Electronic supplementary materials

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Functionalized heterocycle-appended porphyrins: catalysis matters

Inna A. Abdulaeva, Kirill P. Birin, Daria A. Polivanovskaia, Yulia G. Gorbunova, Aslan Yu. Tsivadze

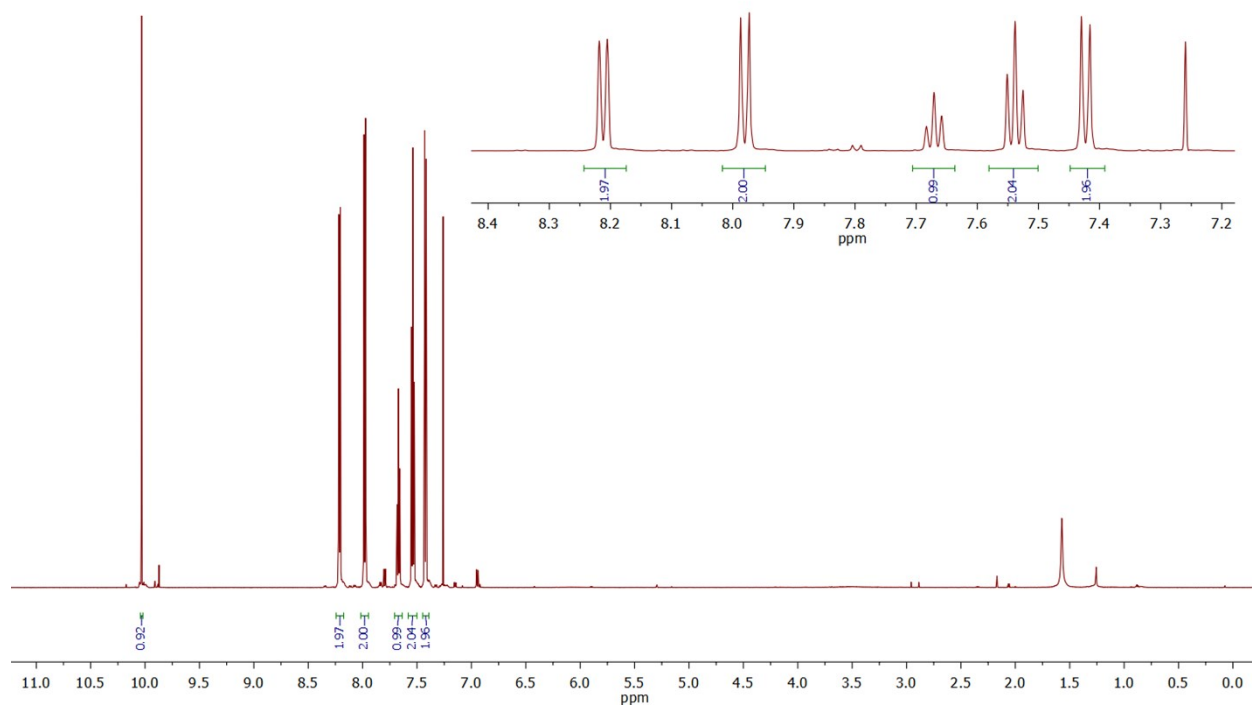## CONTENTS

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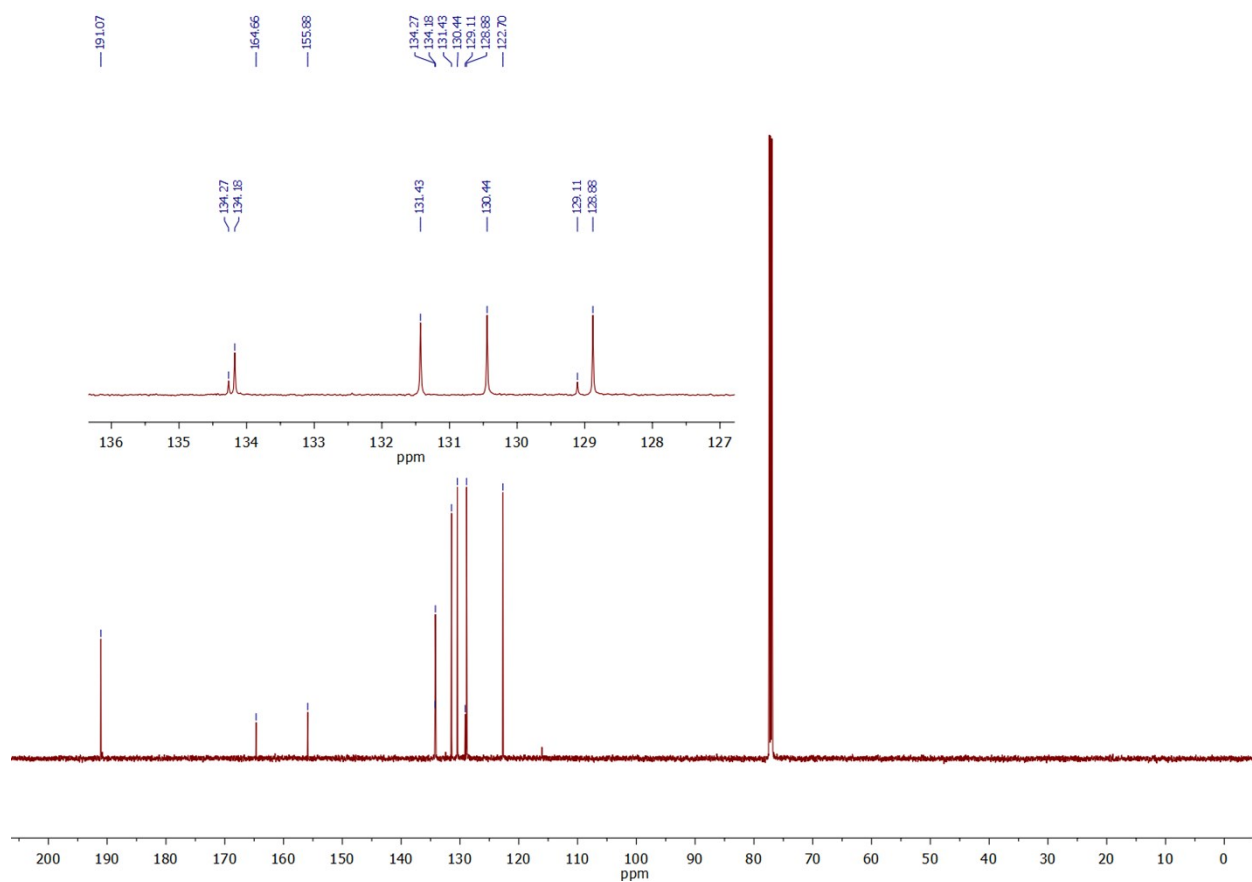Figure S 1. ^{1}H-NMR spectrum of **3e** (CDCl$_3$).

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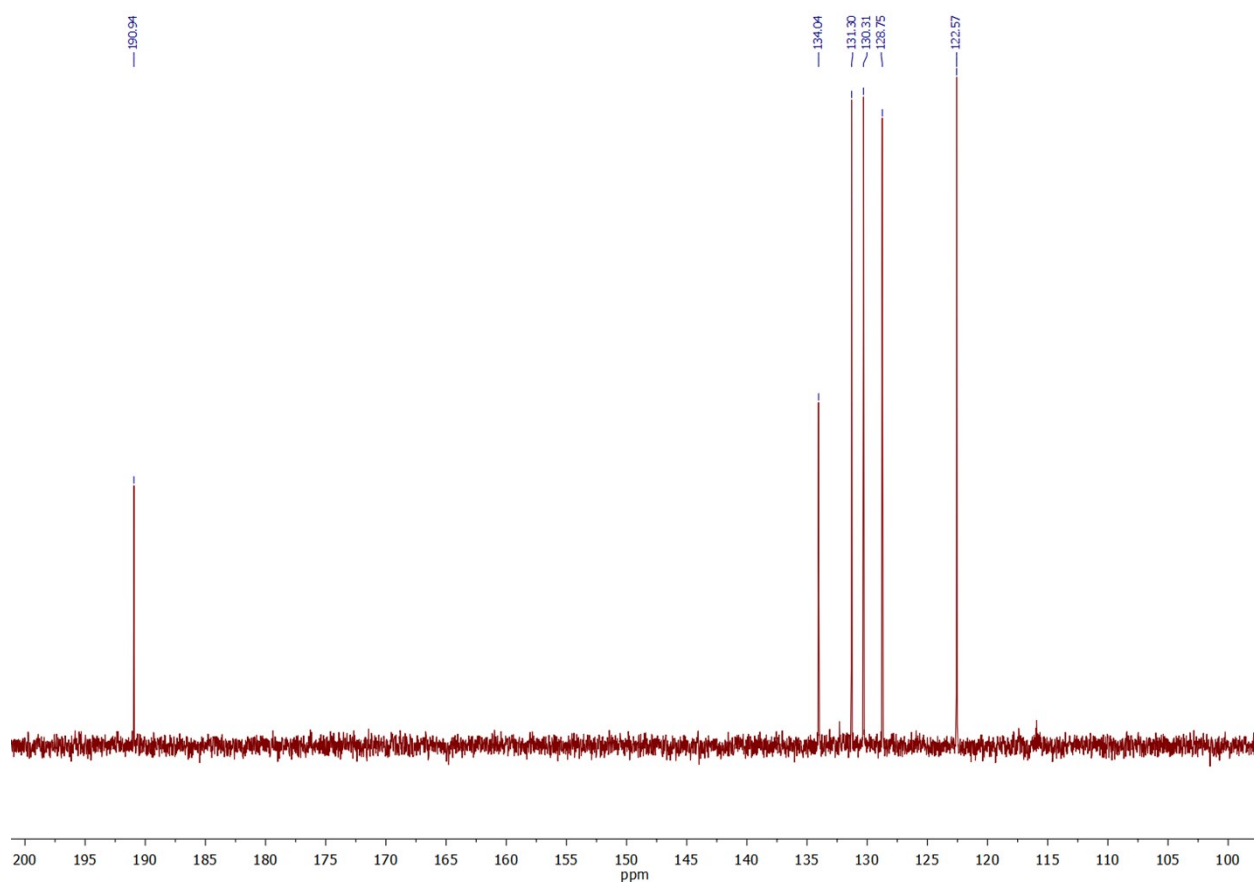
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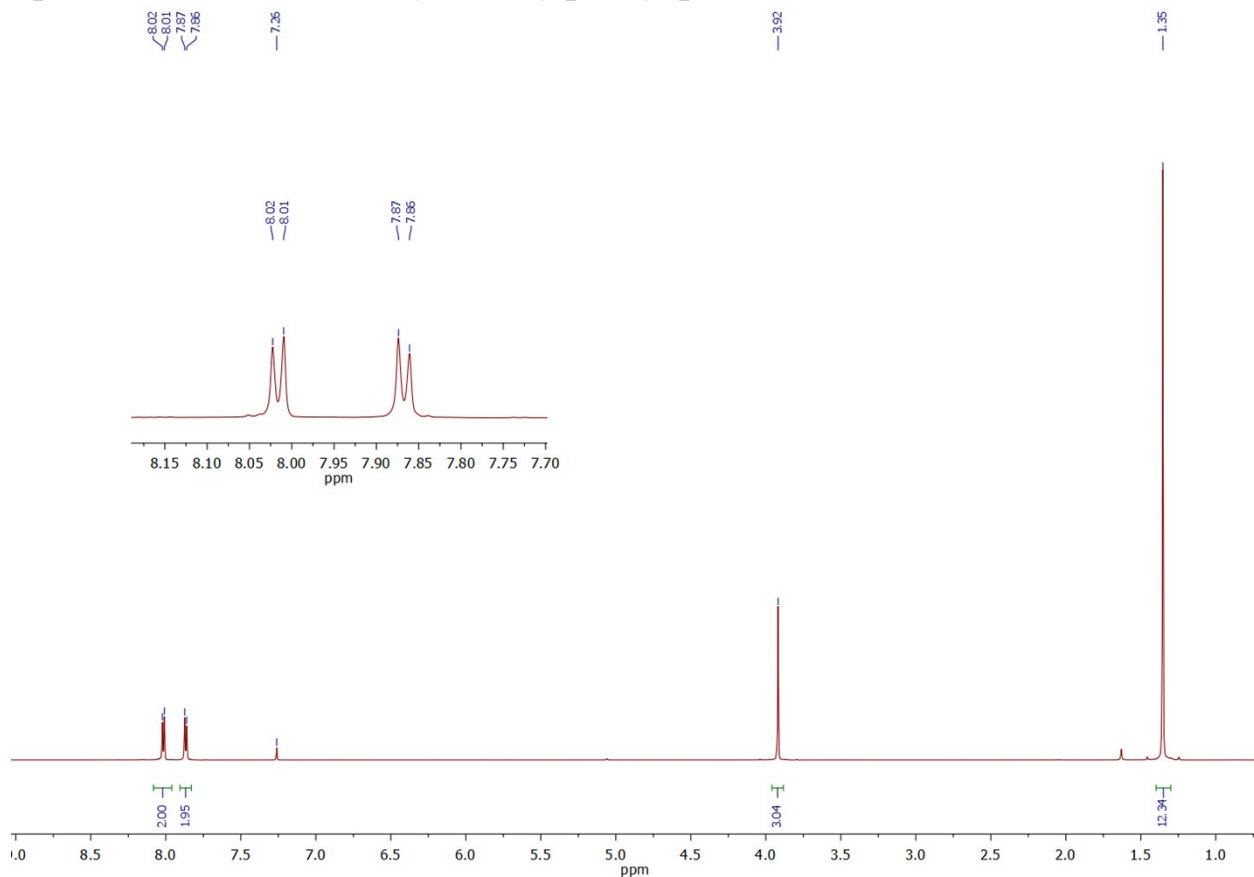

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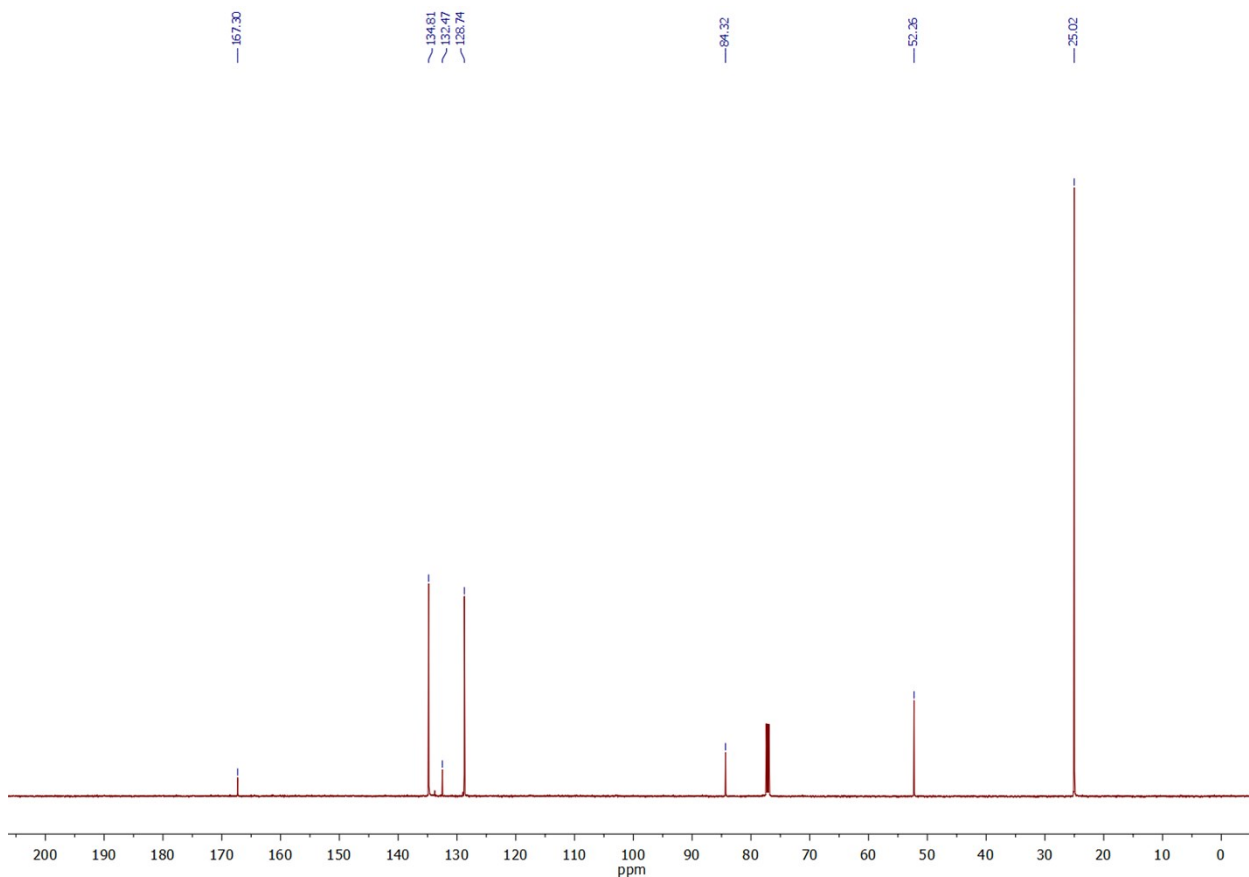
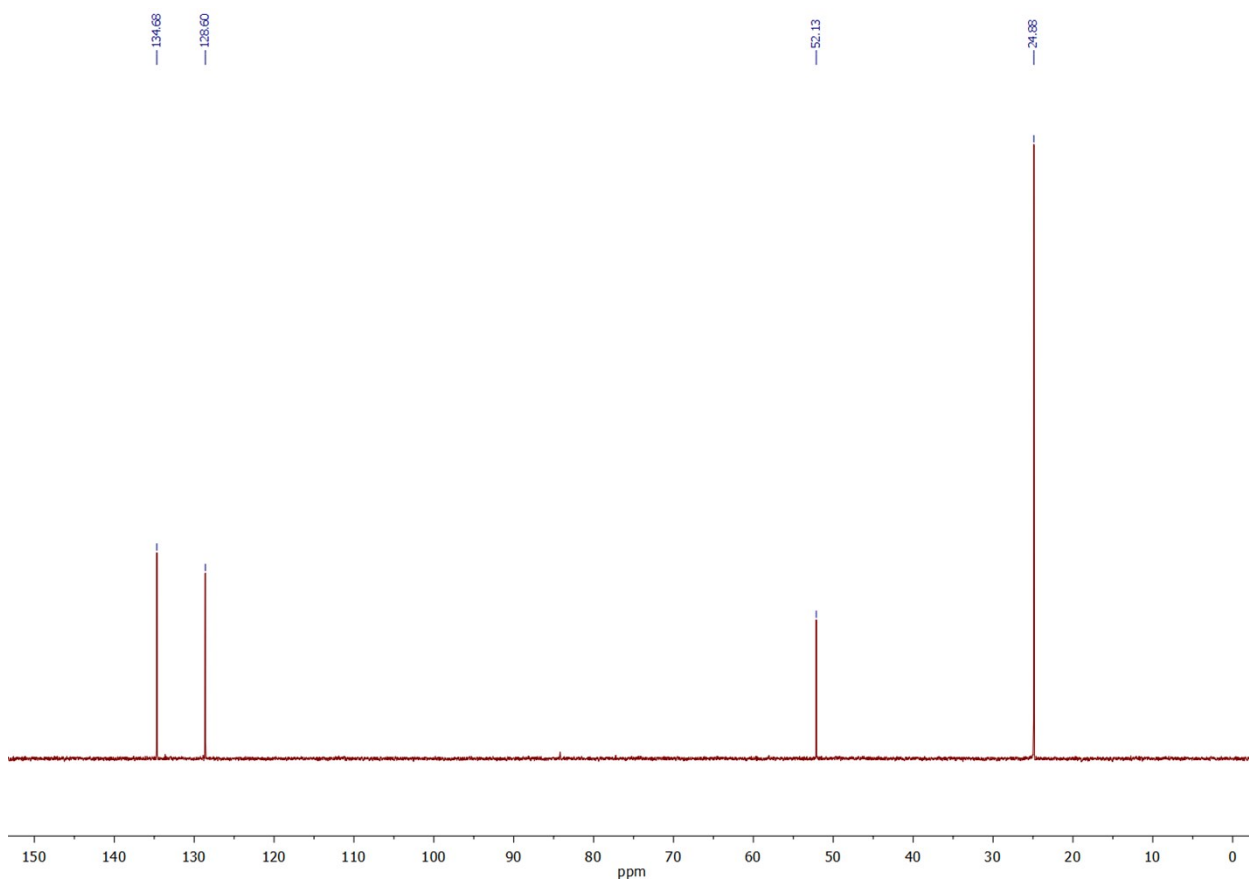*Figure S 5. ^{13}C-NMR spectrum of 4-m*ethoxycarbonylphenyl pinacolborane (CDCl$_3$).

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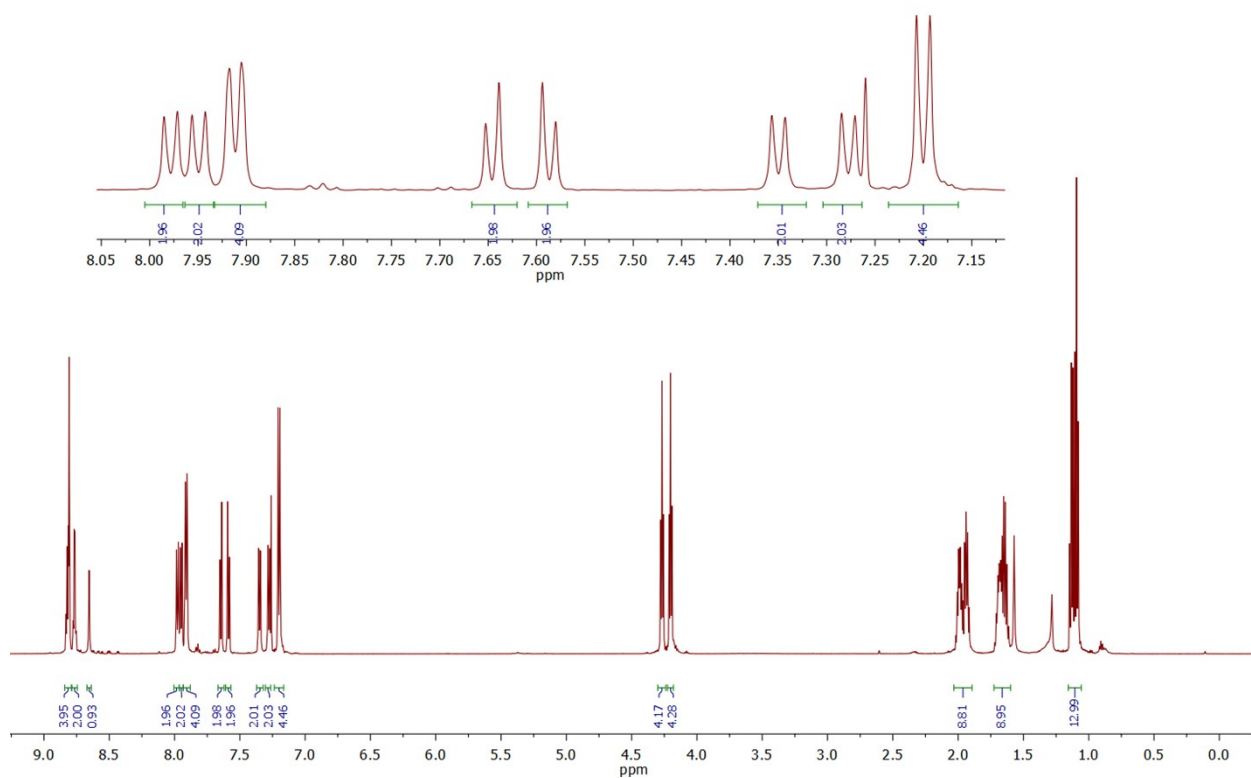
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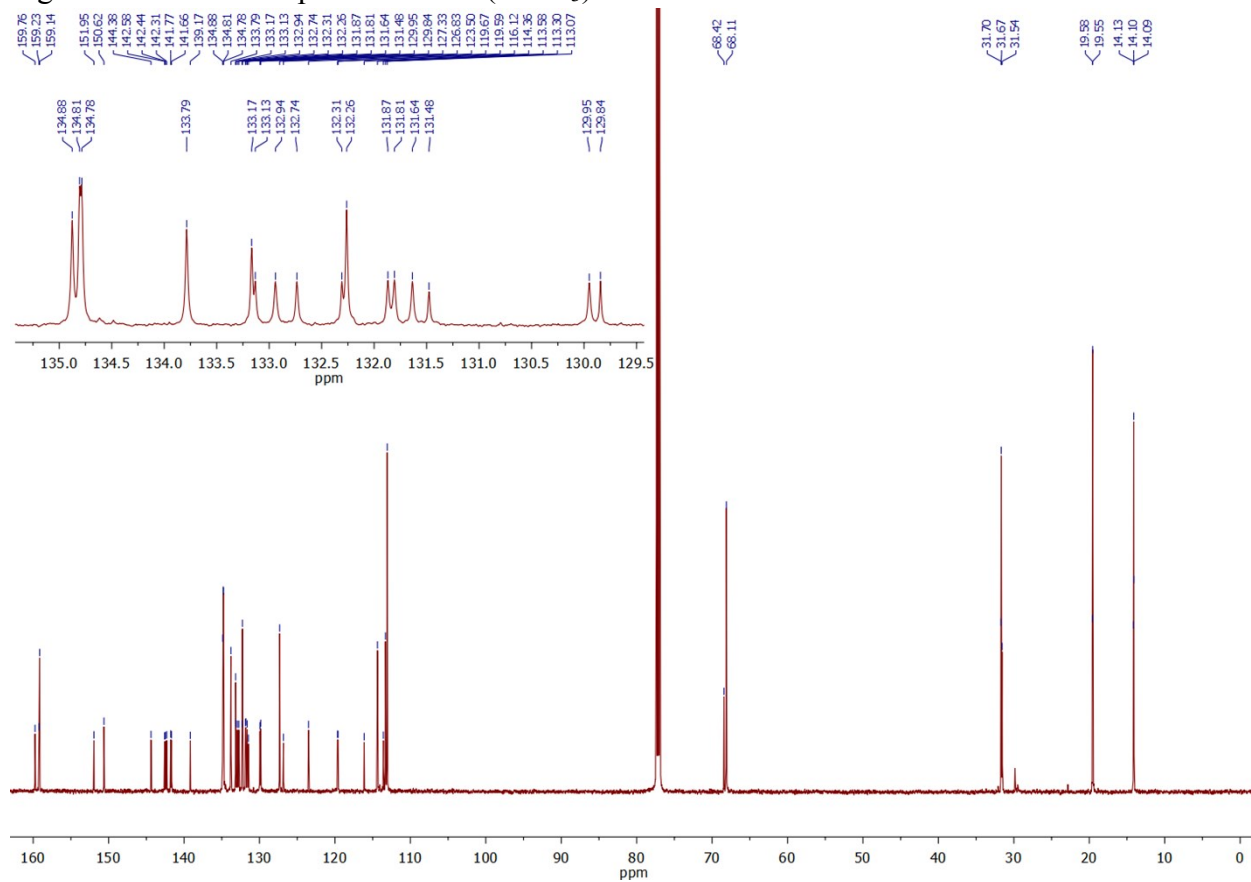

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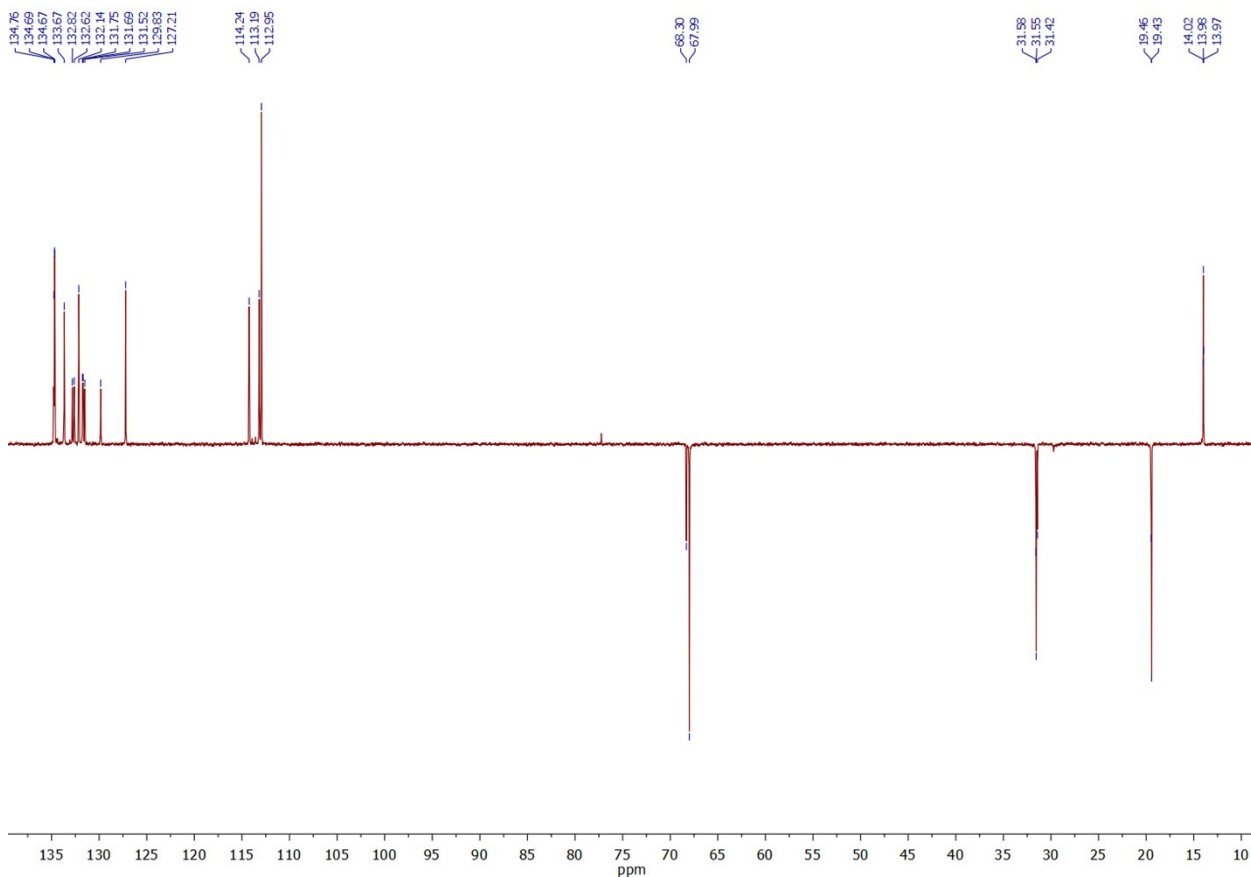
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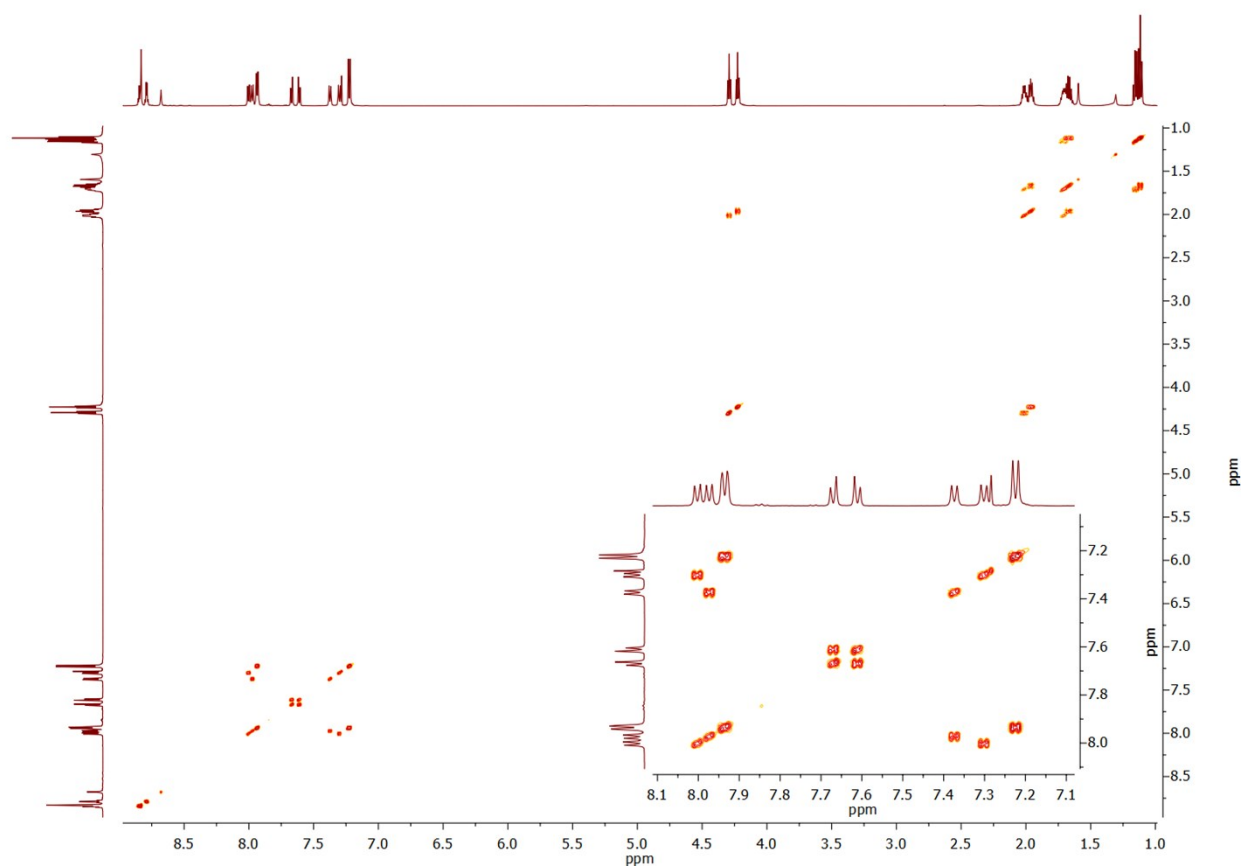
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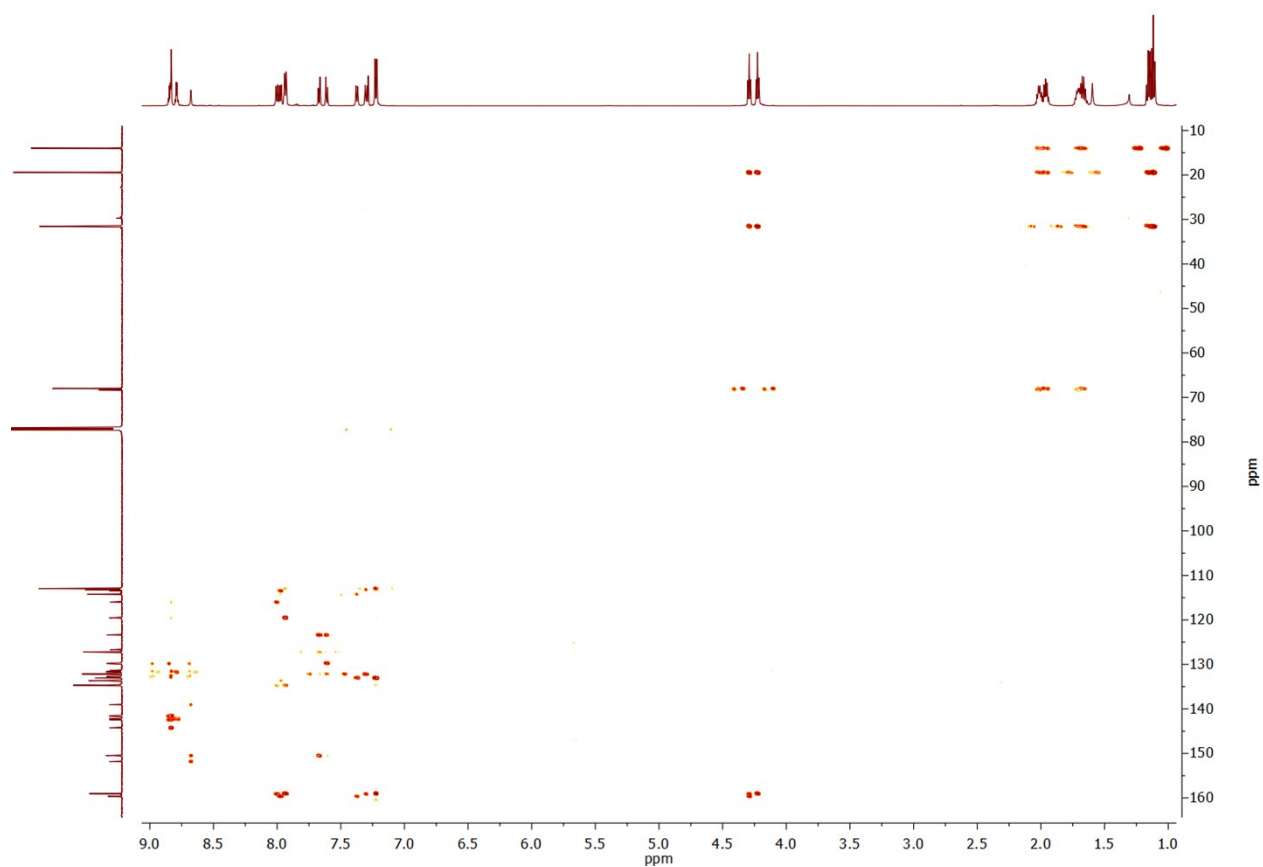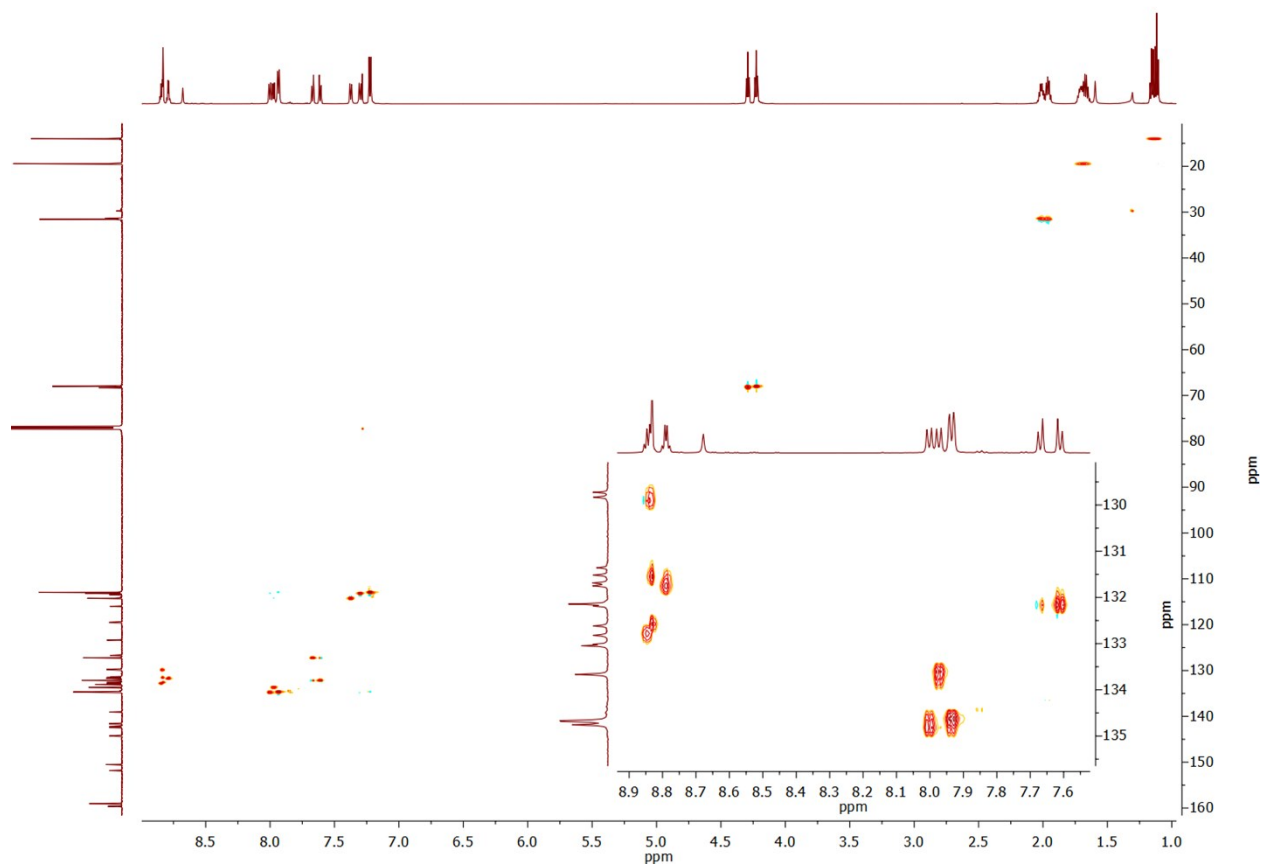
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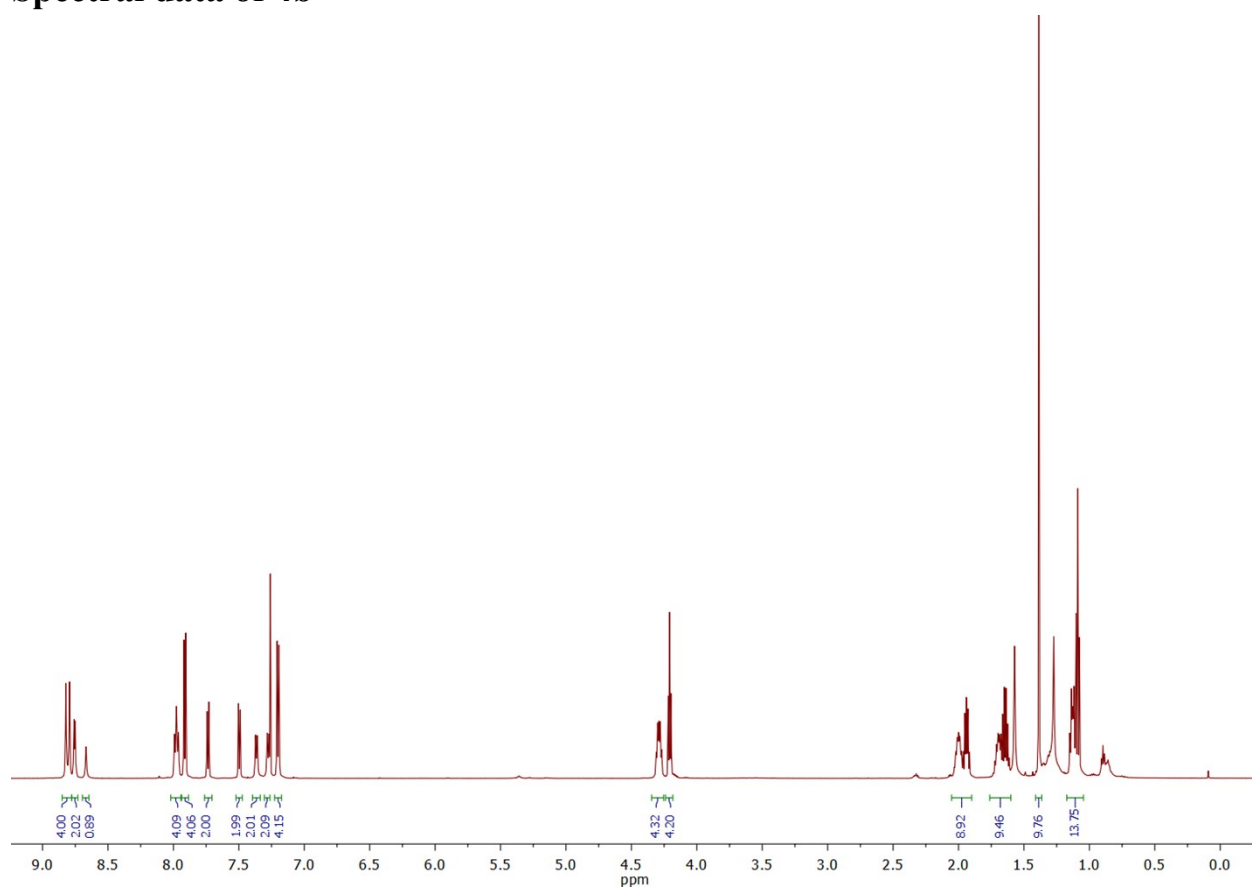
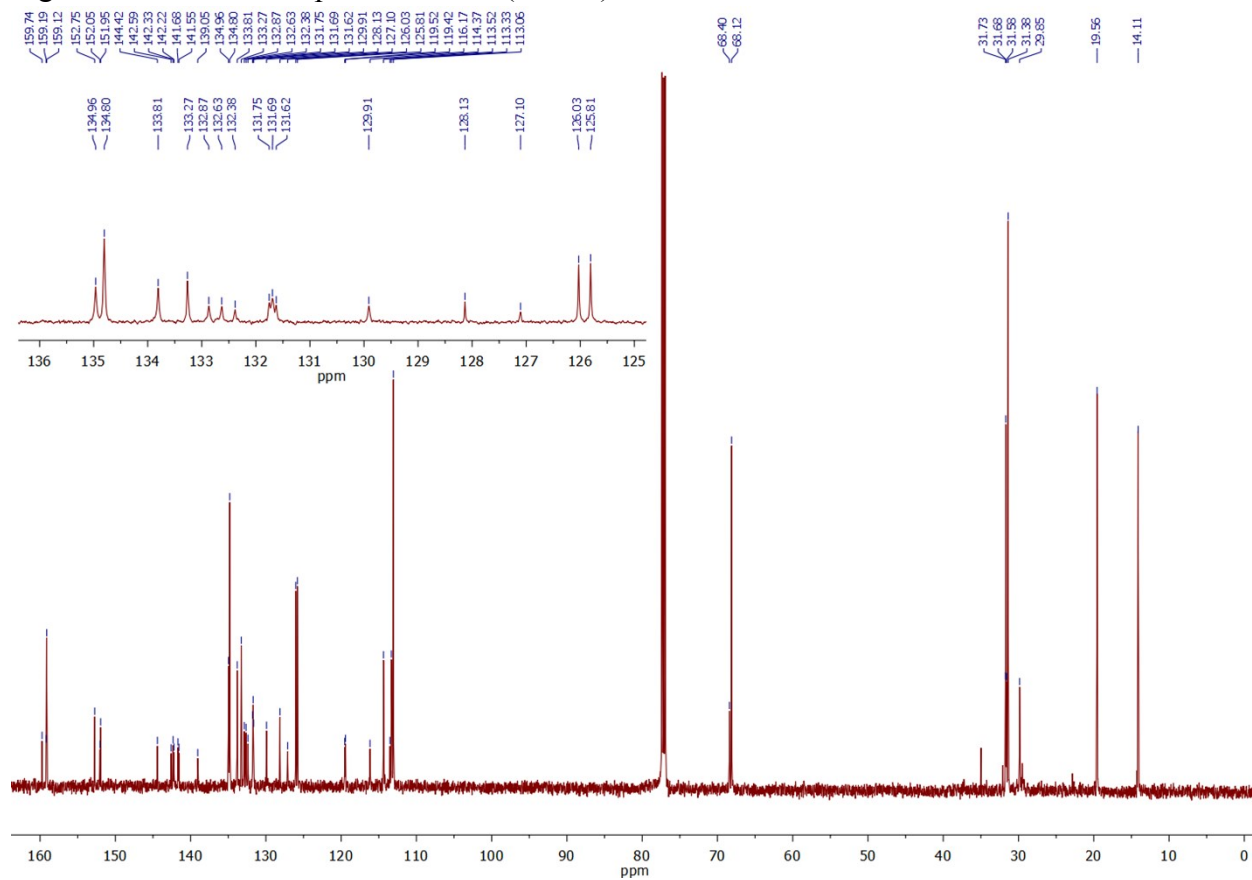Figure S 13. ^{1}H-NMR spectrum of **4b** (CDCl$_3$).
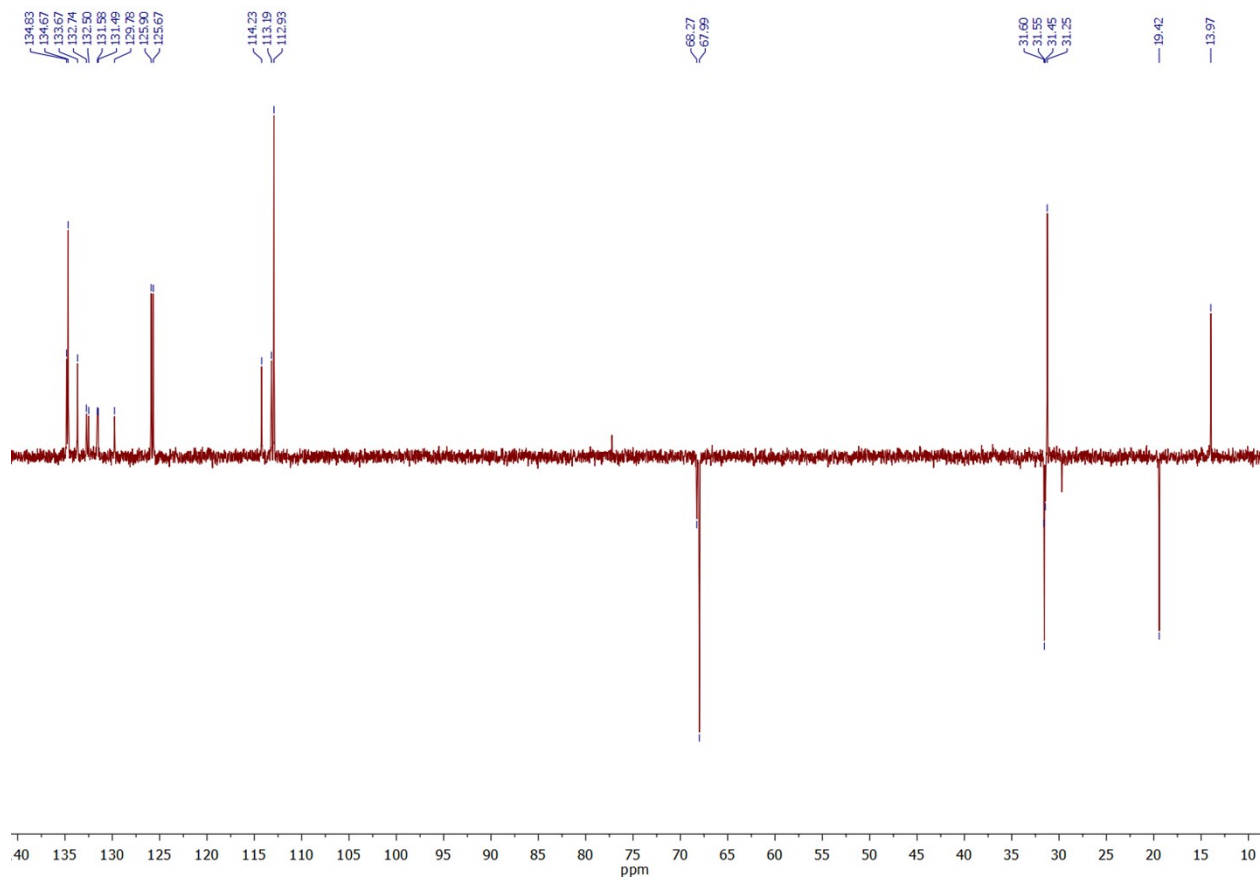

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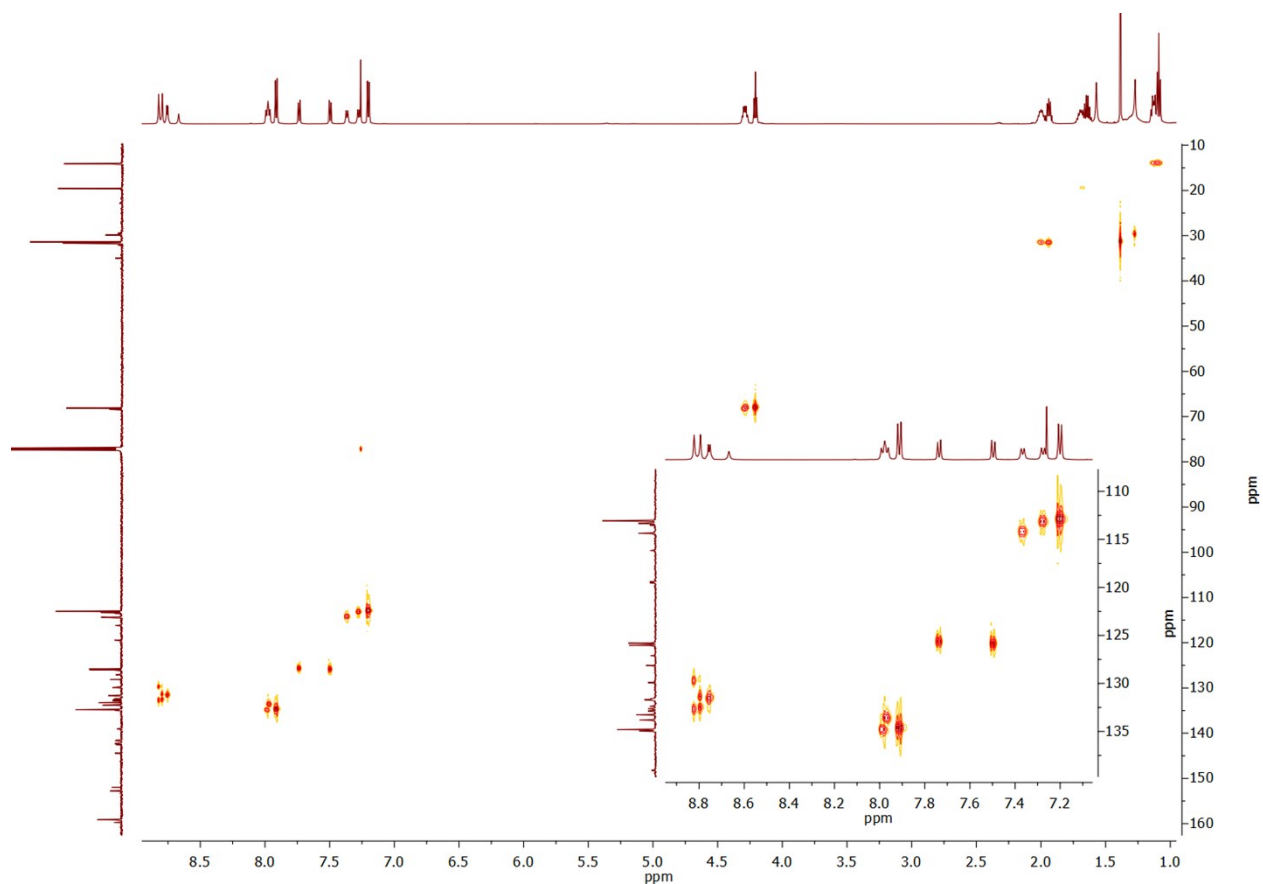
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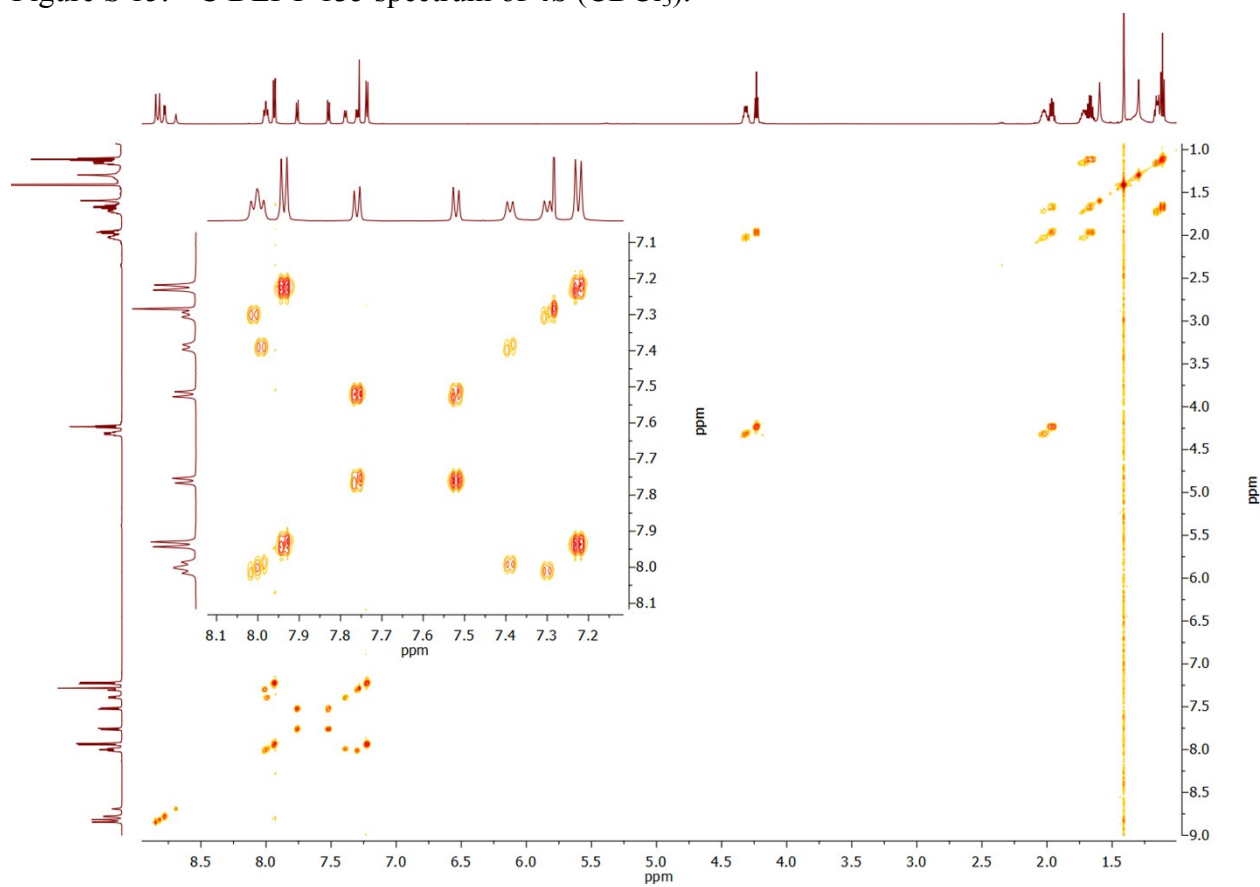
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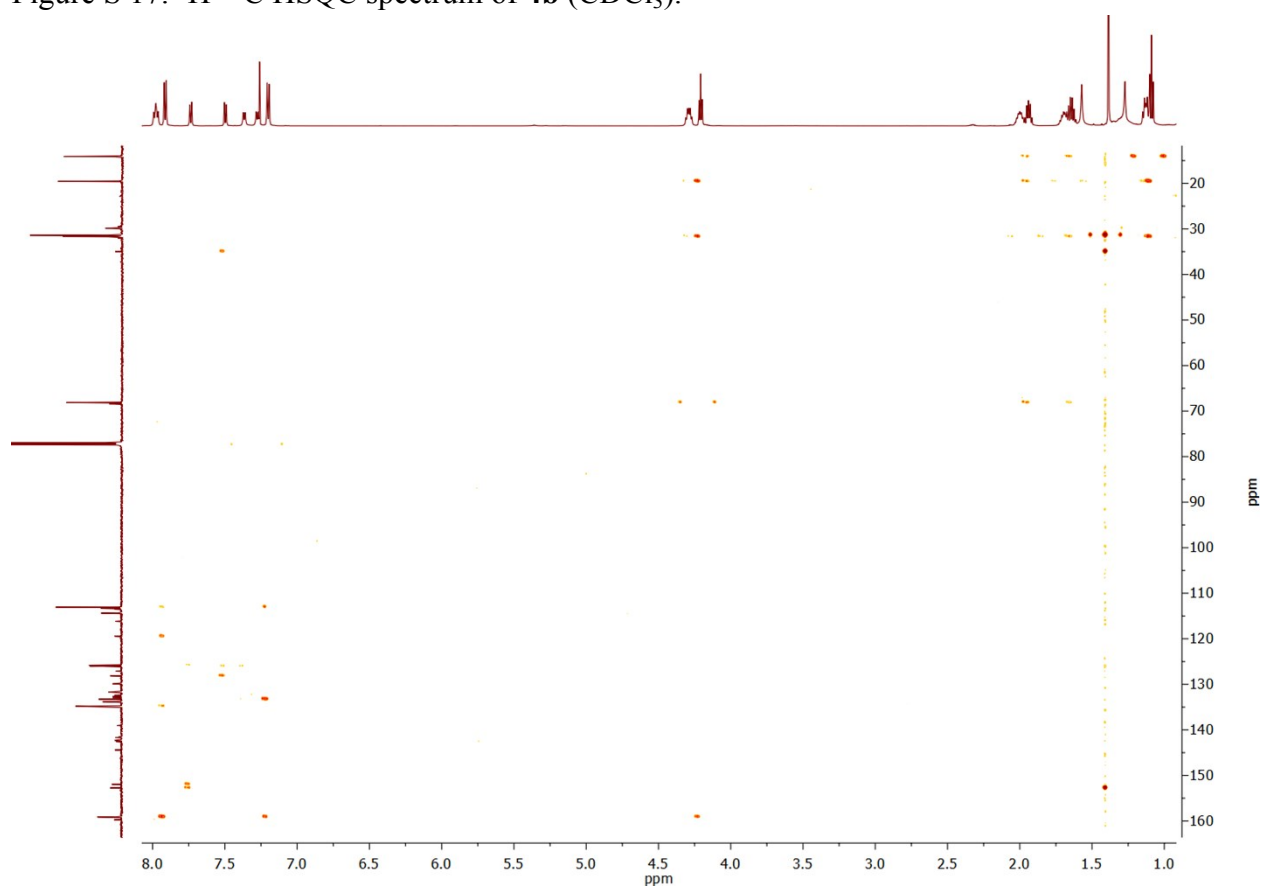
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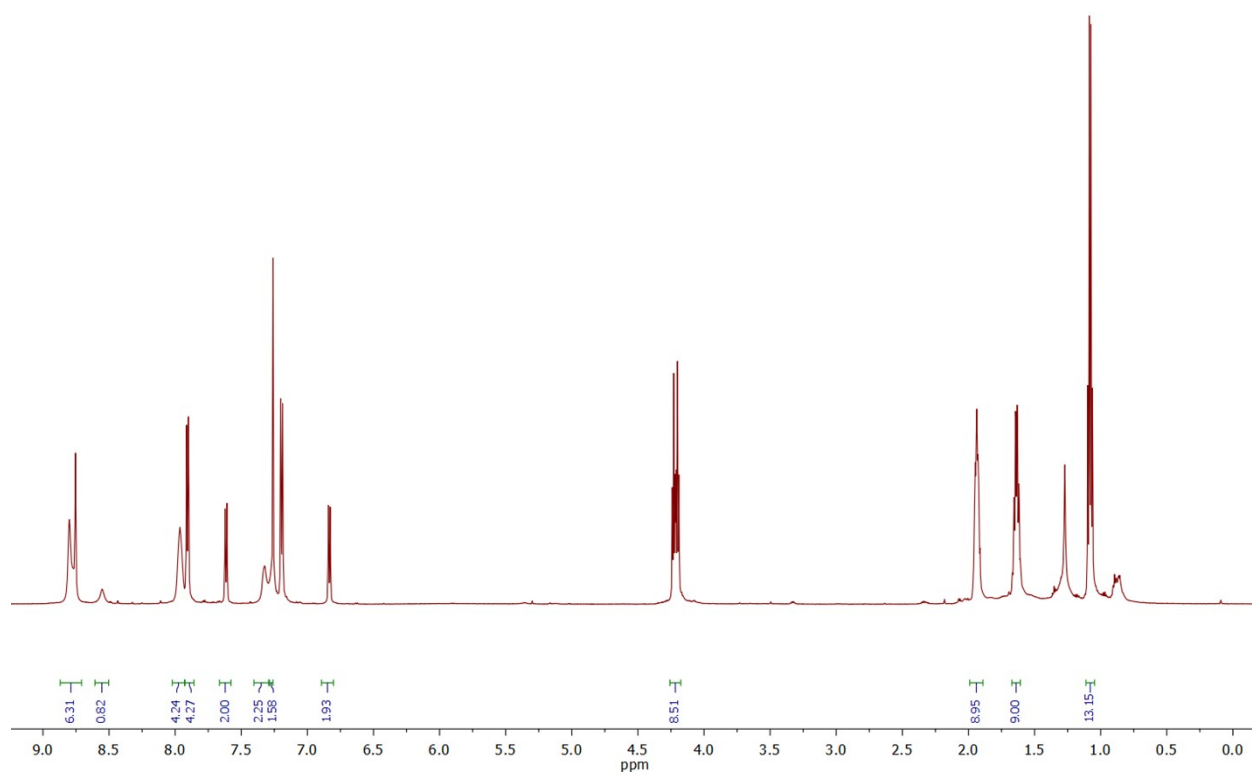
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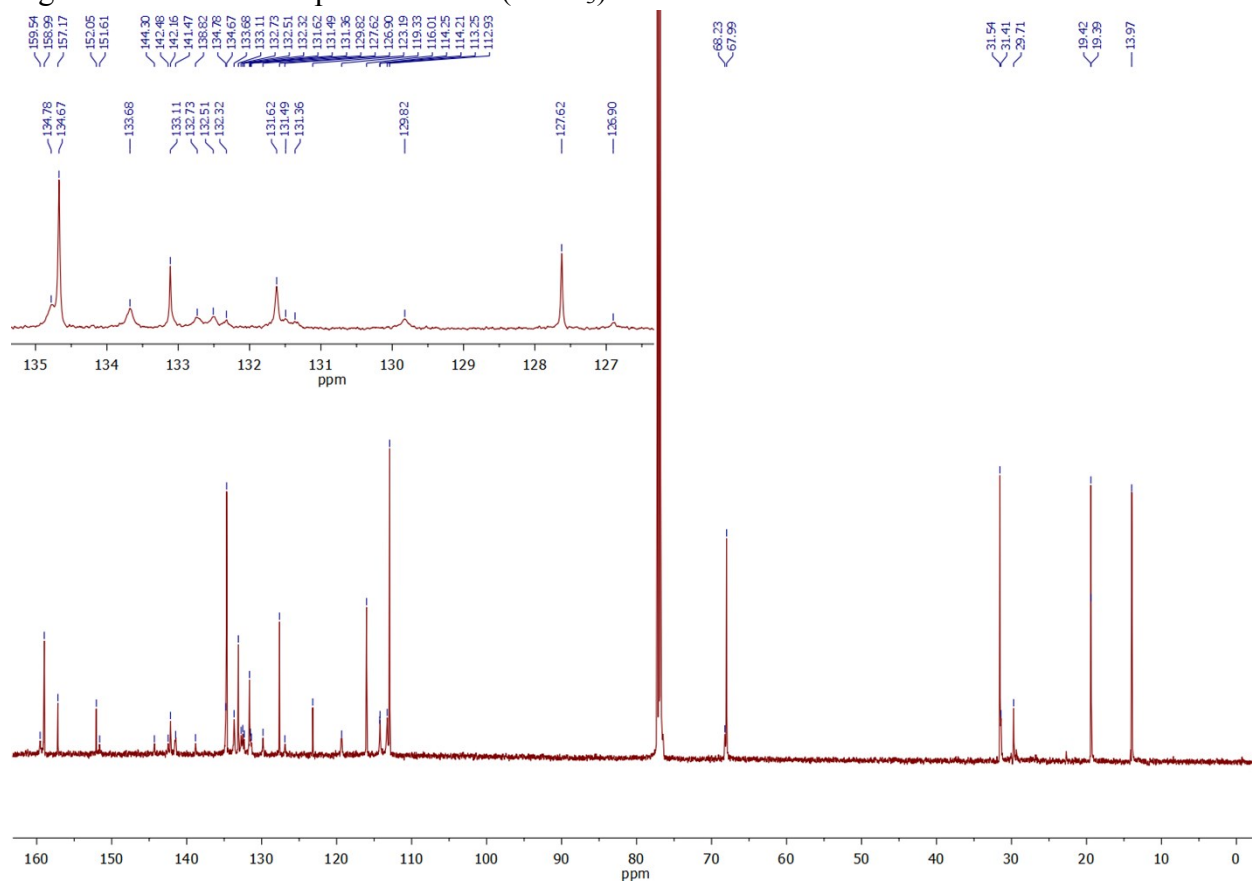

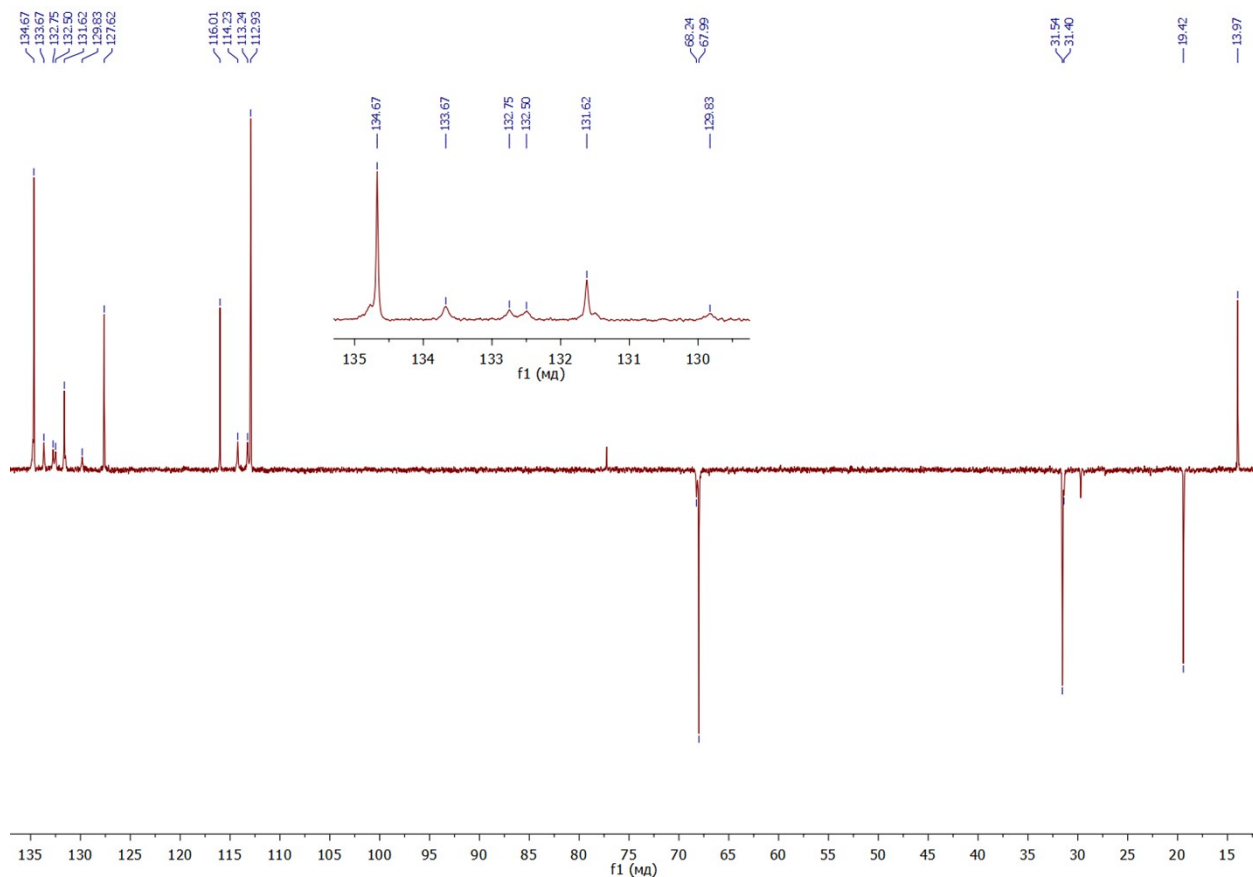Figure S 20. ^{13}C-NMR spectrum of **4c** (CDCl$_3$).

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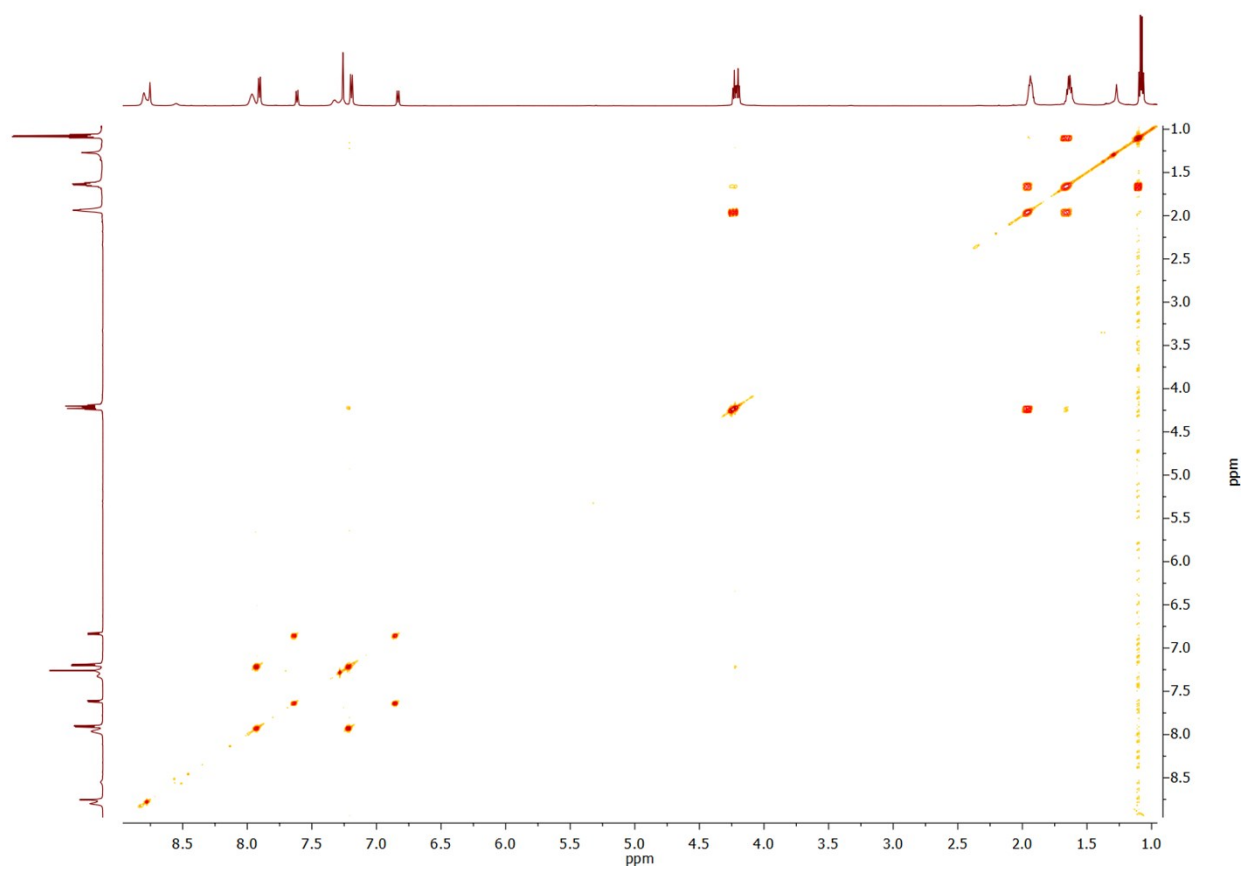Figure S 21. ^{13}C DEPT-135 spectrum of **4c** (CDCl$_3$).

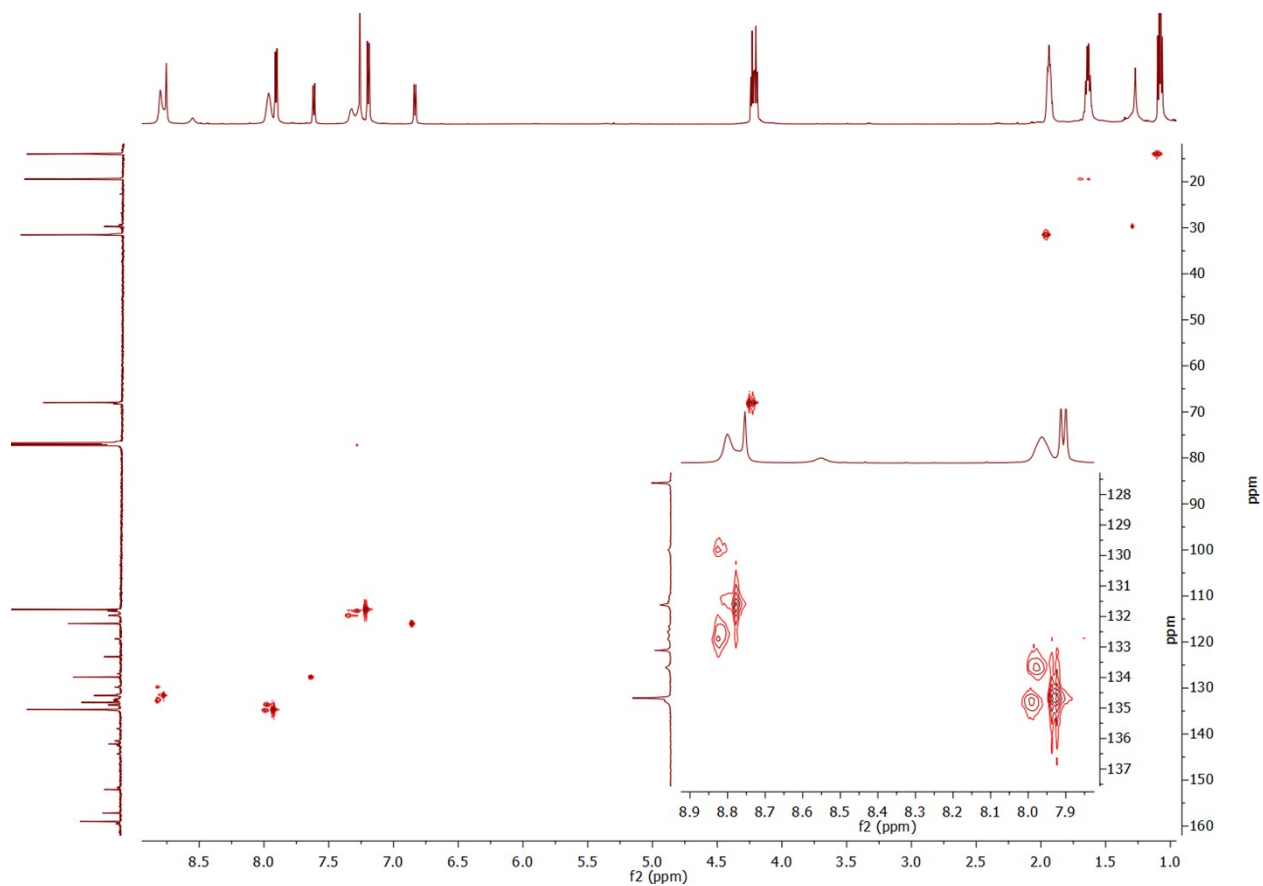Figure S 22. COSY spectrum of **4c** (CDCl$_3$).
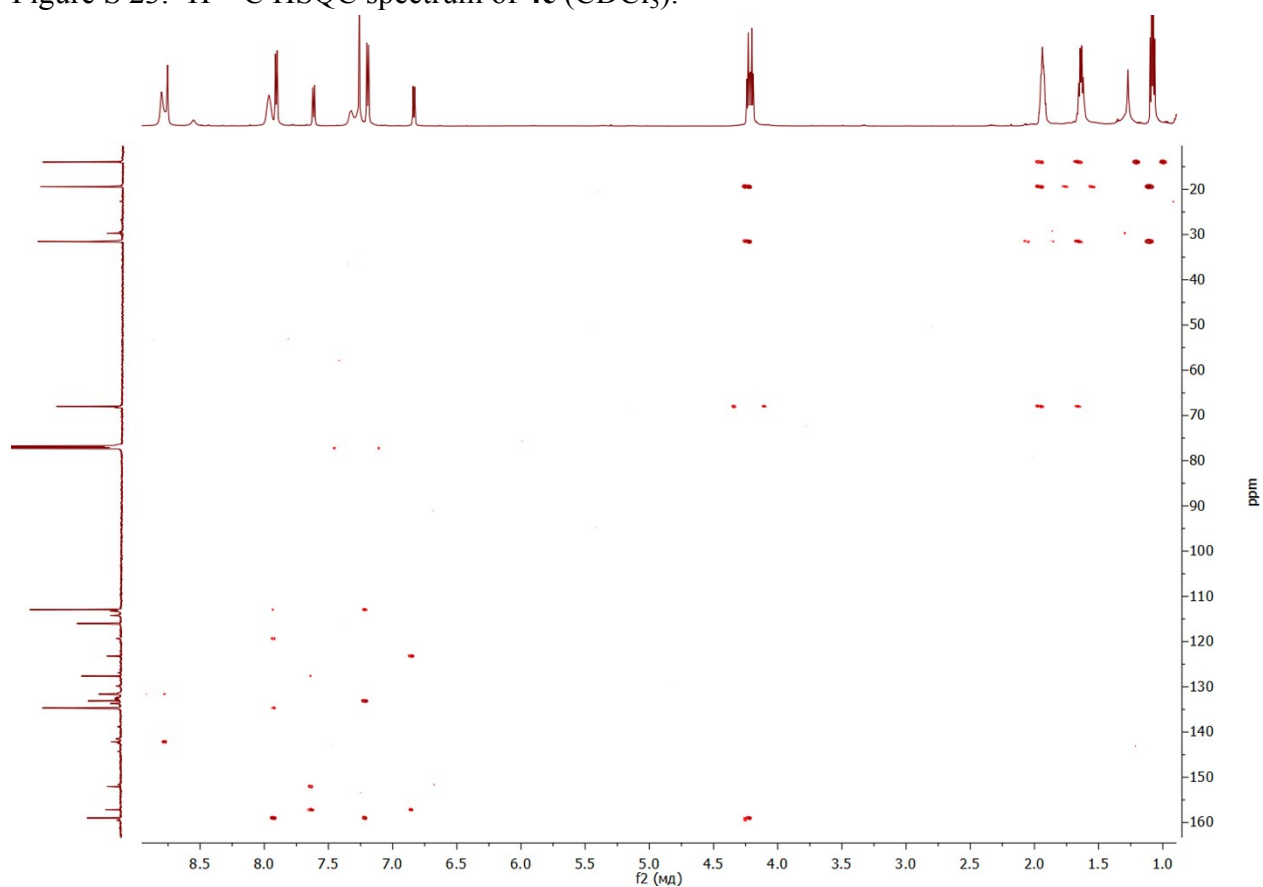
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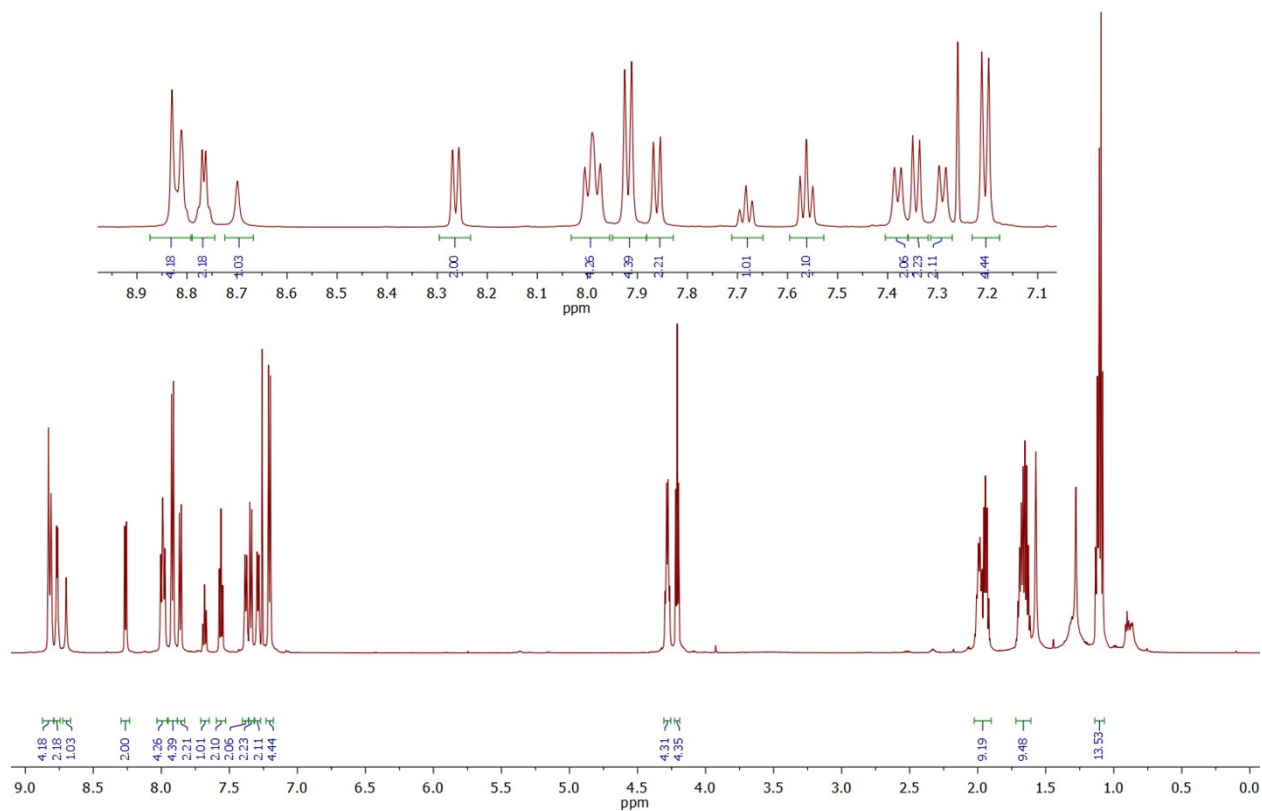
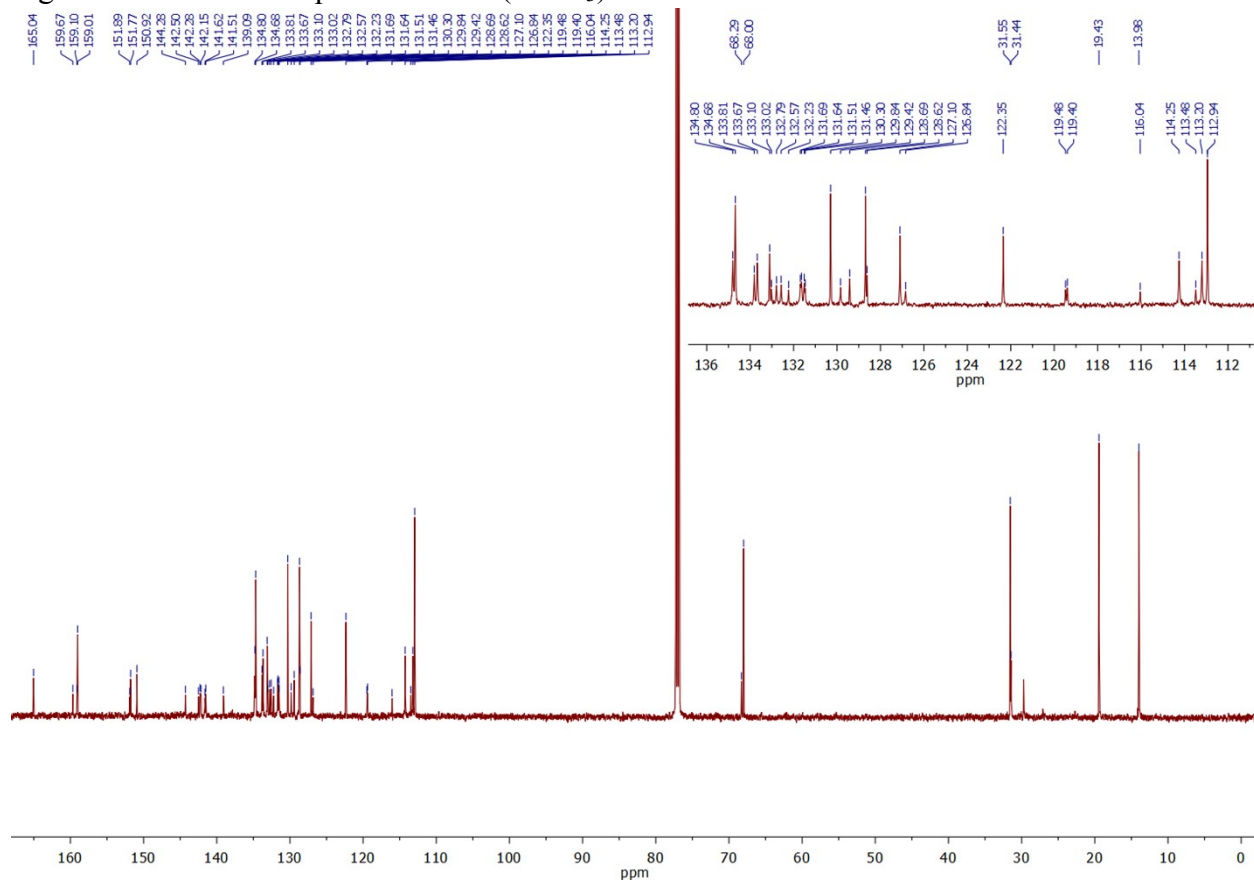# Spectral data of 4e

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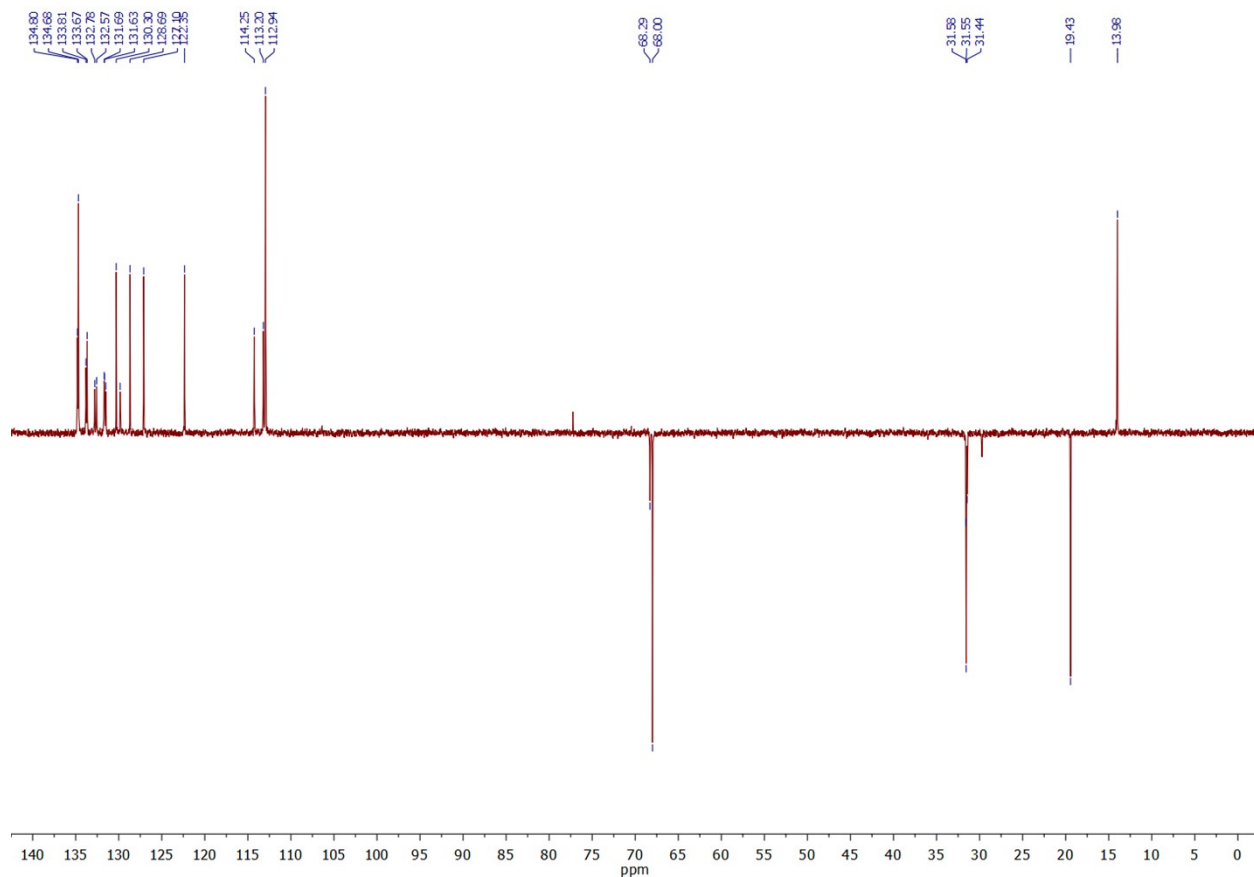Figure S 26. ^{13}C-NMR spectrum of **4e** (CDCl$_3$).

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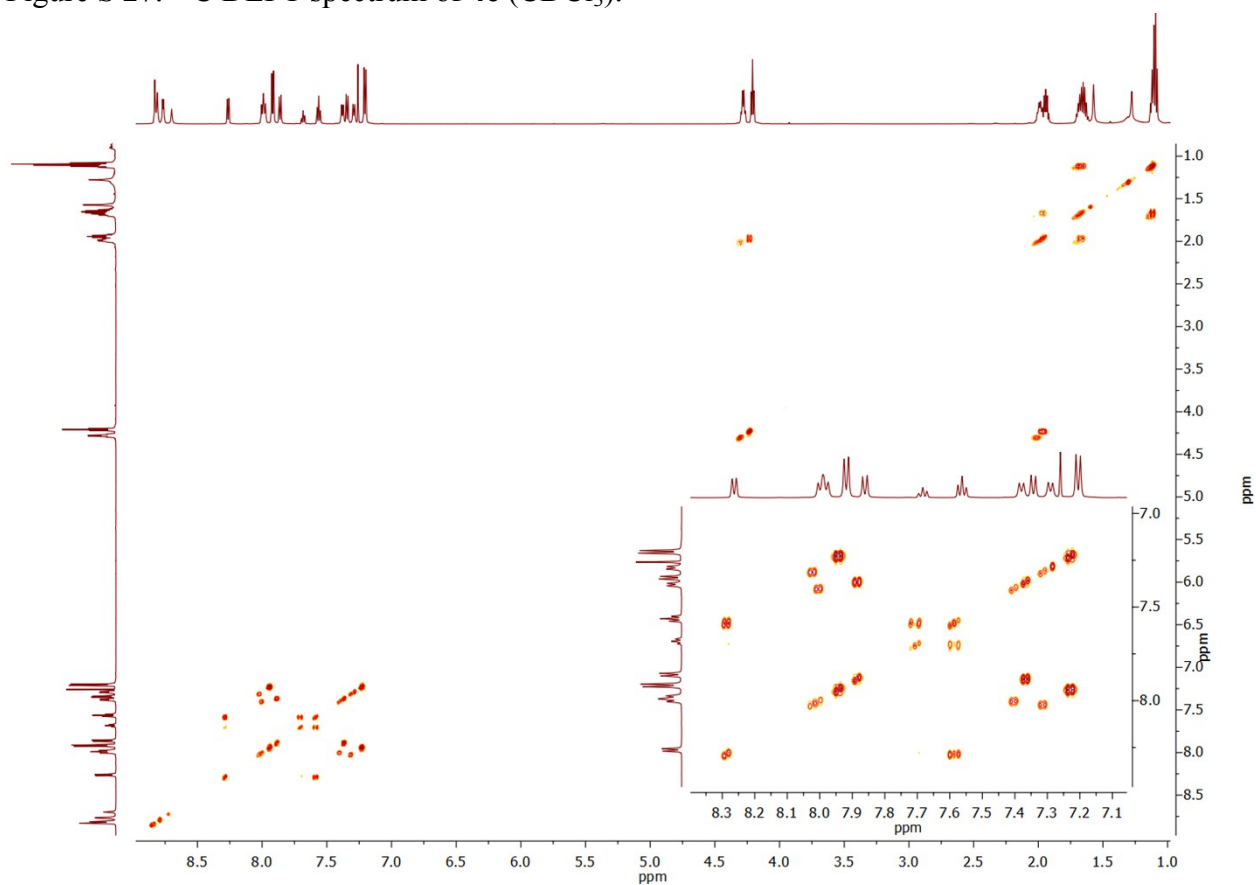
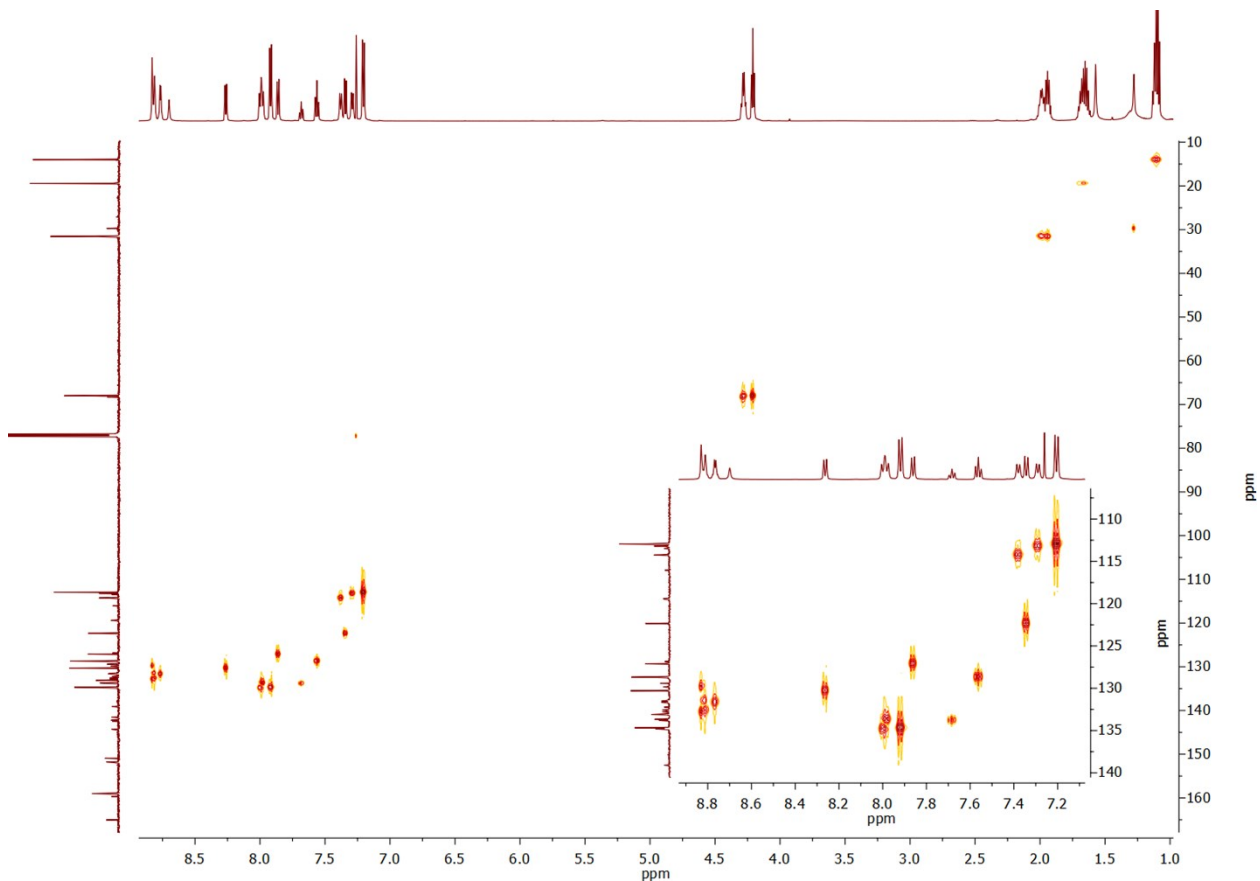

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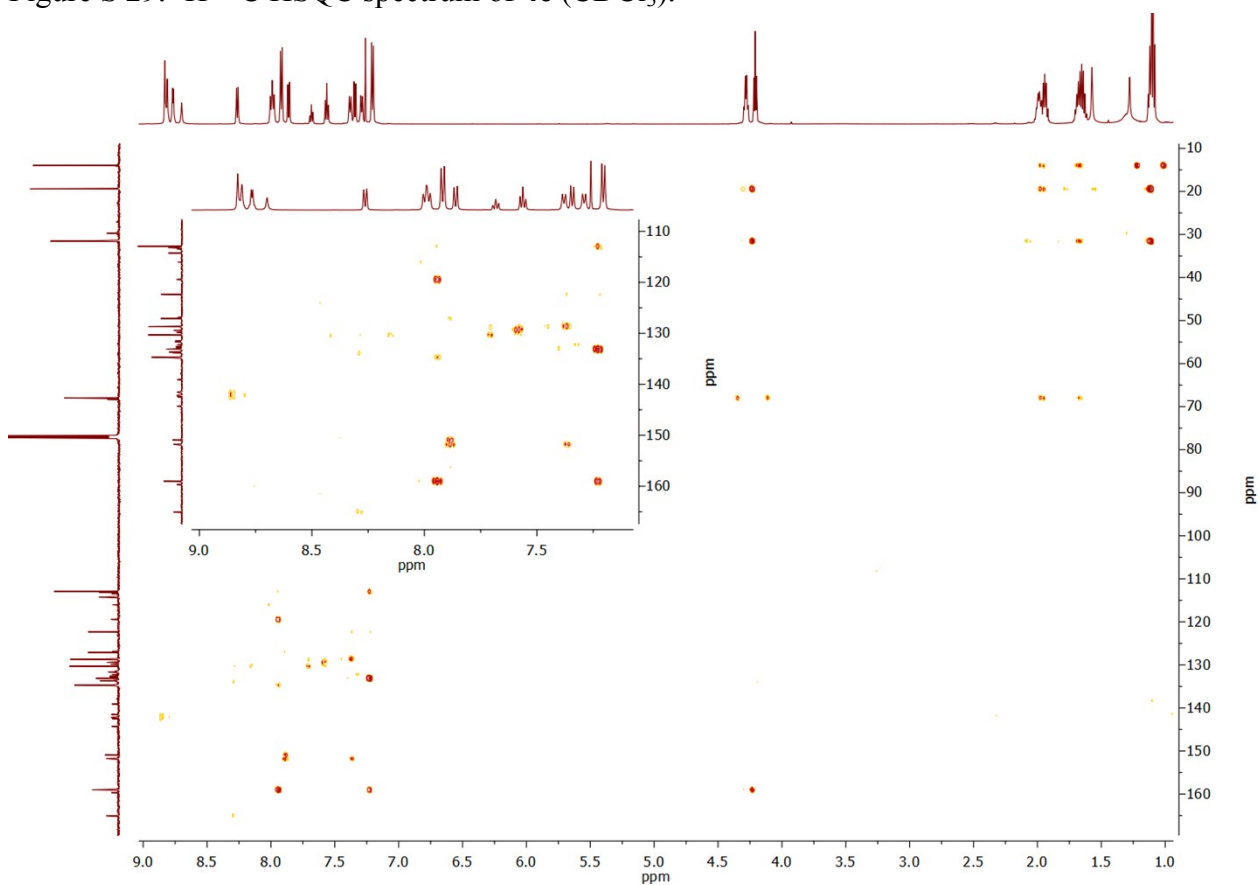15

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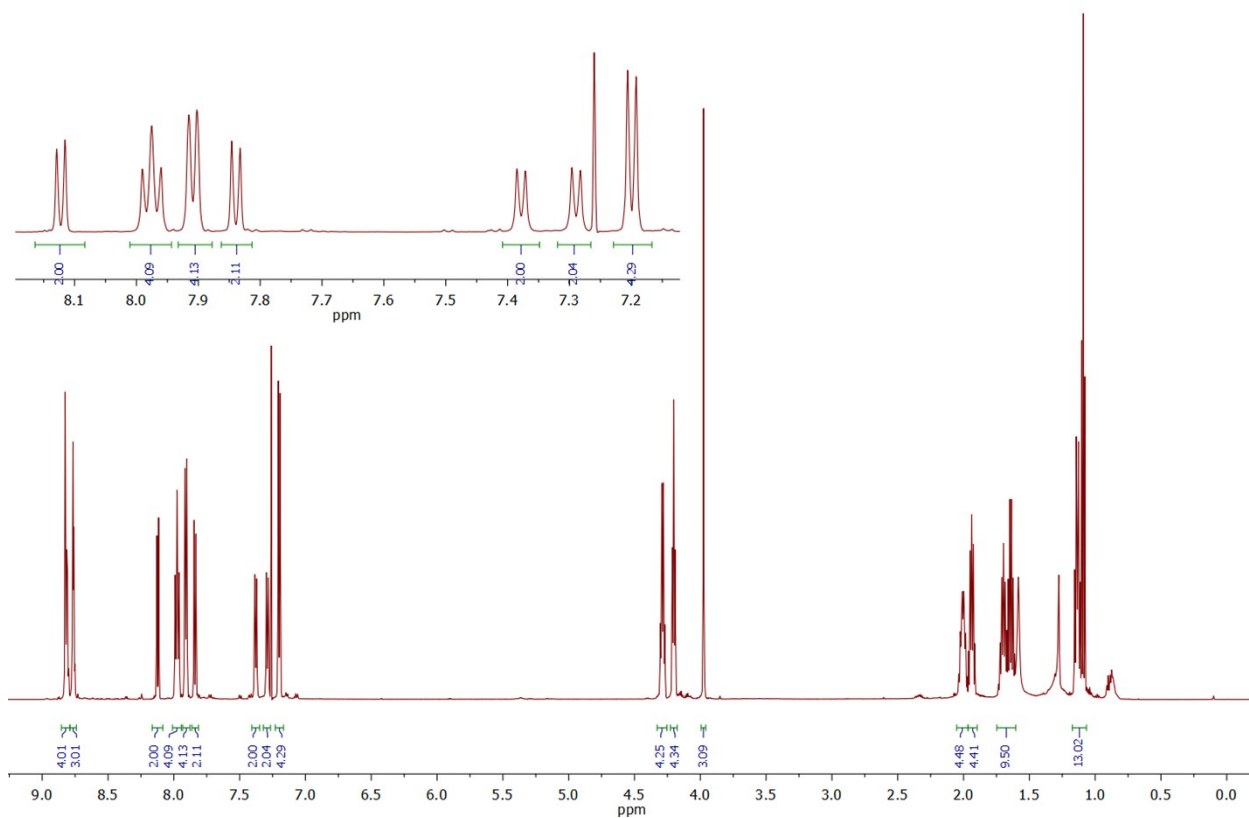
Spectral data of 4f

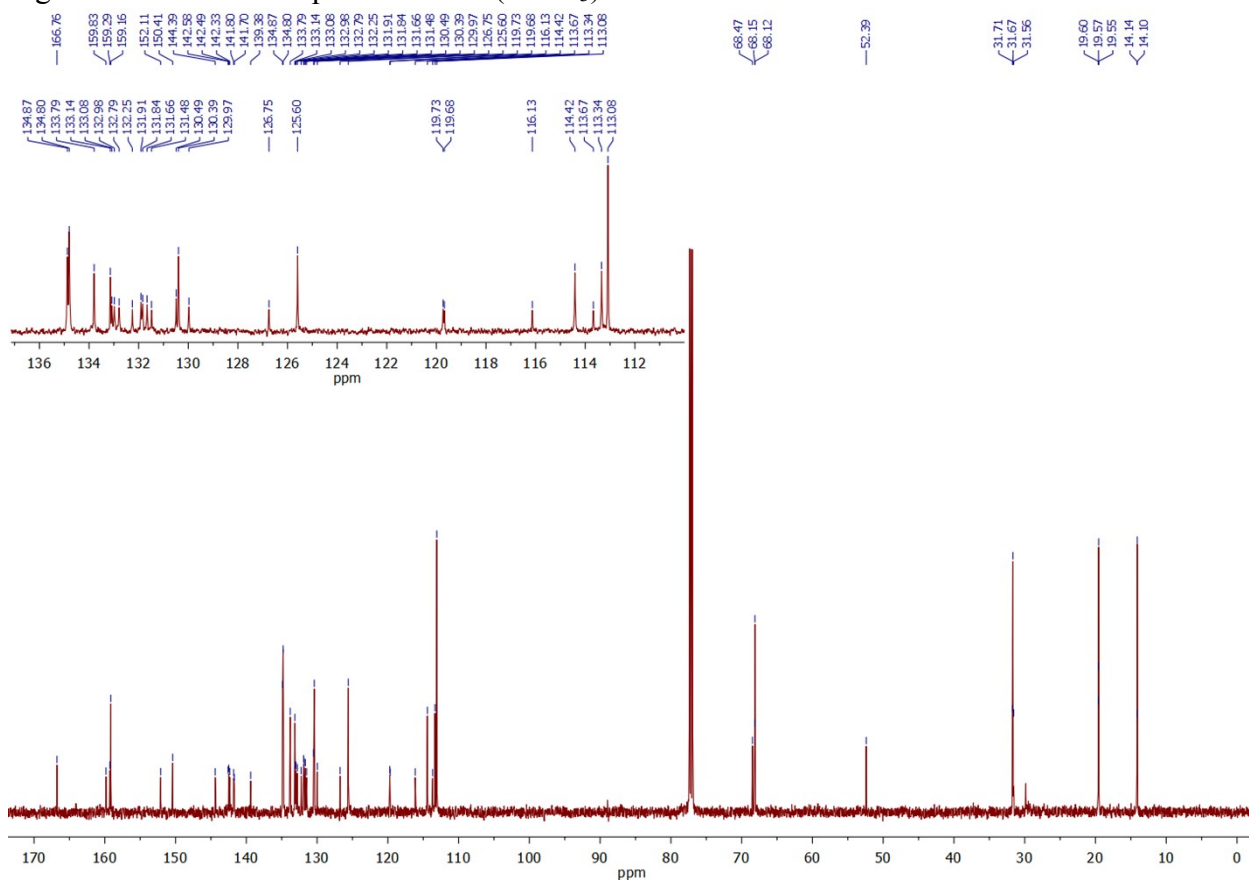Figure S 31. ^{1}H-NMR spectrum of **4f** (CDCl$_3$).

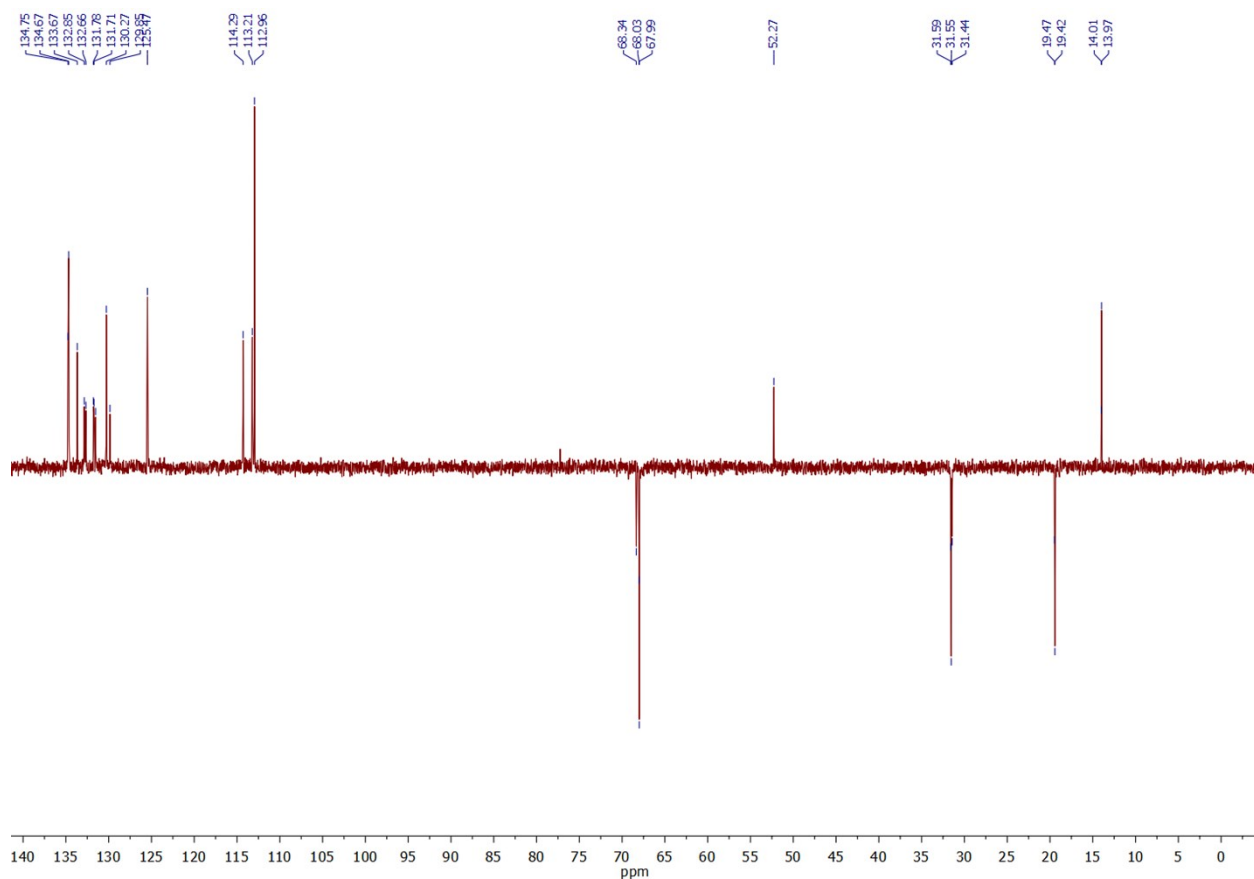Figure S 32. ^{13}C-NMR spectrum of **4f** (CDCl$_3$).

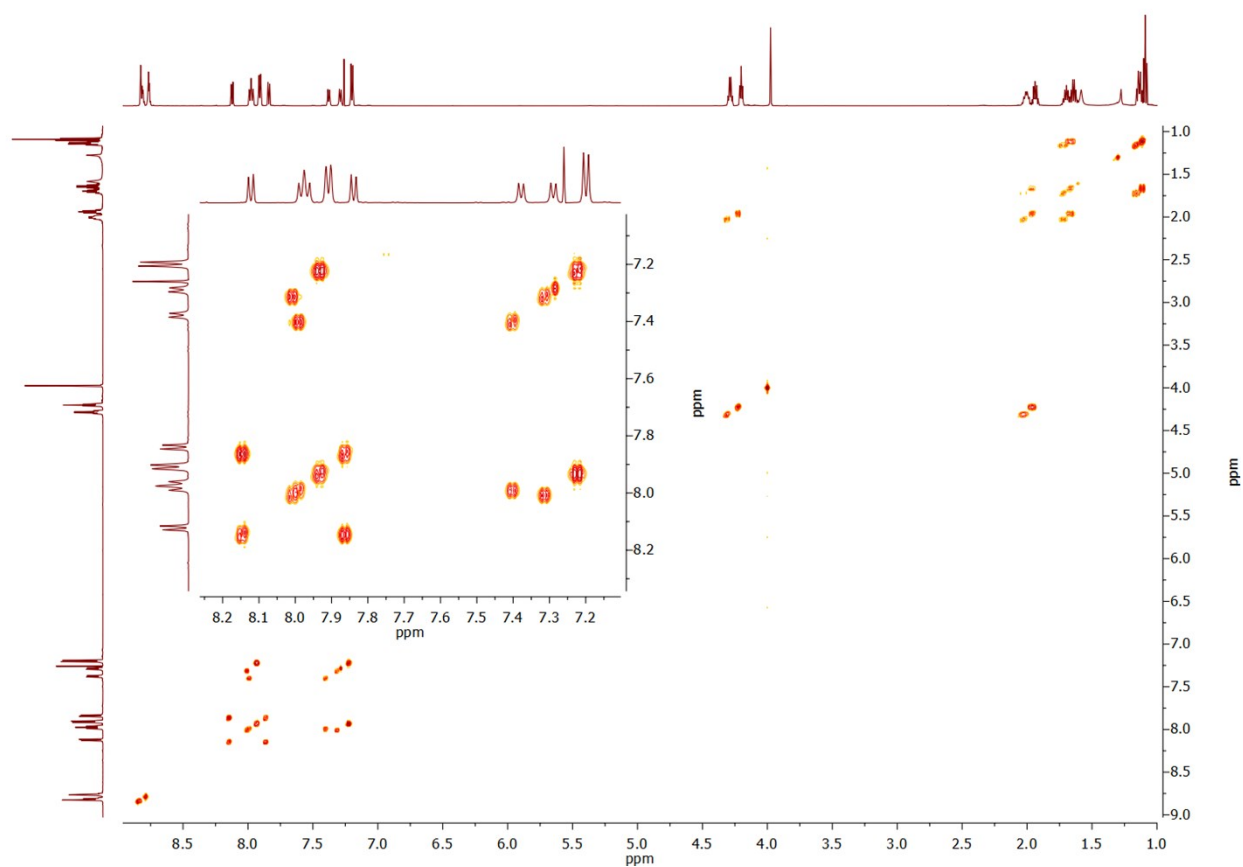Figure S 33. ^{13}C DEPT-135 spectrum of **4f** (CDCl$_3$).
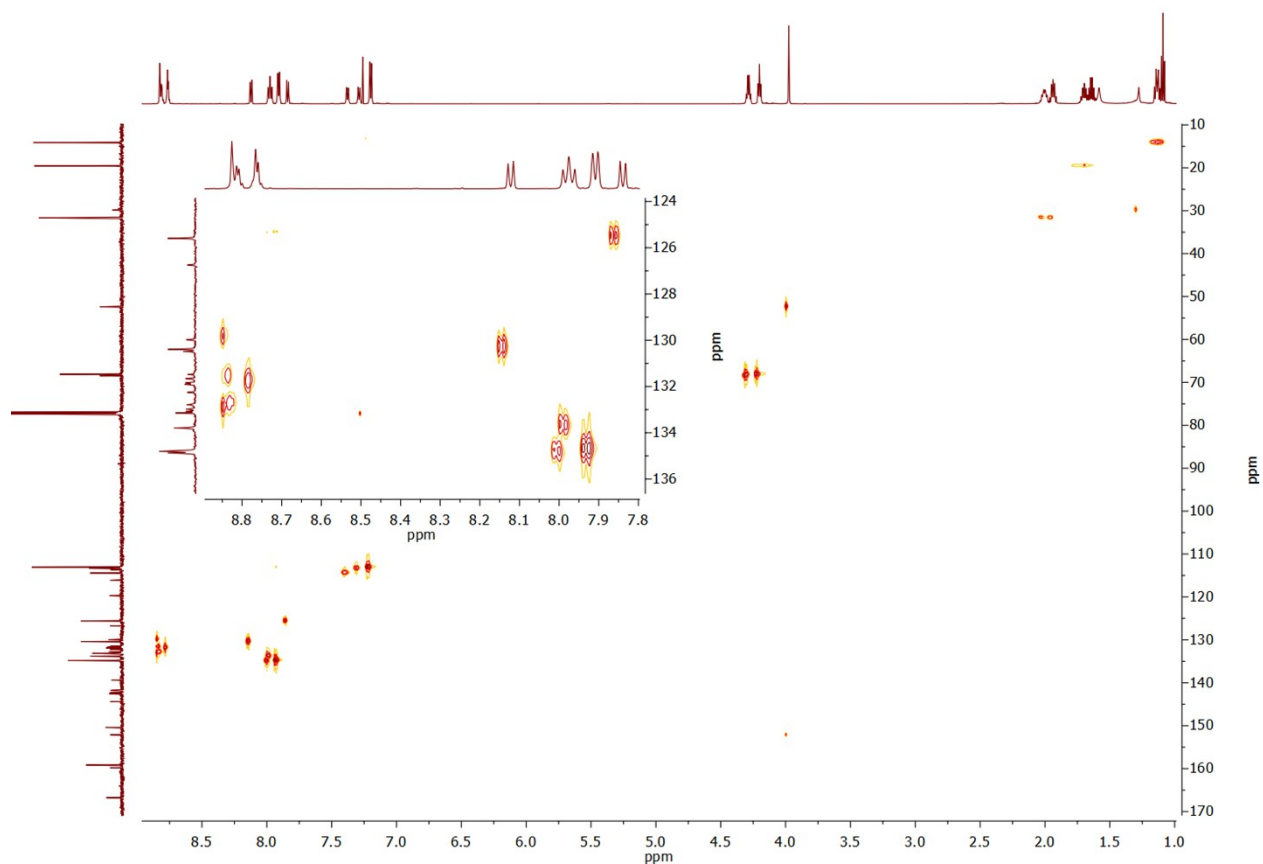

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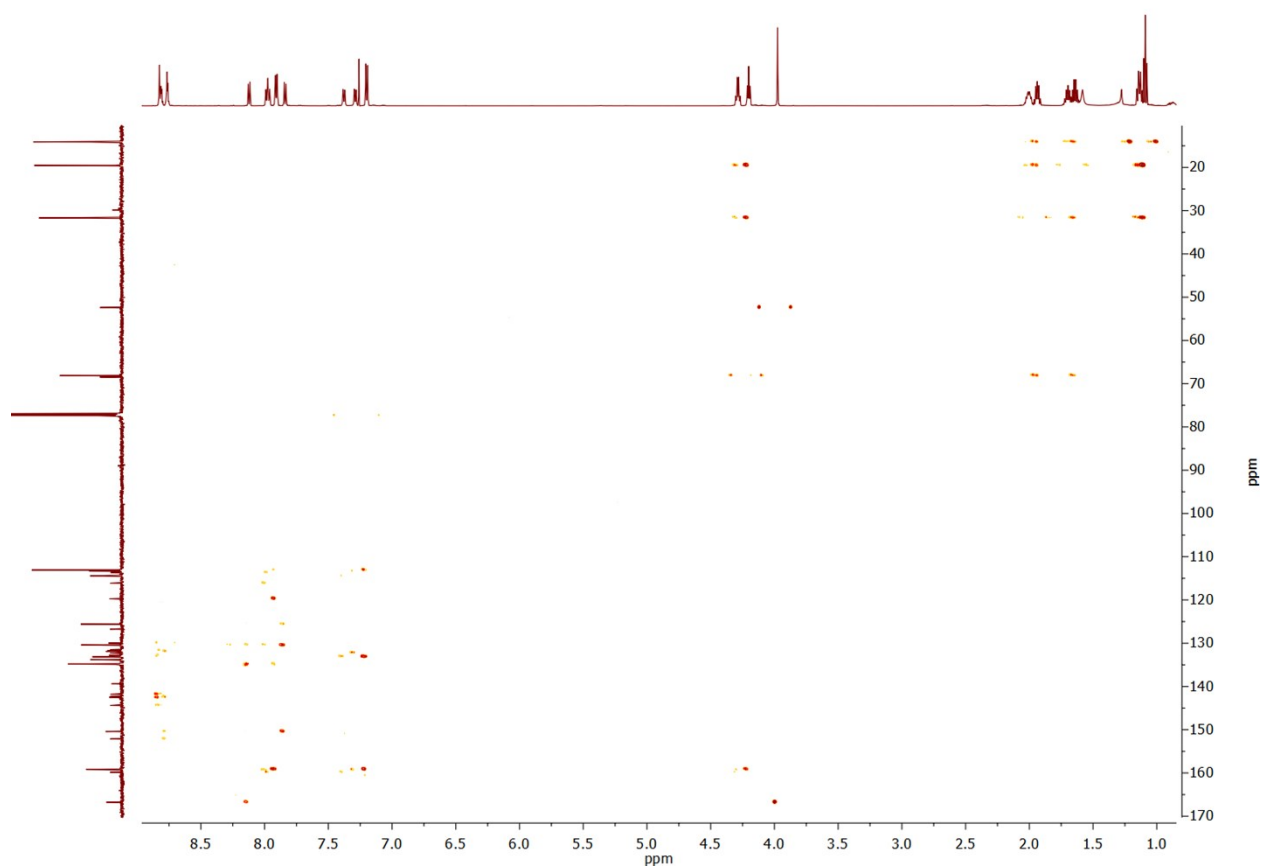
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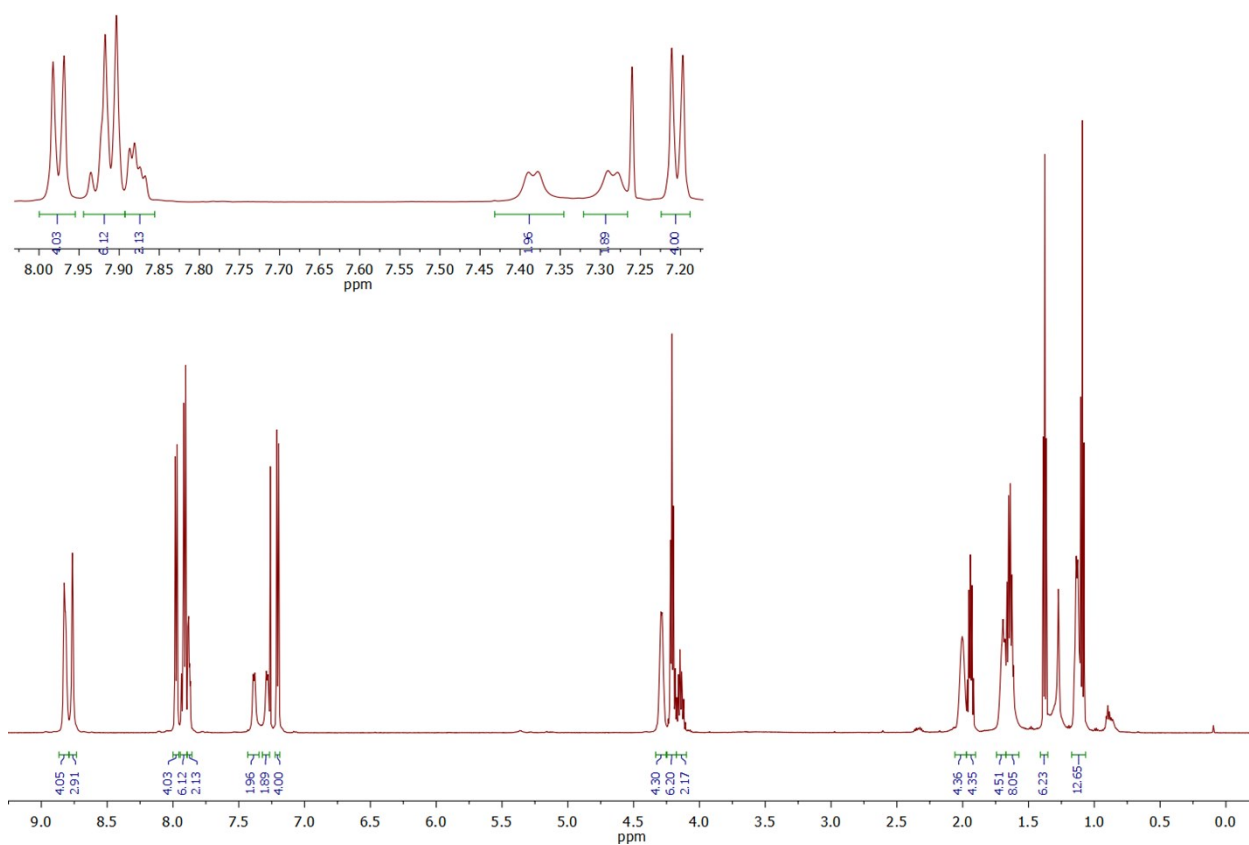
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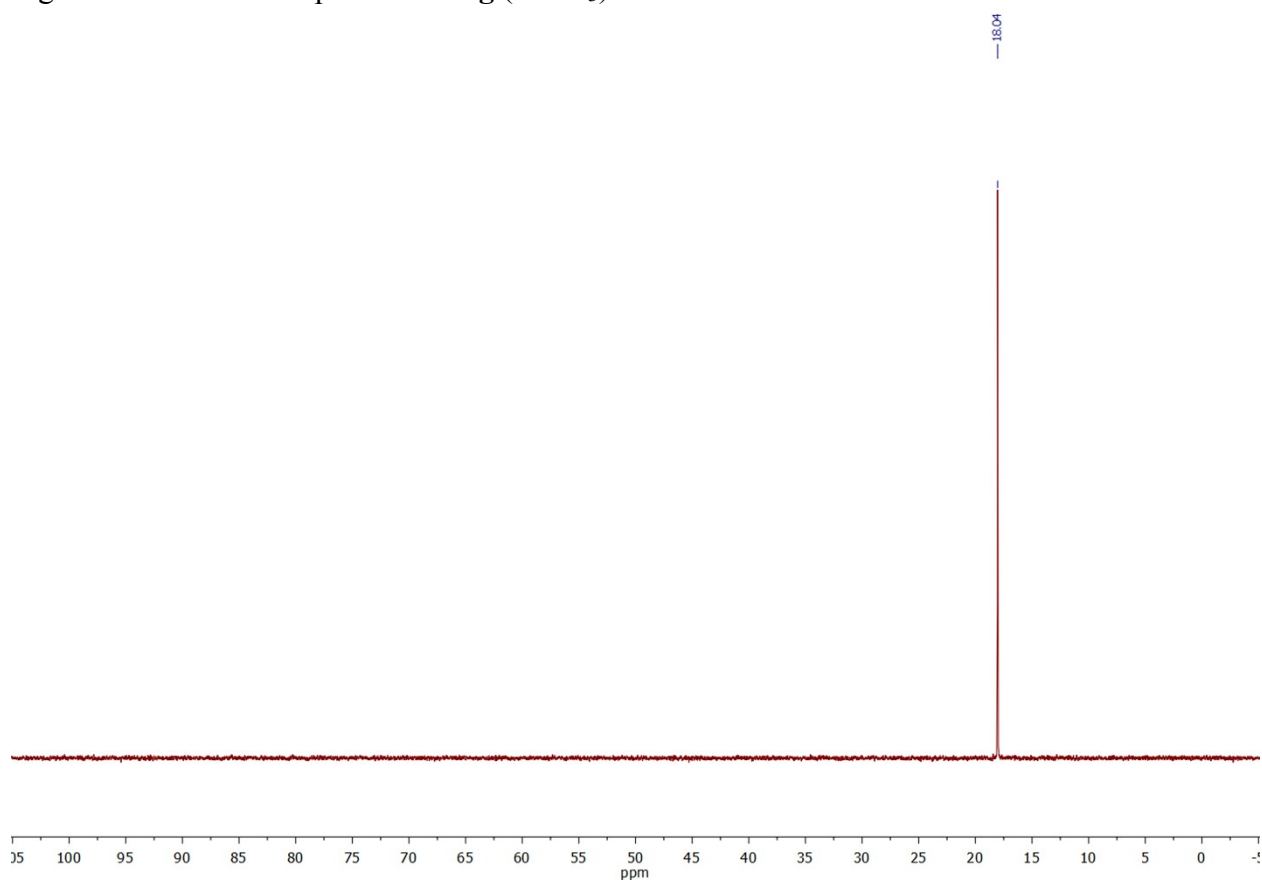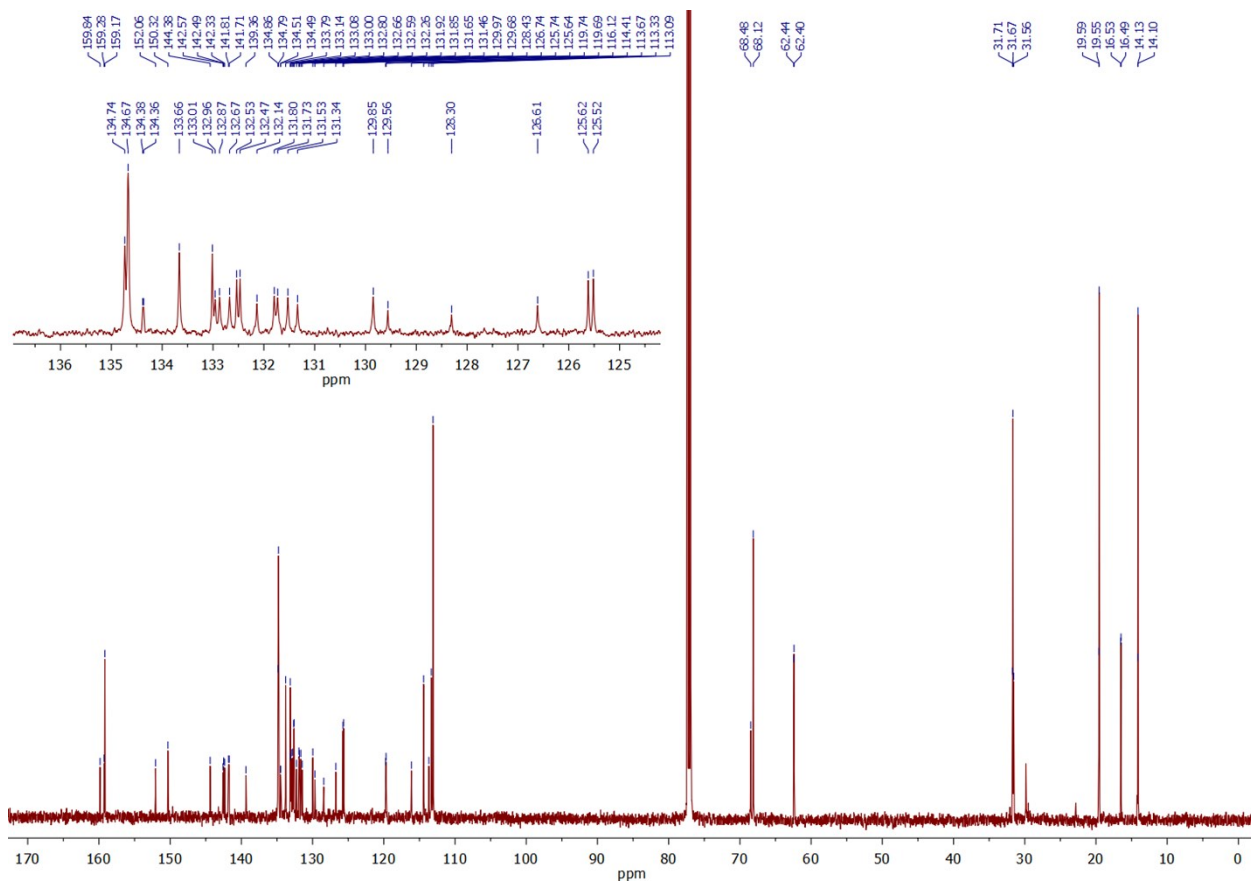Figure S 38. ^{31}P-NMR spectrum of **4g** (CDCl$_3$).

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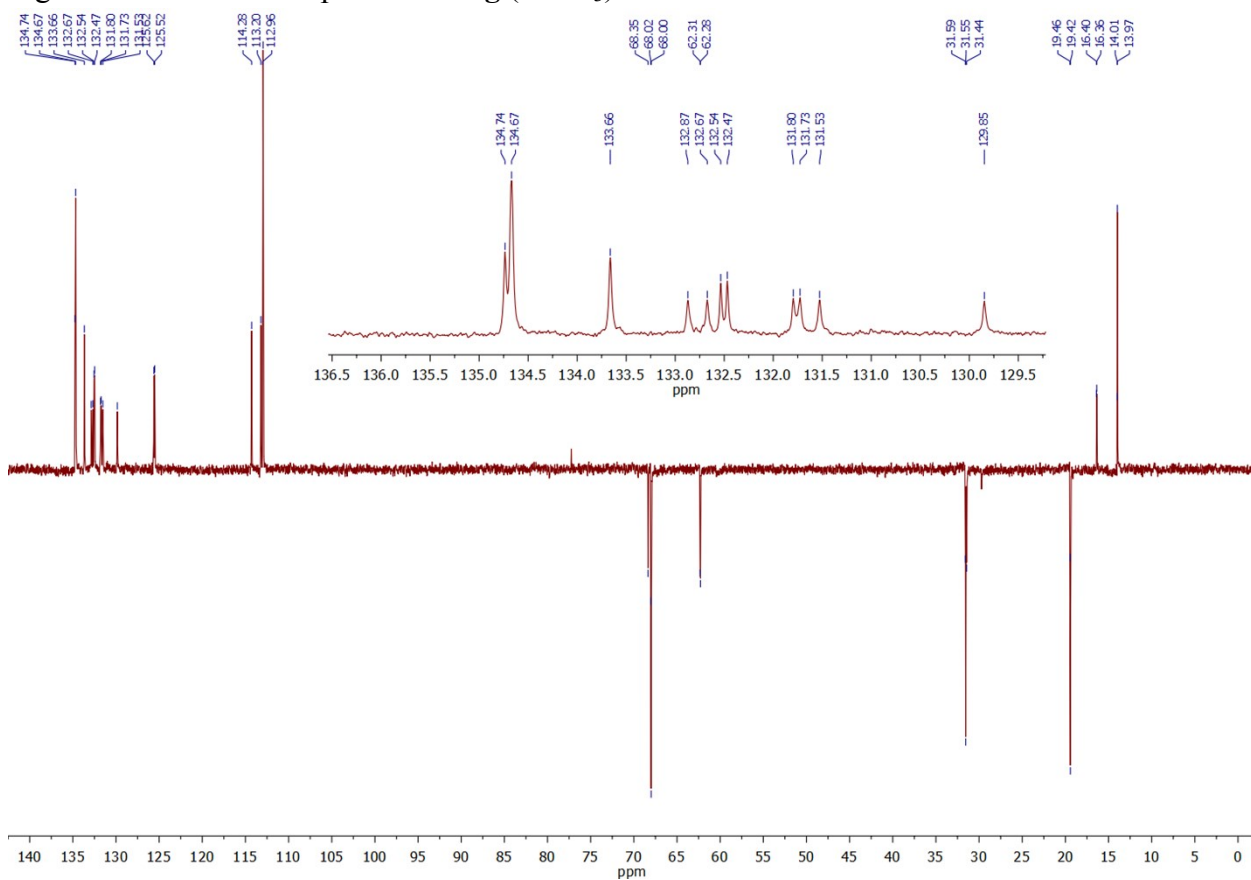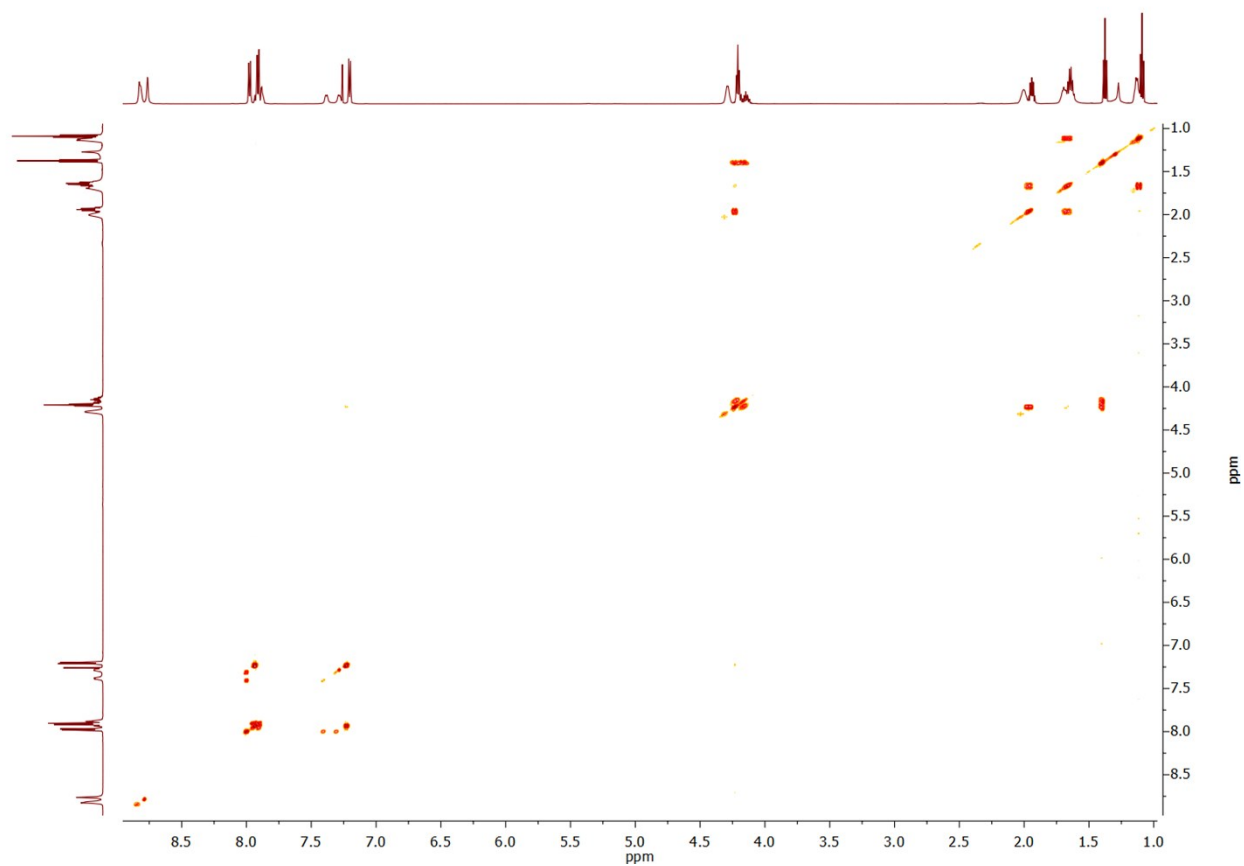

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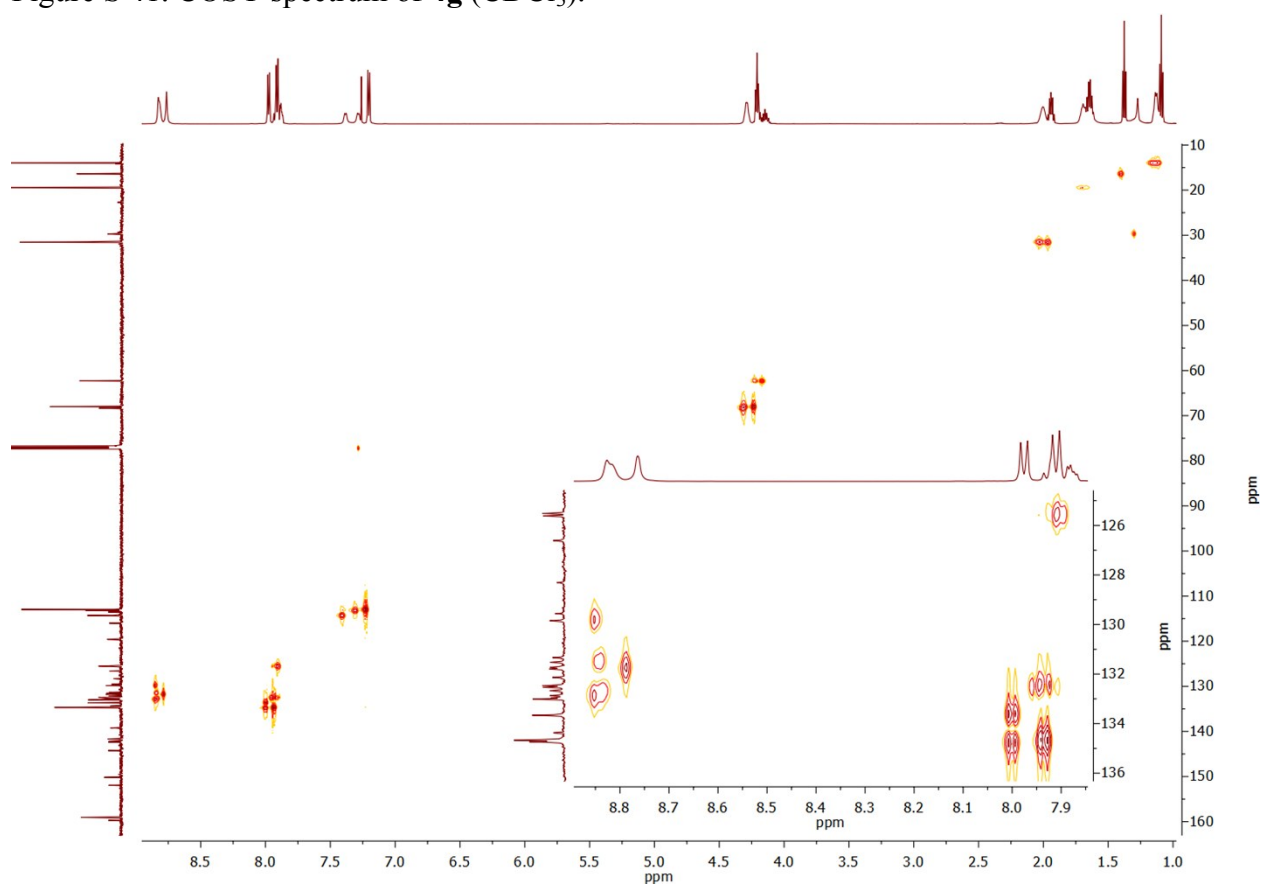
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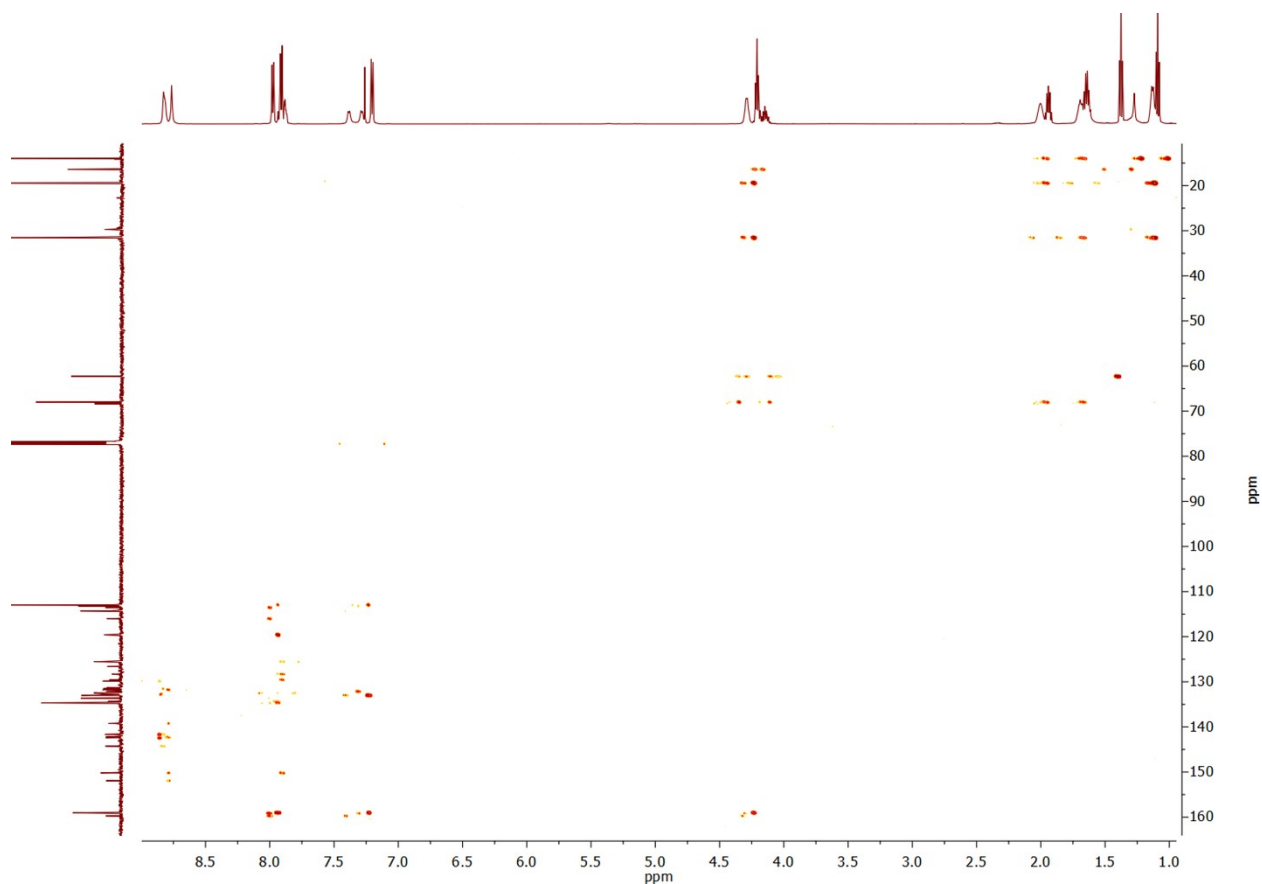Figure S 42. ^{1}H-^{13}C HSQC spectrum of **4g** (CDCl$_3$).

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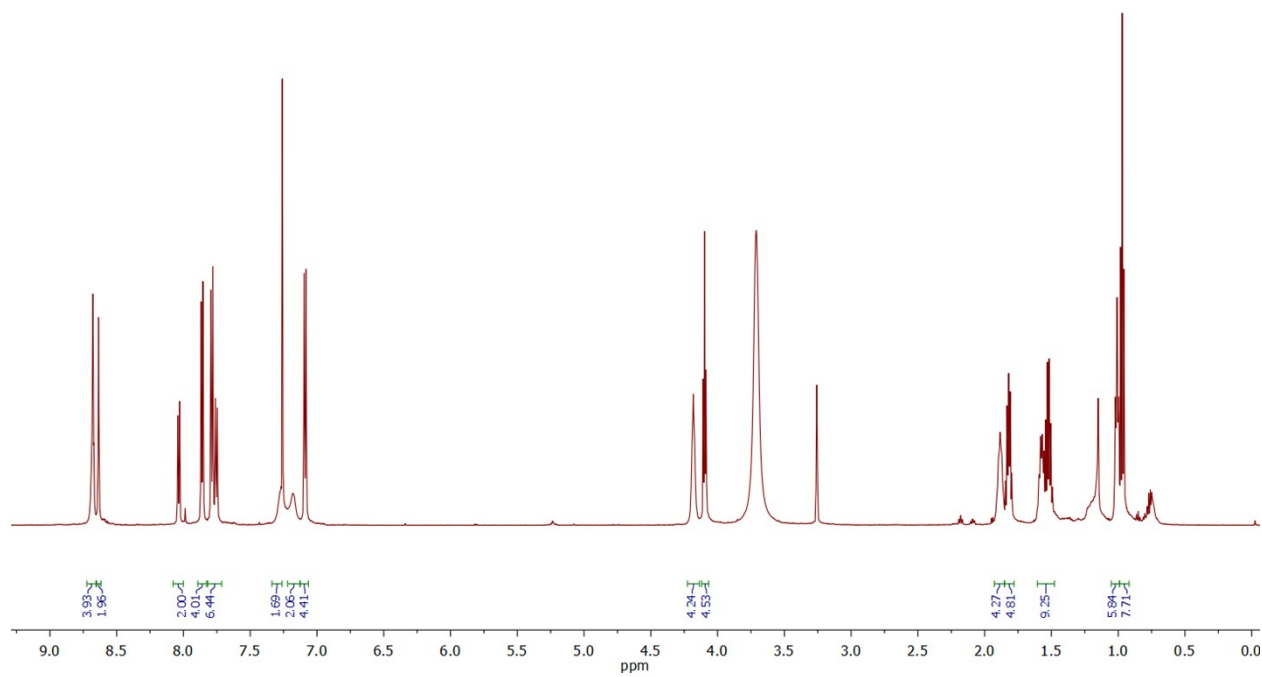
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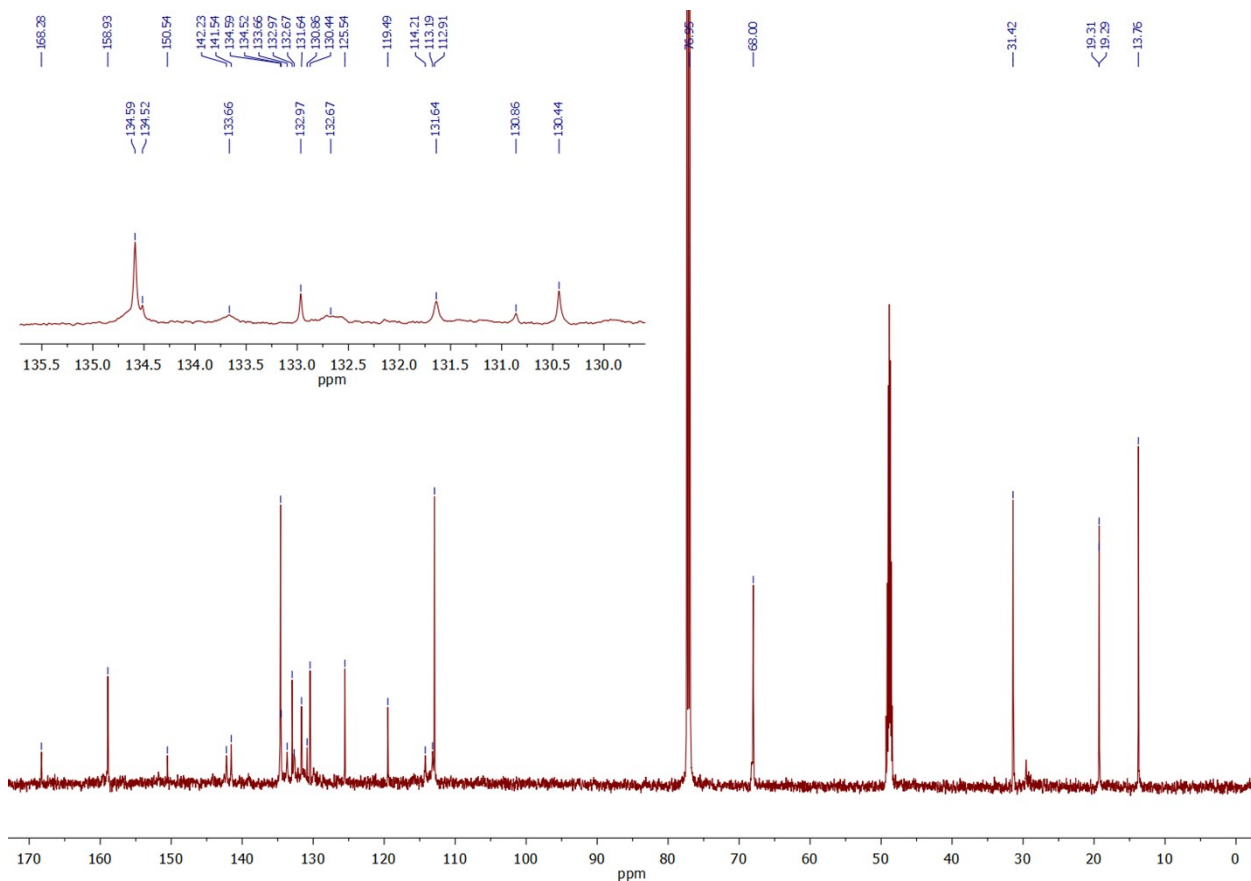Figure S 44. ^1H-NMR spectrum of **4h** (20% MeOD in CDCl$_3$).

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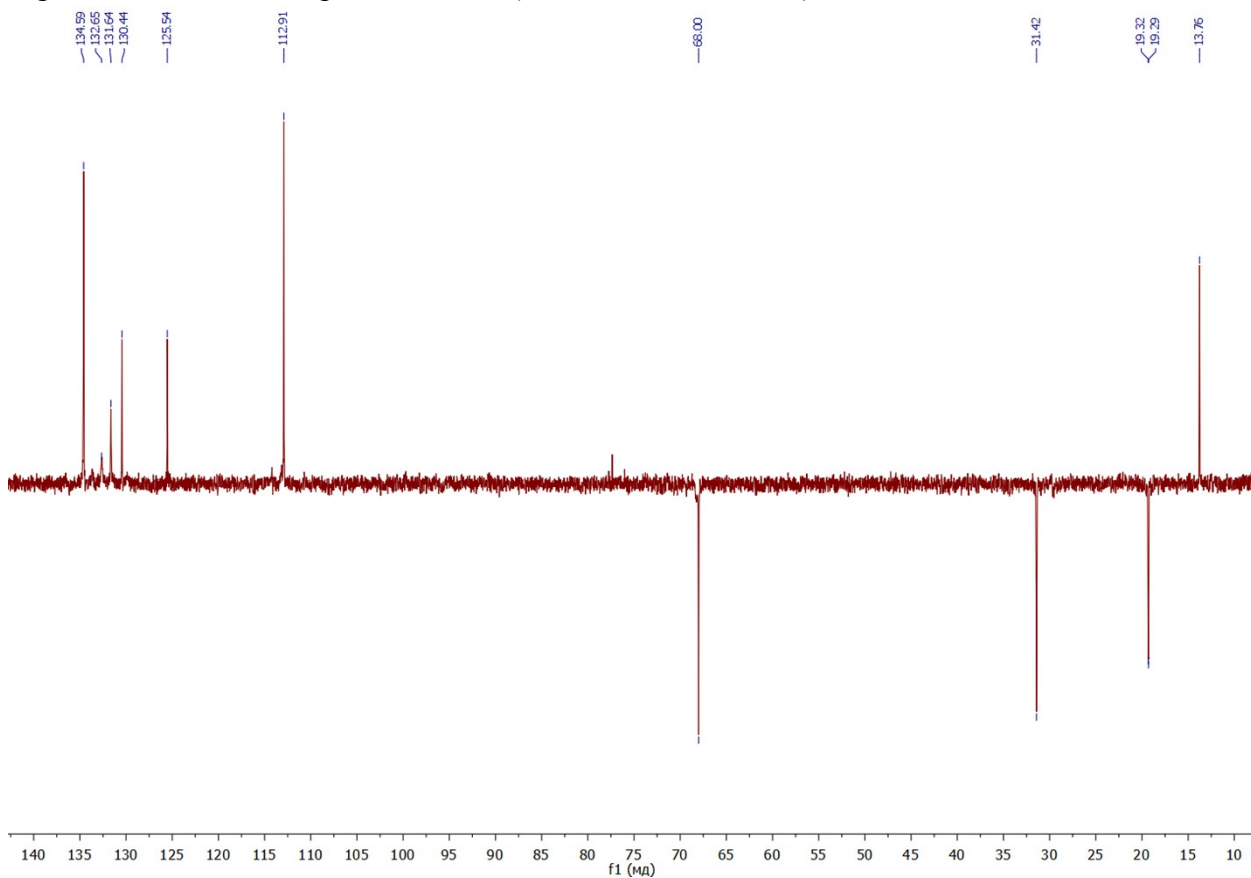

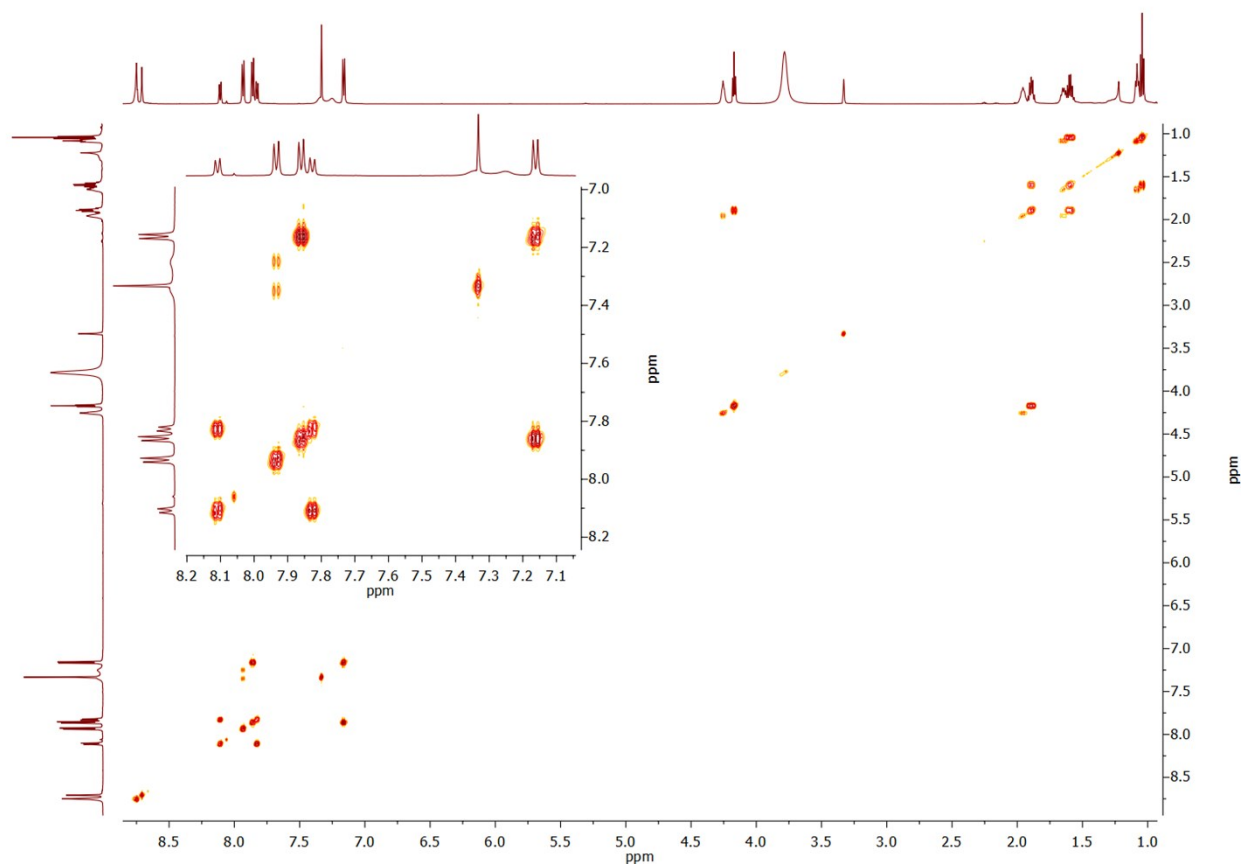Figure S 46. ^{13}C DEPT-135 spectrum of **4h** (20% MeOD in CDCl$_3$).
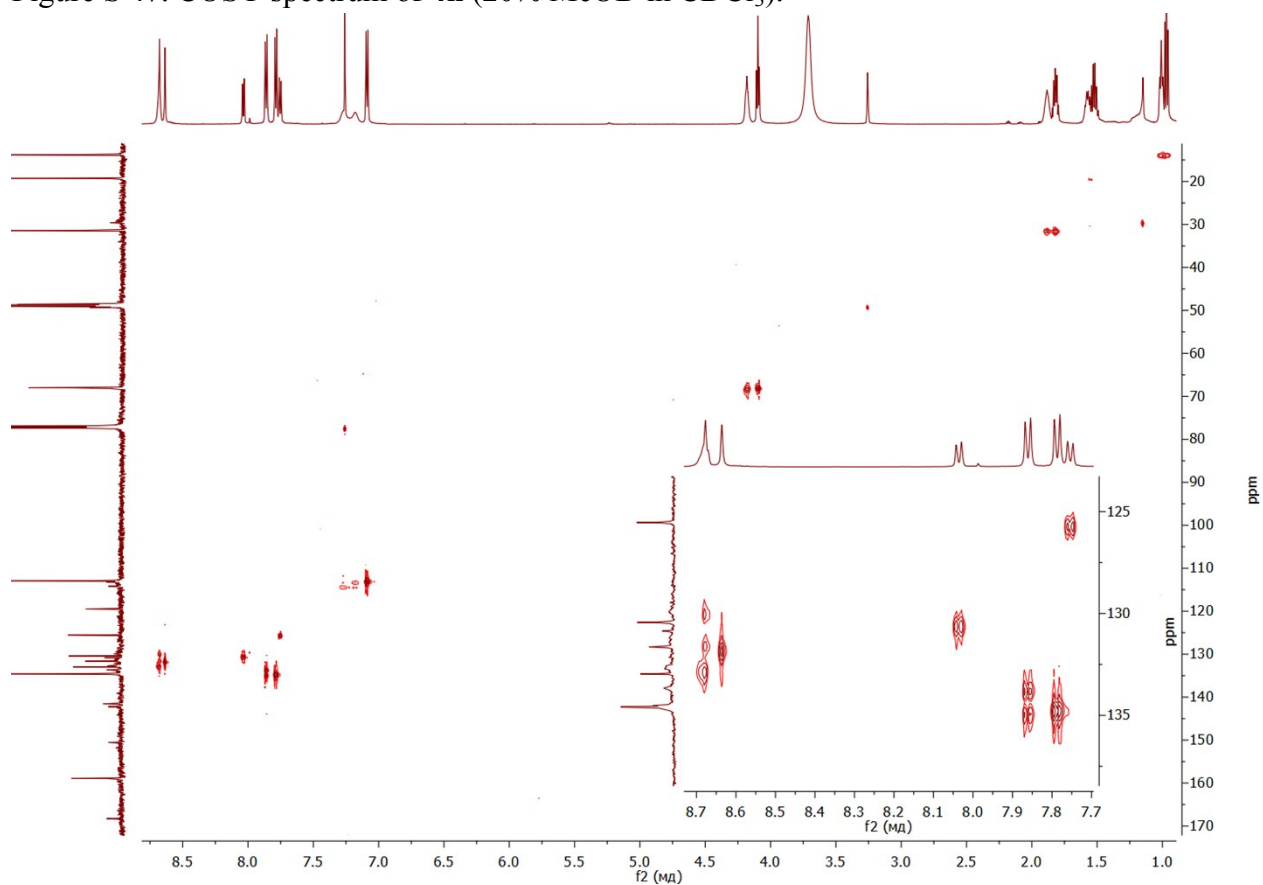
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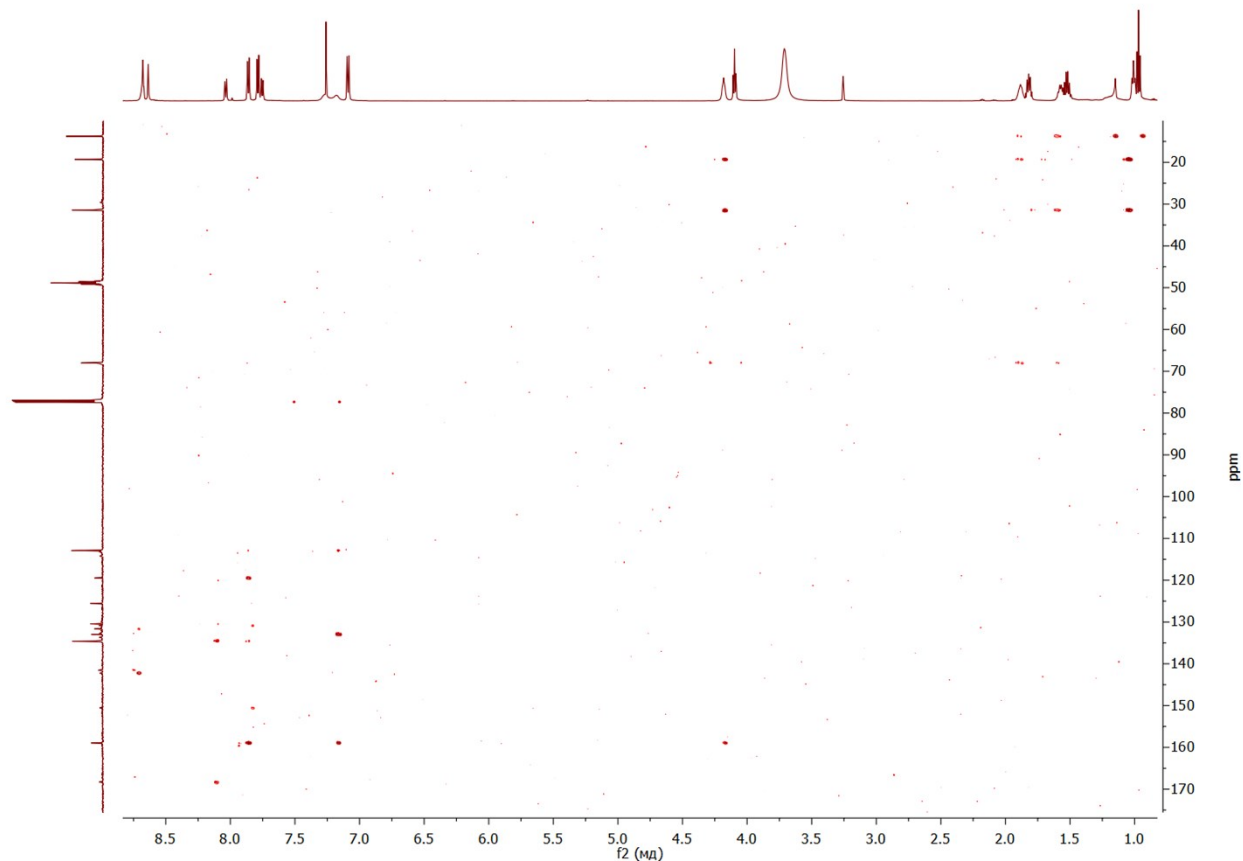Figure S 48. ¹H-¹³C HSQC spectrum of **4h** (20% MeOD in CDCl₃).

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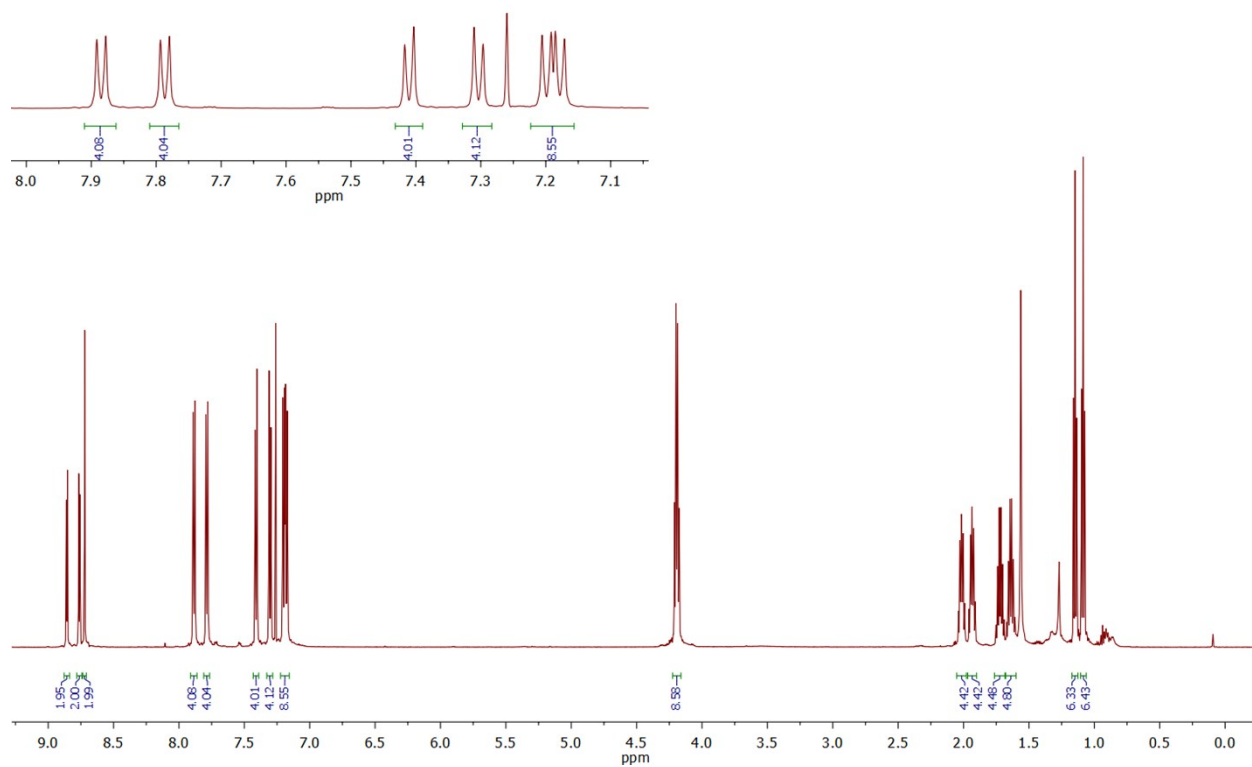
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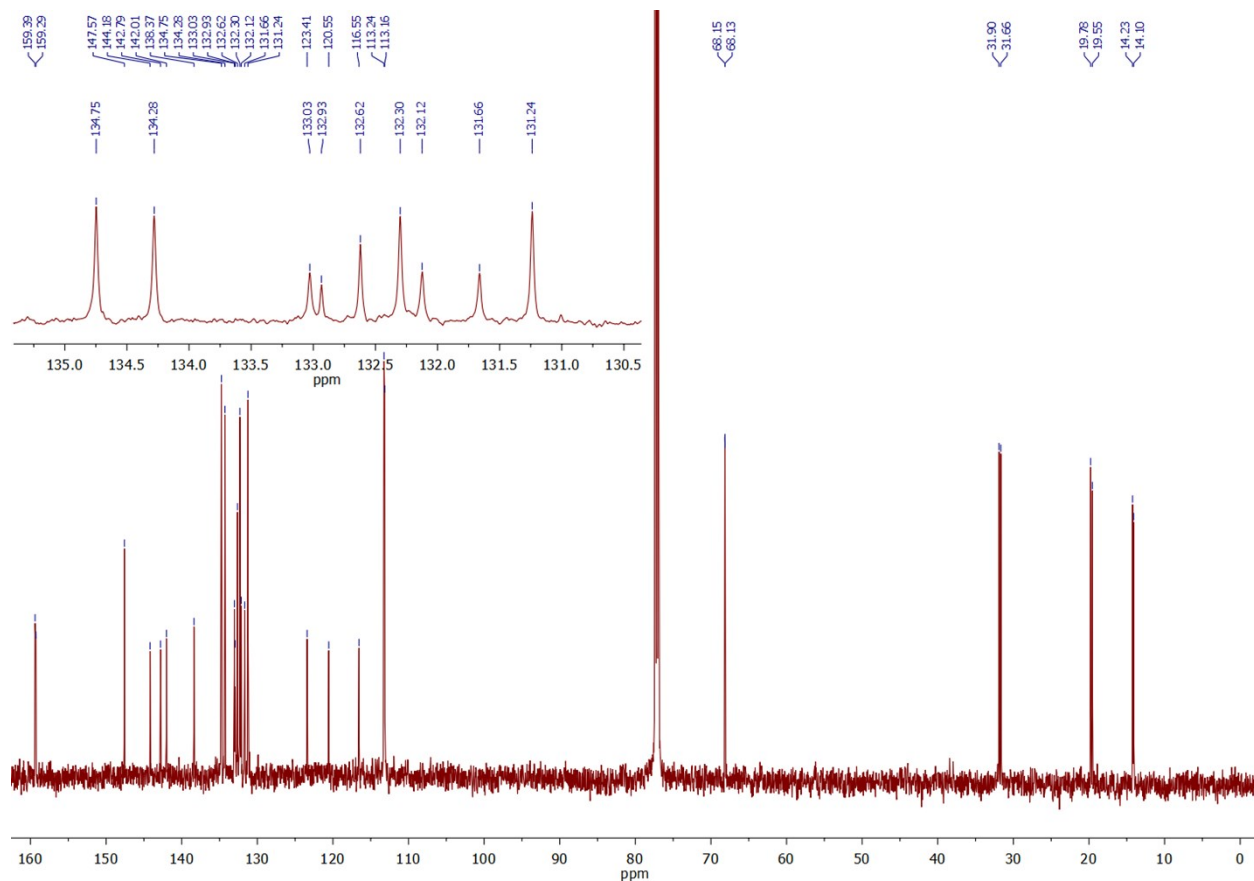
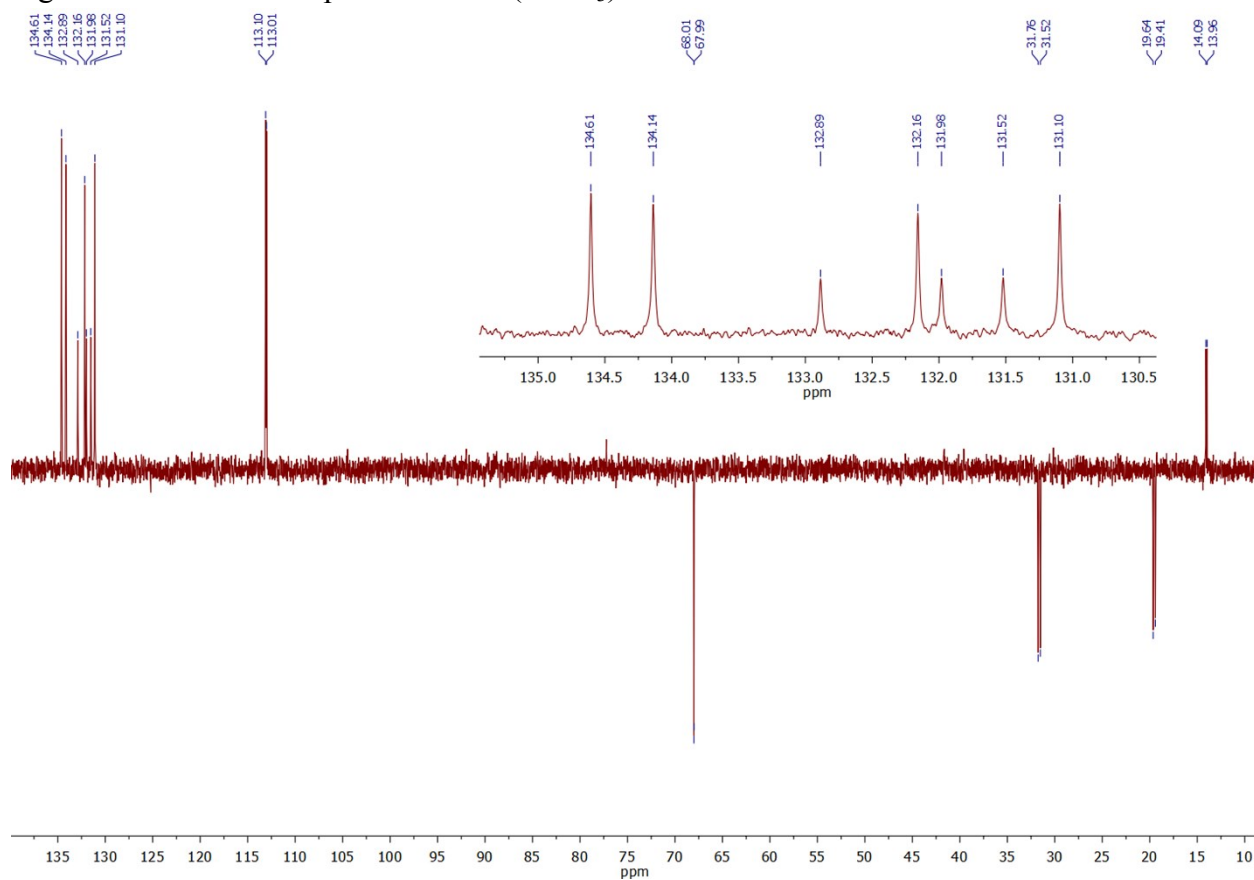Figure S 51. ^{13}C-NMR spectrum of **5a** (CDCl$_3$).
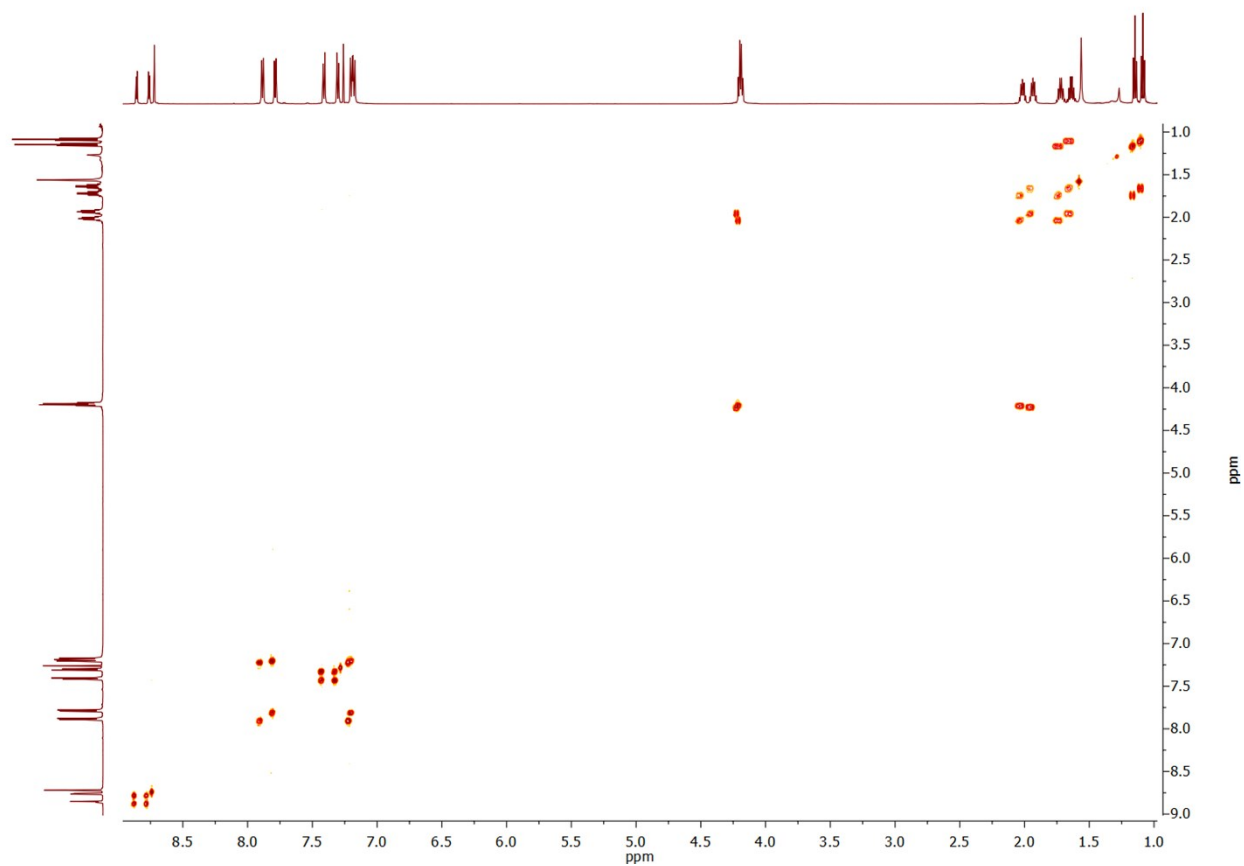

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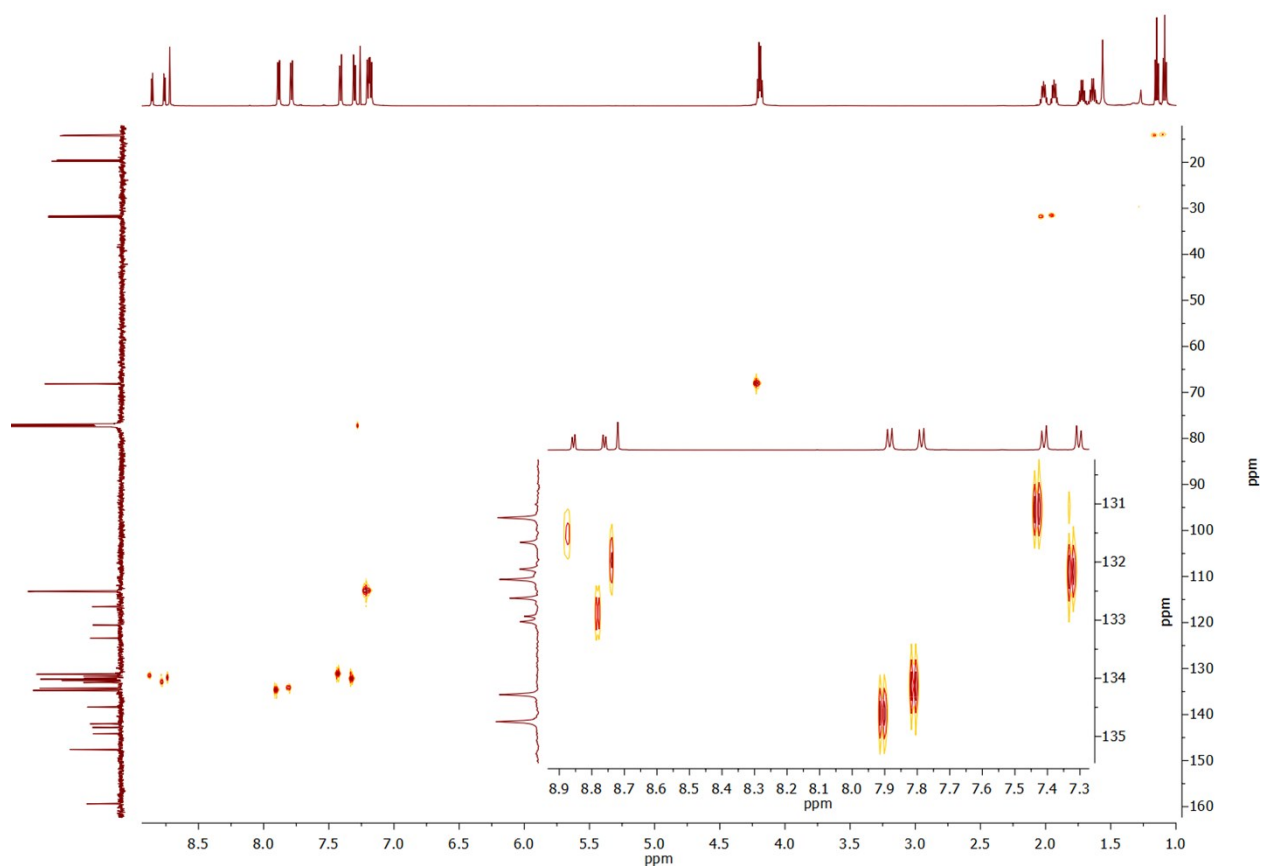
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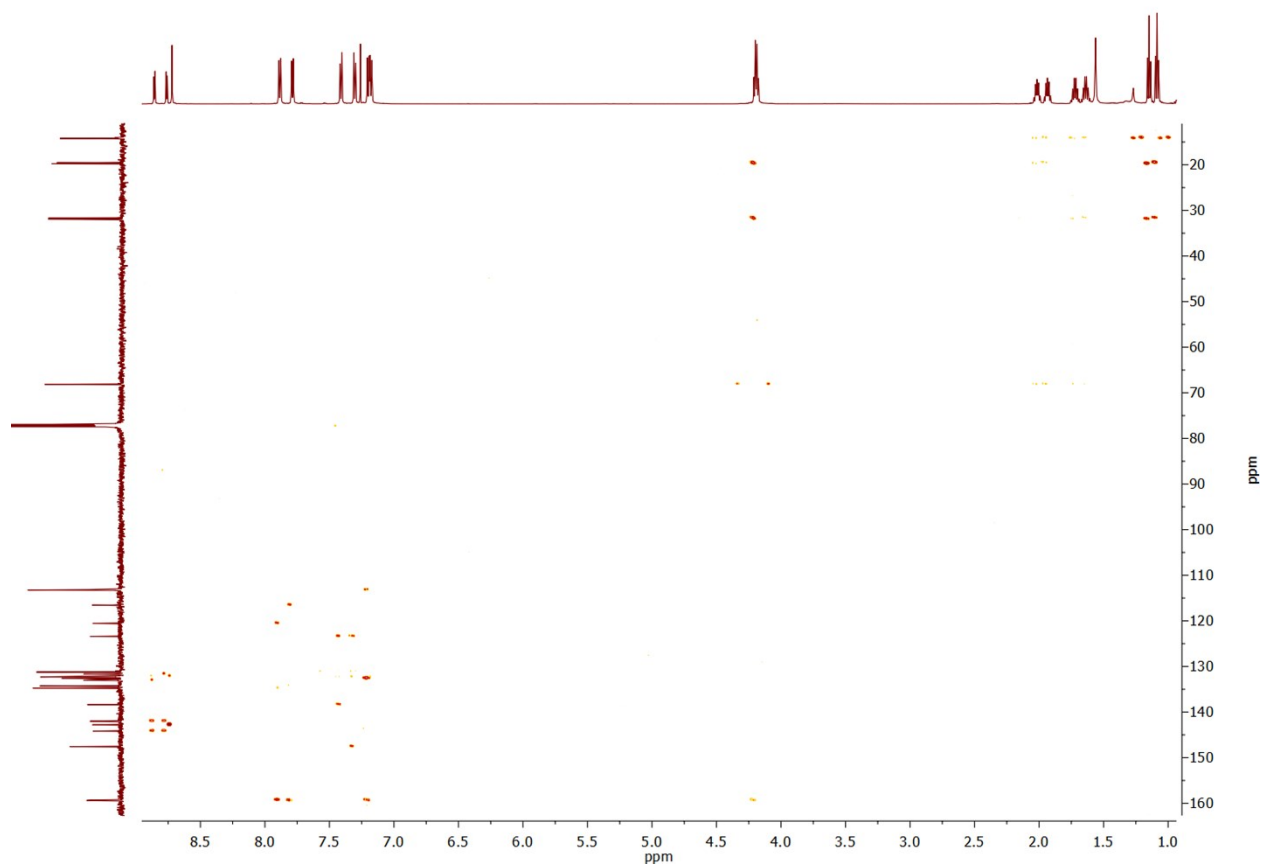Figure S 54. ^{1}H-^{13}C HSQC spectrum of **5a** (CDCl$_3$).

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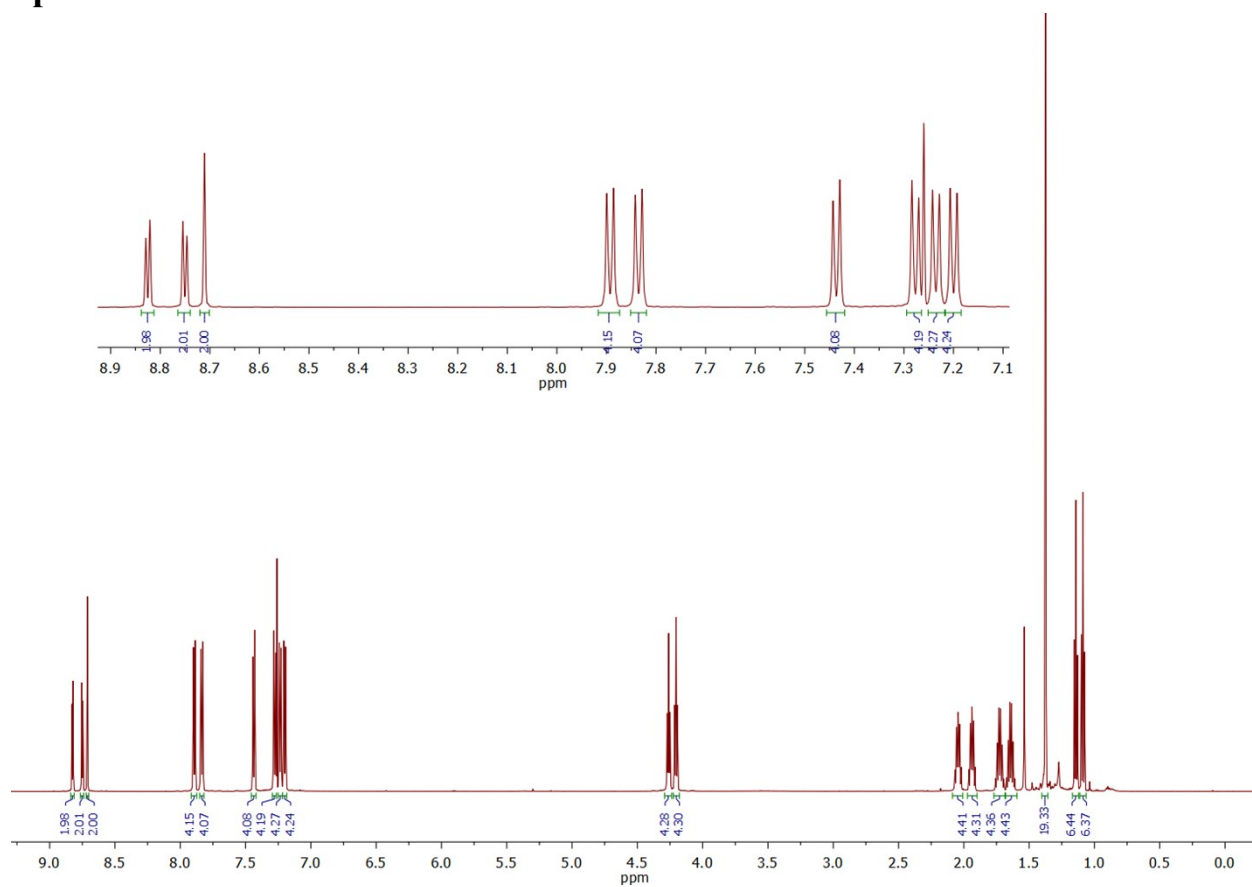
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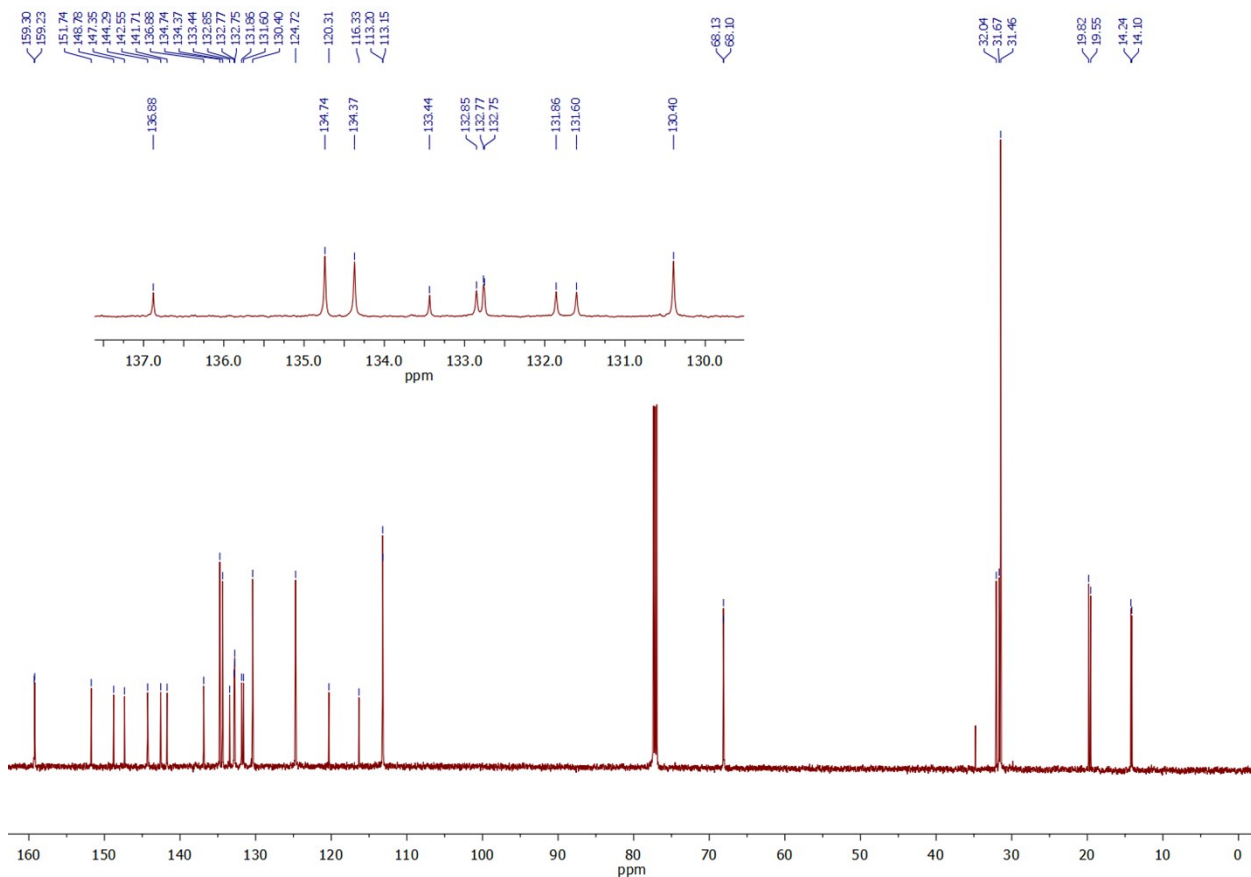Figure S 56. ^{1}H-NMR spectrum of **5b** (CDCl$_3$).
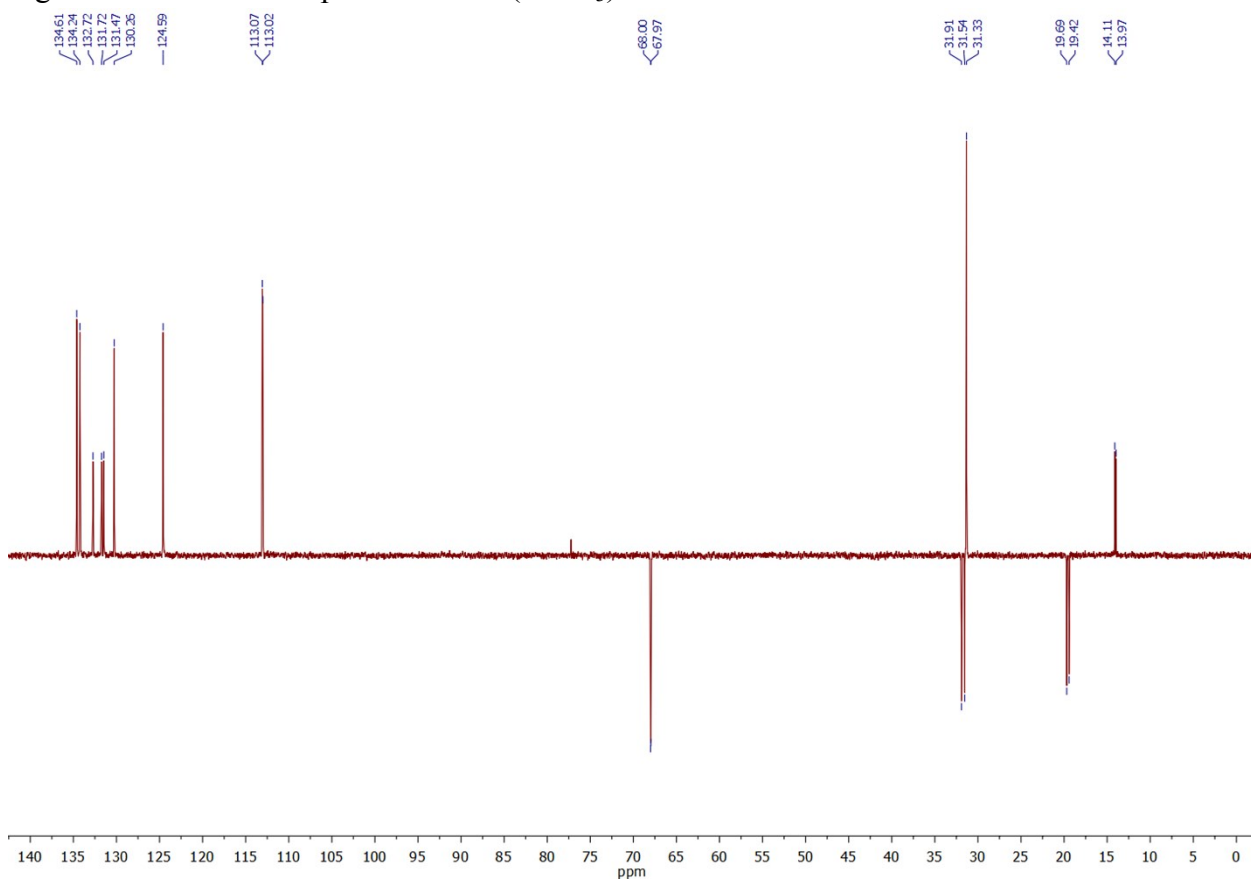
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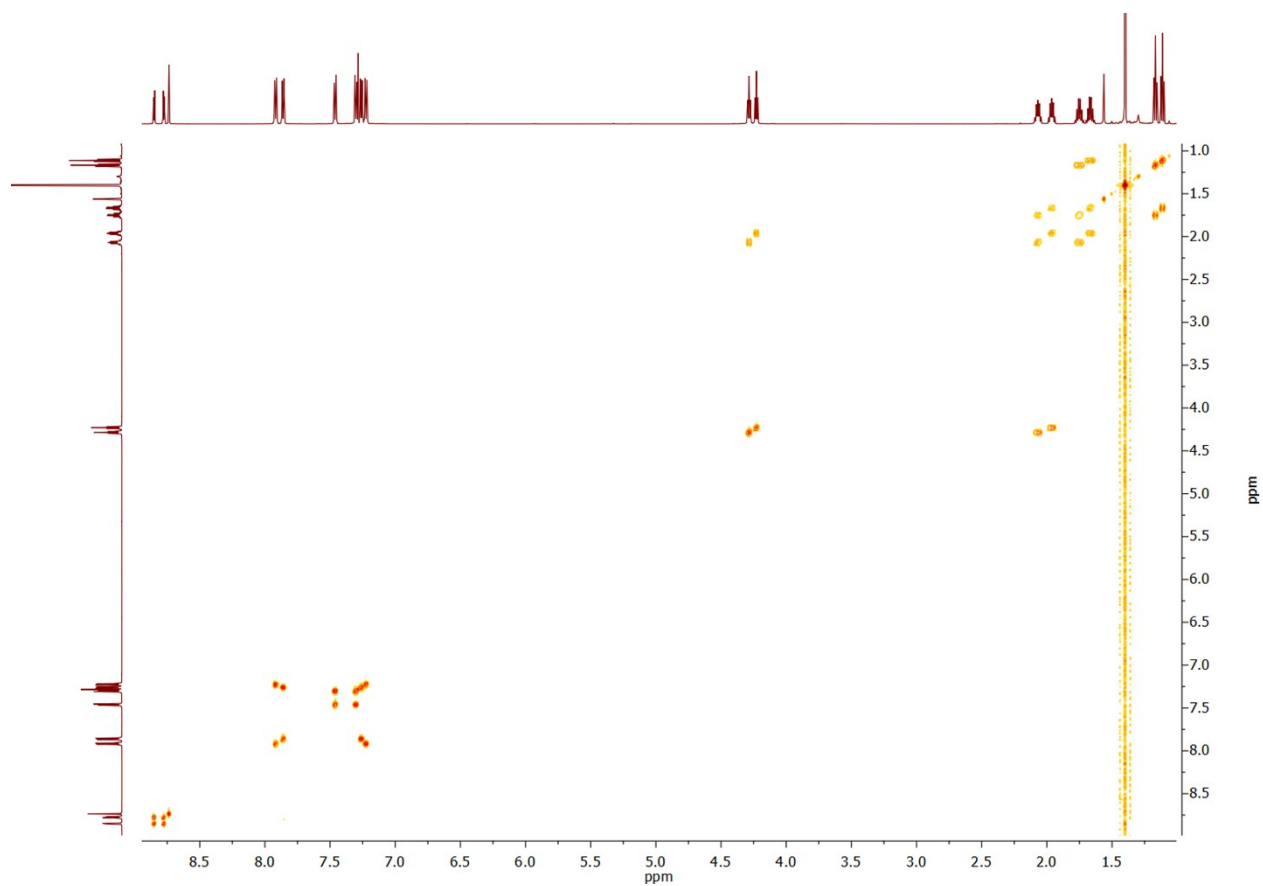Figure S 58. ^{13}C DEPT-135 spectrum of **5b** (CDCl$_3$).
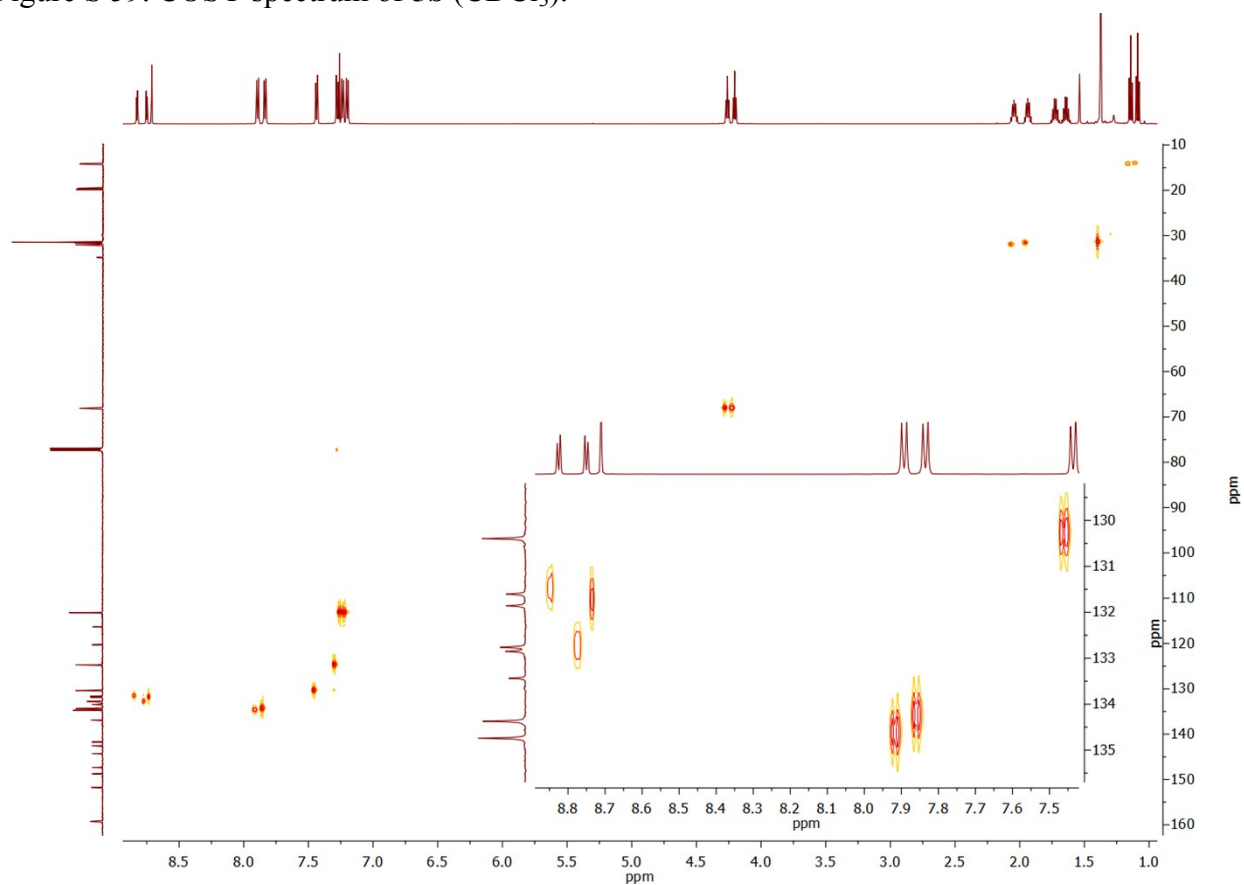
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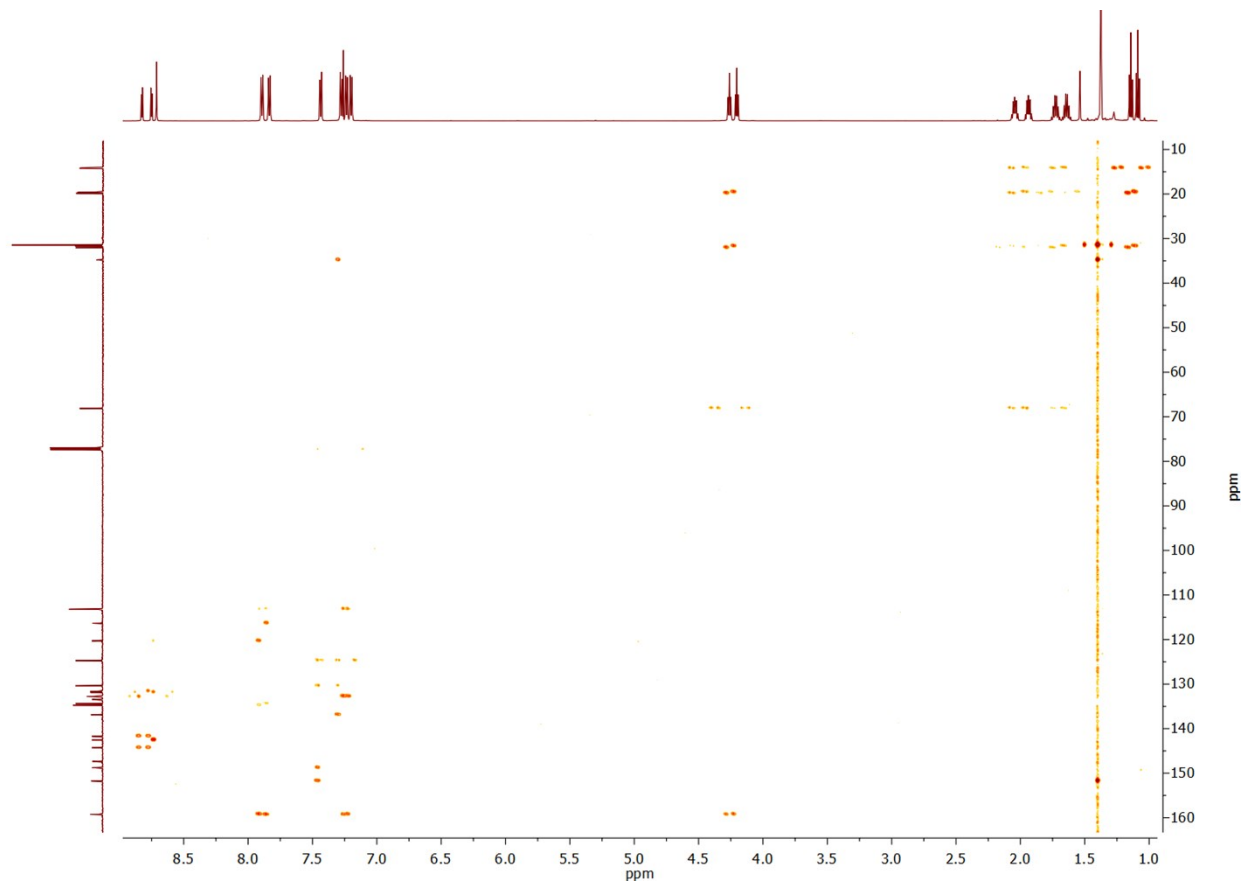Figure S 60. ^{1}H-^{13}C HSQC spectrum of **5b** (CDCl$_3$).

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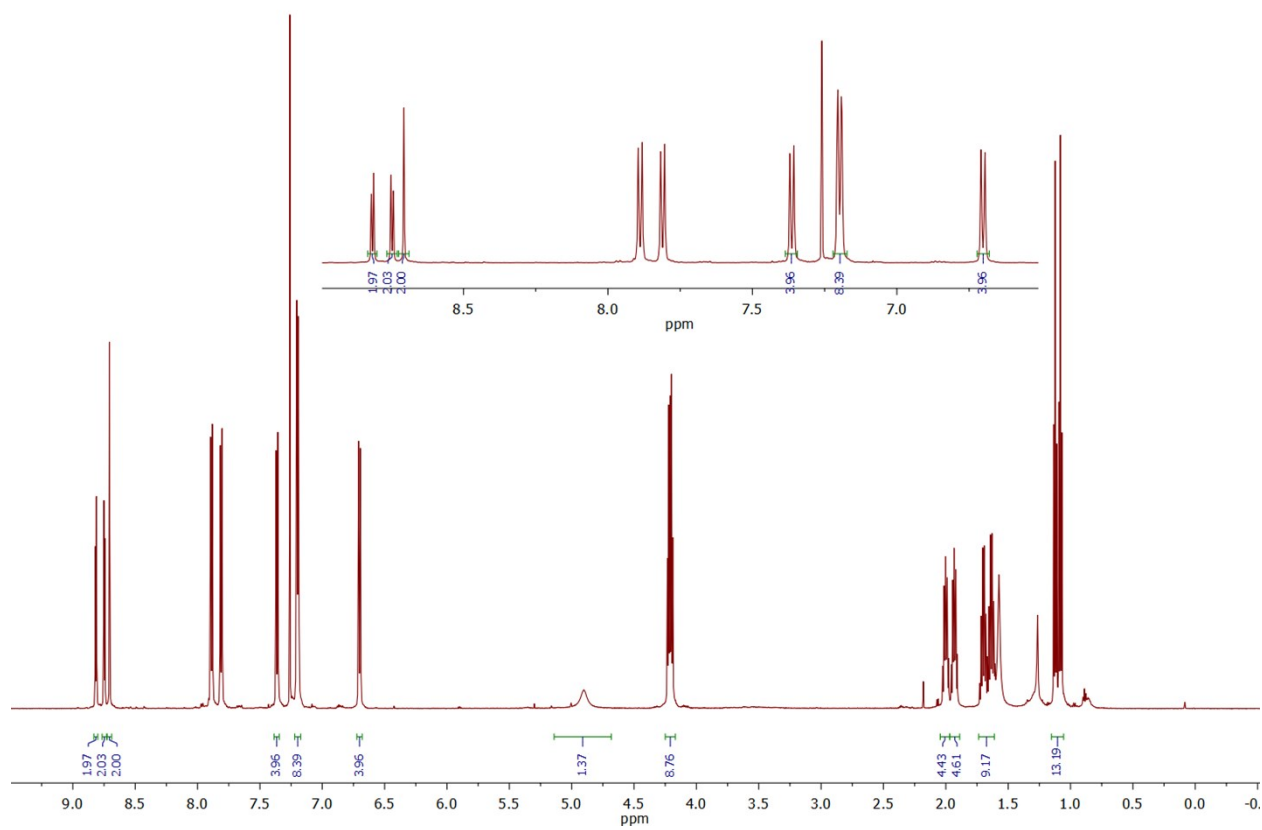
Spectral data of 5c

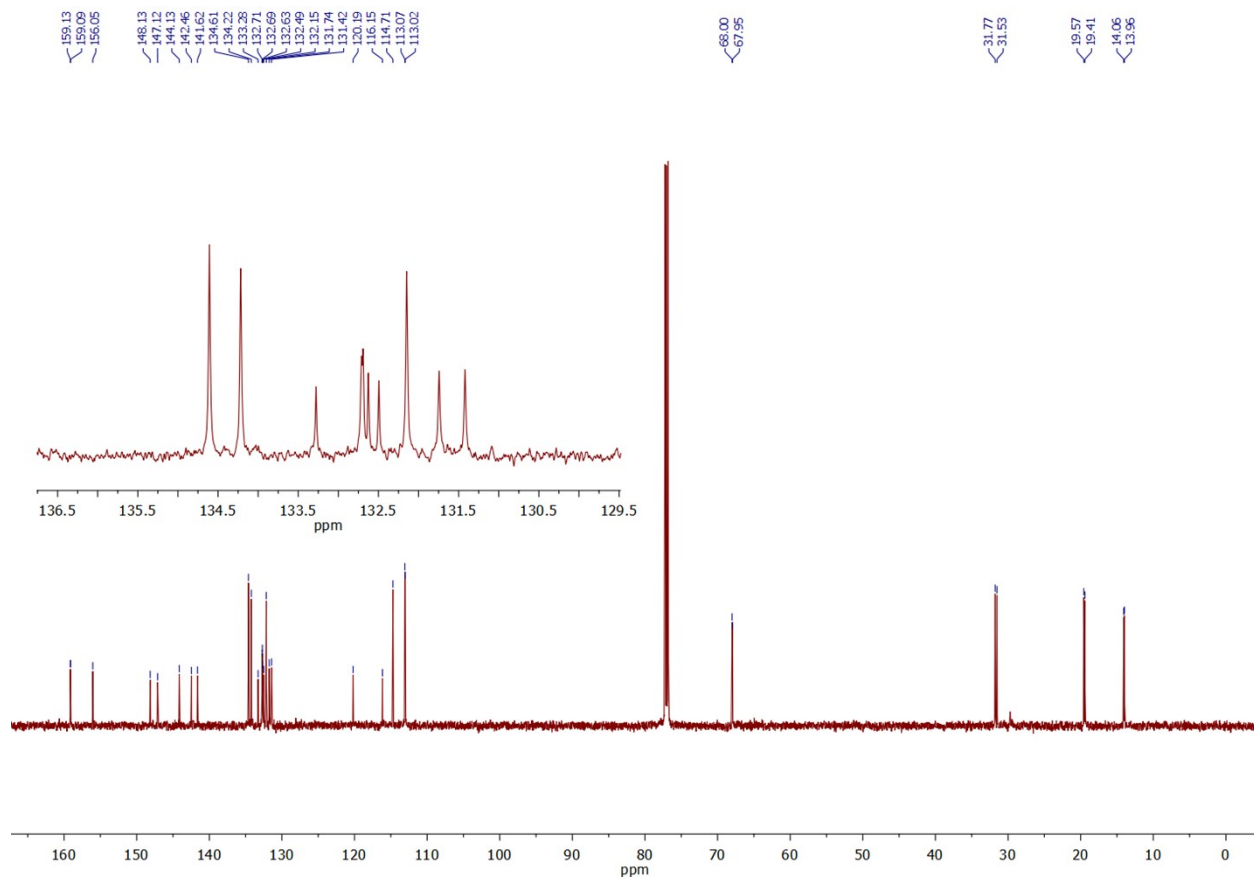Figure S 62. ^{1}H-NMR spectrum of **5c** (CDCl$_3$).

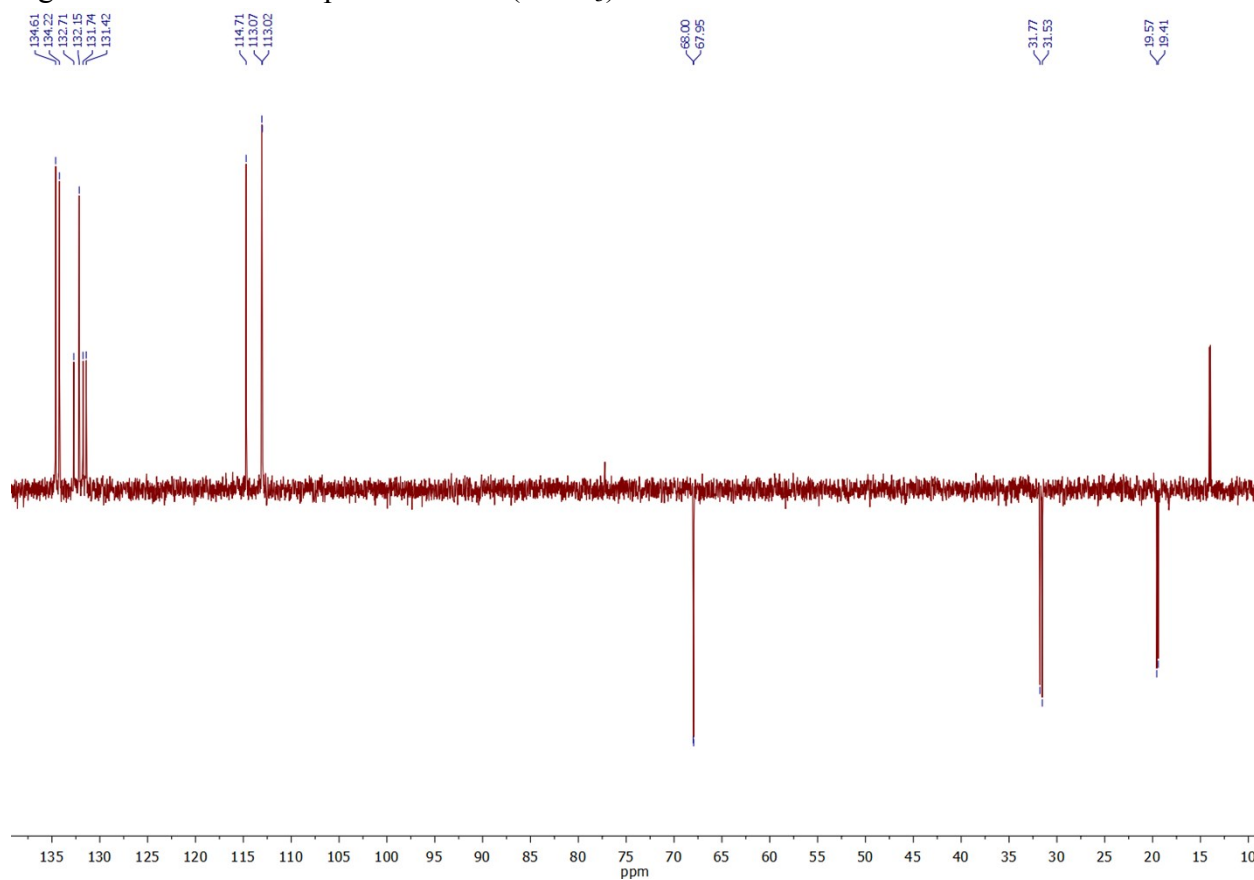Figure S 63. ^{13}C-NMR spectrum of **5c** (CDCl$_3$).

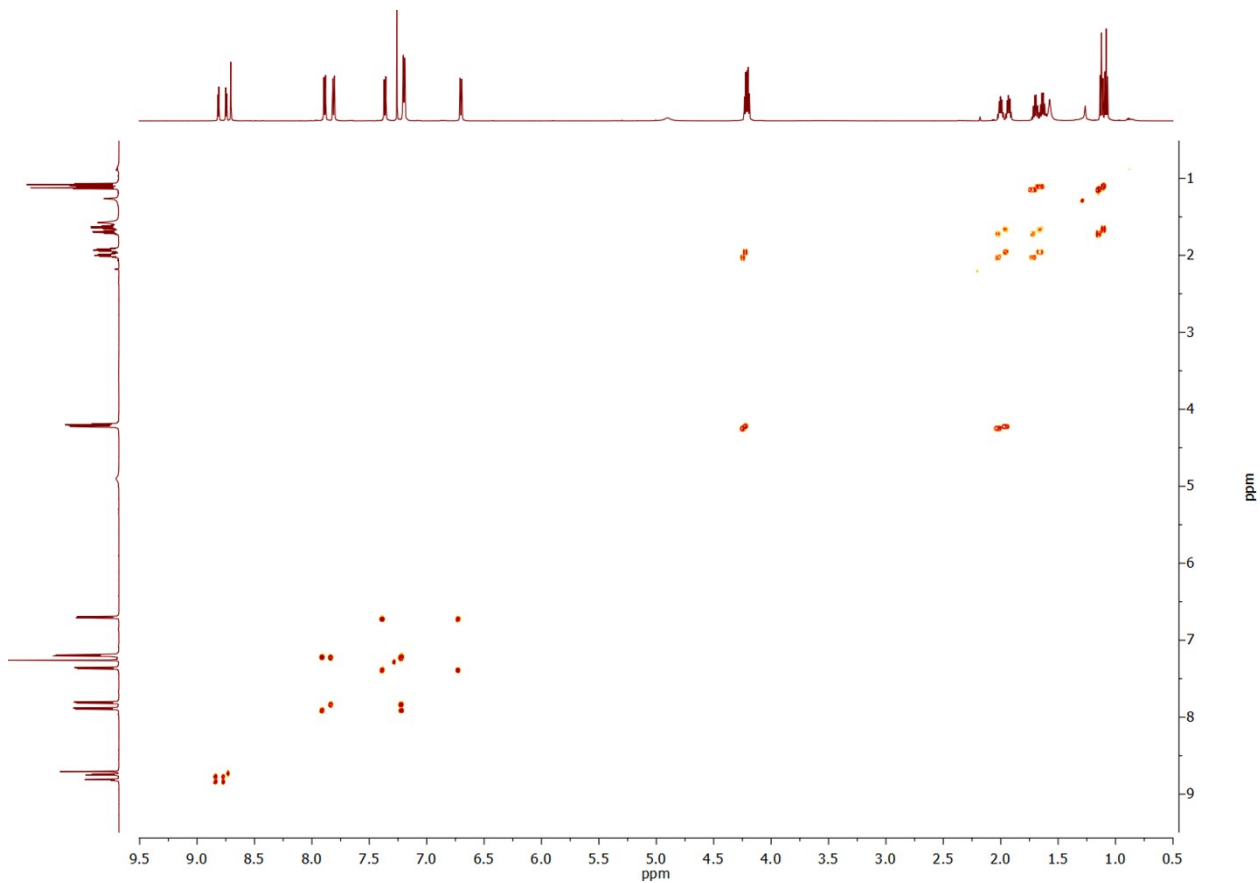Figure S 64. ^{13}C DEPT-135 spectrum of **5c** (CDCl$_3$).
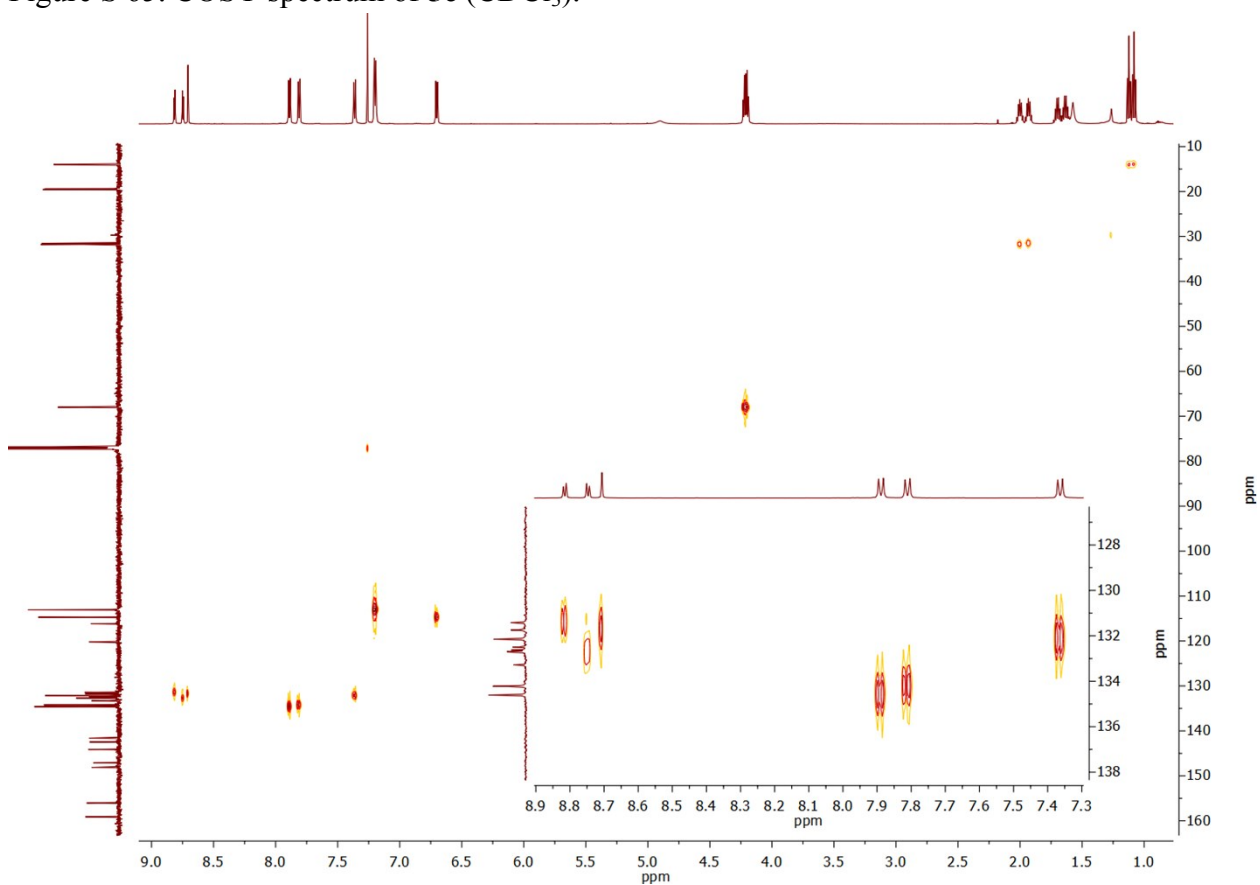
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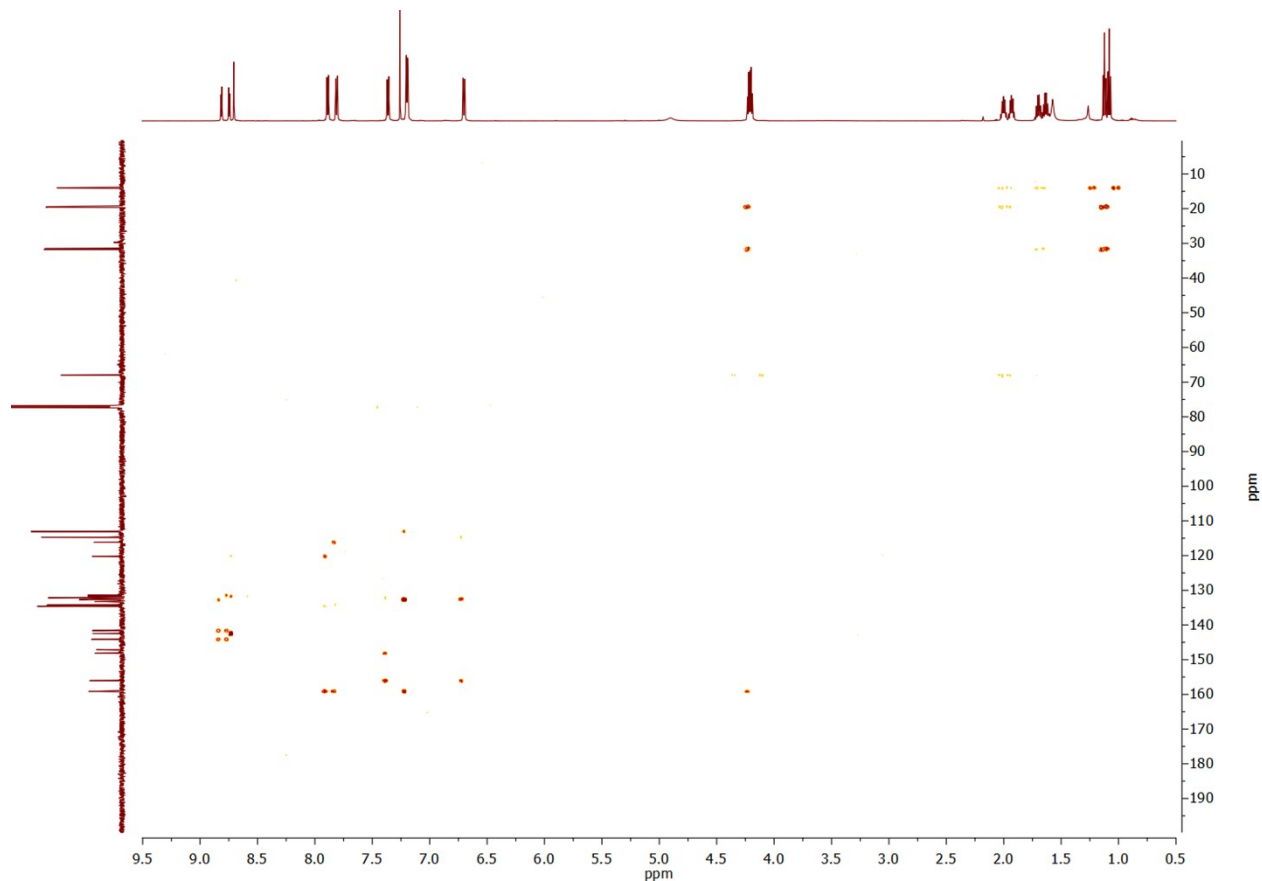
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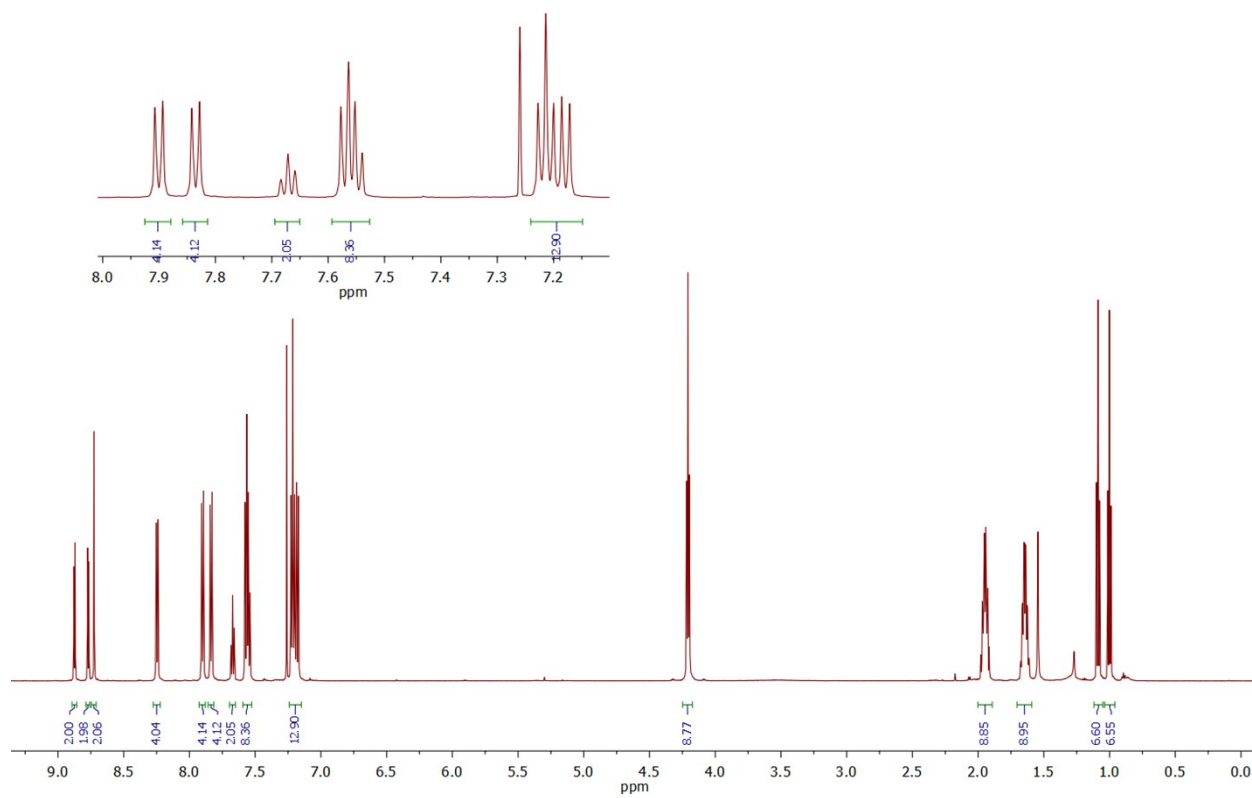
Spectral data of 5e

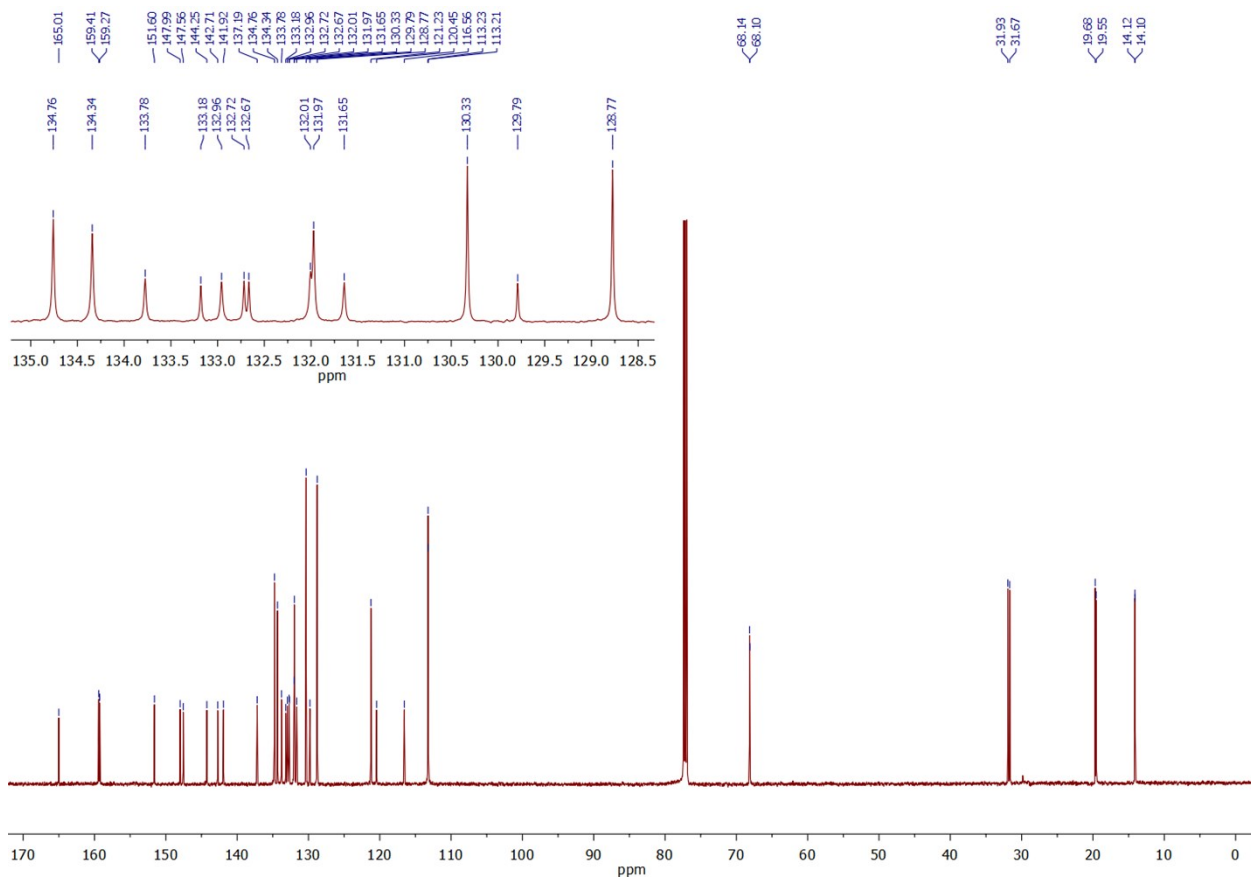Figure S 68. ^{1}H-NMR spectrum of **5e** (CDCl$_3$).
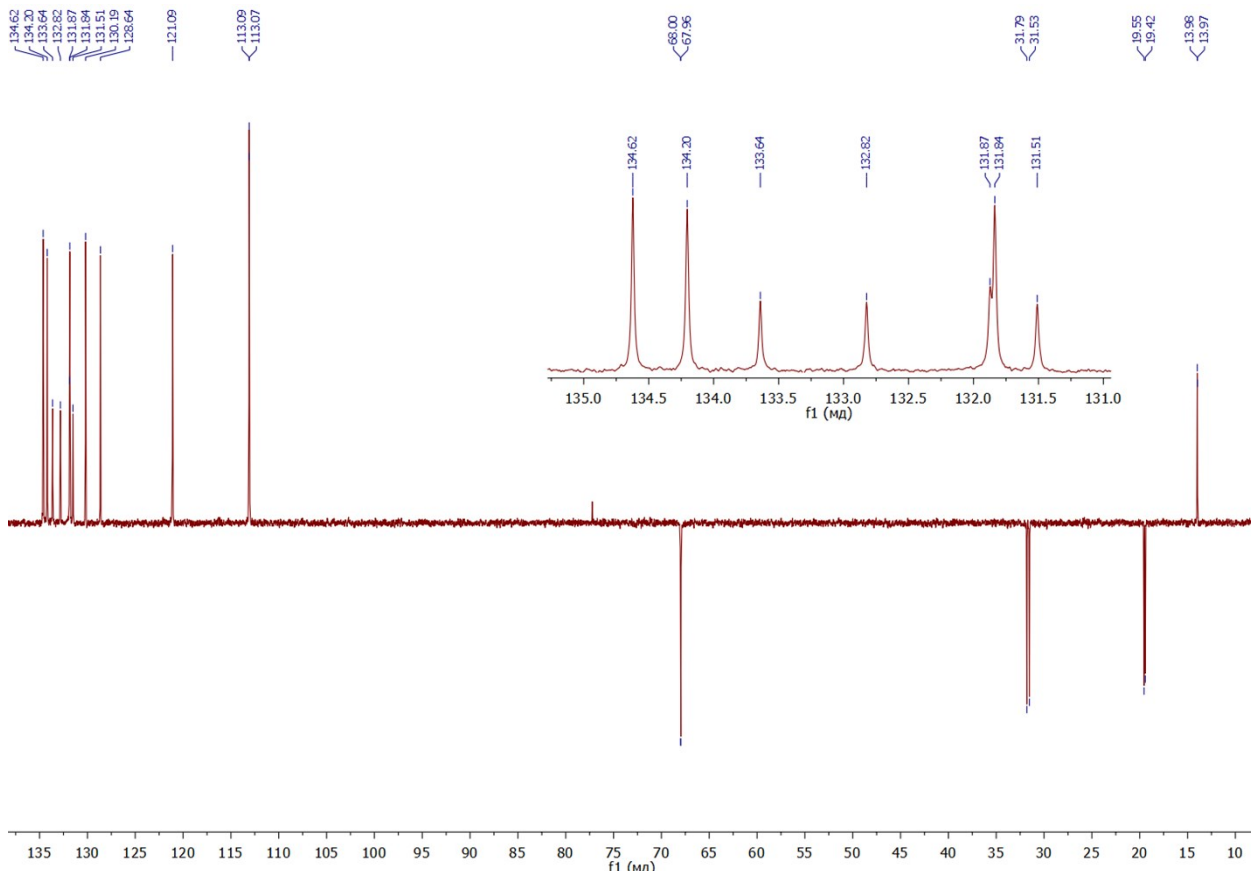
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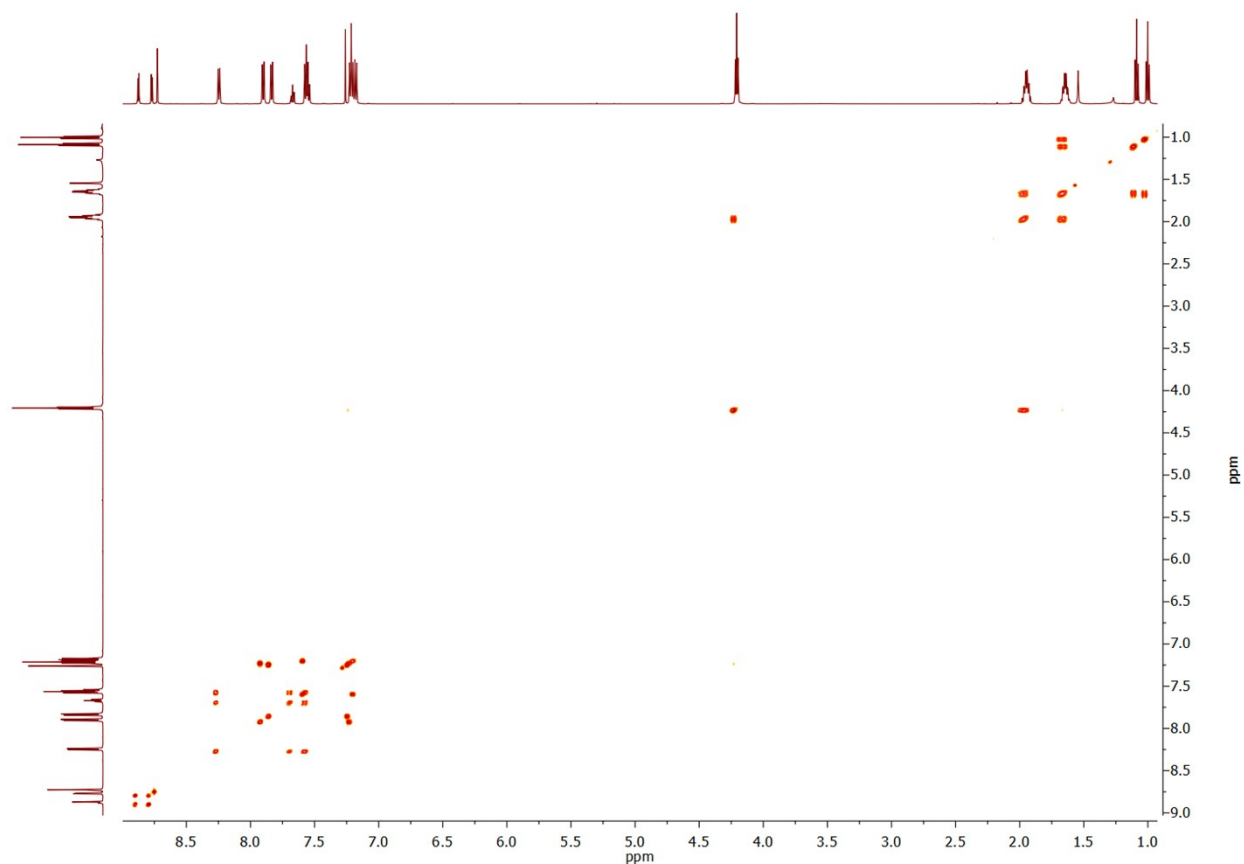Figure S 70. ^{13}C DEPT-135 spectrum of **5e** (CDCl$_3$).
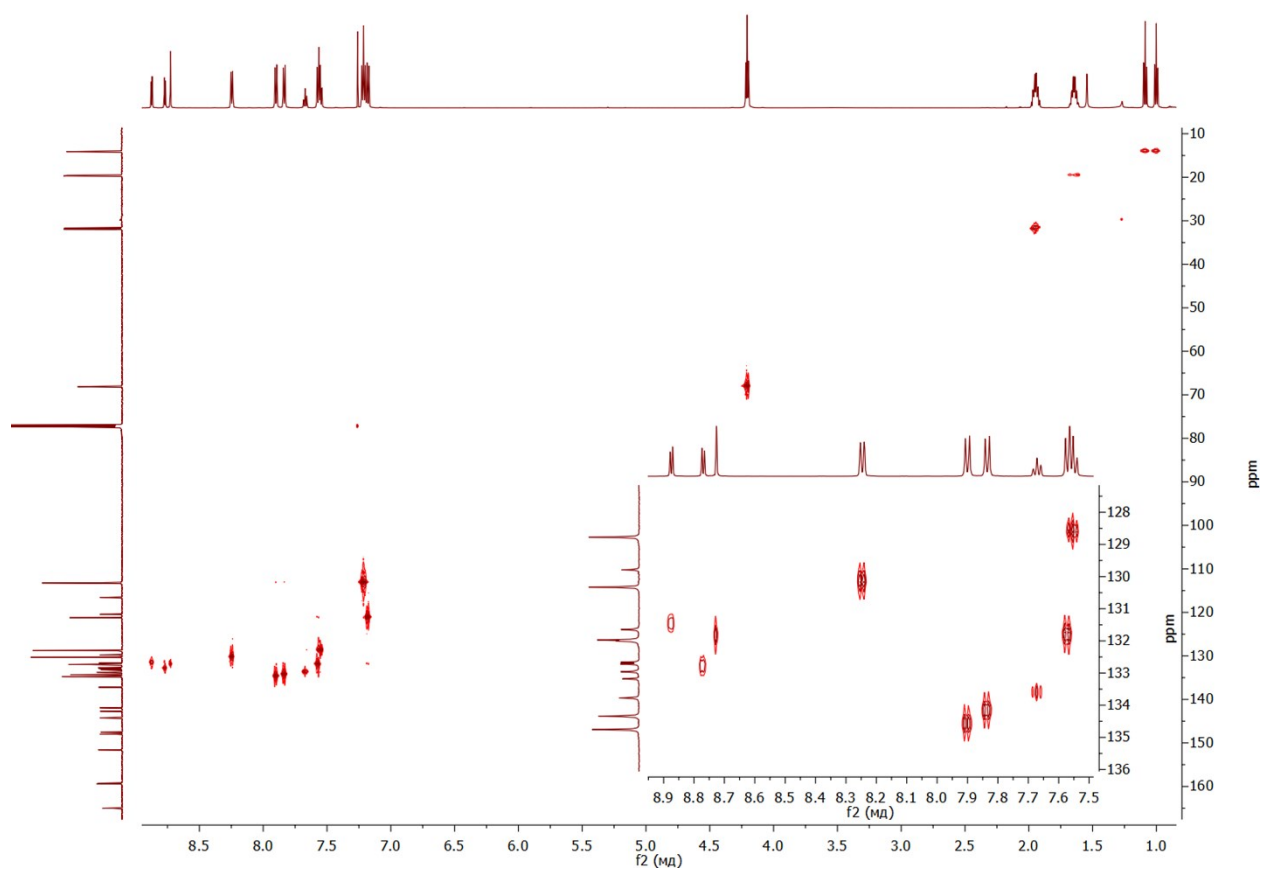
Figure S 71. COSY spectrum of **5e** (CDCl$_3$).

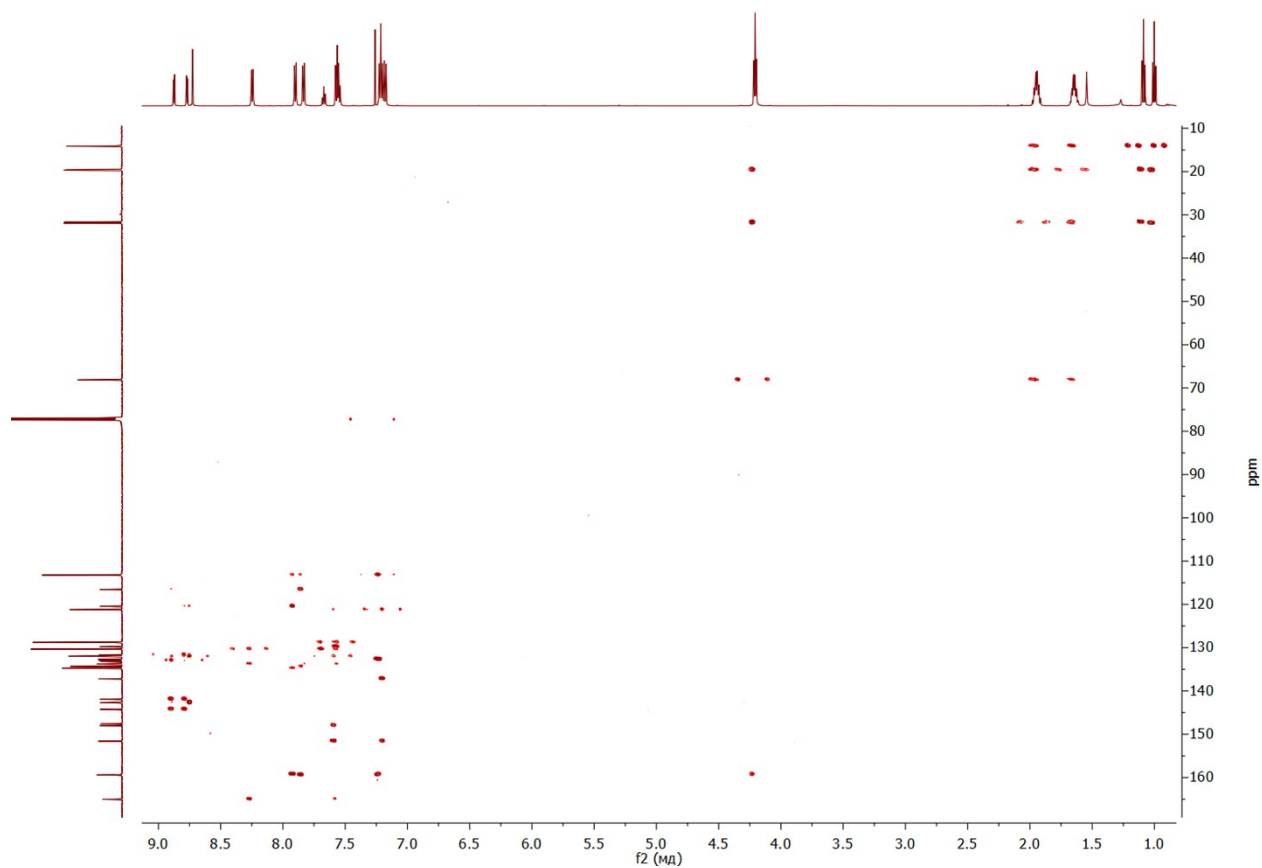Figure S 72. ^{1}H-^{13}C HSQC spectrum of **5e** (CDCl$_3$).

Figure S 73. ^{1}H-^{13}C HMBC spectrum of **5e** (CDCl$_3$).
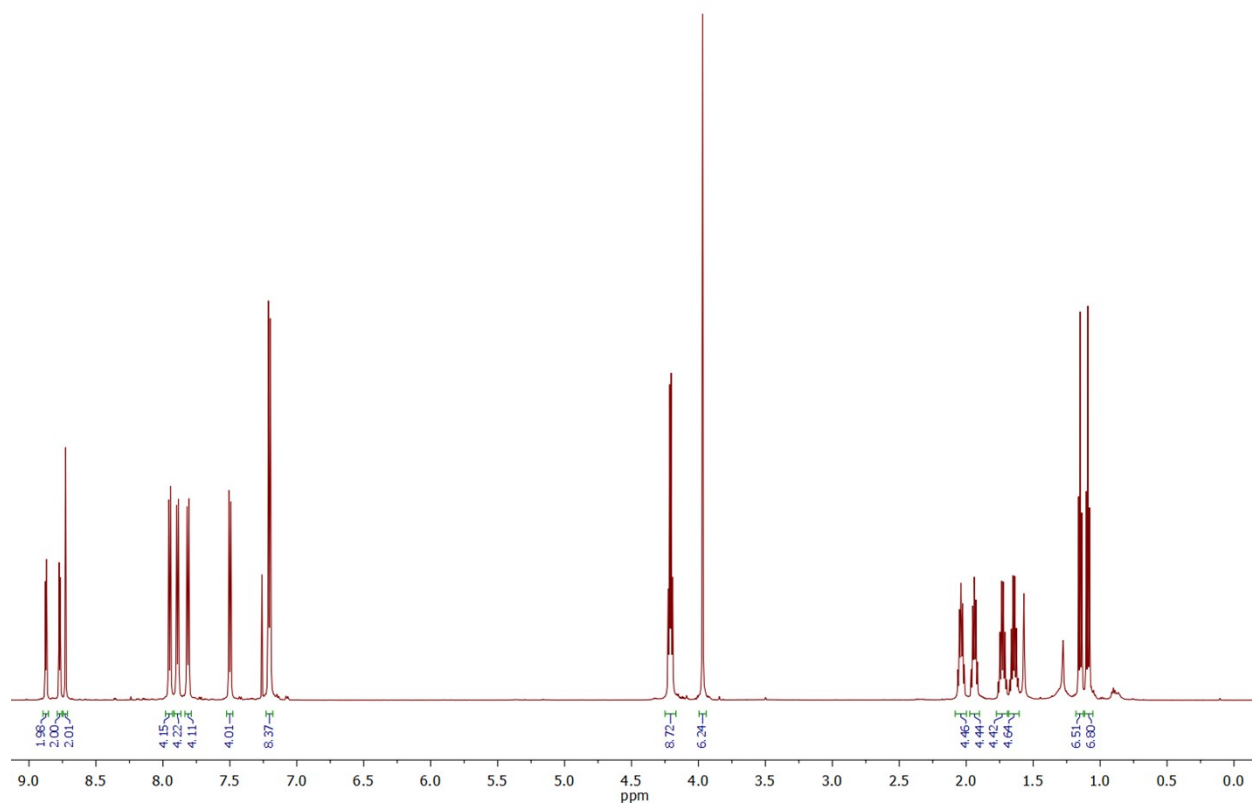
Spectral data of 5f

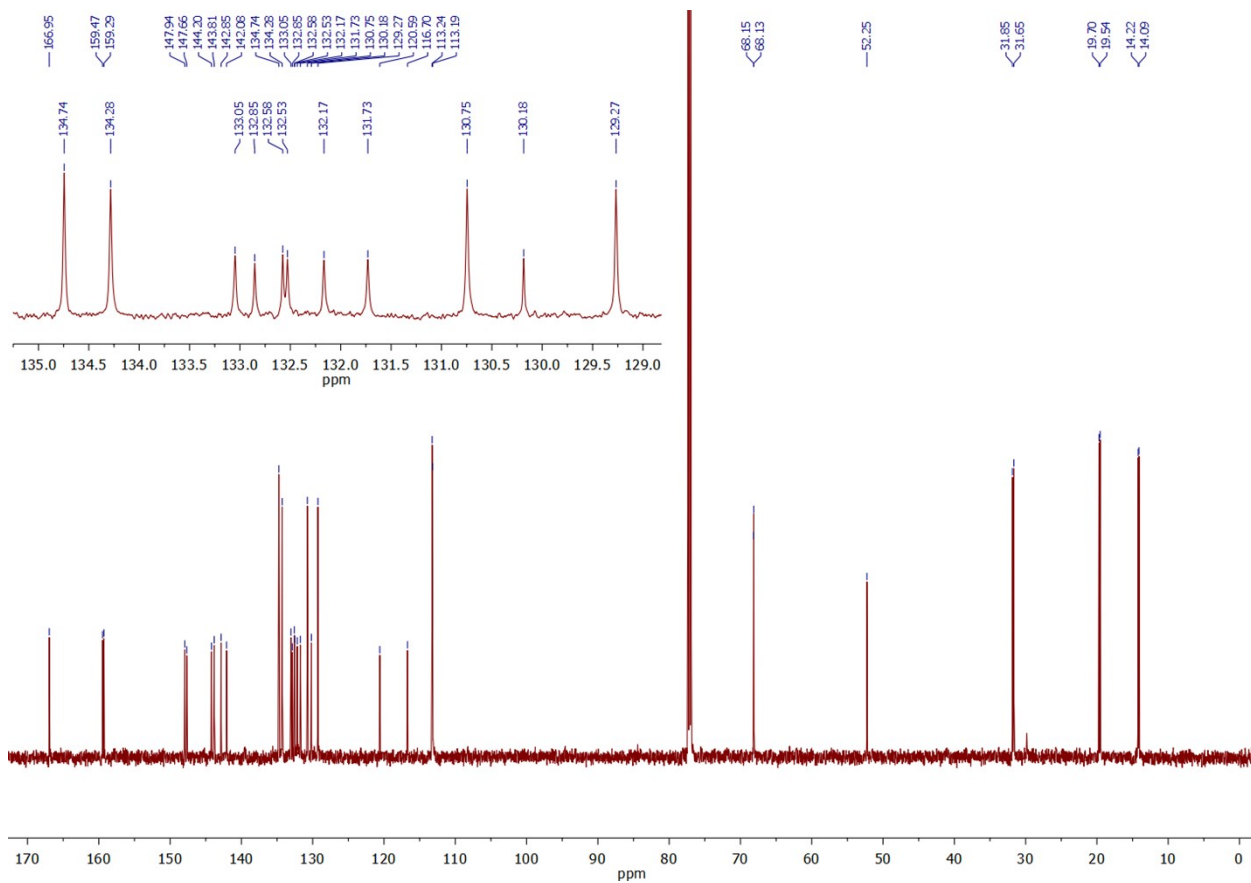Figure S 74. ^{1}H-NMR spectrum of **5f** (CDCl$_3$).
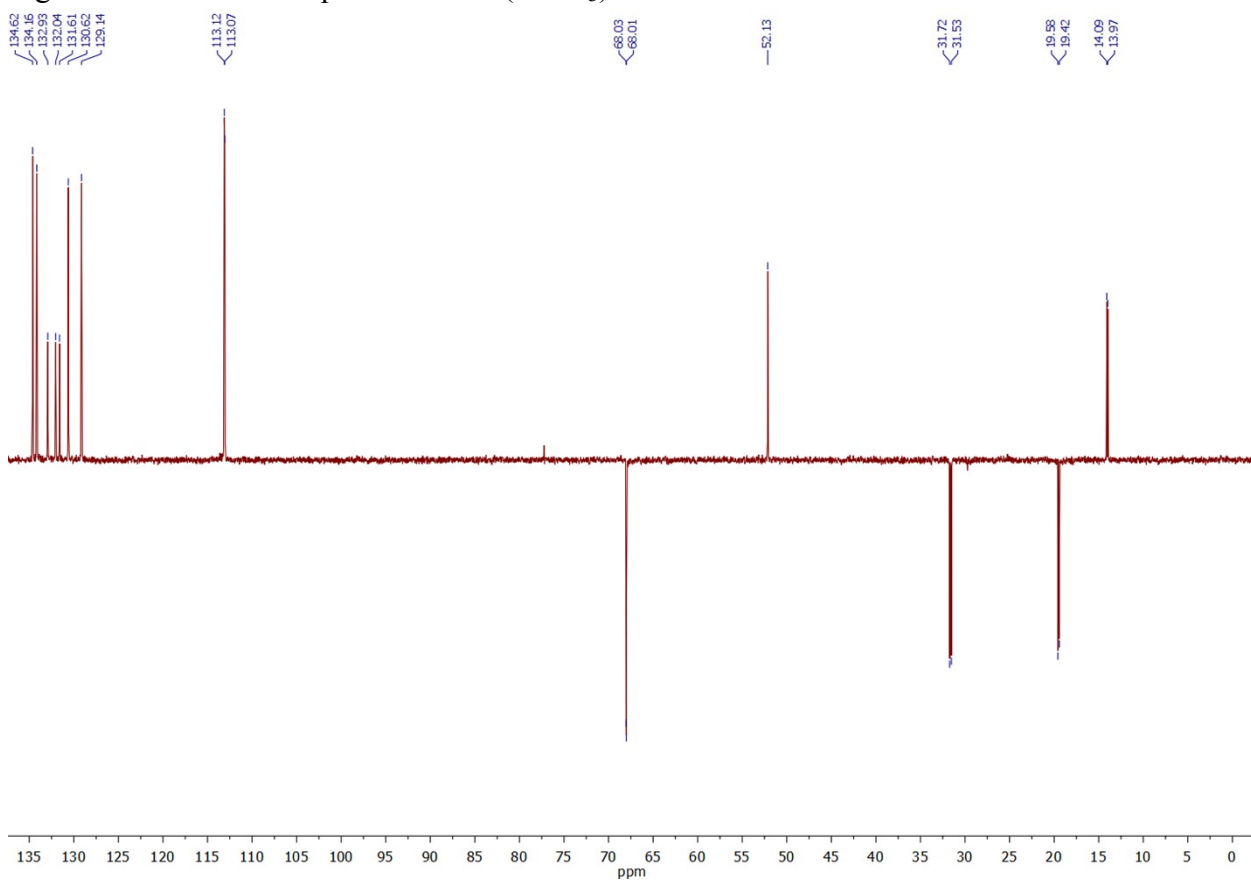
Figure S 75. ^{13}C-NMR spectrum of **5f** (CDCl$_3$).

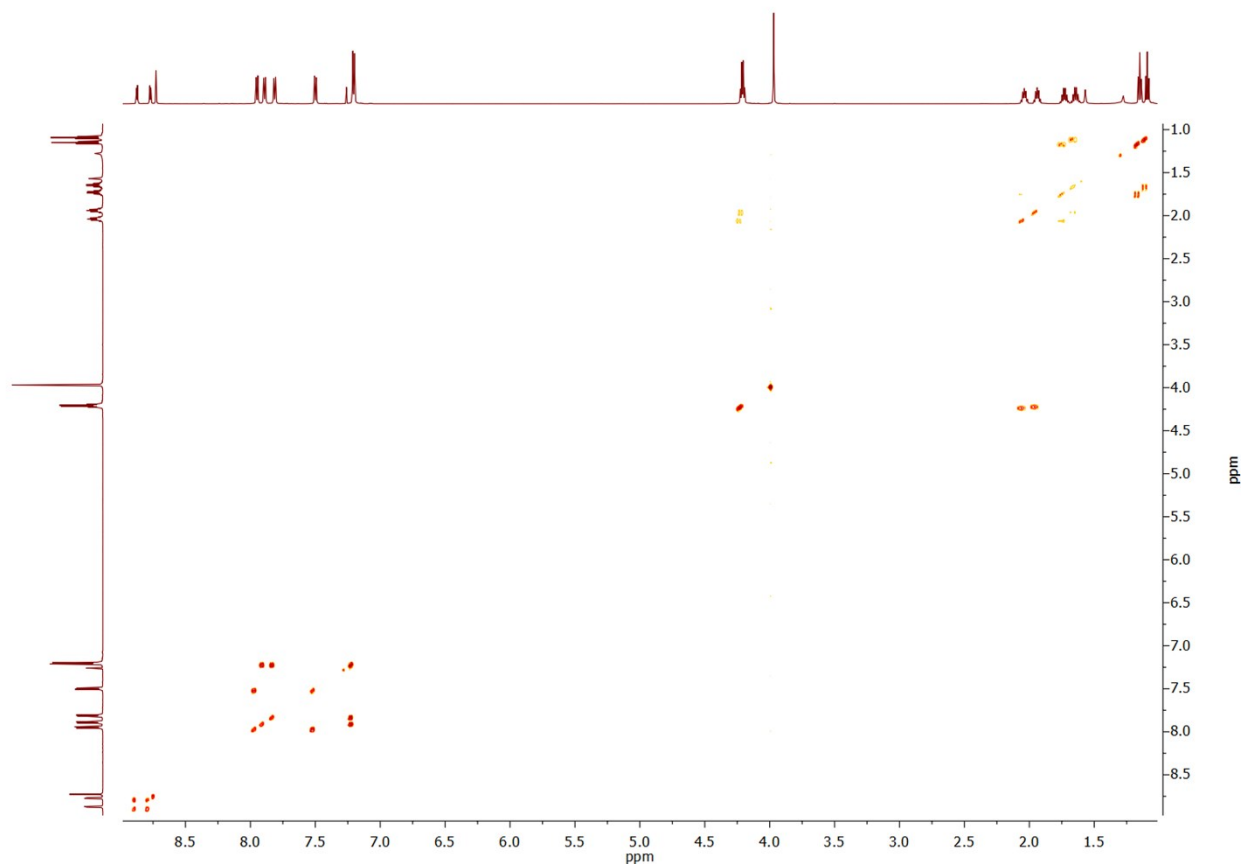Figure S 76. ^{13}C DEPT-135 spectrum of **5f** (CDCl$_3$).
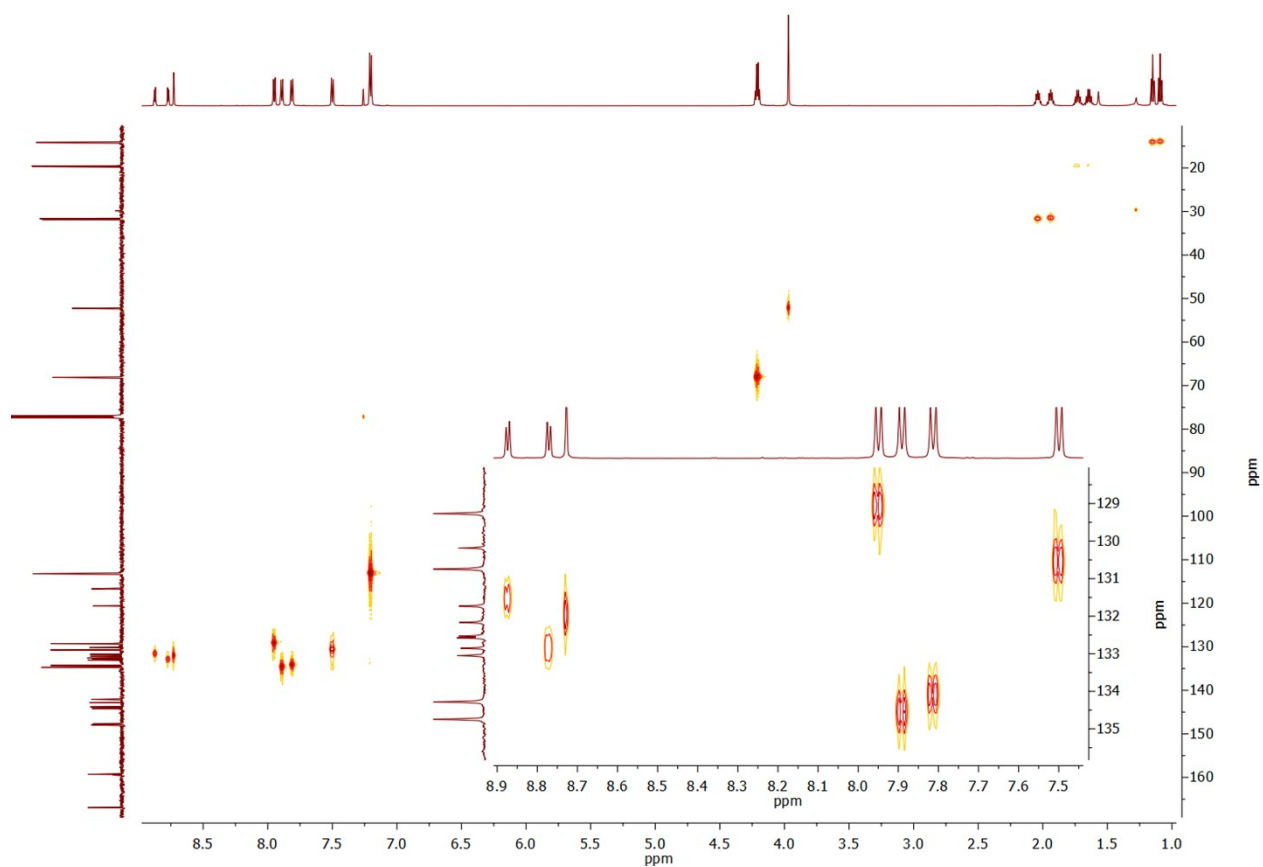
Figure S 77. COSY spectrum of **5f** (CDCl$_3$).

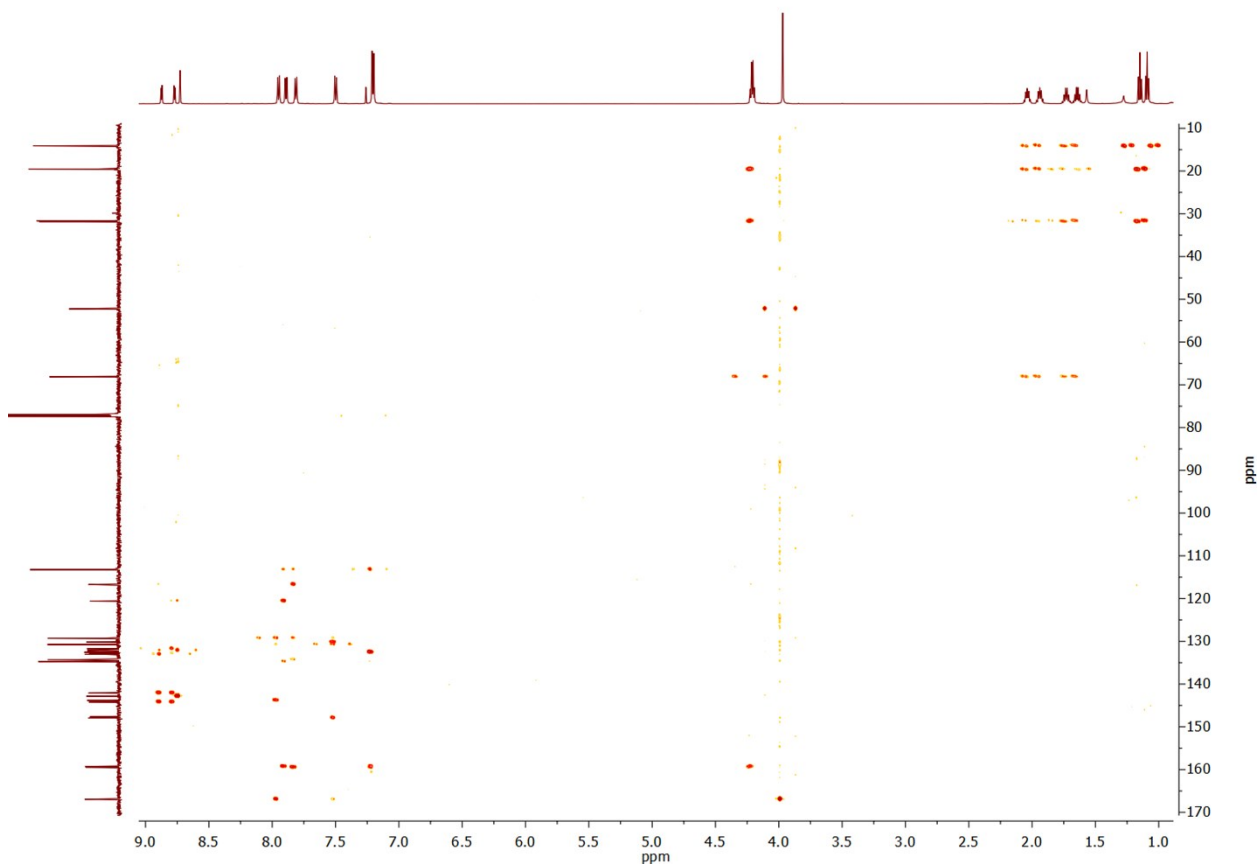Figure S 78. ^{1}H-^{13}C HSQC spectrum of **5f** (CDCl$_3$).

Figure S 79. ^{1}H-^{13}C HMBC spectrum of **5f** (CDCl$_3$).
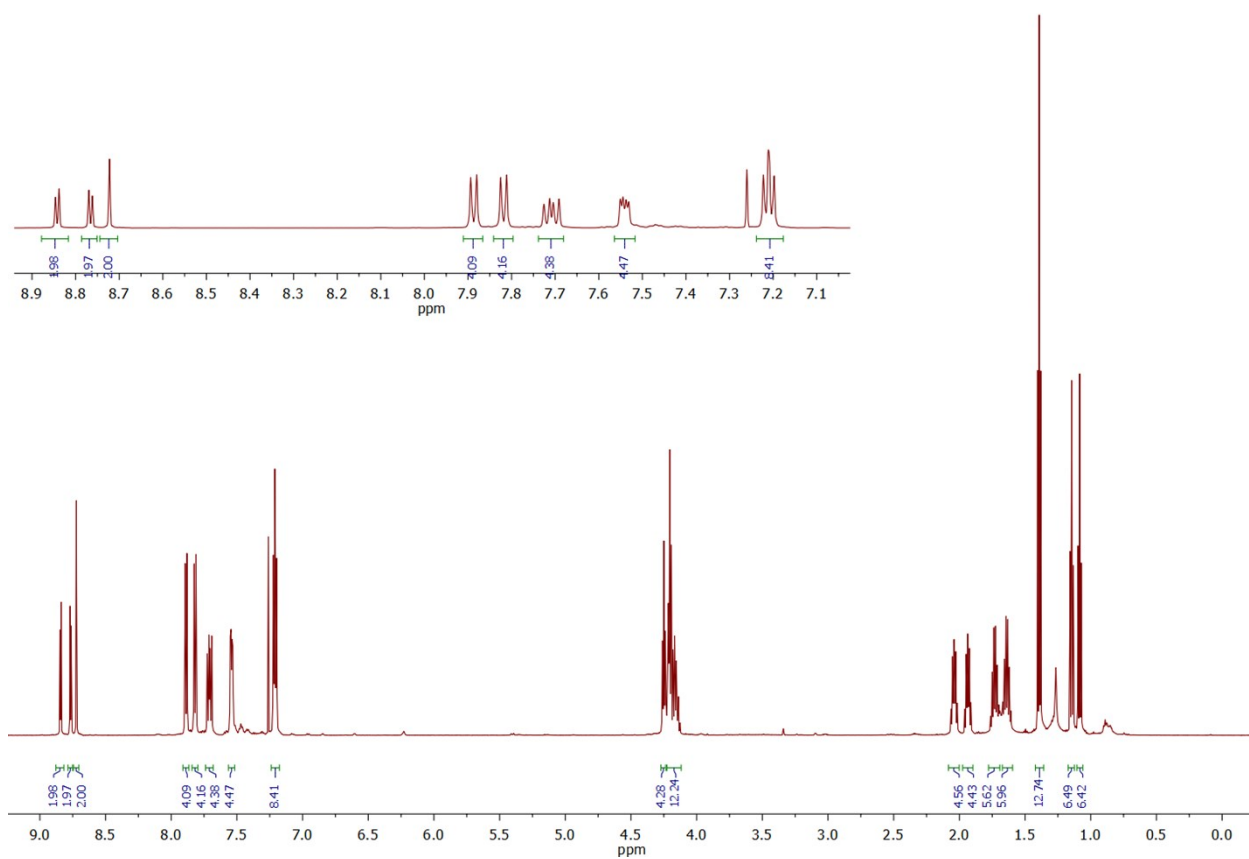
Spectral data of 5g

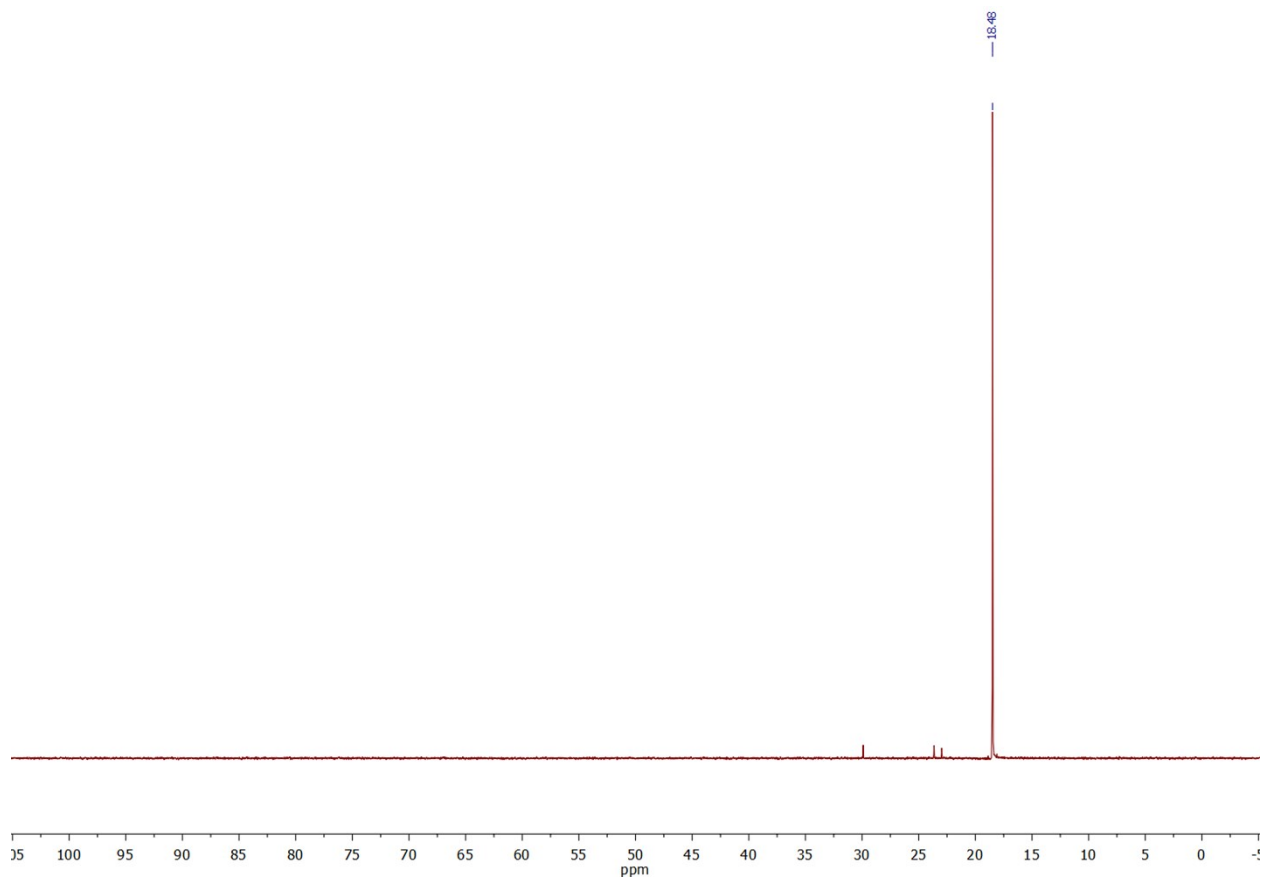Figure S 80. ^{1}H-NMR spectrum of **5g** (CDCl$_3$).

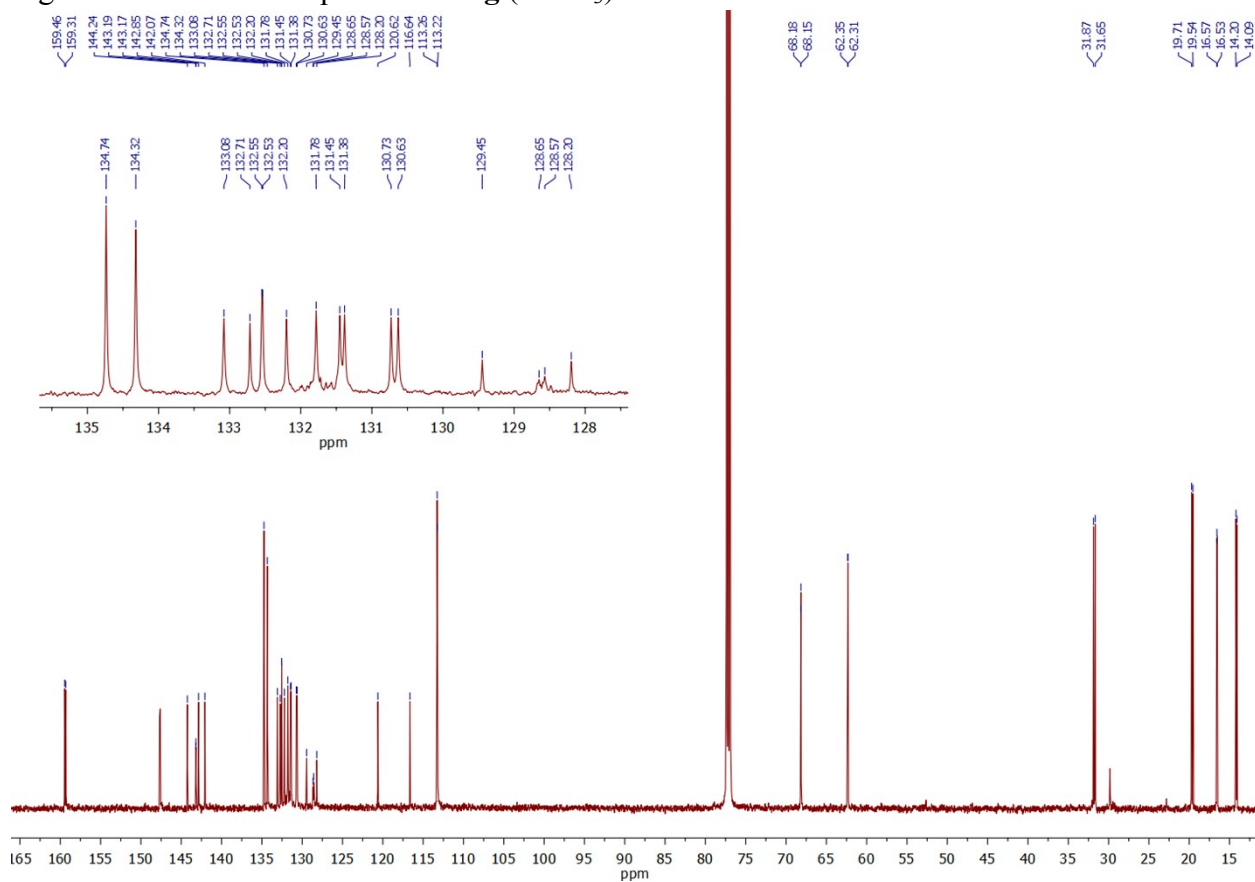Figure S 81. ^{31}P-NMR spectrum of **5g** (CDCl$_3$).
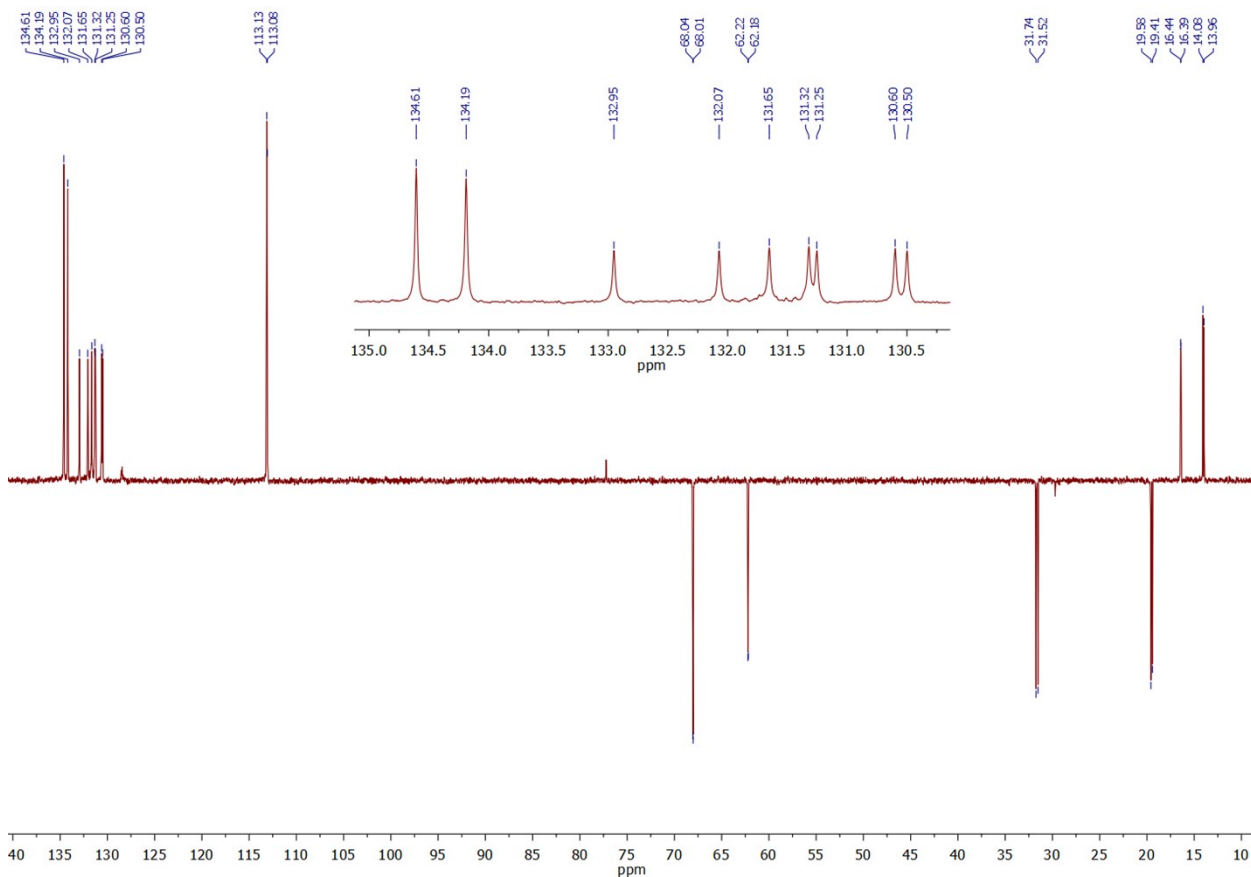

Figure S 82. ^{13}C-NMR spectrum of **5g** (CDCl$_3$).
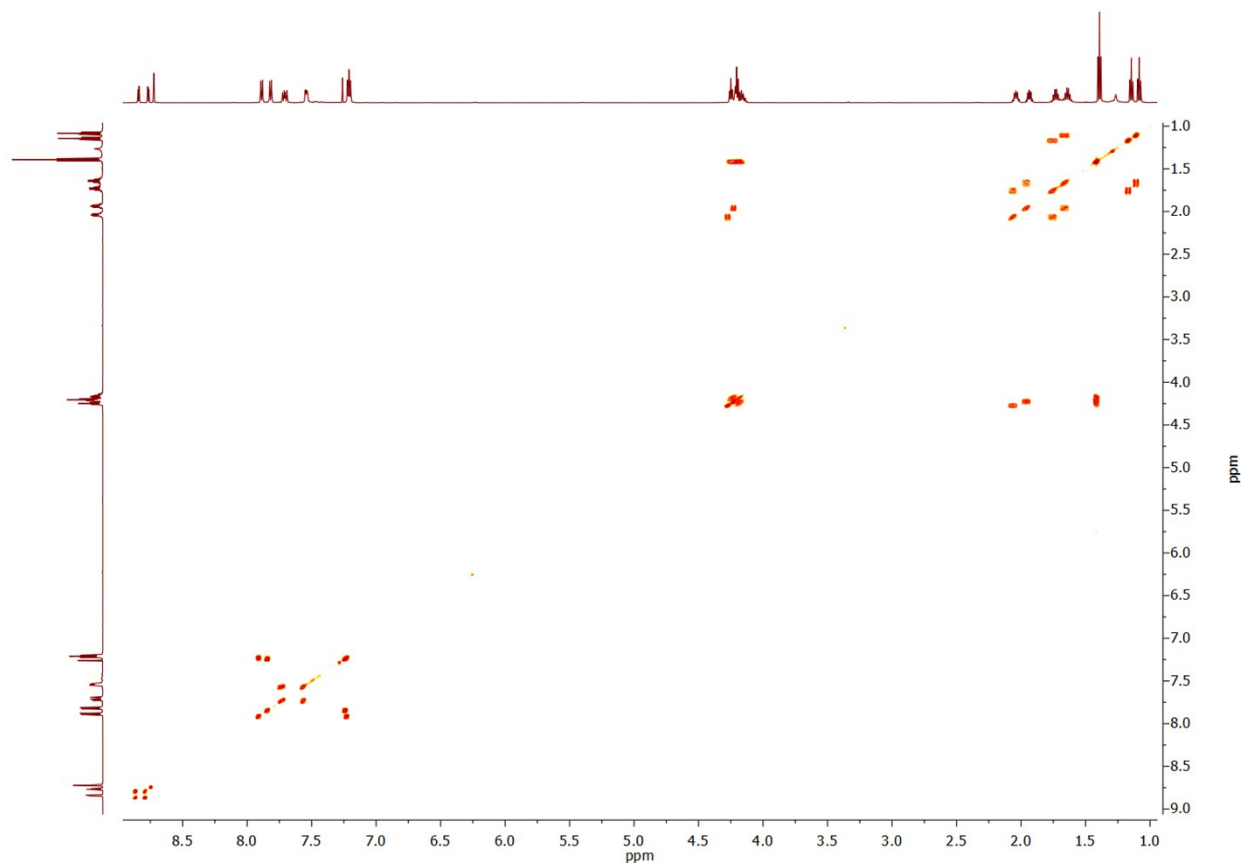
Figure S 83. ^{13}C DEPT spectrum of **5g** (CDCl$_3$).
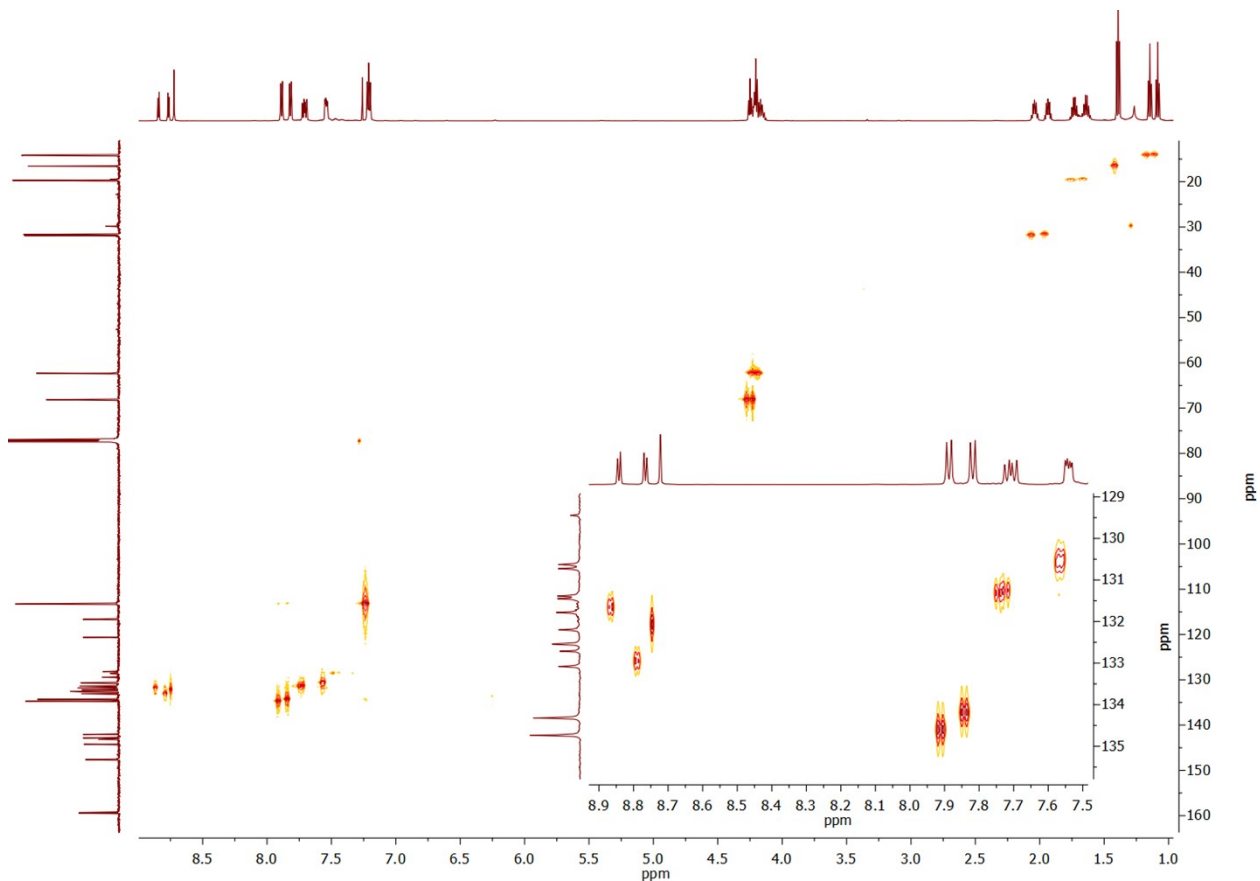

Figure S 84. COSY spectrum of **5g** (CDCl$_3$).

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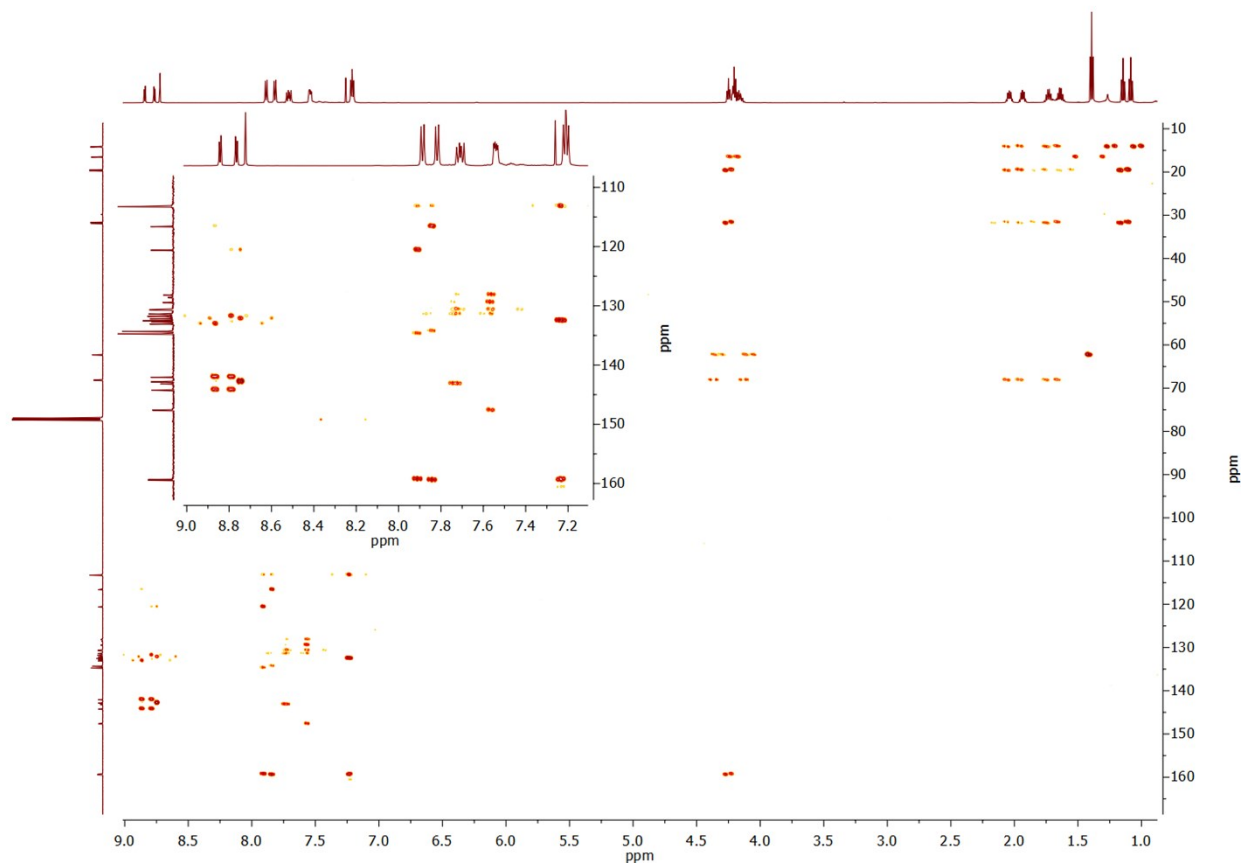Figure S 85. ^{1}H-^{13}C HSQC spectrum of **5g** (CDCl$_3$).

Figure S 86. ^{1}H-^{13}C HMBC spectrum of **5g** (CDCl$_3$).
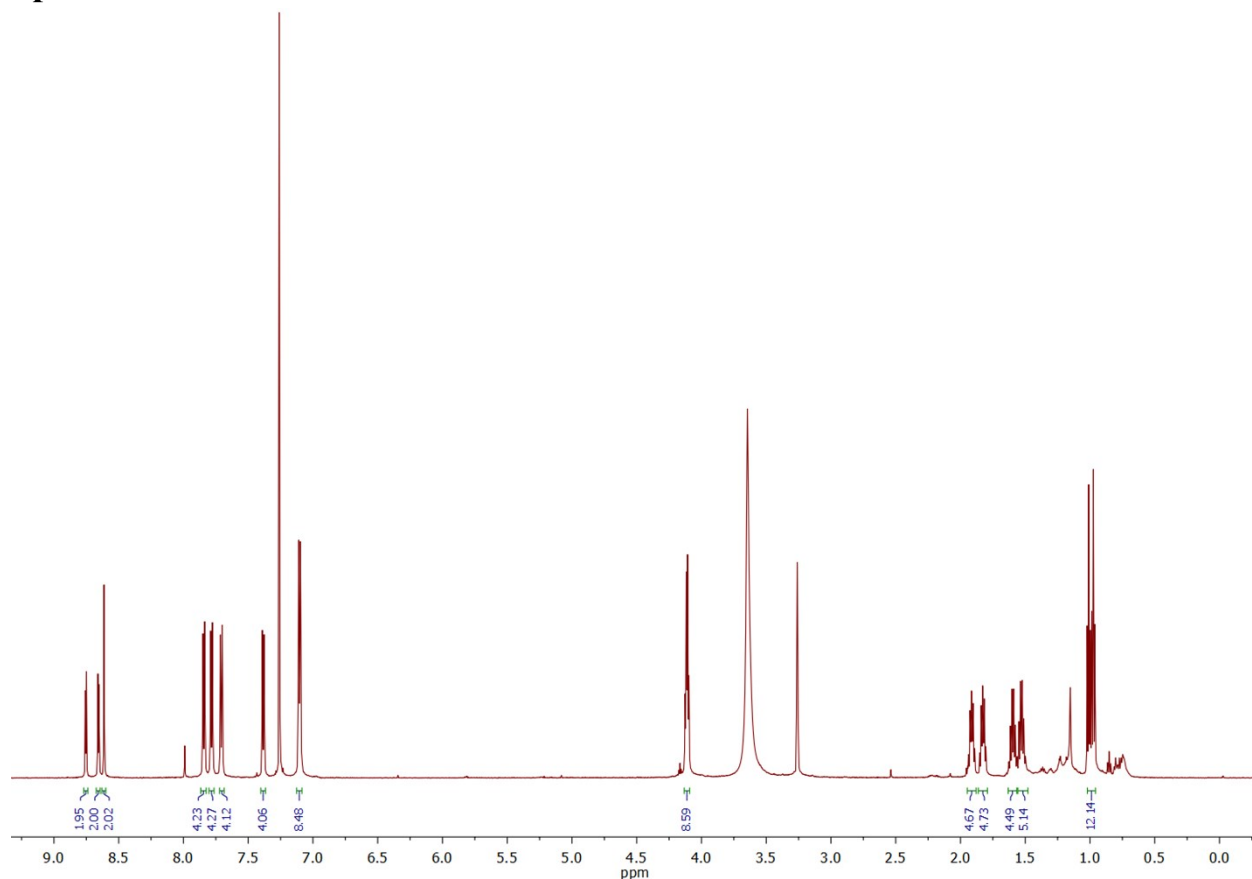
Spectral data of 5h

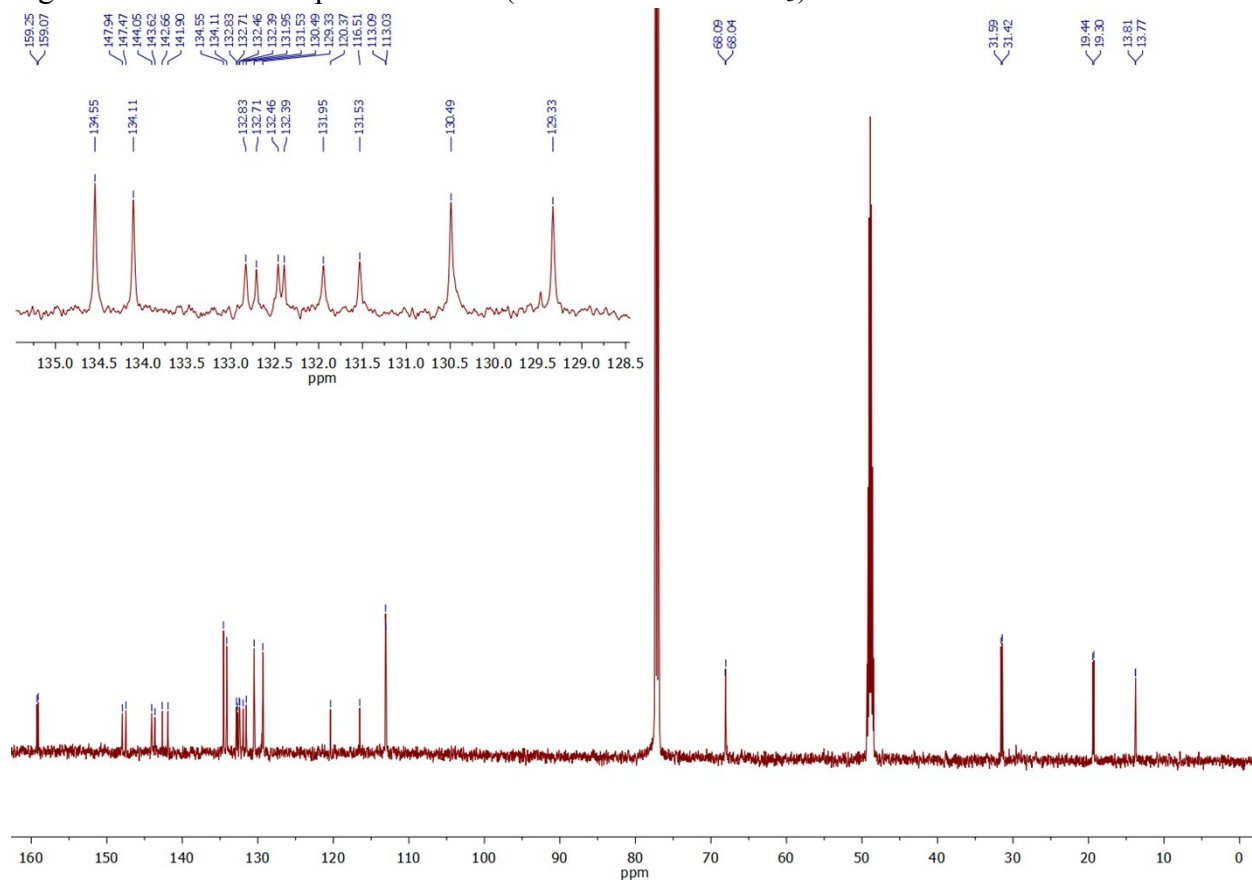Figure S 87. ^{1}H-NMR spectrum of **5h** (20% MeOD in CDCl$_3$).

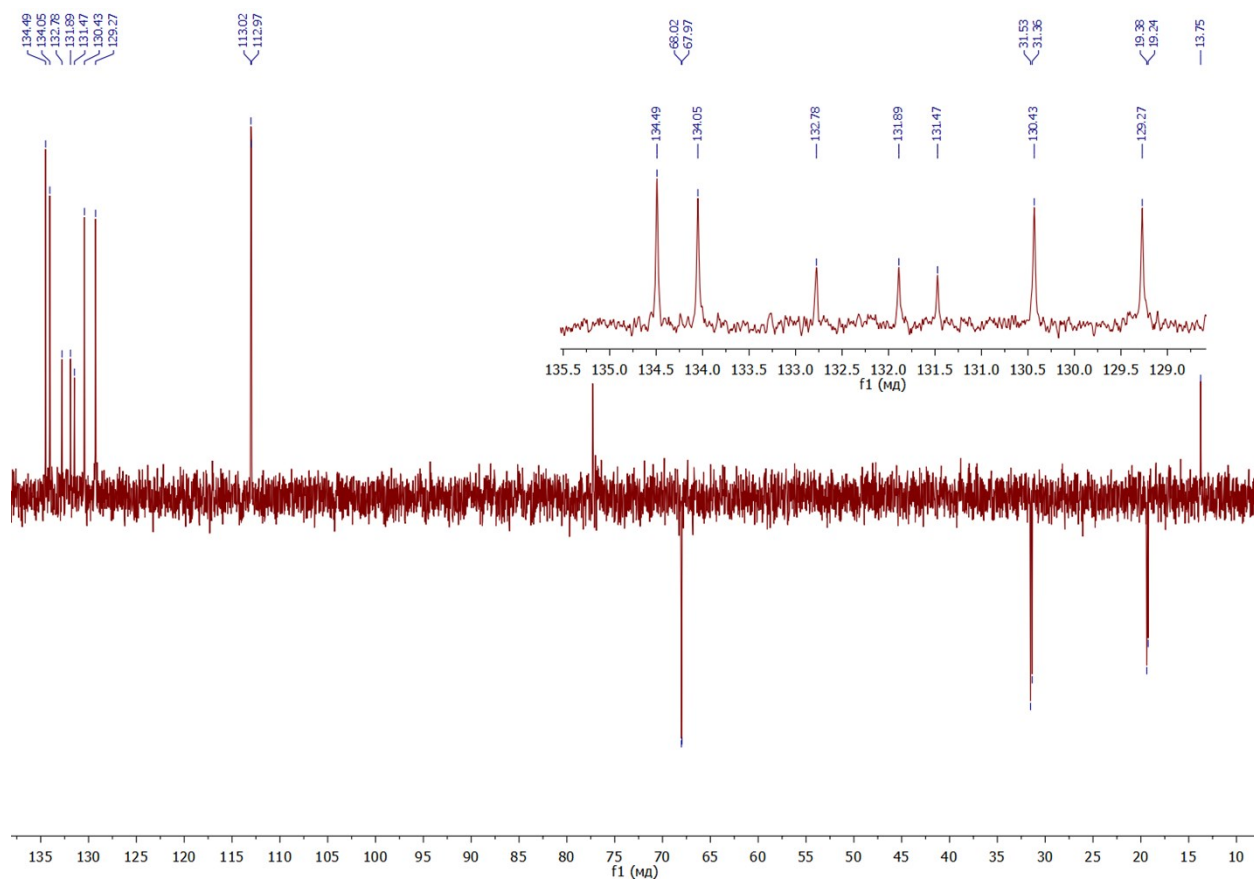Figure S 88. ^{13}C-NMR spectrum of **5h** (20% MeOD in CDCl$_3$).

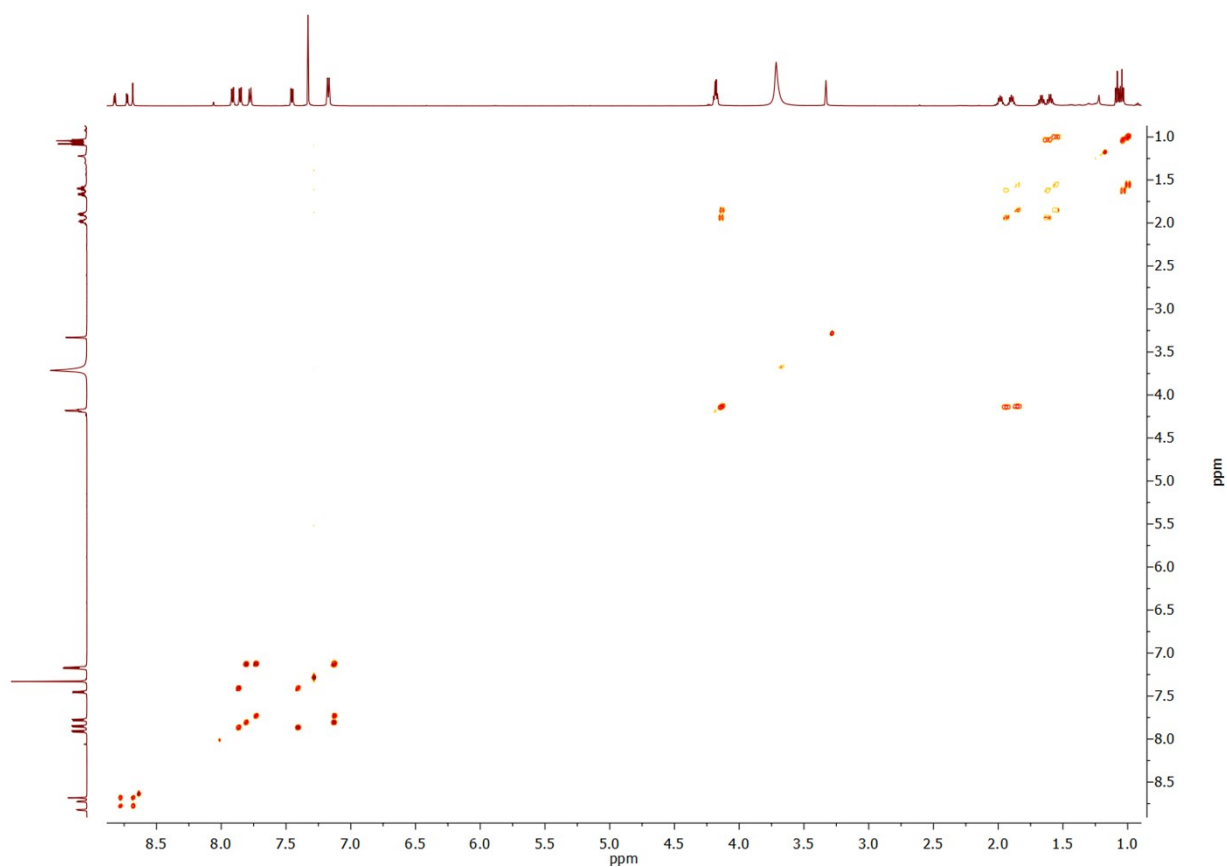Figure S 89. ^{13}C DEPT-135 spectrum of **5h** (20% MeOD in CDCl$_3$).

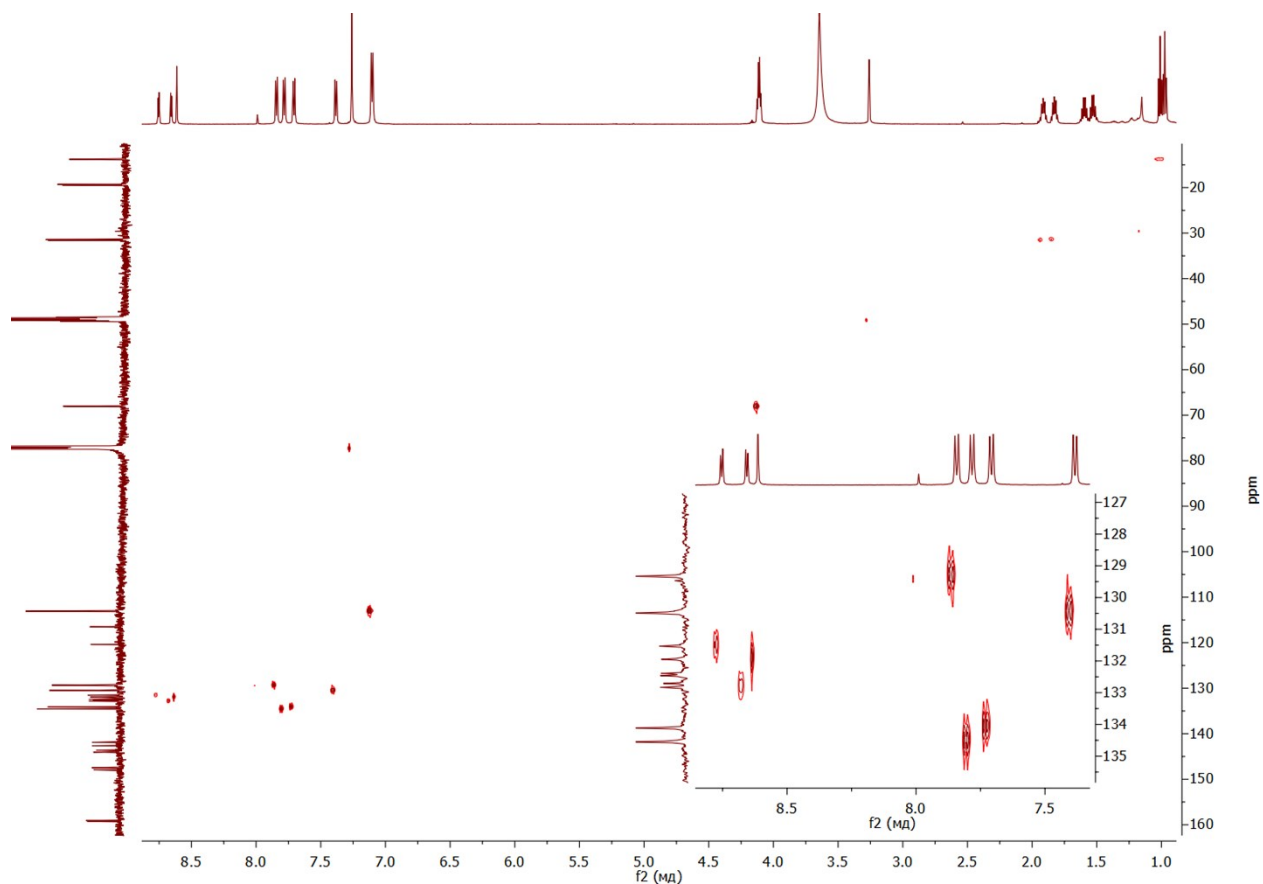Figure S 90. COSY spectrum of **5h** (20% MeOD in CDCl$_3$).

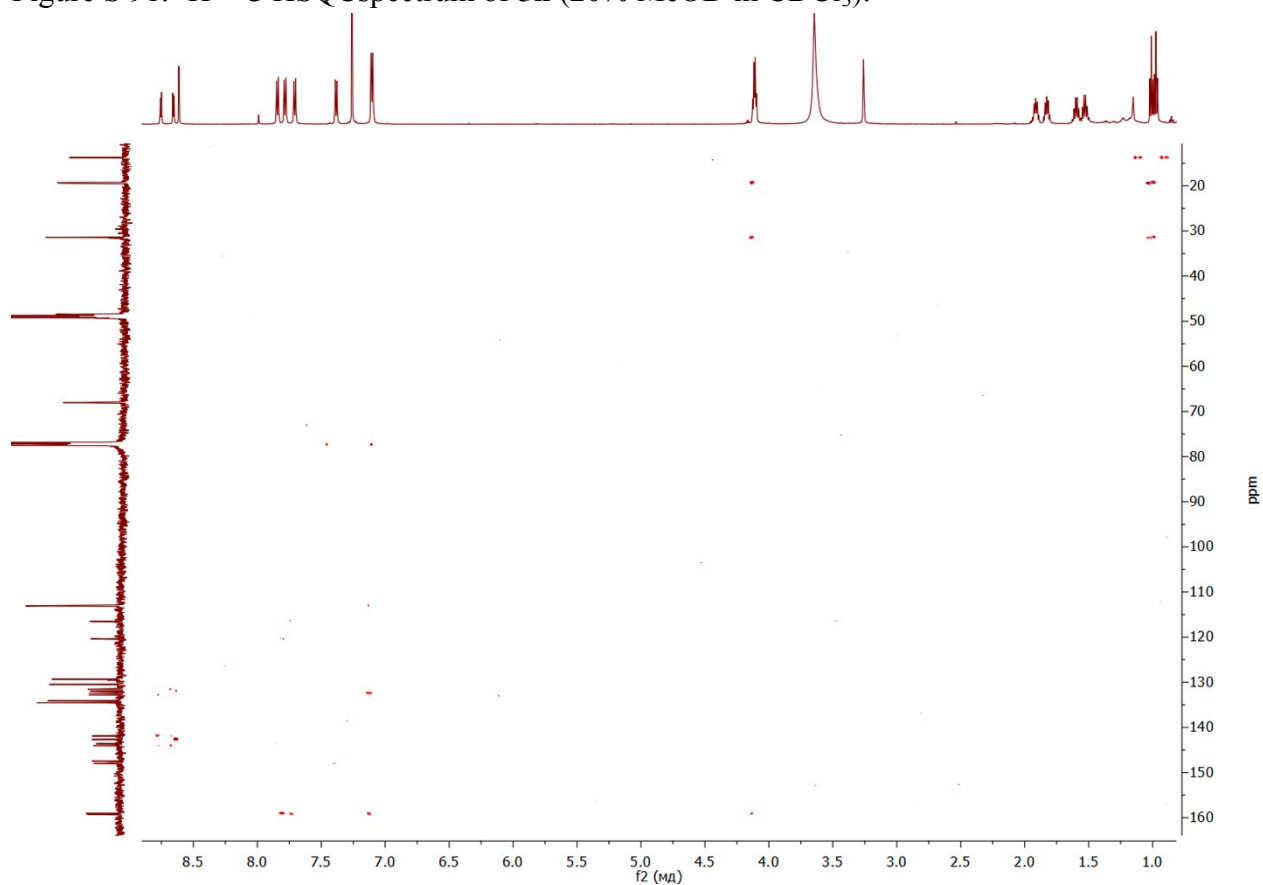Figure S 91. ^{1}H-^{13}C HSQCspectrum of **5h** (20% MeOD in CDCl$_3$).

Figure S 92. ^{1}H-^{13}C HMBC spectrum of **5h** (20% MeOD in CDCl$_3$).
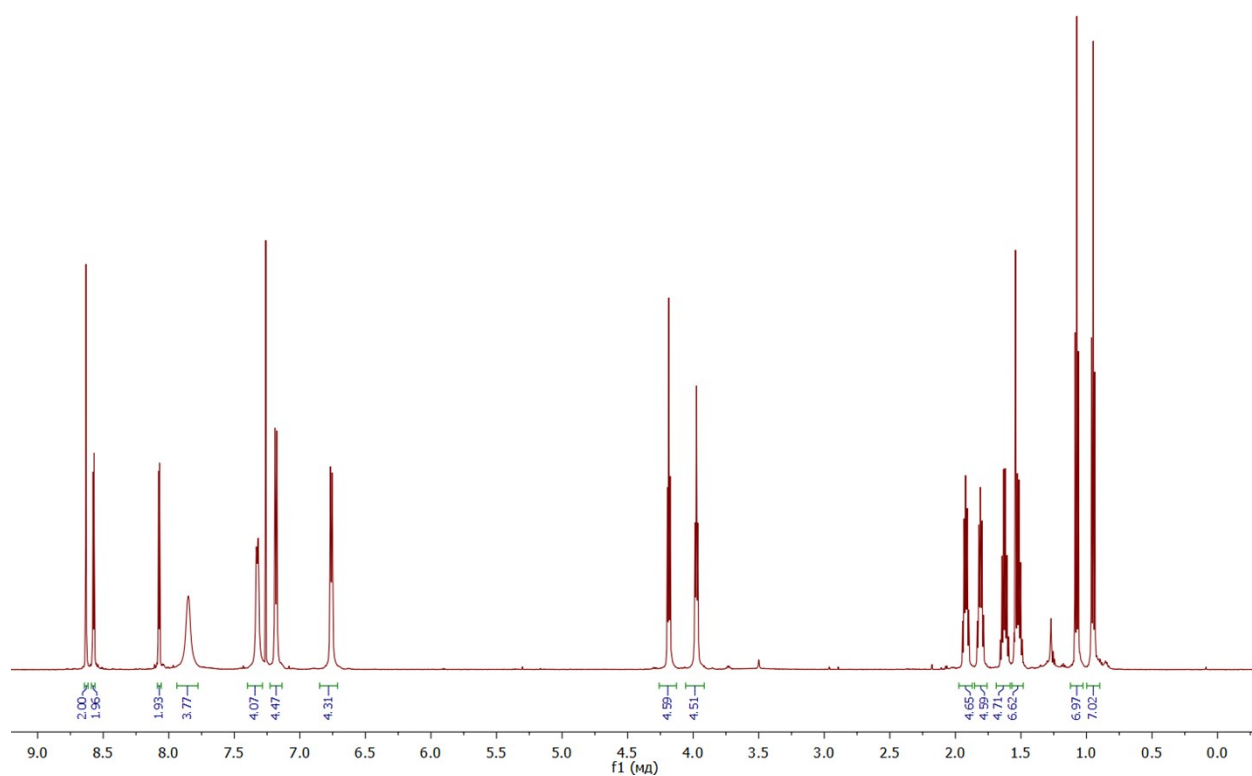
Spectral data of 6

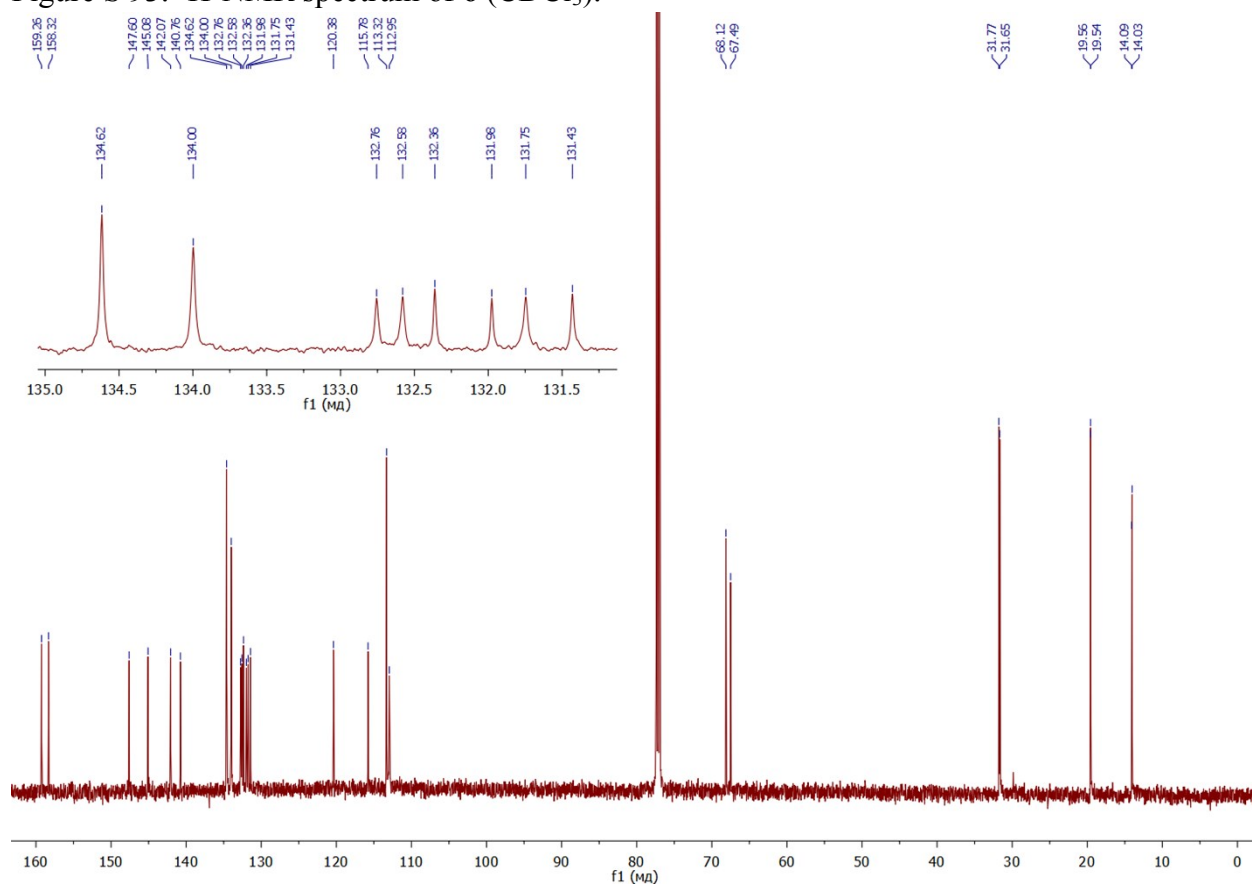Figure S 93. ^{1}H-NMR spectrum of **6** (CDCl$_3$).

Figure S 94. ^{13}C-NMR spectrum of **6** (CDCl$_3$).
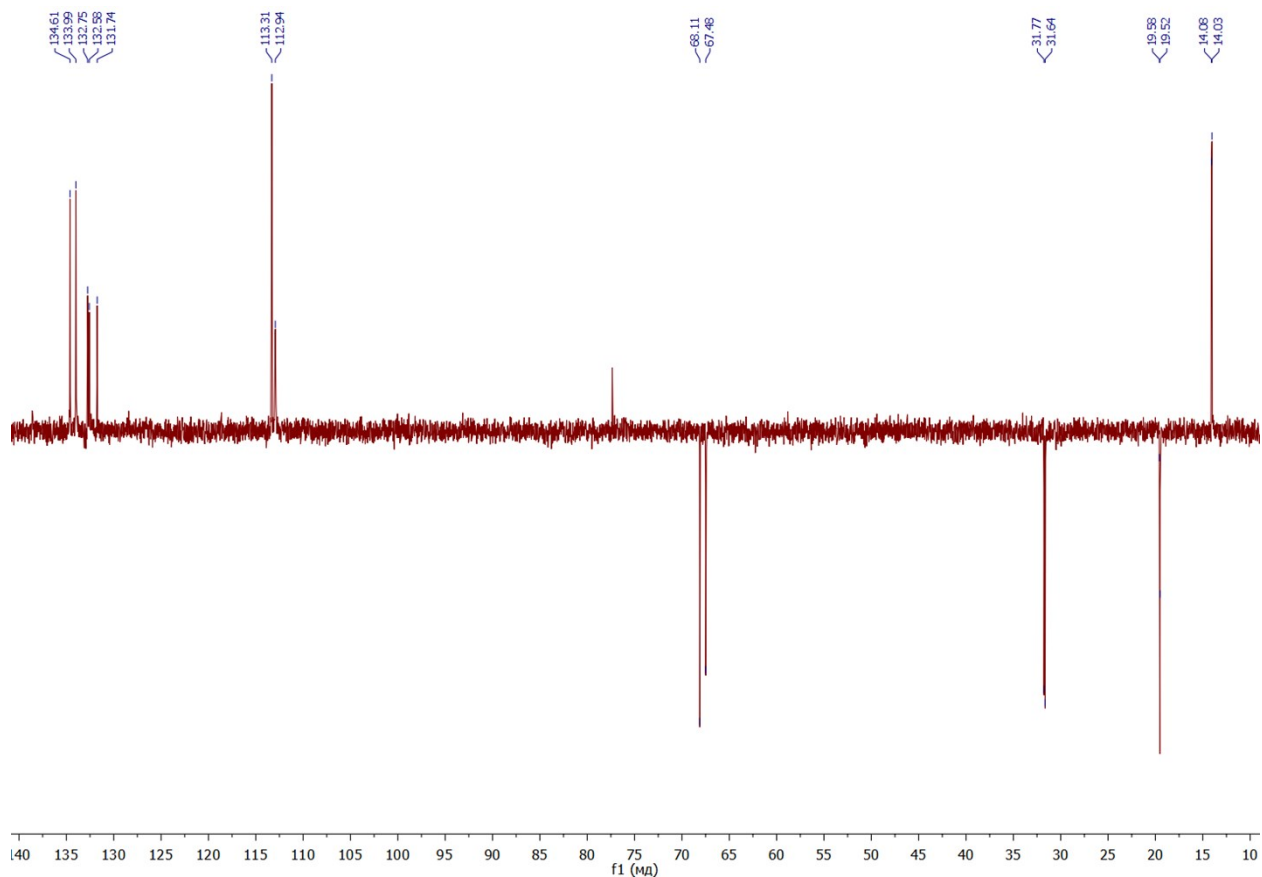
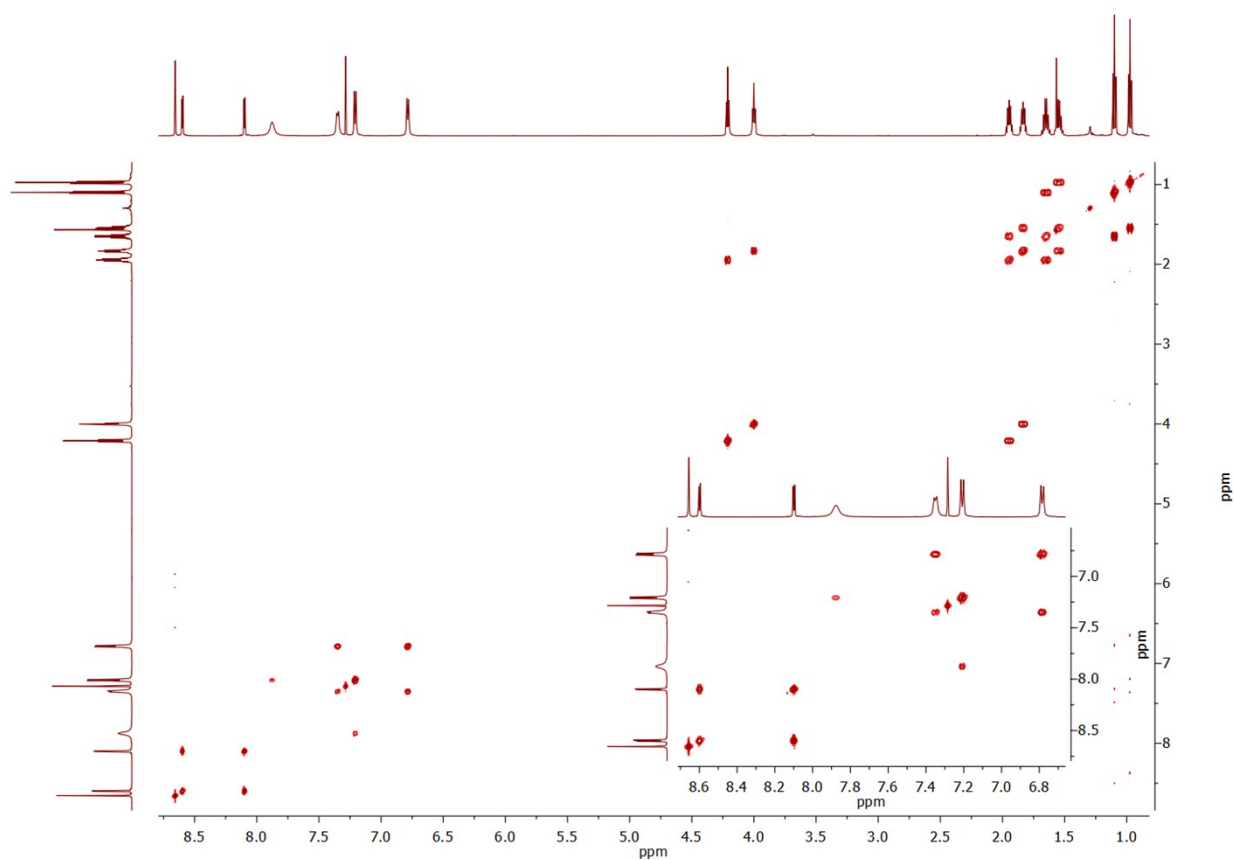Figure S 95. ^{13}C DEPT-135 spectrum of **6** (CDCl$_3$).
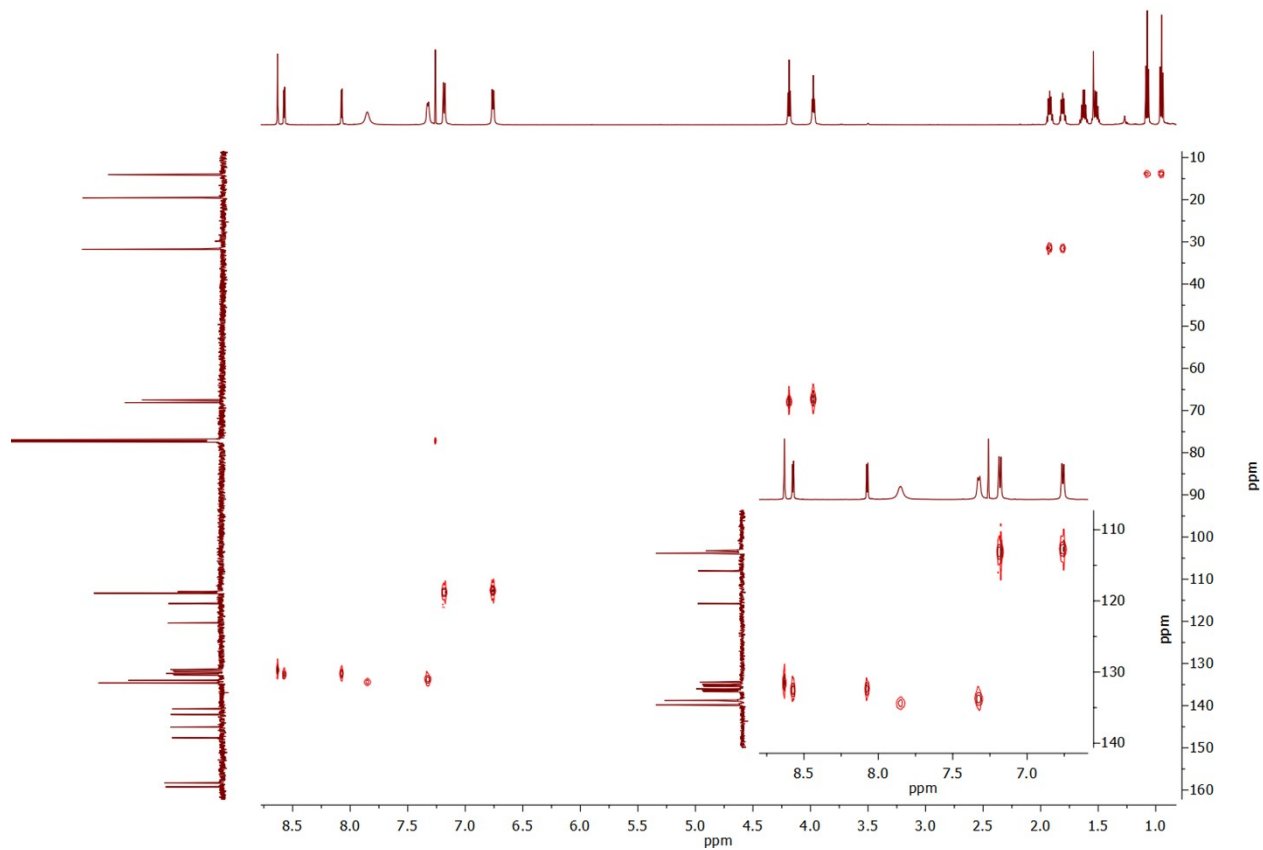

Figure S 96. COSY spectrum of **6** (CDCl$_3$).
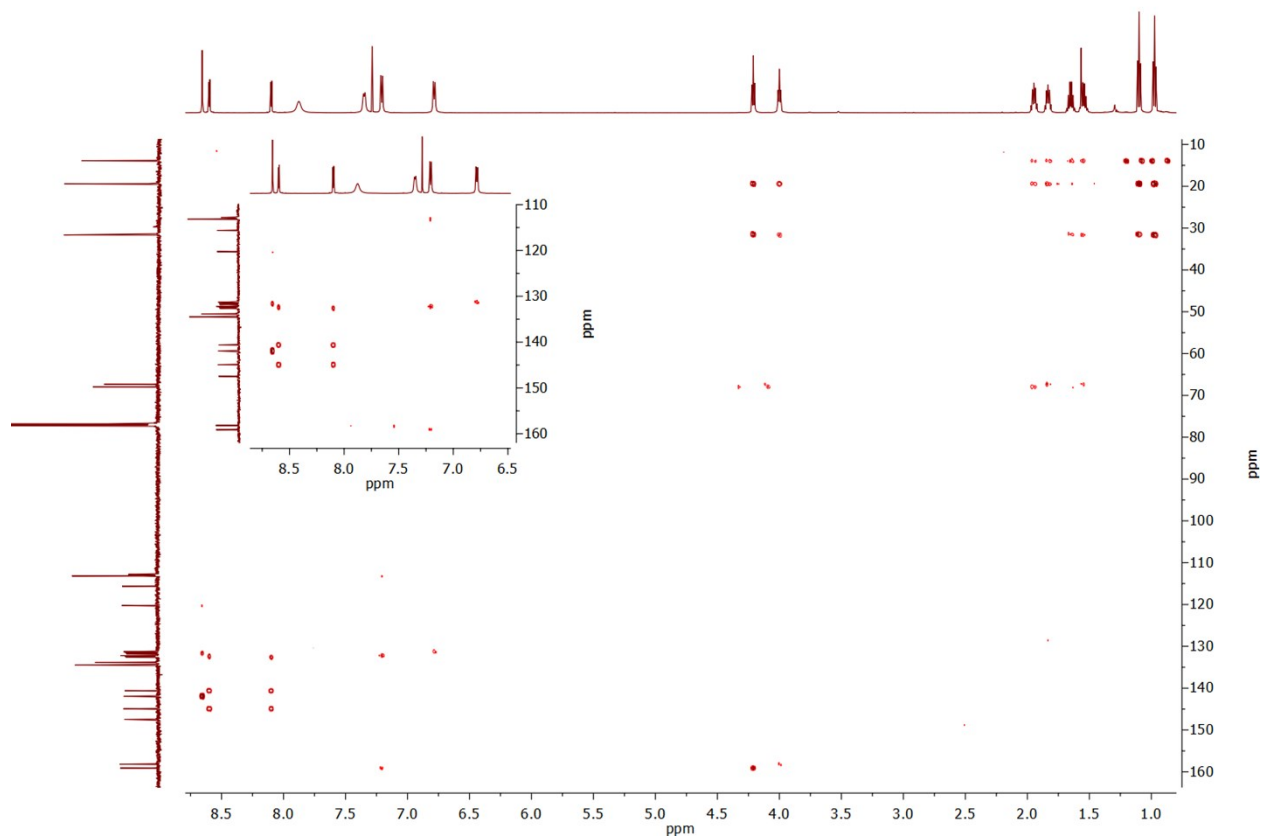
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Figure S 97. ^{1}H-^{13}C HSQC spectrum of **6** (CDCl$_3$).

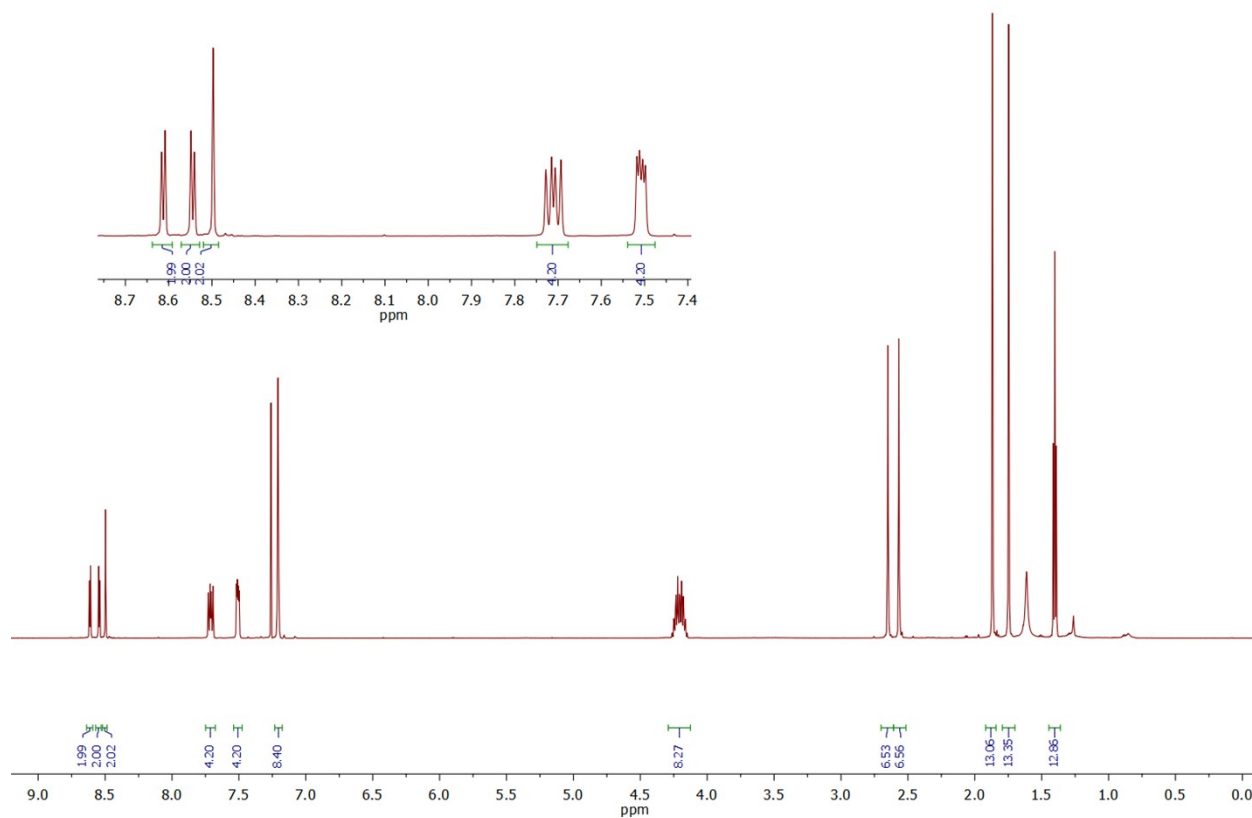Figure S 98. ^{1}H-^{13}C HMBC spectrum of **6** (CDCl$_3$).

Spectral data of 8g

Figure S 99. ¹H-NMR spectrum of **8g** (CDCl₃).
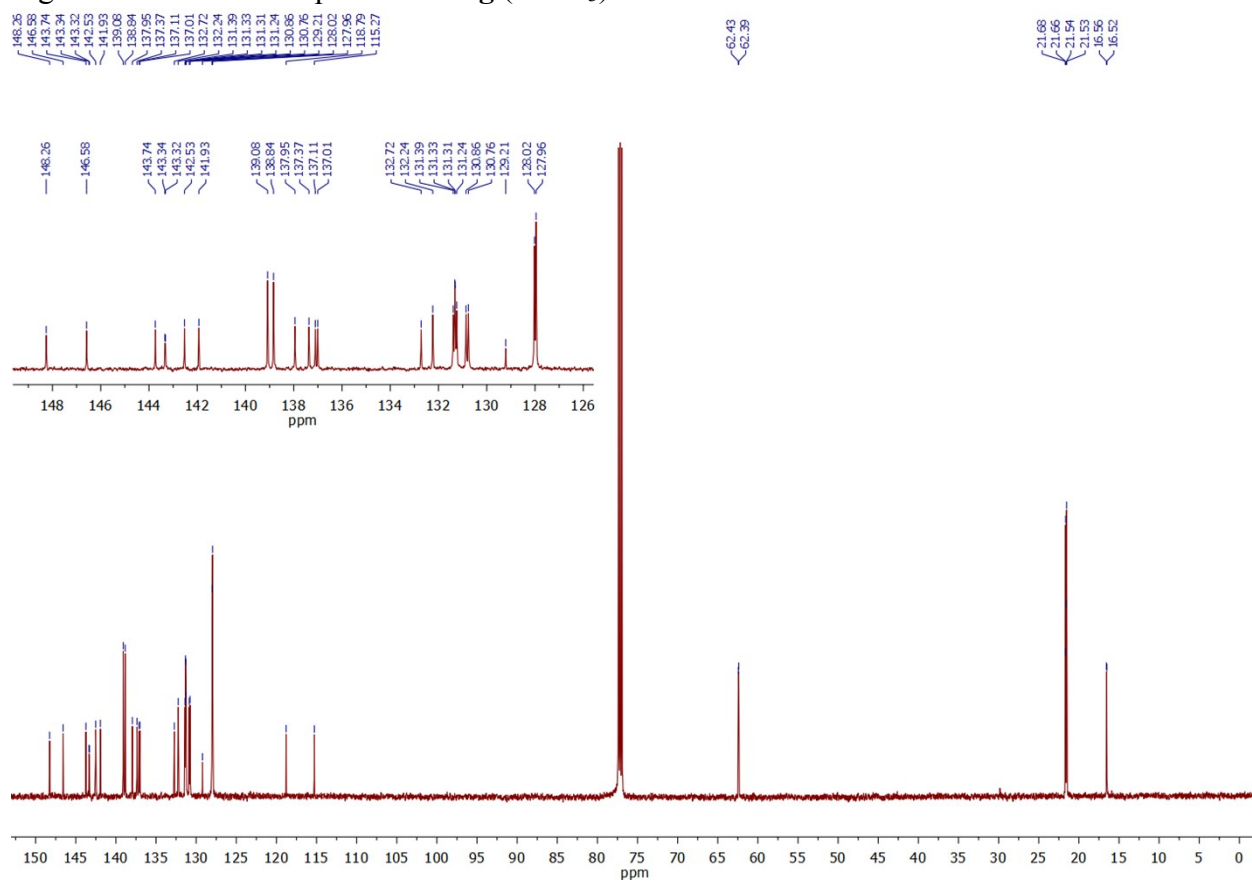

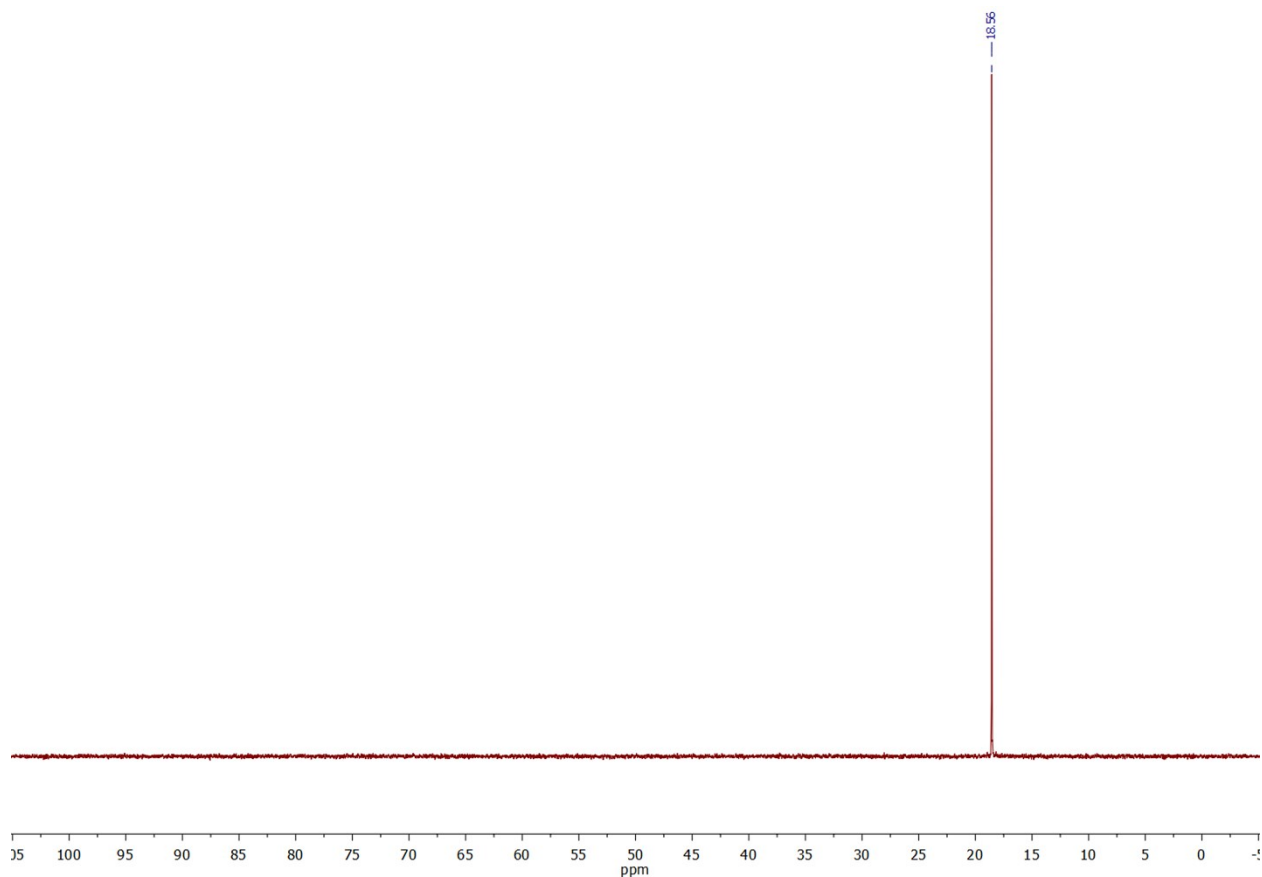Figure S 100. ¹³C-NMR spectrum of **8g** (CDCl₃).
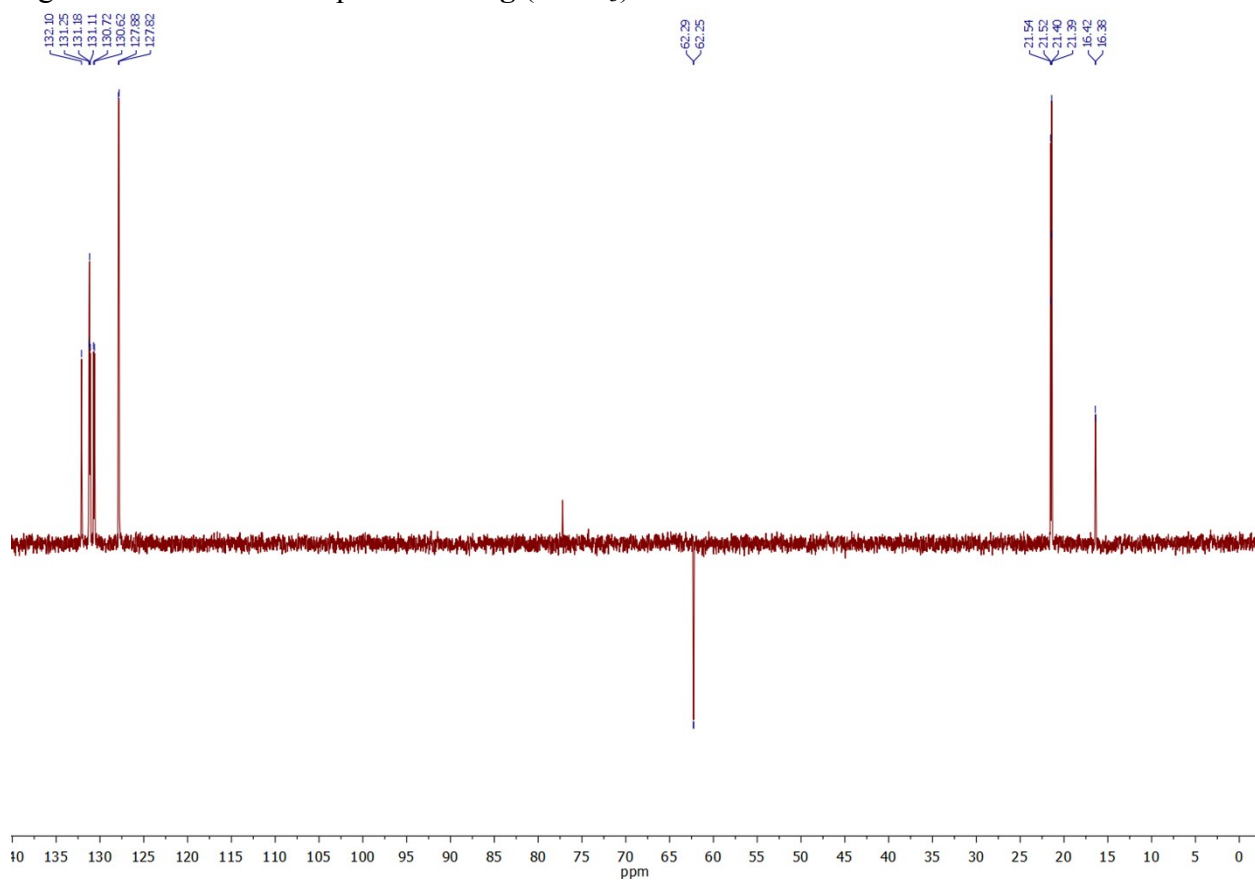
Figure S 101. ^{31}P-NMR spectrum of **8g** (CDCl$_3$).

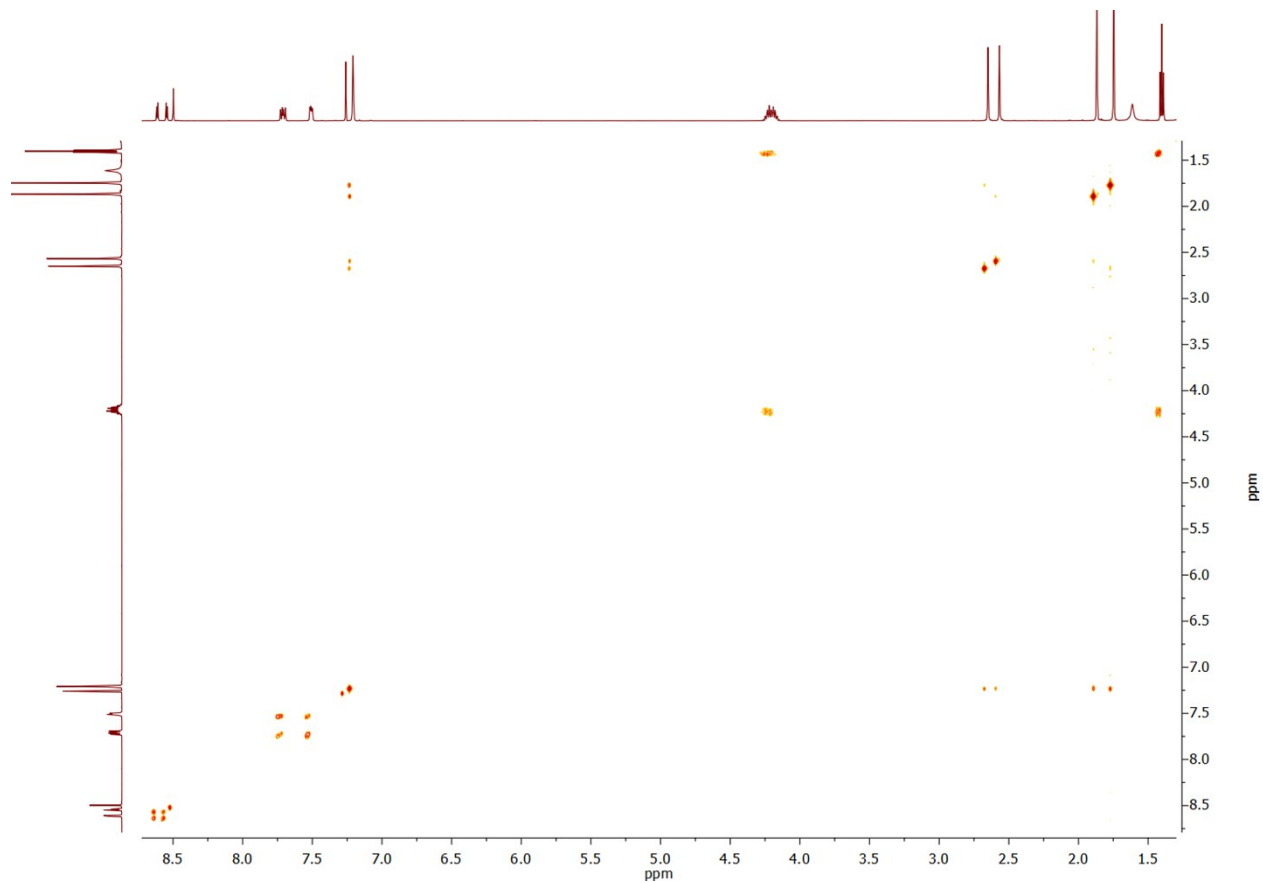Figure S 102. ^{13}C DEPT-135 spectrum of **8g** (CDCl$_3$).
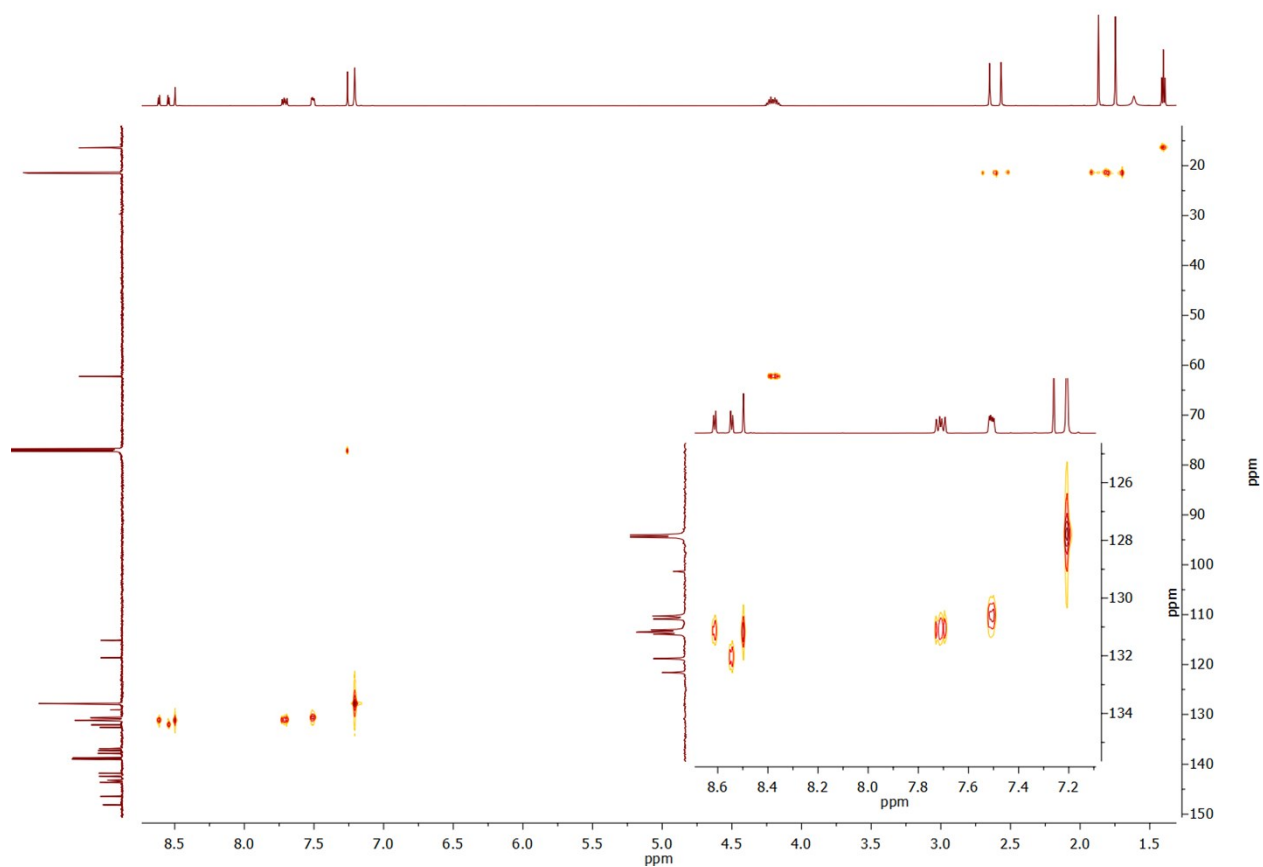
Figure S 103. COSY spectrum of **8g** (CDCl$_3$).

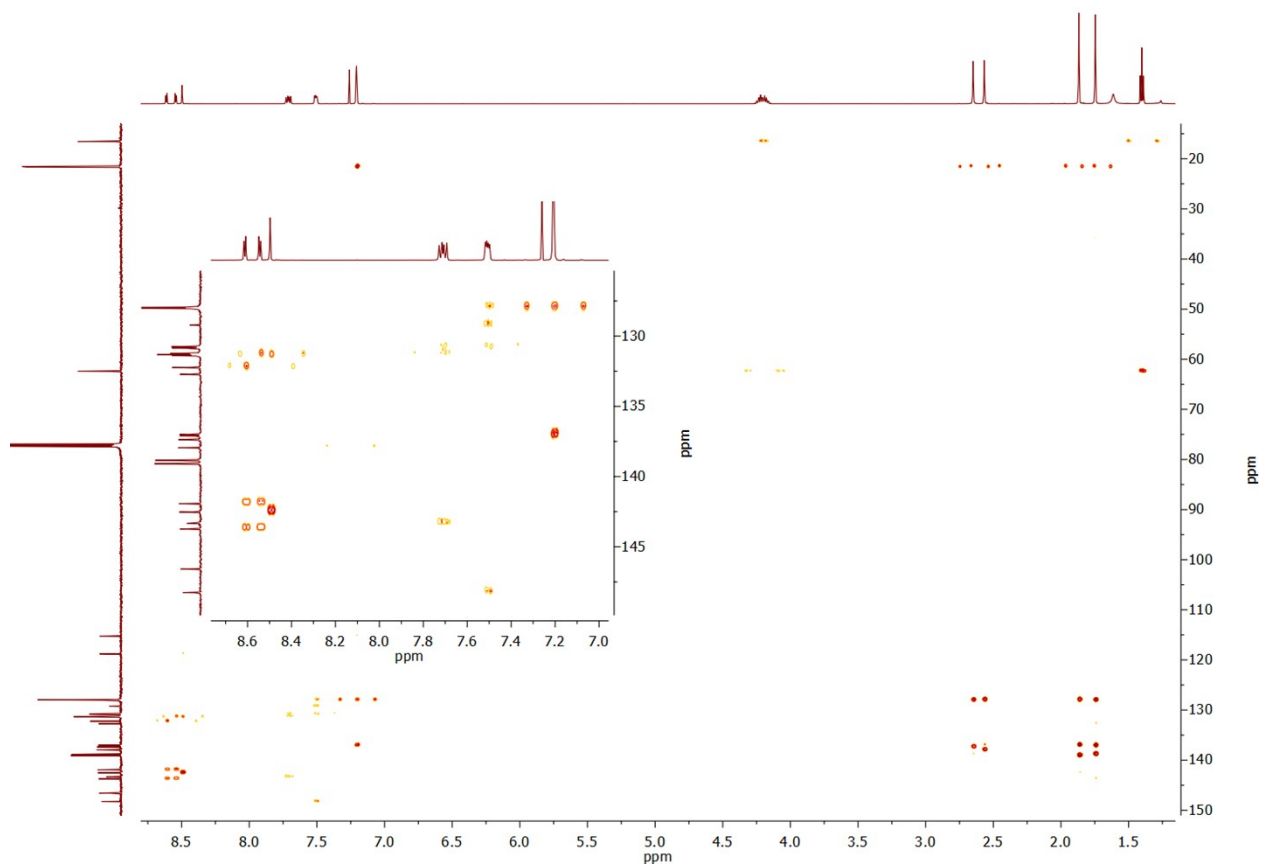Figure S 104. ^{1}H-^{13}C HSQC spectrum of **8g** (CDCl$_3$).

Figure S 105. ^{1}H-^{13}C HMBC spectrum of **8g** (CDCl$_3$).
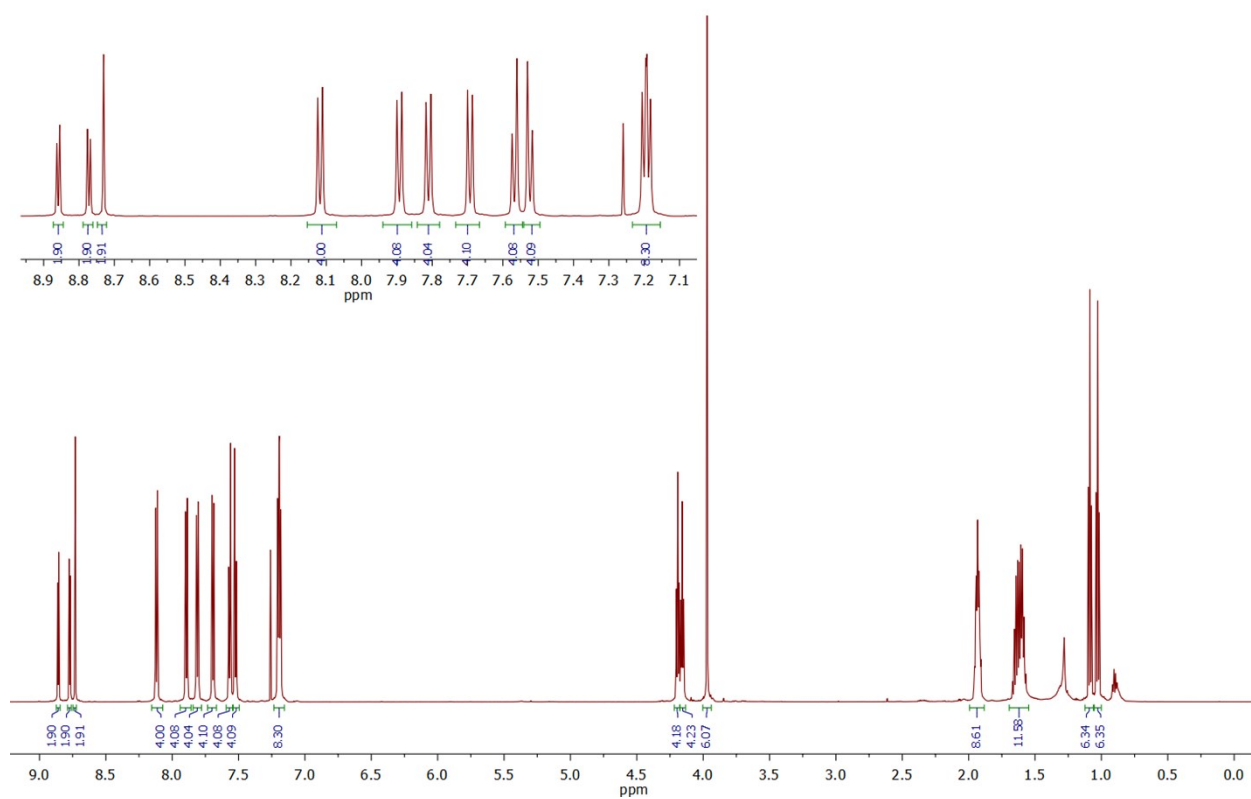
Spectral data of 9

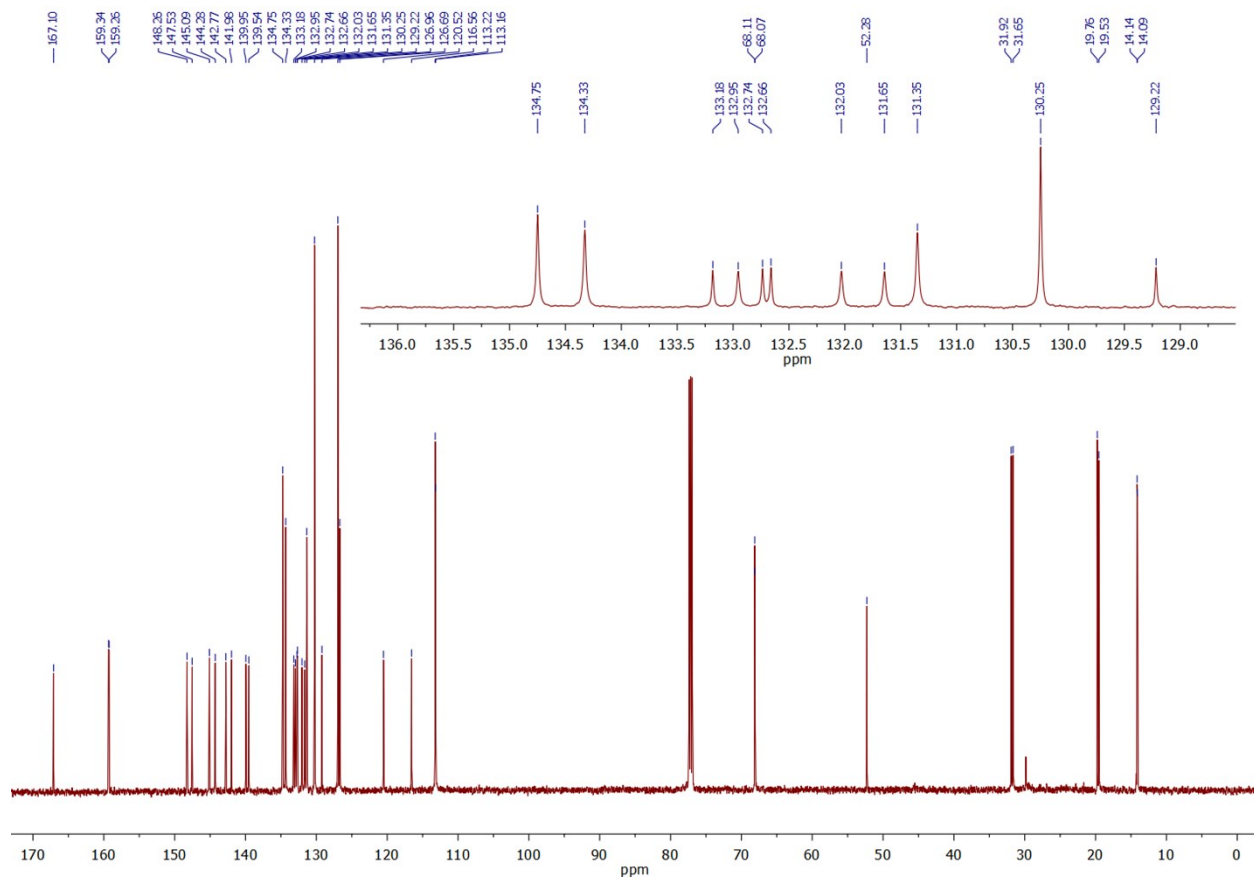Figure S 106. ^{1}H-NMR spectrum of **9** (CDCl$_3$).
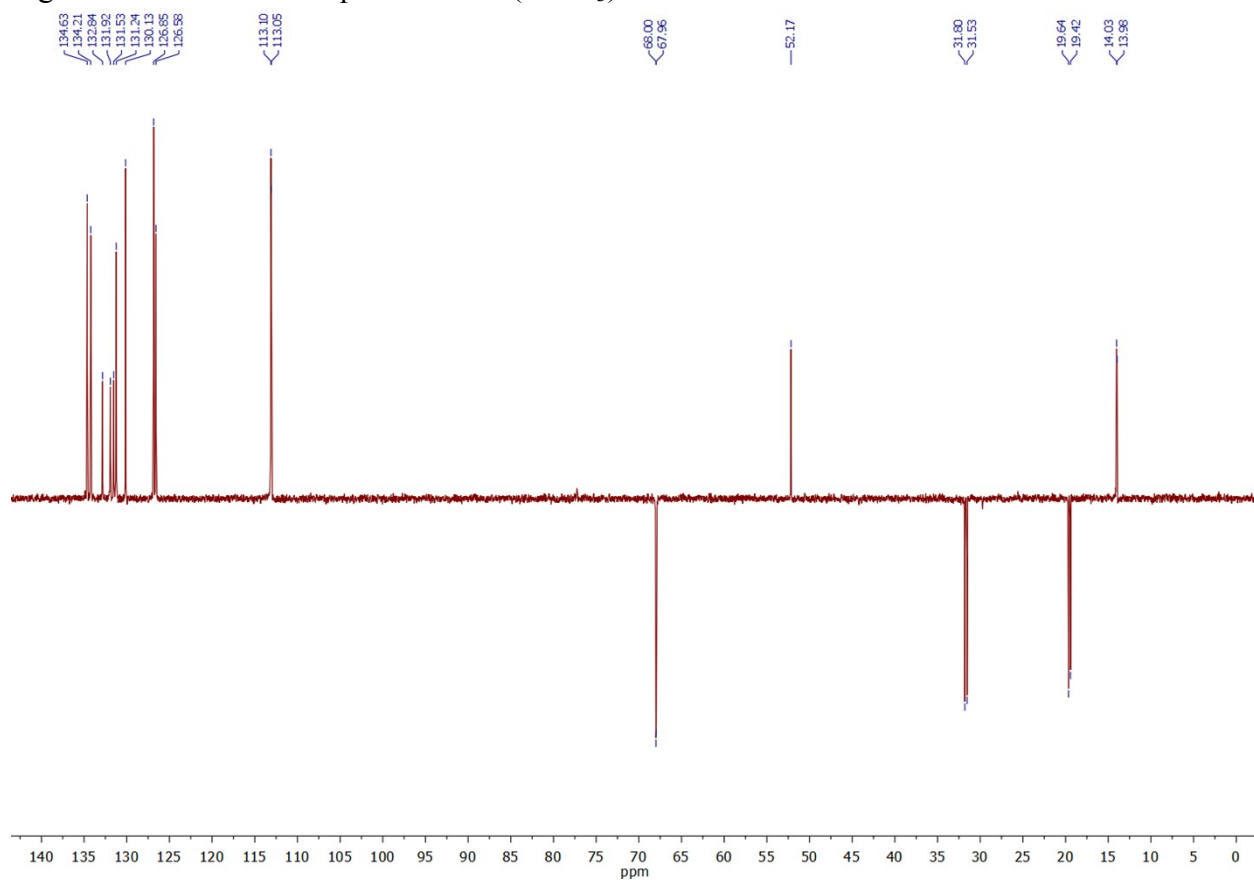
Figure S 107. ^{13}C-NMR spectrum of **9** (CDCl$_3$).

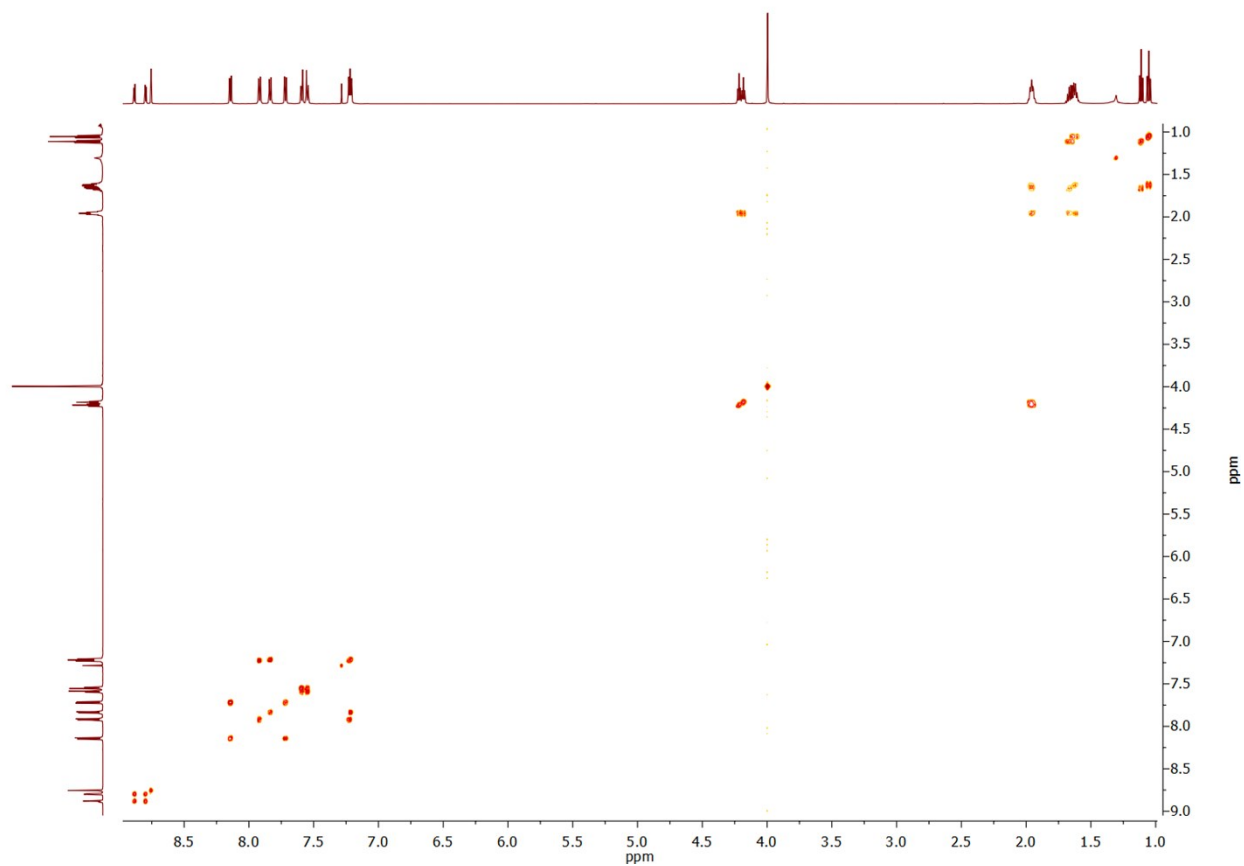Figure S 108. ^{13}C DEPT-135 spectrum of **9** (CDCl$_3$).
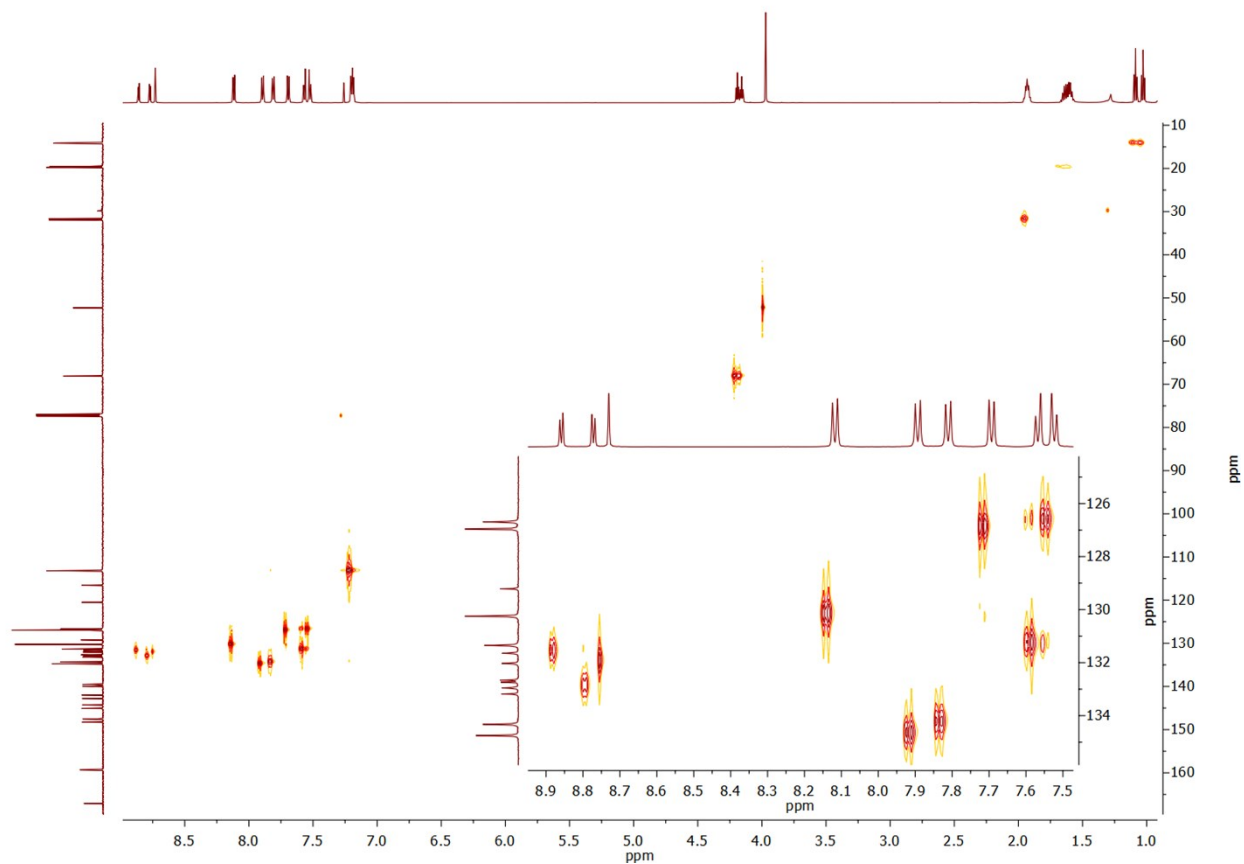
Figure S 109. COSY spectrum of **9** (CDCl$_3$).

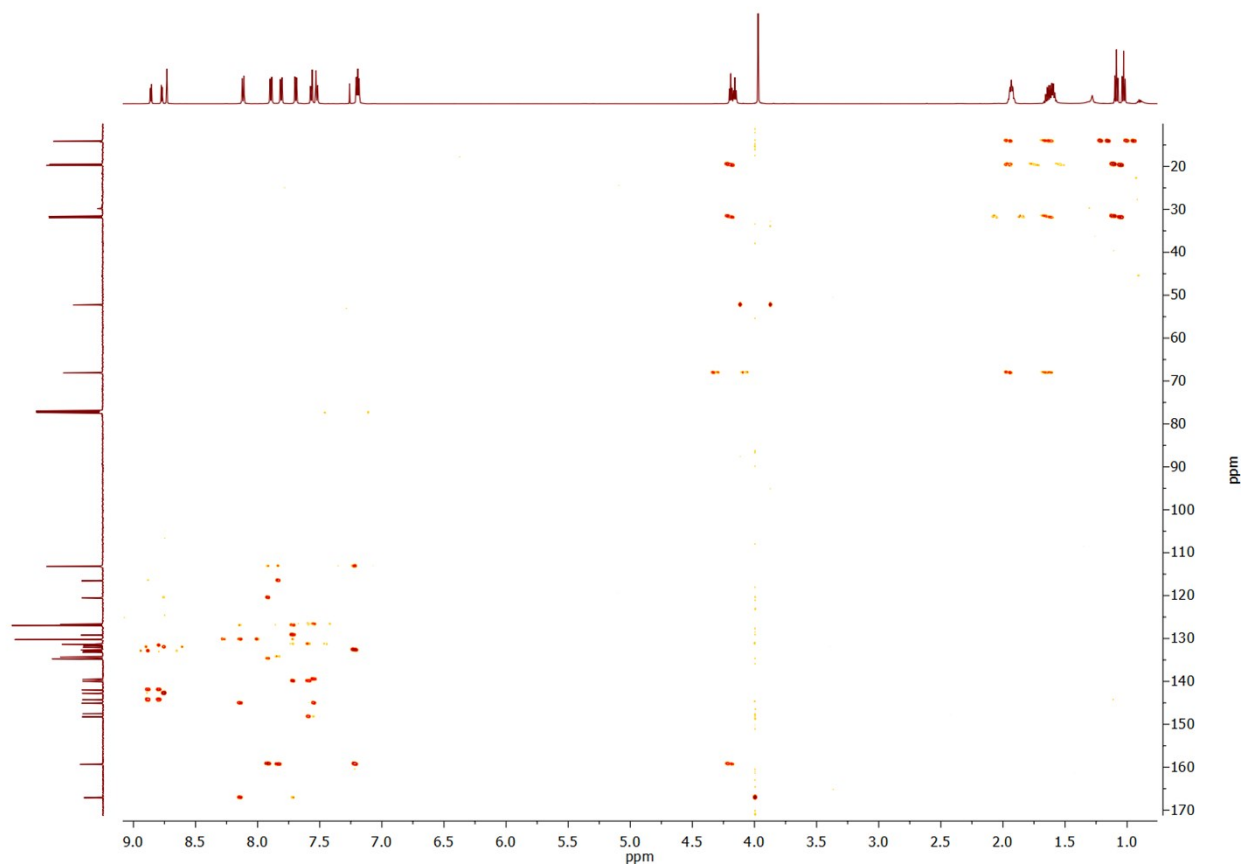Figure S 110. ^{1}H-^{13}C HSQC spectrum of **9** (CDCl$_3$).

Figure S 111. ^{1}H-^{13}C HMBC spectrum of **9** (CDCl$_3$).
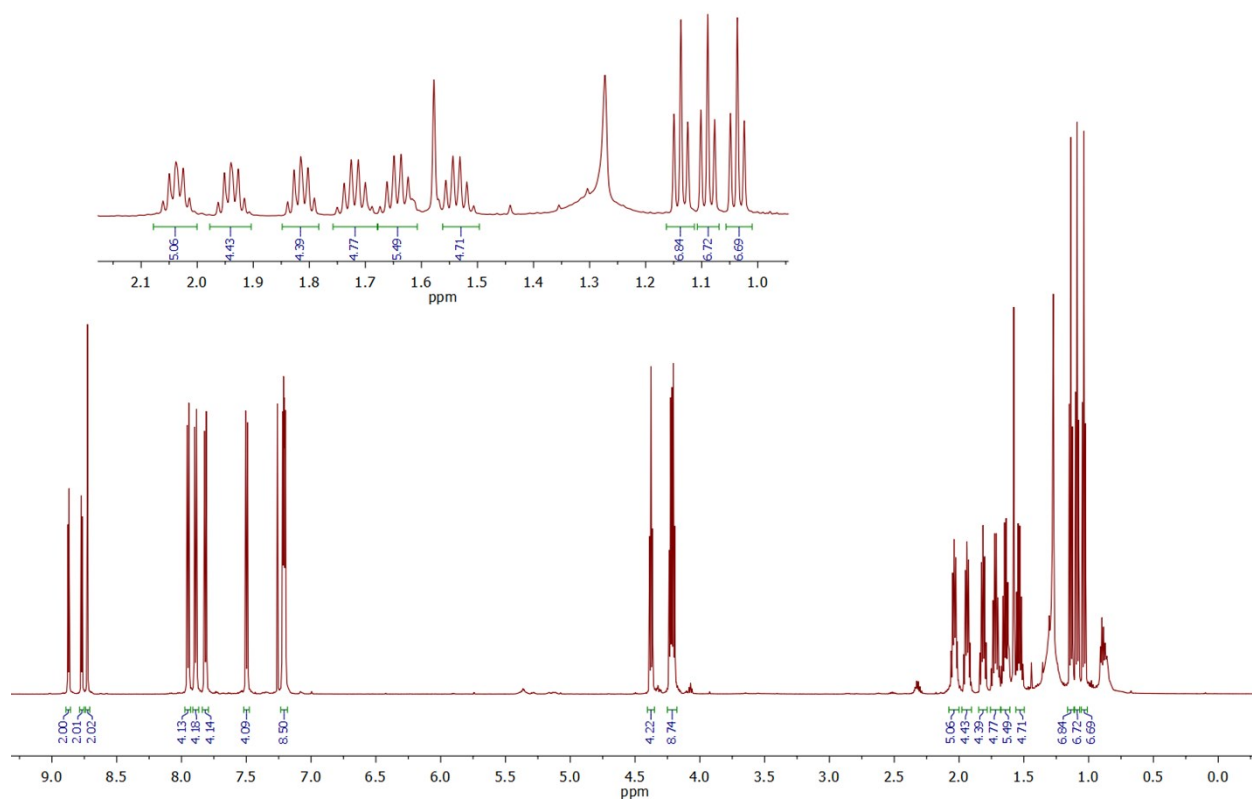
Spectral data of 10

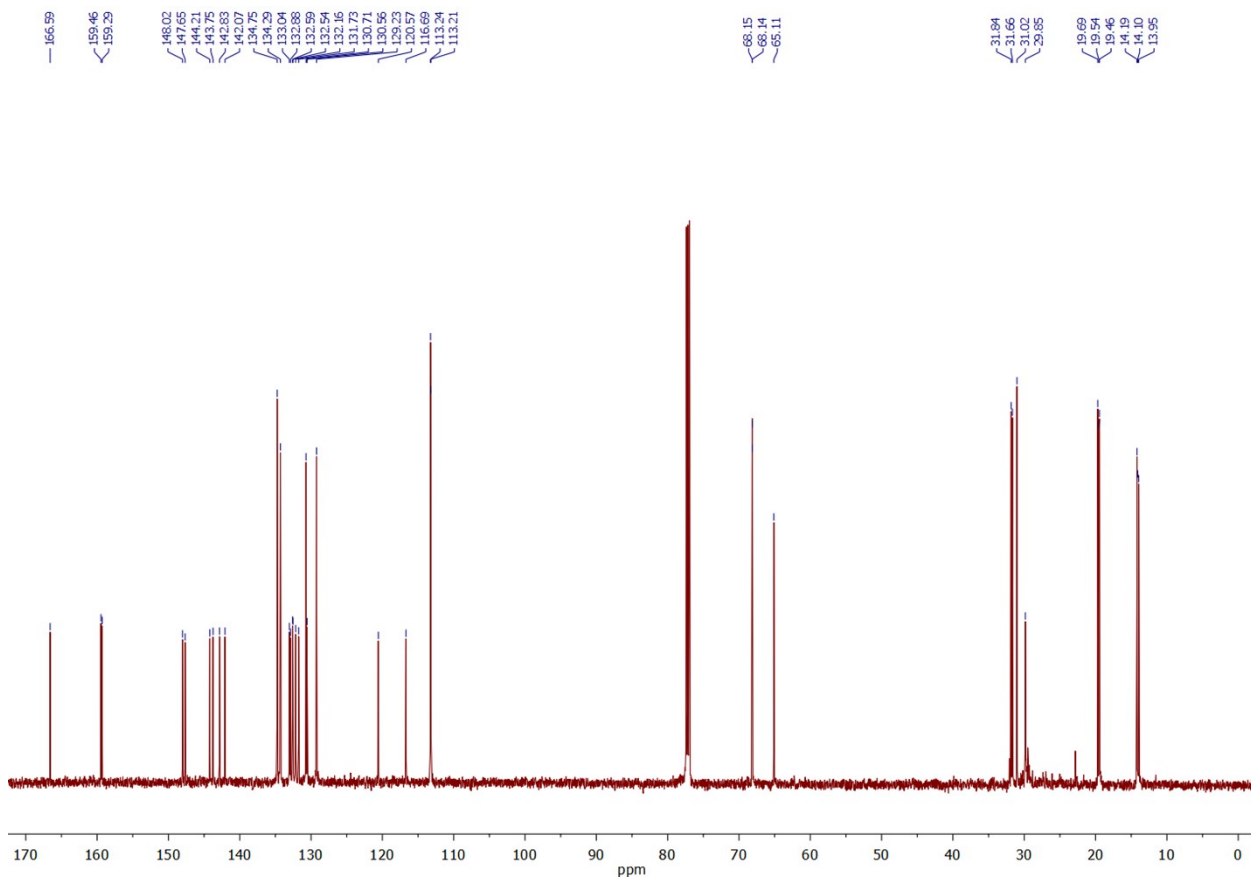Figure S 112. ^{1}H-NMR spectrum of **10** (CDCl$_3$).
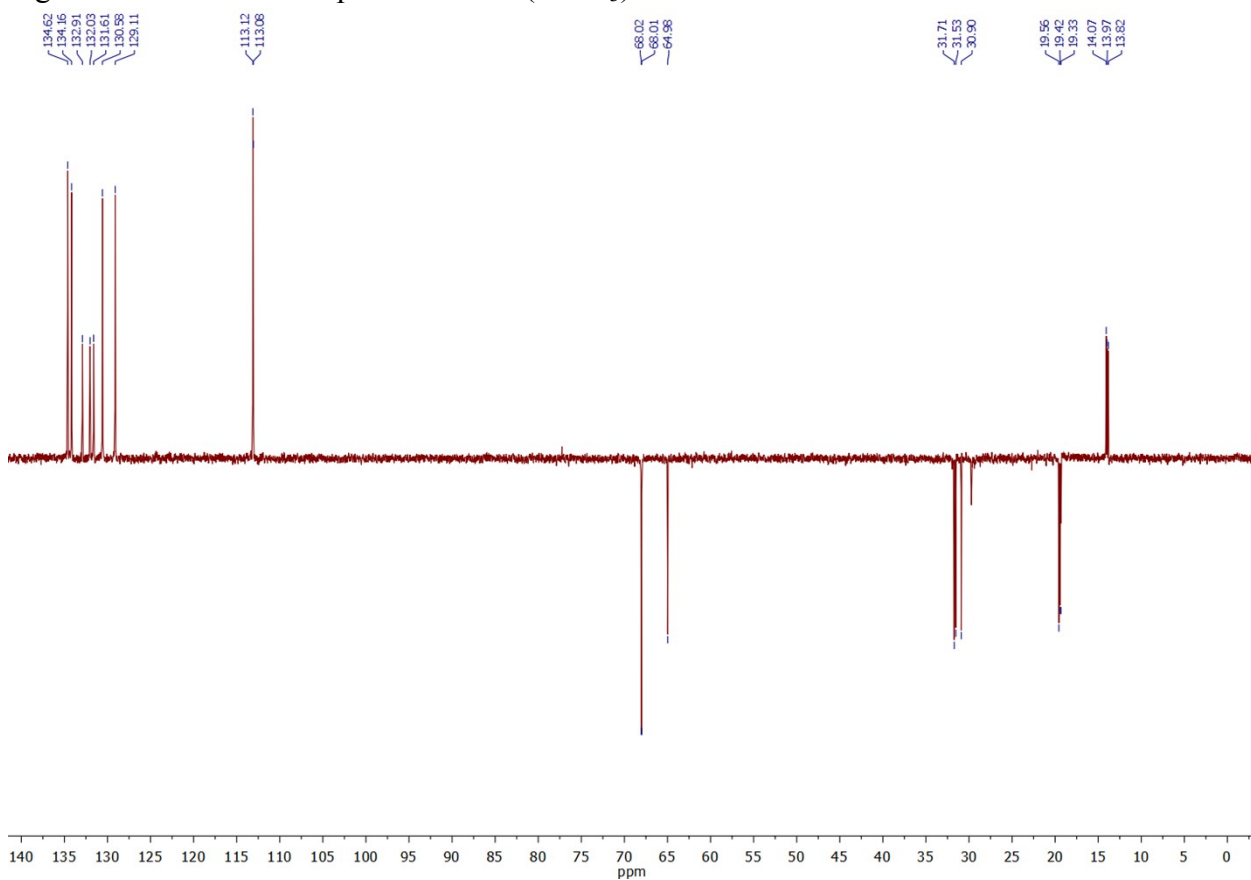
Figure S 113. ^{13}C-NMR spectrum of **10** (CDCl$_3$).

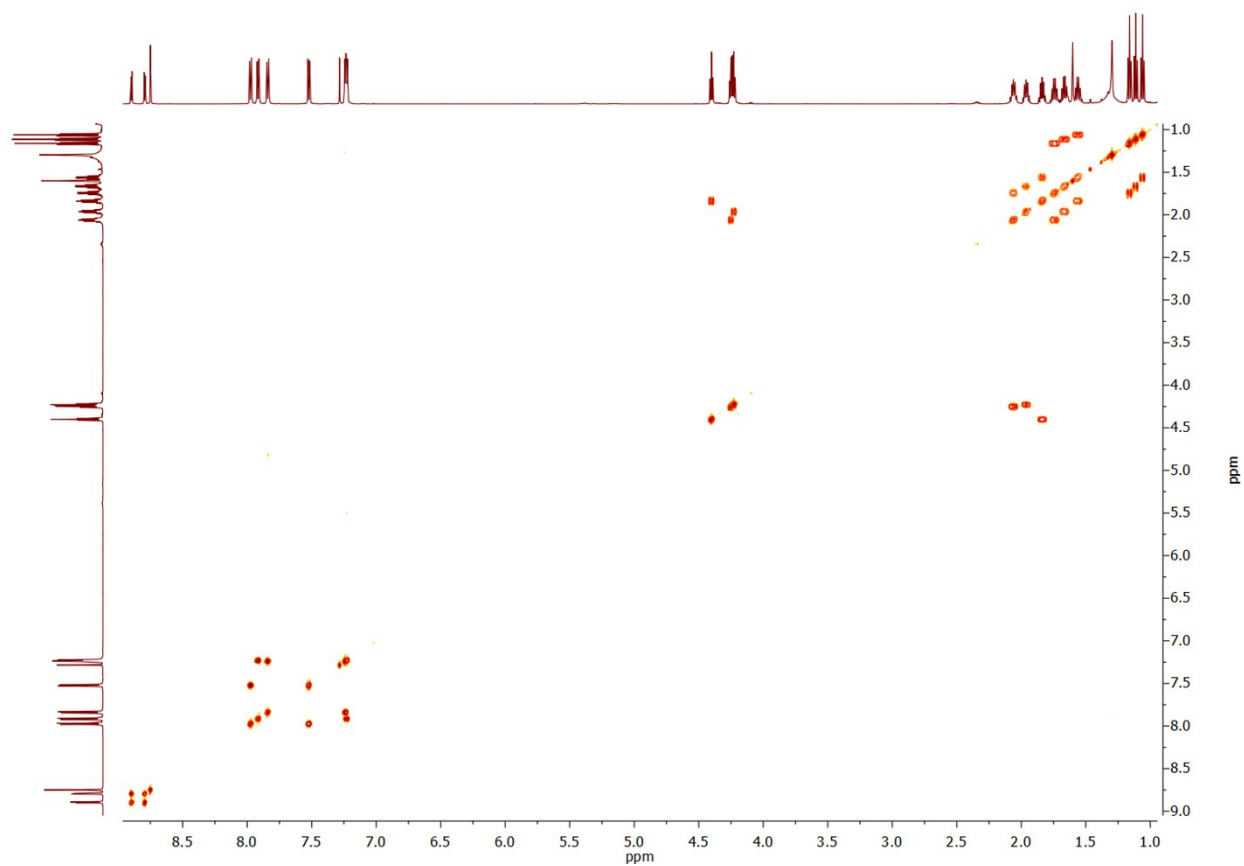Figure S 114. ^{13}C DEPT-135 spectrum of **10** (CDCl$_3$).
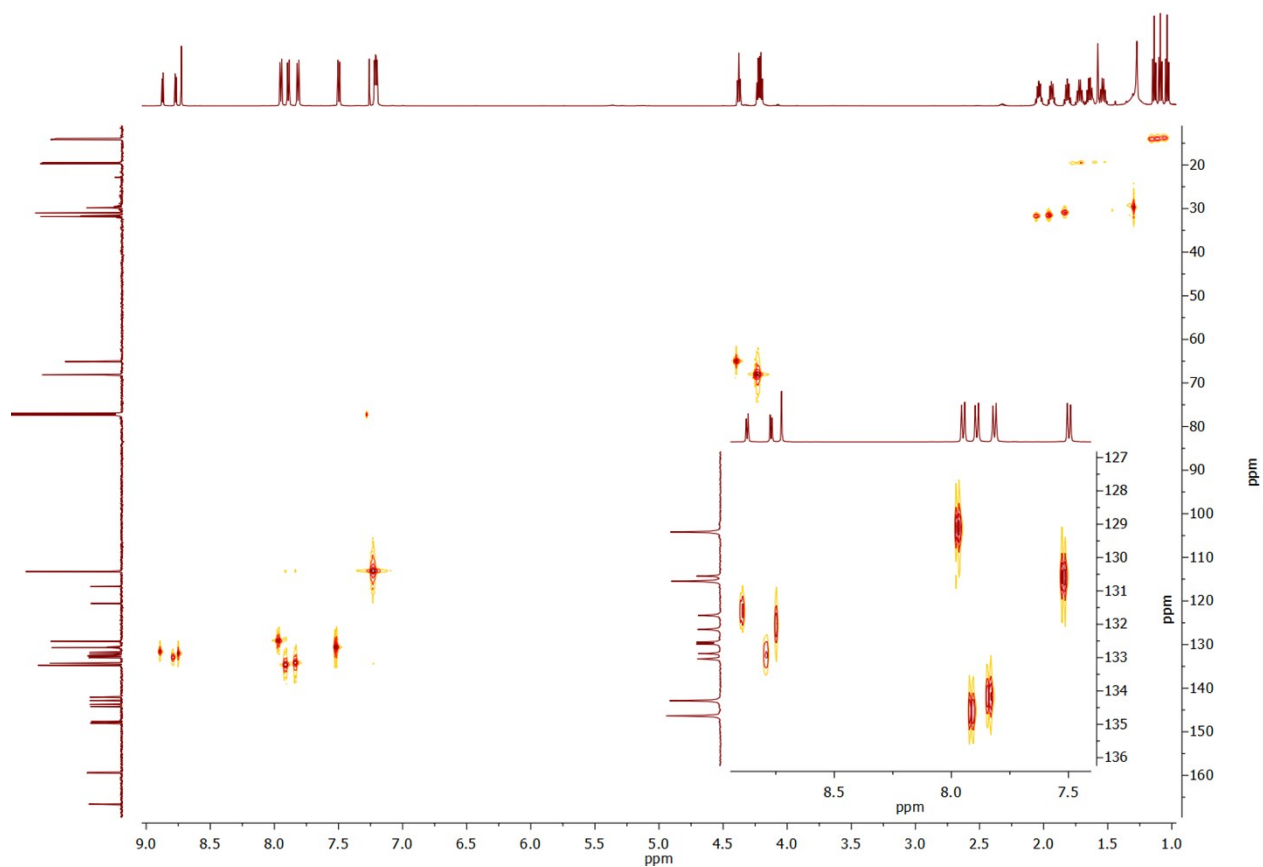
Figure S 115. COSY spectrum of **10** (CDCl$_3$).

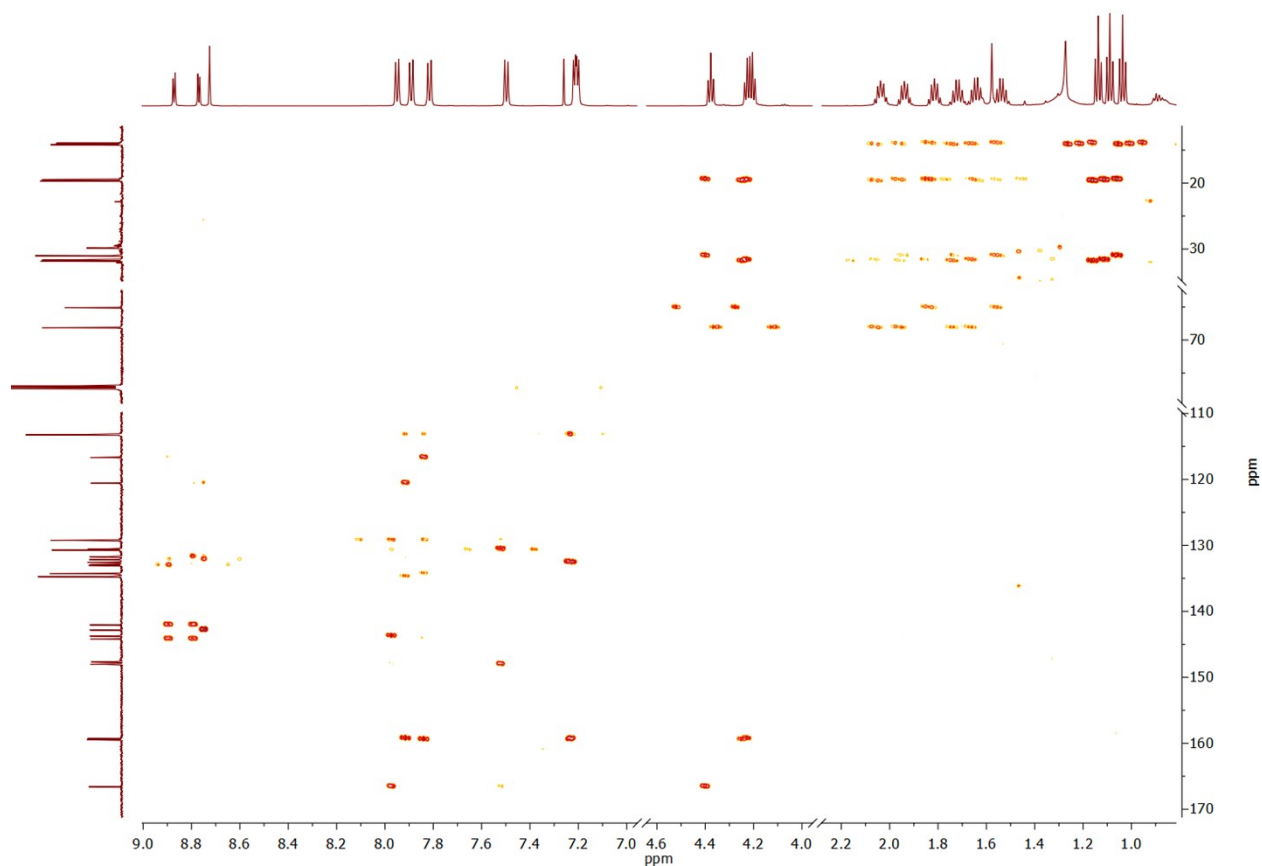Figure S 116. ^{1}H-^{13}C HSQC spectrum of **10** (CDCl$_3$).

Figure S 117. ^{1}H-^{13}C HMBC spectrum of **10** (CDCl$_3$).
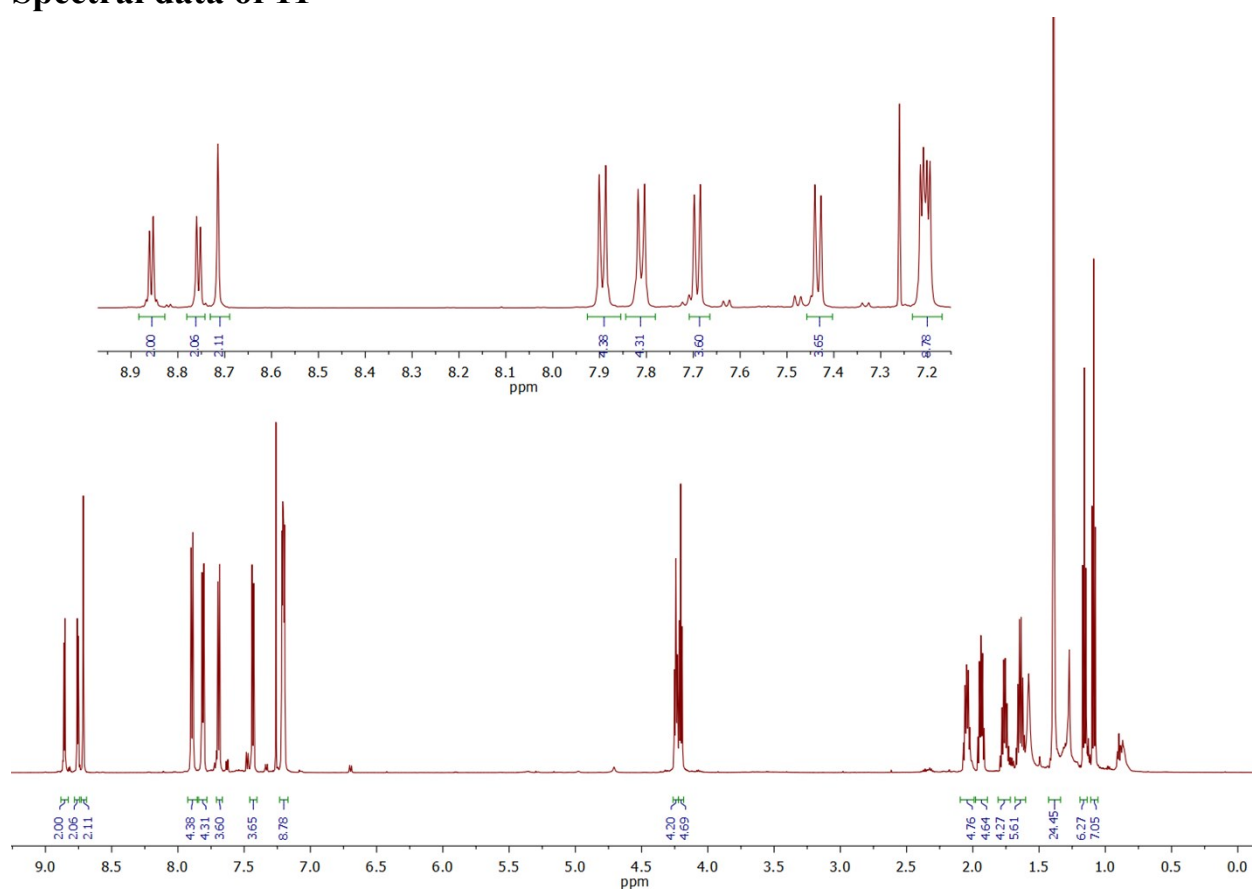
Spectral data of 11

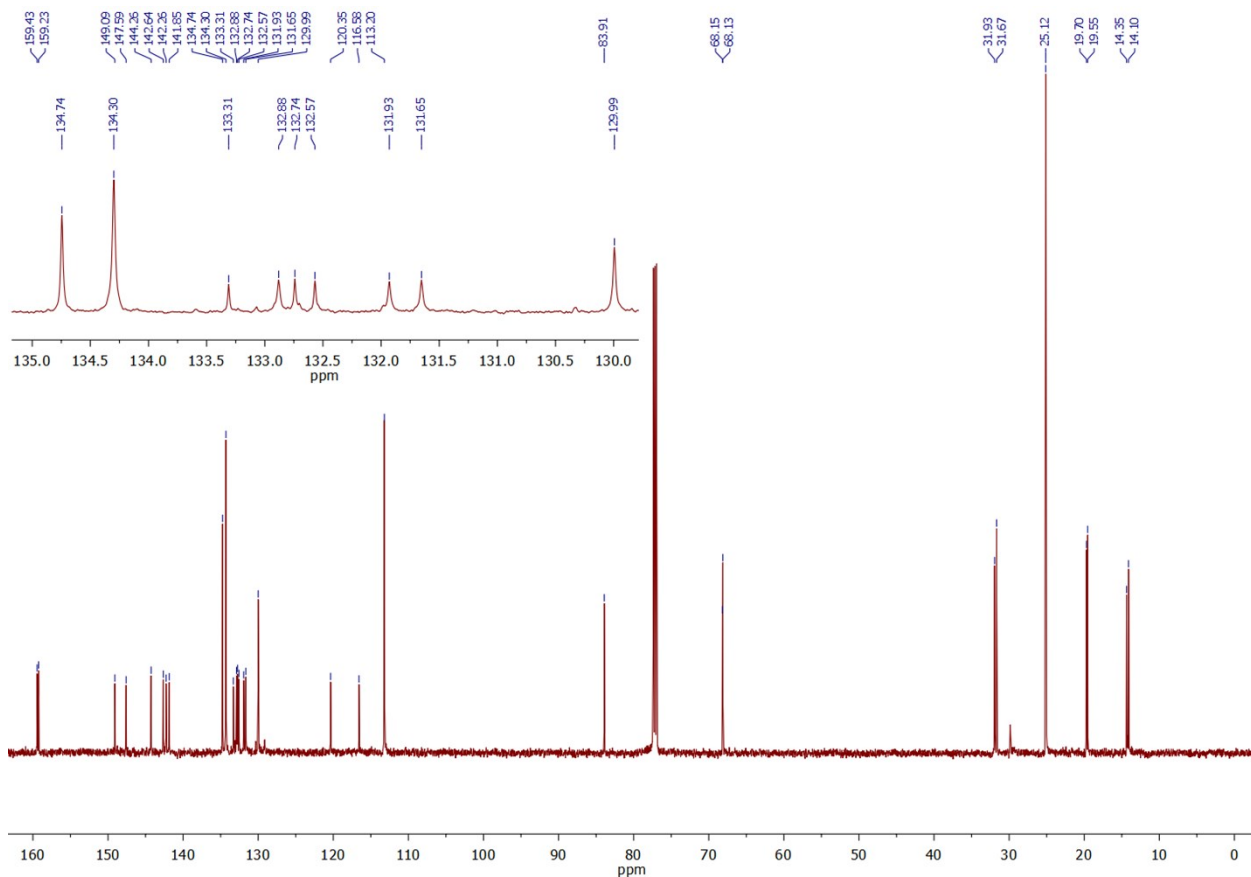Figure S 118. ^{1}H-NMR spectrum of **11** (CDCl$_3$).
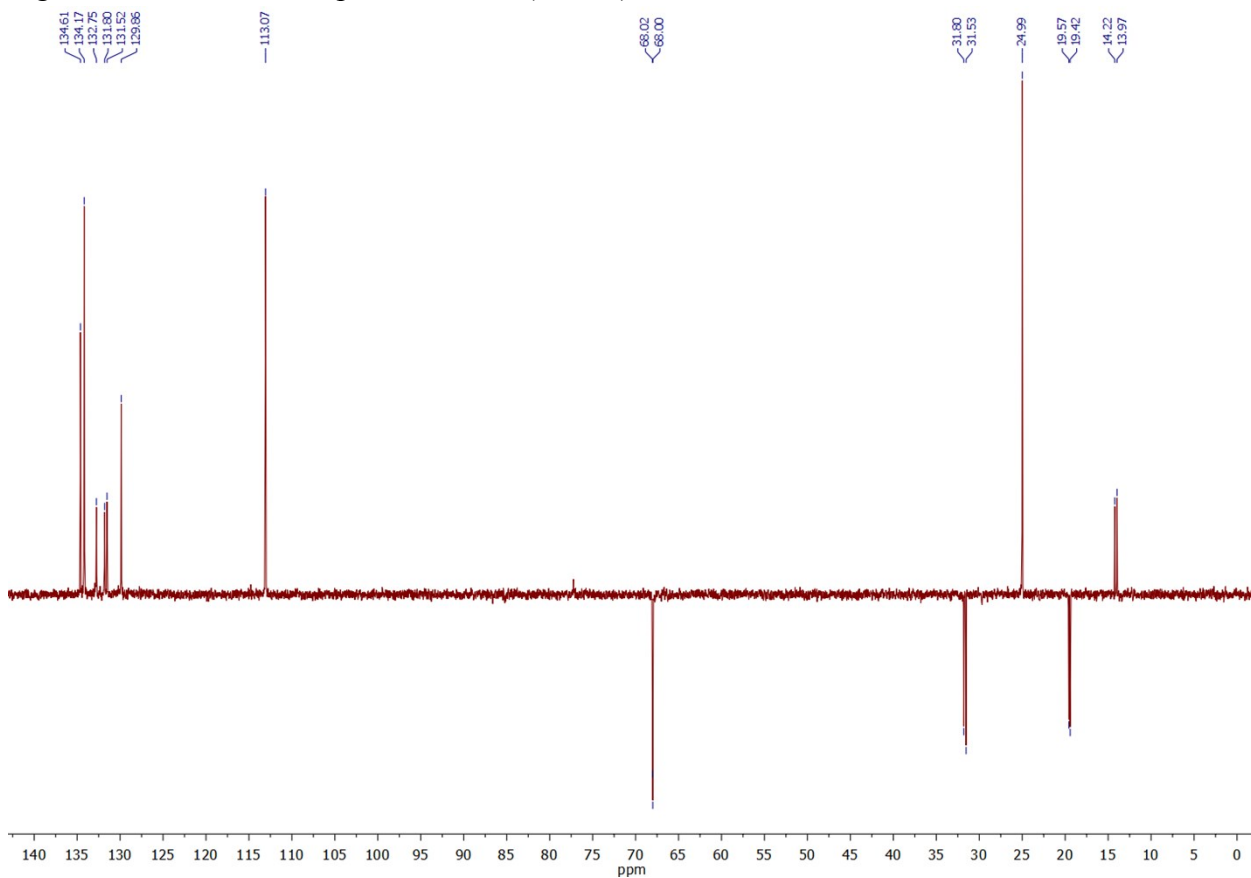
Figure S 119. ^{13}C-NMR spectrum of **11** (CDCl$_3$).

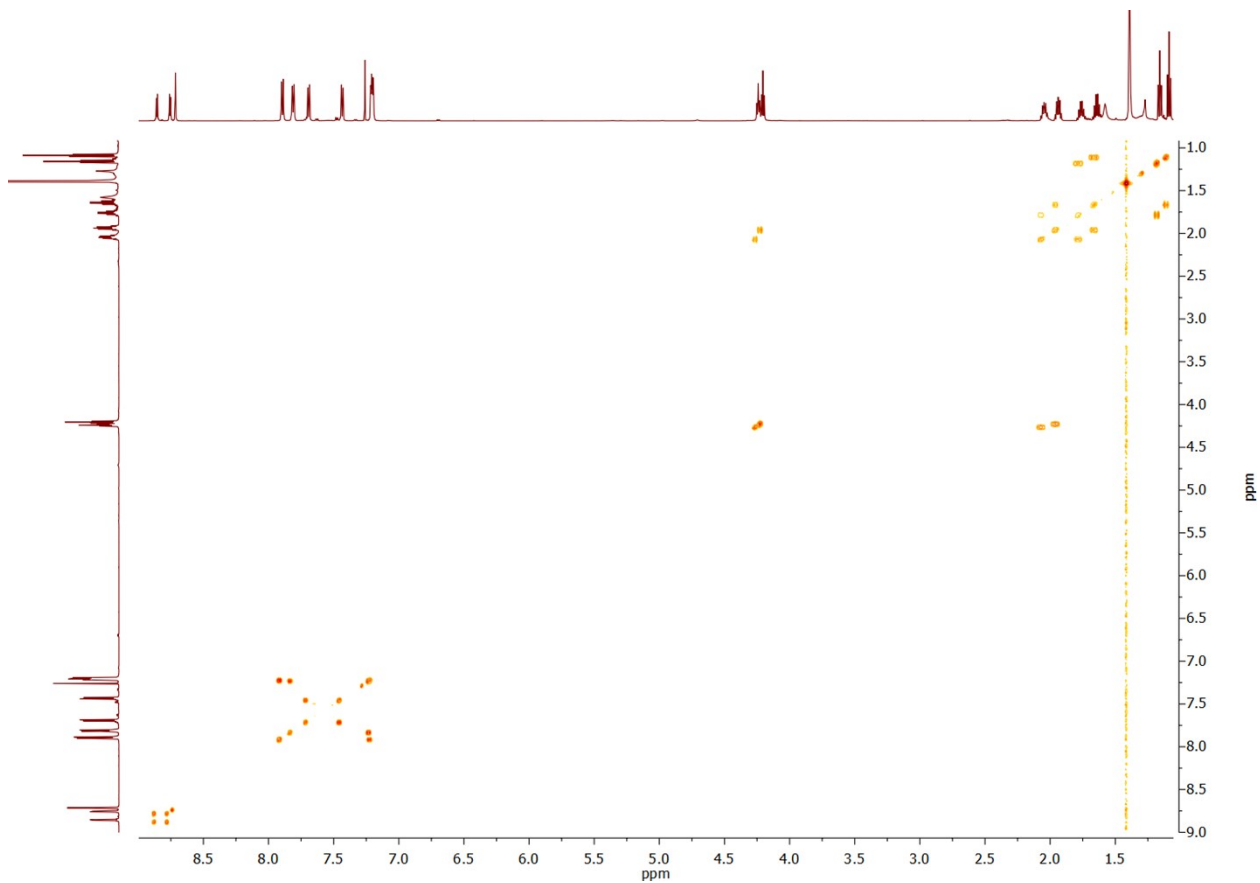Figure S 120. ^{13}C DEPT-135 spectrum of **11** (CDCl$_3$).
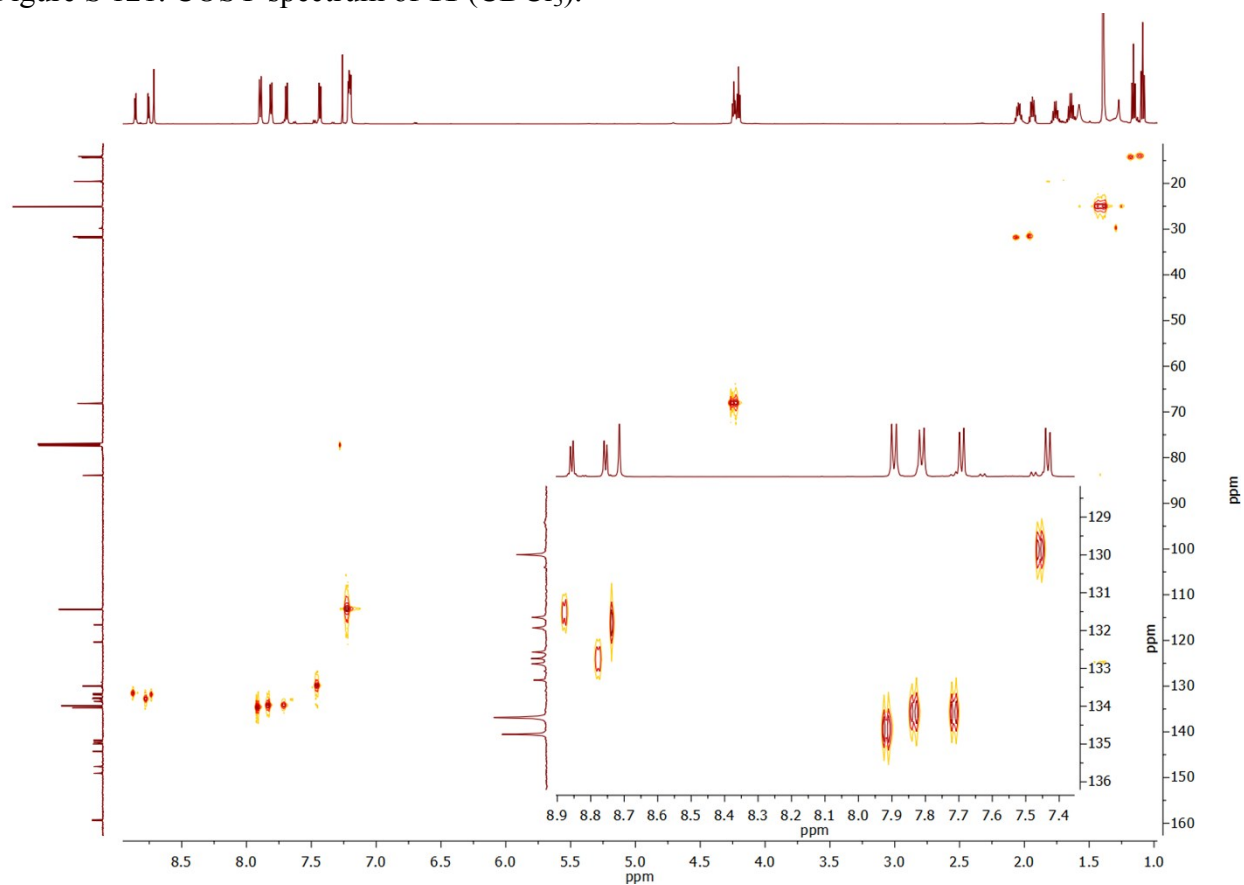
Figure S 121. COSY spectrum of **11** (CDCl$_3$).

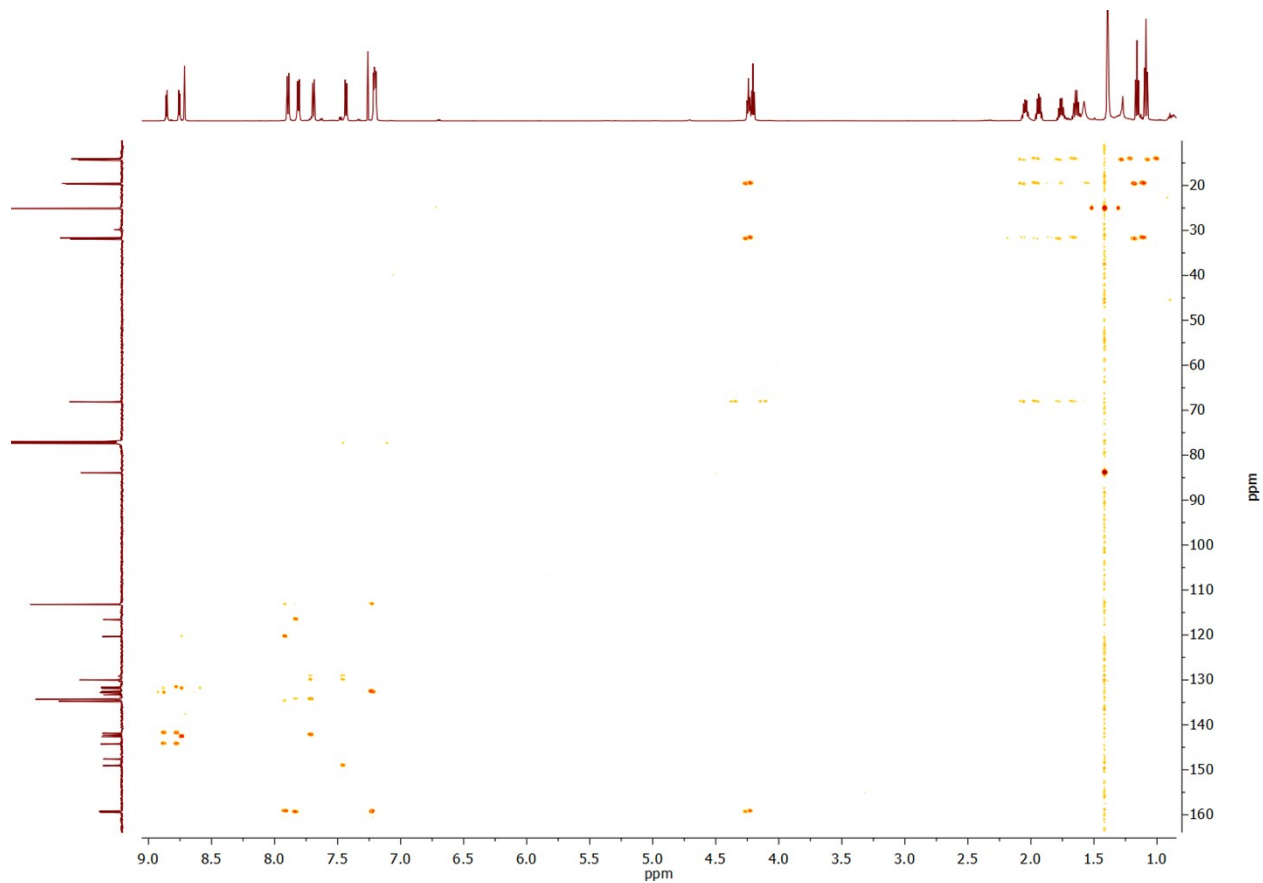

Figure S 122. ^{1}H-^{13}C HSQC spectrum of **11** (CDCl$_3$).

Figure S 123. ^{1}H-^{13}C HMBC spectrum of **11** (CDCl$_3$).