Electronic Supplementary Information
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Nucleoside bearing boron clusters and their phosphoramidites – building blocks for modified oligonucleotide synthesis

Michał Matuszewski,[a] Agnieszka Kiliszek,[b] Wojciech Rypniewski,[b] Zbigniew J. Lesnikowski[c] and Agnieszka B. Olejniczak[*c]

[a] *Institute of Organic Chemistry, Lodz University of Technology, 116 Zeromskiego St., 90-924 Lodz, Poland.*
[b]*Institute of Bioorganic Chemistry PAS, 12/14 Noskowskiego St., 61-704 Poznan, Poland.*
[c]*Institute of Medical Biology PAS, 106 Lodowa St., 92-232 Lodz, Poland.*
E-mail: aolejniczak@cbm.pan.pl

^{1}H-, ^{13}C-, ^{11}B-, ^{11}B{H BB}-,^{31}P-NMR, DEPT-135, IR, MS spectra of 1,2-dicarba-*closo*-dodecaborane derivatives of thymidine: **20**, **21**, **29**, 2'-deoxycytidine: **22**, **23**, **30**, 2'-deoxyadenosine: **12-14**, **24**, **25**, **31**, 2'-deoxyguanosine: **16**, **17**, **26-28**, **32**, and conjugates with opened-cage 7,8-dicarba-*nido*-undecaborate ion **33-36.** CD spectra for **20**, **22**, **24**, **27**, **MALDI-TOF** spectra for **38-41**.

Thymidine derivatives

2'-Deoxycytidine derivatives

2'-Deoxyadenosine derivatives

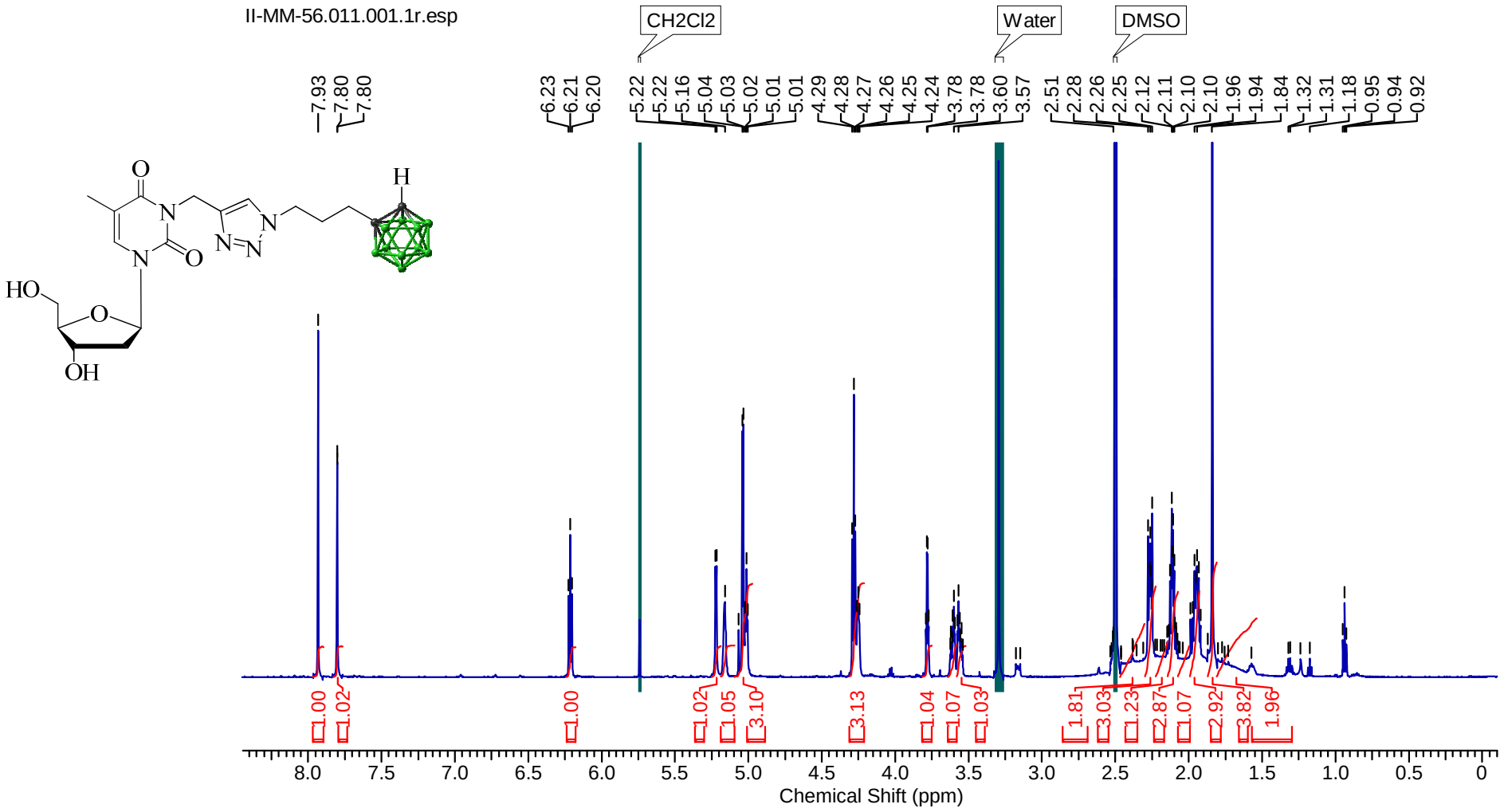


Figure S1. ^{1}H NMR spectrum of conjugate **20**.

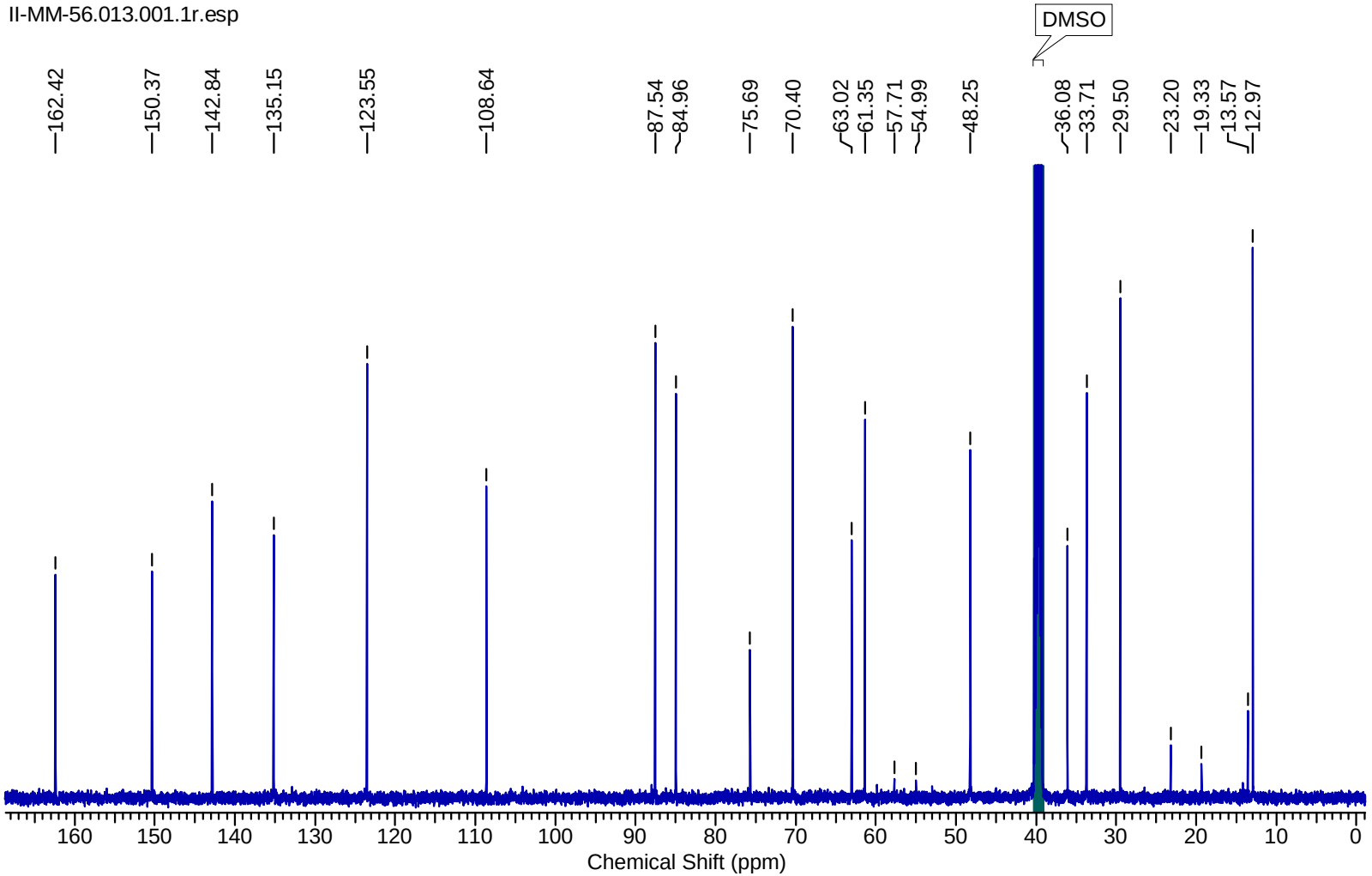


Figure S2. ^{13}C NMR spectrum of conjugate **20**.

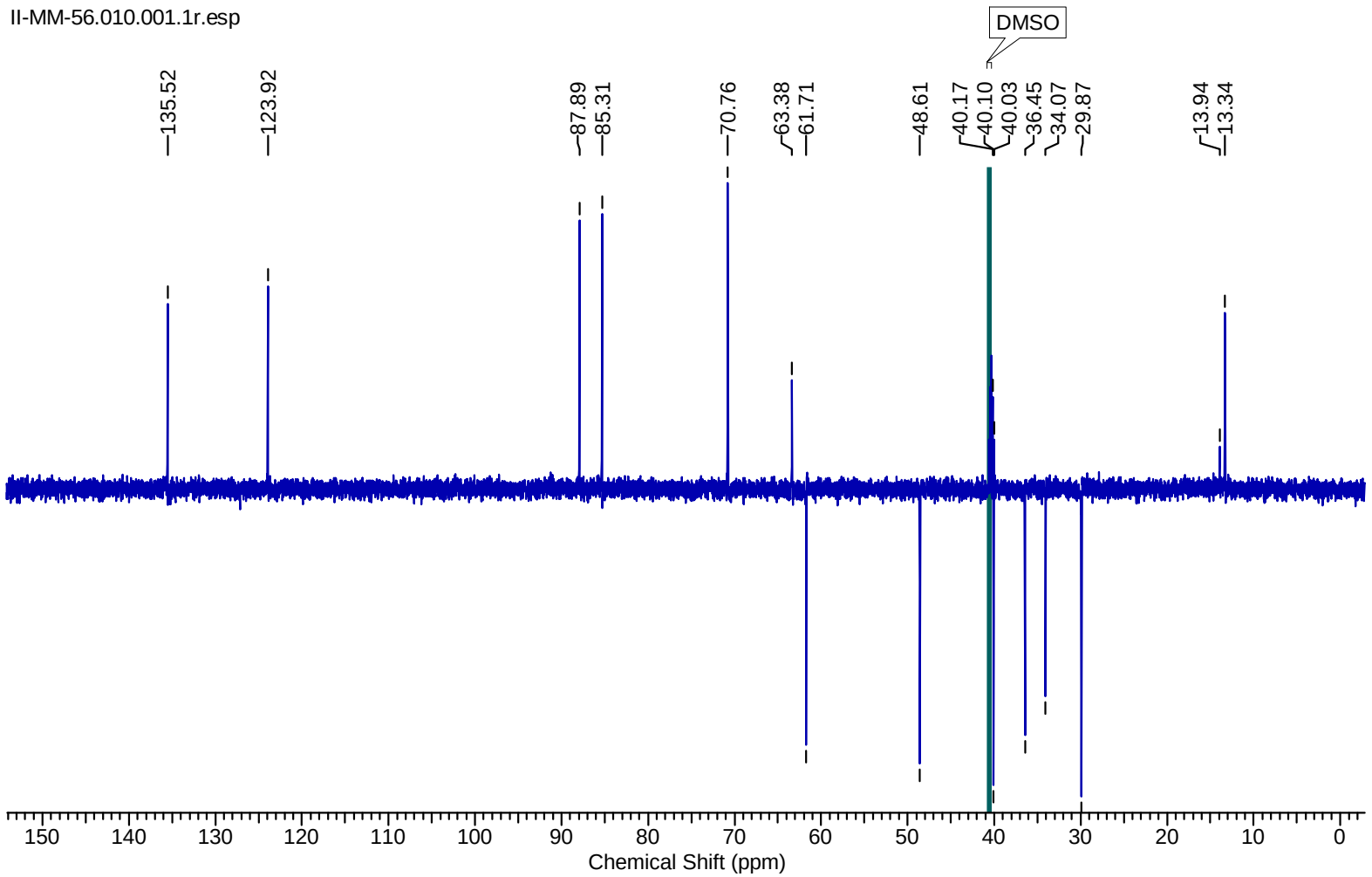


Figure S3. DEPT-135 spectrum of conjugate **20**.

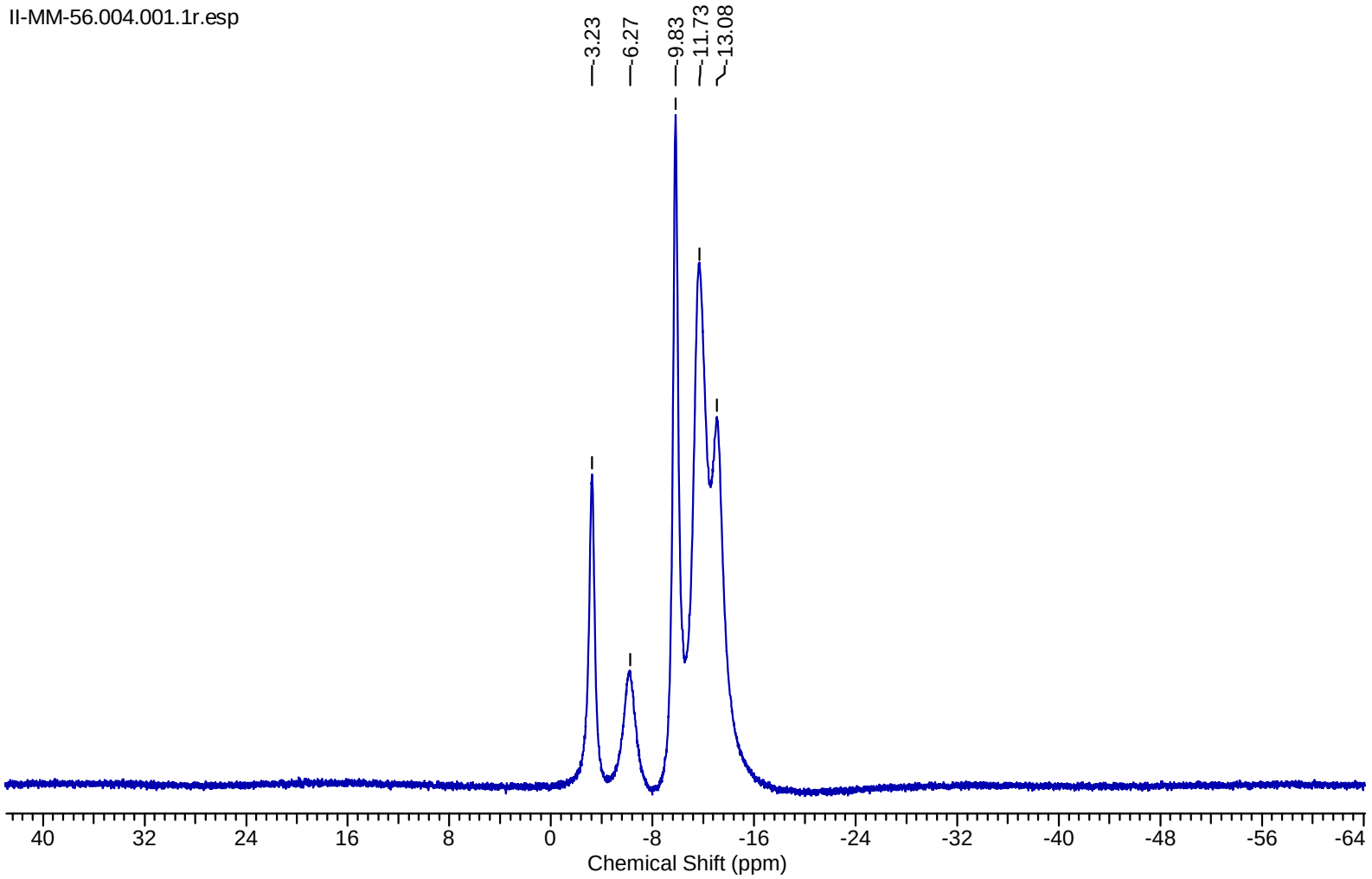


Figure S4. ^{11}B {H BB} NMR spectrum of compound **20**.

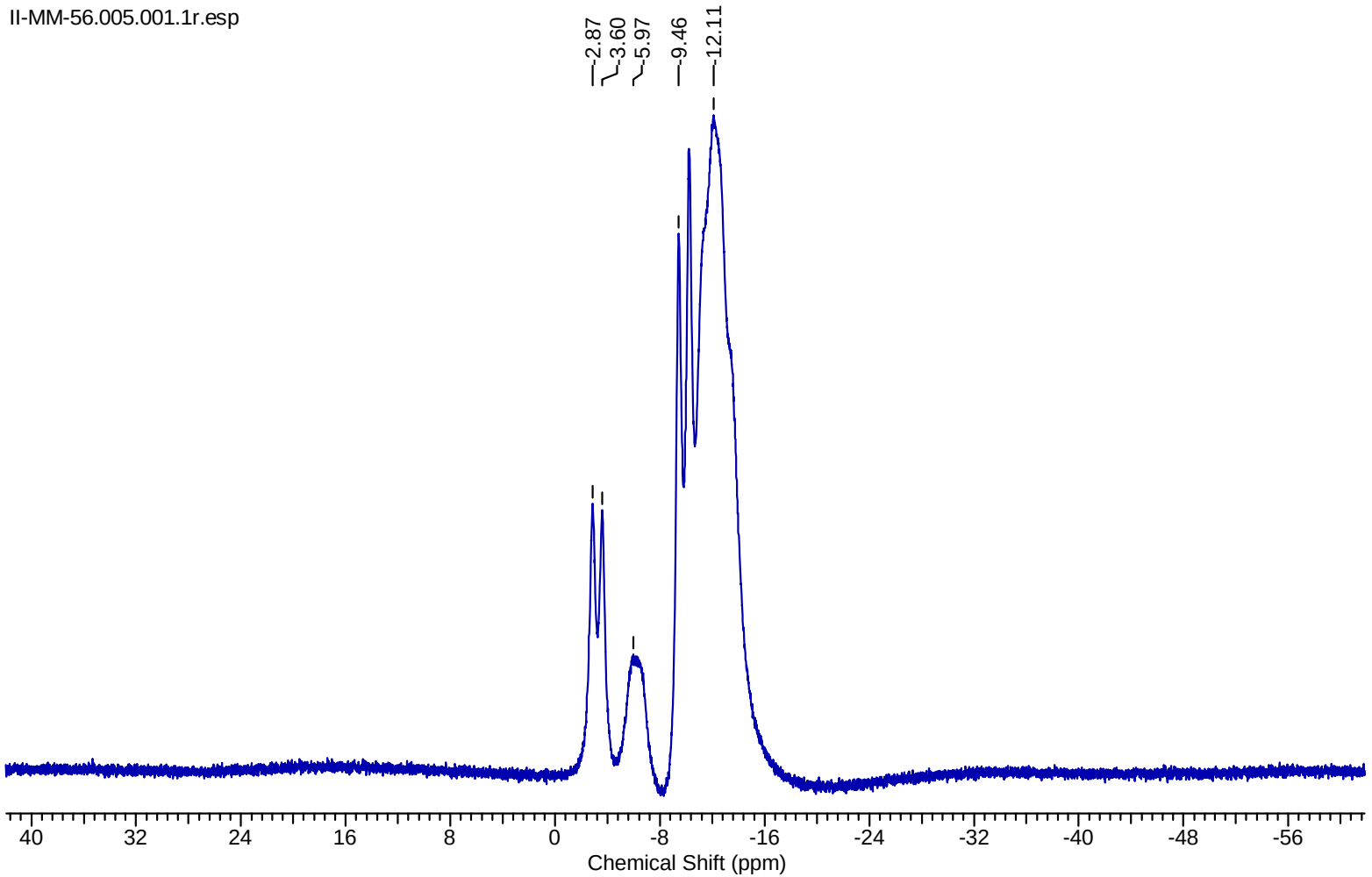


Figure S5. ^{11}B NMR spectrum of compound **20**.

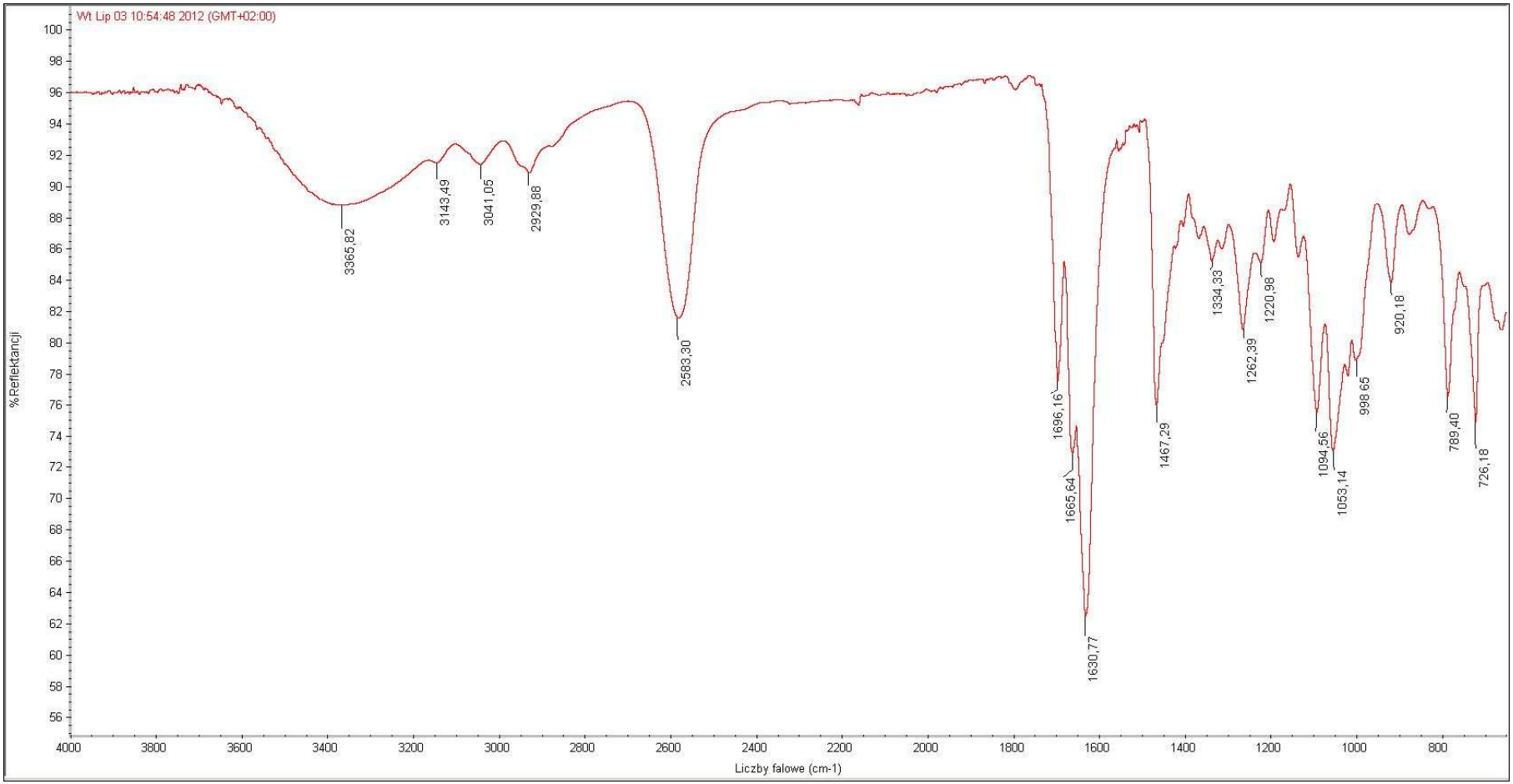
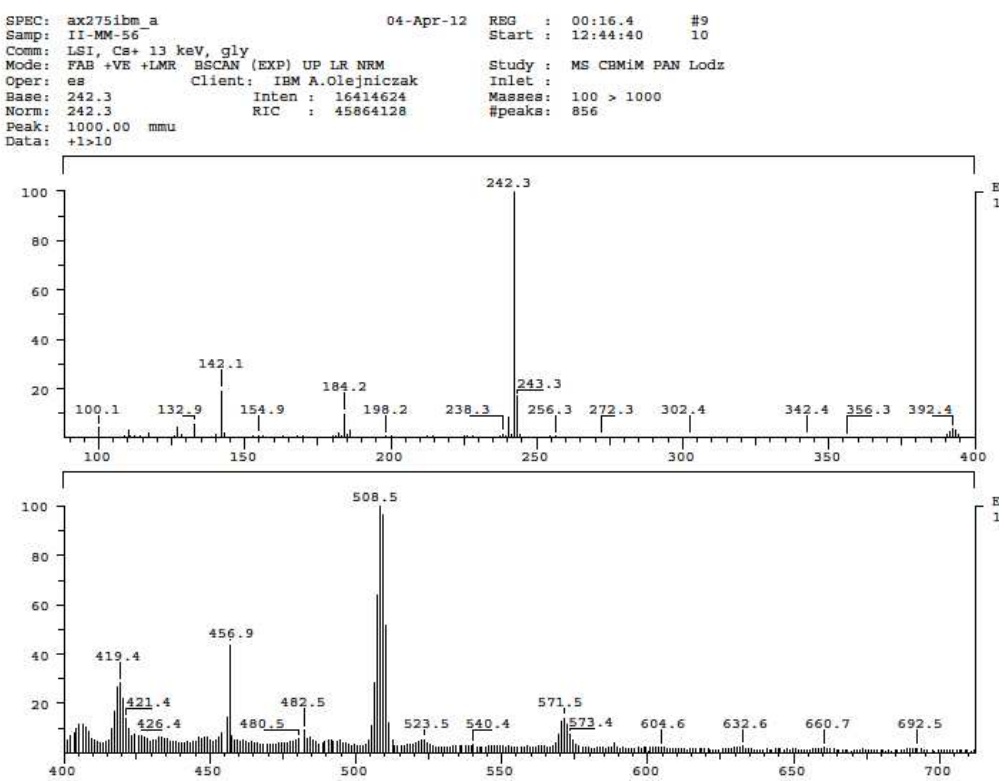


Figure S6. IR spectrum of compound **20**.



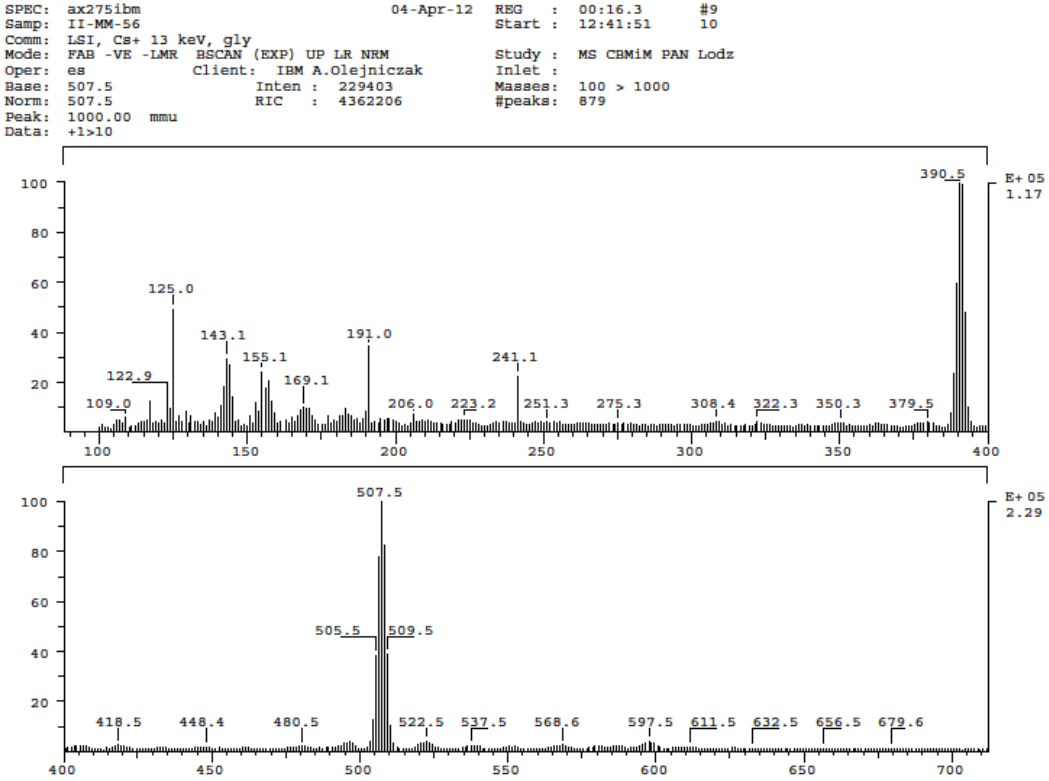


Figure S7. MS-FAB spectra of compound **20**.

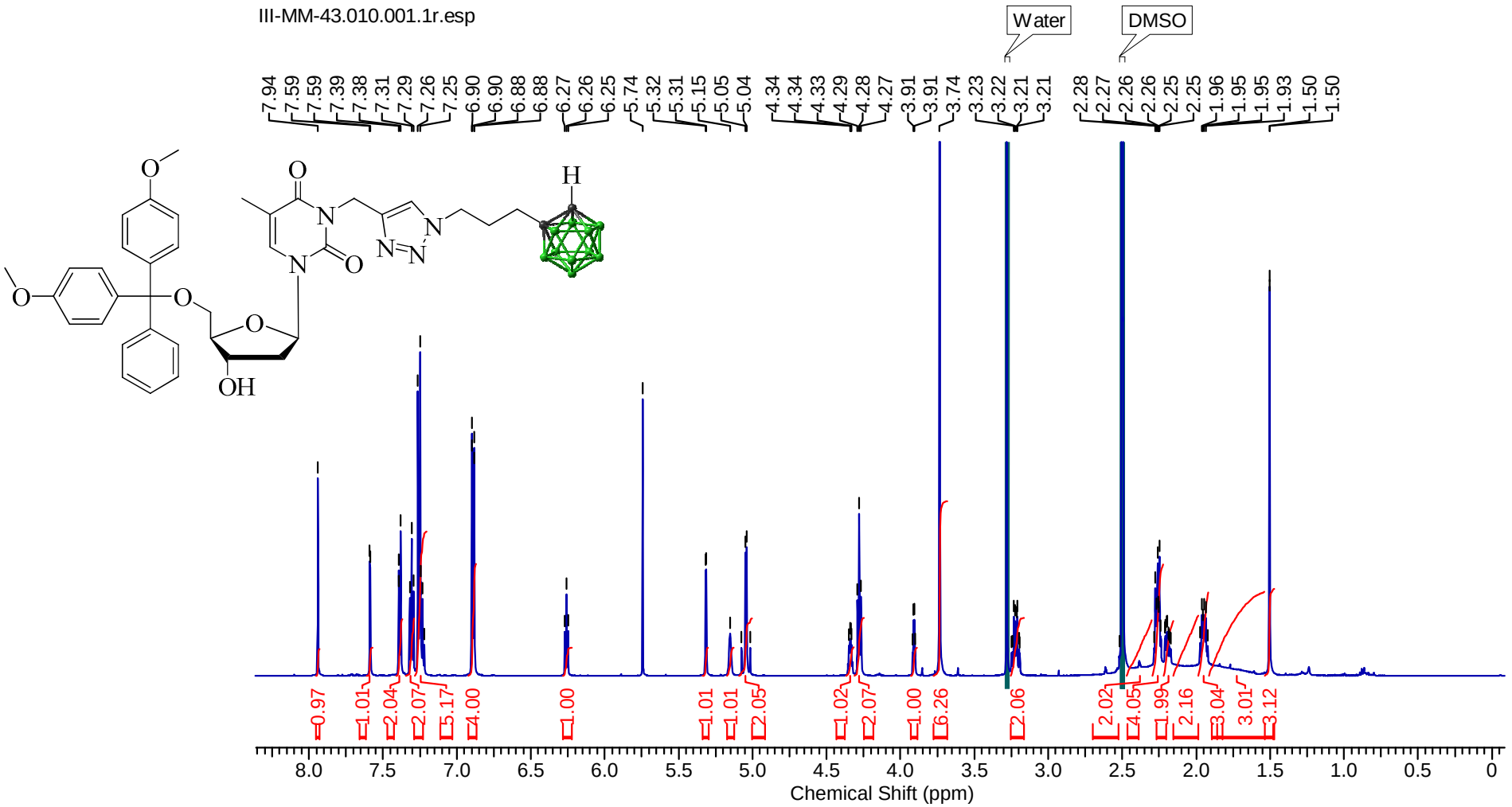


Figure S8. ^{1}H NMR spectrum of compound **21**.

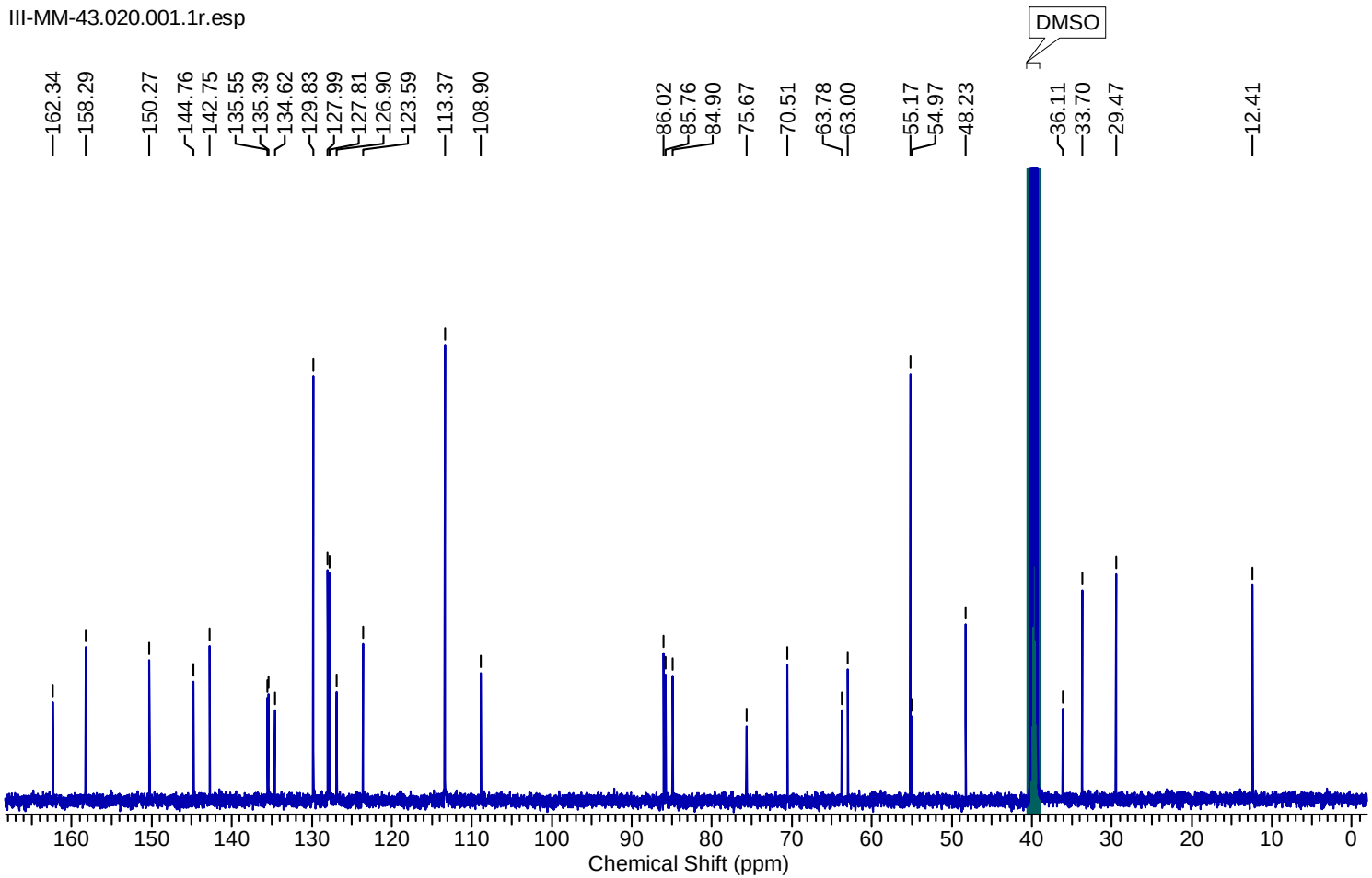


Figure S9. ^{13}C NMR spectrum of compound **21**.

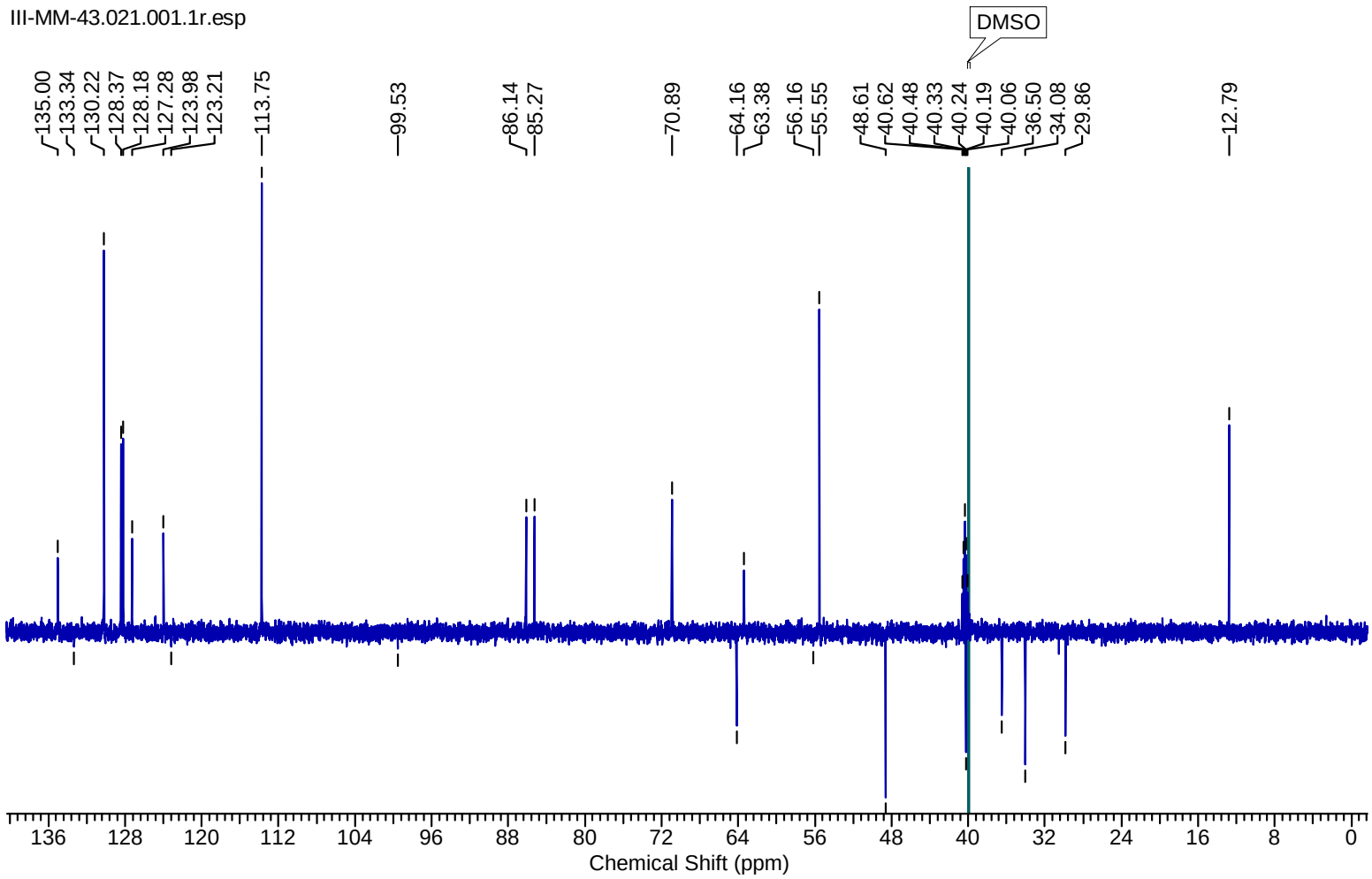


Figure S10. DEPT-135 spectrum of compound **21**.

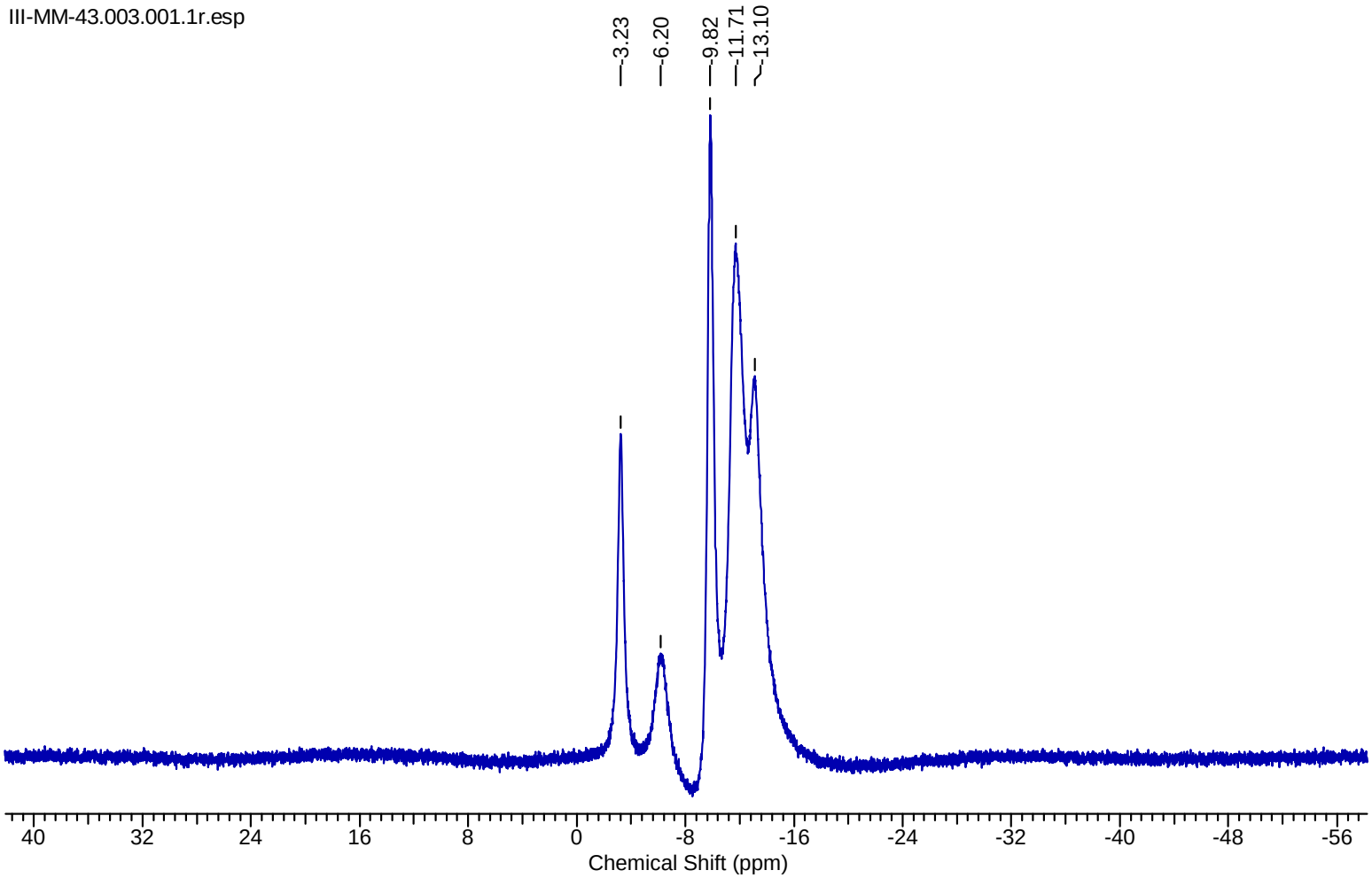


Figure S11. ^{11}B {H BB} NMR spectrum of compound **21**.

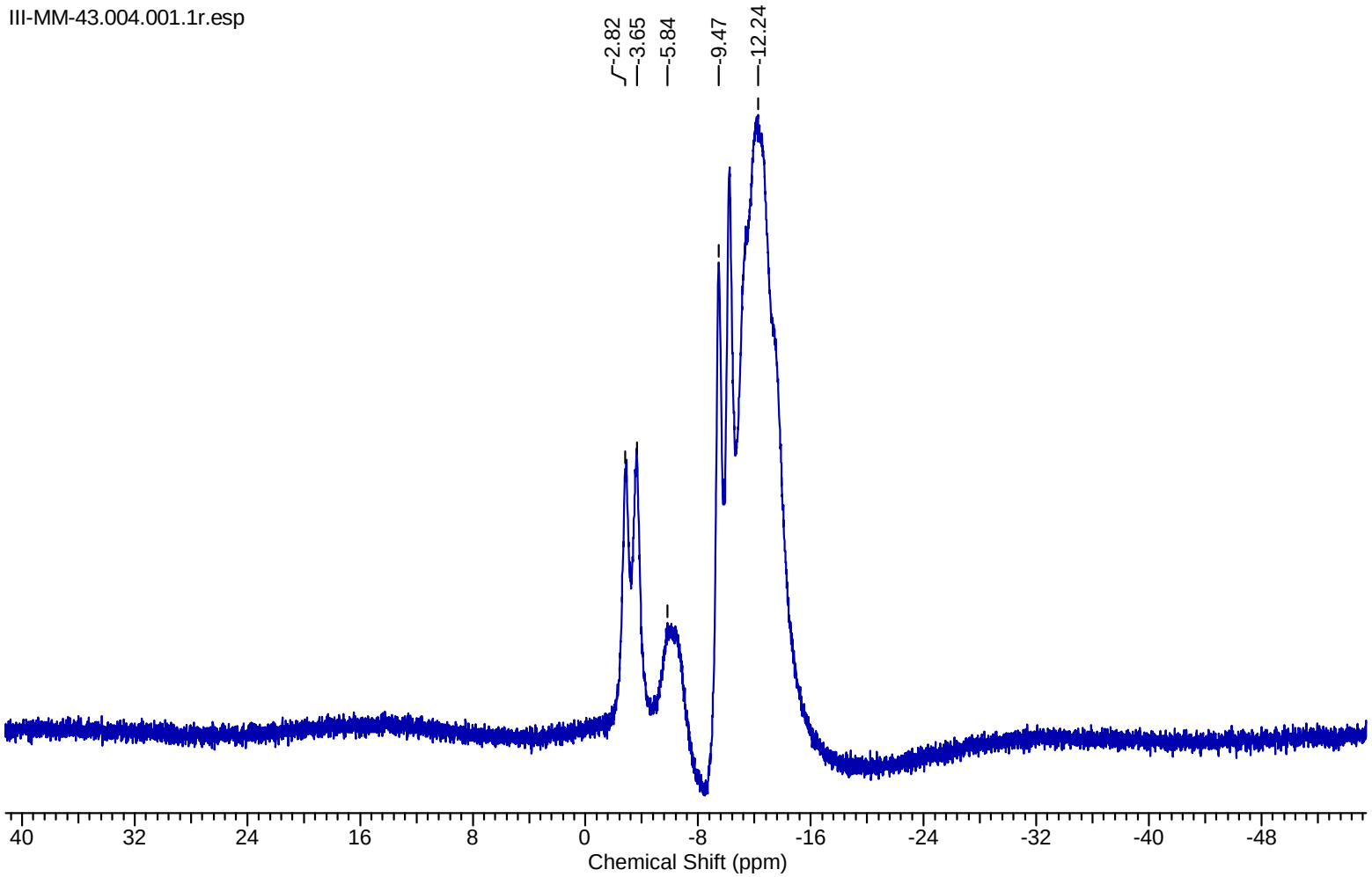


Figure S12. ^{11}B NMR spectrum of compound **21**.

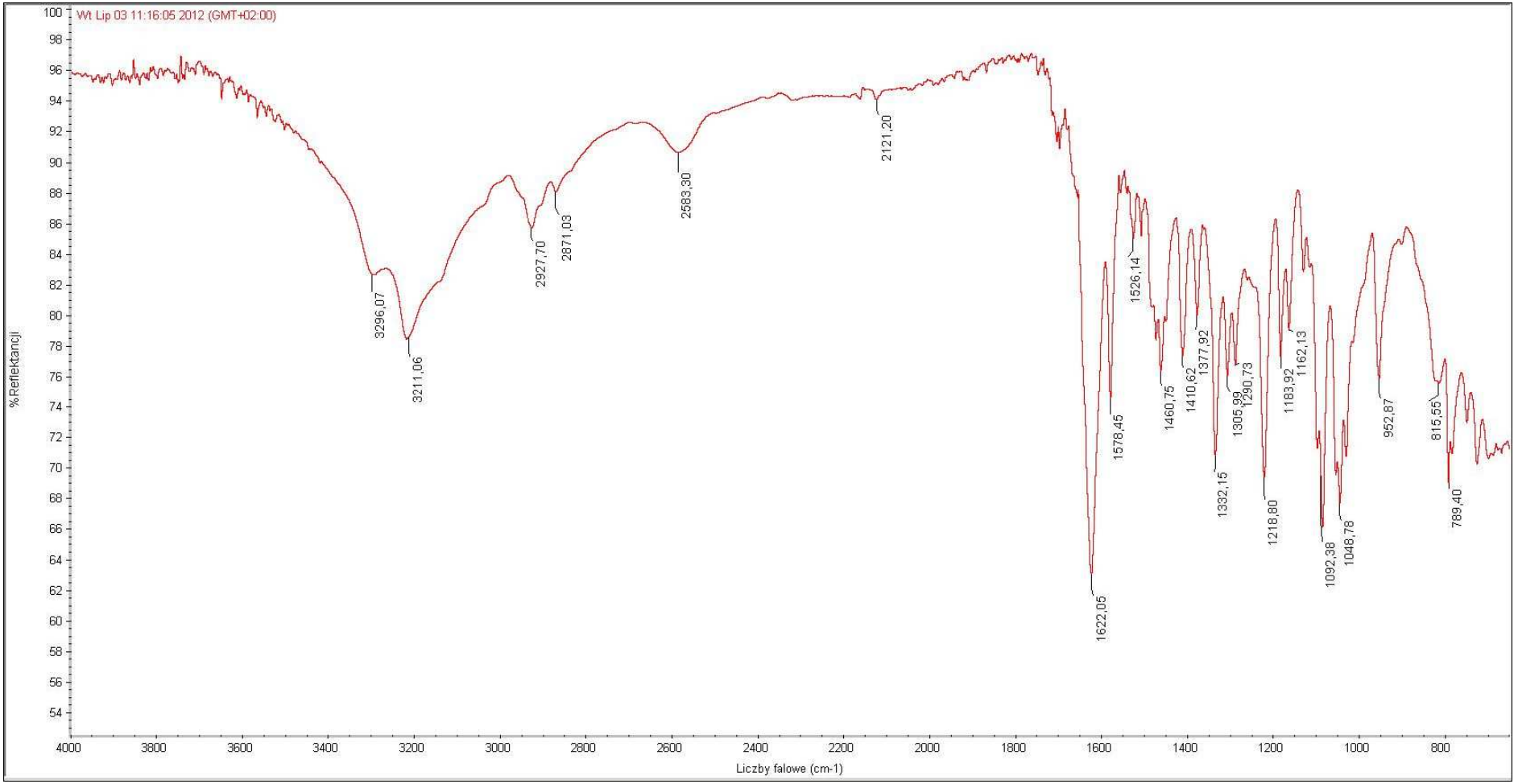
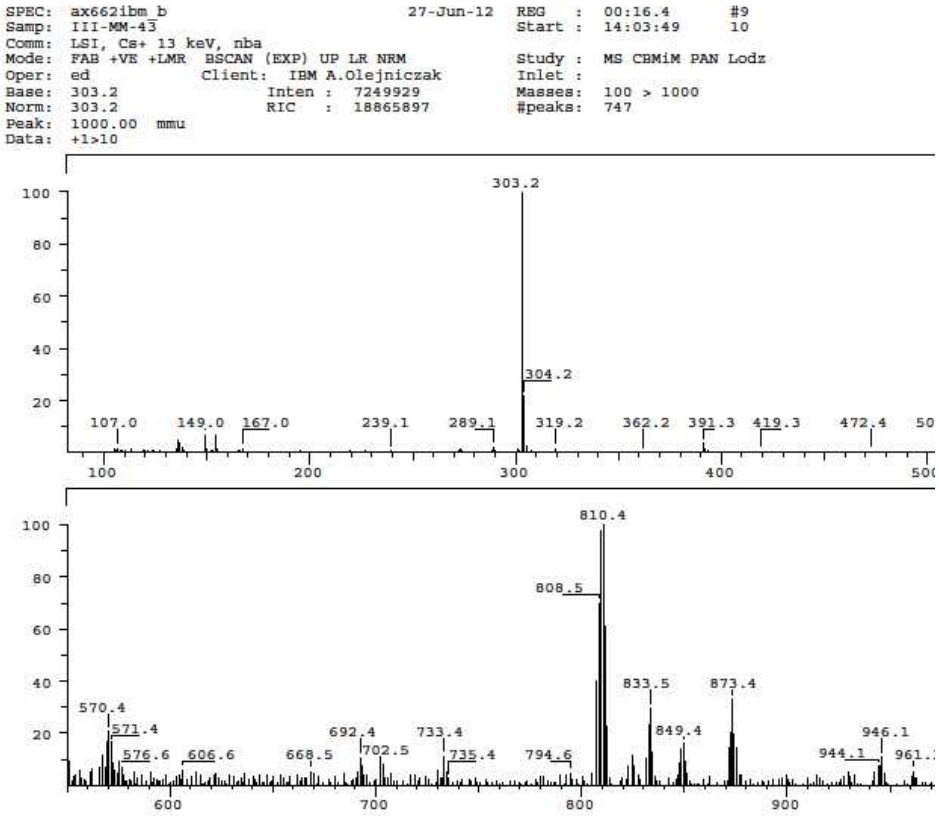


Figure S13. IR spectrum of compound **21**.



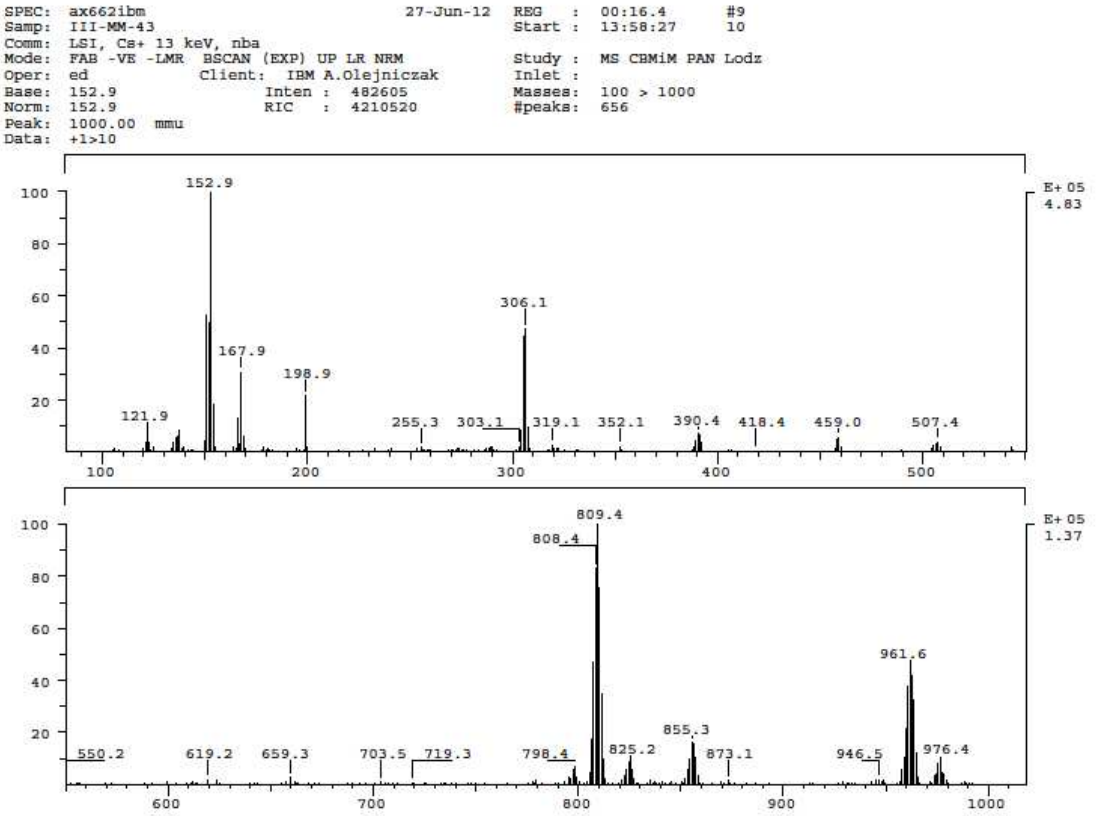


Figure S14. MS-FAB spectra of compound **21**.

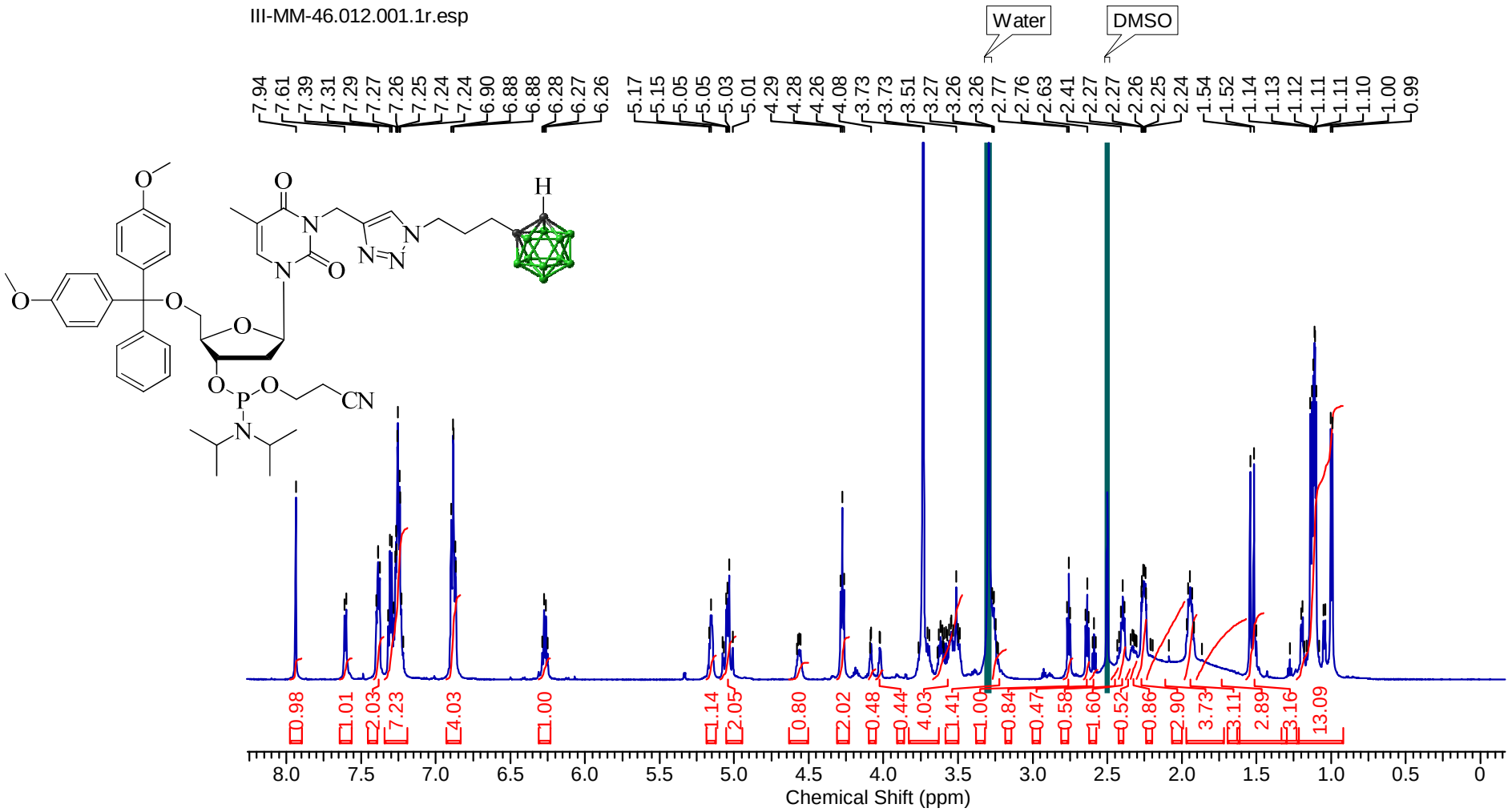


Figure S15. ^{1}H NMR spectrum of compound **29**.

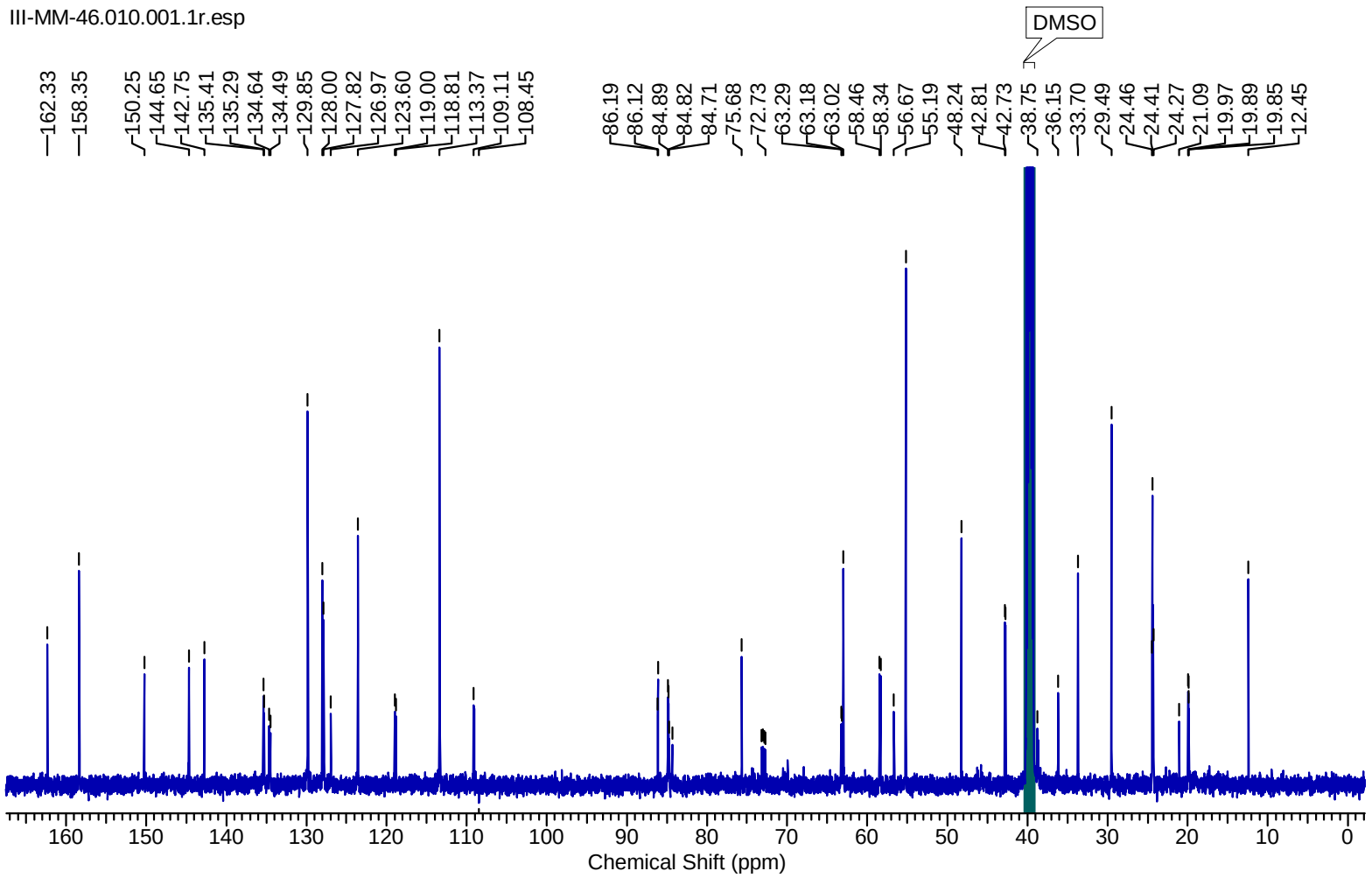


Figure S16. ^{13}C NMR spectrum of compound **29**.

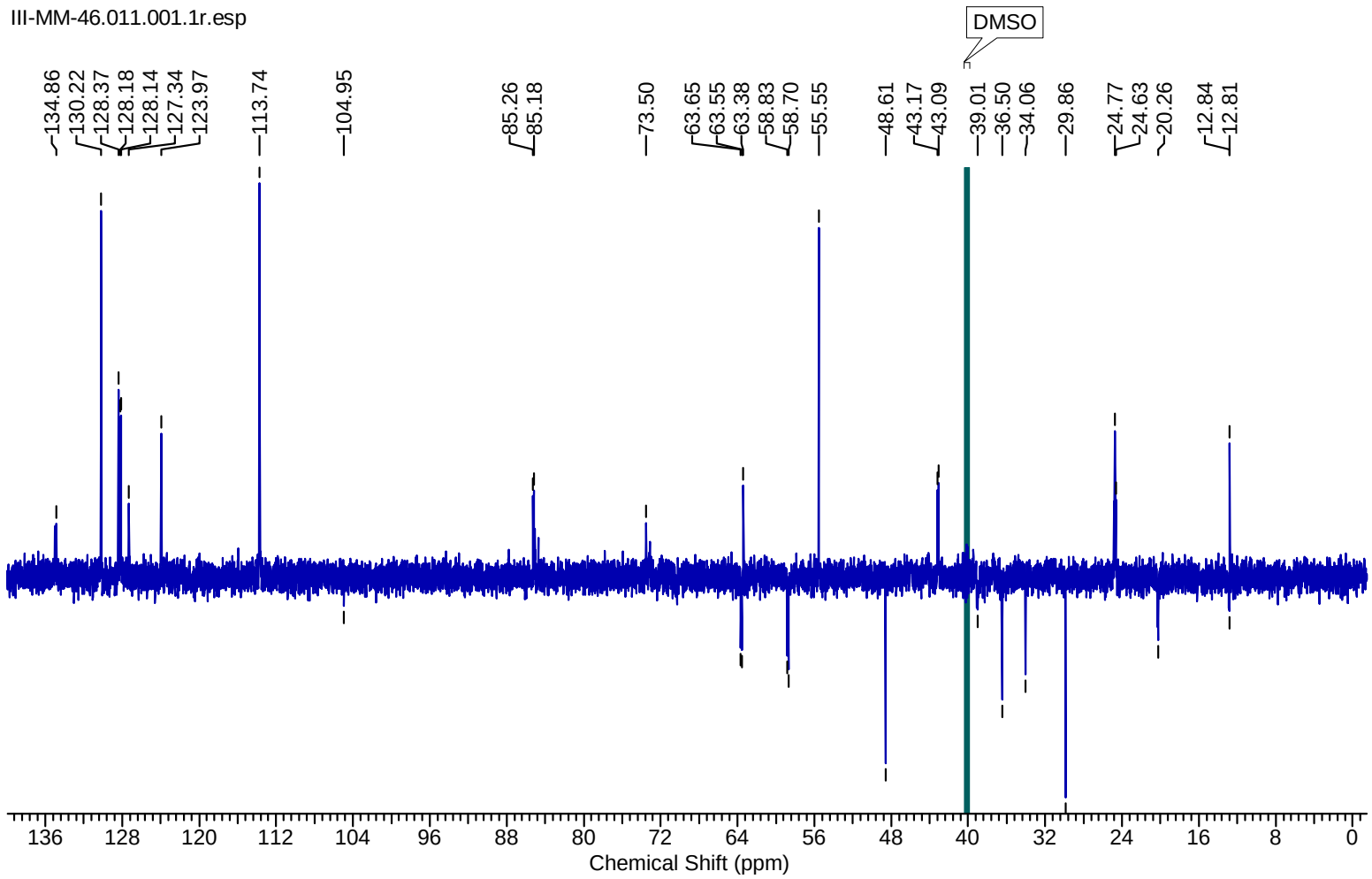


Figure S17. DEPT-135 spectrum of compound **29**.

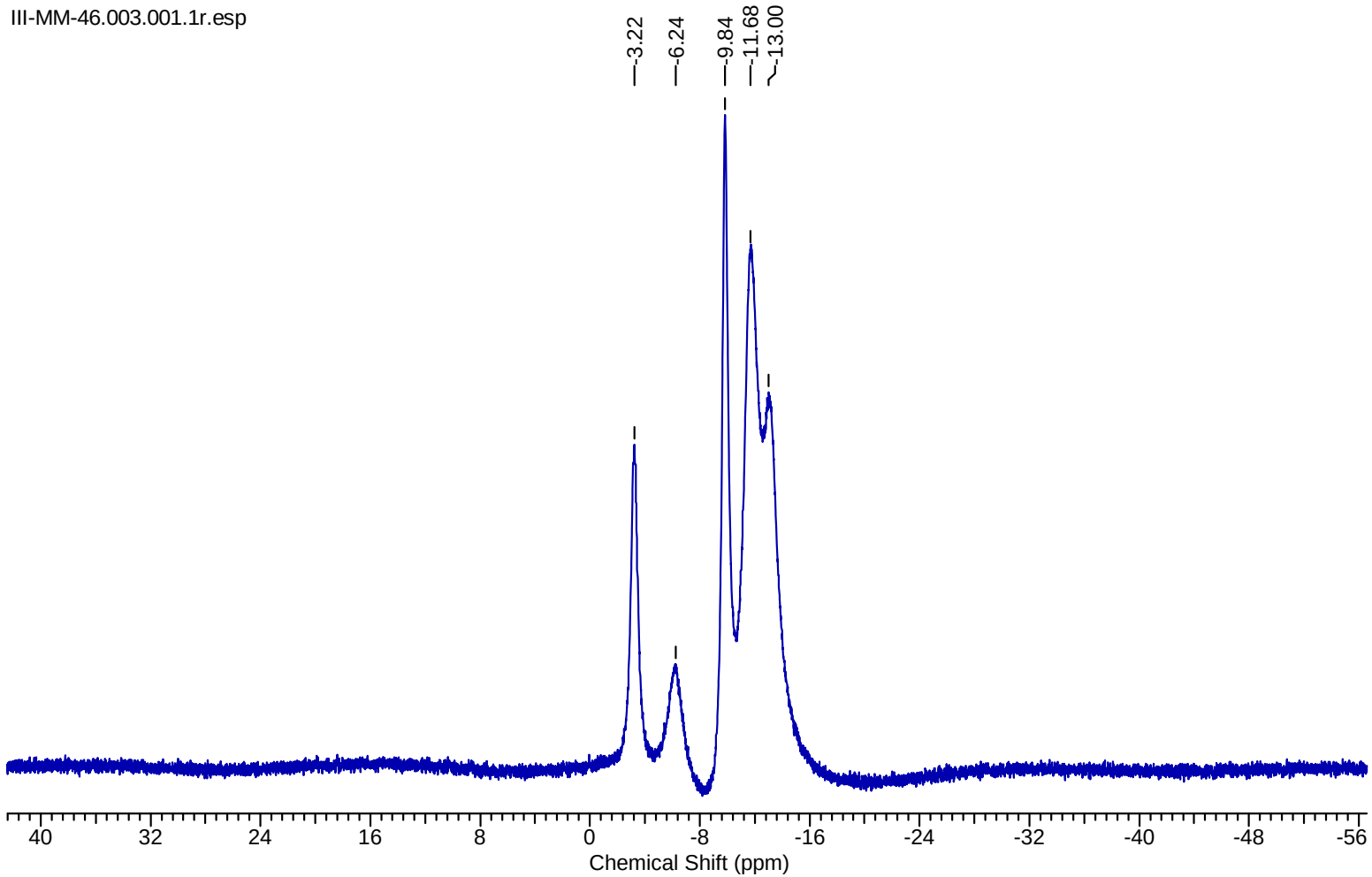


Figure S18. ^{11}B {H BB} NMR spectrum of compound **29**.

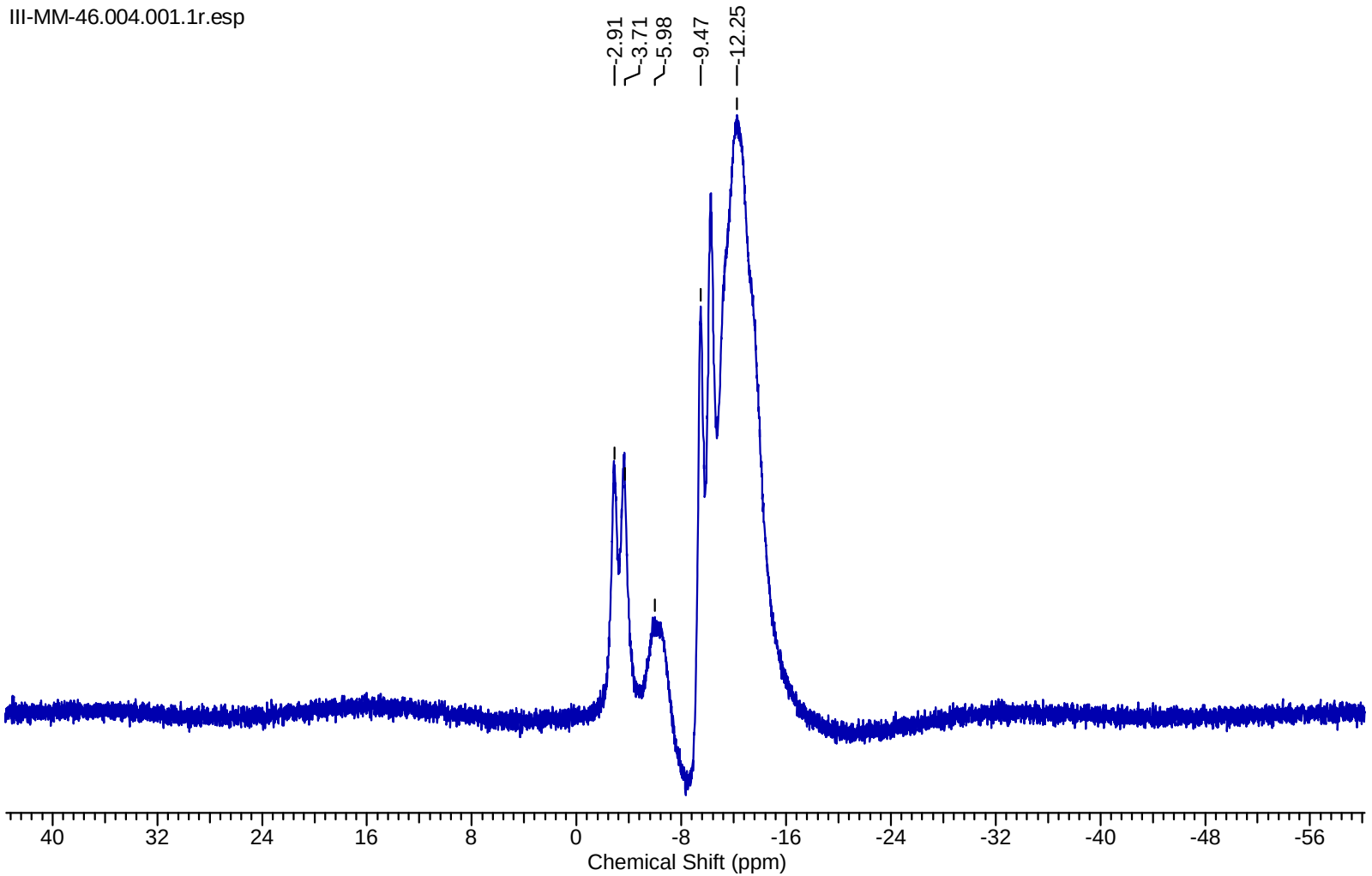


Figure S19. ^{11}B NMR spectrum of compound **29**.

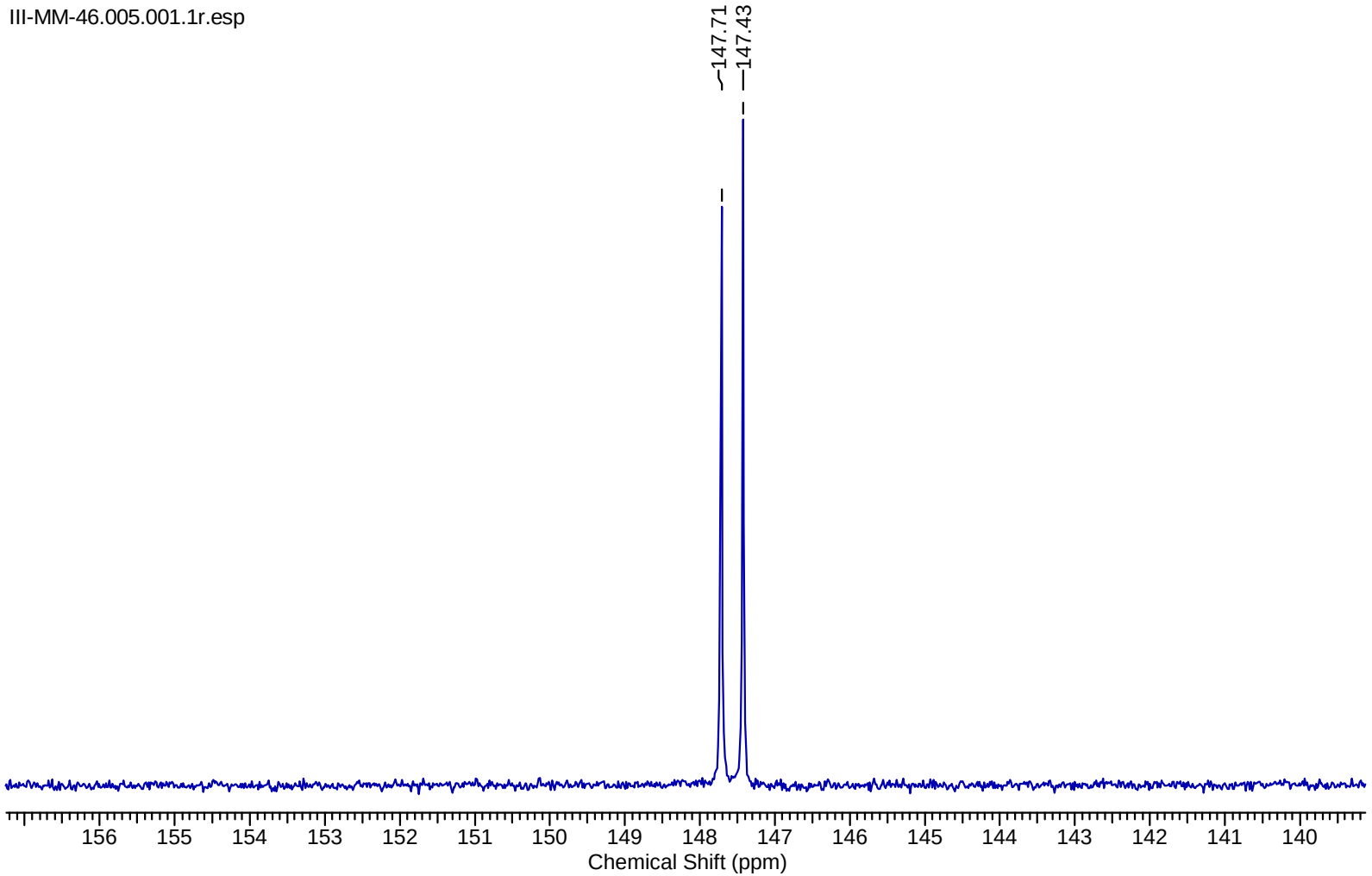


Figure S20. ^{31}P NMR spectrum of compound **29**.

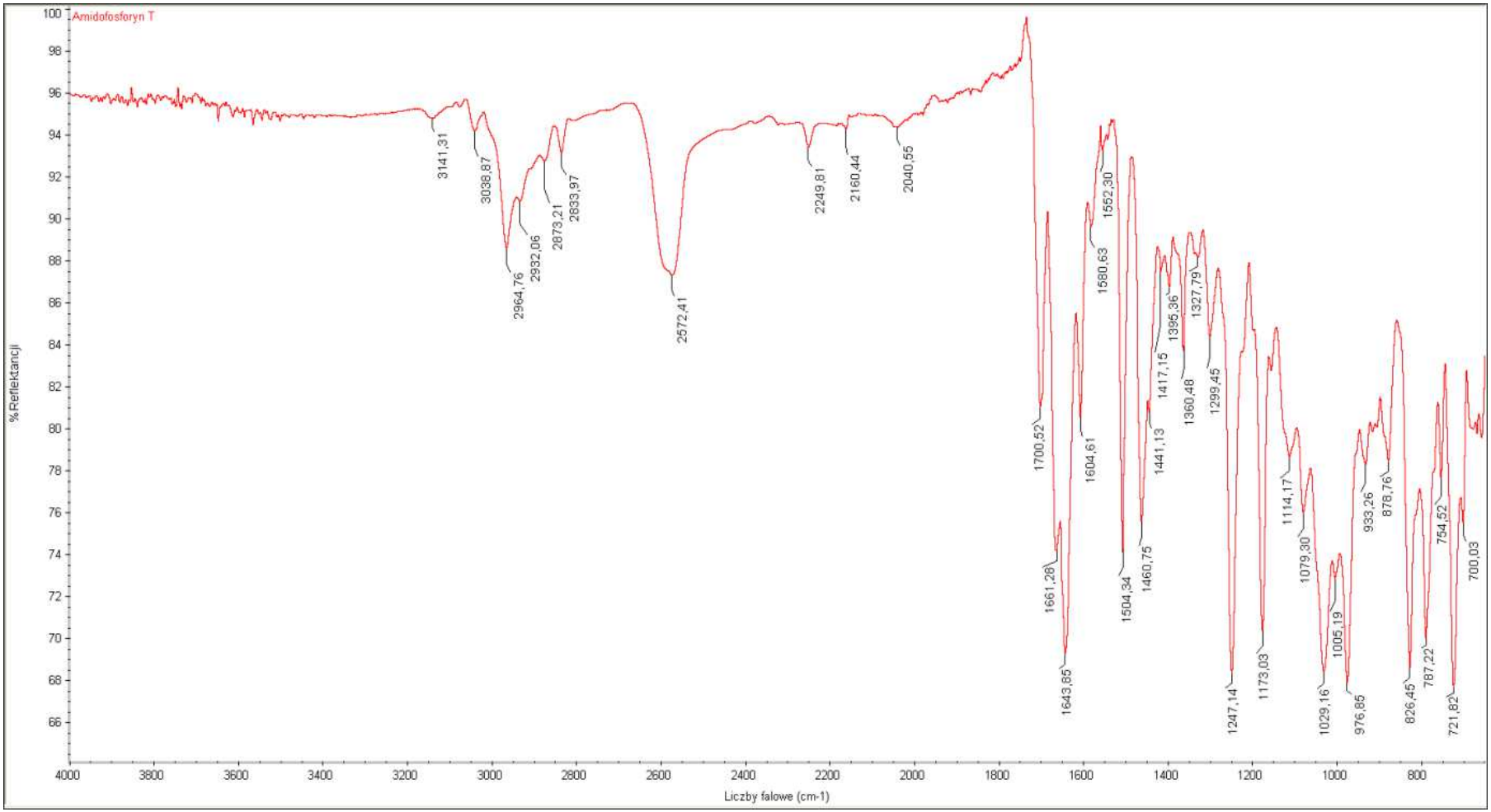
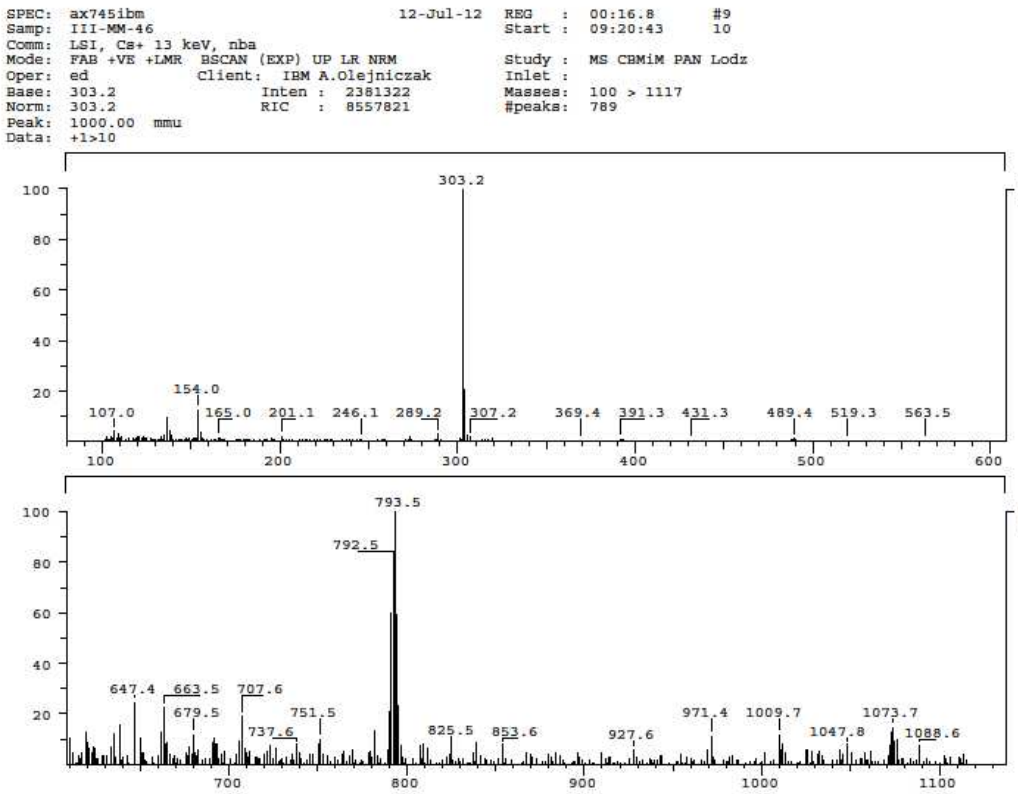


Figure S21. IR spectrum of compound **29**.



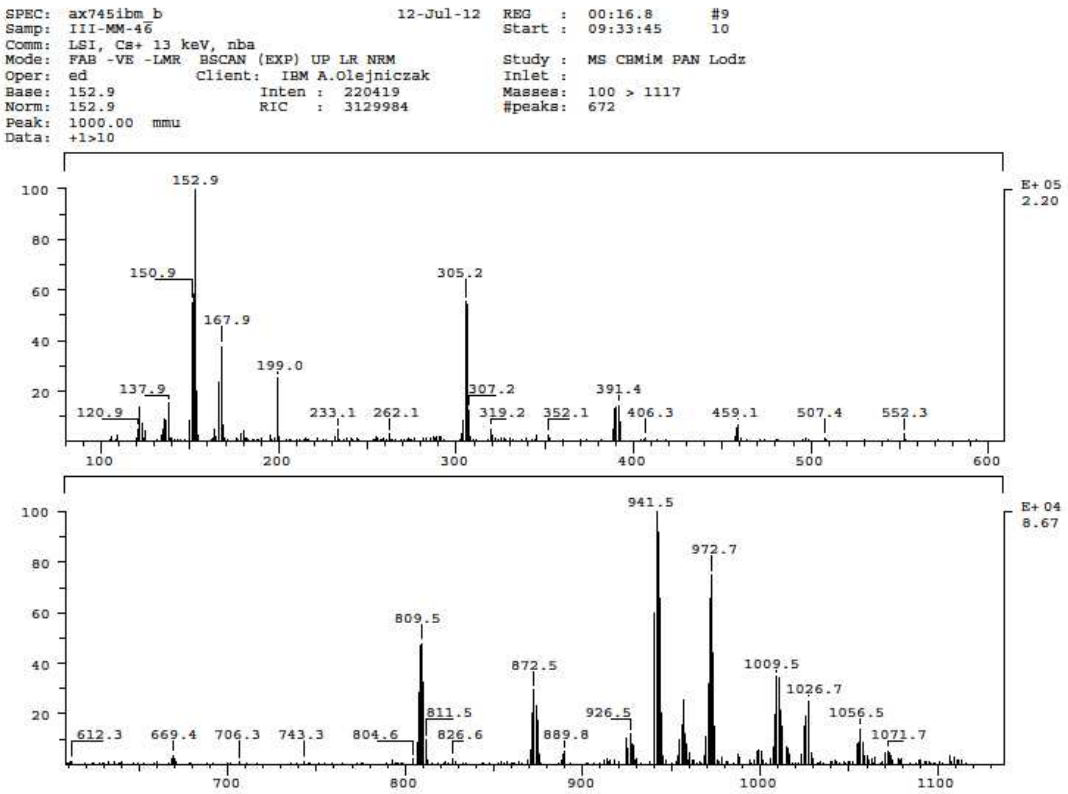


Figure S22. MS-FAB spectra of compound **29**.

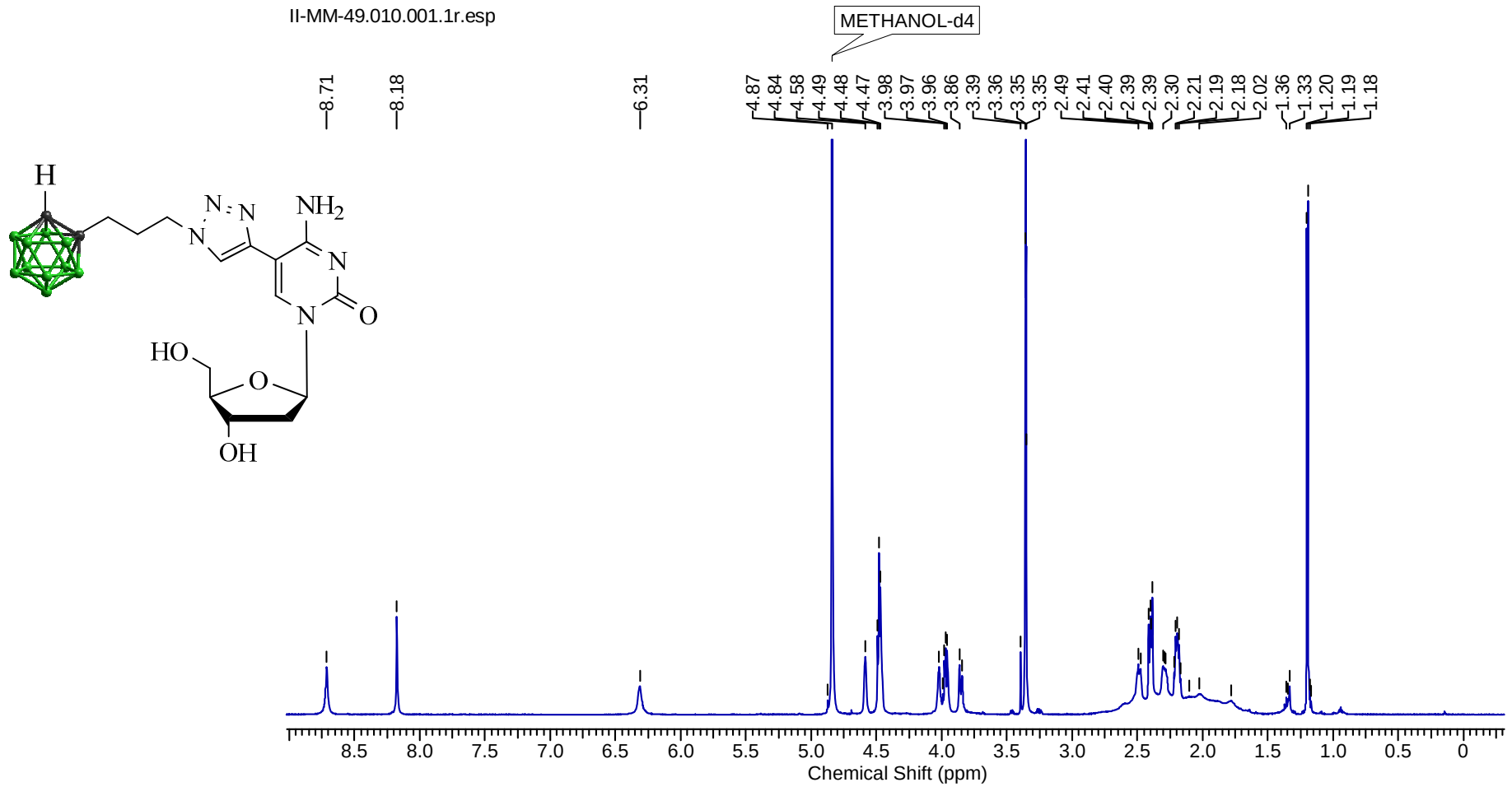


Figure S23. ^{1}H NMR spectrum of compound **22**.

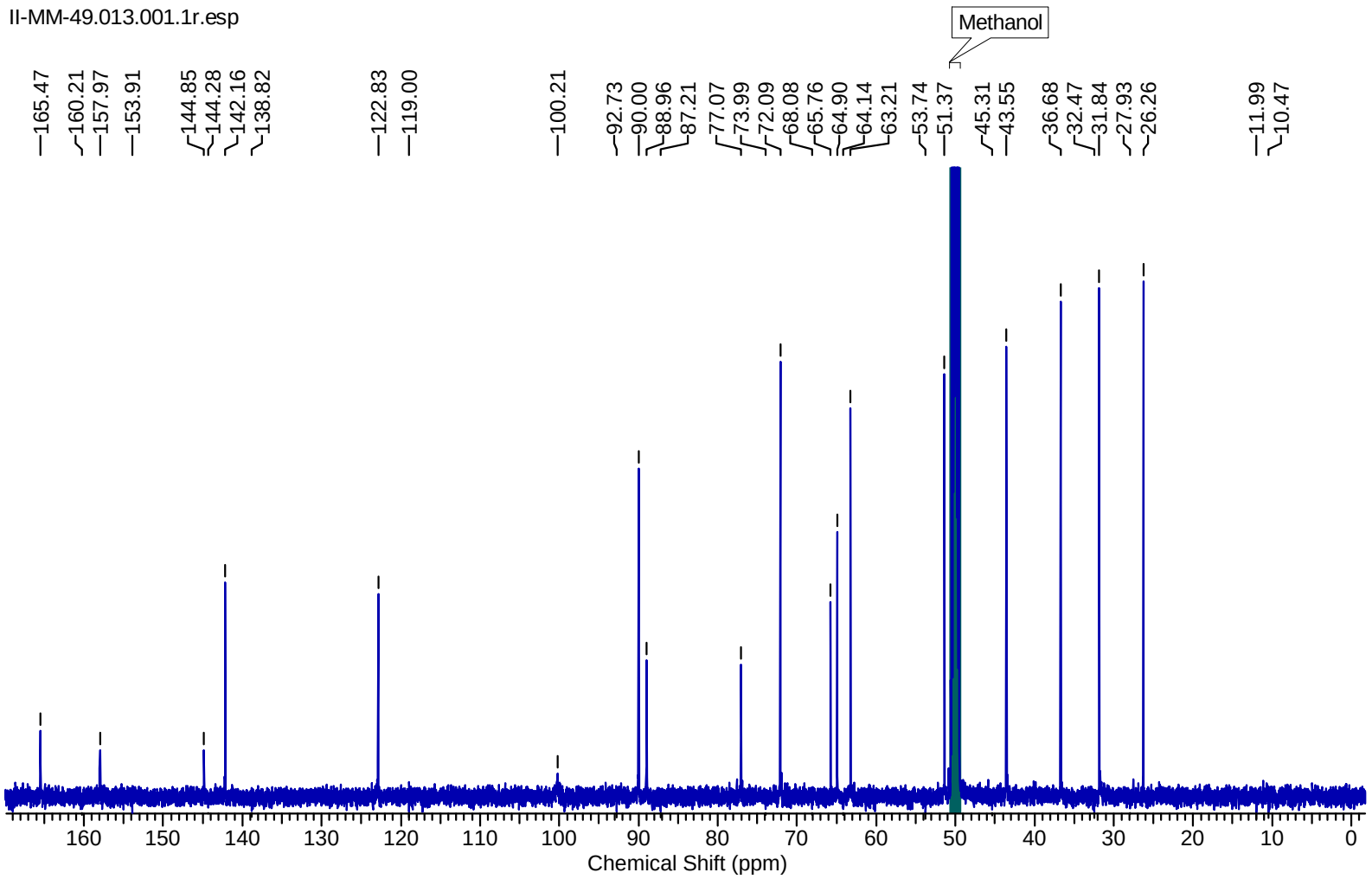


Figure S24. ^{13}C NMR spectrum of compound **22**.

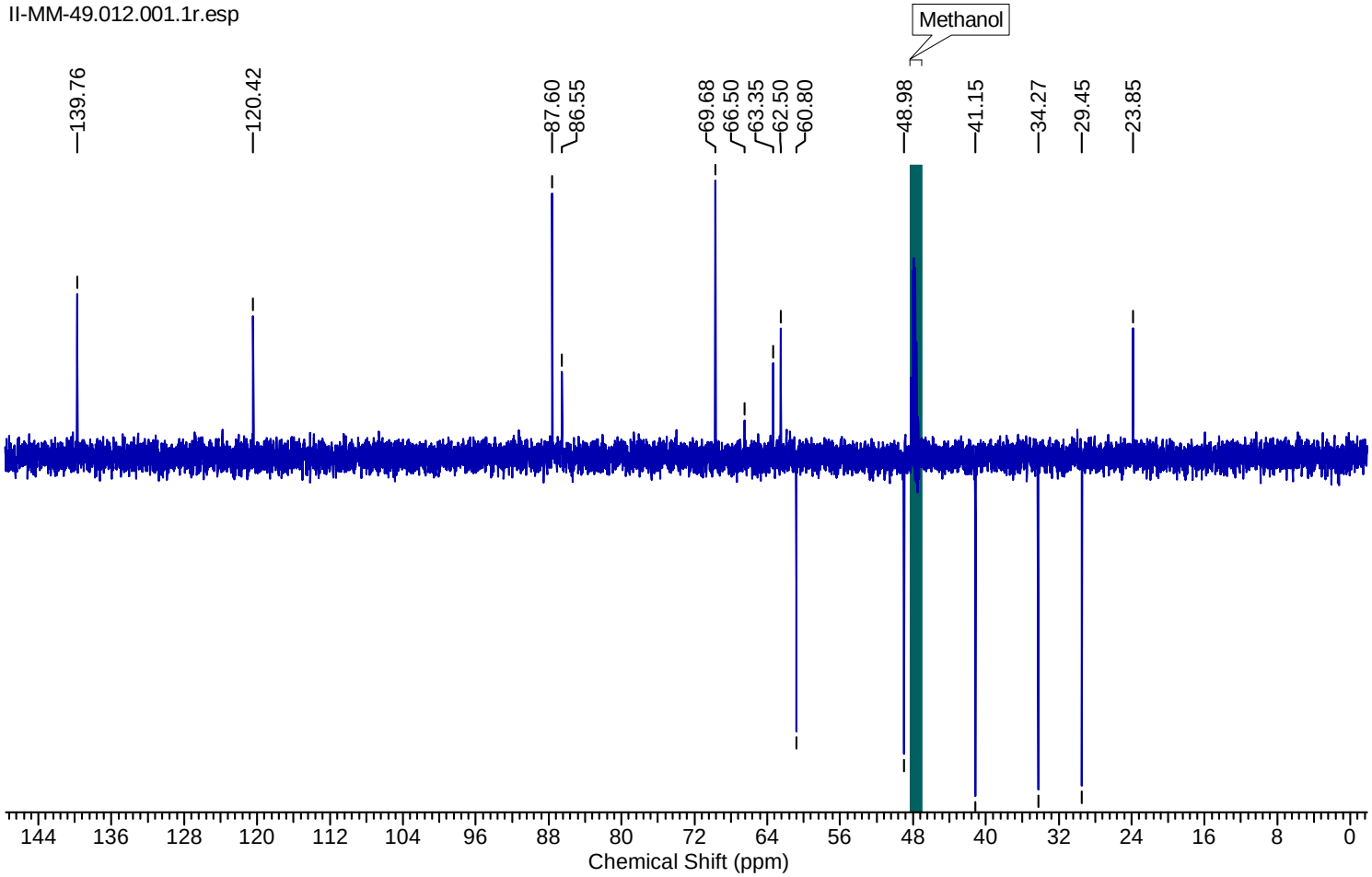


Figure S25. DEPT-135 spectrum of compound **22**.

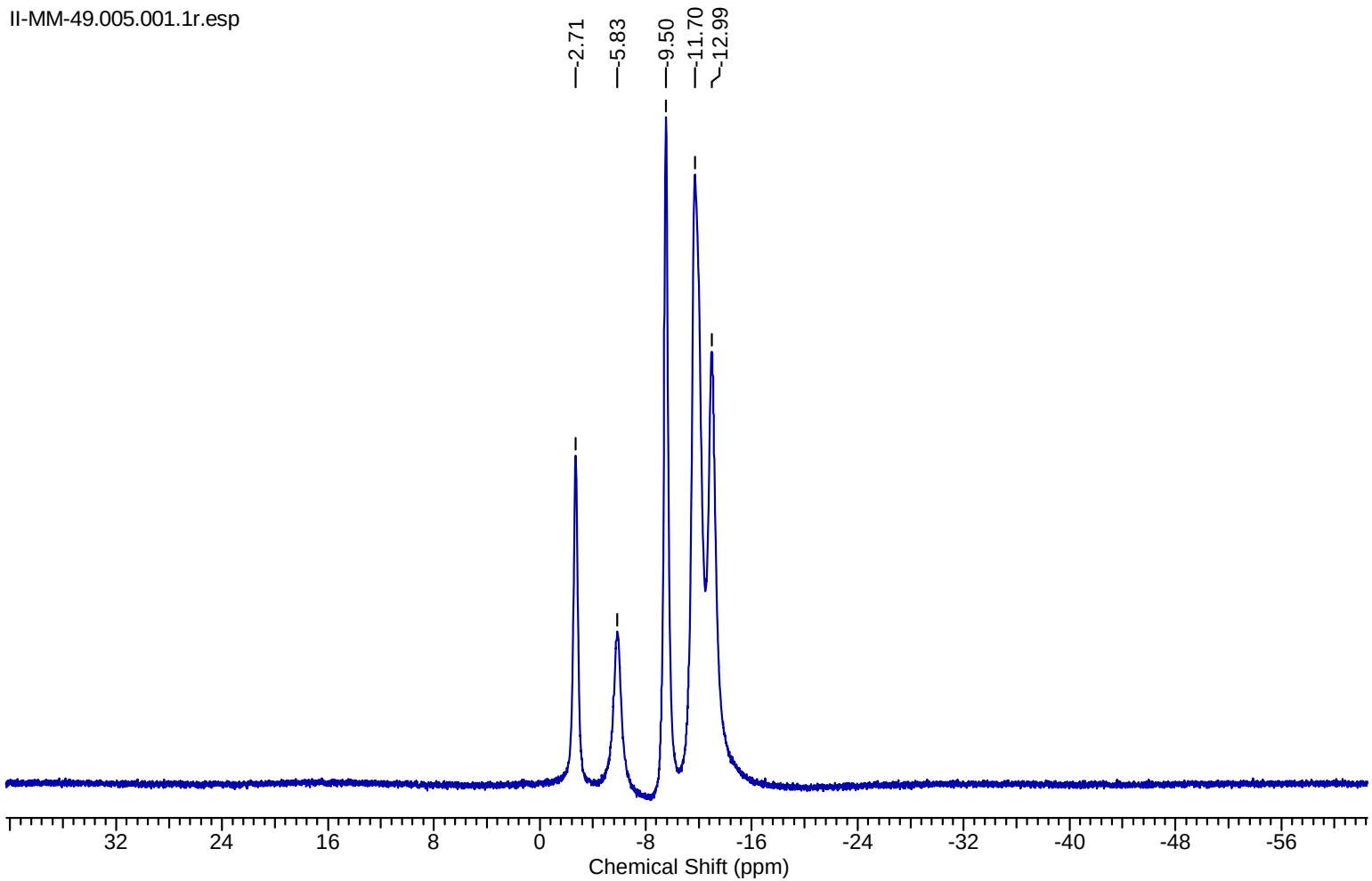


Figure S26. ^{11}B {H BB} NMR spectrum of compound **22**.

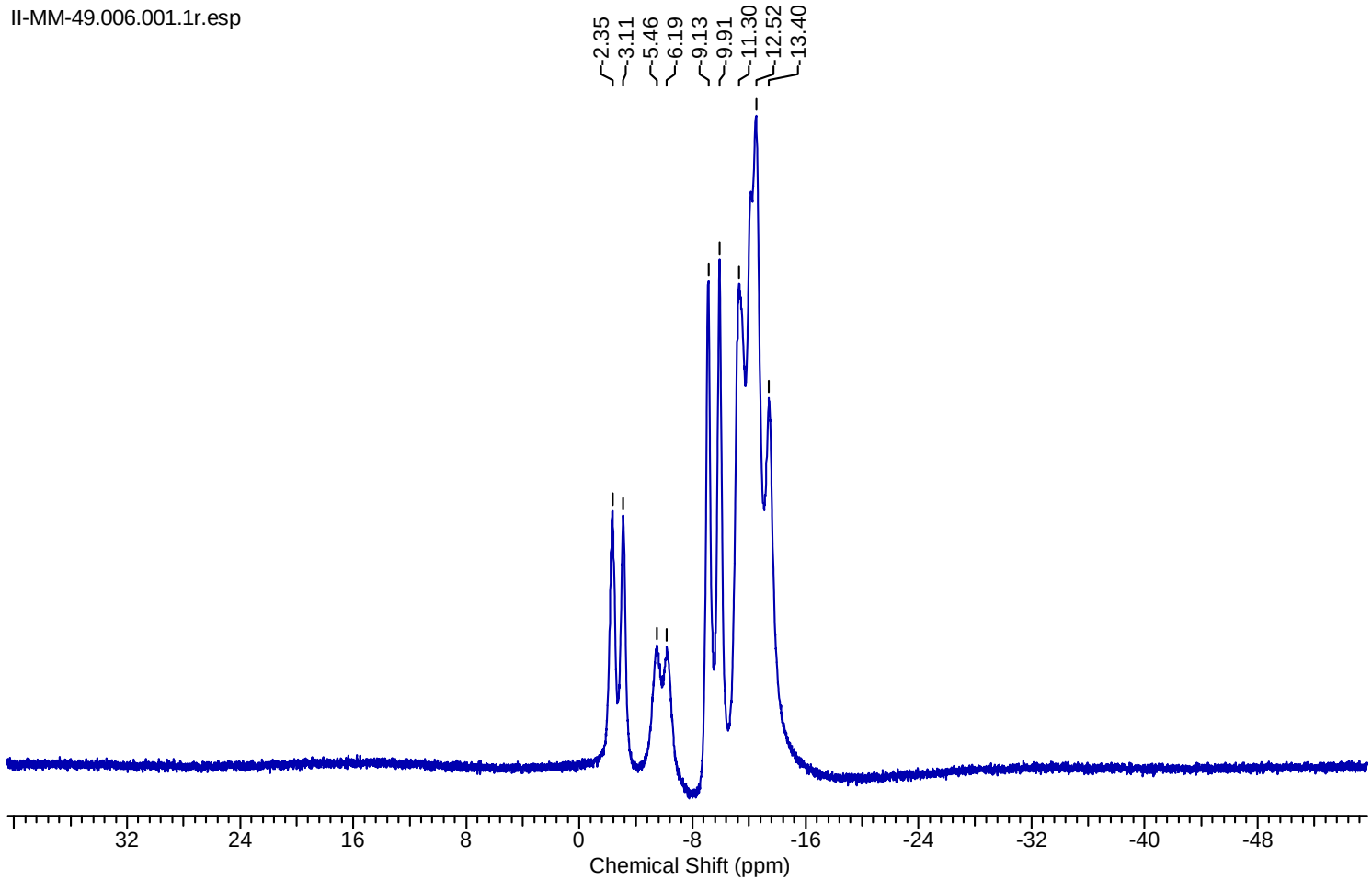


Figure S27. ^{11}B NMR spectrum of compound **22**.

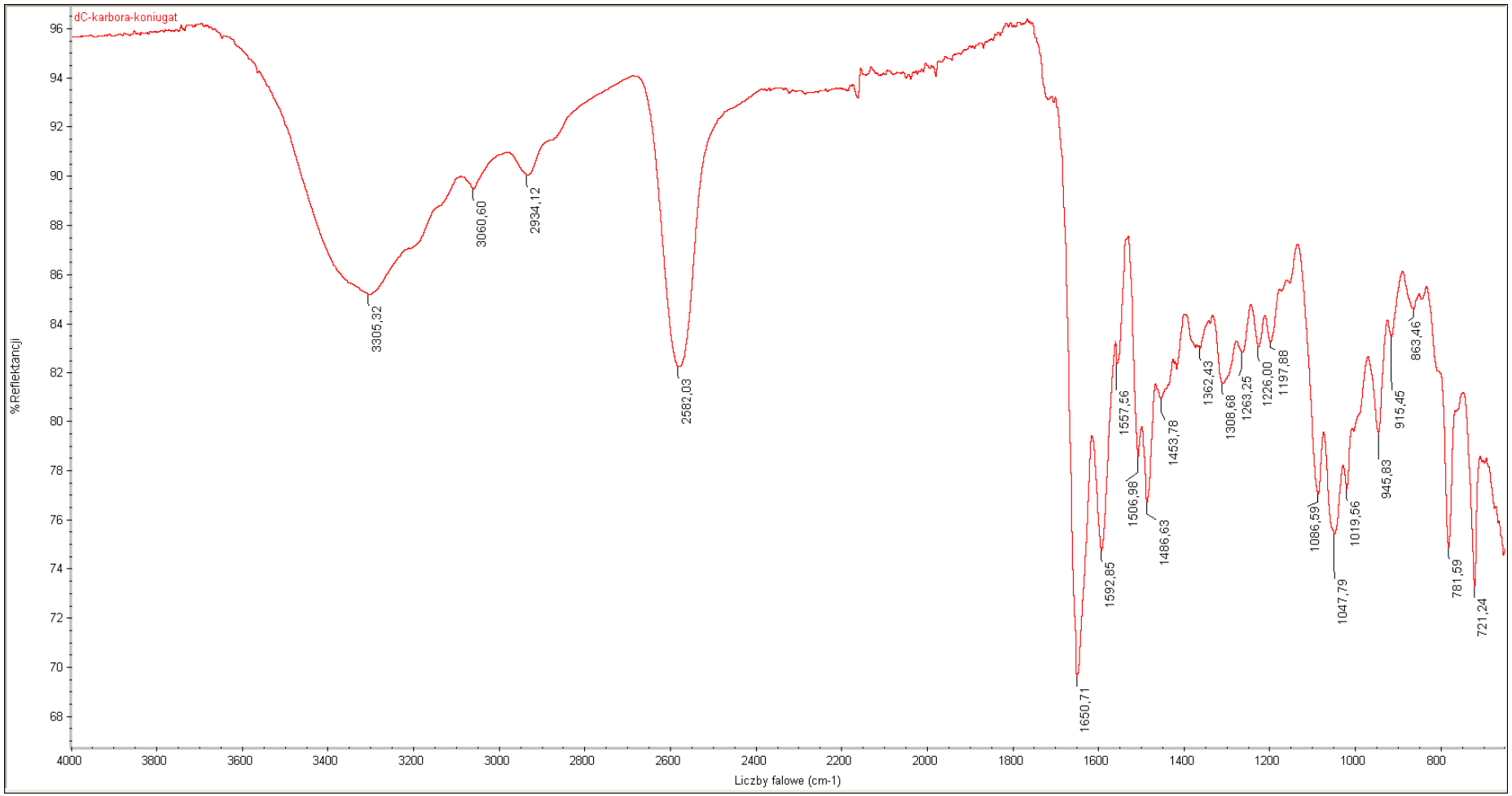
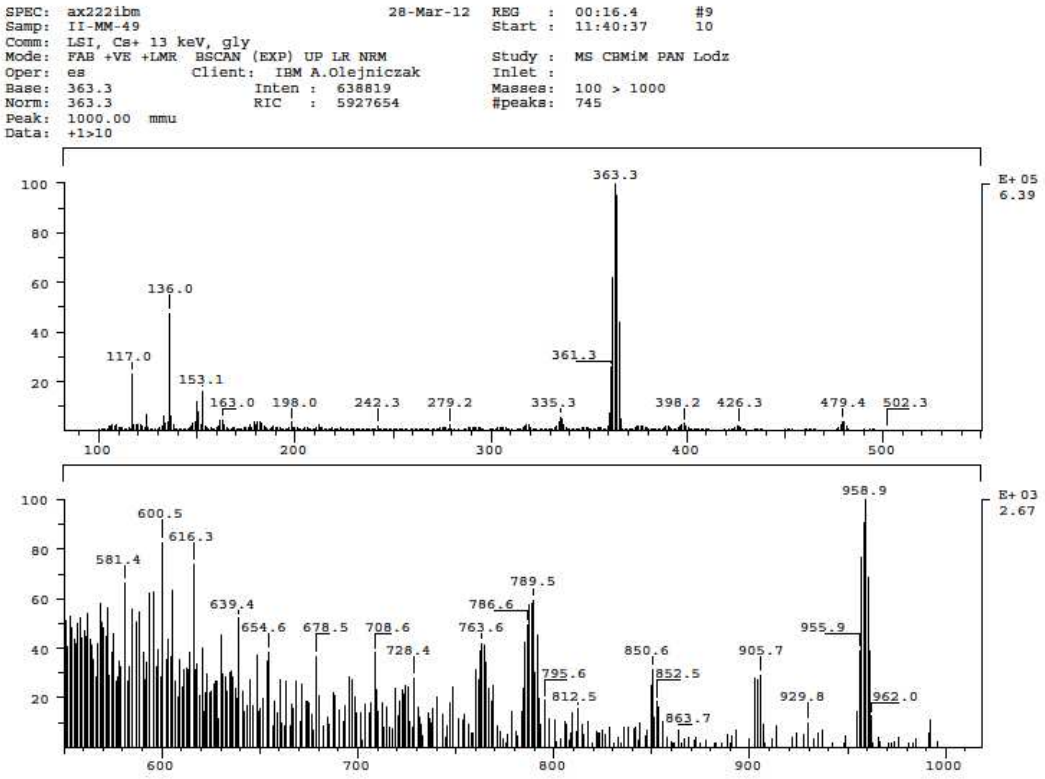


Figure S28. IR spectrum of compound **22**.



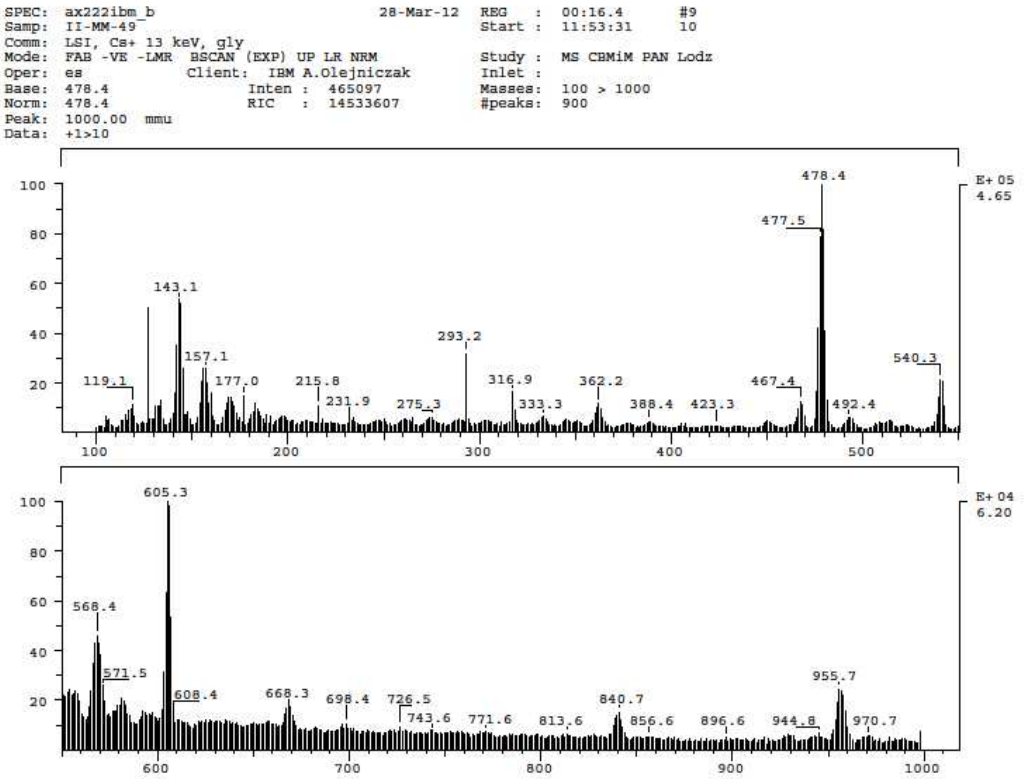


Figure S29. MS-FAB spectra of compound **22**.

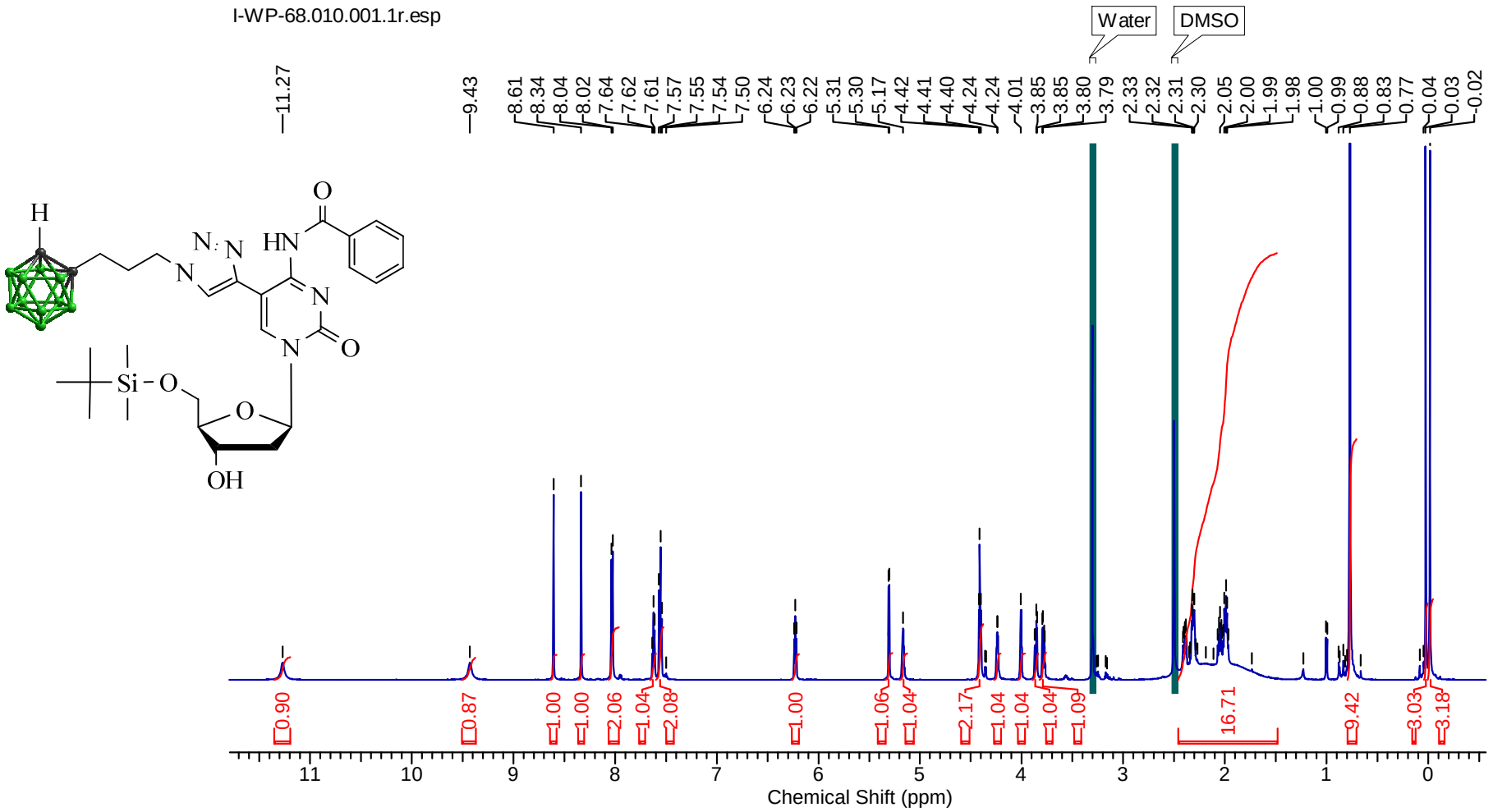


Figure S30. ^{1}H NMR spectrum of compound **23.**

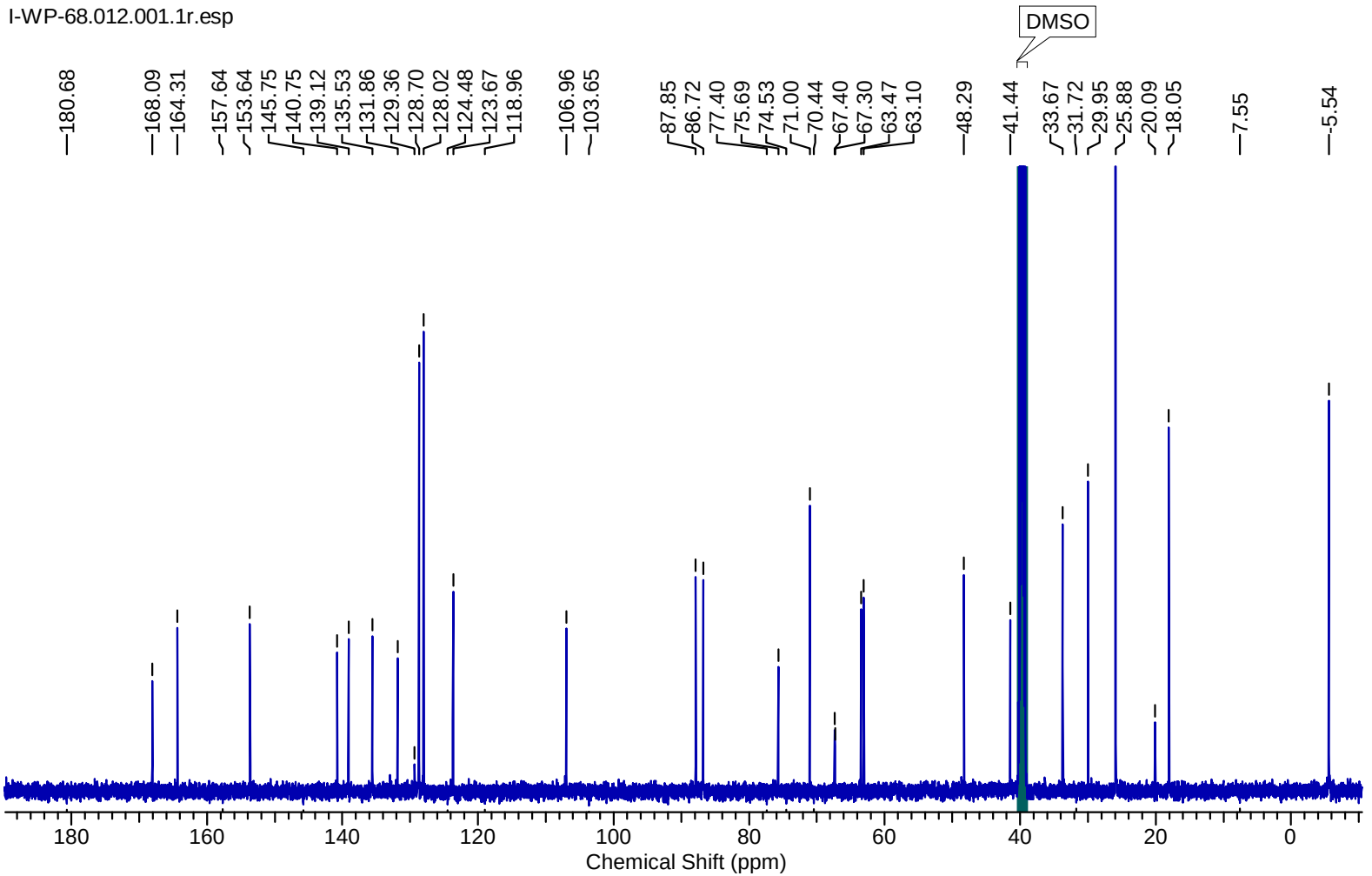


Figure S31. ^{13}C NMR spectrum of compound **23**.

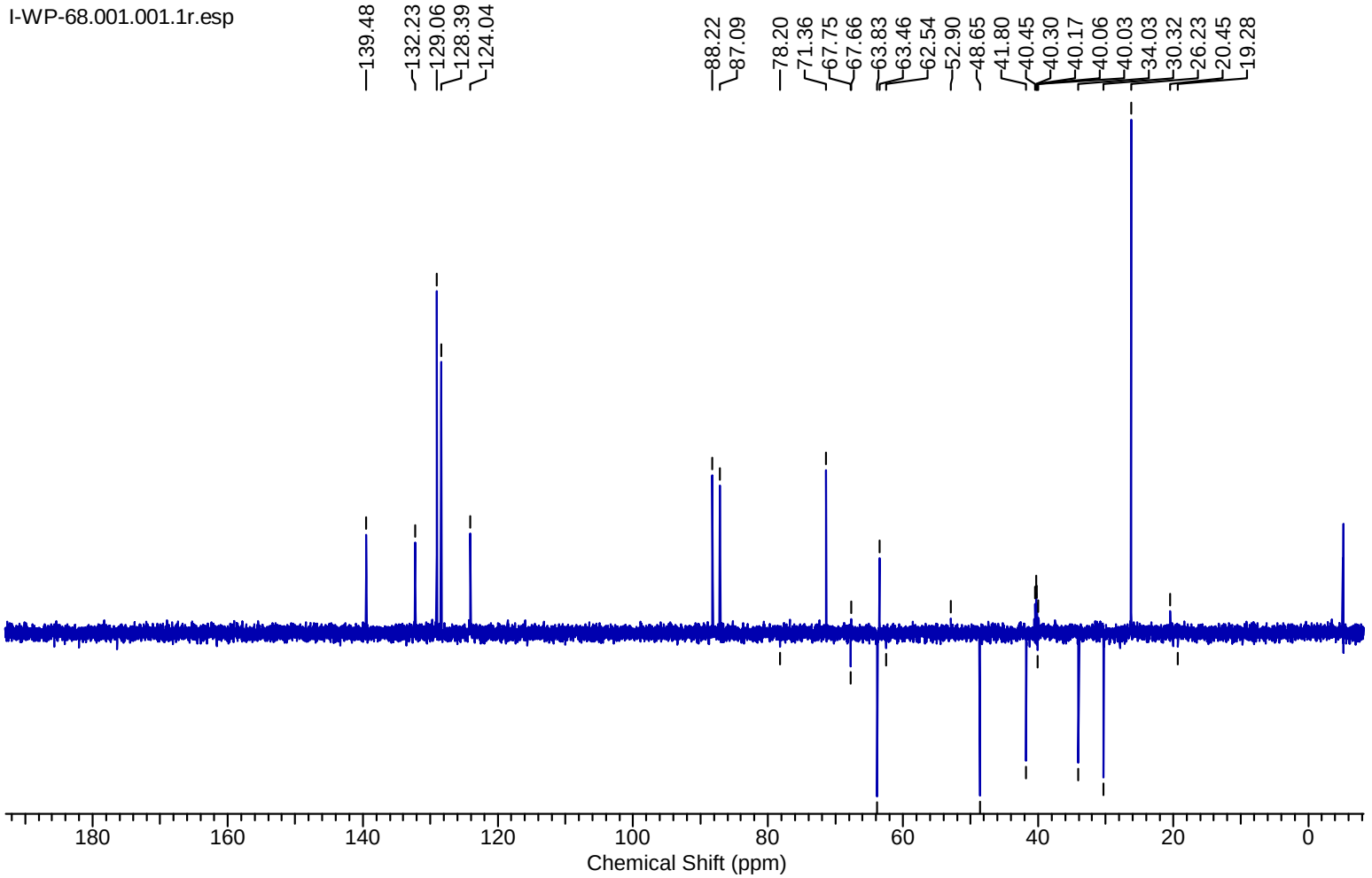


Figure S32. DEPT-135 spectrum of compound **23**.

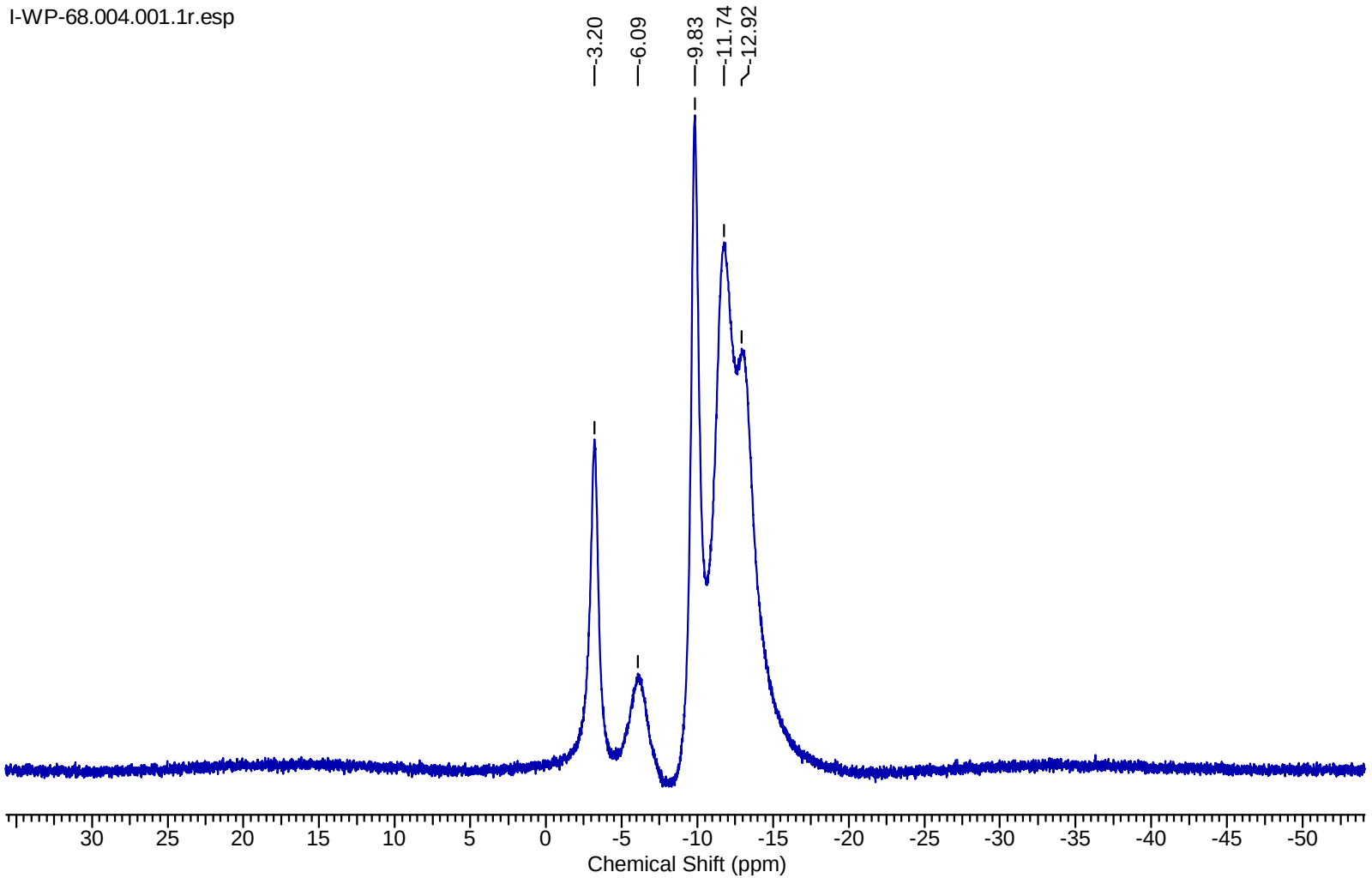


Figure S33. ^{11}B {H BB} NMR spectrum of compound **23**.

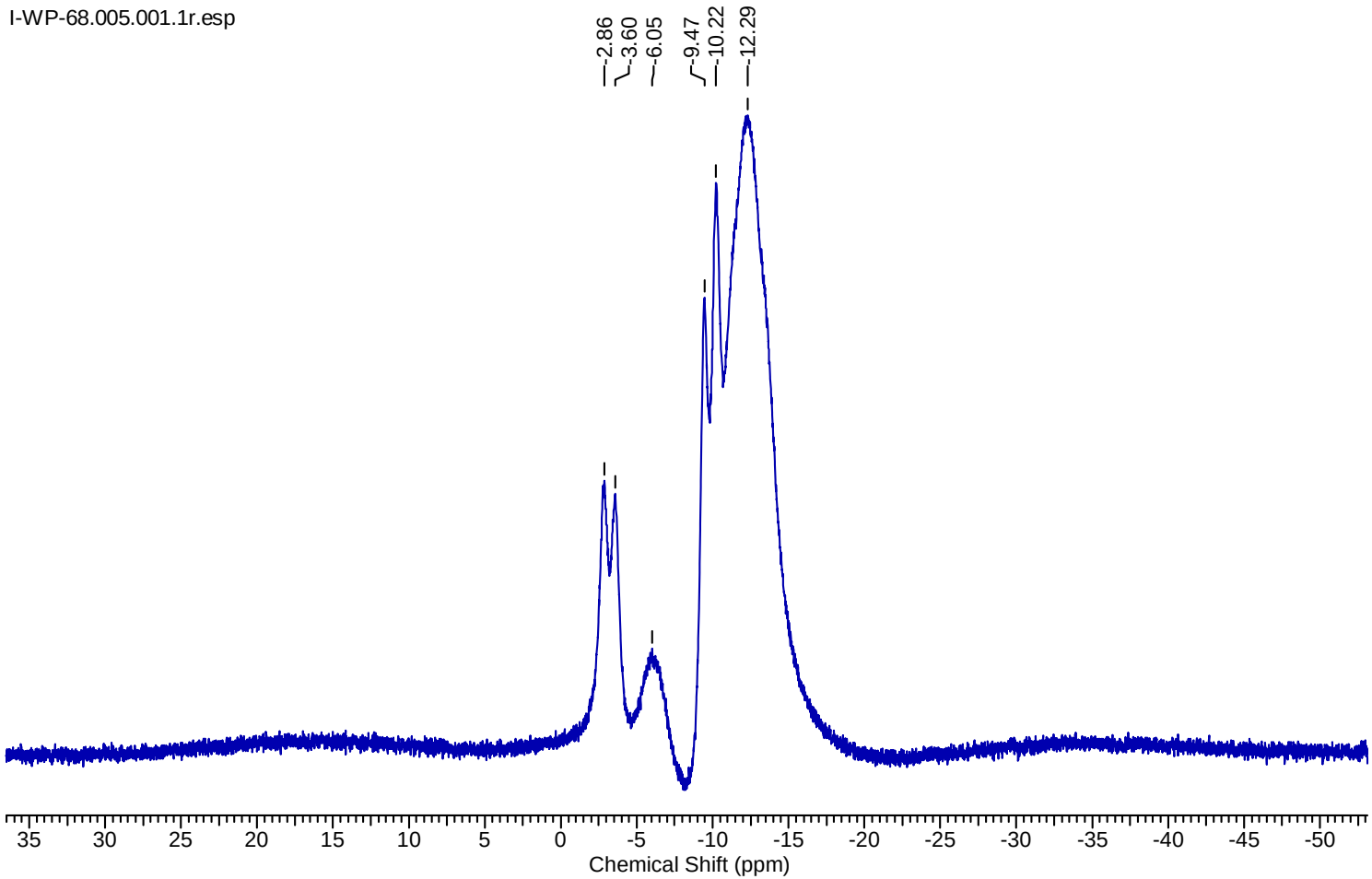


Figure S34. ^{11}B NMR spectrum of compound **23**.

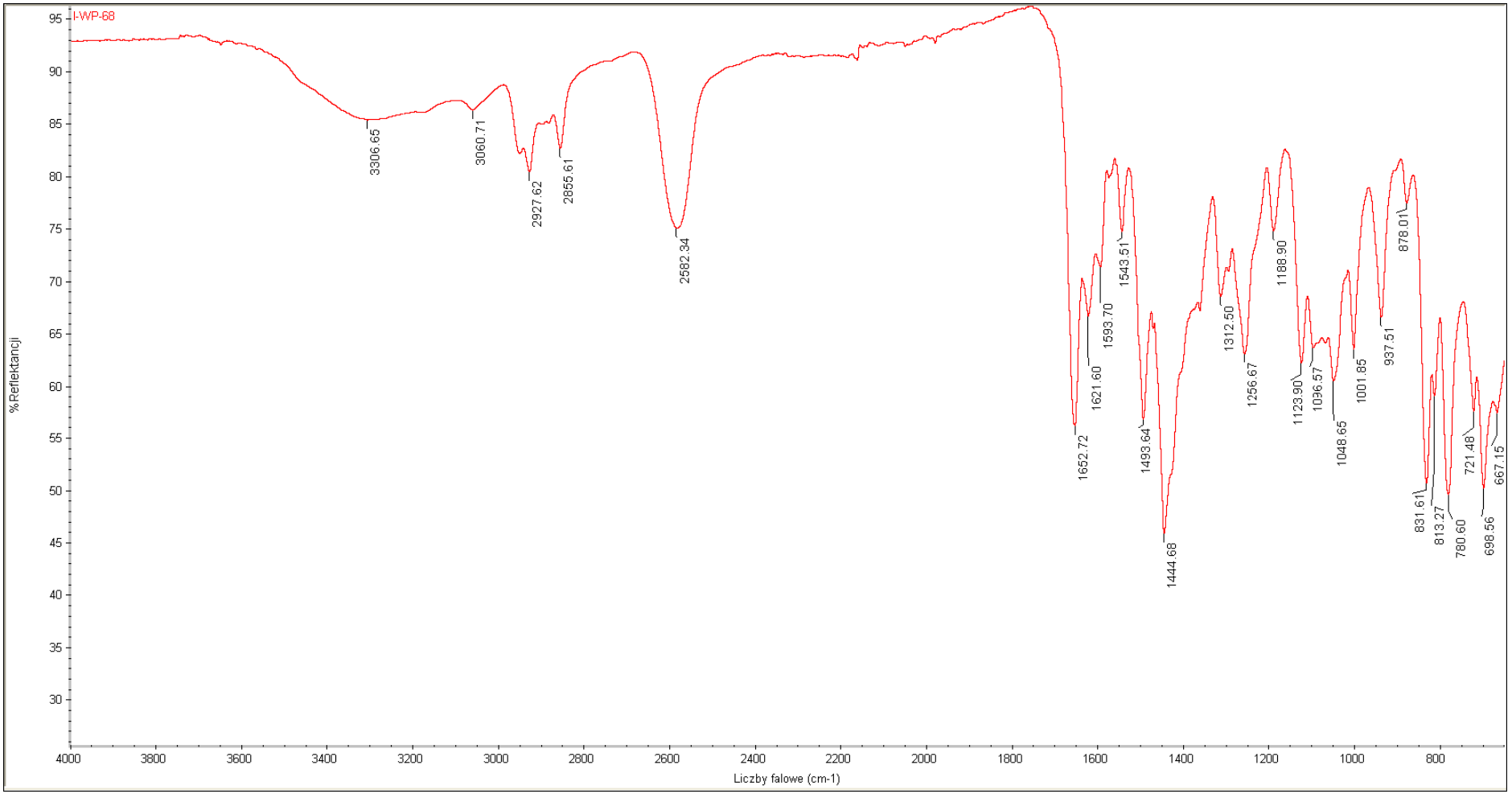


Figure S35. IR spectrum of compound **23**.

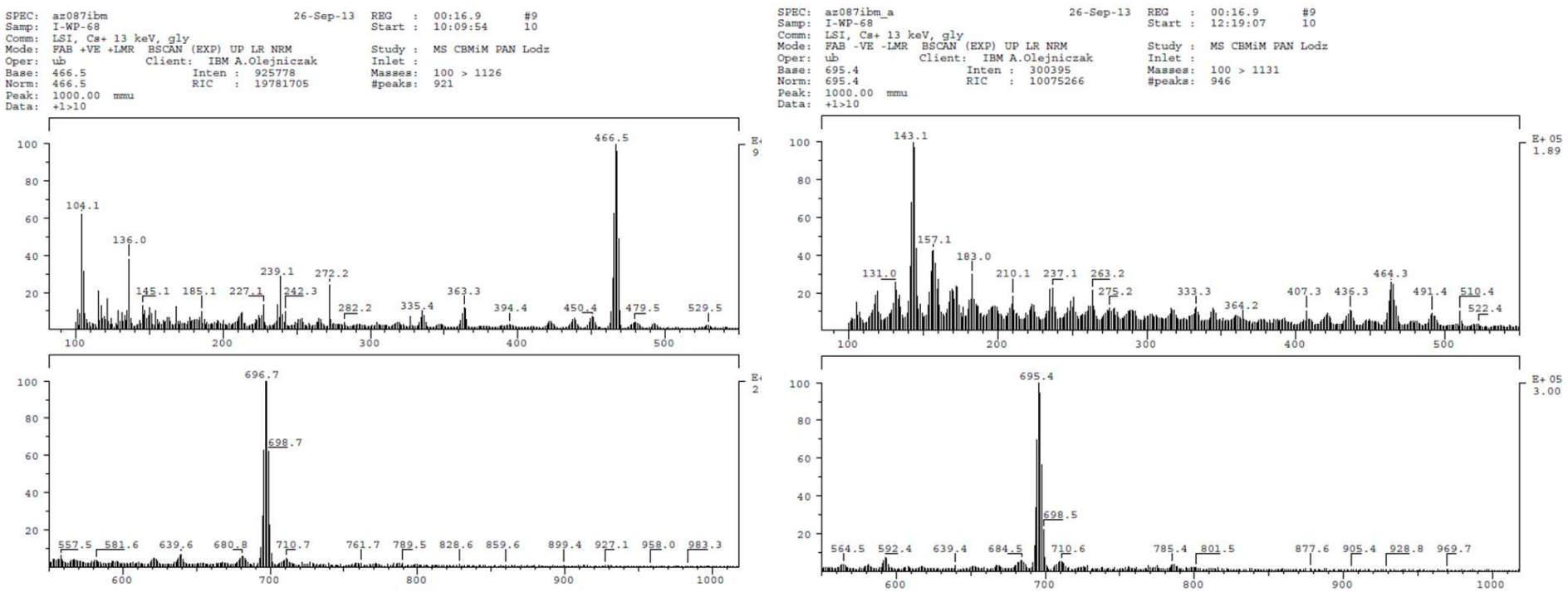


Figure S36. MS-FAB spectra of compound **23**.

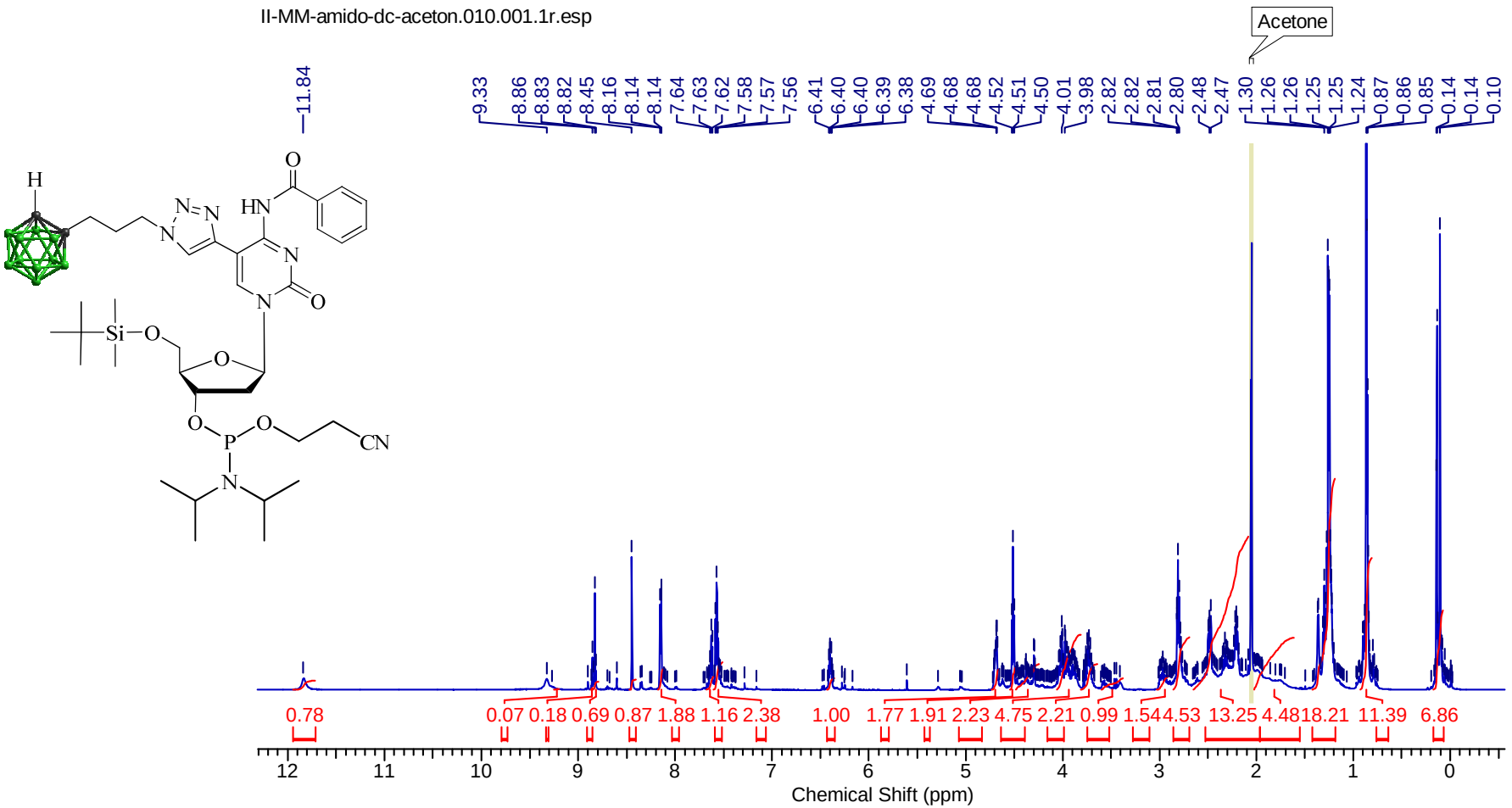


Figure S37. ^{1}H NMR spectrum of compound **30**.

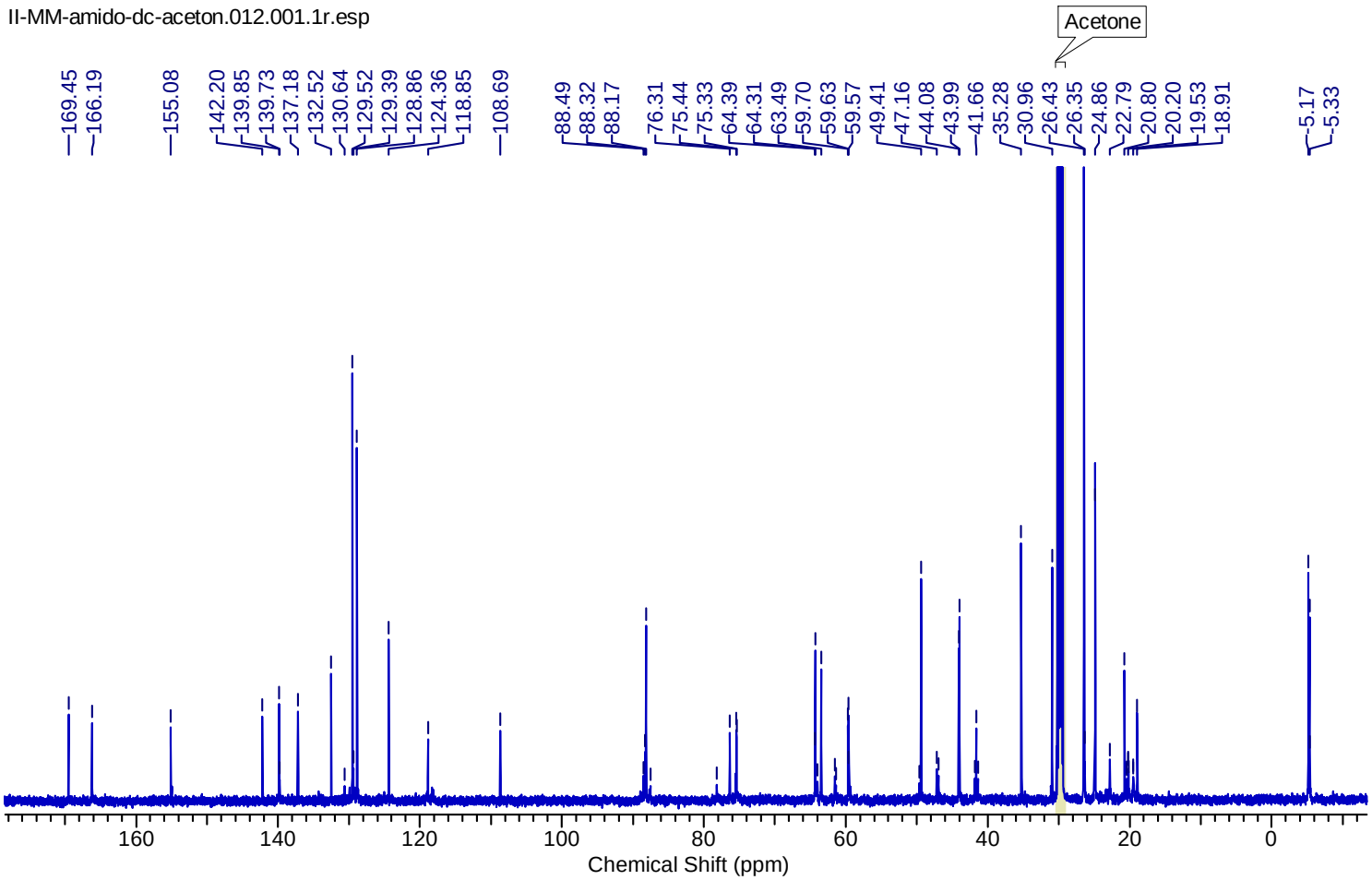


Figure S38. ^{13}C NMR spectrum of compound **30**.

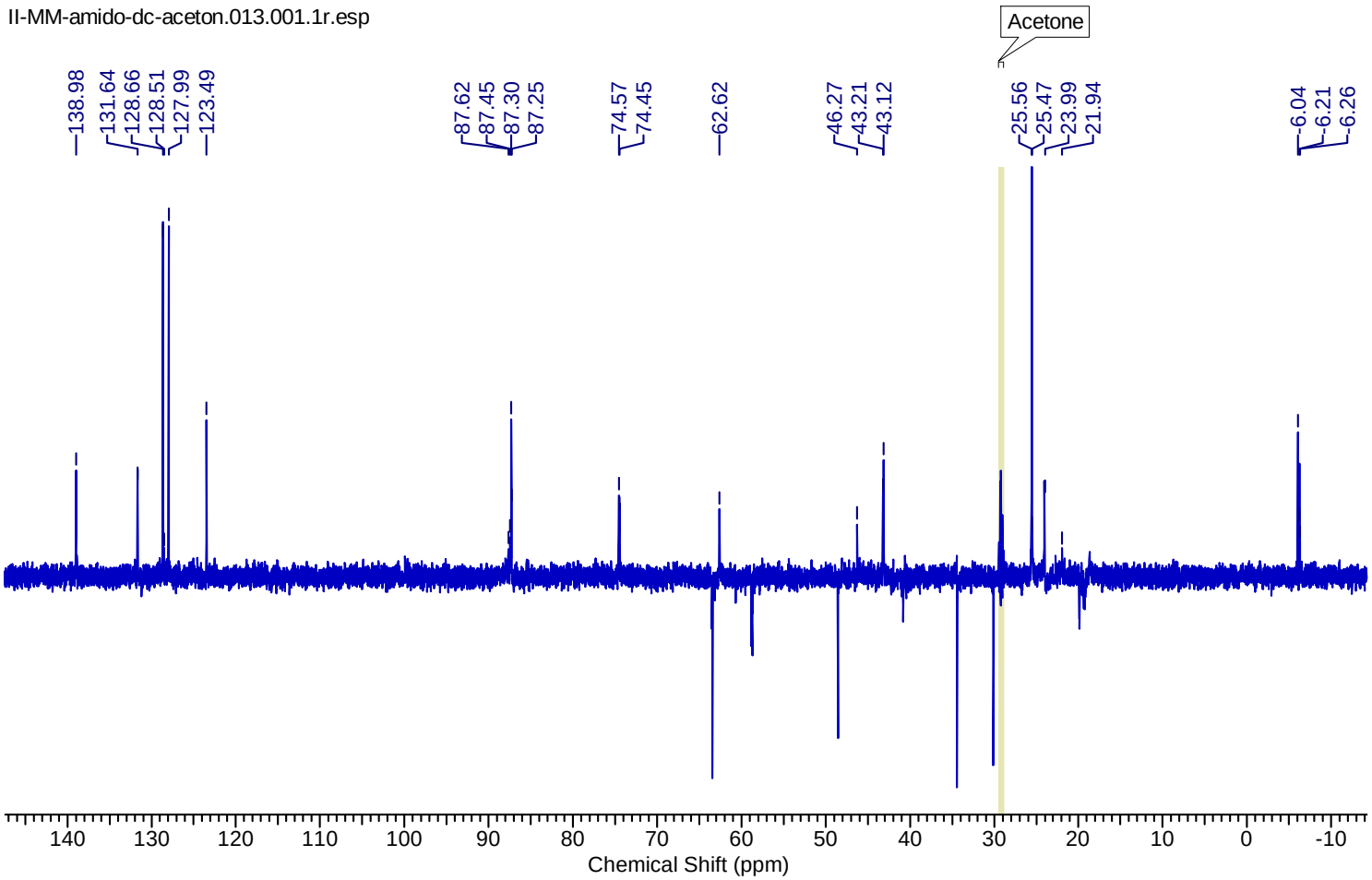


Figure S39. DEPT-135 spectrum of compound **30**.

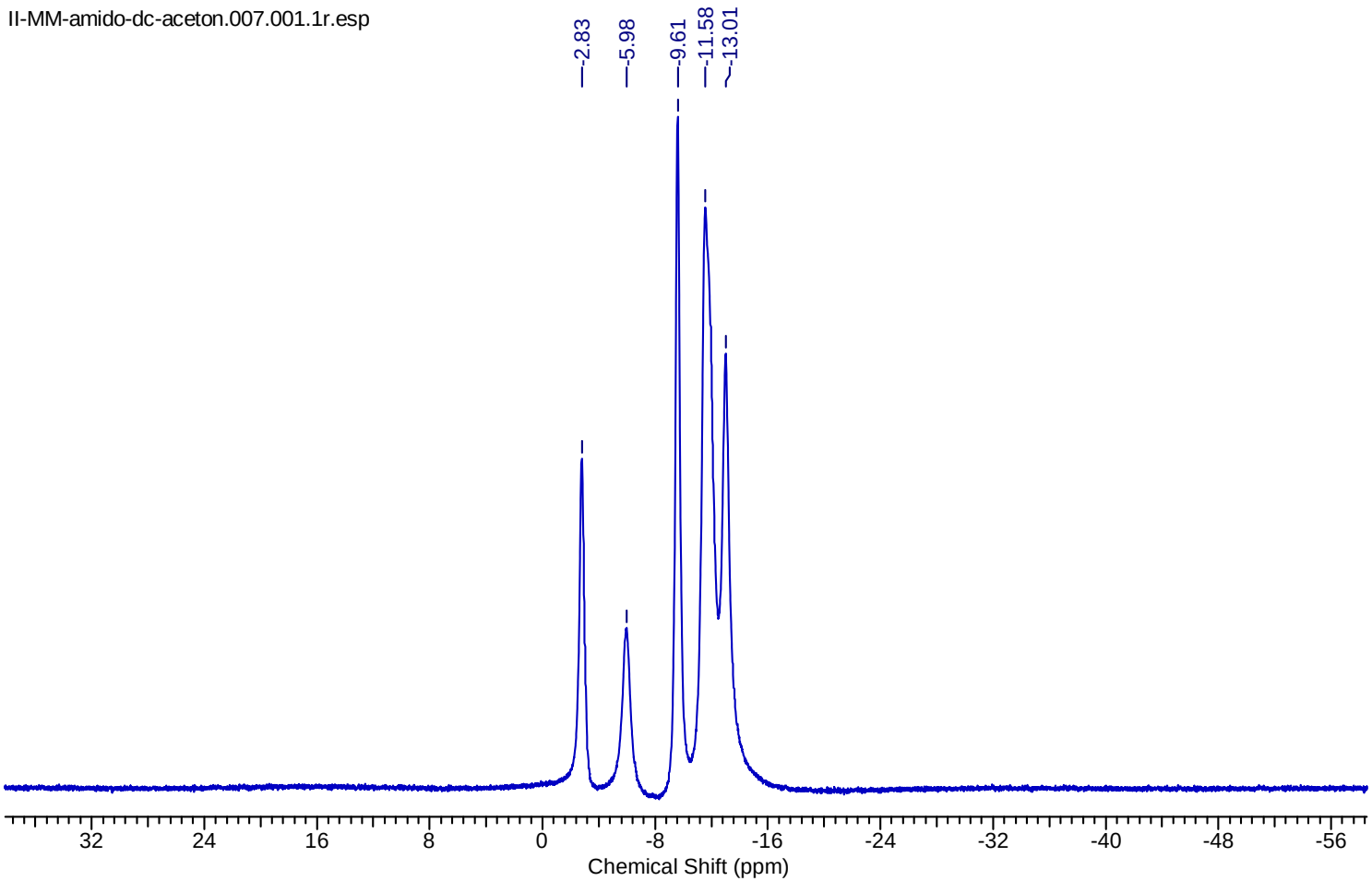


Figure S40. ^{11}B{H BB} NMR spectrum of compound **30**.

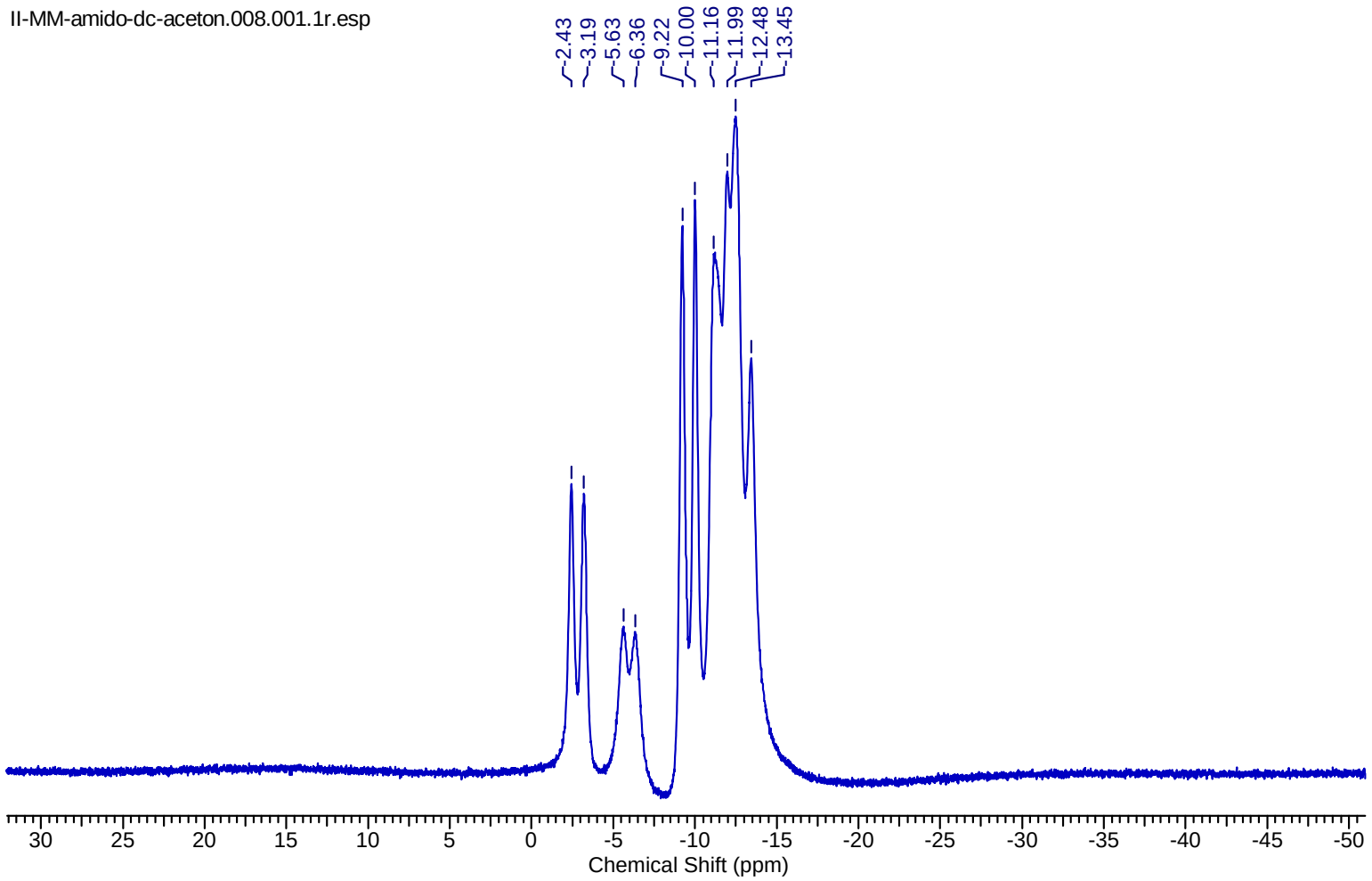


Figure S41. ^{11}B NMR spectrum of compound **30**

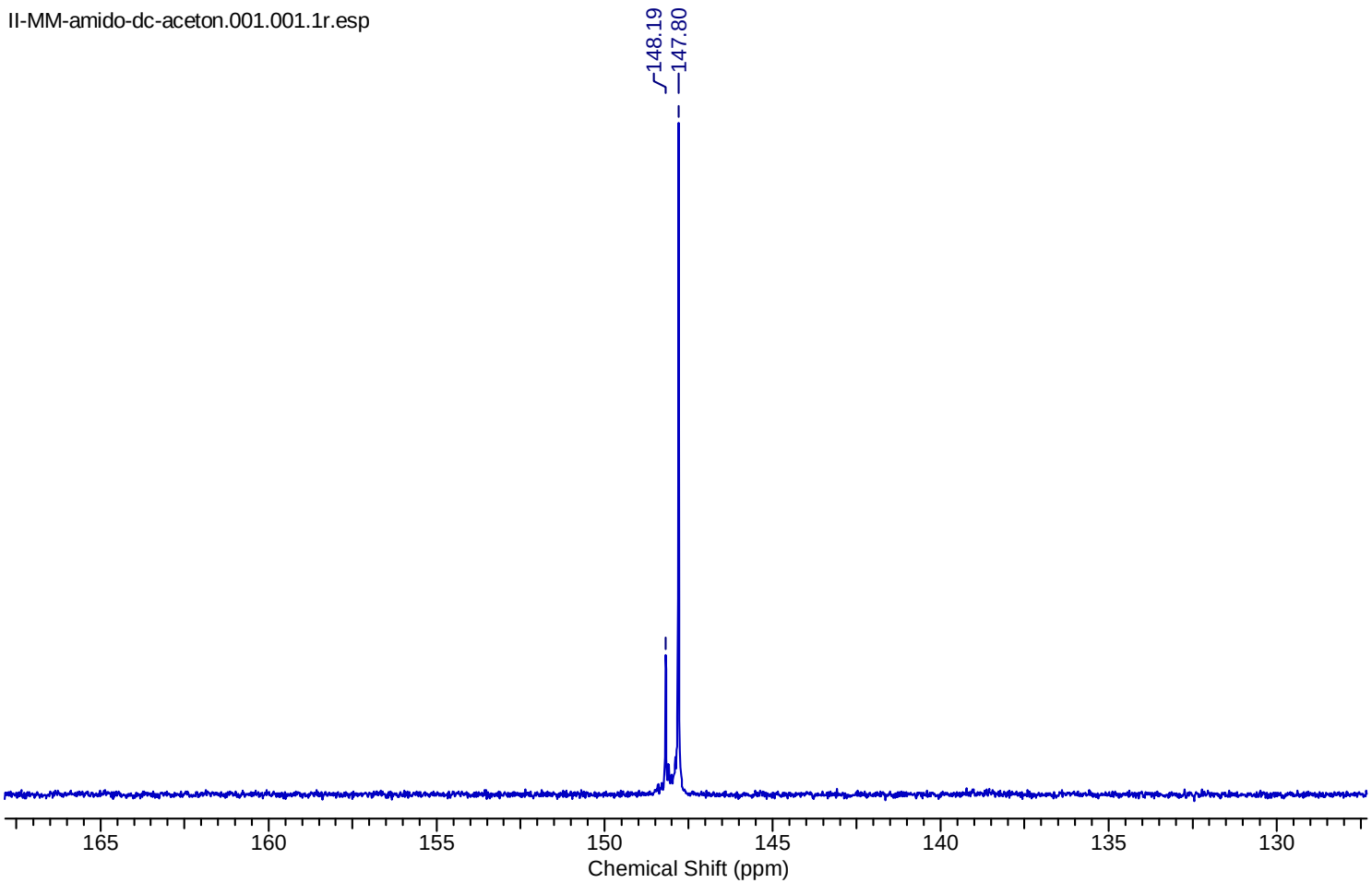


Figure S42. ^{31}P NMR spectrum of compound **30**.

Figure S43. IR spectrum of compound **30**.

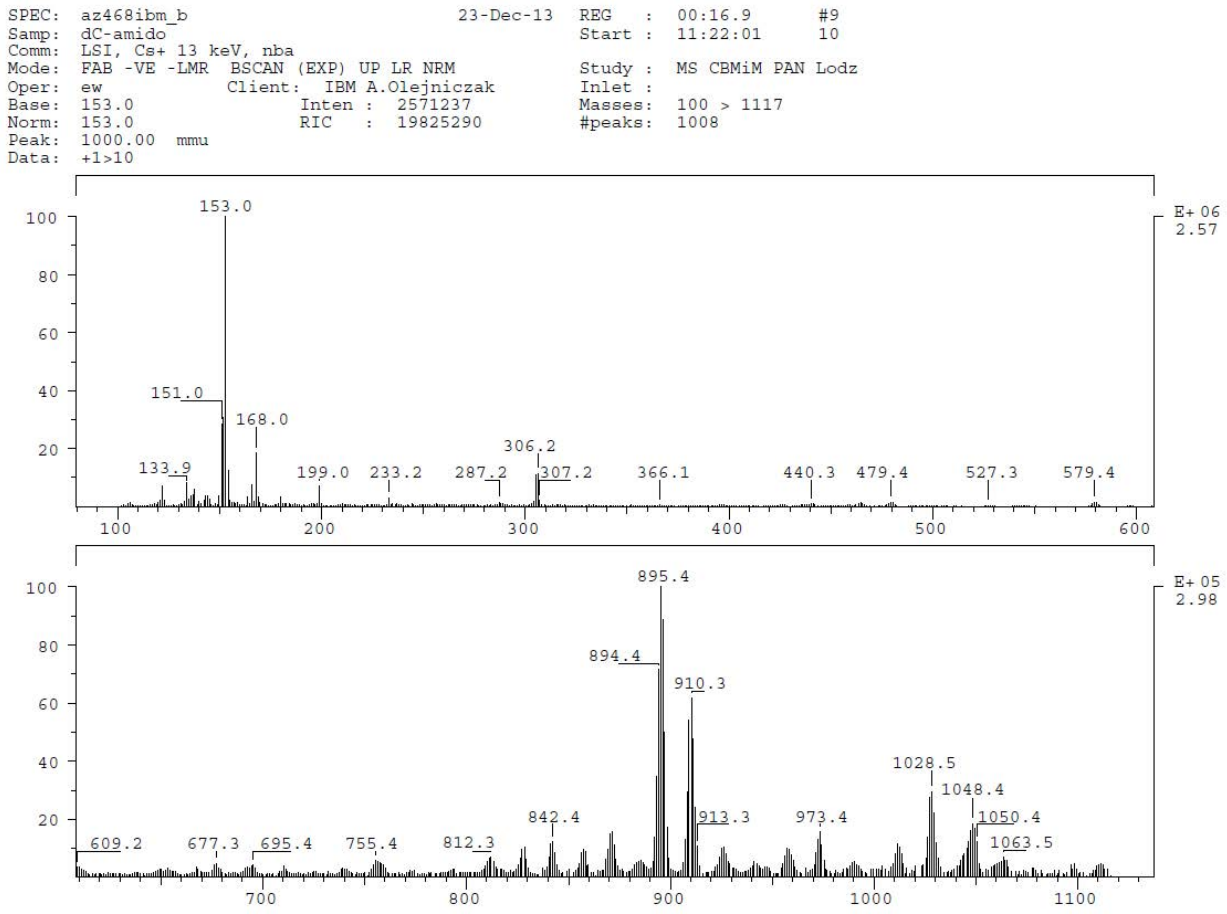


Figure S44. MS-FAB spectrum of compound **30**.

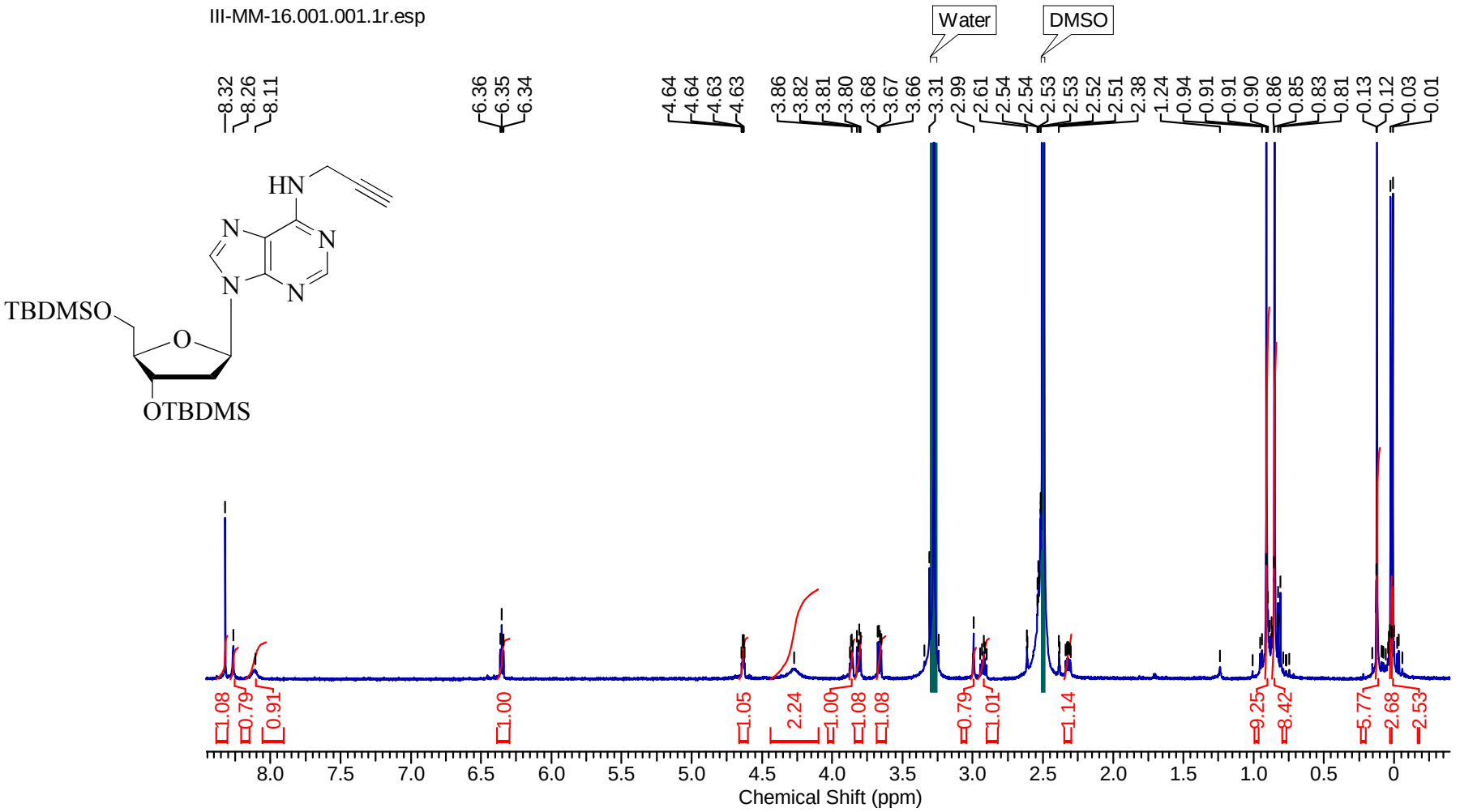


Figure S45. ^{1}H NMR spectrum of compound **12**.

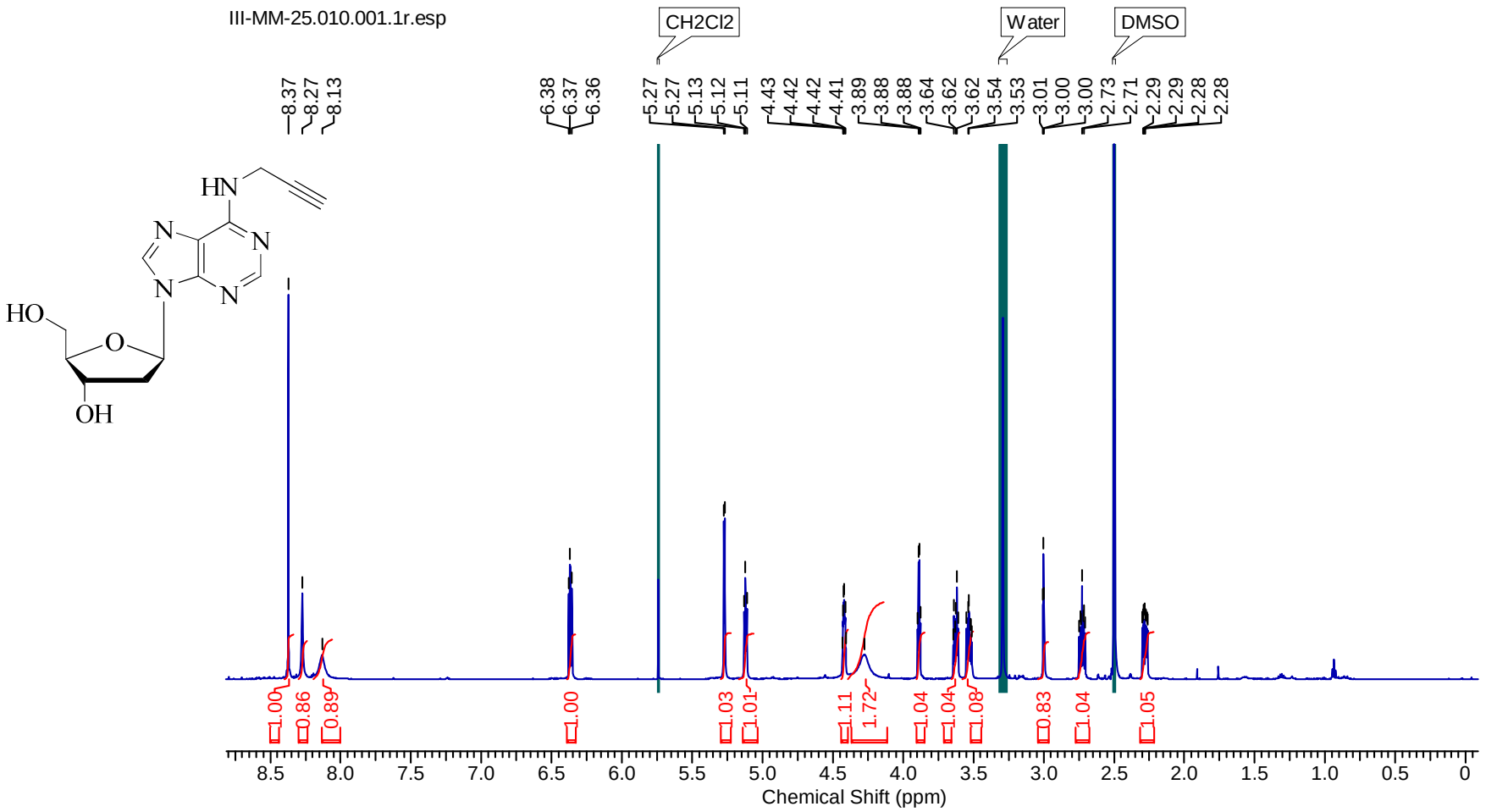


Figure S46. ^{1}H NMR spectrum of compound **13**.

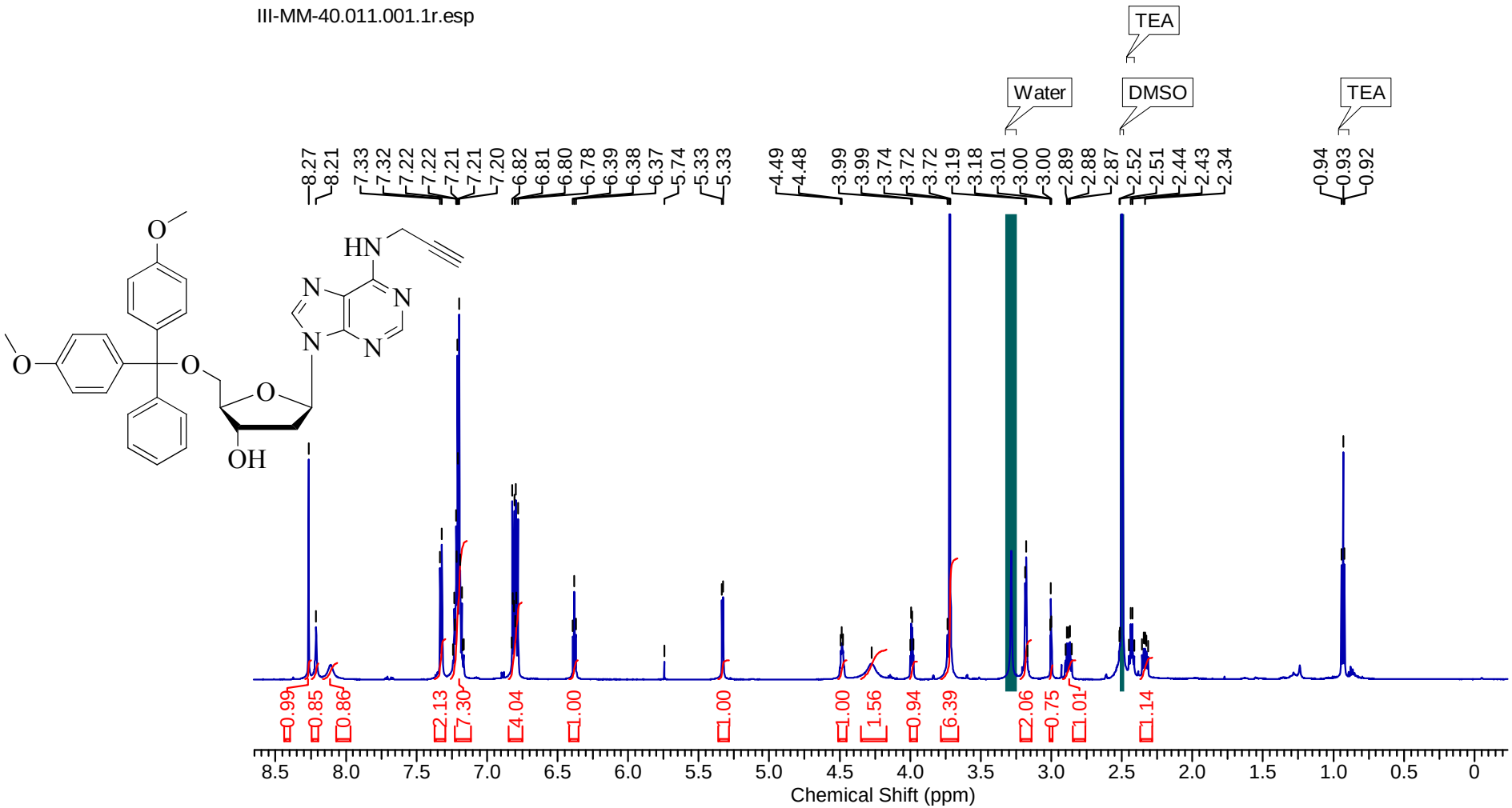


Figure S47. ^{1}H NMR spectrum of compound **14**.

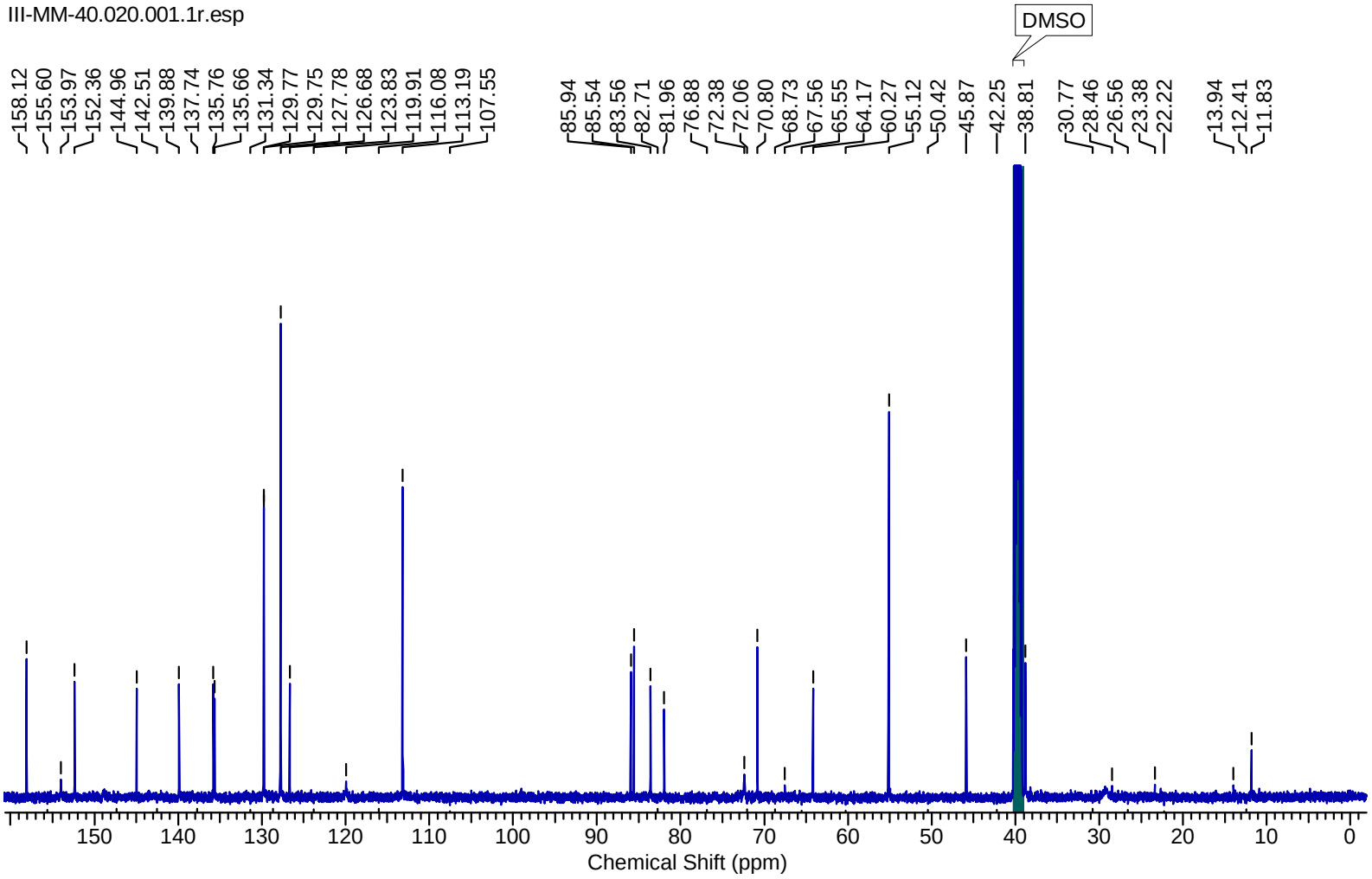


Figure S48. ^{13}C NMR spectrum of compound **14**.

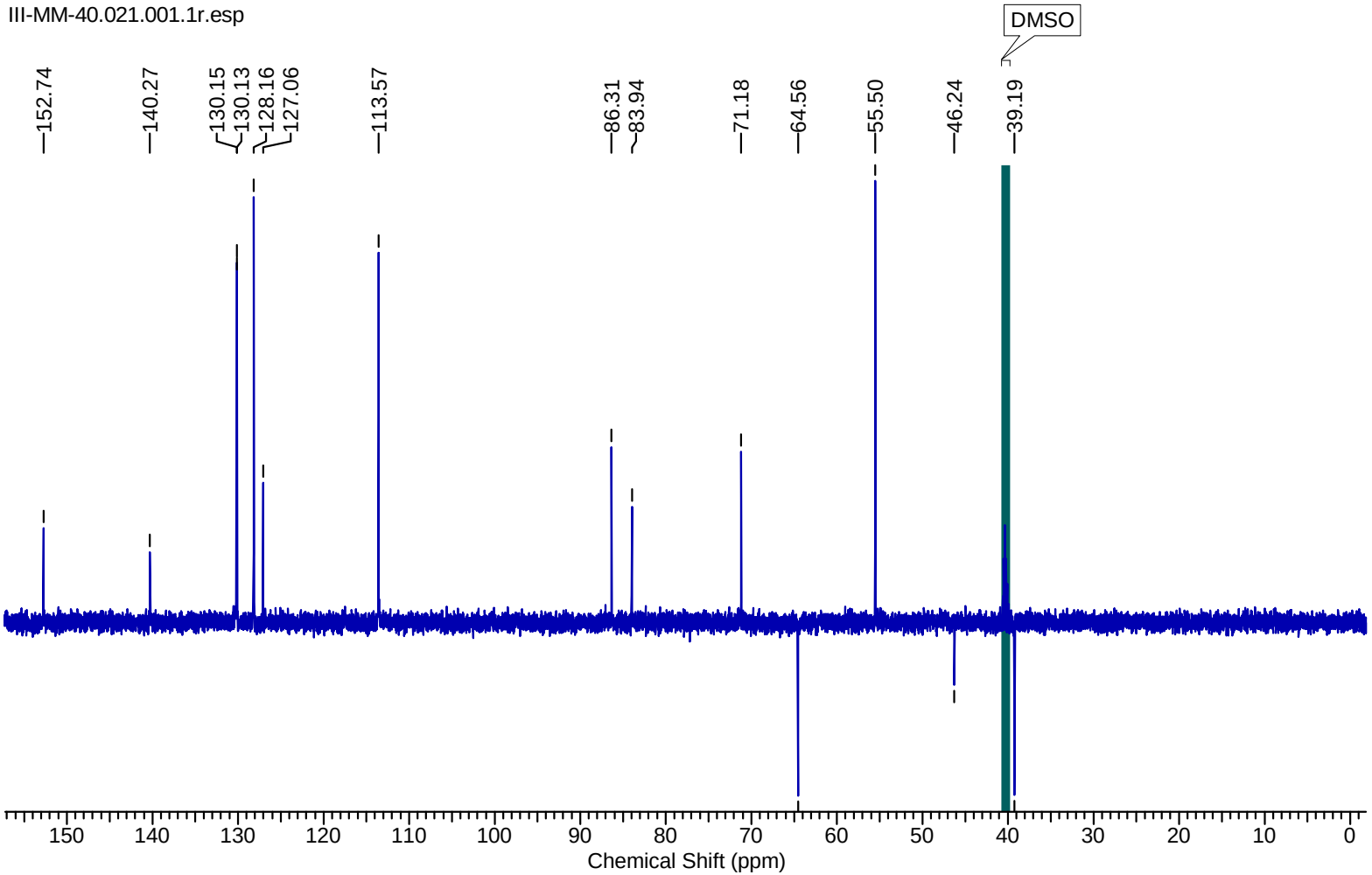


Figure S49. DEPT-135 spectrum of compound **14**.

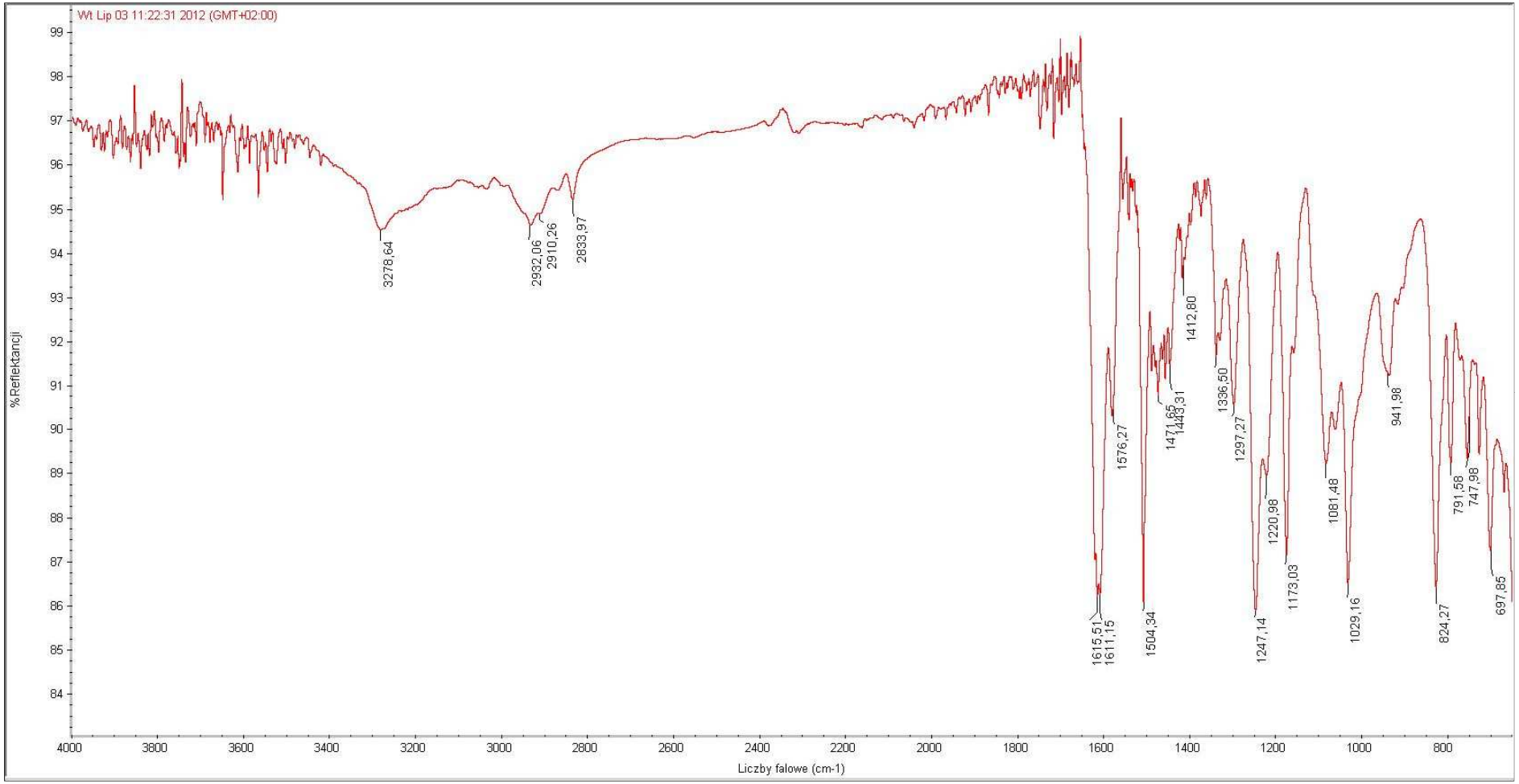
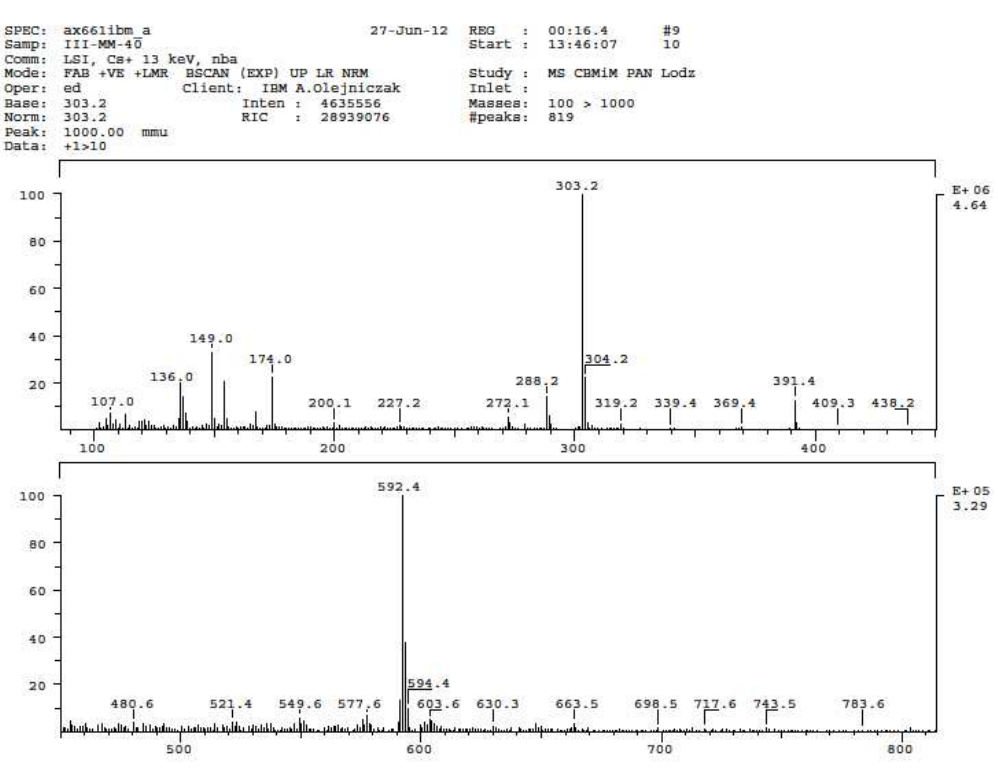


Figure S50. IR spectrum of compound **14**.



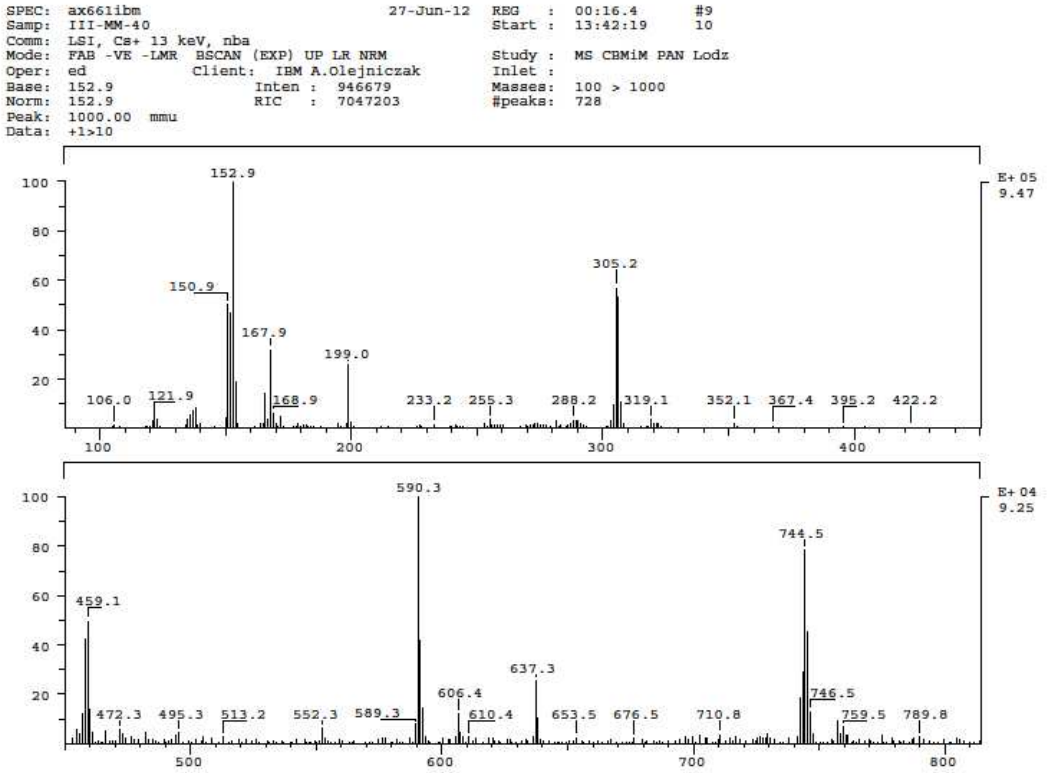


Figure S51. MS-FAB spectra of compound **14**.

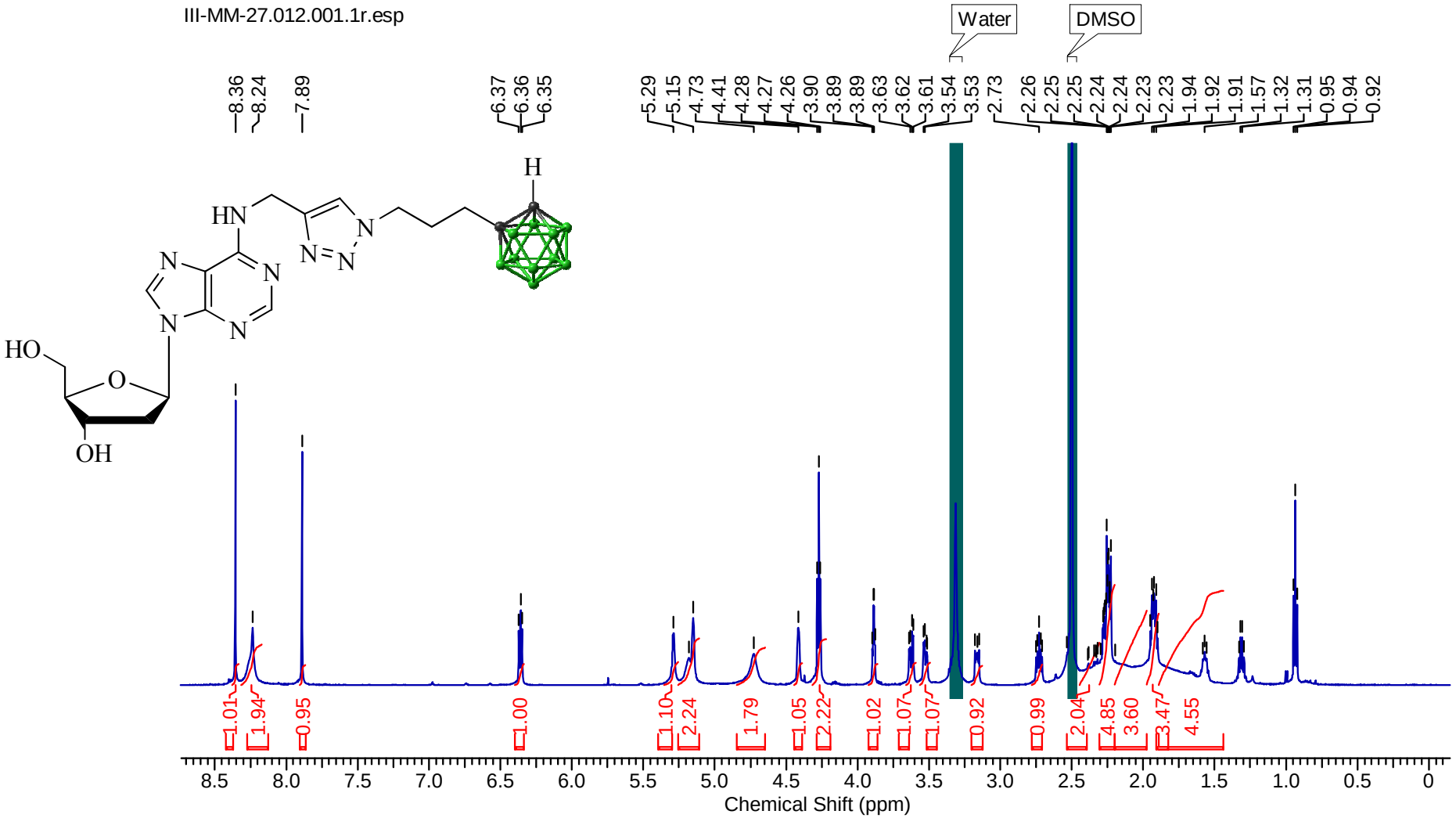


Figure S52. ^{1}H NMR spectrum of compound **24**.

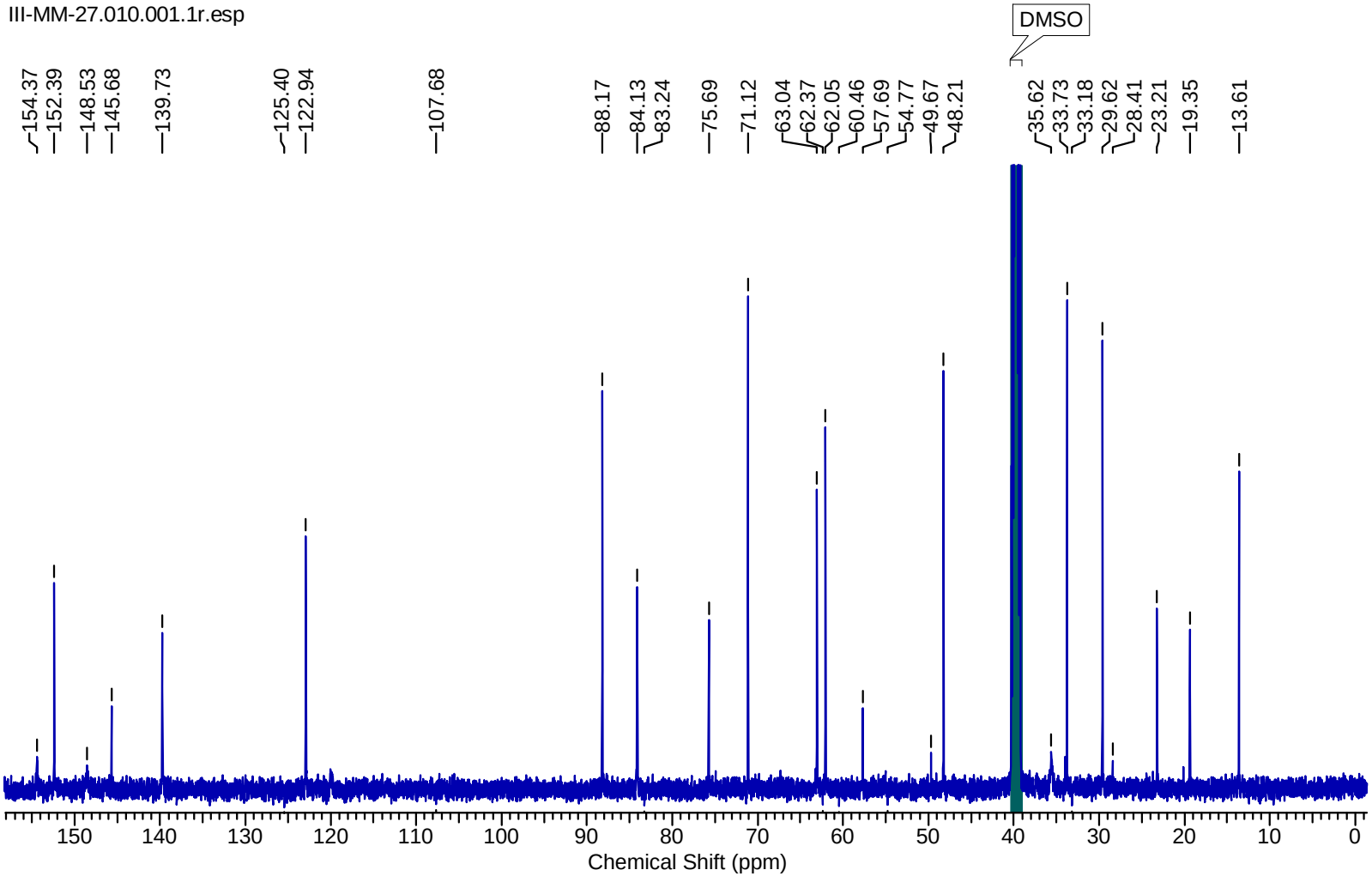


Figure S53. ^{13}C NMR spectrum of compound **24**.

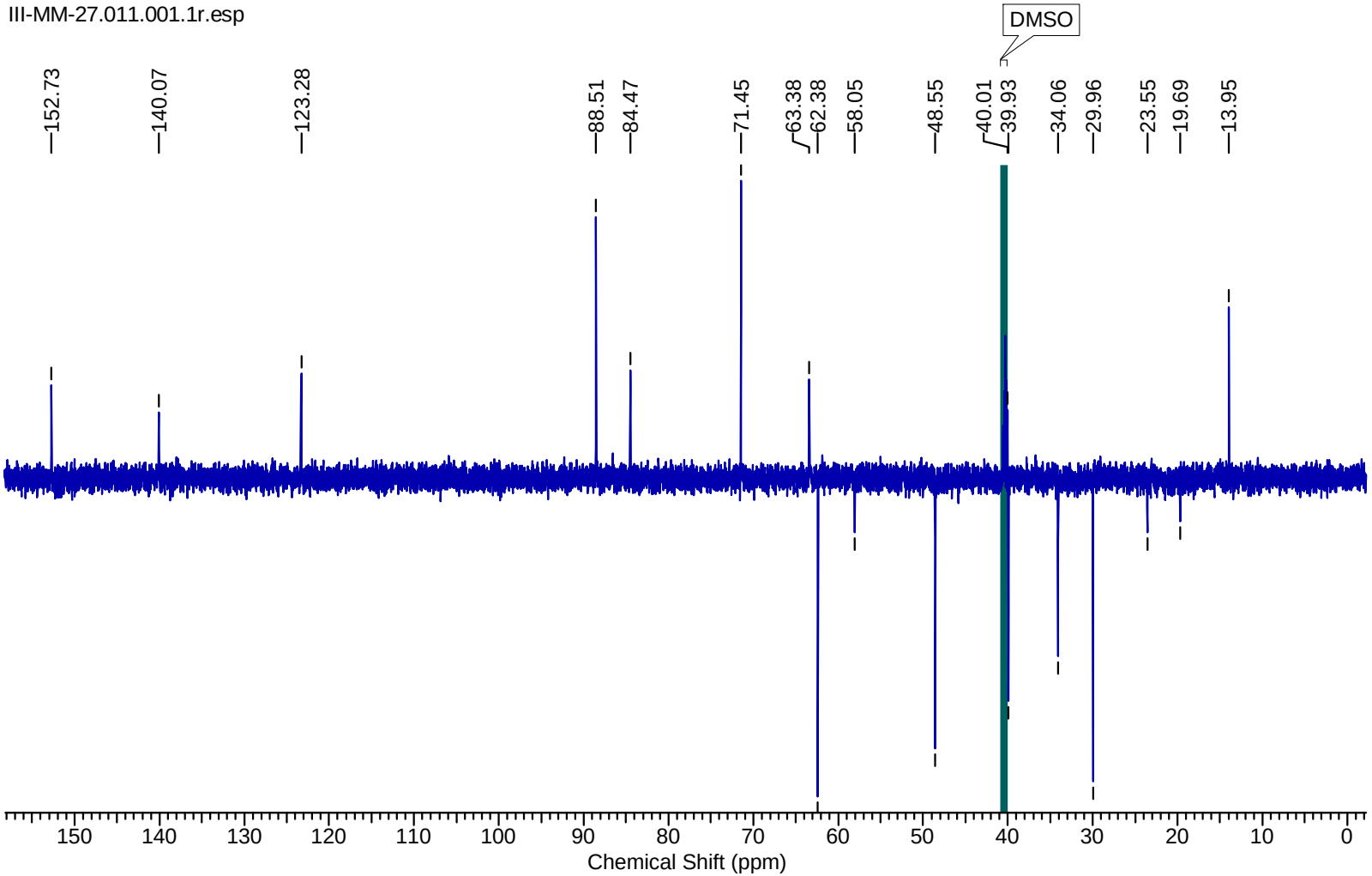


Figure S54. DEPT-135 spectrum of compound **24**.

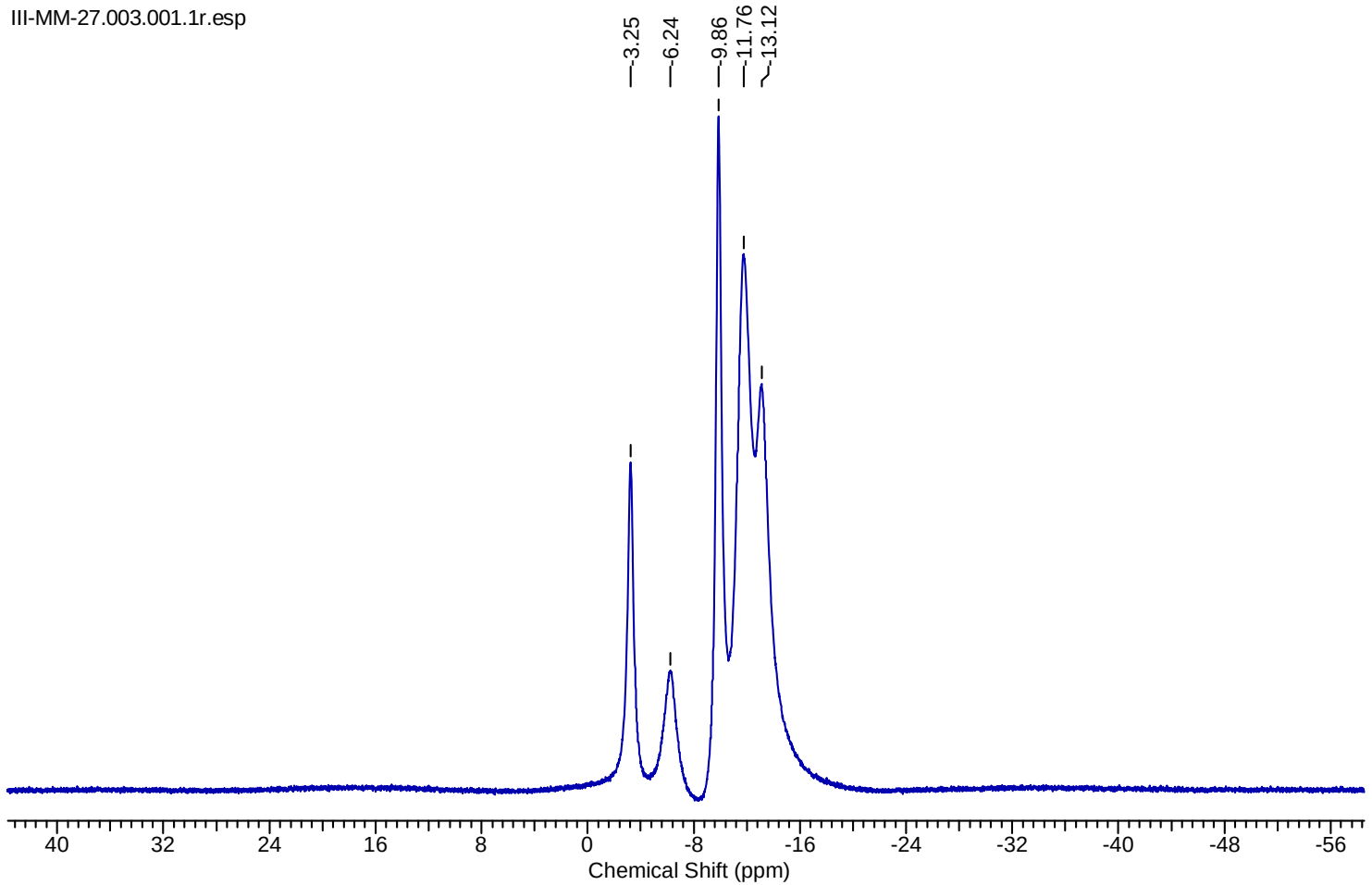


Figure S55. $^{11}B\{^{1}H\ BB\}$ NMR spectrum of compound **24**.

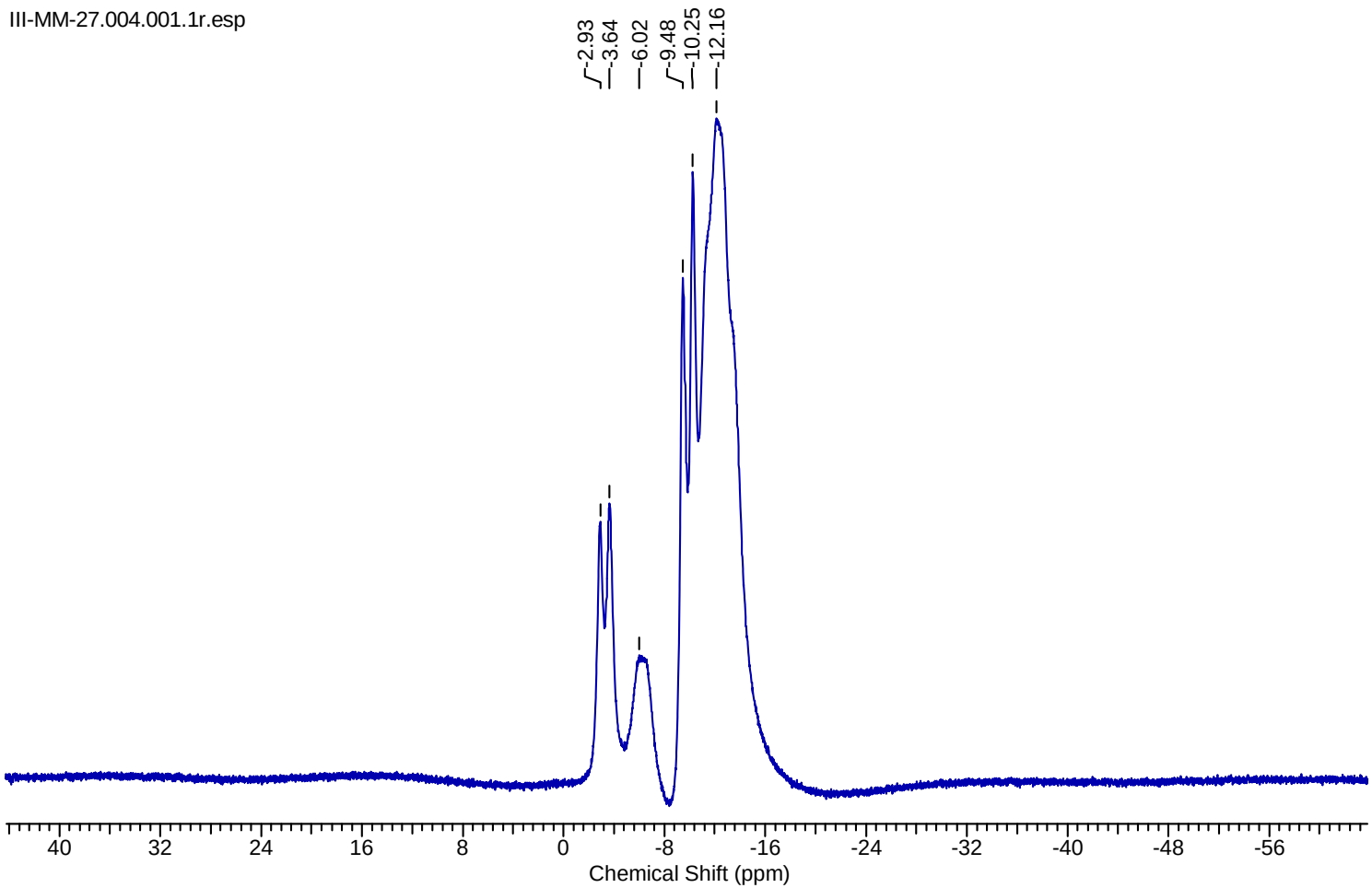


Figure S56. ^{11}B NMR spectrum of compound **24**.

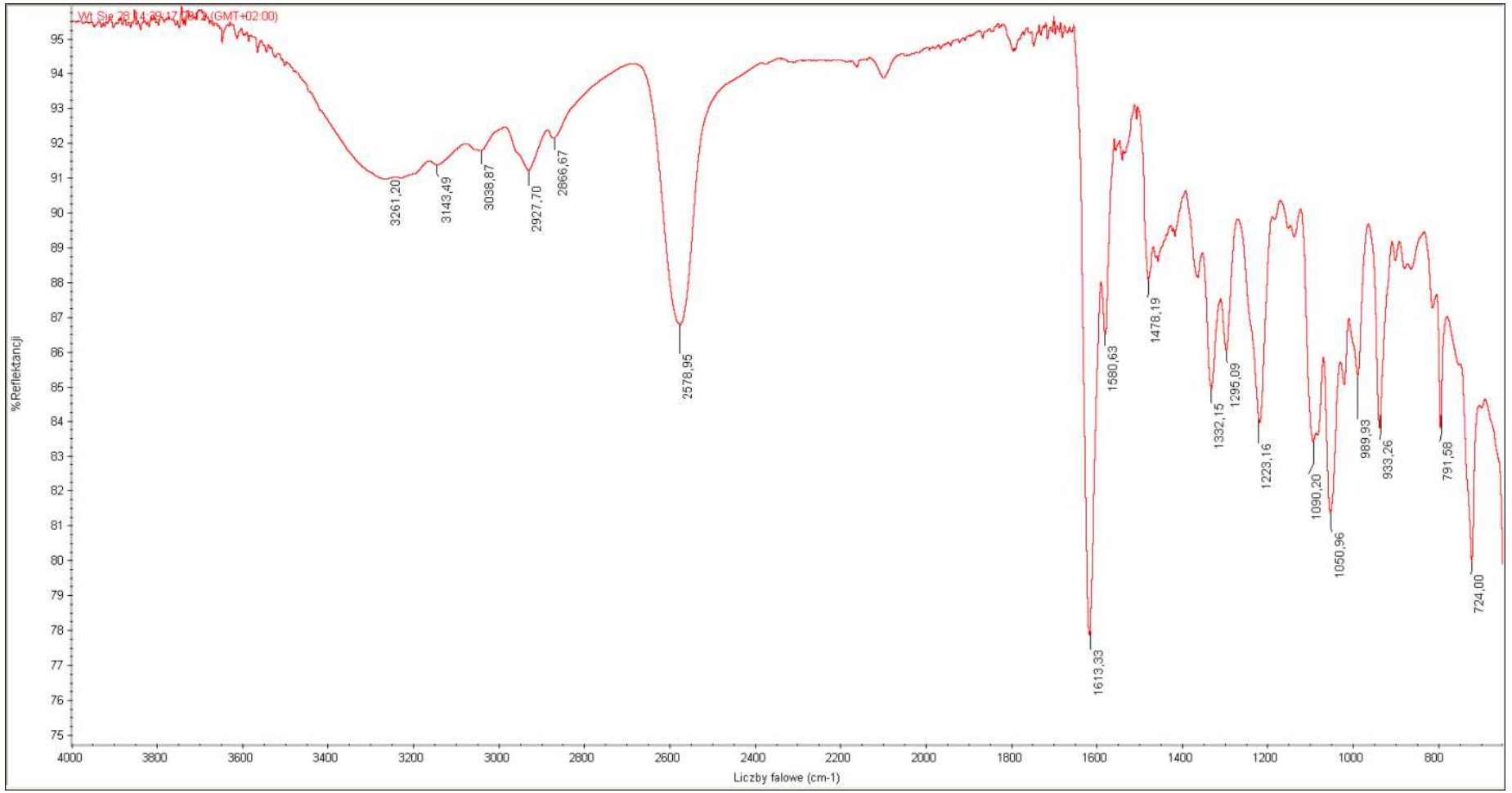
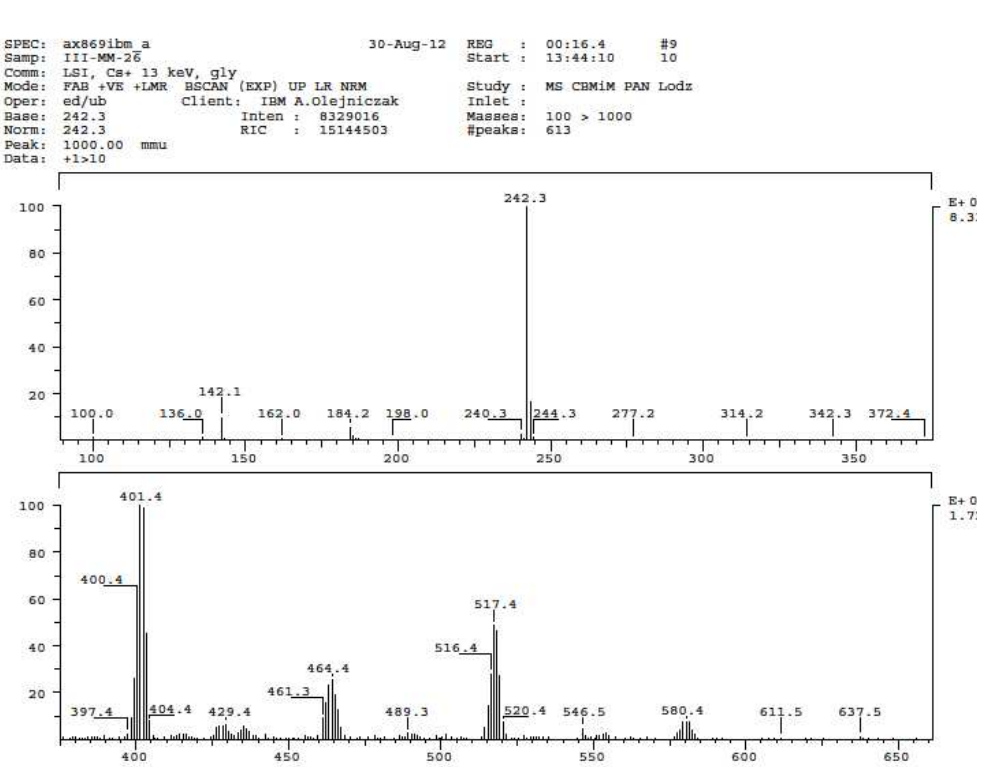


Figure S57. IR spectrum of compound **24**.



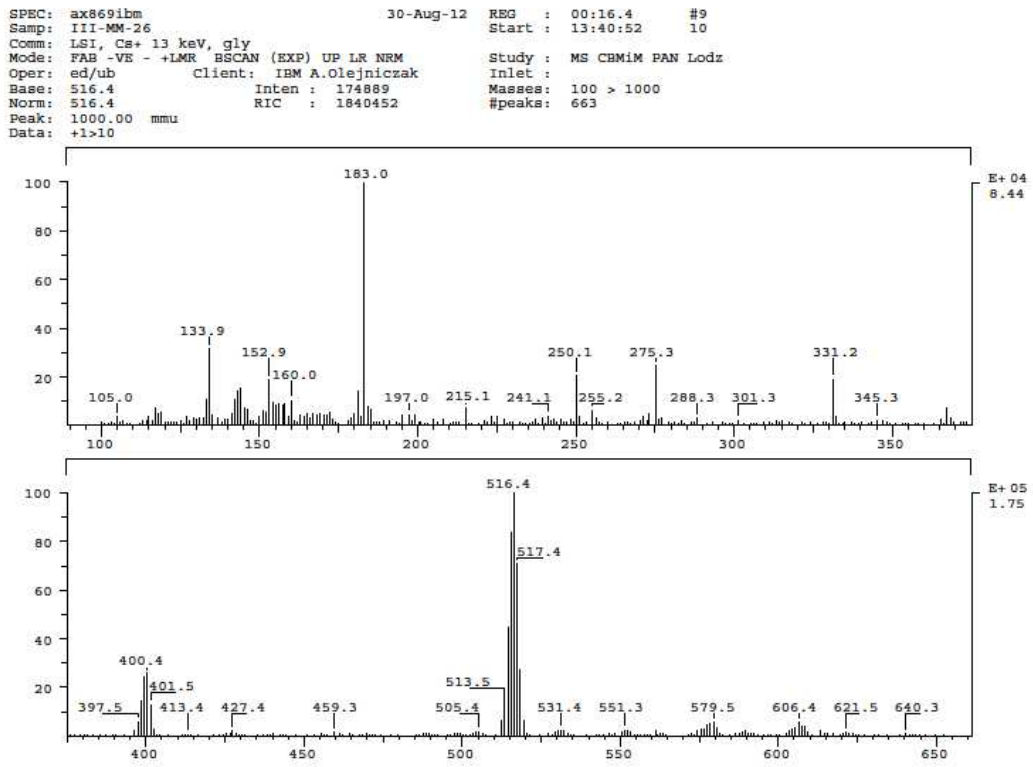


Figure S58. MS-FAB spectra of compound **24**.

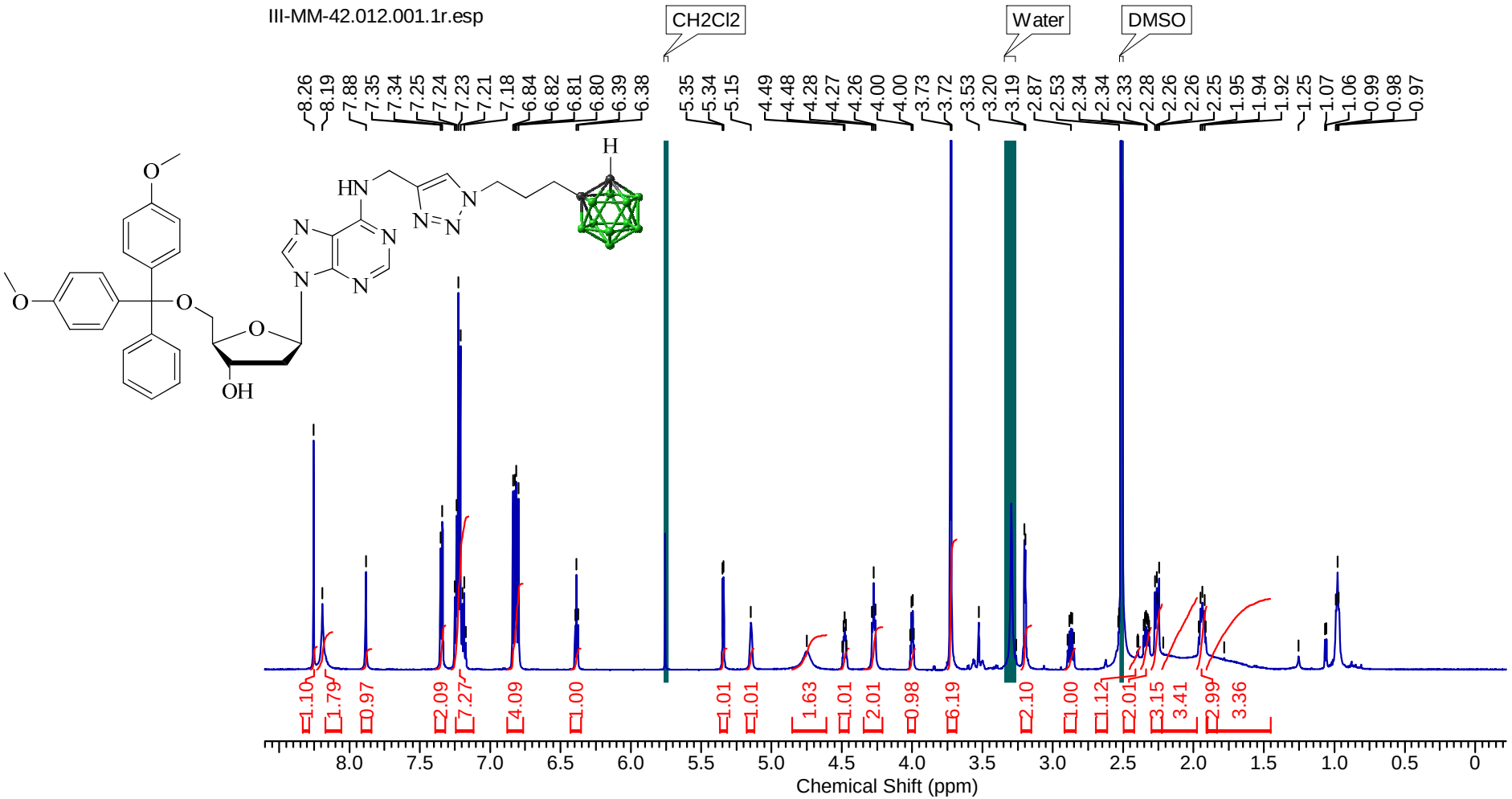


Figure S59. ^{1}H NMR spectrum of compound **25**.

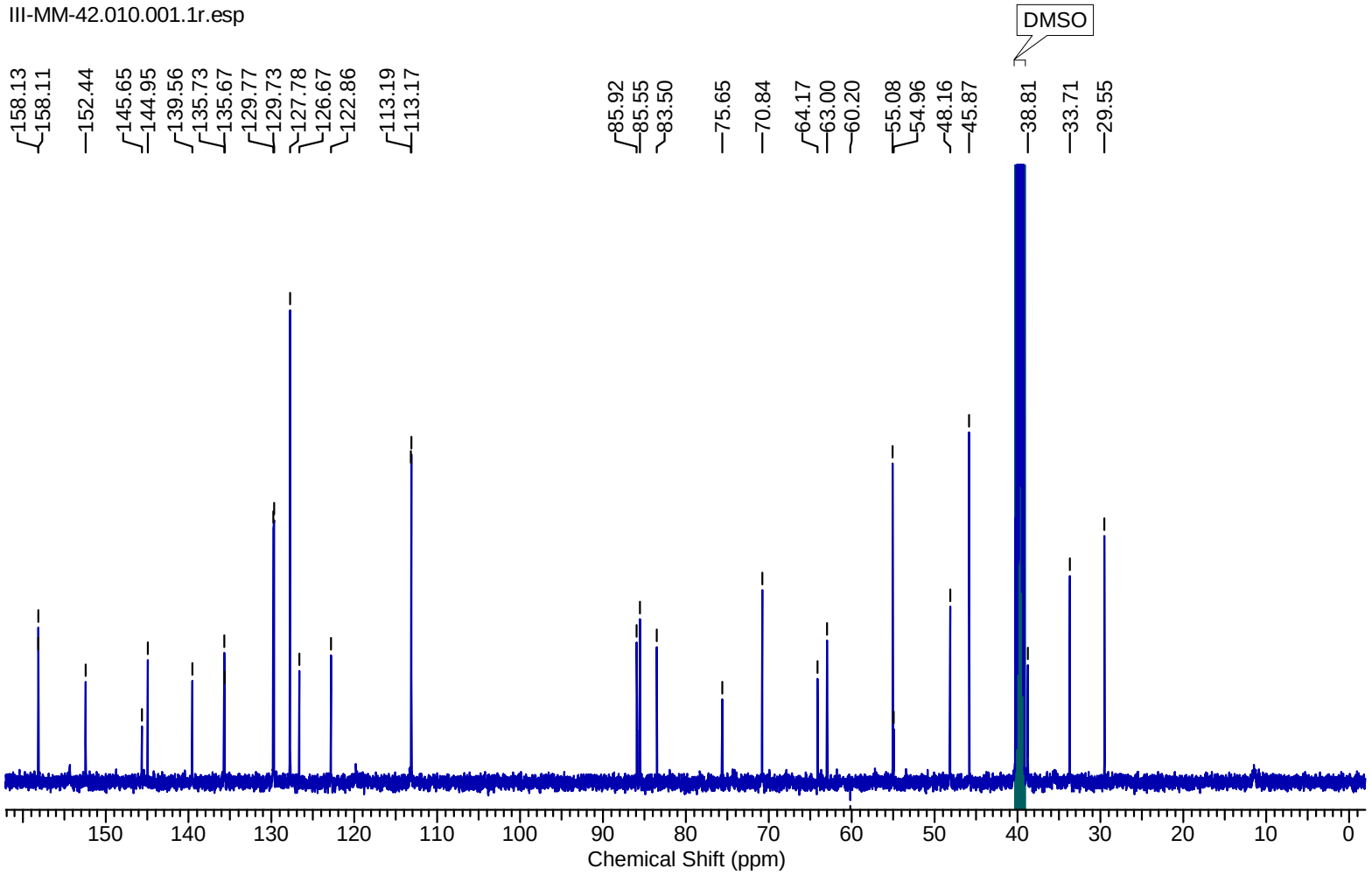


Figure S60. ^{13}C NMR spectrum of compound **25**.

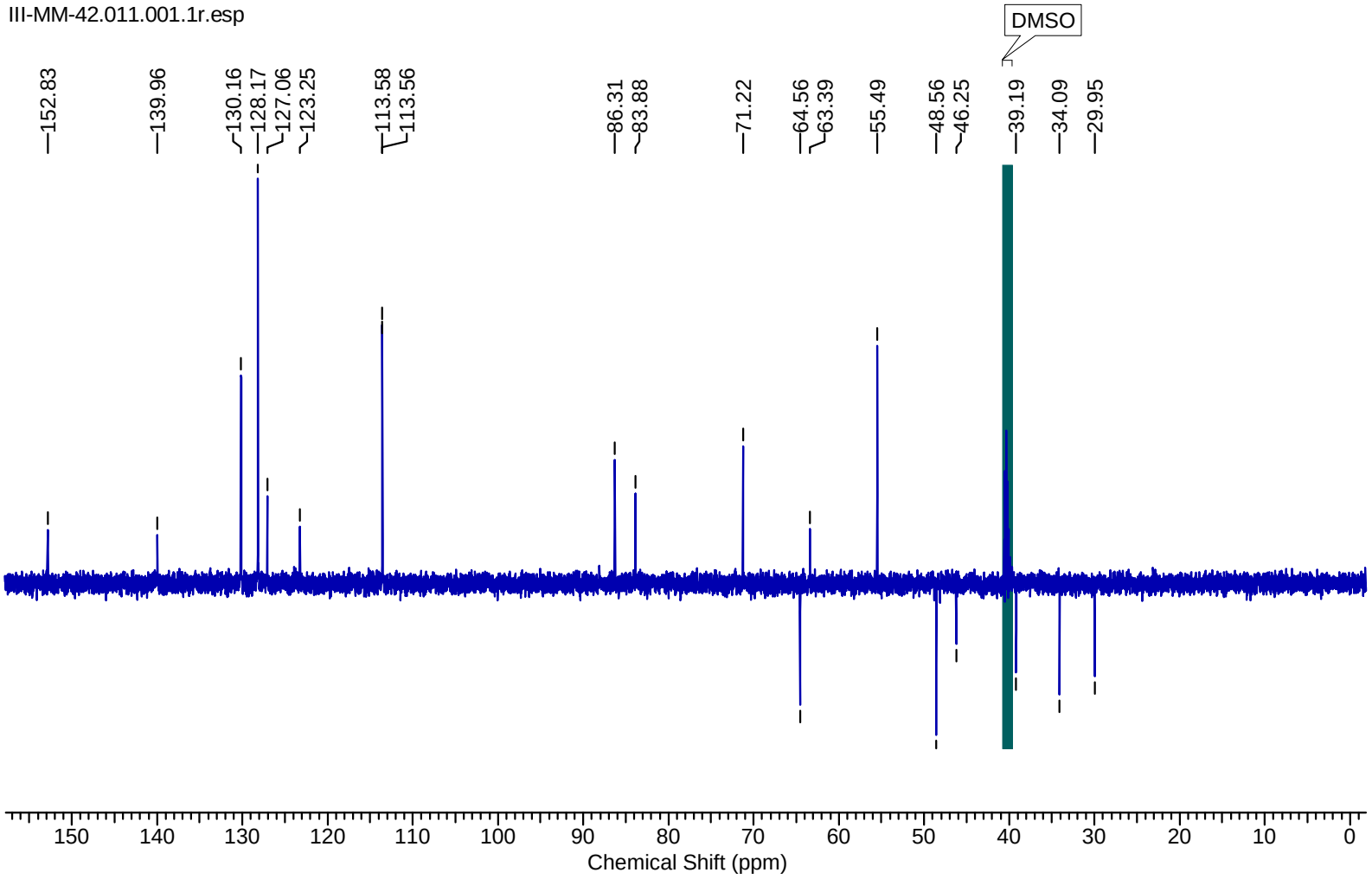


Figure S61. DEPT-135 spectrum of compound **25**.

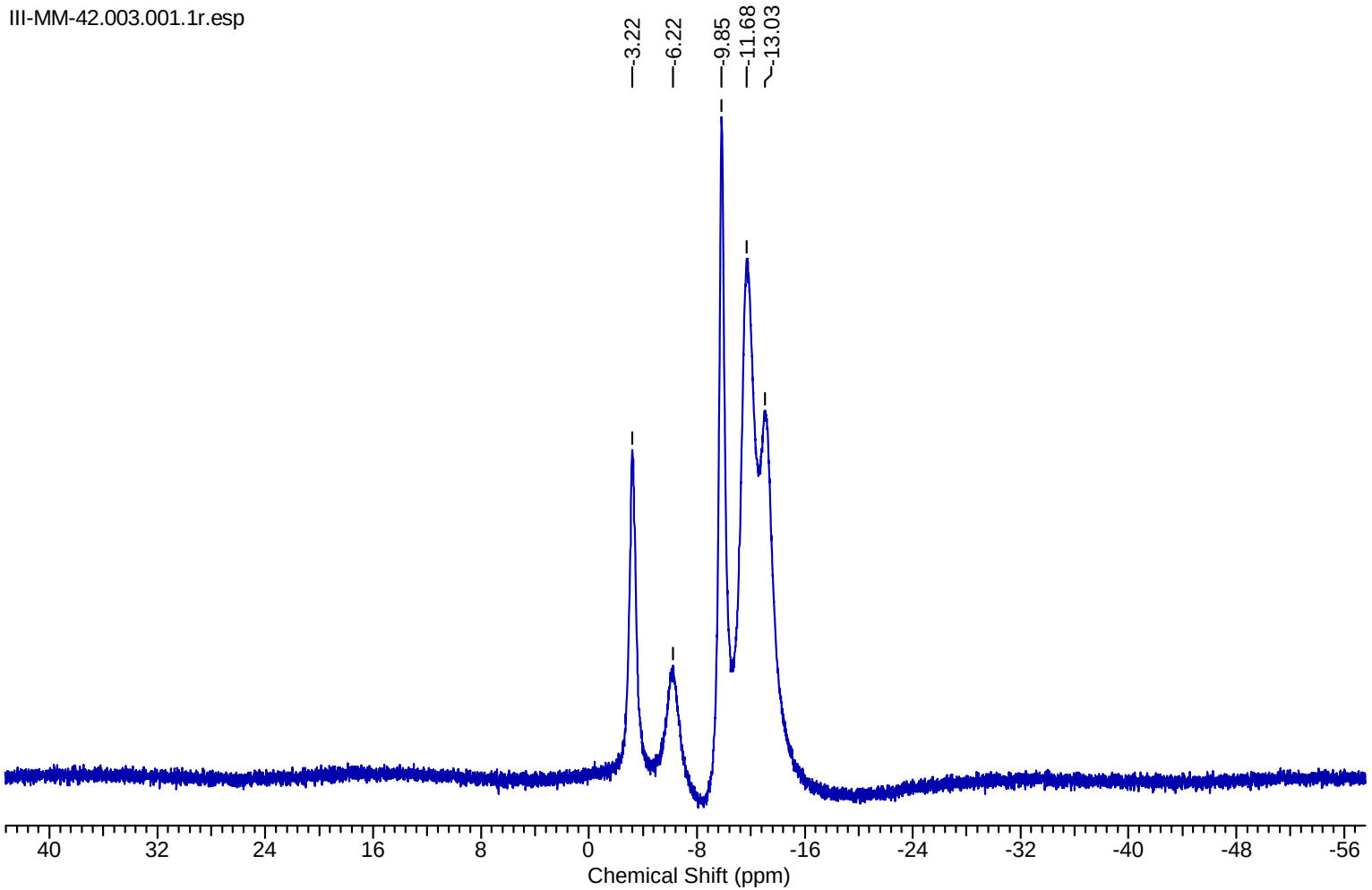


Figure S62. $^{11}B\{^{1}H\ BB\}$ NMR spectrum of compound **25**.

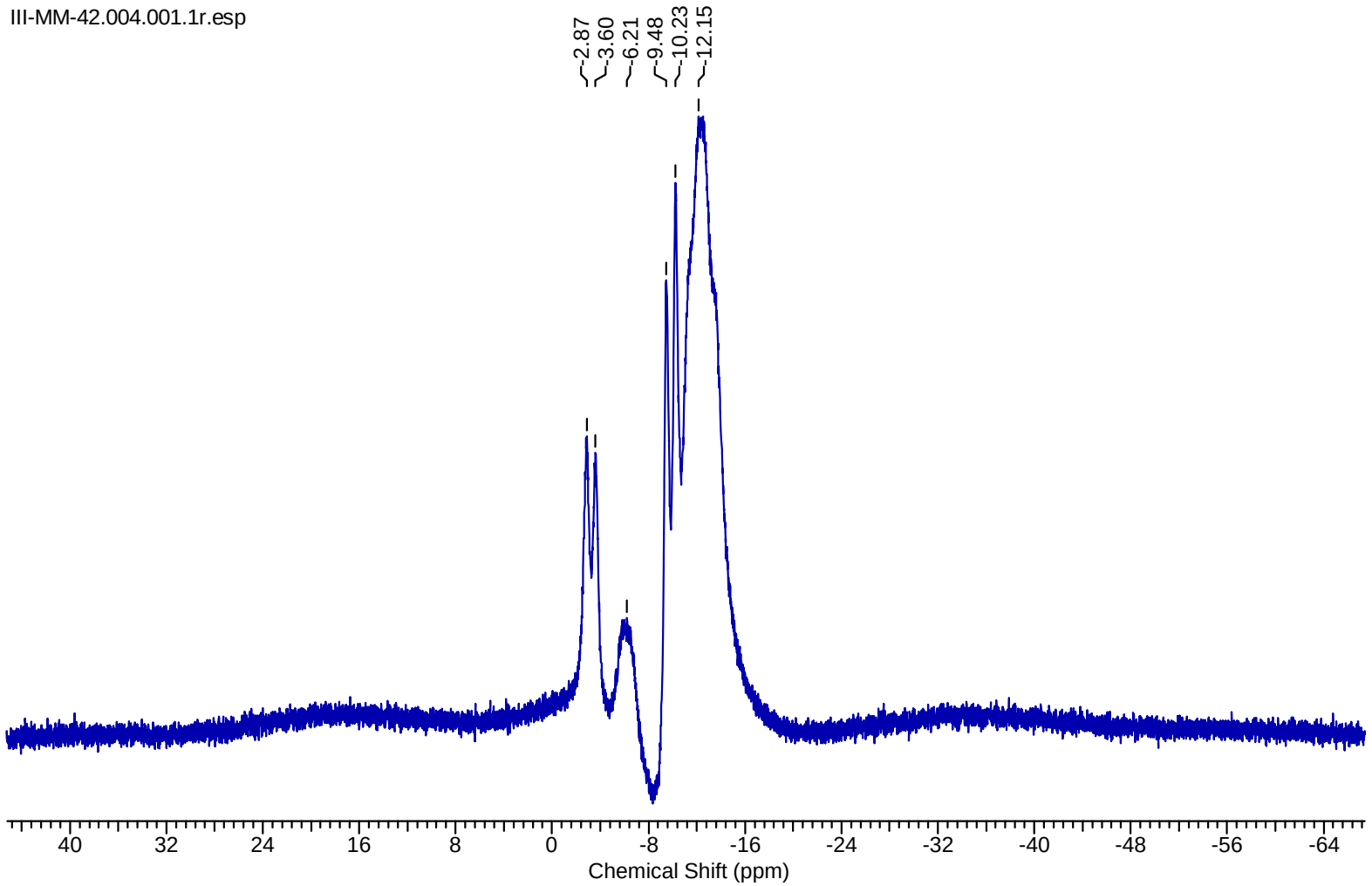


Figure S63. ^{11}B NMR spectrum of compound **25**.

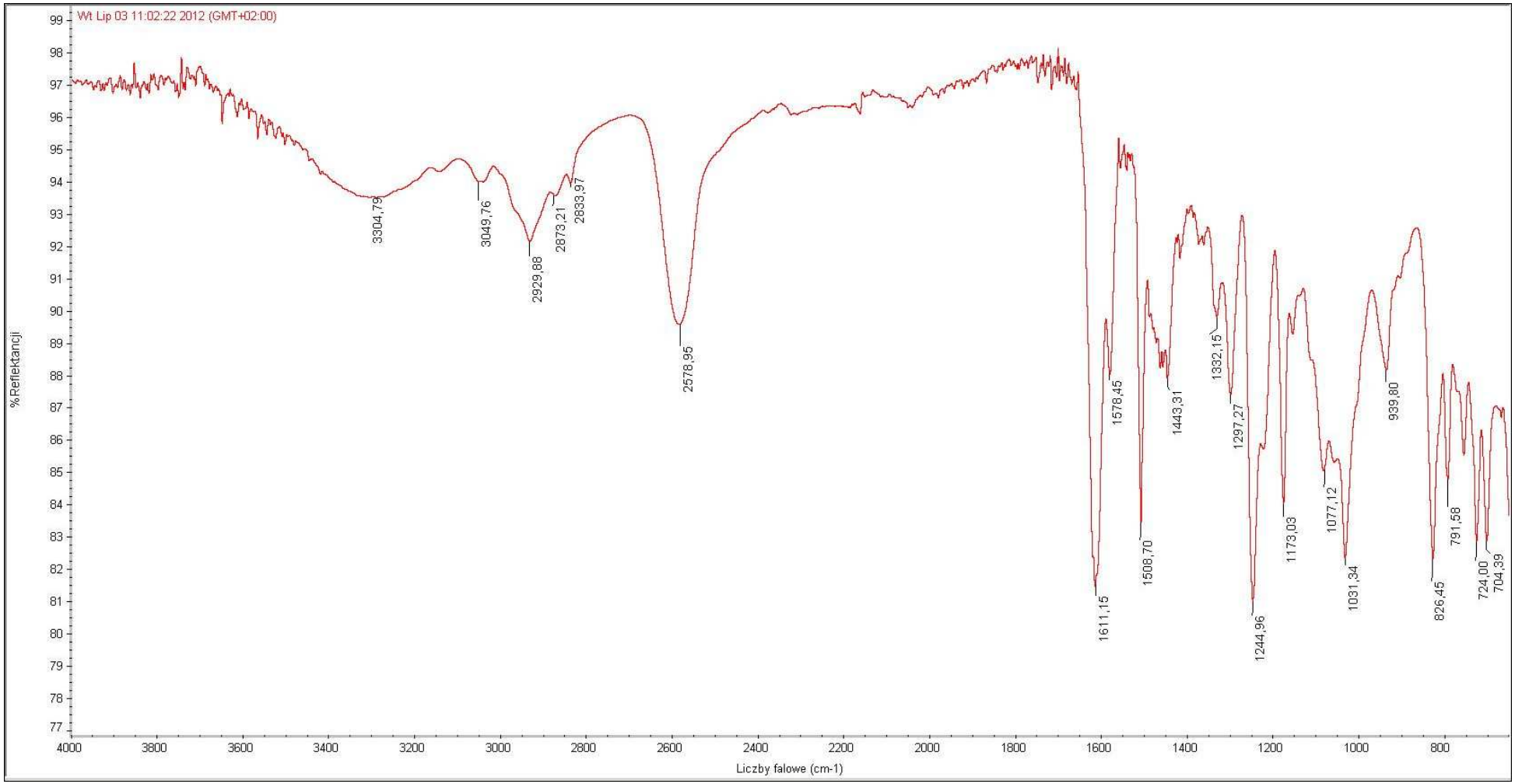
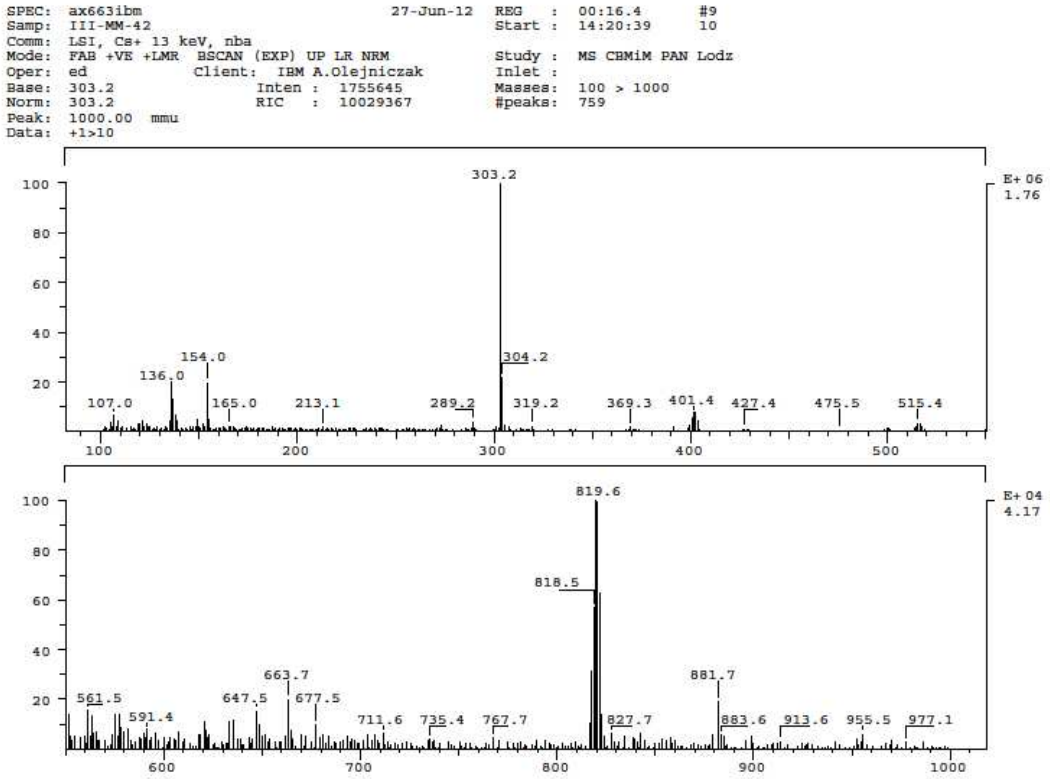


Figure S64. IR spectrum of compound **25**.



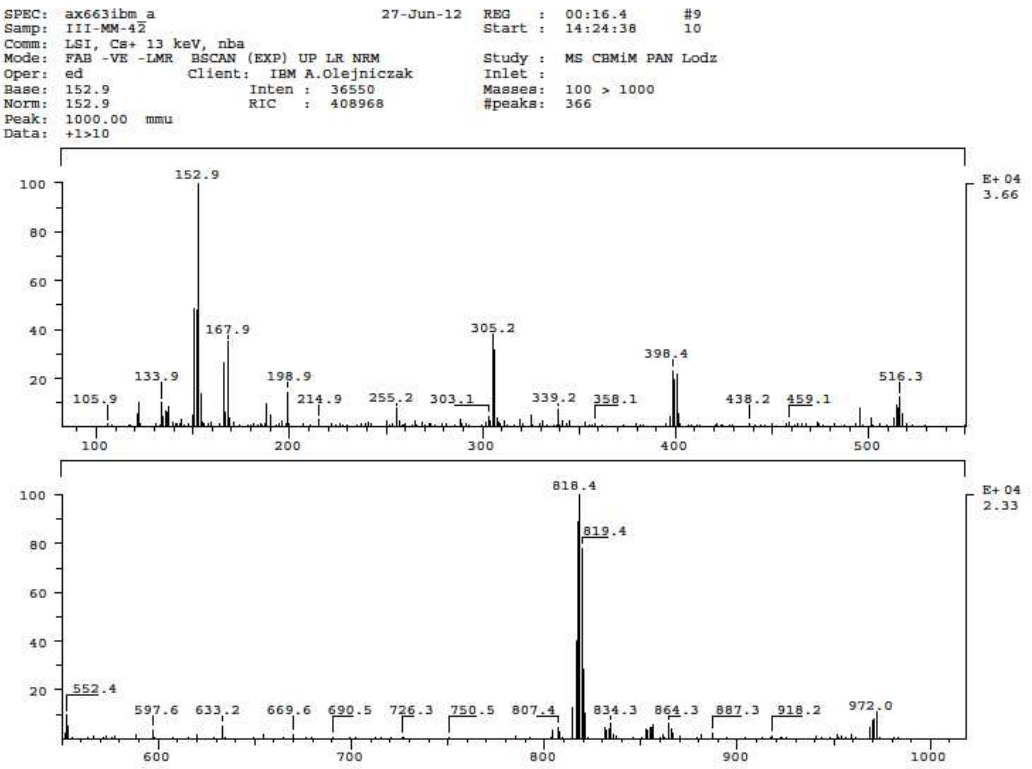


Figure S65. MS spectra of compound **25**.

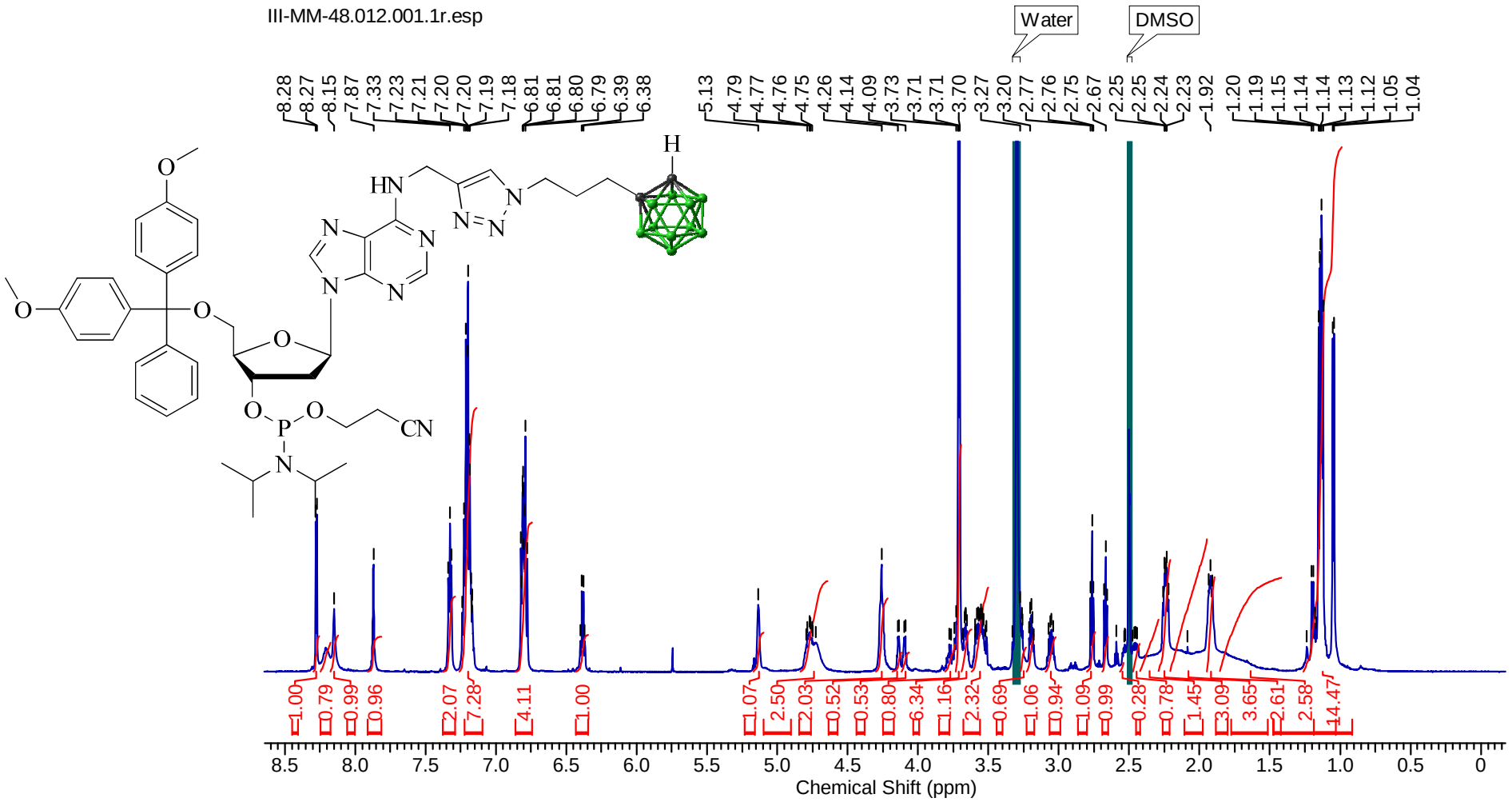


Figure S66. ^{1}H NMR spectrum of compound **31**.

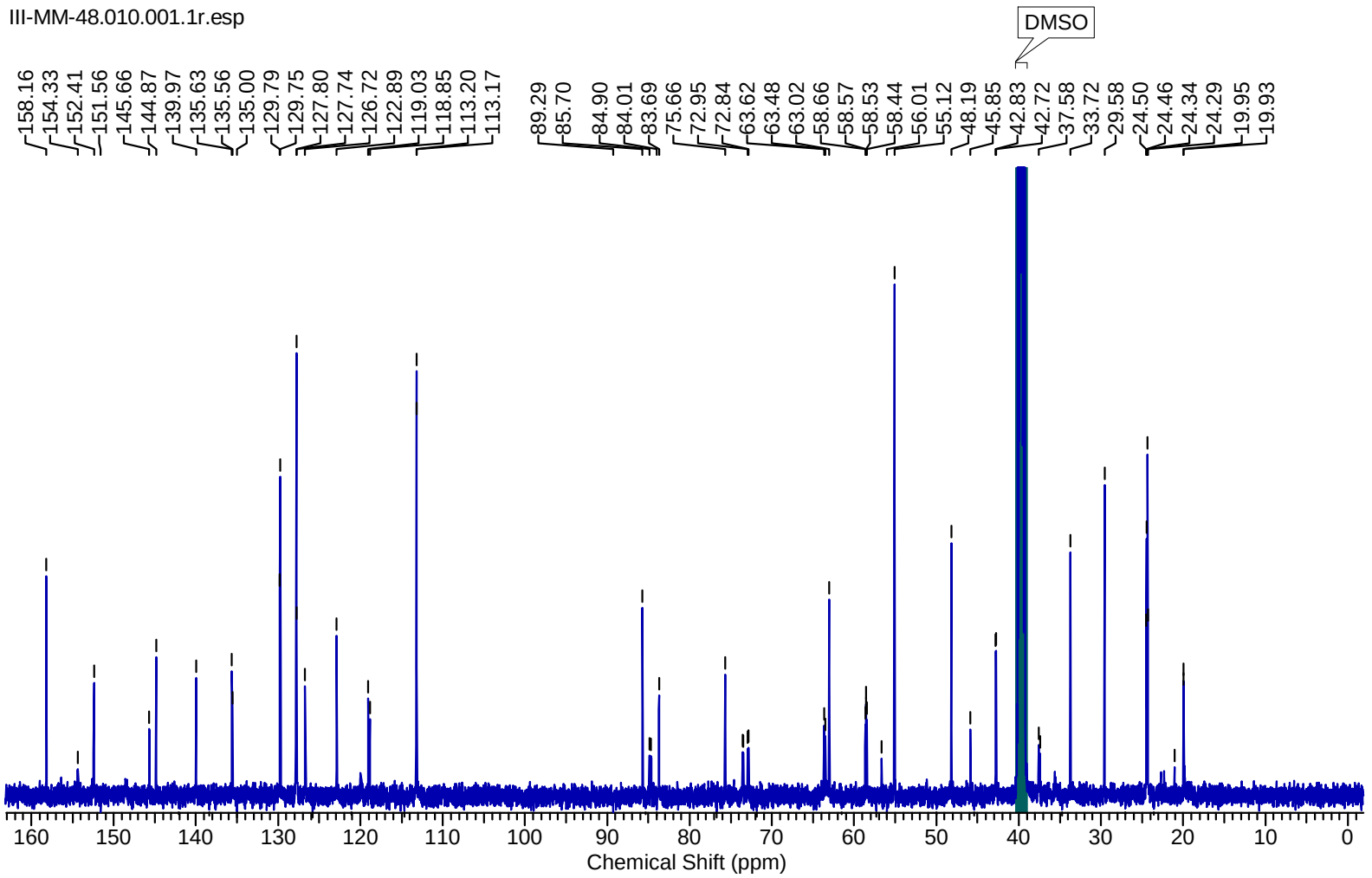


Figure S67. ^{13}C NMR spectrum of compound **31**.

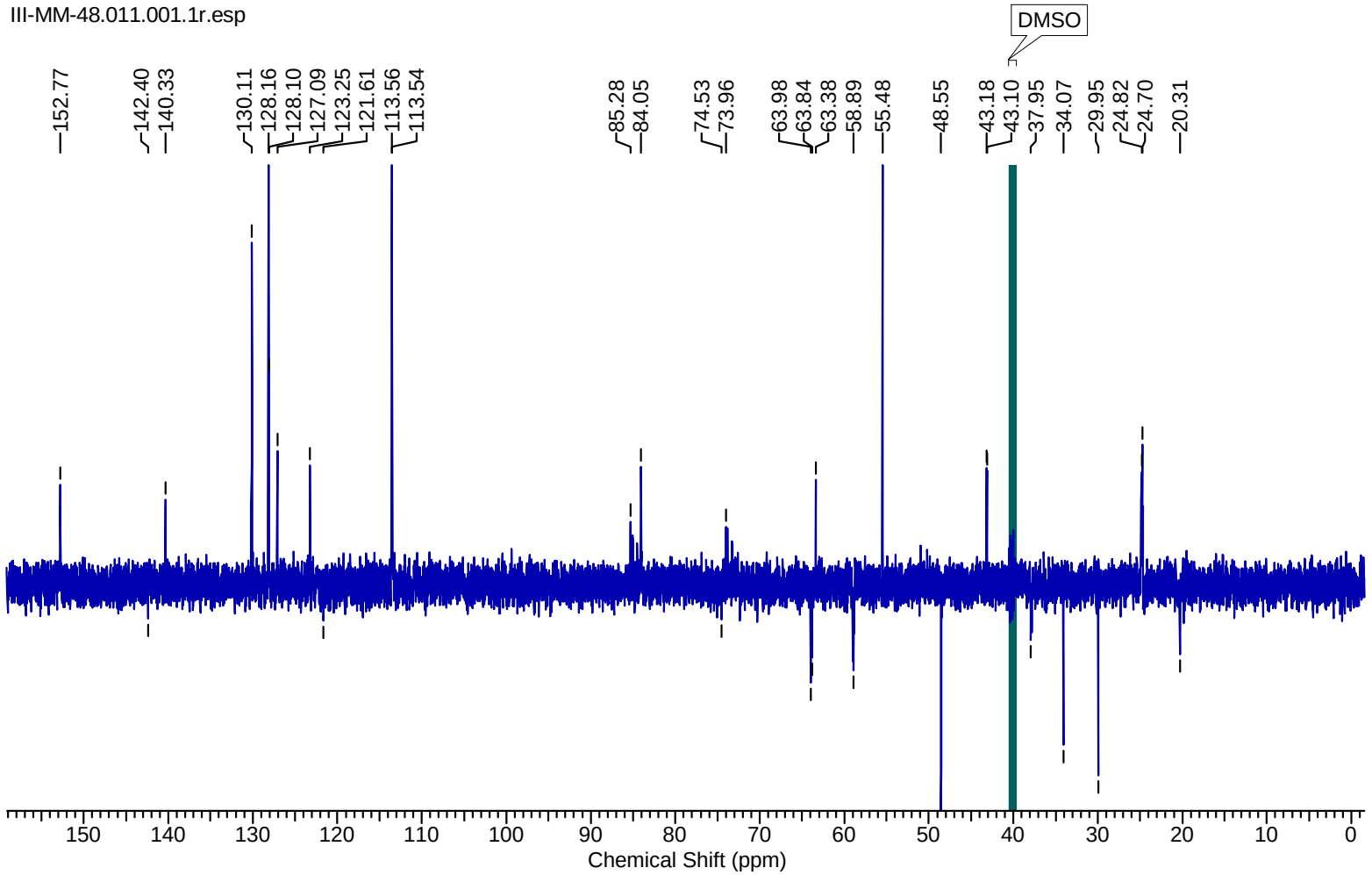


Figure S68. DEPT-135 spectrum of compound **31**.

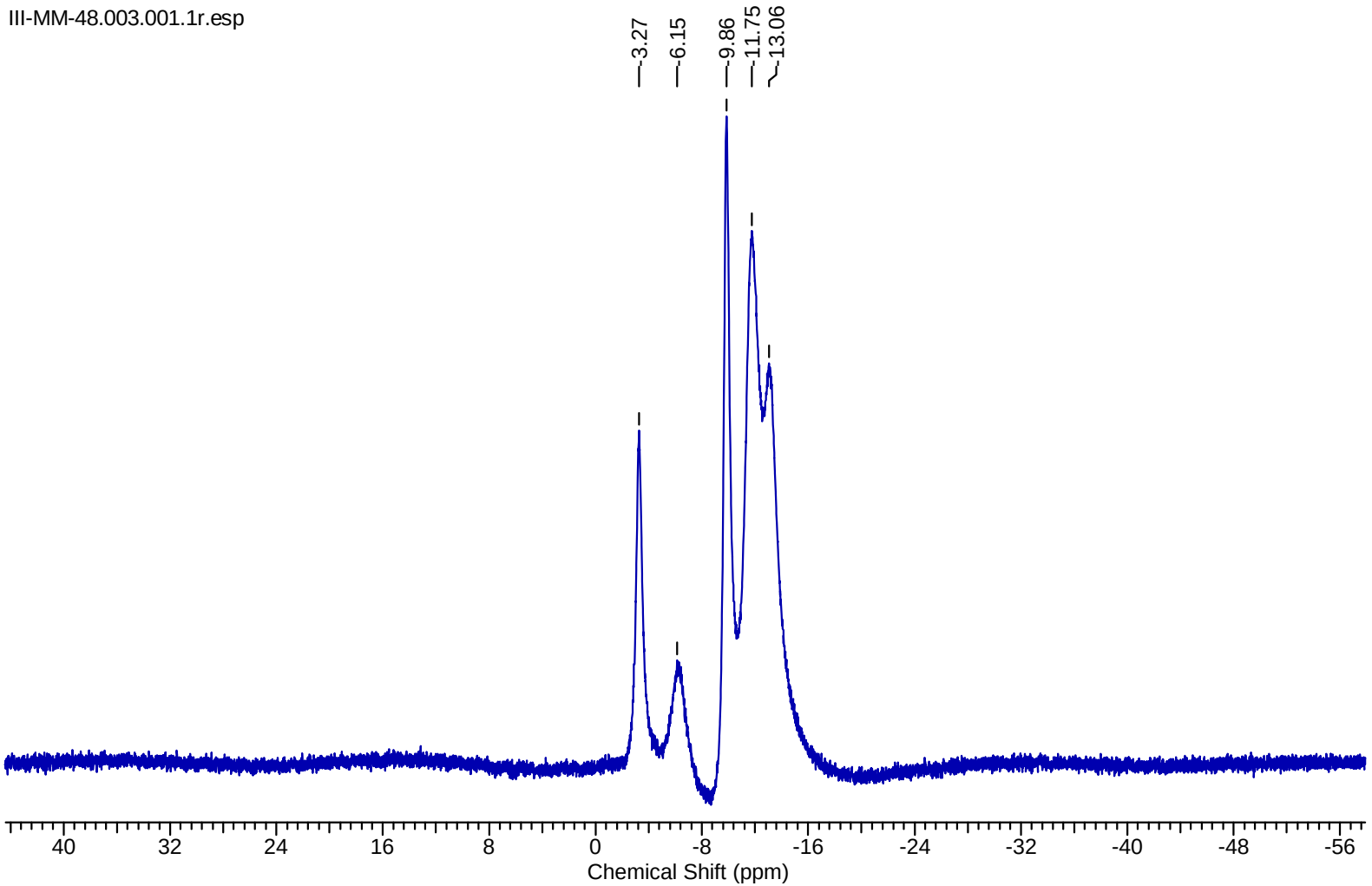


Figure S69. $^{11}B\{^{1}H\ BB\}$ NMR spectrum of compound **31**.

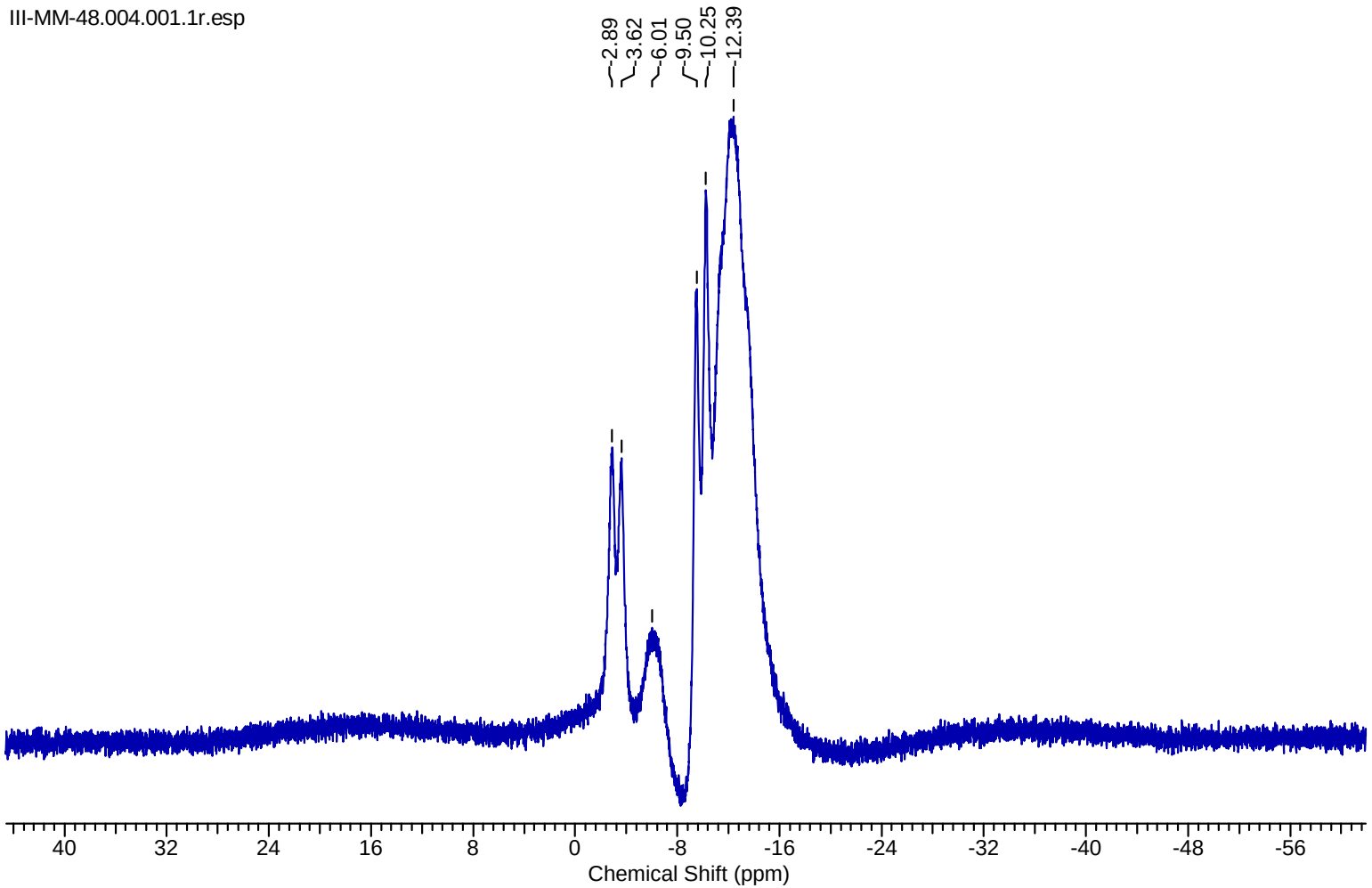


Figure S70. ^{11}B NMR spectrum of compound **31**.

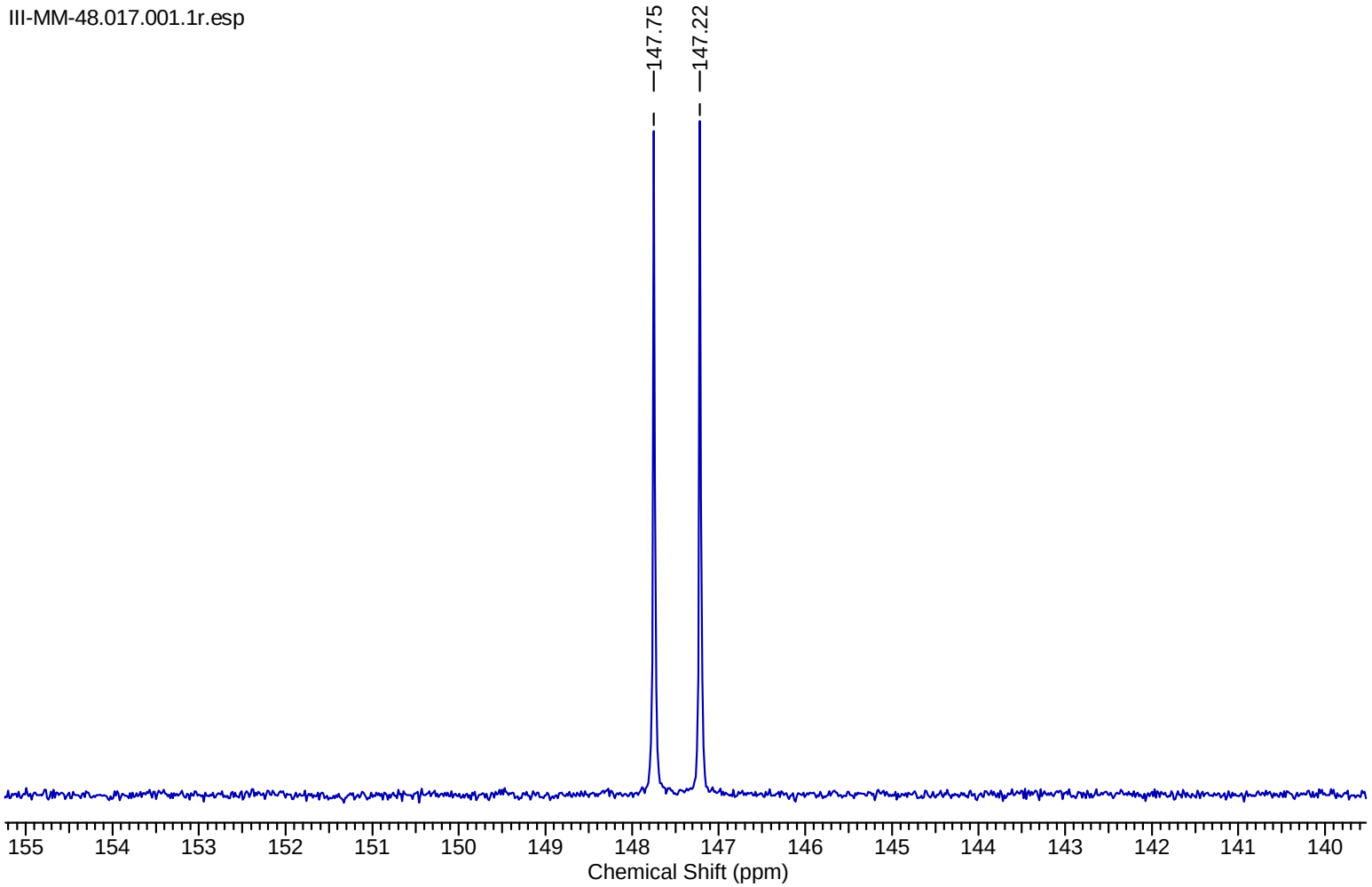


Figure S71. ^{31}P NMR spectrum of compound **31**.

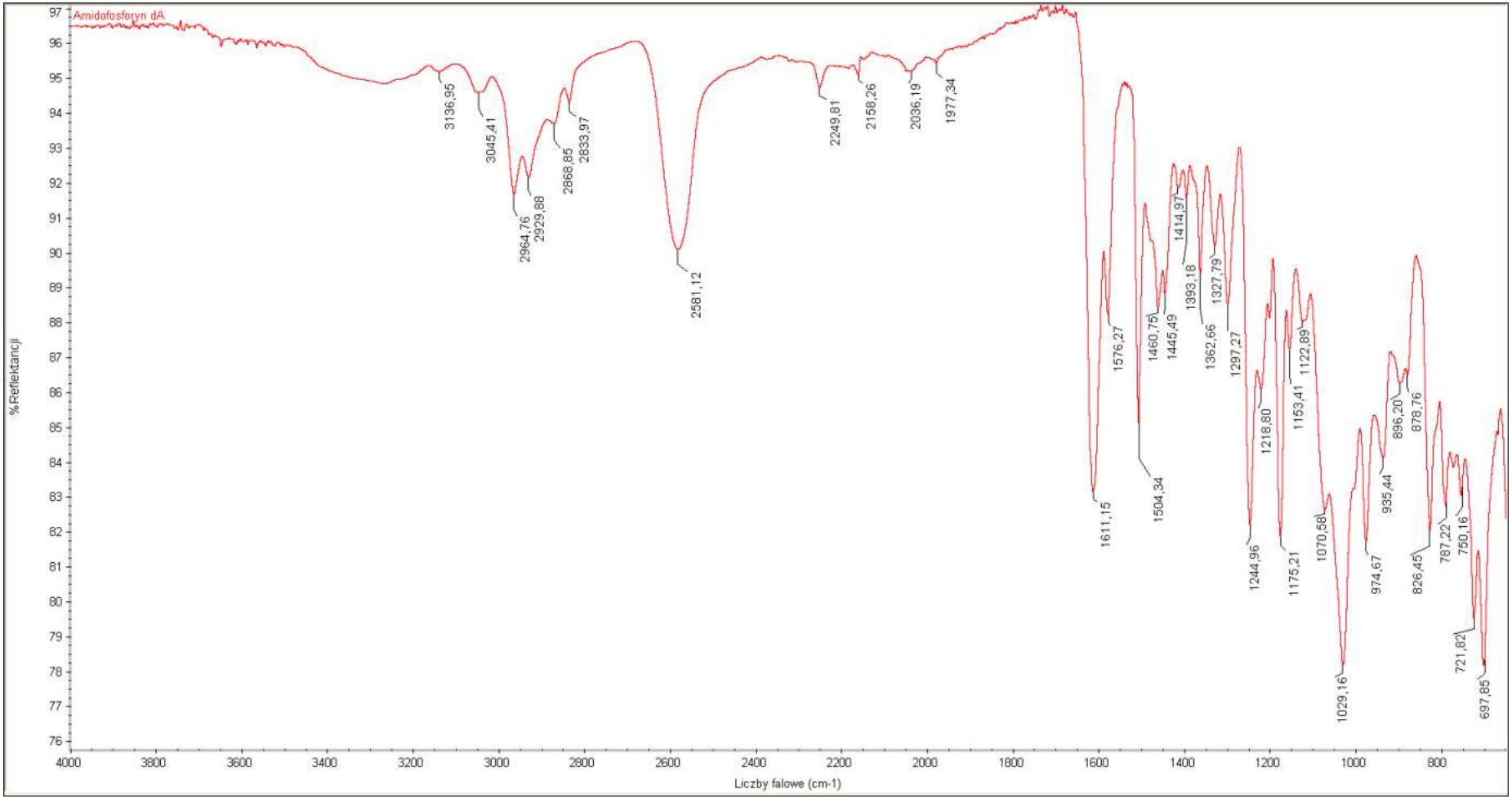
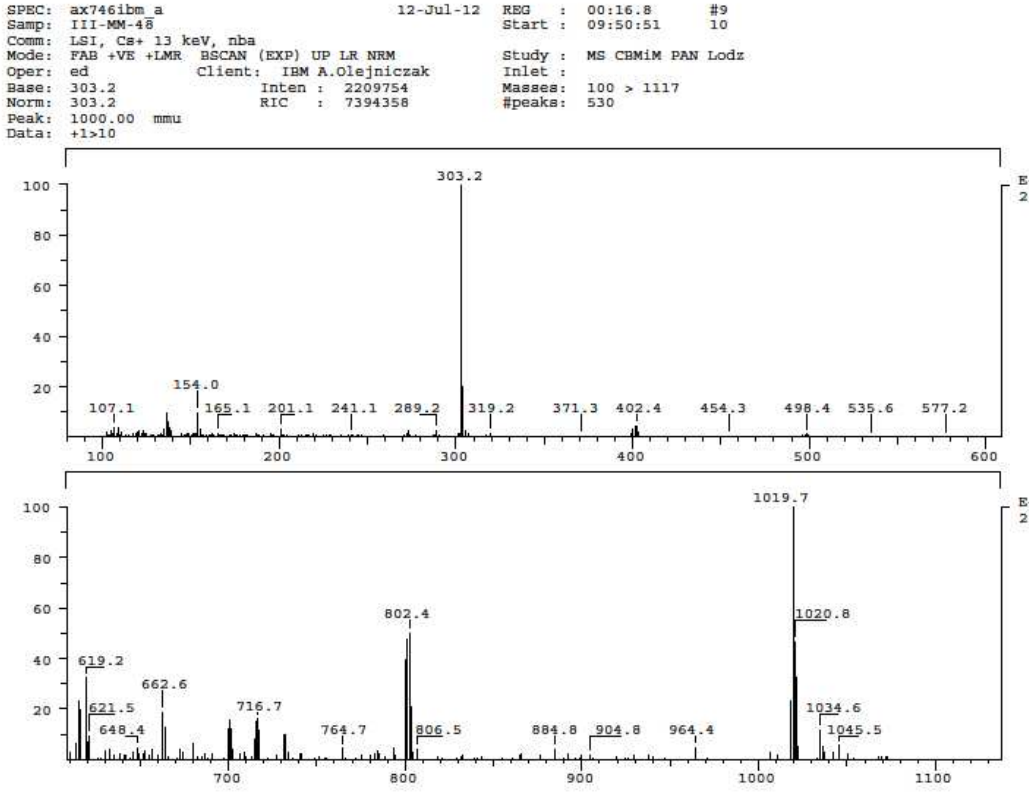


Figure S72. IR spectrum of compound **31**.



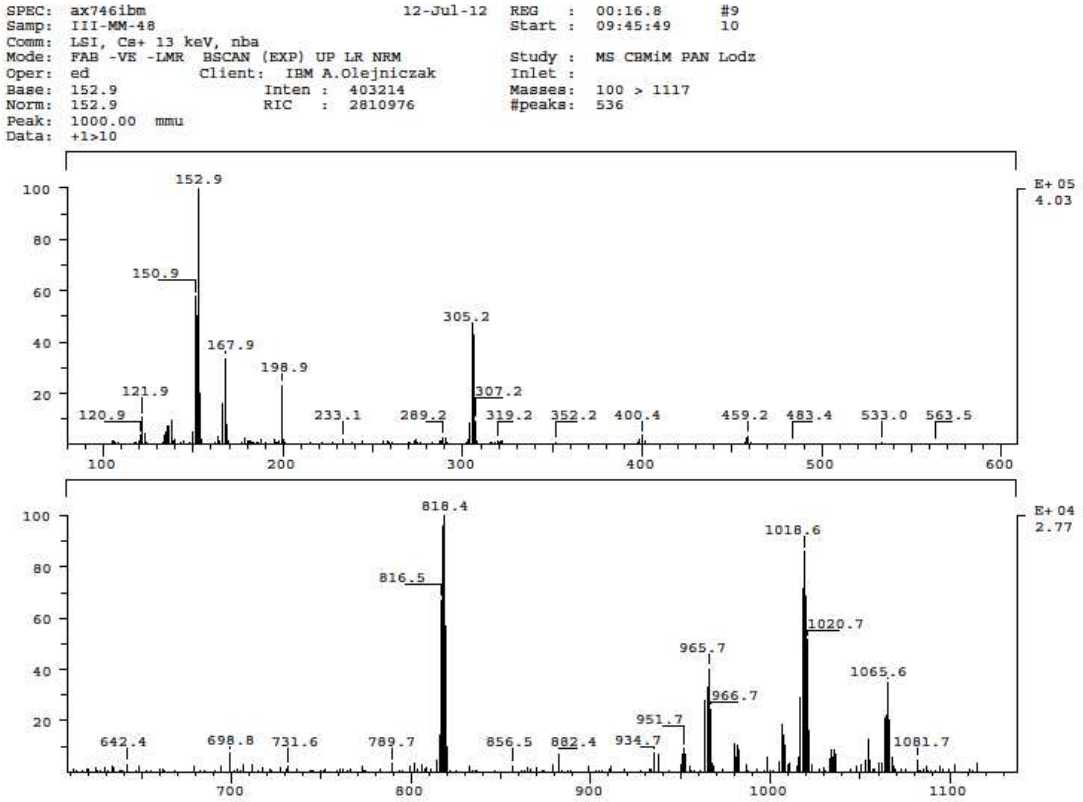


Figure S73. MS-FAB spectra of compound **31**.

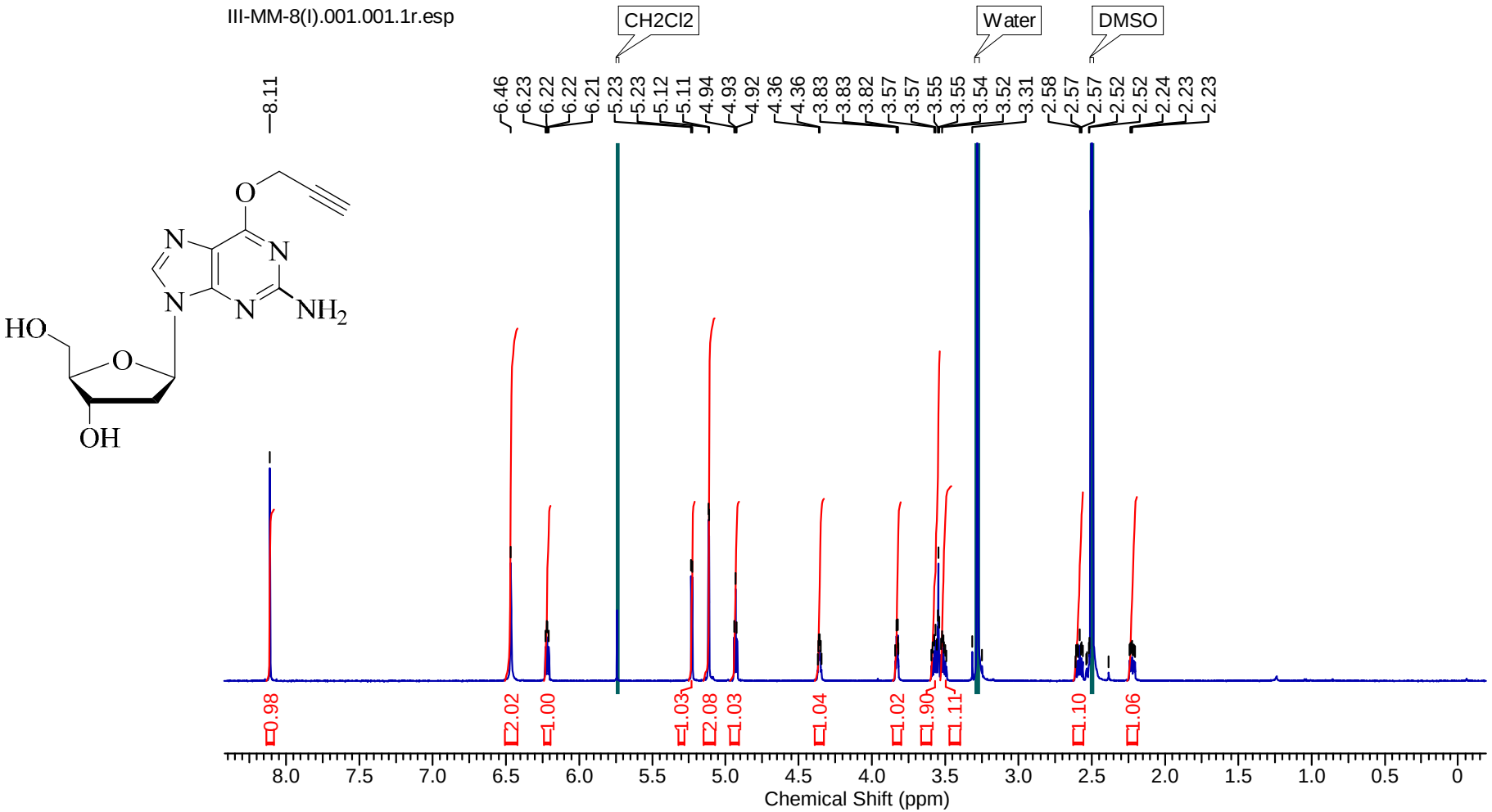


Figure S74. ^{1}H NMR spectrum of compound **16**.

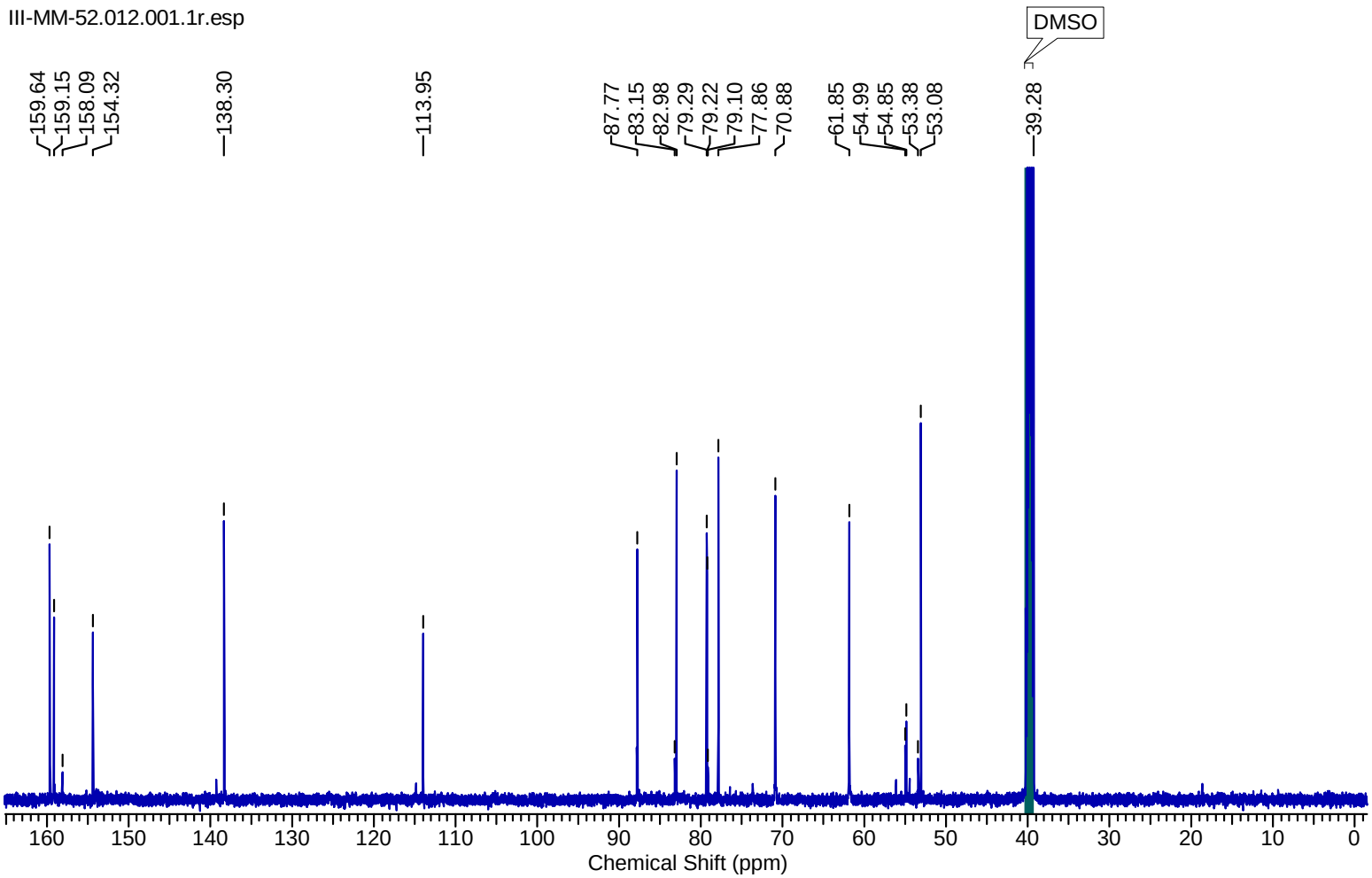


Figure S75. ^{13}C NMR spectrum of compound **16**.

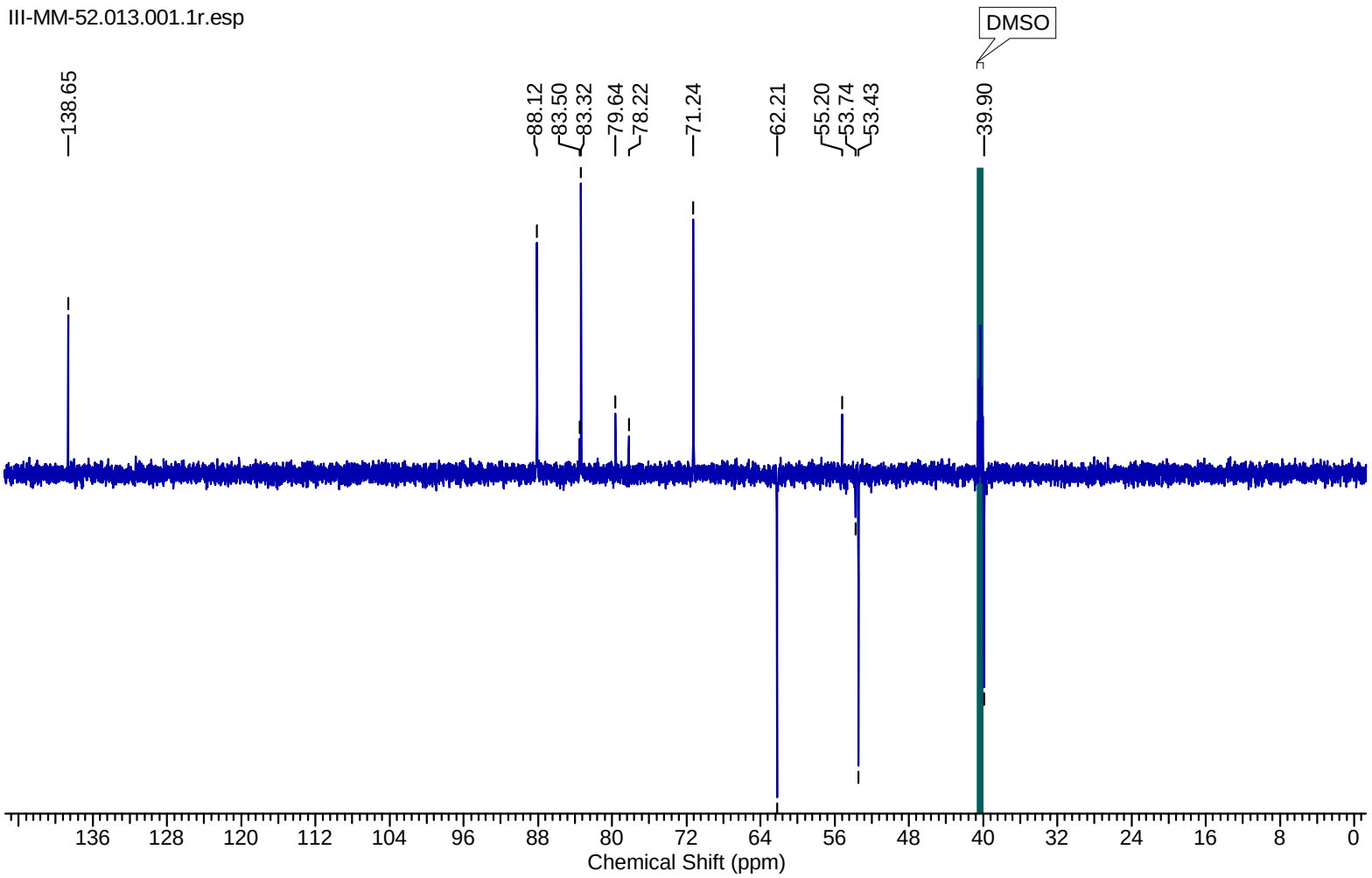


Figure S76. DEPT-135 spectrum of compound **16**.

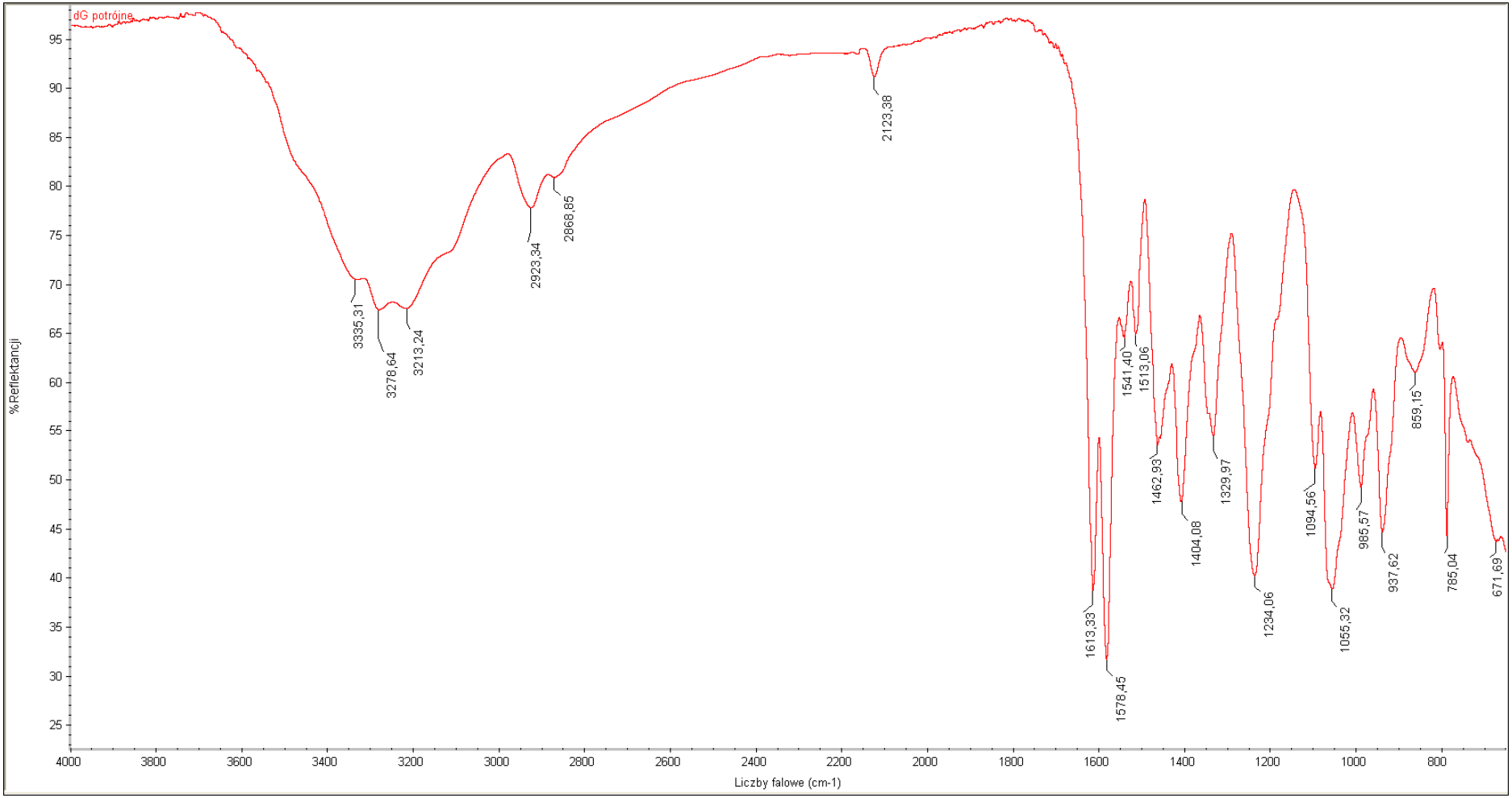


Figure S77. IR spectrum of compound **16**.

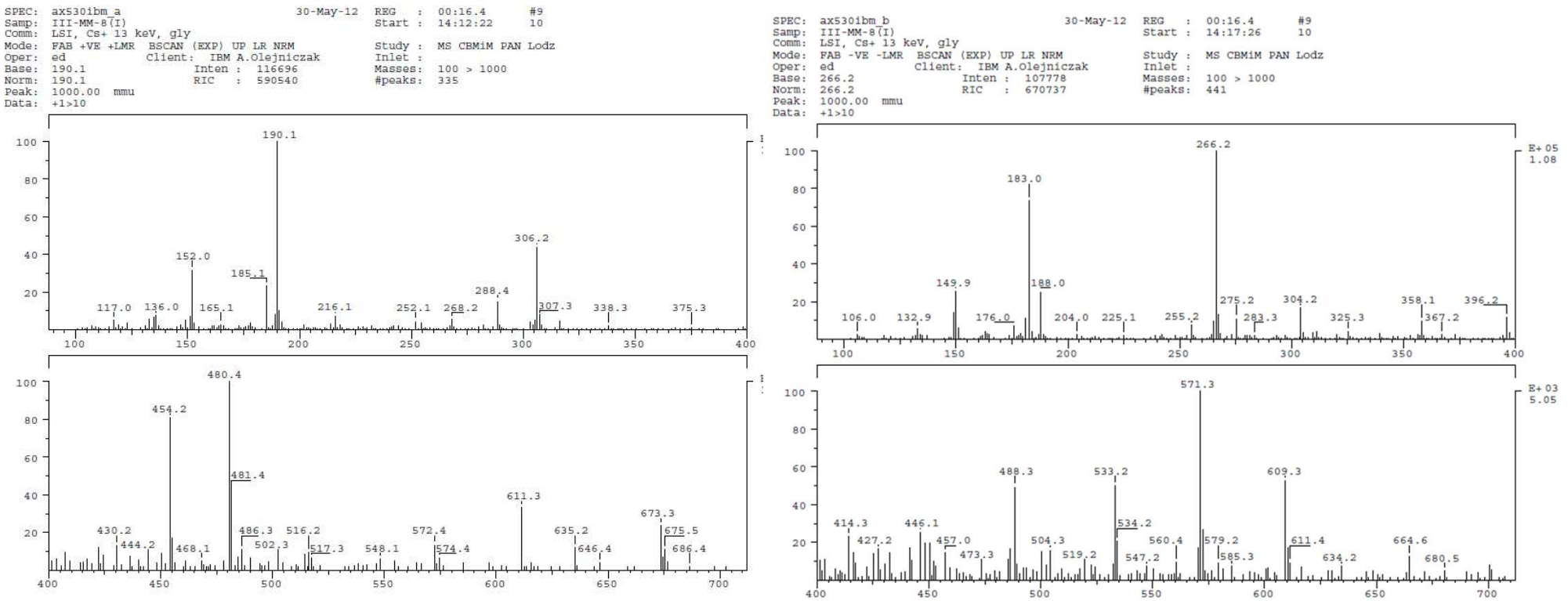


Figure S78. MS-FAB spectra of compound **16**.

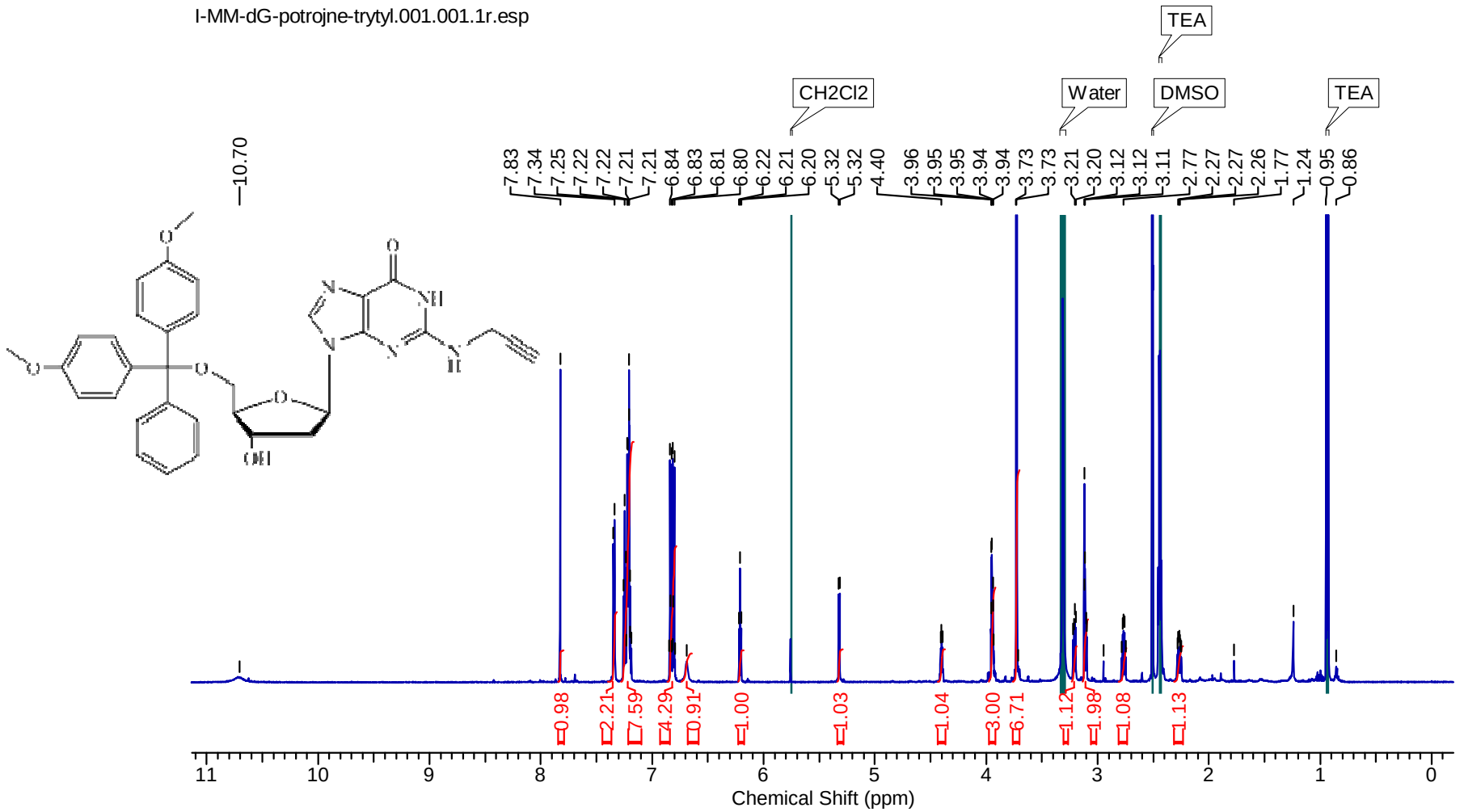


Figure S79. ^{1}H NMR spectrum of compound **17**.

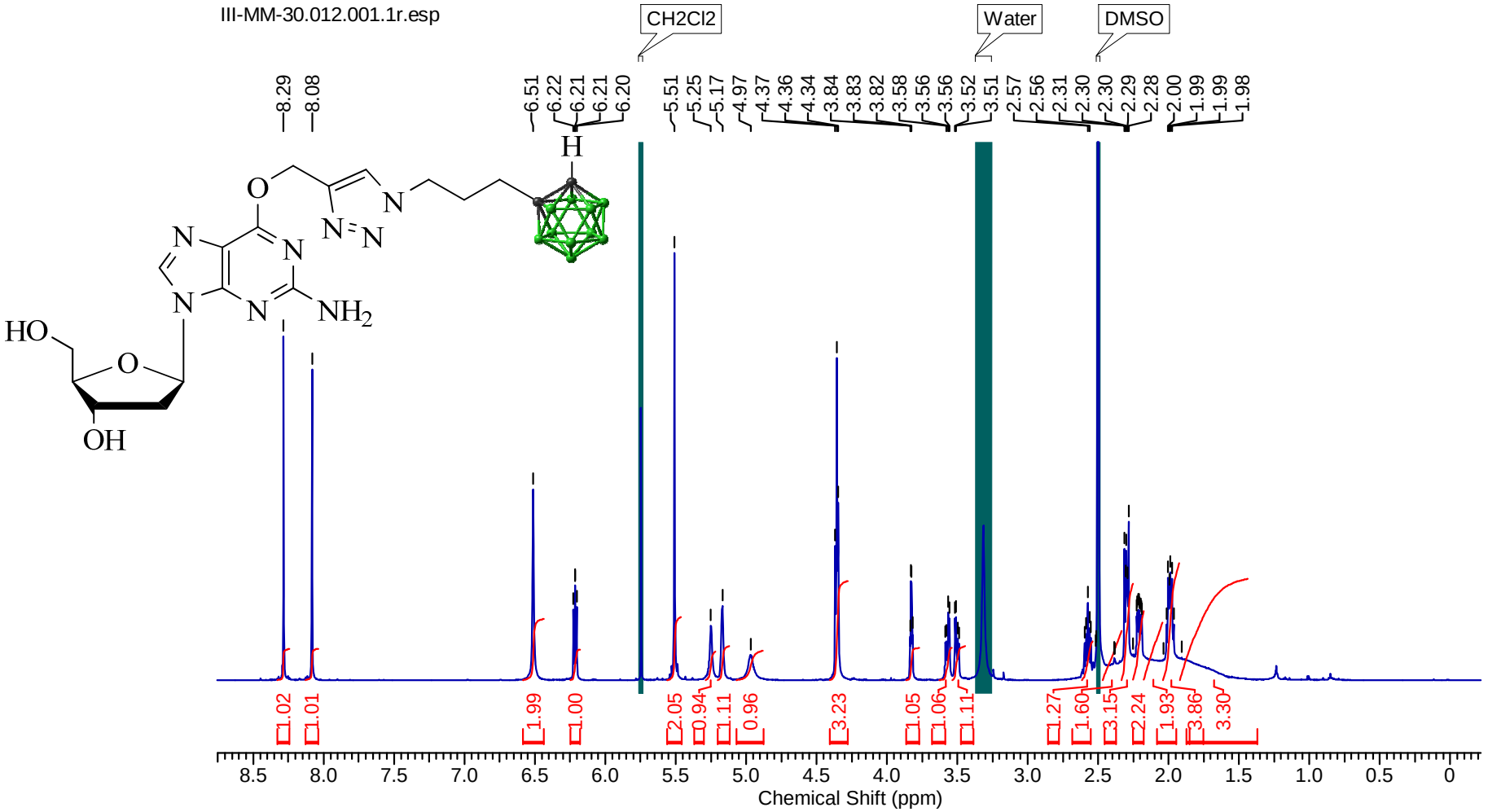


Figure S80. ^{1}H NMR spectrum of compound **26**.

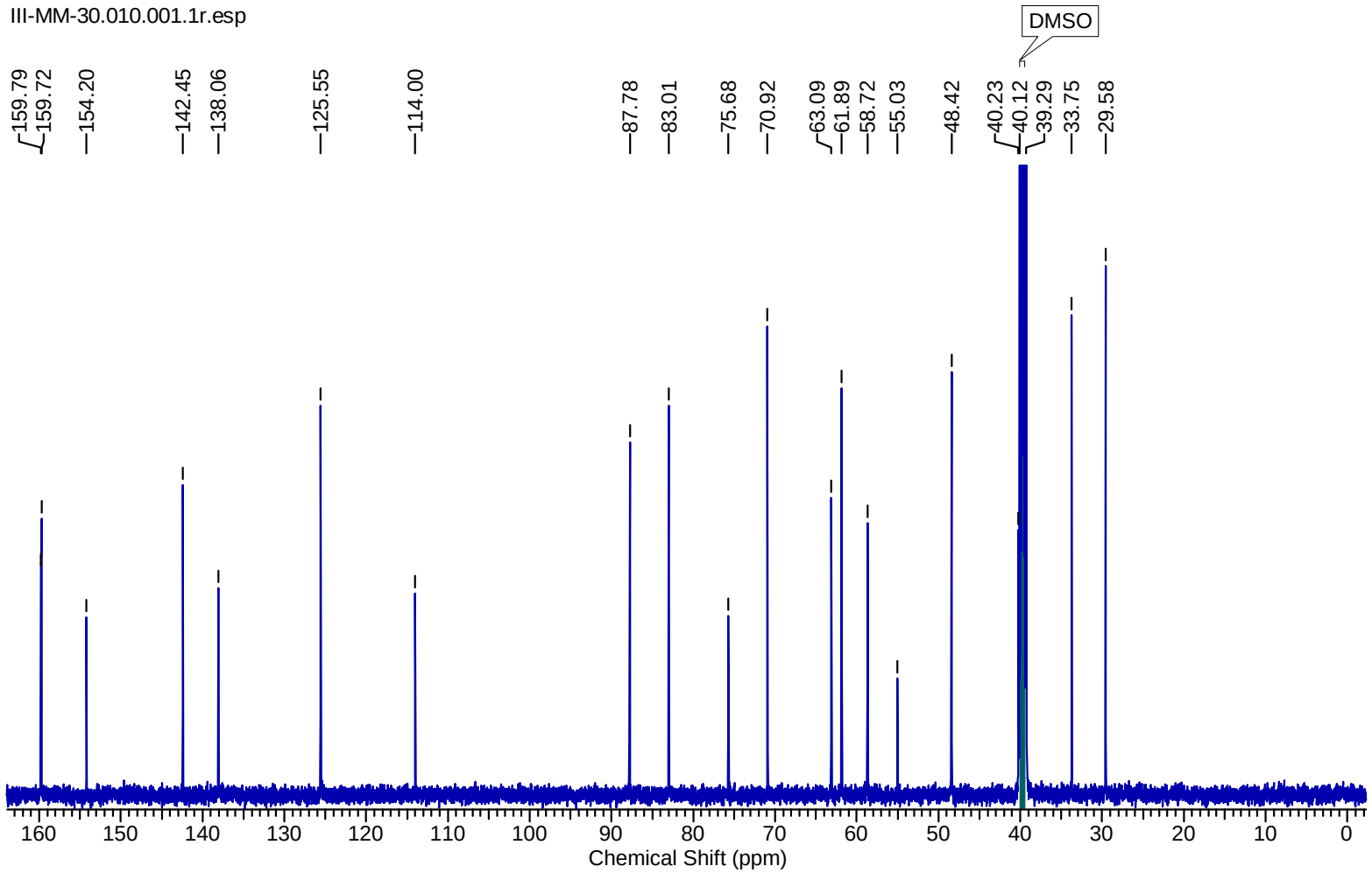


Figure S81. ^{13}C NMR spectrum of compound **26**.

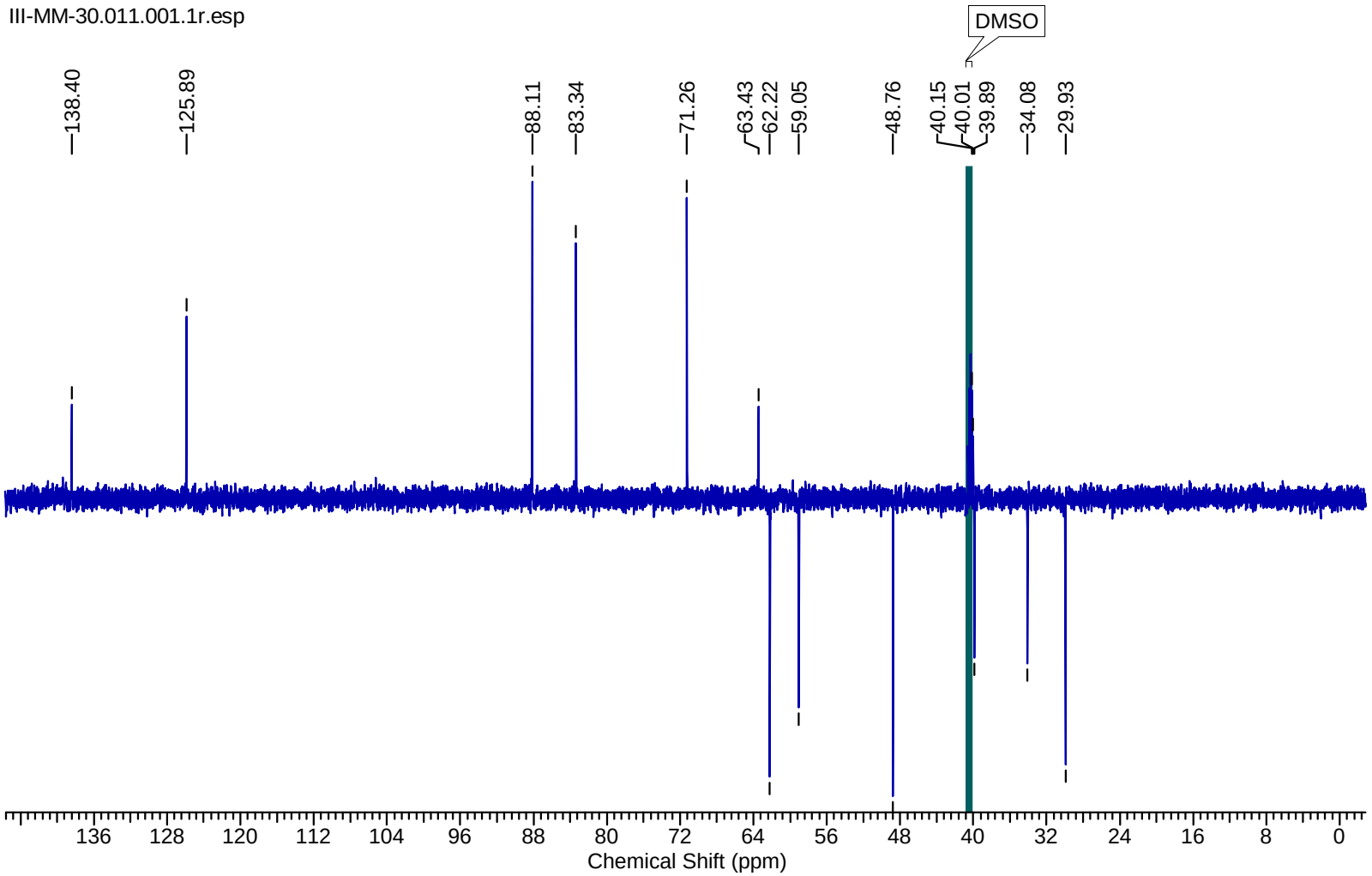


Figure S82. DEPT-135 spectrum of compound **26**.

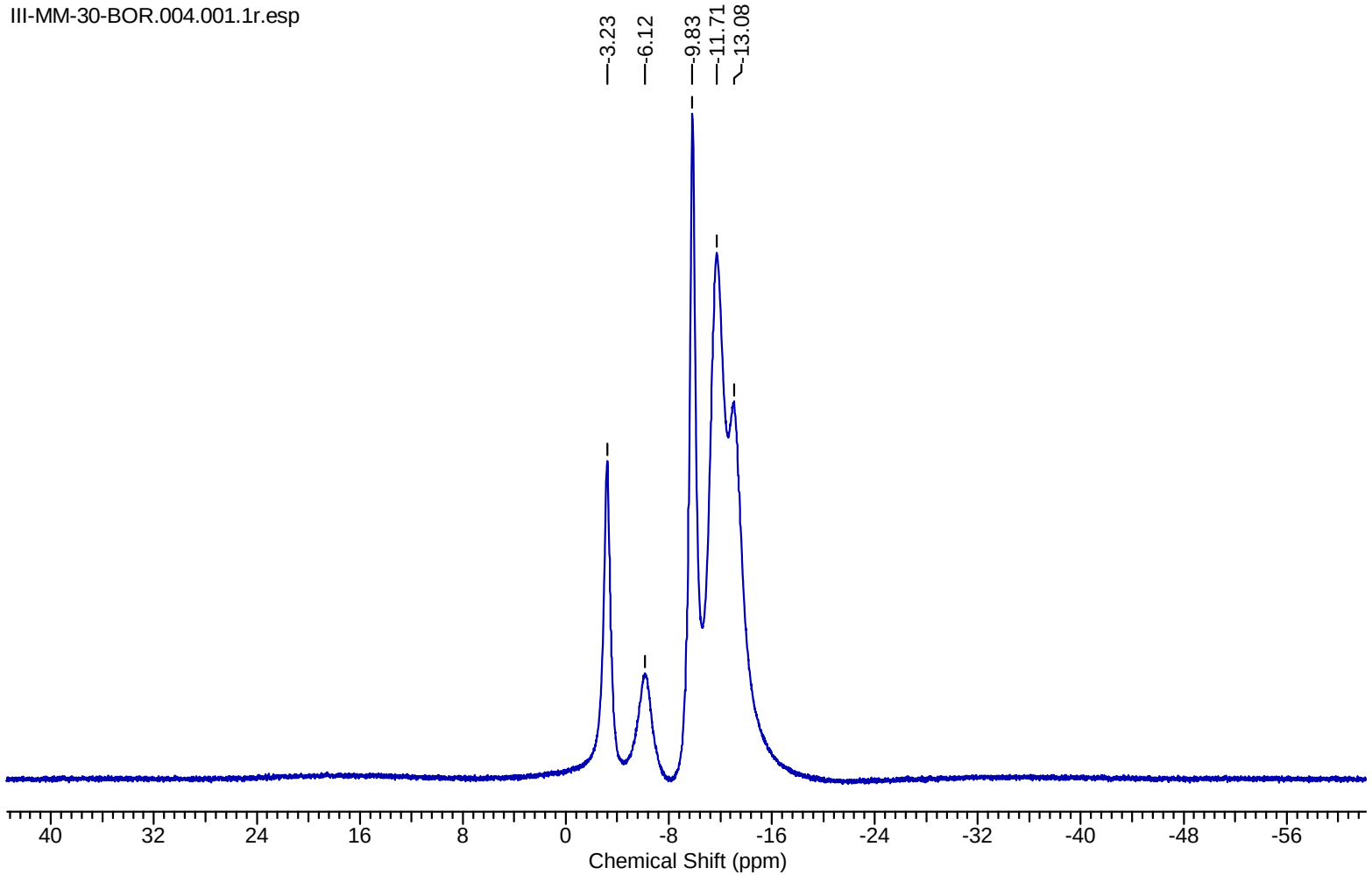


Figure S83. $^{11}B\{^{1}H$ BB$\}$ NMR spectrum of compound **26**.

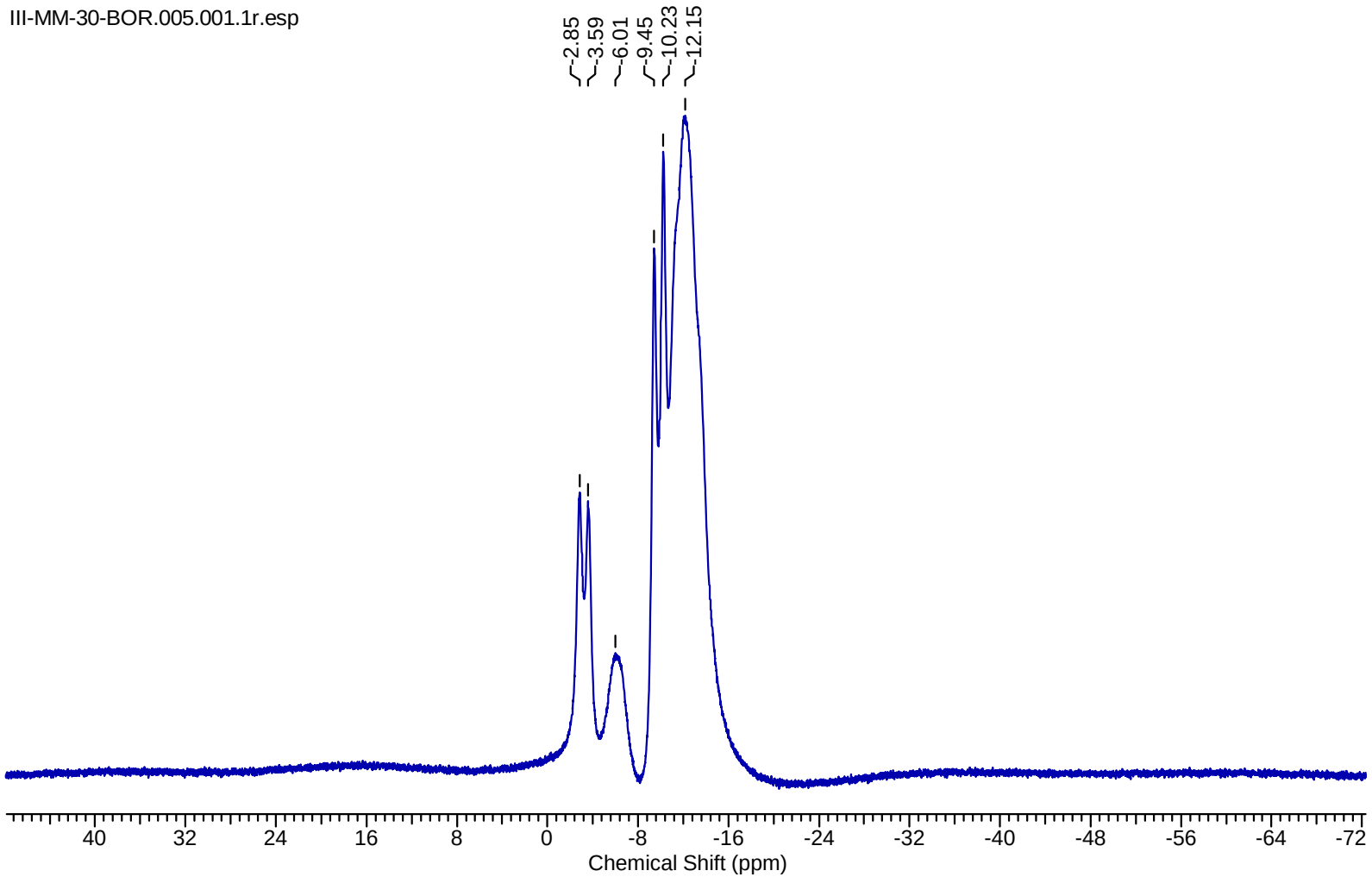


Figure S84. ^{11}B NMR spectrum of compound **26**.

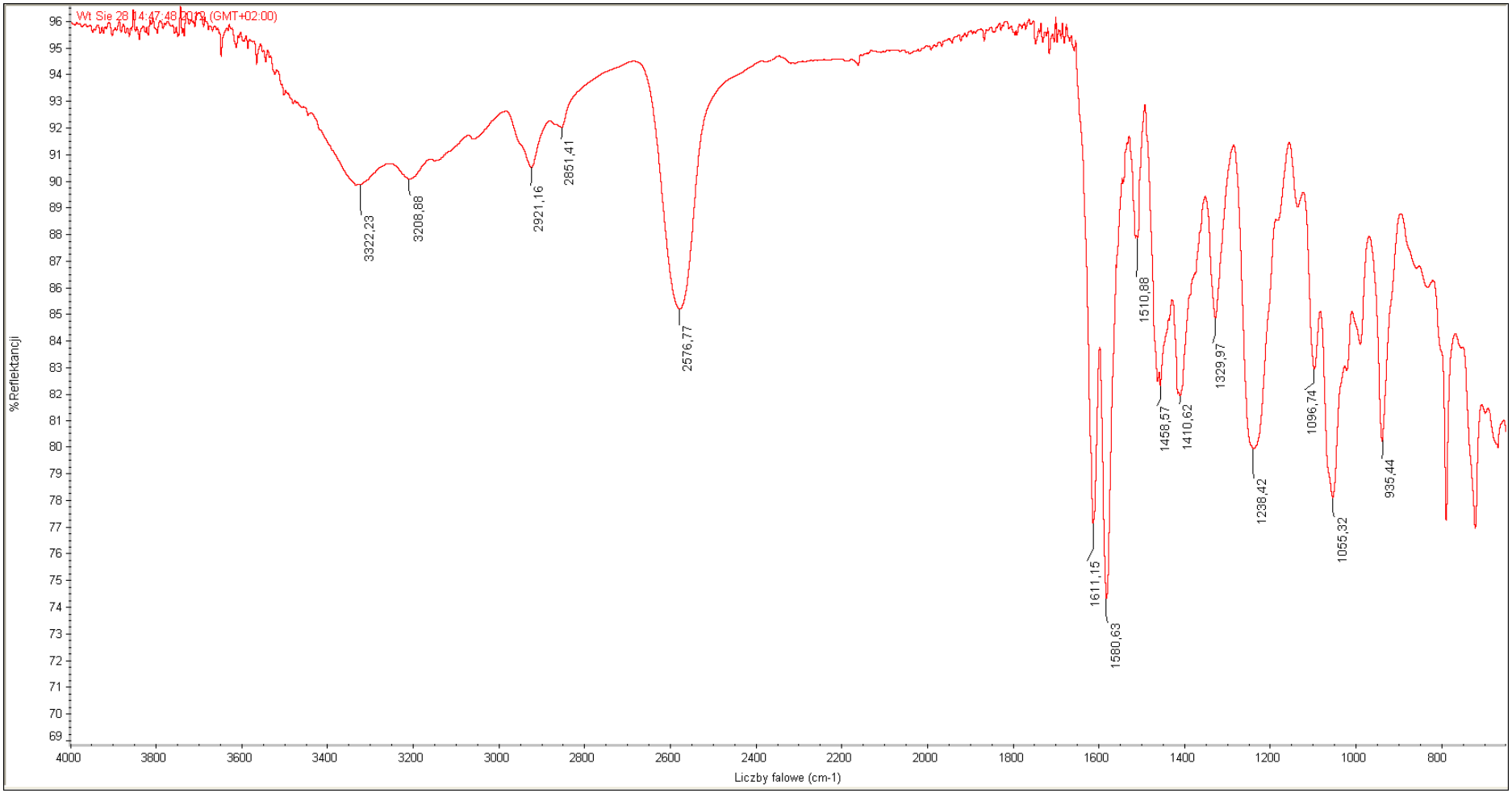


Figure S85. IR spectrum of compound **26**.

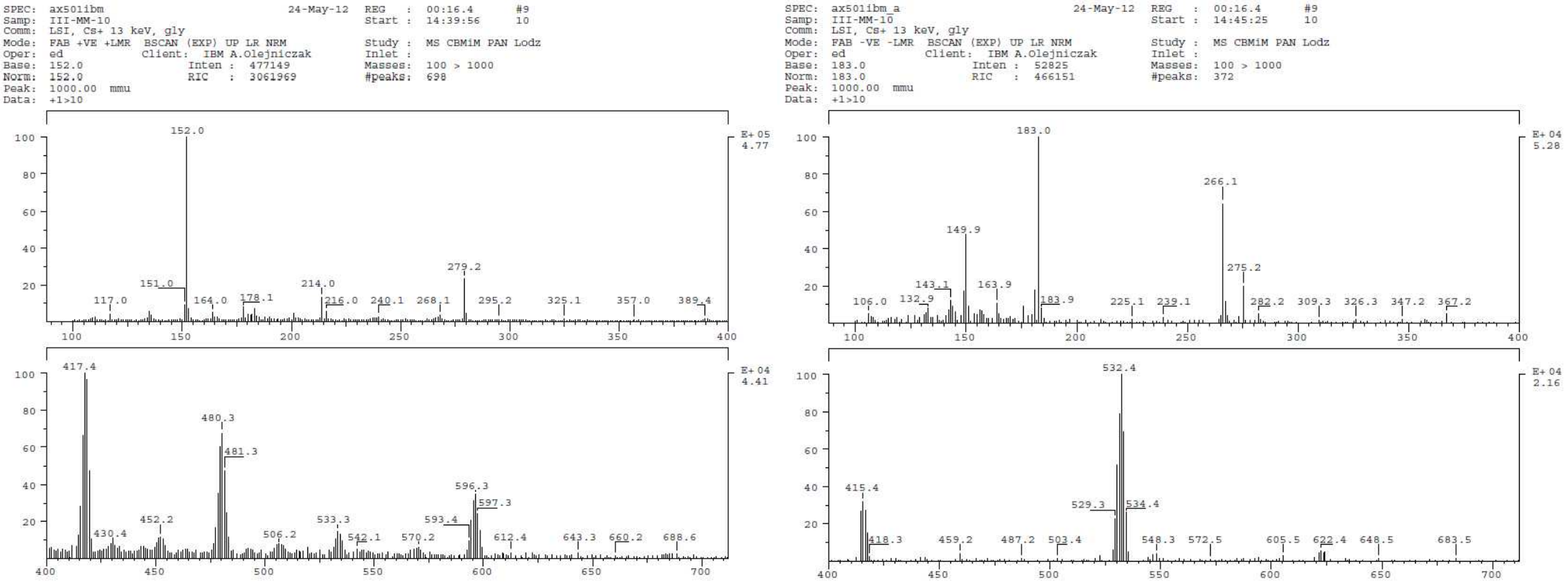


Figure S86. MS-FAB spectra of compound **26**.

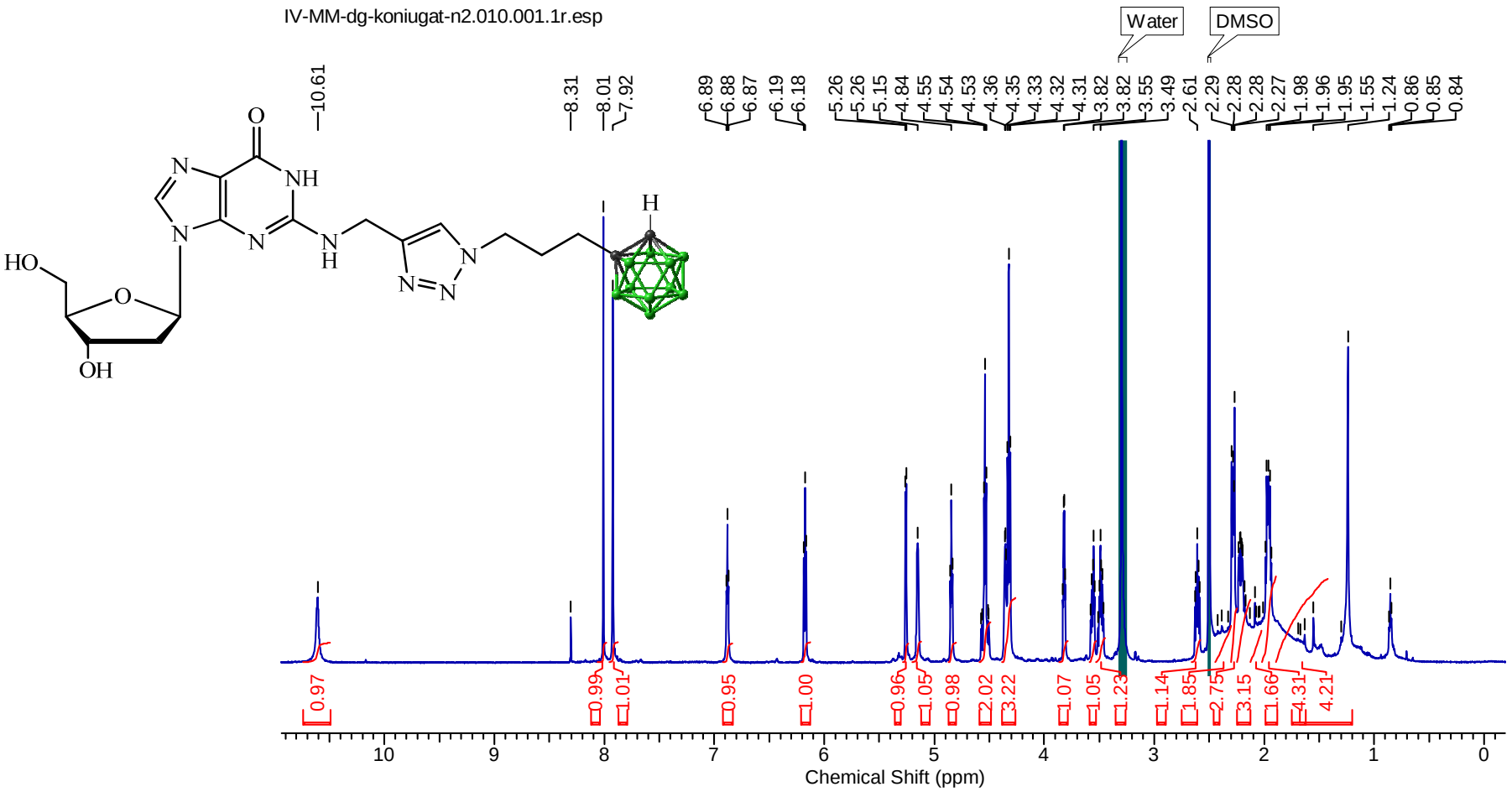


Figure S87. ^{1}H NMR spectrum of compound **27**.

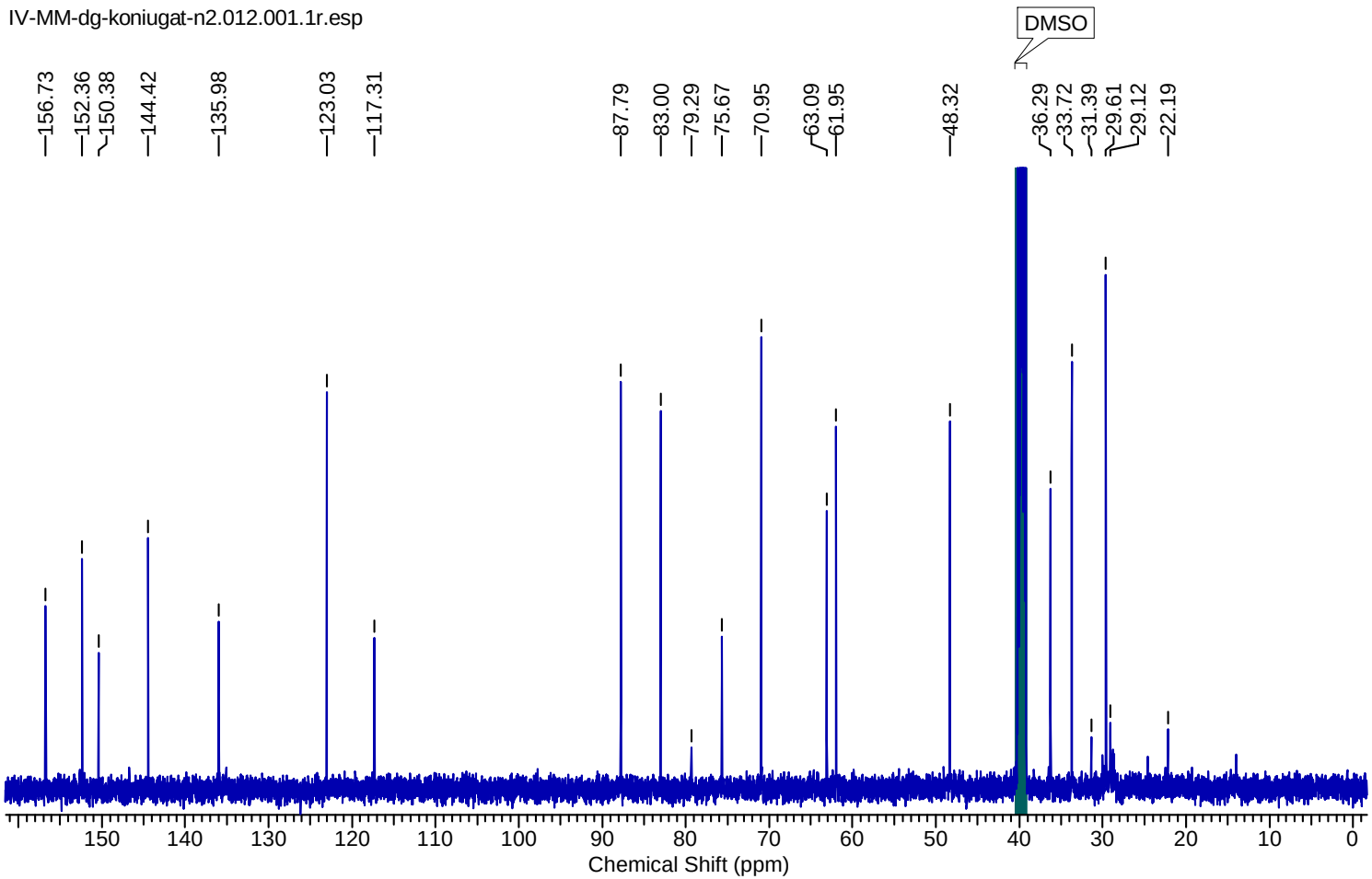


Figure S88. ^{13}C NMR spectrum of compound **27**.

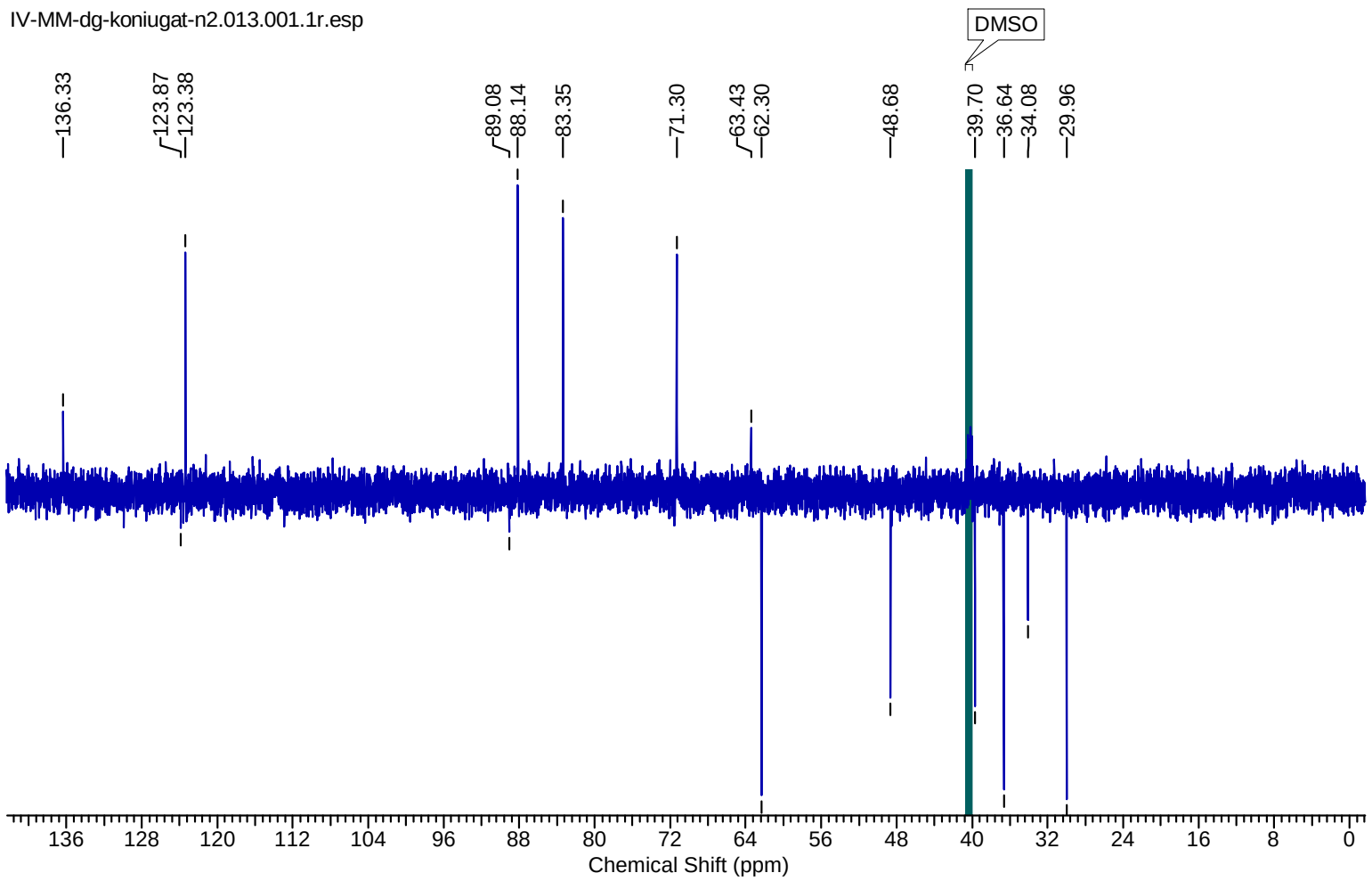


Figure S89. DEPT-135 spectrum of compound **27**.

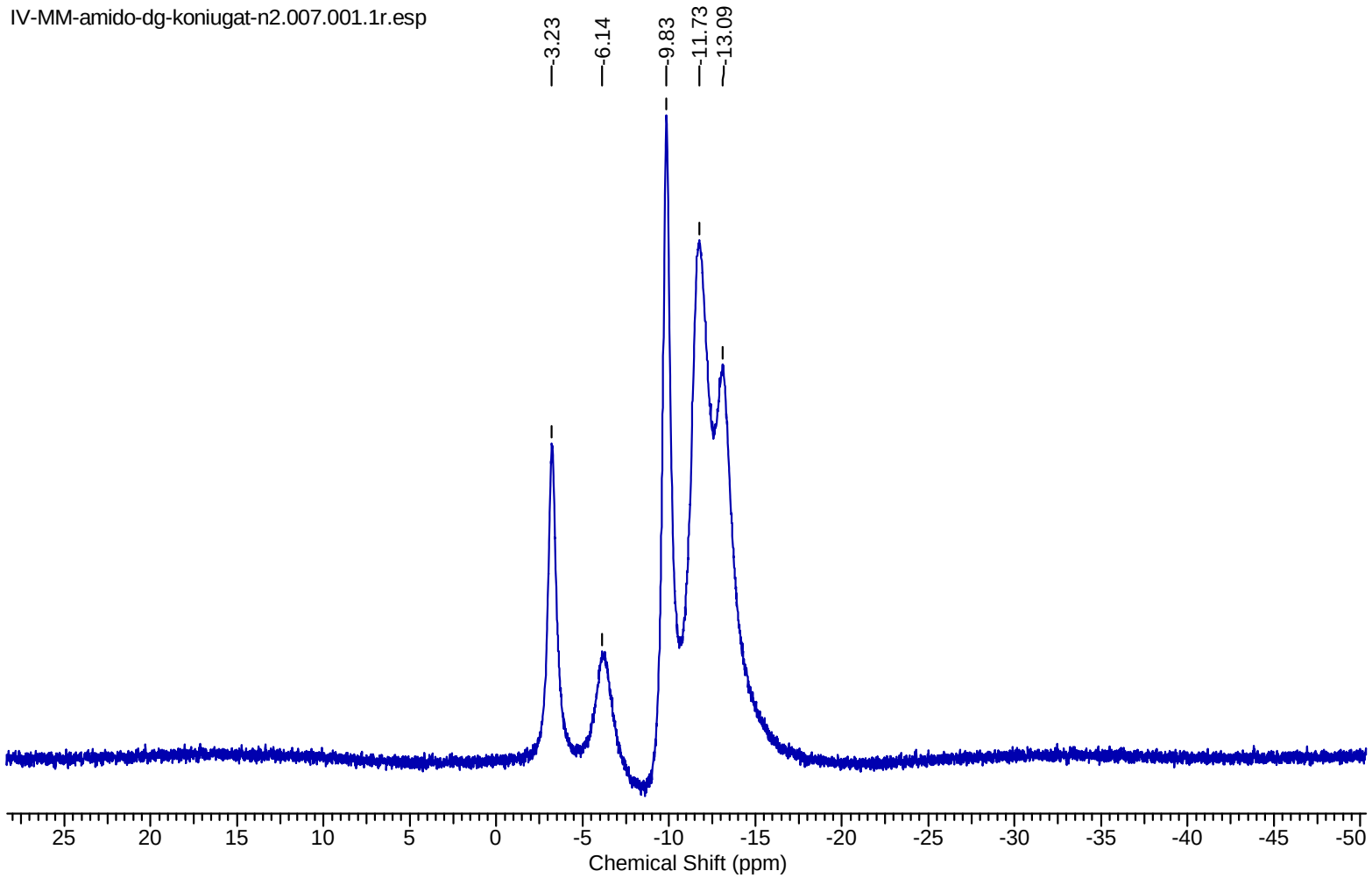


Figure S90. $^{11}B\{^{1}H$ BB$\}$ NMR spectrum of compound **27**.

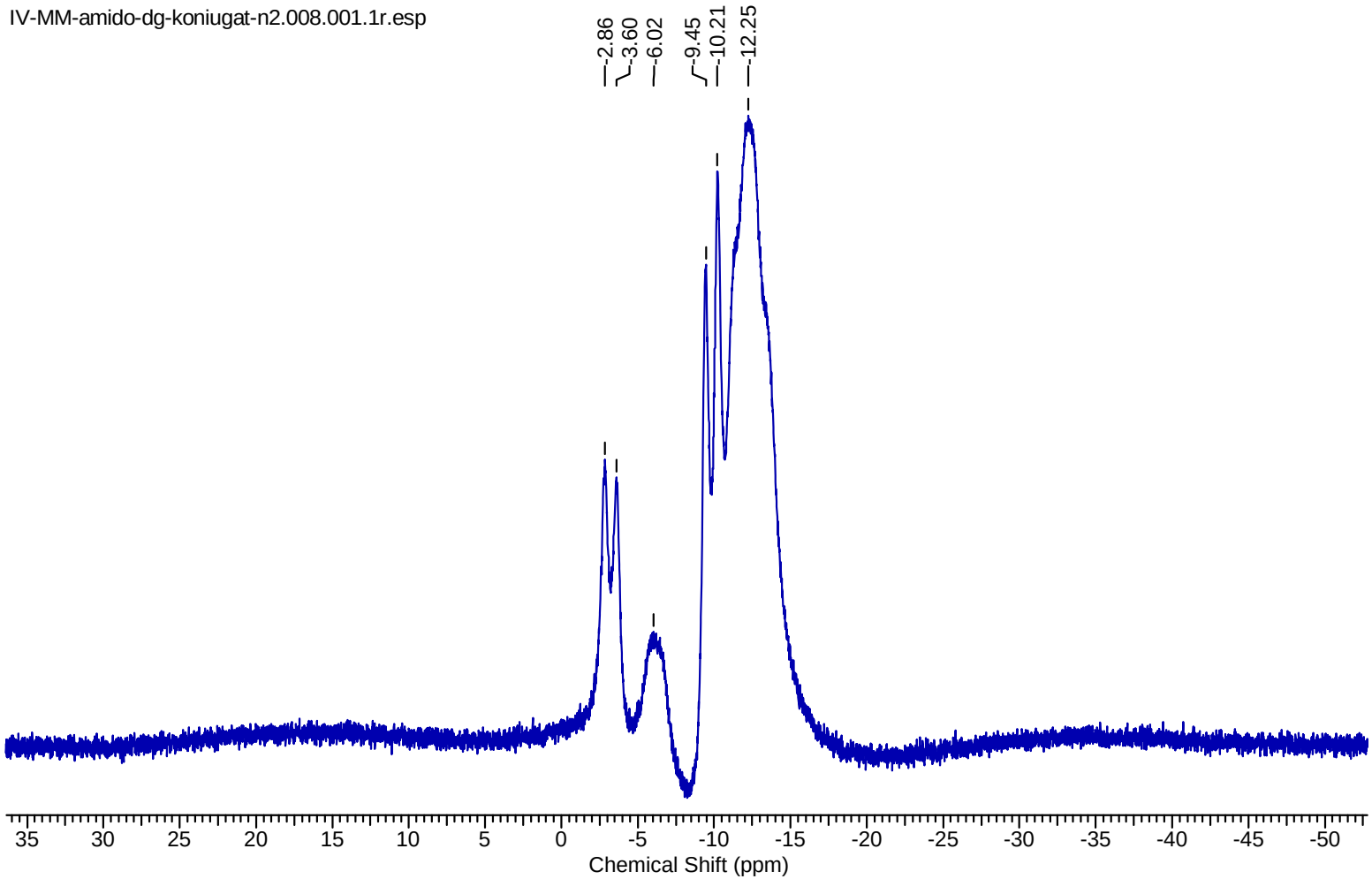


Figure S91. ^{11}B NMR spectrum of compound **27**.

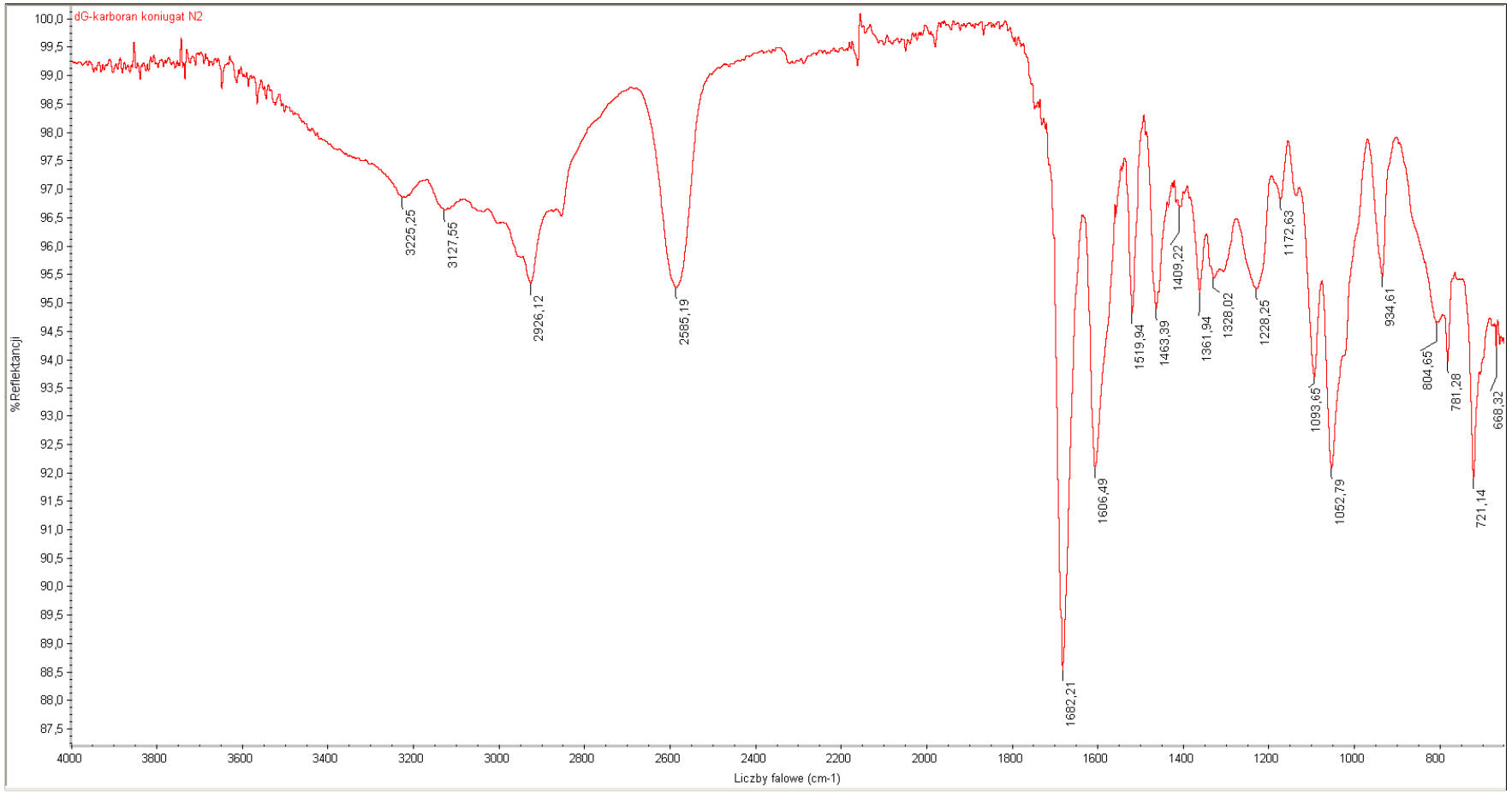


Figure S92. IR spectrum of compound **27**.

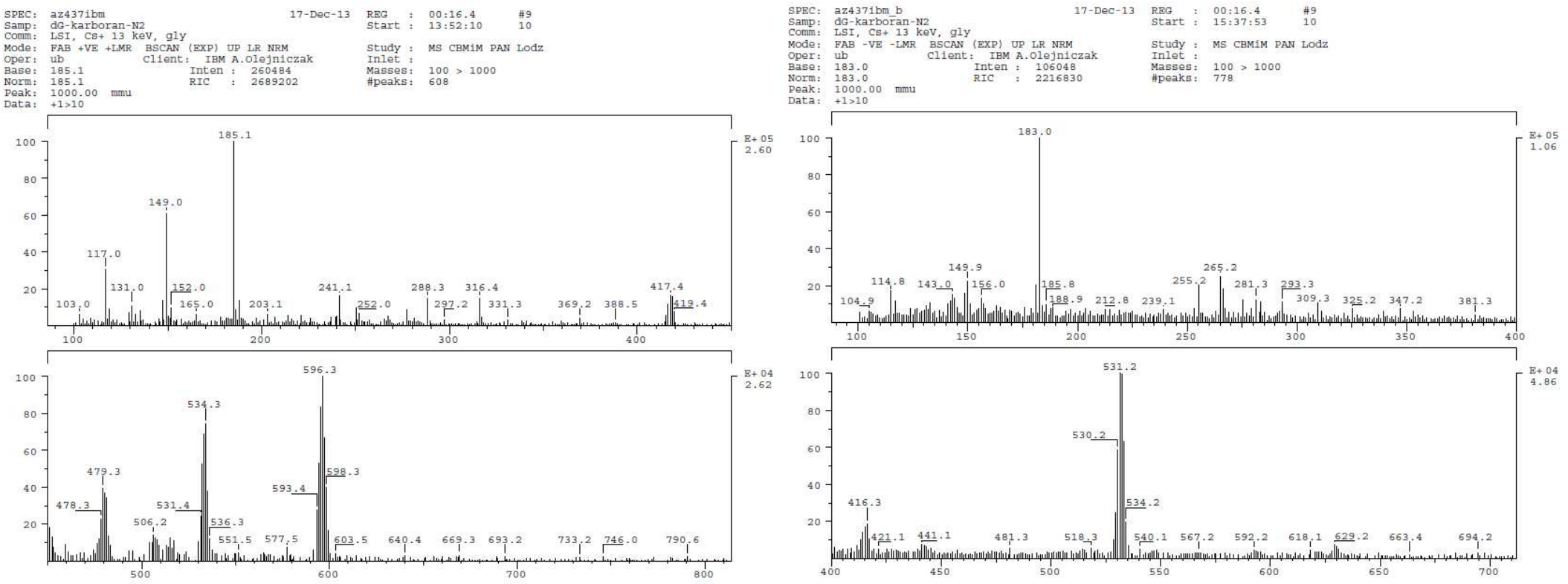


Figure S93. MS-FAB spectra of compound **27**.

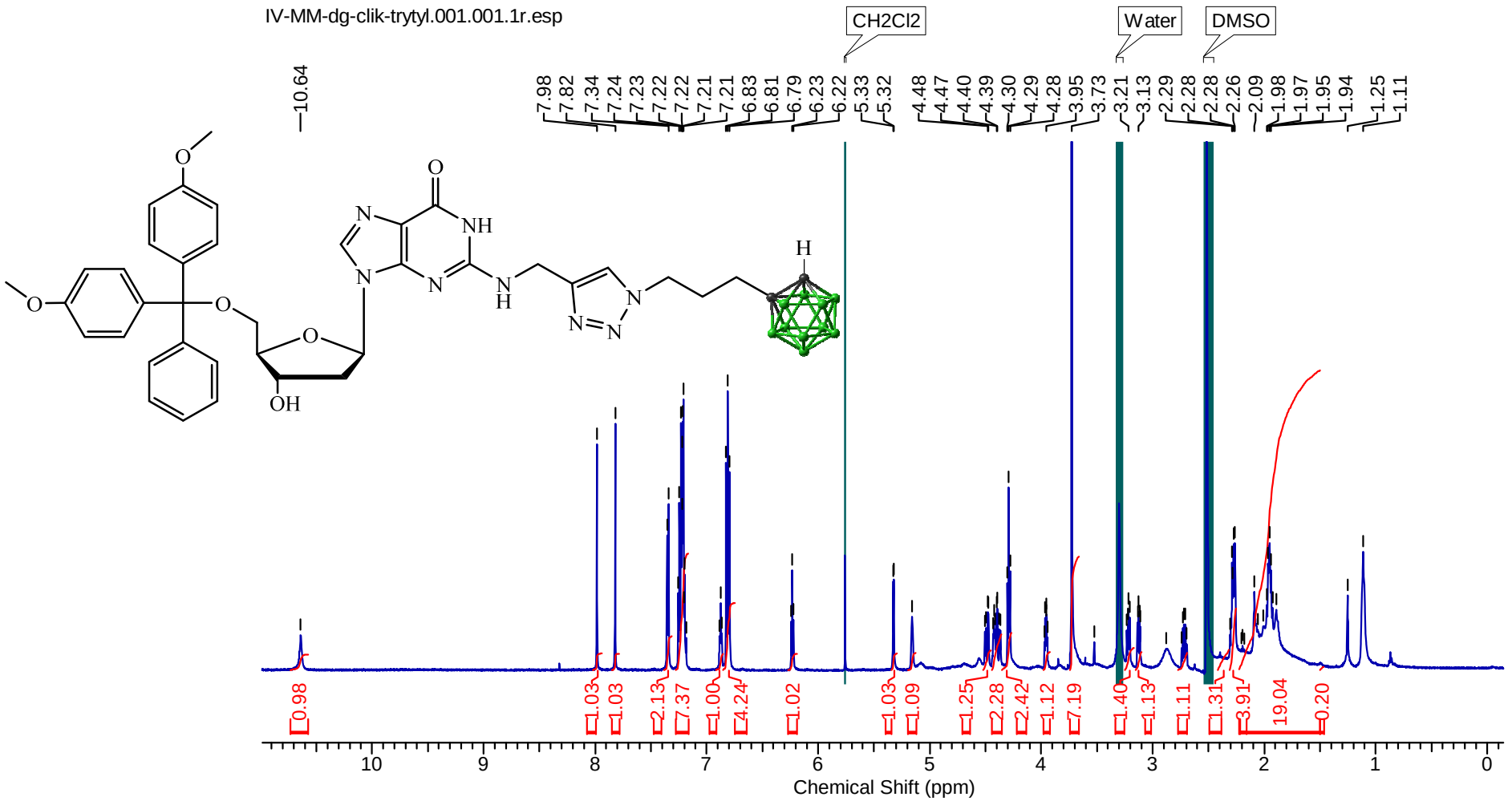


Figure S94. ^{1}H NMR spectrum of compound **28**.

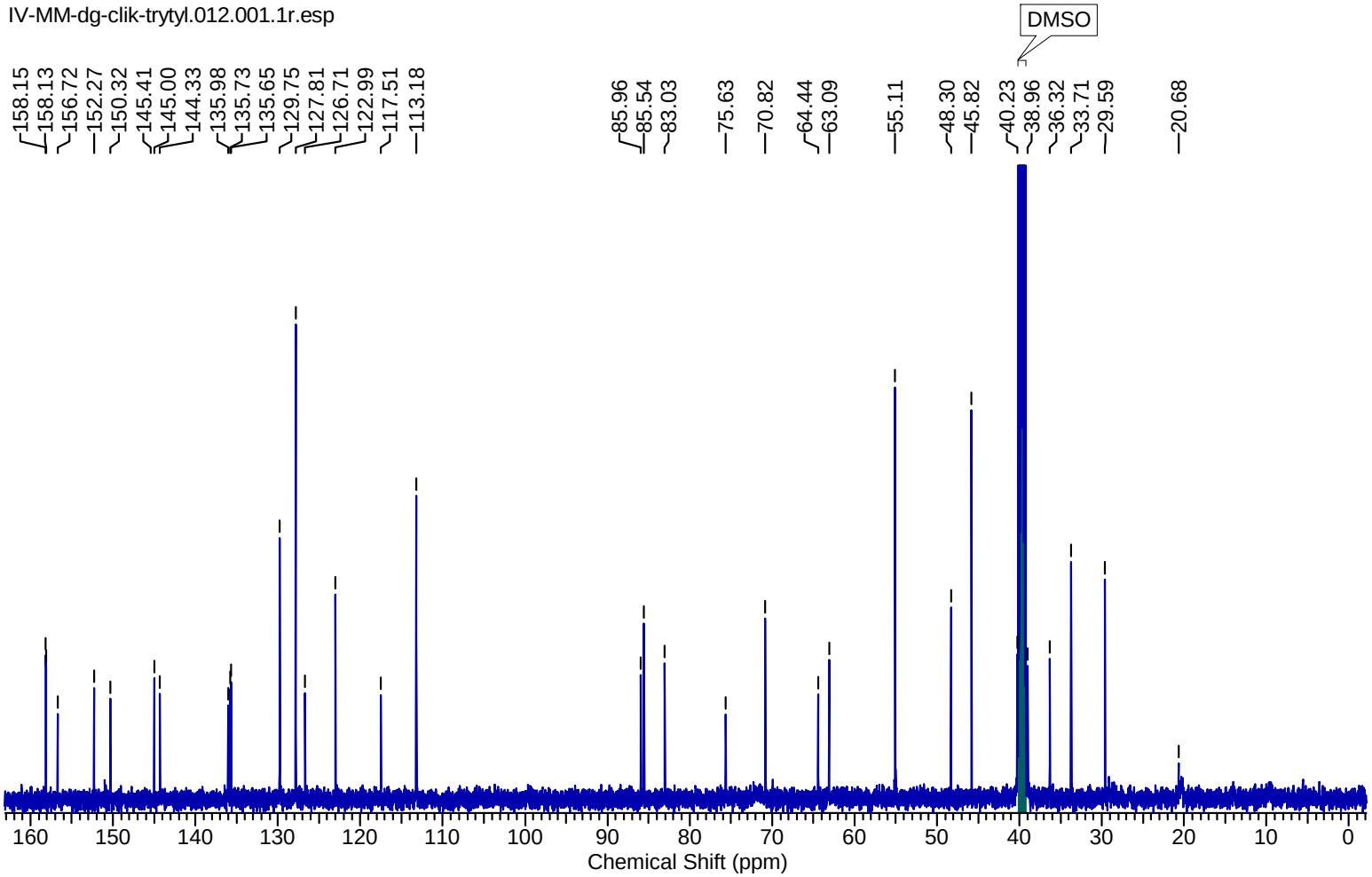


Figure S95. ^{13}C NMR spectrum of compound **28**.

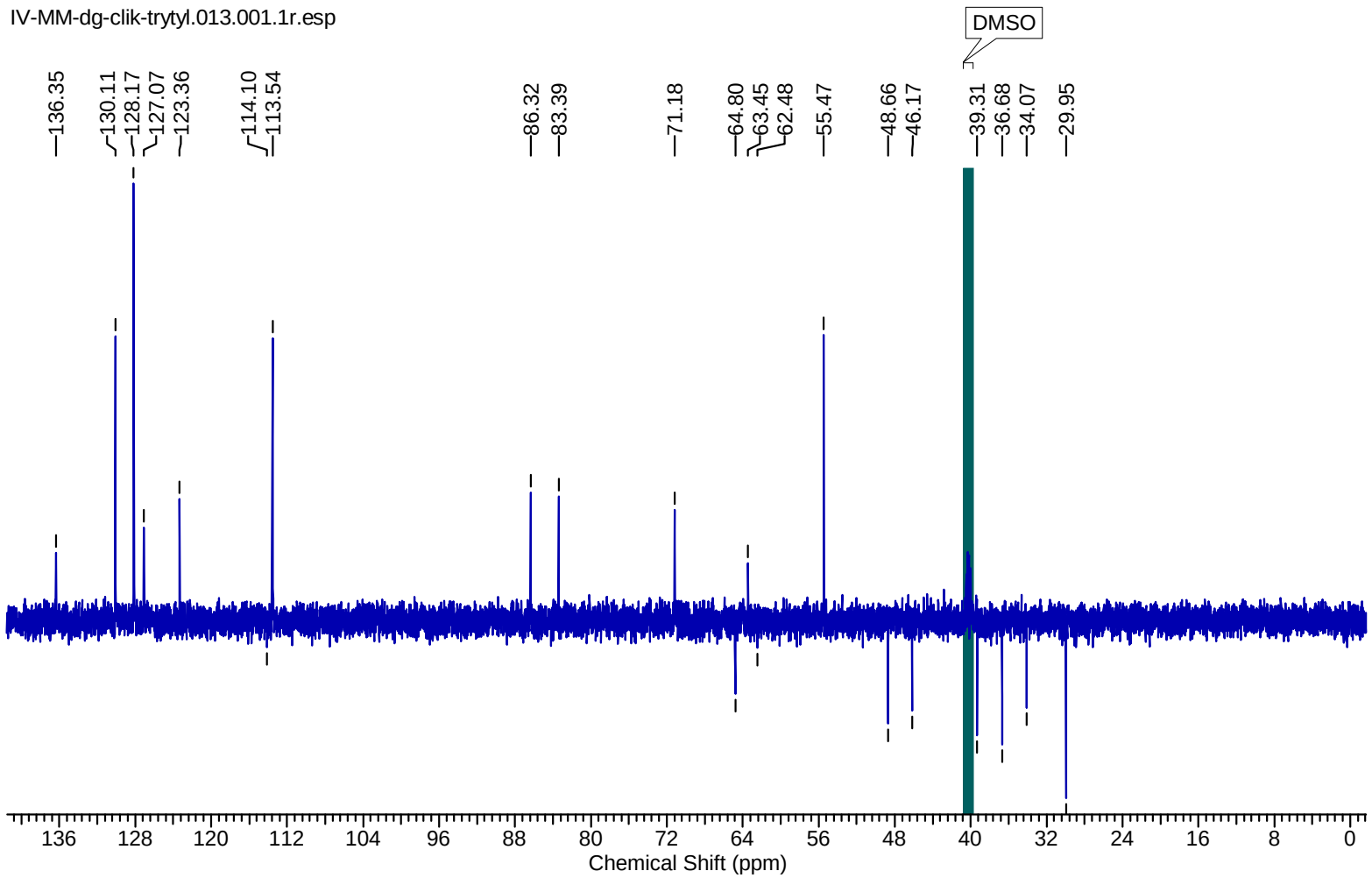


Figure S96. DEPT-135 spectrum of compound **28**.

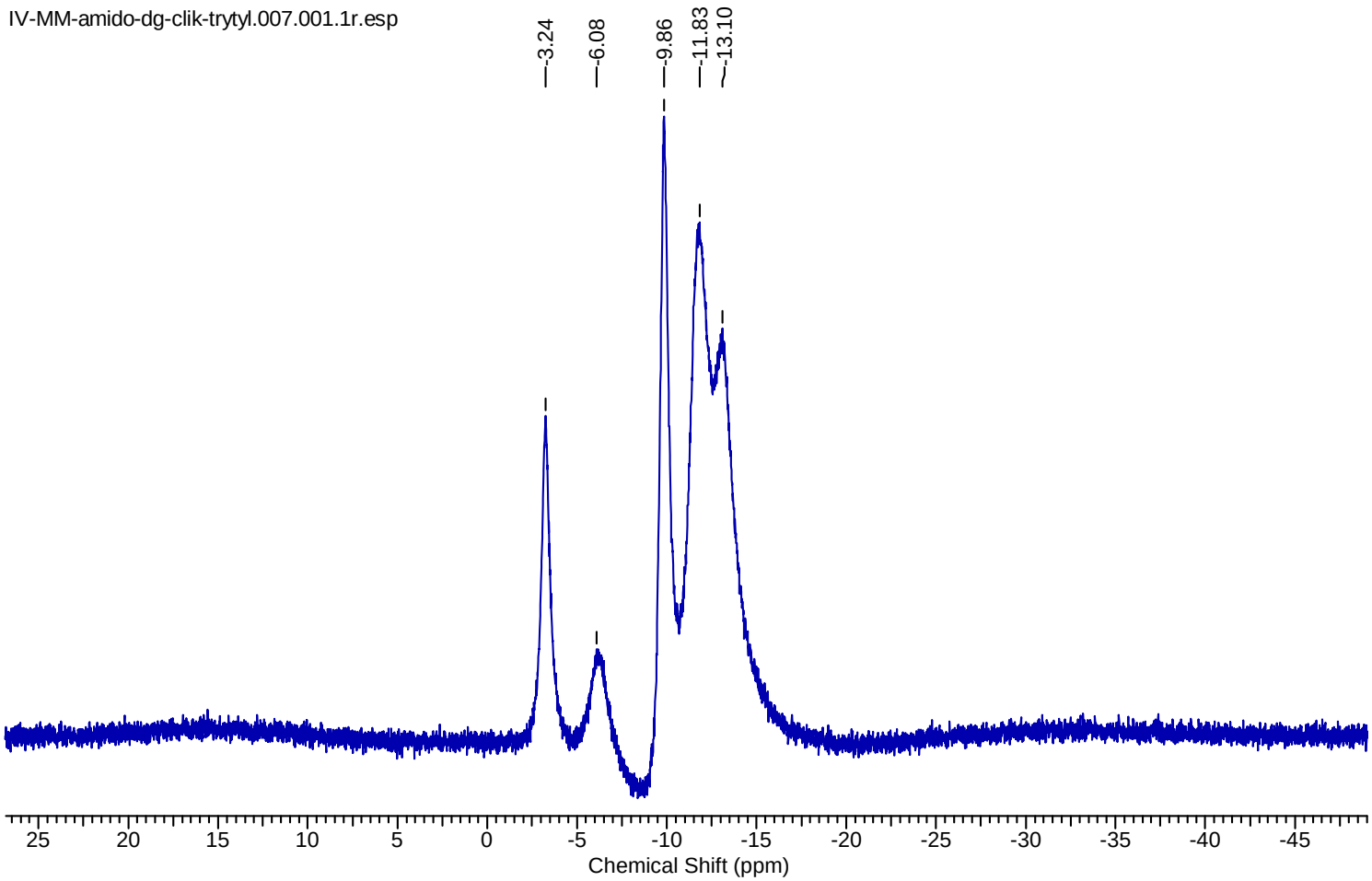


Figure S97. $^{11}B\{^{1}H$ BB$\}$ NMR spectrum of compound **28**.

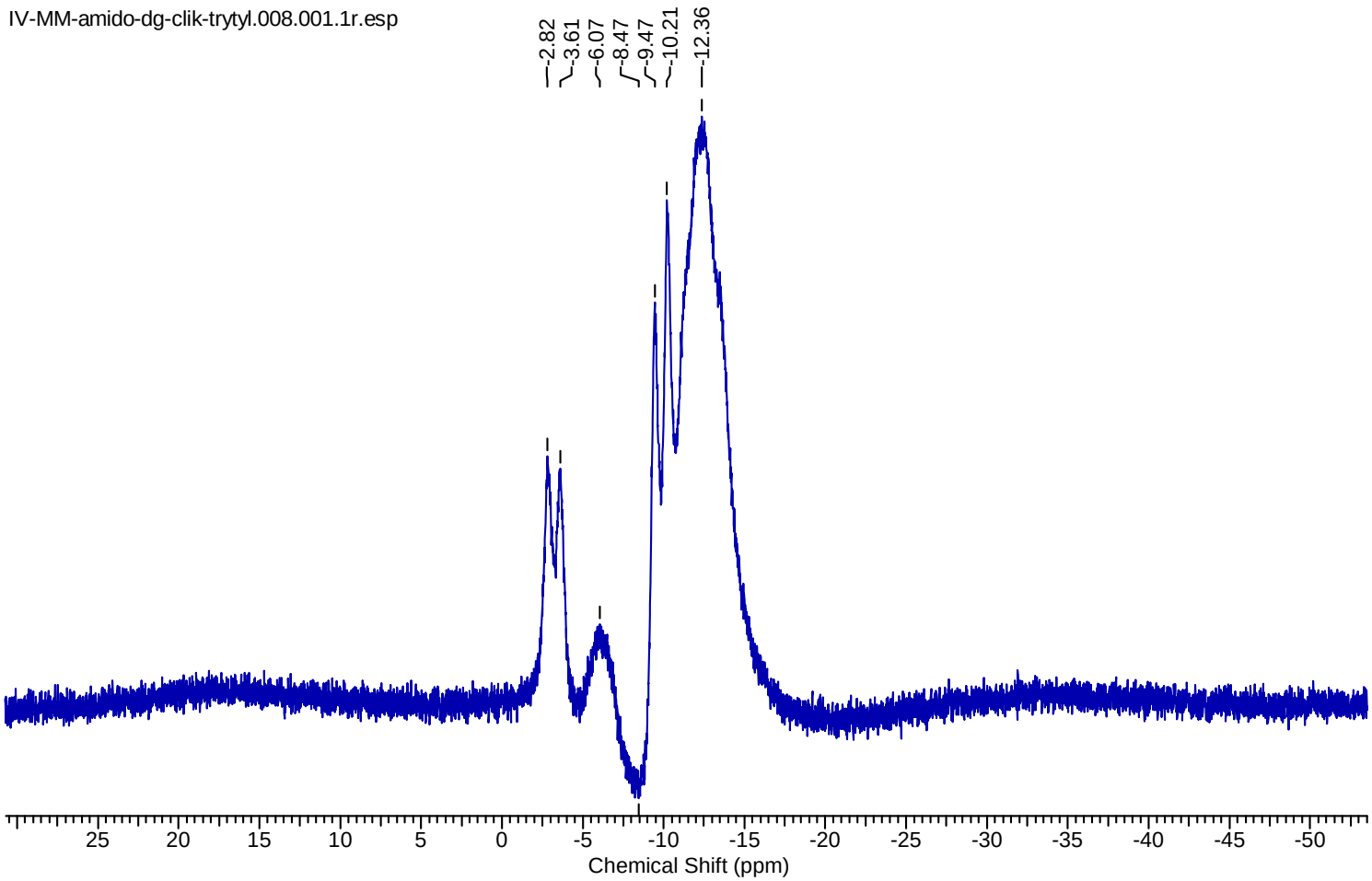


Figure S98. ^{11}B NMR spectrum of compound **28**.

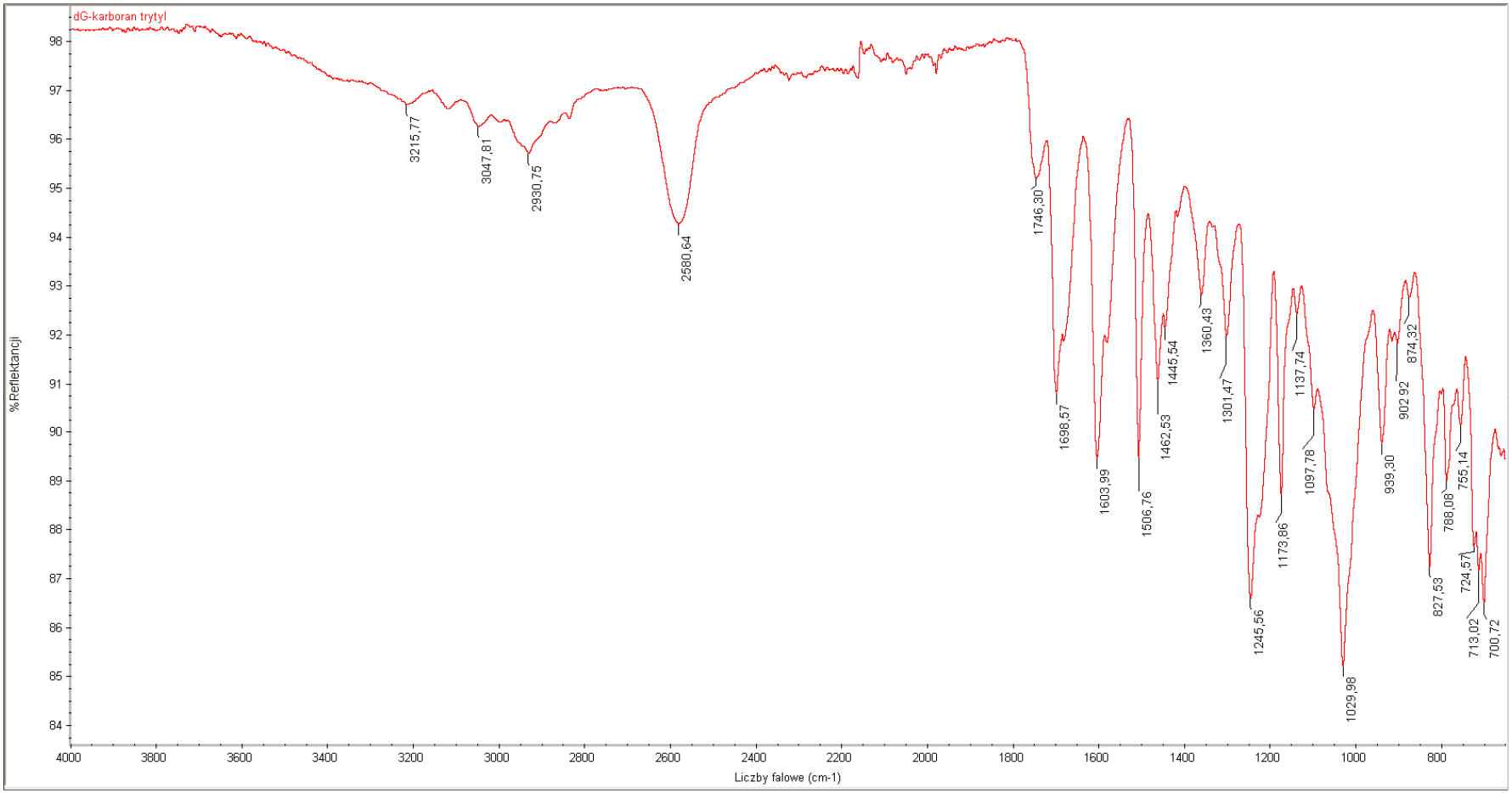


Figure S99. IR spectrum of compound **28**.

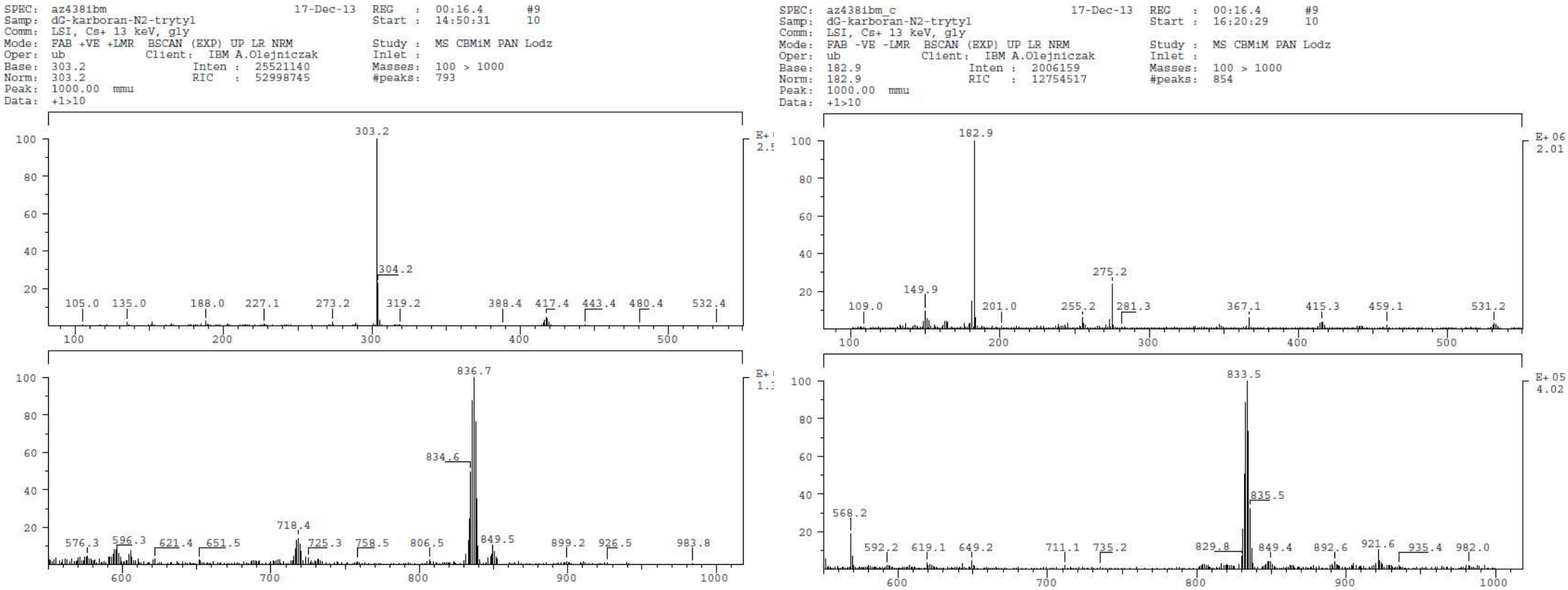


Figure S100. MS-FAB spectra of compound **28**.

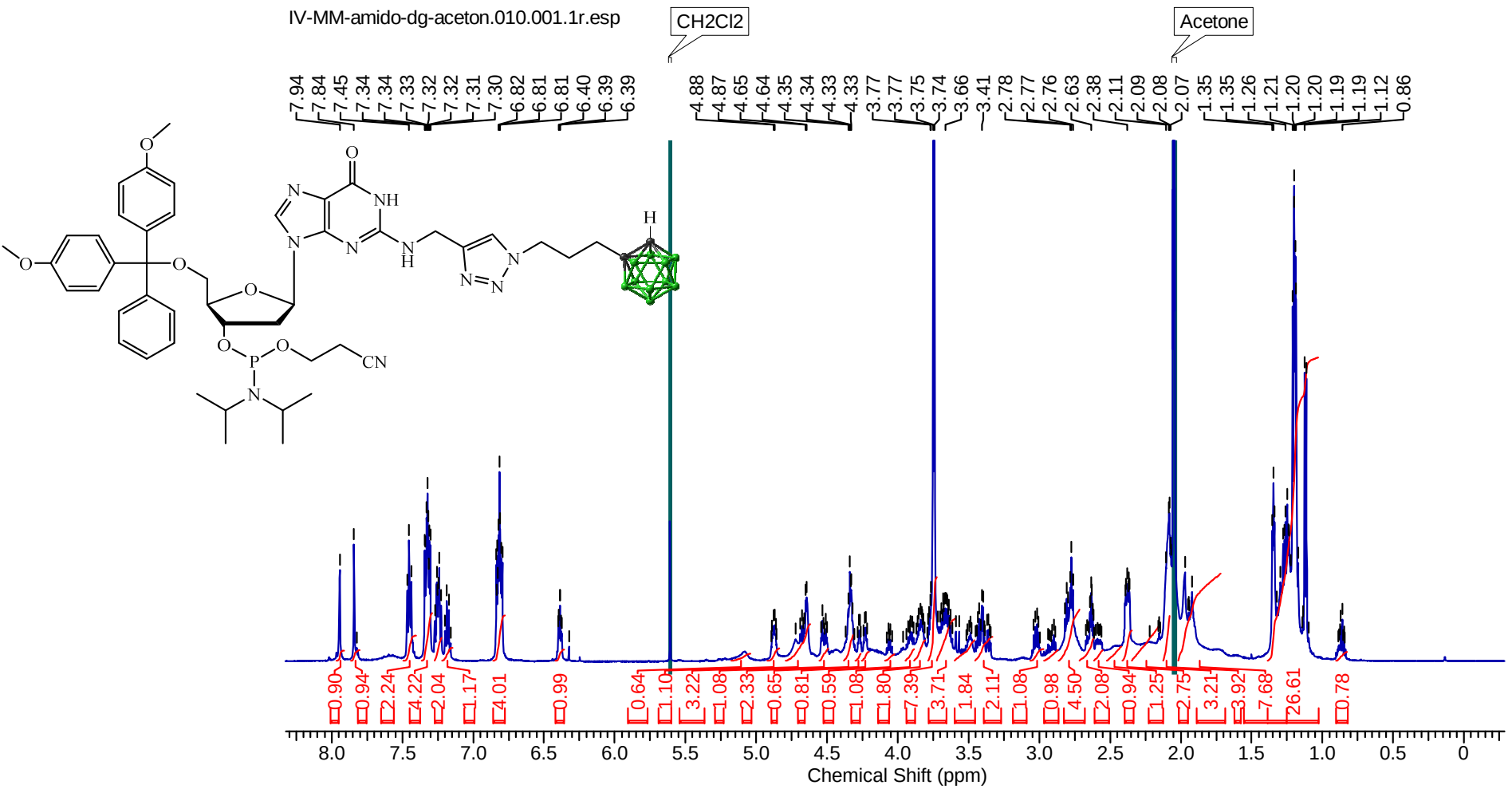


Figure S101. ^{1}H NMR spectrum of compound **32**.

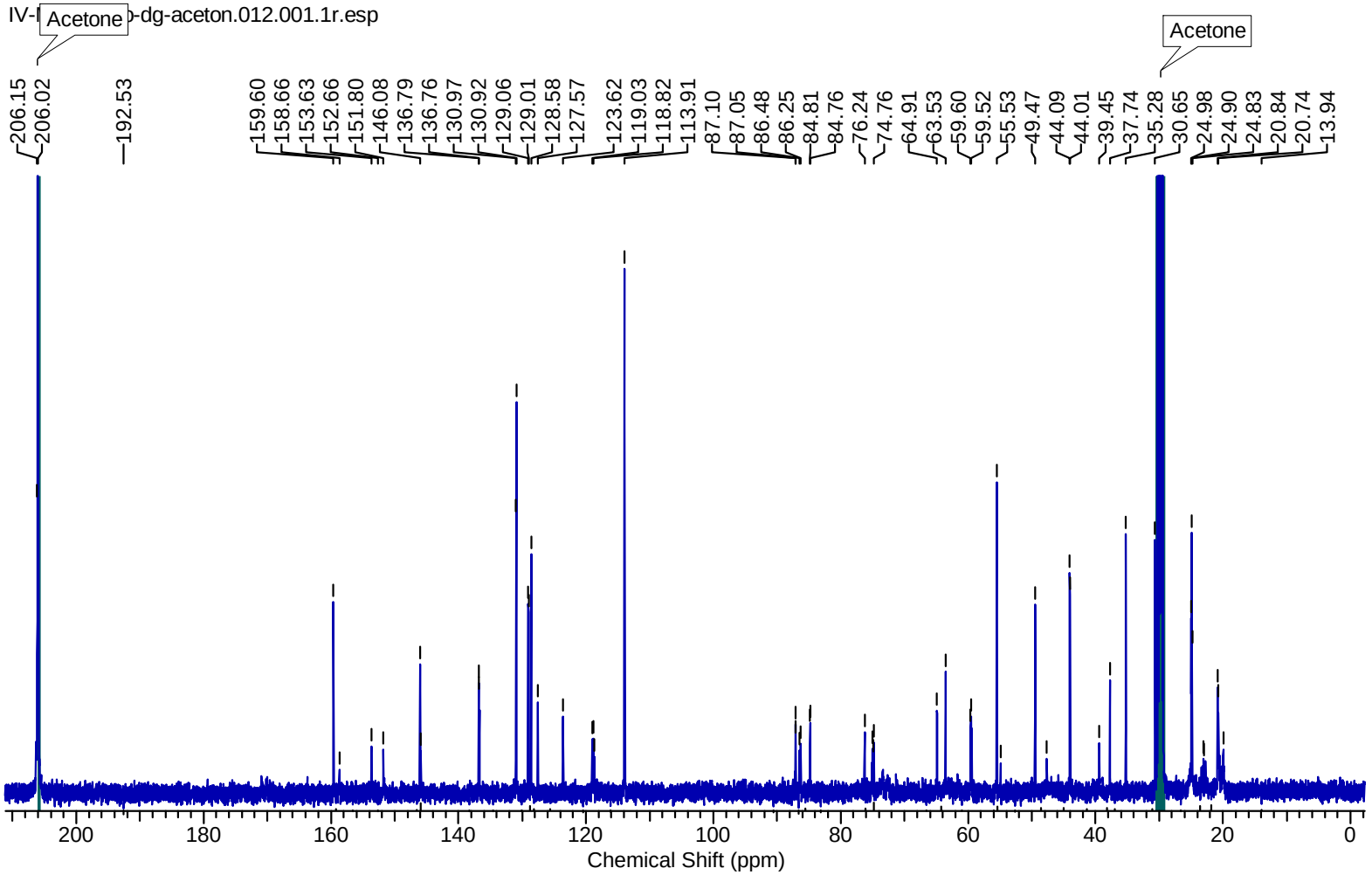


Figure S102. ^{13}C NMR spectrum of compound **32**.

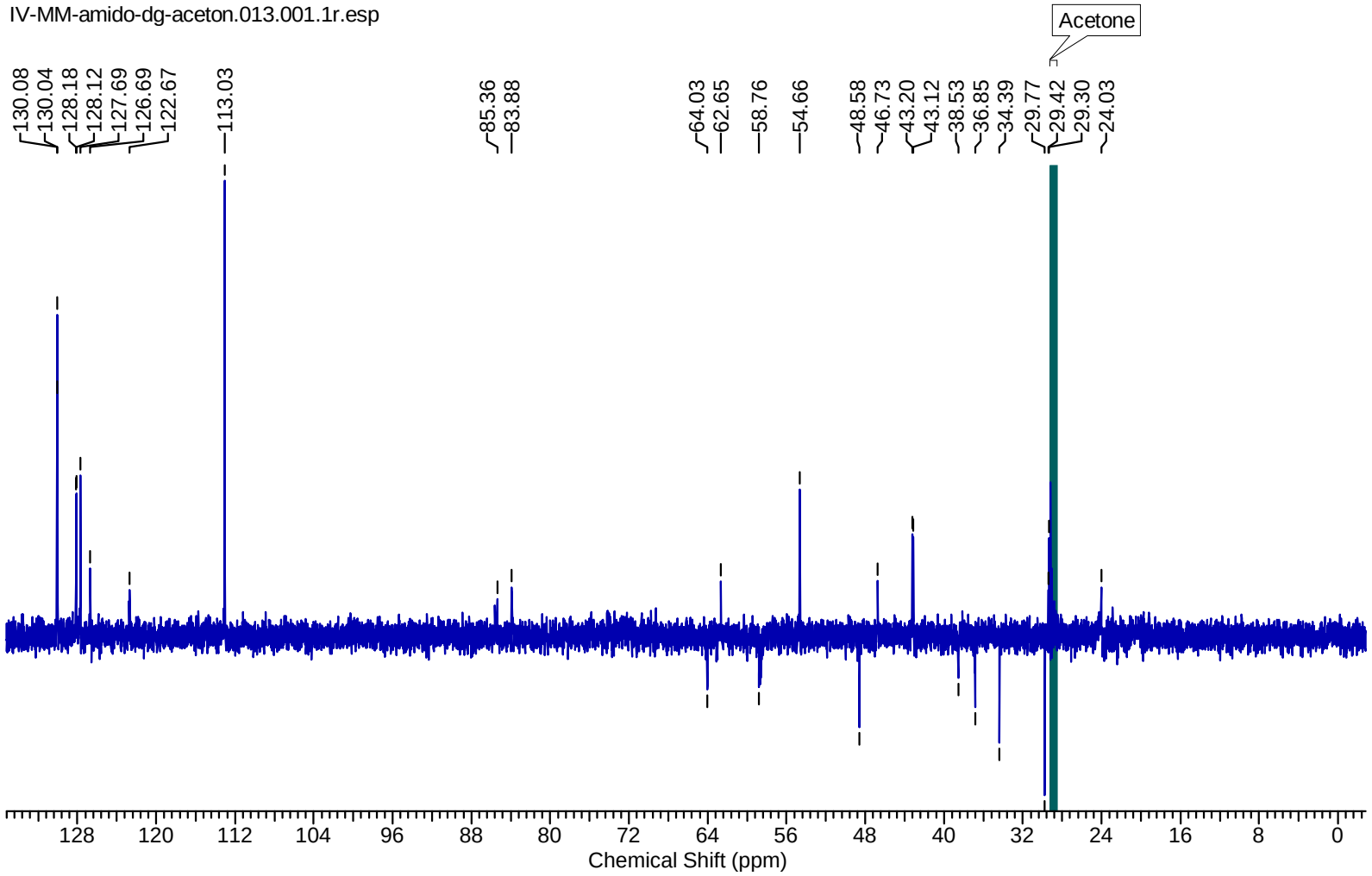


Figure S103. DEPT-135 spectrum of compound **32**.

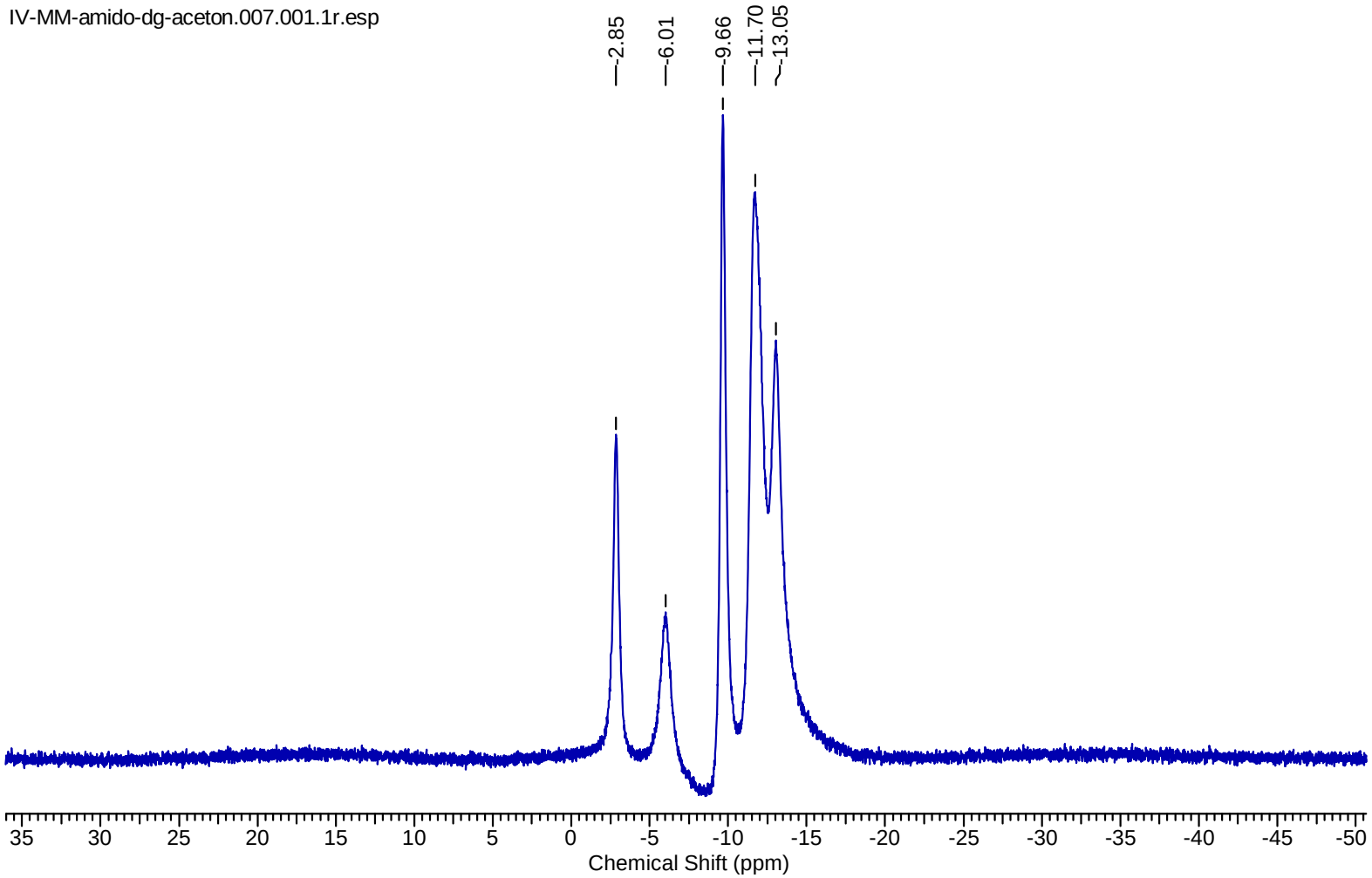


Figure S104. $^{11}B\{^{1}H\ BB\}$ NMR spectrum of compound **32**.

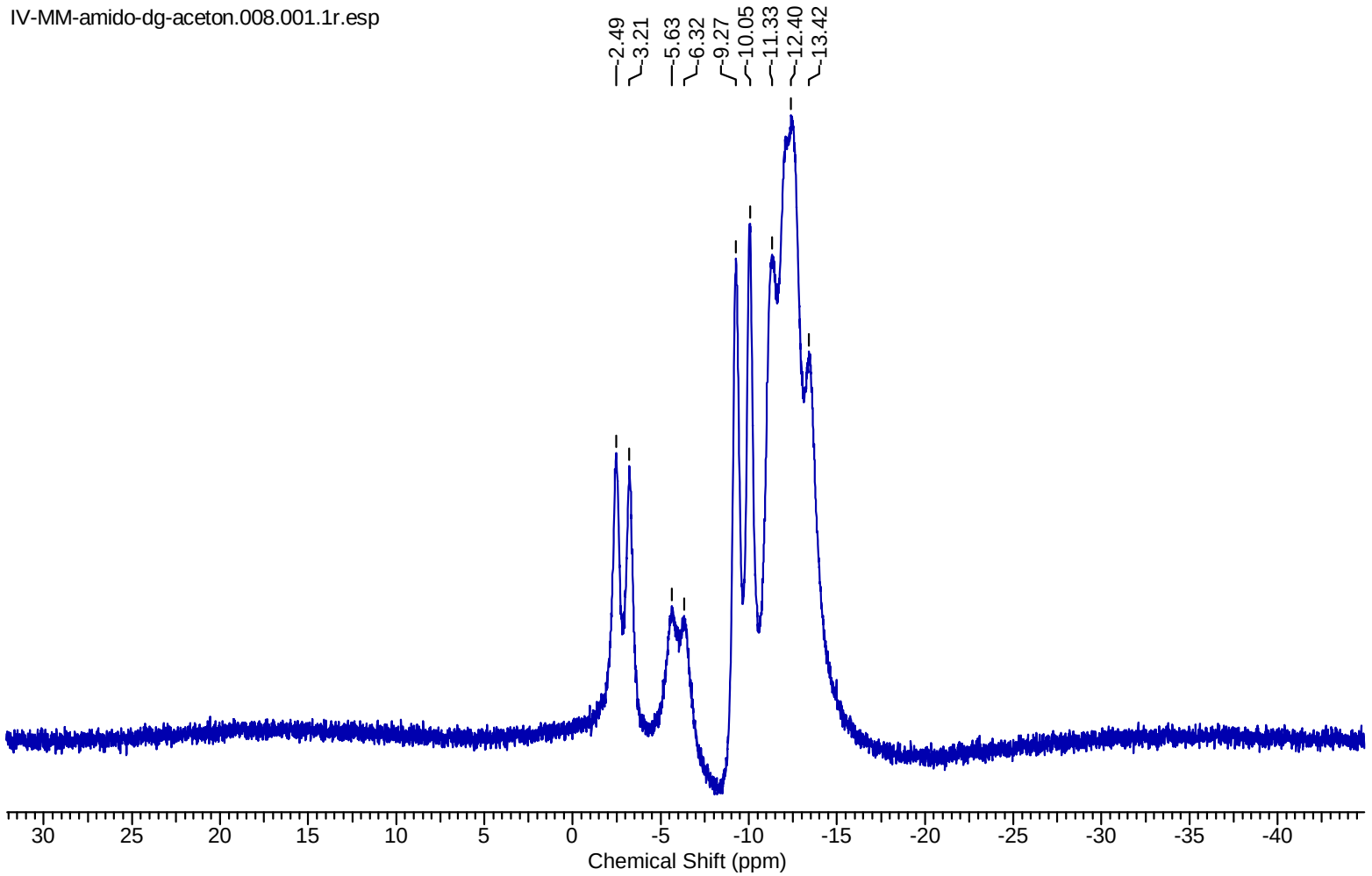


Figure S105. ^{11}B NMR spectrum of compound **32**.

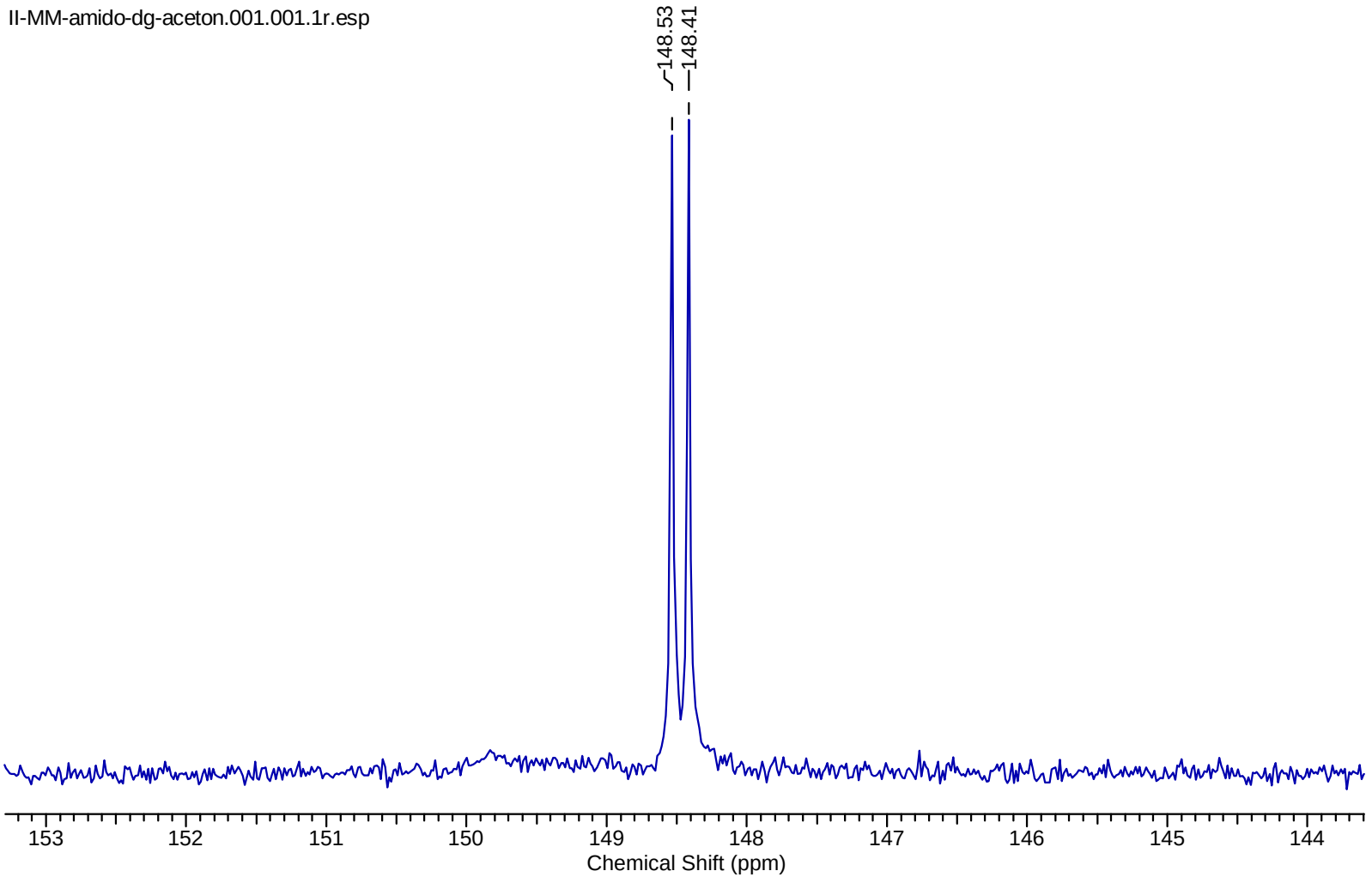


Figure S106. ^{31}P NMR spectrum of compound **32**.

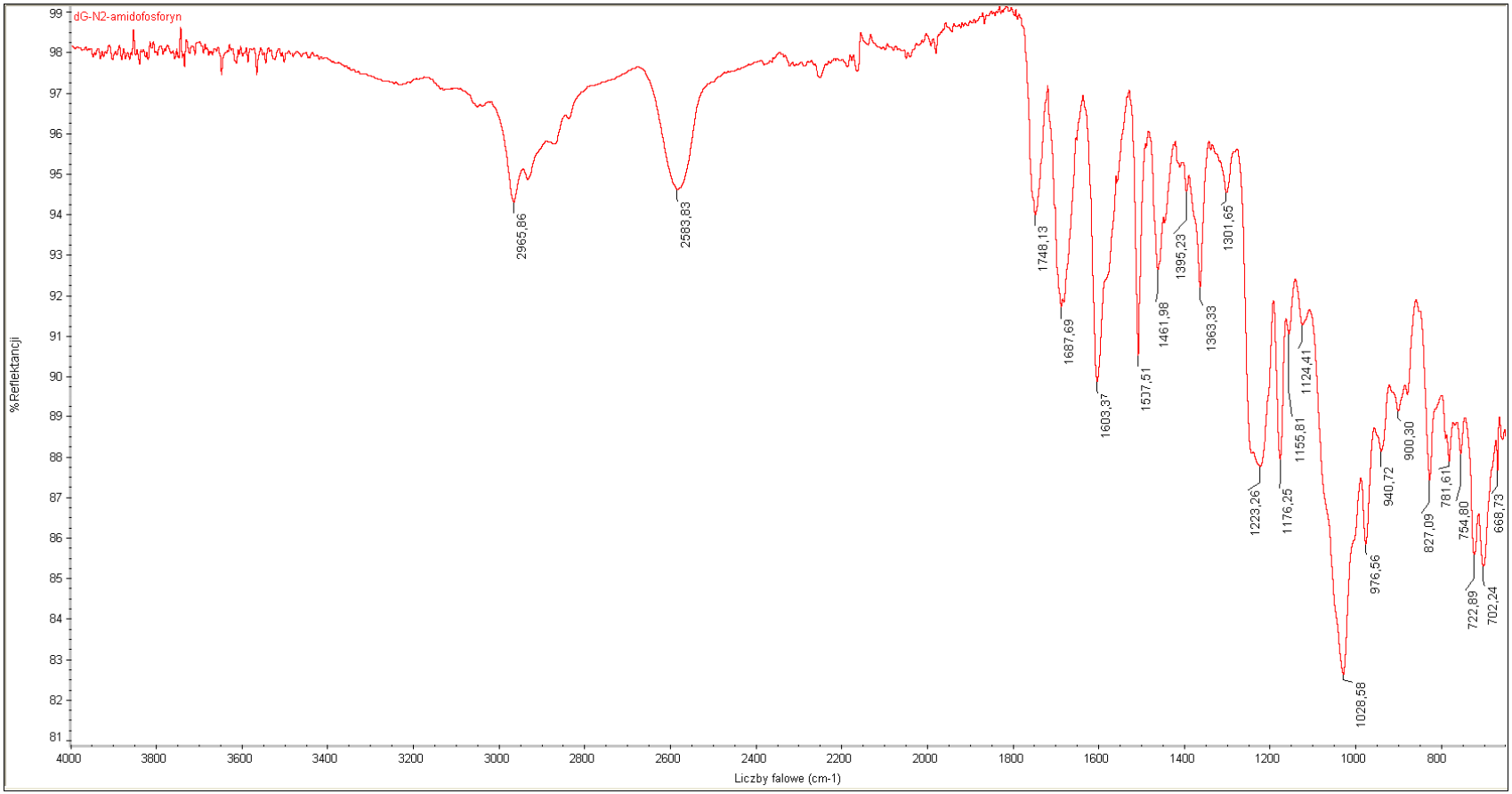
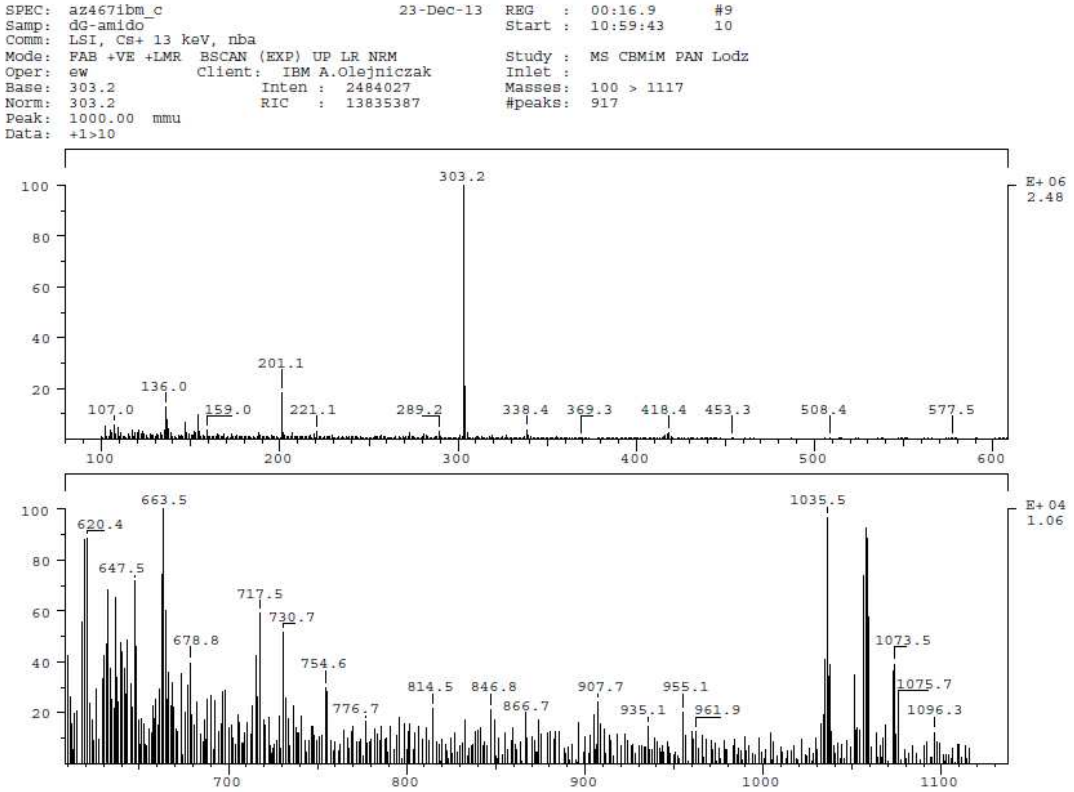


Figure S107. IR spectrum of compound **32**.



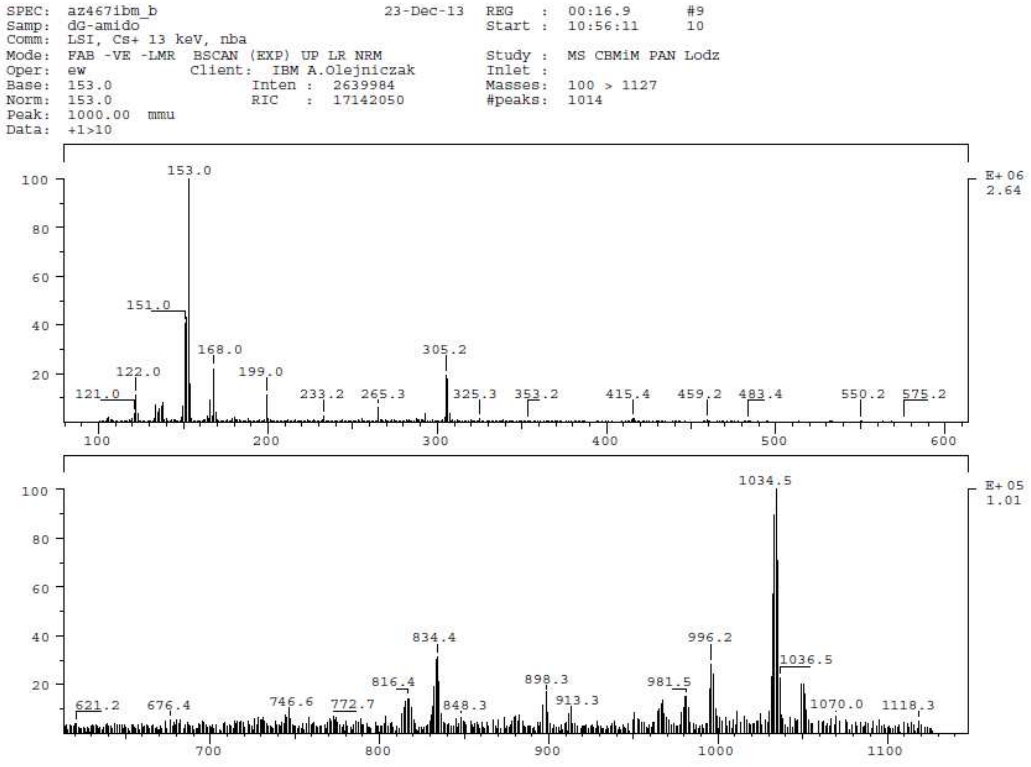


Figure S108. MS-FAB spectra of compound **32**.

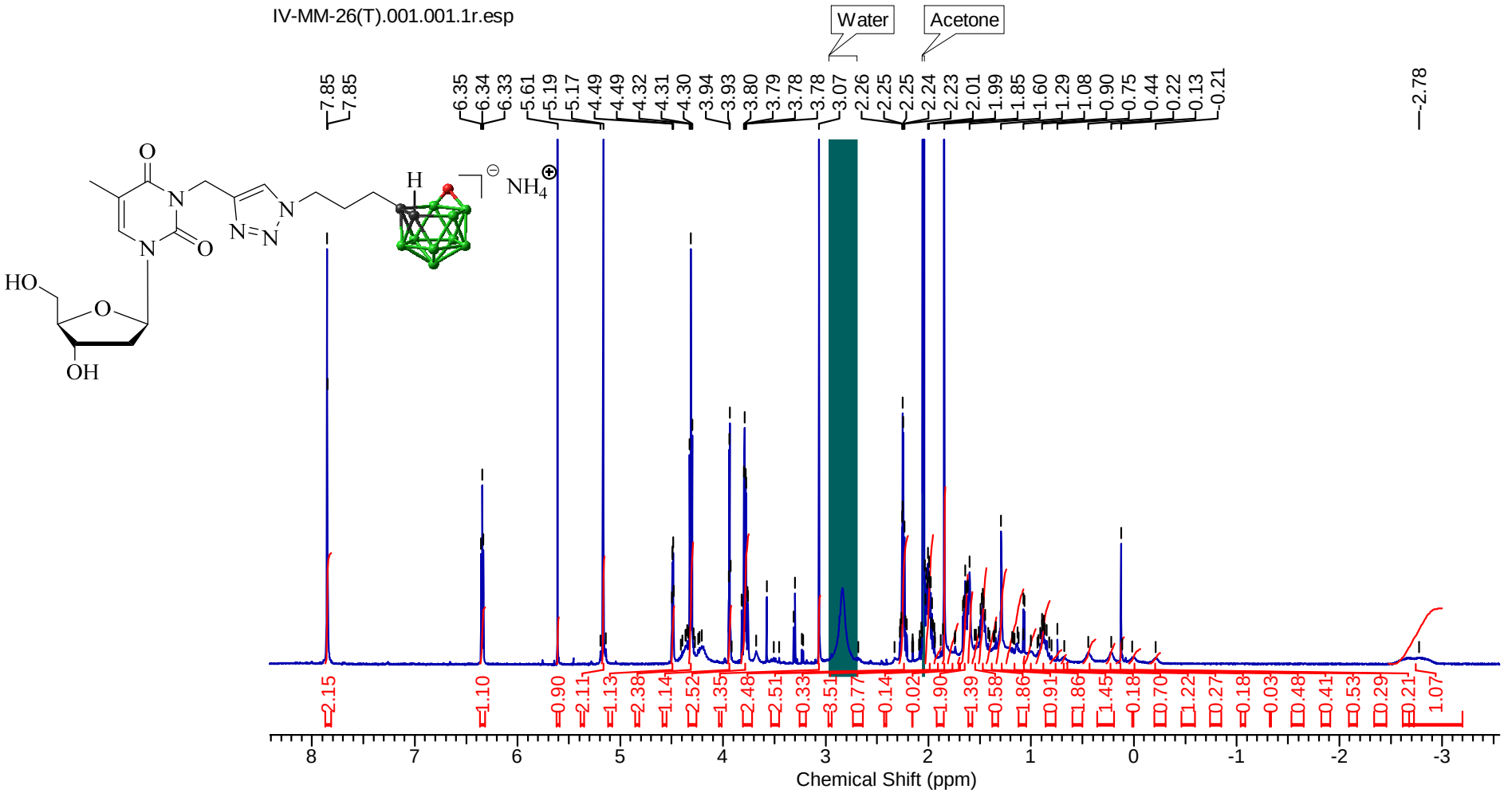


Figure S109. ^{1}H NMR spectrum of compound **33**.

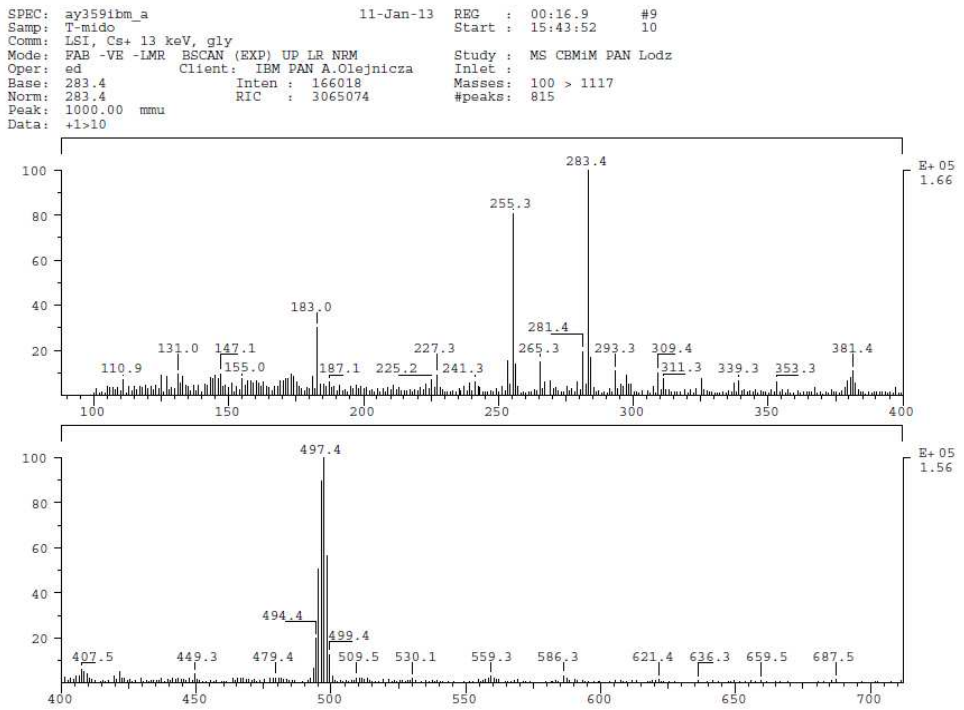


Figure S110. MS-FAB spectrum of compound **33**.

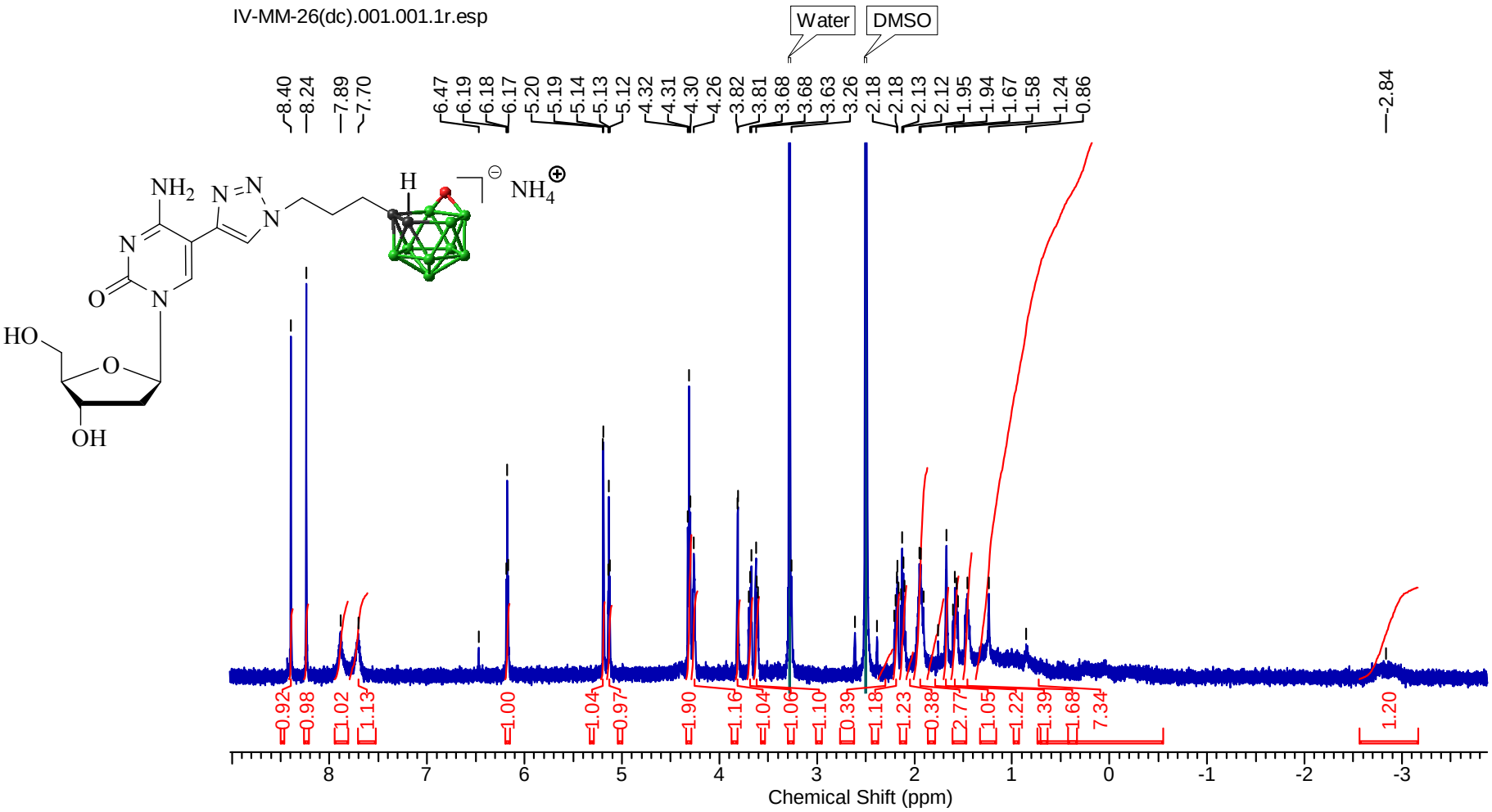


Figure S111. ^{1}H NMR spectrum of compound **34**.

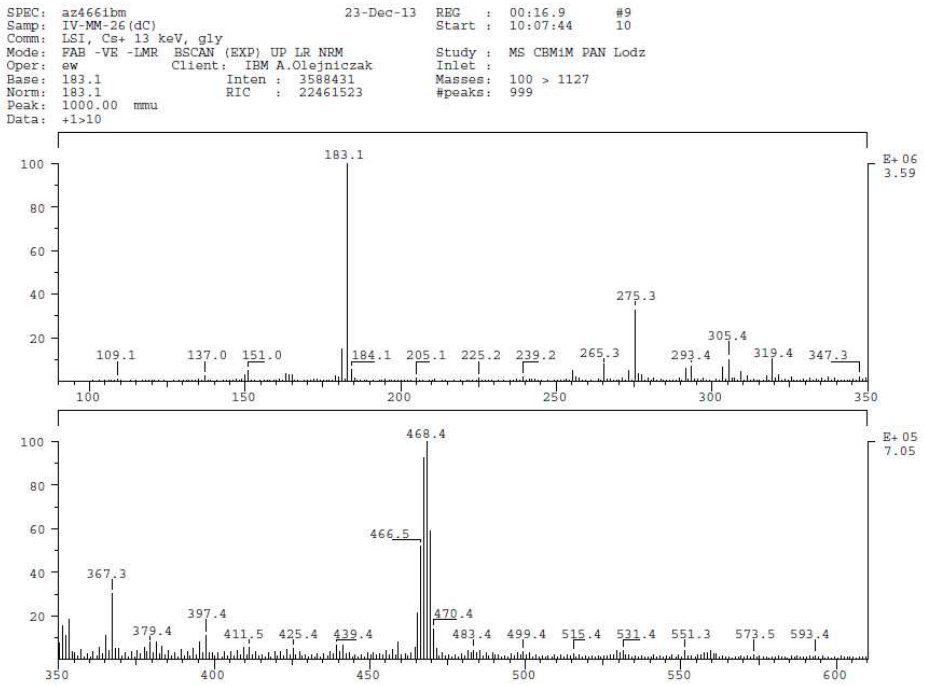


Figure S112. MS-FAB spectrum of compound **34**.

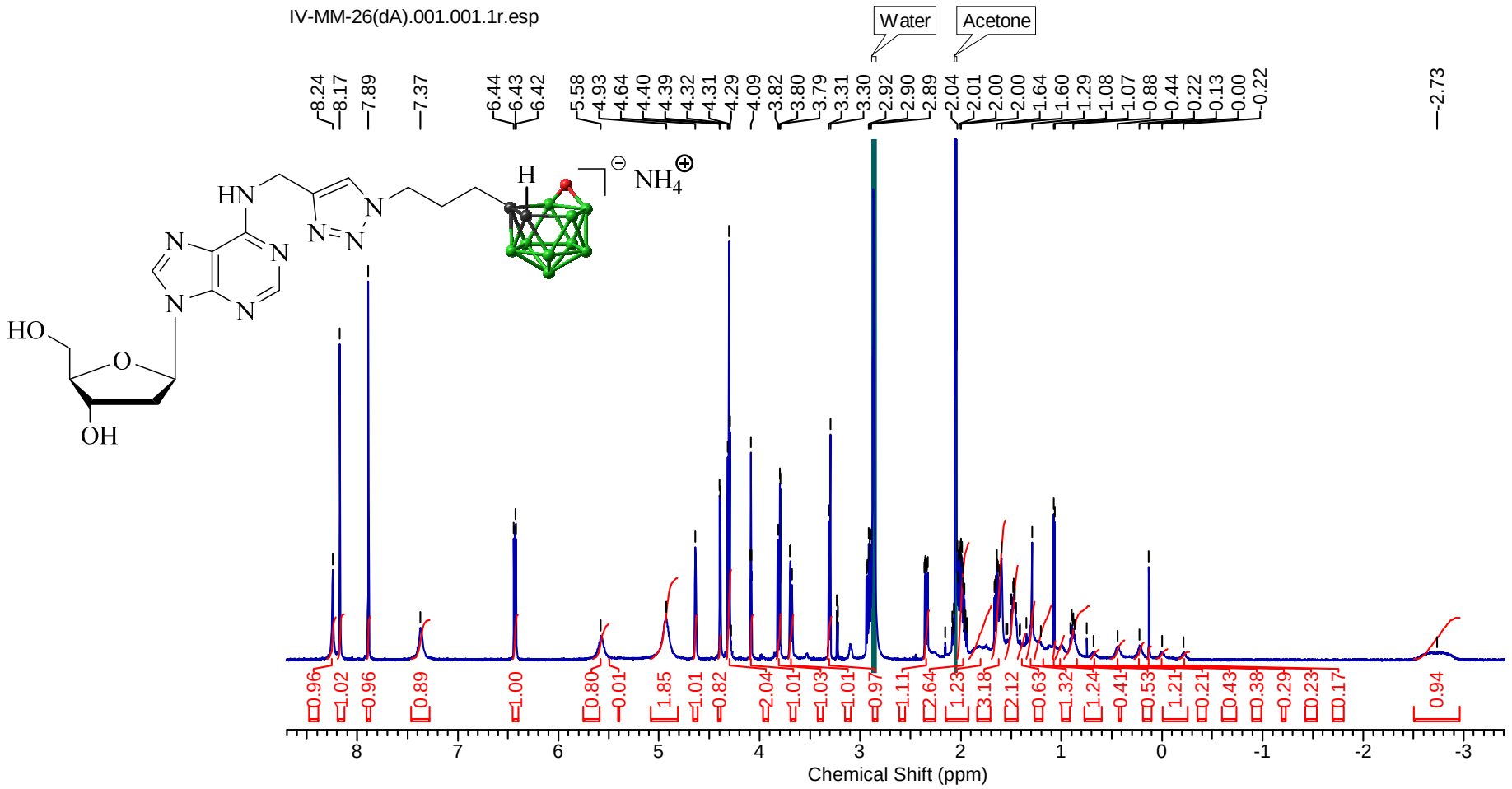


Figure S113. ^{1}H NMR spectrum of compound **35**.

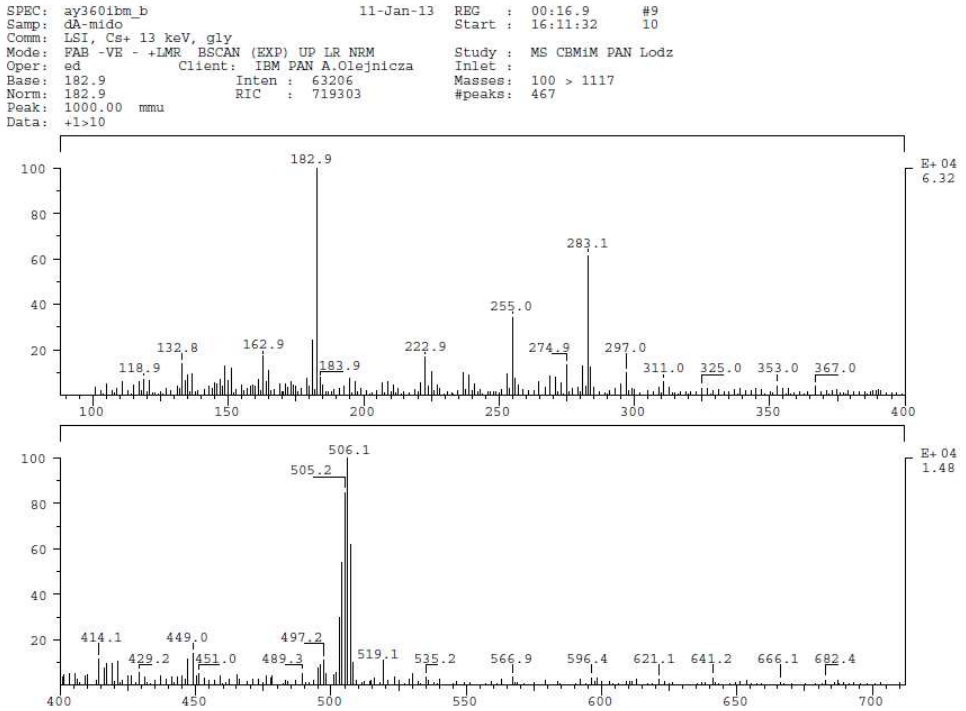


Figure S114. MS-FAB spectrum of compound **35**.

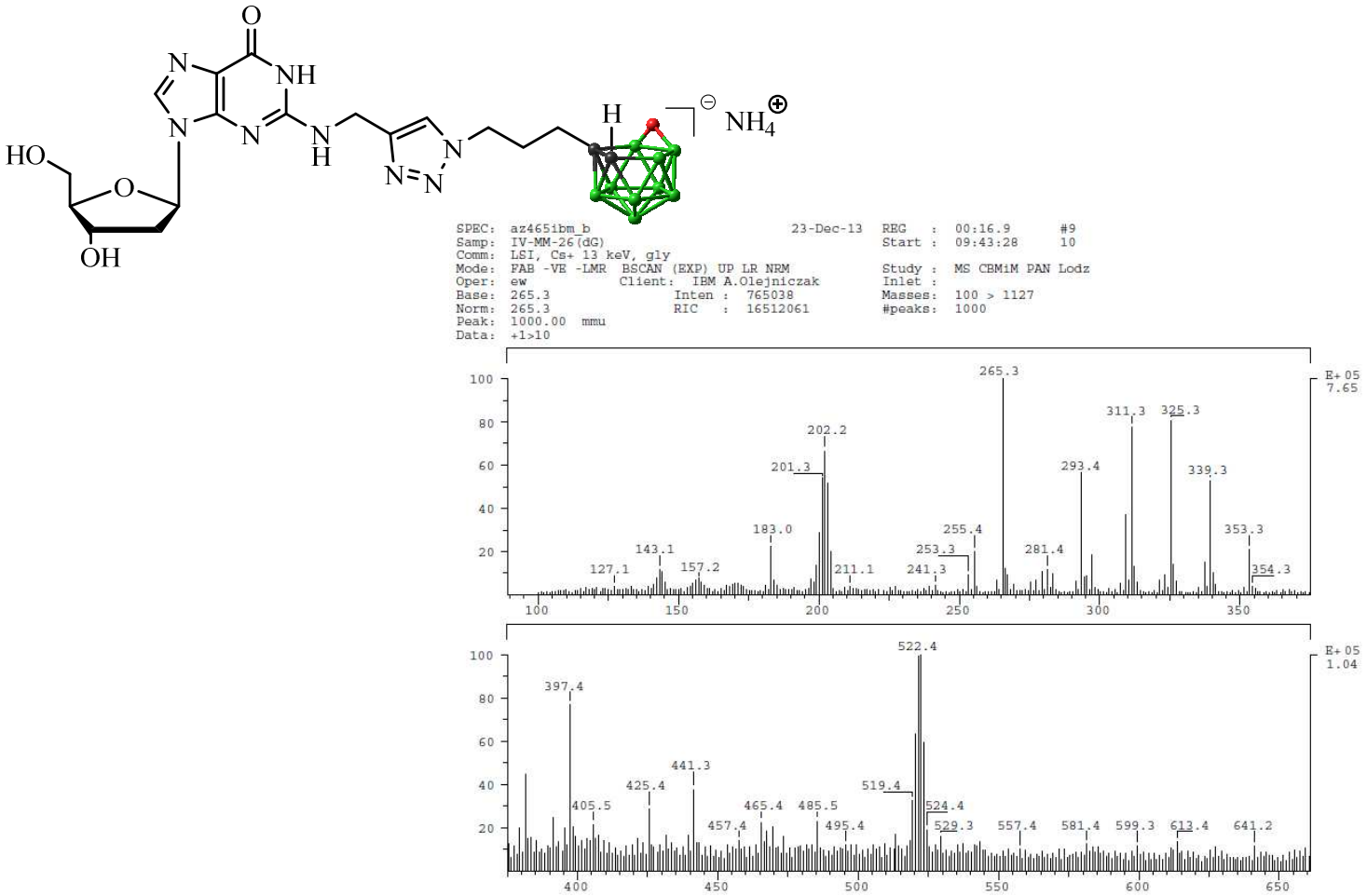


Figure S115. MS-FAB spectrum of compound **36**.

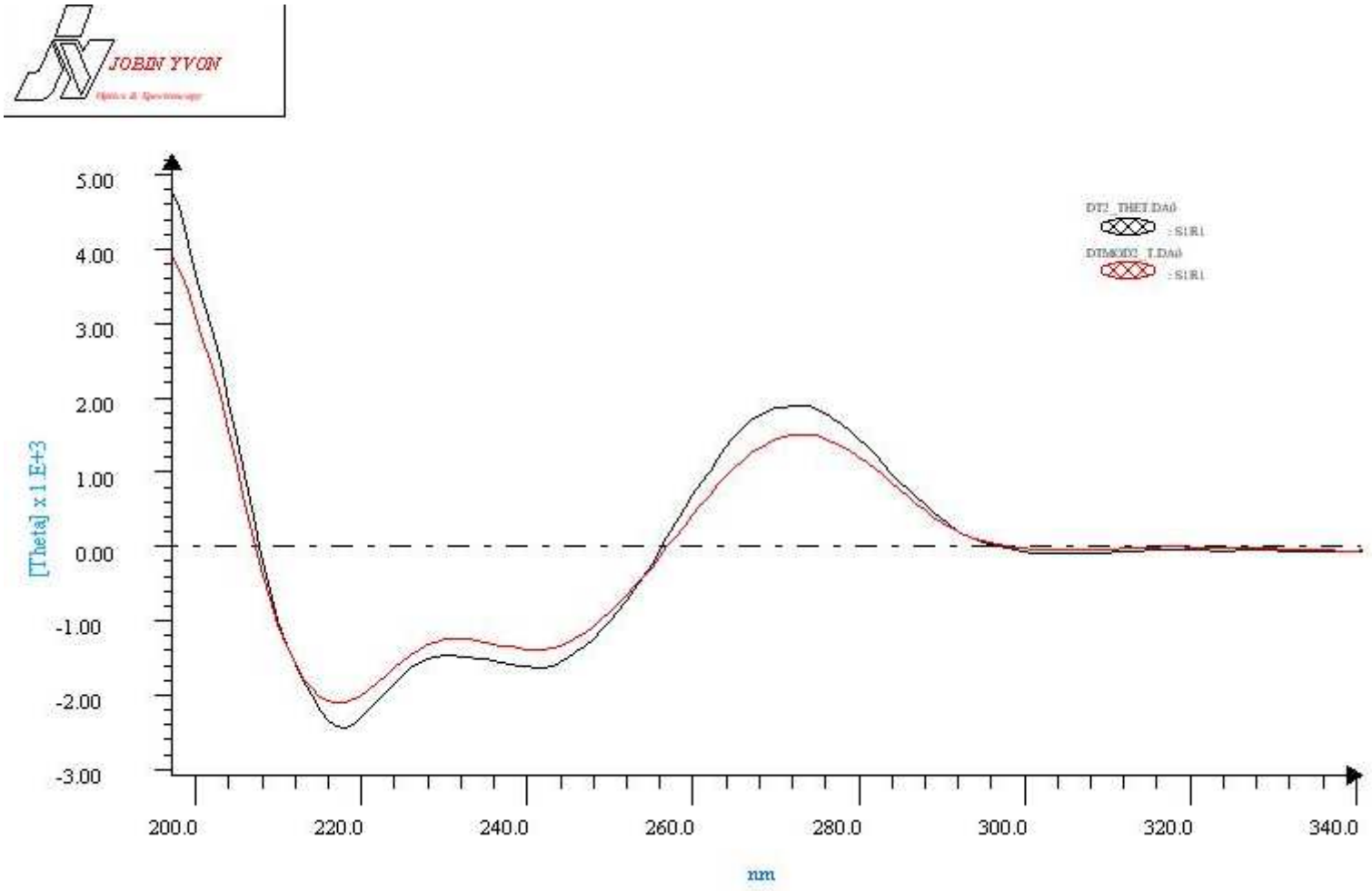


Figure S116. CD spectra of compounds **20** (red) and thymidine (black).

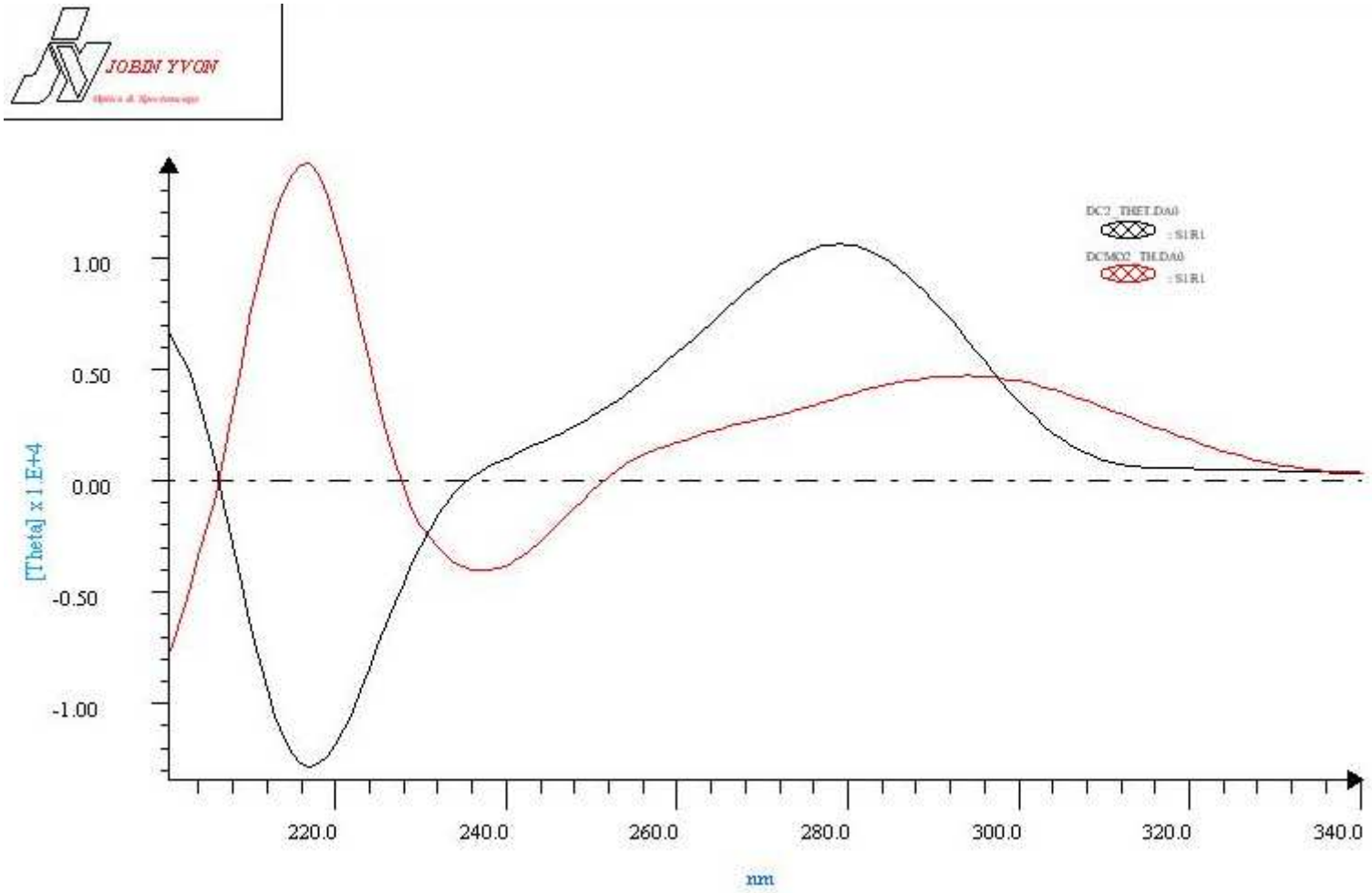


Figure S117. CD spectra of compounds **22** (red) and 2'-deoxycytidine (black).

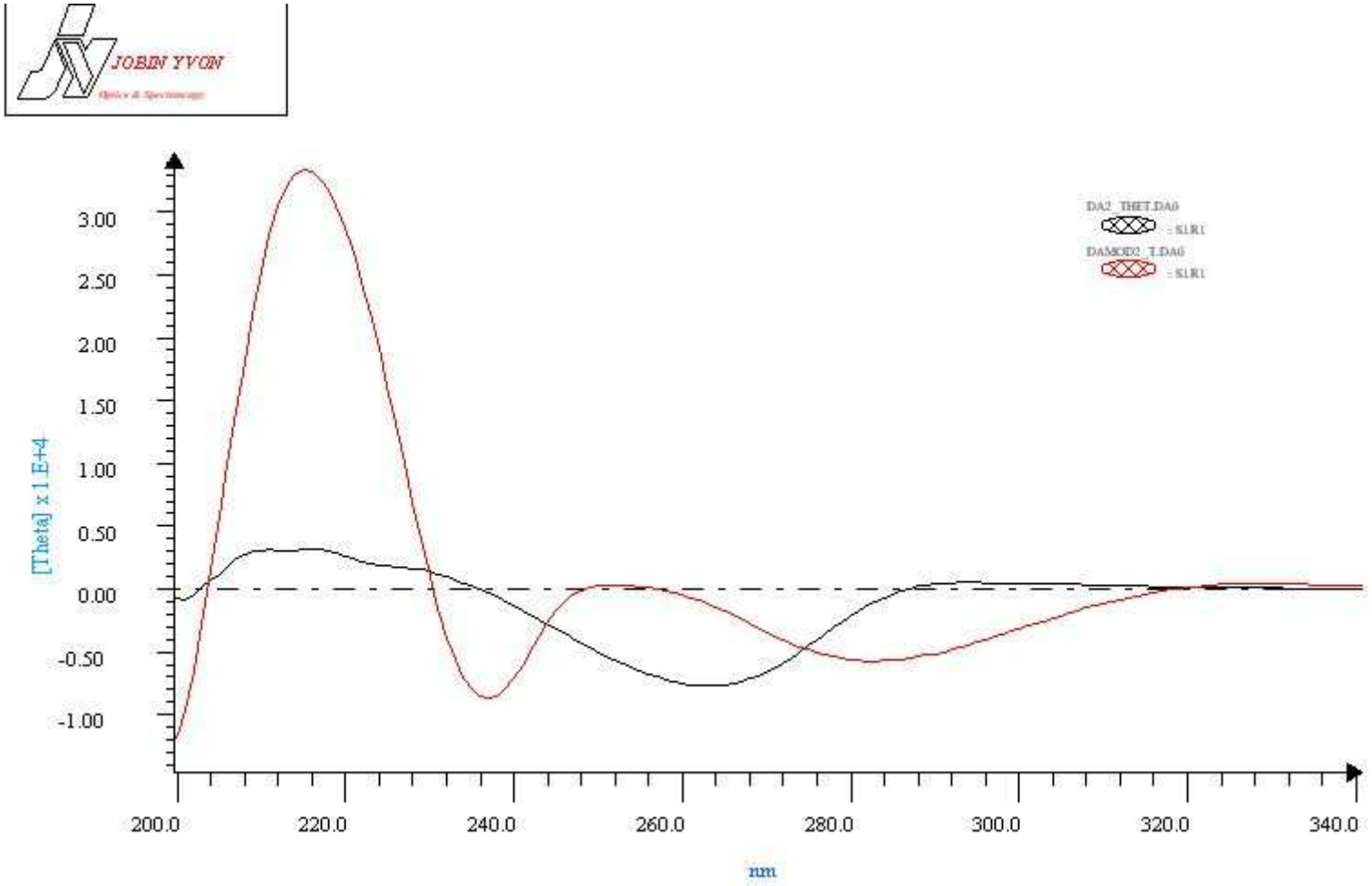


Figure S118. CD spectra of compounds **24** (red) and 2'-deoxyadenosine (black).

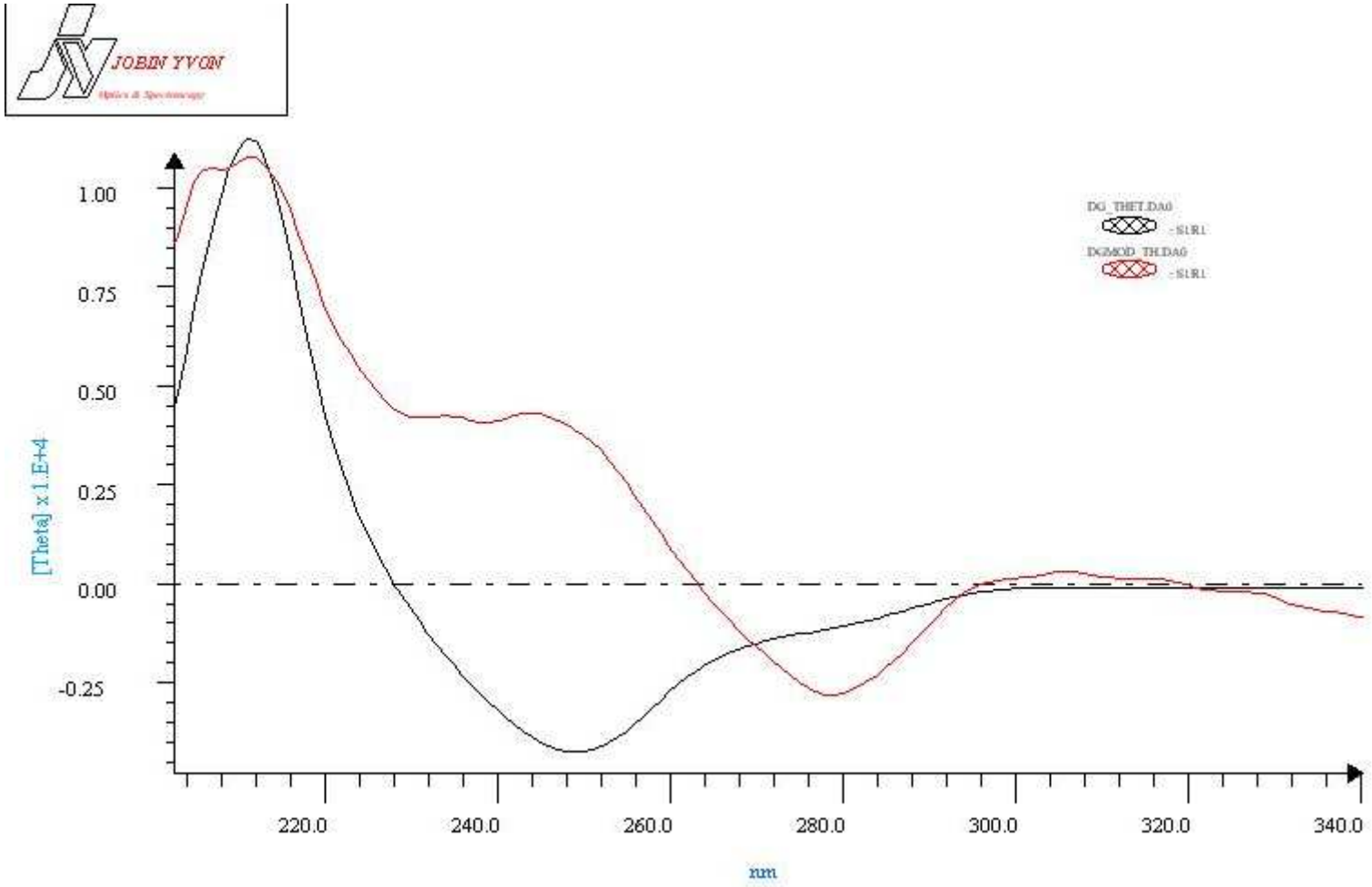


Figure S119. CD spectra of compounds **27** (red) and 2'-deoxyguanosine (black).

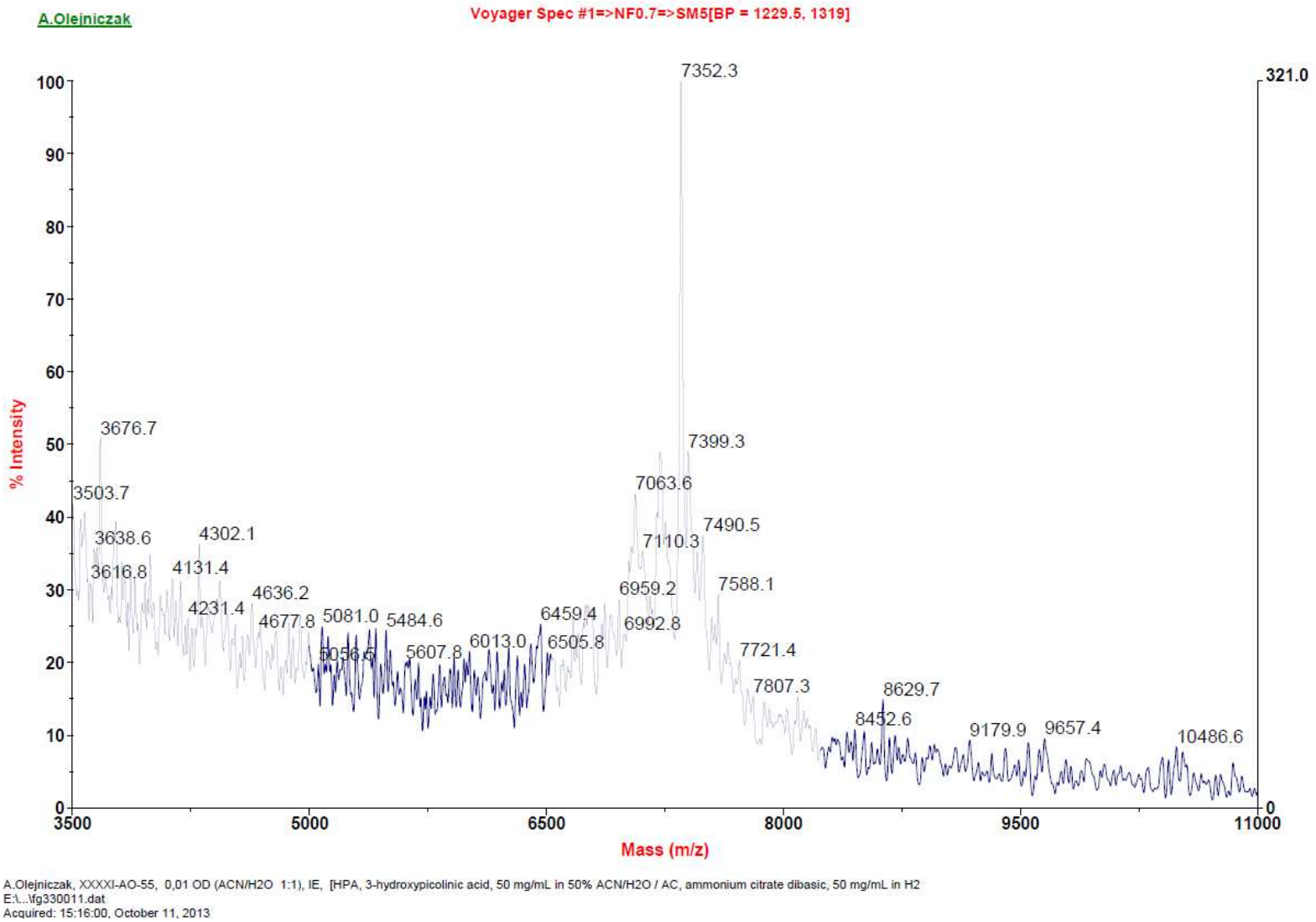


Figure S120. MALDI-TOF spectrum of oligonucleotide **38**.

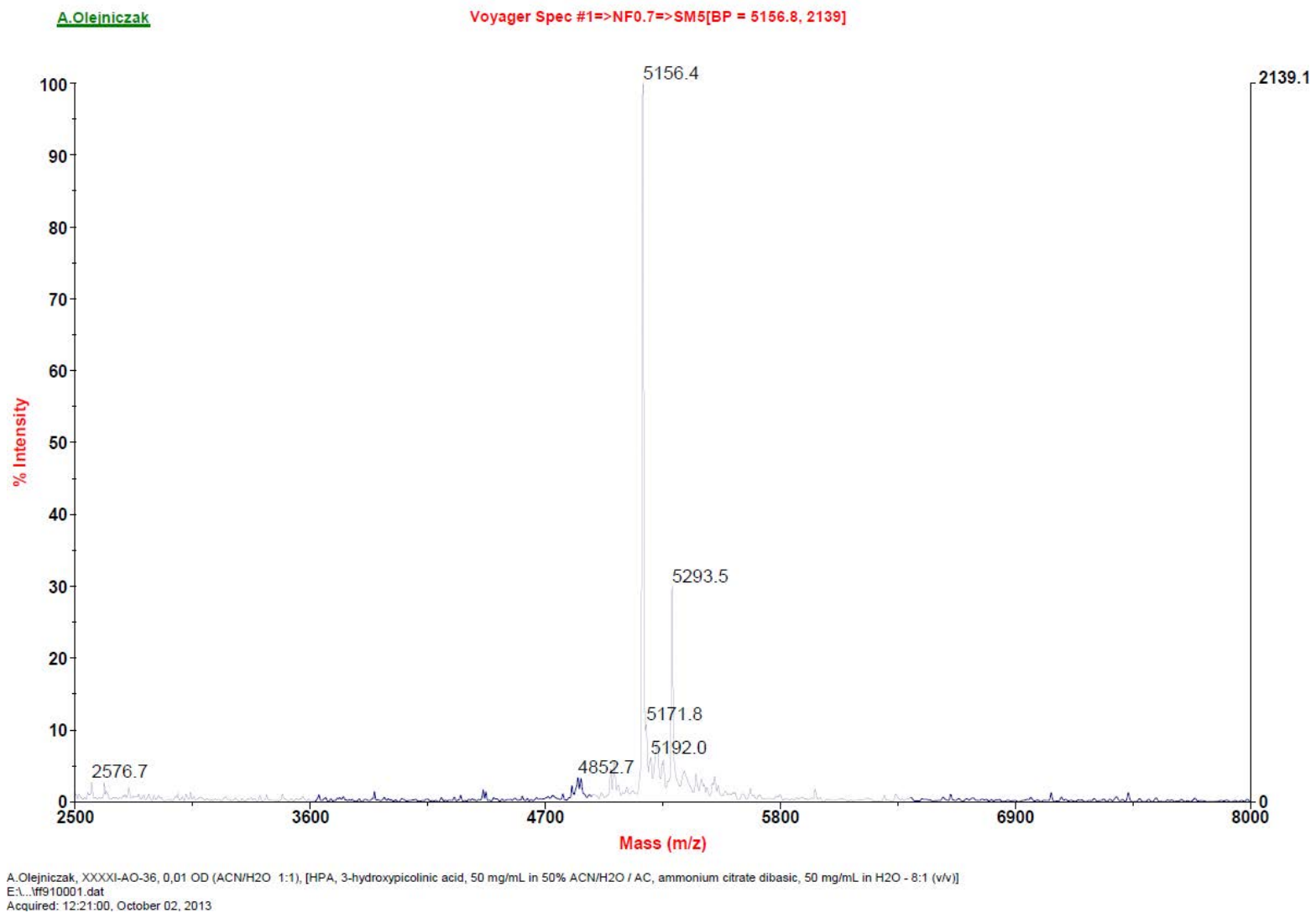


Figure S121. MALDI-TOF spectrum of oligonucleotide **39**.

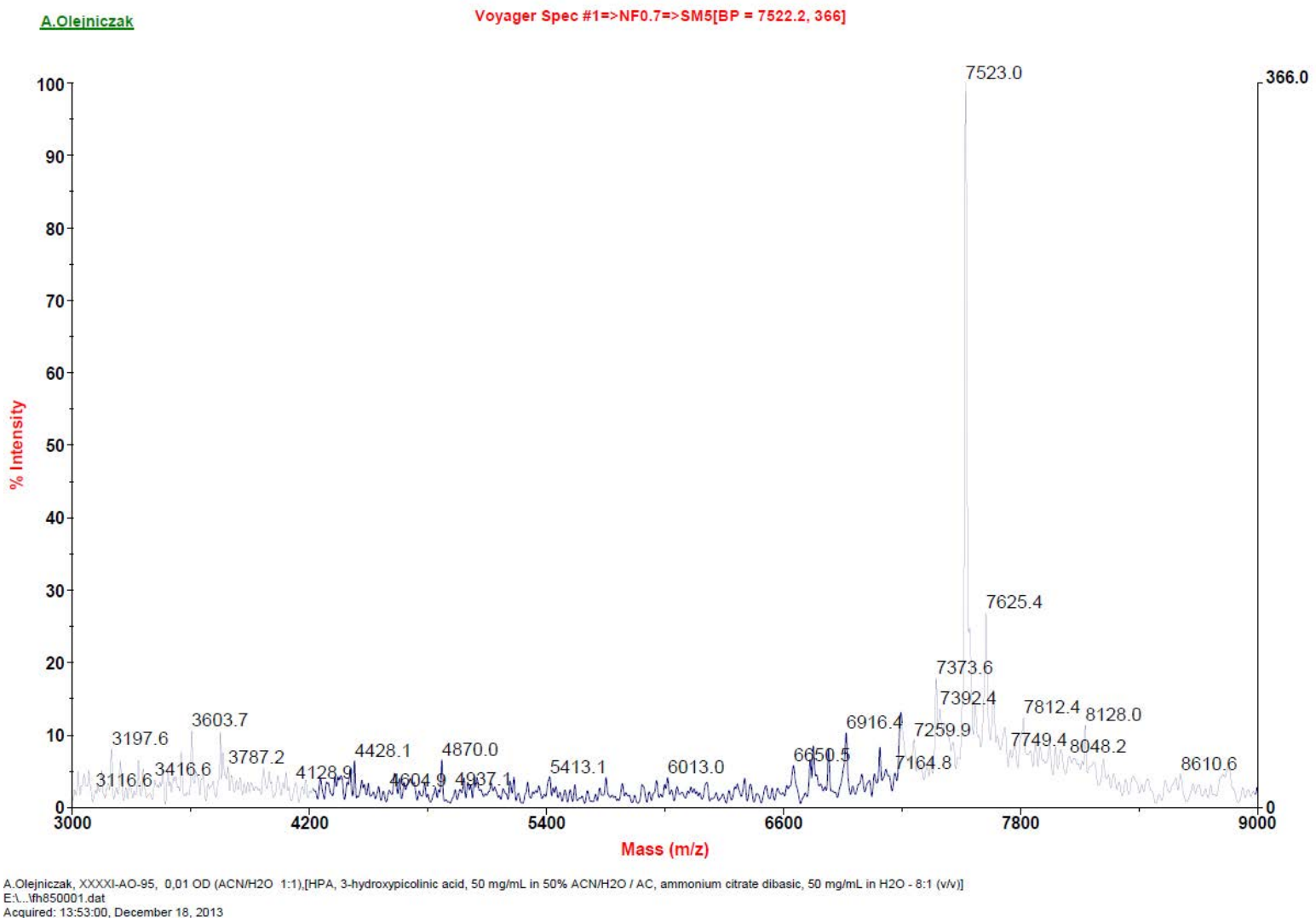


Figure S122. MALDI-TOF spectrum of oligonucleotide **40**.

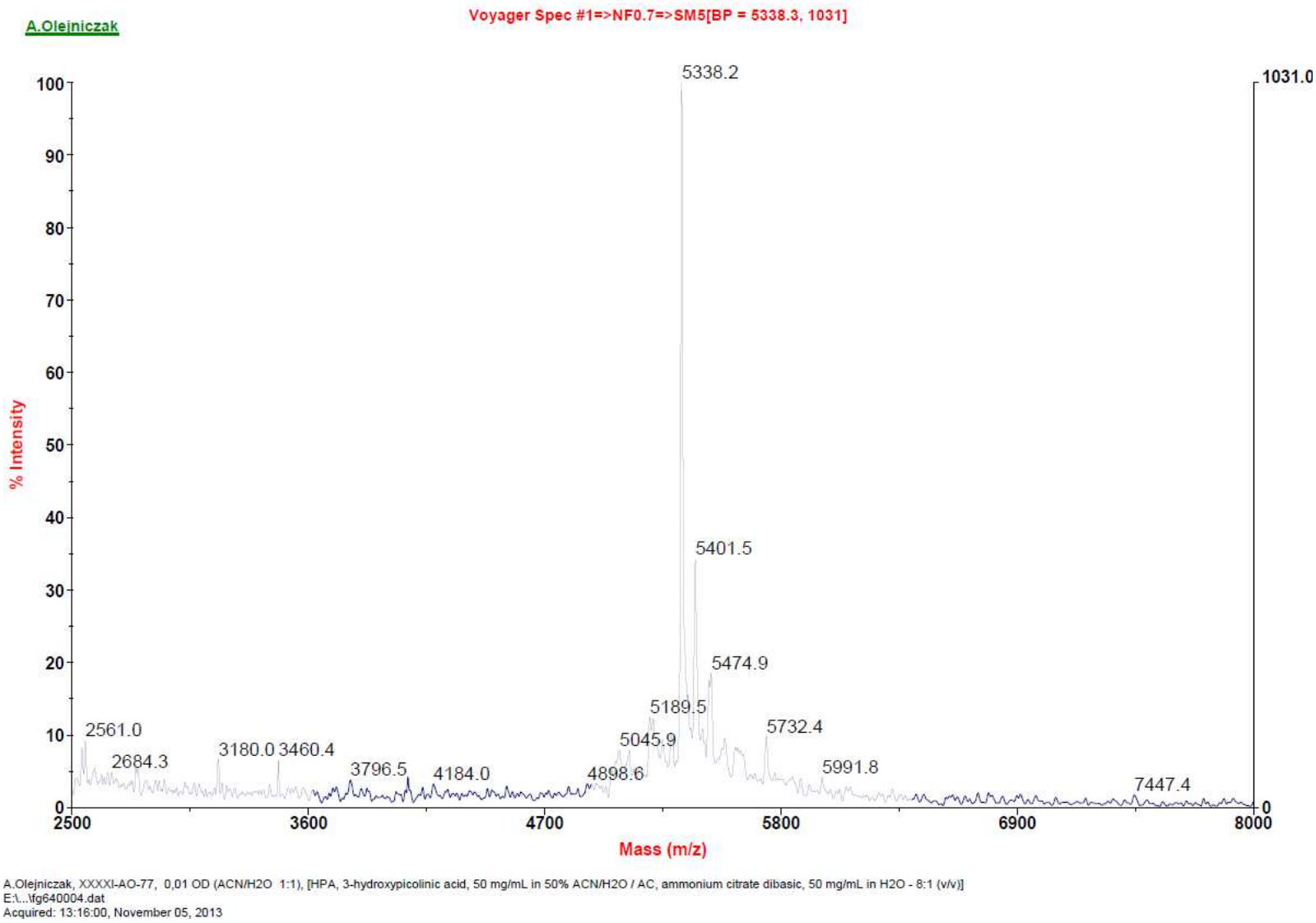


Figure S123. MALDI-TOF spectrum of oligonucleotide **41**.