Supporting Materials for:

Preparation of New Olefin Polymerization Precatalysts by Facile Derivatization of Imino-Enamido $ZrMe_3$ and $HfMe_3$ Complexes

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Figure 1. ^{1}H NMR Spectra of Complex **11** (C_6D_6, 500 MHz).

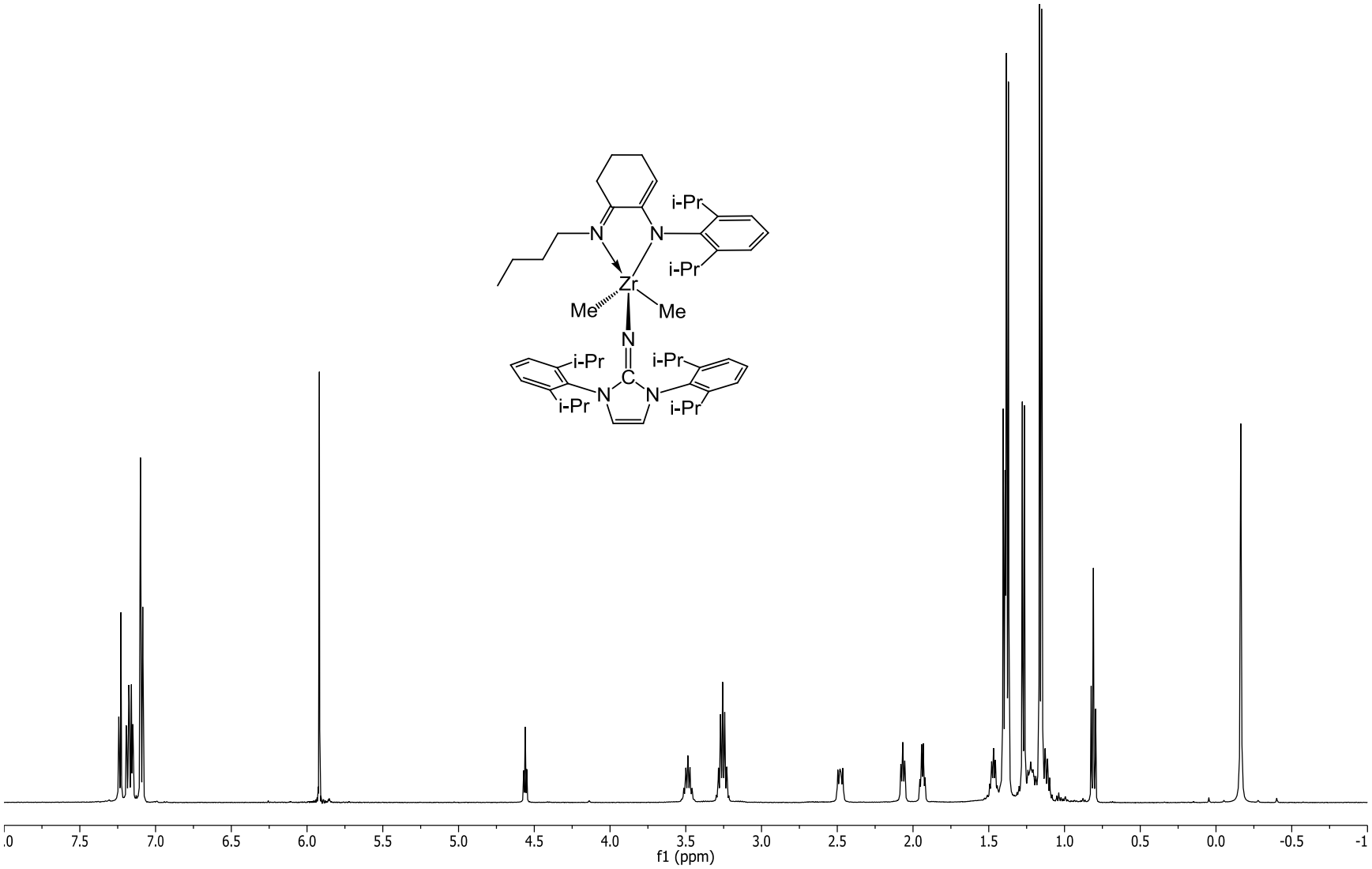


Figure 2. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **11** (C_6D_6, 125 MHz).

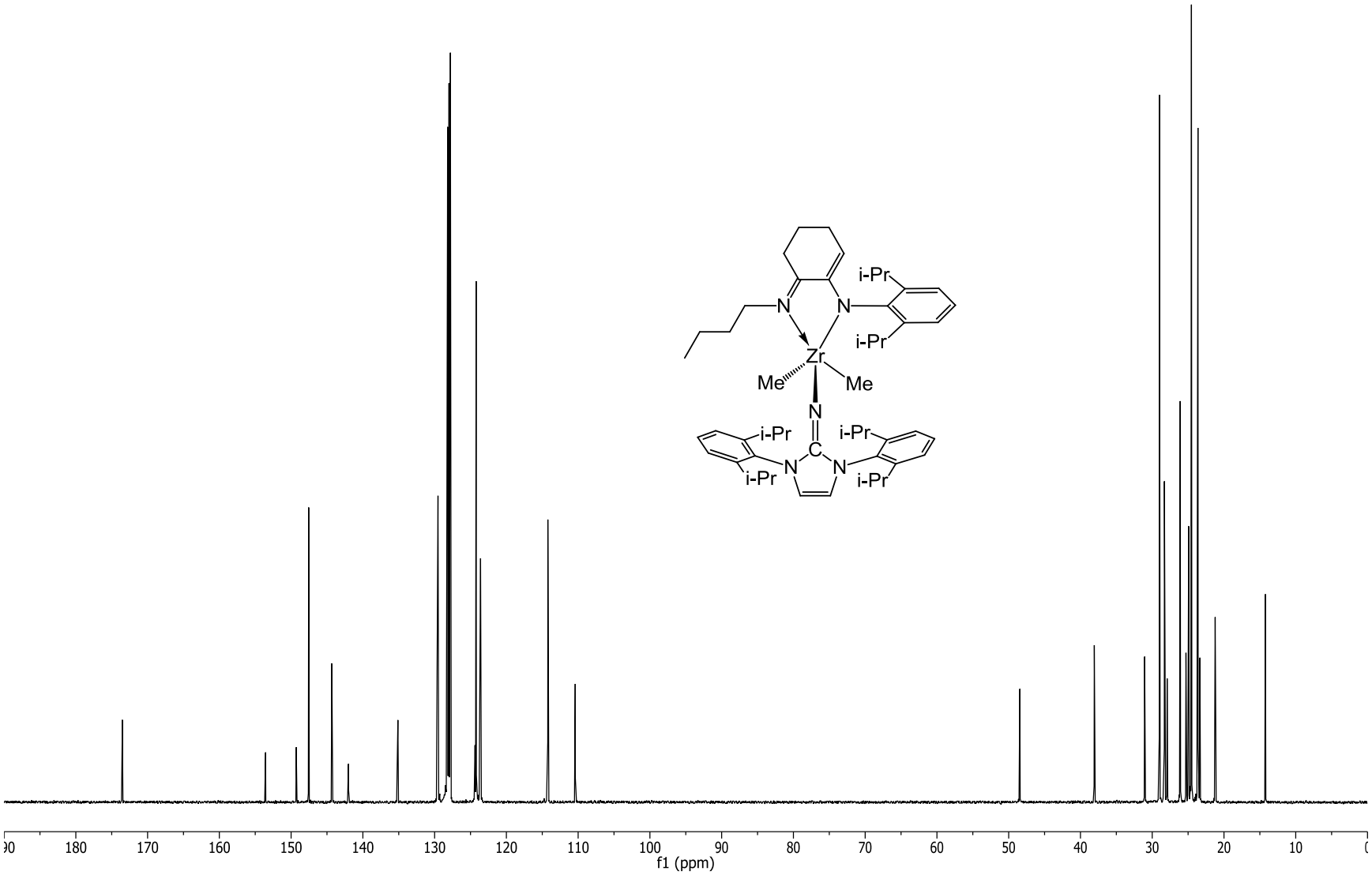


Figure 3. APT NMR Spectrum of Complex **11** (C_6D_6, 125 MHz).

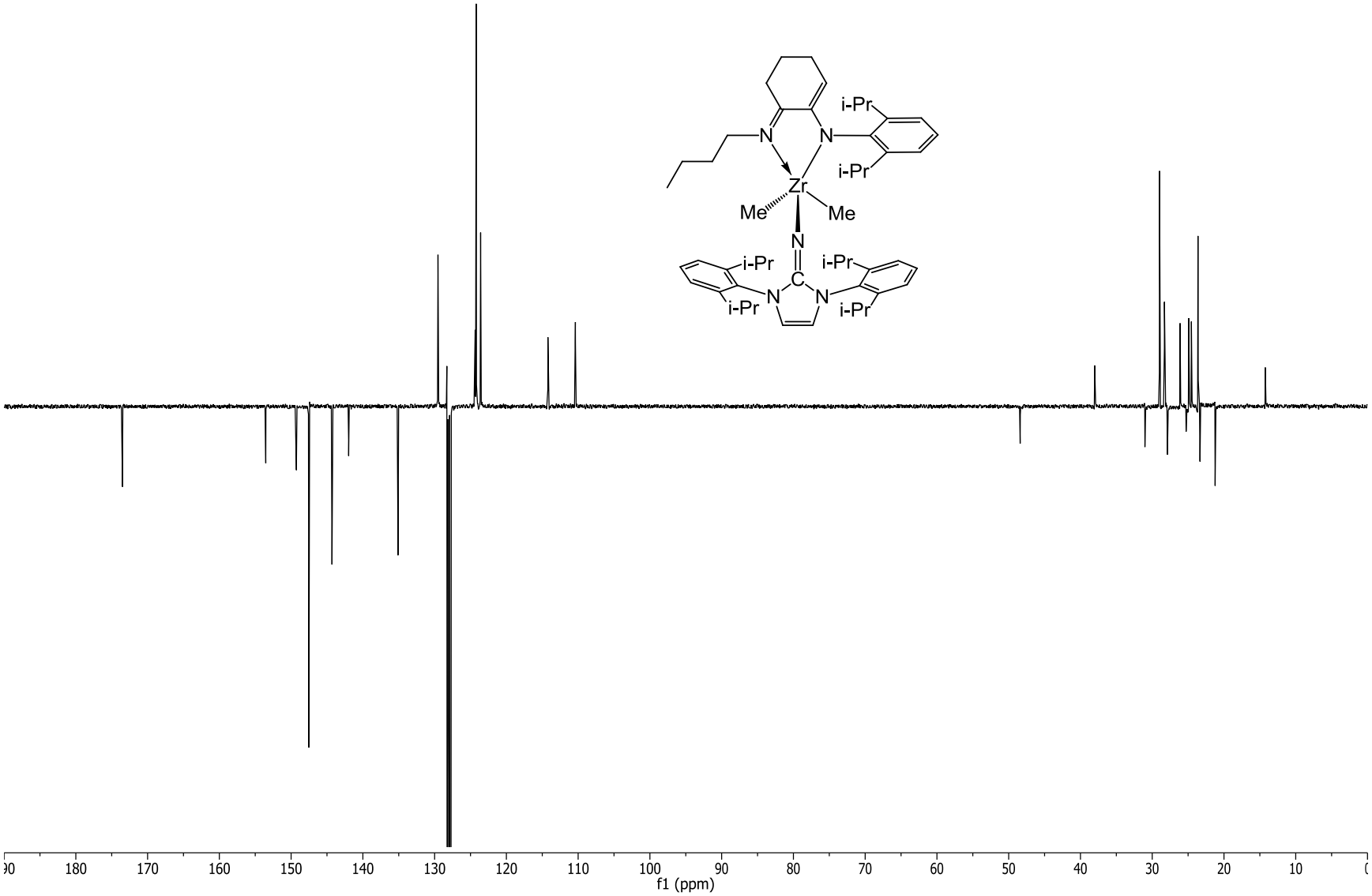


Figure 4. TOCSY1D NMR Spectra of Complex **11** (C_6D_6, 400 MHz) (mix time = 0, 0.08 s).

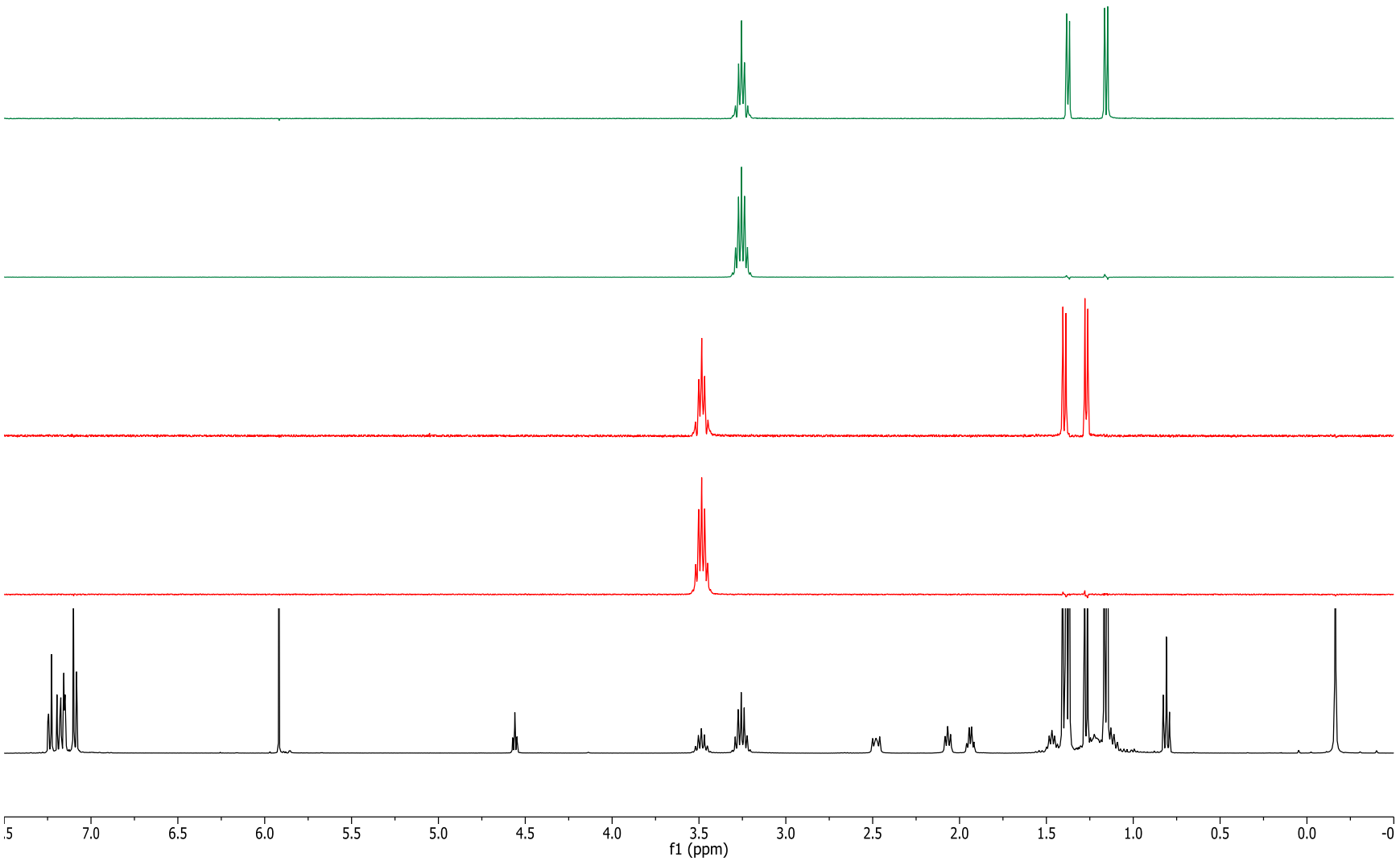


Figure 5. TOCSY1D NMR Spectra of Complex **11** (C_6D_6, 400 MHz) (mix time = 0, 0.08 s).

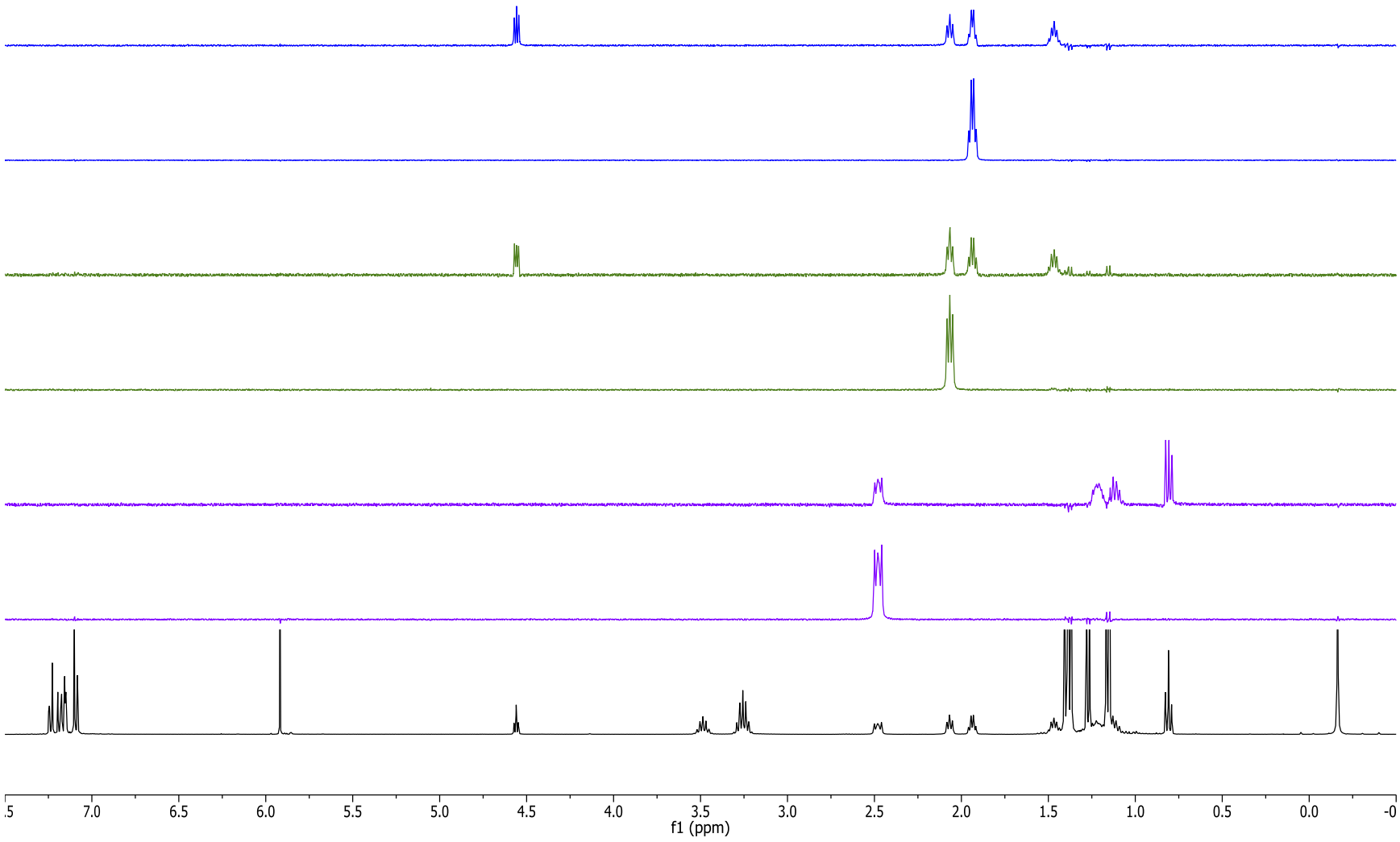


Figure 6. ^{1}H and NOESY1D NMR Spectra of Complex **11** (C_6D_6, 400 MHz, mixing time = 0.8 s).

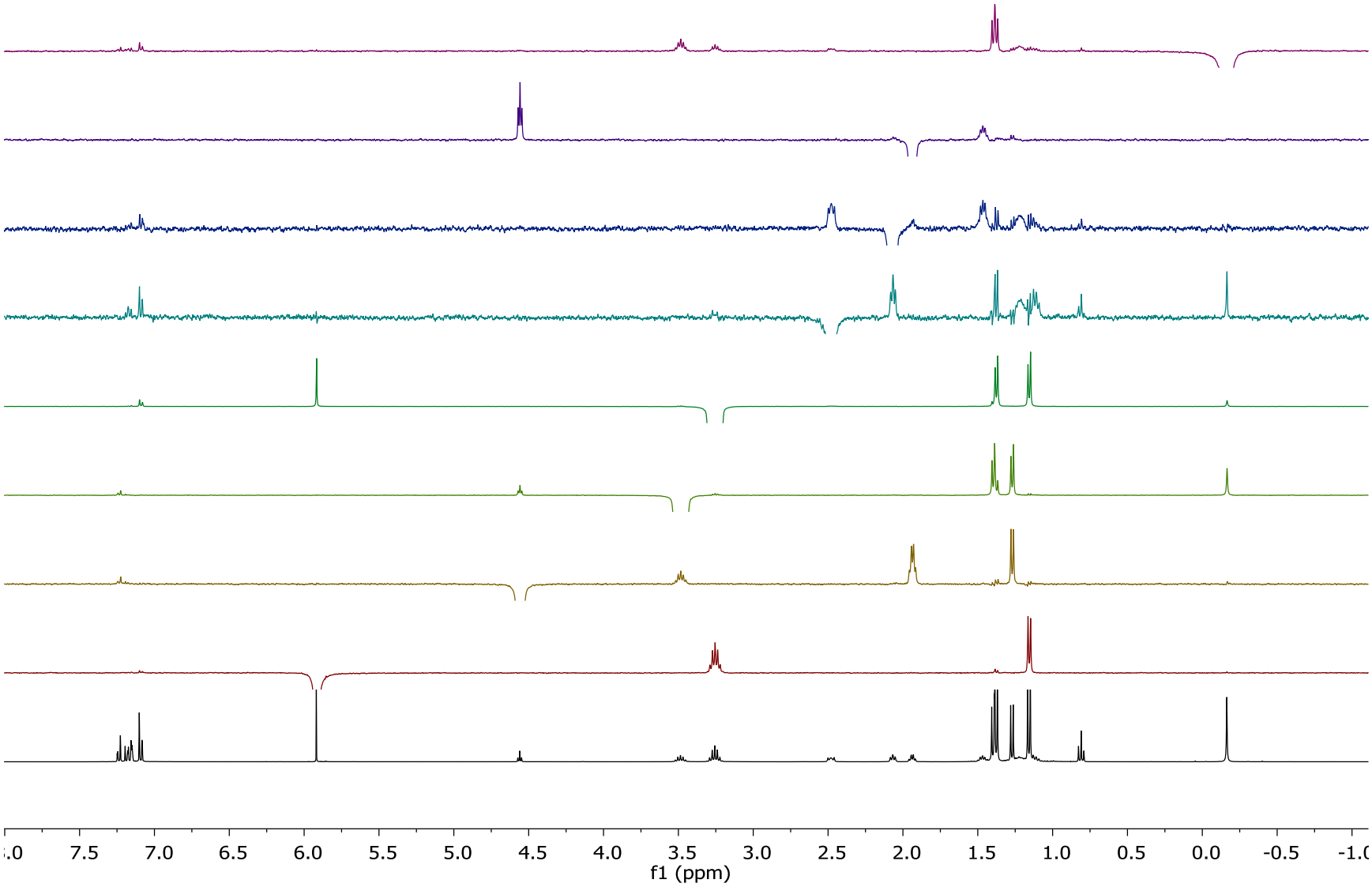


Figure 7. gCOSY NMR Spectrum of Complex **11** (C_6D_6, 500 MHz).

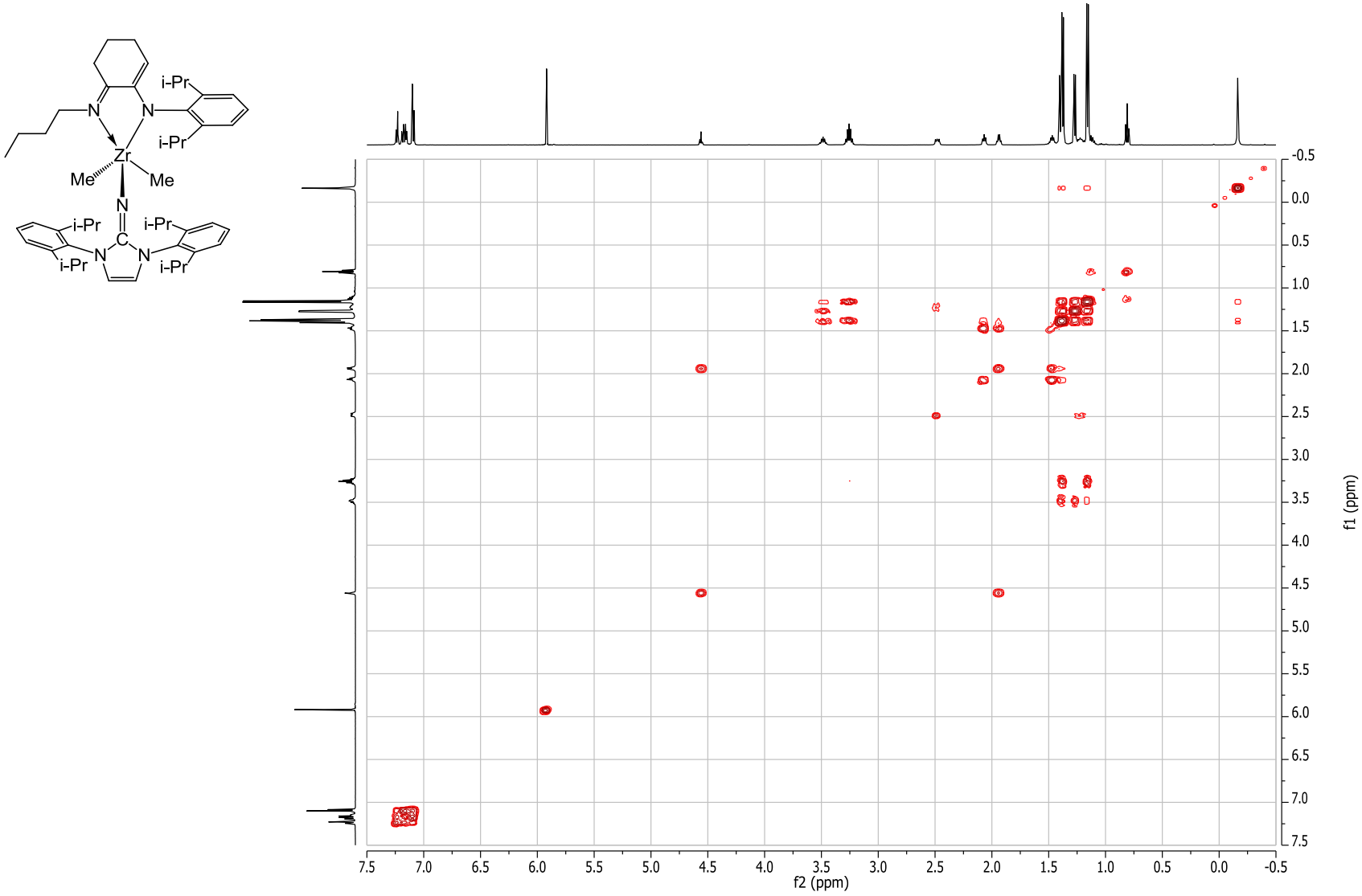


Figure 8. Fragment of gCOSY Spectrum of Complex **11** (C_6D_6, 500 MHz).

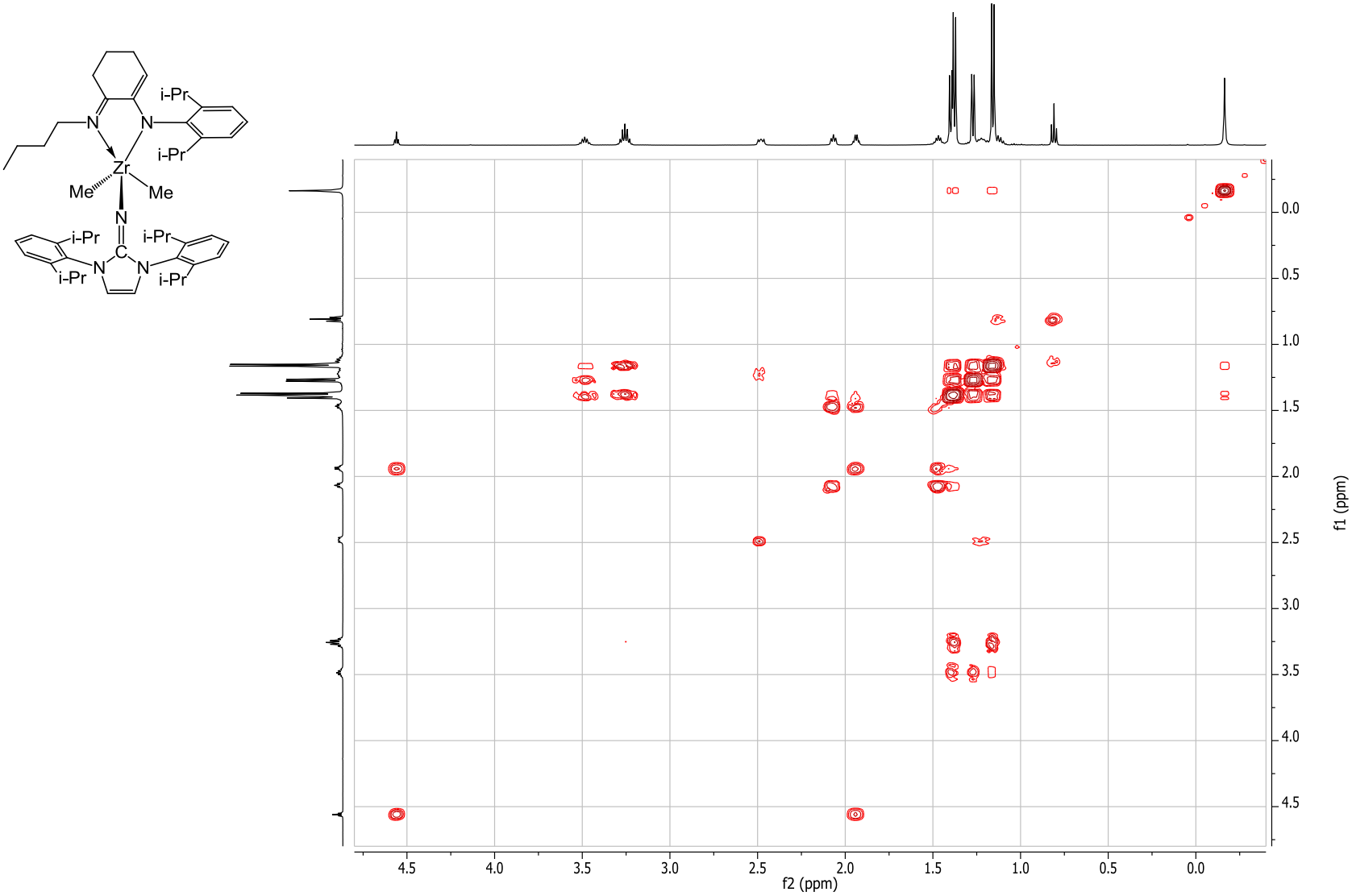


Figure 9. HSQCAD NMR Spectrum of Complex **11** (C_6D_6, 500 MHz).

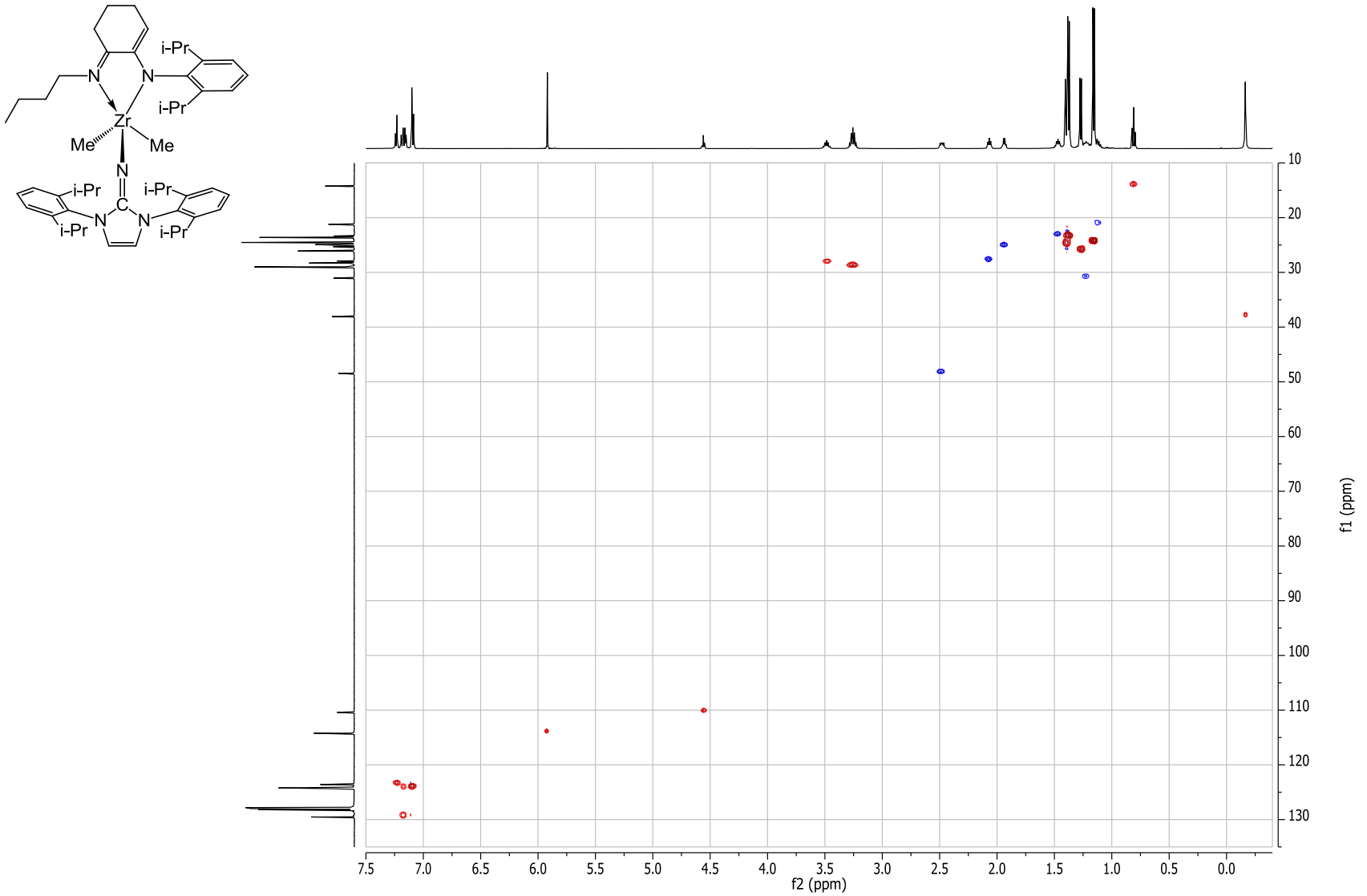


Figure 10. Fragment of gHSQCAD NMR Spectrum of Complex **11** (C_6D_6, 500 MHz).

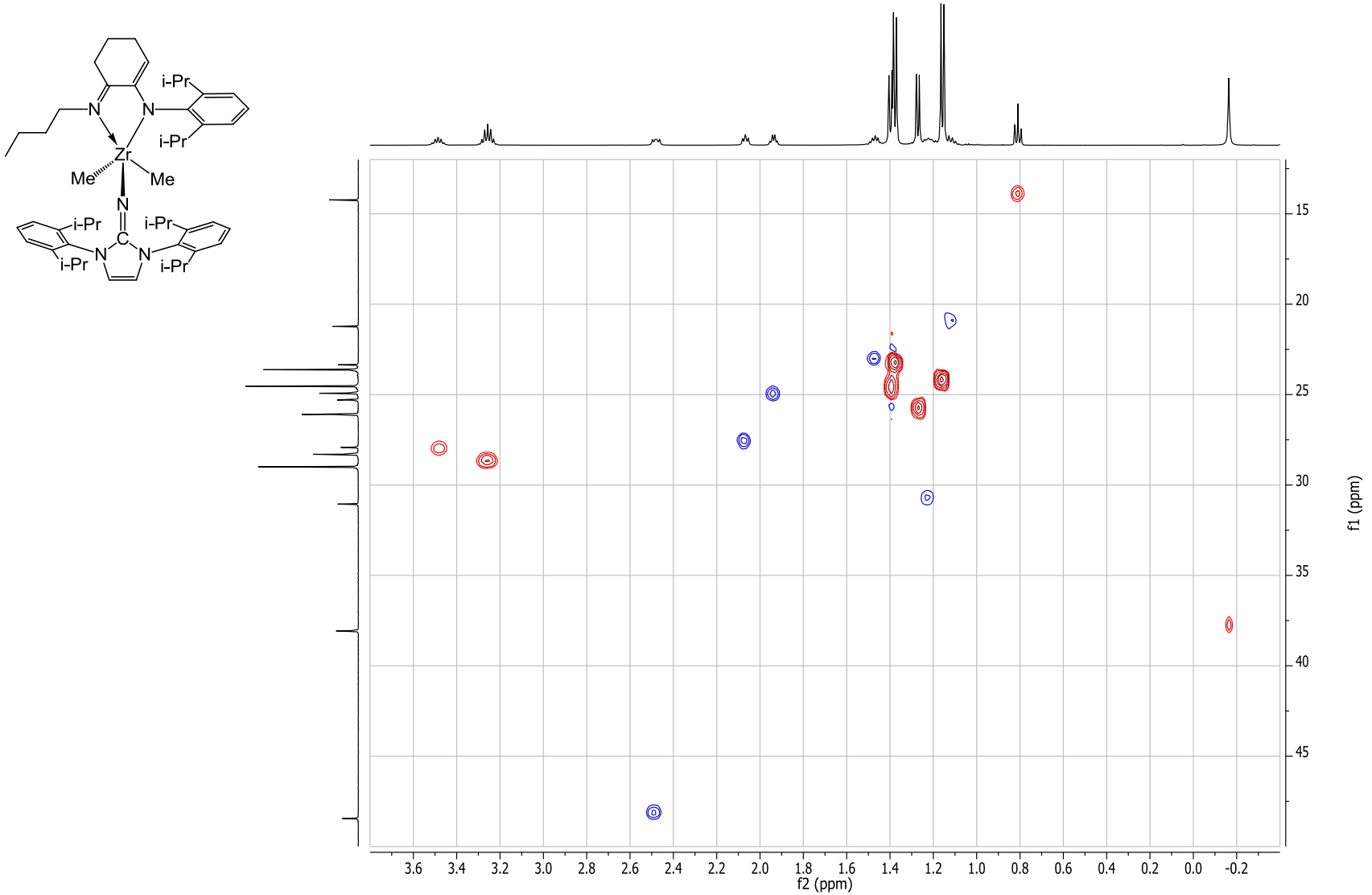


Figure 11. Fragment of gHSQCAD NMR Spectrum of Complex **11** (C_6D_6, 500 MHz).

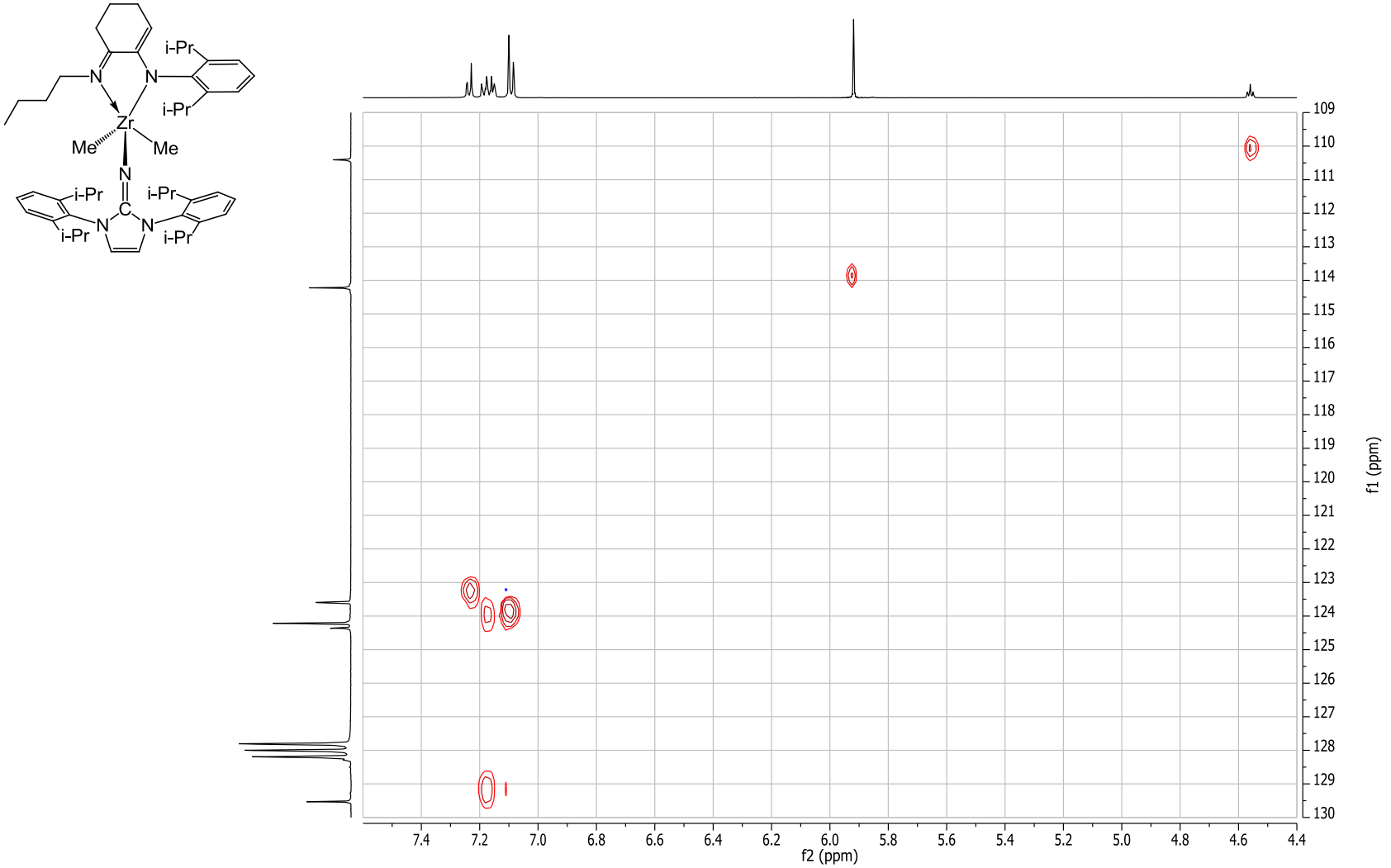


Figure 12. ^{1}H NMR Spectra of Complex **12** (C_6D_6, 400 MHz).

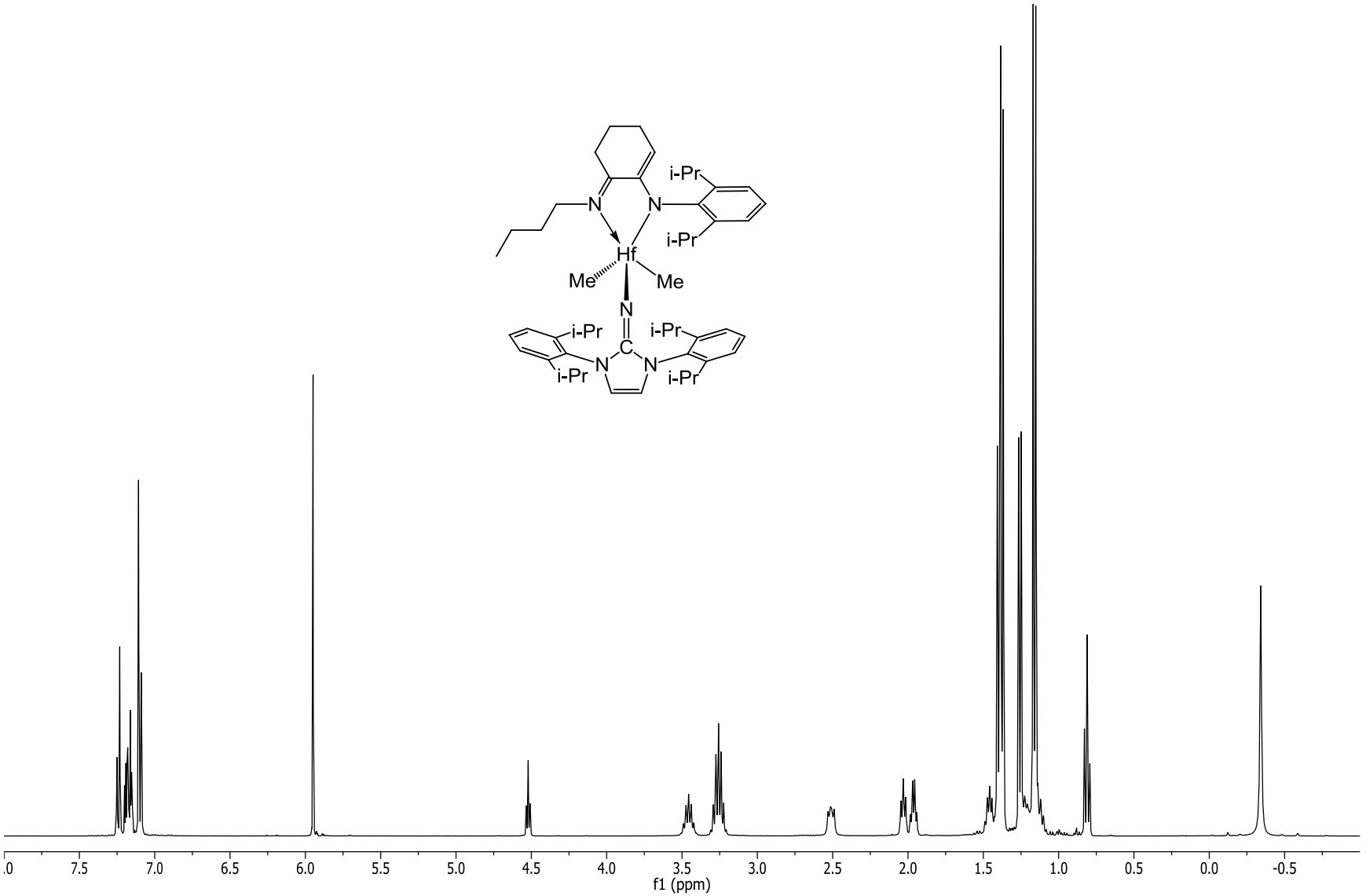


Figure 13. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **12** (C_6D_6, 100 MHz).

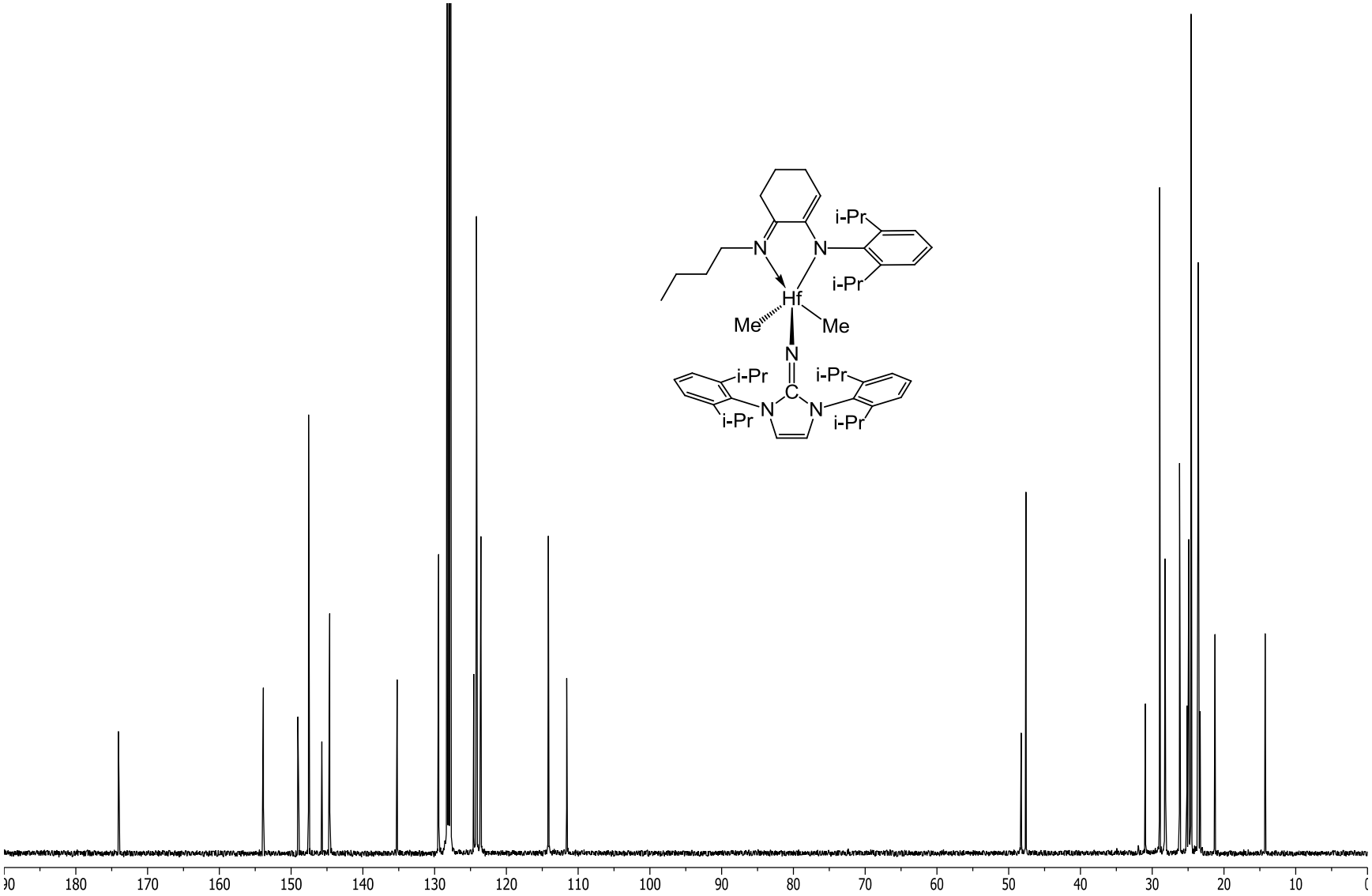


Figure 14. APT NMR Spectrum of Complex **12** (C_6D_6, 100 MHz).

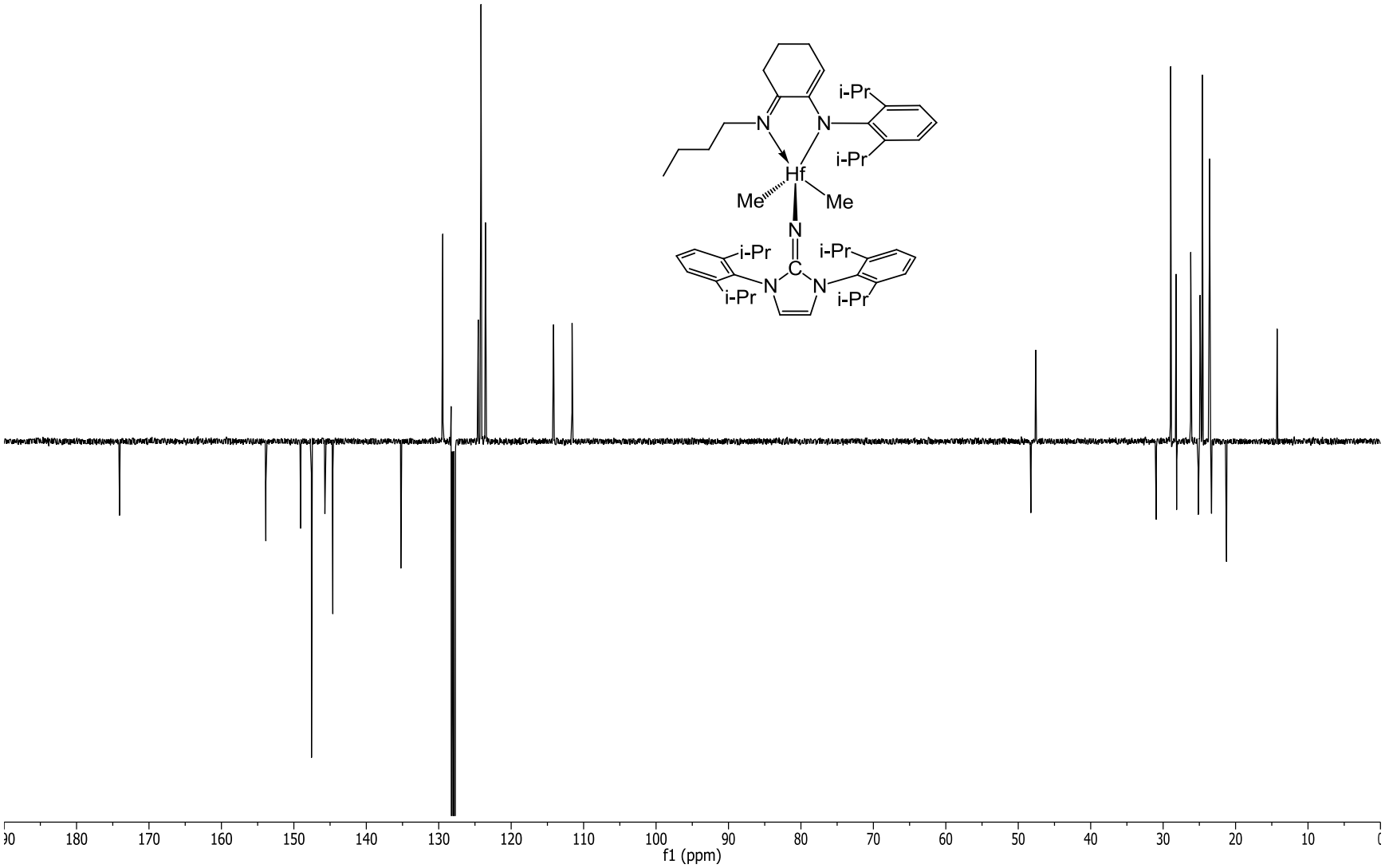


Figure 15. TOCSY1D NMR Spectra of Complex **12** (C_6D_6, 400 MHz) (mix time = 0, 0.03, 0.08 s).

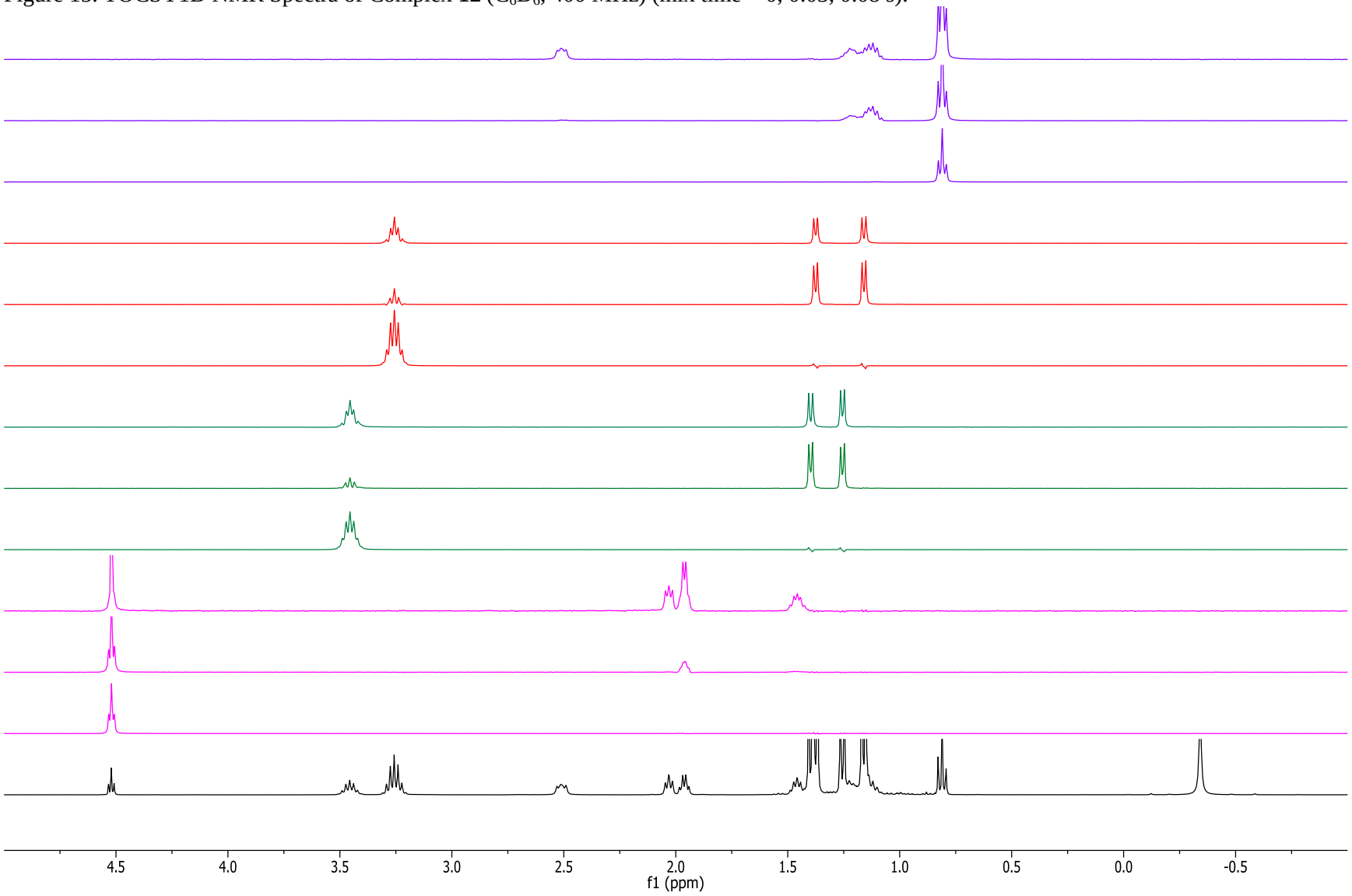


Figure 16. ^{1}H and NOESY1D NMR Spectra of Complex **12** (C_6D_6, 400 MHz, mixing time = 0.8 s).

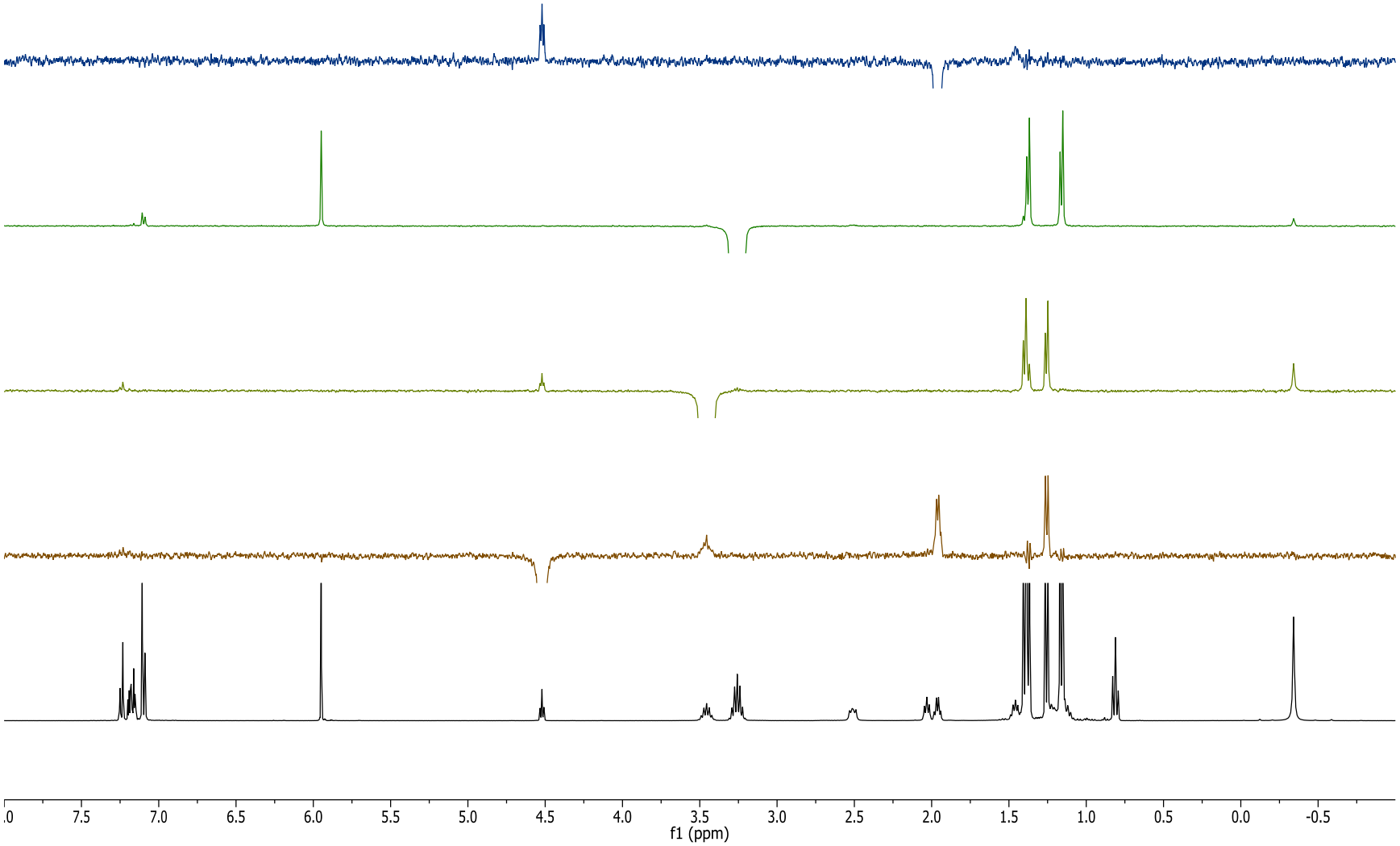


Figure 17. ^{1}H and NOESY1D NMR Spectra of Complex **12** (C_6D_6, 400 MHz, mixing time = 0.8 s) – Continuation.

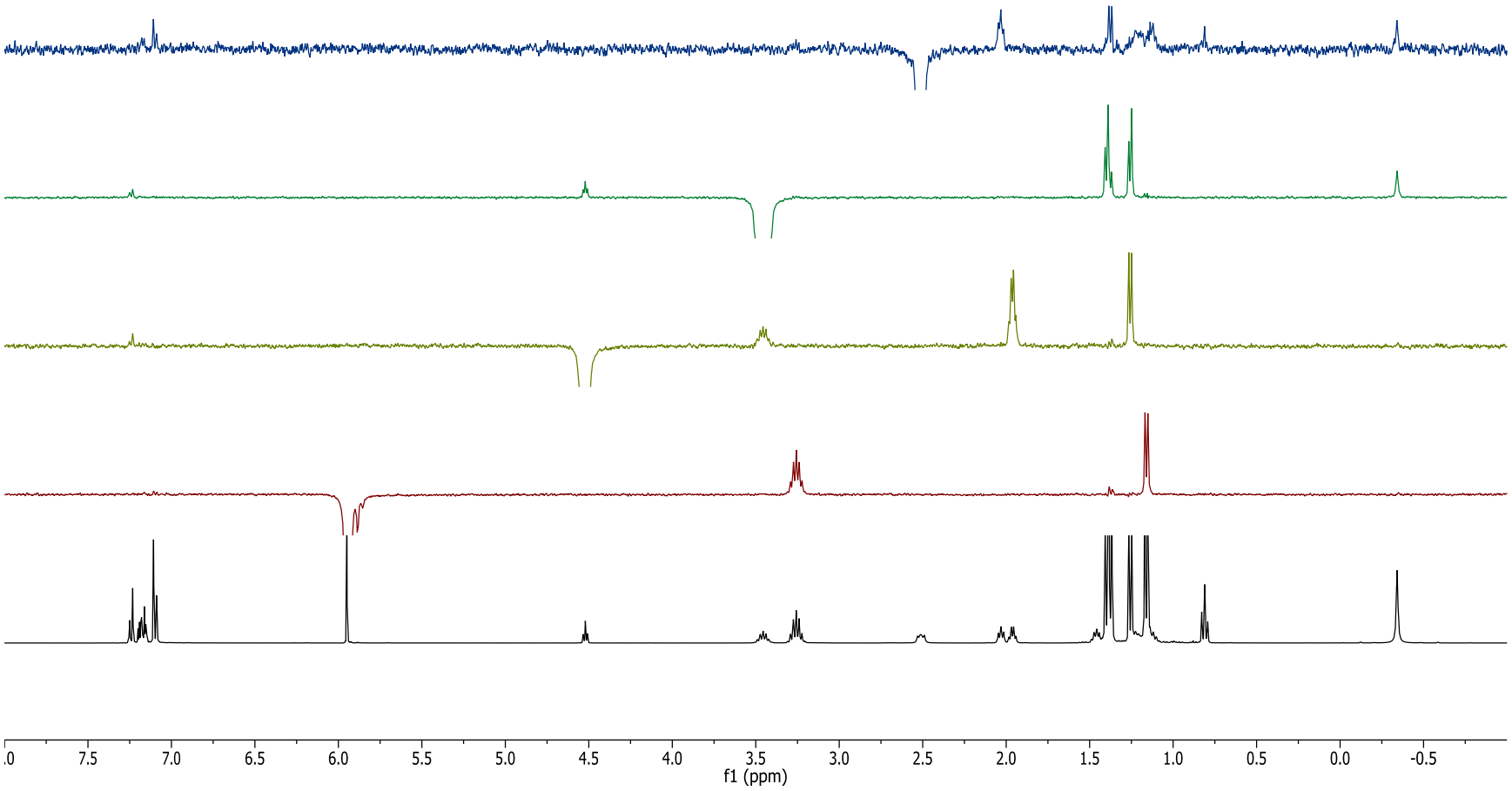


Figure 18. gCOSY NMR Spectrum of Complex **12** (C_6D_6, 400 MHz)

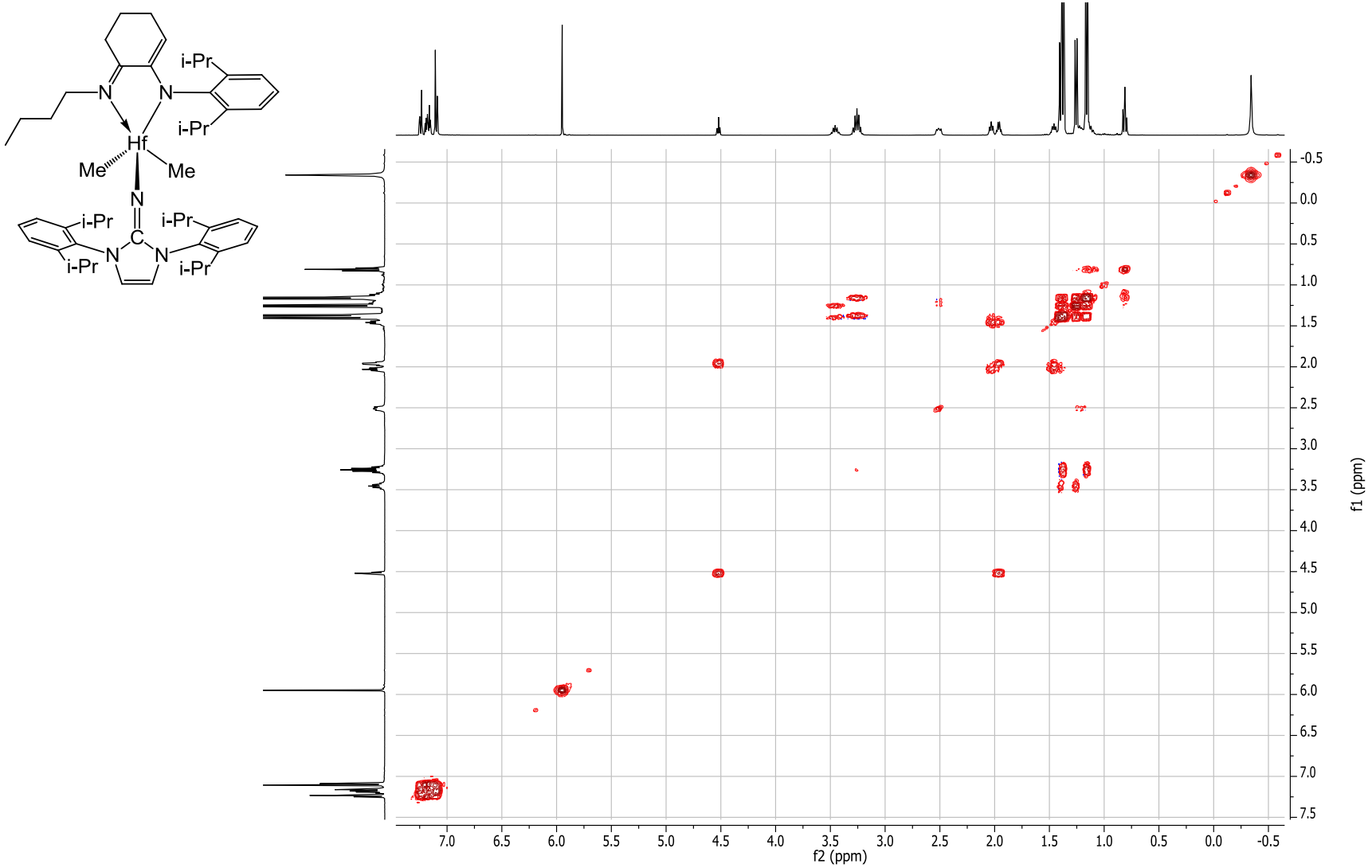


Figure 19. Fragment of gCOSY Spectrum of Complex **12** (C_6D_6, 400 MHz).

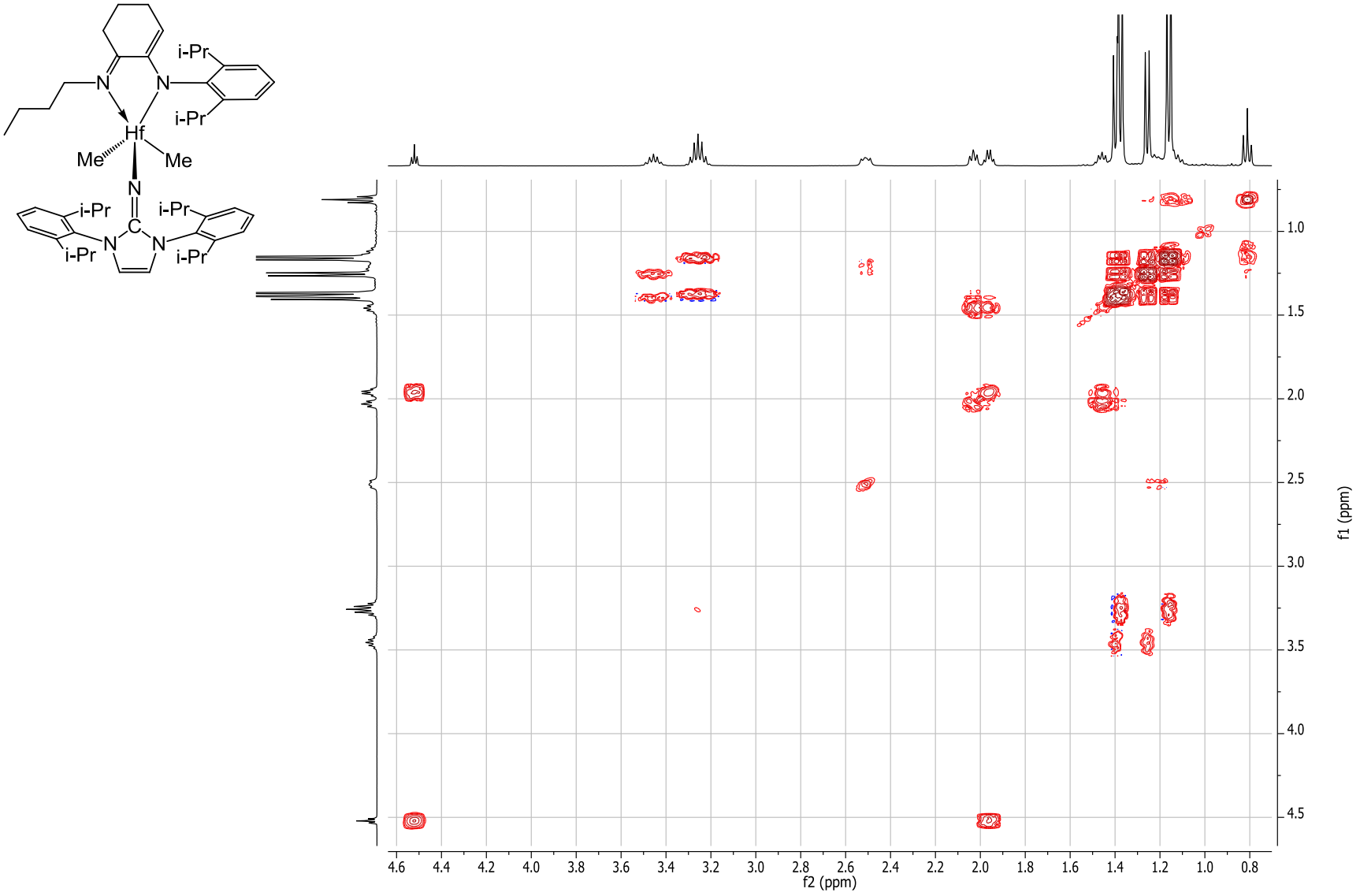


Figure 20. HSQCAD NMR Spectrum of Complex **12** (C_6D_6, 400 MHz).

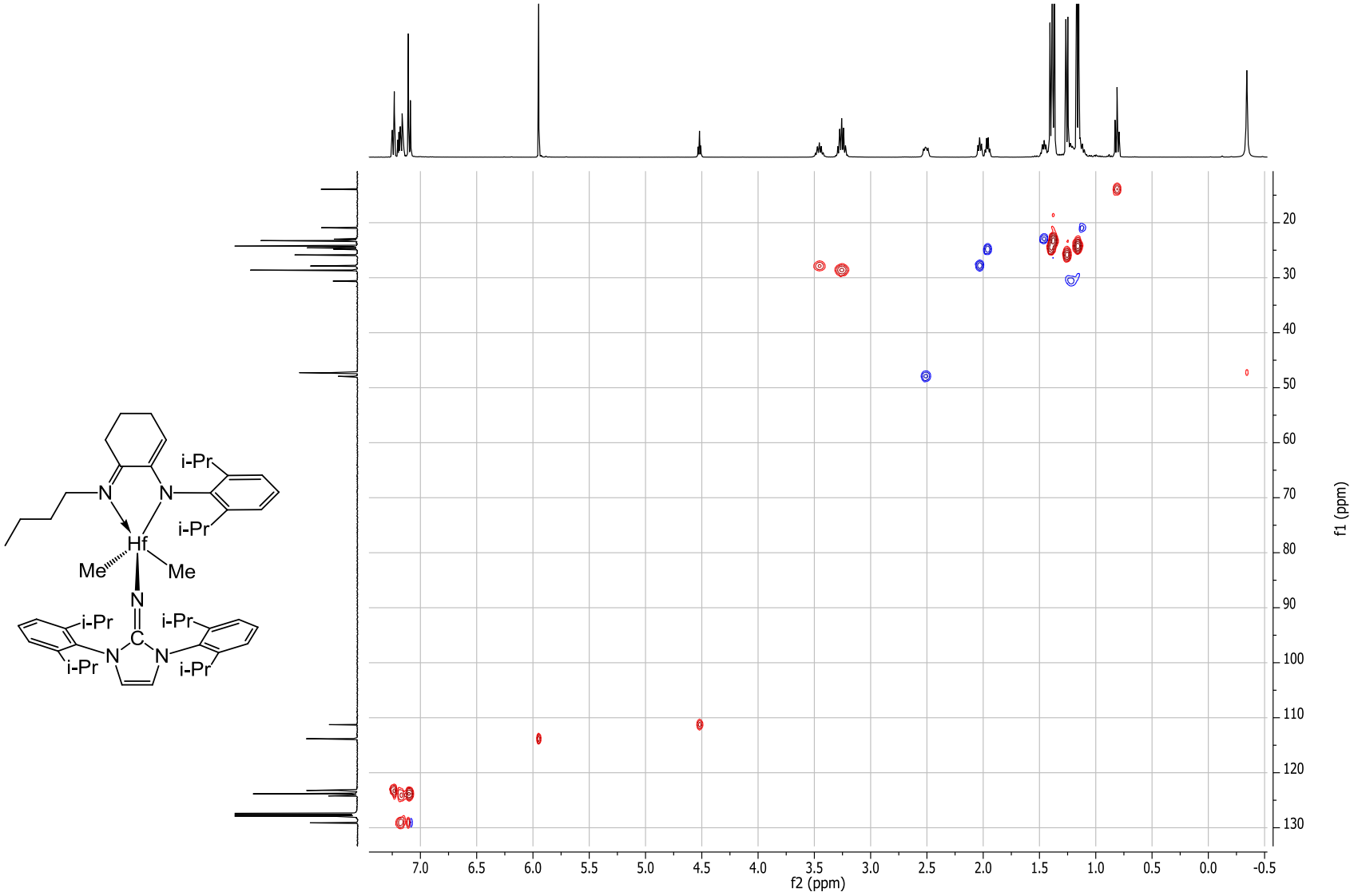


Figure 21. Fragments of gHSQC NMR Spectrum of Complex **12** (C_6D_6, 400 MHz).

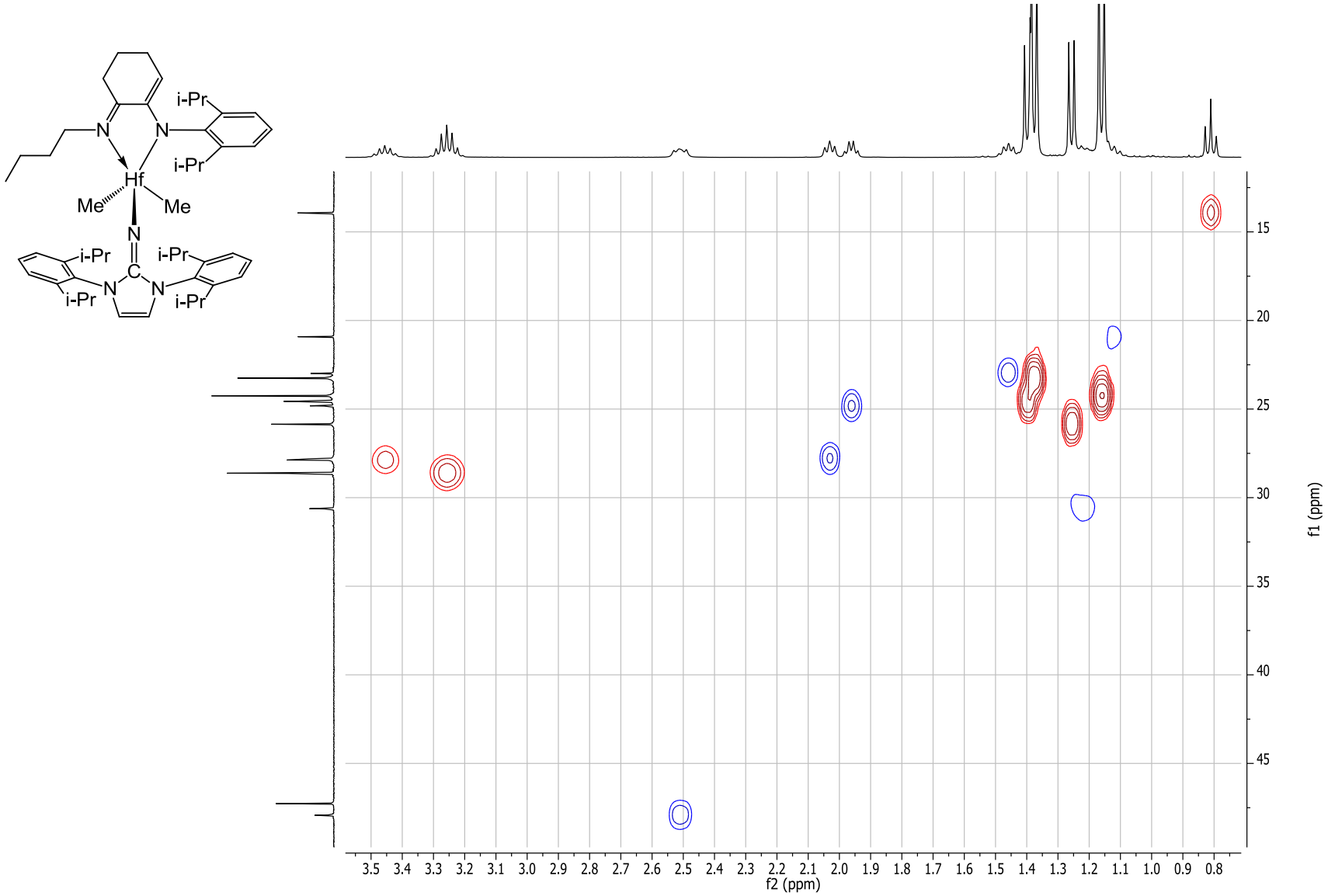


Figure 22. ^{1}H NMR Spectra of Complex **13** (C_6D_6, 400 MHz).

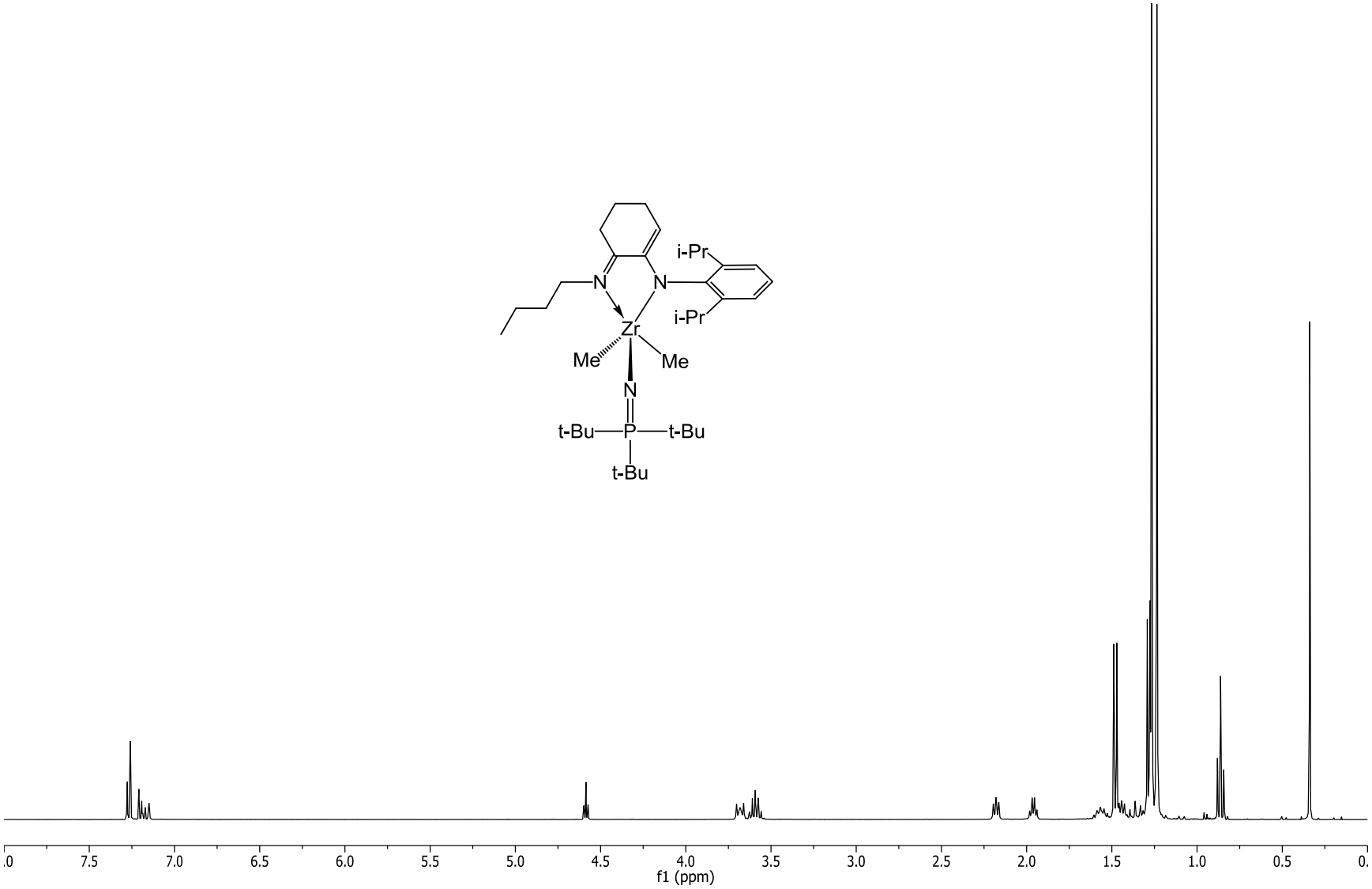


Figure 23. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **13** (C_6D_6, 100 MHz).

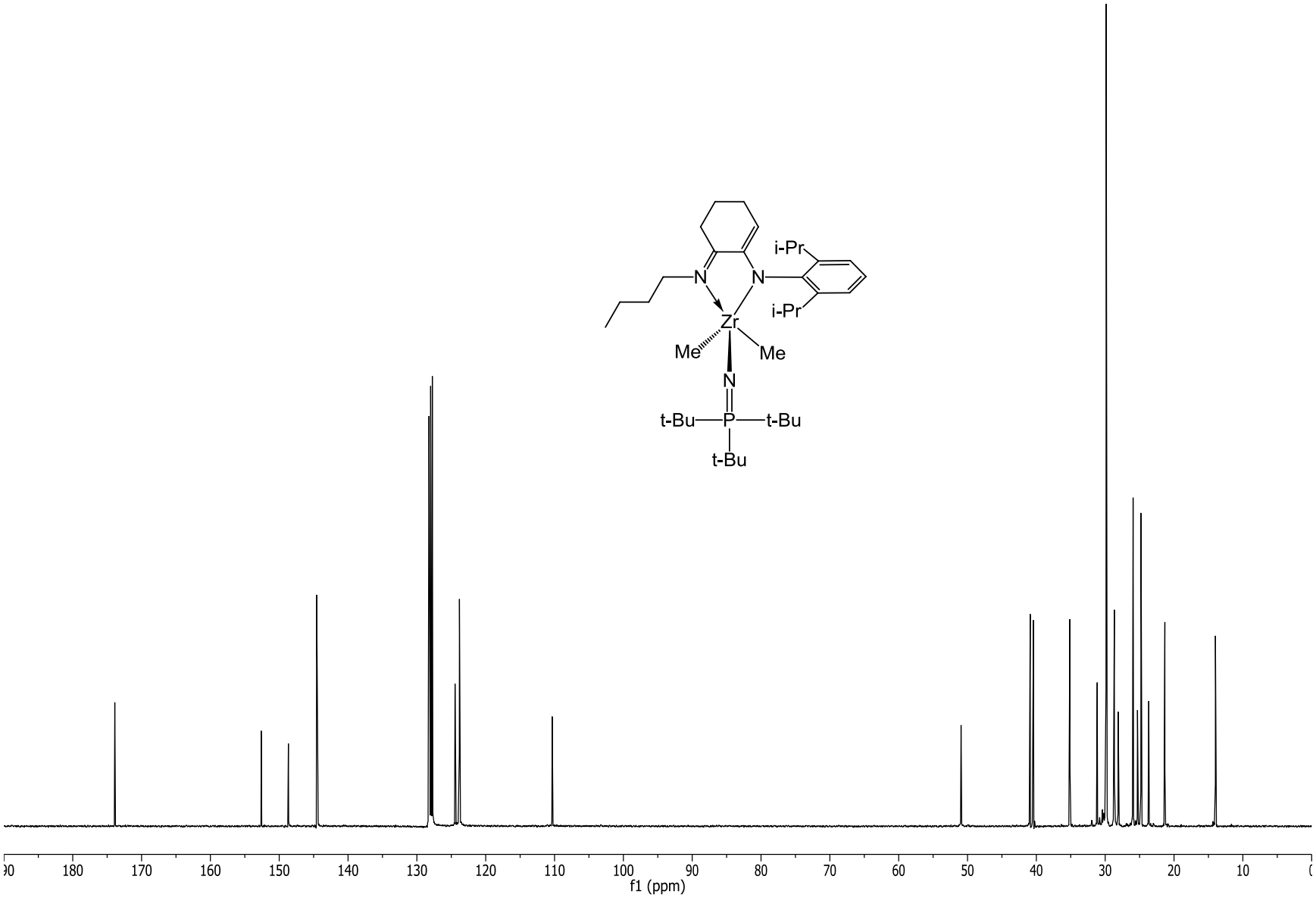


Figure 24. APT NMR Spectrum of Complex **13** (C_6D_6, 100 MHz).

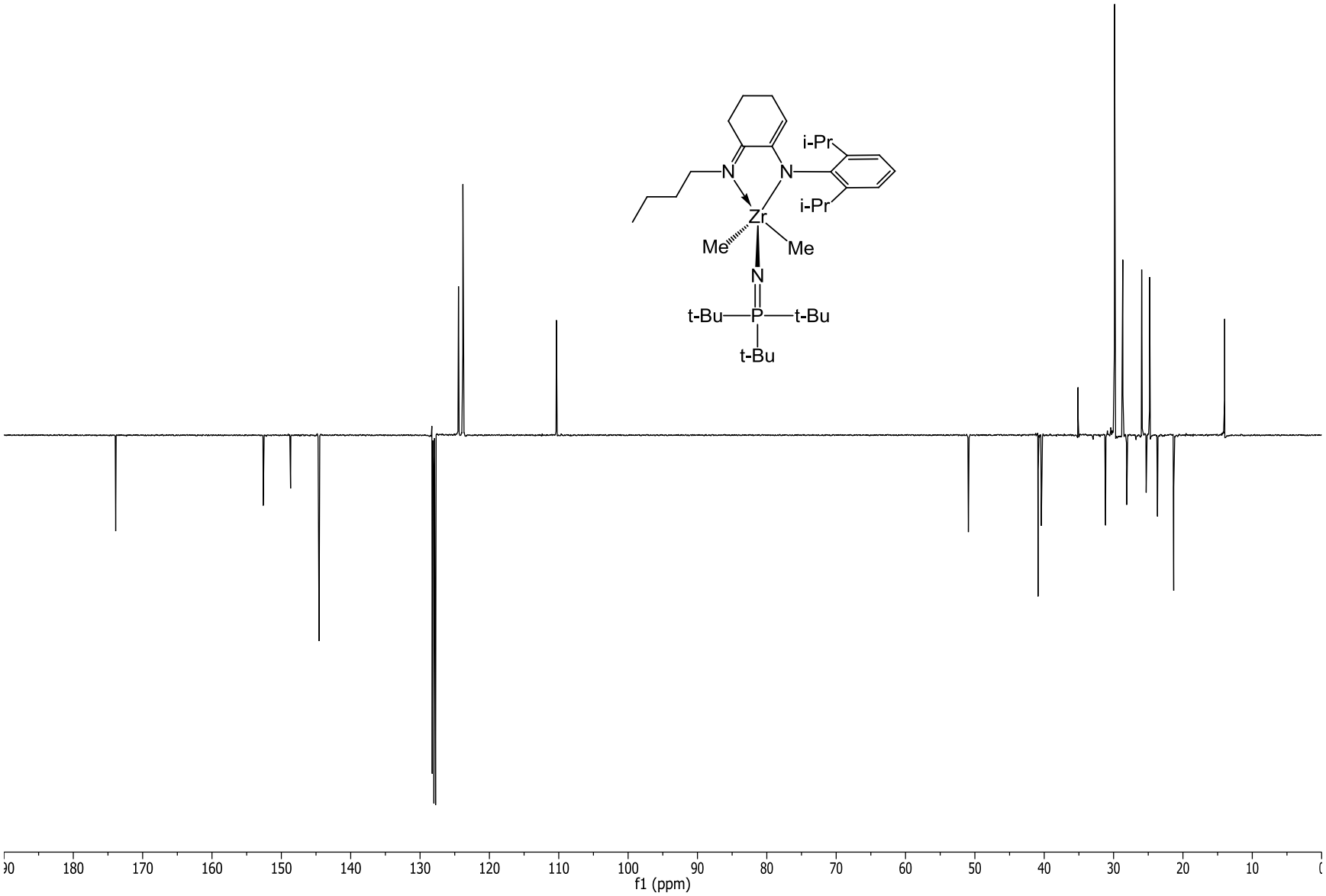


Figure 25. TOCSY1D NMR Spectra of Complex **13** (C_6D_6, 400 MHz) (mix time = 0, 0.03, 0.08 s).

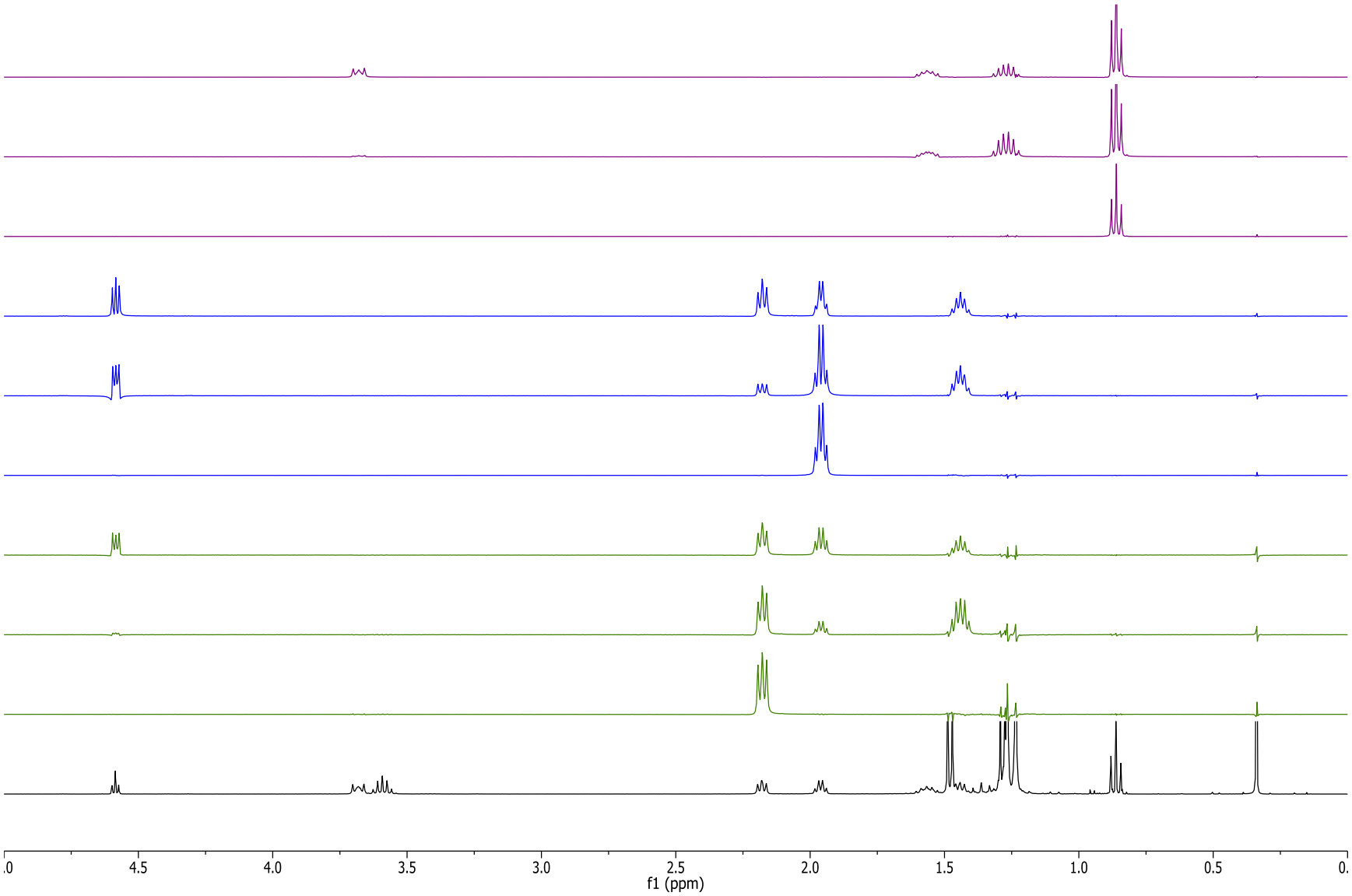


Figure 26. ^{1}H and NOESY1D NMR Spectra of Complex **13** (C_6D_6, 400 MHz, mixing time = 0.8 s).

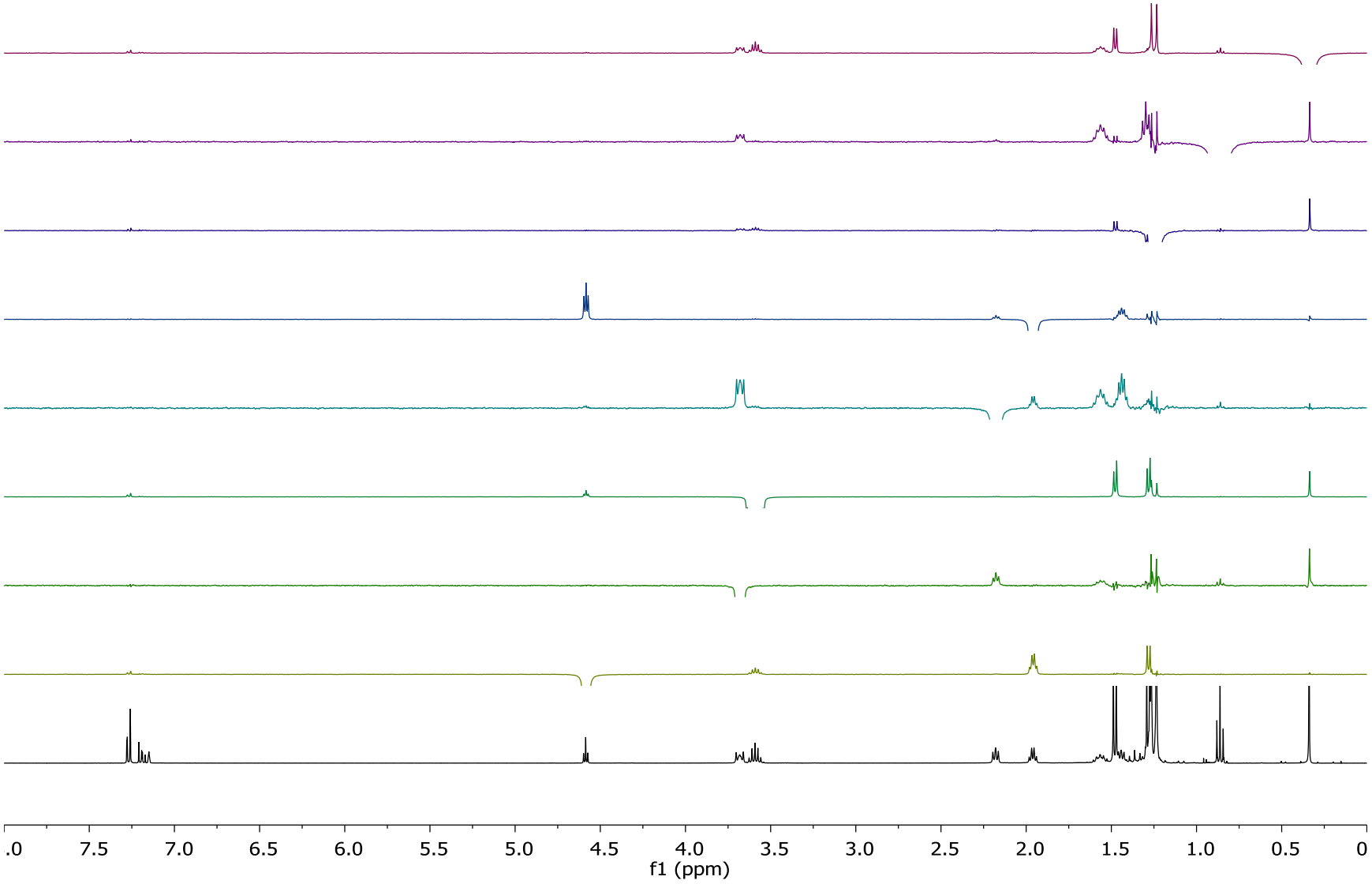


Figure 27. gCOSY NMR Spectrum of Complex **13** (C_6D_6, 400 MHz).

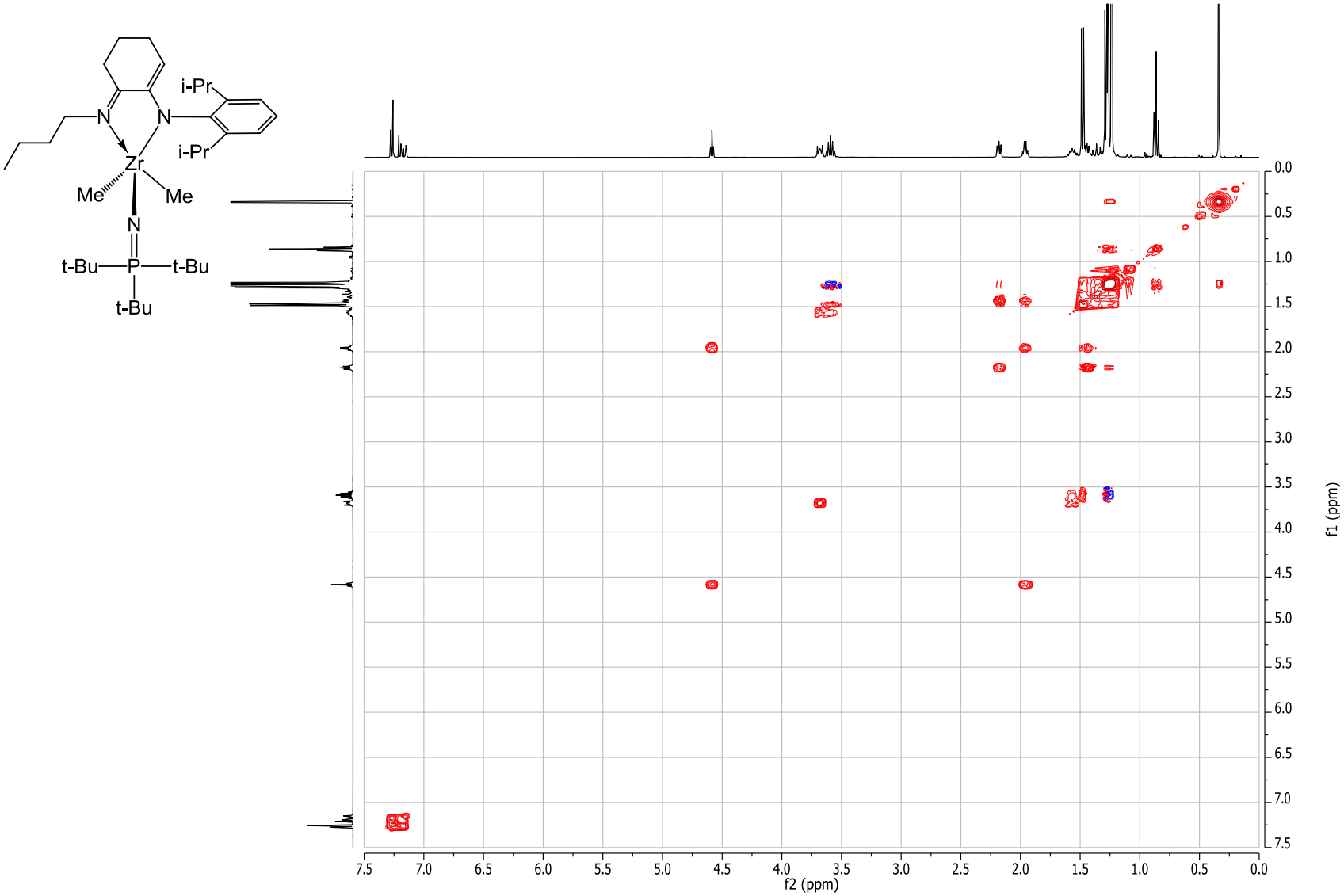


Figure 28. Fragment of gCOSY Spectrum of Complex **13** (C_6D_6, 400 MHz).

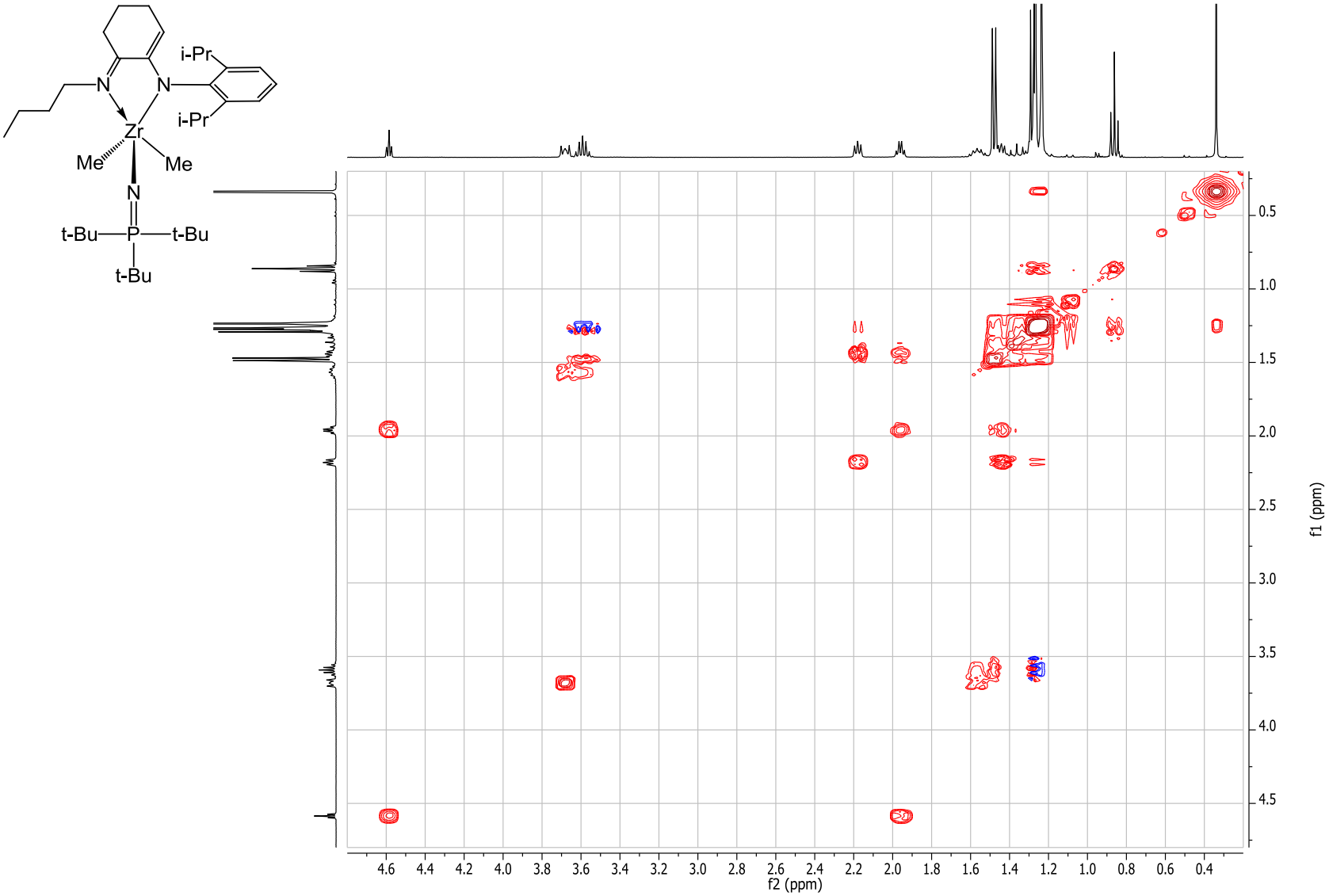


Figure 29. HSQCAD NMR Spectrum of Complex **13** (C_6D_6, 400 MHz).

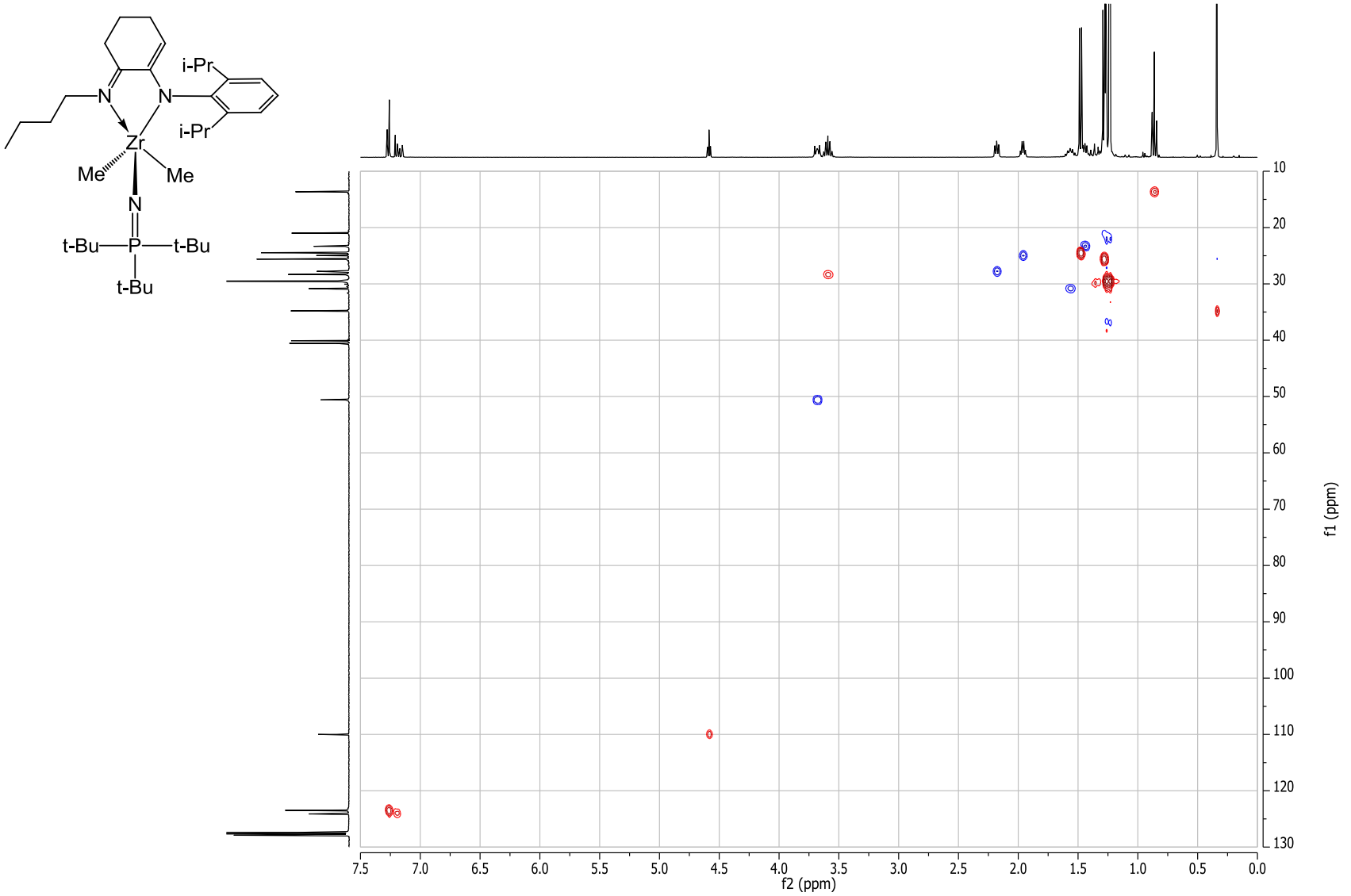


Figure 30. Fragment of gHSQCAD NMR Spectrum of Complex **13** (C_6D_6, 400 MHz).

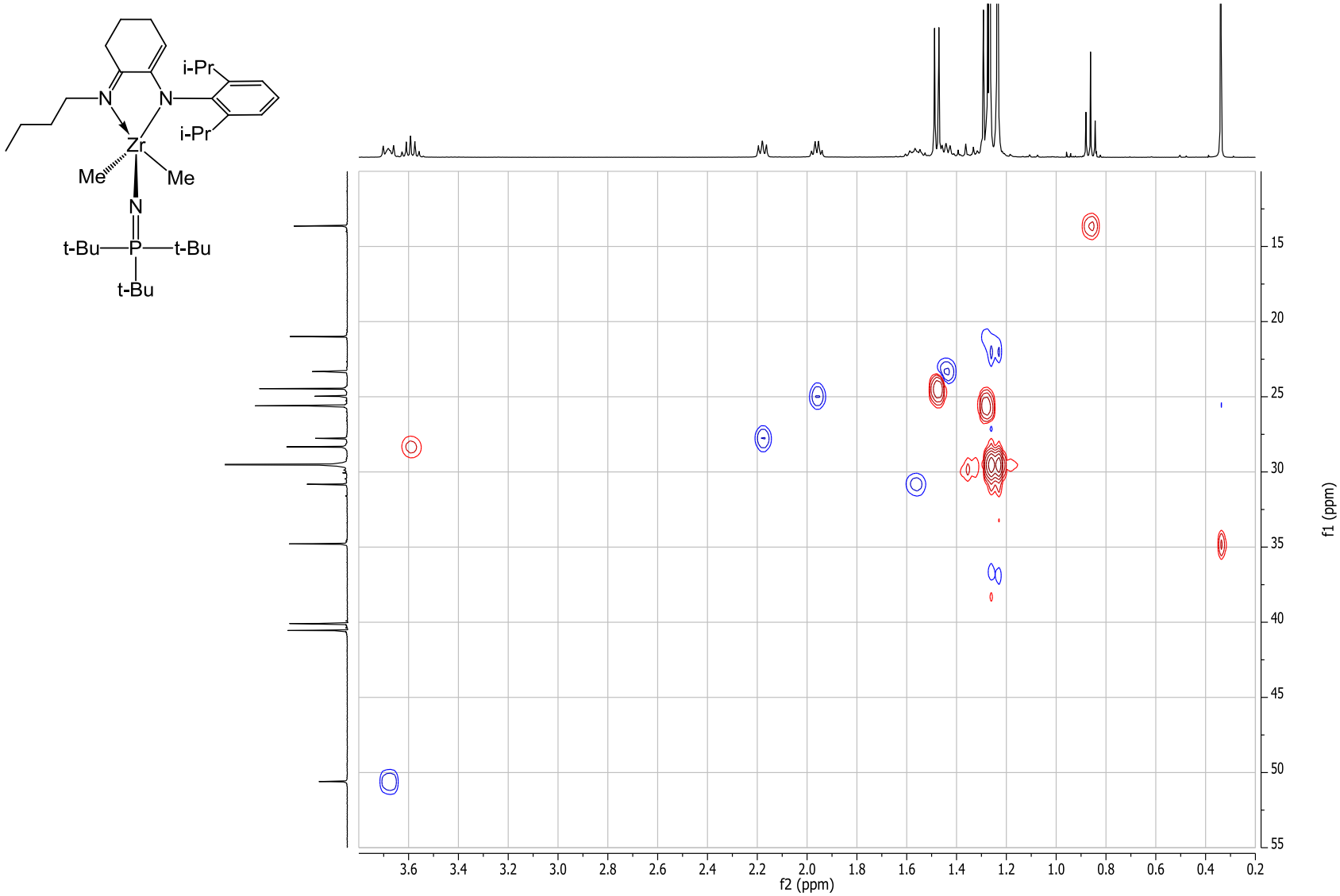


Figure 31: ^{31}P NMR Spectrum of Complex **13** (C_6D_6, 202 MHz).

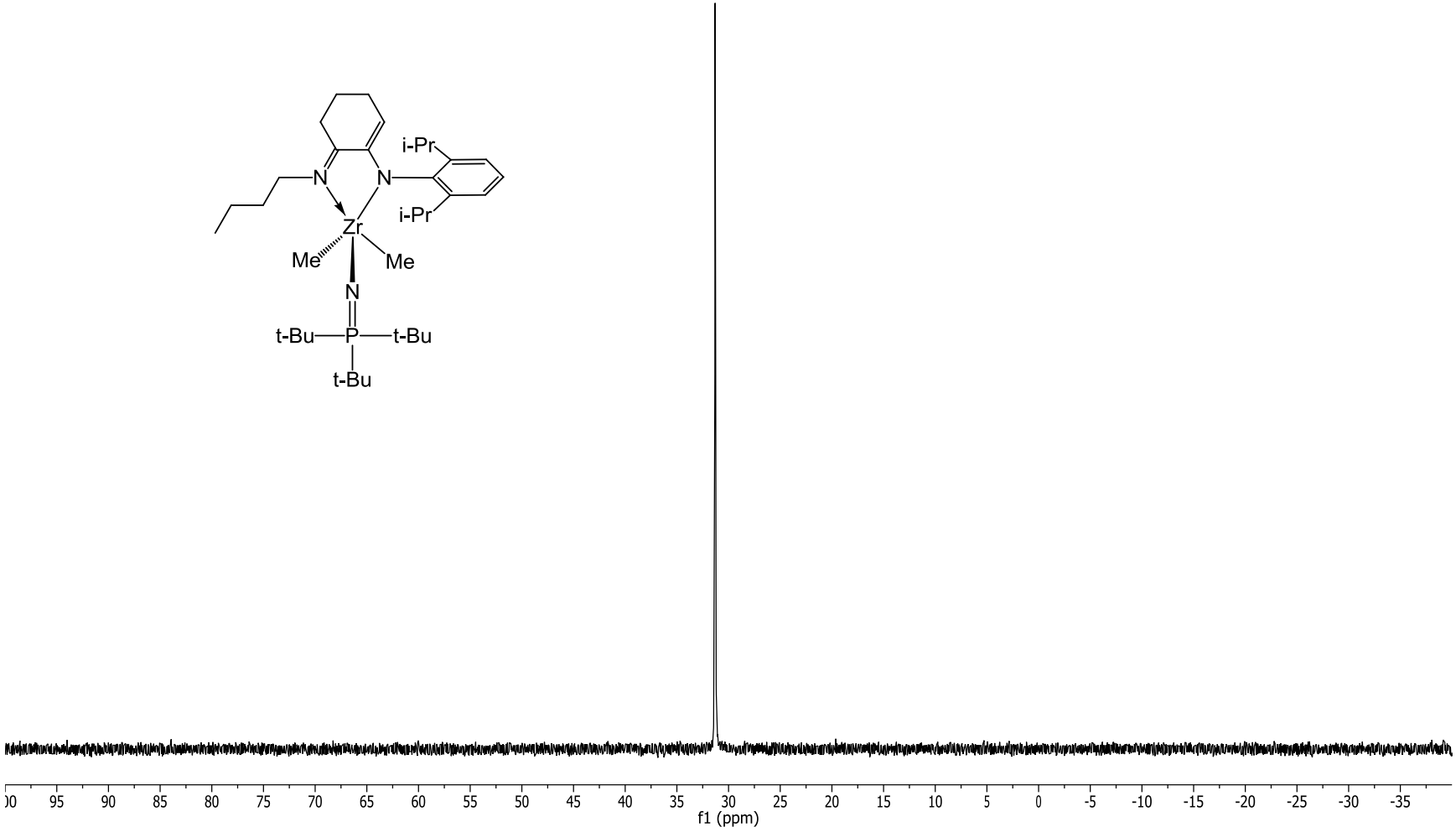


Figure 32. ^{1}H NMR Spectra of Complex **14** (C_6D_6, 500 MHz).

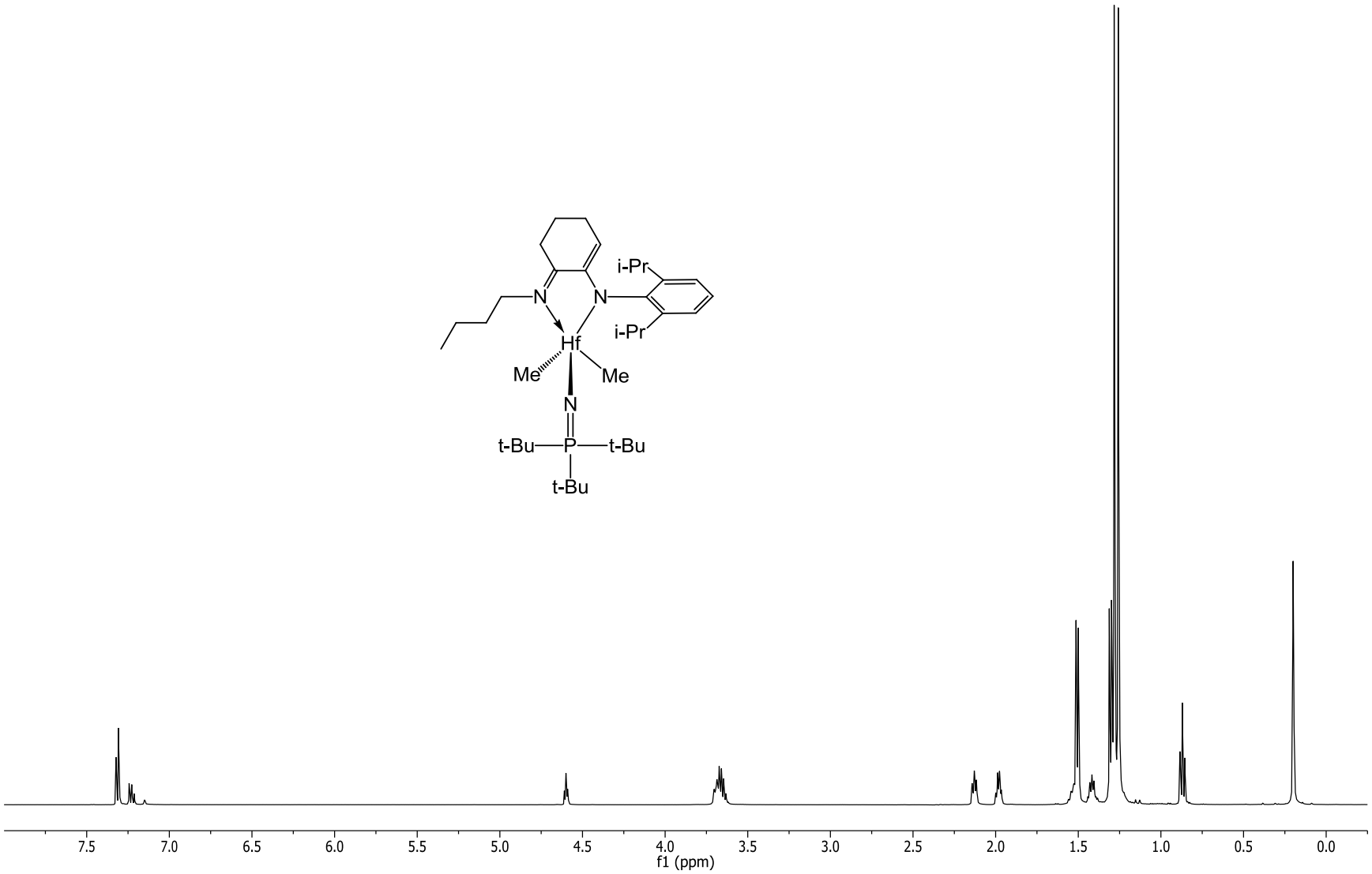


Figure 33. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **14** (C_6D_6, 125 MHz).

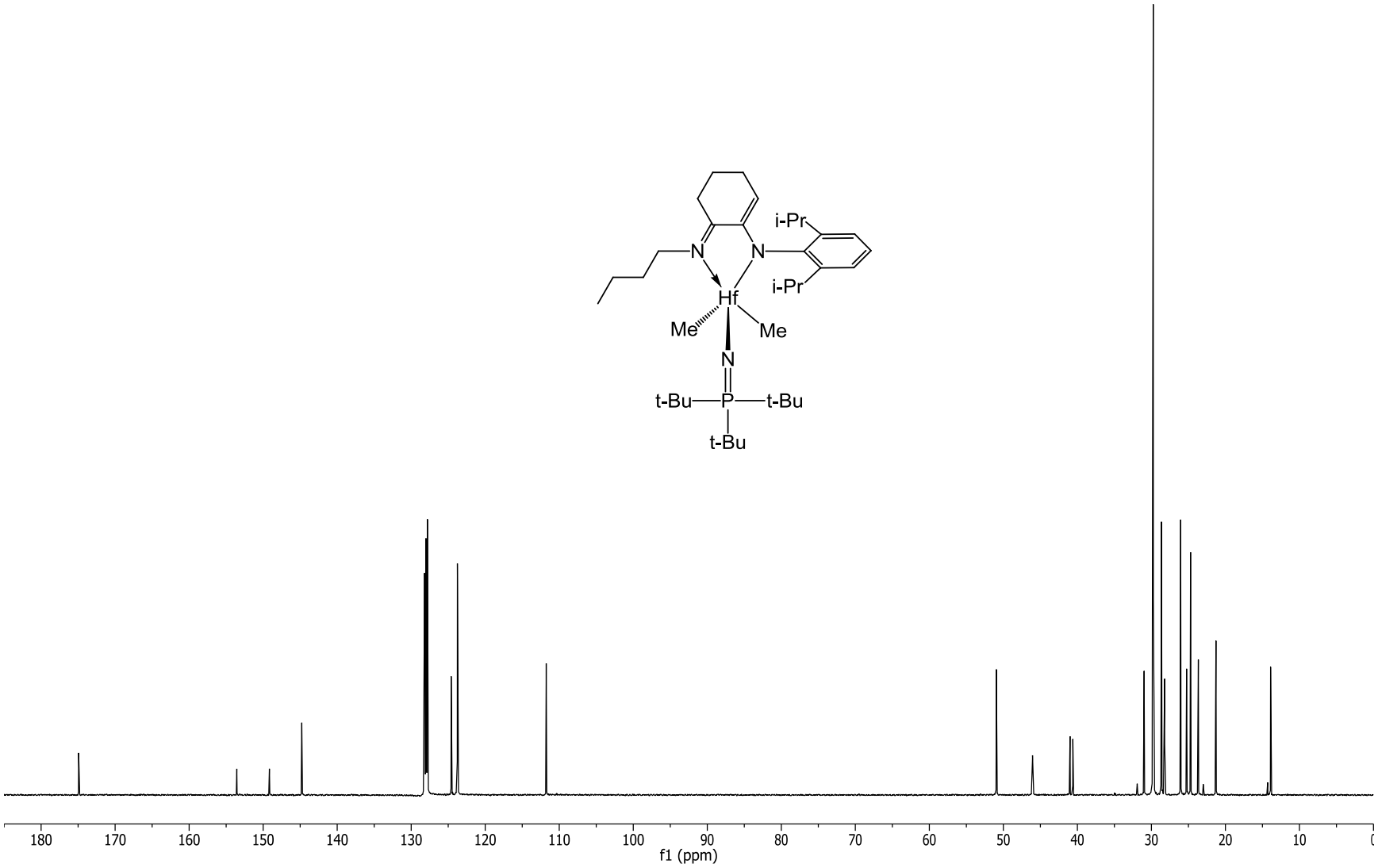


Figure 34. TOCSY1D NMR Spectra of Complex **14** (C_6D_6, 500 MHz) (mix time = 0, 0.03, 0.08 s).

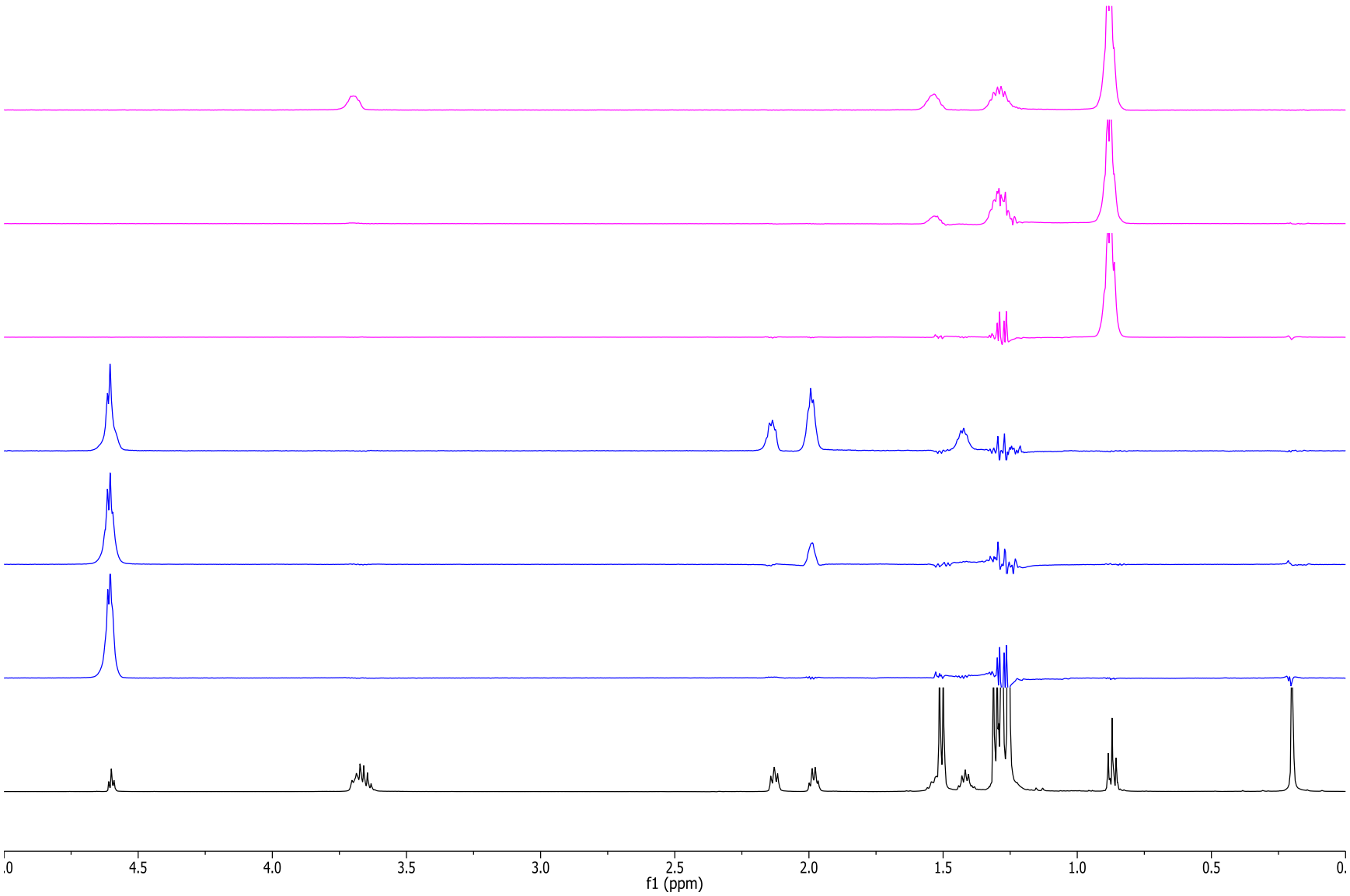


Figure 35. ^{1}H and NOESY1D NMR Spectra of Complex **14** (C_6D_6, 500 MHz, mixing time = 0.8 s).

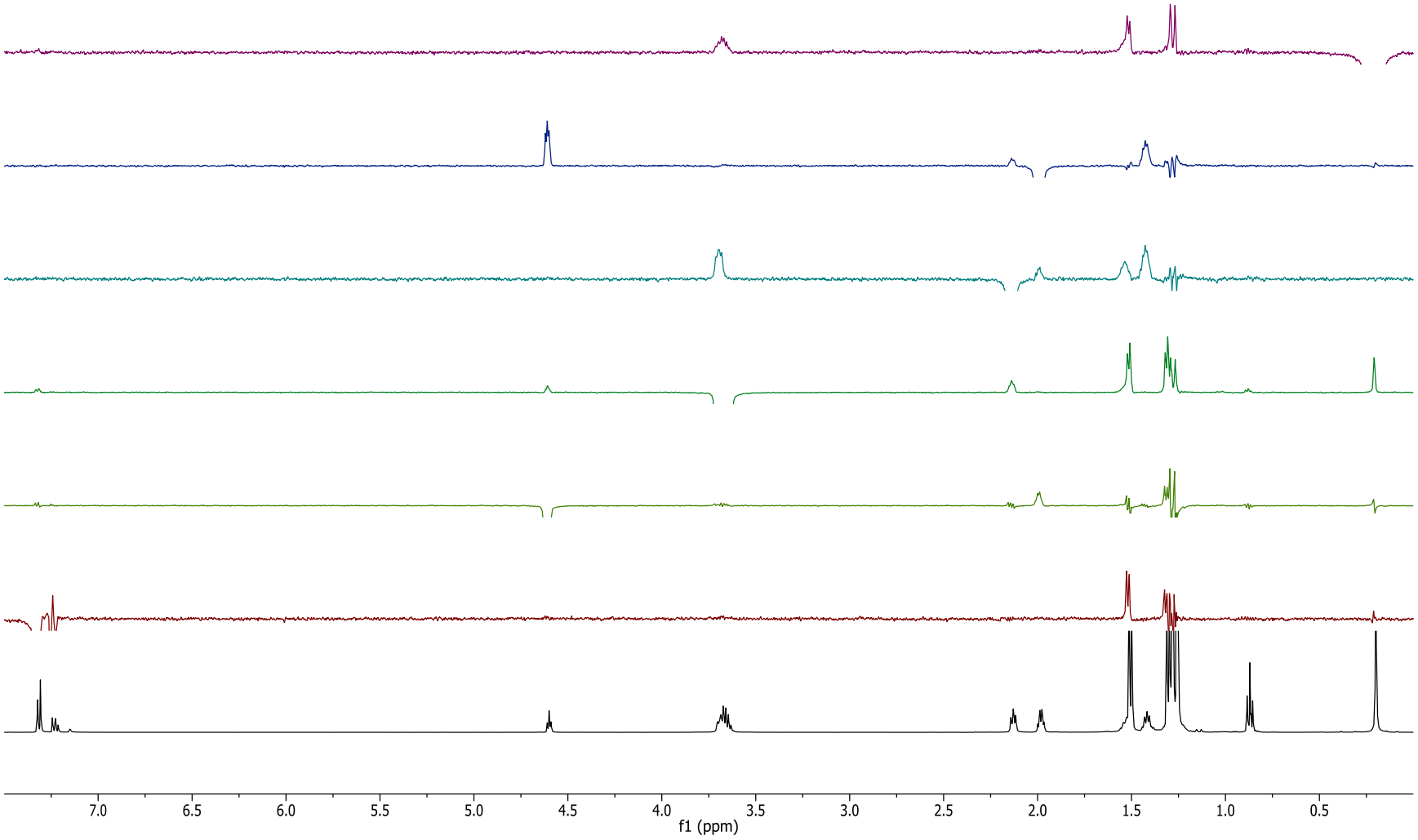


Figure 36. gCOSY NMR Spectrum of Complex **14** (C_6D_6, 500 MHz).

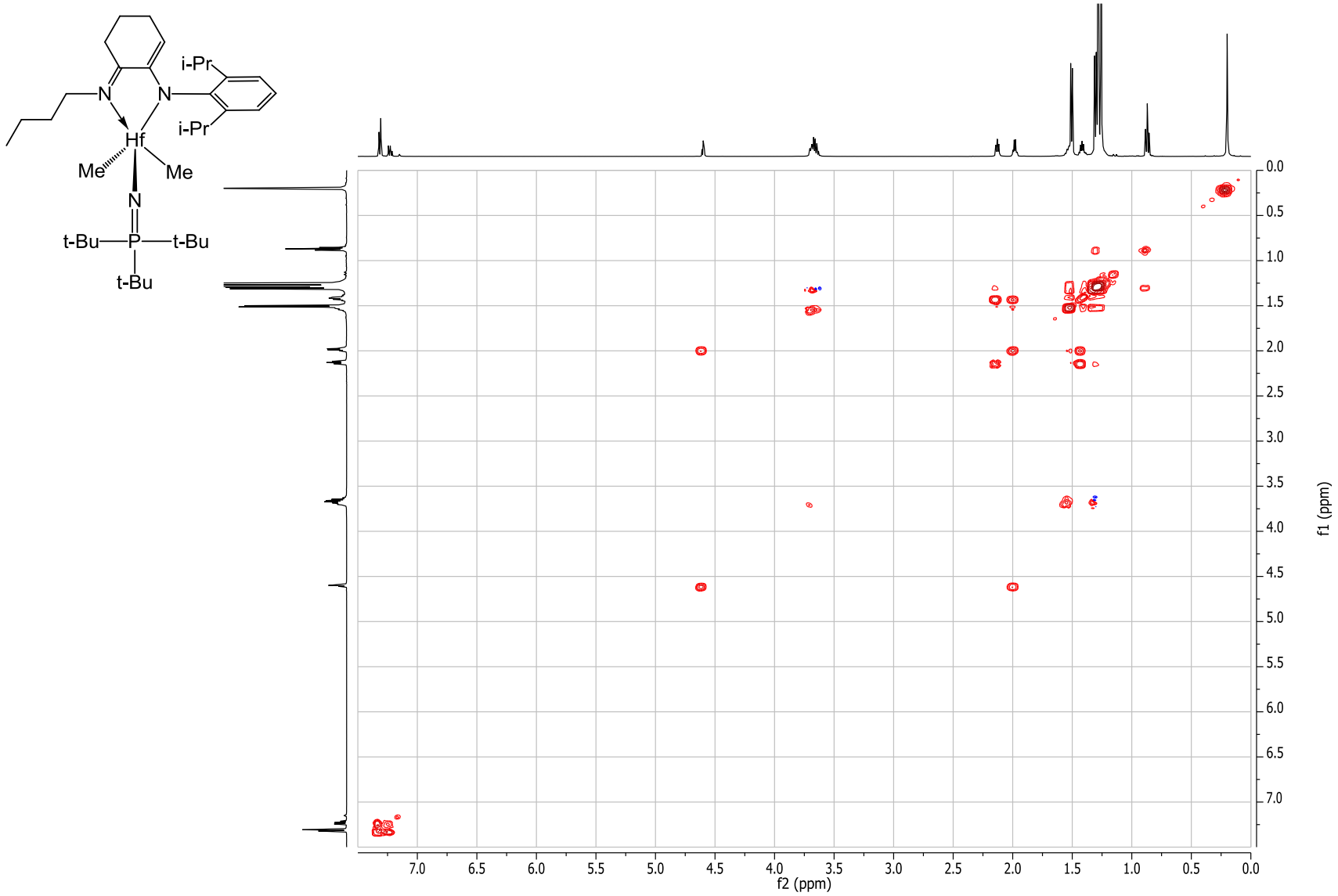


Figure 37. Fragment of gCOSY Spectrum of Complex **14** (C_6D_6, 500 MHz).

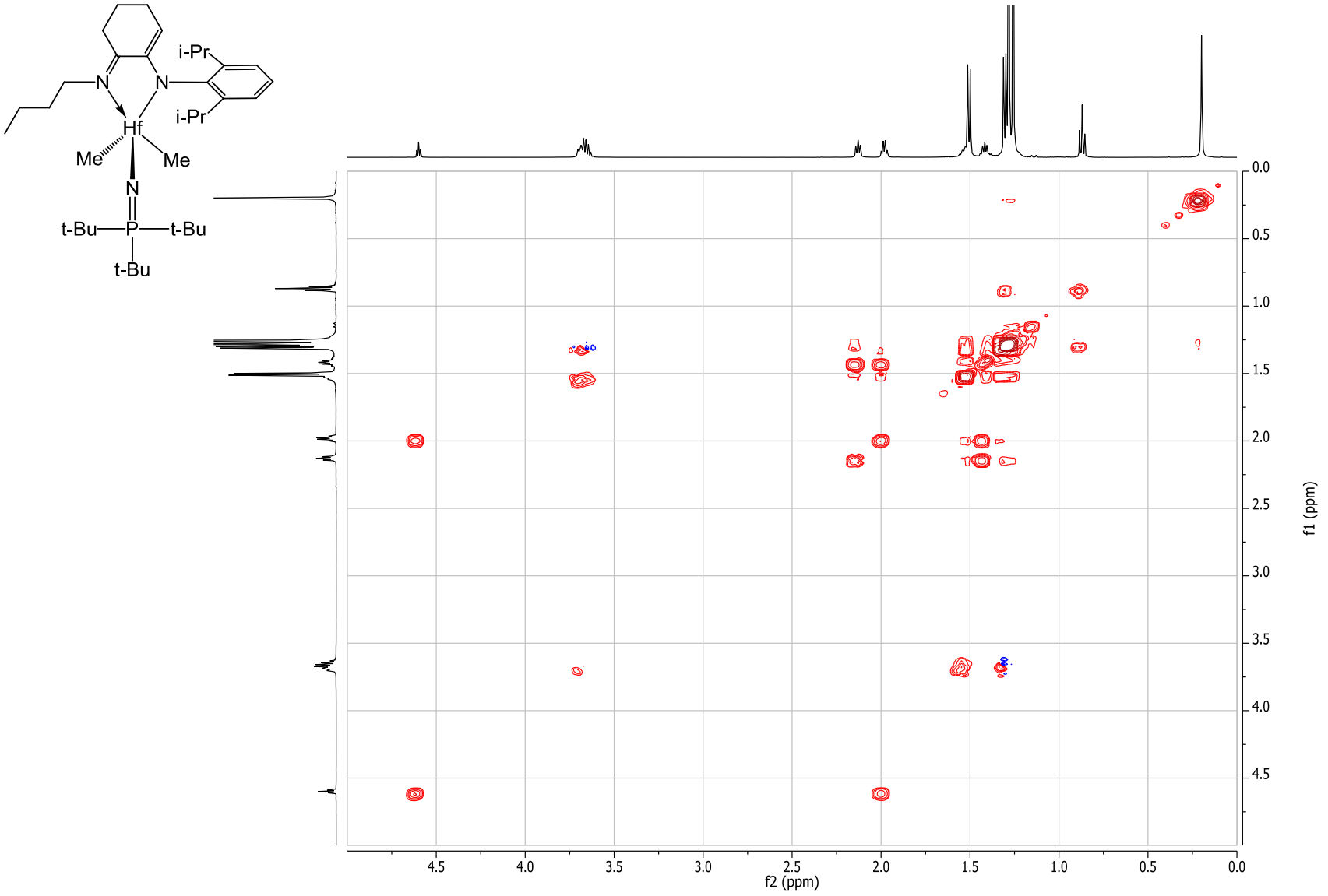


Figure 38. HSQCAD NMR Spectrum of Complex **14** (C_6D_6, 500 MHz).

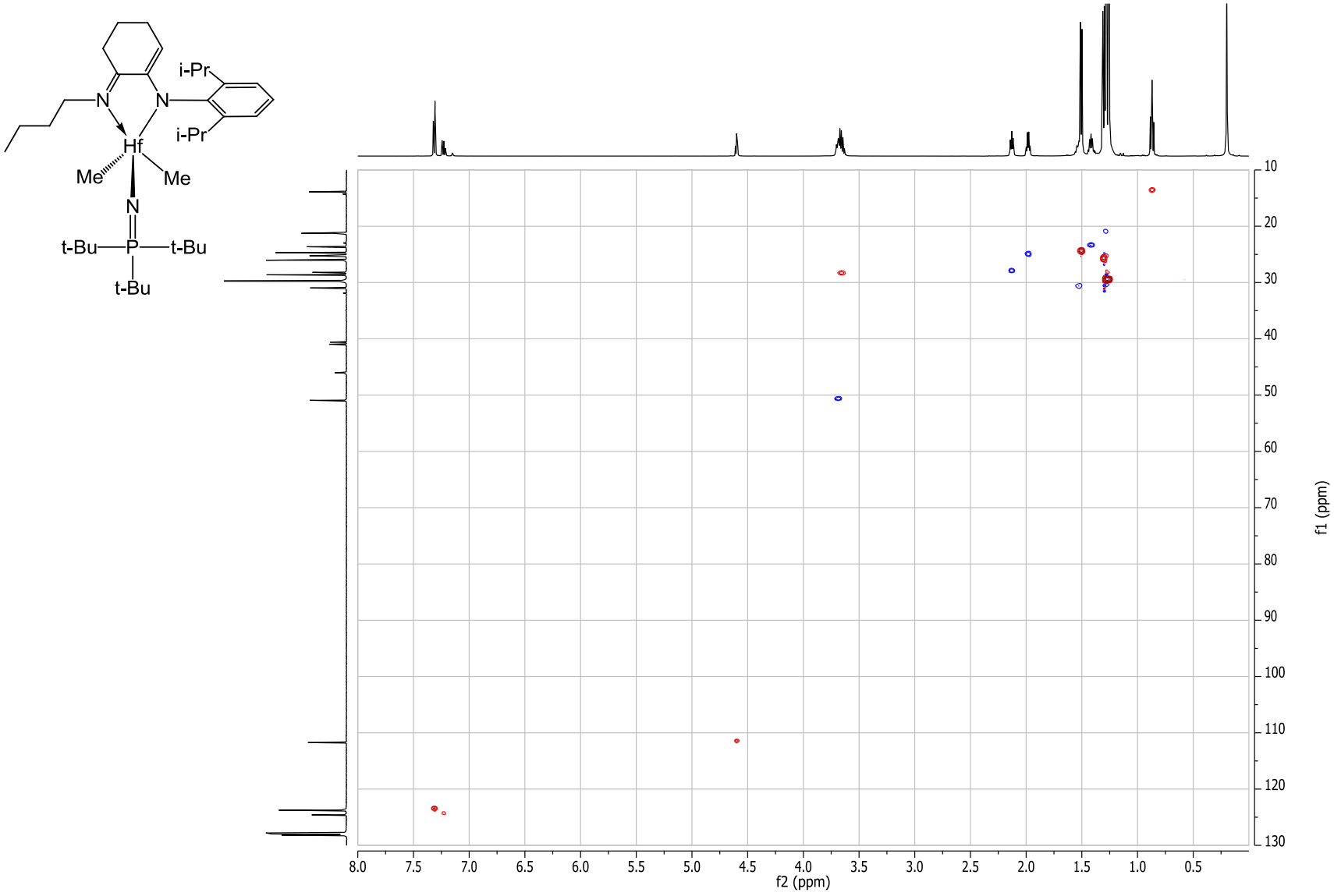


Figure 39. Fragment of gHSQCAD NMR Spectrum of Complex **14** (C_6D_6, 500 MHz).

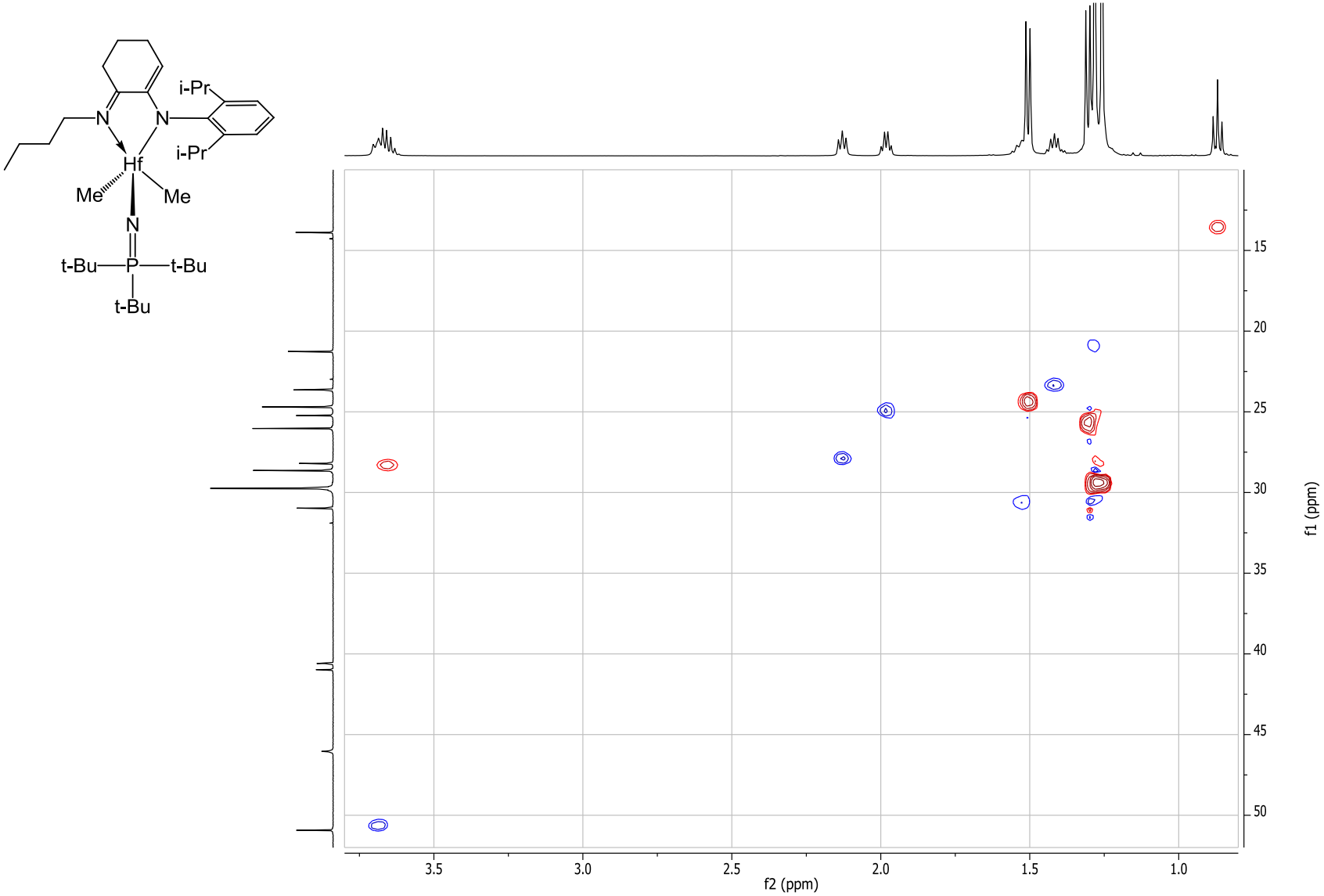


Figure 40.^{31}P NMR Spectrum of Complex **14** (C_6D_6, 202 MHz).

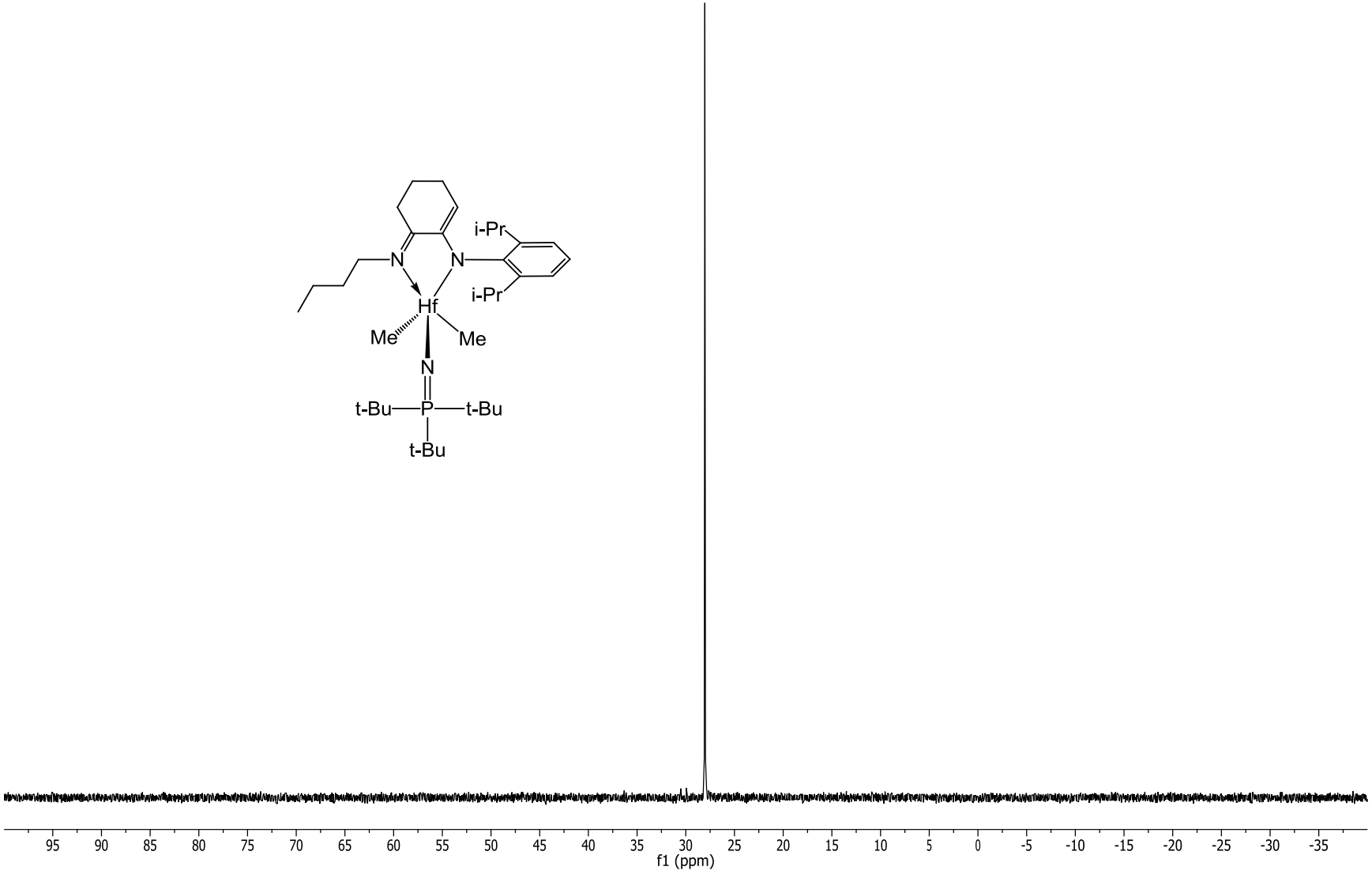


Figure 41. ^{1}H NMR Spectra of Complex **15** (C_6D_6, 400 MHz).

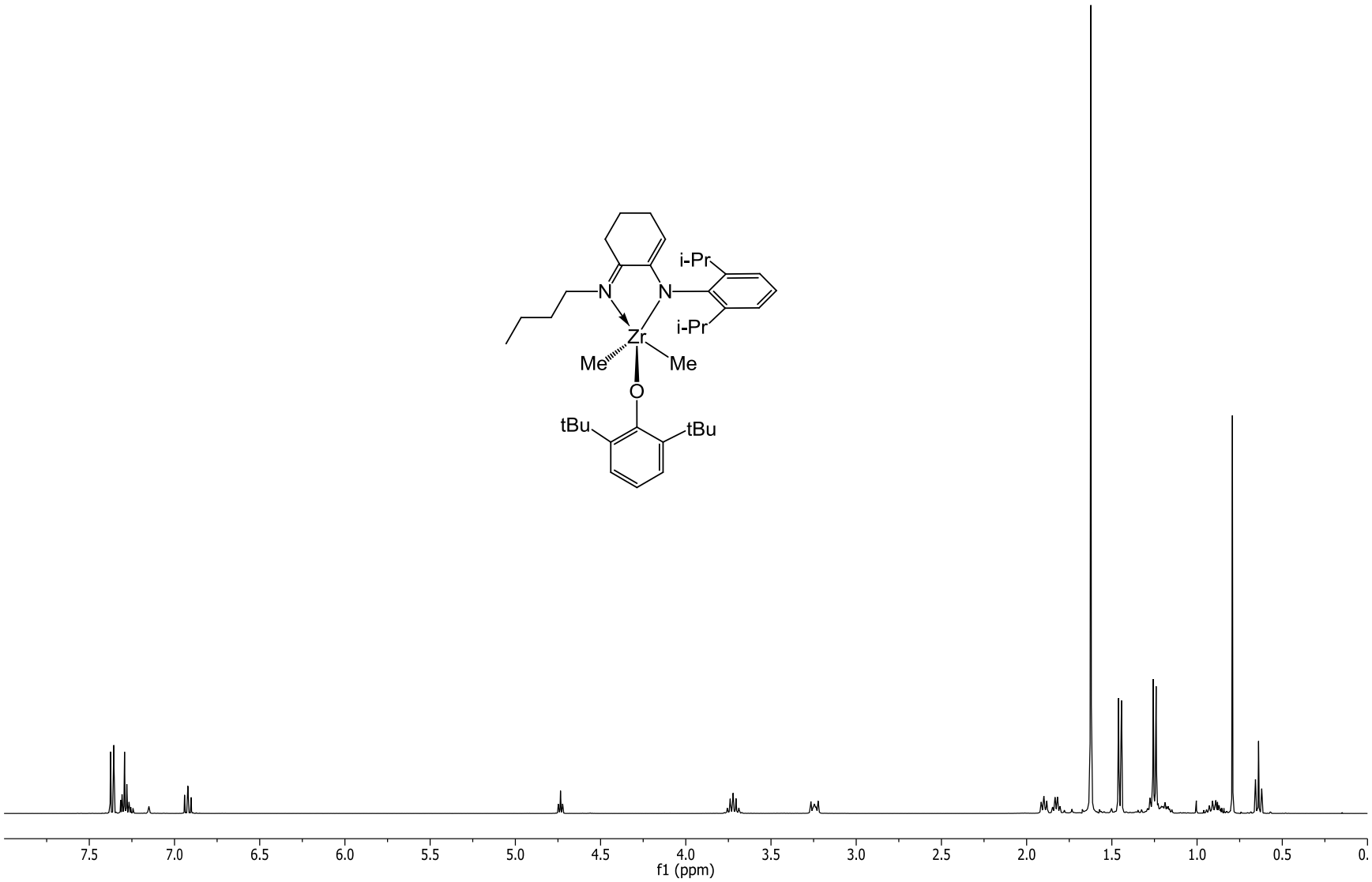


Figure 42. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **15** (C_6D_6, 100 MHz).

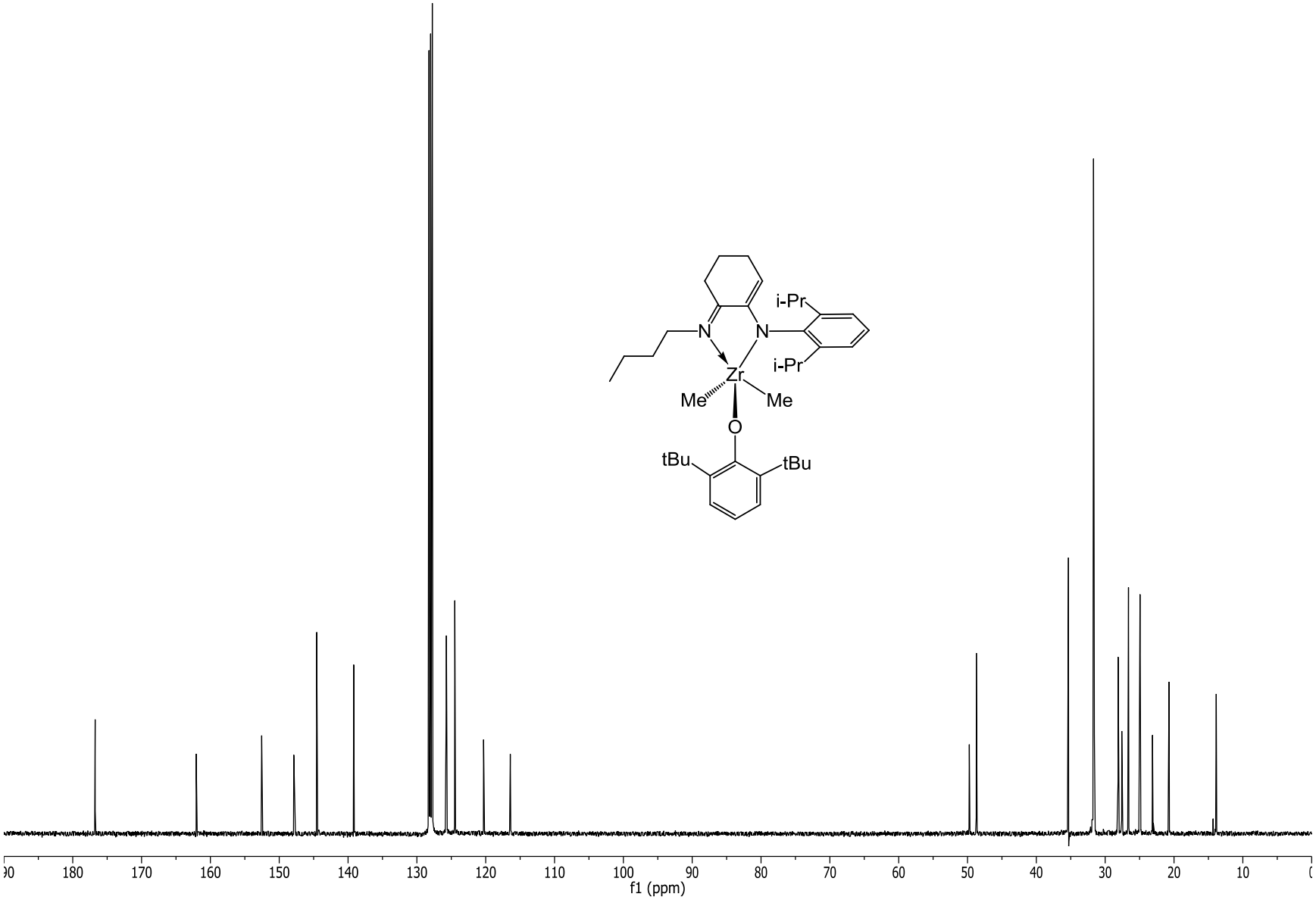


Figure 43. APT NMR Spectrum of Complex **15** (C_6D_6, 100 MHz).

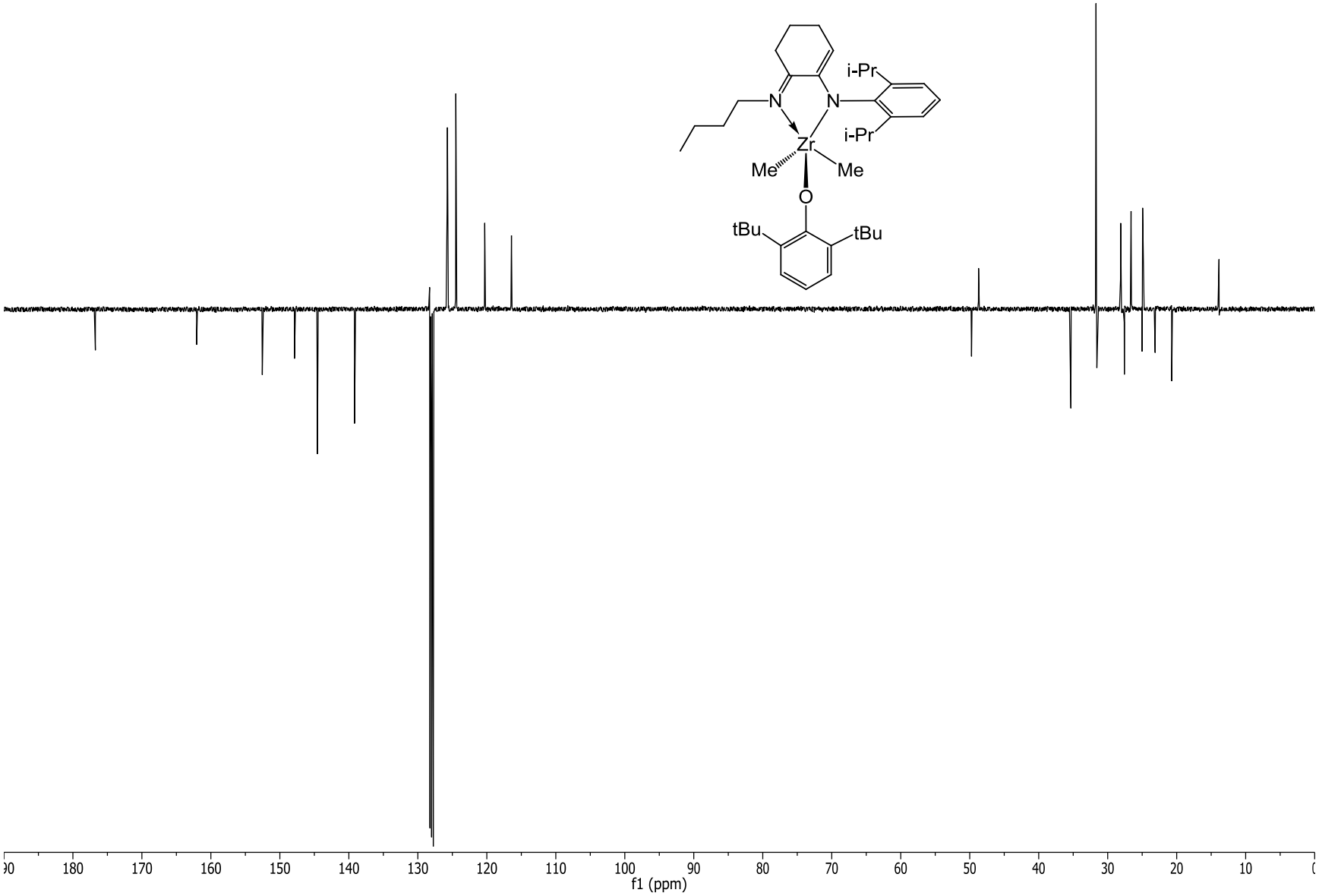


Figure 44. TOCSY1D NMR Spectra of Complex **15** (C_6D_6, 400 MHz) (mix time = 0, 0.03, 0.08 s).

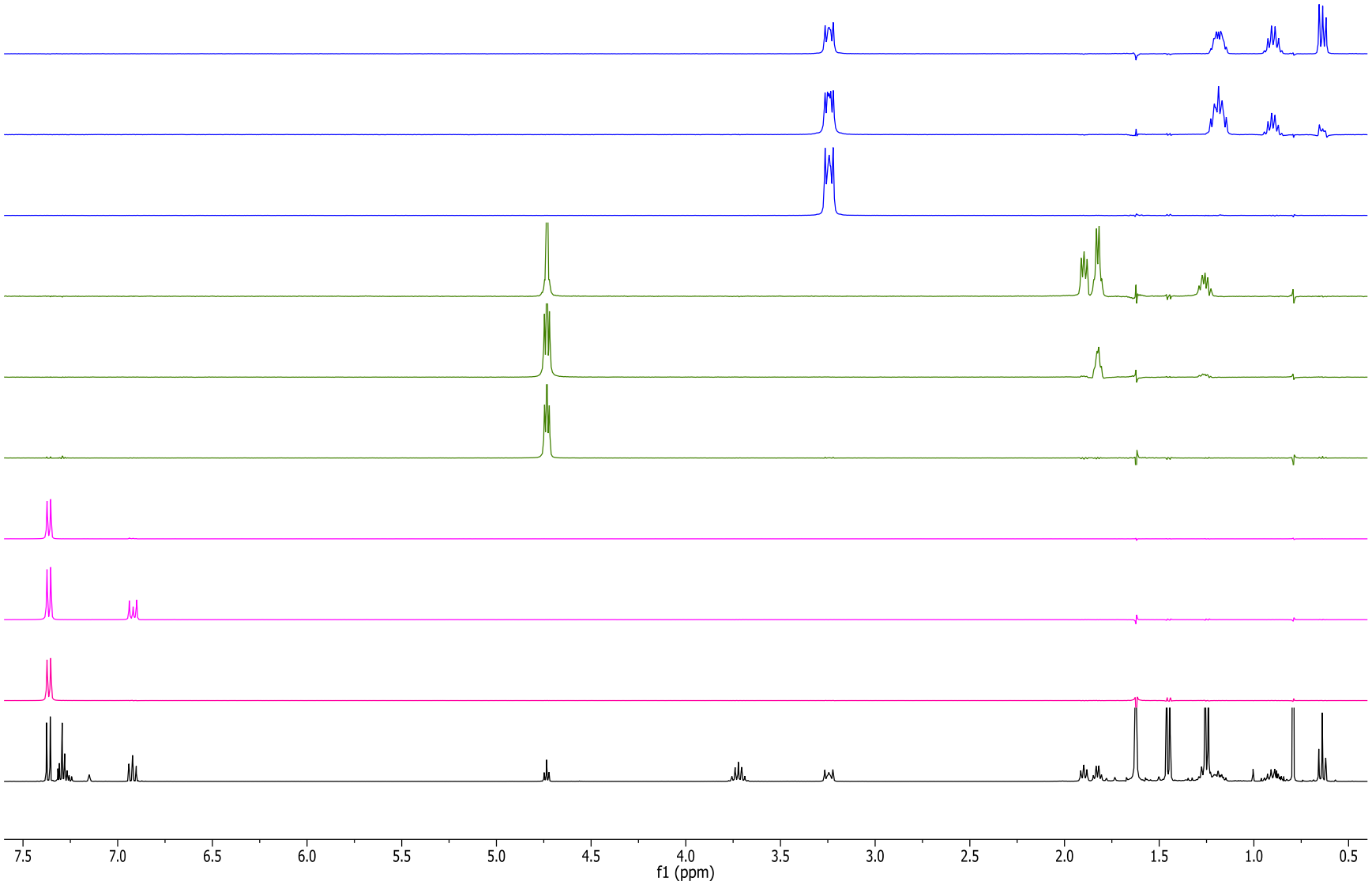


Figure 45. ^{1}H and NOESY1D NMR Spectra of Complex **15** (C_6D_6, 400 MHz, mixing time = 0.8 s).

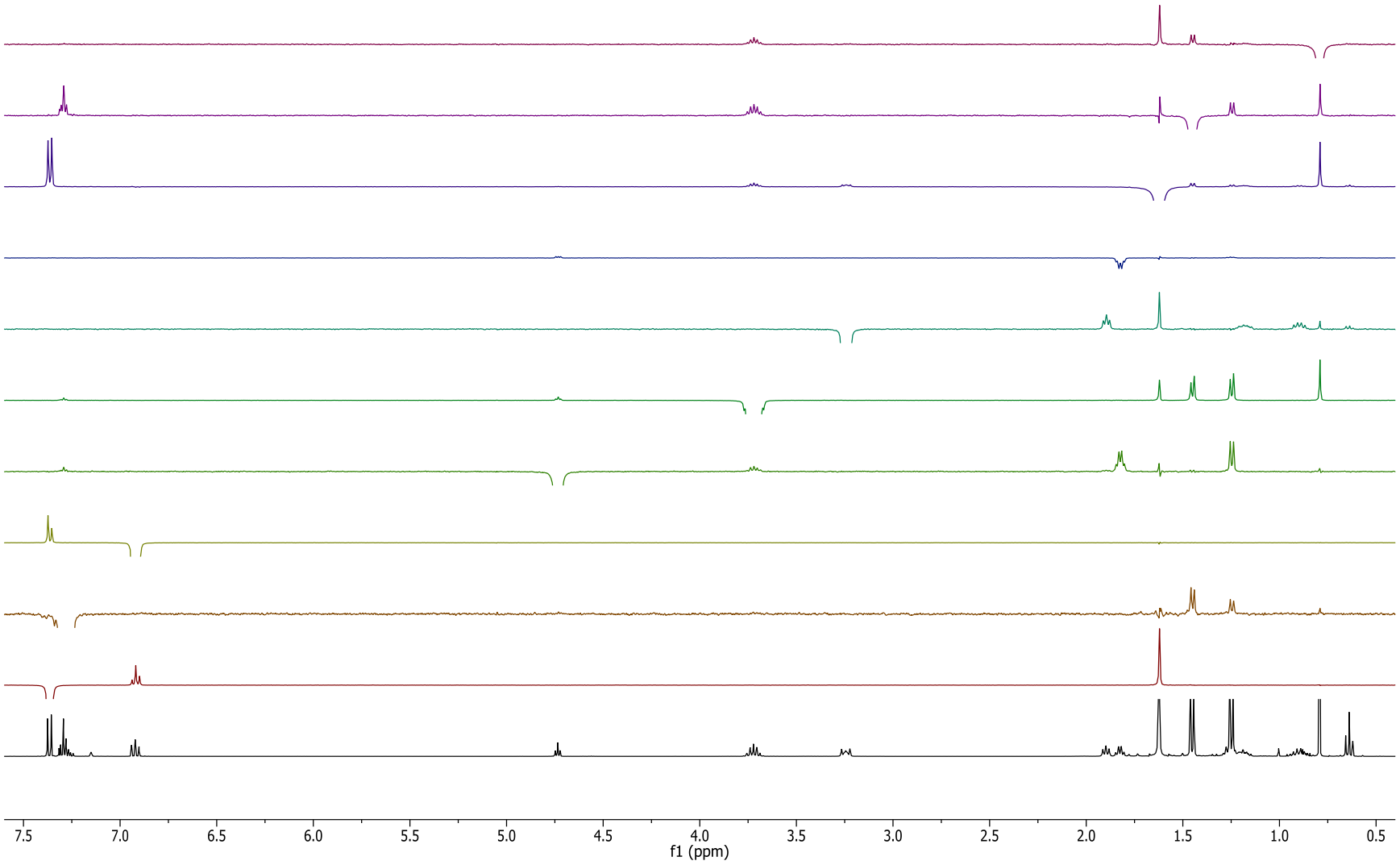


Figure 46. gCOSY NMR Spectrum of Complex **15** (C_6D_6, 400 MHz).

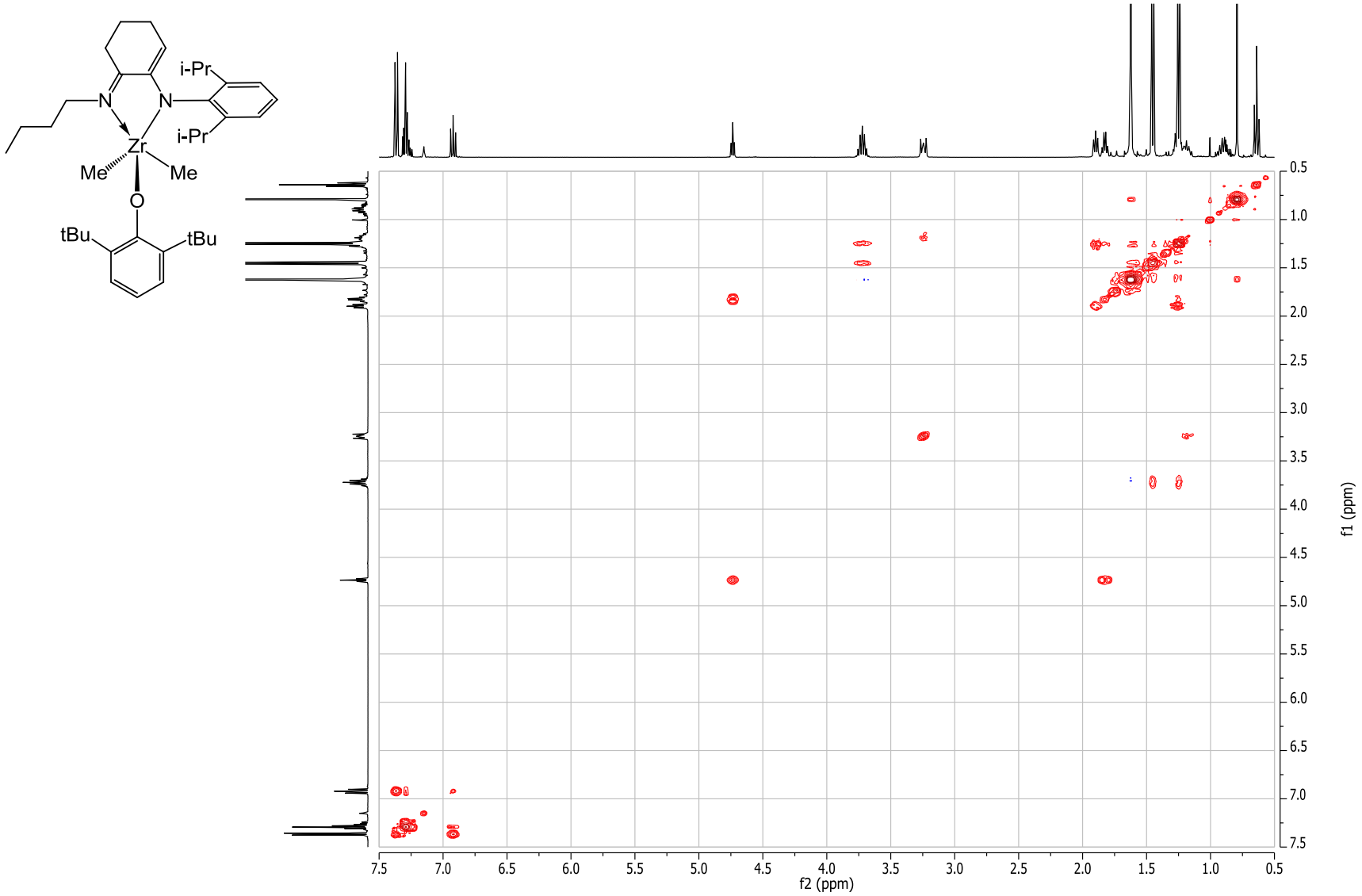


Figure 47. Fragment of gCOSY Spectrum of Complex **15** (C_6D_6, 400 MHz).

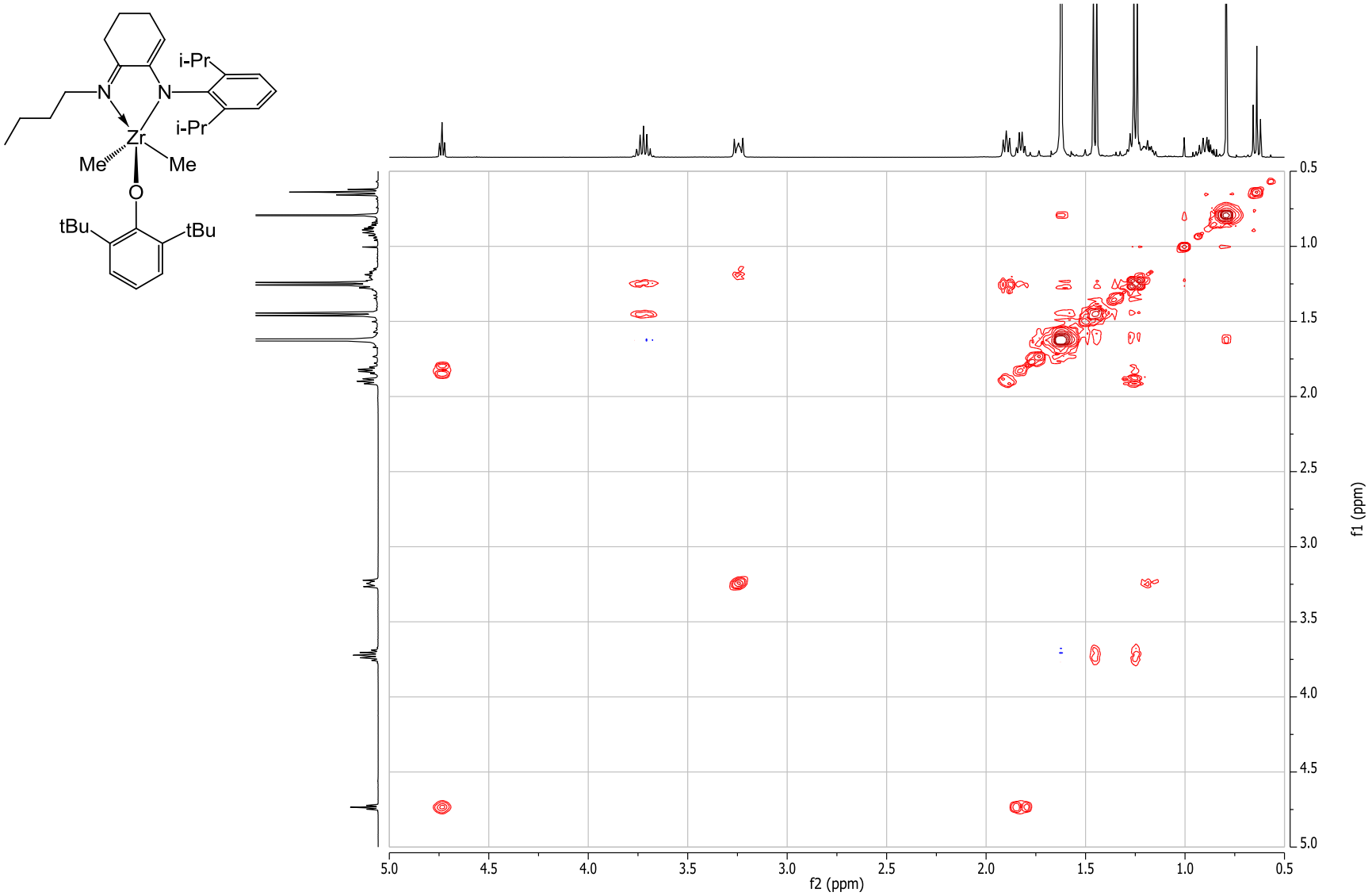


Figure 48. HSQCAD NMR Spectrum of Complex **15** (C_6D_6, 400 MHz).

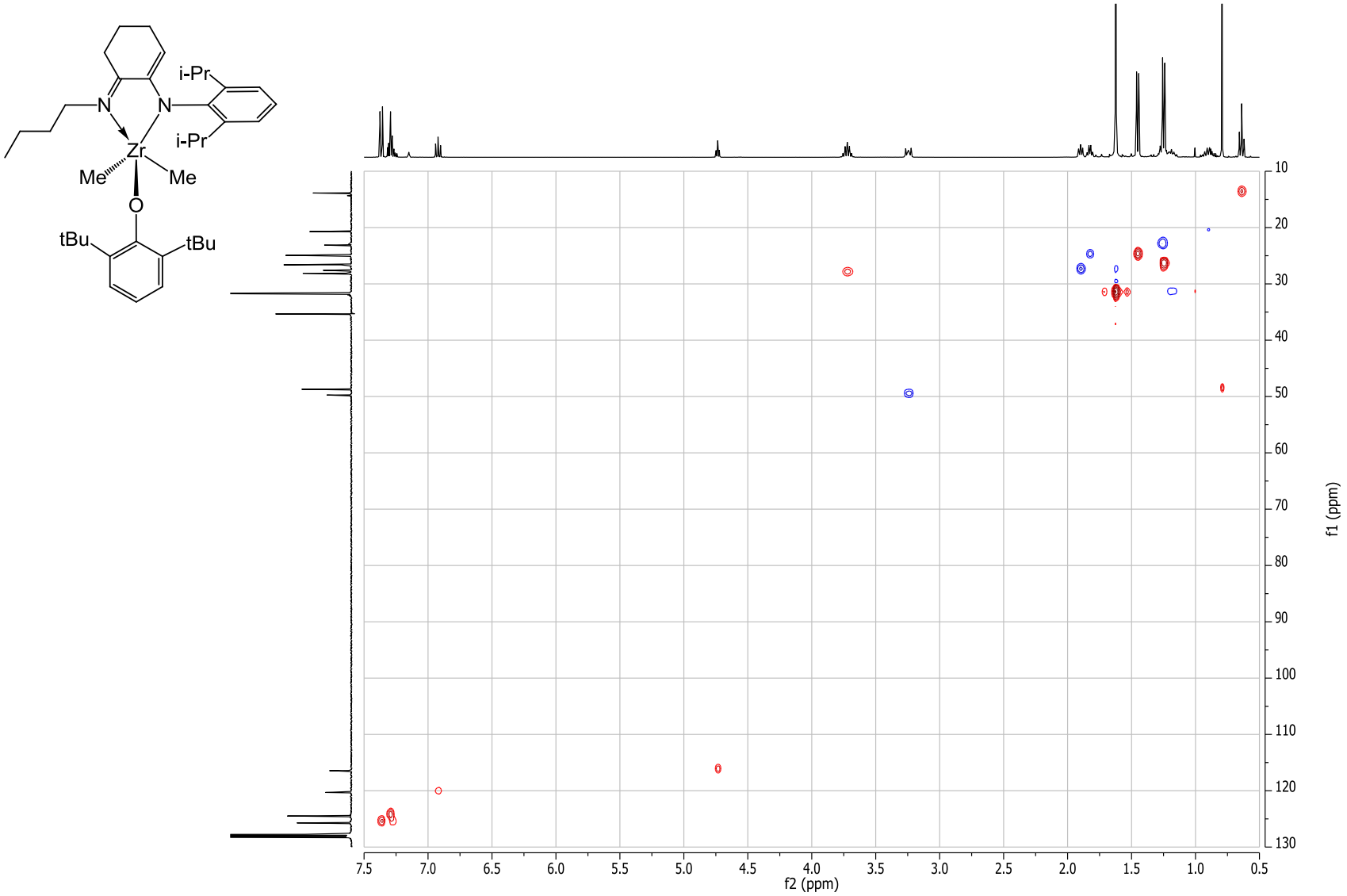


Figure 49. Fragment of gHSQCAD NMR Spectrum of Complex **15** (C_6D_6, 400 MHz).

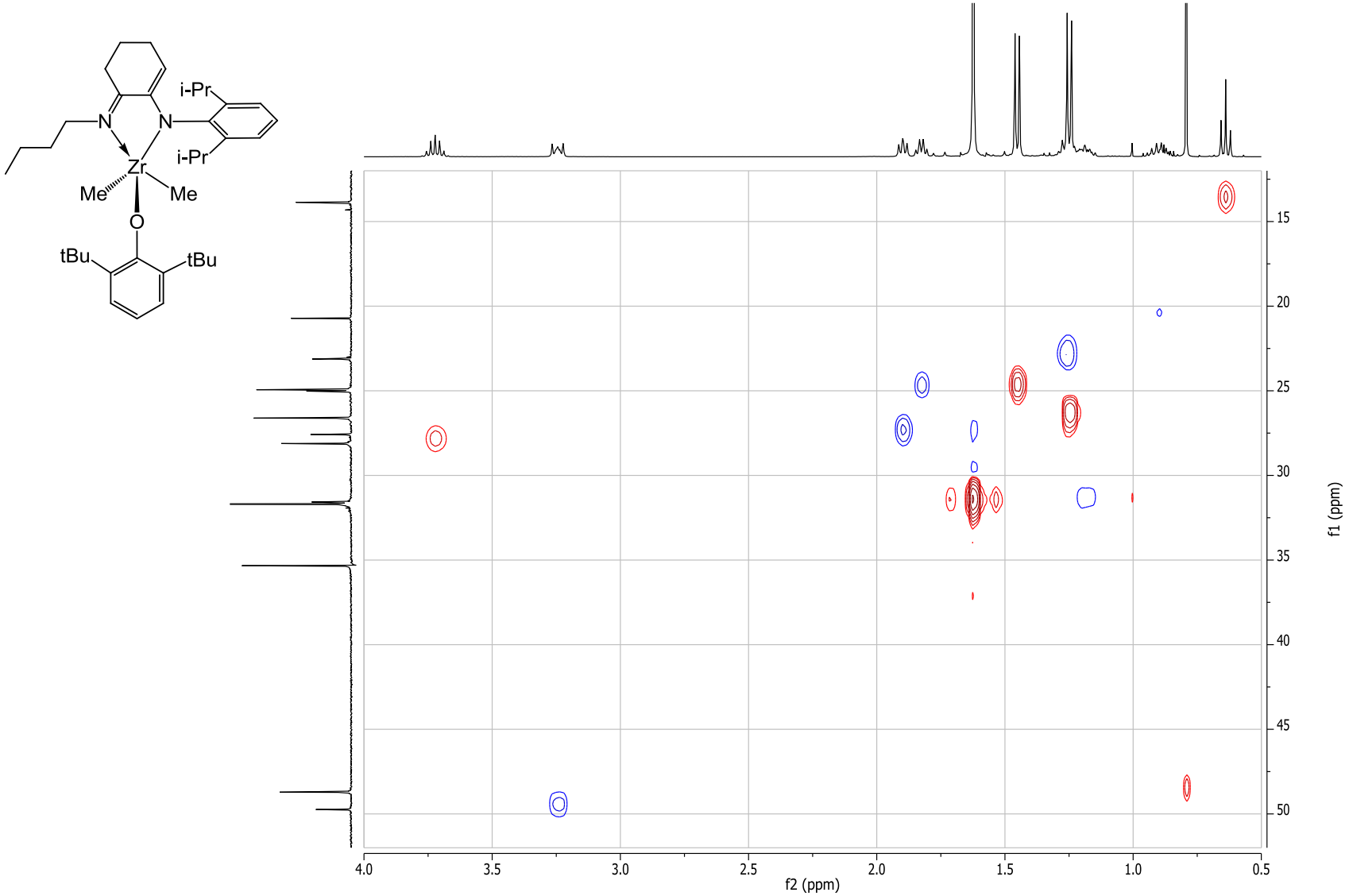


Figure 50. ^{1}H NMR Spectra of Complex **16** (C_6D_6, 500 MHz).

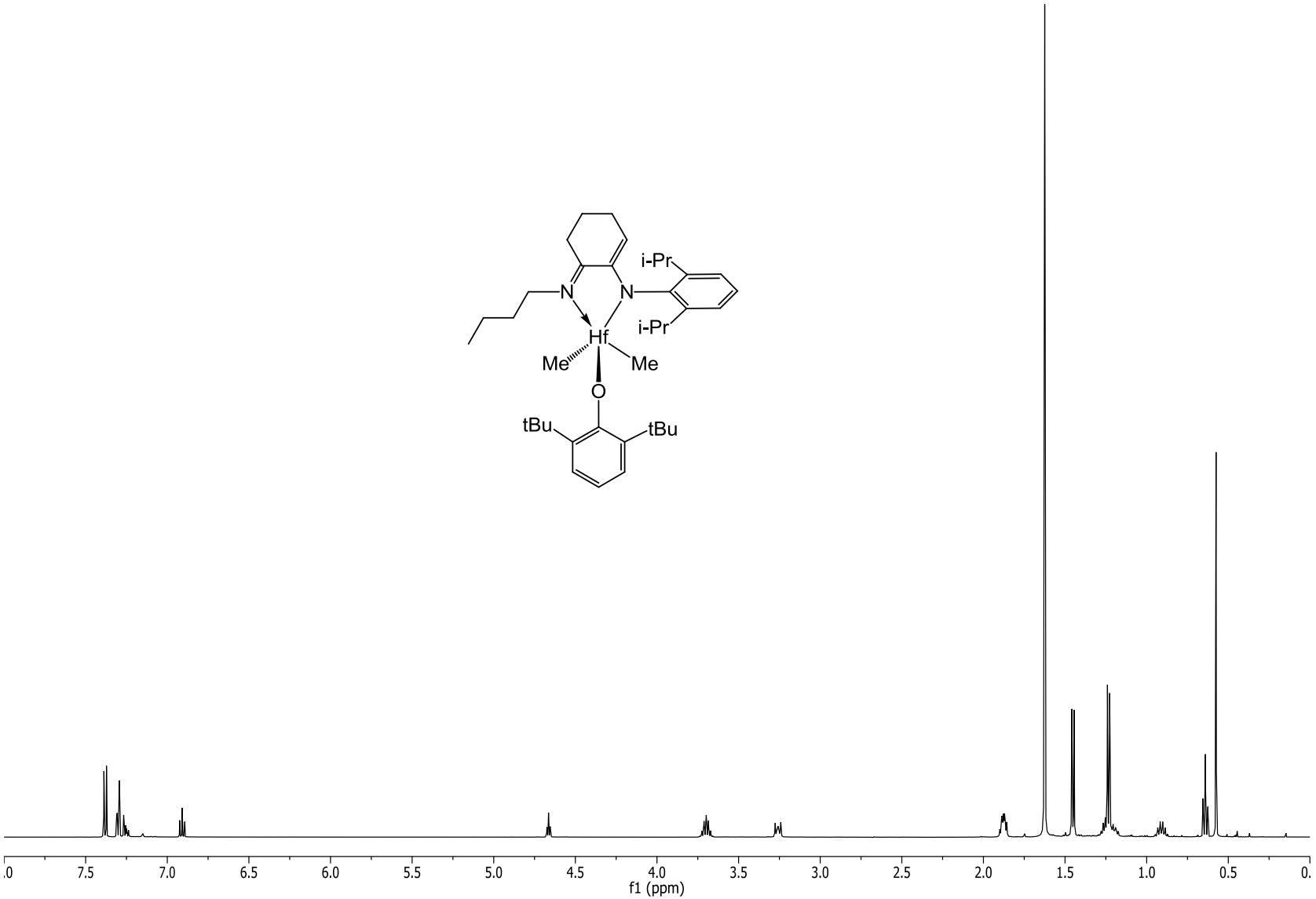


Figure 51. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **16** (C_6D_6, 125 MHz).

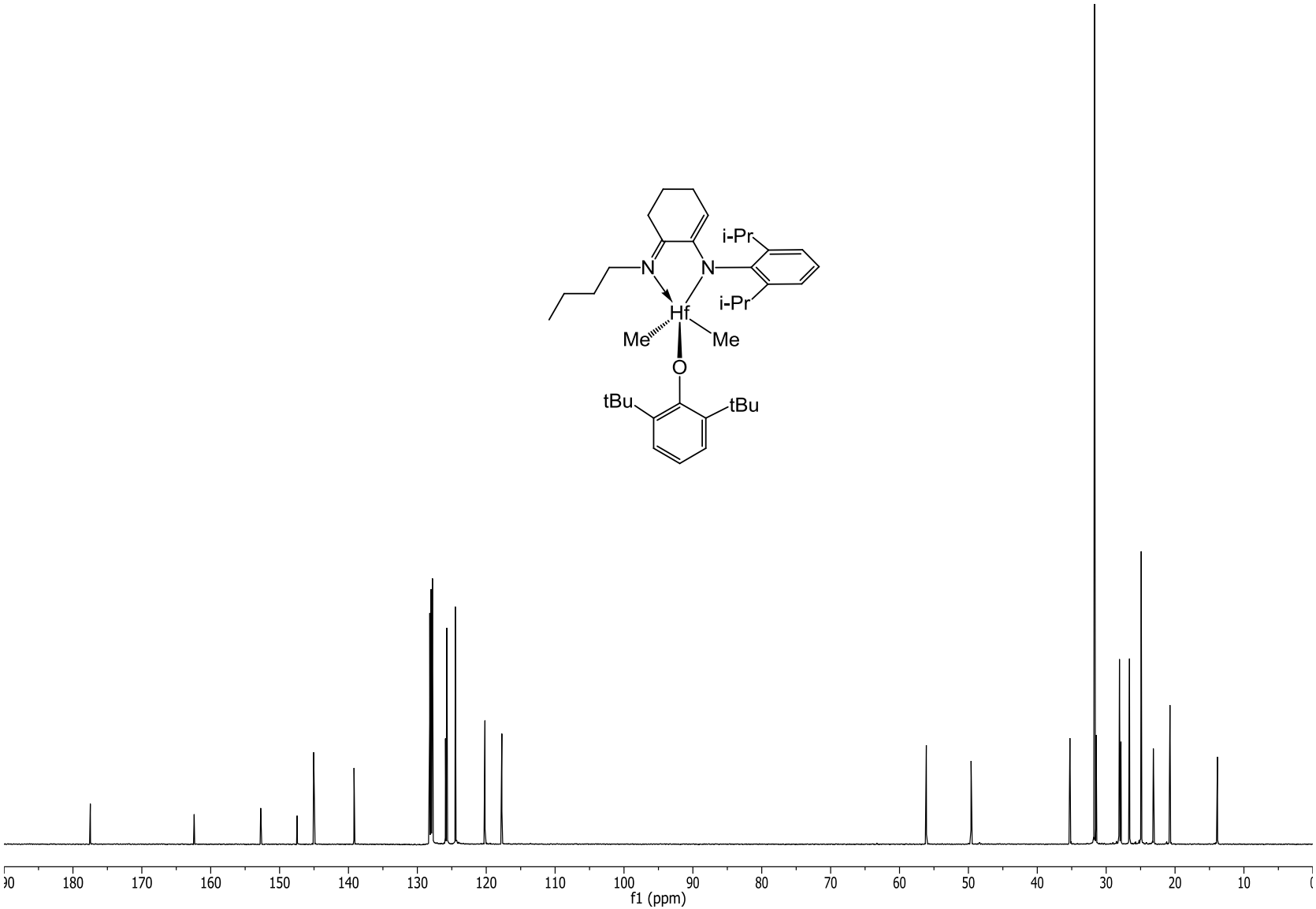


Figure 52. APT NMR Spectrum of Complex **16** (C_6D_6, 125 MHz).

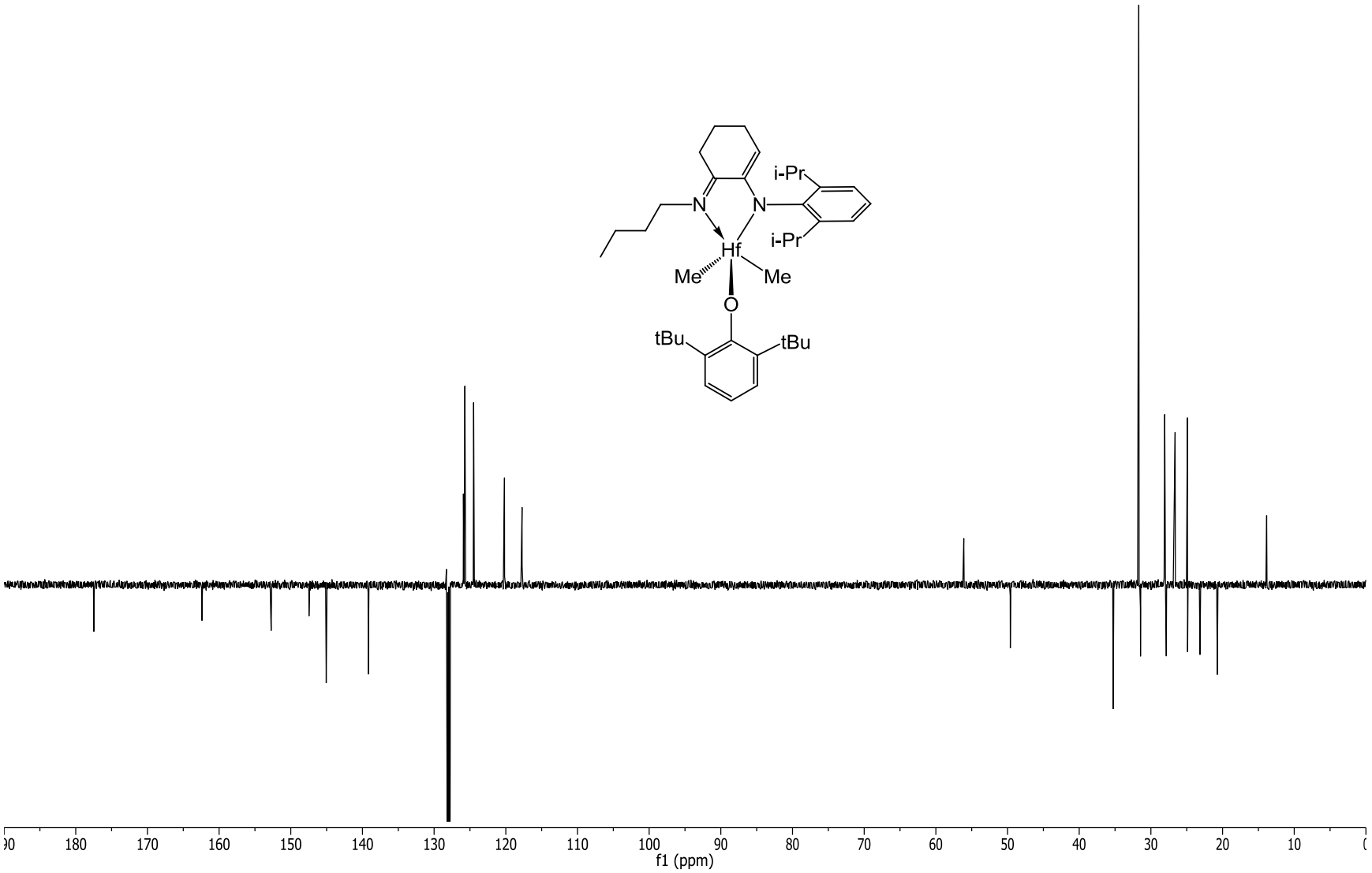


Figure 53. TOCSY1D NMR Spectra of Complex **16** (C_6D_6, 500 MHz) (mix time = 0, 0.03, 0.08 s).

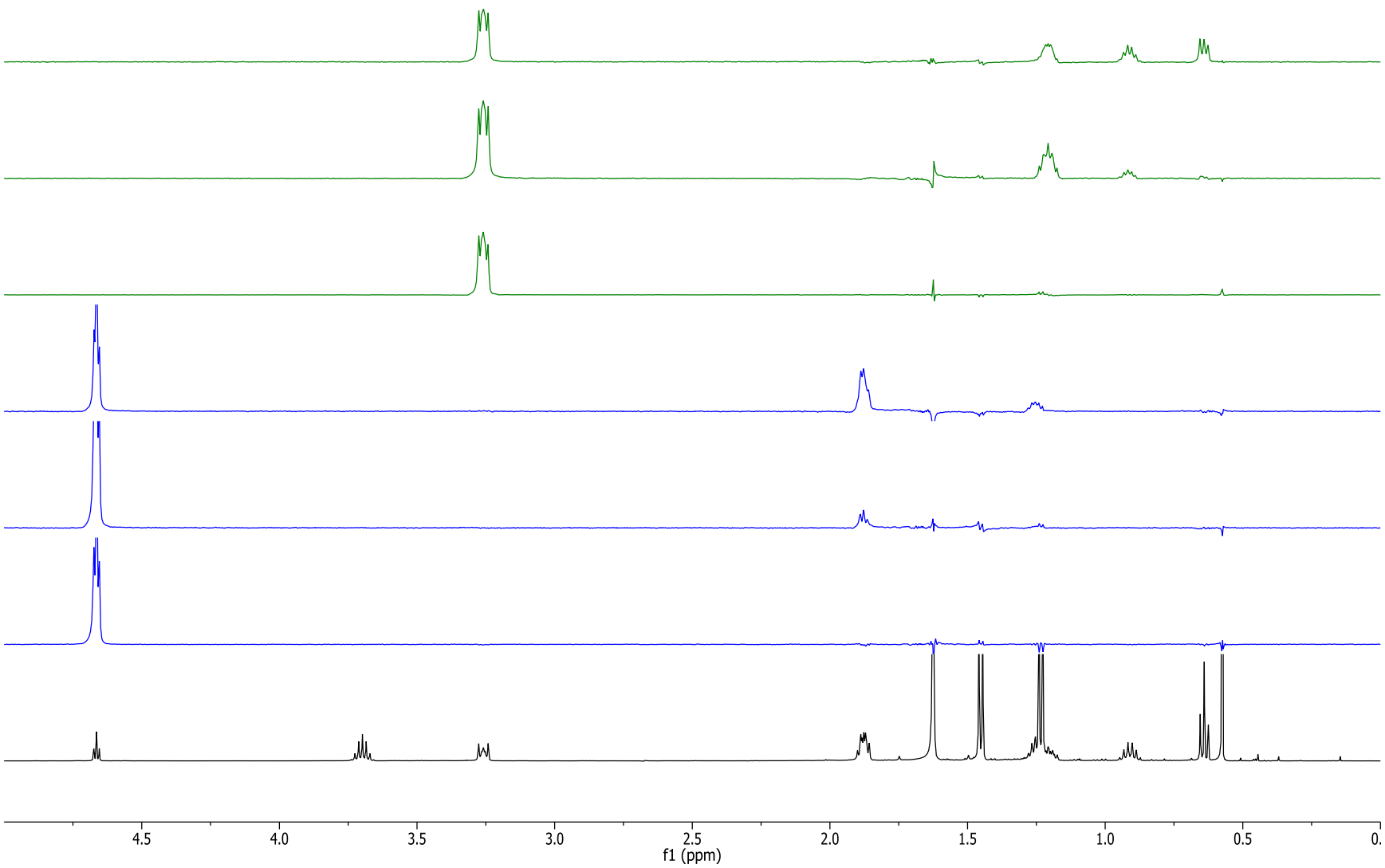


Figure 54. ^{1}H and NOESY1D NMR Spectra of Complex **16** (C_6D_6, 500 MHz, mixing time = 0.8 s).

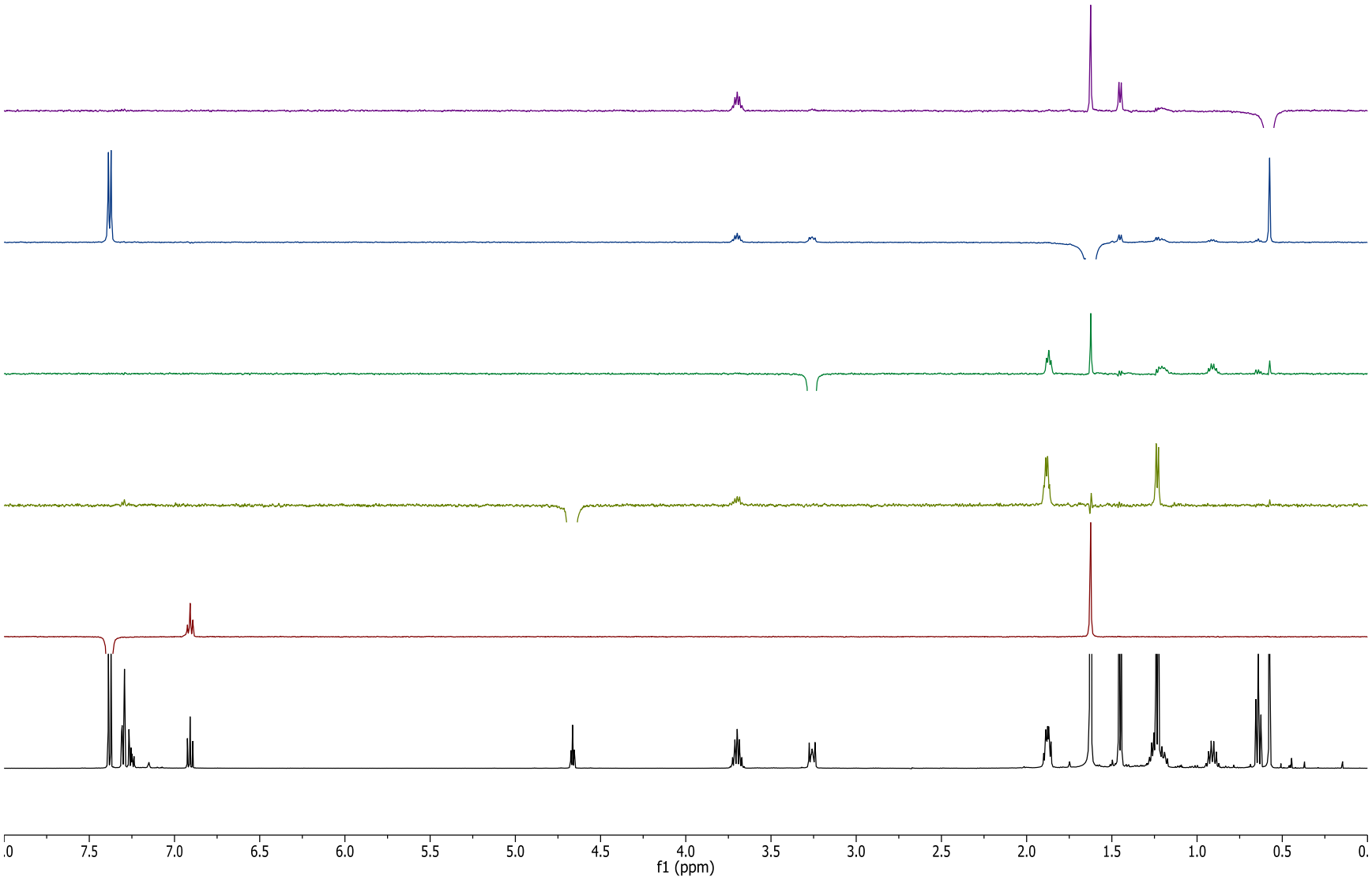


Figure 55. gCOSY NMR Spectrum of Complex **16** (C_6D_6, 500 MHz).

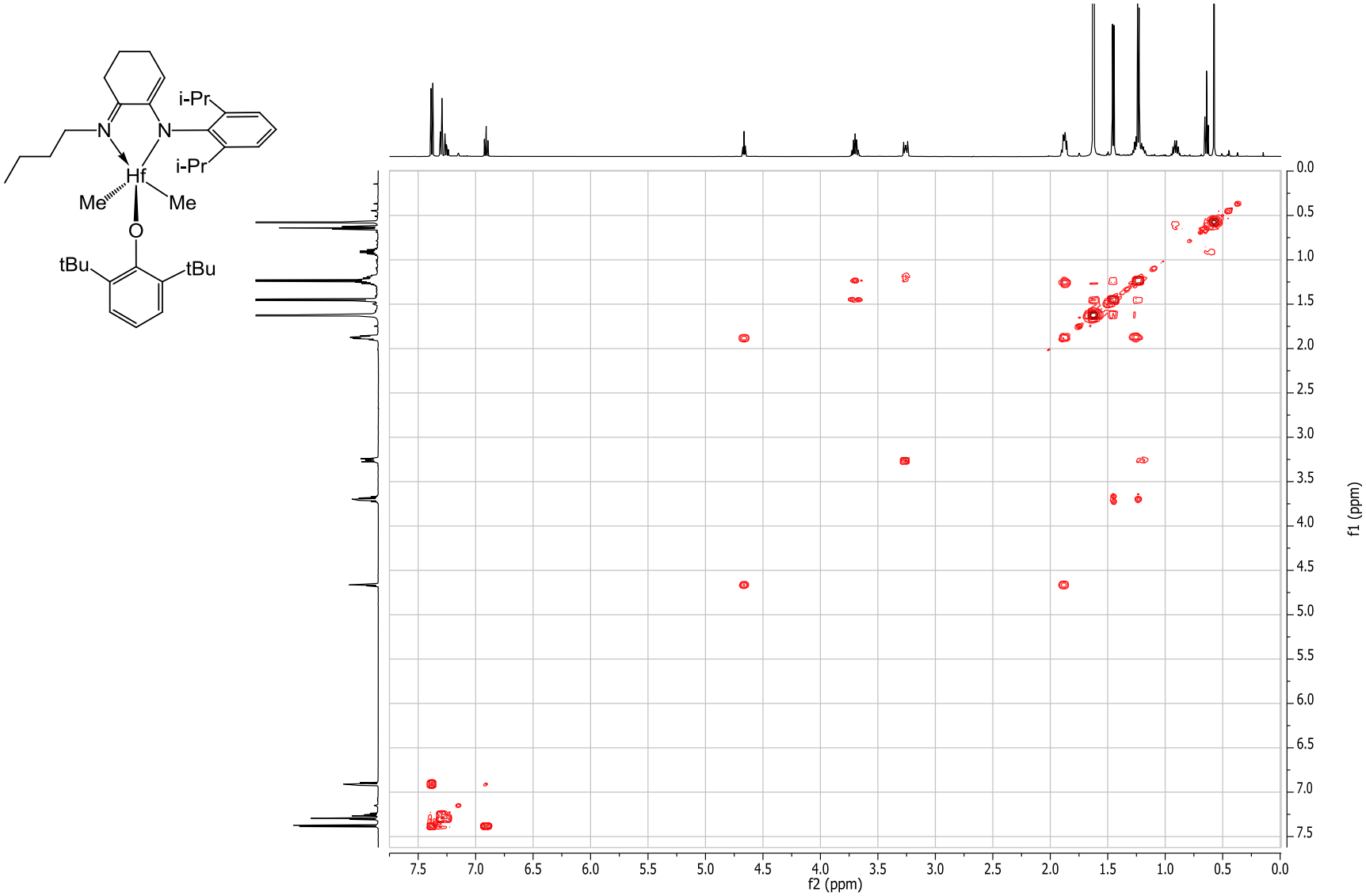


Figure 56. Fragment of gCOSY Spectrum of Complex **16** (C_6D_6, 500 MHz).

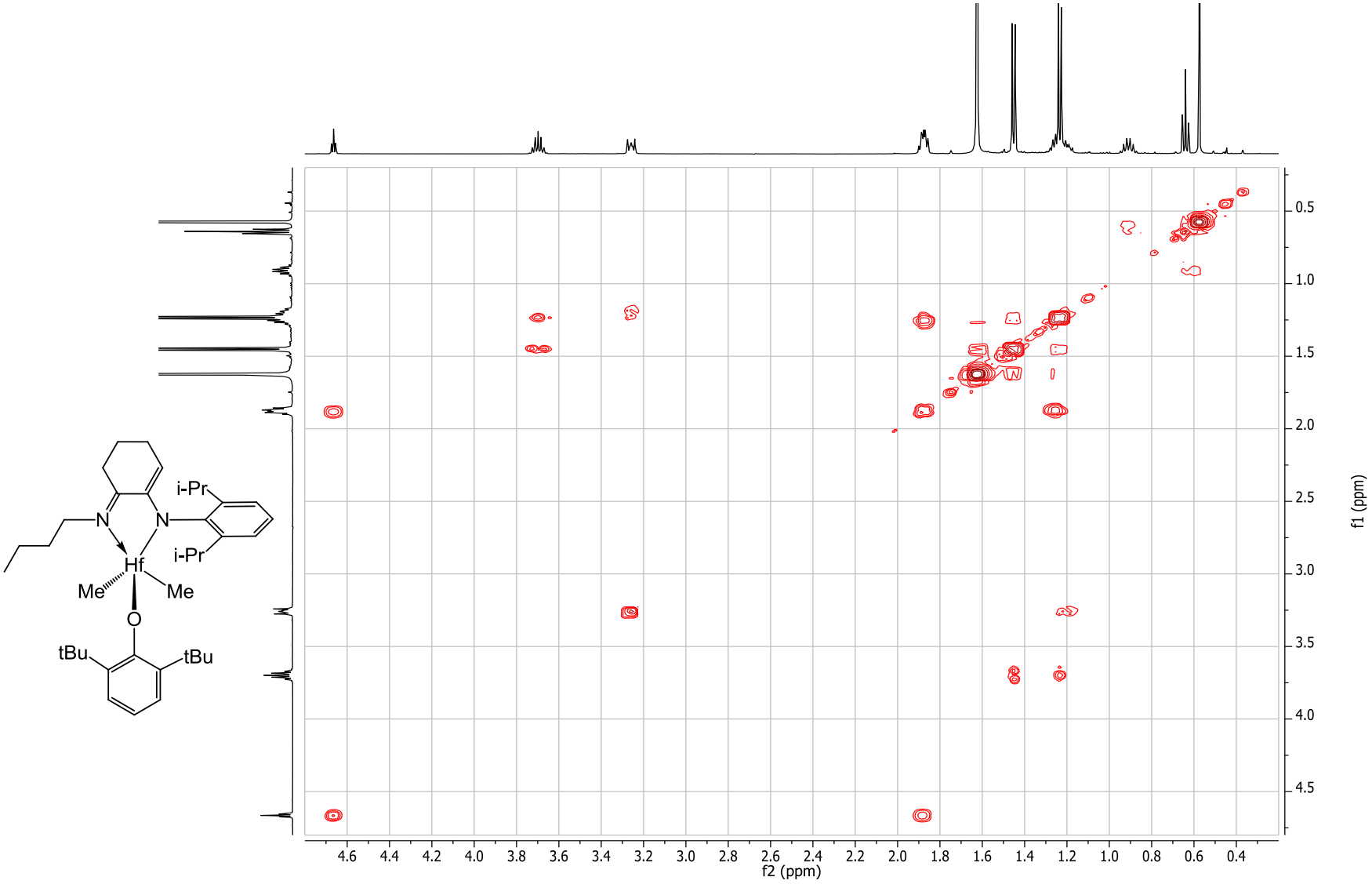


Figure 57. HSQCAD NMR Spectrum of Complex **16** (C_6D_6, 500 MHz).

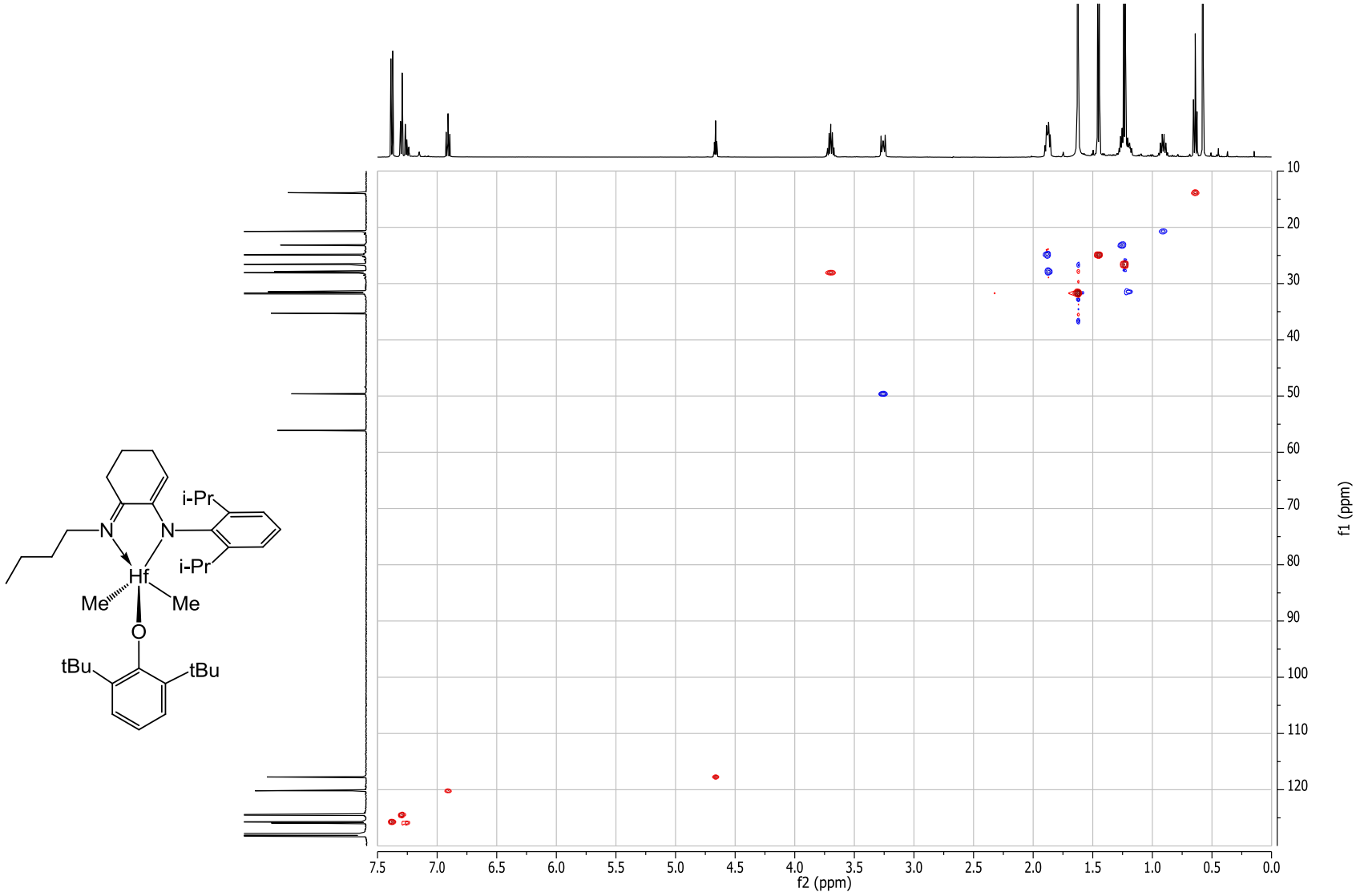


Figure 58. Fragment of gHSQCAD NMR Spectrum of Complex **16** (C_6D_6, 500 MHz).

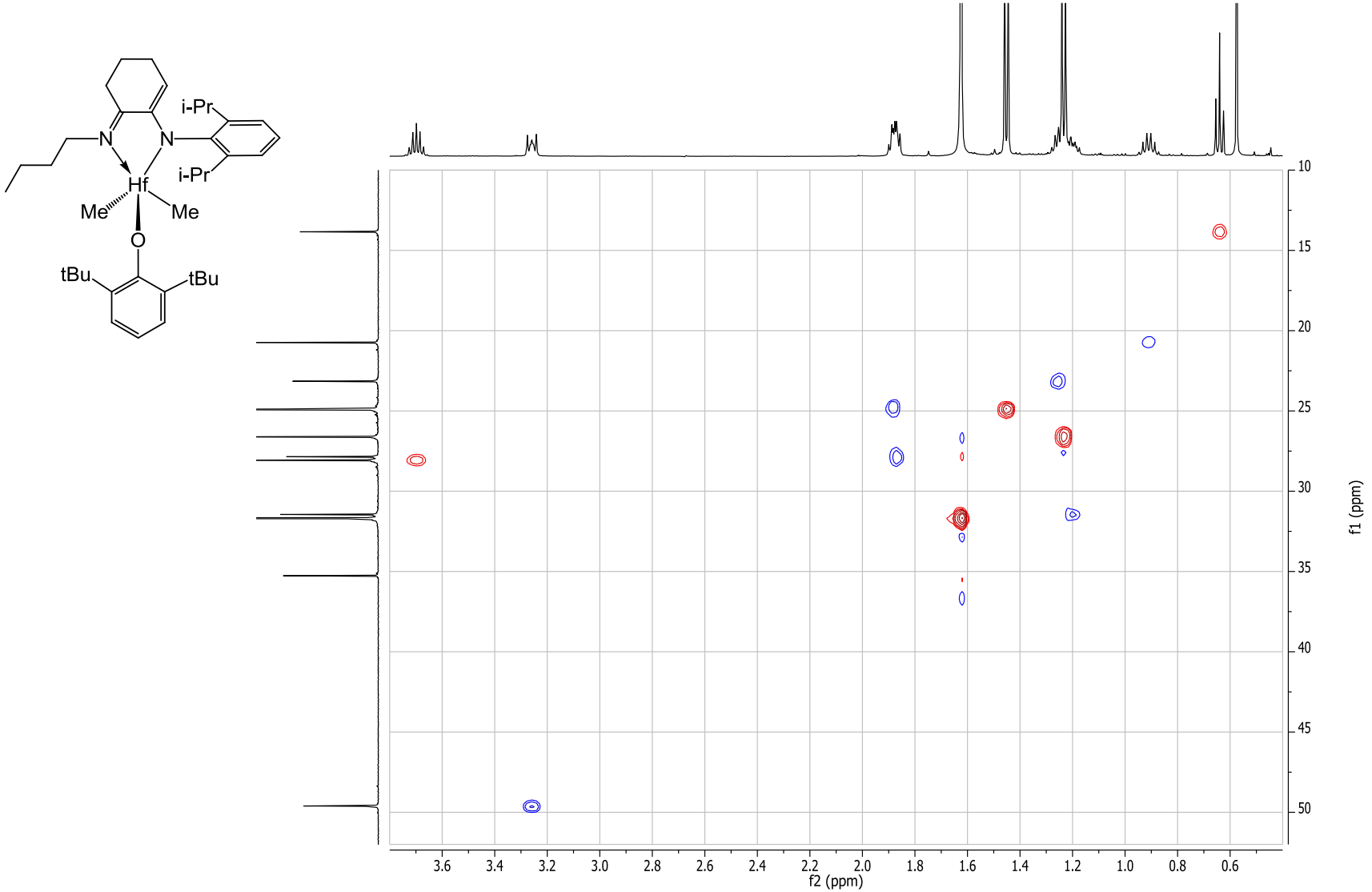


Figure 59. ^{1}H NMR Spectra of Complex **17** (C_6D_6, 400 MHz).

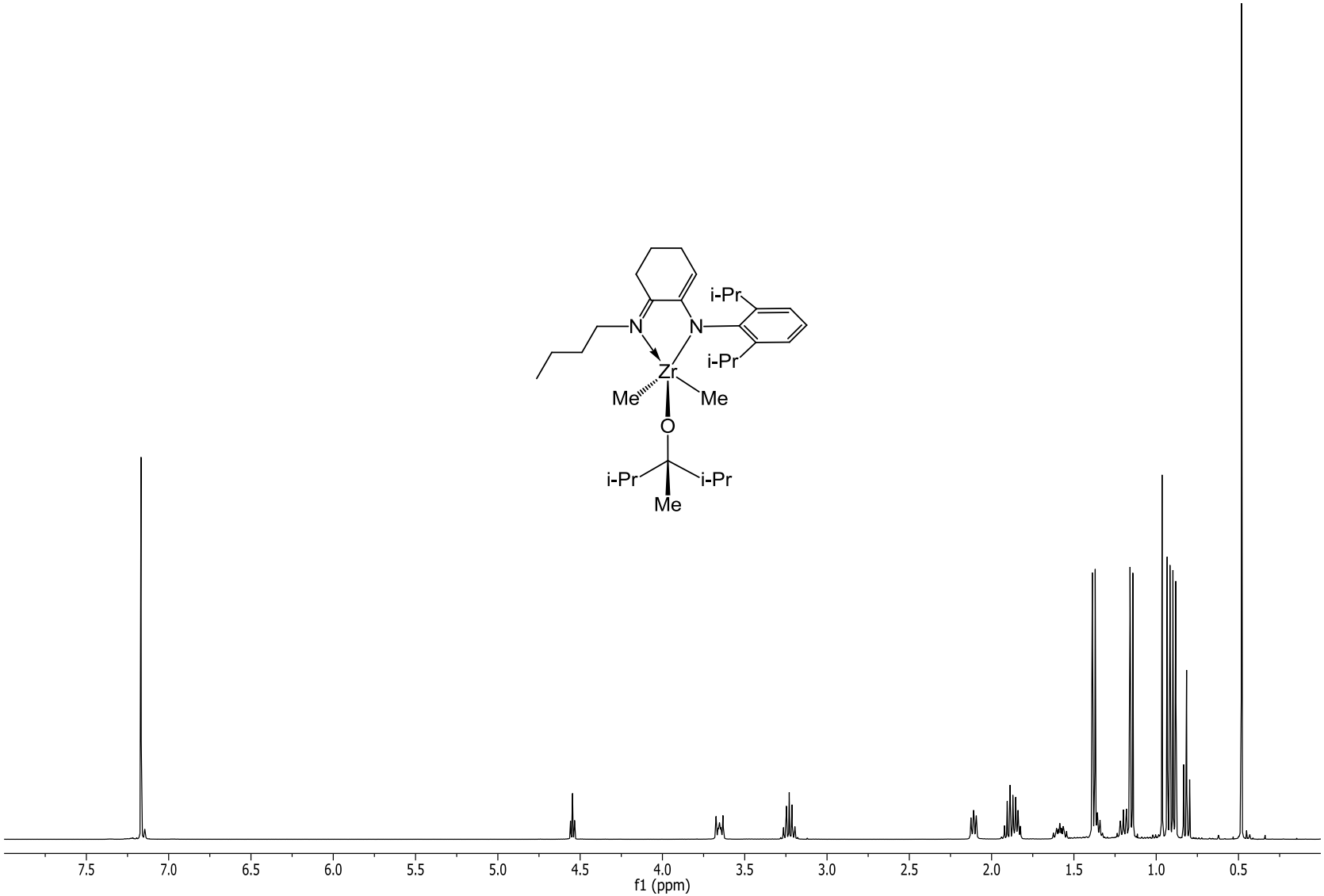


Figure 60. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **17** (C_6D_6, 100 MHz).

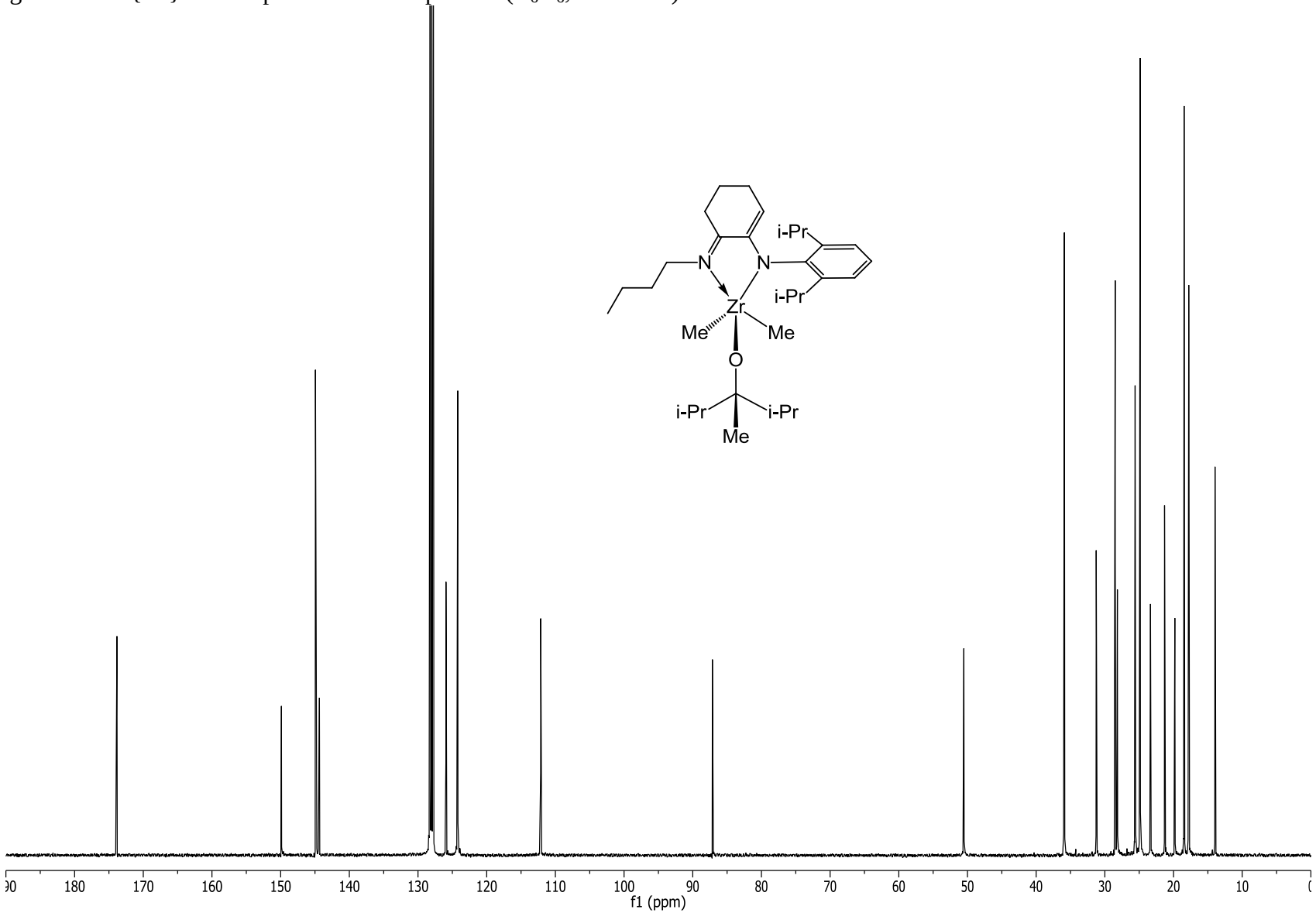


Figure 61. APT NMR Spectrum of Complex **17** (C_6D_6, 100 MHz).

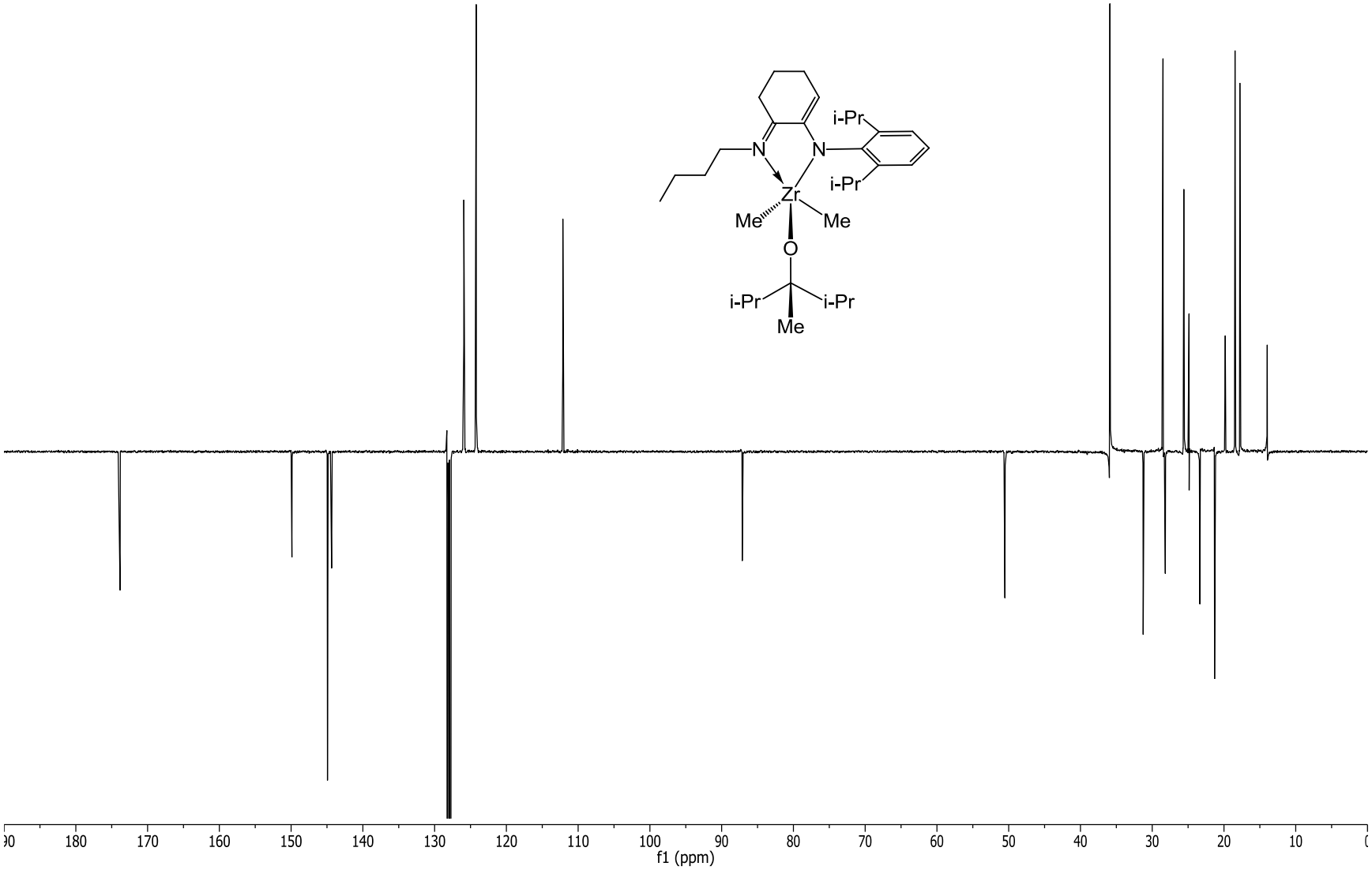


Figure 62. TOCSY1D NMR Spectra of Complex **17** (C_6D_6, 400 MHz) (mix time = 0, 0.03, 0.08 s).

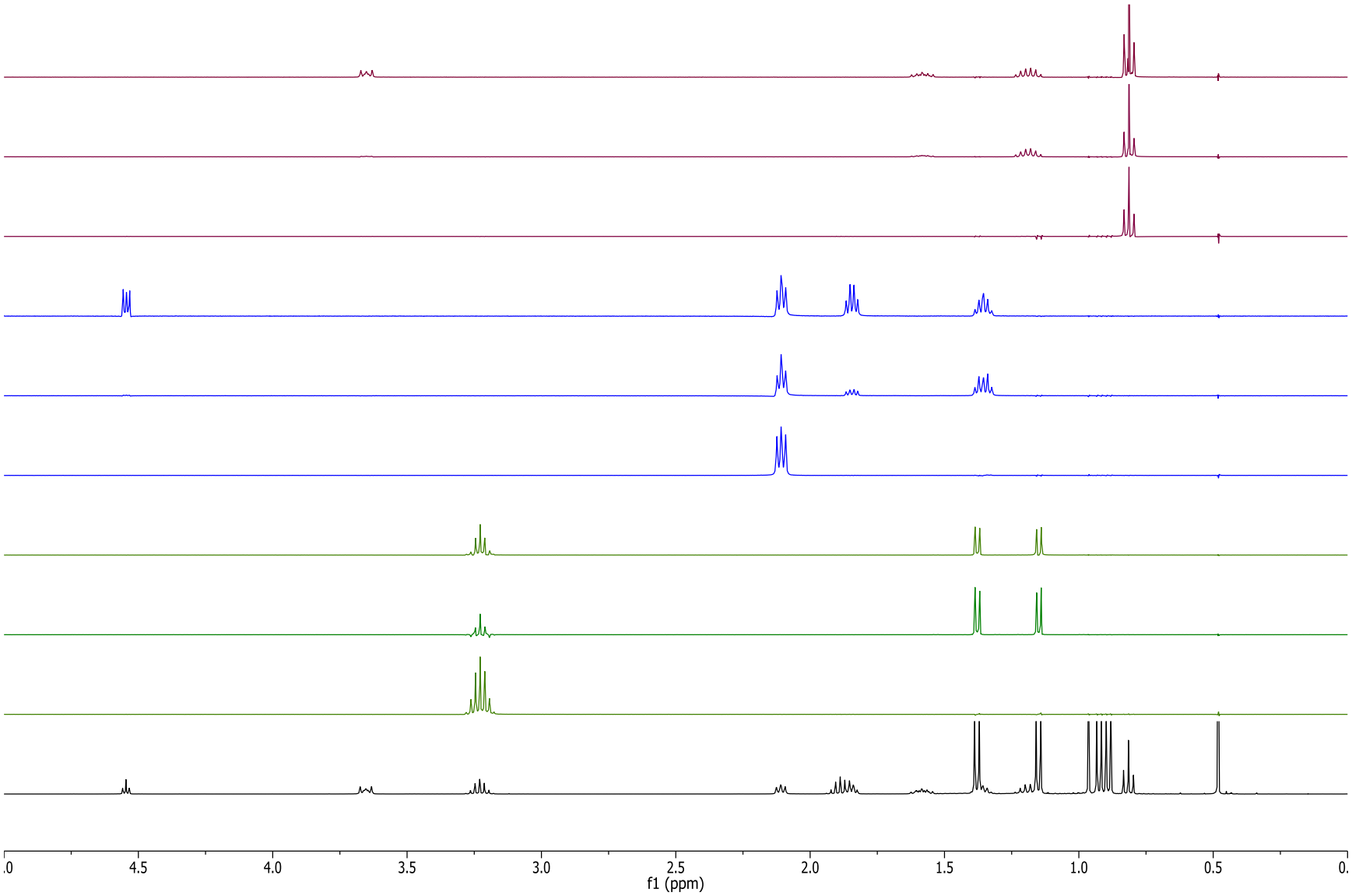


Figure 63. ^{1}H and NOESY1D NMR Spectra of Complex **17** (C_6D_6, 400 MHz, mixing time = 0.8 s).

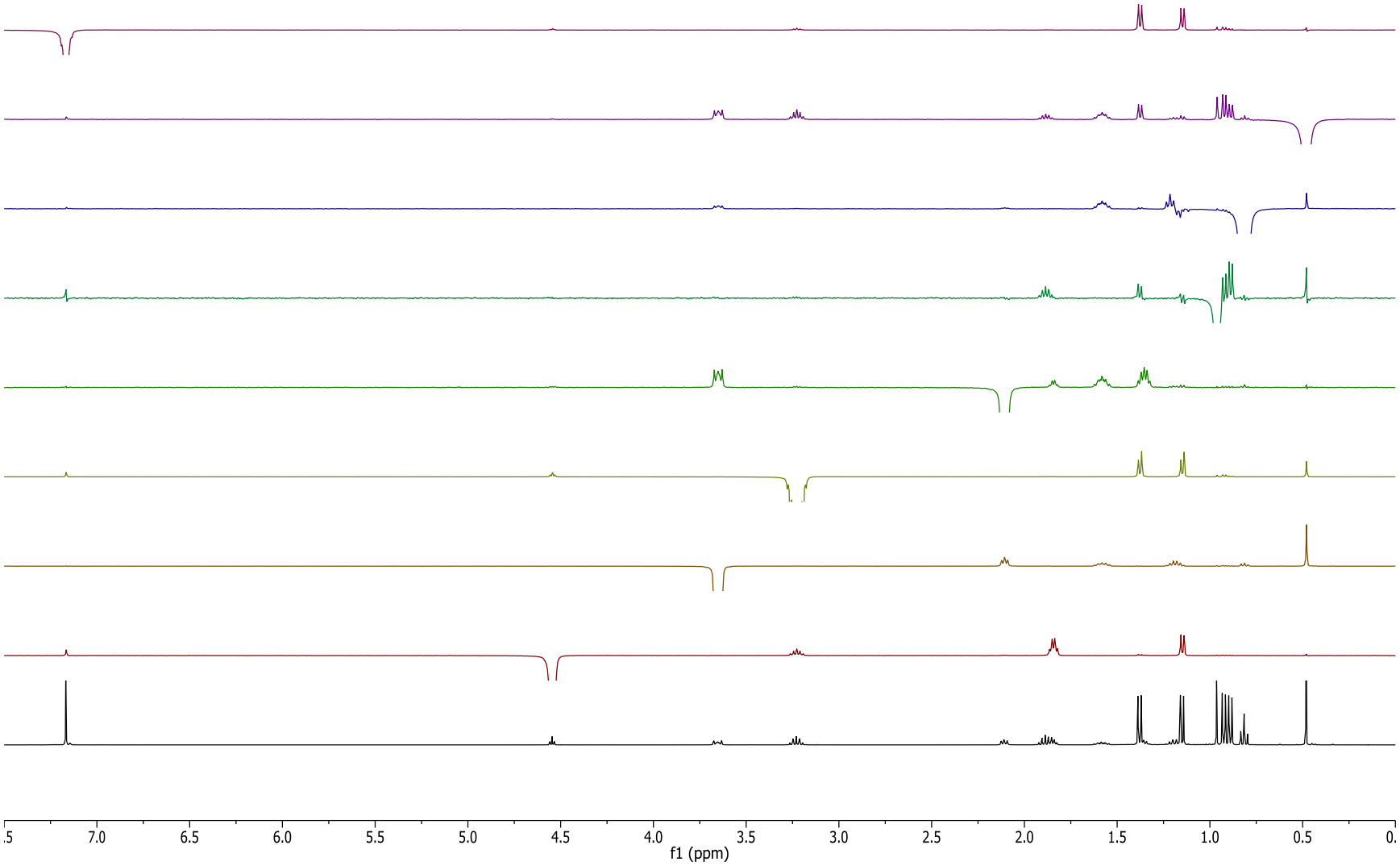


Figure 64. gCOSY NMR Spectrum of Complex **17** (C_6D_6, 400 MHz)

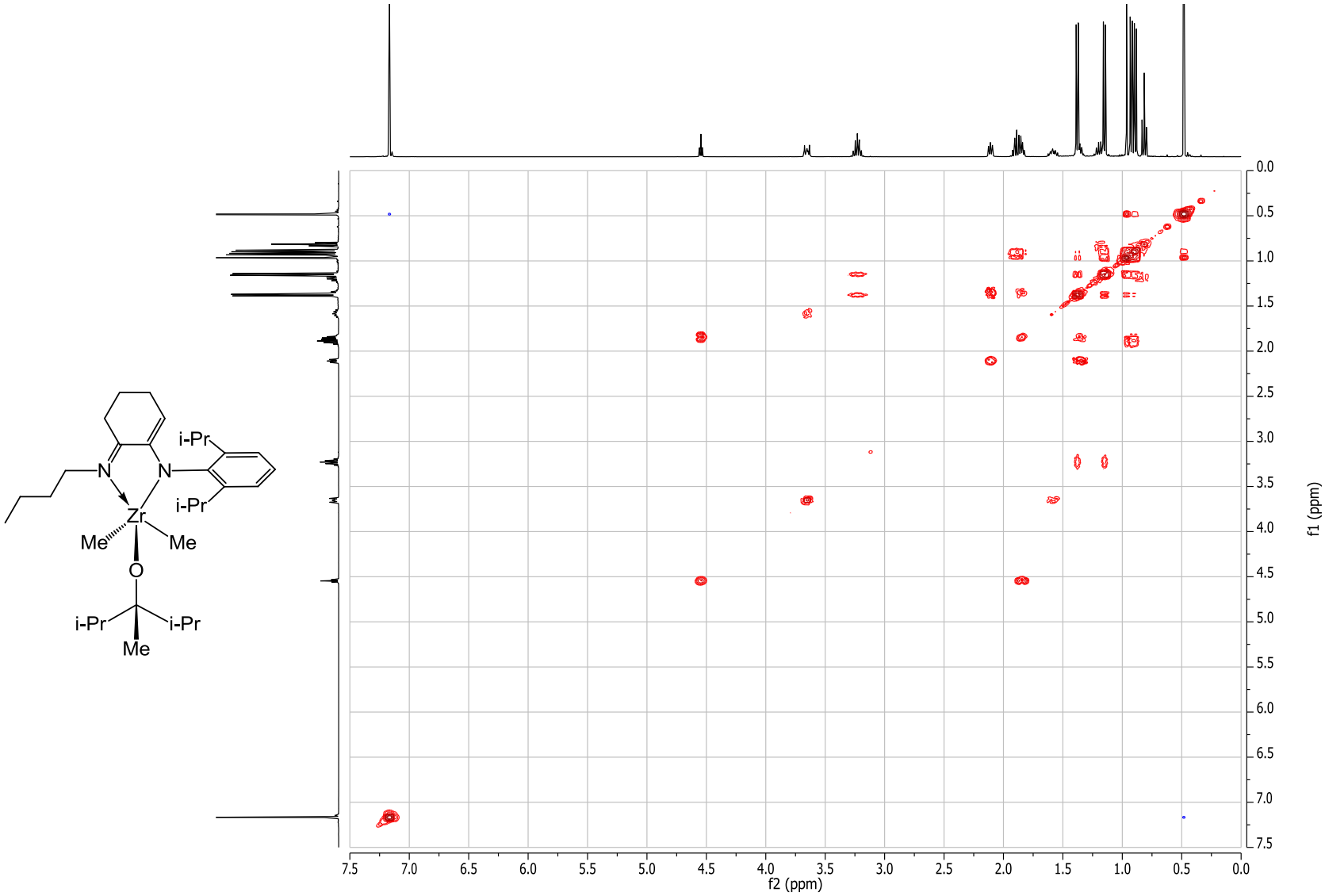


Figure 65. Fragment of gCOSY Spectrum of Complex **17** (C_6D_6, 400 MHz)

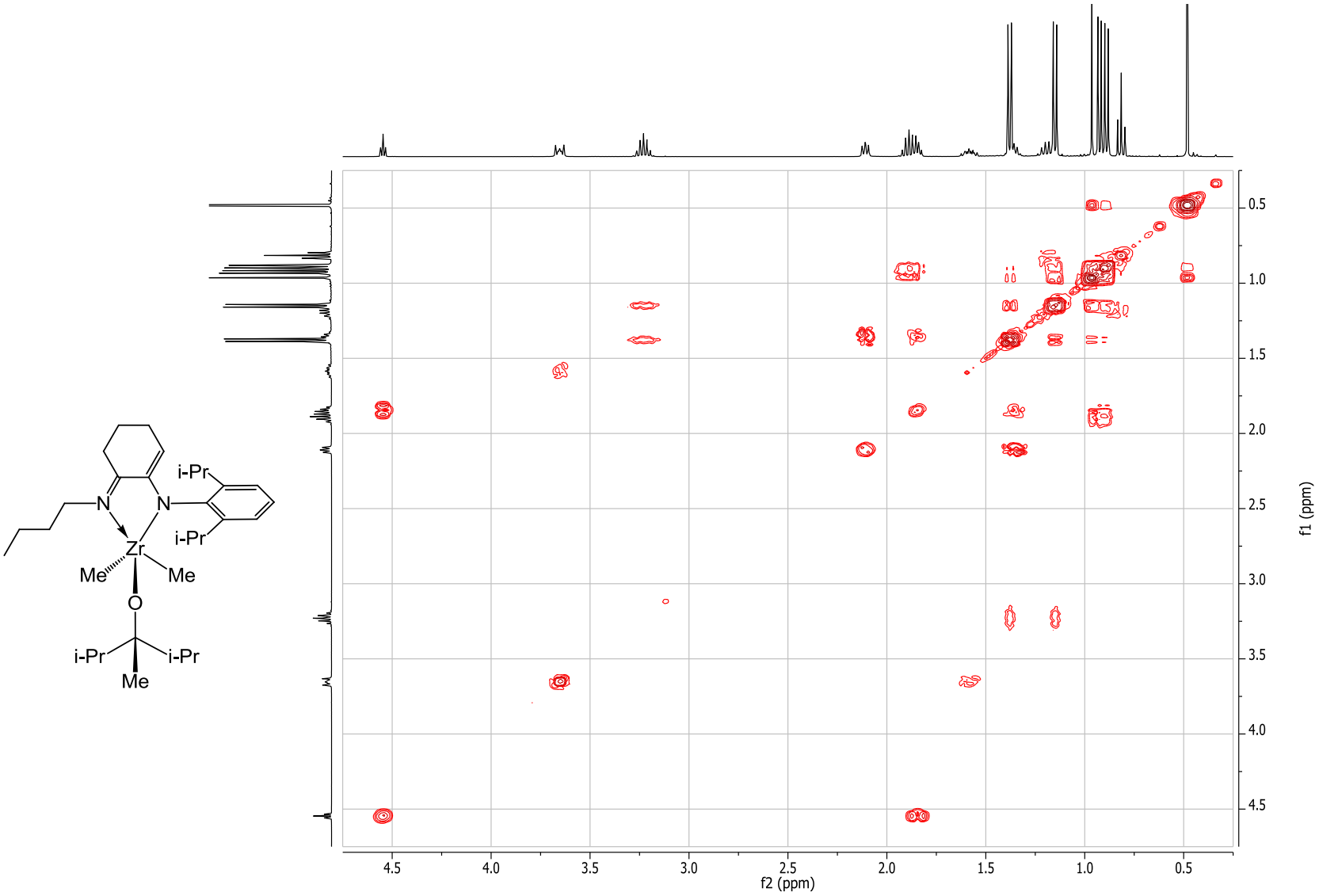


Figure 66. HSQCAD NMR Spectrum of Complex **17** (C_6D_6, 400 MHz)

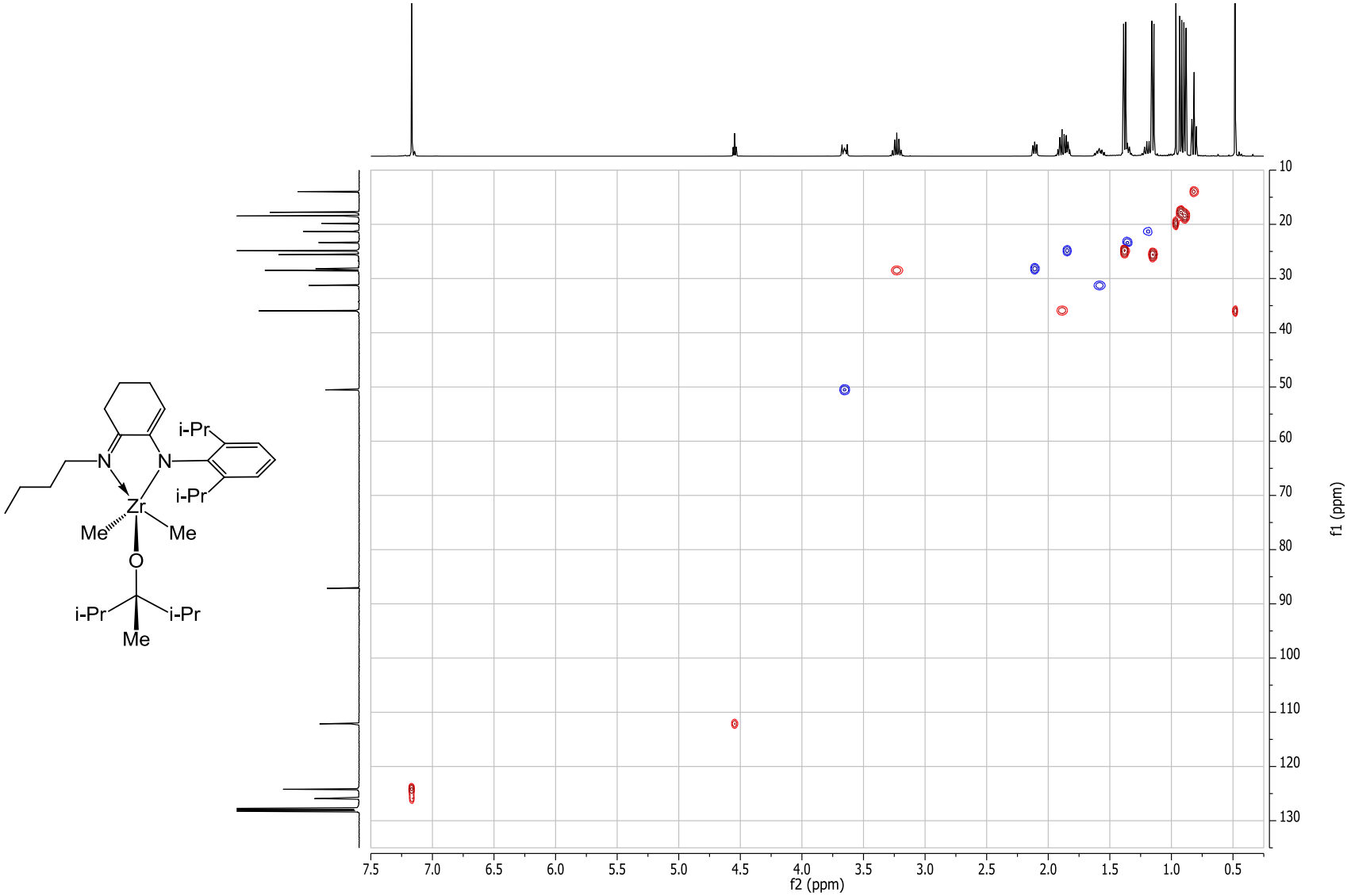


Figure 67. Fragment of gHSQCAD NMR Spectrum of Complex **17** (C_6D_6, 400 MHz).

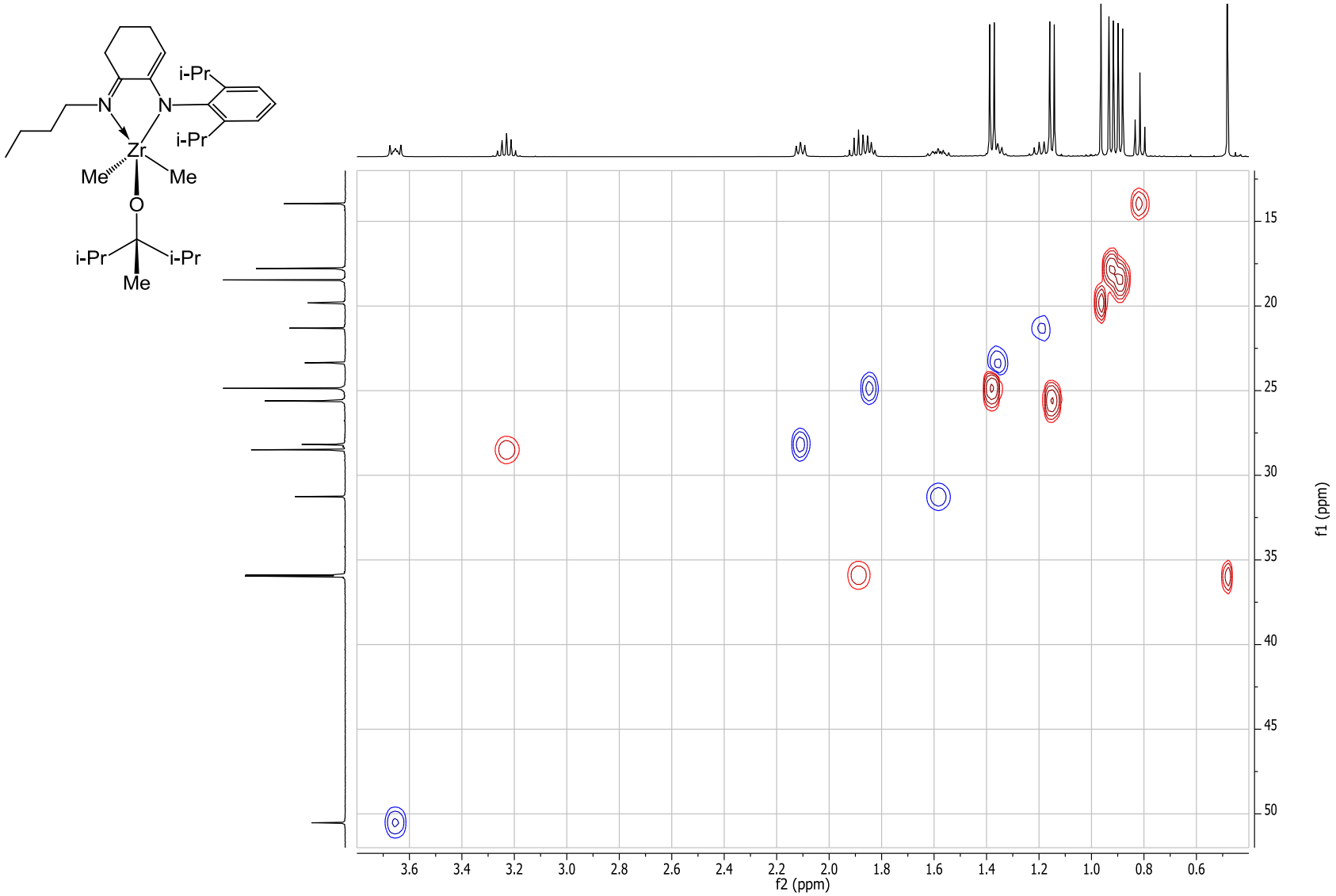


Figure 68. ^{1}H NMR Spectra of Complex **18** (C_6D_6, 500 MHz).

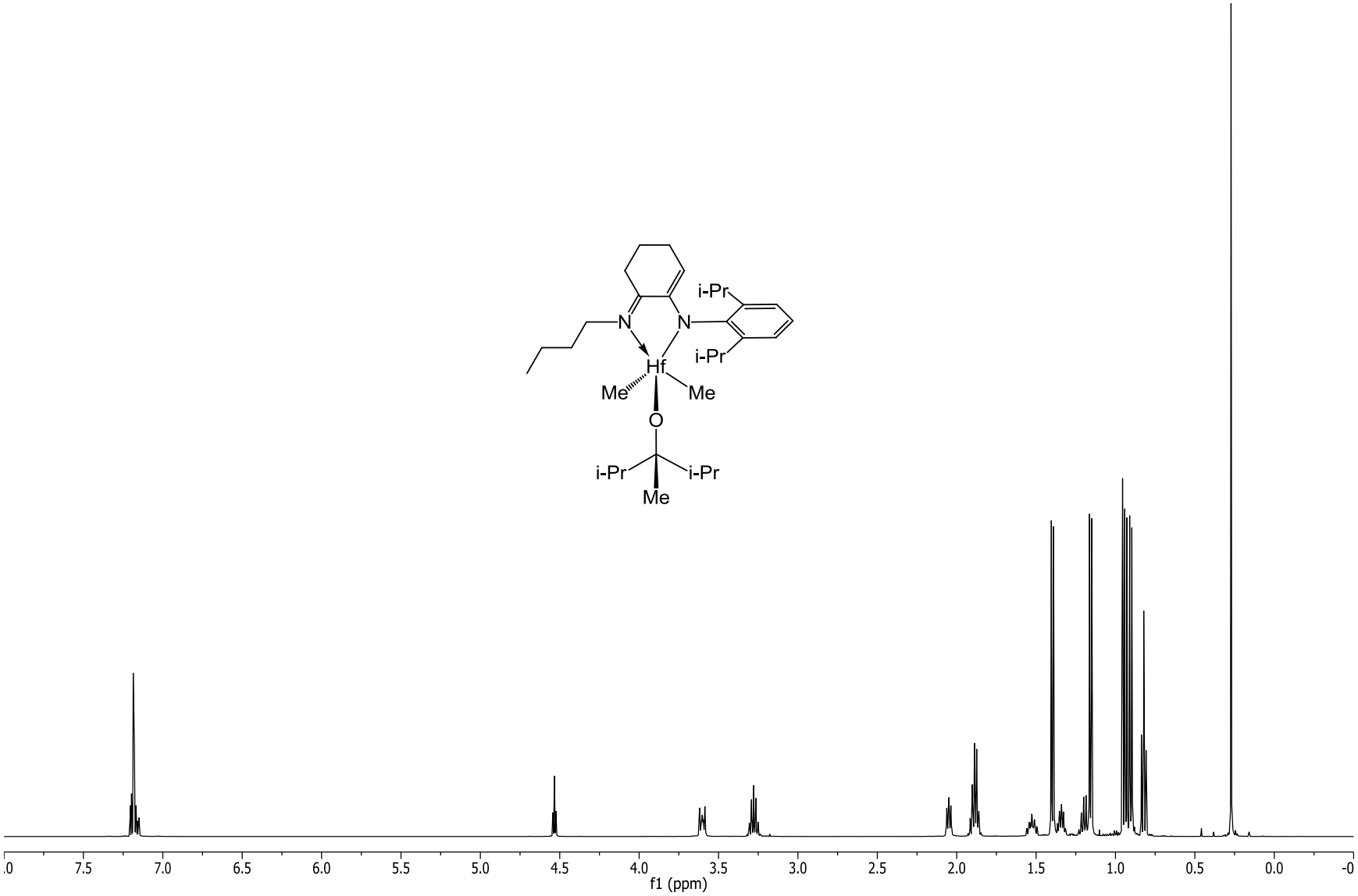


Figure 69. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **18** (C_6D_6, 125 MHz).

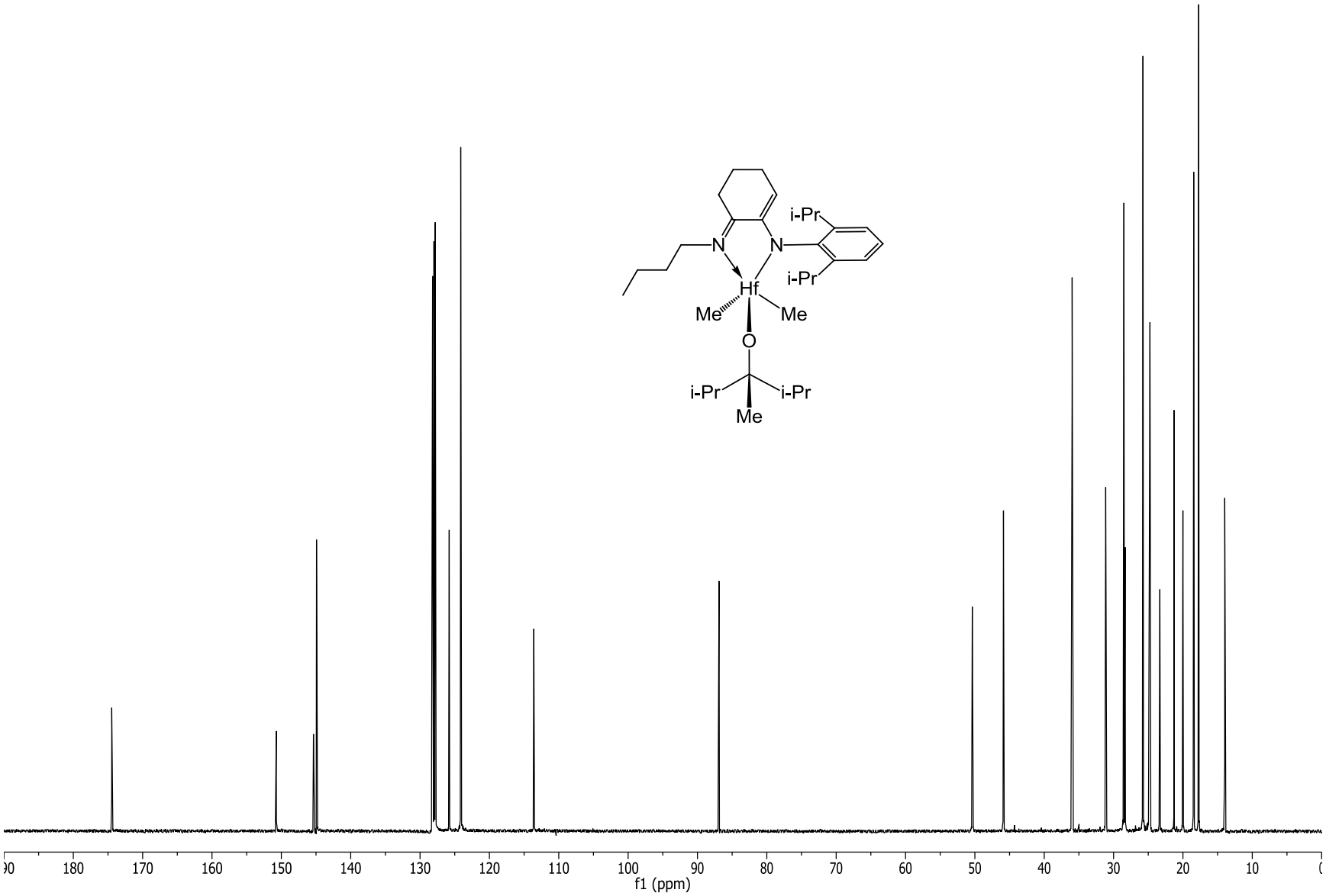


Figure 70. APT NMR Spectrum of Complex **18** (C_6D_6, 125 MHz).

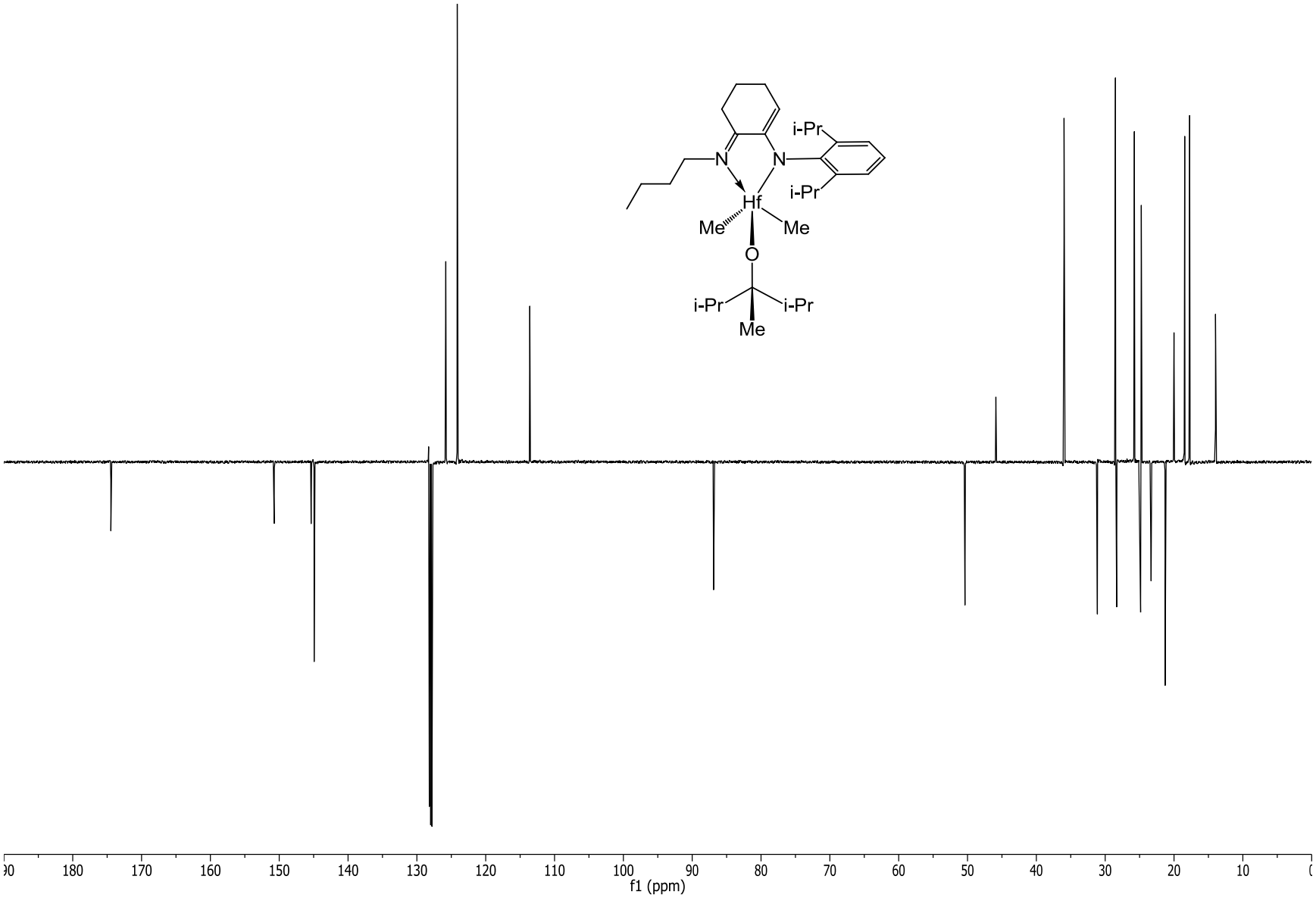


Figure 71. TOCSY1D NMR Spectra of Complex **18** (C_6D_6, 500 MHz) (mix time = 0, 0.03, 0.08 s).

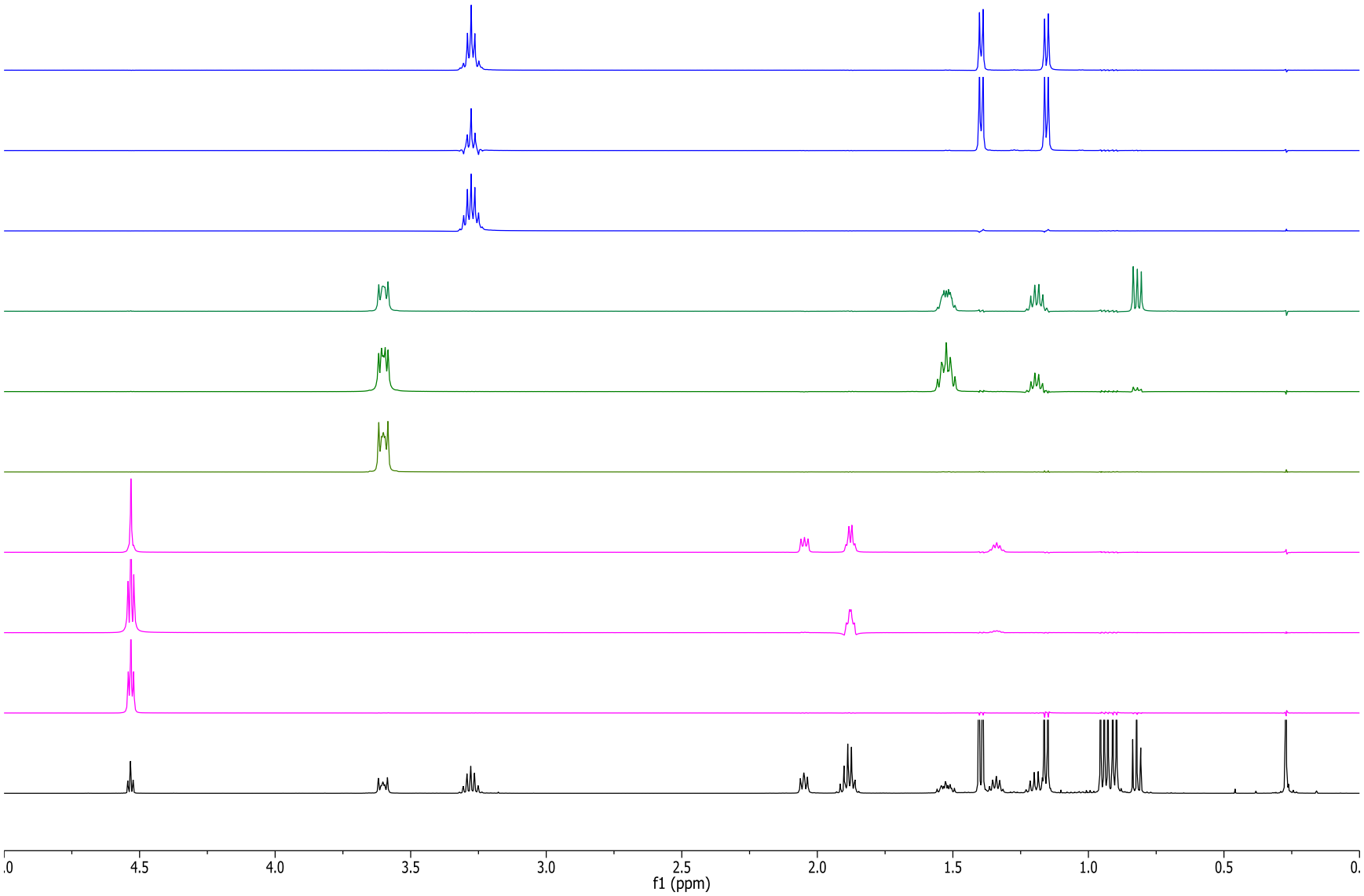


Figure 72. ^{1}H and NOESY1D NMR Spectra of Complex **18** (C_6D_6, 500 MHz, mixing time = 0.8 s).

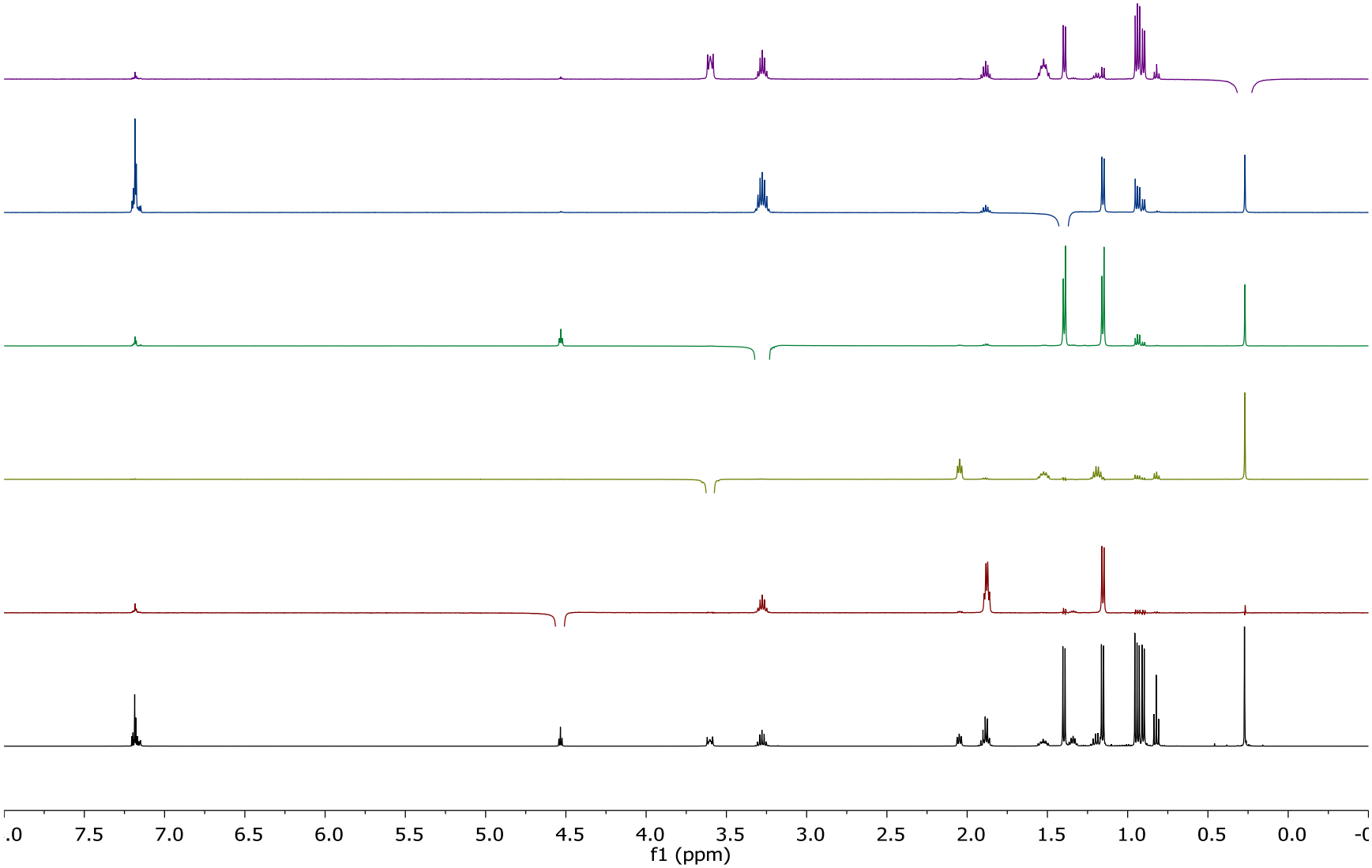


Figure 73. gCOSY NMR Spectrum of Complex **18** (C_6D_6, 500 MHz)

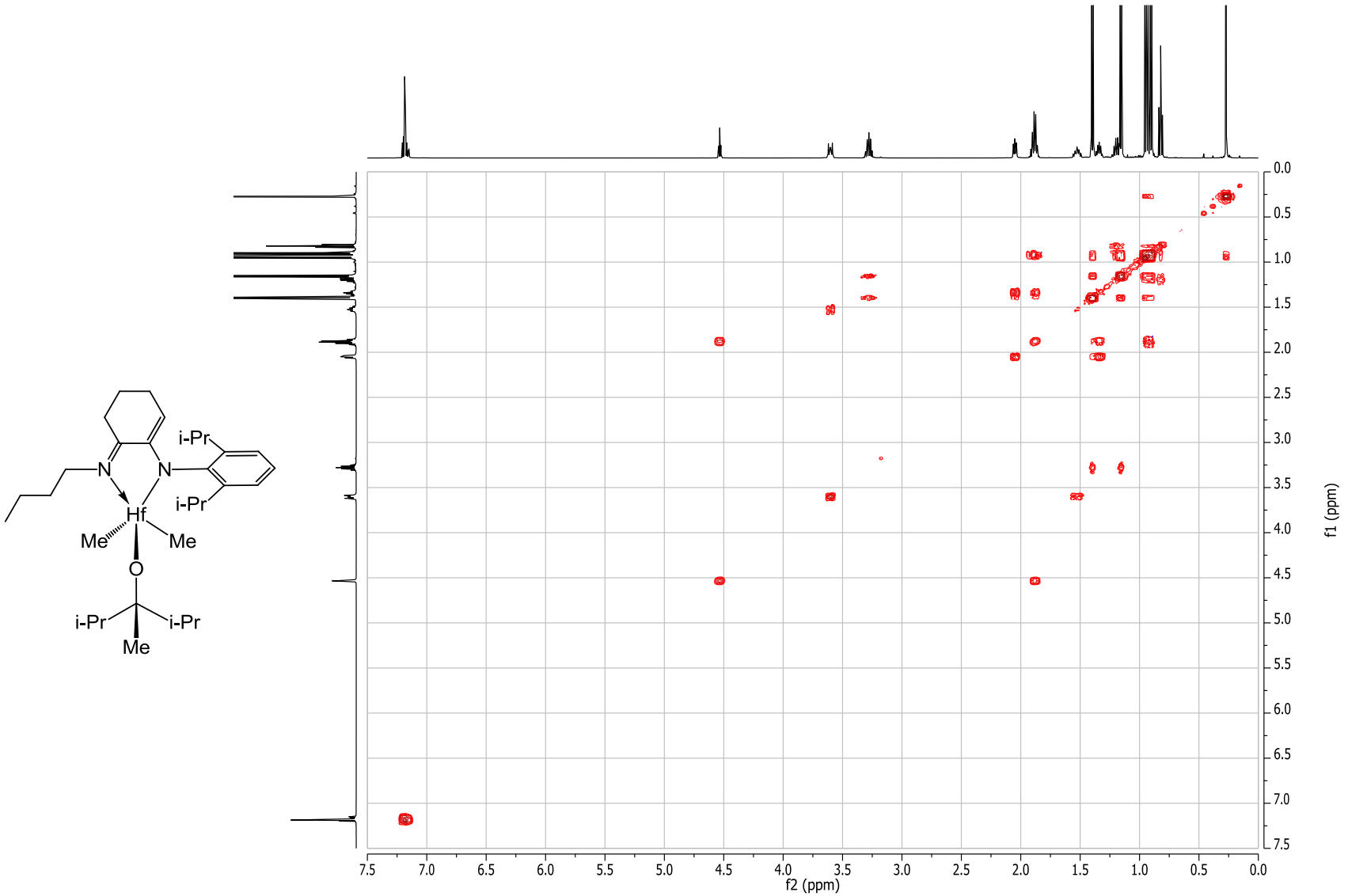


Figure 74. Fragment of gCOSY Spectrum of Complex **18** (C_6D_6, 500 MHz)

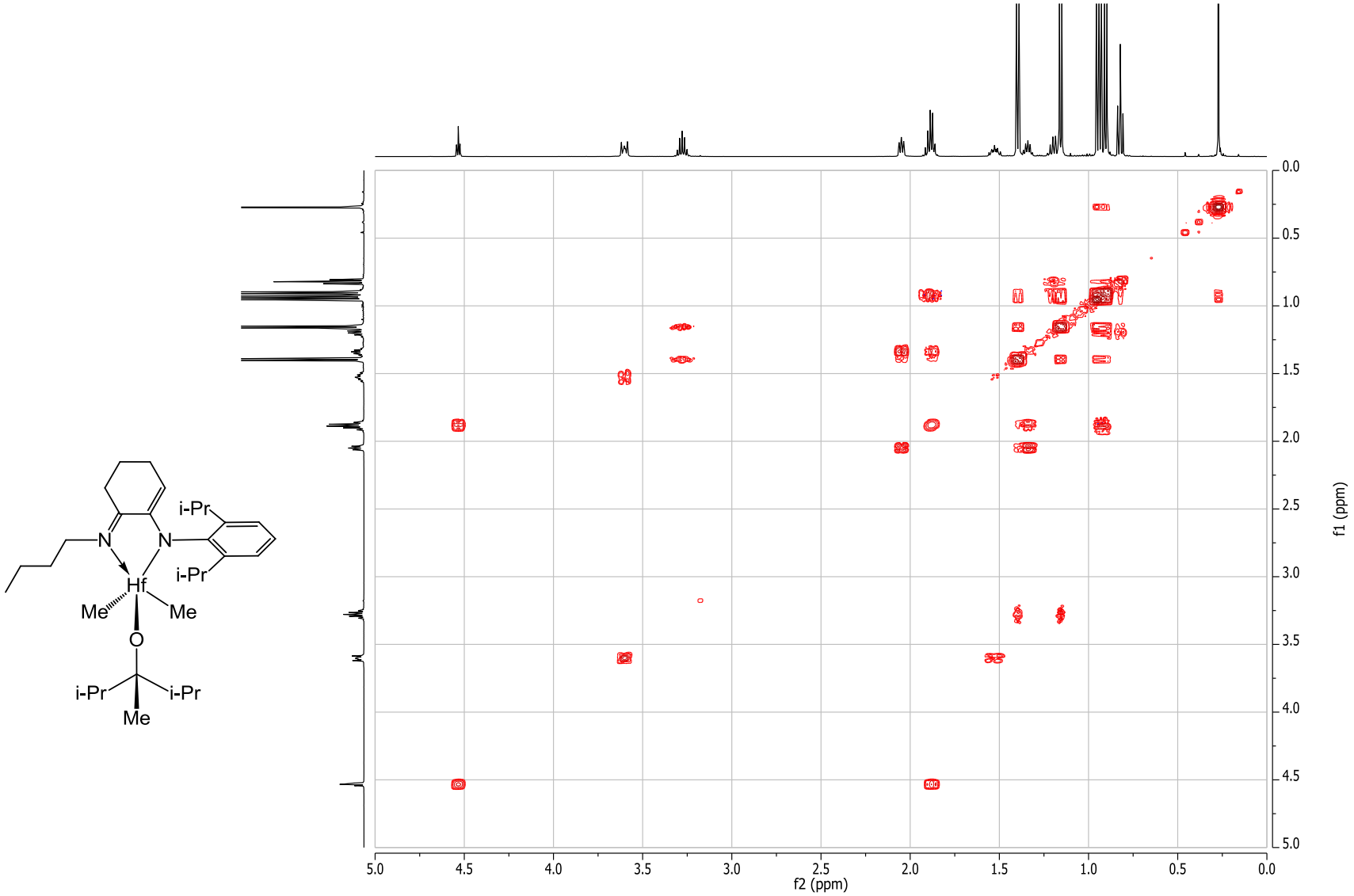


Figure 75. HSQCAD NMR Spectrum of Complex **18** (C_6D_6, 500 MHz)

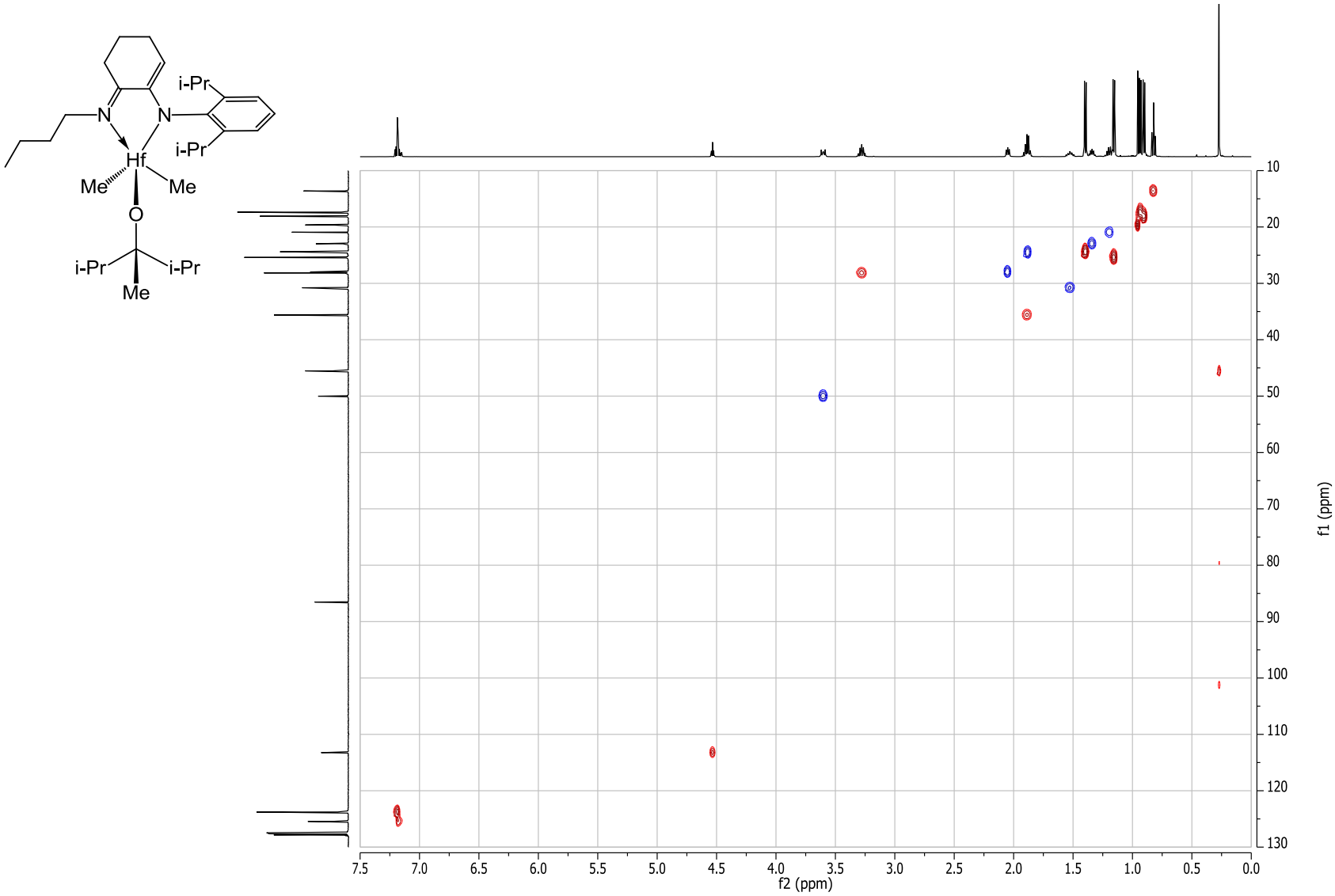


Figure 76. Fragment of gHSQCAD NMR Spectrum of Complex **18** (C_6D_6, 500 MHz)

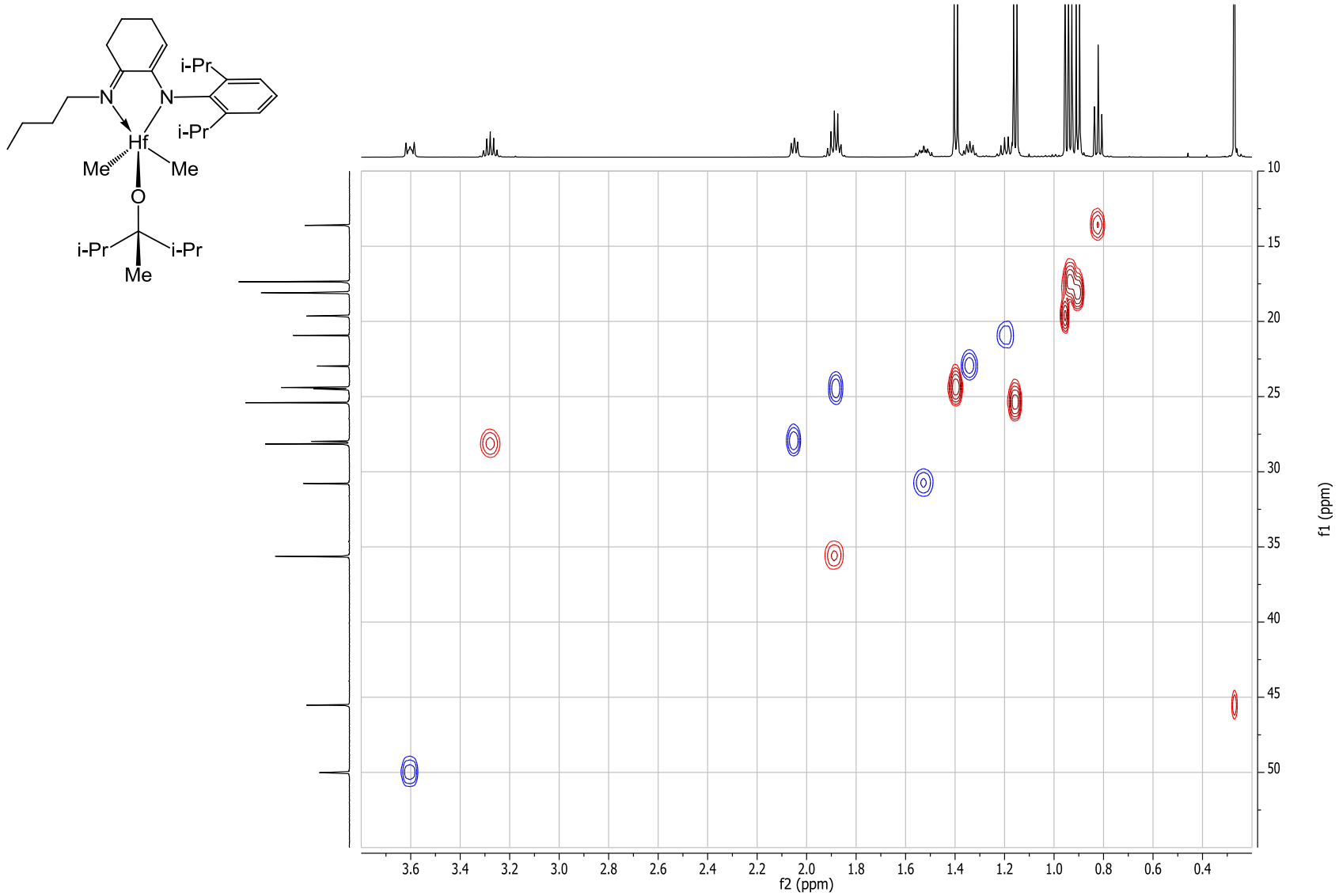


Figure 77. ^{1}H NMR Spectra of Complex **19** (C_6D_6, 500 MHz).

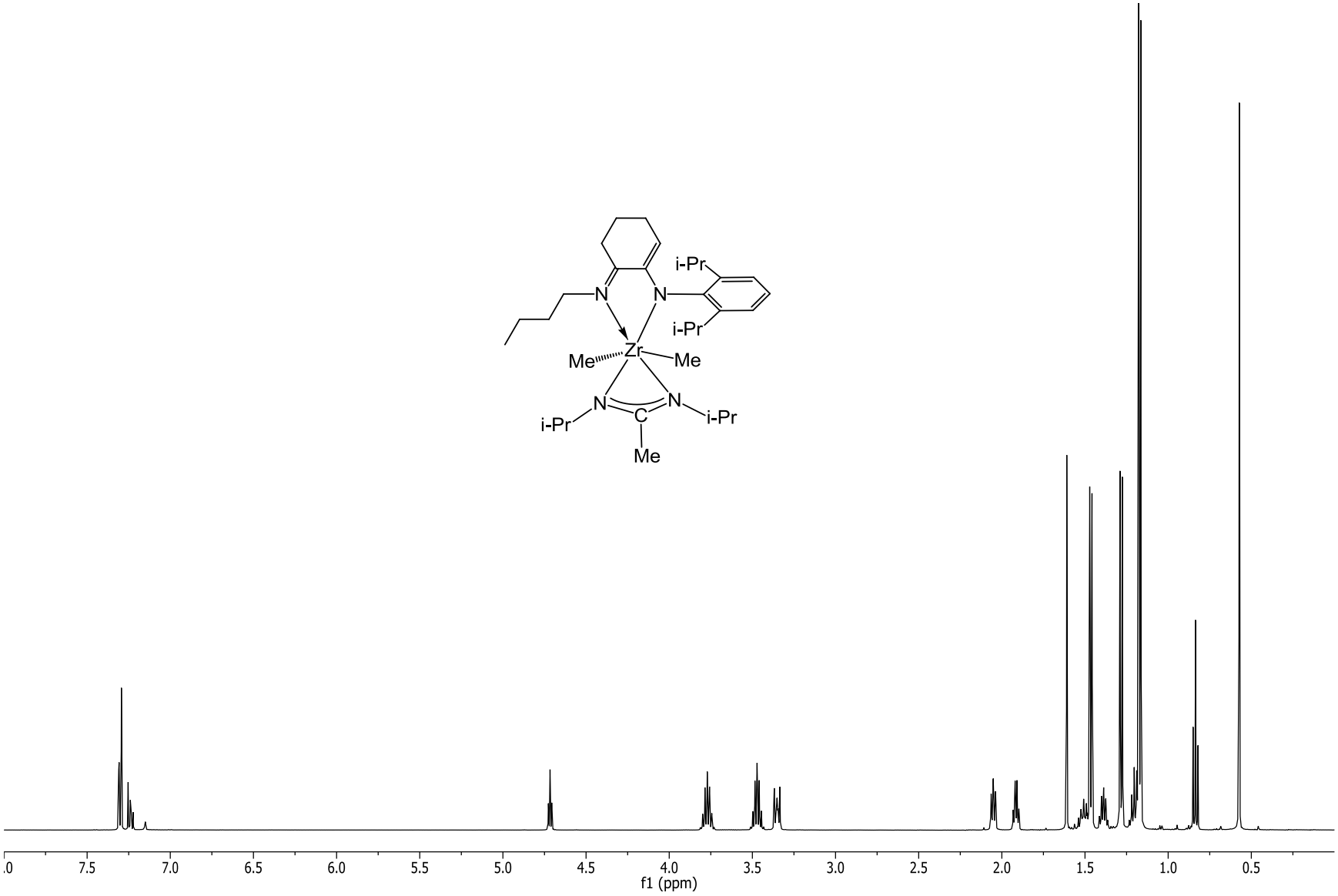


Figure 78. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **19** (C_6D_6, 125 MHz).

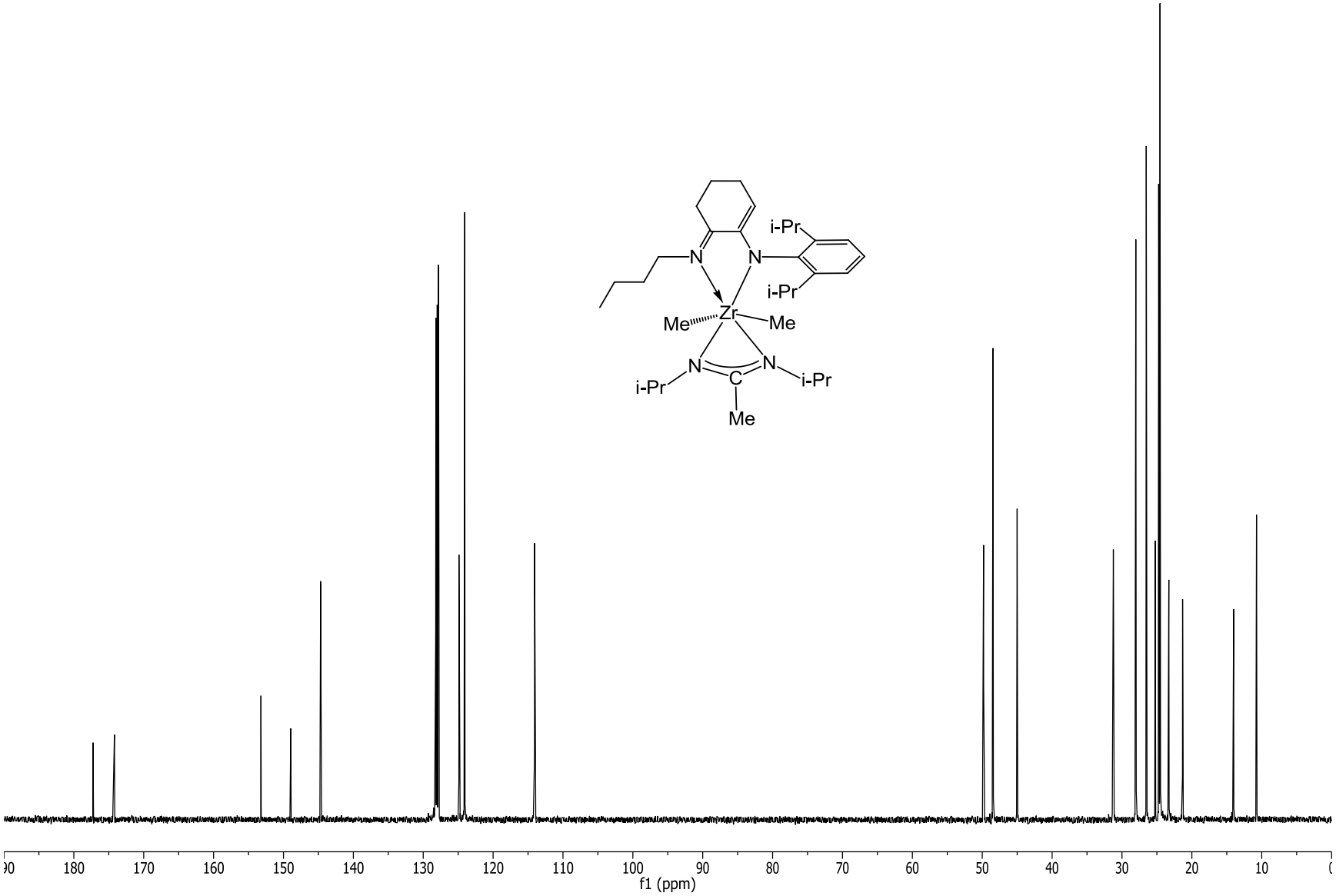


Figure 79. APT NMR Spectrum of Complex **19** (C_6D_6, 125 MHz).

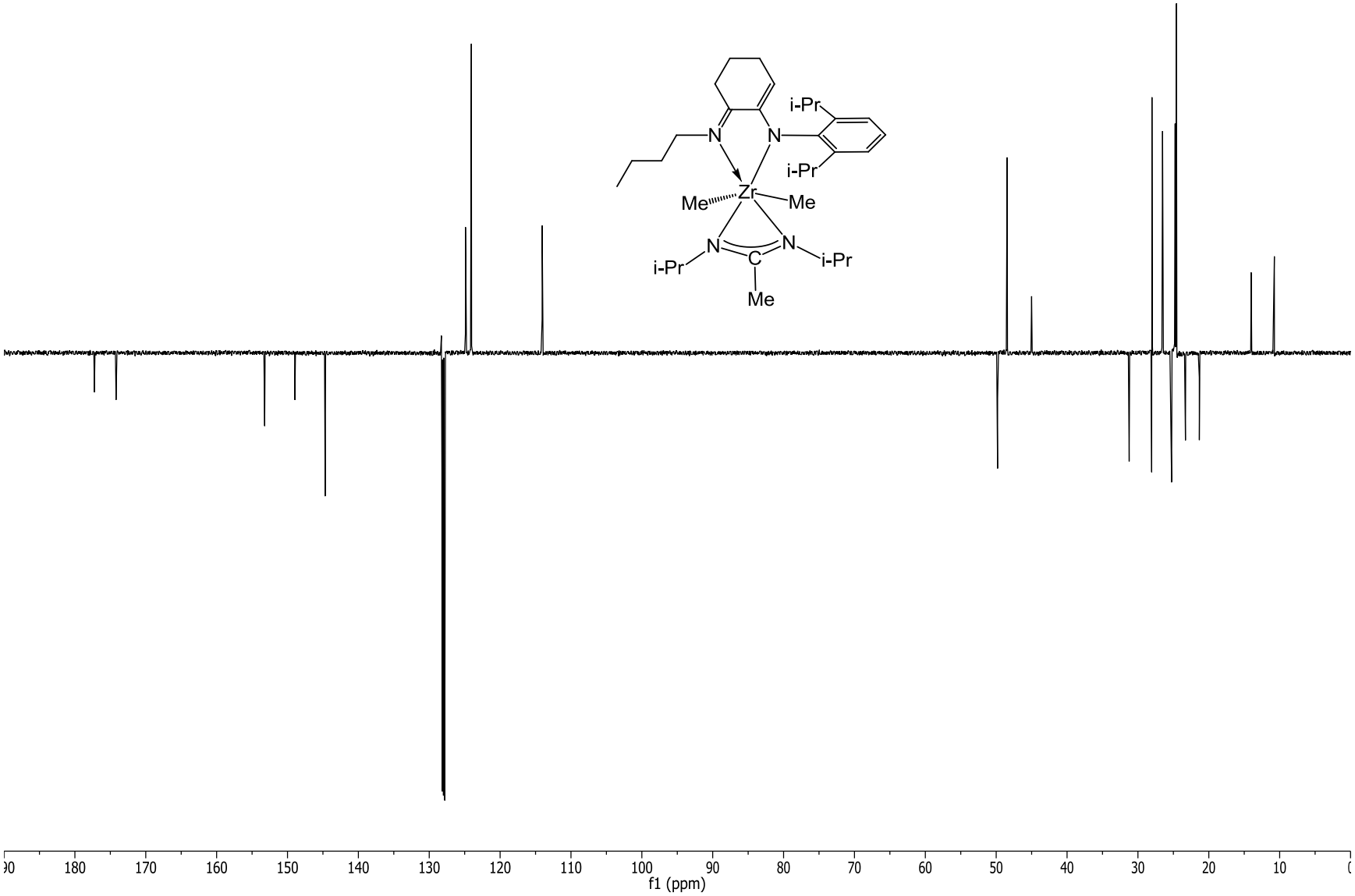


Figure 80. TOCSY1D NMR Spectra of Complex **19** (C_6D_6, 500 MHz) (mix time = 0, 0.03, 0.08 s).

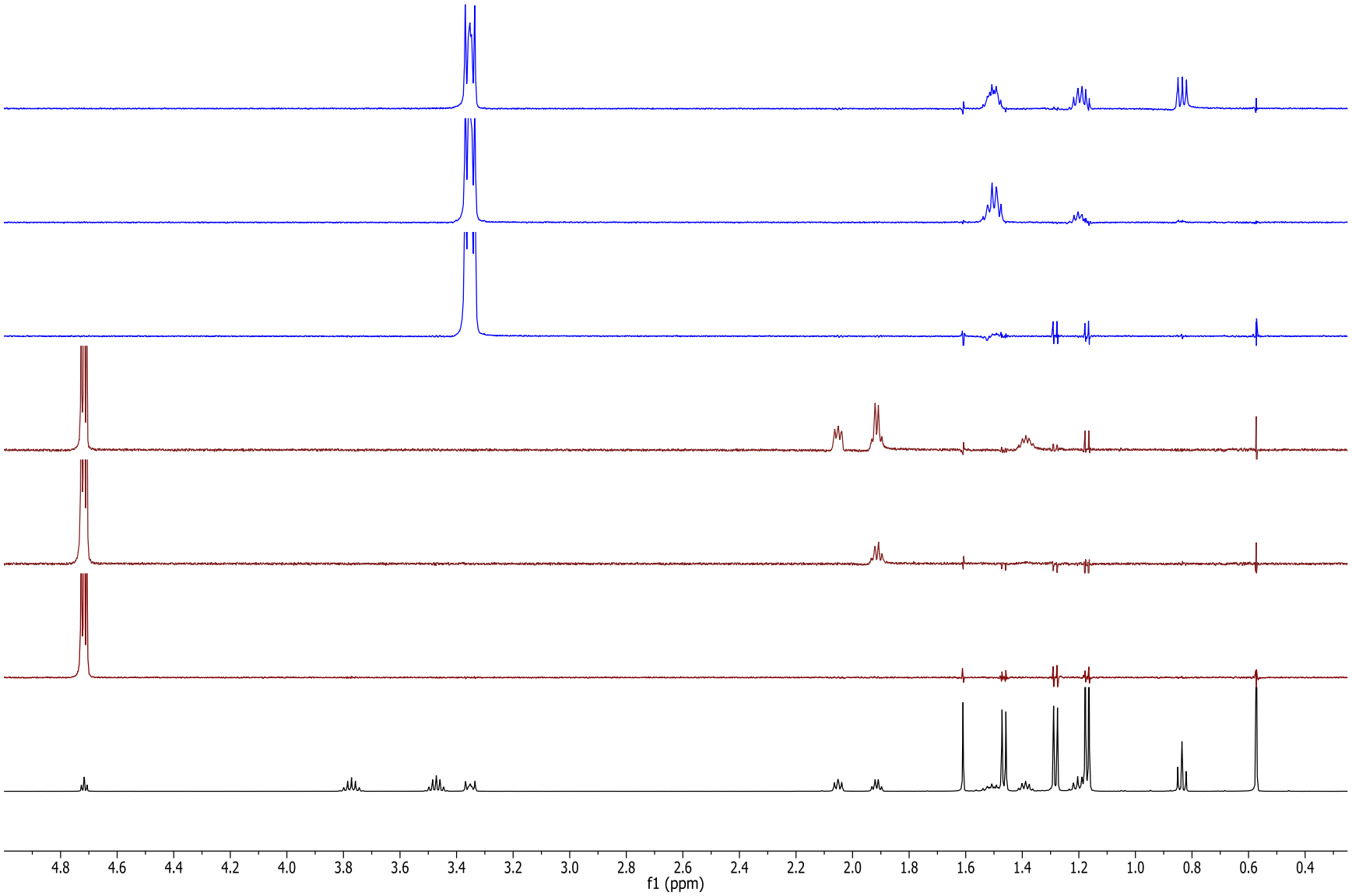


Figure 81. ^{1}H and NOESY1D NMR Spectra of Complex **19** (C_6D_6, 500 MHz, mixing time = 0.8 s).

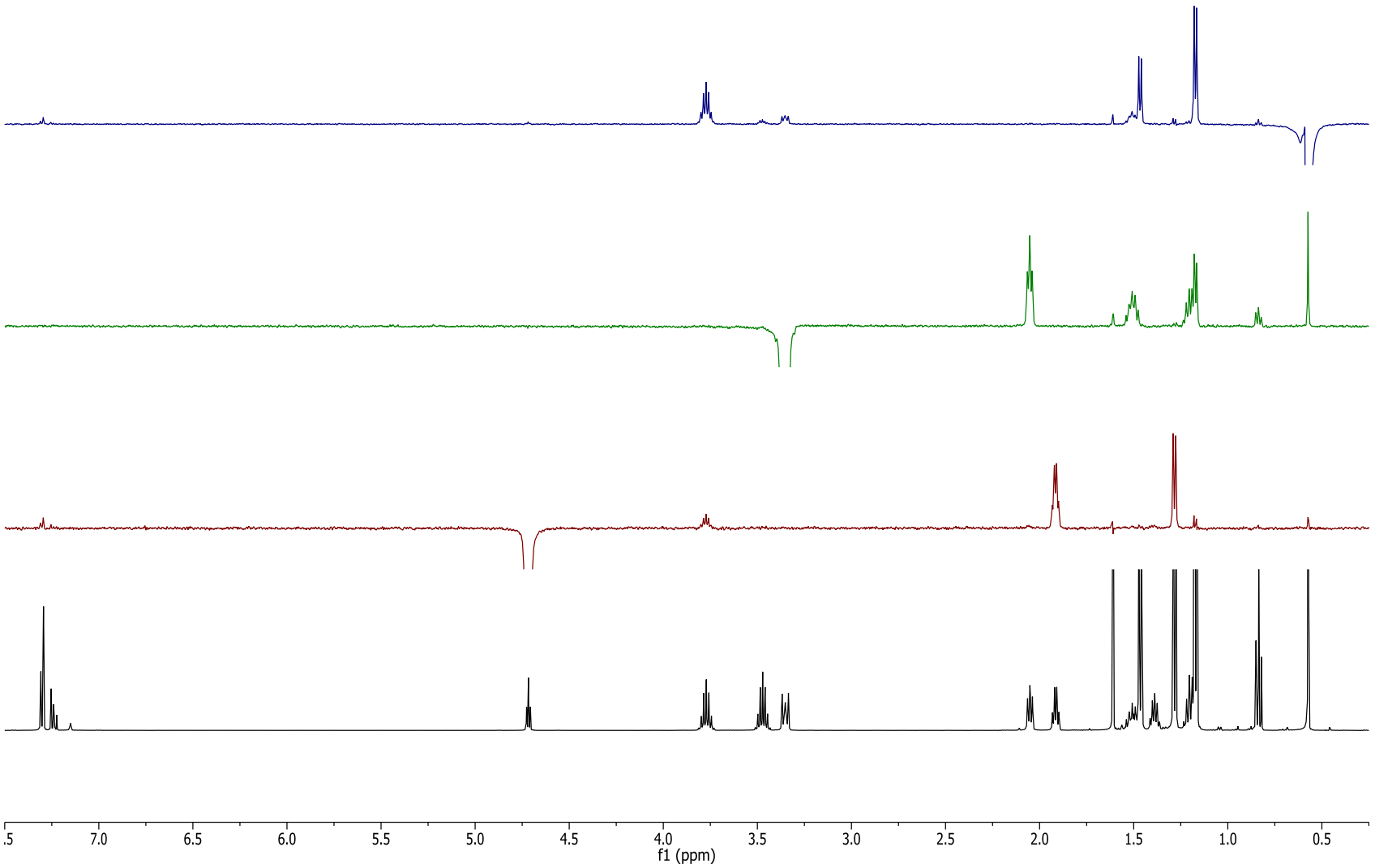


Figure 82. gCOSY NMR Spectrum of Complex **19** (C_6D_6, 500 MHz)

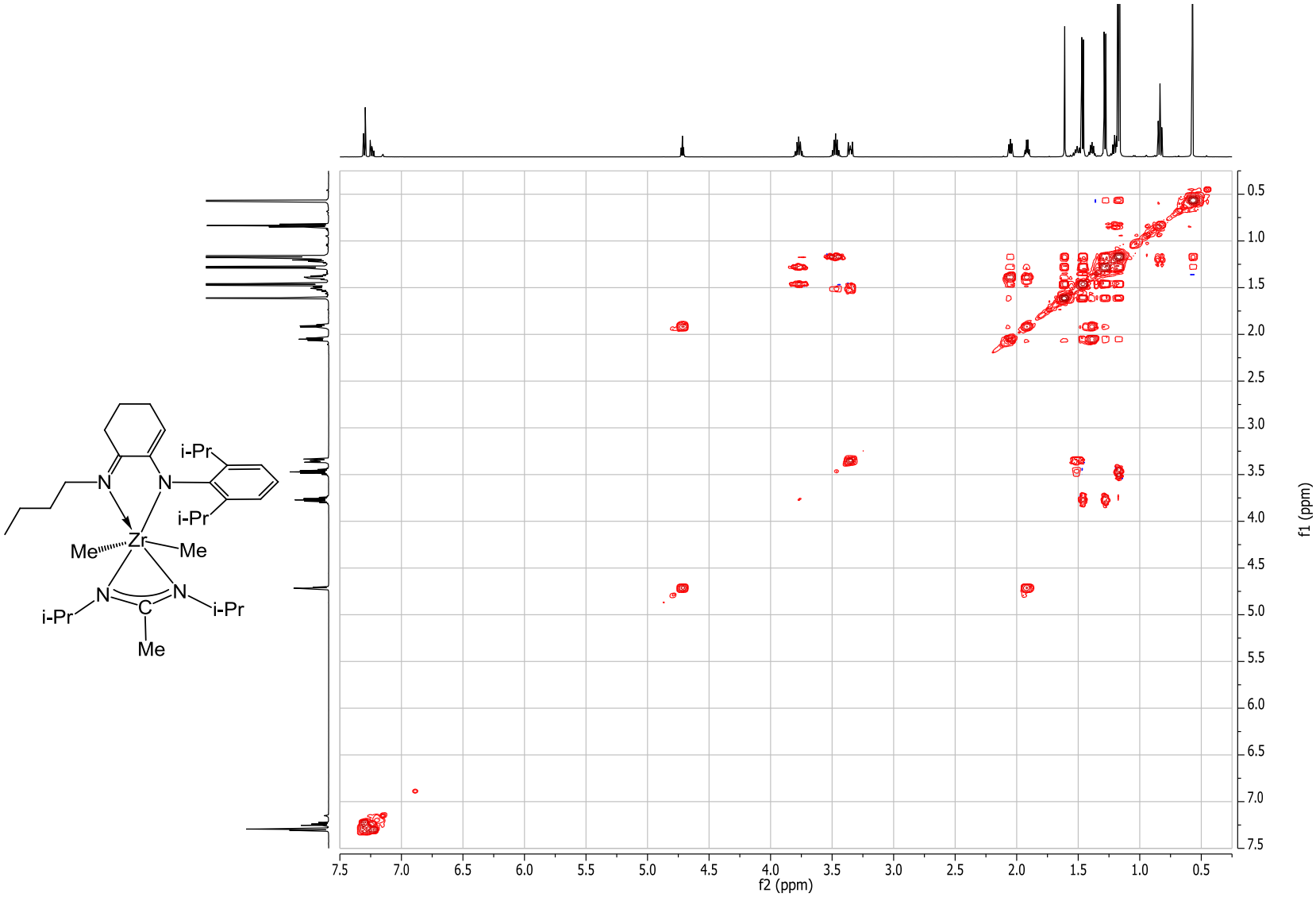


Figure 83. Fragment of gCOSY Spectrum of Complex **19** (C_6D_6, 500 MHz).

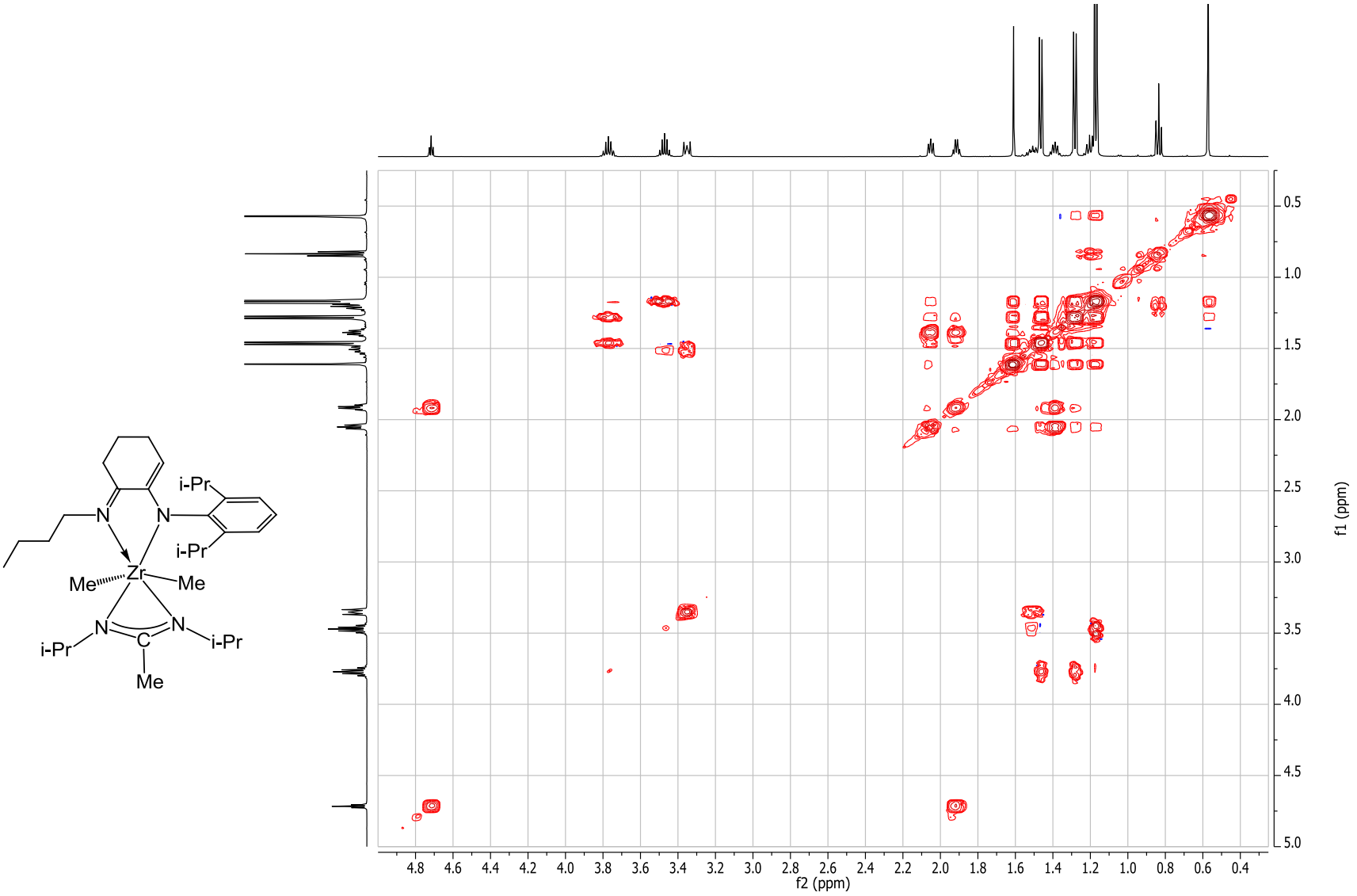


Figure 84. HSQCAD NMR Spectrum of Complex **19** (C_6D_6, 500 MHz).

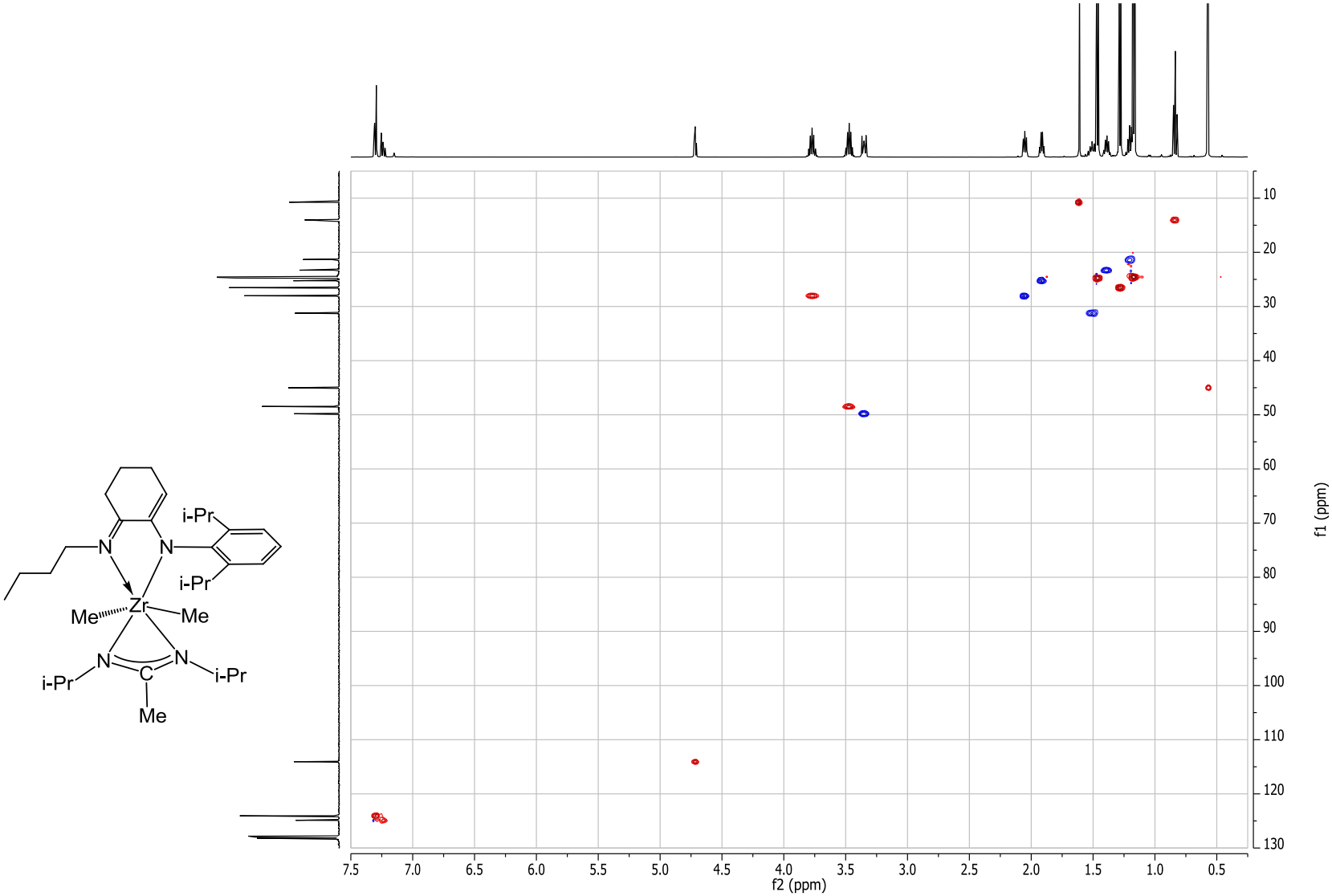


Figure 85. Fragment of gHSQCAD NMR Spectrum of Complex **19** (C_6D_6, 500 MHz).

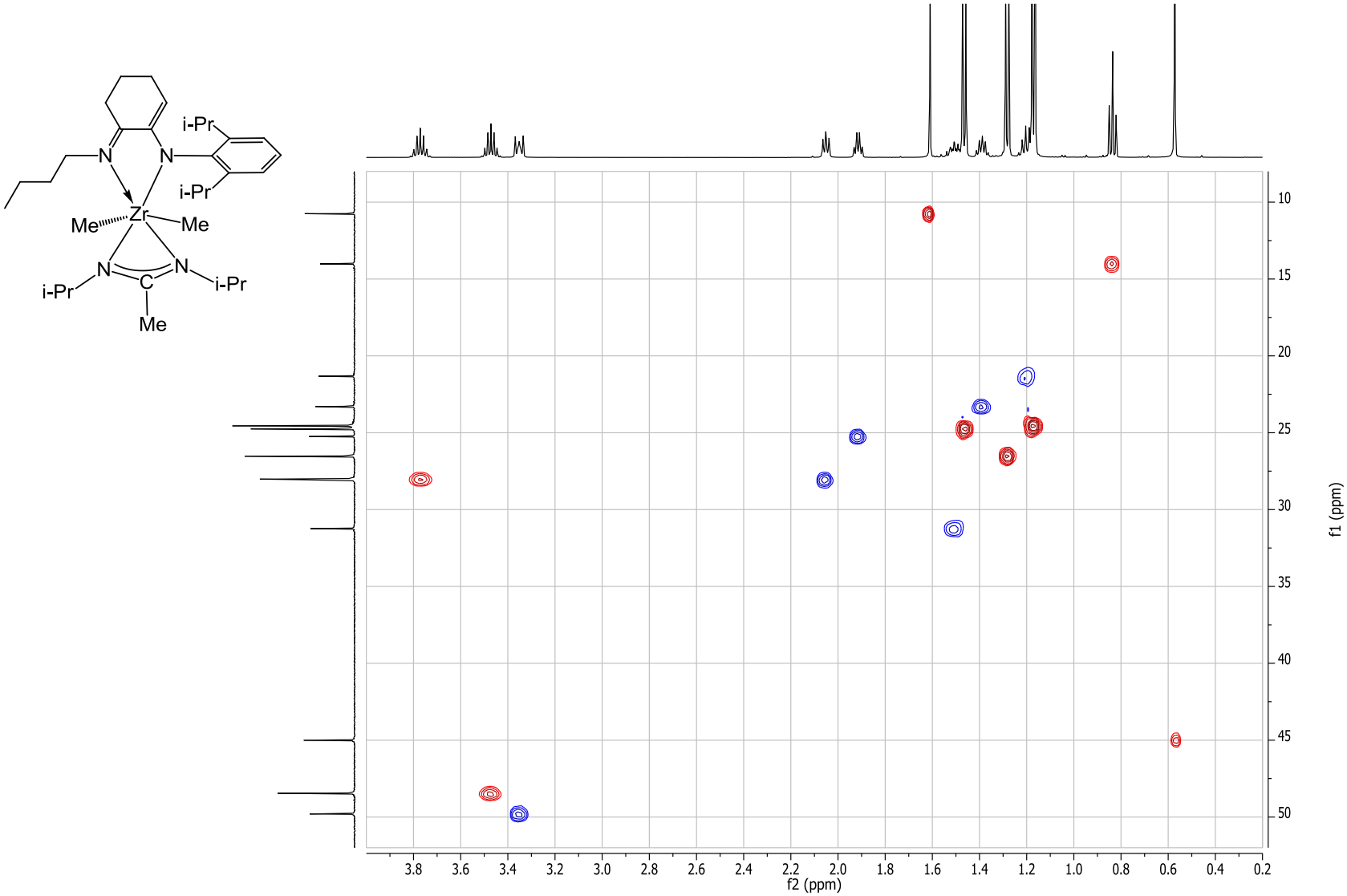


Figure 86. ^{1}H NMR Spectra of Complex **20** (C_6D_6, 400 MHz).

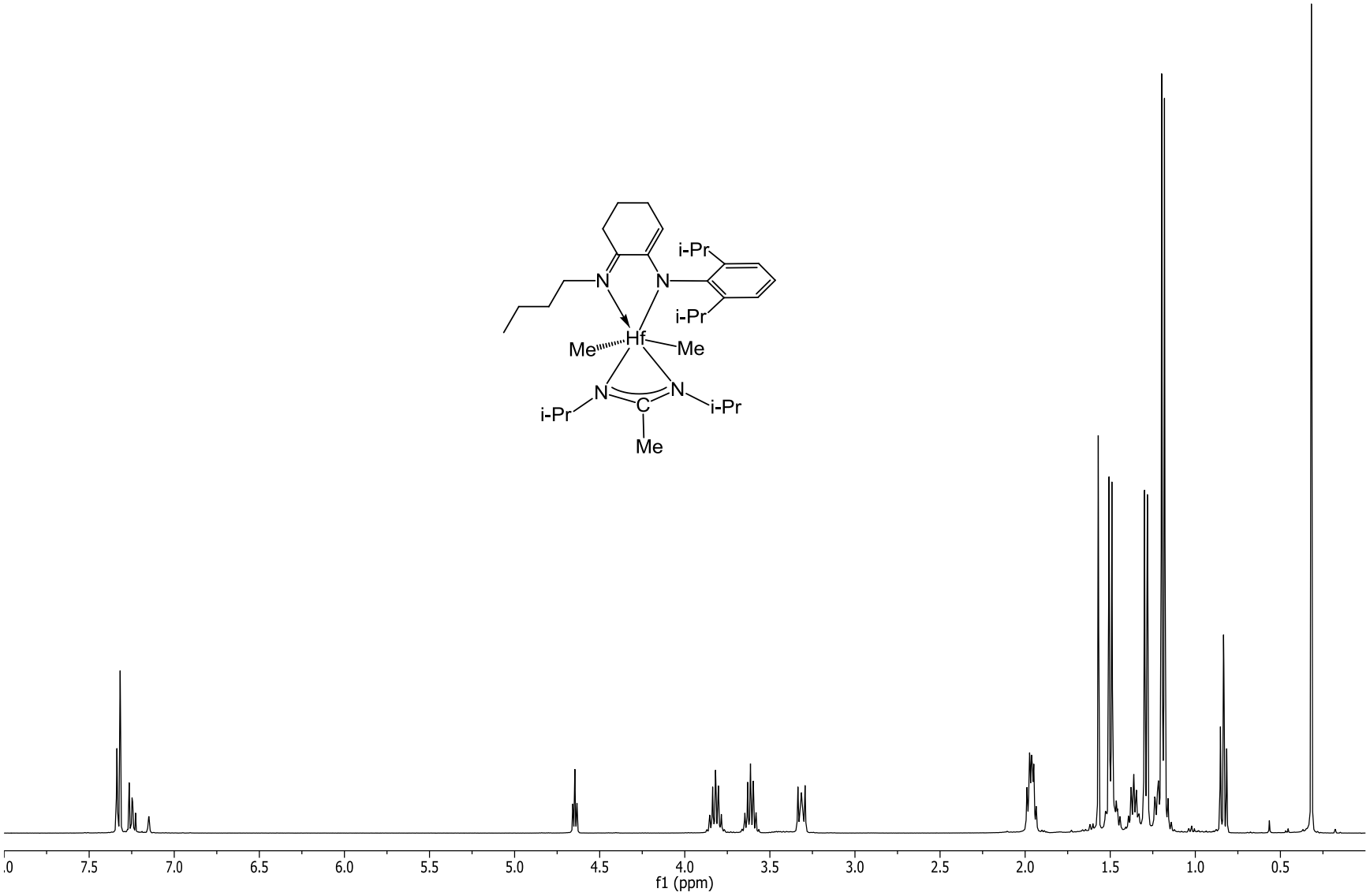


Figure 87. $^{13}C\{^{1}H\}$ NMR Spectrum of Complex **20** (C_6D_6, 100 MHz).

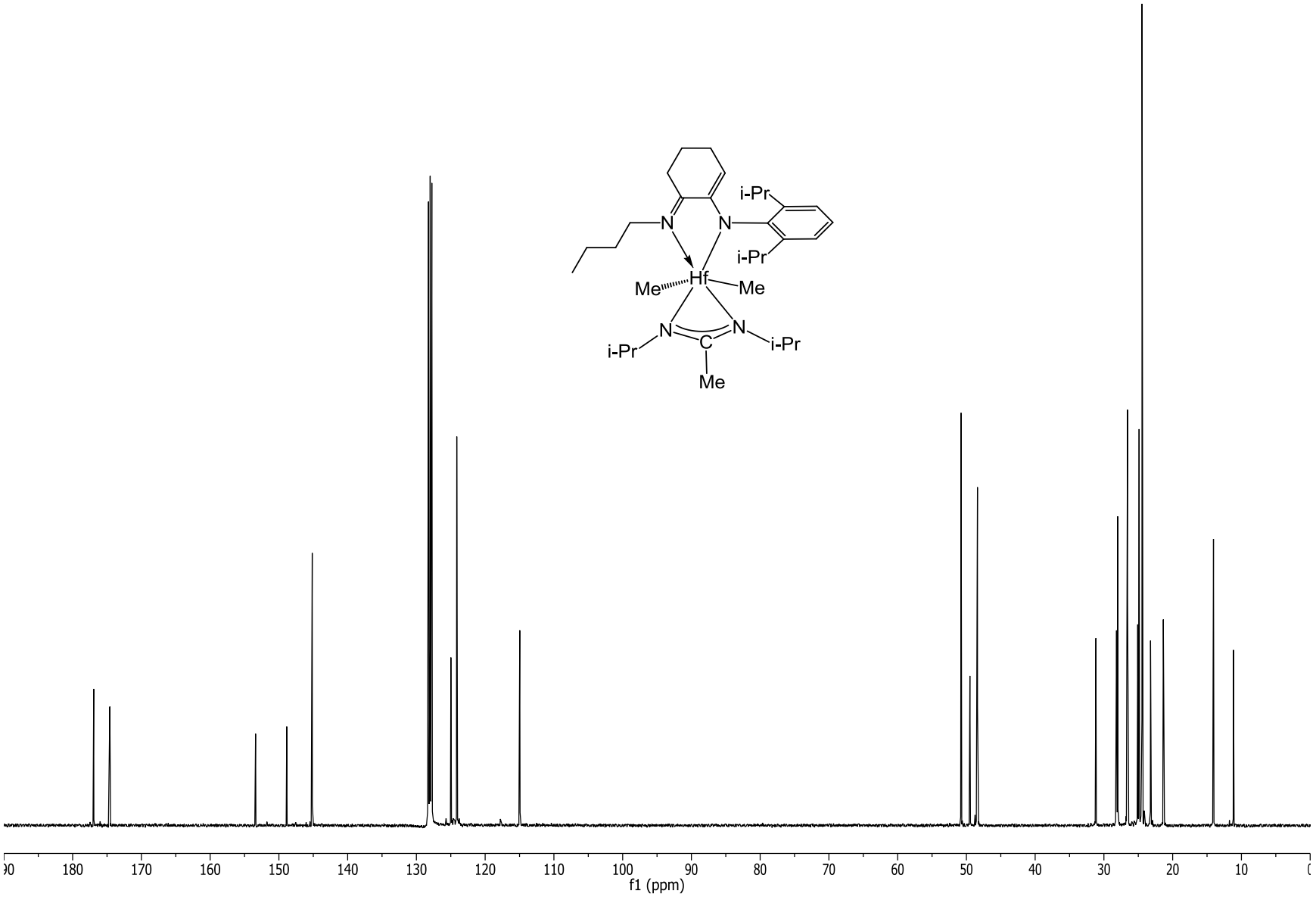


Figure 88. APT NMR Spectrum of Complex **20** (C_6D_6, 100 MHz).

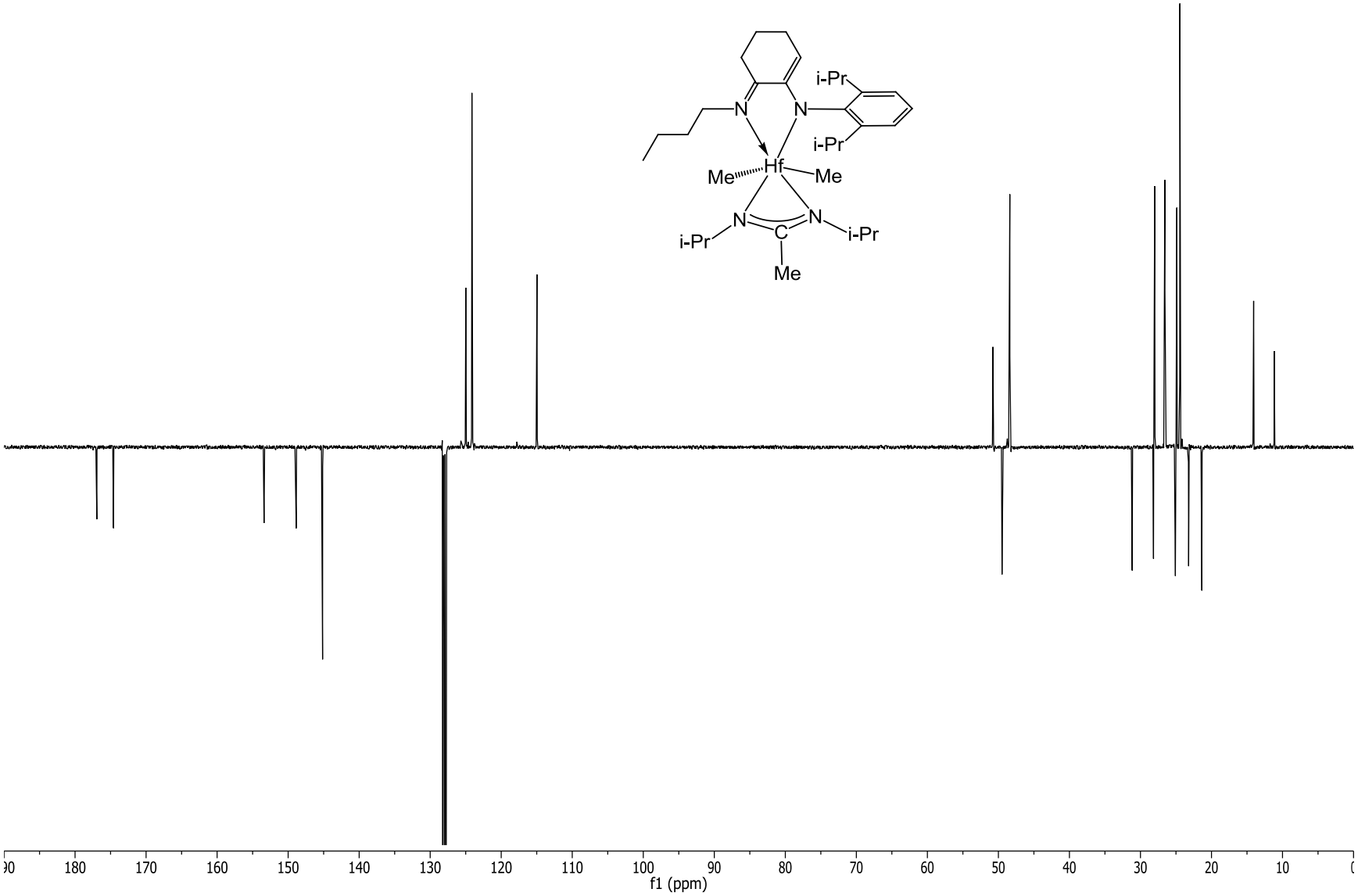


Figure 89. TOCSY1D NMR Spectra of Complex **20** (C_6D_6, 400 MHz) (mix time = 0, 0.03, 0.08 s).

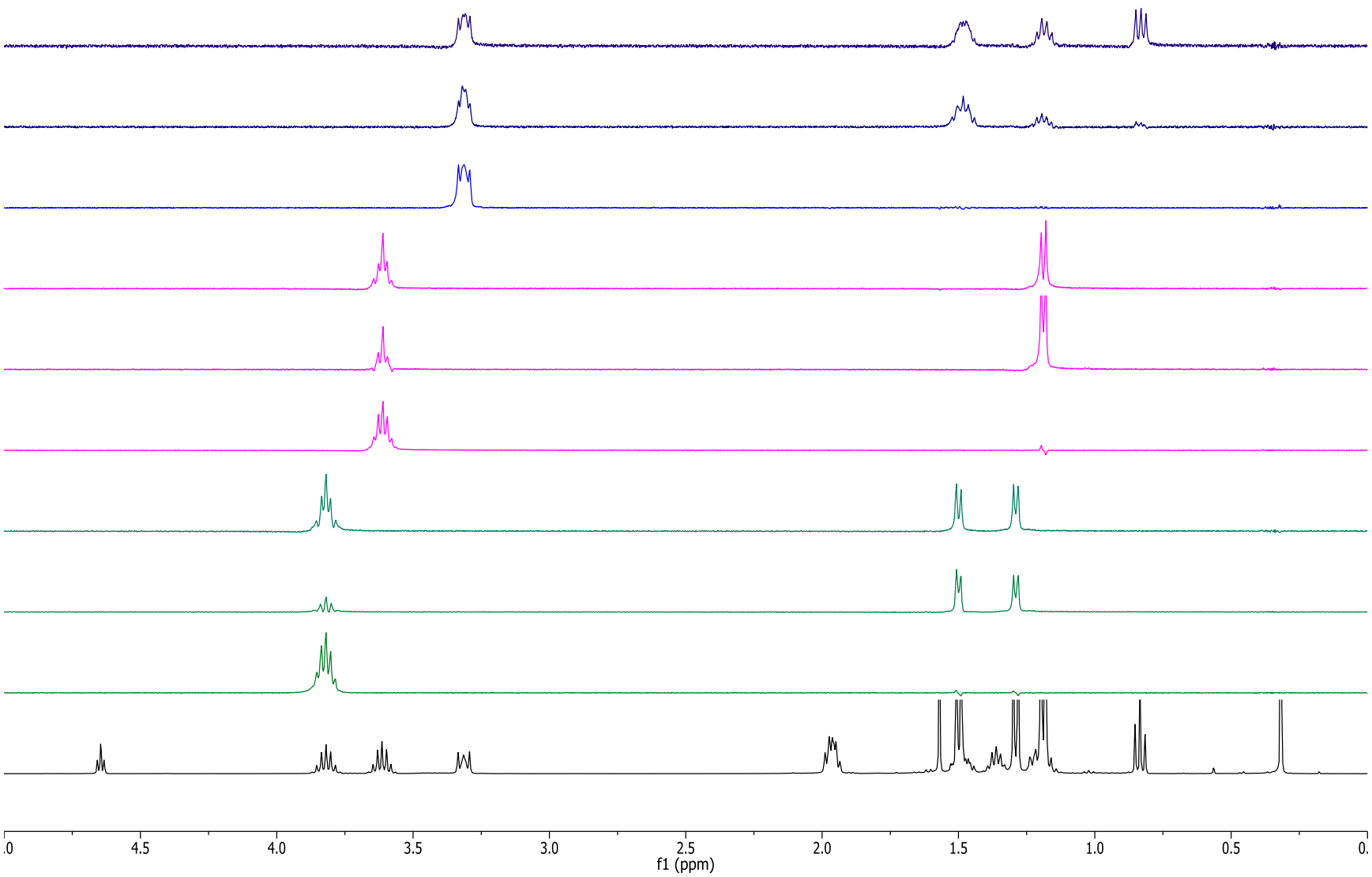


Figure 90. TOCSY1D NMR Spectra of Complex **20** (C_6D_6, 400 MHz) (mix time = 0, 0.03, 0.08 s) – Continuation.

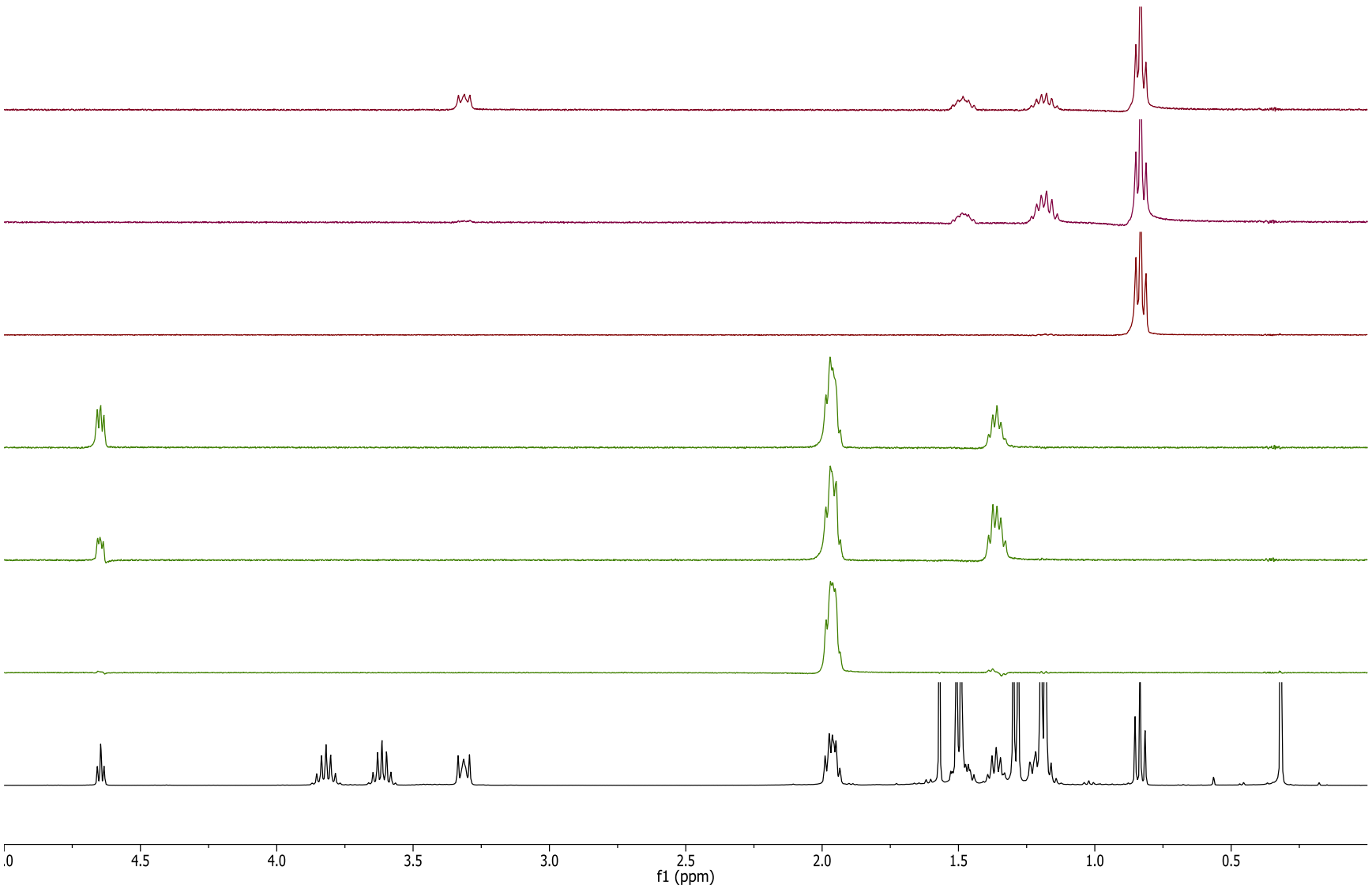


Figure 91. ^{1}H and NOESY1D NMR Spectra of Complex **20** (C_6D_6, 400 MHz, mixing time = 0.8 s).

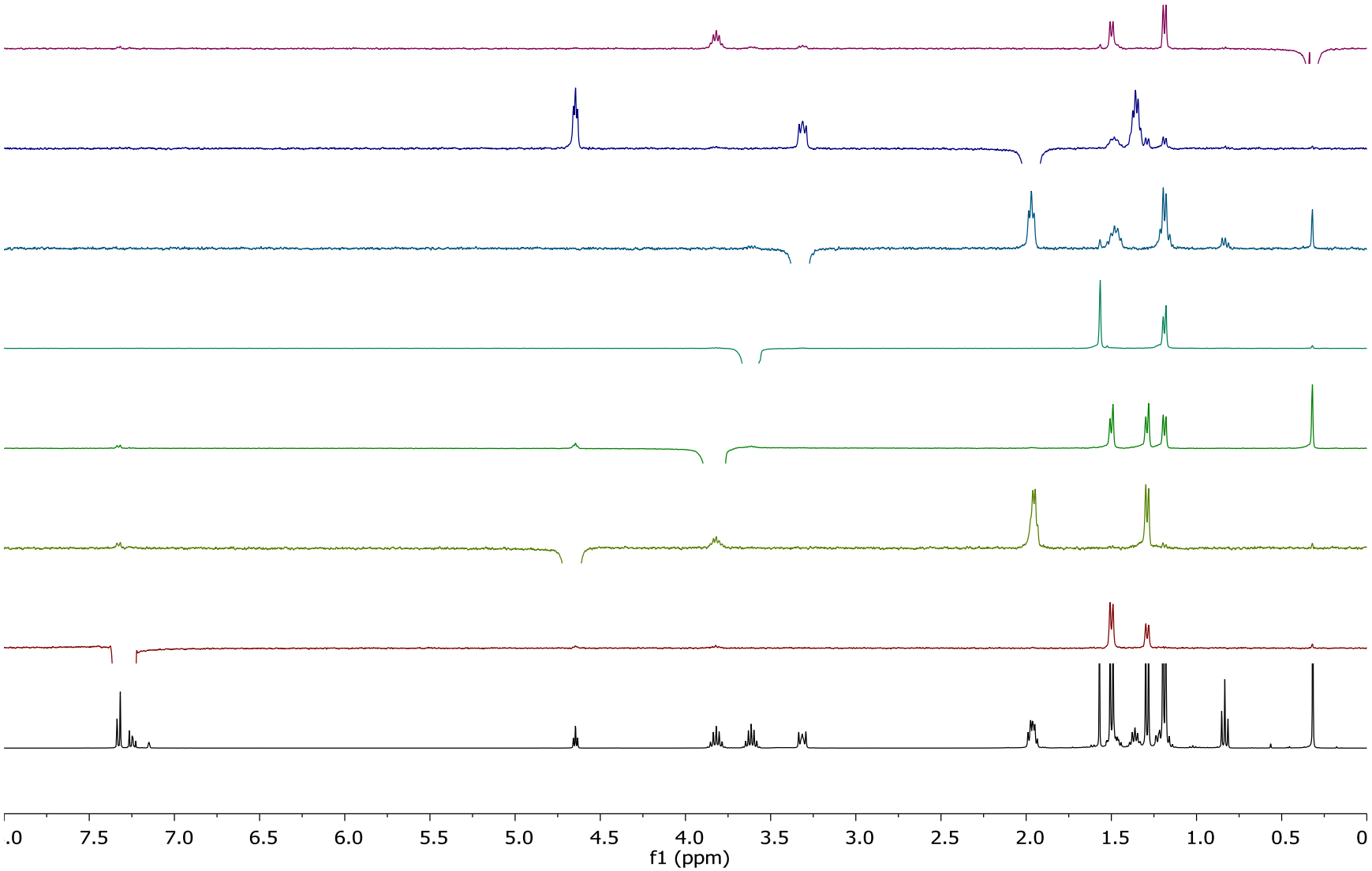


Figure 92. gCOSY NMR Spectrum of Complex **20** (C_6D_6, 400 MHz).

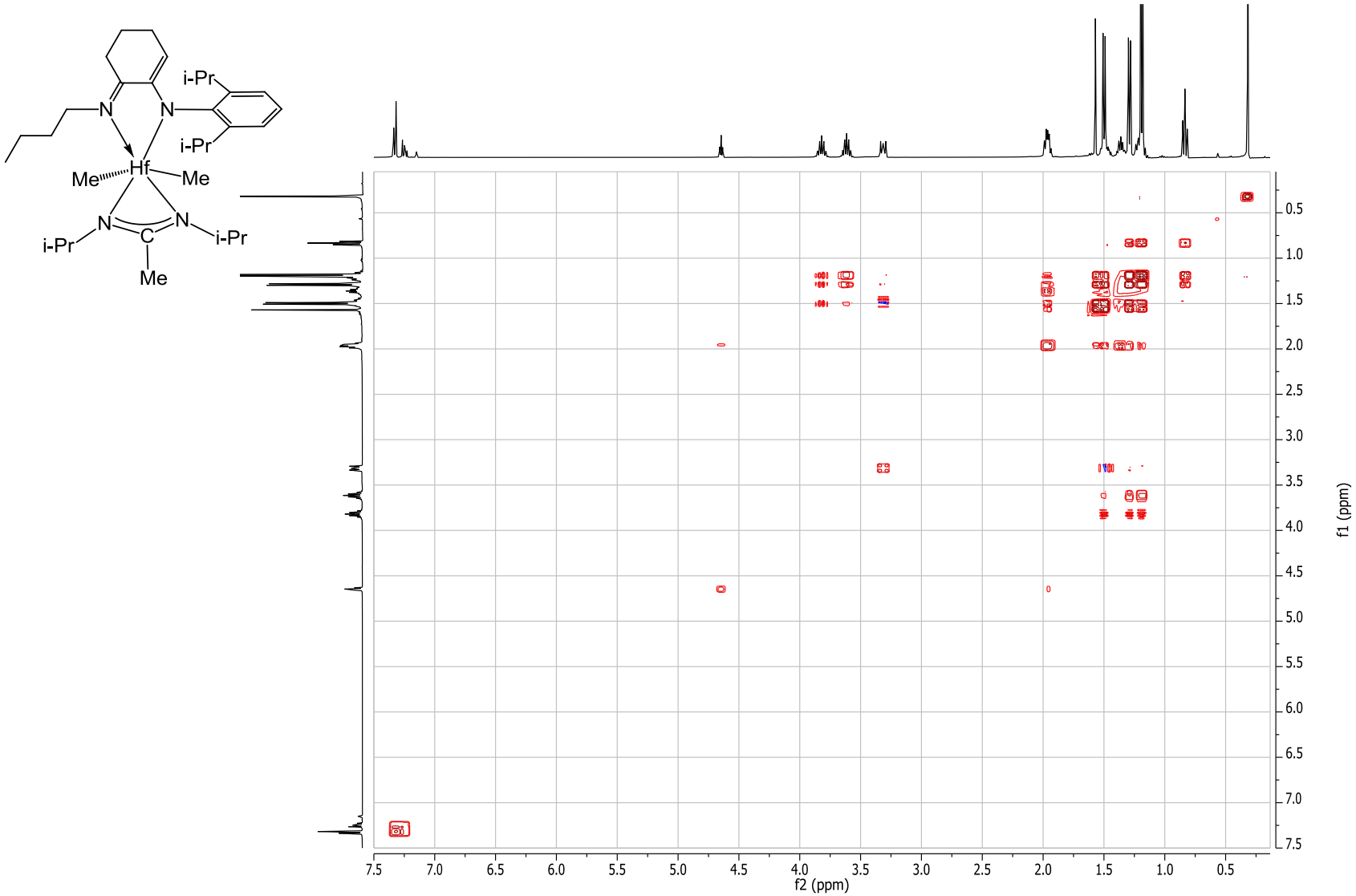


Figure 93. Fragment of gCOSY Spectrum of Complex **20** (C_6D_6, 400 MHz).

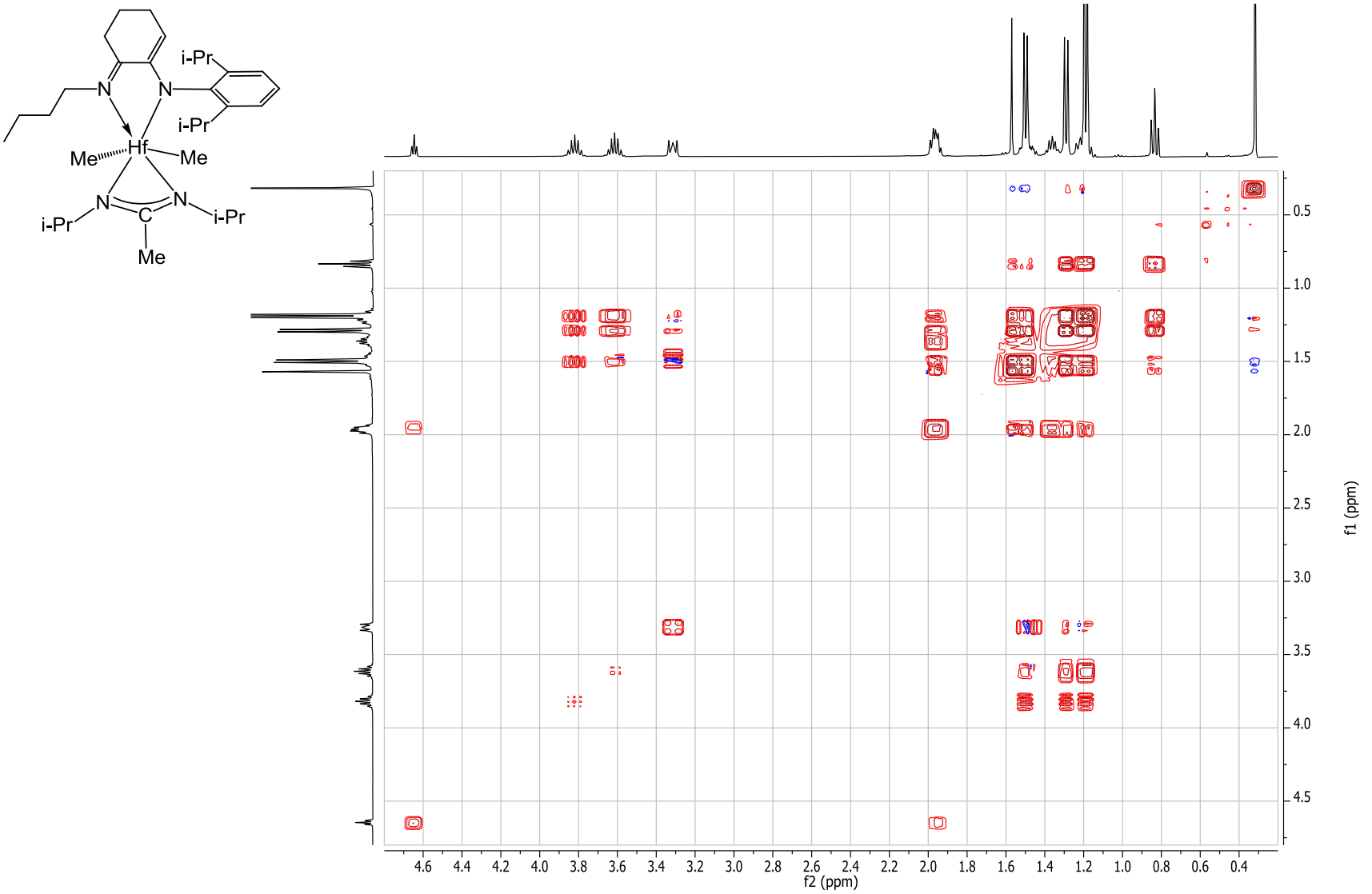


Figure 94. HSQCAD NMR Spectrum of Complex **20** (C_6D_6, 400 MHz).

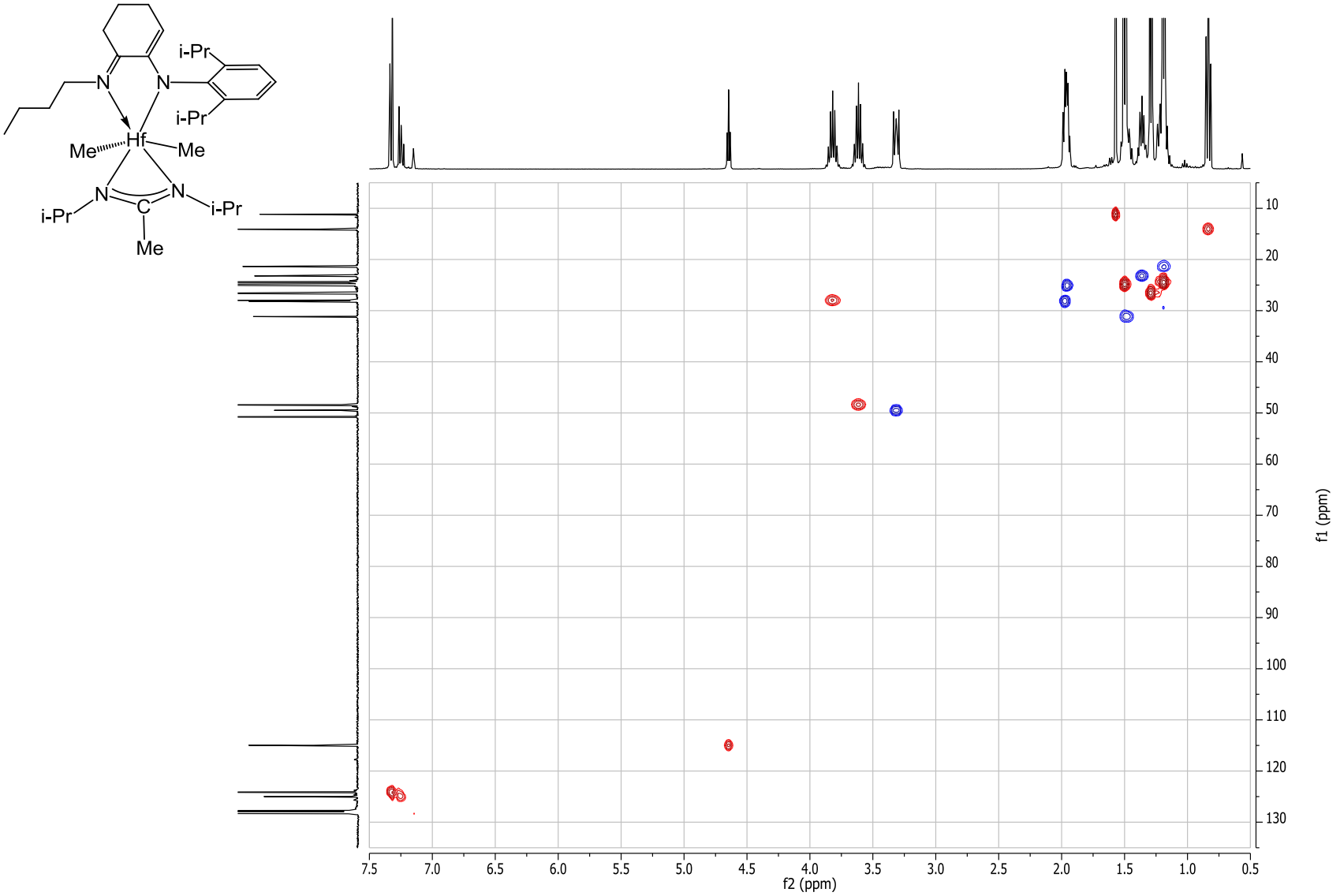


Figure 95. Fragment of gHSQCAD NMR Spectrum of Complex **20** (C_6D_6, 400 MHz).

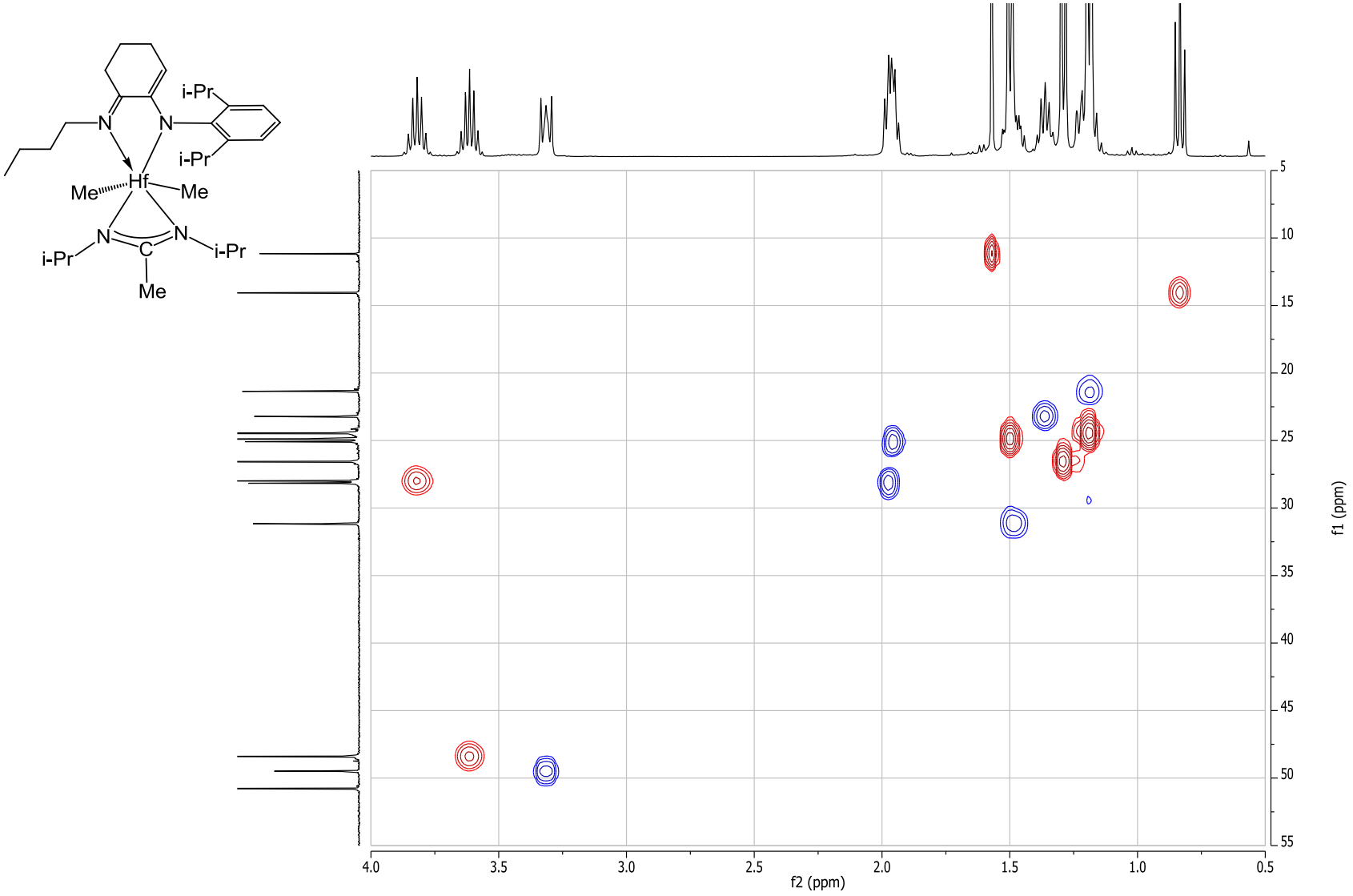


Figure 96. GPC trace for run #1.

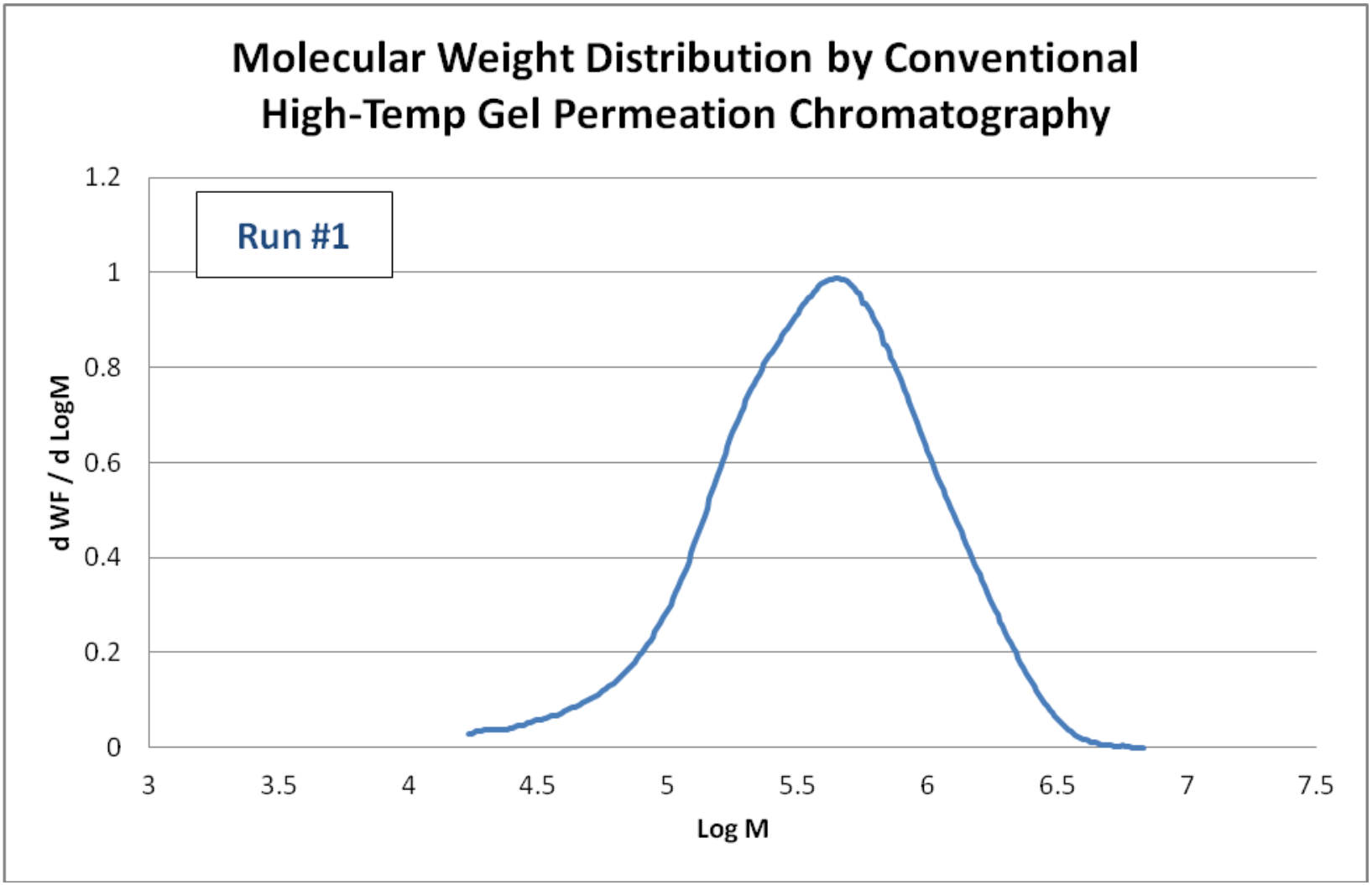


Figure 97. DSC plot for run # 1 .

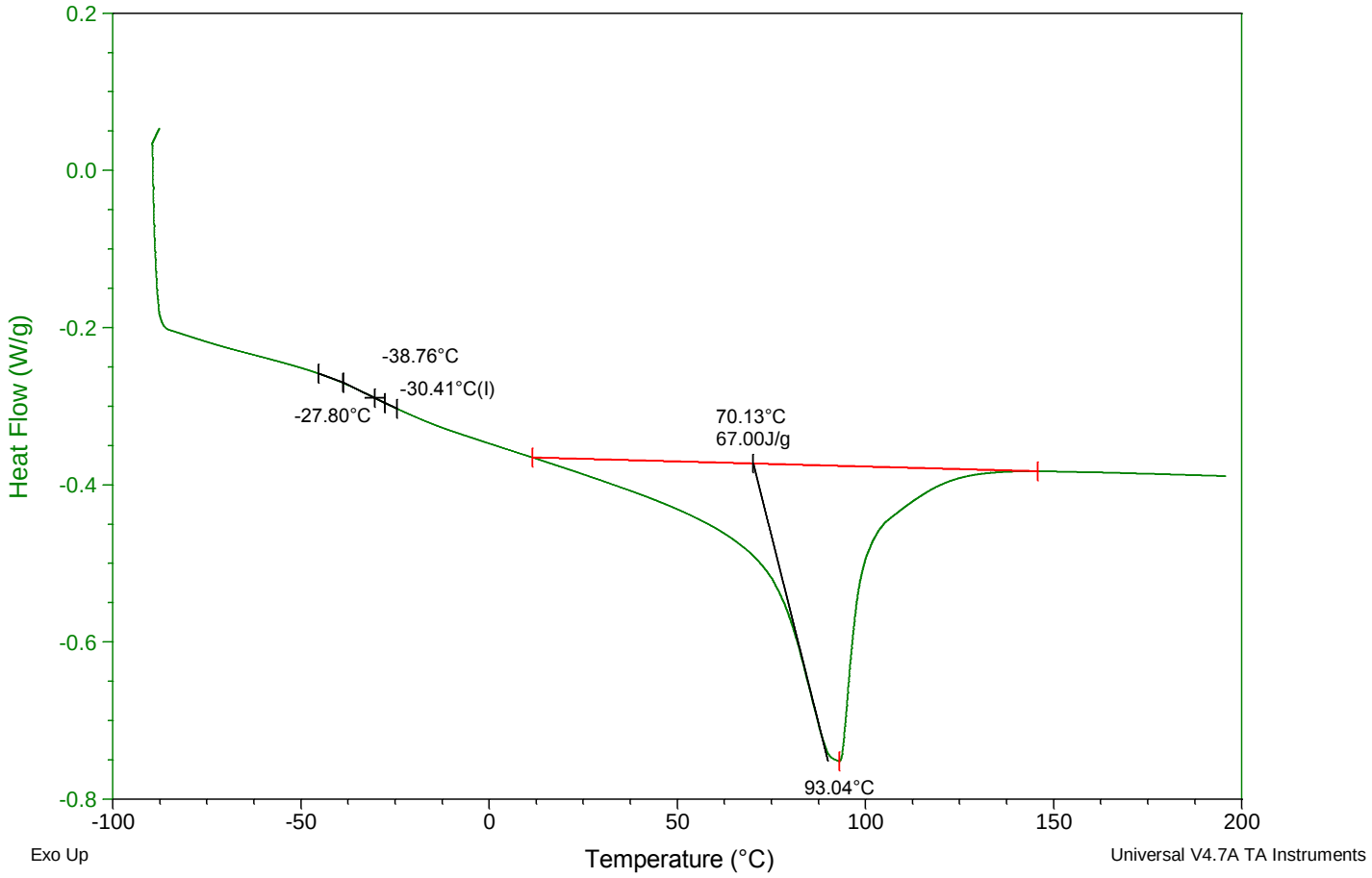


Figure 98. GPC trace for run #2.

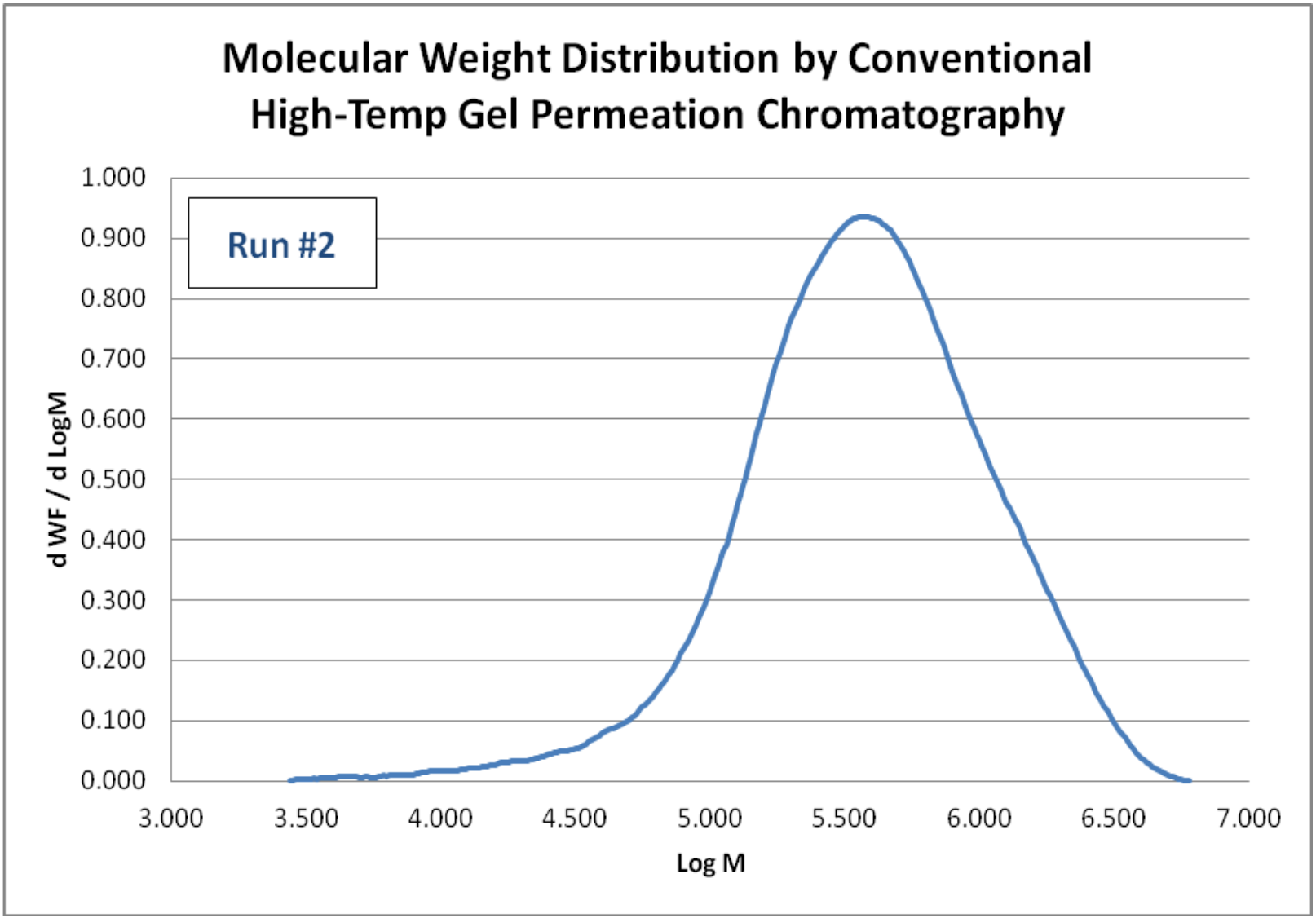


Figure 99. DSC plot for run #2.

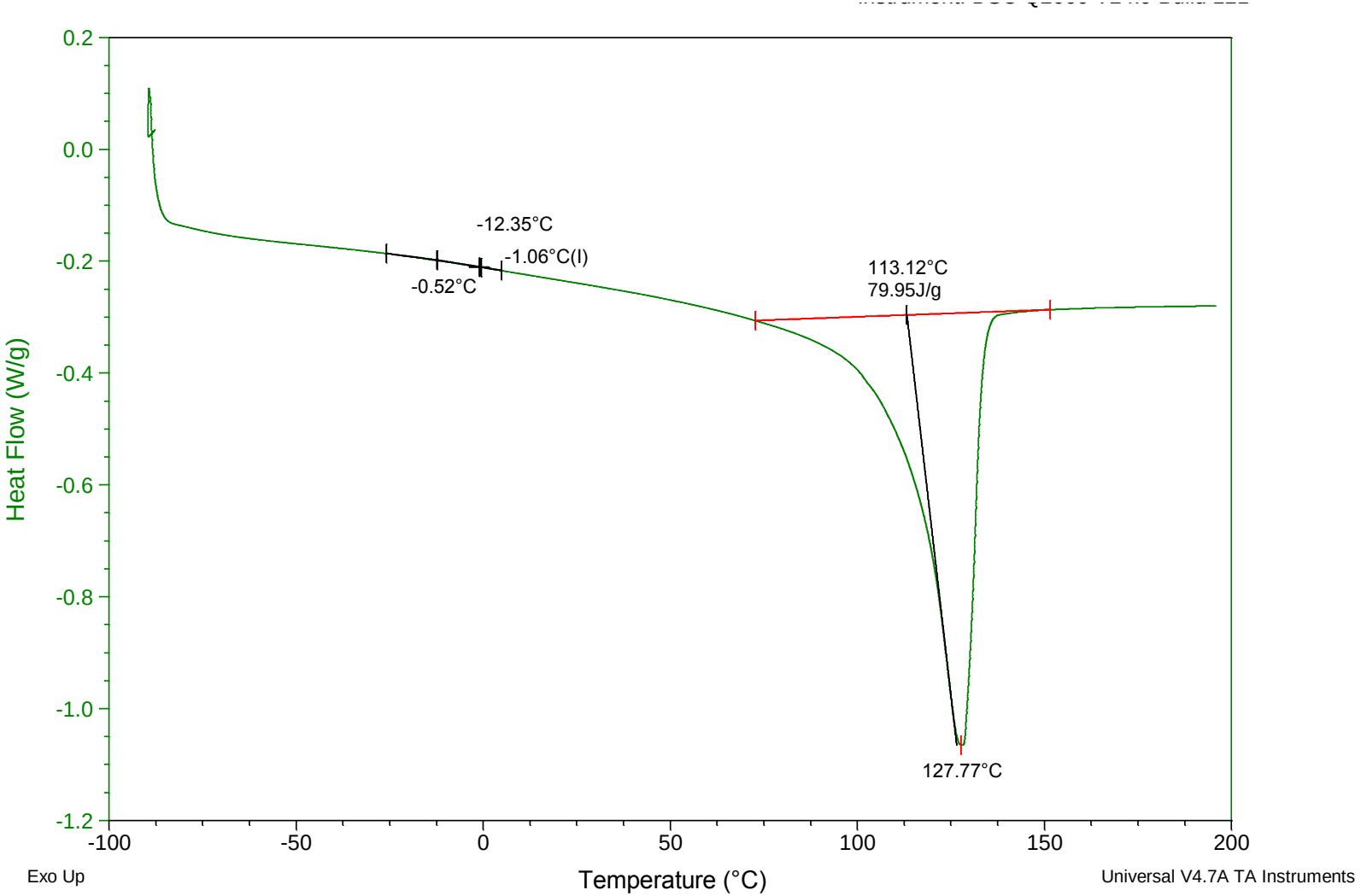


Figure 100. GPC trace for run #3.

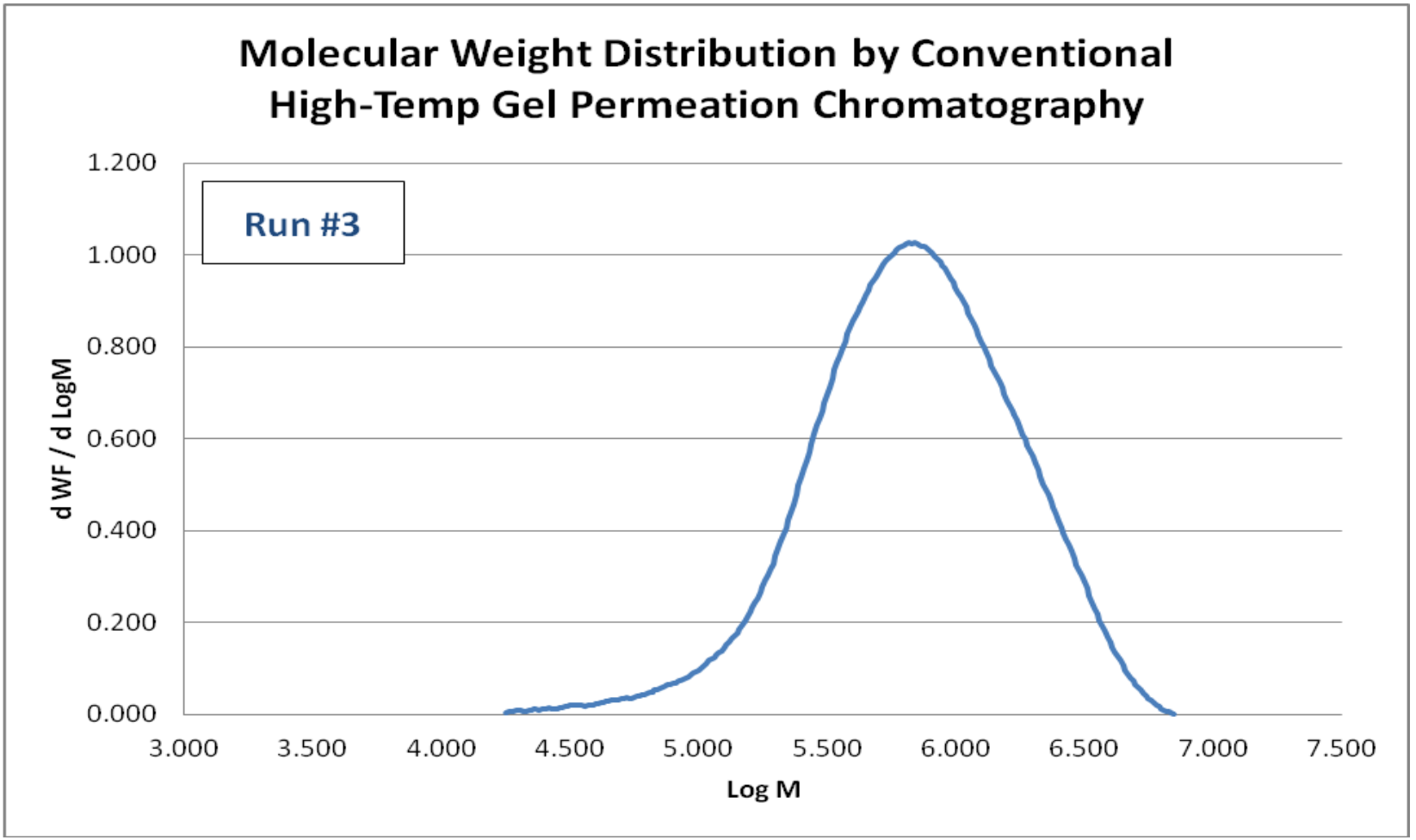


Figure 101. DSC plot for run #3.

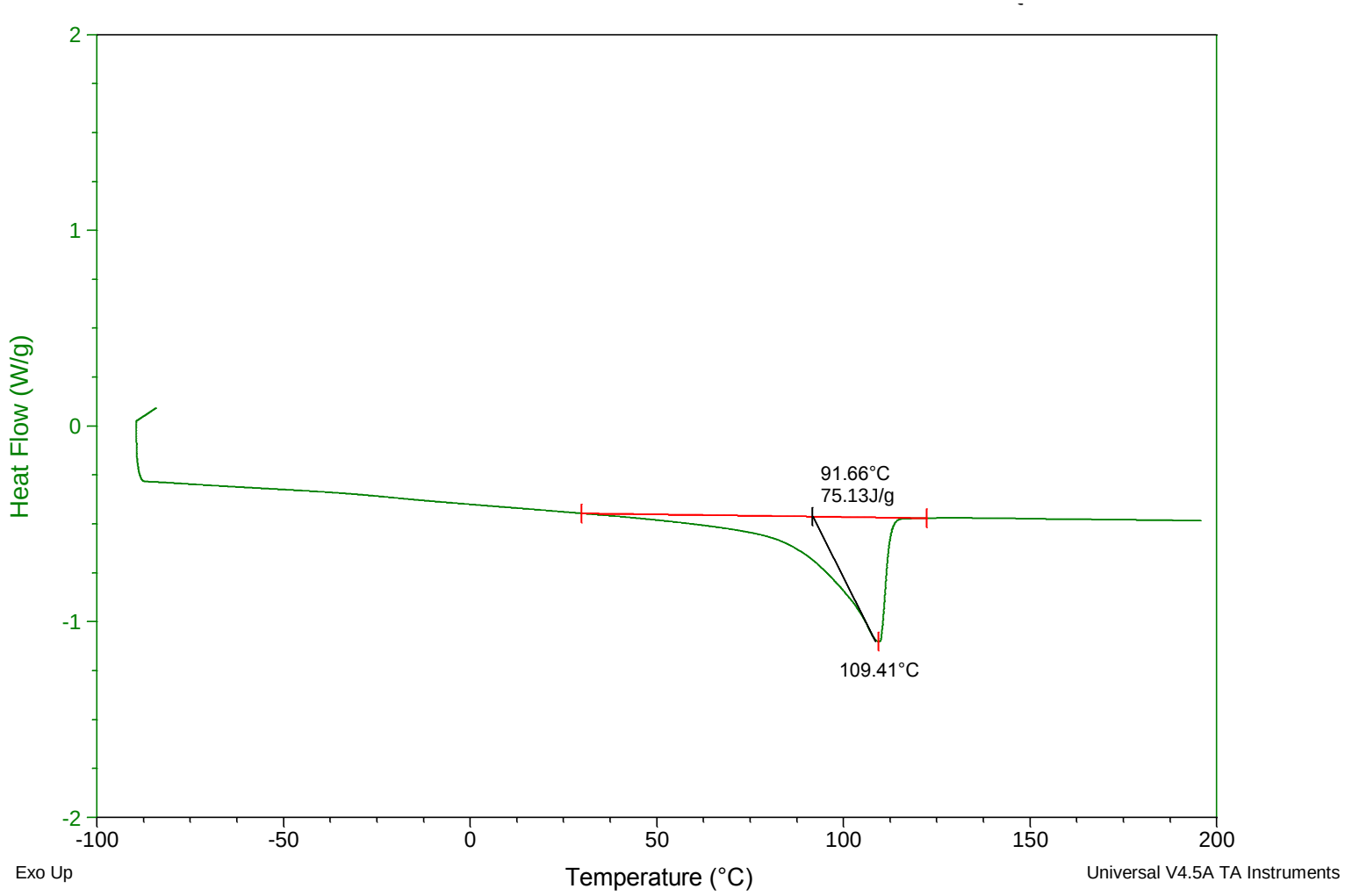


Figure 102. GPC trace for run #4.

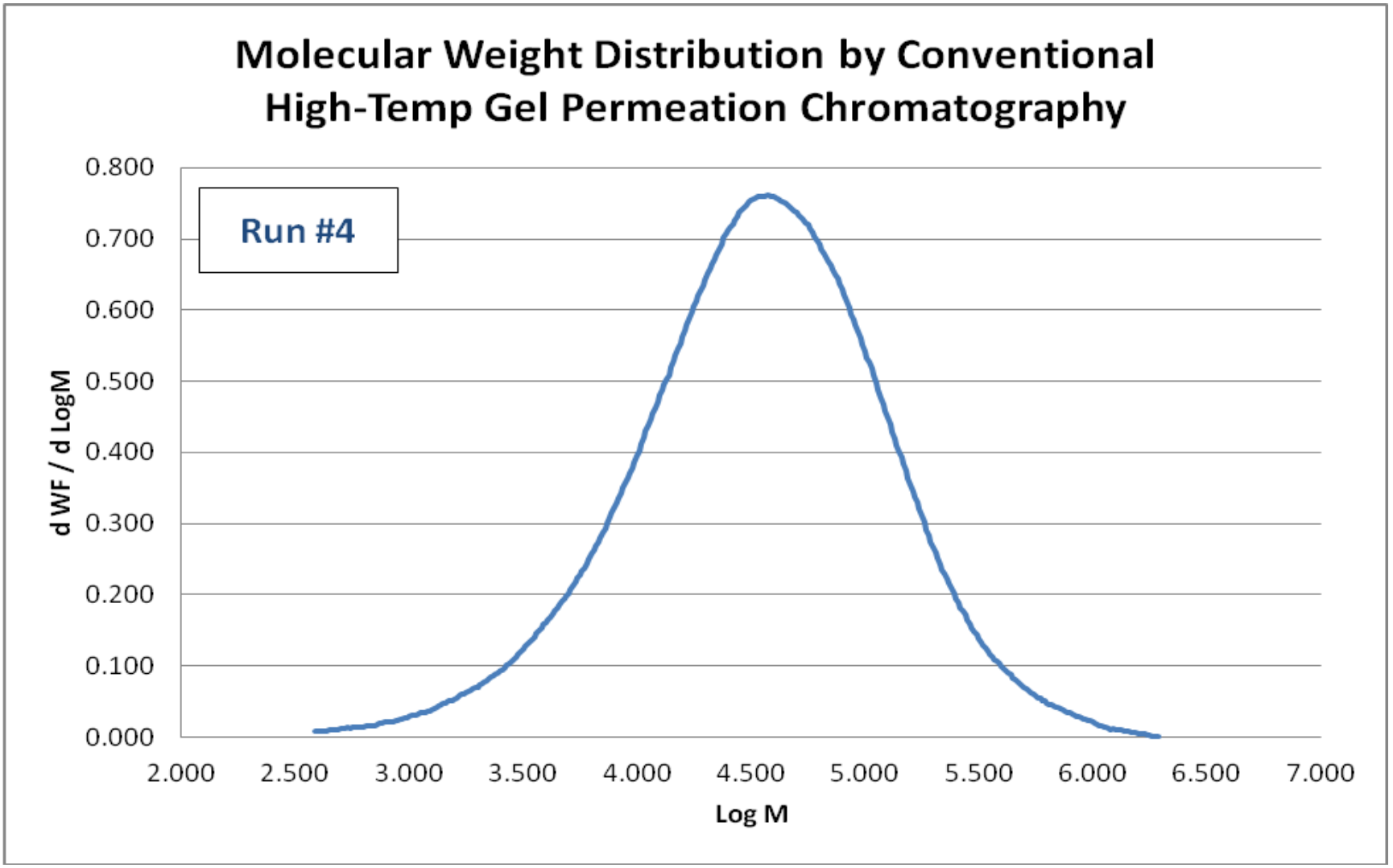


Figure 103. DSC plot for run #4.

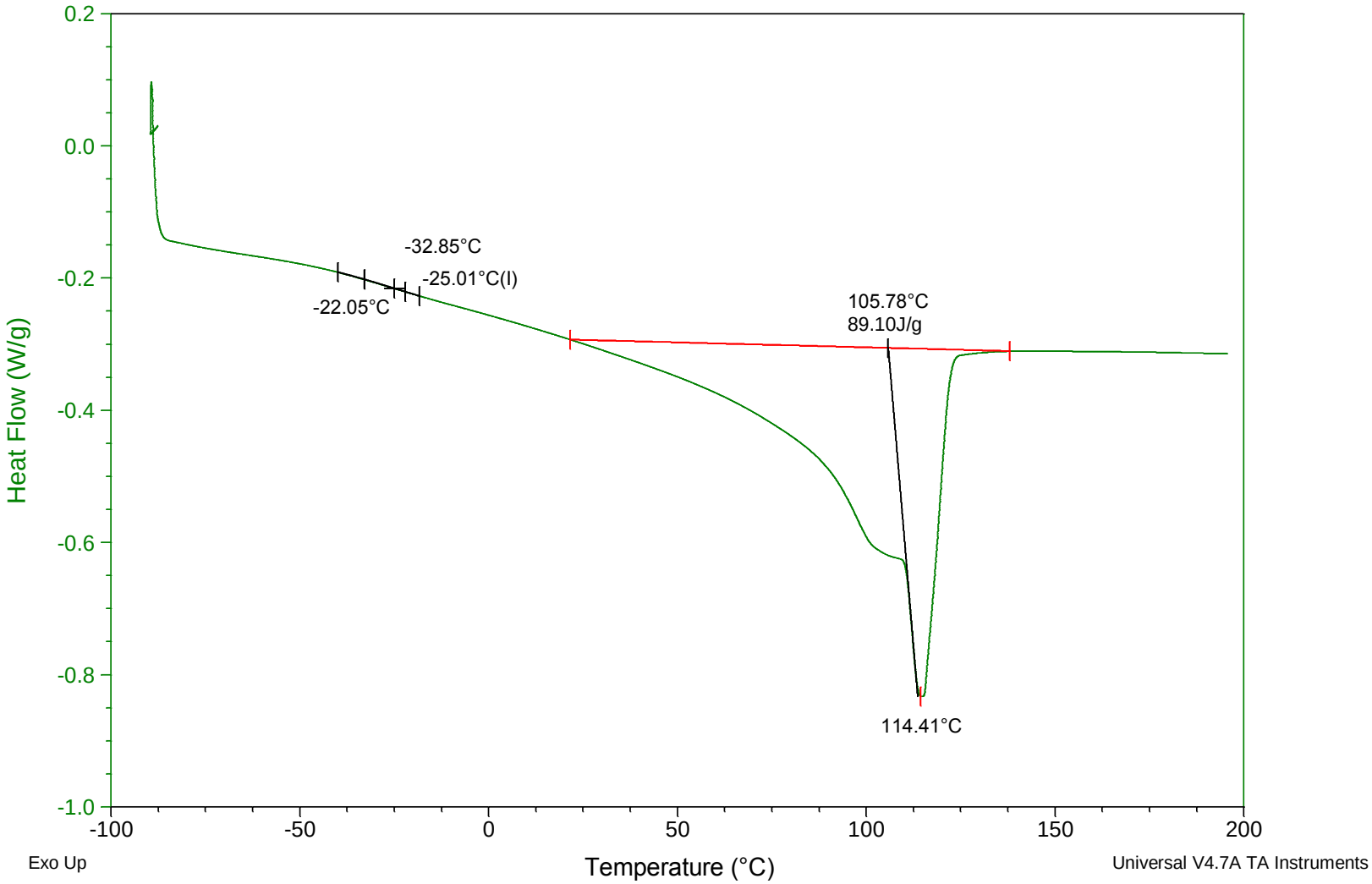


Figure 104. GPC trace for run #5.

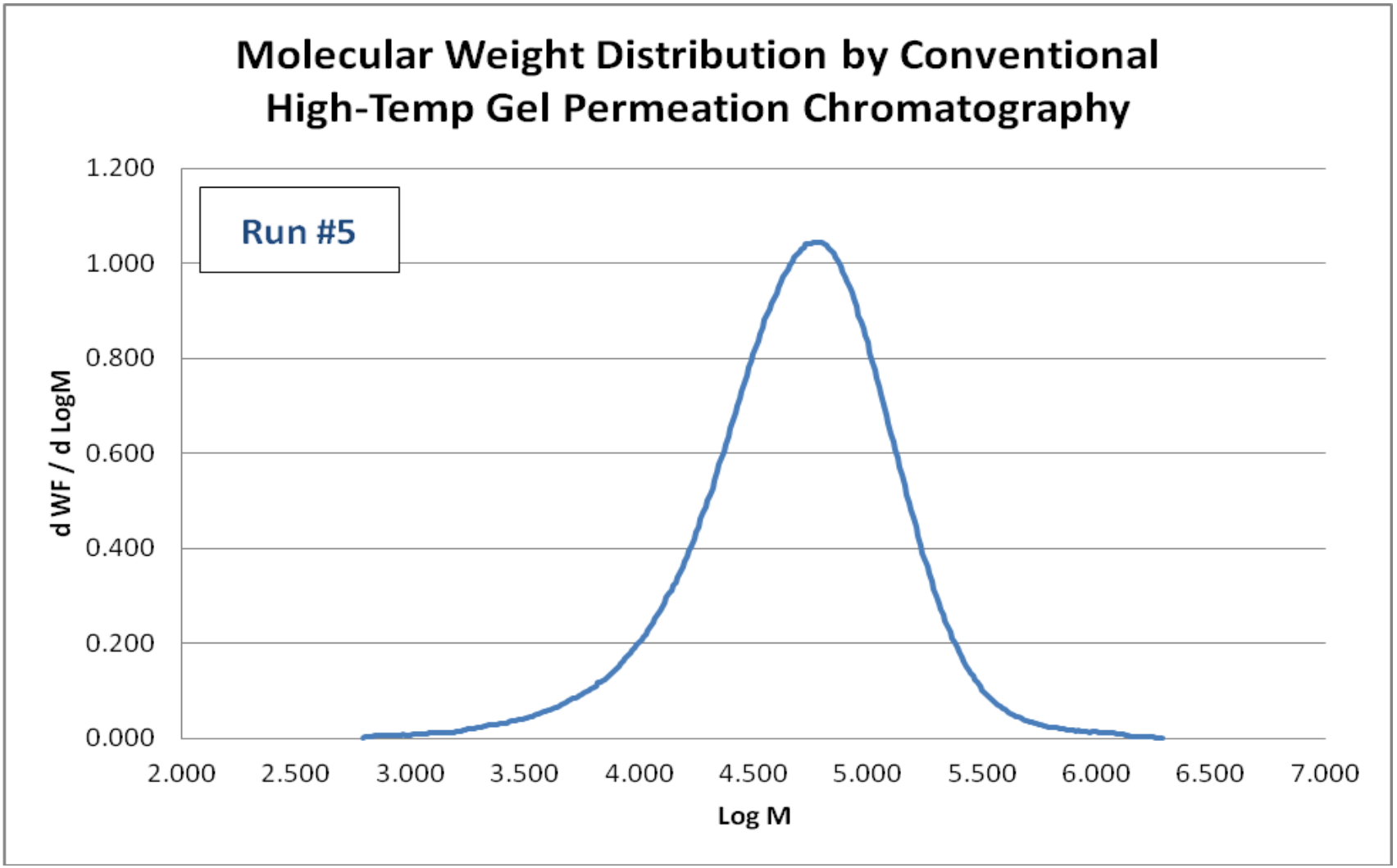


Figure 105. DSC plot for run #5.

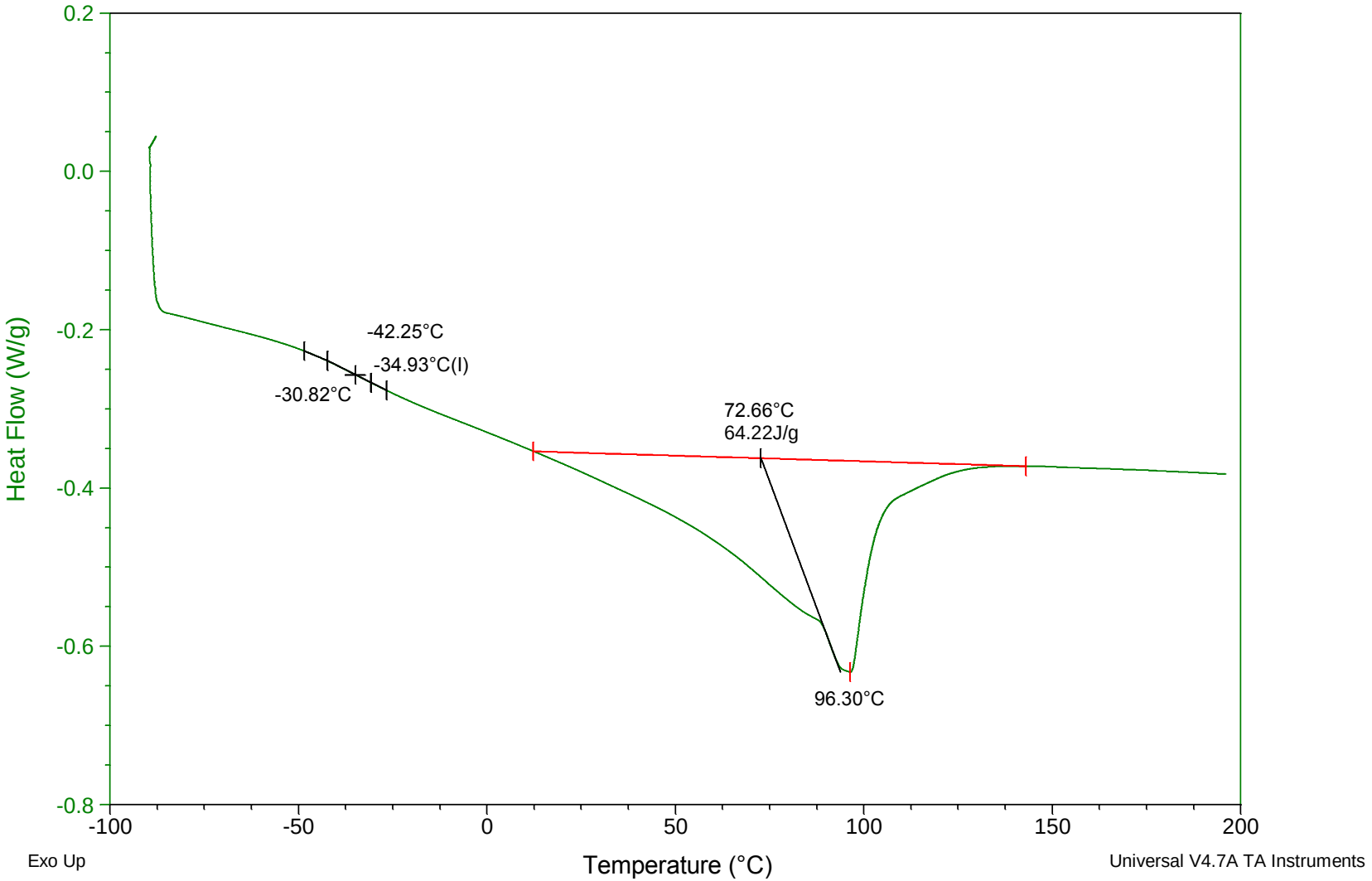


Figure 106. GPC trace for run #6.

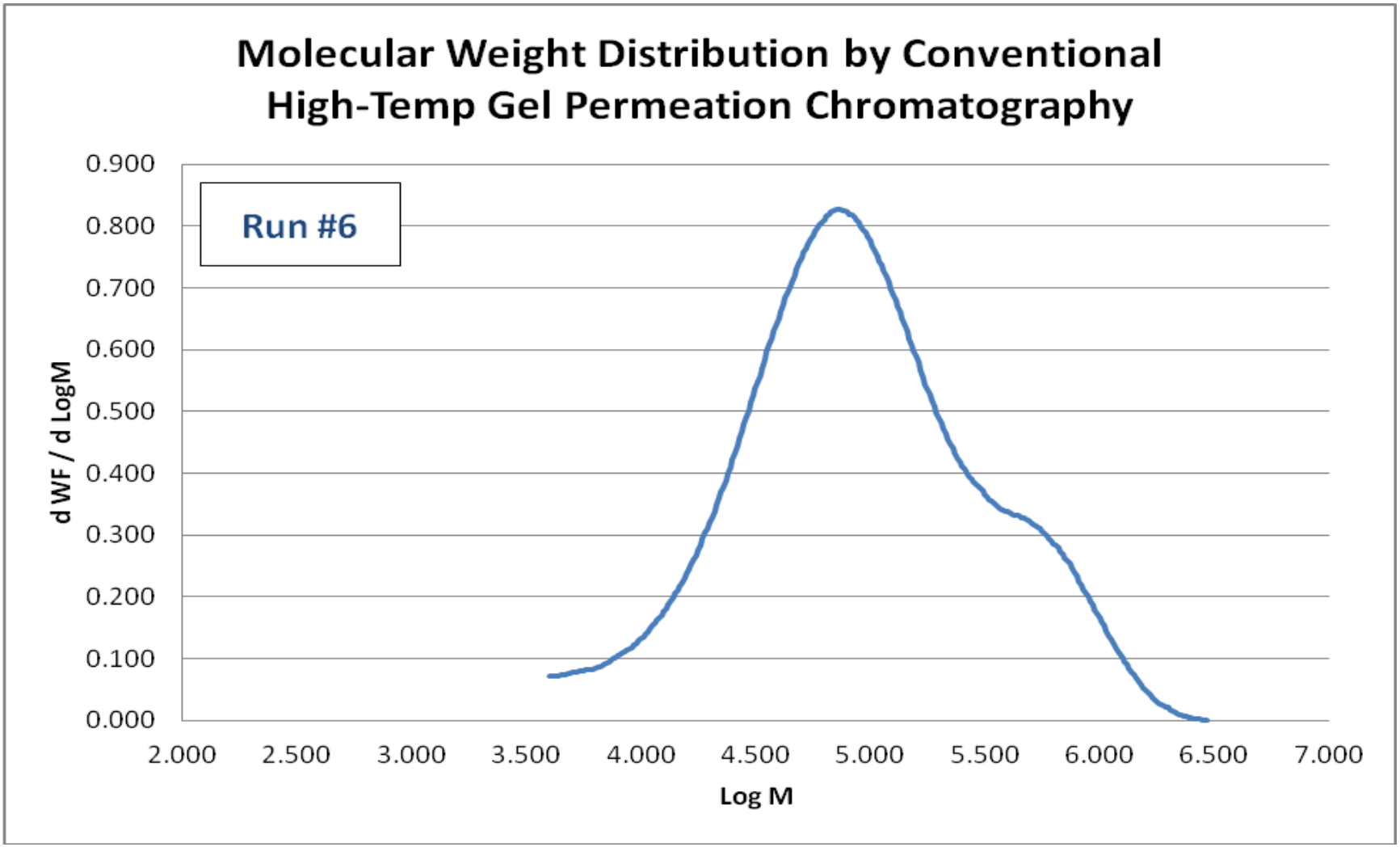


Figure 107. DSC plot for run #6.

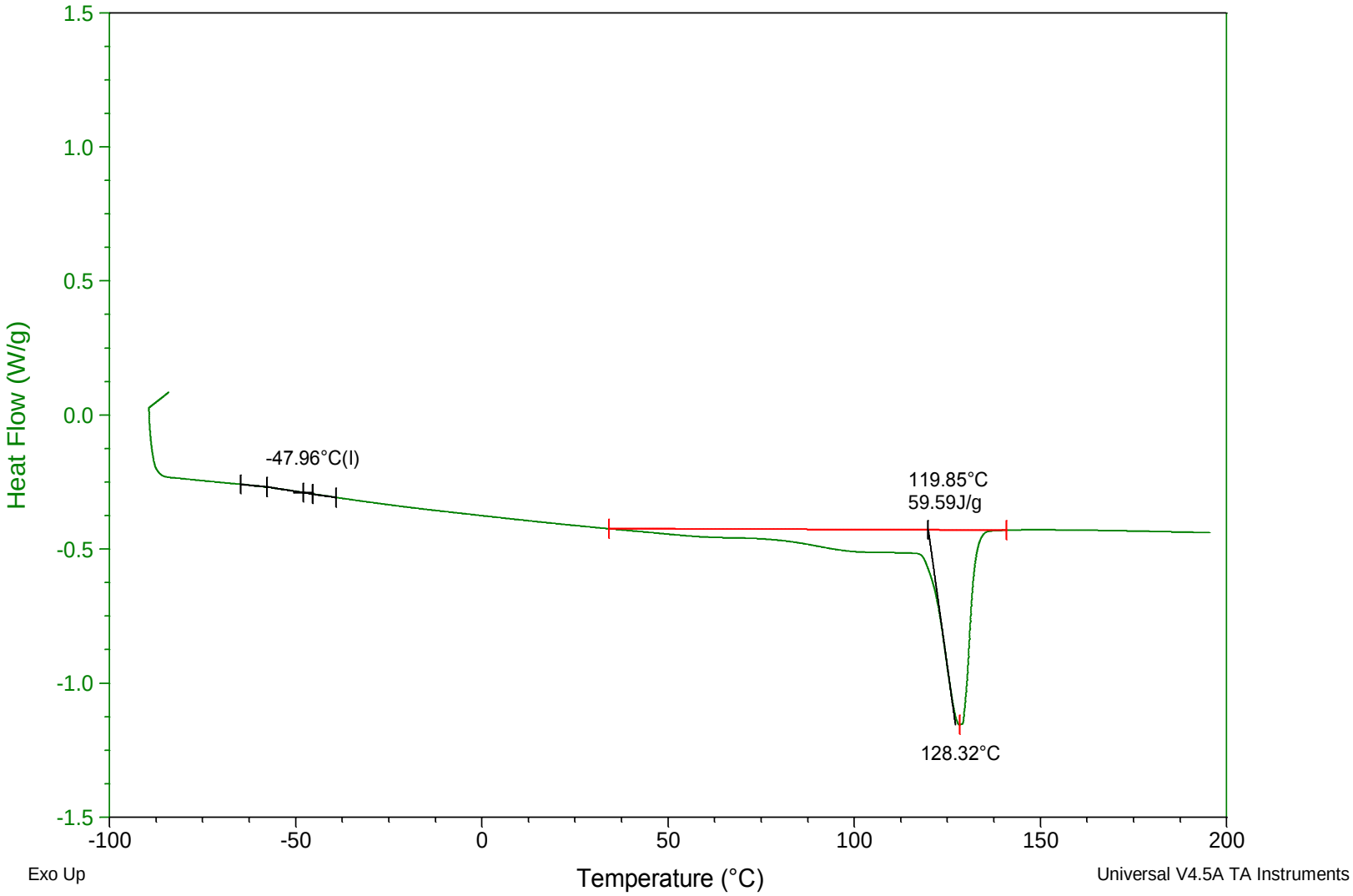


Figure 108. GPC trace for run #7.

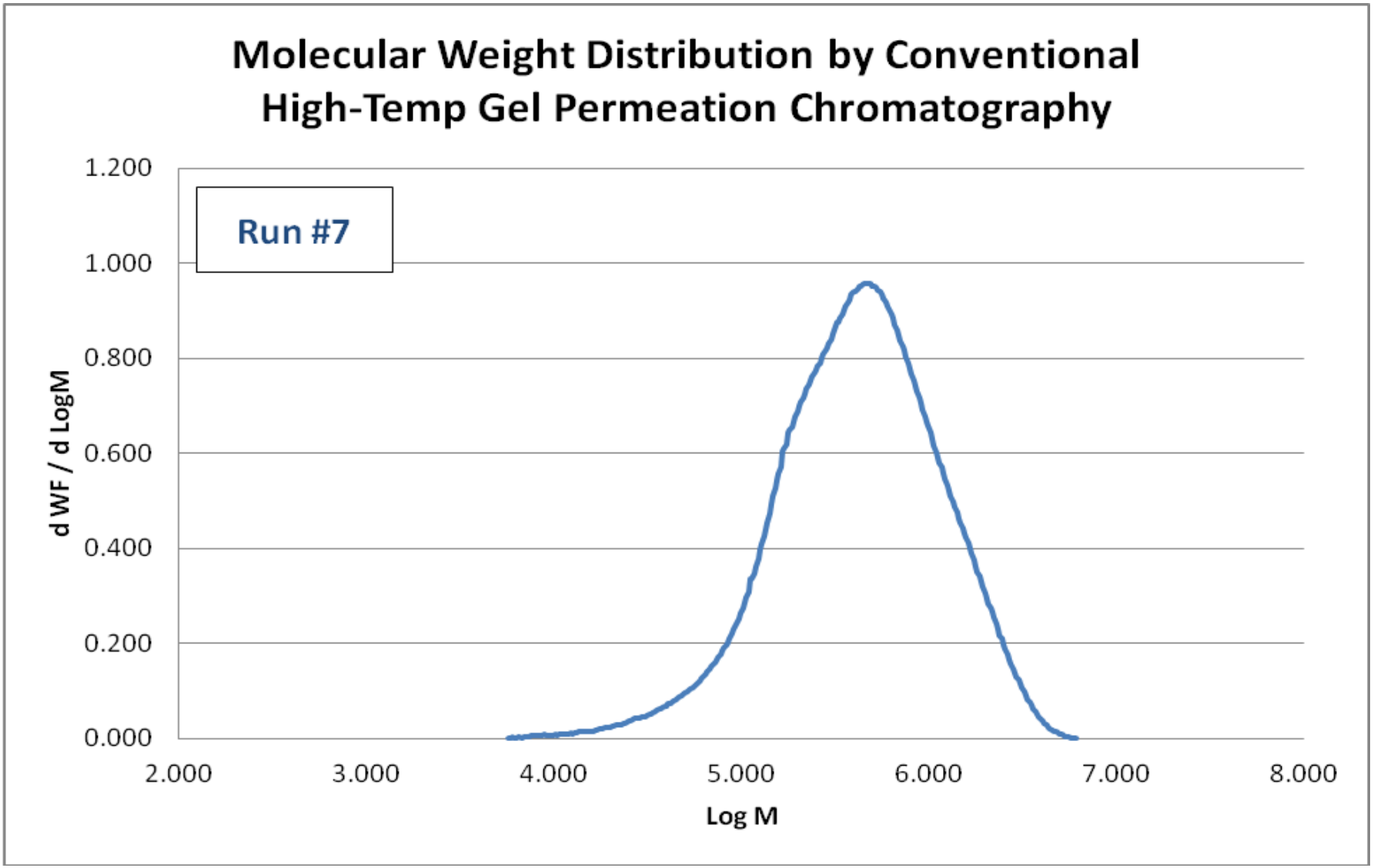


Figure 109. DSC plot for run #7.

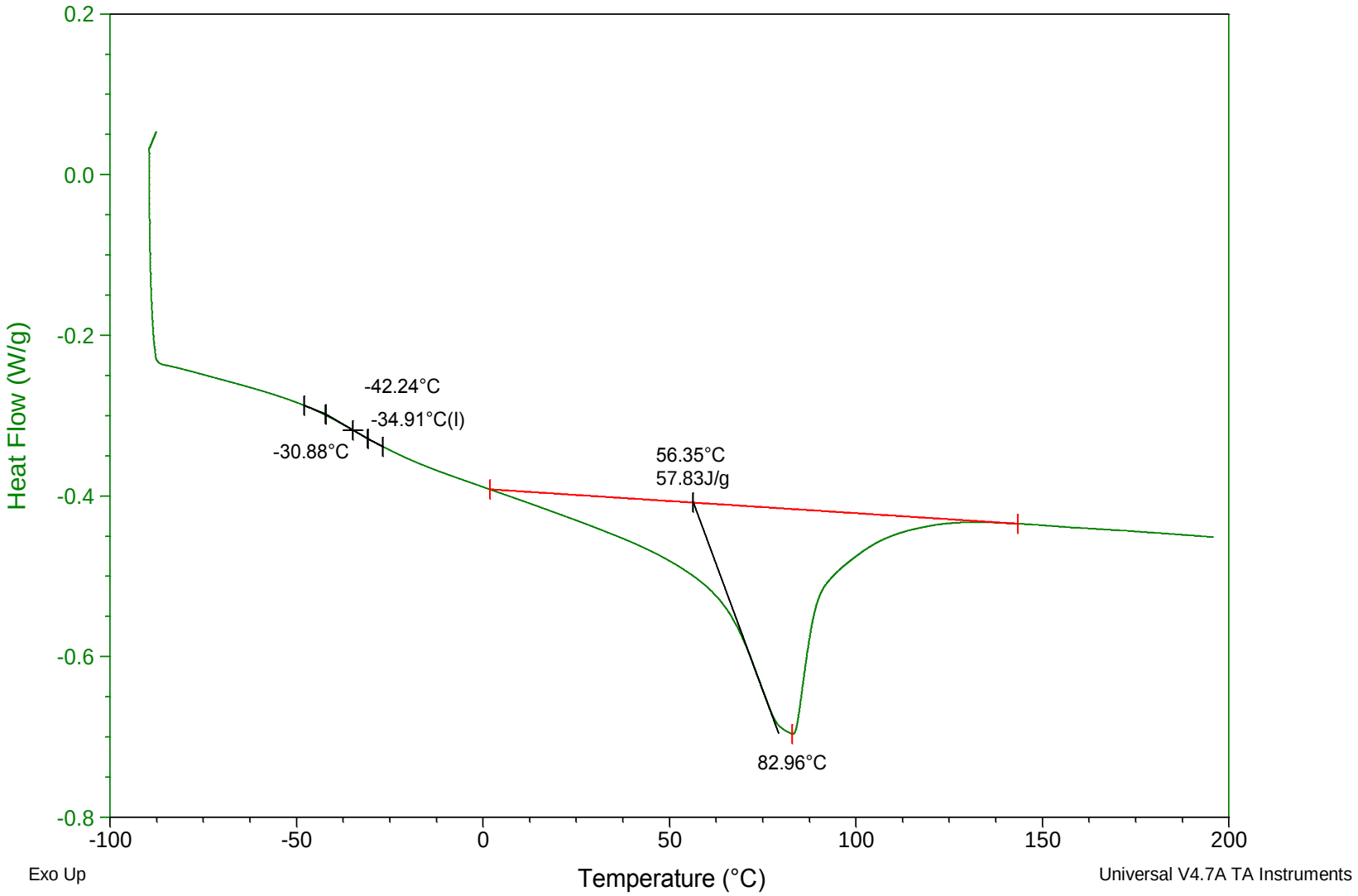


Figure 110. GPC trace for run #8.

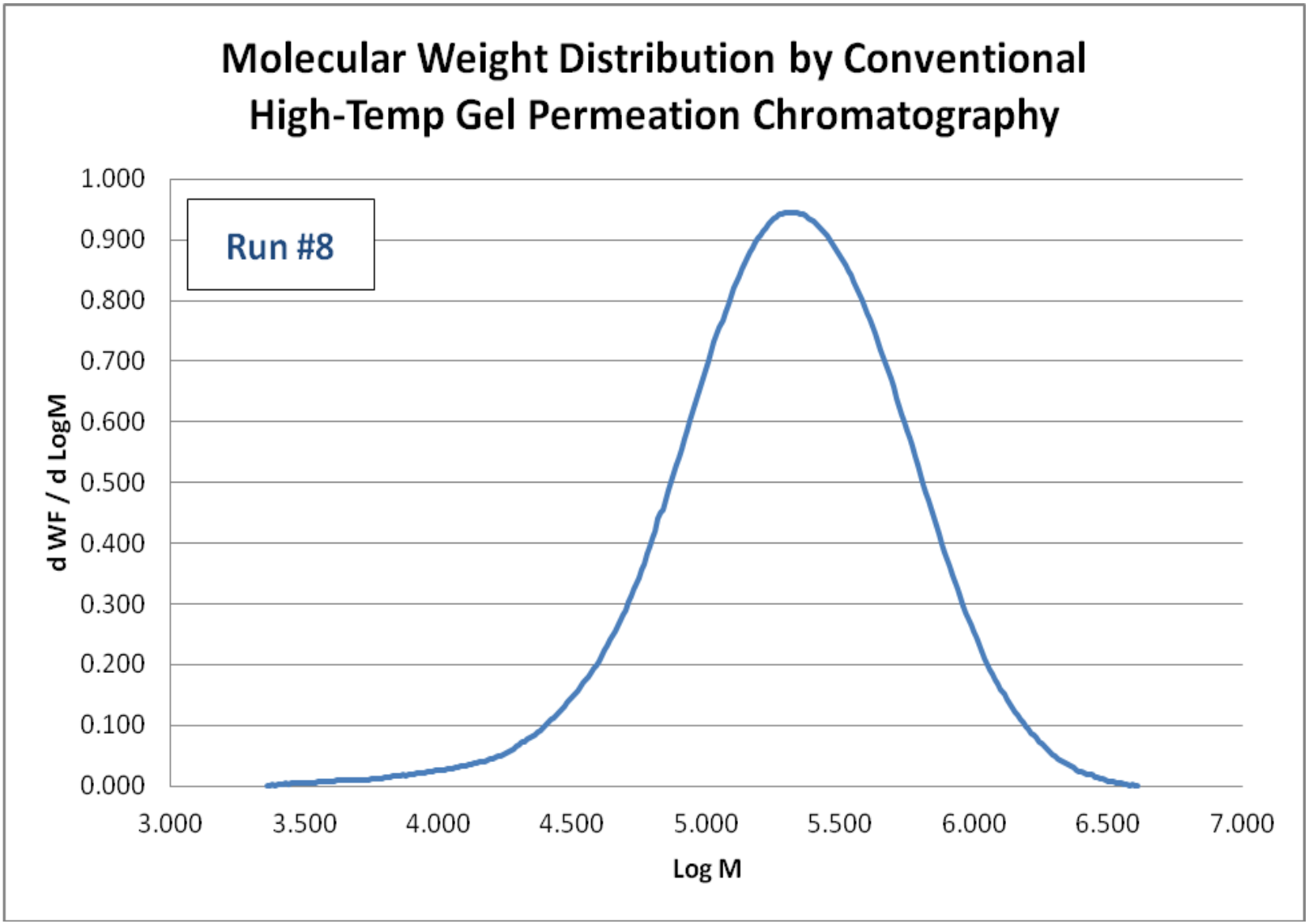


Figure 111. DSC plot for run #8.

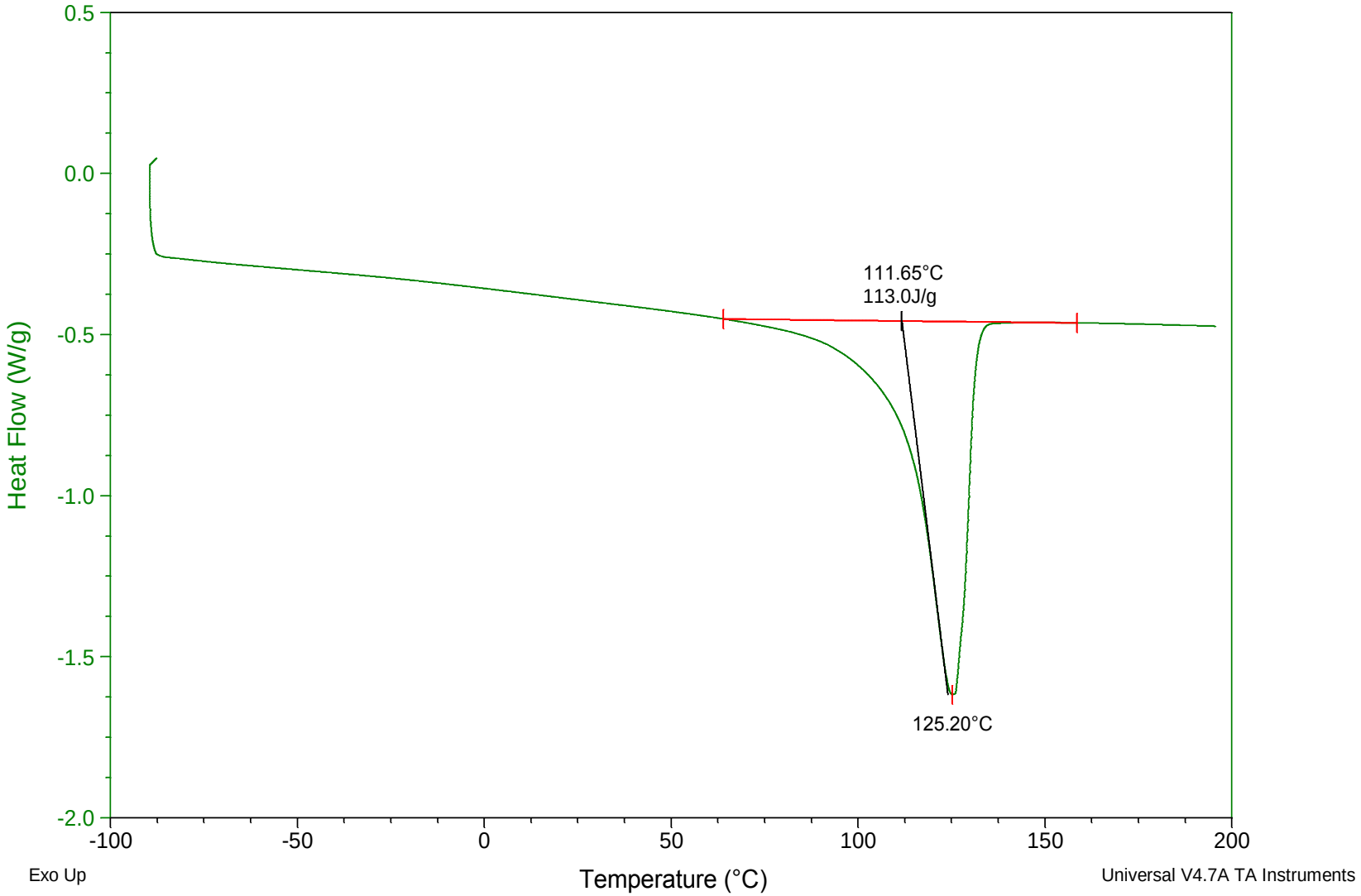


Figure 112. GPC trace for run #9.

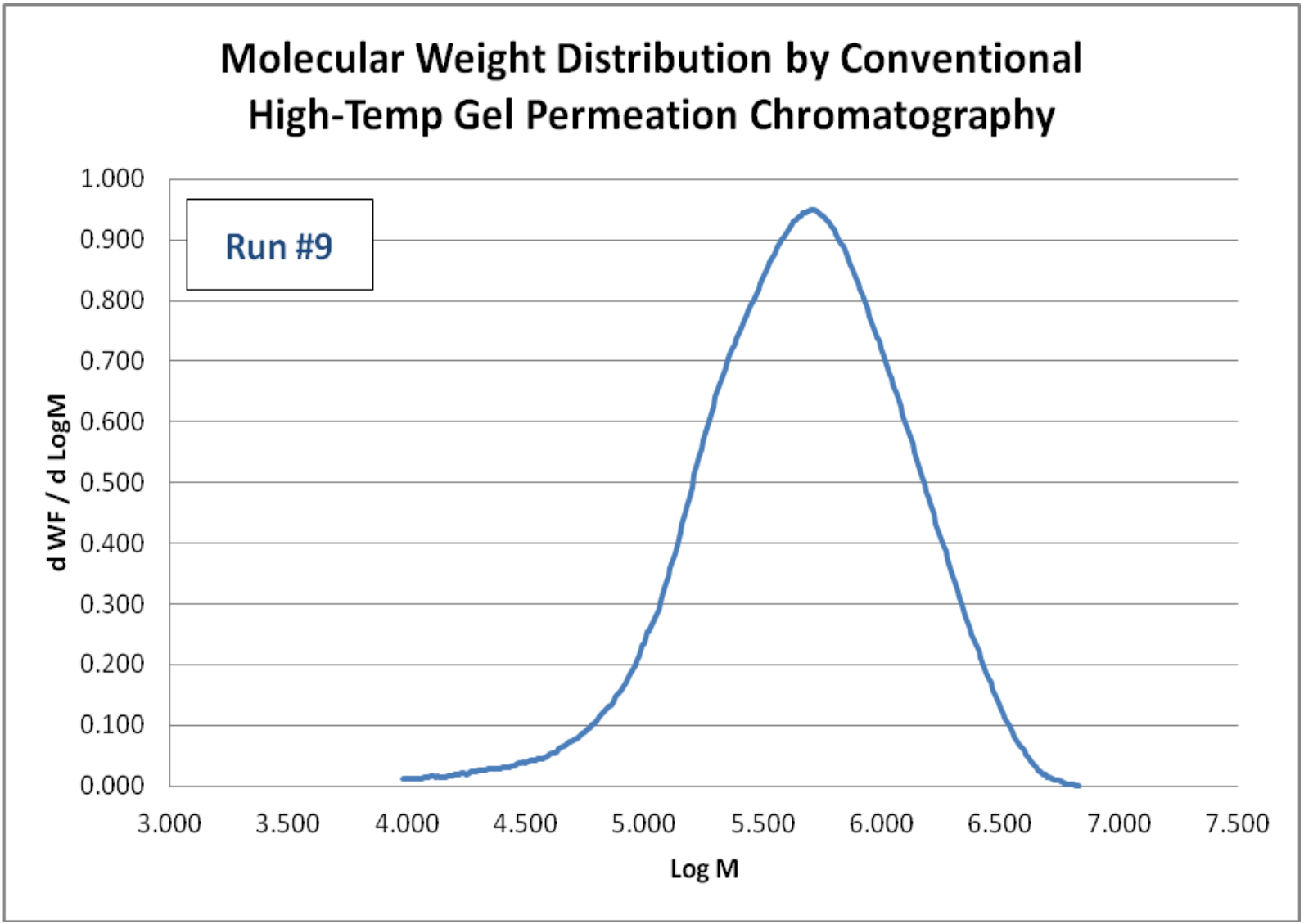


Figure 113. DSC plot for run #9.

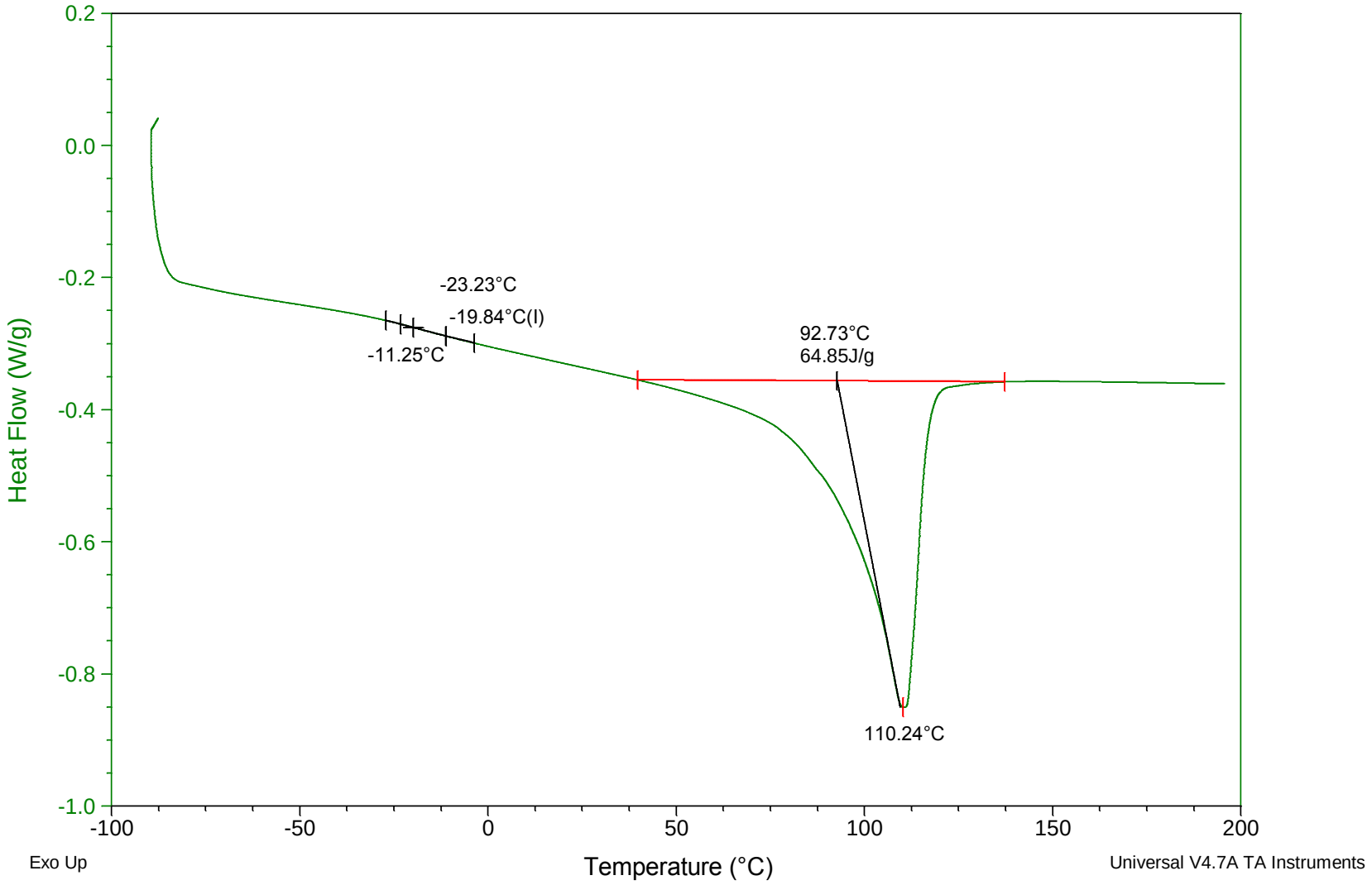


Figure 114. GPC trace for run #10.

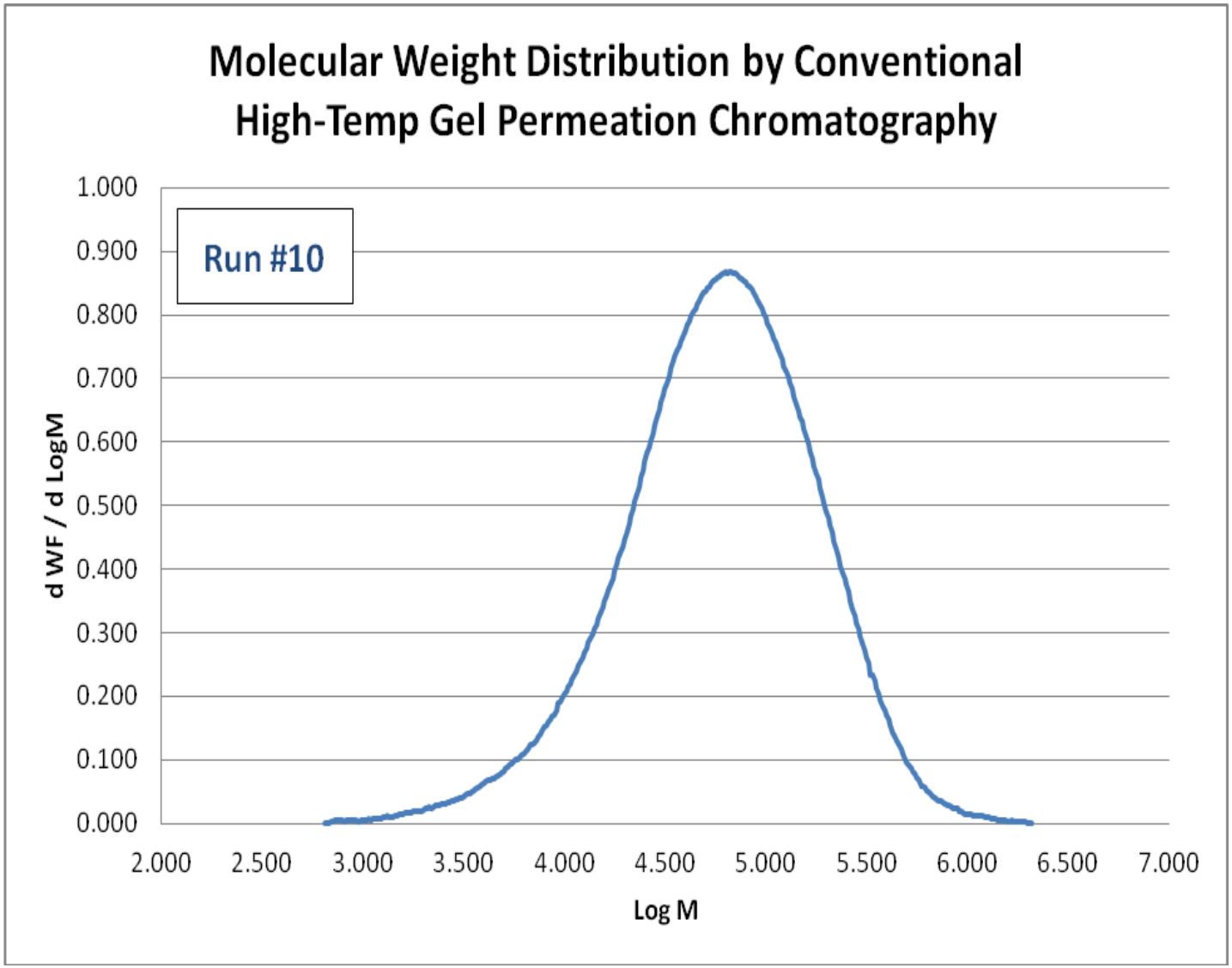


Figure 115. DSC plot for run #10.

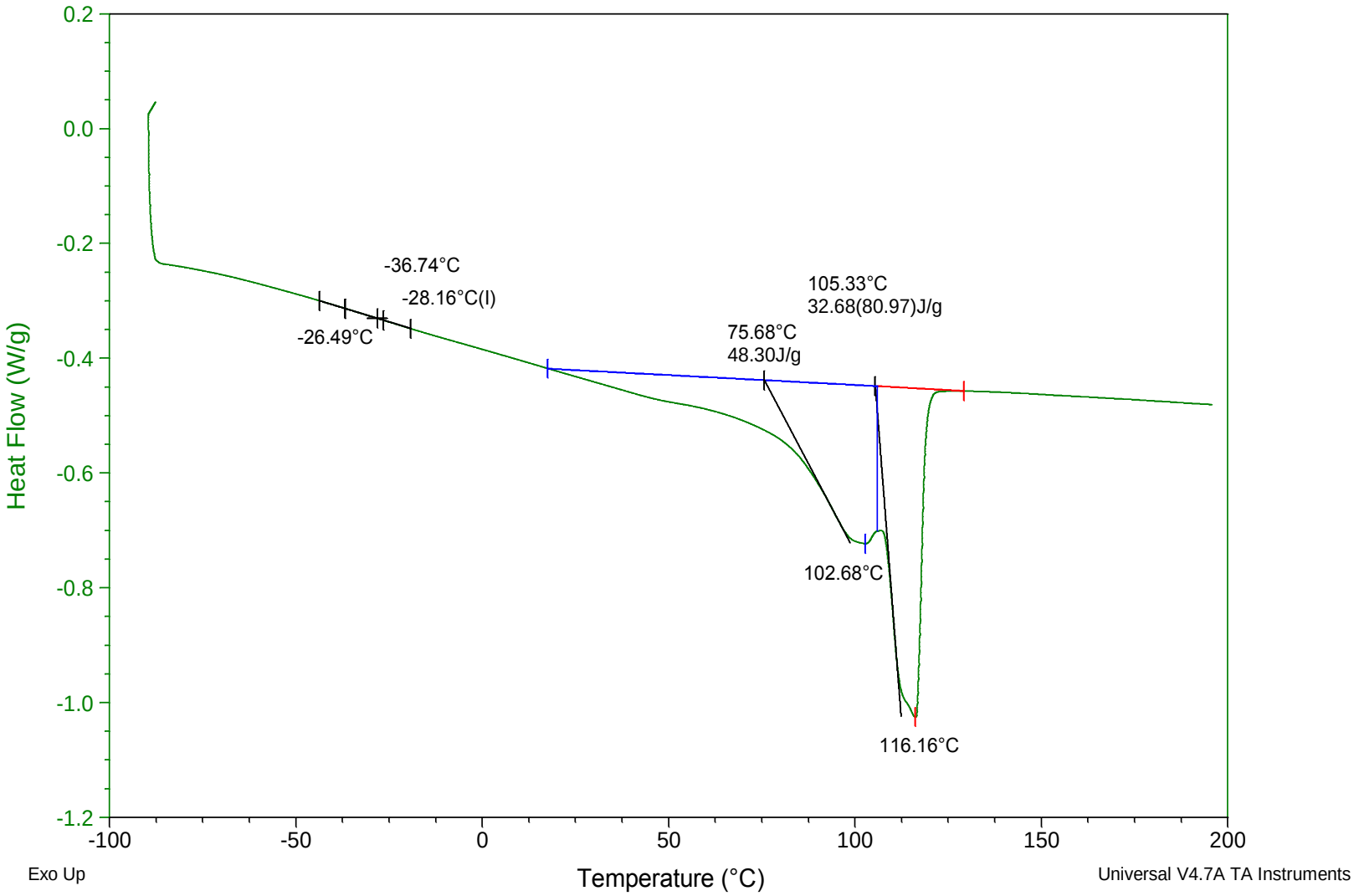


Figure 116. GPC trace for run #11.

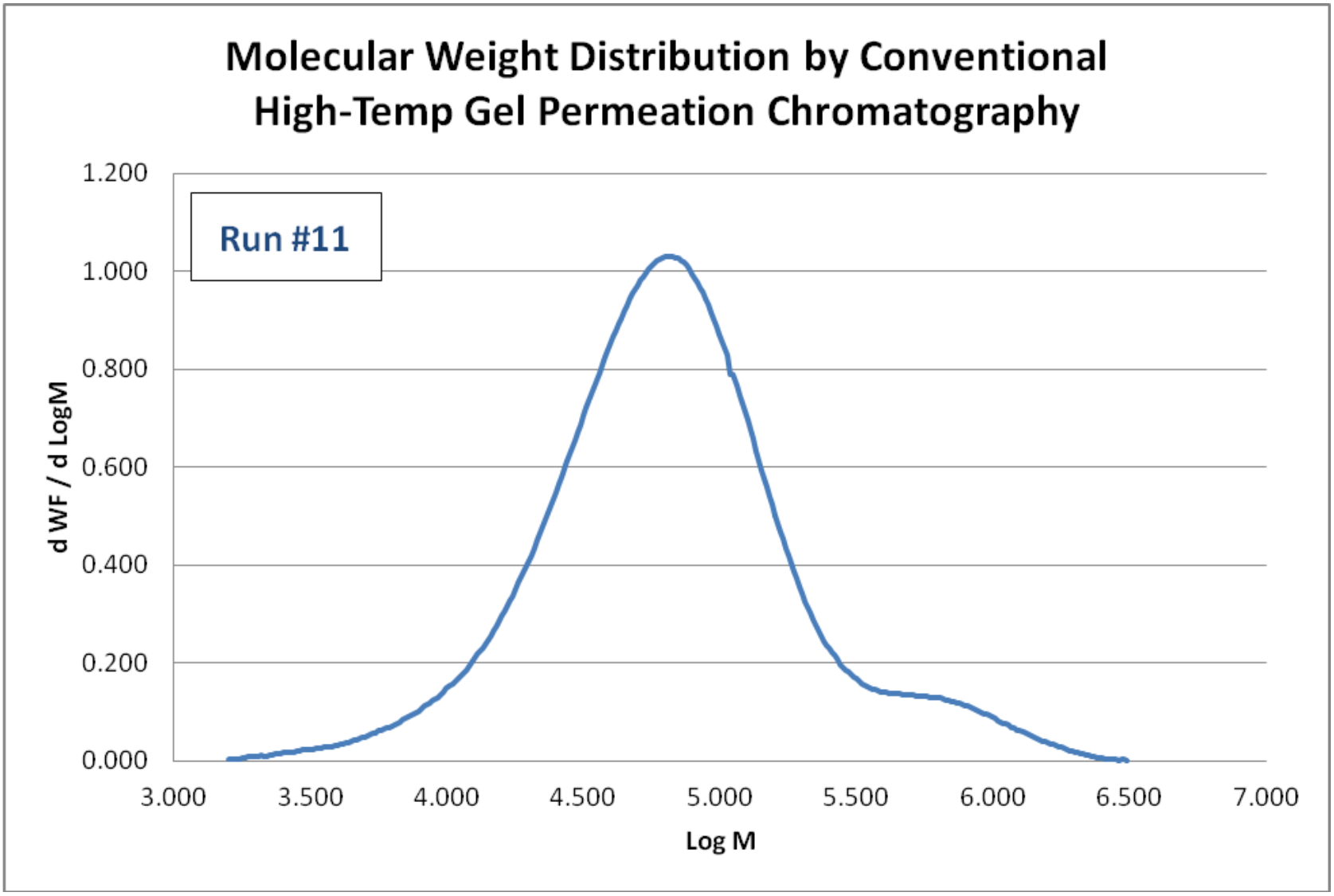


Figure 117. DSC plot for run #11.

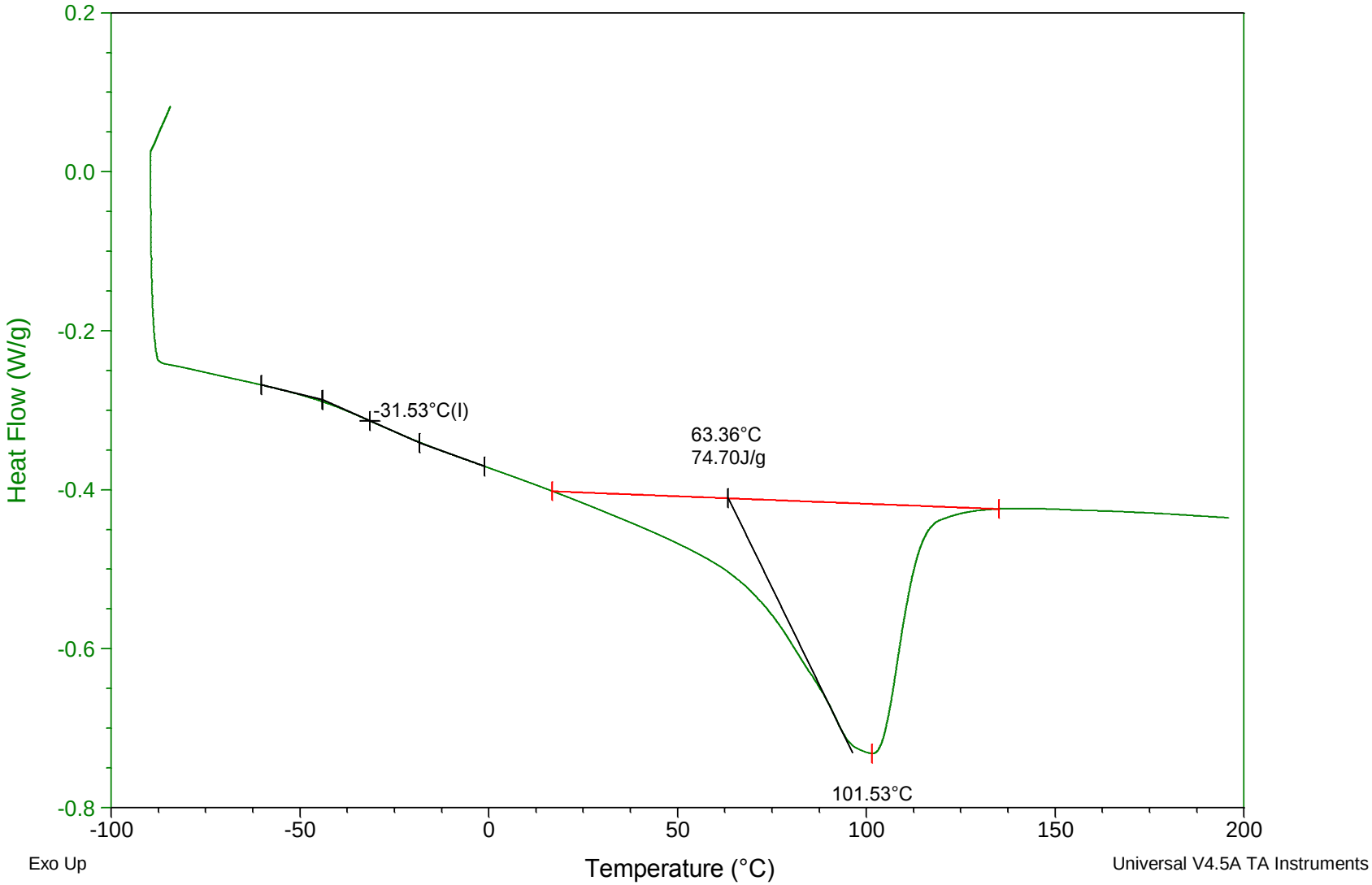


Figure 118. GPC trace for run #12.

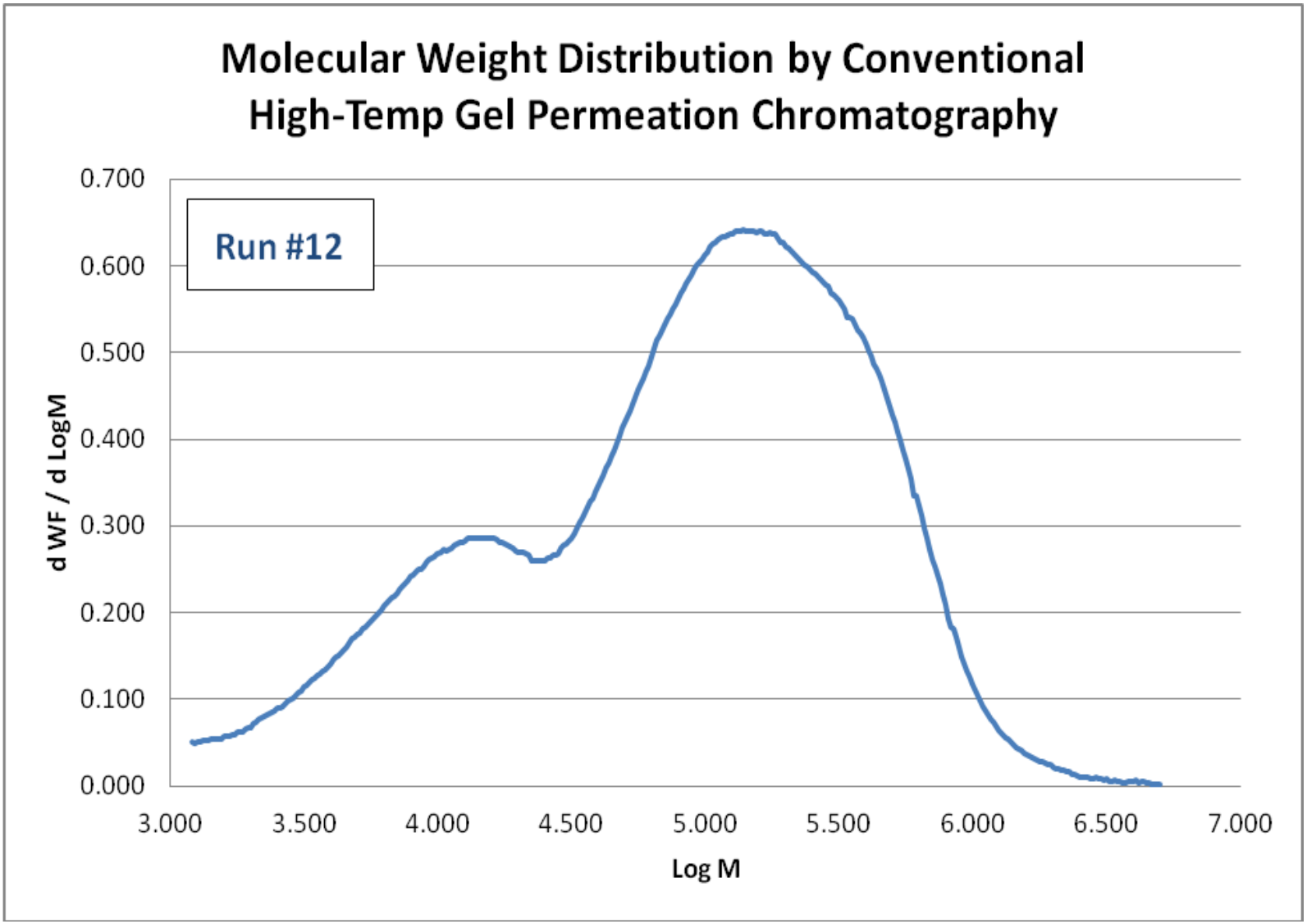


Figure 119. DSC plot for run #12.

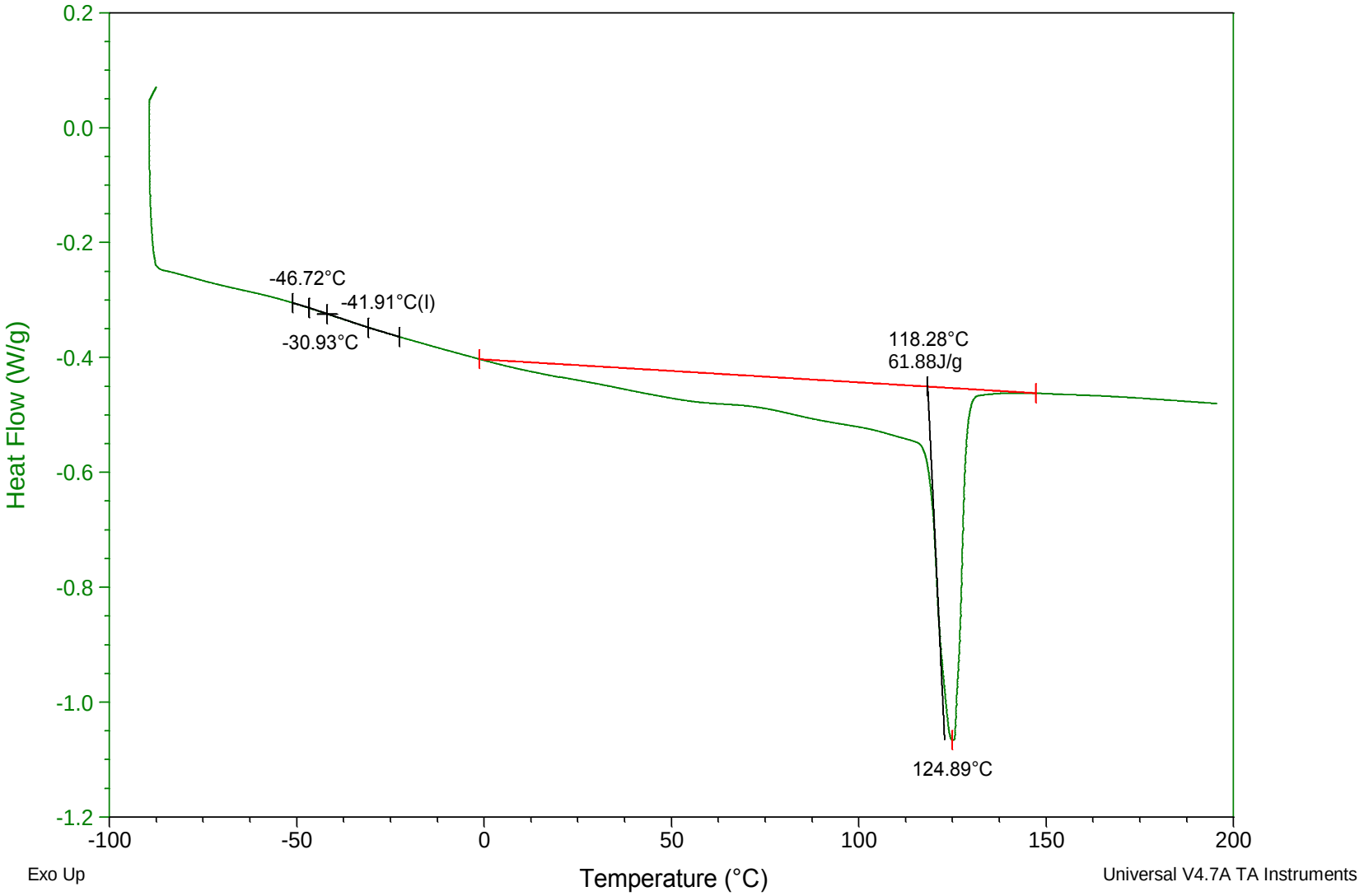


Figure 120. GPC trace for run #13.

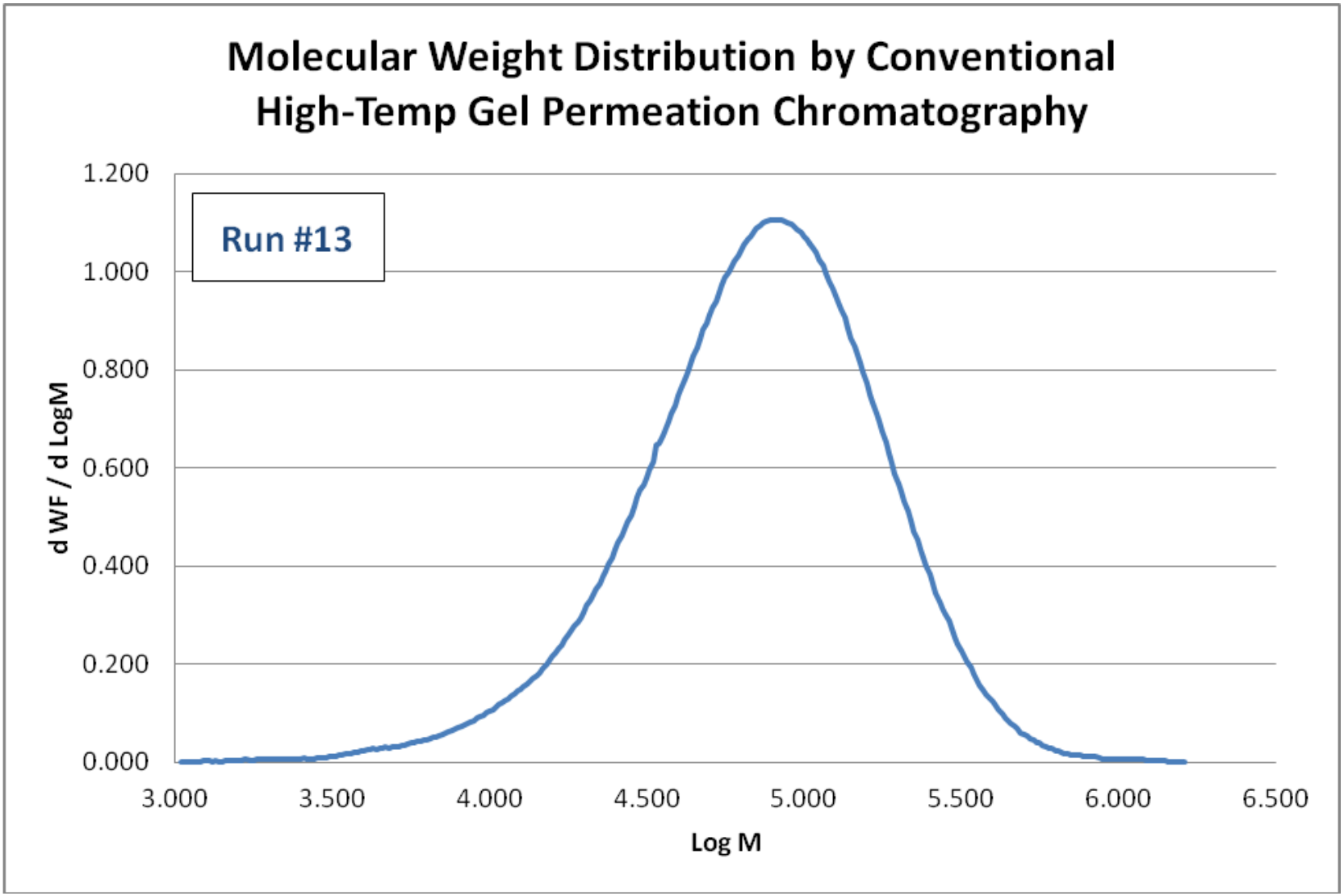


Figure 121. DSC plot for run #13.

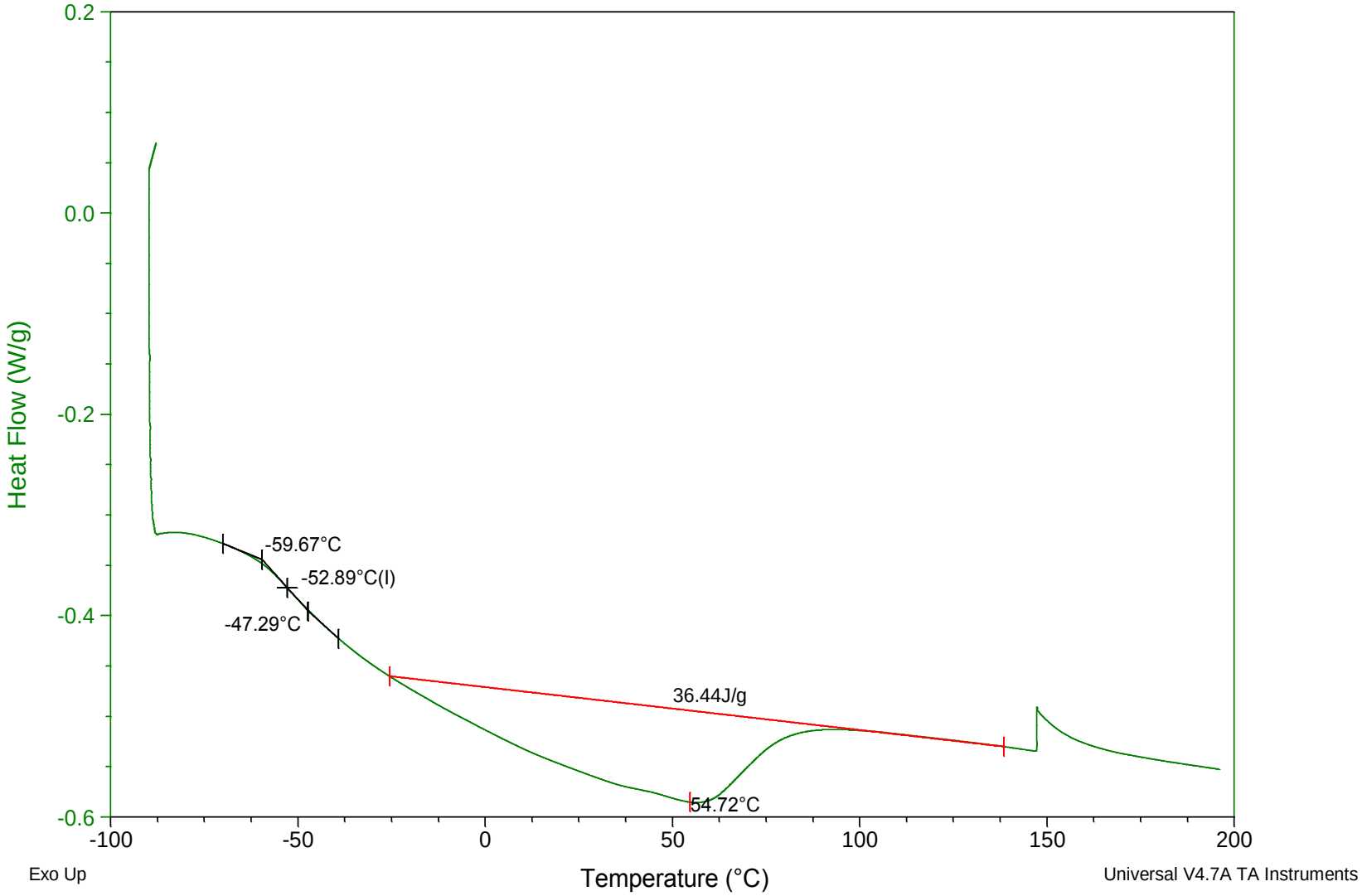


Figure 122. GPC trace for run #14.

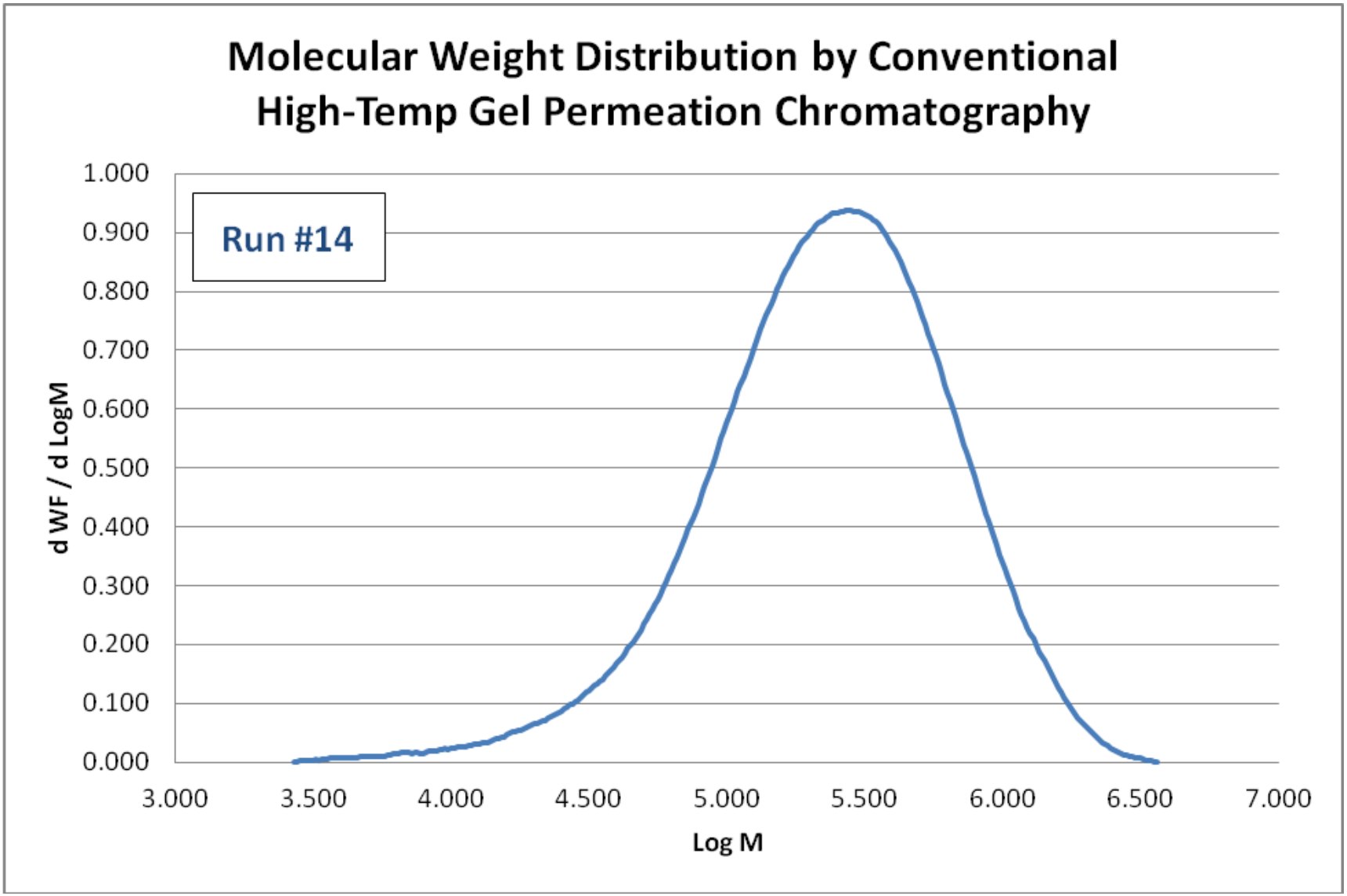


Figure 123. DSC plot for run #14.

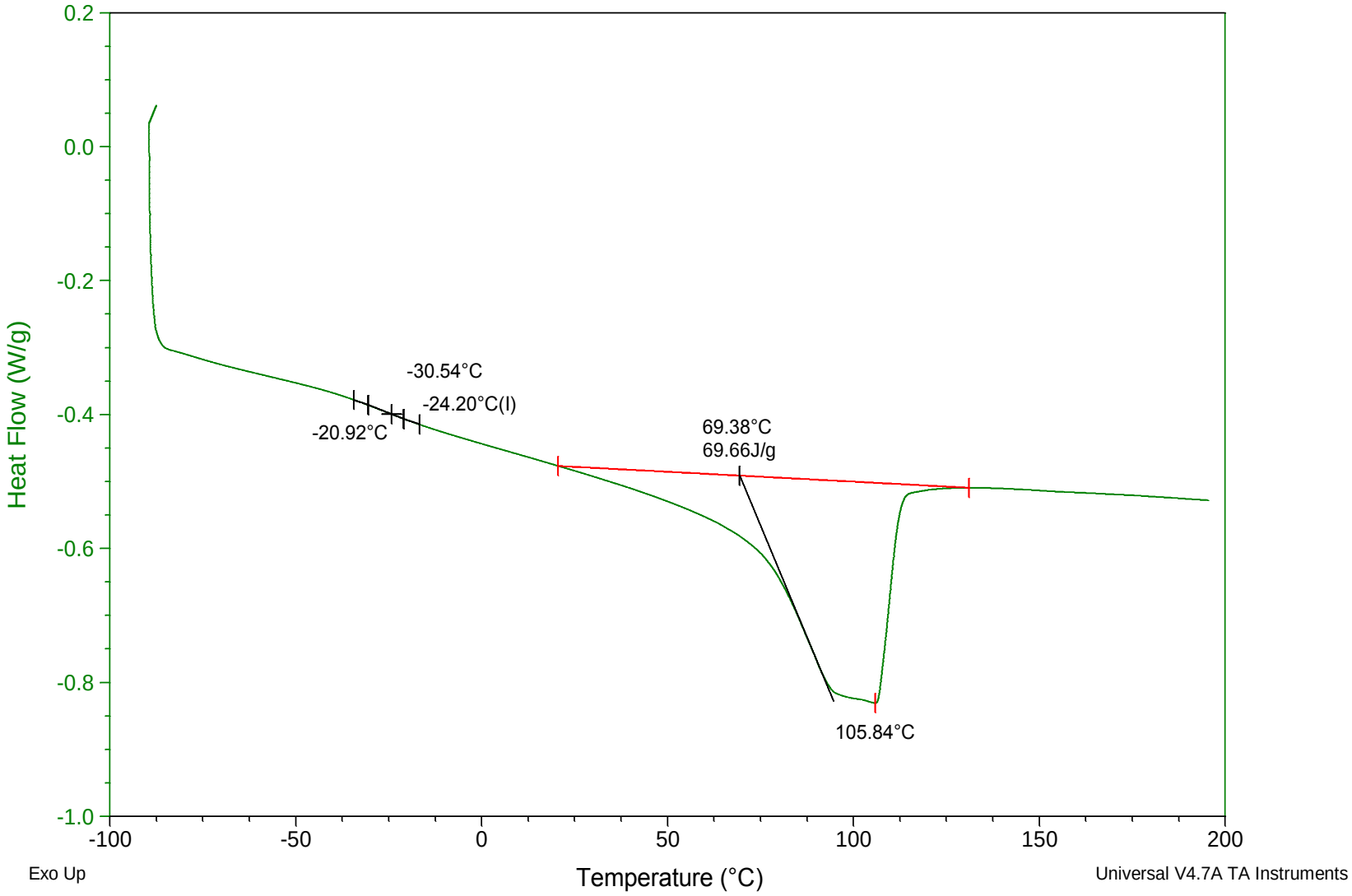


Figure 124. GPC trace for run #15.

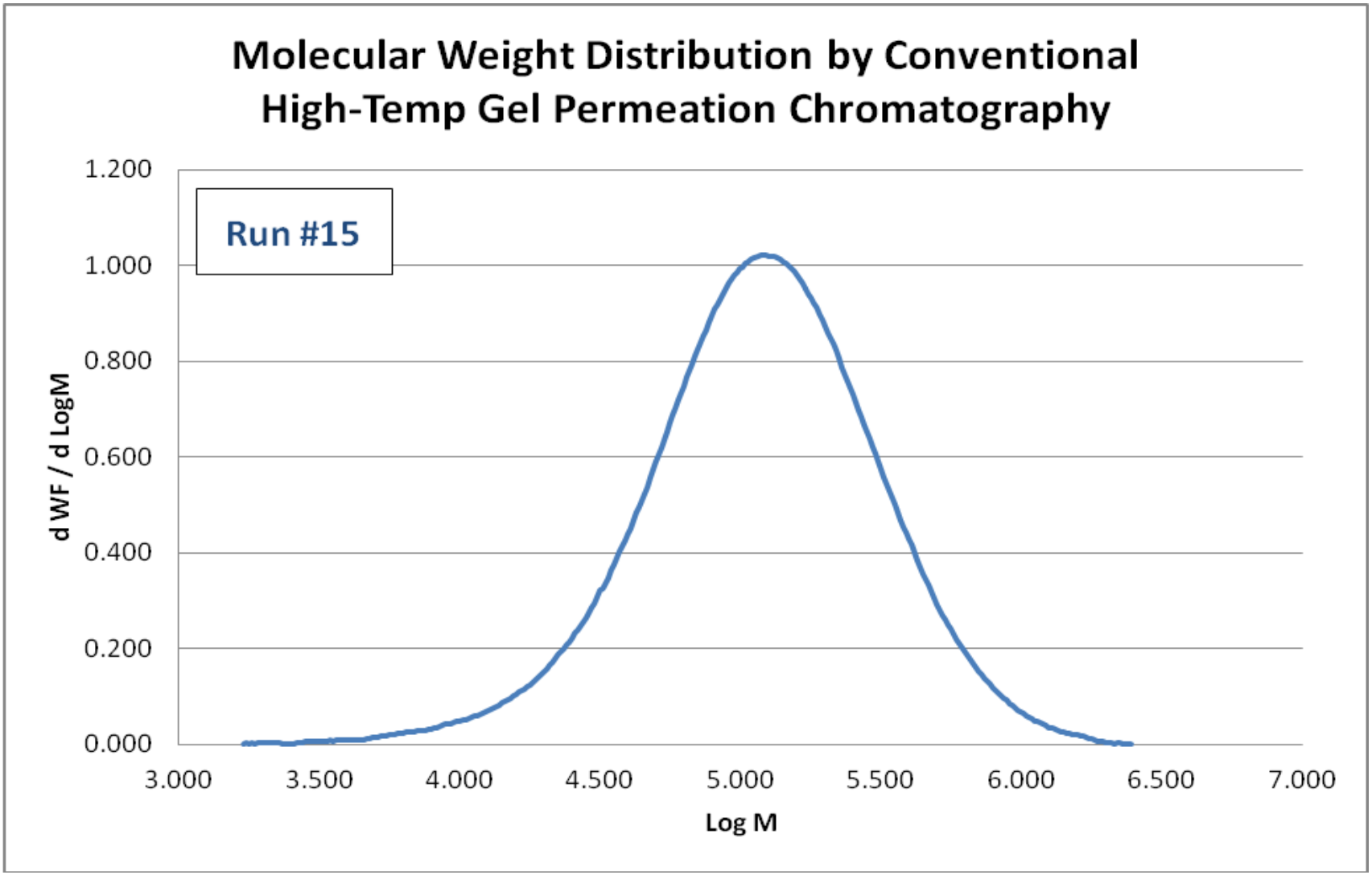


Figure 125. DSC plot for run #15.

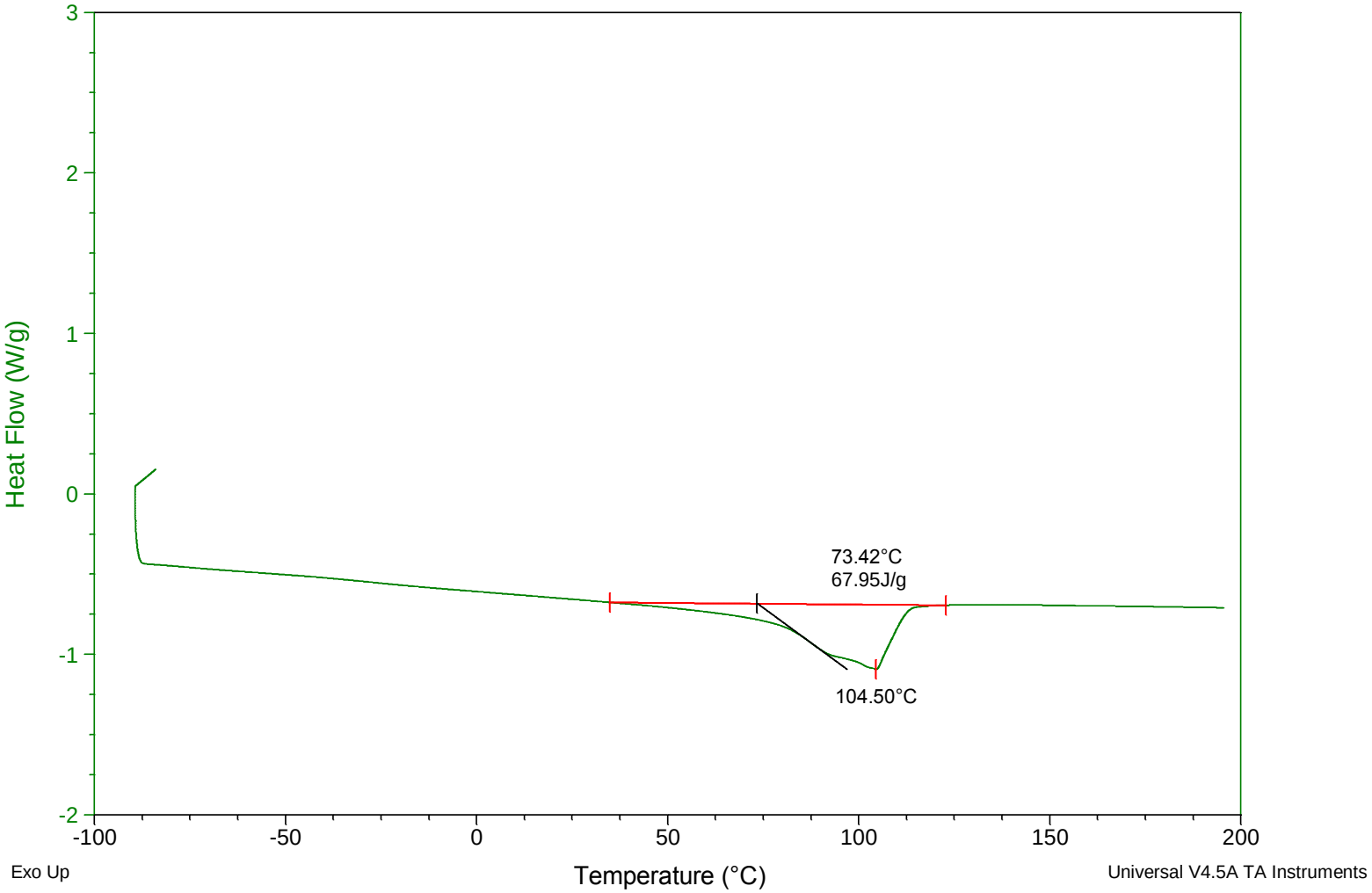


Figure 126. GPC trace for run #16.

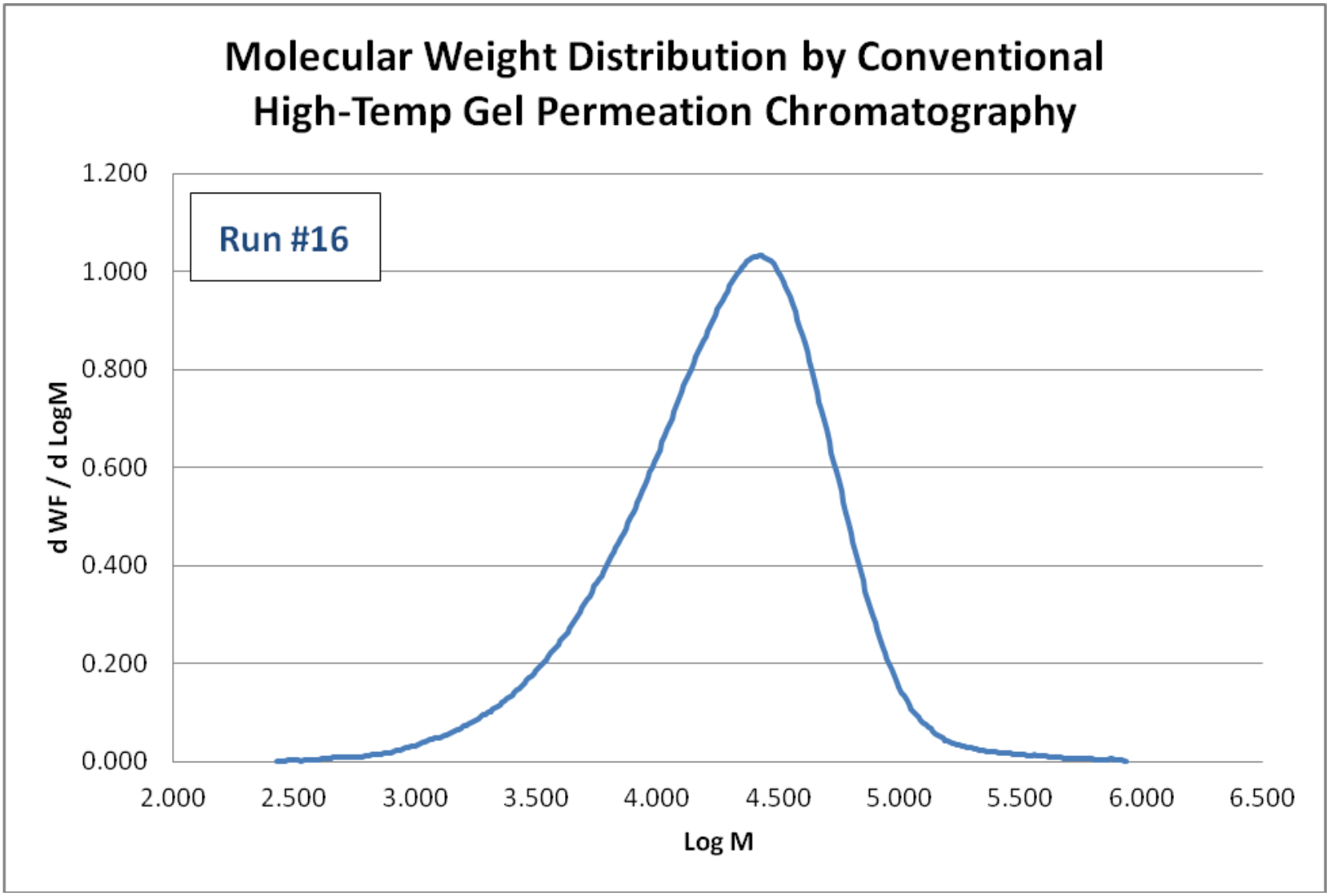


Figure 127. DSC plot for run #16.

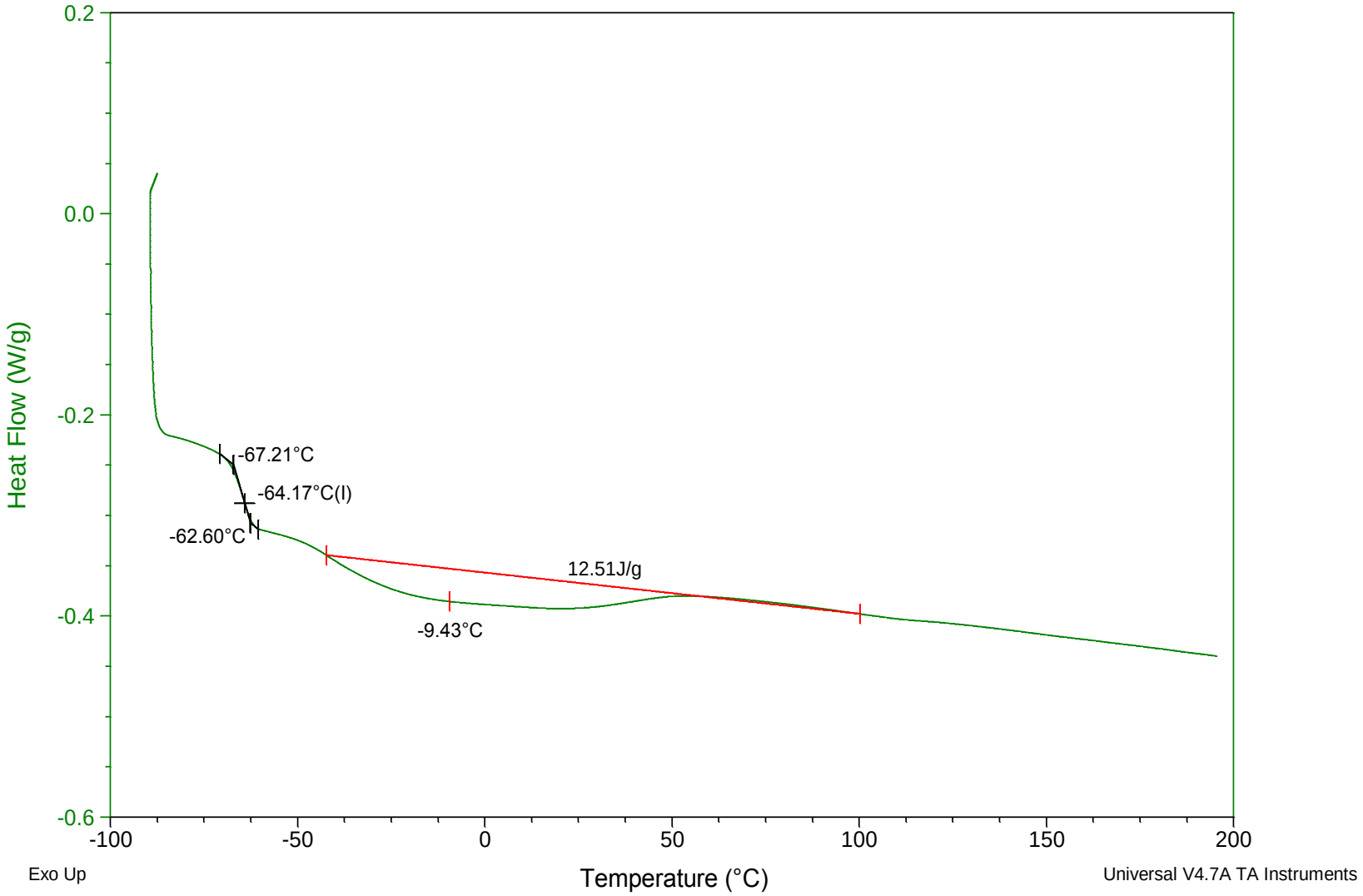


Figure 128. GPC trace for run #17.

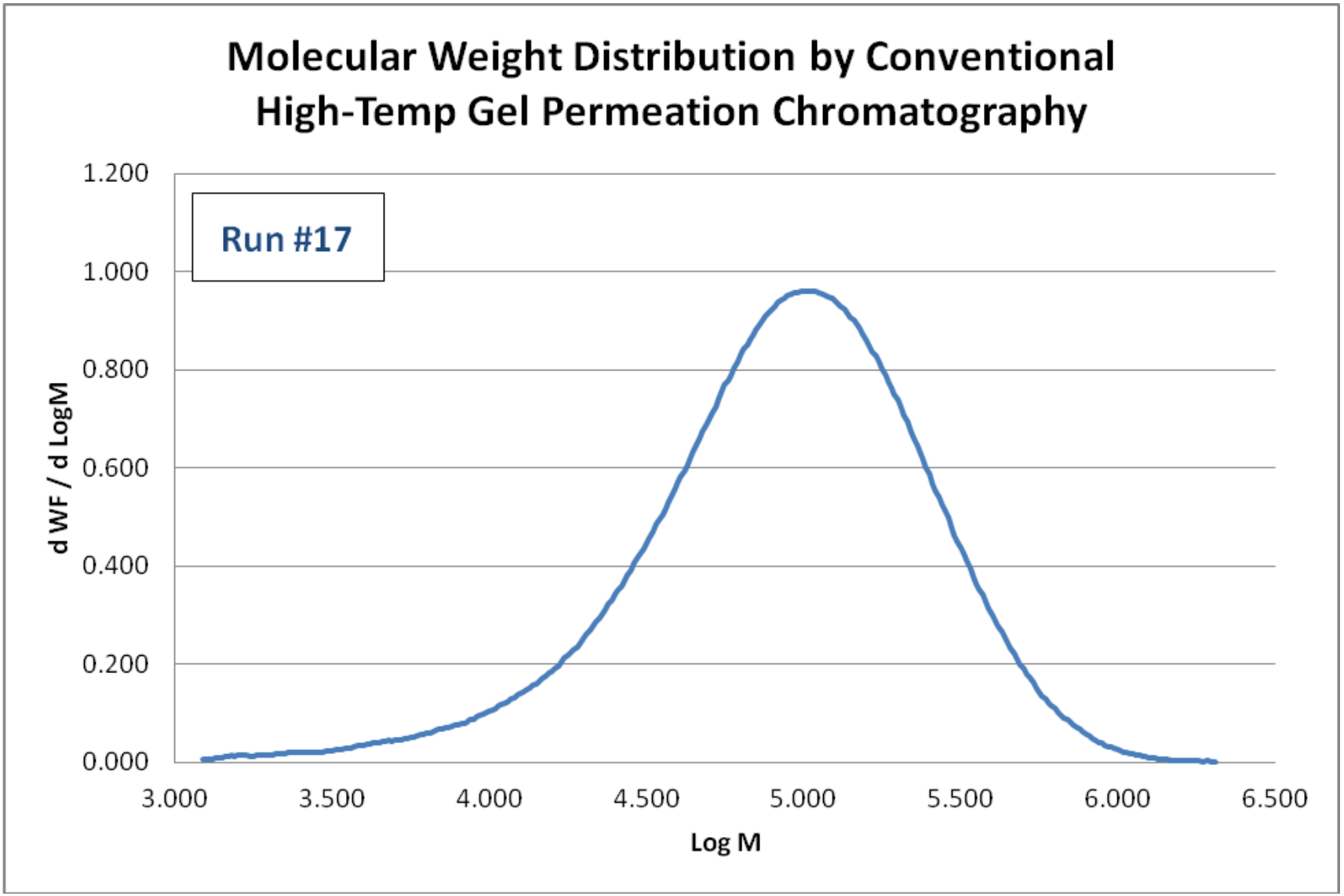


Figure 129. DSC plot for run #17.

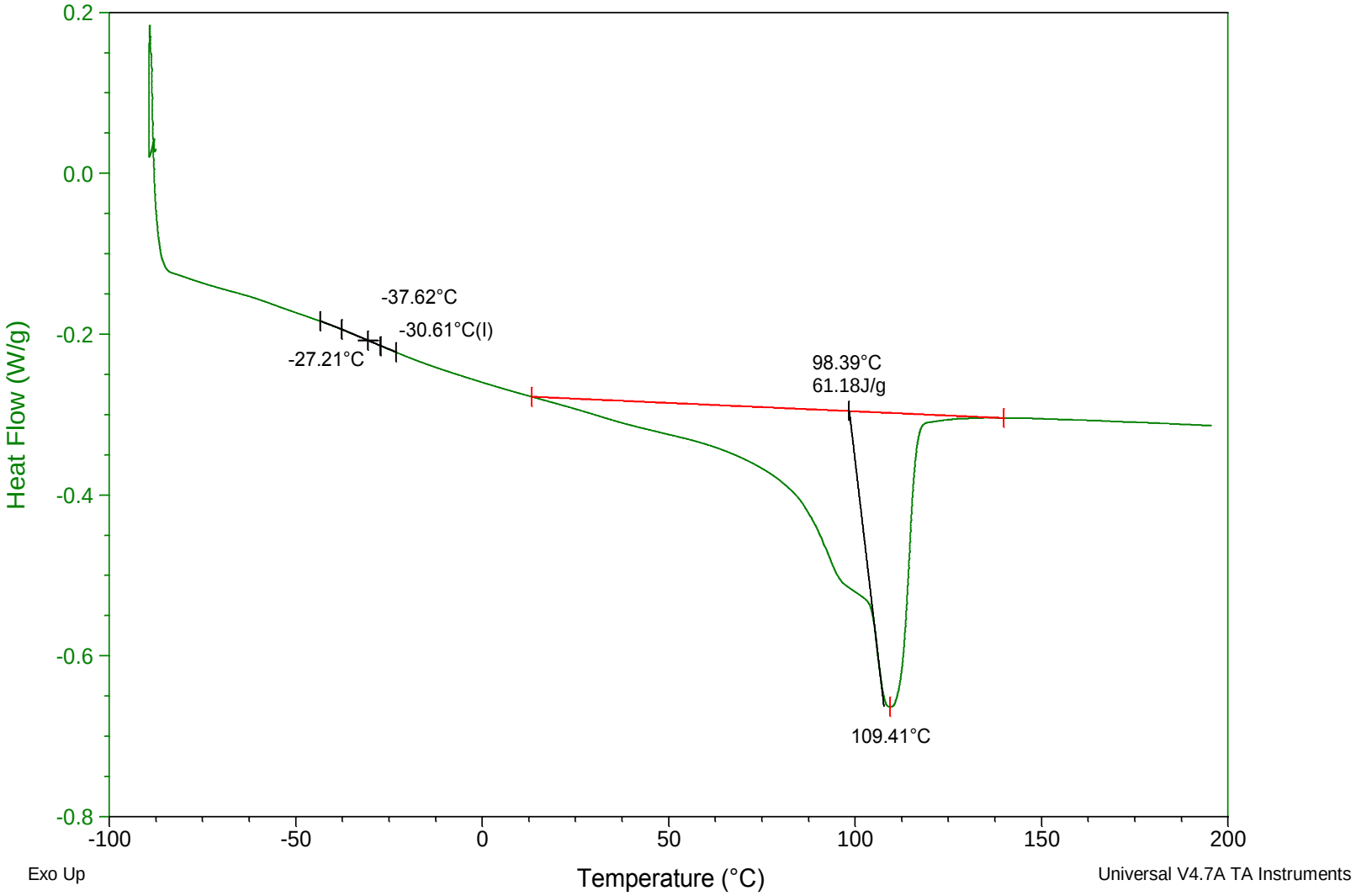


Figure 130. GPC trace for run #18.

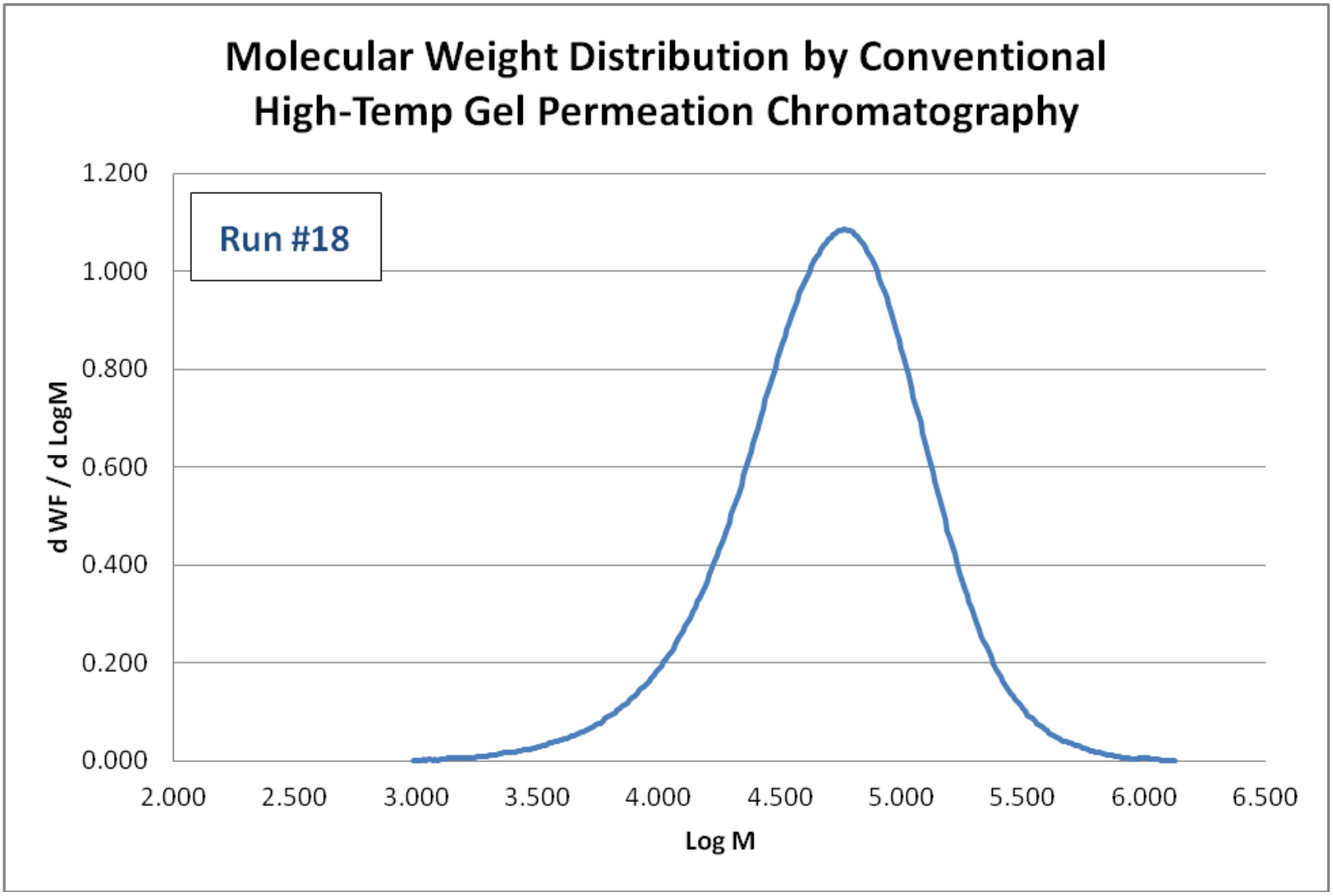


Figure 131. DSC plot for run #18.

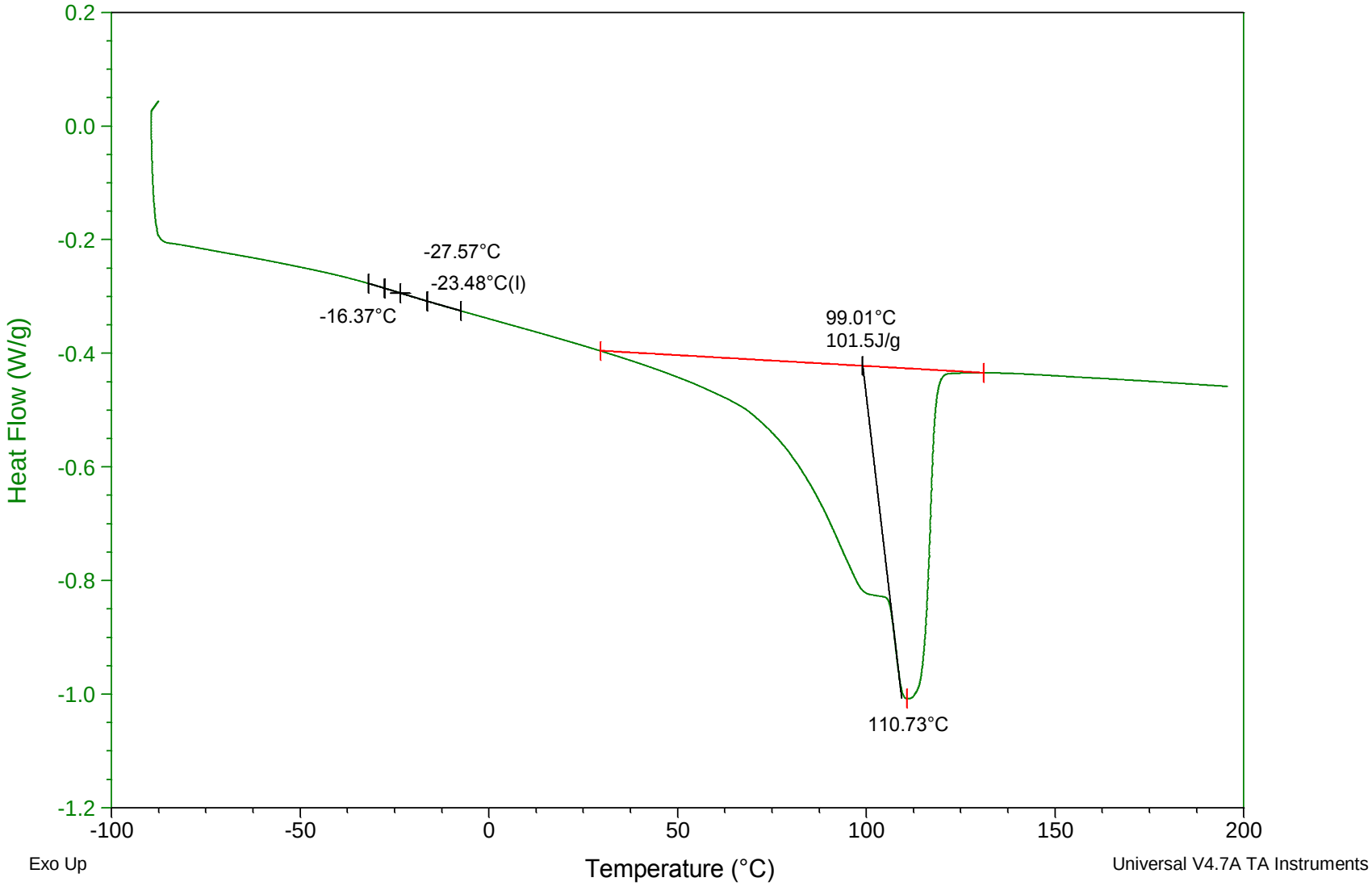


Figure 132. GPC trace for run #19.

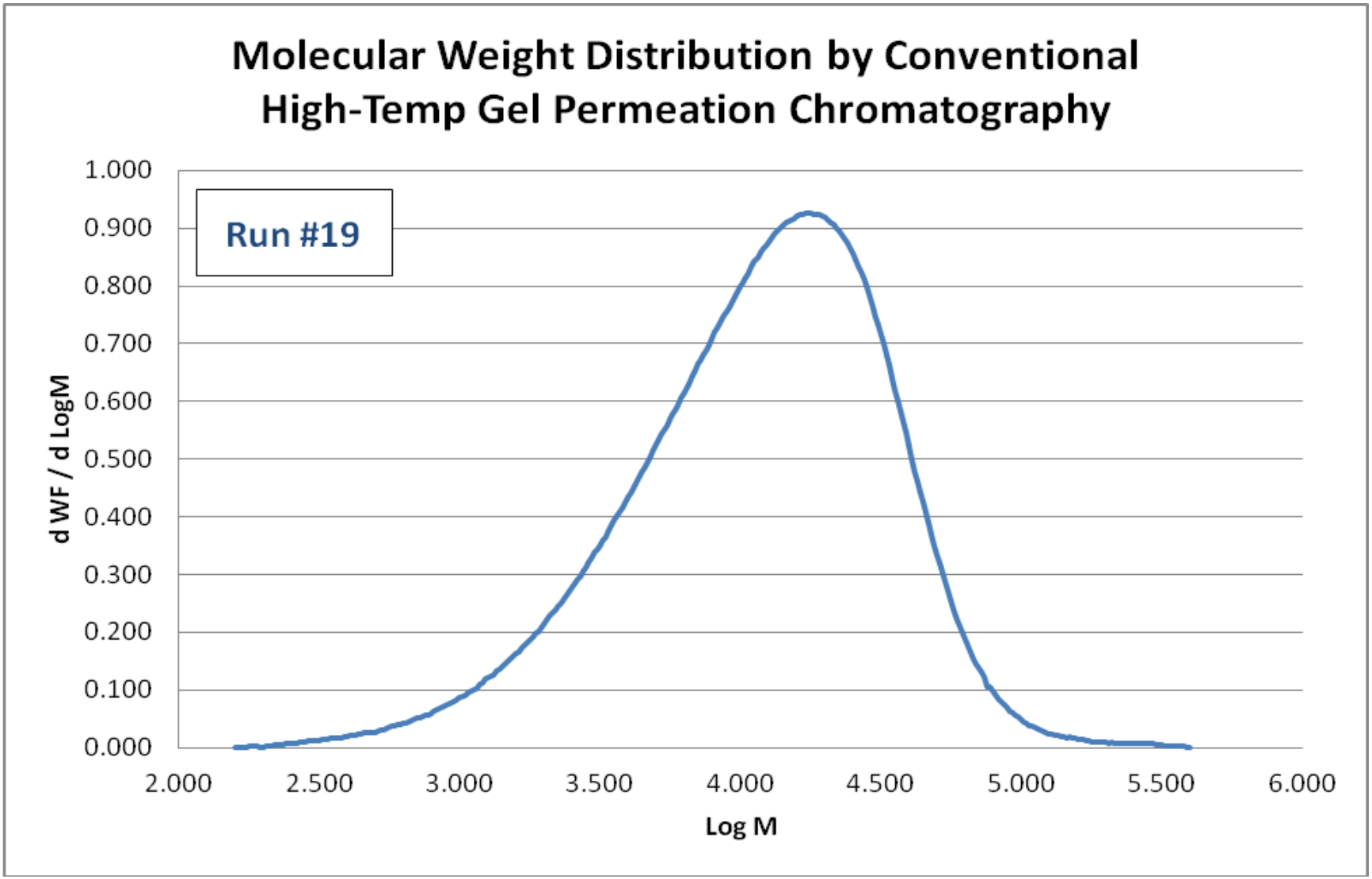
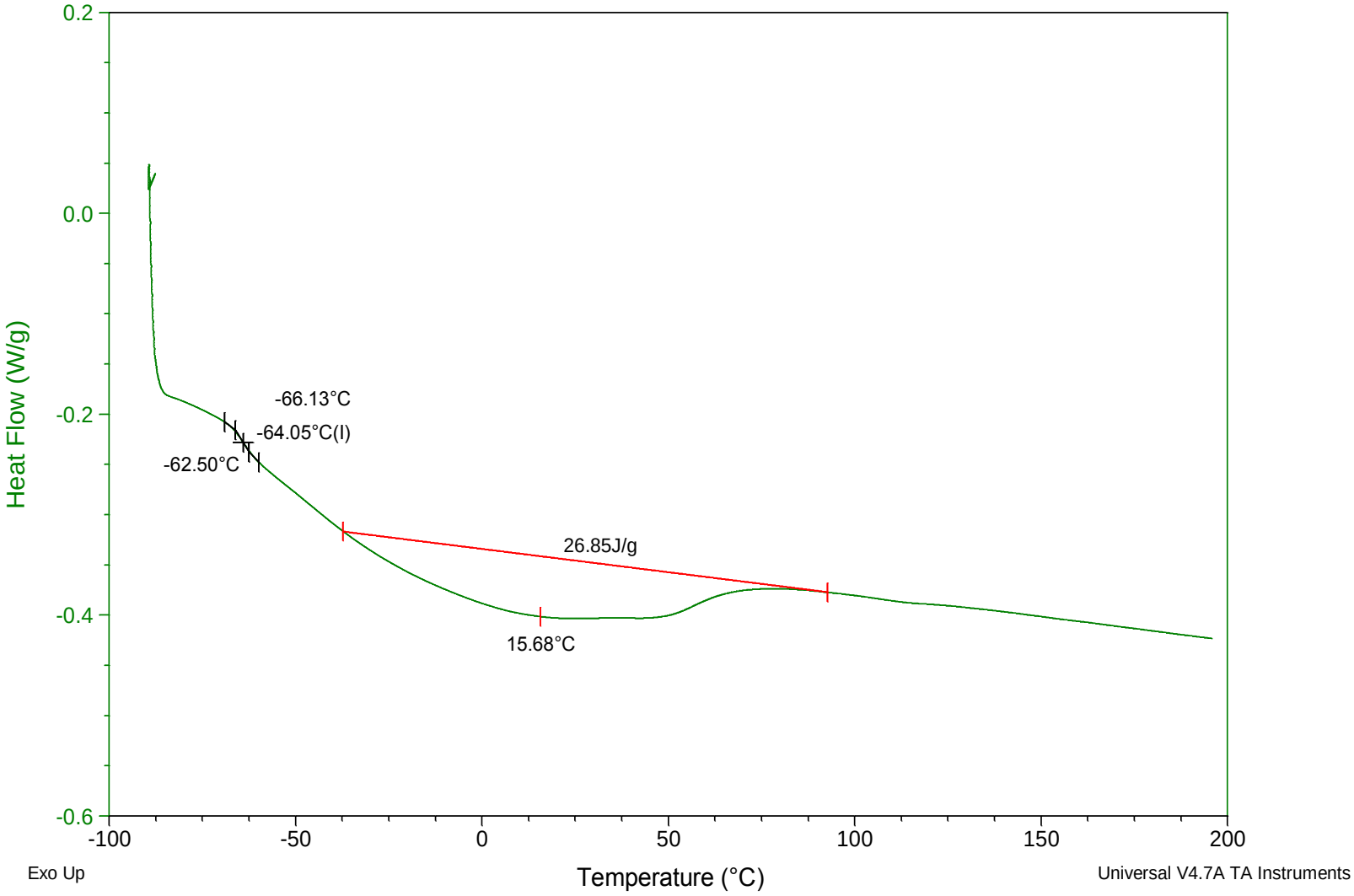


Figure 133. DSC plot for run #19.



FTIR Analytical Description:

Polymer samples were dissolved at a concentration of 30mg/mL in 1,2,4-Trichlorobenzene at 160°C for 1 hr while shaking. A 100µL aliquot of each polymer/TCB solution was deposited into individual cells on a custom silicon wafer at 160°C under nitrogen inerting. The wafer was held at 160°C for 45 minutes, and then pulled from heat and allowed to cool to room temperature. The wafer was then analyzed using a Nicolet Nexus 670 FT-IR ESP infrared spectrometer. Mol% octene within each sample was determined by taking a ratio of the CH_3 area (1382.7-1373.5 wavenumbers) to the CH_2 area (1525-1400 wavenumbers) and normalizing to a standard curve generated through NMR analysis of ethylene-co-1-octene polymer standards.

Figure 134. FTIR Spectrum for Run # 1 (5000 – 400 wavenumbers)

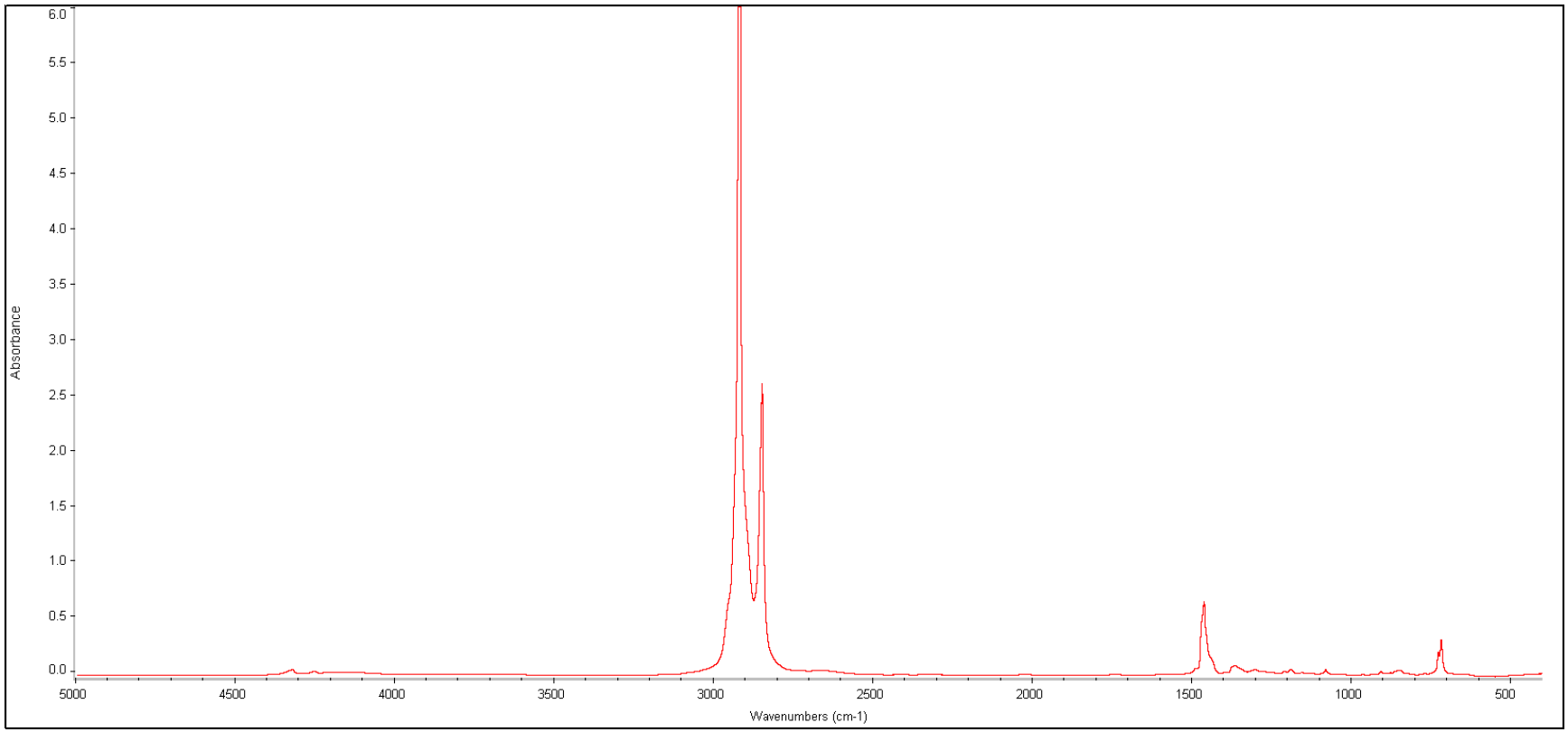


Figure 135. FTIR Spectrum for Run # 1 (1700 – 1200 wavenumbers)

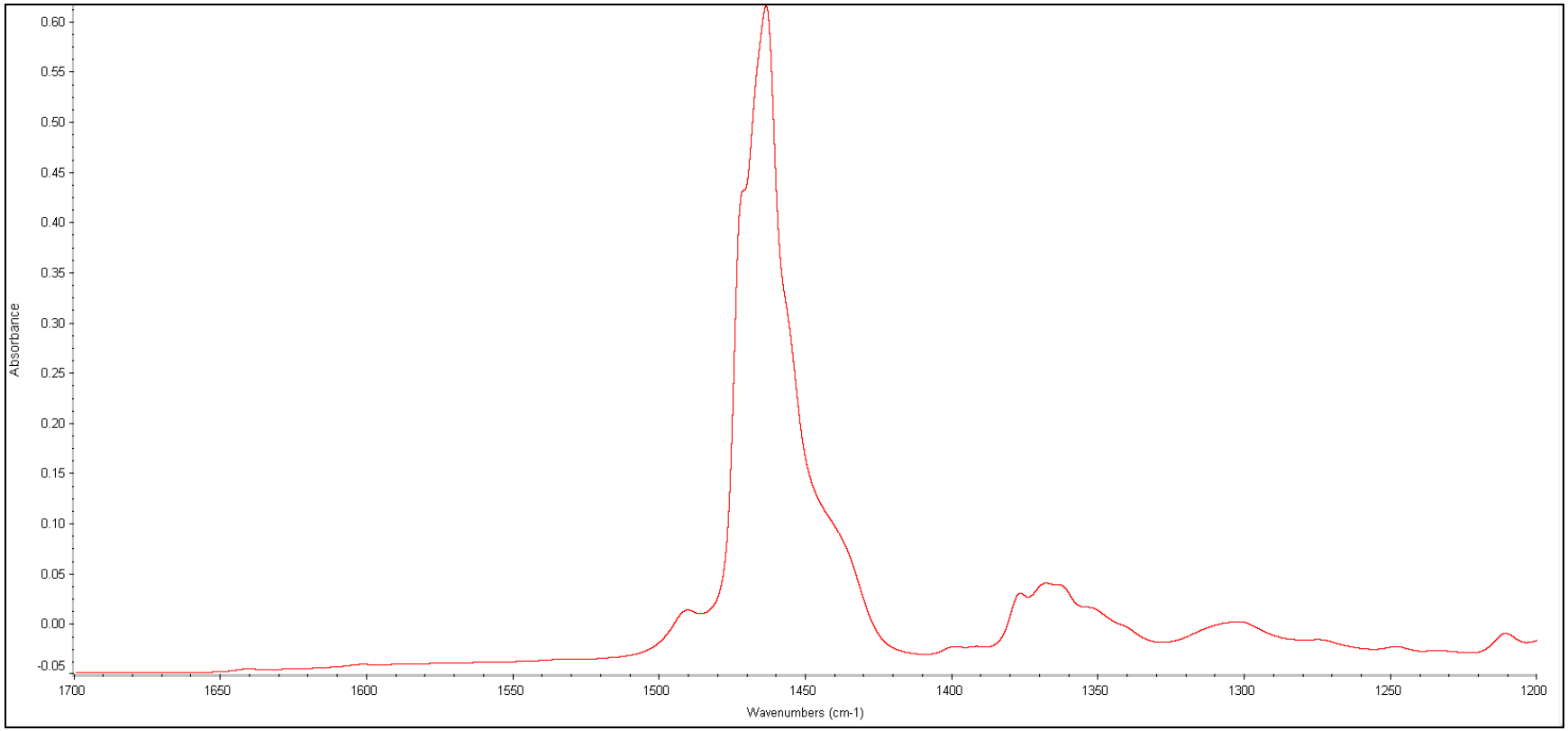


Figure 136. FTIR Spectrum for Run # 2 (5000 – 400 wavenumbers)

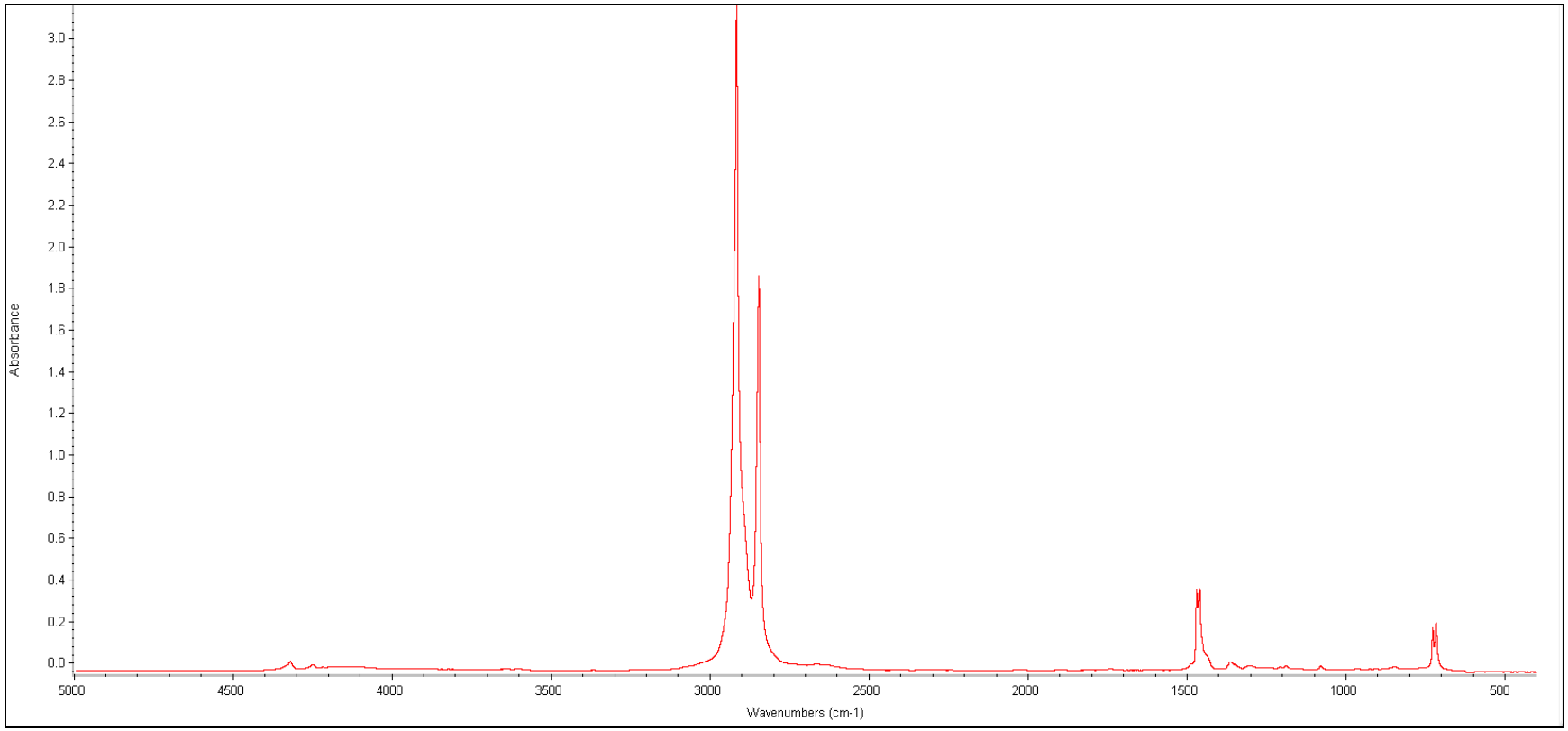


Figure 137. FTIR Spectrum for Run # 2 (1700 – 1200 wavenumbers)

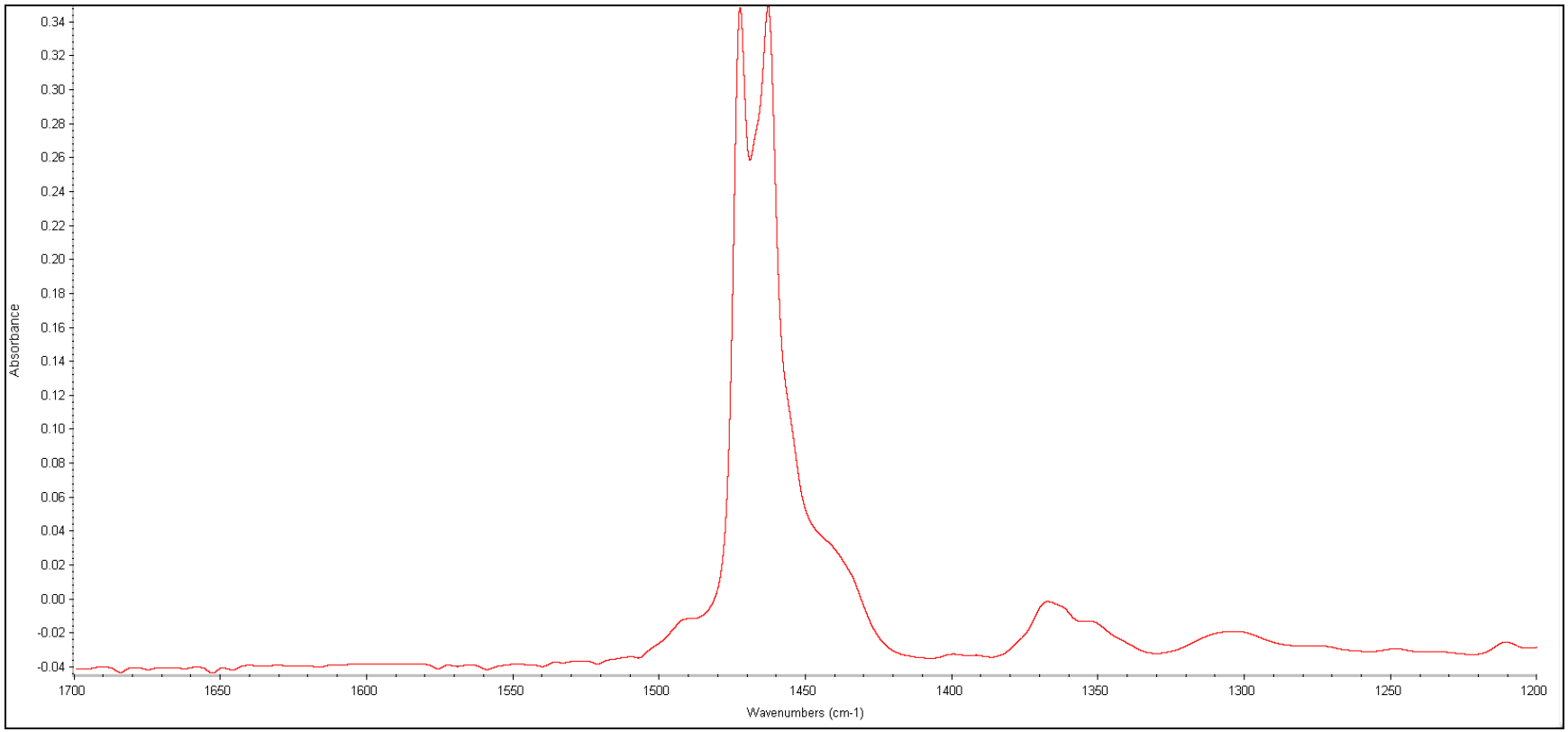


Figure 138. FTIR Spectrum for Run # 13 (5000 – 400 wavenumbers)

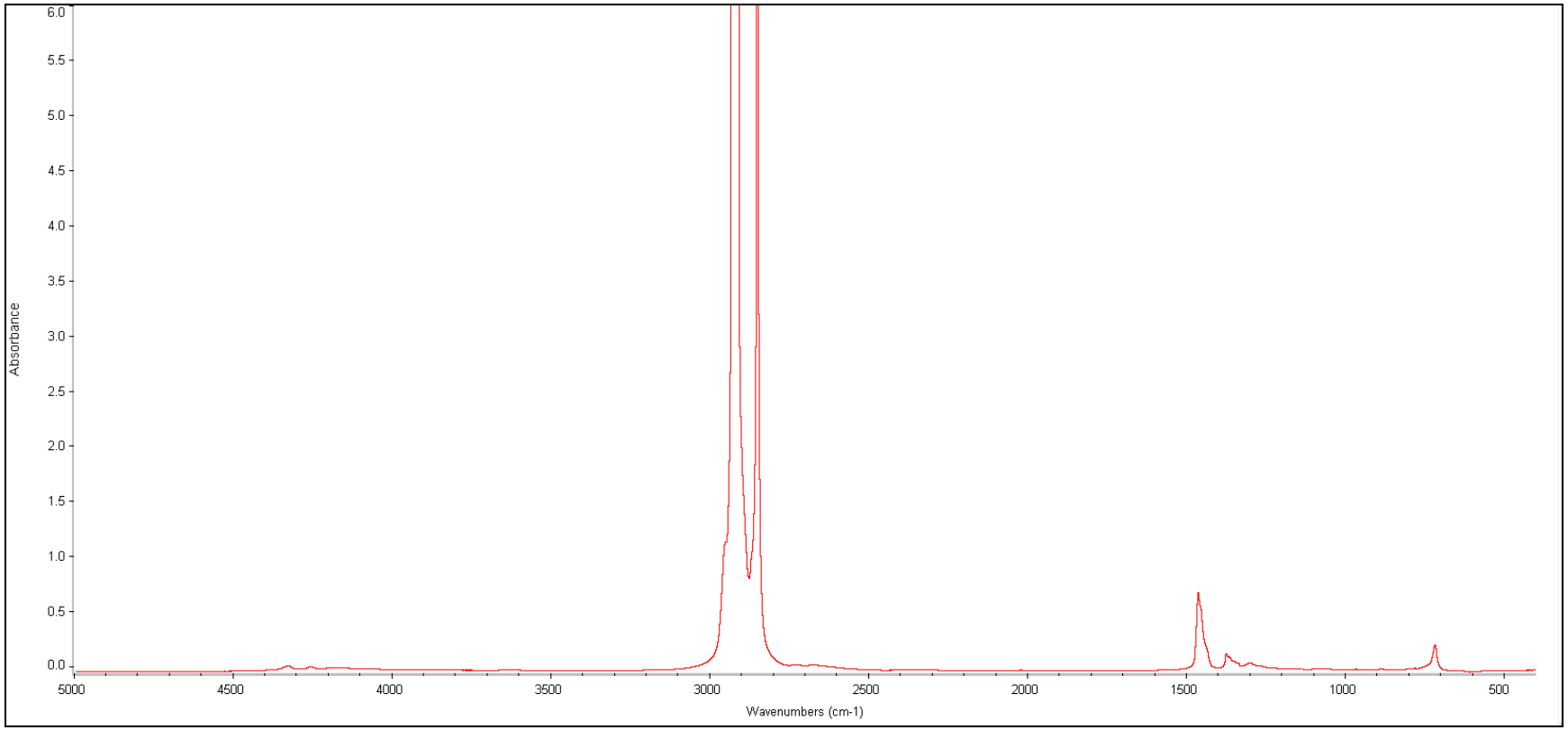


Figure 139. FTIR Spectrum for Run # 13 (1700 – 1200 wavenumbers)