Supporting Information II (SI) for

Ni, Pd, and Pt Complexes of a Chiral Tetradentate Dianionic Thiosemicarbazone-based O^N^N^S Ligand

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Contents: **NMR spectra**

NMR Spectra for (3,5-di-tert-butyl-2-methoxyphenyl)boronic acid Synthesis

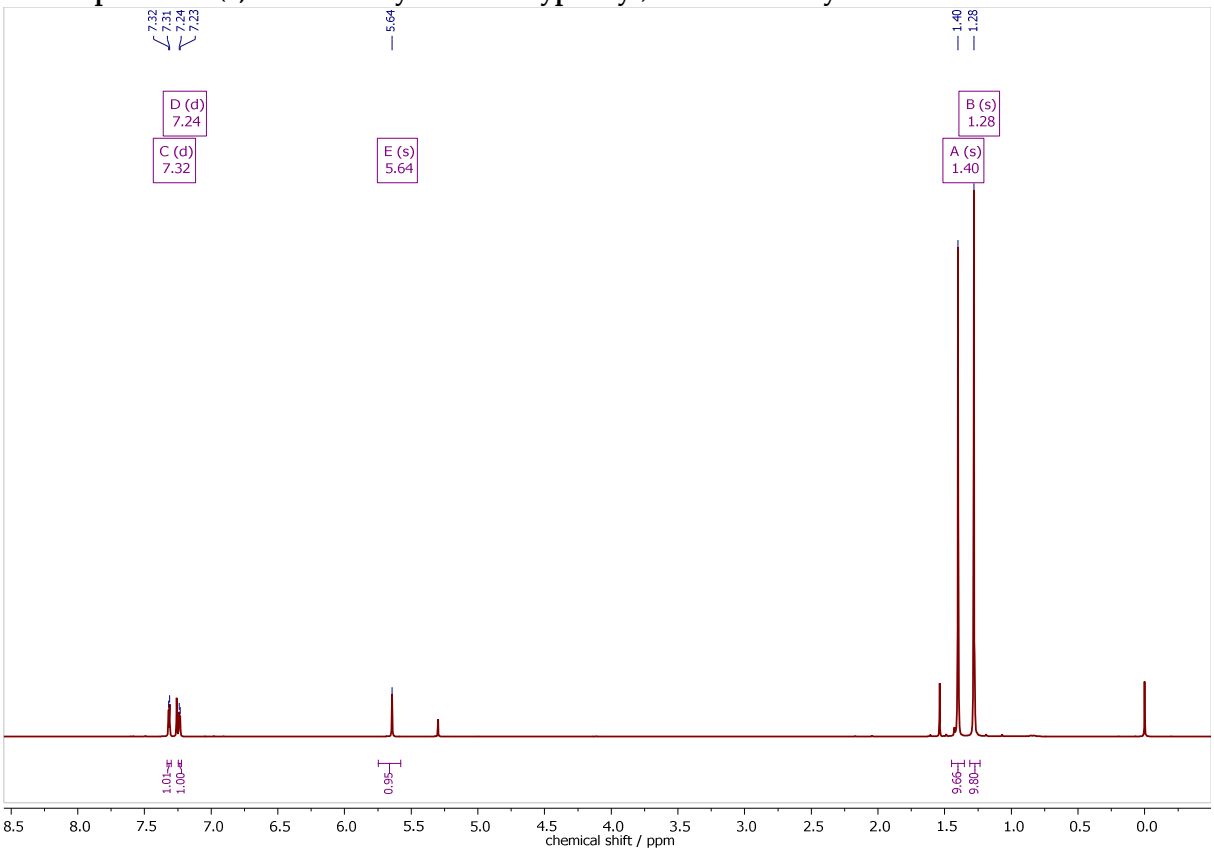

Fig. X1. ^{1}H NMR spectrum of 2-bromo-4,6-di-tert-butylphenol in $CDCl_3$ at 300 MHz.

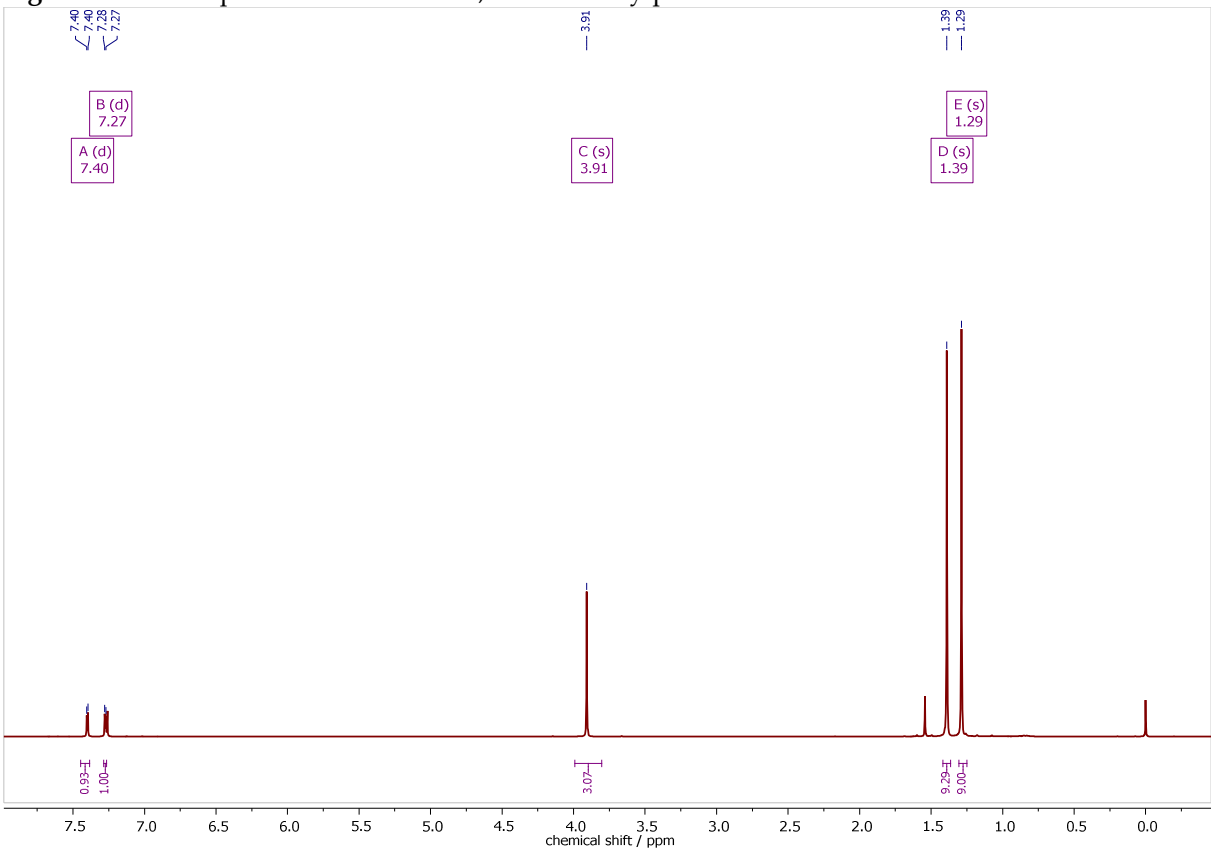

Fig. X2. ^{1}H NMR spectrum of 1-bromo-3,5-di-tert-butyl-2-methoxybenzene in $CDCl_3$ at 300 MHz.

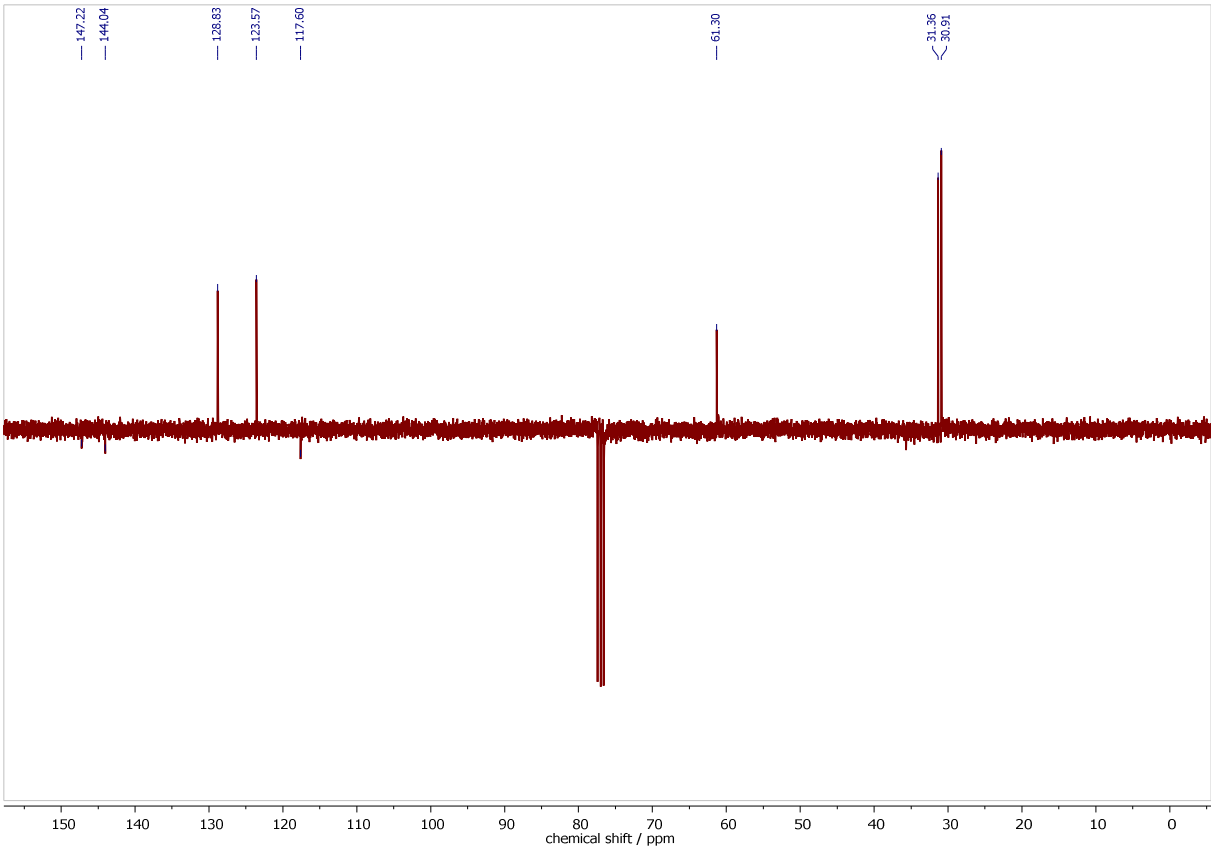

Fig. X3. ^{13}C DEPTQ NMR spectrum 1-bromo-3,5-di-tert-butyl-2-methoxybenzene in $CDCl_3$ at 75 MHz.

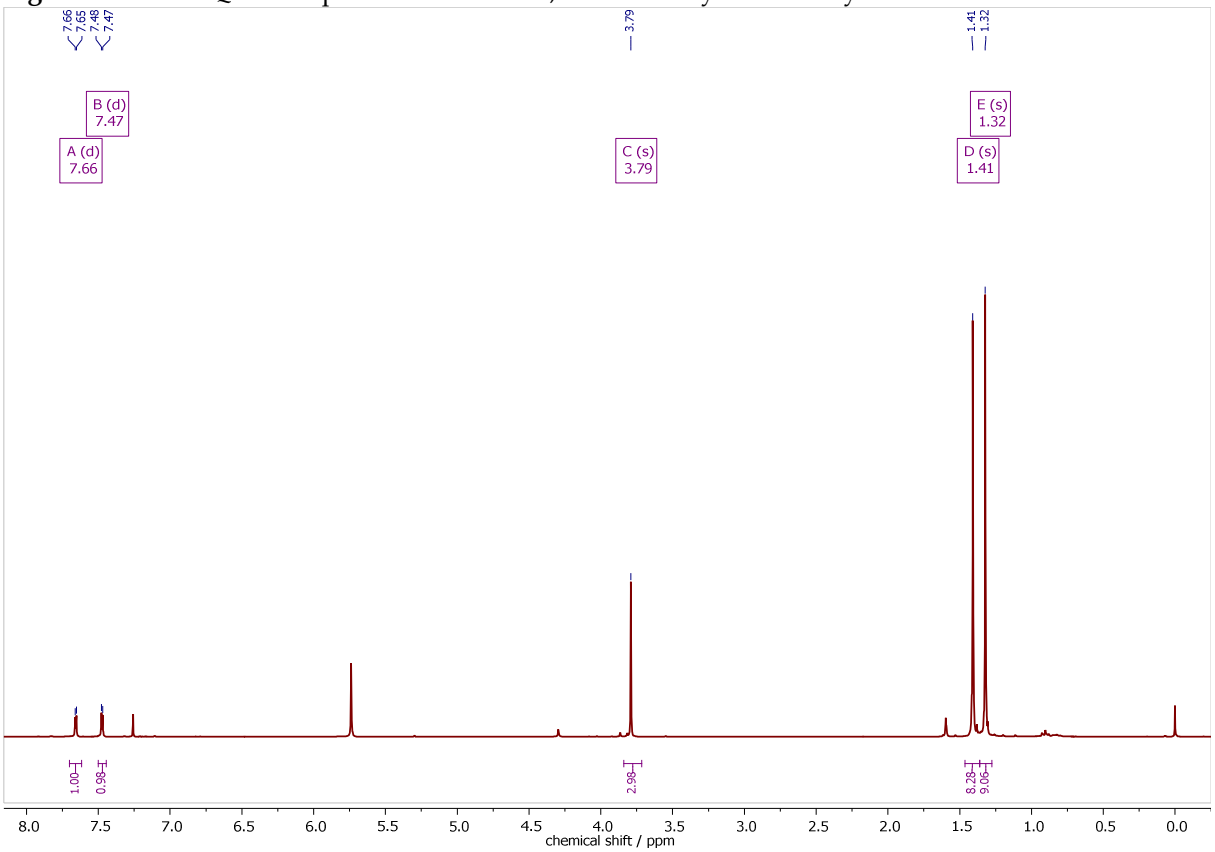

Fig. X4. ^{1}H NMR spectrum of (3,5-di-tert-butyl-2-methoxyphenyl)boronic acid in $CDCl_3$ at 300 MHz.

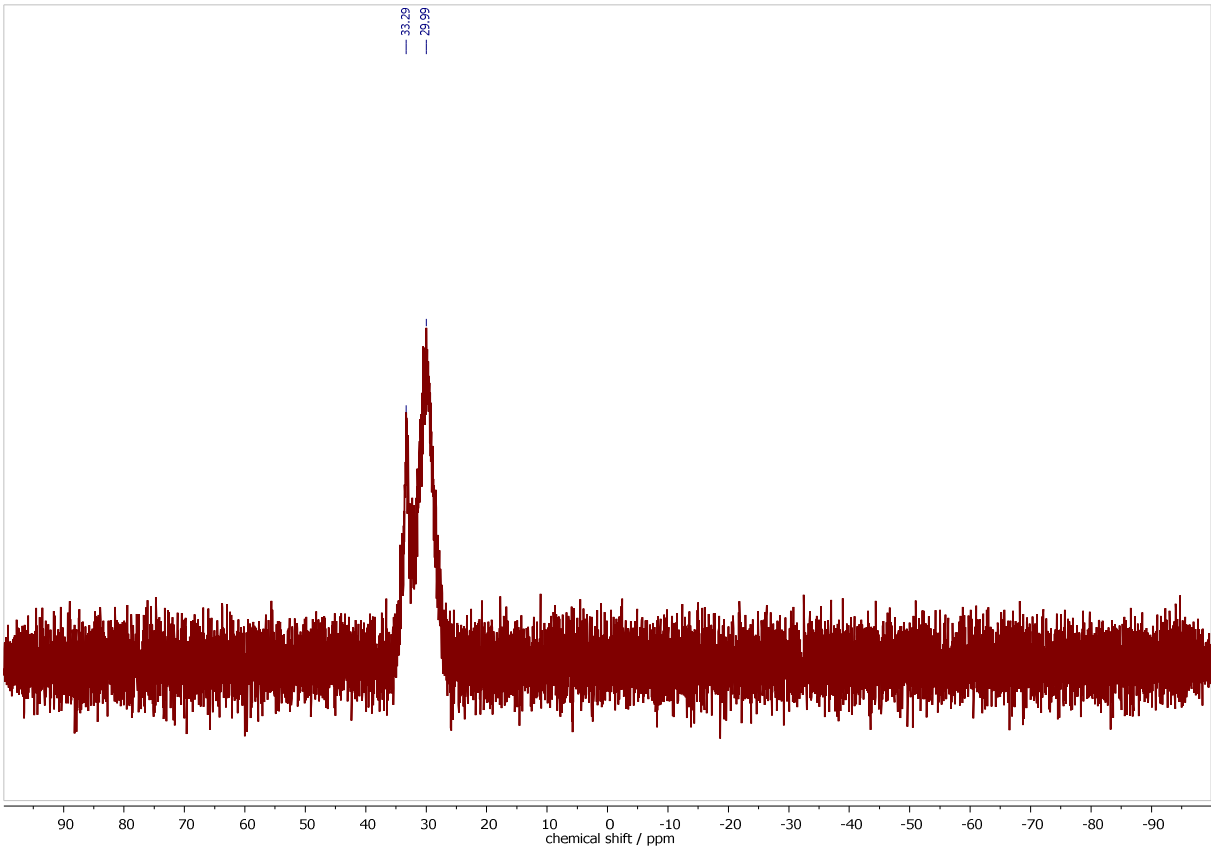

Fig. X5. ^{11}B NMR spectrum of (3,5-di-tert-butyl-2-methoxyphenyl)boronic acid in $CDCl_3$ at 32 MHz.

NMR Spectra of Aldehydes

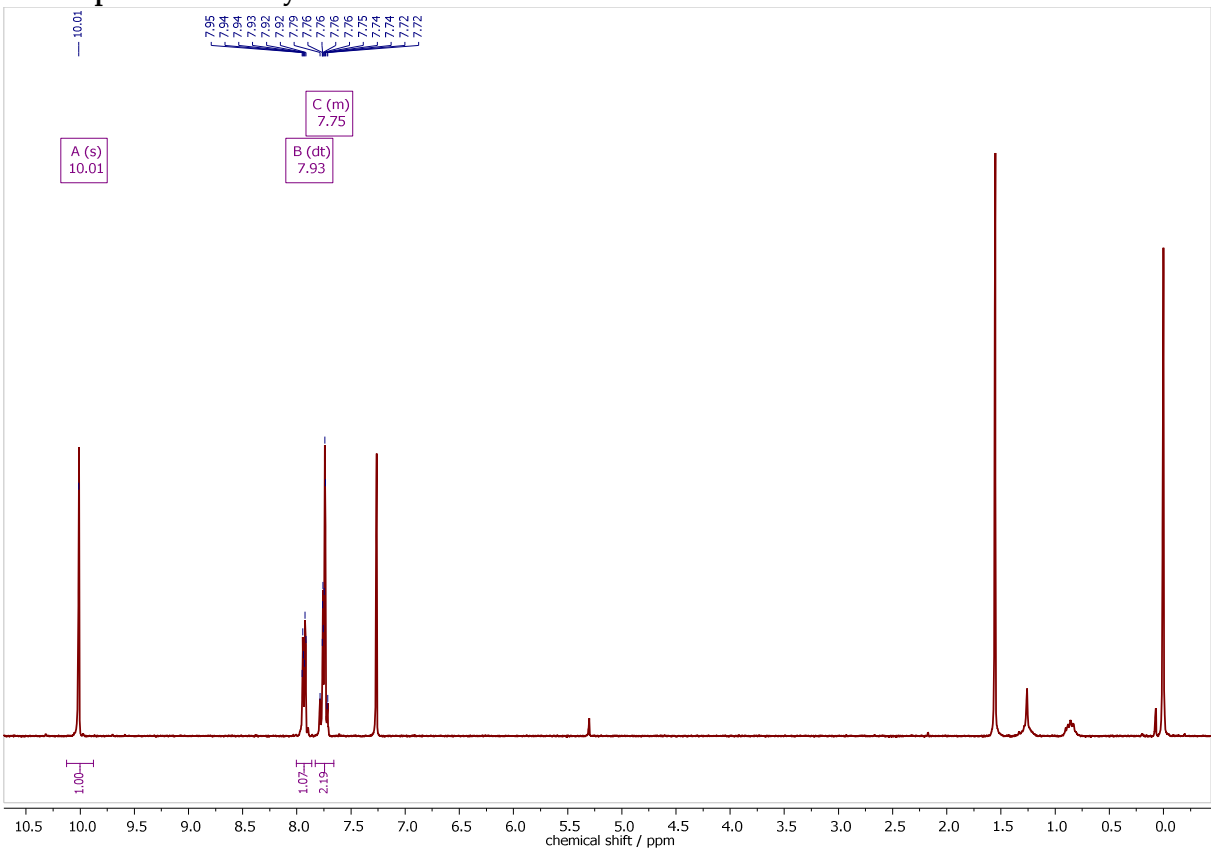

Fig. X6. ^{1}H NMR spectrum of 6-bromopicolinaldehyde in $CDCl_3$ at 300 MHz.

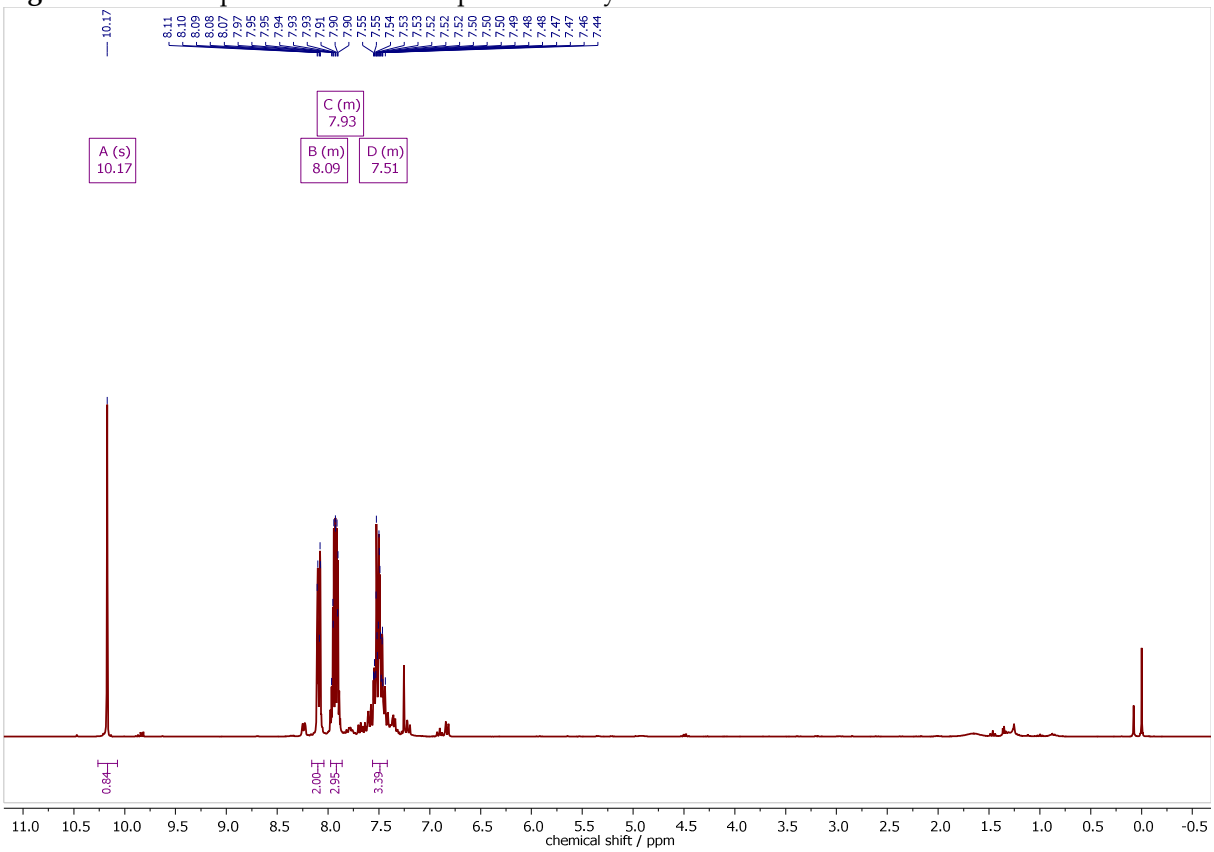

Fig. X7. ^{1}H NMR spectrum of 6-phenylpicolinaldehyde in $CDCl_3$ at 300 MHz.

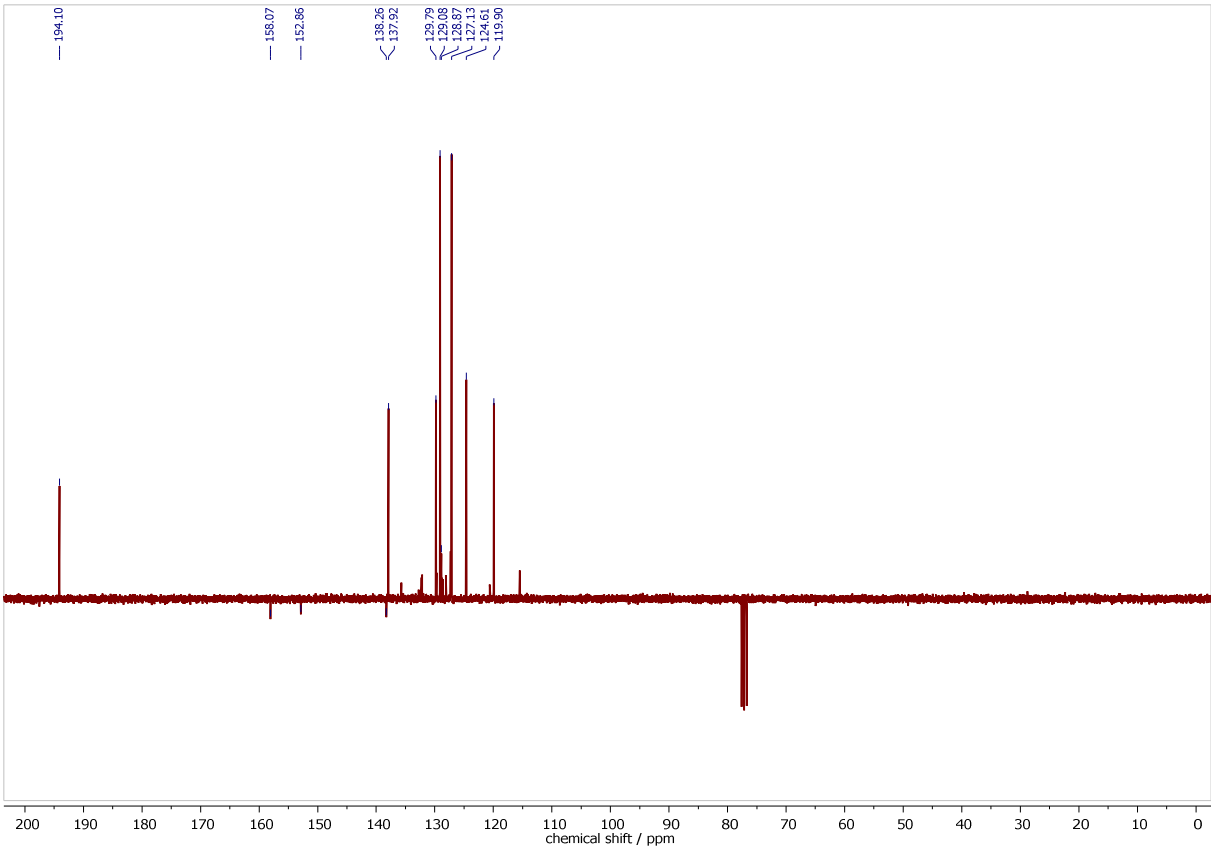

Fig. X8. ^{13}C DEPTQ NMR spectrum of 6-phenylpicolinaldehyde in $CDCl_3$ at 75 MHz.

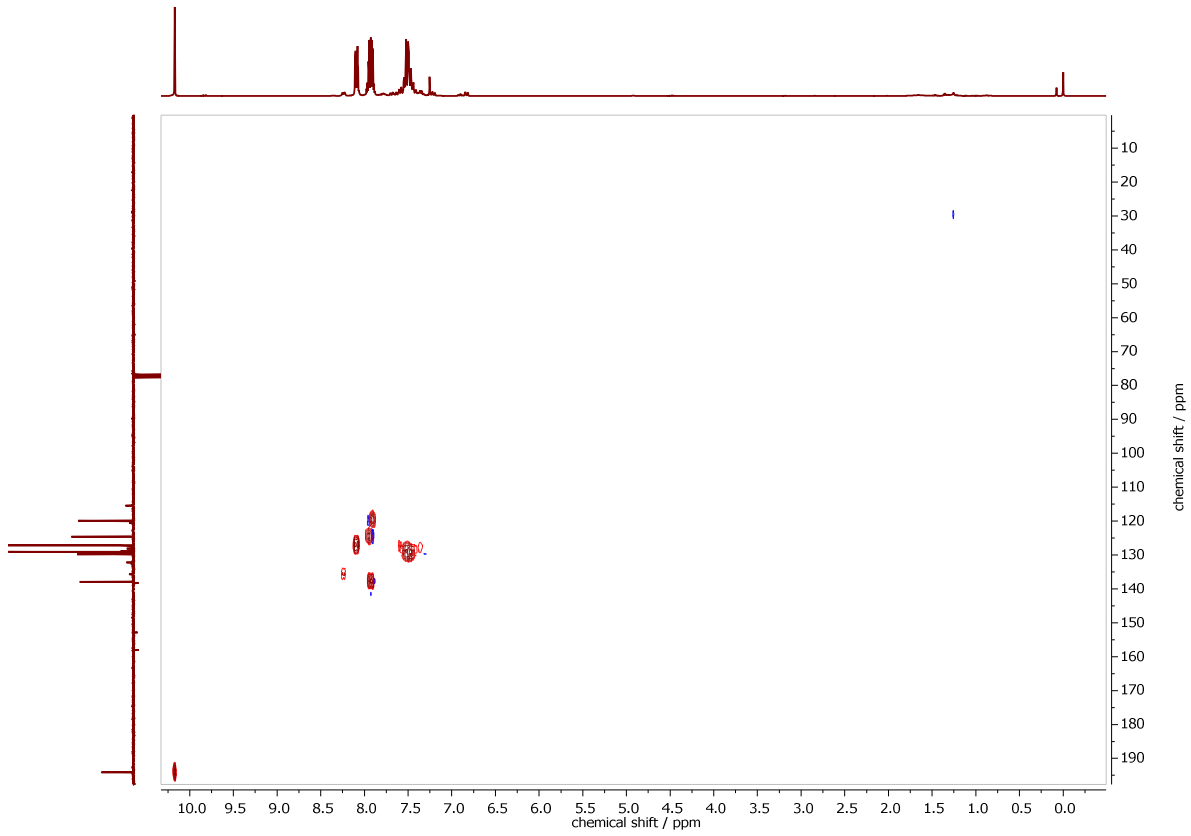

Fig. X9. $^{1}H,^{13}C$ HSQCed NMR spectrum of 6-phenylpicolinaldehyde in $CDCl_3$.

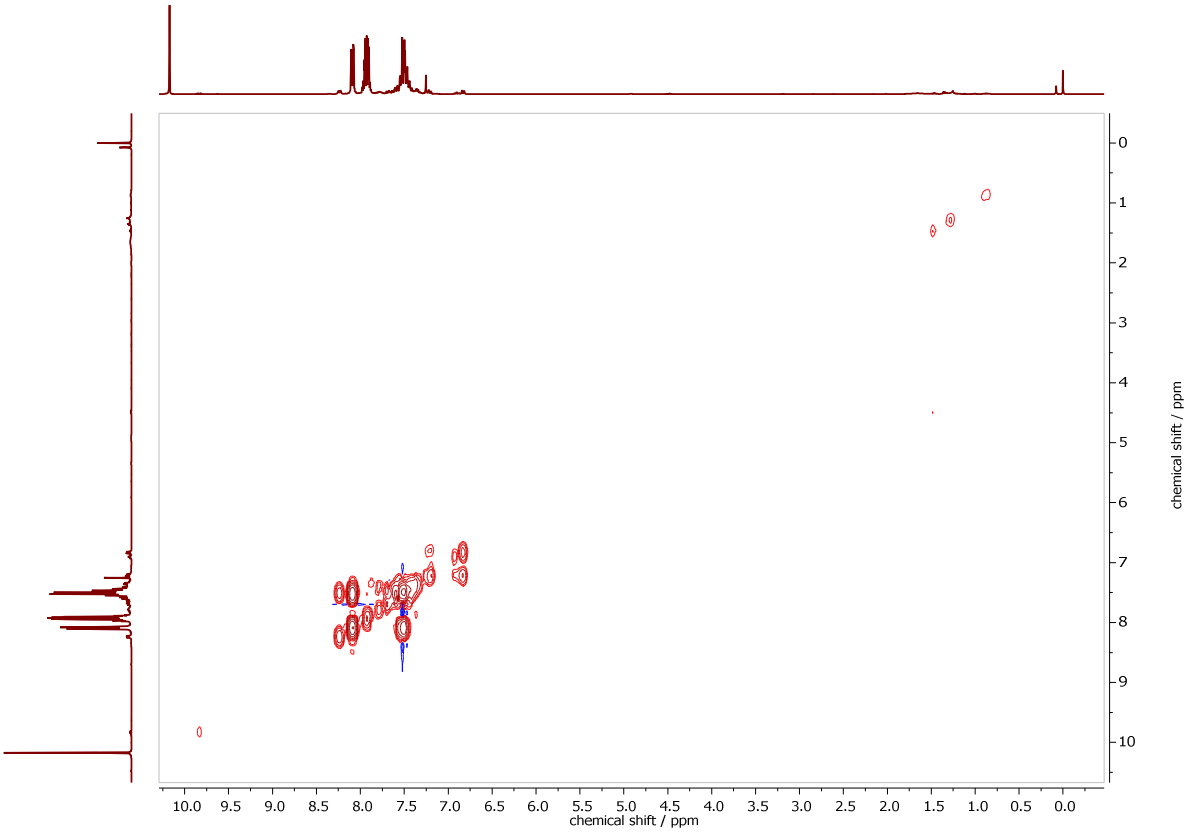

Fig. X10. $^{1}H,^{1}H$ COSY NMR spectrum of 6-phenylpicolinaldehyde in $CDCl_3$.

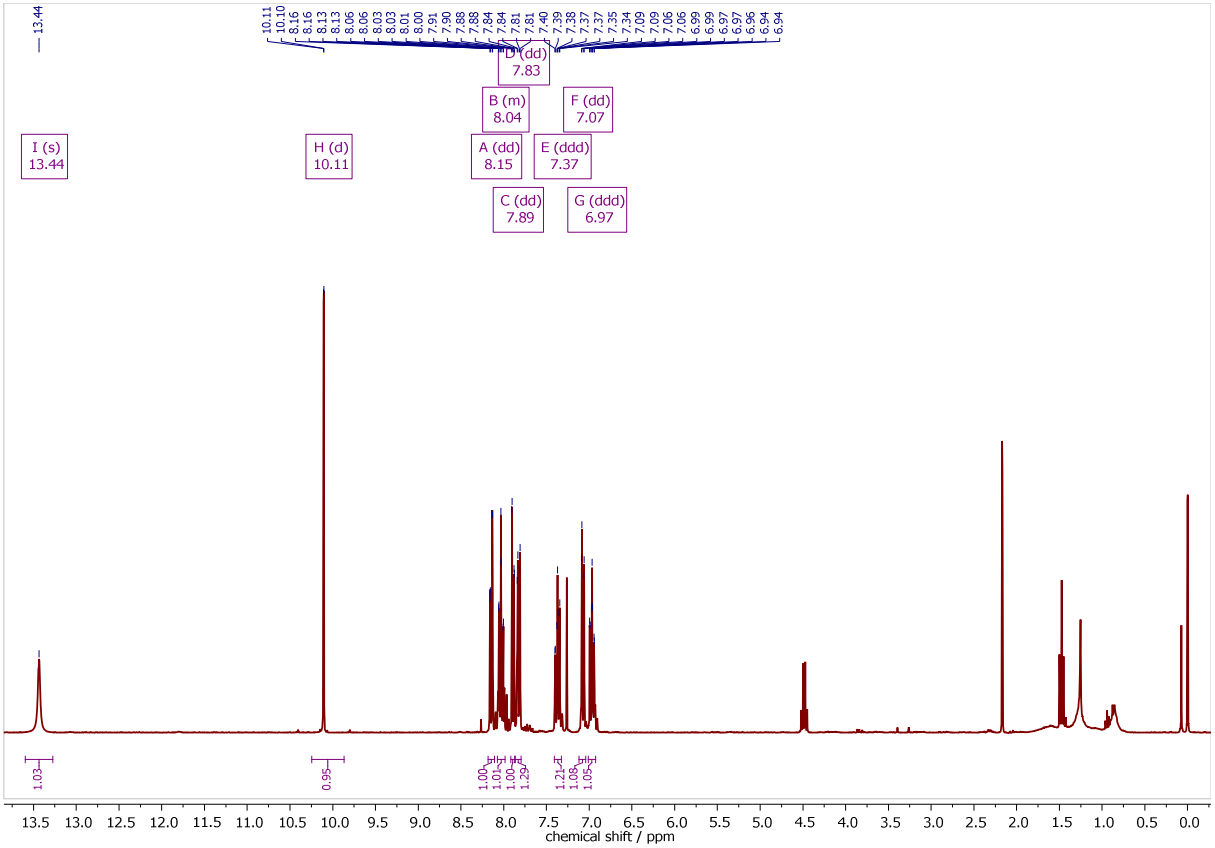

Fig. X11. ^{1}H NMR spectrum of 6-(2-hydroxyphenyl)picolinaldehyde in $CDCl_3$ at 300 MHz.

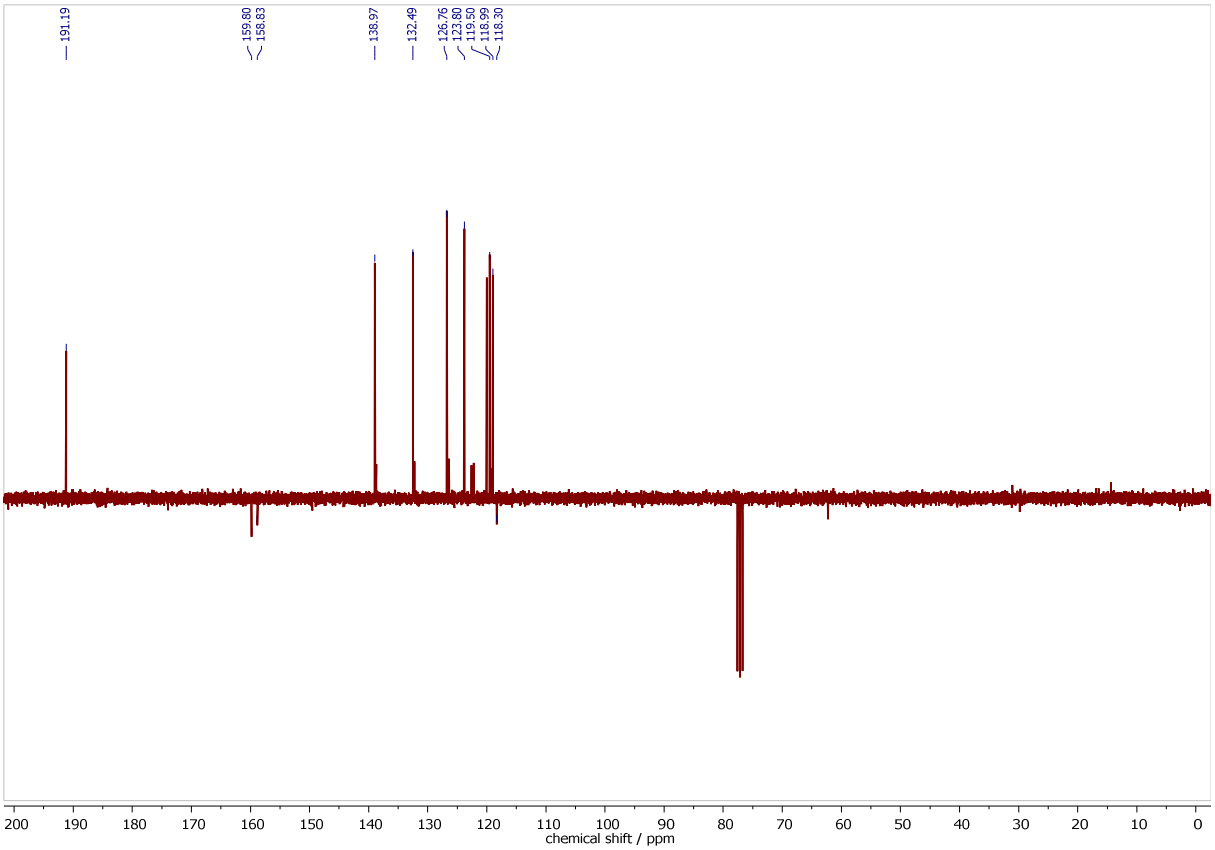

Fig. X12. ^{13}C DEPTQ NMR spectrum of 6-(2-hydroxyphenyl)picolinaldehyde in $CDCl_3$ at 75 MHz.

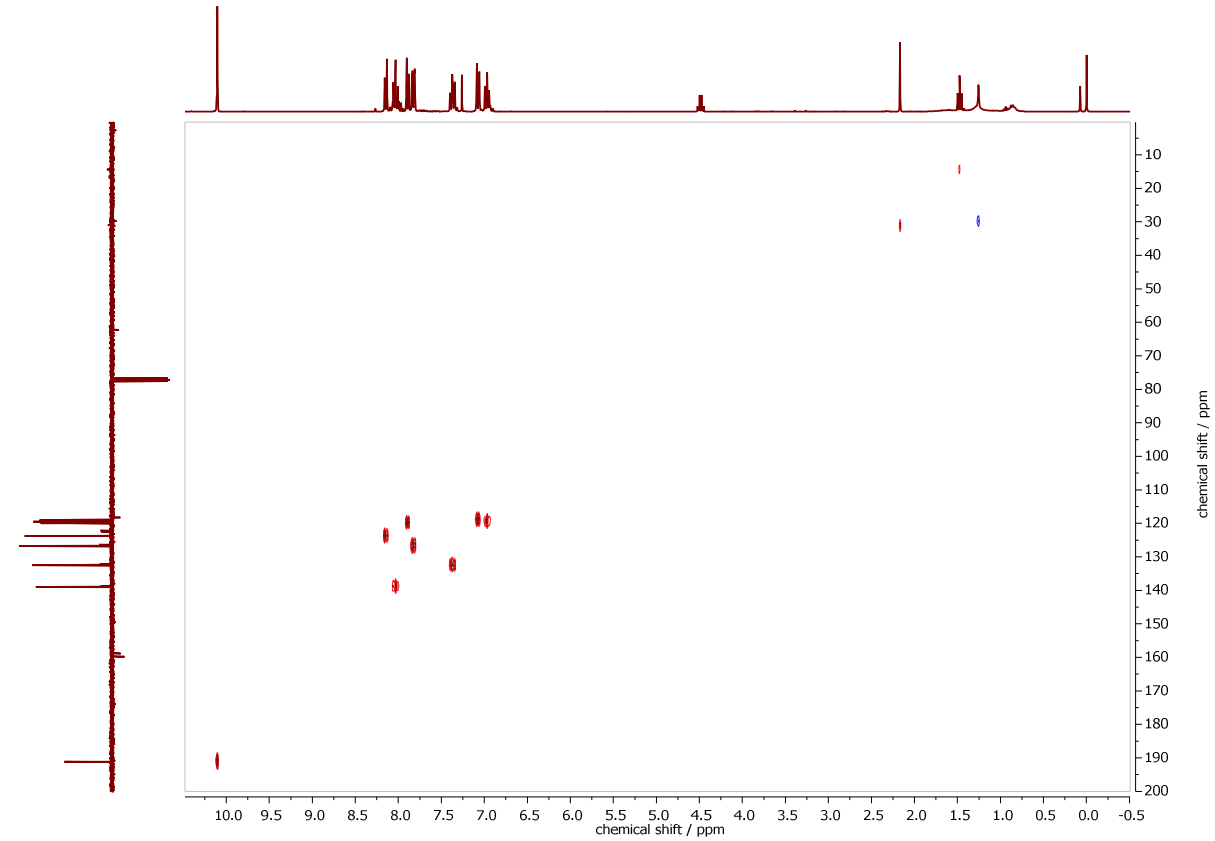

Fig. X13. $^{1}H,^{13}C$ HSQCed NMR spectrum of 6-(2-hydroxyphenyl)picolinaldehyde in $CDCl_3$.

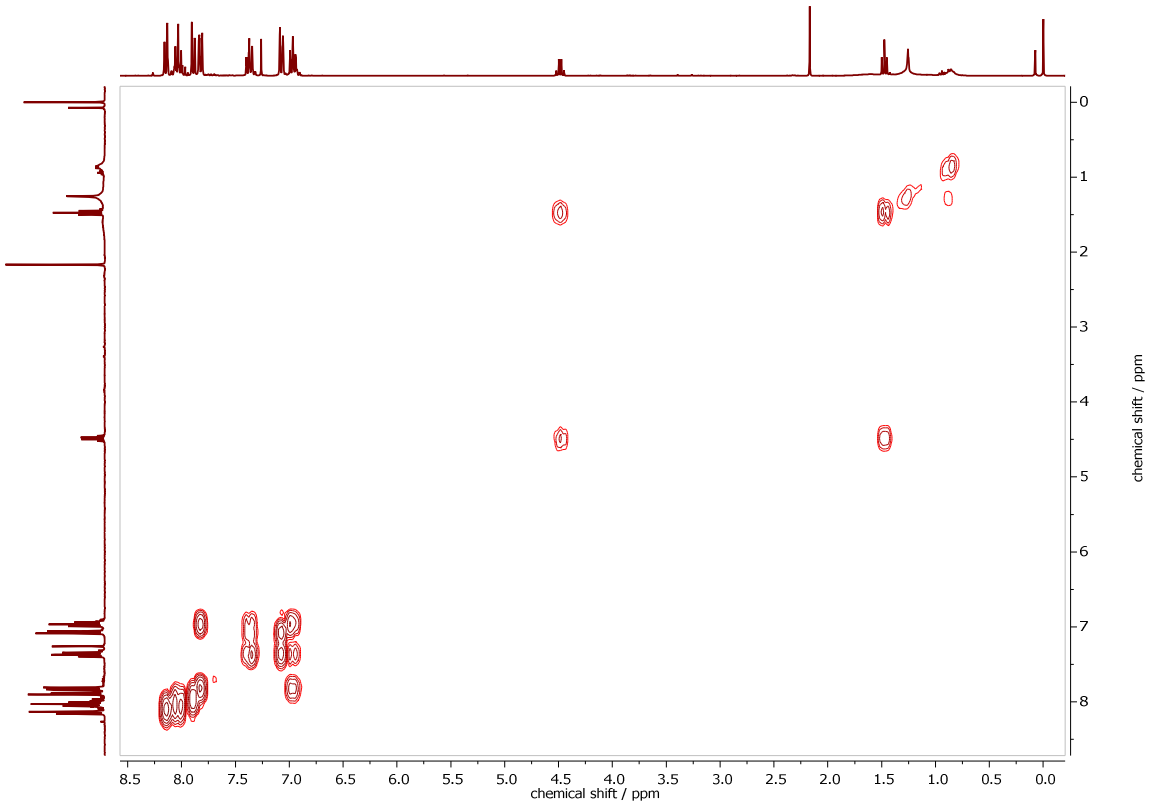

Fig. X14. $^{1}H,^{1}H$ COSY NMR spectrum of 6-(2-hydroxyphenyl)picolinaldehyde in $CDCl_3$.

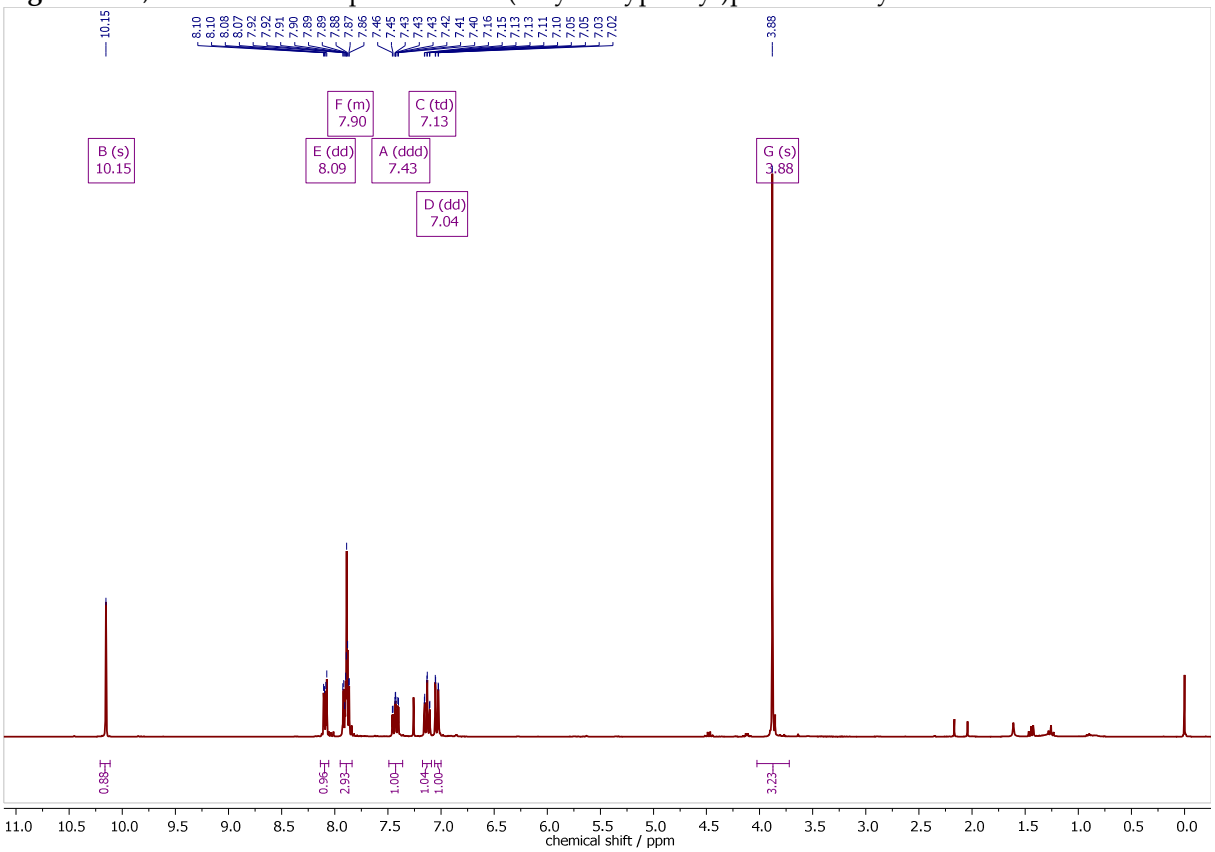

Fig. X15. ^{1}H NMR spectrum of 6-(2-methoxyphenyl)picolinaldehyde in $CDCl_3$ at 300 MHz.

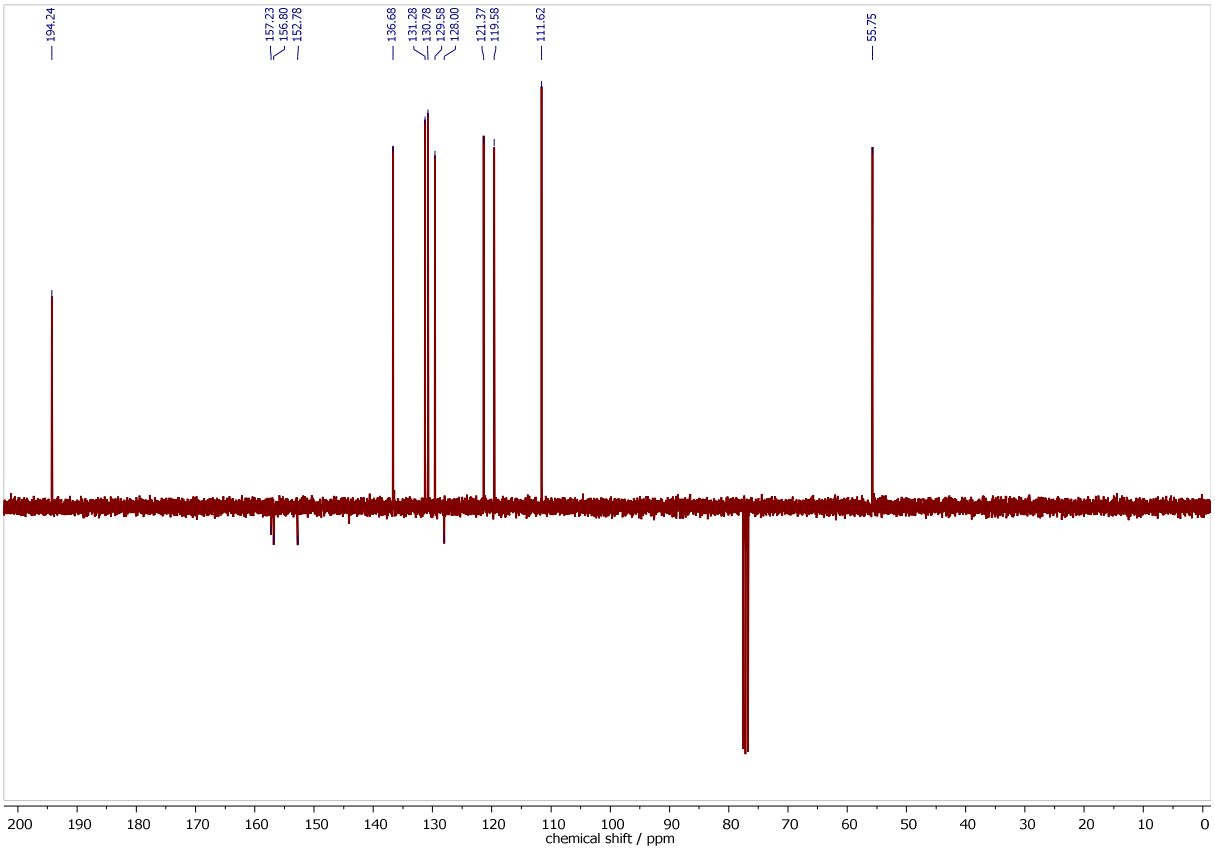

Fig. X16. ^{13}C DEPTQ NMR spectrum of 6-(2-methoxyphenyl)picolinaldehyde in $CDCl_3$ at 75 MHz.

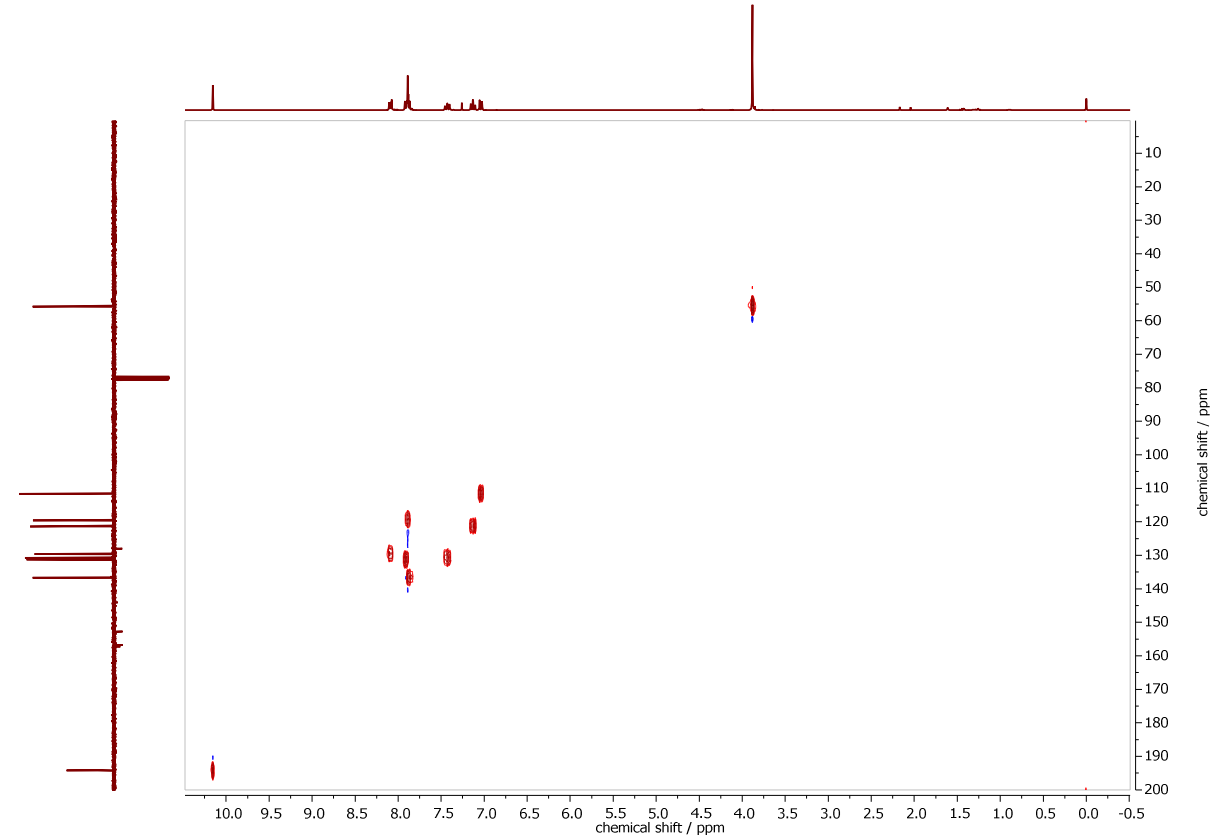

Fig. X17. ^{1}H,^{13}C HSQCed NMR spectrum of 6-(2-methoxyphenyl)picolinaldehyde in $CDCl_3$.

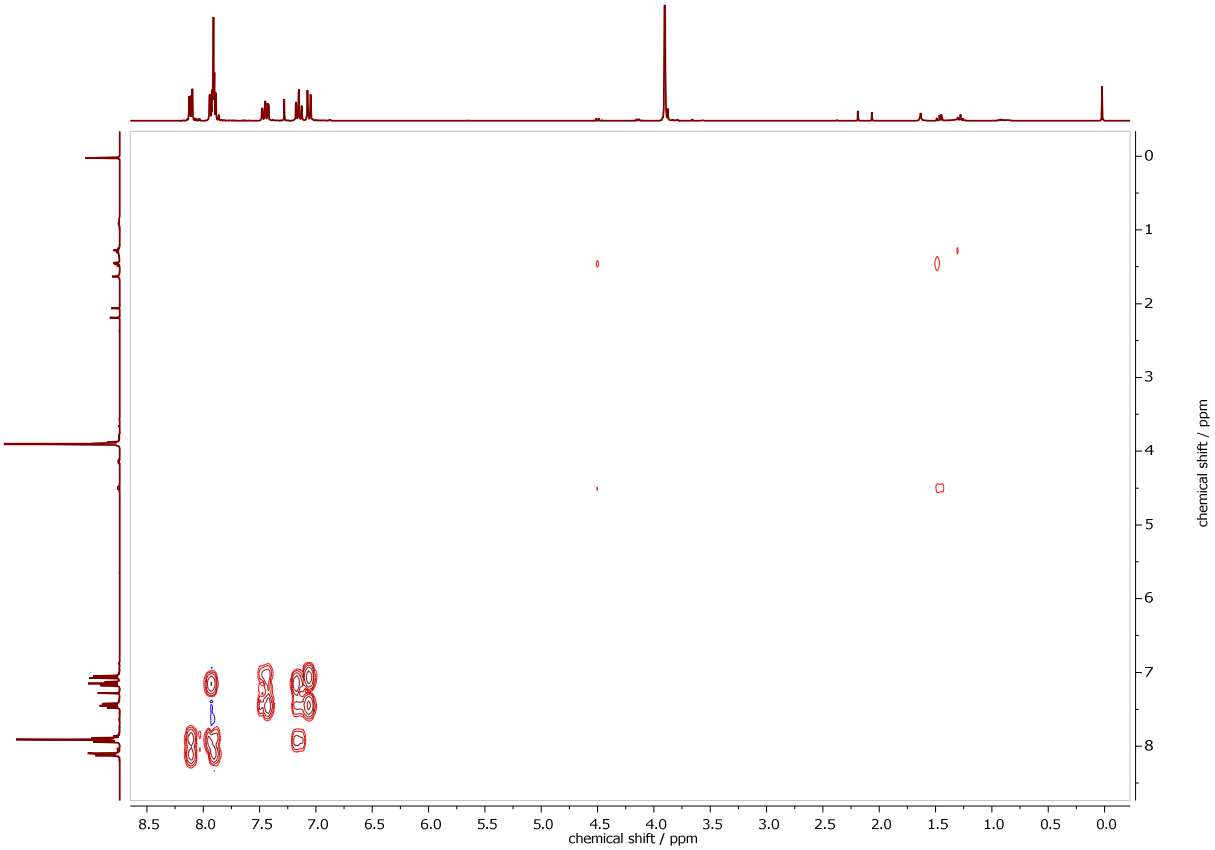

Fig. X18. $^{1}H,^{1}H$ COSY NMR spectrum of 6-(2-methoxyphenyl)picolinaldehyde in $CDCl_3$.

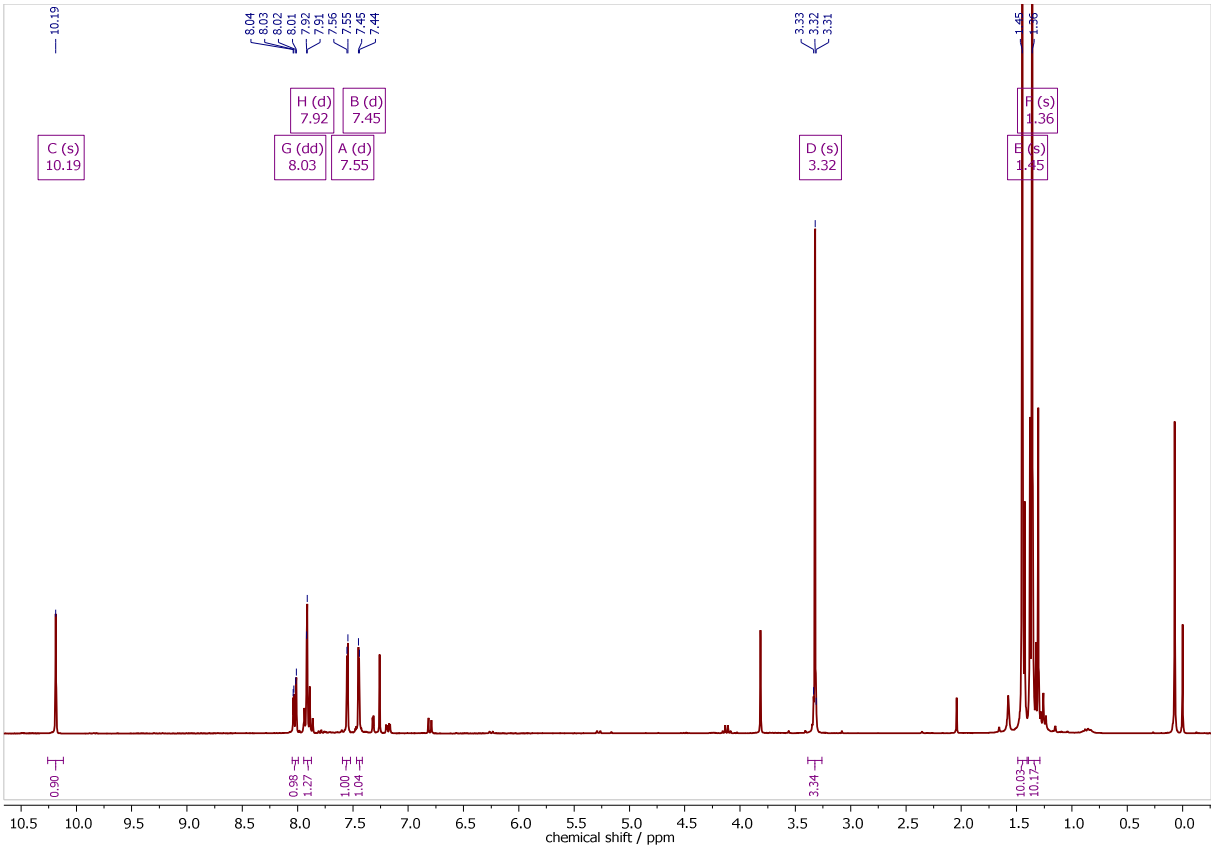

Fig. X19. ^{1}H NMR spectrum of 6-(3,5-di-tert-butyl-2-methoxyphenyl)picolinaldehyde in $CDCl_3$ at 300 MHz.

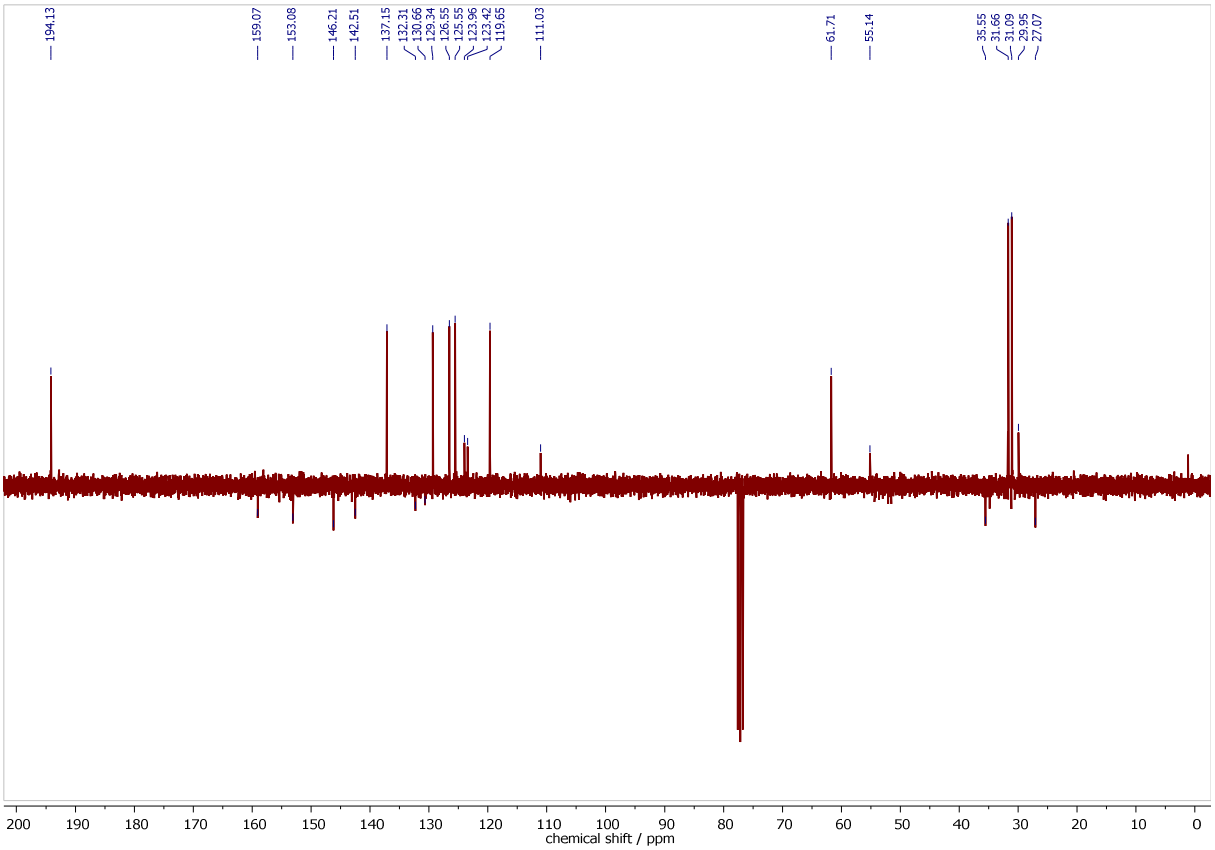

Fig. X20. ^{13}C DEPTQ NMR spectrum of 6-(3,5-di-tert-butyl-2-methoxyphenyl)picolinaldehyde in $CDCl_3$ at 75 MHz.

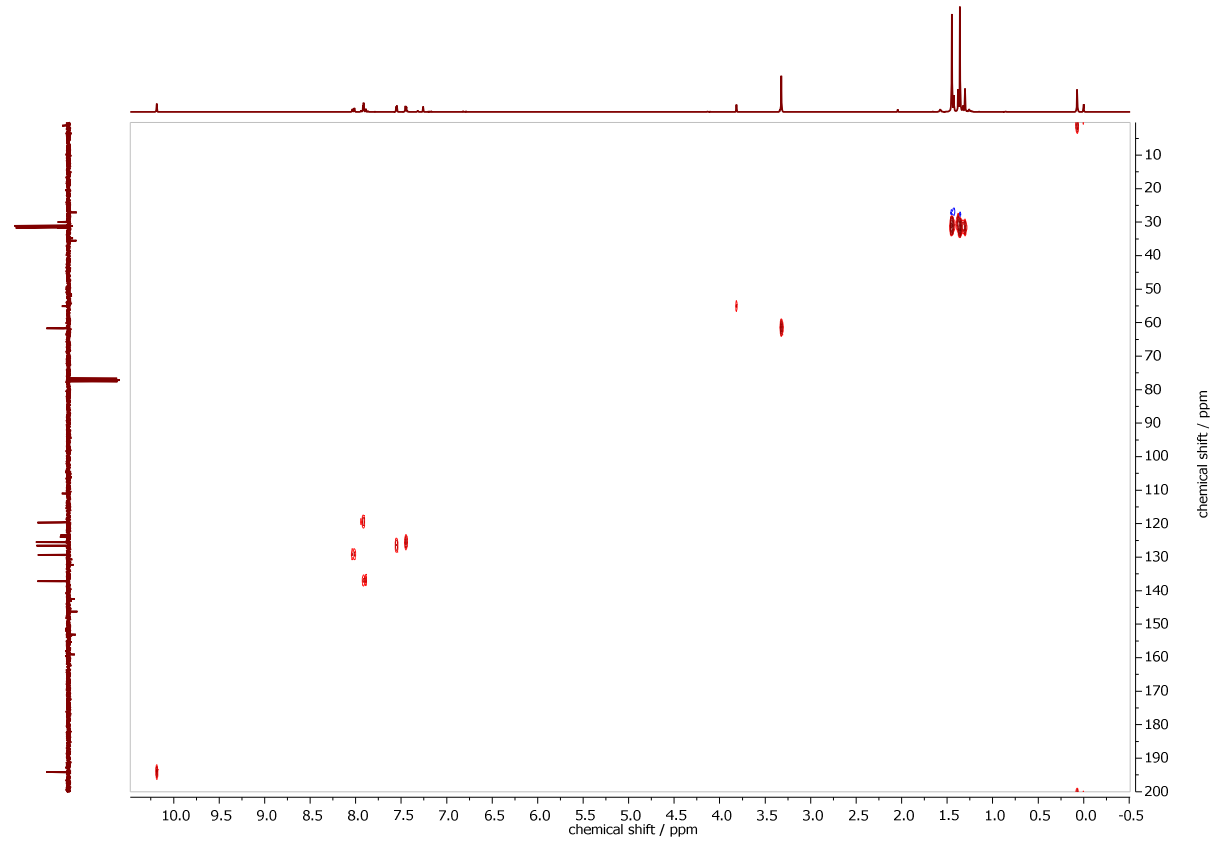

Fig. X21. $^{1}H,^{13}C$ HSQCed NMR spectrum of 6-(3,5-di-tert-butyl-2-methoxyphenyl)picolinaldehyde in $CDCl_3$.

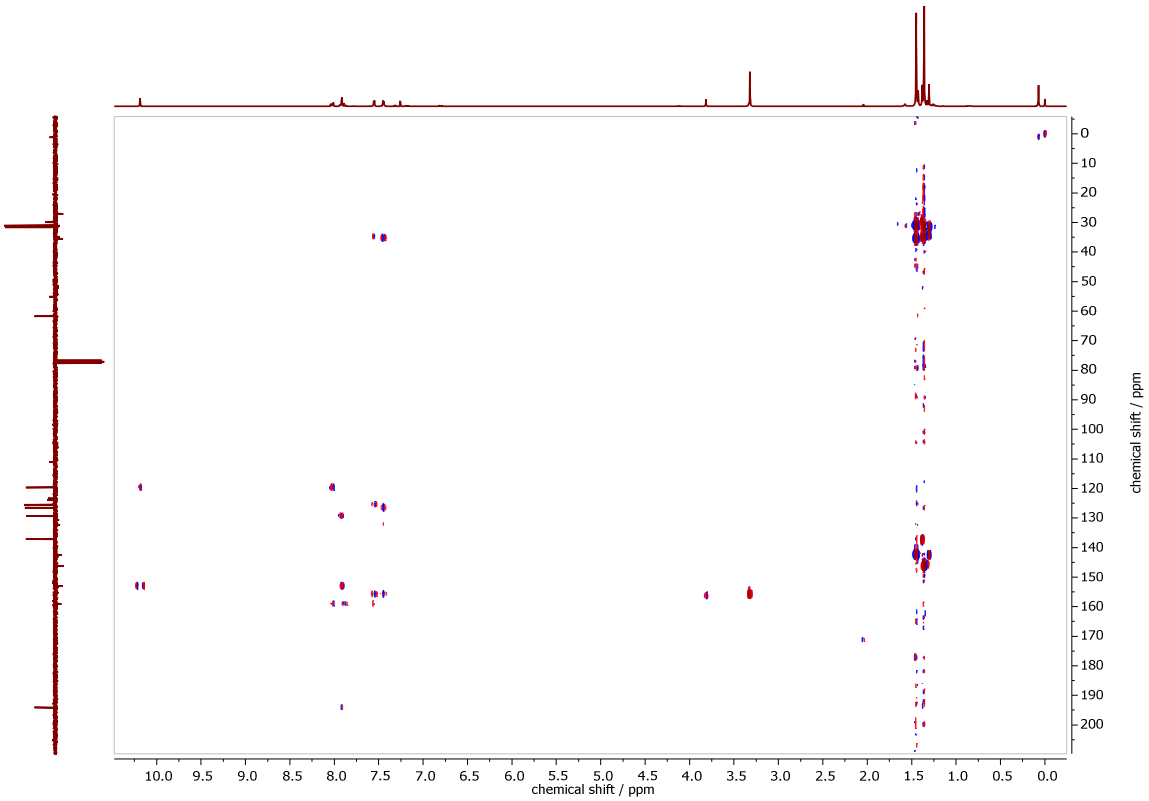

Fig. X22. $^{1}H,^{13}C$ HMBC NMR spectrum of 6-(3,5-di-tert-butyl-2-methoxyphenyl)picolinaldehyde in $CDCl_3$.

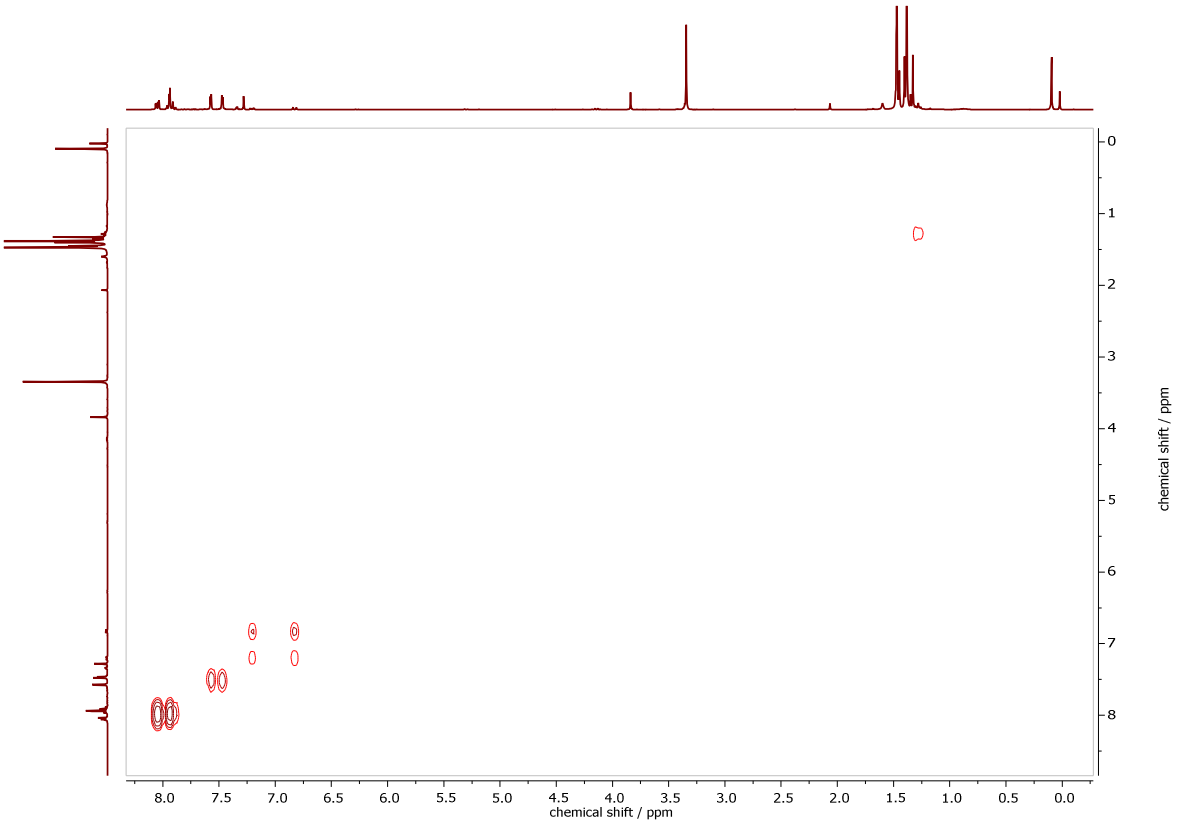

Fig. X23. $^{1}H,^{1}H$ COSY NMR spectrum of 6-(3,5-di-tert-butyl-2-methoxyphenyl)picolinaldehyde in $CDCl_3$.

NMR Spectra of Protoligands

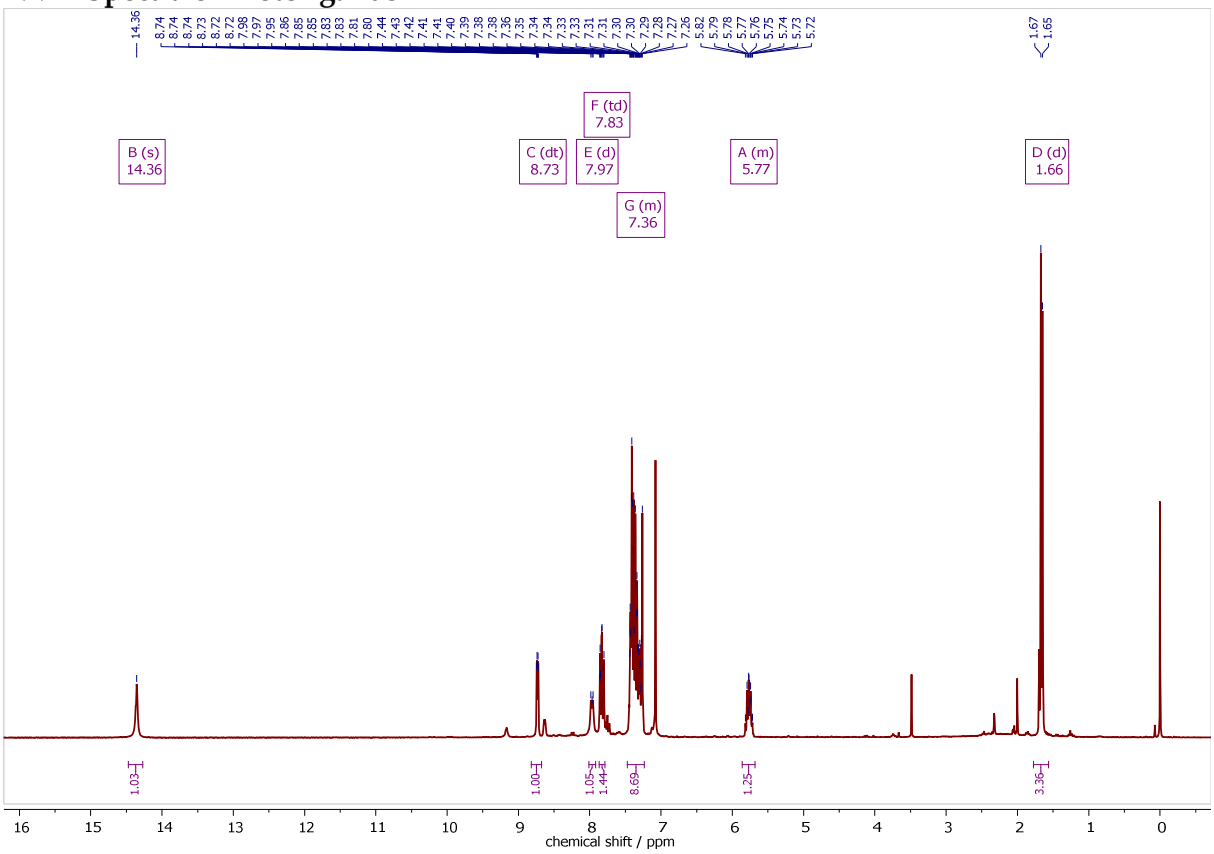

Fig. X24. ^{1}H NMR spectrum of HfpyTSCmB in $CDCl_3$ at 300 MHz.

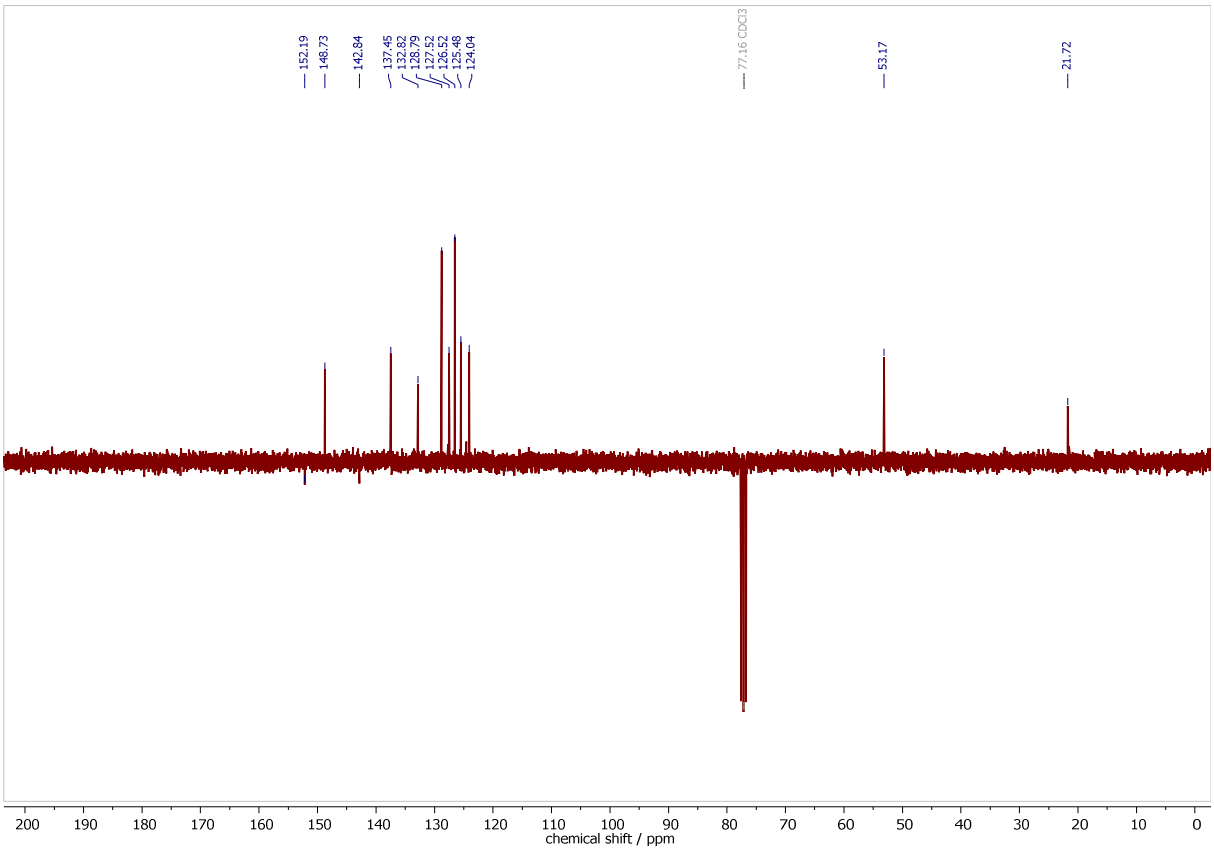

Fig. X25. ^{13}C DEPTQ NMR spectrum of HfpyTSCmB in $CDCl_3$ at 75 MHz.

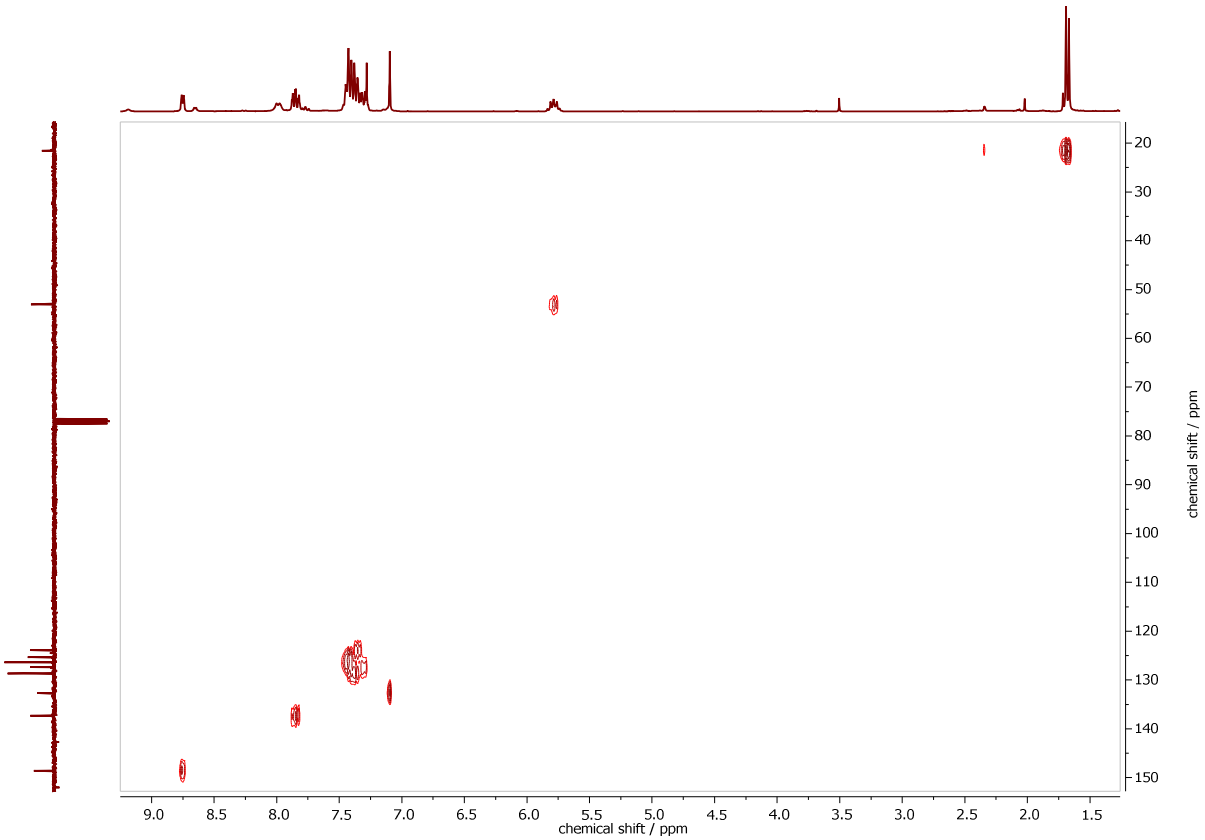

Fig. X26. $^{1}H,^{13}C$ HSQCed NMR spectrum of HfpyTSCmB in $CDCl_3$.

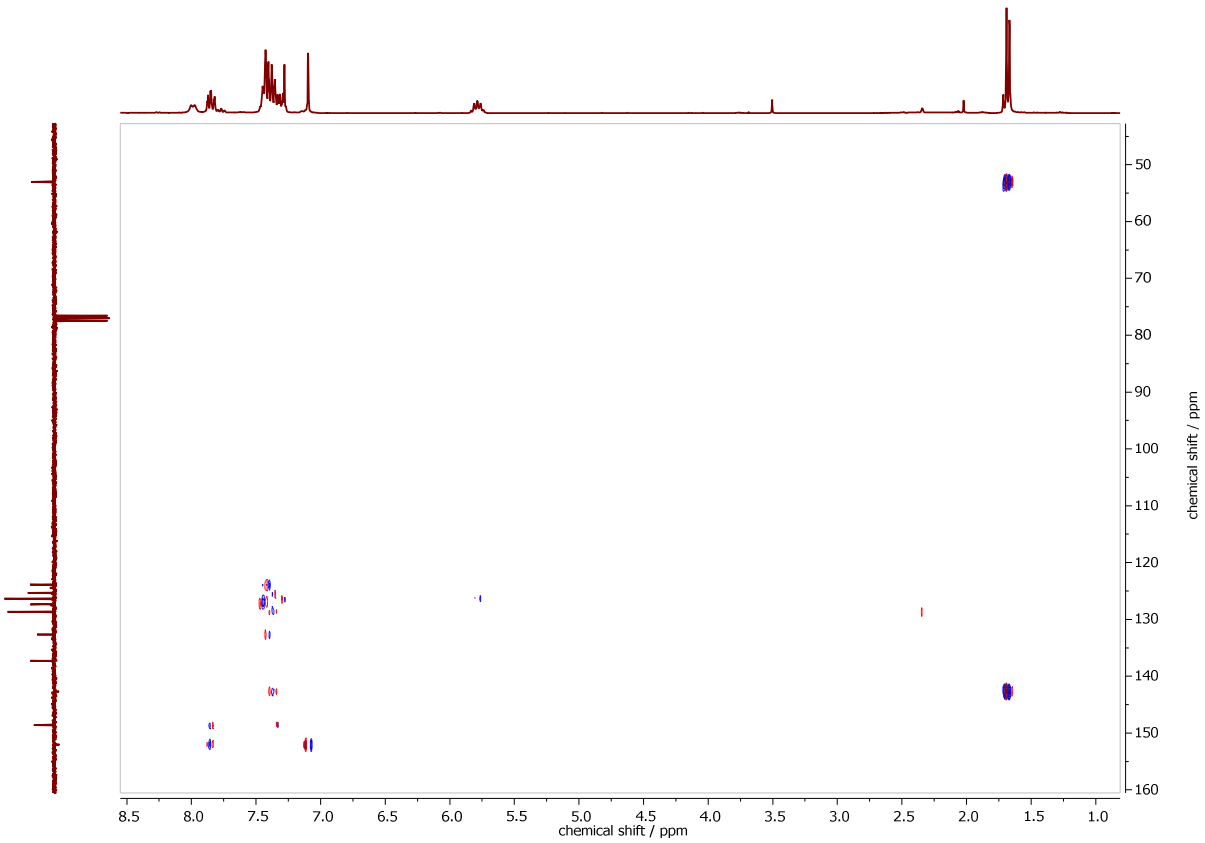

Fig. X27. $^{1}H,^{13}C$ HMBC NMR spectrum of HfpyTSCmB in $CDCl_3$.

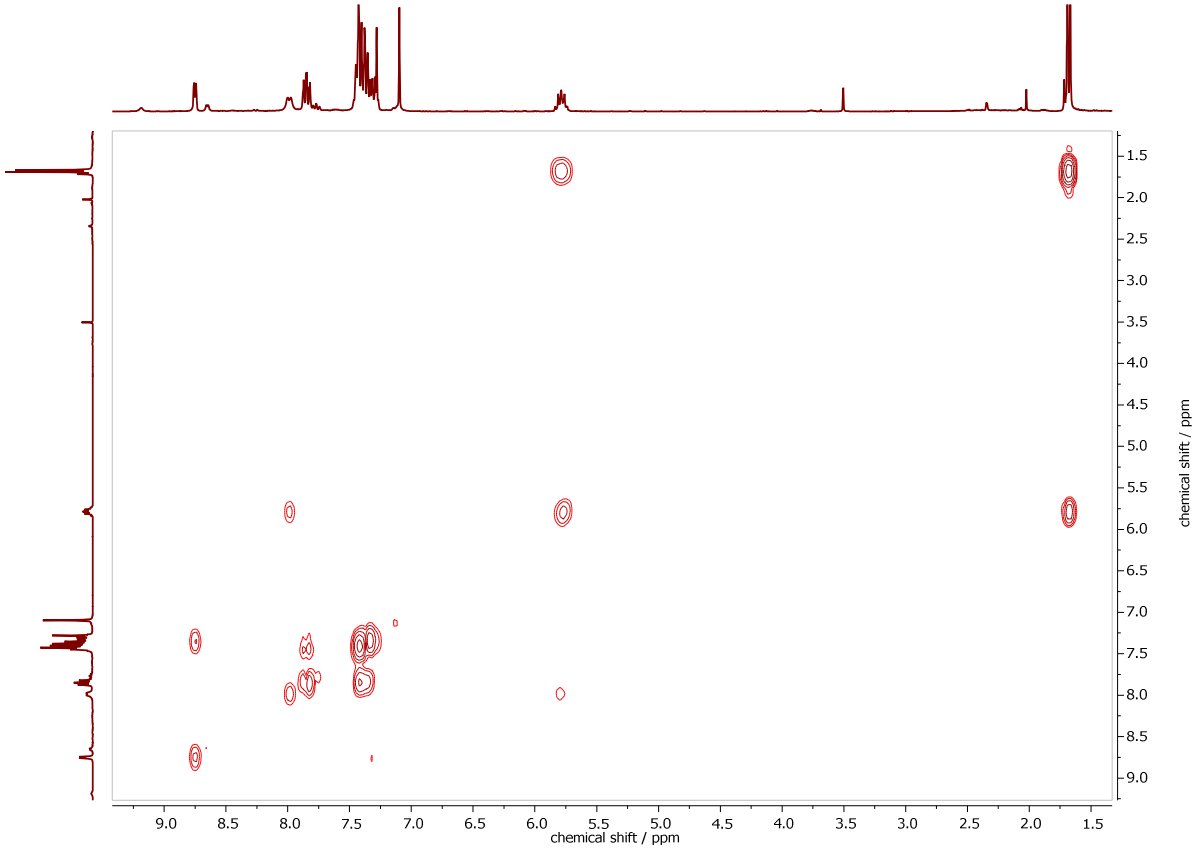

Fig. X28. $^{1}H,^{1}H$ COSY NMR spectrum of HfpyTSCmB in $CDCl_3$.

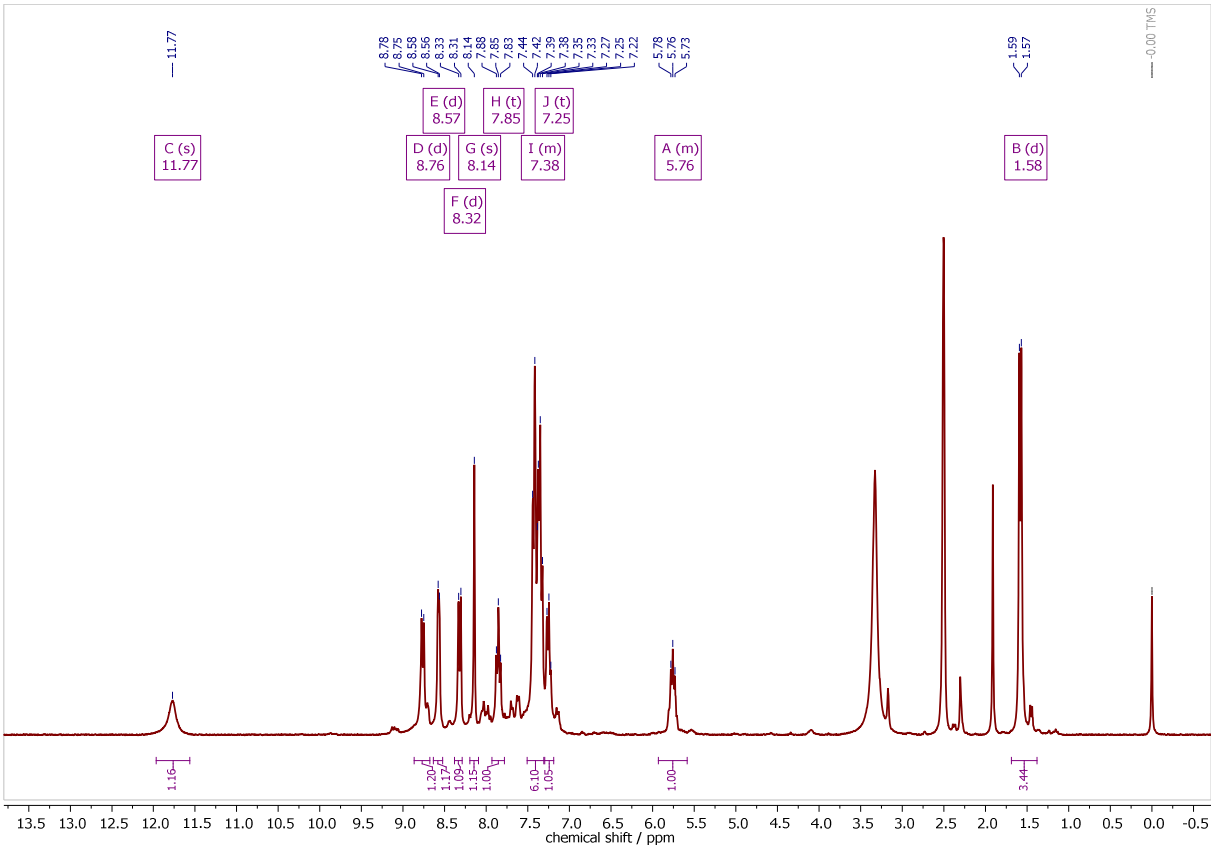

Fig. X29. ^{1}H NMR spectrum of HfpyTSCmB in DMSO-d_6 at 300 MHz.

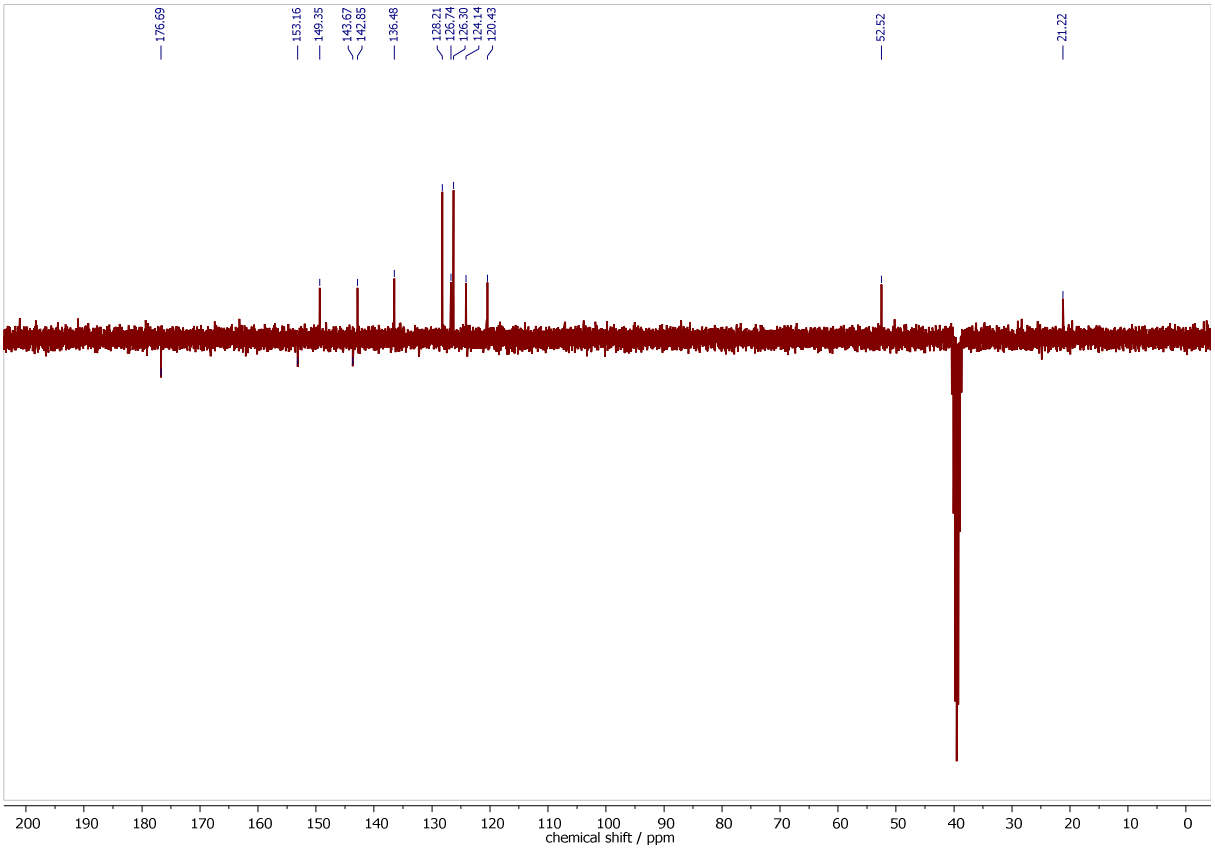

Fig. X30. ^{13}C DEPTQ NMR spectrum of HfpyTSCmB in DMSO-d_6 at 75 MHz.

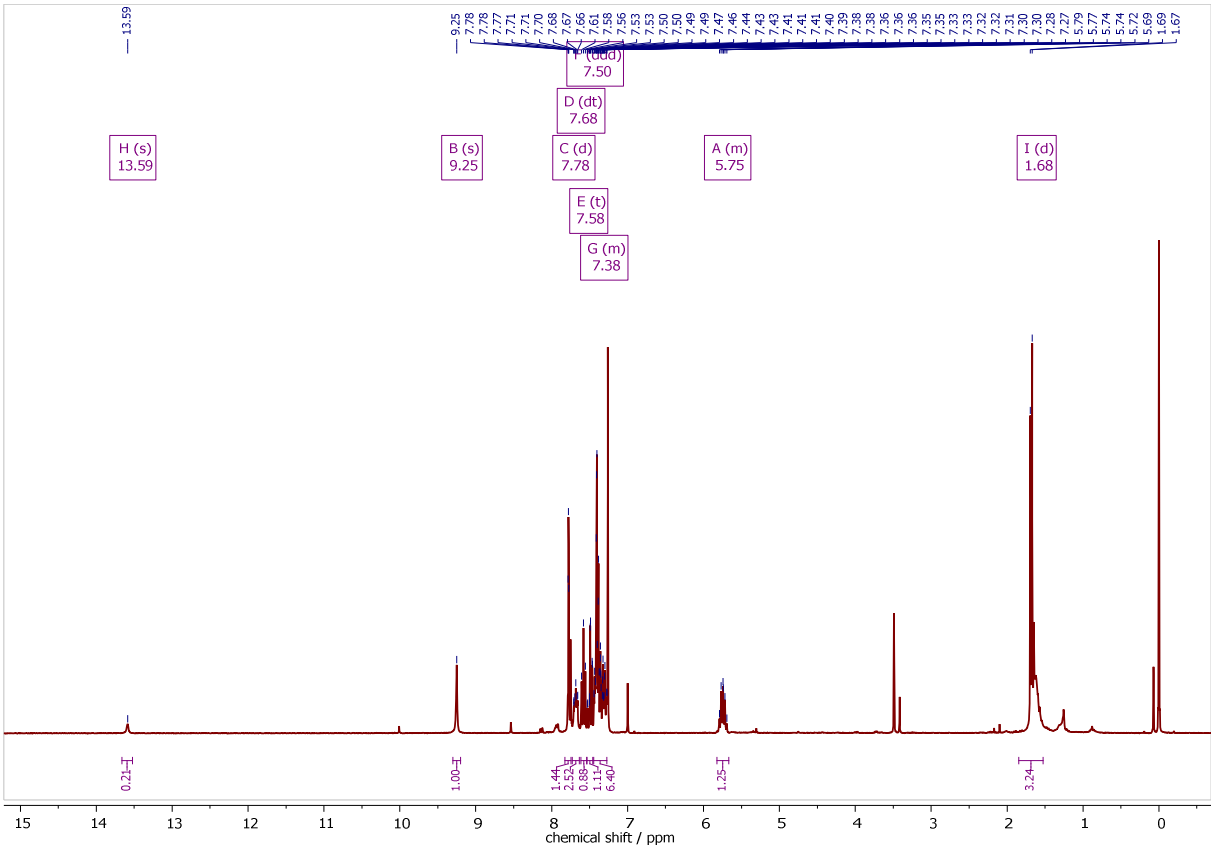

Fig. X31. ^{1}H NMR spectrum of H6-BrfpyTSCmB in $CDCl_3$ at 300 MHz.

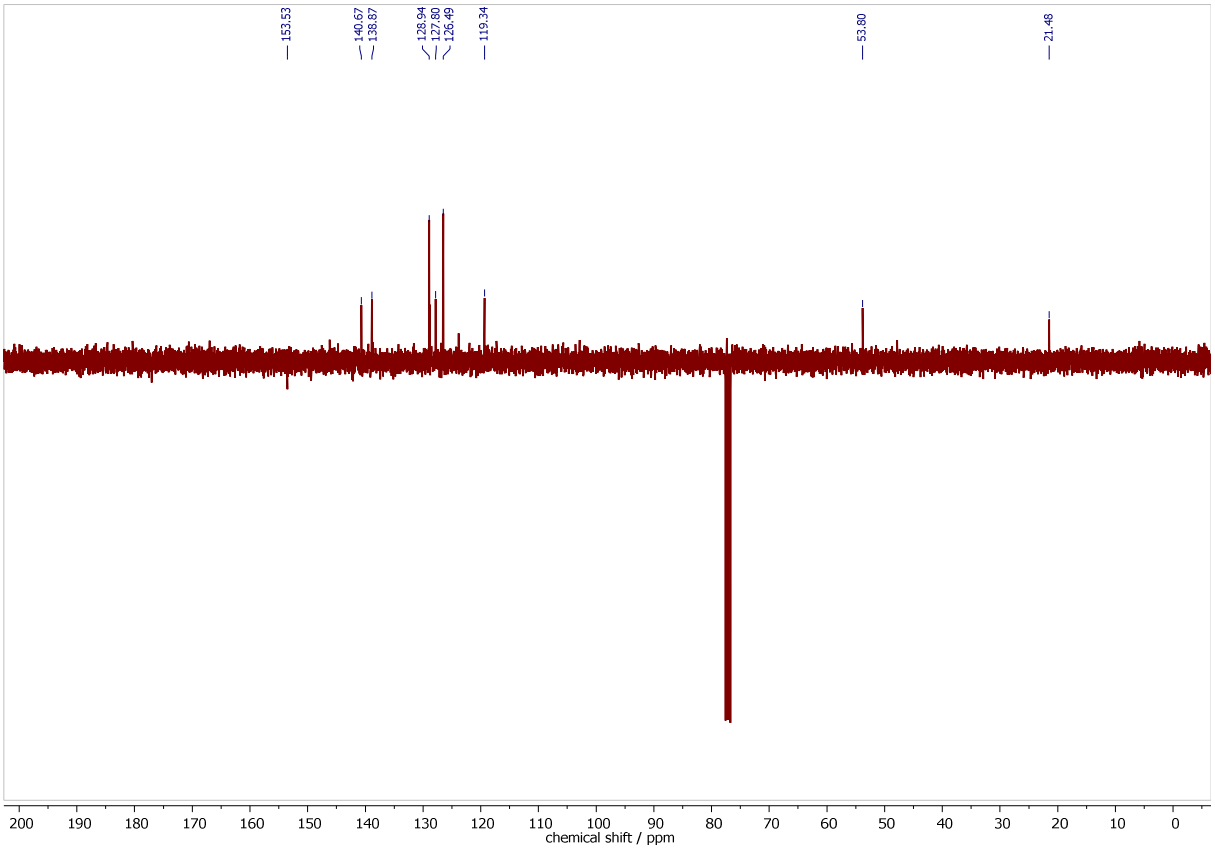

Fig. X32. ^{13}C DEPTQ NMR spectrum of H6-BrfpyTSCmB in $CDCl_3$ at 75 MHz.

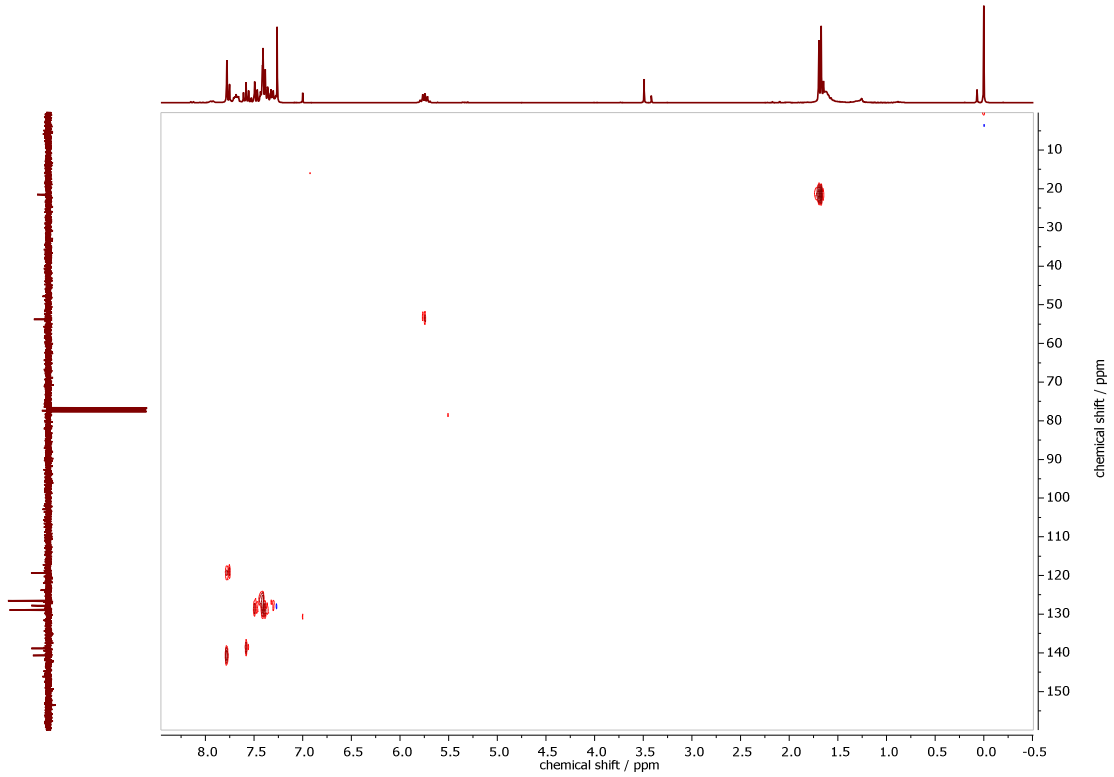

Fig. X33. $^{1}H,^{13}C$ HSQCed NMR spectrum of H6-BrfpyTSCmB in $CDCl_3$.

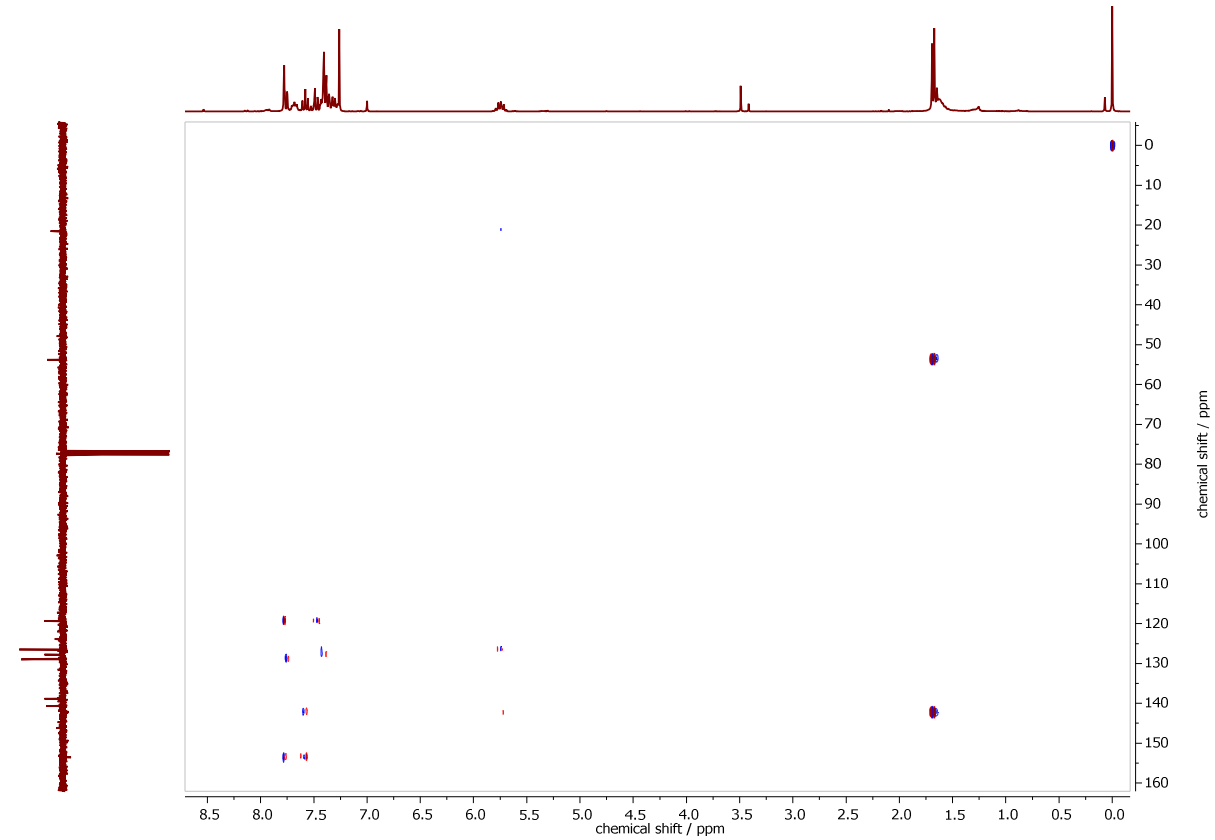

Fig. X34. $^{1}H,^{13}C$ HMBC NMR spectrum of H6-BrfpyTSCmB in $CDCl_3$.

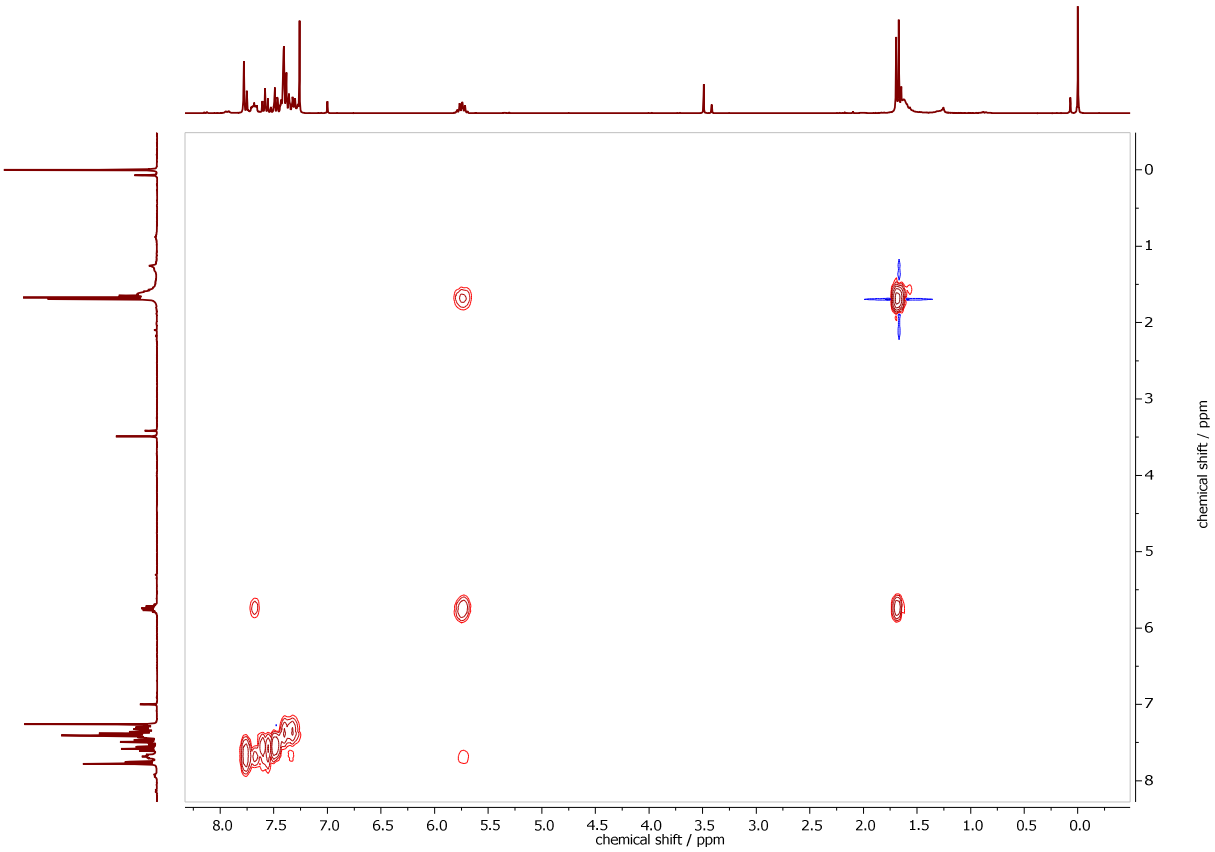

Fig. X35. $^{1}H,^{1}H$ COSY NMR spectrum of H6-BrfpyTSCmB in $CDCl_3$.

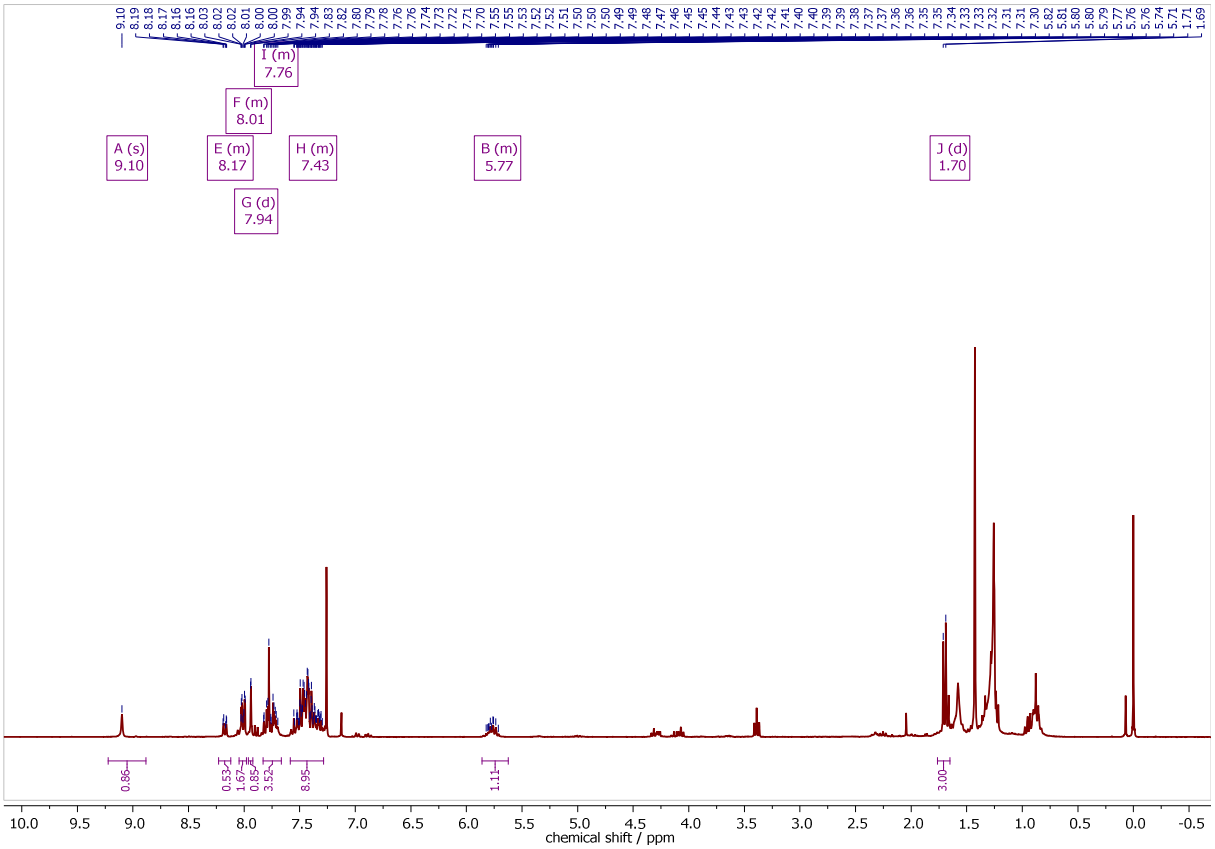

Fig. X36. ^{1}H NMR spectrum of H6-PhfpyTSCmB in $CDCl_3$ at 300 MHz.

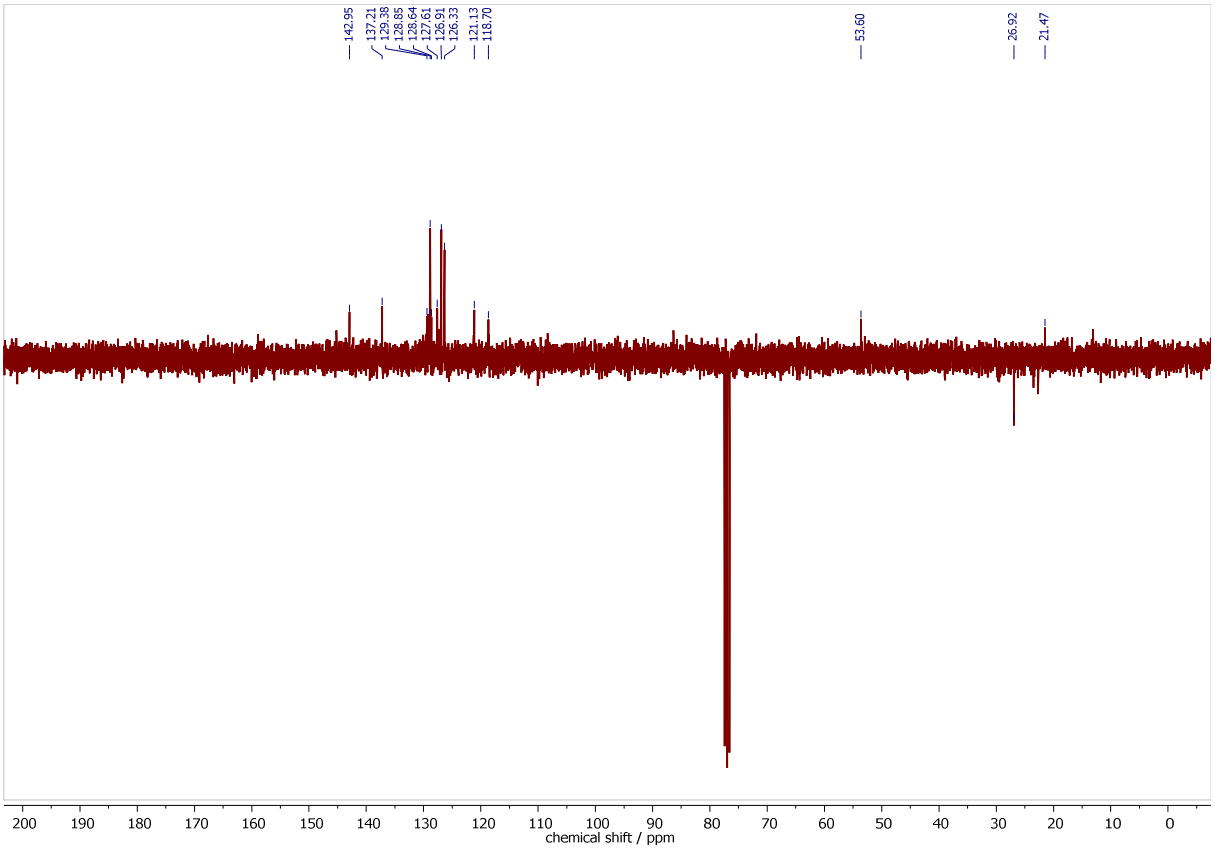

Fig. X37. ^{13}C DEPTQ NMR spectrum of H6-PhfpyTSCmB in $CDCl_3$ at 75 MHz

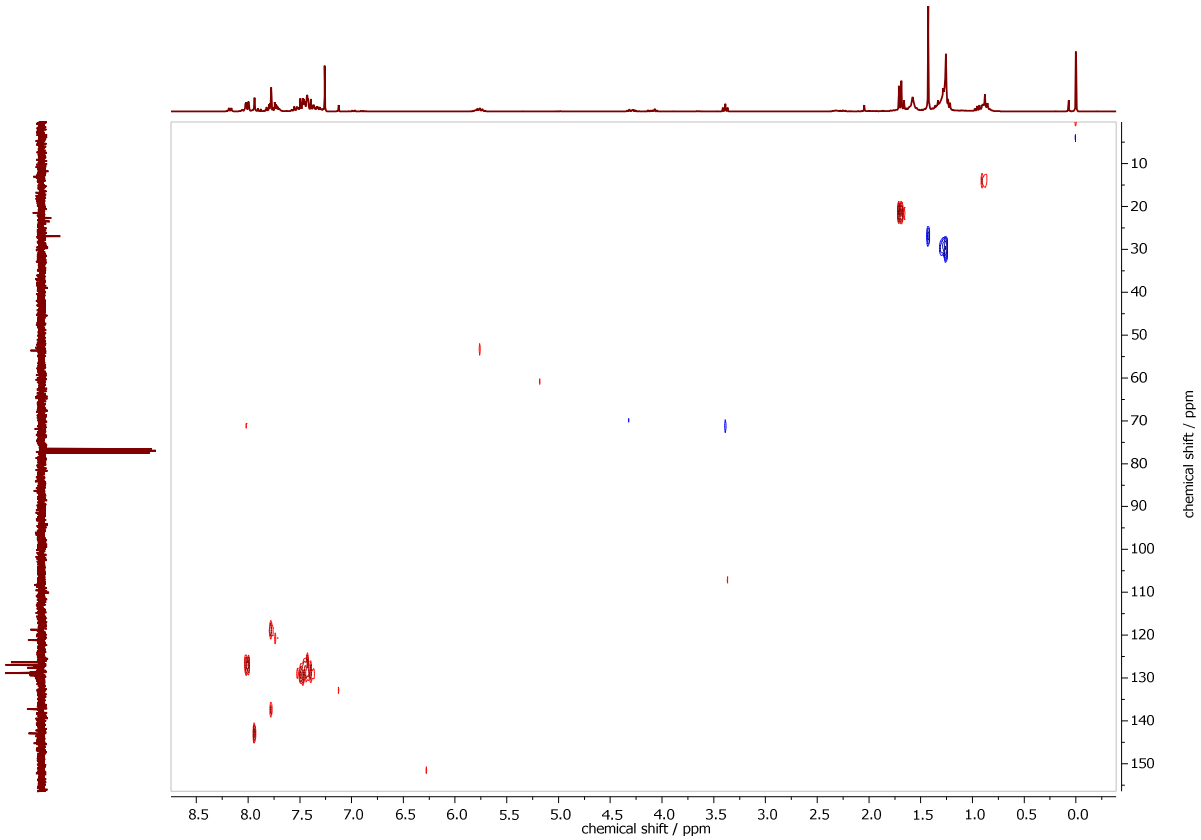

Fig. X38. $^{1}H,^{13}C$ HSQCed NMR spectrum of H6-PhfpyTSCmB in $CDCl_3$.

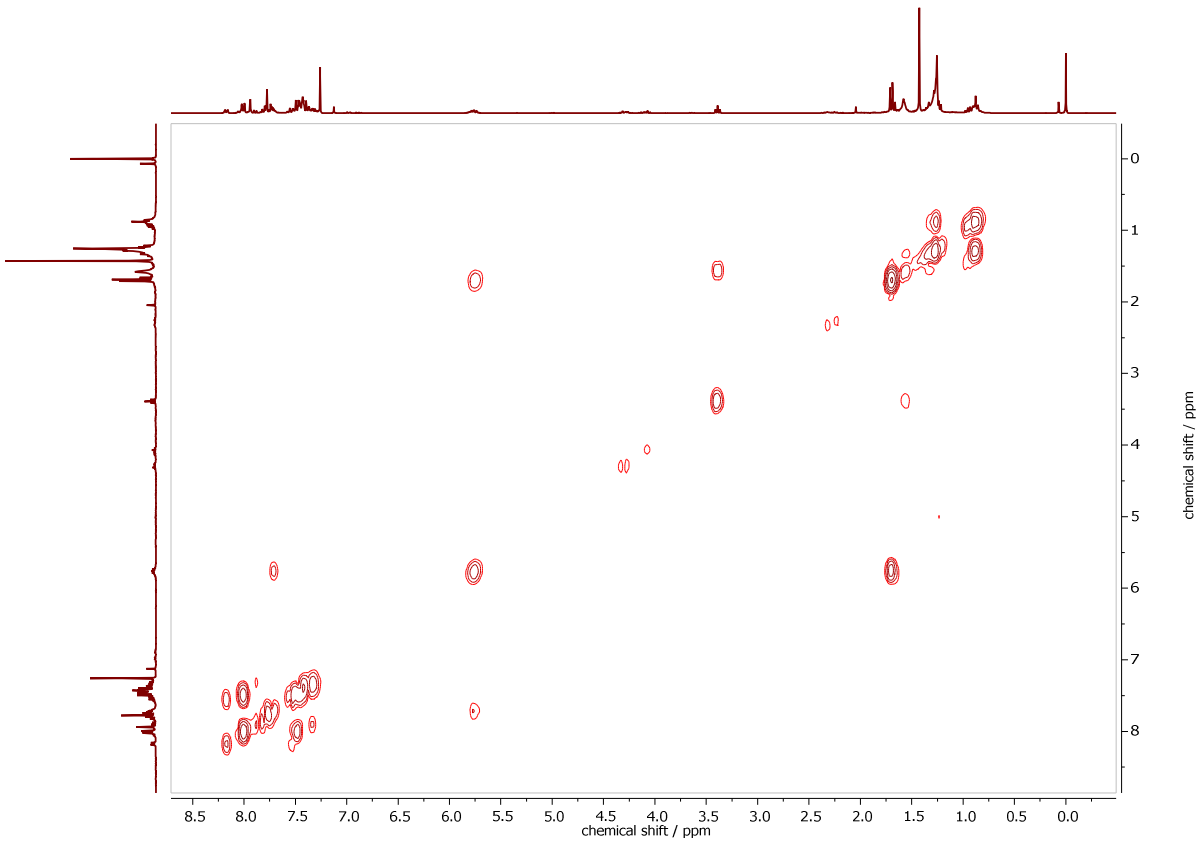

Fig. X39. $^{1}H,^{1}H$ COSY NMR spectrum of H6-PhfpyTSCmB in $CDCl_3$.

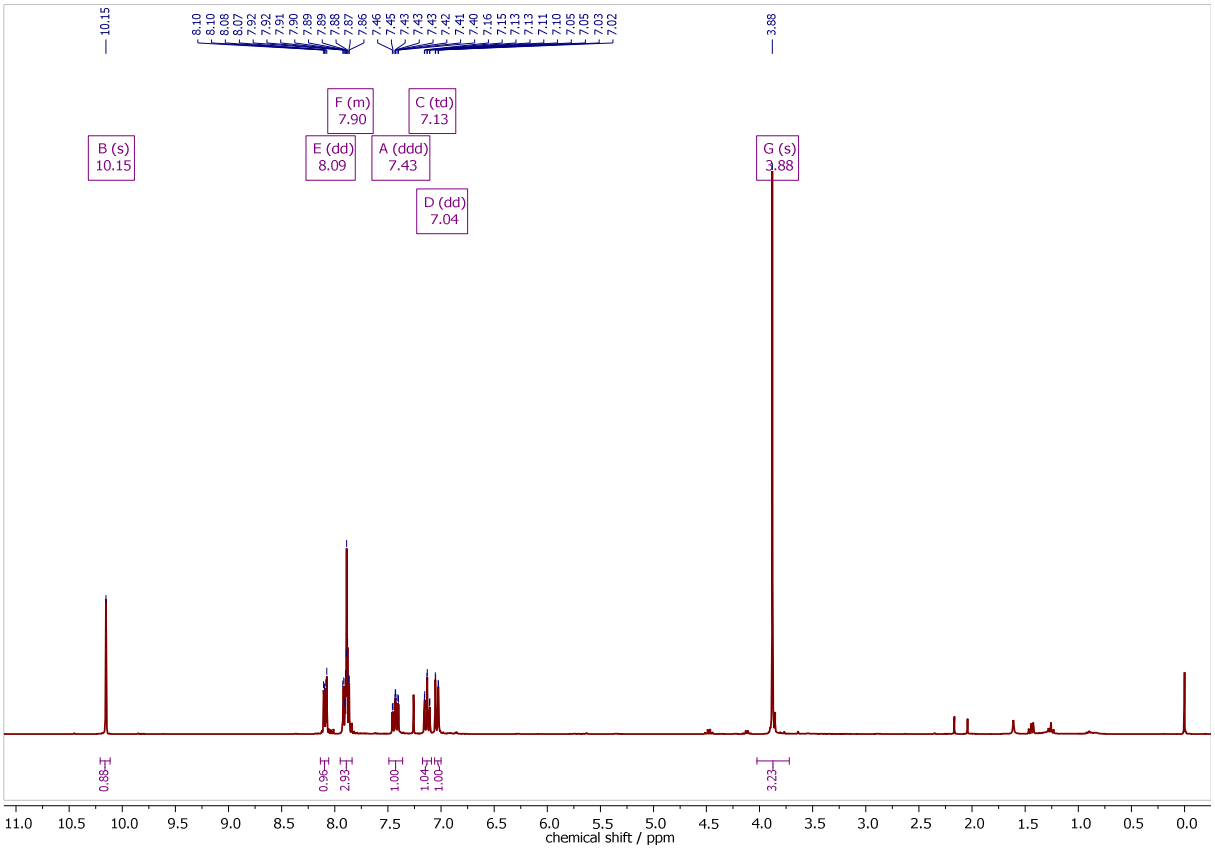

Fig. X40. ^{1}H NMR spectrum of 2-((6-(2-methoxyphenyl)pyridin-2-yl)TSCmB in $CDCl_3$ at 499 MHz.

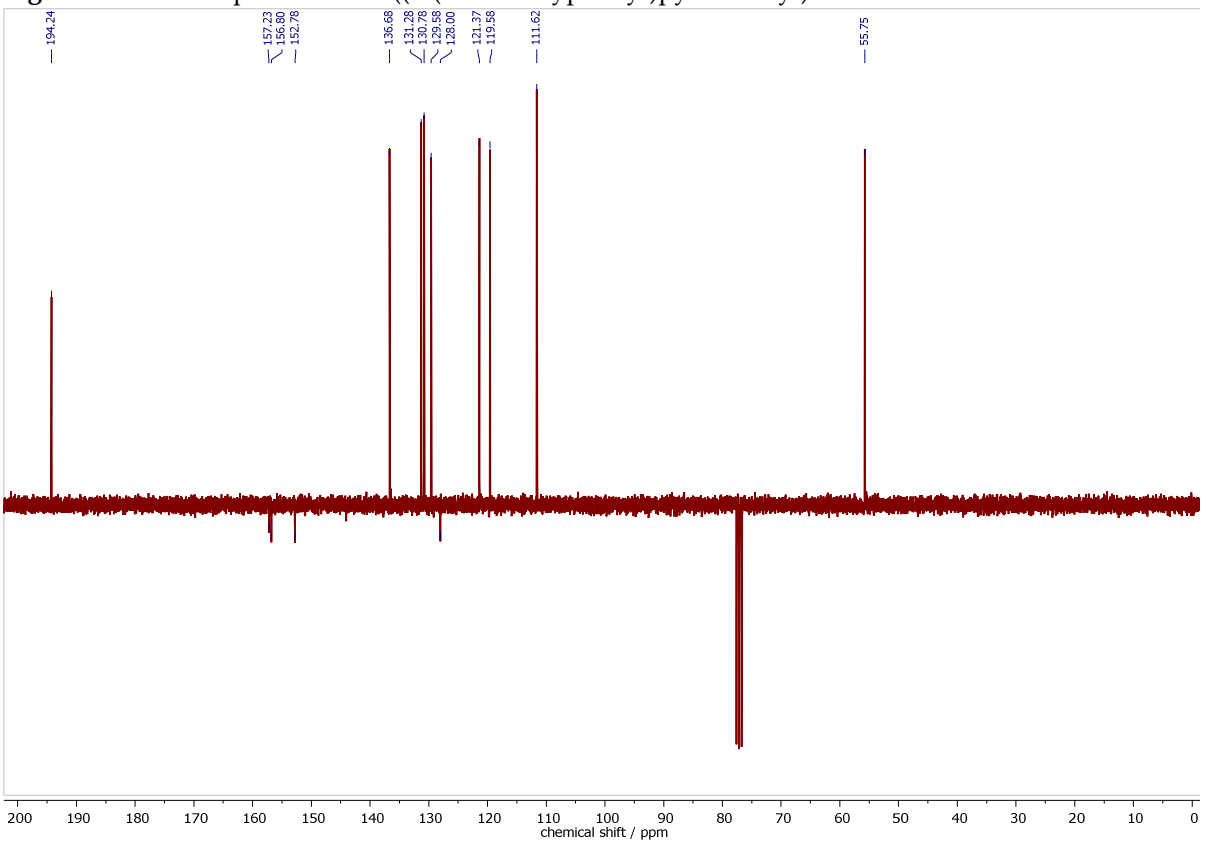

Fig. X41. ^{13}C DEPTQ NMR spectrum of 2-((6-(2-methoxyphenyl)pyridin-2-yl)TSCmB in $CDCl_3$ at 125 MHz

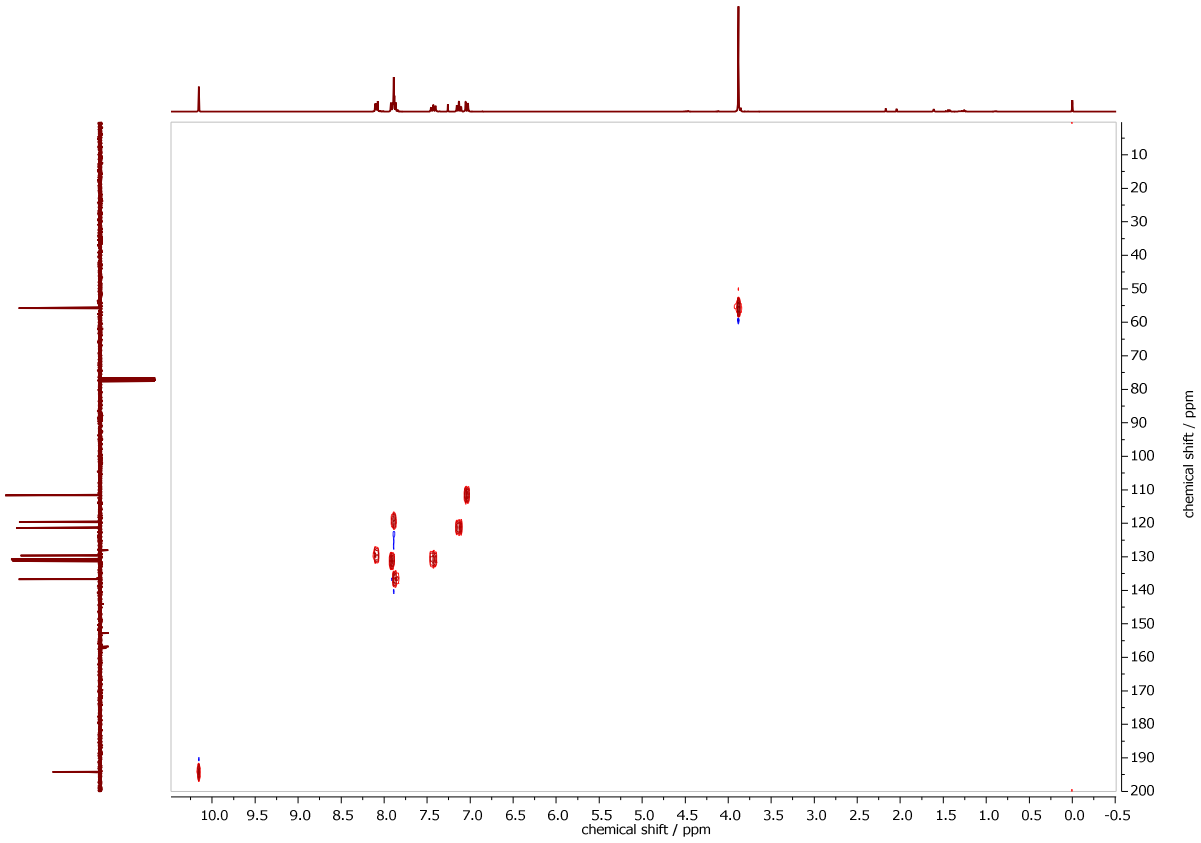

Fig. X42. $^{1}H,^{13}C$ HSQCed NMR spectrum of 2-((6-(2-methoxyphenyl)pyridin-2-yl)TSCmB in $CDCl_3$.

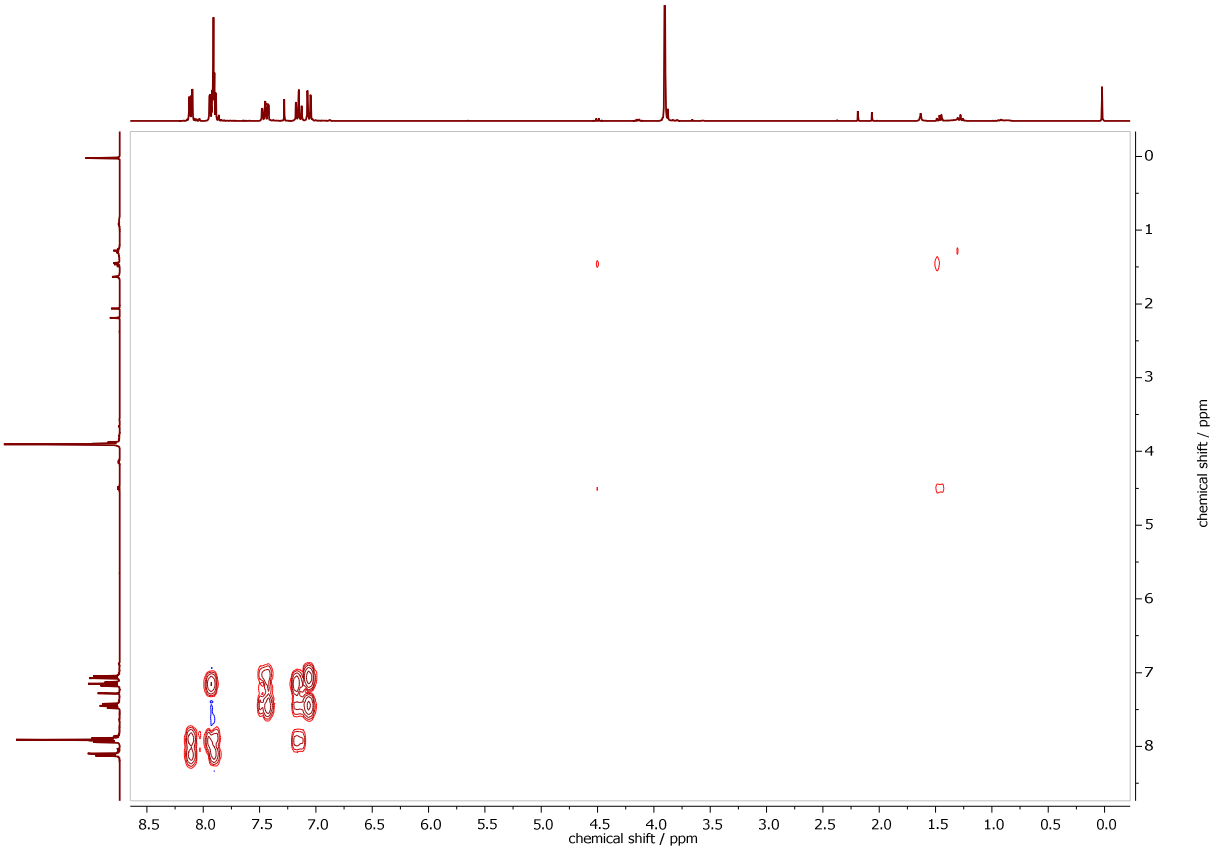

Fig. X43. $^{1}H,^{1}H$ COSY NMR spectrum of 2-((6-(2-methoxyphenyl)pyridin-2-yl)TSCmB in $CDCl_3$.

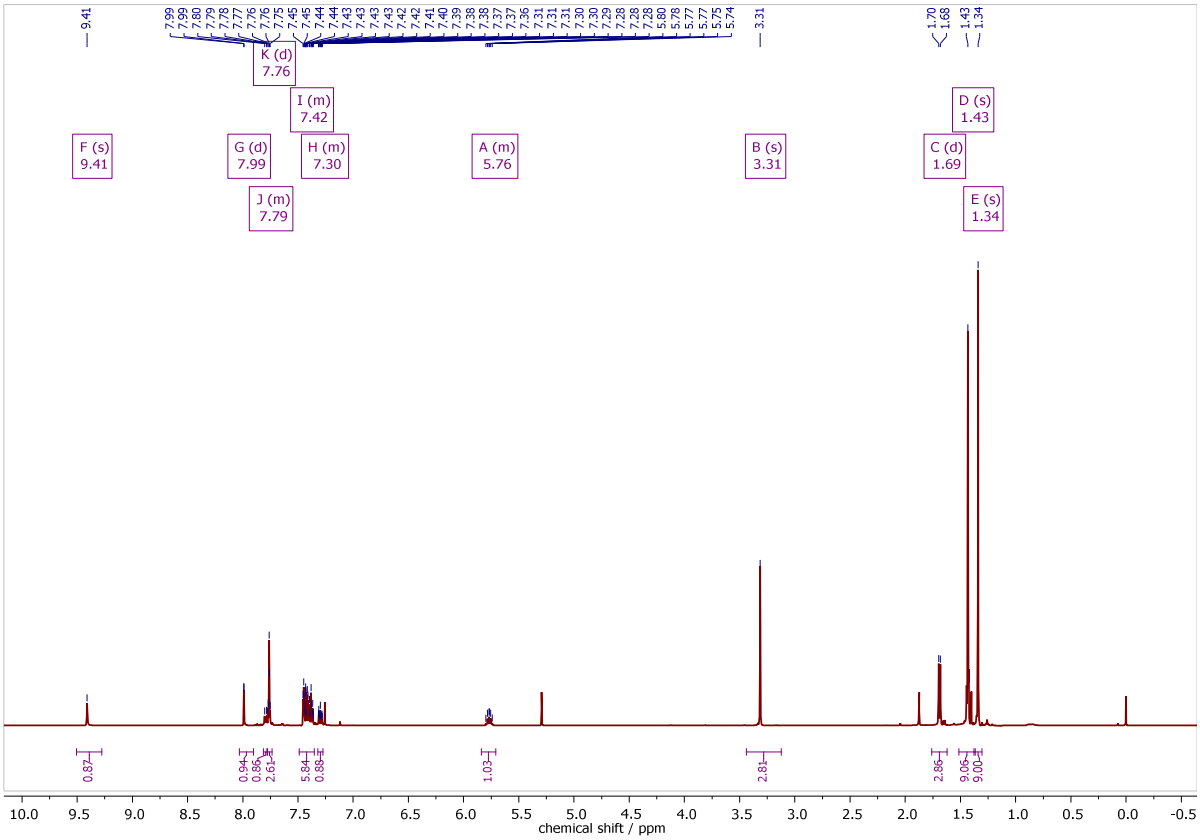

Fig. X44. ^{1}H NMR spectrum of 2-((6-(3,5-di-tert-butyl-2-methoxyphenyl)pyridin-2-yl)methylene) TSCmB in $CDCl_3$ at 499 MHz.

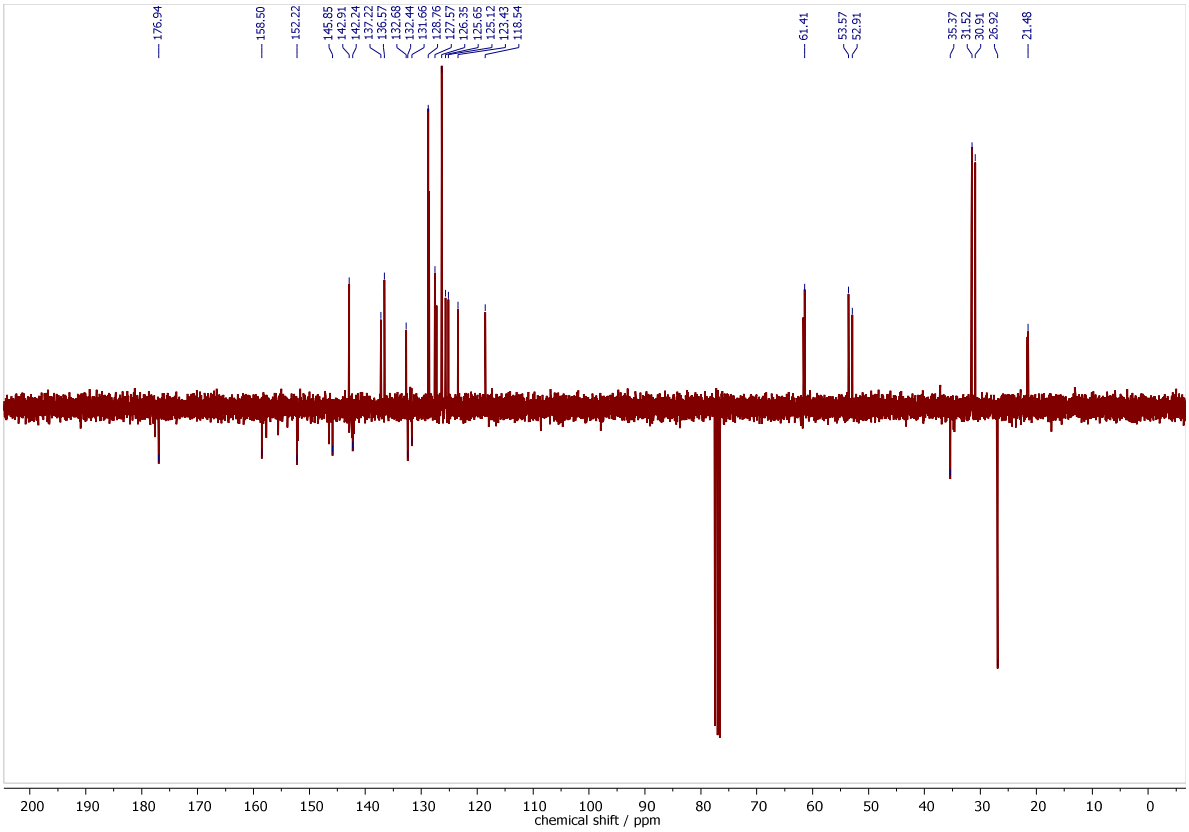

Fig. X45. ^{13}C DEPTQ NMR spectrum of 2-((6-(3,5-di-tert-butyl-2-methoxyphenyl)pyridin-2-yl)methylene) TSCmB in $CDCl_3$ at 499 MHz.

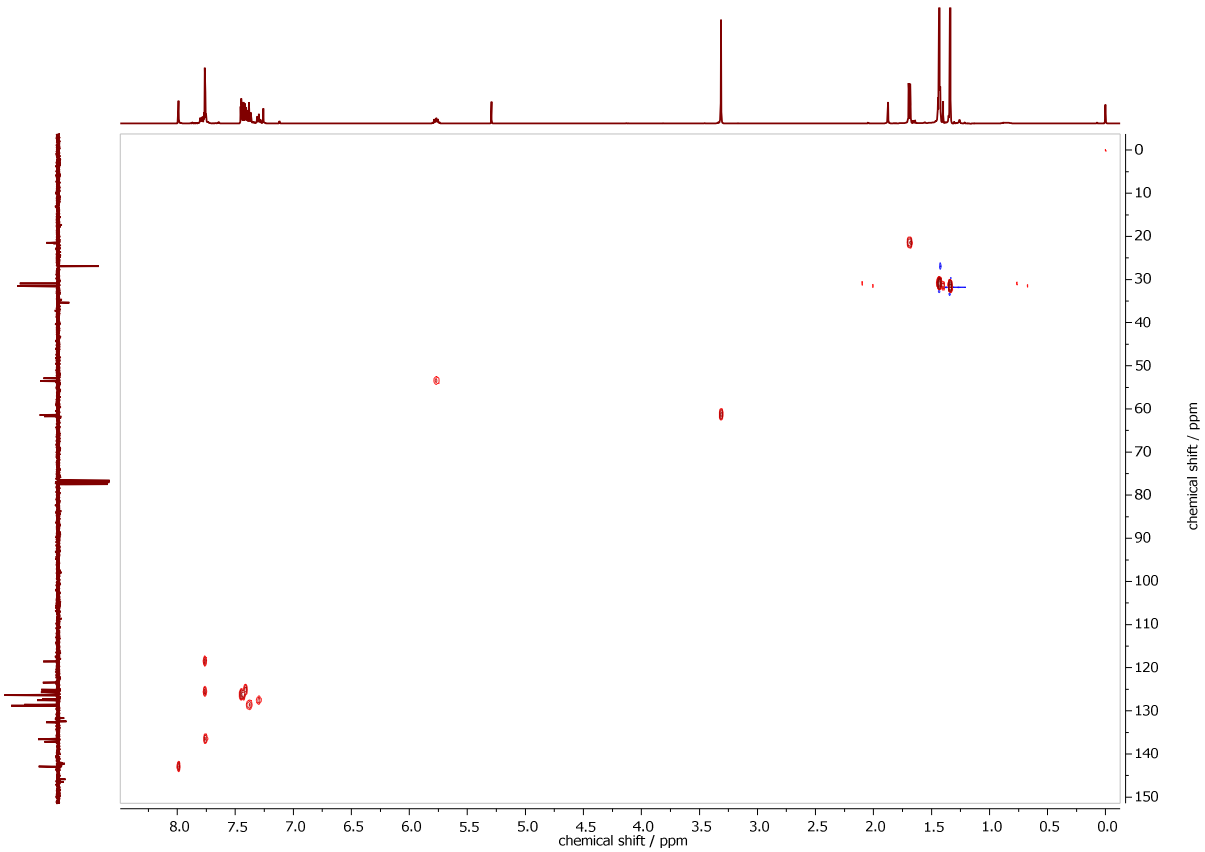

Fig. X46. ^{1}H, ^{13}C HSQCed NMR spectrum of 2-((6-(3,5-di-tert-butyl-2-methoxyphenyl)pyridin-2-yl)methylene) TSCmB in $CDCl_3$.

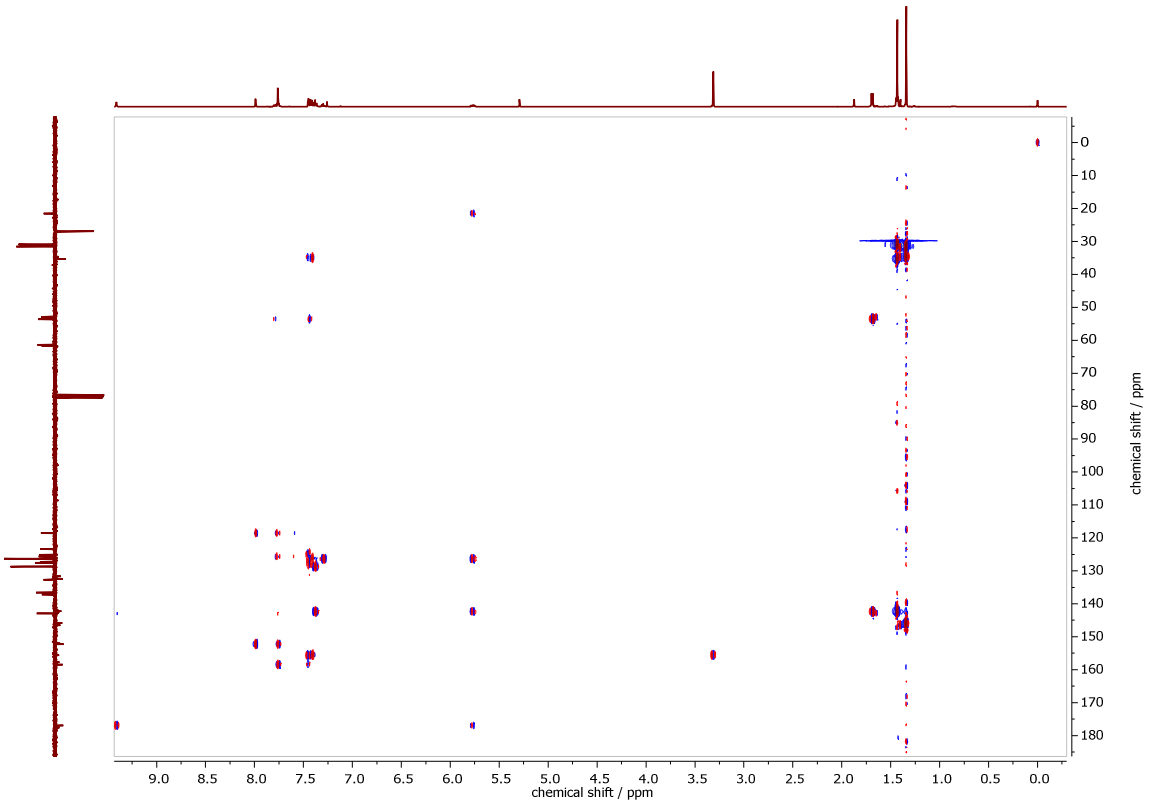

Fig. X47. ^{1}H, ^{13}C HMBC NMR spectrum of 2-((6-(3,5-di-tert-butyl-2-methoxyphenyl)pyridin-2-yl)methylene) TSCmB in $CDCl_3$.

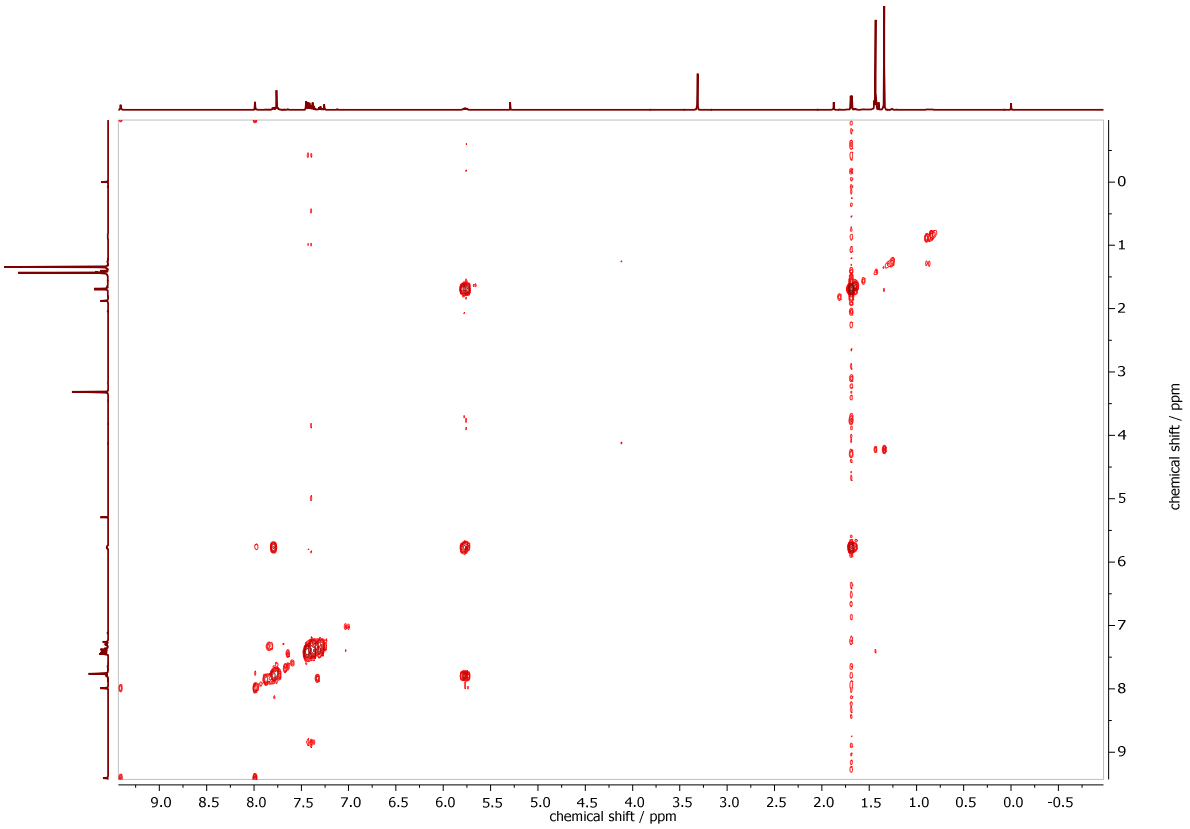

Fig. X48. ^{1}H, ^{1}H COSY NMR spectrum of 2-((6-(3,5-di-tert-butyl-2-methoxyphenyl)pyridin-2-yl)methylene) TSCmB in $CDCl_3$.

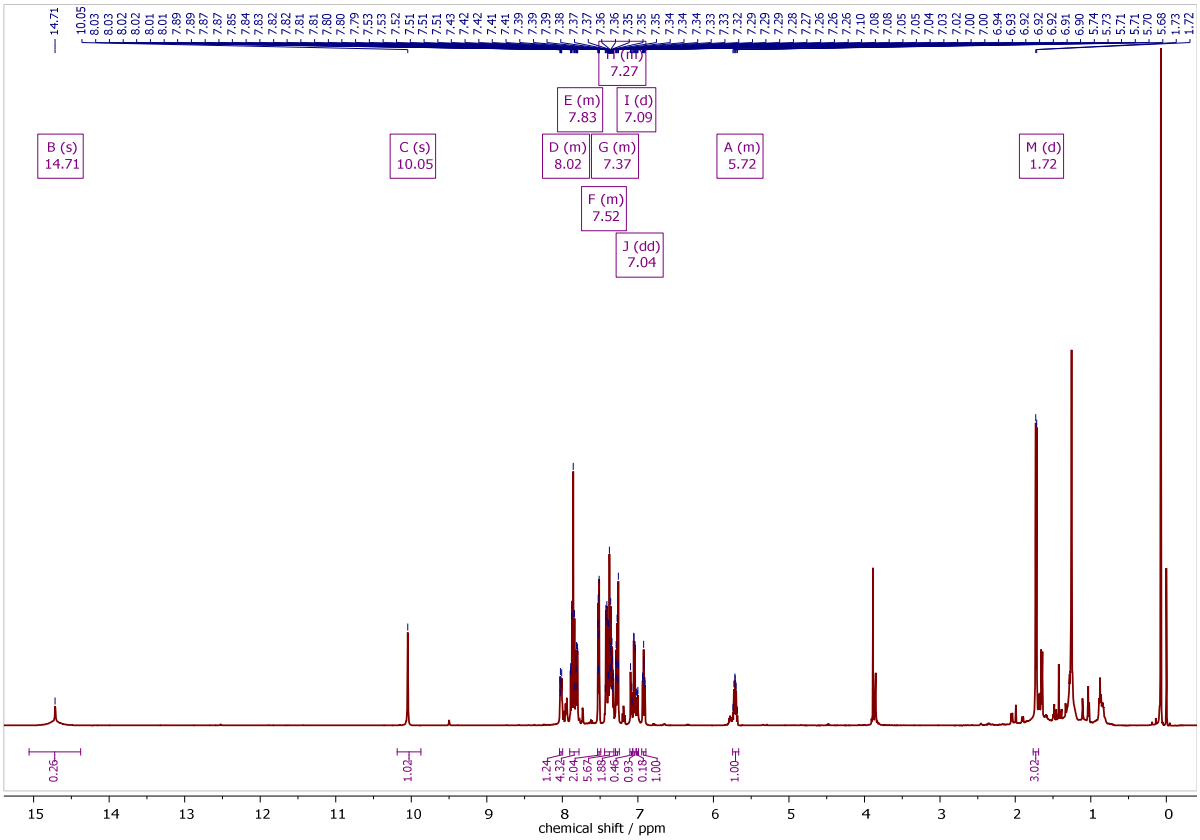

Fig. X49. ^{1}H NMR spectrum H_2L in $CDCl_3$ at 499 MHz.

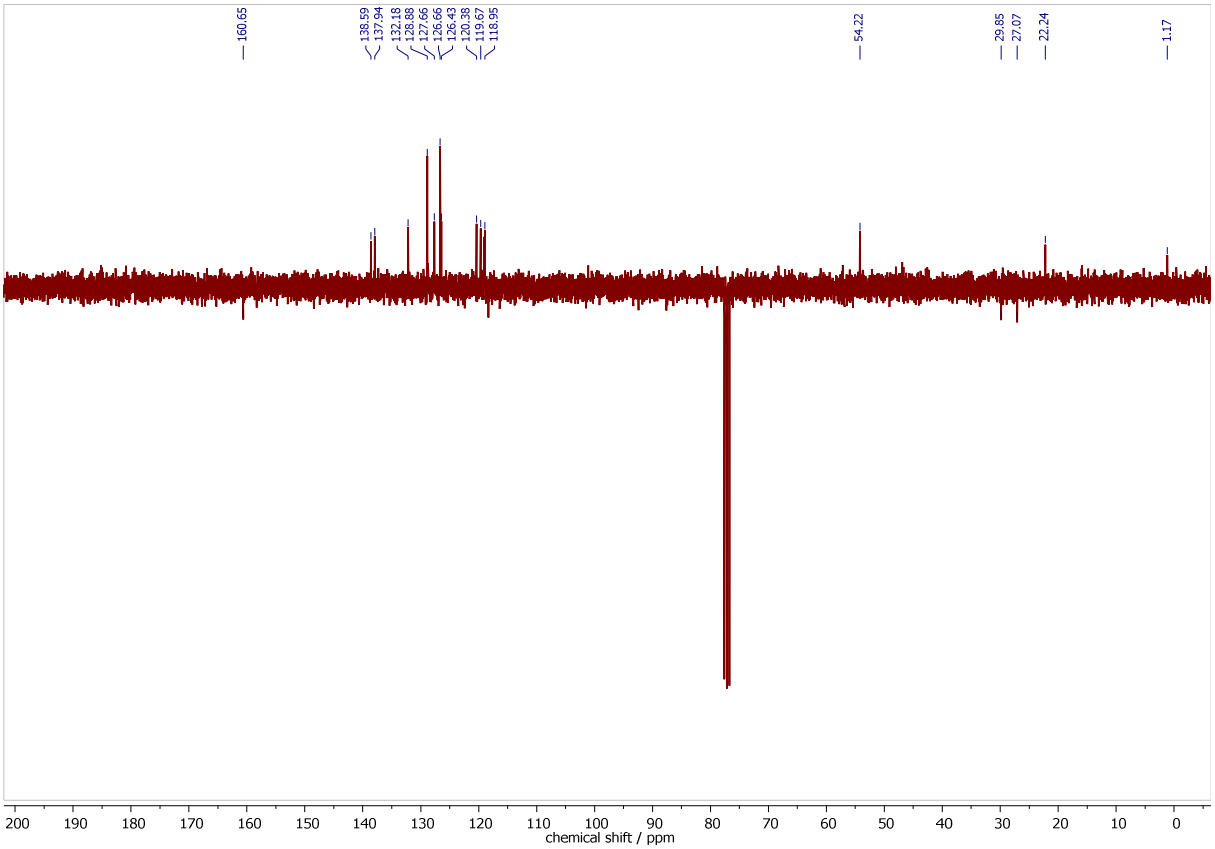

Fig. X50. ^{13}C DEPTQ NMR spectrum of H_2L in $CDCl_3$ at 499 MHz.

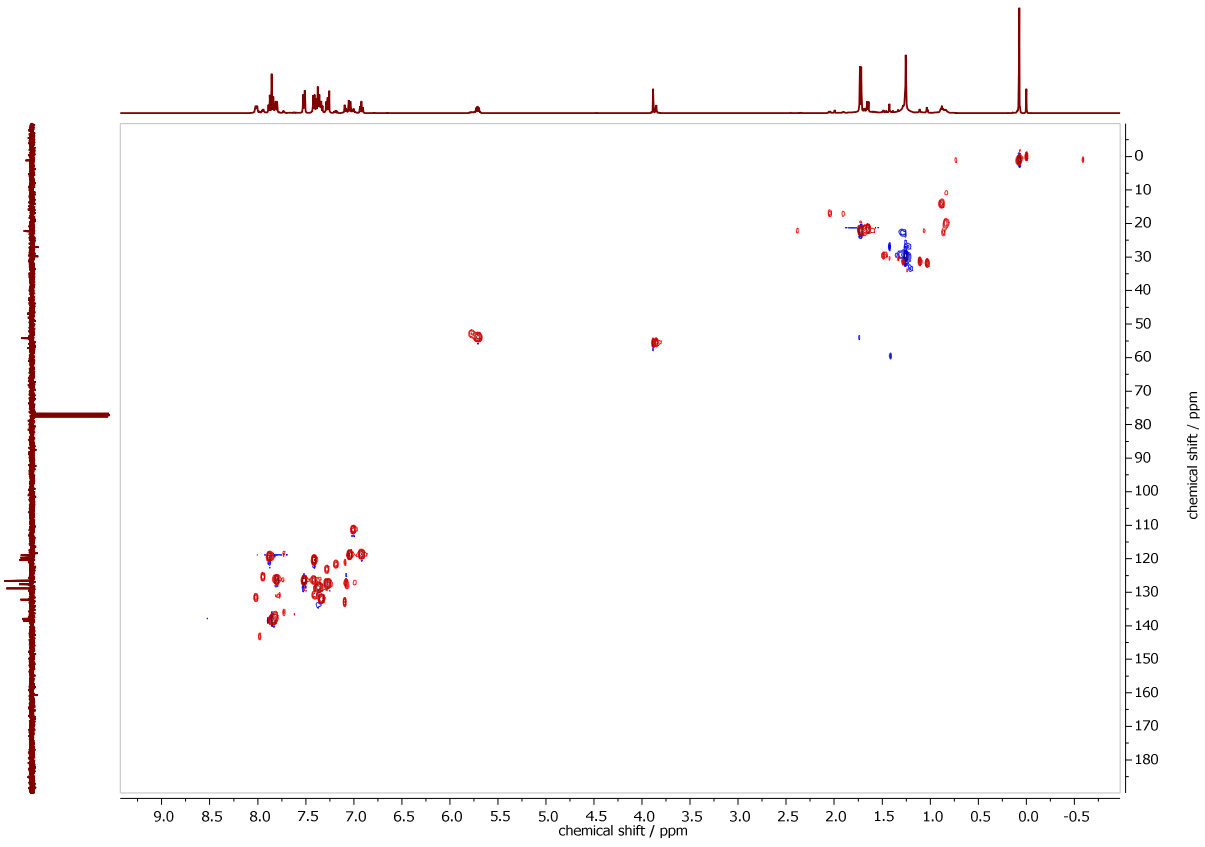

Fig. X51. ^{1}H, ^{13}C HSQCed NMR spectrum of H_2L in $CDCl_3$.

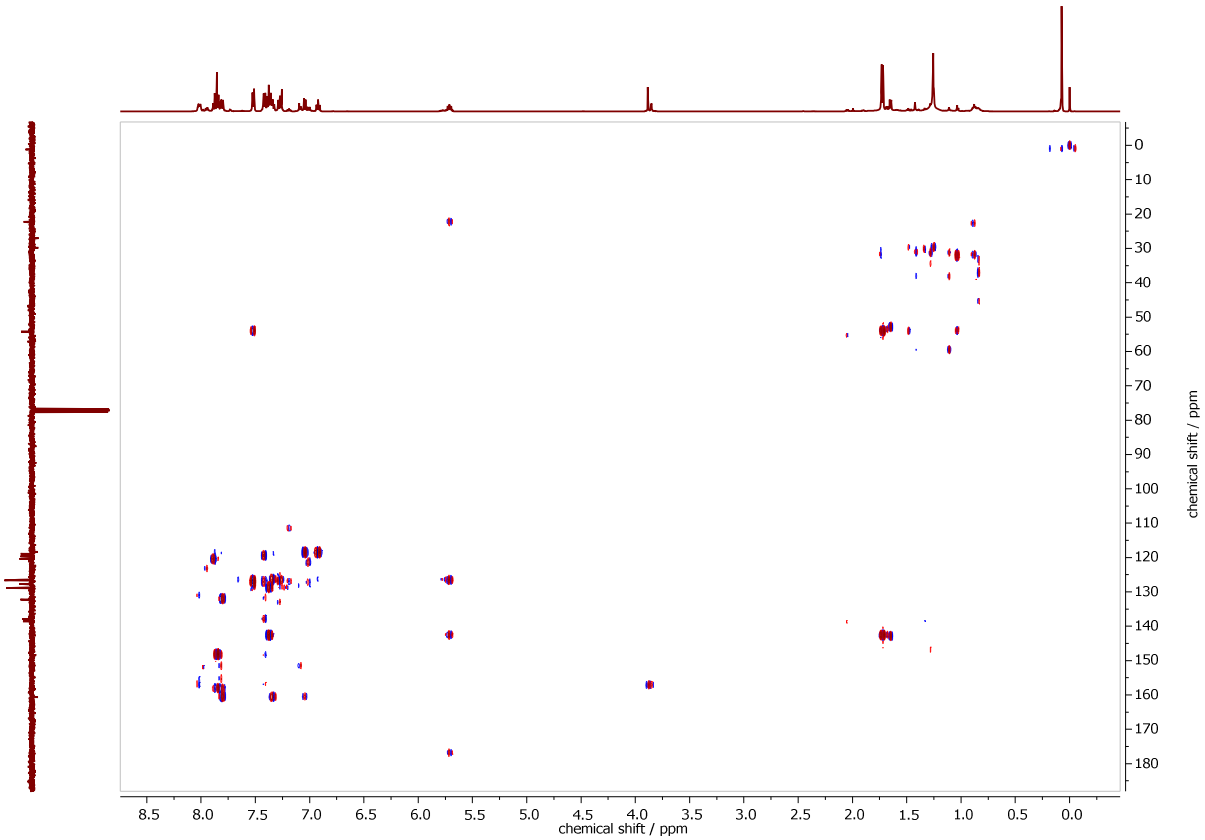

Fig. X52. ^{1}H, ^{13}C HMBC NMR spectrum of H_2L in $CDCl_3$.

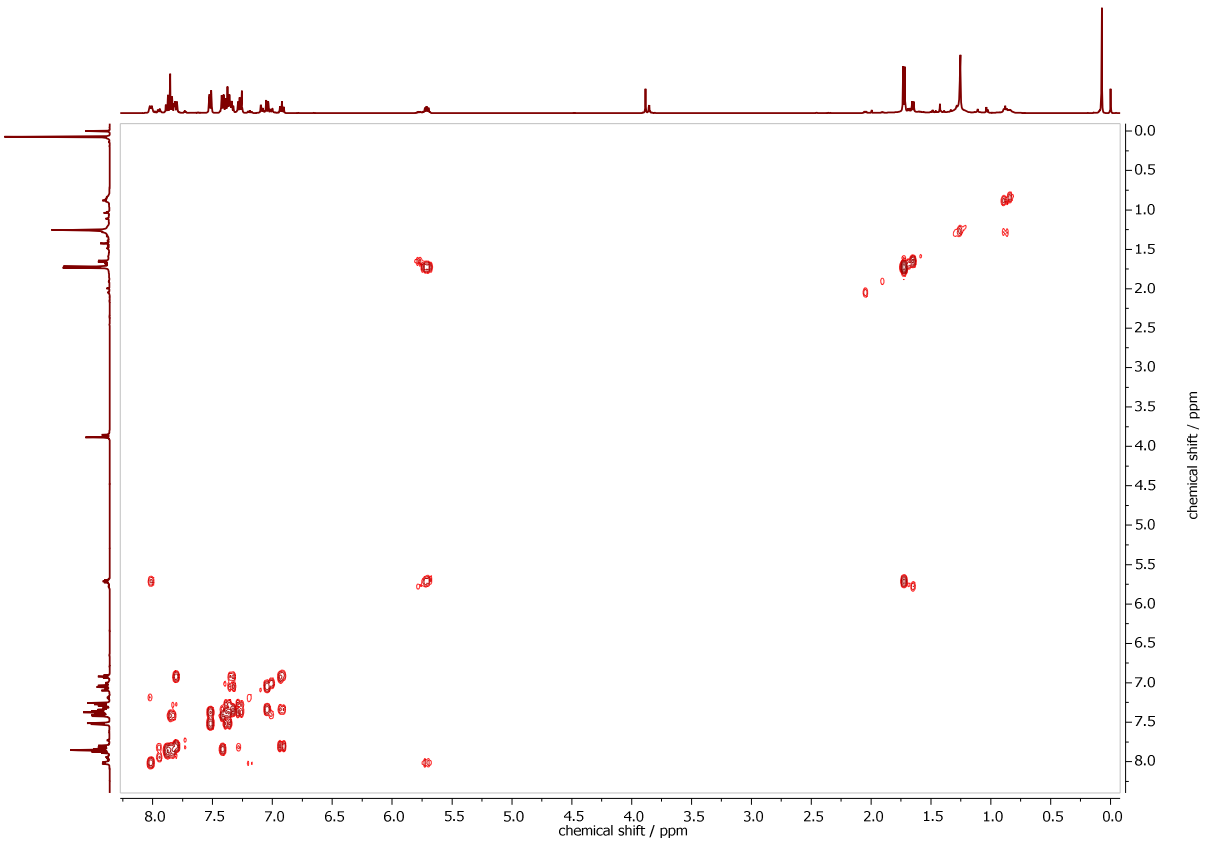

Fig. X53. ^{1}H, ^{1}H COSY NMR spectrum of H_2L in $CDCl_3$.

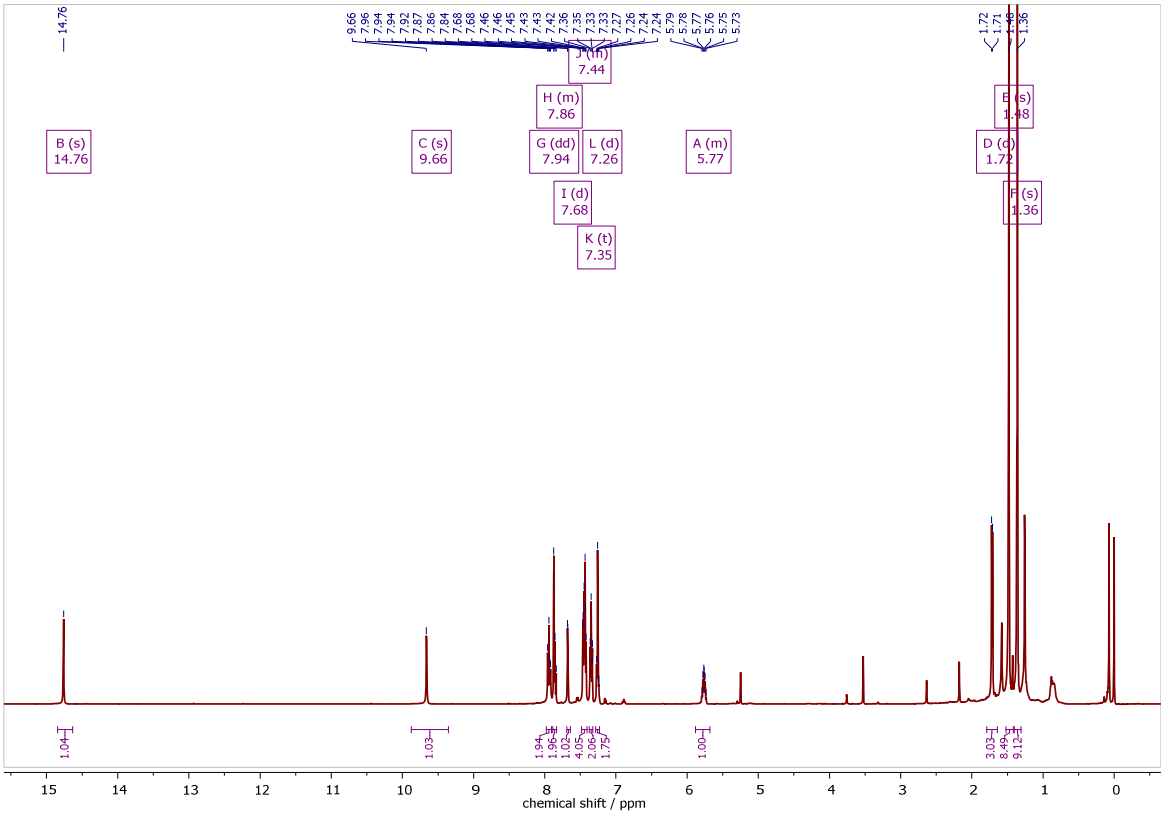

Fig. X54. ^{1}H NMR spectrum of $H_2{}^{tBu}L$ in $CDCl_3$ at 499 MHz.

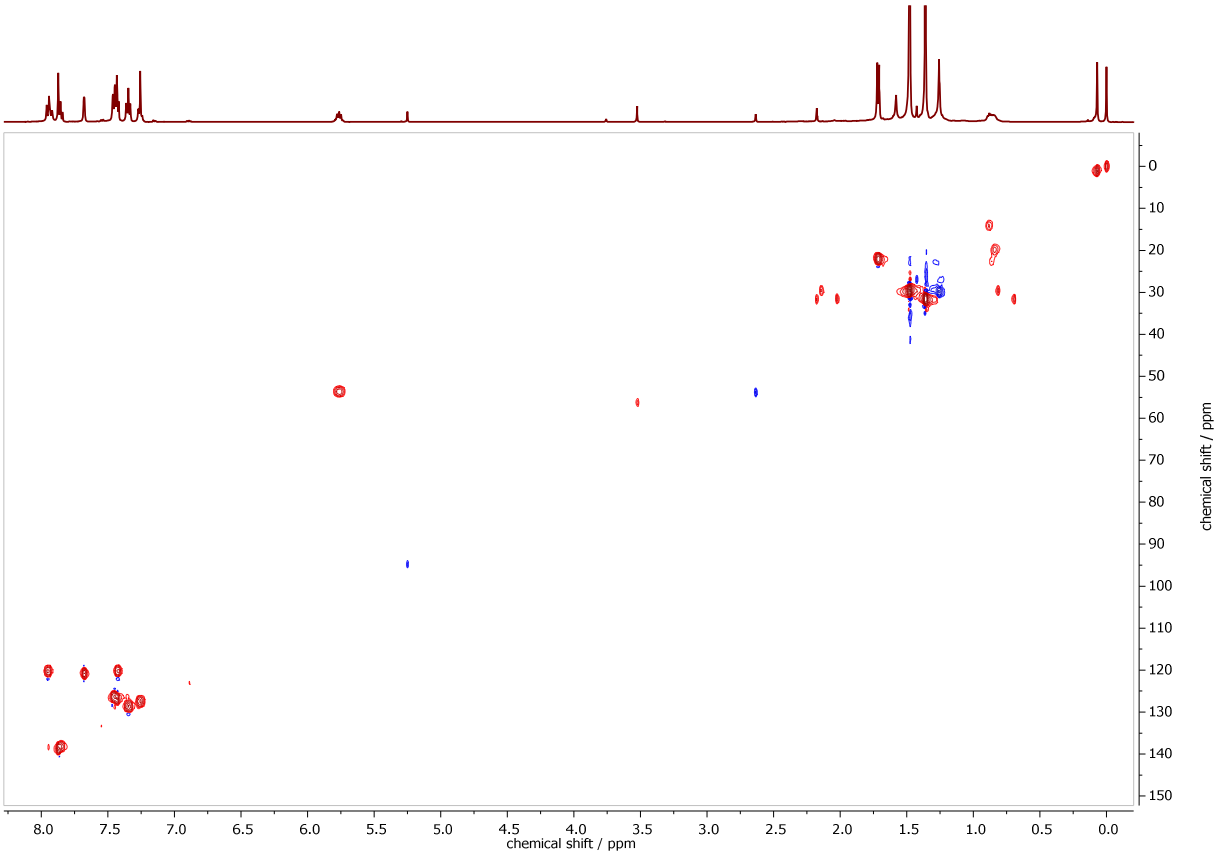

Fig. X55. ^{1}H, ^{13}C HSQCed NMR spectrum of $H_2{}^{tBu}L$ in $CDCl_3$.

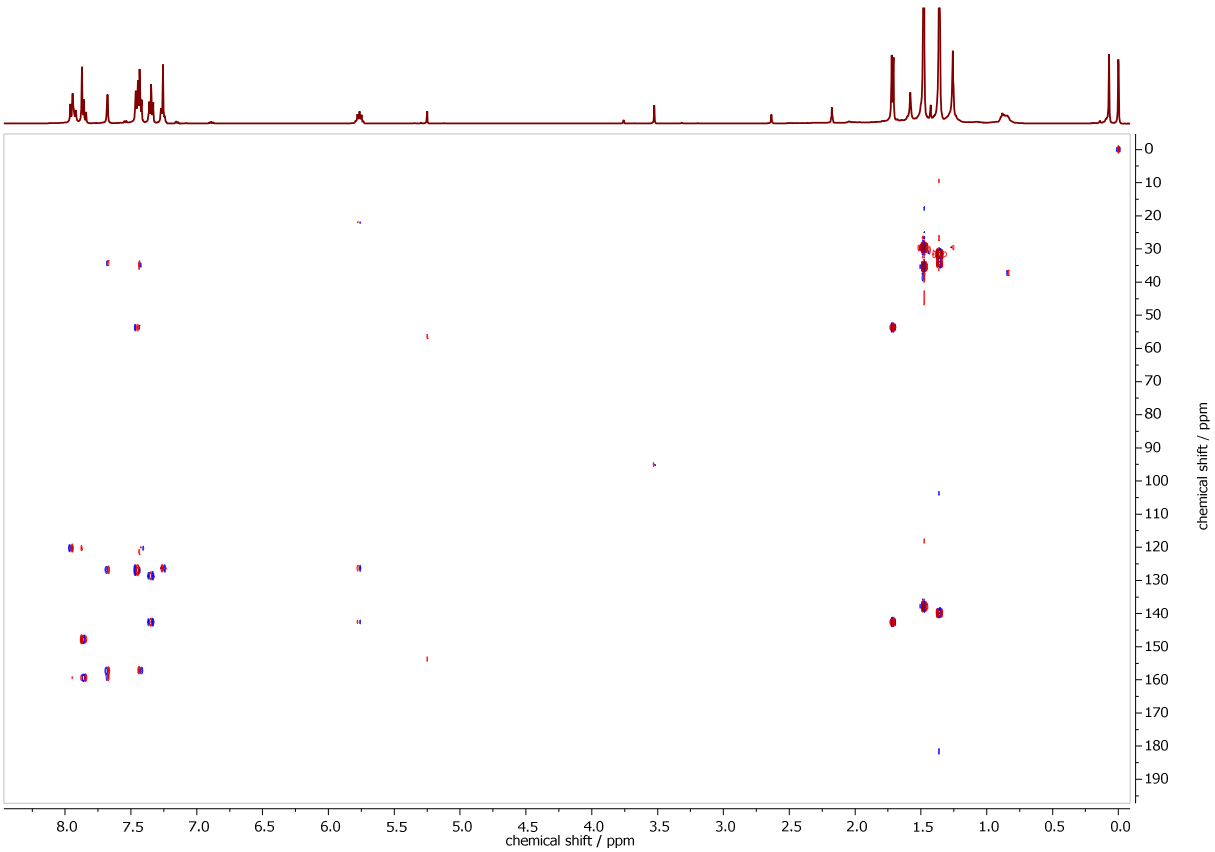

Fig. X56. ^{1}H, ^{13}C HMBC NMR spectrum of $H_2{}^{tBu}L$ in $CDCl_3$.

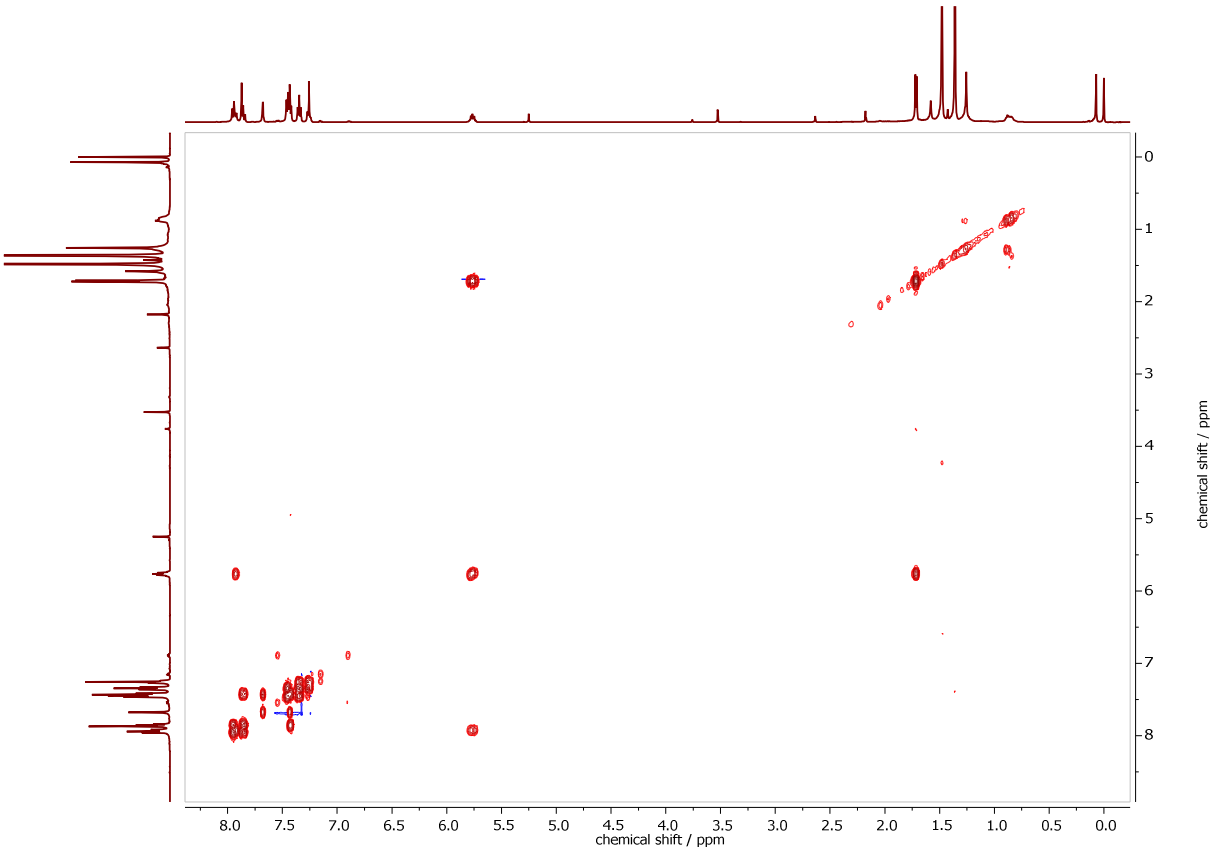

Fig. X57. ^{1}H, ^{1}H COSY NMR spectrum of $H_2{}^{tBu}L$ in $CDCl_3$.

NMR Spectra for [M(L)]

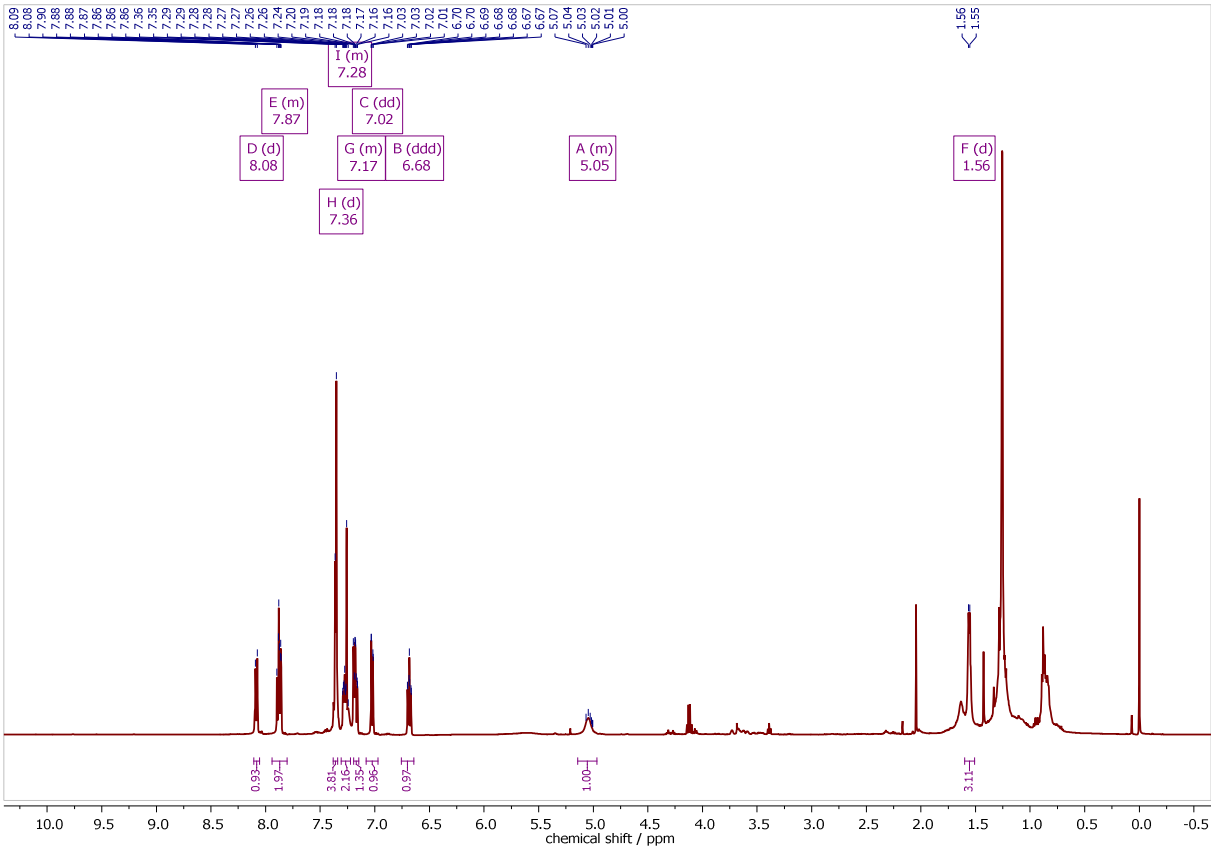

Fig. X58. ^{1}H NMR spectrum of [Ni(L)] in $CDCl_3$ at 499 MHz.

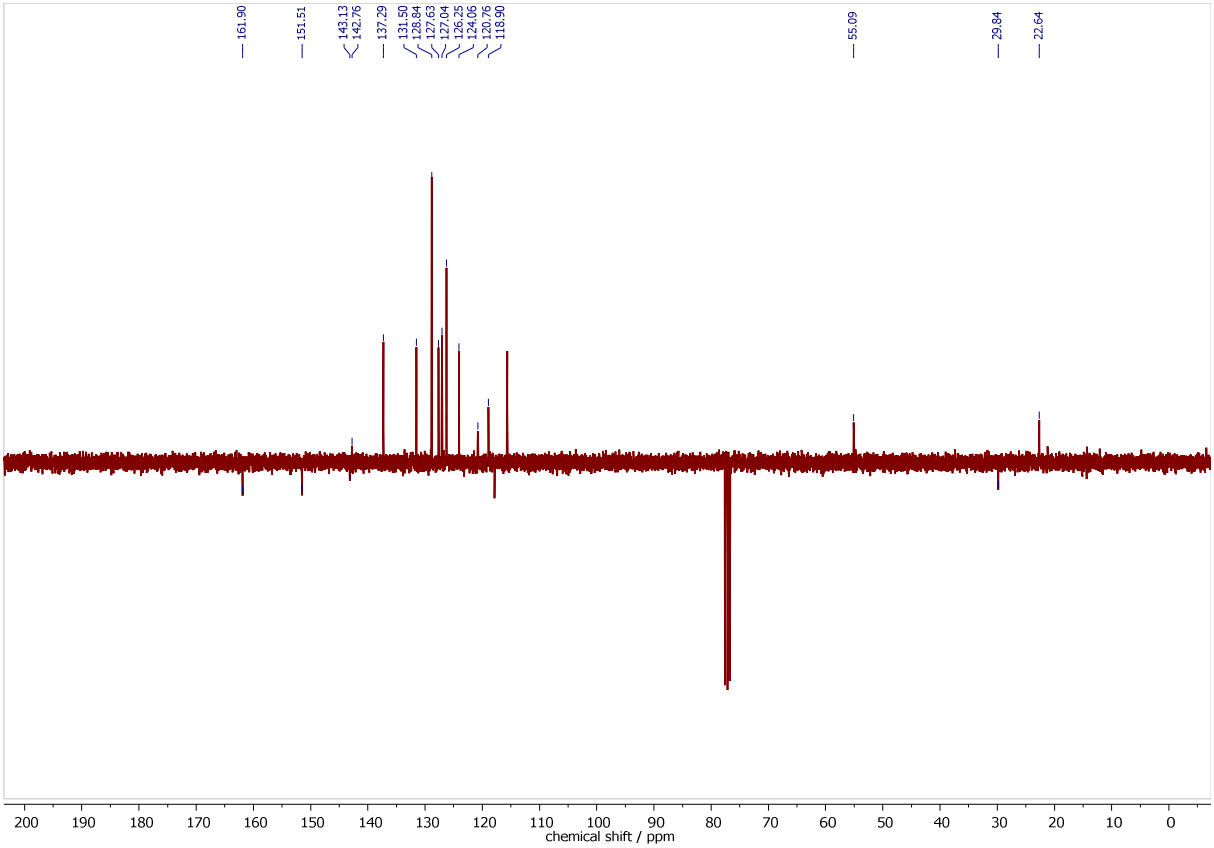

Fig. X59. ^{13}C DEPTQ NMR spectrum of [Ni(L)] in $CDCl_3$ at 75 MHz.

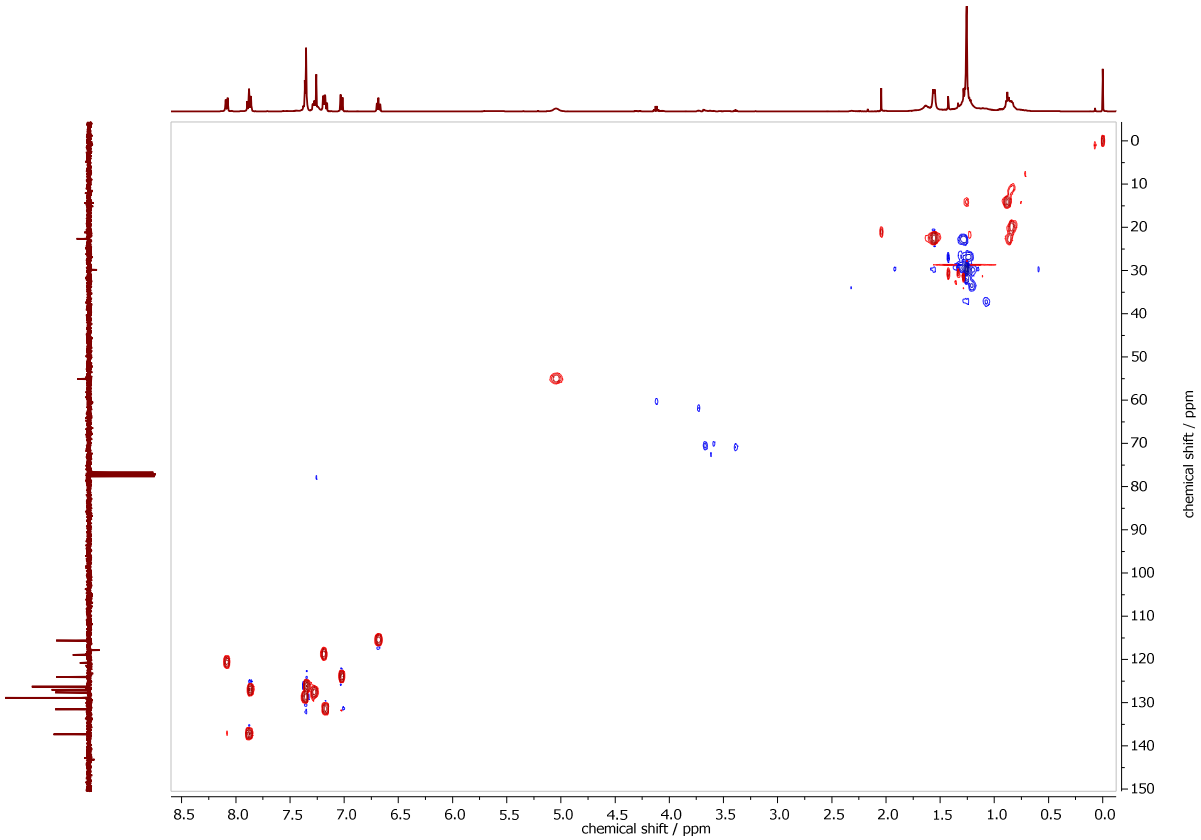

Fig. X60. $^{1}H,^{13}C$ HSQCed NMR spectrum of [Ni(L)] in $CDCl_3$.

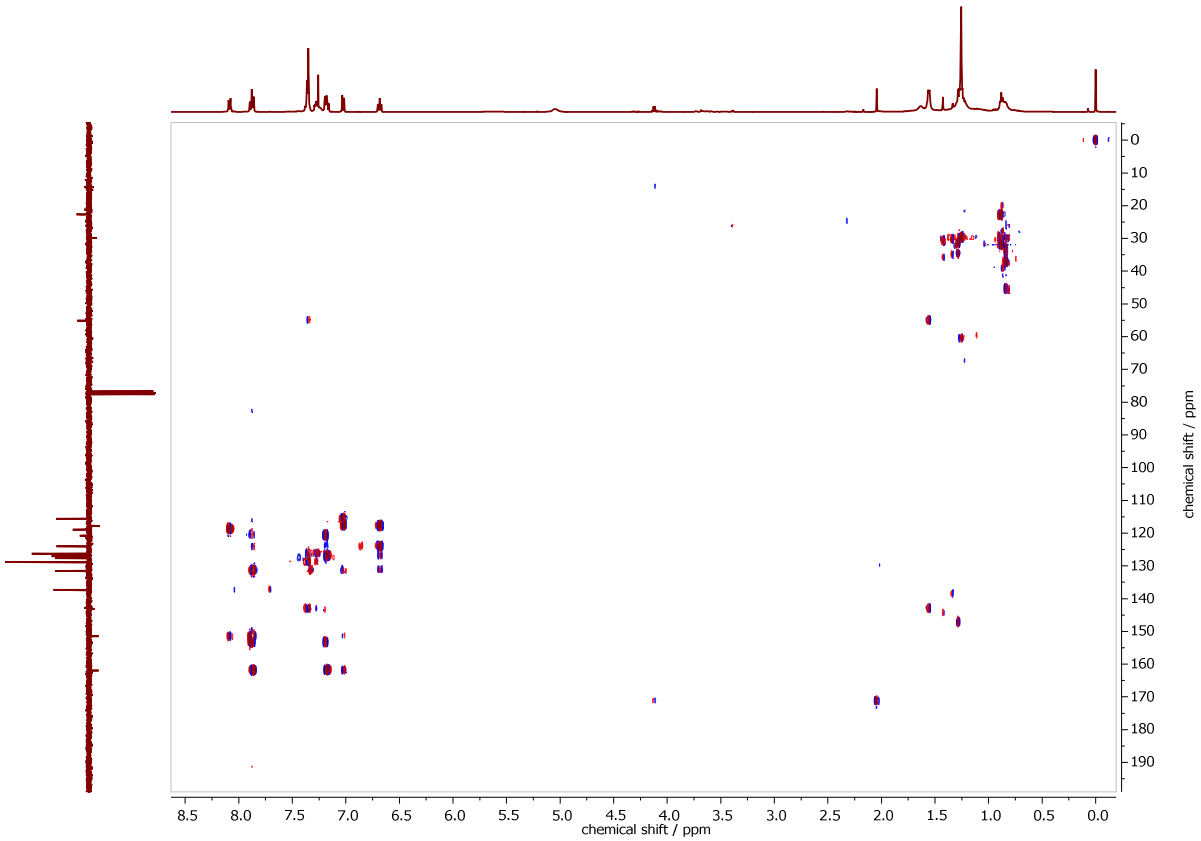

Fig. X61. $^{1}H,^{13}C$ HMBC NMR spectrum of [Ni(L)] in $CDCl_3$.

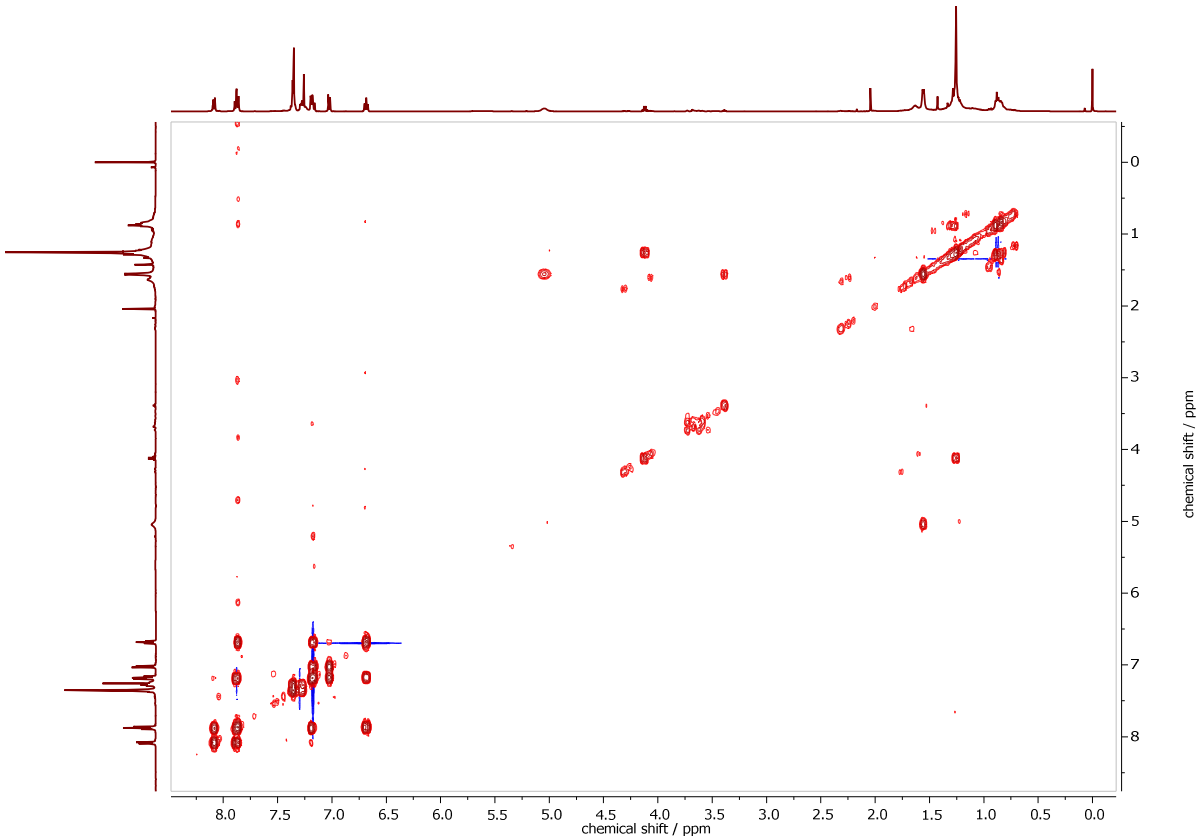

Fig. X62. $^{1}H,^{1}H$ COSY NMR spectrum of [Ni(L)] in $CDCl_3$.

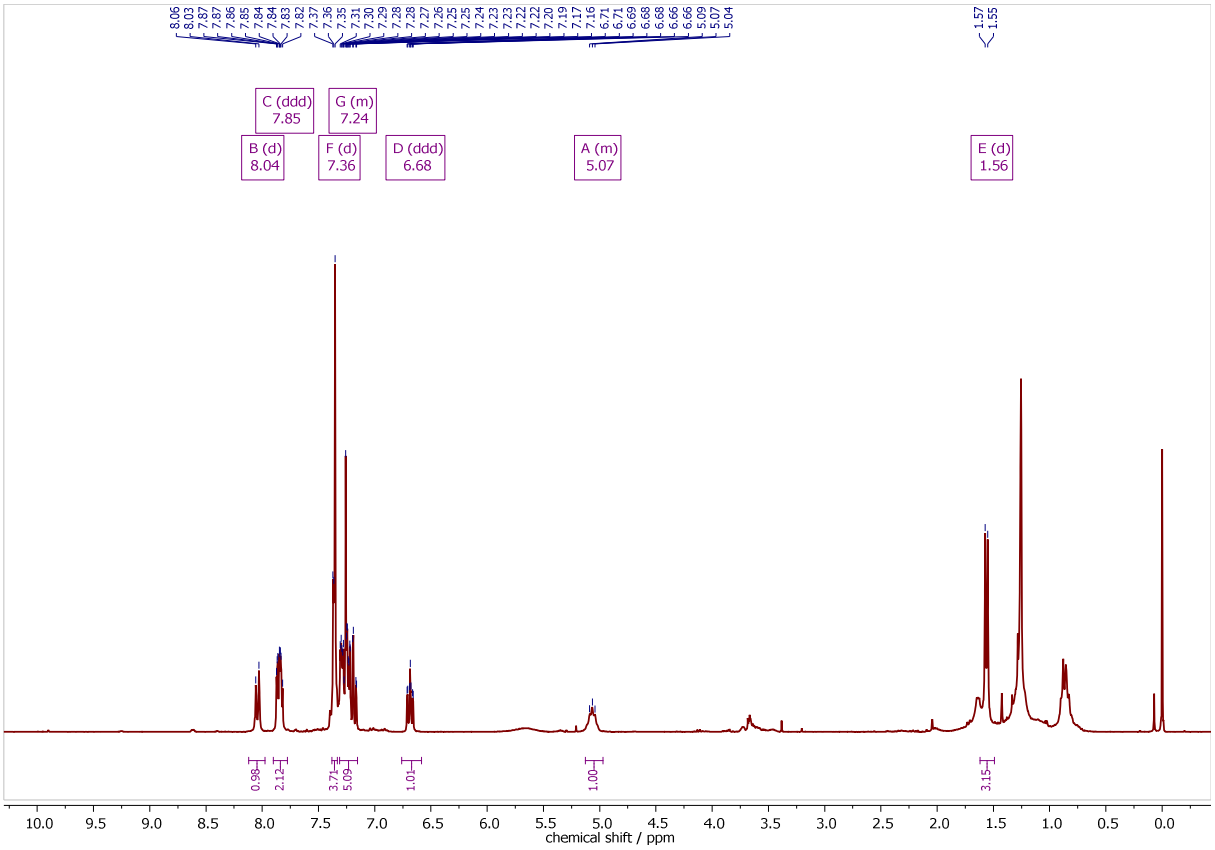

Fig. X63. ^{1}H NMR spectrum of [Pd(L)] in $CDCl_3$ at 300 MHz.

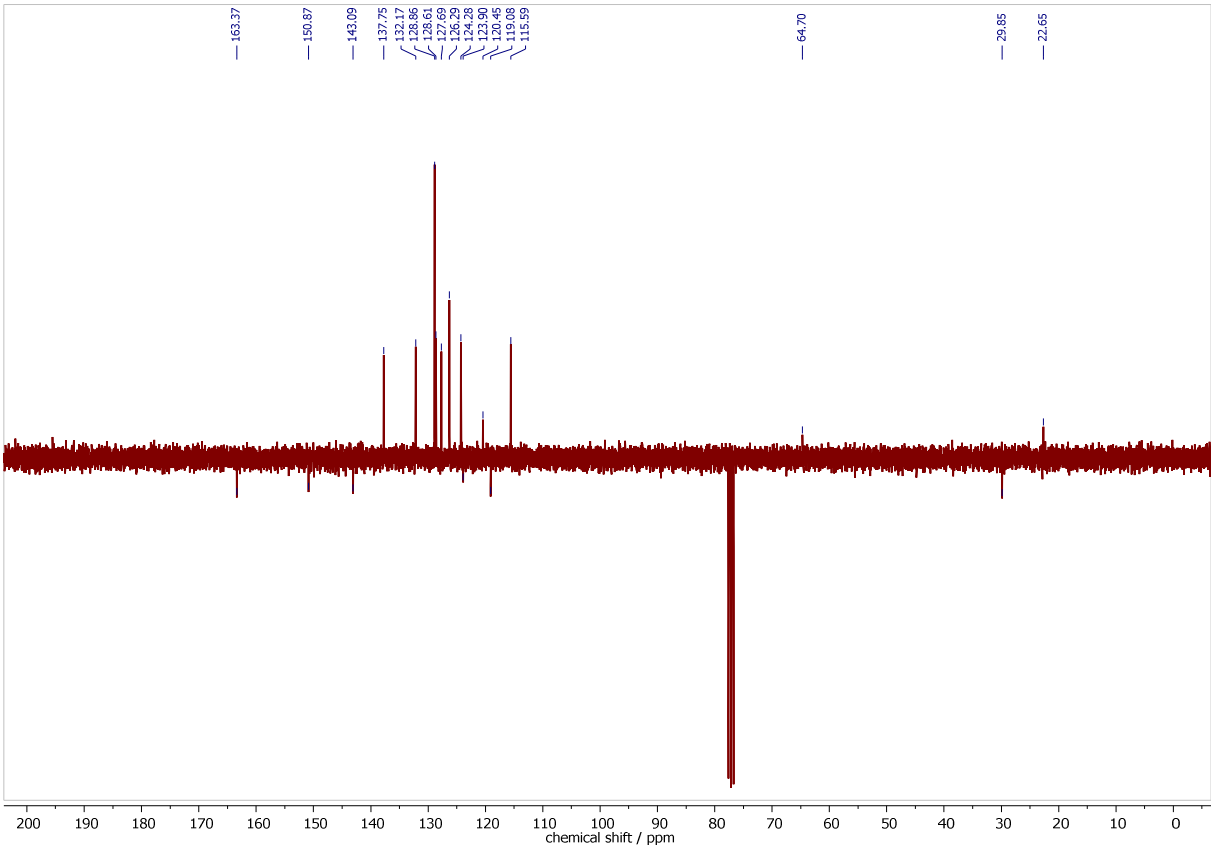

Fig. X64. ^{13}C DEPTQ NMR spectrum of [Pd(L)] in $CDCl_3$ at 75 MHz.

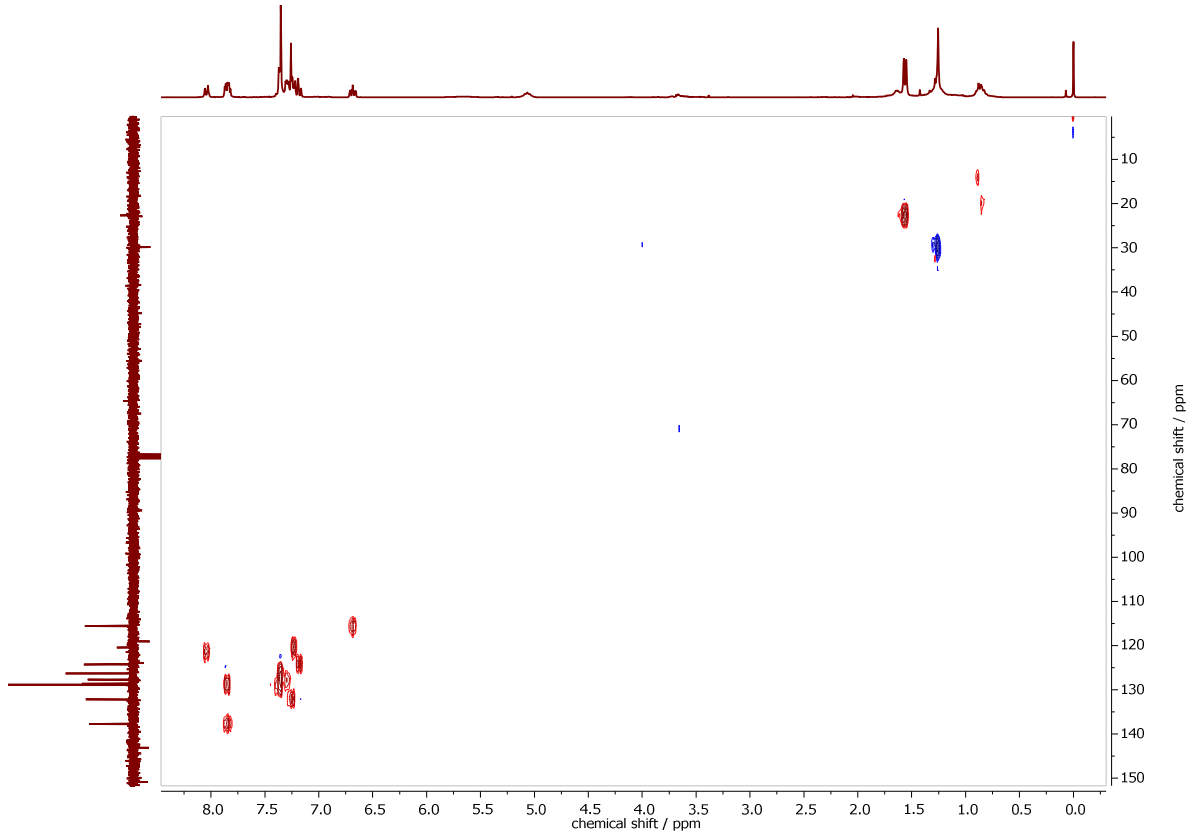

Fig. X65. $^{1}H,^{13}C$ HSQCed NMR spectrum of [Pd(L)] in $CDCl_3$.

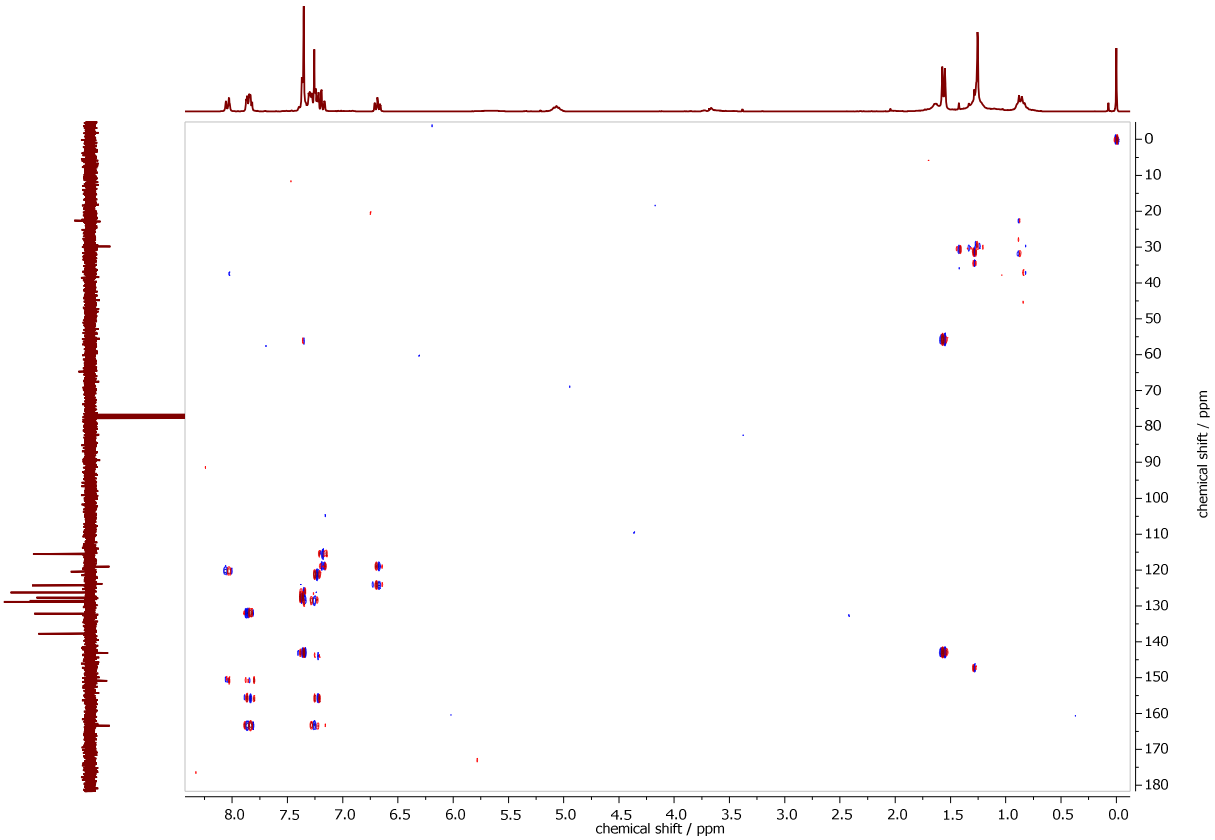

Fig. X66. $^{1}H,^{13}C$ HMBC NMR spectrum of [Pd(L)] in $CDCl_3$.

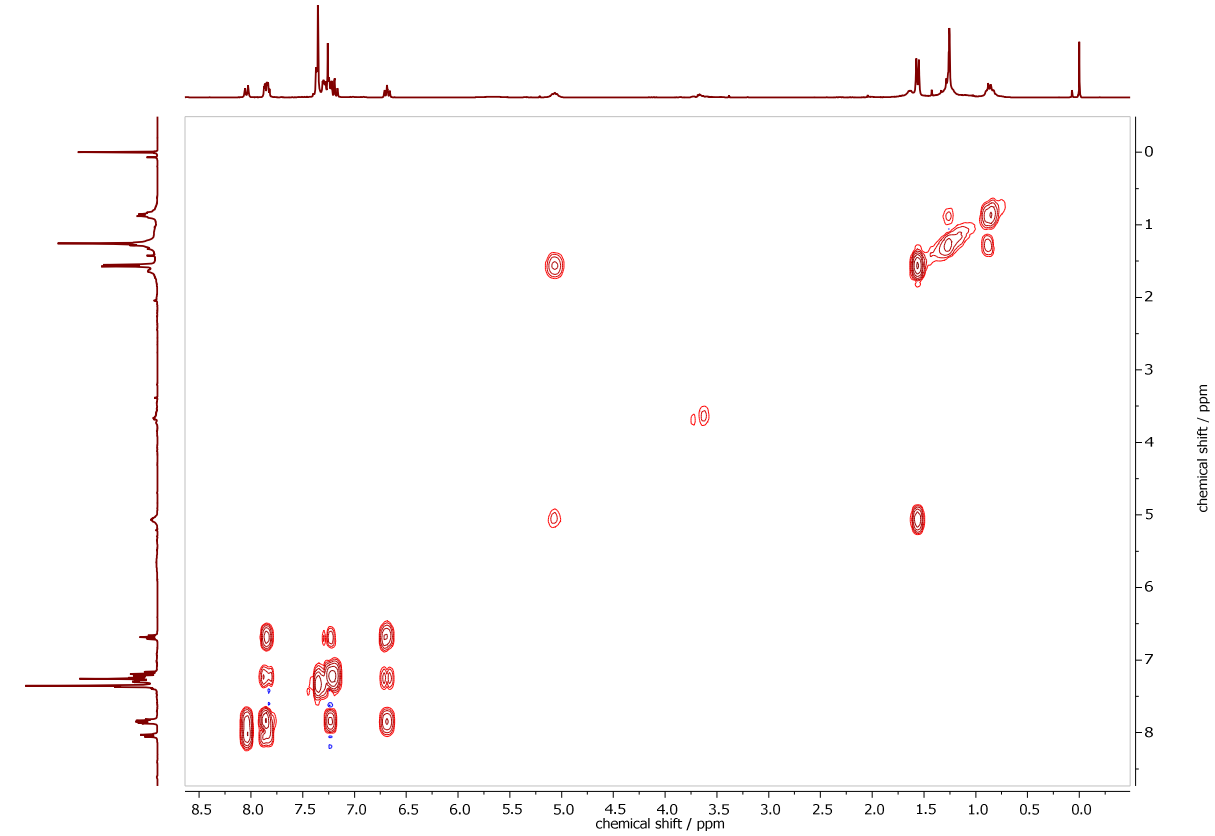

Fig. X67. $^{1}H,^{1}H$ COSY NMR spectrum of [Pd(L)] in $CDCl_3$.

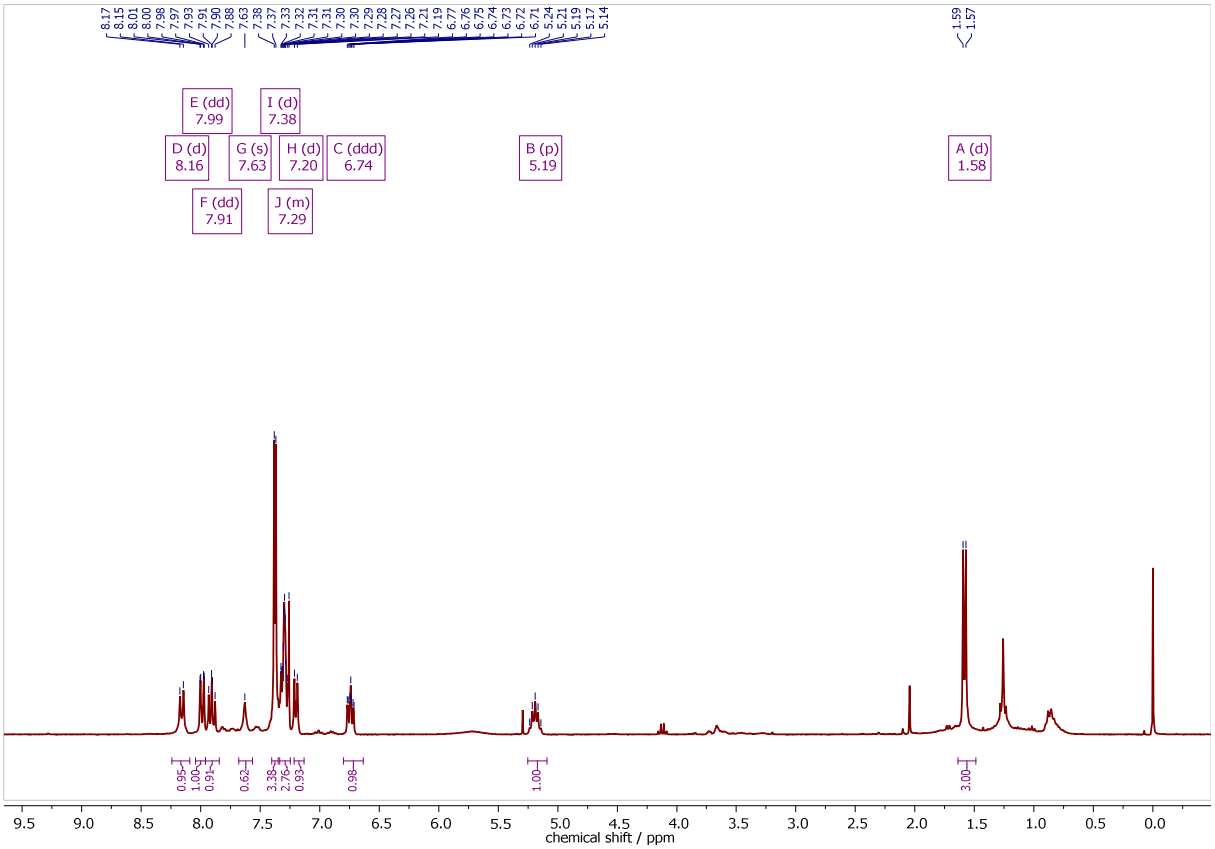

Fig. X68. ^{1}H NMR spectrum of [Pt(L)] in $CDCl_3$ at 300 MHz.

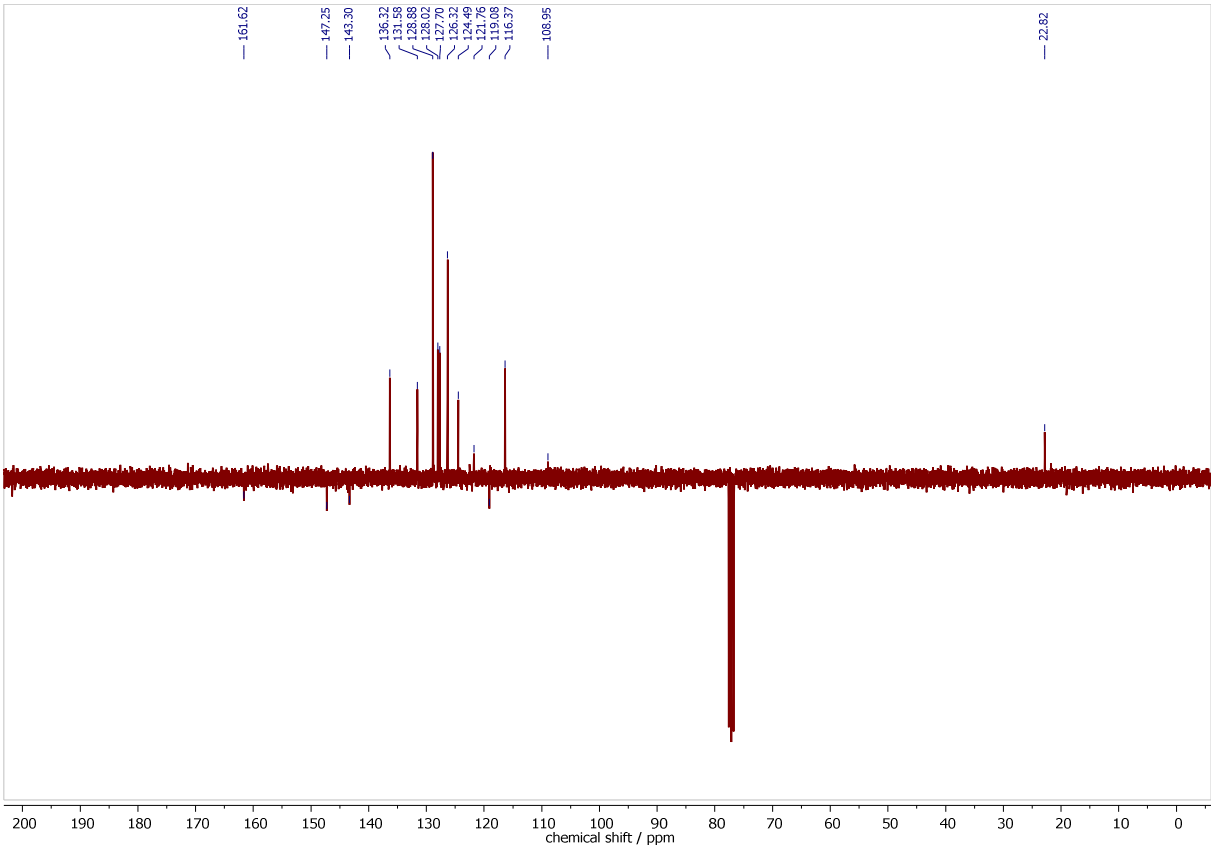

Fig. X69. ^{13}C DEPTQ NMR spectrum of [Pt(L)] in $CDCl_3$ at 75 MHz.

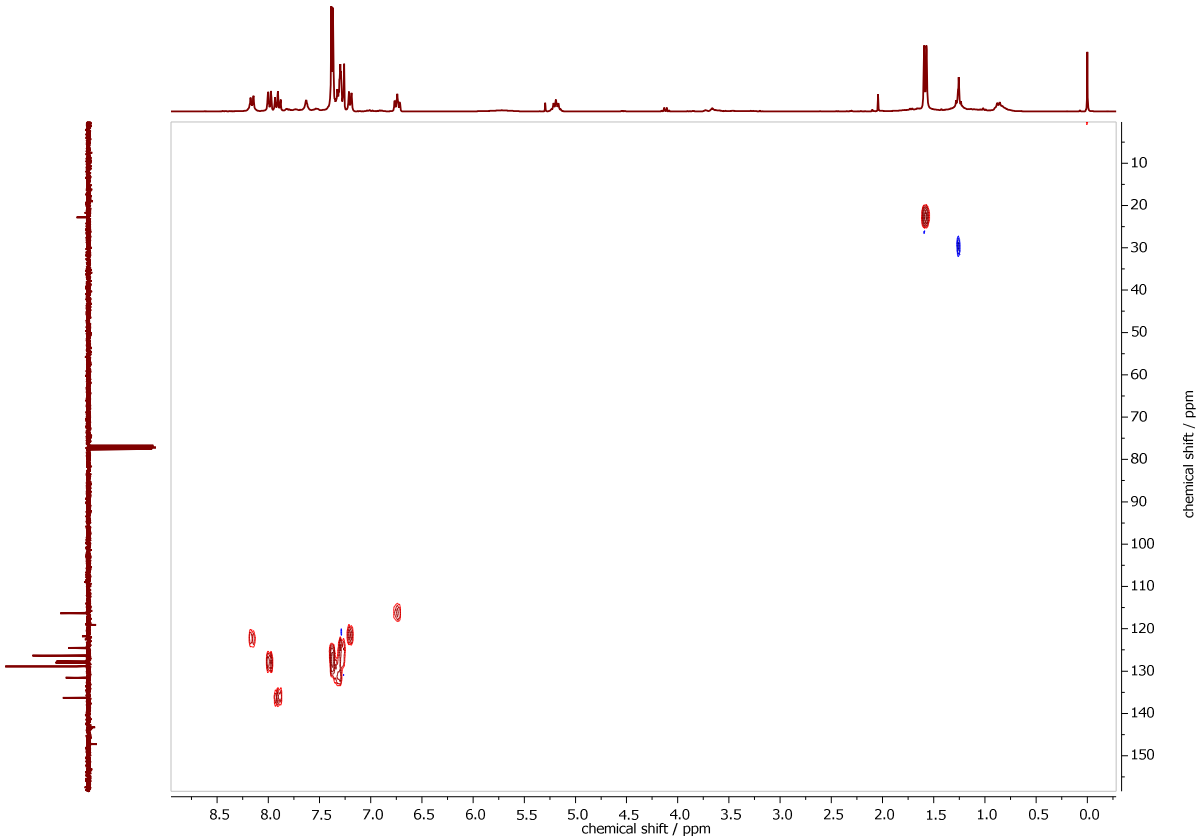

Fig. X70. $^{1}H,^{13}C$ HMBC NMR spectrum of [Pt(L)] in $CDCl_3$.

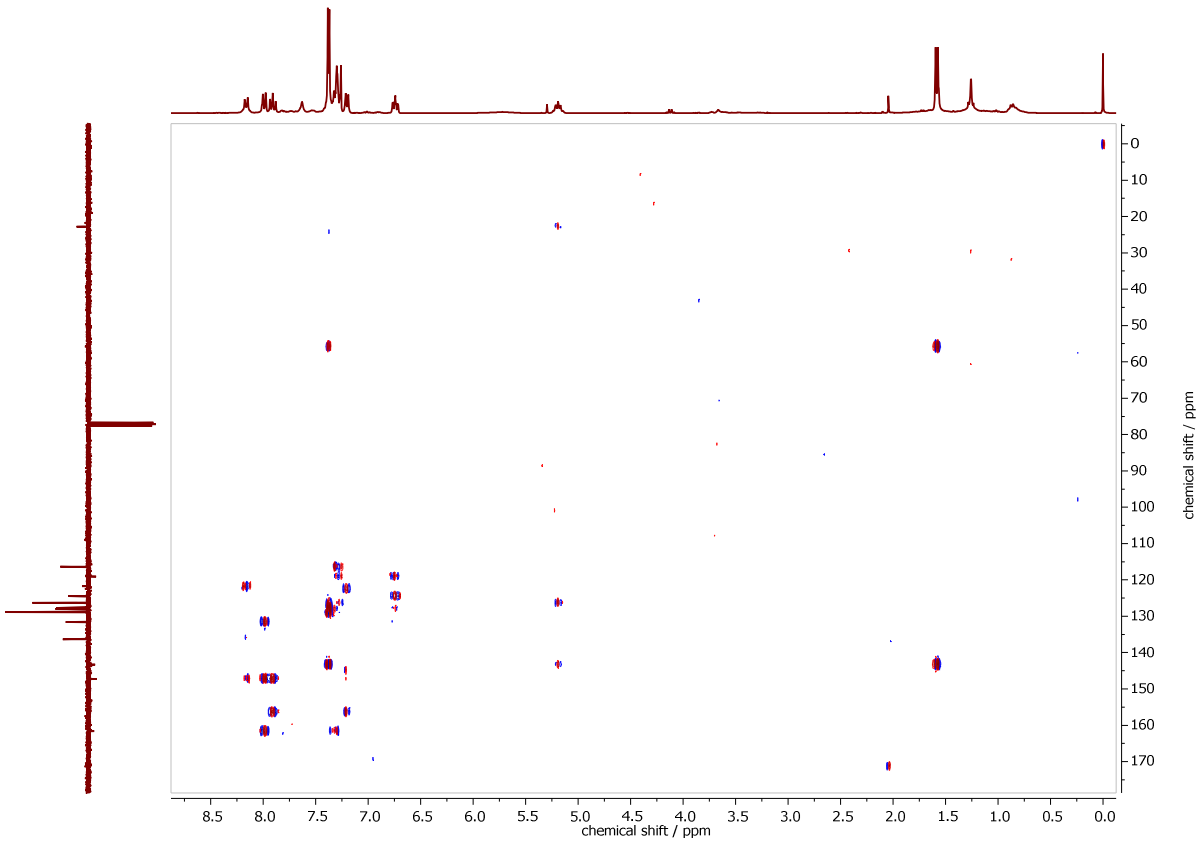

Fig. X71. $^{1}H,^{13}C$ HMBC NMR spectrum of [Pt(L)] in $CDCl_3$.

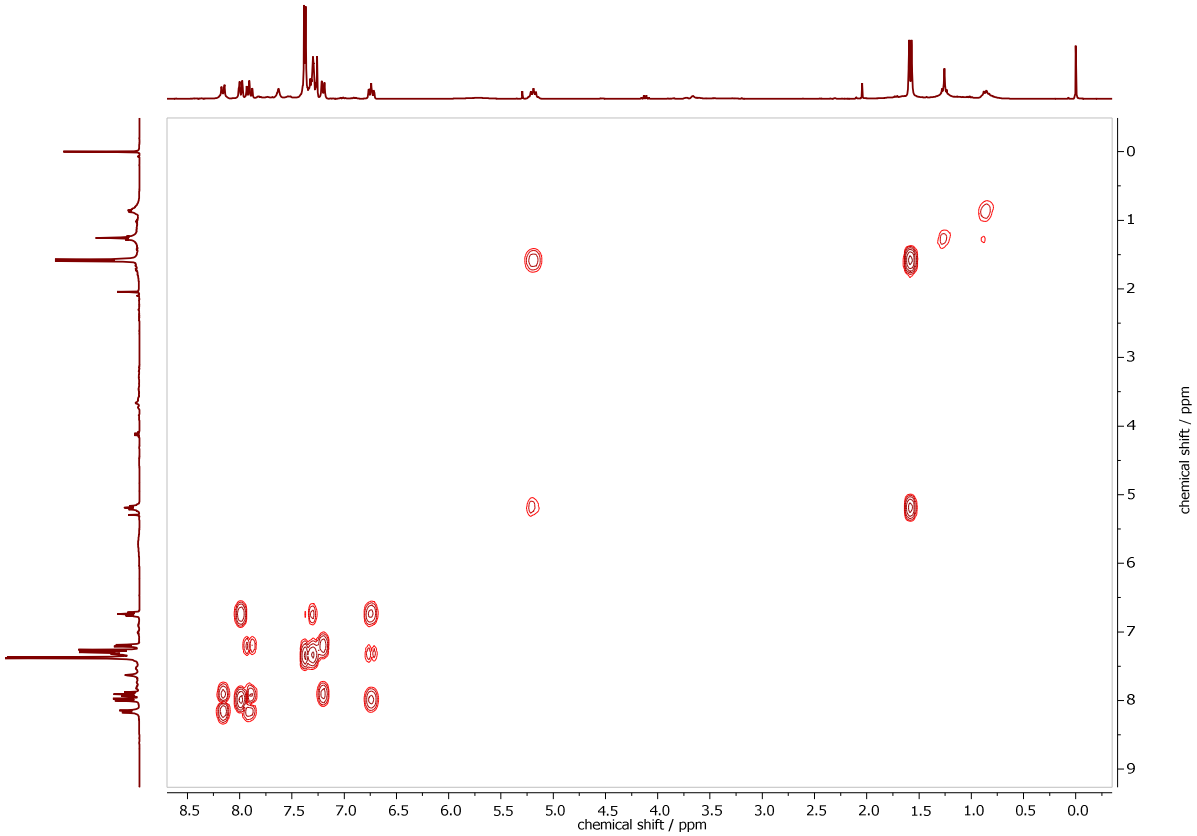

Fig. X72. $^{1}H,^{1}H$ COSY NMR spectrum of [Pt(L)] in $CDCl_3$.

[M(^{tBu}L)] Series

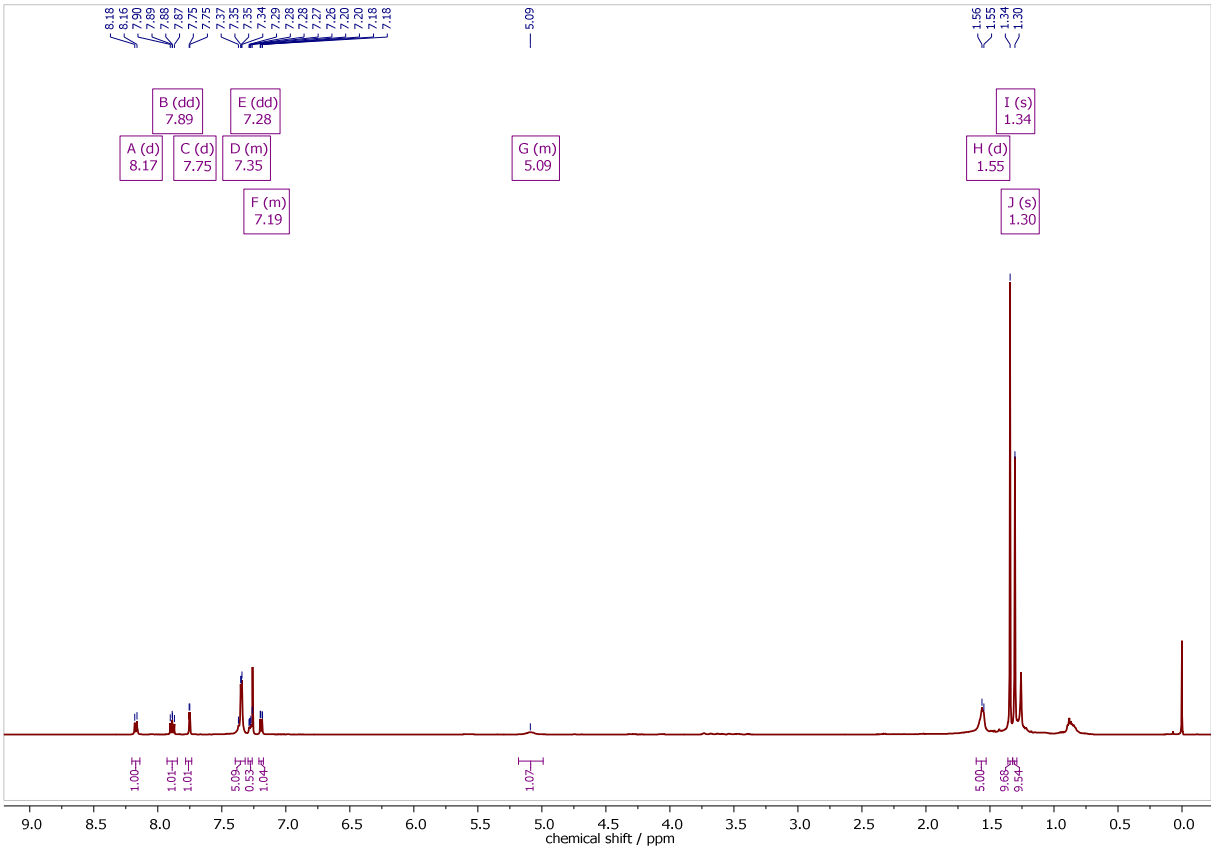

Fig. X73. ^{1}H NMR spectrum of [Ni(^{tBu}L)] in $CDCl_3$ at 499 MHz.

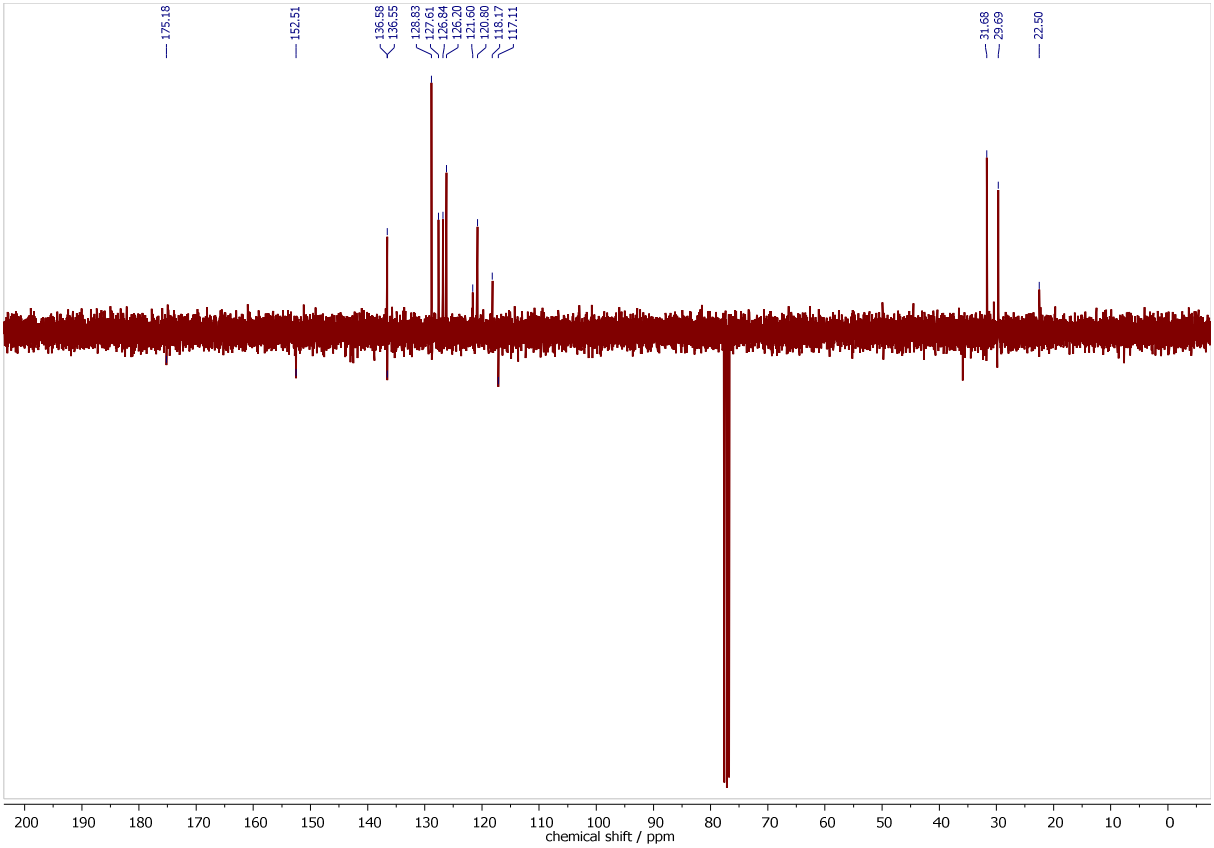

Fig. X74. ^{13}C DEPTQ NMR spectrum of [Ni(^{tBu}L)] in $CDCl_3$ at 75 MHz.

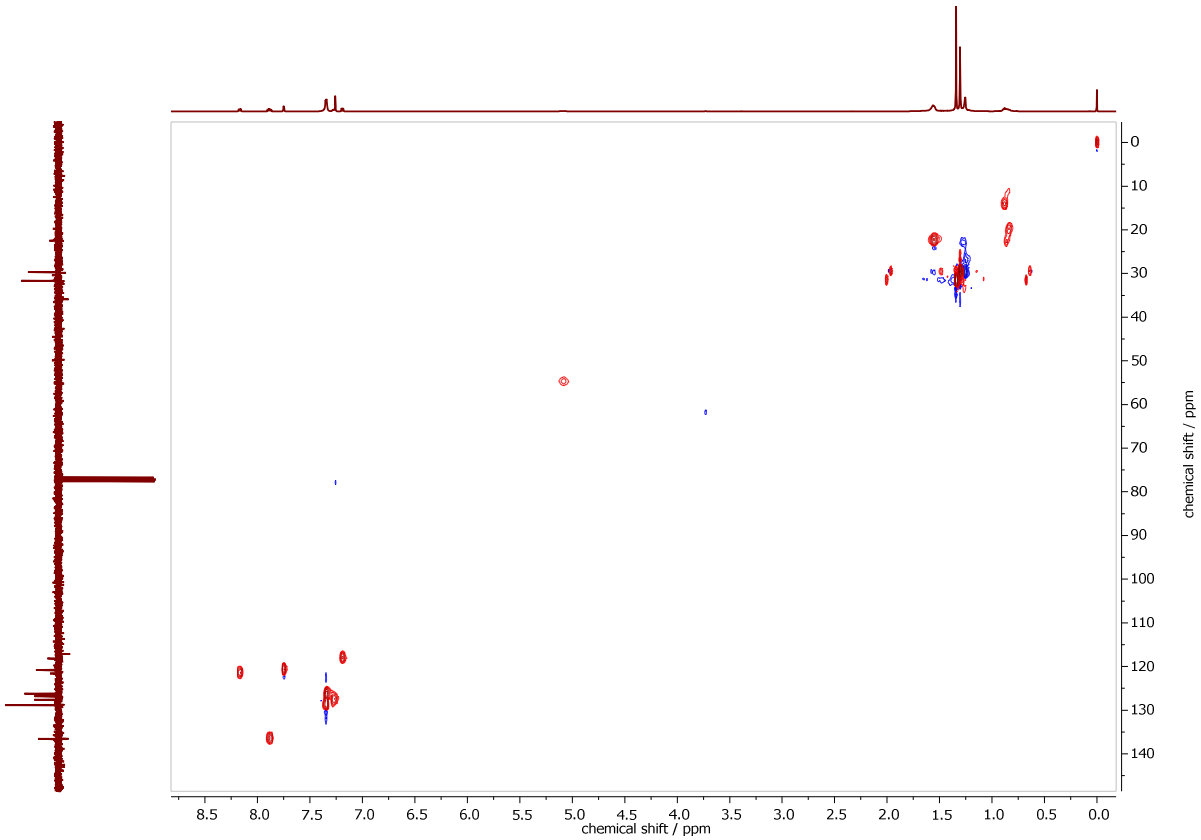

Fig. X75. $^{1}H,^{13}C$ HSQCed NMR spectrum of [Ni(^{tBu}L)] in $CDCl_3$.

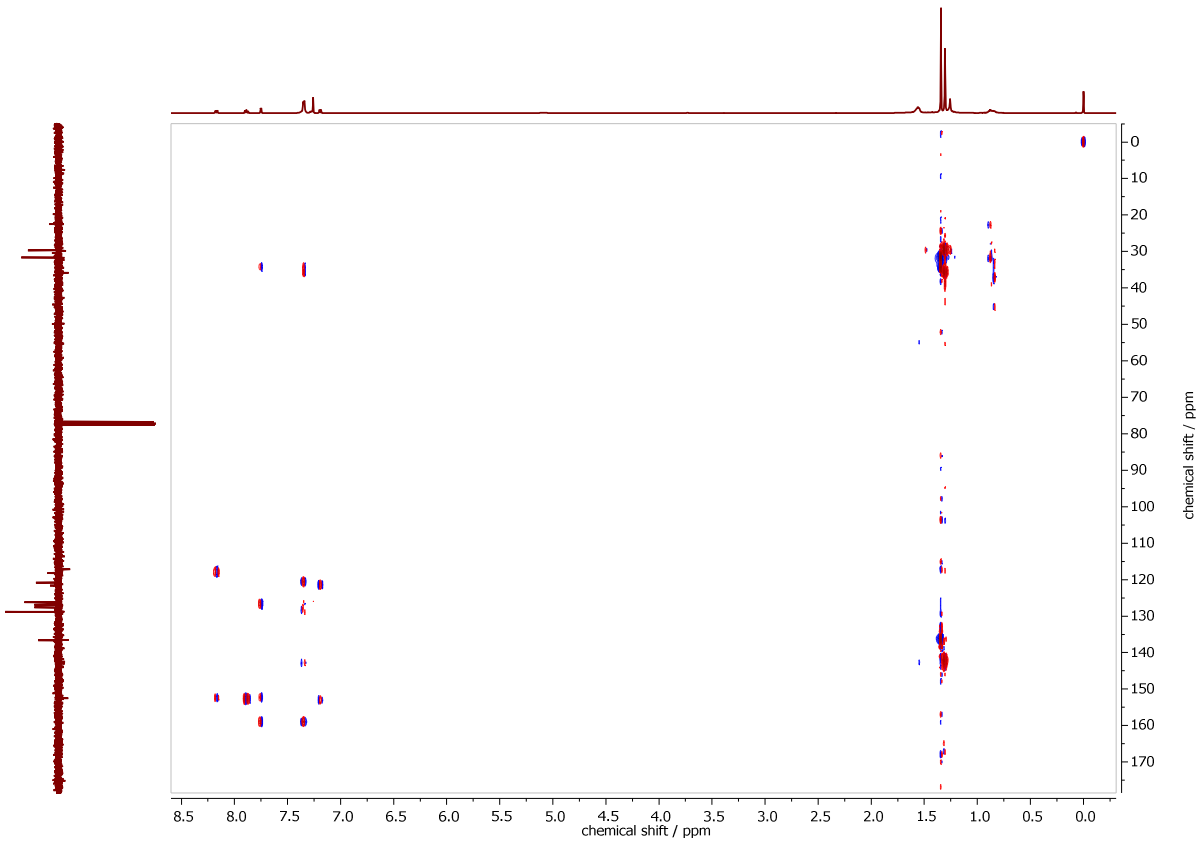

Fig. X76. $^{1}H,^{13}C$ HMBC NMR spectrum of [Ni(^{tBu}L)] in $CDCl_3$.

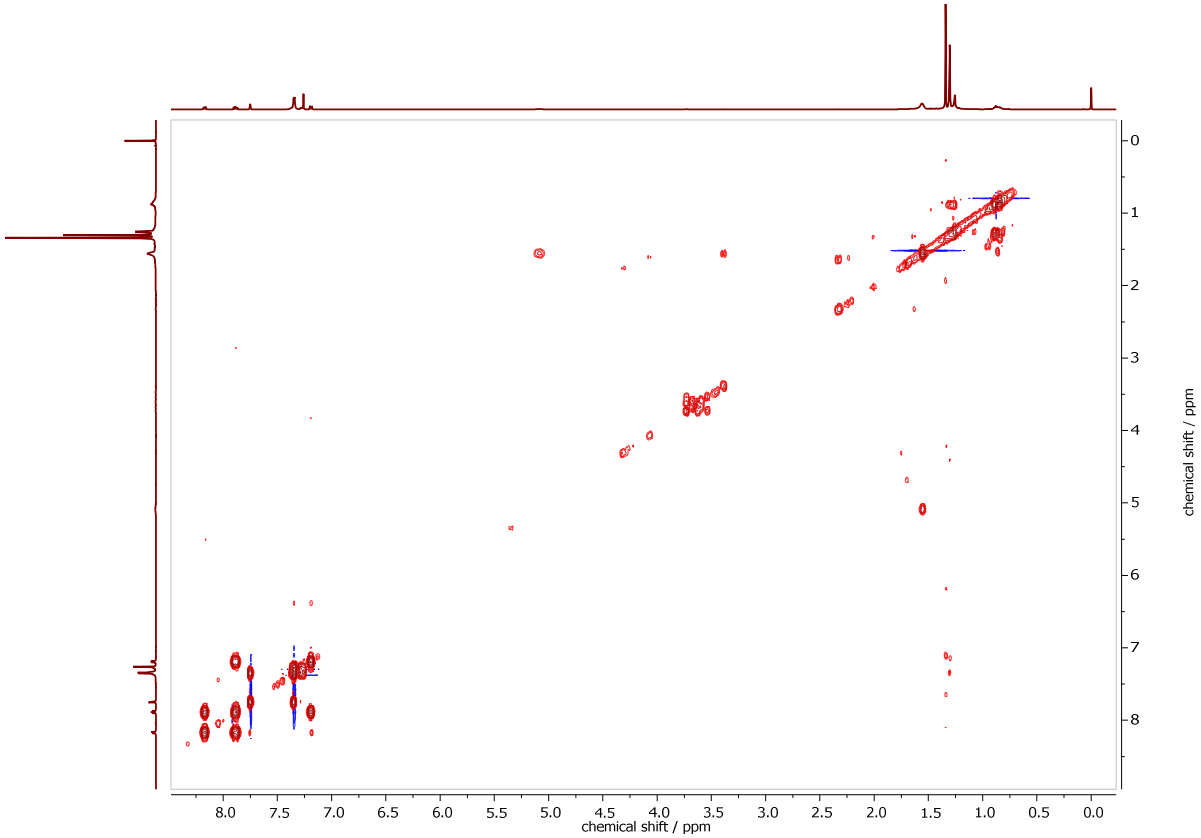

Fig. X77. $^{1}H,^{1}H$ COSY NMR spectrum of [Ni(^{tBu}L)] in $CDCl_3$.

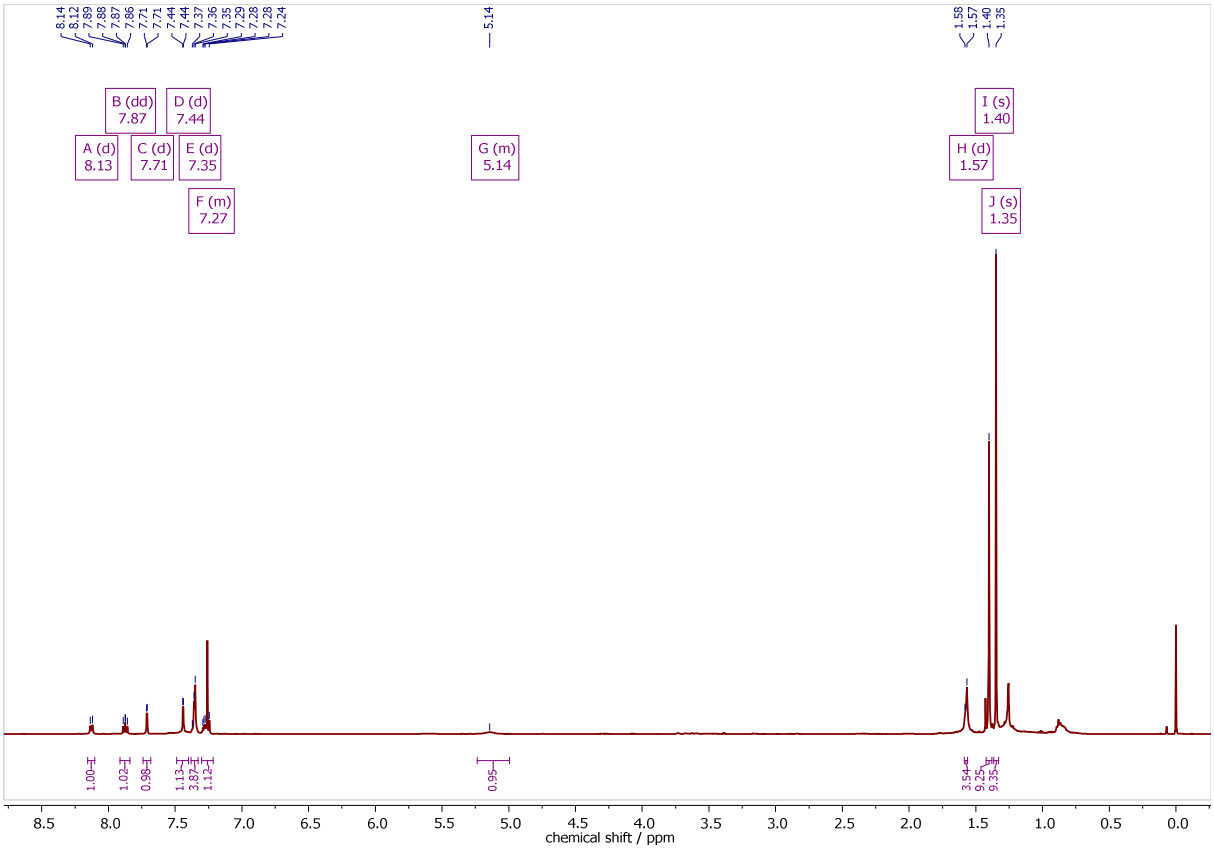

Fig. X78. ^{1}H NMR spectrum of [Pd(^{tBu}L)] in $CDCl_3$ at 300 MHz.

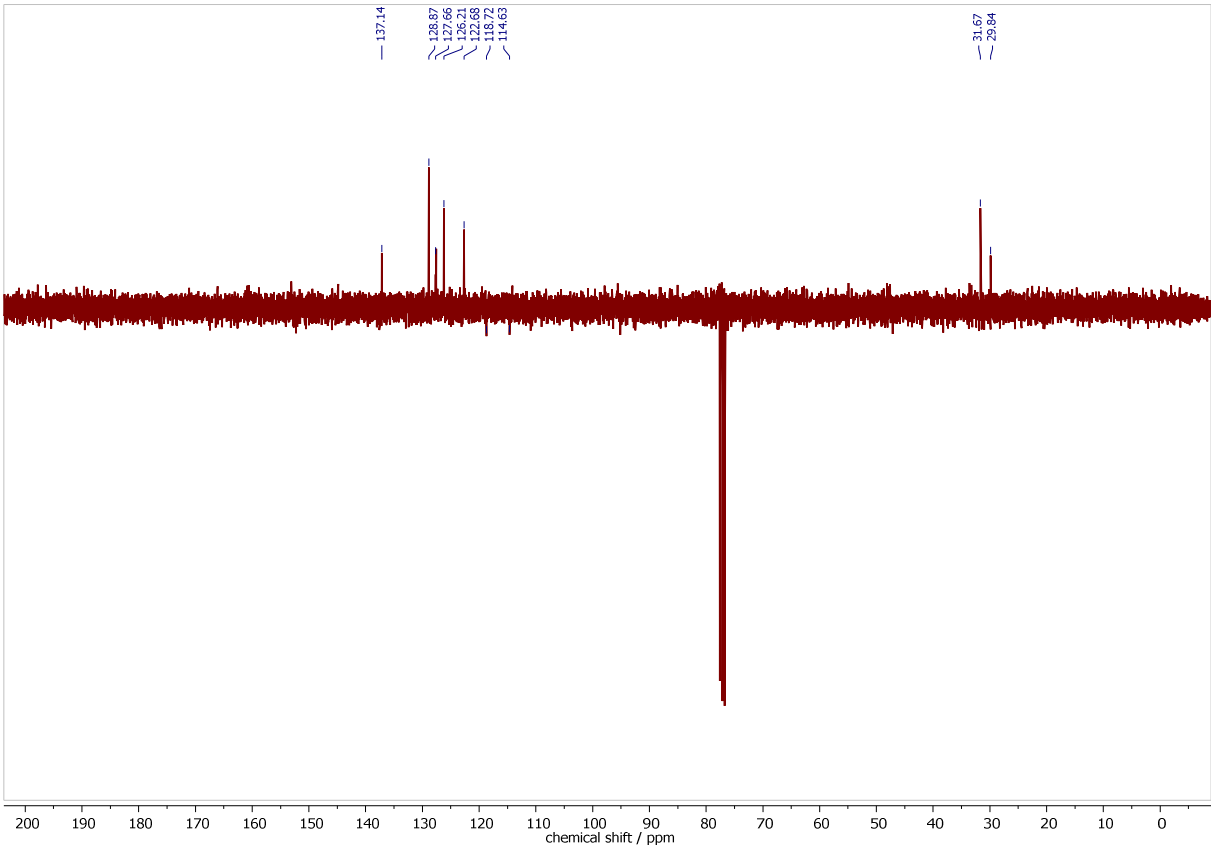

Fig. X79. ^{13}C DEPTQ NMR spectrum of [Pd(^{tBu}L)] in $CDCl_3$ at 75 MHz.

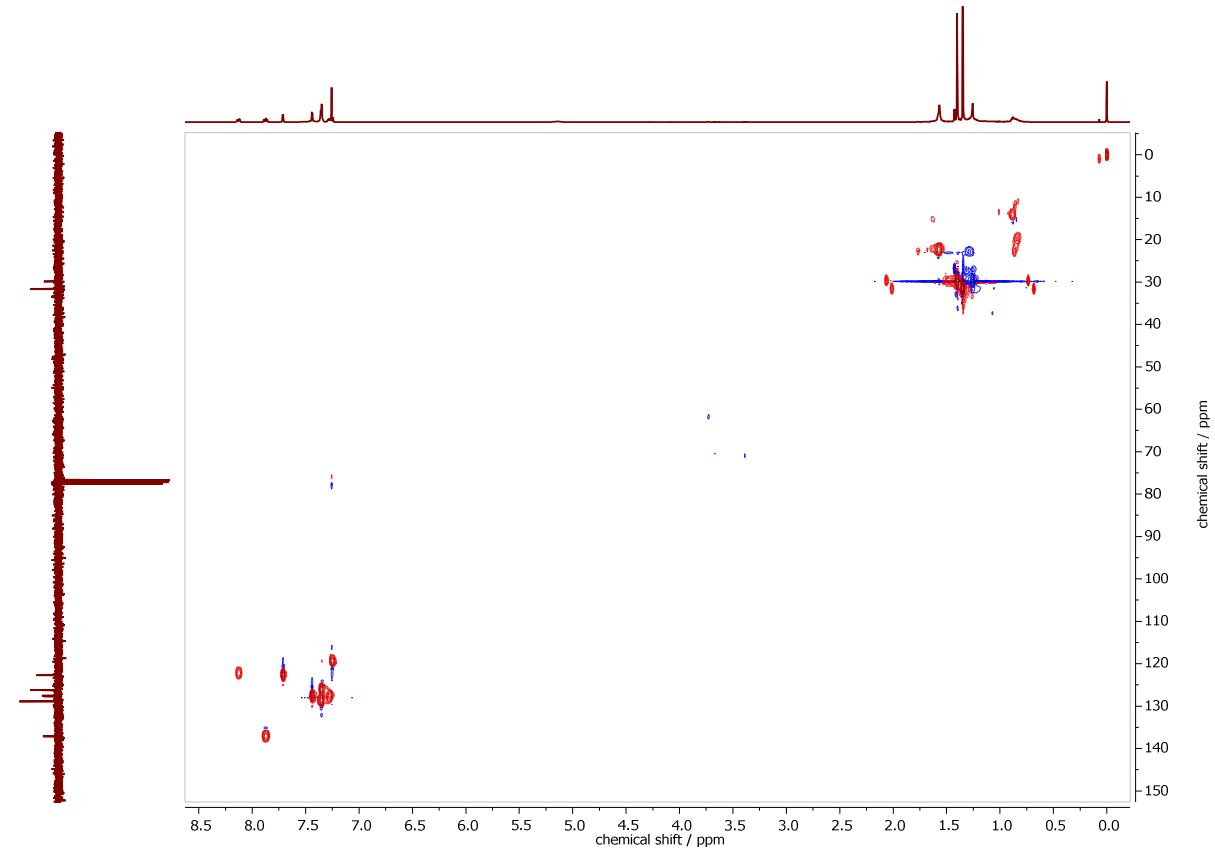

Fig. X80. ^{1}H,^{13}C HSQCed NMR spectrum of [Pd(^{tBu}L)] in $CDCl_3$.

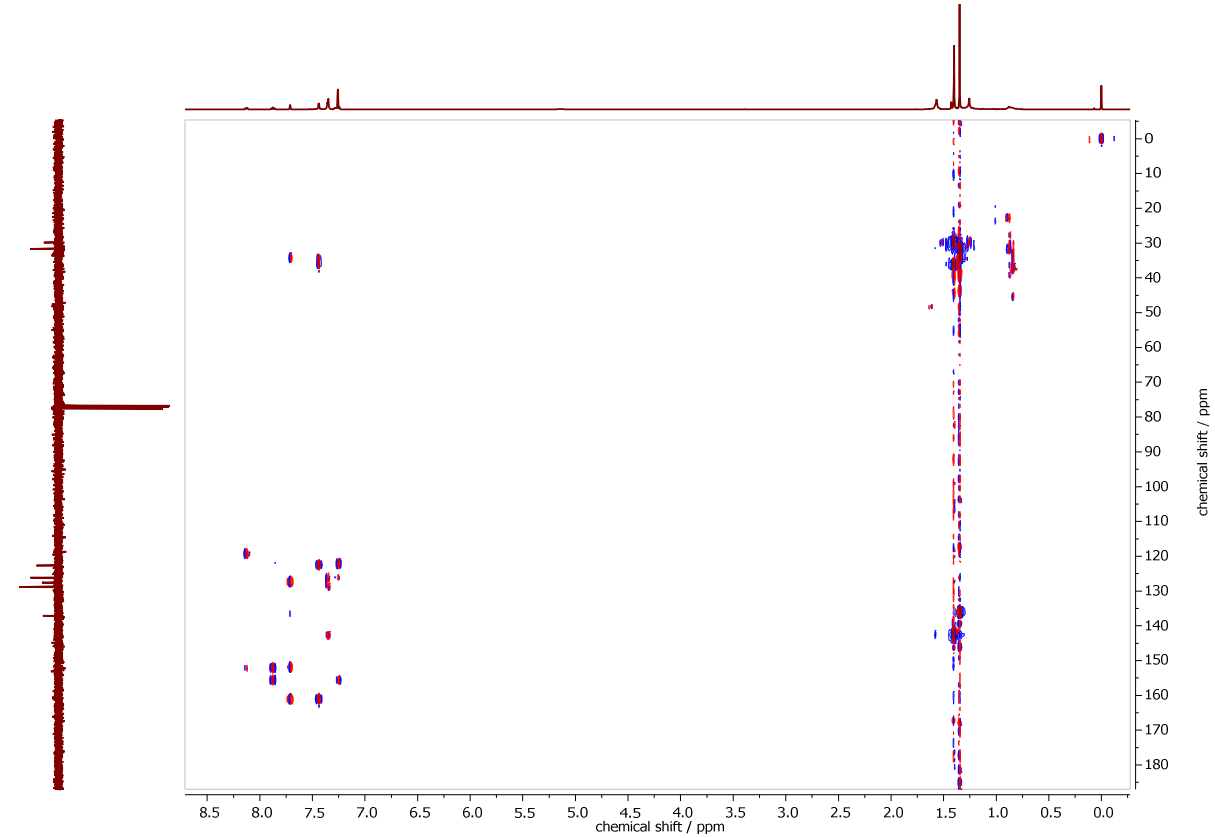

Fig. X81. $^{1}H,^{13}C$ HMBC NMR spectrum of [Pd(^{tBu}L)] in $CDCl_3$.

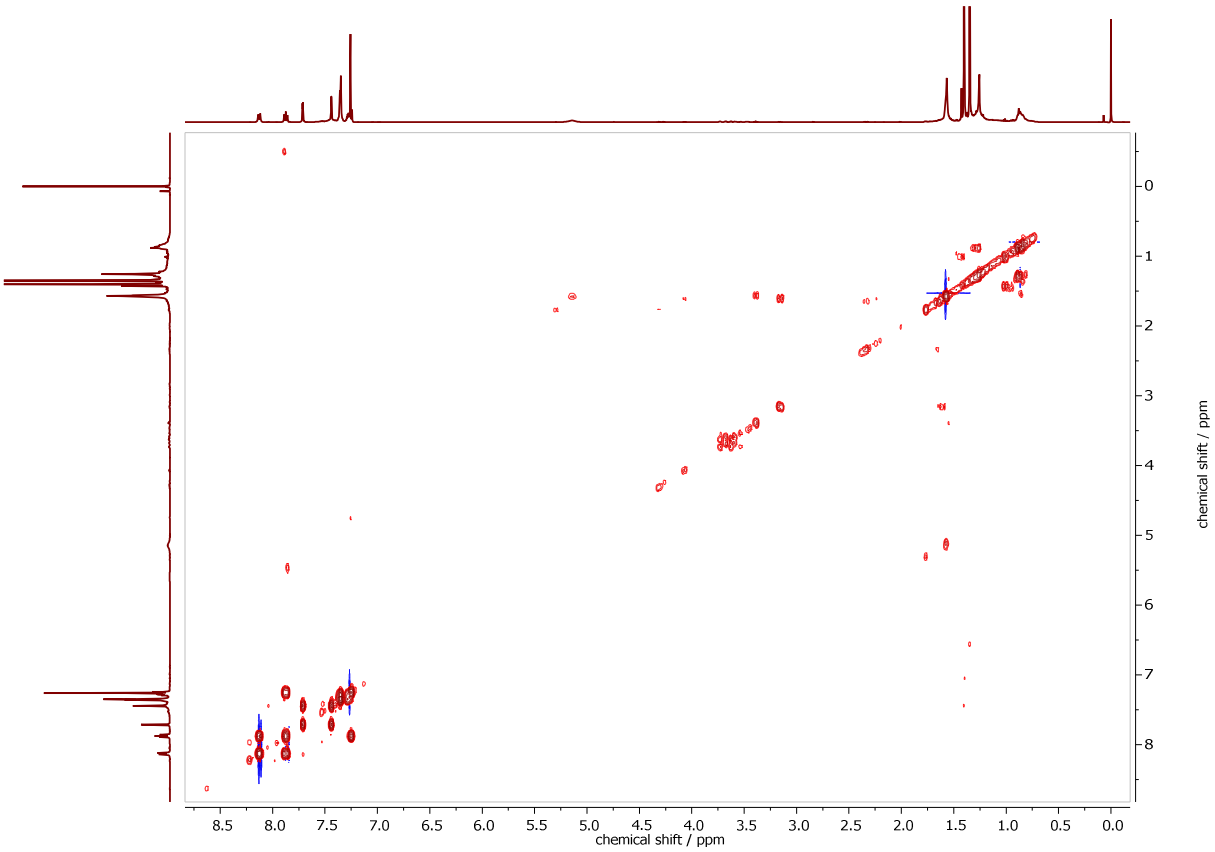

Fig. X82. $^{1}H,^{1}H$ COSY NMR spectrum of [Pd(^{tBu}L)] in $CDCl_3$.

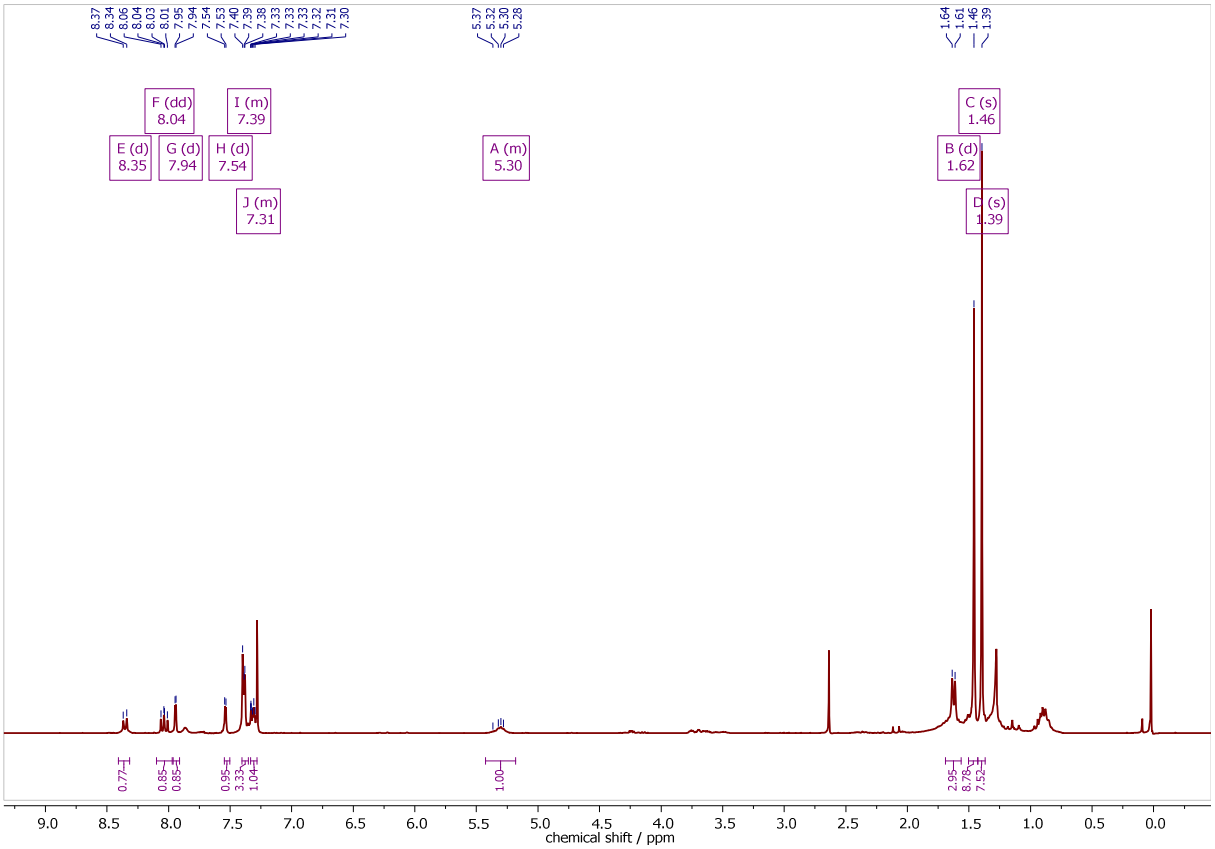

Fig. X83. ^{1}H NMR spectrum of [Pt($^{t\text{Bu}}$L)] in $CDCl_3$ at 300 MHz.

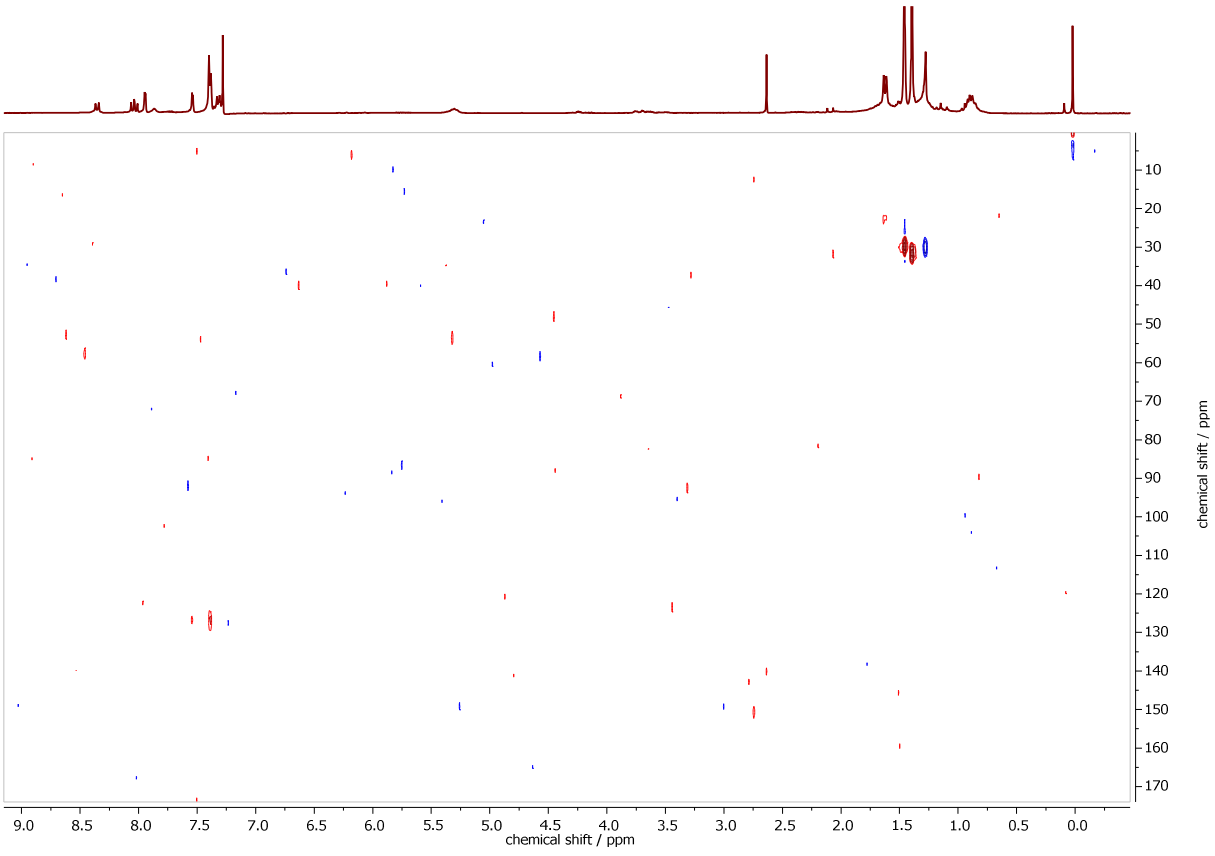

Fig. X84. ^{1}H,^{13}C HSQCed NMR spectrum of [Pt($^{t\text{Bu}}$L)] in $CDCl_3$.

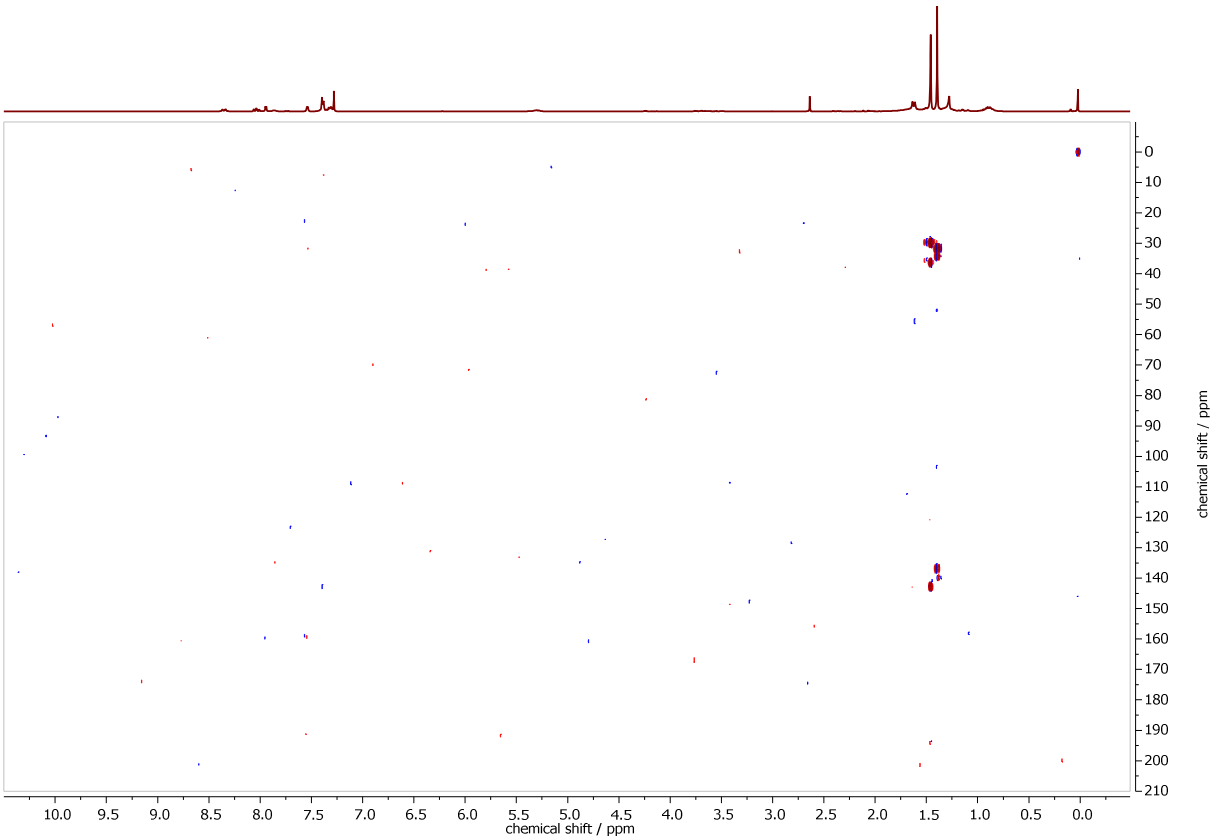

Fig. X85. $^{1}H,^{13}C$ HMBC NMR spectrum of [Pt(^{tBu}L)] in $CDCl_3$.

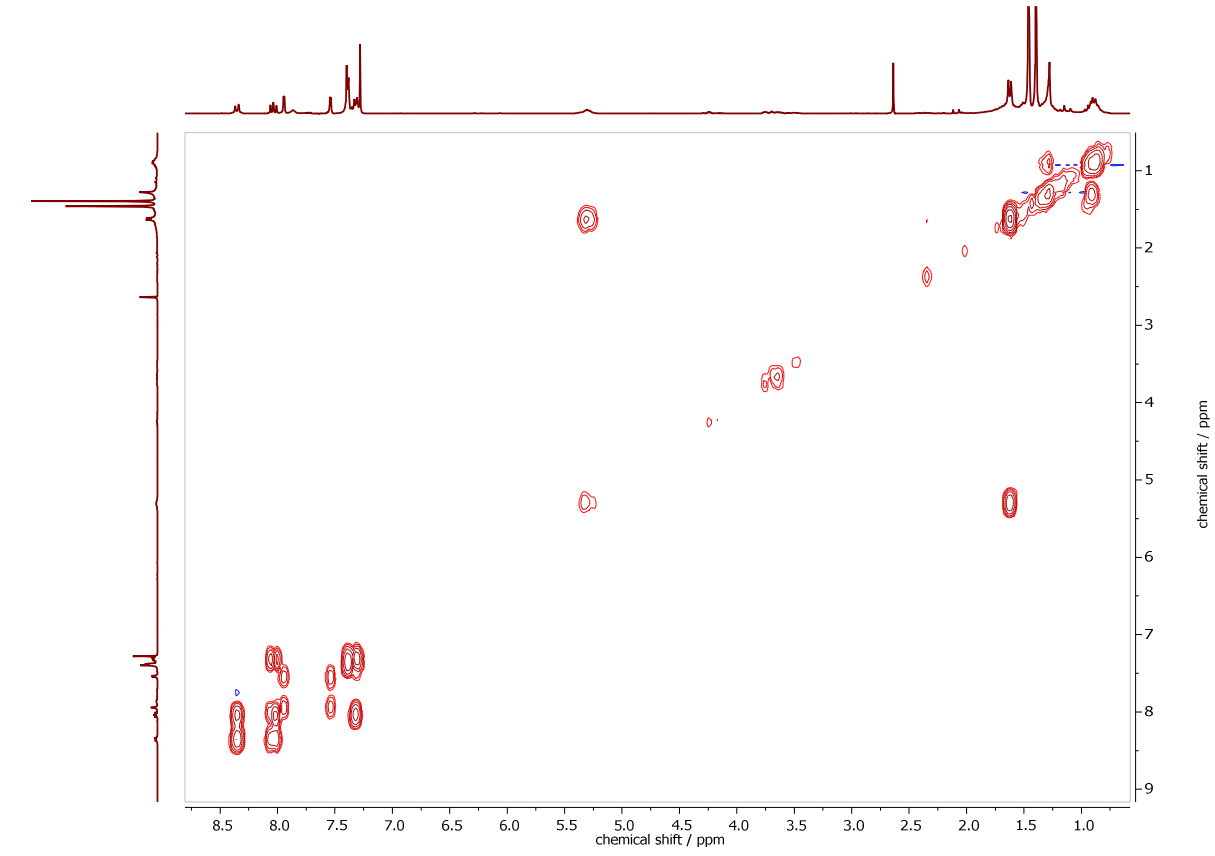

Fig. X86. $^{1}H,^{1}H$ COSY NMR spectrum of [Pt(^{tBu}L)] in $CDCl_3$.