

Supplementary Materials

(copies of spectra)

Article

Isomers of β,β -Dinitro-5,10,15,20-tetraphenylporphyrin Derivatives: Valuable Starting Materials for Further Transformations

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(2,7-dinitro-5,10,15,20-tetraphenylporphyrinato)copper(II) (**3ca**)

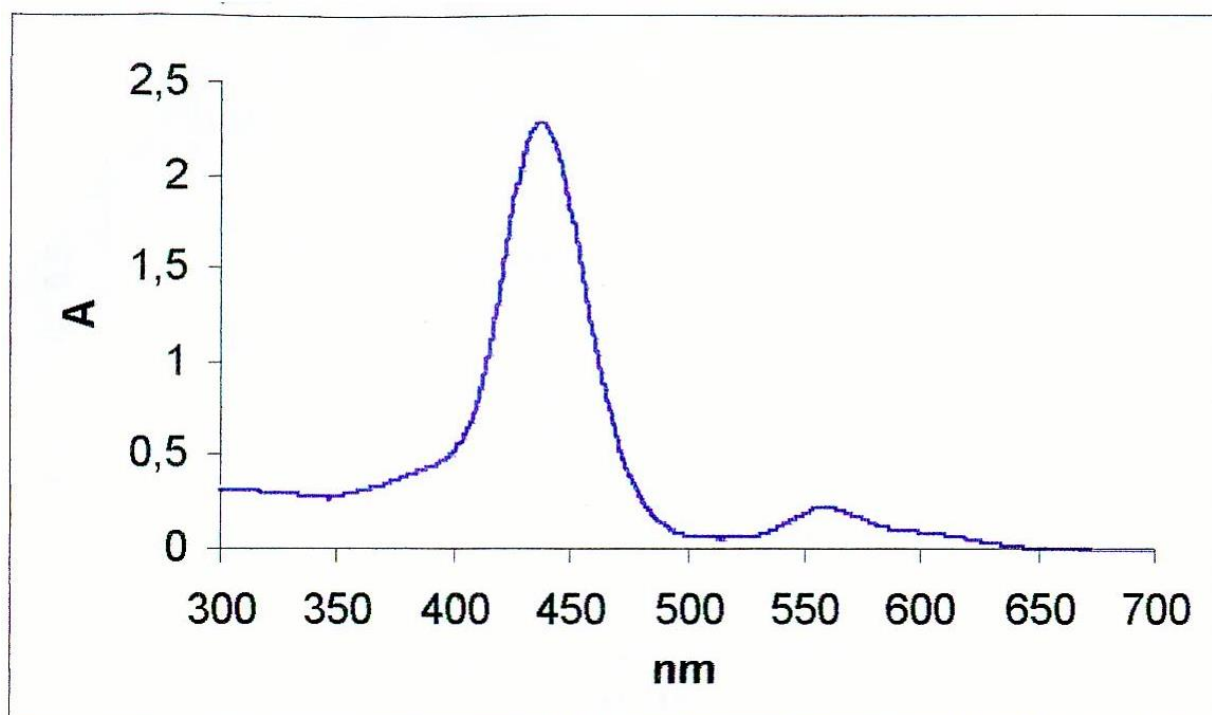


Figure 1. UV-vis spectrum of product **3ca**.

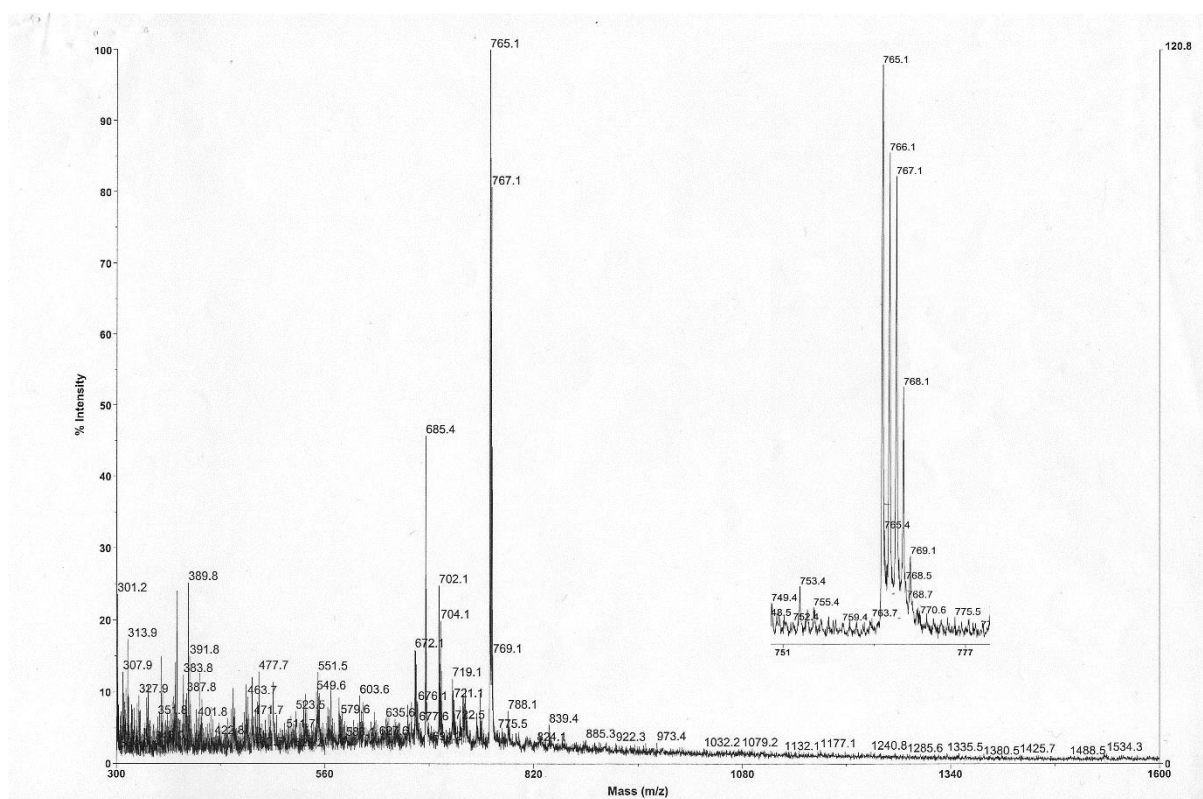


Figure 2. MS spectrum of product **3ca** (ESI technique; positive ions mode).

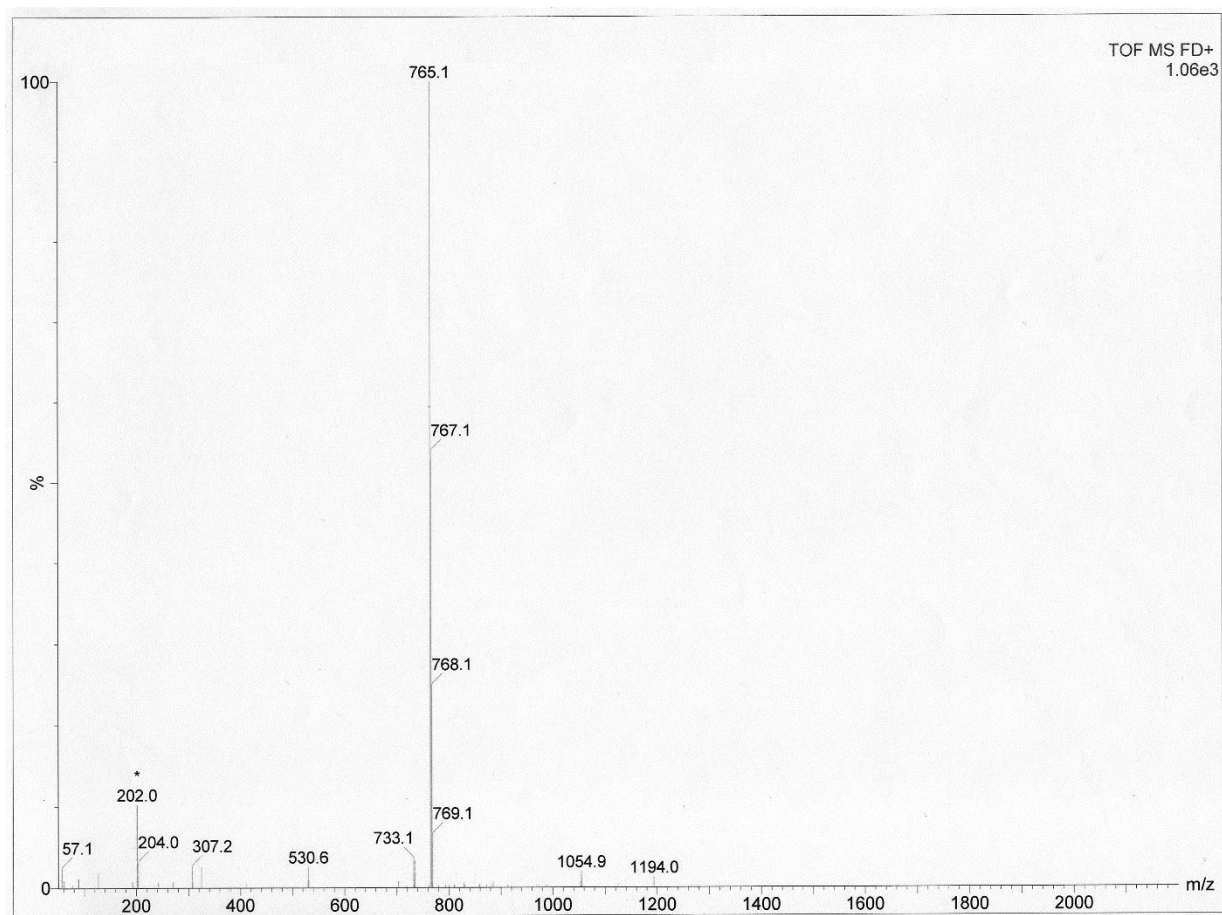


Figure 3. MS spectrum of product **3ca** (FD technique).

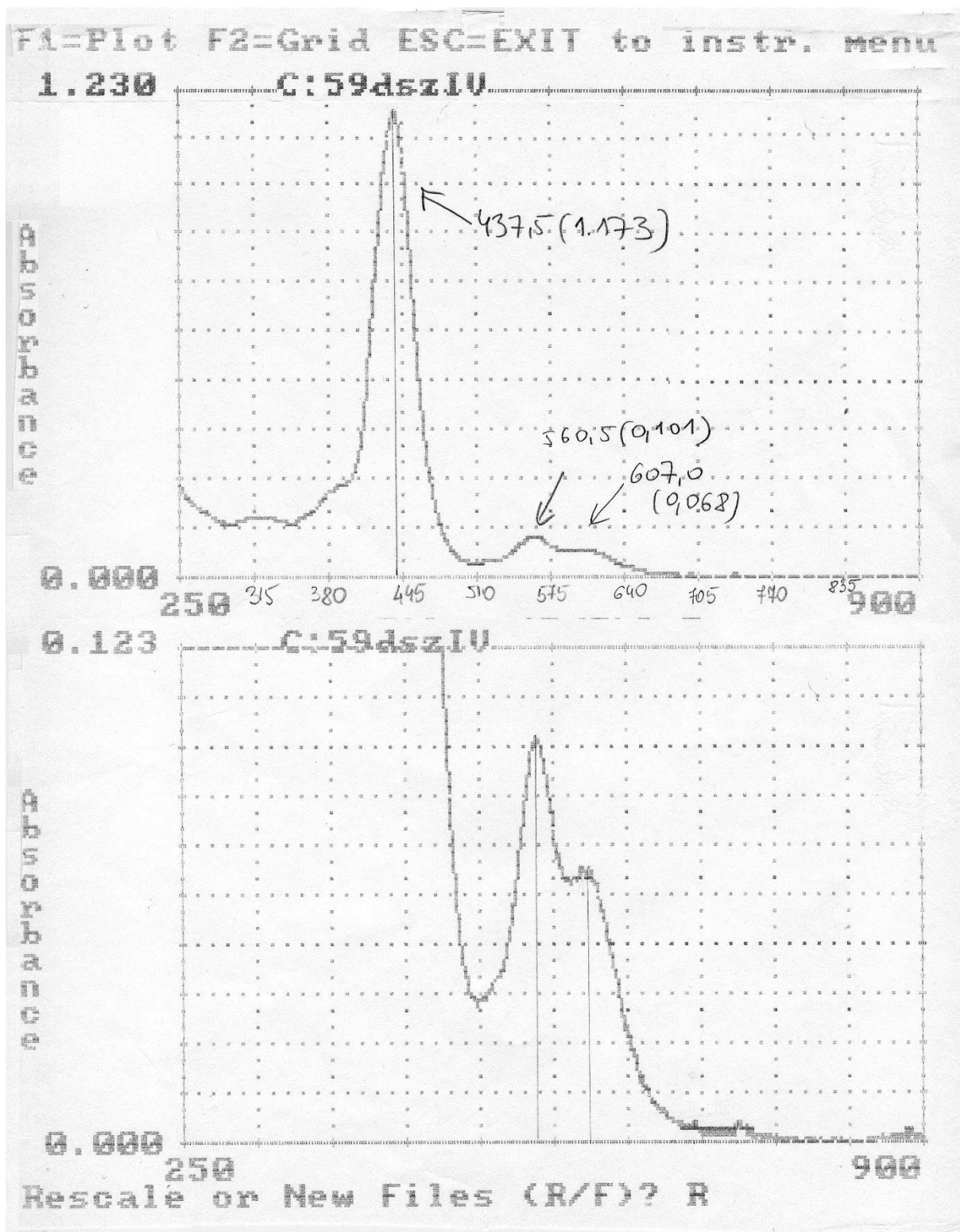
(3,7-dinitro-5,10,15,20-tetraphenylporphyrinato)copper(II) (**3c**)

Figure 4. UV-vis spectrum of product **3cb**.

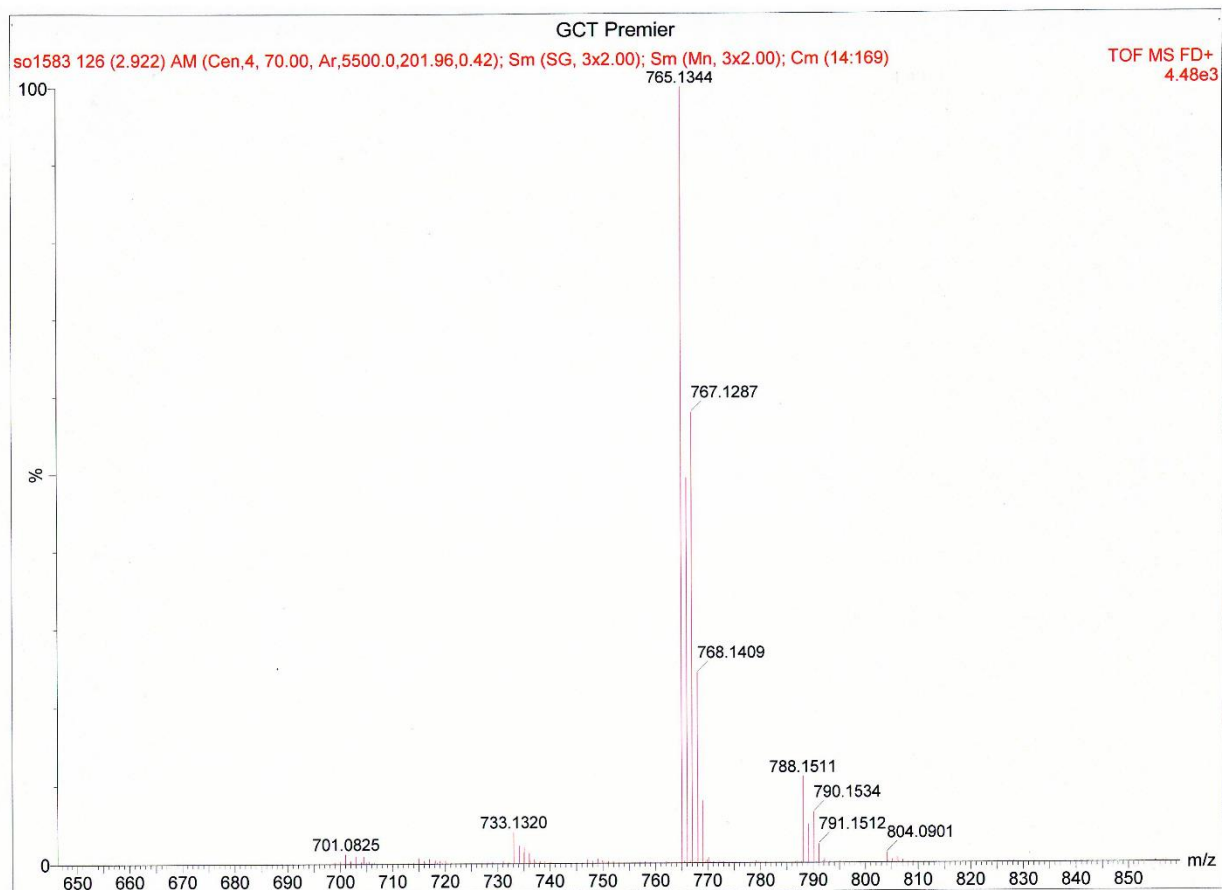


Figure 5. MS spectrum of product **3cb** (FD technique).

(2,8-dinitro-5,10,15,20-tetraphenylporphyrinato)copper(II) (**3cc**)

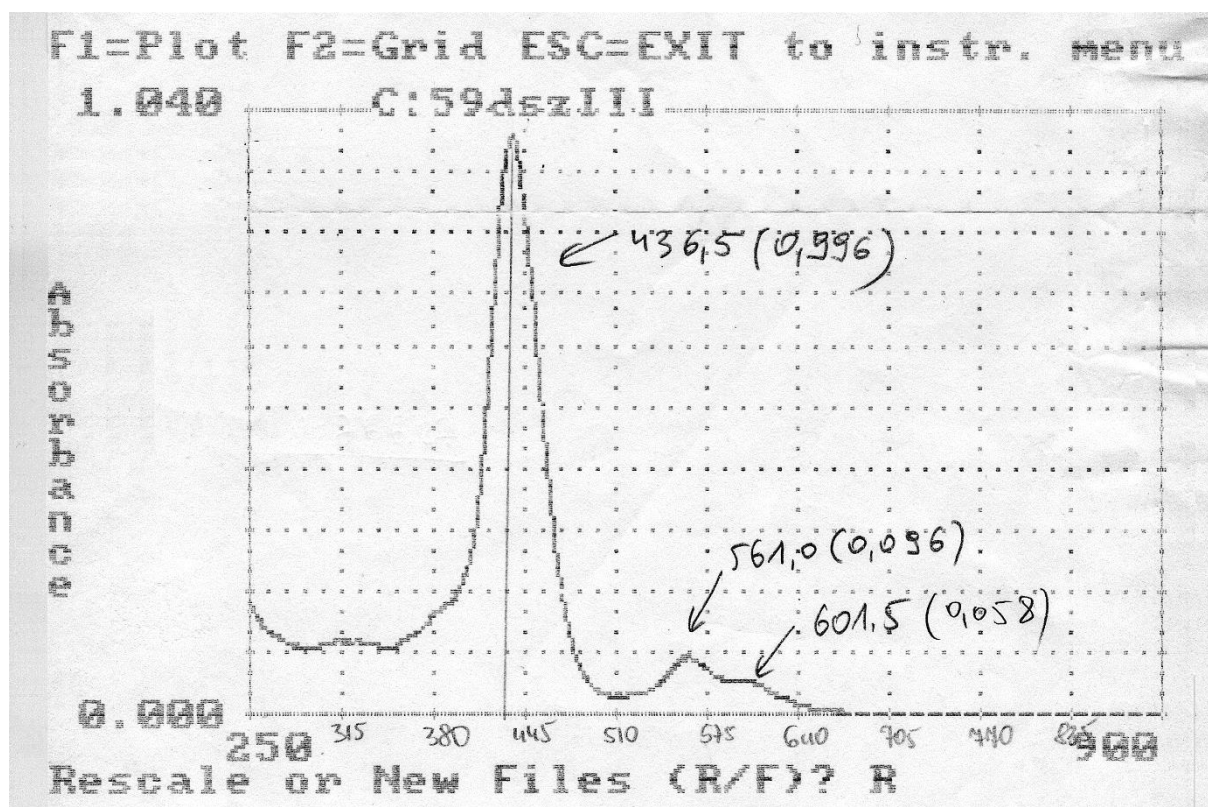


Figure 6. UV-vis spectrum of product **3cc**.

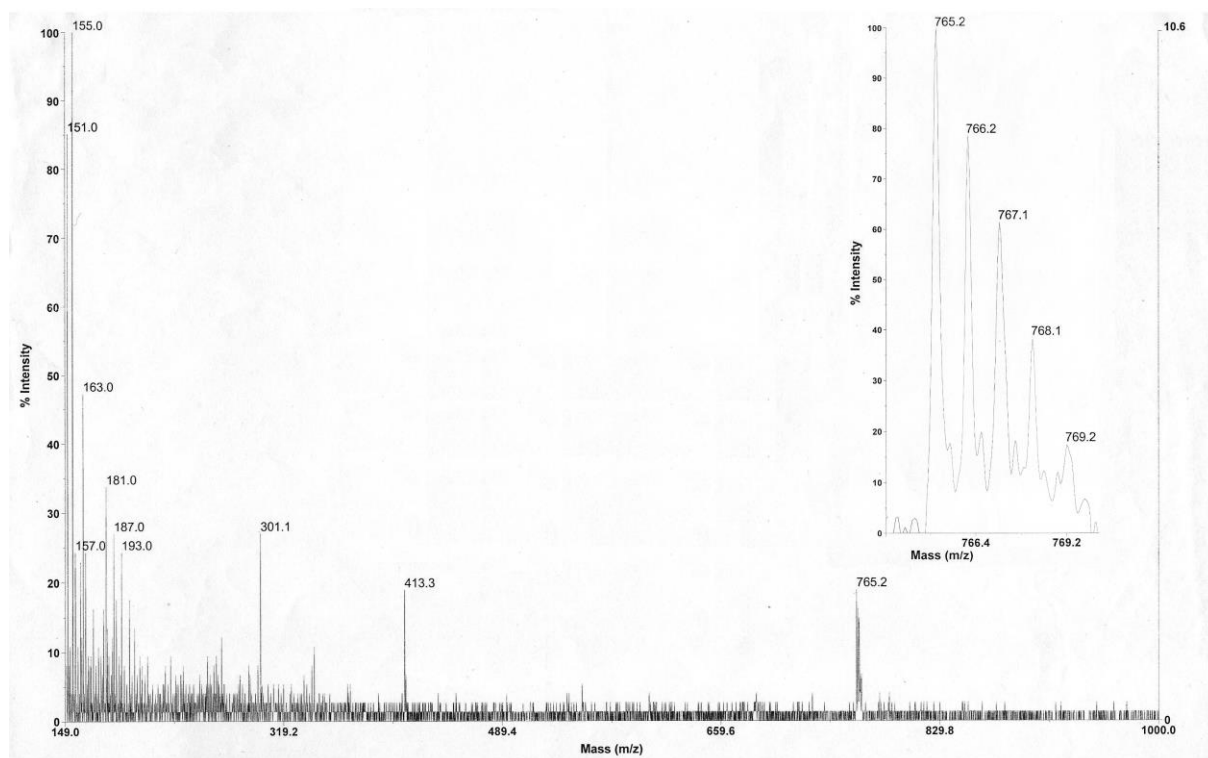


Figure 7. MS spectrum of product **3cc** (FD technique).

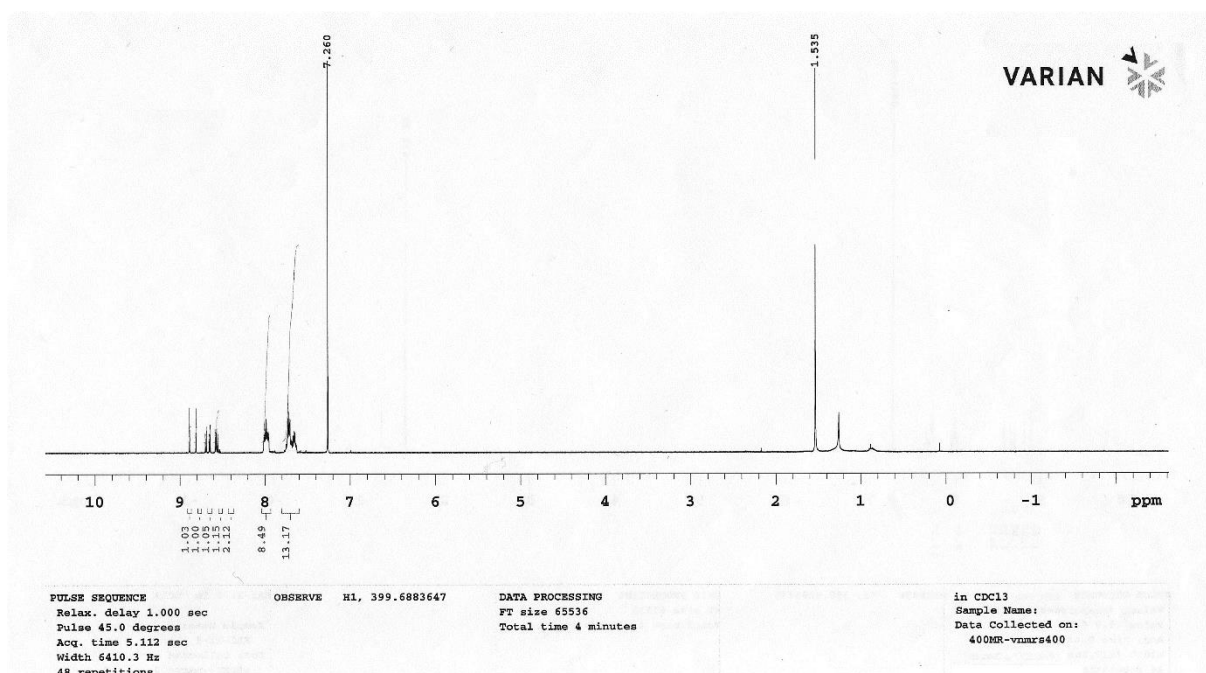
(2,7-dinitro-5,10,15,20-tetraphenylporphyrinato)nickel(II) (**3da**)

Figure 8. ^1H NMR spectrum of product **3da**.

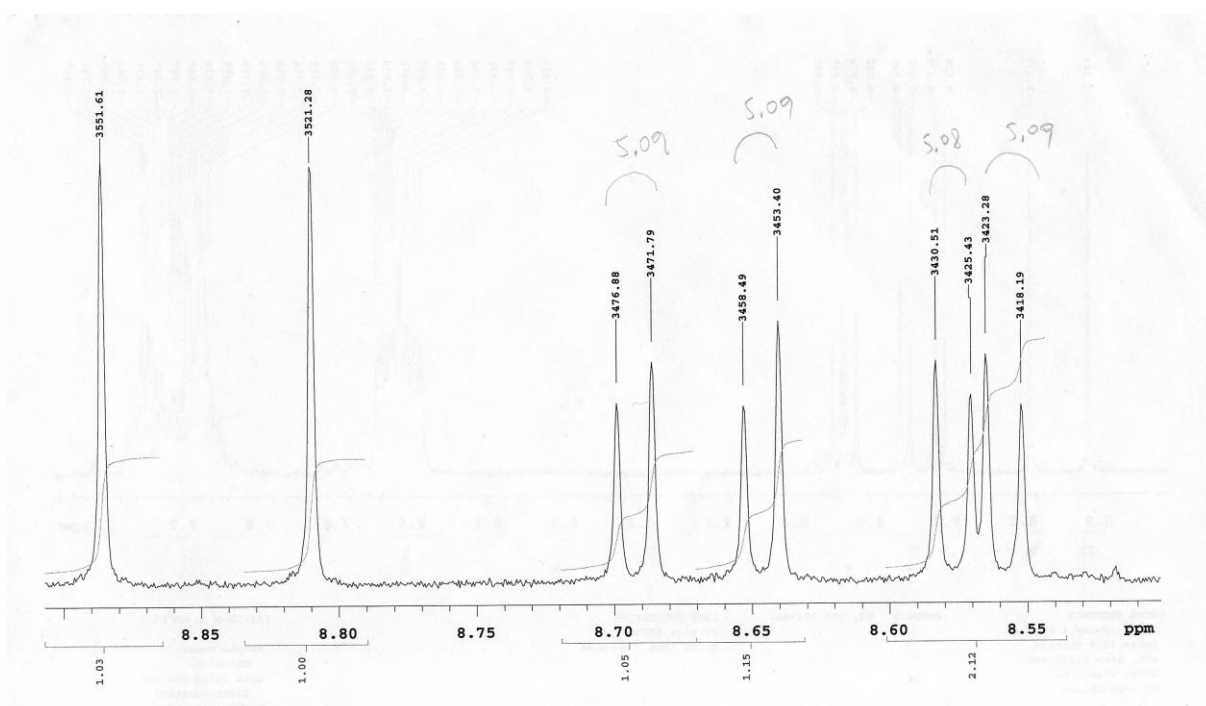


Figure 9. ^1H NMR spectrum of product **3da** (range: 8.50 – 8.90 ppm).

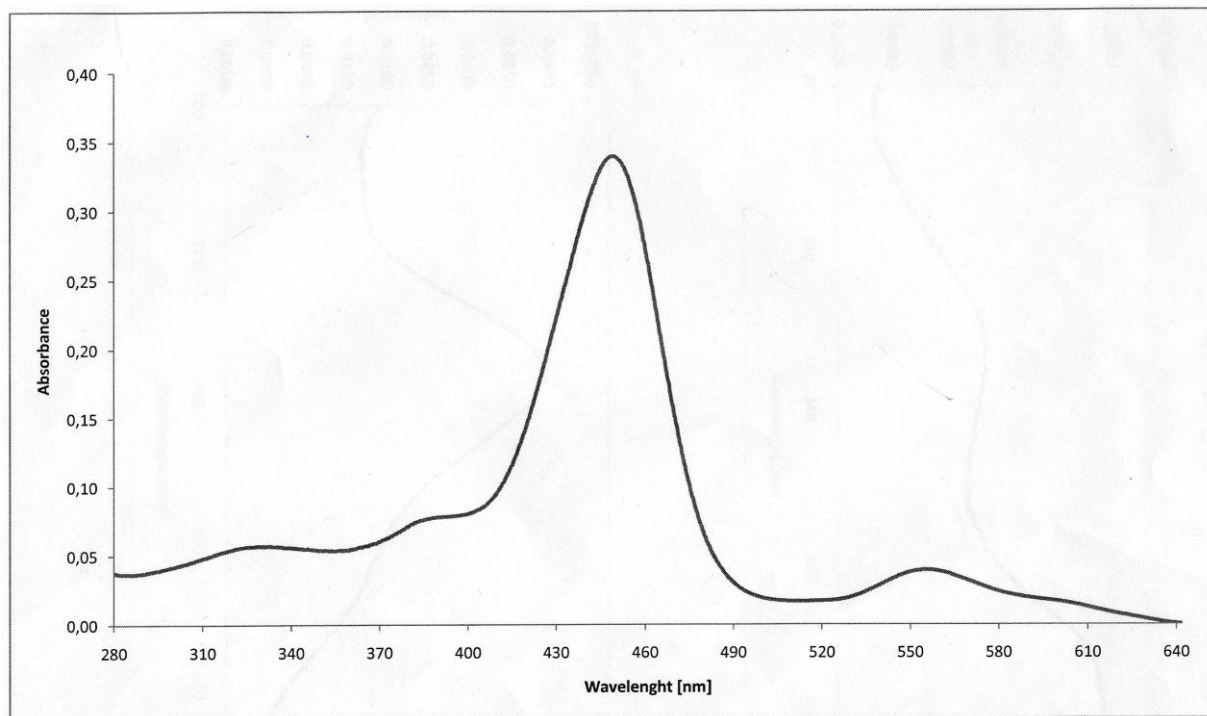


Figure 10. UV-vis spectrum of product **3da**.

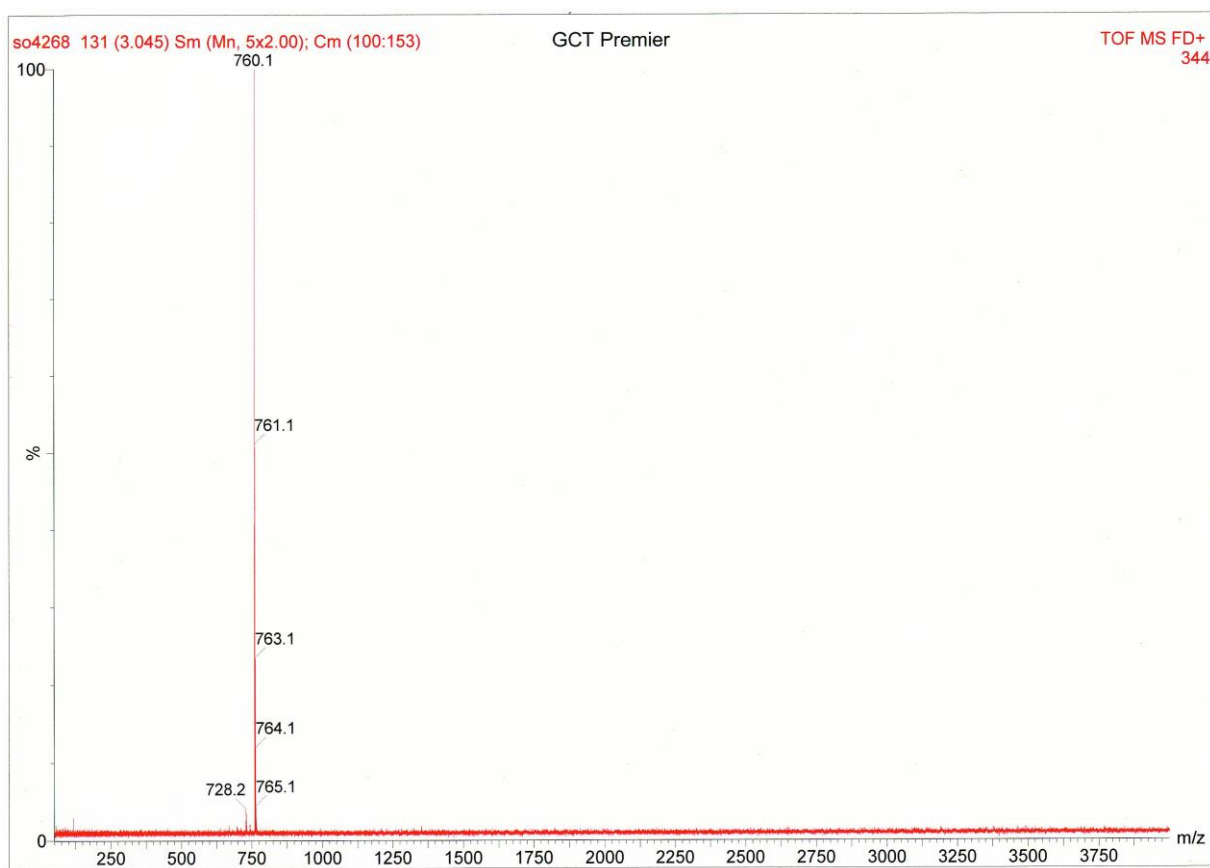


Figure 11. MS spectrum of product **3da** (FD technique).

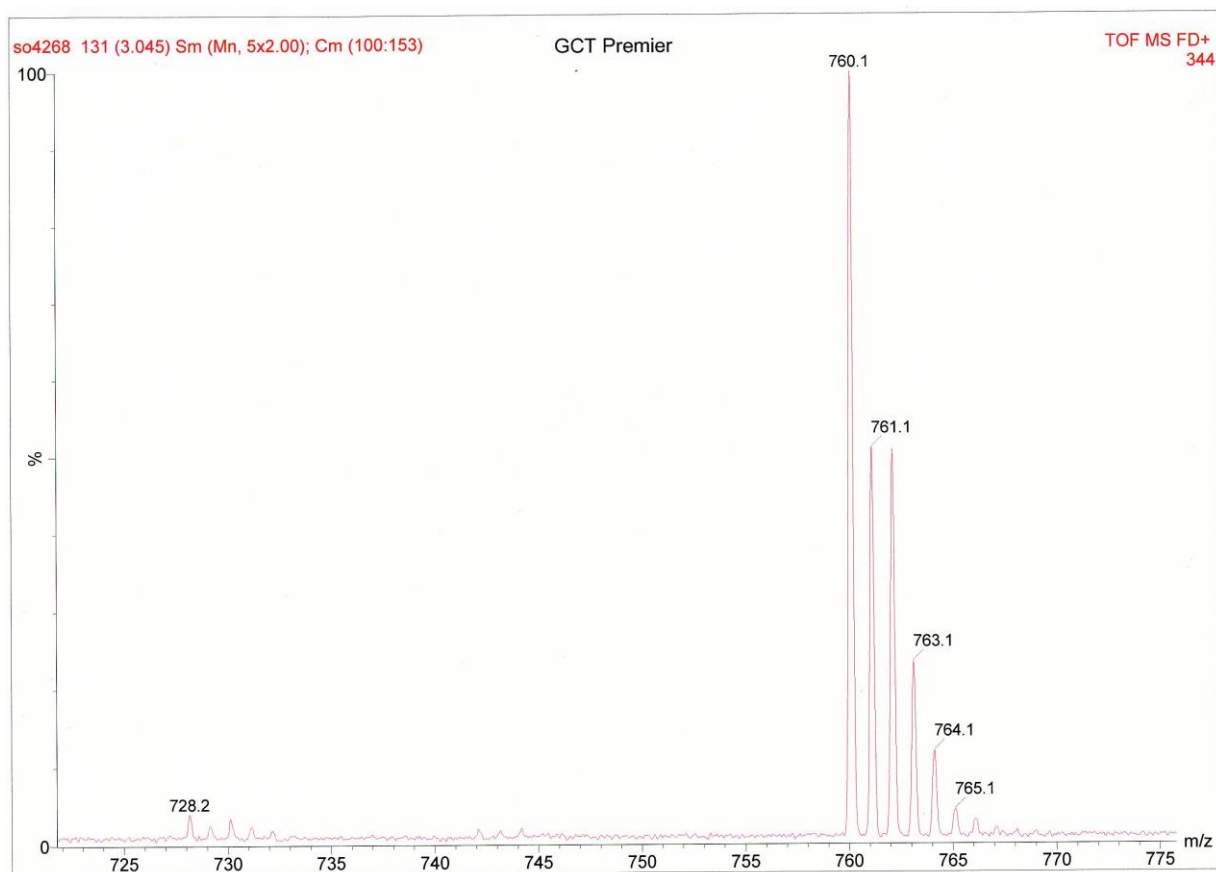


Figure 12. MS spectrum of product **3da** (range: $m/z = 725 - 775$; FD technique).

(3,7-dinitro-5,10,15,20-tetraphenylporphyrinato)nickel(II) (**3db**)

^1H NMR spectrum – see the copy in the text, *Section 2.4*.

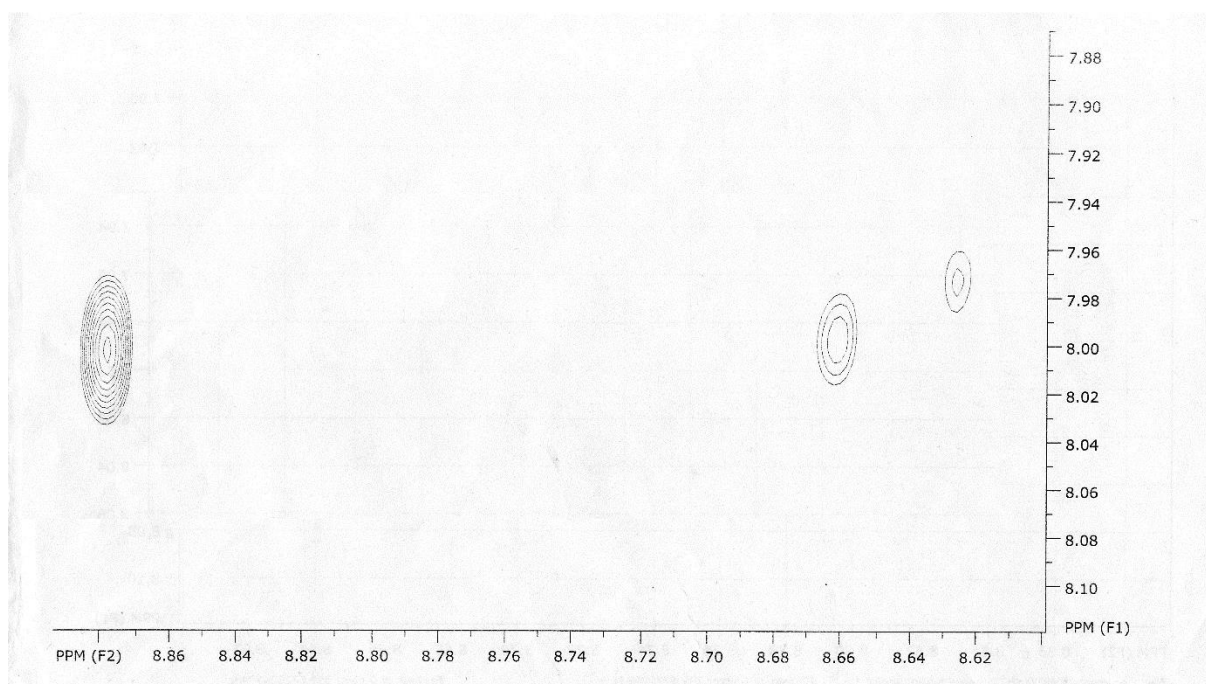


Figure 13. 2D NMR-NOESY spectrum of product **3db** (diagnostic ^1H - ^1H correlations).

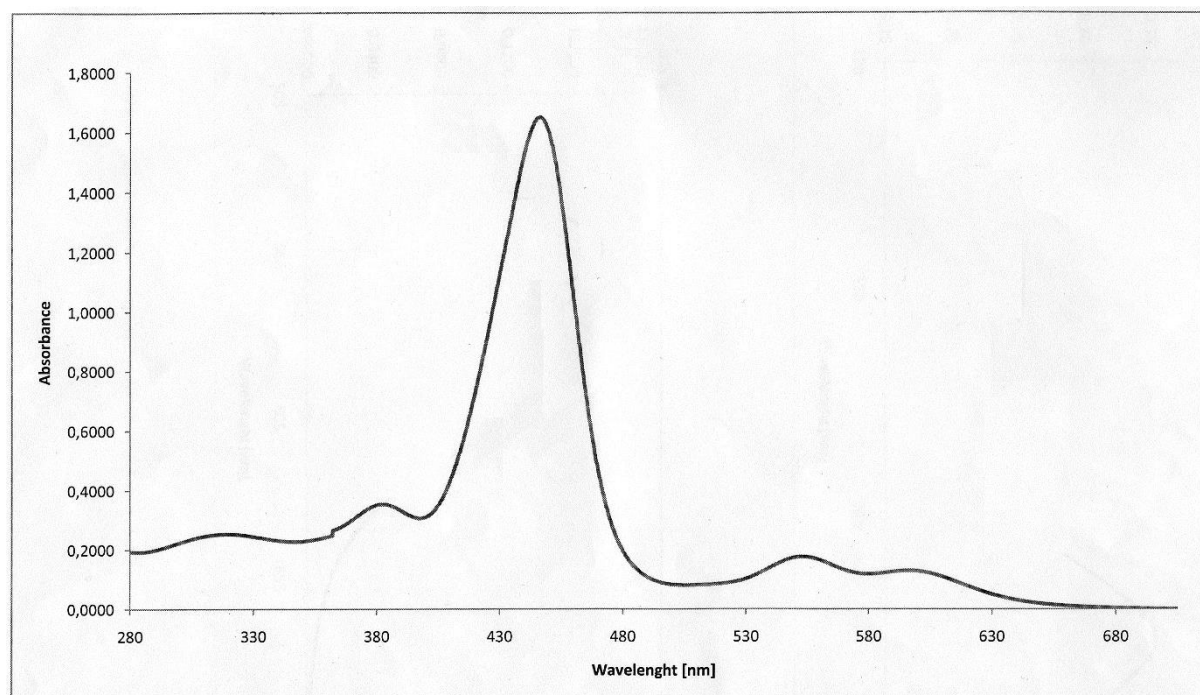


Figure 14. UV-vis spectrum of product **3db**.

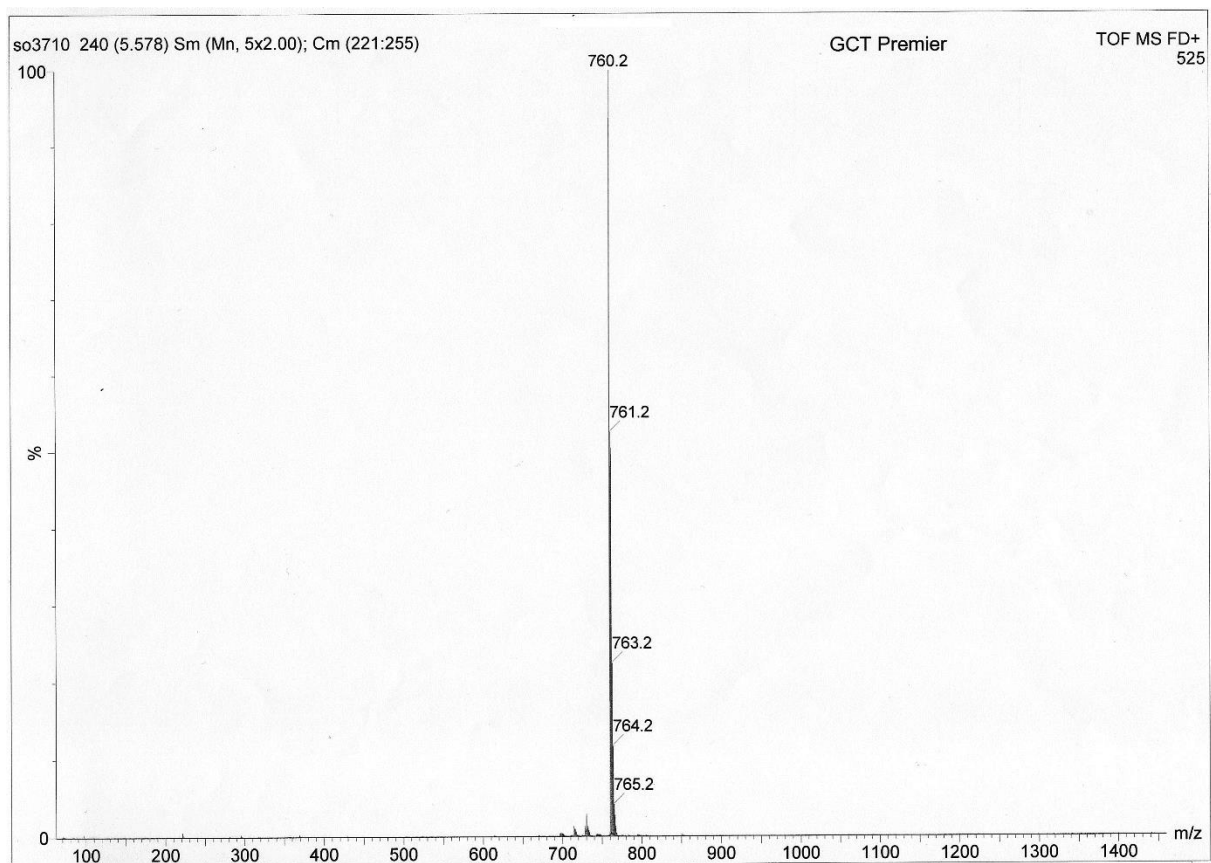


Figure 15. MS spectrum of product **3db** (FD technique).

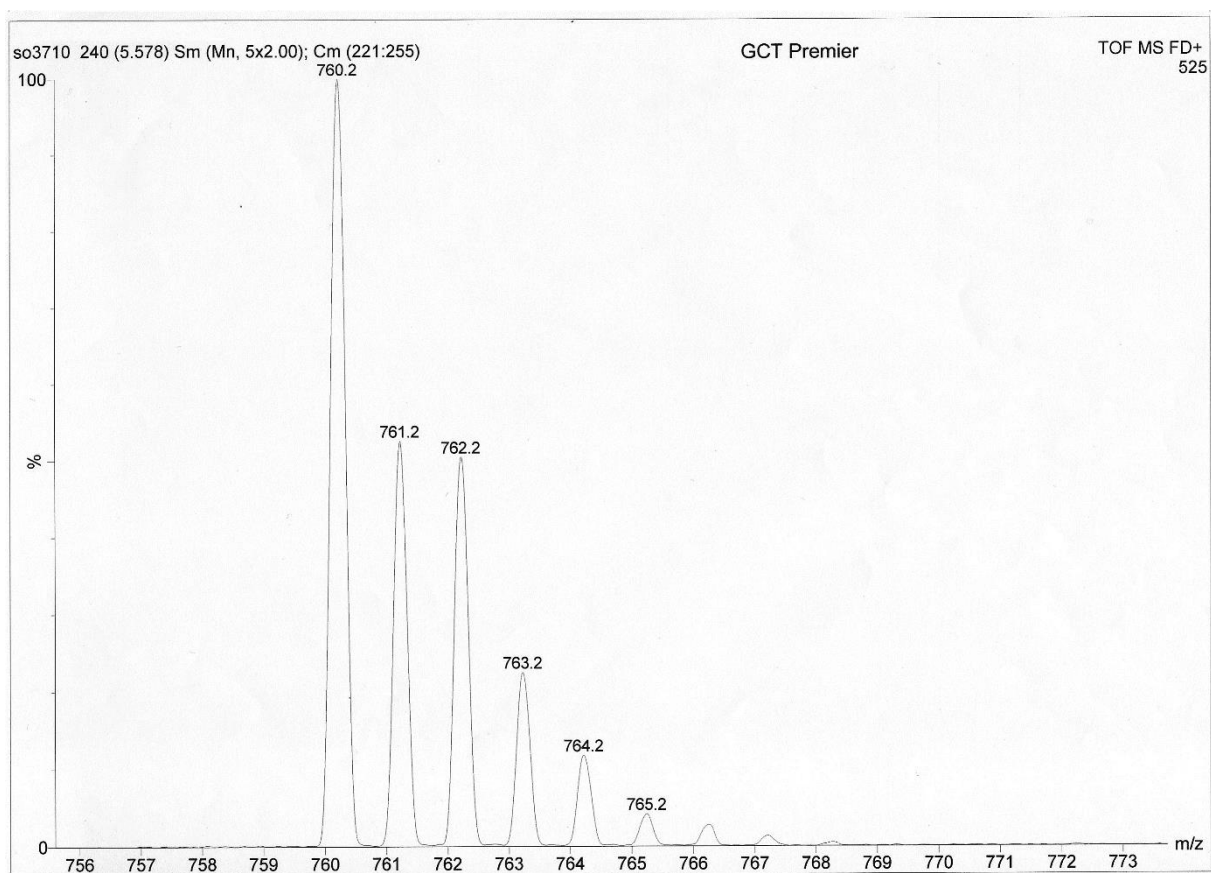


Figure 16. MS spectrum of product **3db** (range: m/z = 755 – 775; FD technique).

2,7-dinitro-5,10,15,20-tetraphenylporphyrin (**4a**)

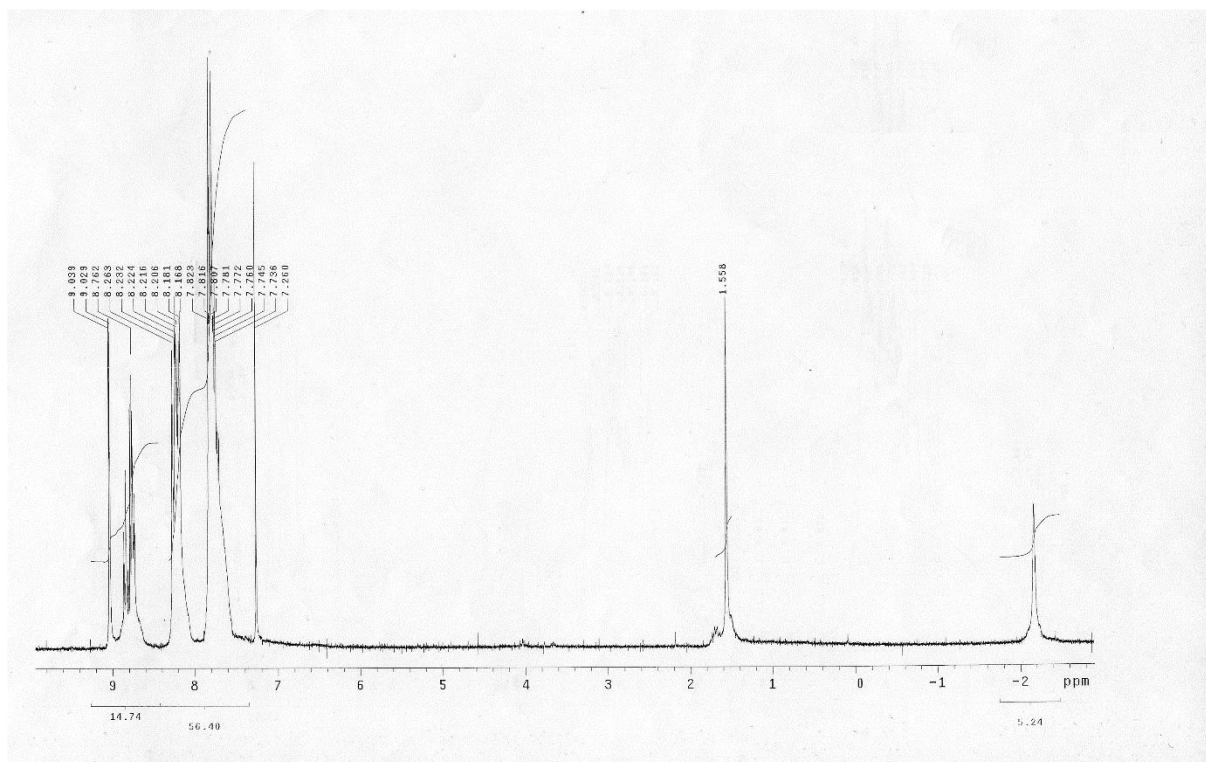


Figure 17. ¹H NMR spectrum of product **4a**.

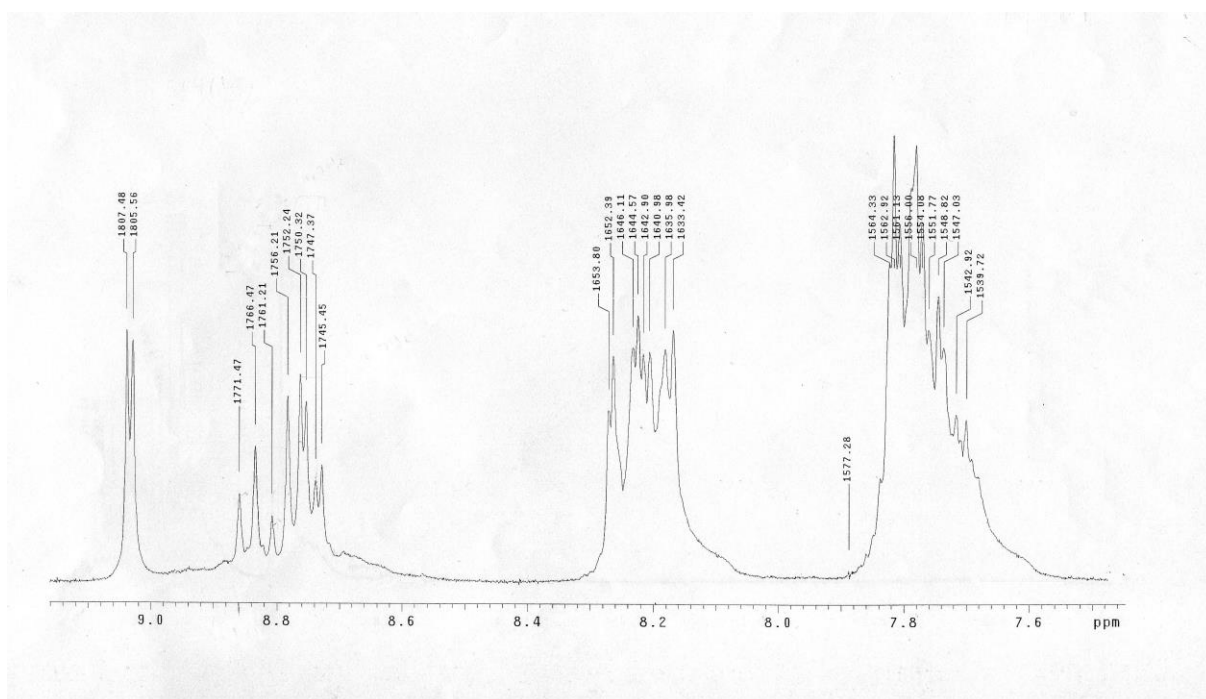


Figure 18. ¹H NMR spectrum of product **4a** (range: 7.50 – 9.10 ppm).

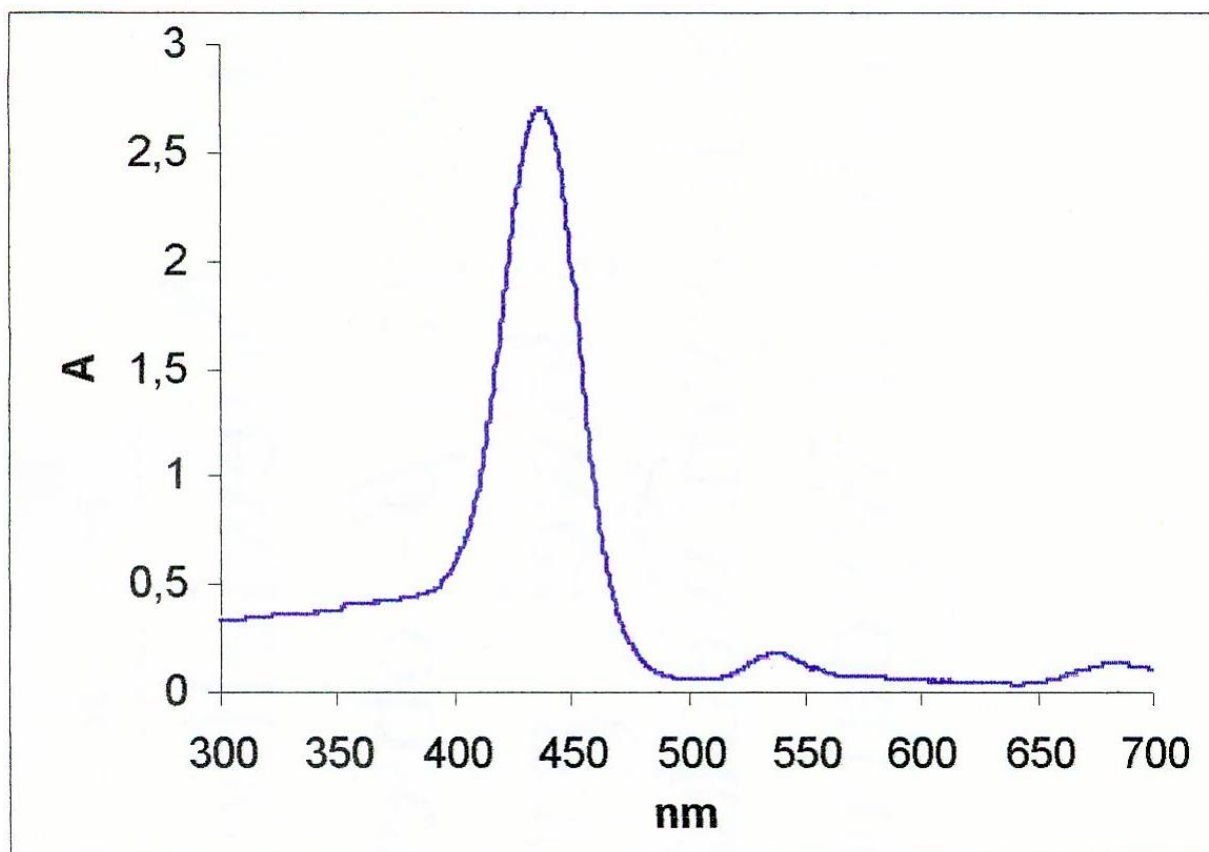


Figure 19. UV-vis spectrum of product **4a**.

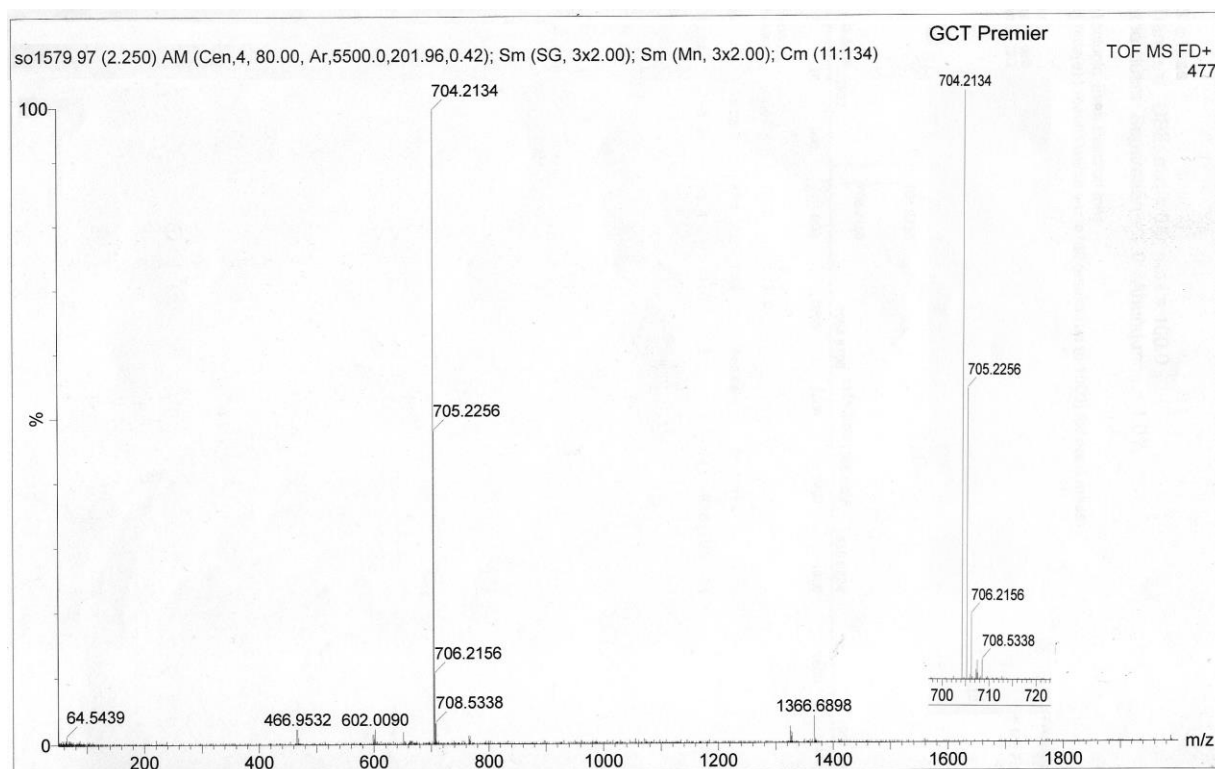


Figure 20. MS spectrum of product **4a** (FD technique).

3,7-dinitro-5,10,15,20-tetraphenylporphyrin (**4b**)

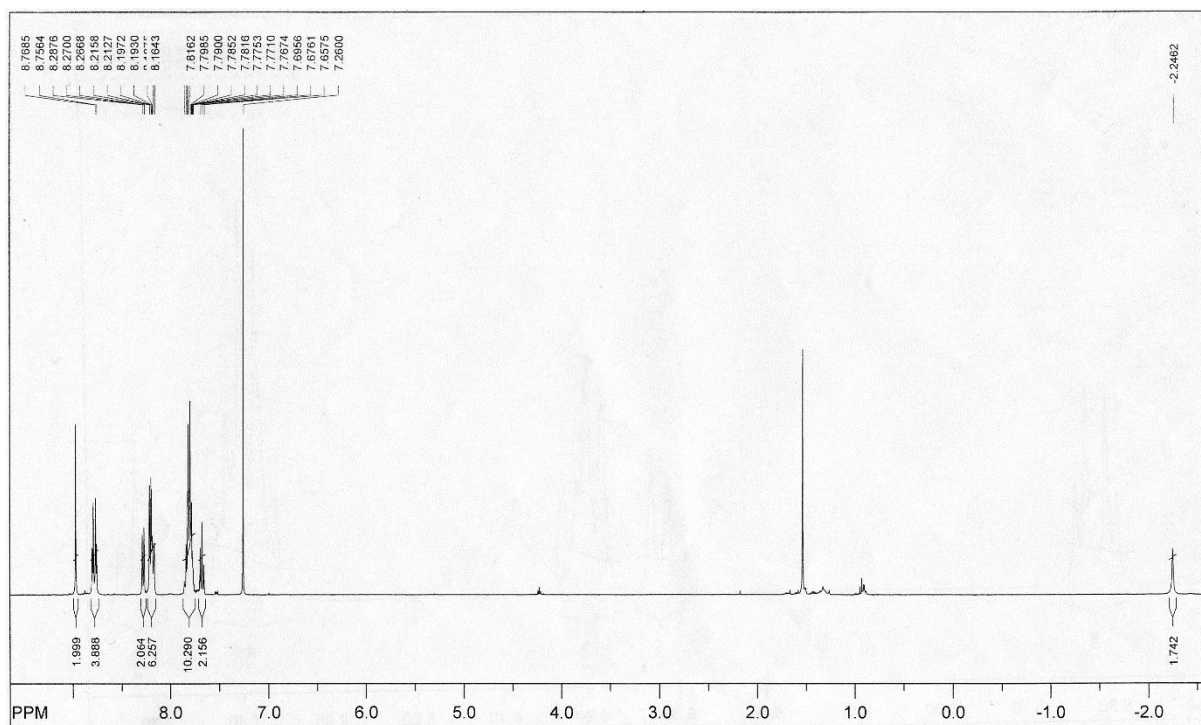


Figure 21. ¹H NMR spectrum of product **4b**.

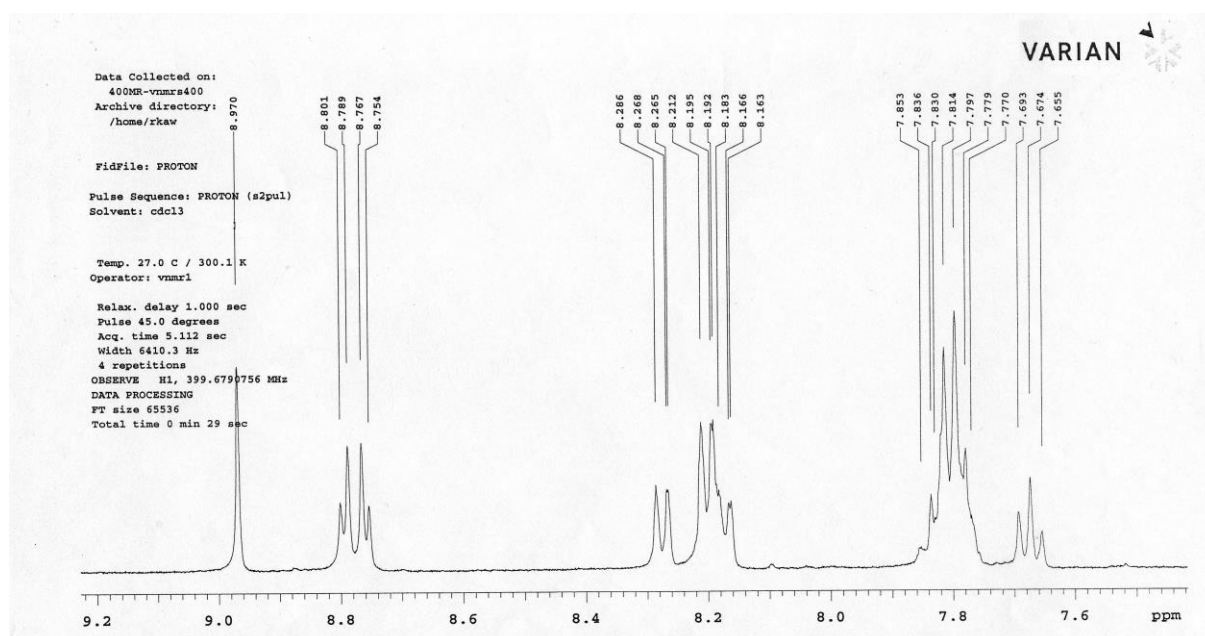


Figure 22. ¹H NMR spectrum of product **4b** (range: 7.50 – 9.20 ppm).

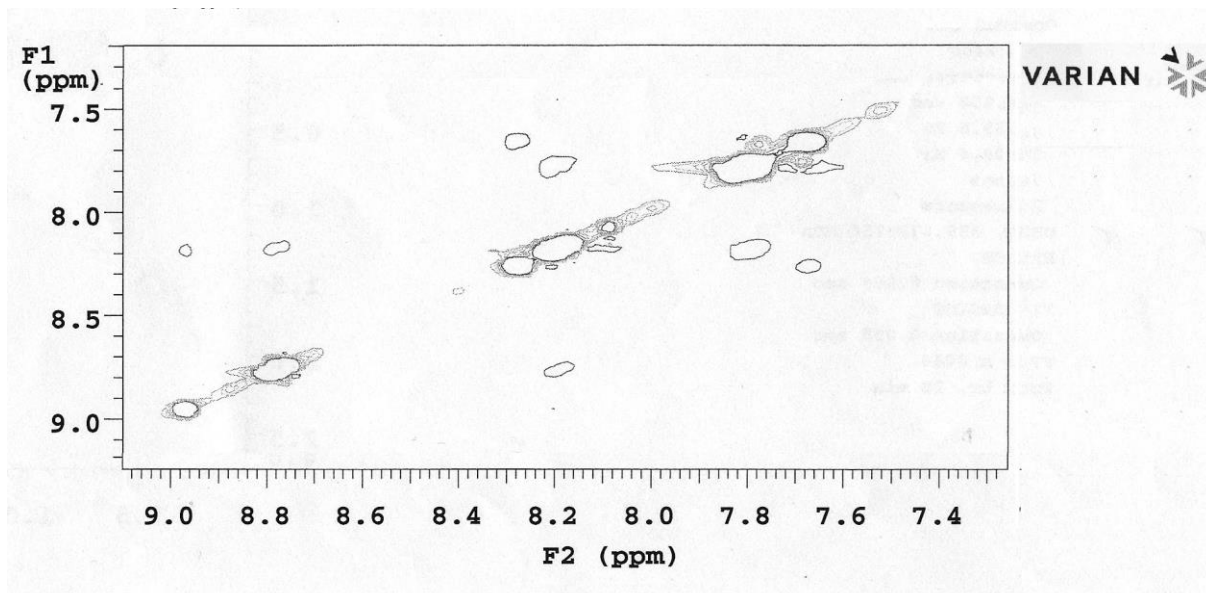


Figure 23. 2D NMR-NOESY spectrum of product **4b** (diagnostic ^1H - ^1H correlations).

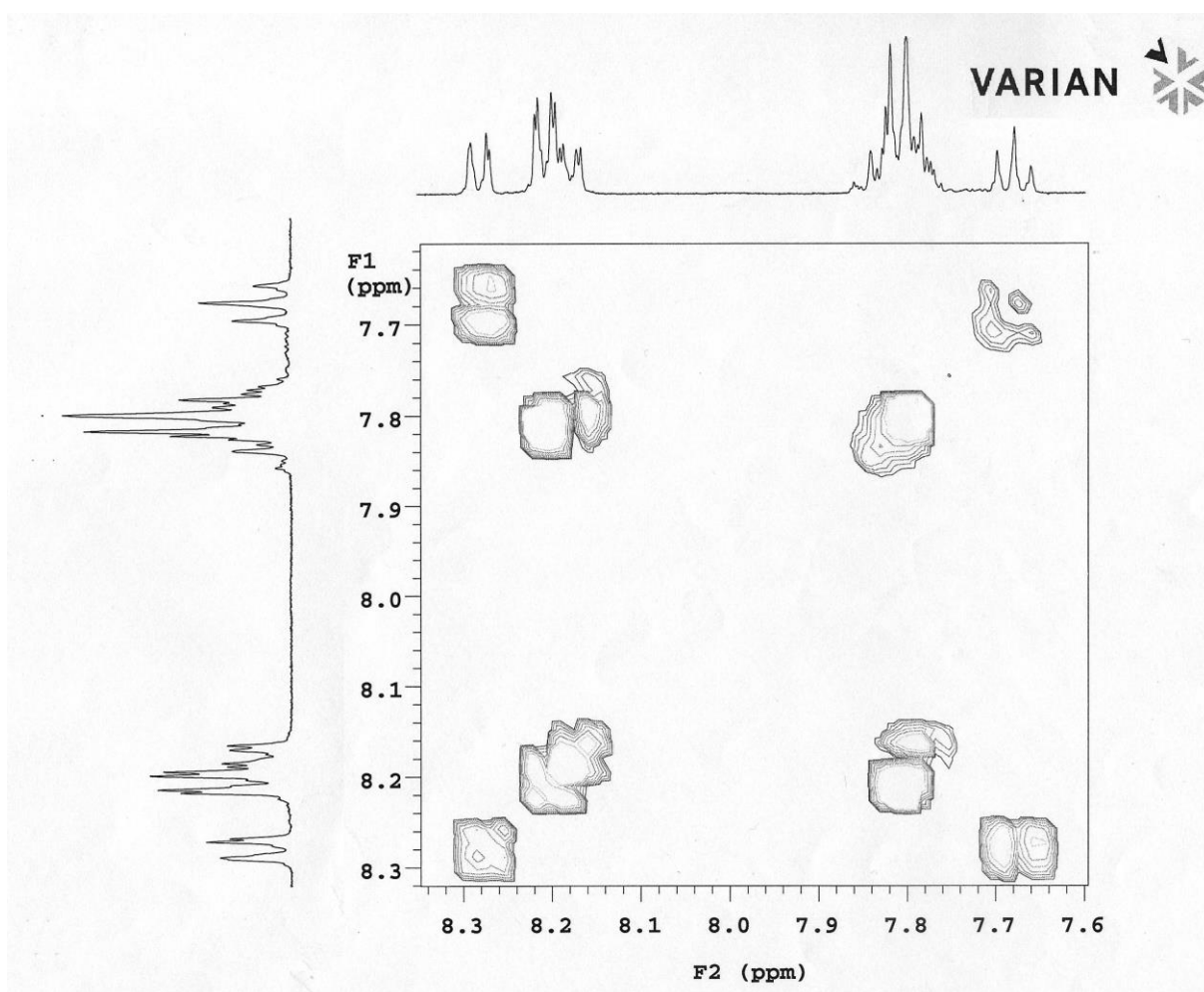


Figure 24. 2D NMR-COSY spectrum of product **4b** (diagnostic ^1H - ^1H correlations).

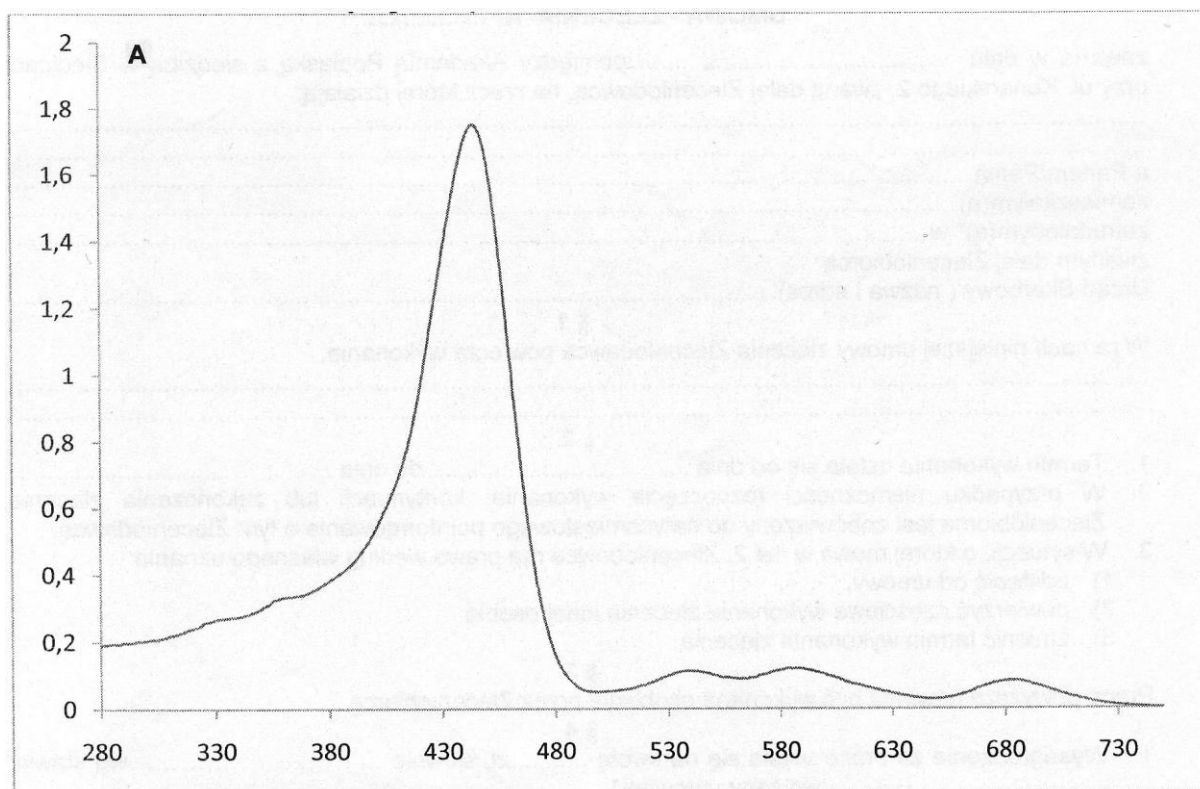


Figure 25. UV-vis spectrum of product **4b**.

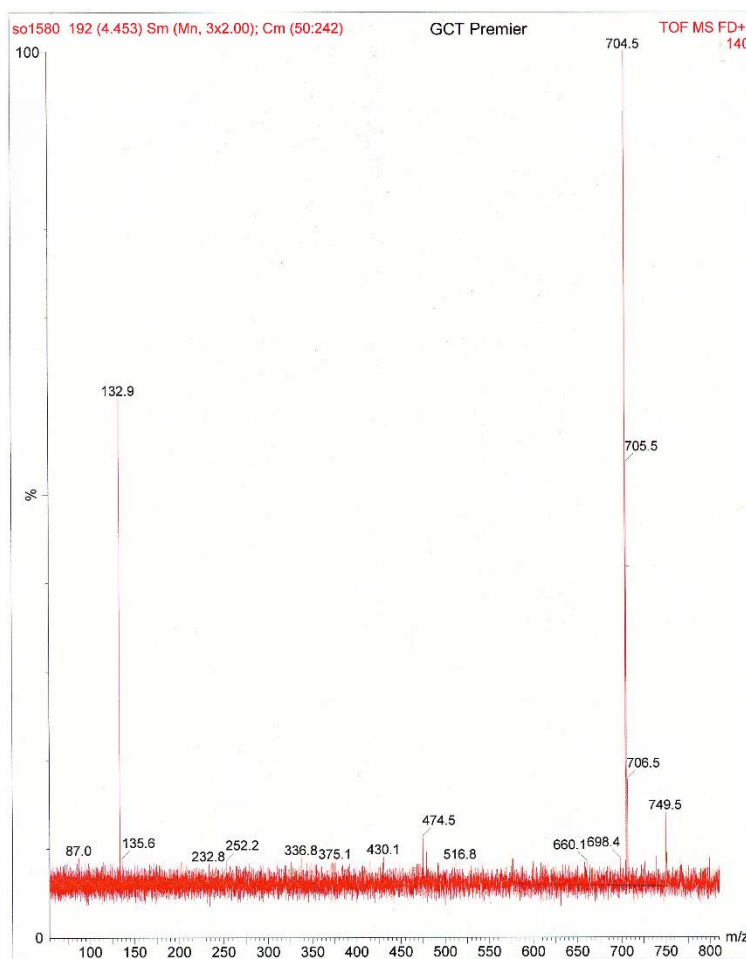


Figure 26. MS spectrum of product **4b** (FD technique).

¹H NMR spectrum of compound 10a in CDCl₃. The spectrum shows peaks at 8.9311, 8.8311, 8.2488, 8.1951, 8.1574, 8.1241, 7.7721, 7.728, 7.7946, 7.8239, 7.7360, 1.5436, -2.4896, and -2.5738 ppm. An inset zooms in on the aromatic region from 8.0 to 9.0 ppm.

1.140

0.000

250 750

Rescale or New Files (R/F)? R

18

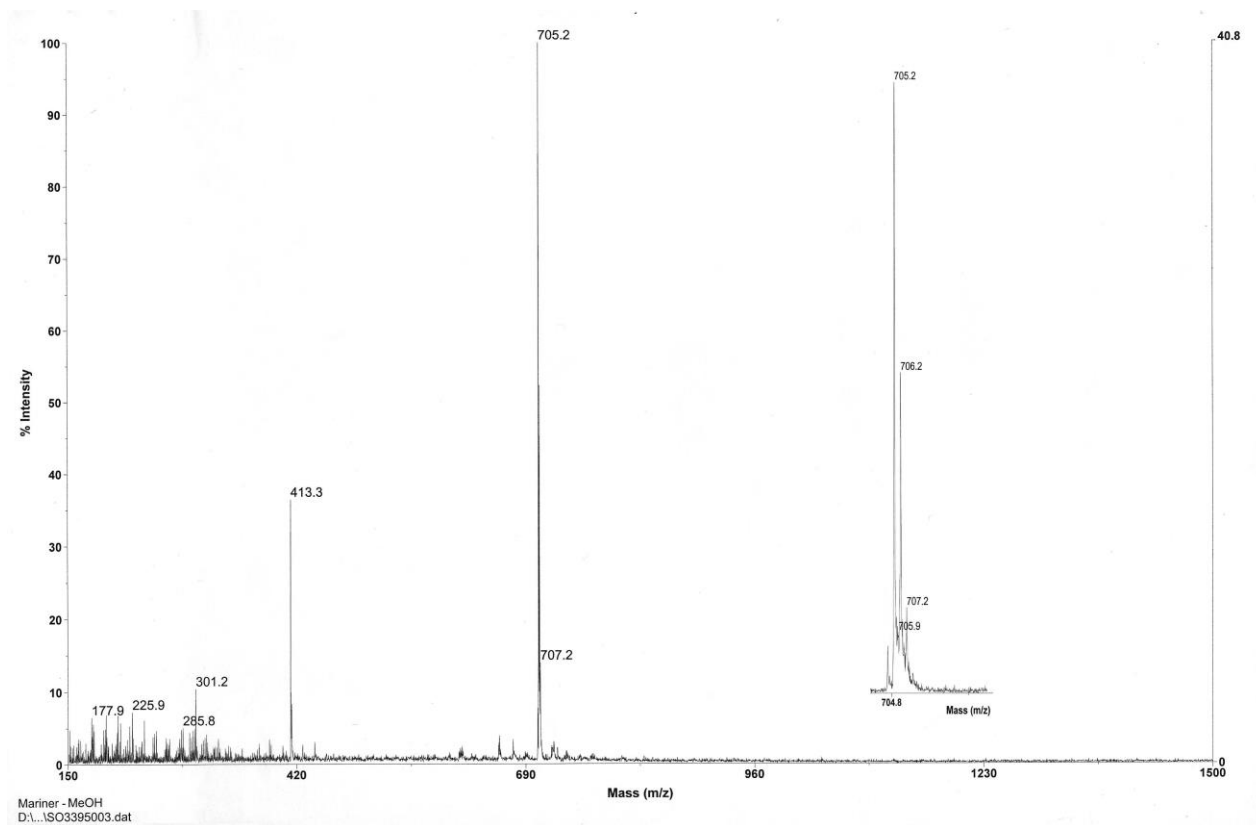


Figure 29. MS spectrum of product **4c** (ESI technique).

[2,7-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrinato]copper(II) (**6a**)

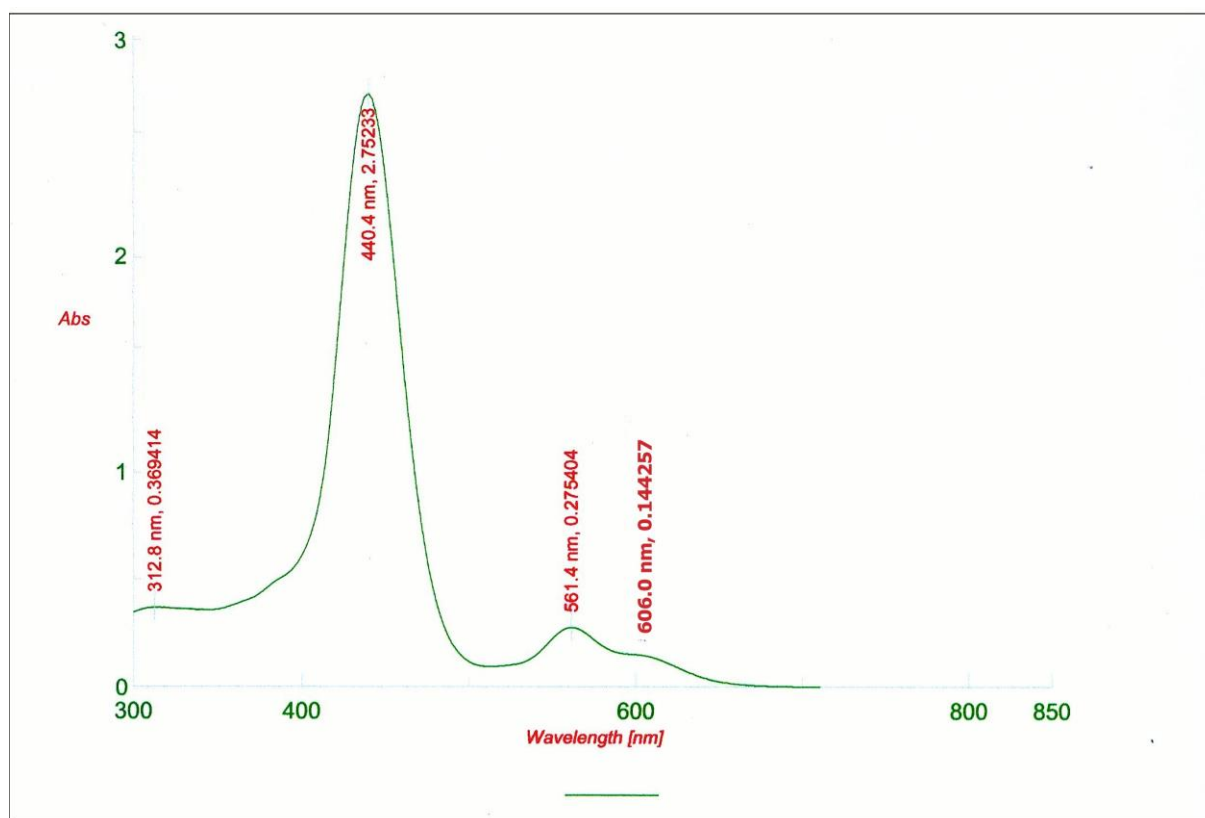


Figure 30. UV-vis spectrum of product **6a**.

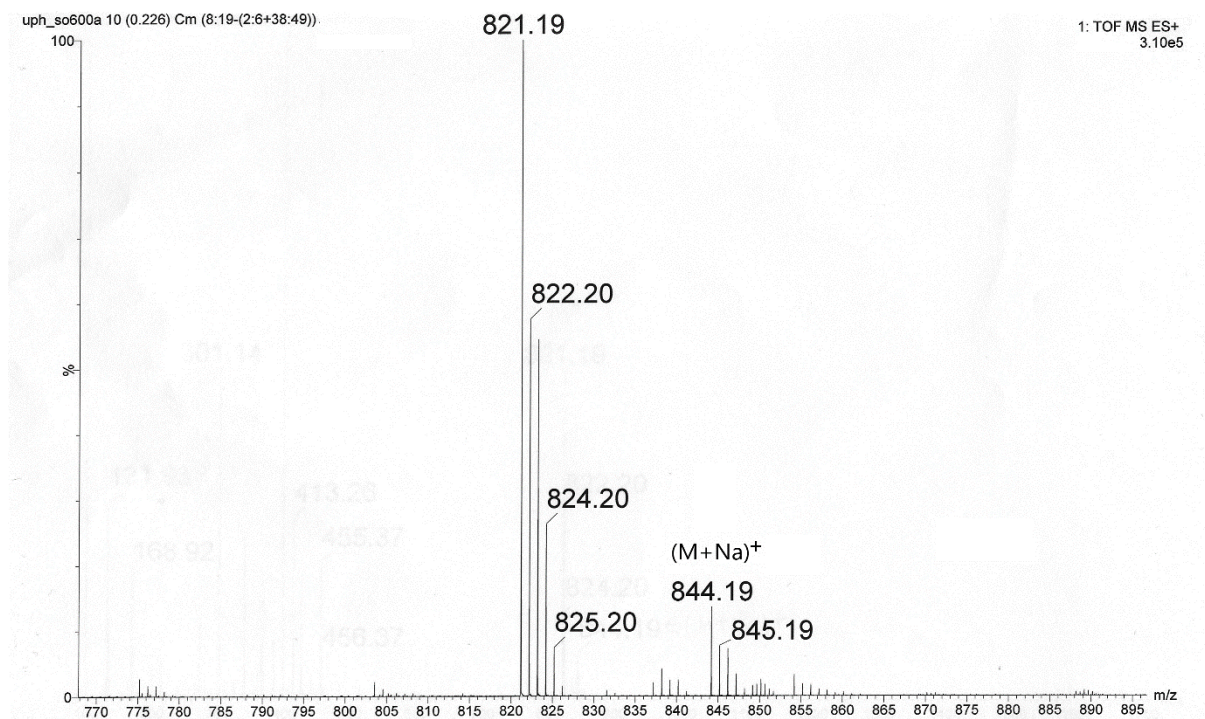


Figure 31. MS spectrum of product **6a** (ESI technique).

[3,7-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrinato]copper(II) (**7a**)

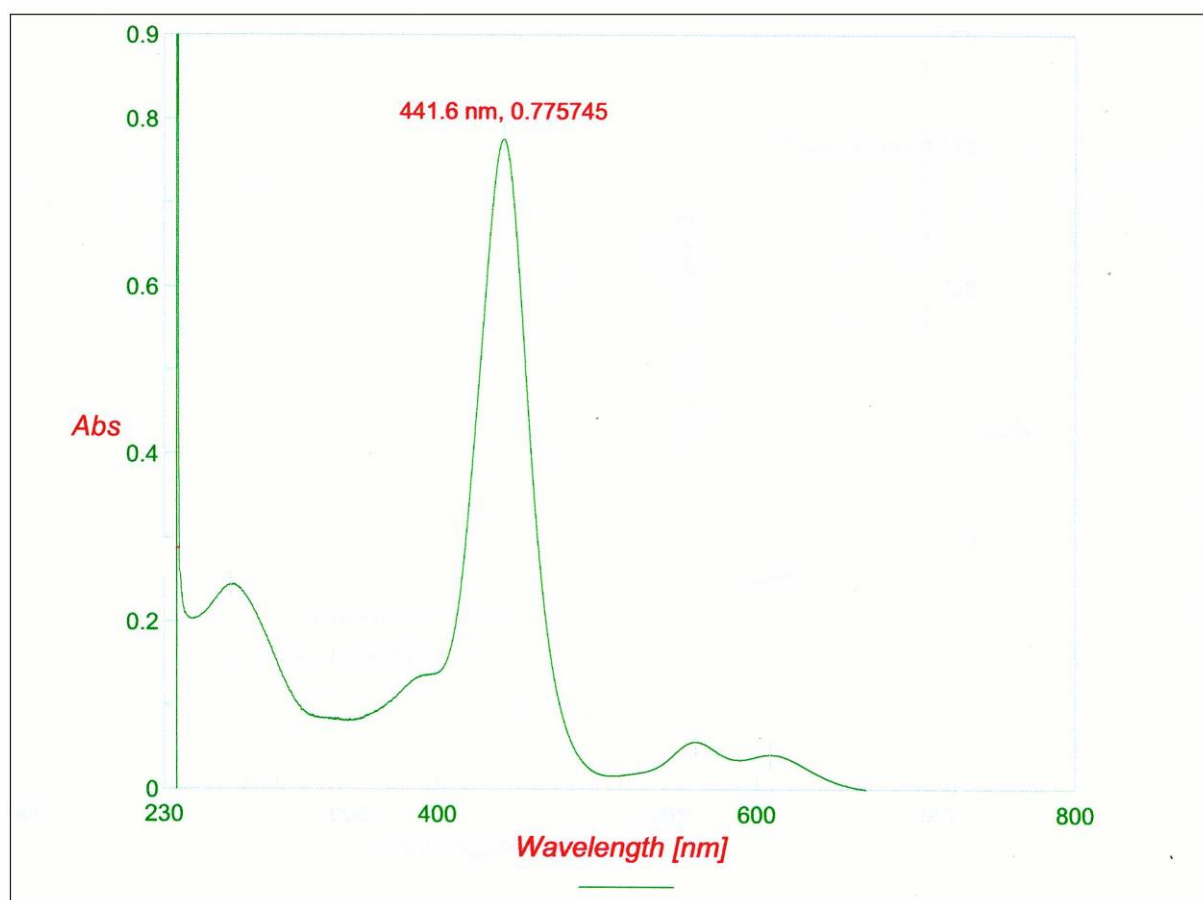


Figure 32. UV-vis spectrum of product **7a**.

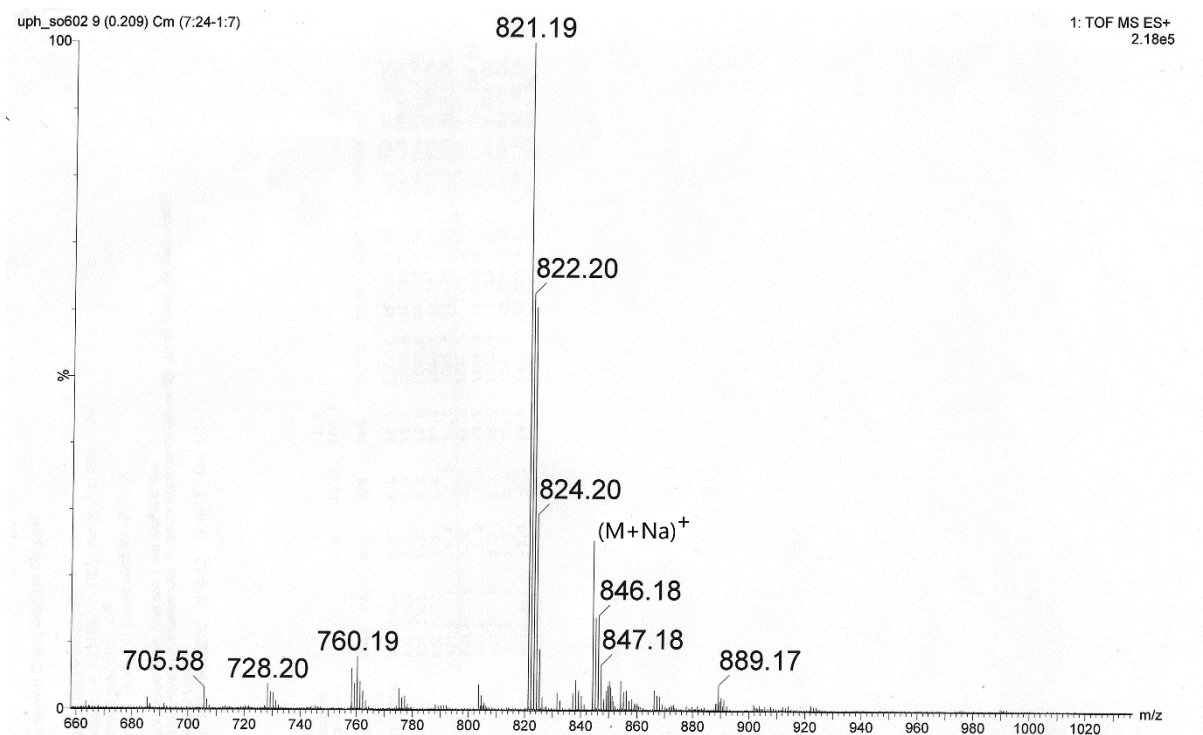


Figure 33. MS spectrum of product **7a** (ESI technique).

[2,8-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrinato]copper(II) (**8a**)
and
[2,12-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrinato]copper(II) (**9a**)

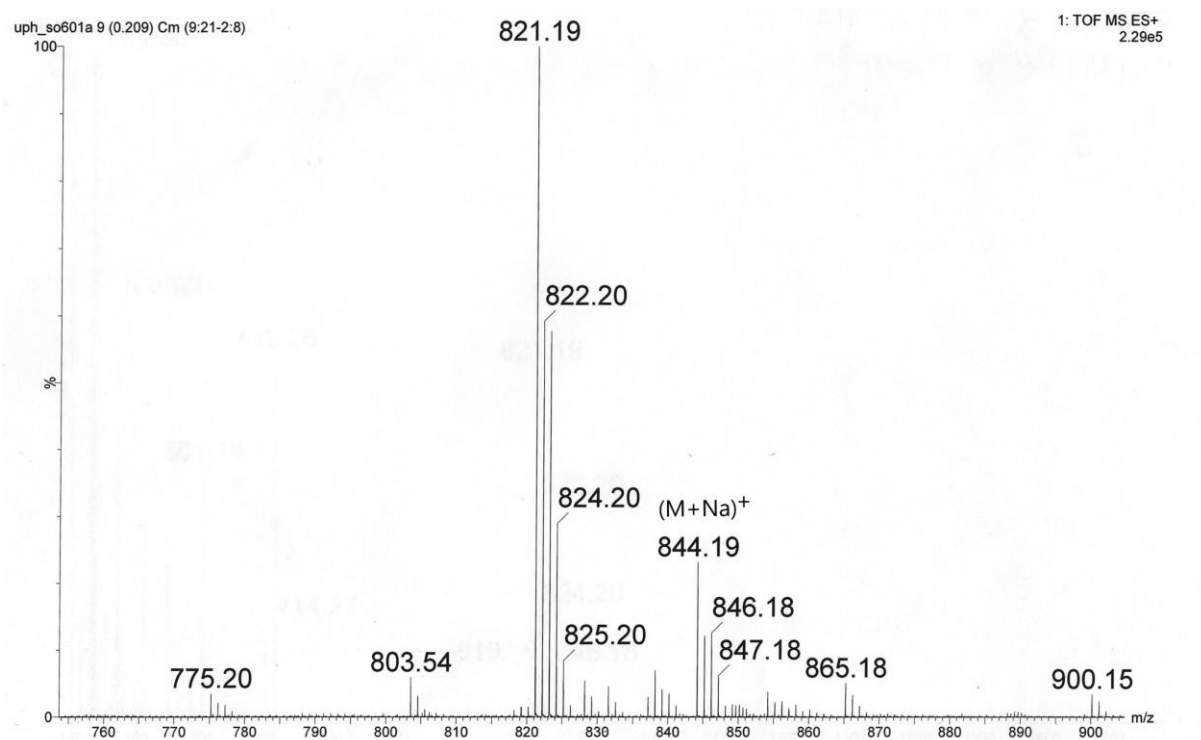


Figure 34. MS spectrum of products **8a** and **9a** (an inseparable mixture; ESI technique).

[2,13-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrinato]copper(II) (**10a**)

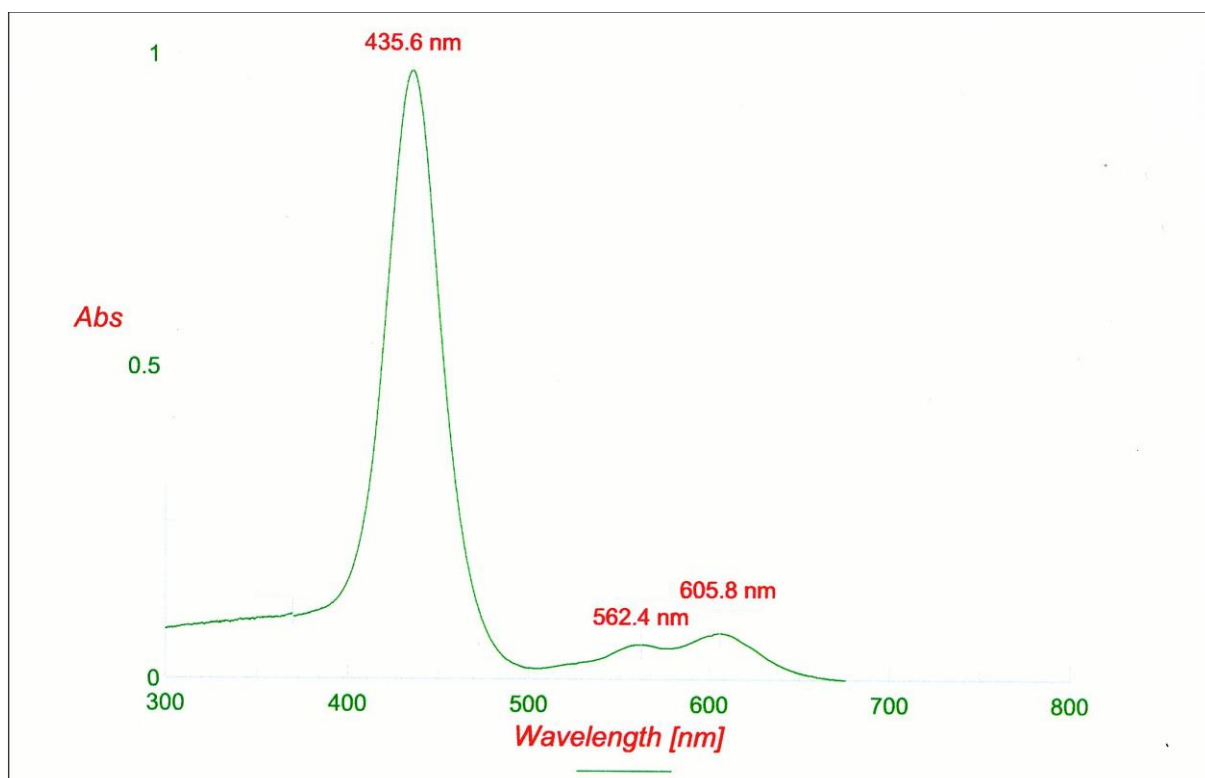


Figure 35. UV-vis spectrum of product **10a**.

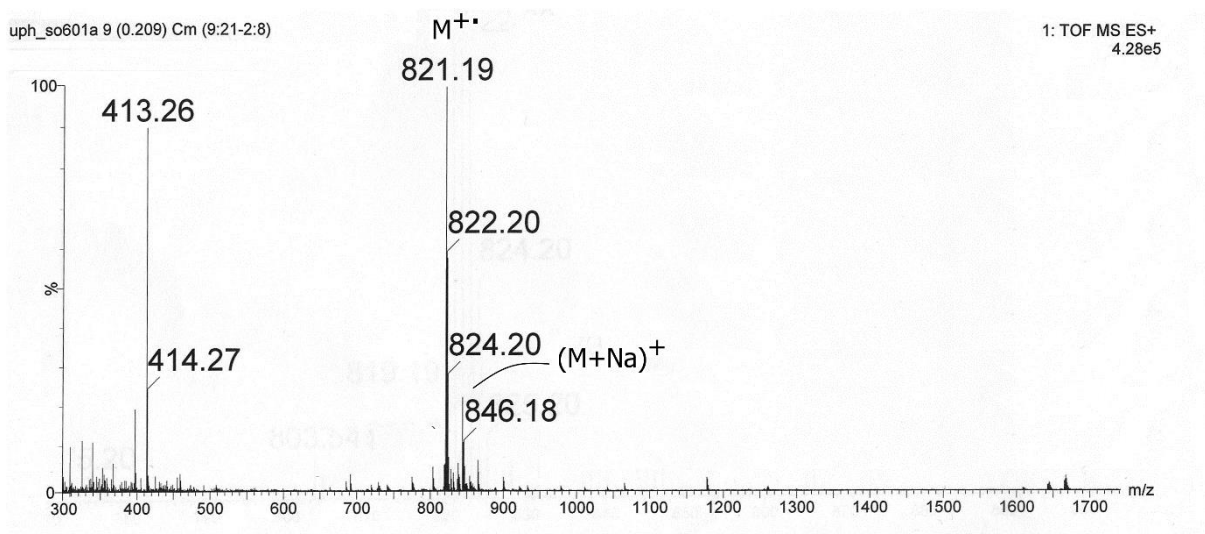


Figure 36. MS spectrum of product **10a** (ESI technique).

(2,7-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrin (**6b**))

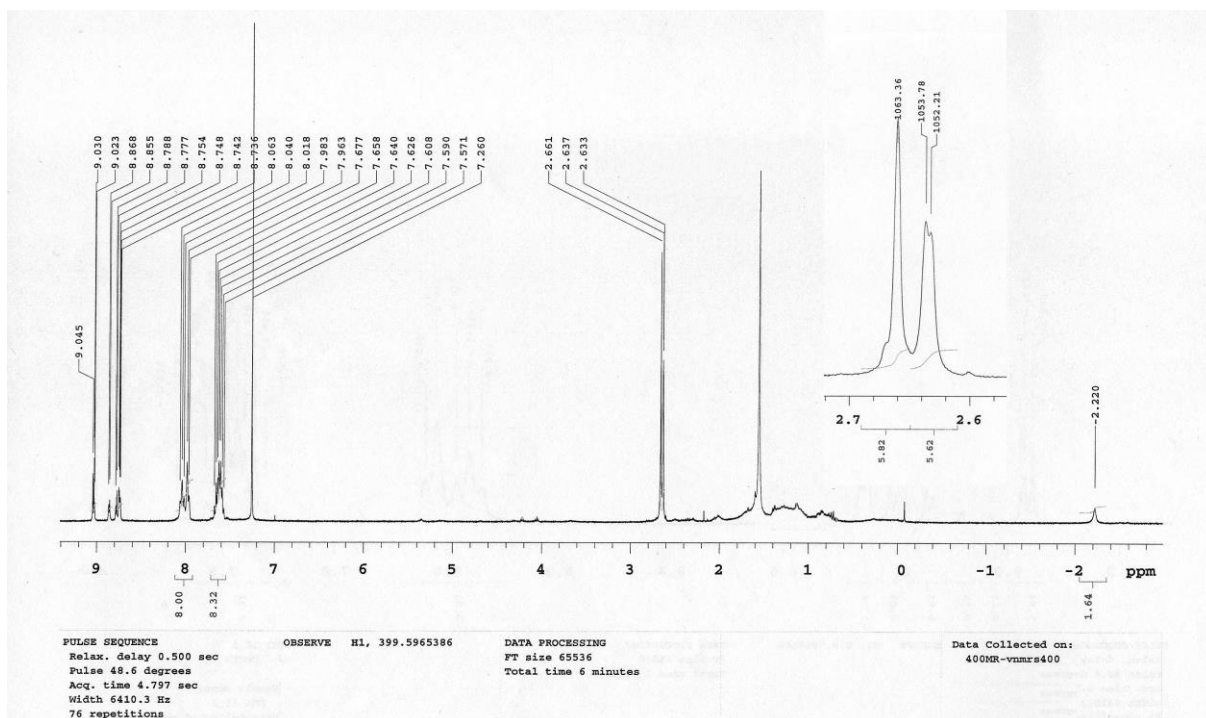


Figure 37. ¹H NMR spectrum of product **6b**.

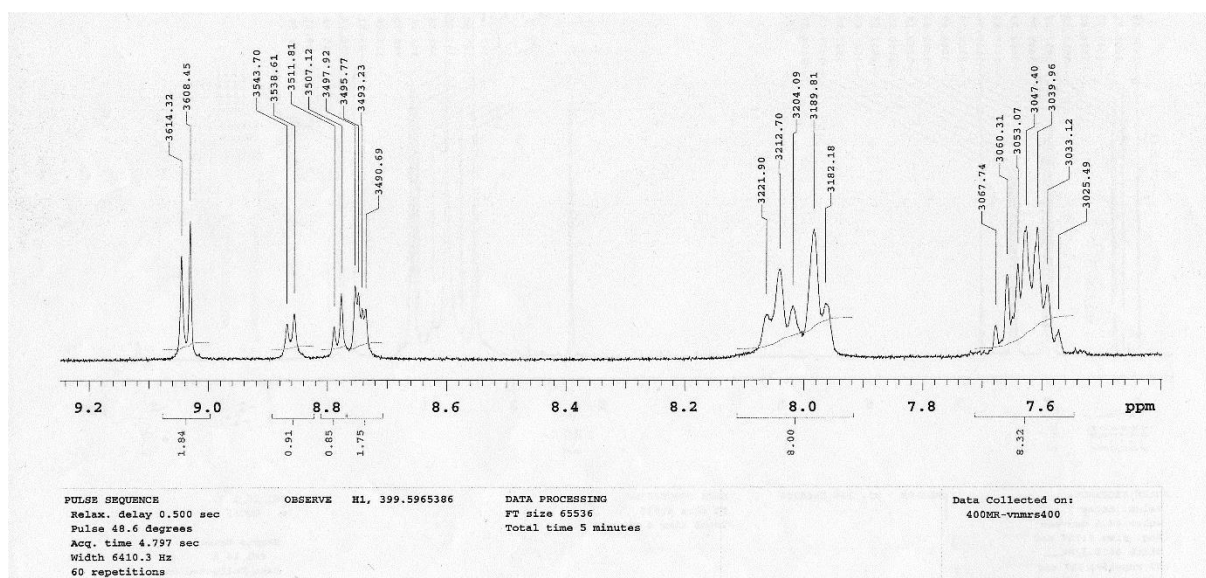


Figure 38. ¹H NMR spectrum of product **6b** (range: 7.40 – 9.20 ppm).

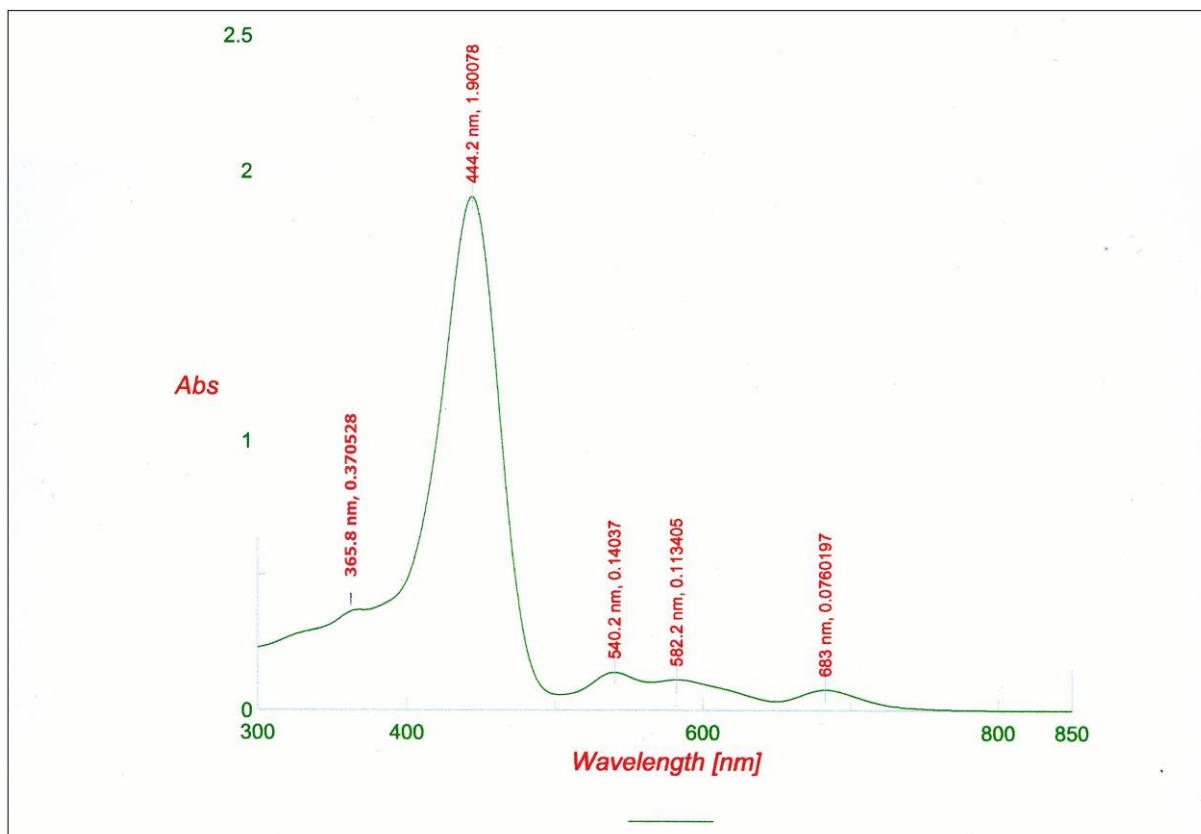


Figure 39. UV-vis spectrum of product **6b**.

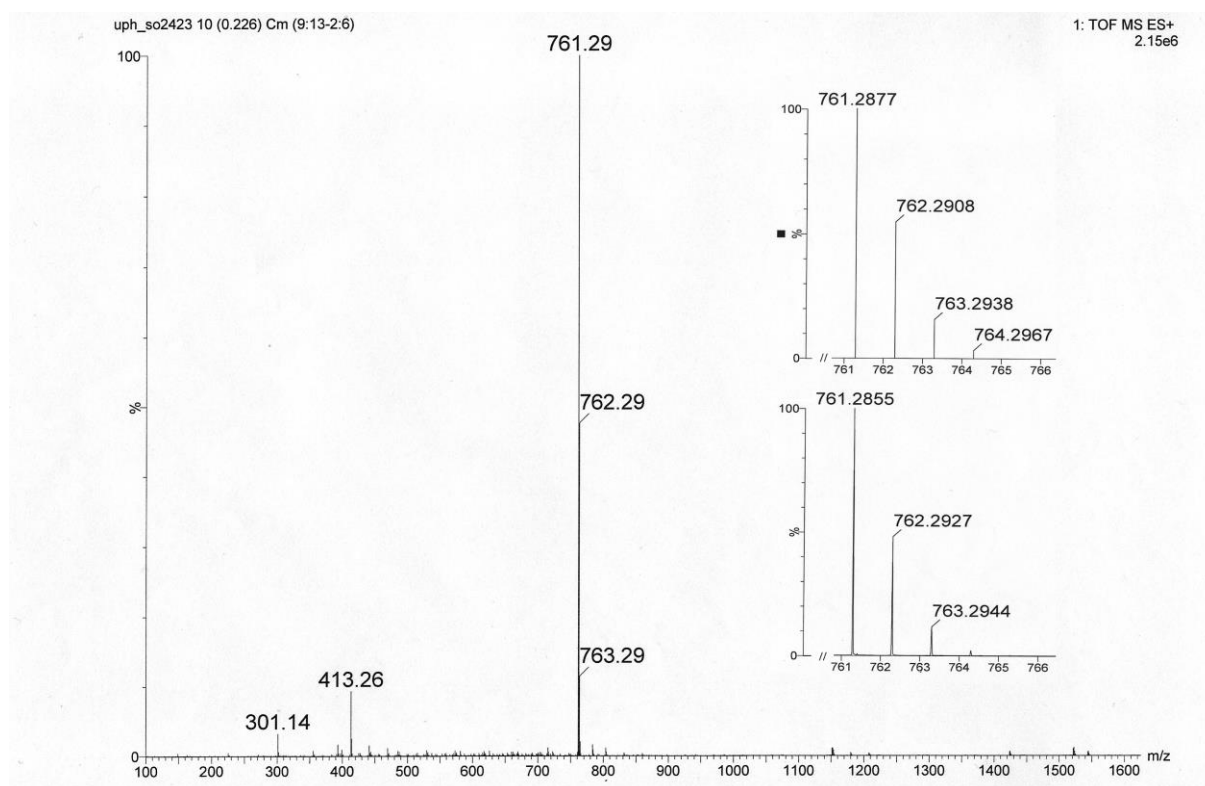


Figure 40. MS spectrum of product **6b** (ESI technique).

(3,7-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrin (**7b**))

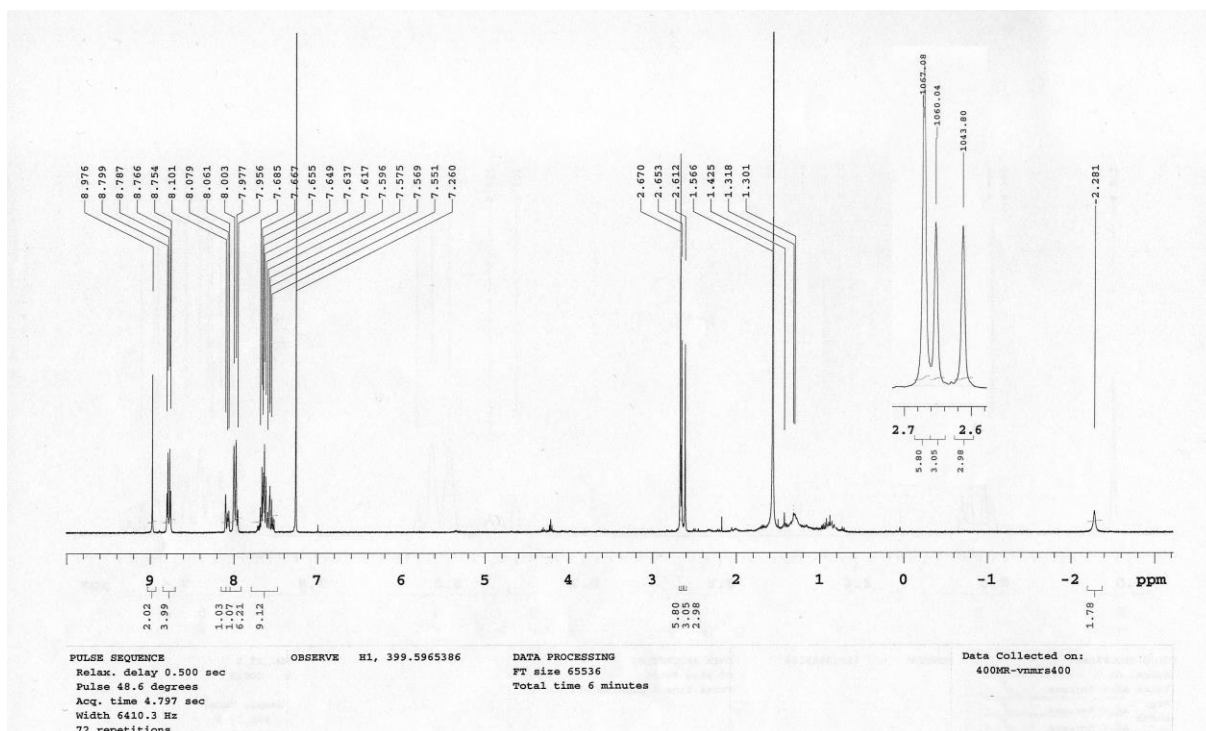


Figure 41. ¹H NMR spectrum of product **7b**.

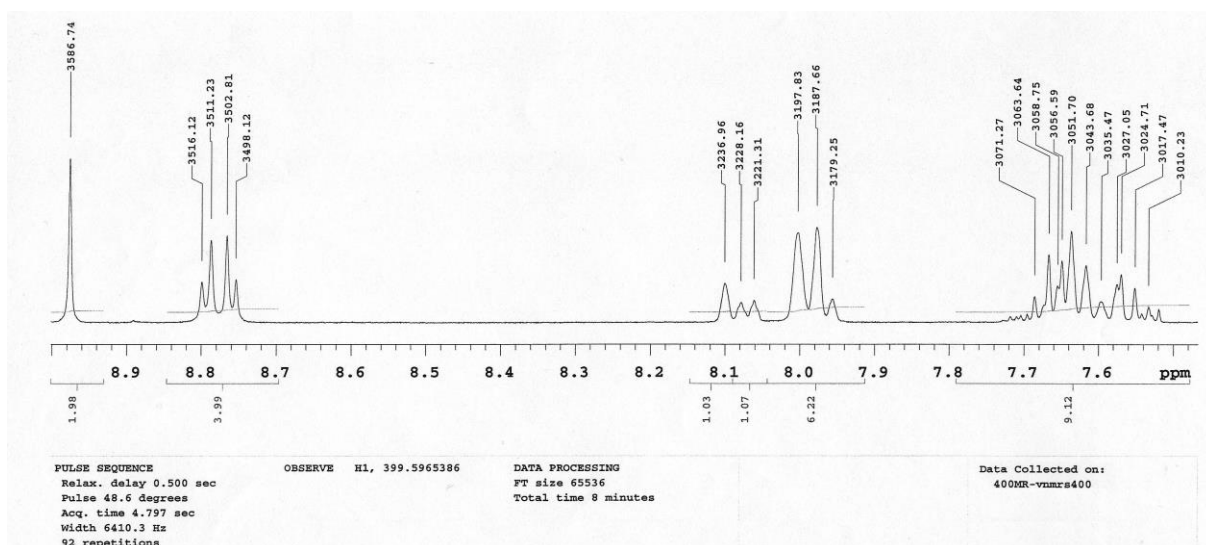


Figure 42. ¹H NMR spectrum of product **7b** (range: 7.50 – 9.00 ppm).

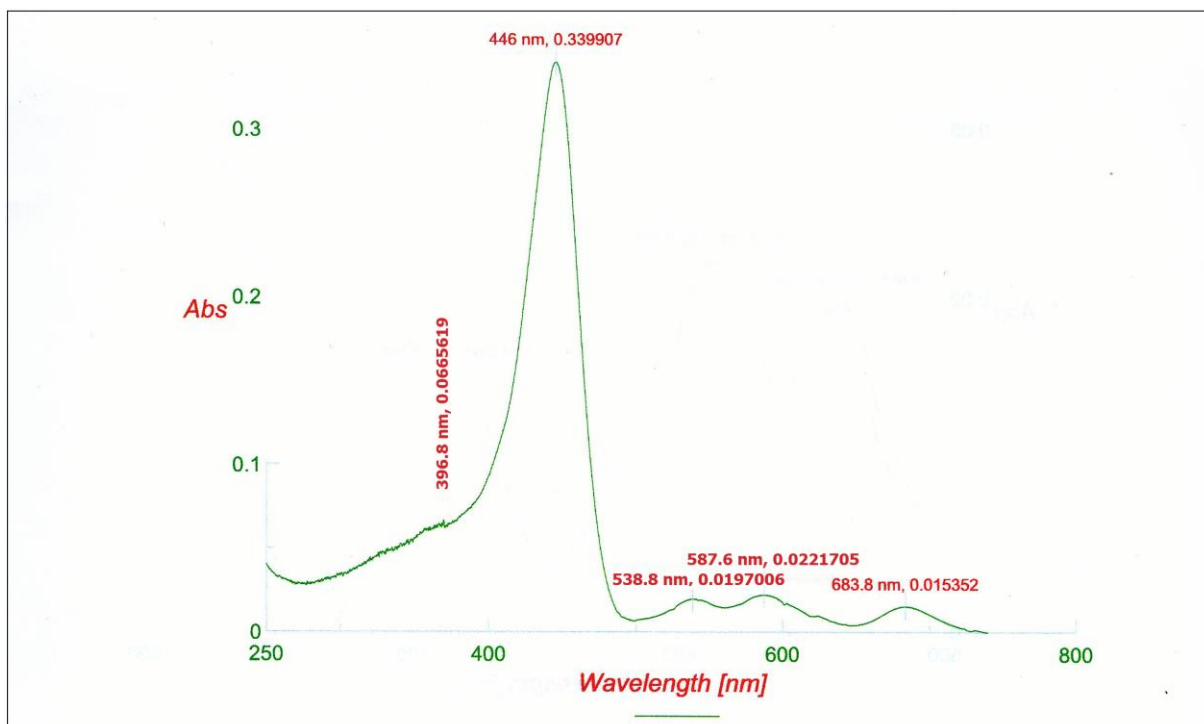


Figure 43. UV-vis spectrum of product **7b**.

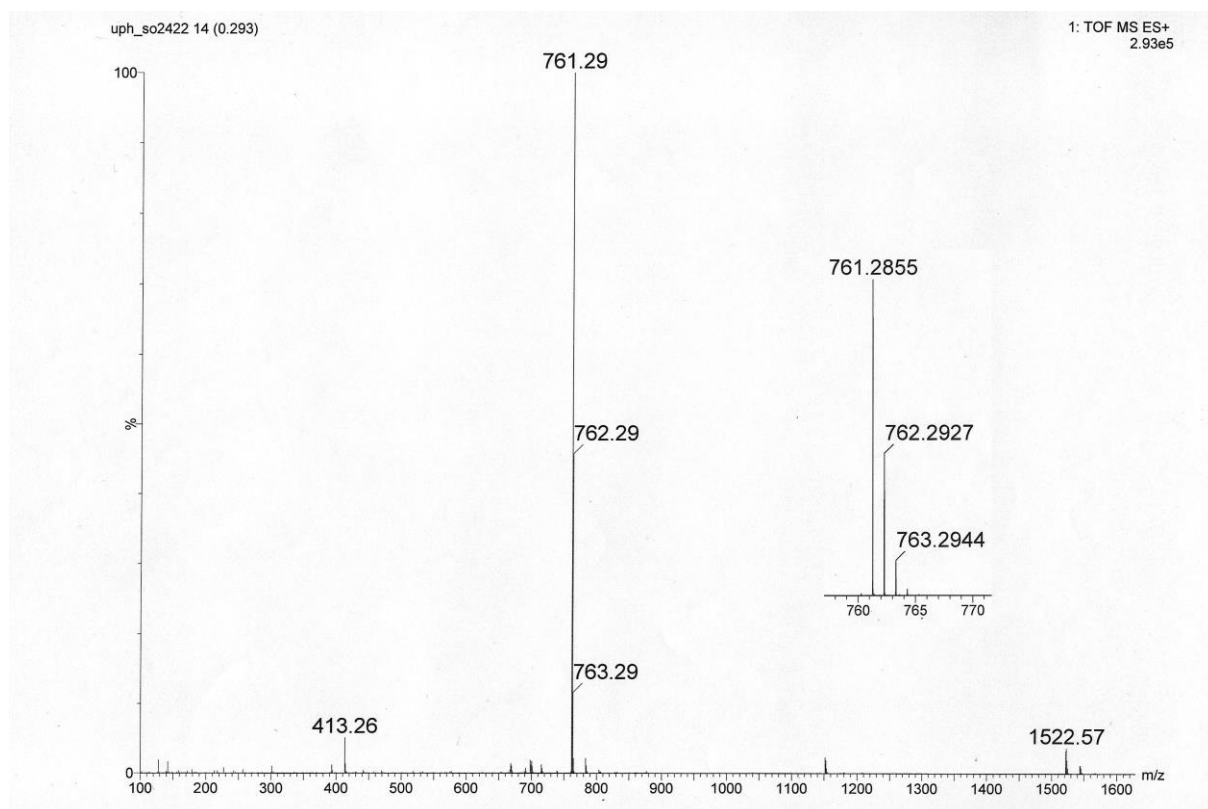


Figure 44. MS spectrum of product **7b** (ESI technique).

(2,8-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrin (**8b**))

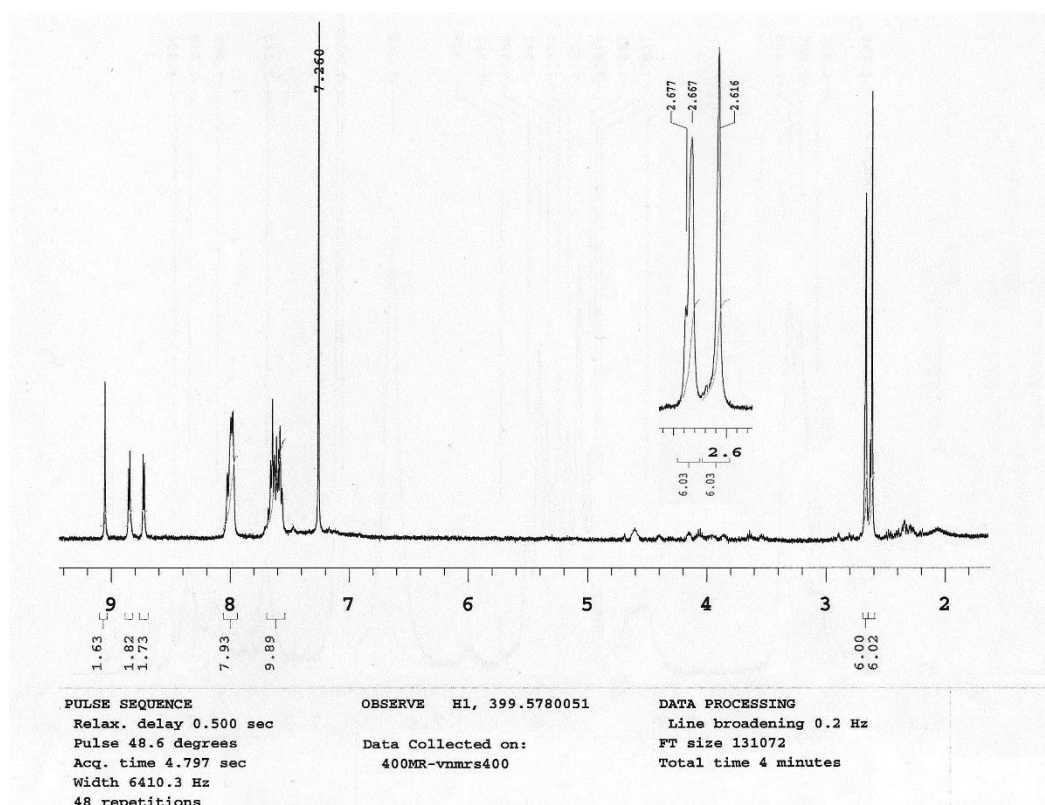


Figure 45. ¹H NMR spectrum of product **8b**.

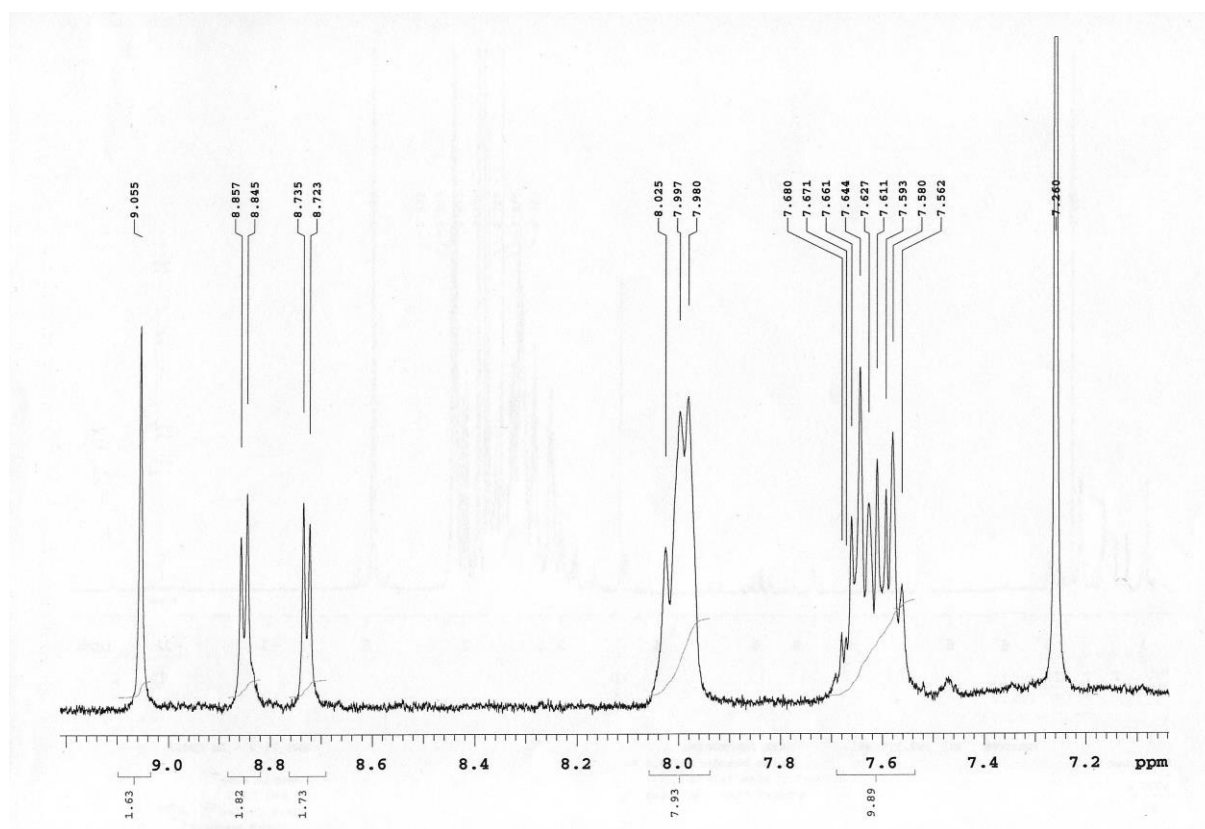


Figure 46. ¹H NMR spectrum of product **8b** (range: 7.10 – 9.20 ppm).

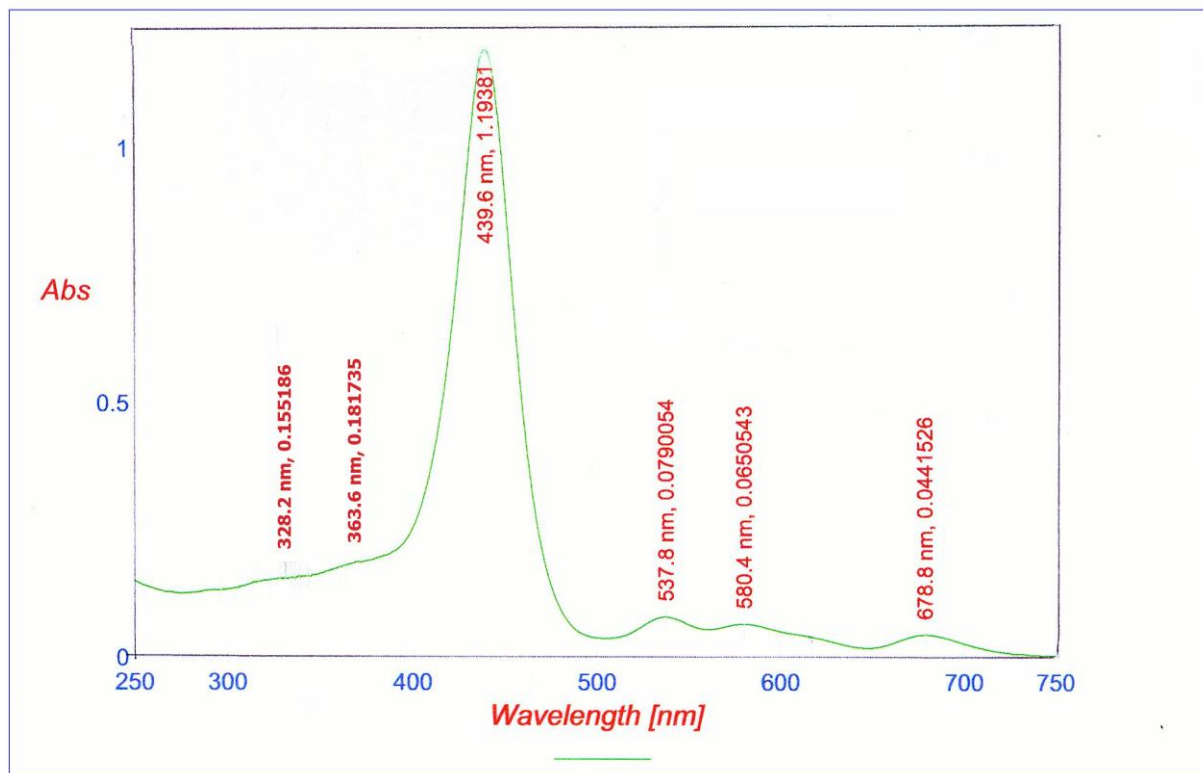


Figure 47. UV-vis spectrum of product **8b**.

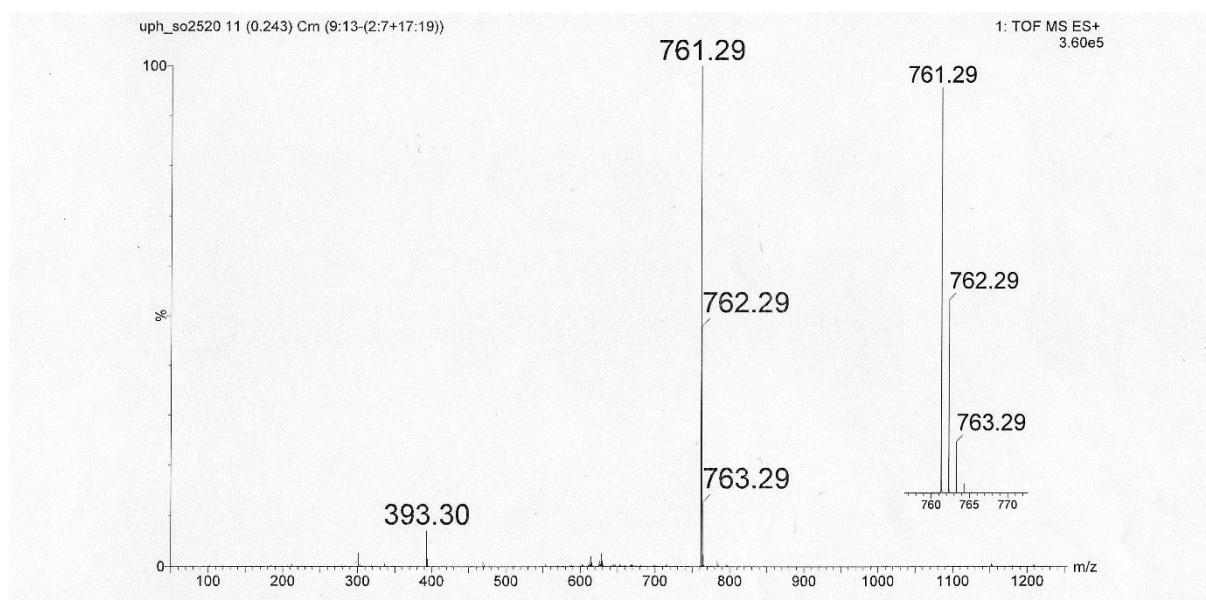


Figure 48. MS spectrum of product **8b** (ESI technique).

(2,12-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrin (**9b**))

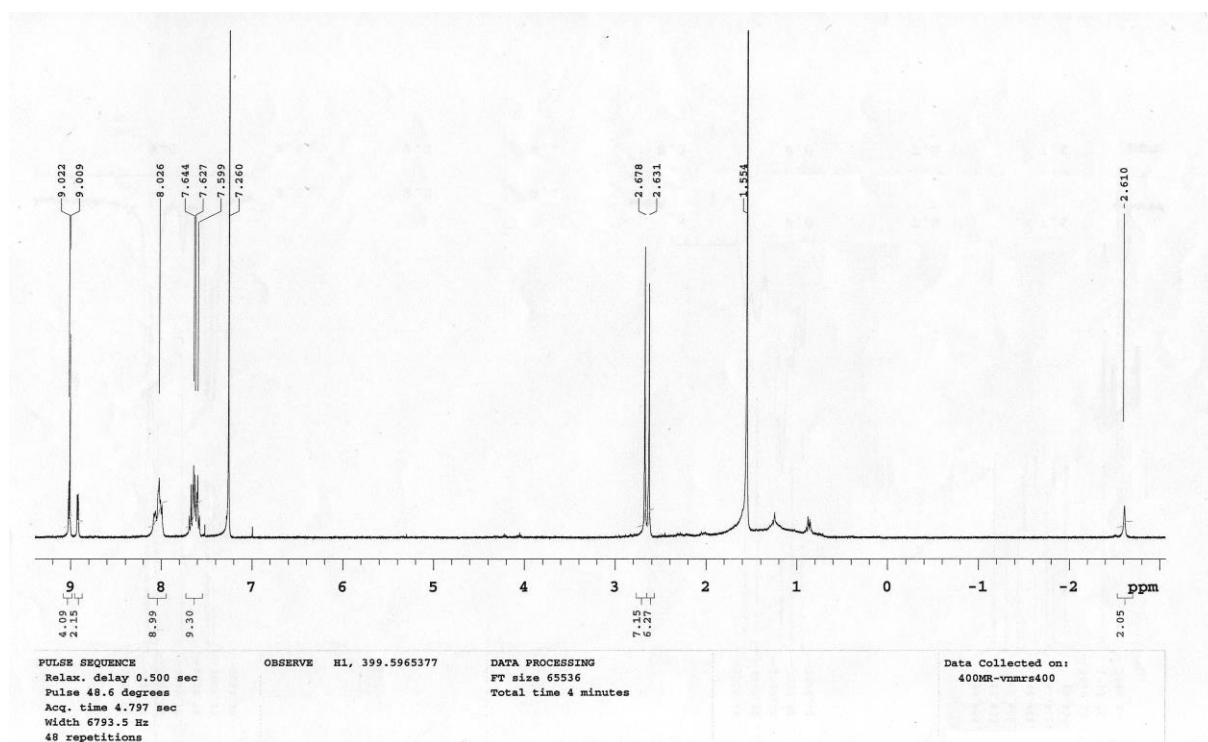


Figure 49. ¹H NMR spectrum of product **9b**.

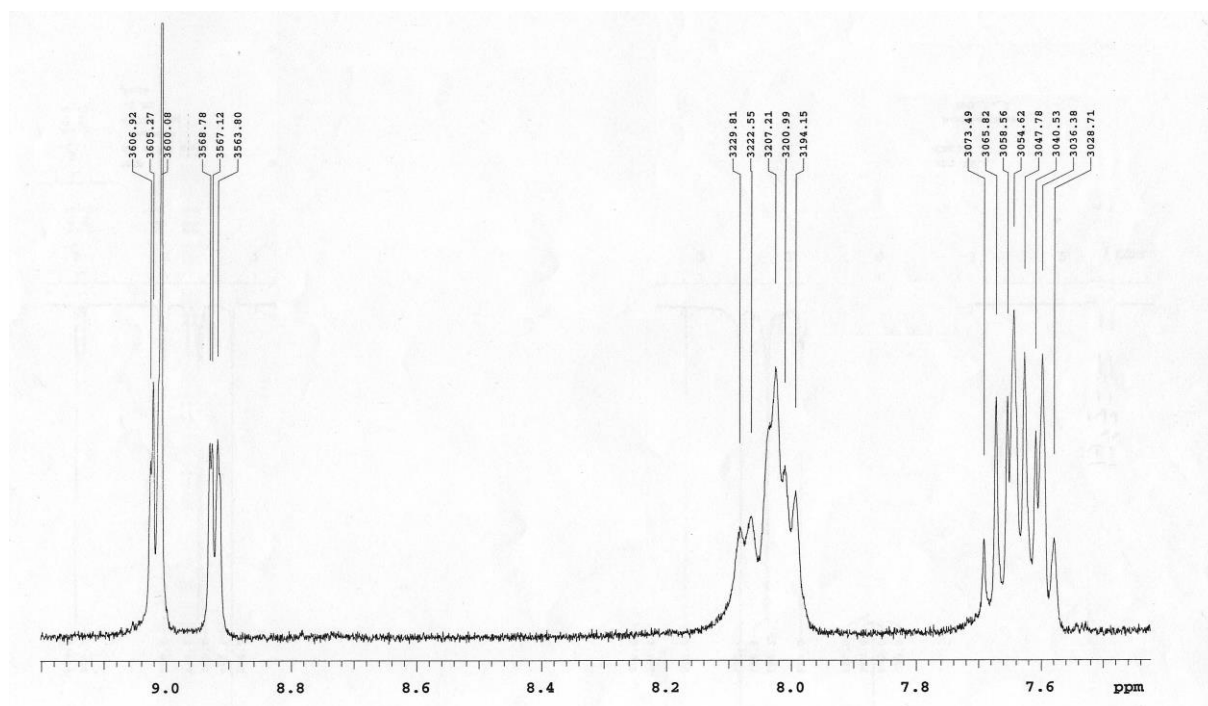


Figure 50. ¹H NMR spectrum of product **9b** (range: 7.50 – 9.20 ppm).

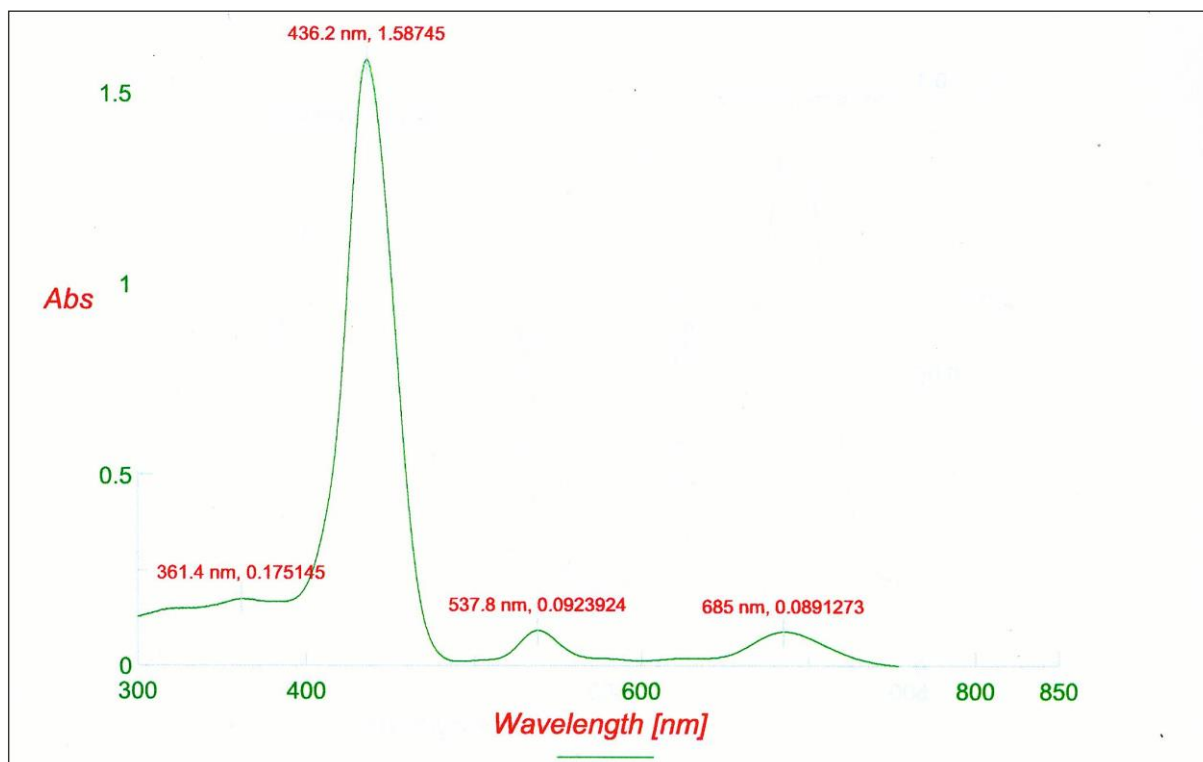


Figure 51. UV-vis spectrum of product **9b**.

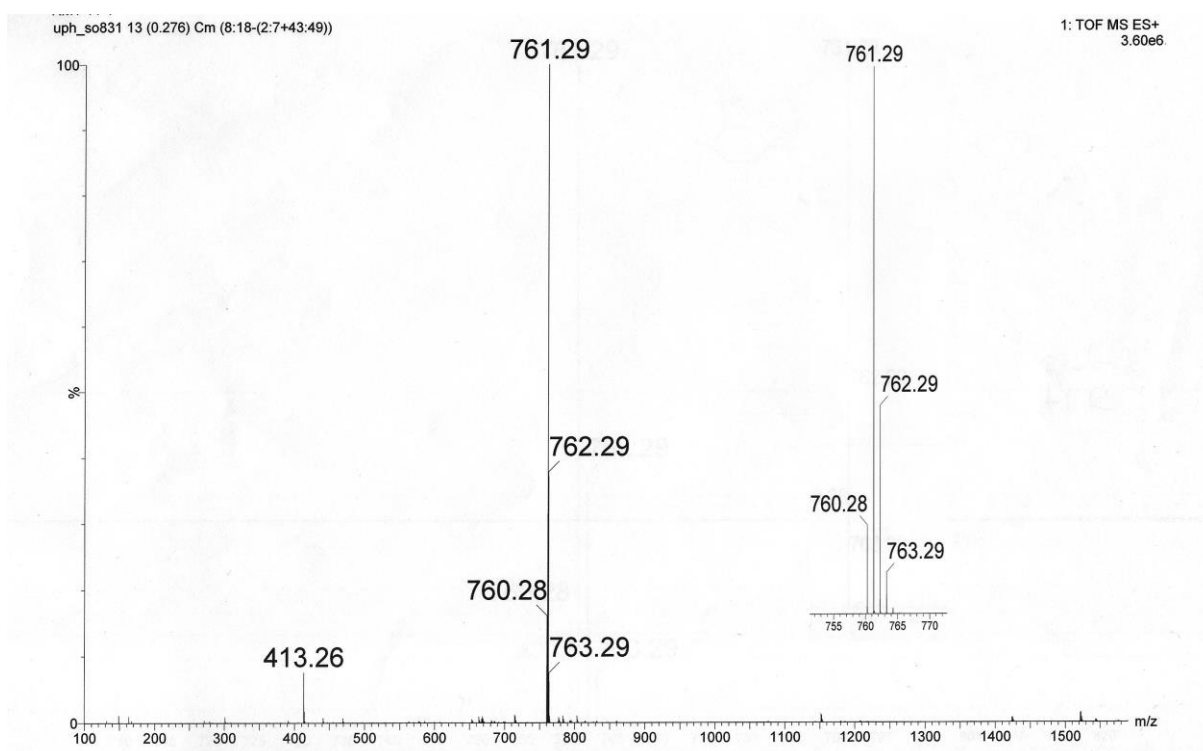


Figure 52. MS spectrum of product **9b** (ESI technique).

(2,13-dinitro-5,10,15,20-tetrakis(3-methylphenyl)porphyrin (**10b**))

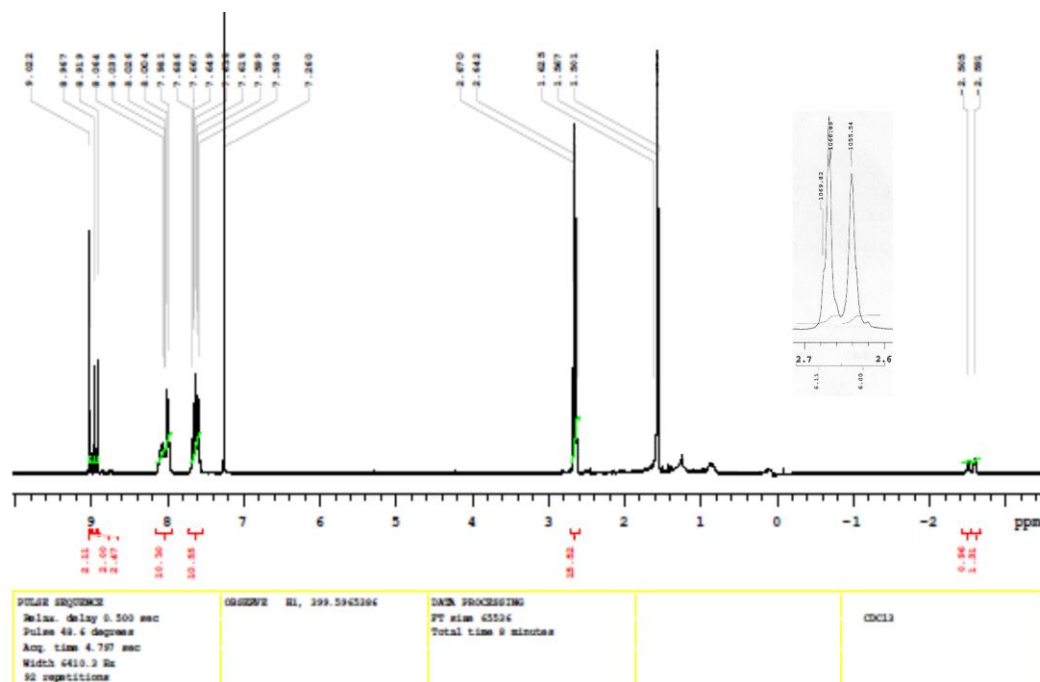


Figure 53. ¹H NMR spectrum of product **10b**.

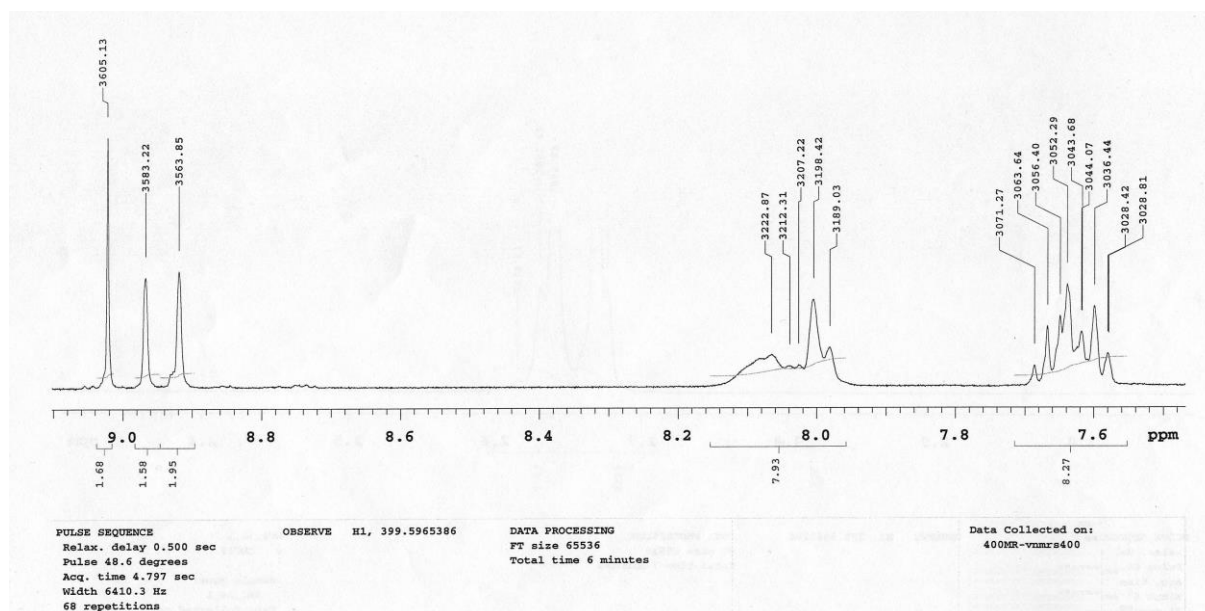


Figure 54. ¹H NMR spectrum of product **10b** (range: 7.50 – 9.10 ppm).

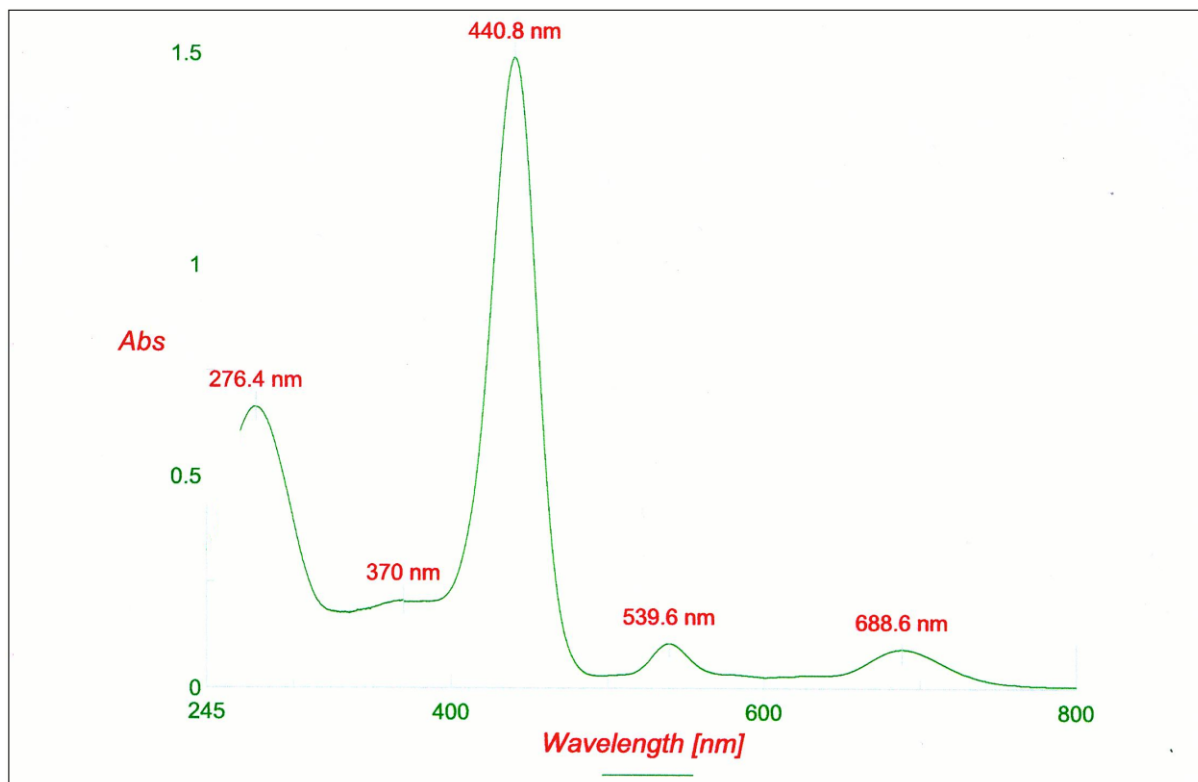


Figure 55. UV-vis spectrum of product **10b**.

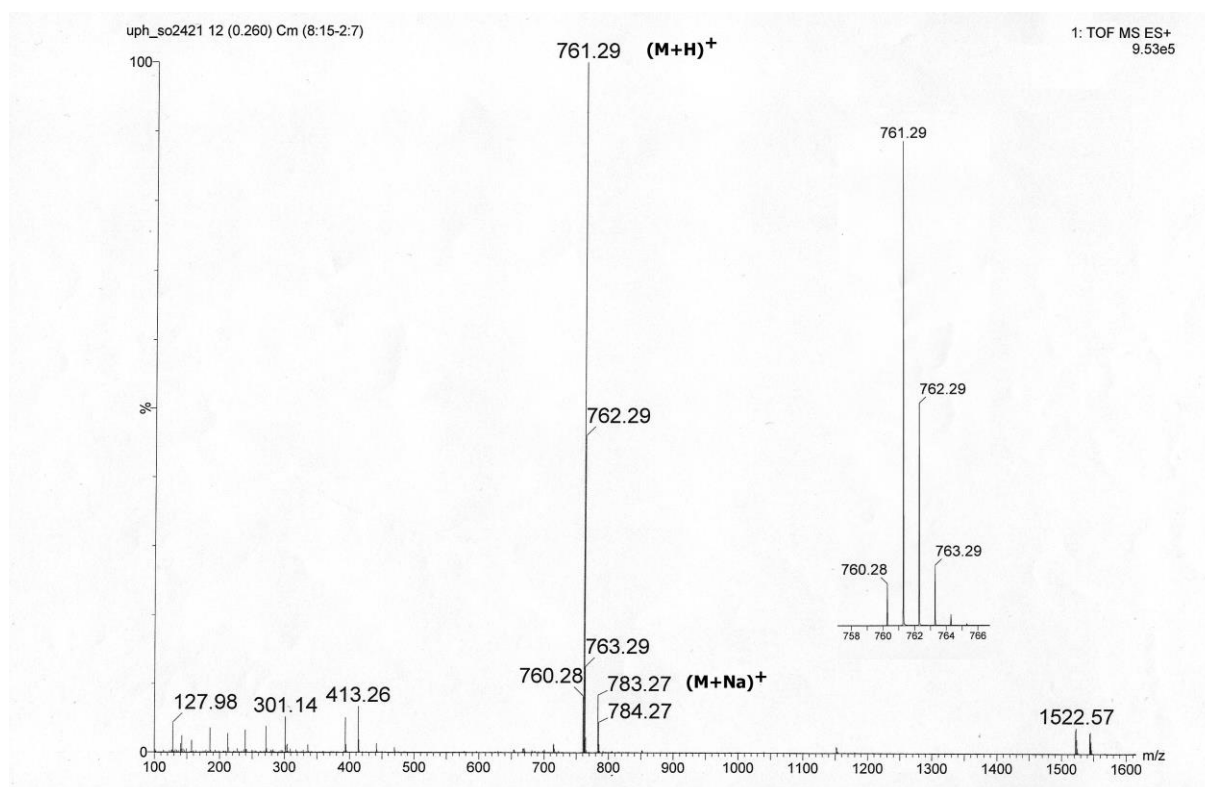


Figure 56. MS spectrum of product **10b** (ESI technique).