1H NMR spectrum of extended divalent α -D-mannopyranoside-terminated dendrimer (27) in methanol- d_4



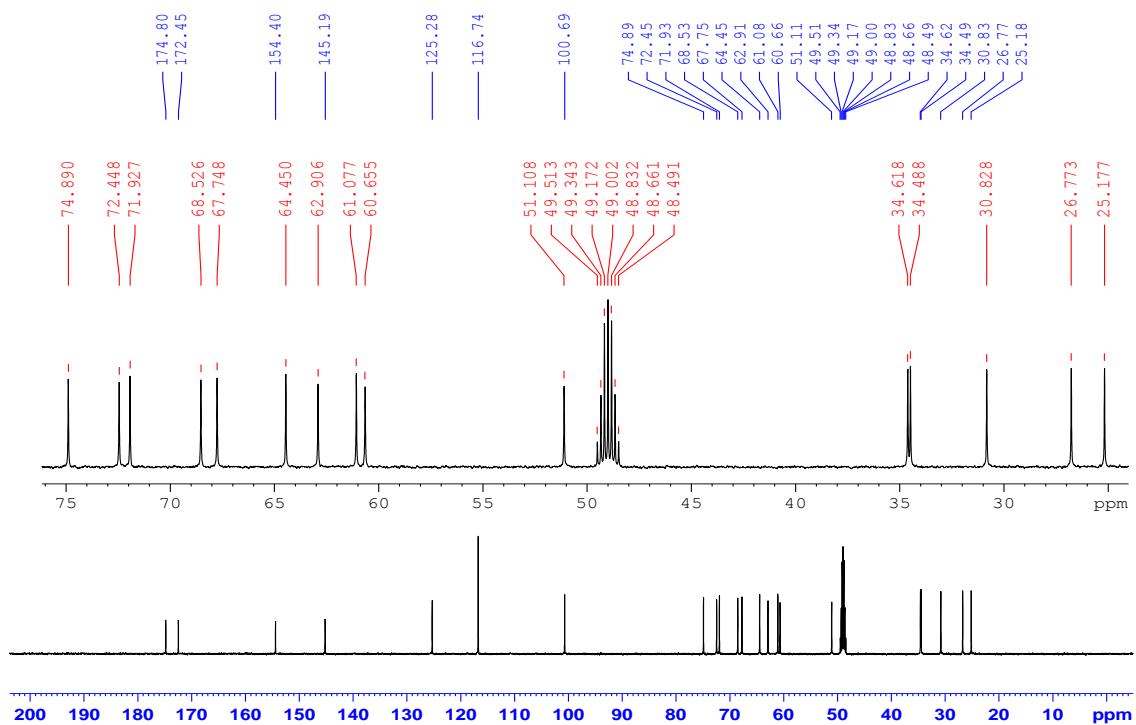
Expansion of part of the 500.13 MHz ^1H NMR spectrum of extended divalent α -D-mannopyranoside-terminated dendrimer (27) in methanol- d_4



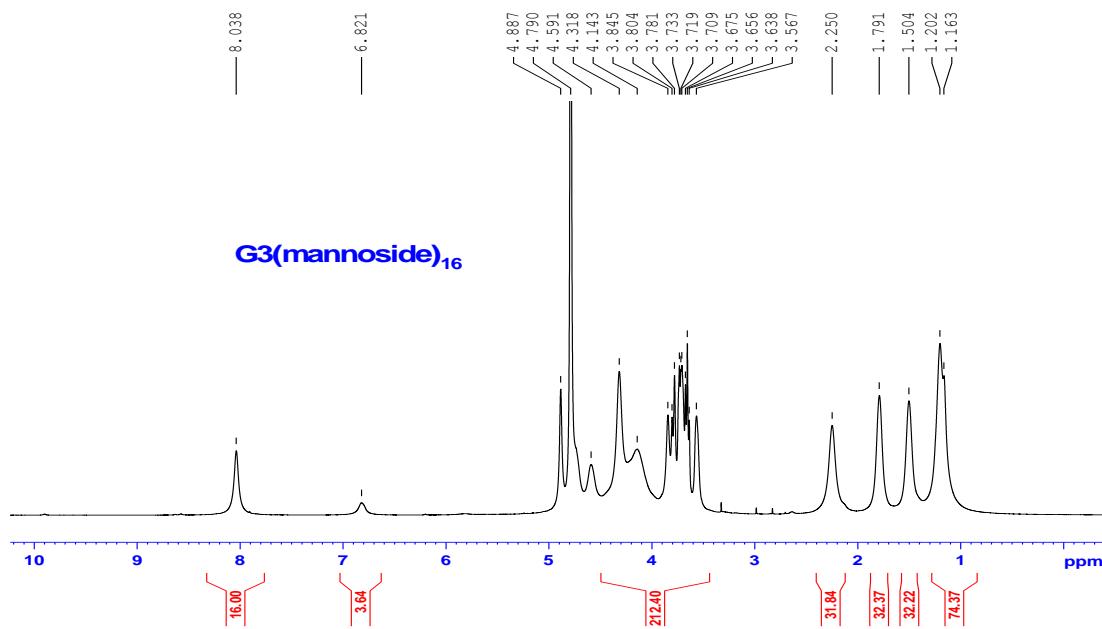
125.7 MHz ^{13}C NMR spectrum of extended divalent α -D-mannopyranoside-terminated dendrimer (27) in methanol- d_4



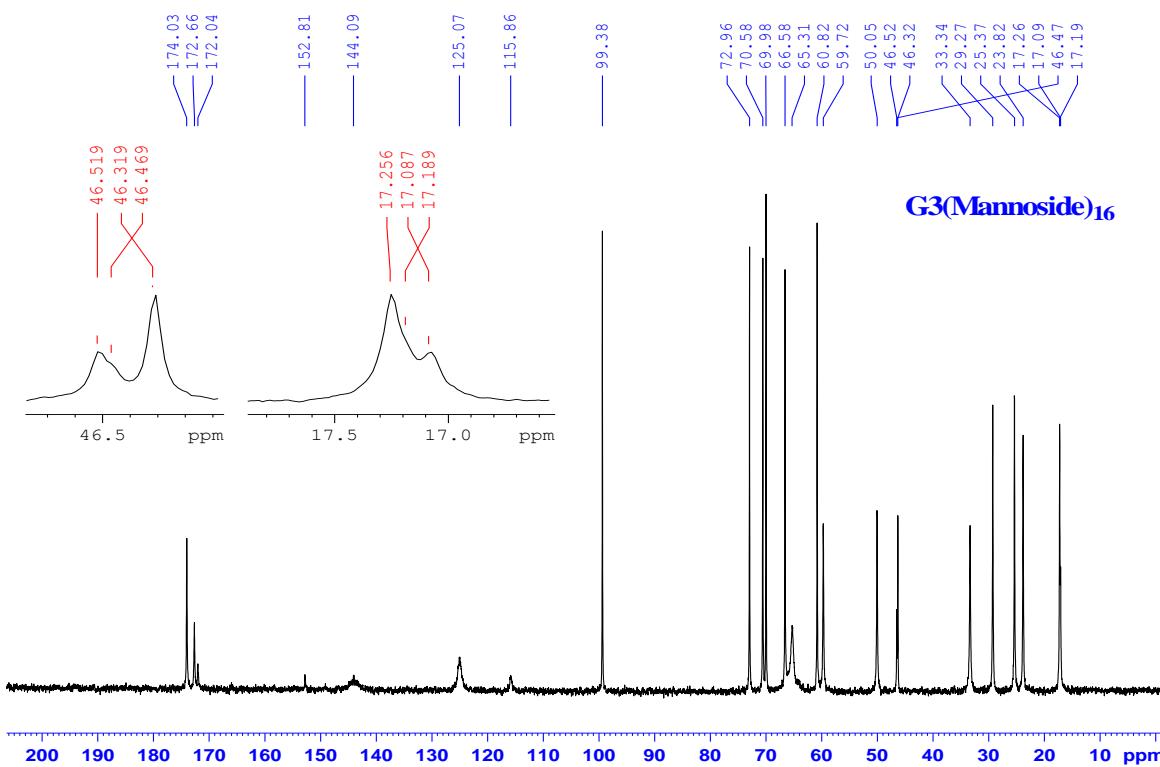
Expansion of part of the 125.7 MHz ^{13}C NMR spectrum of extended divalent α -D-mannopyranoside-terminated dendrimer (27) in methanol- d_4



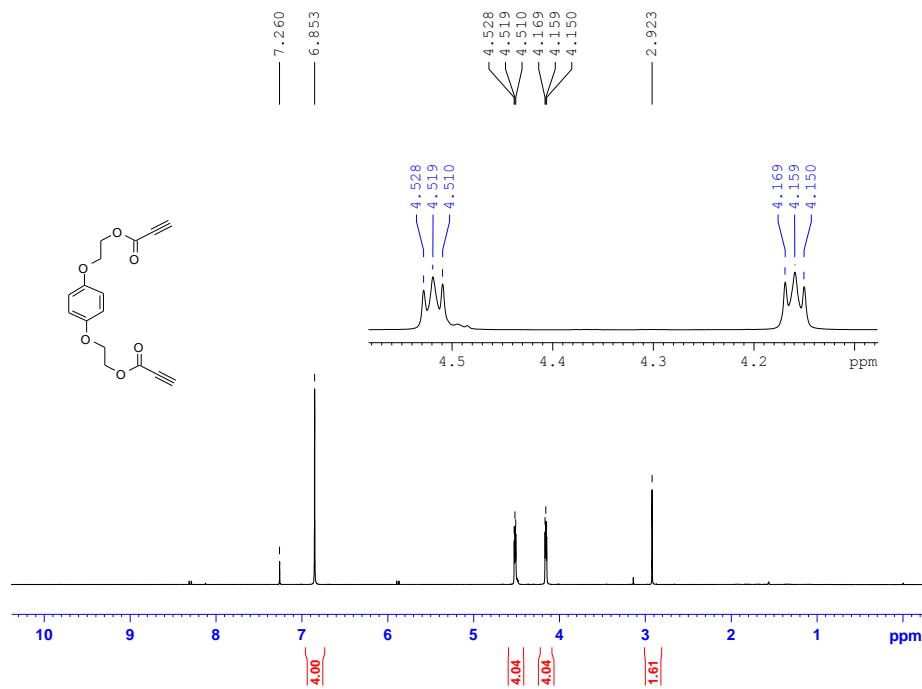
500.13 MHz ^1H NMR spectrum of third generation dendrimer bearing 16 mannose residues (28) in water- d_2



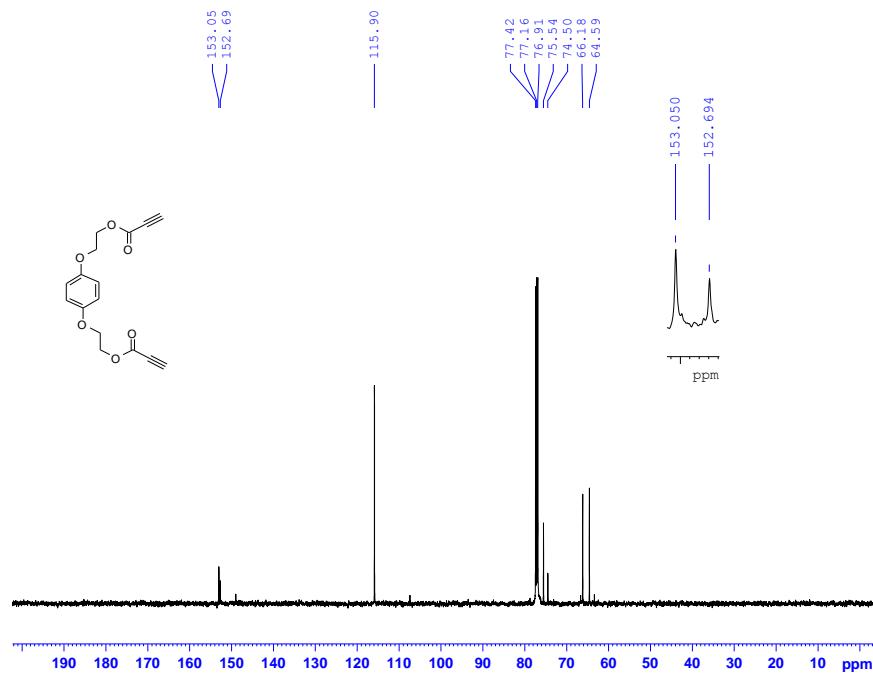
125.7 MHz ^{13}C NMR spectrum of third generation dendrimer bearing 16 mannose residues (28) in water- d_2



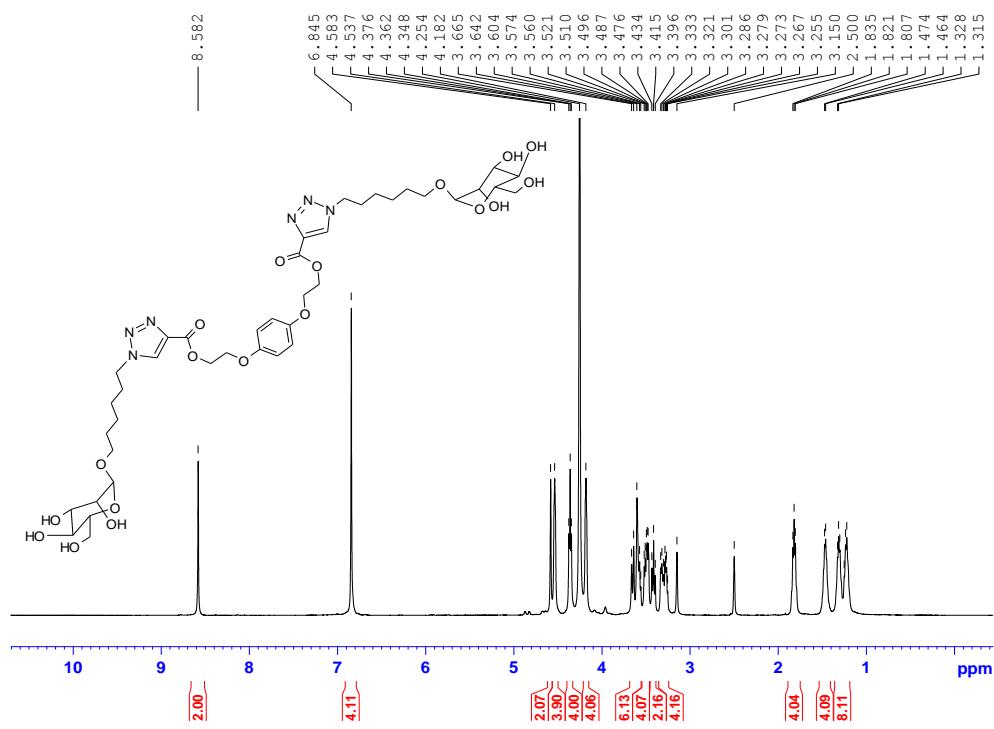
500.13 MHz ^1H NMR spectrum of bis(2-(2-propynyoxy)ethoxy)benzene (29) in chloroform-*d*



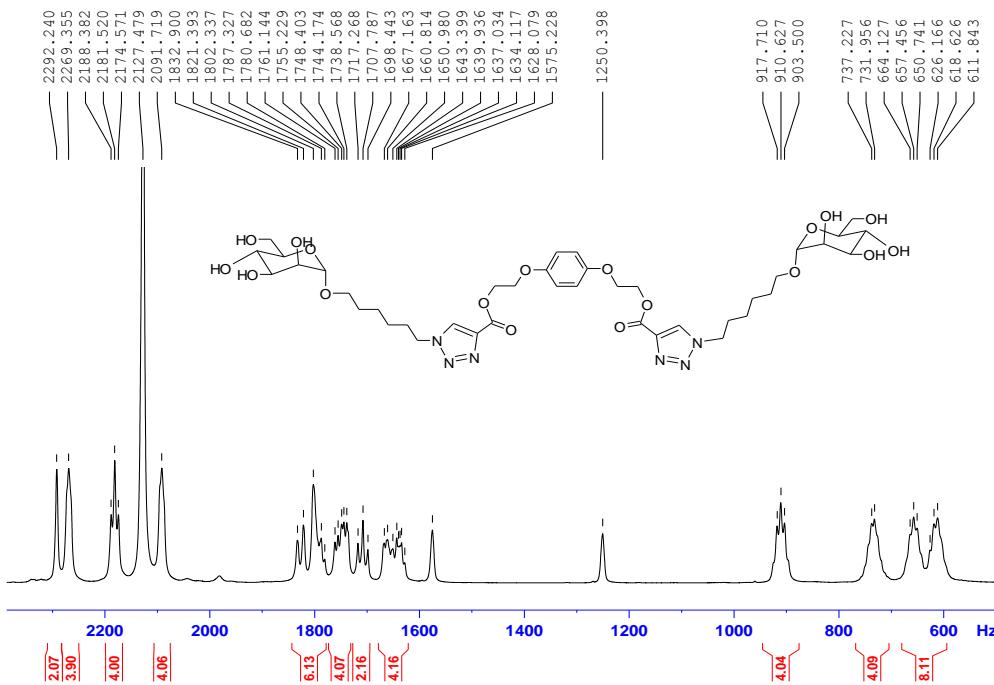
125.7 MHz ^{13}C NMR spectrum of bis(2-(2-propynyoxy)ethoxy)benzene (29) in chloroform-*d*



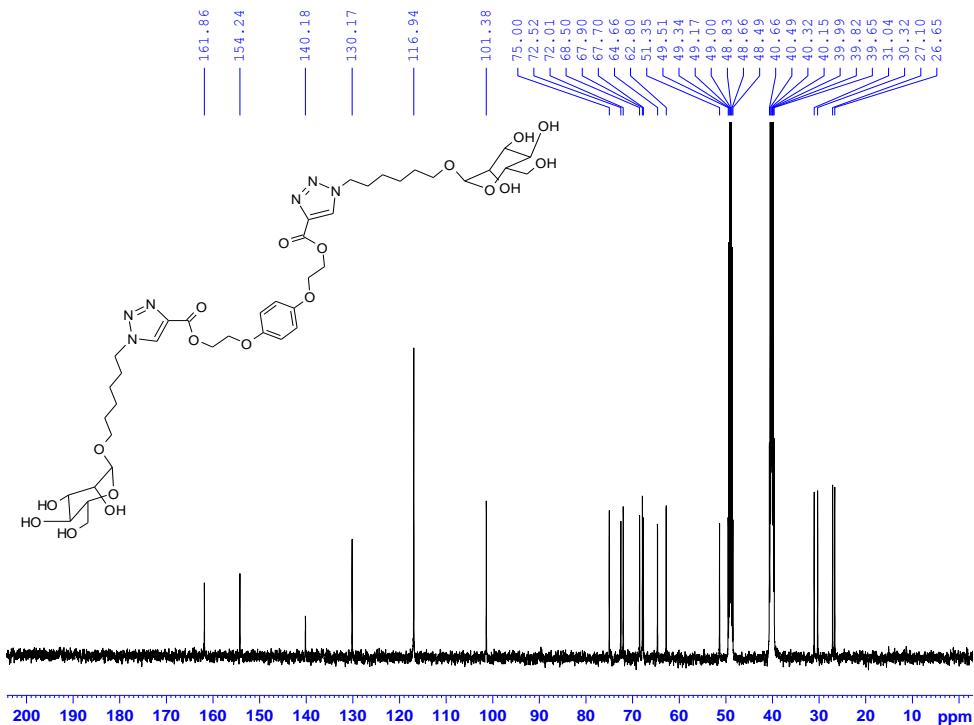
500.13 MHz ^1H NMR spectrum of divalent α -D-mannopyranoside-terminated dendrimer with a hexyl linker (30) in $\text{DMSO}-d_6$ / methanol- d_4



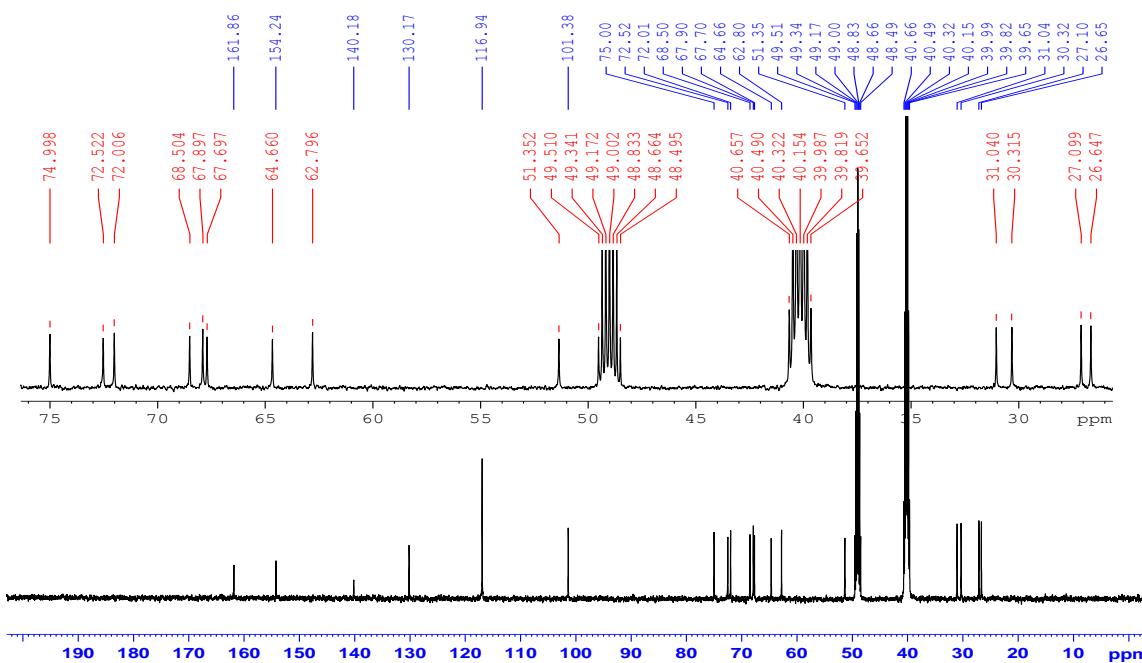
Expansion of part of the 500.13 MHz ^1H NMR spectrum of divalent α -D-mannopyranoside-terminated dendrimer with a hexyl linker (30) in $\text{DMSO}-d_6$ / methanol- d_4



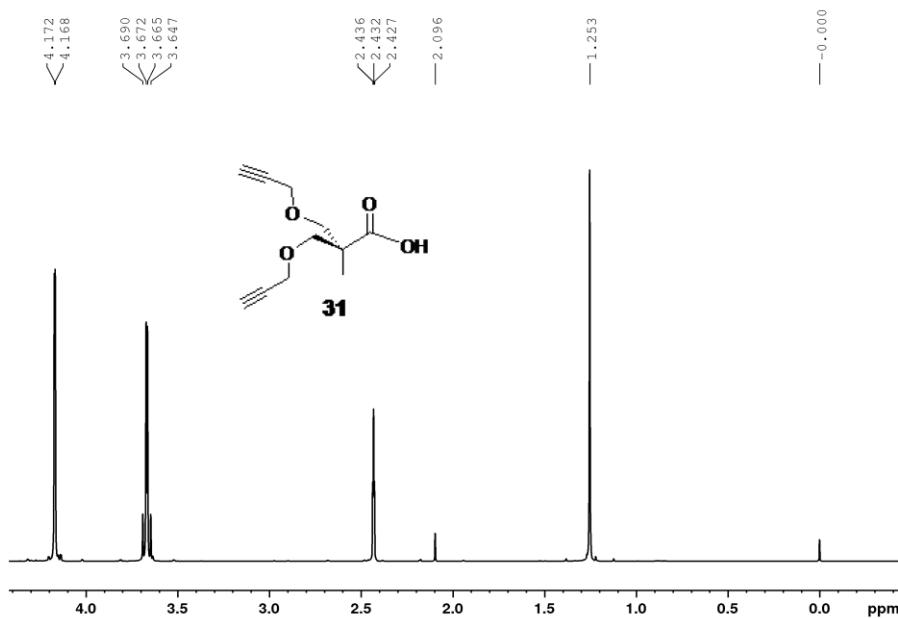
125.7 MHz ^{13}C NMR spectrum of divalent α -D-mannopyranoside-terminated dendrimer with a hexyl linker (30) in $\text{DMSO}-d_6$ / methanol- d_4



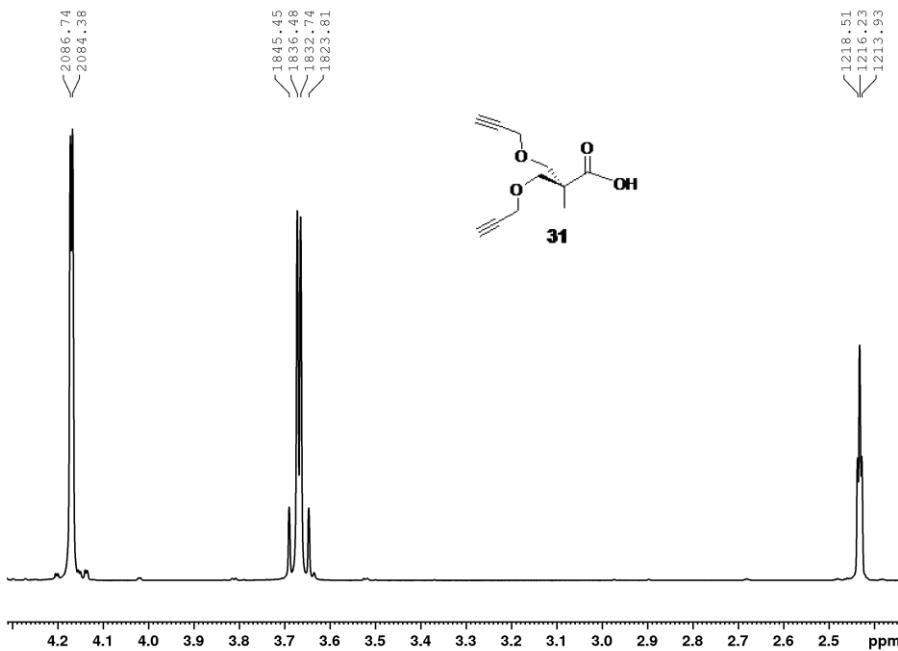
125.7 MHz ^{13}C NMR spectrum of divalent α -D-mannopyranoside-terminated dendrimer with a hexyl linker (30) in $\text{DMSO}-d_6$ / methanol- d_4



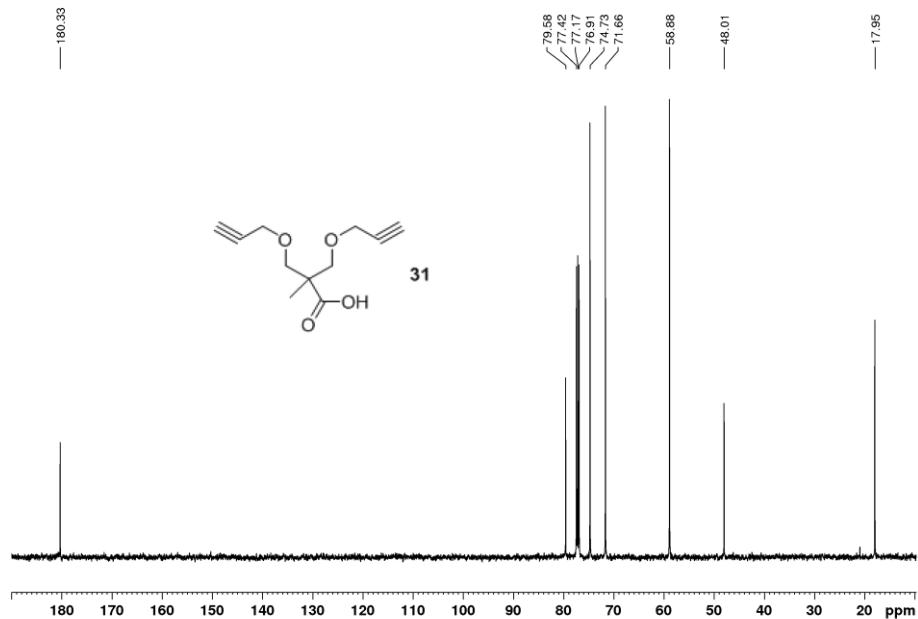
500.13 MHz ^1H NMR spectrum of 2,2'-bis-(2-propynylloxymethyl)propanoic acid (31**) in chloroform-*d***



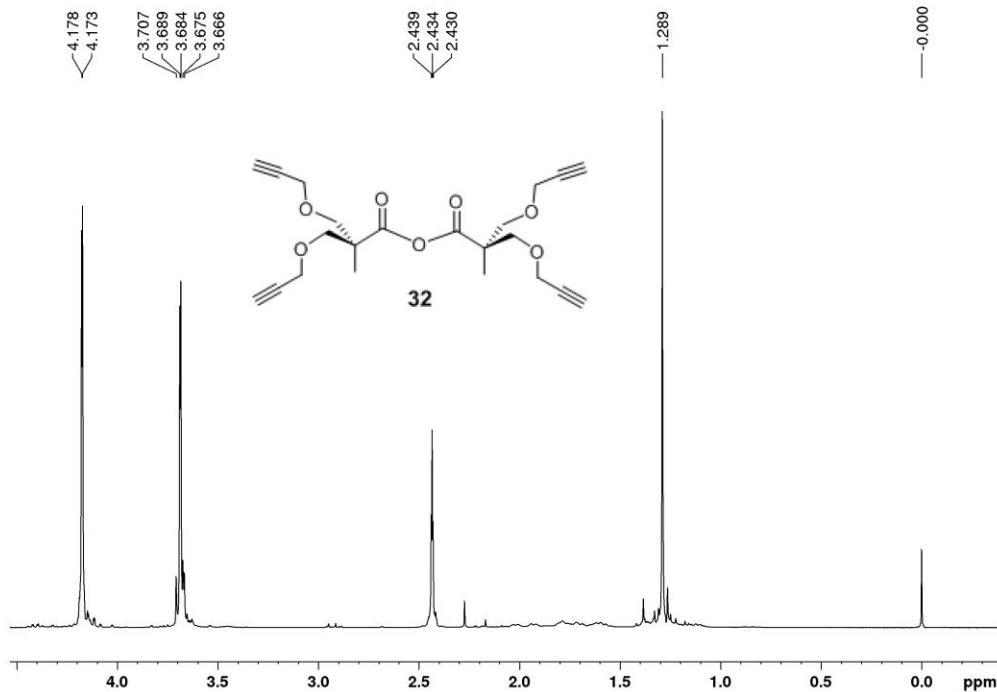
Expansion of part of the 500.13 MHz ^1H NMR spectrum of 2,2'-bis-(2-propynylloxymethyl)-propanoic acid (31**) in chloroform-*d***



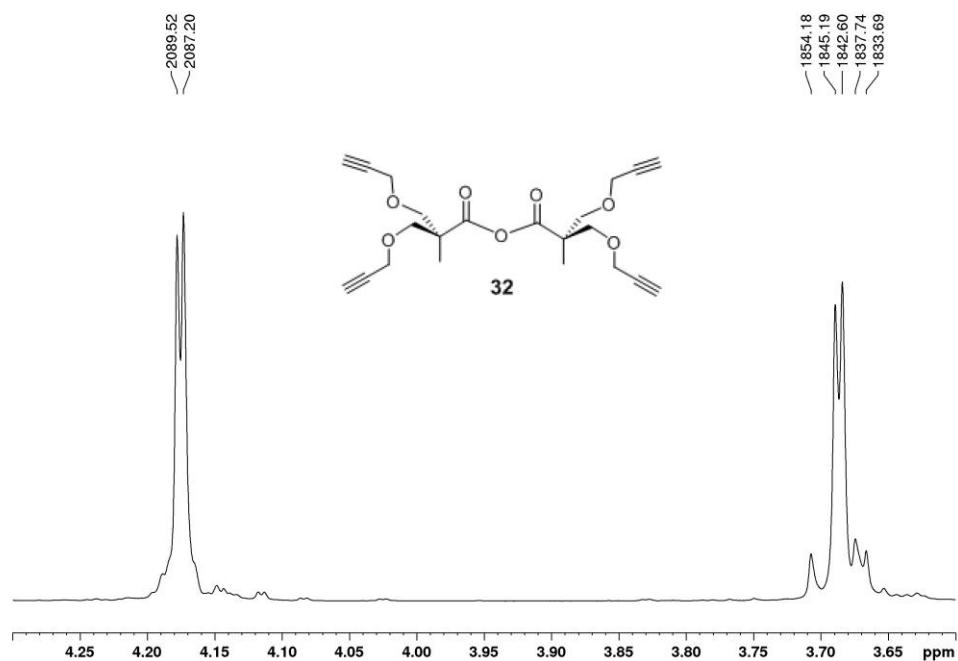
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis-(2-propynyloxymethyl)propanoic acid (31) in chloroform-*d*



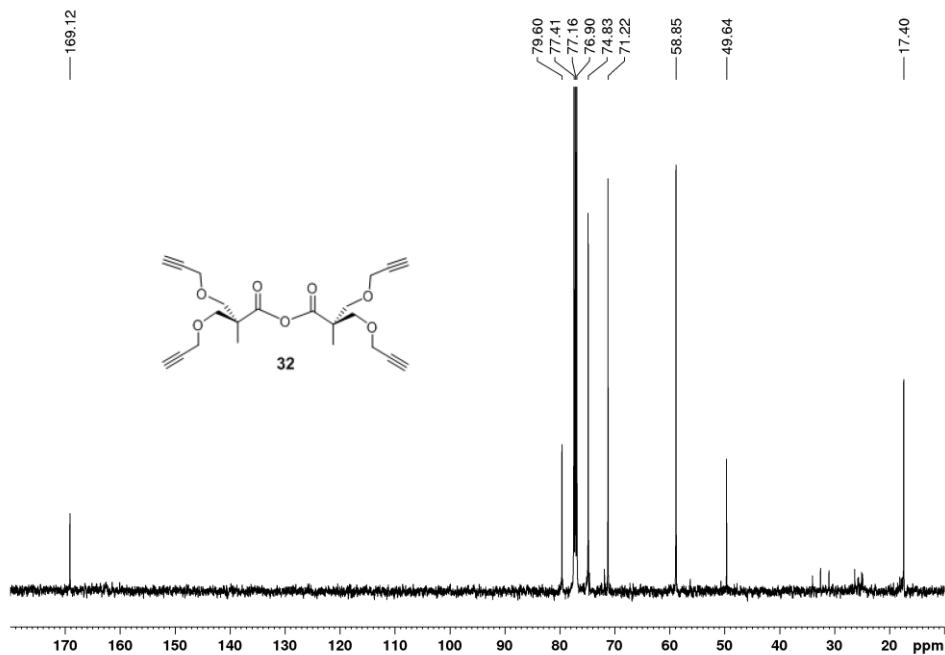
500.13 MHz ^1H NMR spectrum of 2,2'-bis-(2-propynyloxymethyl)propanoyl anhydride (32) in chloroform-*d*



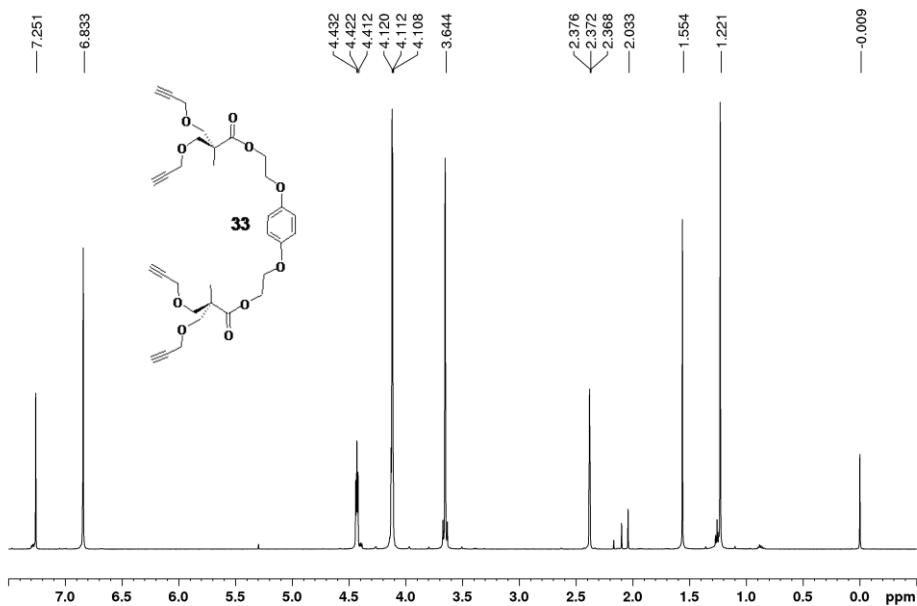
Expansion of part of the 500.13 MHz ^1H NMR spectrum of 2,2'-bis-(2-propynylloxymethyl)-propanoyl anhydride (32) in chloroform-*d*



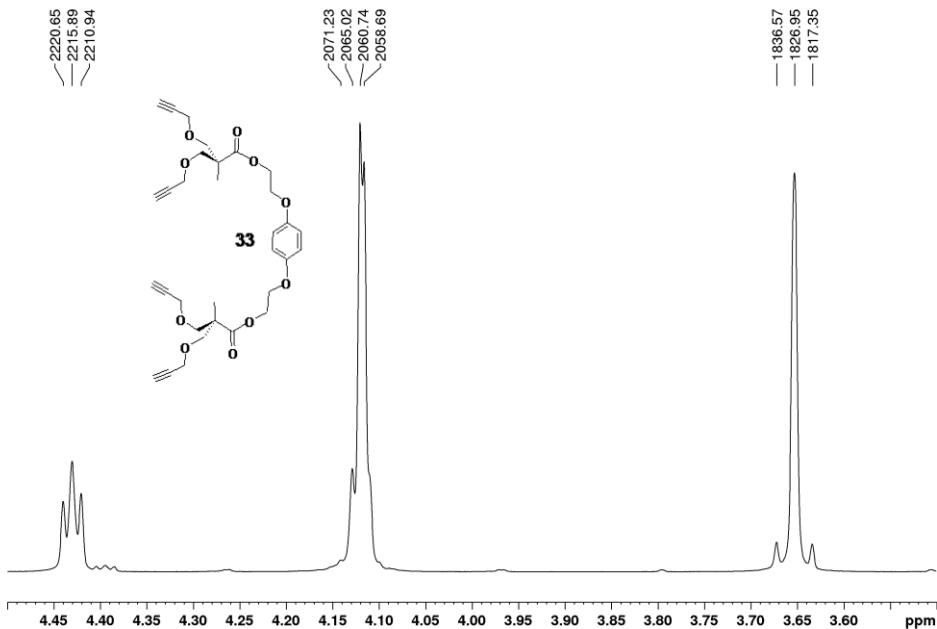
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis-(2-propynylloxymethyl)propanoyl anhydride (32) in chloroform-*d*



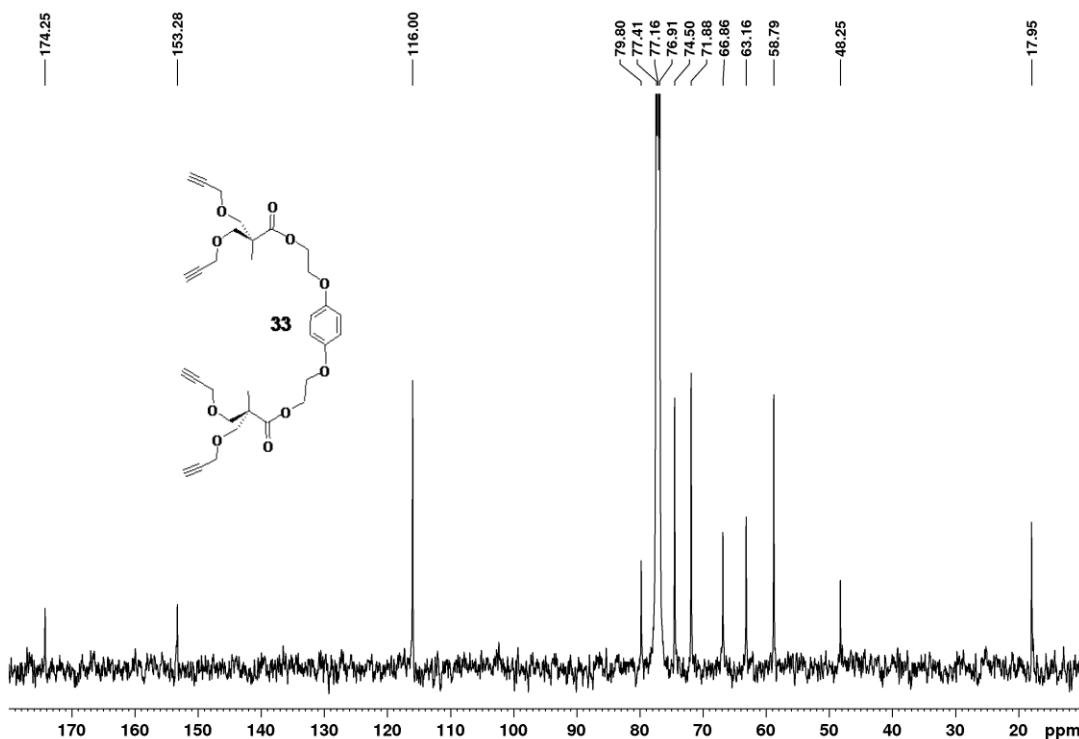
500.13 MHz ^1H NMR spectrum of 1,4-bis-2-(2,2'-bis-(2-propynyloxy)methyl)-propanoyloxyethoxybenzene (33) in chloroform-*d*



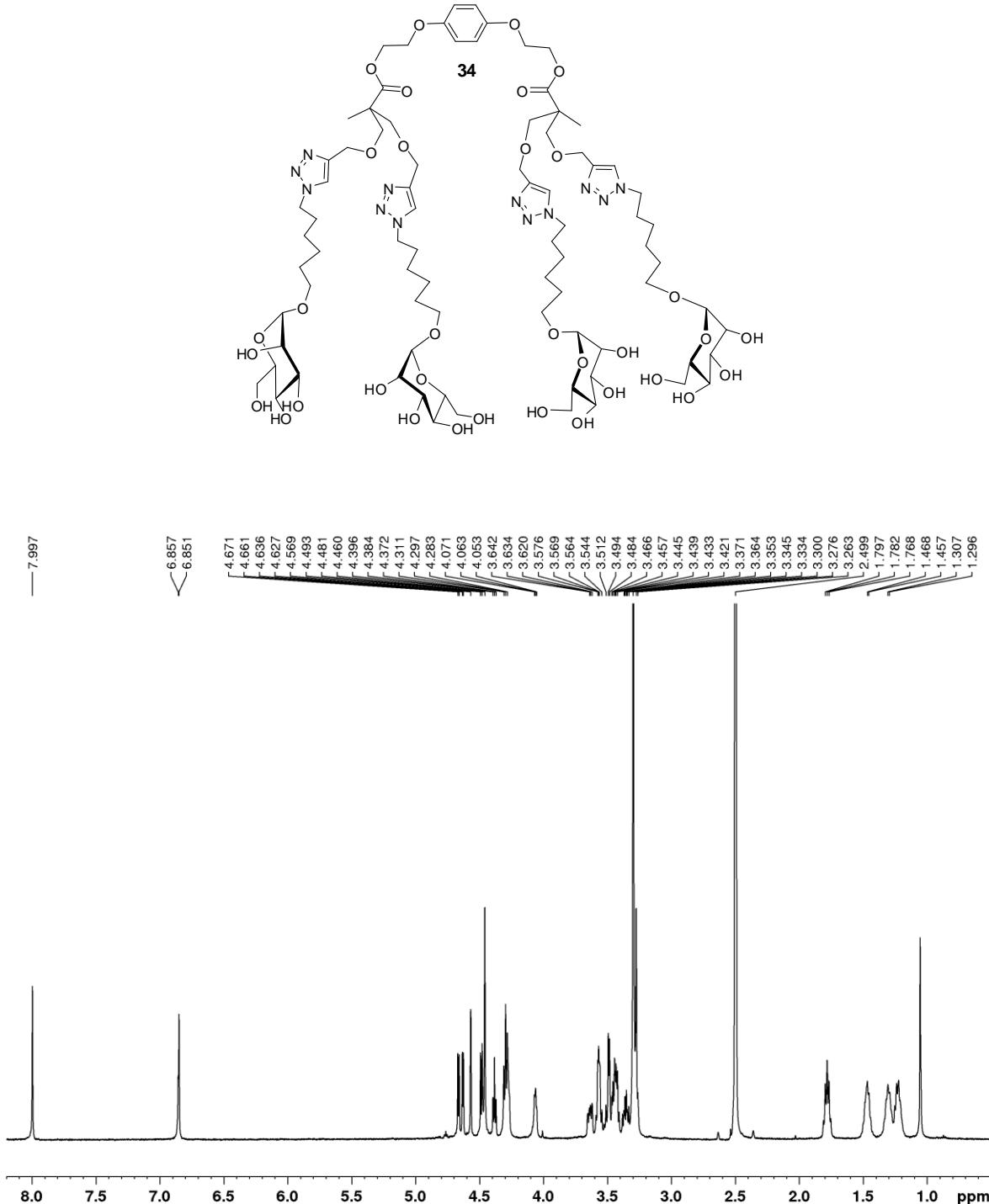
Expansion of part of the 500.13 MHz ^1H NMR spectrum of 1,4-bis-2-(2,2'-bis-(2-propynyloxy)methyl)-propanoyloxyethoxybenzene (33) in chloroform-*d*



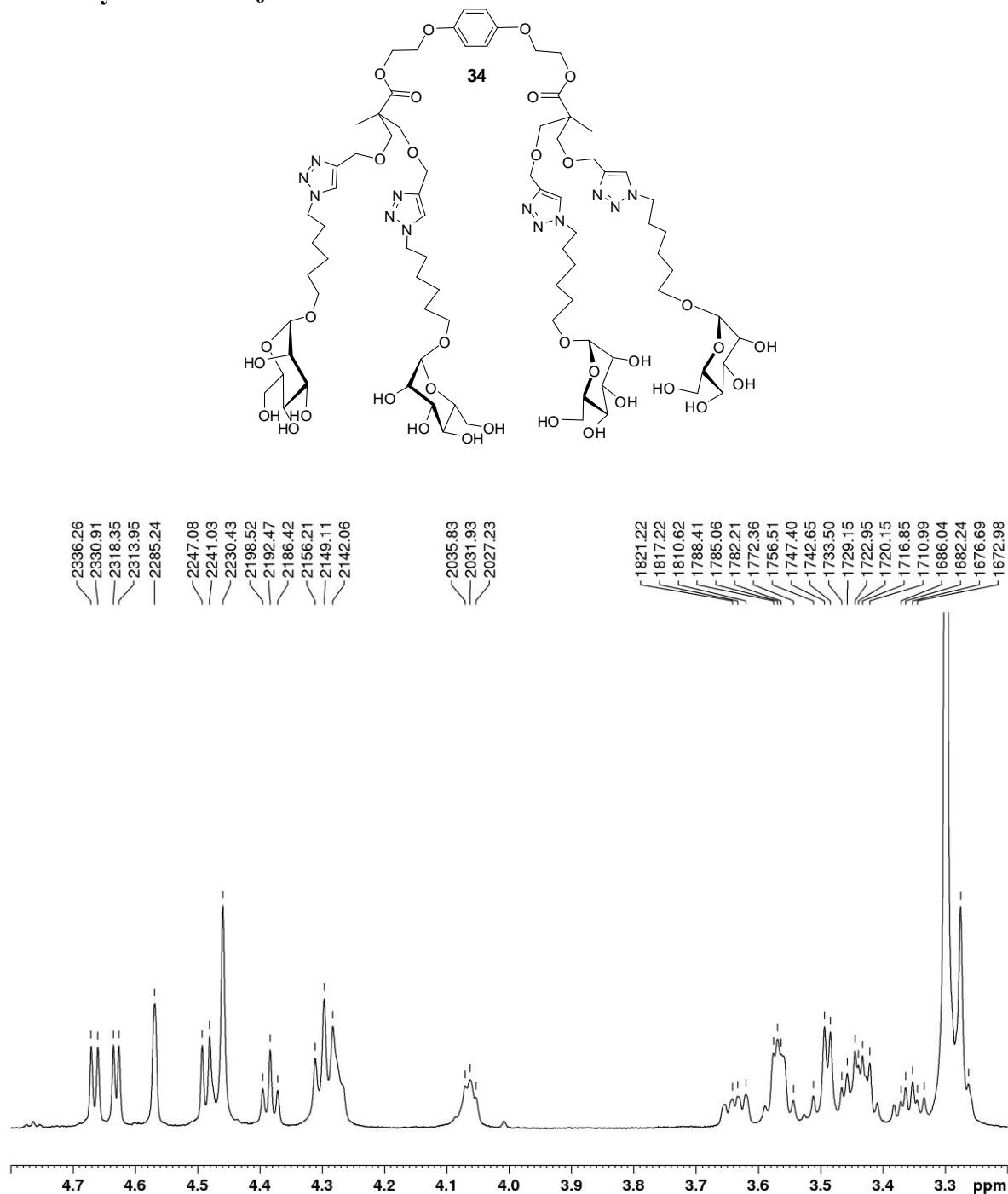
125.7 MHz ^{13}C NMR spectrum of 1,4-bis-2-(2,2'-bis-(2-propynylloxy)methyl)propanoyloxy)-ethoxy)benzene (33) in chloroform-*d*



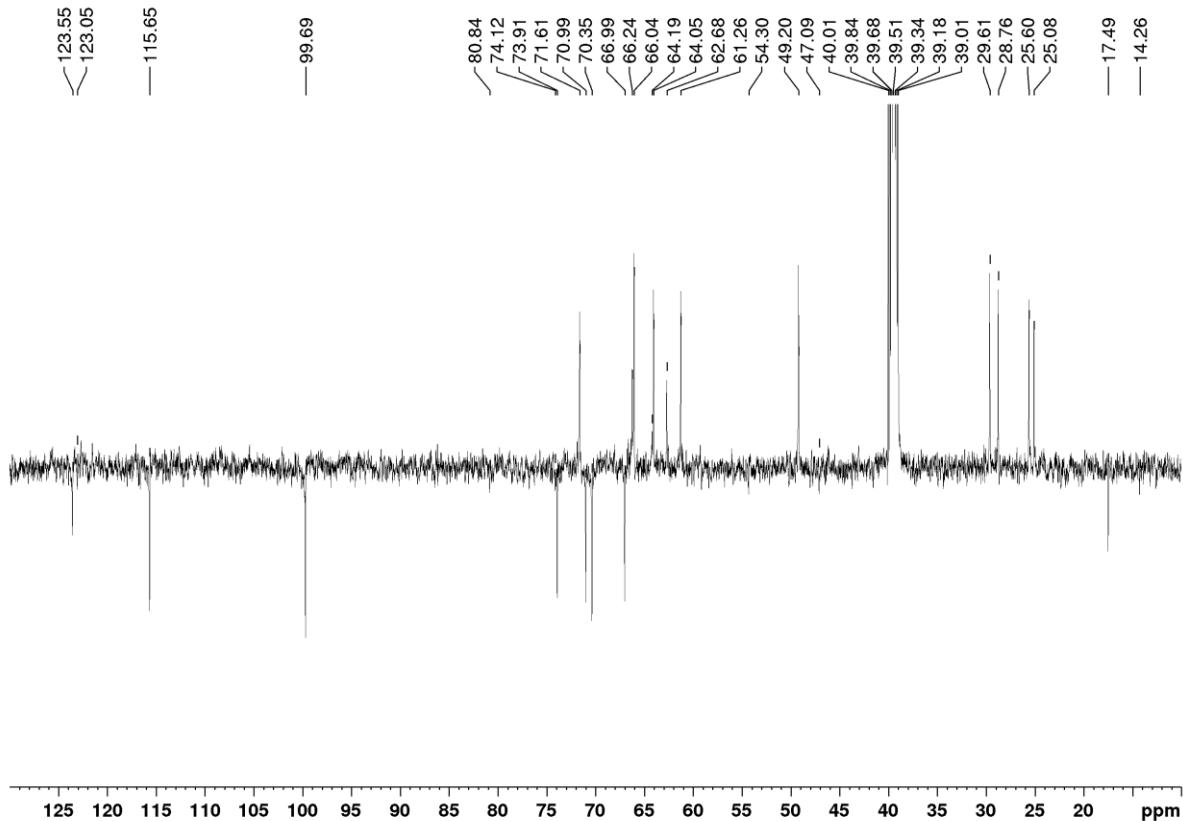
500.13 MHz ^1H NMR spectrum of tetramannoside polyester dendrimer (34**) in dimethyl sulfoxide- d_6**



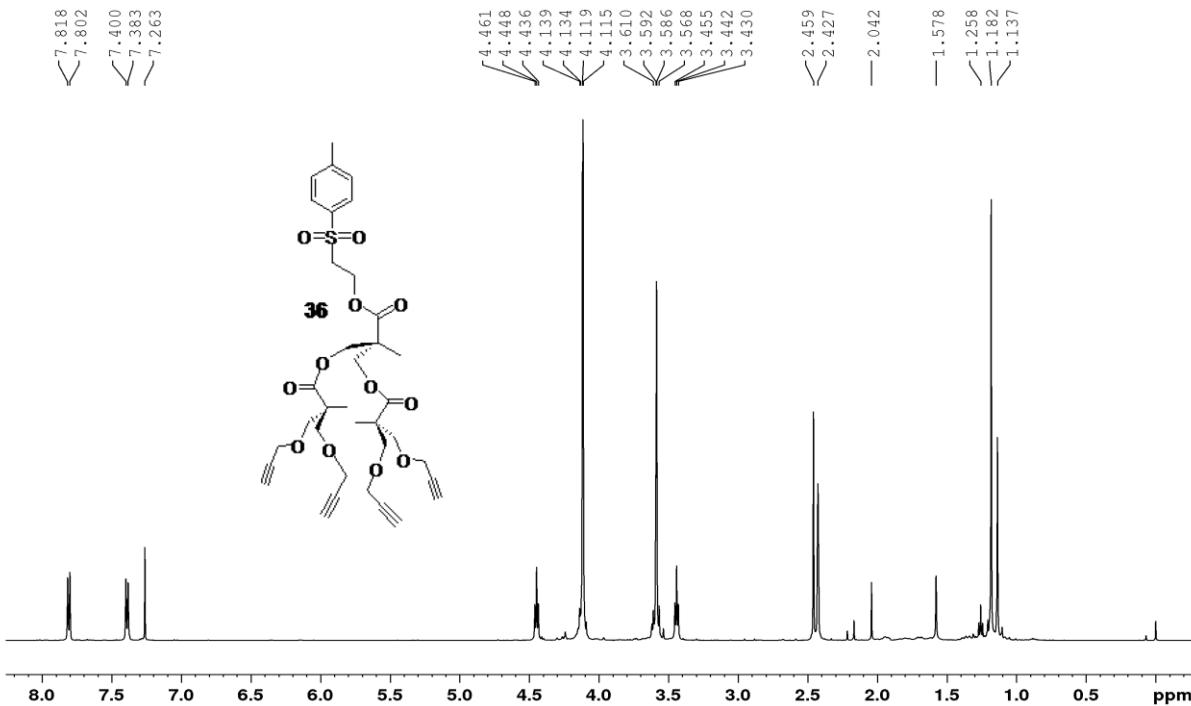
Expansion of part of the 500.13 MHz ^1H NMR spectrum of tetramannoside polyester dendrimer (34) in dimethyl sulfoxide- d_6



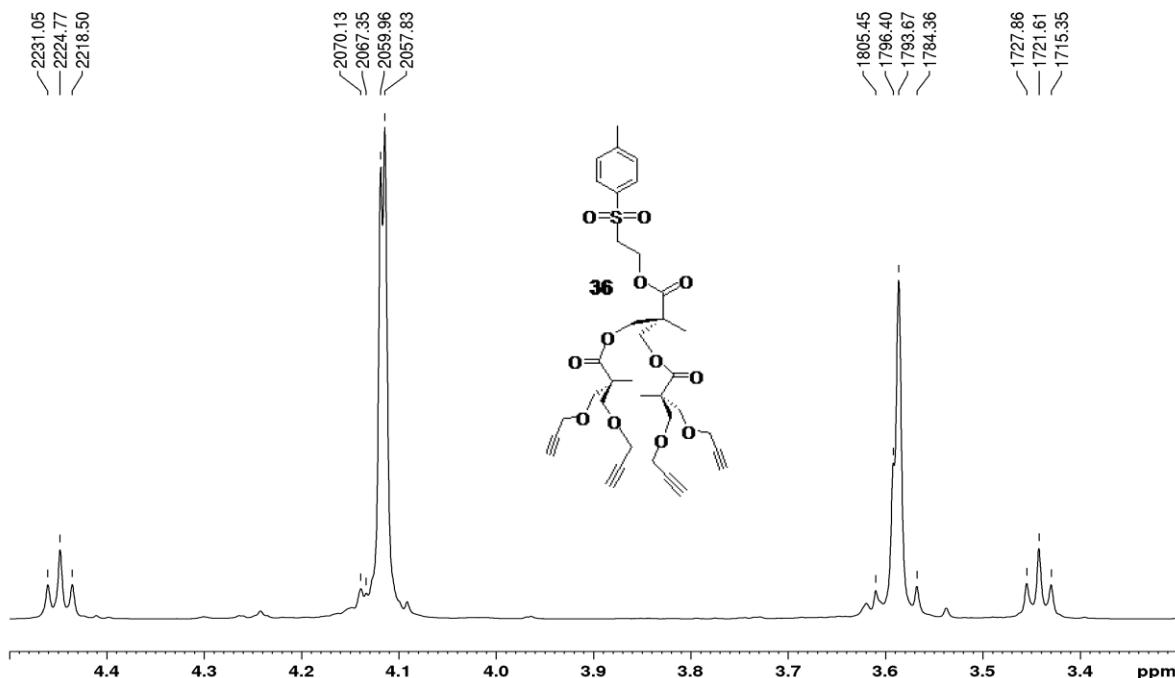
125.7 MHz ^{13}C DeptQ spectrum of tetramannoside polyester dendrimer (34) in dimethyl sulfoxide- d_6



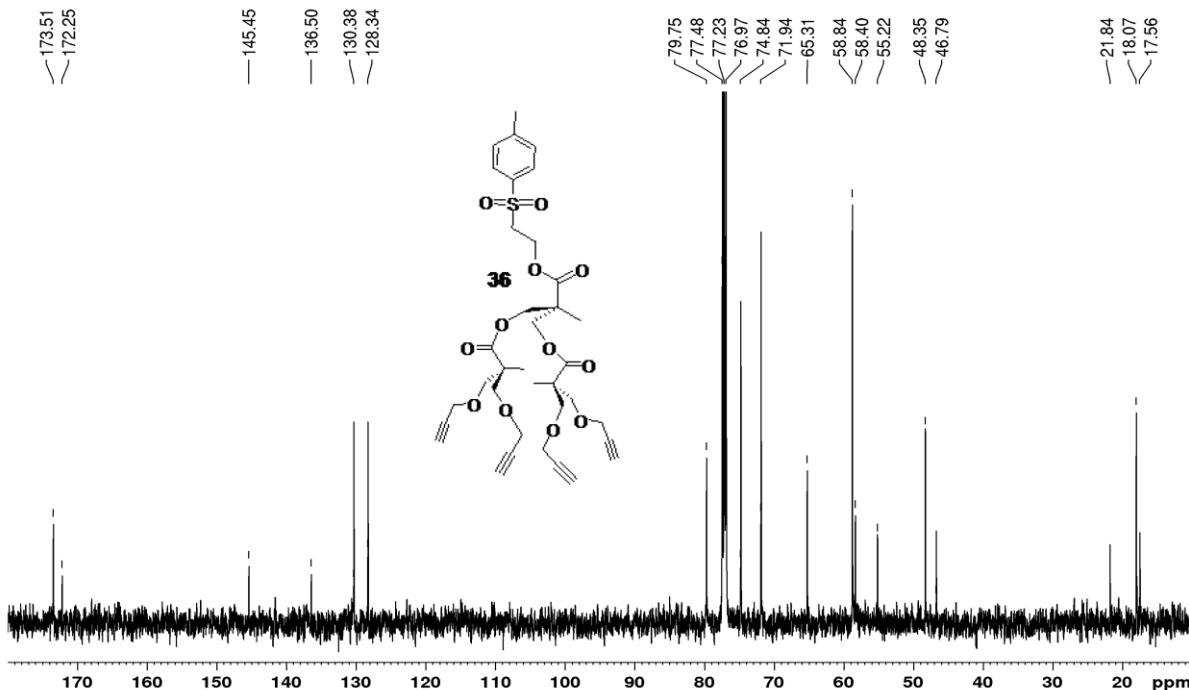
500.13 MHz ^1H NMR spectrum of 2-(*p*-toluenesulfonyl)ethyl 2,2'-bis(2,2'-bis-(2-propynylloxymethyl)propanoyloxymethyl)-propanoate (36**) in chloroform-*d***



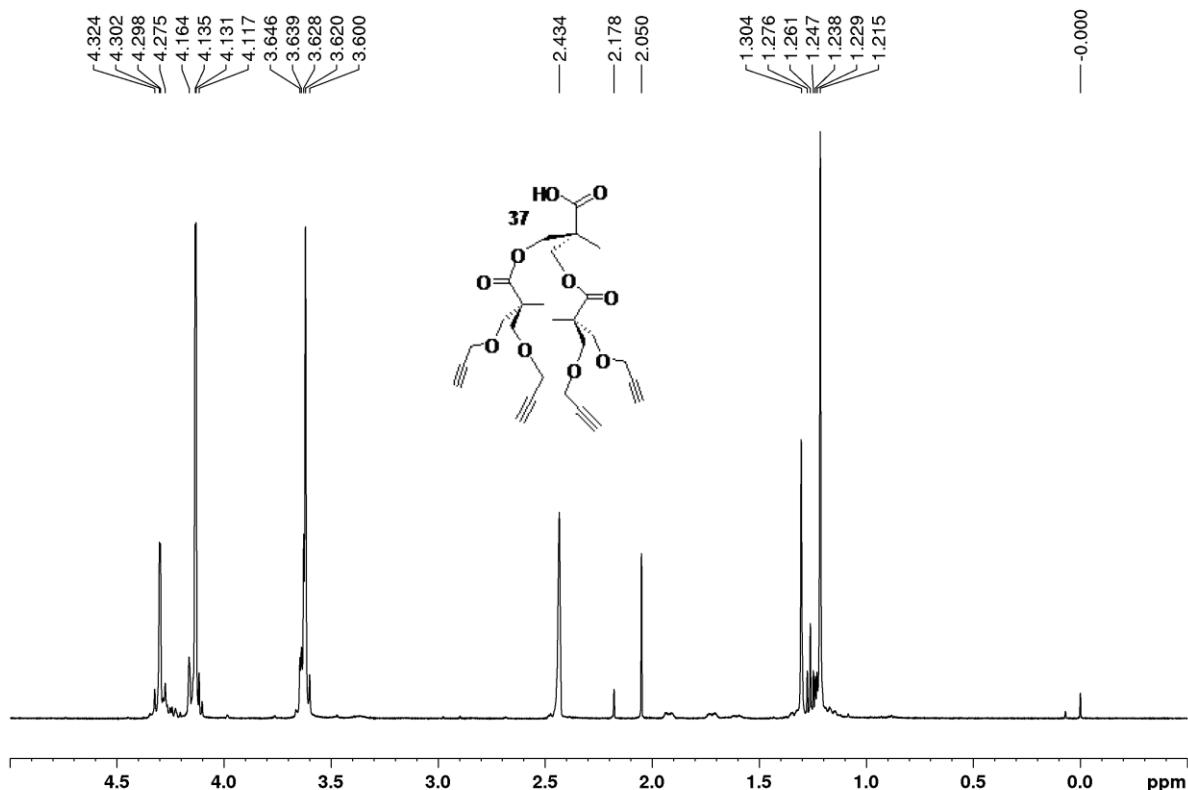
Expansion of part of the 500.13 MHz ^1H NMR spectrum of 2-(p-toluenesulfonyl)ethyl 2,2'-bis(2,2'-bis(2-propynylloxymethyl)propanoyloxy)methyl)-propanoate (36**) in chloroform-**



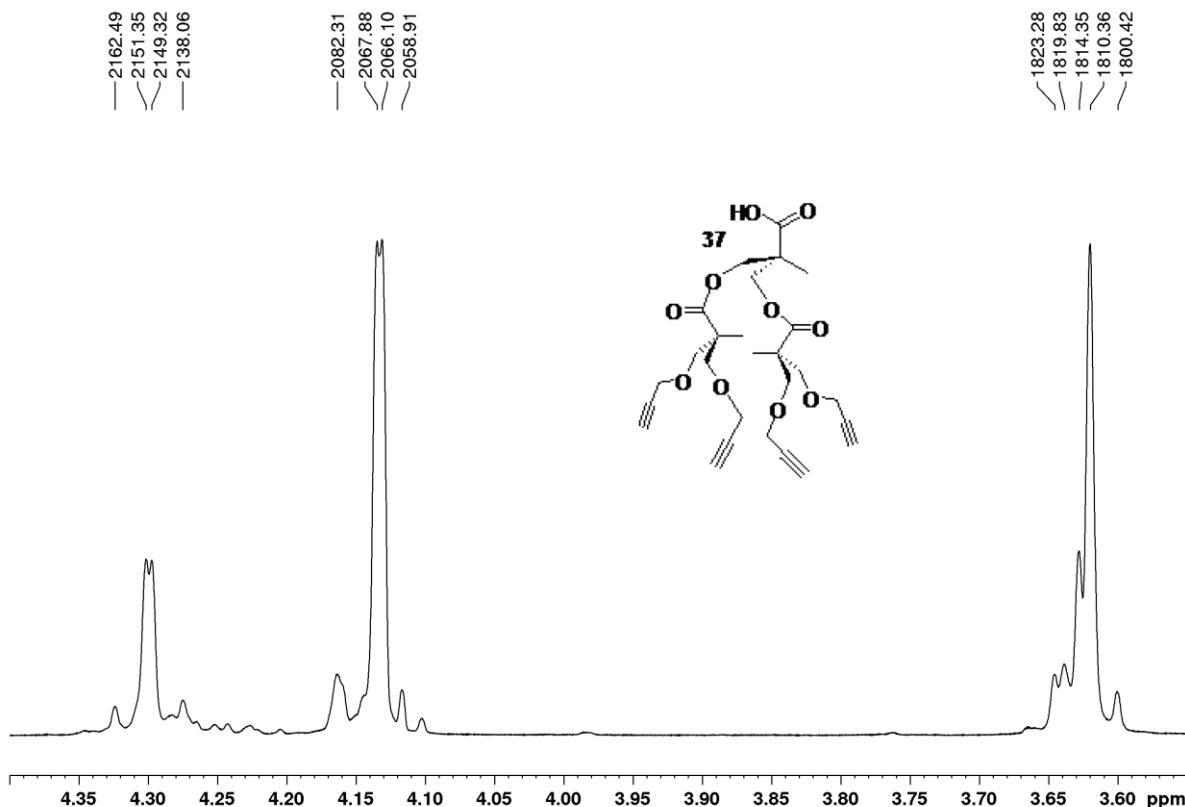
125.7 MHz ^{13}C NMR spectrum of 2-(p-toluenesulfonyl)ethyl 2,2'-bis(2,2'-bis(2-propynylloxymethyl)propanoyloxymethyl)-propanoate (36**) in chloroform-*d***



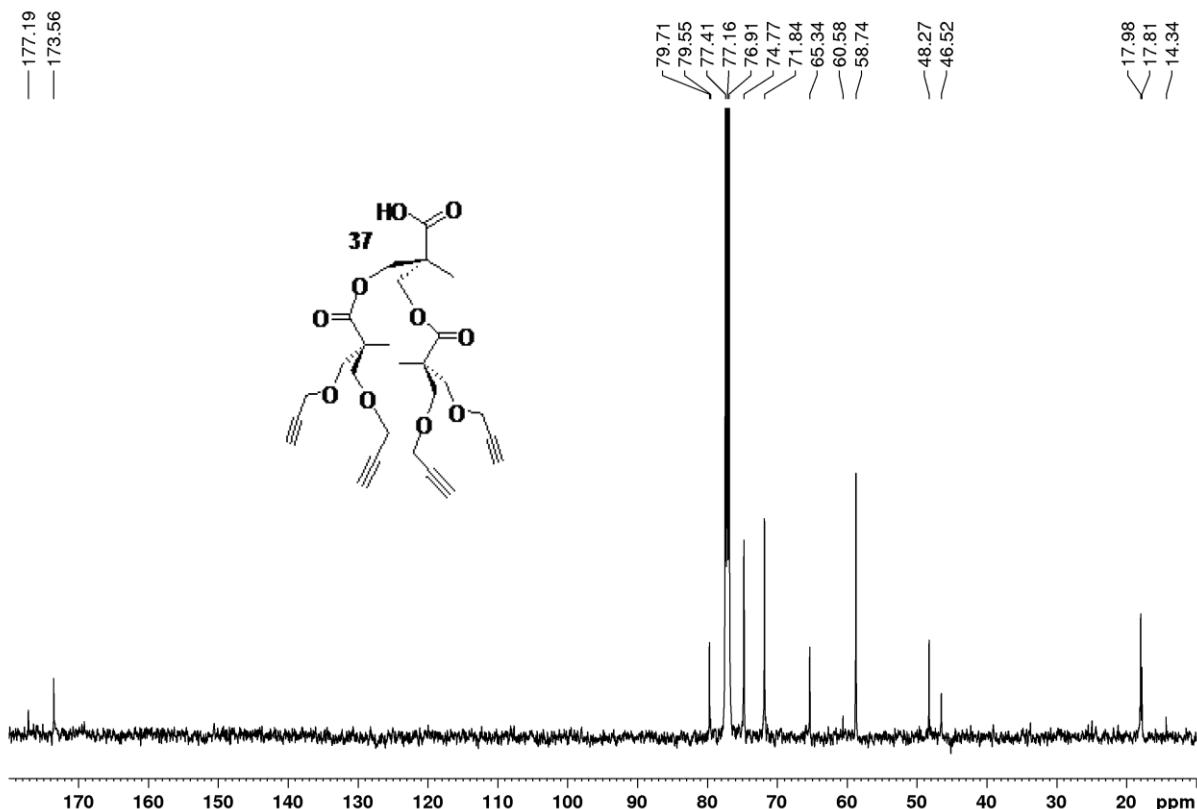
500.13 MHz ^1H NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynylloxymethyl)propanoyloxymethyl)-propanoic acid (37) in chloroform-*d*



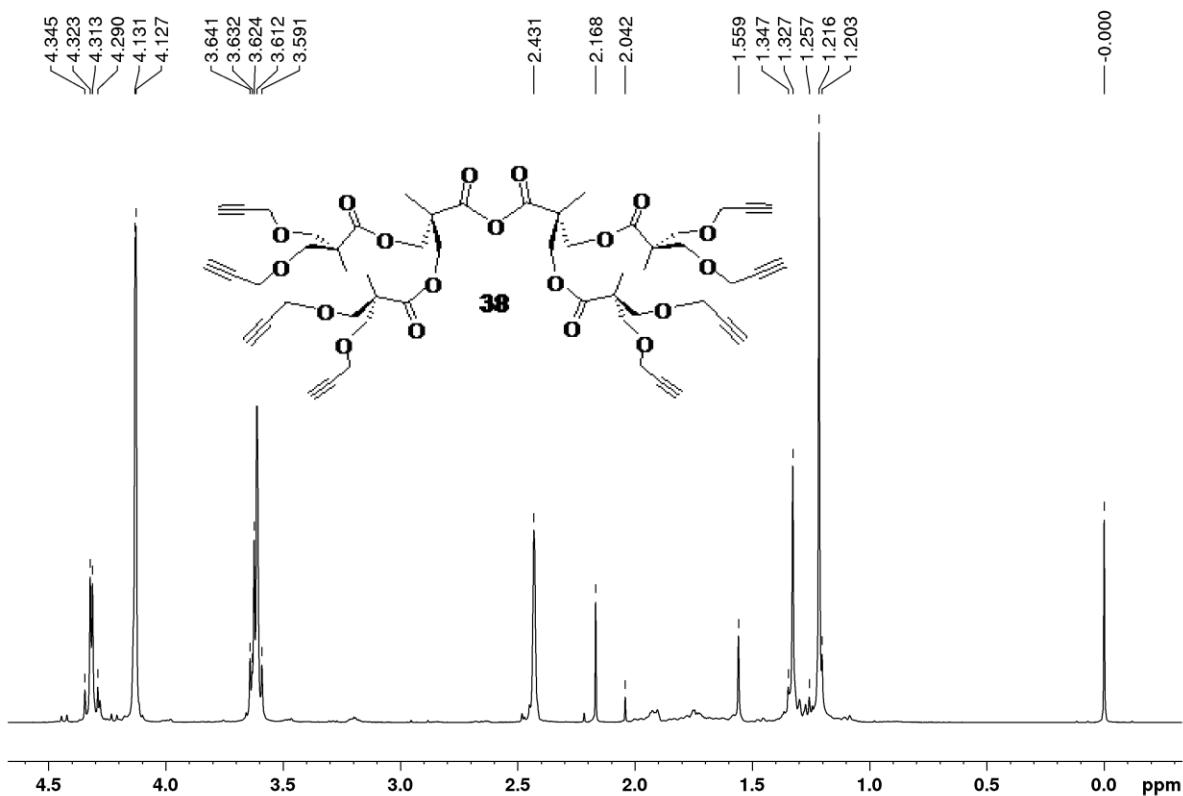
Expansion of part of the 500.13 MHz ^1H NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynyoxy-methyl)propanoyloxymethyl)propanoic acid (37**) in chloroform-*d***



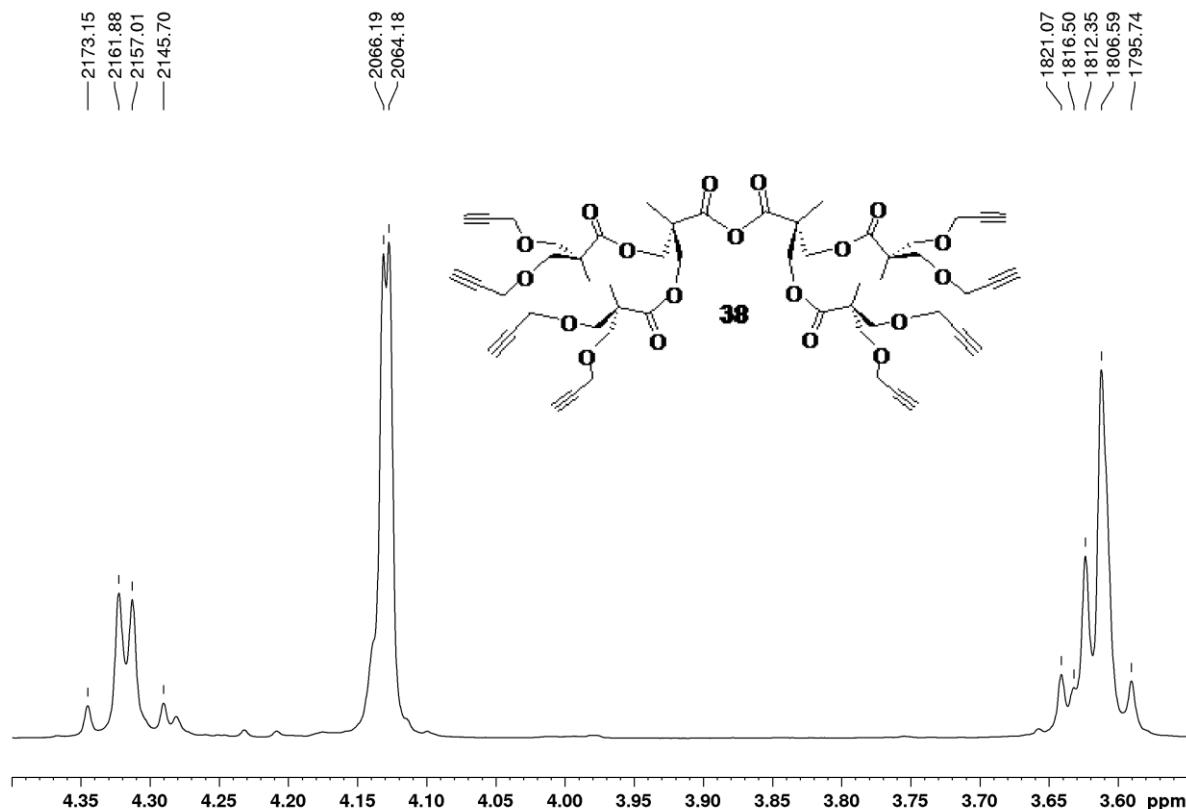
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynyloxymethyl)propanoyloxymethyl)-propanoic acid (37) in chloroform-*d*



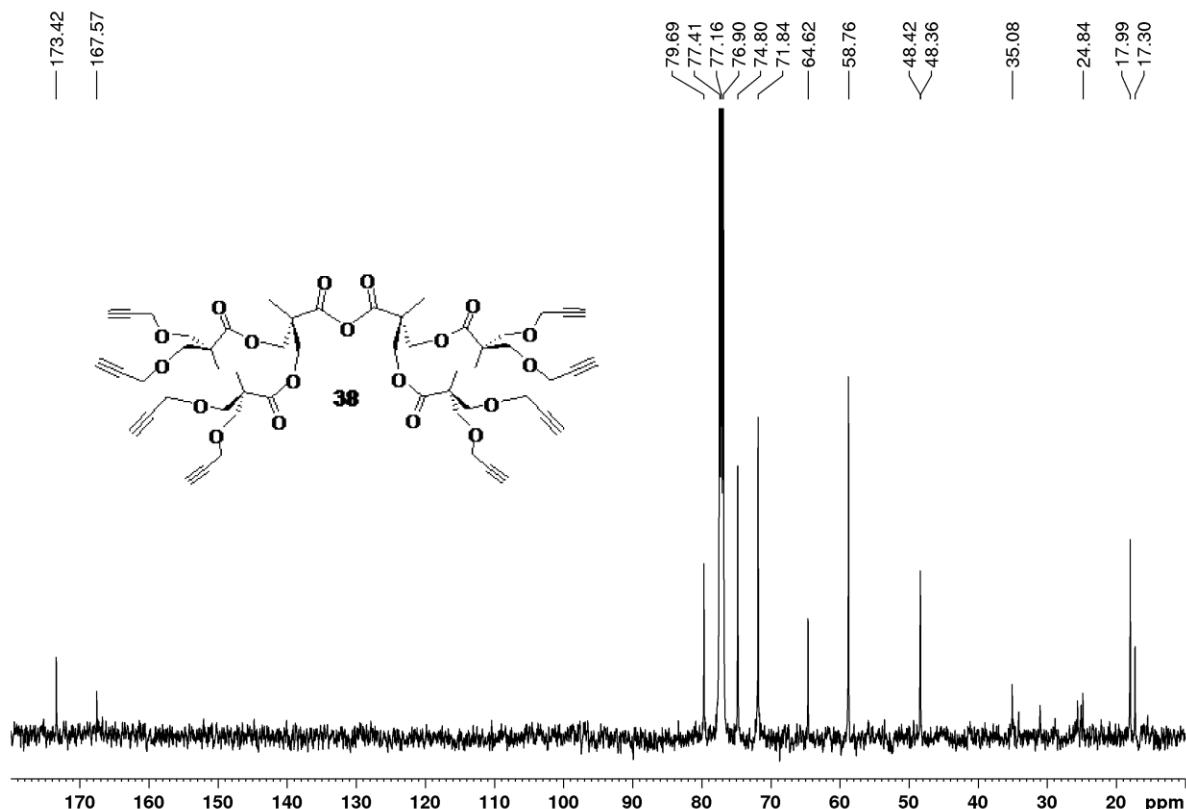
500.13 MHz ^1H NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynylloxymethyl)propanoyloxymethyl)-propanoic anhydride (38**) in chloroform-*d***

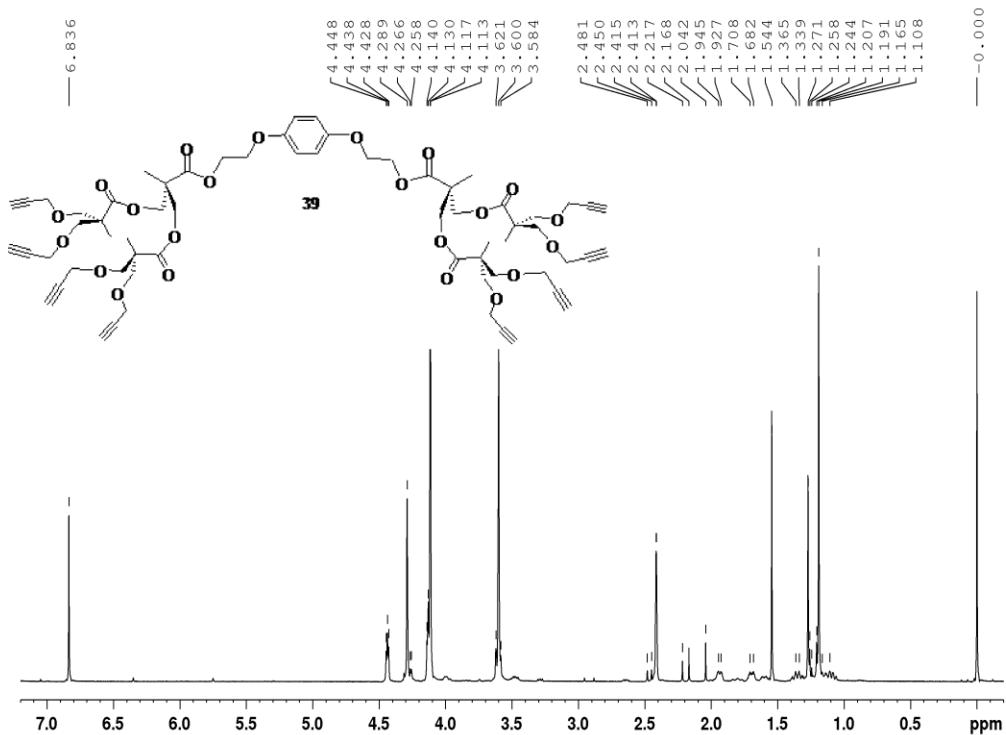


Expansion of part of the 500.13 MHz ^1H NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynyoxy-methyl)propanoyloxymethyl)propanoic anhydride (38**) in chloroform-*d***

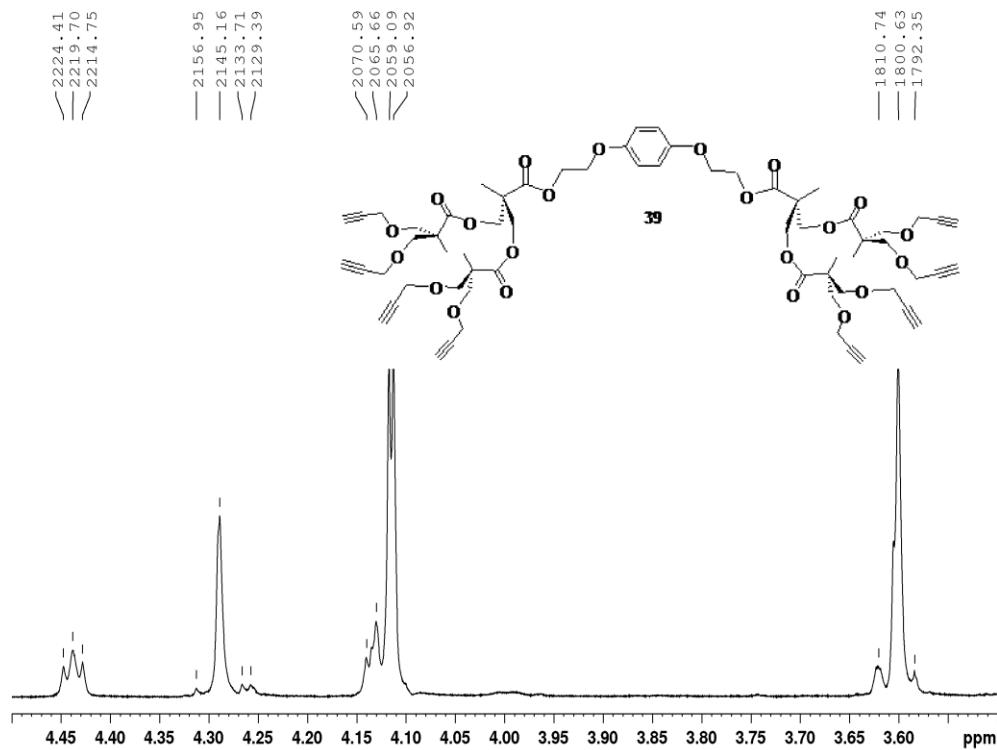


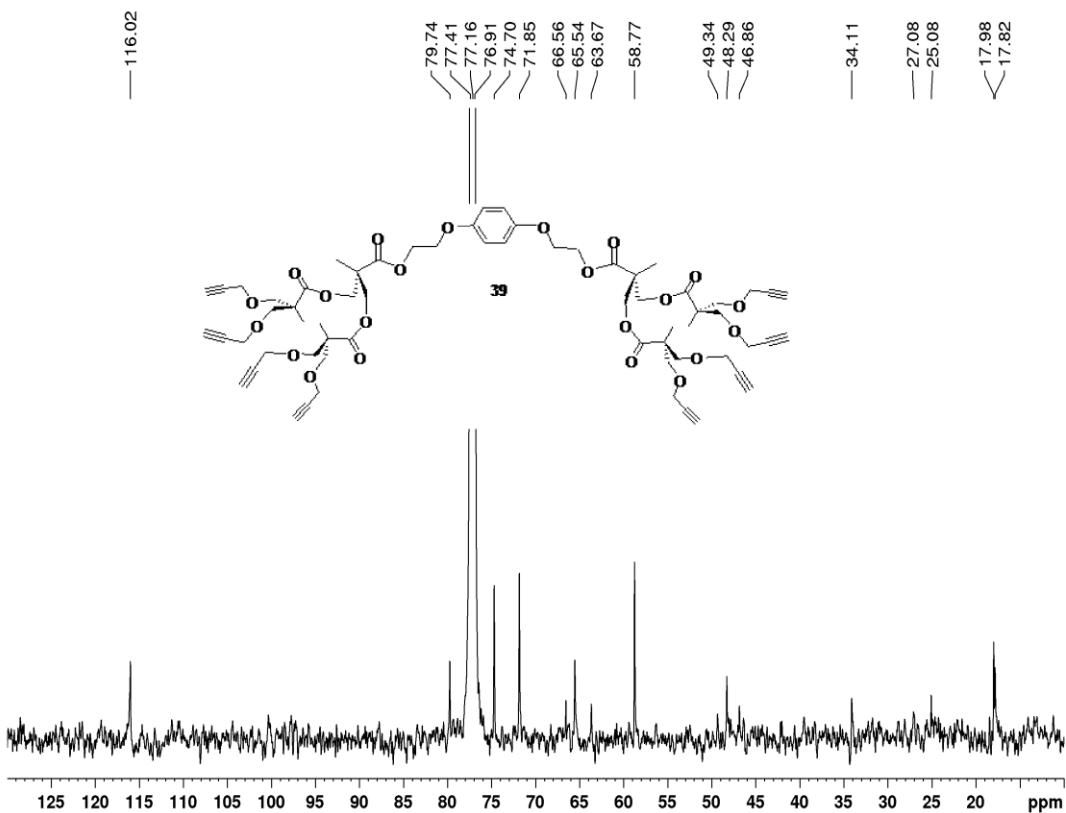
125.7 MHz ^{13}C NMR spectrum of 2,2'-bis(2,2'-bis-(2-propynylloxymethyl)propanoyloxymethyl)-propanoic anhydride (38) in chloroform-*d*



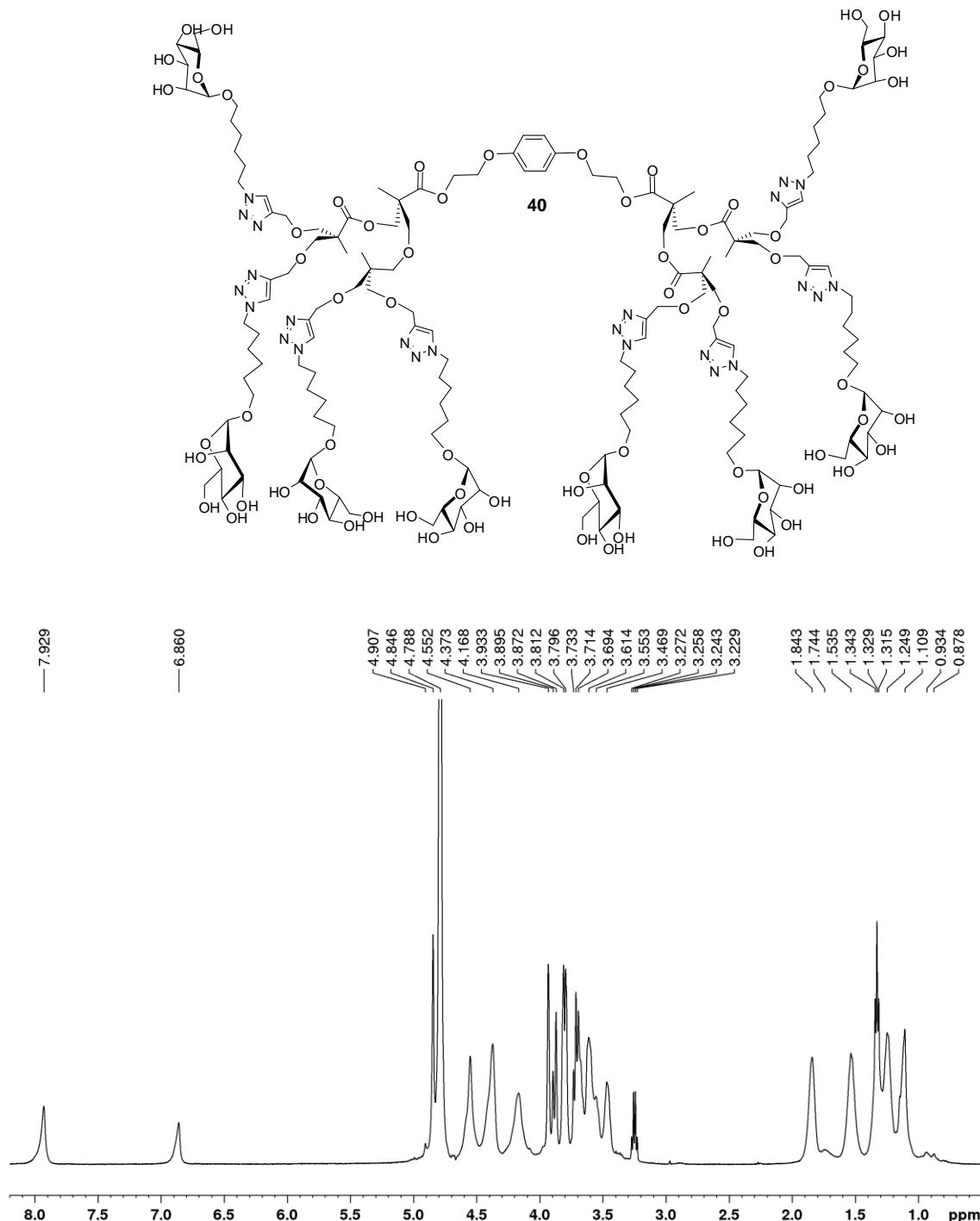
500.13 MHz ^1H NMR spectrum of octapropargylated polyester dendrimer (39**) in chloroform-*d***

Expansion of part of the 500.13 MHz ^1H NMR spectrum of octapropargylated polyester dendrimer (39**) in chloroform-*d***

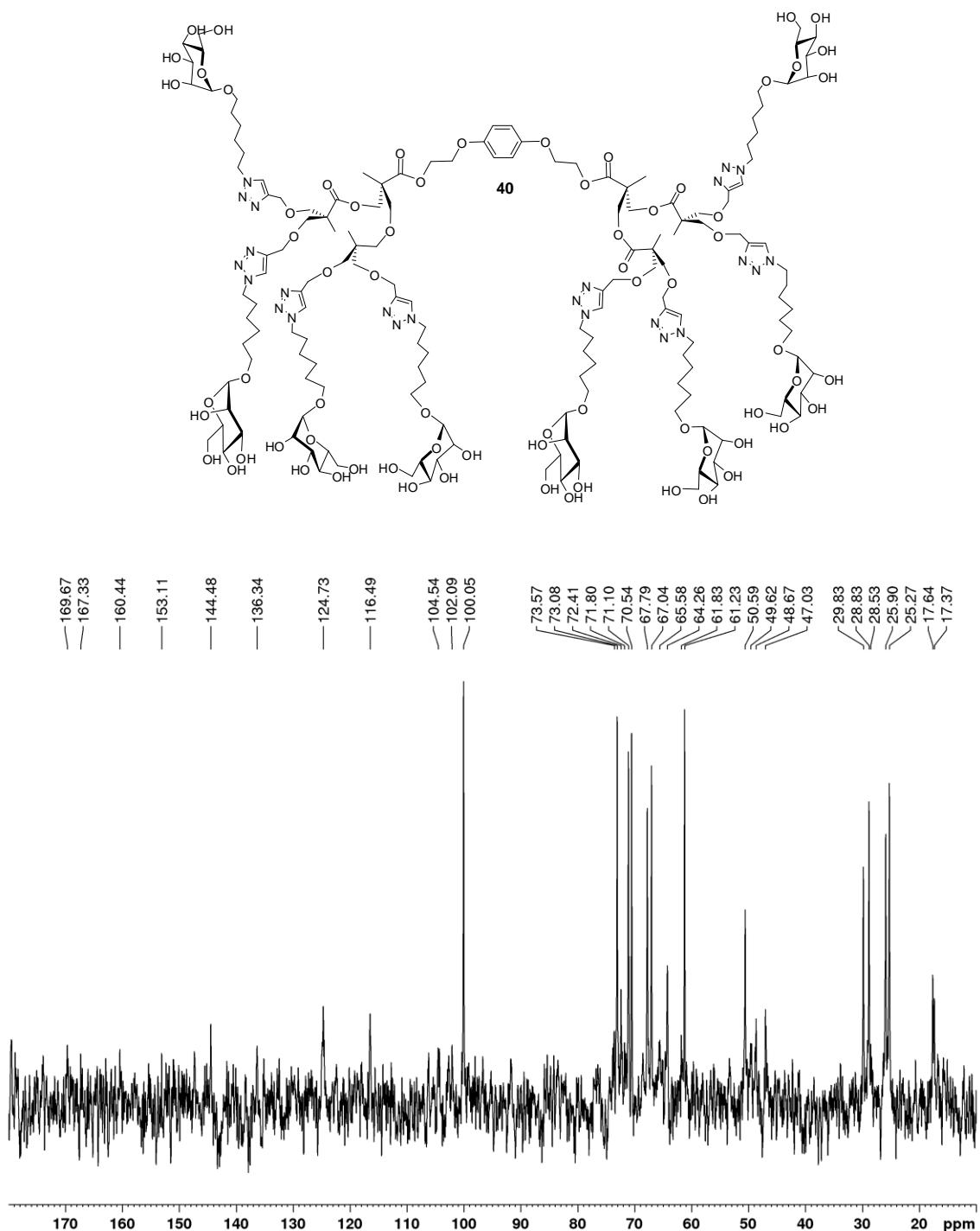


125.7 MHz ^{13}C NMR spectrum of octapropargylated polyester dendrimer (39**) in chloroform-*d***

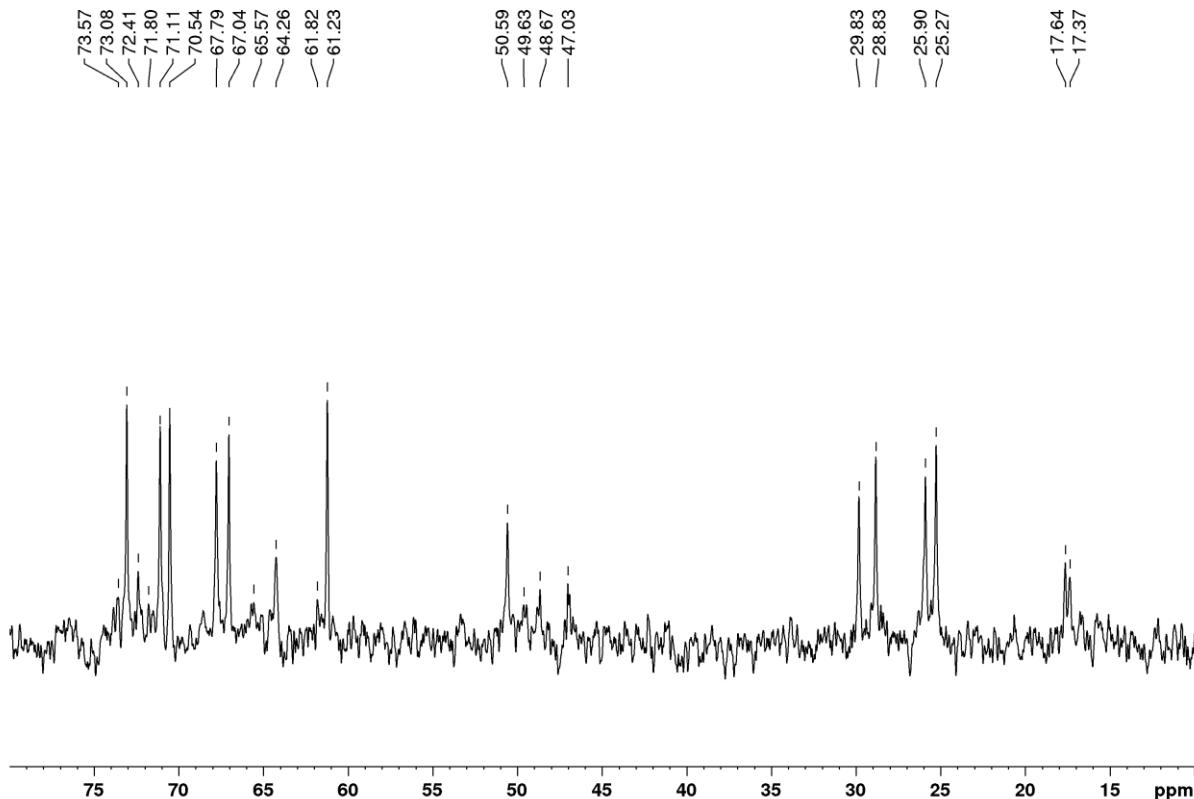
500.13 MHz ^1H NMR spectrum of octavalent mannose-terminated polyester dendrimer (40**) in water- d_2**



125.7 MHz ^{13}C NMR spectrum of octavalent mannose-terminated polyester dendrimer (40**) in water- d_2**



Expansion of part of the 125.7 MHz ^{13}C NMR spectrum of octavalent mannose-terminated polyester dendrimer (40**) in water- d_2**



125.7 MHz ^{13}C DEPT Q NMR spectrum of octavalent mannose-terminated polyester dendrimer (40) in water- d_2

