

Supporting information

Functionalization of *N,N*-Dialkylferrocenesulfonamides toward Substituted Derivatives

Min Wen,^a William Erb,^{a*} Florence Mongin,^a Yury S. Halauko,^{b*} Oleg A. Ivashkevich,^c
Vadim E. Matulis,^c Thierry Roisnel^a and Vincent Dorcet^a

^a *Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226,
F-35000 Rennes, France*

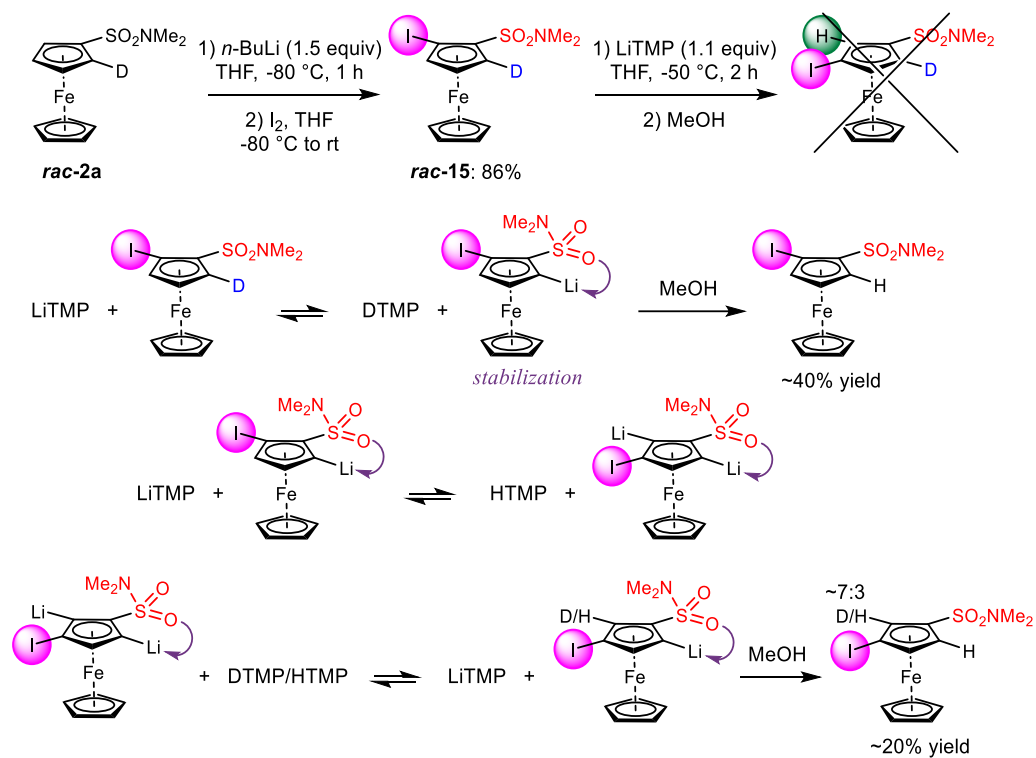
^b *UNESCO Chair of Belarusian State University, 14 Leningradskaya Str., Minsk 220030, Belarus*

^c *Research Institute for Physico-Chemical Problems of Belarusian State University,
14 Leningradskaya Str., Minsk 220030, Belarus*

E-mails: william.erb@univ-rennes1.fr, hys@tut.by

Table of Contents

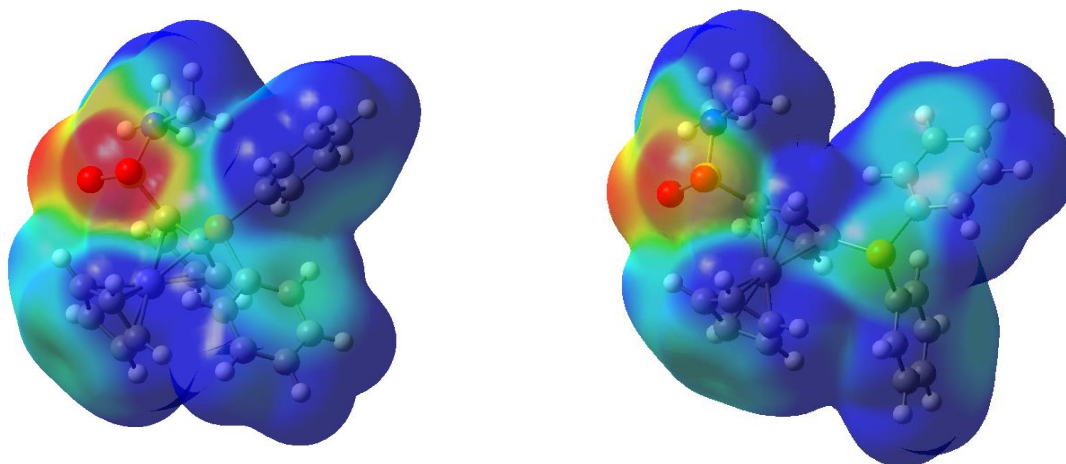
Putative reaction sequence to rationalize the unsuccessful attempt to use deuterium as protecting group in the ‘halogen dance’ reaction	p. S2
Selected calculated NPA charges of potential donor centers	p. S2
Molecular electrostatic potential mapped on an SCF density (isoval = 0.0004)	p. S3
Calculated values of the Gibbs energies $\Delta_{\text{acid}}G$ [kcal mol ⁻¹] for the deprotonation at the corresponding positions of the investigated compounds (gas-phase acidities)	p. S3
NMR spectra of compounds 2a-j , 4a,b , 4c1 , 4c2 , 4d-g , 5 , 6a-c , 7 , 8 , 9 , 10a-c , 11 , 12 , 13a,b , 14 , 15 , 16a,b , 17ab and 18a,b	p. S4-S149
NMR NOESY correlations of compounds 2b , 2d-f , 2h,i , 4b , 4c1 , 4c2 , 4e , 4g , 5 , 6a-c , 9 , 10a-c , 11 , 13a,b , 16b and 18a,b	p. S150-S151



Scheme S1. Putative reaction sequence to rationalize the unsuccessful attempt to use deuterium as protecting group in the ‘halogen dance’ reaction

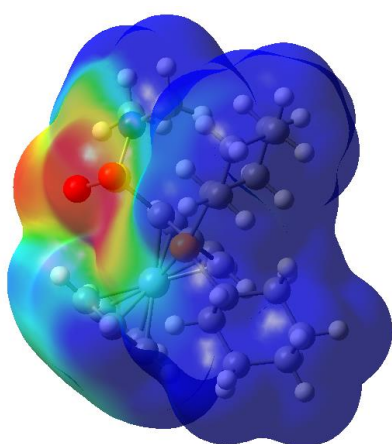
Table S1. Selected calculated NPA charges of potential donor centers

Structure	P	O(1)	O(2)	N
2h	+0.956	-0.939	-0.956	-0.717
2i	+0.938	-0.944	-0.947	-0.718
18a	+0.934	-0.949	-0.952	-0.713
18b	+0.906	-0.951	-0.951	-0.712

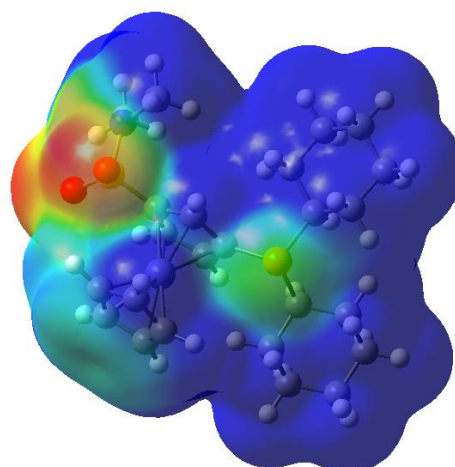


2h

18a



2i



18b

−0.055  0.0

Figure S1. Molecular electrostatic potential mapped on an SCF density (isoval = 0.0004).

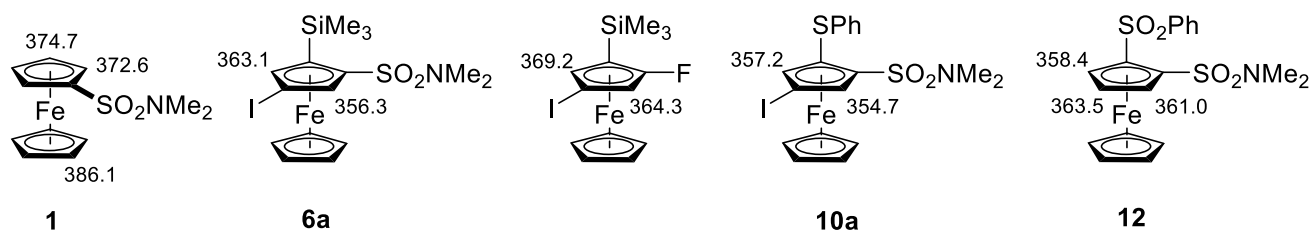


Figure S2. Calculated values of the Gibbs energies $\Delta_{\text{acid}}G$ [kcal mol⁻¹] for the deprotonation at the corresponding positions of the investigated compounds (gas-phase acidities).

NMR spectra

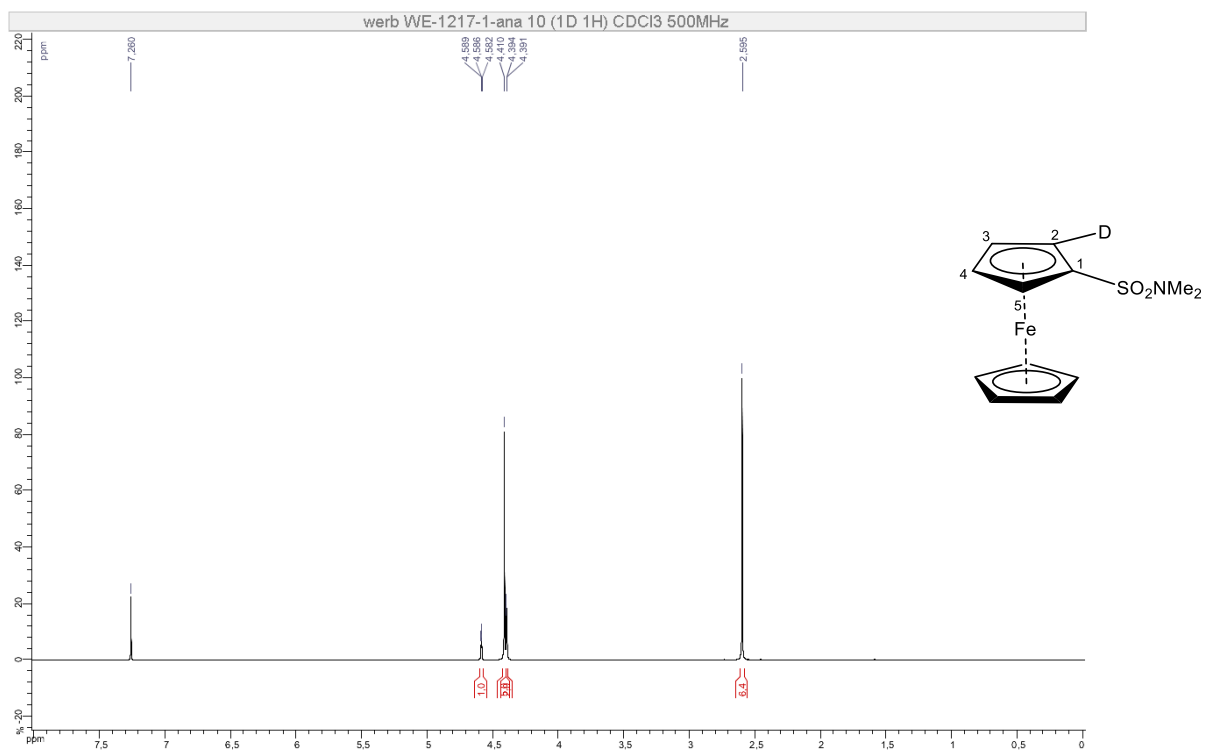


Figure S3. ^1H NMR (500 MHz, CDCl_3) of **2a** (racemic mixture)

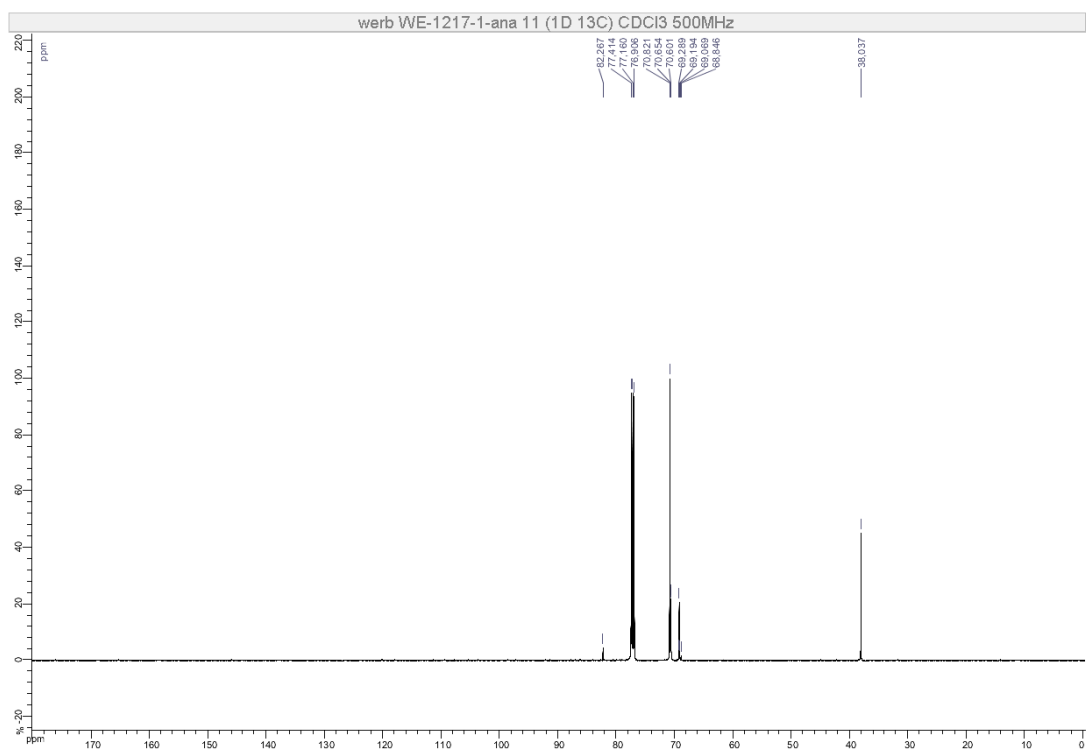


Figure S4. ^{13}C NMR (126 MHz, CDCl_3) of **2a** (racemic mixture)

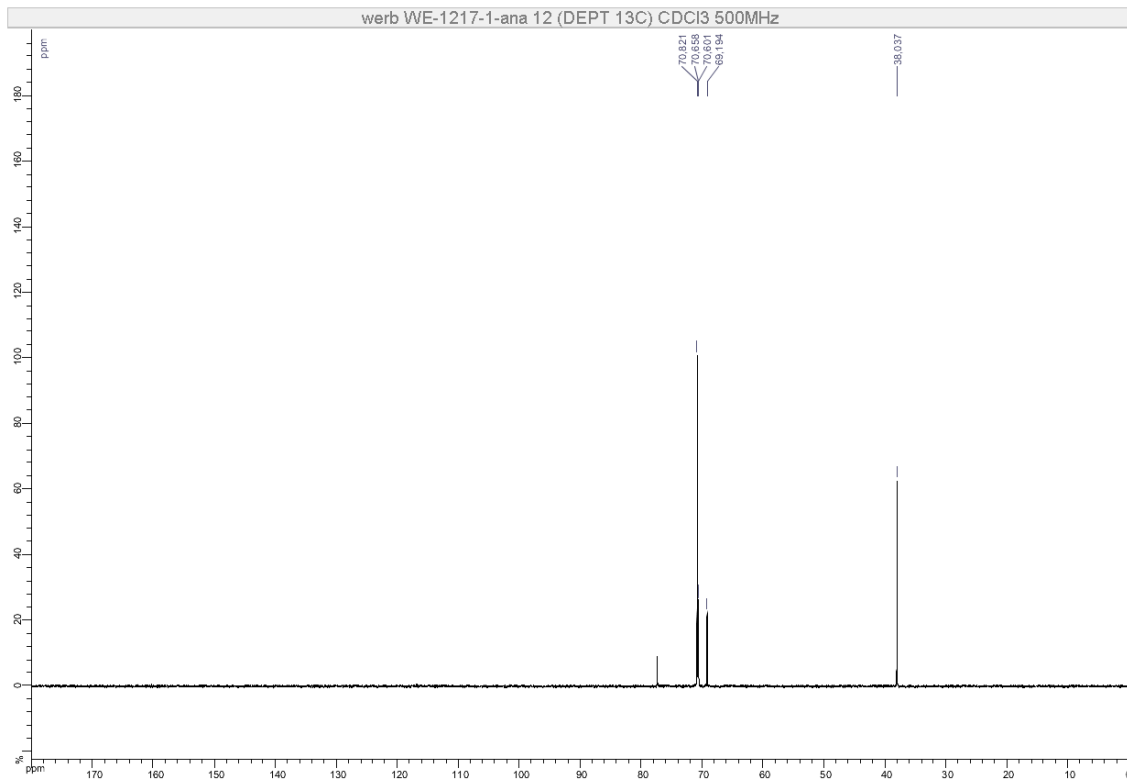


Figure S5. DEPT 135 (126 MHz, CDCl₃) of **2a** (racemic mixture)

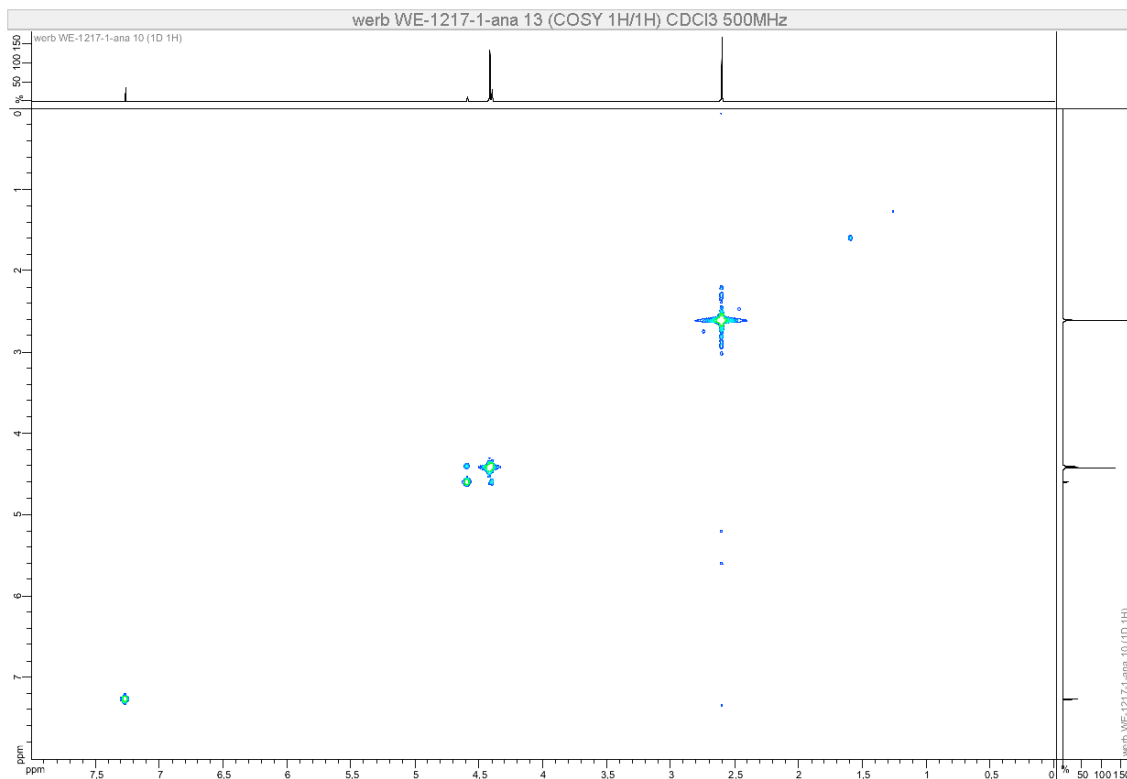


Figure S6. COSY (500 MHz, CDCl₃) of **2a** (racemic mixture)

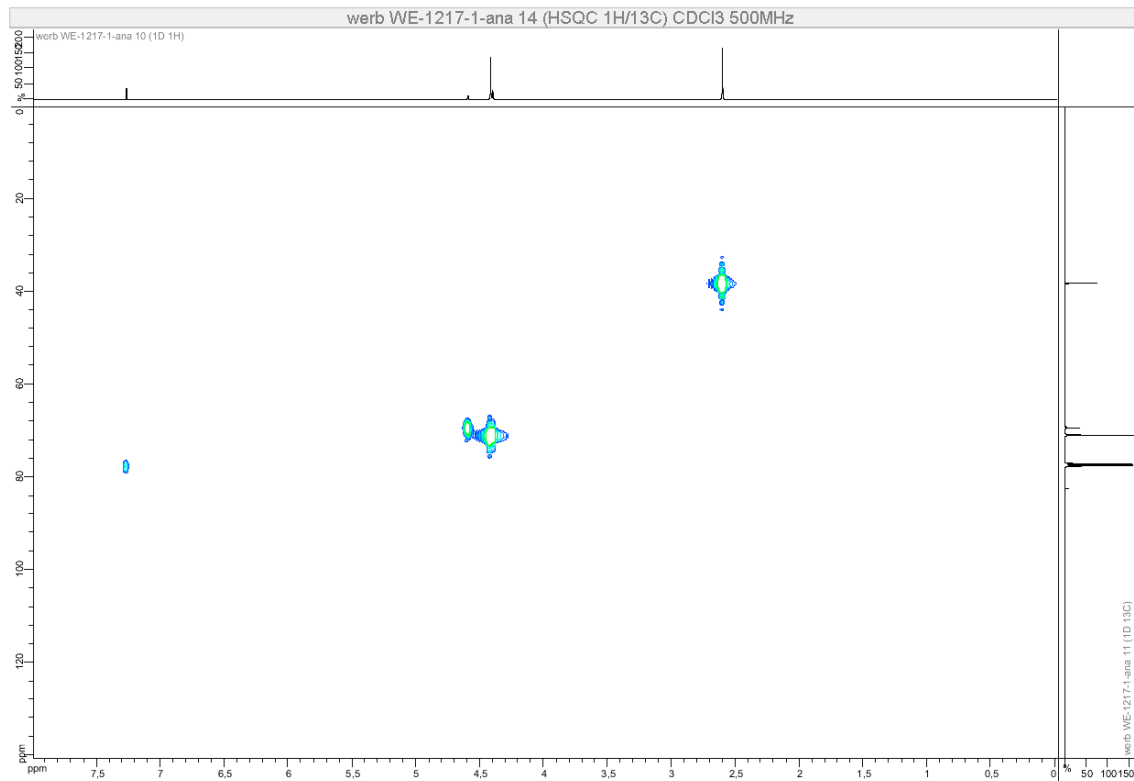


Figure S7. HSQC (500 MHz, CDCl₃) of **2a** (racemic mixture)

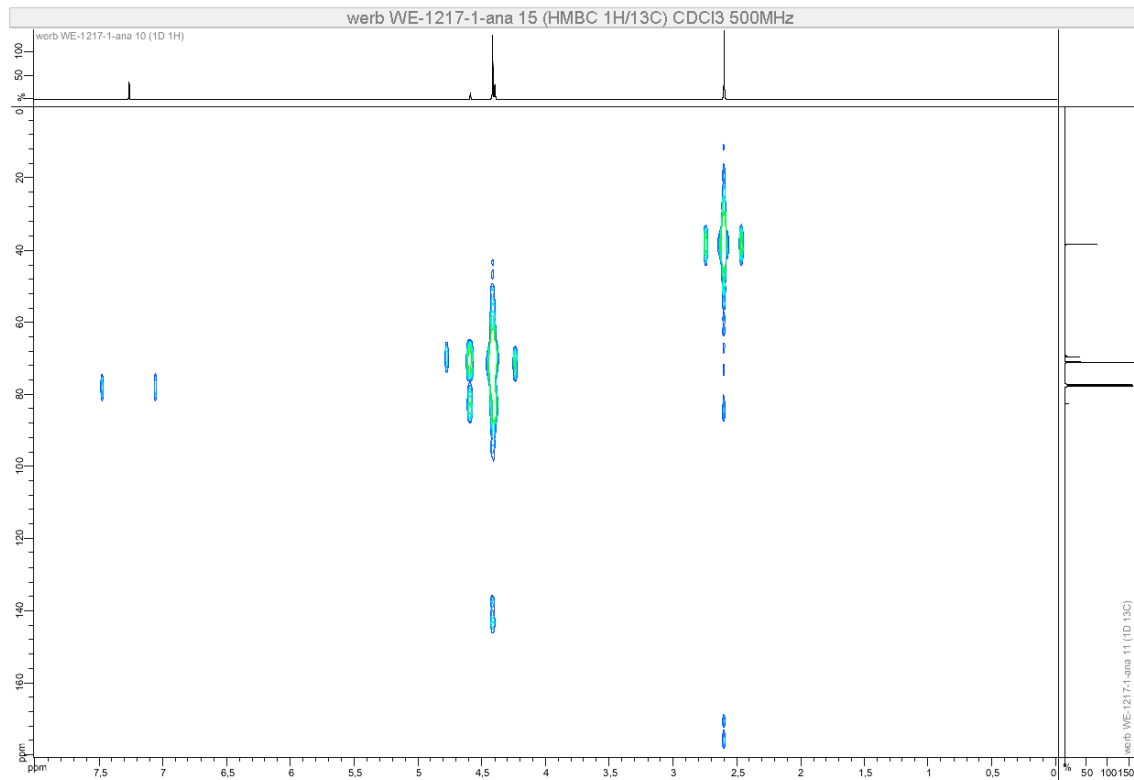


Figure S8. HMBC (500 MHz, CDCl₃) of **2a** (racemic mixture)

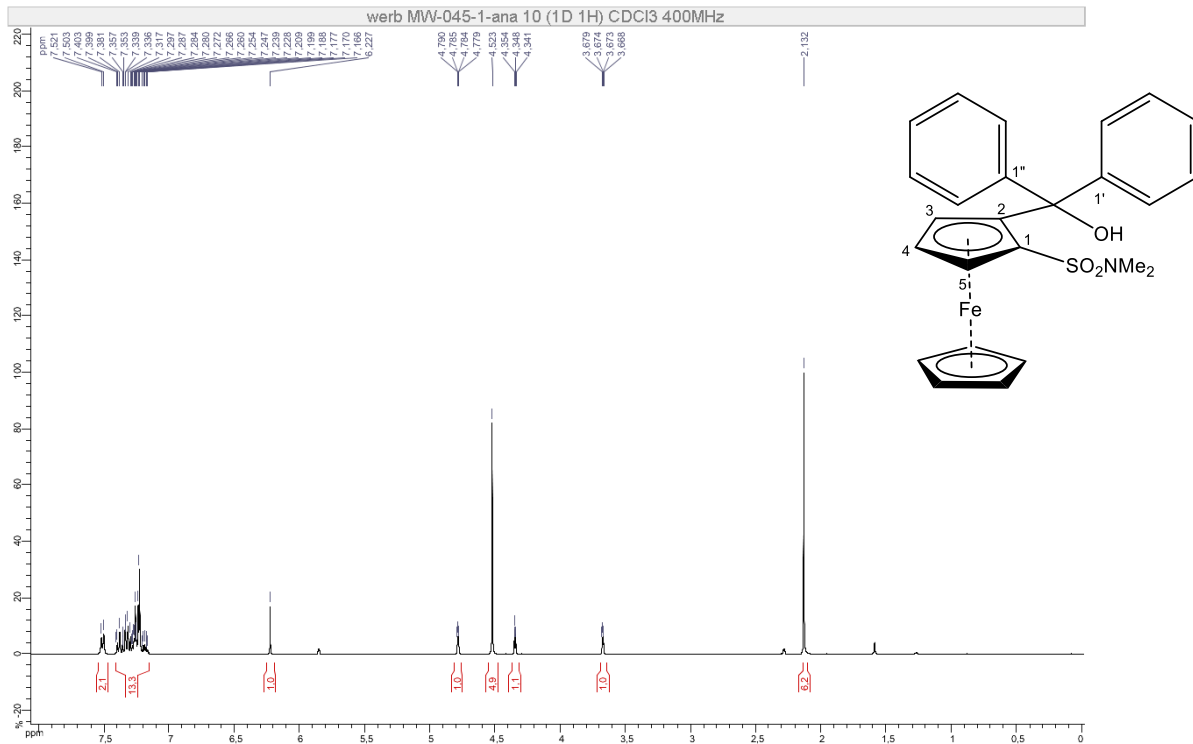


Figure S9. ^1H NMR (400 MHz, CDCl_3) of **2b** (racemic mixture)

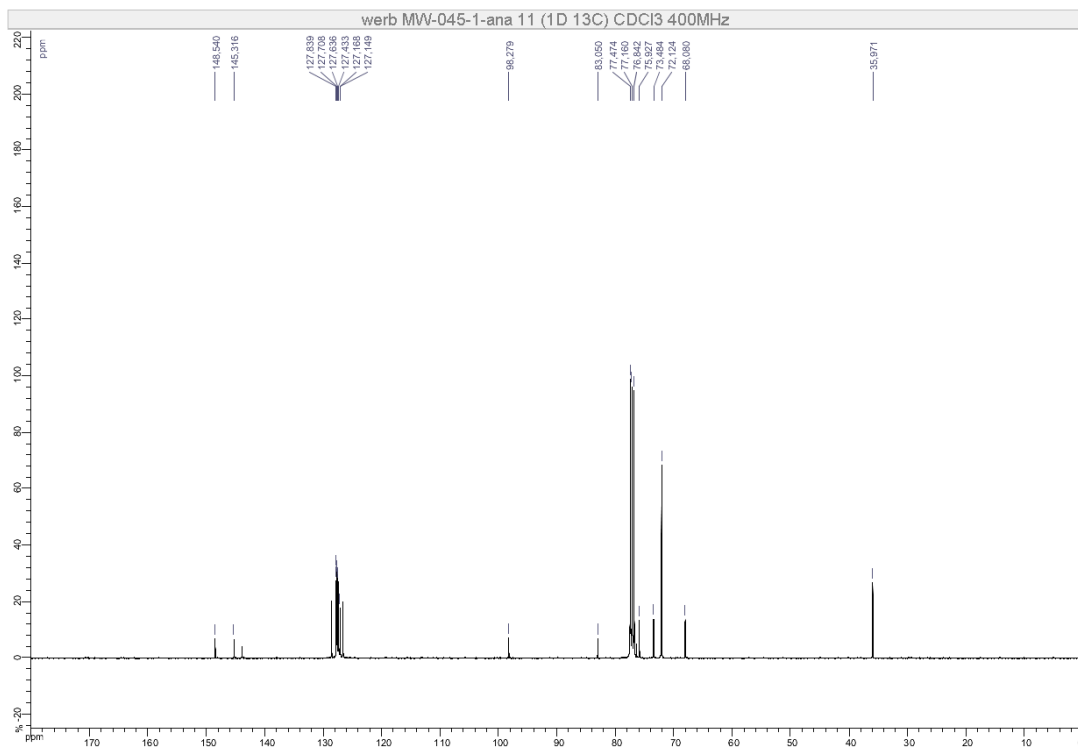


Figure S10. ^{13}C NMR (101 MHz, CDCl_3) of **2b** (racemic mixture)

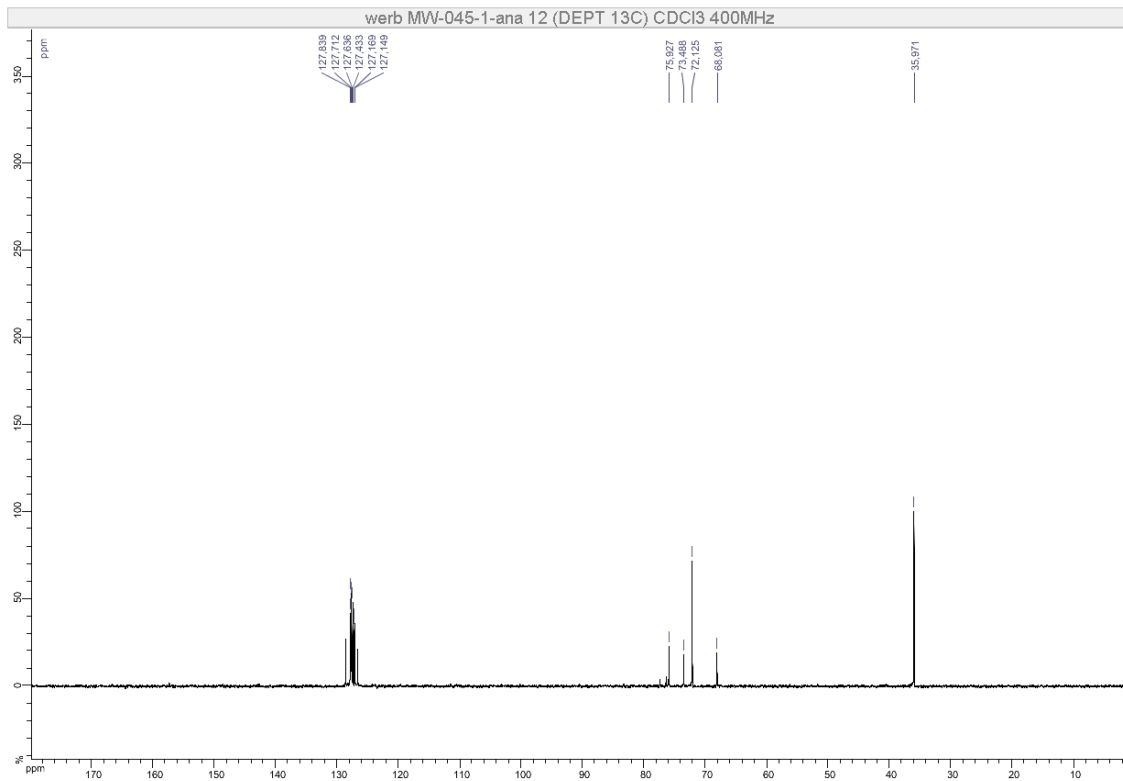


Figure S11. DEPT 135 (101 MHz, CDCl₃) of **2b** (racemic mixture)

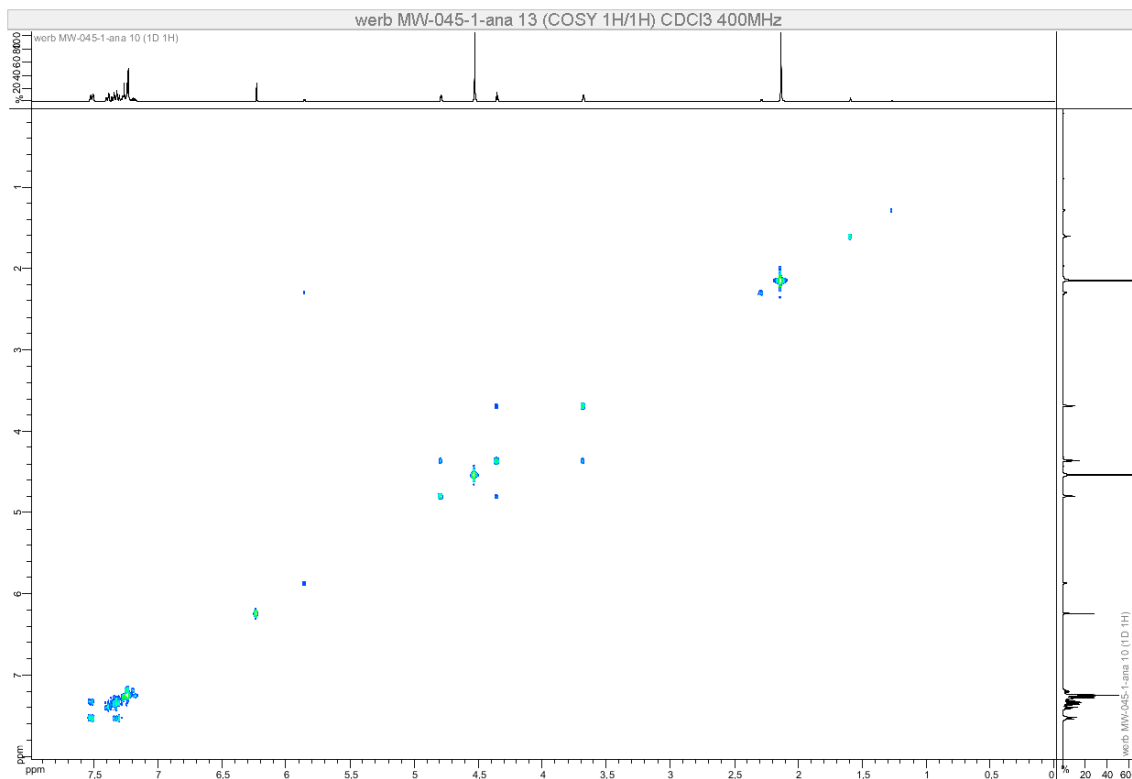


Figure S12. COSY (400 MHz, CDCl₃) of **2b** (racemic mixture)

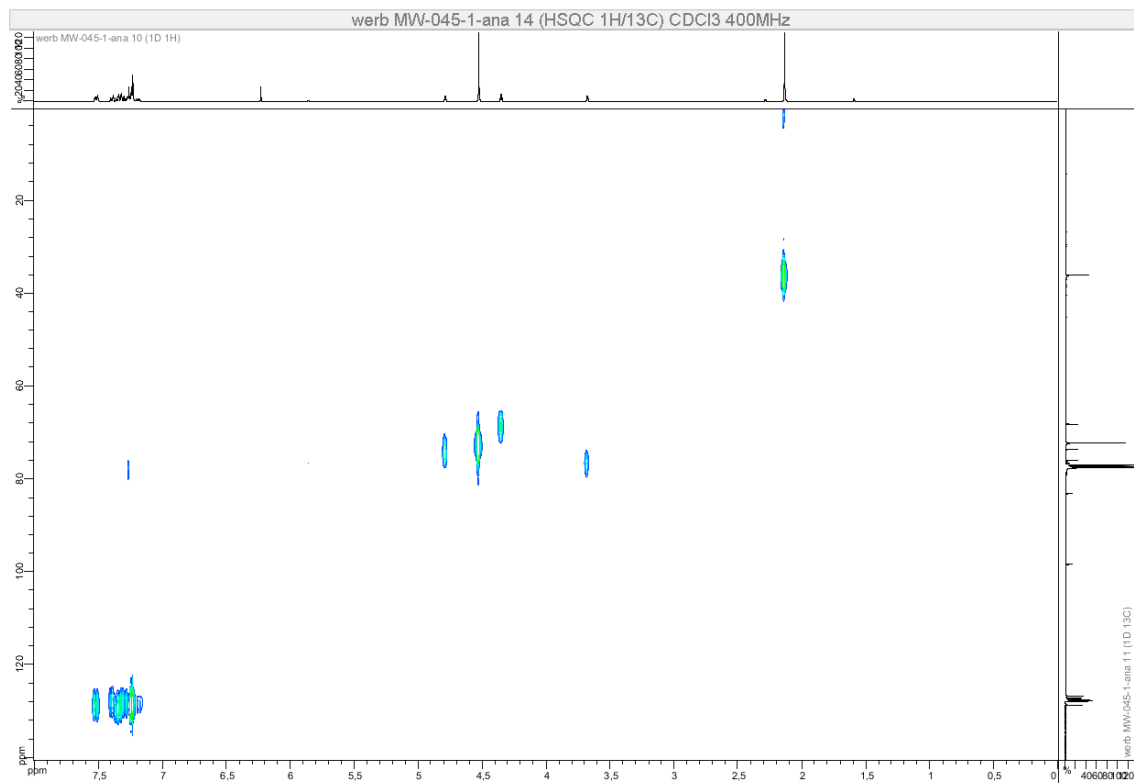


Figure S13. HSQC (400 MHz, CDCl₃) of **2b** (racemic mixture)

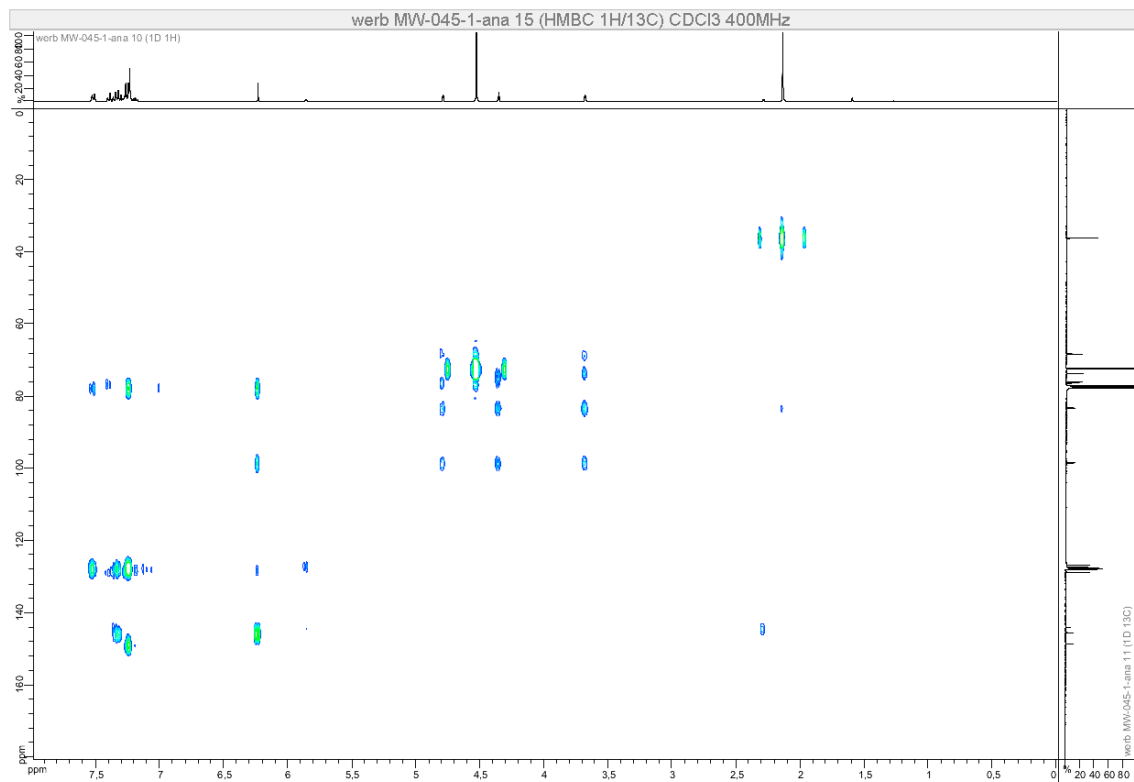


Figure S14. HMBC (400 MHz, CDCl₃) of **2b** (racemic mixture)

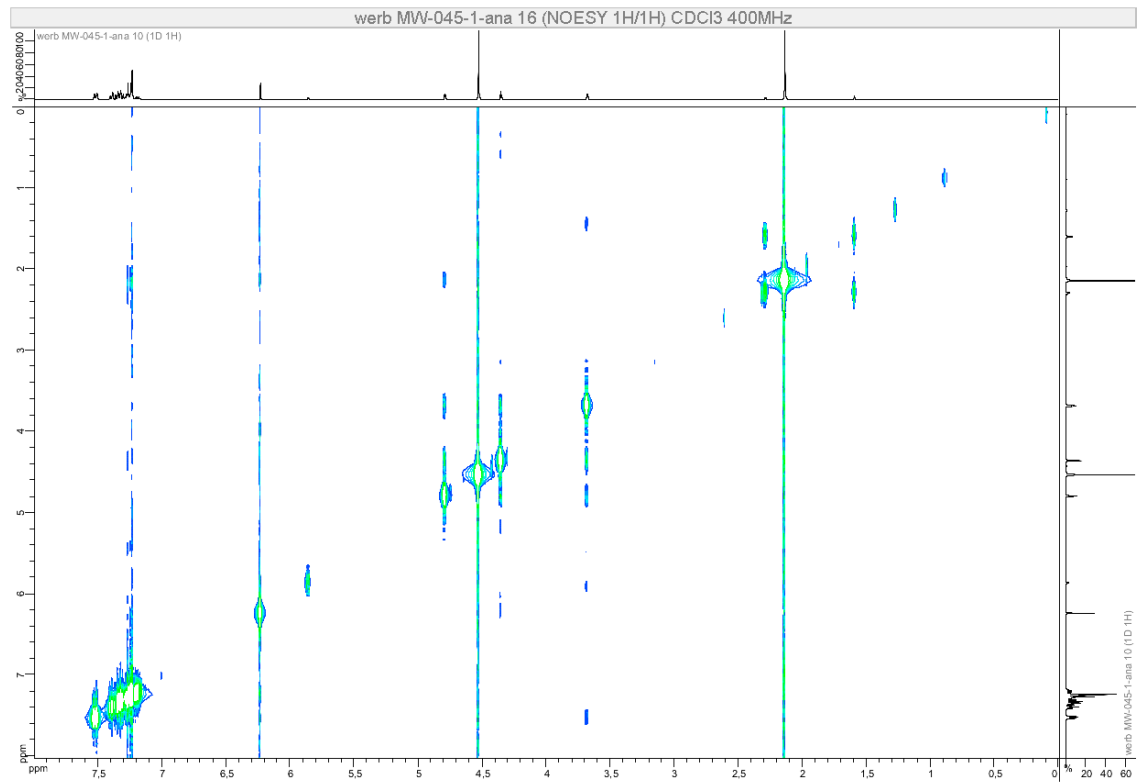
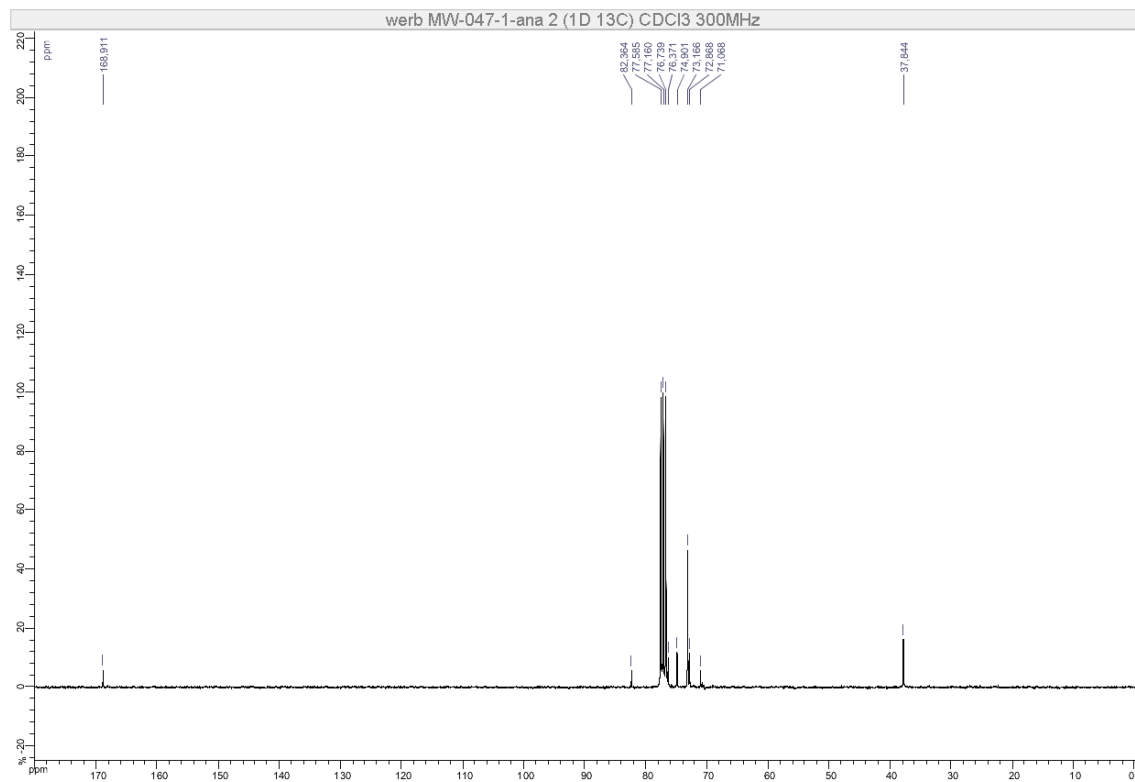
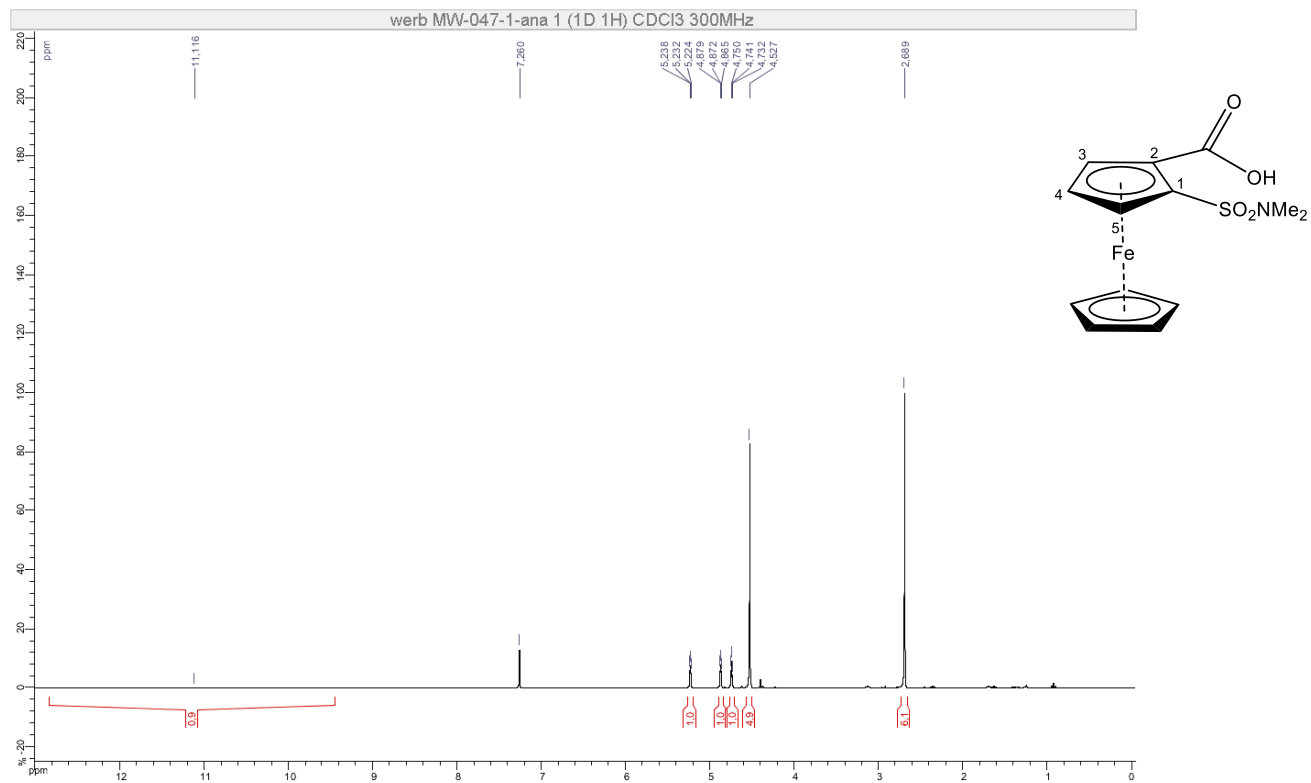


Figure S15. NOESY (400 MHz, CDCl₃) of **2b** (racemic mixture)



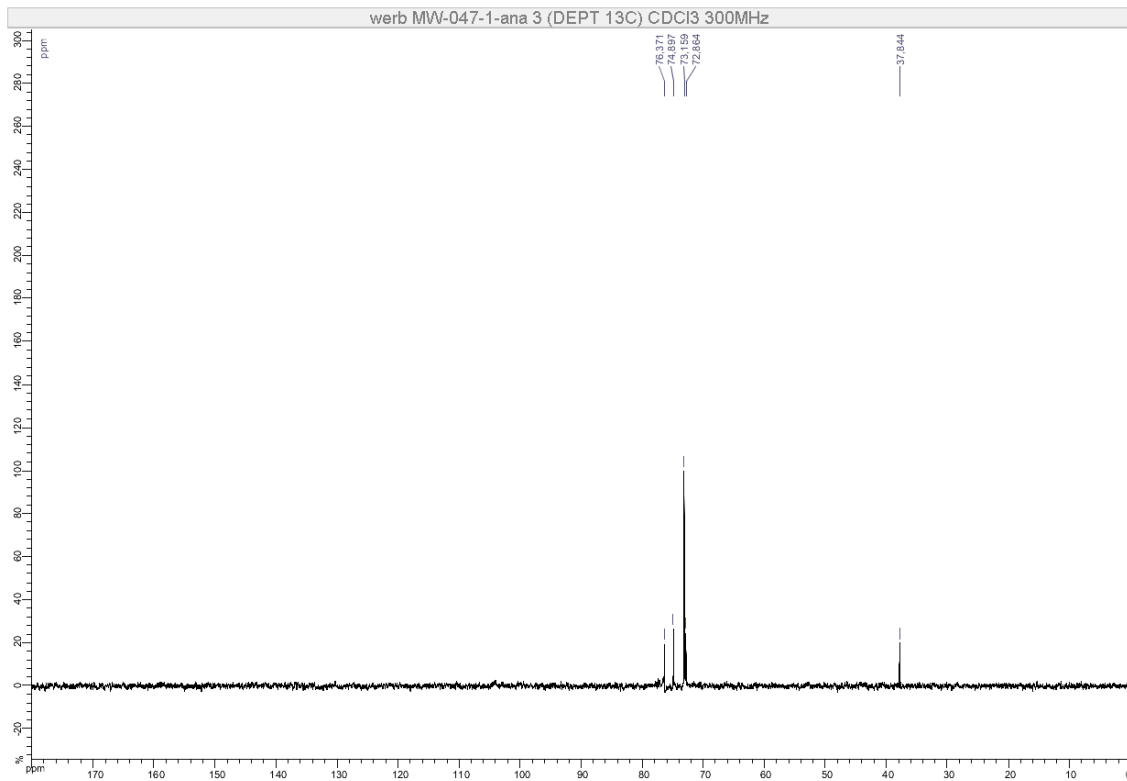


Figure S18. DEPT 135 (75 MHz, CDCl₃) of **2c** (racemic mixture)

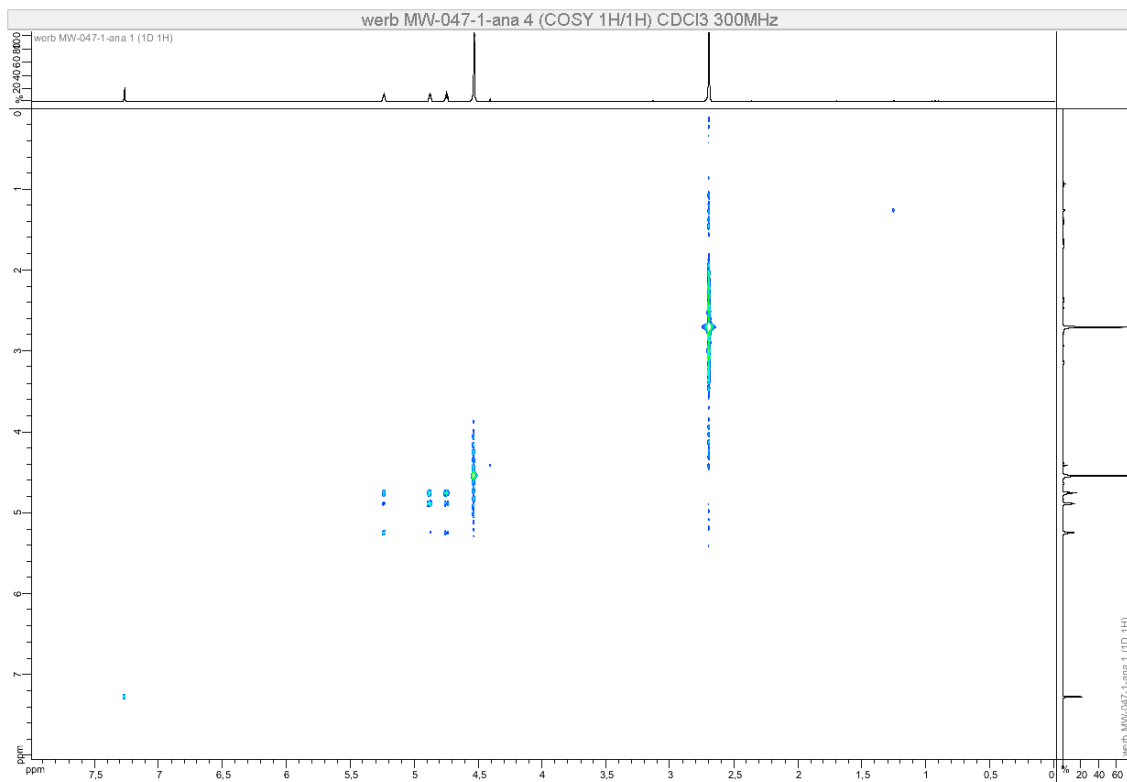


Figure S19. COSY (300 MHz, CDCl₃) of **2c** (racemic mixture)

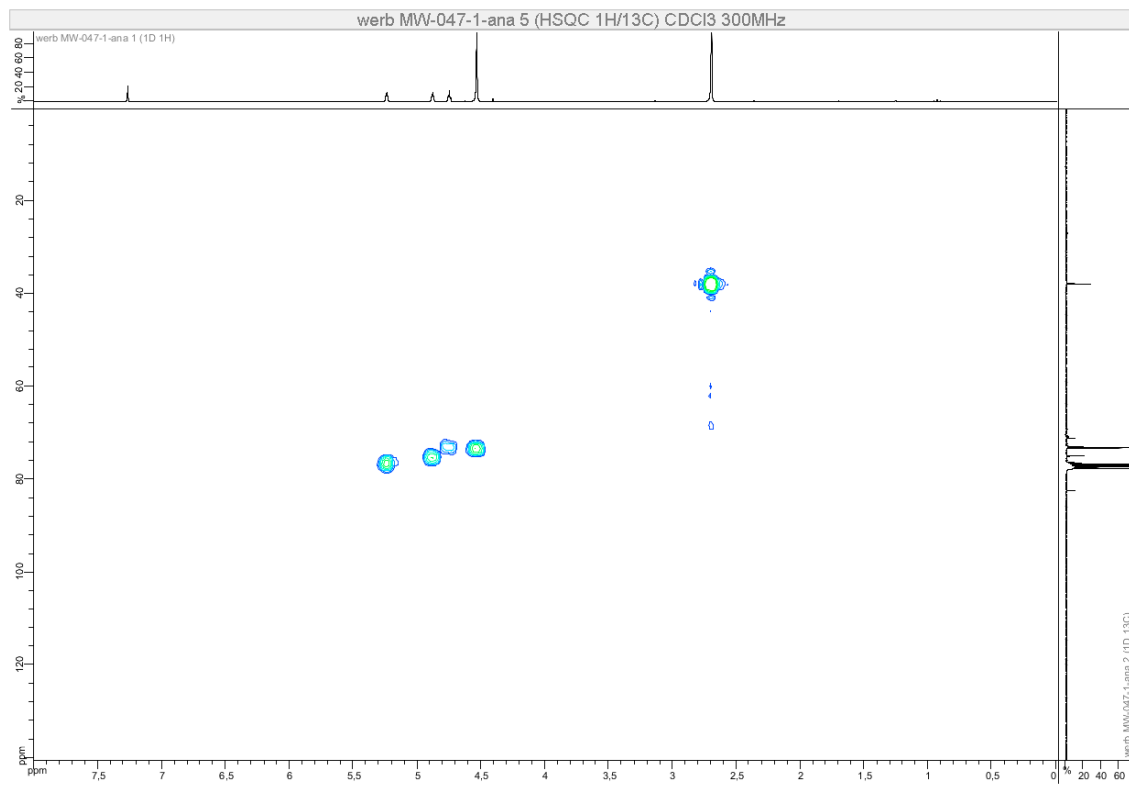


Figure S20. HSQC (300 MHz, CDCl₃) of **2c** (racemic mixture)

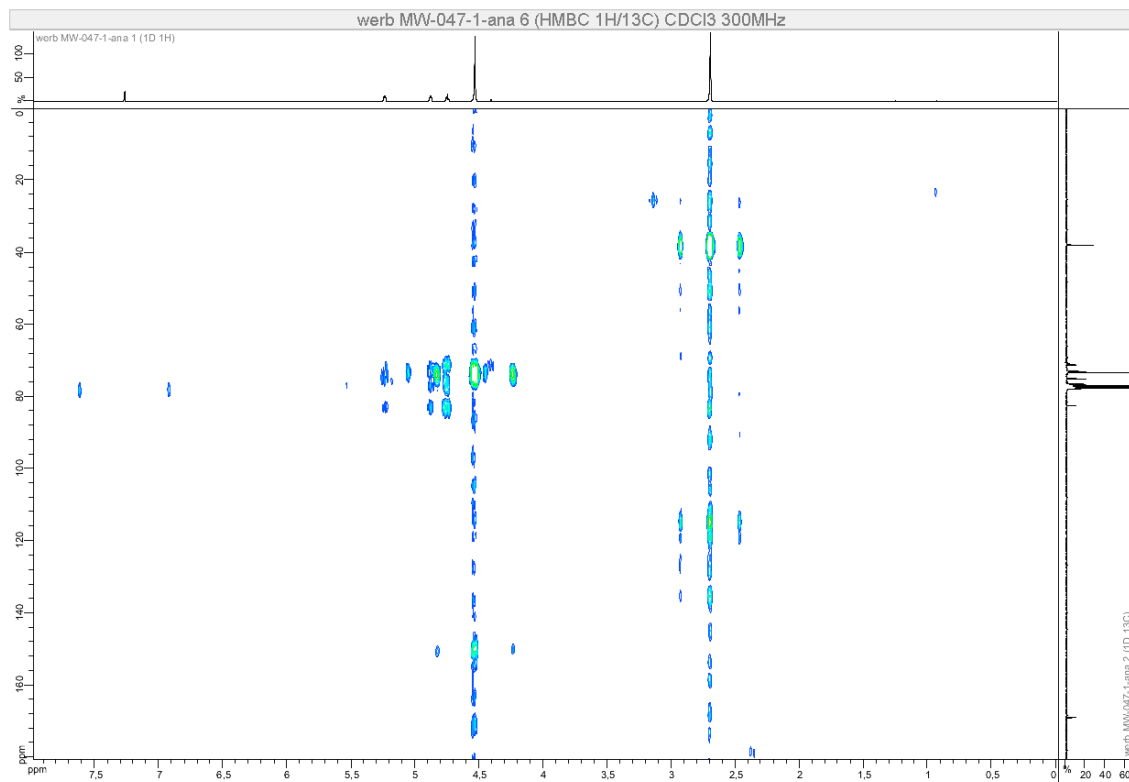


Figure S21. HMBC (300 MHz, CDCl₃) of **2c** (racemic mixture)

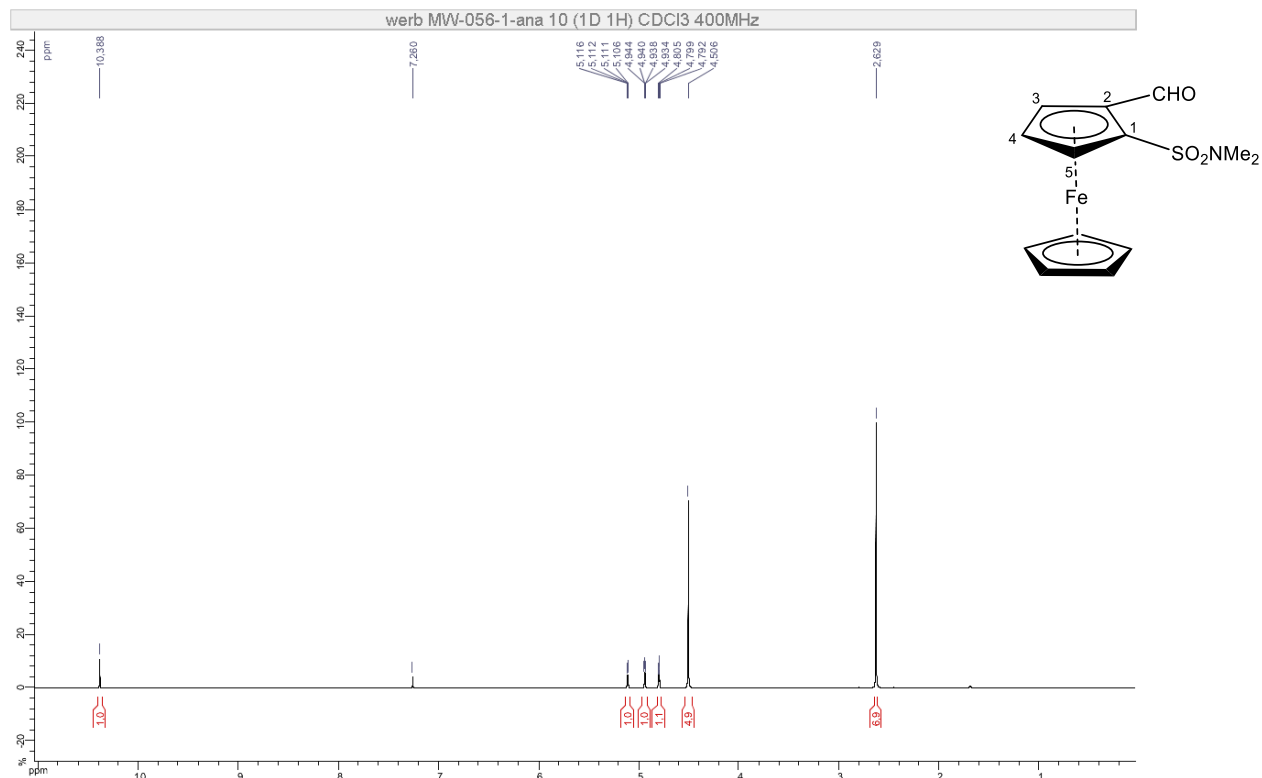


Figure S22. ¹H NMR (400 MHz, CDCl₃) of **2d** (racemic mixture)

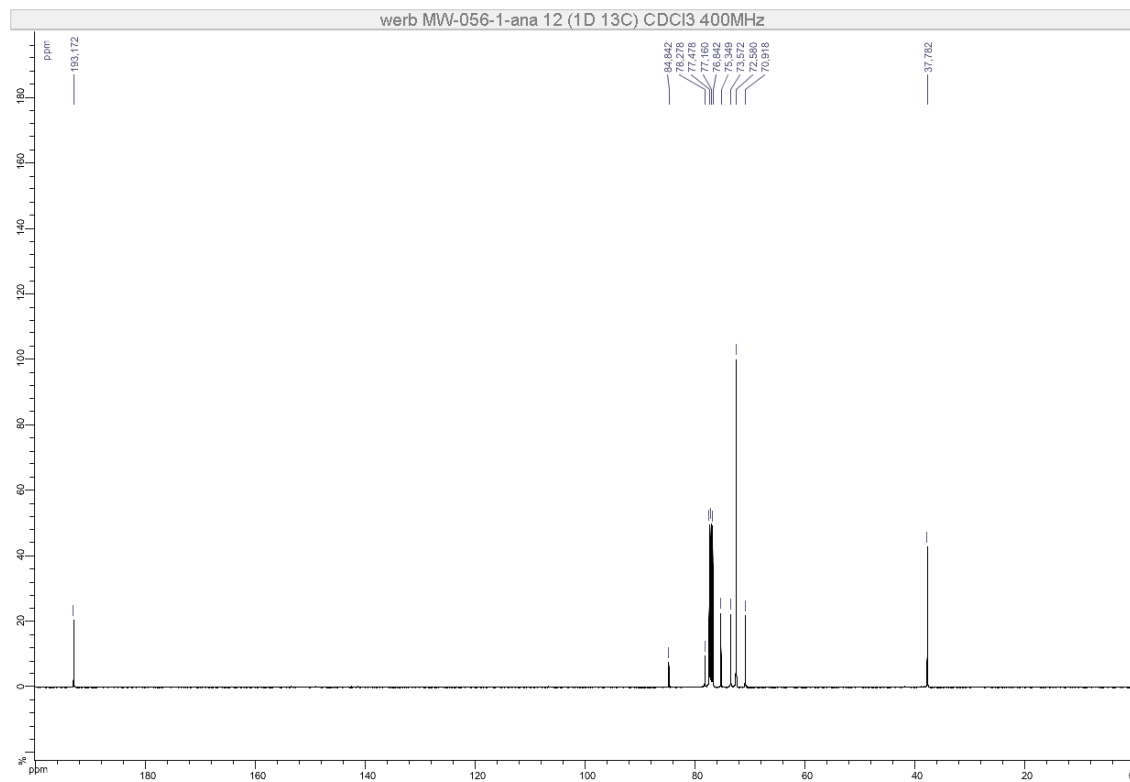


Figure S23. ¹³C NMR (101 MHz, CDCl₃) of **2d** (racemic mixture)

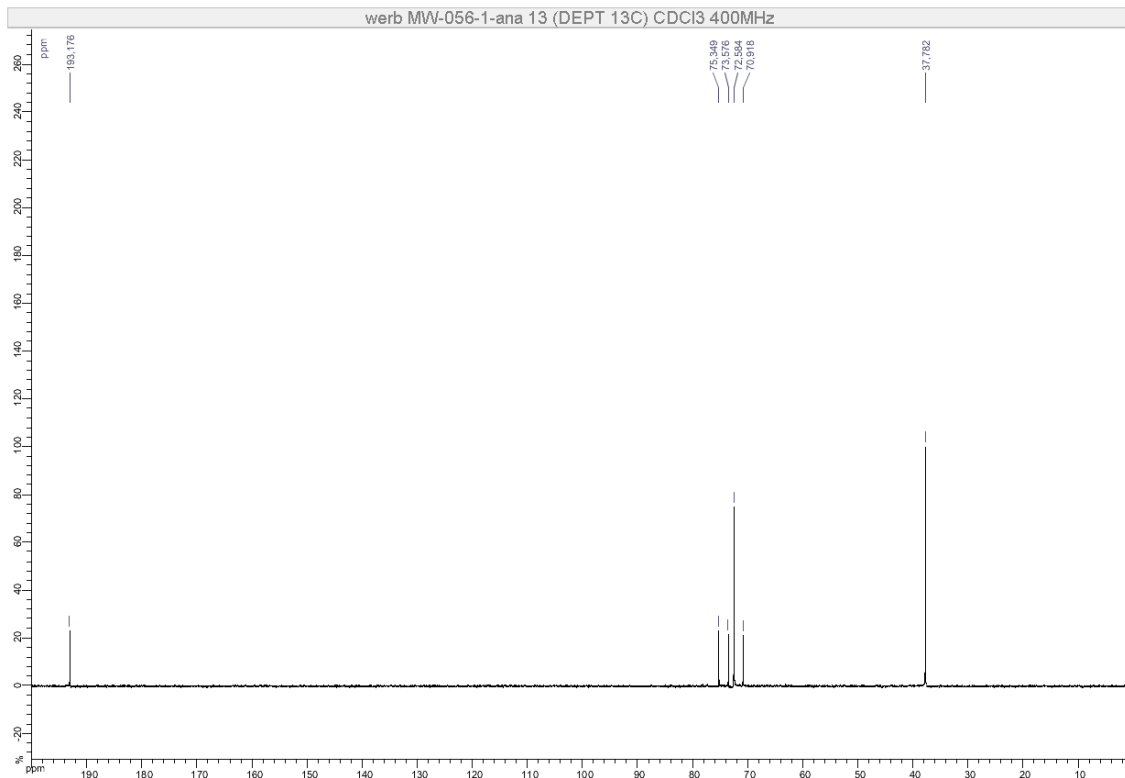


Figure S24. DEPT 135 (101 MHz, CDCl₃) of **2d** (racemic mixture)

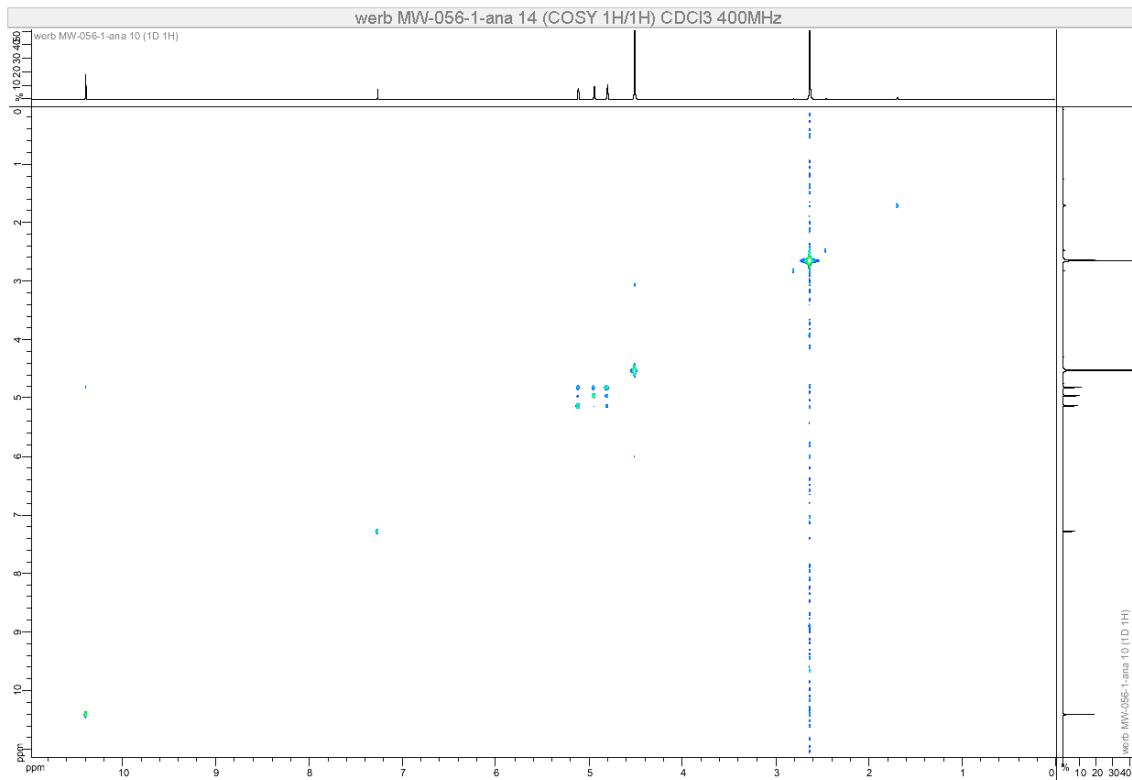


Figure S25. COSY (400 MHz, CDCl₃) of **2d** (racemic mixture)

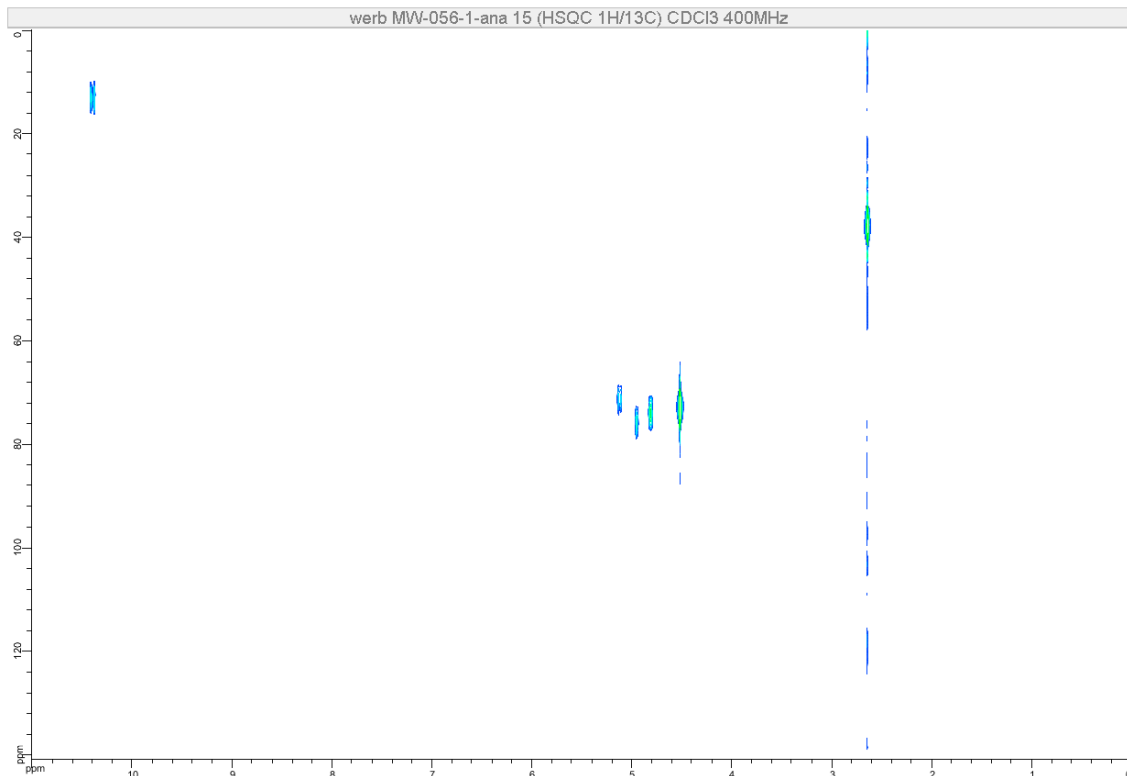


Figure S26. HSQC (400 MHz, CDCl₃) of **2d** (racemic mixture)

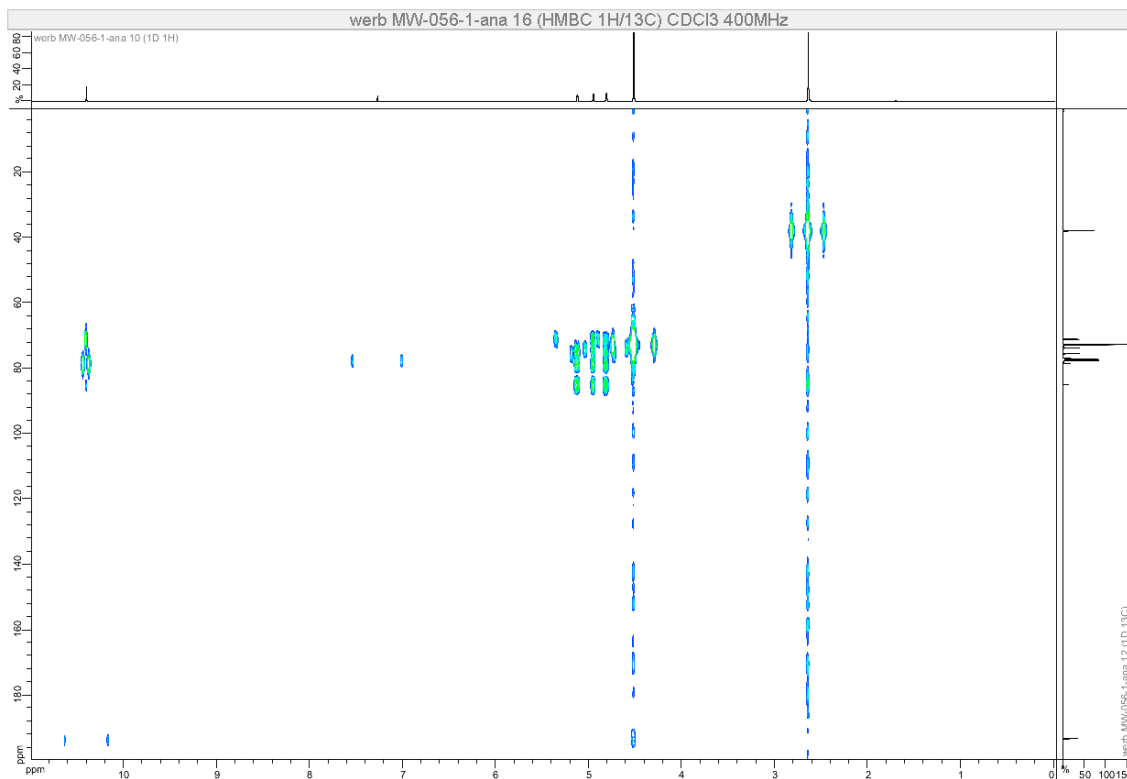


Figure S27. HMBC (400 MHz, CDCl₃) of **2d** (racemic mixture)

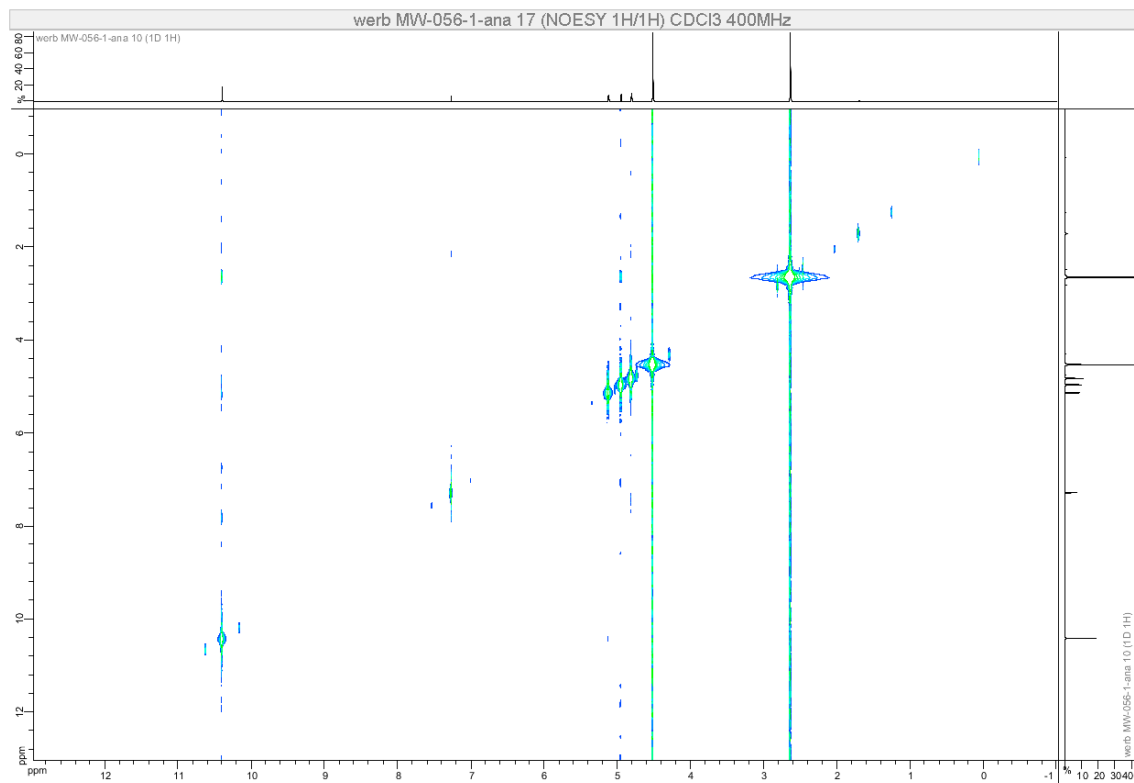


Figure S28. NOESY (400 MHz, CDCl_3) of **2d** (racemic mixture)

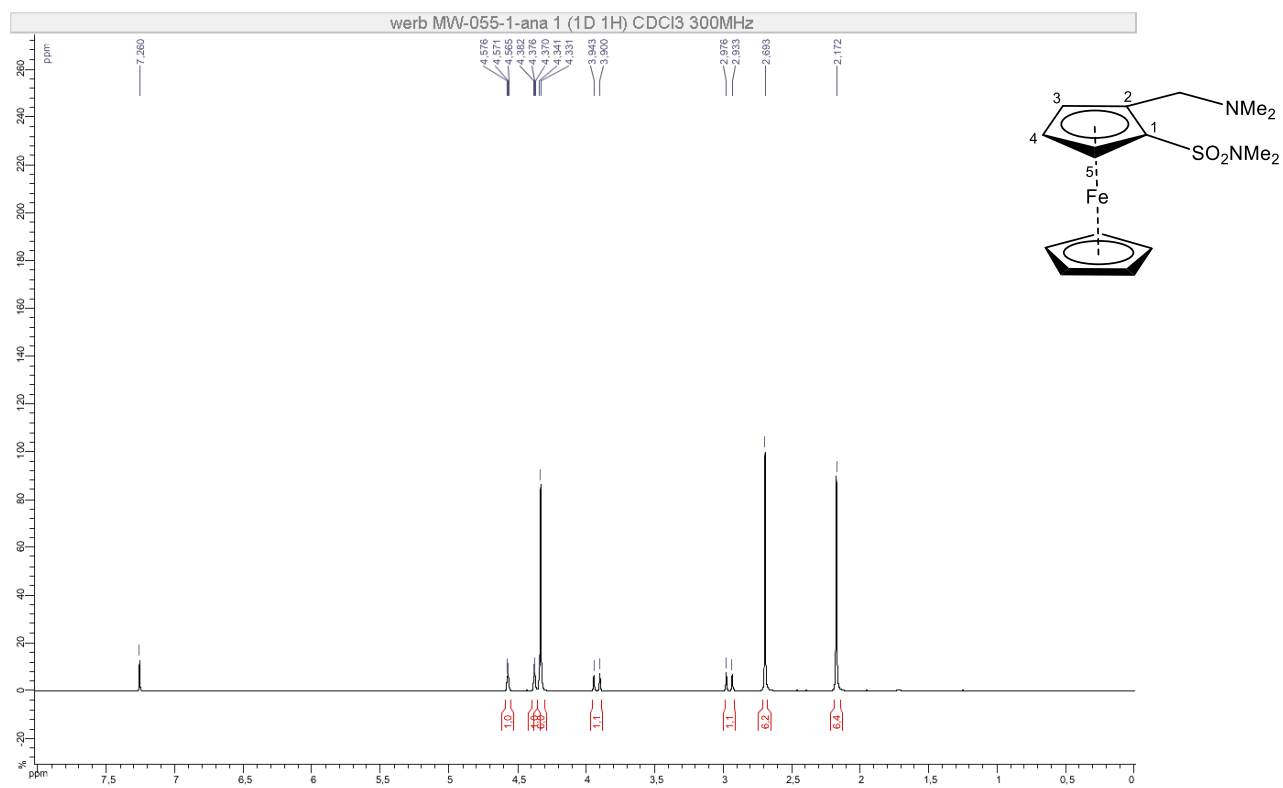


Figure S29. ¹H NMR (500 MHz, CDCl₃) of **2e** (racemic mixture)

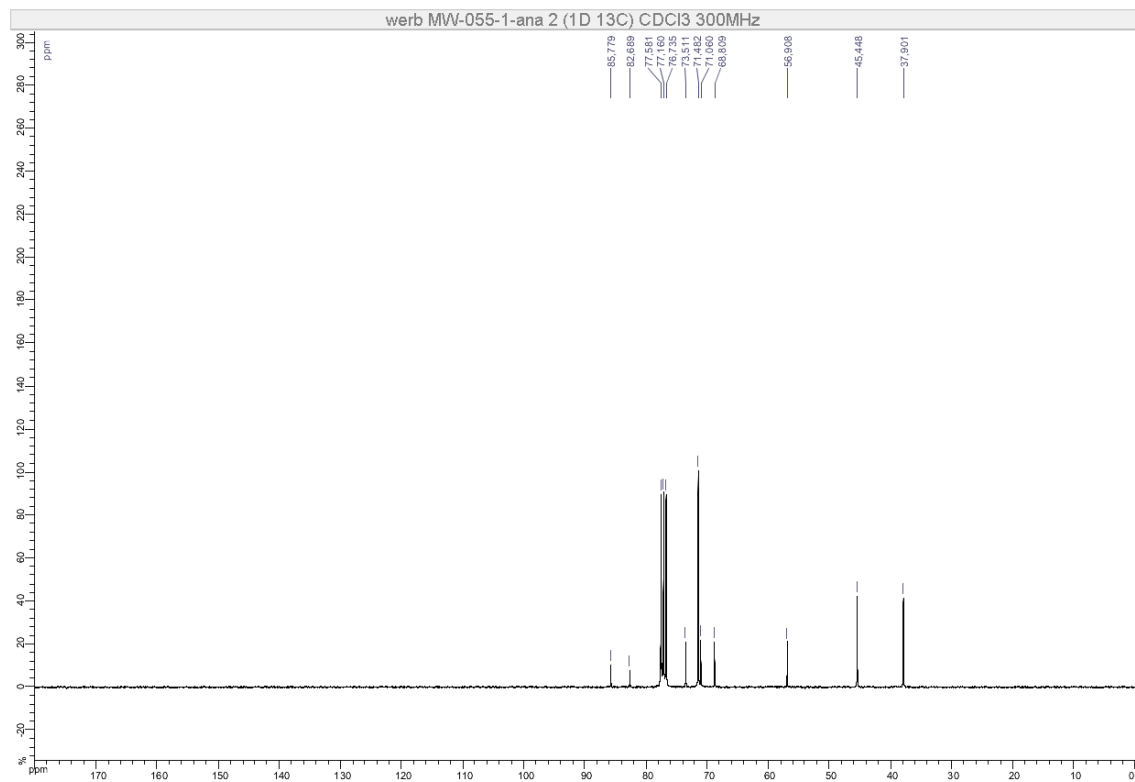


Figure S30. ¹³C NMR (75 MHz, CDCl₃) of **2e** (racemic mixture)

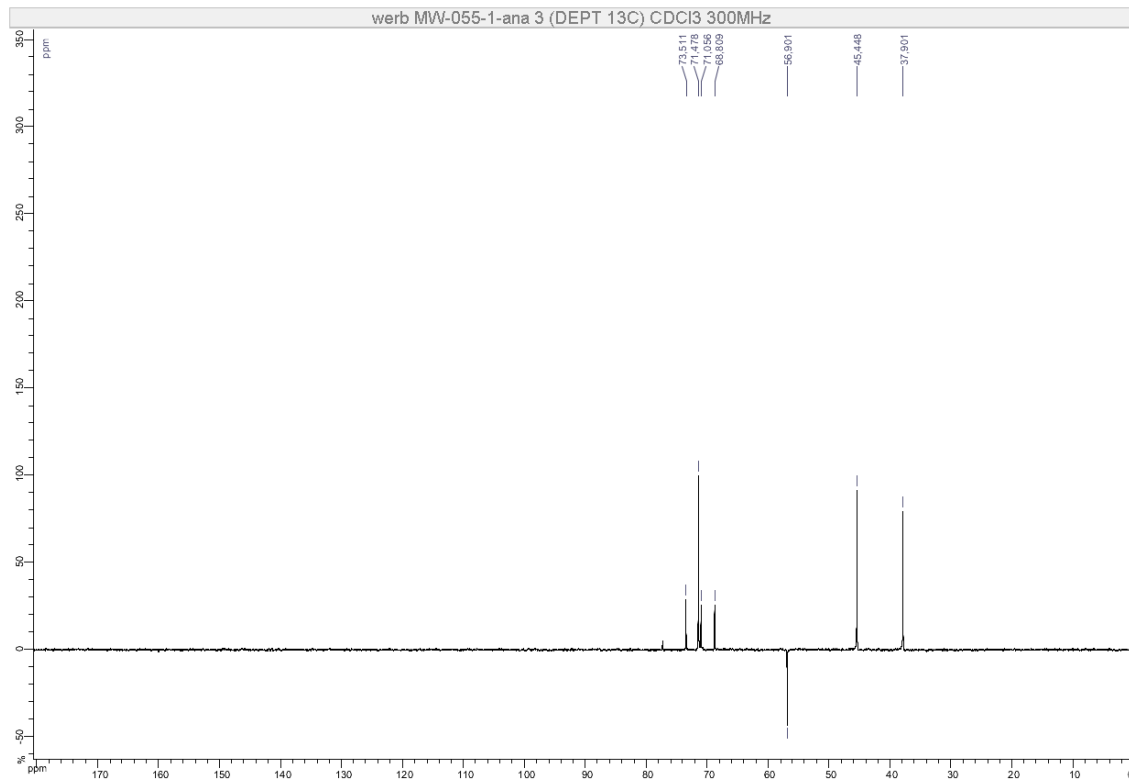


Figure S31. DEPT 135 (75 MHz, CDCl₃) of **2e** (racemic mixture)

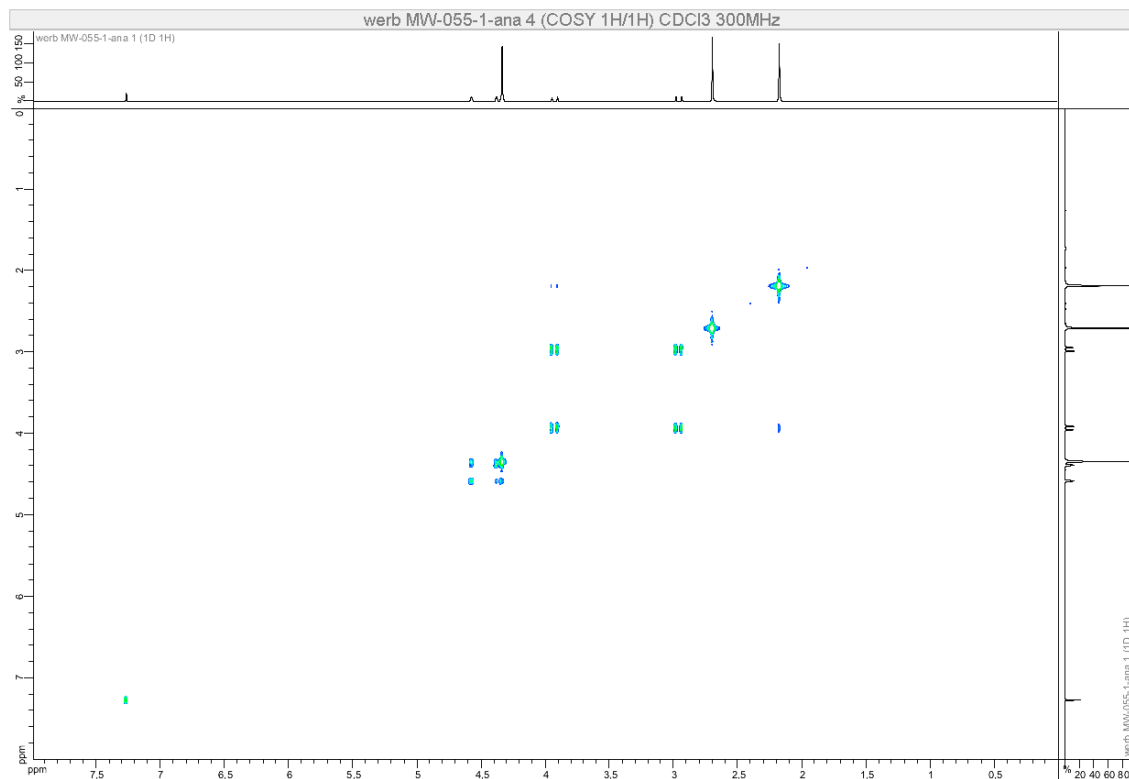


Figure S32. COSY (300 MHz, CDCl₃) of **2e** (racemic mixture)

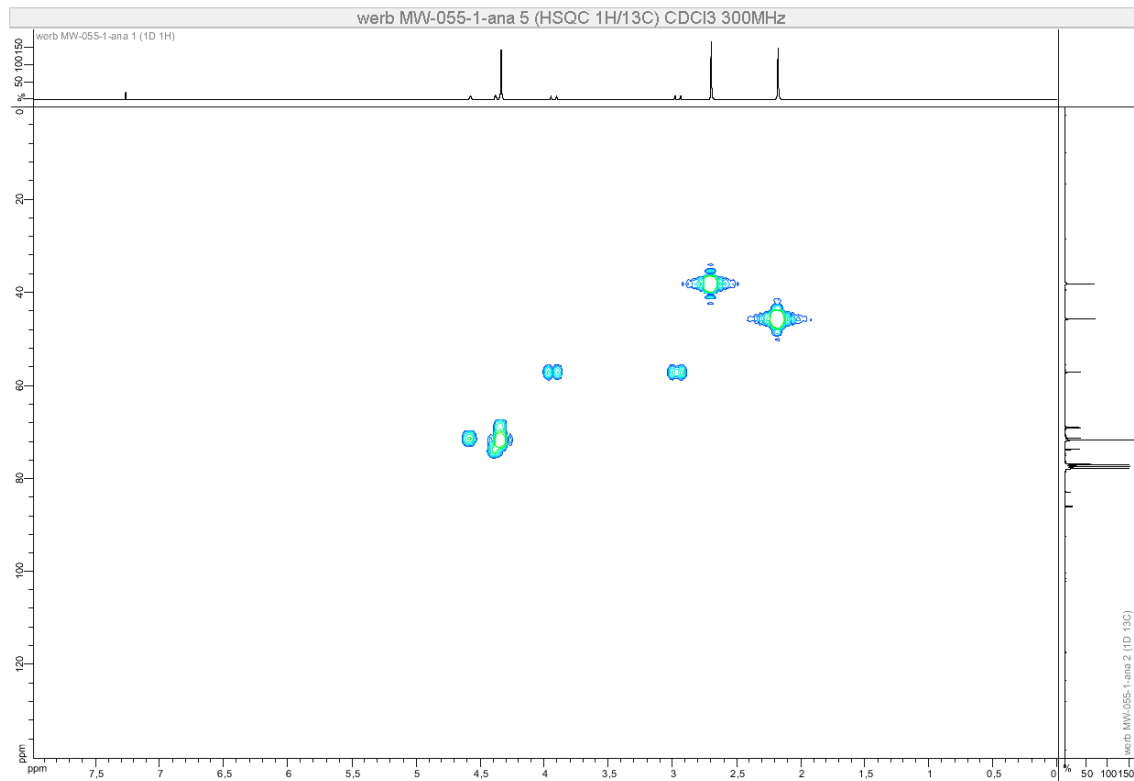


Figure S33. HSQC (300 MHz, CDCl₃) of **2e** (racemic mixture)

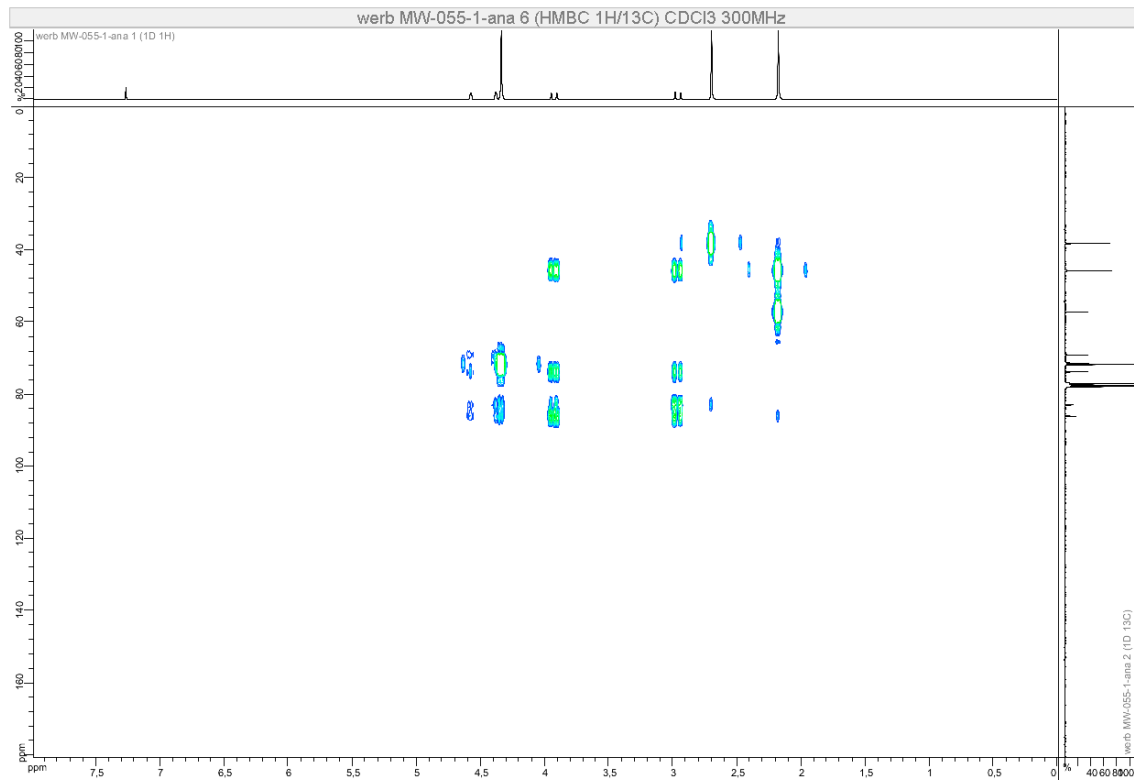


Figure S34. HMBC (300 MHz, CDCl₃) of **2e** (racemic mixture)

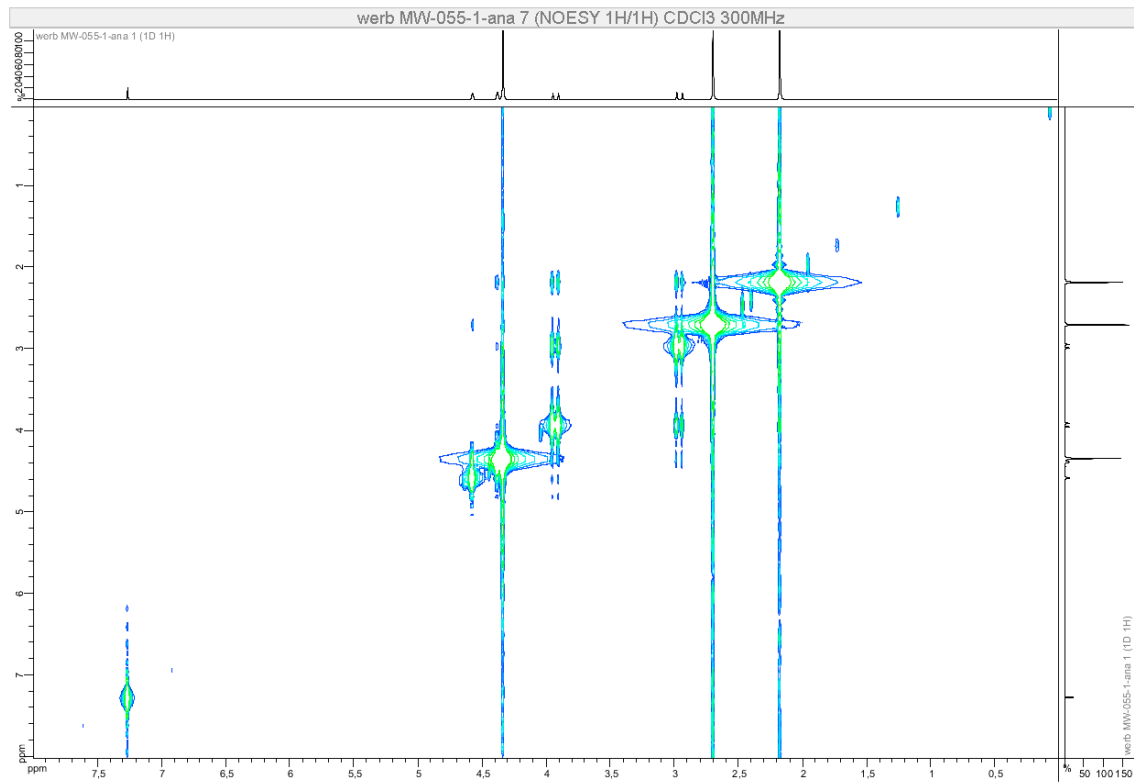


Figure S35. NOESY (300 MHz, CDCl₃) of **2e** (racemic mixture)

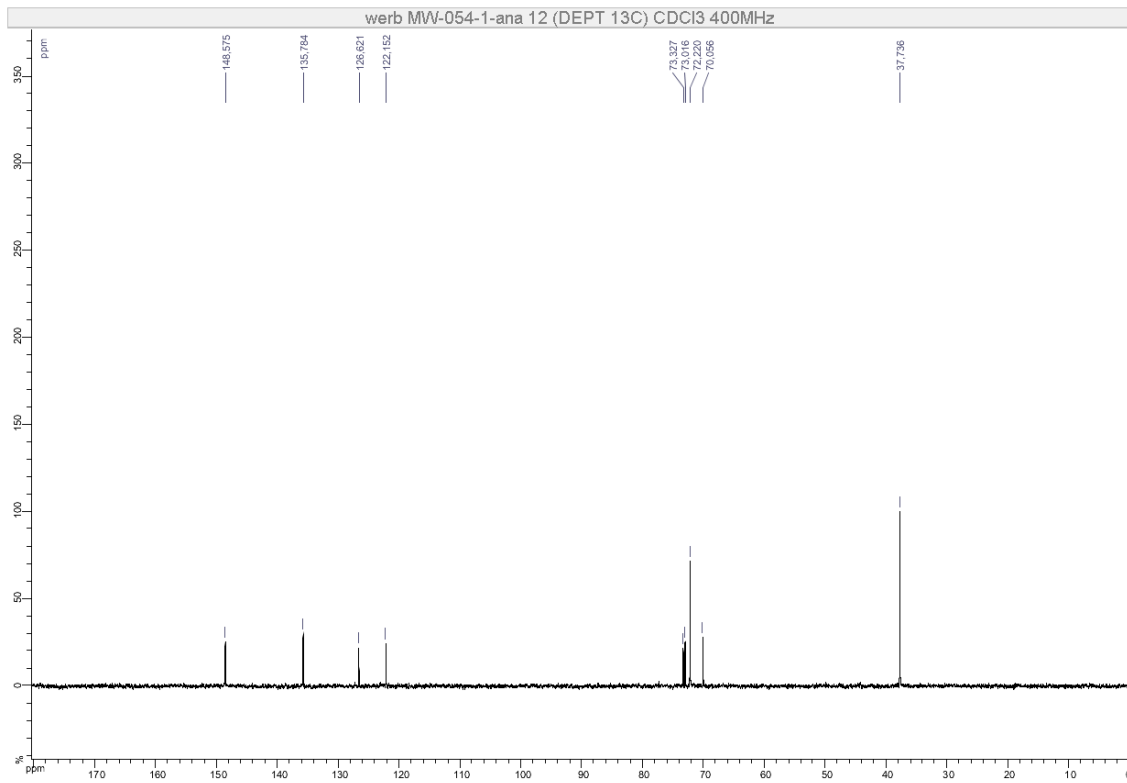


Figure S38. DEPT 135 (101 MHz, CDCl₃) of **2f** (racemic mixture)

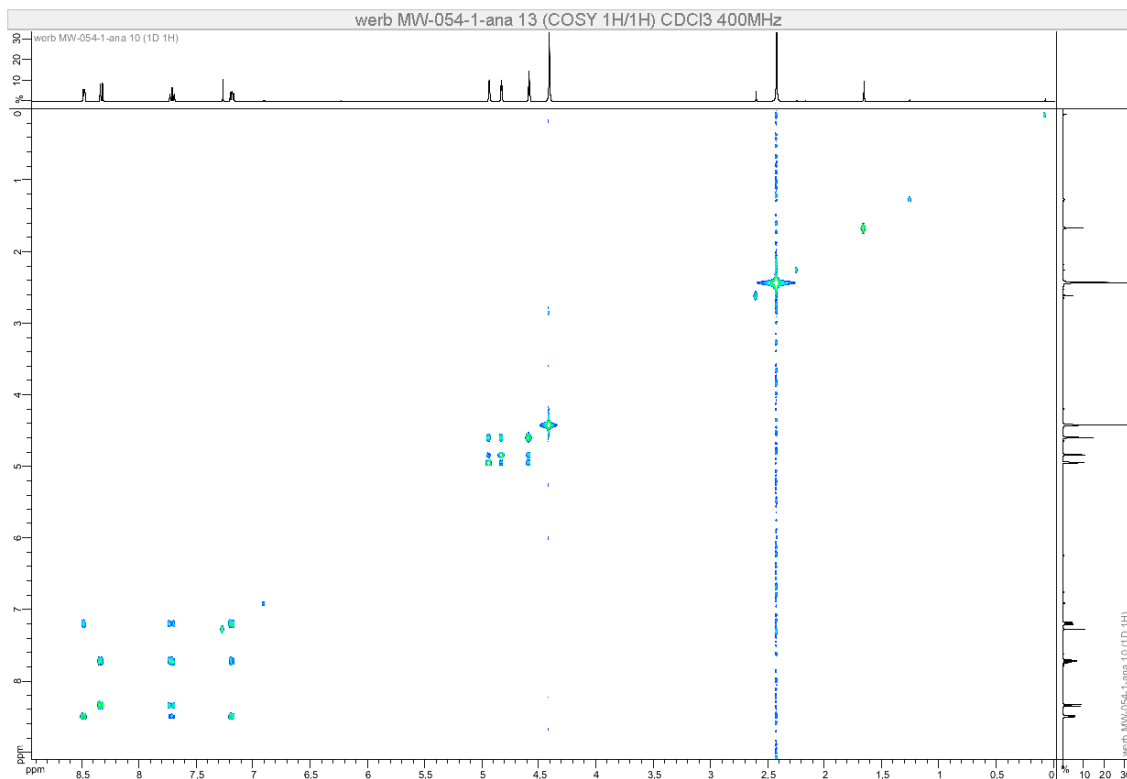


Figure S39. COSY (400 MHz, CDCl₃) of **2f** (racemic mixture)

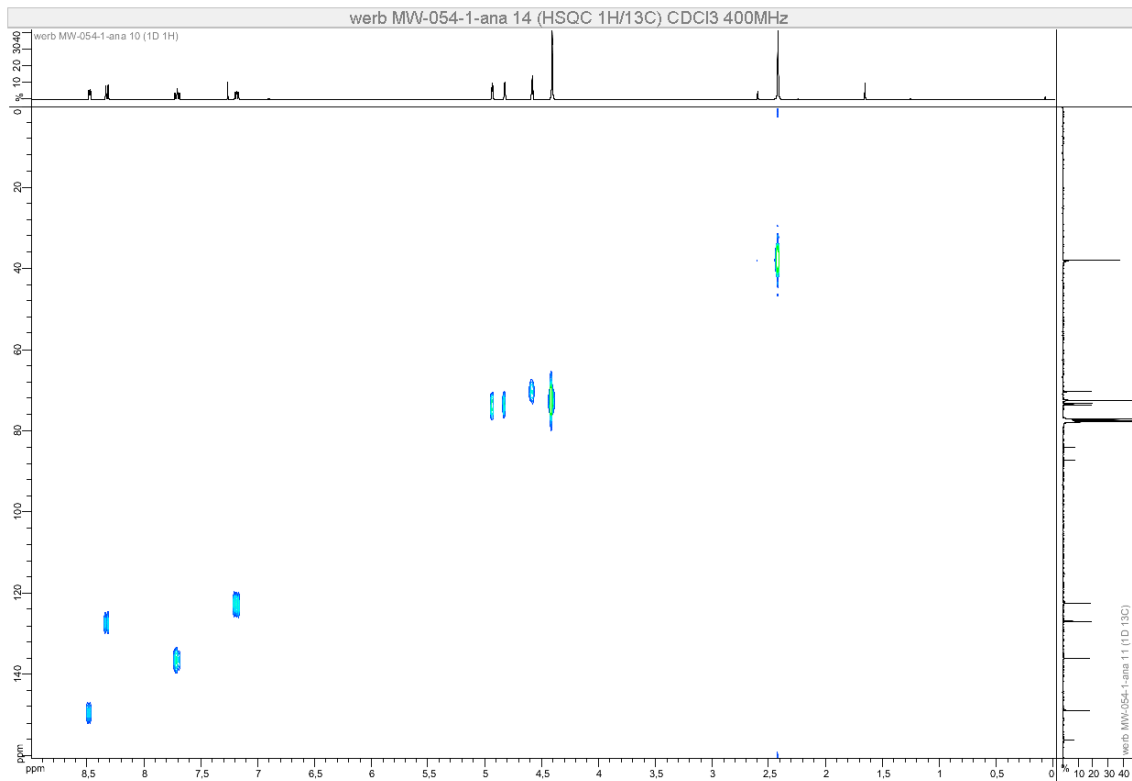


Figure S40. HSQC (400 MHz, CDCl₃) of **2f** (racemic mixture)

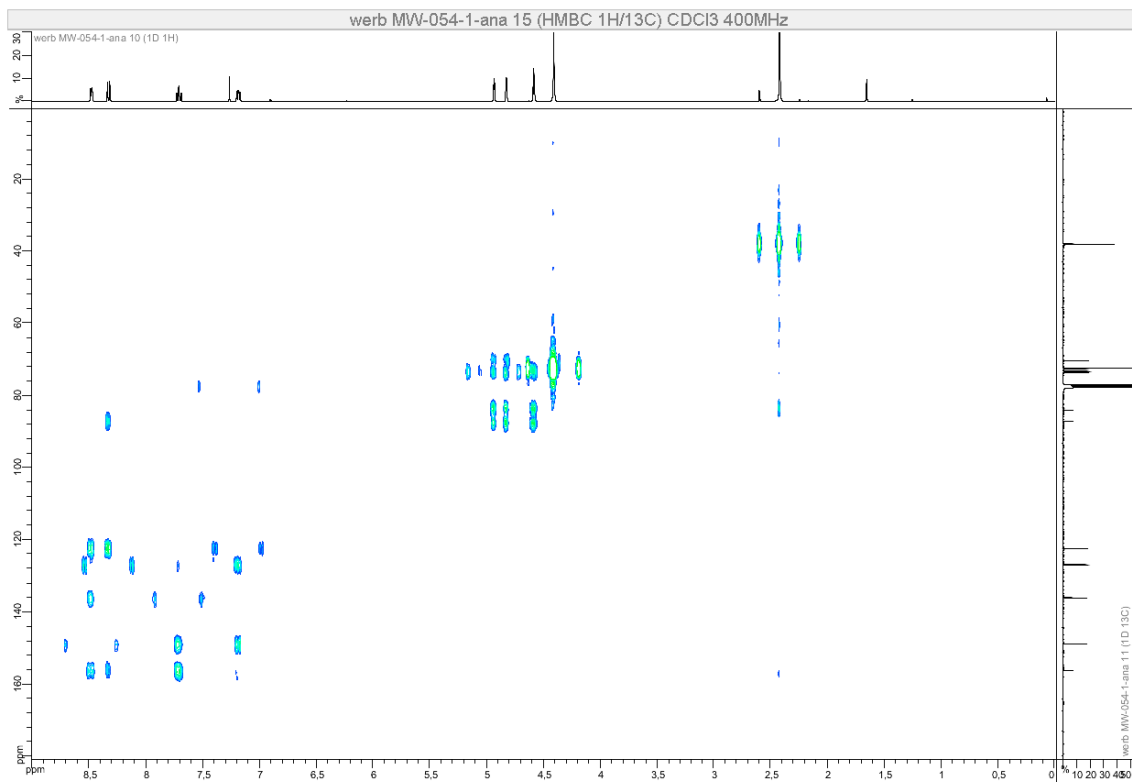


Figure S41. HMBC (400 MHz, CDCl₃) of **2f** (racemic mixture)

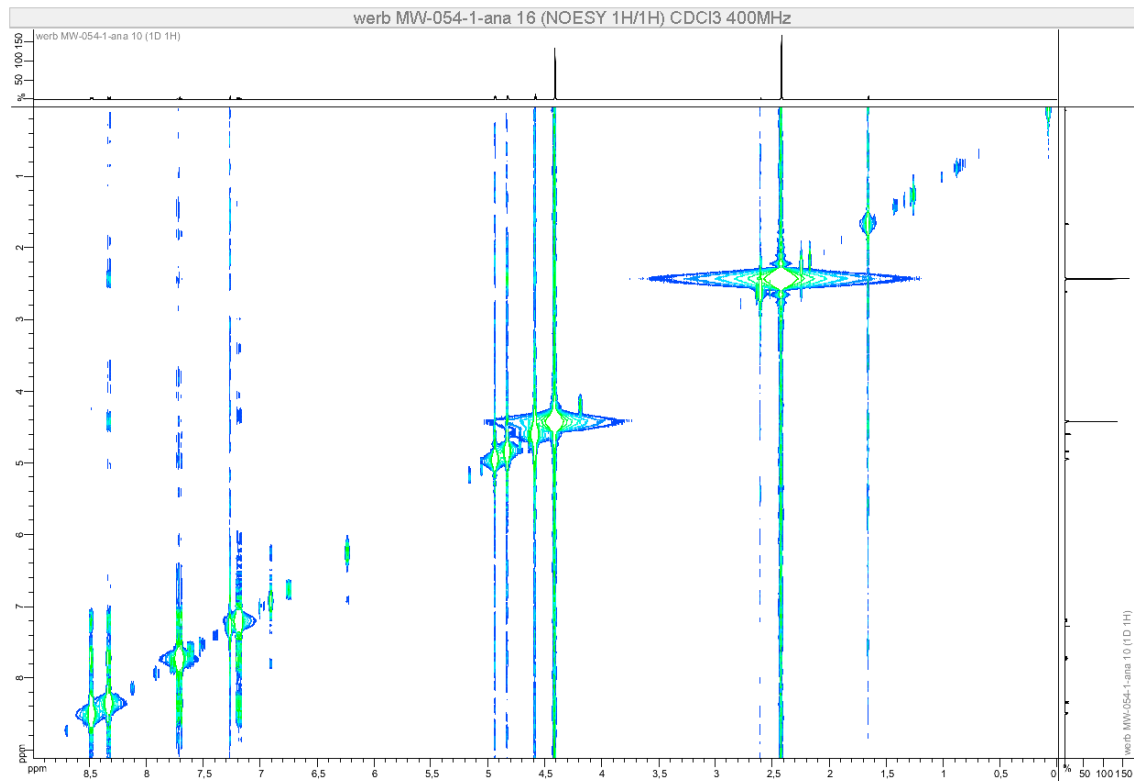
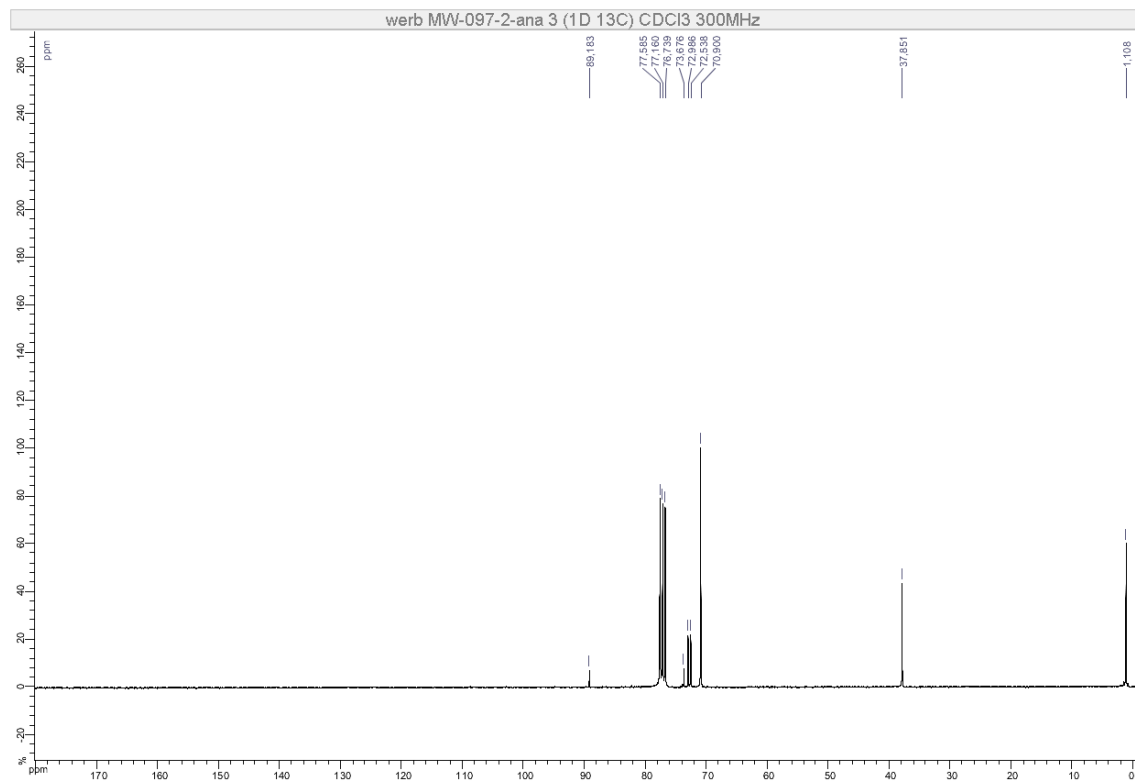
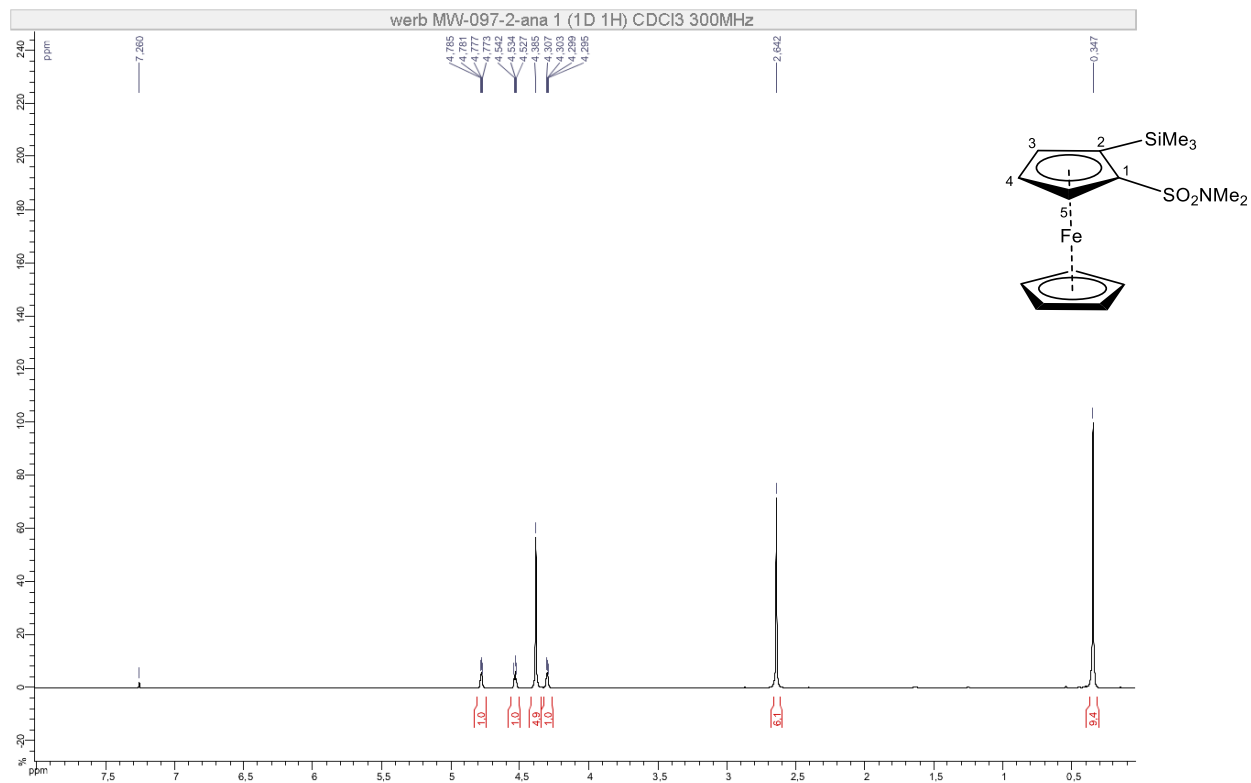


Figure S42. NOESY (400 MHz, CDCl₃) of **2f** (racemic mixture)



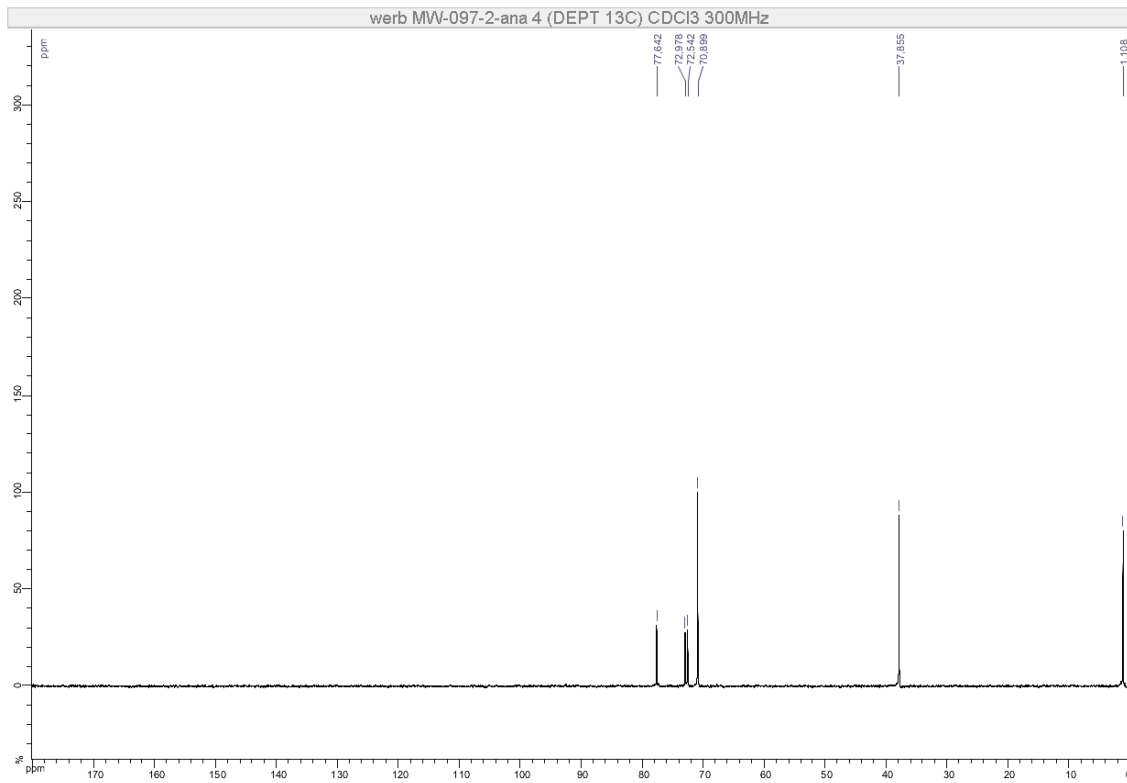


Figure S45. DEPT 135 (75 MHz, CDCl_3) of **2g** (racemic mixture)

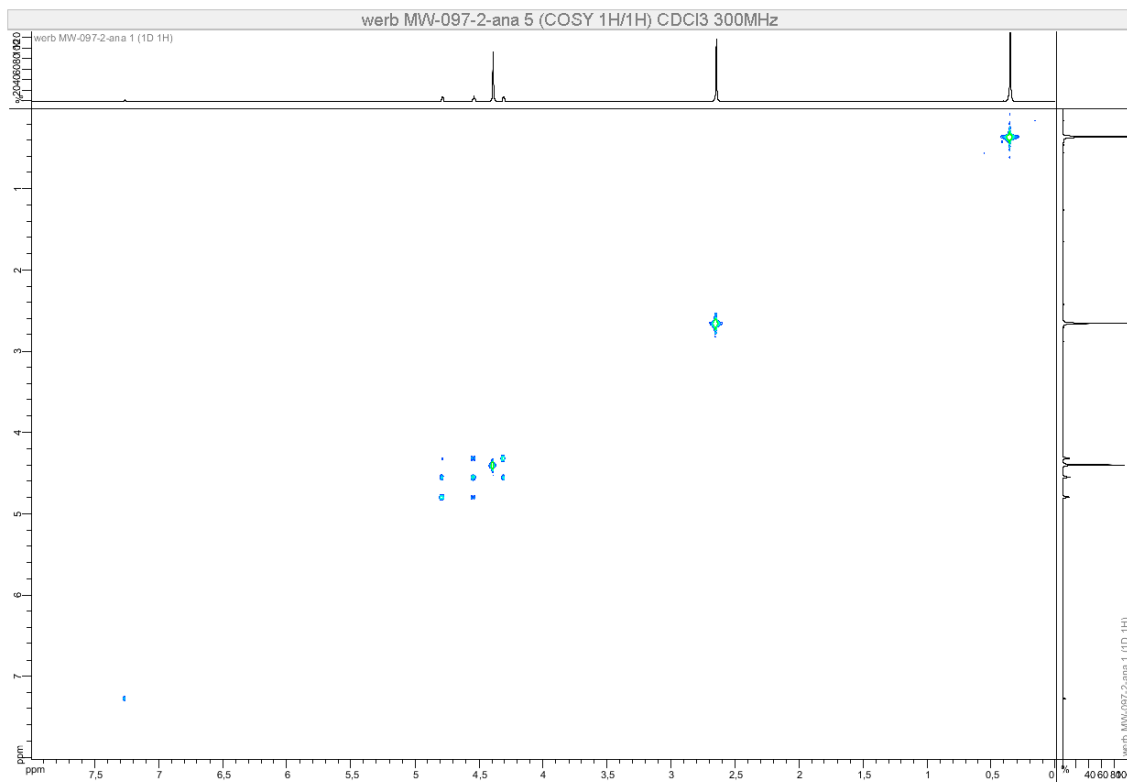


Figure S46. COSY (300 MHz, CDCl_3) of **2g** (racemic mixture)

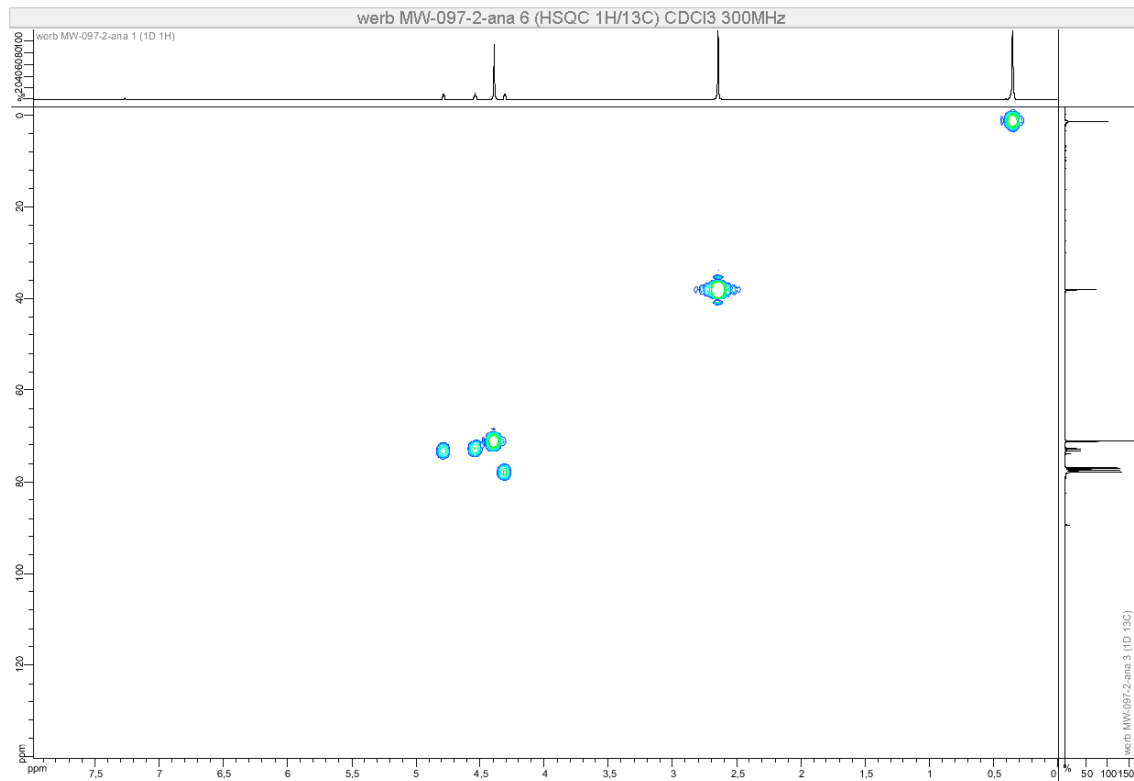


Figure S47. HSQC (300 MHz, CDCl₃) of **2g** (racemic mixture)

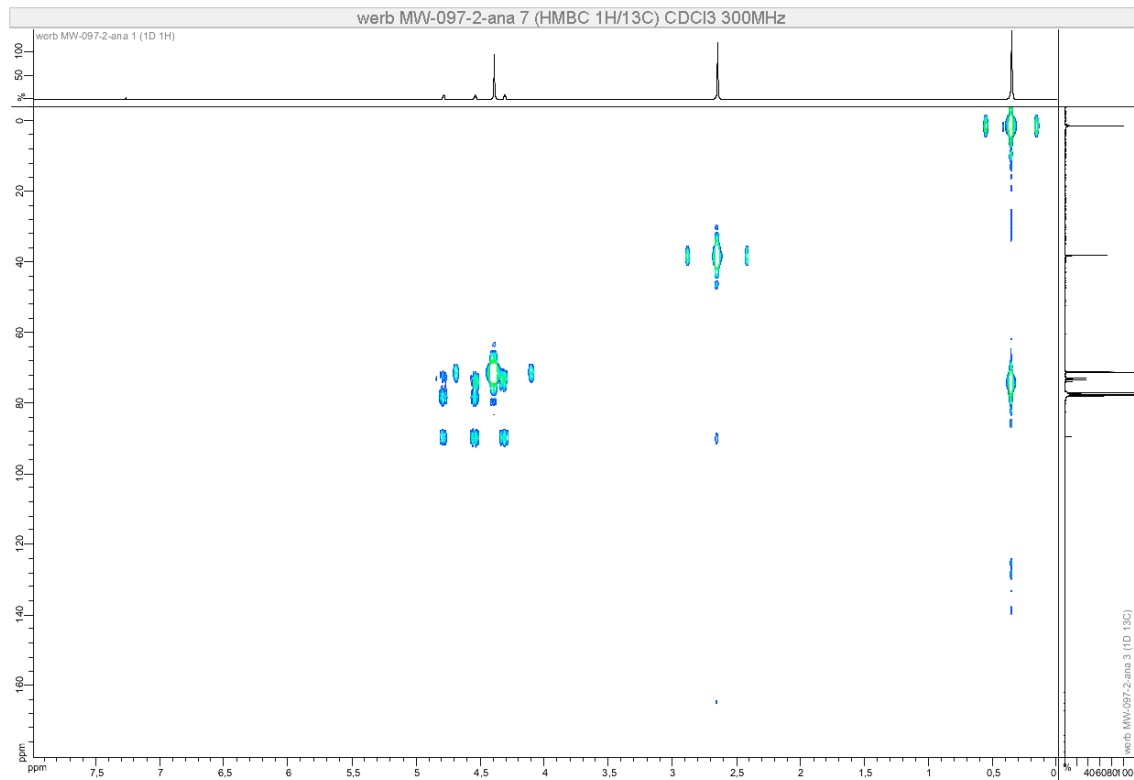
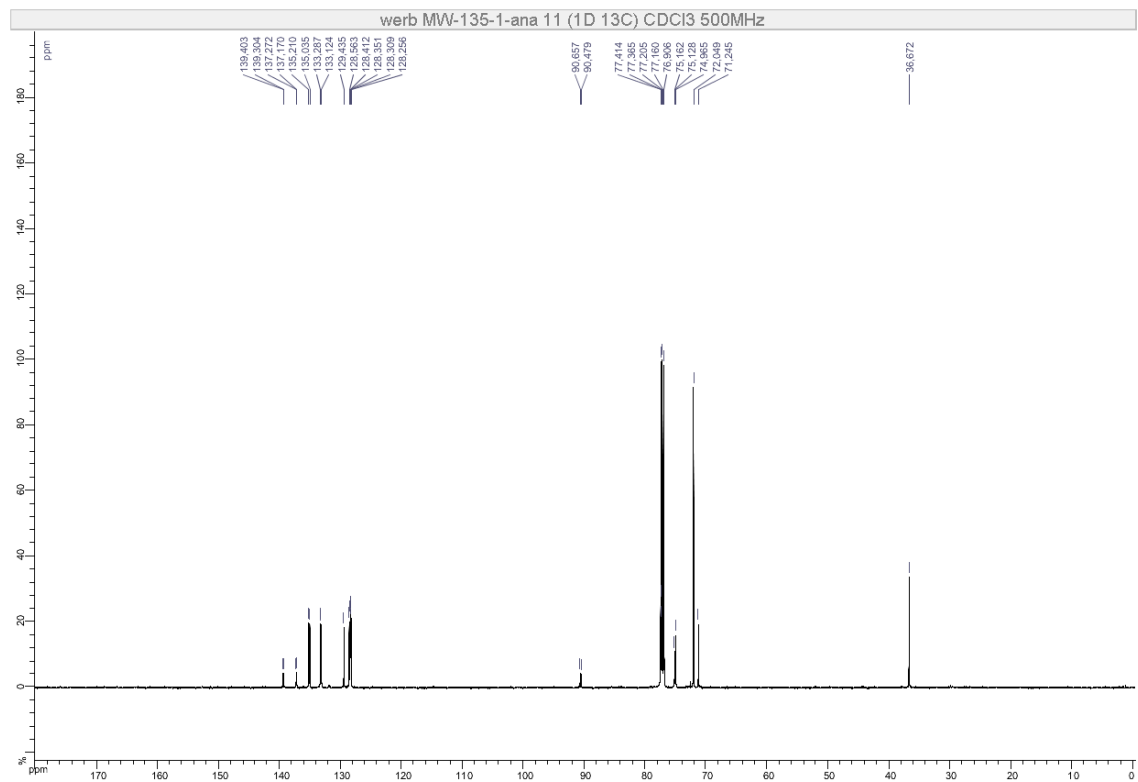
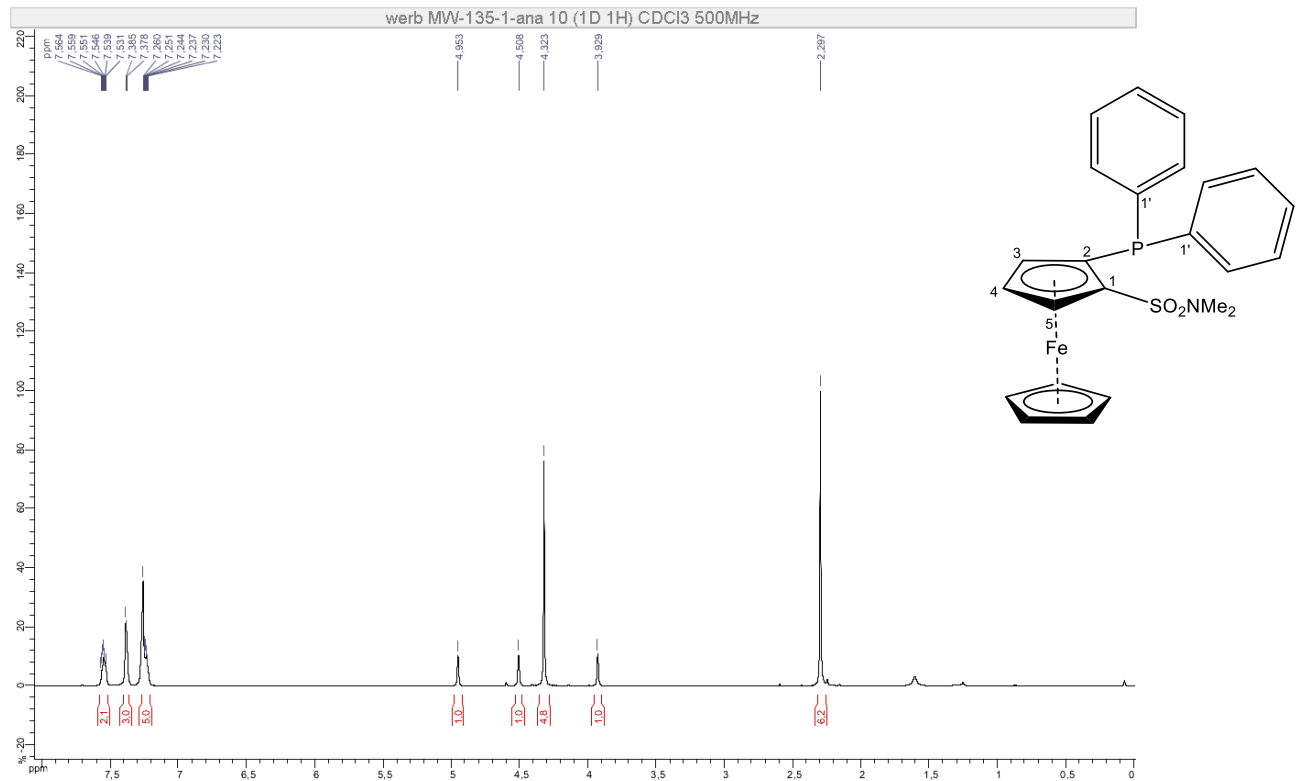


Figure S48. HMBC (300 MHz, CDCl₃) of **2g** (racemic mixture)



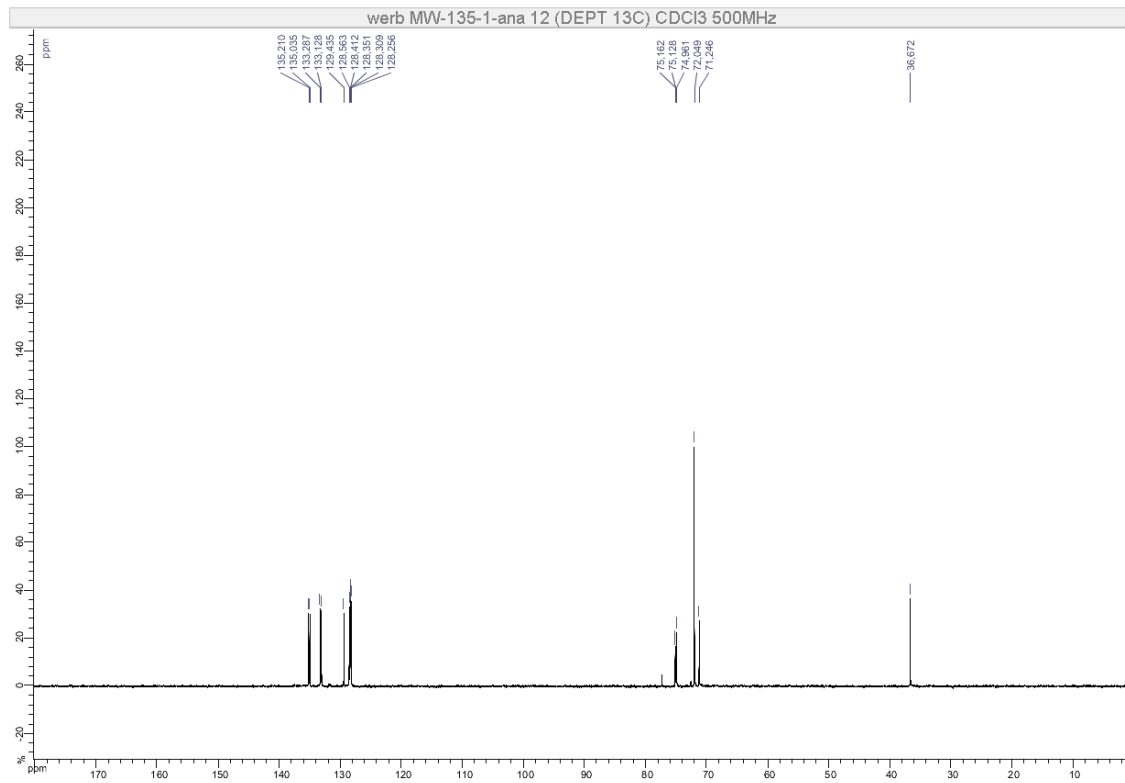


Figure S51. DEPT 135 (126 MHz, CDCl₃) of **2h** (racemic mixture)

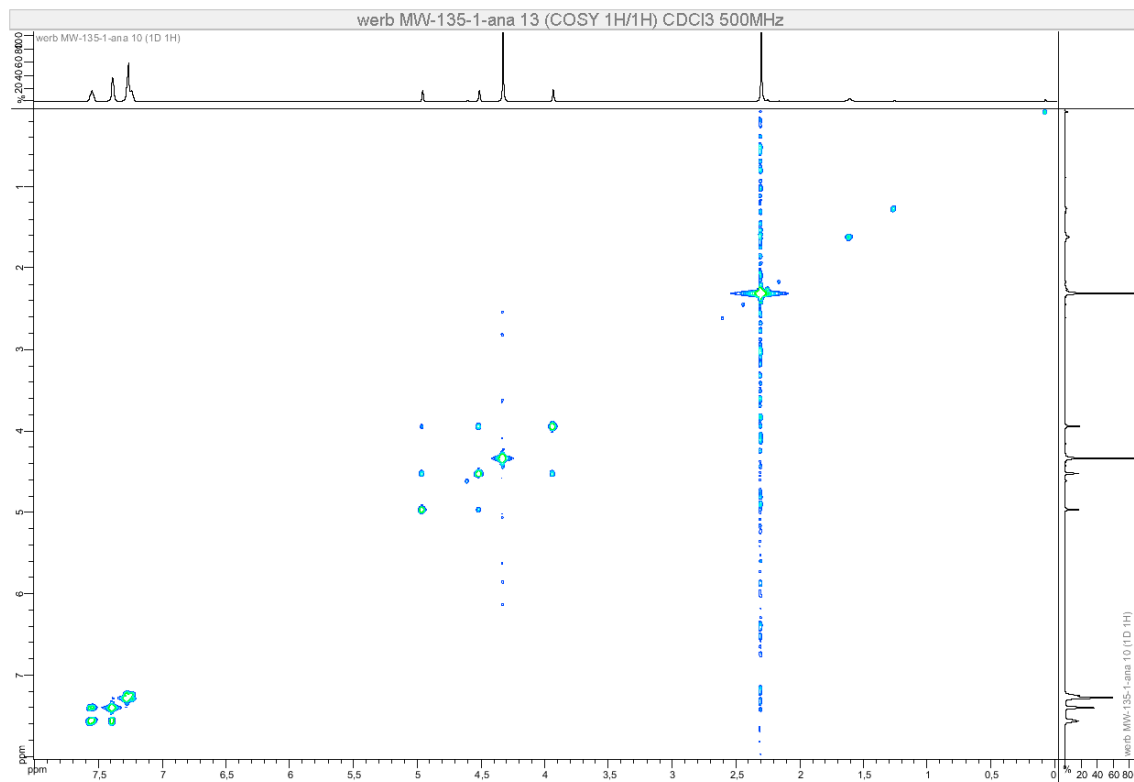


Figure S52. COSY (500 MHz, CDCl₃) of **2h** (racemic mixture)

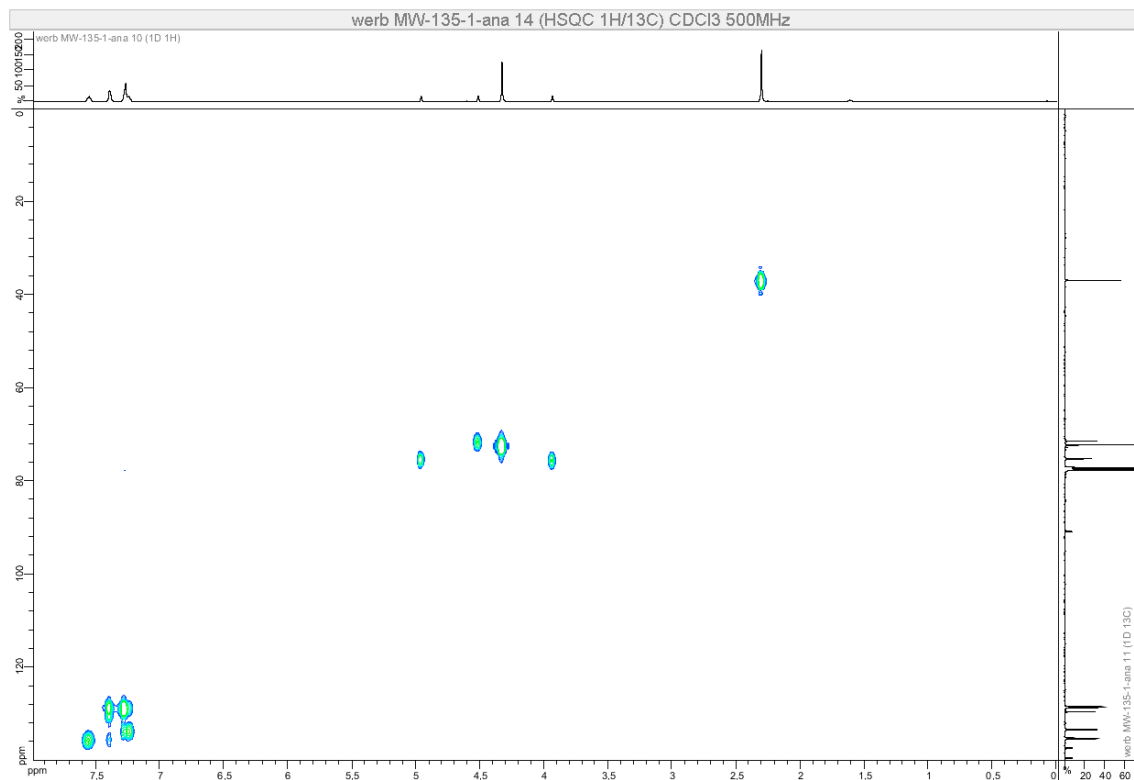


Figure S53. HSQC (500 MHz, CDCl₃) of **2h** (racemic mixture)

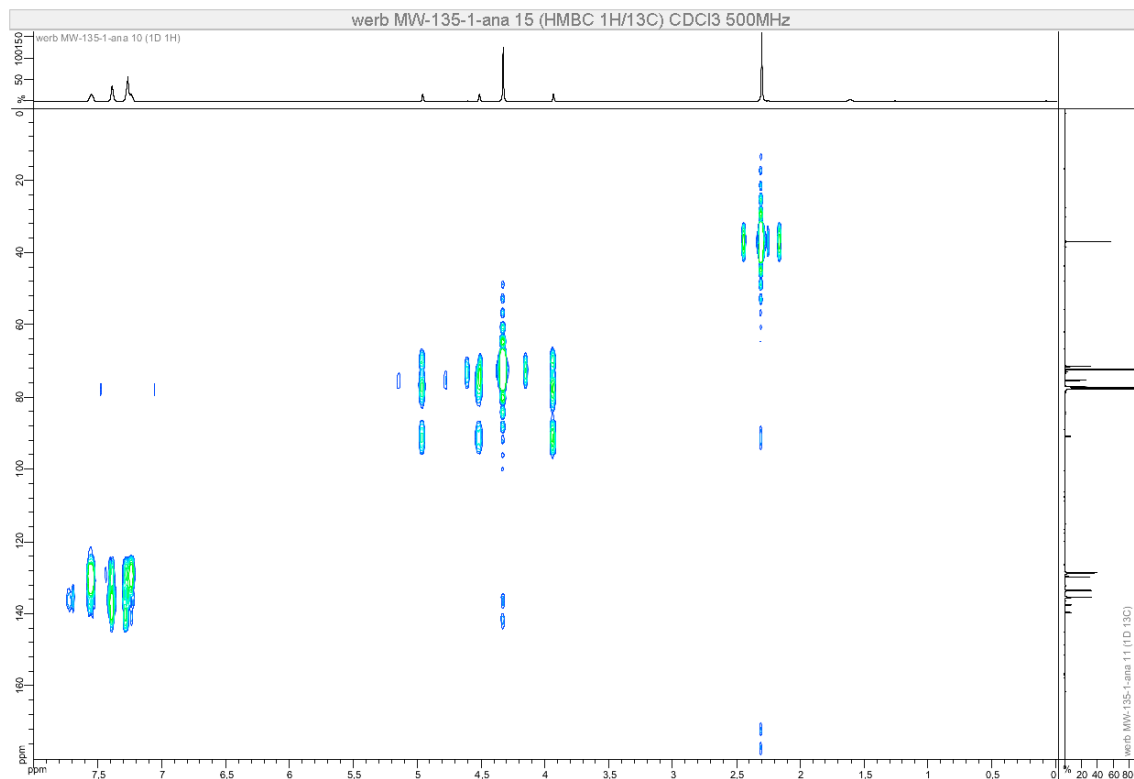


Figure S54. HMBC (500 MHz, CDCl₃) of **2h** (racemic mixture)

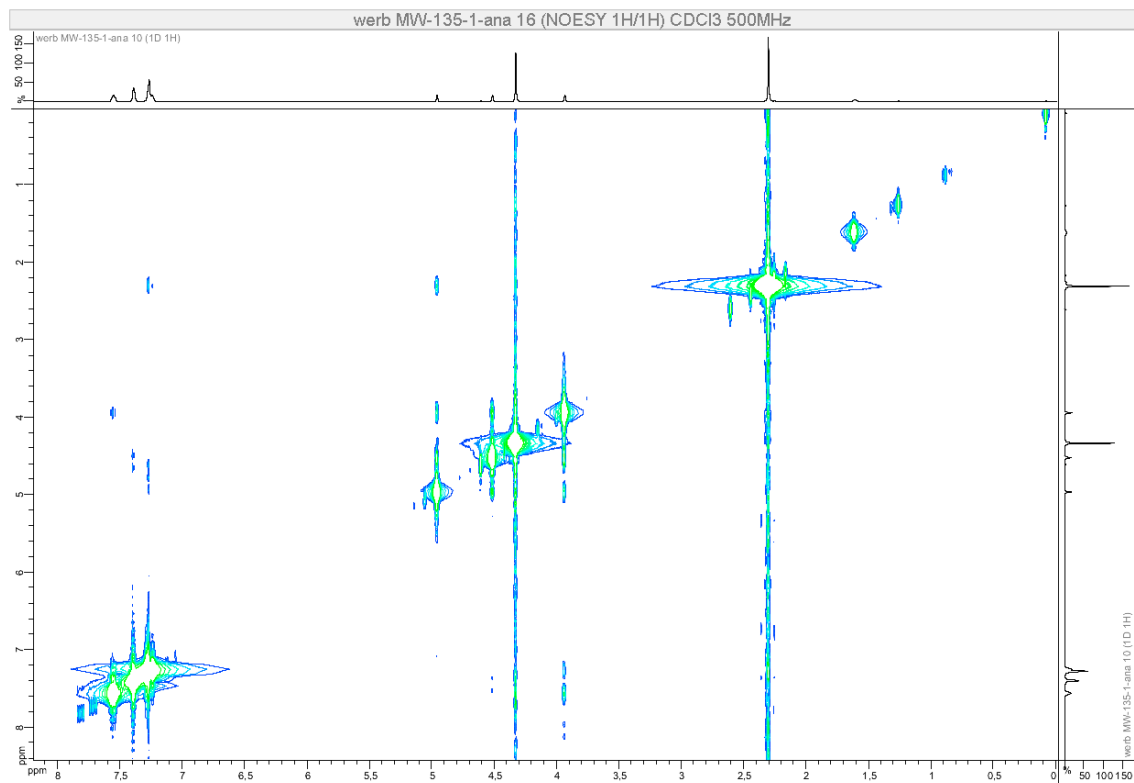


Figure S55. NOESY (500 MHz, CDCl₃) of **2h** (racemic mixture)

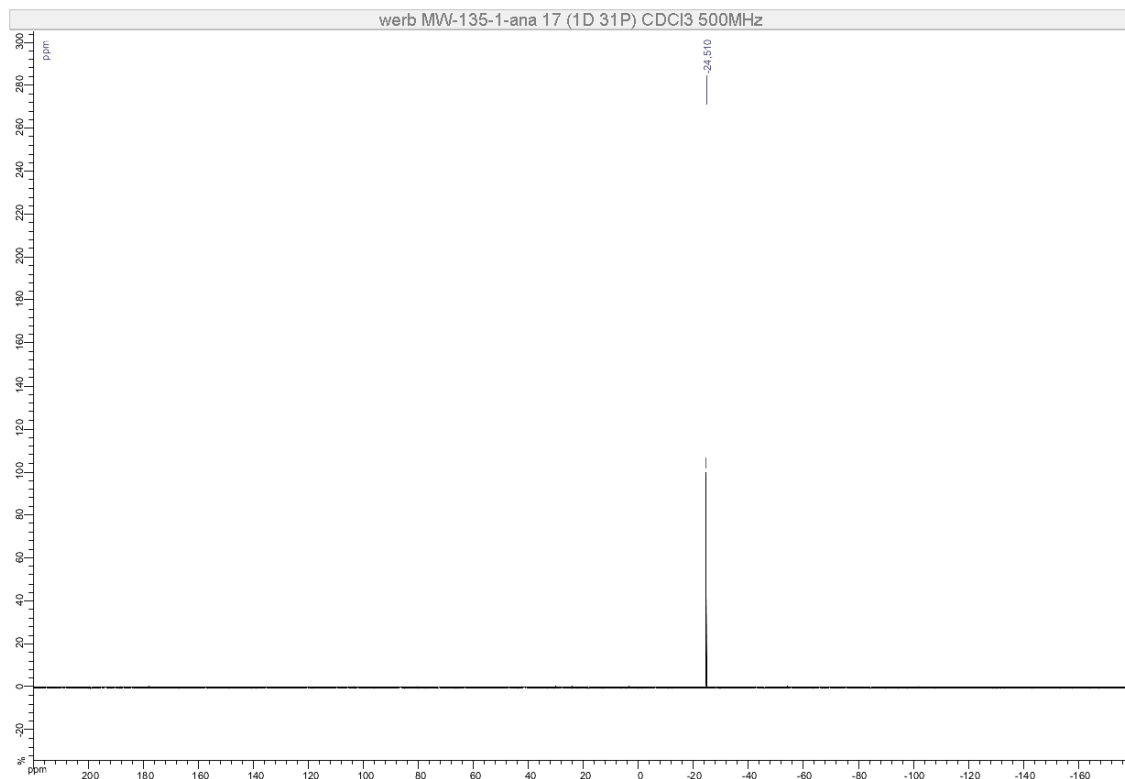


Figure S56. ³¹P NMR (202 MHz, CDCl₃) of **2h** (racemic mixture)

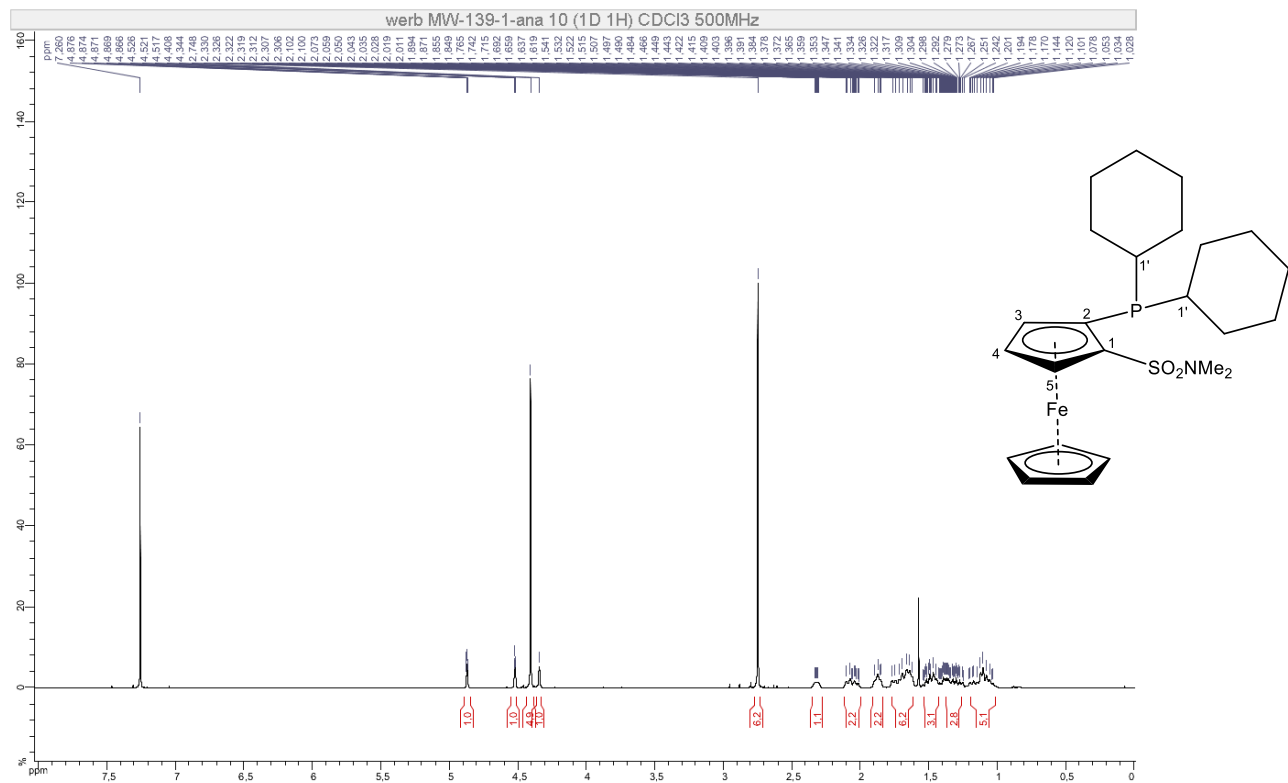


Figure S57. ^1H NMR (500 MHz, CDCl_3) of **2i** (racemic mixture)

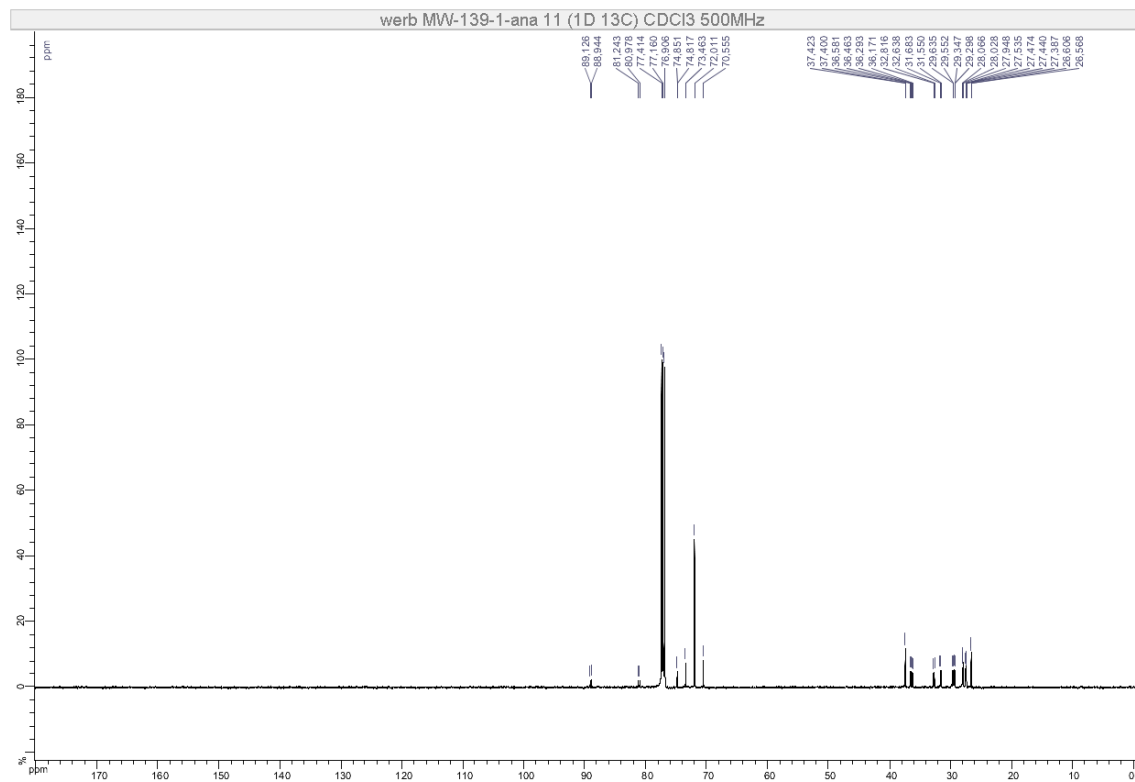


Figure S58. ^{13}C NMR (126 MHz, CDCl_3) of **2i** (racemic mixture)

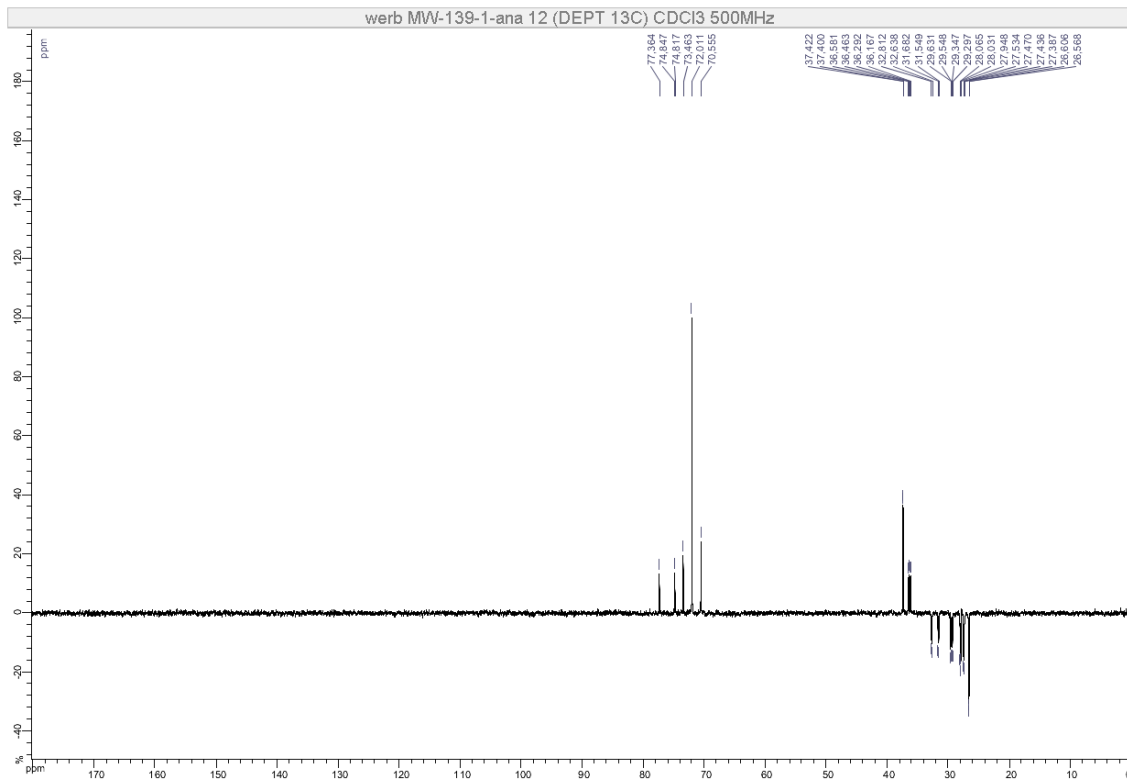


Figure S59. DEPT 135 (126 MHz, CDCl₃) of **2i** (racemic mixture)

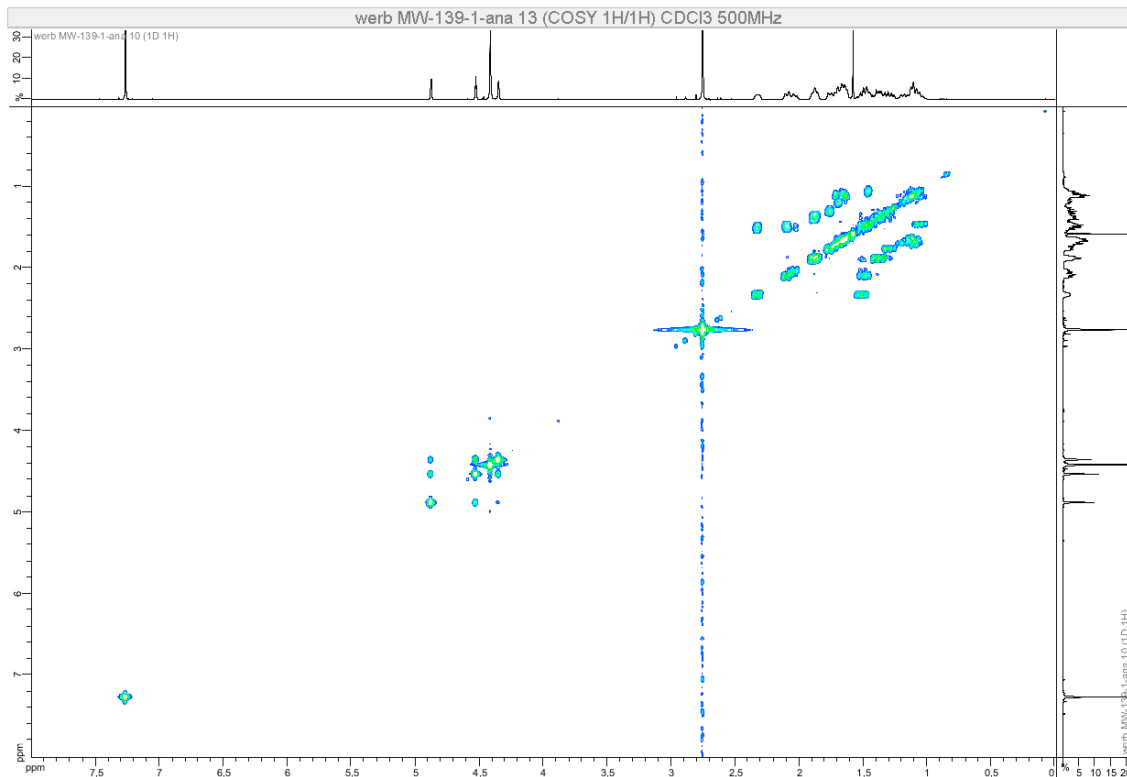


Figure S60. COSY (500 MHz, CDCl₃) of **2i** (racemic mixture)

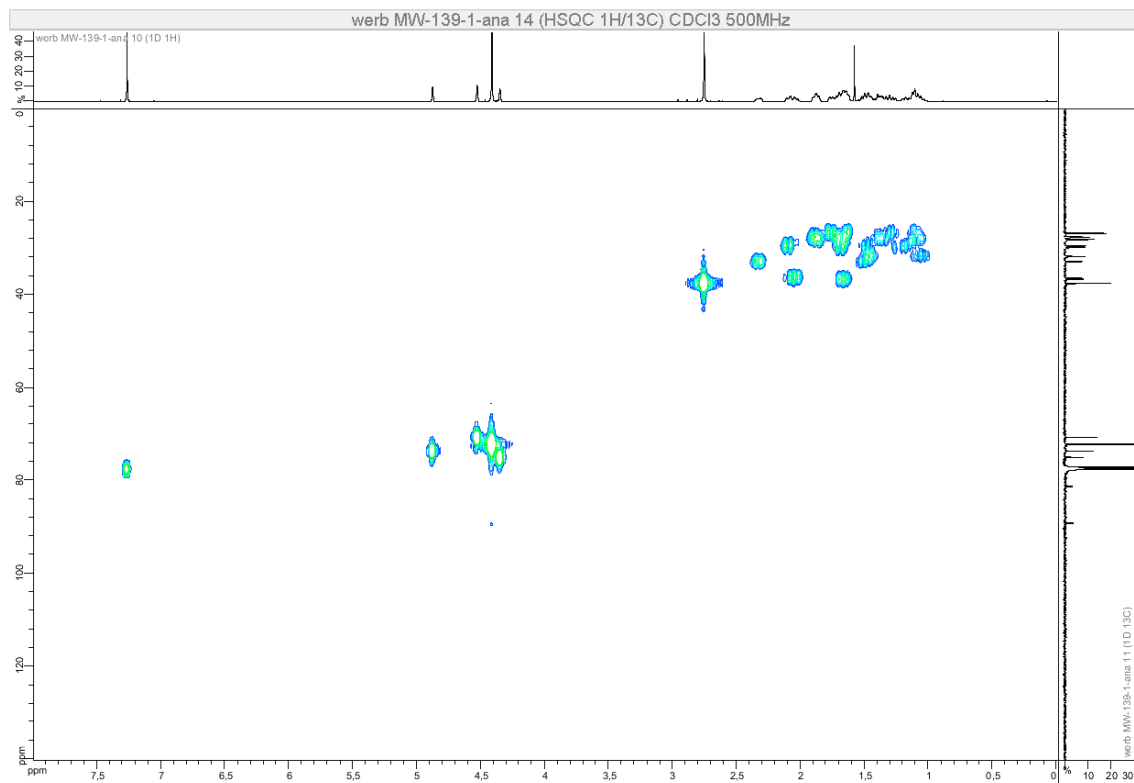


Figure S61. HSQC (500 MHz, CDCl₃) of **2i** (racemic mixture)

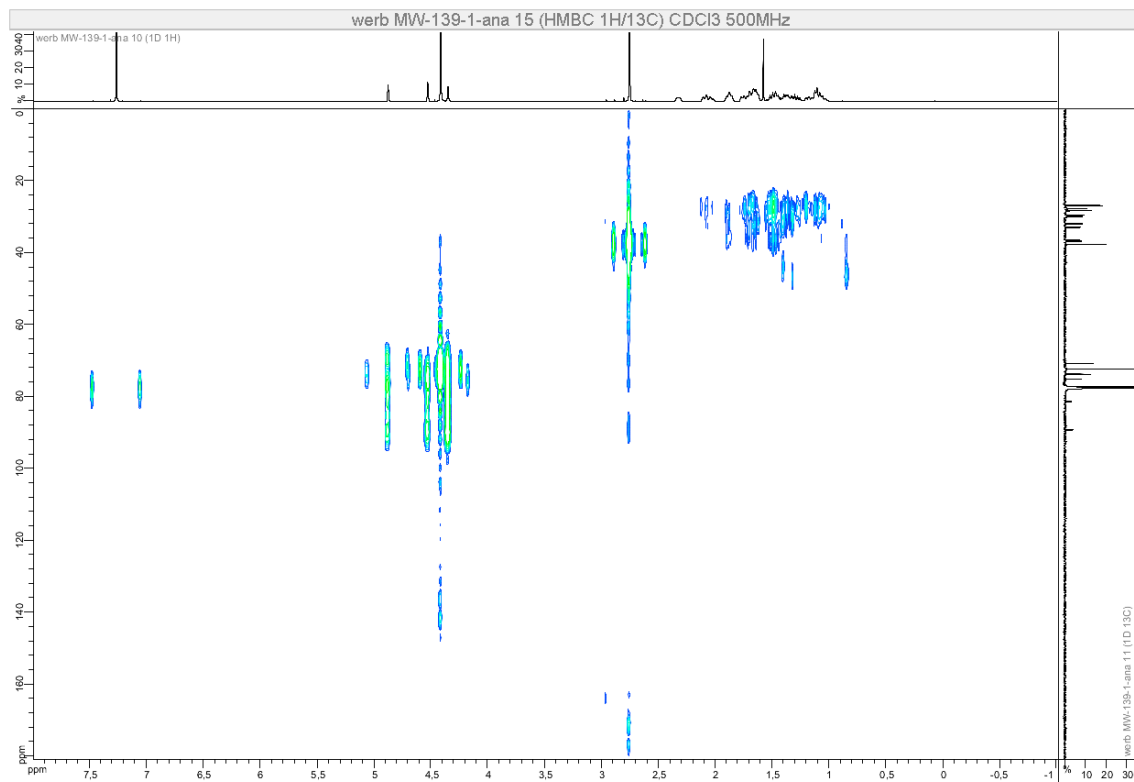


Figure S62. HMBC (500 MHz, CDCl₃) of **2i** (racemic mixture)

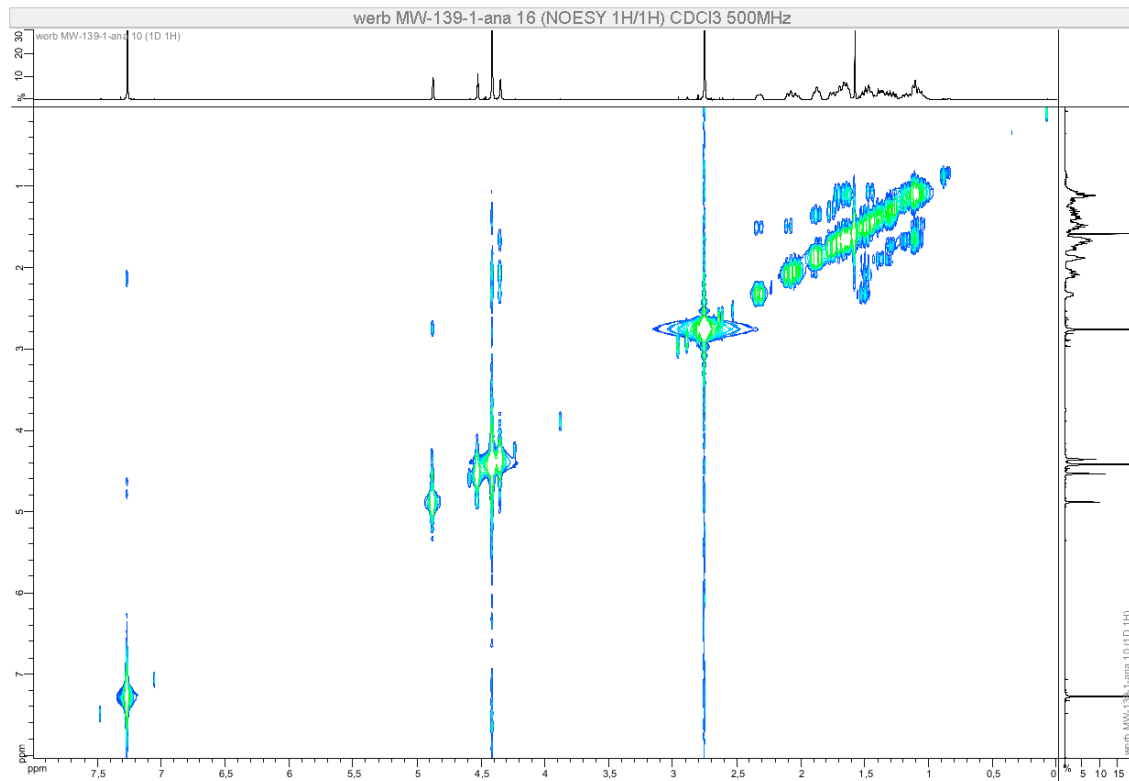


Figure S63. NOESY (500 MHz, CDCl₃) of **2i** (racemic mixture)

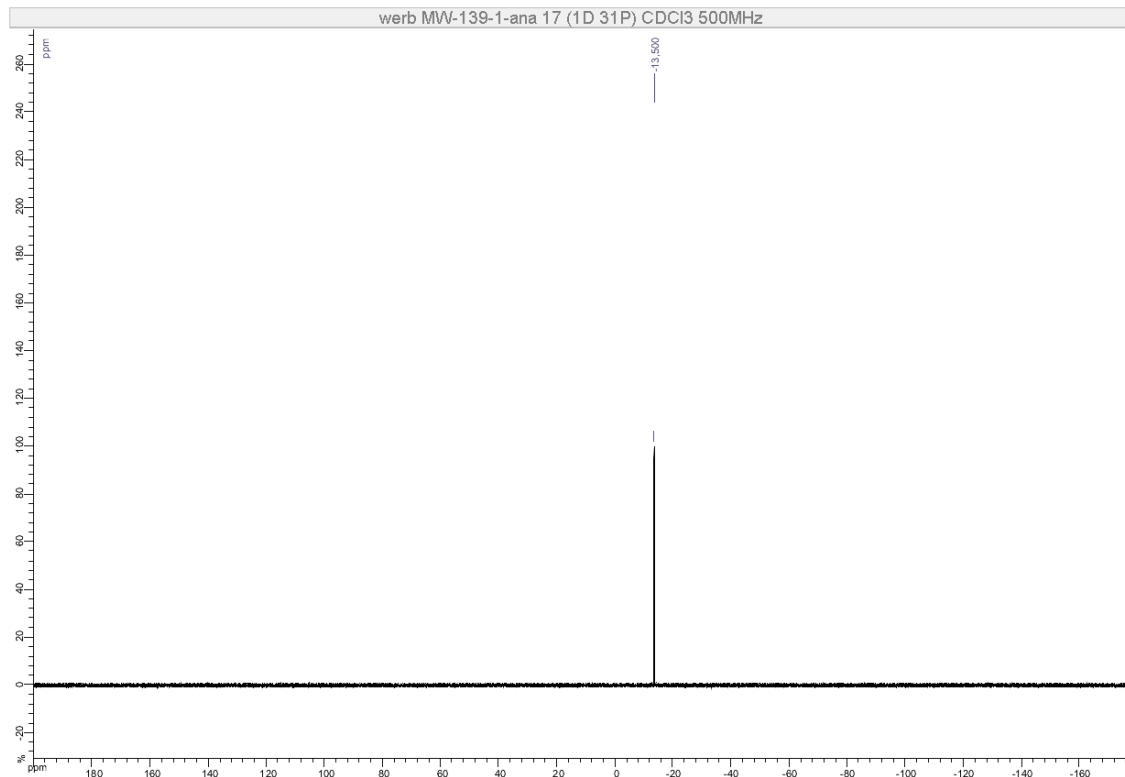


Figure S64. ³¹P NMR (202 MHz, CDCl₃) of **2i** (racemic mixture)

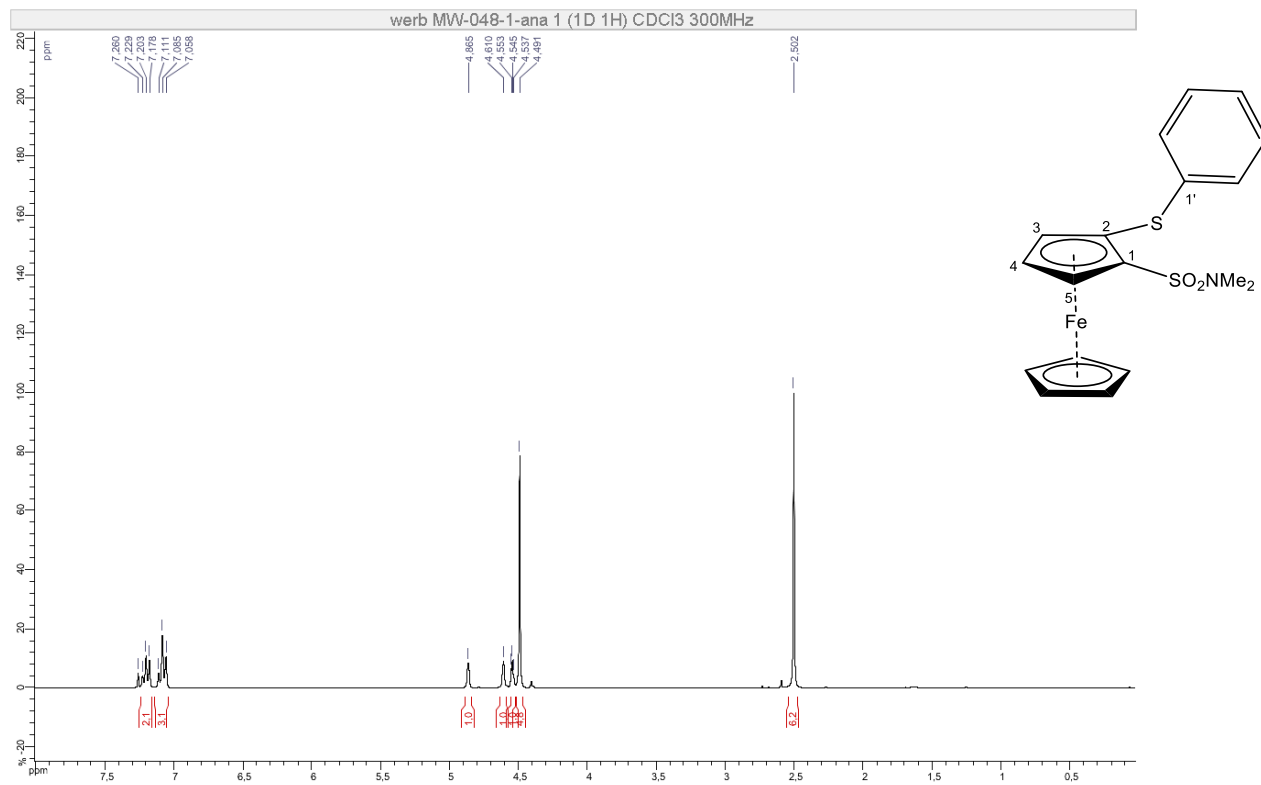


Figure S65. ¹H NMR (300 MHz, CDCl₃) of **2j** (racemic mixture)

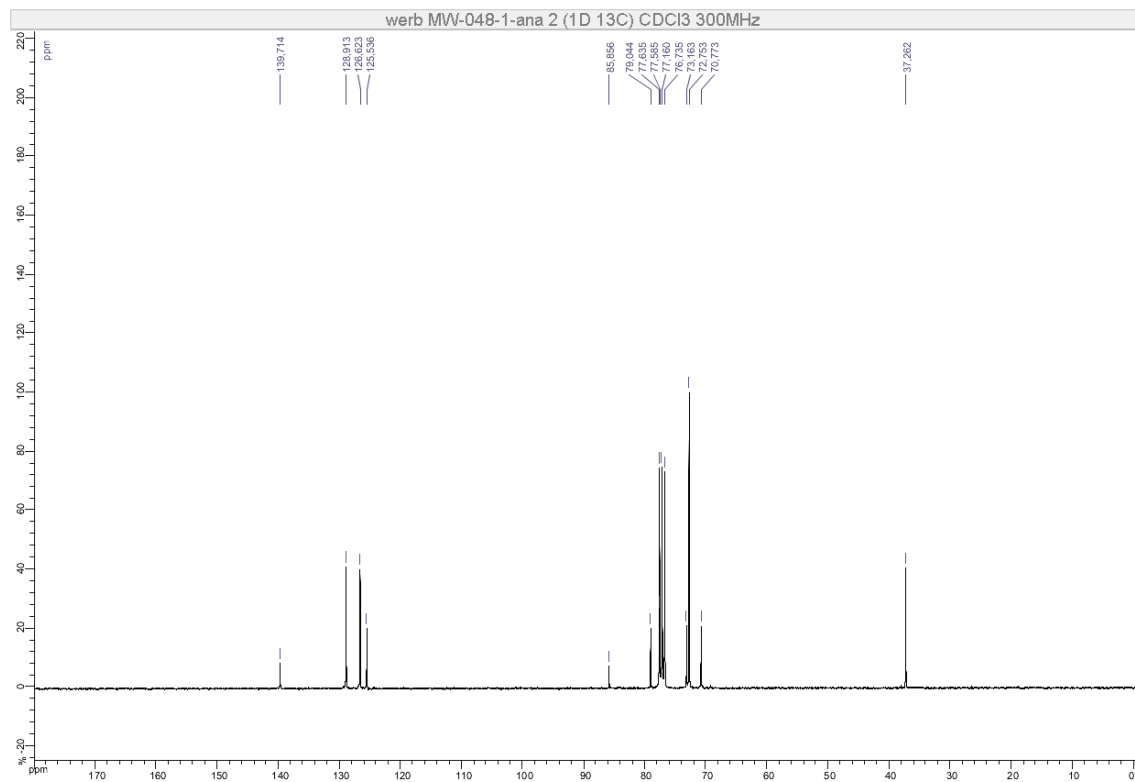


Figure S66. ¹³C NMR (75 MHz, CDCl₃) of **2j** (racemic mixture)

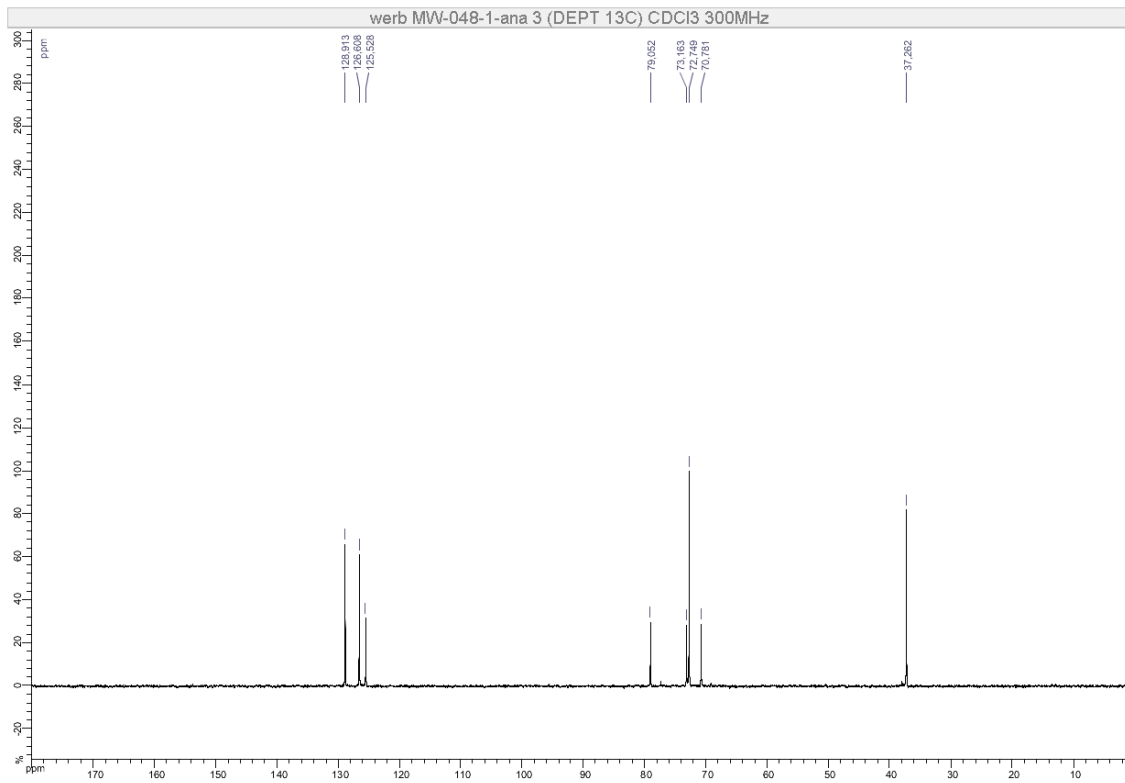


Figure S67. DEPT 135 (75 MHz, CDCl₃) of **2j** (racemic mixture)

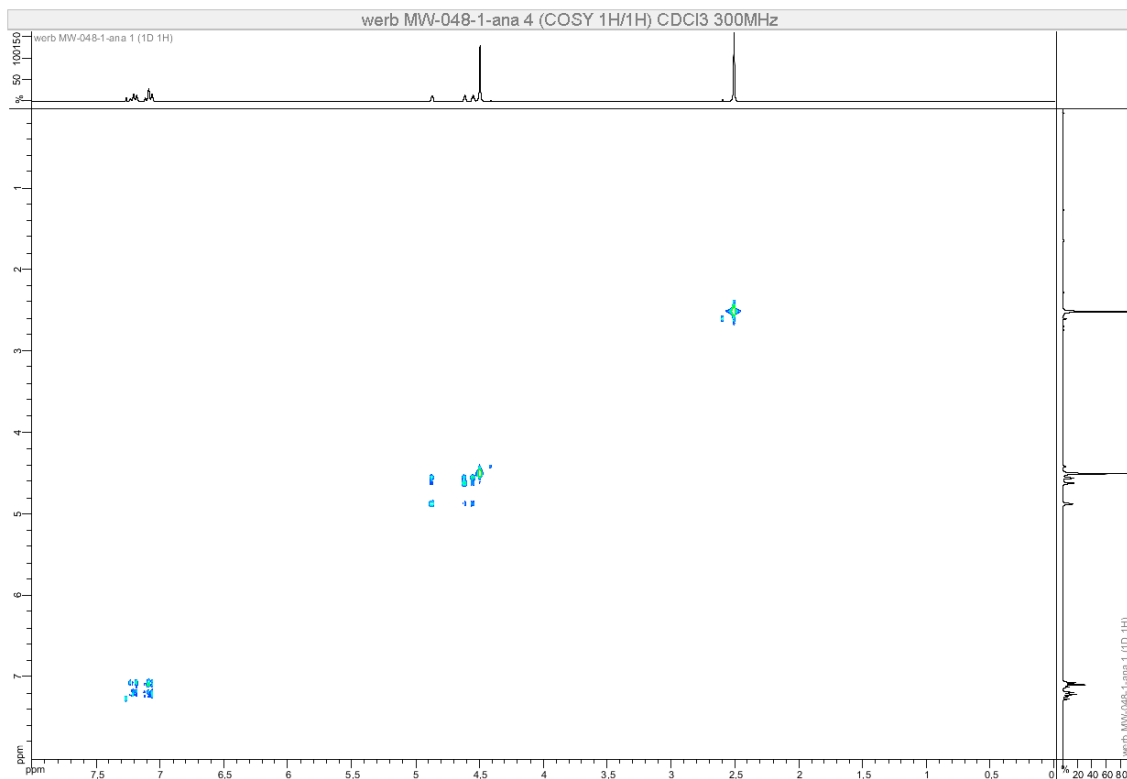


Figure S68. COSY (300 MHz, CDCl₃) of **2j** (racemic mixture)

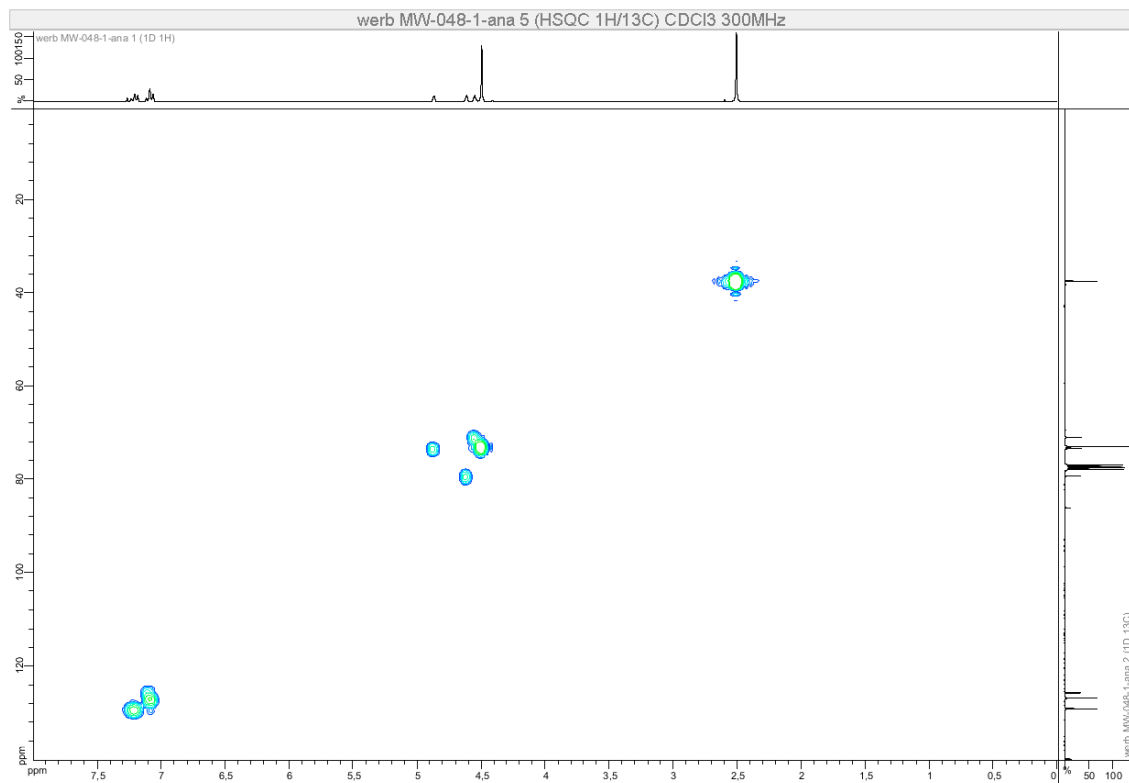


Figure S69. HSQC (300 MHz, CDCl₃) of **2j** (racemic mixture)

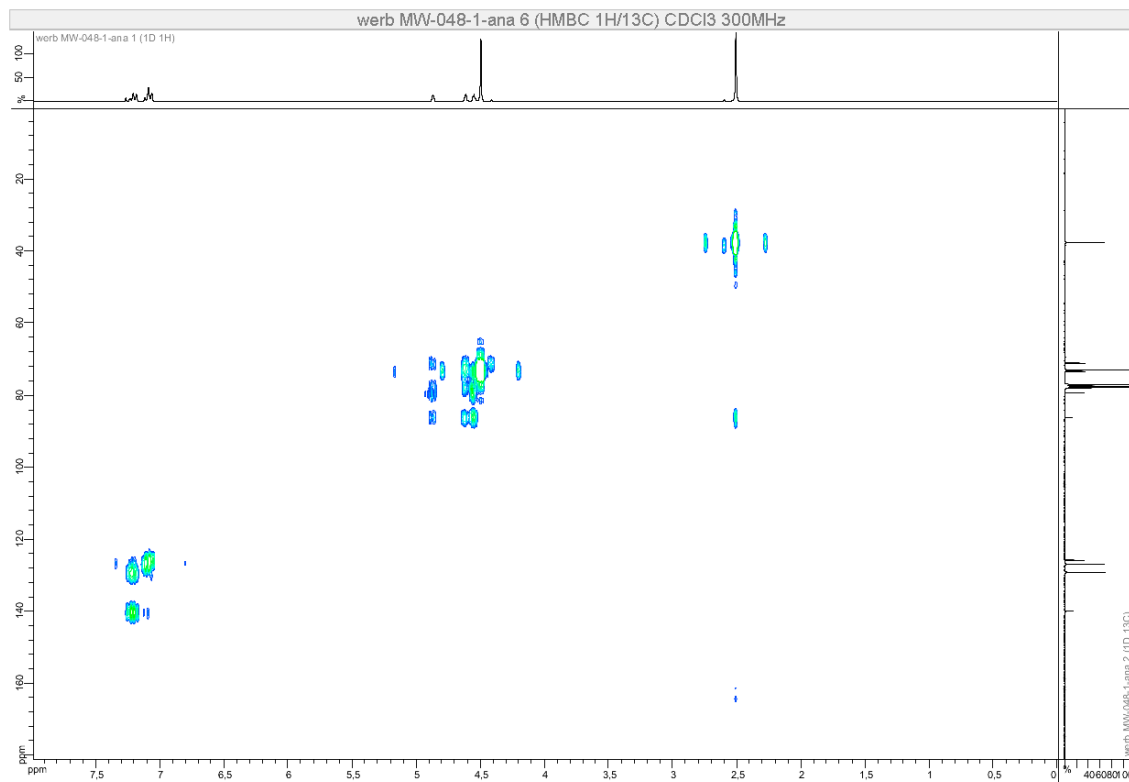


Figure S70. HMBC (300 MHz, CDCl₃) of **2j** (racemic mixture)

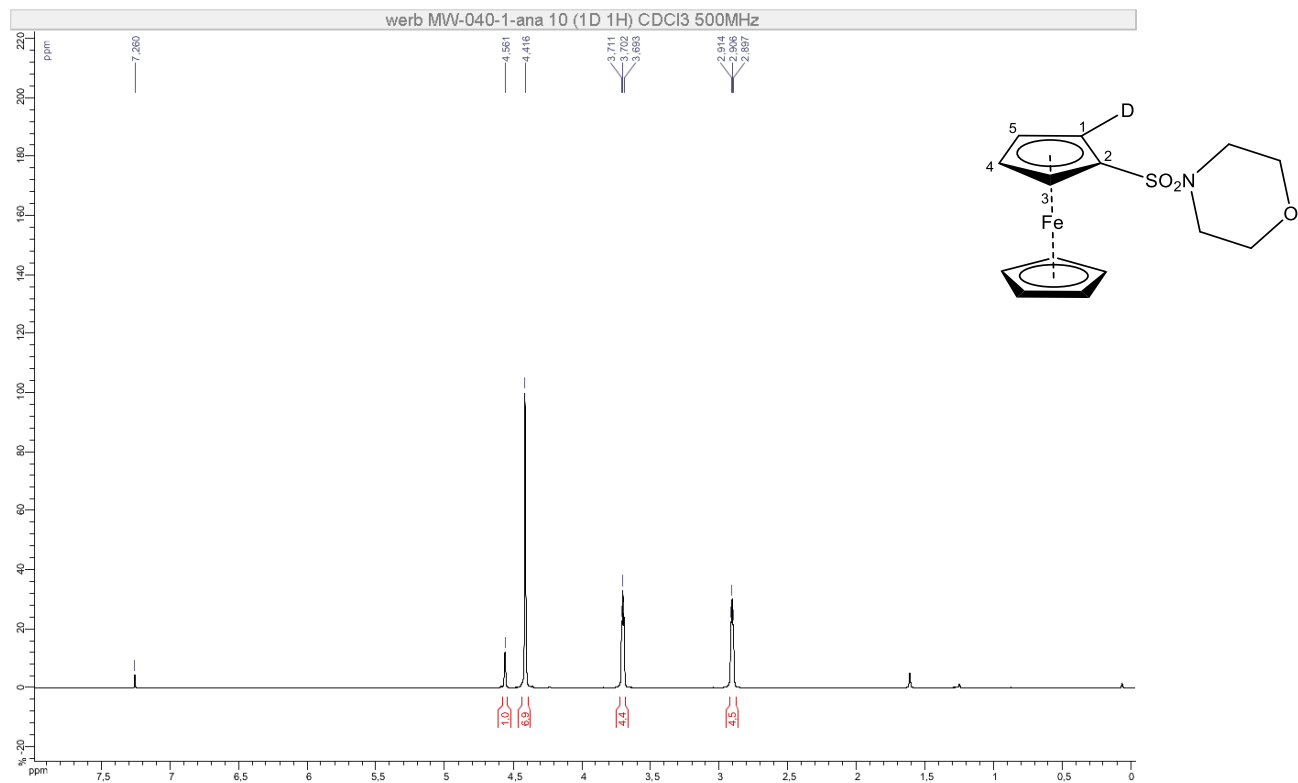


Figure S71. ^1H NMR (300 MHz, CDCl_3) of **4a** (racemic mixture)

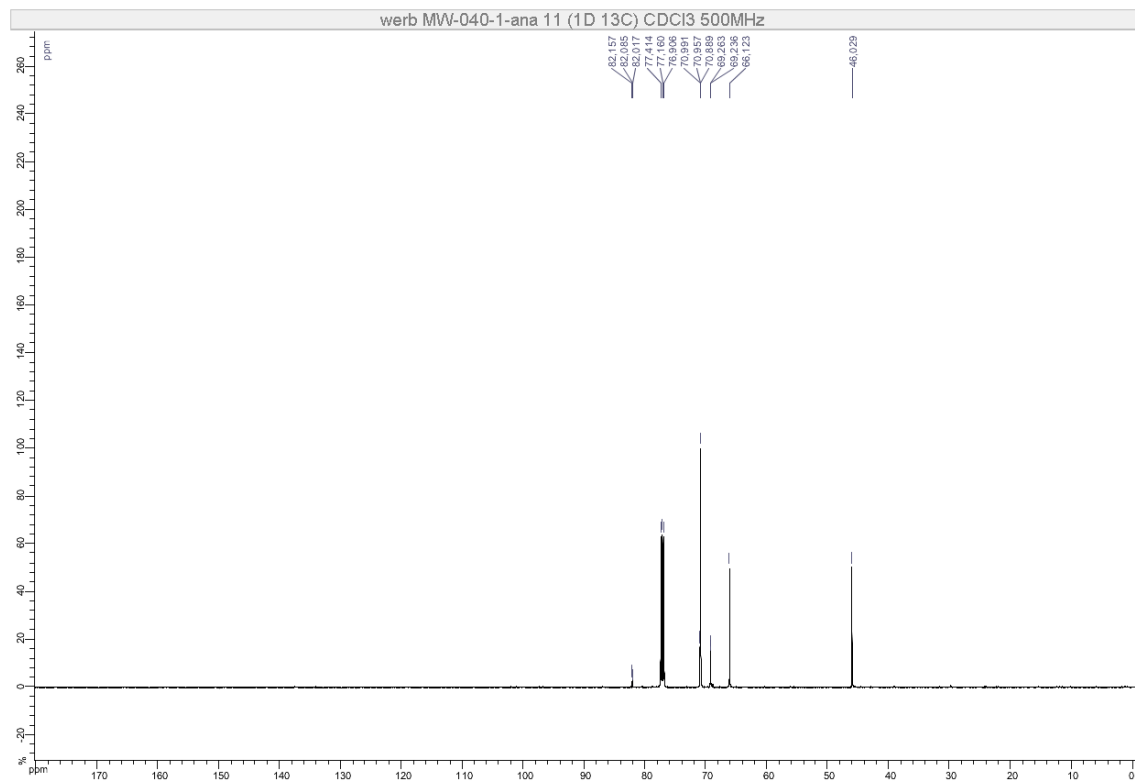


Figure S72. ^{13}C NMR (75 MHz, CDCl_3) of **4a** (racemic mixture)

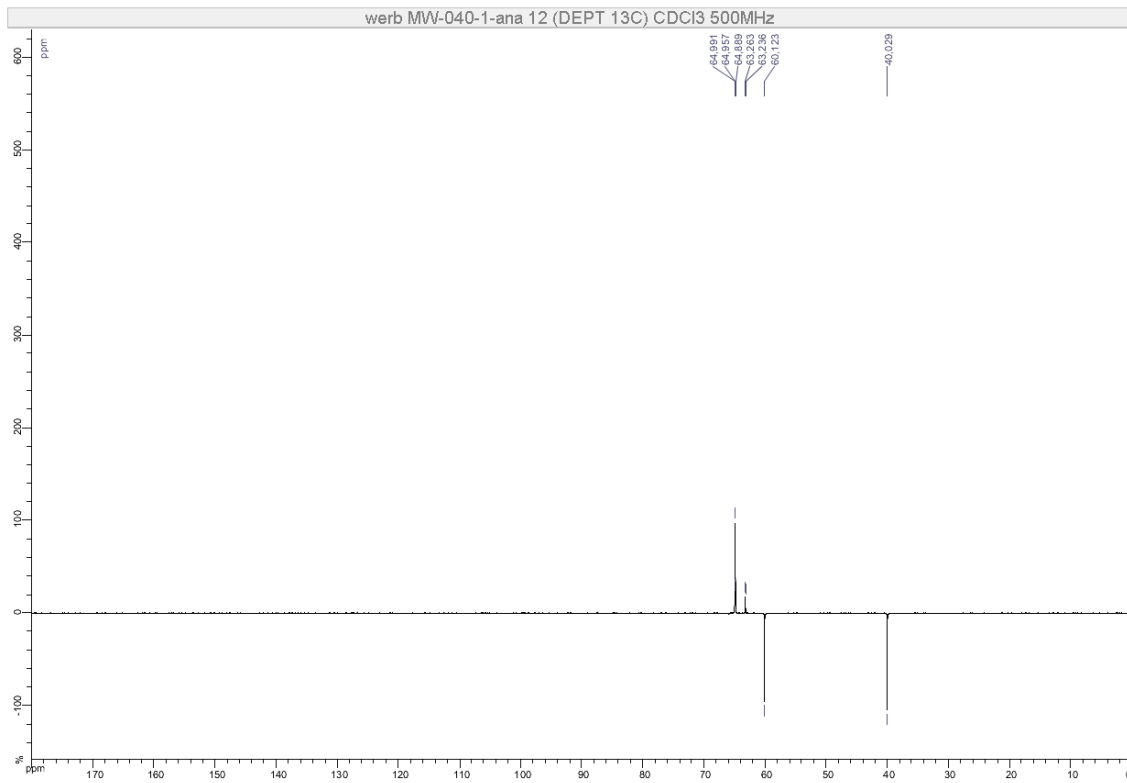


Figure S73. DEPT 135 (75 MHz, CDCl₃) of **4a** (racemic mixture)

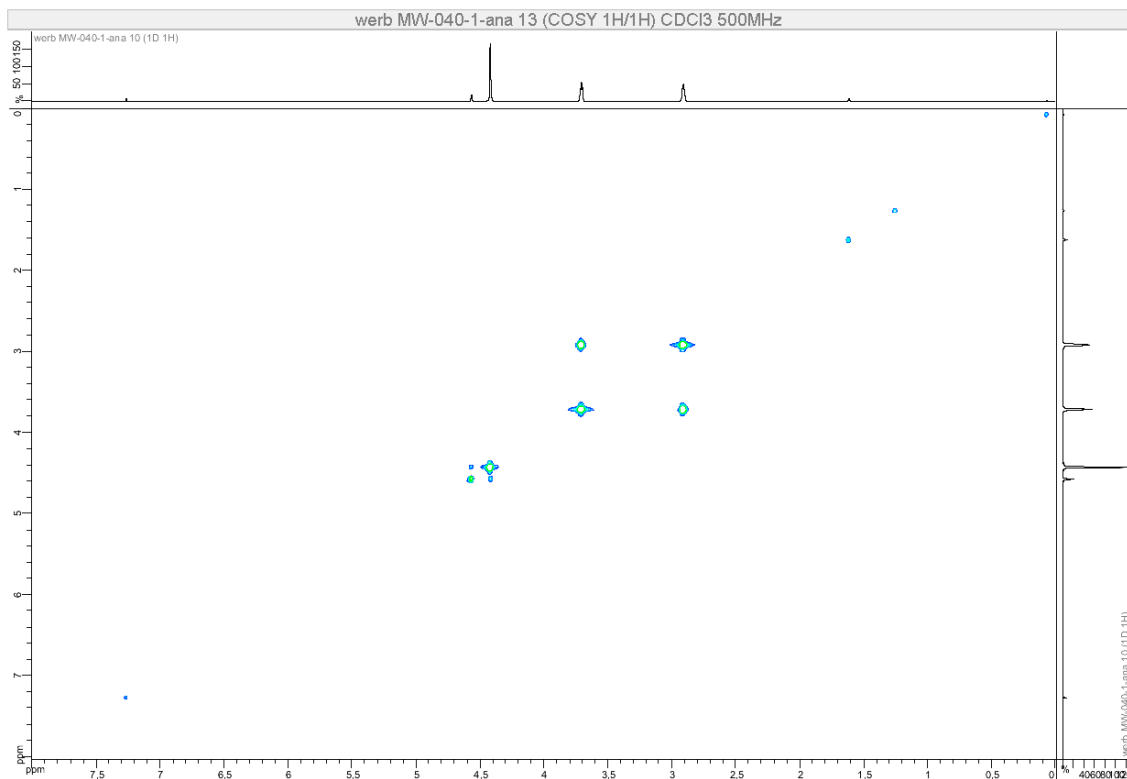


Figure S74. COSY (300 MHz, CDCl₃) of **4a** (racemic mixture)

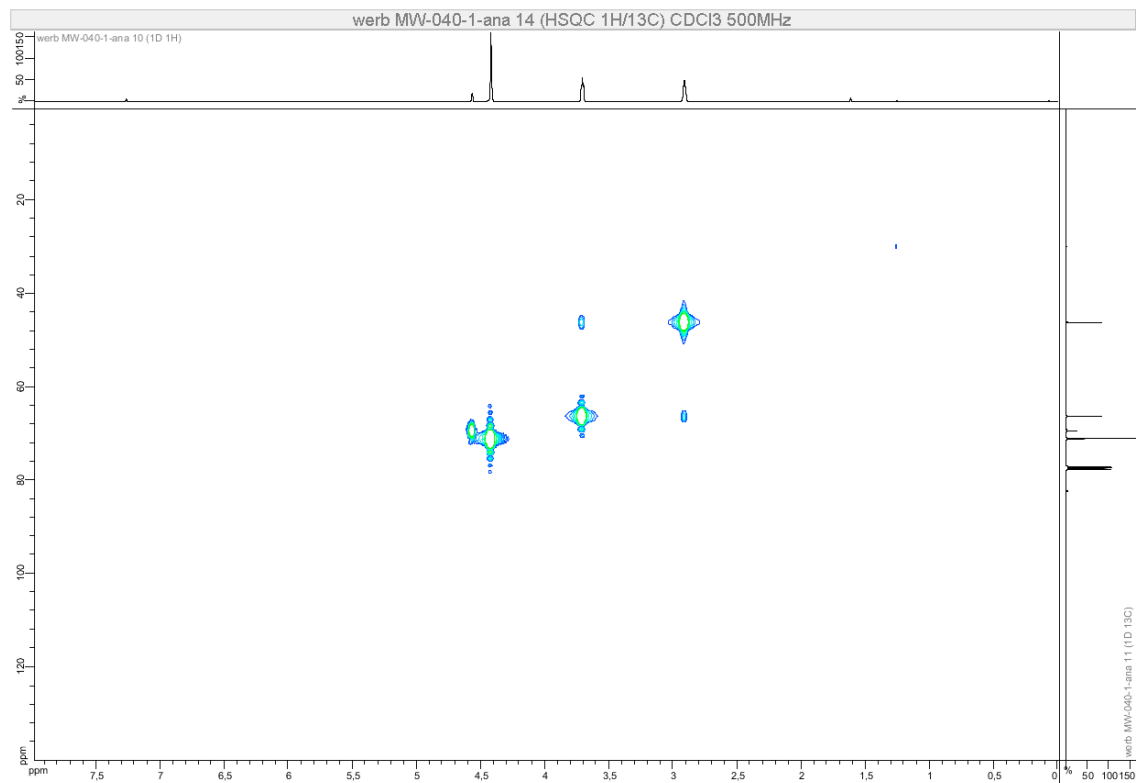


Figure S75. HSQC (300 MHz, CDCl₃) of **4a** (racemic mixture)

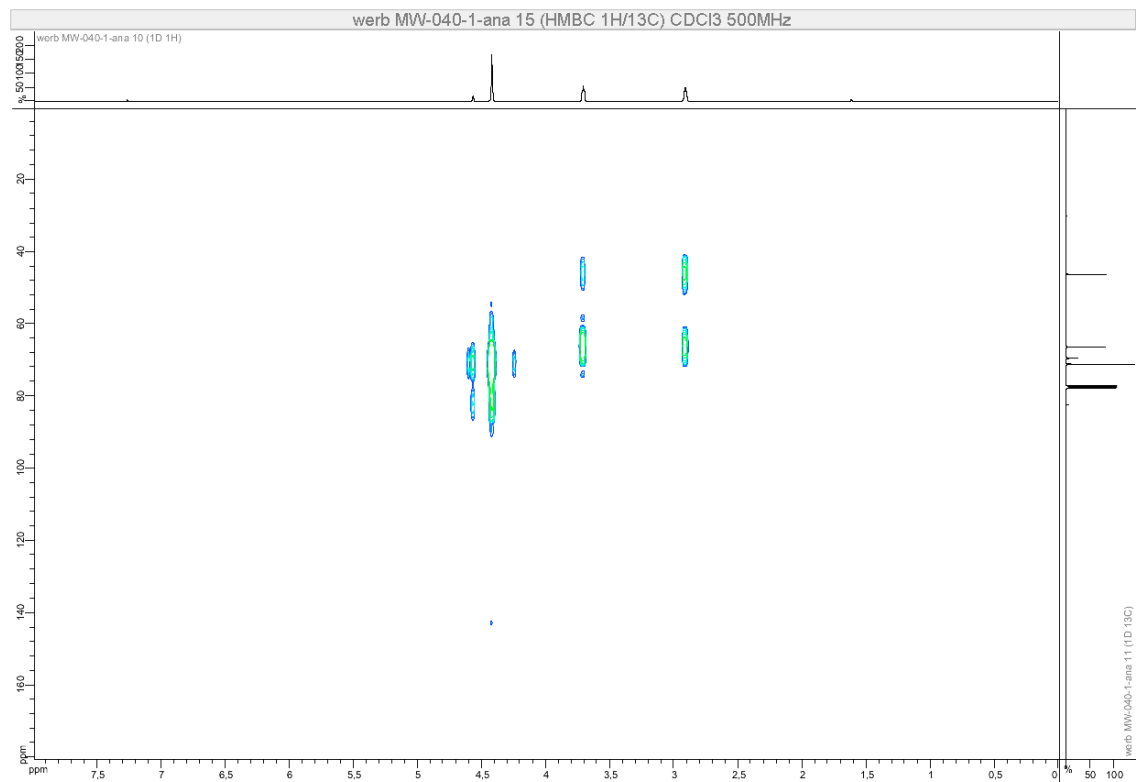
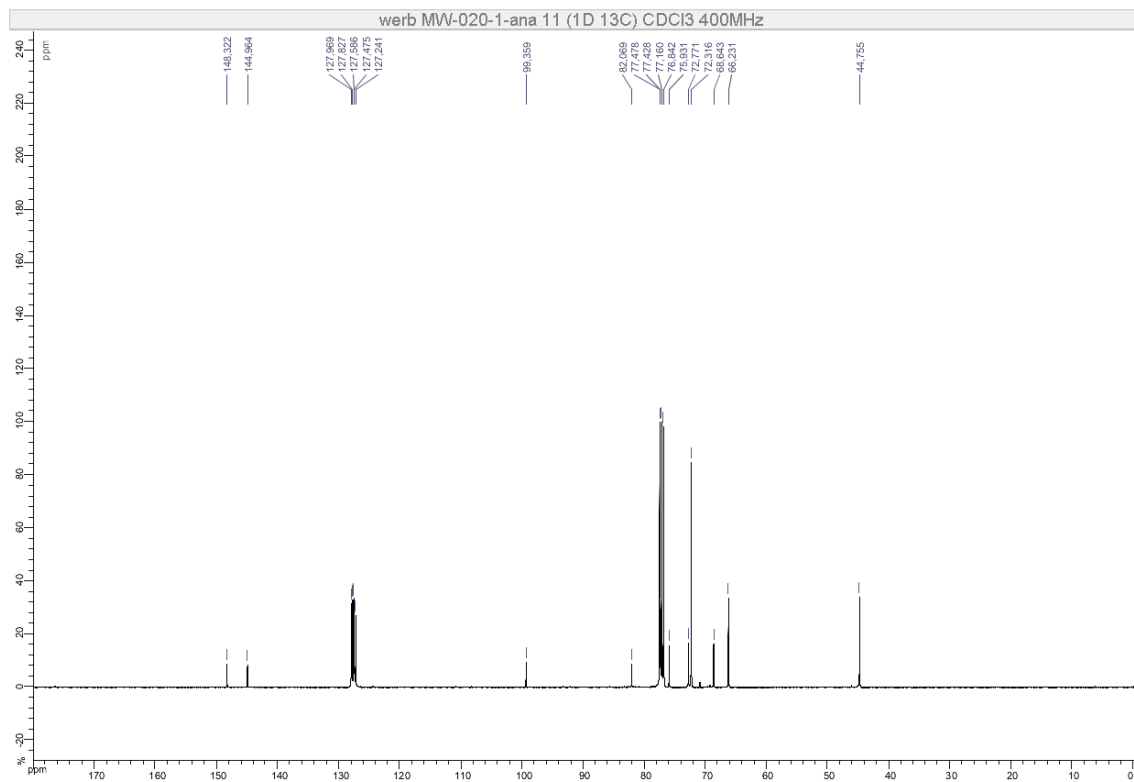
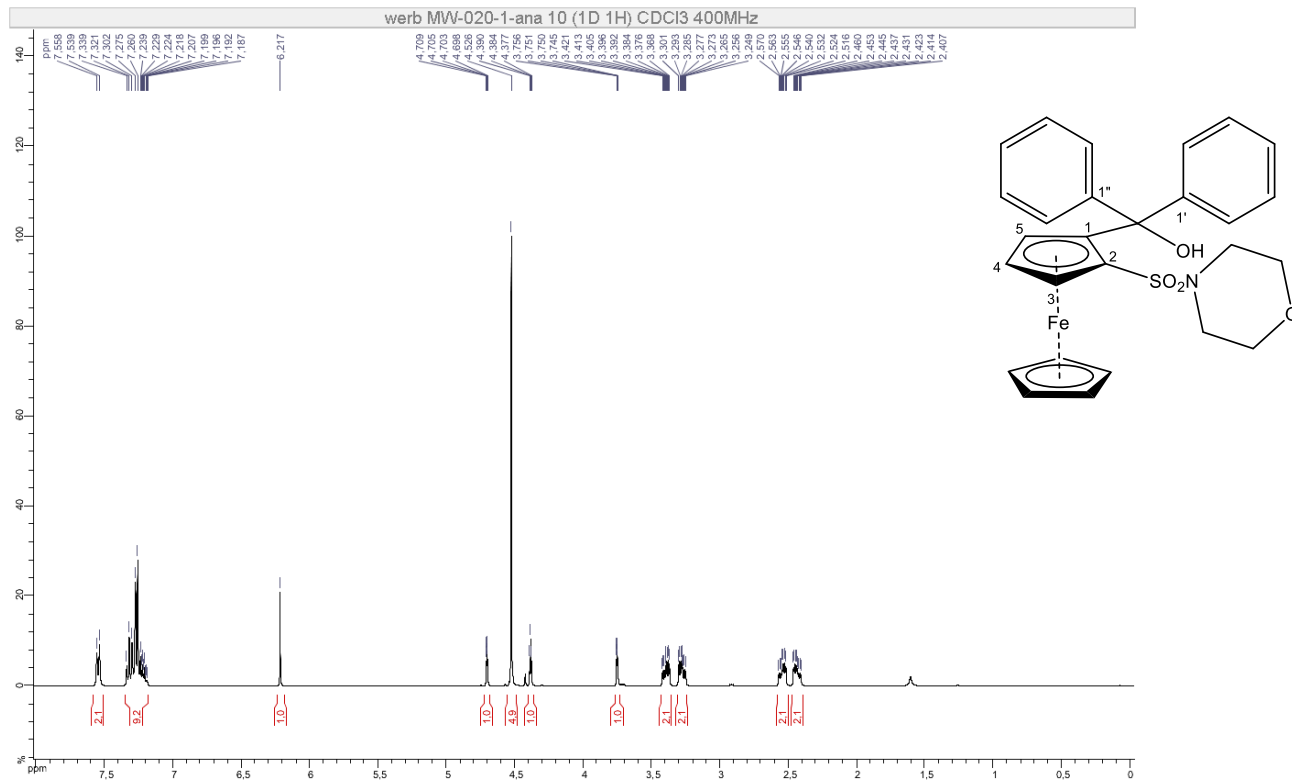


Figure S76. HMBC (300 MHz, CDCl₃) of **4a** (racemic mixture)



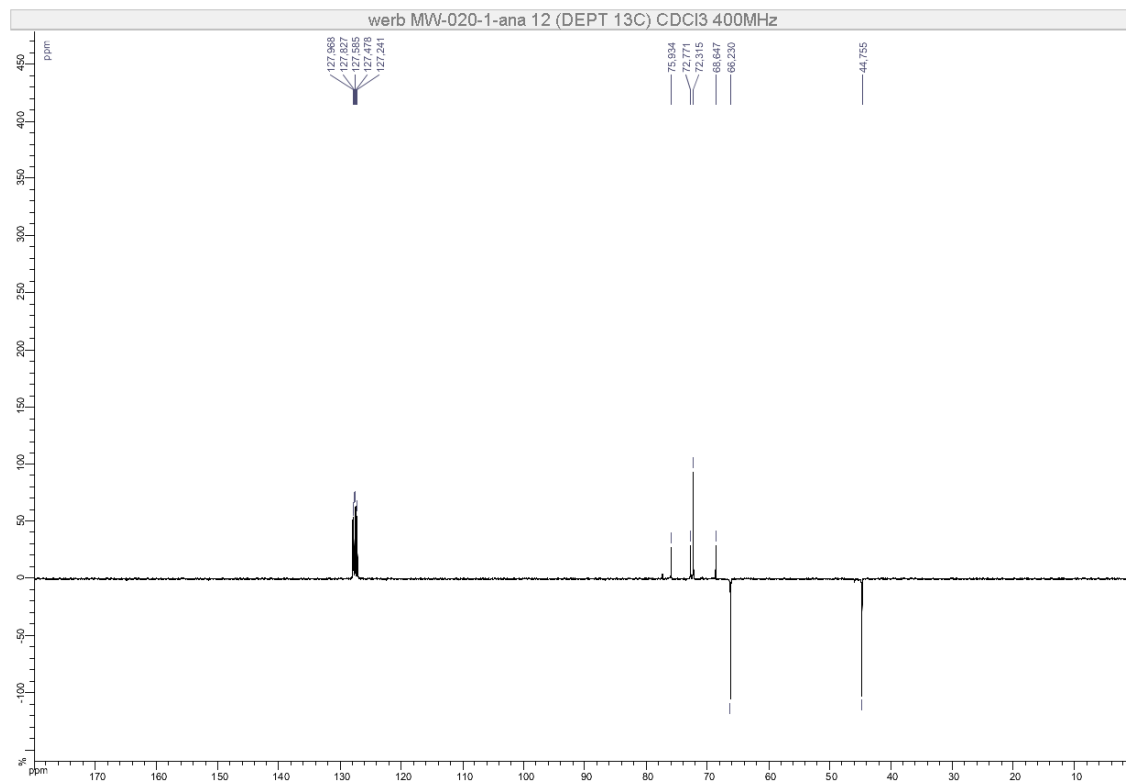


Figure S79. DEPT 135 (101 MHz, CDCl₃) of **4b** (racemic mixture)

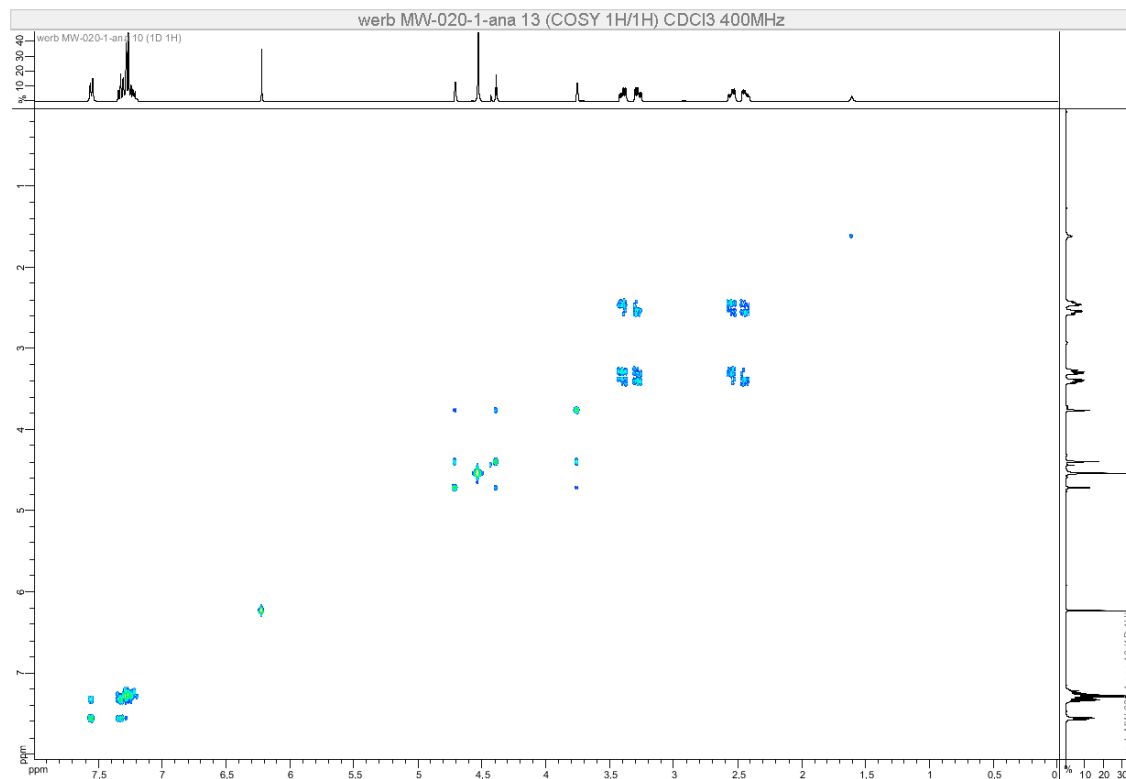


Figure S80. COSY (400 MHz, CDCl₃) of **4b** (racemic mixture)

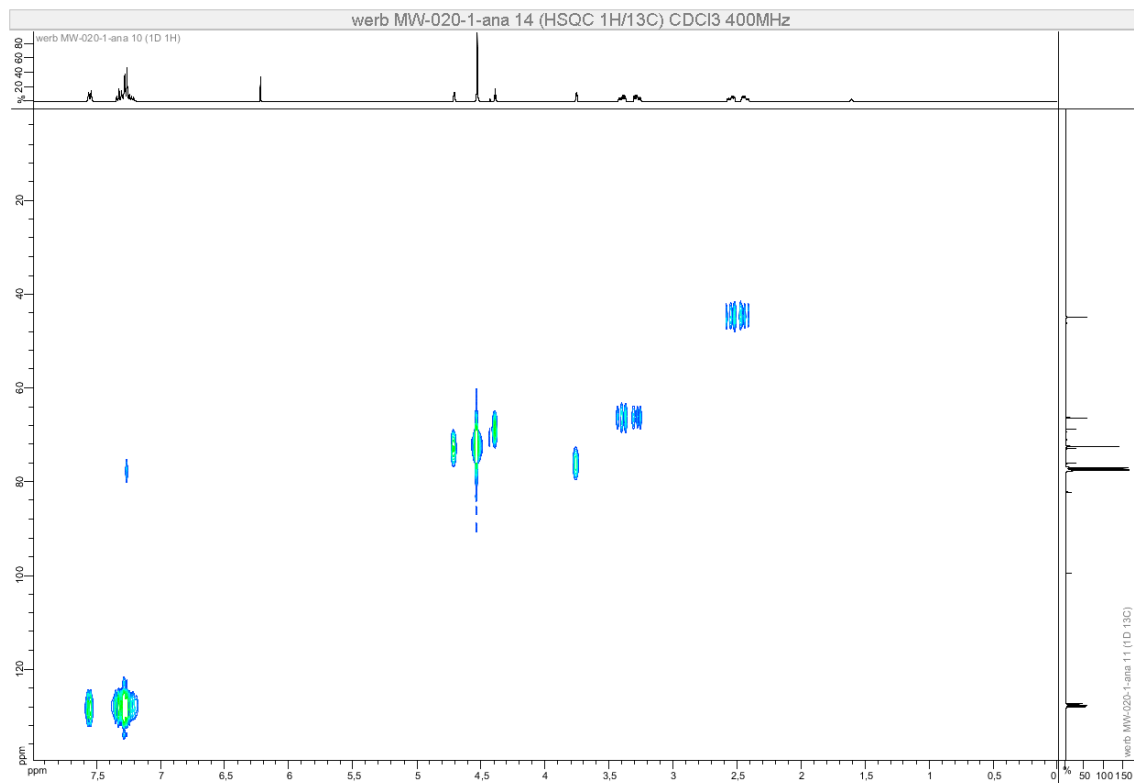


Figure S81. HSQC (400 MHz, CDCl_3) of **4b** (racemic mixture)

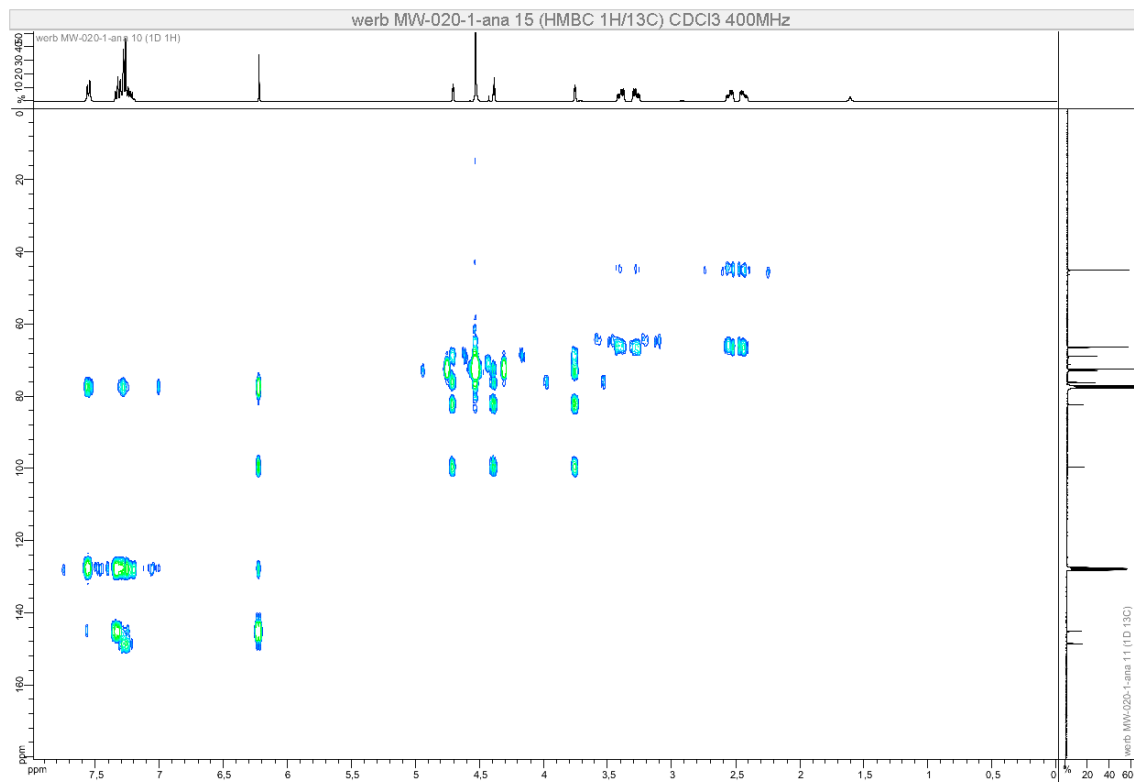


Figure S82. HMBC (400 MHz, CDCl_3) of **4b** (racemic mixture)

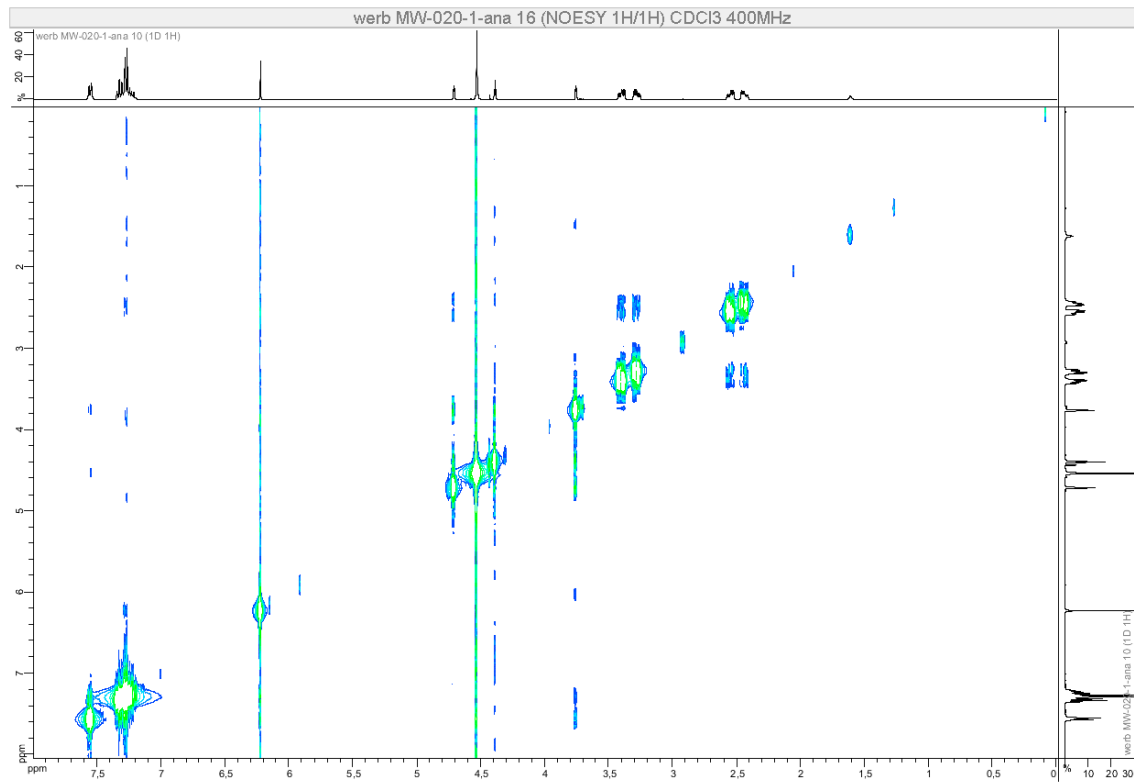
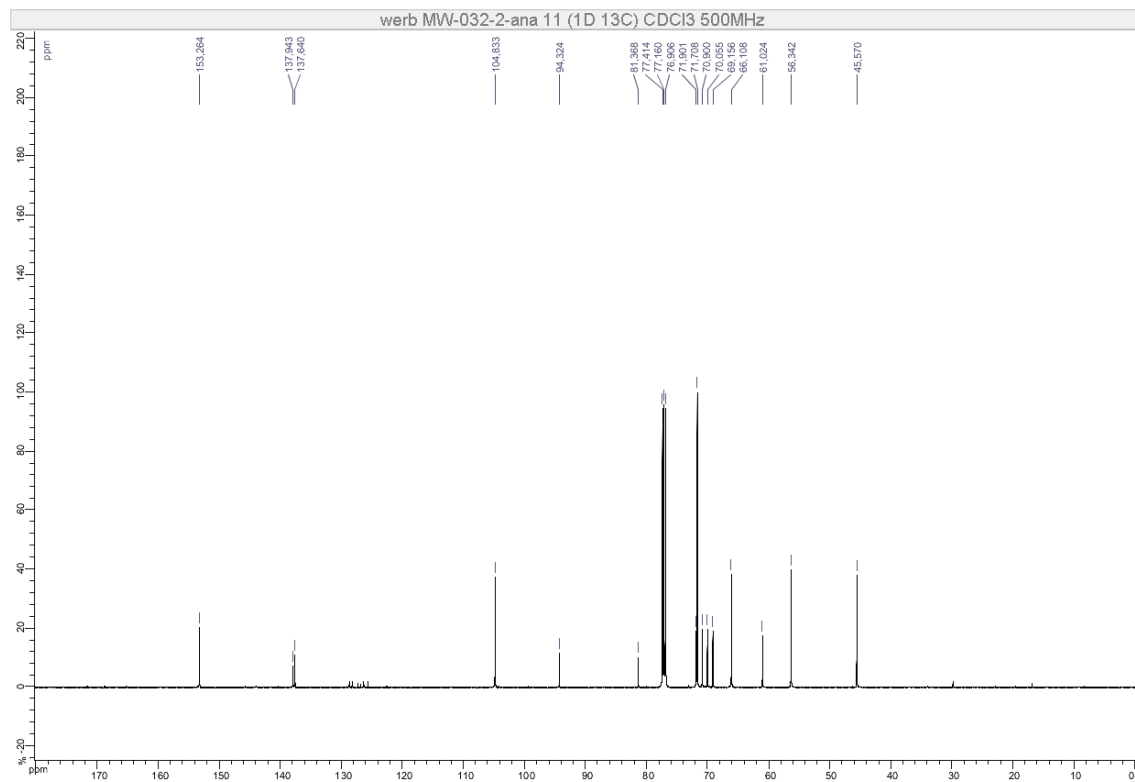
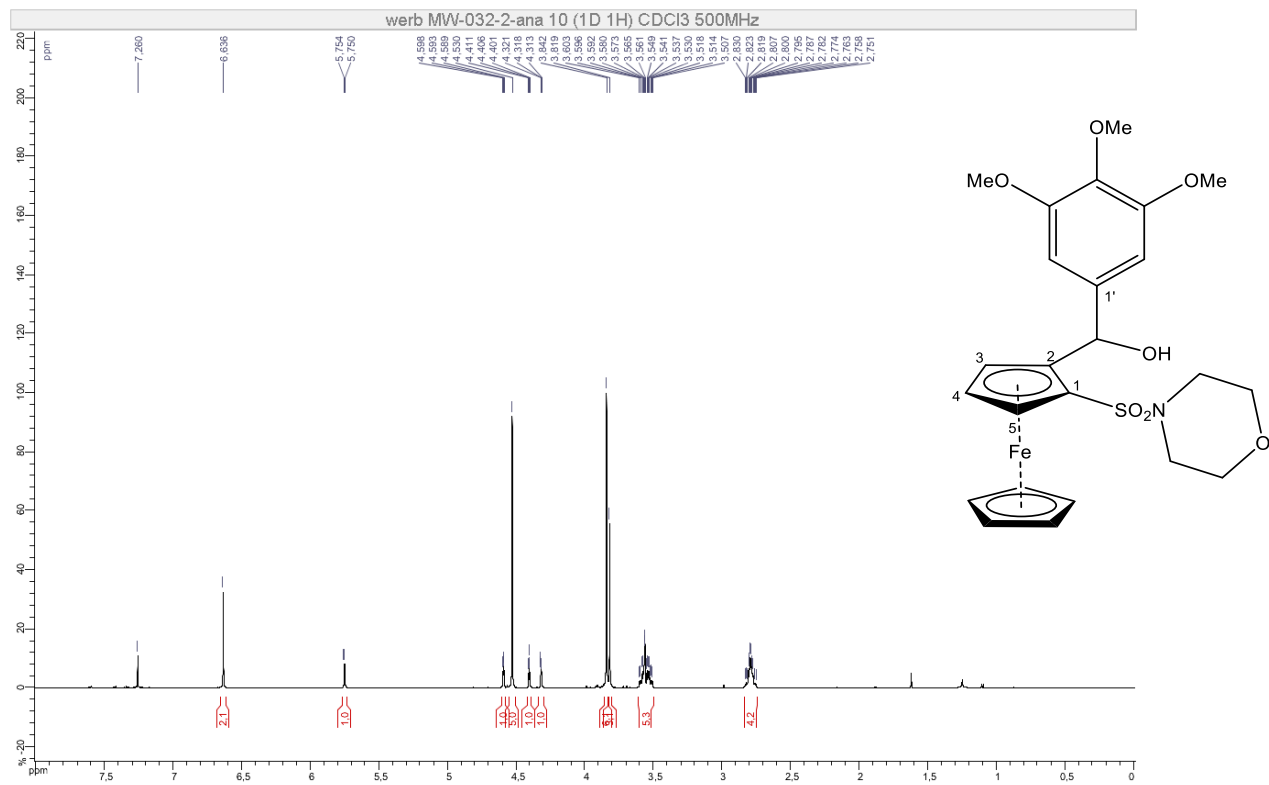


Figure S83. NOESY (400 MHz, CDCl_3) of **4b** (racemic mixture)



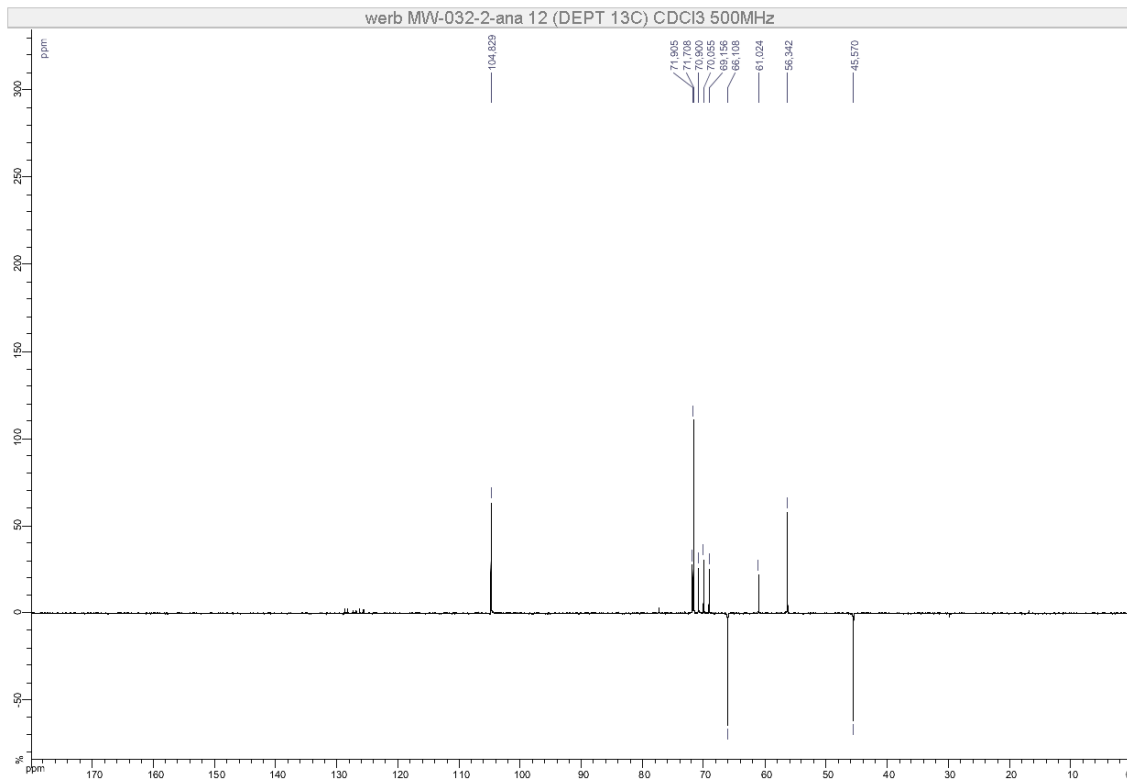


Figure S86. DEPT 135 (126 MHz, CDCl₃) of **4c1** (racemic mixture)

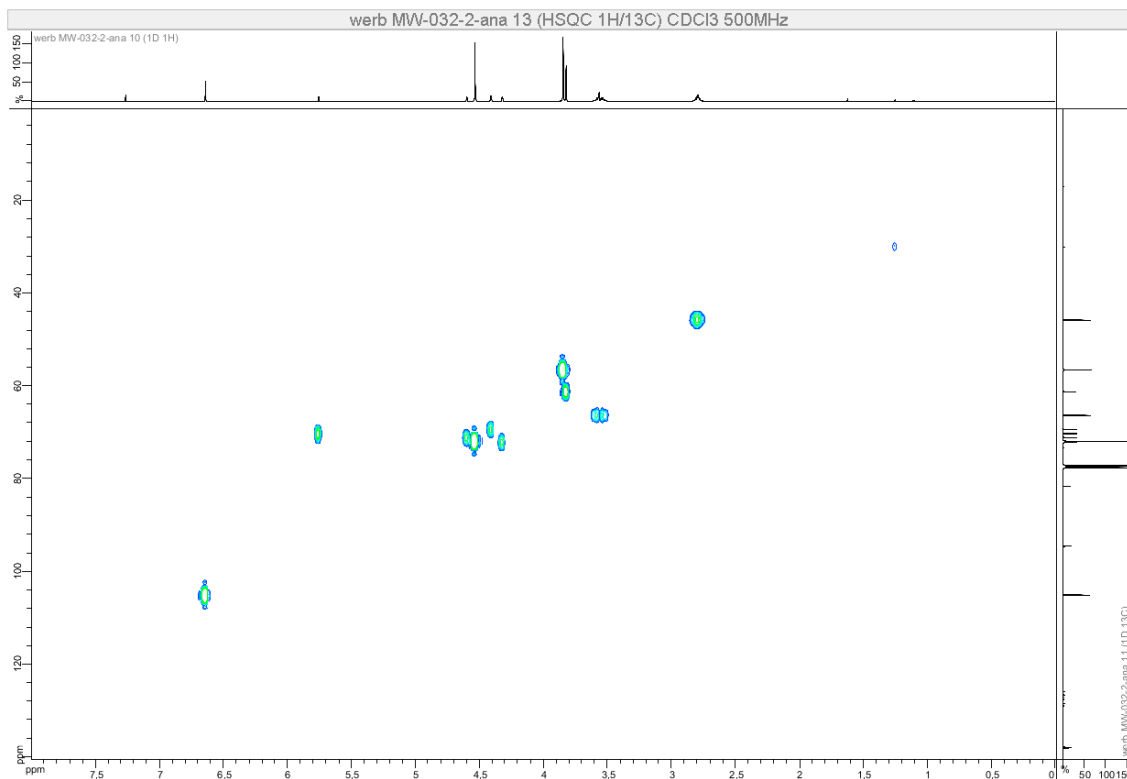


Figure S87. HSQC (500 MHz, CDCl₃) of **4c1** (racemic mixture)

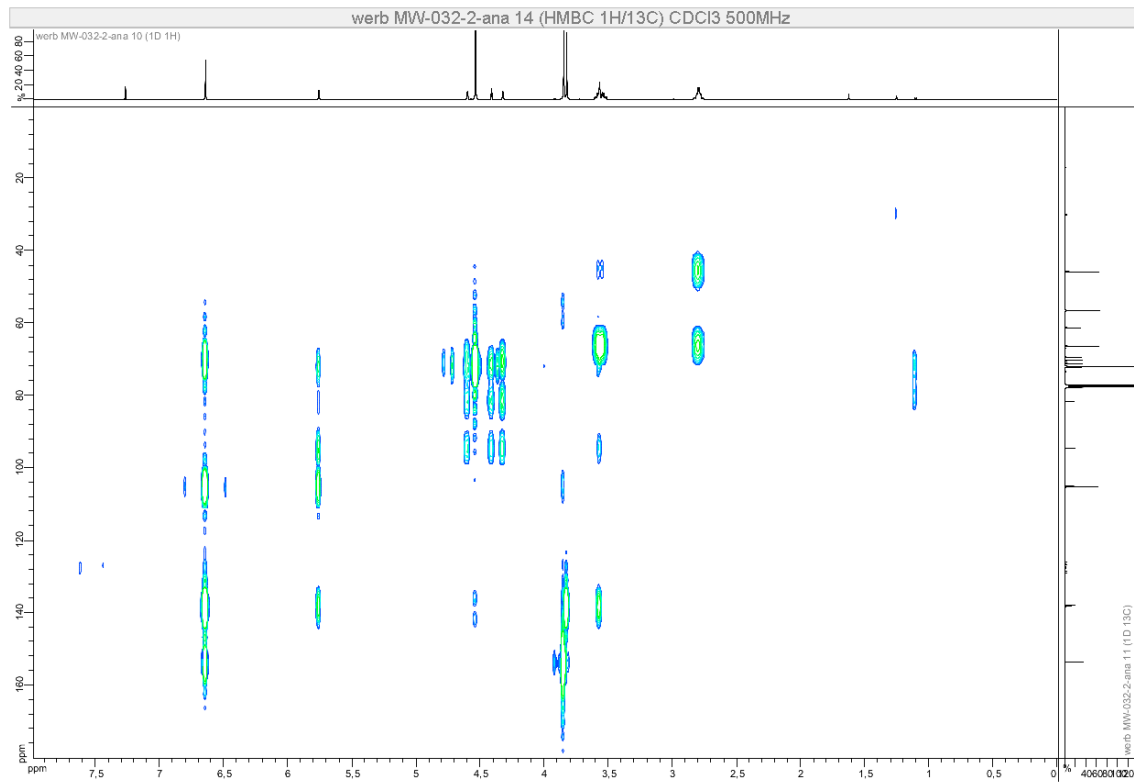


Figure S88. HMBC (500 MHz, CDCl₃) of **4c1** (racemic mixture)

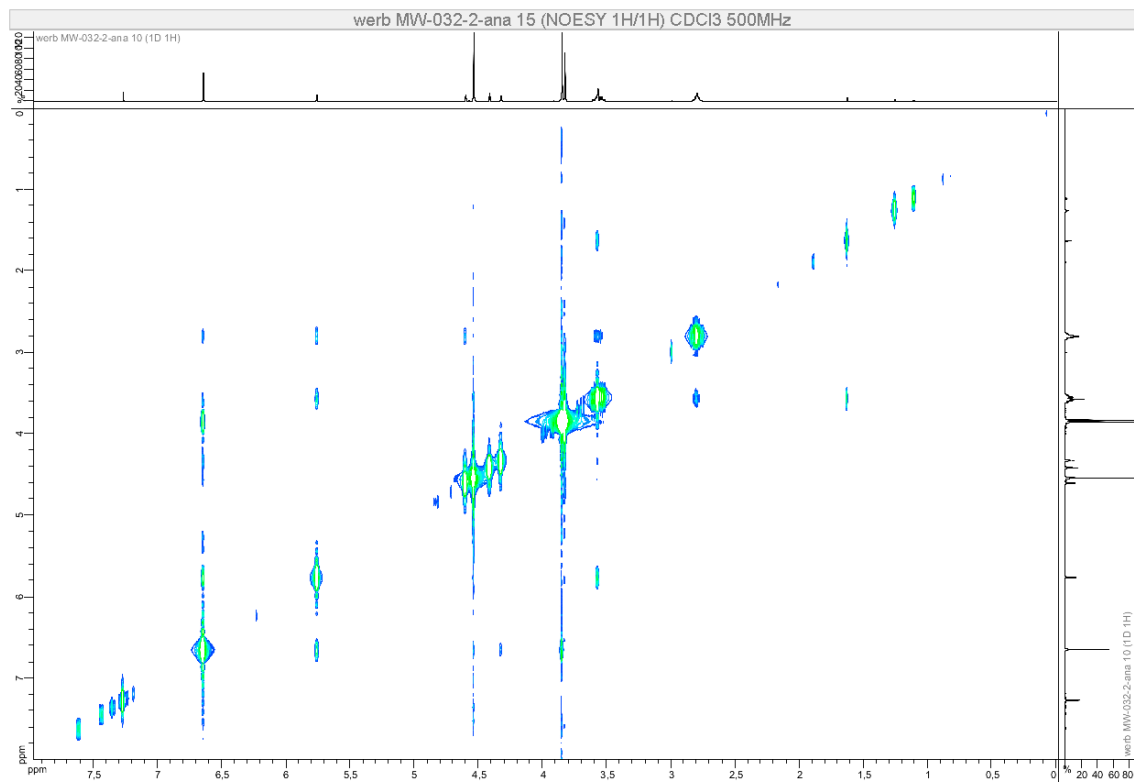


Figure S89. NOESY (500 MHz, CDCl₃) of **4c1** (racemic mixture)

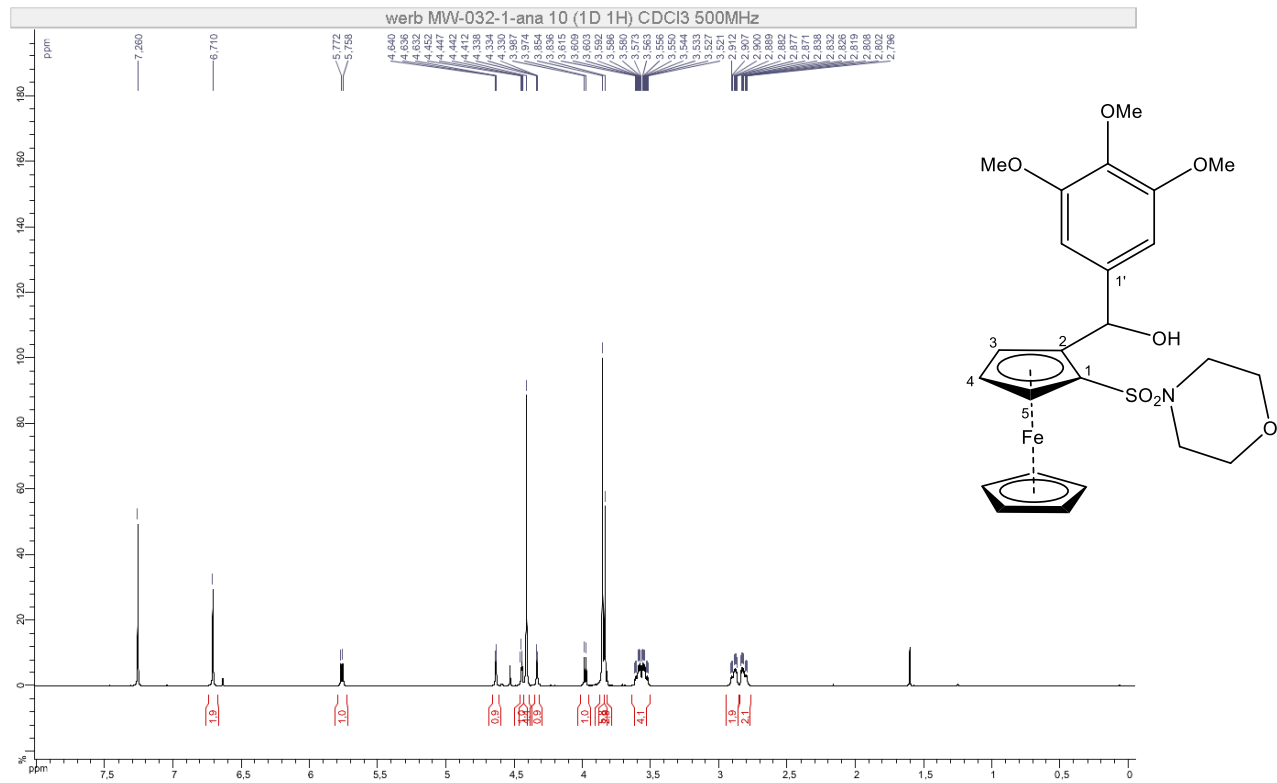


Figure S90. ^1H NMR (500 MHz, CDCl_3) of **4c2** (racemic mixture)

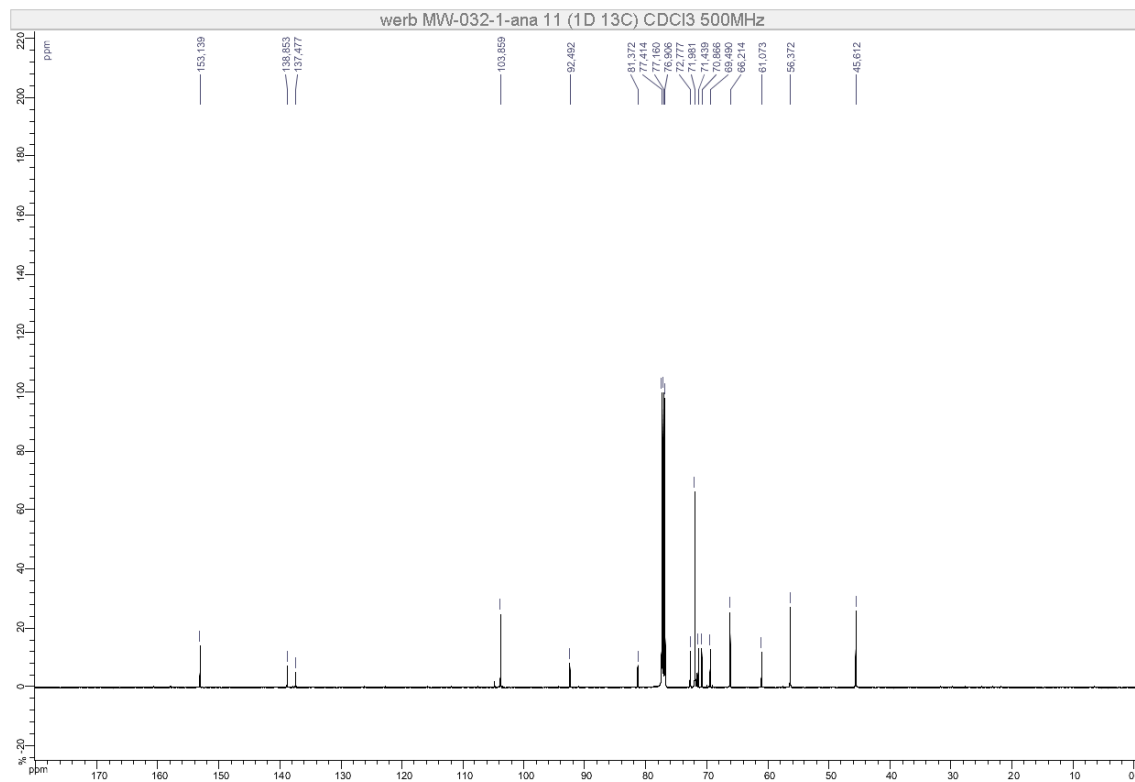


Figure S91. ^{13}C NMR (126 MHz, CDCl_3) of **4c2** (racemic mixture)

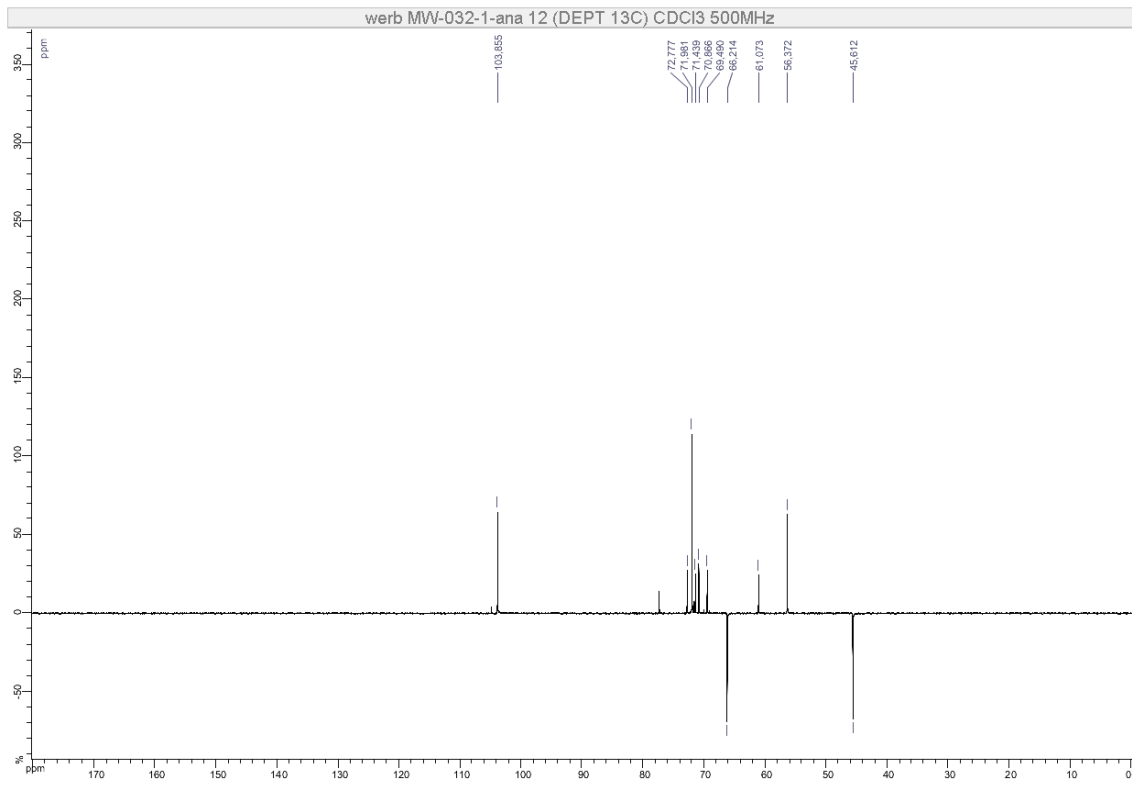


Figure S92. DEPT 135 (126 MHz, CDCl₃) of **4c2** (racemic mixture)

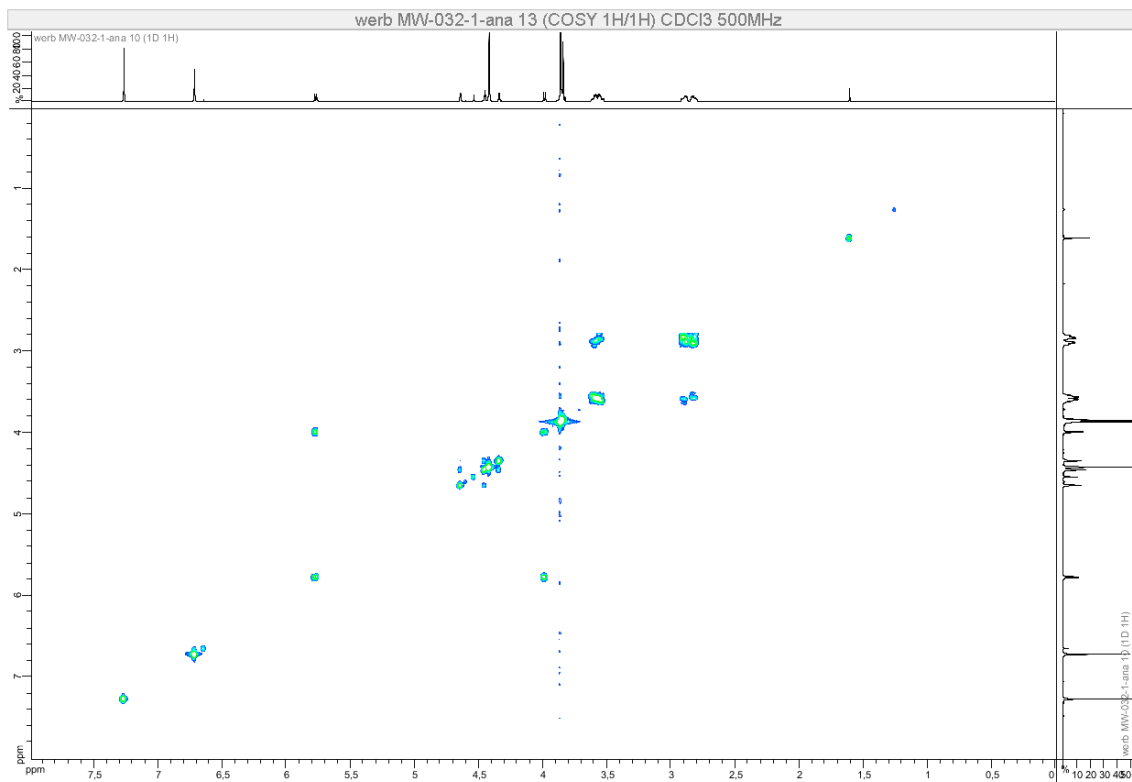


Figure S93. COSY (500 MHz, CDCl₃) of **4c2** (racemic mixture)

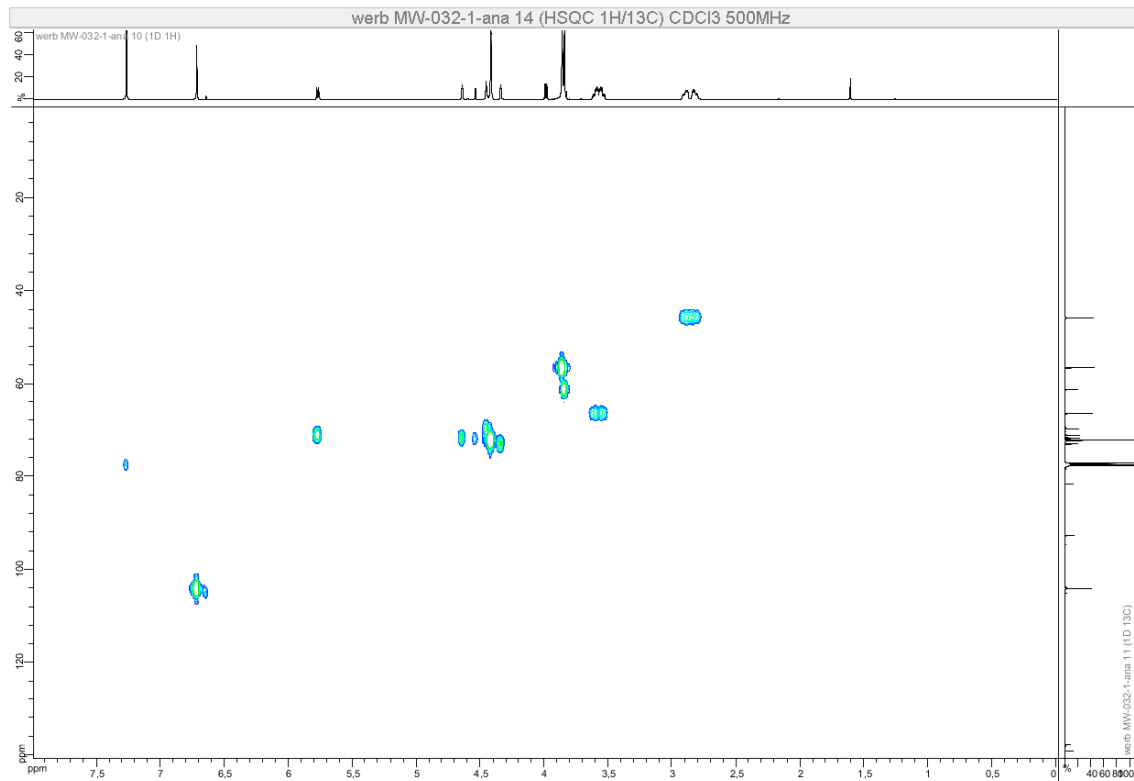


Figure S94. HSQC (500 MHz, CDCl₃) of **4c2** (racemic mixture)

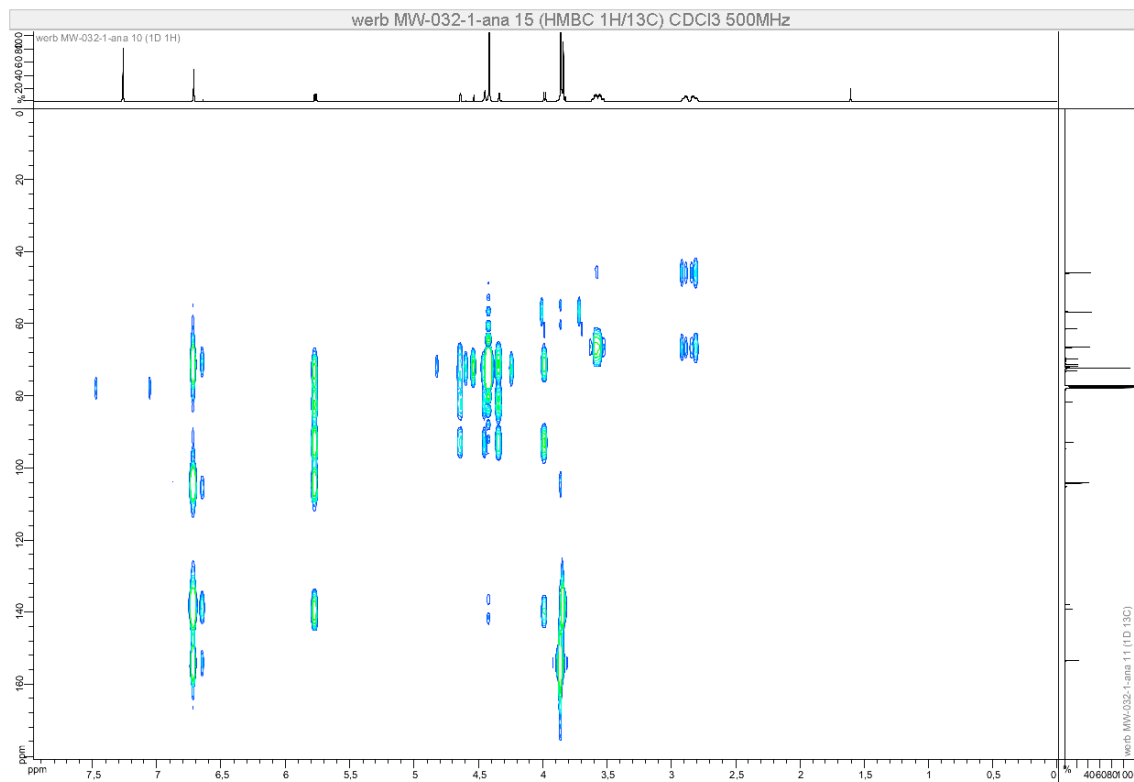


Figure S95. HMBC (500 MHz, CDCl₃) of **4c2** (racemic mixture)

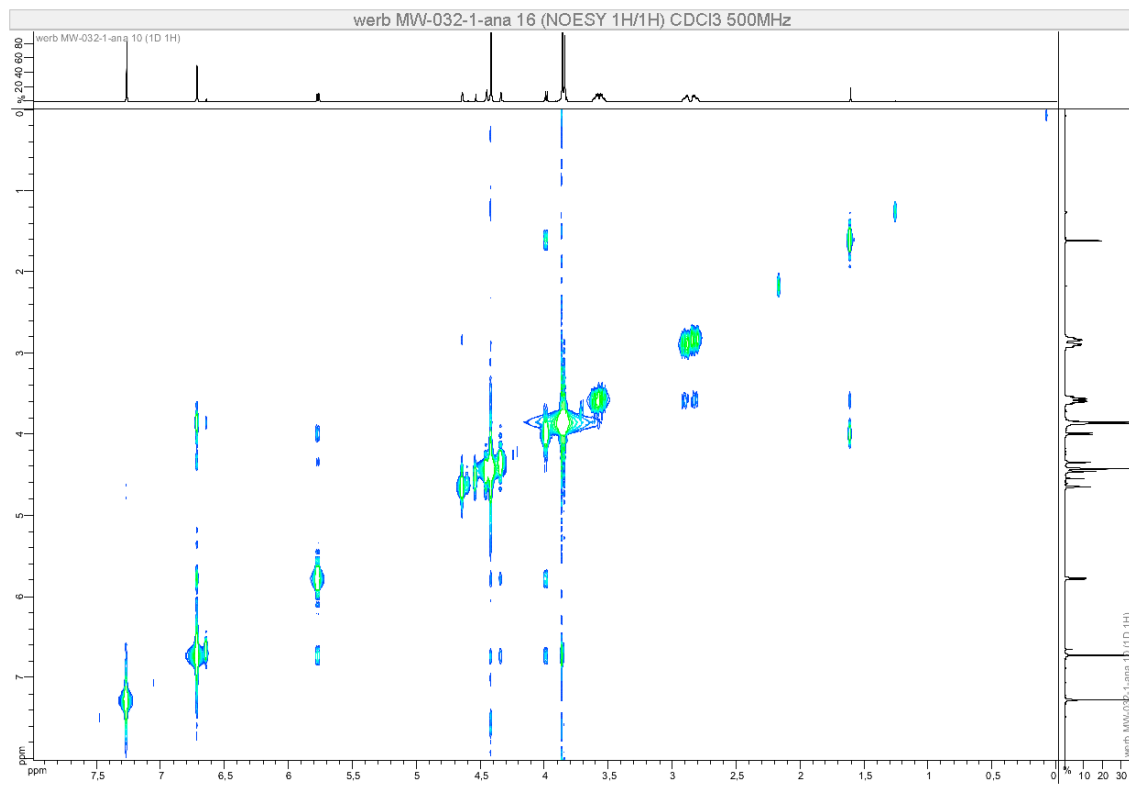


Figure S96. NOESY (500 MHz, CDCl₃) of **4c2** (racemic mixture)

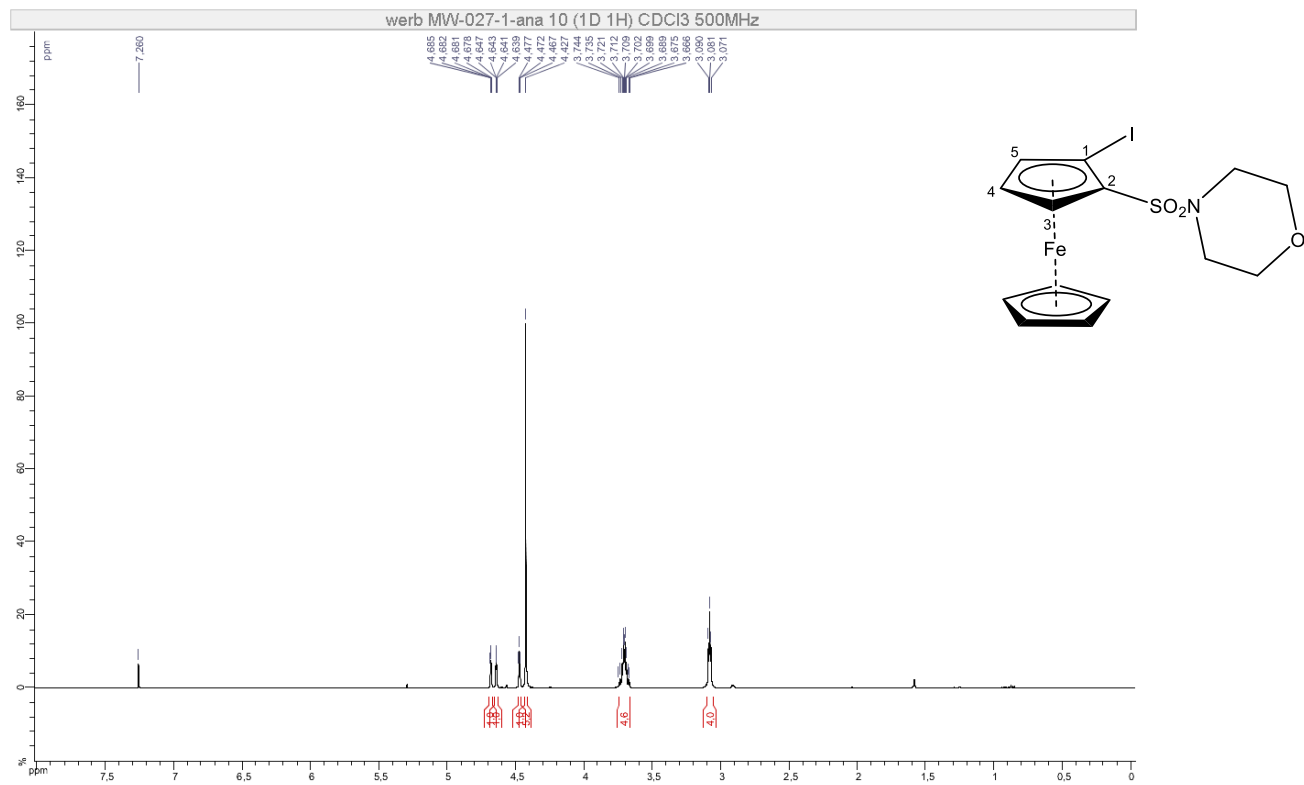


Figure S97. ^1H NMR (300 MHz, CDCl_3) of **4d** (racemic mixture)

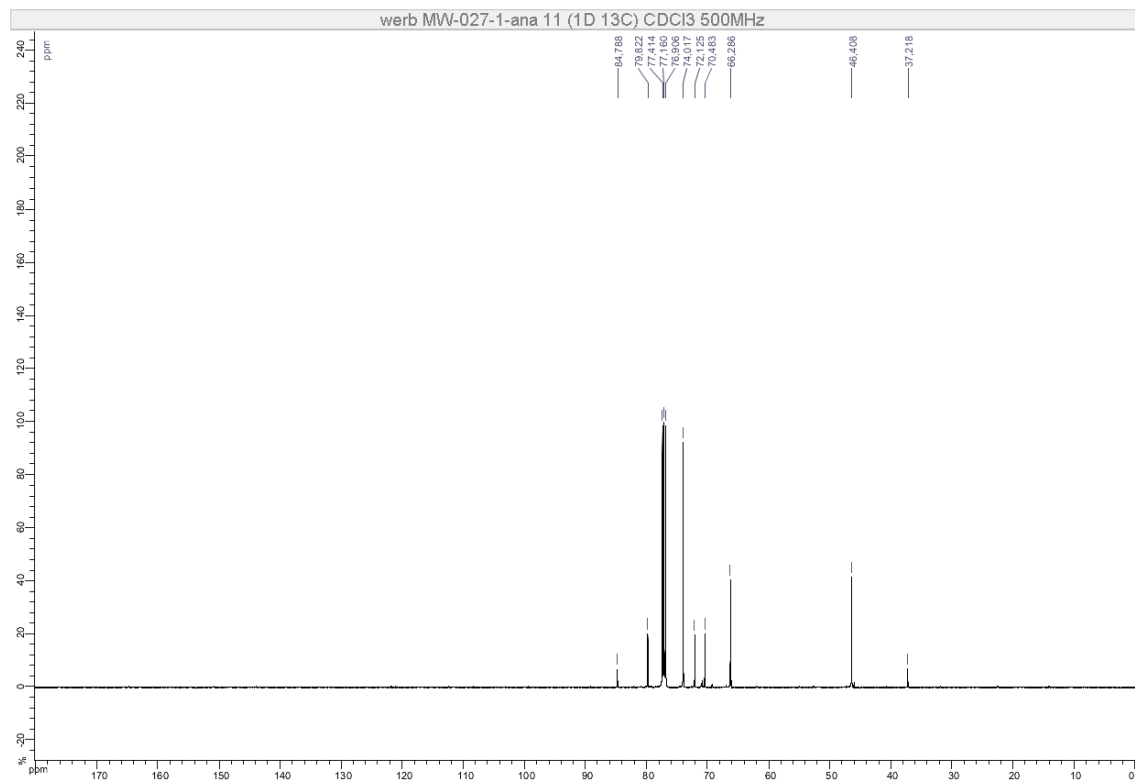


Figure S98. ^{13}C NMR (75 MHz, CDCl_3) of **4d** (racemic mixture)

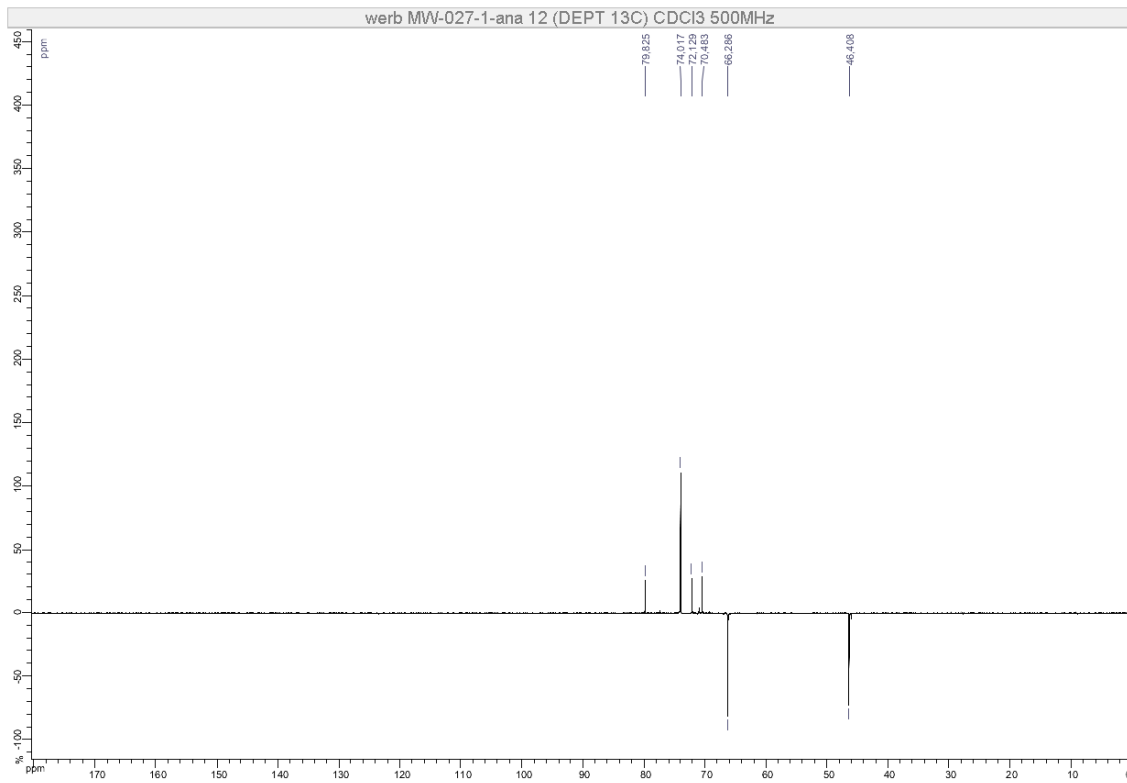


Figure S99. DEPT 135 (75 MHz, CDCl₃) of **4d** (racemic mixture)

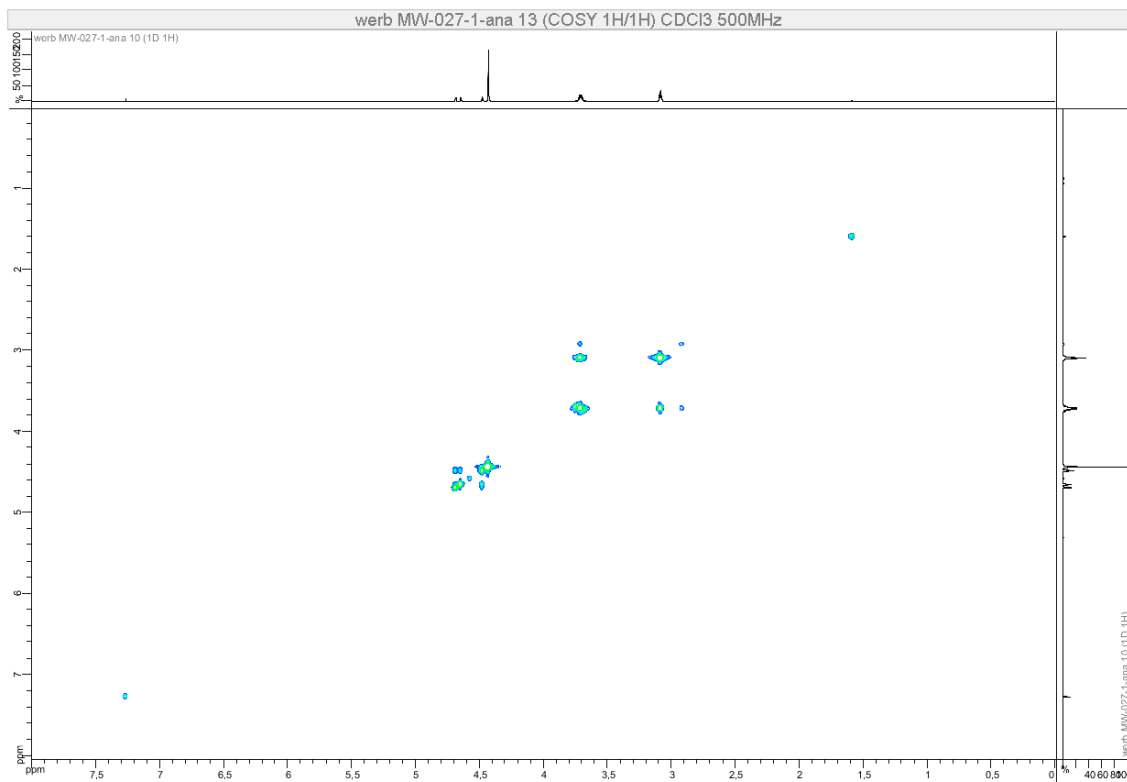


Figure S100. COSY (300 MHz, CDCl₃) of **4d** (racemic mixture)

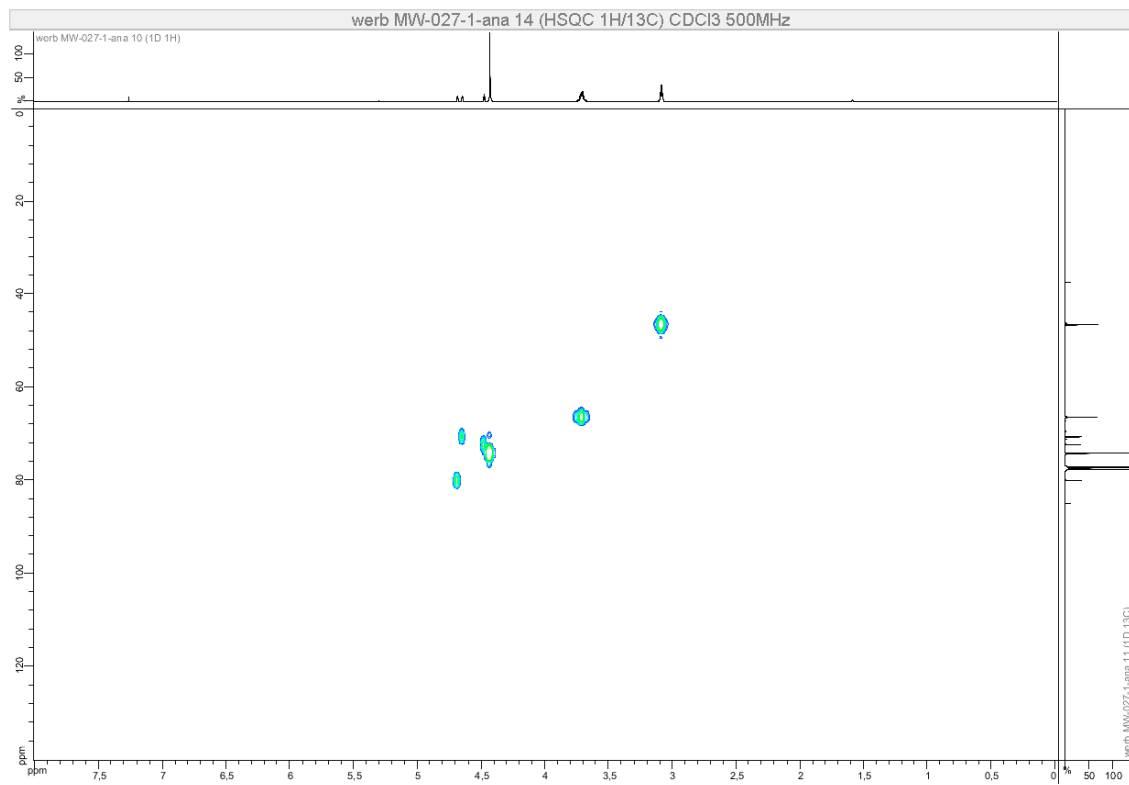


Figure S101. HSQC (300 MHz, CDCl₃) of **4d** (racemic mixture)

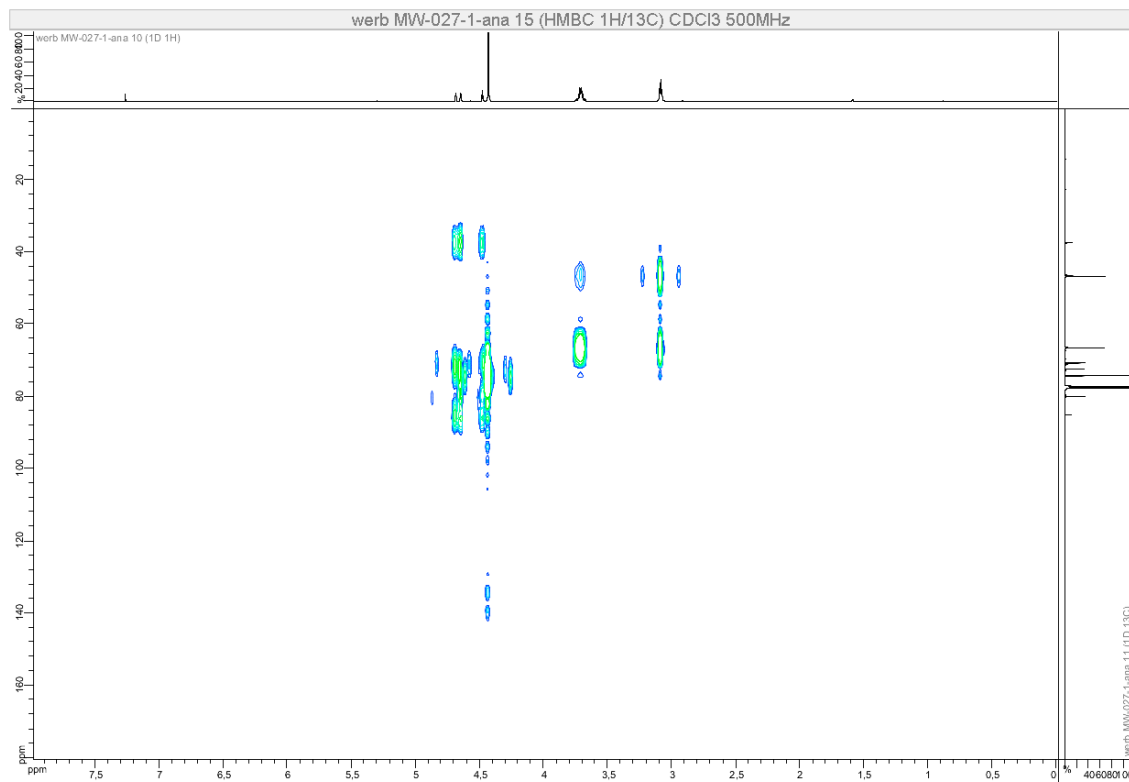


Figure S102. HMBC (300 MHz, CDCl₃) of **4d** (racemic mixture)

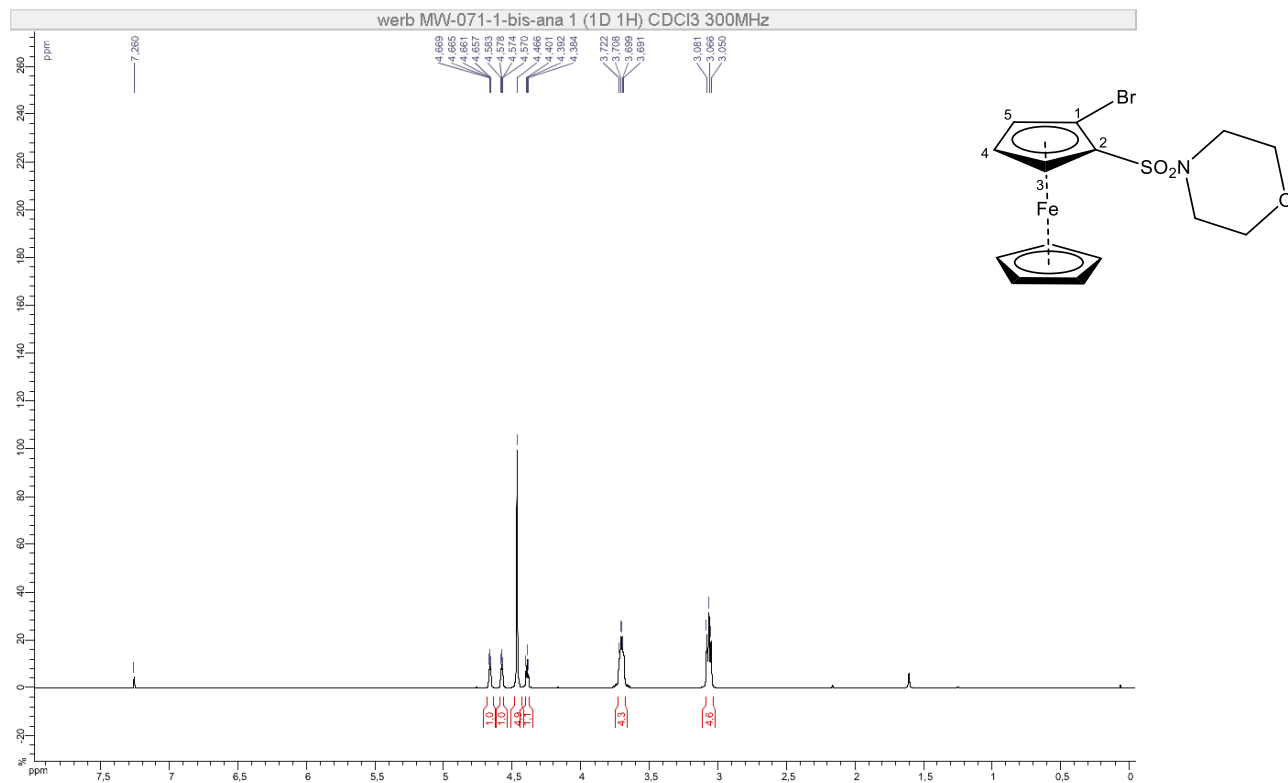


Figure S103. ¹H NMR (300 MHz, CDCl₃) of **4e** (racemic mixture)

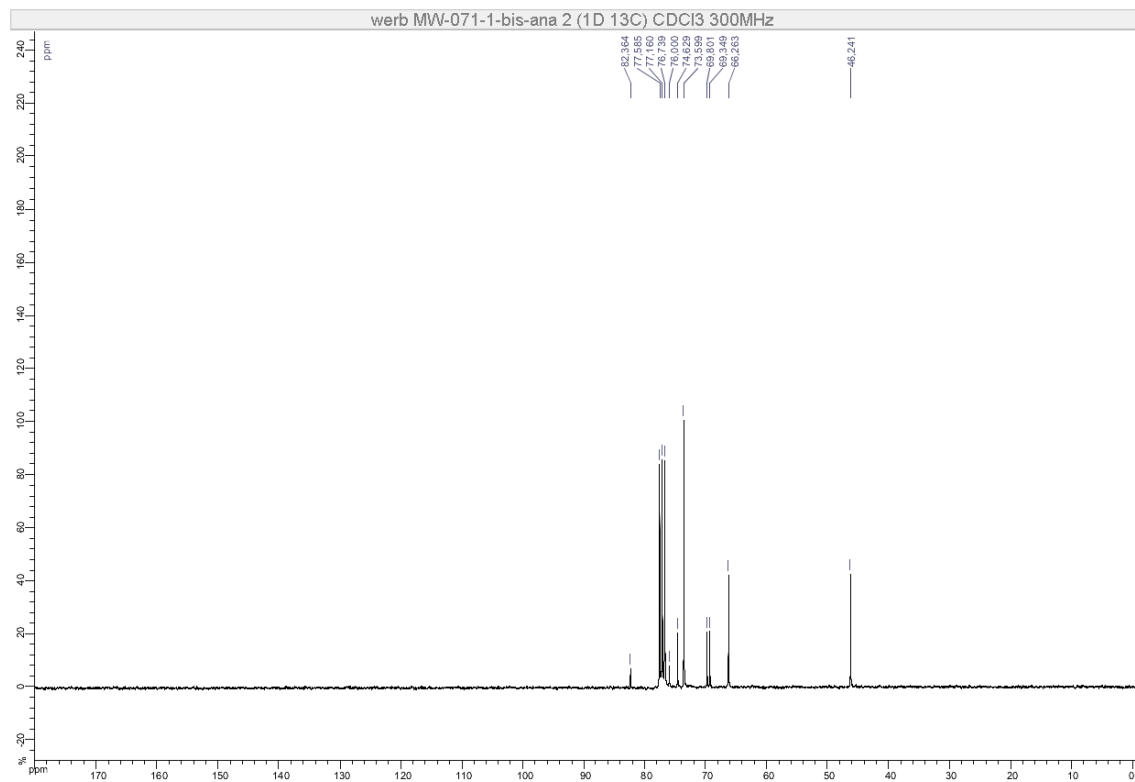


Figure S104. ¹³C NMR (75 MHz, CDCl₃) of **4e** (racemic mixture)

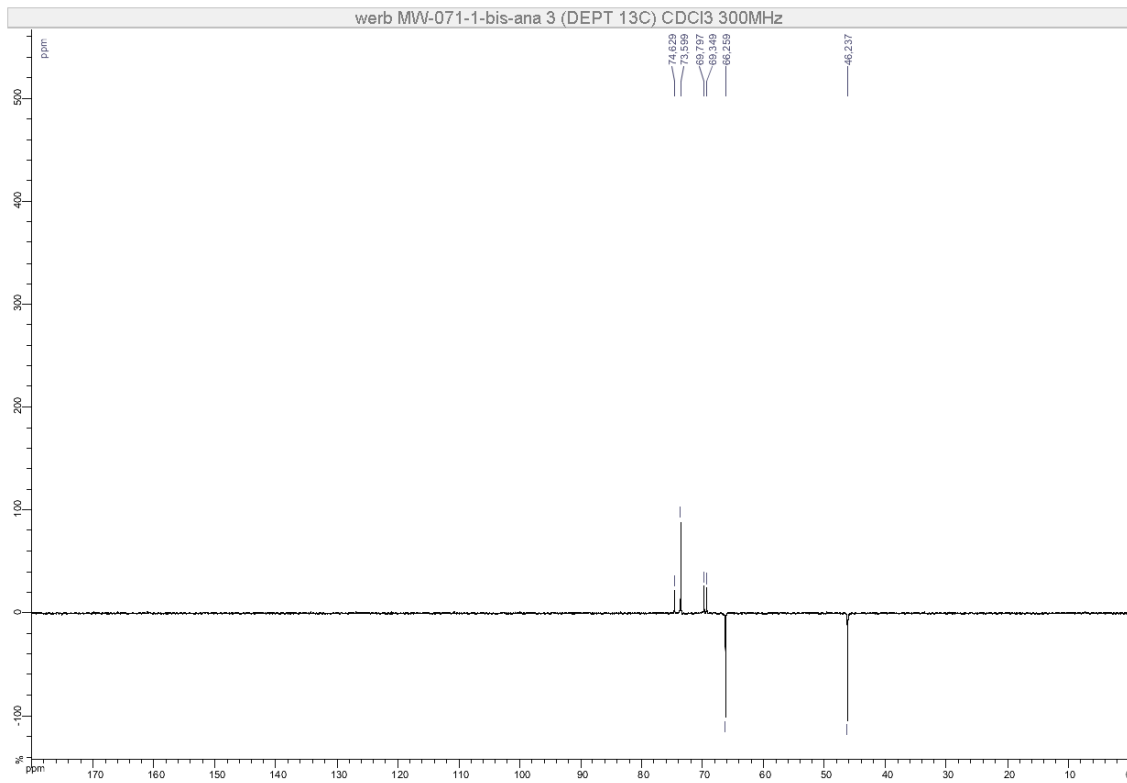


Figure S105. DEPT 135 (75 MHz, CDCl_3) of **4e** (racemic mixture)

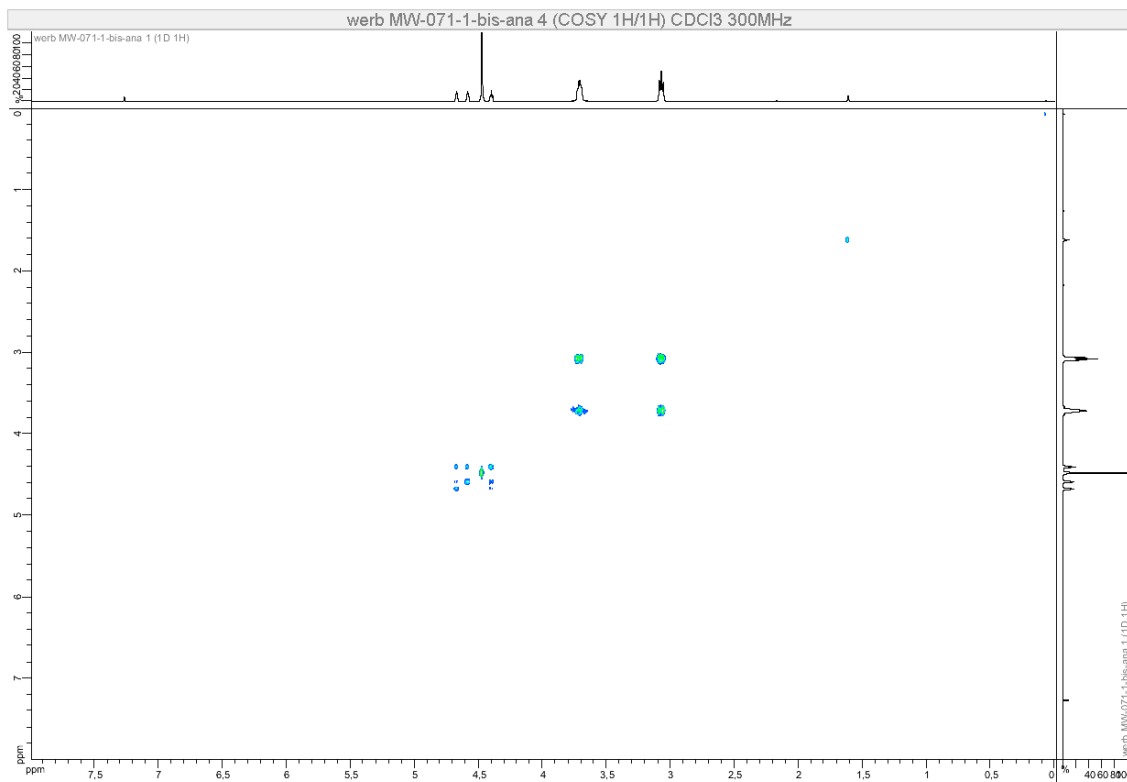


Figure S106. COSY (300 MHz, CDCl_3) of **4e** (racemic mixture)

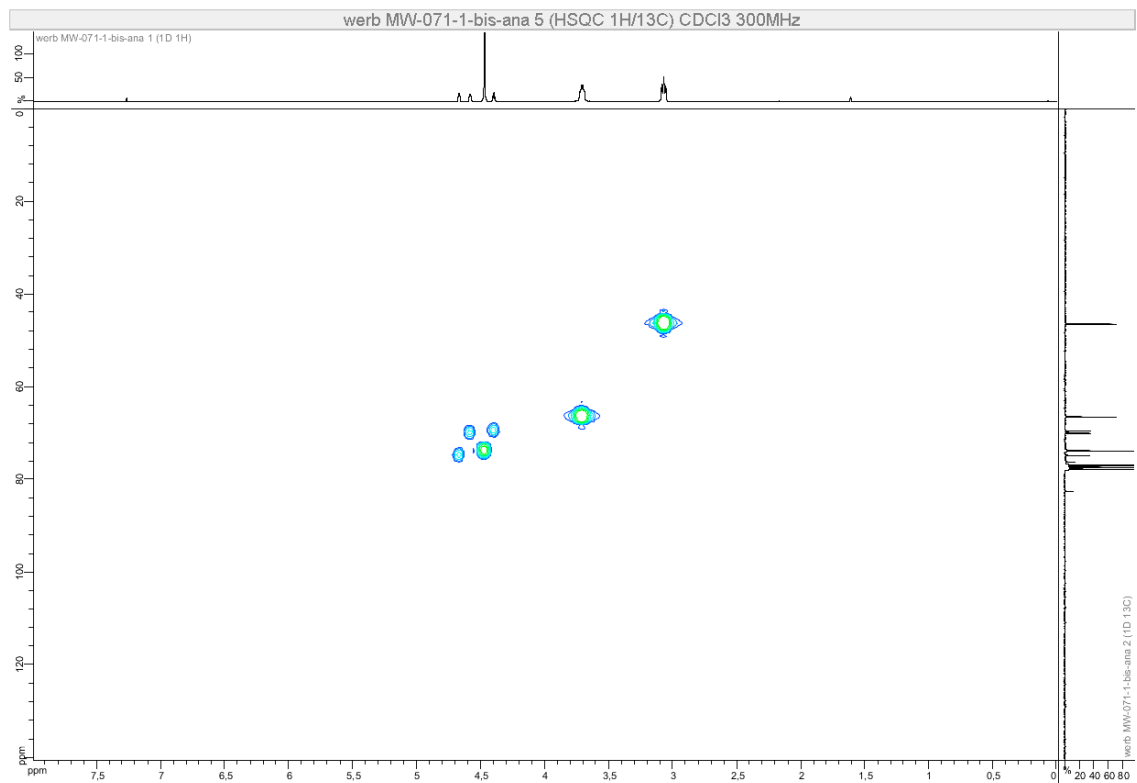


Figure S107. HSQC (300 MHz, CDCl_3) of **4e** (racemic mixture)

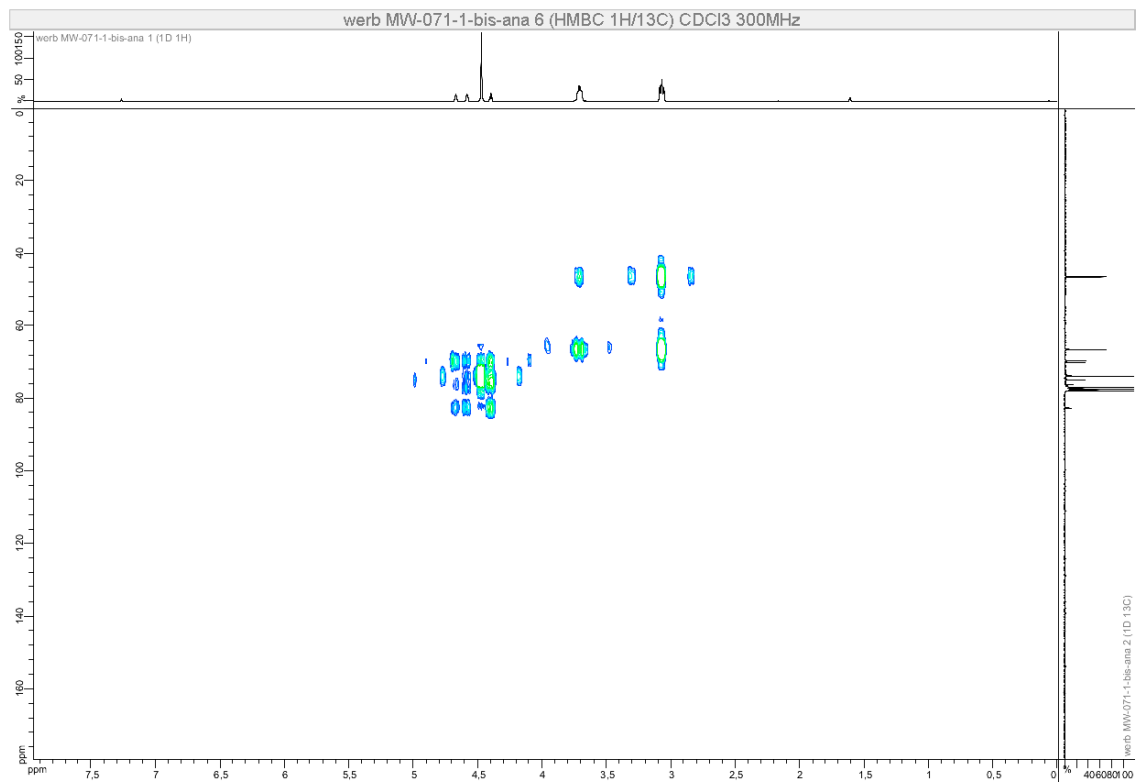


Figure S108. HMBC (300 MHz, CDCl_3) of **4e** (racemic mixture)

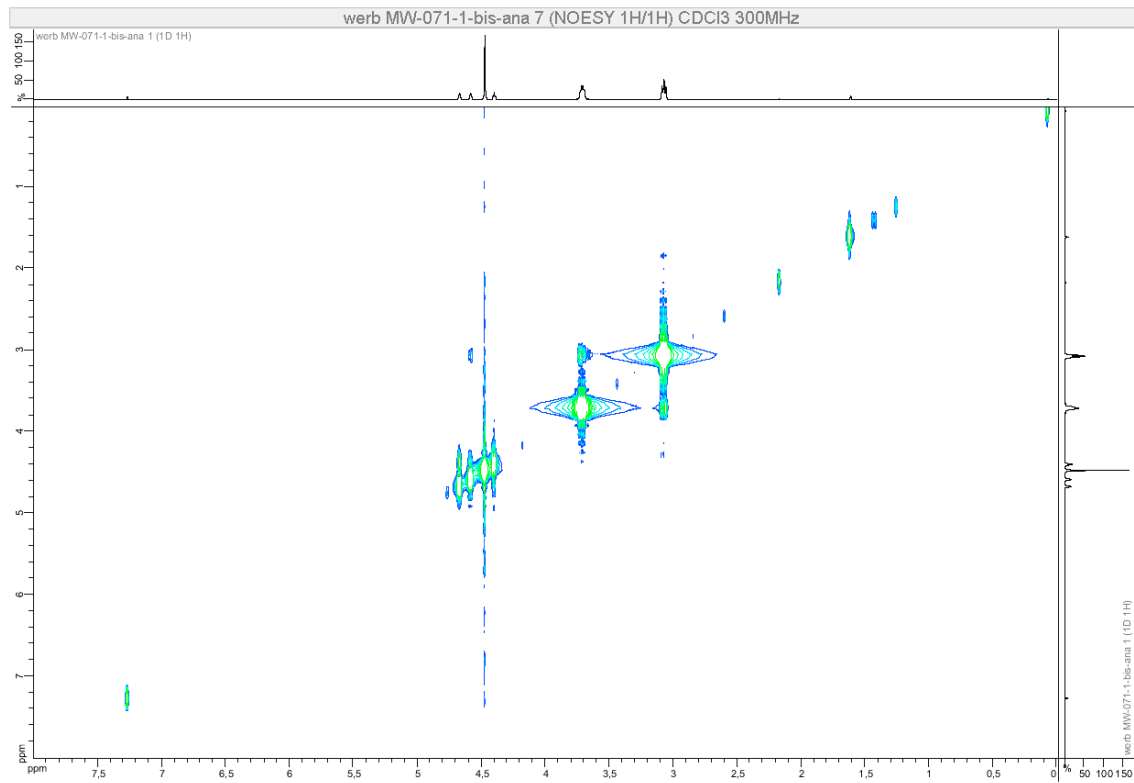


Figure S109. NOESY (300 MHz, CDCl_3) of **4e** (racemic mixture)

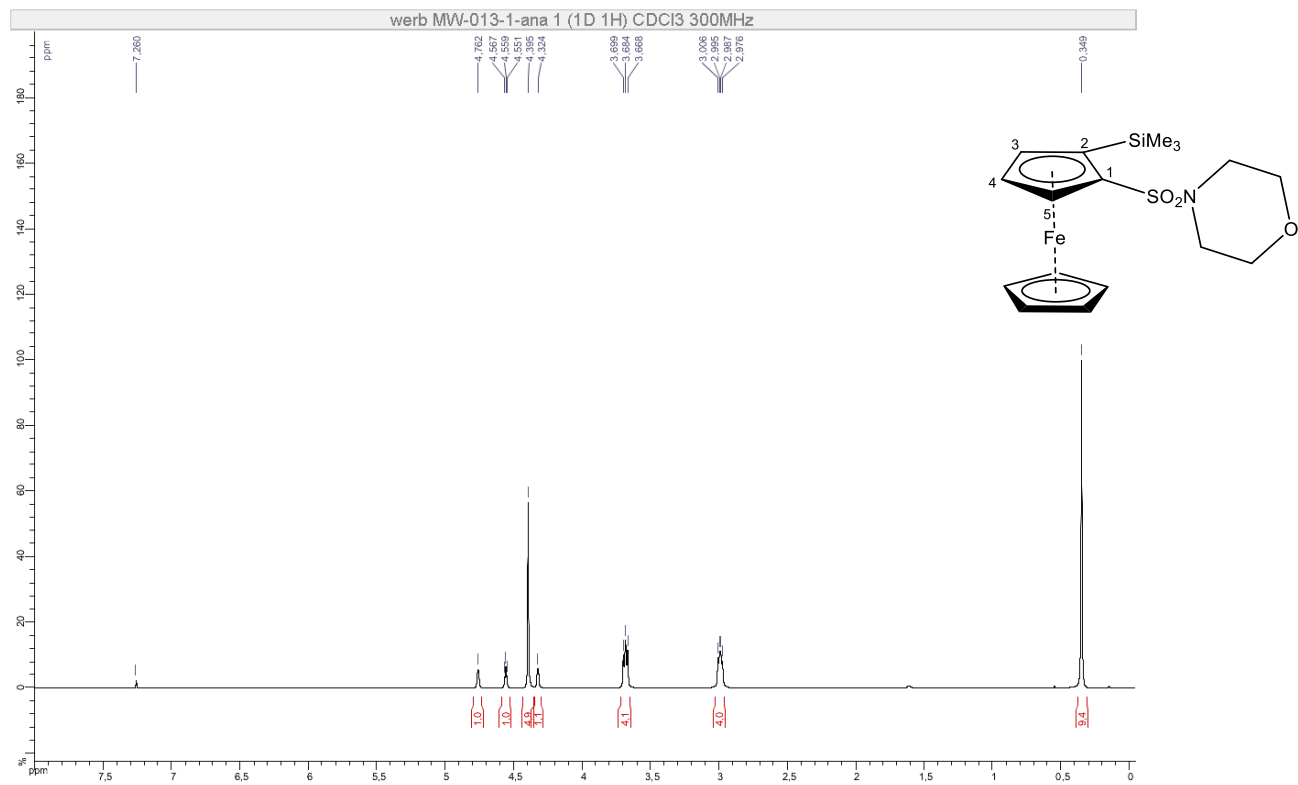


Figure S110. ¹H NMR (300 MHz, CDCl₃) of **4f** (racemic mixture)

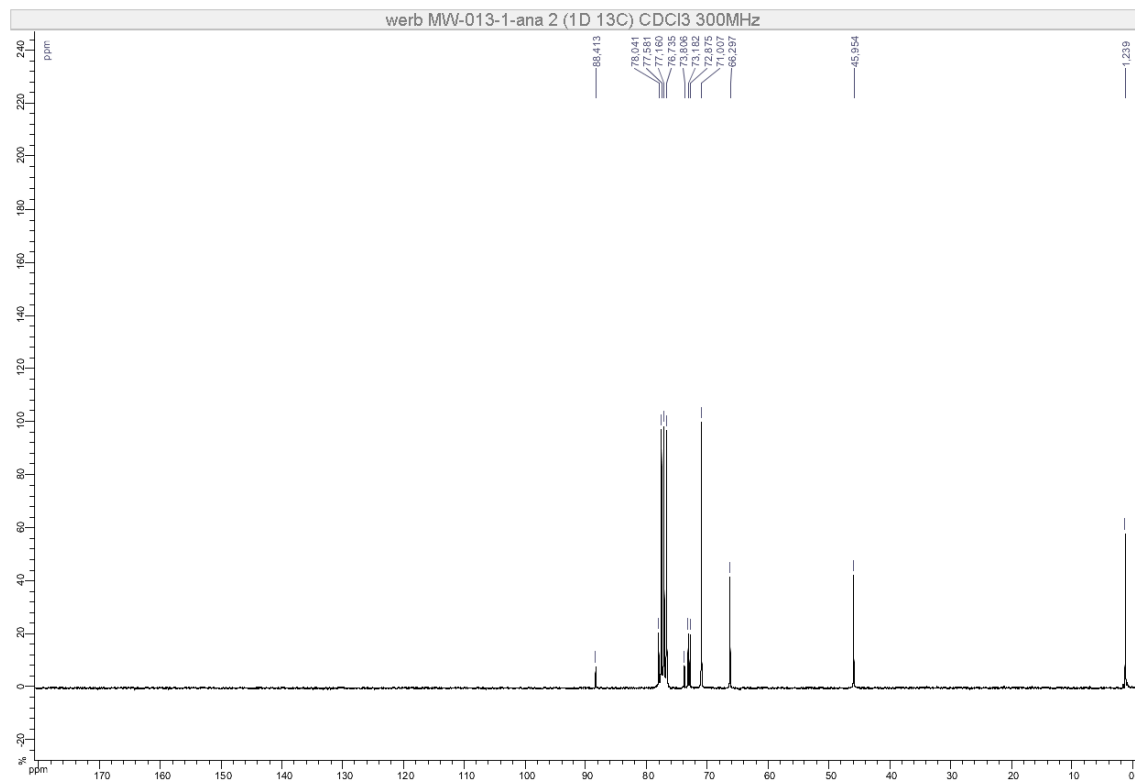


Figure S111. ¹³C NMR (75 MHz, CDCl₃) of **4f** (racemic mixture)

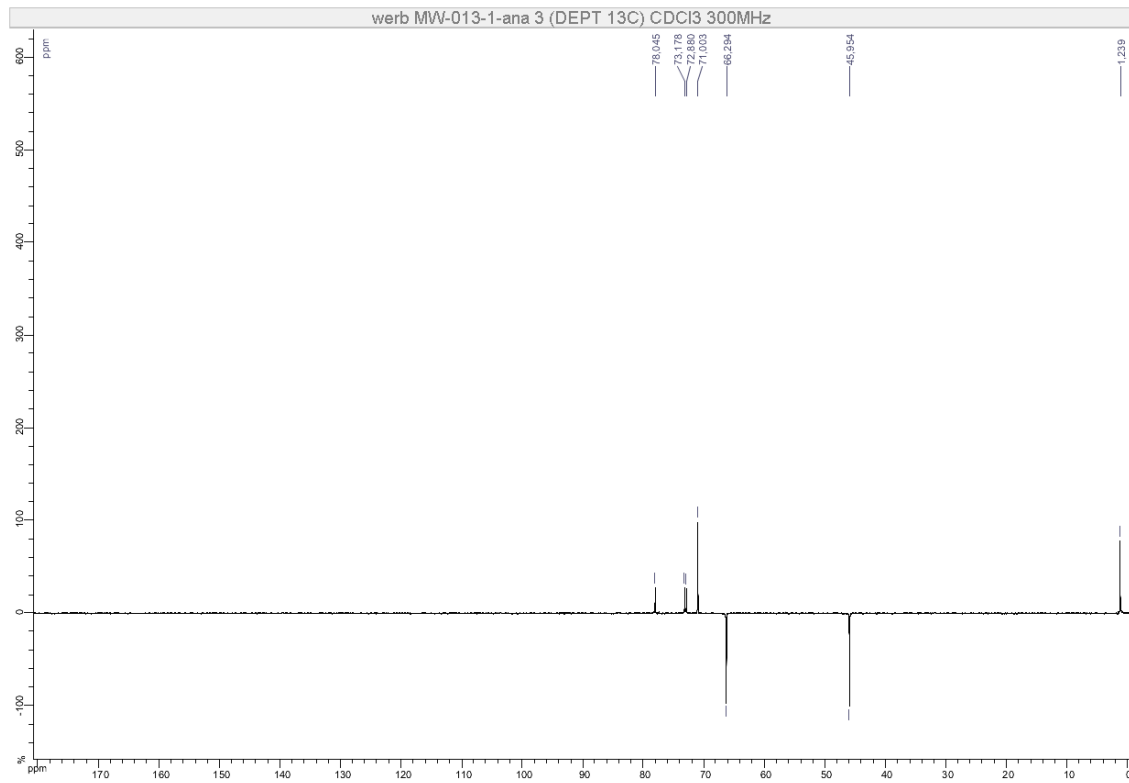


Figure S112. DEPT 135 (75 MHz, CDCl₃) of **4f** (racemic mixture)

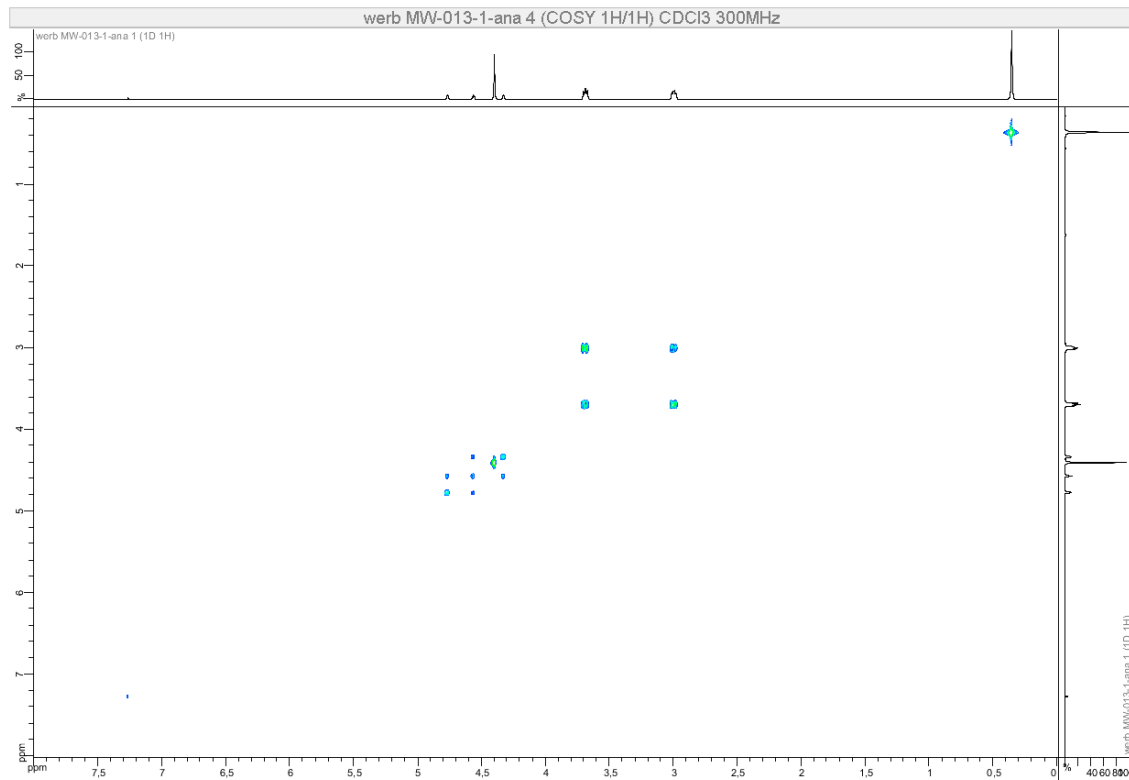


Figure S113. COSY (300 MHz, CDCl₃) of **4f** (racemic mixture)

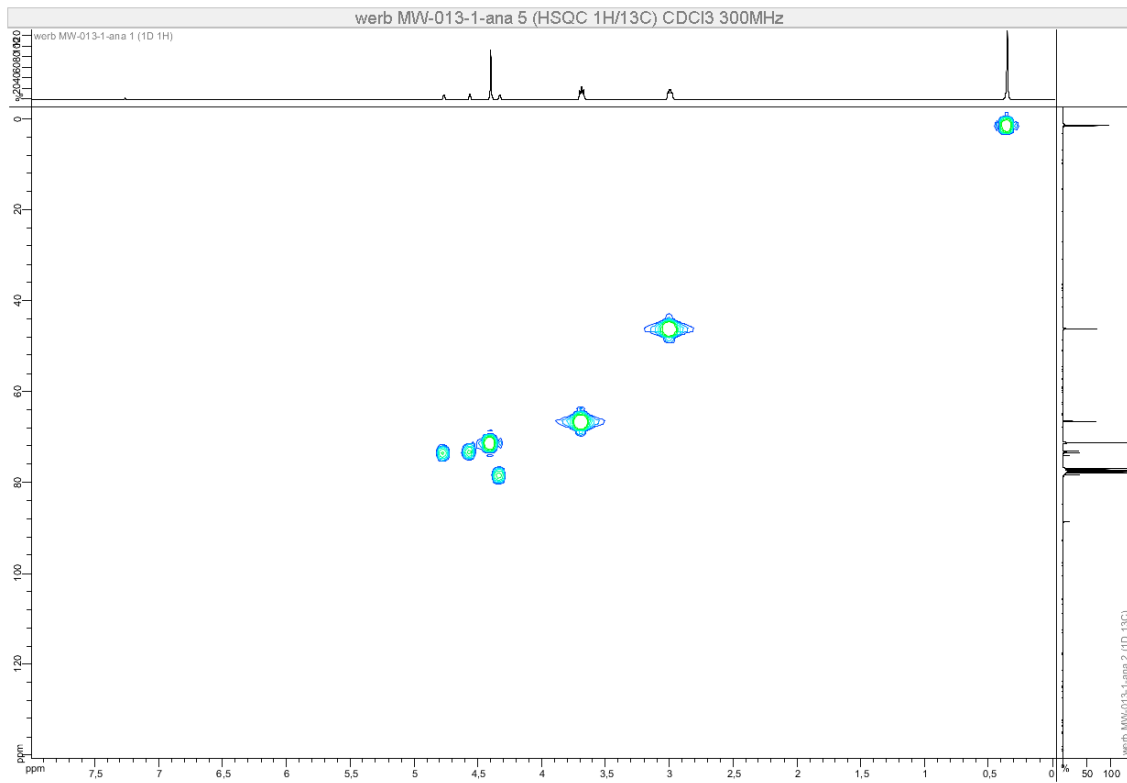


Figure S114. HSQC (300 MHz, CDCl₃) of **4f** (racemic mixture)

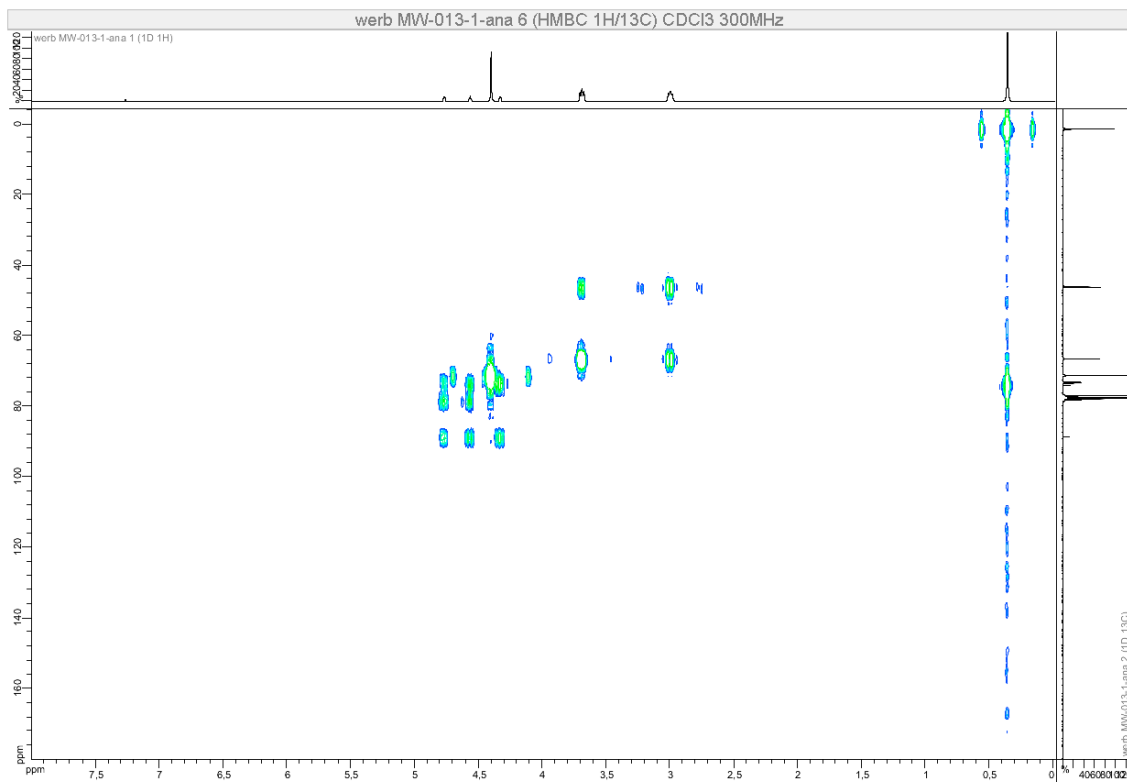


Figure S115. HMBC (300 MHz, CDCl₃) of **4f** (racemic mixture)

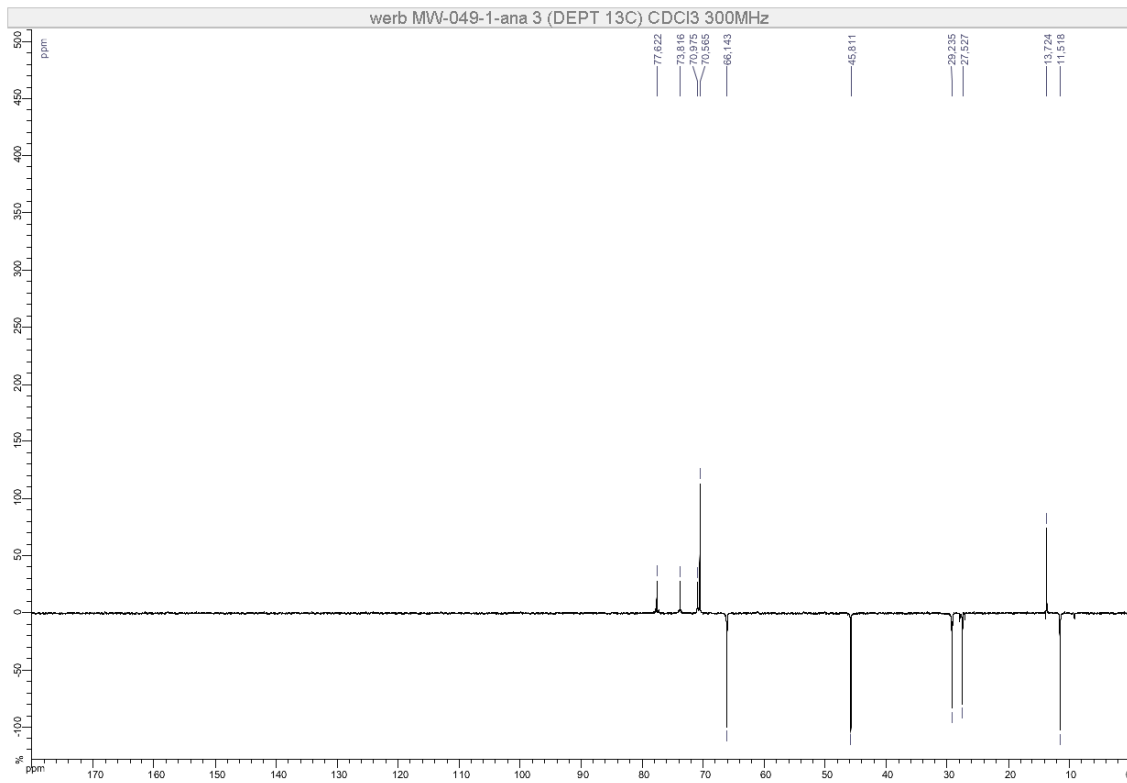


Figure S118. DEPT 135 (75 MHz, CDCl₃) of **4g** (racemic mixture)

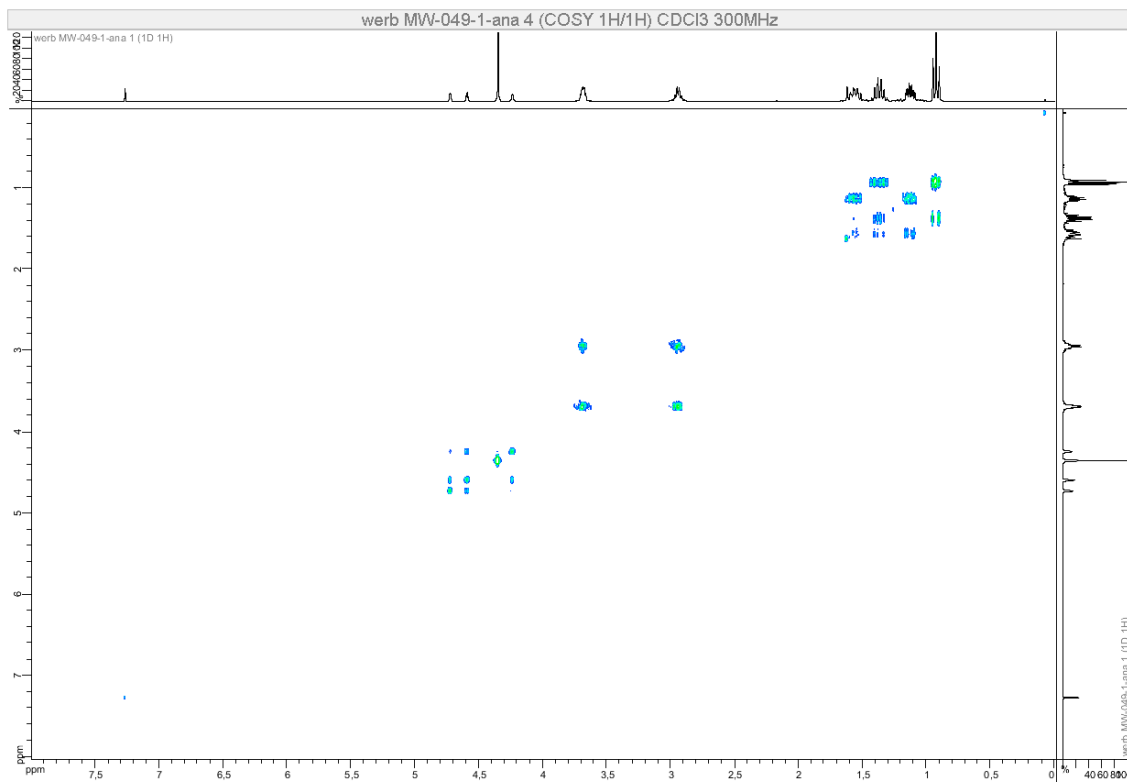


Figure S119. COSY (300 MHz, CDCl₃) of **4g** (racemic mixture)

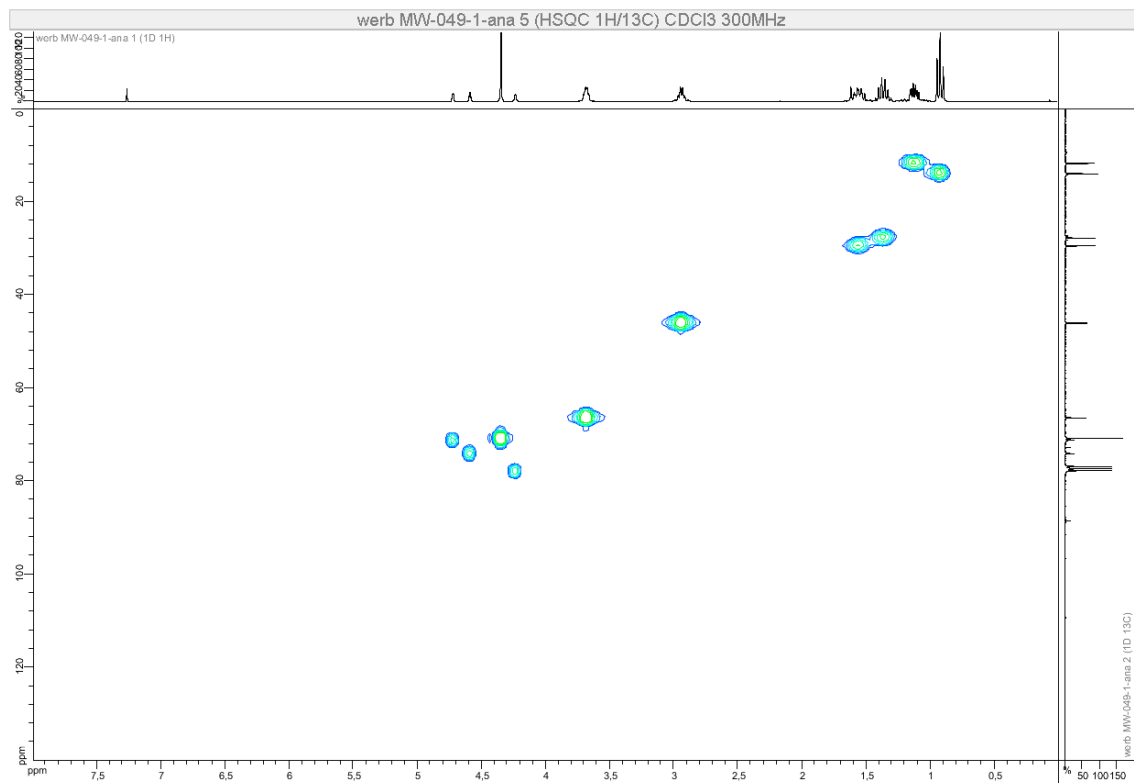


Figure S120. HSQC (300 MHz, CDCl₃) of **4g** (racemic mixture)

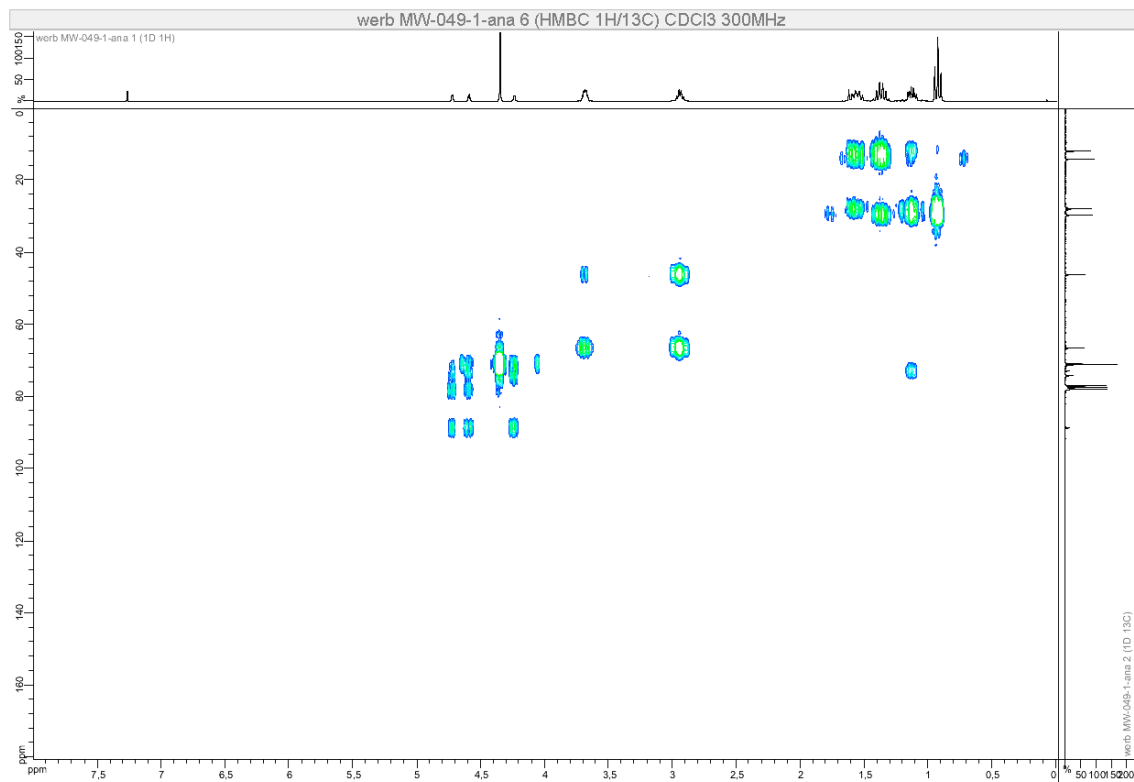


Figure S121. HMBC (300 MHz, CDCl₃) of **4g** (racemic mixture)

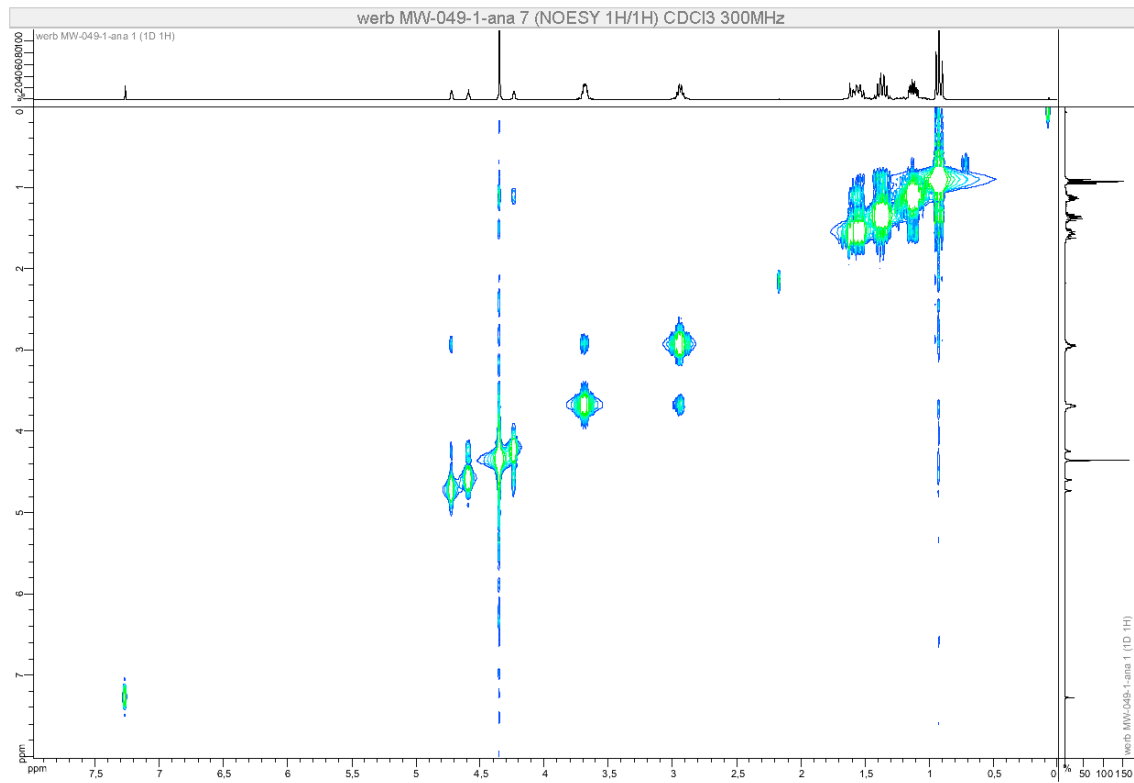


Figure S122. NOESY (300 MHz, CDCl_3) of **4g** (racemic mixture)

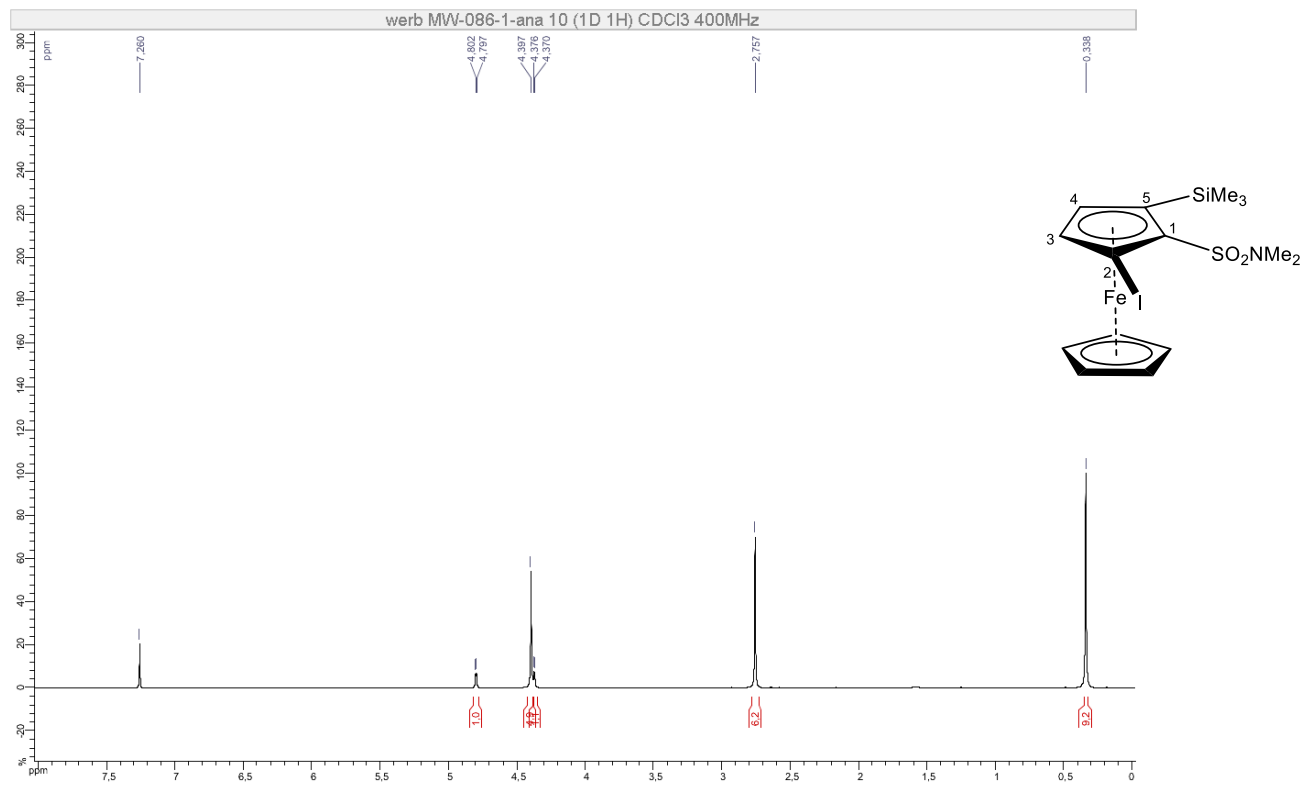


Figure S123. ^1H NMR (400 MHz, CDCl_3) of **5** (racemic mixture)

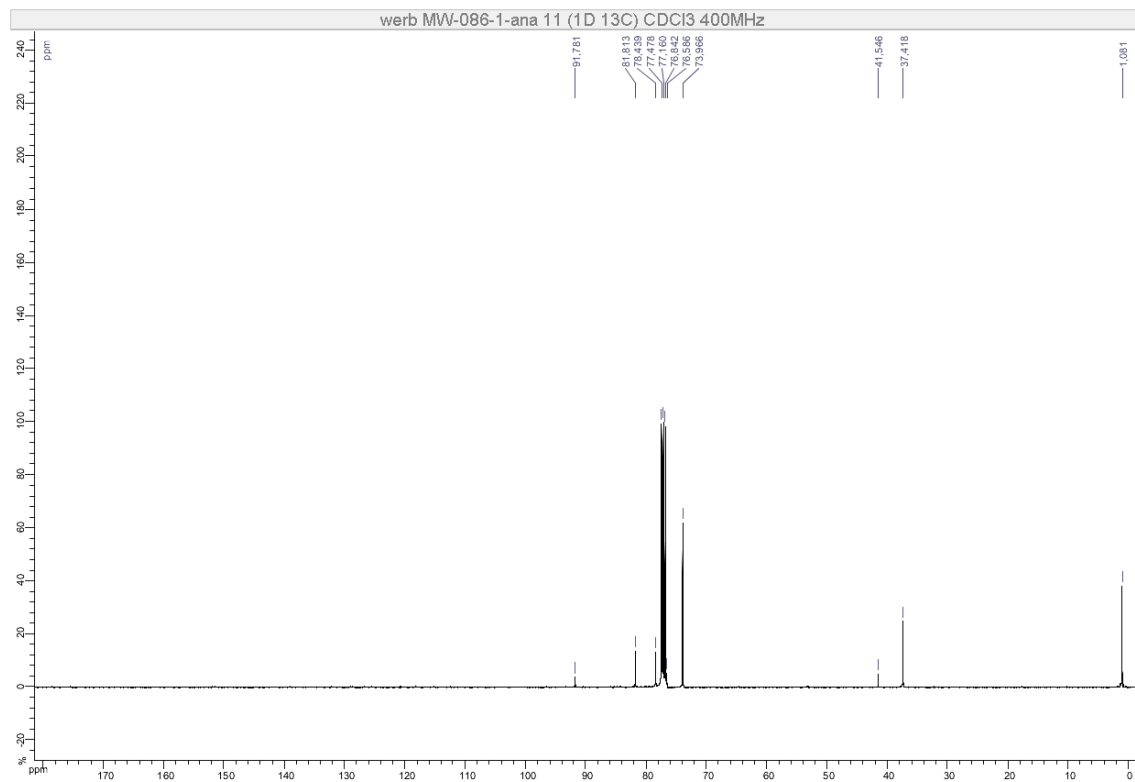


Figure S124. ^{13}C NMR (101 MHz, CDCl_3) of **5** (racemic mixture)

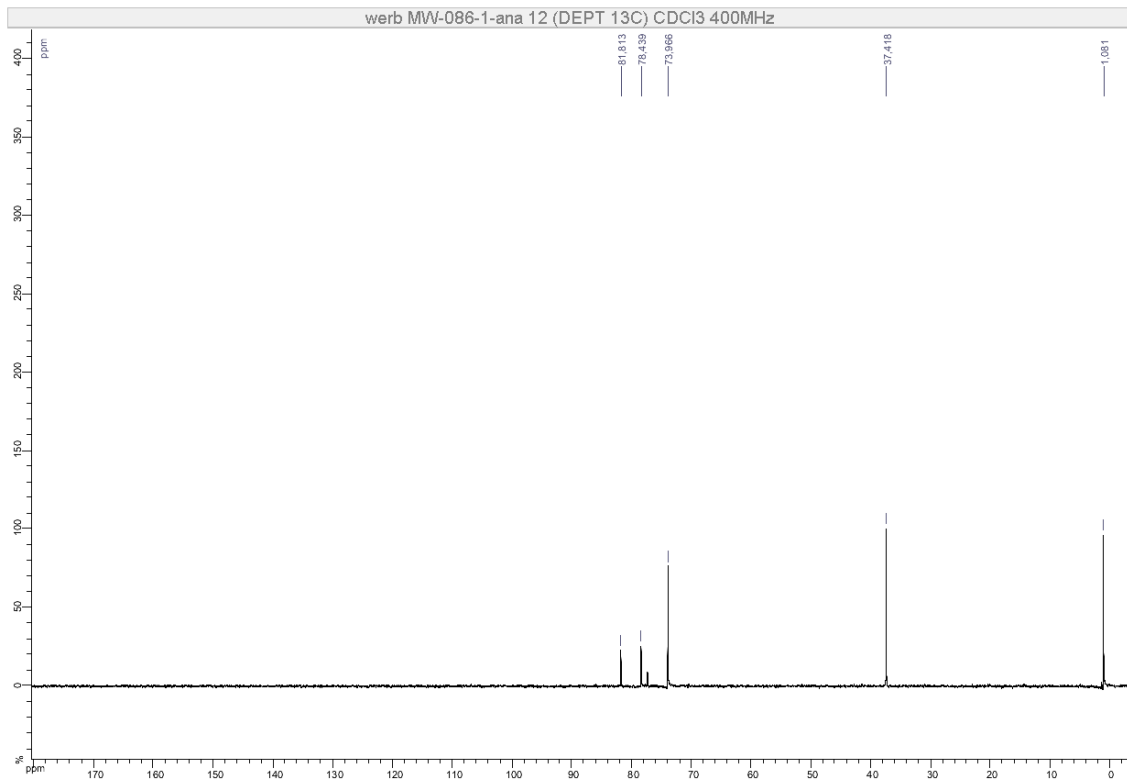


Figure S125. DEPT 135 (101 MHz, CDCl₃) of **5** (racemic mixture)

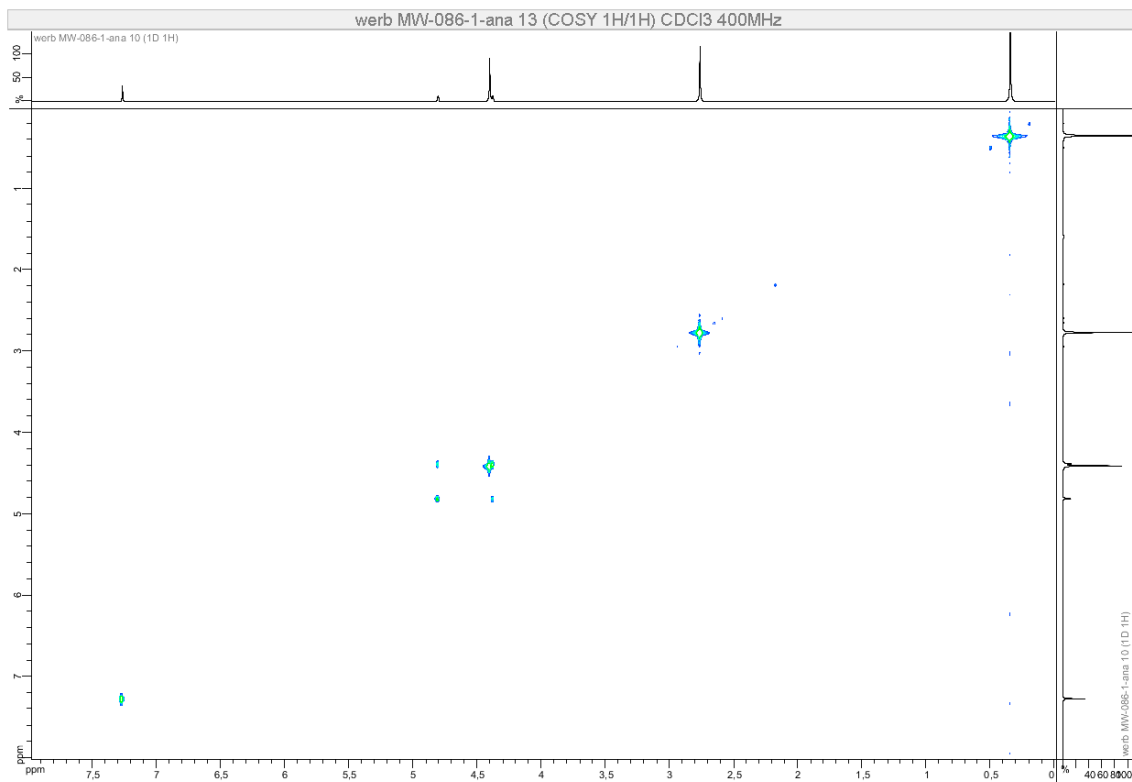


Figure S126. COSY (400 MHz, CDCl₃) of **5** (racemic mixture)

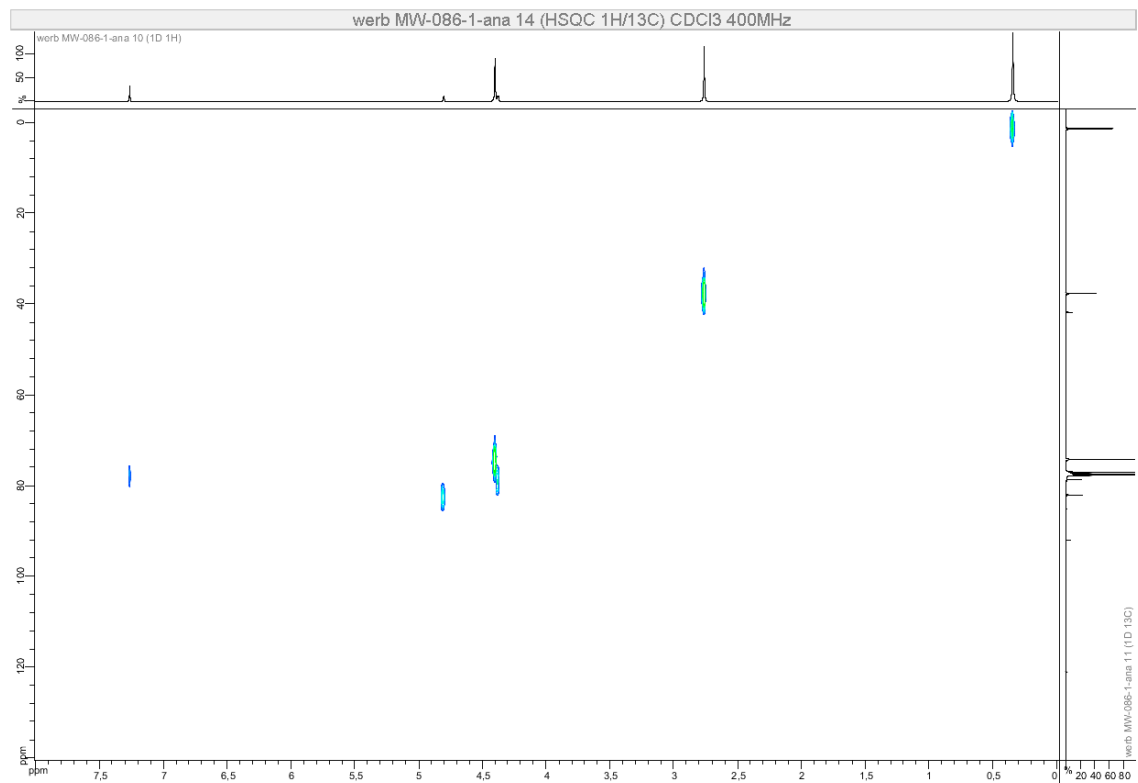


Figure S127. HSQC (400 MHz, CDCl₃) of **5** (racemic mixture)

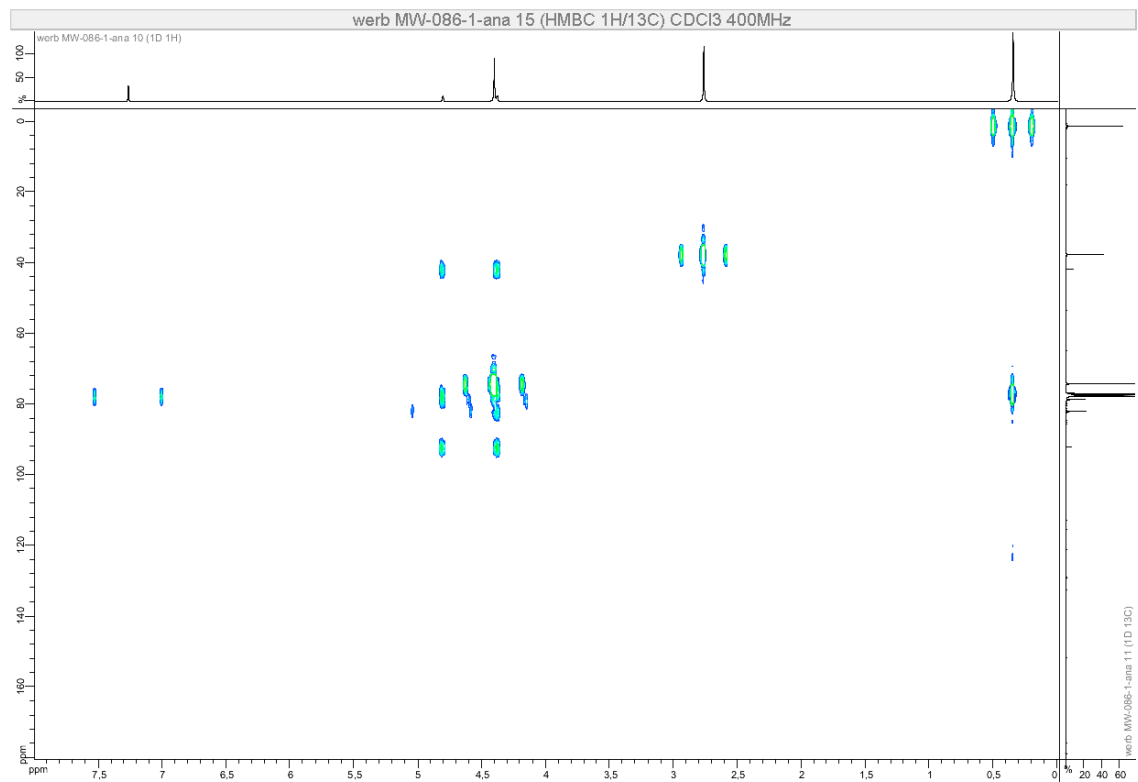


Figure S128. HMBC (400 MHz, CDCl₃) of **5** (racemic mixture)

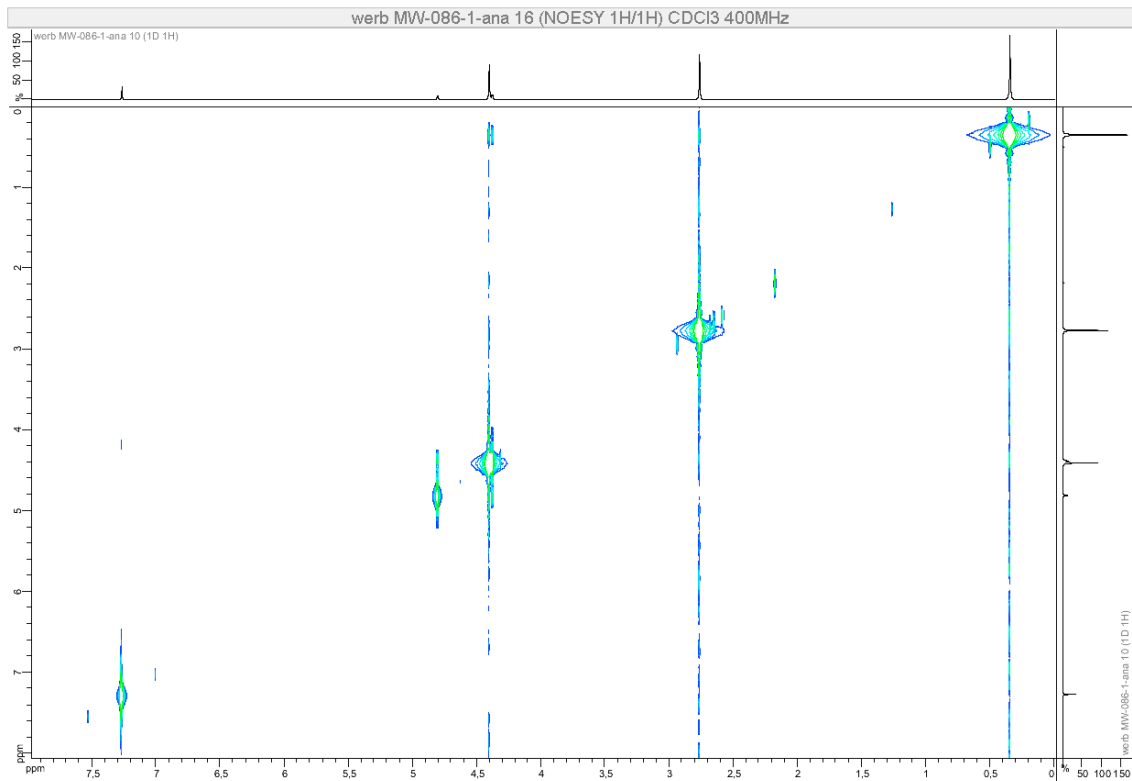
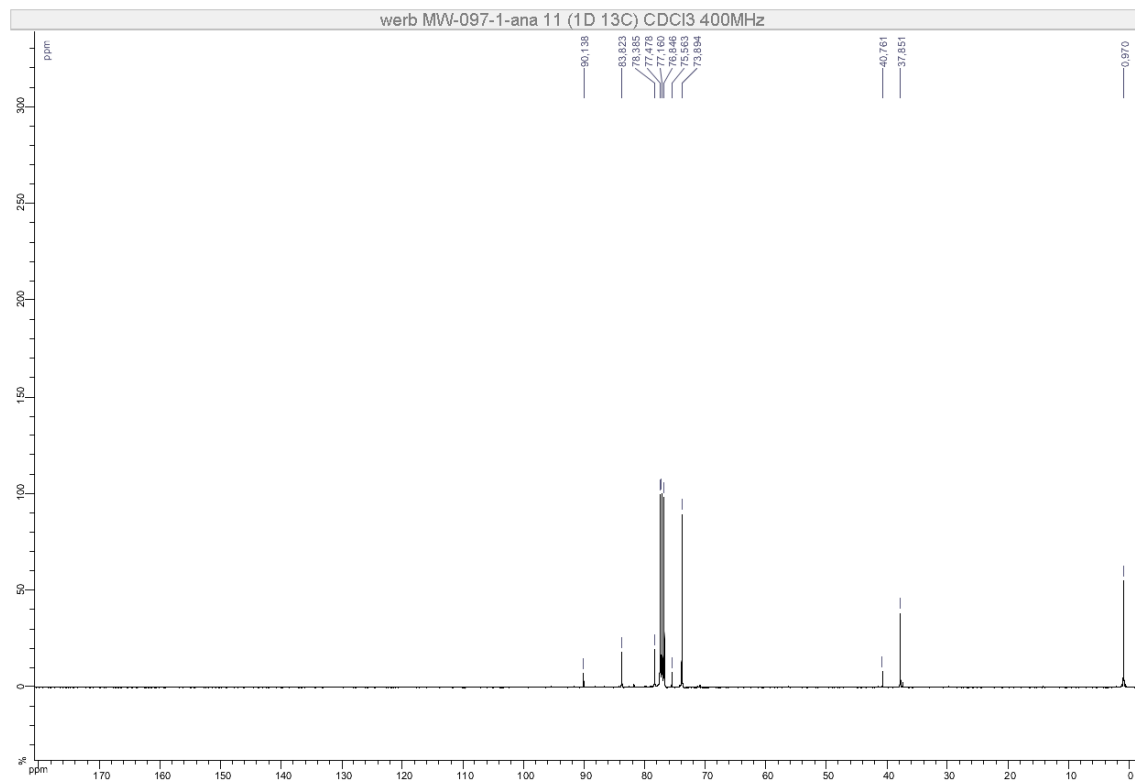
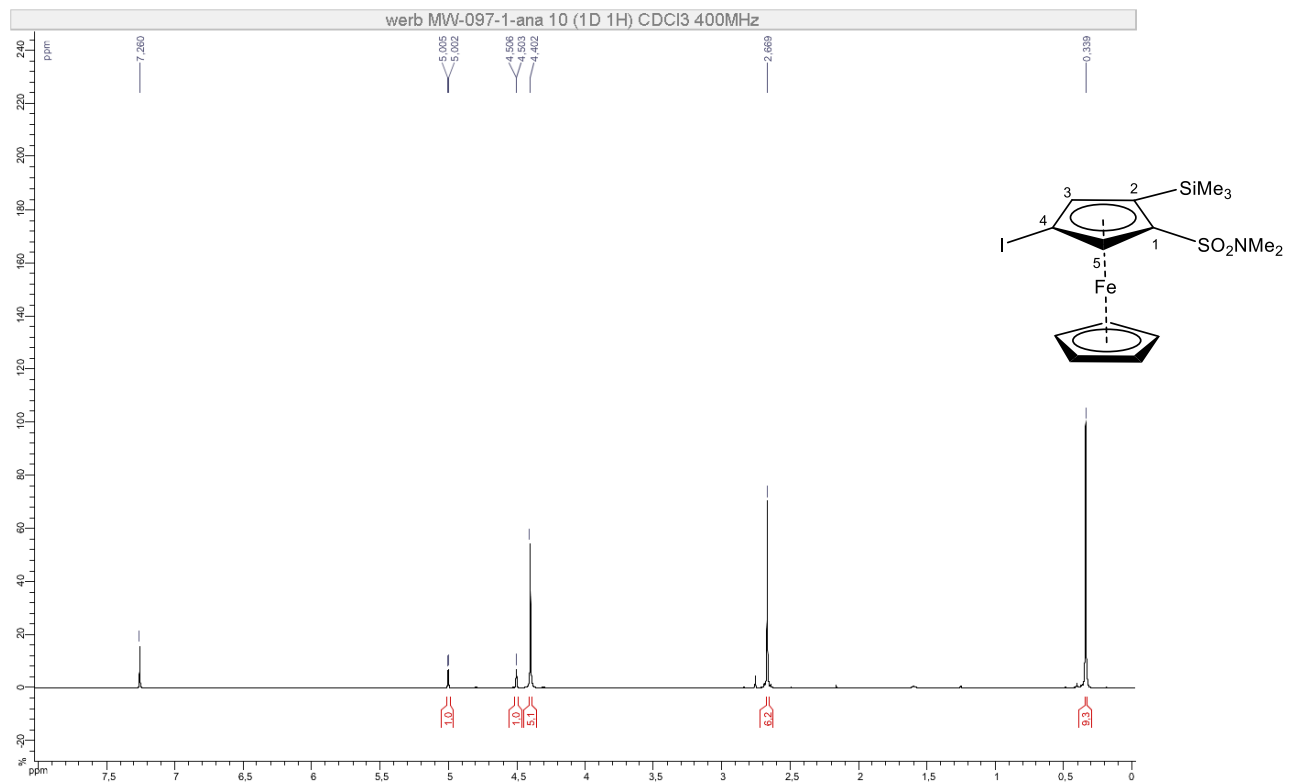


Figure S129. NOESY (400 MHz, CDCl₃) of **5** (racemic mixture)



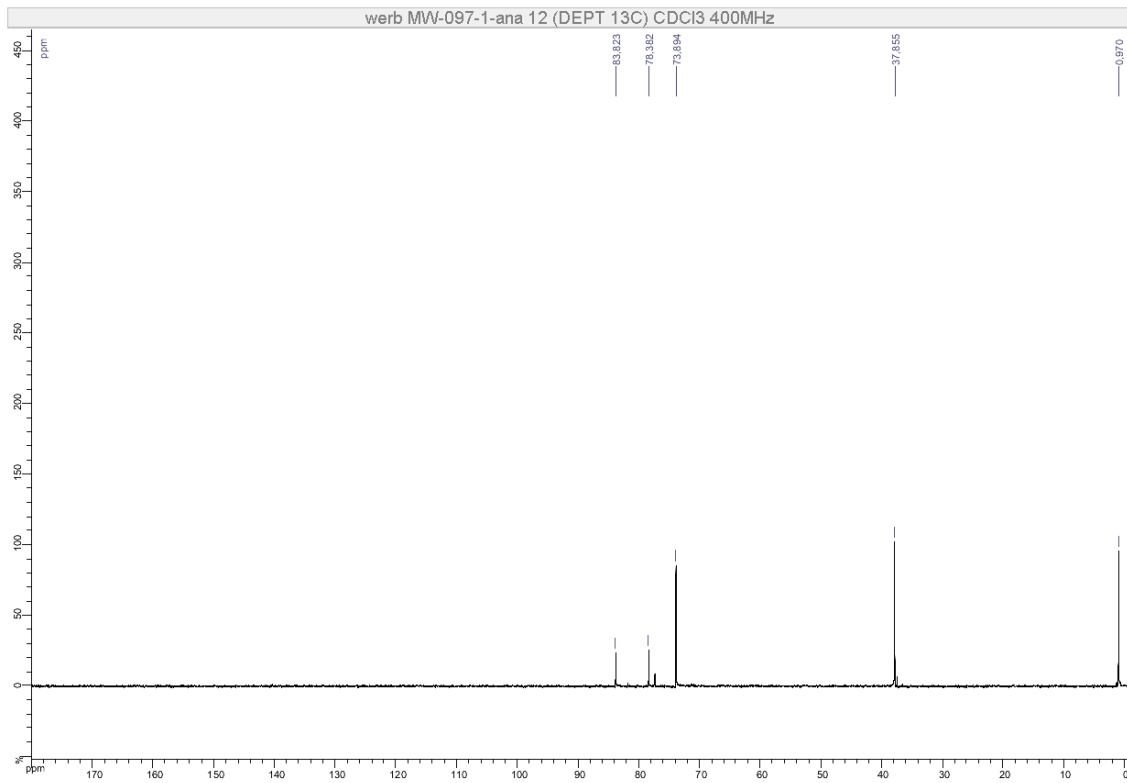


Figure S132. DEPT 135 (101 MHz, CDCl₃) of **6a** (racemic mixture)

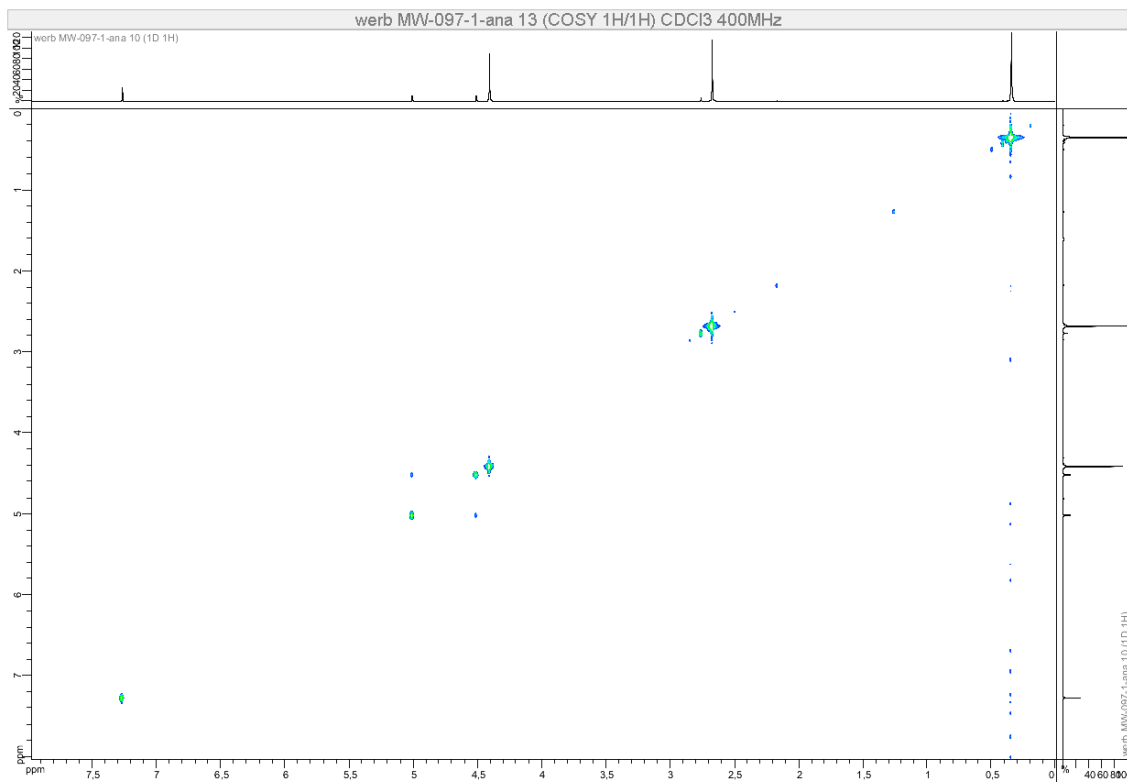


Figure S133. COSY (400 MHz, CDCl₃) of **6a** (racemic mixture)

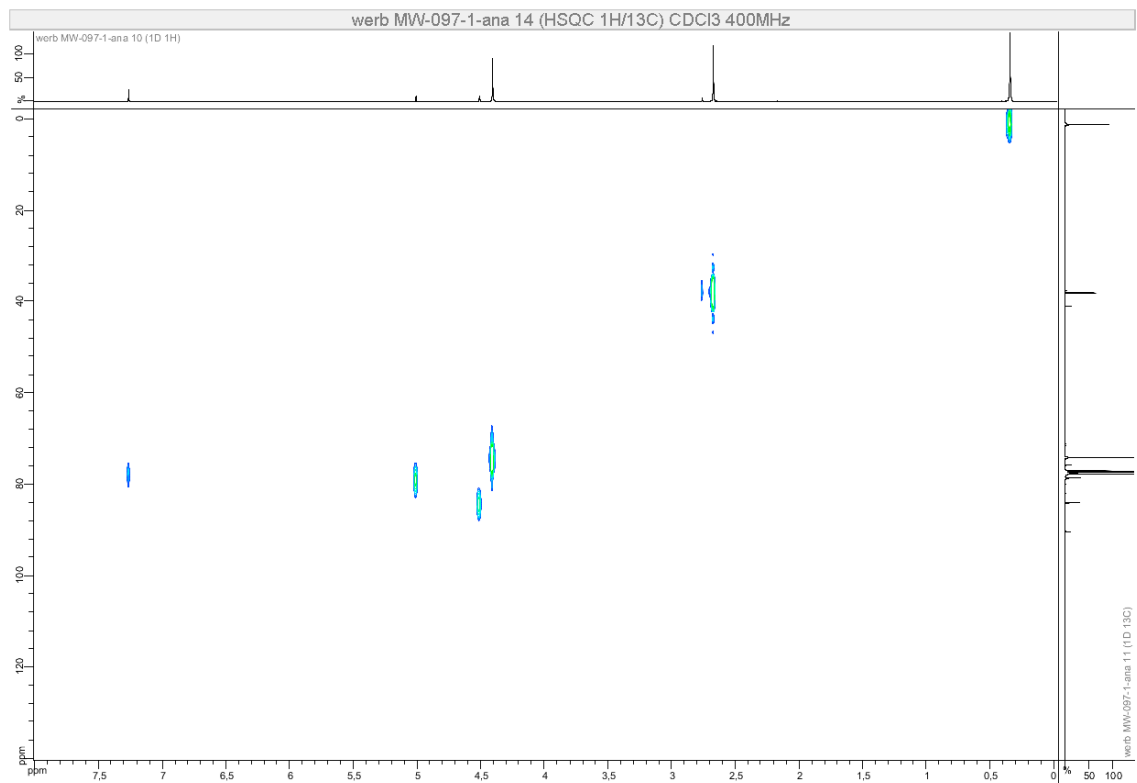


Figure S134. HSQC (400 MHz, CDCl₃) of **6a** (racemic mixture)

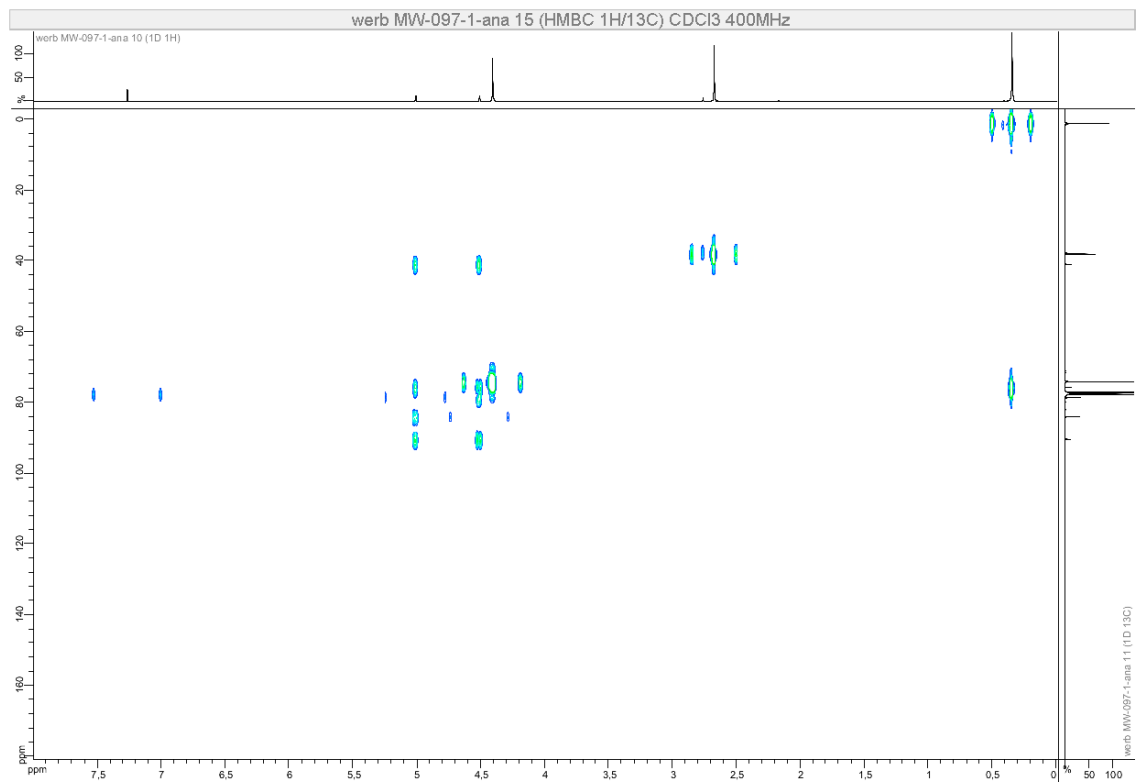


Figure S135. HMBC (400 MHz, CDCl₃) of **6a** (racemic mixture)

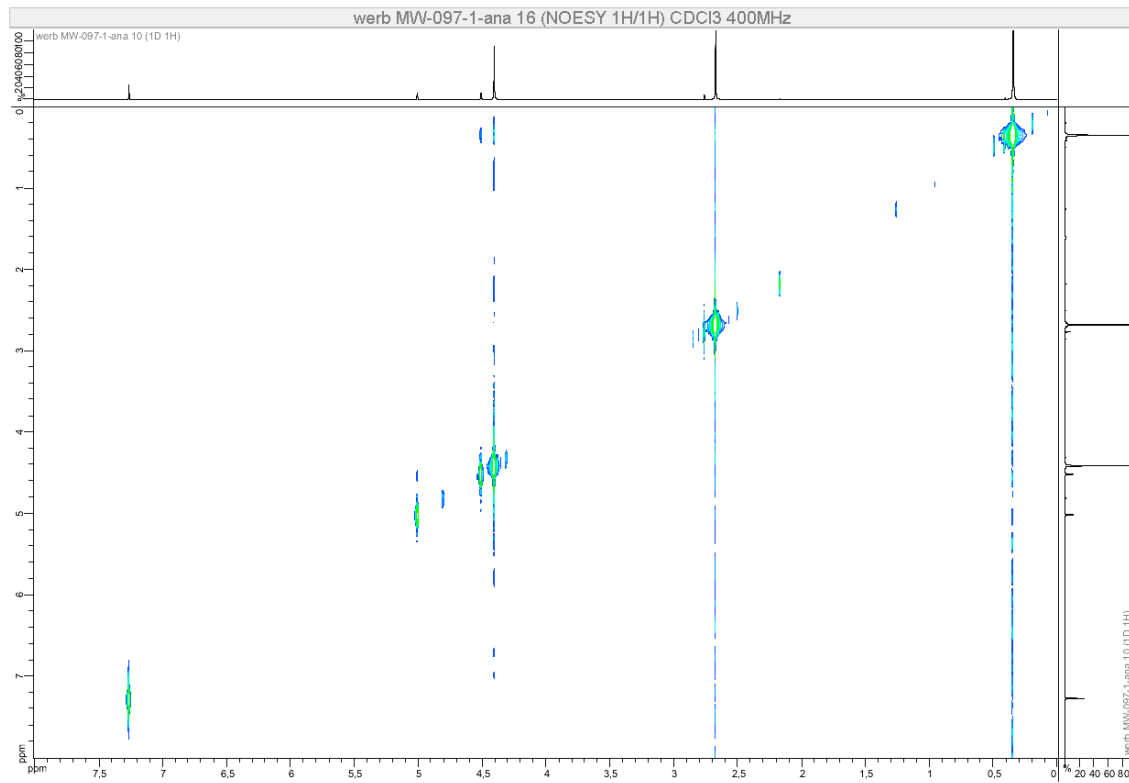
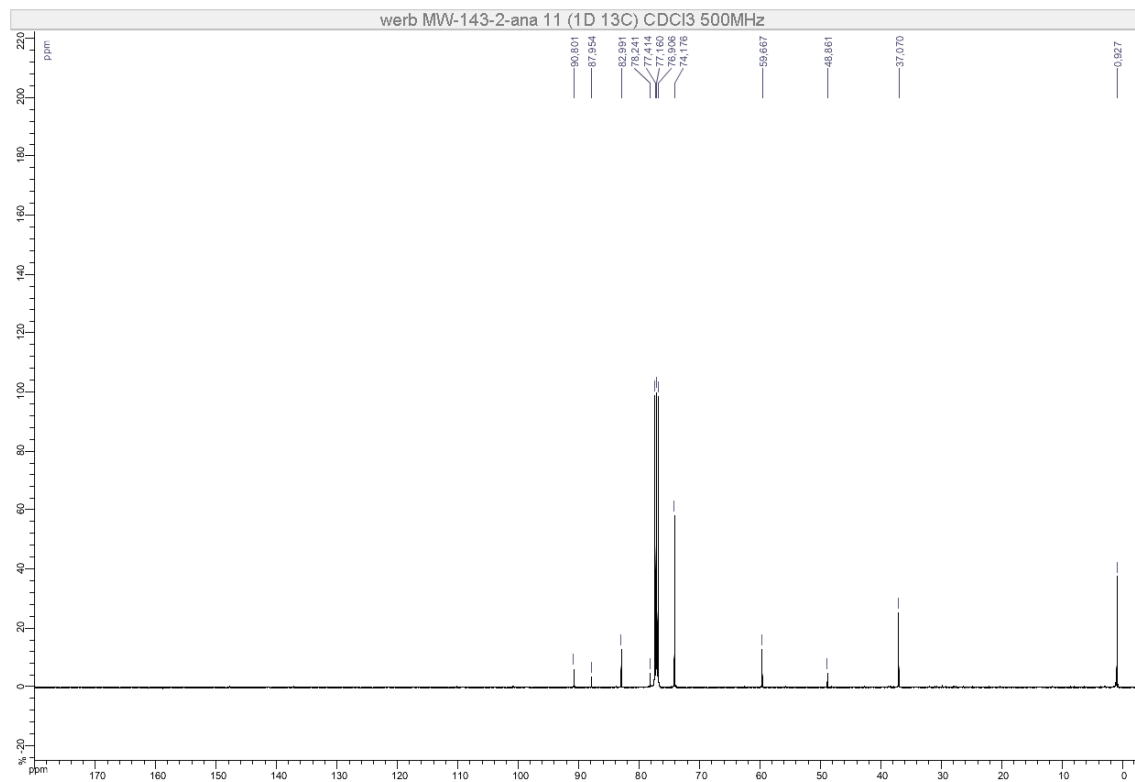
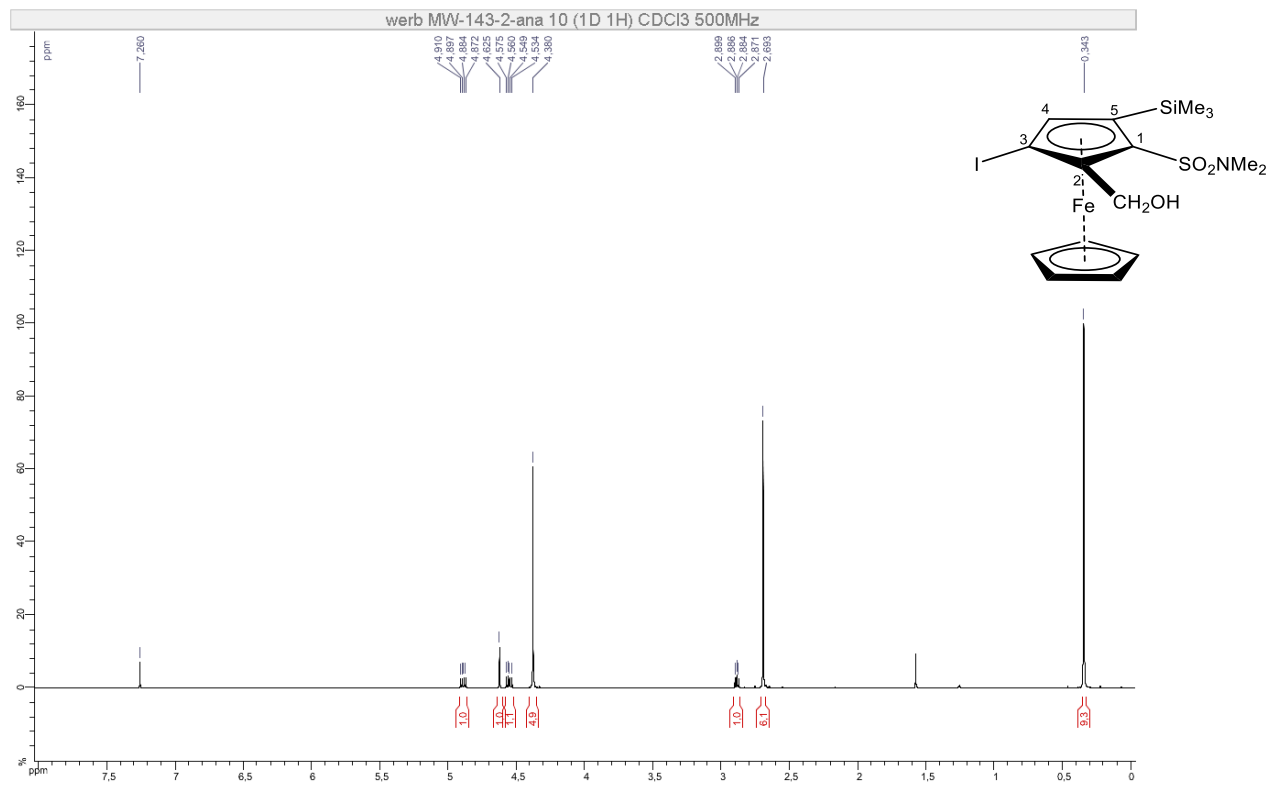


Figure S136. NOESY (400 MHz, CDCl₃) of **6a** (racemic mixture)



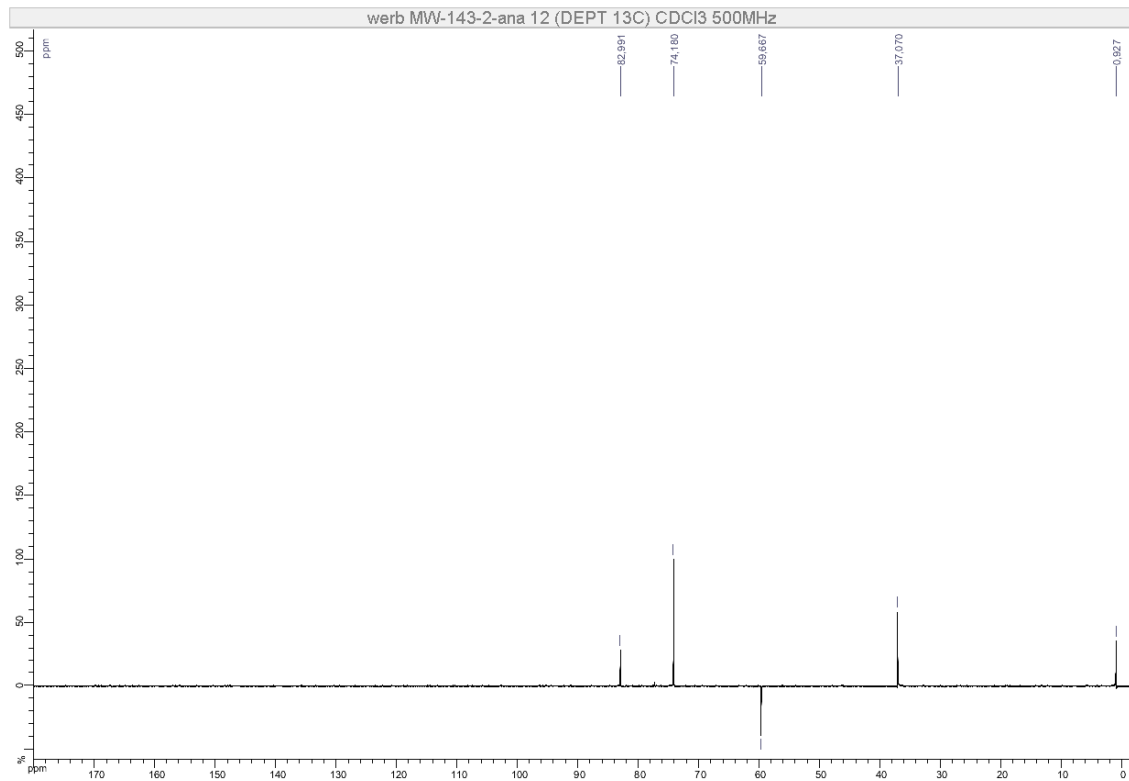


Figure S139. DEPT 135 (126 MHz, CDCl₃) of **6b** (racemic mixture)

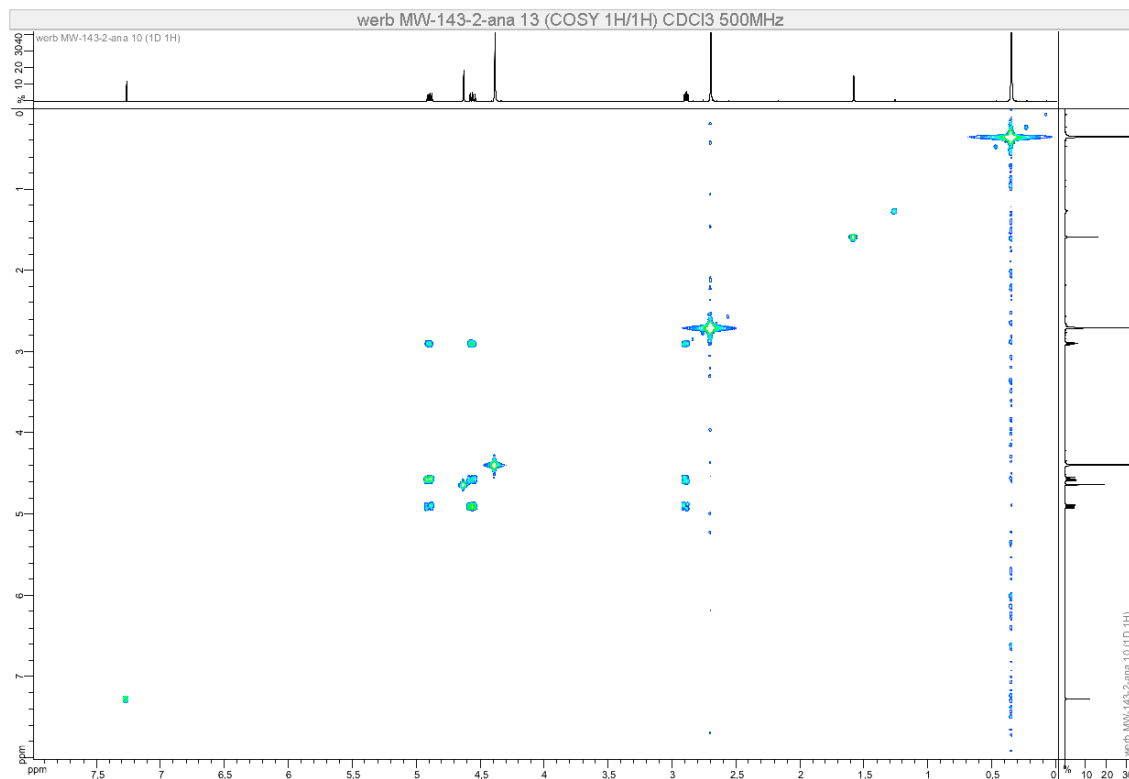


Figure S140. COSY (500 MHz, CDCl₃) of **6b** (racemic mixture)

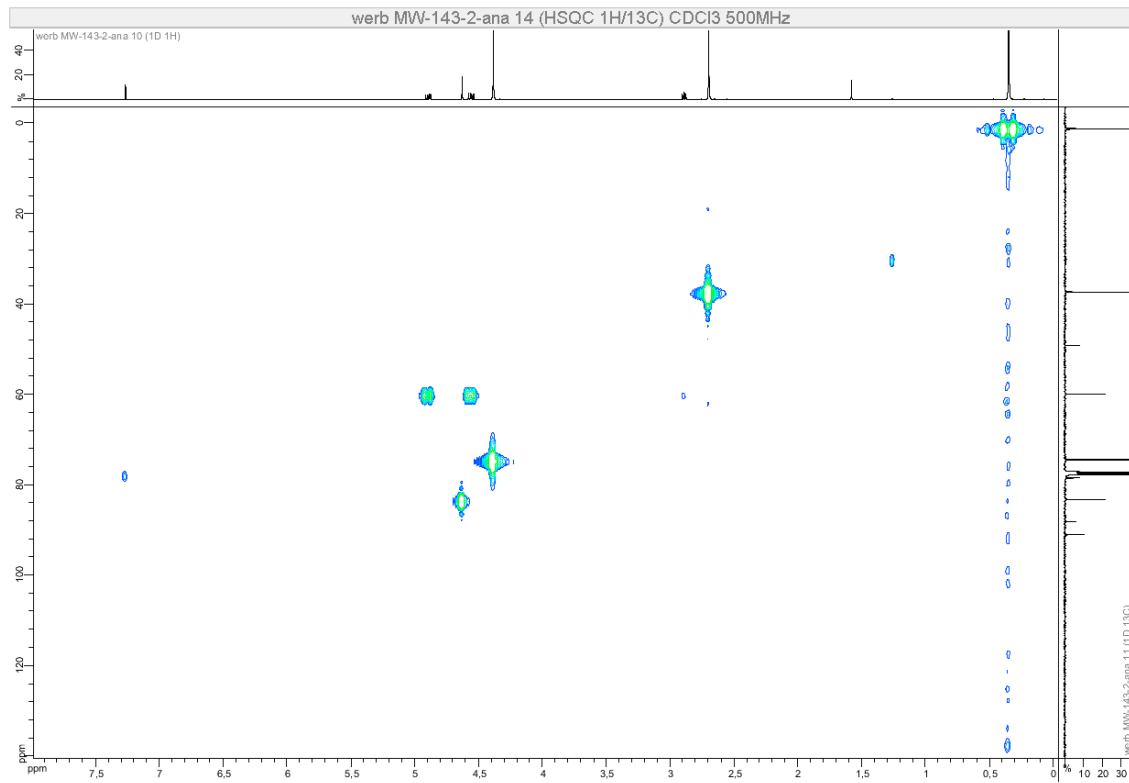


Figure S141. HSQC (500 MHz, CDCl₃) of **6b** (racemic mixture)

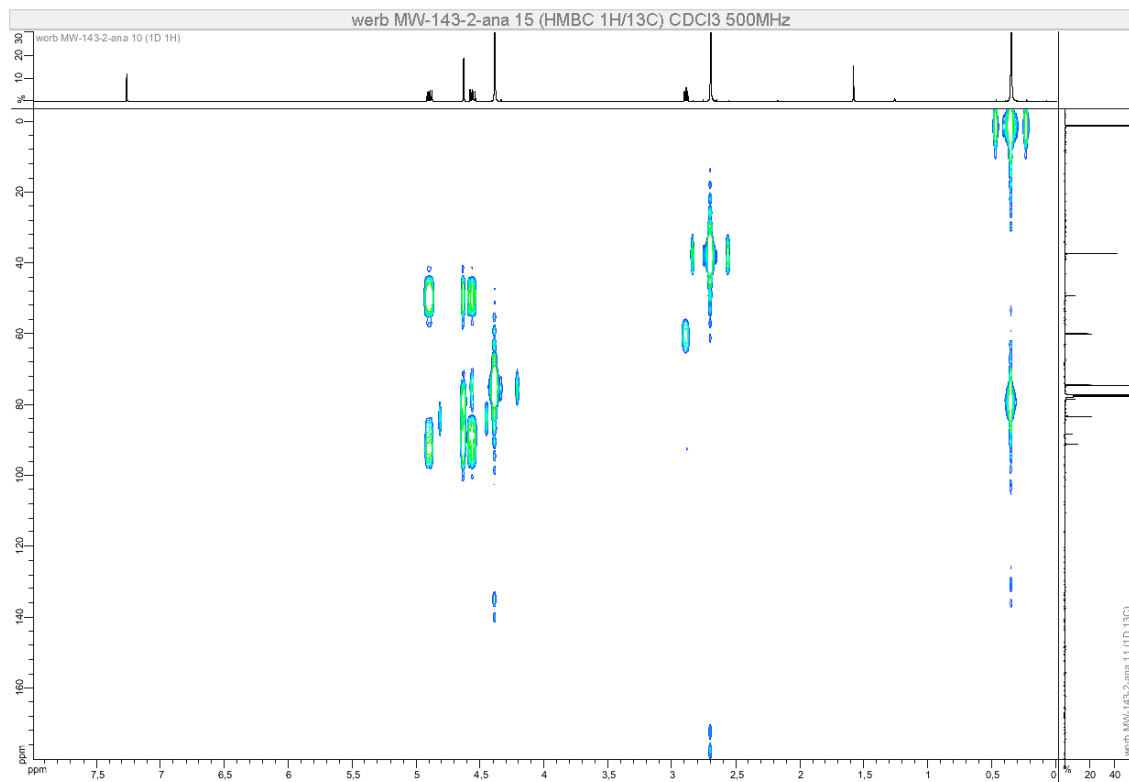


Figure S142. HMBC (500 MHz, CDCl₃) of **6b** (racemic mixture)

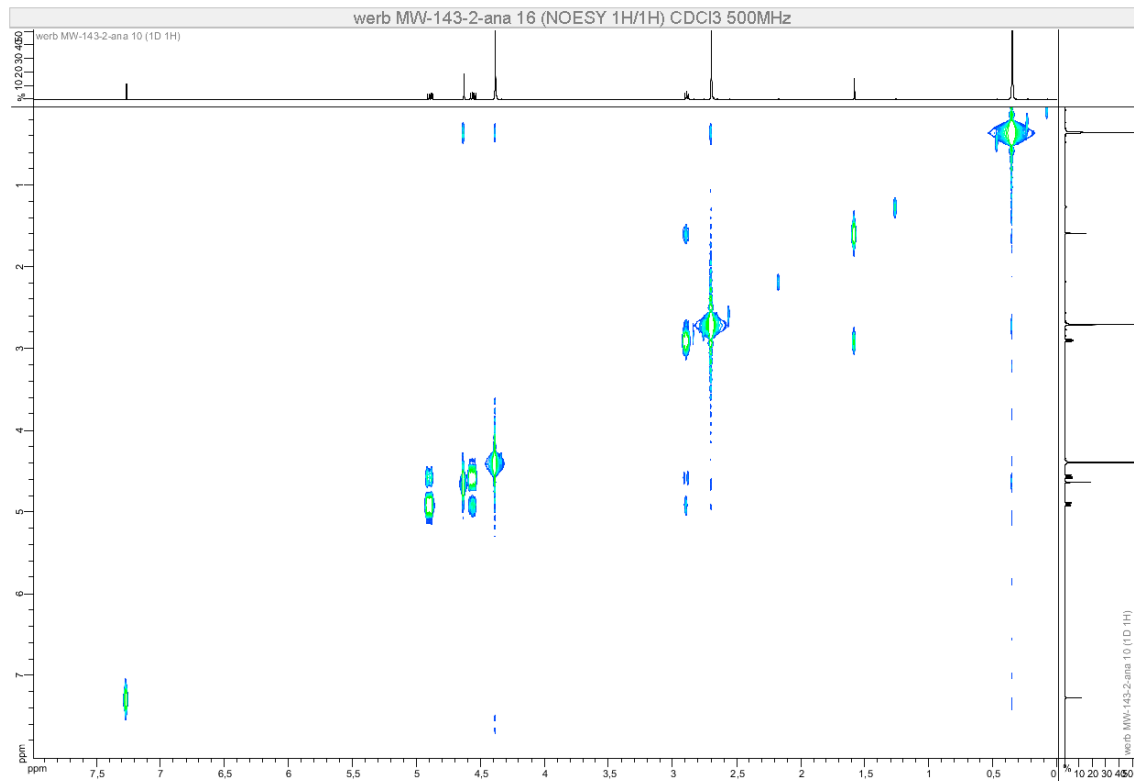


Figure S143. NOESY (500 MHz, CDCl_3) of **6b** (racemic mixture)

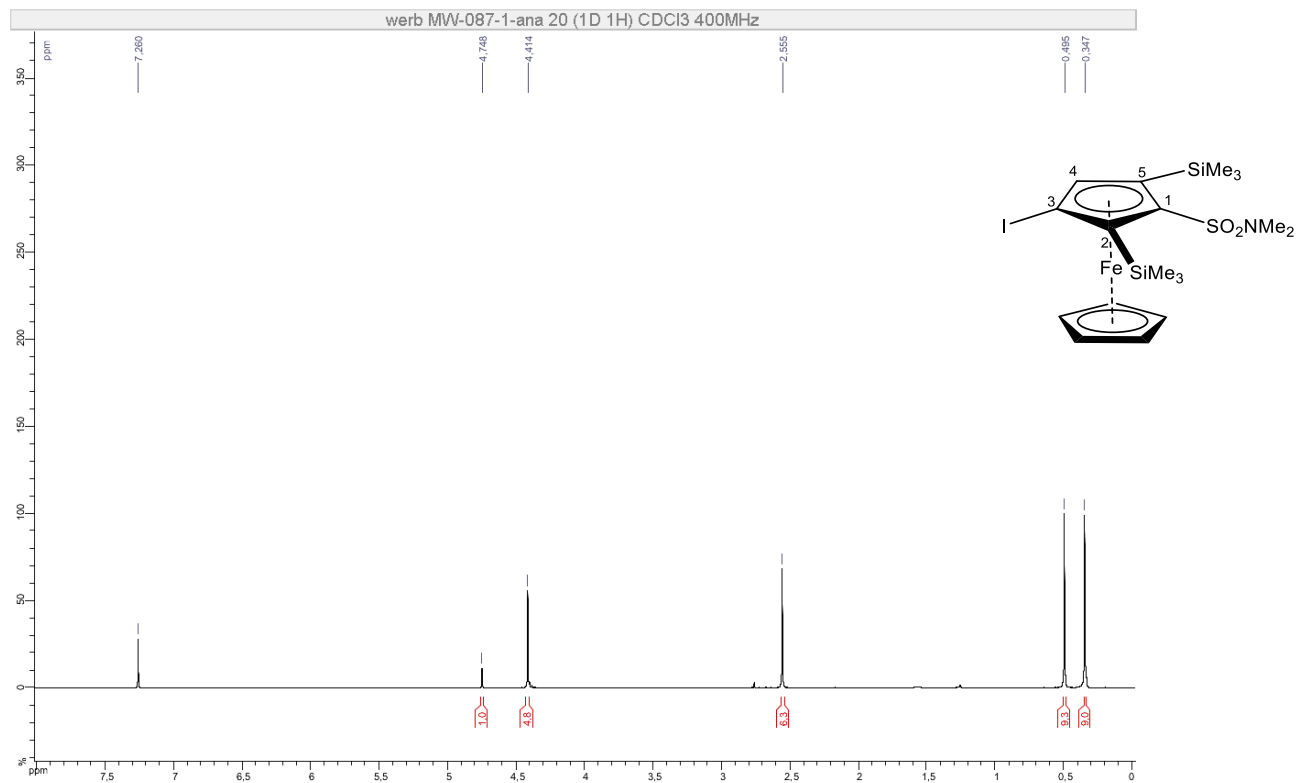


Figure S144. ^1H NMR (400 MHz, CDCl_3) of **6c** (racemic mixture)

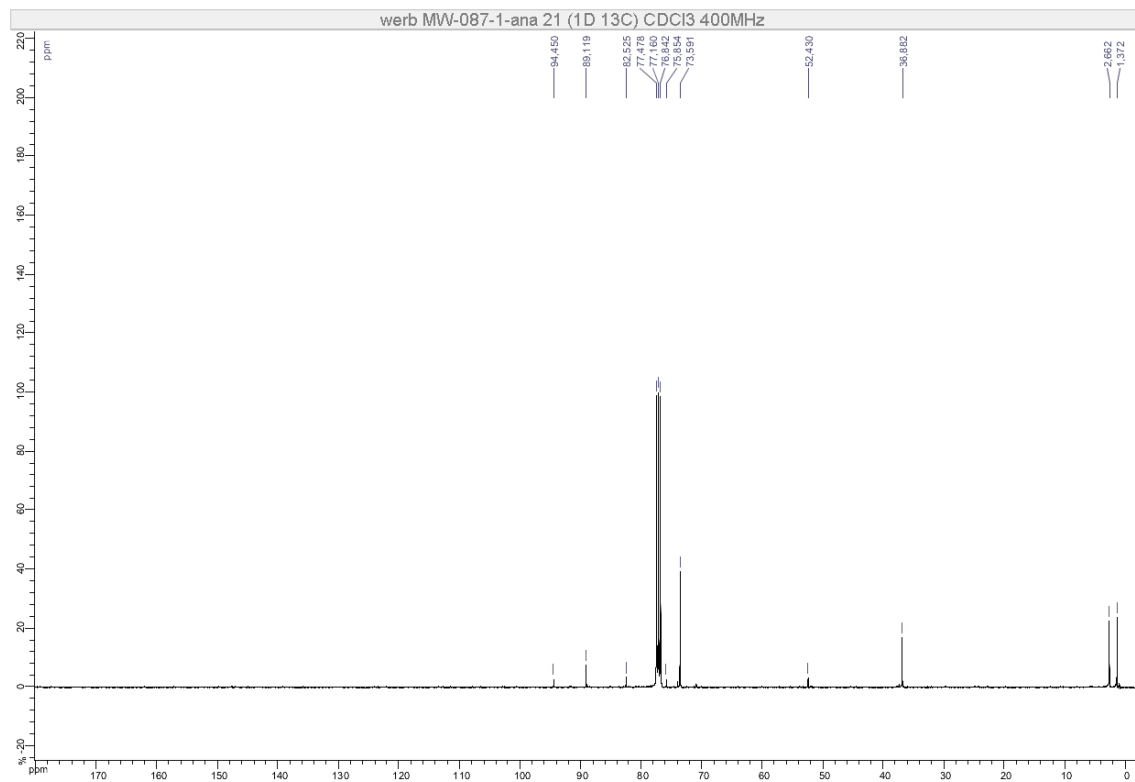


Figure S145. ^{13}C NMR (101 MHz, CDCl_3) of **6c** (racemic mixture)

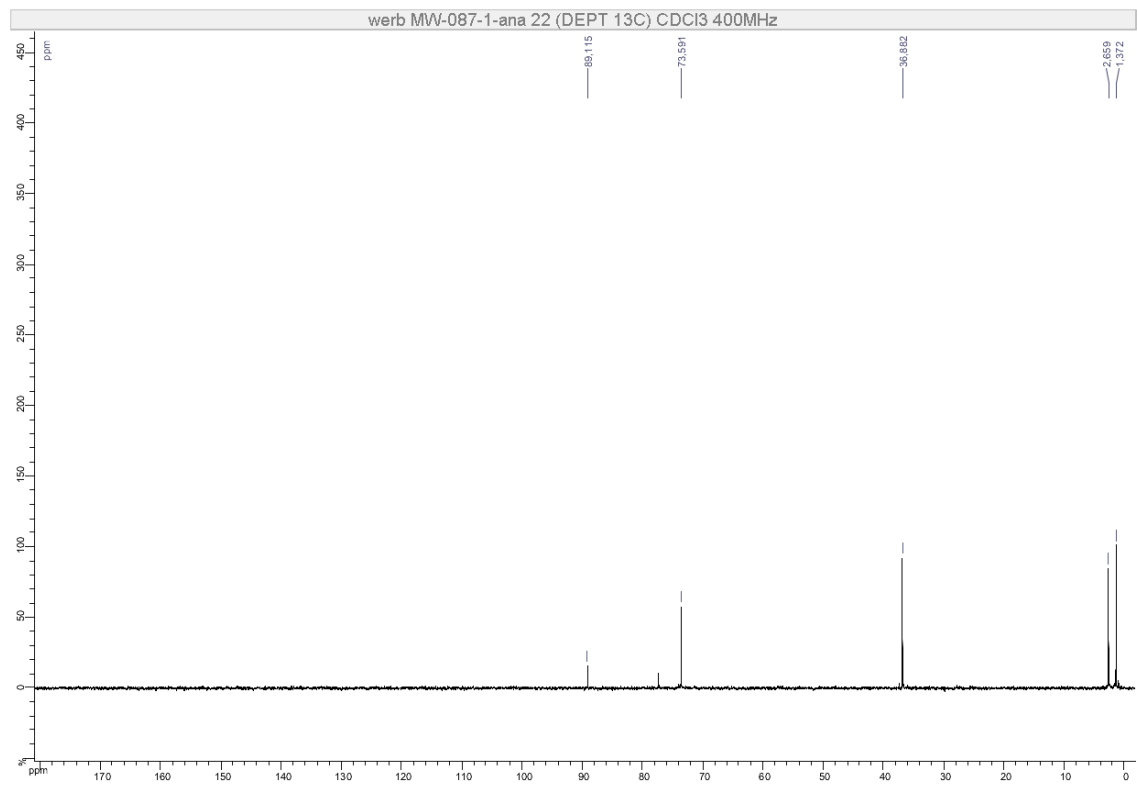


Figure S146. DEPT 135 (101 MHz, CDCl₃) of **6c** (racemic mixture)

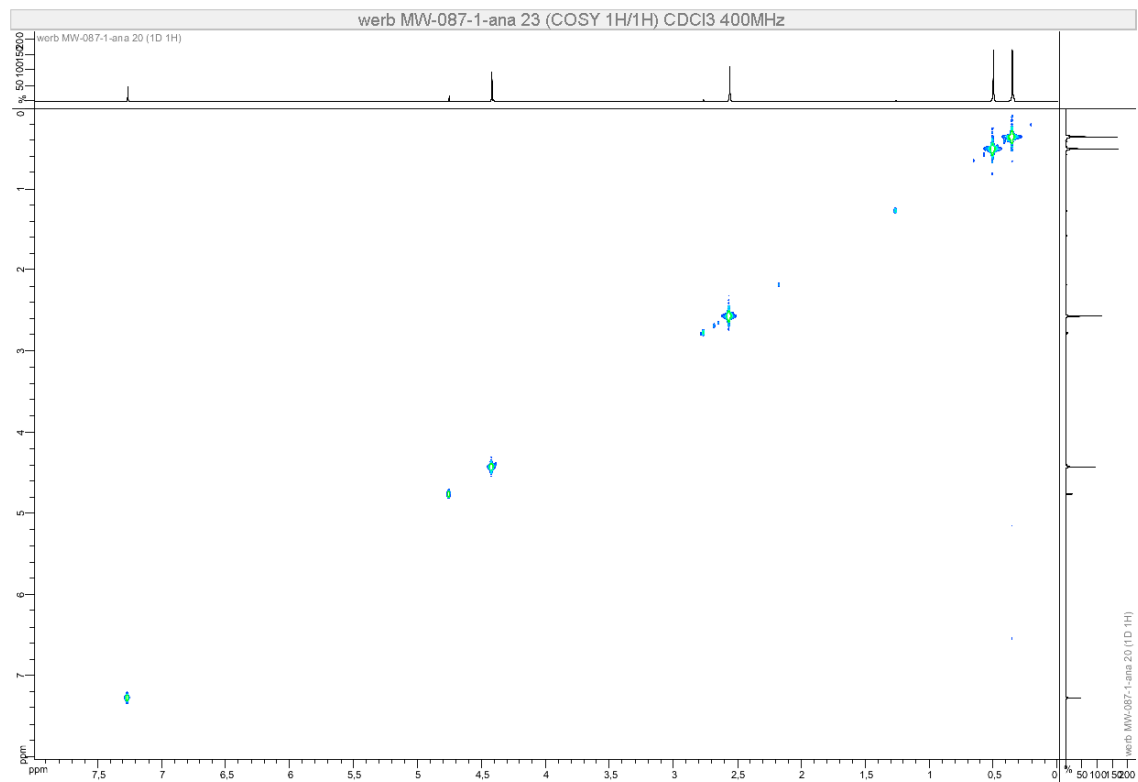


Figure S147. COSY (400 MHz, CDCl₃) of **6c** (racemic mixture)

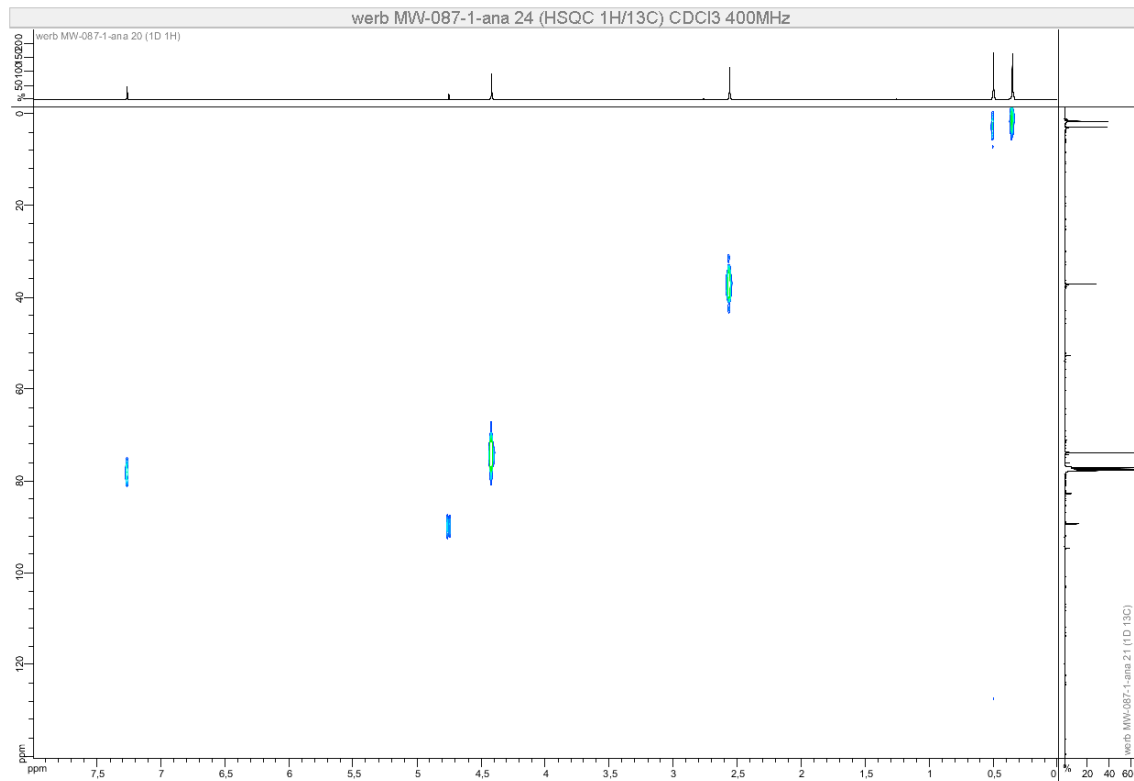


Figure S148. HSQC (400 MHz, CDCl₃) of **6c** (racemic mixture)

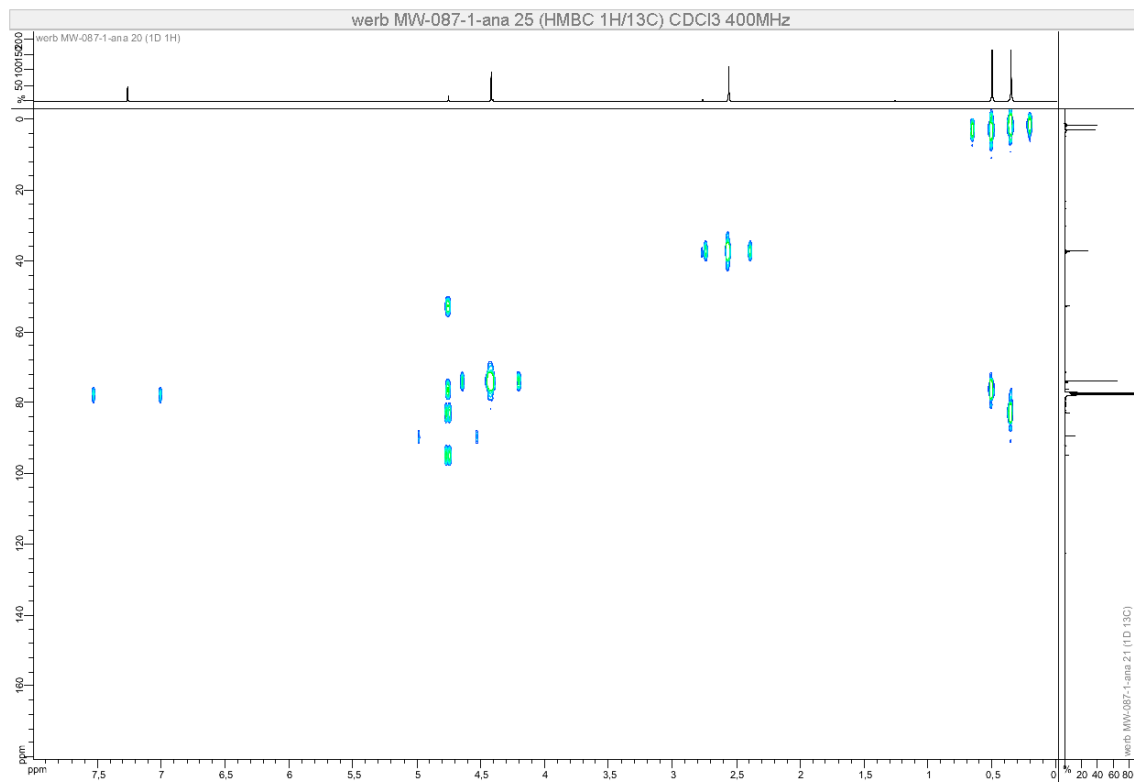


Figure S149. HMBC (400 MHz, CDCl₃) of **6c** (racemic mixture)

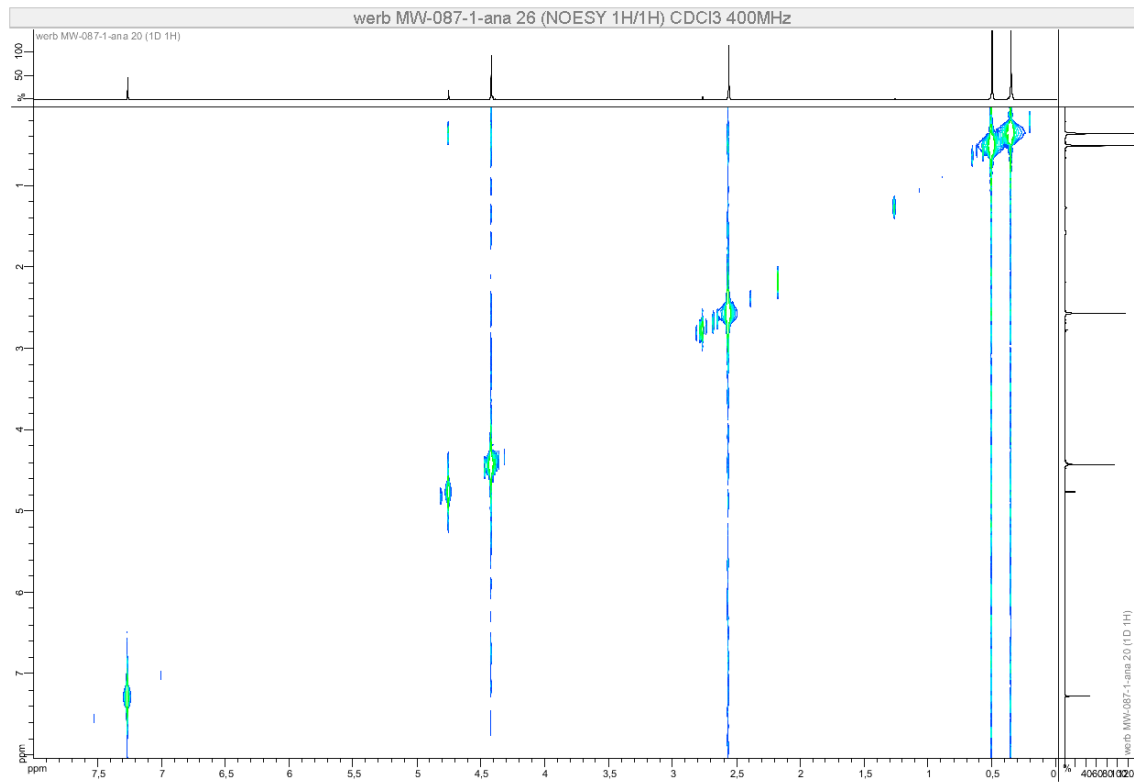
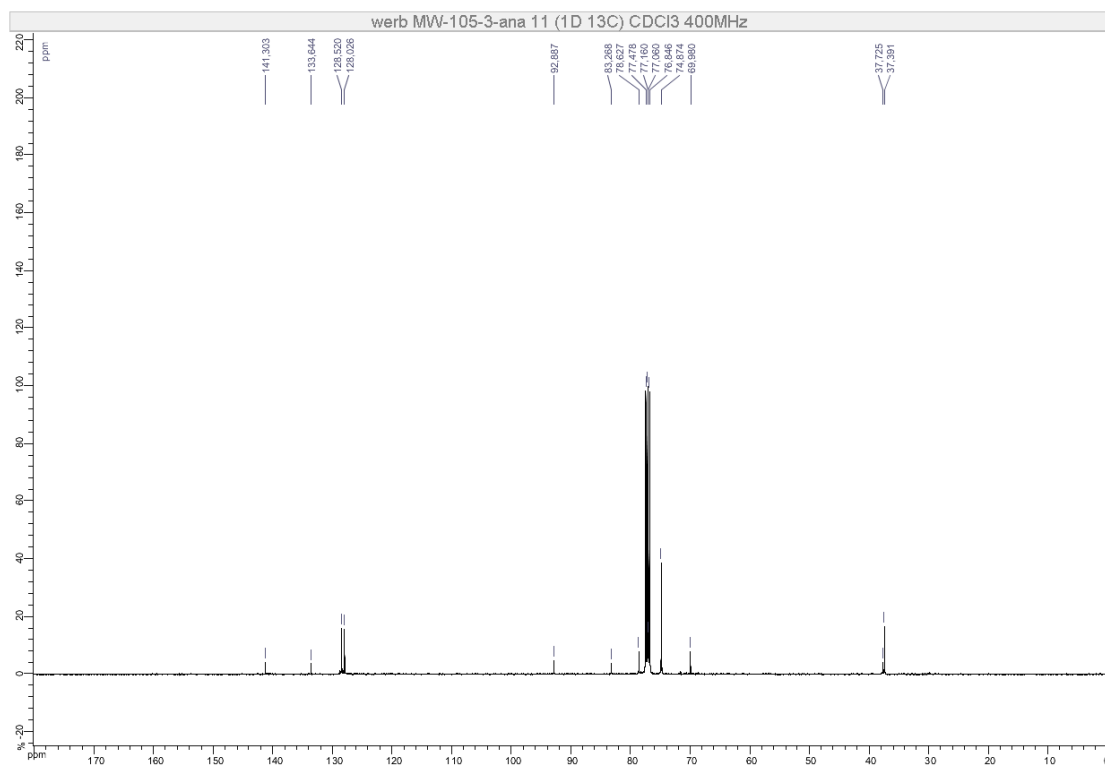
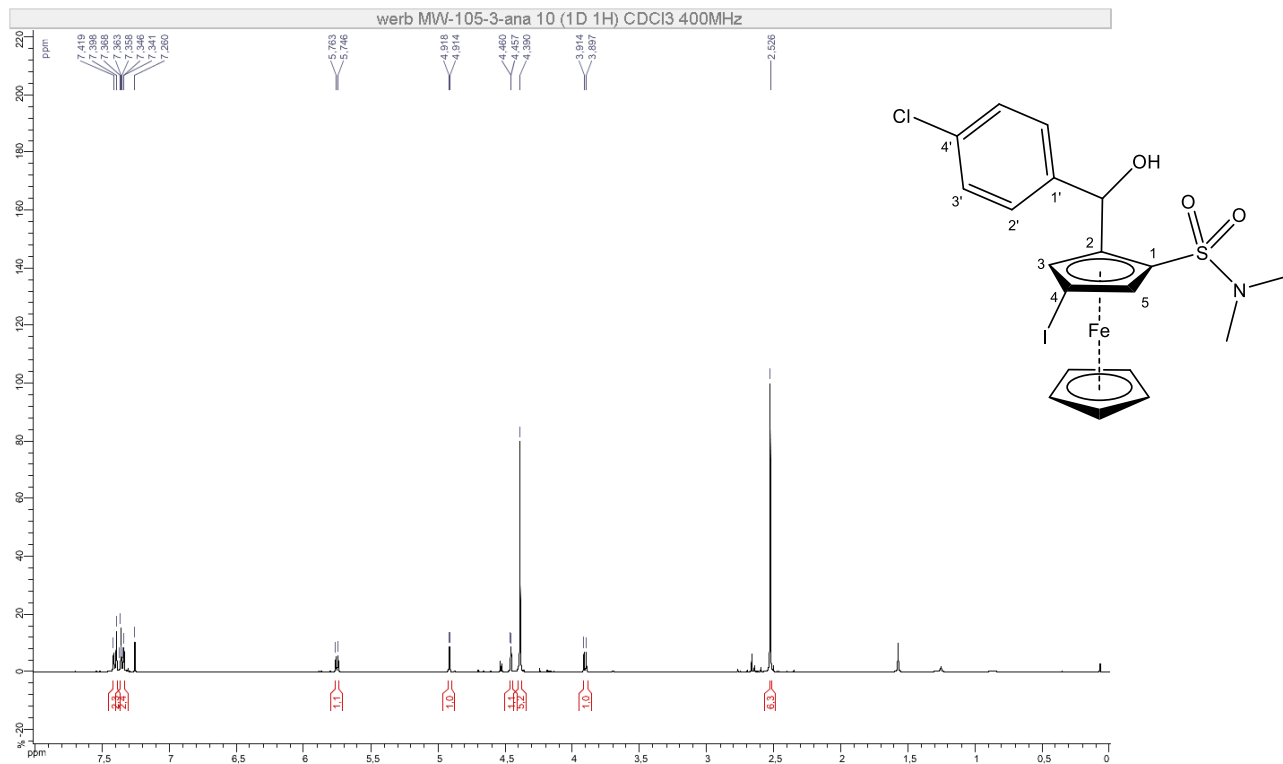


Figure S150. NOESY (400 MHz, CDCl₃) of **6c** (racemic mixture)



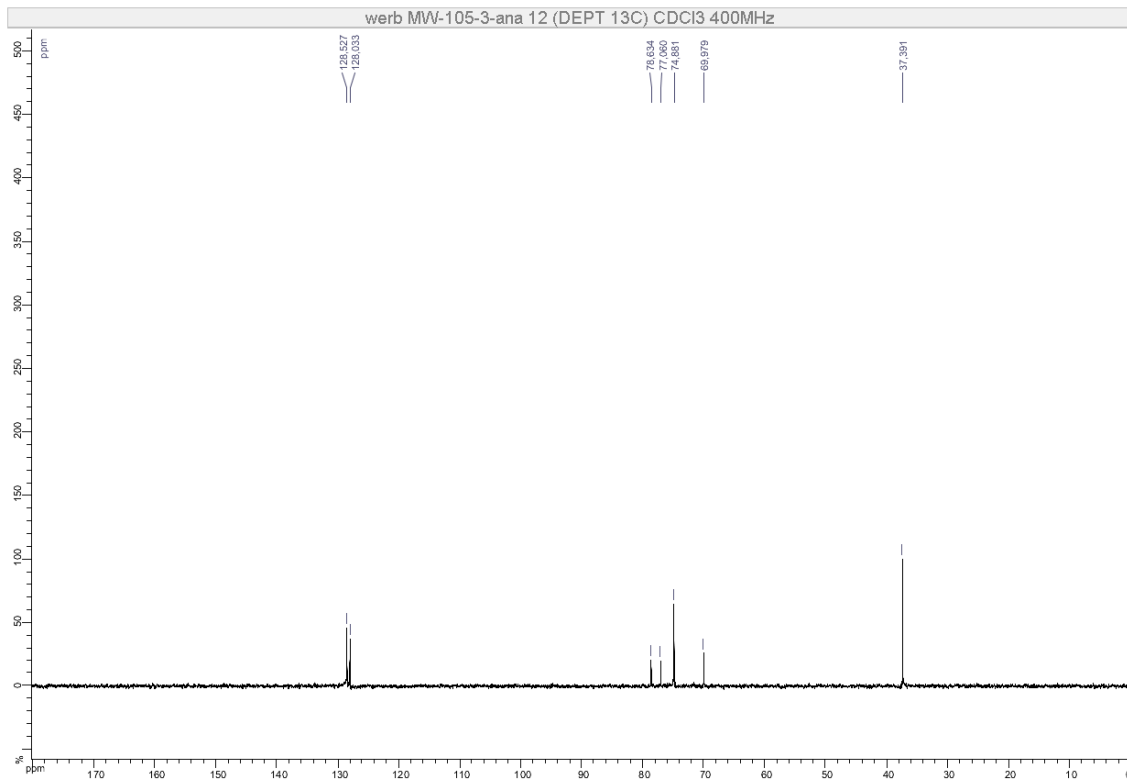


Figure S153. DEPT 135 (101 MHz, CDCl₃) of **7** (main diastereoisomer, racemic mixture)

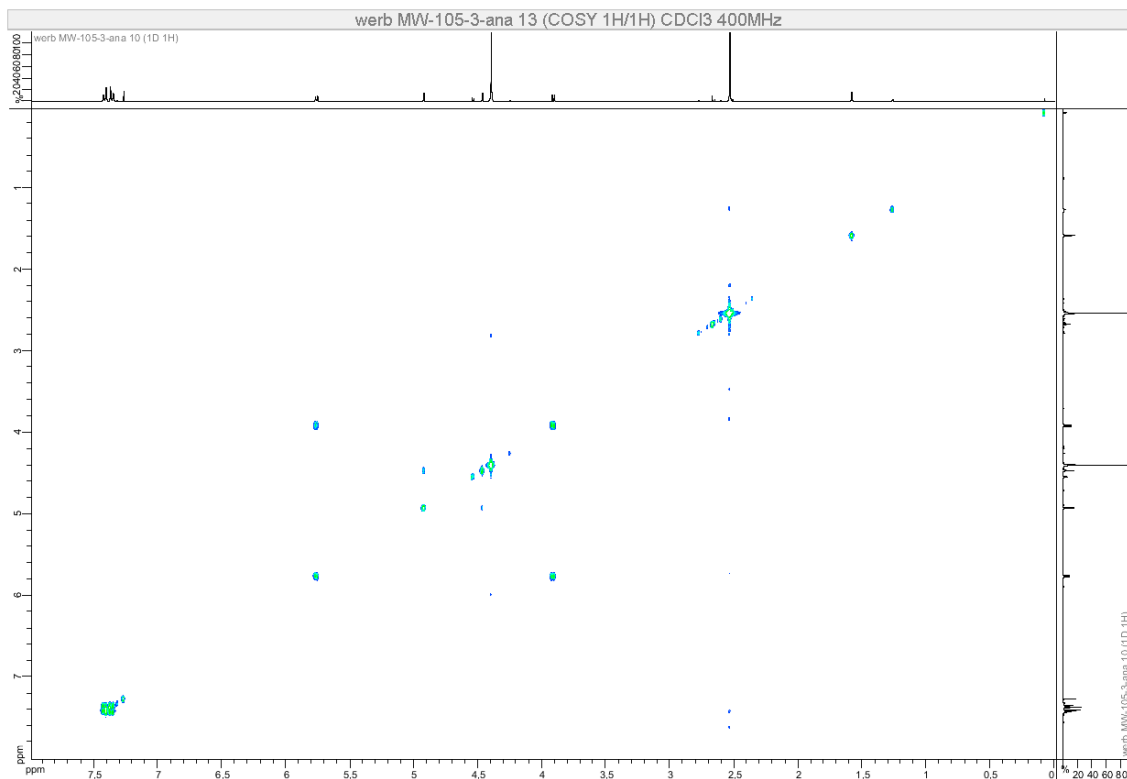


Figure S154. COSY (400 MHz, CDCl₃) of **7** (main diastereoisomer, racemic mixture)

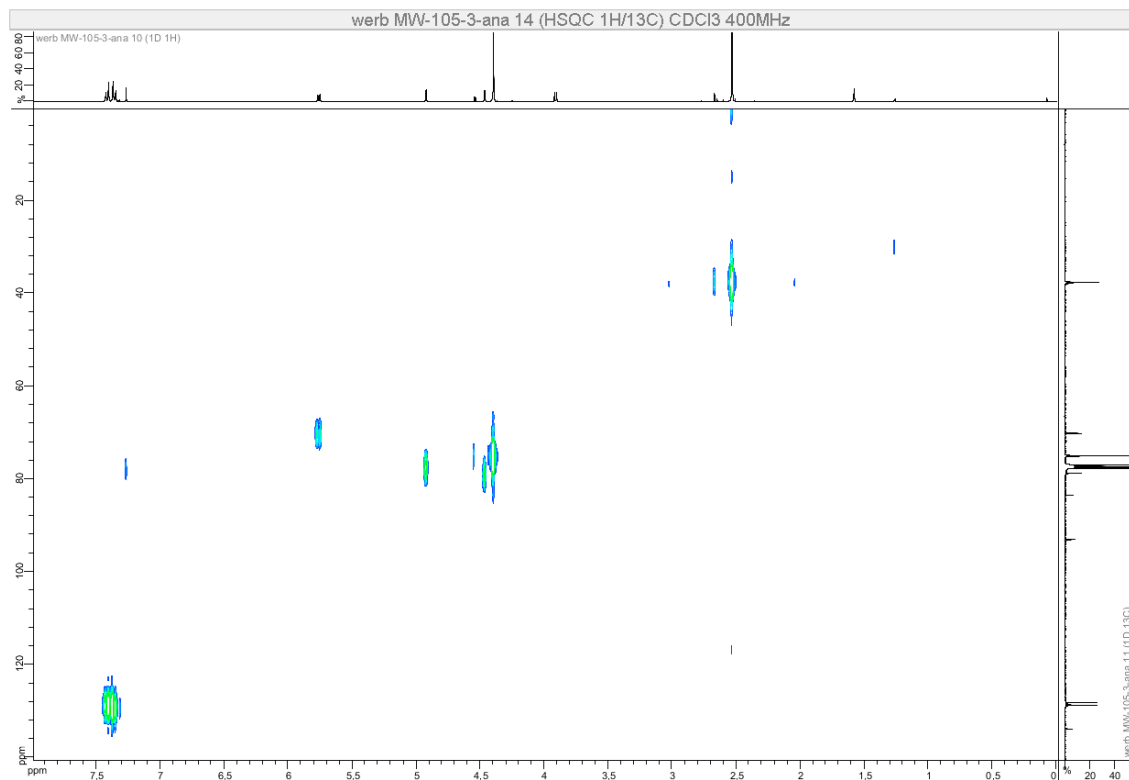


Figure S155. HSQC (400 MHz, CDCl₃) of **7** (main diastereoisomer, racemic mixture)

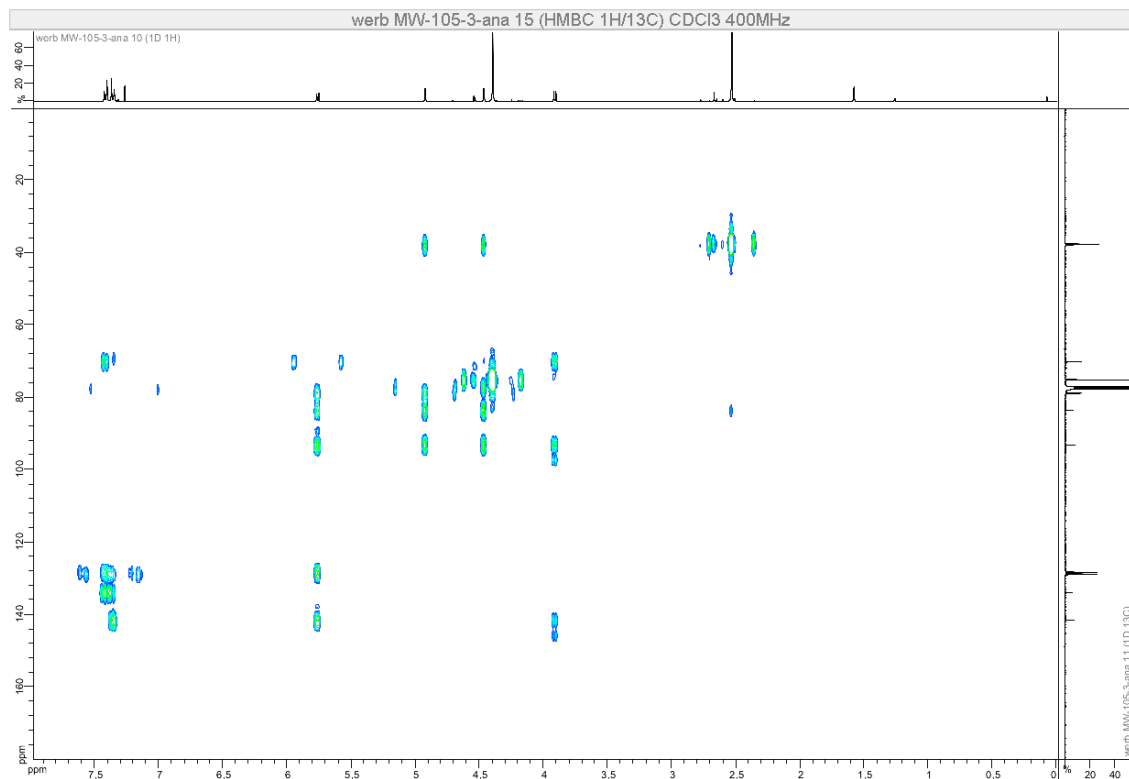


Figure S156. HMBC (400 MHz, CDCl₃) of **7** (main diastereoisomer, racemic mixture)

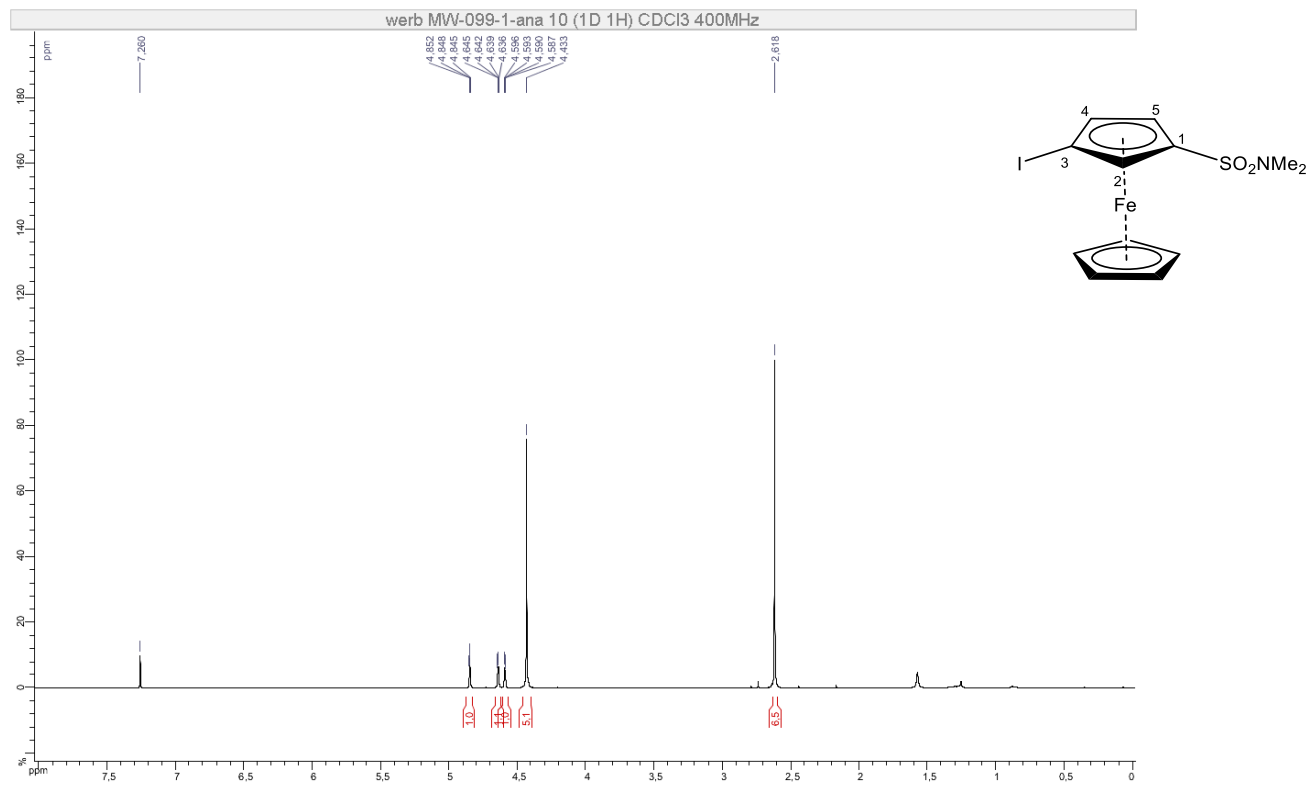


Figure S157. ¹H NMR (400 MHz, CDCl₃) of **8** (racemic mixture)

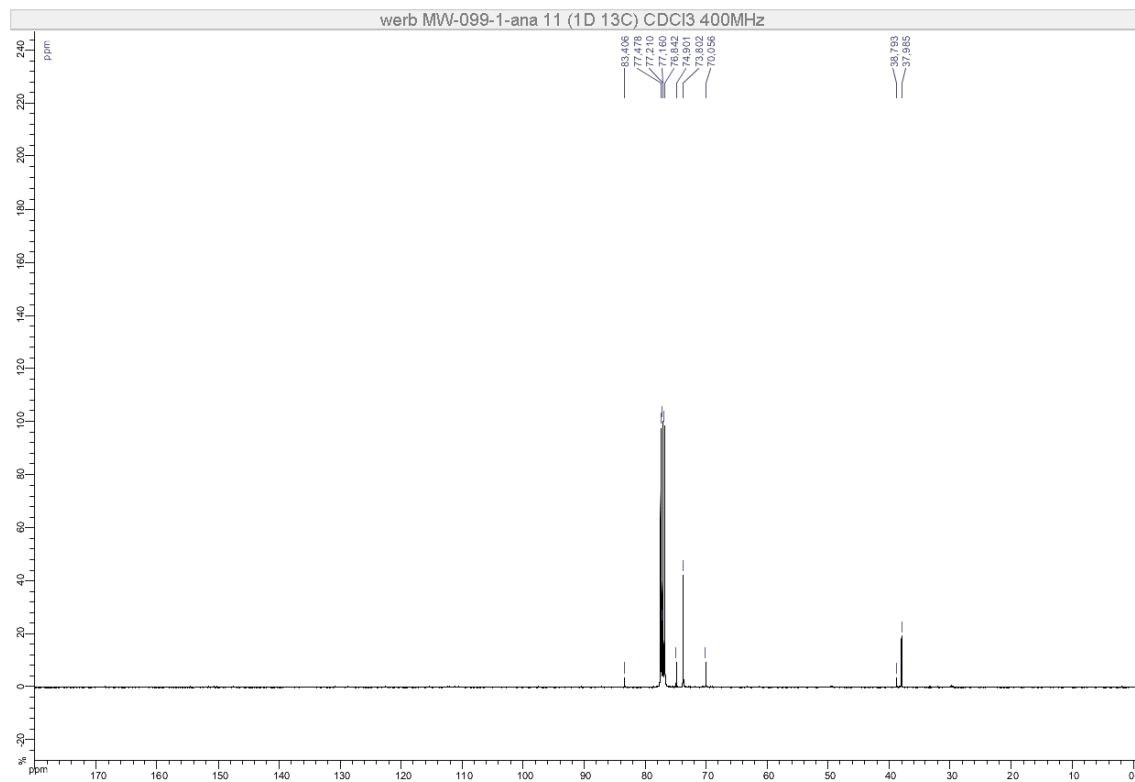


Figure S158. ¹³C NMR (101 MHz, CDCl₃) of **8** (racemic mixture)

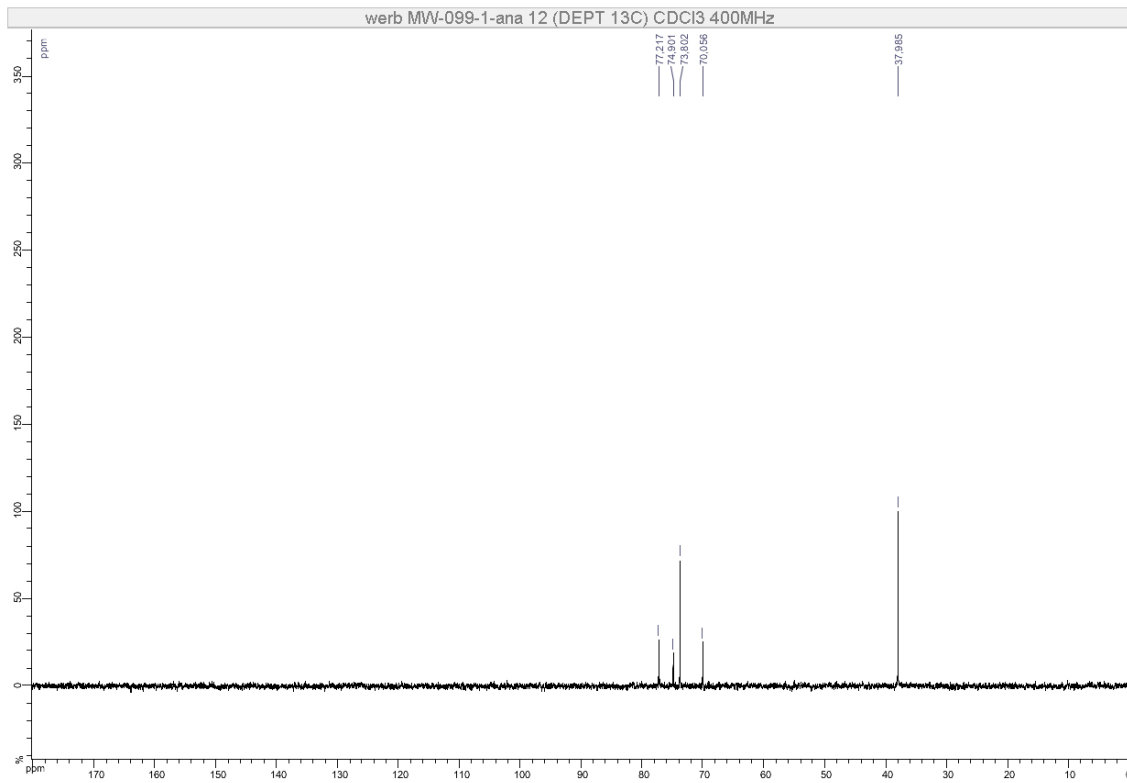


Figure S159. DEPT 135 (101 MHz, CDCl₃) of **8** (racemic mixture)

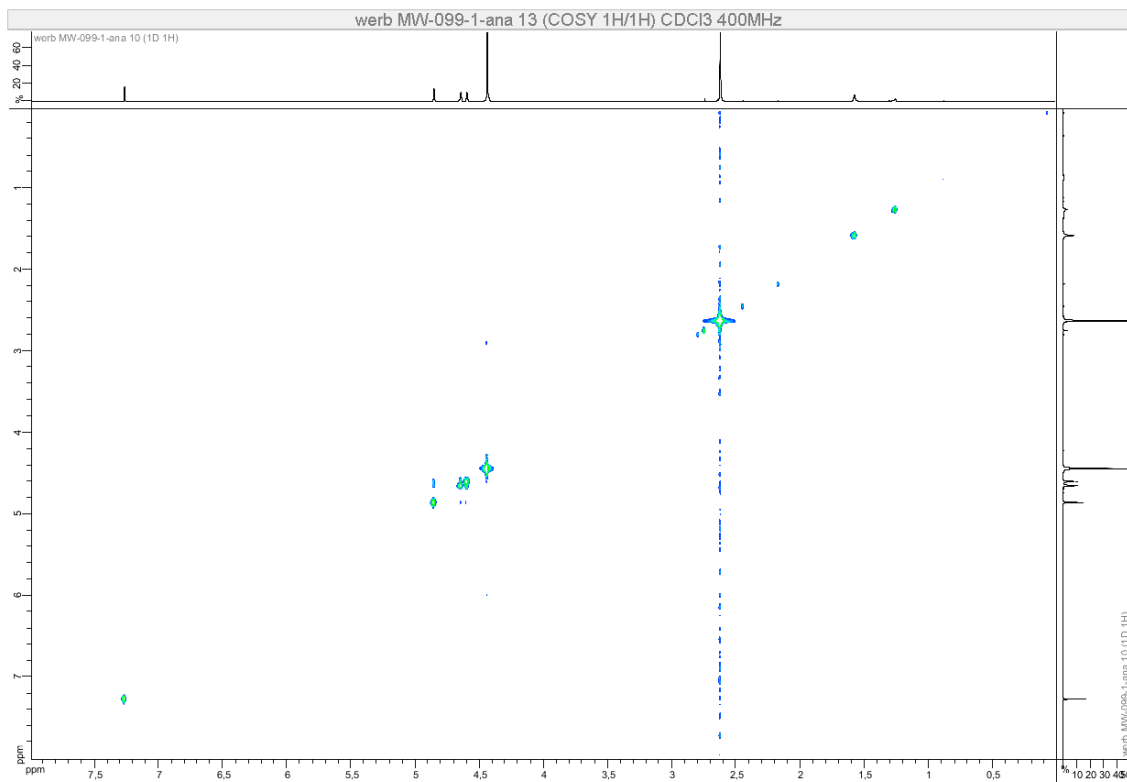


Figure S160. COSY (400 MHz, CDCl₃) of **8** (racemic mixture)

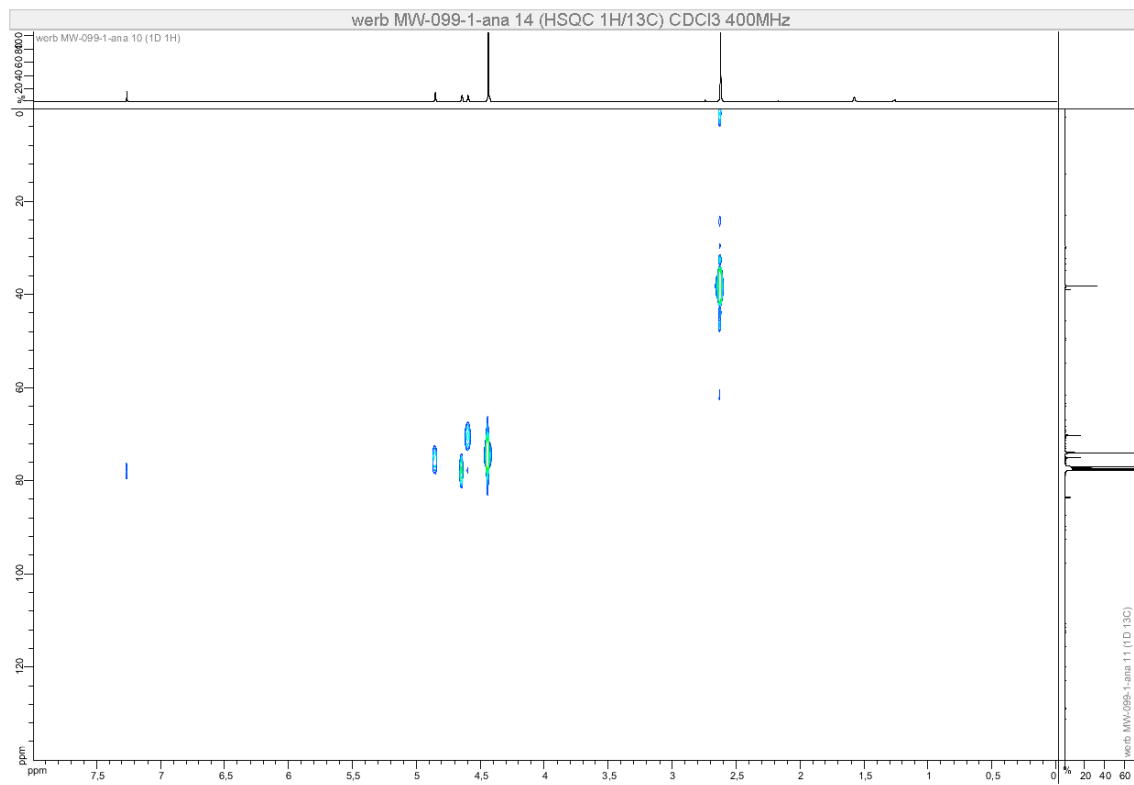


Figure S161. HSQC (400 MHz, CDCl₃) of **8** (racemic mixture)

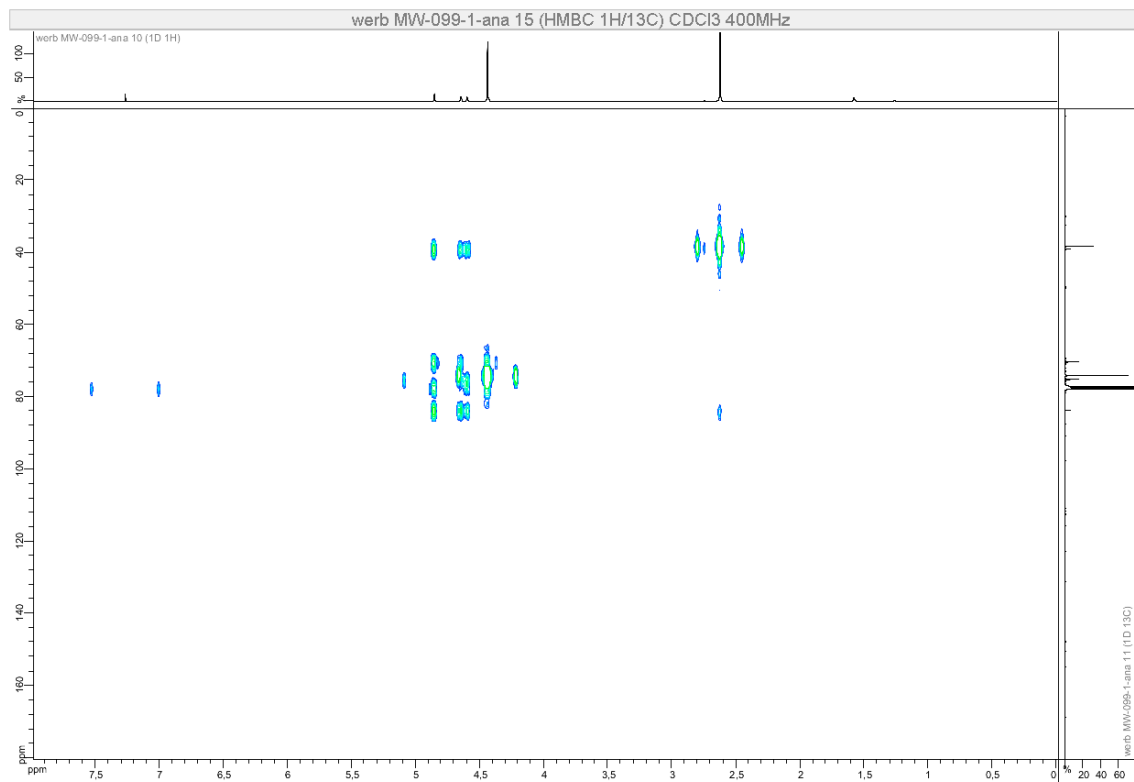
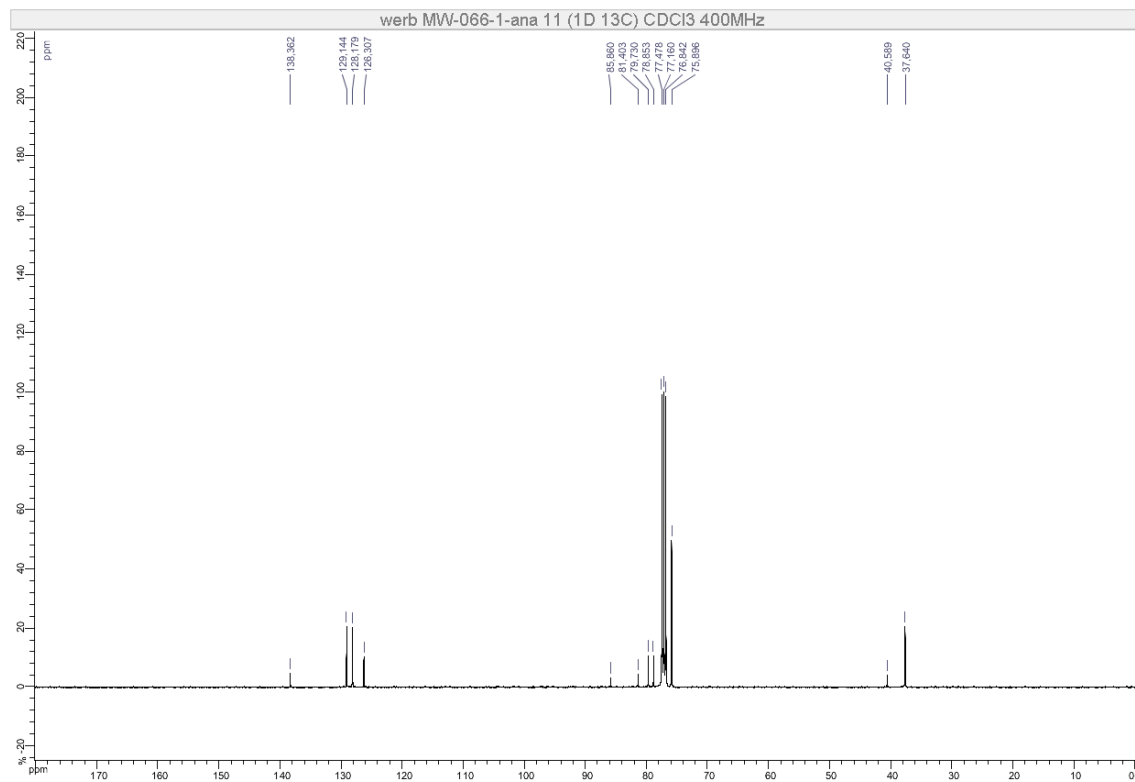
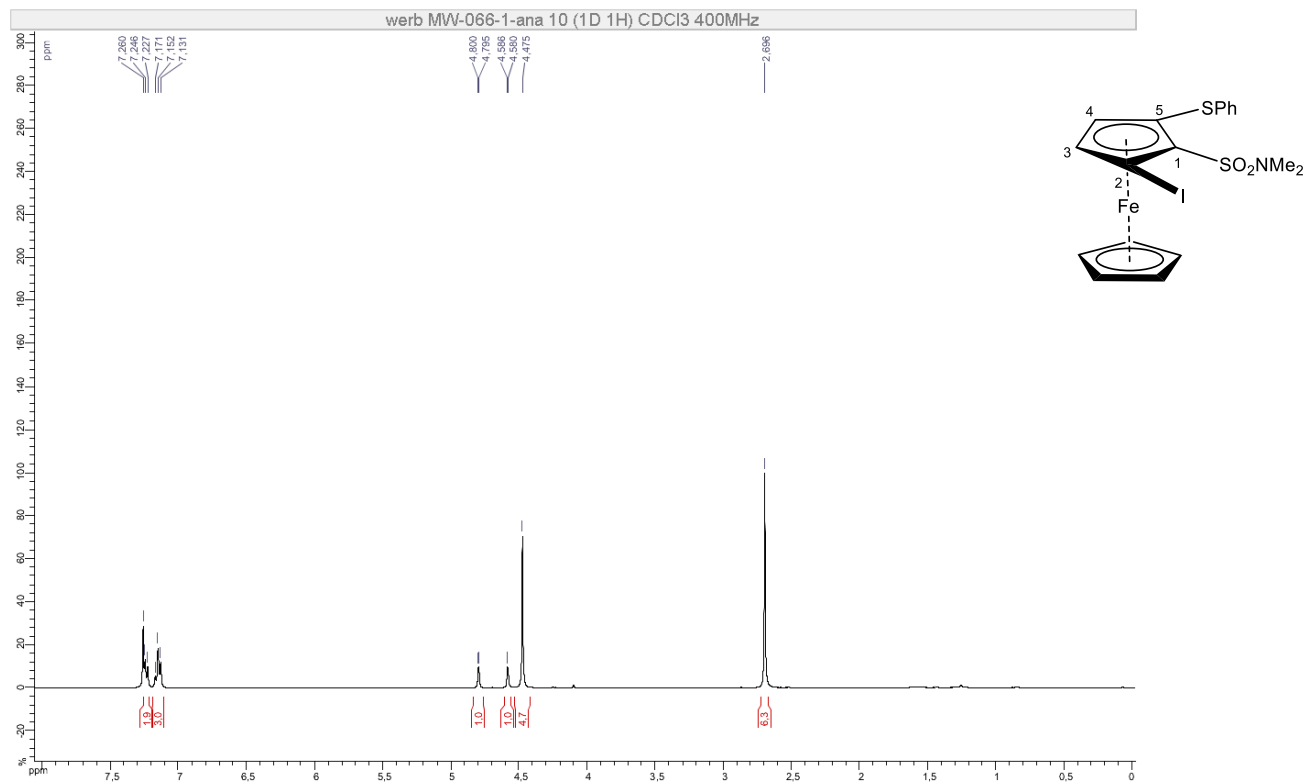


Figure S162. HMBC (400 MHz, CDCl₃) of **8** (racemic mixture)



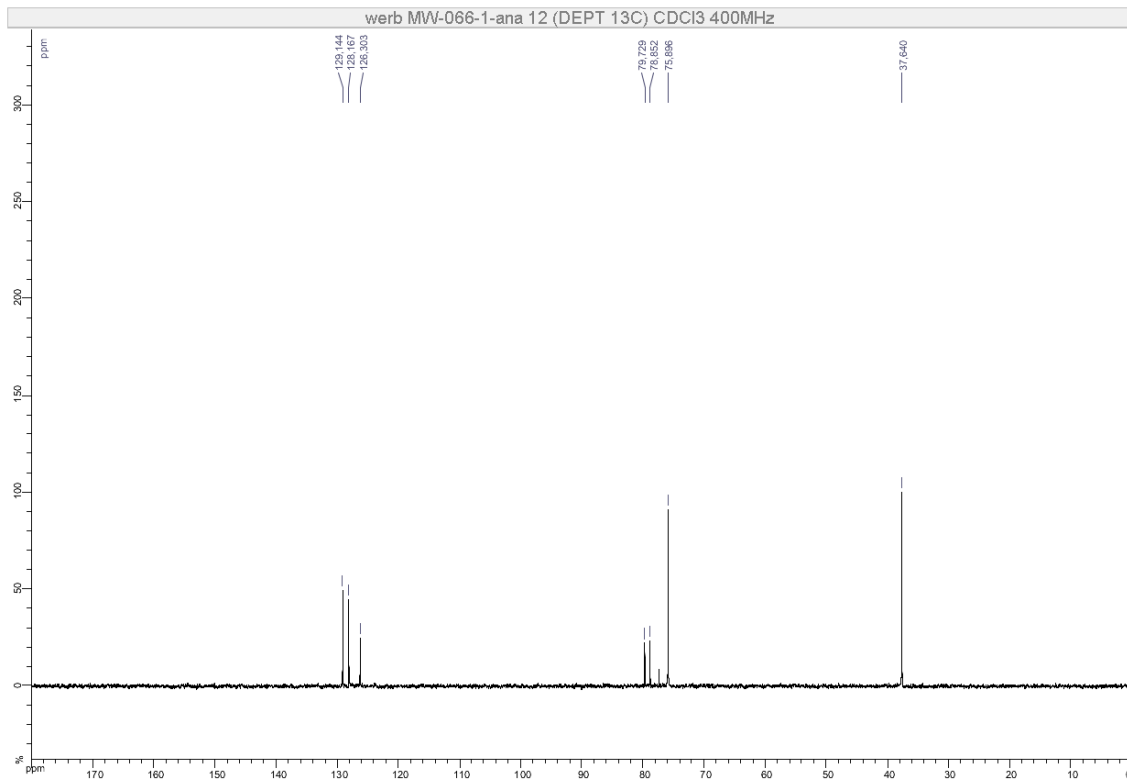


Figure S165. DEPT 135 (101 MHz, CDCl₃) of **9** (racemic mixture)

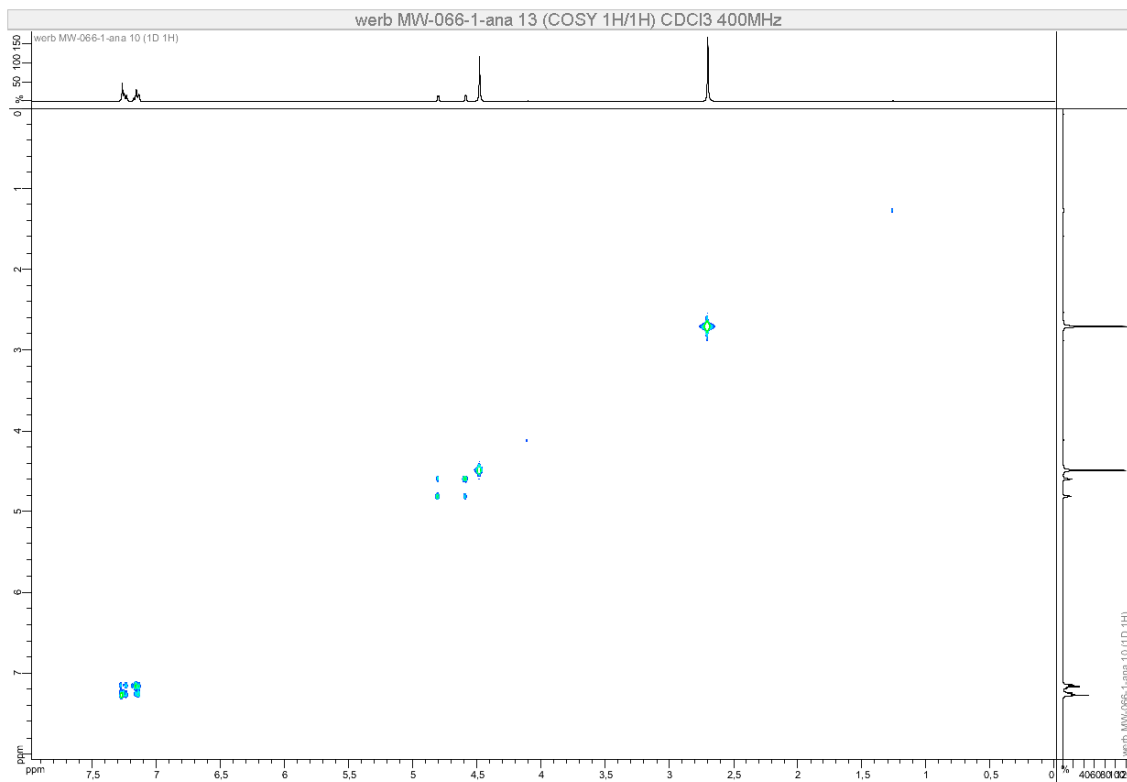


Figure S166. COSY (400 MHz, CDCl₃) of **9** (racemic mixture)

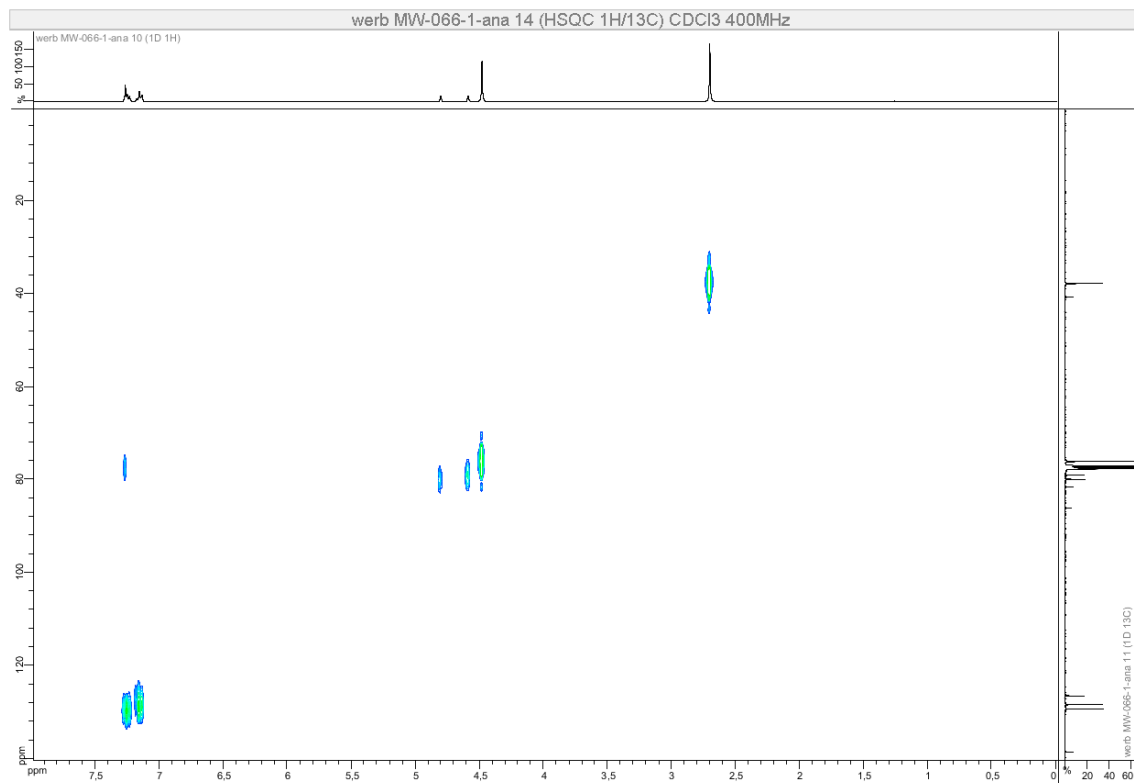


Figure S167. HSQC (400 MHz, CDCl₃) of **9** (racemic mixture)

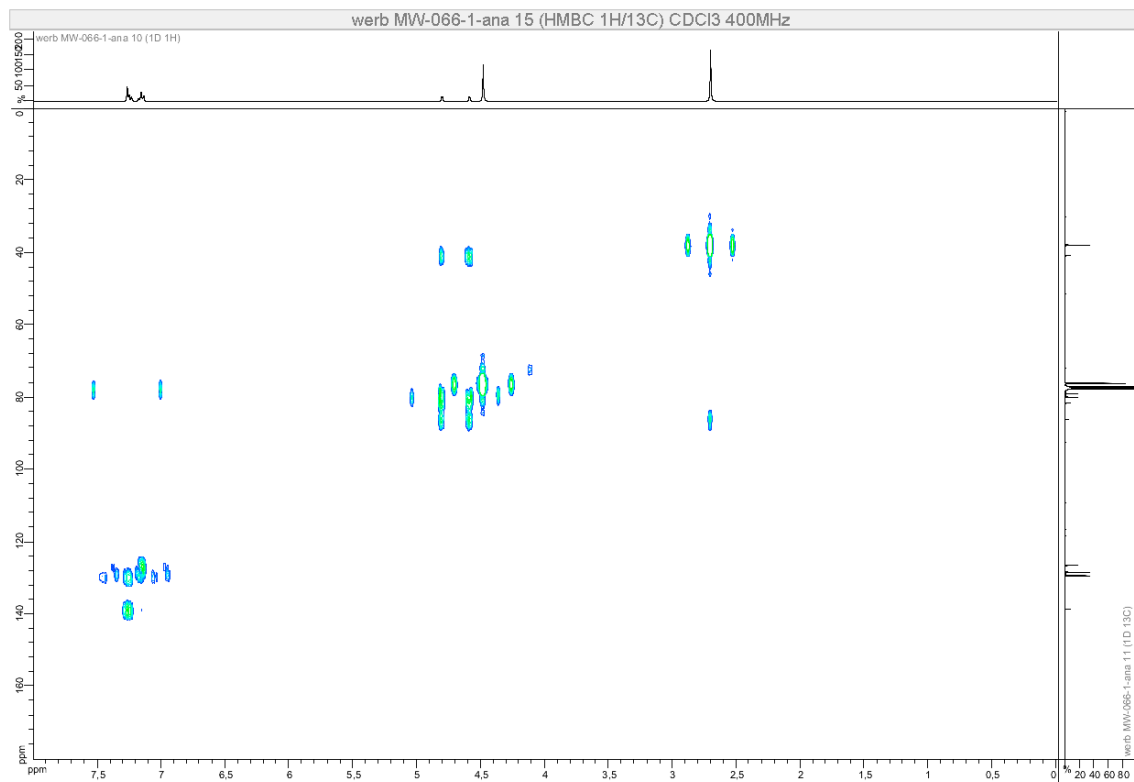


Figure S168. HMBC (400 MHz, CDCl₃) of **9** (racemic mixture)

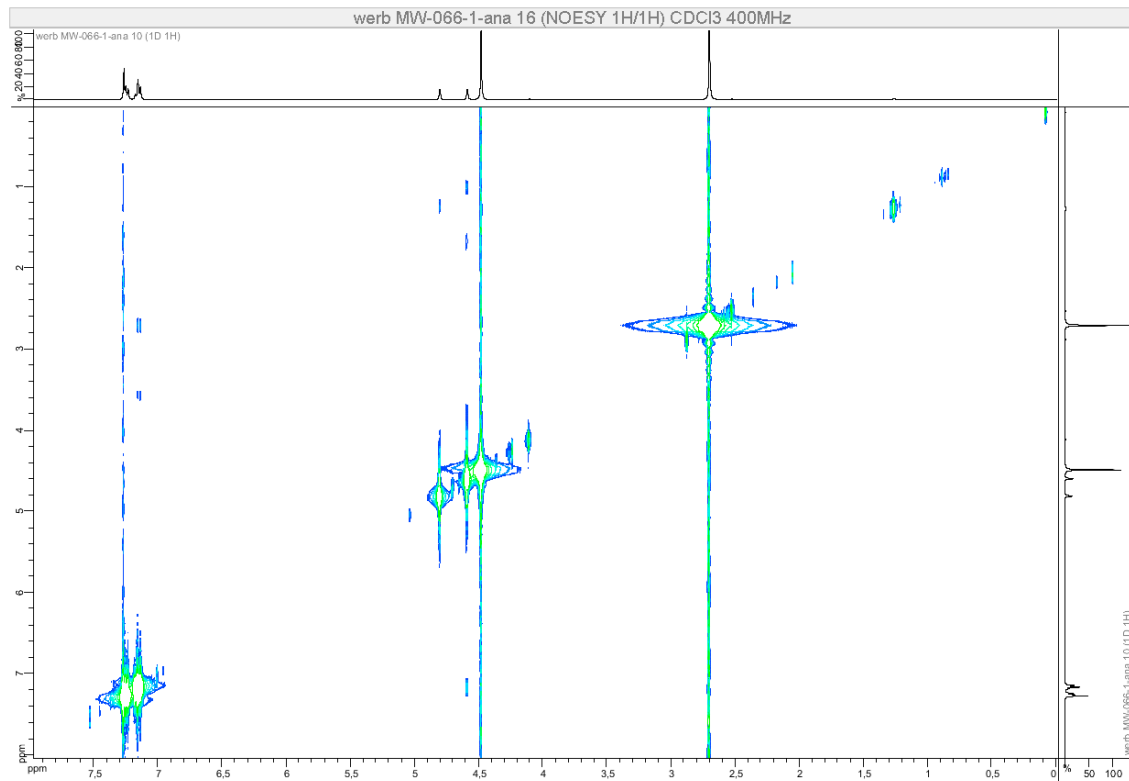


Figure S169. NOESY (400 MHz, CDCl₃) of **9** (racemic mixture)

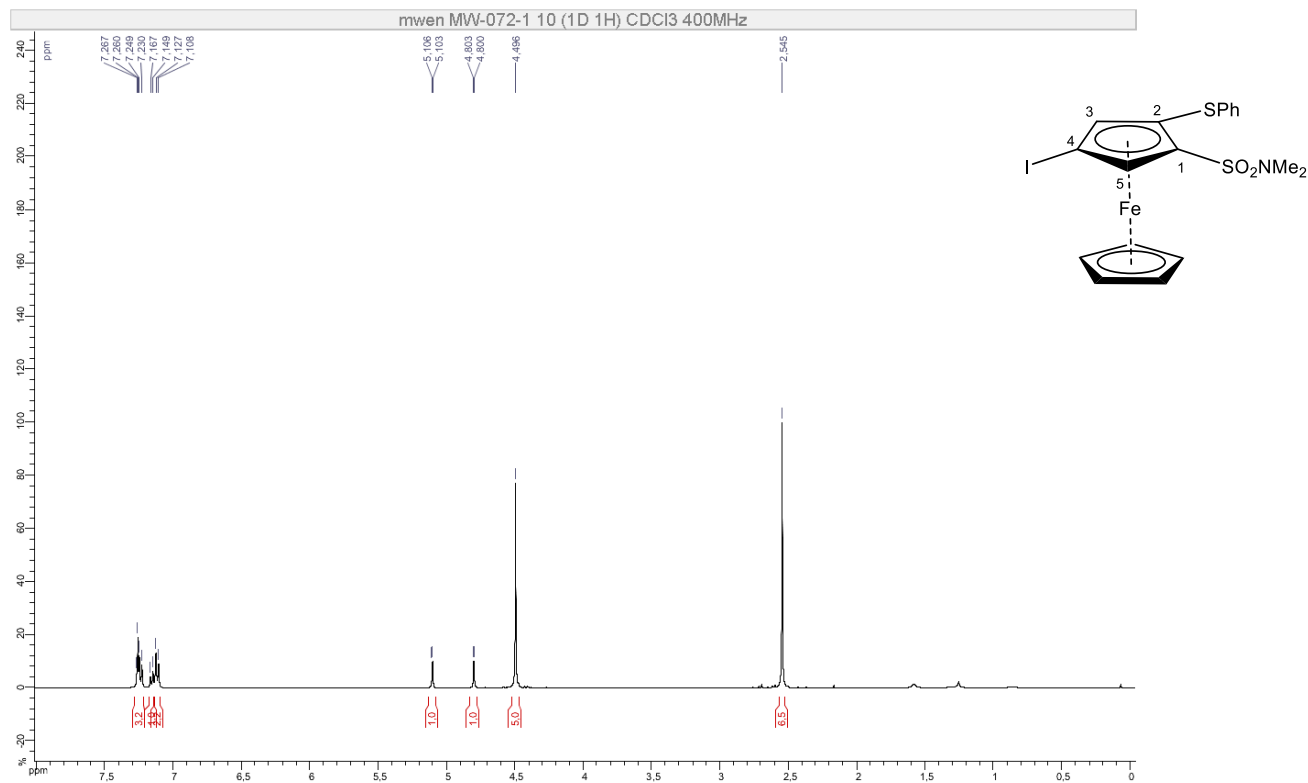


Figure S170. ¹H NMR (400 MHz, CDCl₃) of **10a** (racemic mixture)

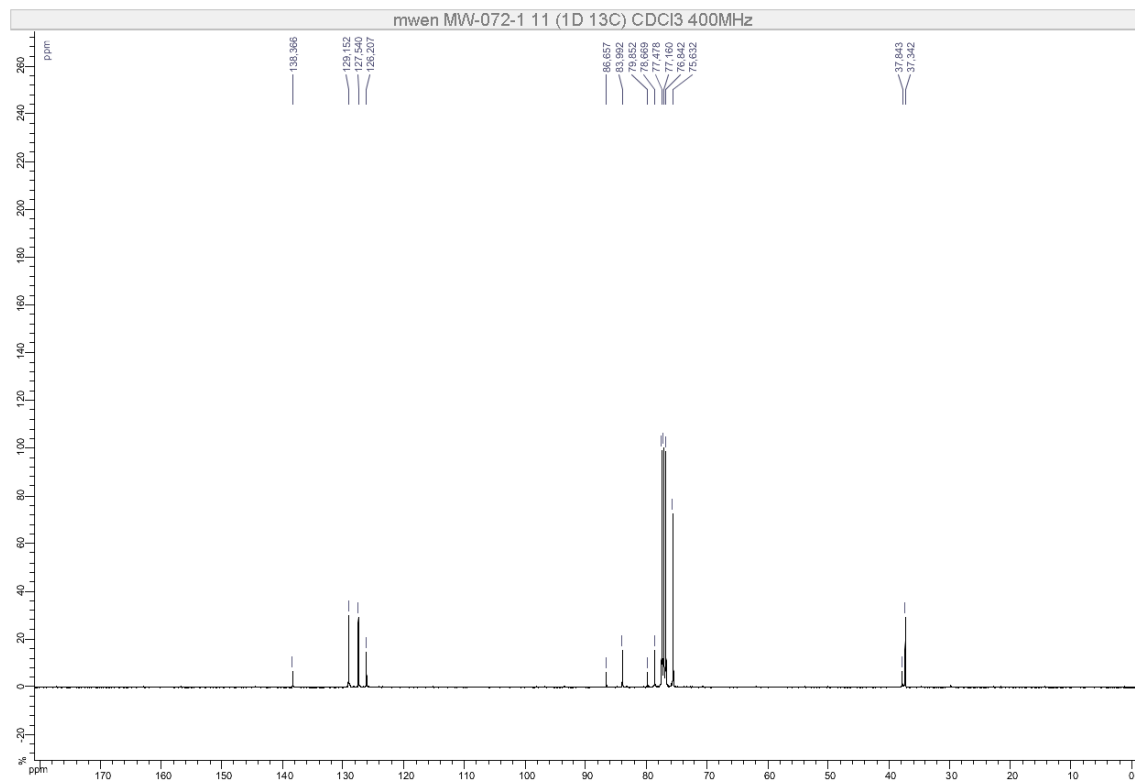


Figure S171. ¹³C NMR (101 MHz, CDCl₃) of **10a** (racemic mixture)

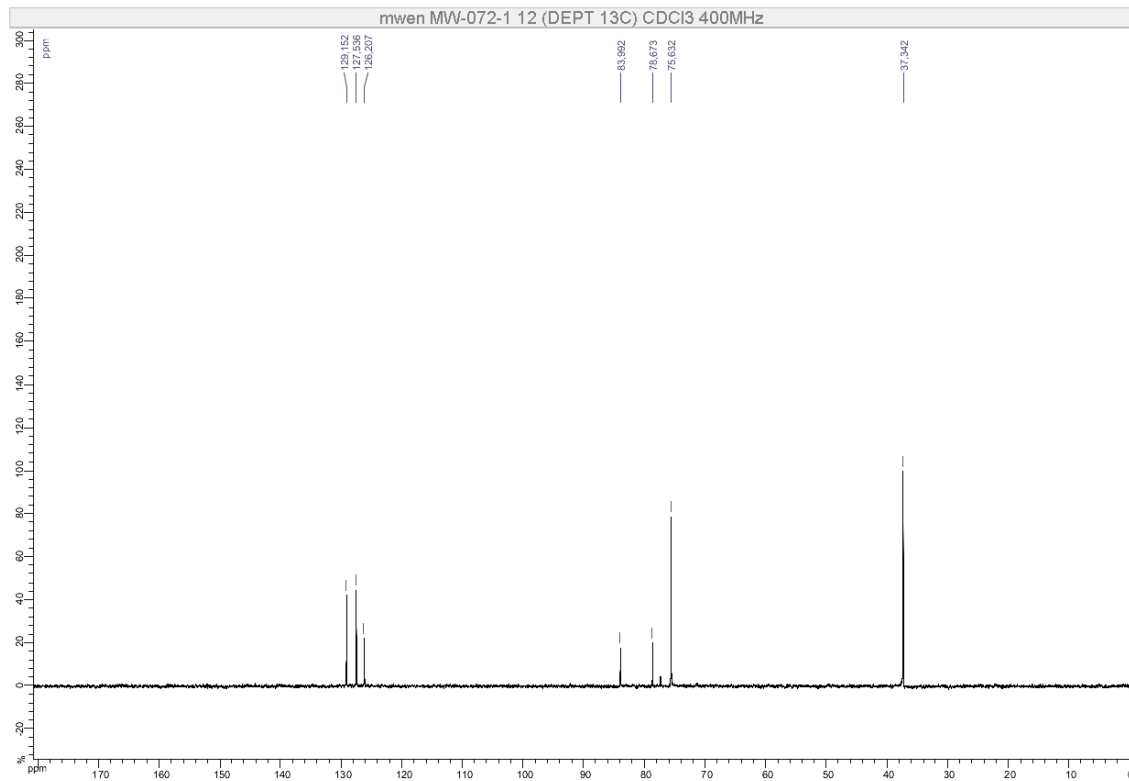


Figure S172. DEPT 135 (101 MHz, CDCl₃) of **10a** (racemic mixture)

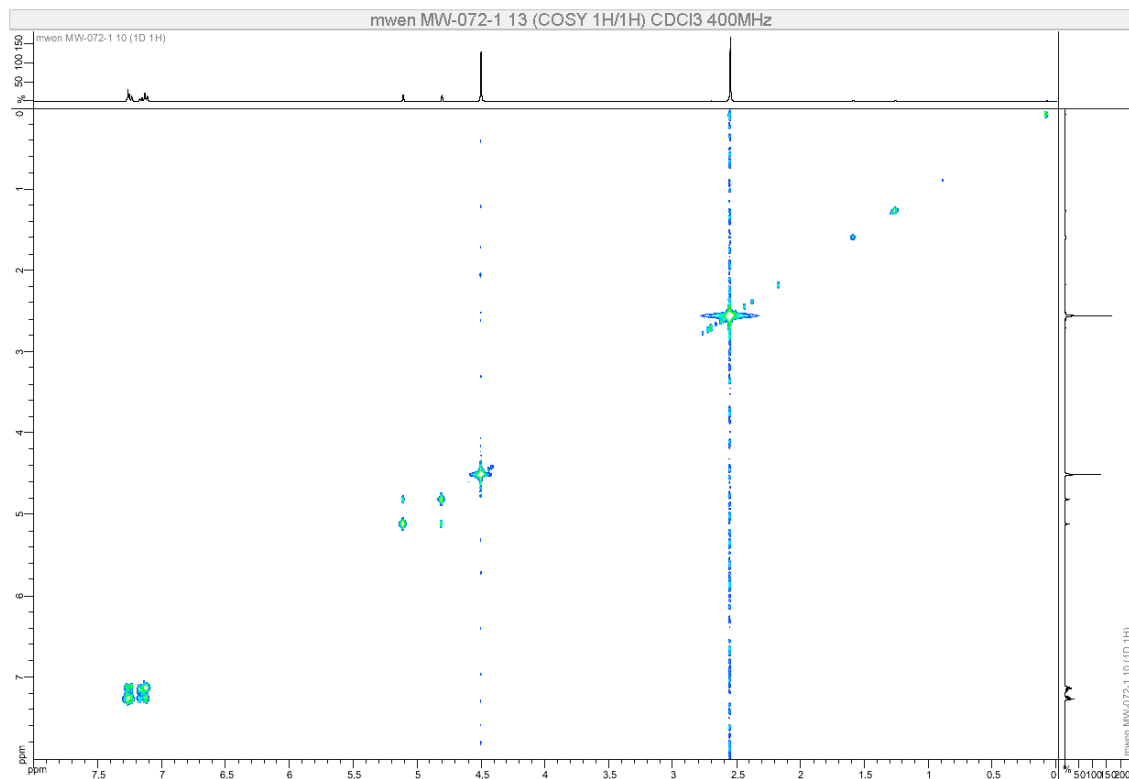


Figure S173. COSY (400 MHz, CDCl₃) of **10a** (racemic mixture)

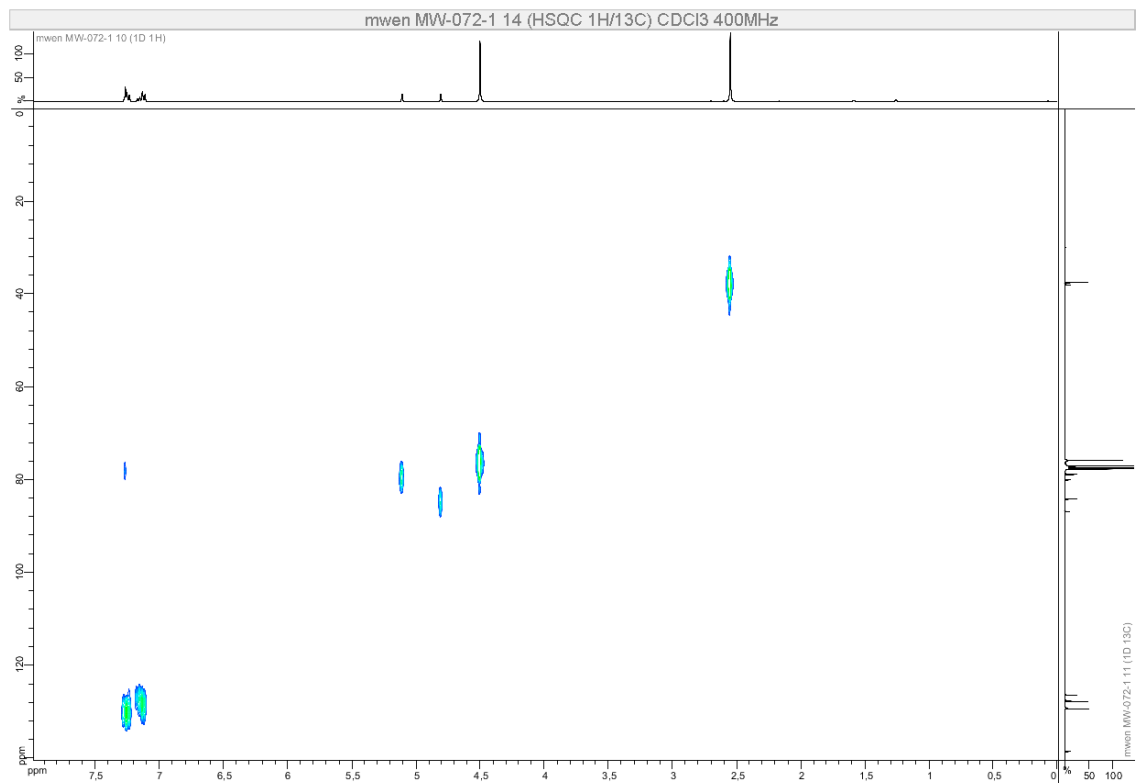


Figure S174. HSQC (400 MHz, CDCl₃) of **10a** (racemic mixture)

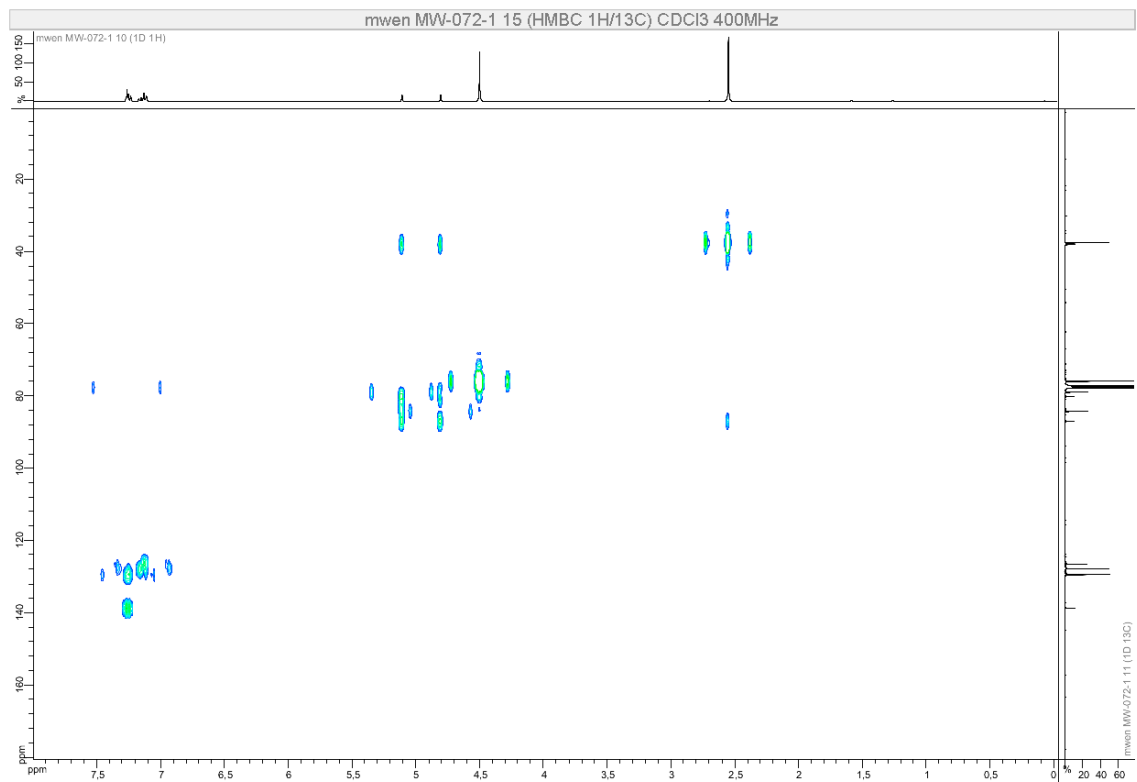


Figure S175. HMBC (400 MHz, CDCl₃) of **10a** (racemic mixture)

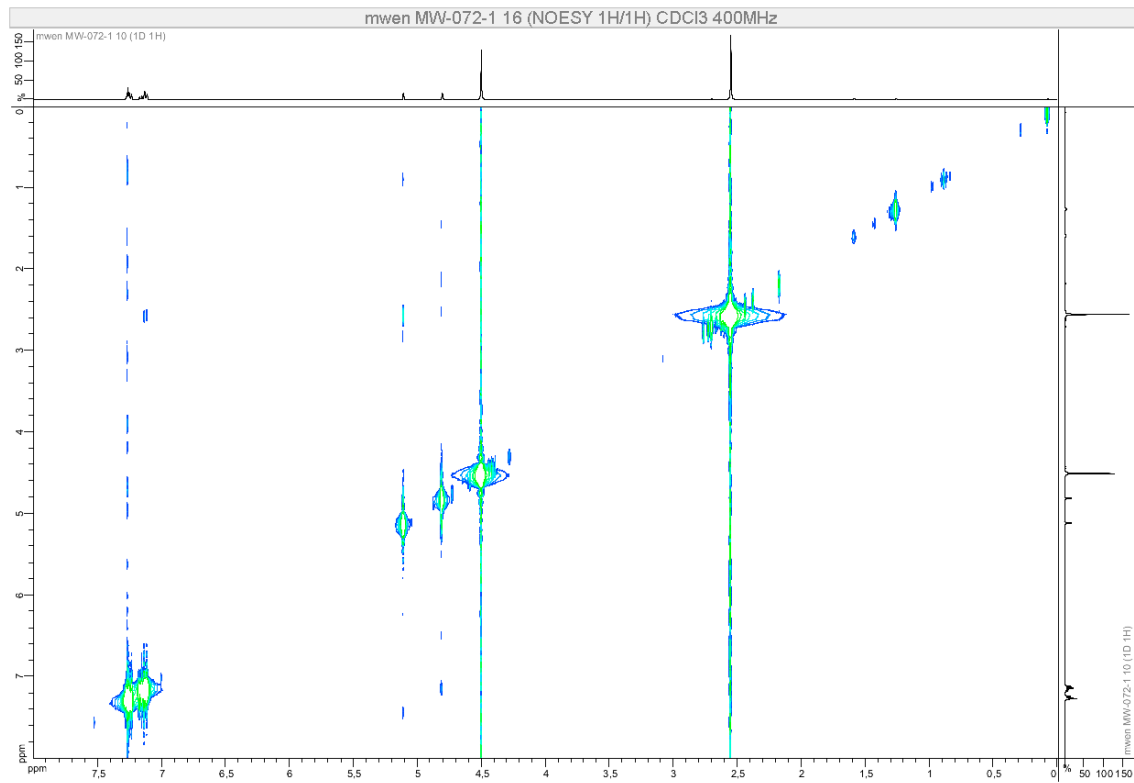
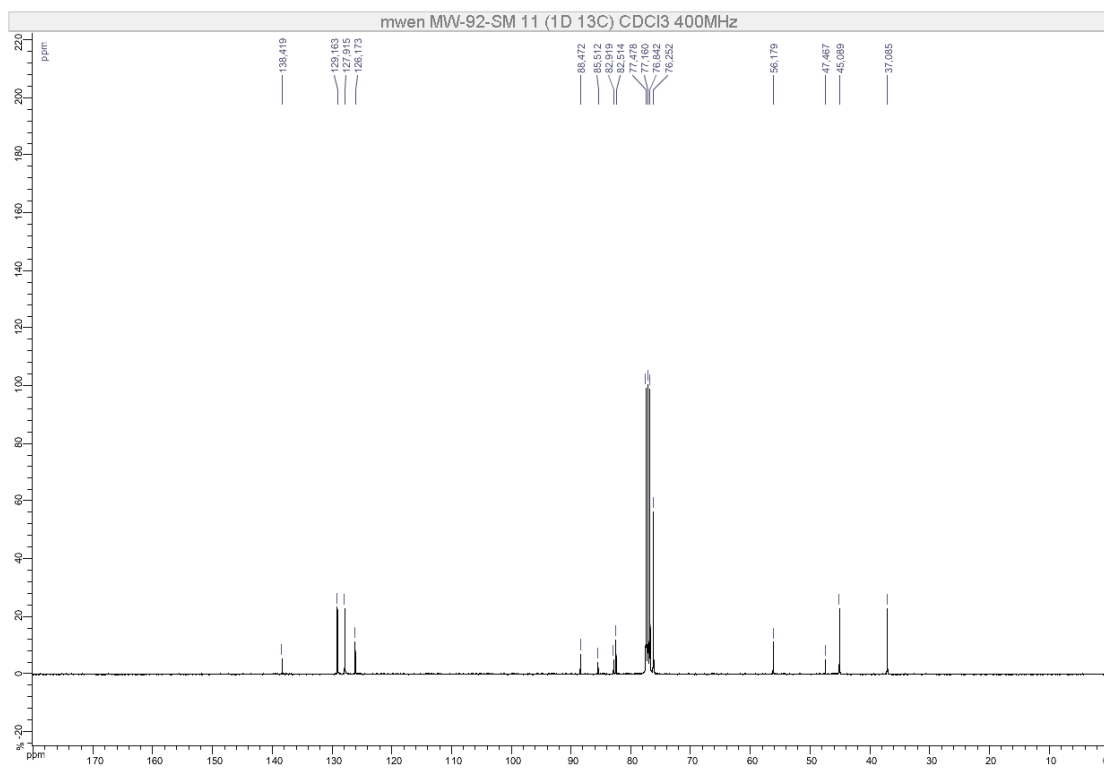
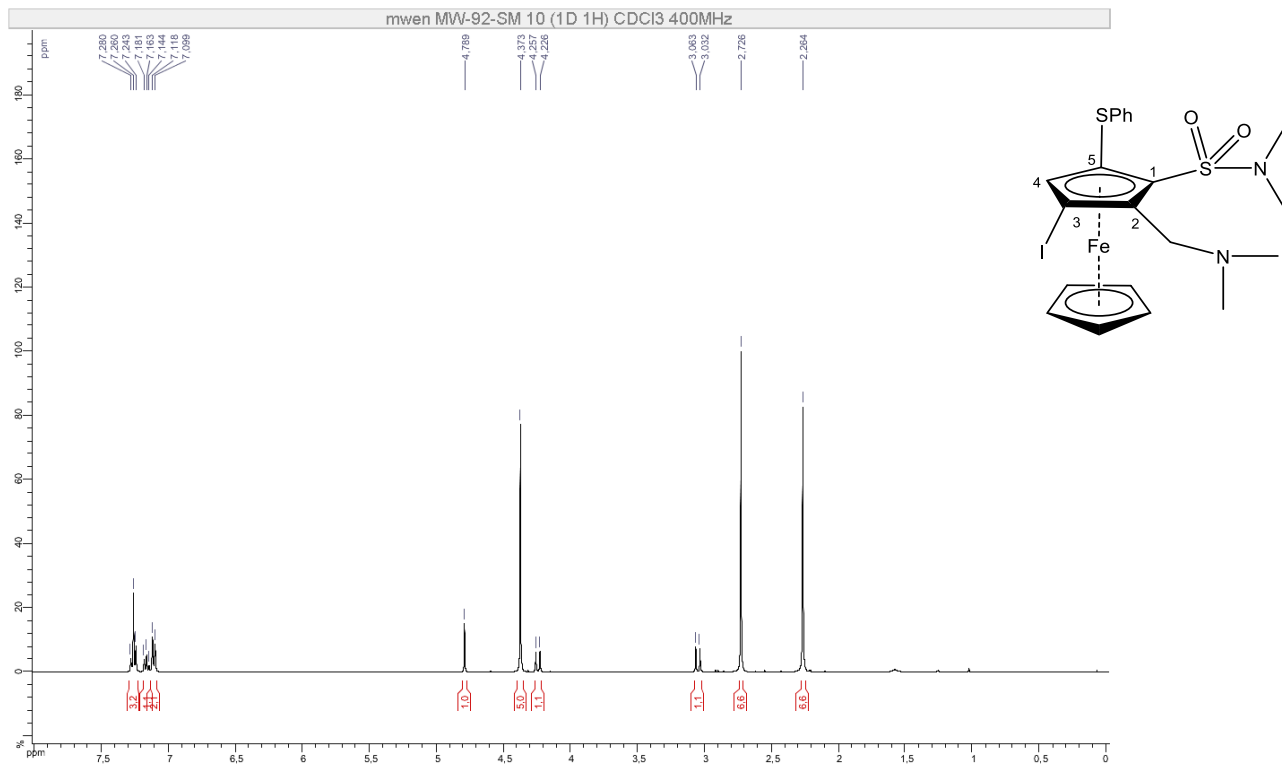


Figure S176. NOESY (400 MHz, CDCl₃) of **10a** (racemic mixture)



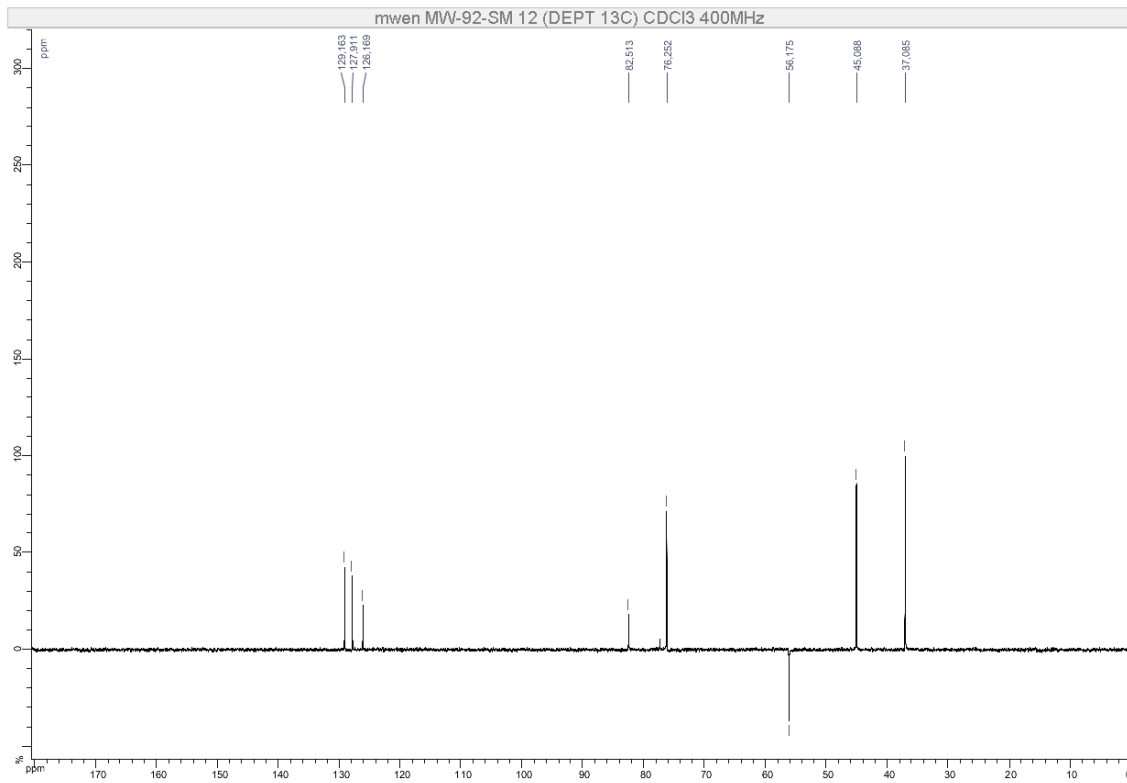


Figure S179. DEPT 135 (101 MHz, CDCl₃) of **10b** (racemic mixture)

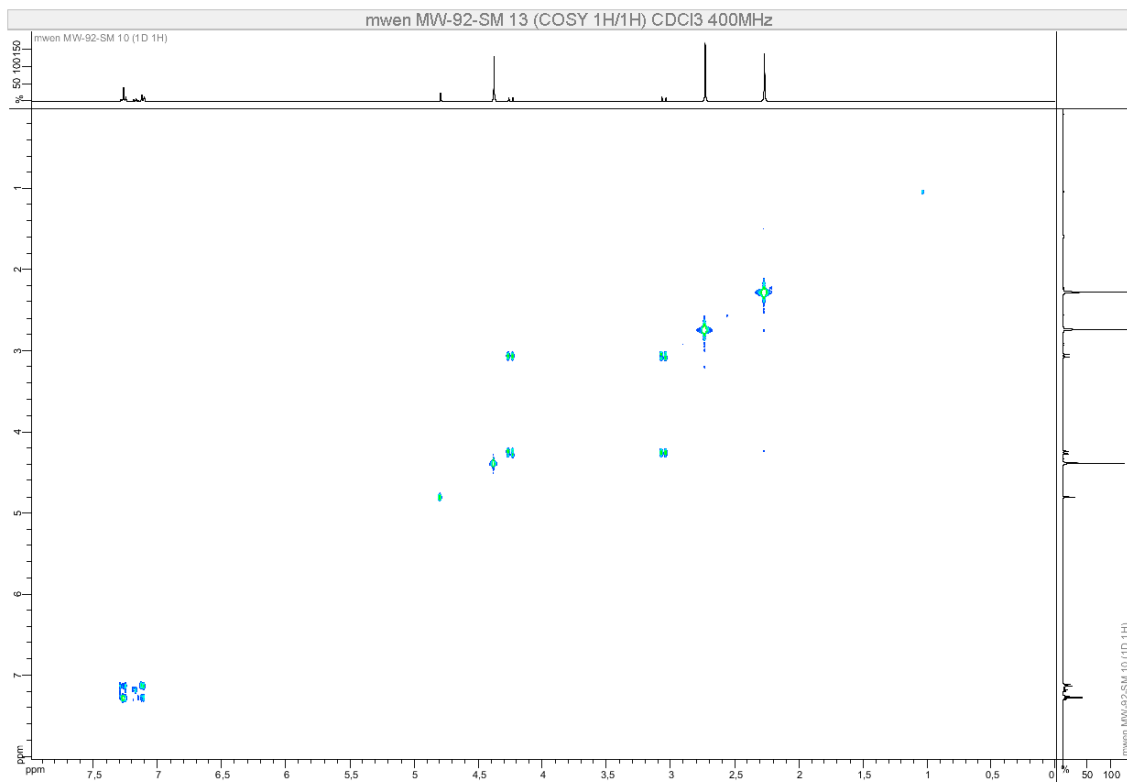


Figure S180. COSY (400 MHz, CDCl₃) of **10b** (racemic mixture)

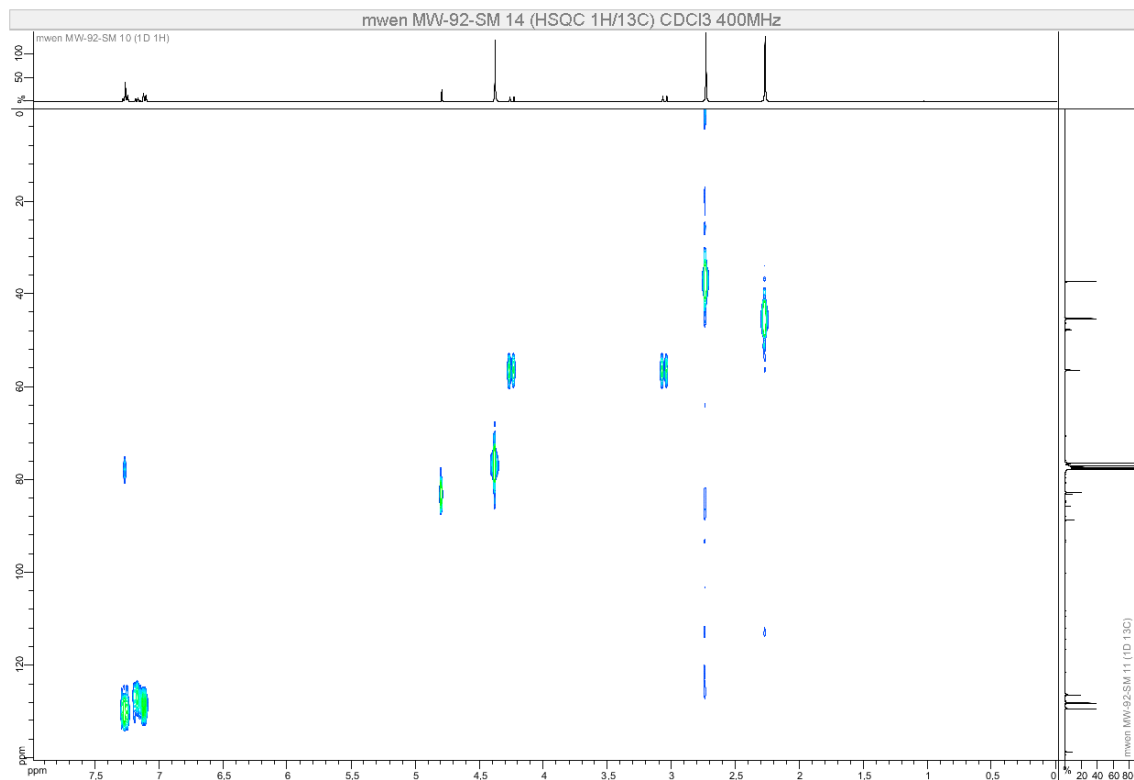


Figure S181. HSQC (400 MHz, CDCl₃) of **10b** (racemic mixture)

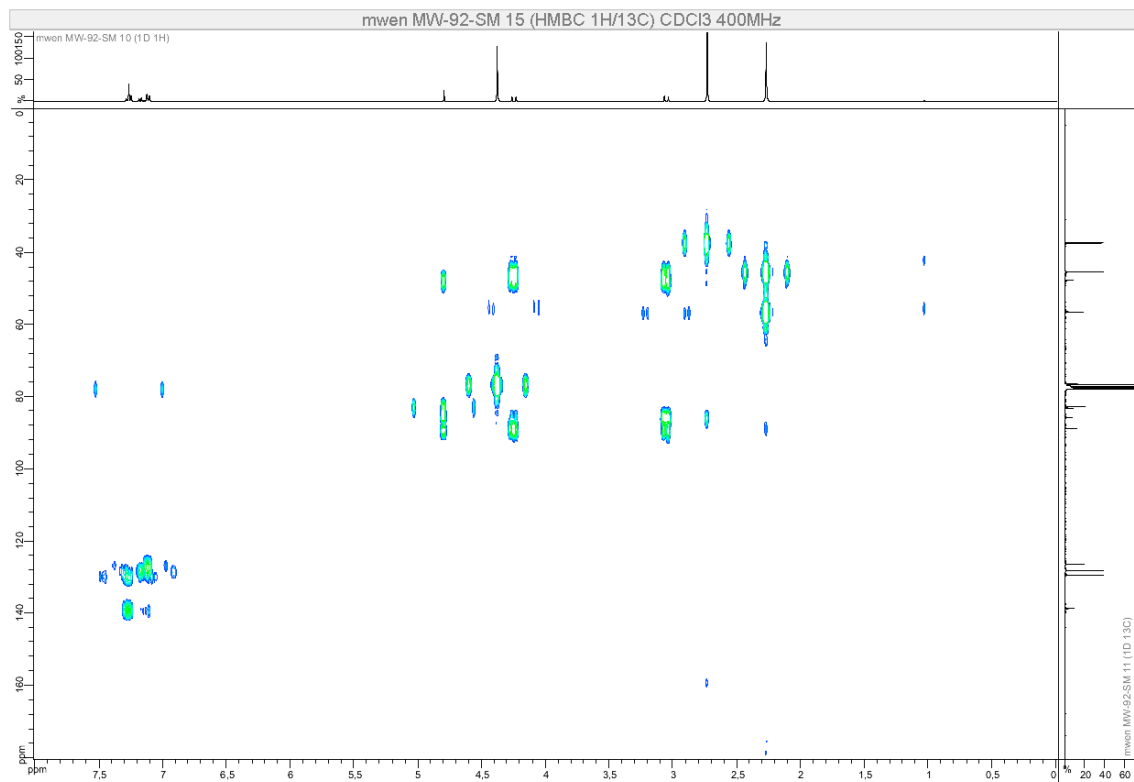


Figure S182. HMBC (400 MHz, CDCl₃) of **10b** (racemic mixture)

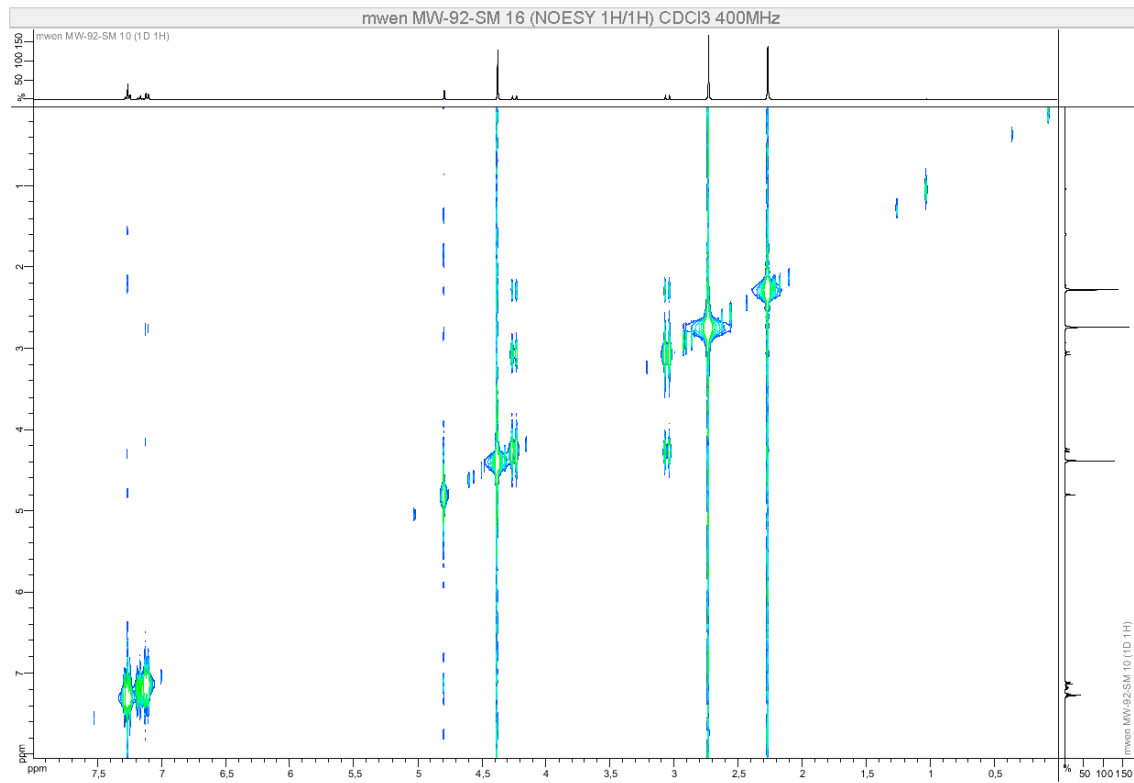
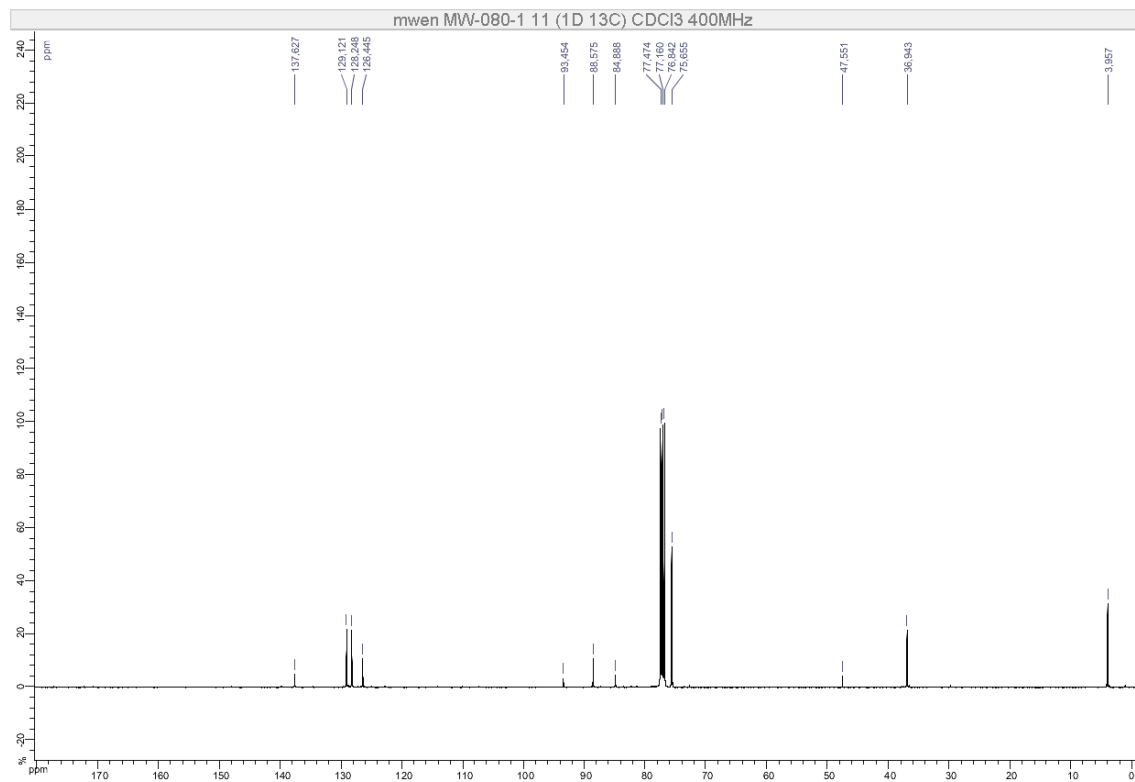
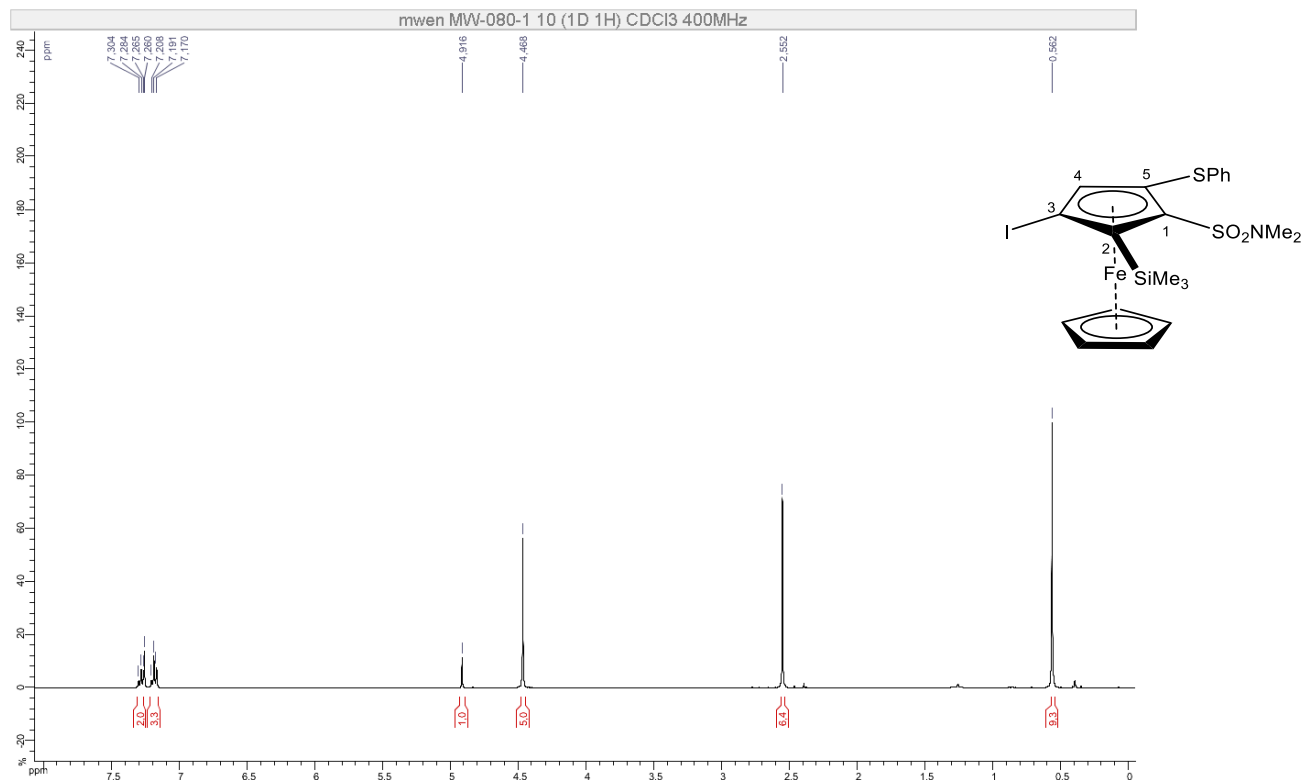


Figure S183. NOESY (400 MHz, CDCl₃) of **10b** (racemic mixture)



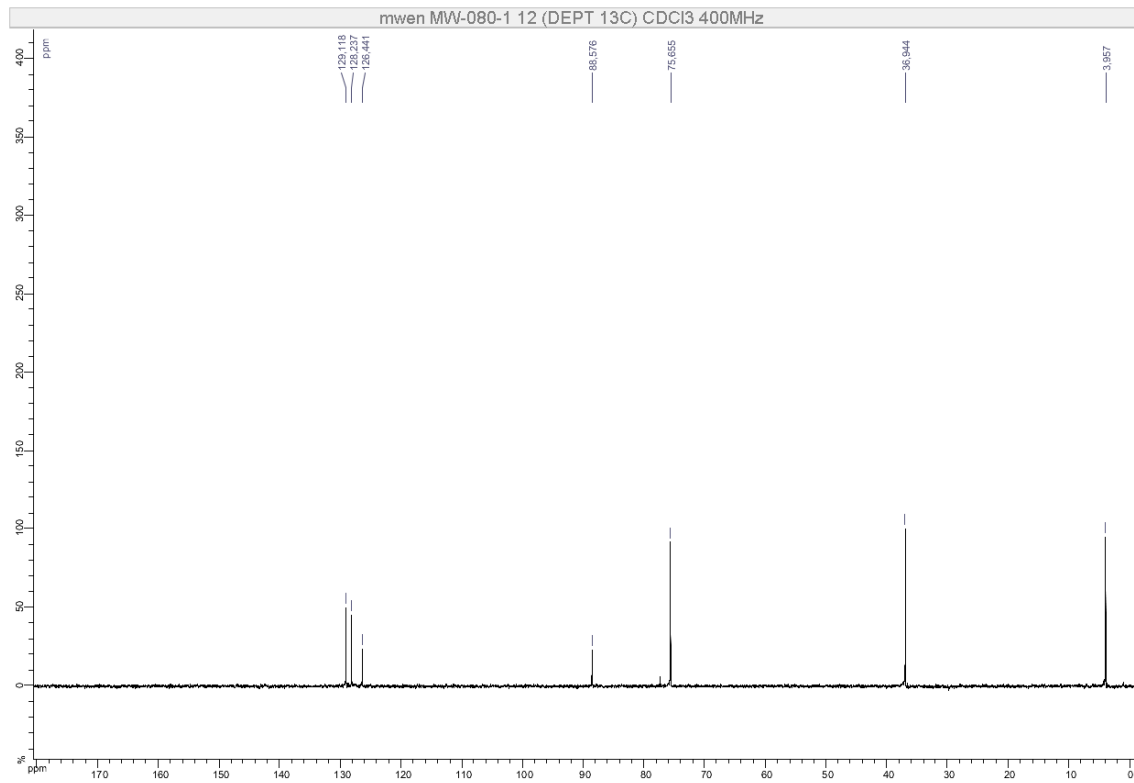


Figure S186. DEPT 135 (101 MHz, CDCl₃) of **10c** (racemic mixture)

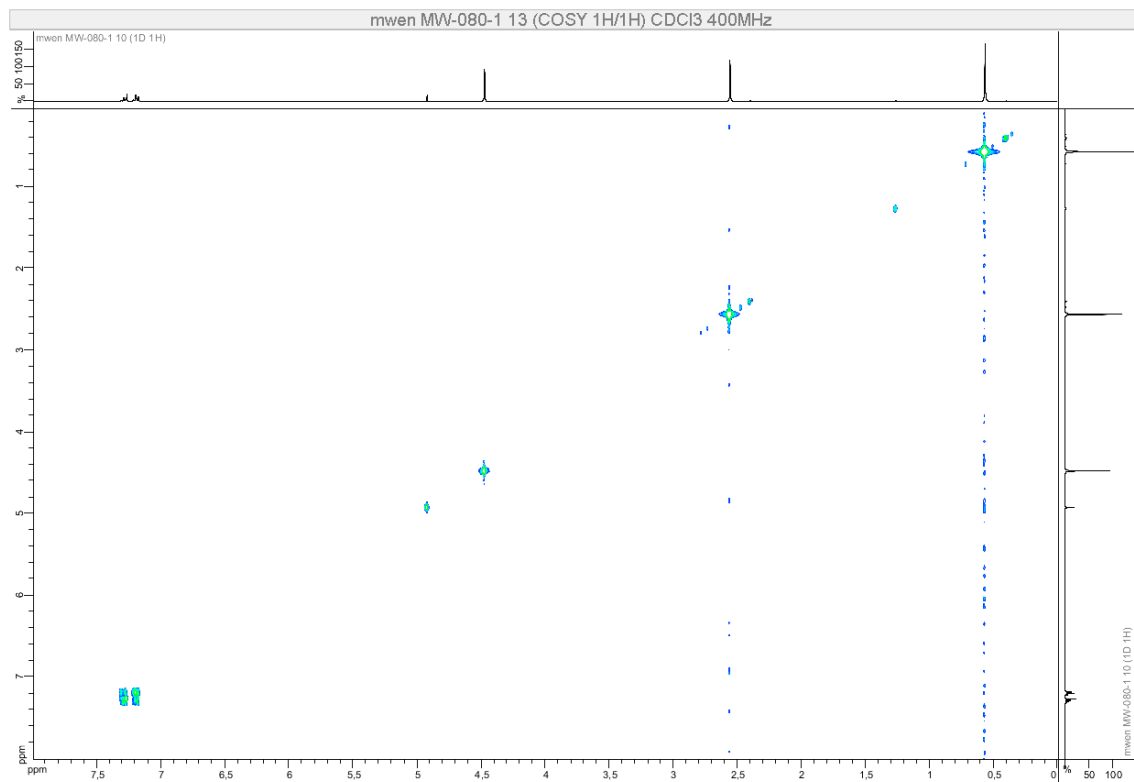


Figure S187. COSY (400 MHz, CDCl₃) of **10c** (racemic mixture)

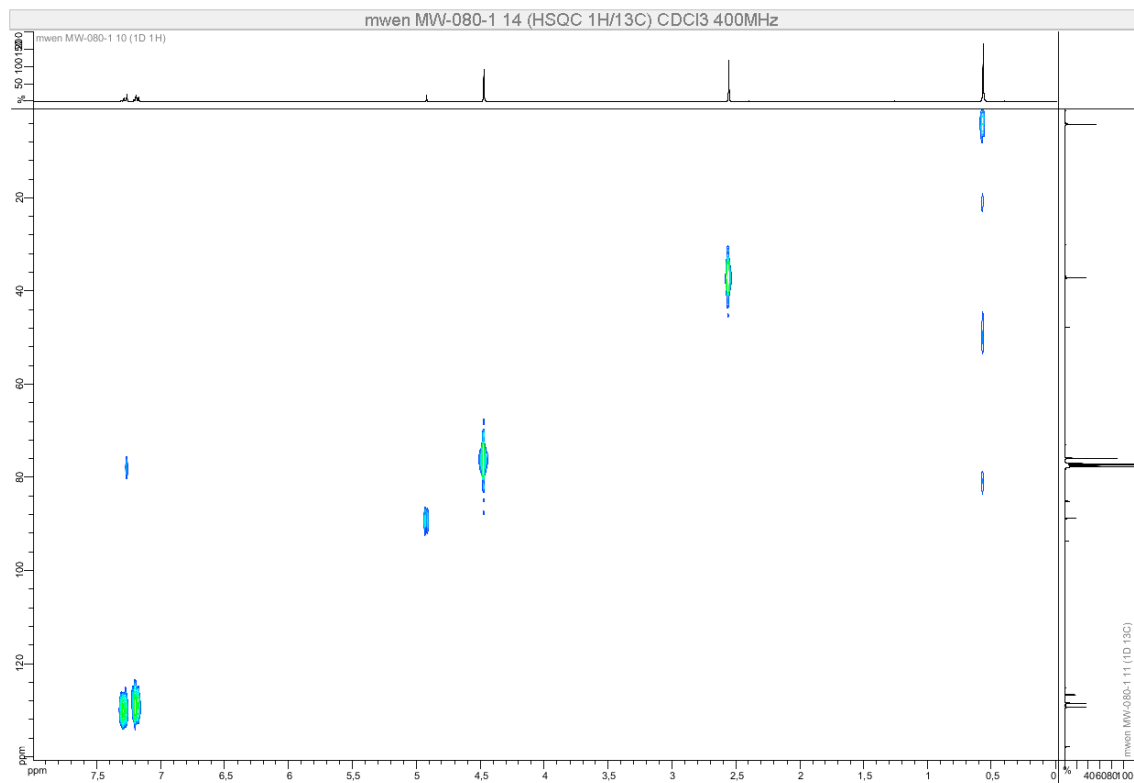


Figure S188. HSQC (400 MHz, CDCl₃) of **10c** (racemic mixture)

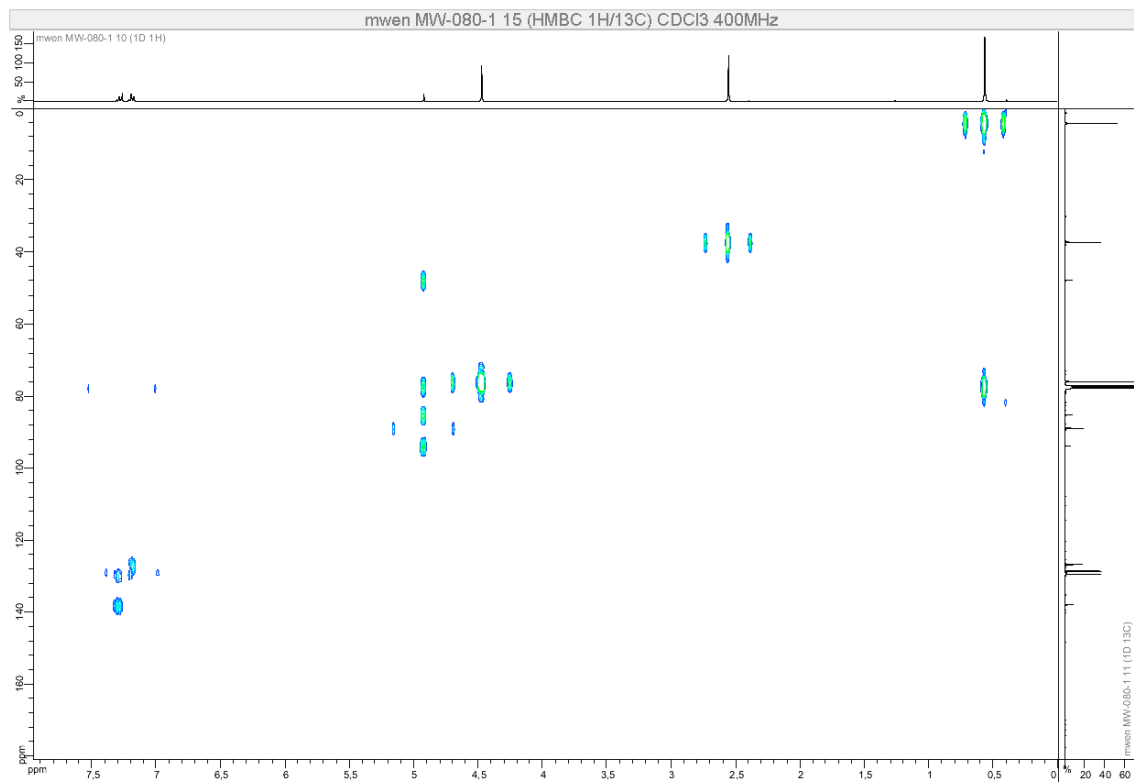


Figure S189. HMBC (400 MHz, CDCl₃) of **10c** (racemic mixture)

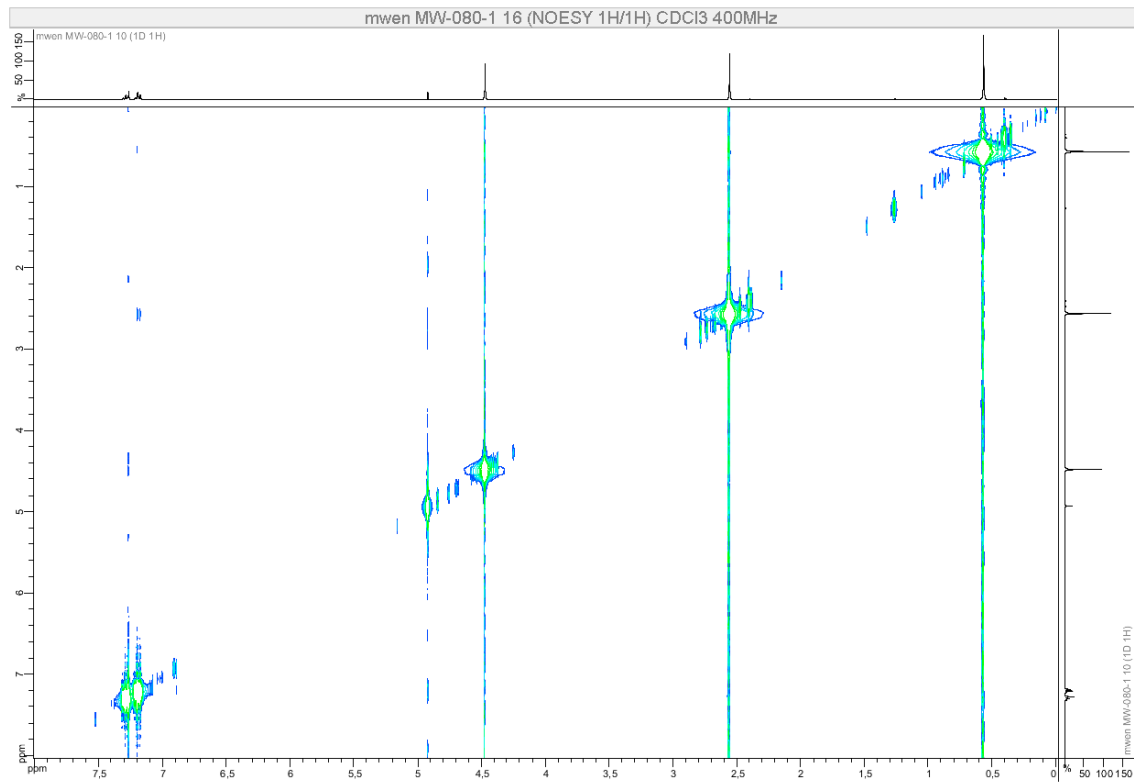


Figure S190. NOESY (400 MHz, CDCl_3) of **10c** (racemic mixture)

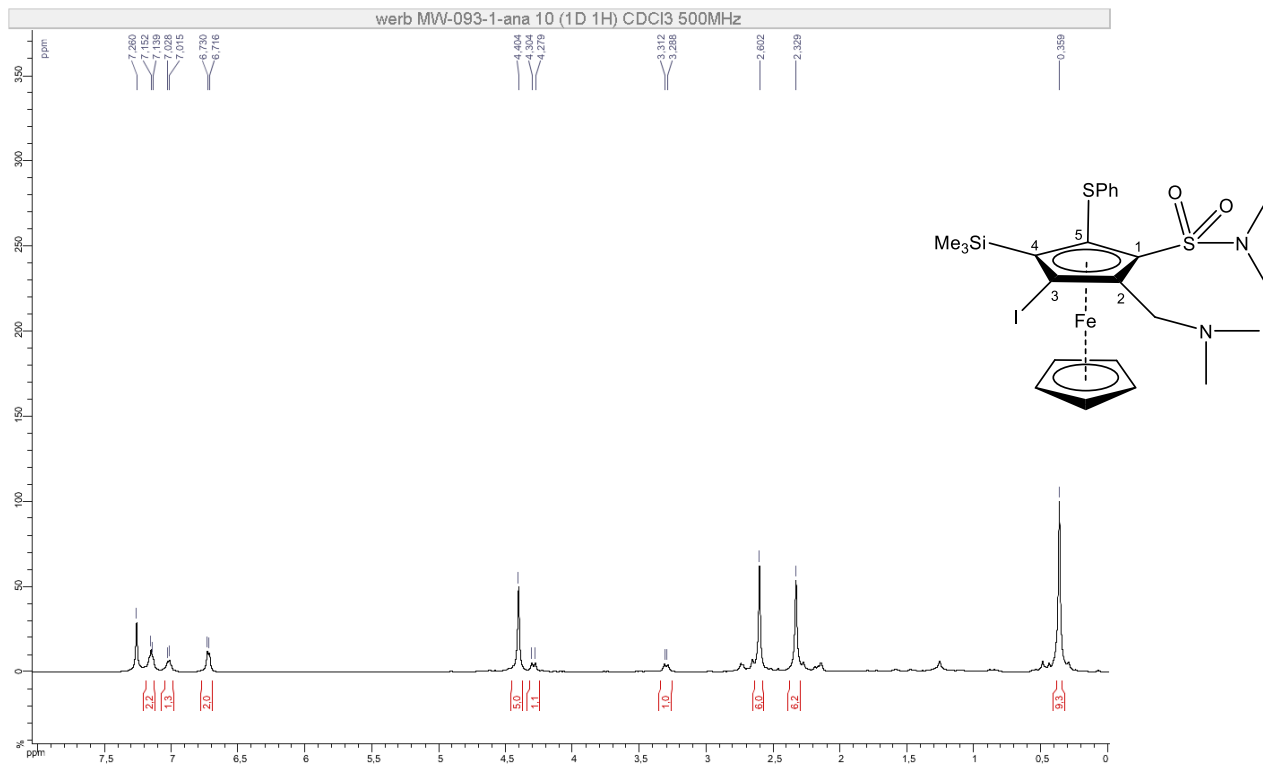


Figure S191. ¹H NMR (500 MHz, CDCl₃) of **11** (racemic mixture)

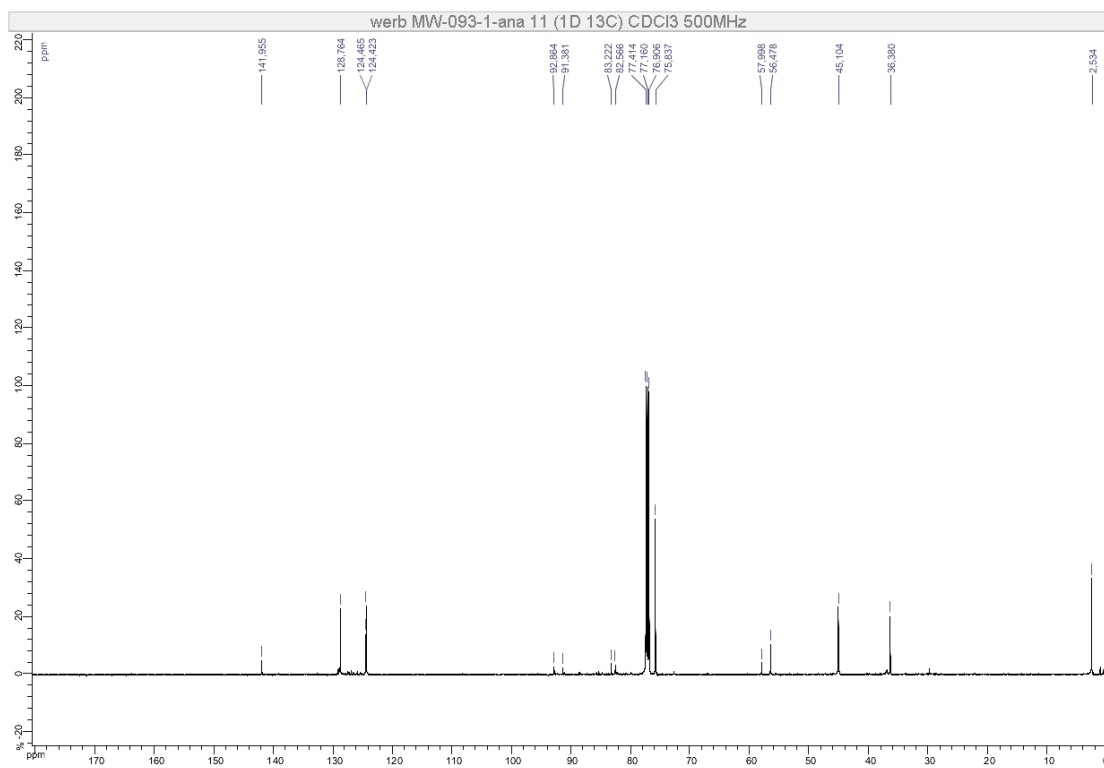


Figure S192. ¹³C NMR (126 MHz, CDCl₃) of **11** (racemic mixture)

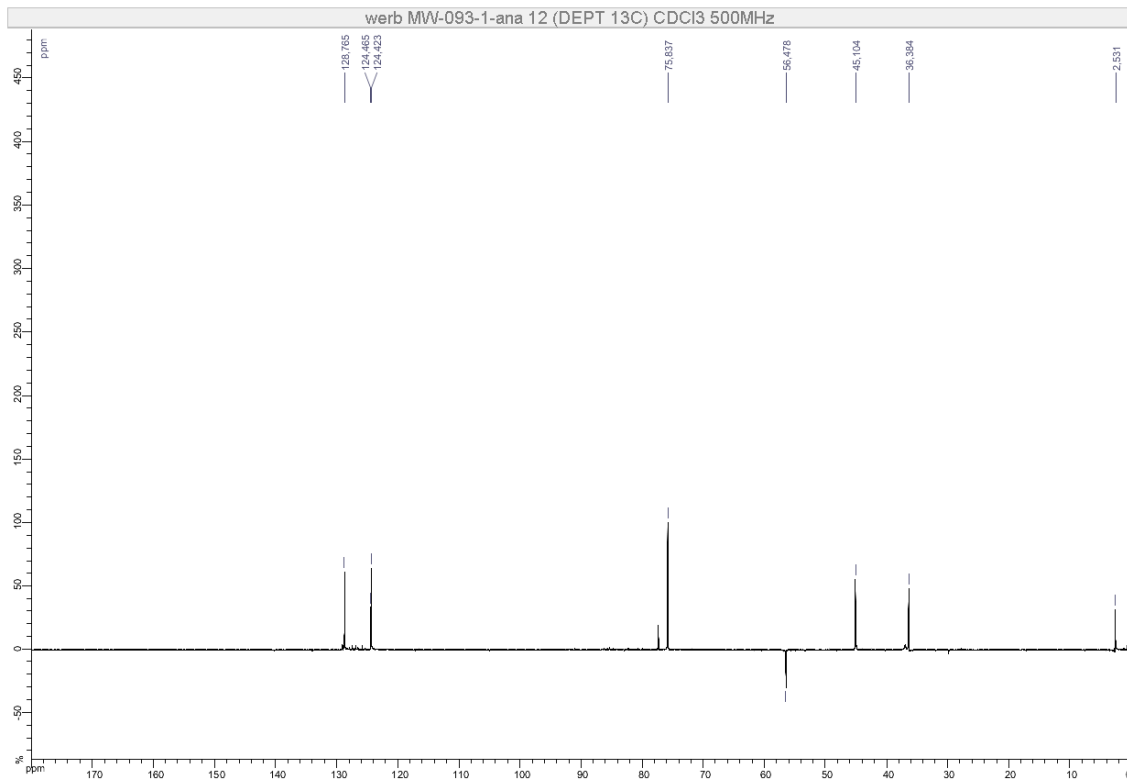


Figure S193. DEPT 135 (126 MHz, CDCl₃) of **11** (racemic mixture)

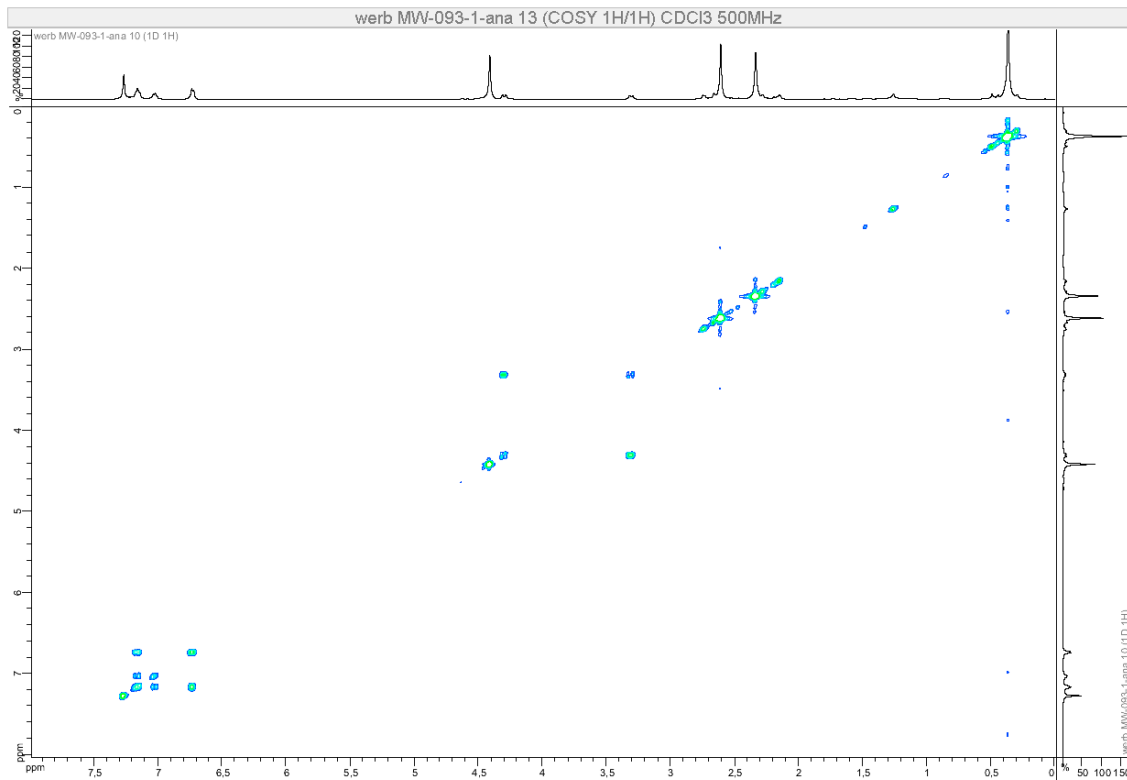


Figure S194. COSY (500 MHz, CDCl₃) of **11** (racemic mixture)

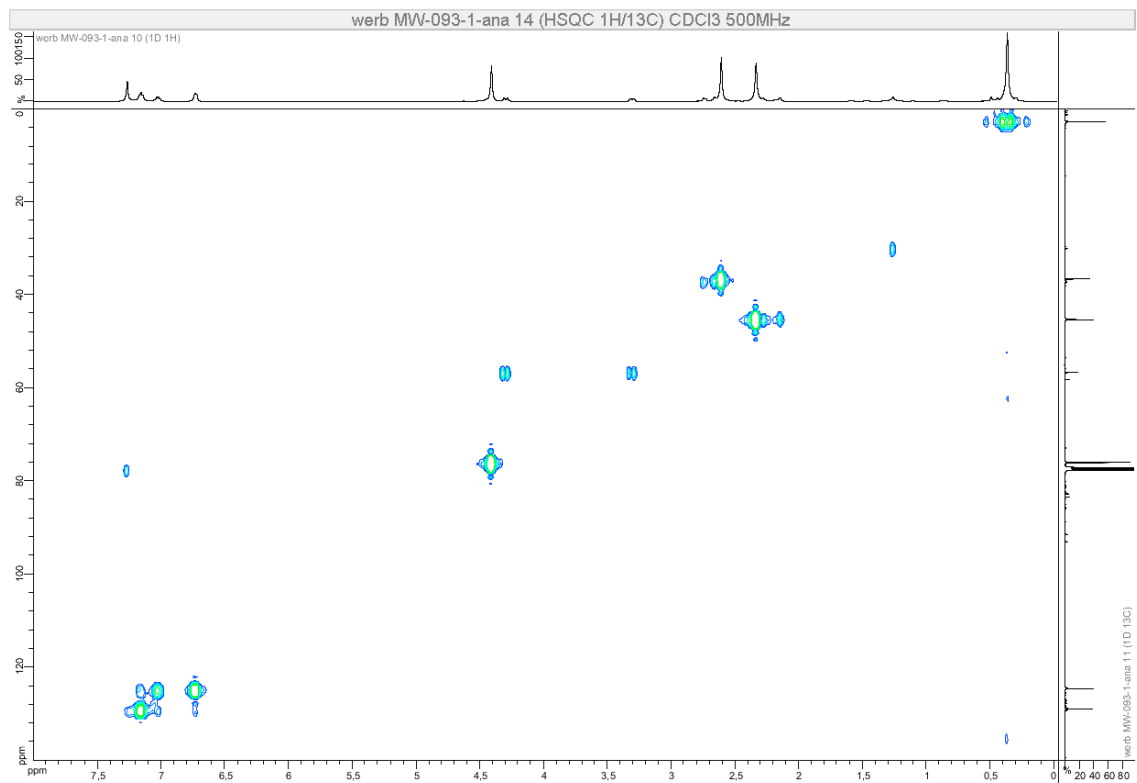


Figure S195. HSQC (500 MHz, CDCl₃) of **11** (racemic mixture)

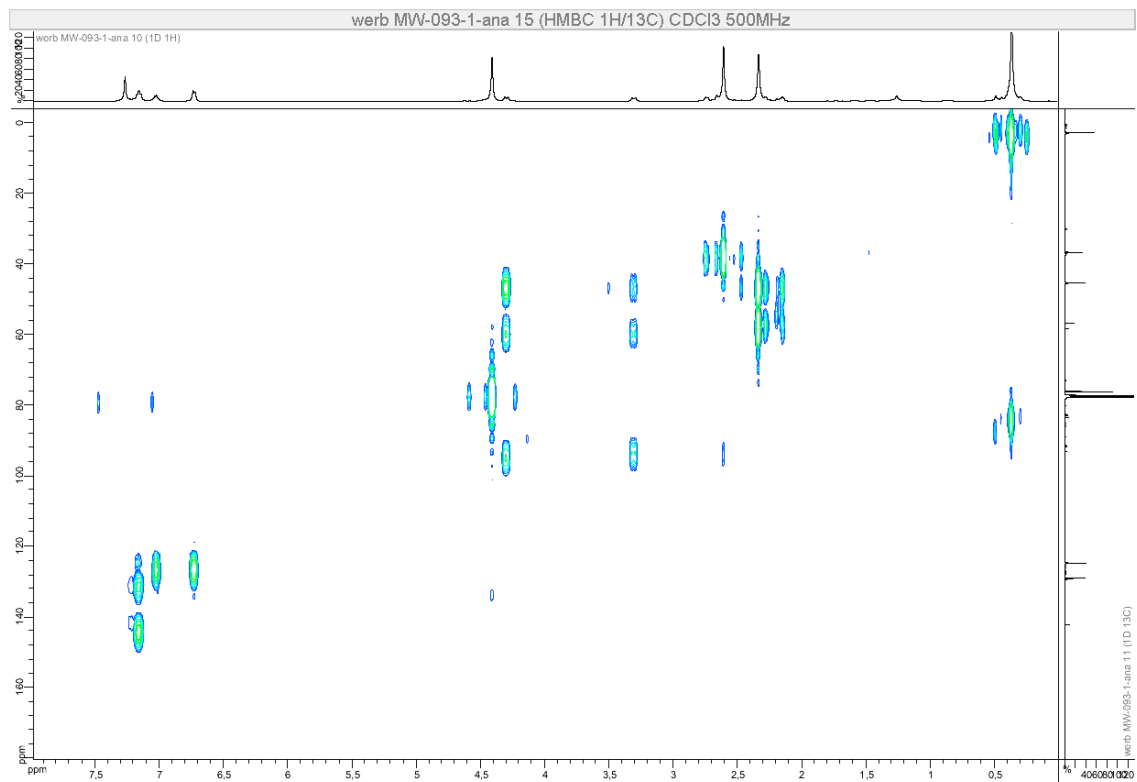


Figure S196. HMBC (500 MHz, CDCl₃) of **11** (racemic mixture)

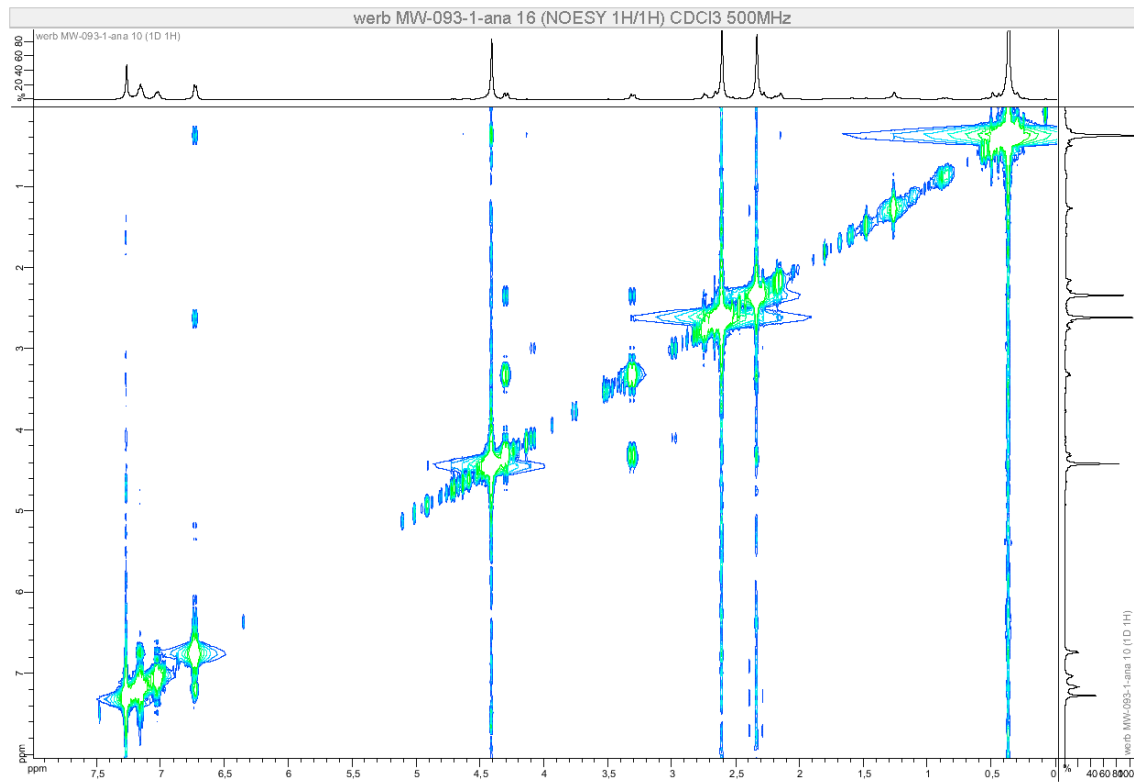
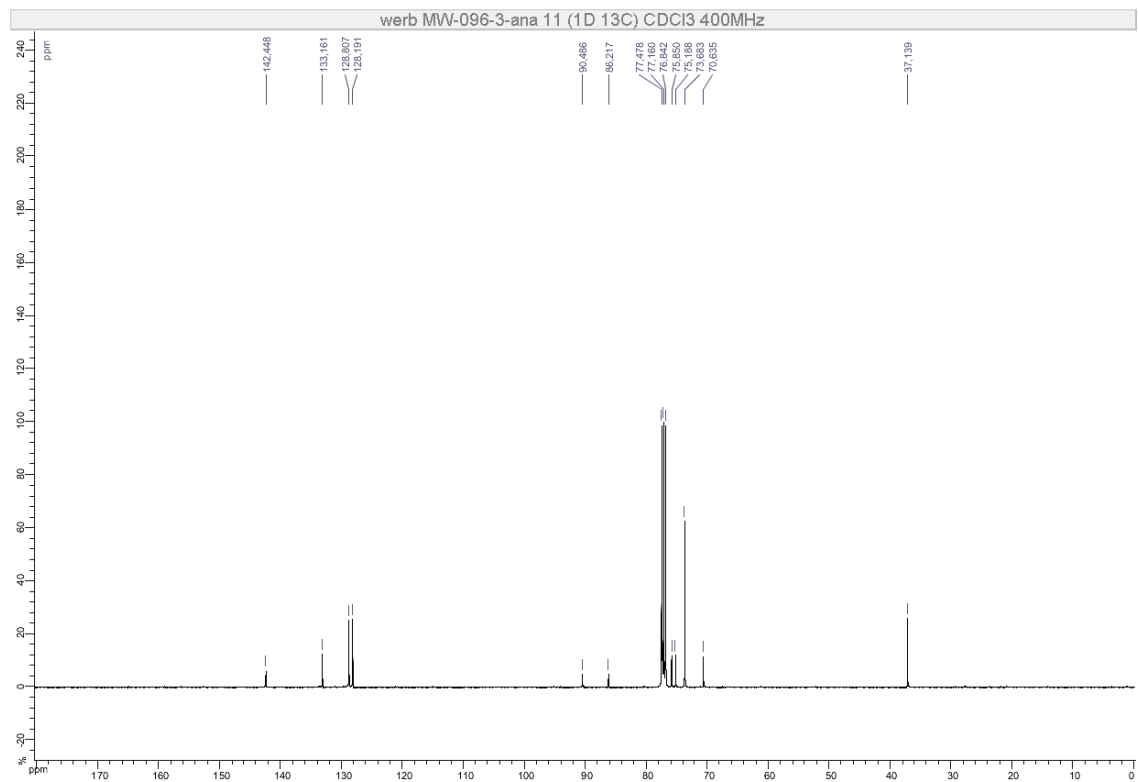
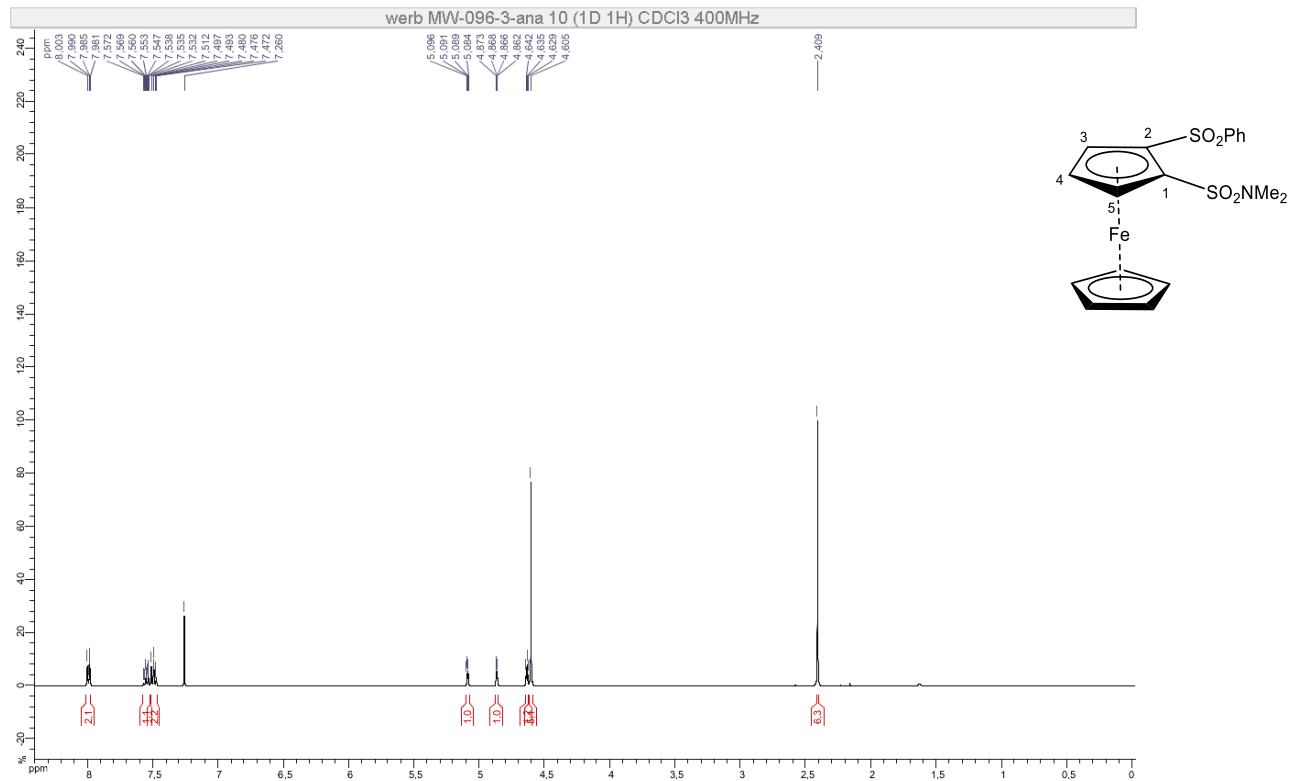


Figure S197. NOESY (500 MHz, CDCl₃) of **11** (racemic mixture)



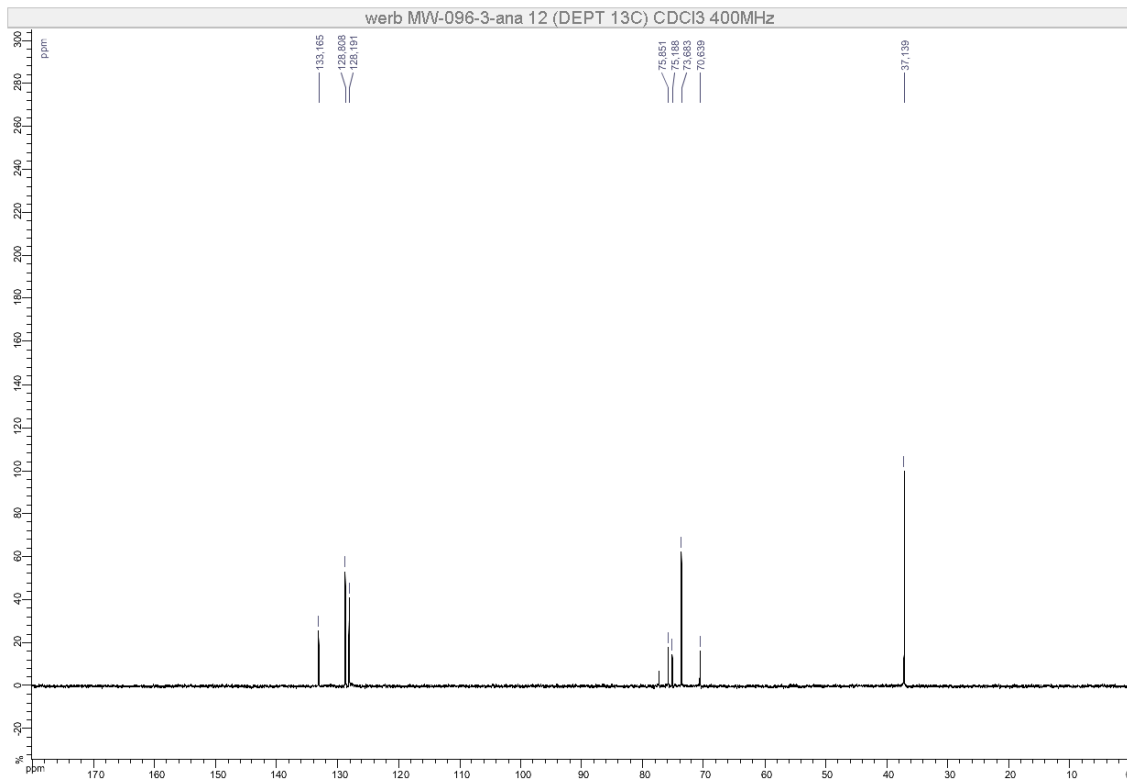


Figure S200. DEPT 135 (101 MHz, CDCl₃) of **12** (racemic mixture)

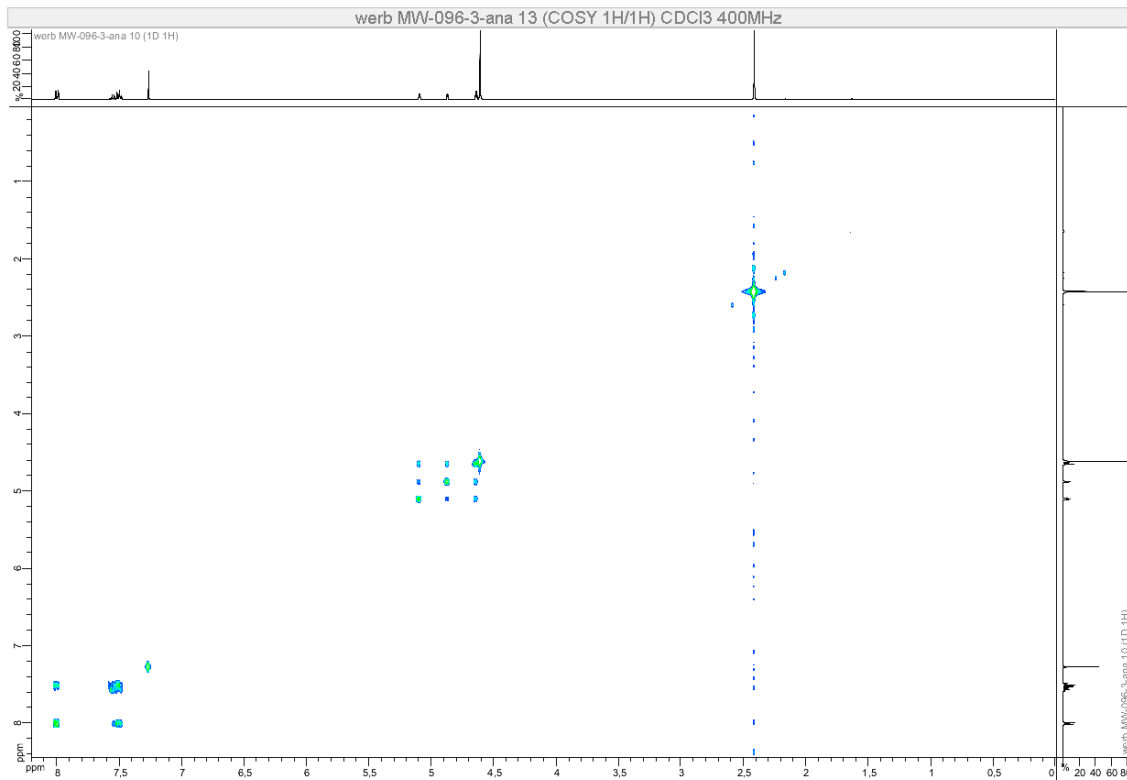


Figure S201. COSY (400 MHz, CDCl₃) of **12** (racemic mixture)

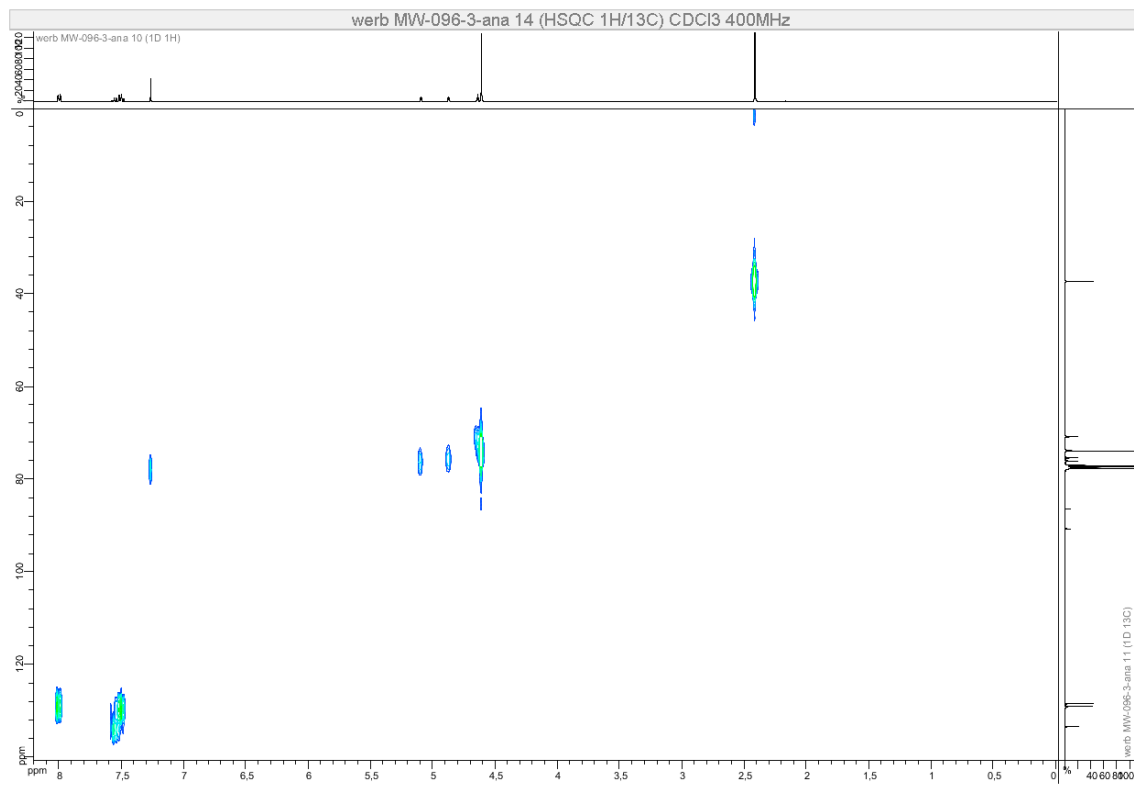


Figure S202. HSQC (400 MHz, CDCl_3) of **12** (racemic mixture)

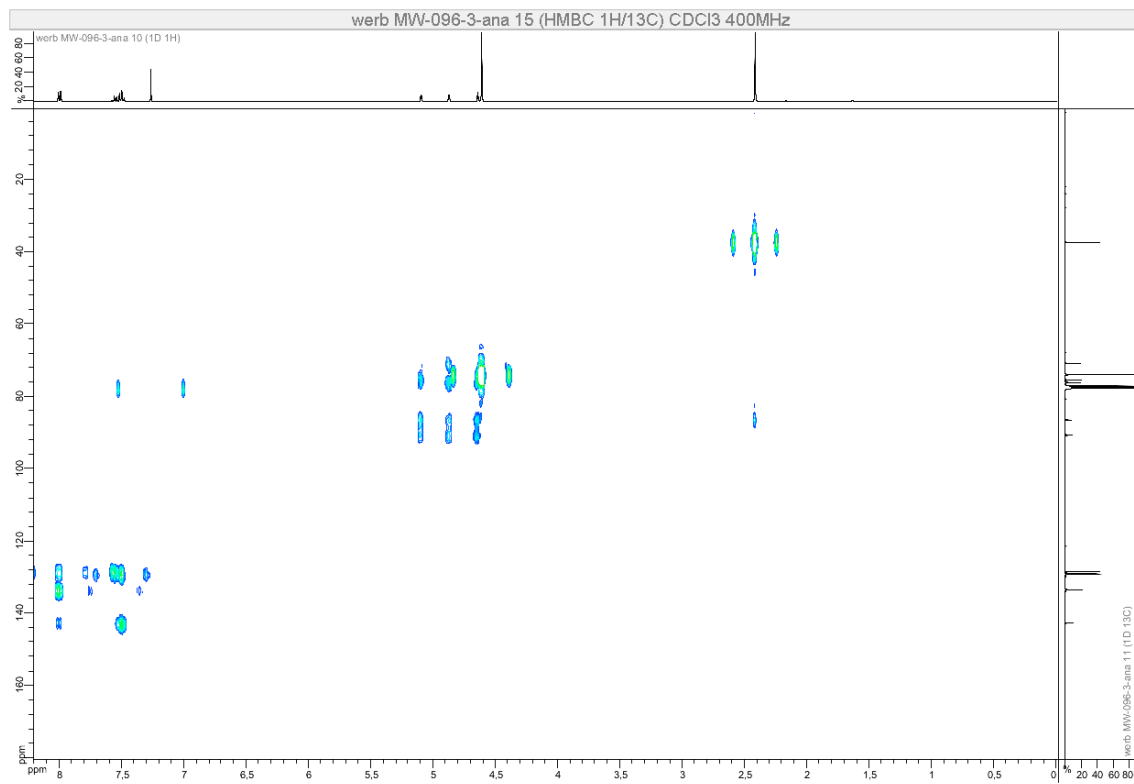
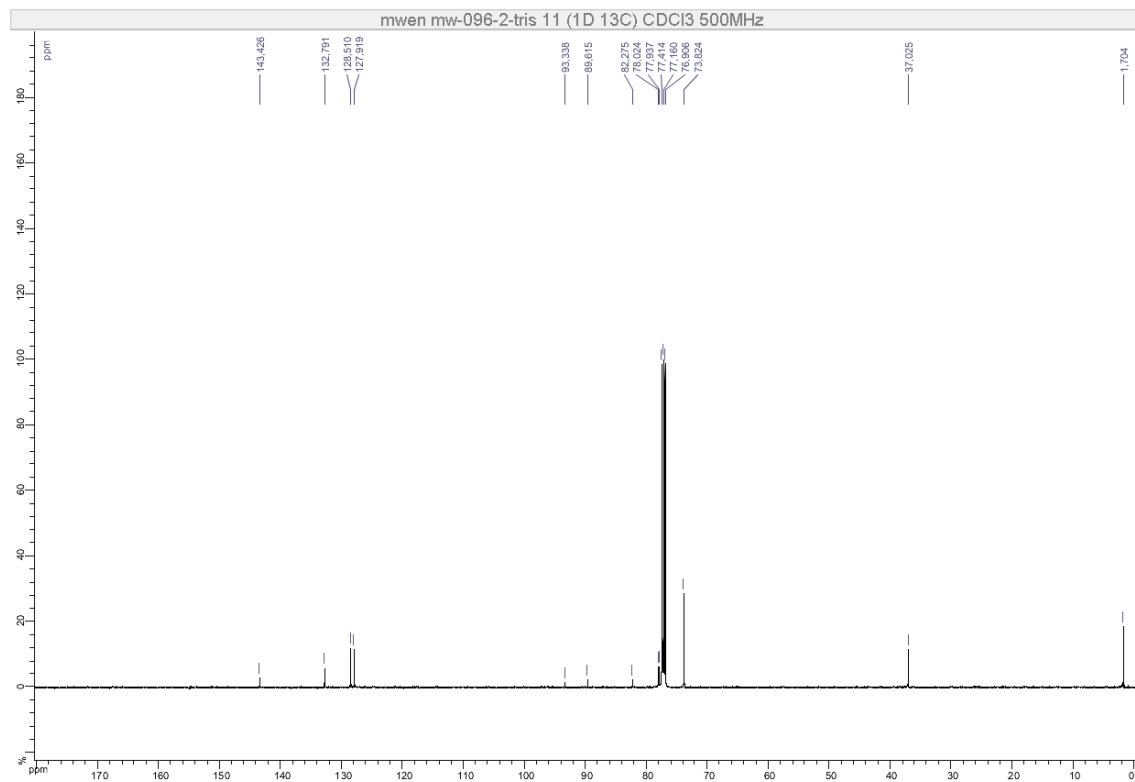
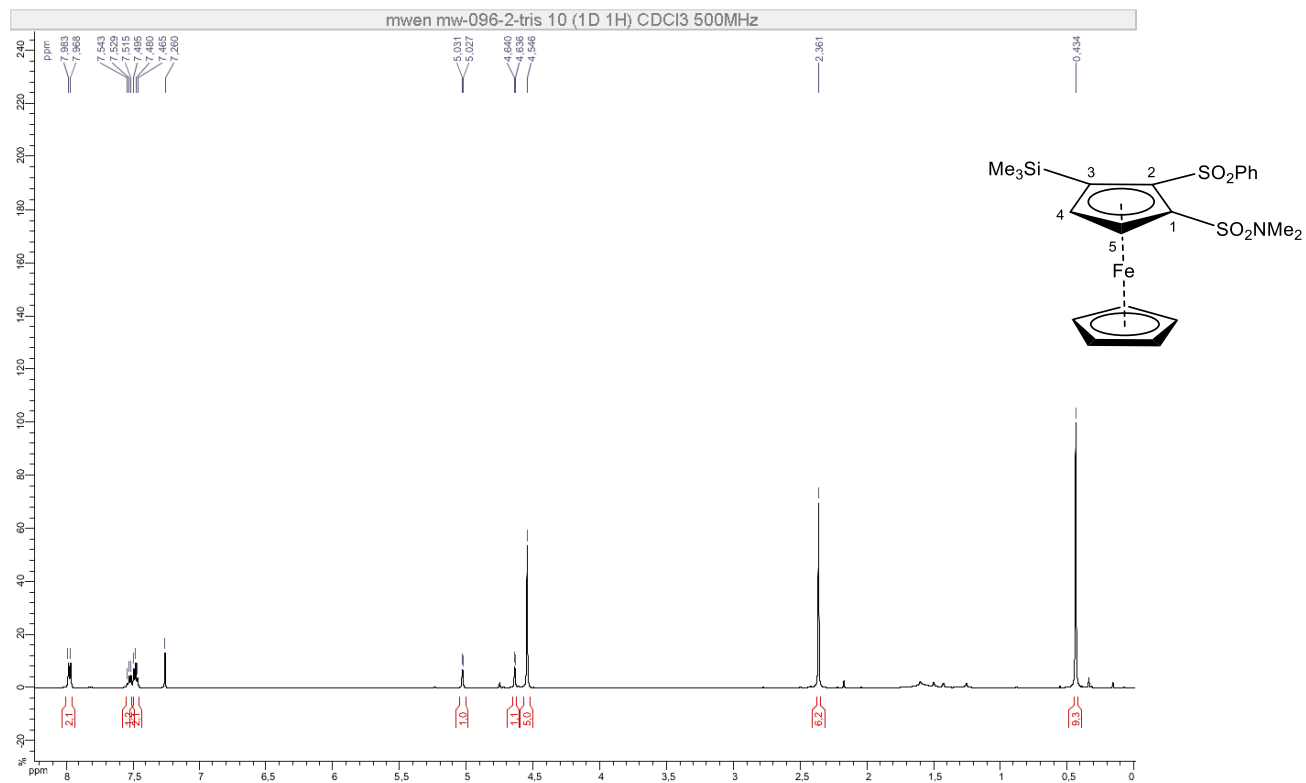


Figure S203. HMBC (400 MHz, CDCl_3) of **12** (racemic mixture)



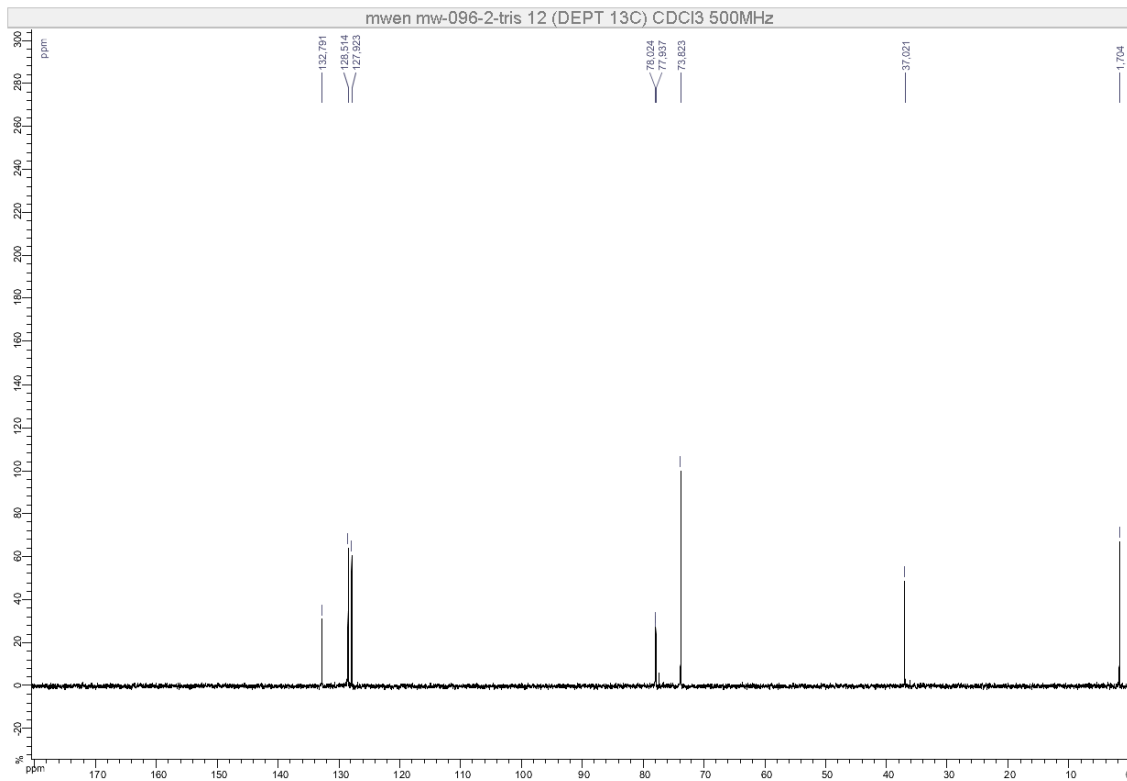


Figure S206. DEPT 135 (126 MHz, CDCl₃) of **13a** (racemic mixture)

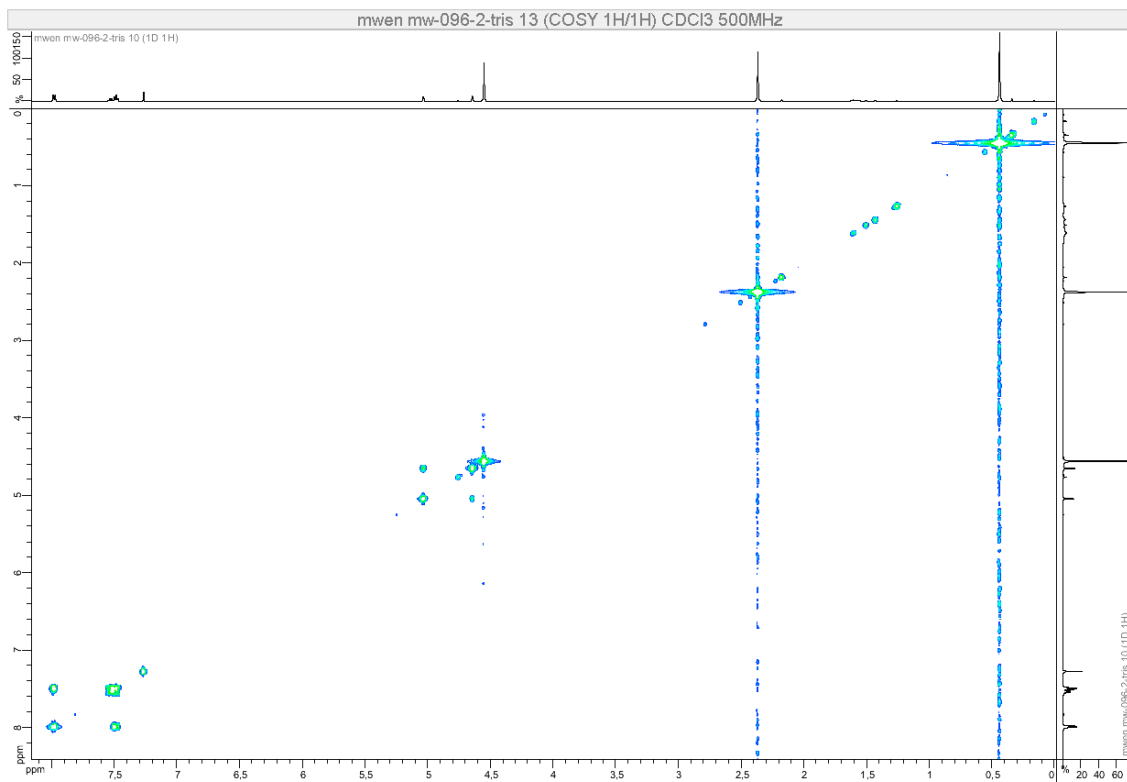


Figure S207. COSY (500 MHz, CDCl₃) of **13a** (racemic mixture)

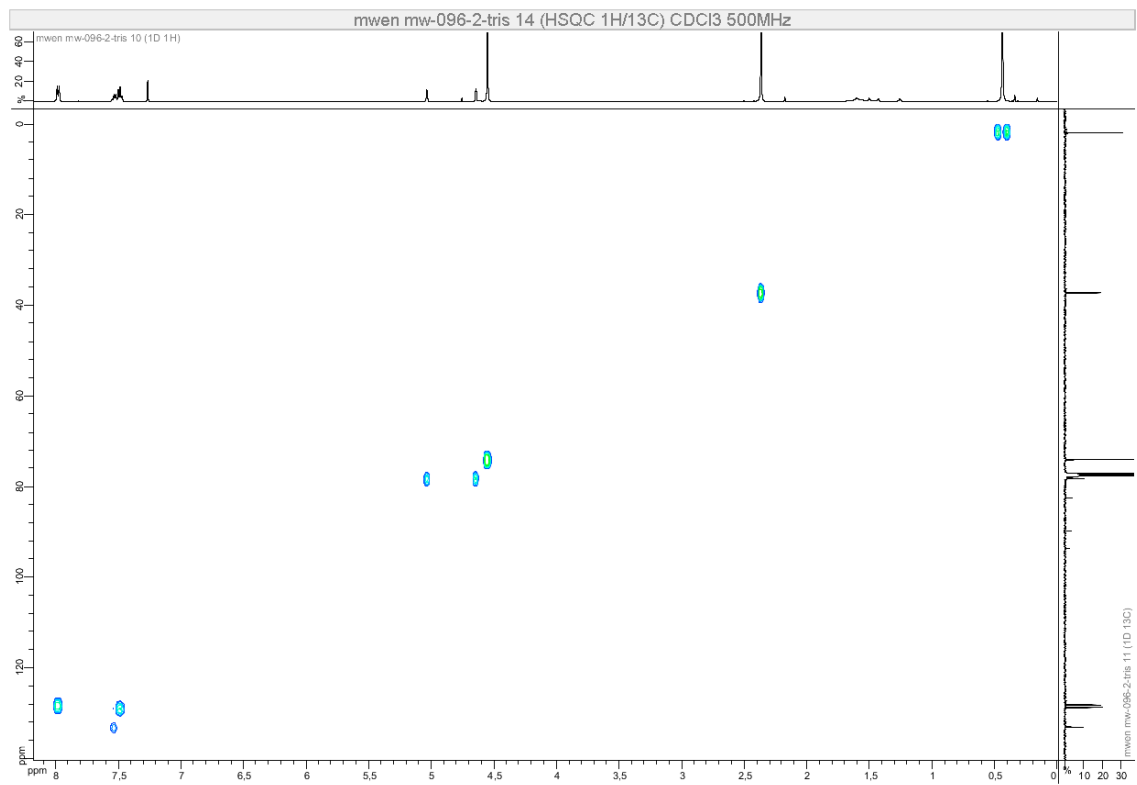


Figure S208. HSQC (500 MHz, CDCl₃) of **13a** (racemic mixture)

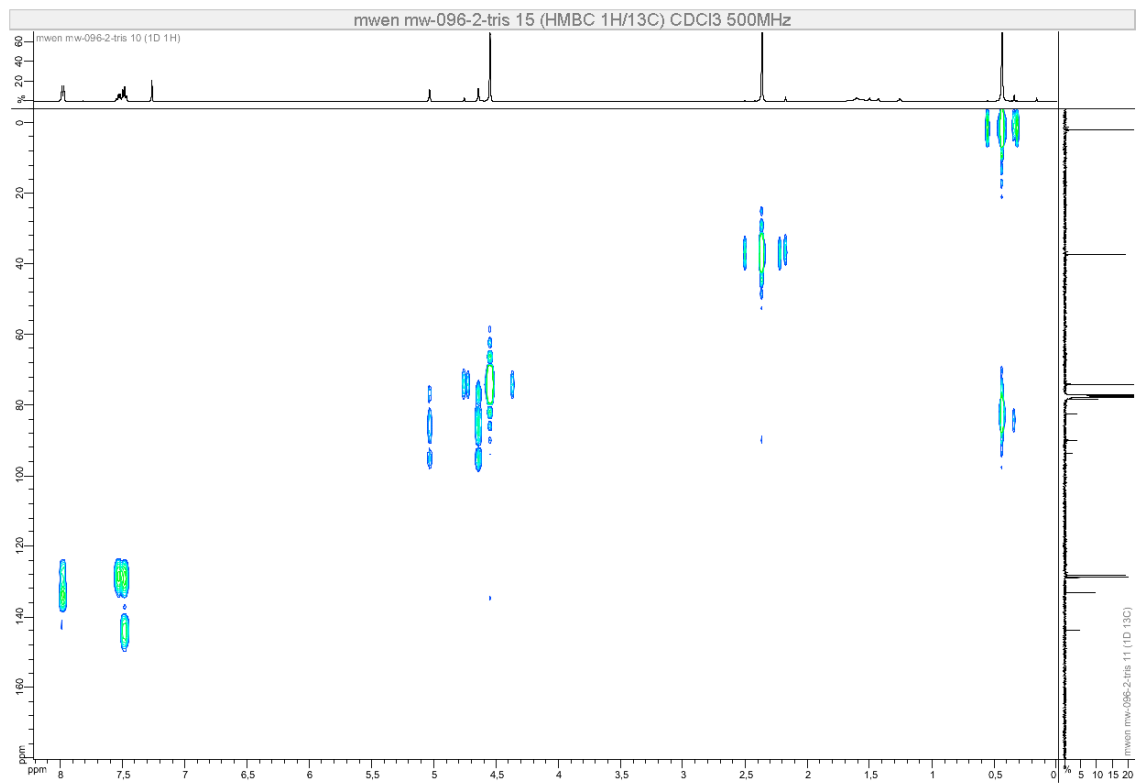


Figure S209. HMBC (500 MHz, CDCl₃) of **13a** (racemic mixture)

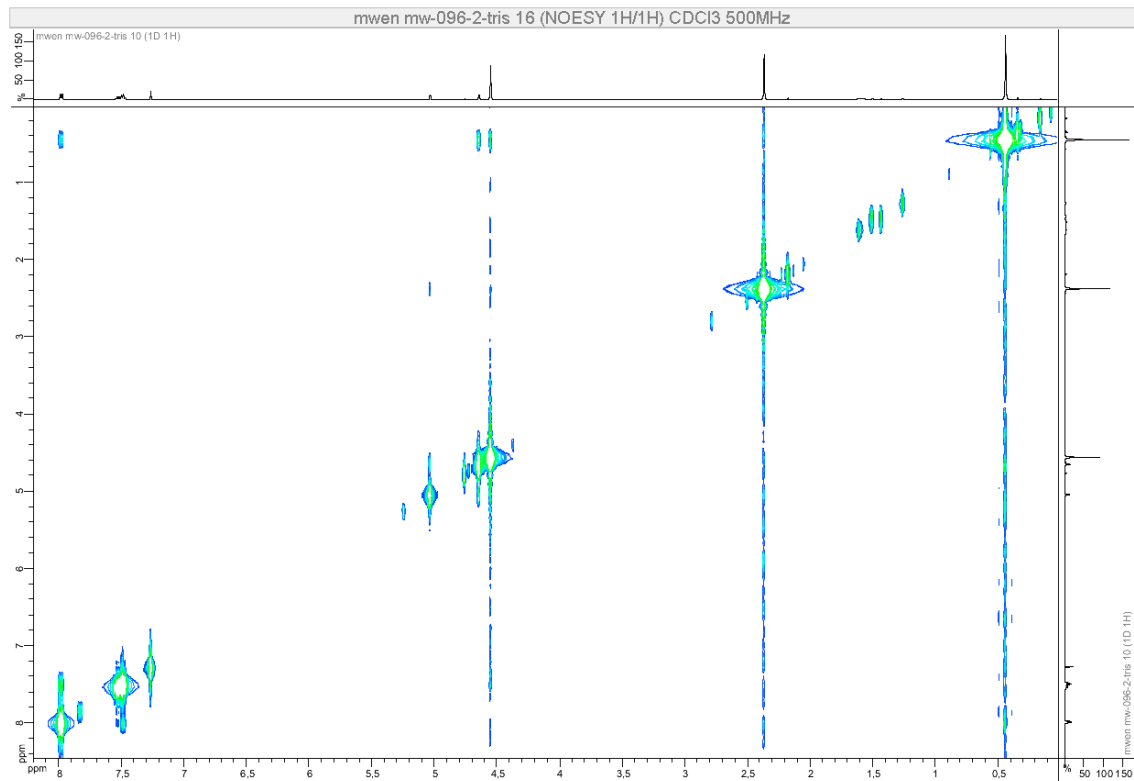


Figure S210. NOESY (500 MHz, CDCl₃) of **13a** (racemic mixture)

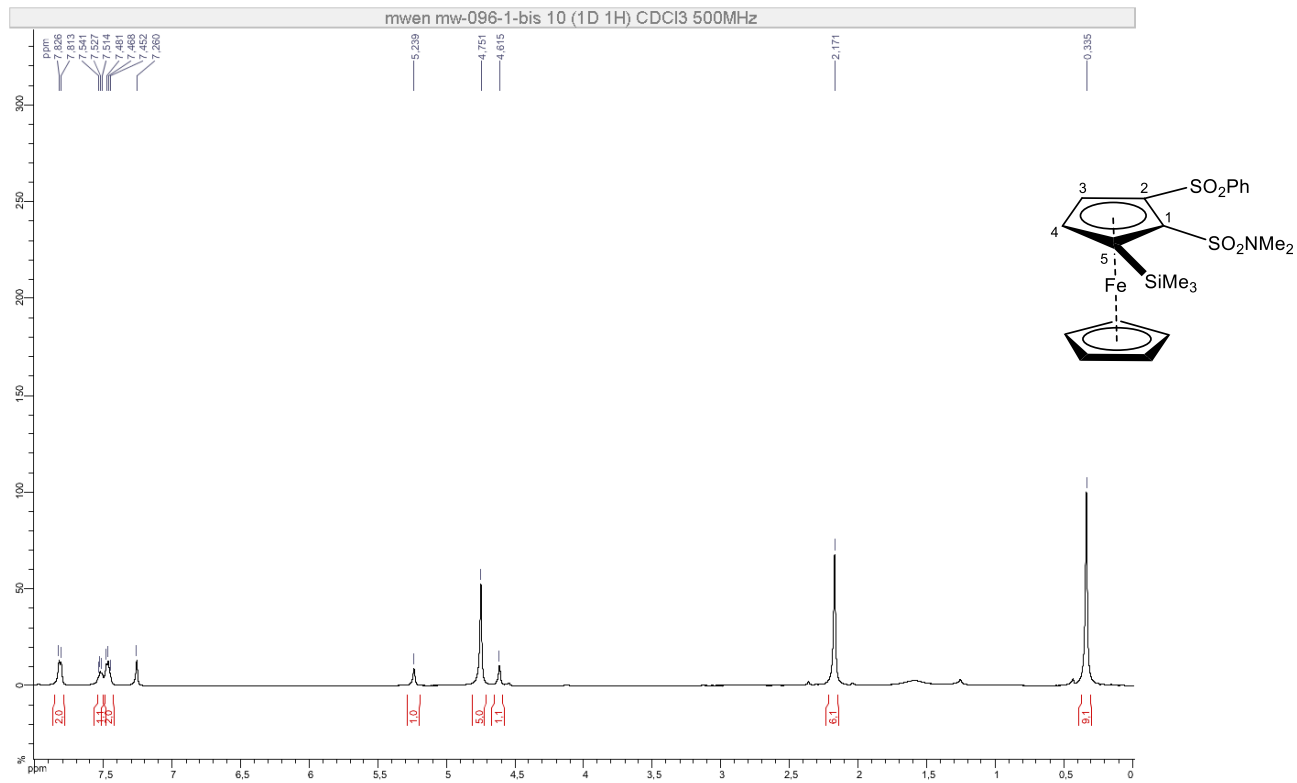


Figure S211. ¹H NMR (500 MHz, CDCl₃) of **13b** (racemic mixture)

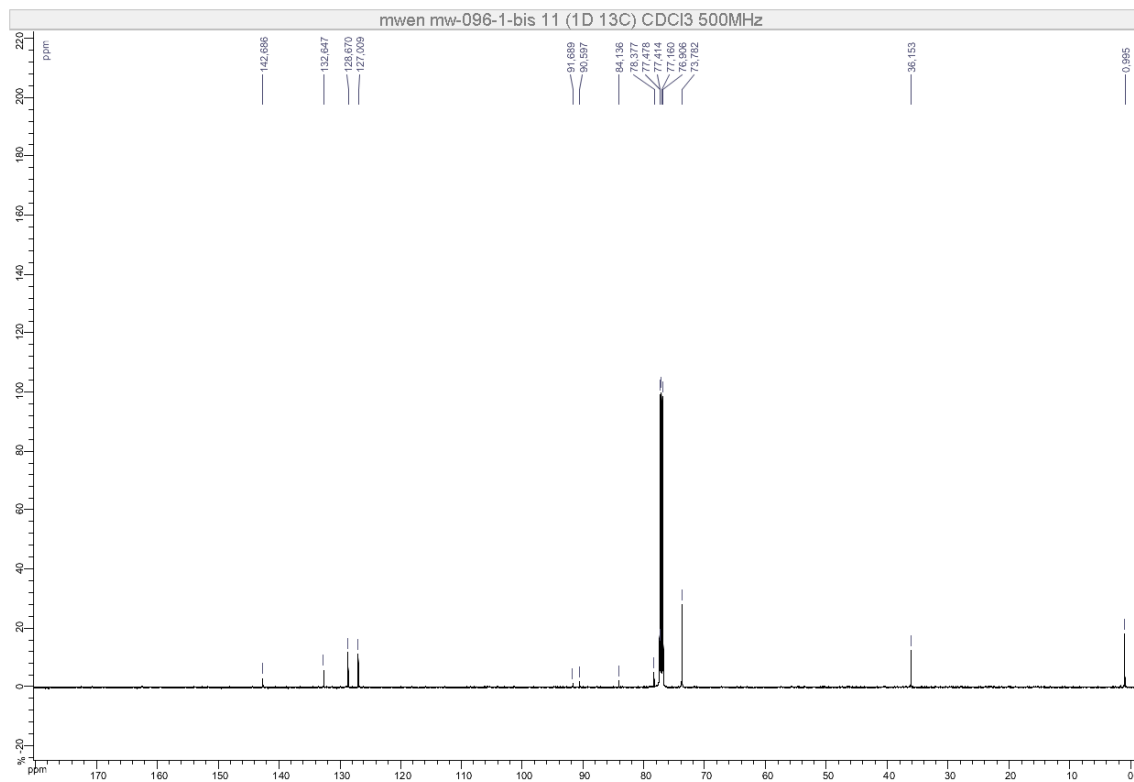


Figure S212. ¹³C NMR (126 MHz, CDCl₃) of **13b** (racemic mixture)

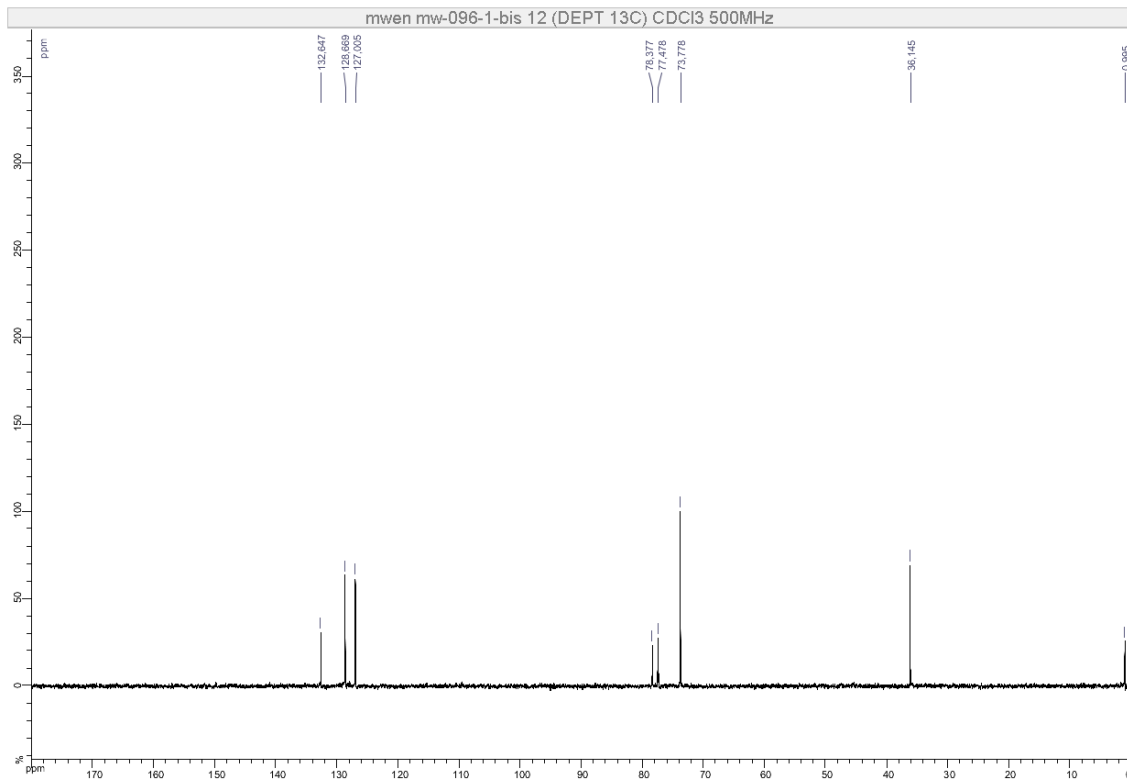


Figure S213. DEPT 135 (126 MHz, CDCl₃) of **13b** (racemic mixture)

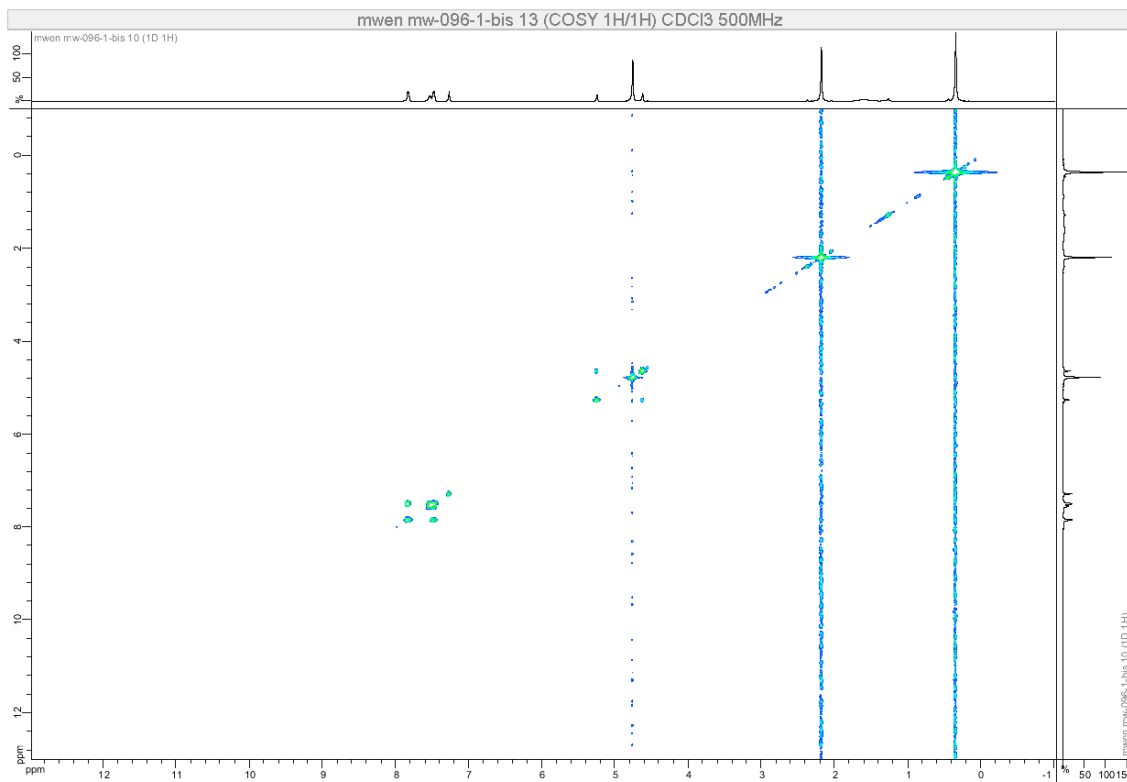


Figure S214. COSY (500 MHz, CDCl₃) of **13b** (racemic mixture)

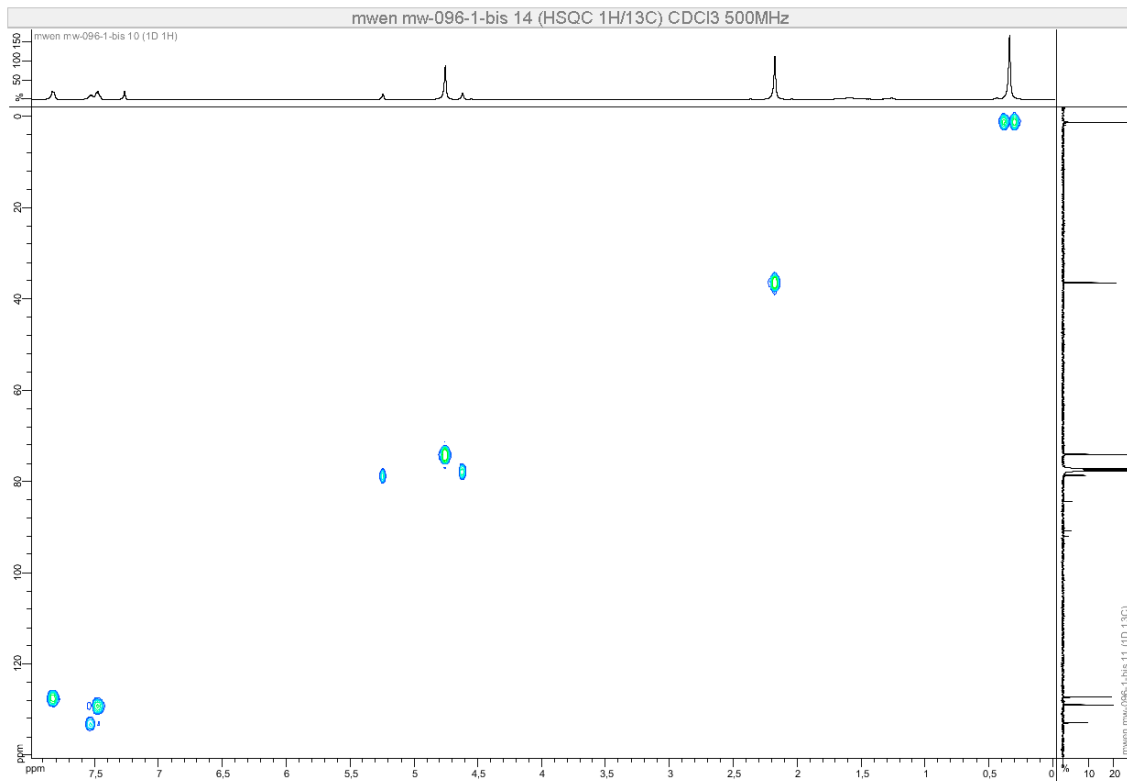


Figure S215. HSQC (500 MHz, CDCl₃) of **13b** (racemic mixture)

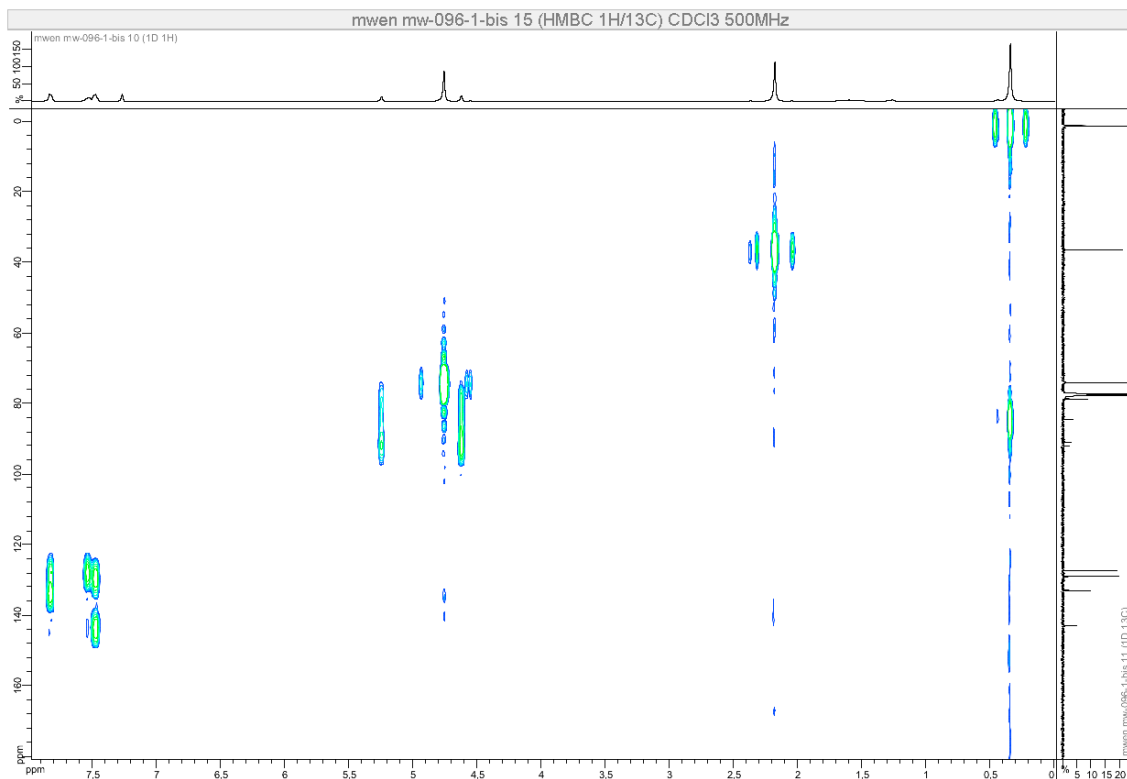


Figure S216. HMBC (500 MHz, CDCl₃) of **13b** (racemic mixture)

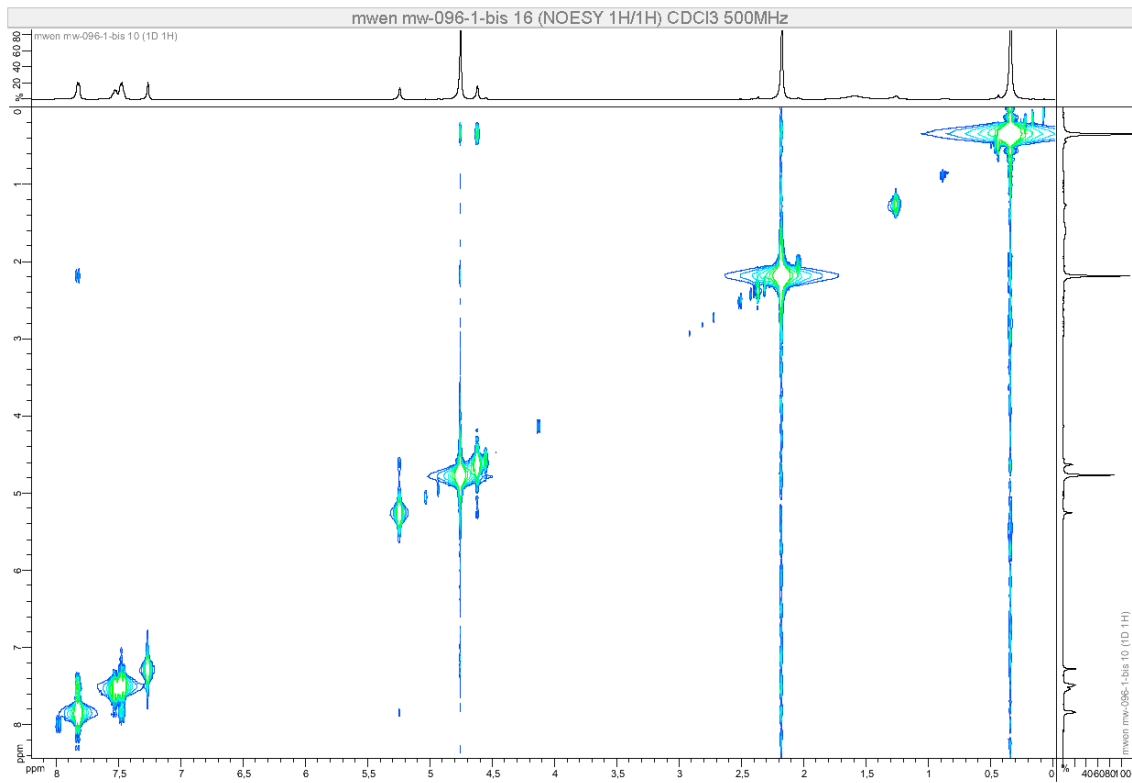


Figure S217. NOESY (500 MHz, CDCl₃) of **13b** (racemic mixture)

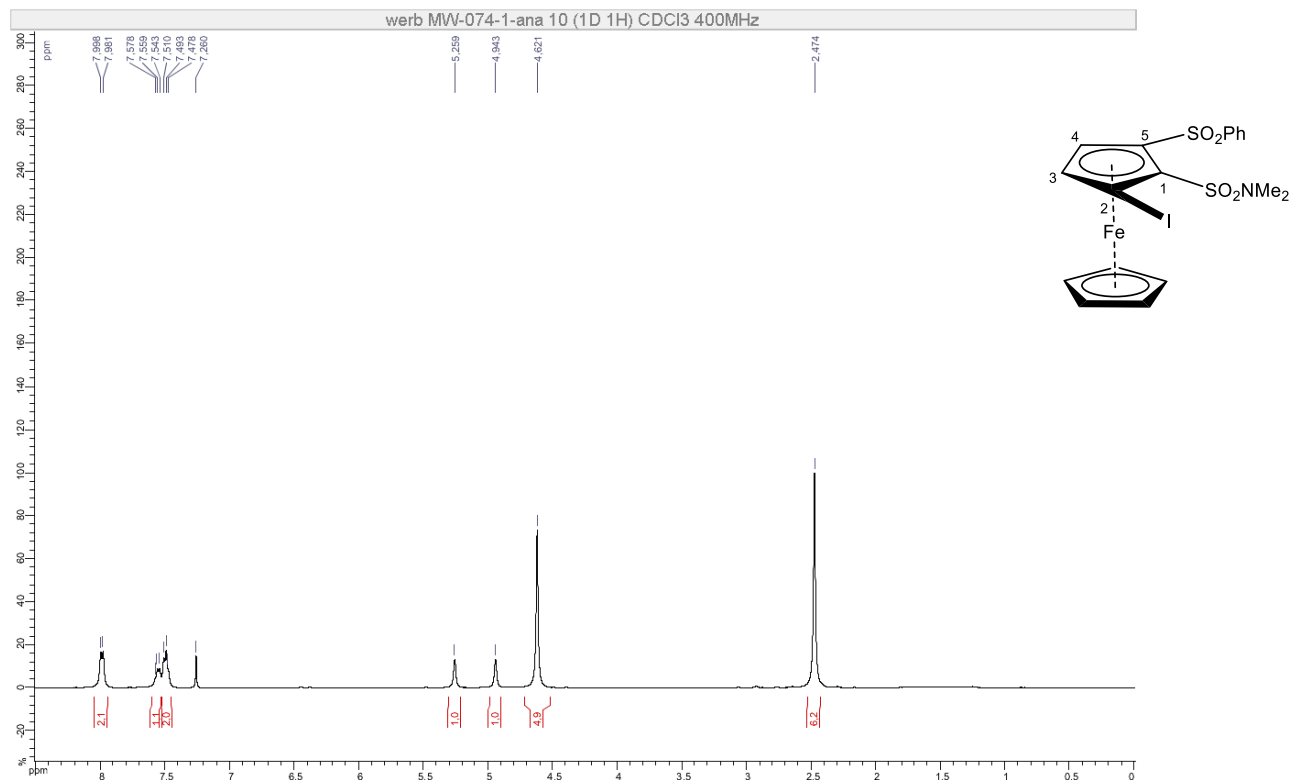


Figure S218. ¹H NMR (400 MHz, CDCl₃) of **14** (racemic mixture)

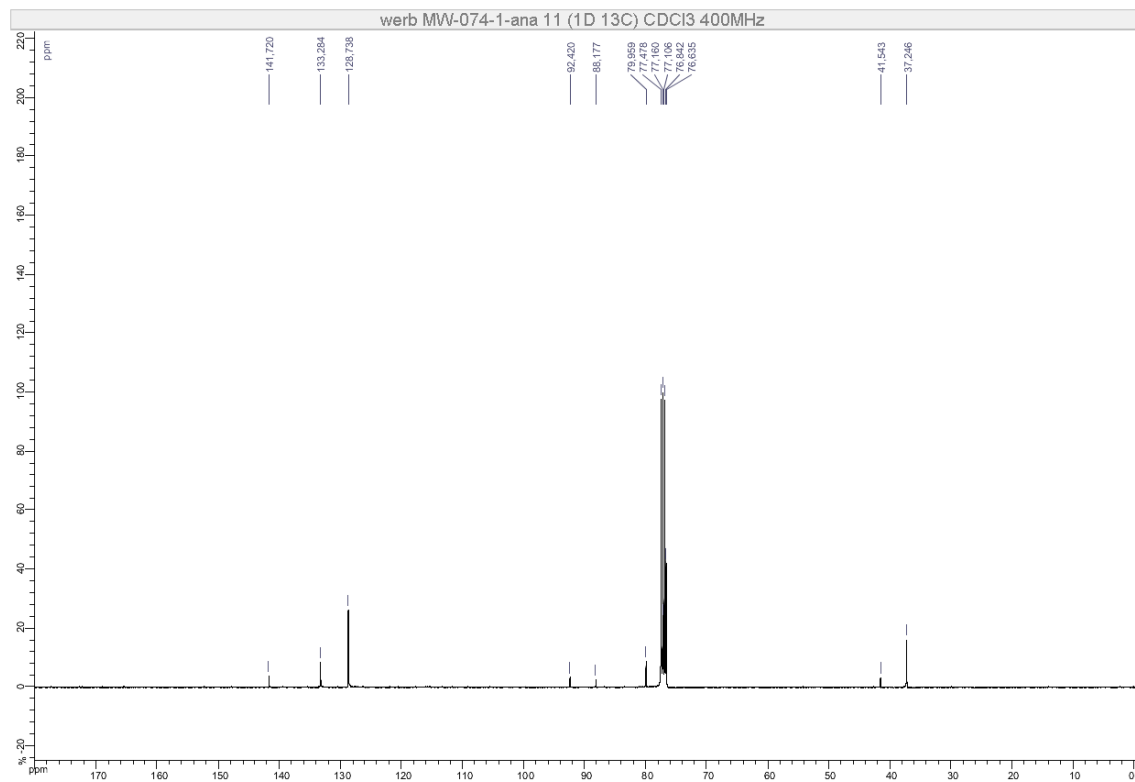


Figure S219. ¹³C NMR (101 MHz, CDCl₃) of **14** (racemic mixture)

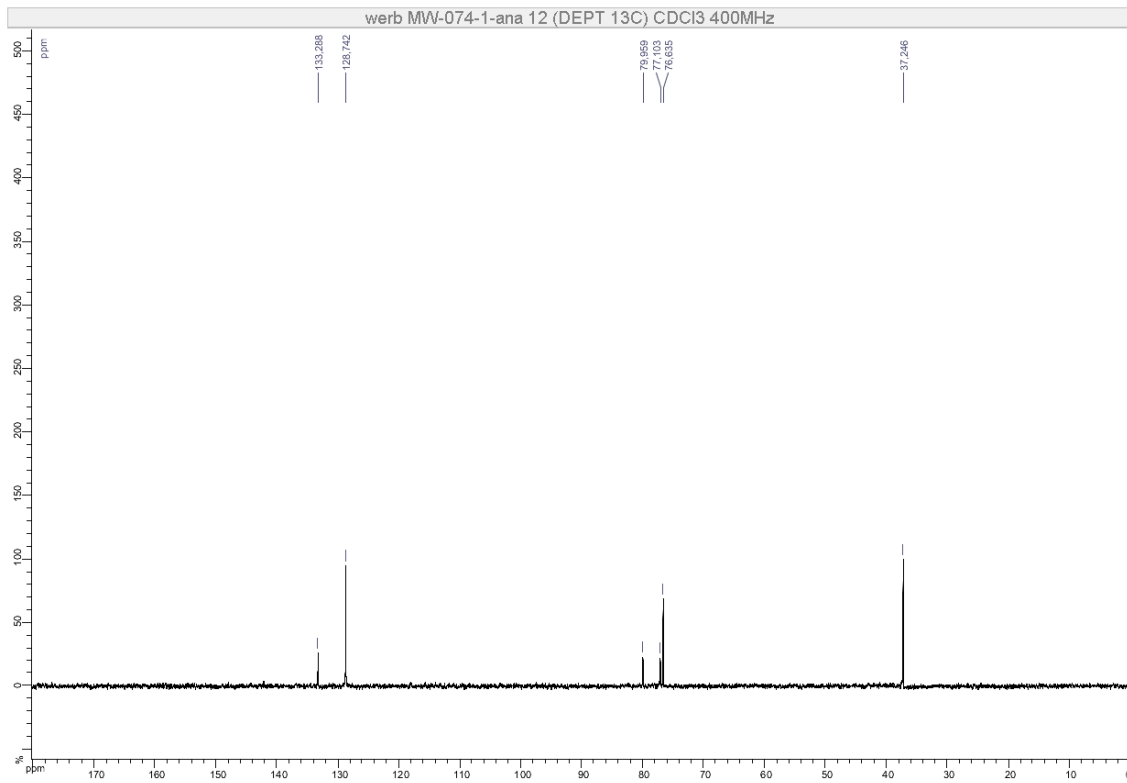


Figure S220. DEPT 135 (101 MHz, CDCl₃) of **14** (racemic mixture)

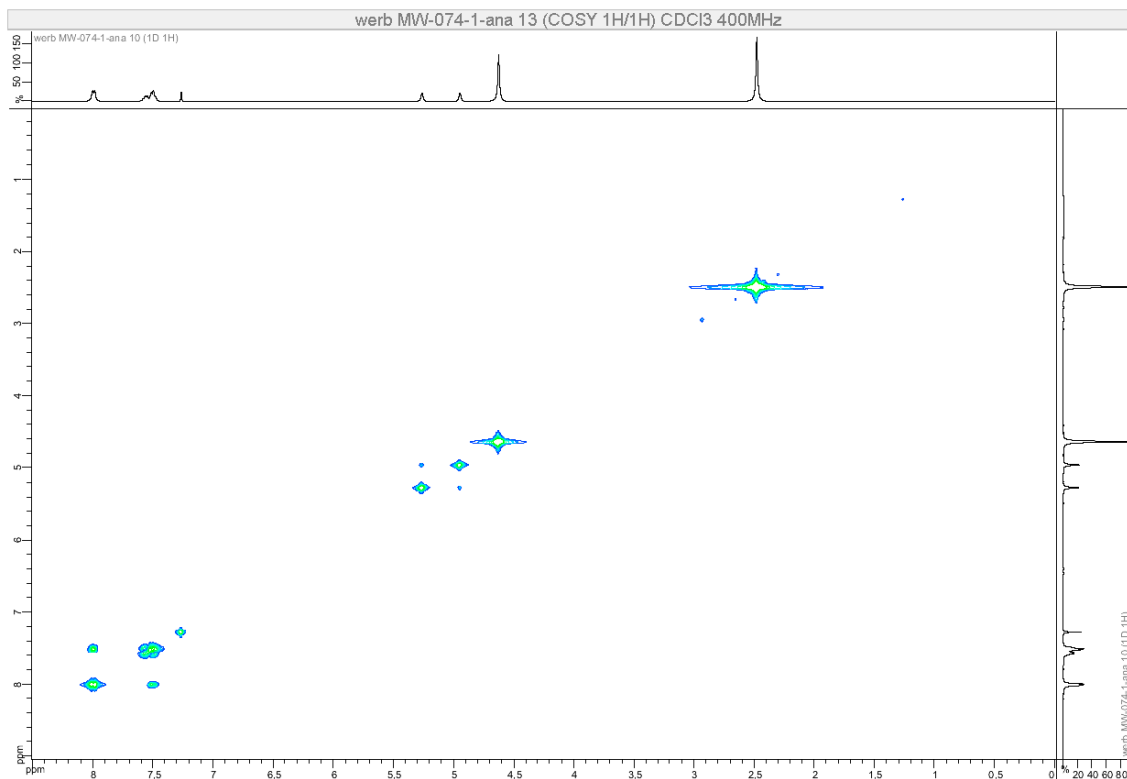


Figure S221. COSY (400 MHz, CDCl₃) of **14** (racemic mixture)

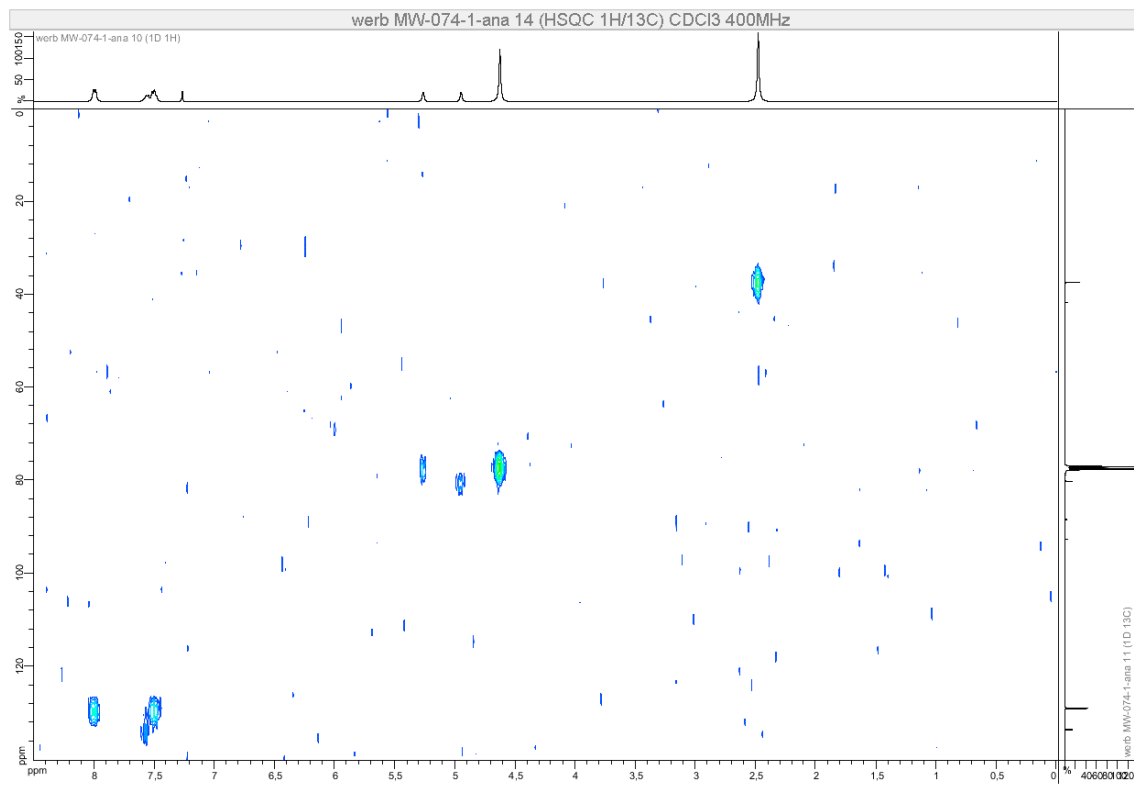


Figure S22. HSQC (400 MHz, CDCl_3) of **14** (racemic mixture)

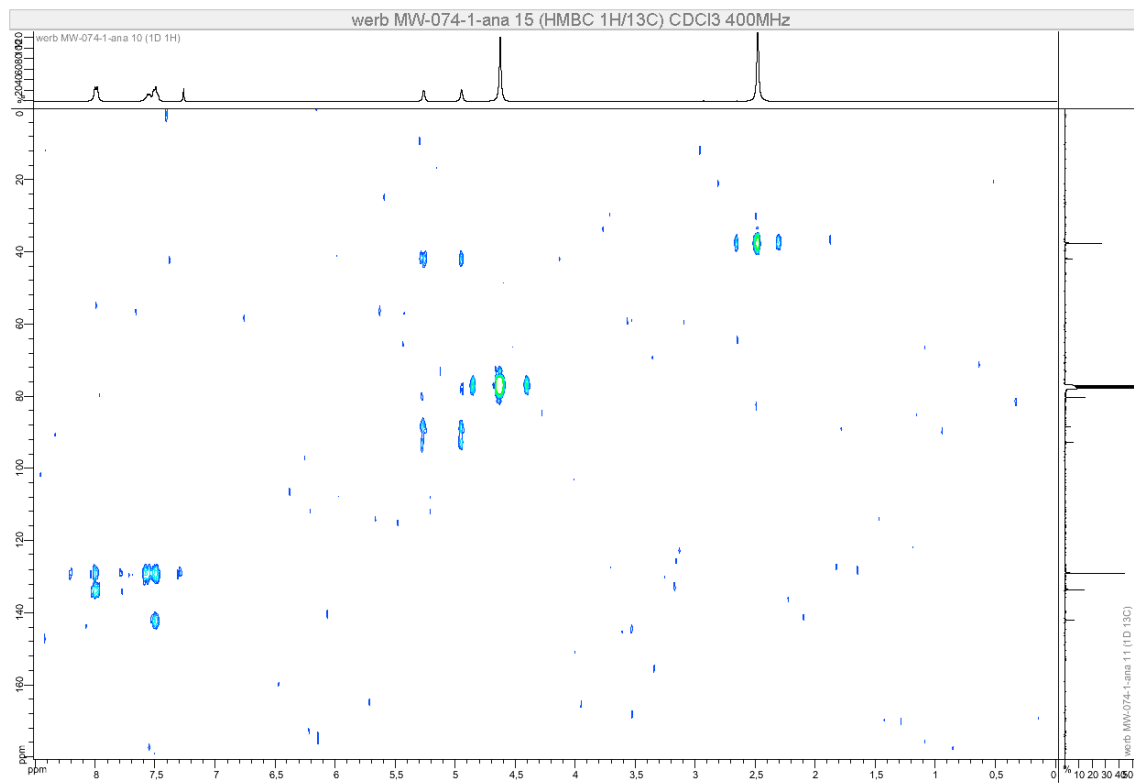
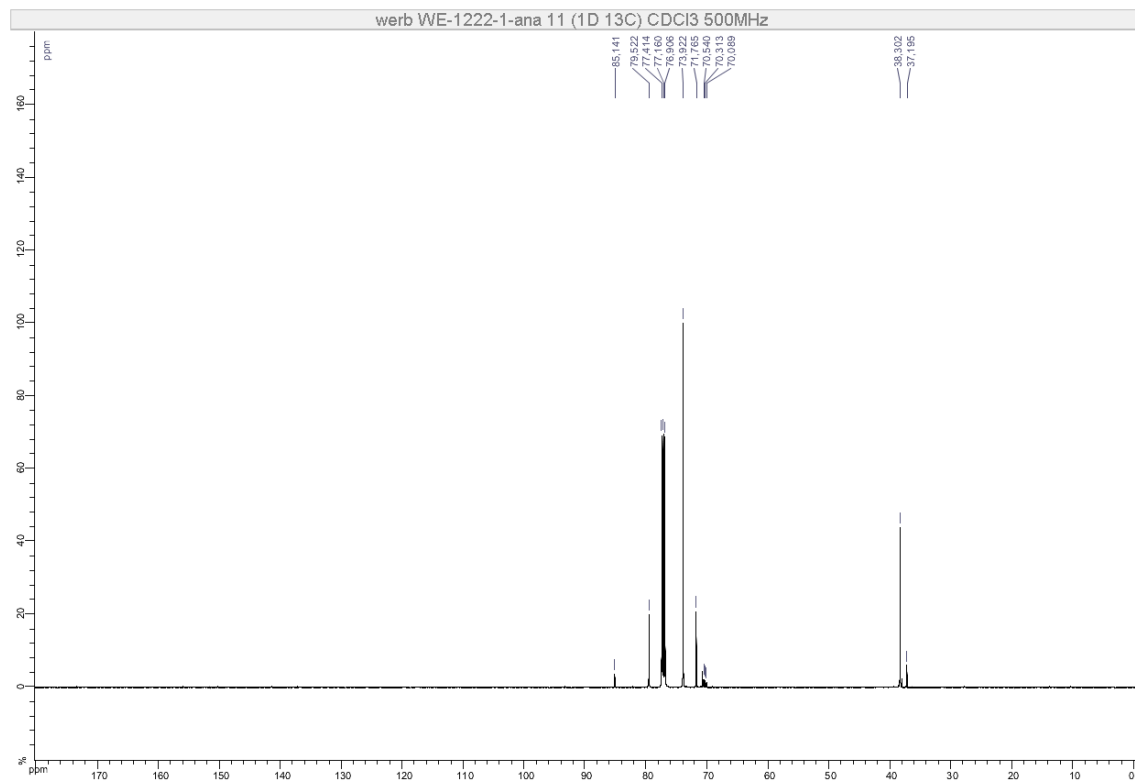
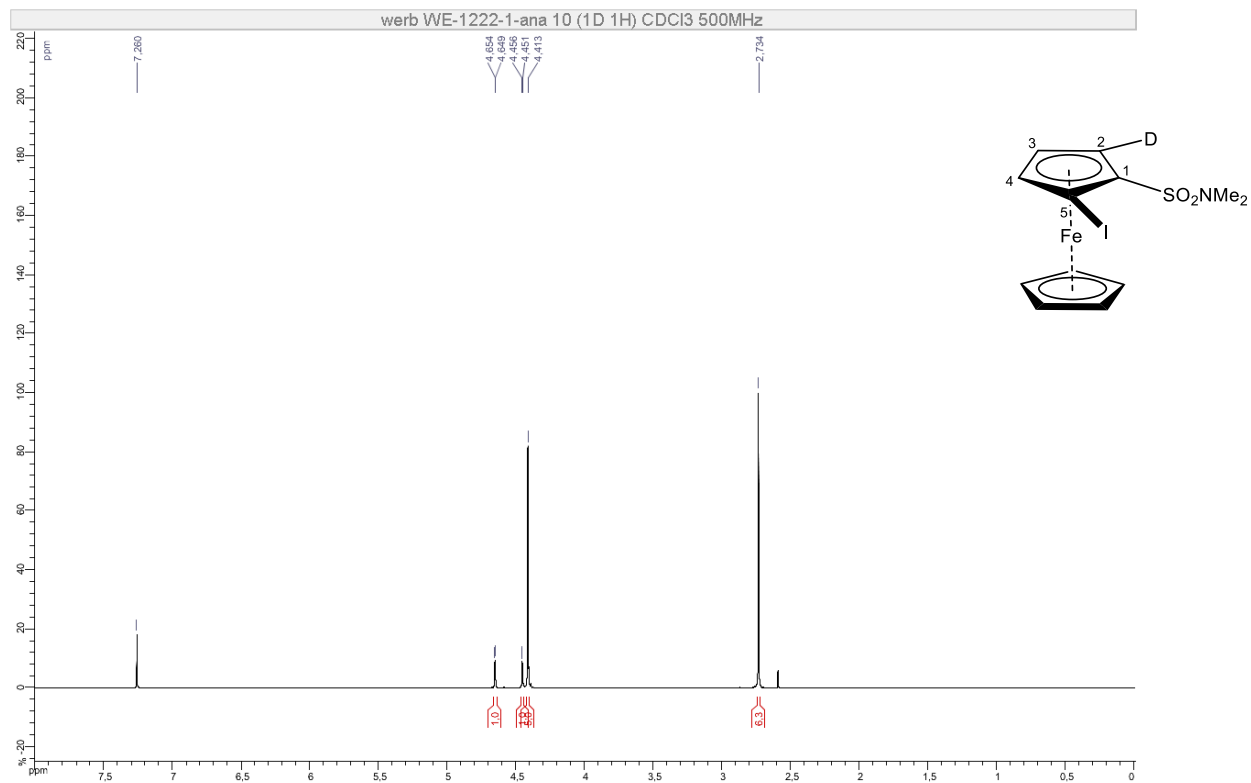


Figure S23. HMBC (400 MHz, CDCl_3) of **14** (racemic mixture)



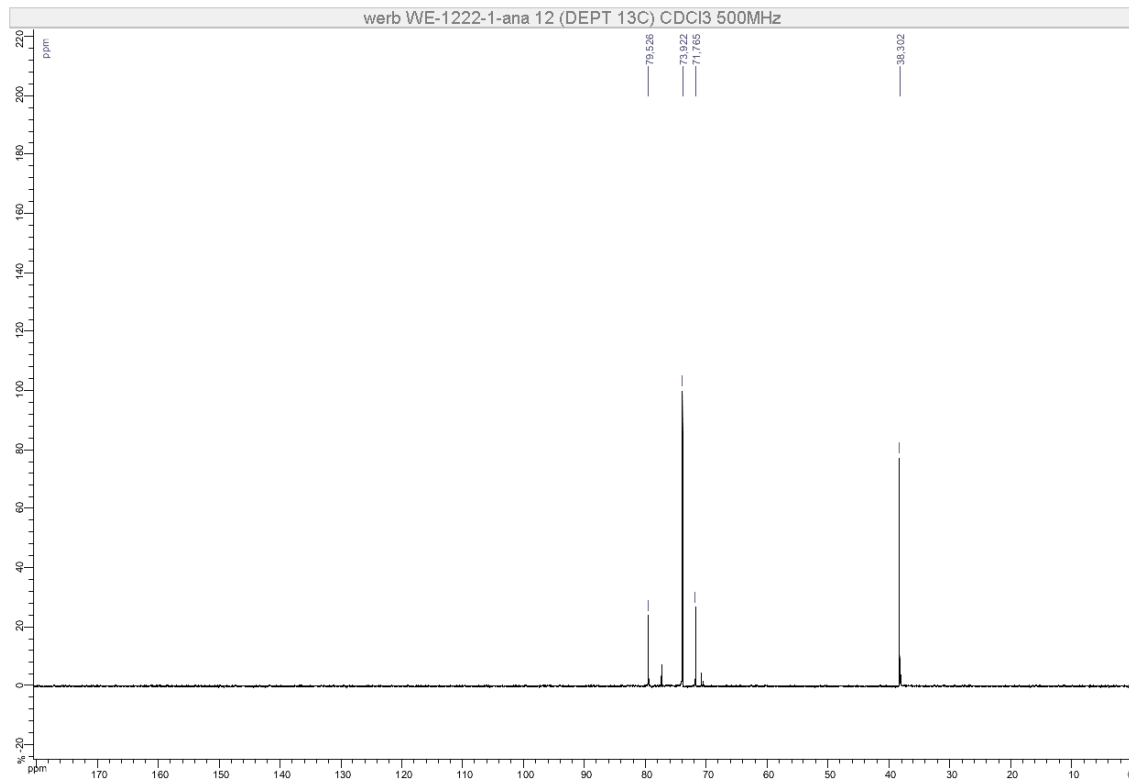


Figure S226. DEPT 135 (126 MHz, CDCl₃) of **15** (racemic mixture)

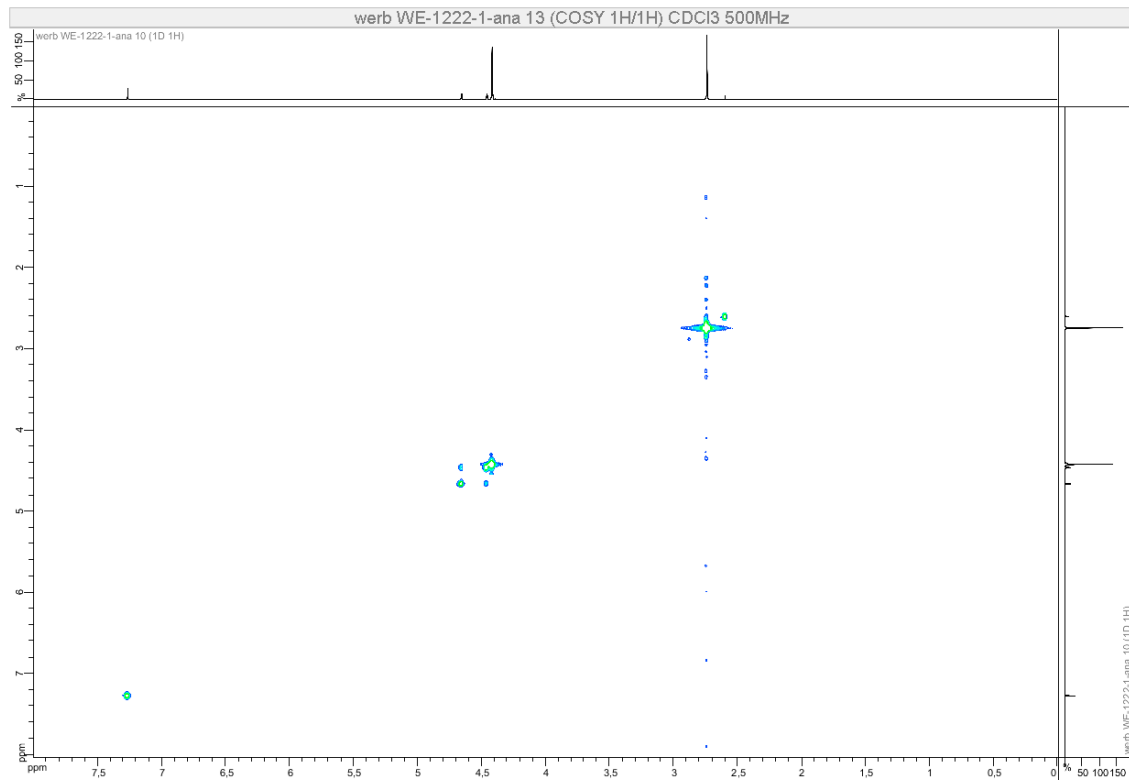


Figure S227. COSY (500 MHz, CDCl₃) of **15** (racemic mixture)

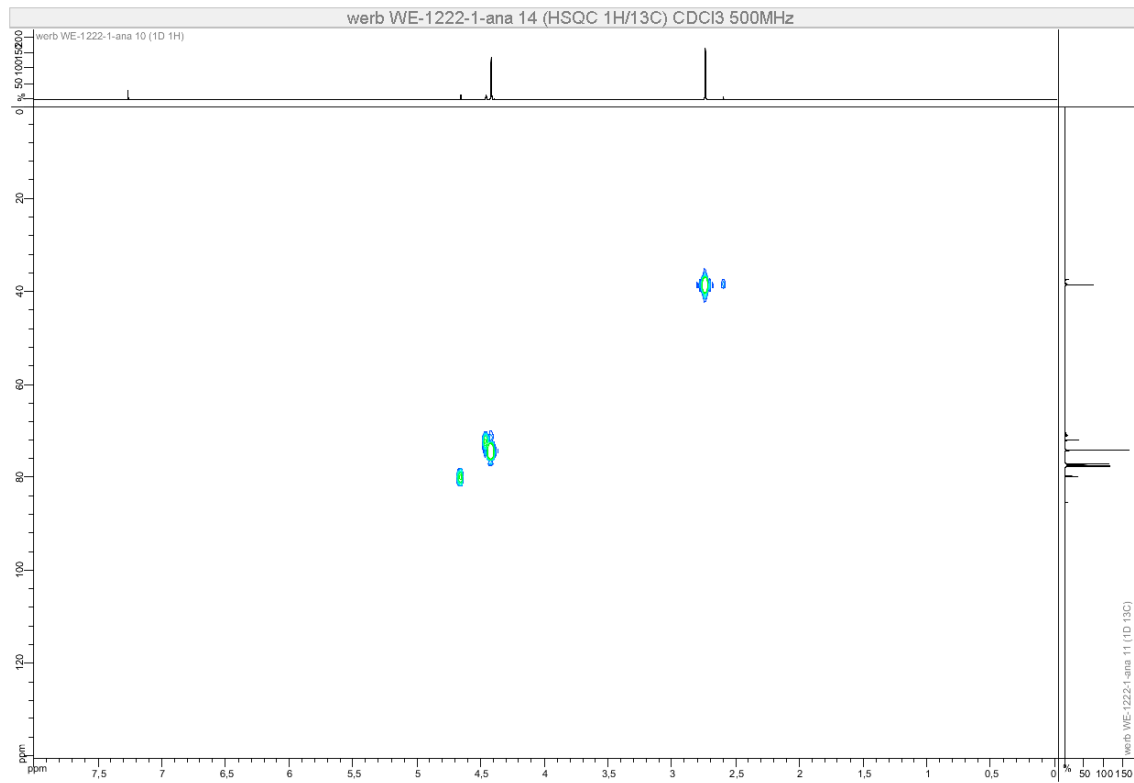


Figure S228. HSQC (500 MHz, CDCl₃) of **15** (racemic mixture)

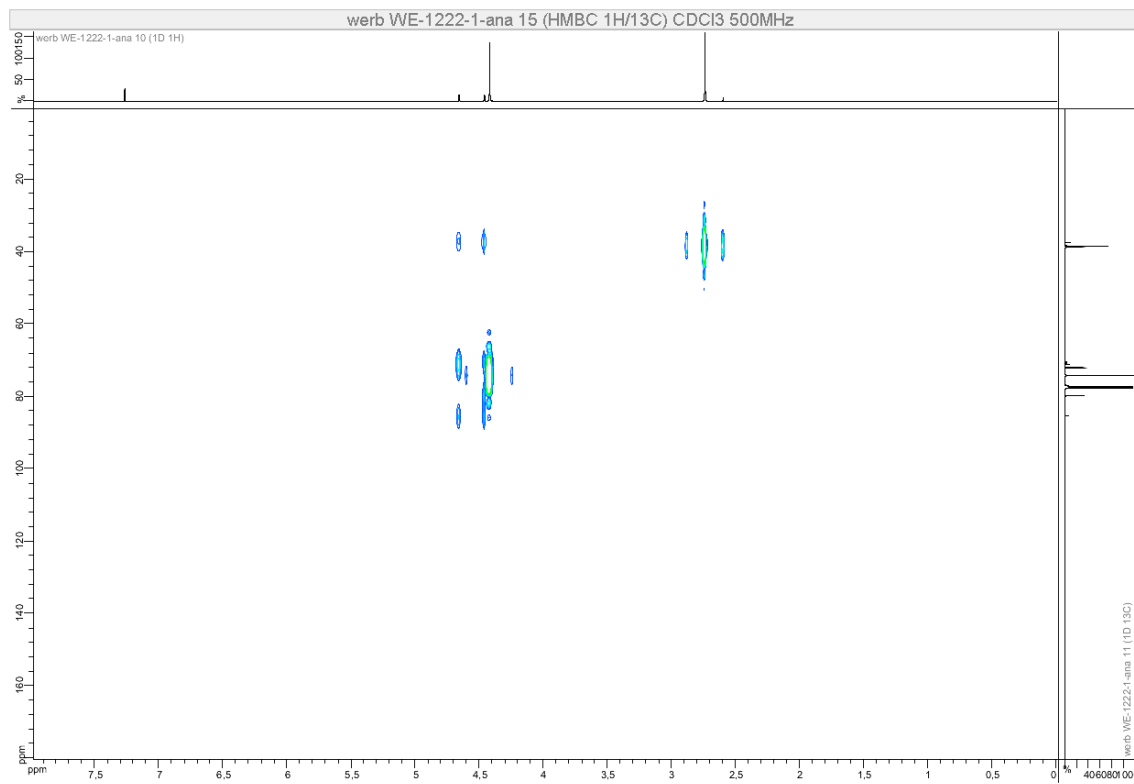
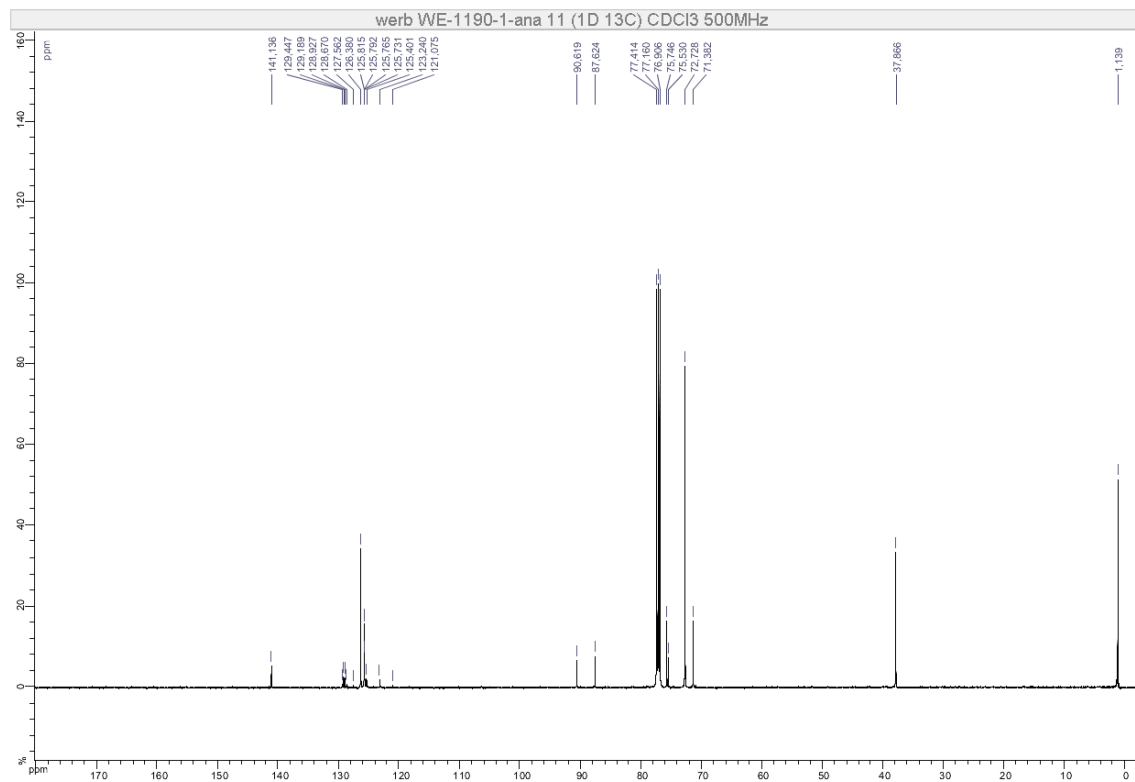
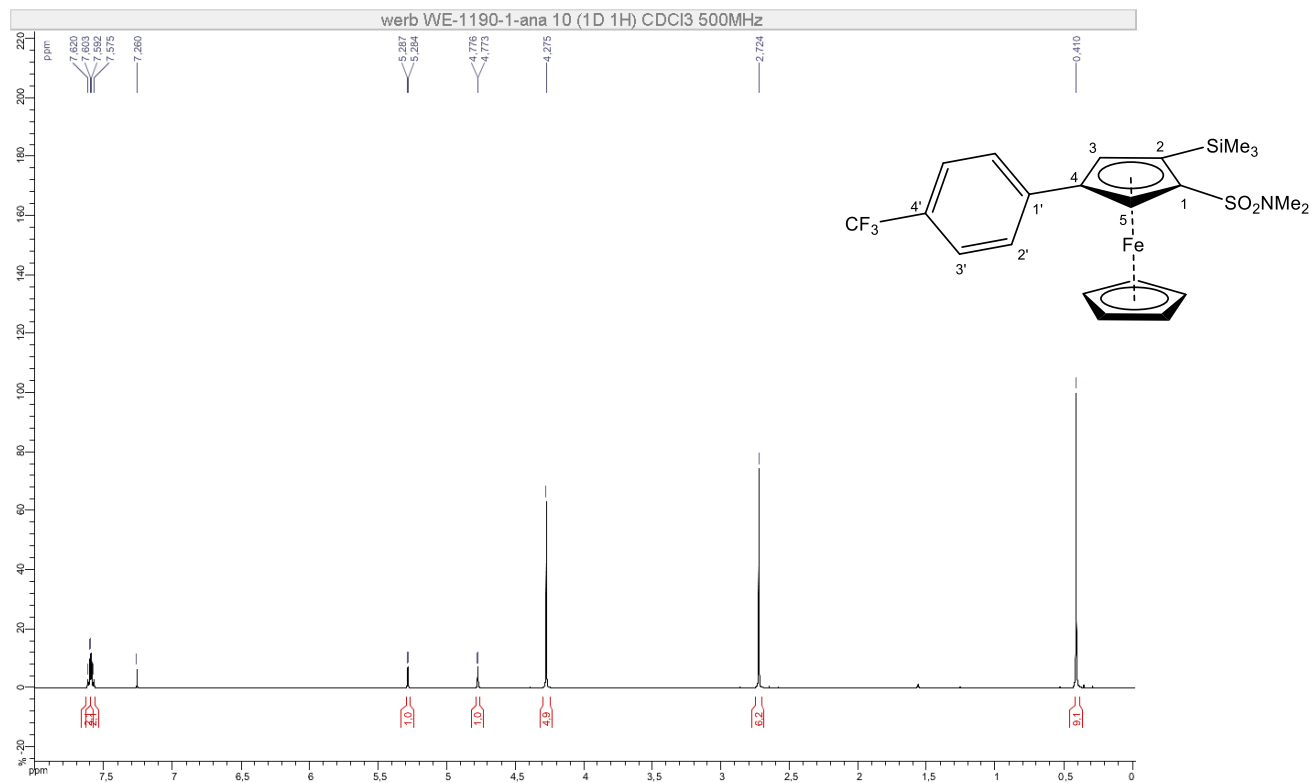


Figure S229. HMBC (500 MHz, CDCl₃) of **15** (racemic mixture)



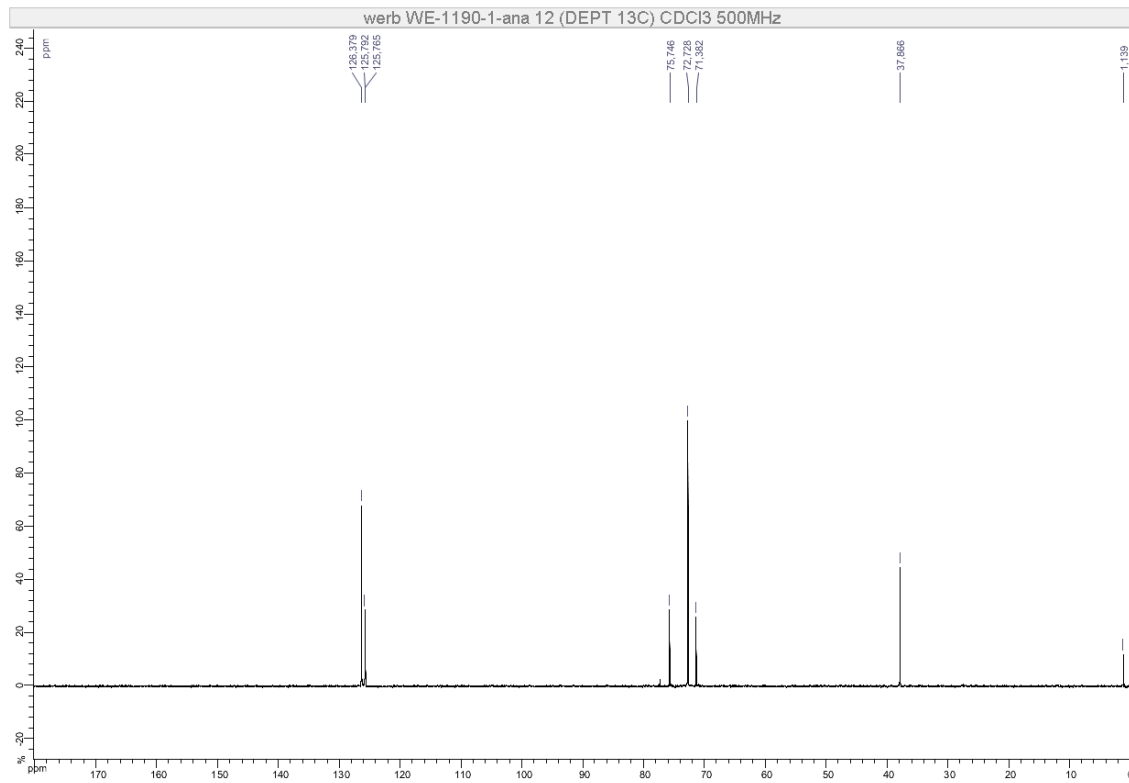


Figure S232. DEPT 135 (500 MHz, CDCl₃) of **16a** (racemic mixture)

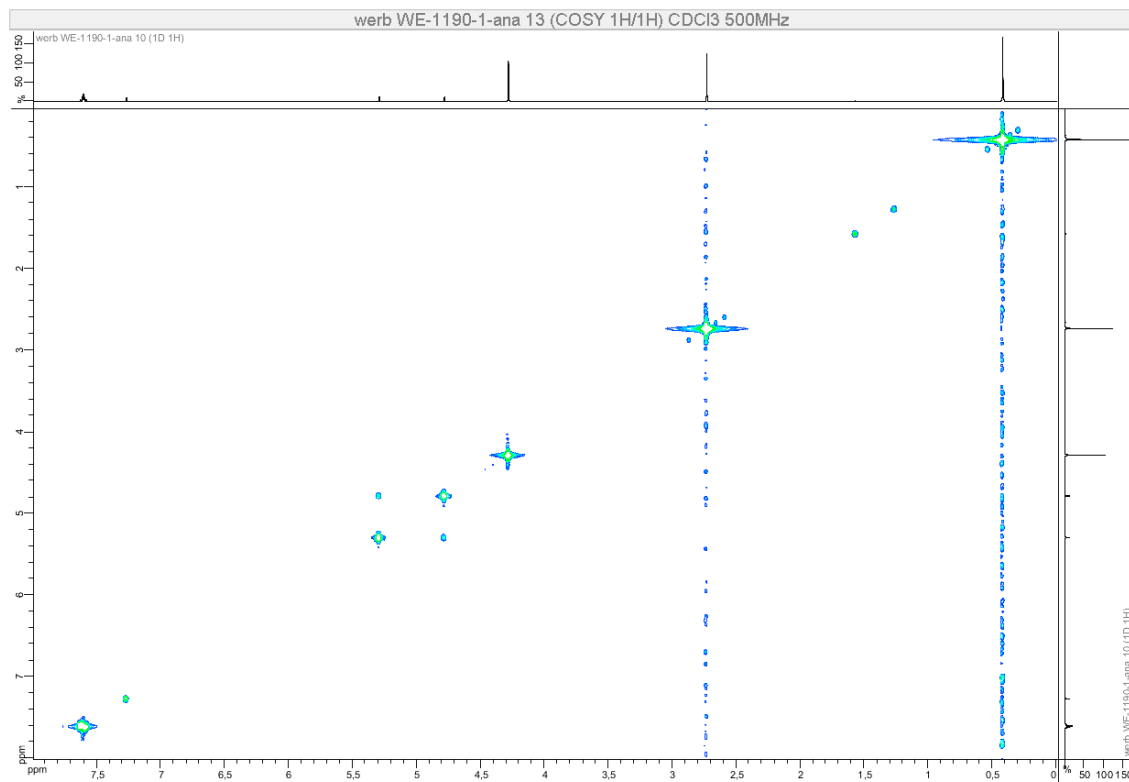


Figure S233. COSY (500 MHz, CDCl₃) of **16a** (racemic mixture)

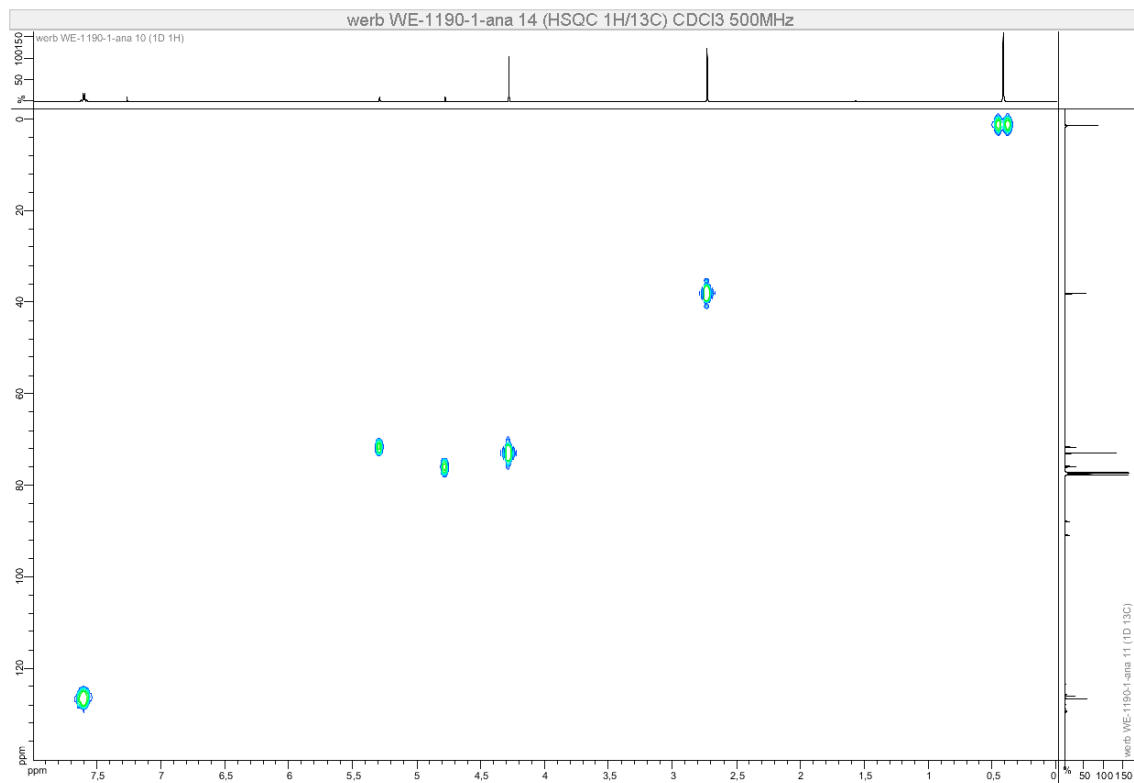


Figure S234. HSQC (500 MHz, CDCl₃) of **16a** (racemic mixture)

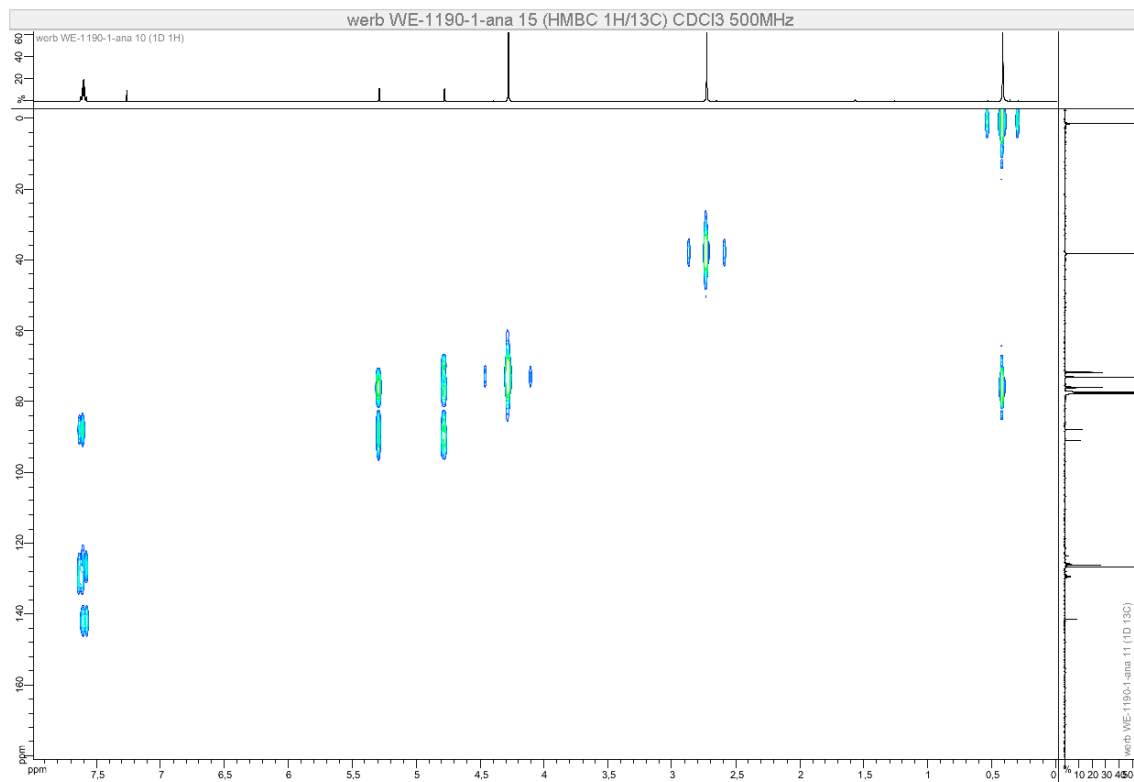


Figure S235. HMBC (500 MHz, CDCl₃) of **16a** (racemic mixture)

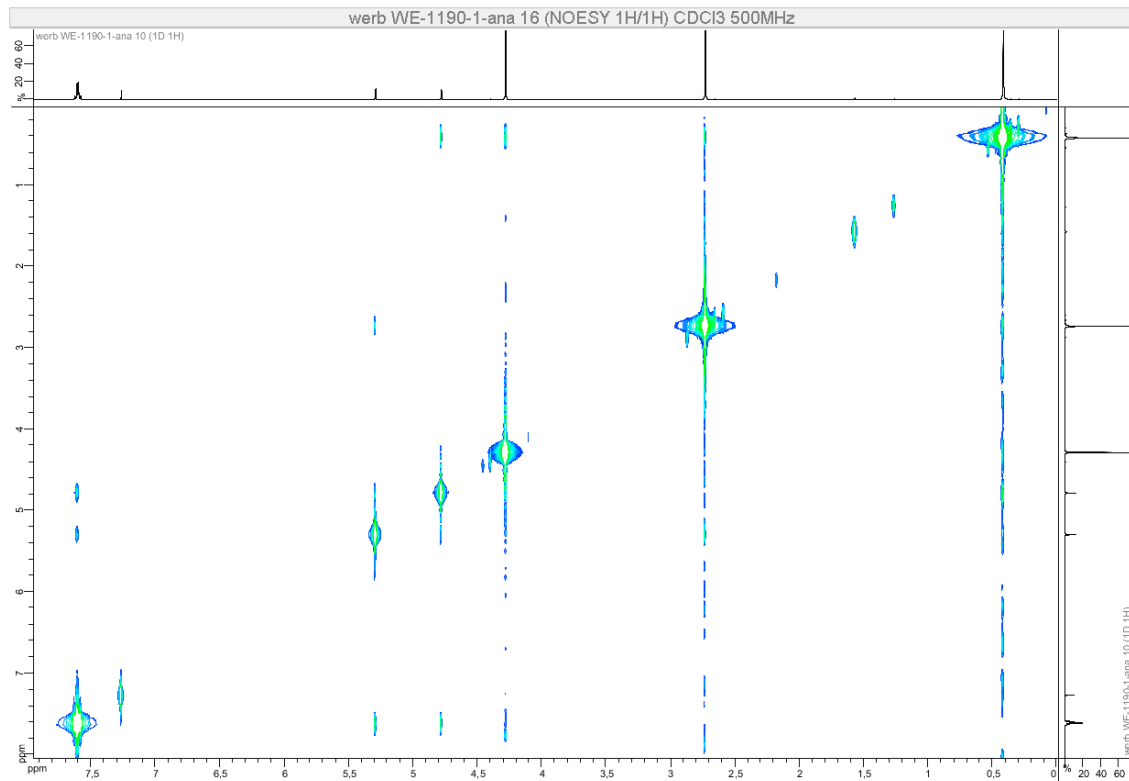


Figure S236. NOESY (500 MHz, CDCl₃) of **16a** (racemic mixture)

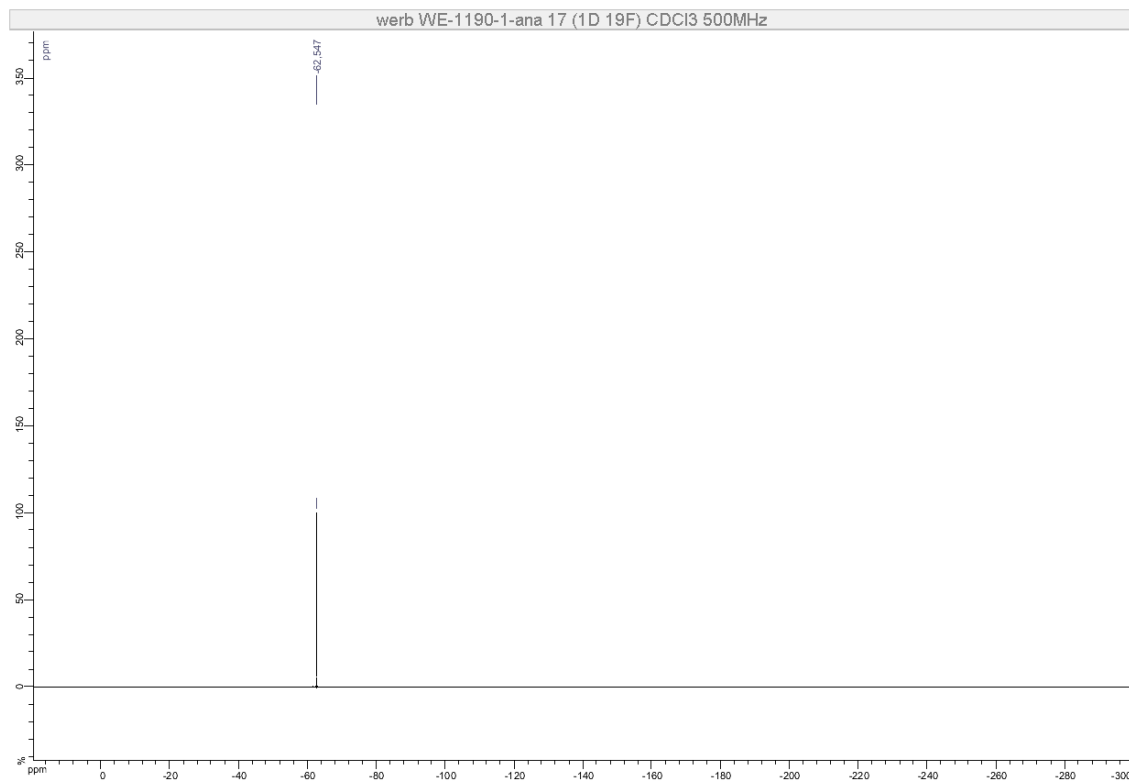


Figure S237. ¹⁹F NMR (470 MHz, CDCl₃) of **16a** (racemic mixture)

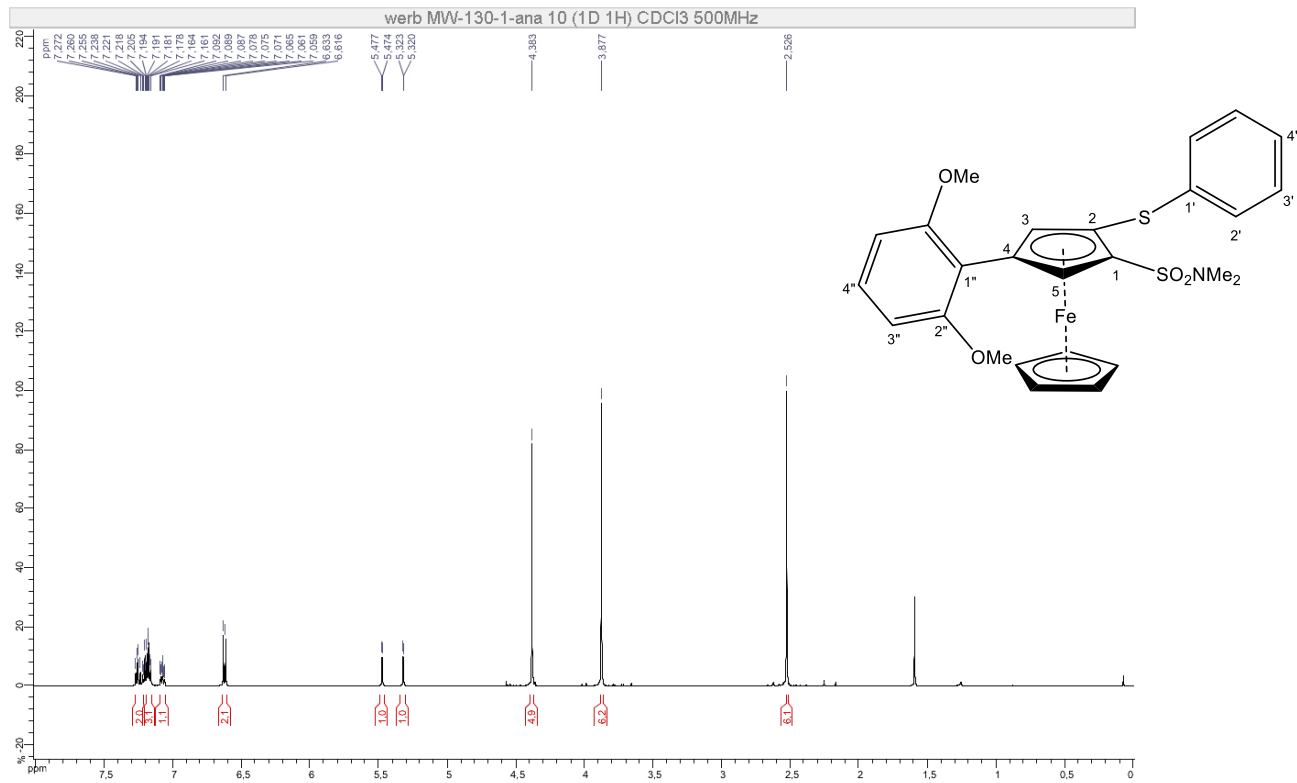


Figure S238. ¹H NMR (500 MHz, CDCl₃) of **16b** (racemic mixture)

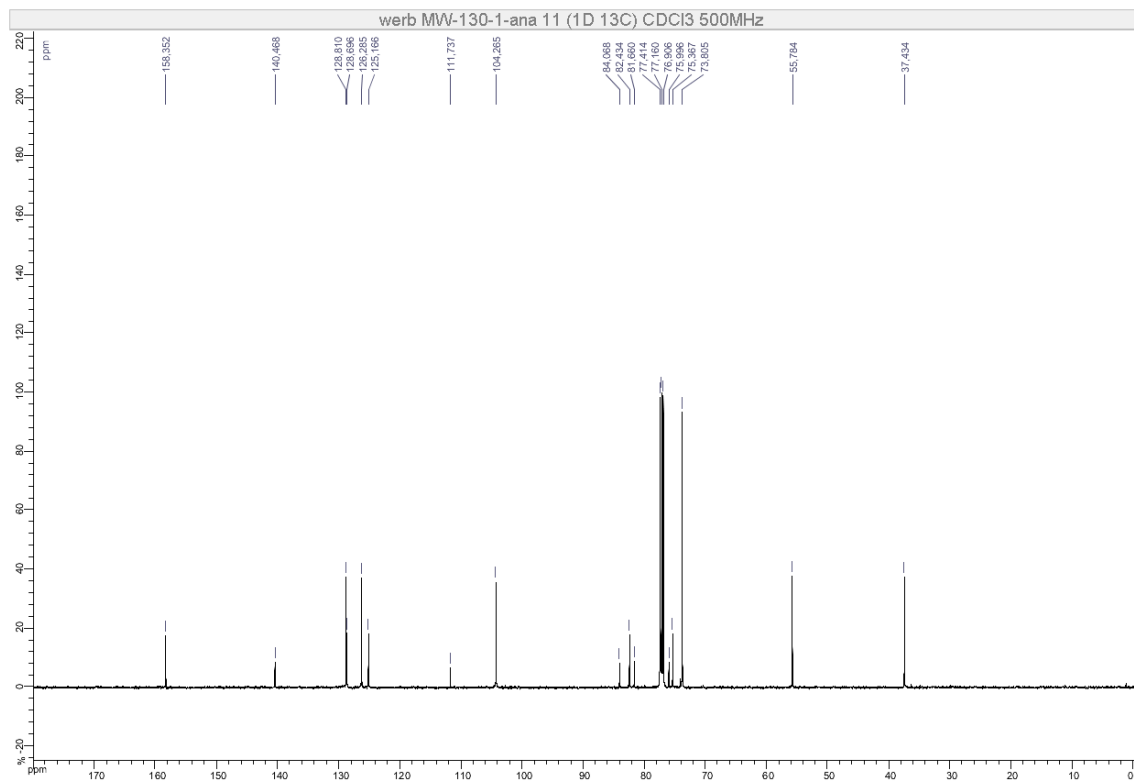


Figure S239. ¹³C NMR (126 MHz, CDCl₃) of **16b** (racemic mixture)

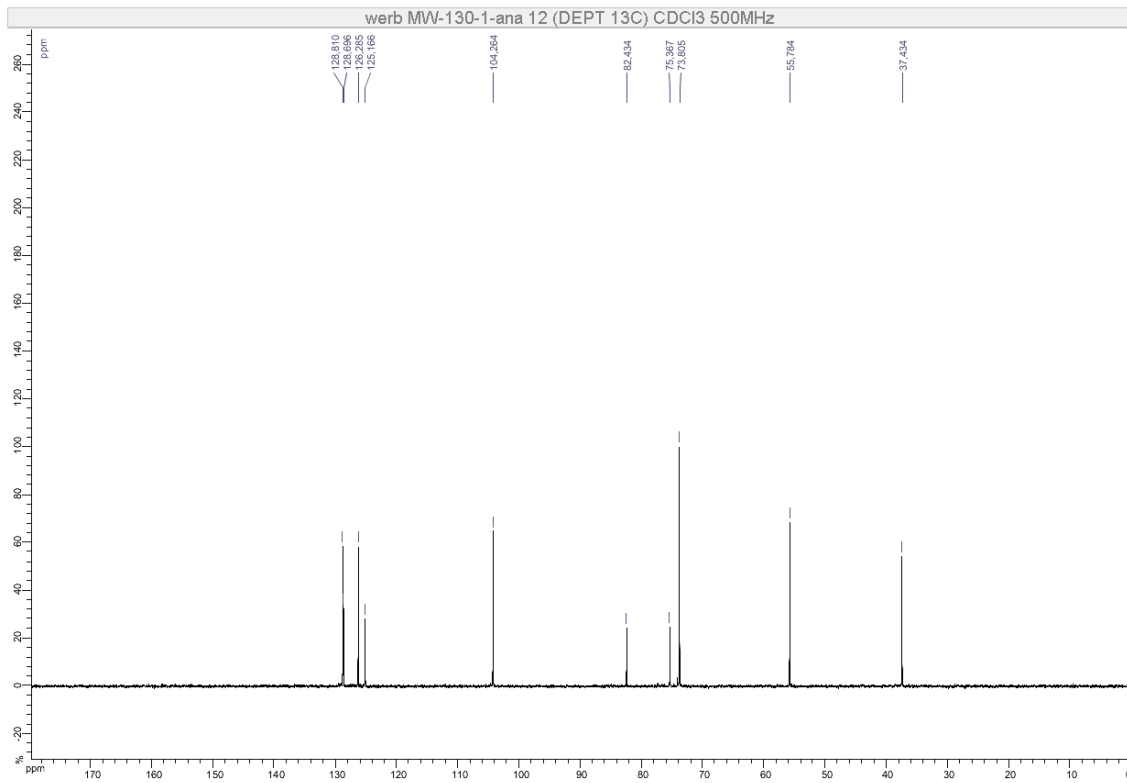


Figure S240. DEPT 135 (126 MHz, CDCl₃) of **16b** (racemic mixture)

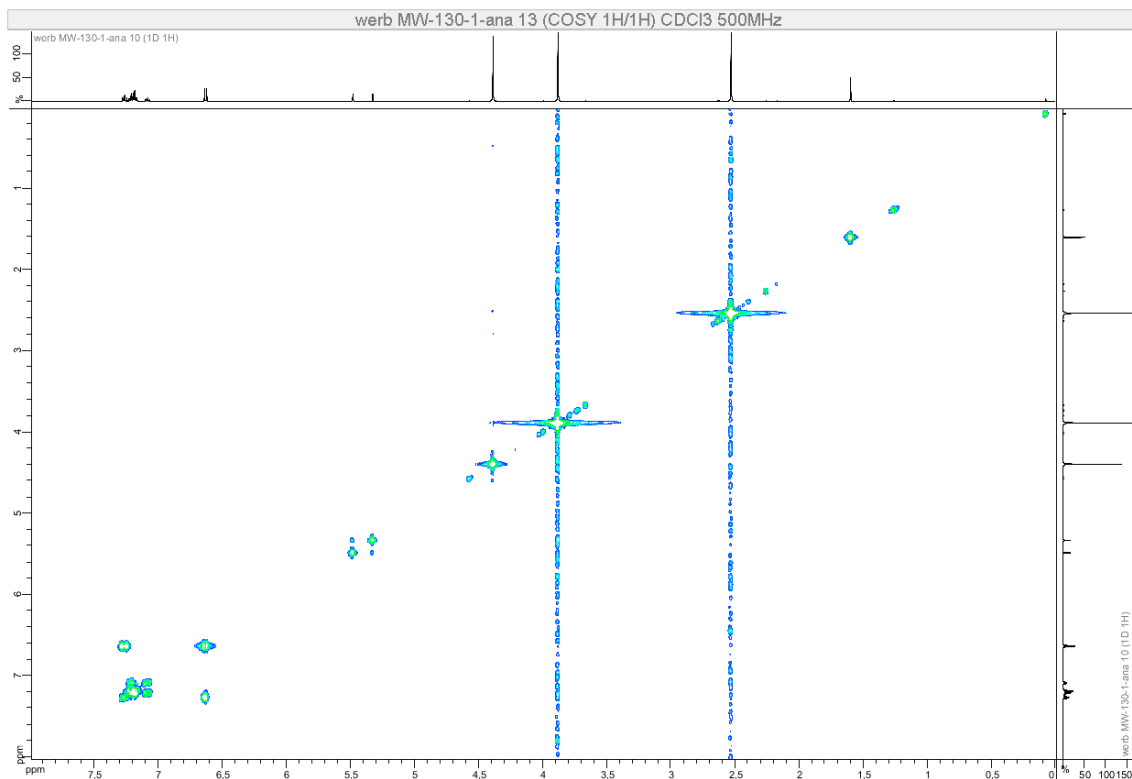


Figure S241. COSY (500 MHz, CDCl₃) of **16b** (racemic mixture)

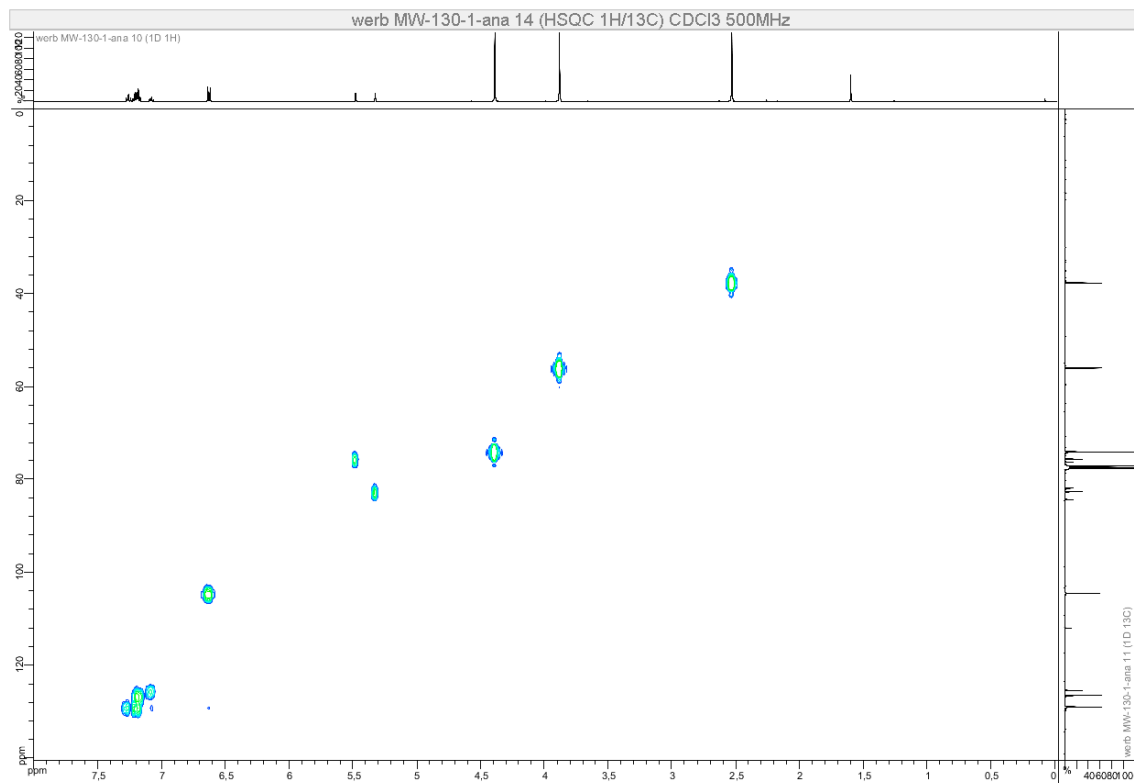


Figure S242. HSQC (500 MHz, CDCl₃) of **16b** (racemic mixture)

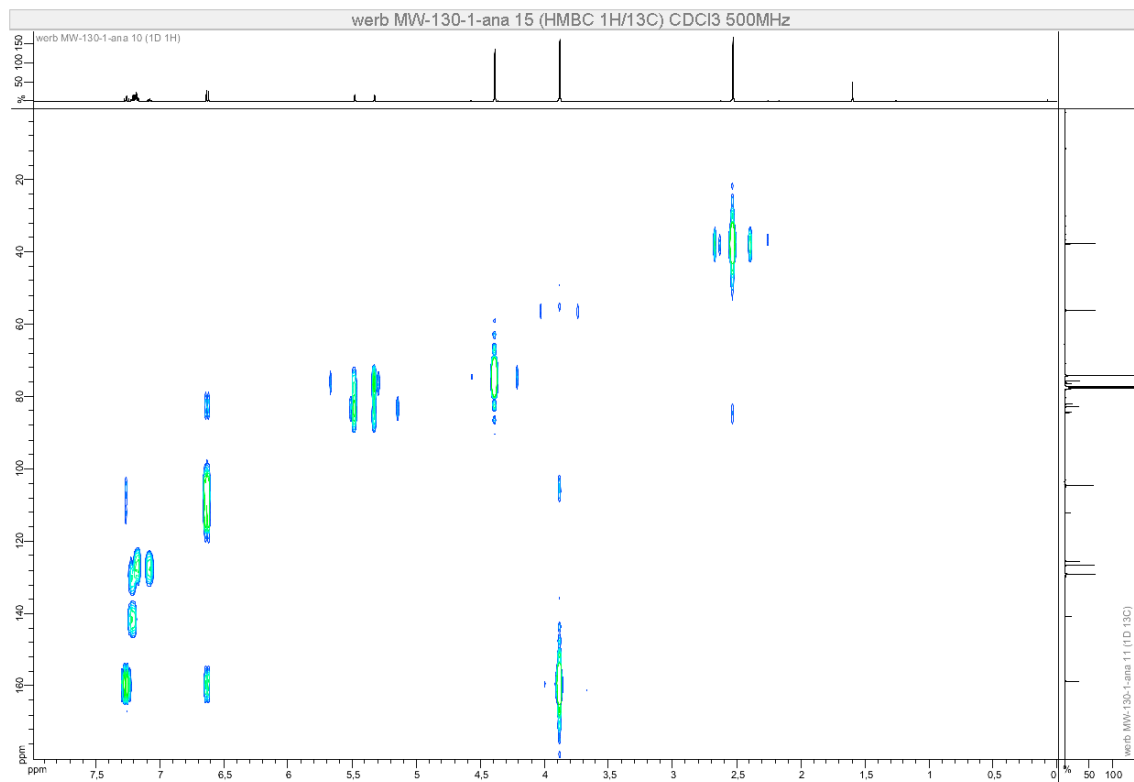


Figure S243. HMBC (500 MHz, CDCl₃) of **16b** (racemic mixture)

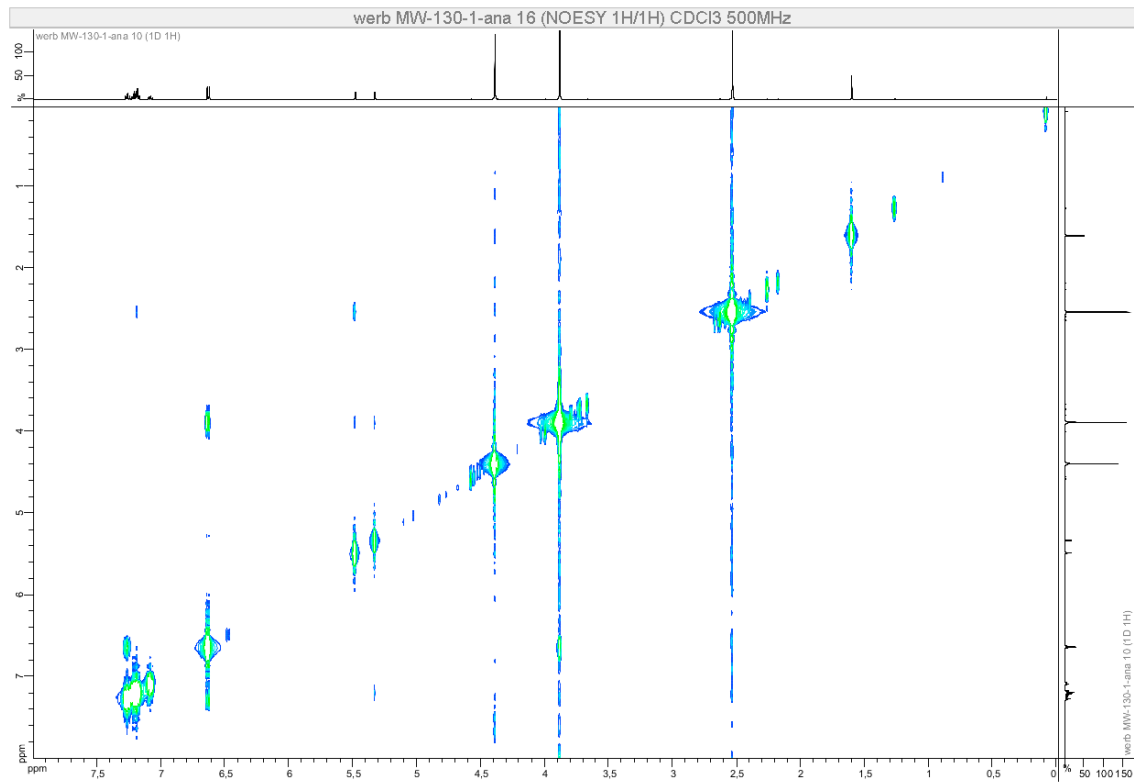


Figure S244. NOESY (500 MHz, CDCl₃) of **16b** (racemic mixture)

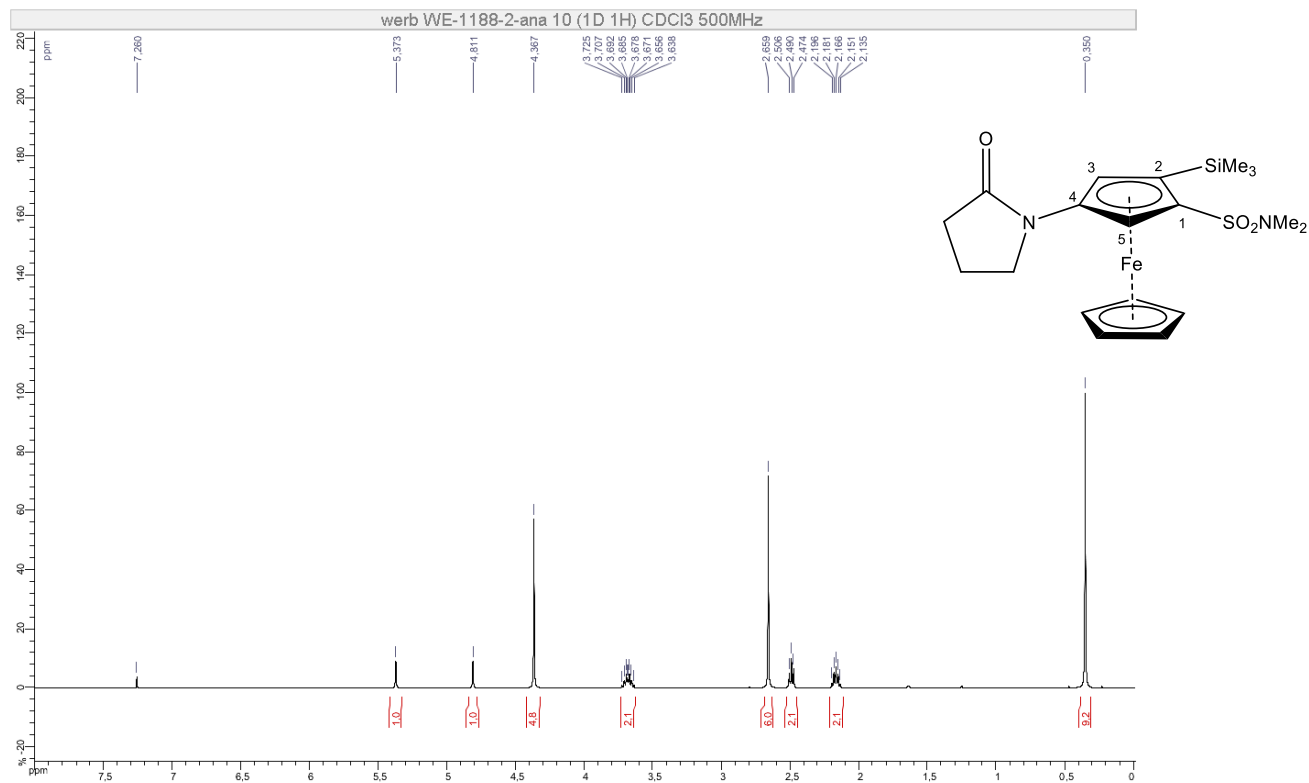


Figure S245. ^1H NMR (500 MHz, CDCl_3) of **17a** (racemic mixture)

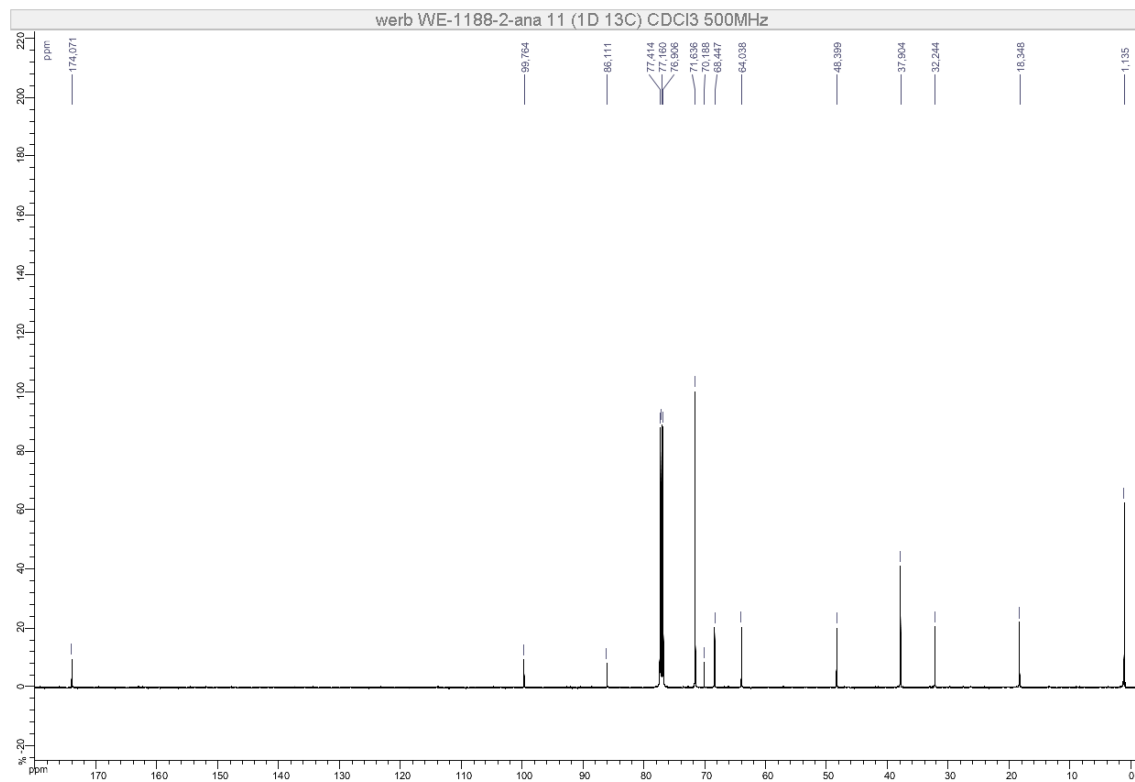


Figure S246. ^{13}C NMR (126 MHz, CDCl_3) of **17a** (racemic mixture)

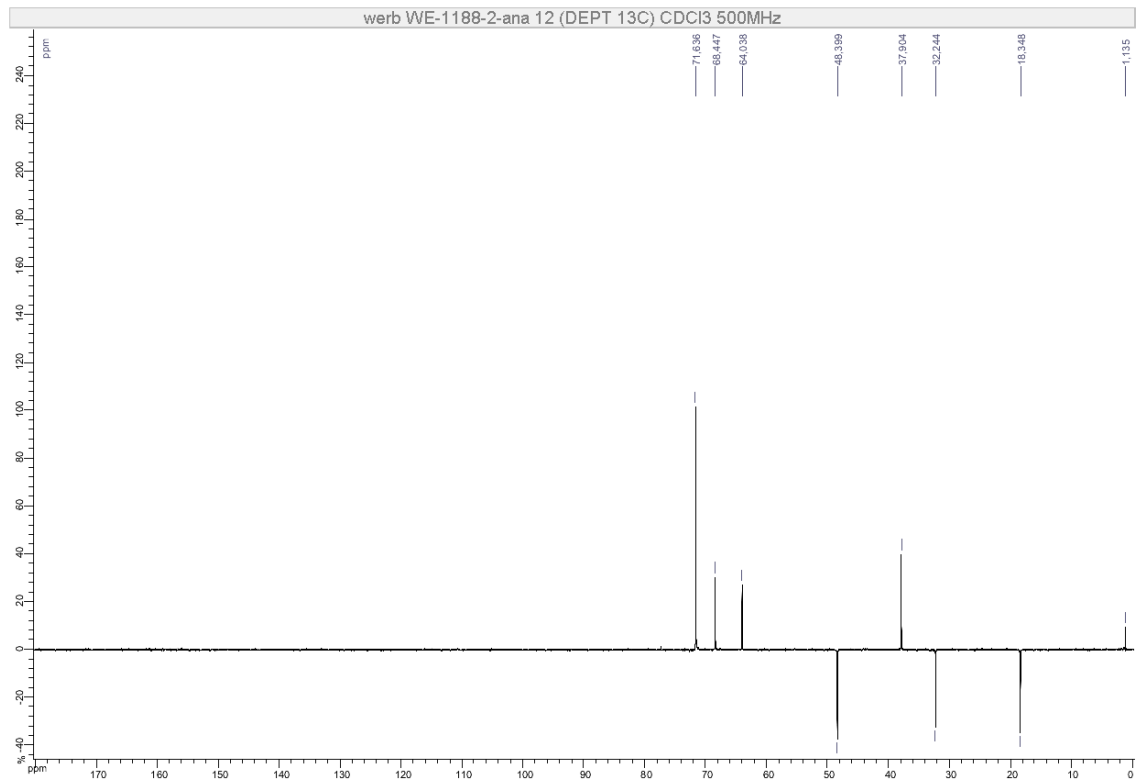


Figure S247. DEPT 135 (126 MHz, CDCl₃) of **17a** (racemic mixture)

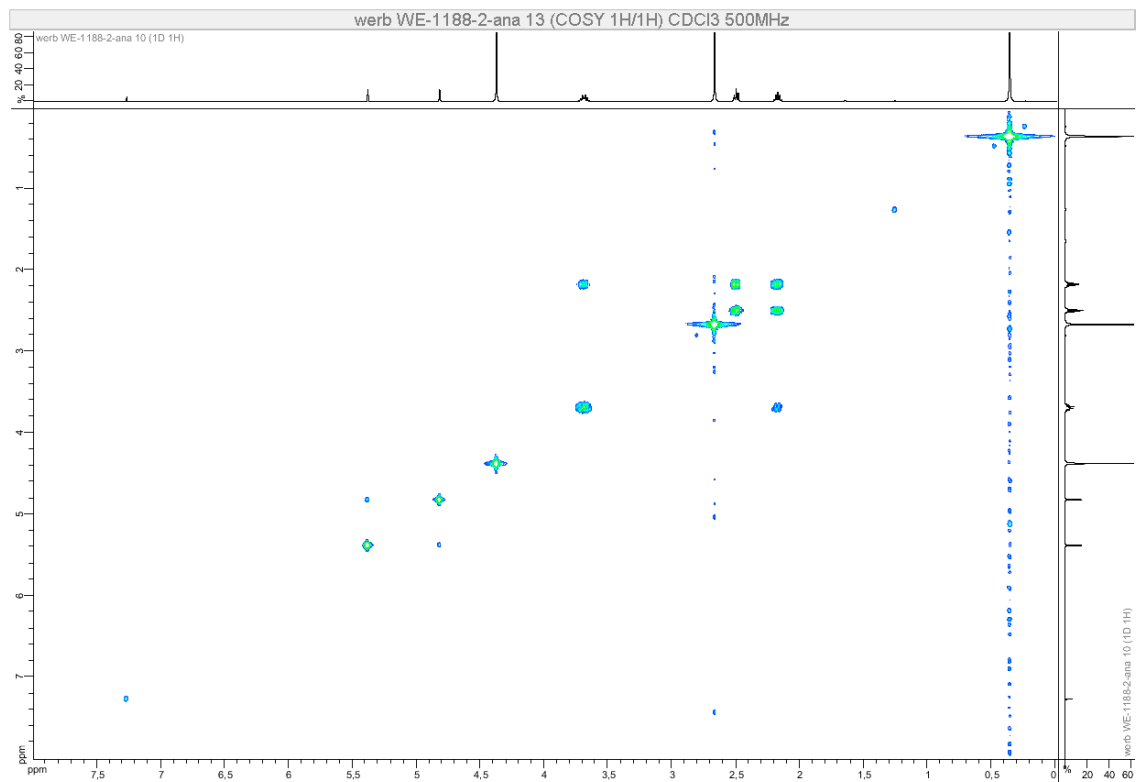


Figure S248. COSY (500 MHz, CDCl₃) of **17a** (racemic mixture)

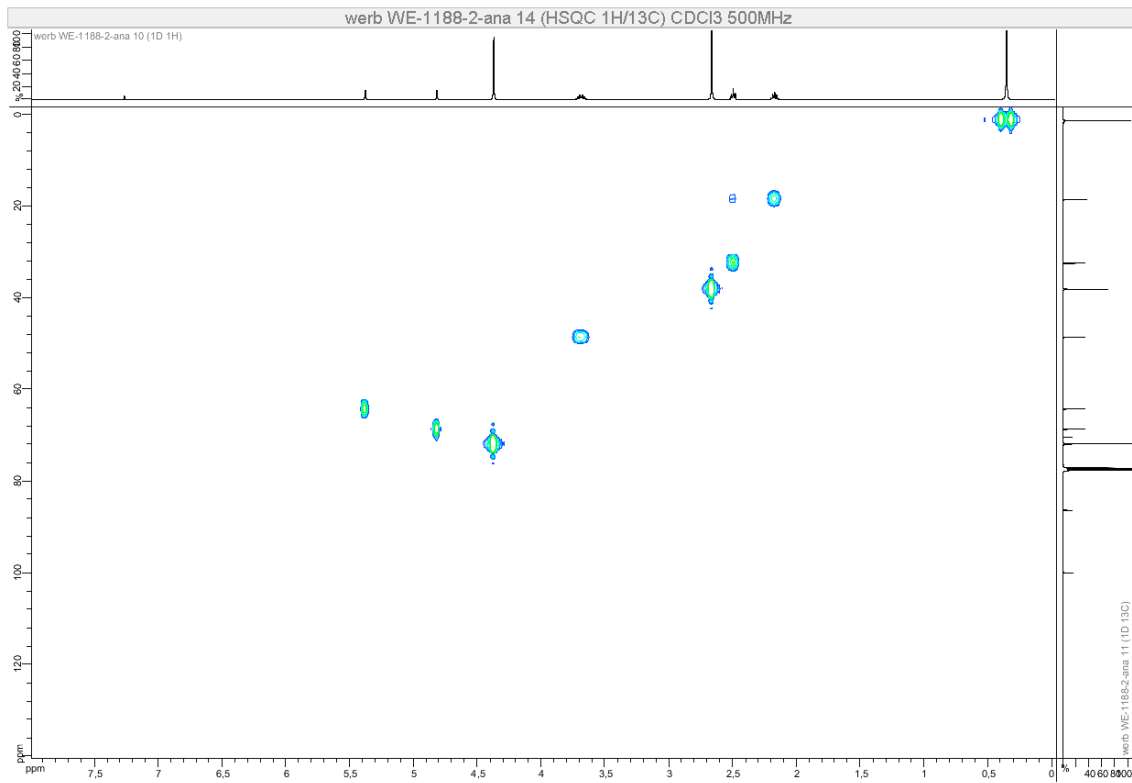


Figure S249. HSQC (500 MHz, CDCl₃) of **17a** (racemic mixture)

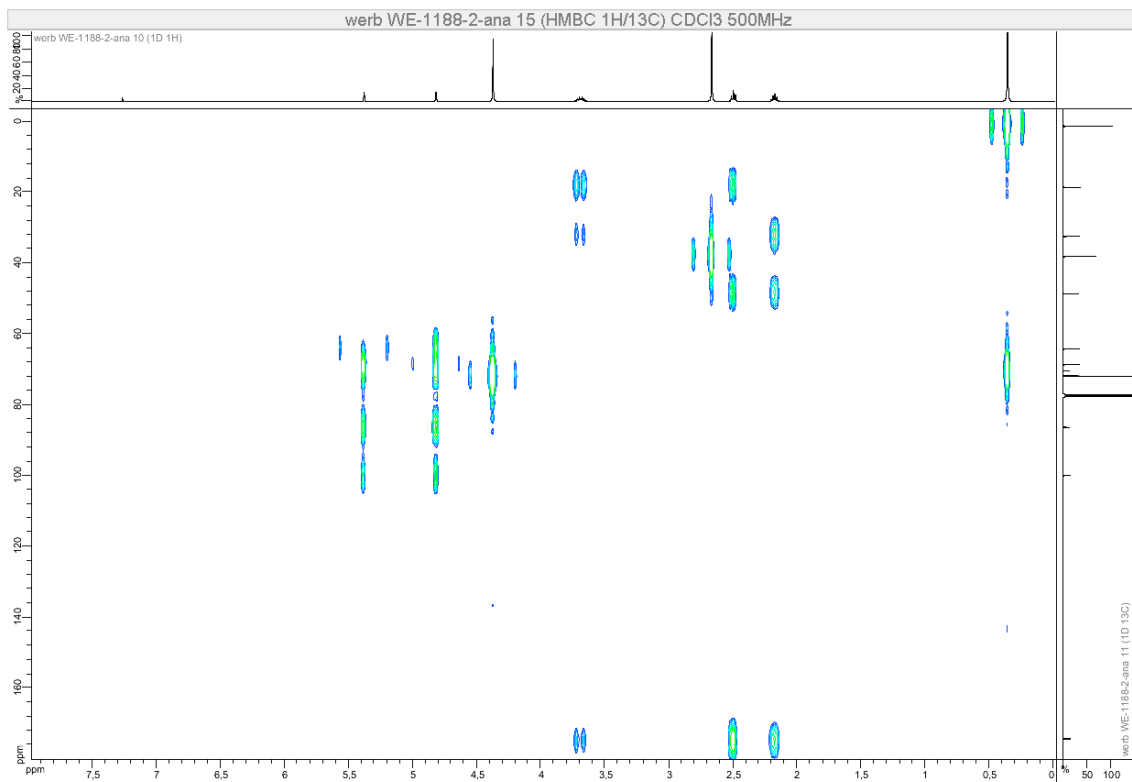


Figure S250. HMBC (500 MHz, CDCl₃) of **17a** (racemic mixture)

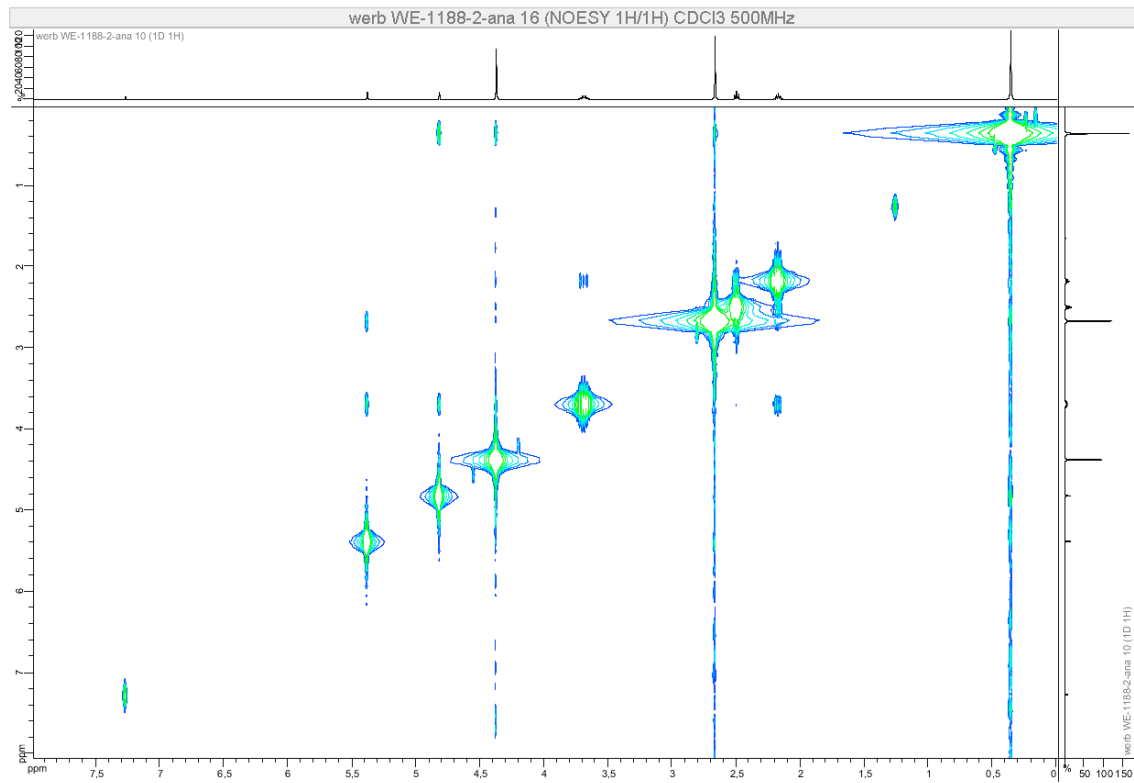


Figure S251. NOESY (500 MHz, CDCl_3) of **17a** (racemic mixture)

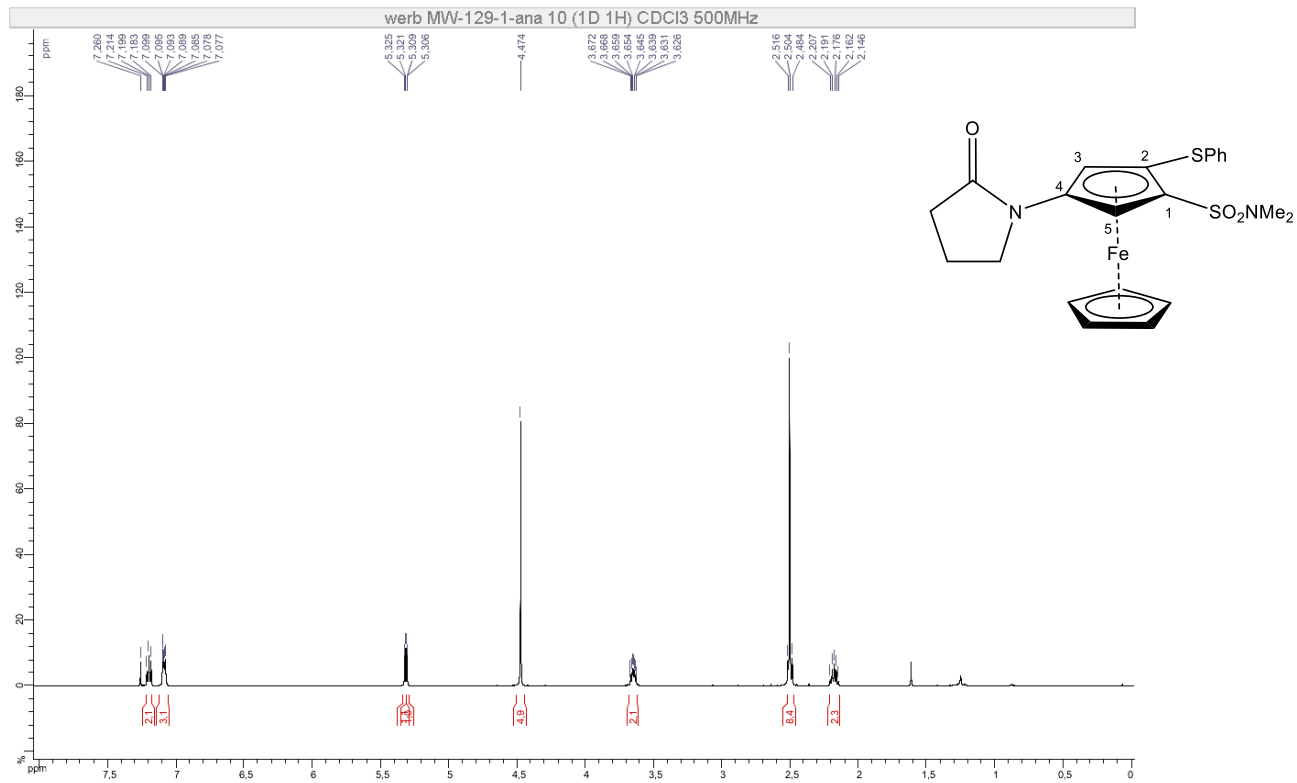


Figure S252. ¹H NMR (500 MHz, CDCl₃) of **17b** (racemic mixture)

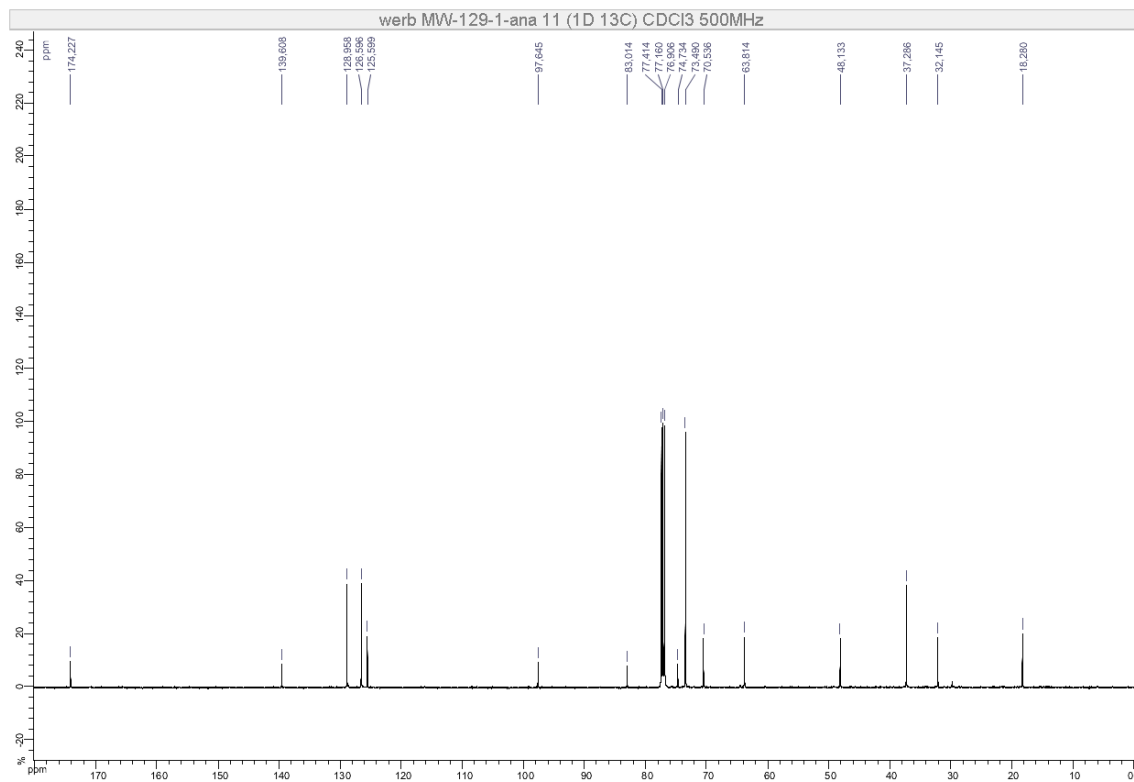


Figure S253. ¹³C NMR (126 MHz, CDCl₃) of **17b** (racemic mixture)

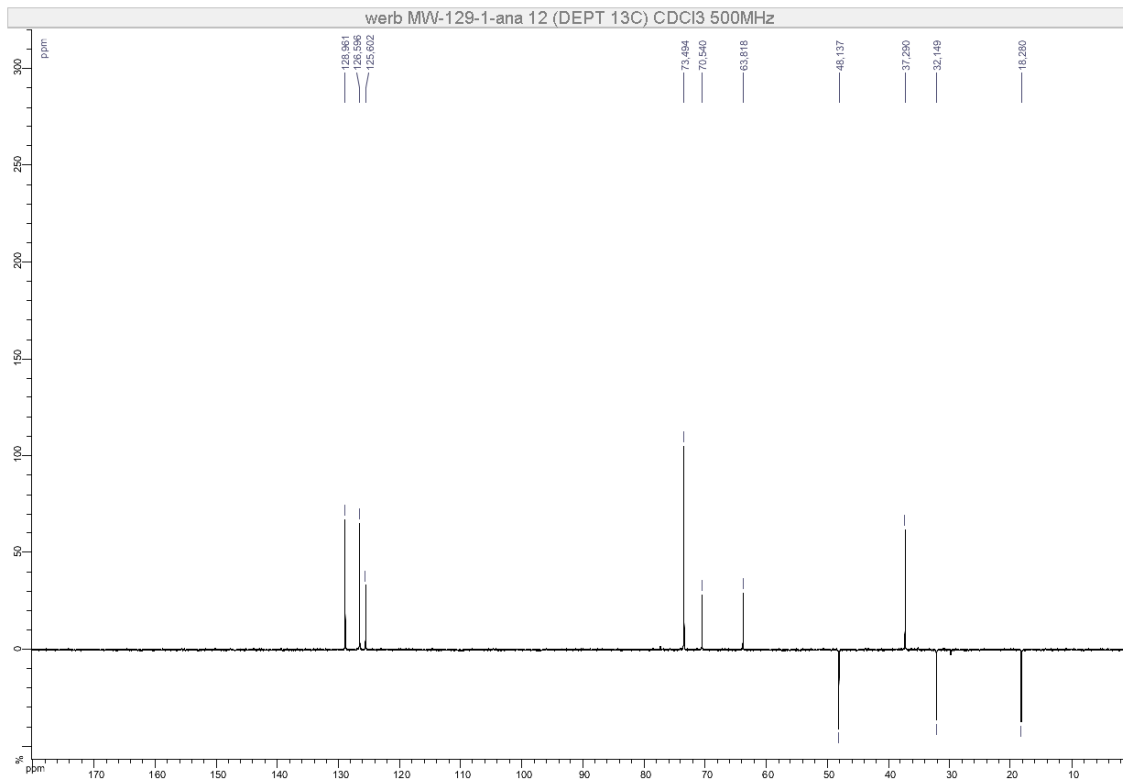


Figure S254. DEPT 135 (126 MHz, CDCl₃) of **17b** (racemic mixture)

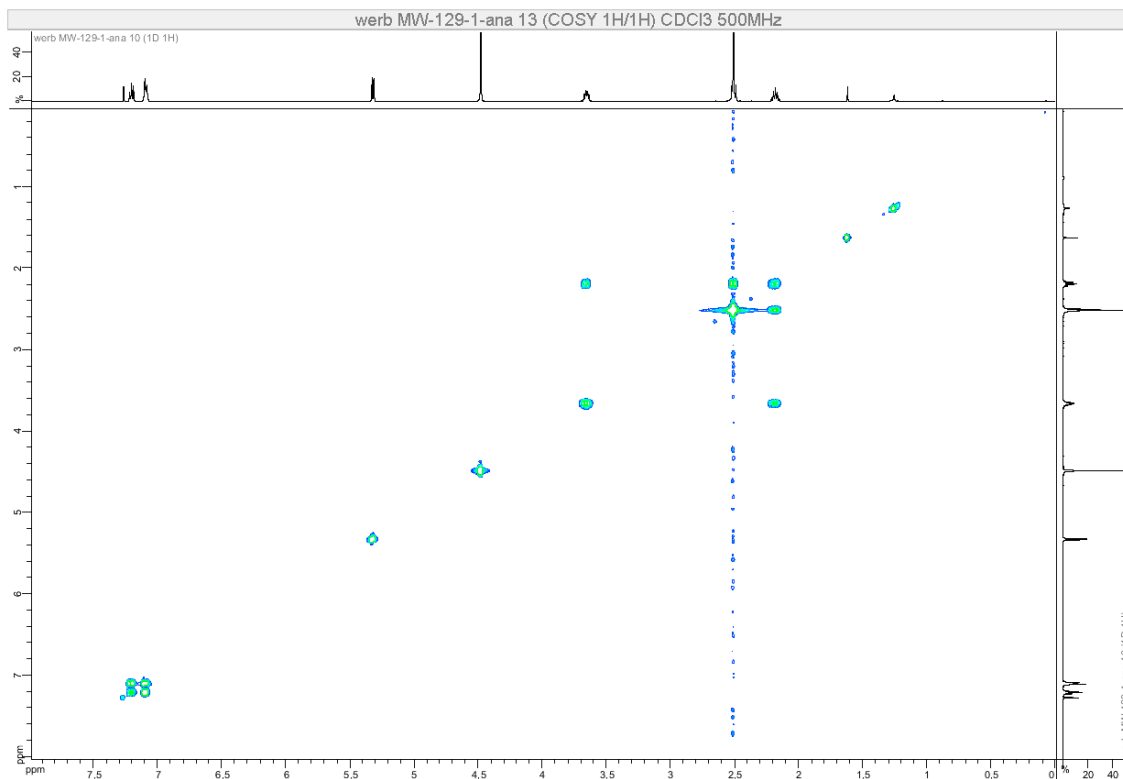


Figure S255. COSY (500 MHz, CDCl₃) of **17b** (racemic mixture)

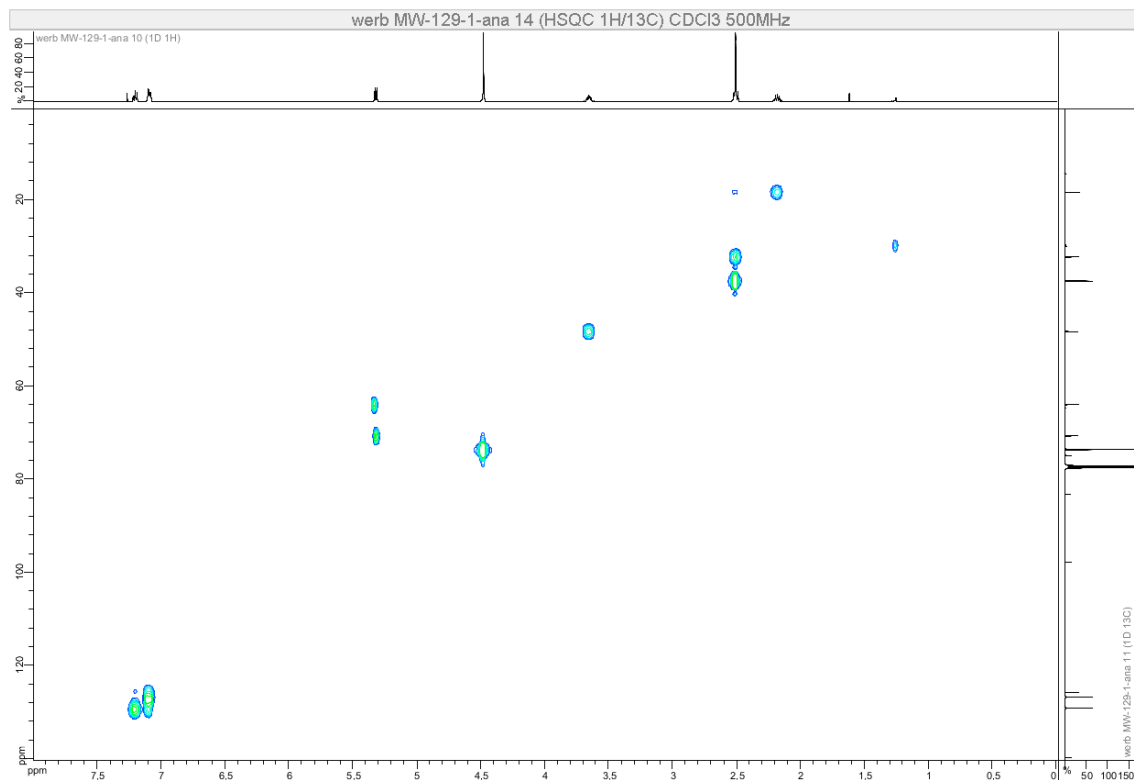


Figure S256. HSQC (500 MHz, CDCl₃) of **17b** (racemic mixture)

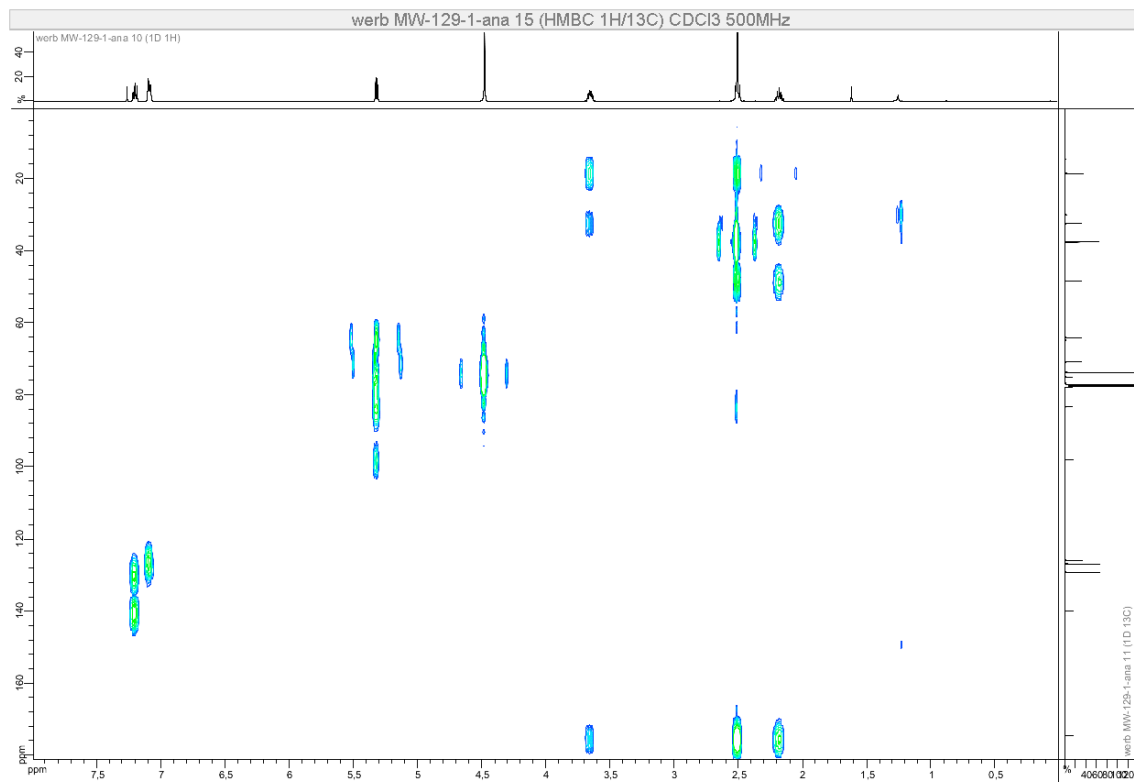
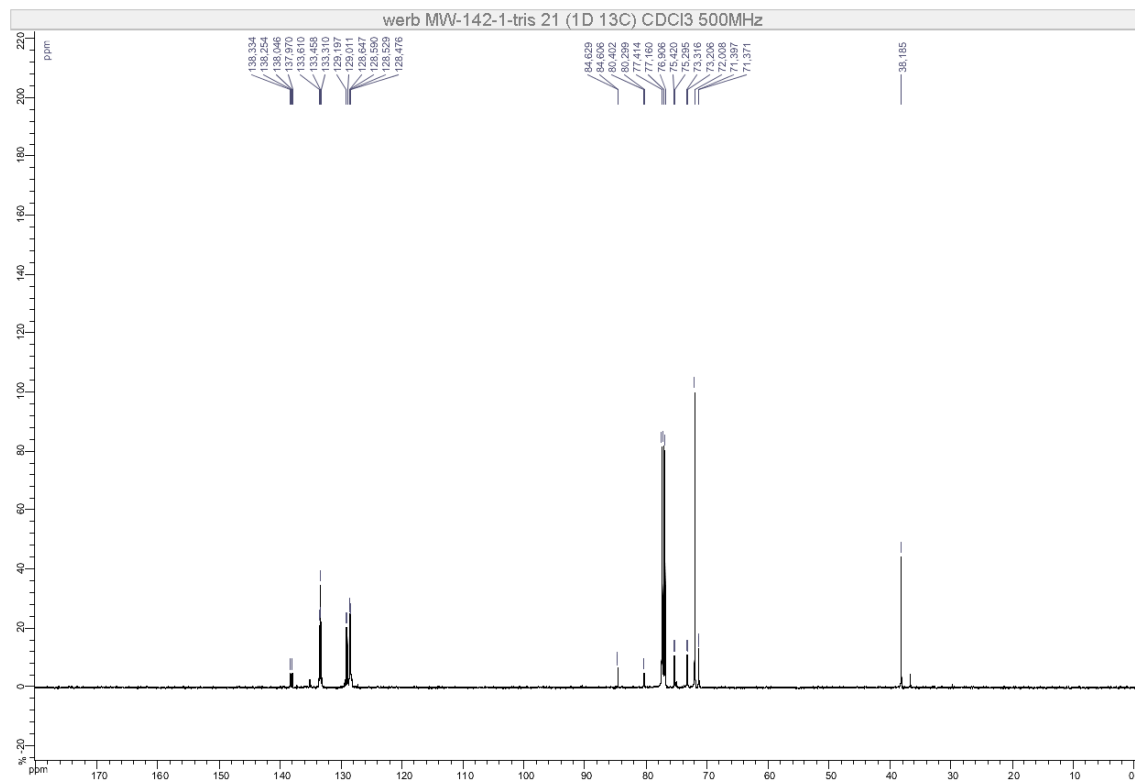
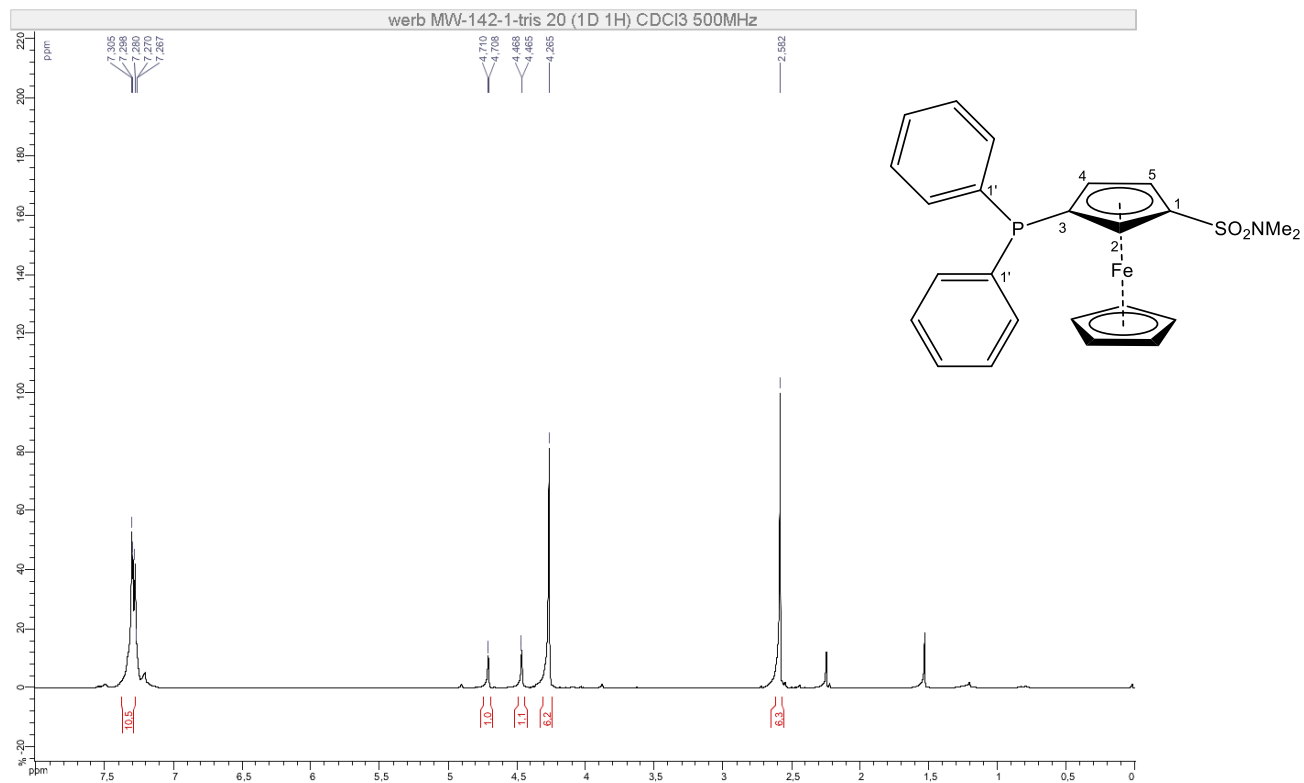


Figure S257. HMBC (500 MHz, CDCl₃) of **17b** (racemic mixture)



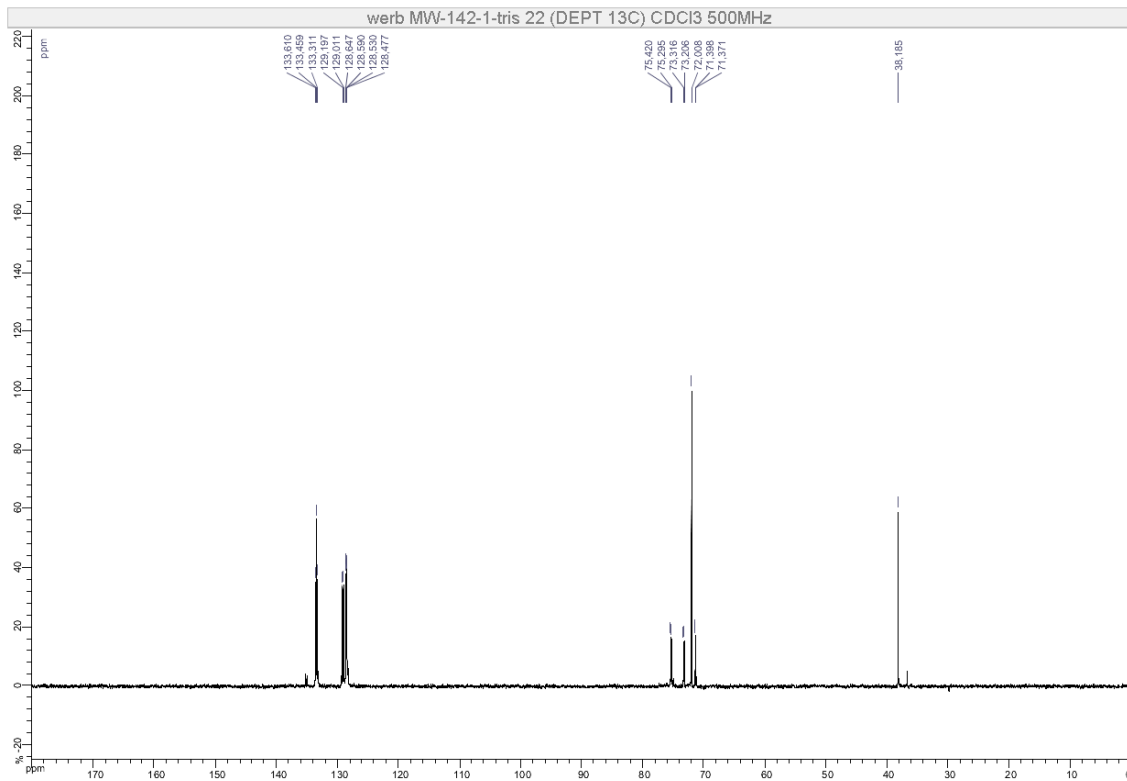


Figure S260. DEPT 135 (126 MHz, CDCl₃) of **18a** (racemic mixture)

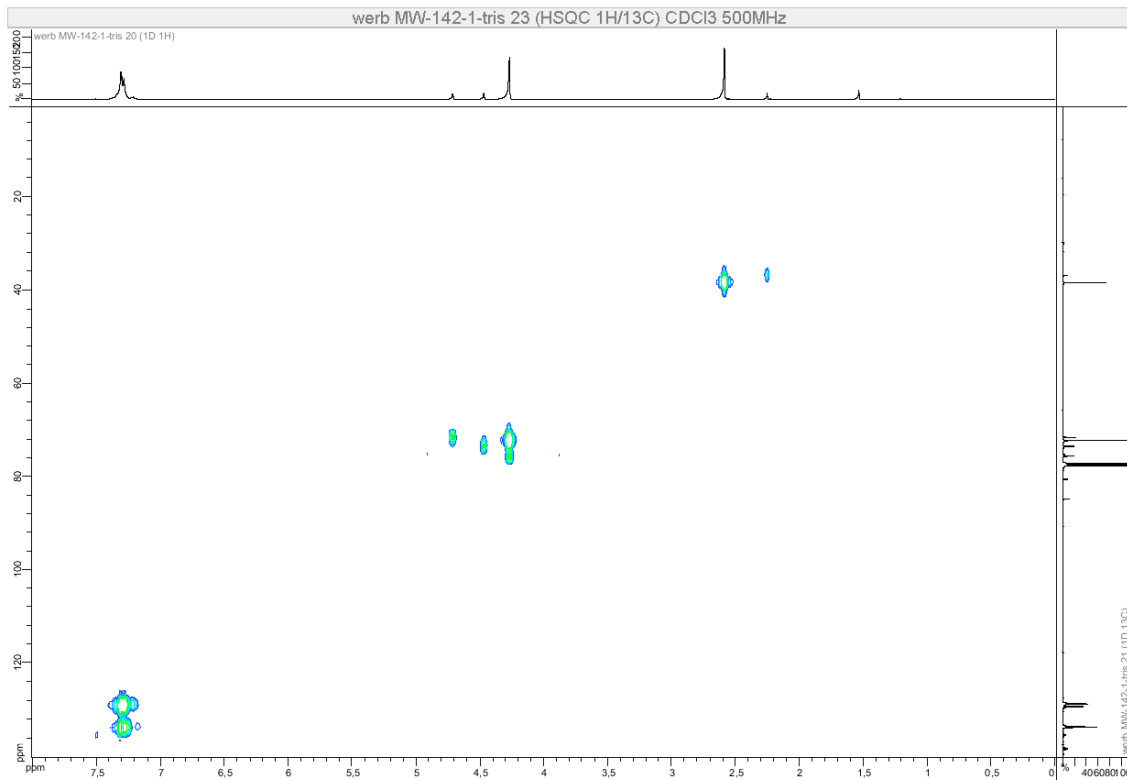


Figure S261. HSQC (500 MHz, CDCl₃) of **18a** (racemic mixture)

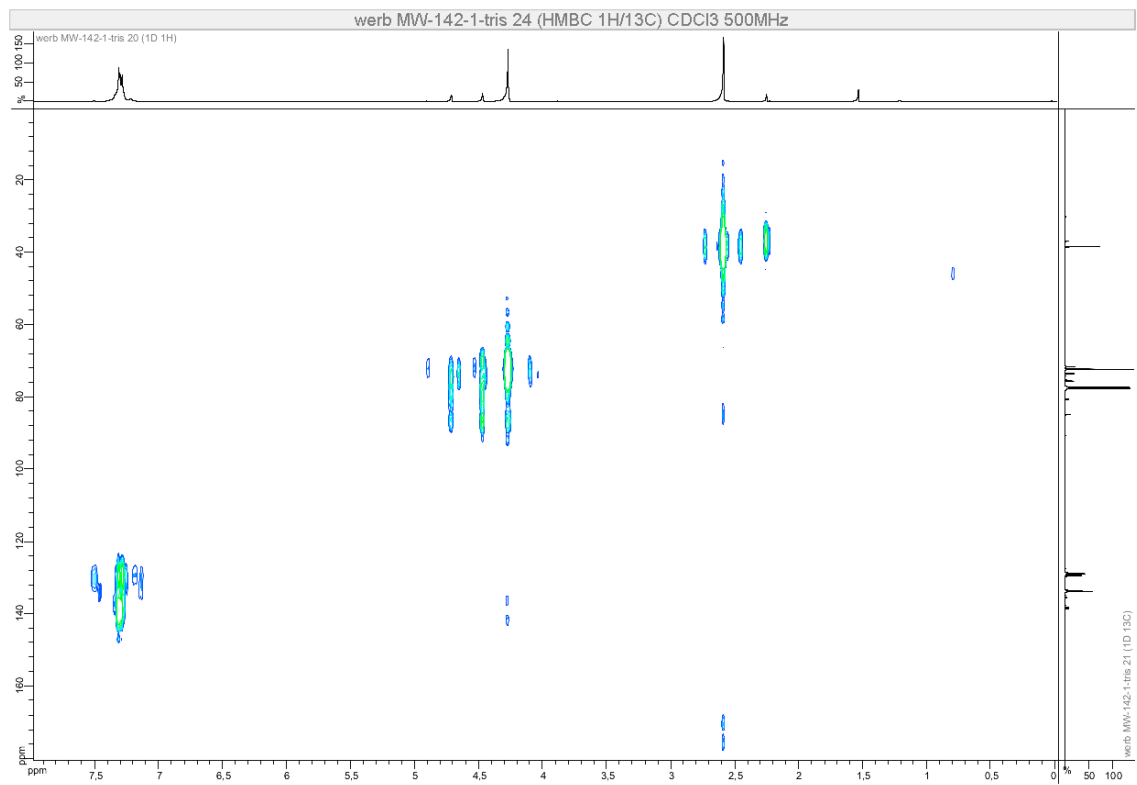


Figure S262. HMBC (500 MHz, CDCl₃) of **18a** (racemic mixture)

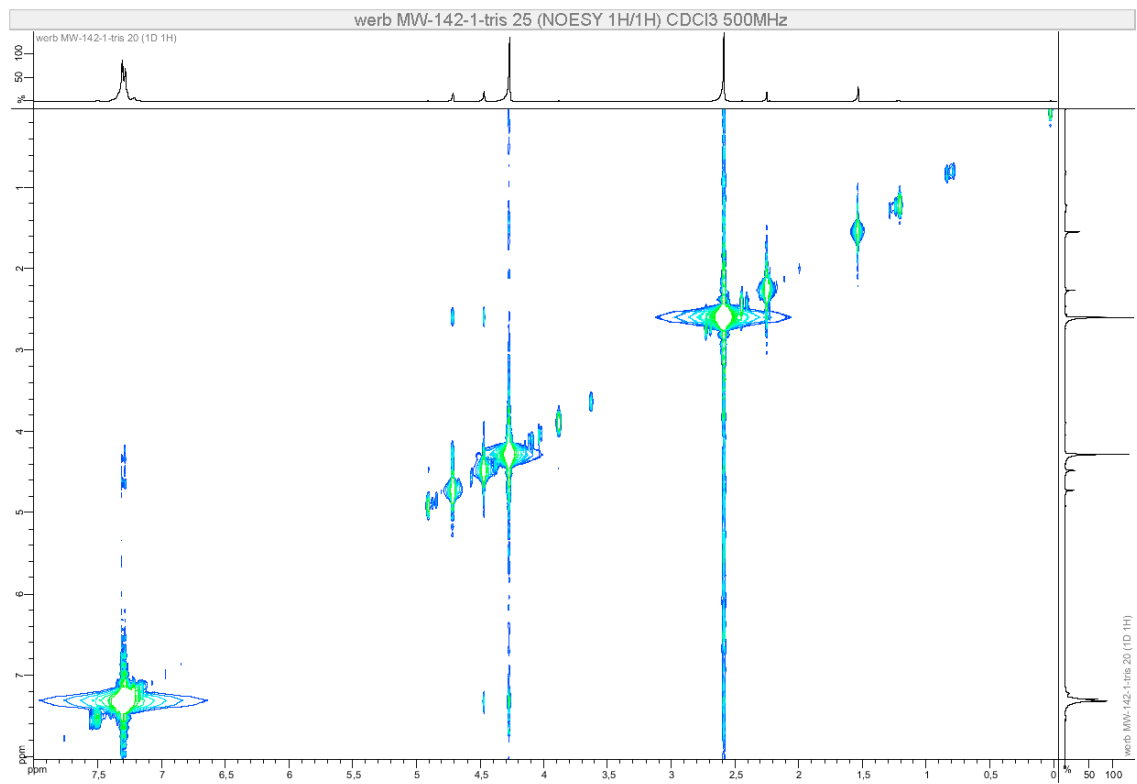


Figure S263. NOESY (500 MHz, CDCl₃) of **18a** (racemic mixture)

^{31}P NMR (202 MHz, CDCl_3)

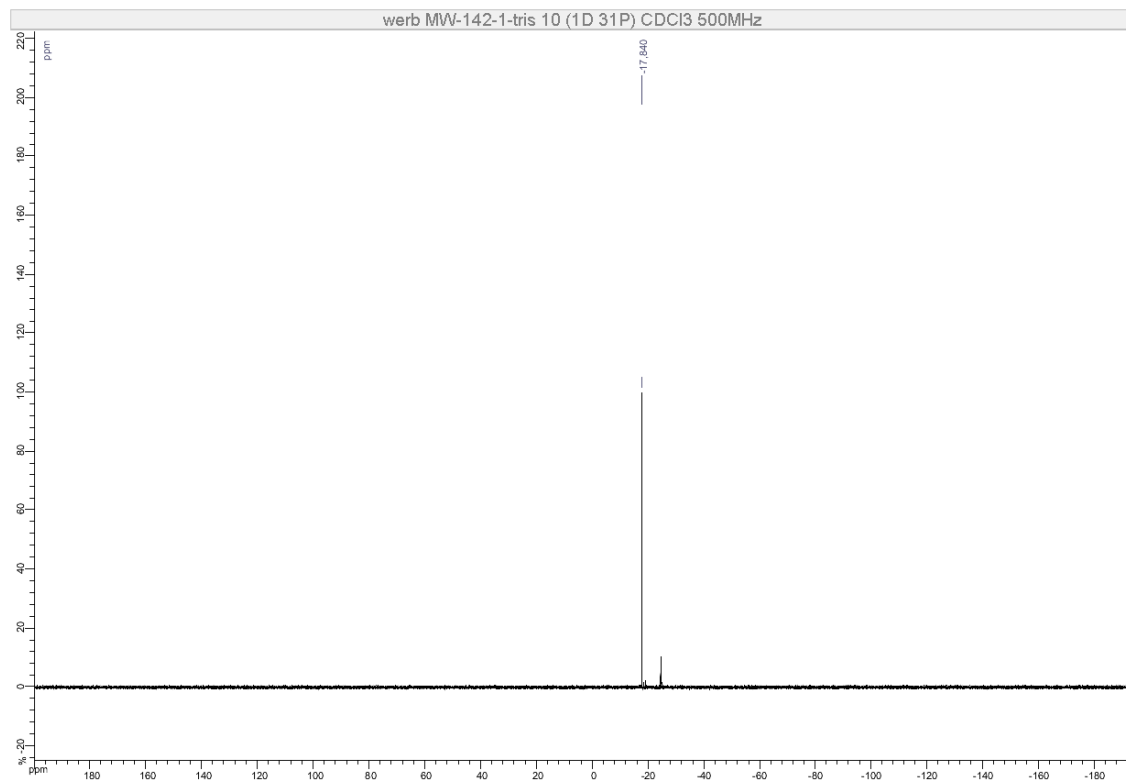


Figure S264. ^{31}P NMR (202 MHz, CDCl_3) of **18a** (racemic mixture)

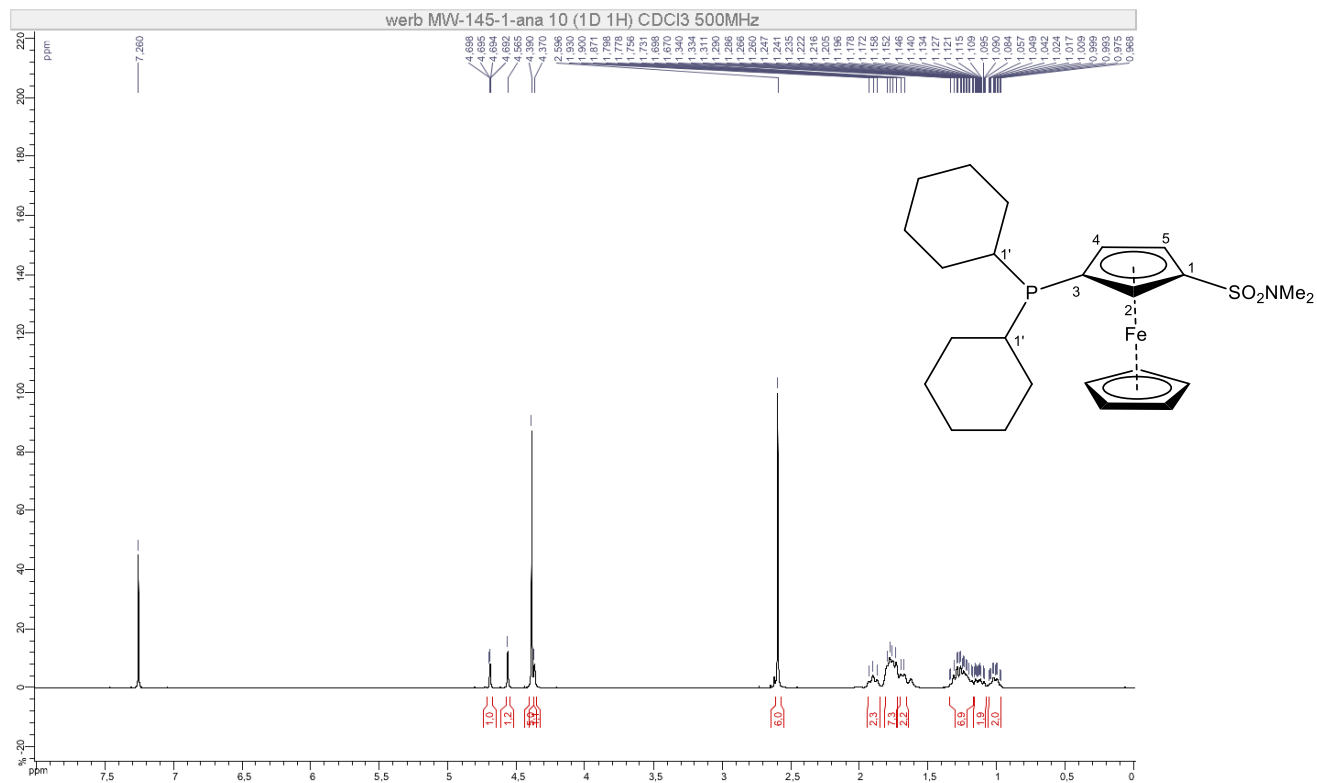


Figure S265. ¹H NMR (500 MHz, CDCl₃) of **18b** (racemic mixture)

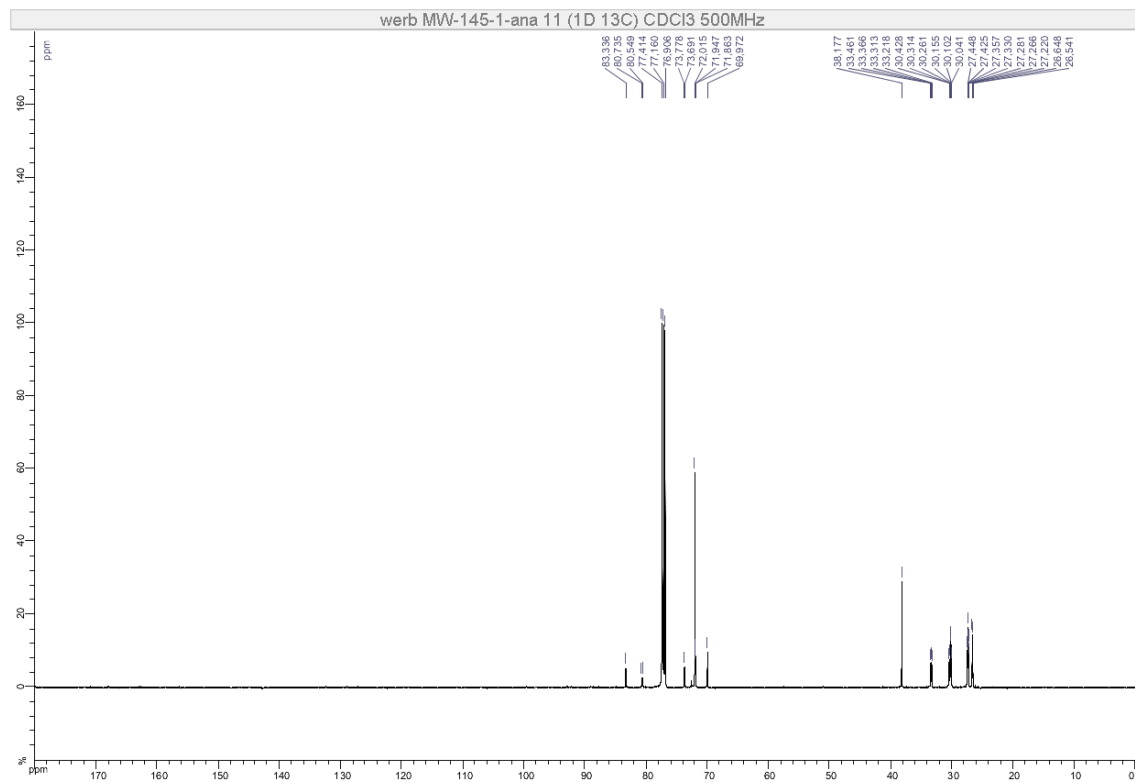


Figure S266. ¹³C NMR (126 MHz, CDCl₃) of **18b** (racemic mixture)

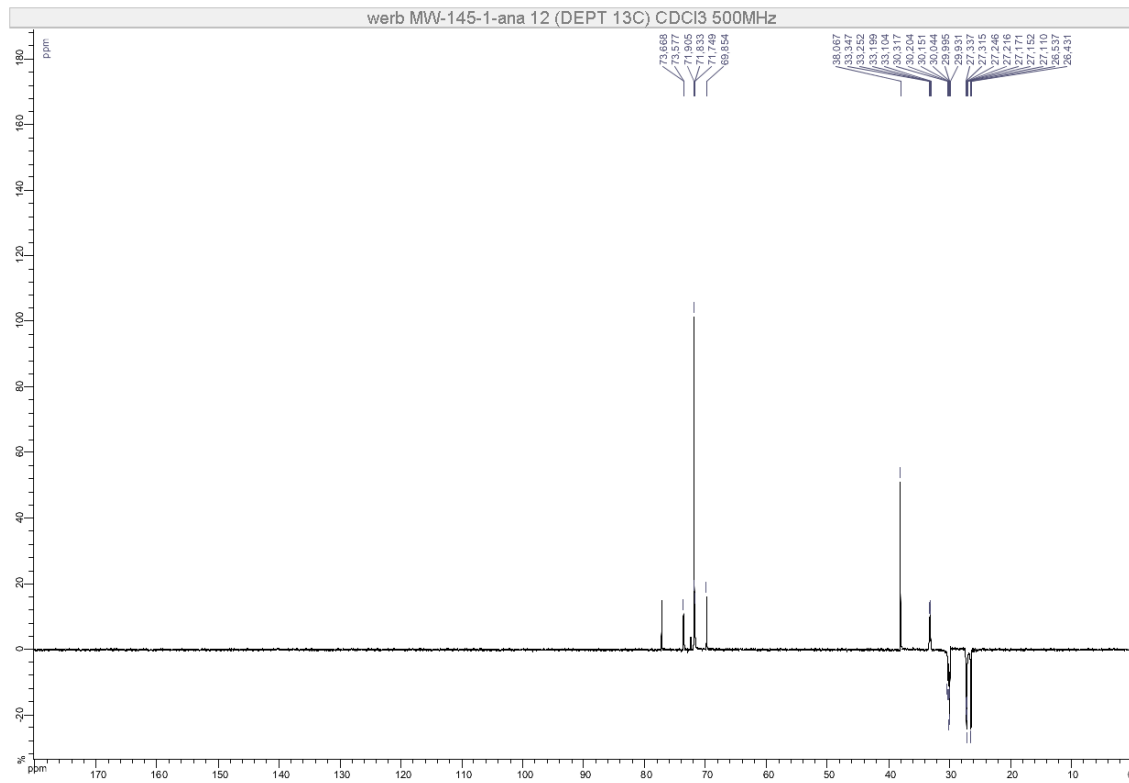


Figure S267. DEPT 135 (126 MHz, CDCl₃) of **18b** (racemic mixture)

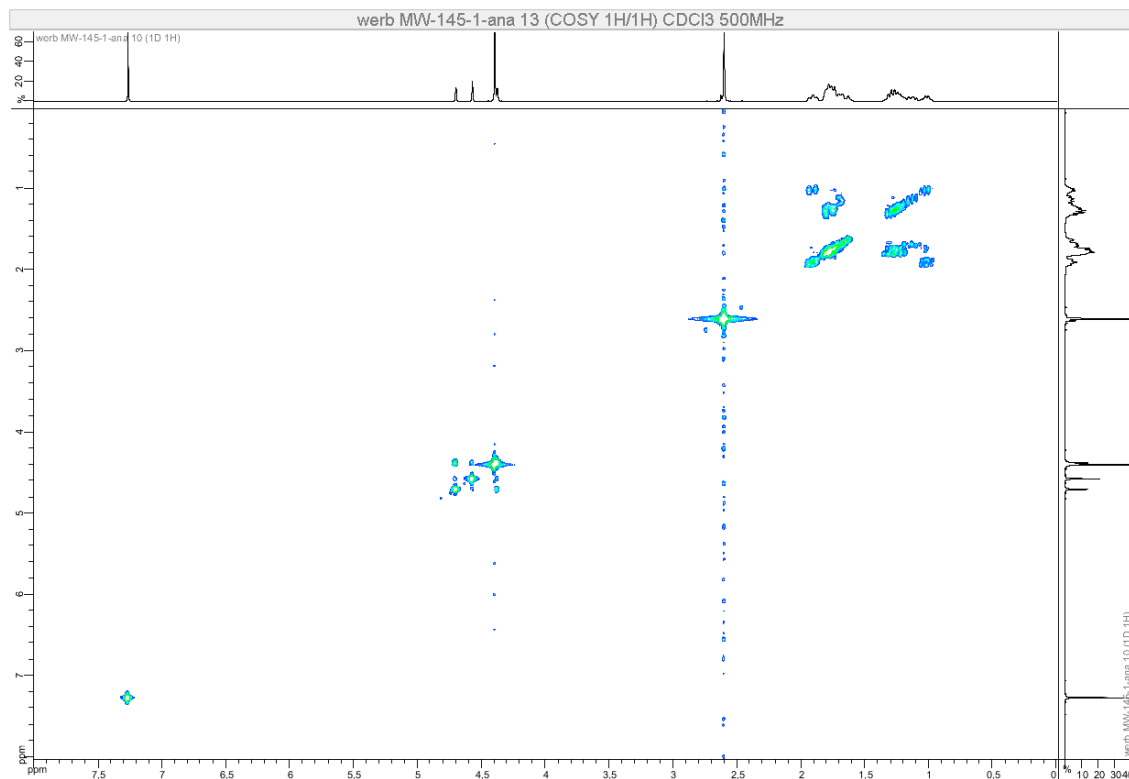


Figure S268. COSY (500 MHz, CDCl₃) of **18b** (racemic mixture)

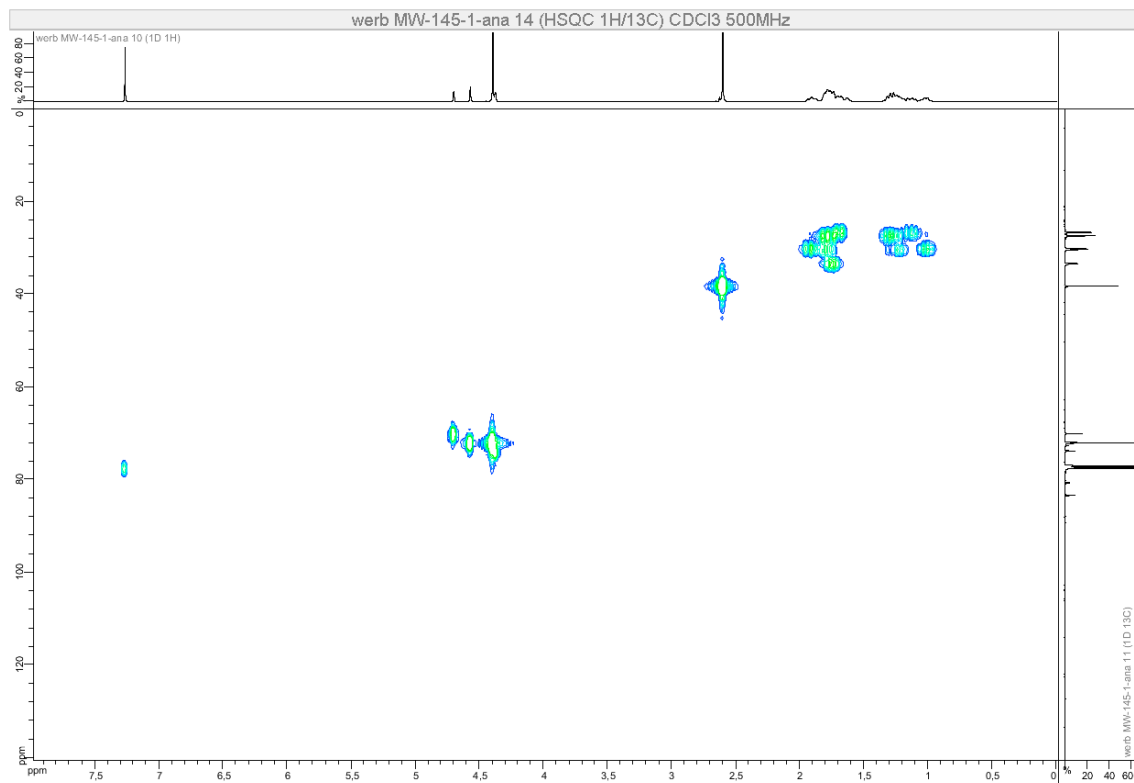


Figure S269. HSQC (500 MHz, CDCl₃) of **18b** (racemic mixture)

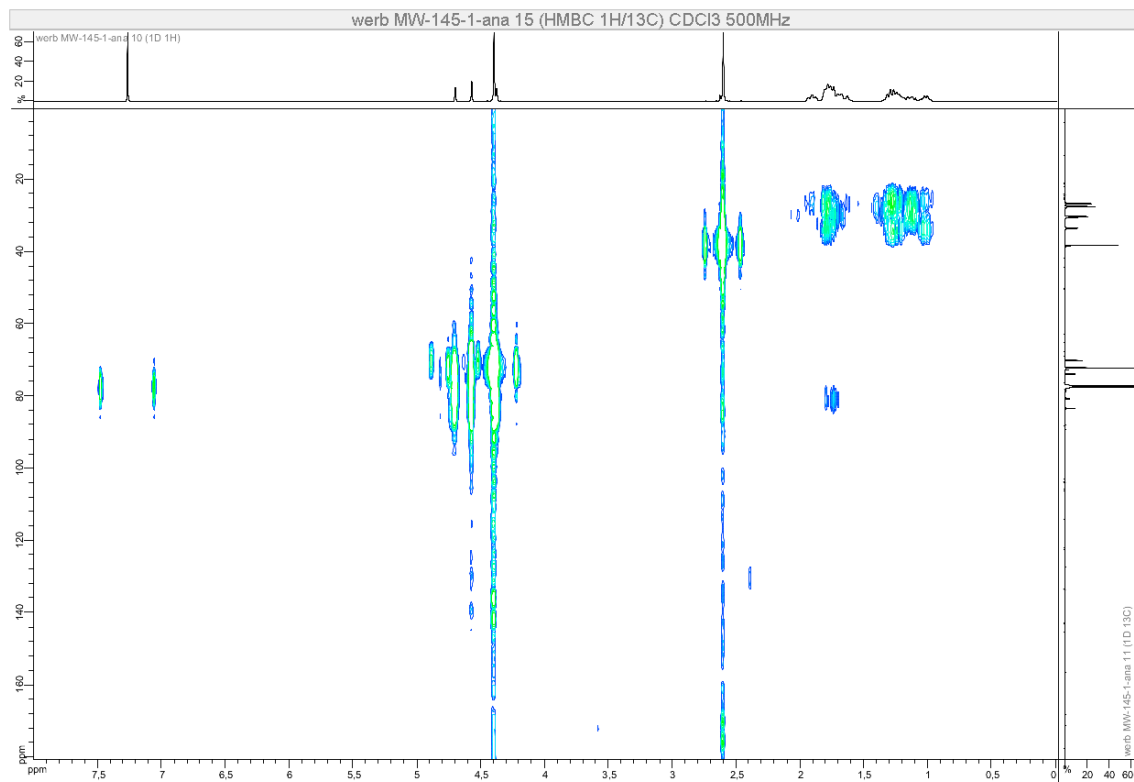


Figure S270. HMBC (500 MHz, CDCl₃) of **18b** (racemic mixture)

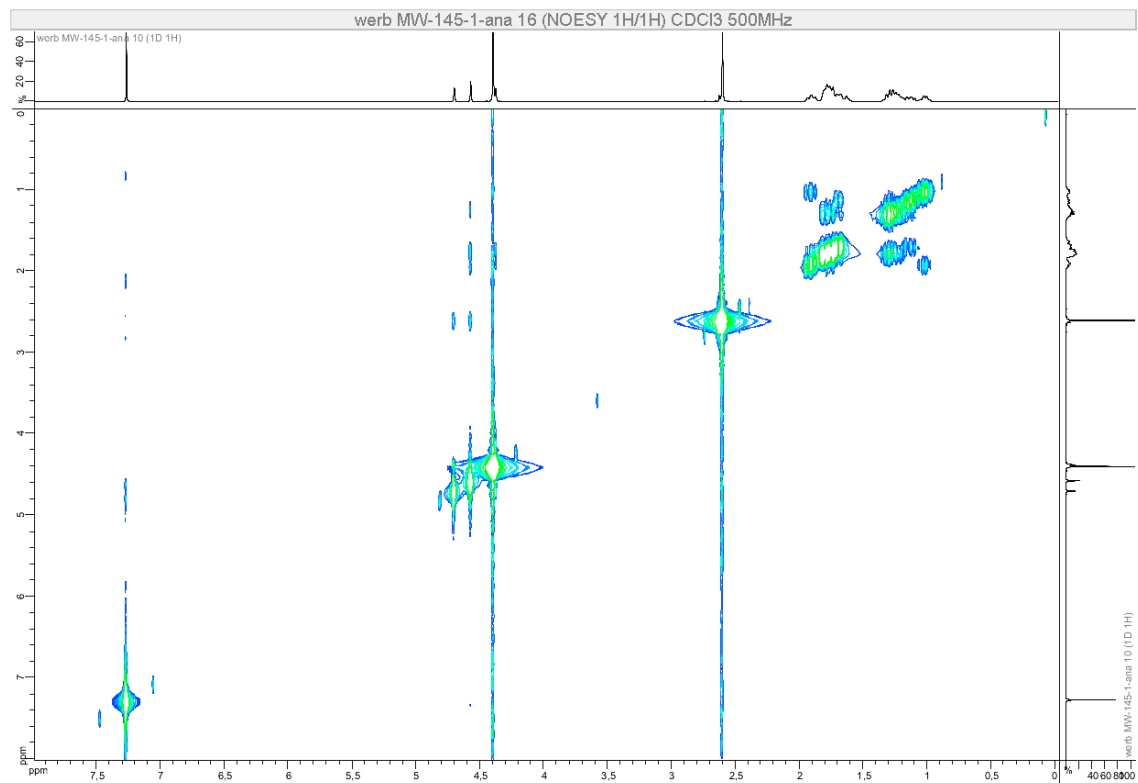


Figure S271. NOESY (500 MHz, CDCl₃) of **18b** (racemic mixture)

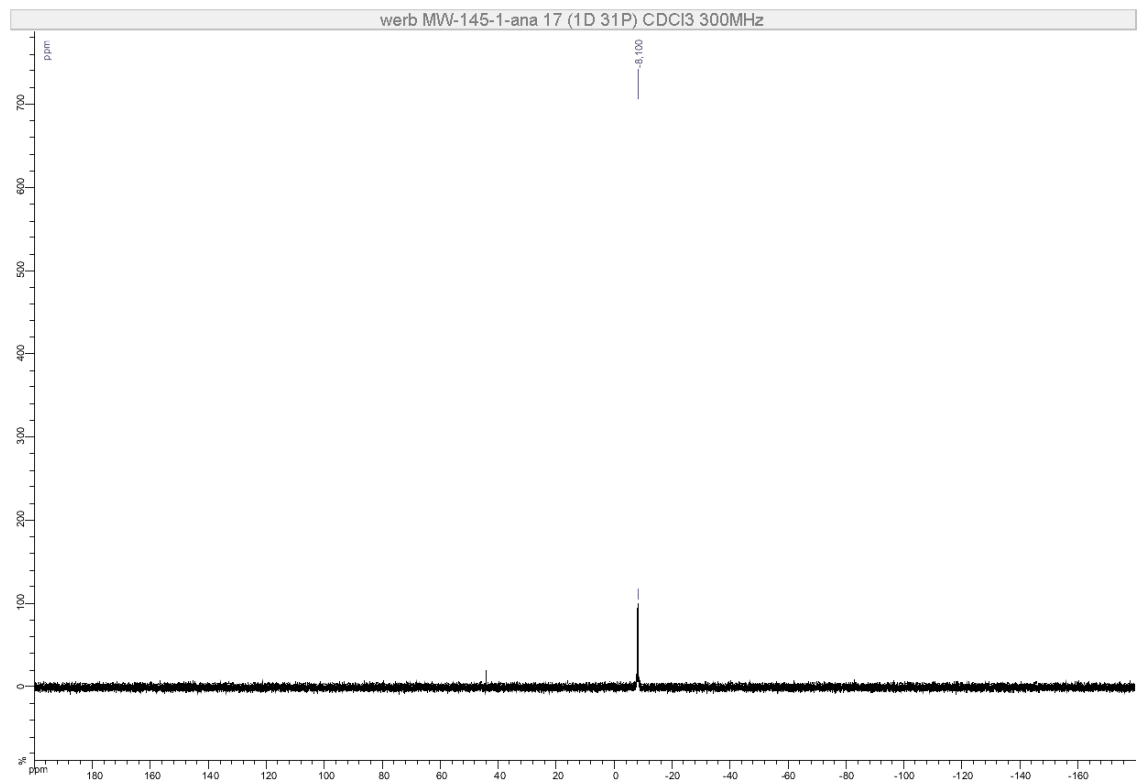
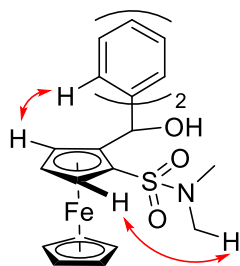
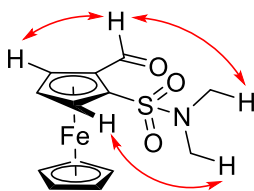


Figure S272. ³¹P NMR (202 MHz, CDCl₃) of **18b** (racemic mixture)

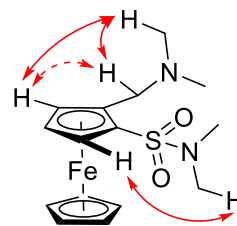
Compound 2b



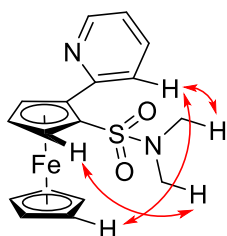
Compound 2d



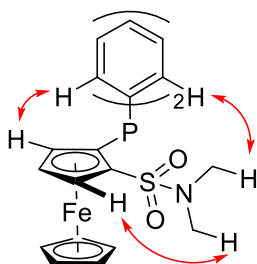
Compound 2e



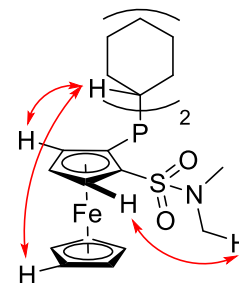
Compound 2f



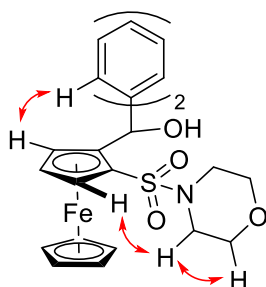
Compound 2h



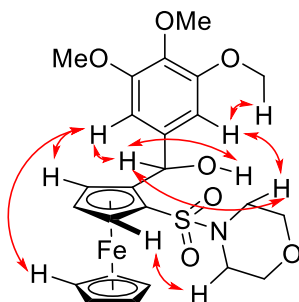
Compound 2i



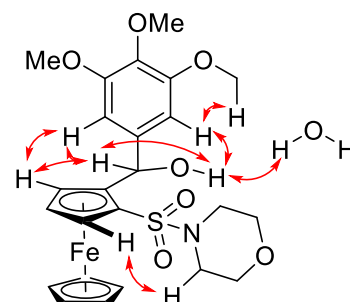
Compound 4b



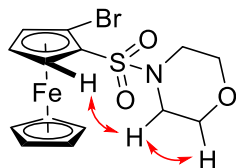
Compound 4c1



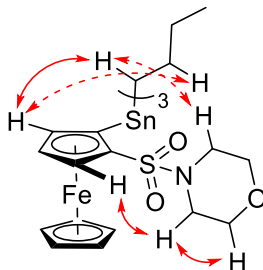
Compound 4c2



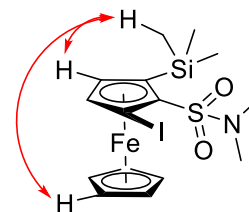
Compound 4e



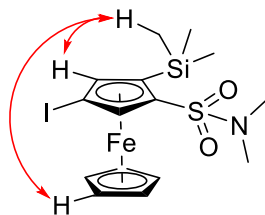
Compound 4g



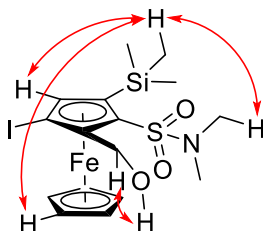
Compound 5



Compound 6a



Compound 6b



Compound 6c

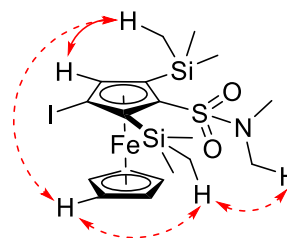


Figure S273. NMR NOESY correlations

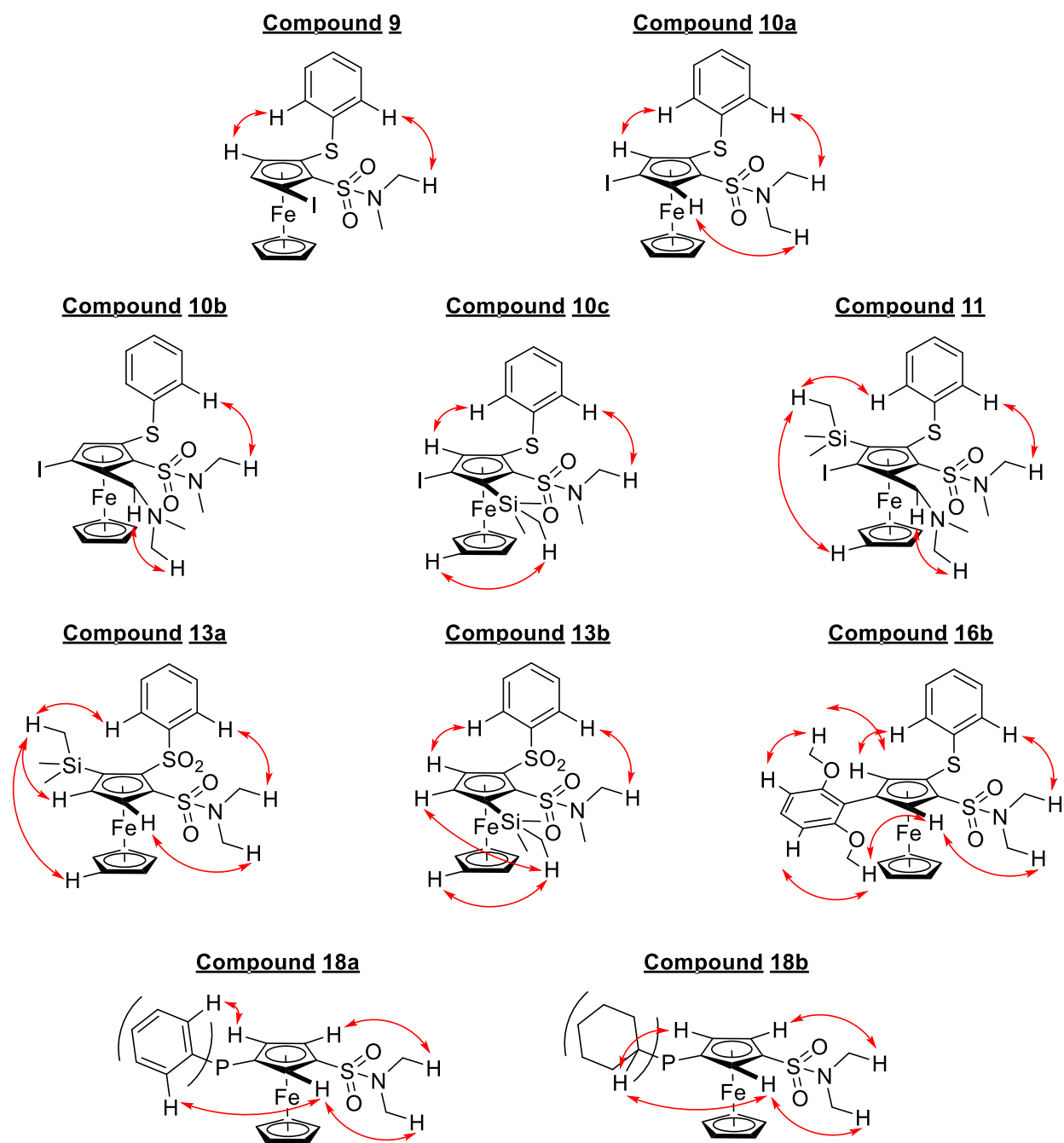


Figure S273 (continued). NMR NOESY correlations