

Supporting Information for

“BisTEGylated poly(*p*-benzamide)s: Combining organo-solubility with shape-persistence”

Synthesis and characterization of polymers

Gel permeation chromatography of polymers

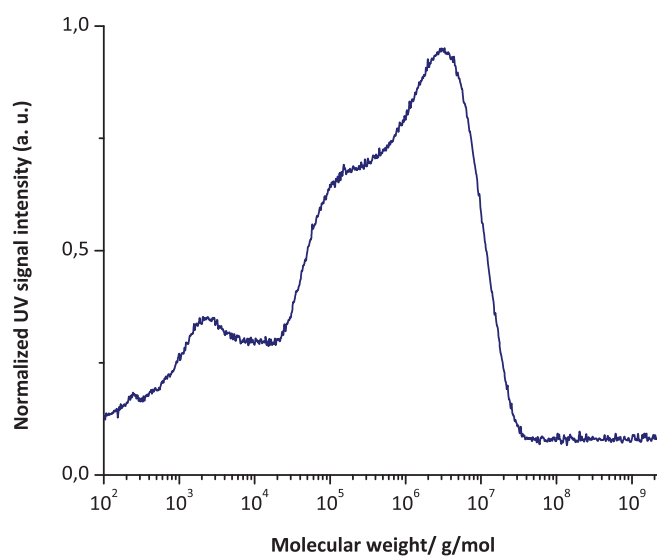


Figure S1. GPC elugram of polymer **13b**.

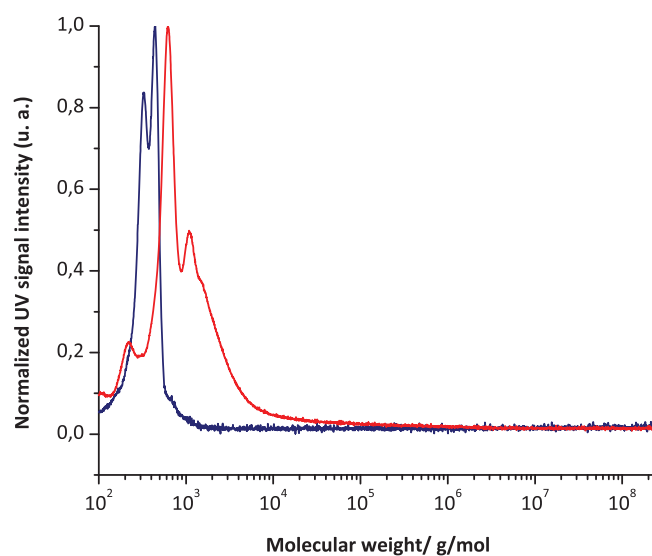


Figure S2. GPC elugram of polymerization of monomer **14a** in diglyme (*red*) and THF (*blue*).

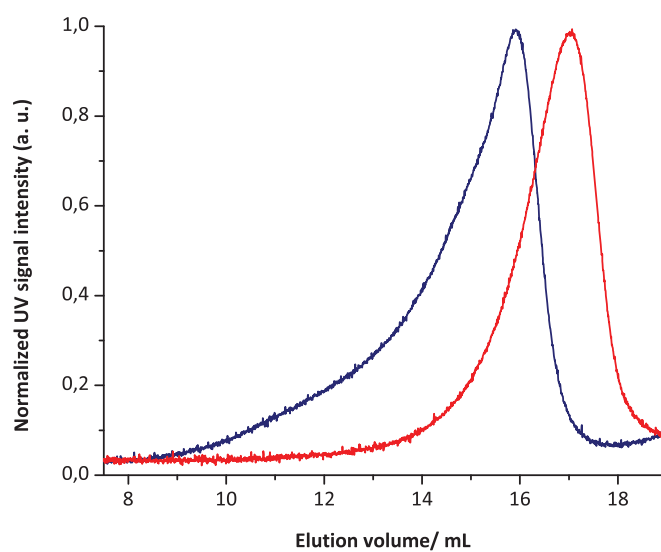


Figure S3. GPC elugram of protected (*red*) and unprotected (*blue*) polymer **14b**.

Bis-TEGylated poly(*p*-benzamide) (13a)

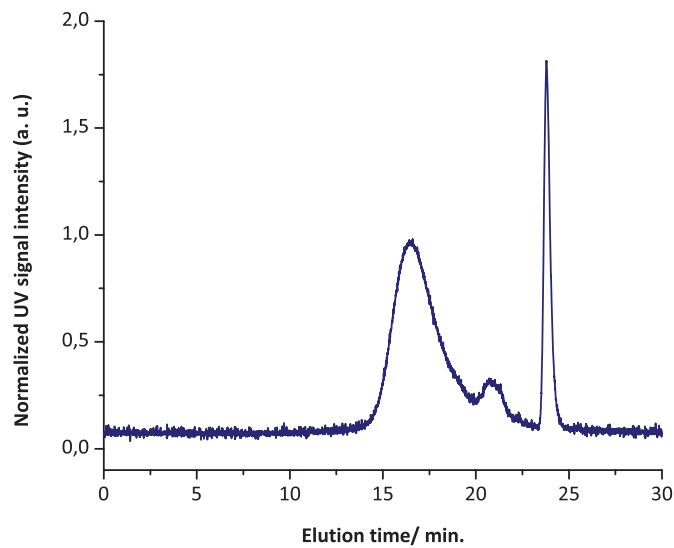


Figure S4. Entire GPC elugram of polymer **13a**, showing no peak at short elution time which would indicate aggregation (toluene at 23.8 min.).

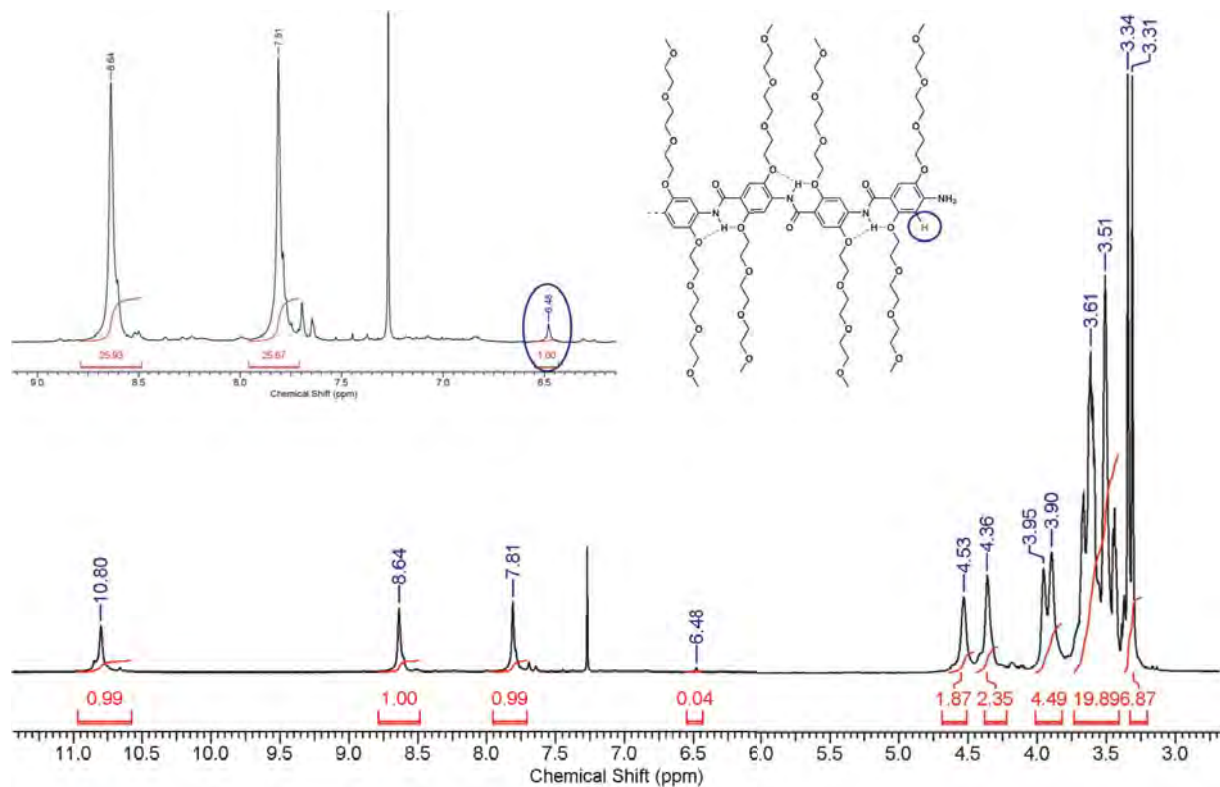


Figure S5. ^1H NMR spectrum (400 MHz) of polymer **13a** in CDCl_3 , end group analysis indicates a polymer containing 25 repeat units (*inset*).

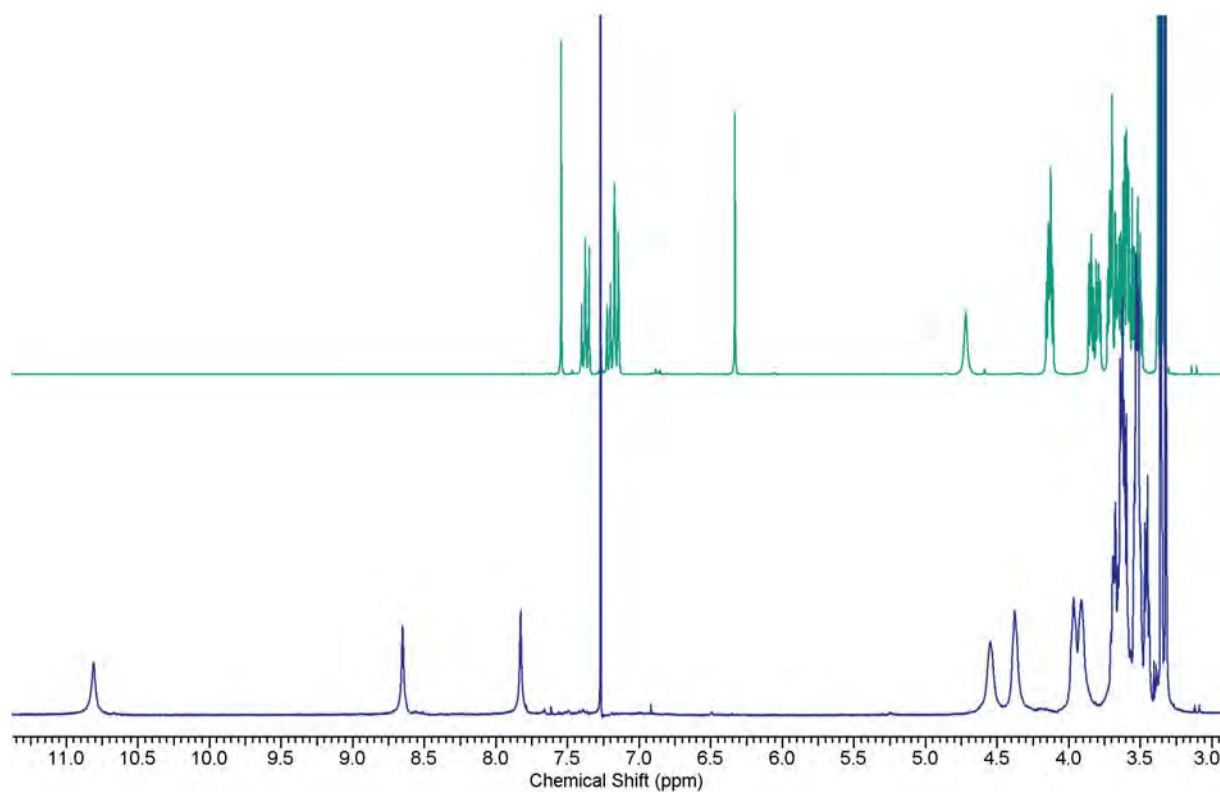


Figure S6. ^1H NMR spectra (300 MHz) of monomer **9a** (green) and polymer **13a** (blue) in CDCl_3 .

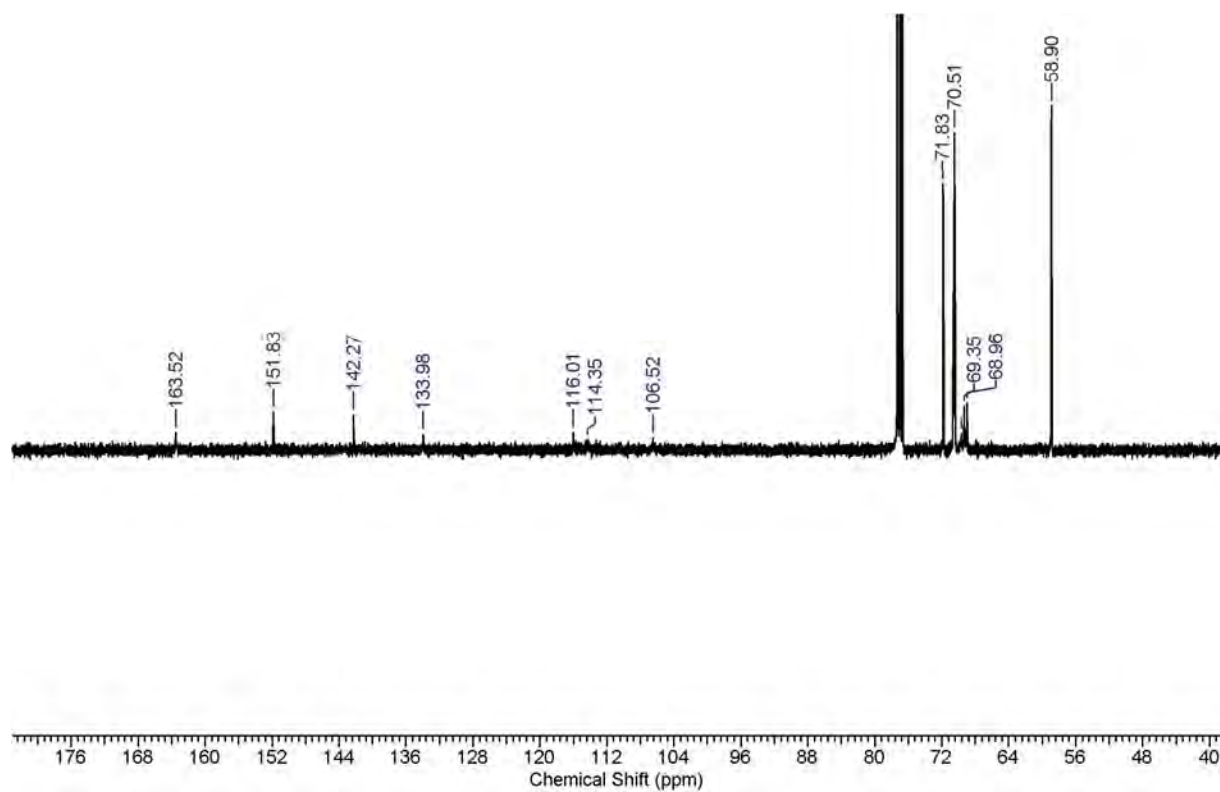


Figure S7. ¹³C NMR spectrum (100 MHz) of **13a** in CDCl₃.

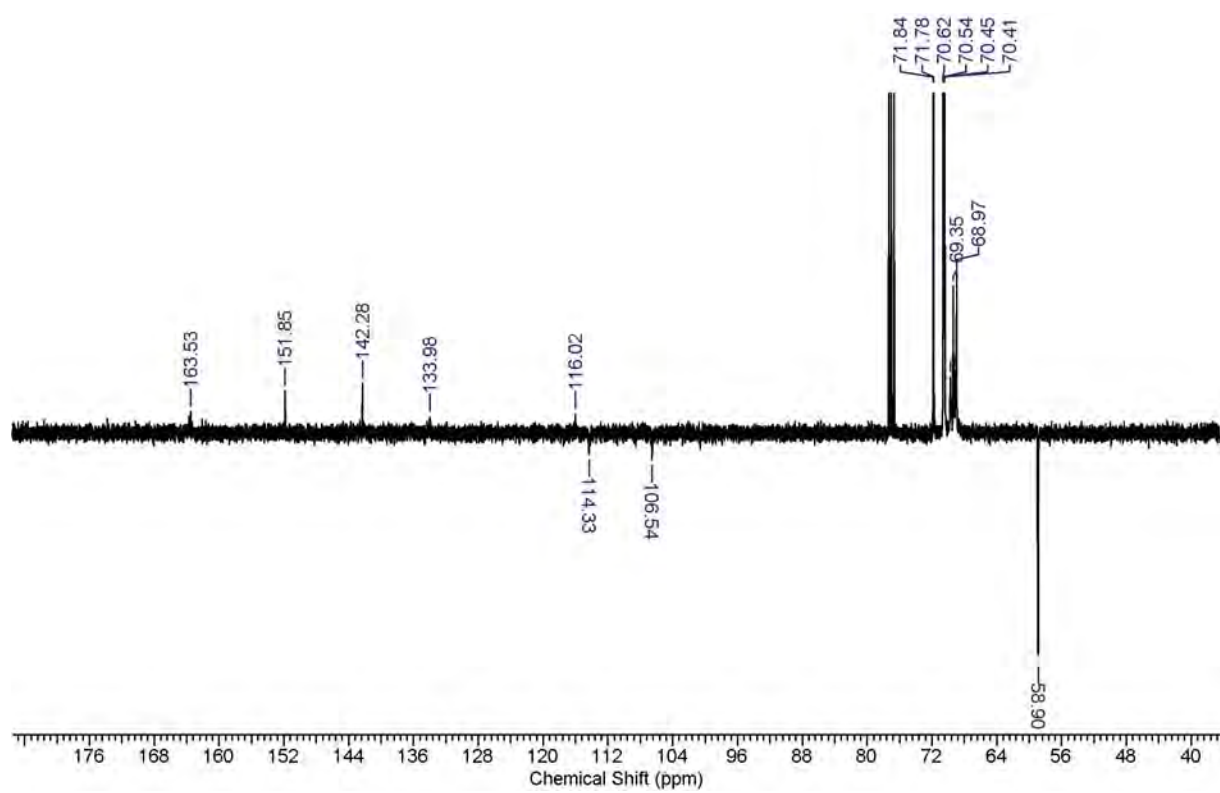


Figure S8. APT spectrum (100 MHz) of **13a** in CDCl₃.

N-protected, mono-TEGylated poly(*p*-benzamide) (**14b**)

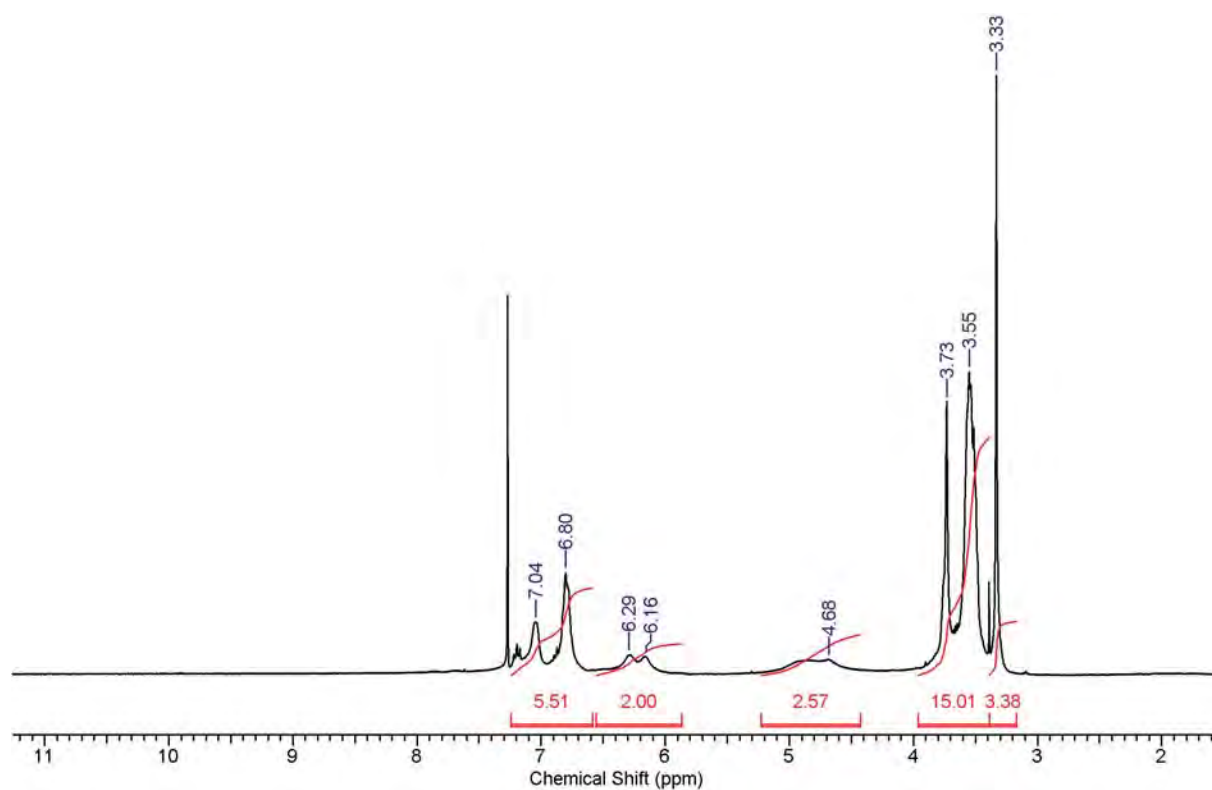


Figure S9. ¹H NMR spectrum (300 MHz) of **14b** in CDCl₃.

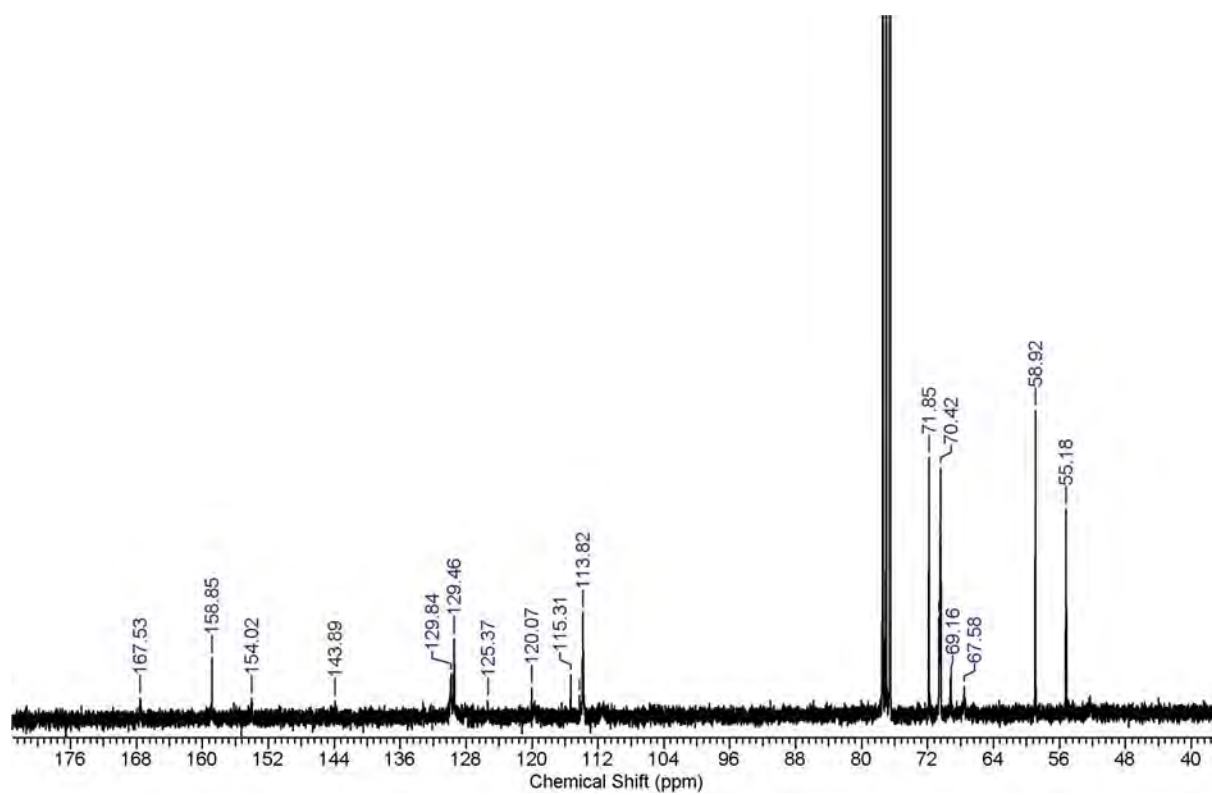


Figure S10. ¹³C NMR spectrum (75 MHz) of **14b** in CDCl₃.

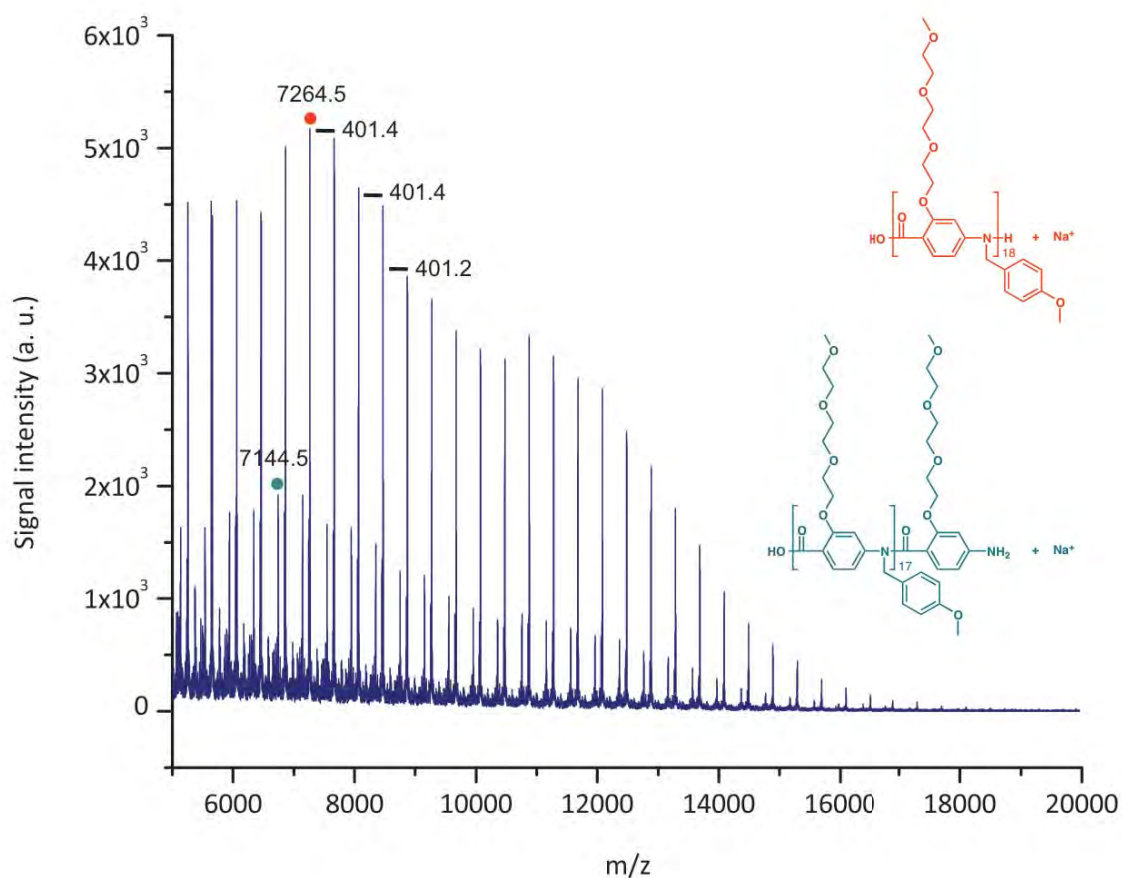


Figure S11. MALDI-ToF mass spectrum of **14b**.

UV-vis measurements

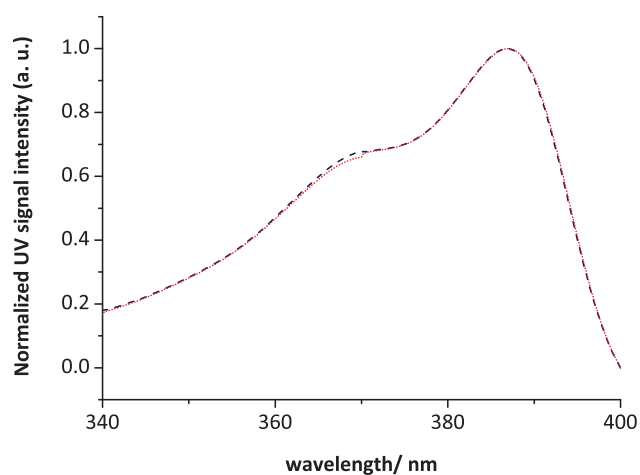


Figure S12. UV-vis measurement at 25°C of a chloroform solution (10 mg/mL) of polymer **13a** before and after filtration. The solutions were diluted to $c = 0.05$ mg/mL before the measurement.
 Red: unfiltered, blue: filtered through a PTFE filter (0.2 μm).

DLS measurements

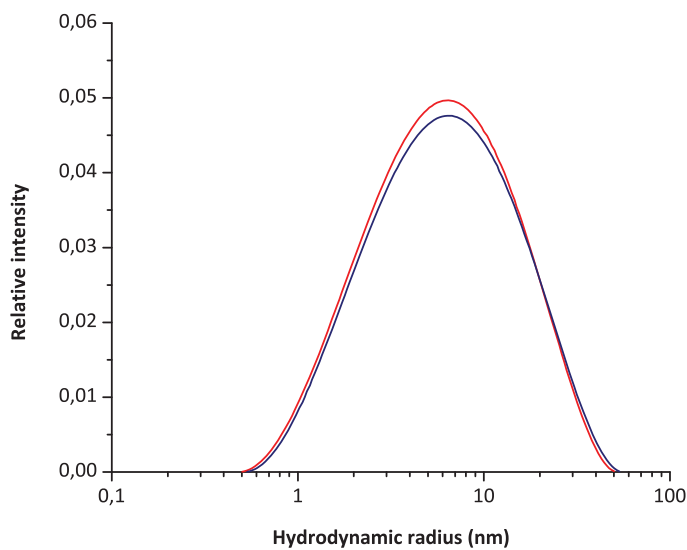


Figure S13. Hydrodynamic radii of polymer **13a** after 0h (*red*) and 12h (*blue*), calculated by the CONTIN method.

Methyl-2,5-dihydroxy-4-nitrobenzoate (**3**)

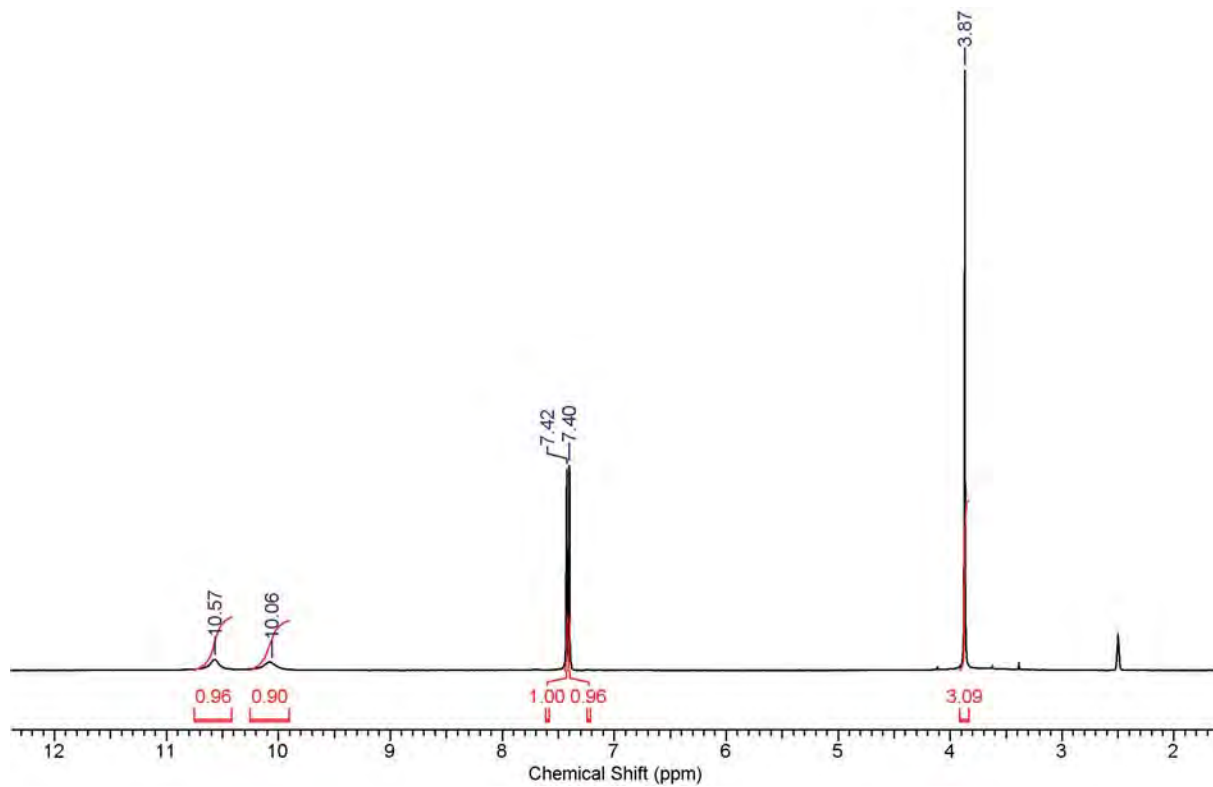


Figure S14. ¹H NMR spectrum (300 MHz) of **3** in DMSO-*d*₆.

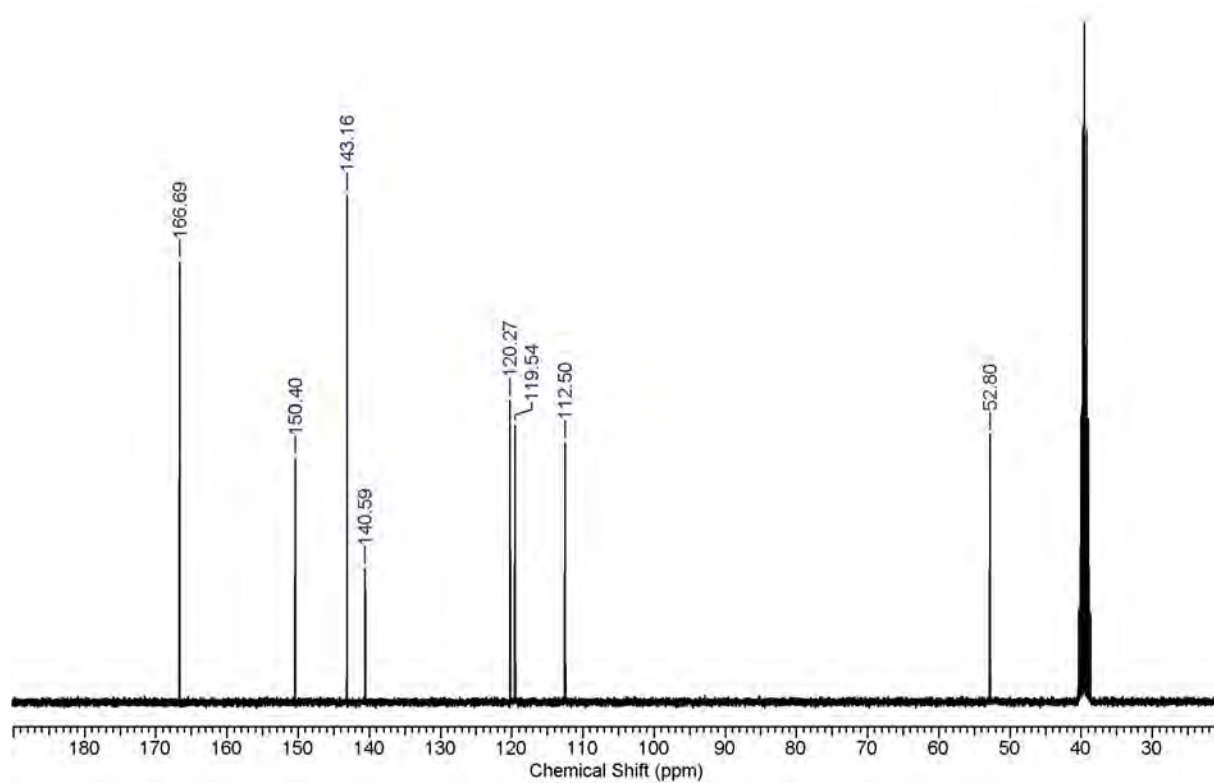


Figure S15. ¹³C NMR spectrum (75 MHz) of **3** in DMSO-*d*₆.

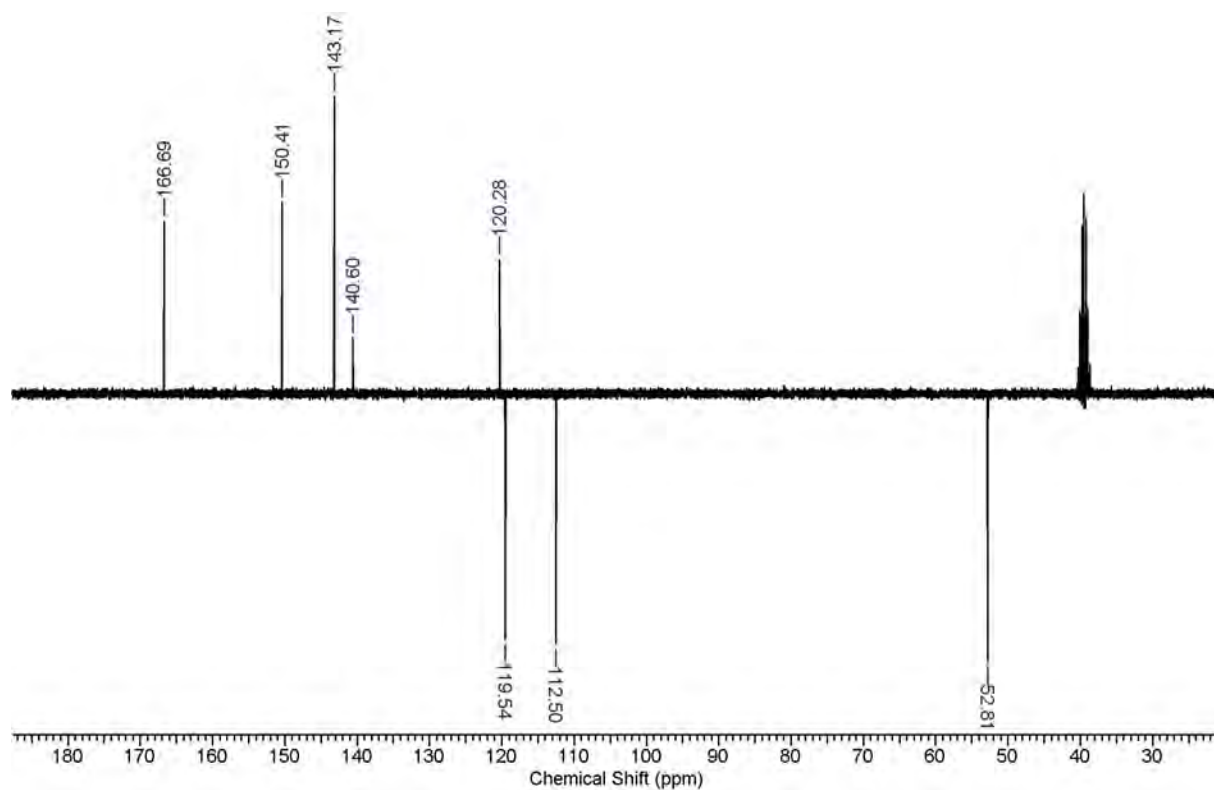


Figure S16. APT spectrum (75 MHz) of **3** in DMSO-*d*₆.

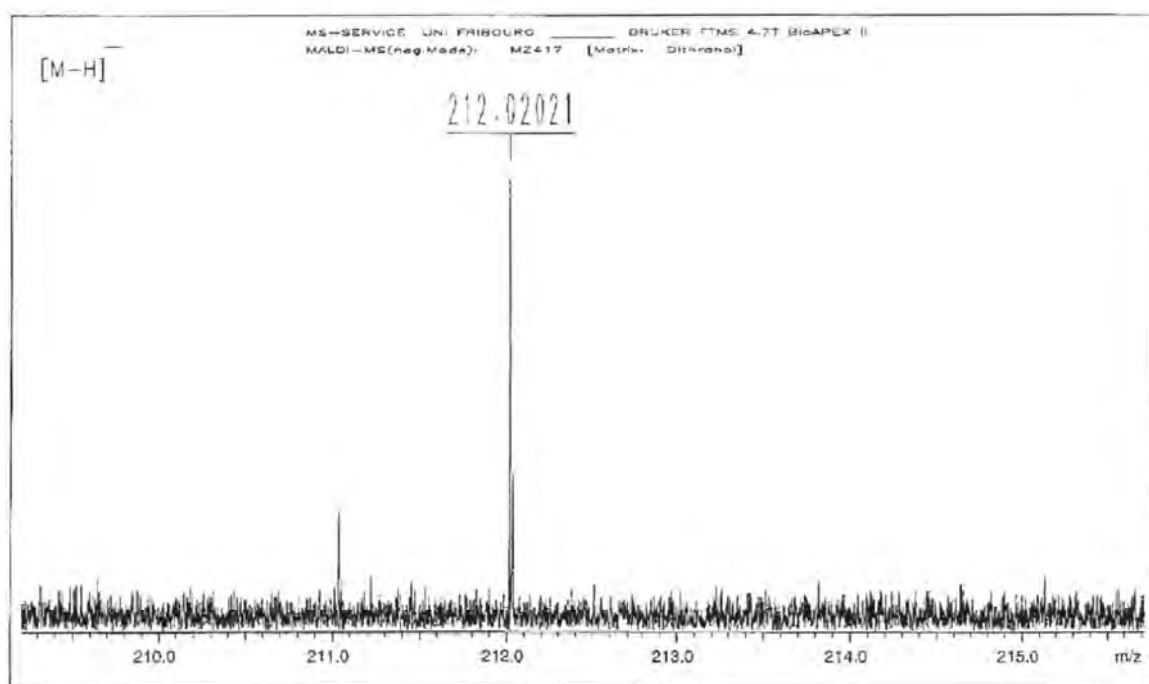


Figure S17. High resolution-mass spectrum of **3** (ESI-).

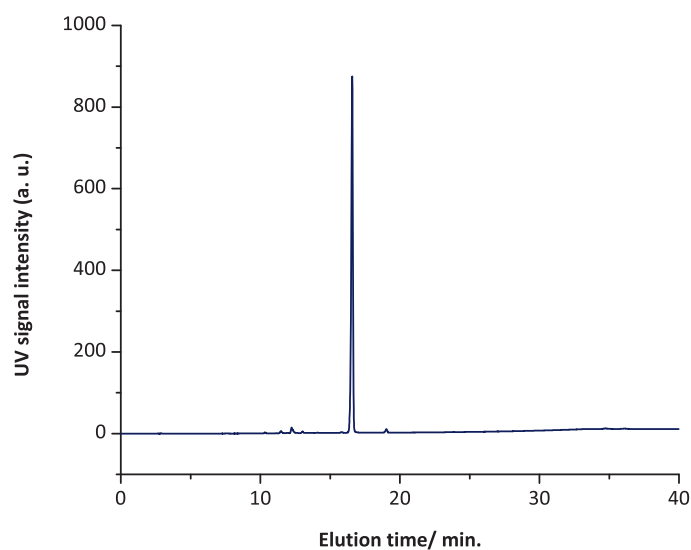


Figure S18. RP-HPLC elugram of **3**.

Methyl-2-hydroxy-4-nitrobenzoate (**4**)

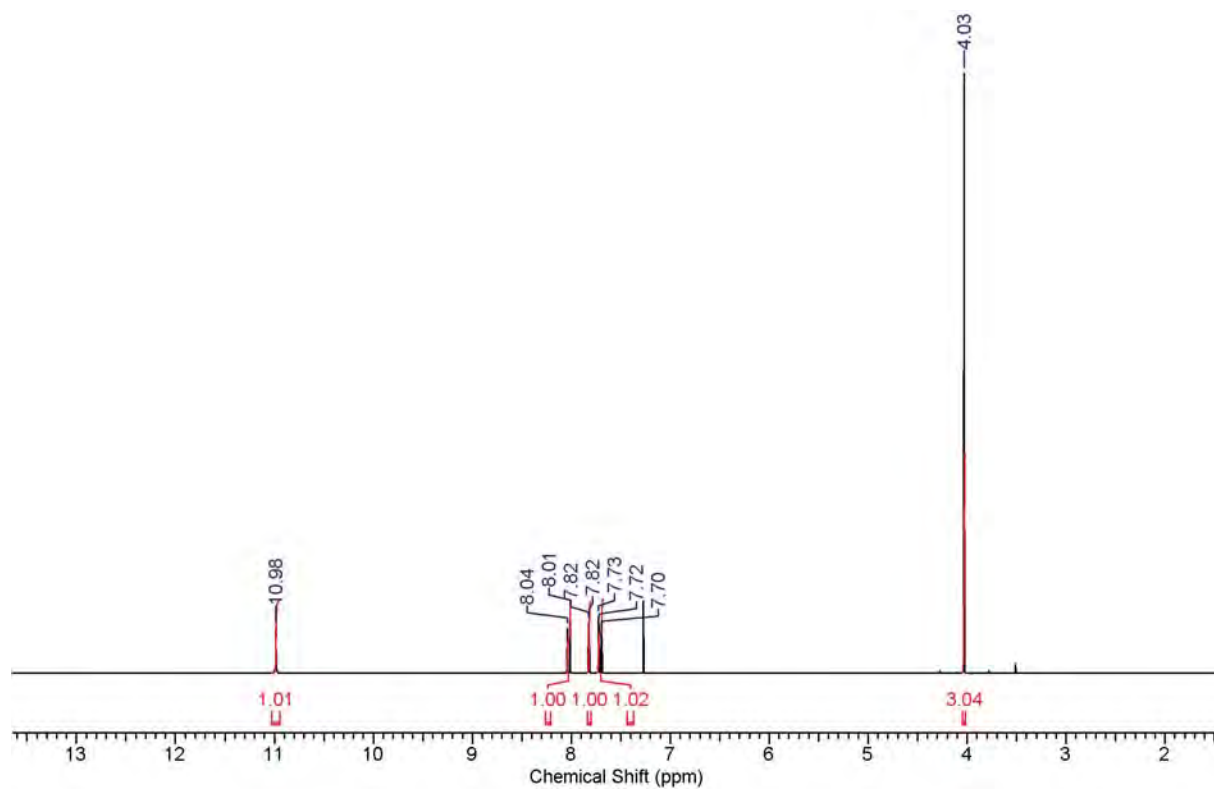


Figure S19. ¹H NMR spectrum (300 MHz) of **4** in CDCl₃.

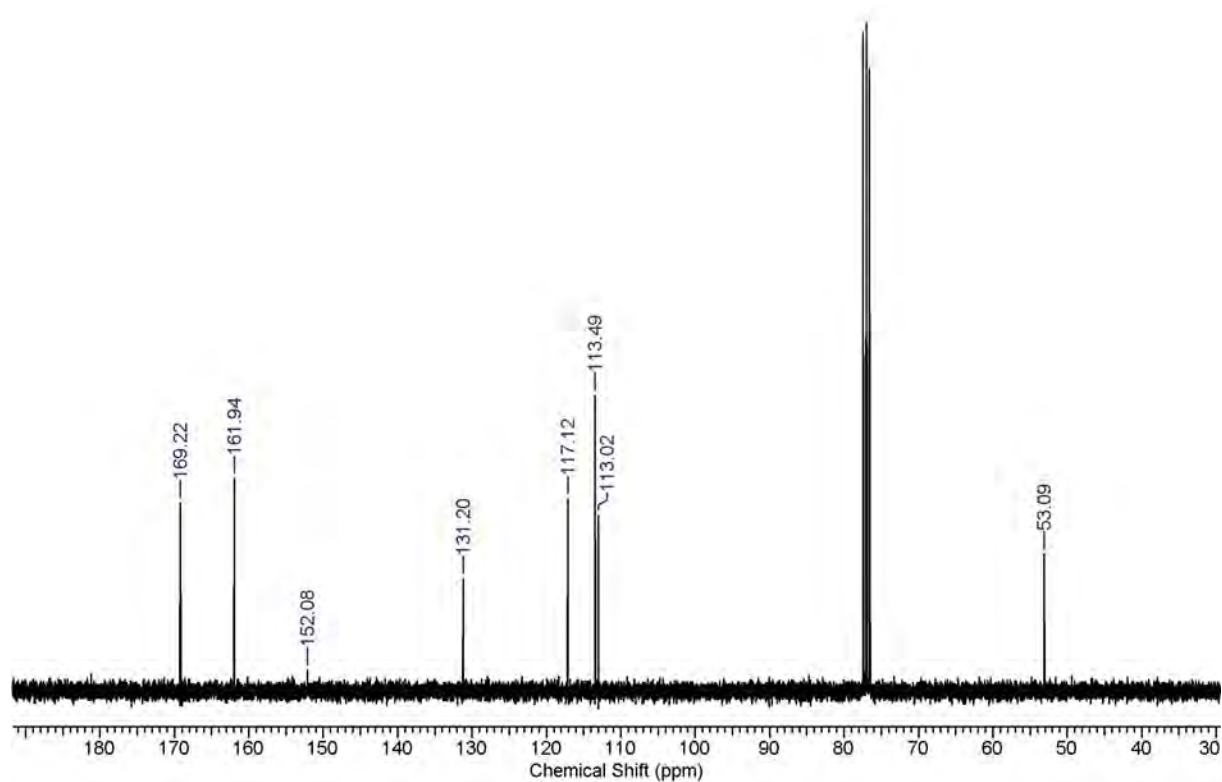


Figure S20. ¹³C NMR spectrum (75 MHz) of **4** in CDCl₃.

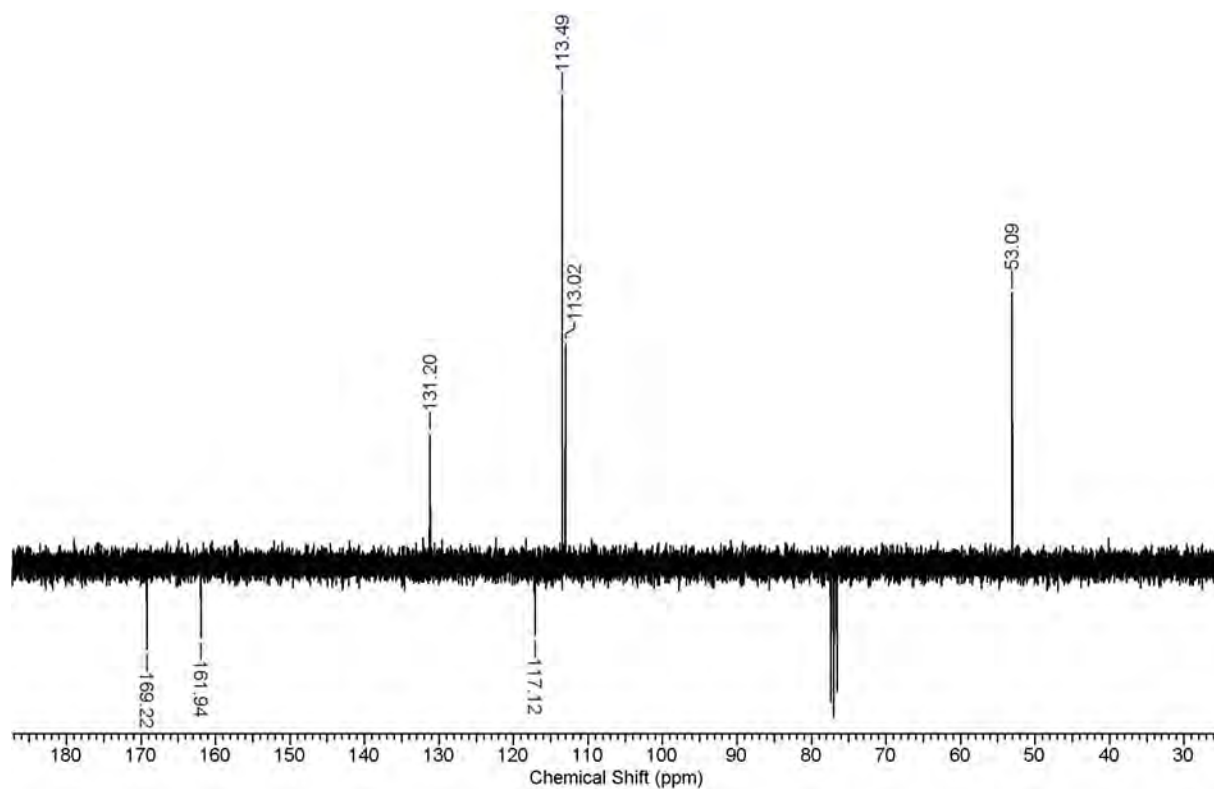


Figure S21. APT spectrum (75 MHz) of **4** in CDCl_3 .

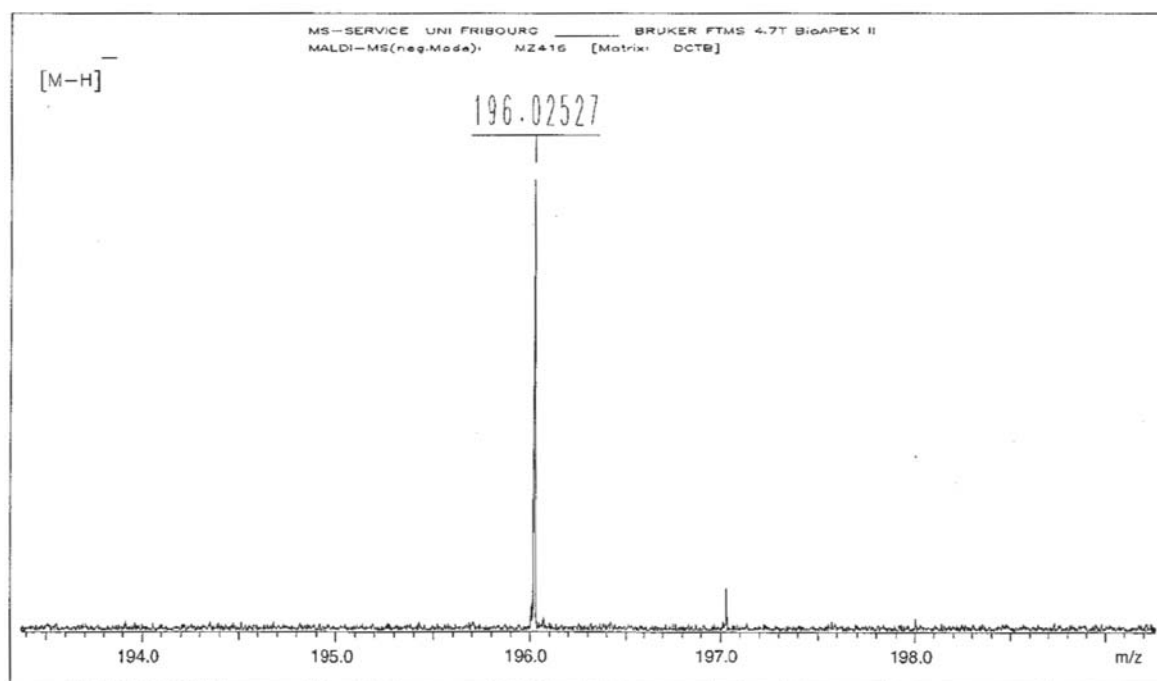


Figure S22. High resolution-mass spectrum of **4** (ESI-).

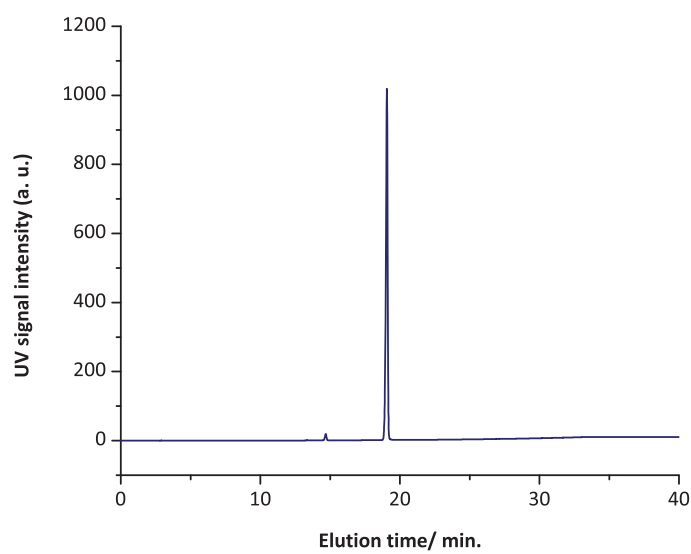


Figure S23. RP-HPLC elugram of **4**.

Triethyleneglycol bromide (5**)**

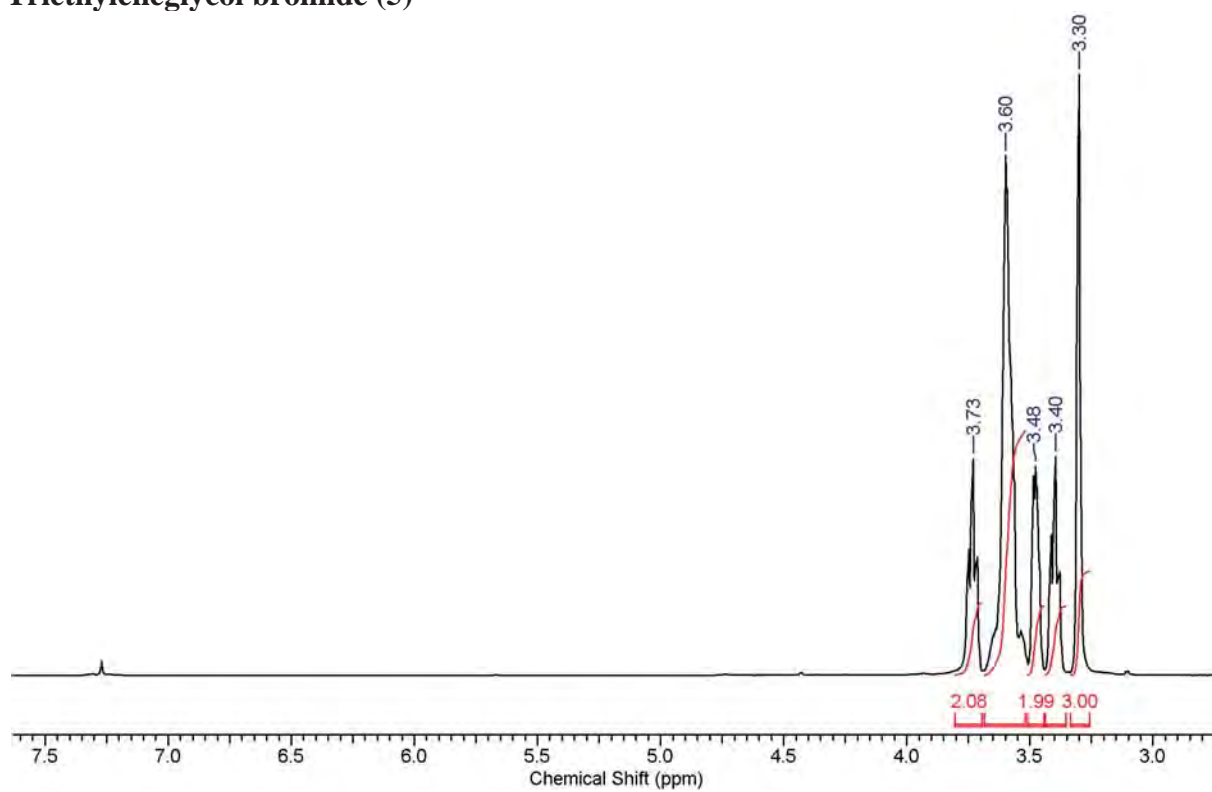


Figure S24. ¹H NMR spectrum (300 MHz) of **5** in CDCl₃.

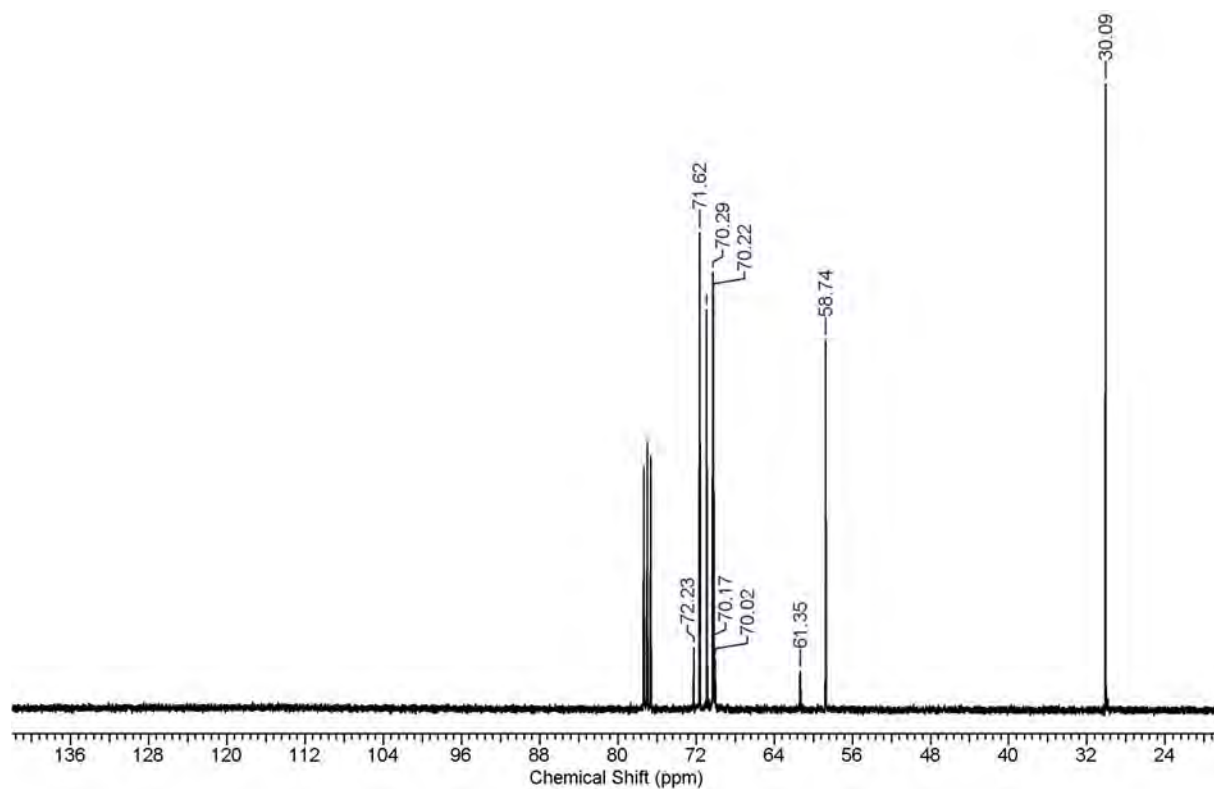


Figure S25. ^{13}C NMR spectrum (75 MHz) of **5** in CDCl_3 .

Methyl-2,5-bis (2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4-nitrobenzoate (**6a**)

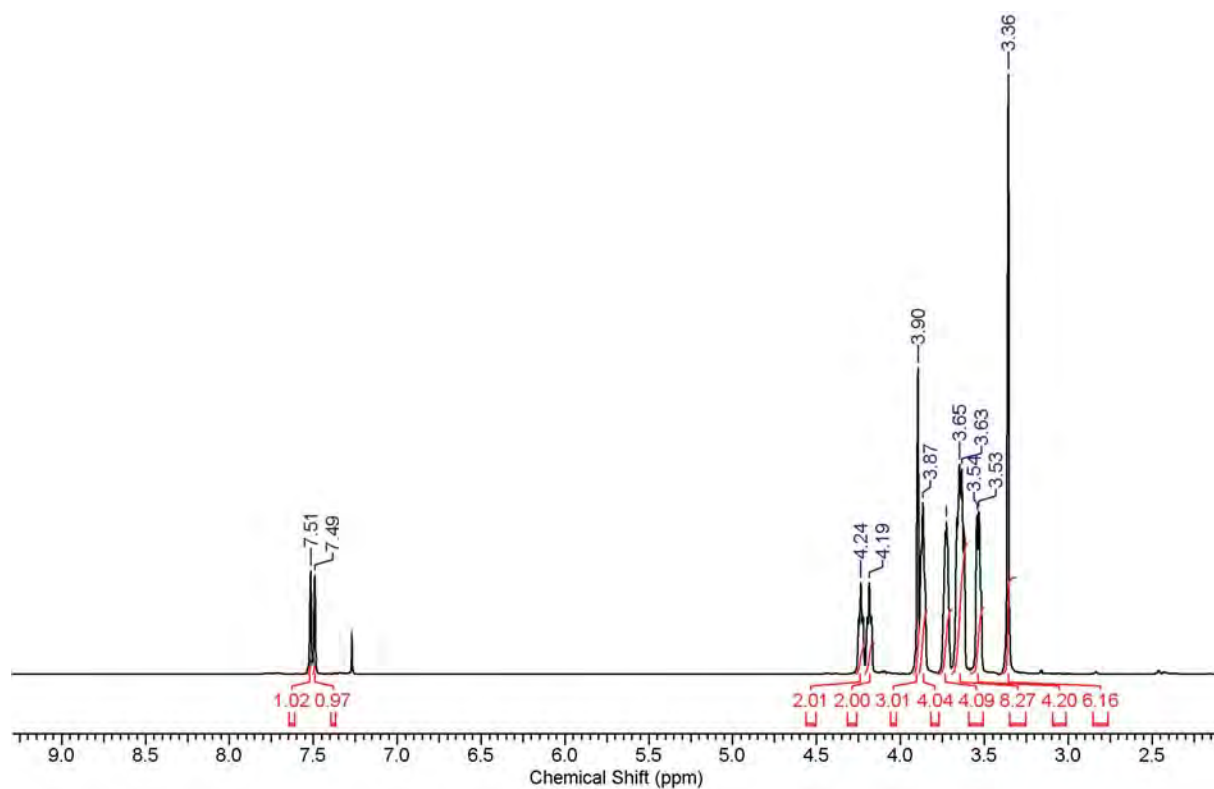


Figure S26. ^1H NMR spectrum (360 MHz) of **6a** in CDCl_3 after purification via column chromatography.

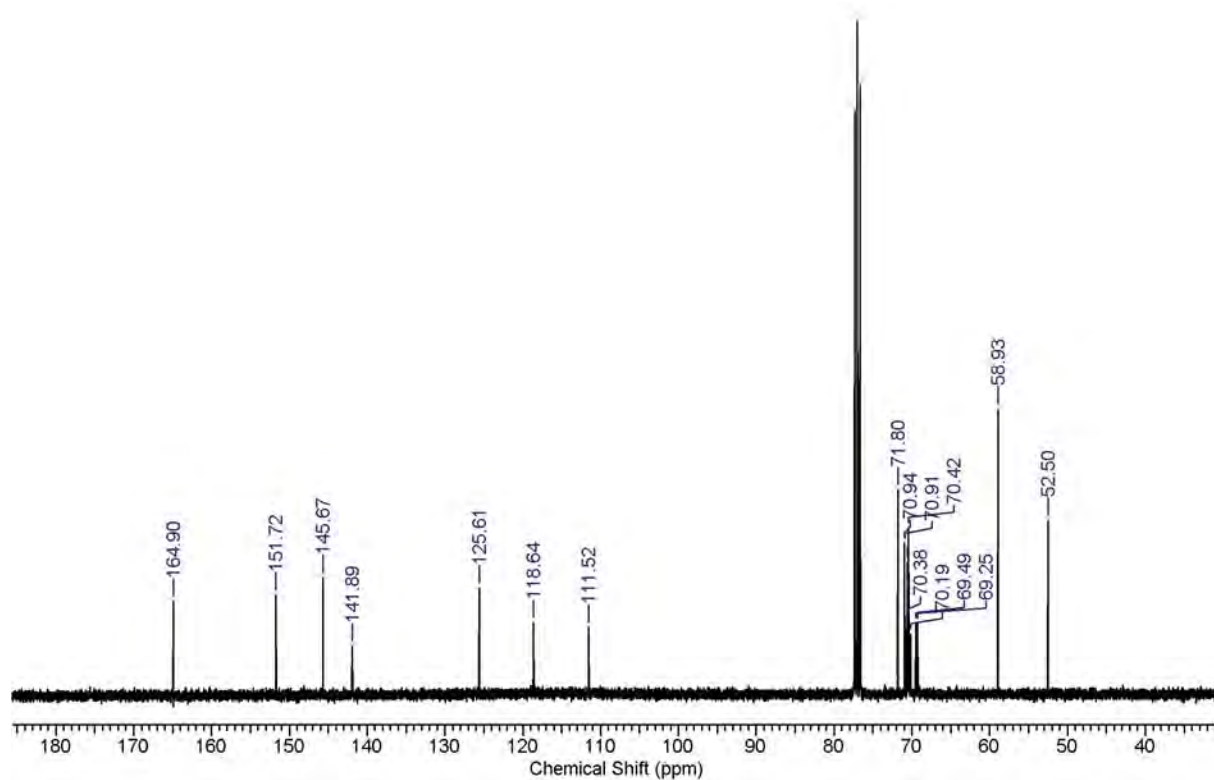


Figure S27. ¹³C NMR spectrum (90 MHz) of **6a** in CDCl₃ after purification via column chromatography.

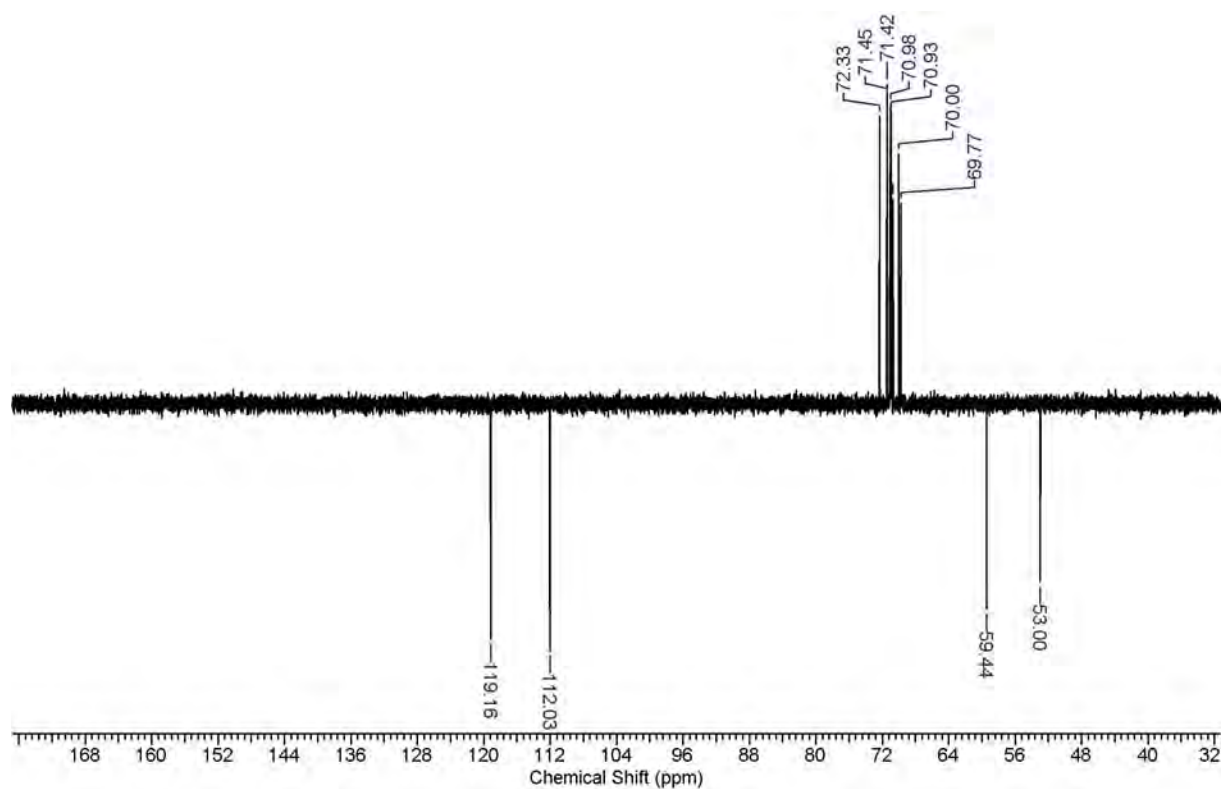


Figure S28. DEPT spectrum (90 MHz) of **6a** in CDCl₃ after purification via column chromatography.

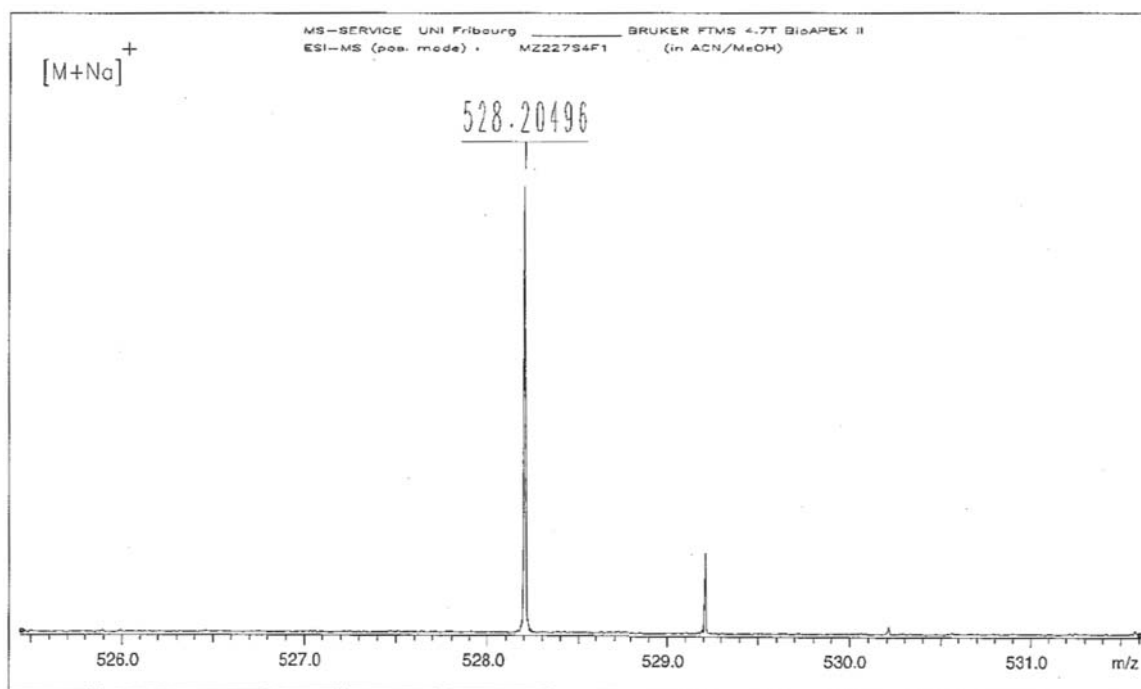


Figure S29. High resolution-mass spectrum of **6a** (ESI+) after purification *via* column chromatography.

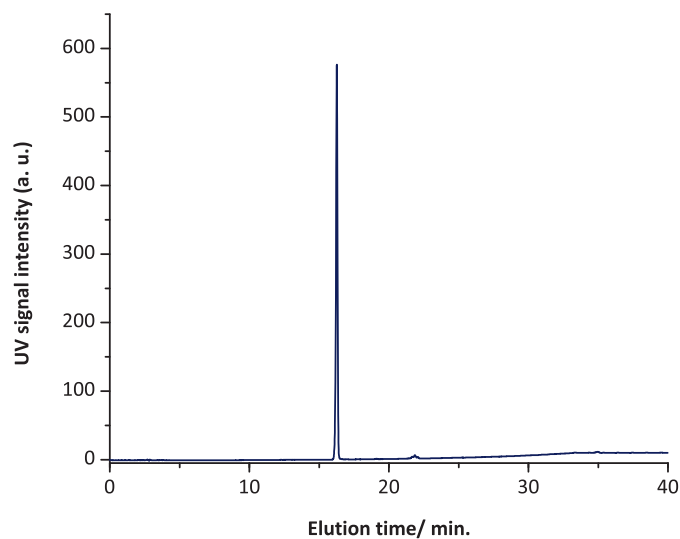


Figure S30. RP-HPLC elugram of **6a** after purification *via* column chromatography.

Methyl 2-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4-nitrobenzoate (**6b**)

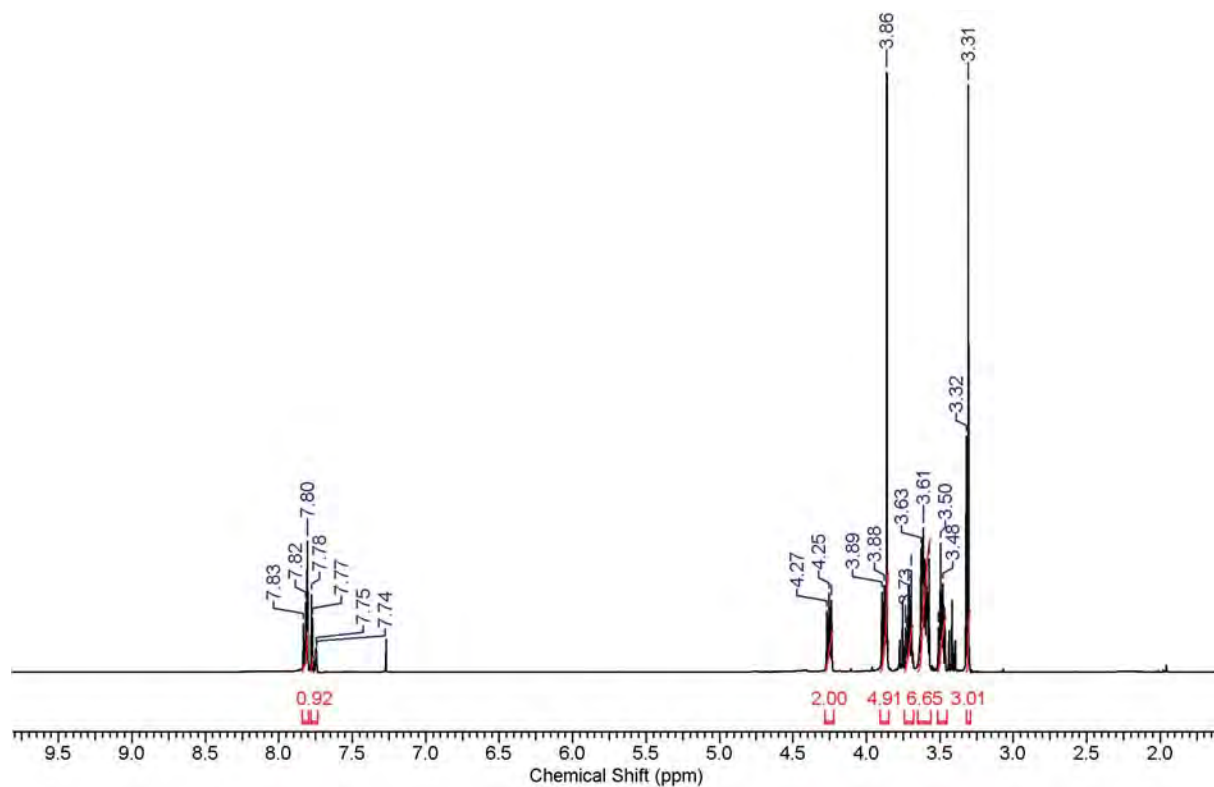


Figure S31. ¹H NMR spectrum (300 MHz) of **6b** in CDCl₃ after purification via column chromatography.

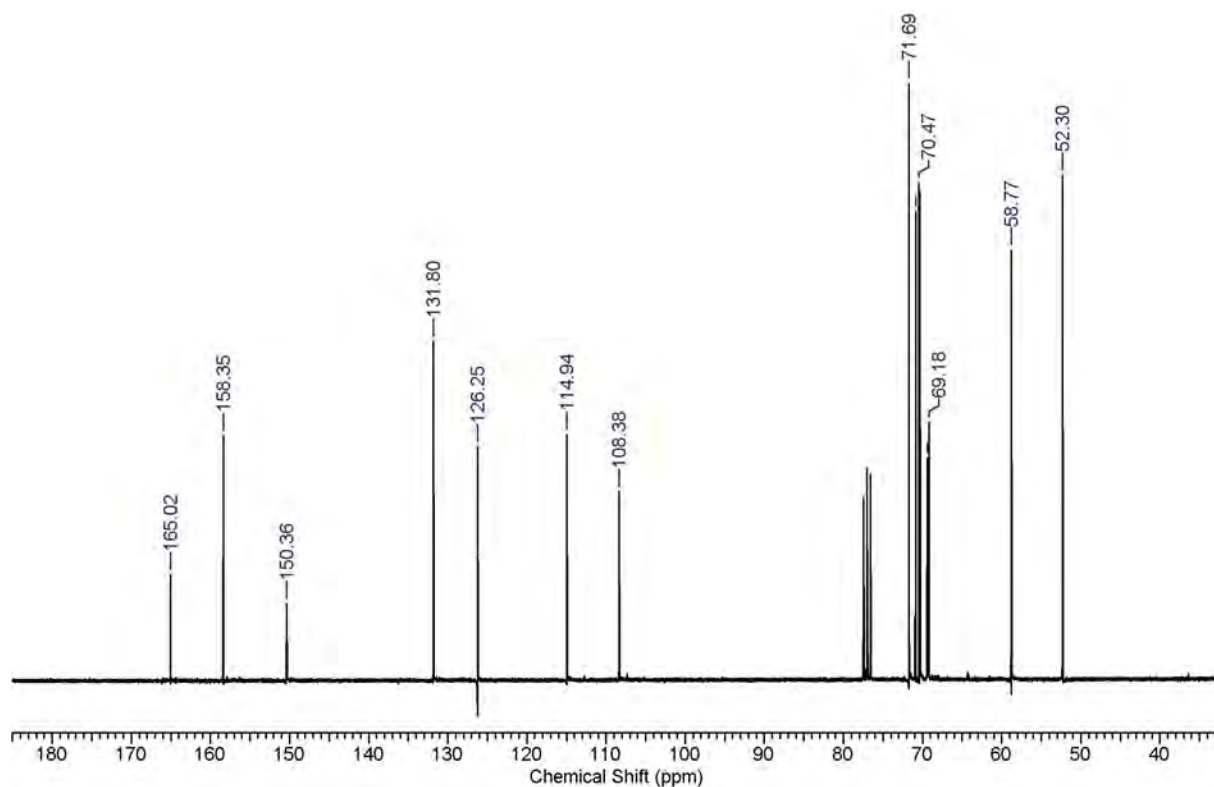


Figure S32. ¹³C NMR spectrum (75 MHz) of **6b** in CDCl₃ after purification via column chromatography.

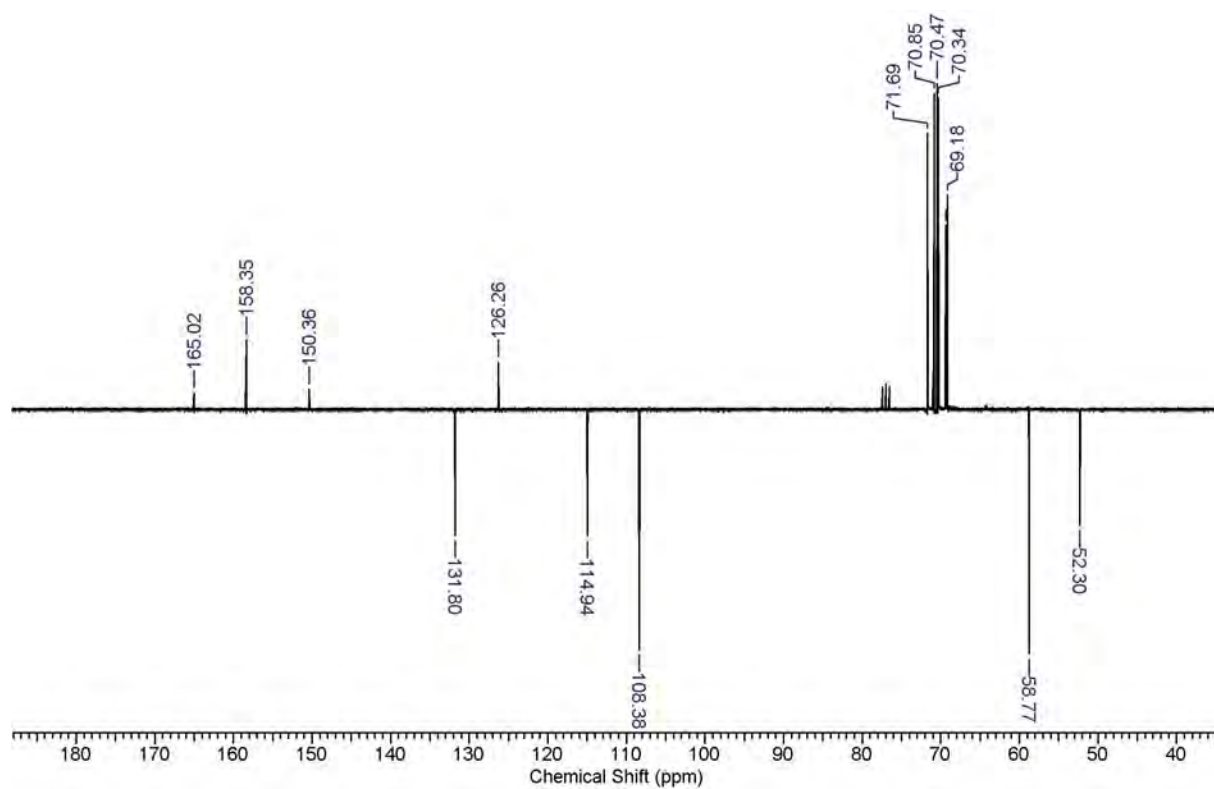


Figure S33. APT spectrum (75 MHz) of **6b** in CDCl_3 after purification *via* column chromatography.

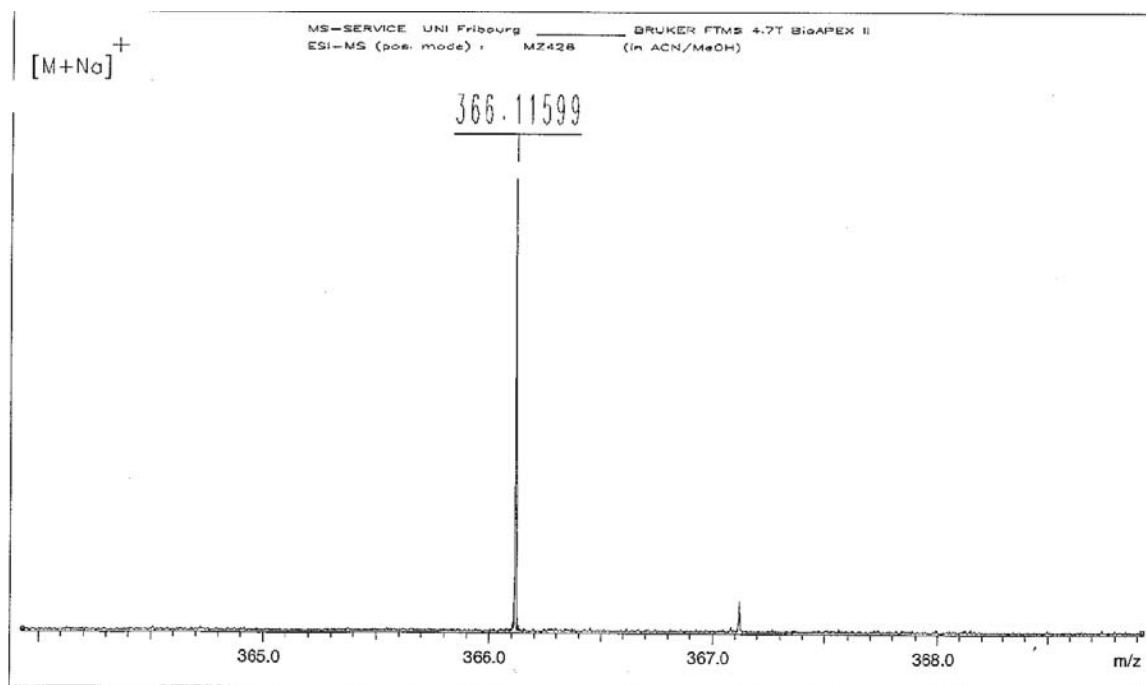


Figure S34. High resolution-mass spectrum of **6b** (ESI^+) after purification *via* column chromatography.

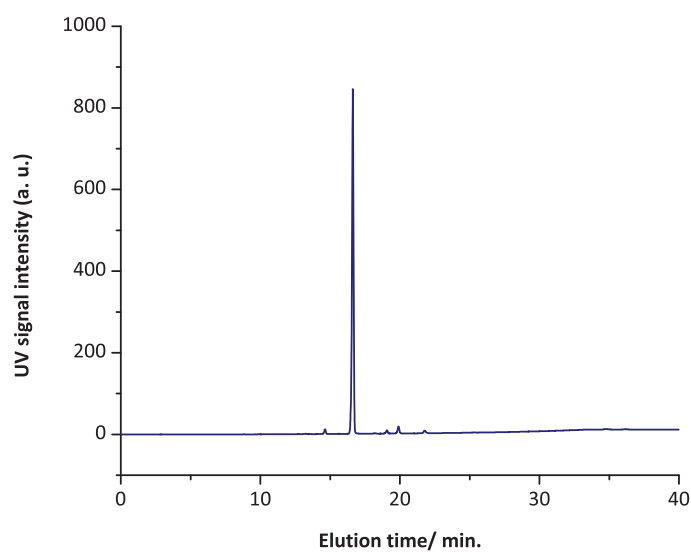


Figure S35. RP-HPLC elugram of **6b** after purification *via* column chromatography.

2,5-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4-nitrobenzoic acid (7a**)**

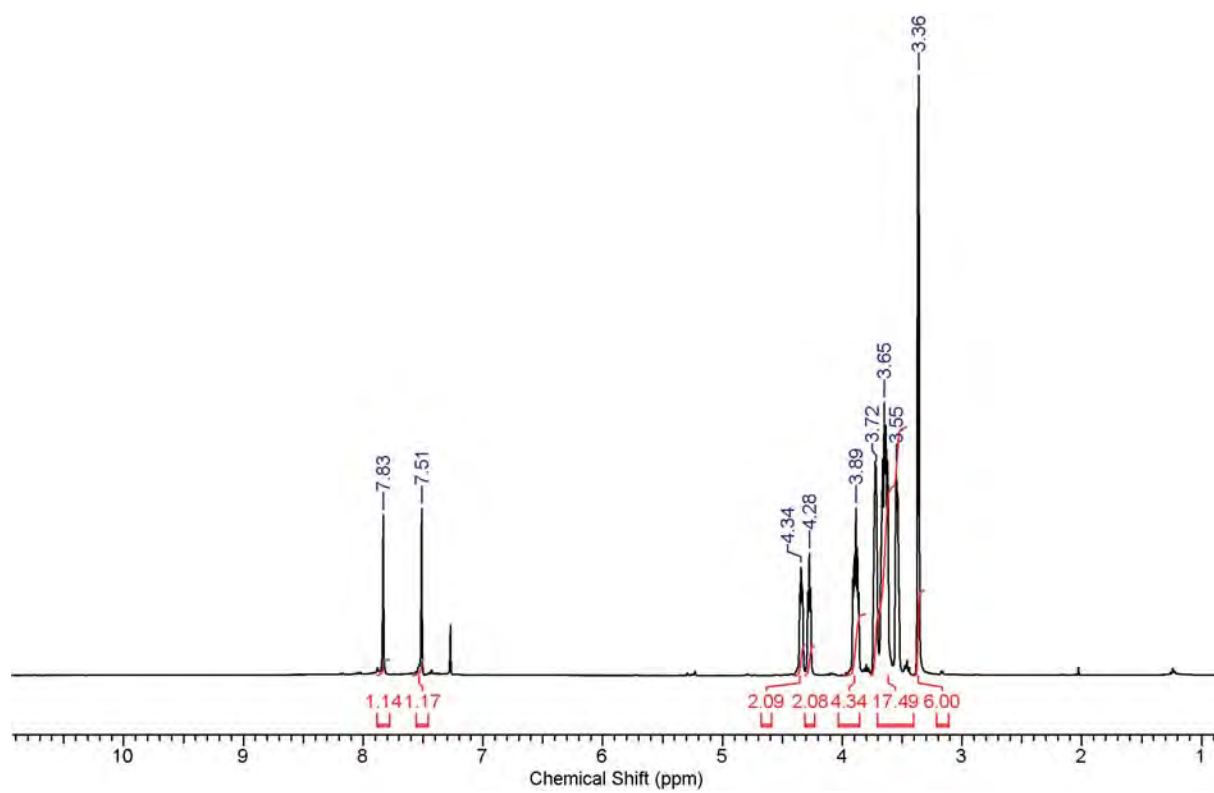


Figure S36. ¹H NMR spectrum (360 MHz) of **7a** in CDCl₃.

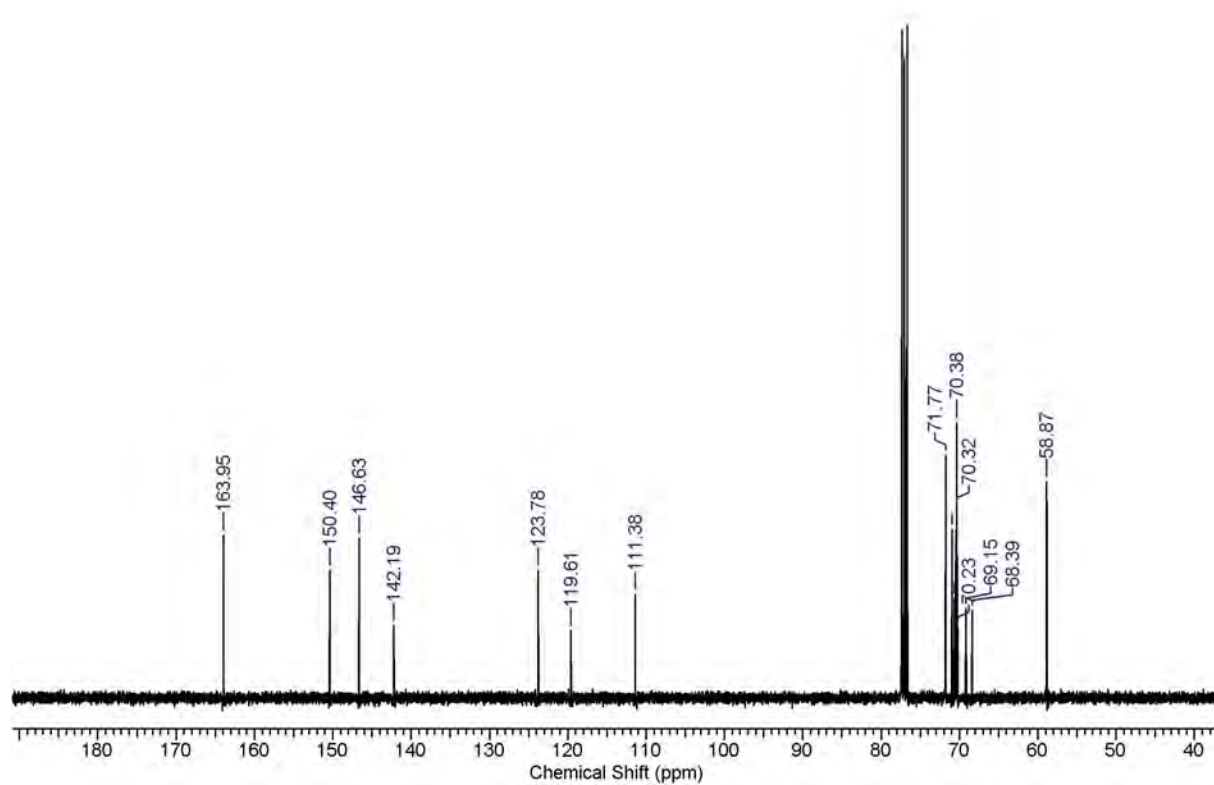


Figure S37. ^{13}C NMR spectrum (90 MHz) of **7a** in CDCl_3 .

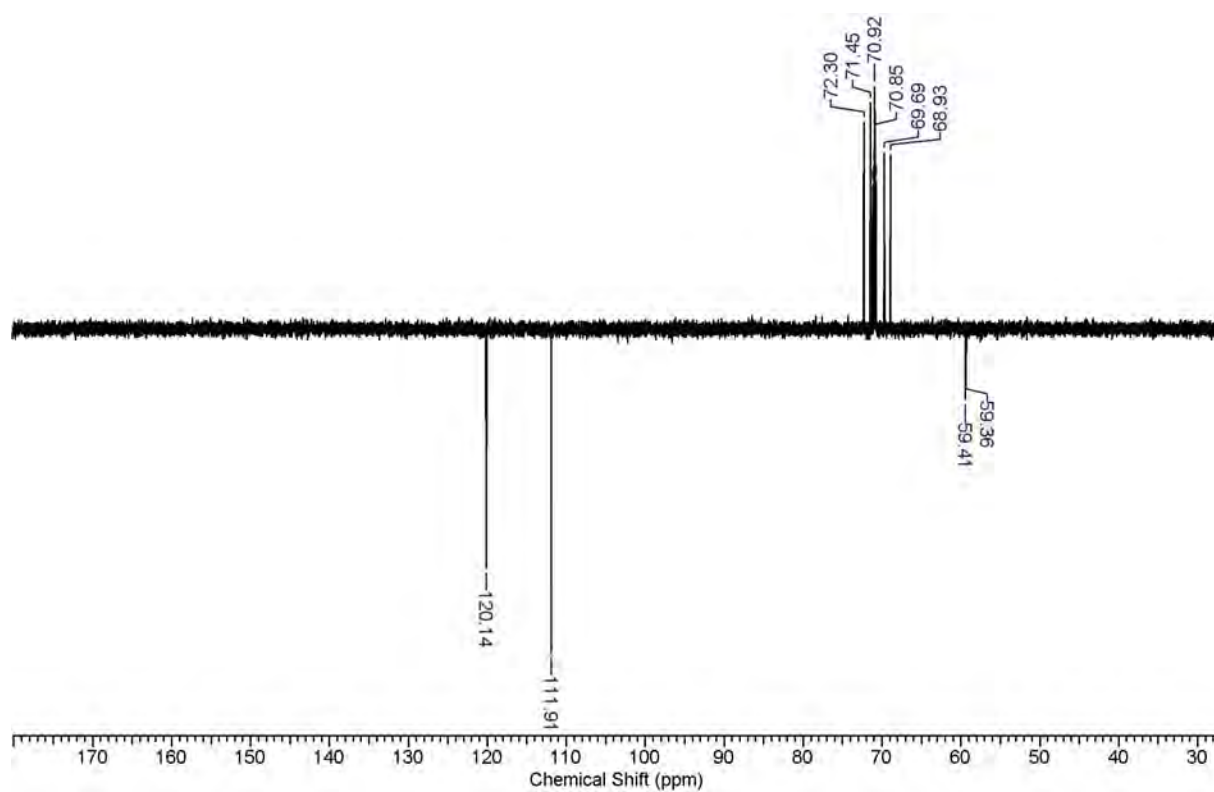


Figure S38. DEPT spectrum (360 MHz) of **7a** in CDCl_3 .

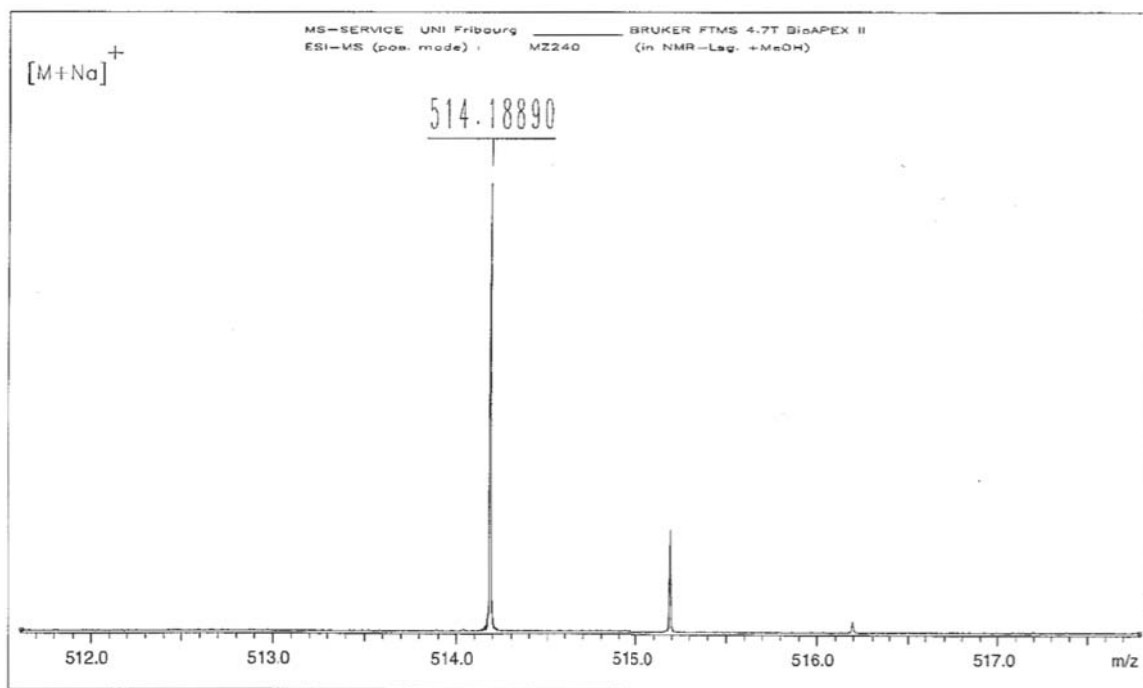


Figure S39. High resolution-mass spectrum of **7a** (ESI+).

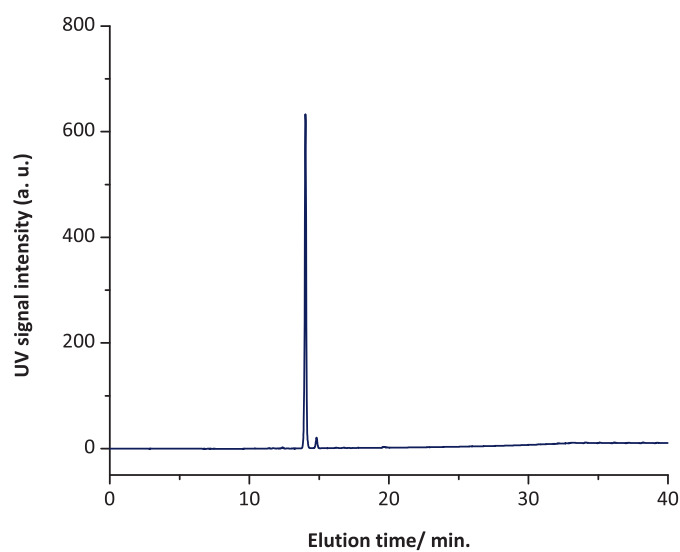


Figure S40. RP-HPLC elugram of **7a**.

2-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4-nitrobenzoic acid (**7b**)

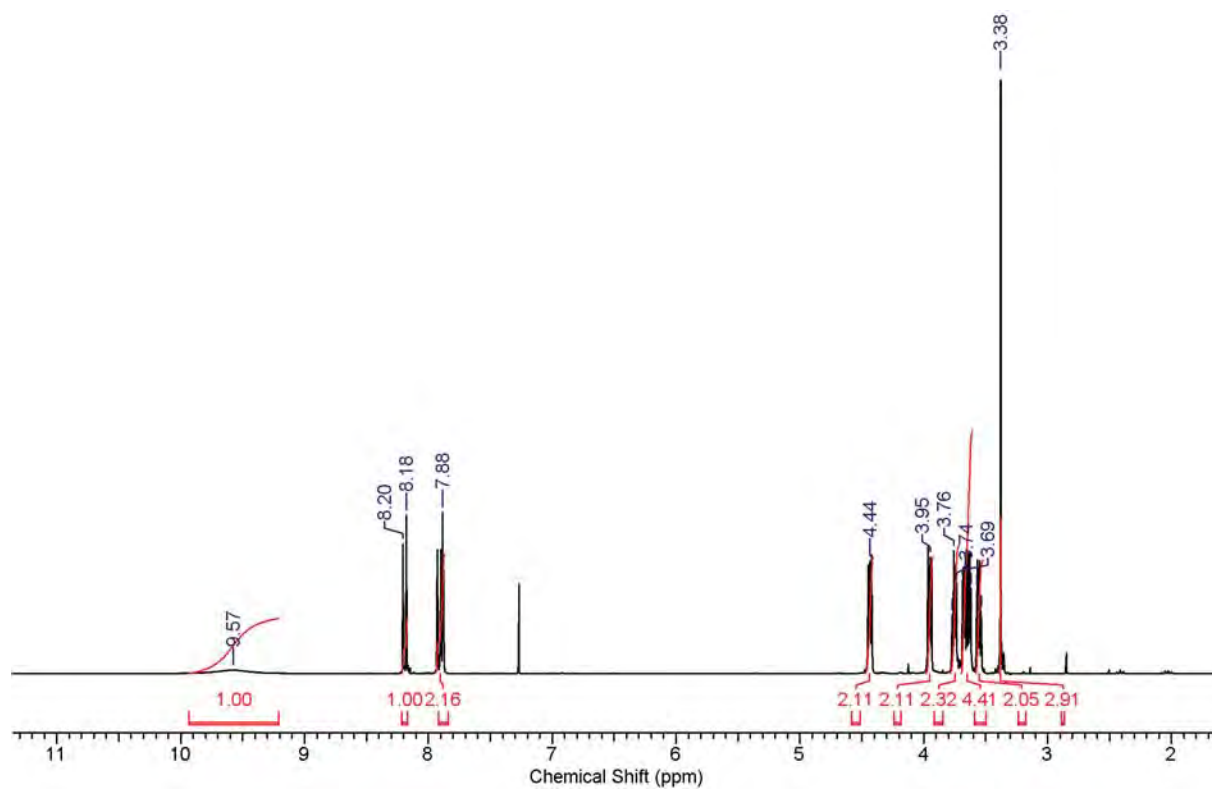


Figure S41. ¹H NMR spectrum (300 MHz) of **7b** in CDCl₃.

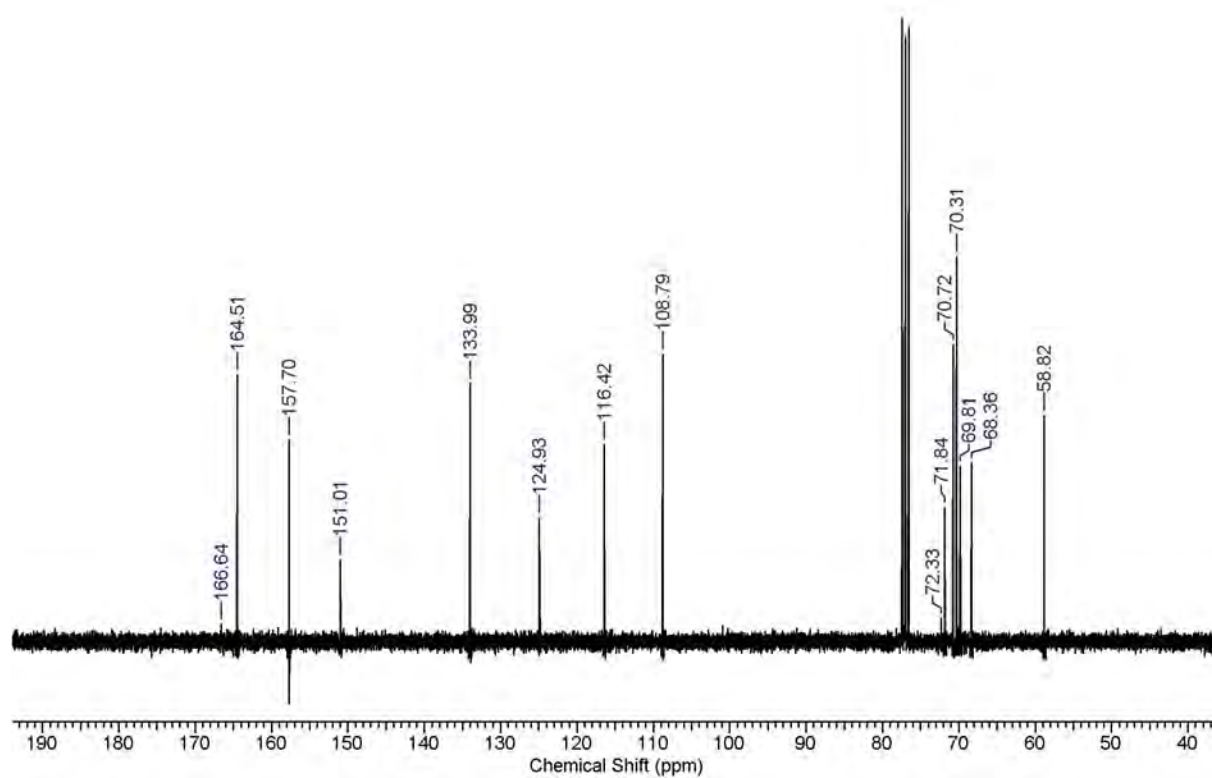


Figure S42. ¹³C NMR spectrum (75 MHz) of **7b** in CDCl₃.

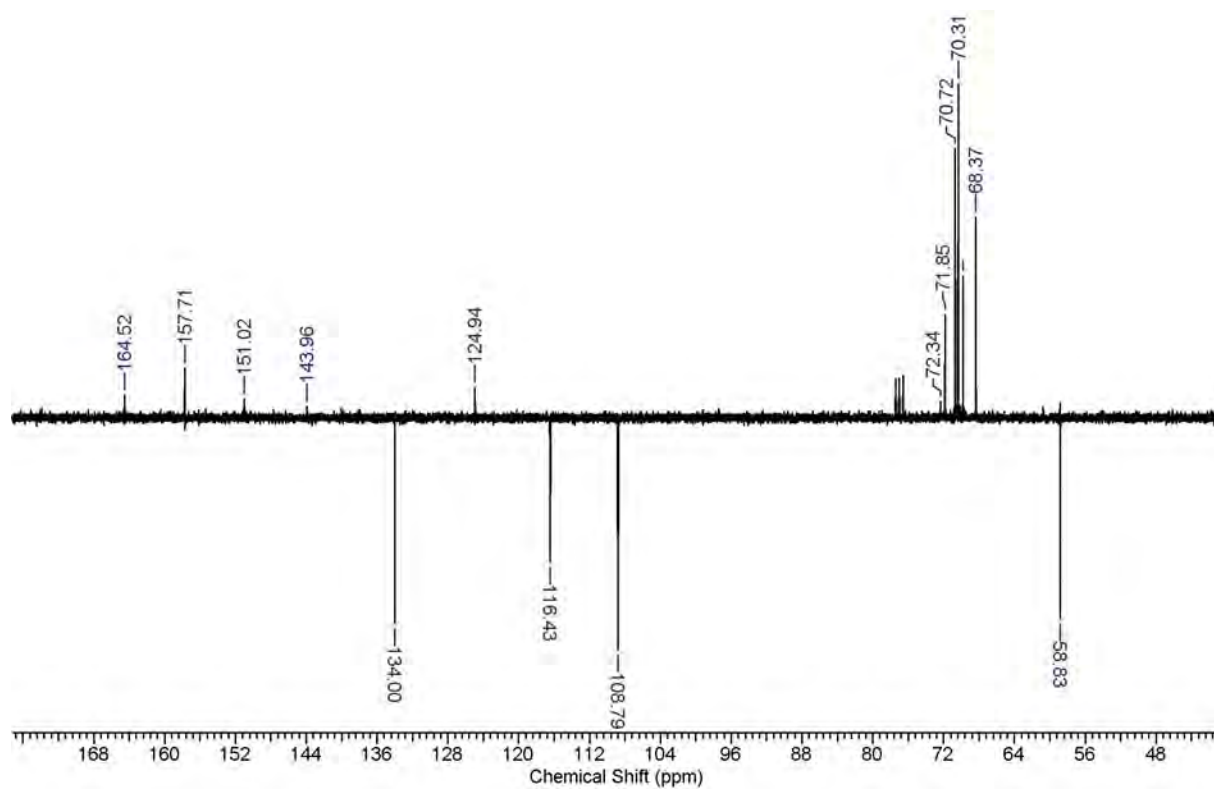


Figure S43. APT spectrum (75 MHz) of **7b** in CDCl_3 .

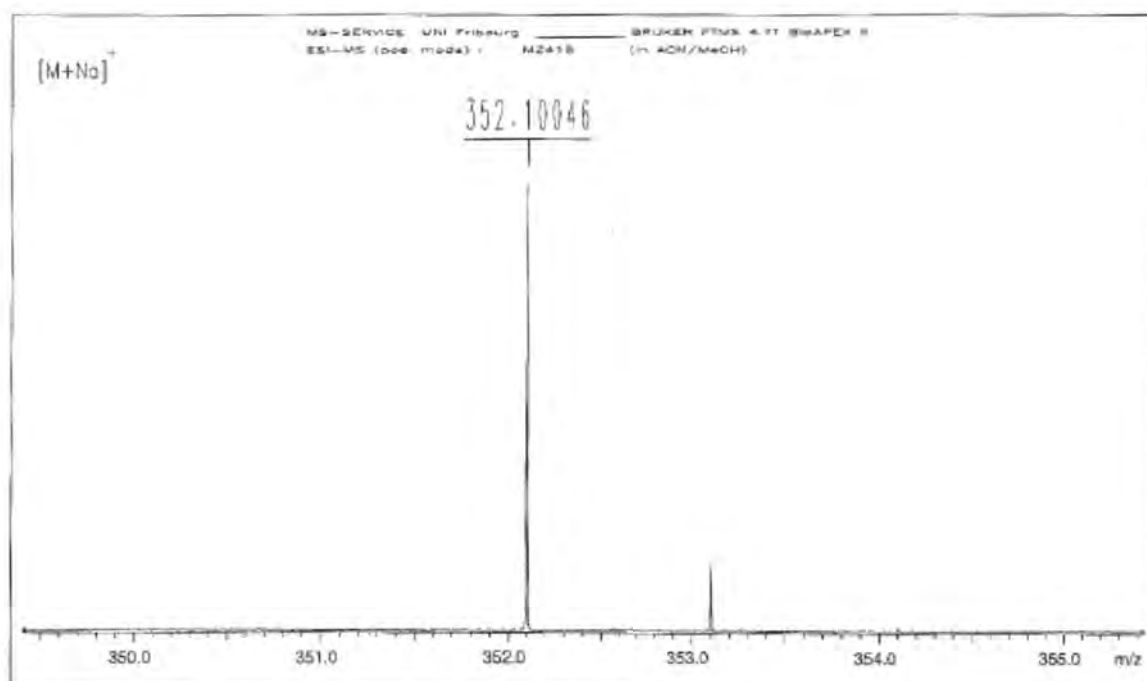


Figure S44. High resolution-mass spectrum of **7b** (ESI+).

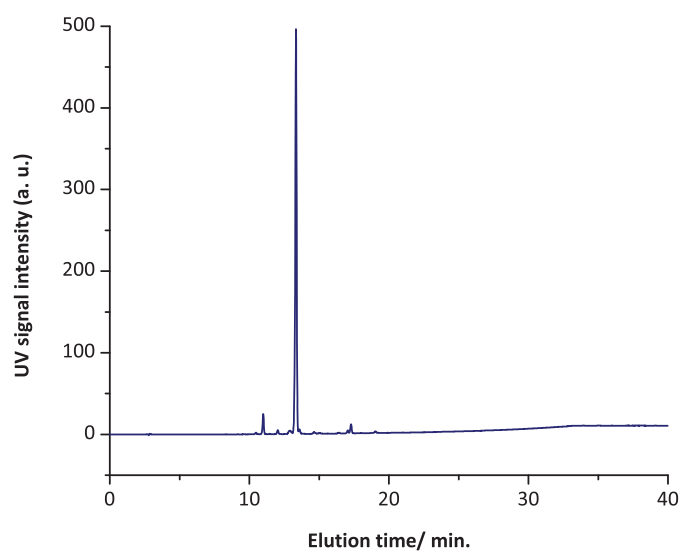


Figure S45. RP-HPLC elugram of **7b**.

Phenyl 2,5-bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4-nitrobenzoate (**8a**)

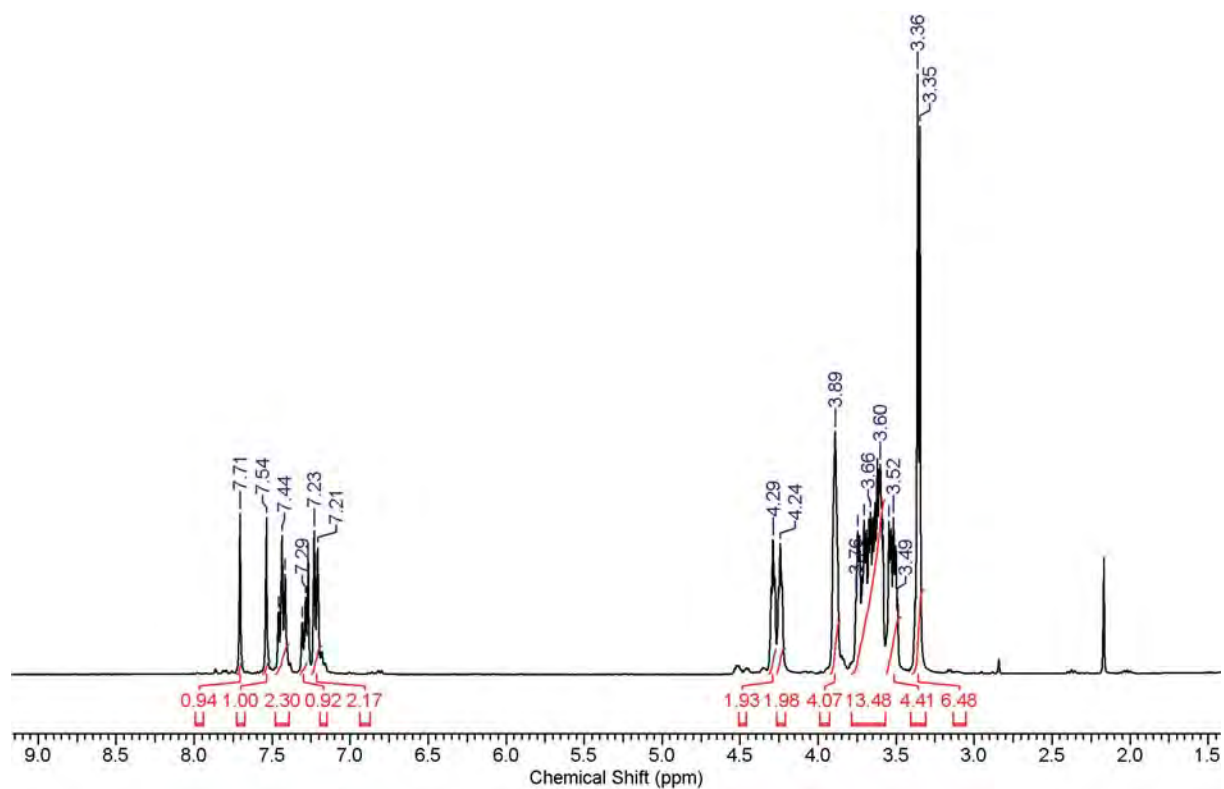


Figure S46. ¹H NMR spectrum (360 MHz) of **8a** in CDCl₃.

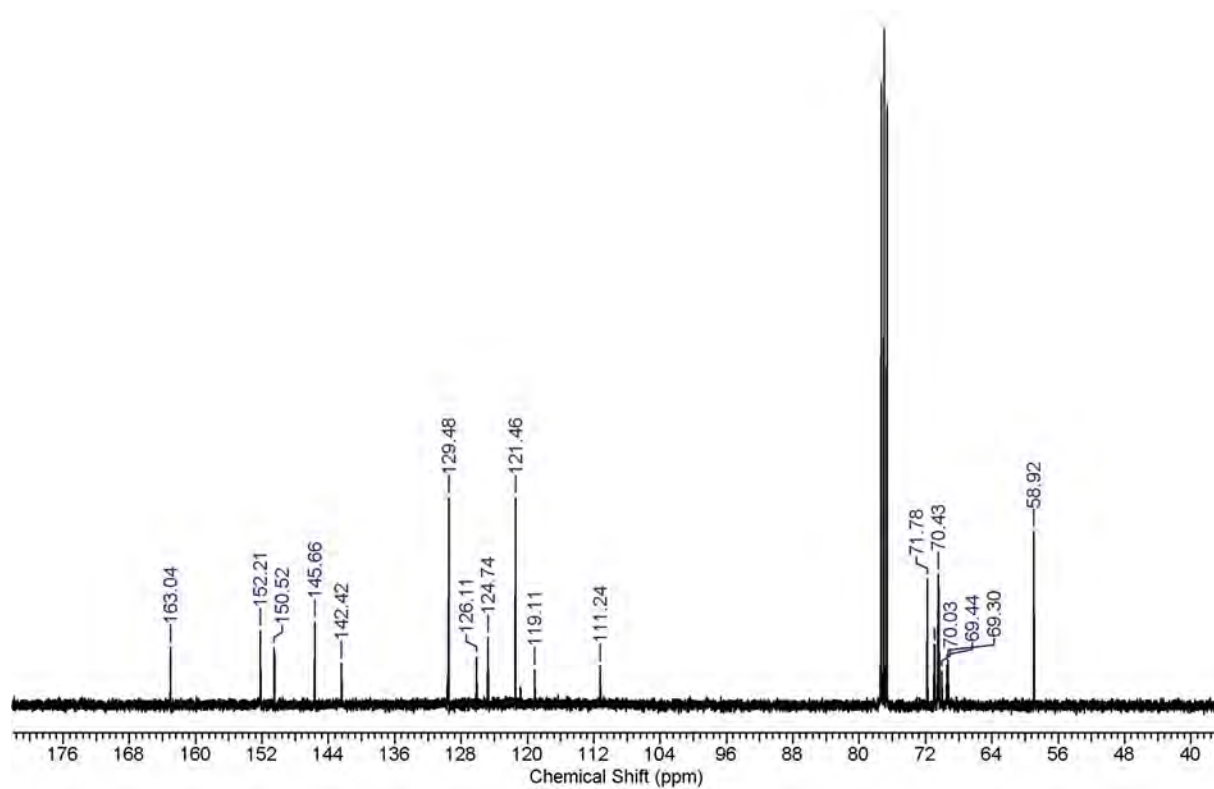


Figure S47. ¹³C NMR spectrum (90 MHz) of **8a** in CDCl₃.

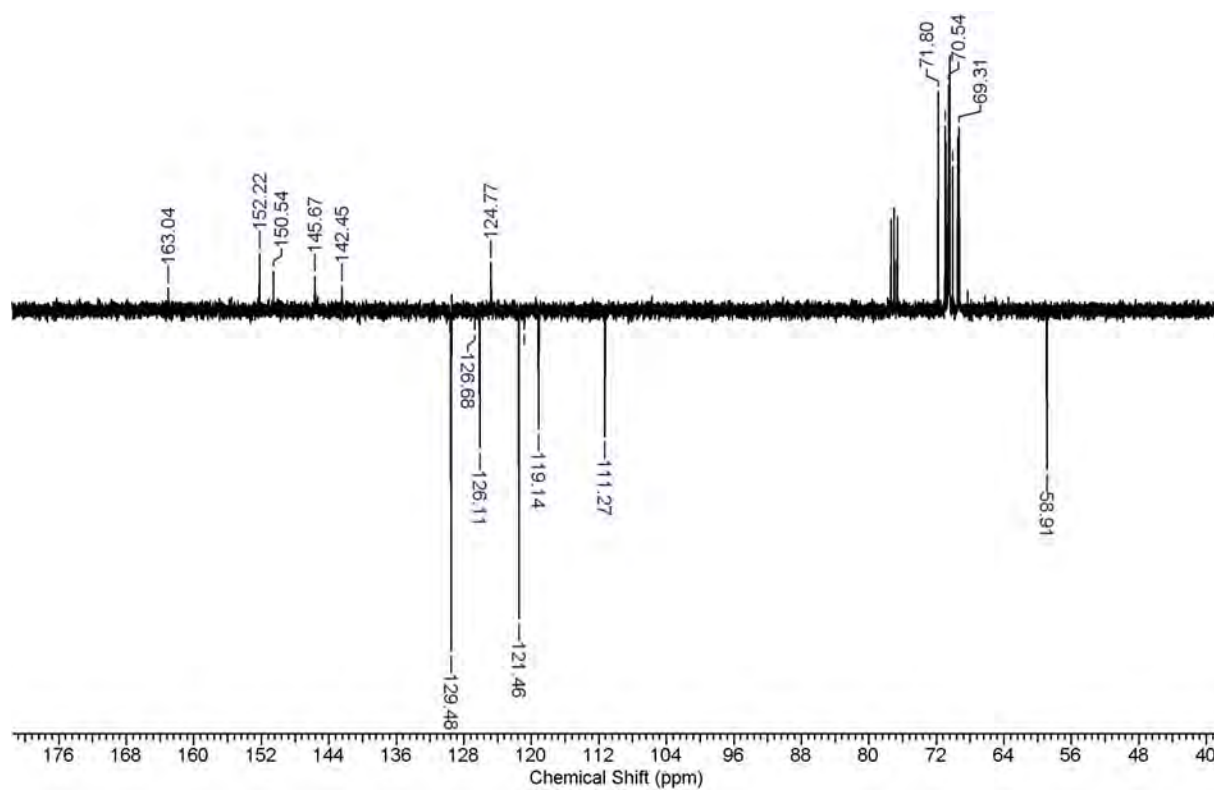


Figure S48. APT spectrum (90 MHz) of **8a** in CDCl₃.

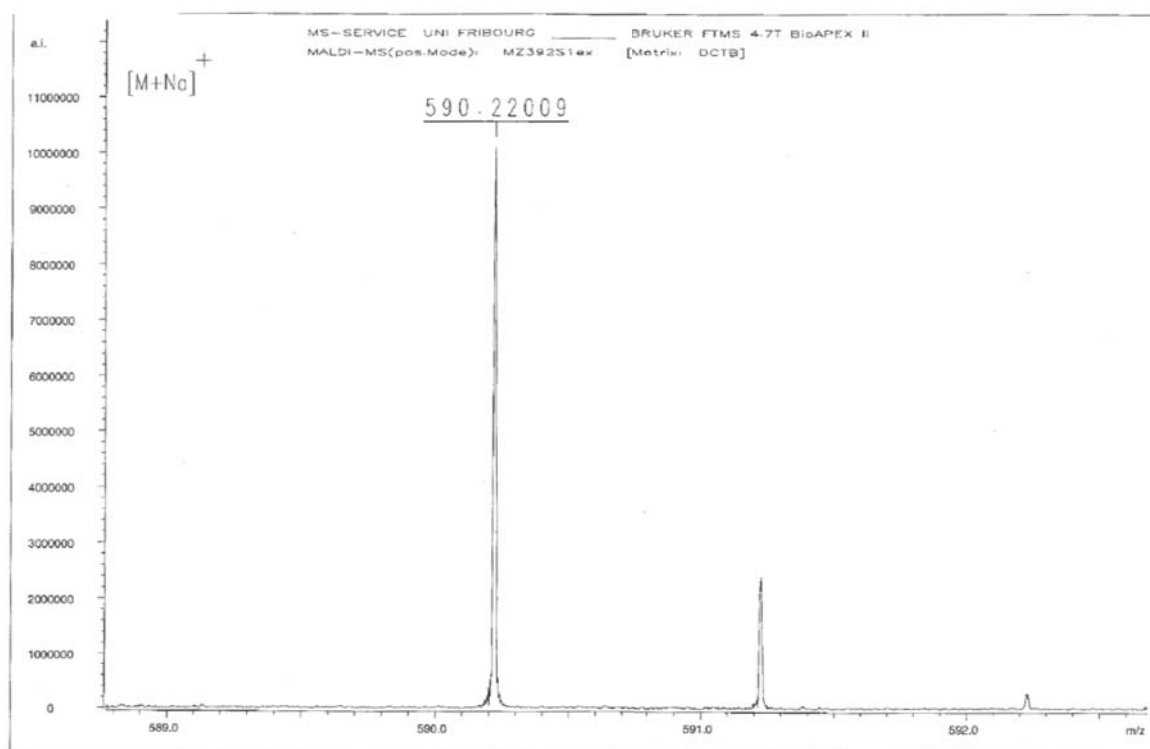


Figure S49. High resolution-mass spectrum of **8a** (ESI+).

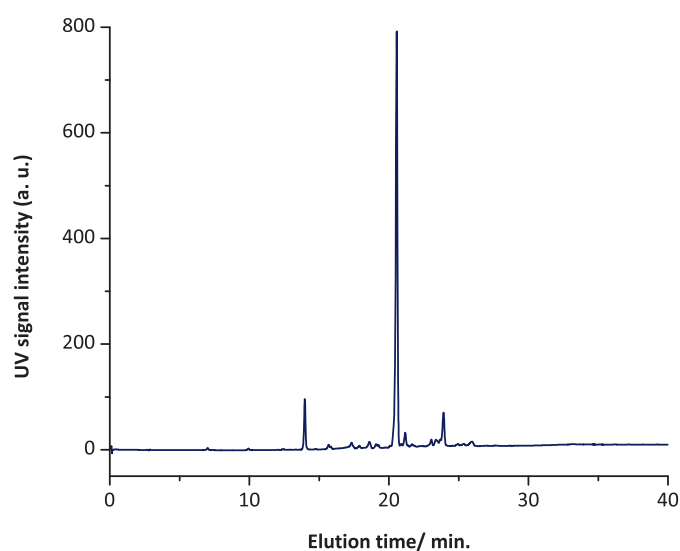


Figure S50. RP-HPLC elugram of crude **8a**.

Phenyl 2-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4-nitrobenzoate (**8b**)

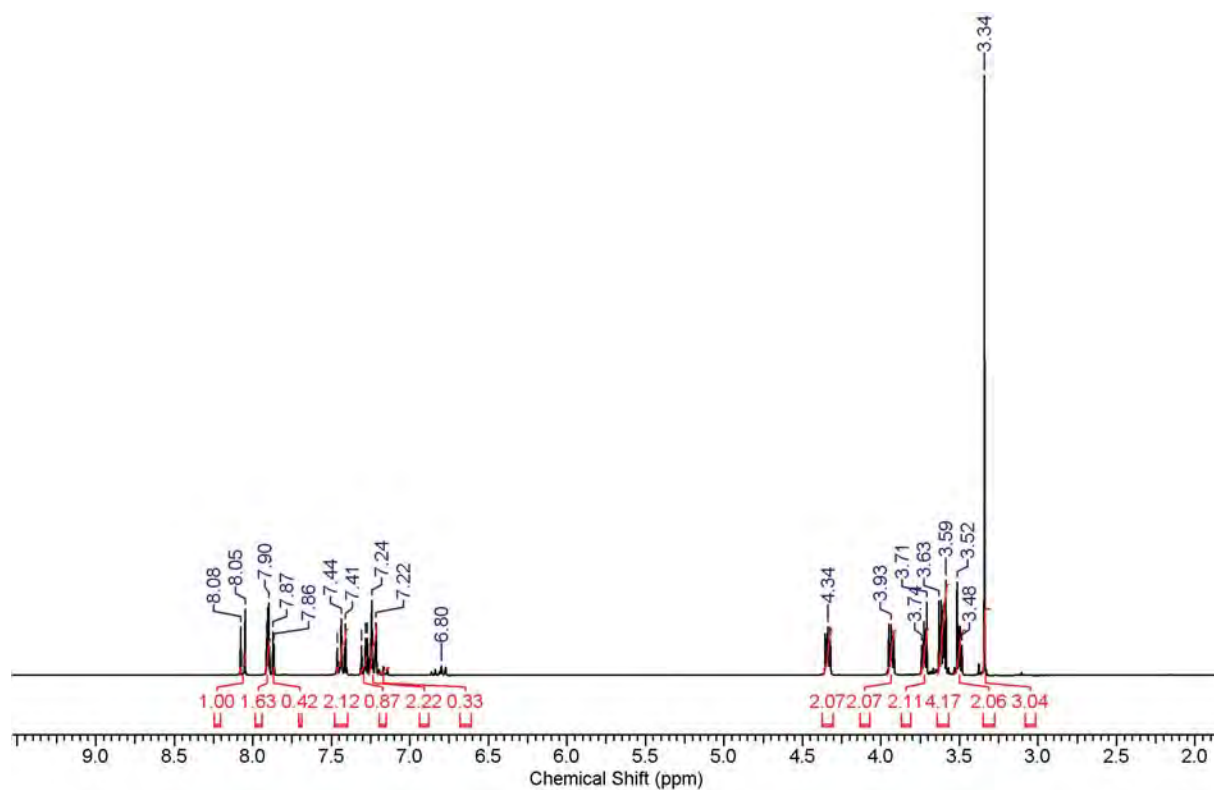


Figure S51. ¹H NMR spectrum (300 MHz) of **8b** in CDCl₃.

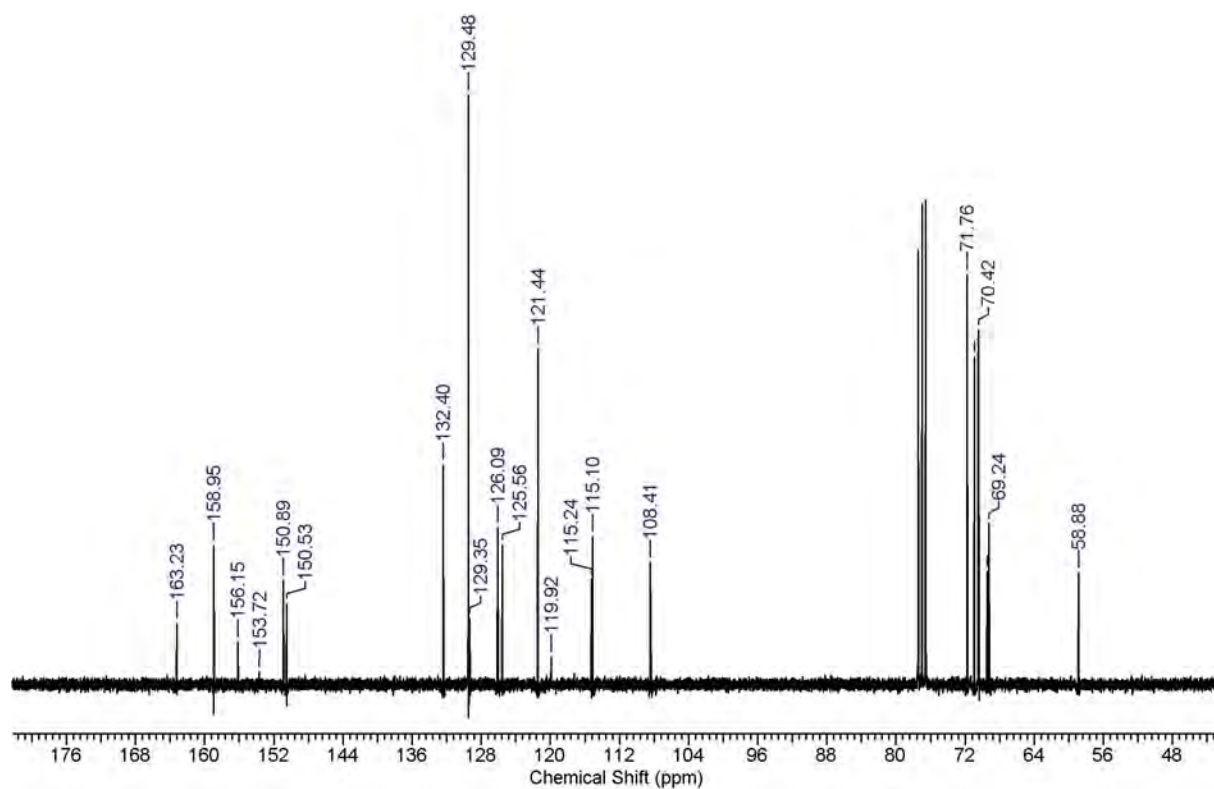


Figure S52. ¹³C NMR spectrum (75 MHz) of **8b** in CDCl₃.

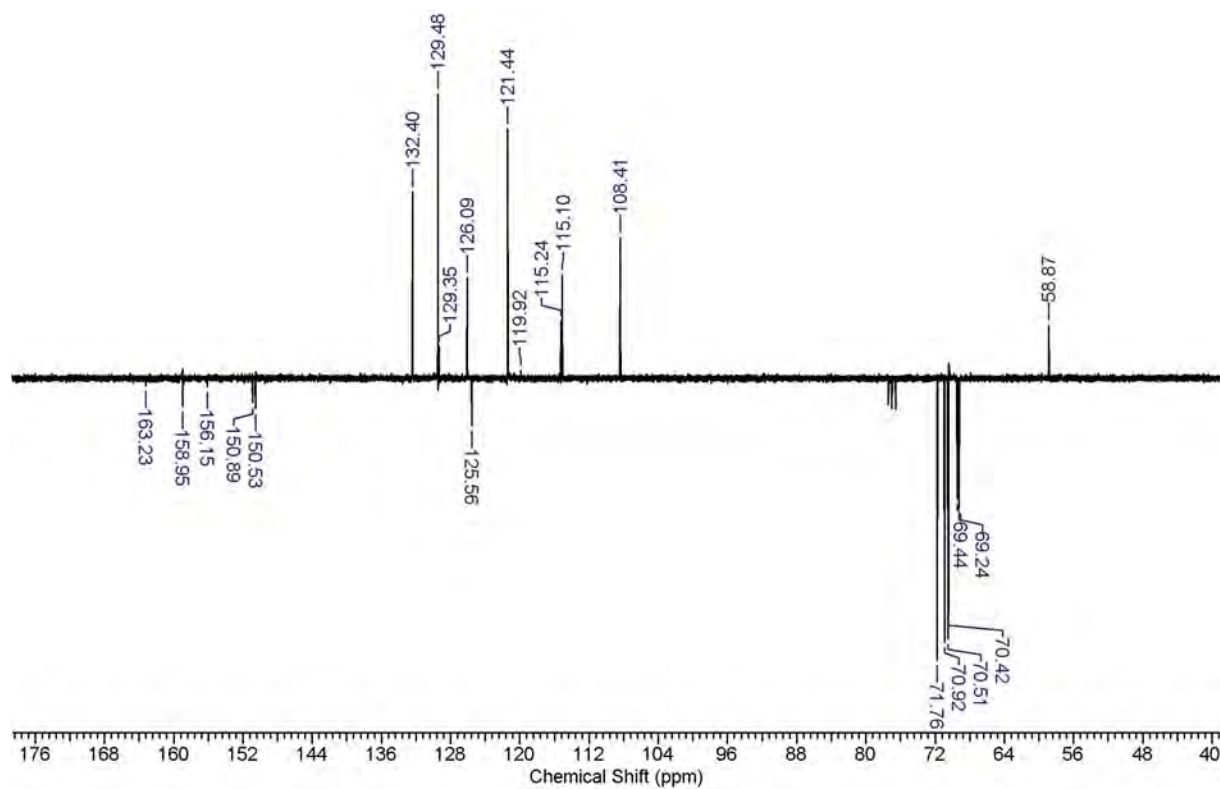


Figure S53. APT NMR spectrum (75 MHz) of **8b** in CDCl_3 .

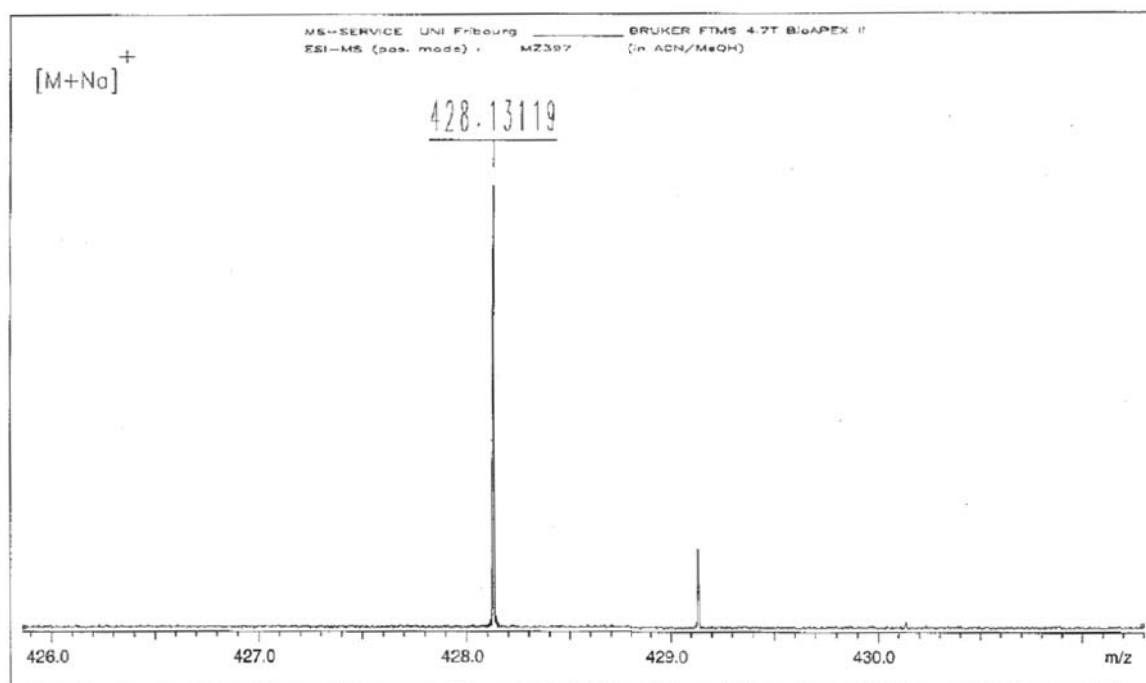


Figure S54. High resolution-mass spectrum of **8a** (ESI+).

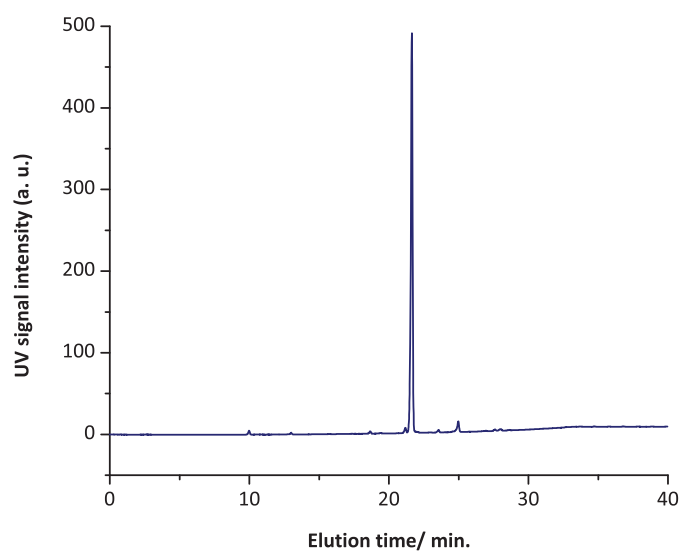


Figure S55. RP-HPLC elugram of crude **8b**.

Phenyl 4-amino-2,5-bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzoate (**9a**)

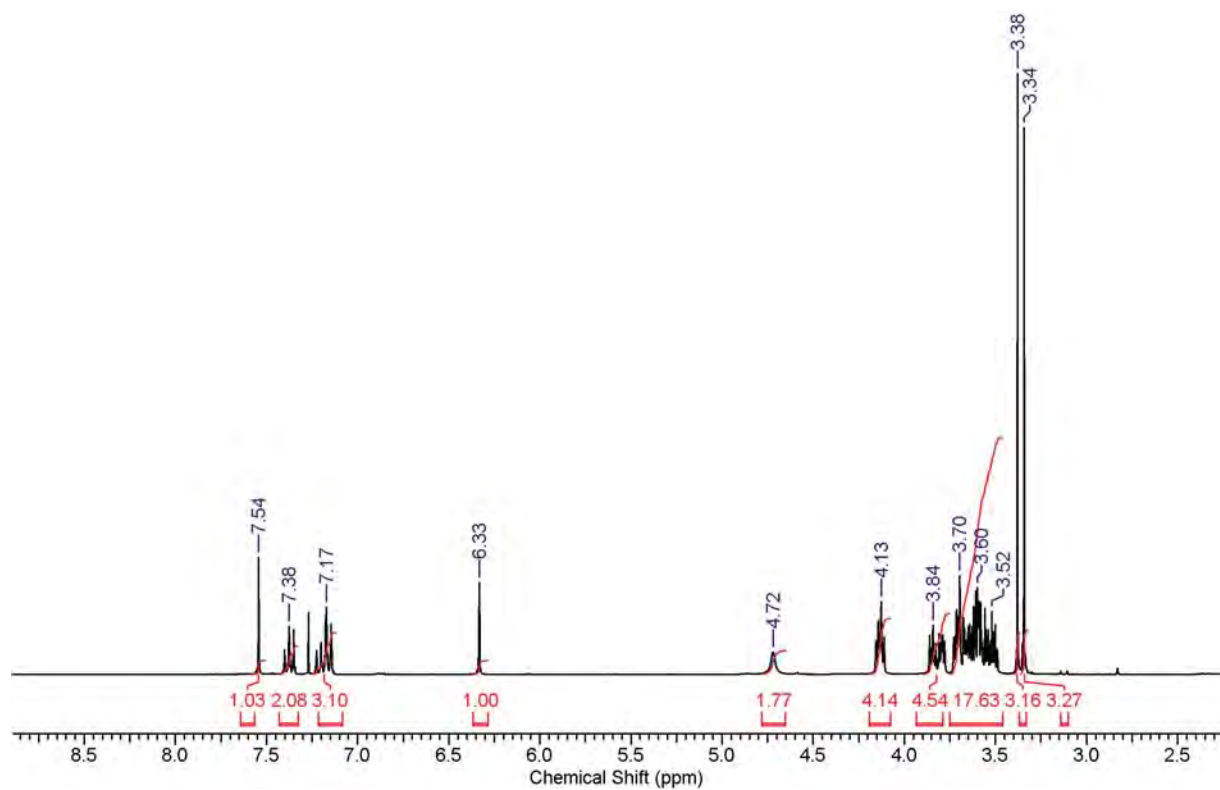


Figure S56. ¹H NMR spectrum (300 MHz) of **9a** in CDCl₃ after purification *via* recycling HPLC.

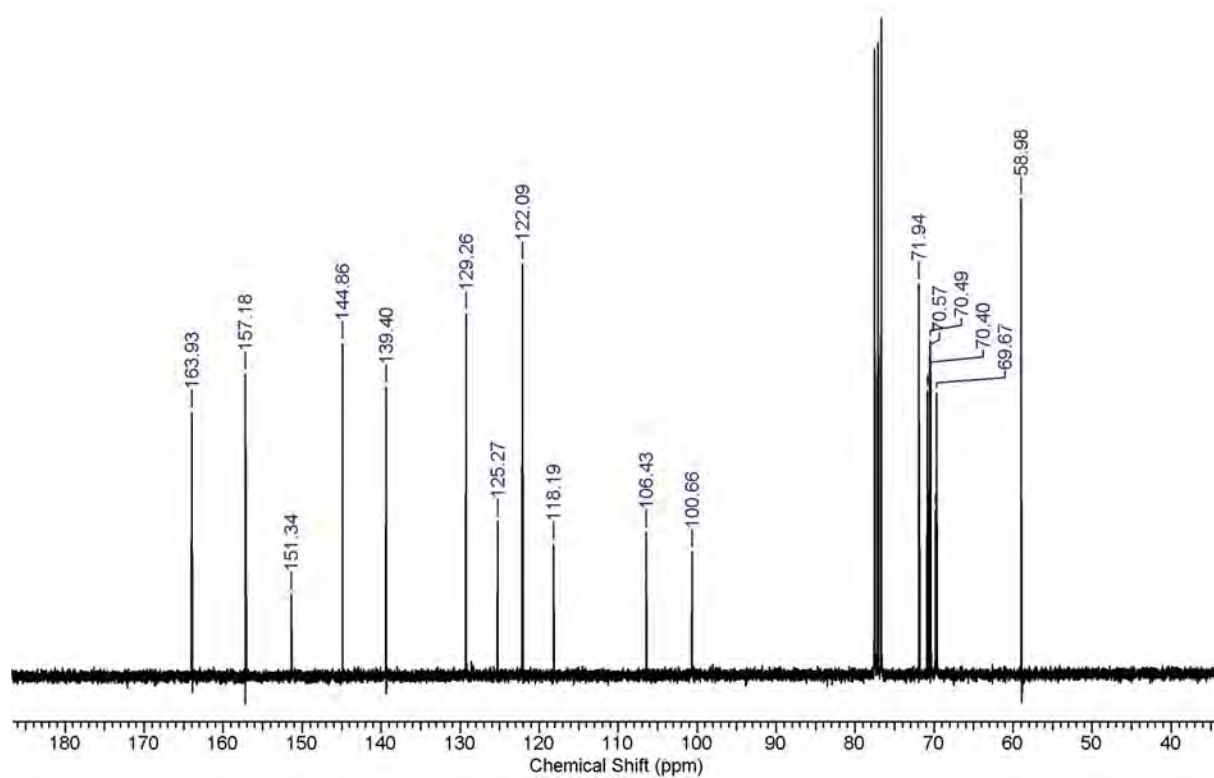


Figure S57. ¹³C NMR spectrum (75 MHz) of **9a** in CDCl₃ after purification *via* recycling HPLC.

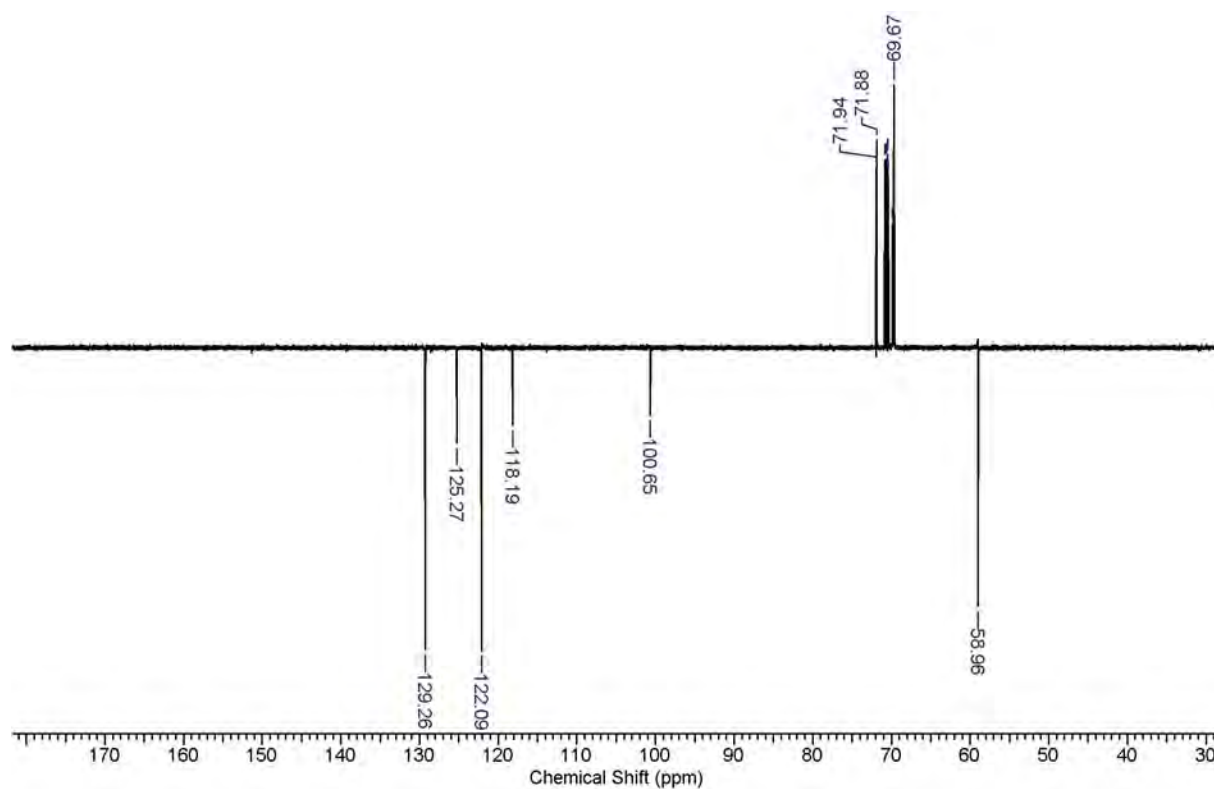


Figure S58. DEPT spectrum (75 MHz) of **9a** in CDCl₃ after purification *via* recycling HPLC.

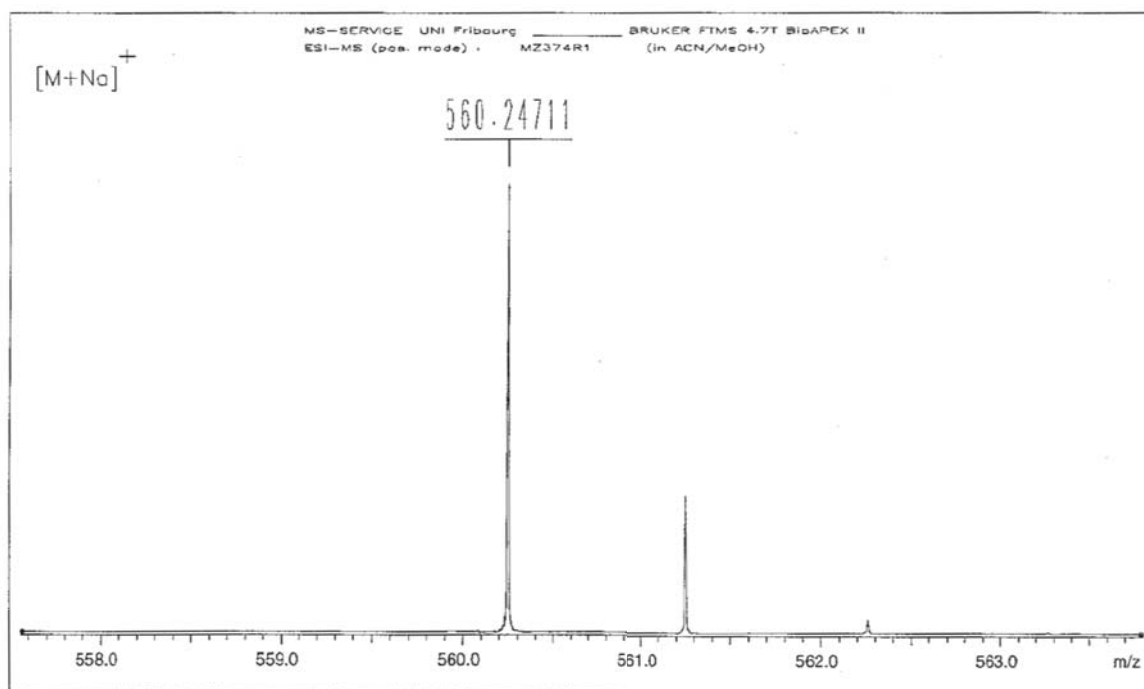


Figure S59. High resolution-mass spectrum of **9a** (ESI⁺) after purification *via* recycling HPLC.

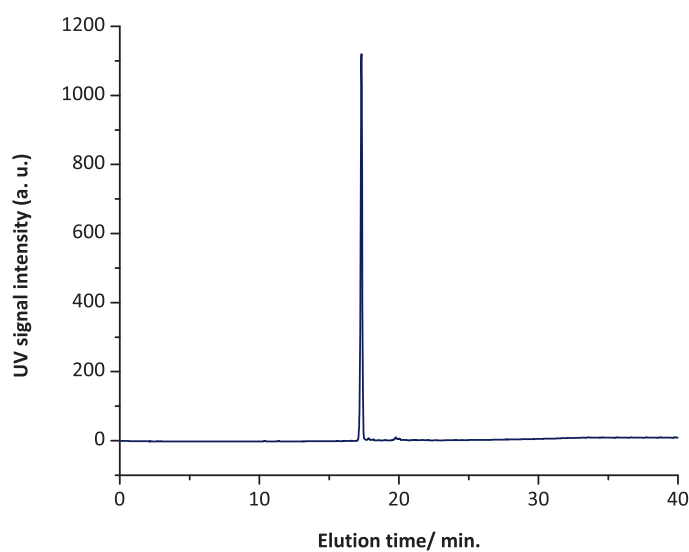


Figure S60. RP-HPLC elugram of **9a** after purification *via* recycling HPLC.

Phenyl 4-amino-2-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzoate (**9b**)

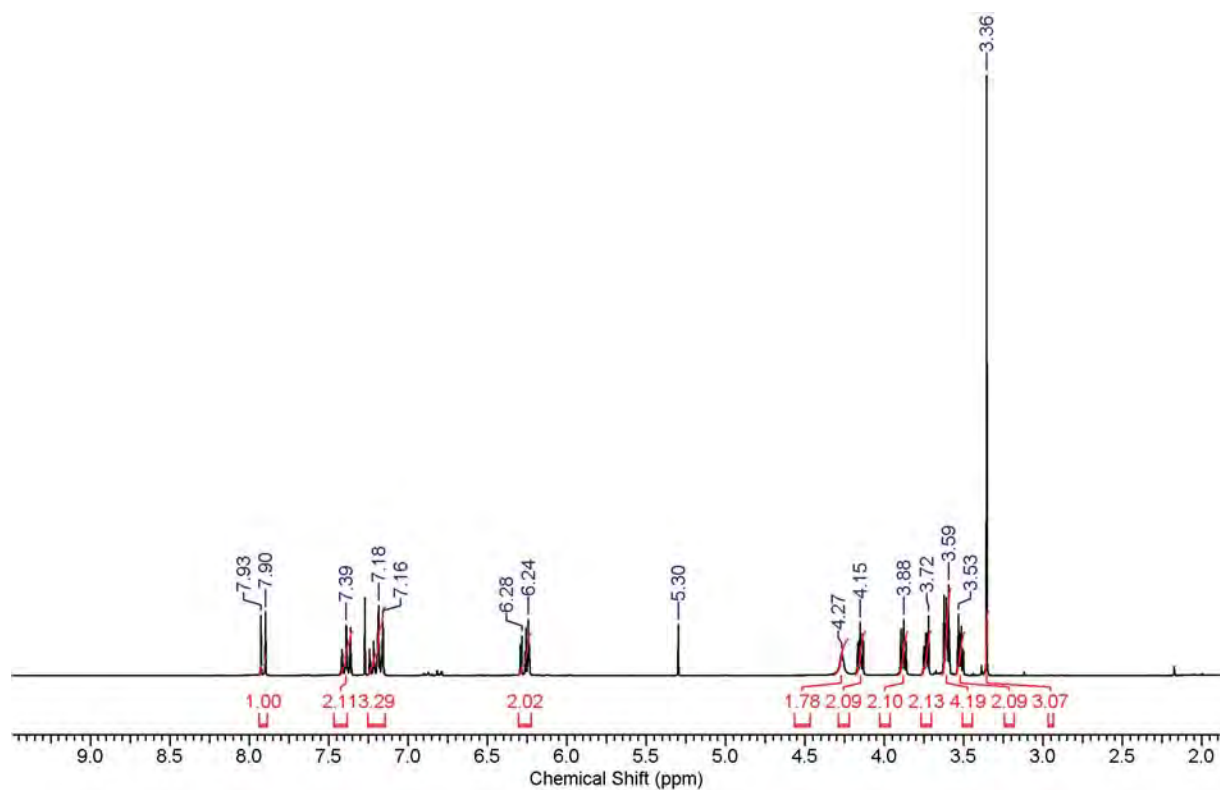


Figure S61. ^1H NMR spectrum (300 MHz) of **9b** in CDCl_3 after purification *via* column chromatography.

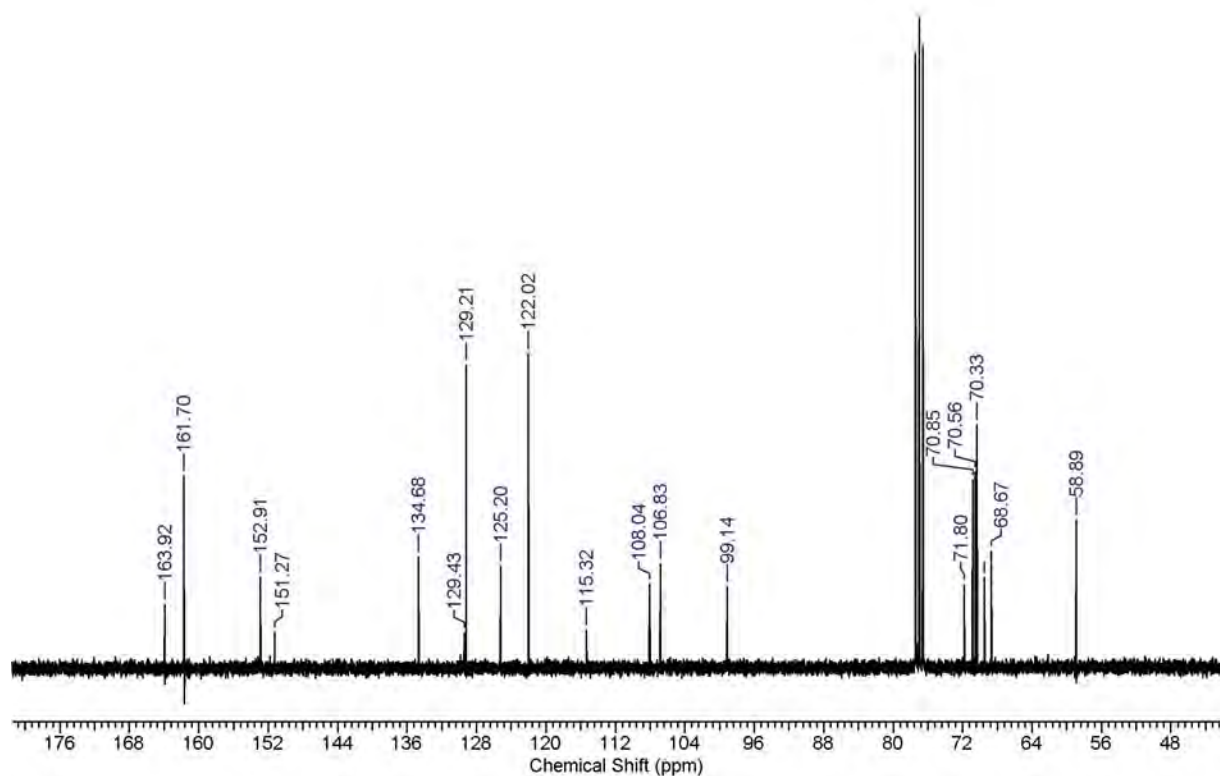


Figure S62. ^{13}C NMR spectrum (75 MHz) of **9b** in CDCl_3 after purification *via* column chromatography.

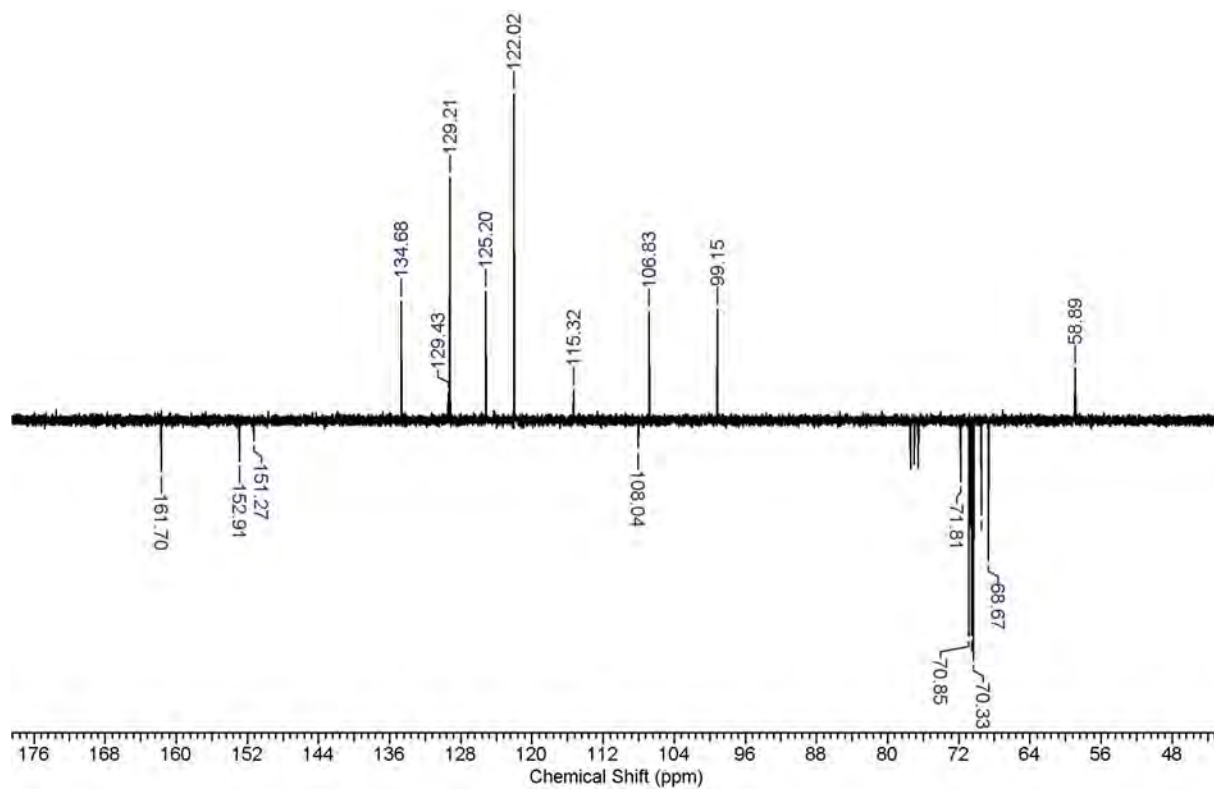


Figure S63. APT spectrum (75 MHz) of **9b** in CDCl_3 after purification *via* column chromatography.

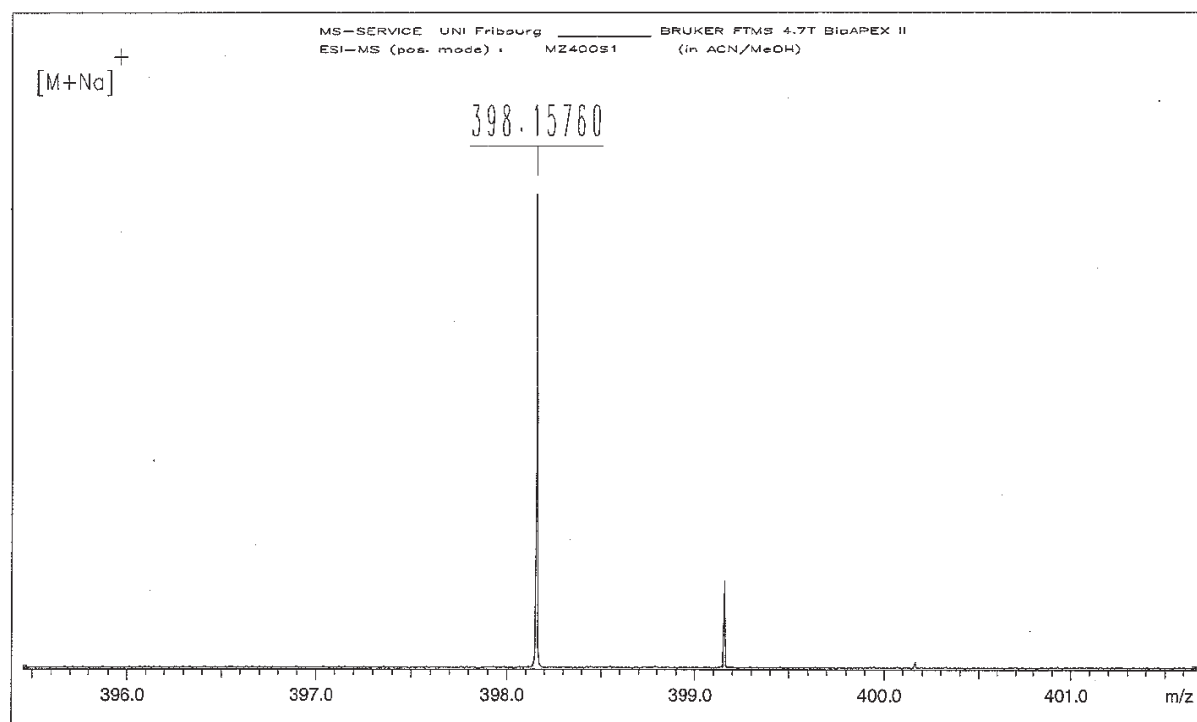


Figure S64. High resolution-mass spectrum of **9b** (ESI+) after purification *via* column chromatography.

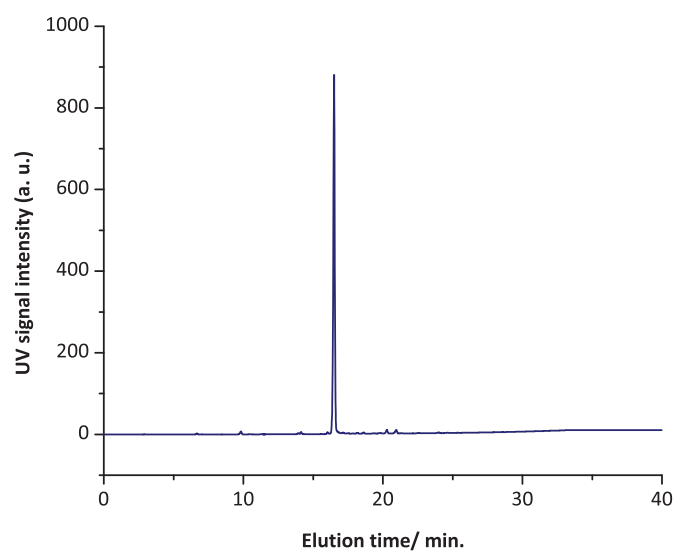


Figure S65. RP-HPLC of **9b** after purification *via* column chromatography.

Phenyl 4-((4-methoxybenzyl)amino)-2,5-bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzoate (**10a**)

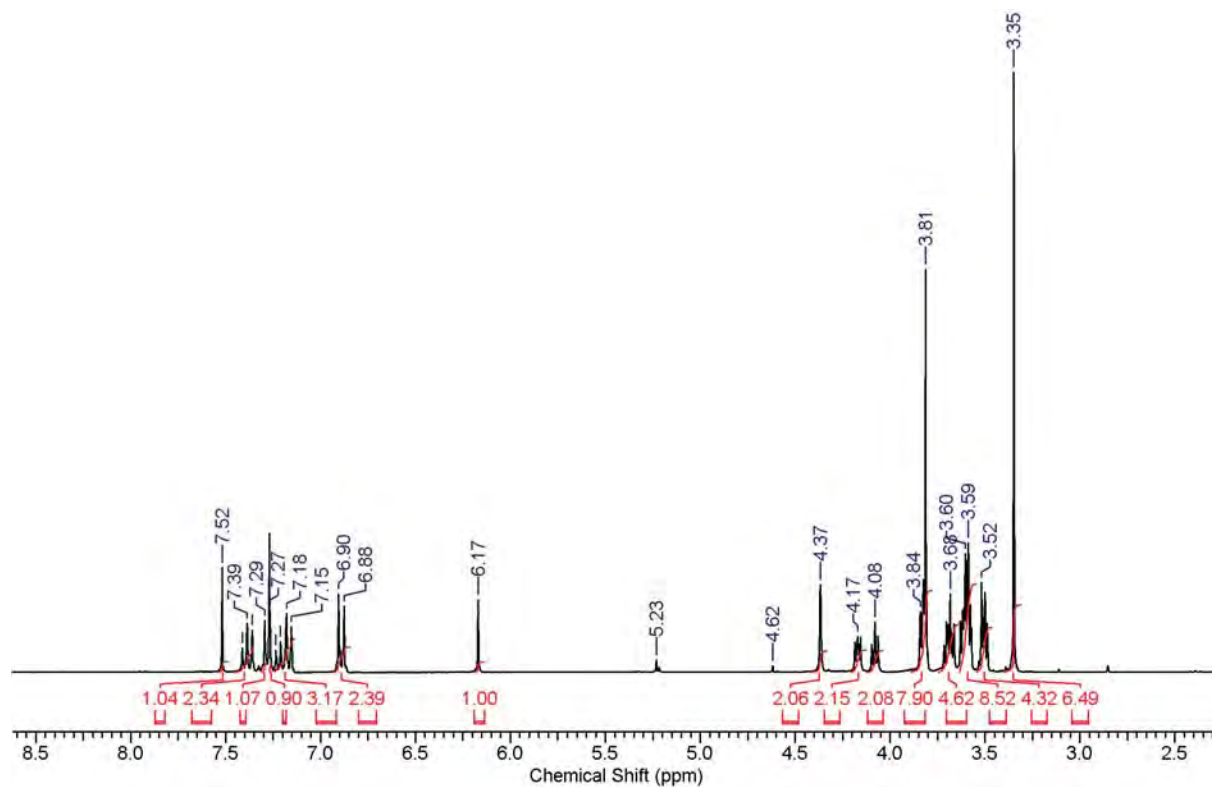


Figure S66. ¹H NMR spectrum (300 MHz) of **10a** in CDCl₃ after purification *via* recycling HPLC.

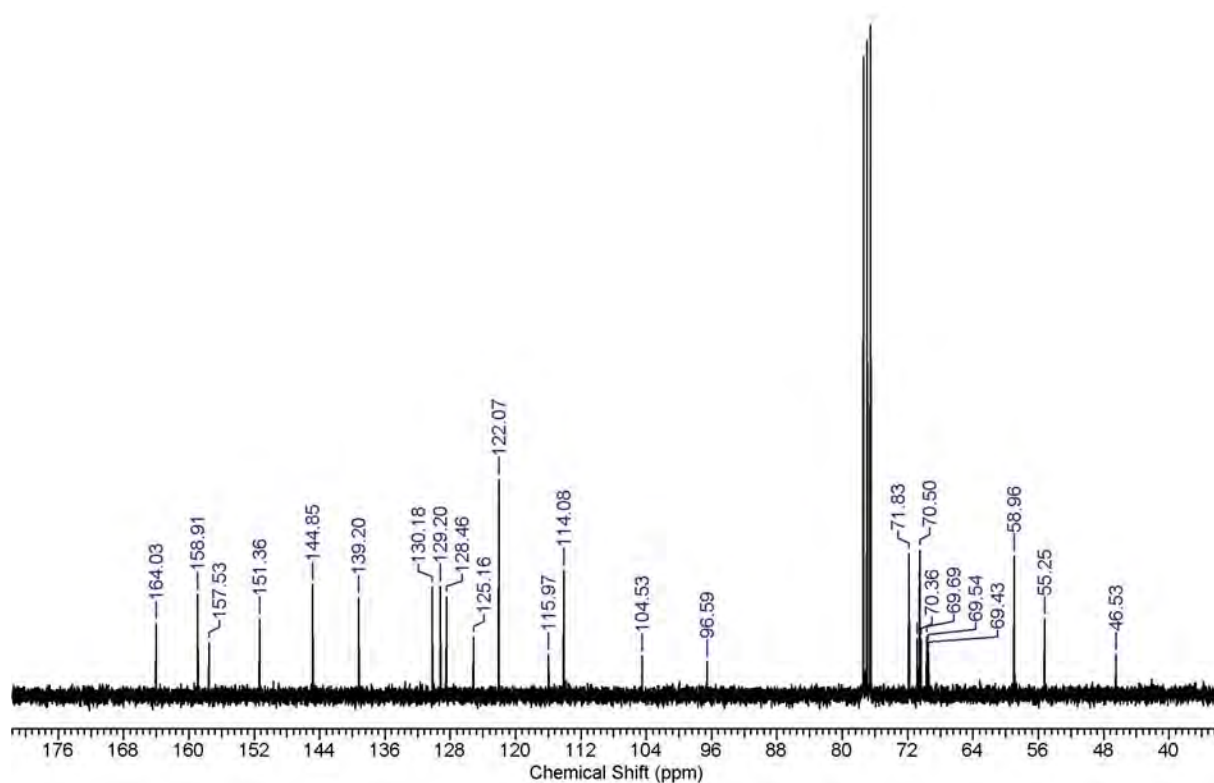


Figure S67. ¹³C NMR spectrum (75 MHz) of **10a** in CDCl₃ after purification *via* recycling HPLC.

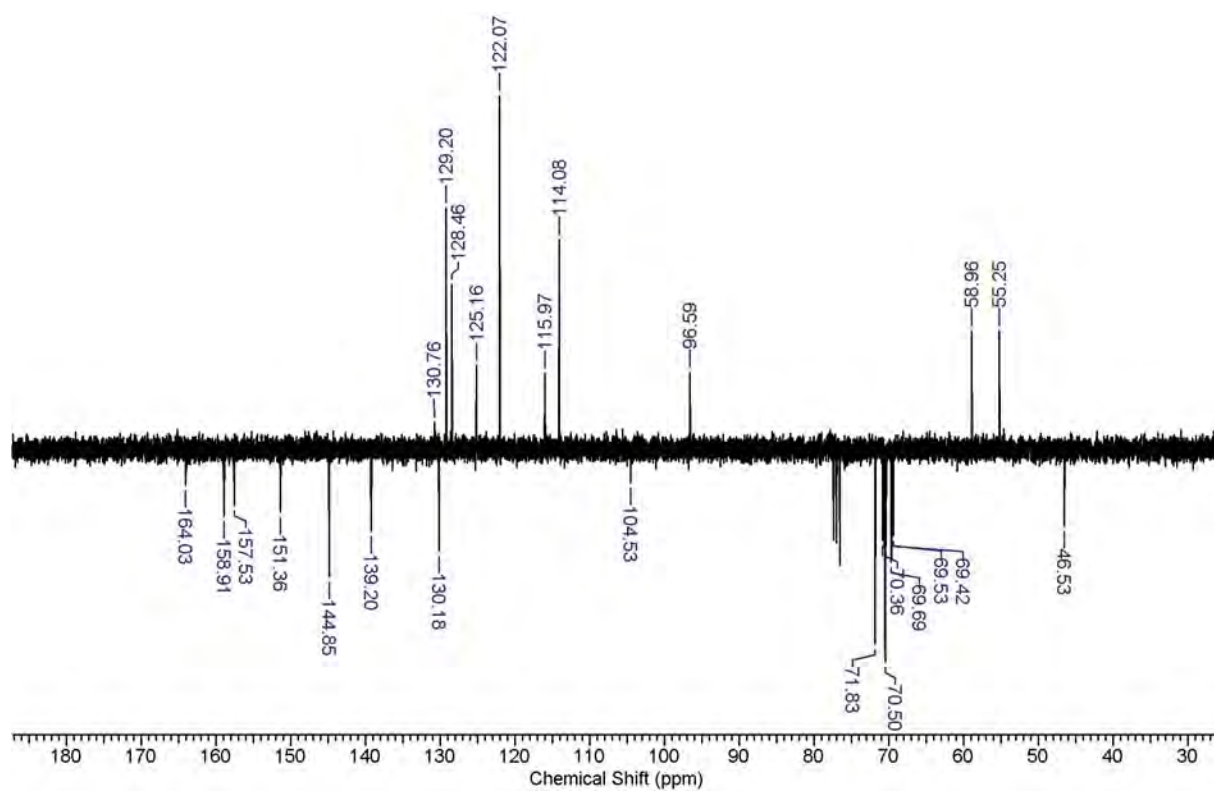


Figure S68. APT spectrum (75 MHz) of **10a** in CDCl₃ after purification *via* recycling HPLC.

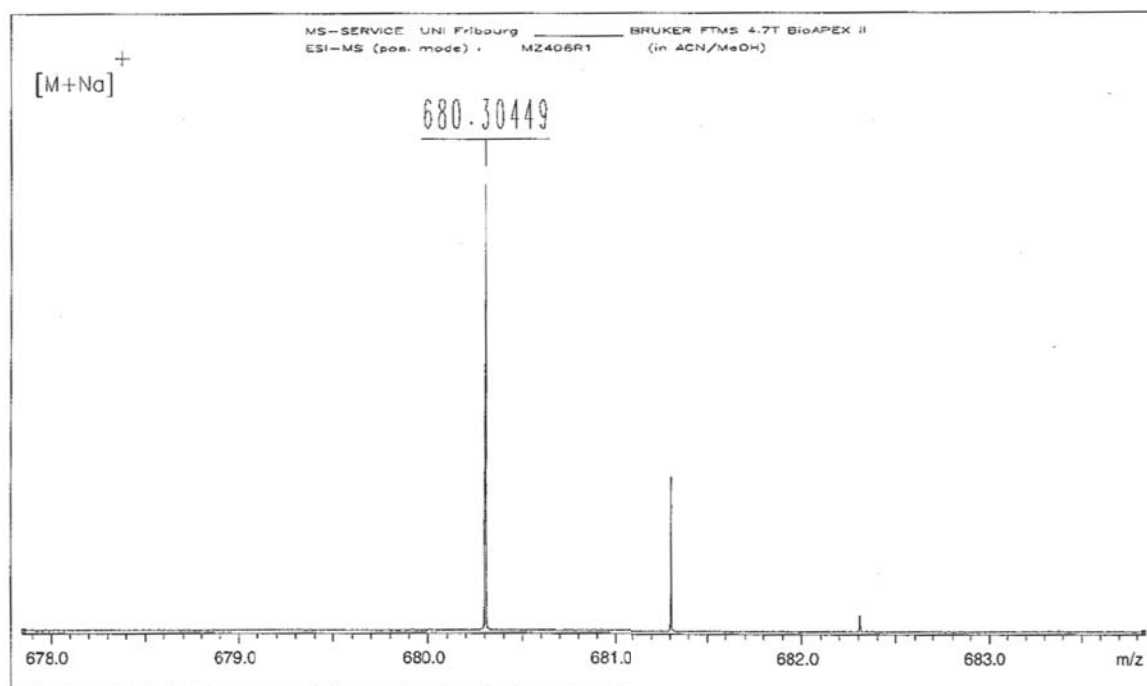


Figure S69. High resolution-mass spectrum of **10a** (ESI+) after purification *via* recycling HPLC.

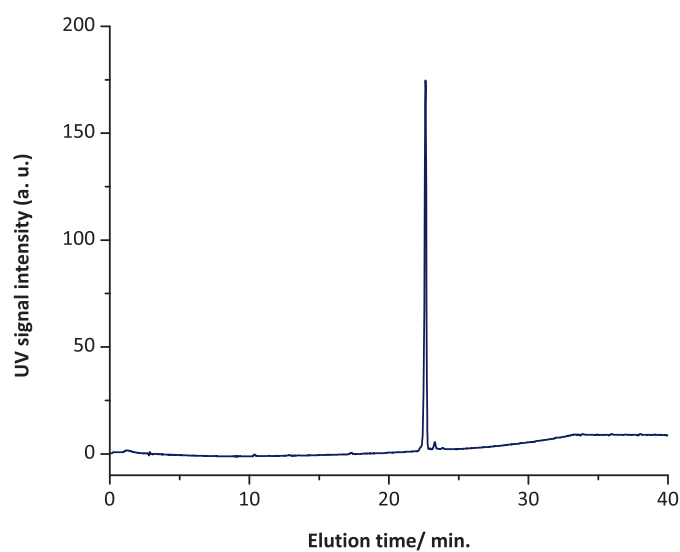


Figure S70. RP-HPLC elugram of **10a** after purification *via* recycling HPLC.

Phenyl 4-((4-methoxybenzyl)amino)-2-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy) benzoate
(10b)

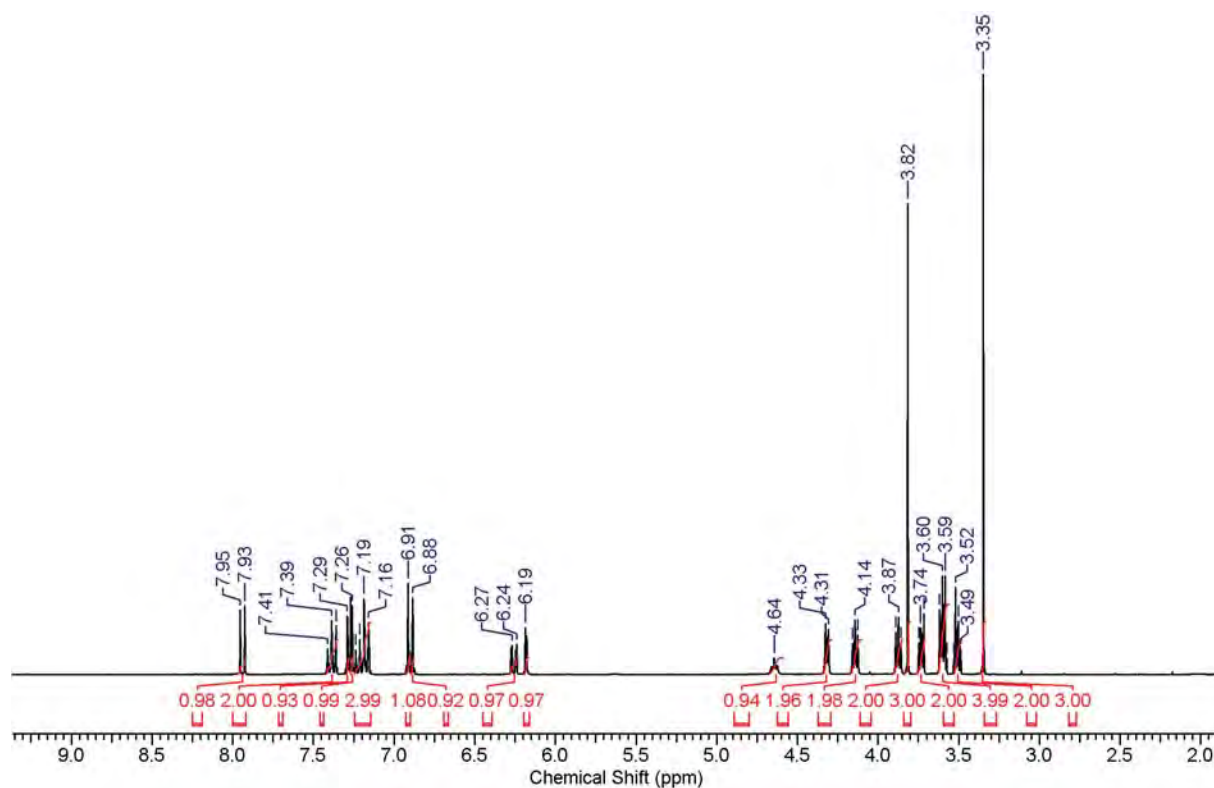


Figure S71. ^1H NMR spectrum (300 MHz) of **10b** in CDCl_3 after purification *via* recycling HPLC.

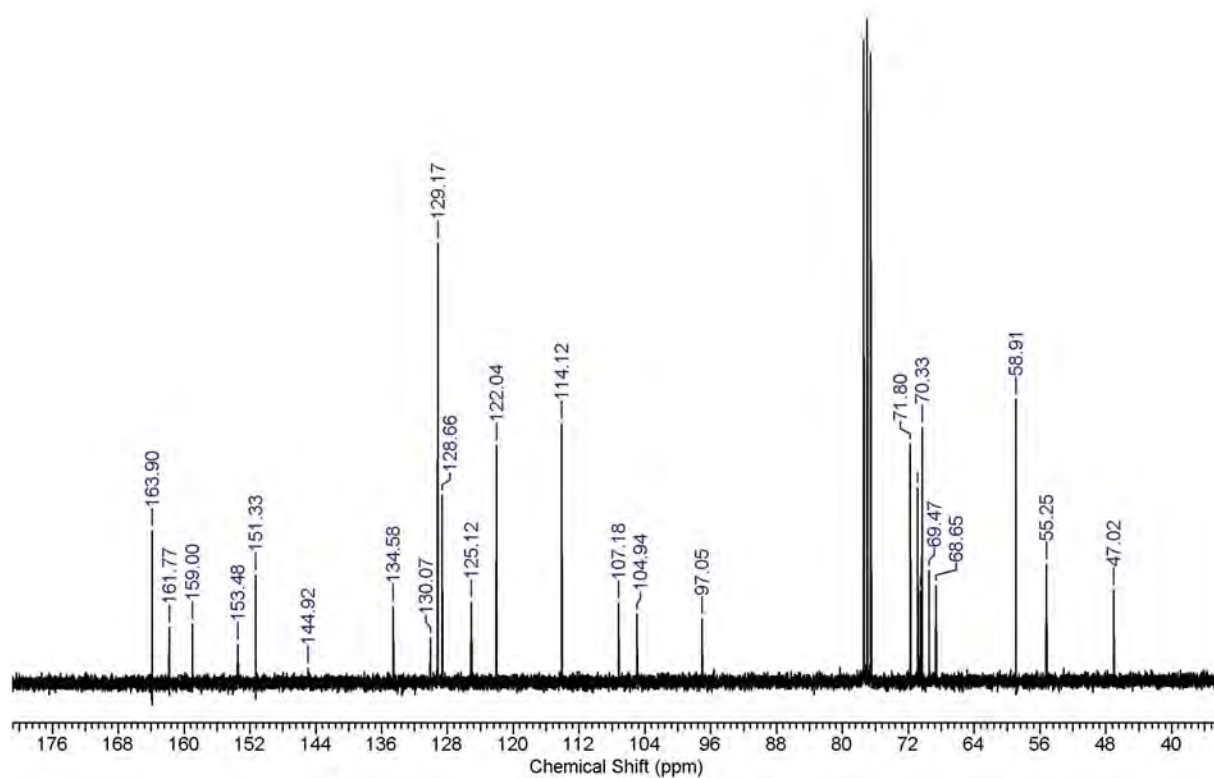


Figure S72. ^{13}C NMR spectrum (75 MHz) of **10b** in CDCl_3 after purification *via* recycling HPLC.

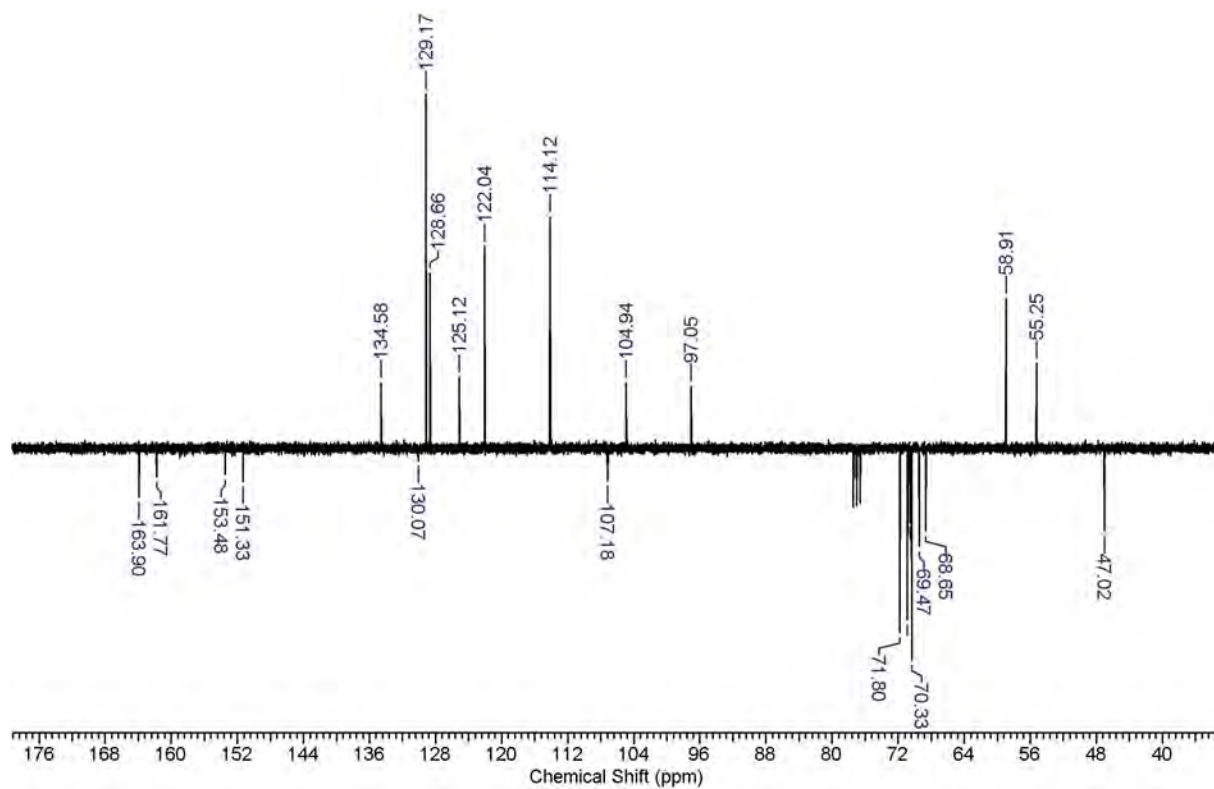


Figure S73. APT spectrum (75 MHz) of **10a** in CDCl_3 after purification *via* recycling HPLC.

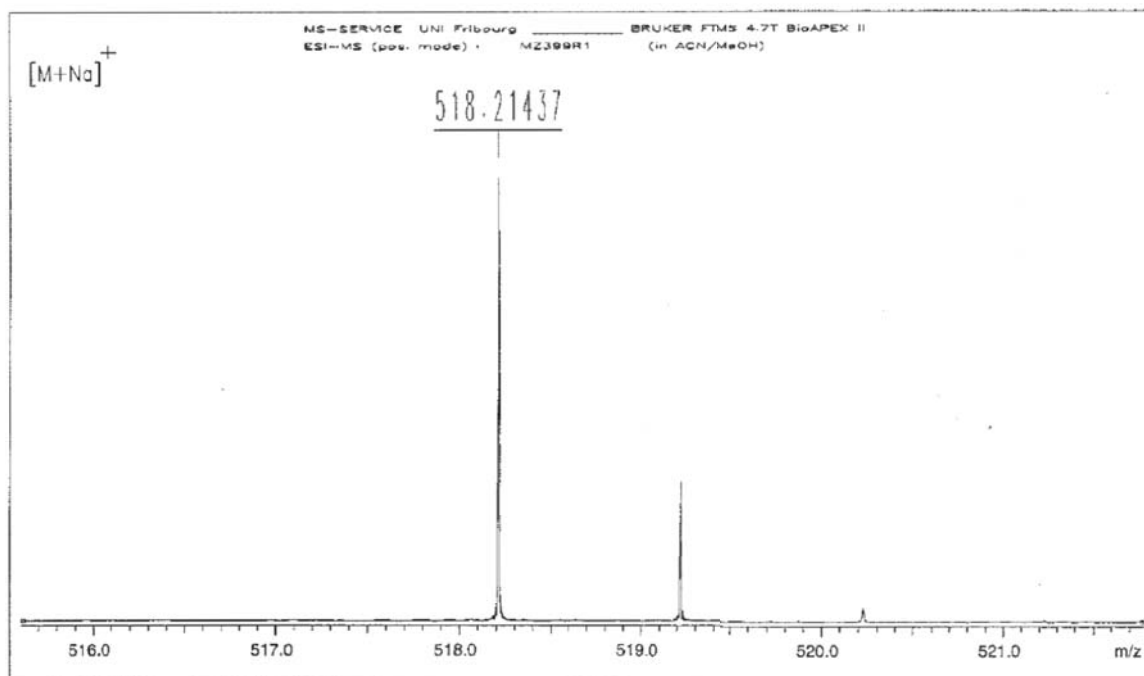


Figure S74. High resolution-mass spectrum of **10b** after purification *via* recycling HPLC.

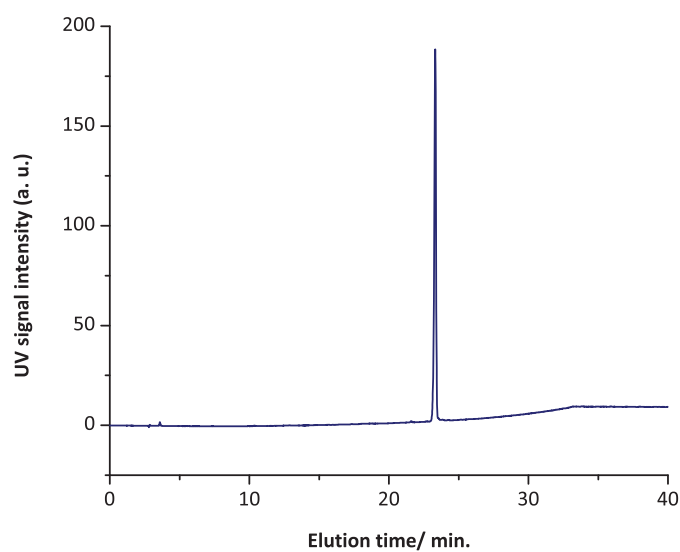


Figure S75. RP-HPLC elugram of **10b** after purification *via* recycling HPLC.

4-Amino-2,5-bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzoic acid (11**)**

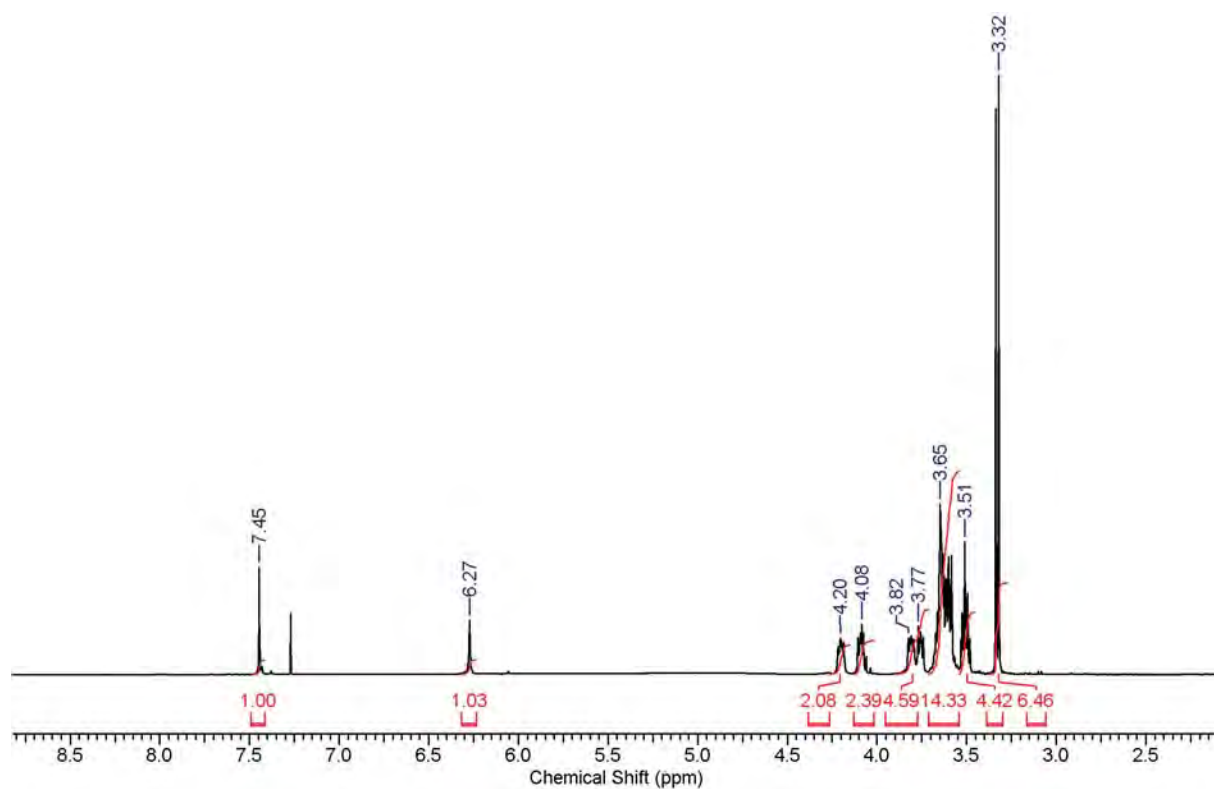


Figure S75. ^1H NMR spectrum (360 MHz) of **11** in CDCl_3 .

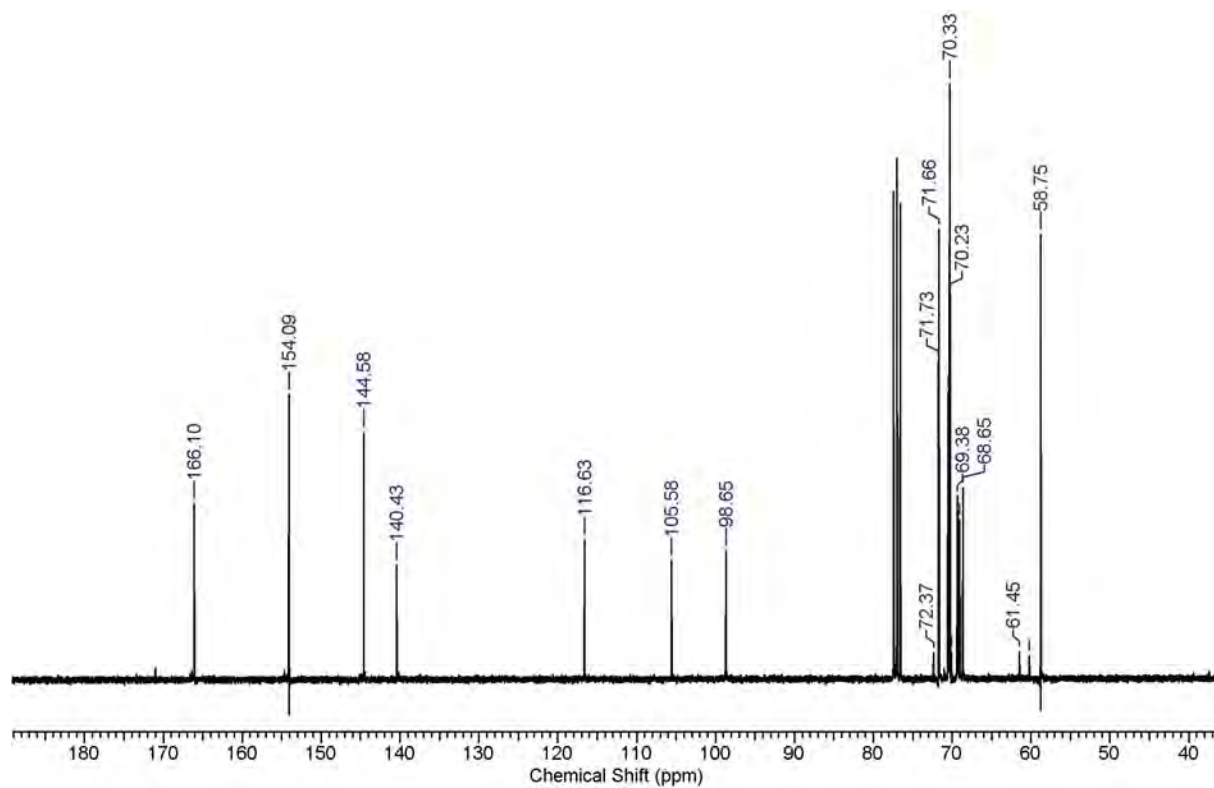


Figure S76. ^{13}C NMR spectrum (90 MHz) of **11** in CDCl_3 .

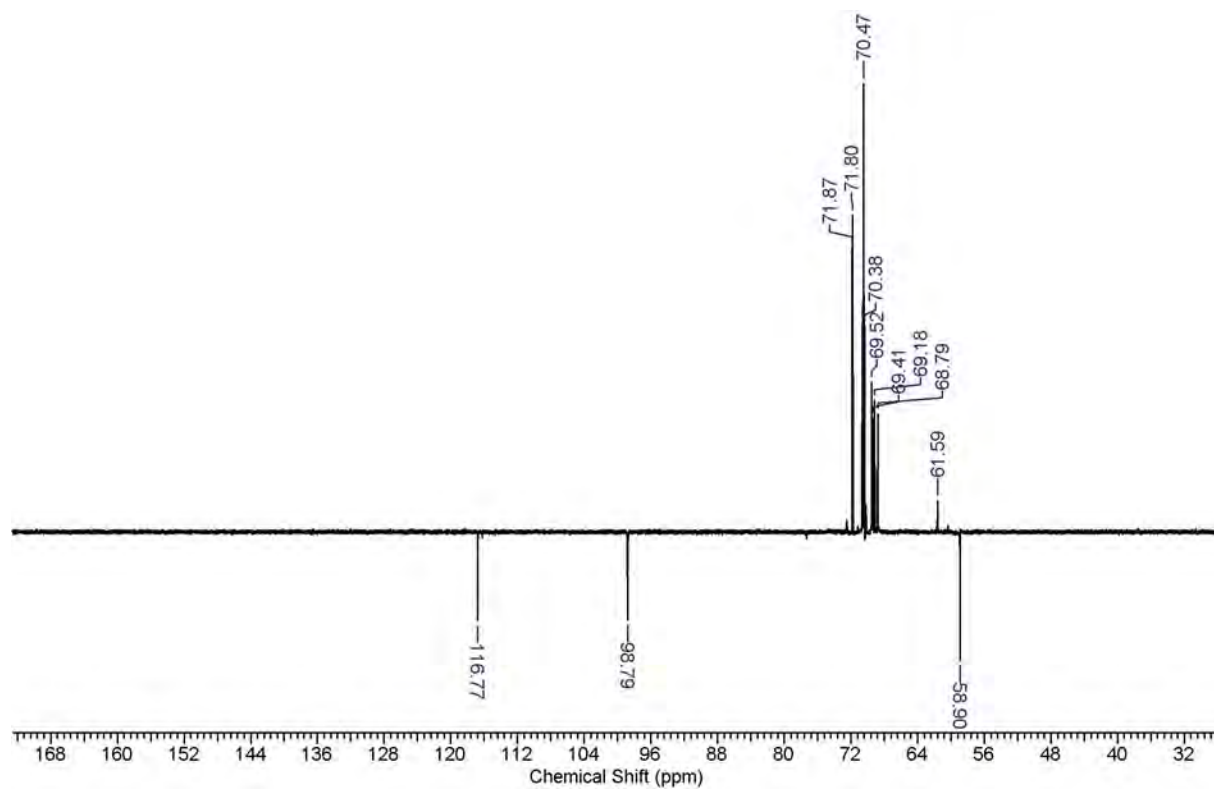


Figure S77. DEPT spectrum (90 MHz) of **11** in CDCl_3 .

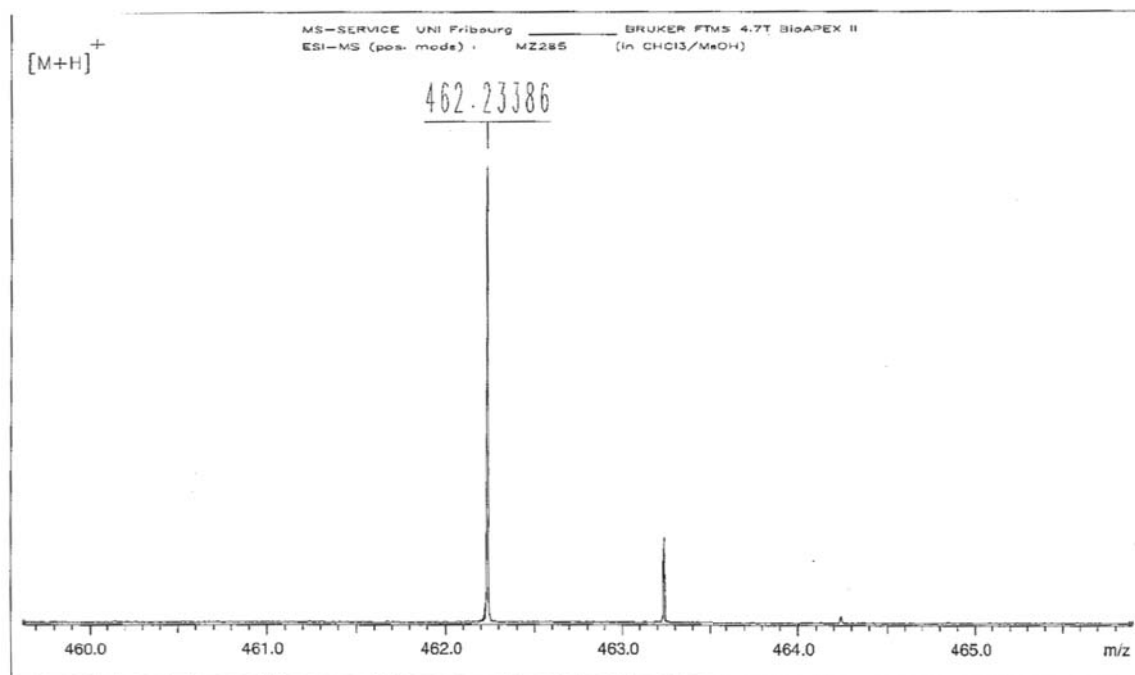


Figure S78. High resolution-mass spectrum of **11** (ESI+).

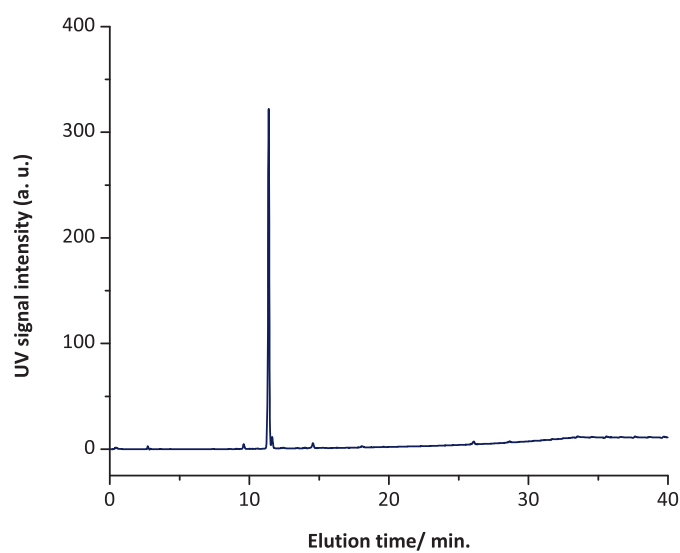


Figure S79. RP-HPLC elugram of **11**.