

Synthesis, characterization and spectroscopic properties of water soluble coumarins substituted with oligomeric alkoxy functions

H. Surya Prakash Rao,* Mohan Babu. B and Avinash Desai

Department of Chemistry, Pondicherry University, Pondicherry – 605 014 INDIA

hspc.che@pondiuni.edu.in

Supplementary data

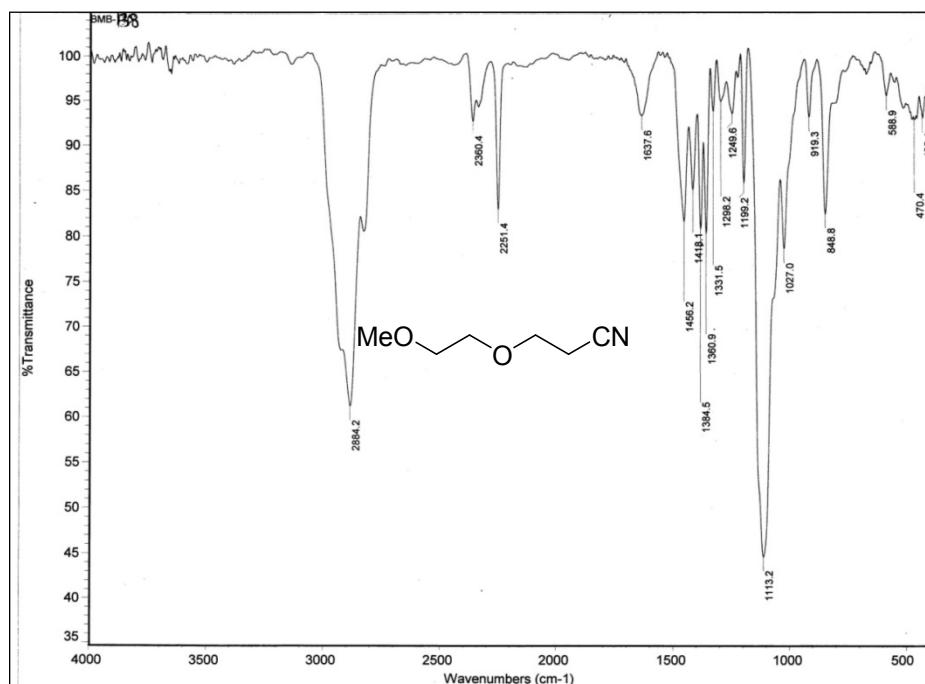


Figure 7. IR (KBr) spectrum of 3-(2-methoxyethoxy)propanenitrile **6a**.

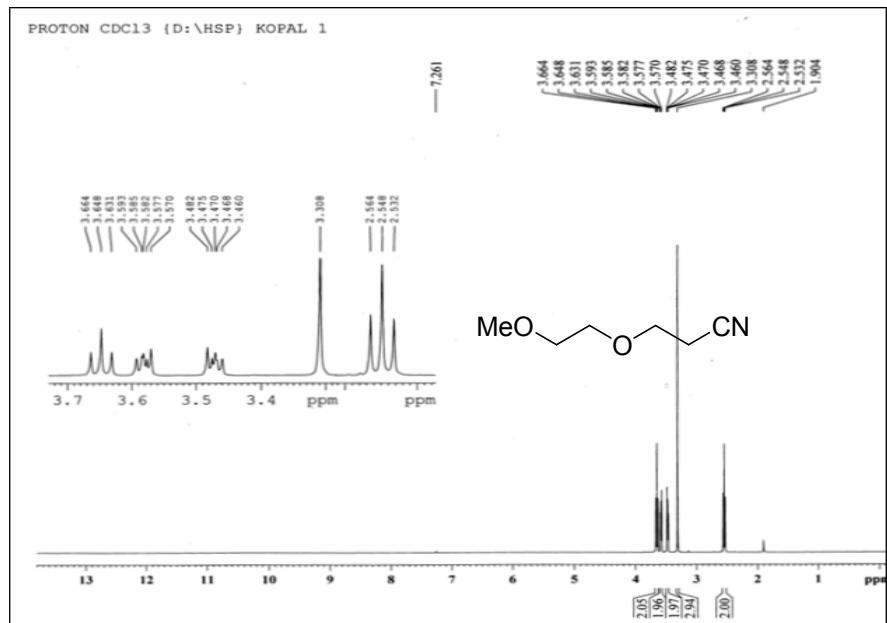


Figure 8. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 3-(2-methoxyethoxy)propanenitrile **6a**.

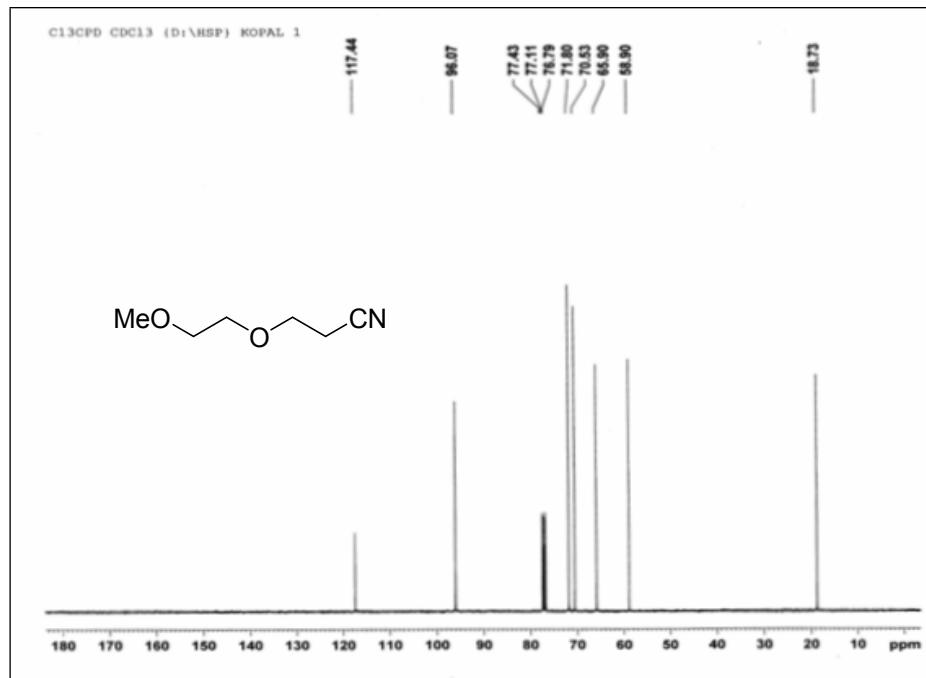


Figure 9. ¹³C NMR (100 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 3-(2-methoxyethoxy)propanenitrile **6a**.

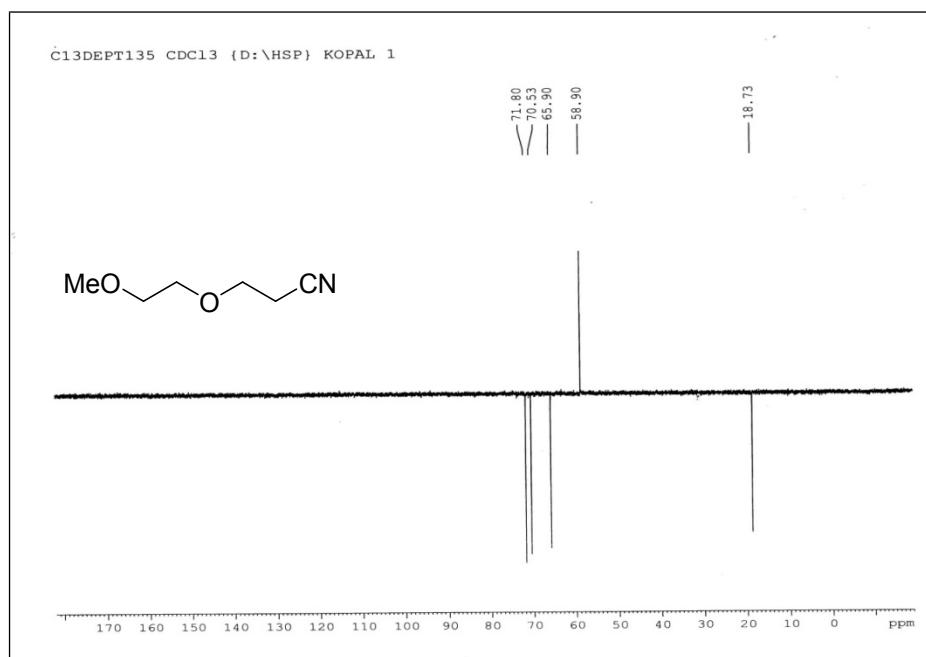


Figure 10. DEPT-135 NMR (100 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 3-(2-methoxyethoxy)propanenitrile **6a**.

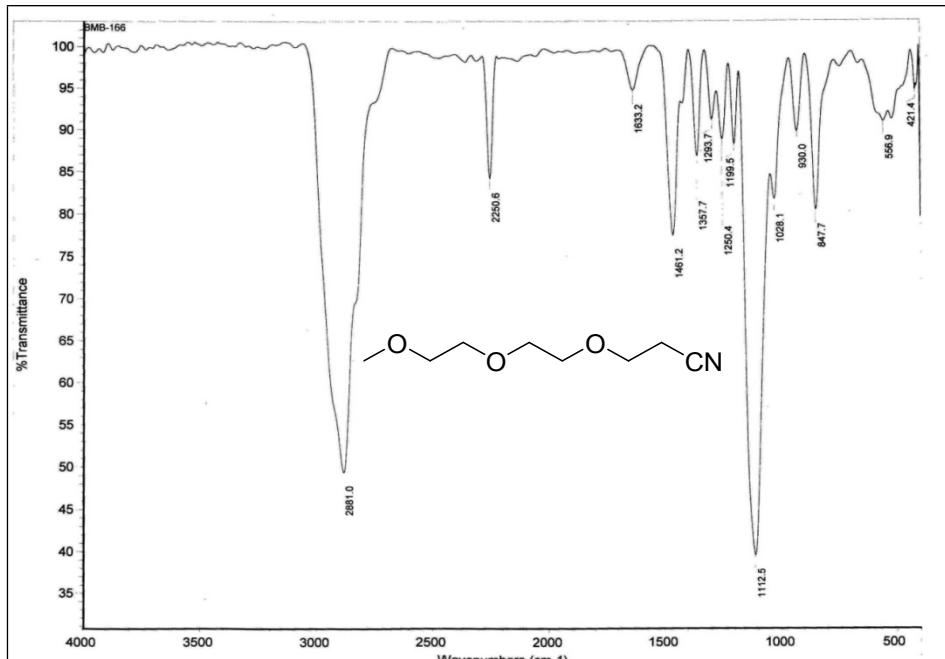


Figure 11. IR (KBr) spectrum of 3-(2-(2-methoxyethoxy)ethoxy)propanenitrile **6b.**

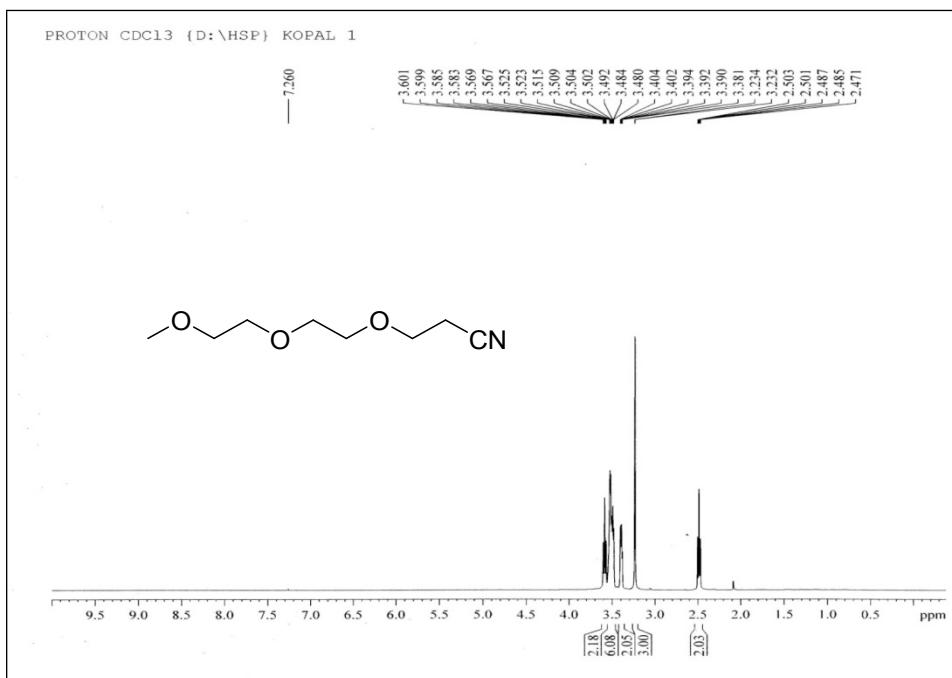


Figure 12. ¹H NMR (400 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 3-(2-(2-methoxyethoxy)ethoxy)propanenitrile **6b.**

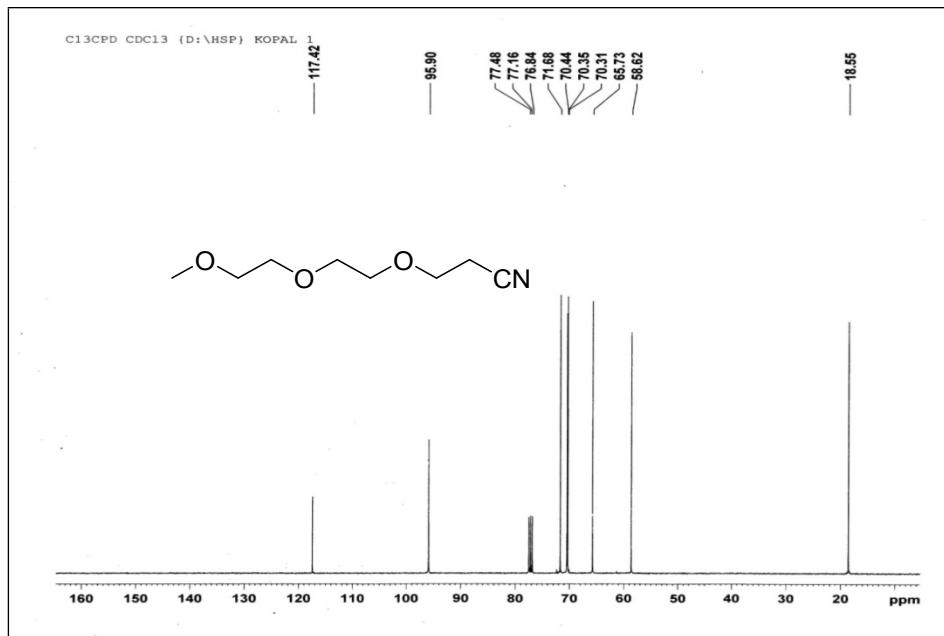


Figure 13. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 3-(2-(2-methoxyethoxy)ethoxy)propanenitrile **6b**.

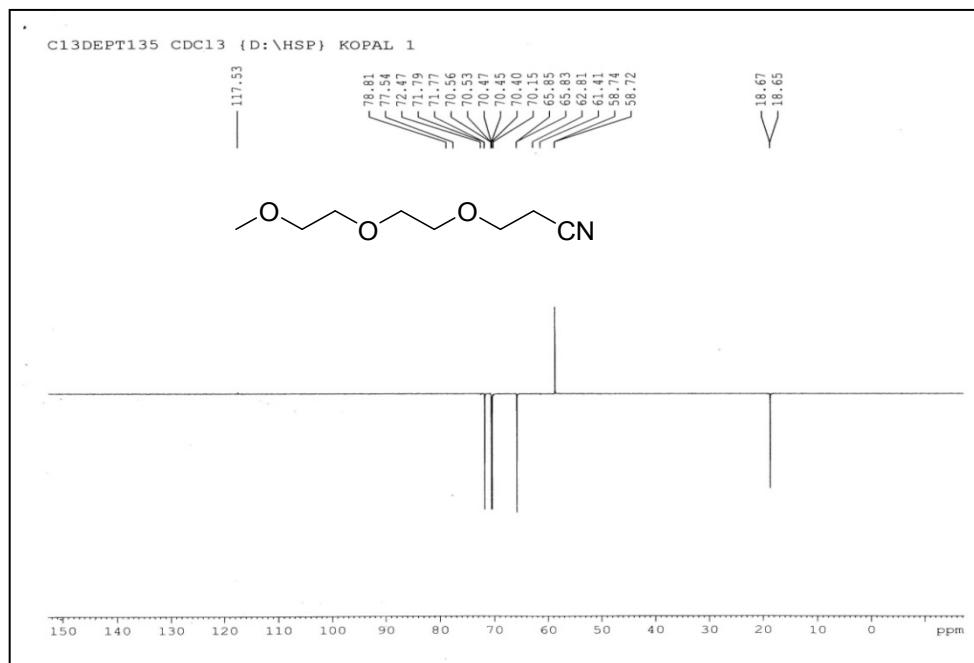


Figure 14. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 3-(2-(2-methoxyethoxy)ethoxy)propanenitrile **6b**.

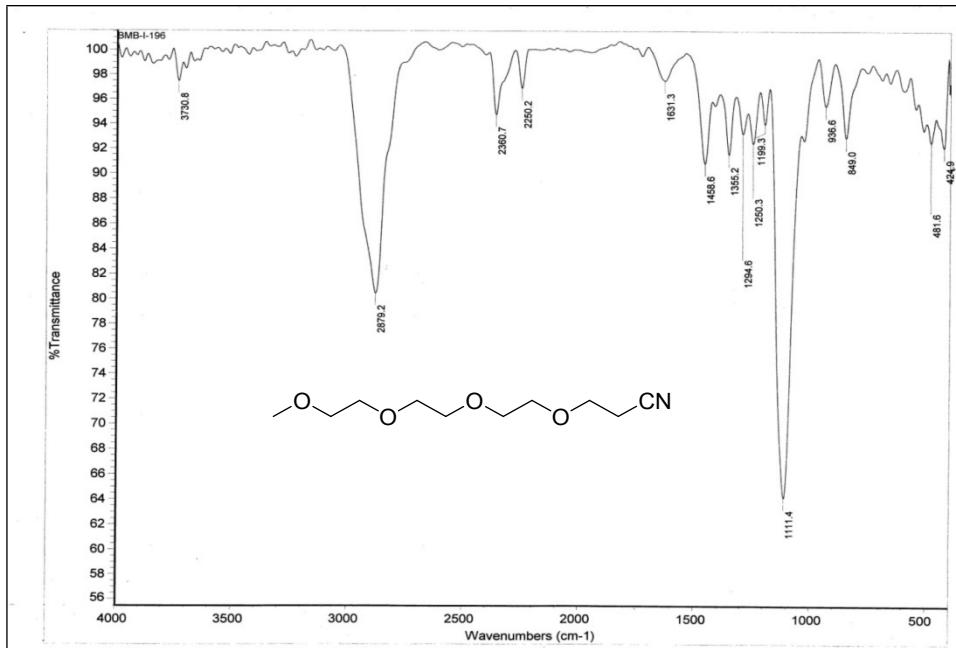


Figure 15. IR (KBr) spectrum of 2,5,8,11-tetraoxatetradecane-14-nitrile **6c**.

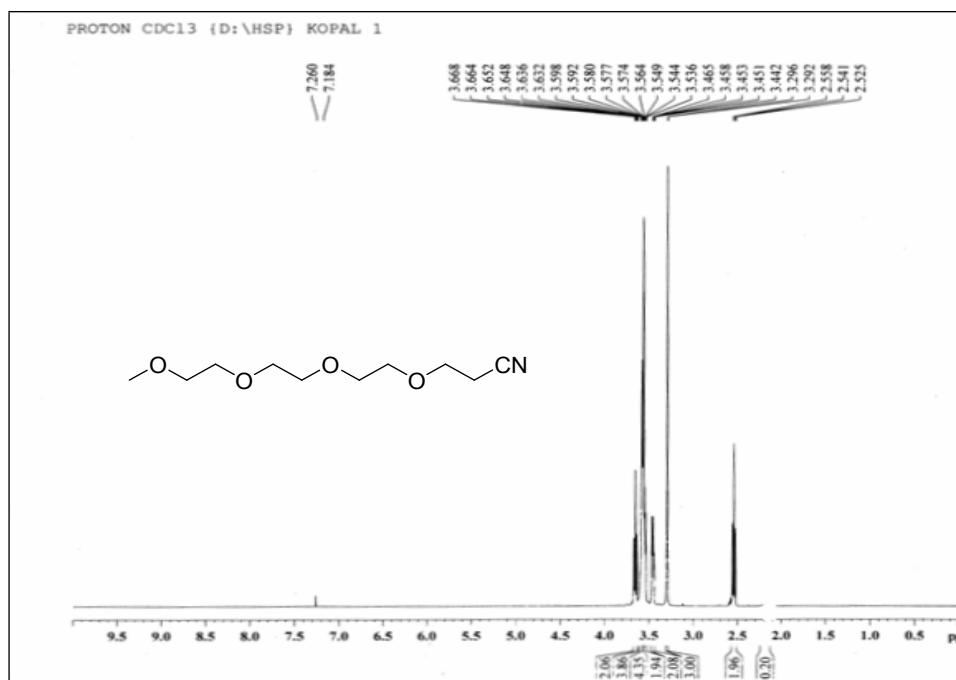


Figure 16. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 2,5,8,11-tetraoxatetradecane-14-nitrile **6c**.

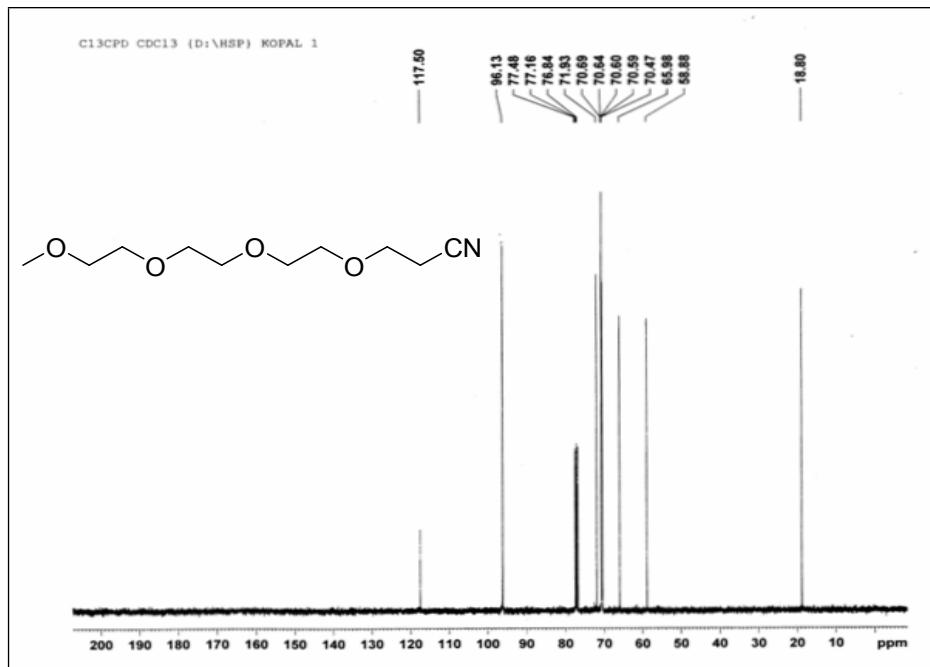


Figure 17. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 2,5,8,11-tetraoxatetradecane-14-nitrile **6c**.

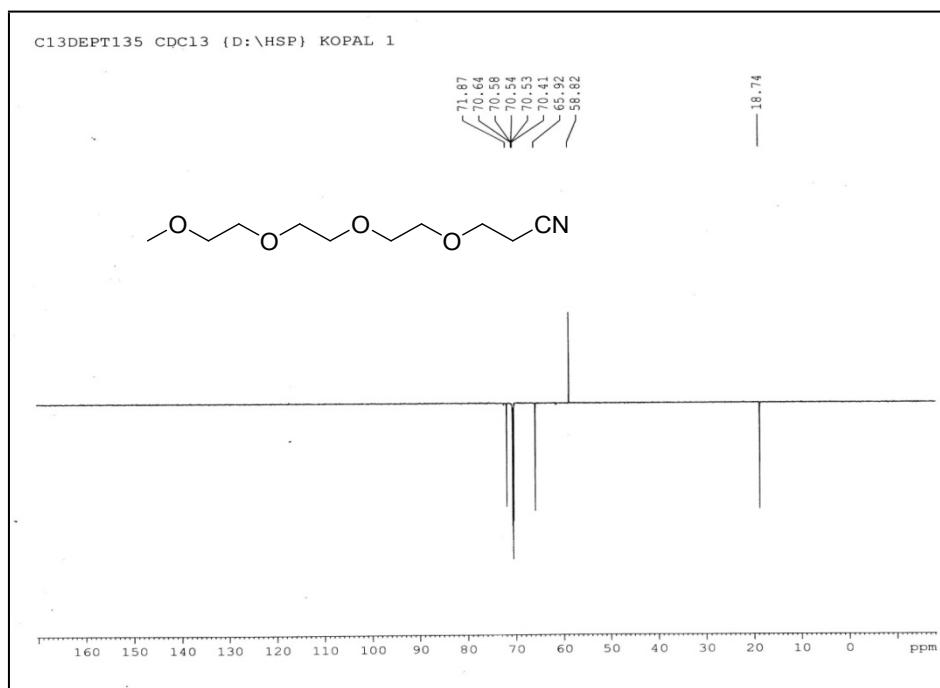


Figure 18. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 2,5,8,11-tetraoxatetradecane-14-nitrile **6c**.

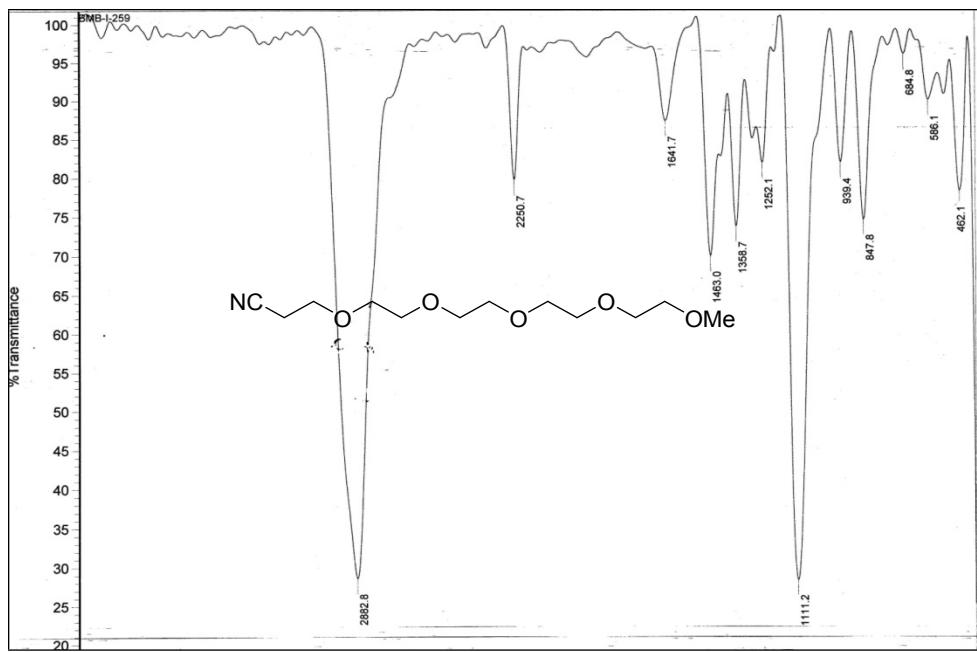


Figure 19. IR (KBr) spectrum of 2,5,8,11,14-pentaoxaheptadecane-17-nitrile **6d**.

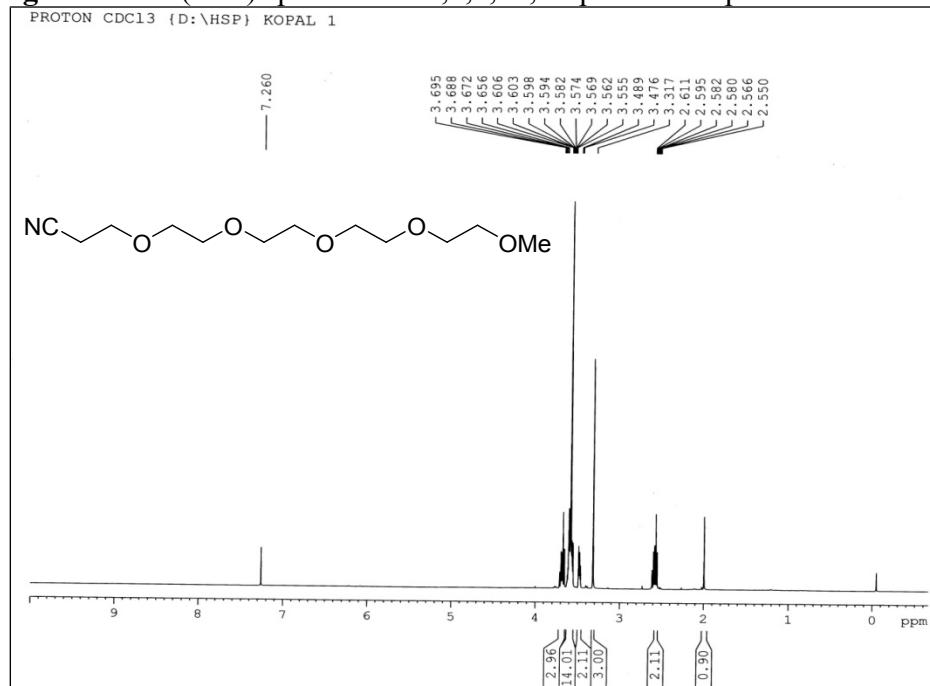


Figure 20. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 2,5,8,11,14-pentaoxaheptadecane-17-nitrile **6d**.

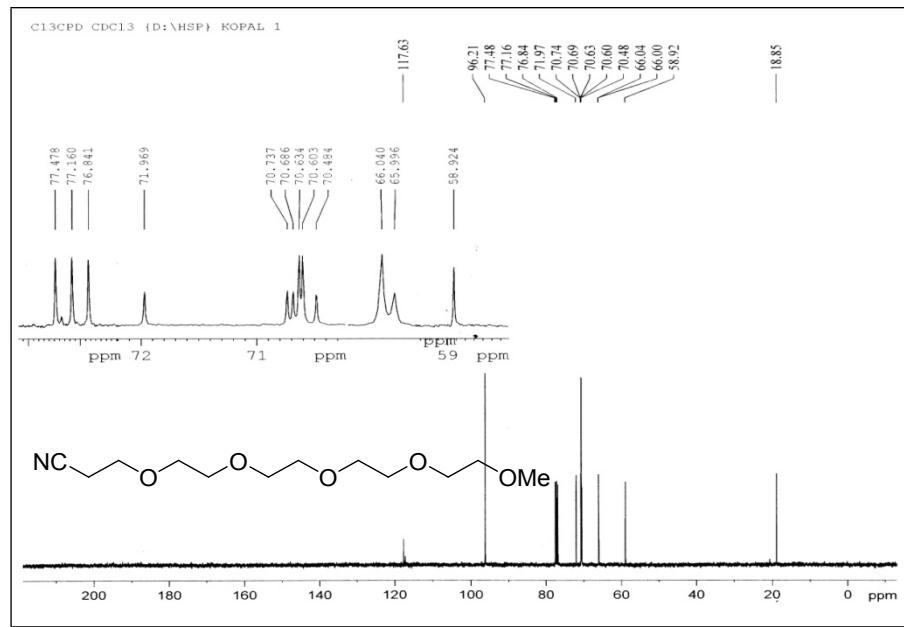


Figure 21. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 2,5,8,11,14-pentaoxaheptadecane-17-nitrile **6d**.

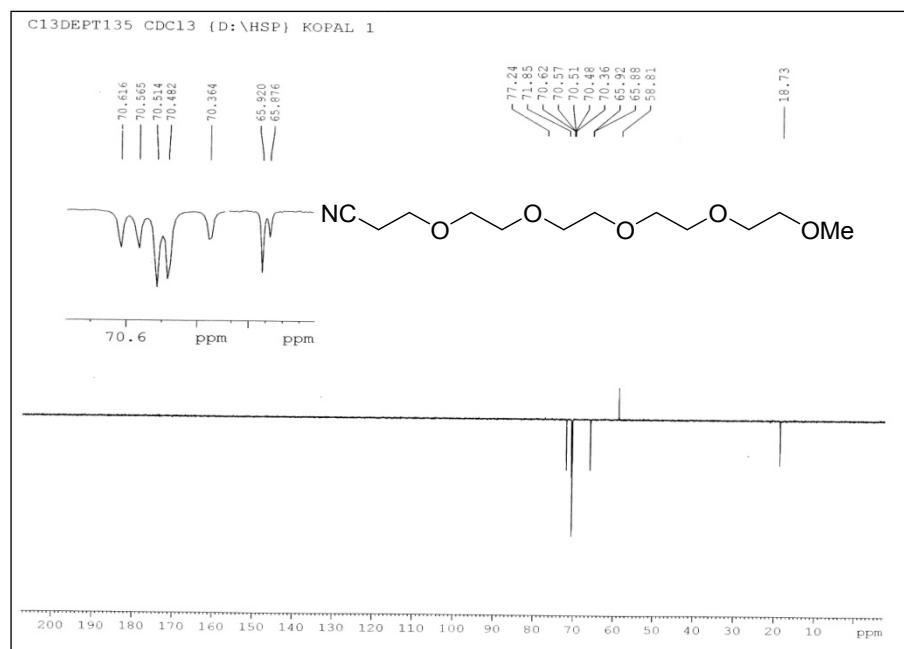


Figure 22. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 2,5,8,11,14-pentaoxaheptadecane-17-nitrile **6d**.

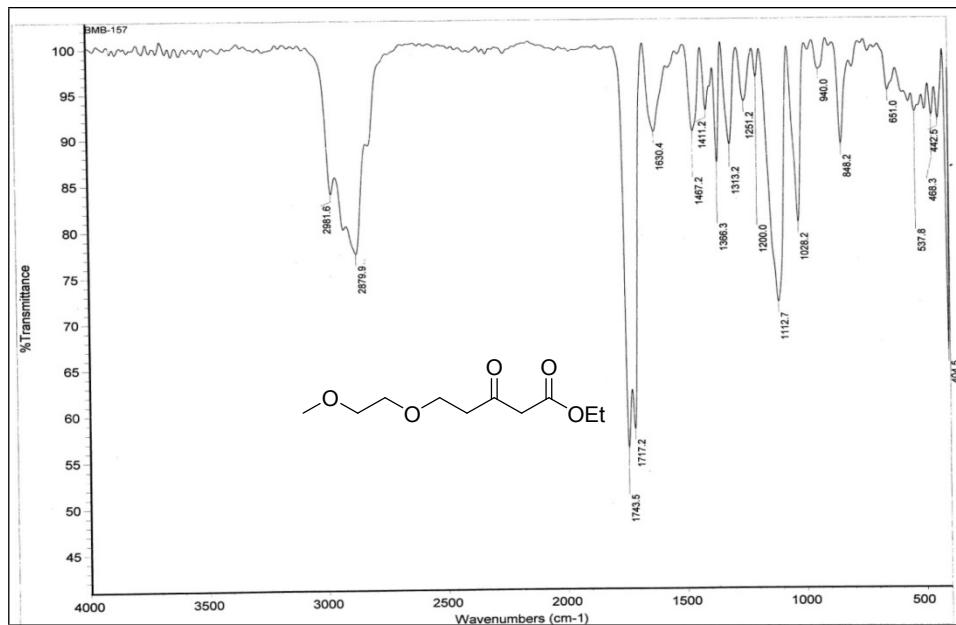


Figure 23. IR (KBr) spectrum of ethyl 5-(2-methoxyethoxy)-3-oxopentanoate **7a**.

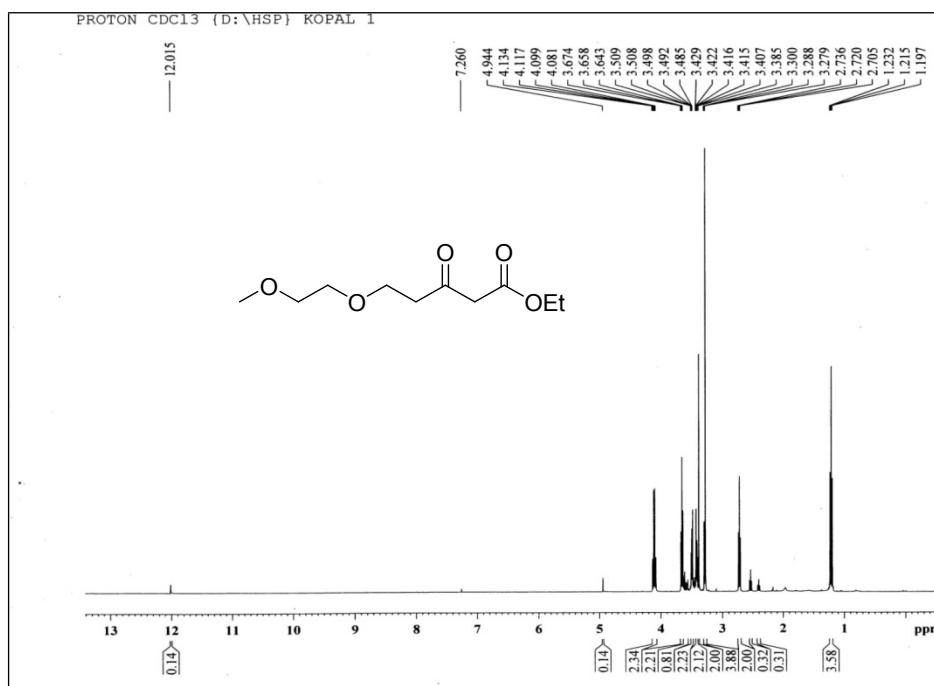


Figure 24. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 5-(2-methoxyethoxy)-3-oxopentanoate **7a**.

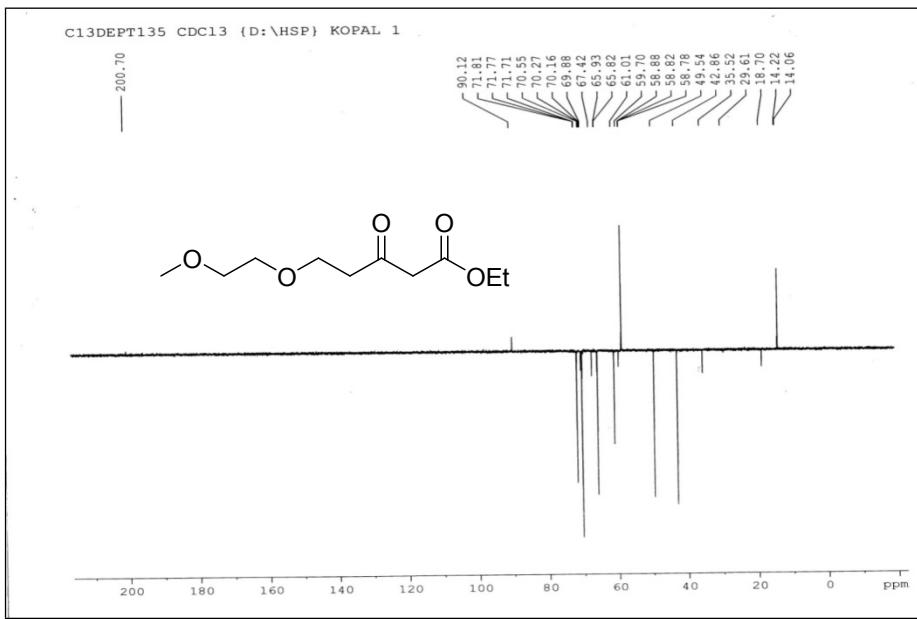
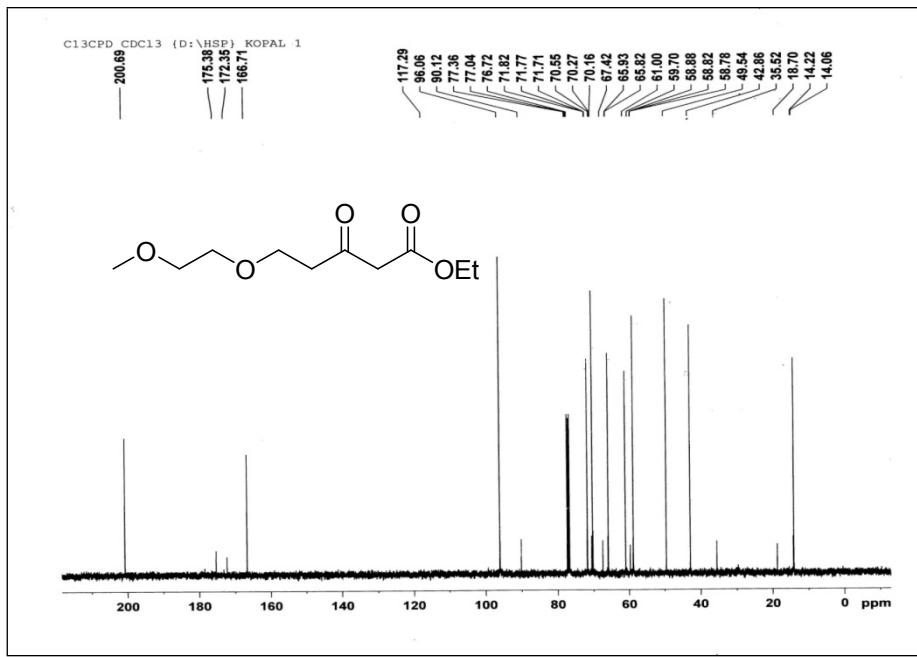


Figure 26. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 5-(2-methoxyethoxy)-3-oxopentanoate **7a**.

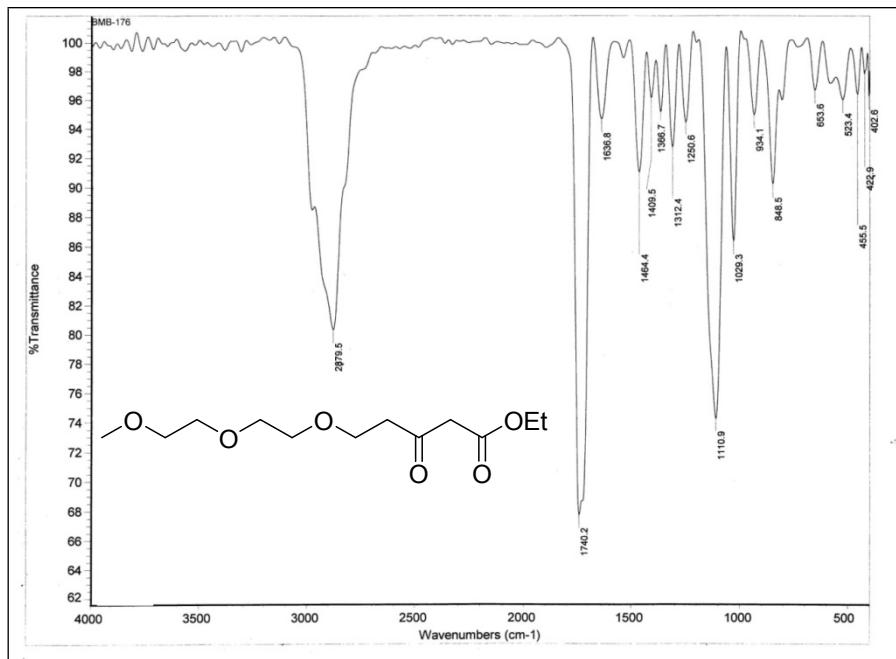


Figure 27. IR (KBr) spectrum of ethyl 5-(2-(2-methoxyethoxy)ethoxy)-3-oxopentanoate **7b**.

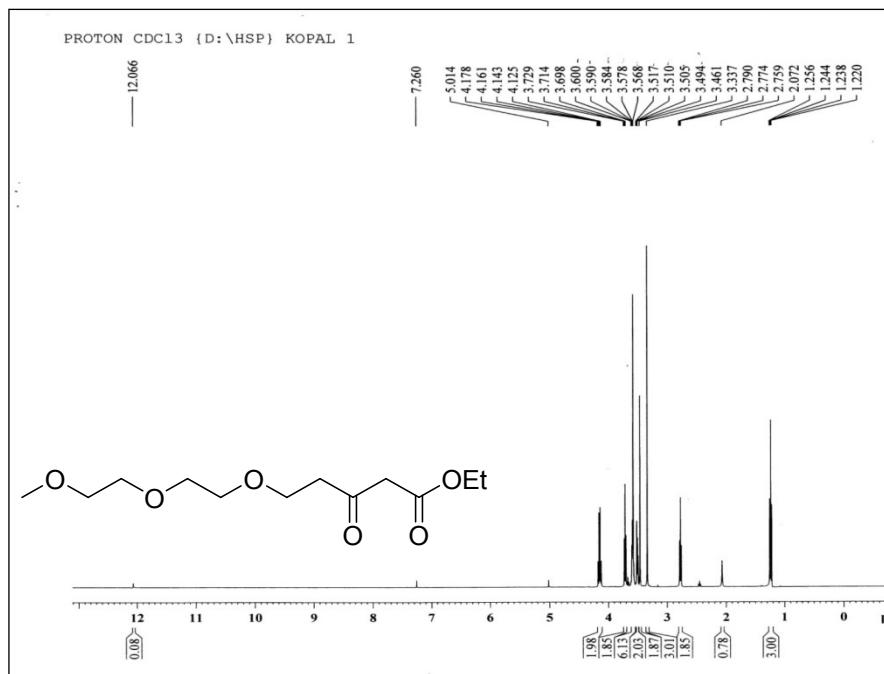


Figure 28. ^1H (400 MHz, $\text{CCl}_4+\text{CDCl}_3$, 1:1) spectrum of ethyl 5-(2-(2-methoxyethoxy)ethoxy)-3-oxopentanoate **7b**.

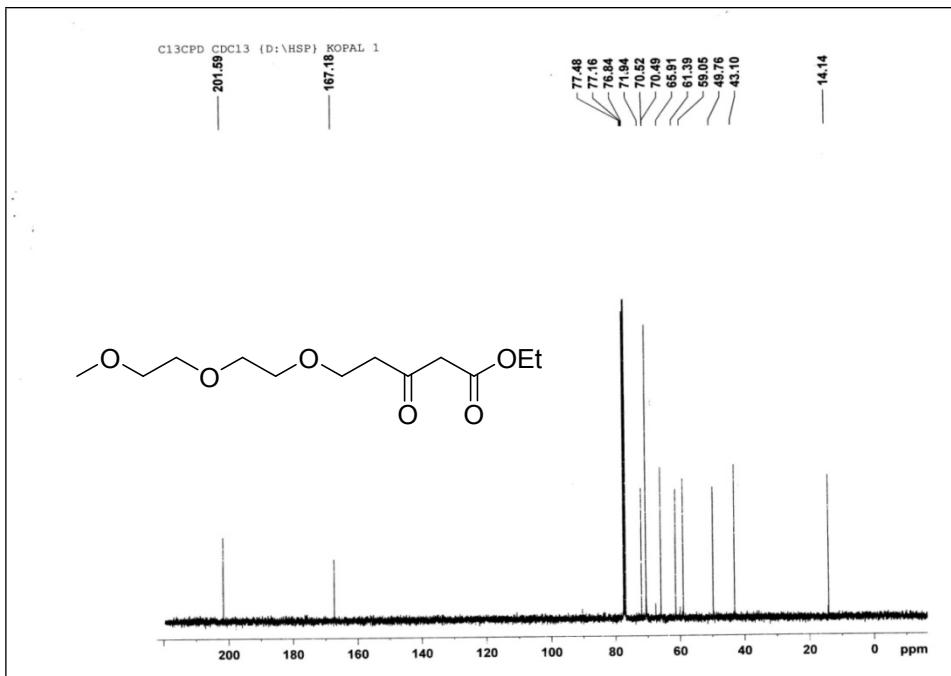


Figure 29. ¹³C NMR (100 MHz, CCl₄ + CDCl₃, 1:1) spectrum of ethyl 5-(2-(2-methoxyethoxy)ethoxy)-3-oxopentanoate **7b**.

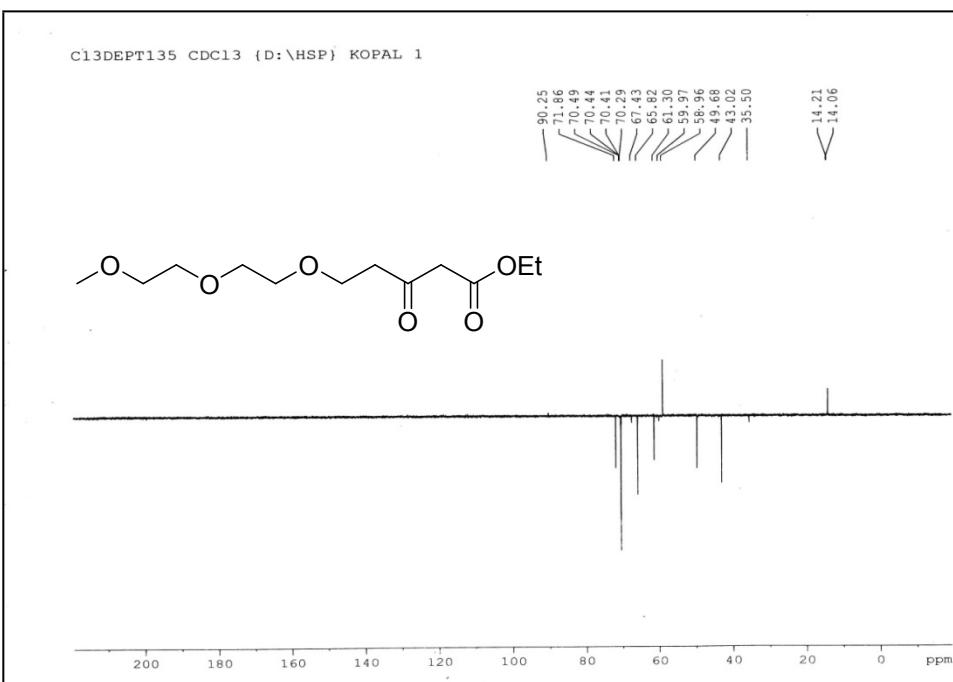


Figure 30. DEPT-135 NMR (100 MHz, CCl₄ + CDCl₃, 1:1) spectrum of ethyl 5-(2-(2-methoxyethoxy)ethoxy)-3-oxopentanoate **7b**.

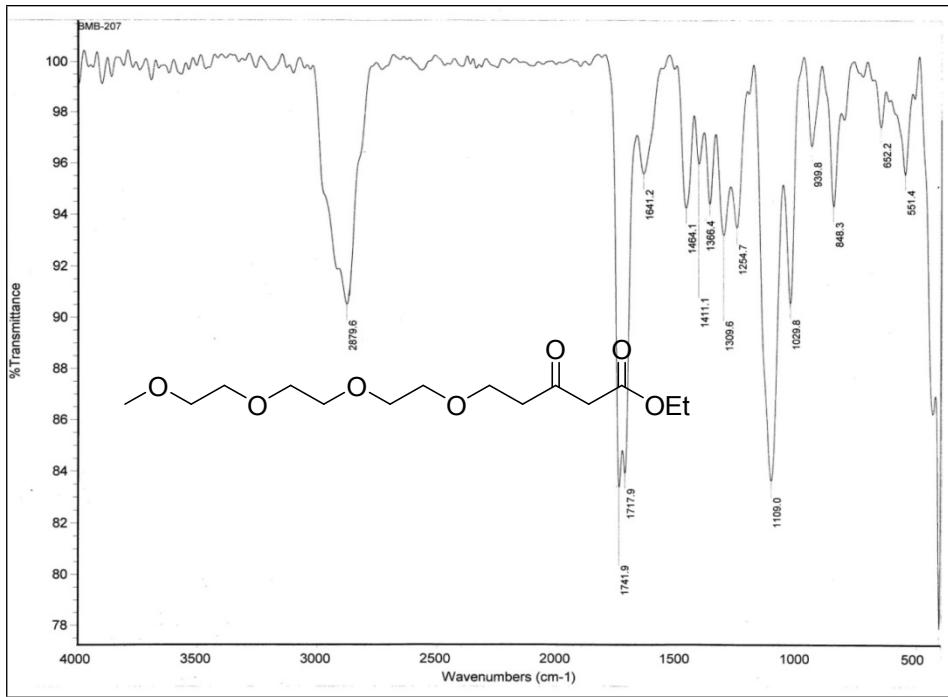


Figure 31. IR (KBr) spectrum of ethyl 14-oxo-2,5,8,11-tetraoxahexadecan-16-oate **7c**.

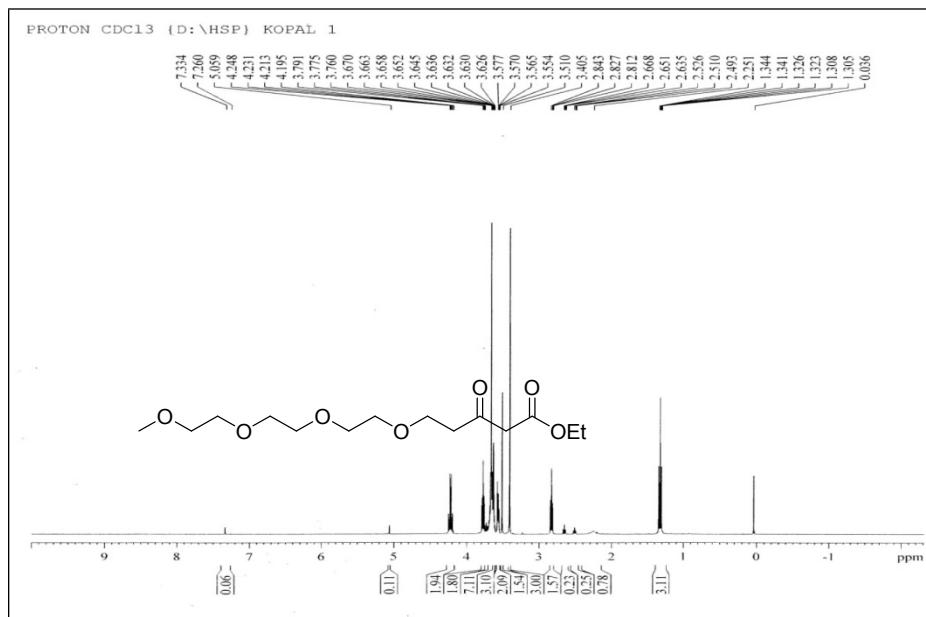


Figure 32. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 14-oxo-2,5,8,11-tetraoxahexadecan-16-oate **7c**.

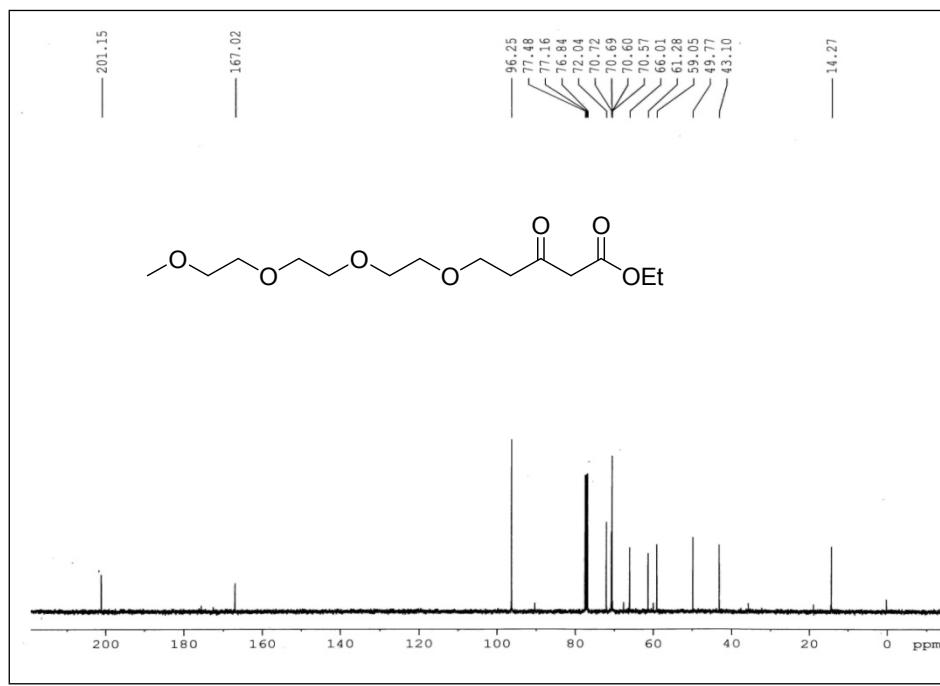


Figure 33. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 14-oxo-2,5,8,11-tetraoxahexadecan-16-oate **7c**.

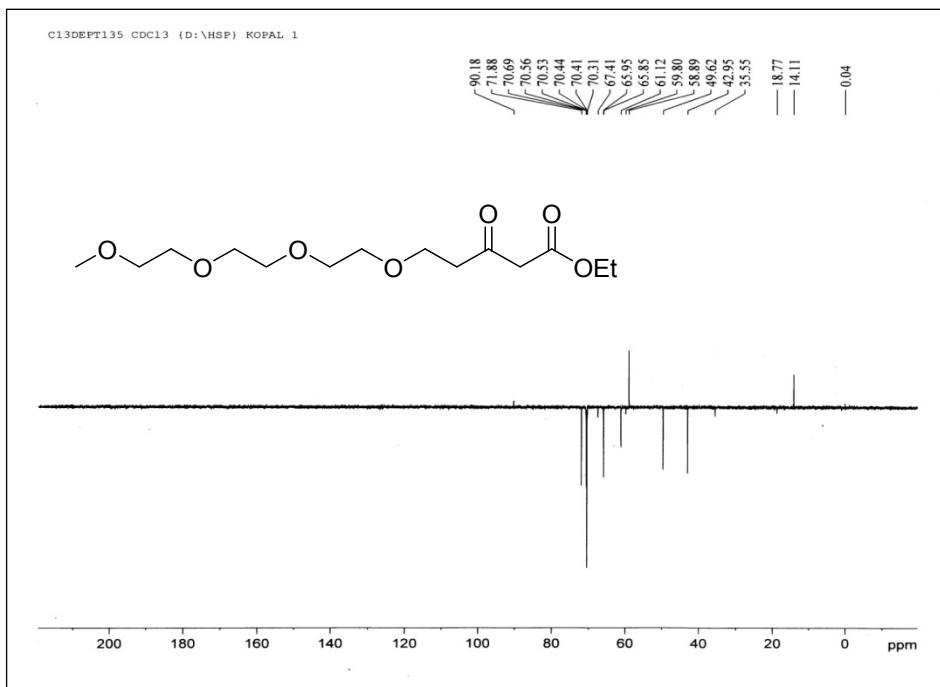


Figure 34. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 14-oxo-2,5,8,11-tetraoxahexadecan-16-oate **7c**.

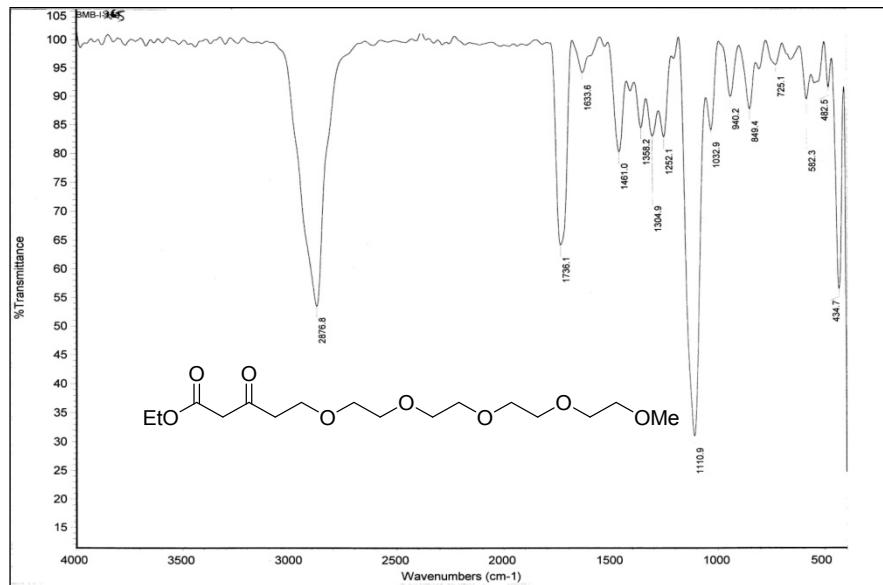


Figure 35. IR (KBr) spectrum of ethyl 17-oxo-2,5,8,11,14-pentaoxanonadecan-19-oate 7d.

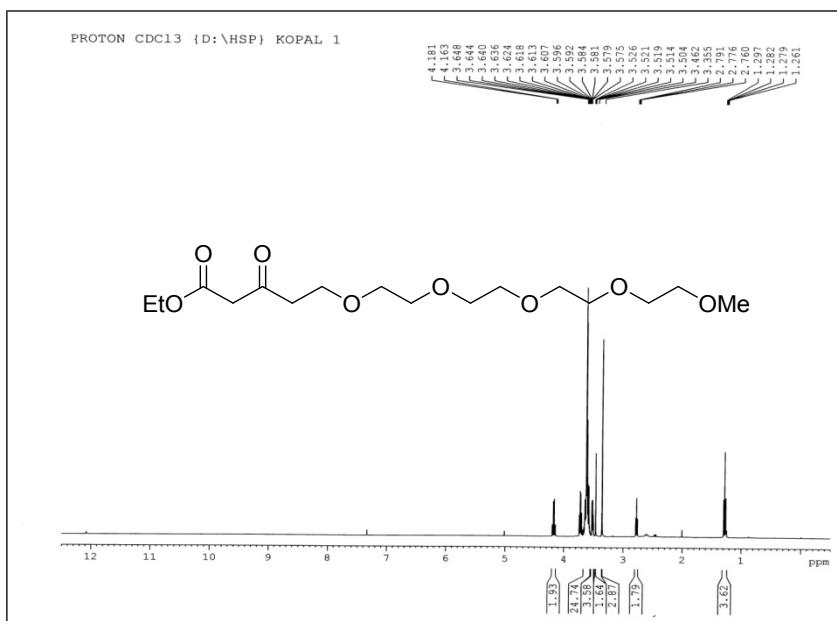


Figure 36. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 17-oxo-2,5,8,11,14-pentaoxanonadecan-19-oate **7d**.

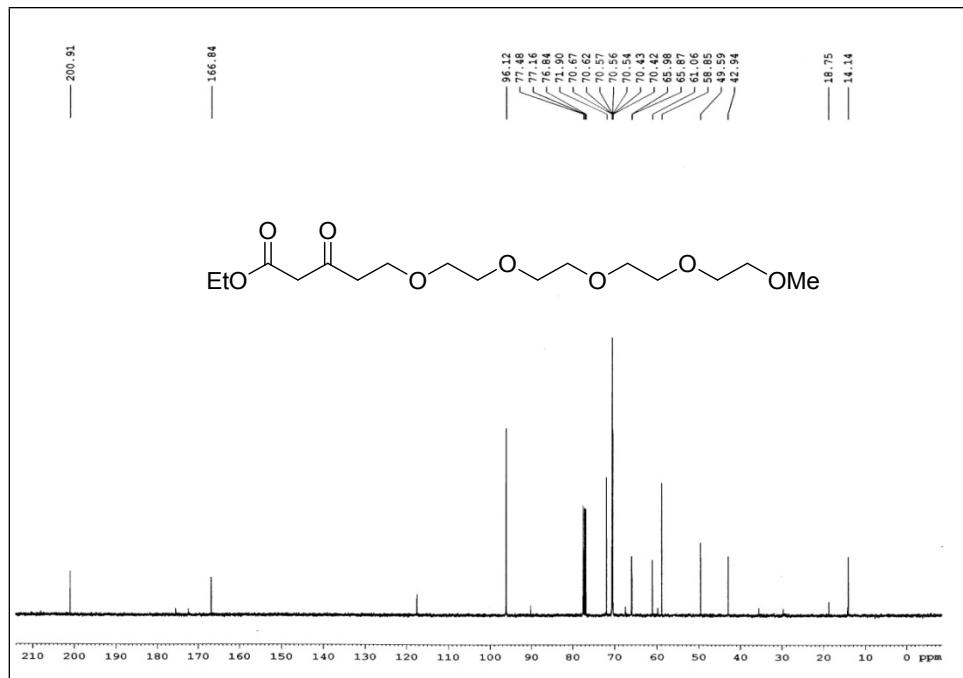


Figure 37. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 17-oxo-2,5,8,11,14-pentaoxanonadecan-19-oate **7d**.

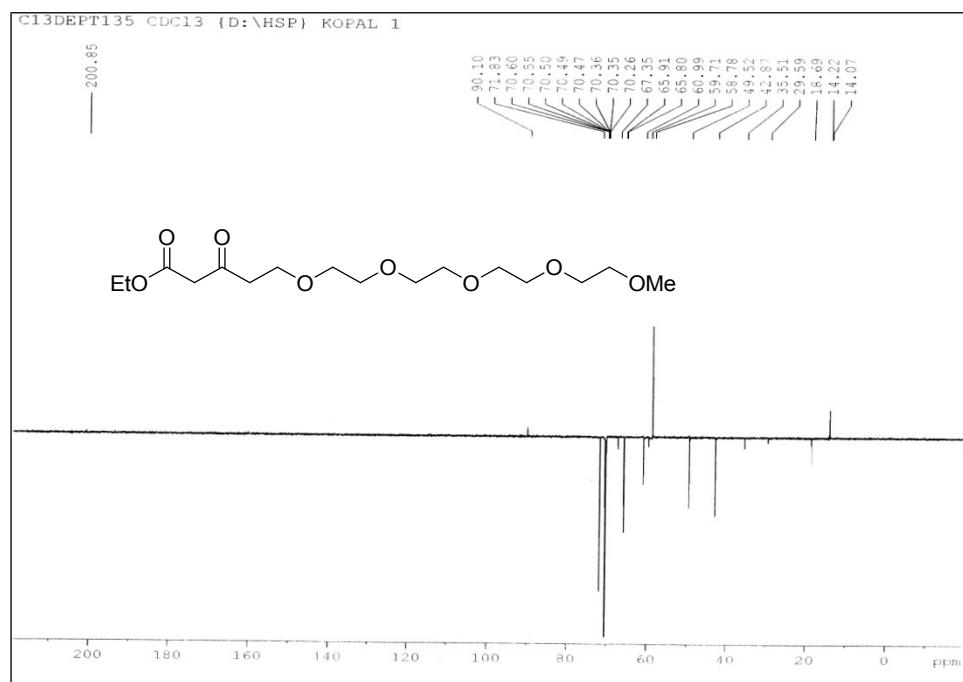


Figure 38. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of ethyl 17-oxo-2,5,8,11,14-pentaoxanonadecan-19-oate **7d**.

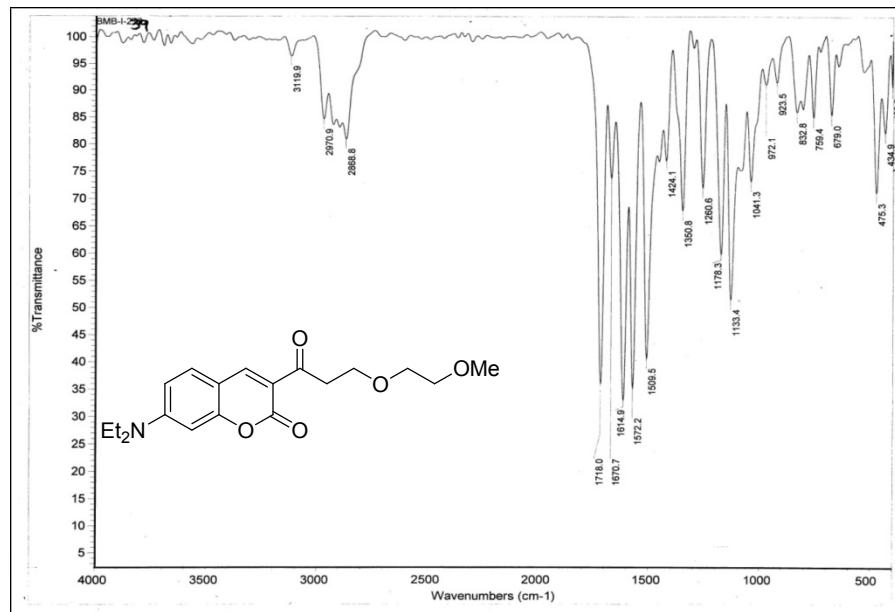


Figure 39. IR (KBr) spectrum of 7-(diethylamino)-3-[3-(2-methoxyethoxy)propanoyl]-2H-chromen-2-one **4a**.

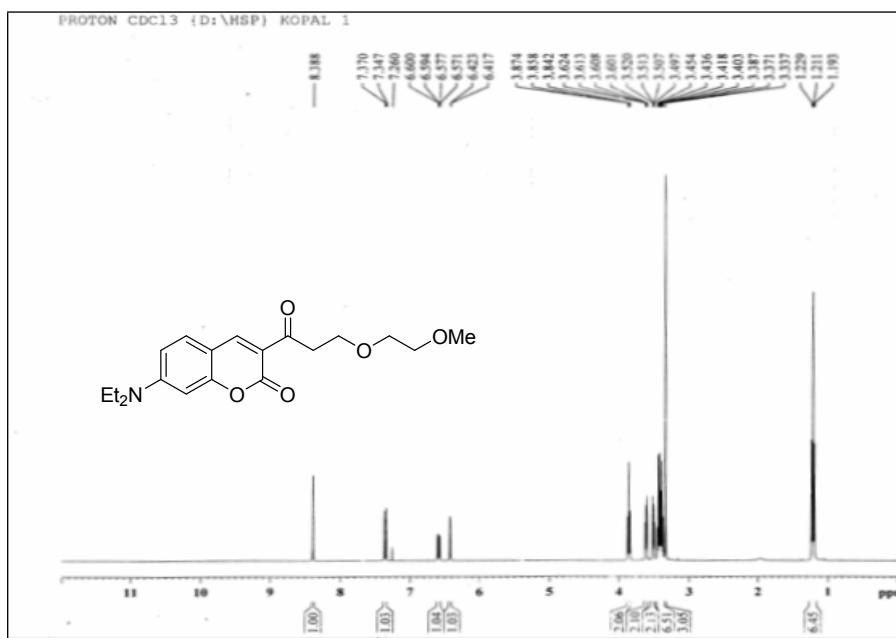


Figure 40. ¹H NMR (400 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 7-(diethylamino)-3-[3-(2-methoxyethoxy)propanoyl]-2H-chromen-2-one **4a**.

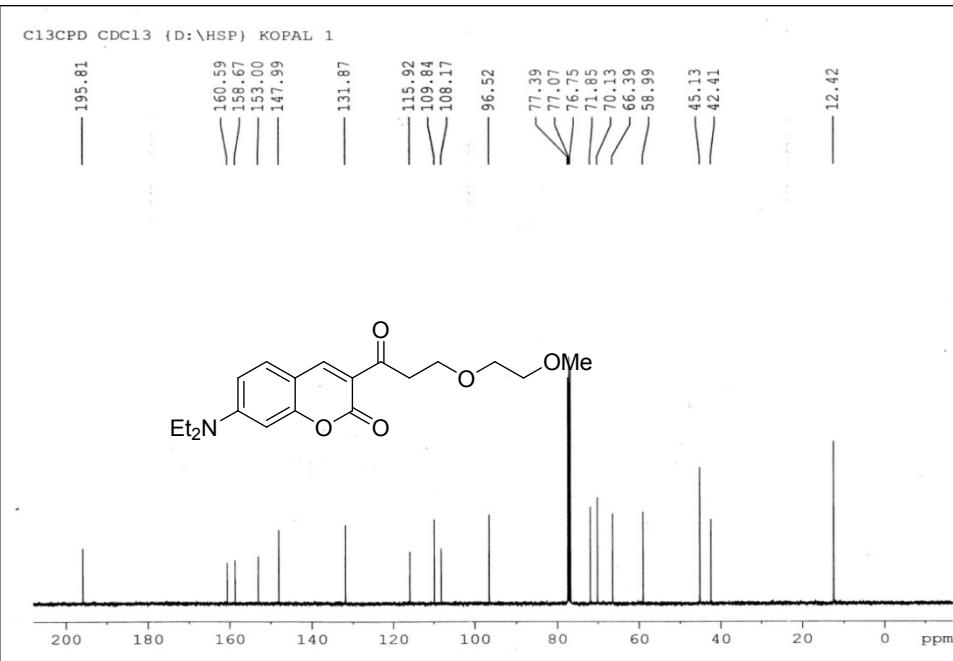


Figure 41. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(diethylamino)-3-[3-(2-methoxyethoxy)propanoyl]-2H-chromen-2-one **4a**.

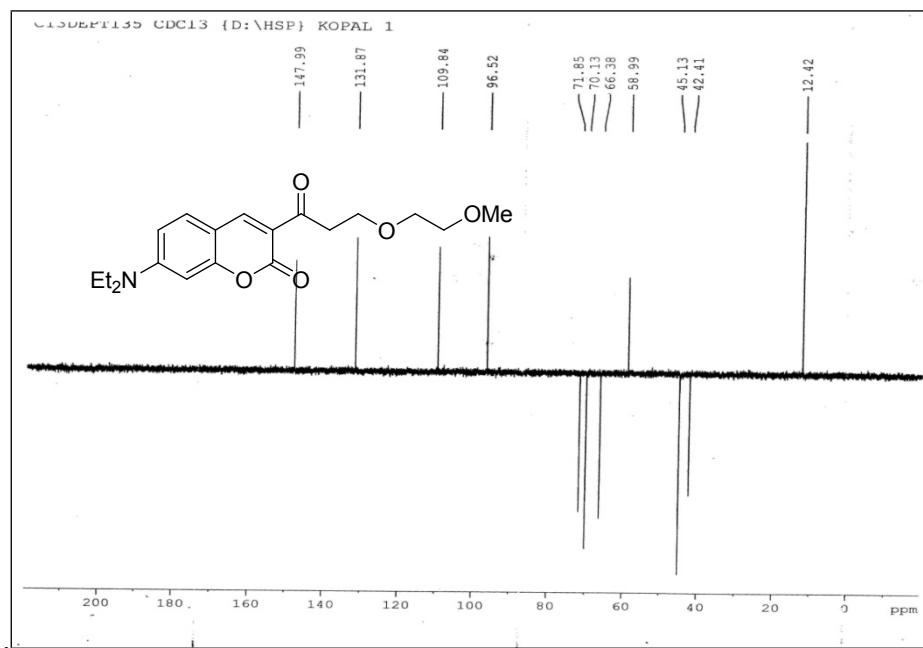


Figure 42. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(diethylamino)-3-[3-(2-methoxyethoxy)propanoyl]-2H-chromen-2-one **4a**.

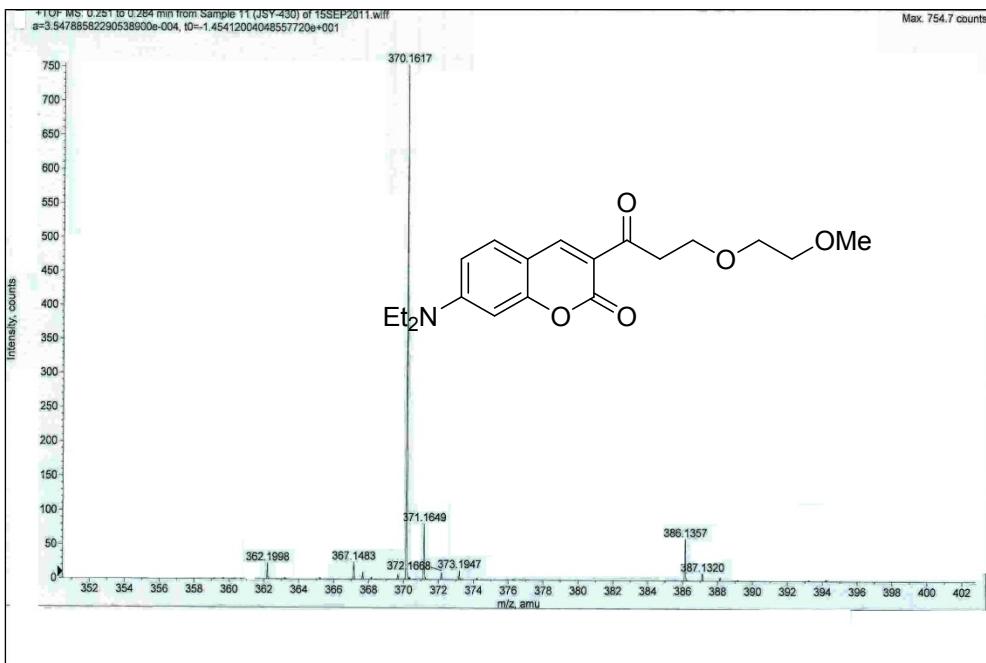


Figure 43. ESI-MS (HRMS) spectrum of 7-(diethylamino)-3-[3-(2-methoxyethoxy)propanoyl]-2H-chromen-2-one **4a**.

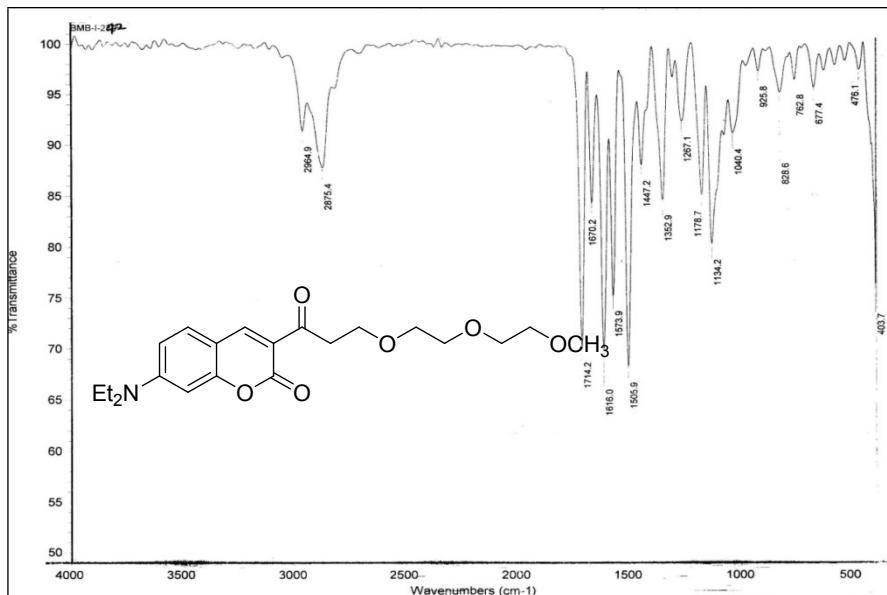


Figure 44. IR (KBr) spectrum of 7-(dimethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]propanoyl]-2H-chromen-2-one **4b**.

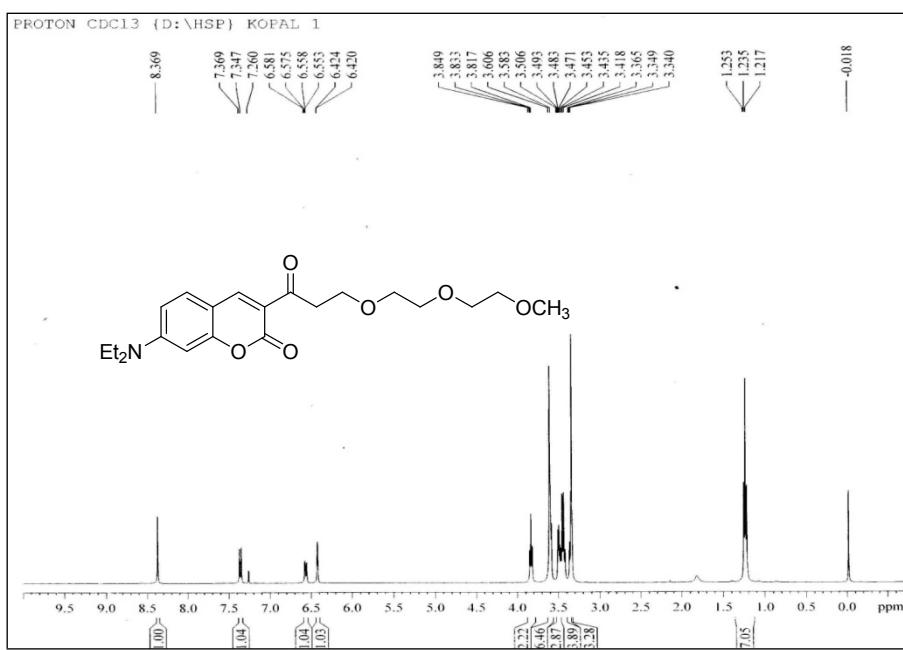


Figure 45. ^1H NMR (400 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(dimethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]propanoyl]-2H-chromen-2-one **4b**.

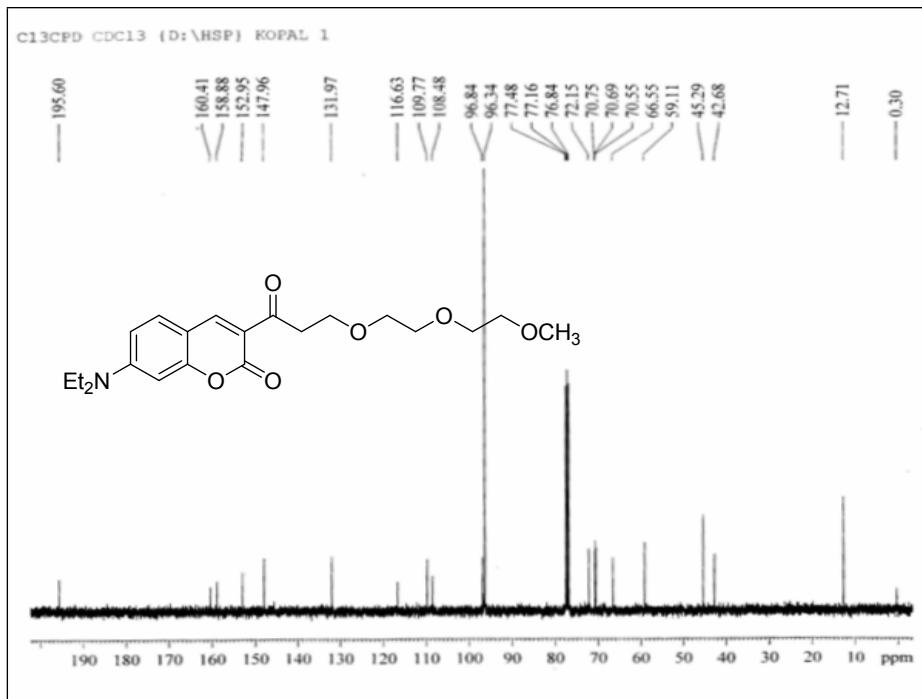


Figure 46. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(dimethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]propanoyl]-2*H*-chromen-2-one **4b**.

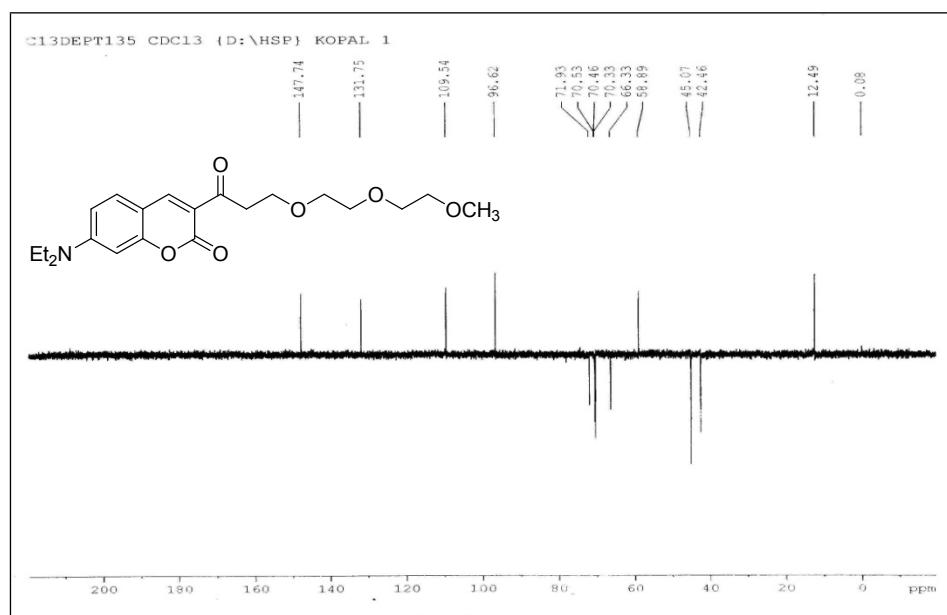


Figure 47. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(dimethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]propanoyl]-2*H*-chromen-2-one **4b**.

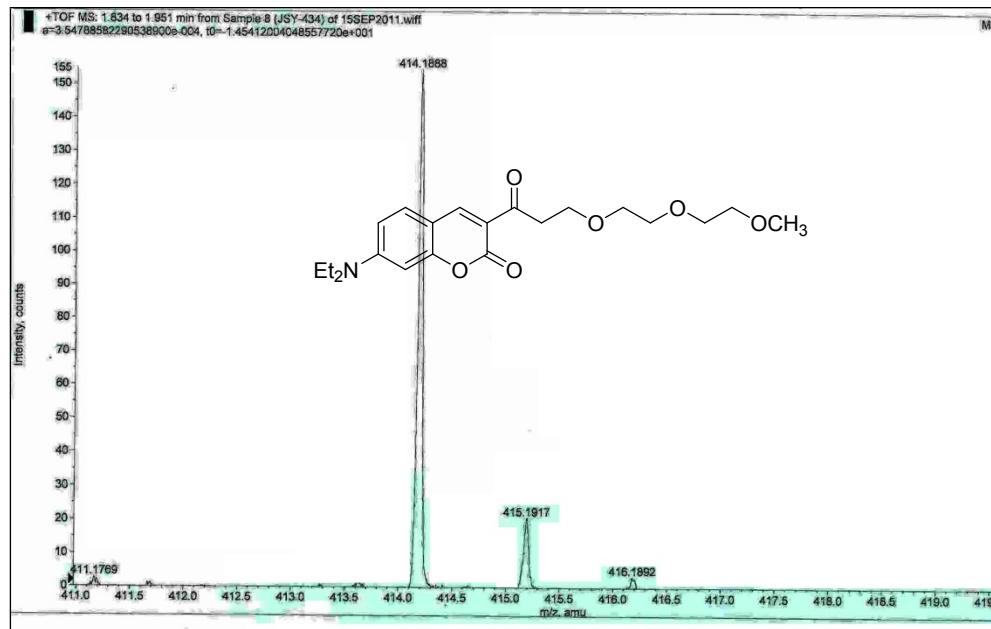


Figure 48. ESI-MS (HRMS) spectrum of 7-(dimethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]propanoyl]-2H-chromen-2-one **4b**.

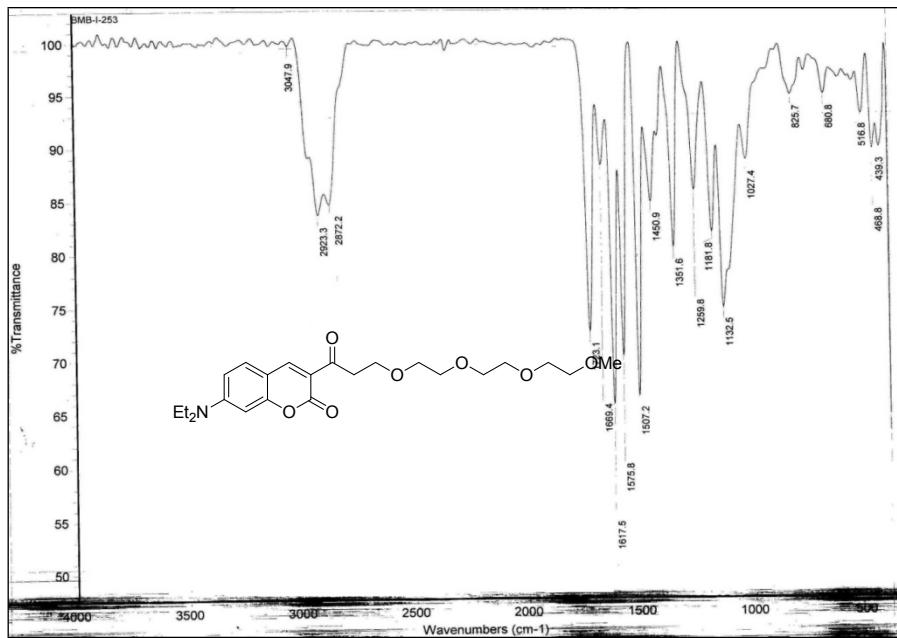


Figure 49. IR (KBr) spectrum of 7-(diethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4c**.

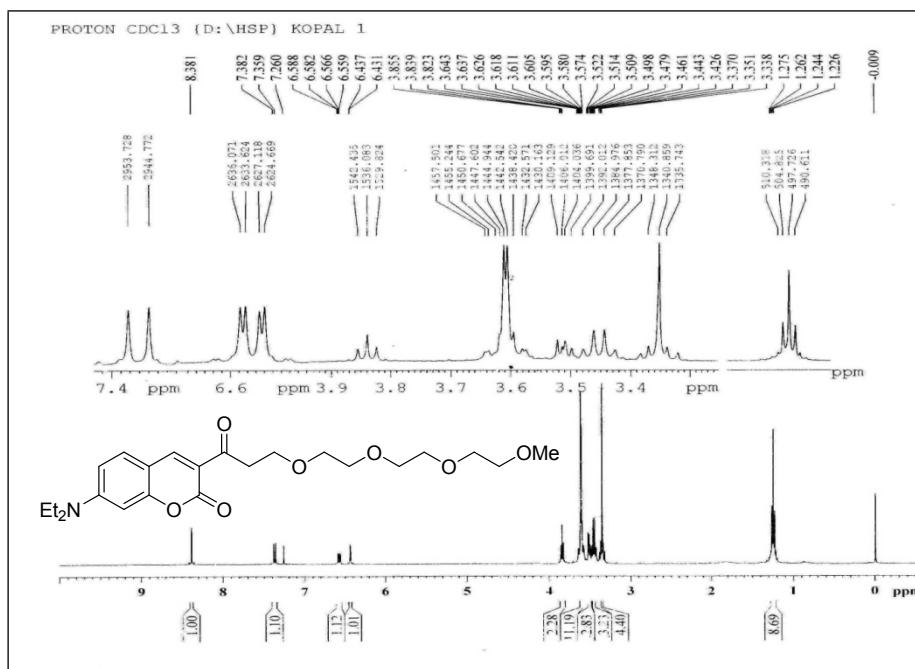


Figure 50. ¹H NMR (400 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 7-(diethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4c**.

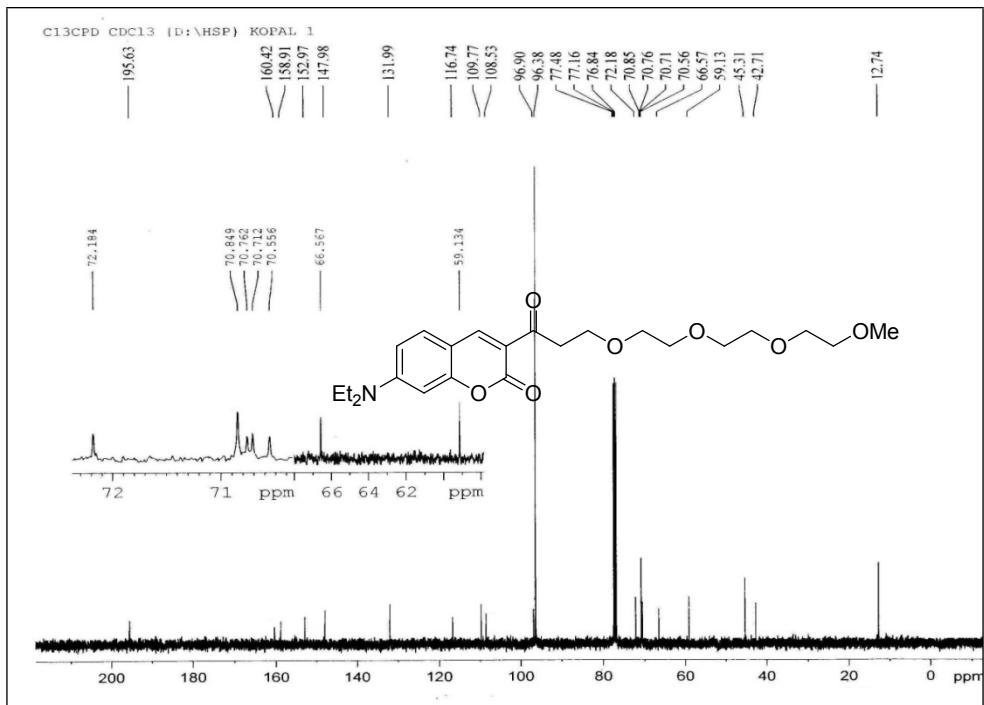


Figure 51. ¹³C NMR (100 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 7-(diethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4c**.

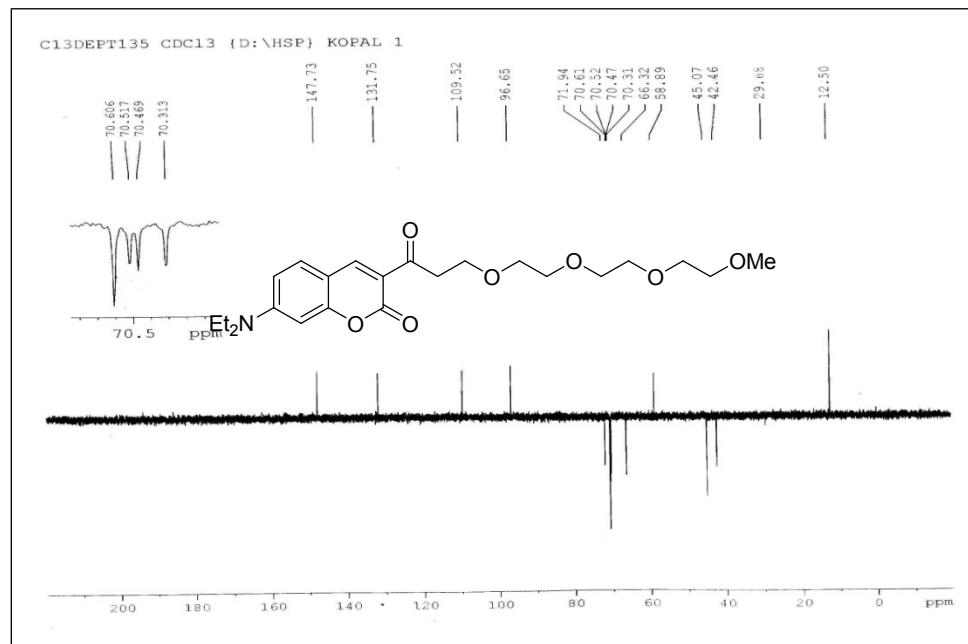


Figure 52. DEPT-135 NMR (100 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 7-(diethylamino)-3-[3-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4c**.

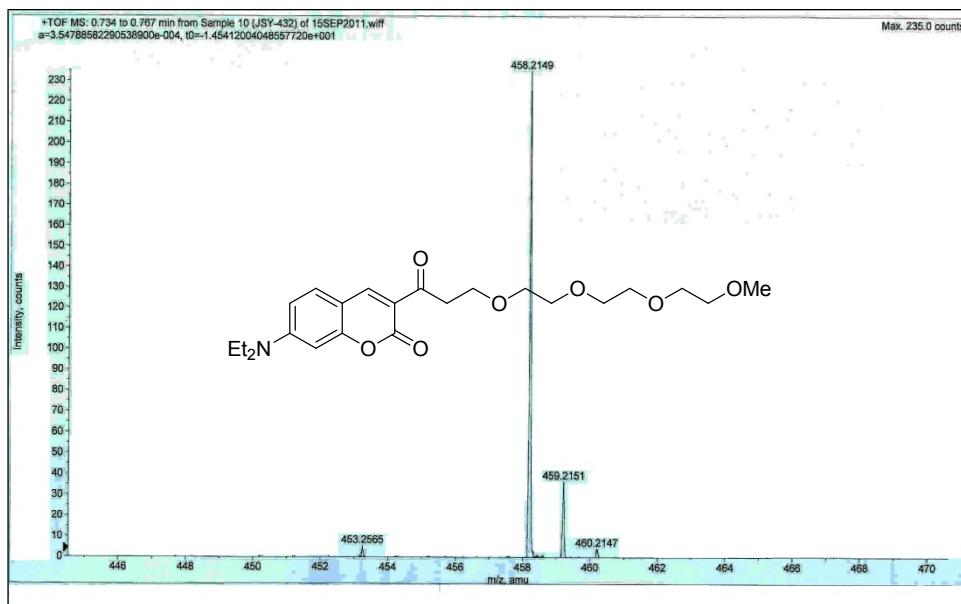


Figure 53. ESI-MS (HRMS) spectrum of 7-(diethylamino)-3-[3-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4c**.

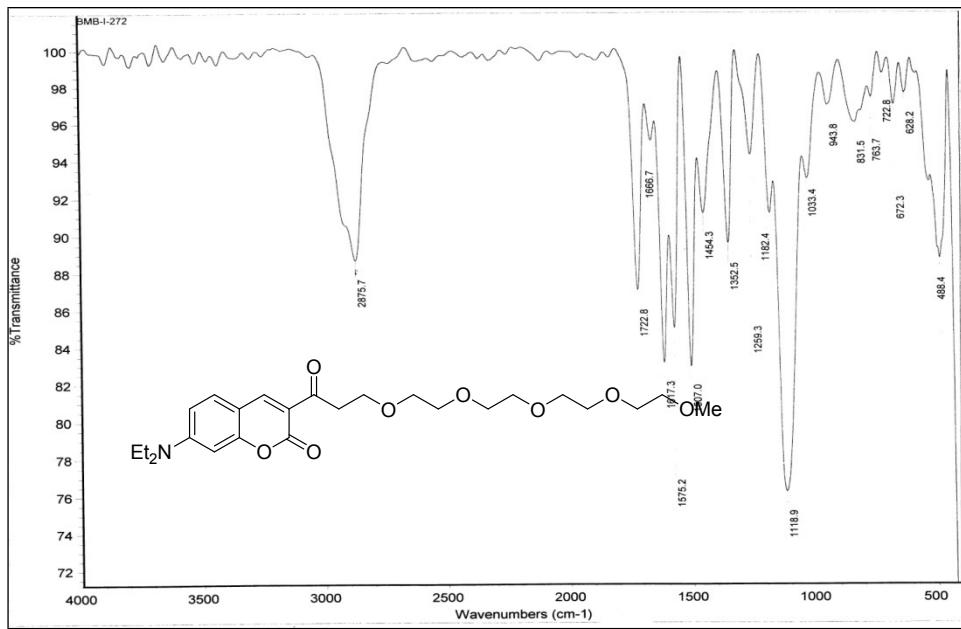


Figure 54. IR (KBr) spectrum of 7-(diethylamino)-3-[3-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4d**.



Figure 55. ¹H NMR (400 MHz, CCl₄ + CDCl₃, 1:1) spectrum of 7-(diethylamino)-3-[3-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4d**.

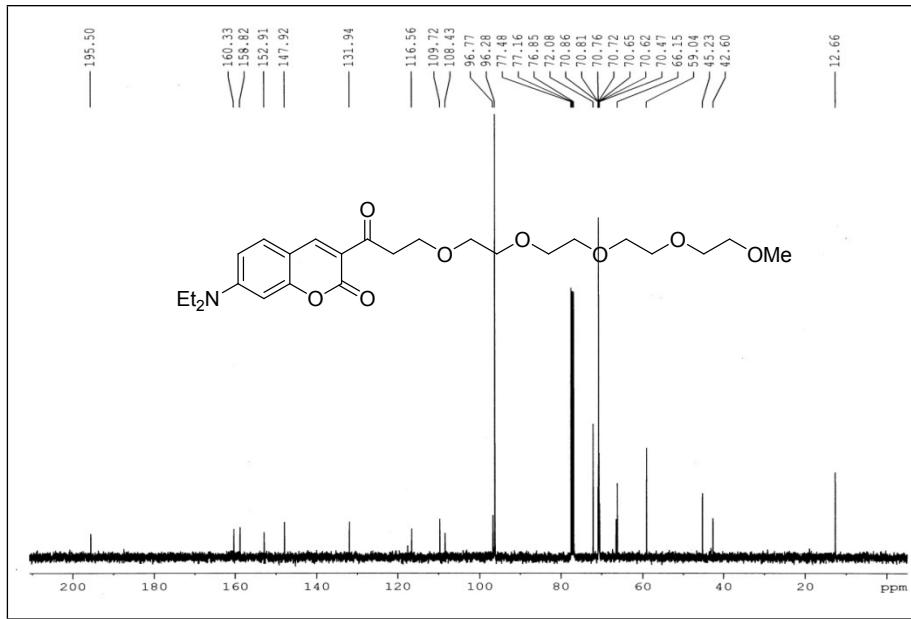


Figure 56. ^{13}C NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(diethylamino)-3-[3-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2*H*-chromen-2-one **4d**.

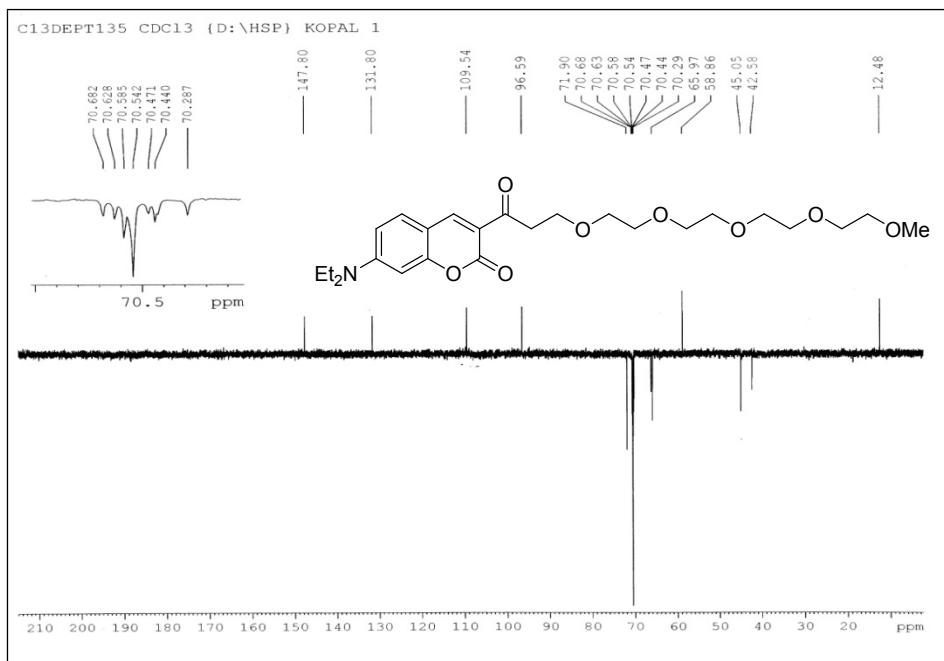


Figure 57. DEPT-135 NMR (100 MHz, $\text{CCl}_4 + \text{CDCl}_3$, 1:1) spectrum of 7-(diethylamino)-3-[3-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]ethoxy]propanoyl]-2*H*-chromen-2-one **4d**

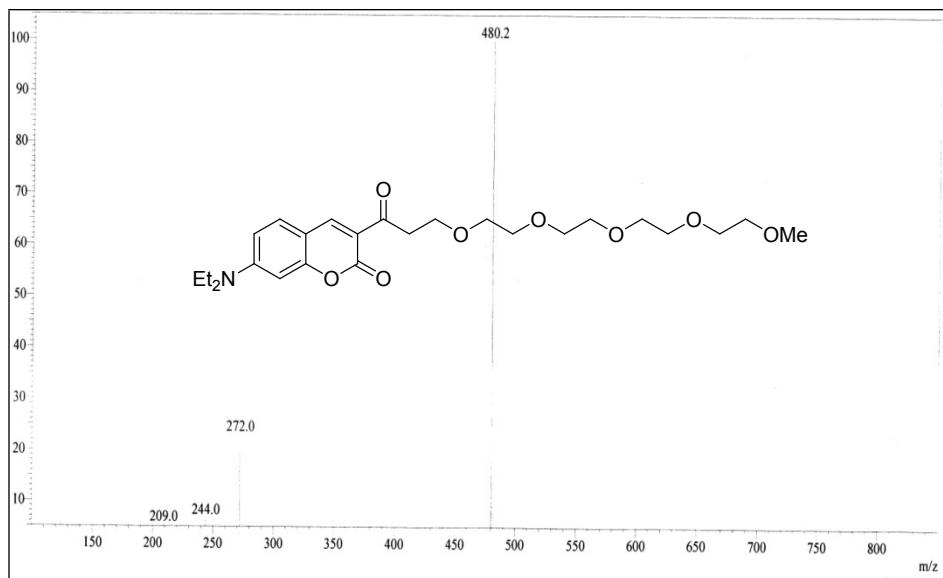


Figure 58. ESI-MS (HRMS) spectrum of 7-(diethylamino)-3-[3-[2-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]propanoyl]-2H-chromen-2-one **4d**.

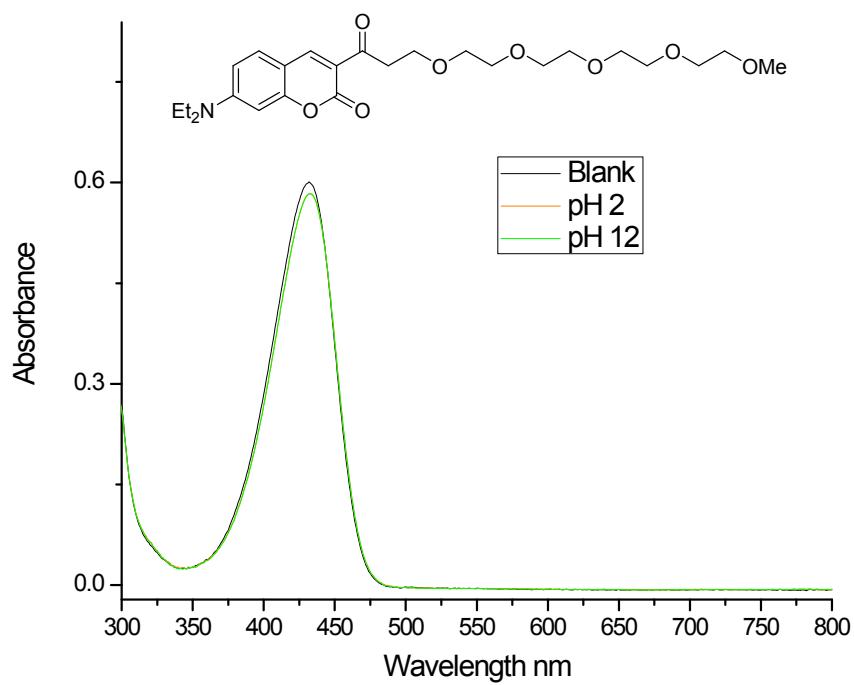


Figure 59. Uv spectrum of **4d** recorded at pH 7, pH 2 and pH 12