Supplementary information

Synthesis and Conformational Analysis of Naphthoxazine-Fused Phenanthrene Derivatives

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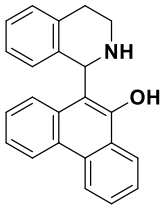
1-(9-Hydroxyphenanthr-10-yl)-1,2,3,4-tetrahydroisoquinoline (3)



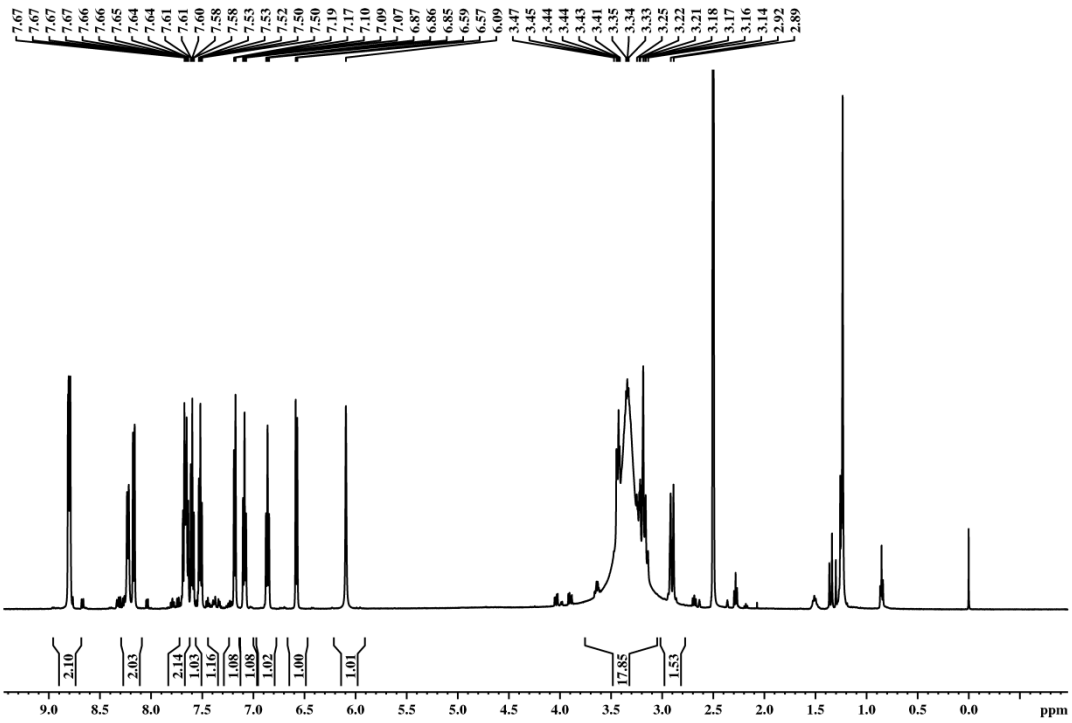


Figure S1. ^{1}H NMR spectrum of **3**

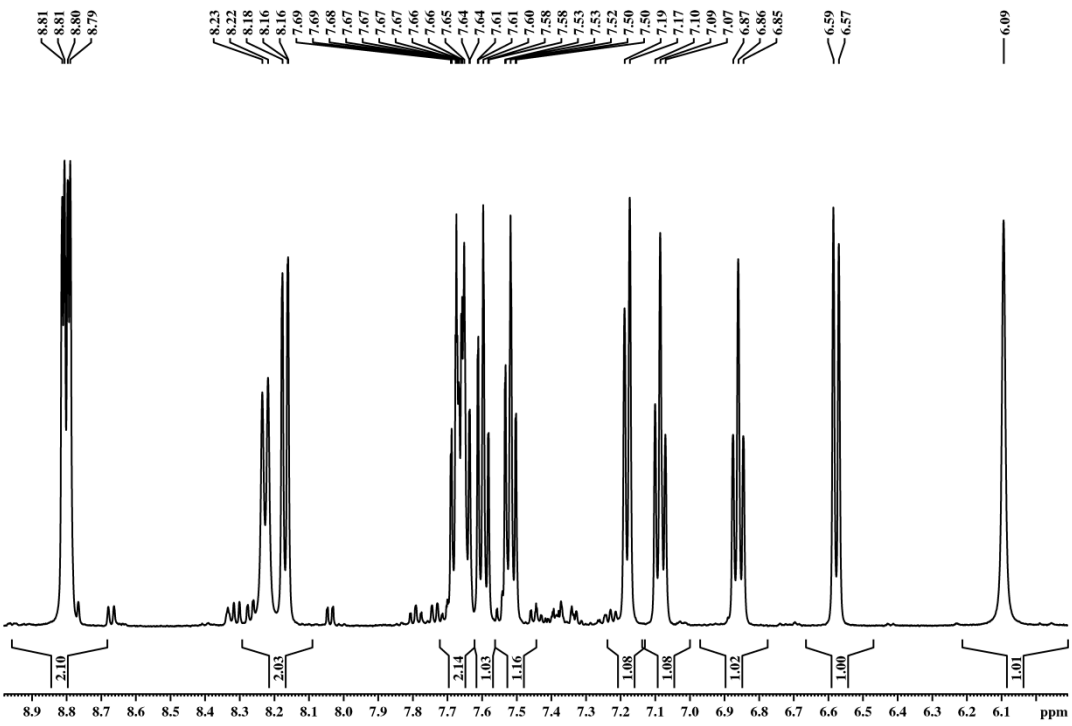


Figure S2. ^{1}H NMR spectrum of **3**, expansion

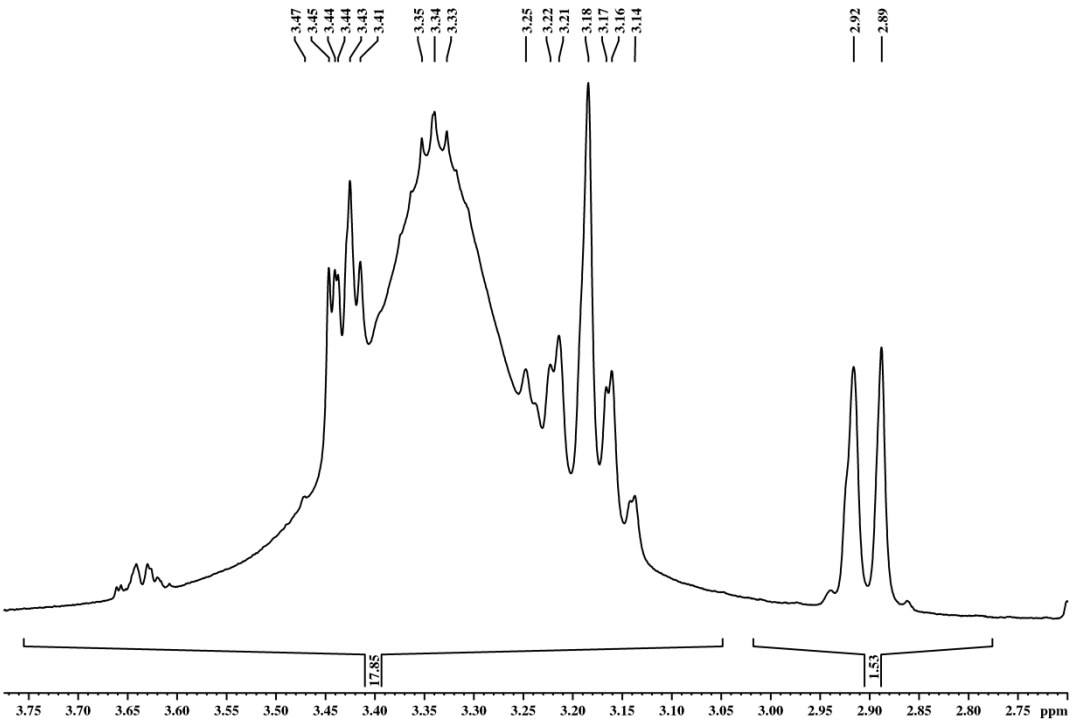


Figure S3. ^{1}H NMR spectrum of **3**, expansion

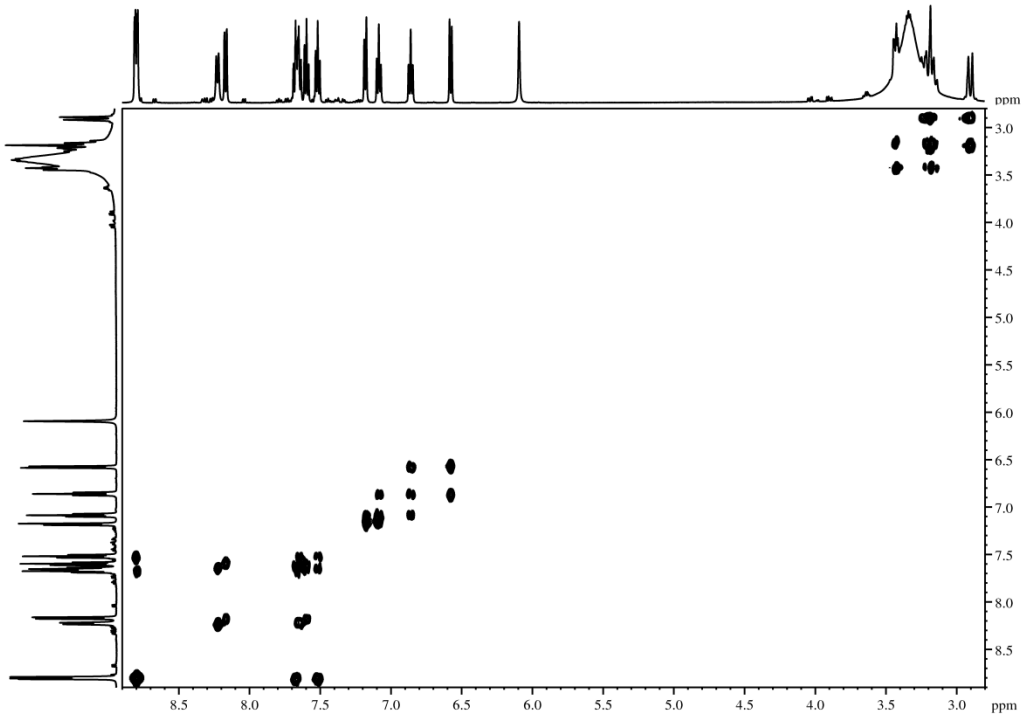


Figure S4. H,H-COSY NMR spectrum of **3**

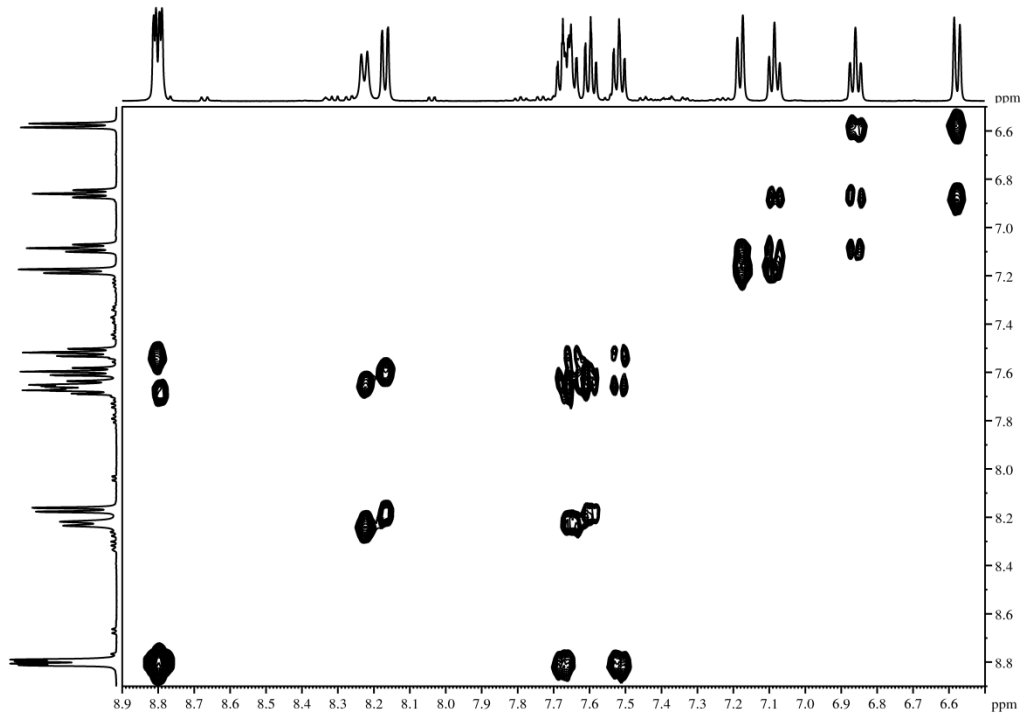


Figure S5. H,H-COSY NMR spectrum of **3**, expansion

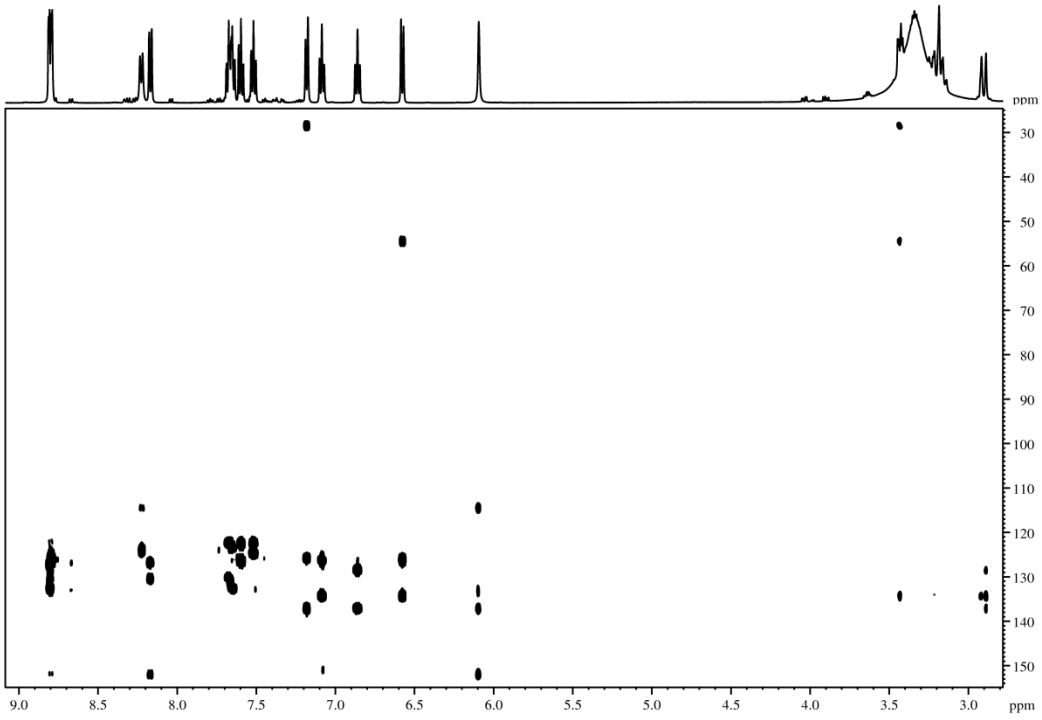


Figure S6. HMBC NMR spectrum of **3**

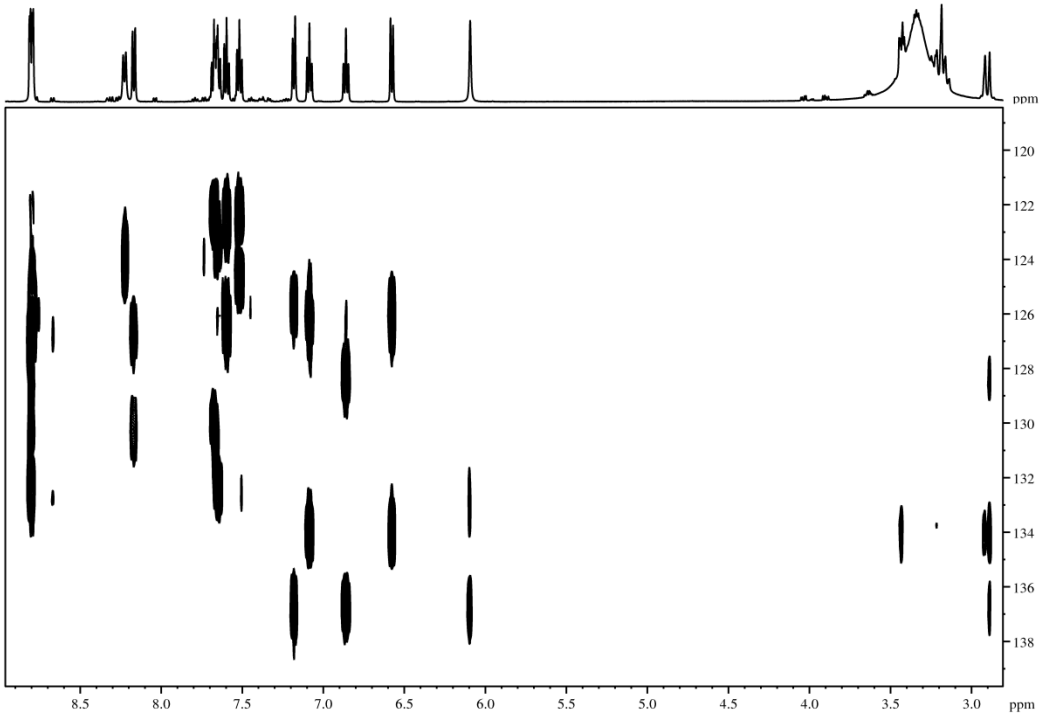


Figure S7. HMBC NMR spectrum of **3**, expansion

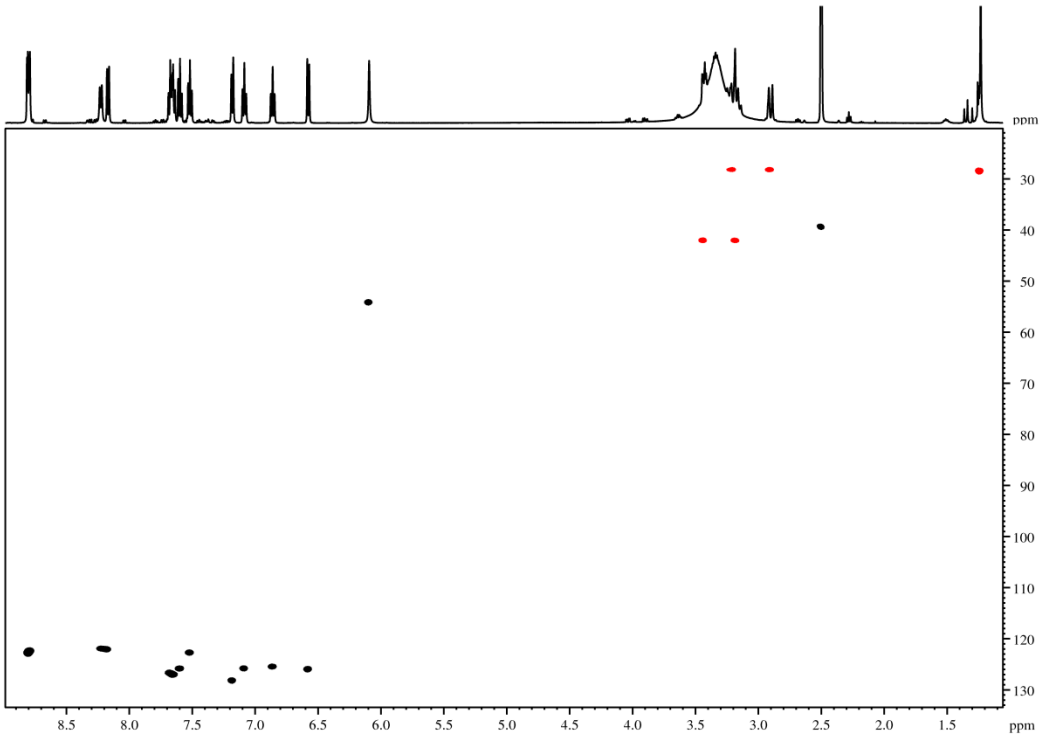


Figure S8. edited HSQC NMR spectrum of **3** (black: positive, red: negative signals)

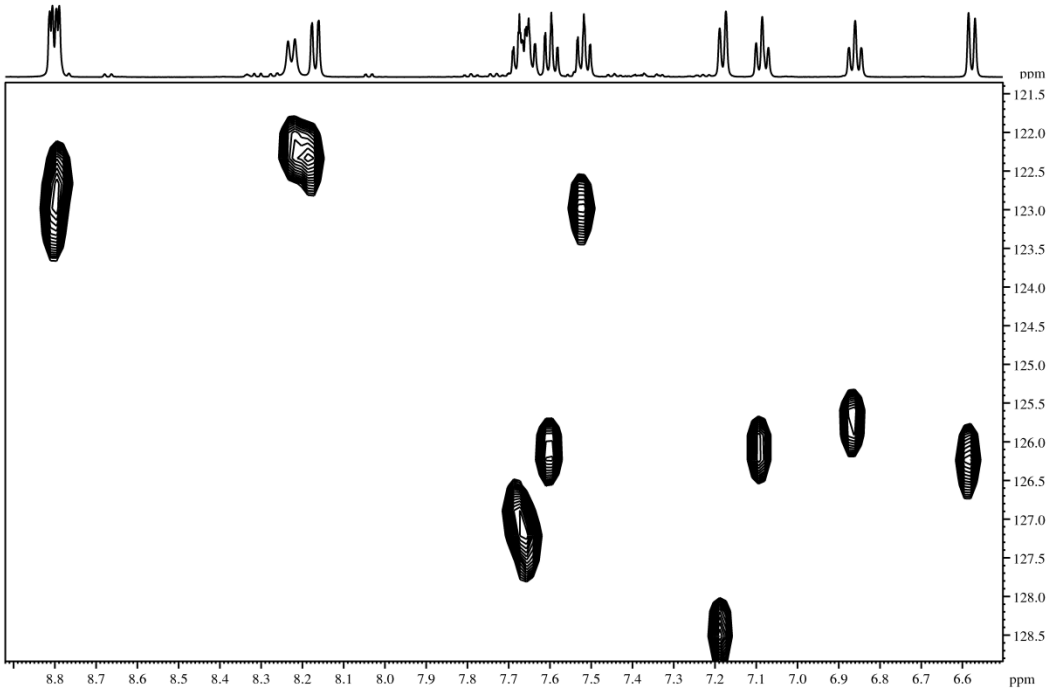
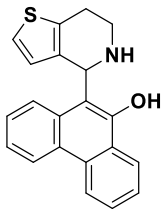


Figure S9. edited HSQC NMR spectrum of **3**, expansion (black: positive, red: negative signals)

***4-(9-Hydroxyphenanthr-10-yl)-4,5,6,7-tetrahydrothieno[3,2-c]pyridine* (5).**



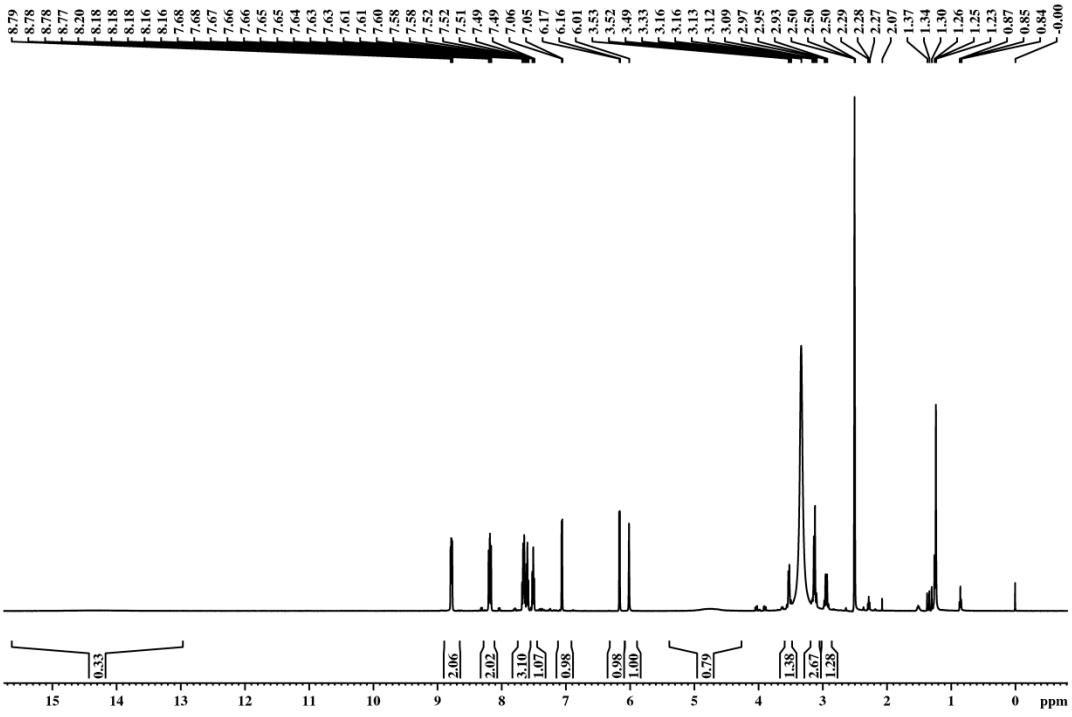


Figure S10. ^{1}H NMR spectrum of **5**

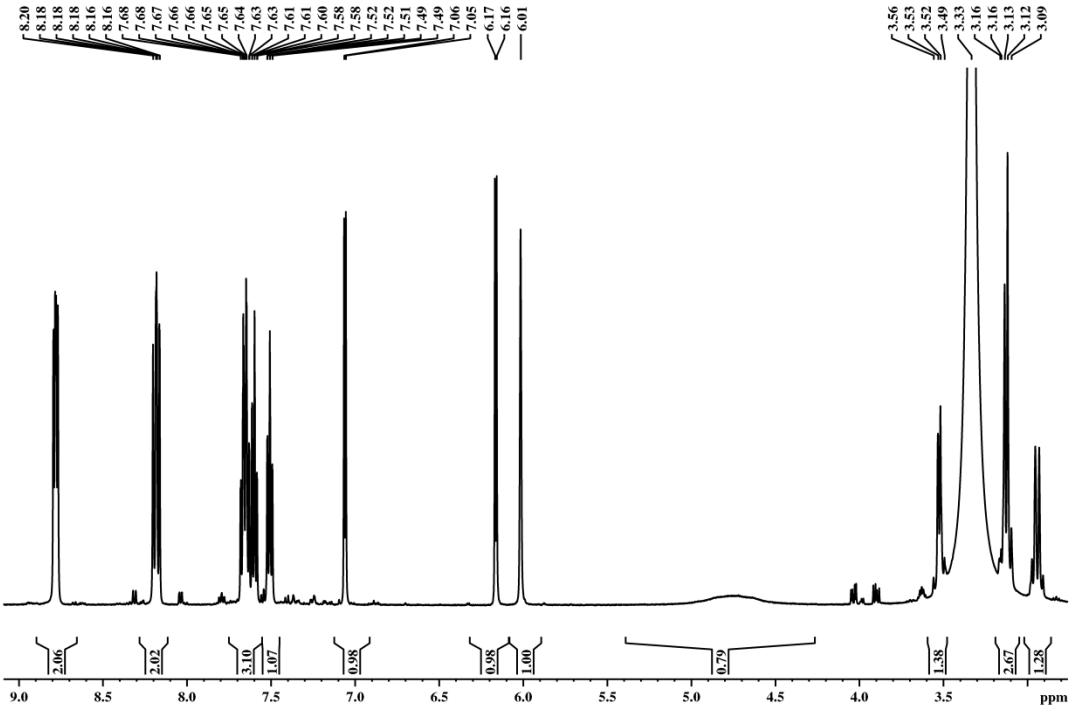


Figure S11. ^{1}H NMR spectrum of **5**, expansion

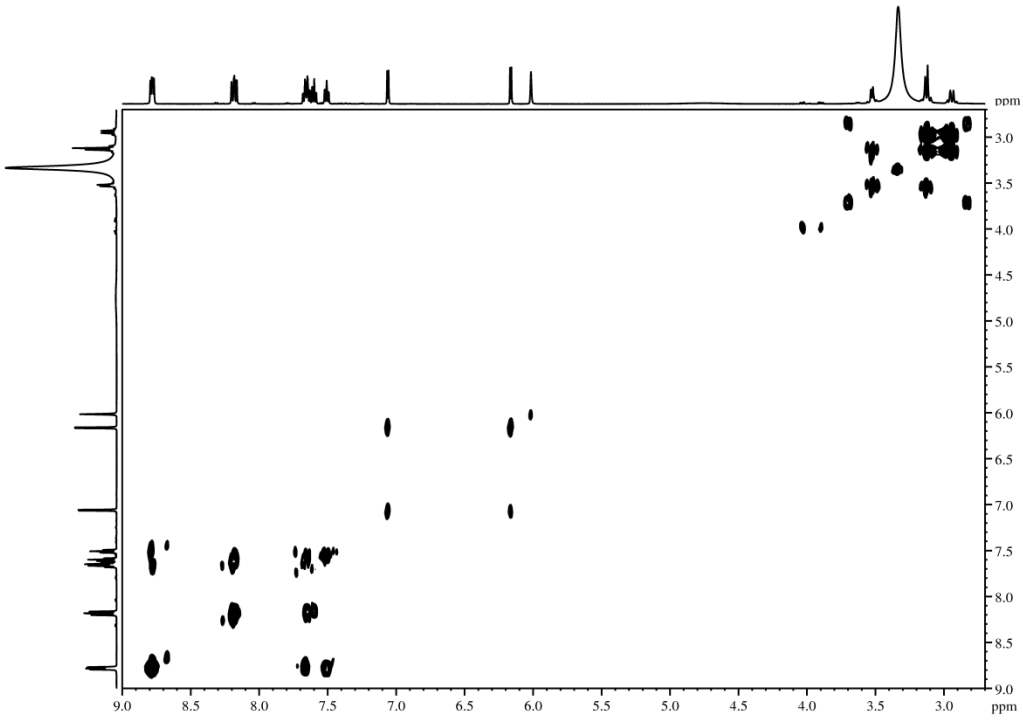


Figure S12. H,H-COSY NMR spectrum of **5**

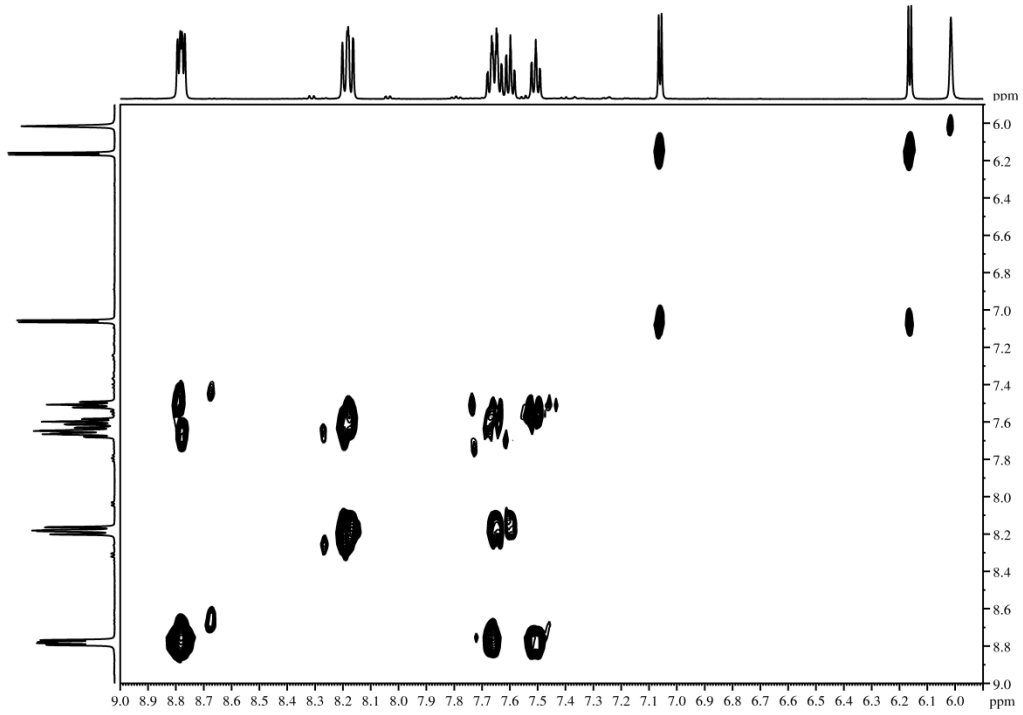


Figure S13. H,H-COSY NMR spectrum of **5**, expansion

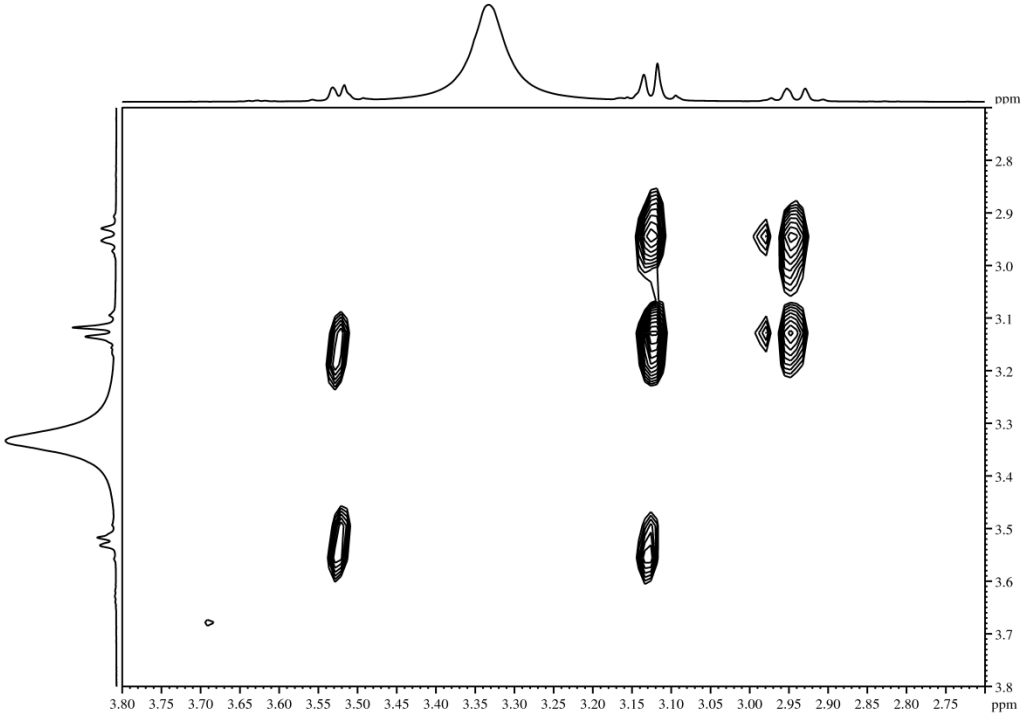


Figure S14. H,H-COSY NMR spectrum of **5**, expansion

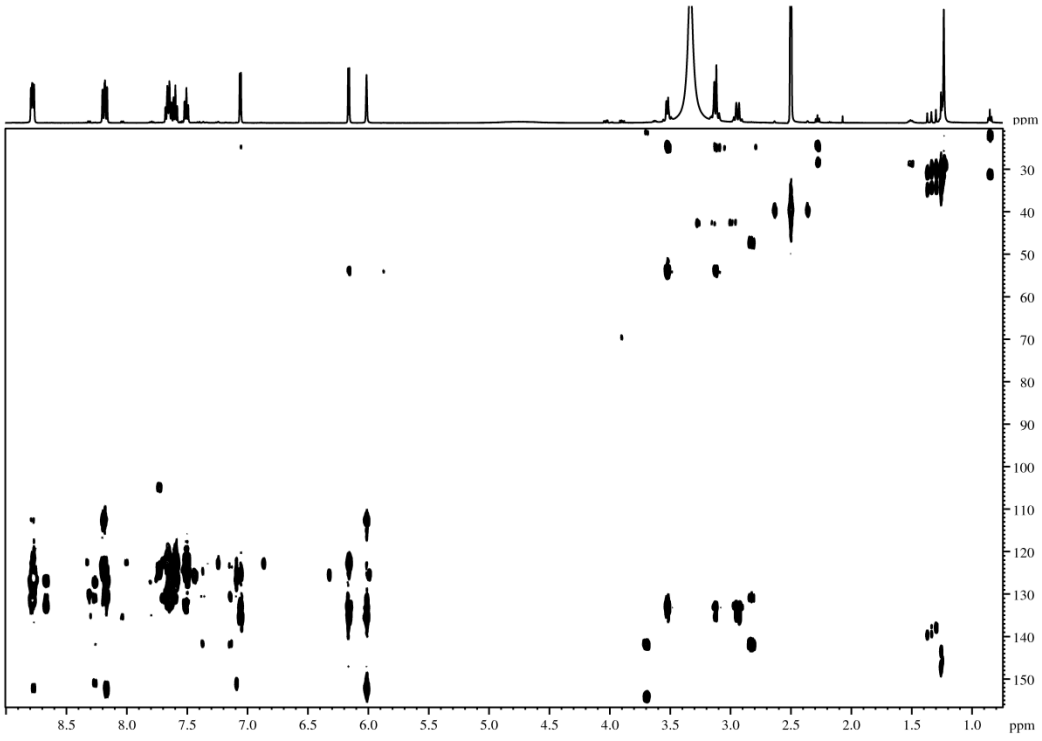


Figure S15. HMBC NMR spectrum of **5**

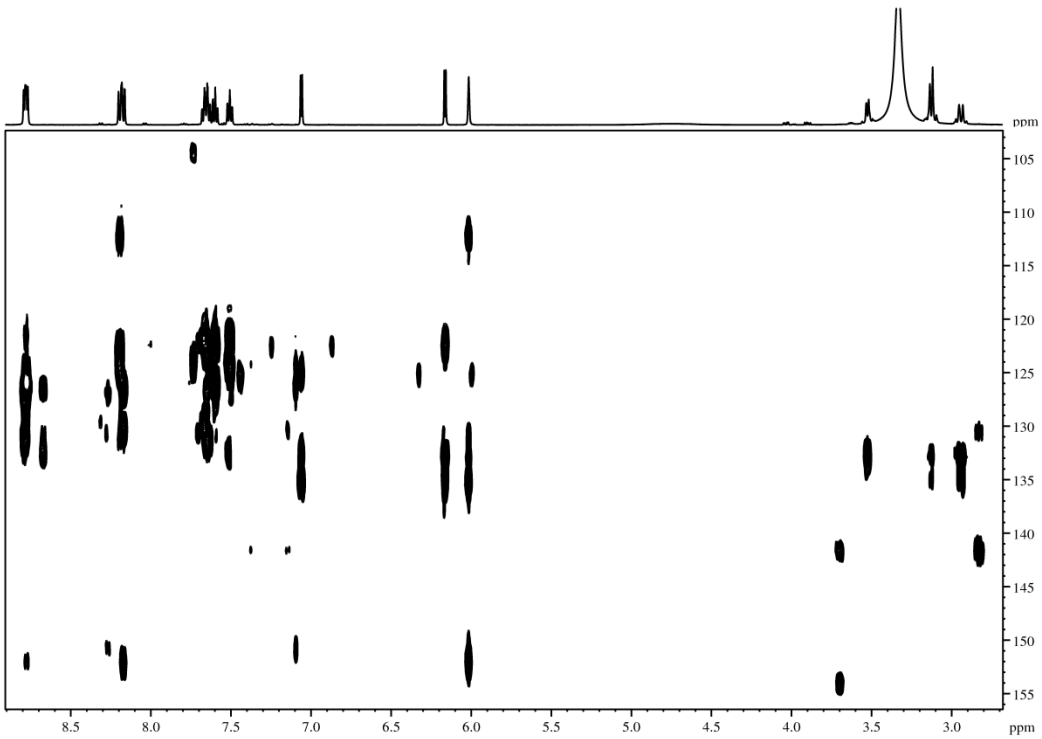


Figure S16. HMBC NMR spectrum of **5**, expansion

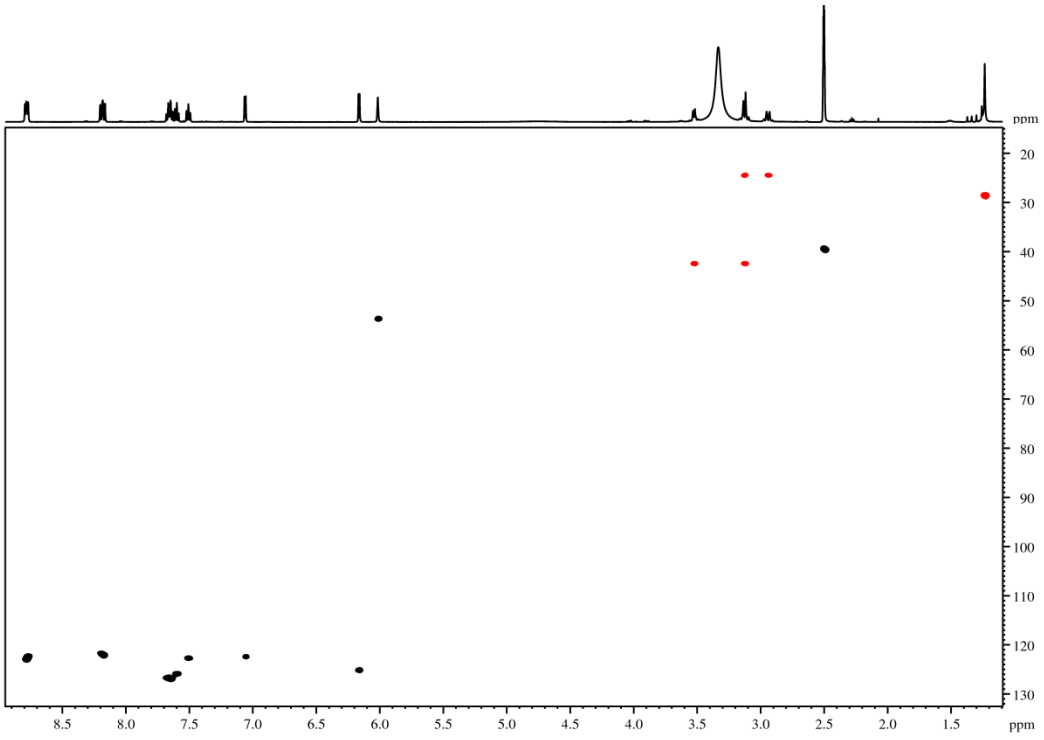


Figure S17. edited HSQC NMR spectrum of **5** (black: positive, red: negative signals)

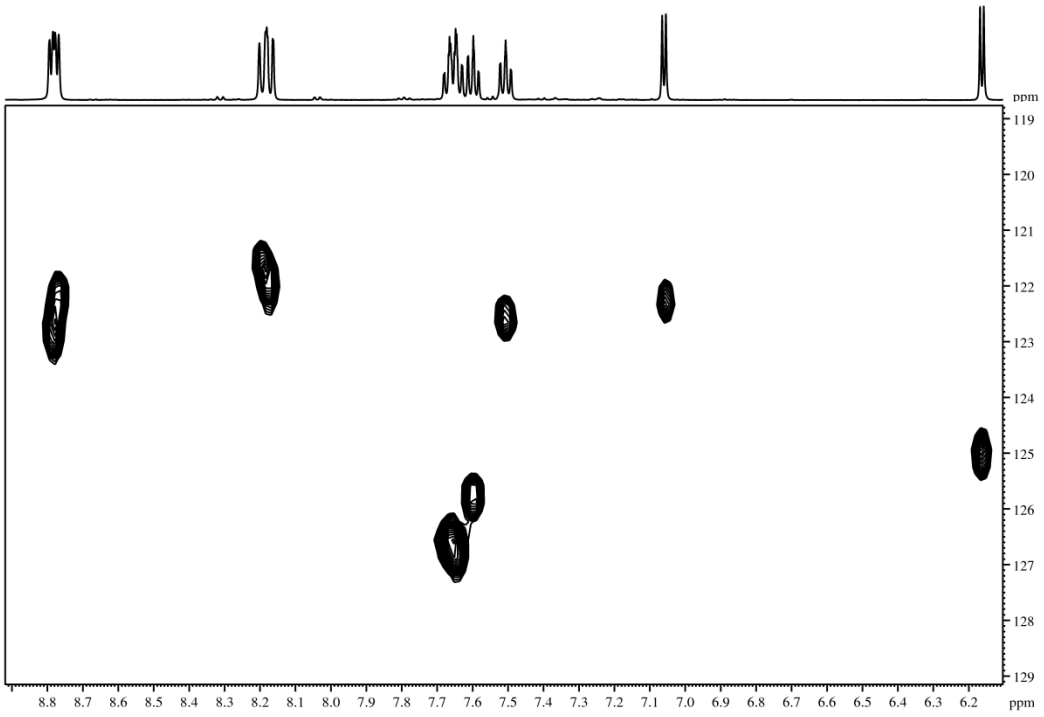
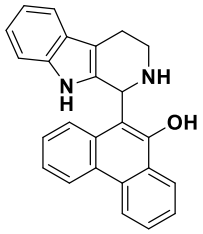


Figure S18. edited HSQC NMR spectrum of **5**, expansion (black: positive, red: negative signals)

1-(9-Hydroxyphenanthr-10-yl)-1,2,3,4-tetrahydro-β-carboline (7)



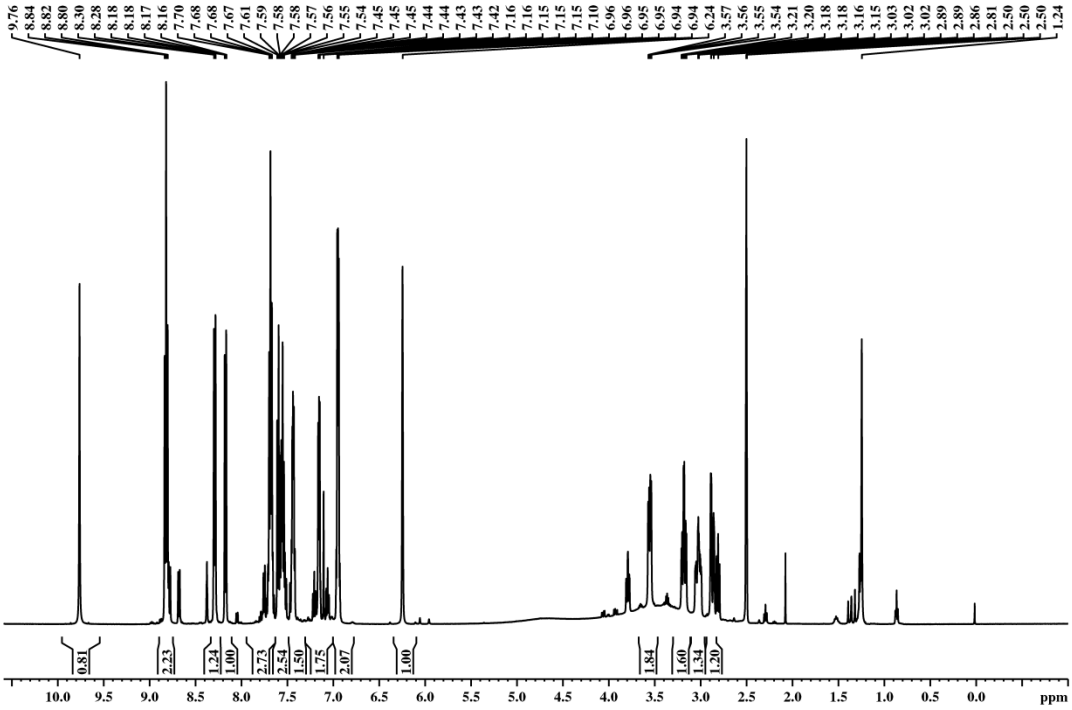


Figure S19. ^{1}H NMR spectrum of **7**

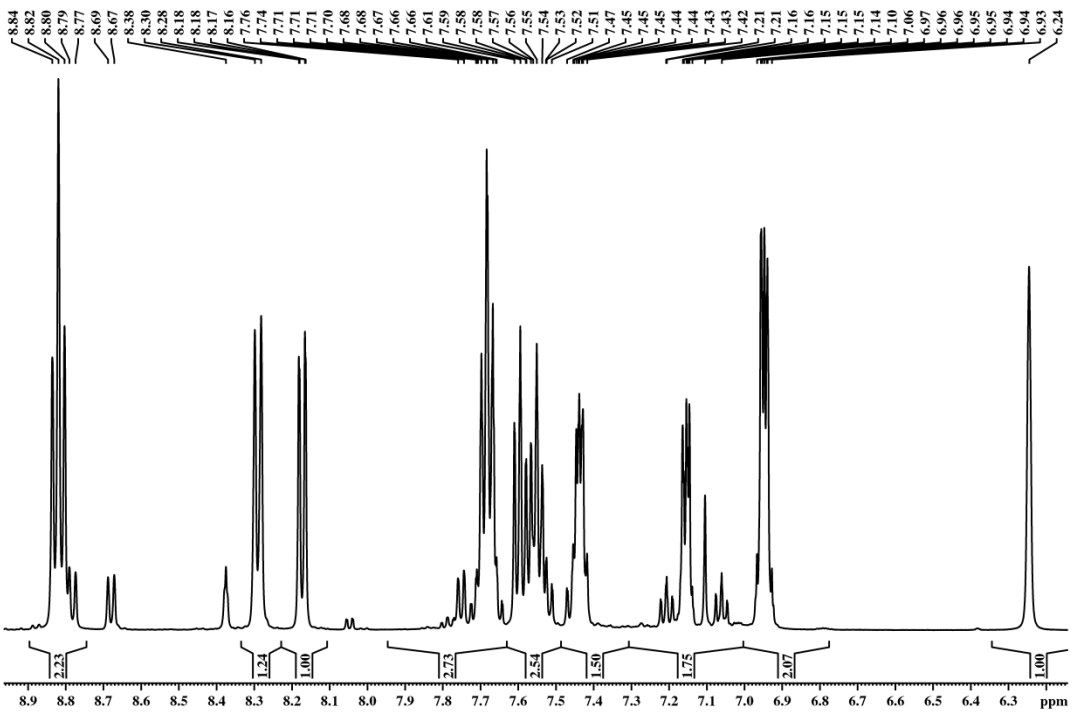


Figure S20. ^{1}H NMR spectrum of **7**, expansion

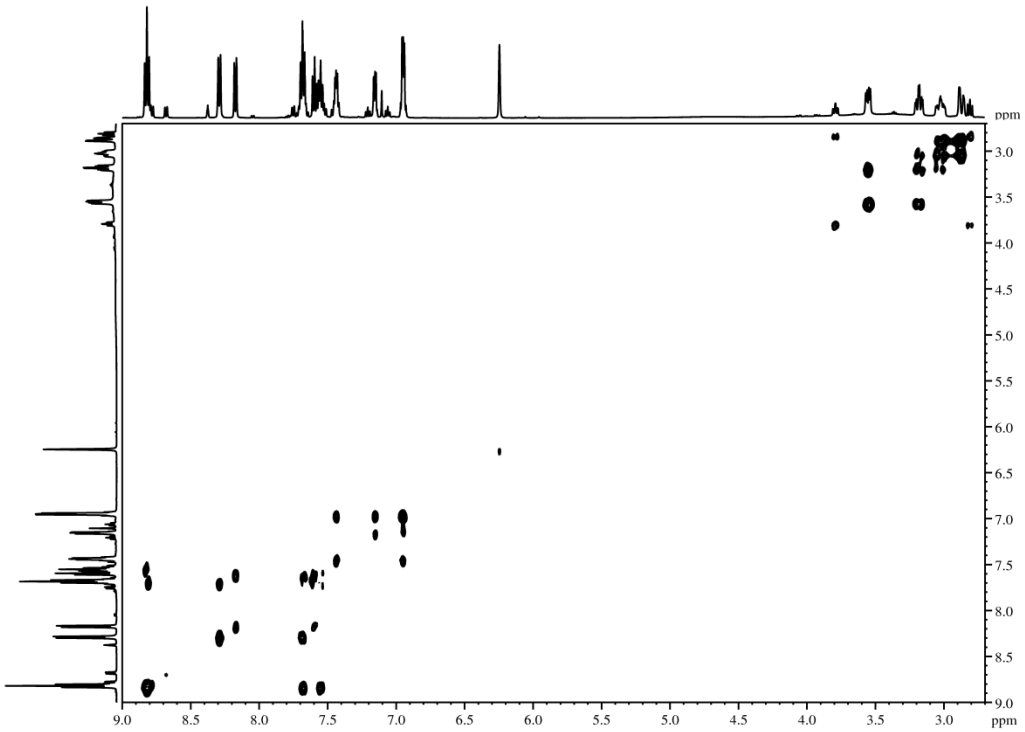


Figure S20. H,H-COSY NMR spectrum of **7**

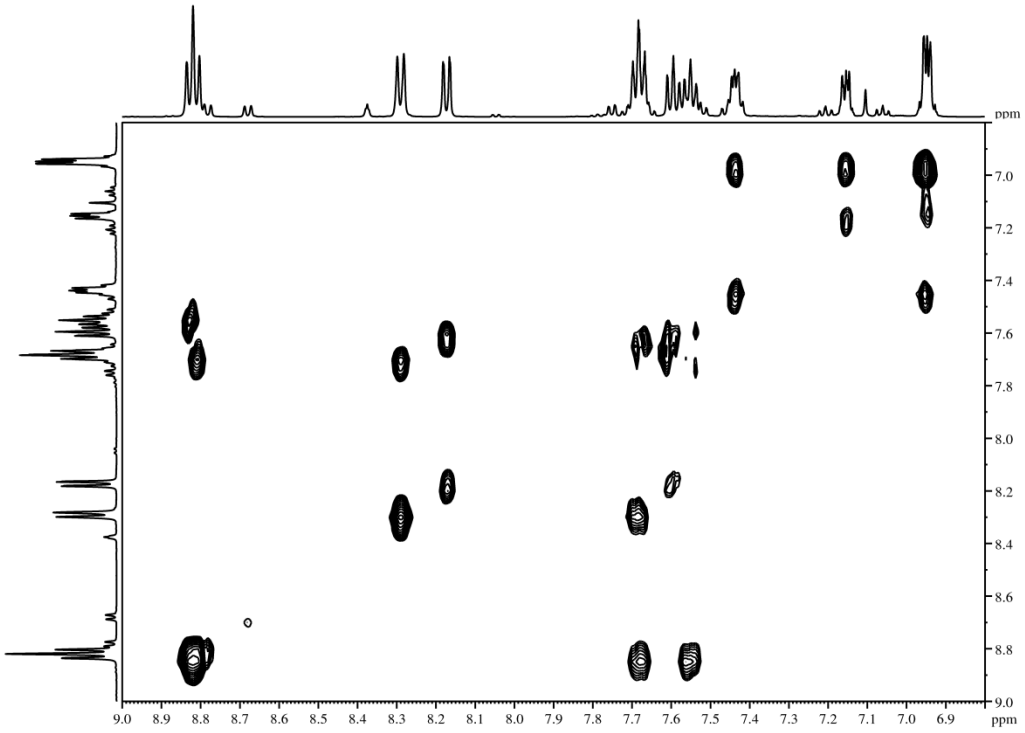


Figure S21. H,H-COSY NMR spectrum of **7**, expansion

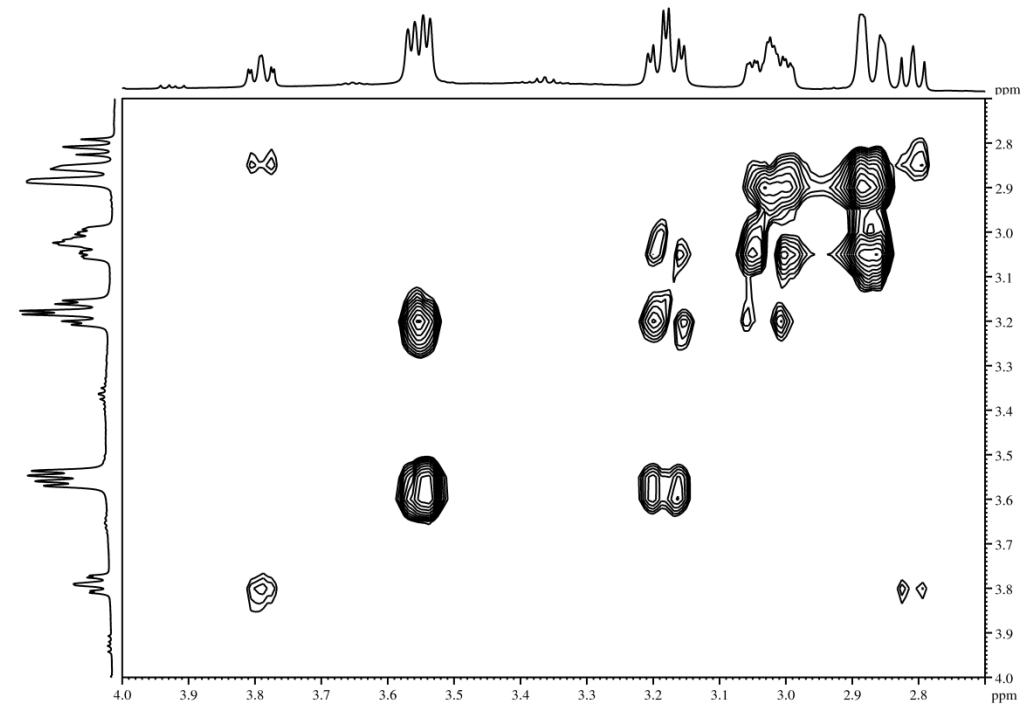


Figure S22. H,H-COSY NMR spectrum of **7**, expansion

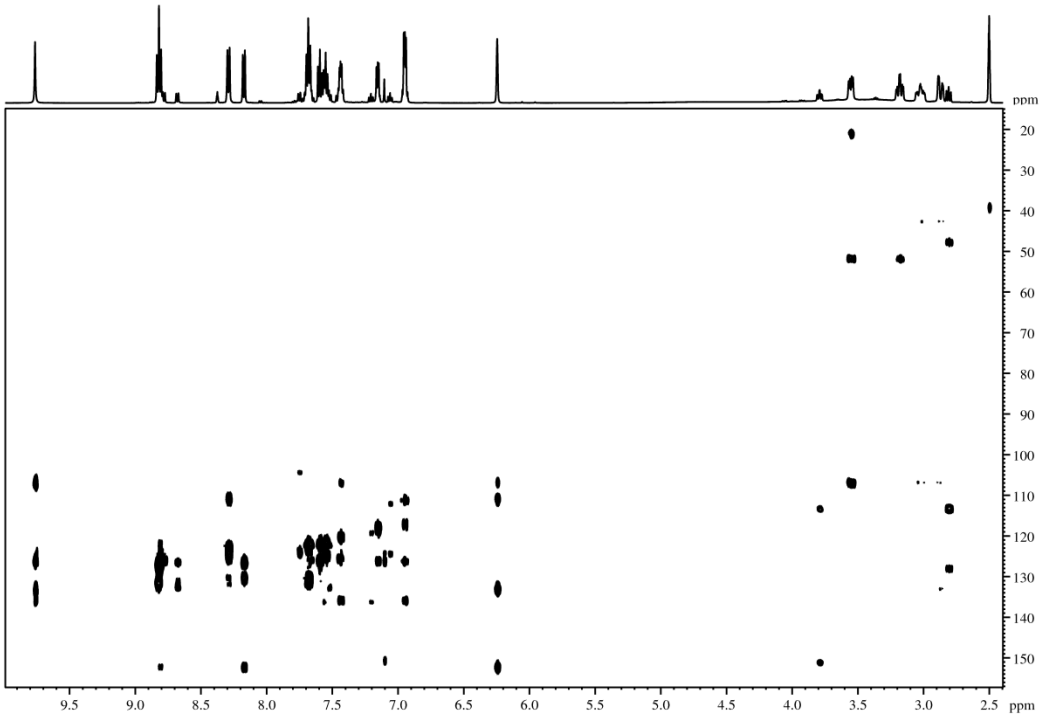


Figure S23. HMBC NMR spectrum of **7**

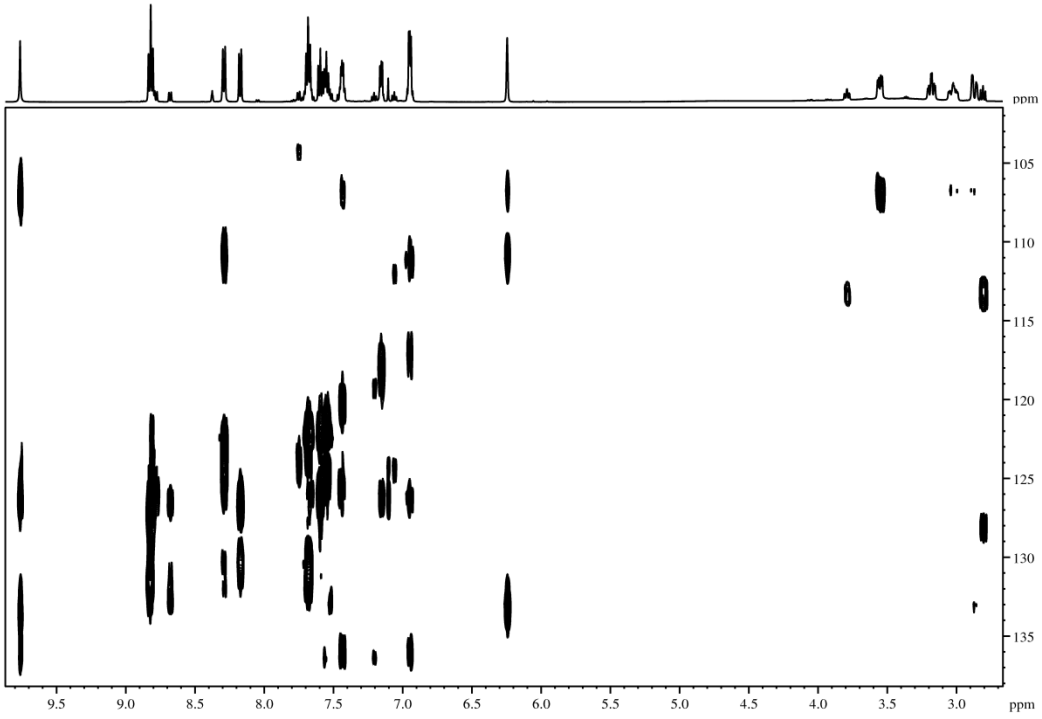


Figure S24. HMBC NMR spectrum of **7**, expansion

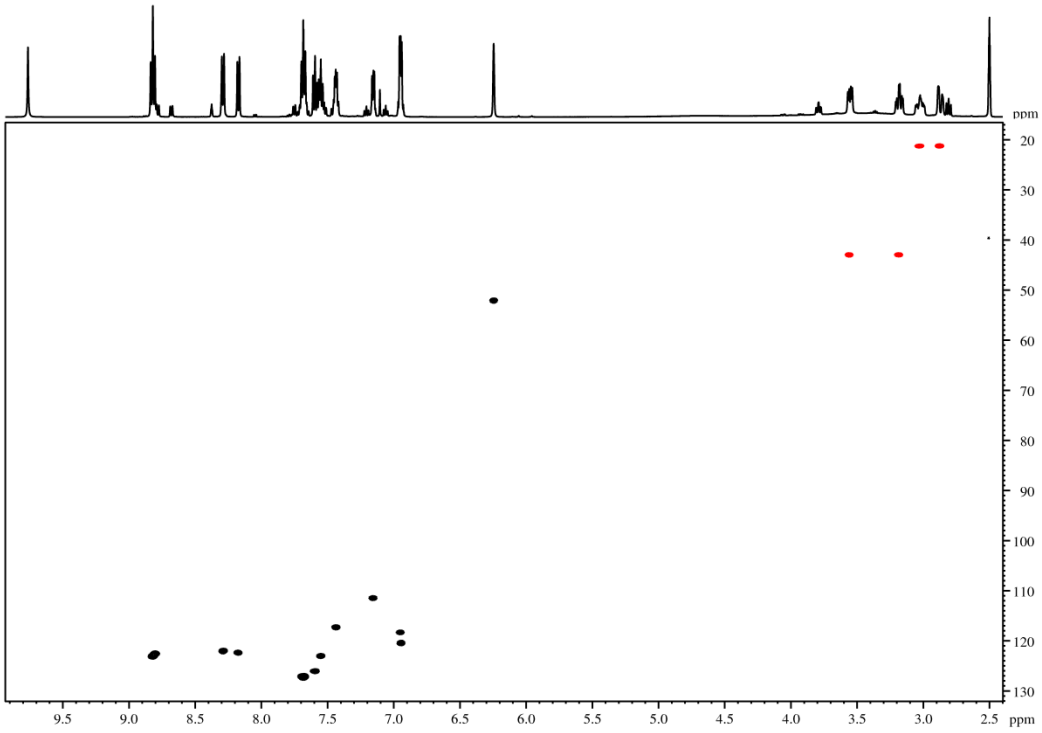


Figure S25. edited HSQC NMR spectrum of **7** (black: positive, red: negative signals)

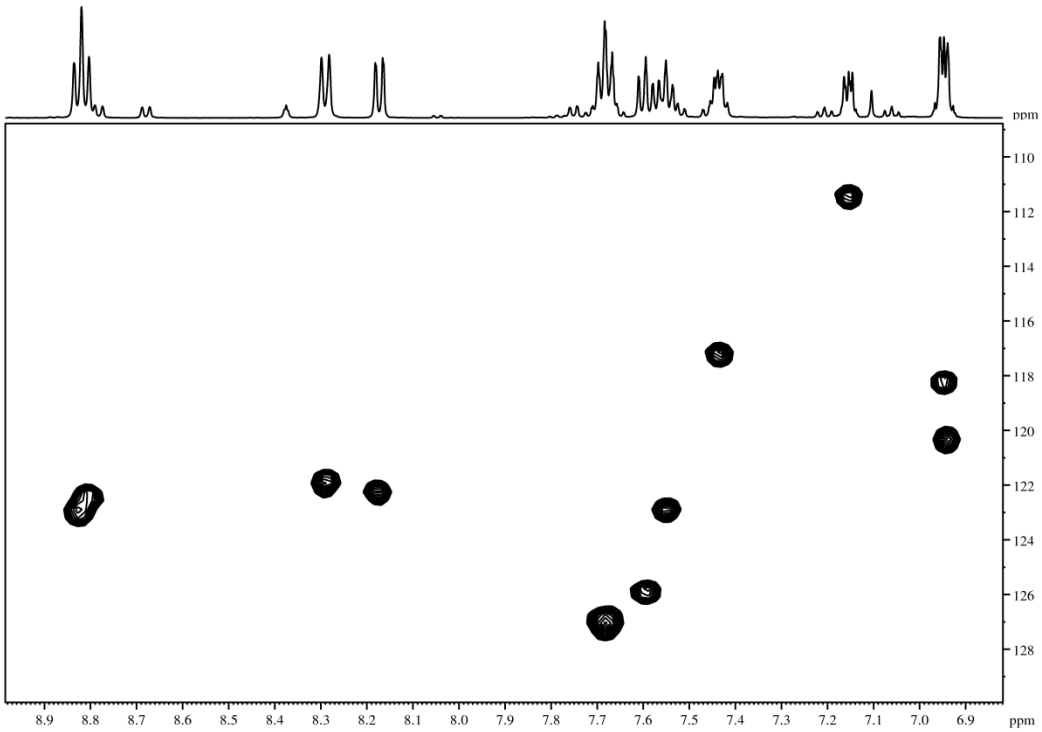
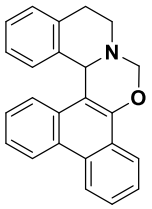


Figure S26. edited HSQC NMR spectrum of **7**, expansion (black: positive, red: negative signals)

Phenanthr[9,10-e][1,3]oxazino[4,3-a]isoquinoline (8)



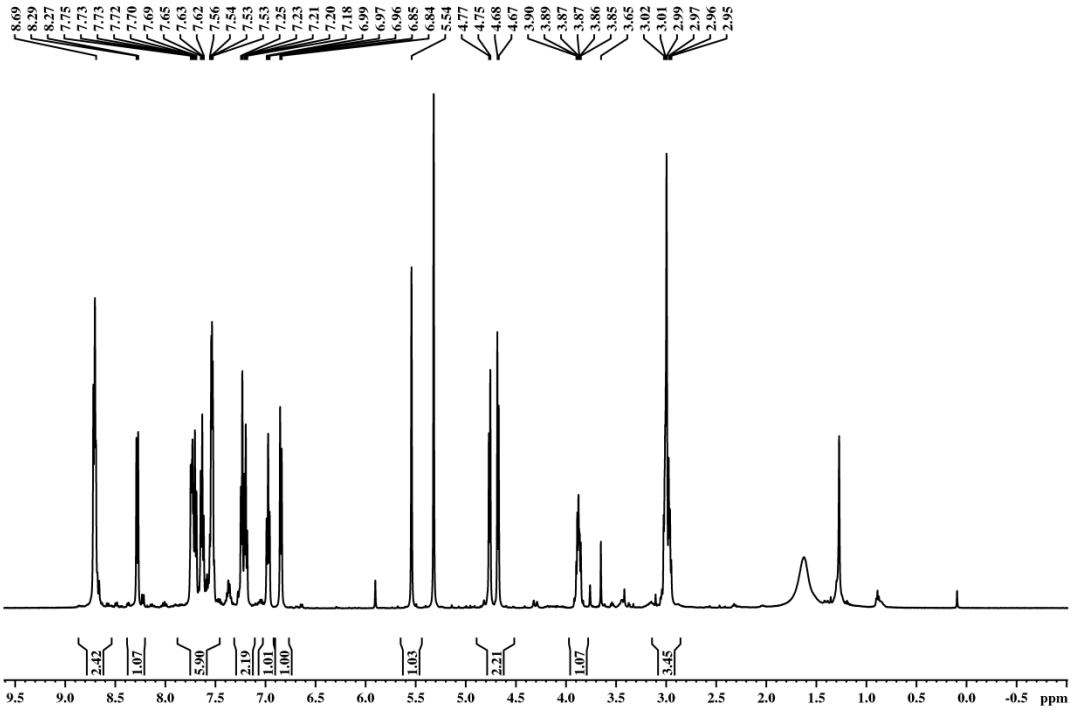


Figure S27. ^{1}H NMR spectrum of **8**

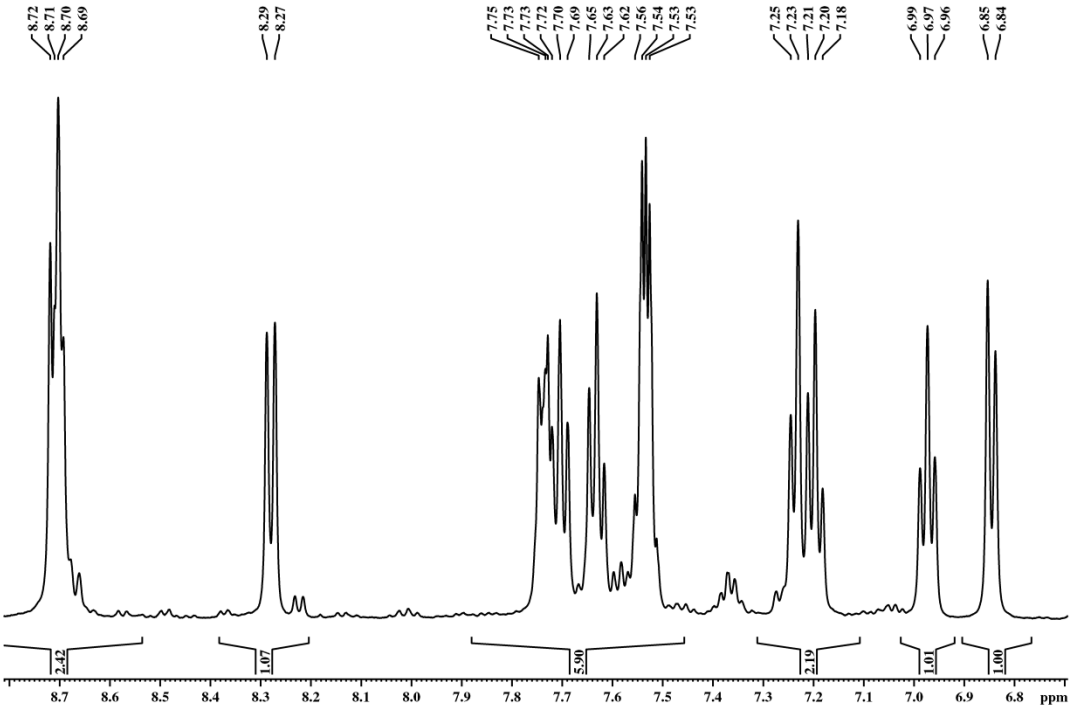


Figure S28. ^{1}H NMR spectrum of **8**, expansion

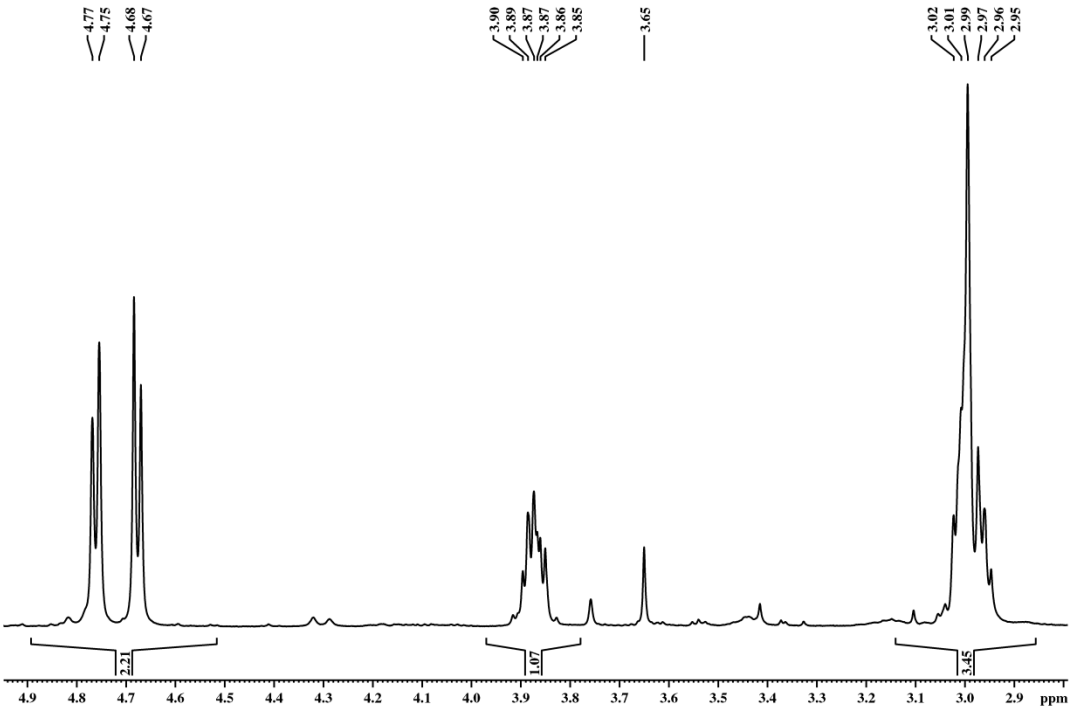


Figure S29. ^{1}H NMR spectrum of **8**, expansion

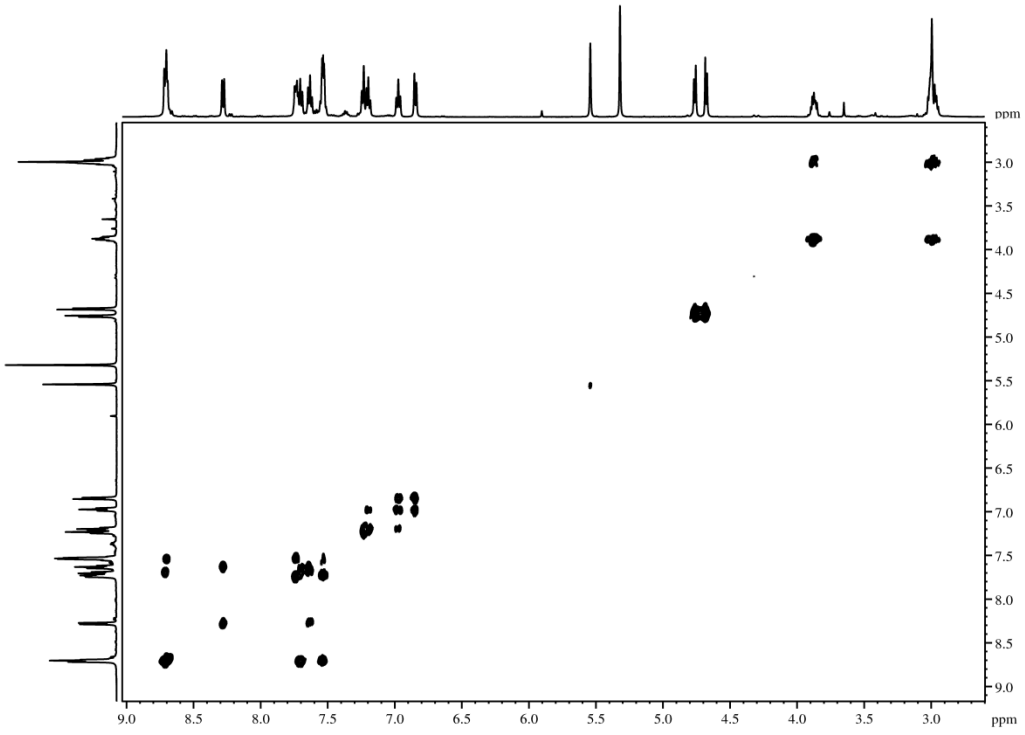


Figure S30. H,H-COSY NMR spectrum of **8**

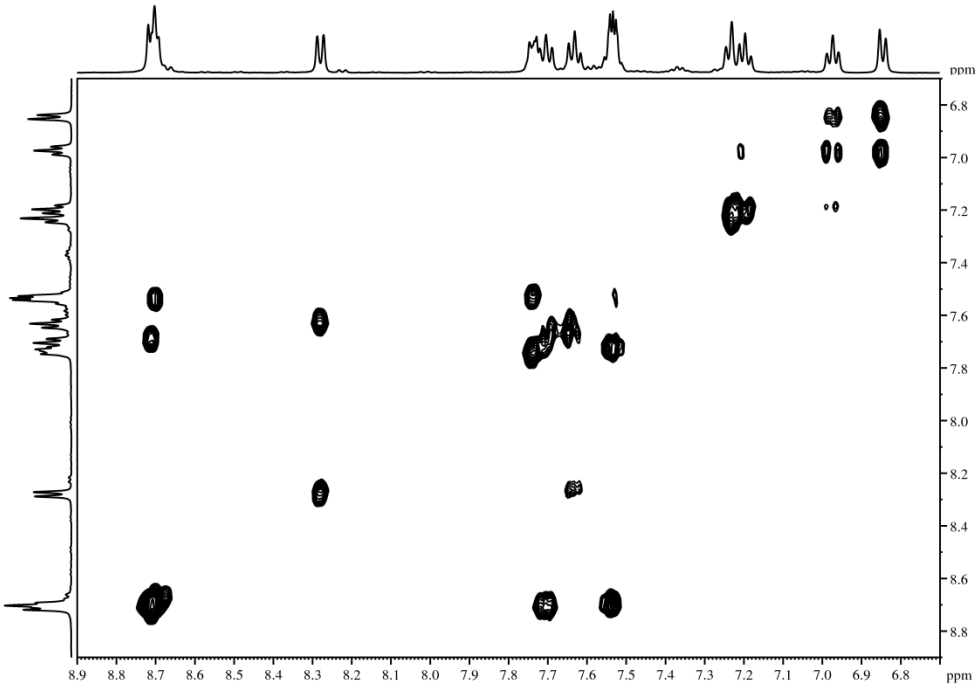


Figure S31. H,H-COSY NMR spectrum of **8**, expansion

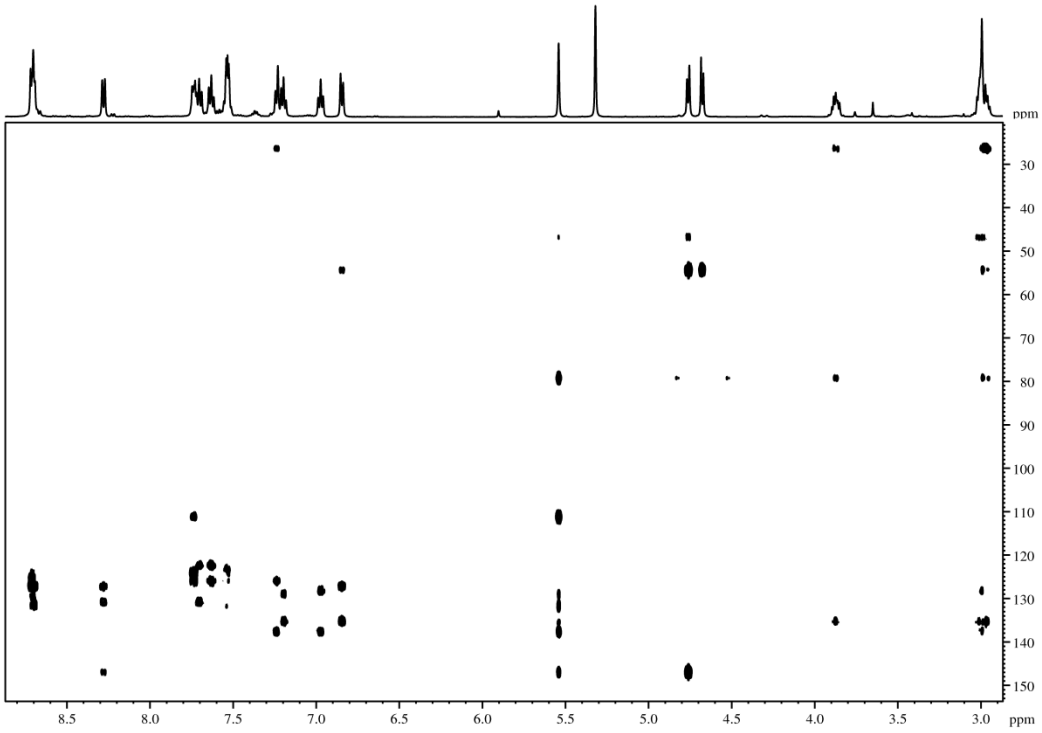


Figure S32. HMBC NMR spectrum of **8**

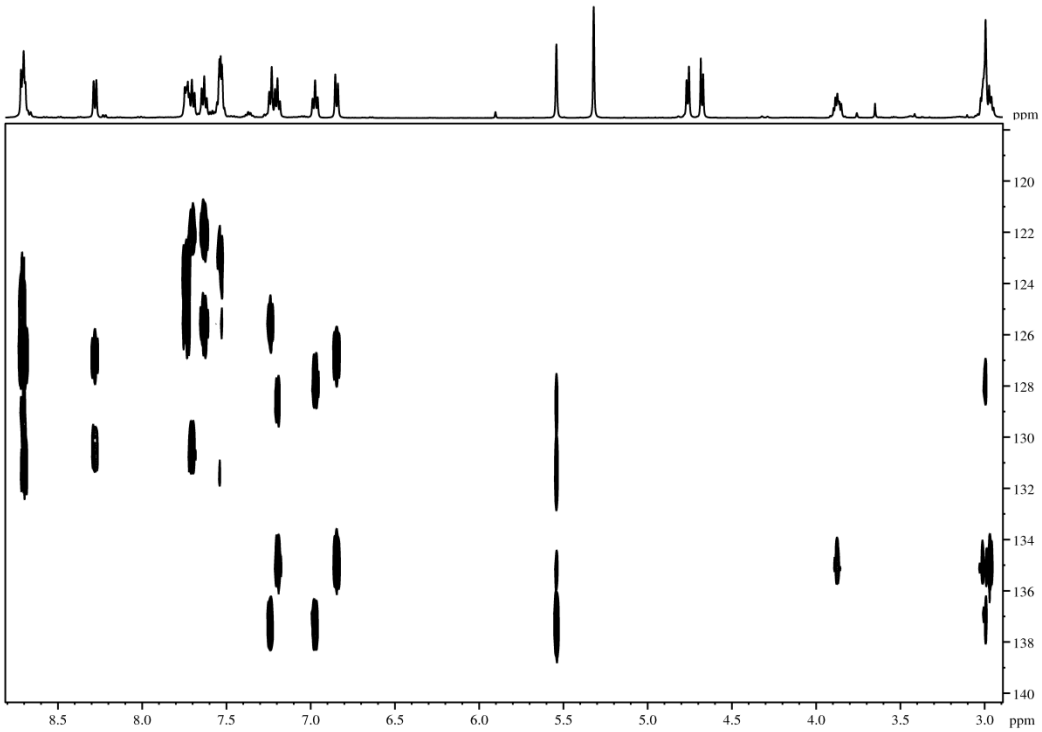


Figure S33. HMBC NMR spectrum of **8**, expansion

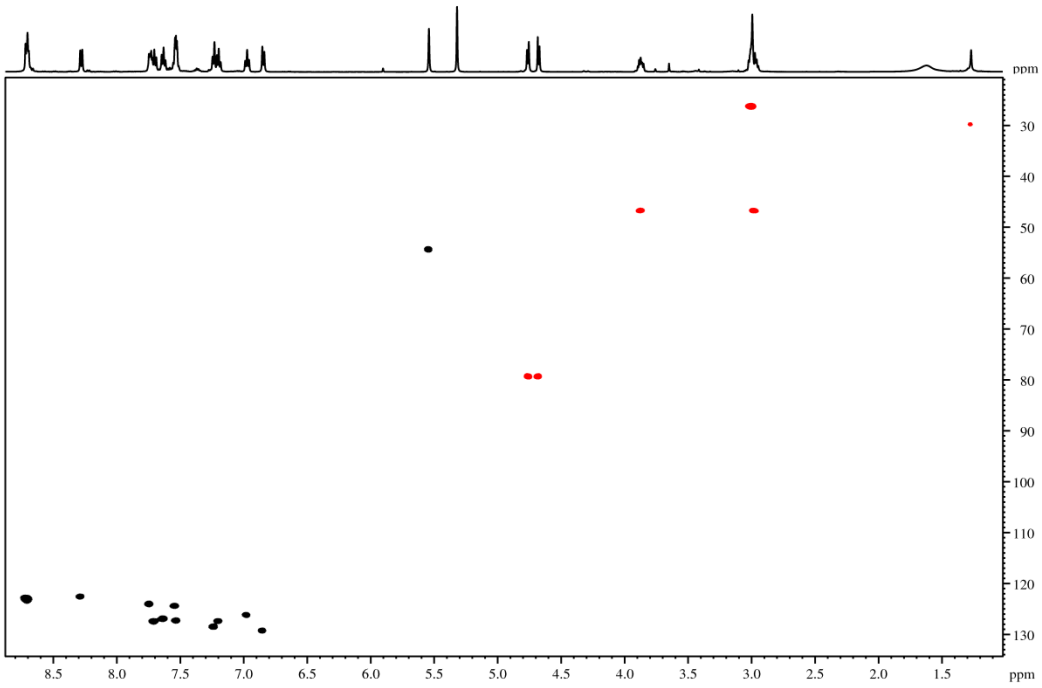


Figure S34. edited HSQC NMR spectrum of **8** (black: positive, red: negative signals)

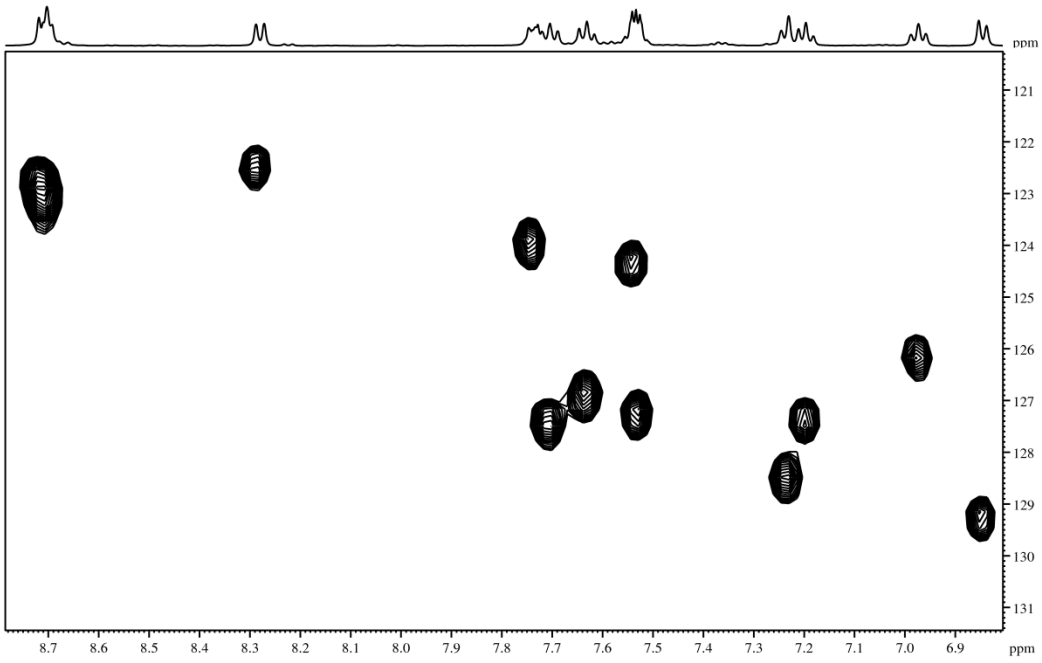
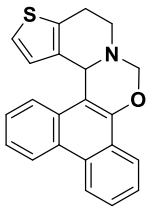


Figure S35. edited HSQC NMR spectrum of **8**, expansion (black: positive, red: negative signals)

Phenanthr[9,10-e][1,3]oxazino[4,3-a]thieno[3,2-c]pyridine (9)



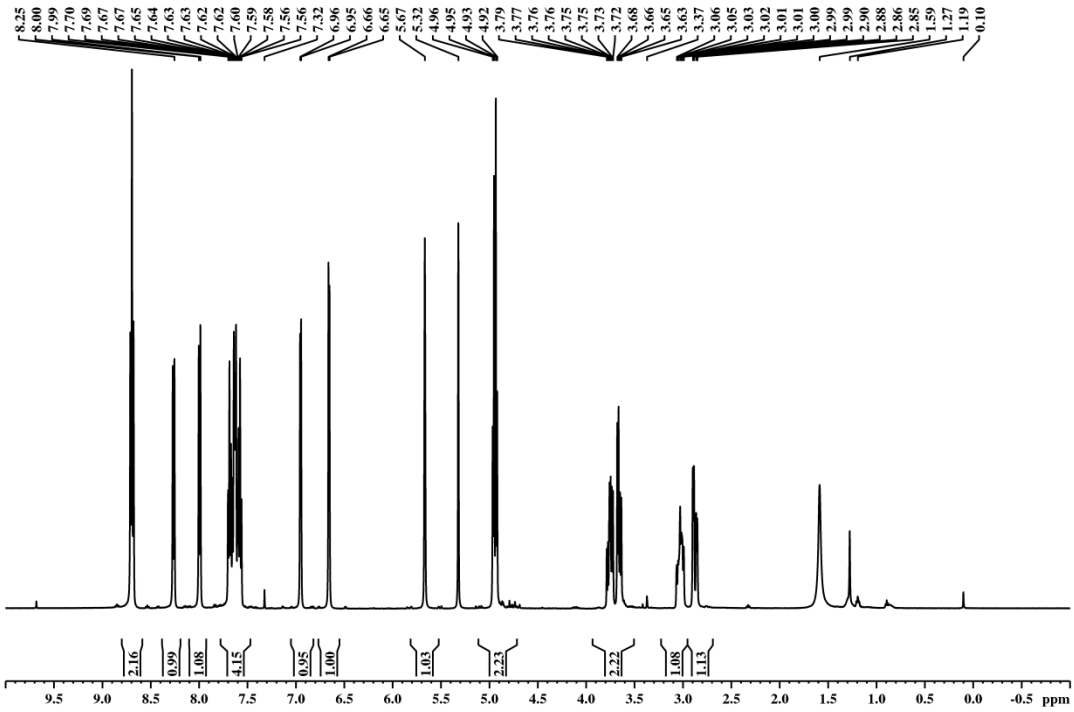


Figure S36. ^{1}H NMR spectrum of **9**

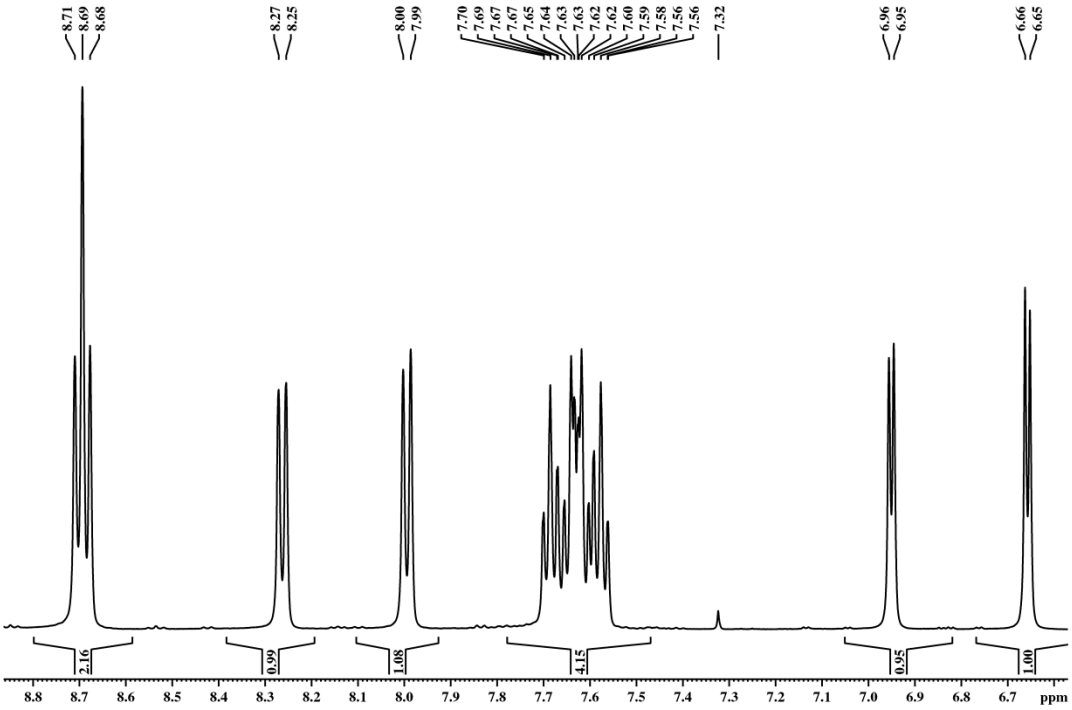


Figure S37. ^{1}H NMR spectrum of **9**, expansion

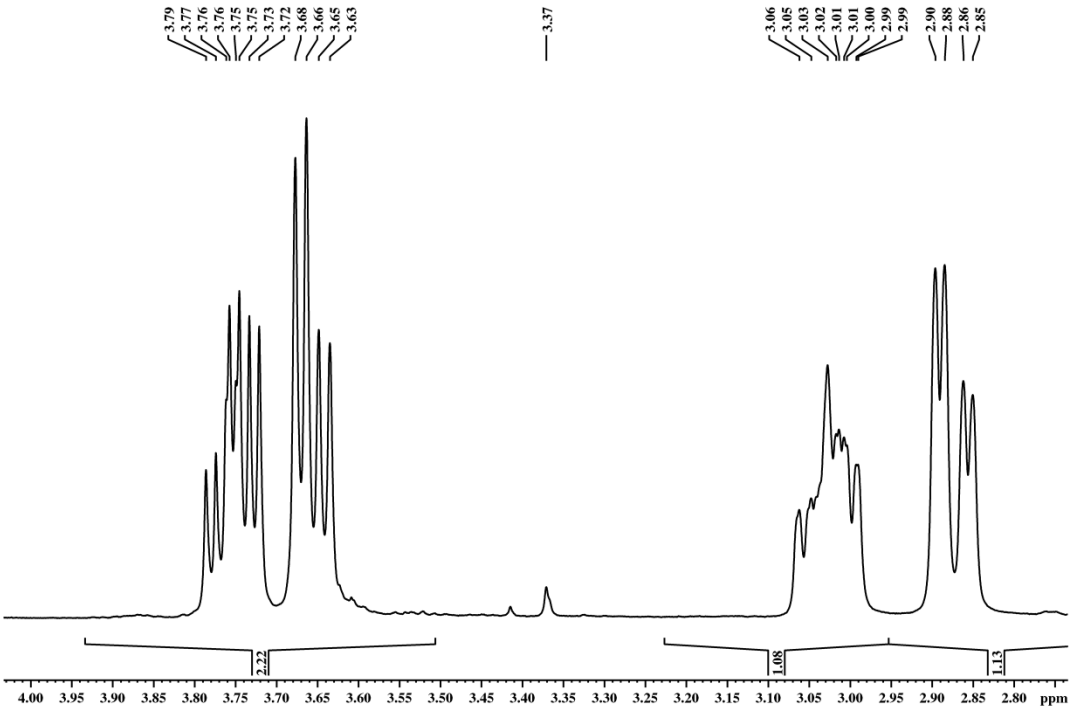


Figure S38. ^{1}H NMR spectrum of **9**, expansion

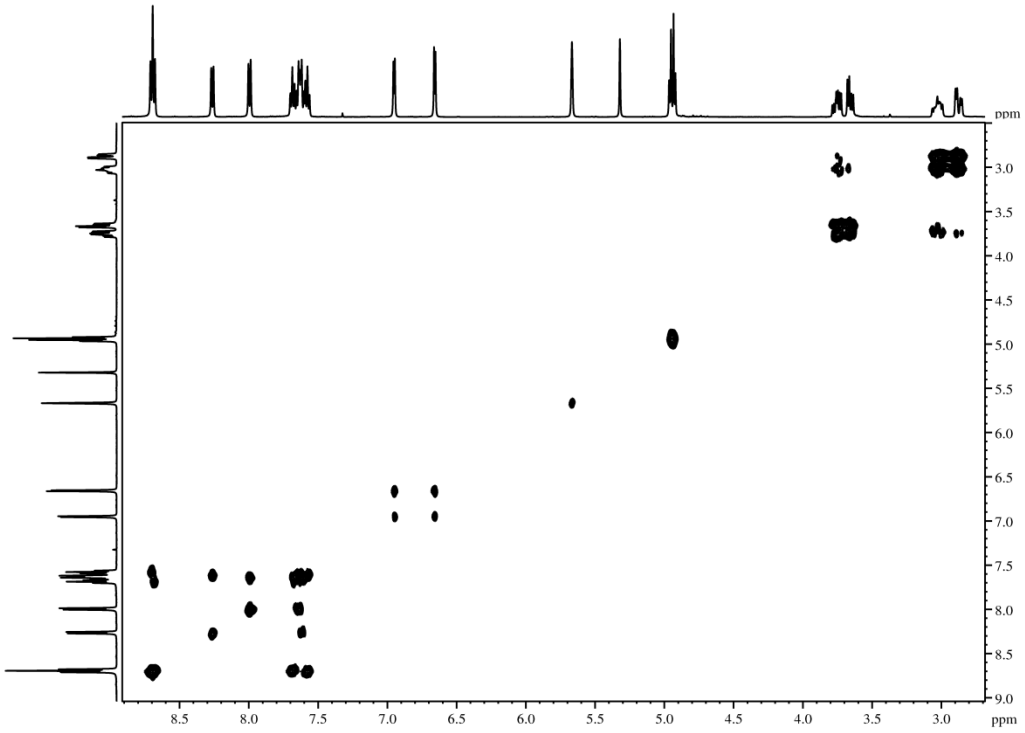


Figure S39. H,H-COSY NMR spectrum of **9**

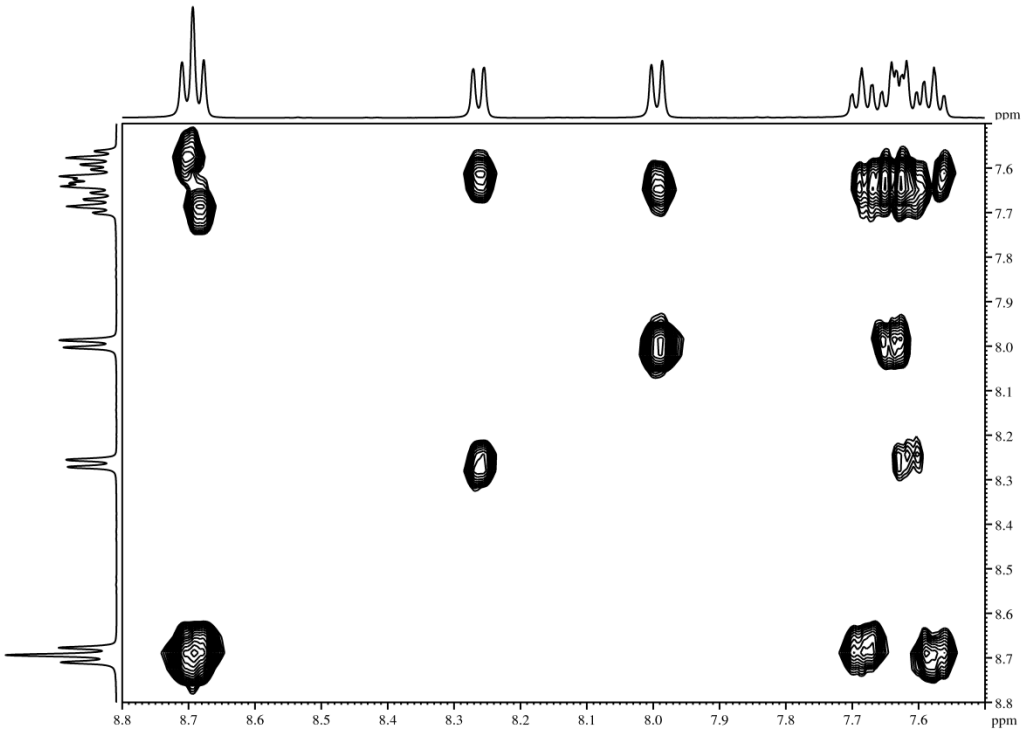


Figure S40. H,H-COSY NMR spectrum of **9**, expansion

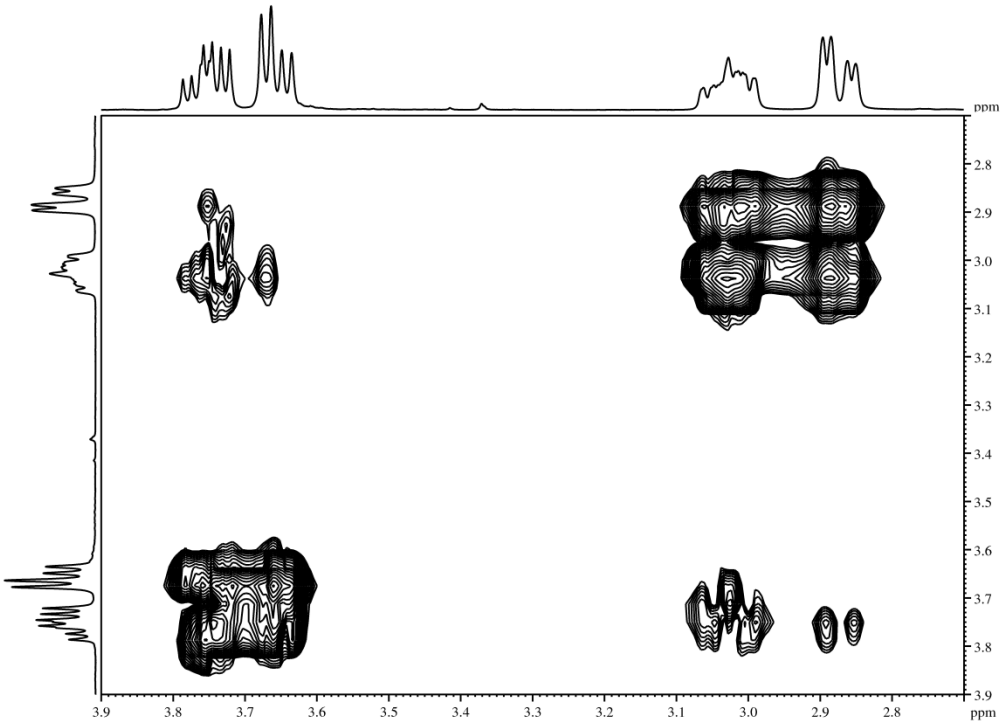


Figure S41. H,H-COSY NMR spectrum of **9**, expansion

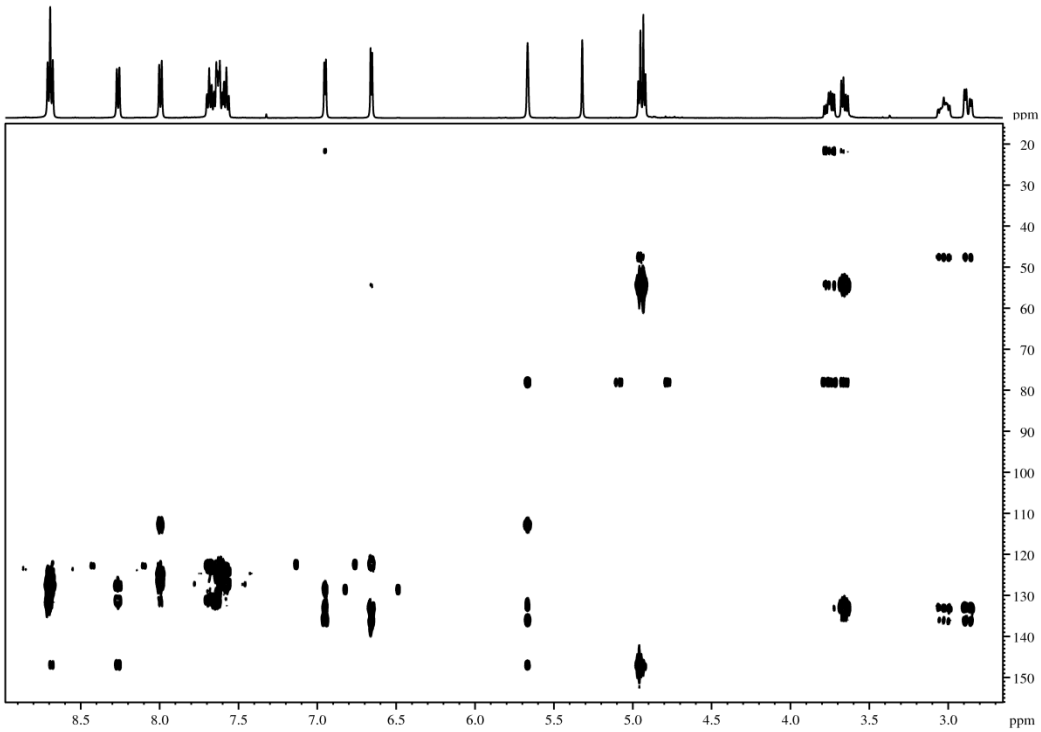


Figure S42. HMBC NMR spectrum of **9**

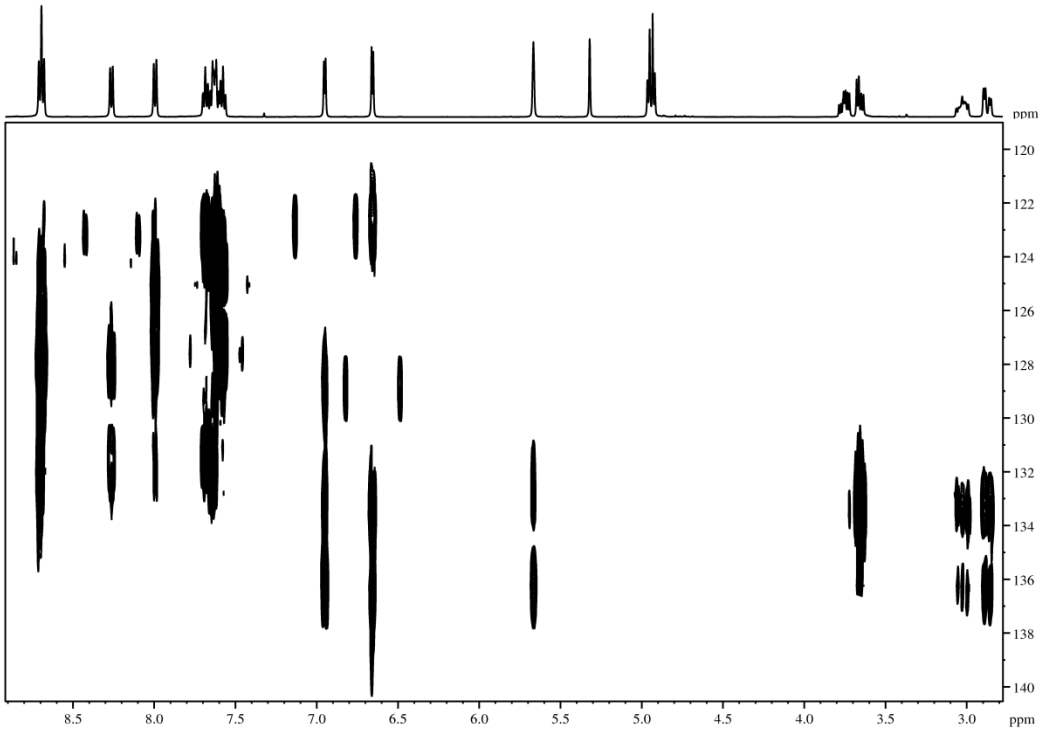


Figure S43. HMBC NMR spectrum of **9**, expansion

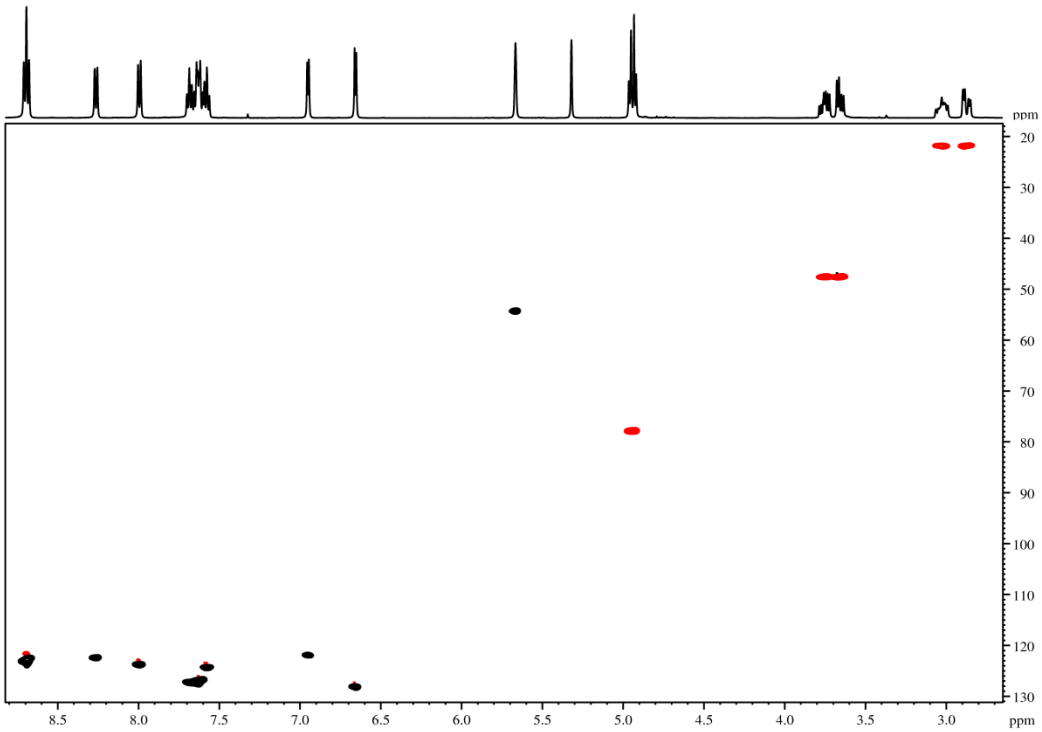


Figure S44. edited HSQC NMR spectrum of **9** (black: positive, red: negative signals)

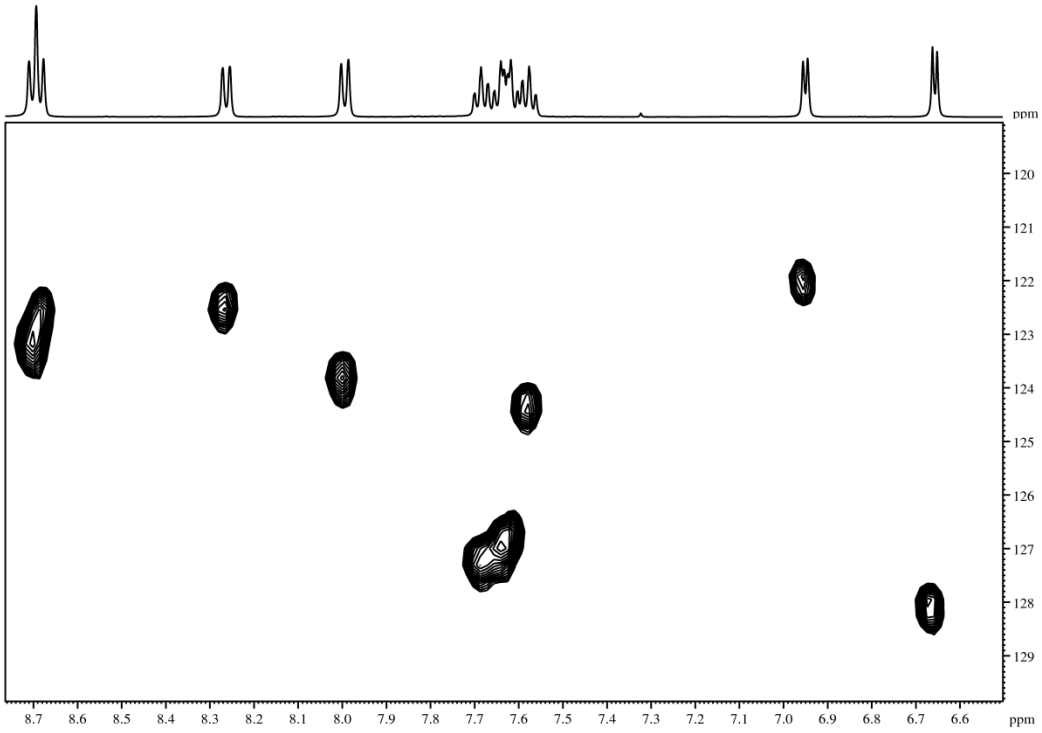
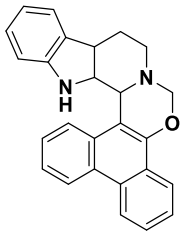


Figure S45. edited HSQC NMR spectrum of **9**, expansion (black: positive, red: negative signals)

Phenanthr[9,10-e][1,3]oxazino[4,3-a]-β-carboline (10)



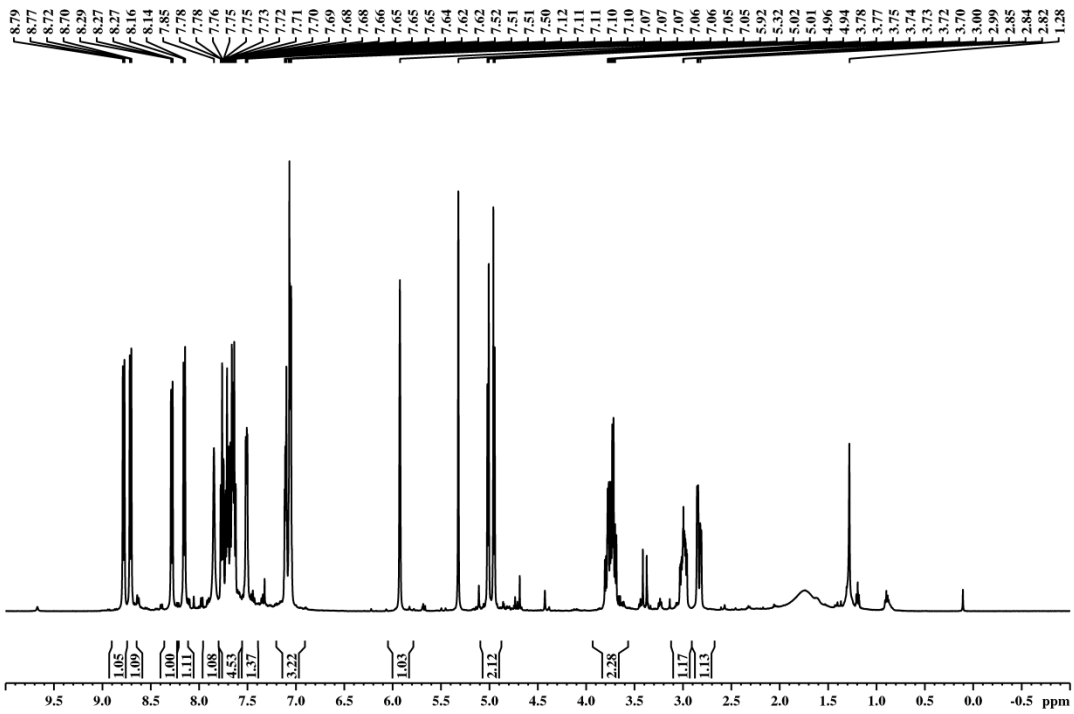


Figure S46. ^{1}H NMR spectrum of **10**

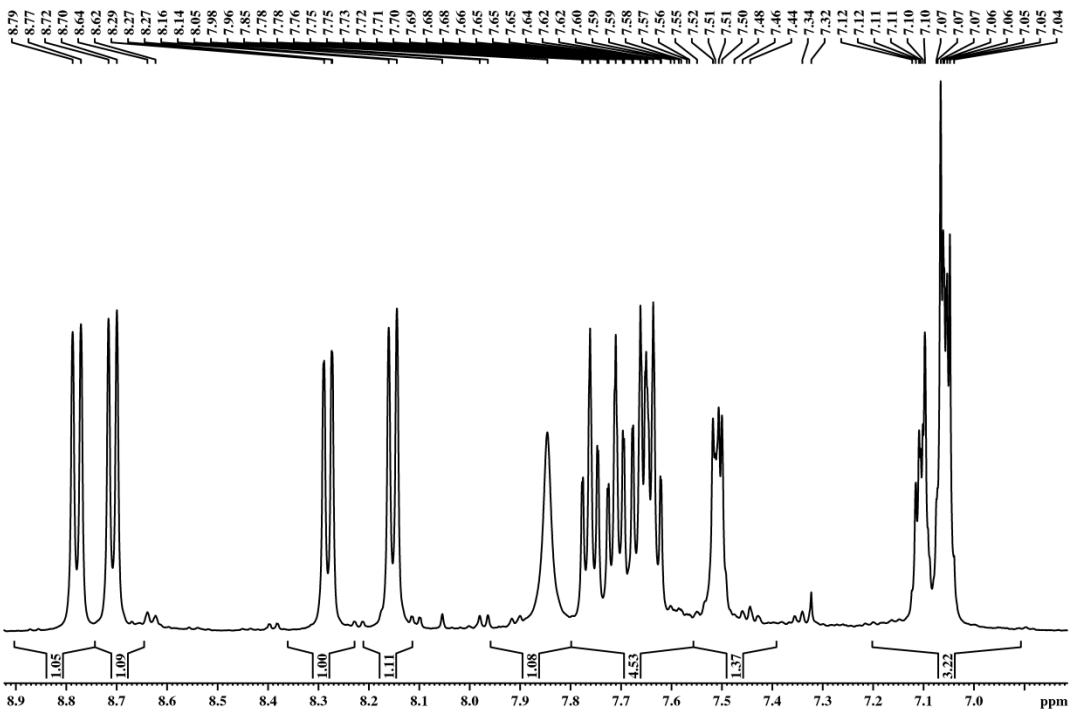


Figure S47. ^{1}H NMR spectrum of **10**, expansion

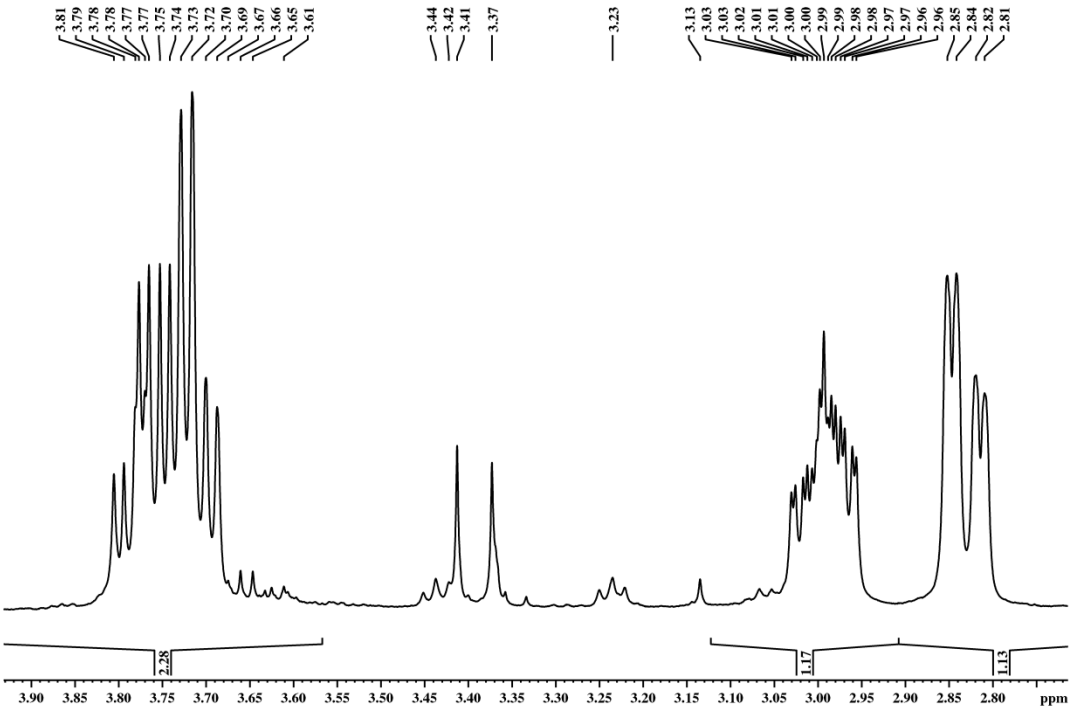


Figure S49. ^{1}H NMR spectrum of **10**, expansion

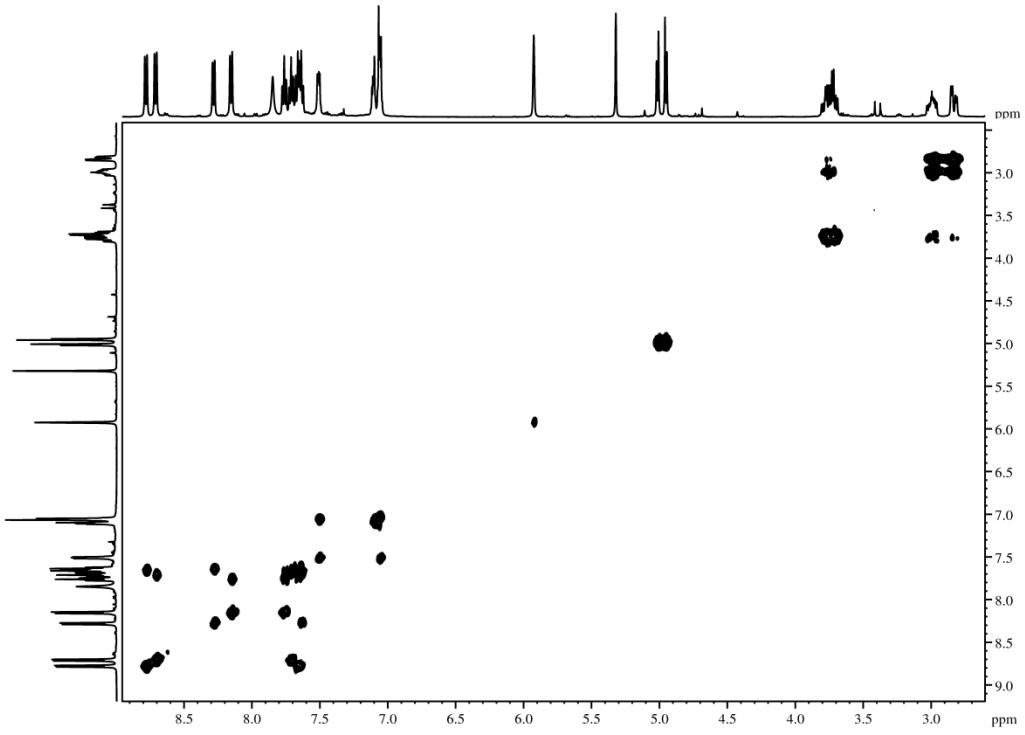


Figure S50. H,H-COSY NMR spectrum of **10**

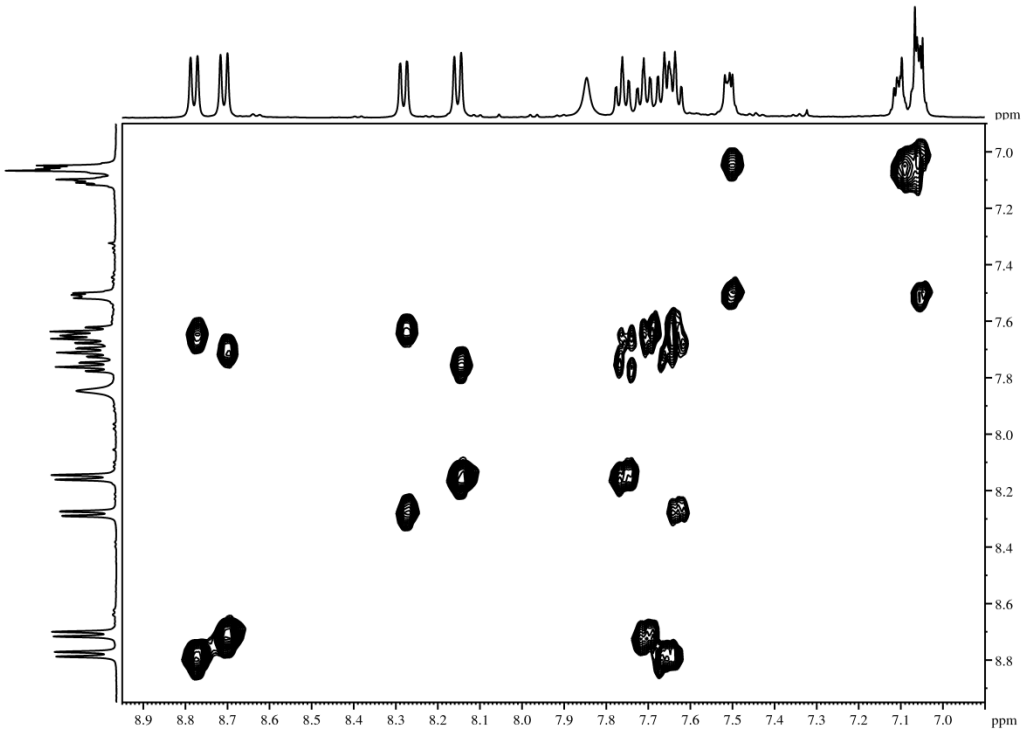


Figure S51. H,H-COSY NMR spectrum of **10**, expansion

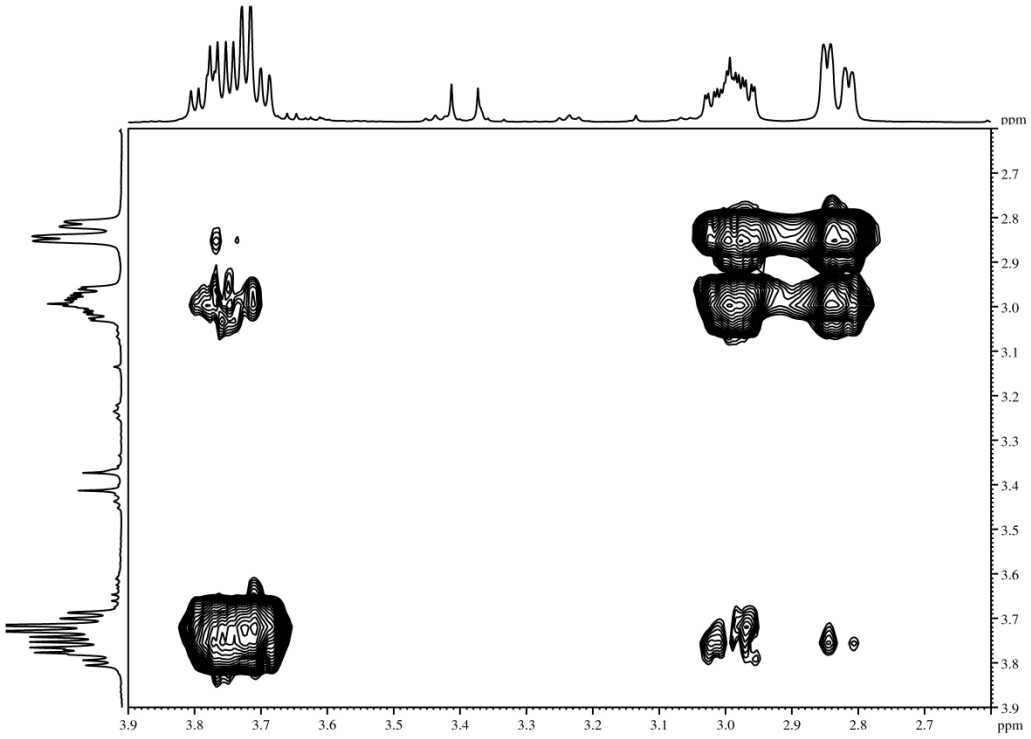


Figure S52. H,H-COSY NMR spectrum of **10**, expansion

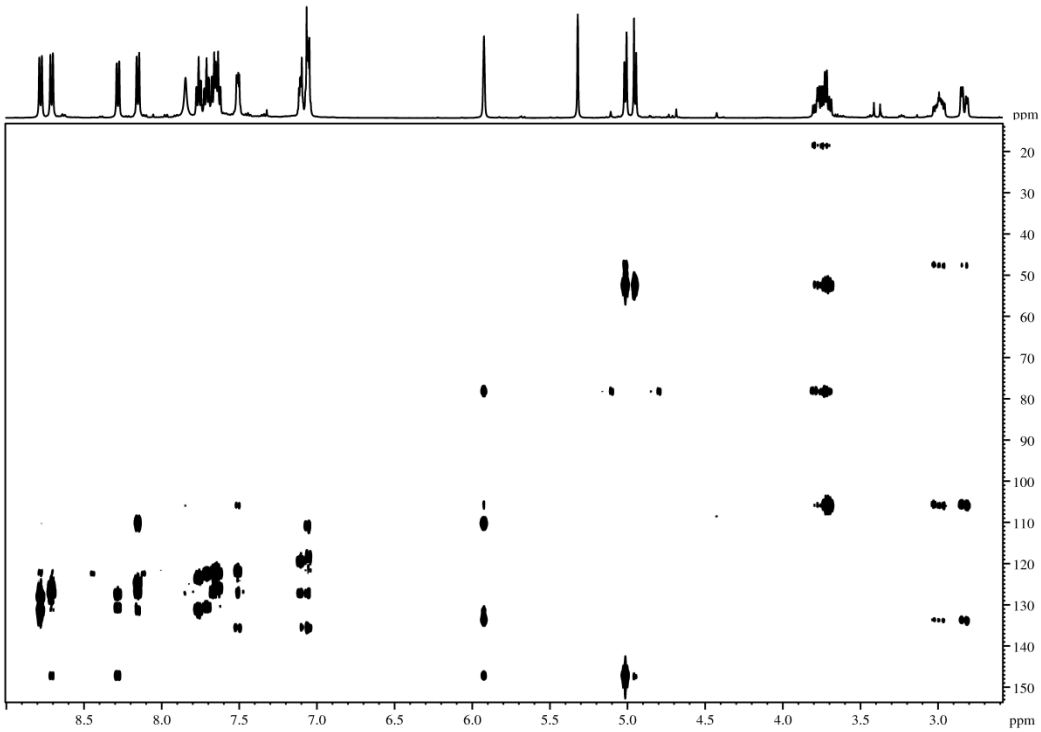


Figure S53. HMBC NMR spectrum of **10**

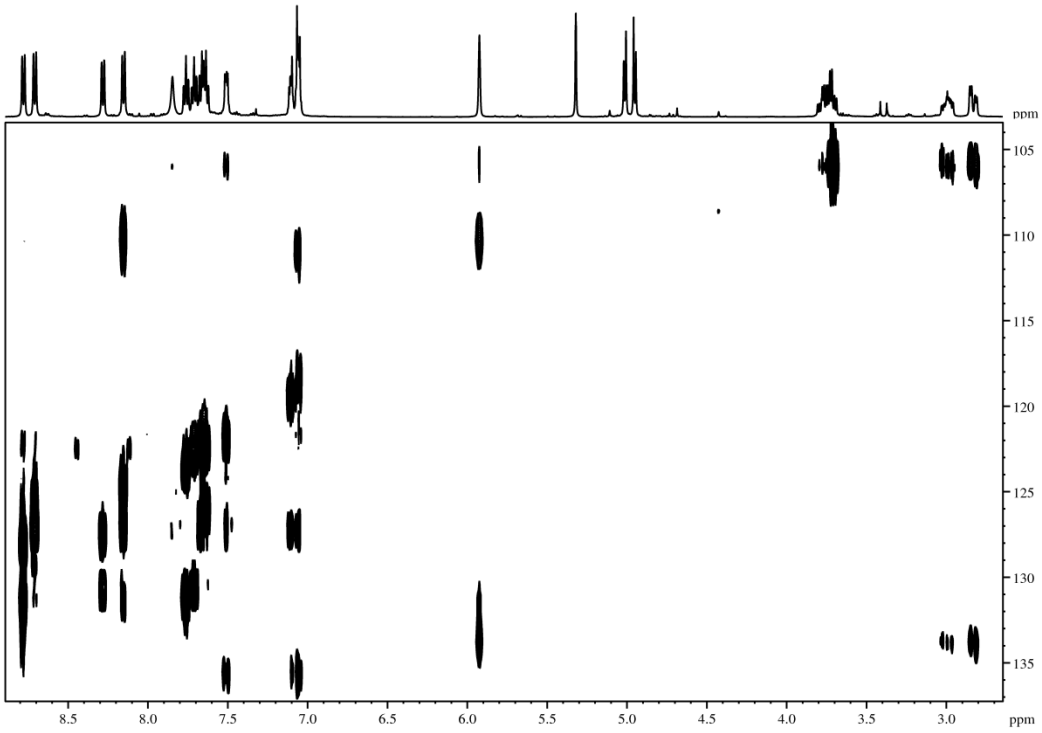


Figure S54. HMBC NMR spectrum of **10**, expansion

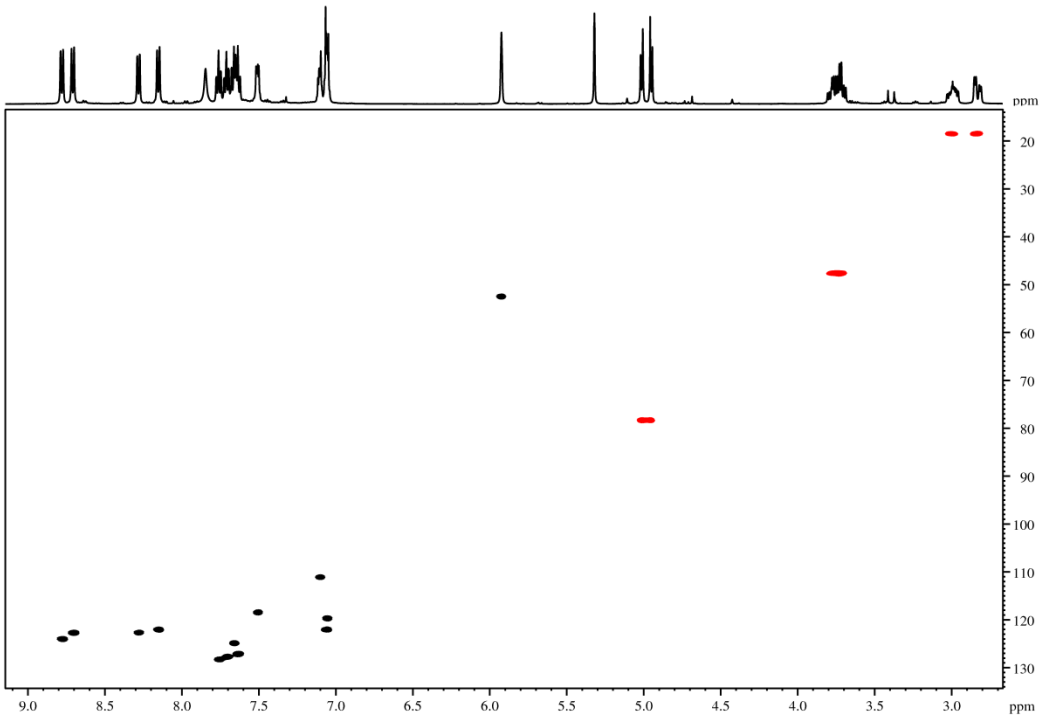


Figure S55. edited HSQC NMR spectrum of **10** (black: positive, red: negative signals)

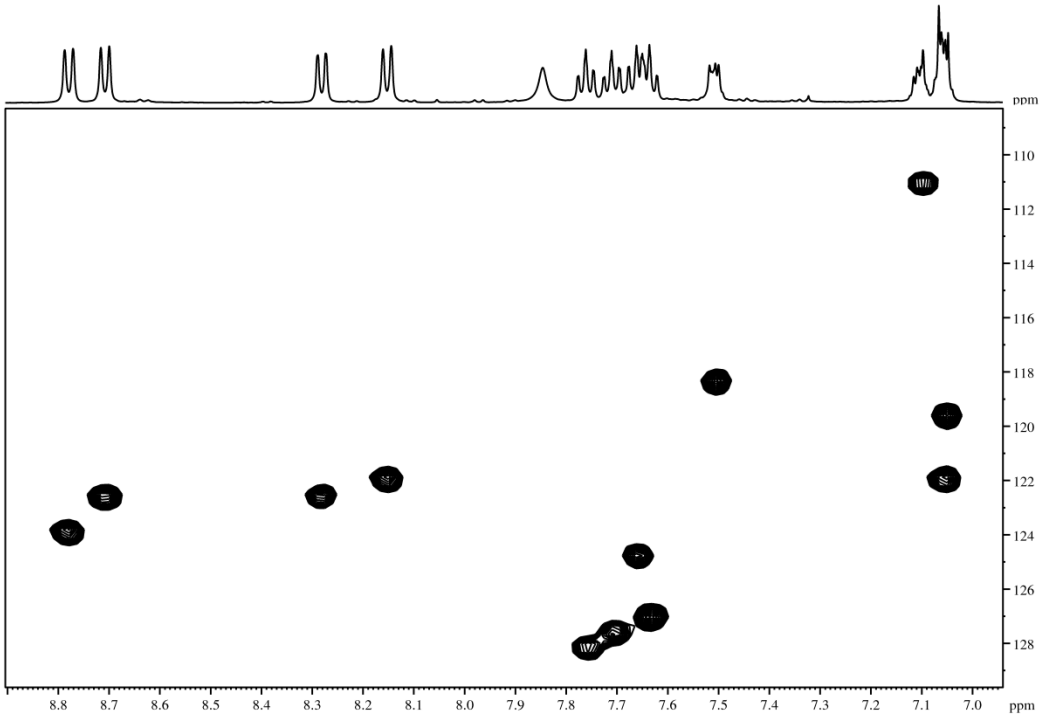
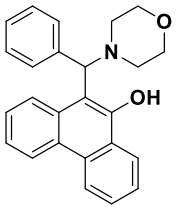


Figure S56. edited HSQC NMR spectrum of **10**, expansion (black: positive, red: negative signals)

10-[(Phenyl)-morpholin-4-yl-methyl]-9-phenanthrol (13)



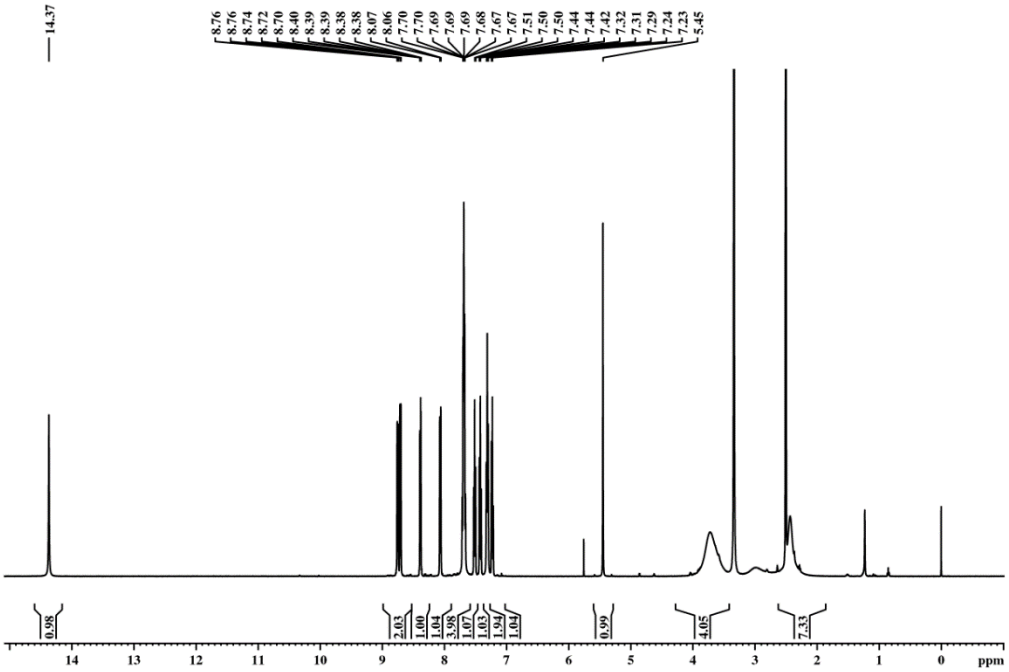


Figure S57. ^{1}H NMR spectrum of **13**

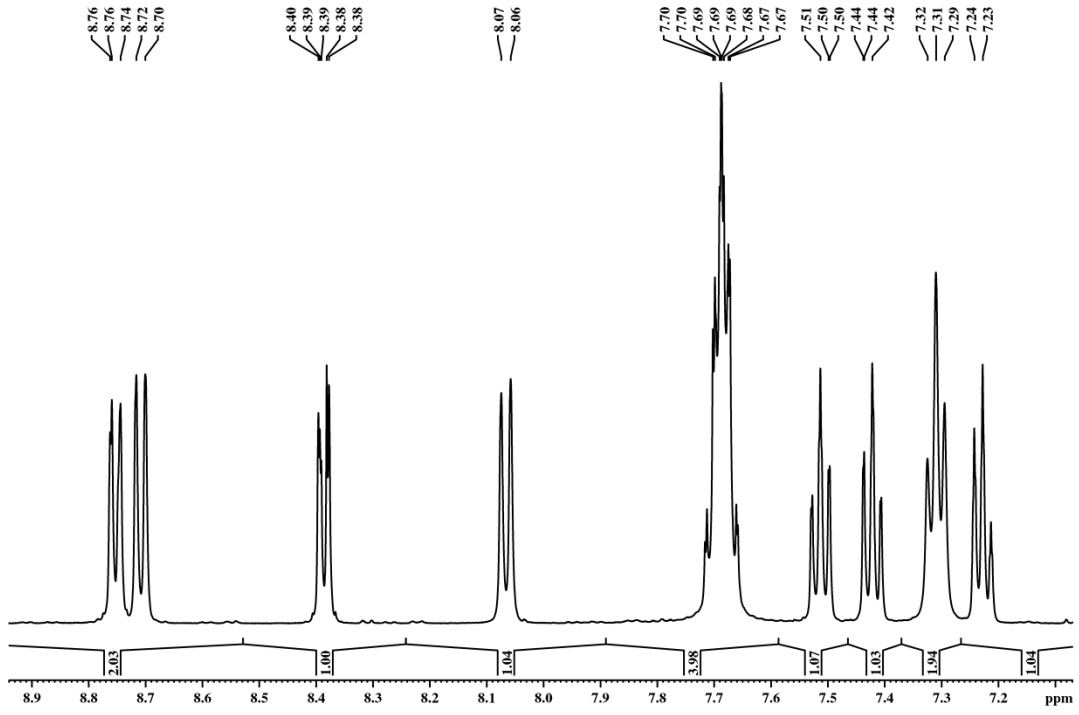


Figure S58. ^{1}H NMR spectrum of **13**, expansion

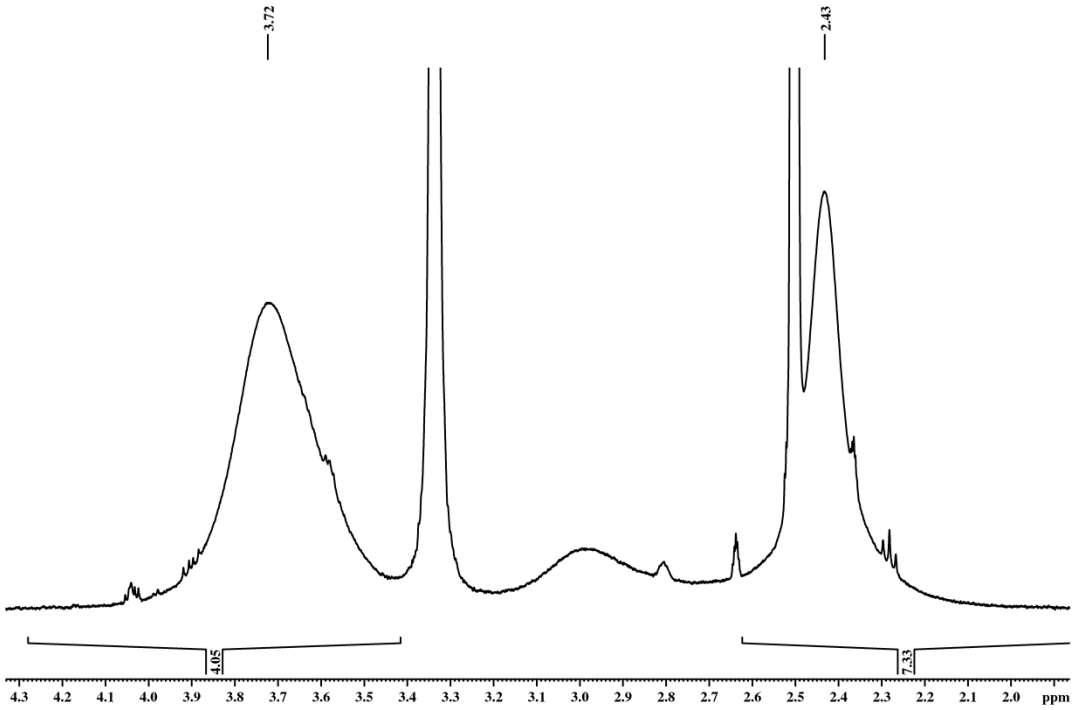


Figure S59. ^{1}H NMR spectrum of **13**, expansion

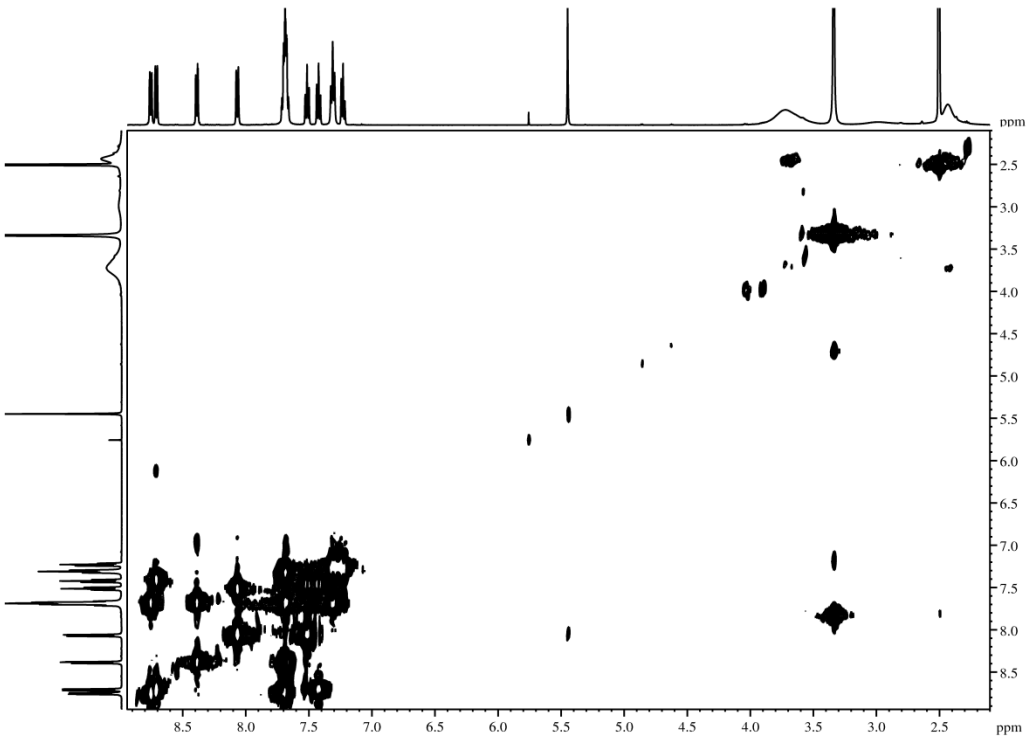


Figure S60. H,H-COSY NMR spectrum of **13**

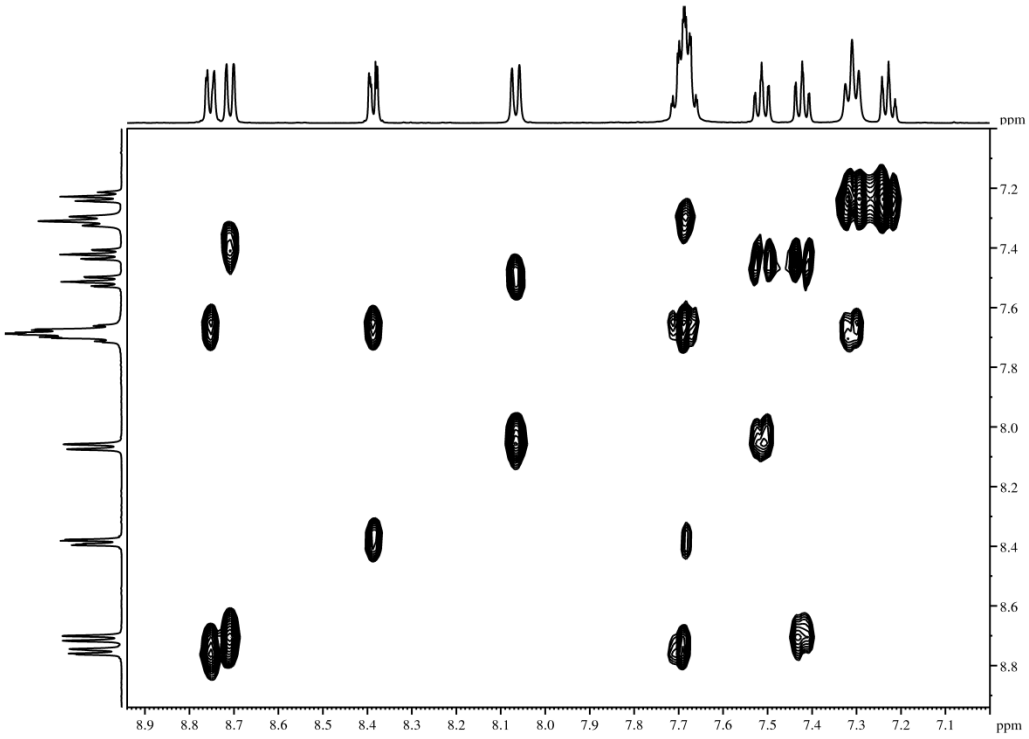


Figure S61. H,H-COSY NMR spectrum of **13**, expansion

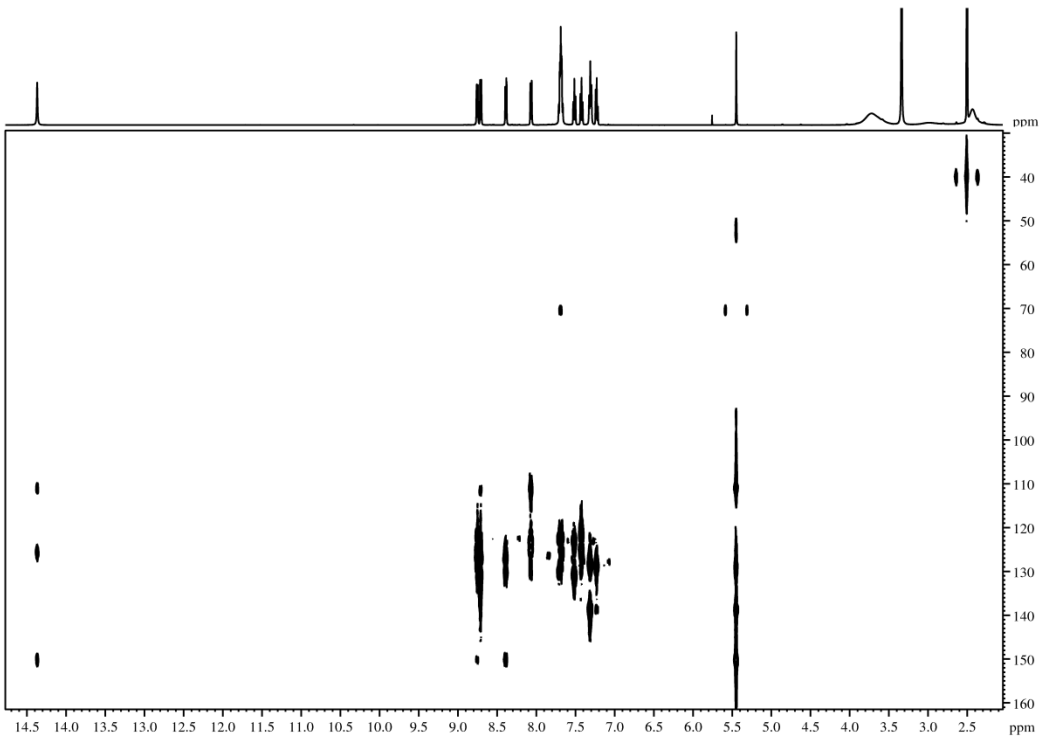


Figure S62. HMBC NMR spectrum of **13**

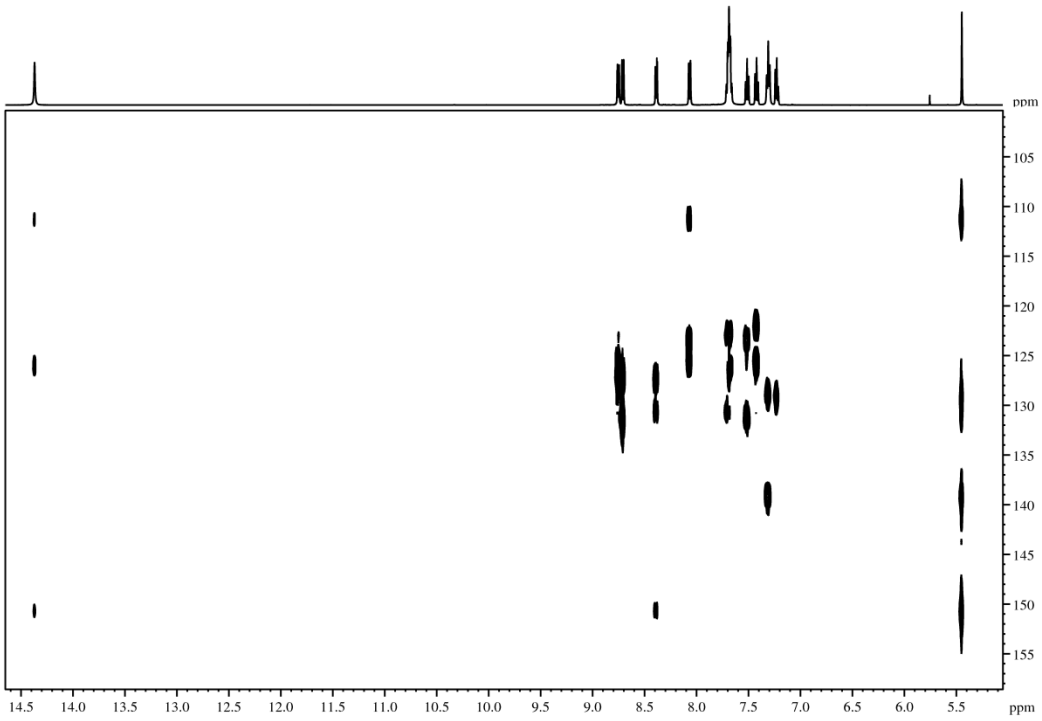


Figure S63. HMBC NMR spectrum of **13**, expansion

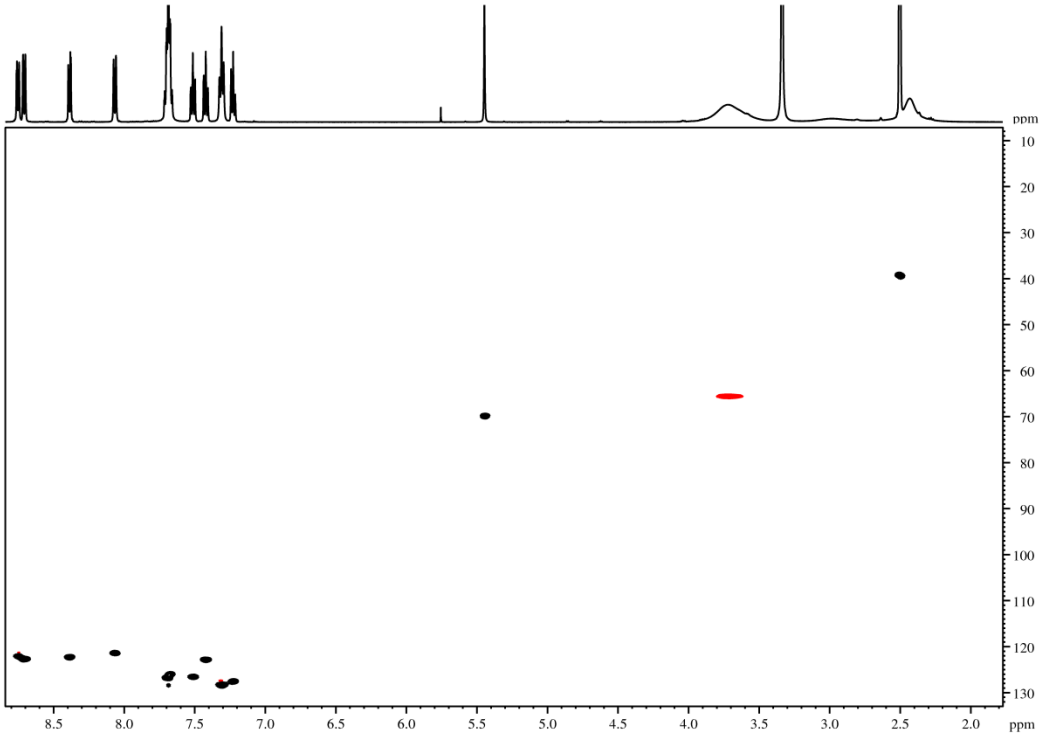


Figure S64. edited HSQC NMR spectrum of **13** (black: positive, red: negative signals)

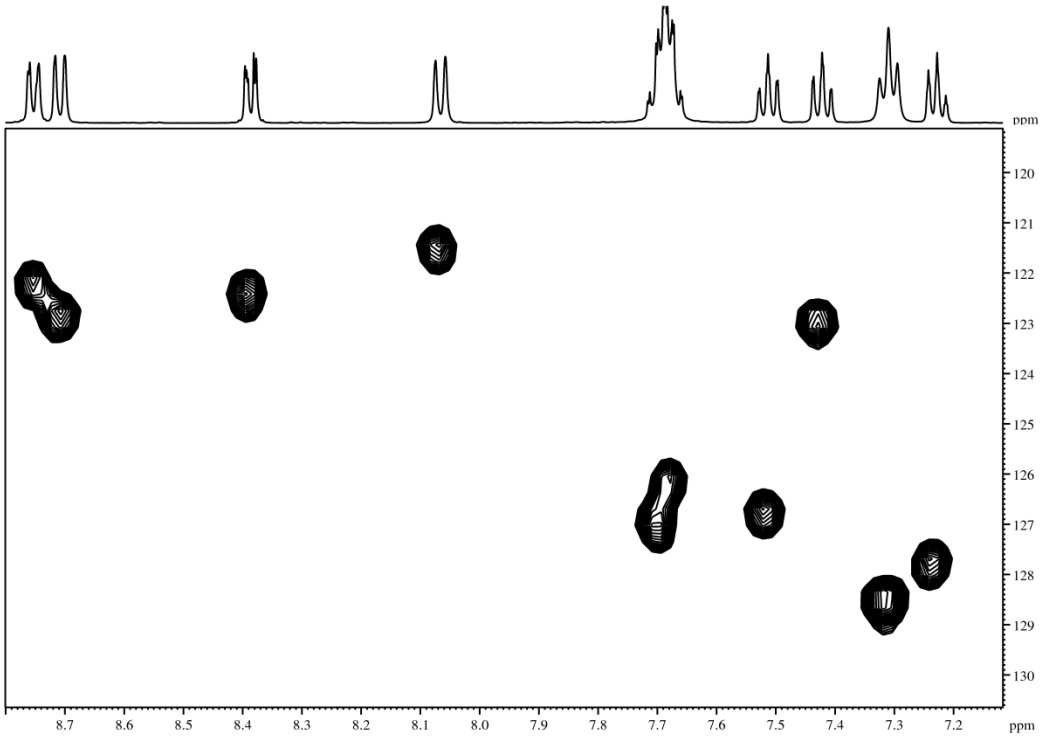
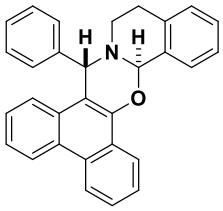


Figure S65. edited HSQC NMR spectrum of **13**, expansion (black: positive, red: negative signals)

9aR*,17S*-15-(Phenyl)-phenanthr[9,10-e]oxazino[2,3-a]isoquinoline (14)



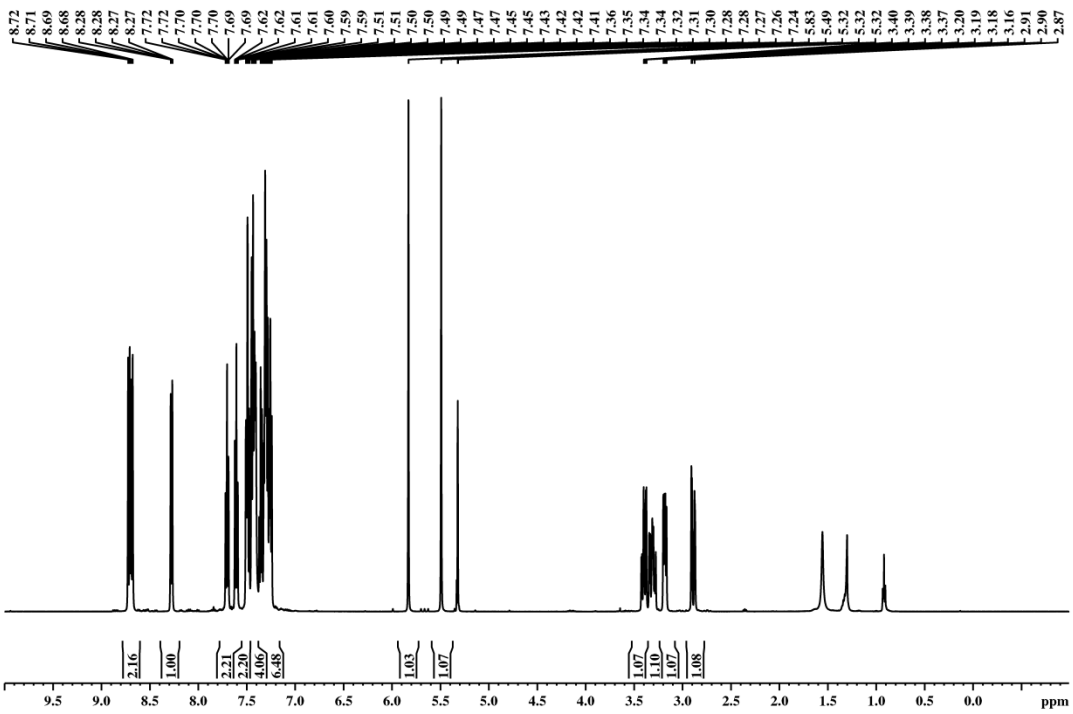


Figure S66. ^{1}H NMR spectrum of **14**

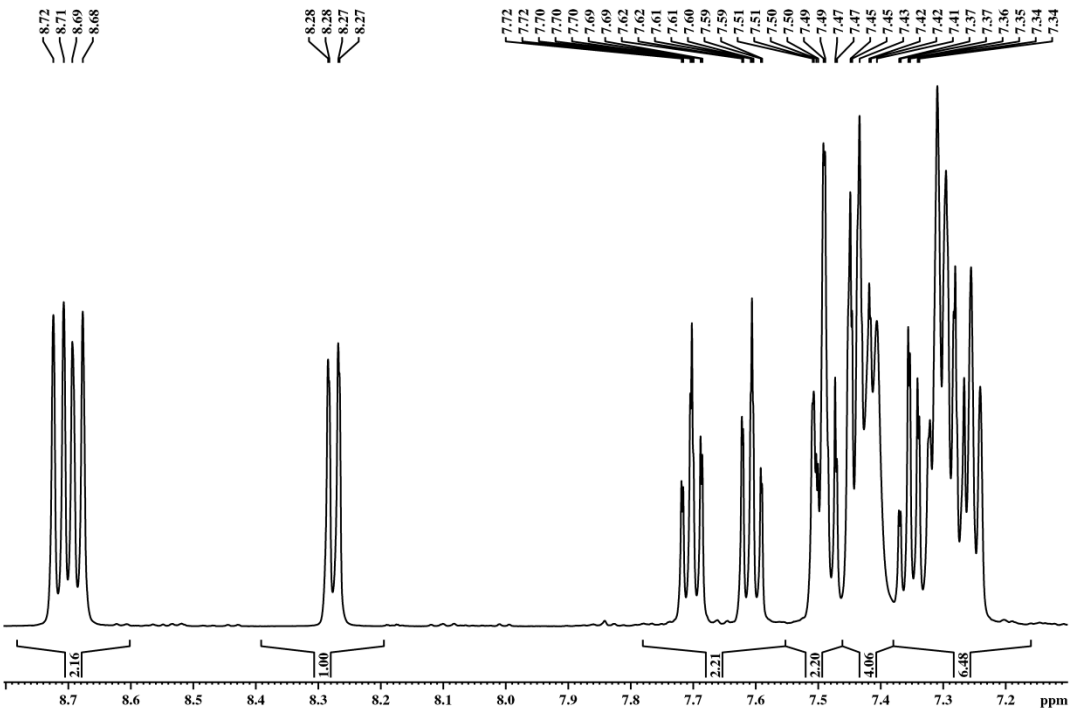


Figure S67. ^{1}H NMR spectrum of **14**, expansion

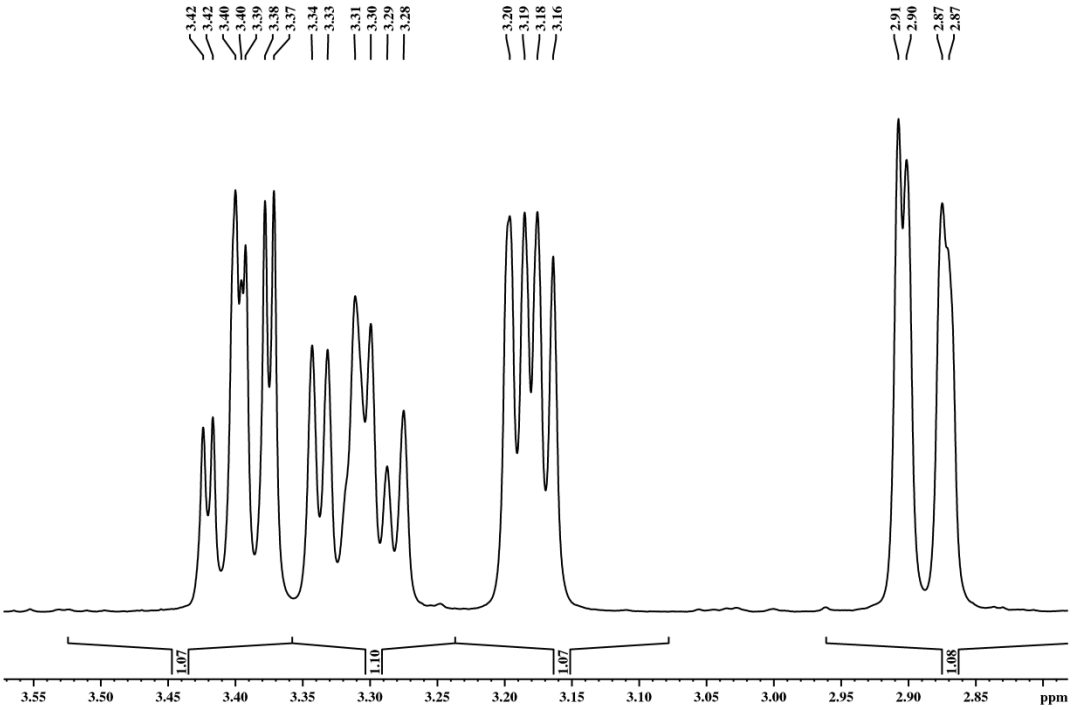


Figure S68. ^{1}H NMR spectrum of **14**, expansion

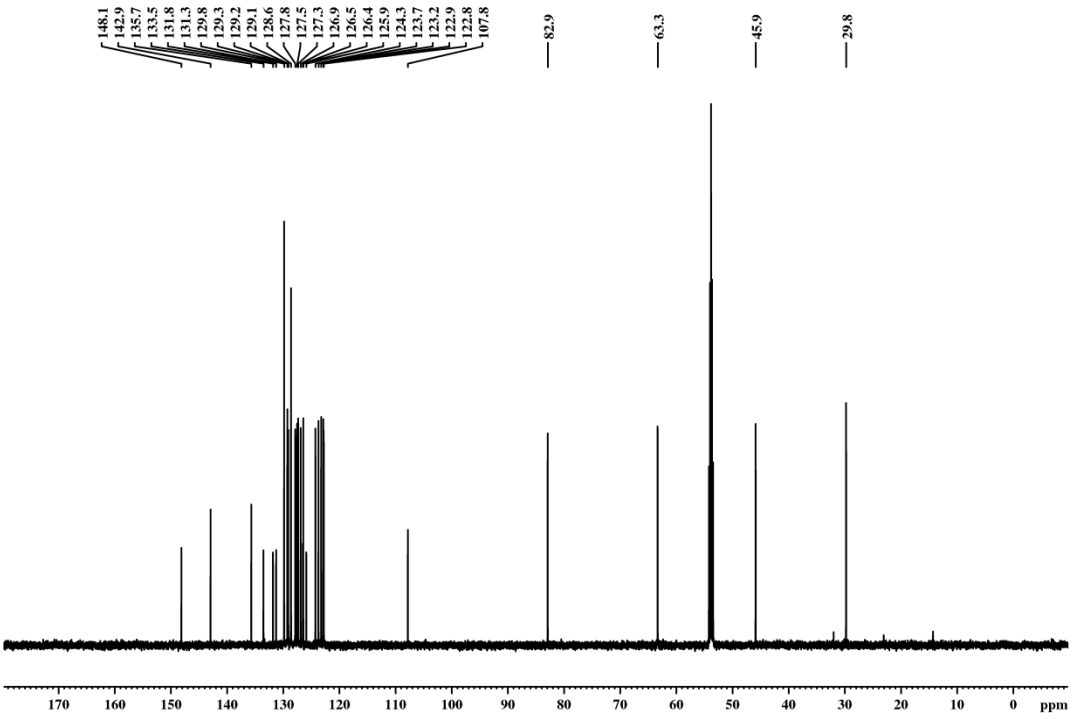


Figure S69. ^{13}C NMR spectrum of **14**

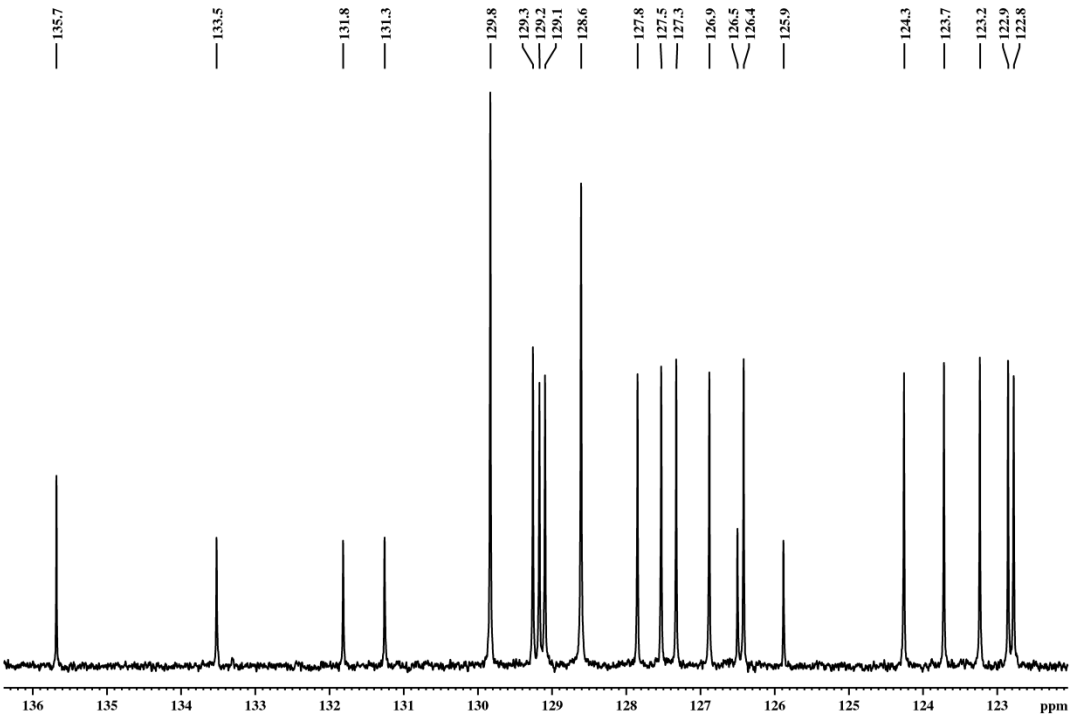


Figure S70. ^{13}C NMR spectrum of **14**, expansion

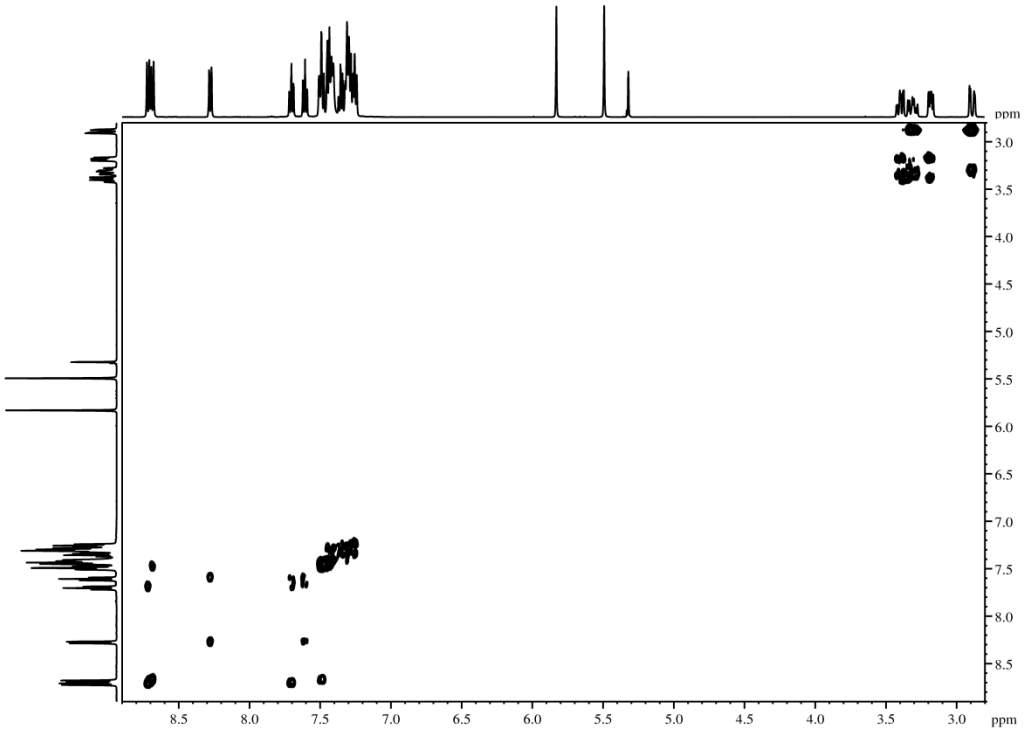


Figure S71. H,H-COSY NMR spectrum of **14**

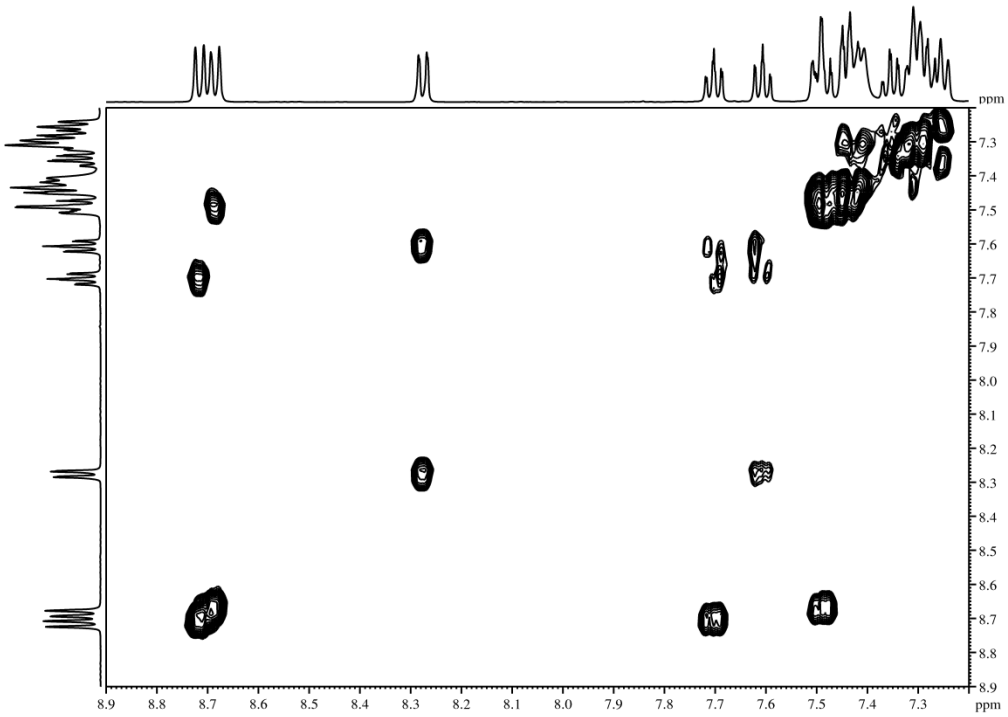


Figure S72. H,H-COSY NMR spectrum of **14**, expansion

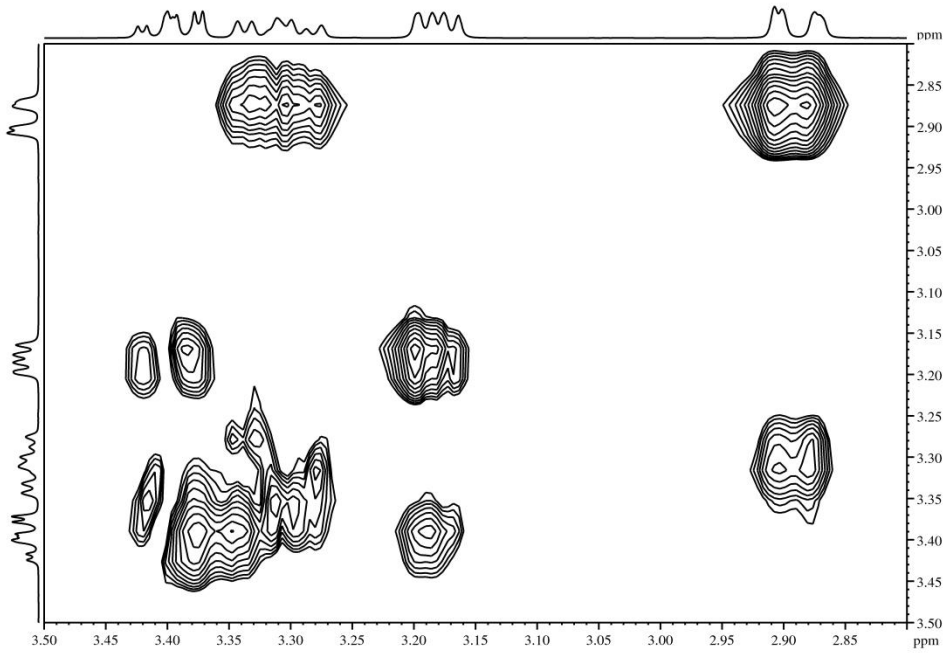


Figure S73. H,H-COSY NMR spectrum of **14**, expansion

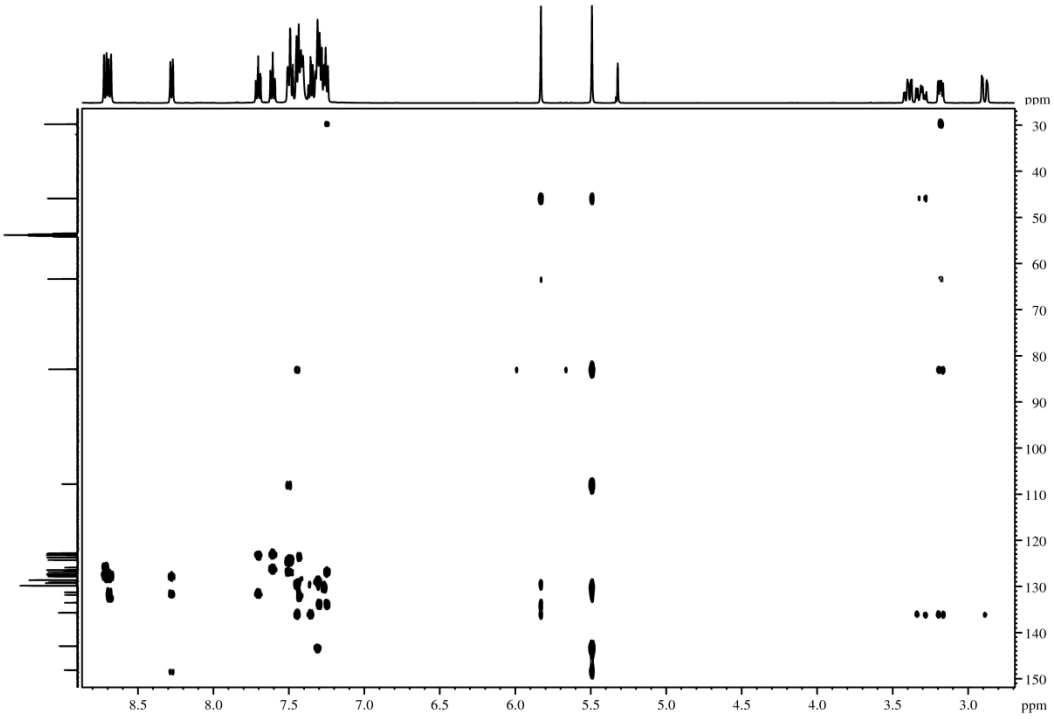


Figure S74. HMBC NMR spectrum of **14**

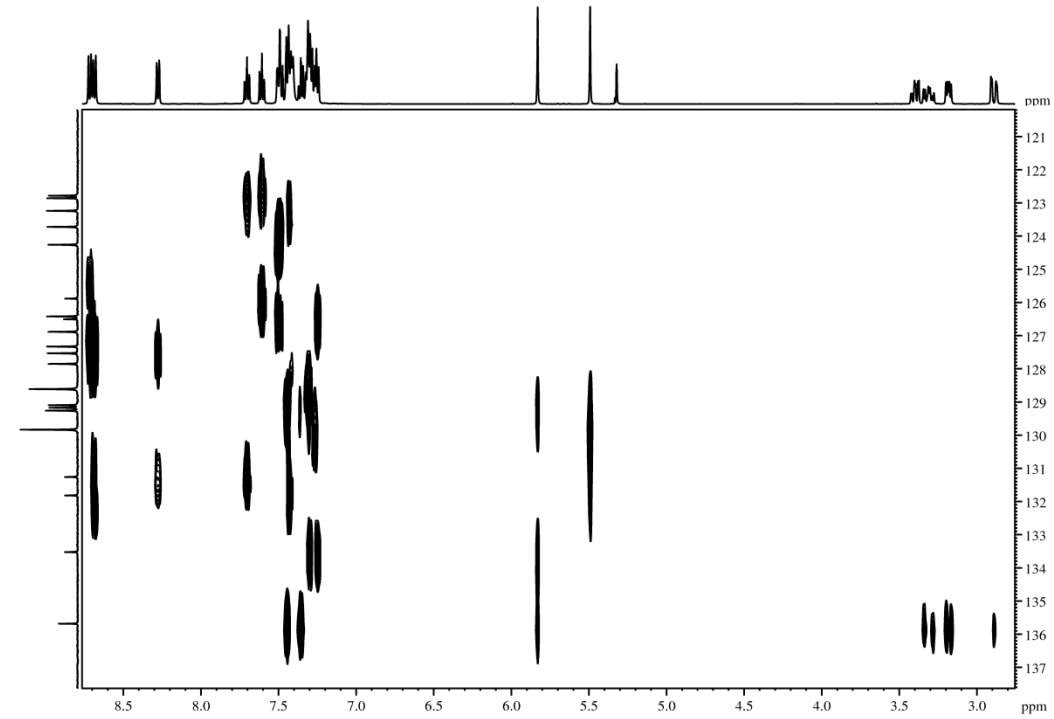


Figure S75. HMBC NMR spectrum of **14**, expansion

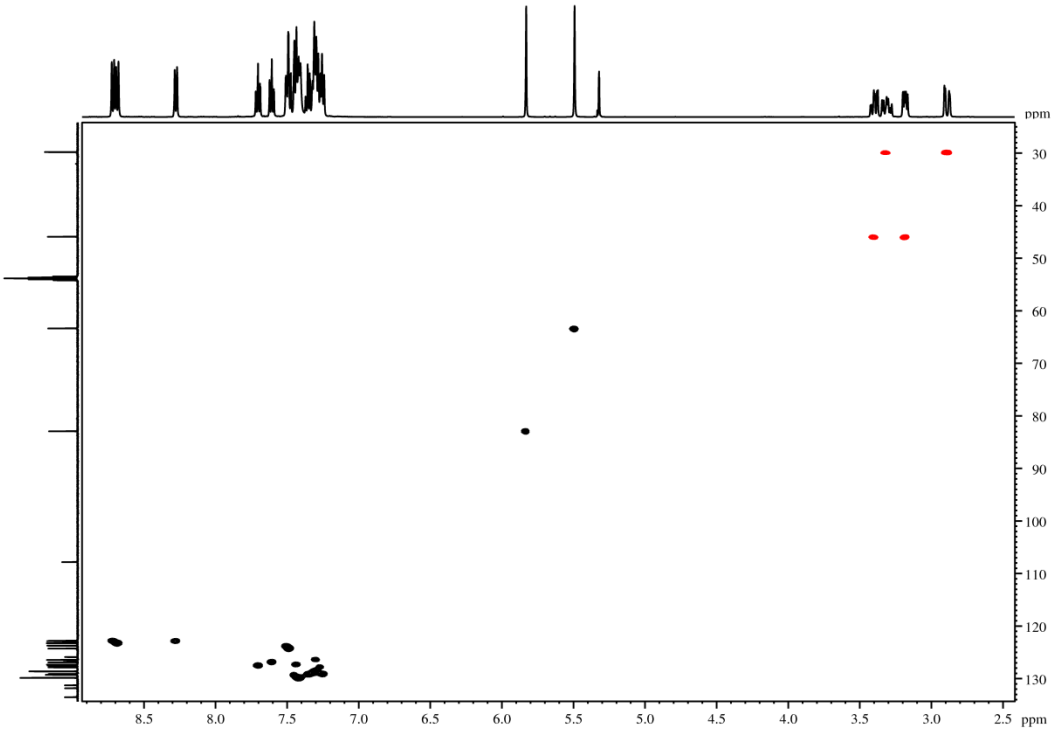


Figure S76. edited HSQC NMR spectrum of **14** (black: positive, red: negative signals)

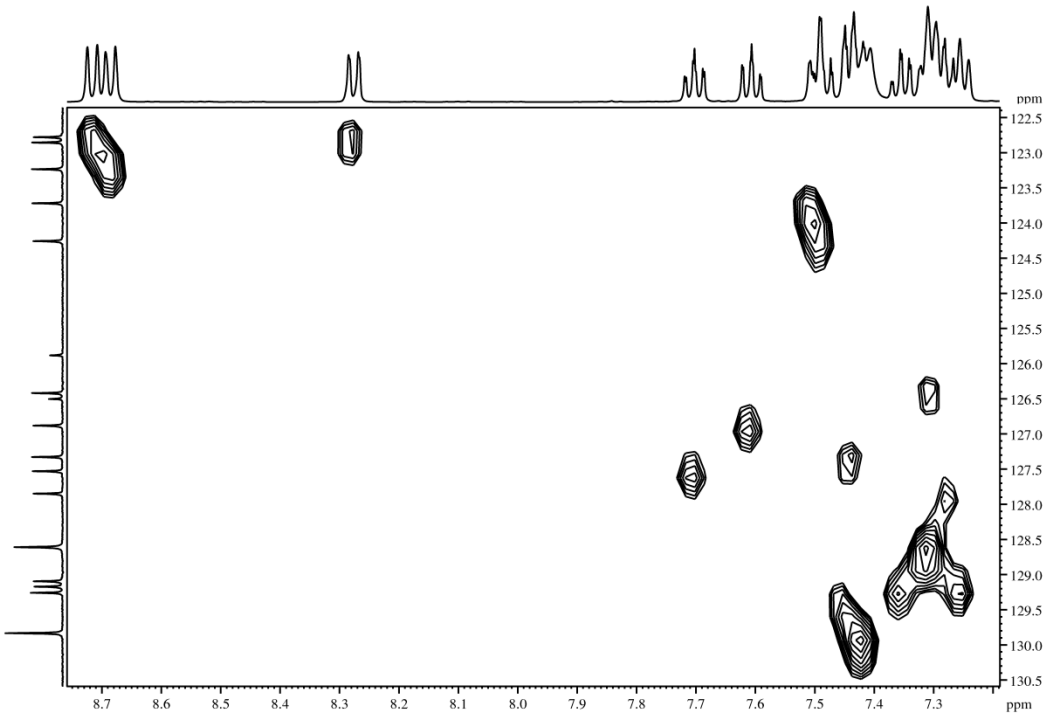


Figure S77. edited HSQC NMR spectrum of **14**, expansion (black: positive, red: negative signals)

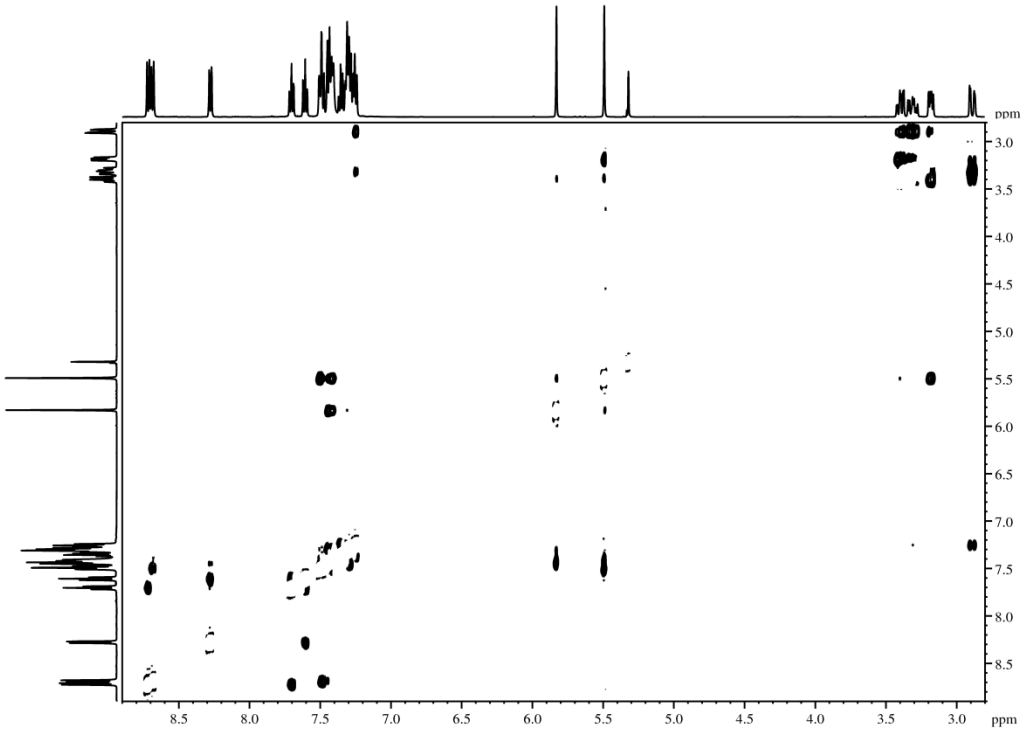
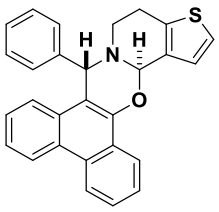


Figure S78. Phase-sensitive NOESY NMR spectrum of **14** (only positive signals, mixing time 800 ms)

9aR*,16S*-16-(Phenyl)-phenanthr[9,10-e]oxazino[2,3-a]thieno[3,2-c]pyridine (15)



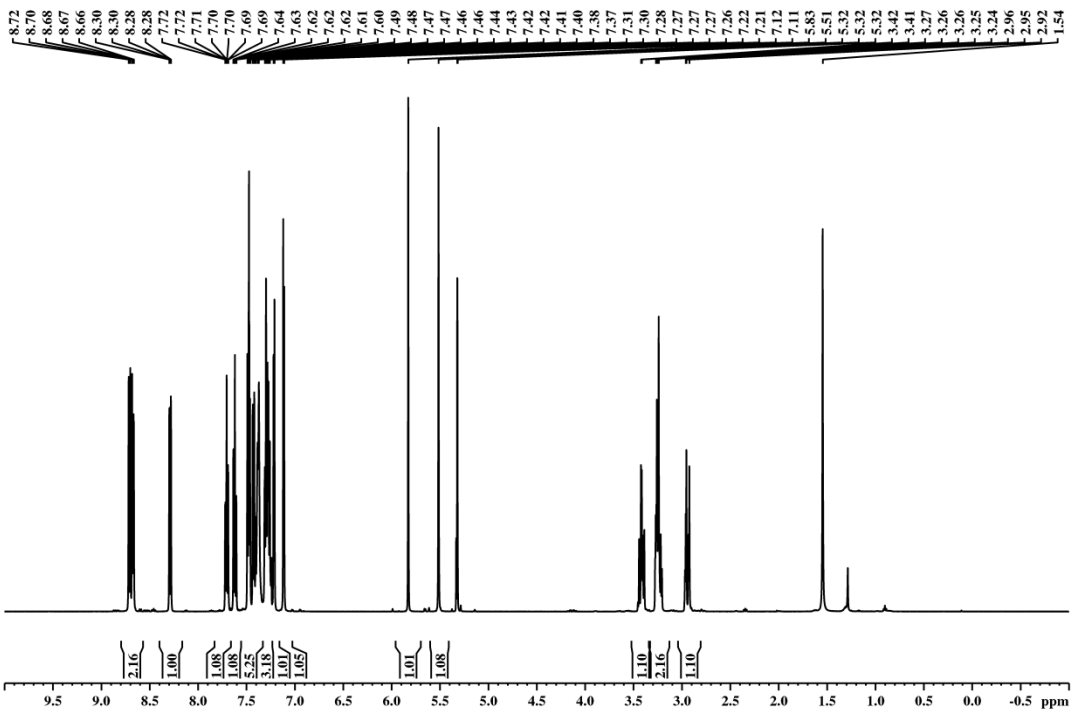


Figure S79. ^{1}H NMR spectrum of **15**

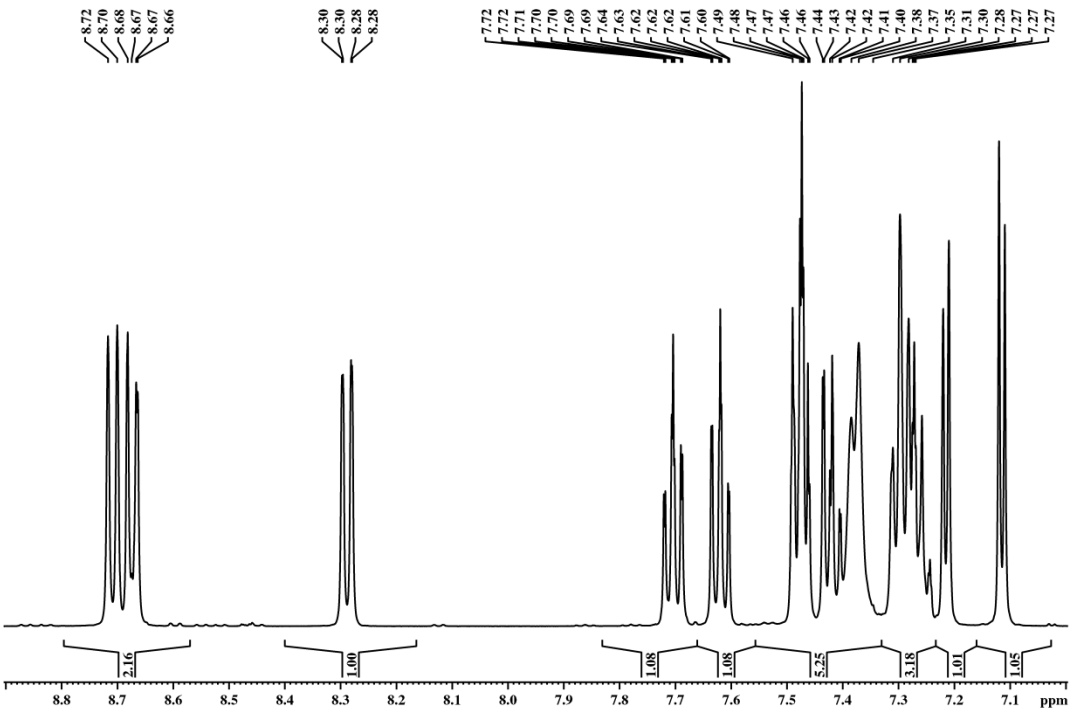


Figure S80. ^{1}H NMR spectrum of **15**, expansion

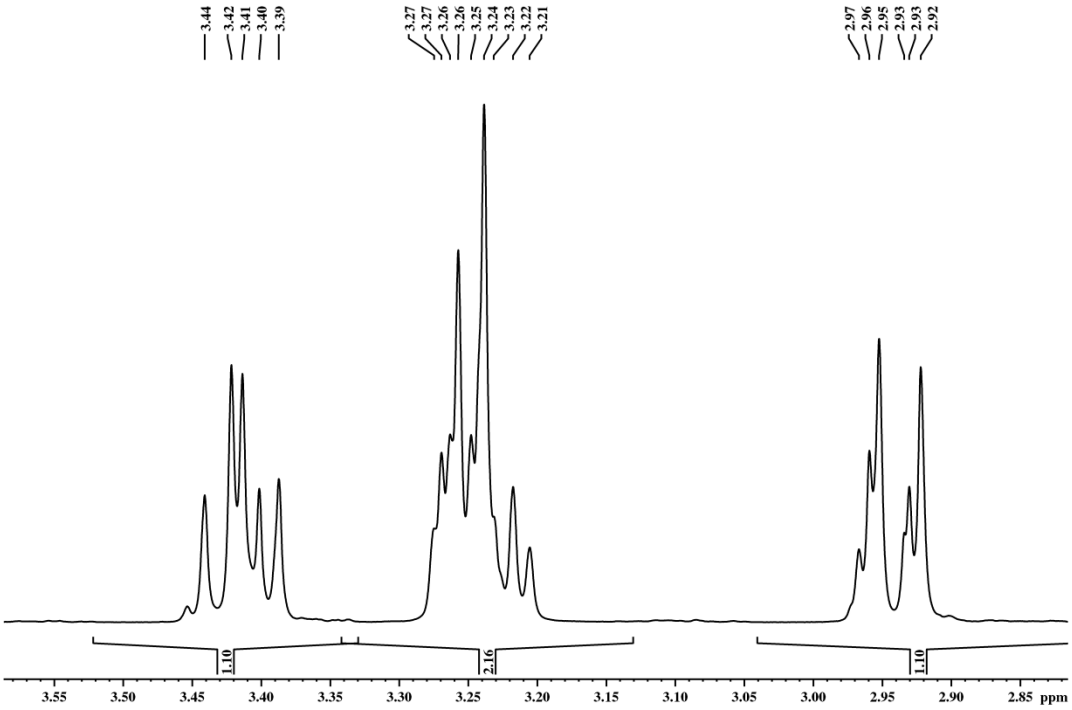


Figure S81. ^{1}H NMR spectrum of **15**, expansion

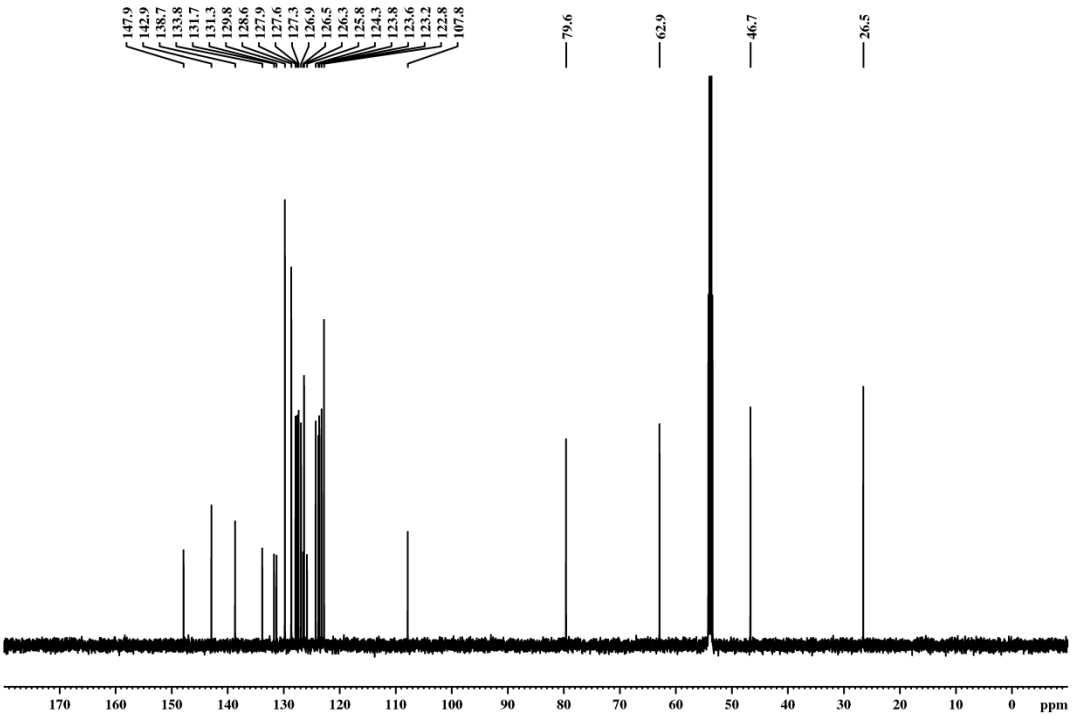


Figure S82. ^{13}C NMR spectrum of **15**

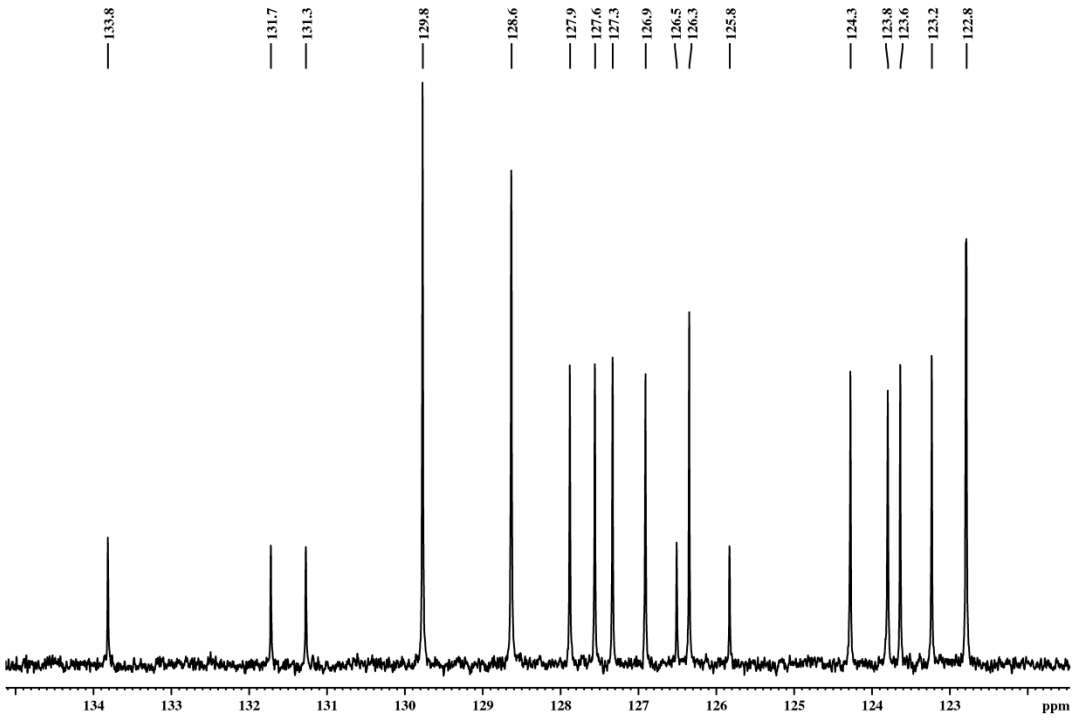


Figure S83. ^{13}C NMR spectrum of **15**, expansion

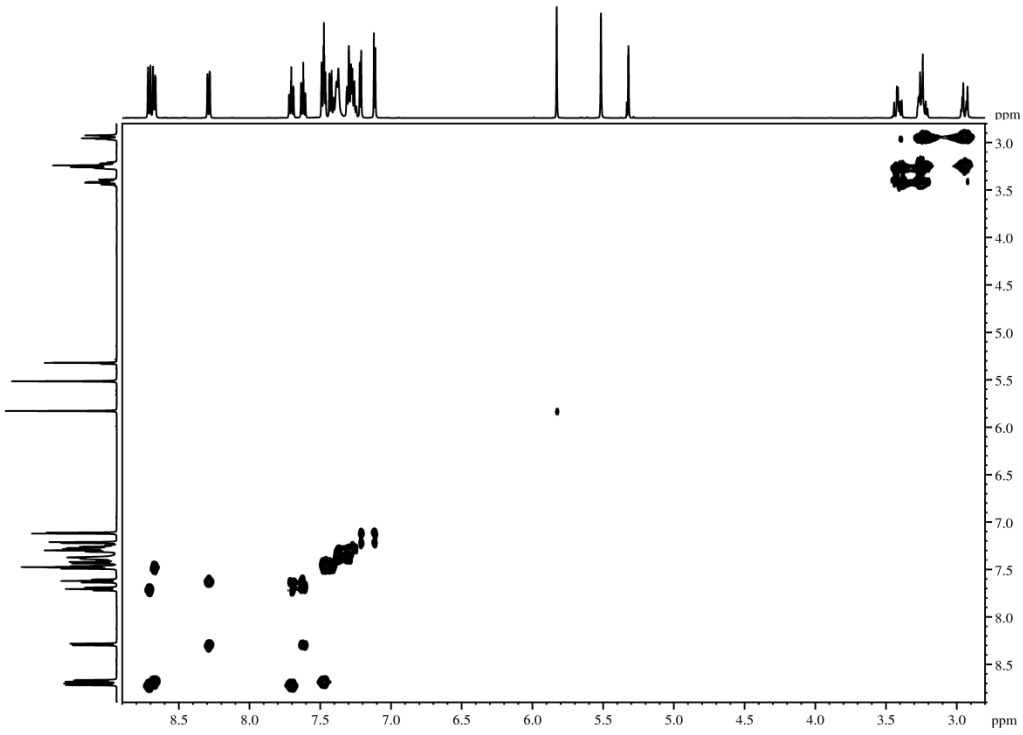


Figure S84. H,H-COSY NMR spectrum of **15**

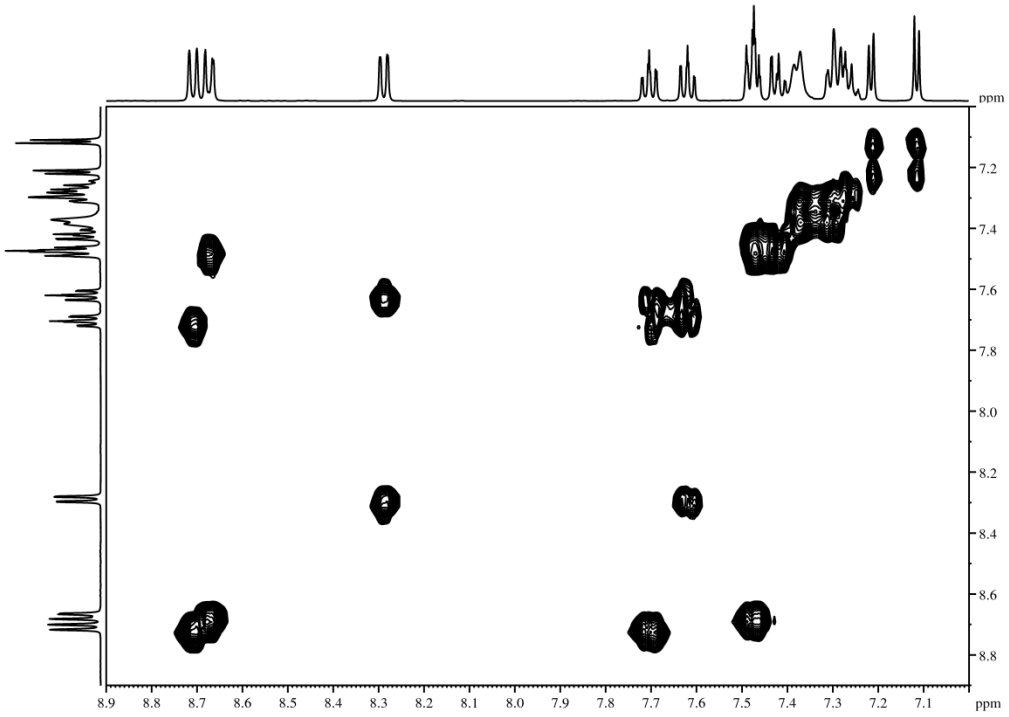


Figure S85. H,H-COSY NMR spectrum of **15**, expansion

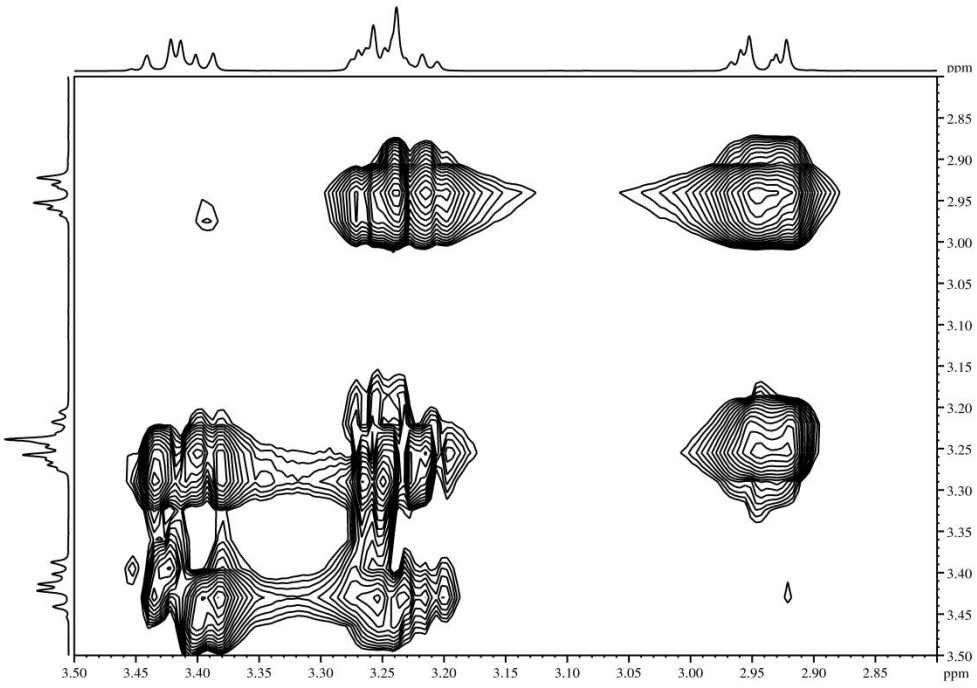


Figure S86. H,H-COSY NMR spectrum of **15**, expansion

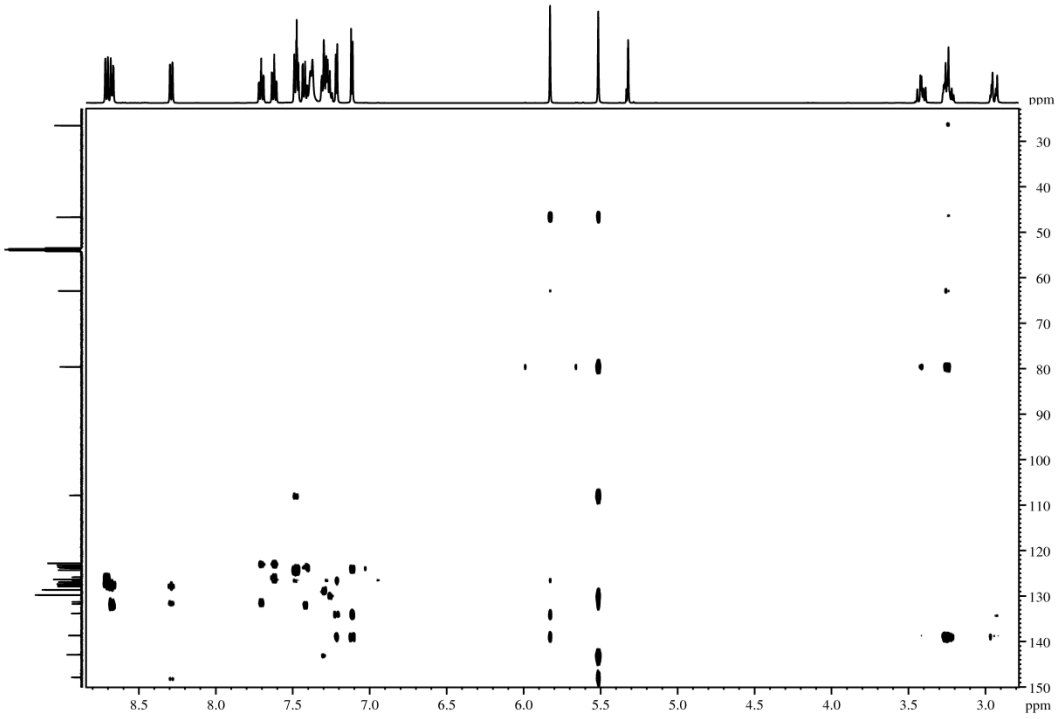


Figure S87. HMBC NMR spectrum of **15**

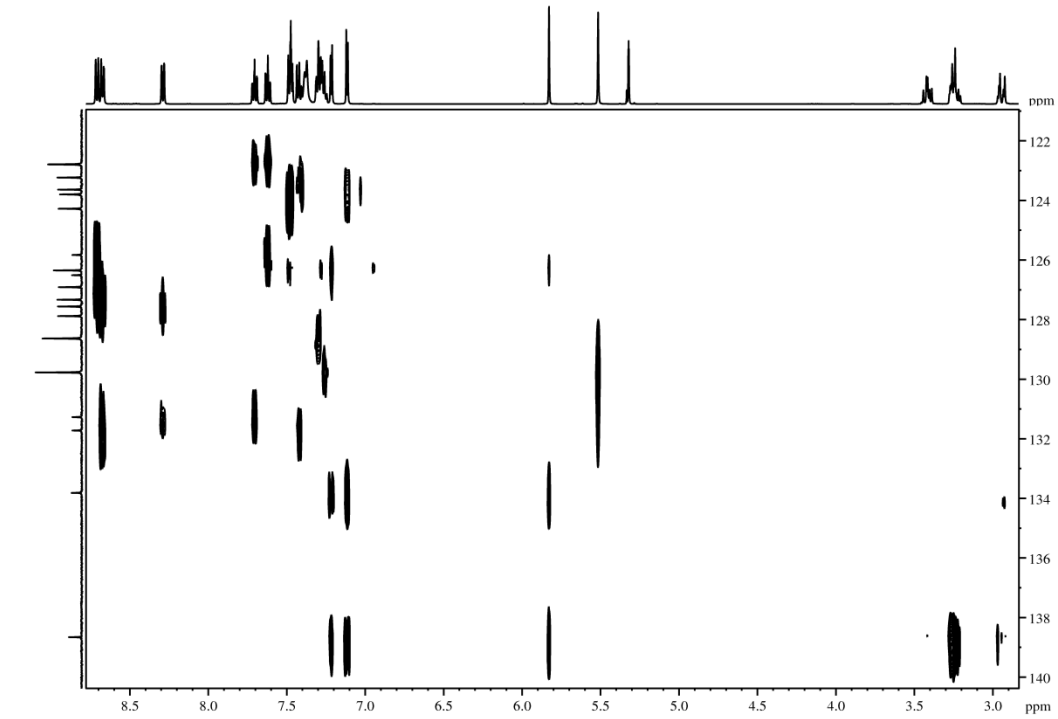


Figure S88. HMBC NMR spectrum of **15**, expansion

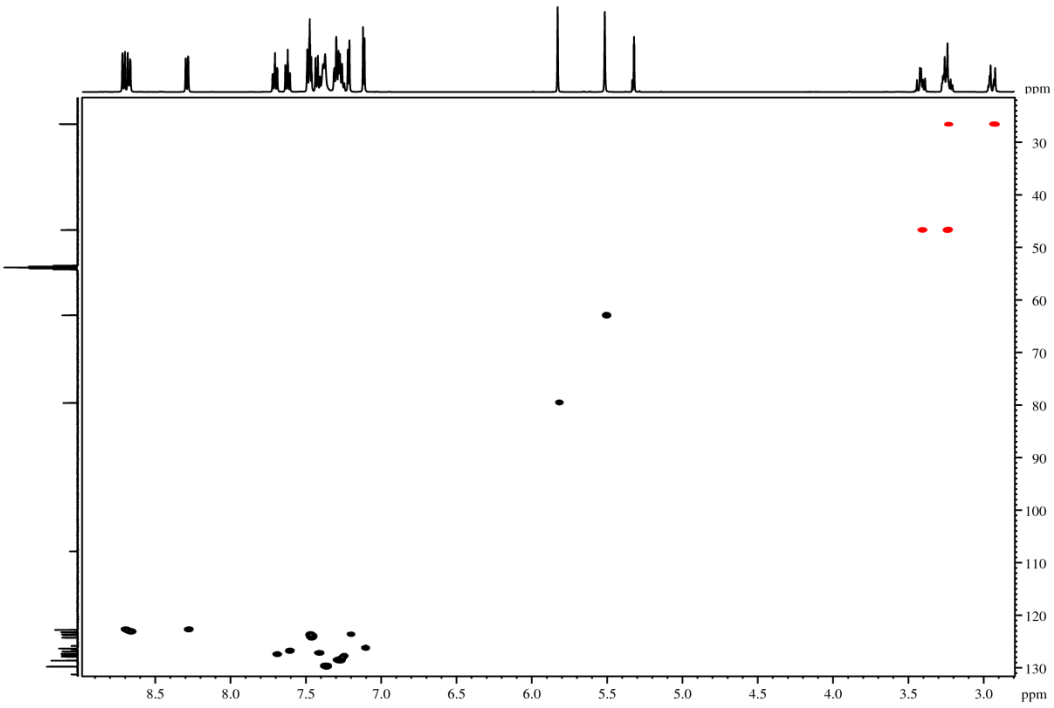


Figure S89. edited HSQC NMR spectrum of **15** (black: positive, red: negative signals)

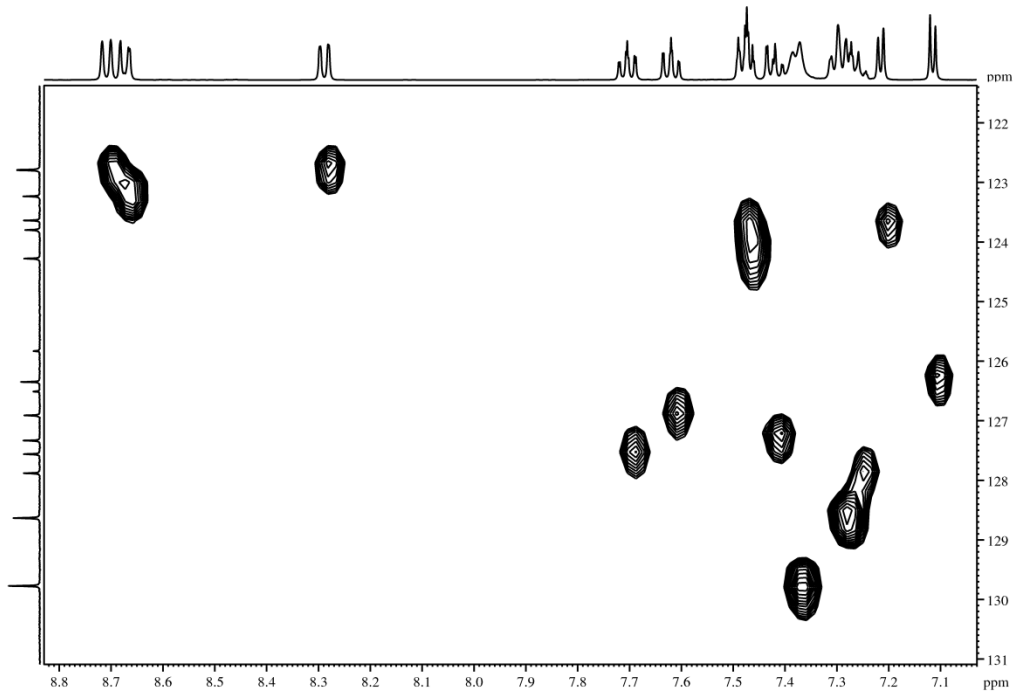


Figure S90. edited HSQC NMR spectrum of **15**, expansion (black: positive, red: negative signals)

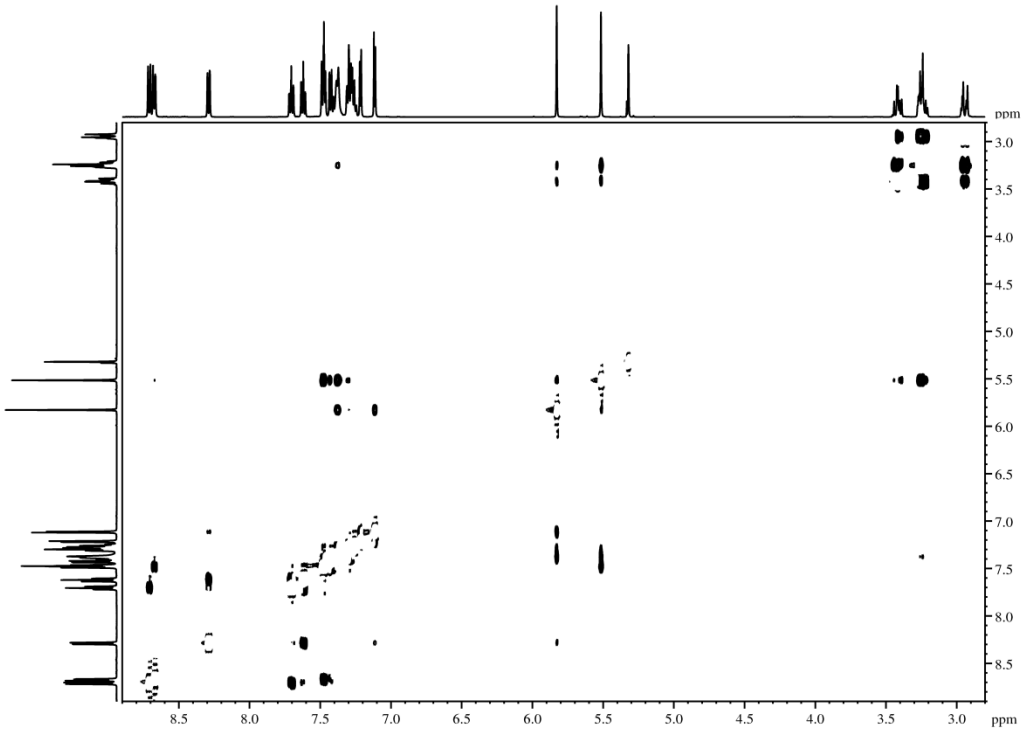
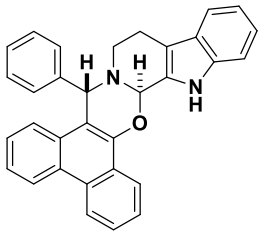


Figure S91. Phase-sensitive NOESY NMR spectrum of **15** (only positive signals, mixing time 800 ms)

9aR*,18S*-19-(Phenyl)-phenanthr[9,10-e]oxazino[2,3-a]-β-carboline (16).



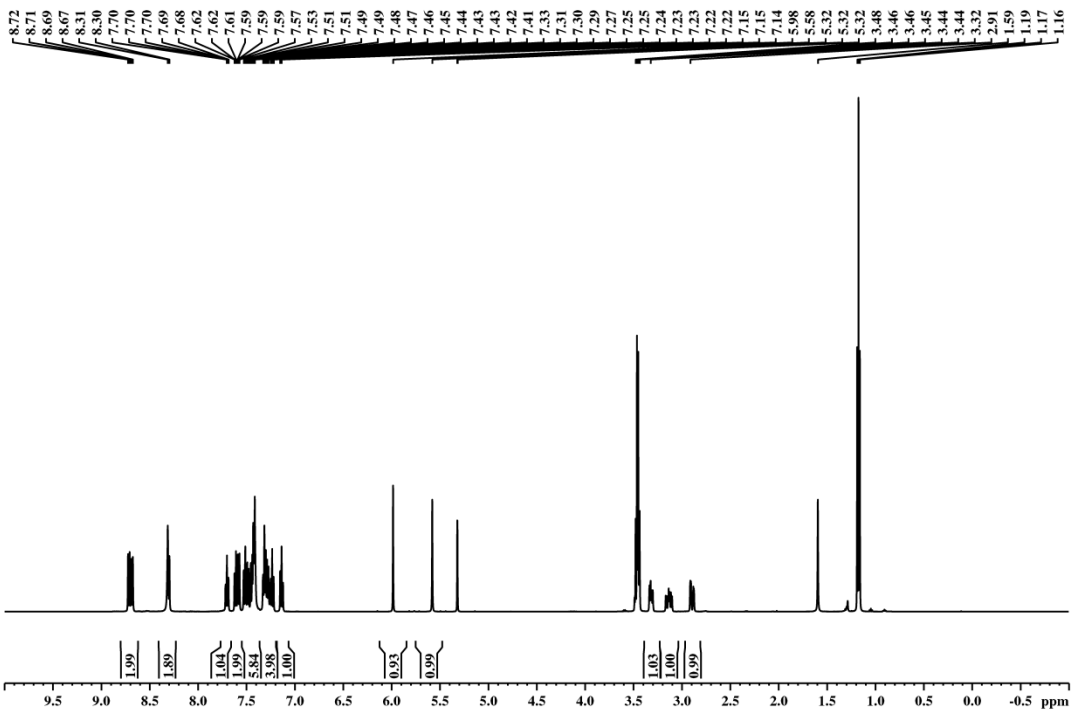


Figure S92. ^{1}H NMR spectrum of **16**

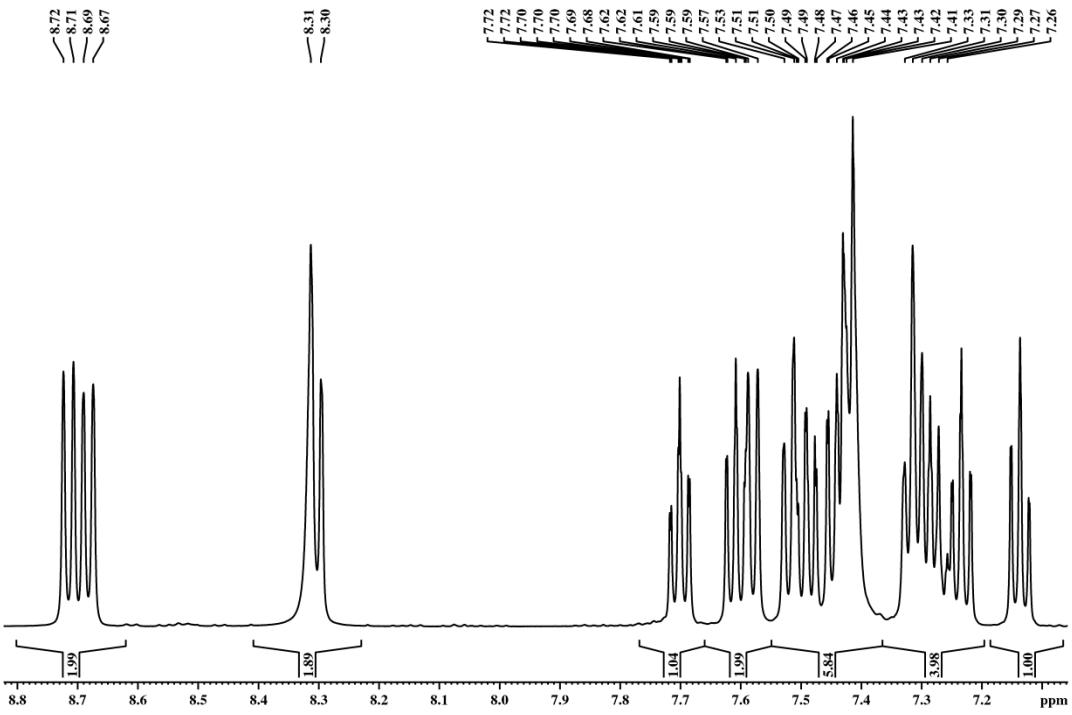


Figure S93. ^{1}H NMR spectrum of **16**, expansion

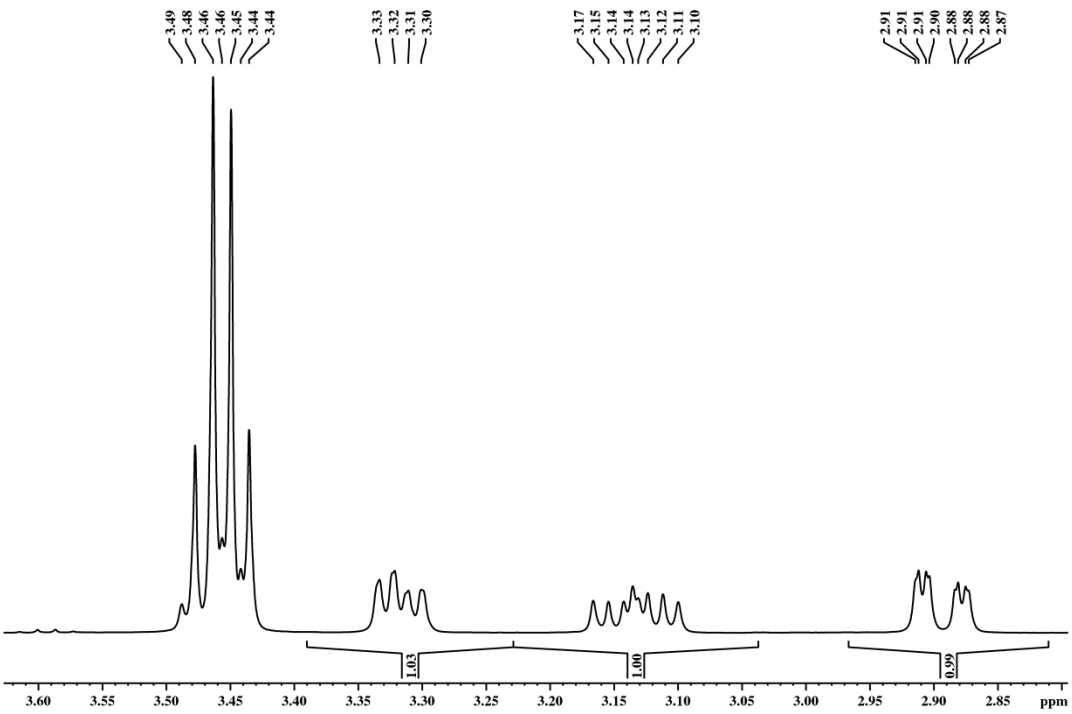


Figure S94. ^{1}H NMR spectrum of **16**, expansion

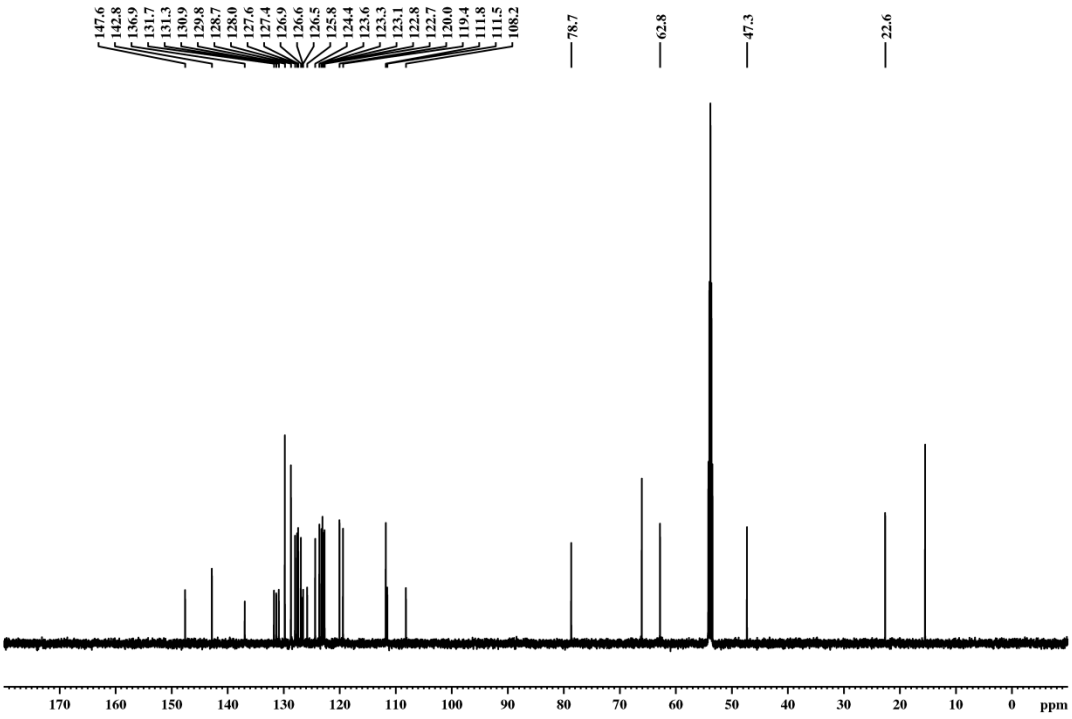


Figure S95. ^{13}C NMR spectrum of **16**

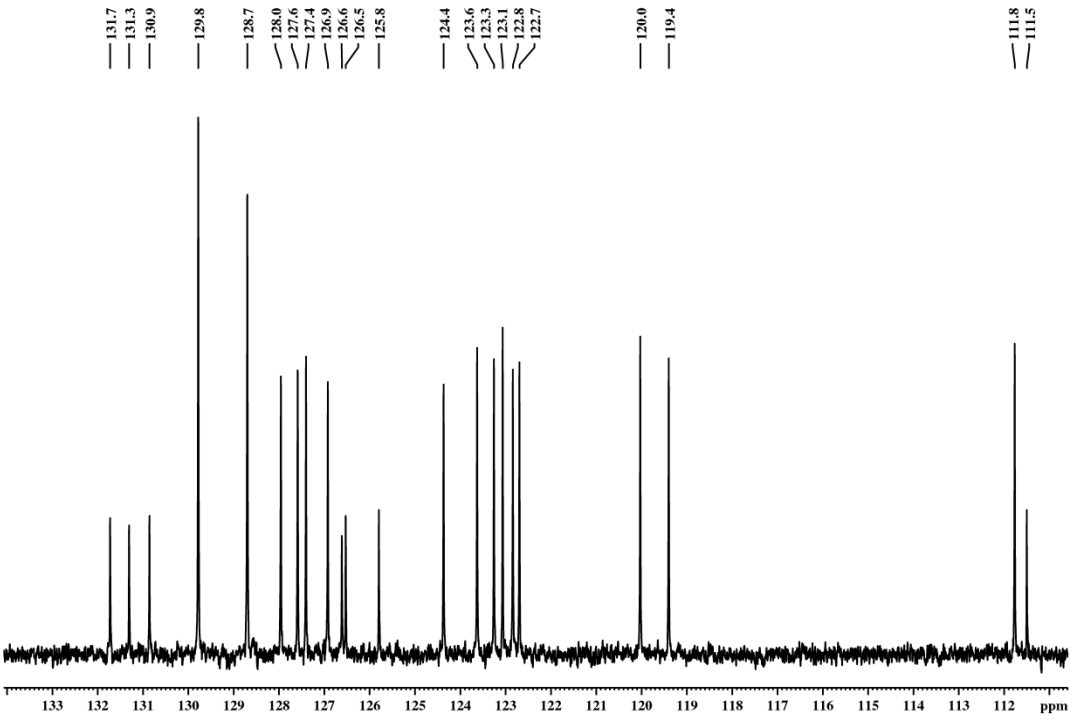


Figure S96. ^{13}C NMR spectrum of **16**, expansion

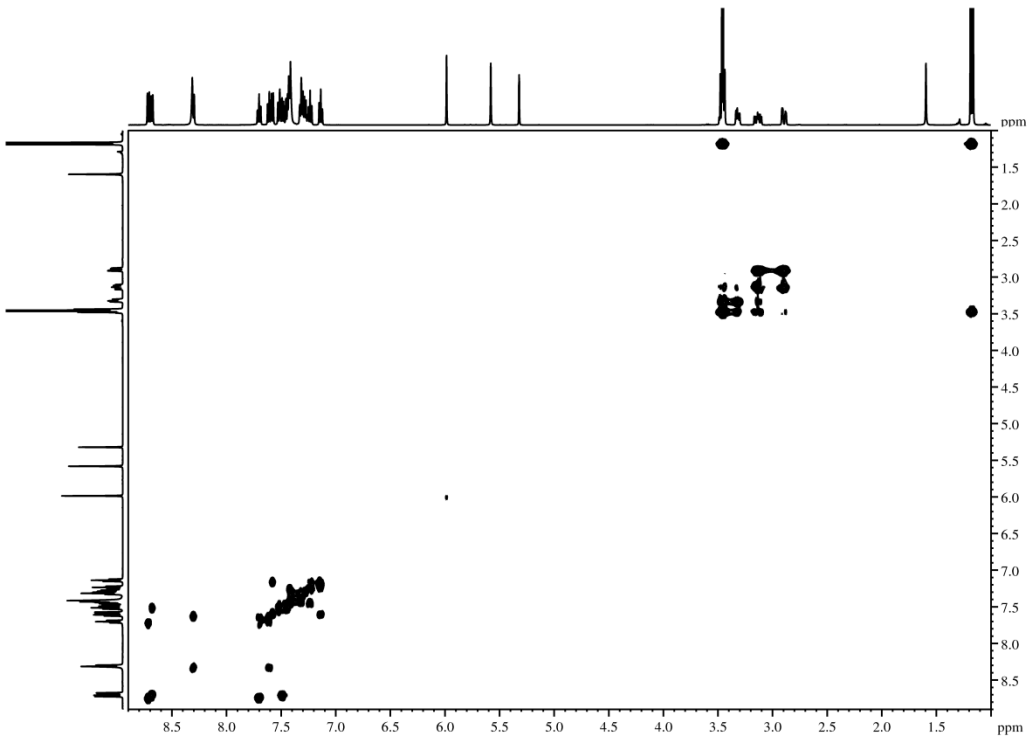


Figure 97. H,H-COSY NMR spectrum of **16**

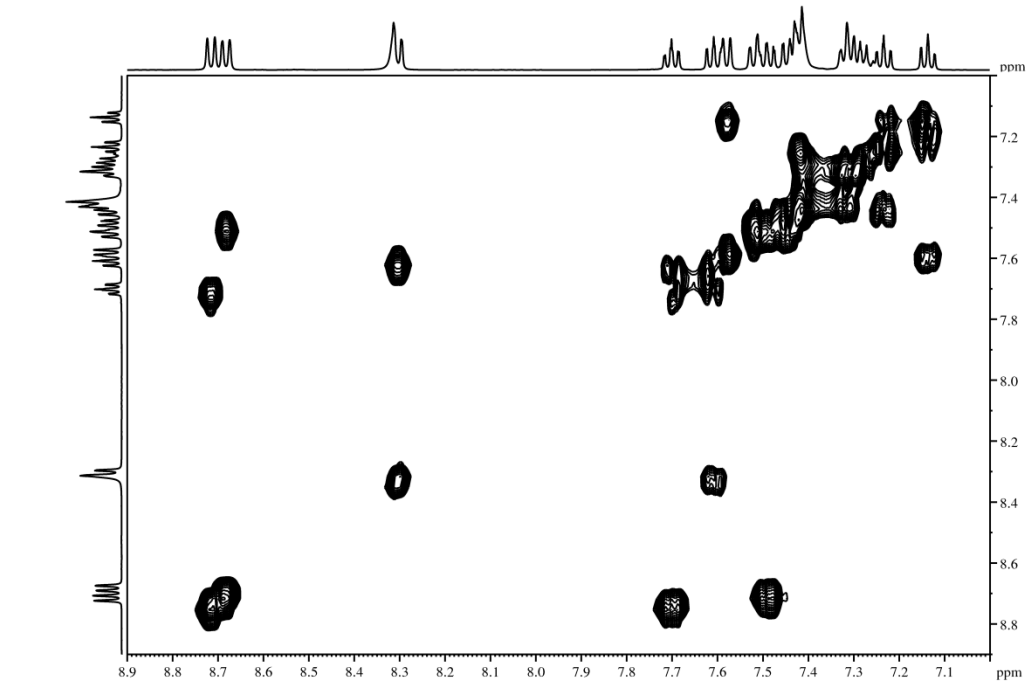


Figure S98. H,H-COSY NMR spectrum of **16**, expansion

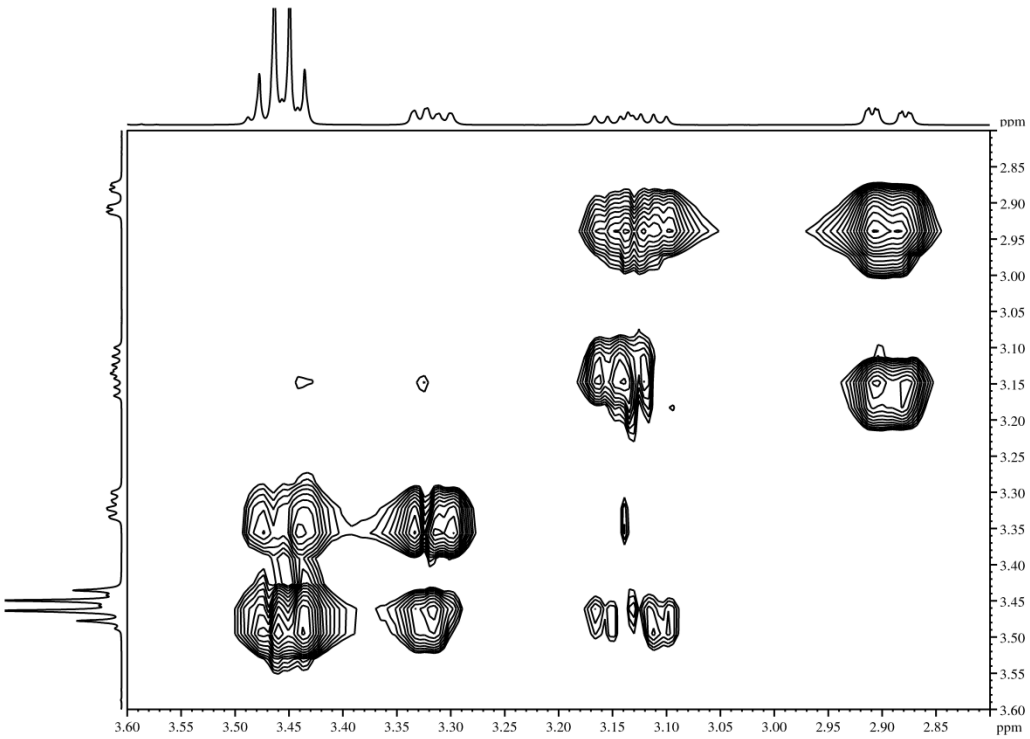


Figure S99. H,H-COSY NMR spectrum of **16**, expansion

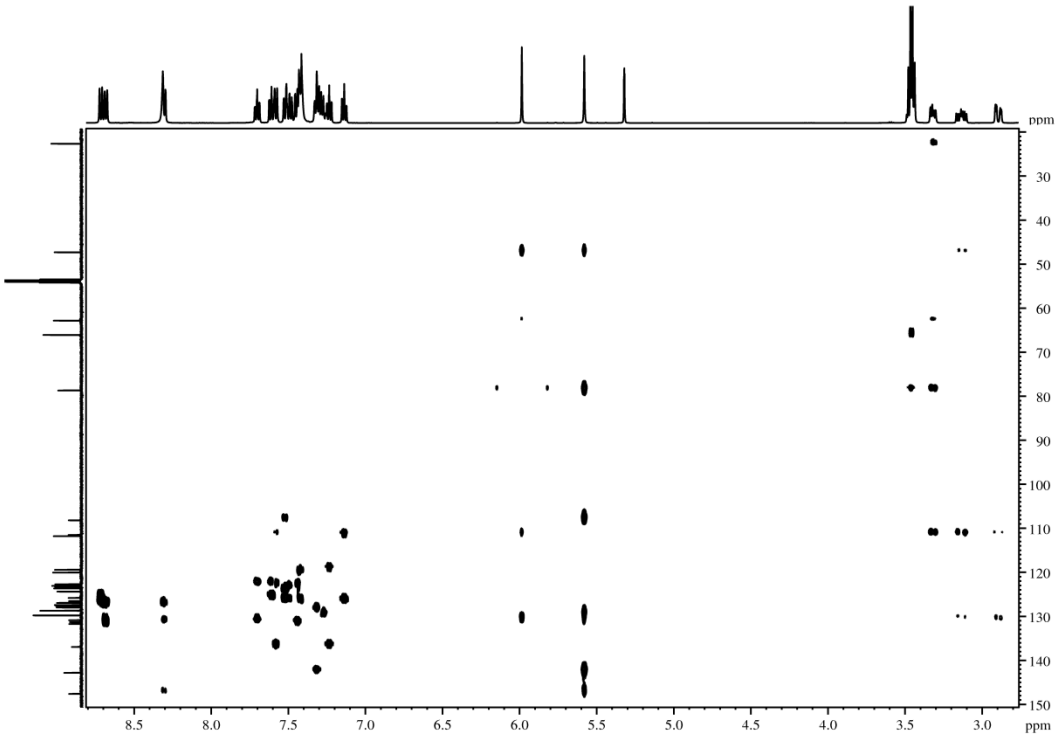


Figure S100. HMBC NMR spectrum of **16**

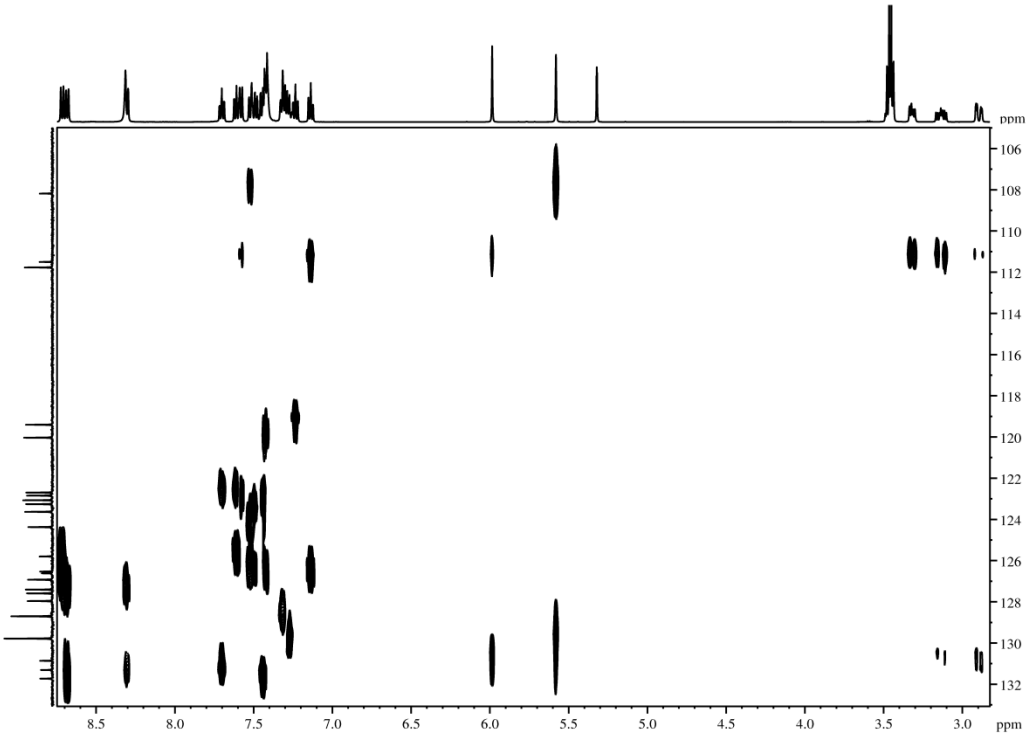


Figure S101. HMBC NMR spectrum of **16**, expansion

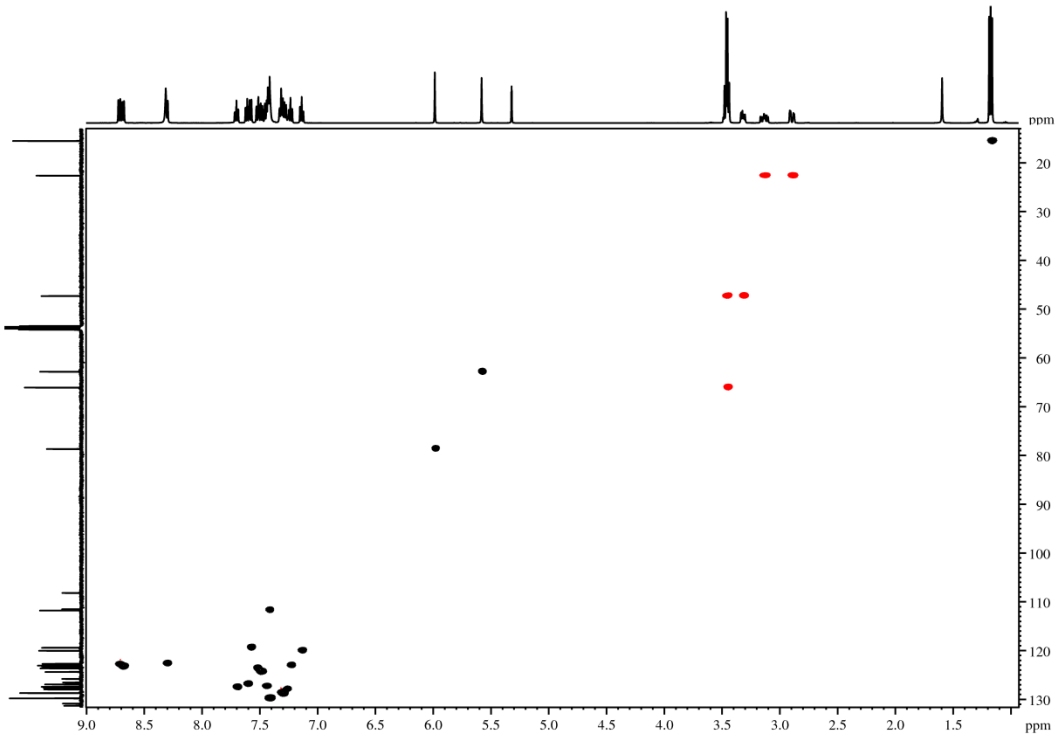


Figure S102. edited HSQC NMR spectrum of **16** (black: positive, red: negative signals)

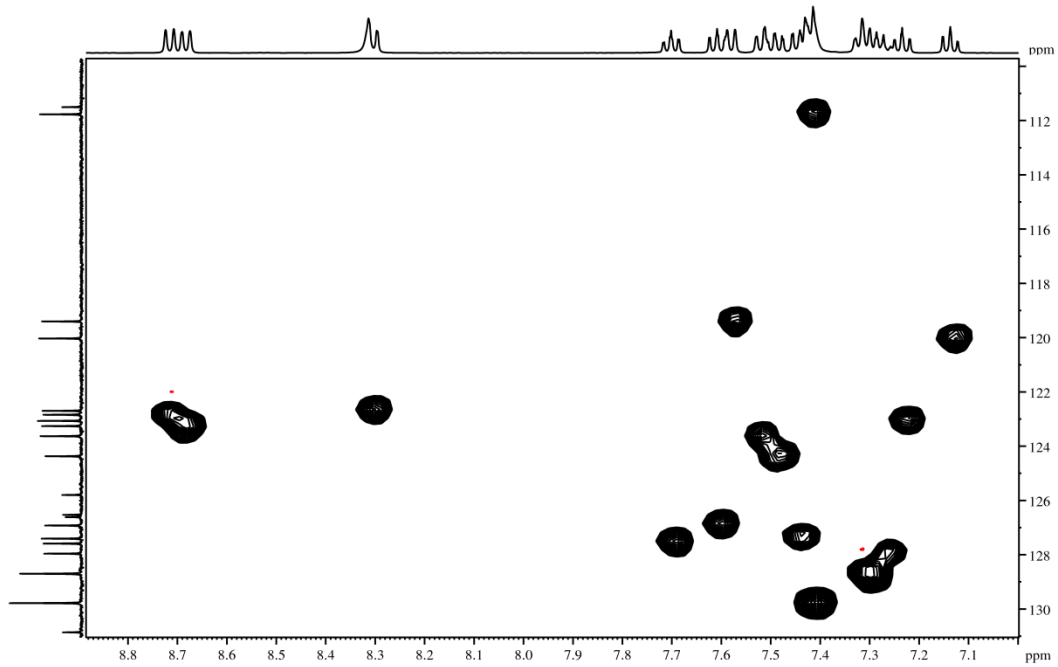


Figure S103. edited HSQC NMR spectrum of **16**, expansion (black: positive, red: negative signals)

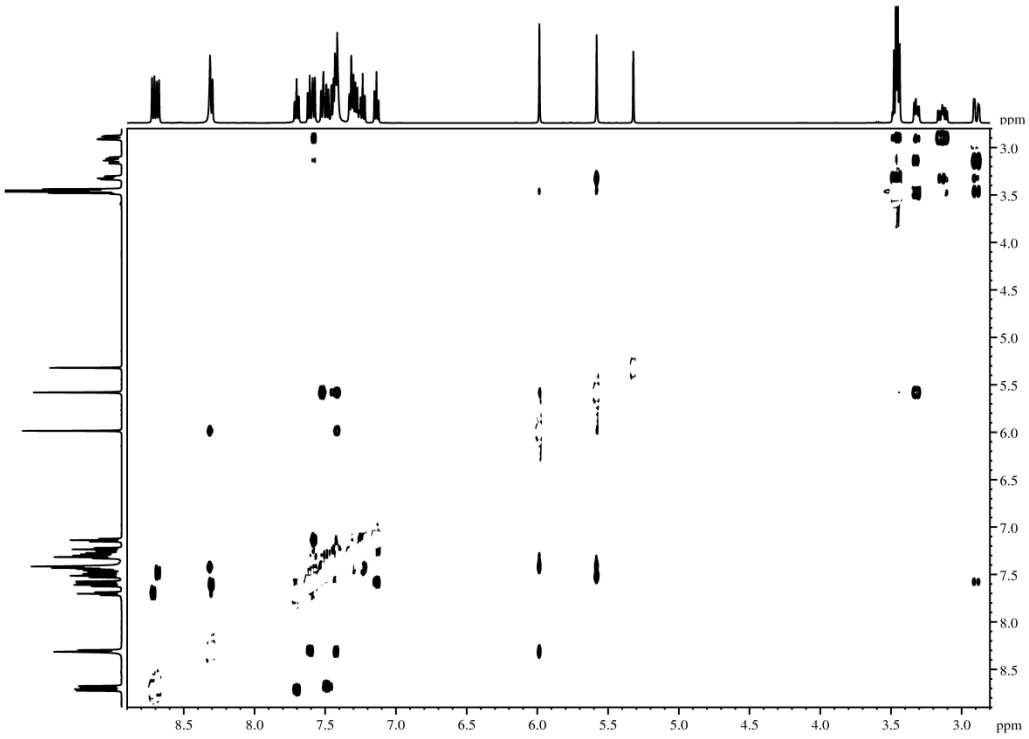
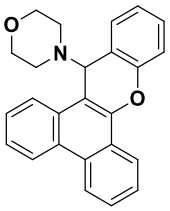


Figure S104. Phase-sensitive NOESY NMR spectrum of **16** (only positive signals, mixing time 800 ms)

14-Morpholin-4-yl-dibenzo[a,c]xanthene (19)



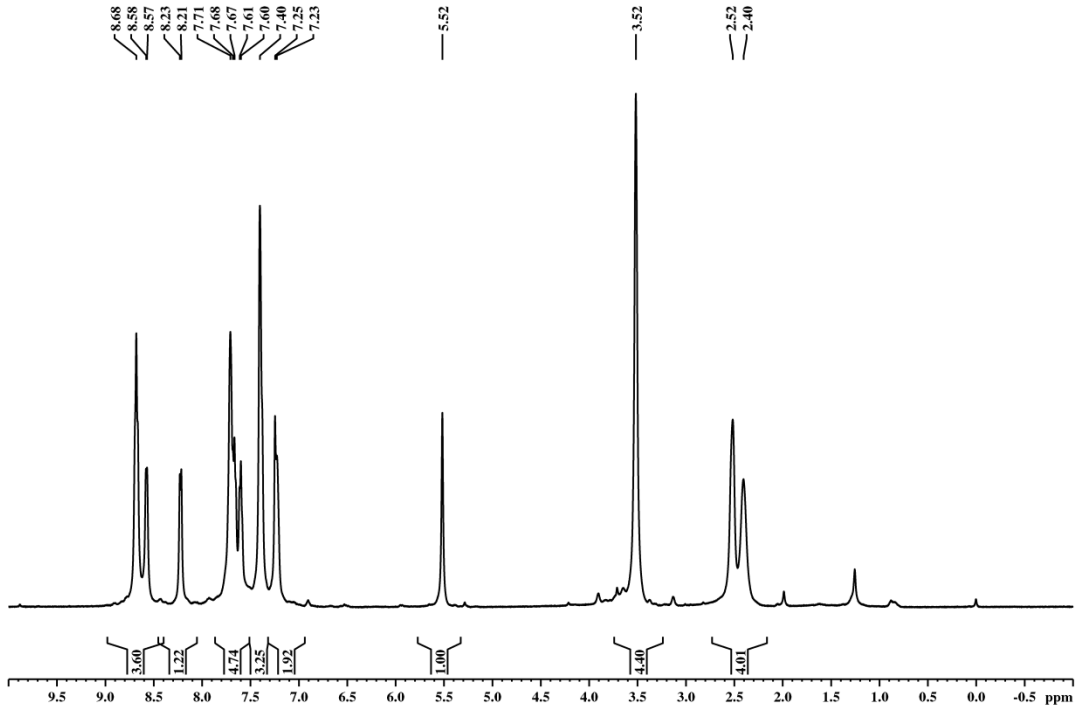


Figure S105. ^{1}H NMR spectrum of **19**

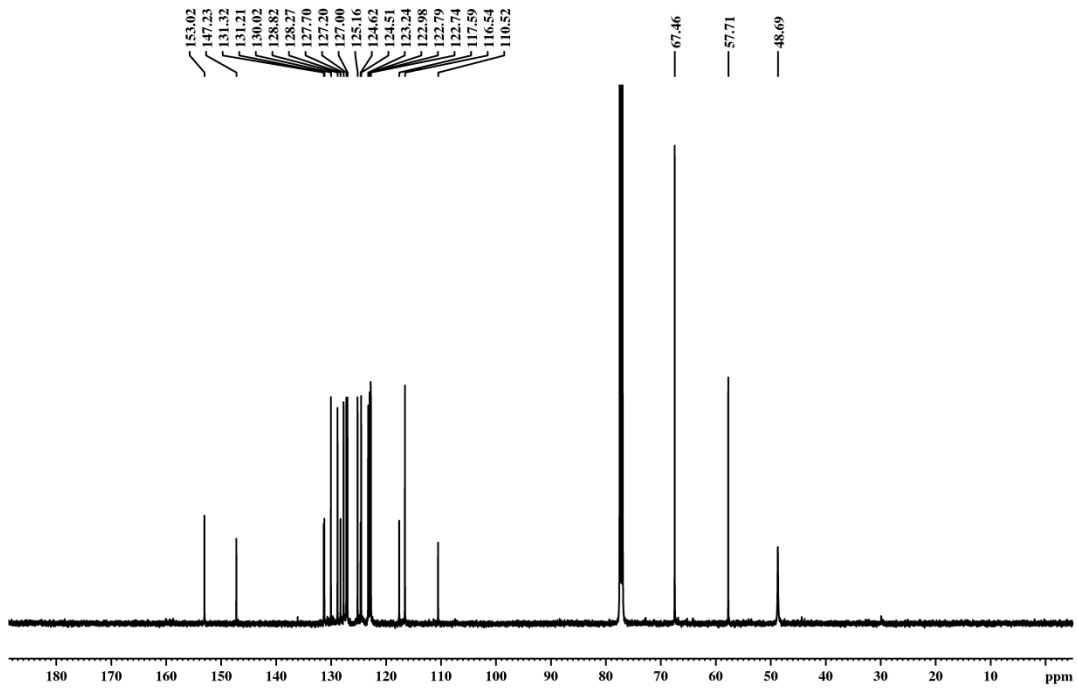


Figure S106. ^{13}C NMR spectrum of **19**

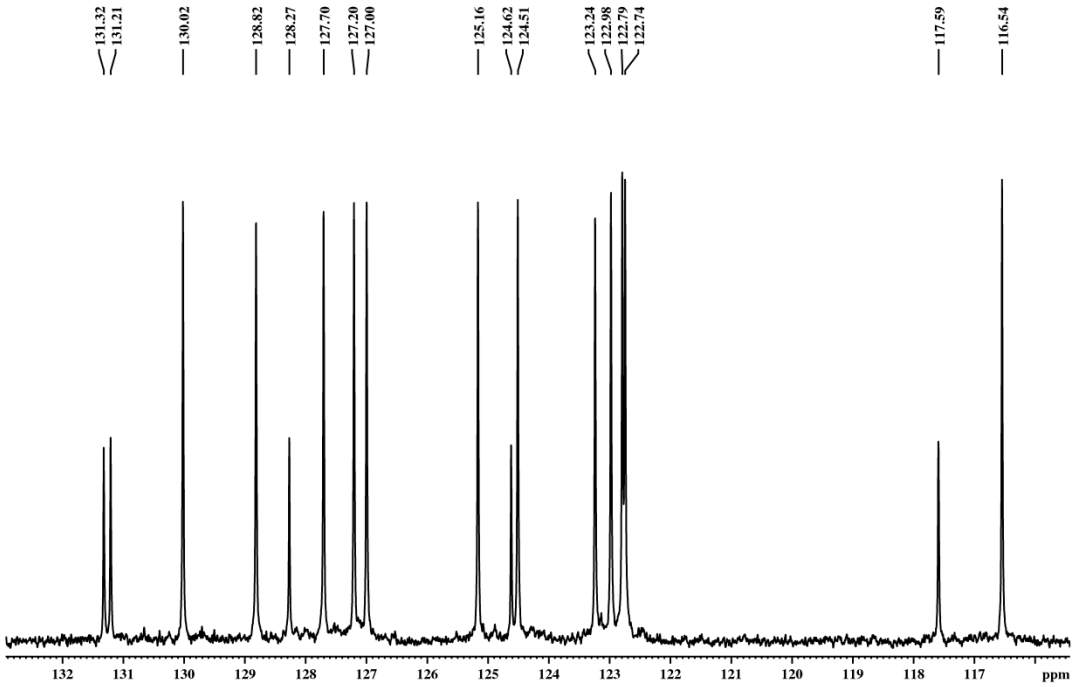


Figure S107. ^{13}C NMR spectrum of **19**, expansion

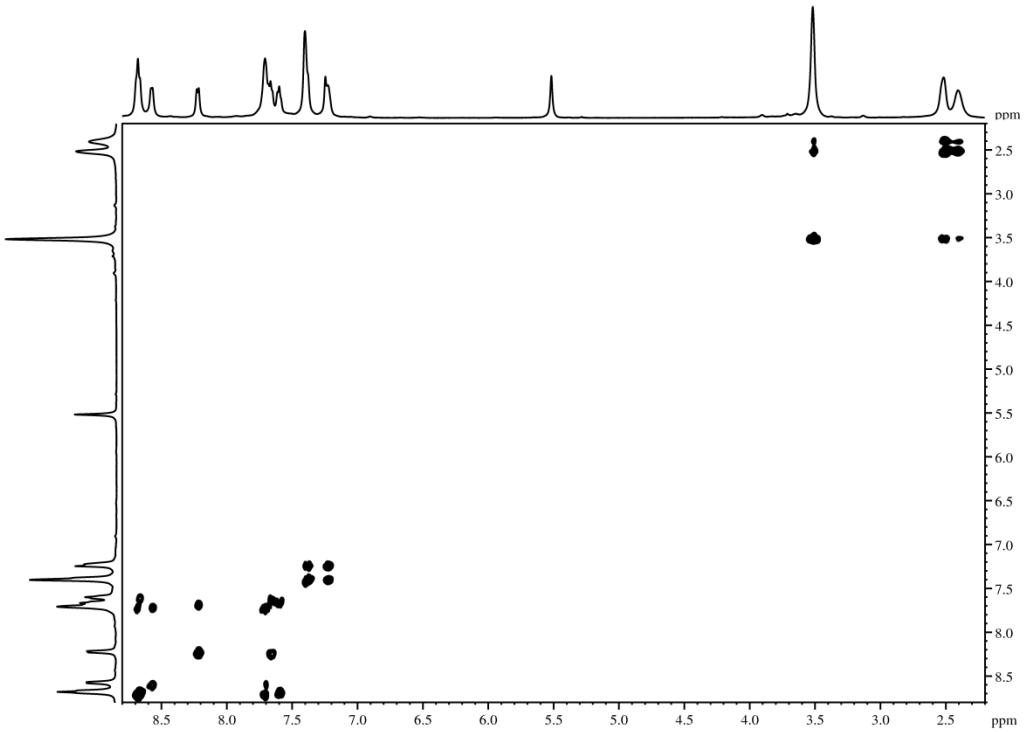


Figure S108. H,H-COSY NMR spectrum of **19**

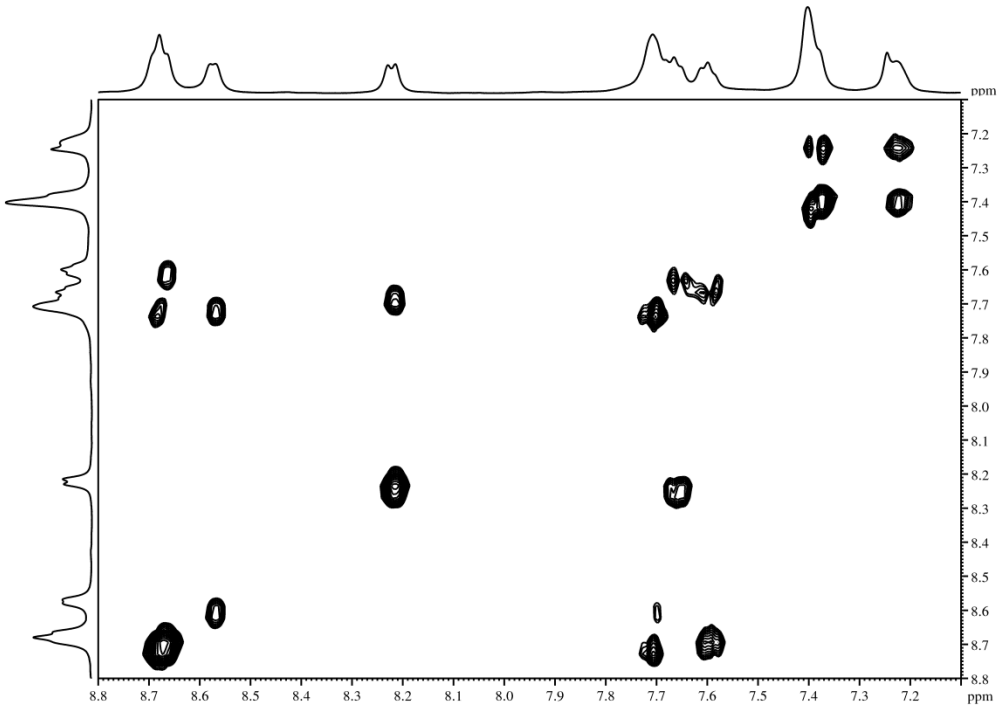


Figure S109. H,H-COSY NMR spectrum of **19**, expansion

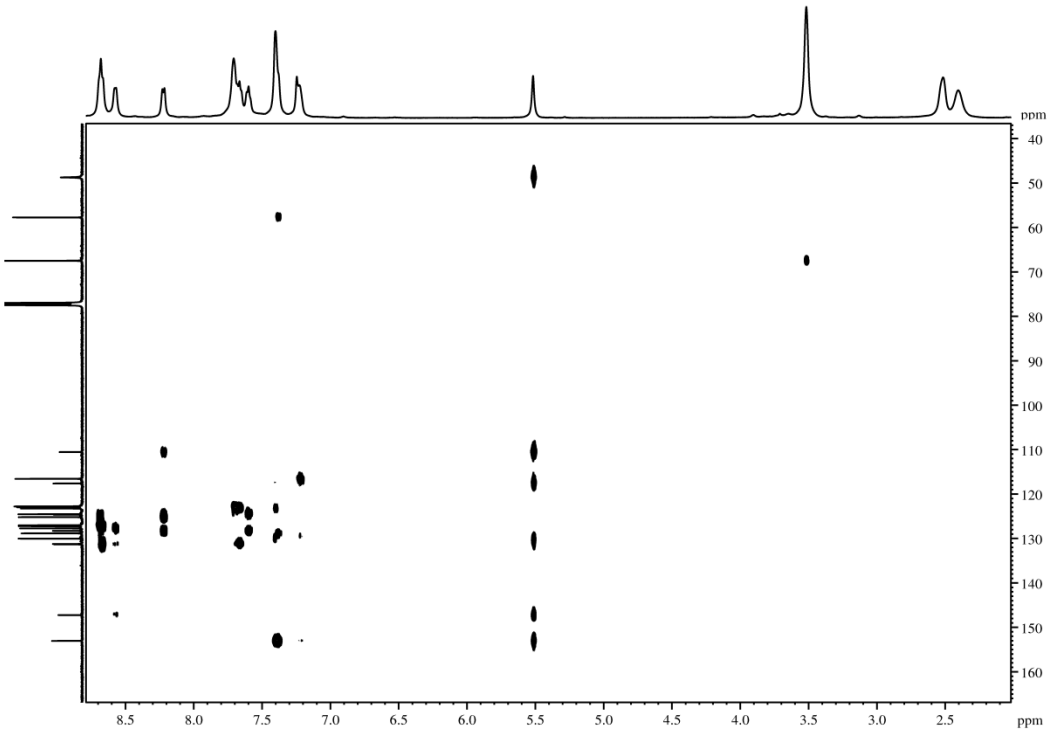


Figure S110. HMBC NMR spectrum of **19**

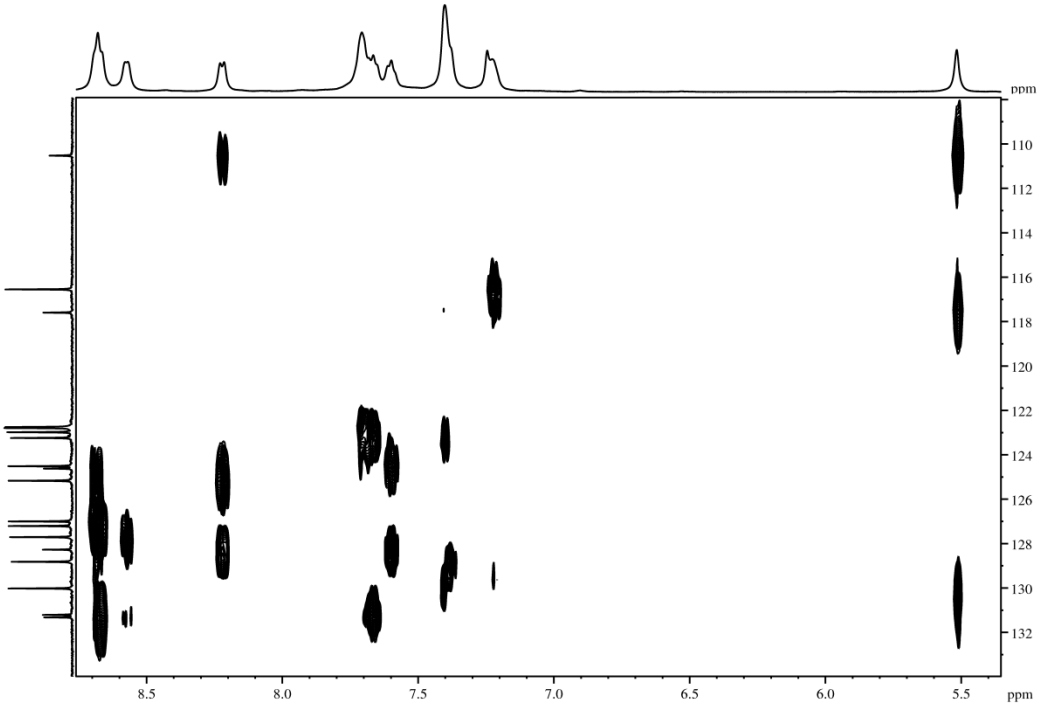


Figure S111. HMBC NMR spectrum of **19**, expansion

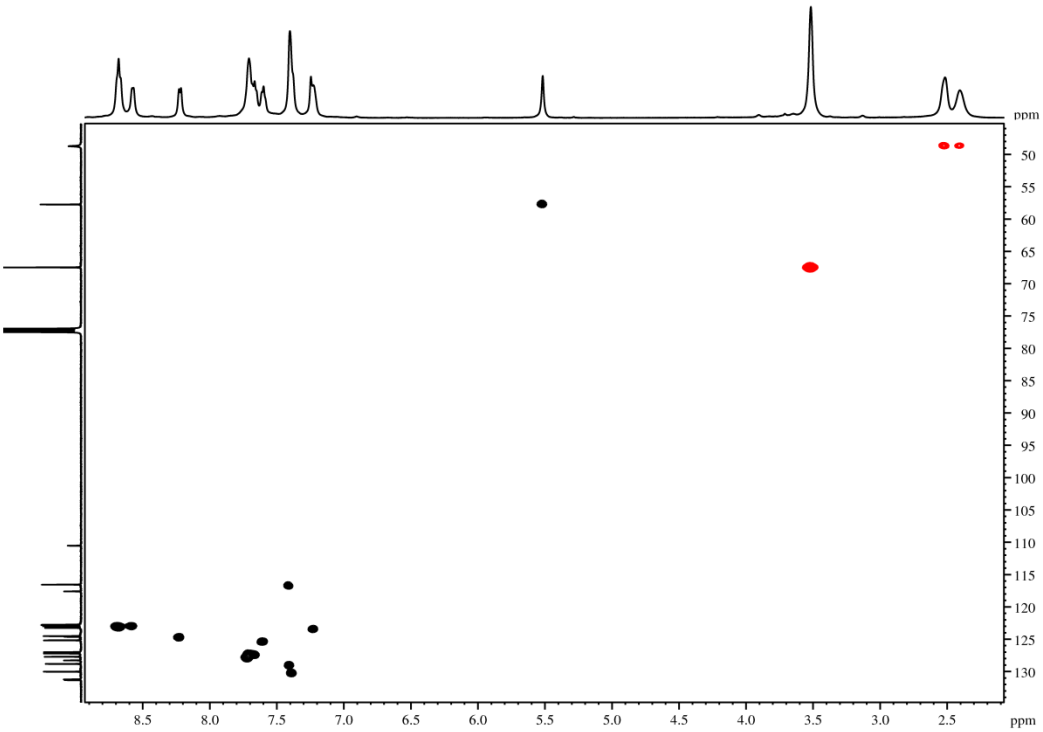


Figure S112. edited HSQC NMR spectrum of **19** (black: positive, red: negative signals)

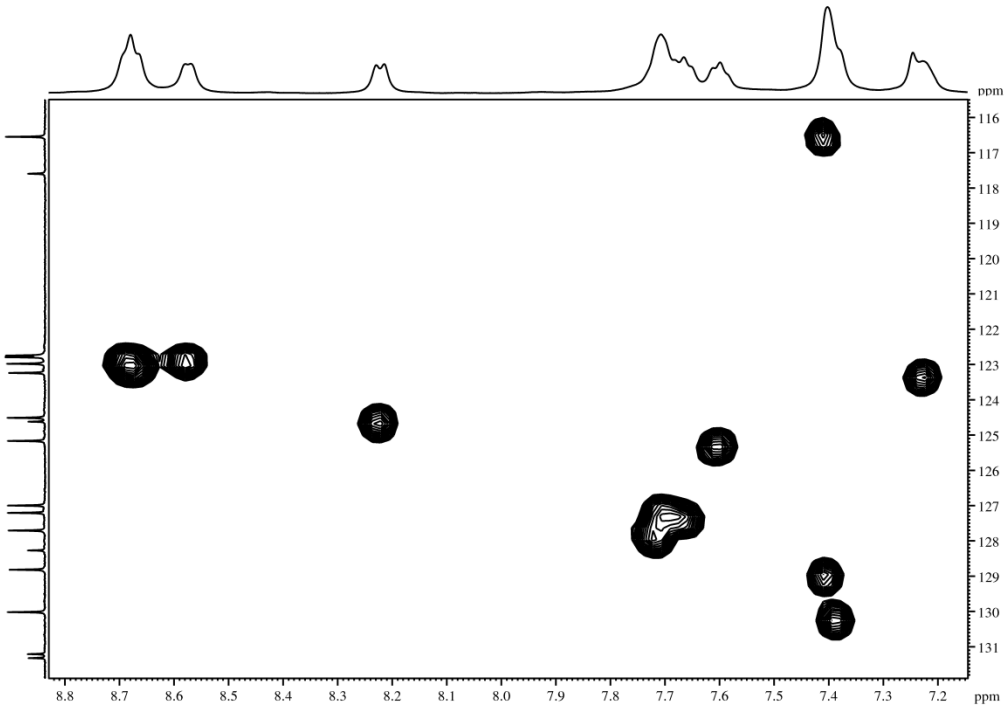
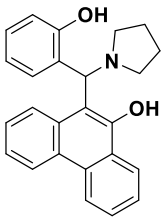


Figure S113. edited HSQC NMR spectrum of **19**, expansion (black: positive, red: negative signals)

10-[(2-Hydroxyphenyl)-pyrrolidin-1-yl-methyl]-9- phenanthrol (21).



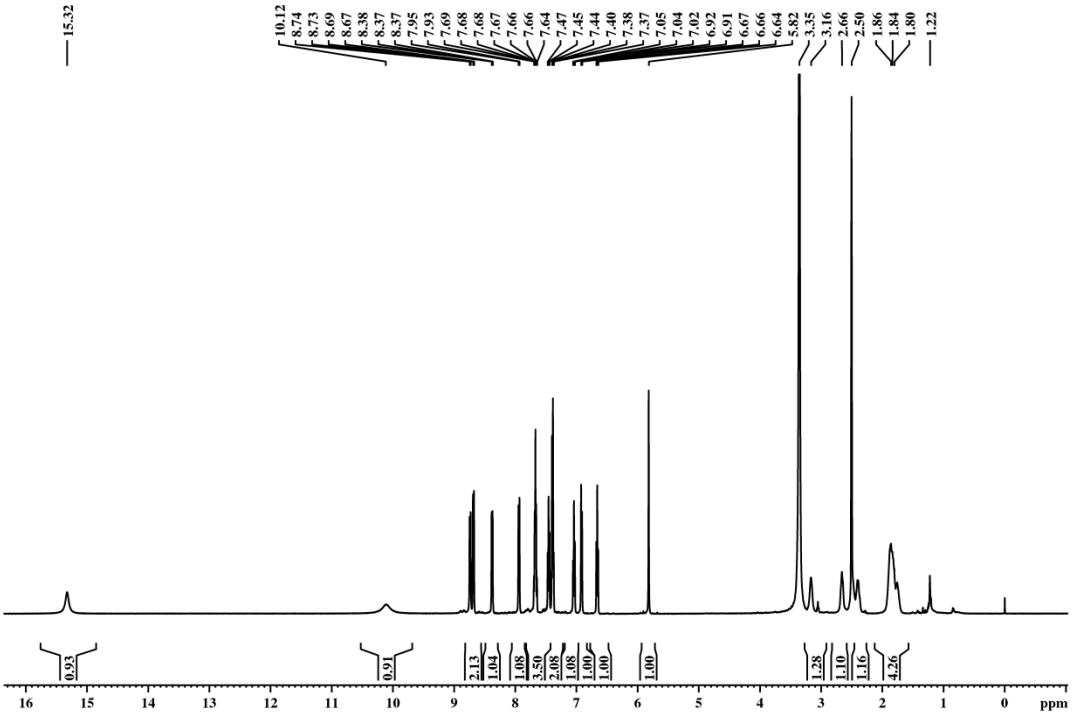


Figure S114. ^{1}H NMR spectrum of **21**

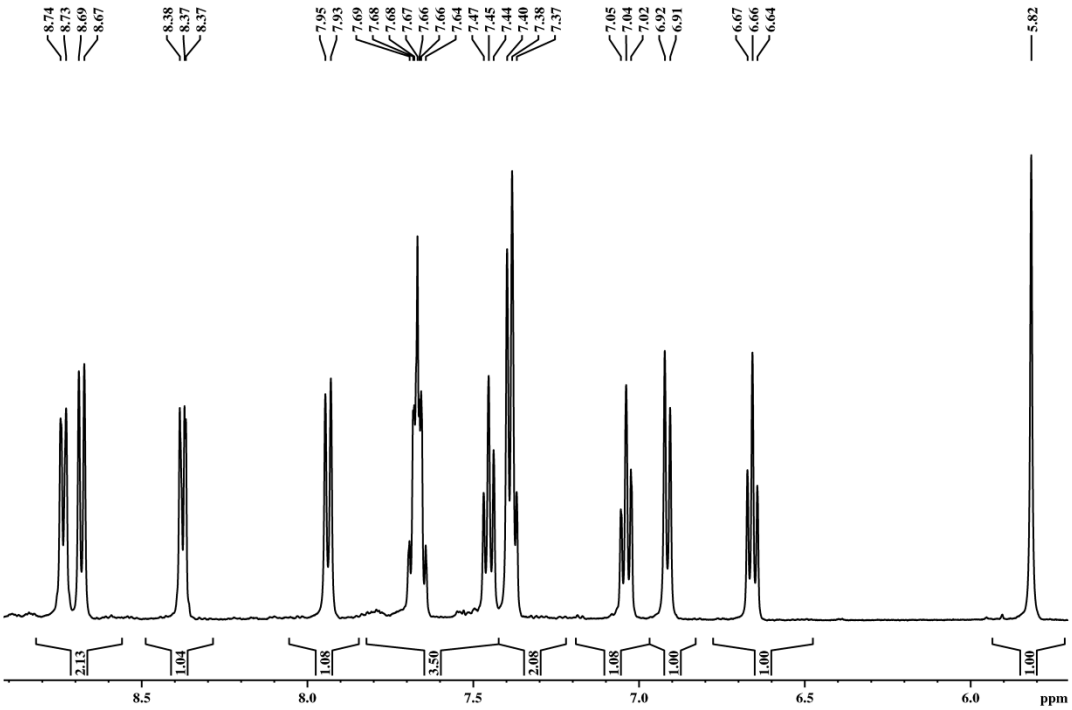


Figure S115. ^{1}H NMR spectrum of **21**, expansion

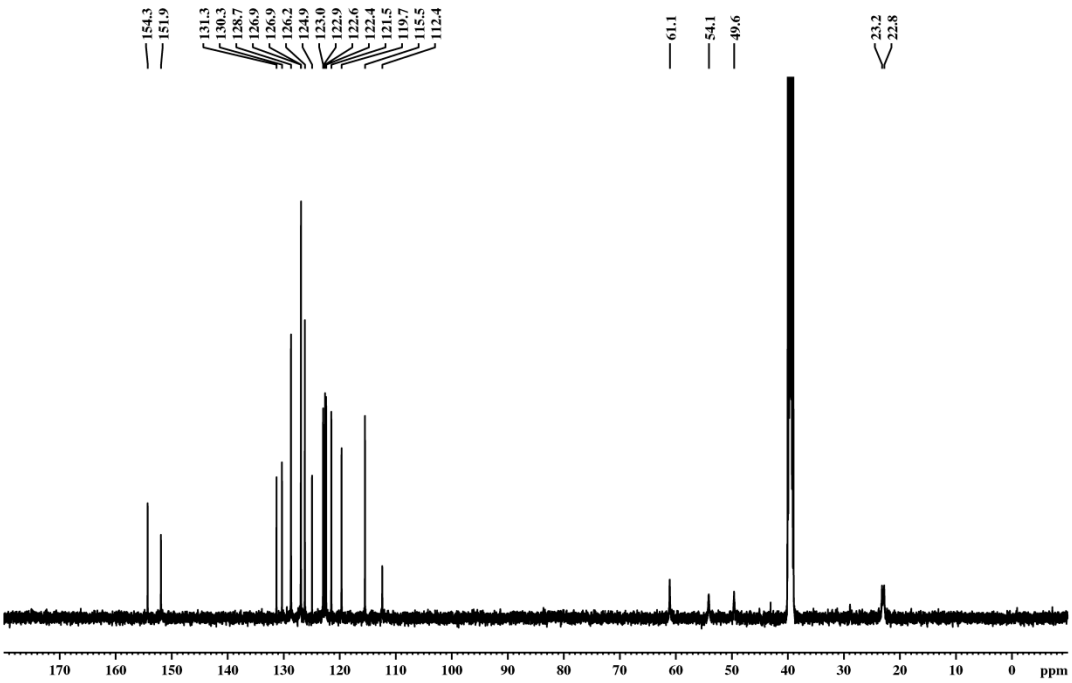


Figure S116. ^{13}C NMR spectrum of **21**

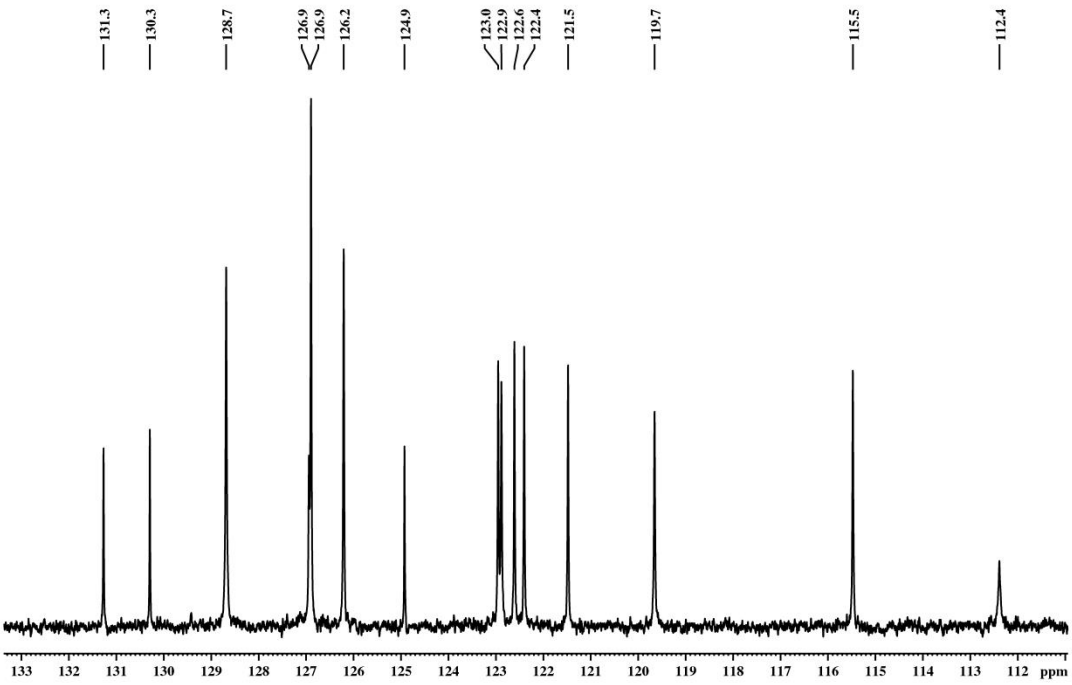


Figure S117. ^{13}C NMR spectrum of **21**, expansion

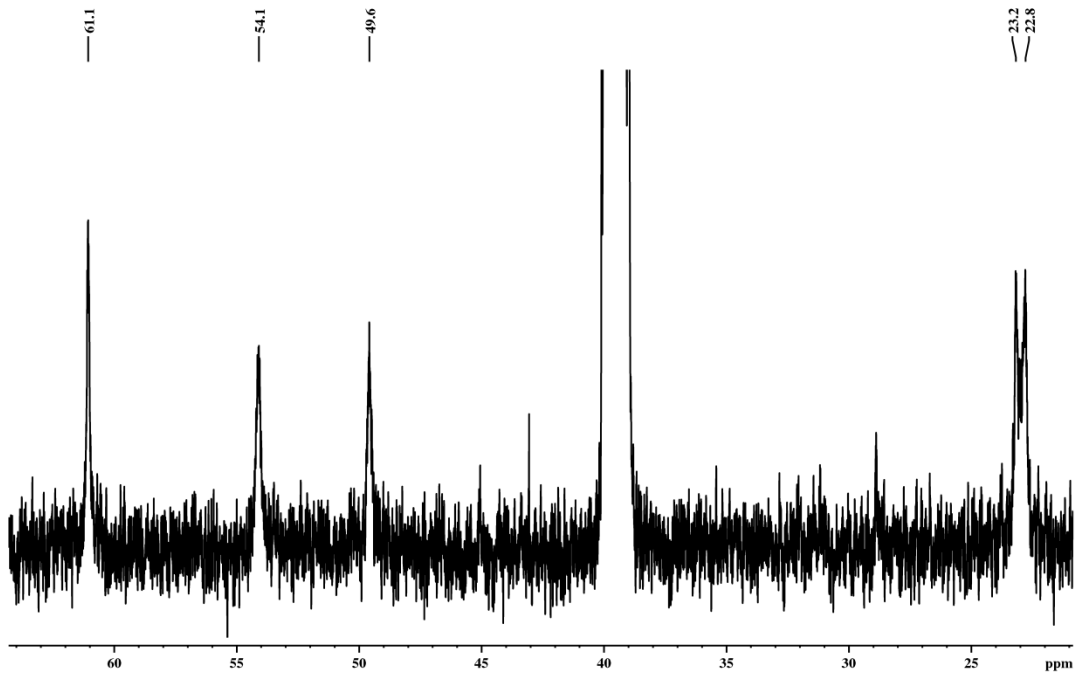


Figure S118. ^{13}C NMR spectrum of **21**, expansion

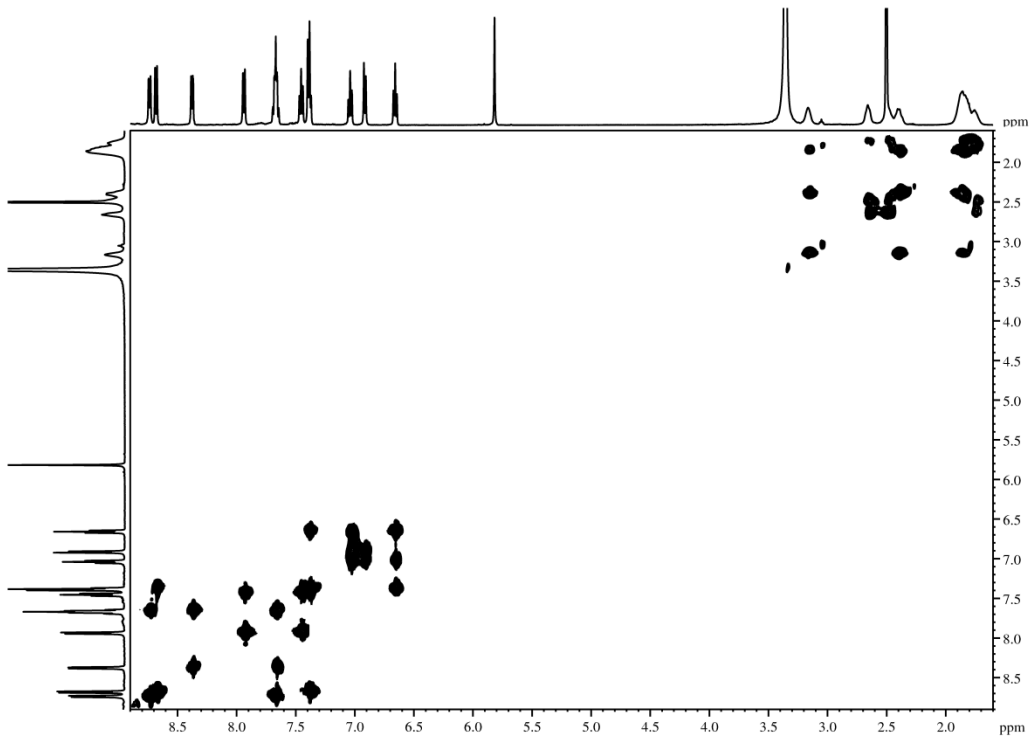


Figure S119. H,H-COSY NMR spectrum of **21**

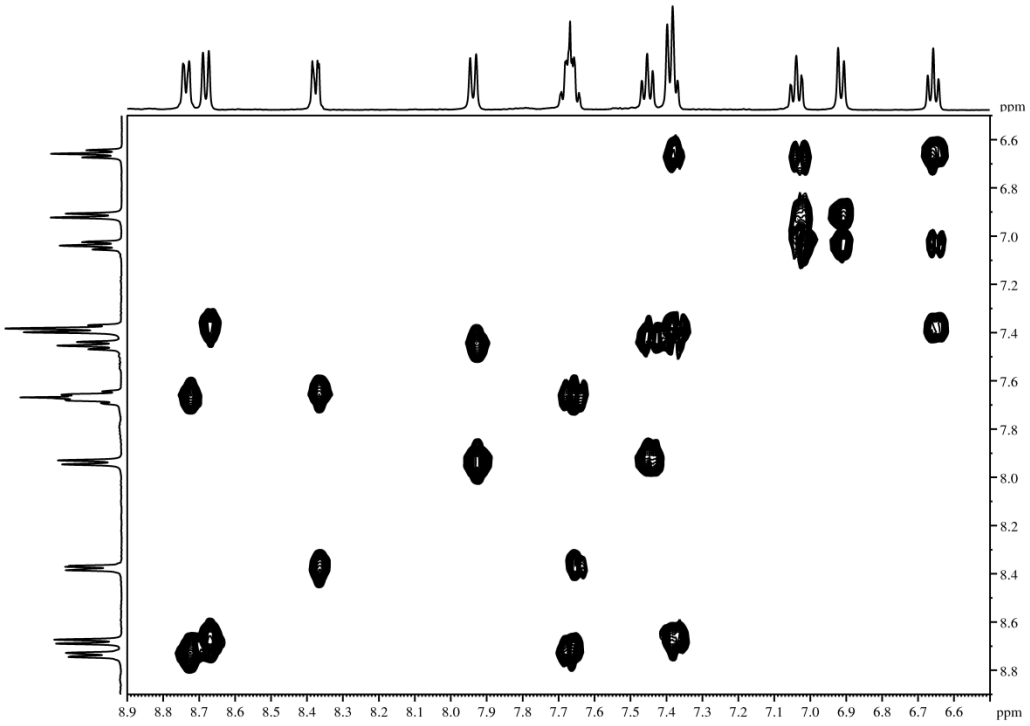


Figure S120. H,H-COSY NMR spectrum of **21**, expansion

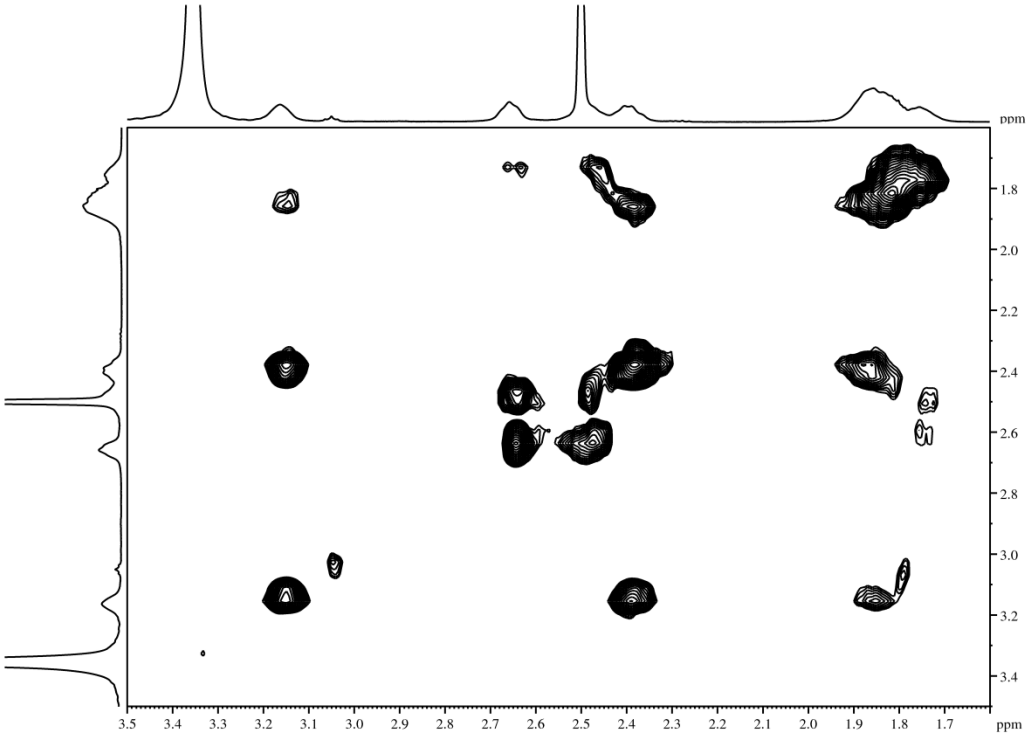


Figure S121. H,H-COSY NMR spectrum of **21**, expansion

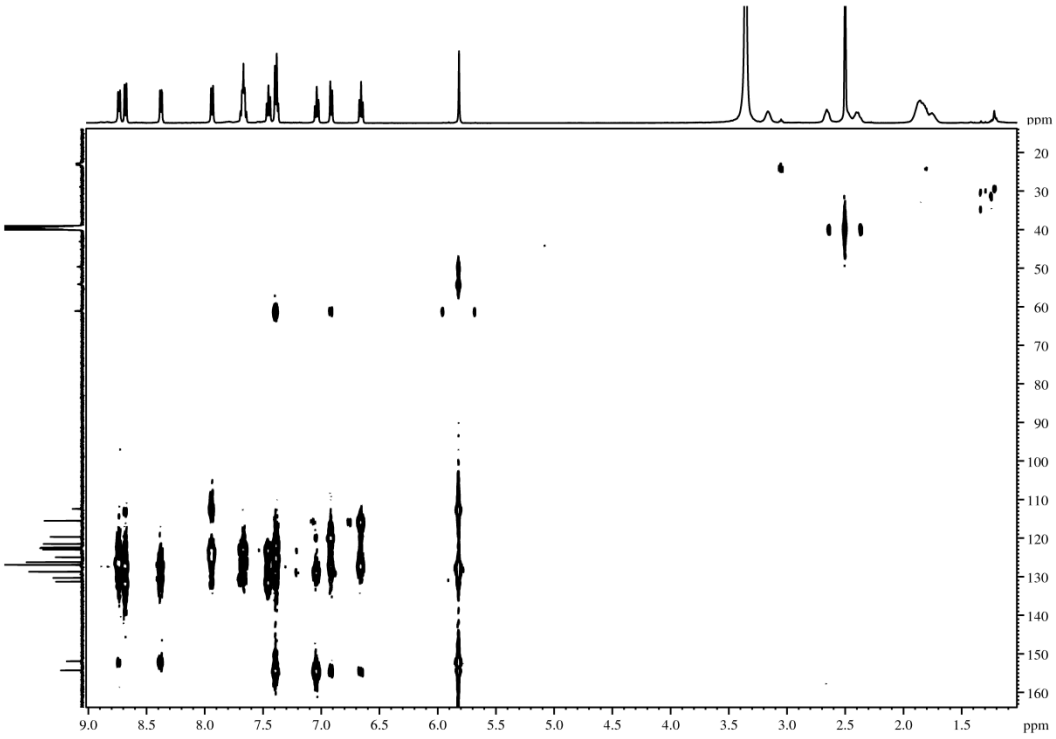


Figure S122. HMBC NMR spectrum of **21**

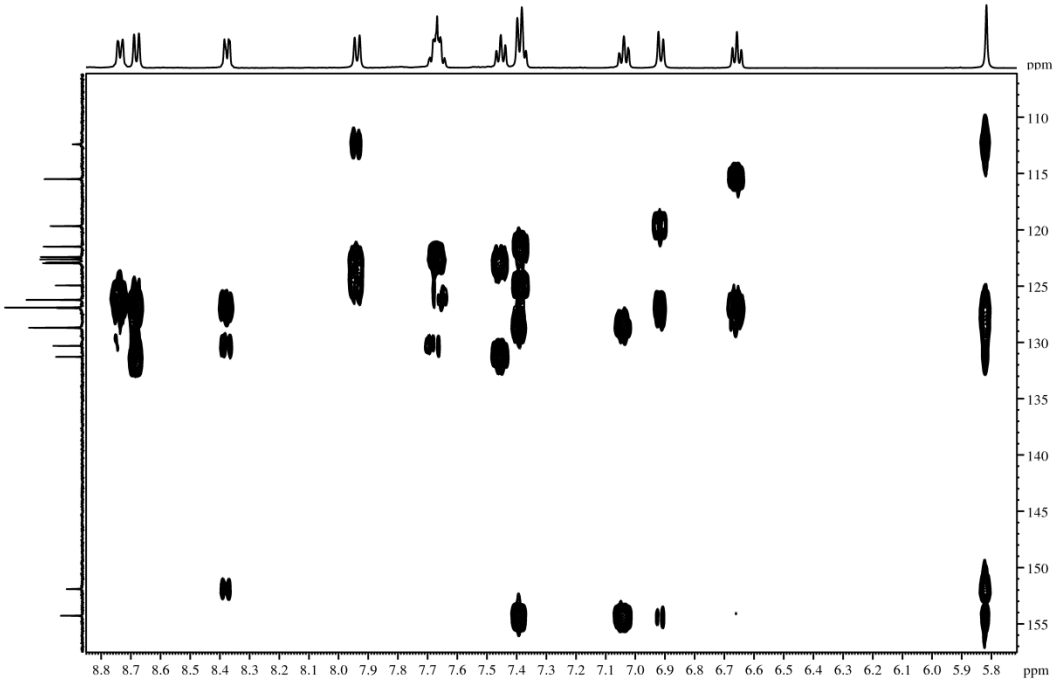


Figure S123. HMBC NMR spectrum of **21**, expansion

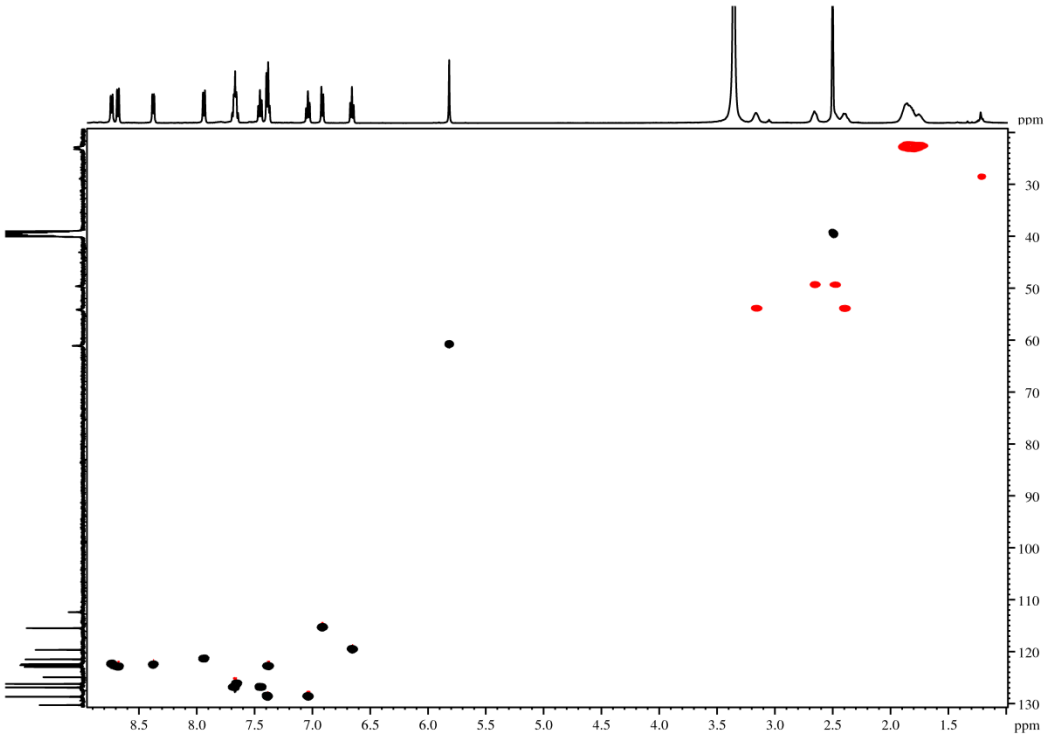


Figure S124. edited HSQC NMR spectrum of **21** (black: positive, red: negative signals)

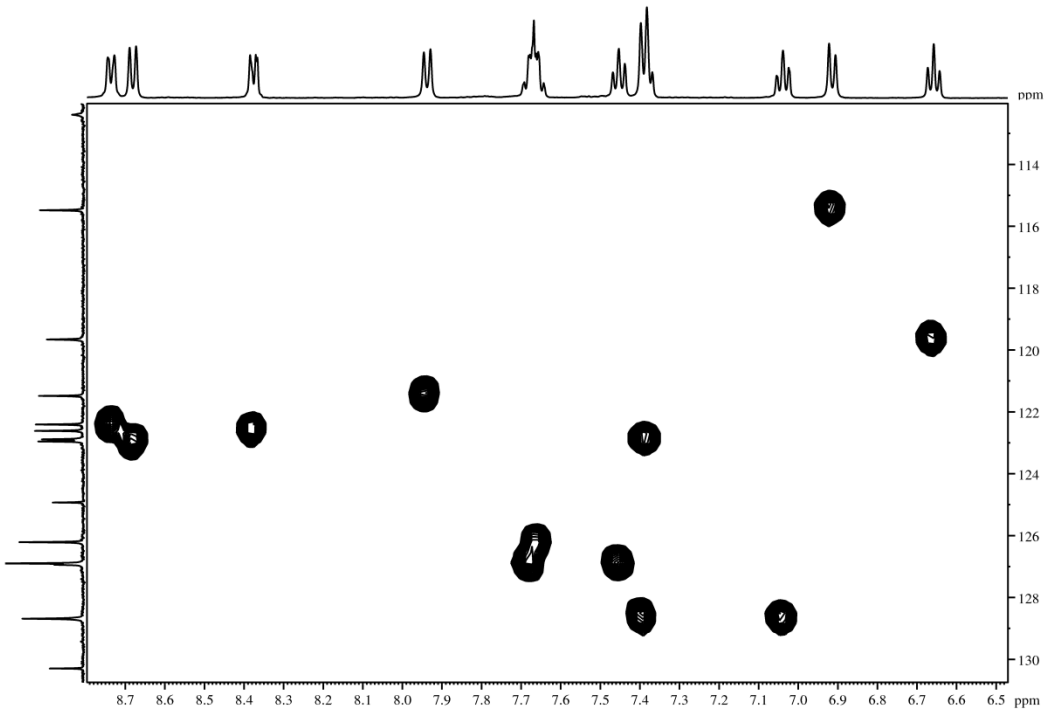
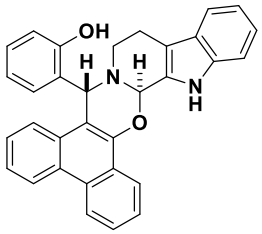


Figure S125. edited HSQC NMR spectrum of **21**, expansion (black: positive, red: negative signals)

9aR*,18S*-19-(2-Hydroxyphenyl)-phenanthr[9,10-e]oxazino[2,3-a]–β–carboline (24).



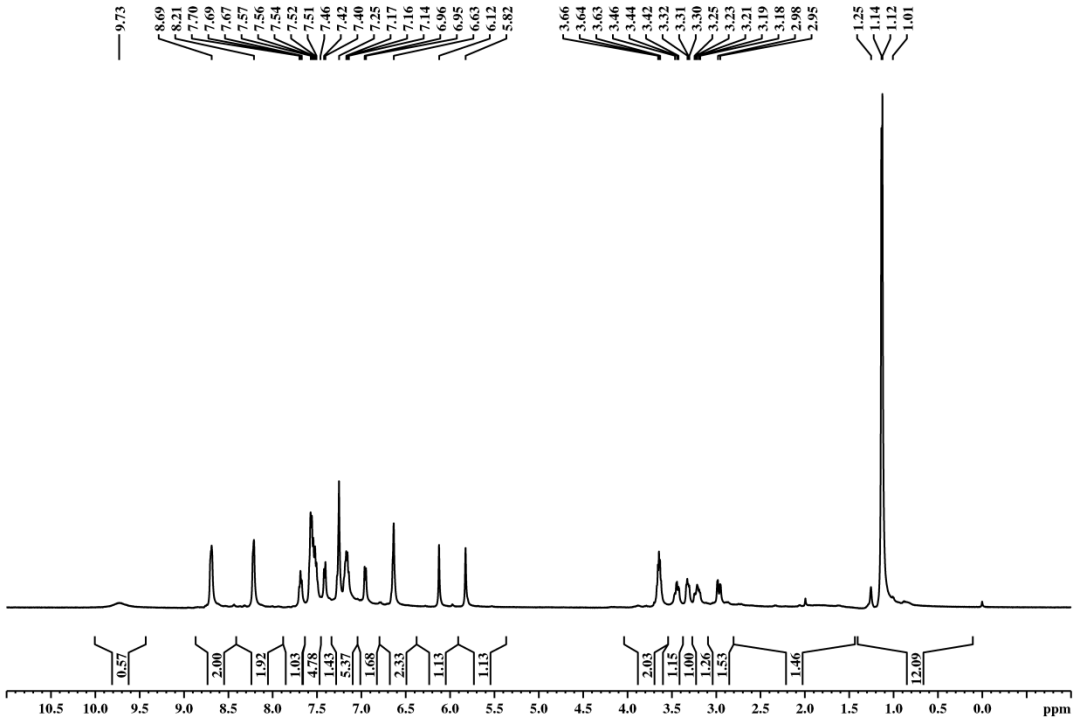


Figure S126. ^{1}H NMR spectrum of **24a**

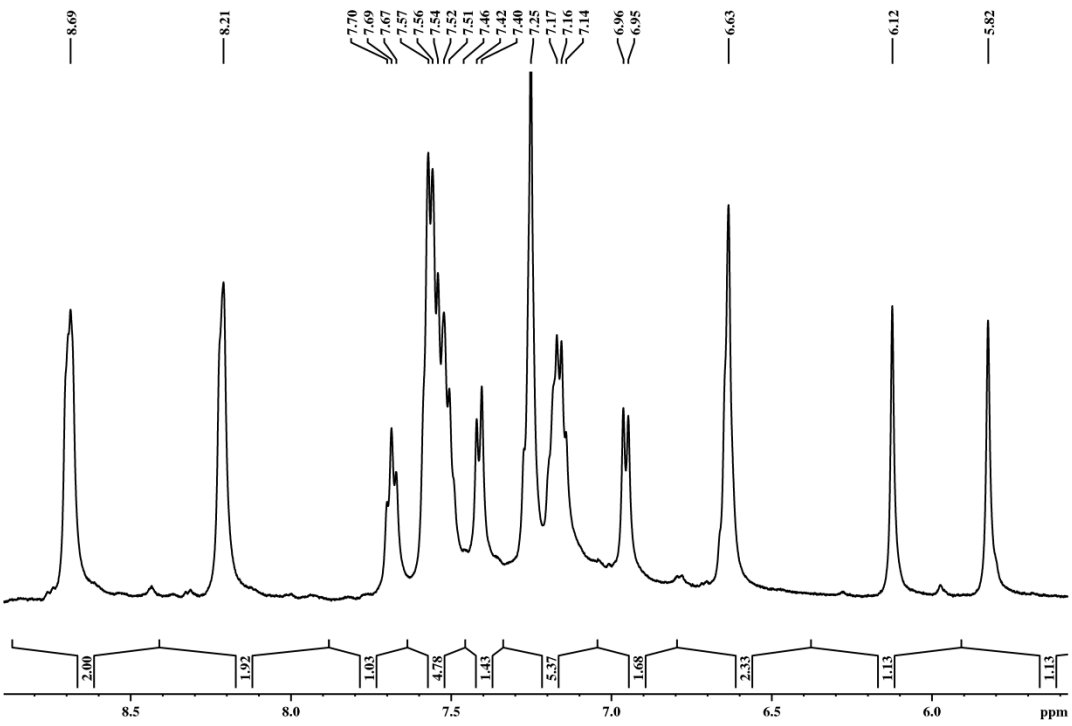


Figure S127. ^{1}H NMR spectrum of **24a**, expansion

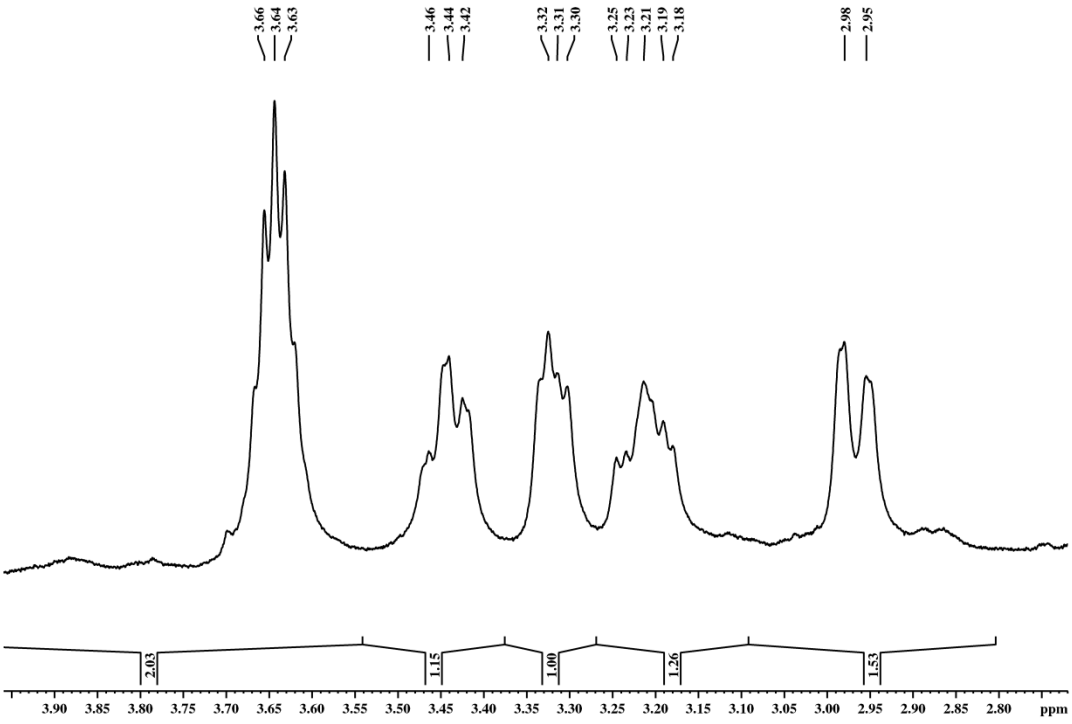


Figure S128. ^{1}H NMR spectrum of **24a**, expansion

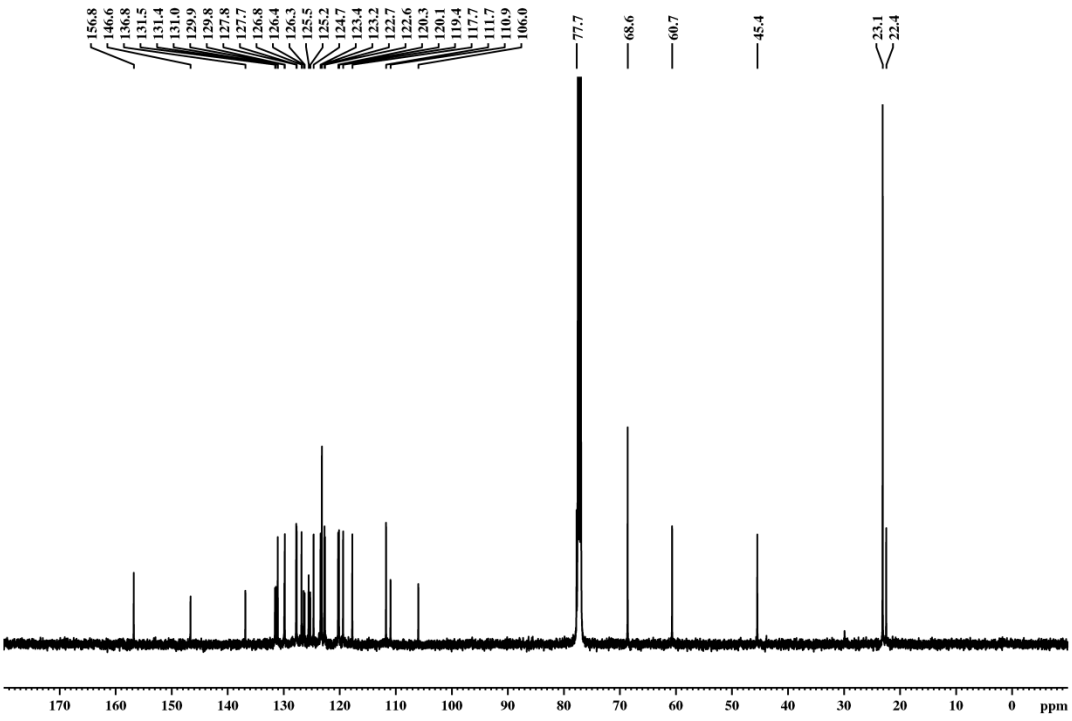


Figure S129. ^{13}C NMR spectrum of **24a**

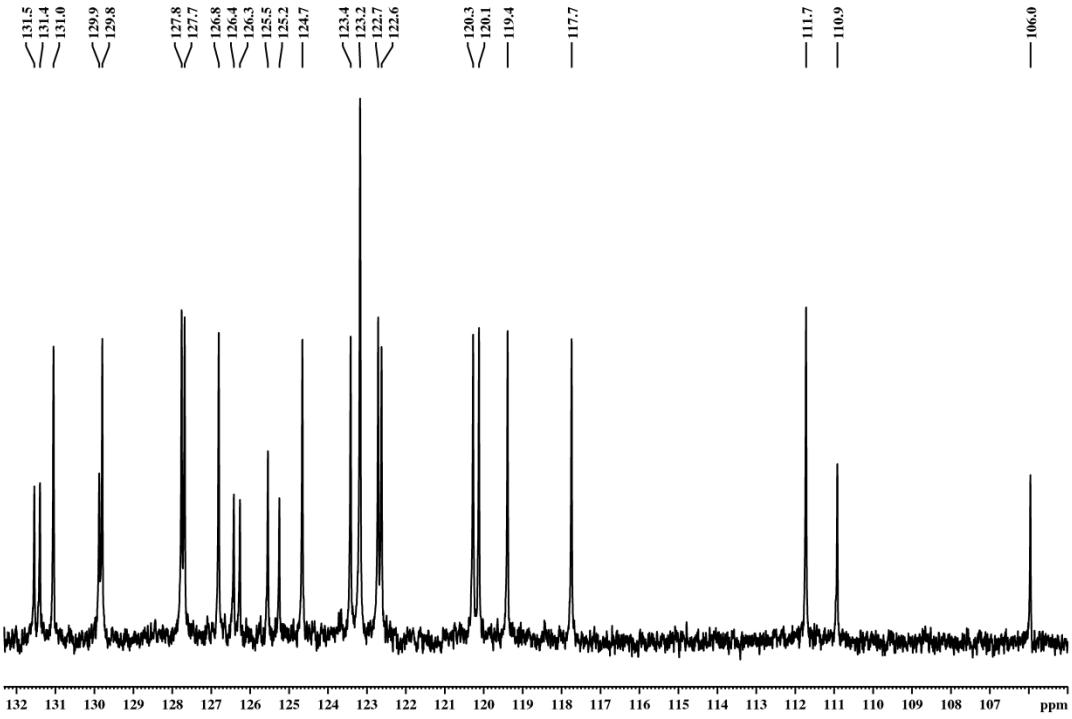


Figure S130. ^{13}C NMR spectrum of **24a**, expansion

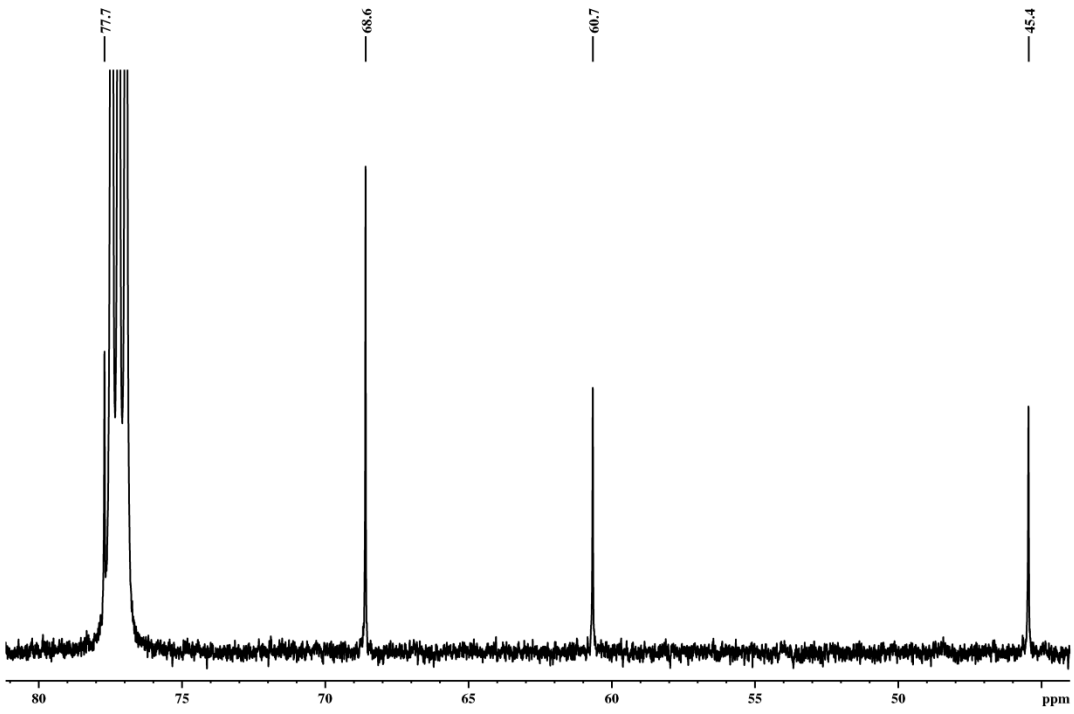


Figure S131. ^{13}C NMR spectrum of **24a**, expansion

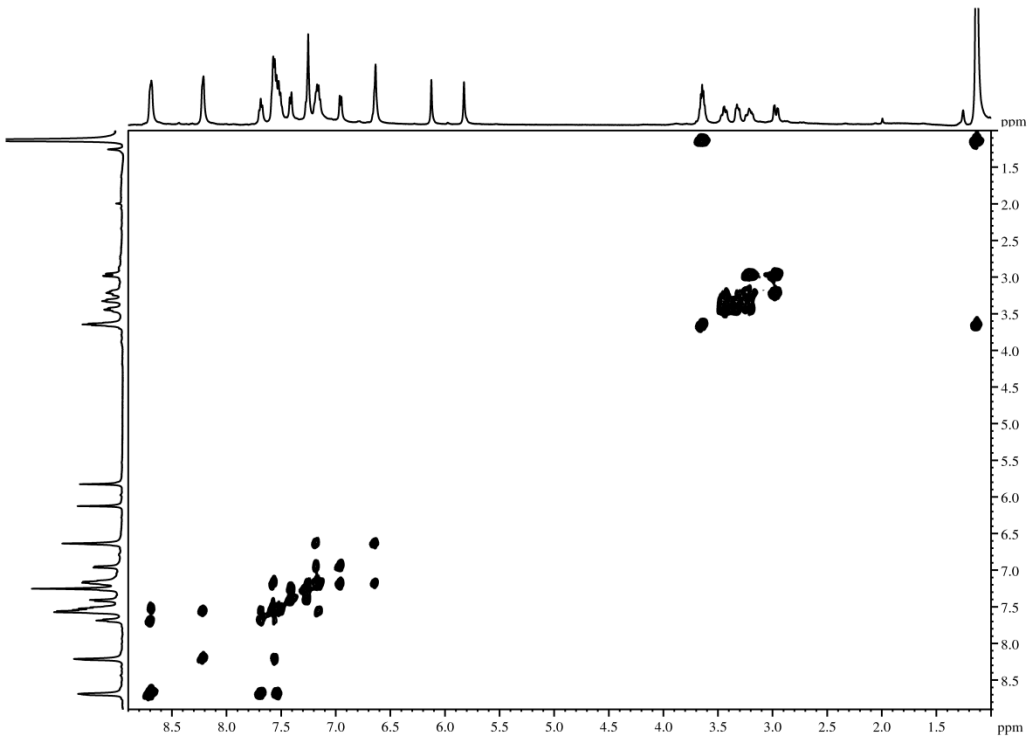


Figure S132. H,H-COSY NMR spectrum of **24a**

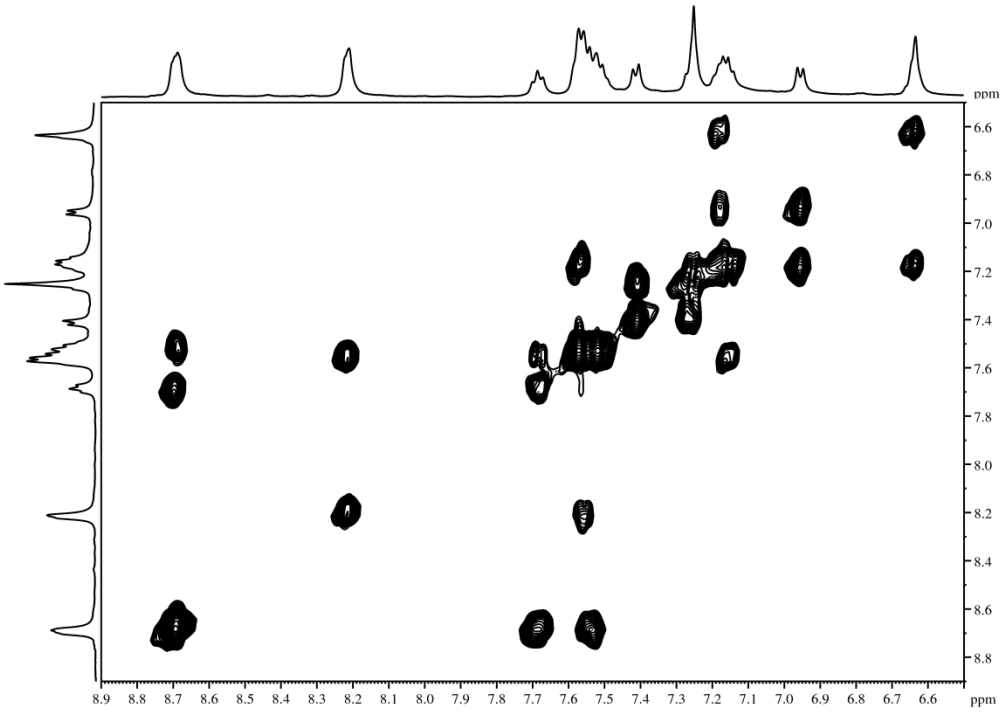


Figure S133. H,H-COSY NMR spectrum of **24a**, expansion

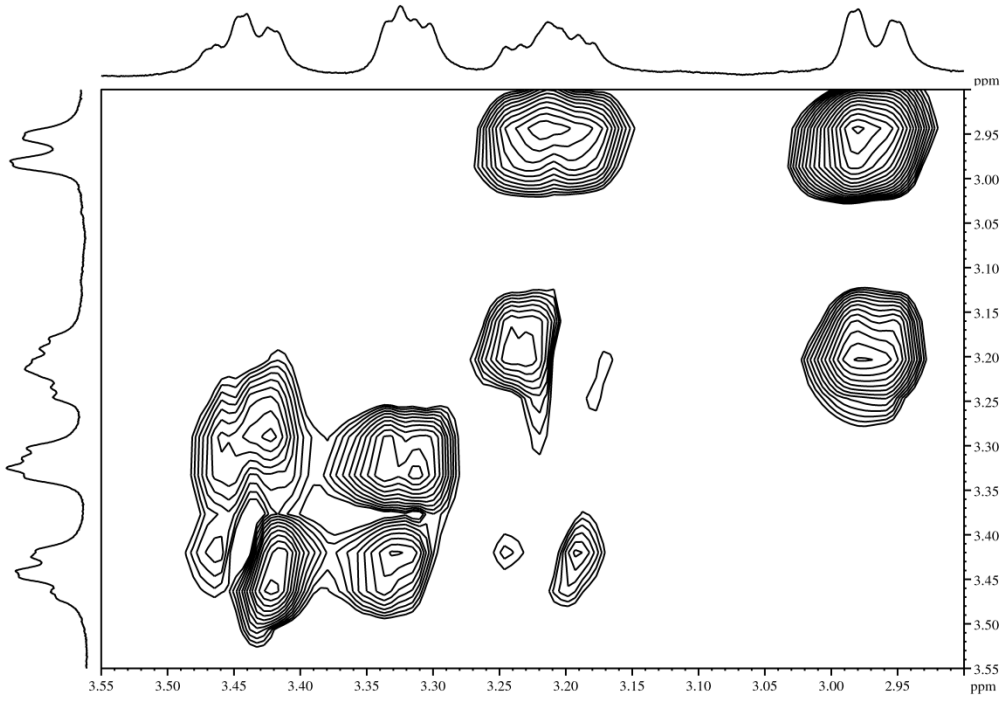


Figure S134. H,H-COSY NMR spectrum of **24a**, expansion

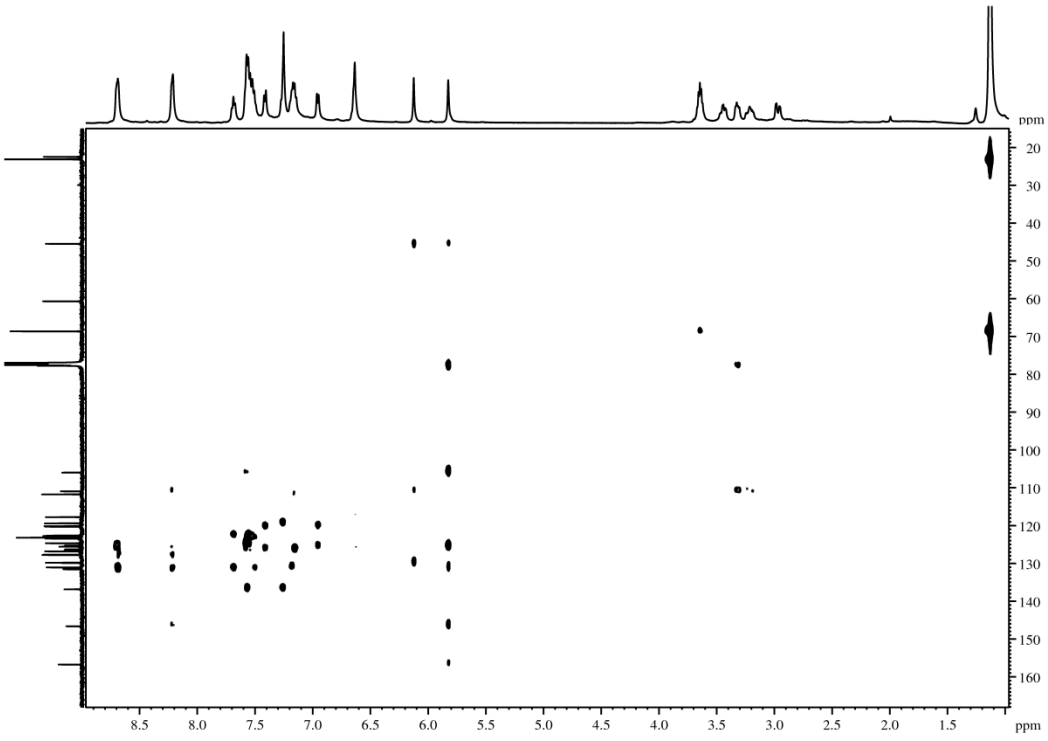


Figure S135. HMBC NMR spectrum of **24a**

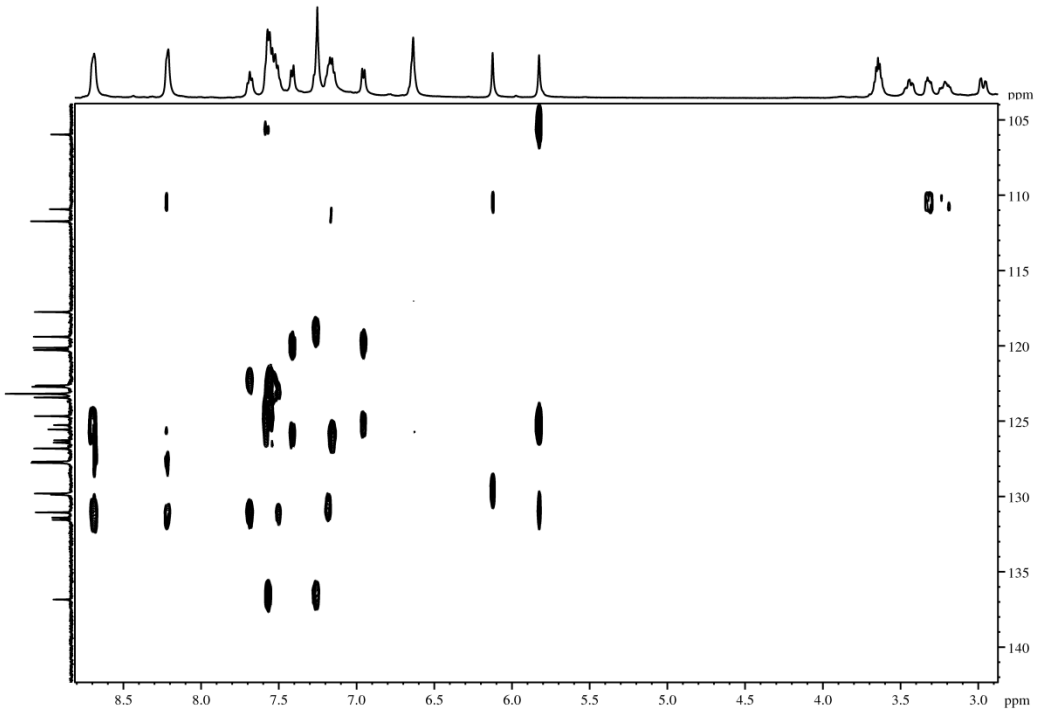


Figure S136. HMBC NMR spectrum of **24a**, expansion

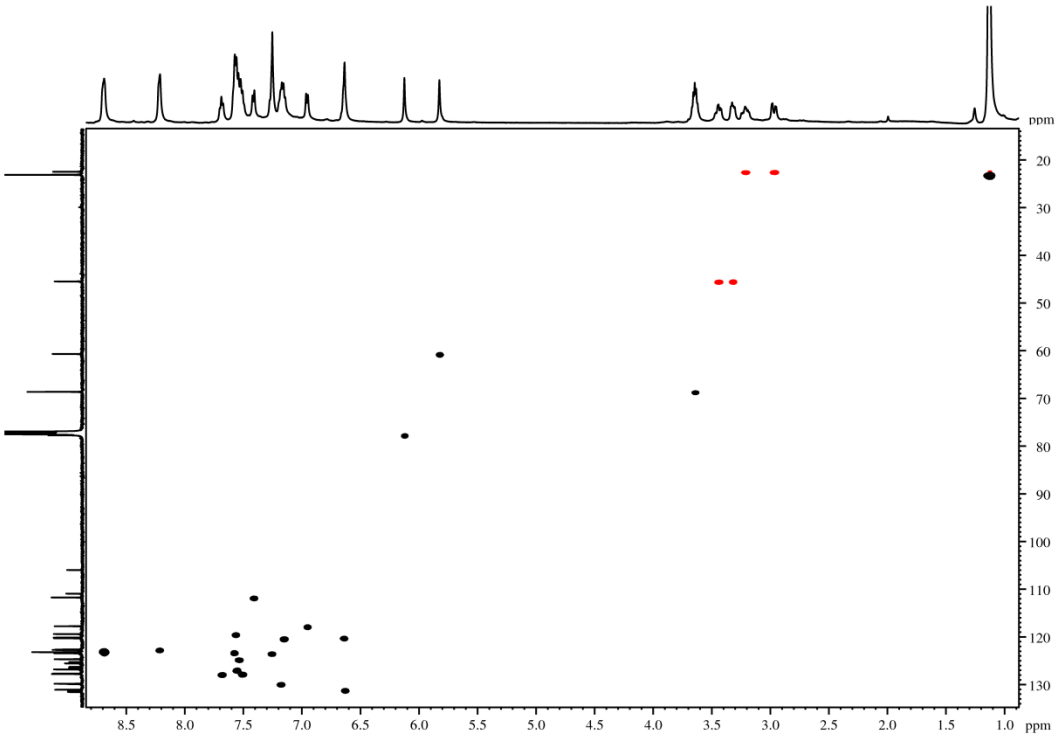


Figure S137. edited HSQC NMR spectrum of **24a** (black: positive, red: negative signals)

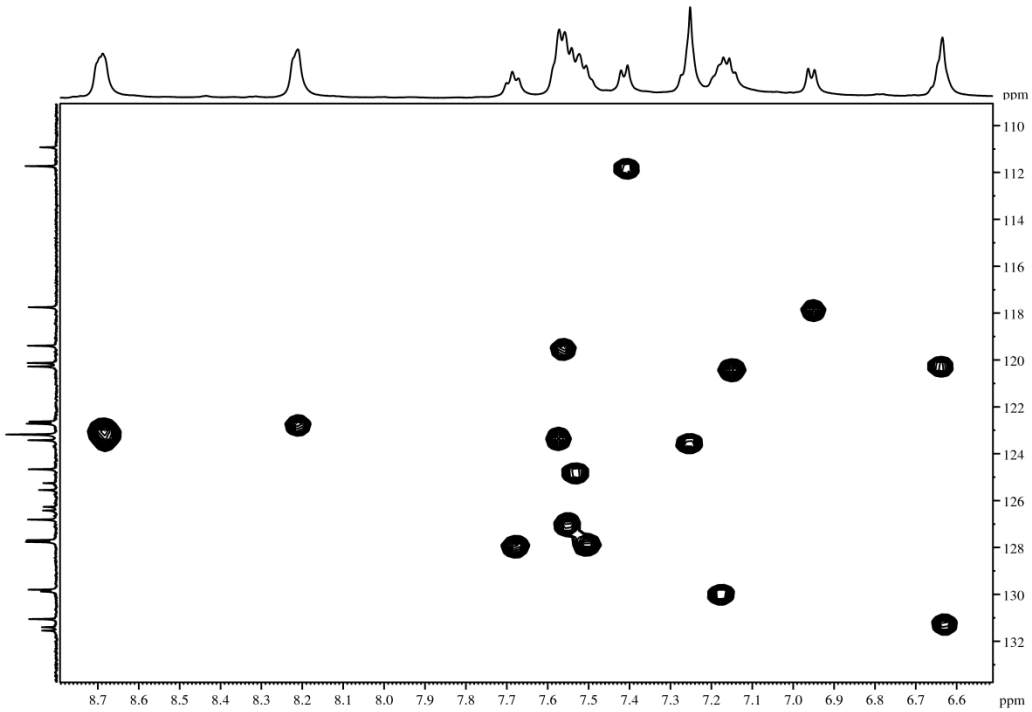


Figure S138. edited HSQC NMR spectrum of **24a**, expansion (black: positive, red: negative signals)

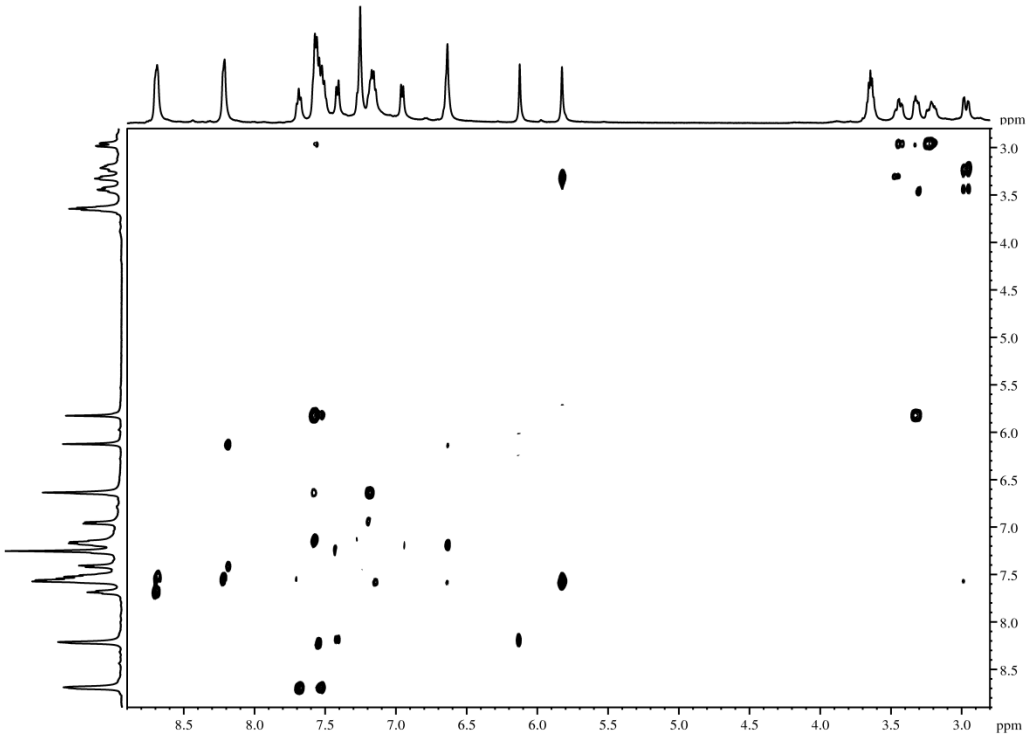
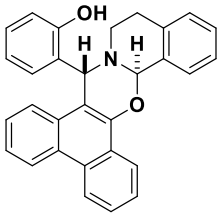


Figure S139. Phase-sensitive NOESY NMR spectrum of **24a** (only positive signals, mixing time 800 ms)

9aR*,17S*-15-(2-Hydroxyphenyl)-phenanthr[9,10-e]oxazino[2,3-a]isoquinoline (26)



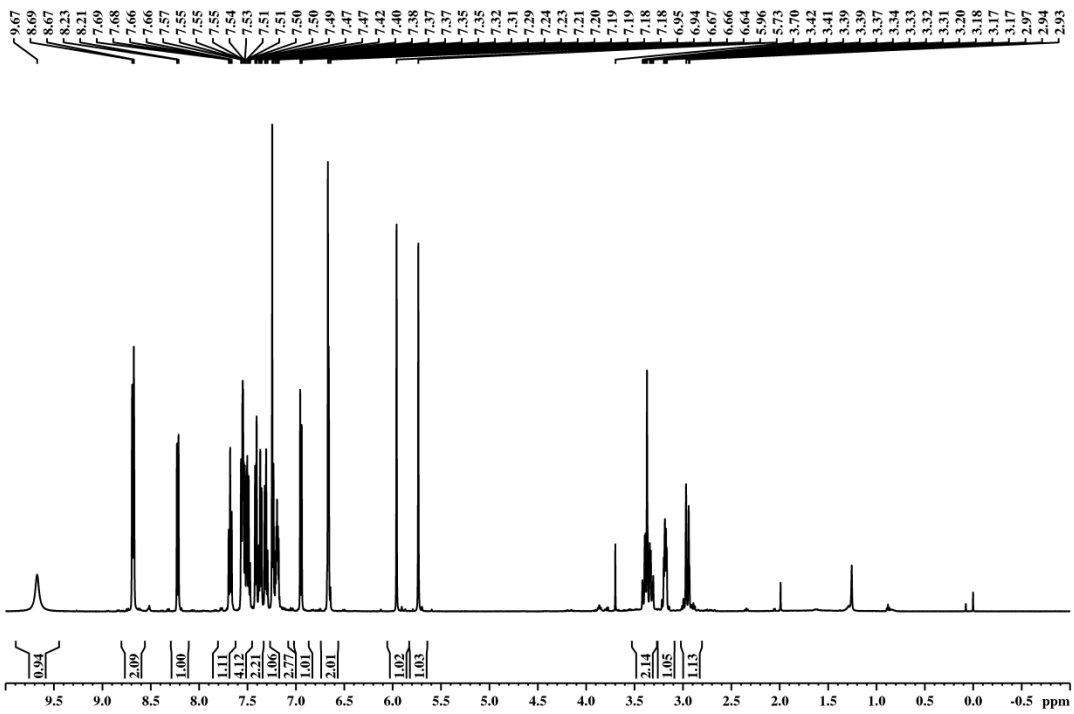


Figure S140. ^{1}H NMR spectrum of **26a**

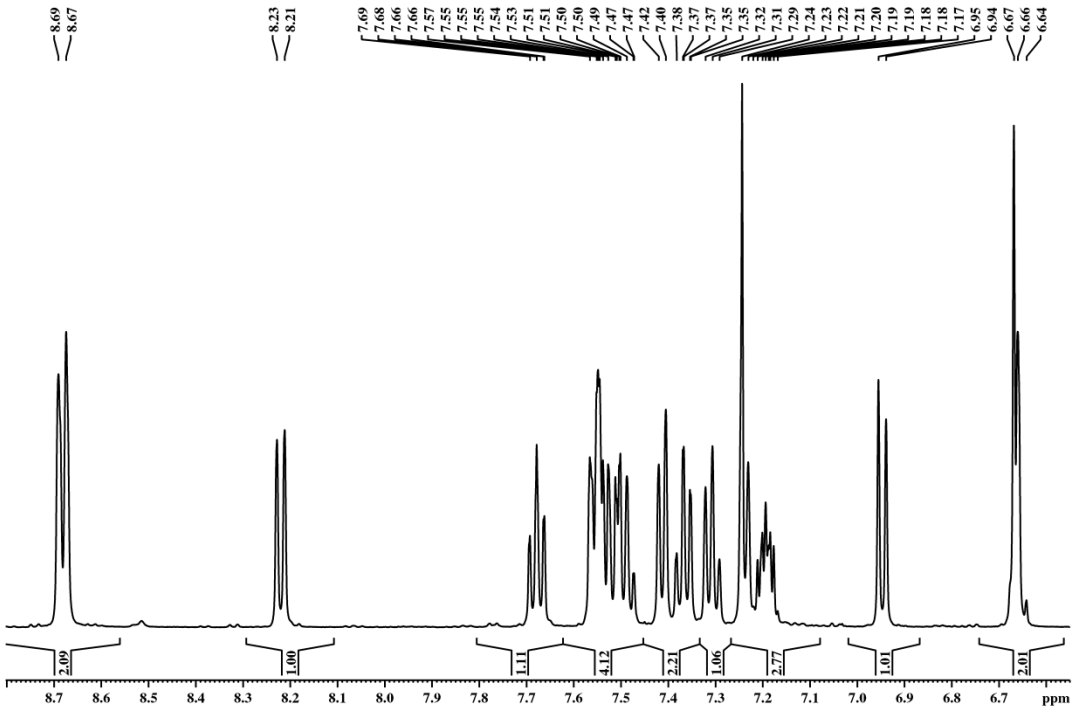


Figure S141. ^{1}H NMR spectrum of **26a**, expansion

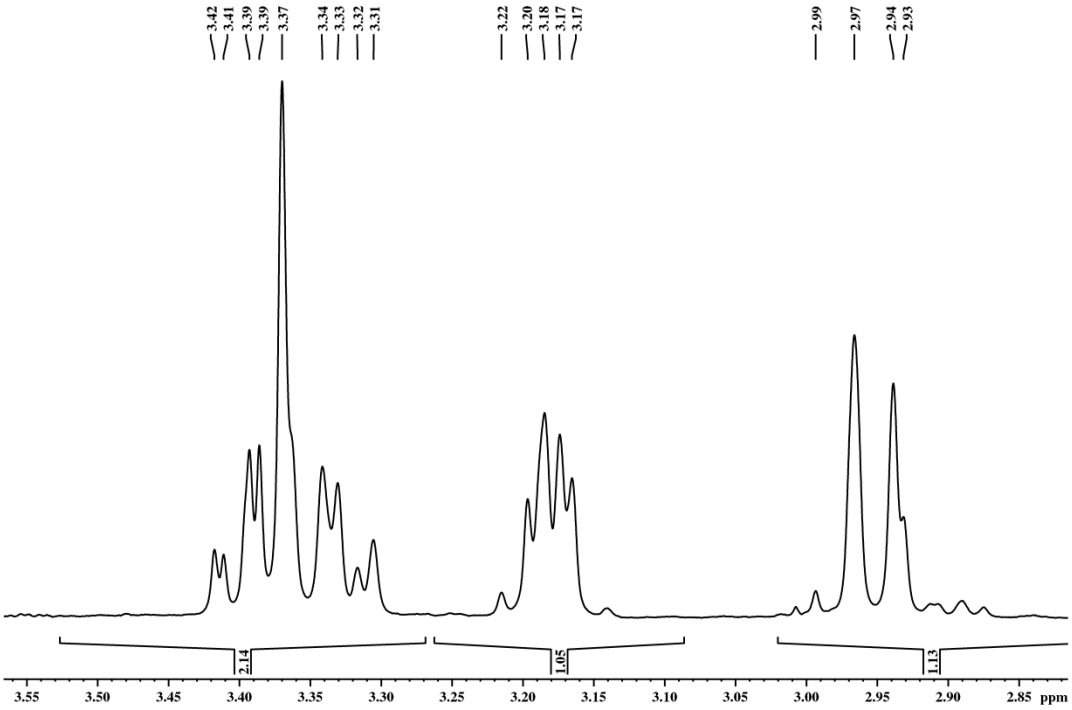


Figure S142. ^{1}H NMR spectrum of **26a**, expansion

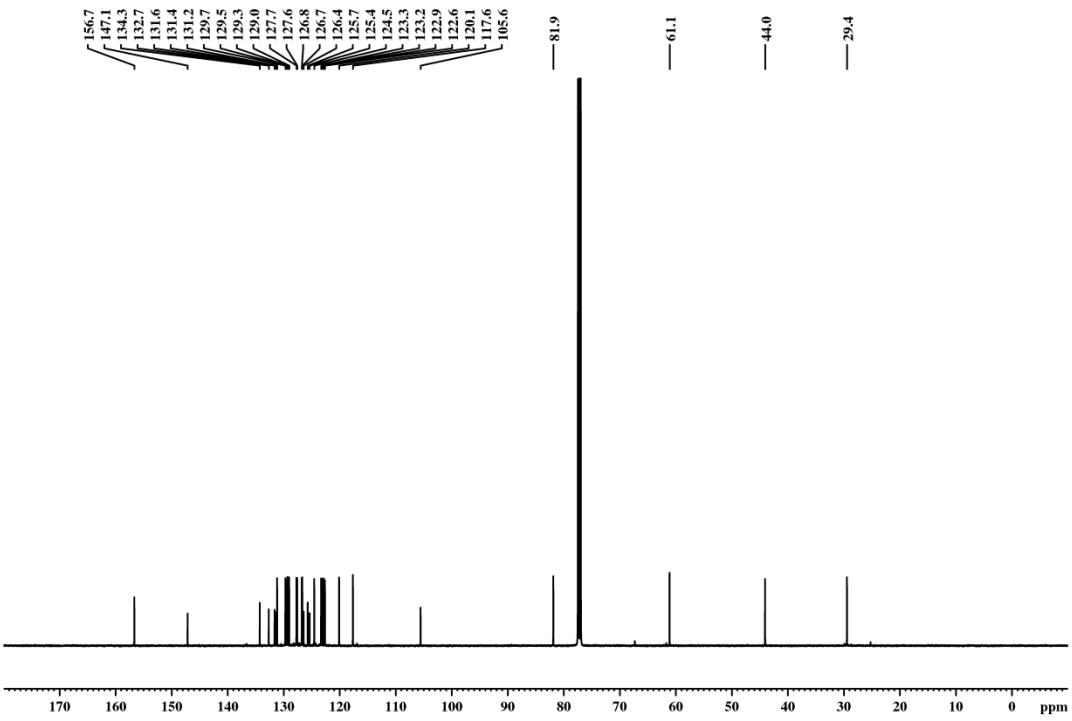


Figure S143. ^{13}C NMR spectrum of **26a**

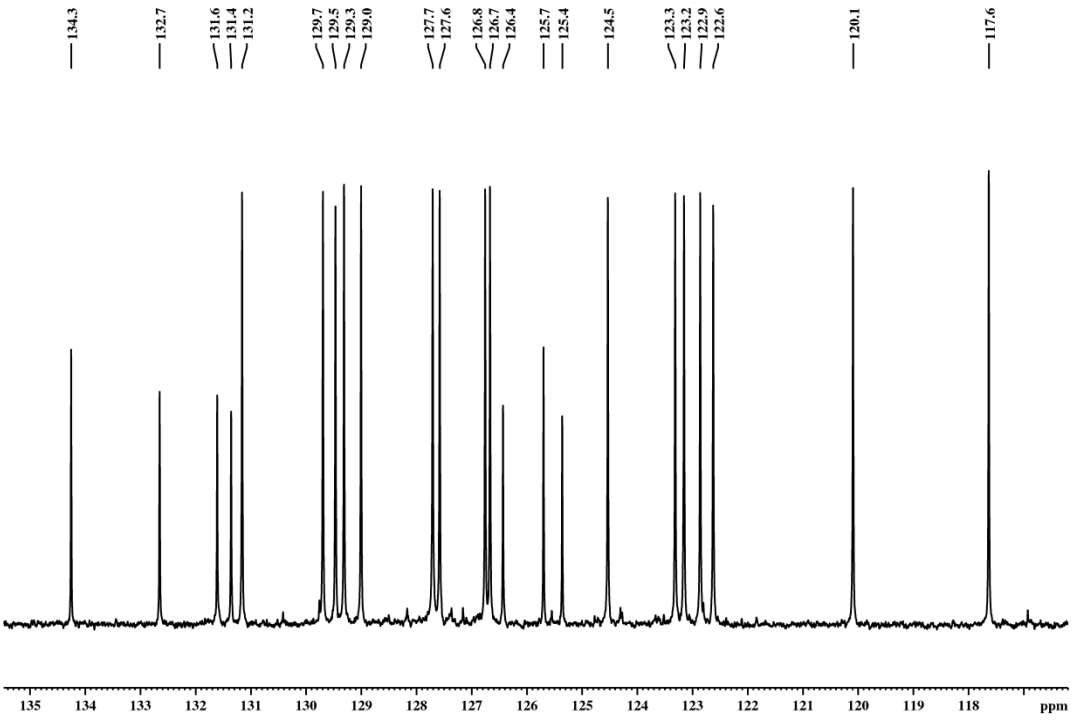


Figure S144. ^{13}C NMR spectrum of **26a**, expansion

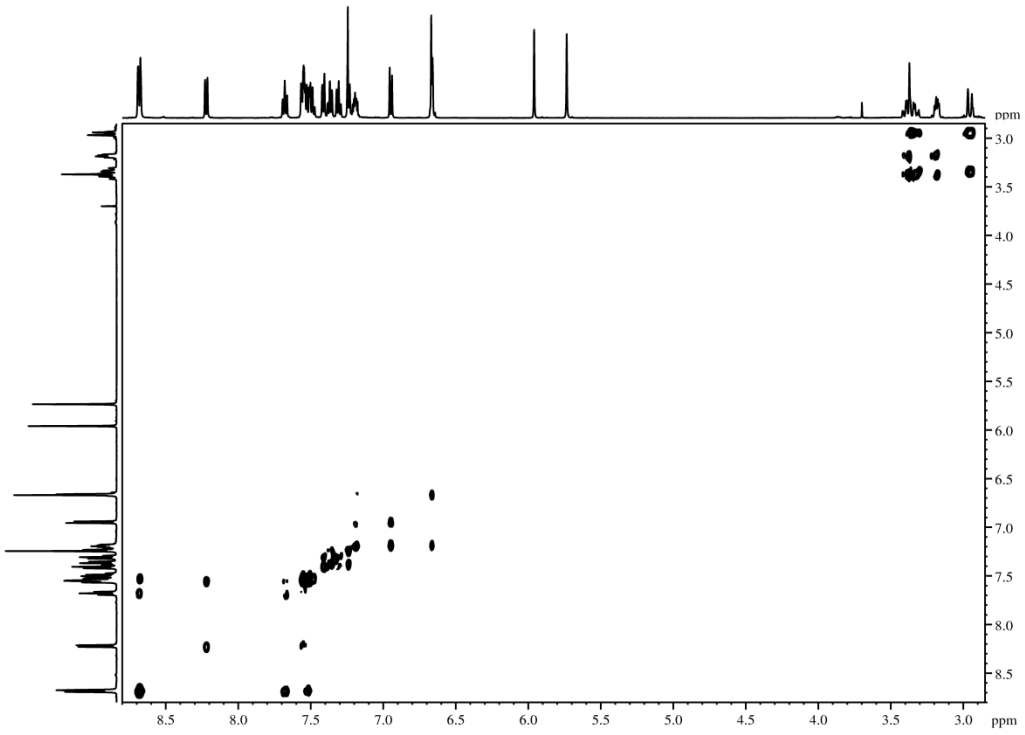


Figure S145. H,H-COSY NMR spectrum of **26a**

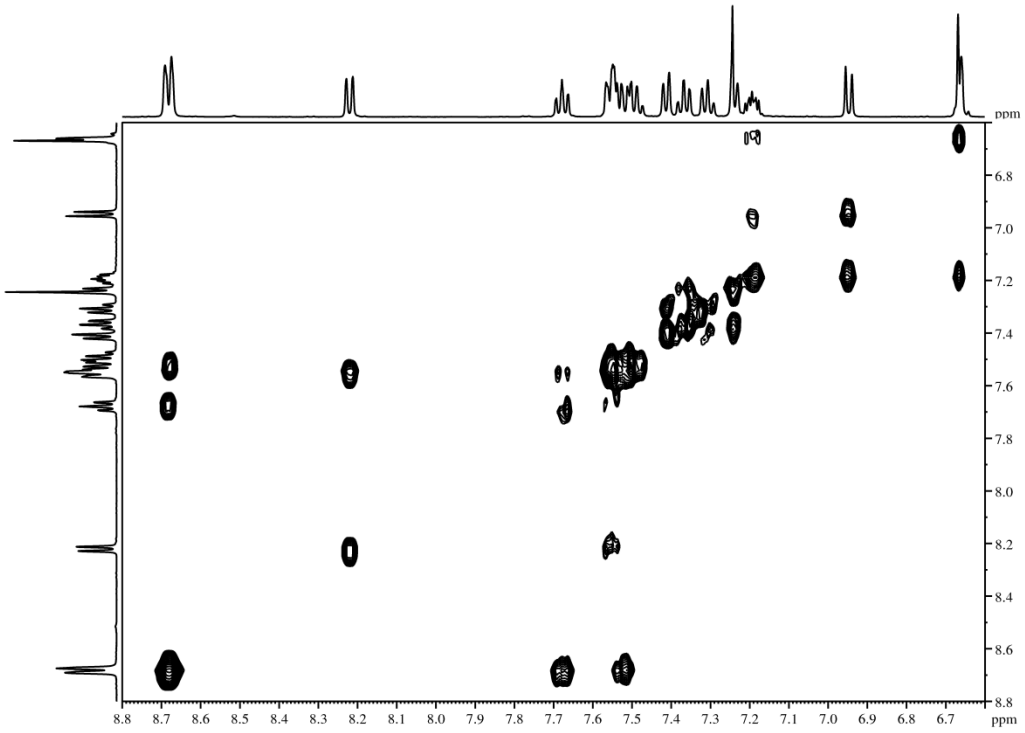


Figure S146. H,H-COSY NMR spectrum of **26a**, expansion

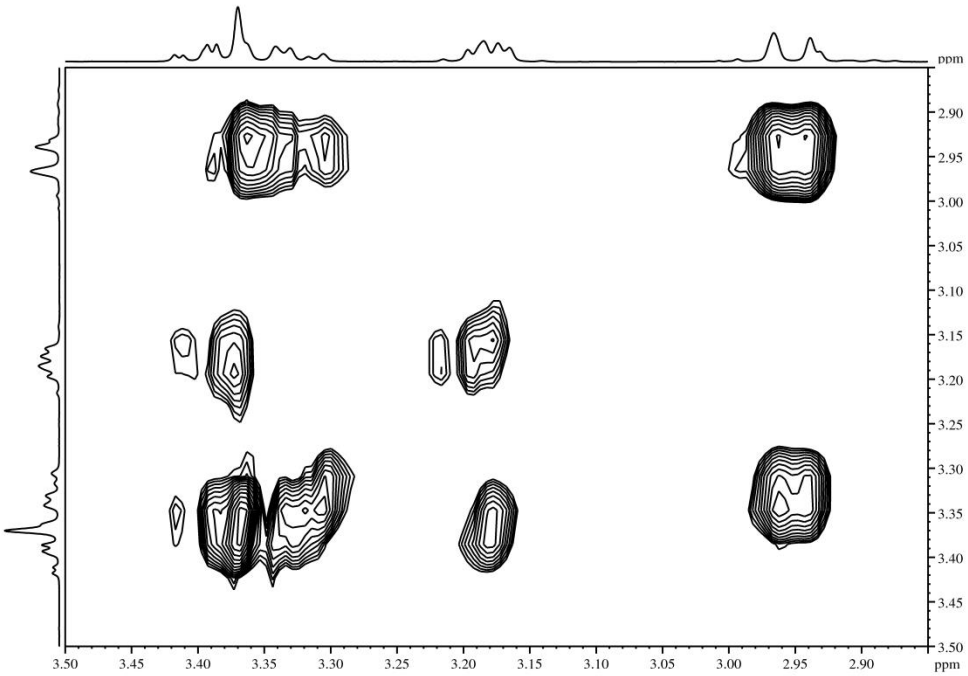


Figure S147. H,H-COSY NMR spectrum of **26a**, expansion

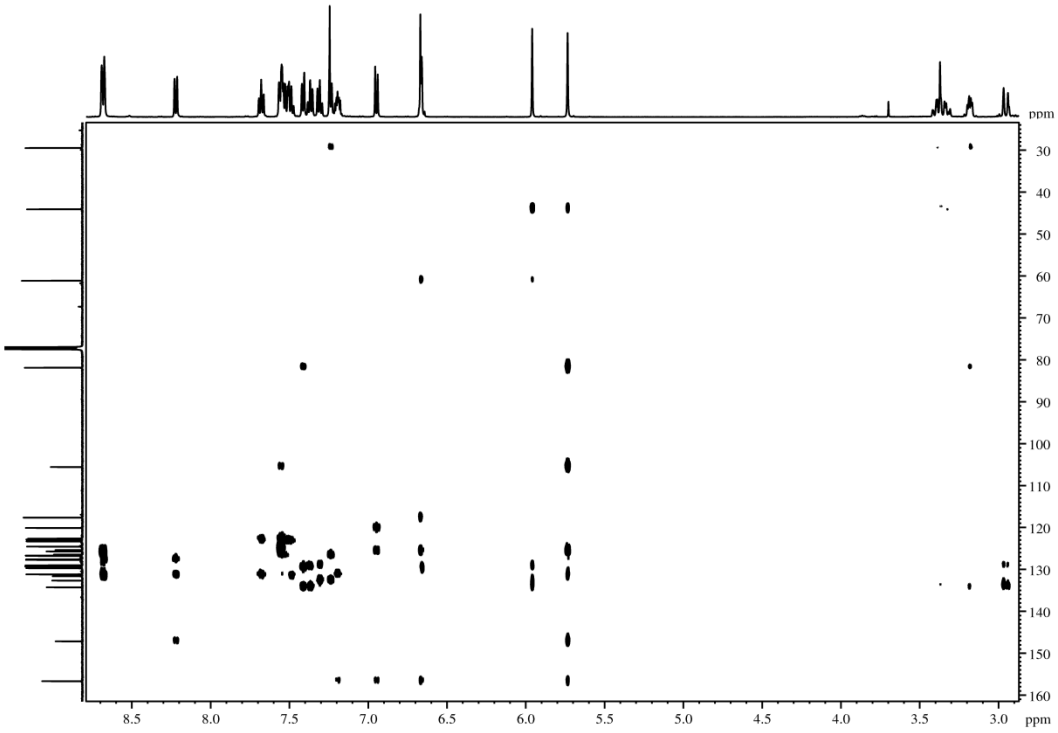


Figure S148. HMBC NMR spectrum of **26a**

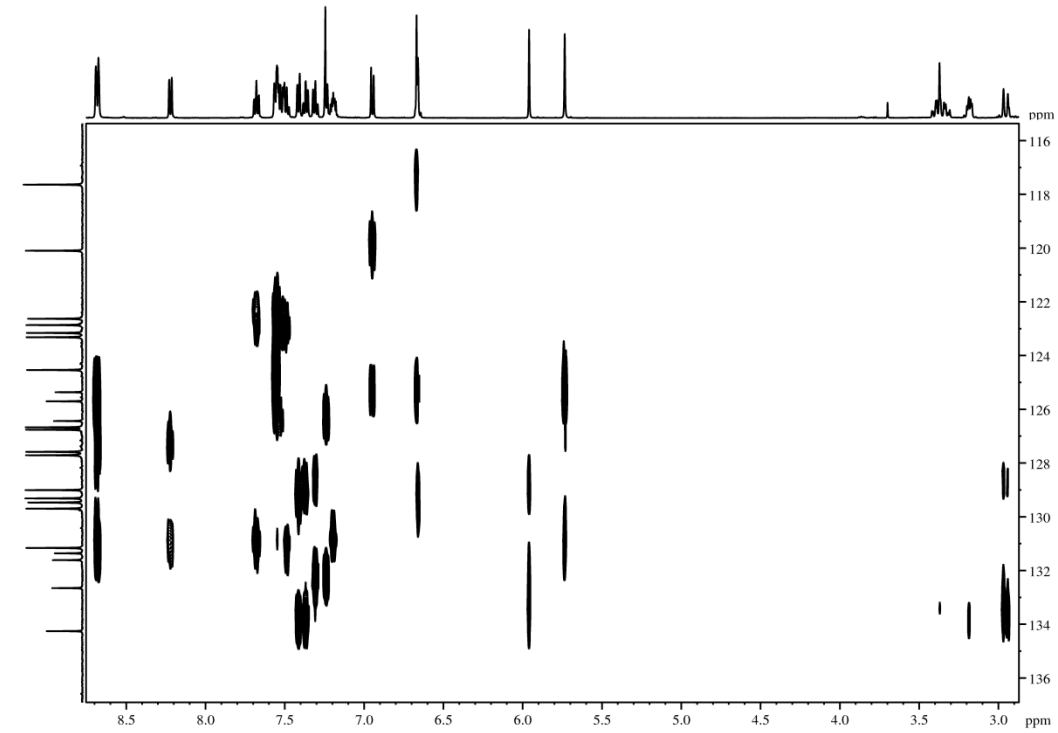


Figure S149. HMBC NMR spectrum of **26a**, expansion

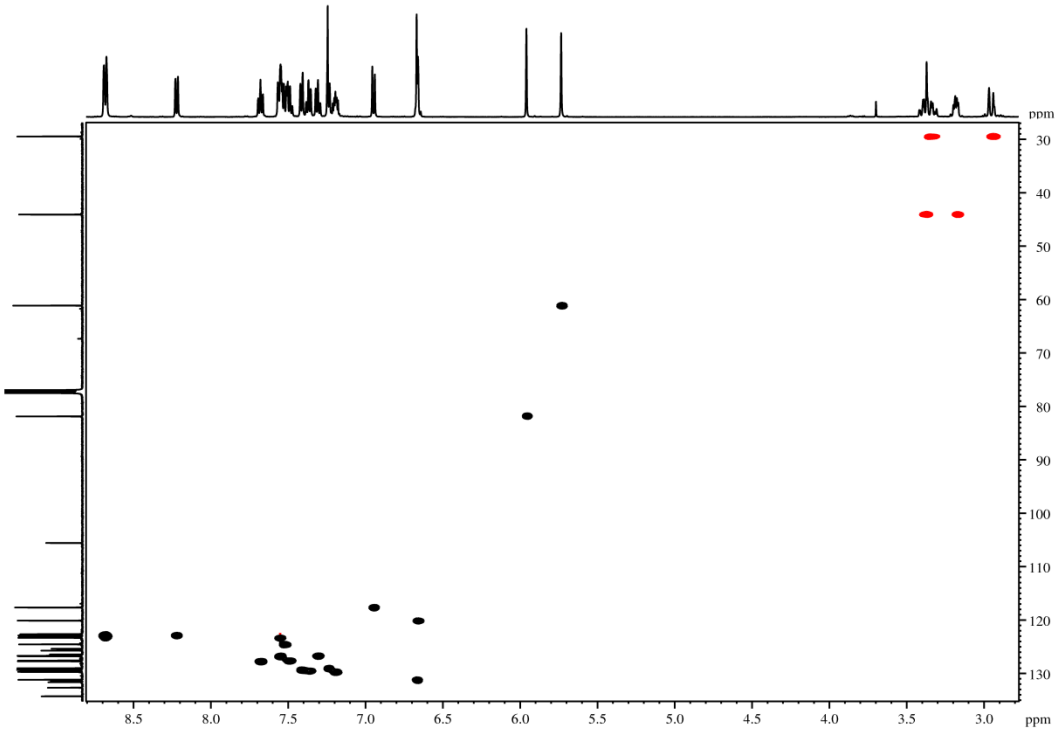


Figure S150. edited HSQC NMR spectrum of **26a** (black: positive, red: negative signals)

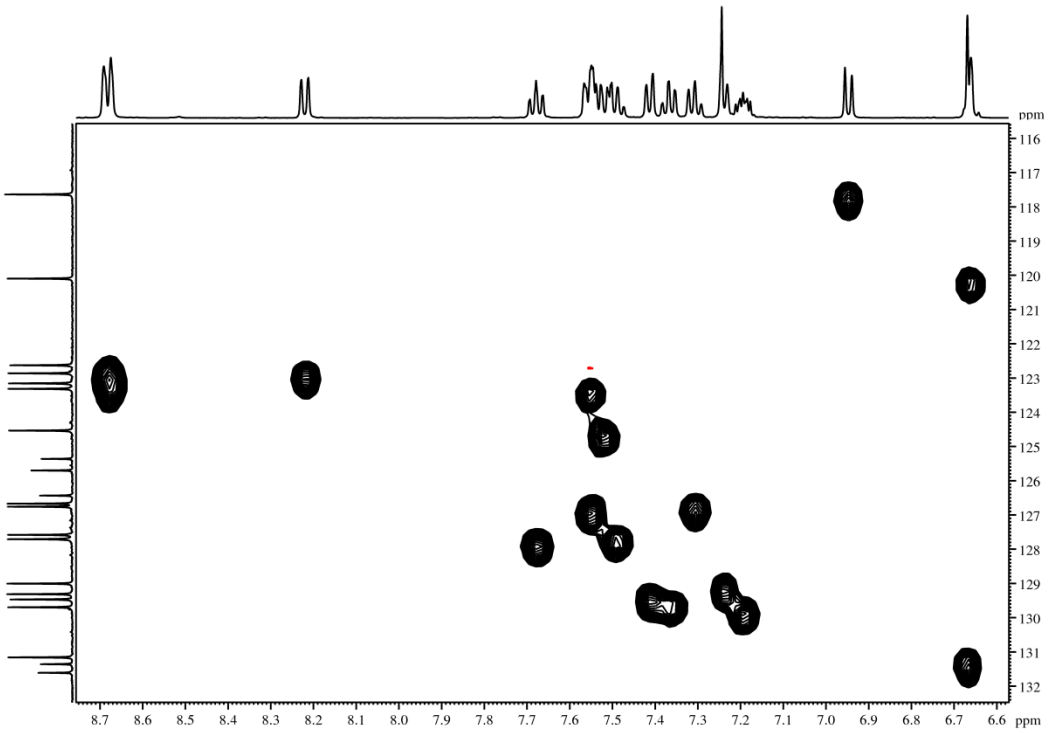


Figure S151. edited HSQC NMR spectrum of **26a**, expansion (black: positive, red: negative signals)

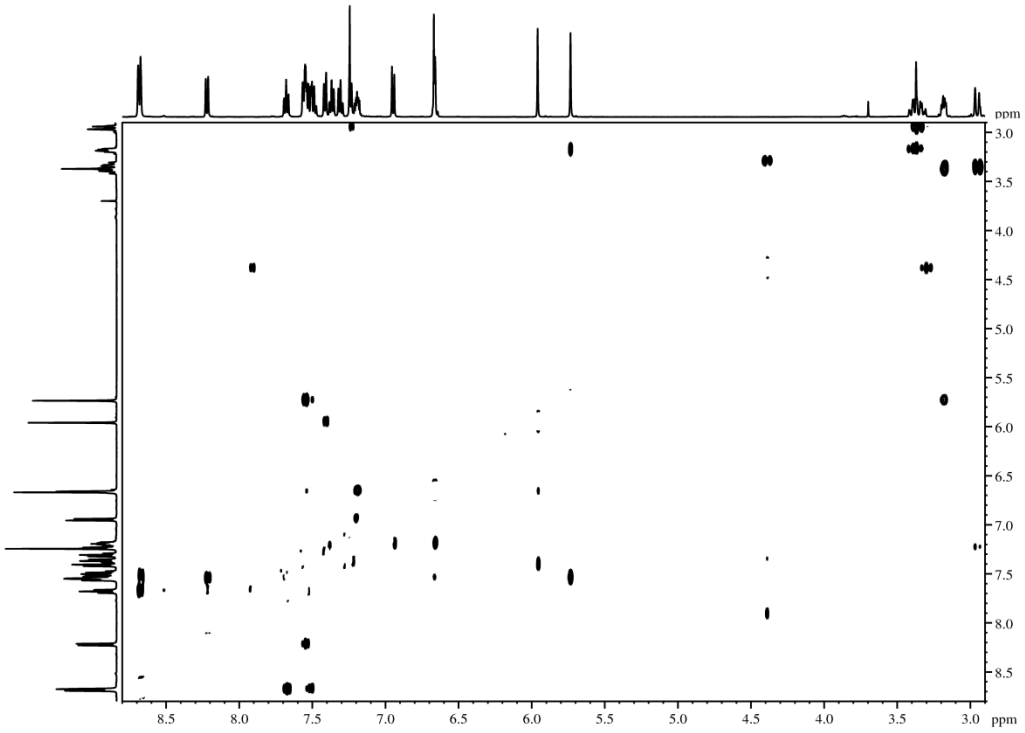
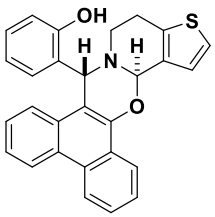


Figure S152. Phase-sensitive NOESY NMR spectrum of **26a** (only positive signals, mixing time 800 ms)

9aR*,16S*-16-(2-Hydroxyphenyl)-phenanthr[9,10-e]oxazino[2,3-a]thieno[3,2-c]pyridine (28)



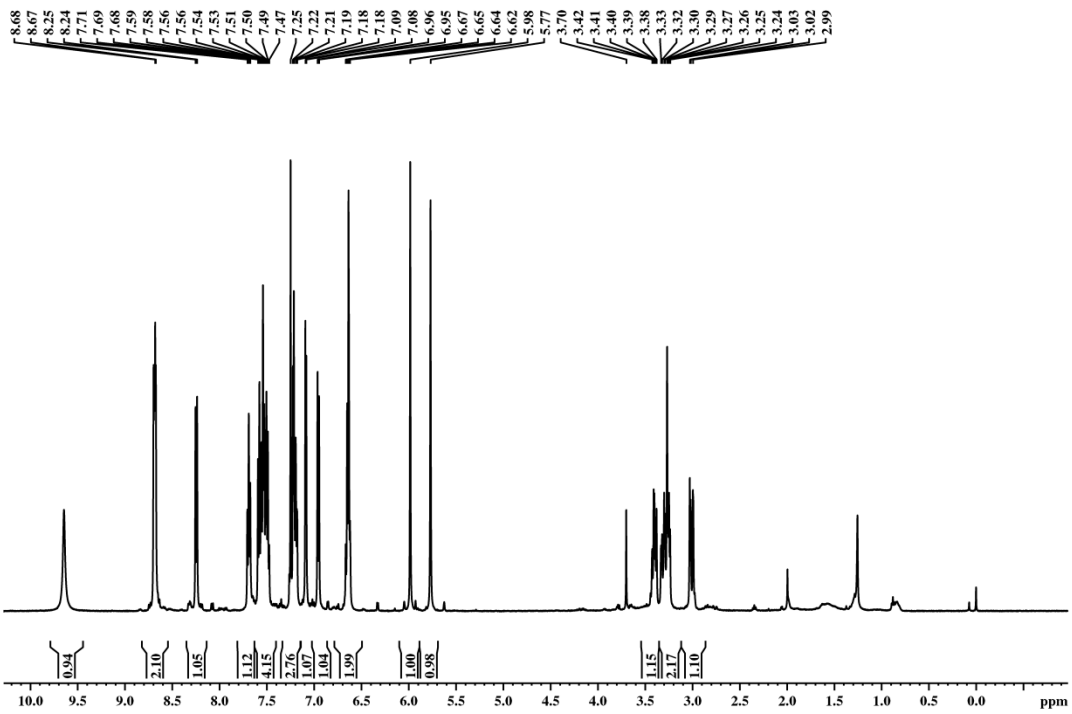


Figure S153. ^{1}H NMR spectrum of **28a**

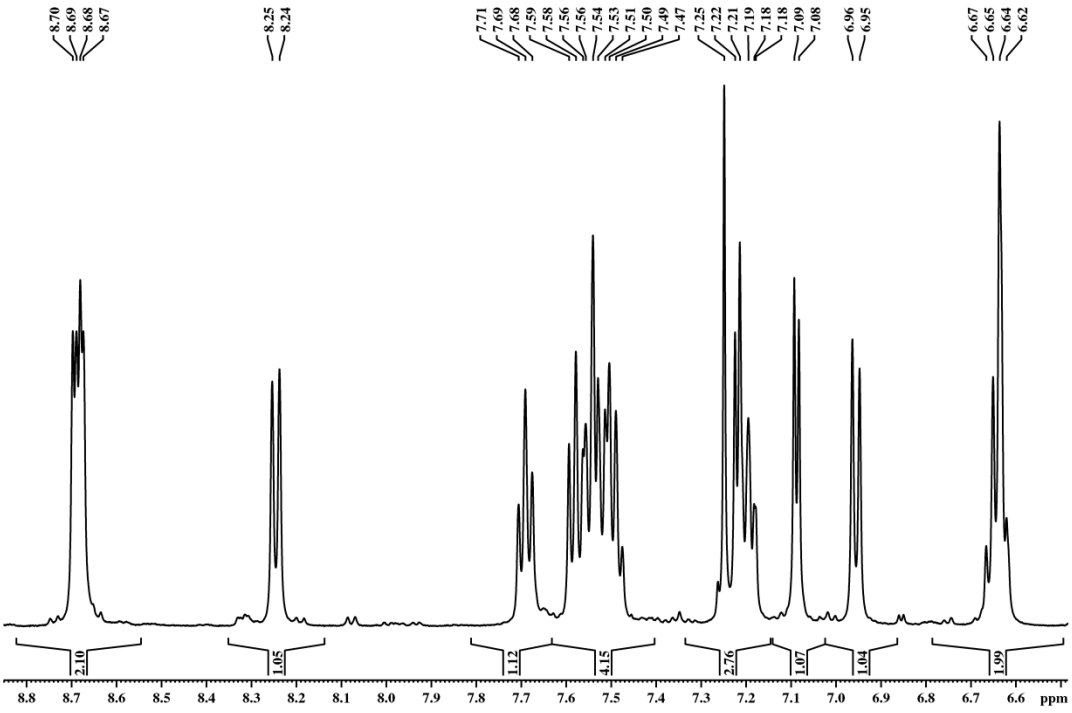


Figure S154. ^{1}H NMR spectrum of **28a**, expansion

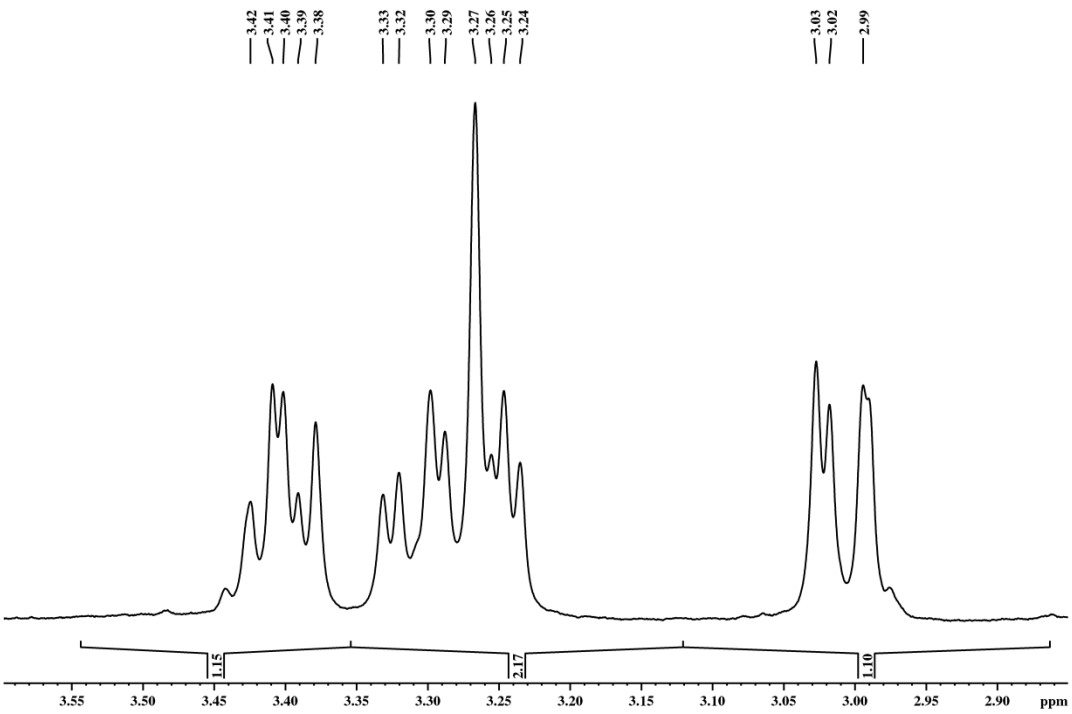


Figure S155. ^{1}H NMR spectrum of **28a**, expansion

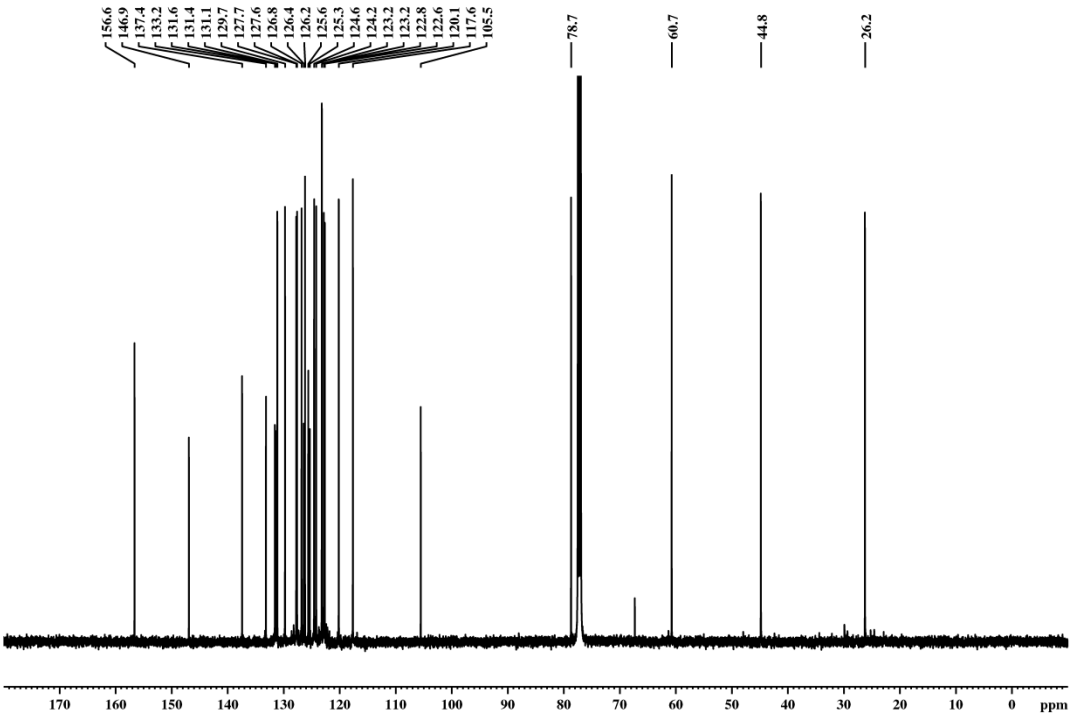


Figure S156. ^{13}C NMR spectrum of **28a**

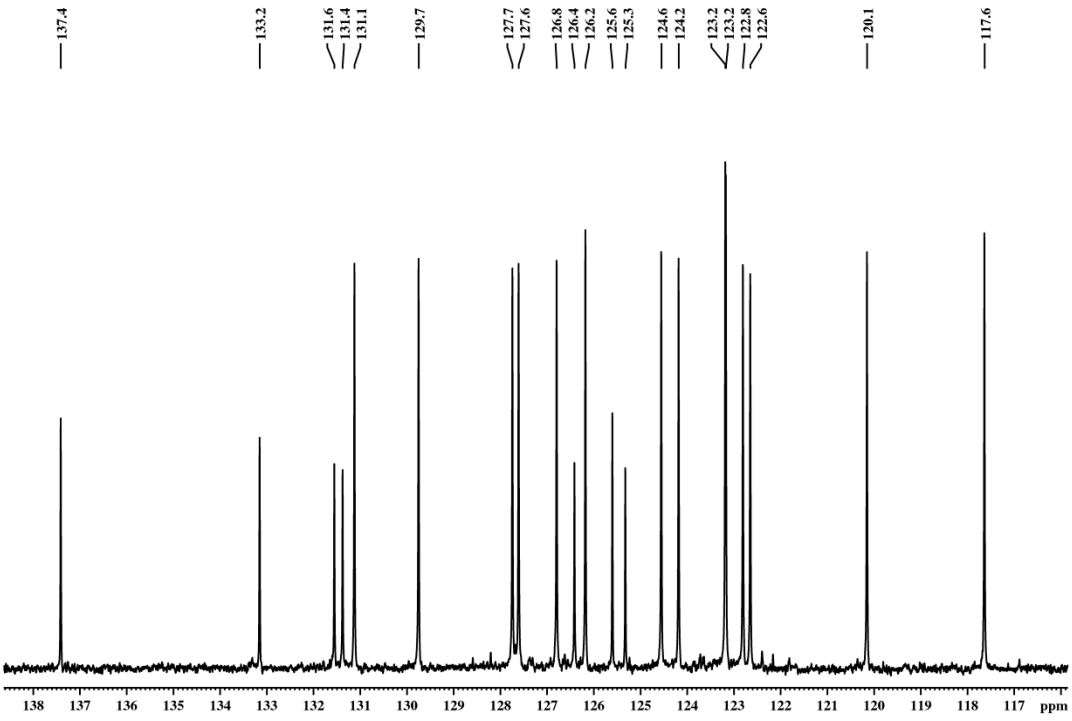


Figure S157. ^{13}C NMR spectrum of **28a**, expansion

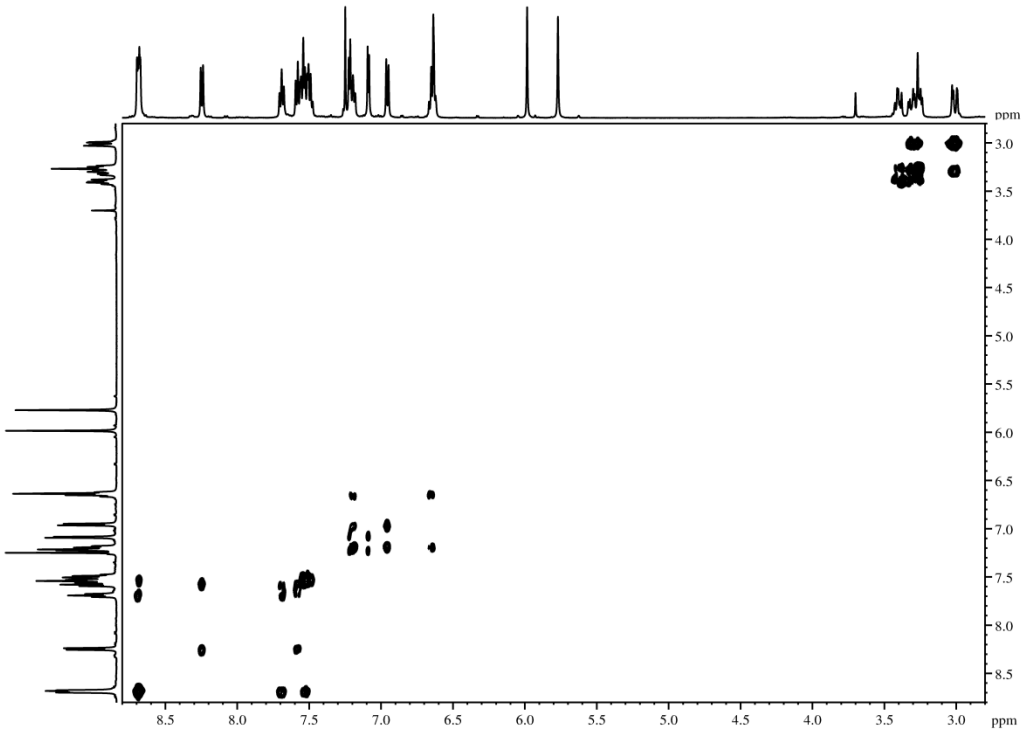


Figure S158. H,H-COSY NMR spectrum of **28a**

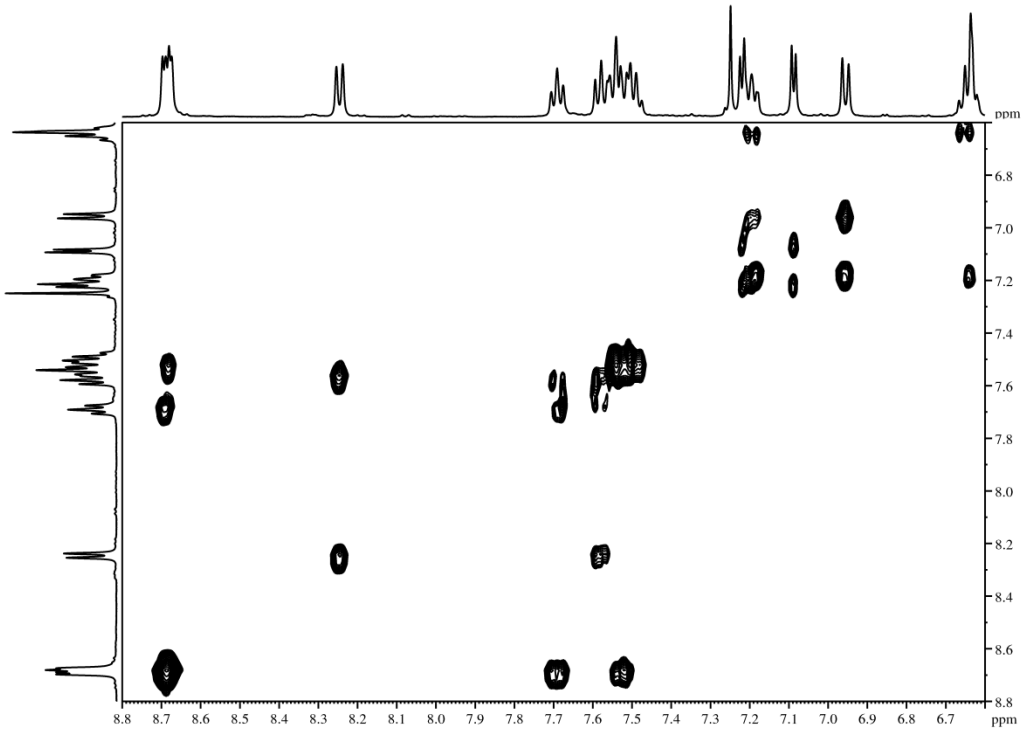


Figure S159. H,H-COSY NMR spectrum of **28a**, expansion

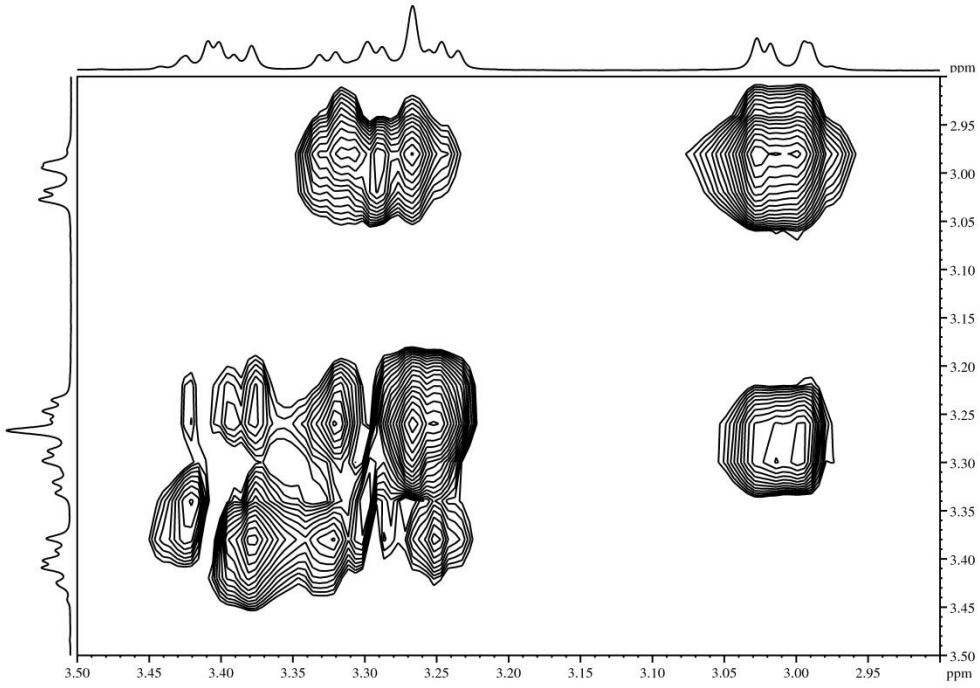


Figure S160. H,H-COSY NMR spectrum of **28a**, expansion

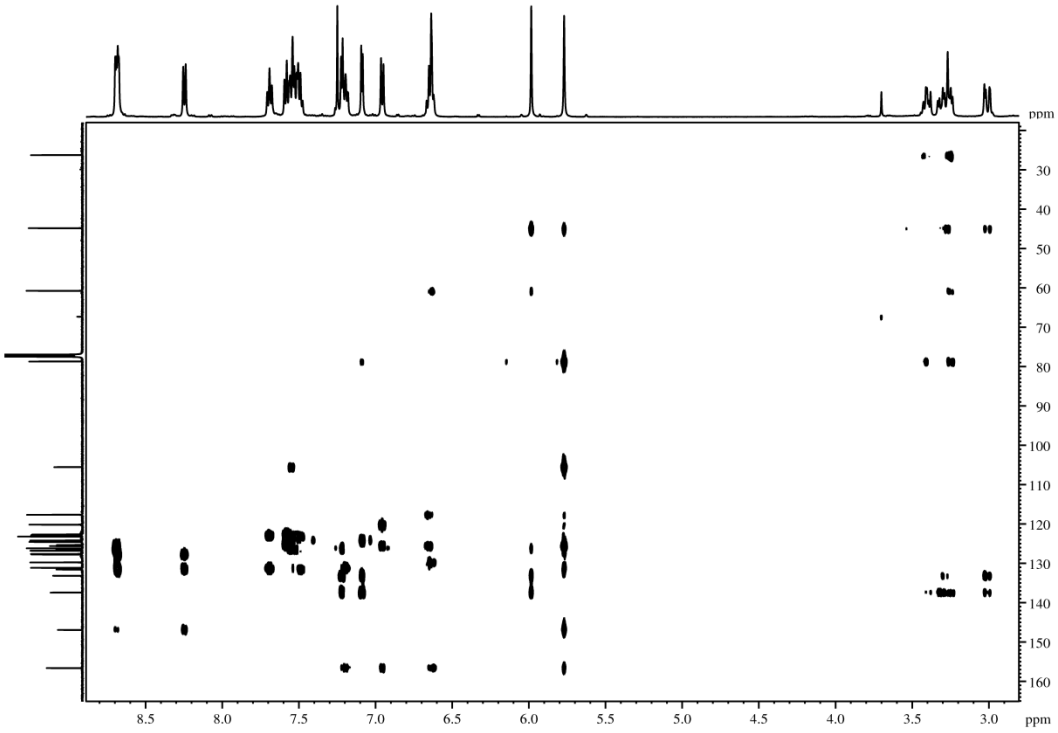


Figure S161. HMBC NMR spectrum of **28a**

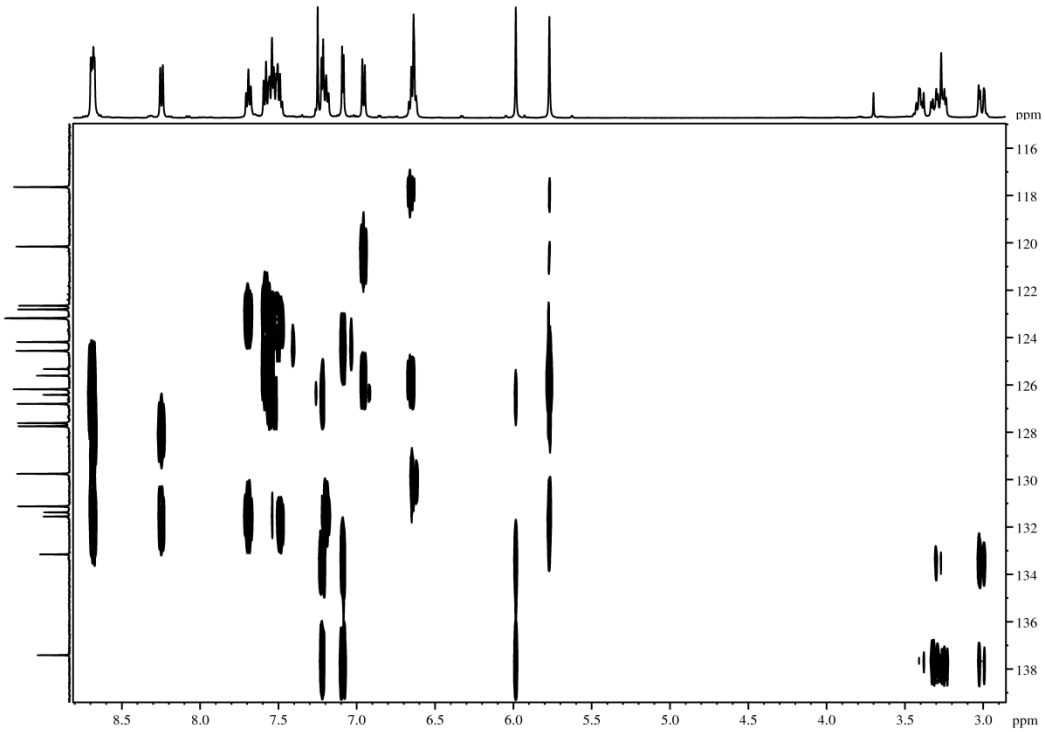


Figure S162. HMBC NMR spectrum of **28a**, expansion

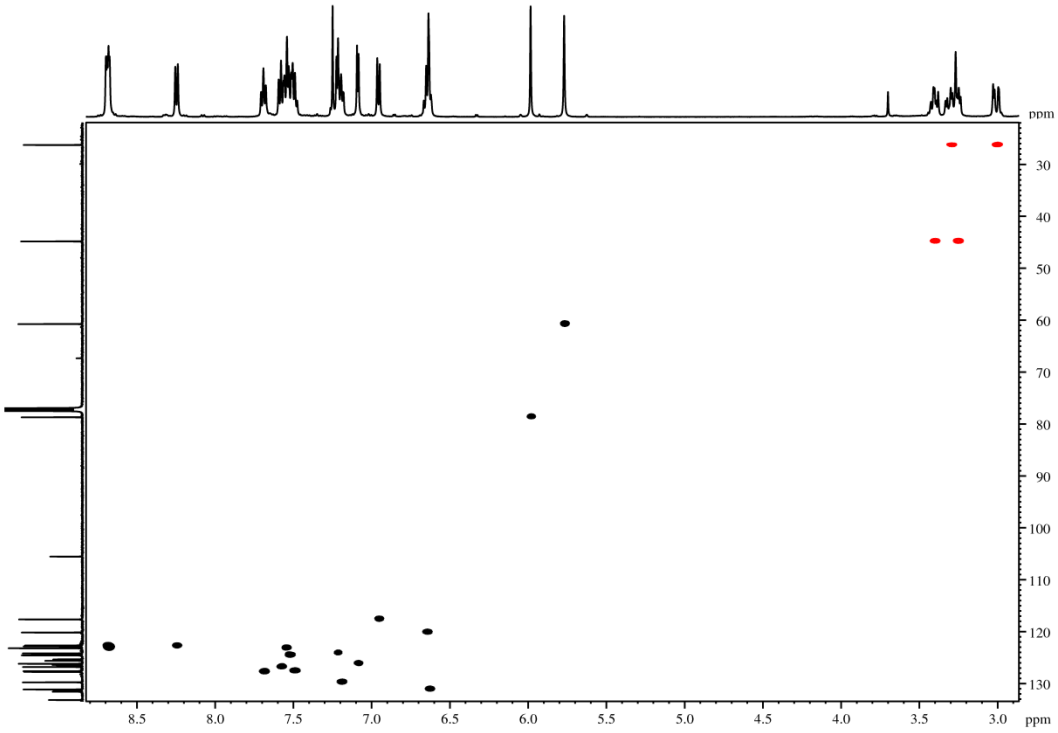


Figure S163. edited HSQC NMR spectrum of **28a** (black: positive, red: negative signals)

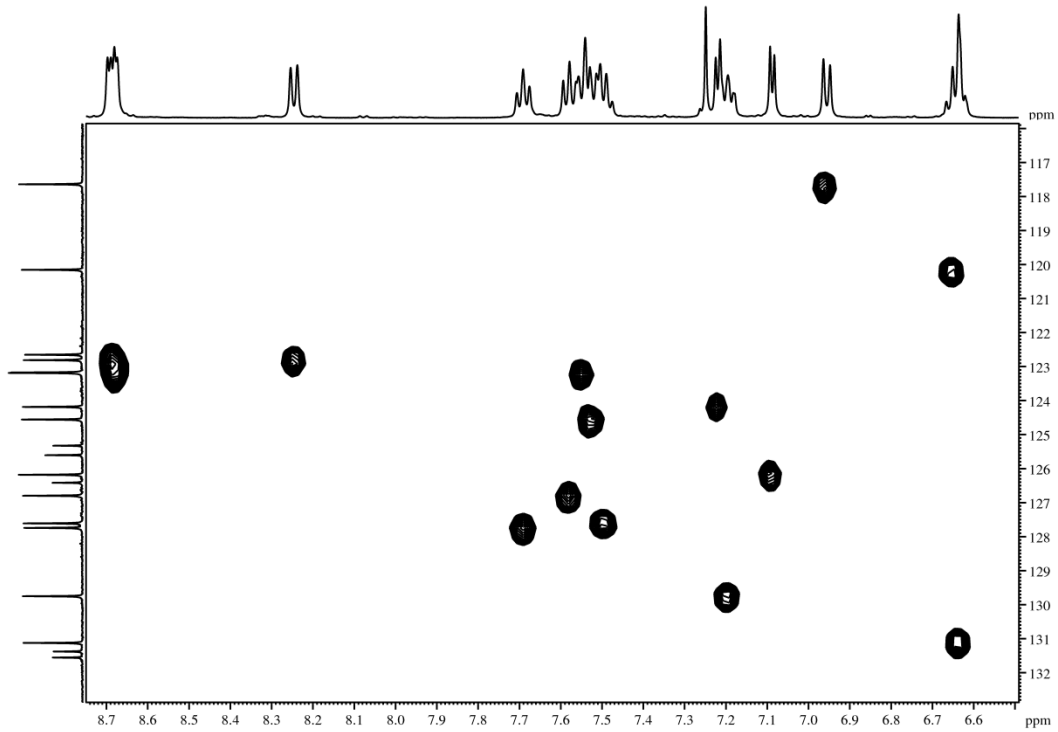


Figure S164. edited HSQC NMR spectrum of **28a**, expansion (black: positive, red: negative signals)

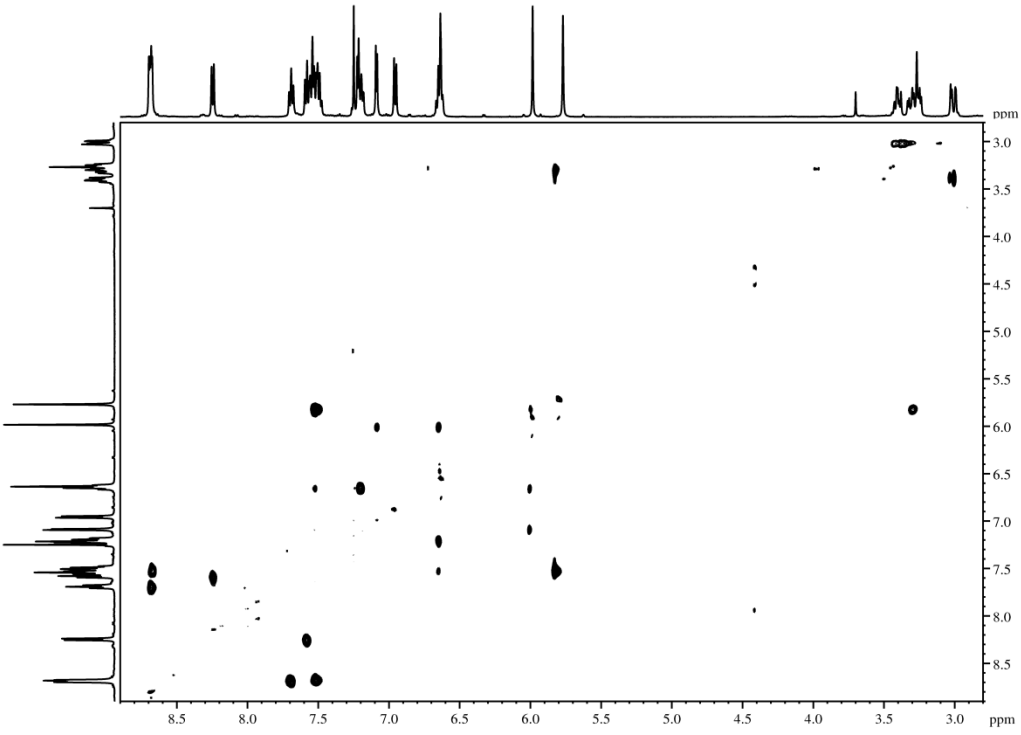


Figure S165. Phase-sensitive NOESY NMR spectrum of **28a** (only positive signals, mixing time 800 ms)