

Supporting Information

TfOH-Promoted Multichannel Transformations of Trifluoromethyl Side Chain Substituted Thiophene and Furan Families to Access Antimicrobial Agents

Olesya V. Khoroshilova,¹ Lia R. Nikiforova,² Julia V. Salmova,² Artem O. Taraskin,²
Kristina E. Borovkova,² Daria V. Spiridonova,³ Aleksander V. Vasilyev^{1,4*}

¹ *Department of Organic Chemistry, Institute of Chemistry, Saint Petersburg State University, Universitetskaya nab., 7/9, Saint Petersburg, 199034, Russia*

² *RMC «HOME OF PHARMACY» Leningrad region., Vsevolozhsk district, p. Kuzmolovsky, 245, 188663, Russia*

³ *Research Center for X-ray Diffraction Studies, Research Park, Saint Petersburg State University, Universitetskiy pr. 26, Saint Petersburg, Petrodvoretz, 198504, Russia*

⁴ *Department of Chemistry, Saint Petersburg State Forest Technical University, Institutsky per., 5, Saint Petersburg, 194021, Russia*

*Corresponding author: A.V. Vasilyev; e-mail: aleksvasil@mail.ru, a.vasilyev@spbu.ru

Contents

1. Copies of ¹ H, ¹³ C{ ¹ H}, ¹³ C{ ¹⁹ F}, ¹⁹ F{ ¹ H}, COSY H-H, NOESY H-H, HSQC C-H, HOESY F-H, DEPT NMR Spectra of compounds 1-14.....	S2
2. Copies of ¹ H NMR Spectra of the compounds previously obtained by ourselves.....	S131
3. X-ray data.....	S134
4. Biological study data.....	S140

Copies of ^1H , $^{13}\text{C}\{^1\text{H}\}$, $^{13}\text{C}\{^{19}\text{F}\}$, $^{19}\text{F}\{^1\text{H}\}$, COSY H-H, NOESY H-H, HSQC C-H, HOESY F-H, DEPT NMR Spectra of compounds 1-14

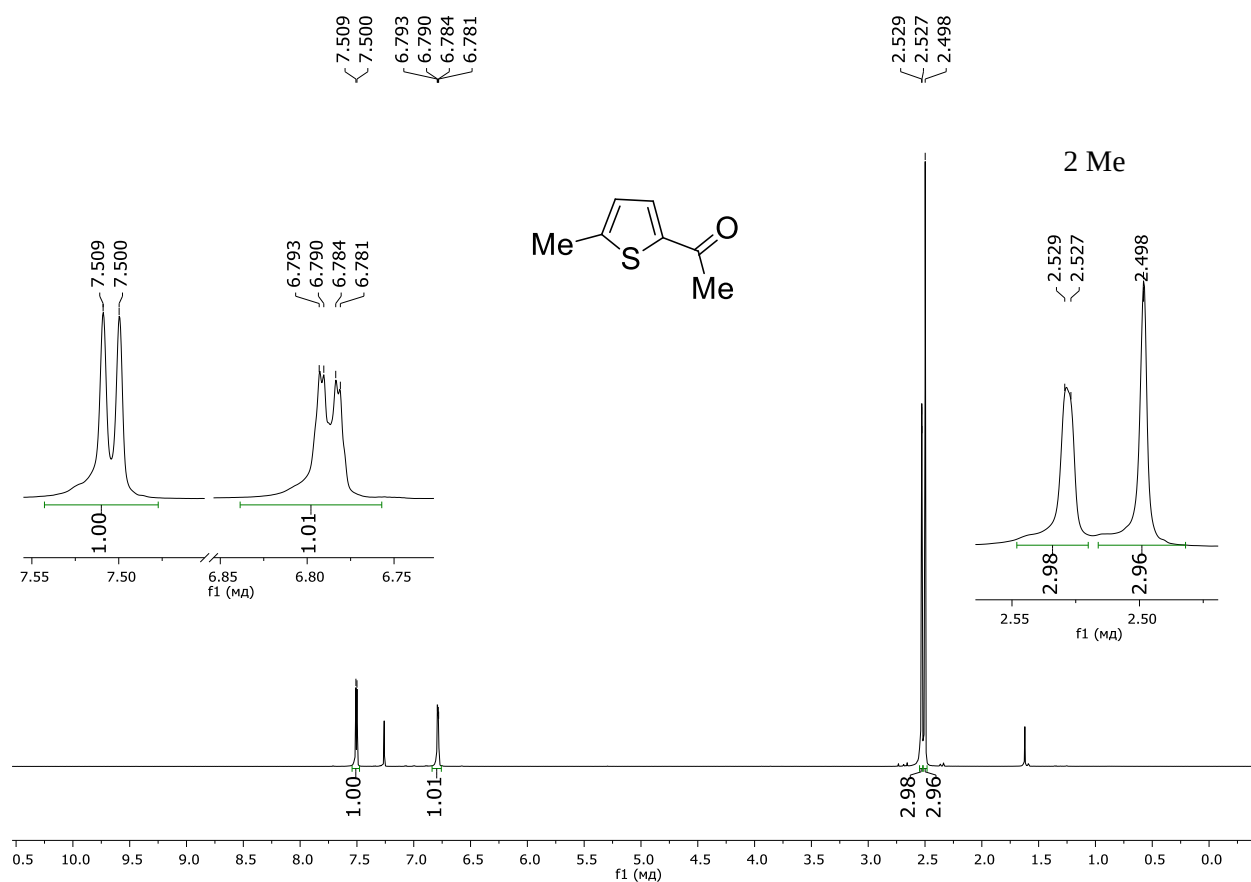


Fig. S1. ^1H NMR spectrum of 1-(5-methylthiophen-2-yl)ethanone (CDCl₃, 400 MHz).

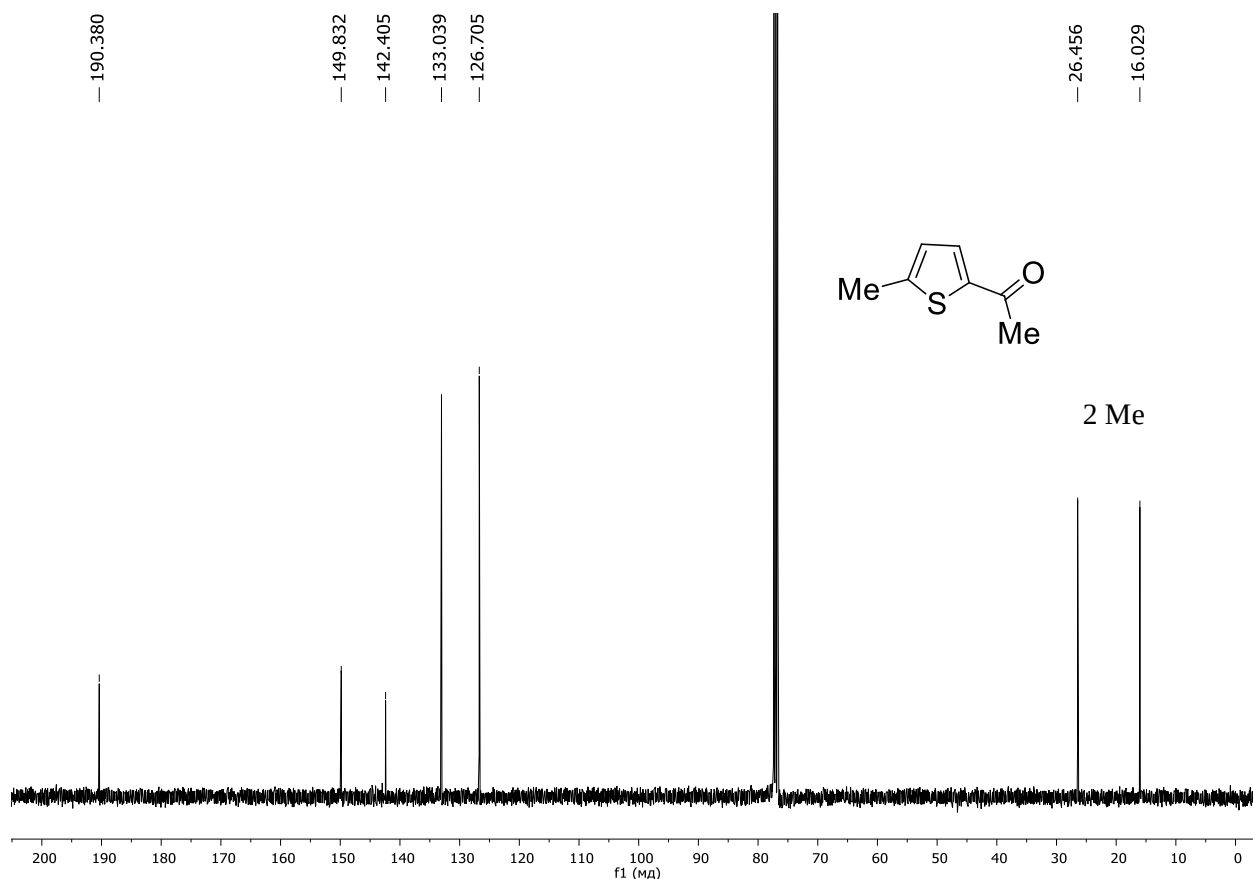


Fig. S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (5-methylthiophen-2-yl)ethanone (CDCl_3 , 100 MHz).

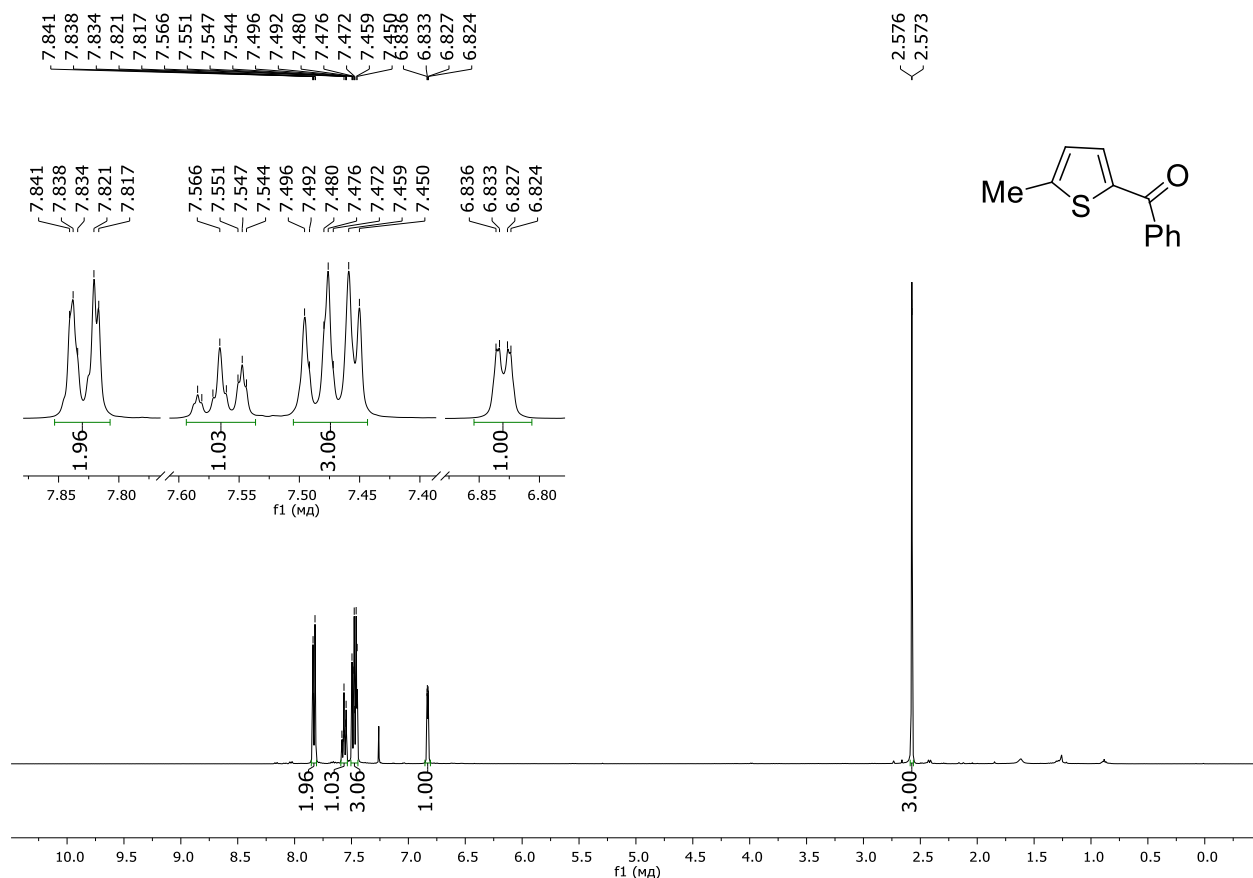


Fig. S3. ^1H NMR spectrum of (5-methylthiophen-2-yl)(phenyl)methanone (CDCl_3 , 400 MHz).

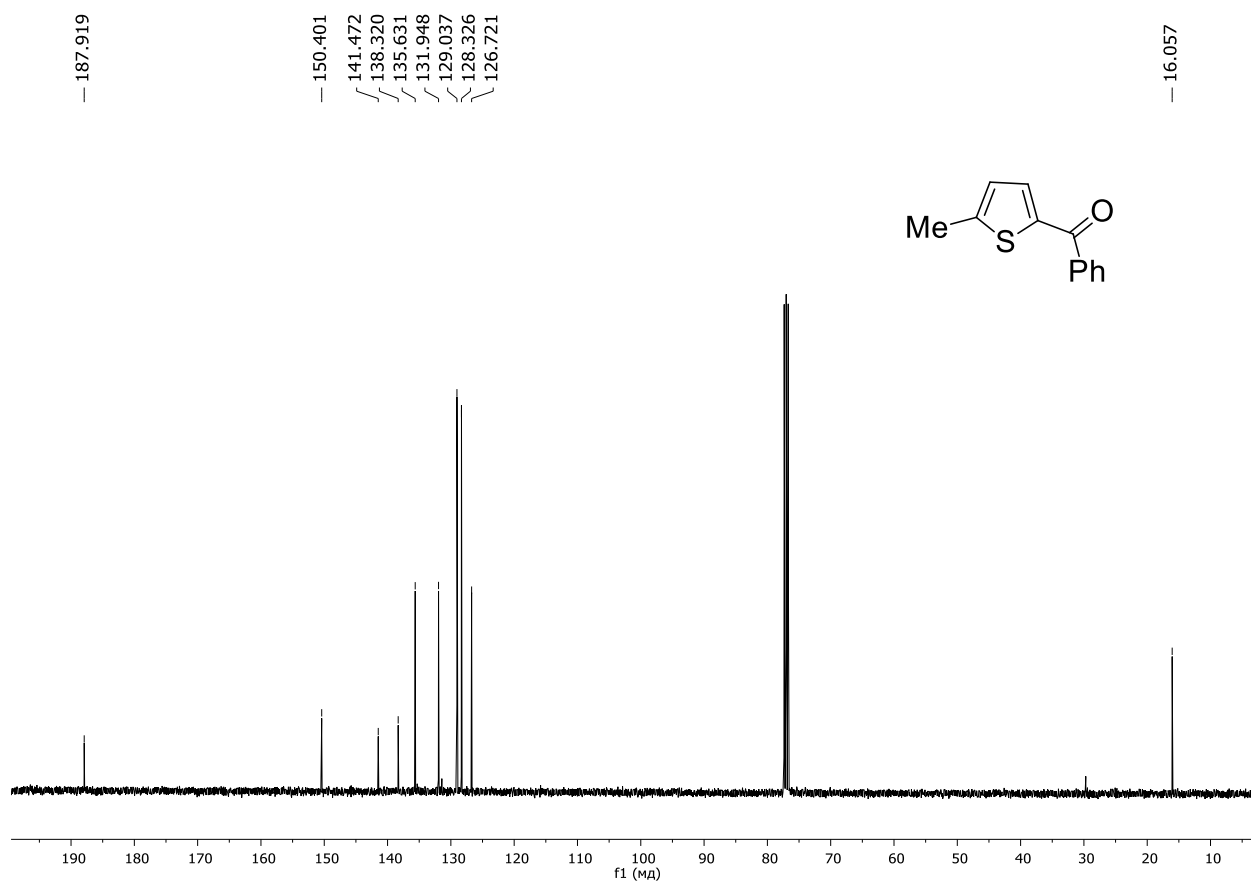


Fig. S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (5-methylthiophen-2-yl)(phenyl)methanone (CDCl_3 , 100 MHz).

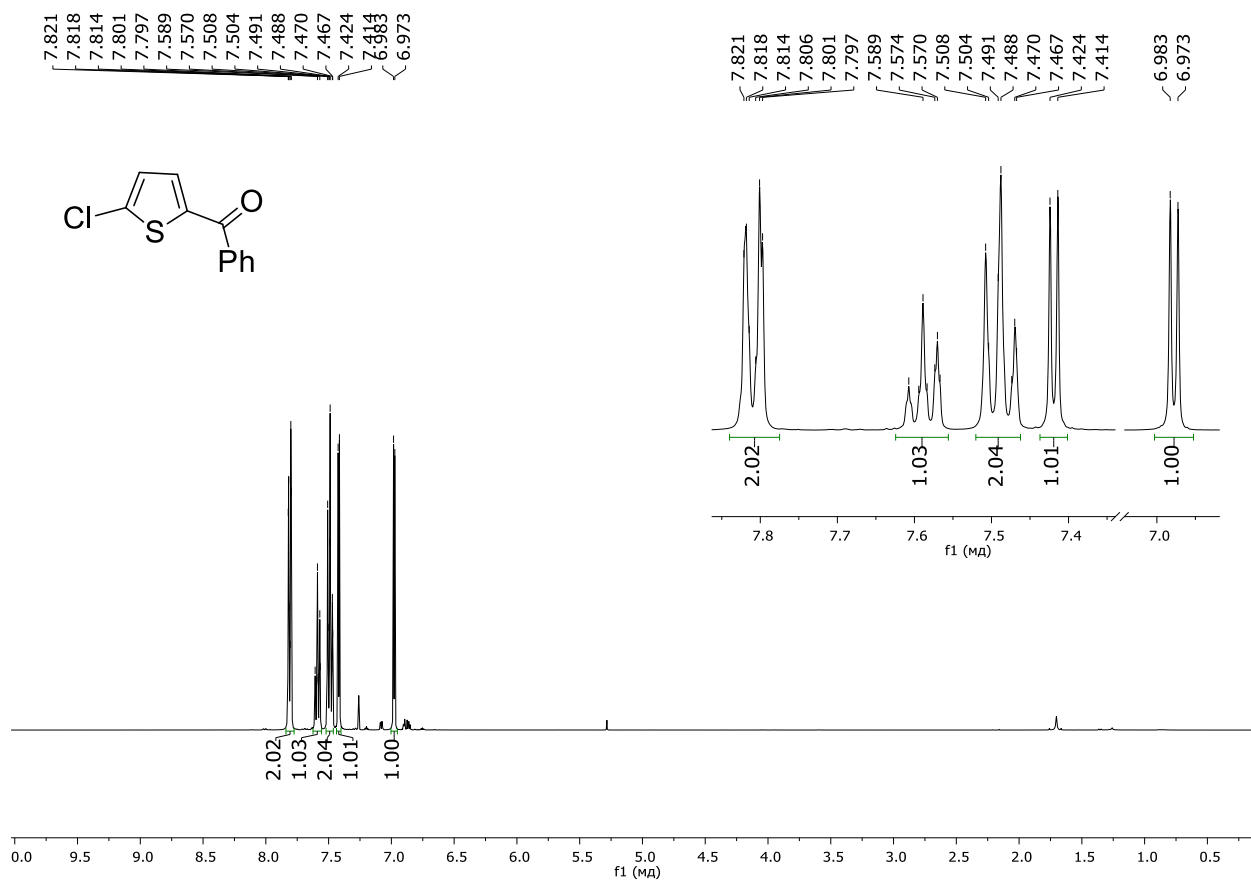


Fig. S5. ^1H NMR spectrum of (5-chlorothiophen-2-yl)(phenyl)methanone (CDCl_3 , 400 MHz).

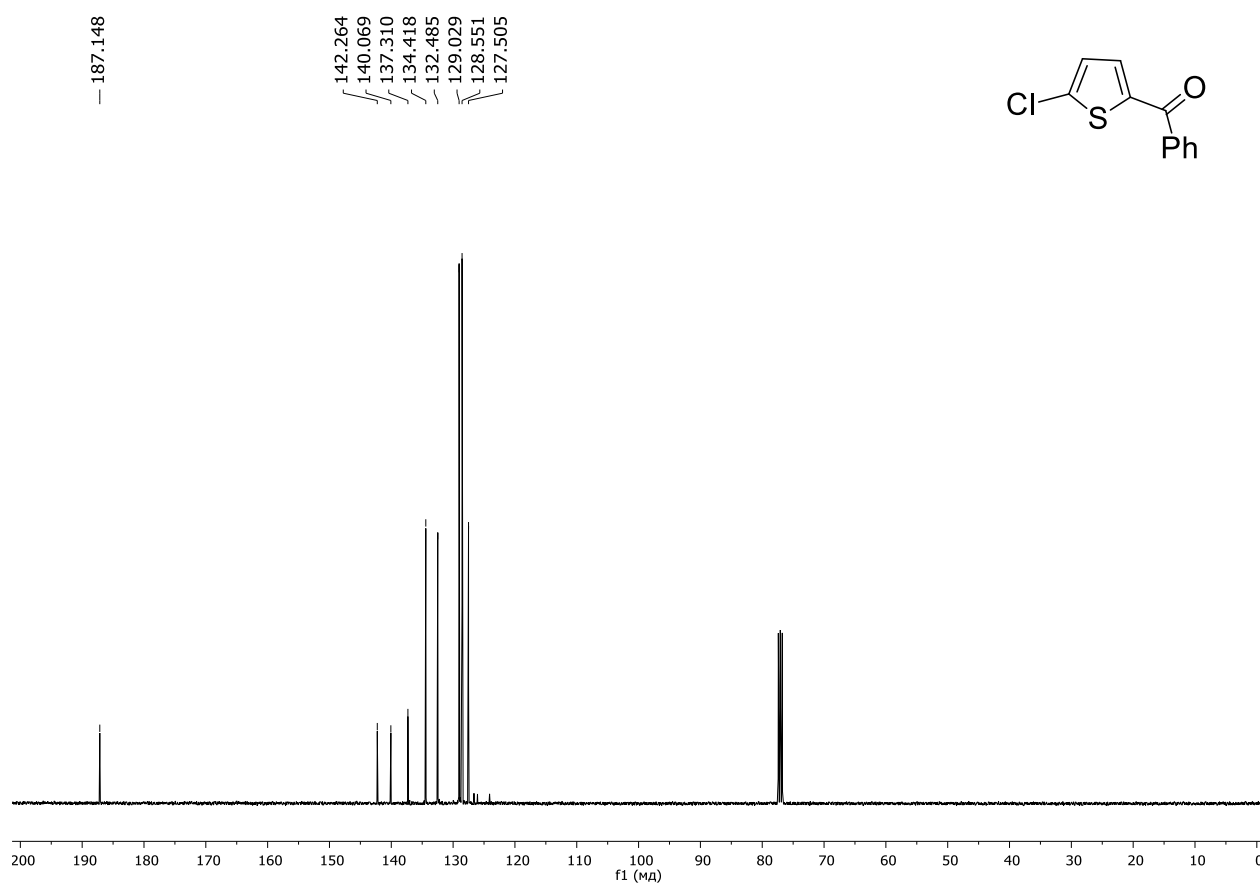


Fig. S6. ¹³C{¹H} NMR spectrum of (5-chlorothiophen-2-yl)(phenyl)methanone (CDCl₃, 100 MHz).

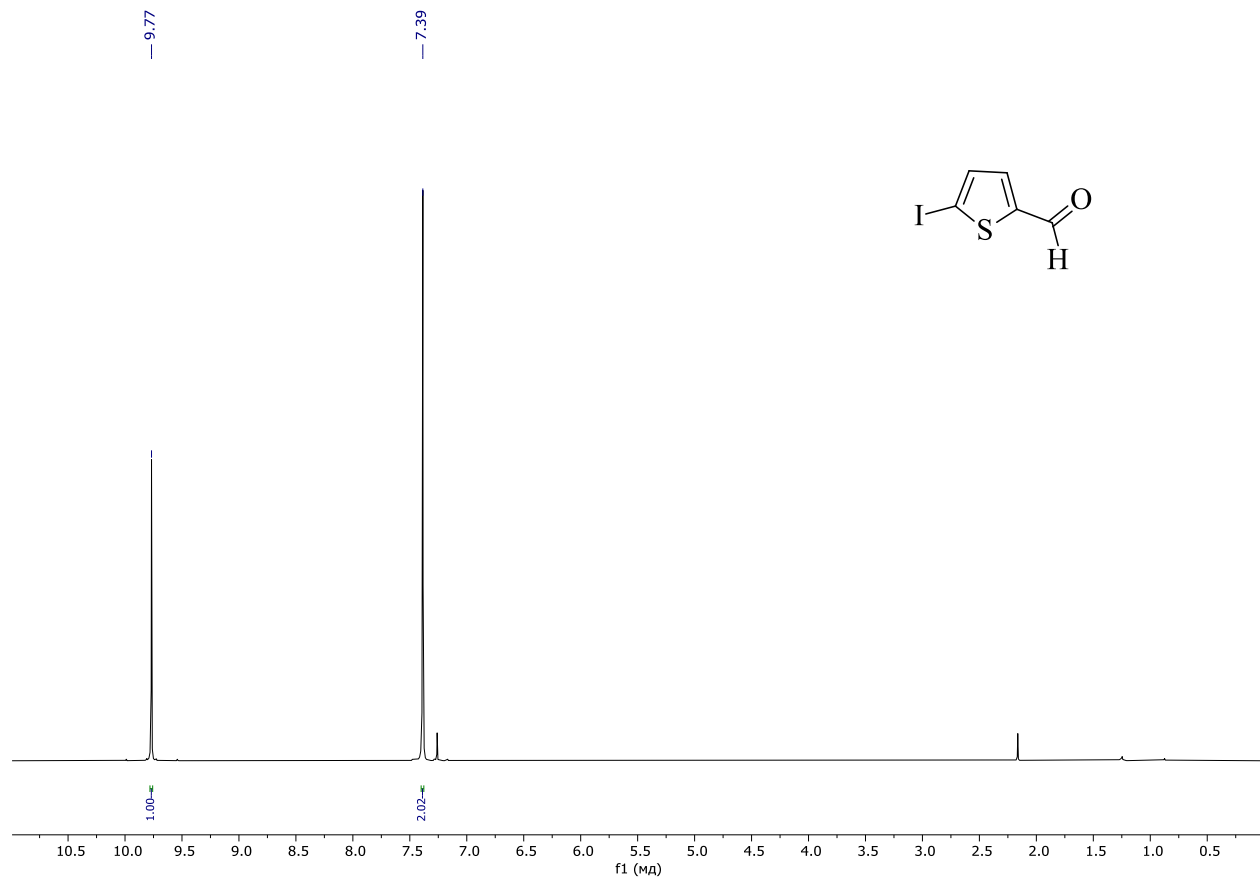


Fig. S7. ¹H NMR spectrum of 5-iodothiophene-2-carbaldehyde (CDCl₃, 400 MHz).

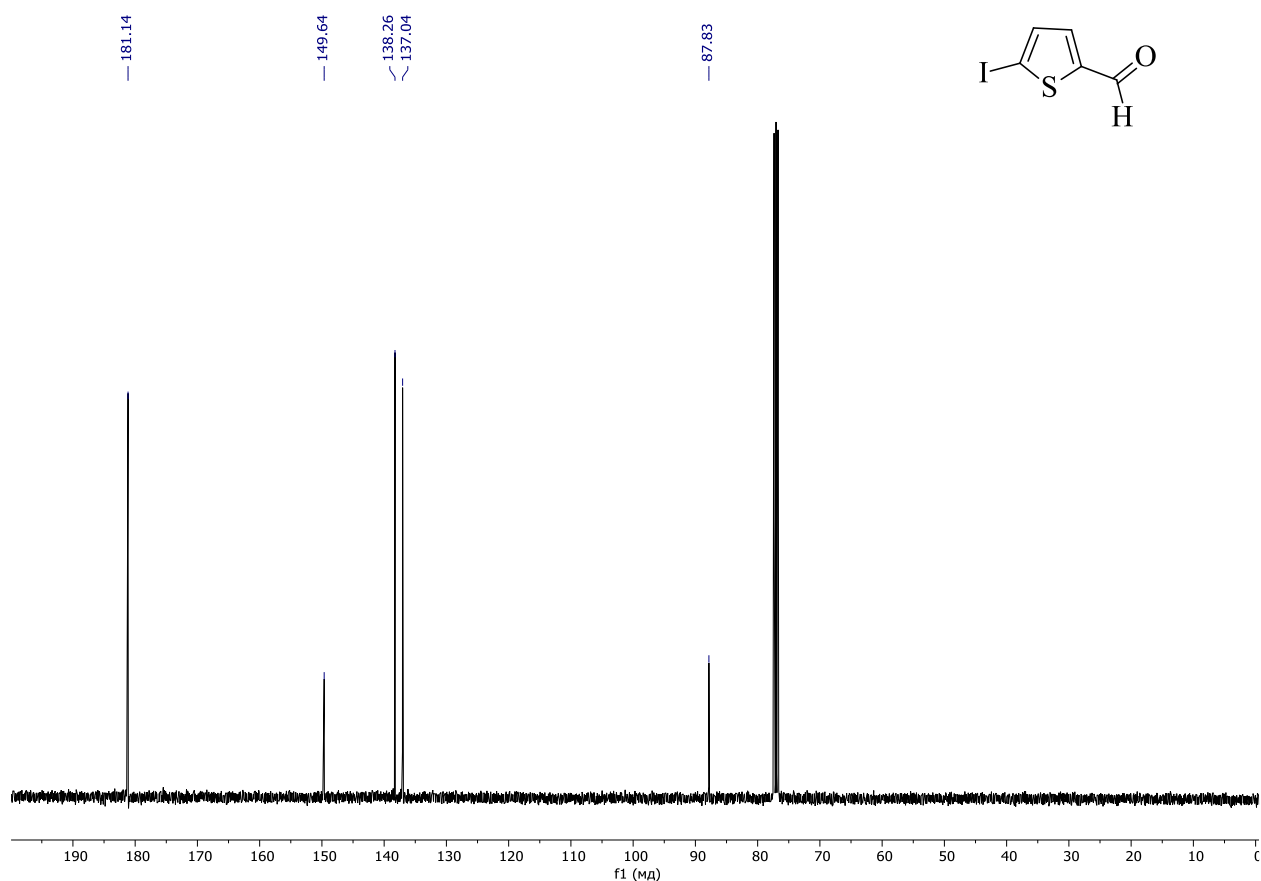


Fig. S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 5-iodothiophene-2-carbaldehyde (CDCl_3 , 100 MHz).

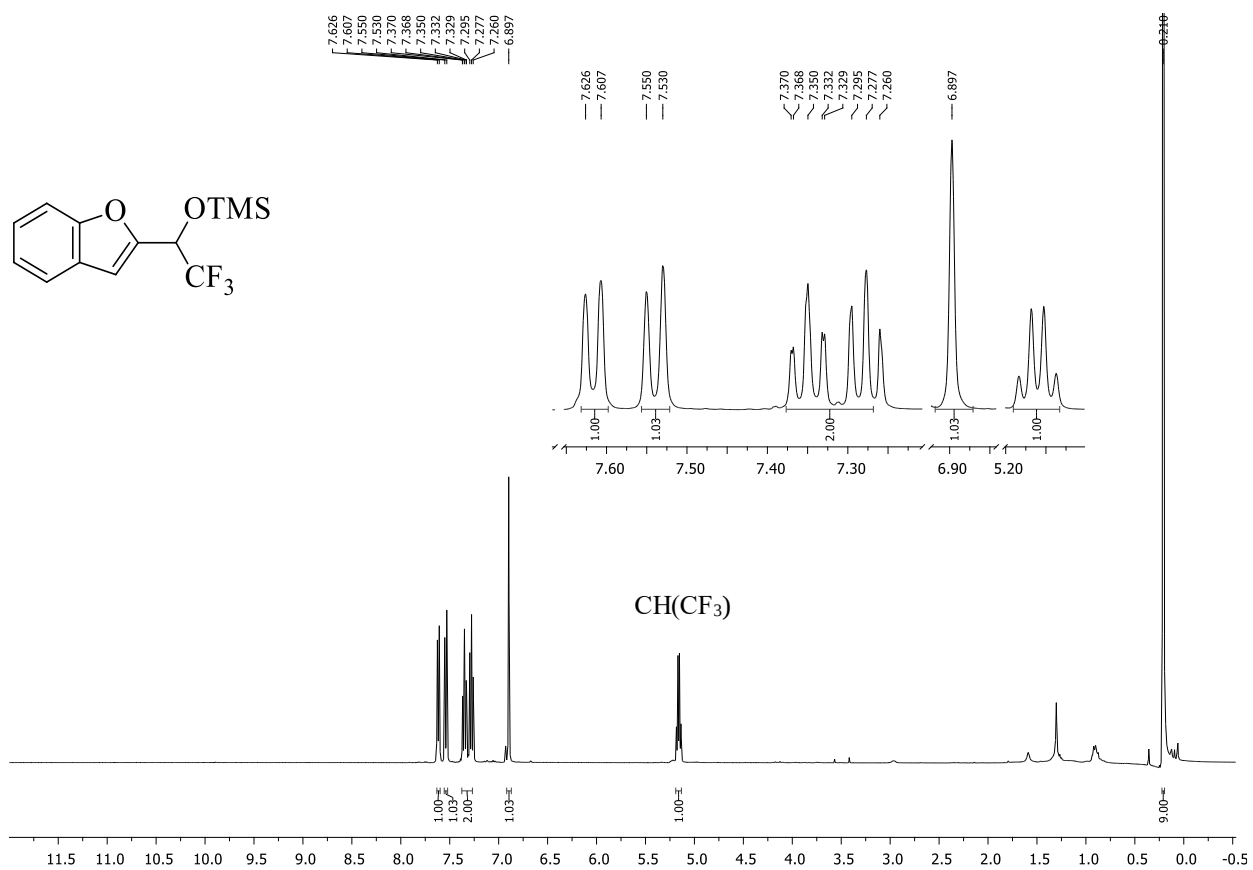


Fig. S9. ^1H NMR spectrum of the compound **1a** (CDCl_3 , 400 MHz).

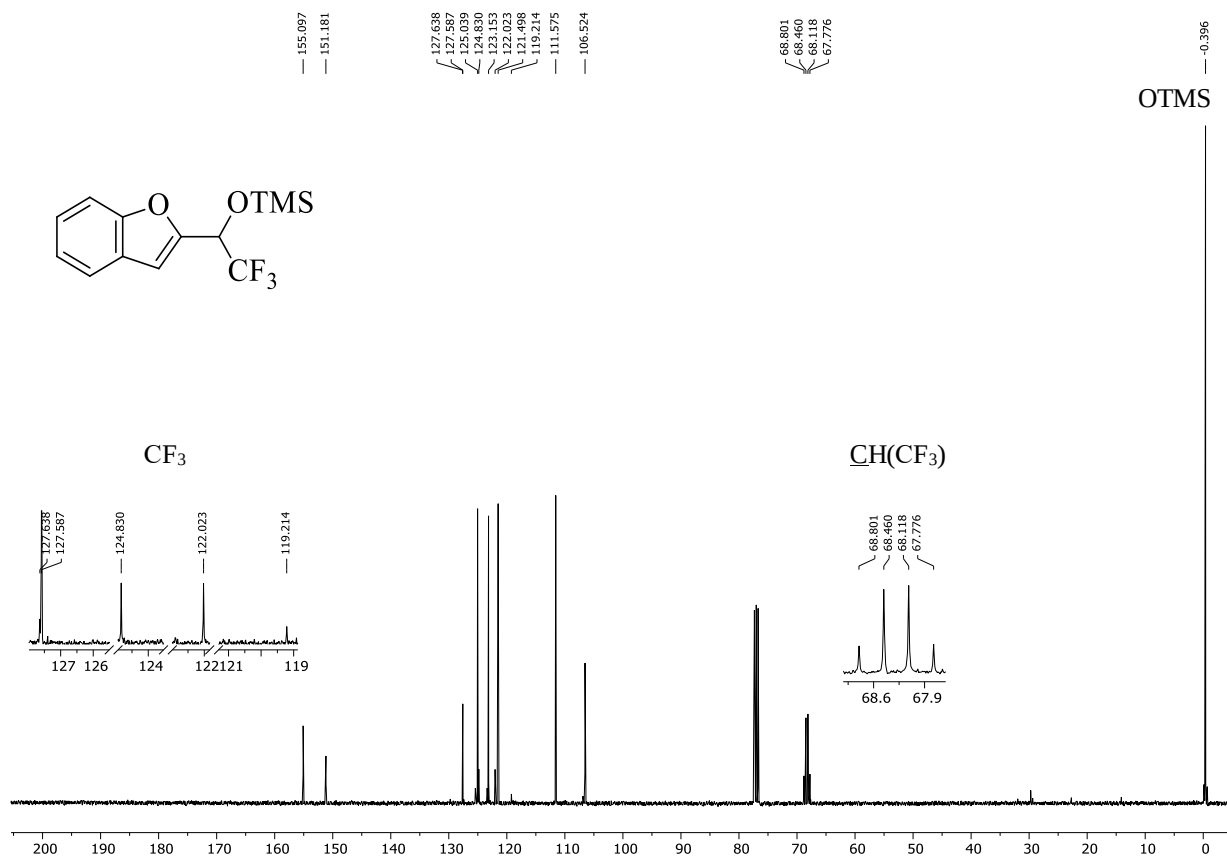


Fig. S10. ¹³C{¹H} NMR spectrum of the compound **1a** (CDCl₃, 101 MHz).

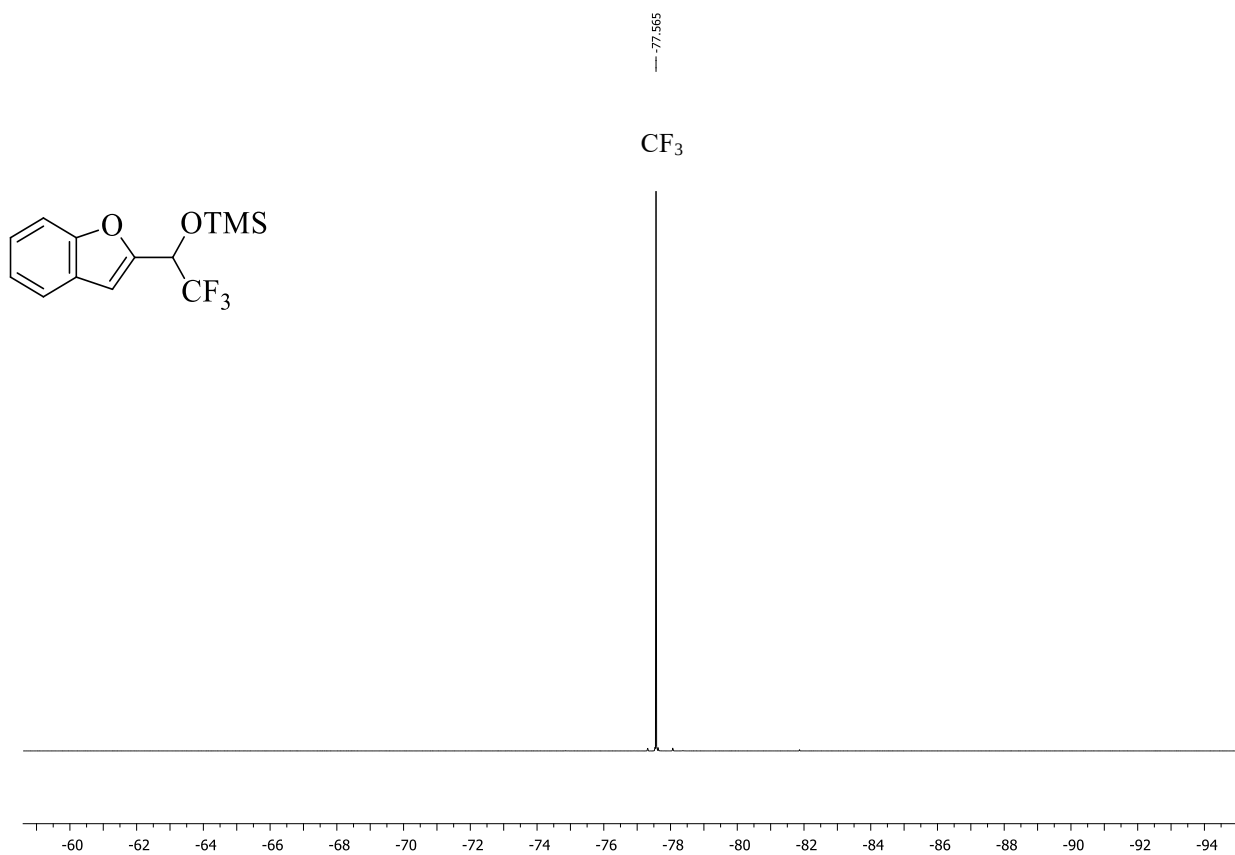


Fig. S11. ¹⁹F{¹H} NMR spectrum of the compound **1a** (CDCl₃, 376 MHz)

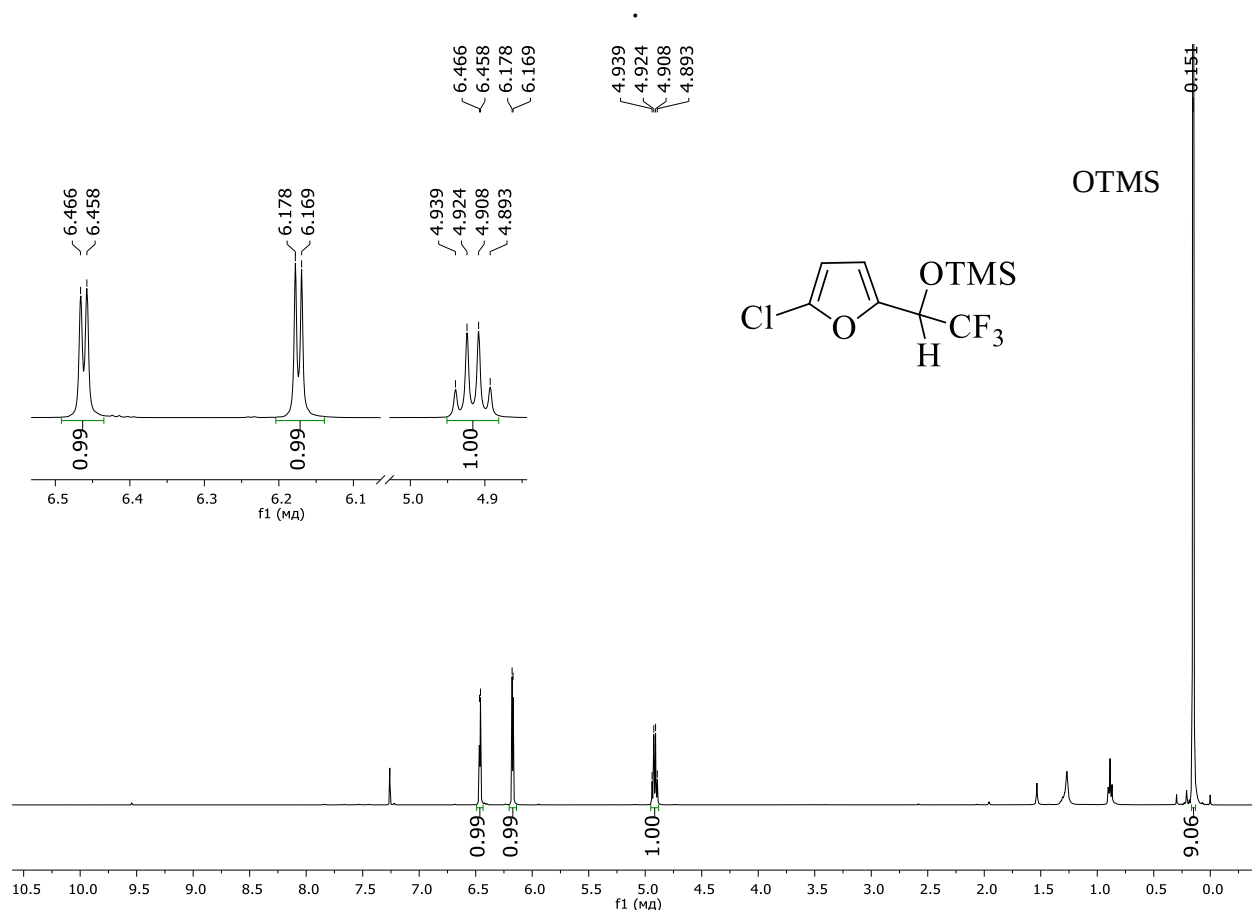


Fig. S12. ¹H NMR spectrum of the compound **1c** (CDCl₃, 400 MHz).

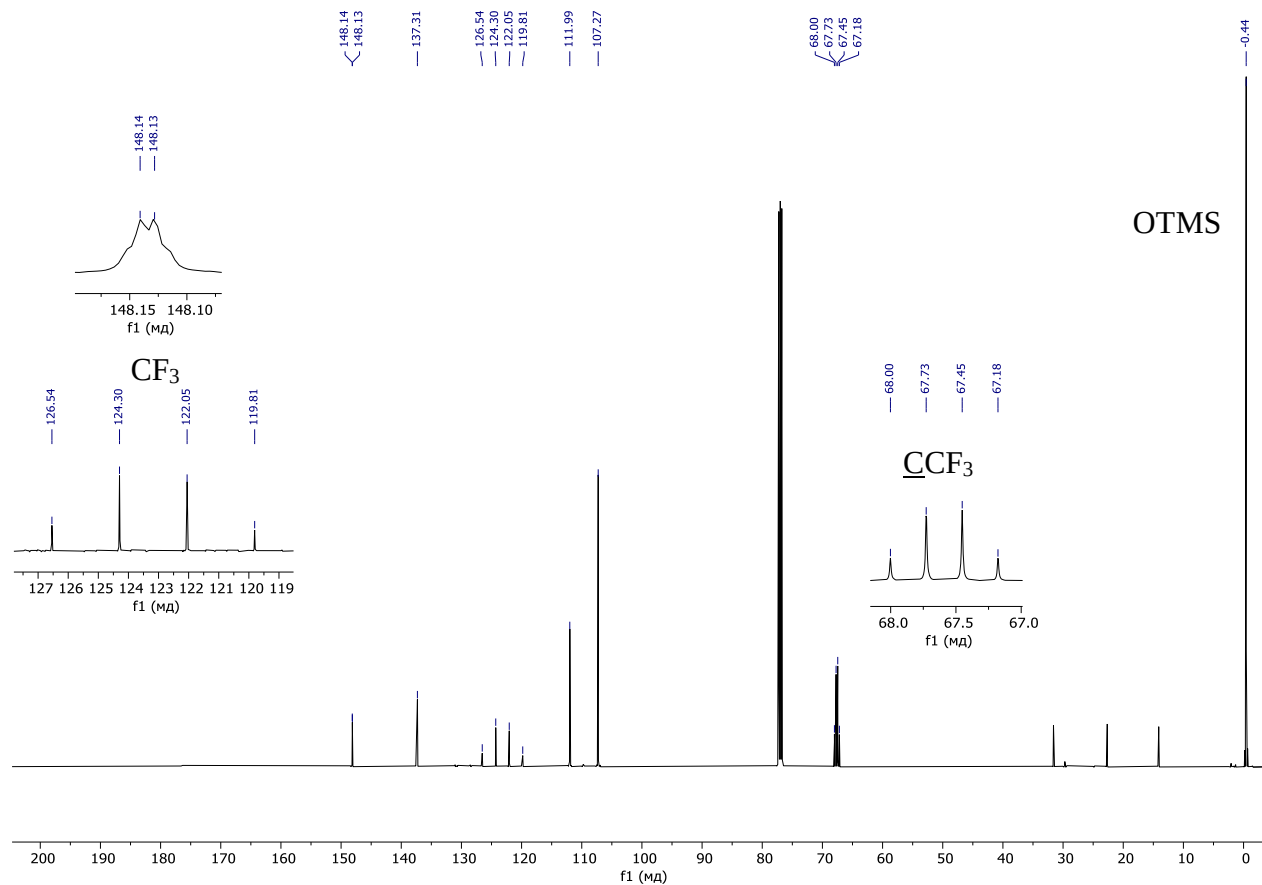


Fig. S13. ¹³C{¹H} NMR spectrum of the compound **1c** (CDCl₃, 101 MHz).

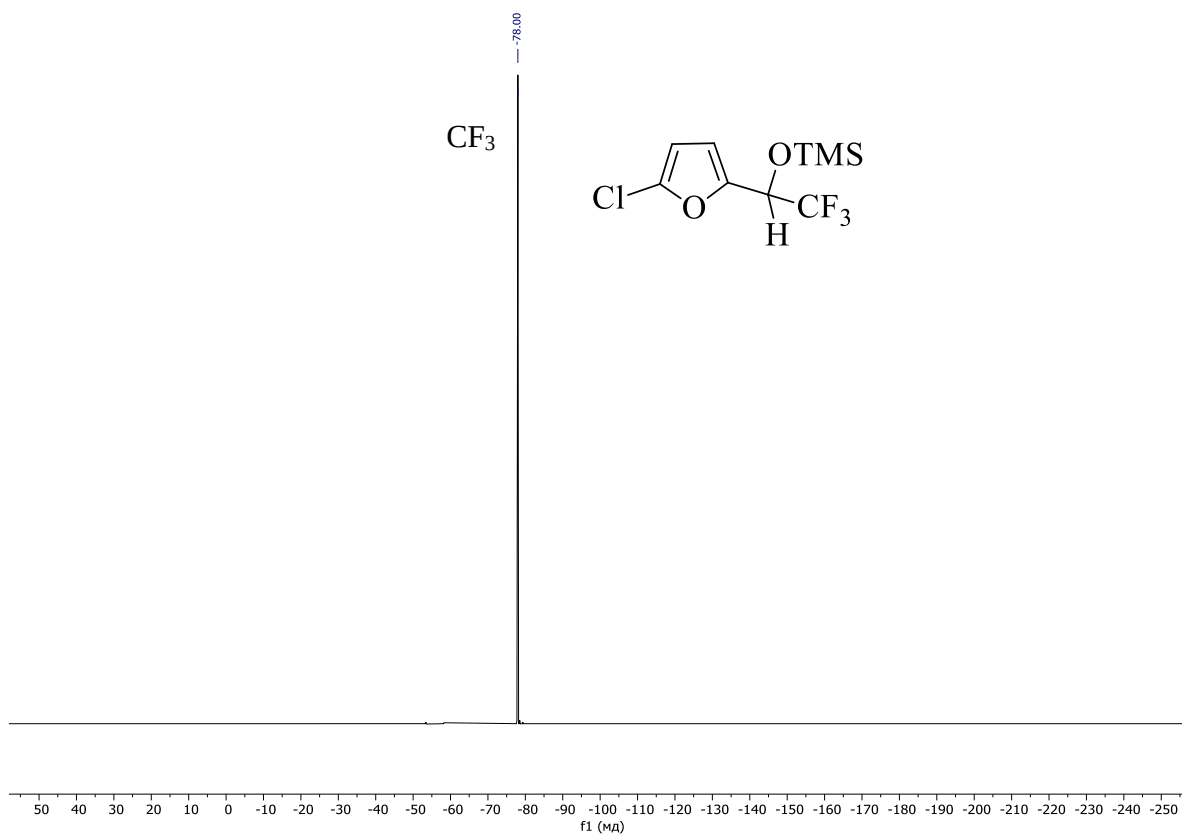


Fig. S14. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **1c** (CDCl₃, 376 MHz).

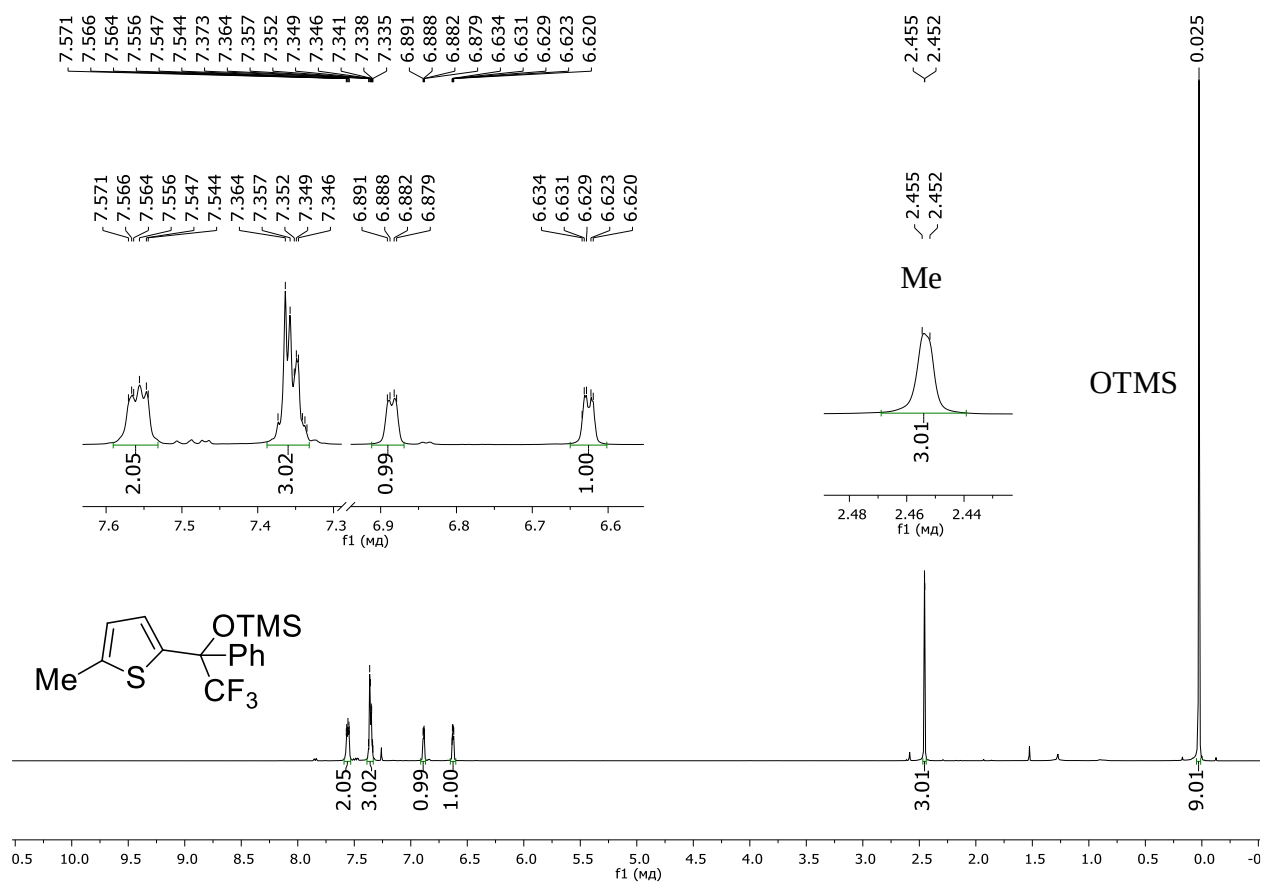
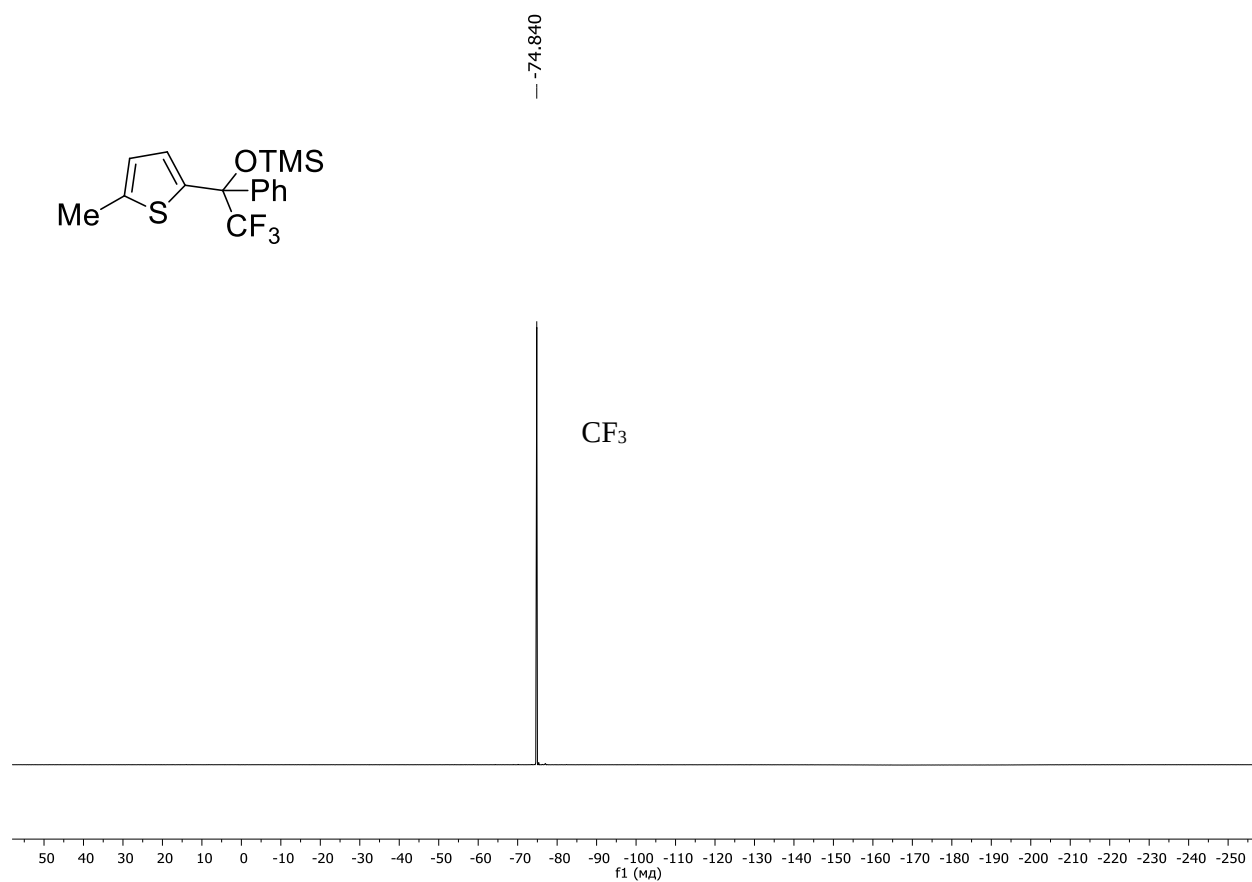
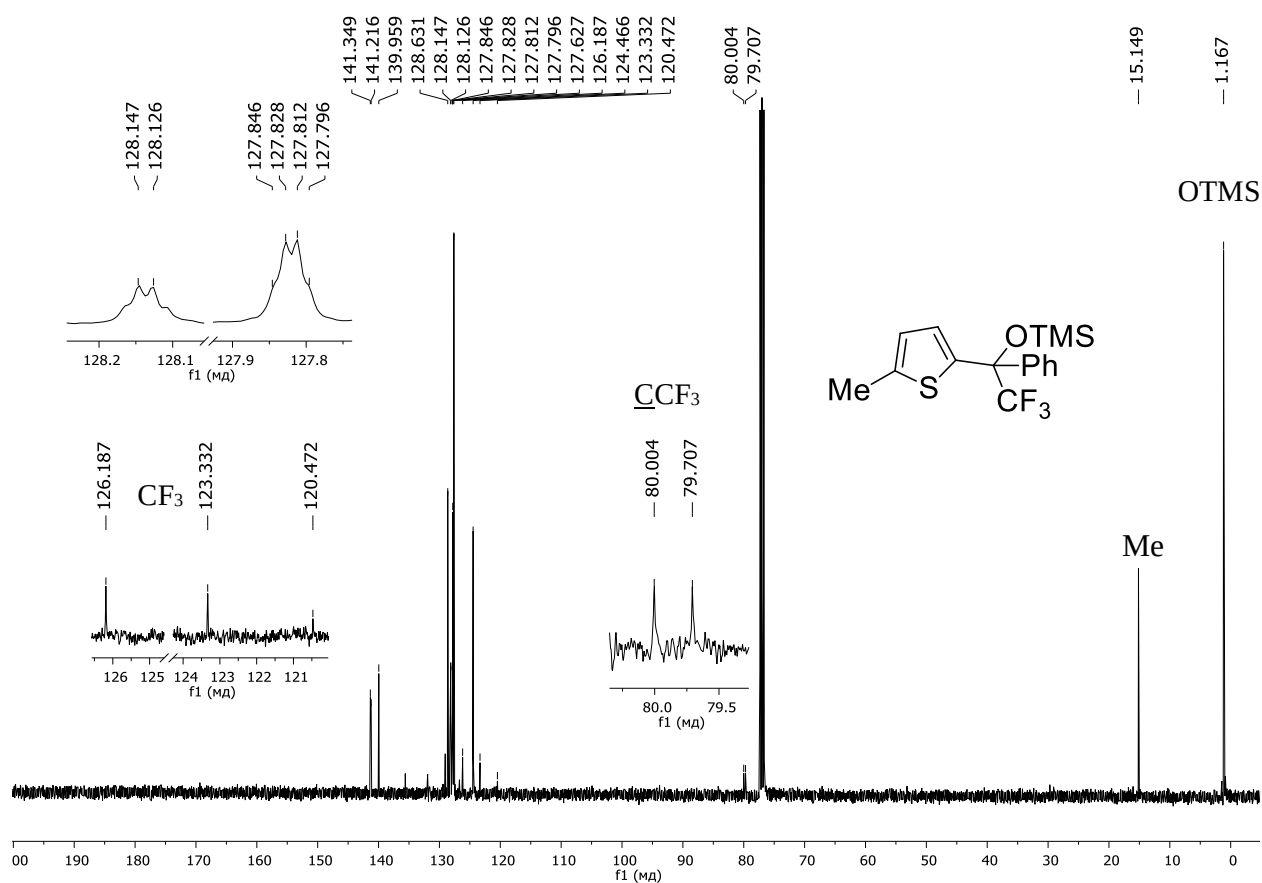


Fig. S15. ^1H NMR spectrum of the compound **1h** (CDCl₃, 400 MHz).



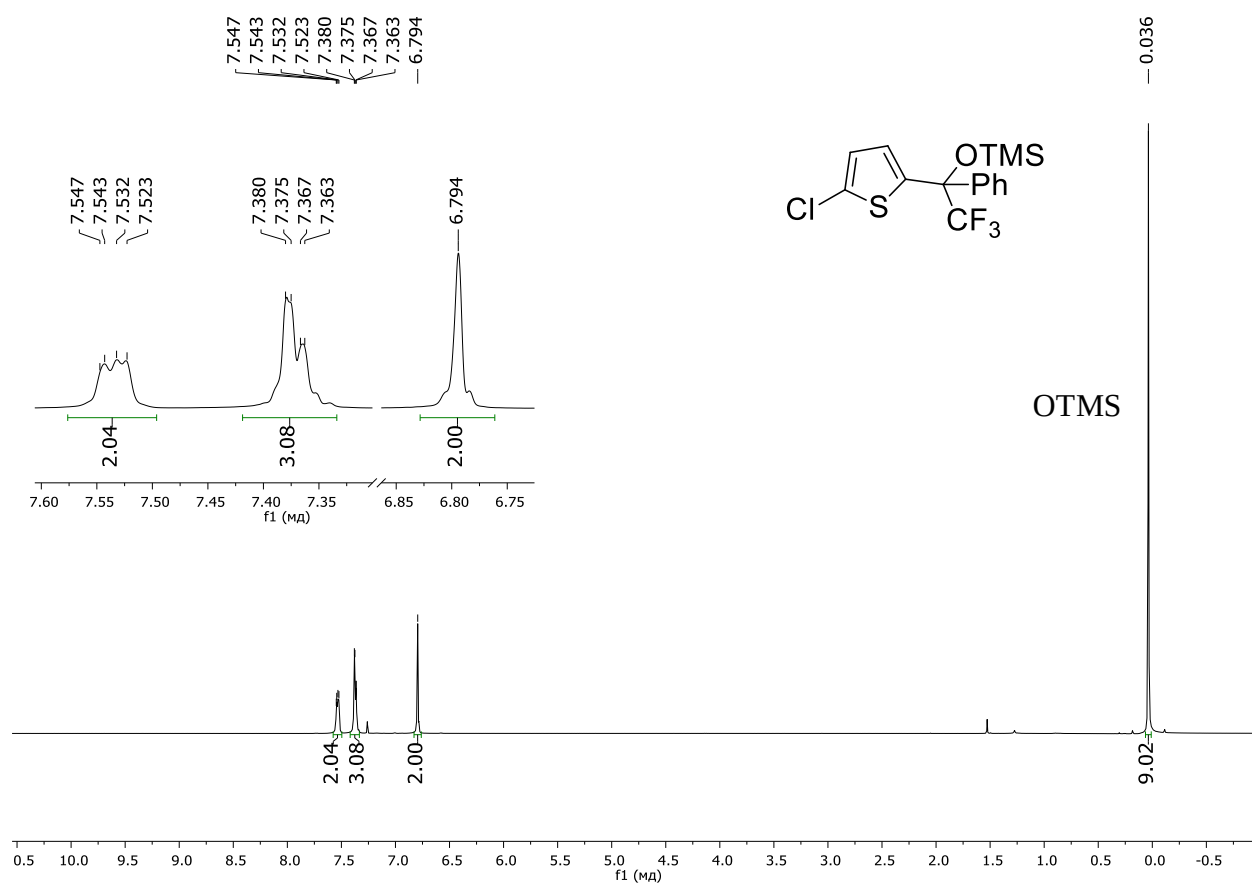


Fig. S18. ¹H NMR spectrum of the compound **1i** (CDCl₃, 400 MHz).

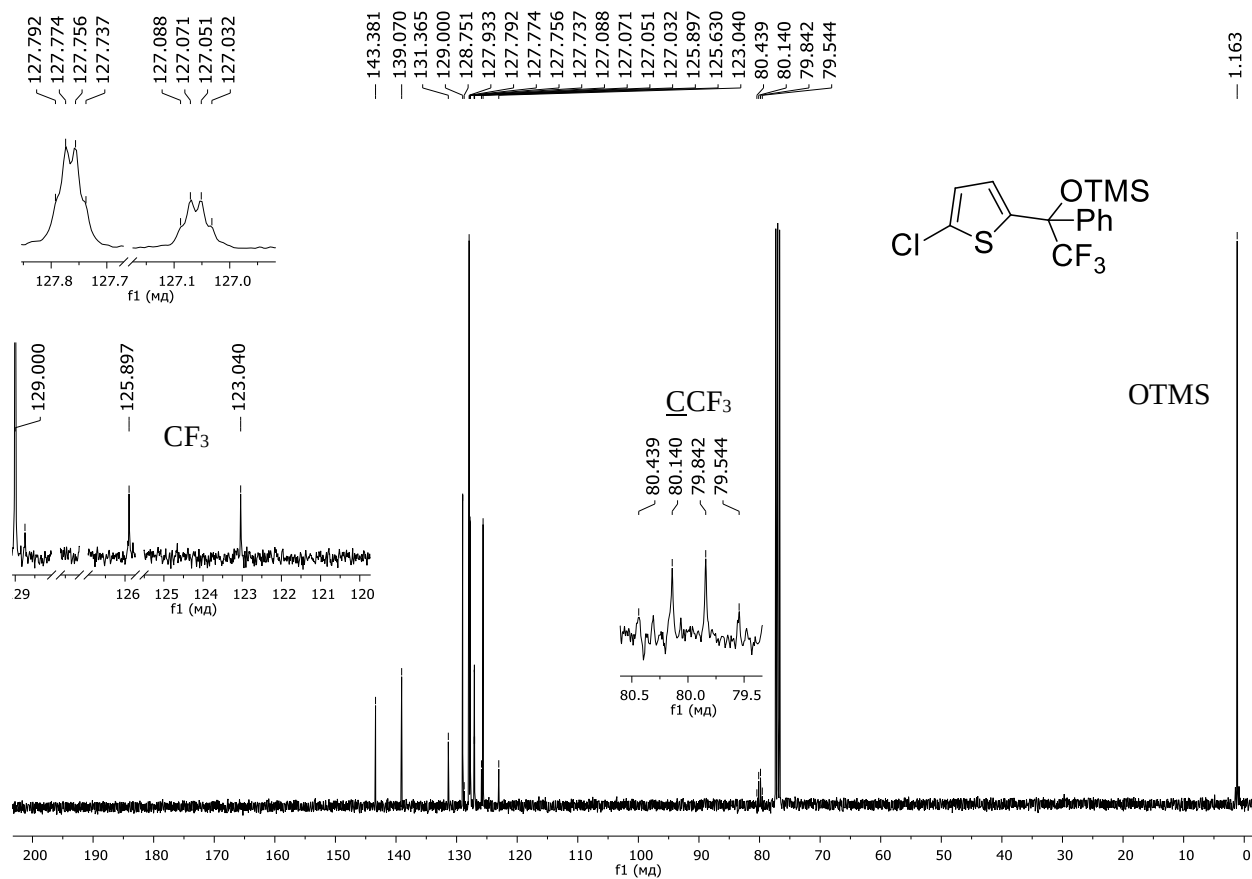


Fig. S19. ¹³C{¹H} NMR spectrum of the compound **1i** (CDCl₃, 100 MHz).

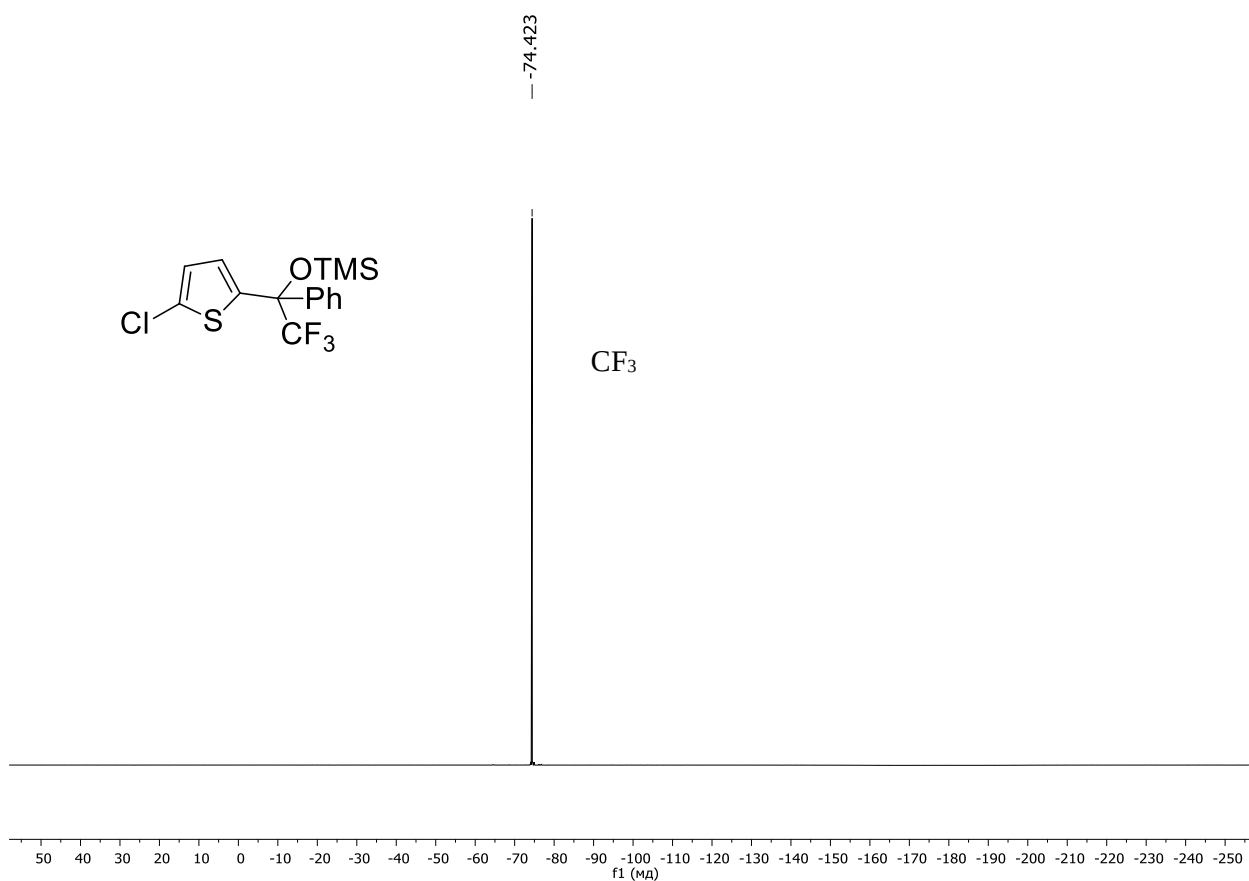


Fig. S20. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **1i** (CDCl_3 , 376 MHz).

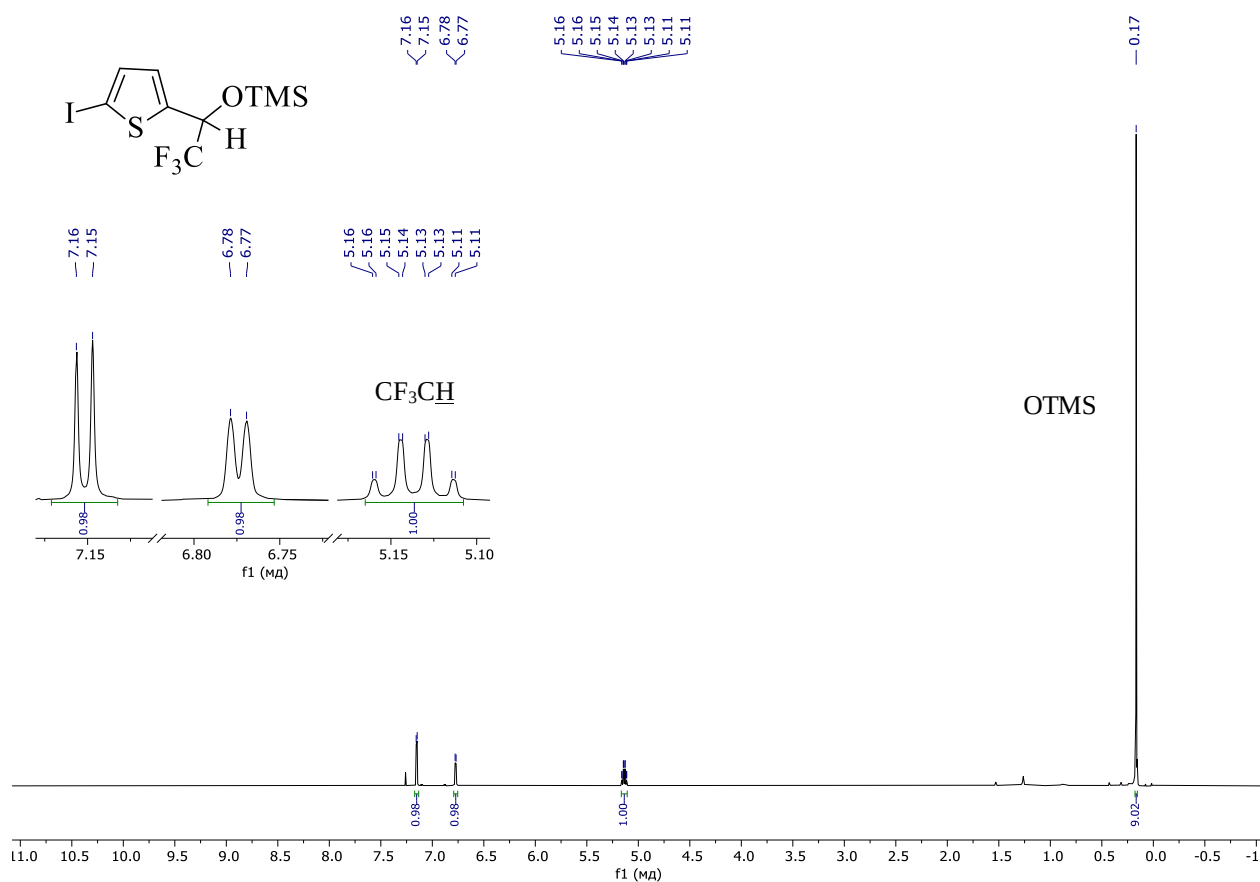


Fig. S21. ^1H NMR spectrum of the compound **1k** (CDCl_3 , 400 MHz).

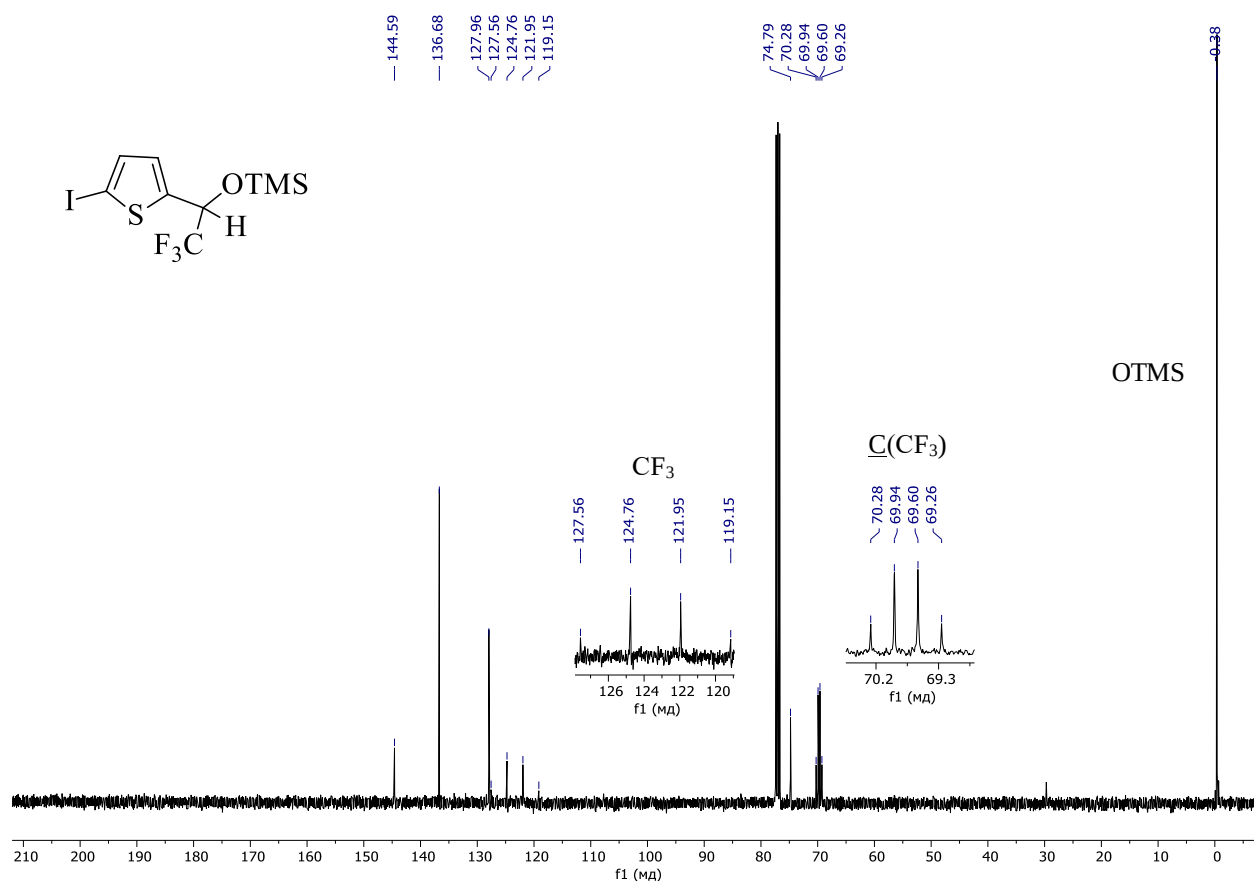


Fig. S22. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **1k** (CDCl₃, 101 MHz).

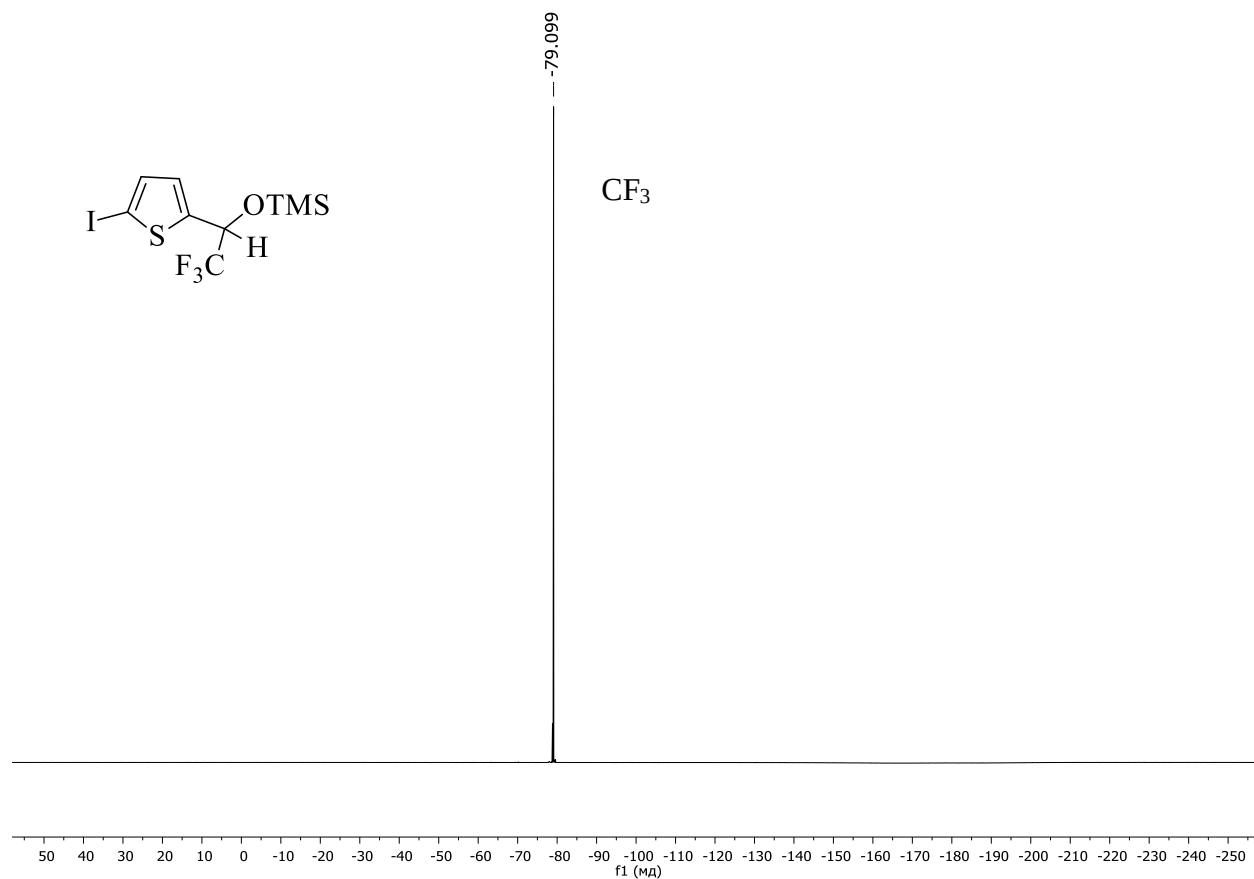


Fig. S23. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **1k** (CDCl₃, 376 MHz).

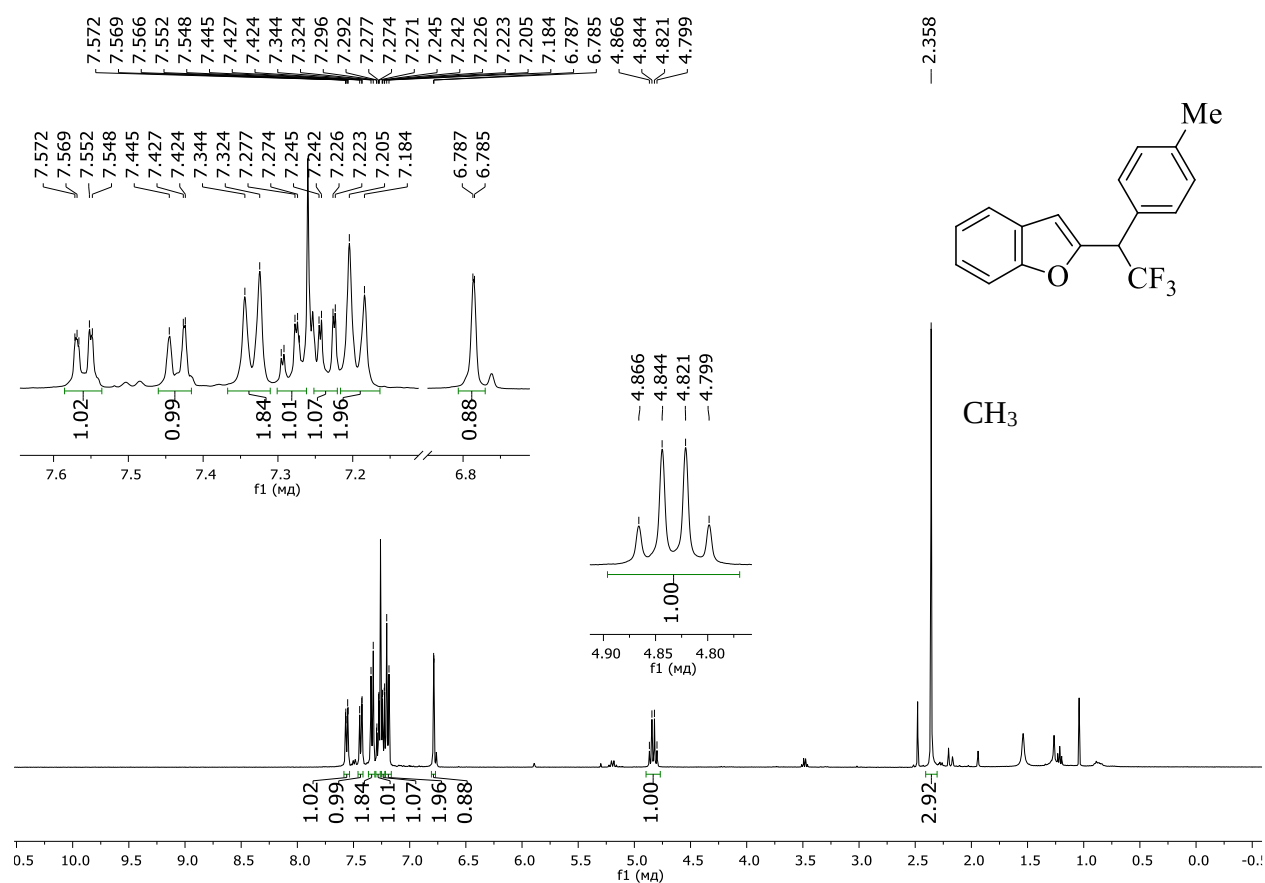


Fig. S24. ¹H NMR spectrum of the compound **2aa** (CDCl₃, 400 MHz).

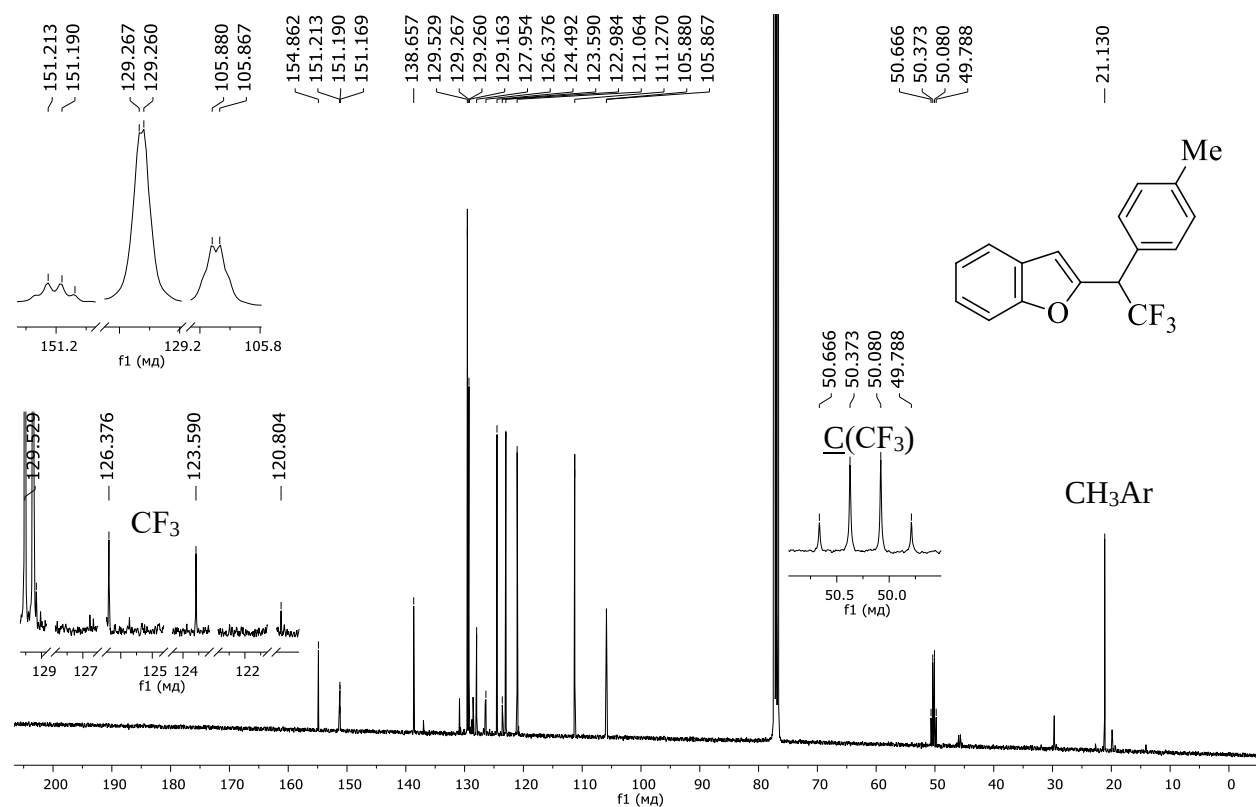


Fig. S25. ¹³C{¹H} NMR spectrum of the compound **2aa** (CDCl₃, 101 MHz).

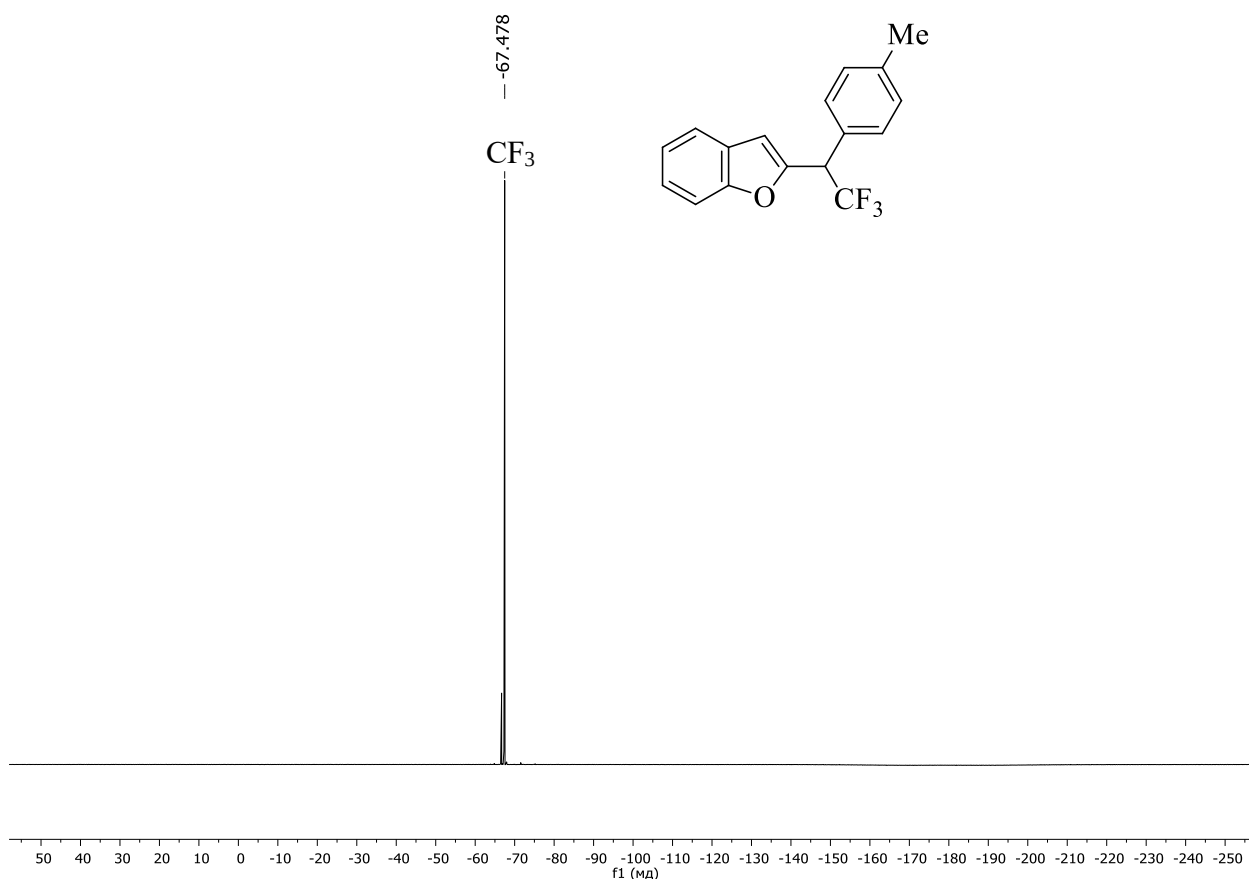


Fig. S26. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2aa** (CDCl_3 , 376 MHz).

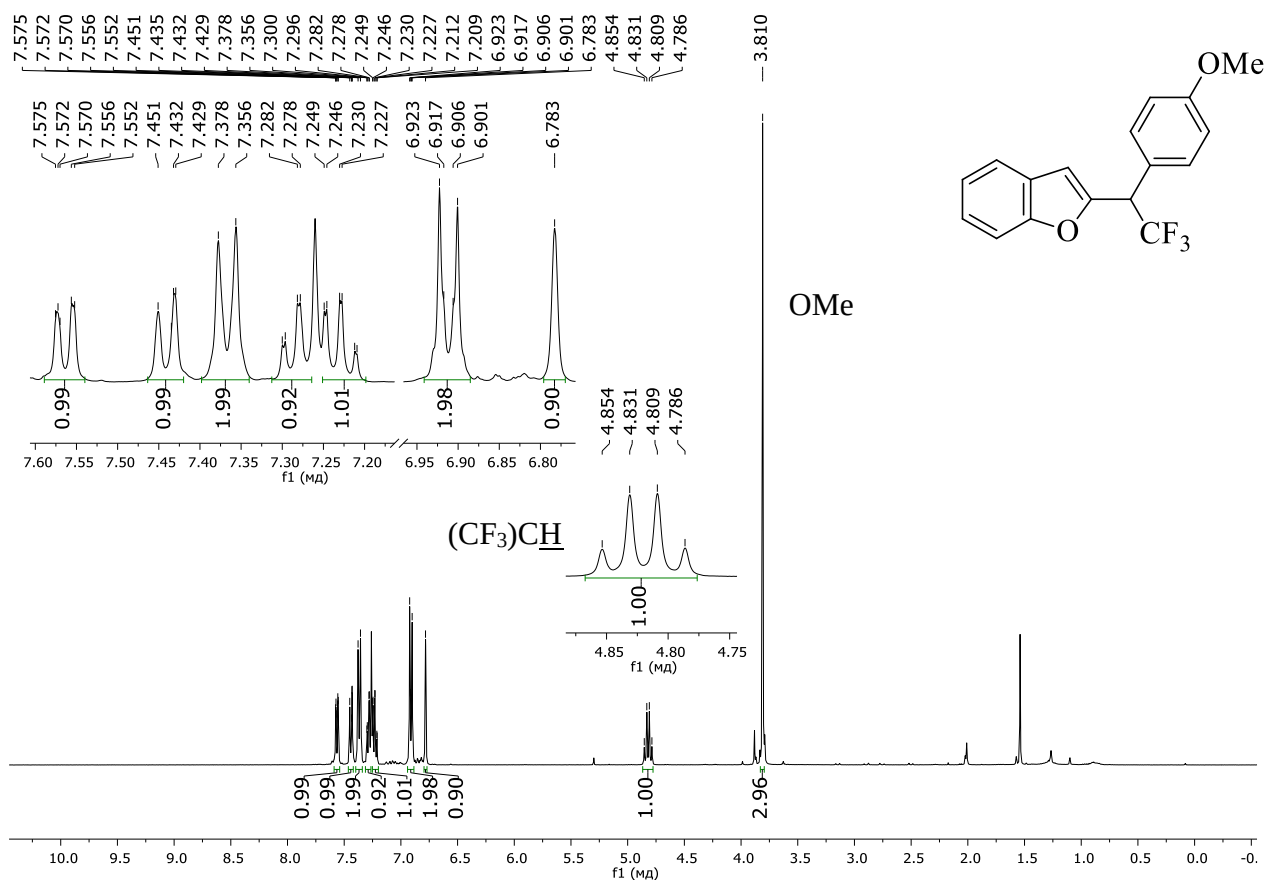


Fig. S27. ^1H NMR spectrum of the compound **2ab** (CDCl_3 , 400 MHz).

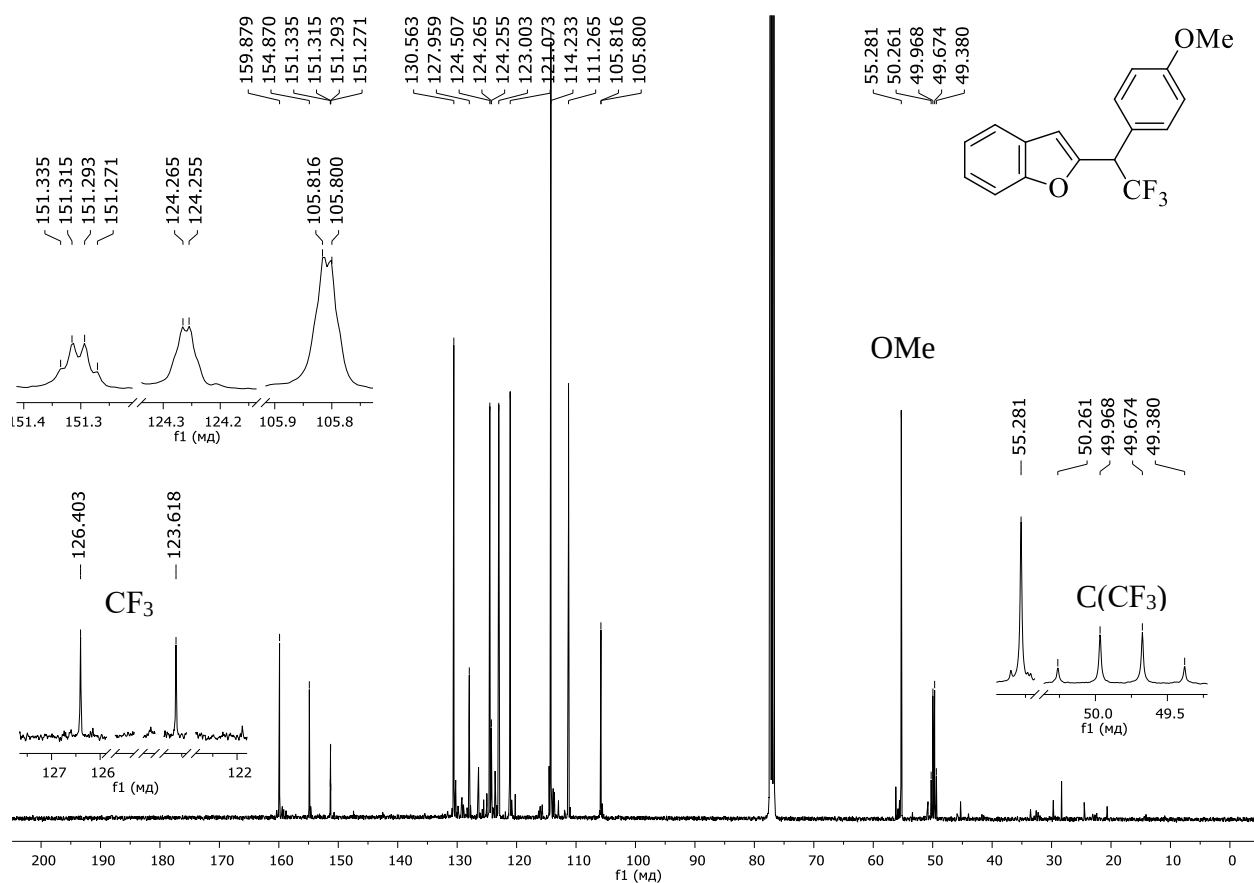


Fig. S28. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2ab** (CDCl_3 , 101 MHz).

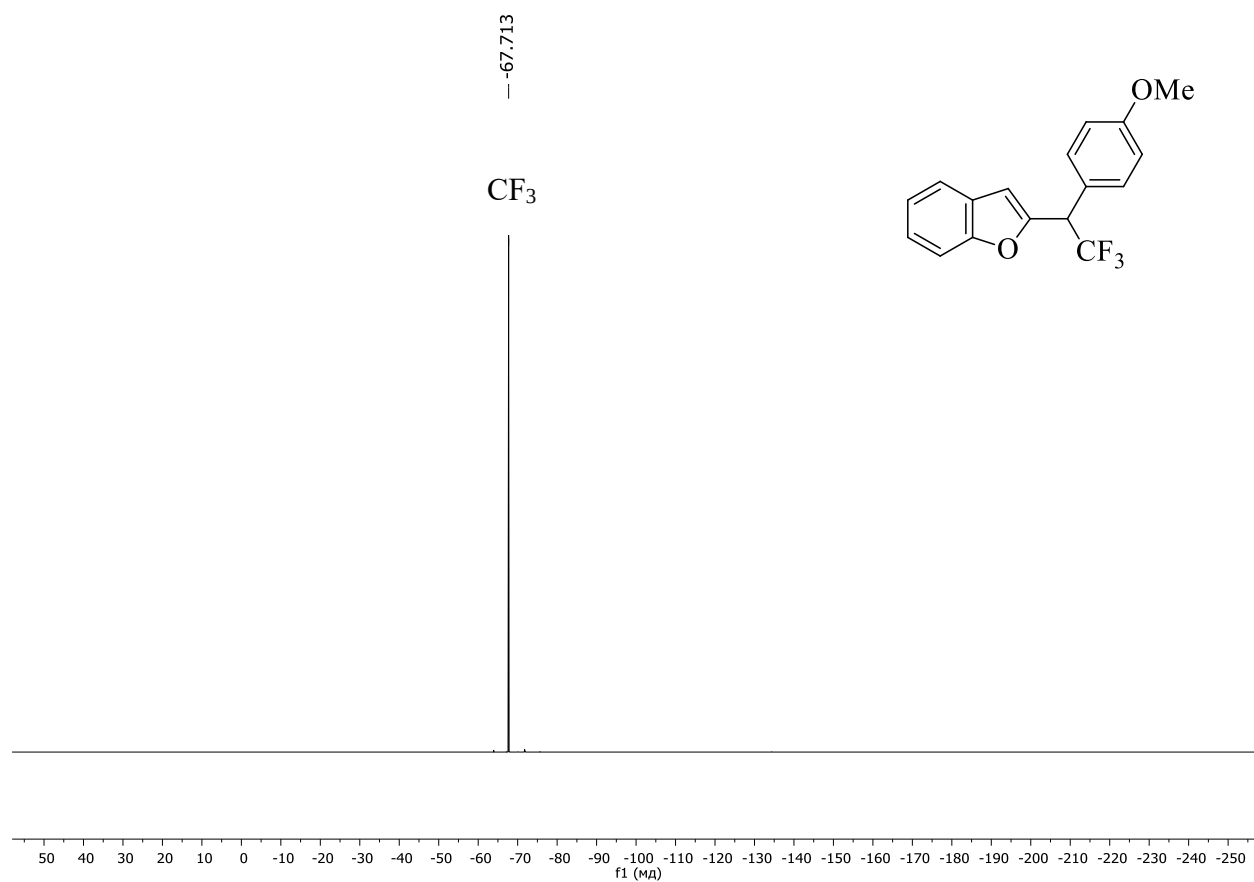


Fig. S29. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ab** (CDCl_3 , 376 MHz).

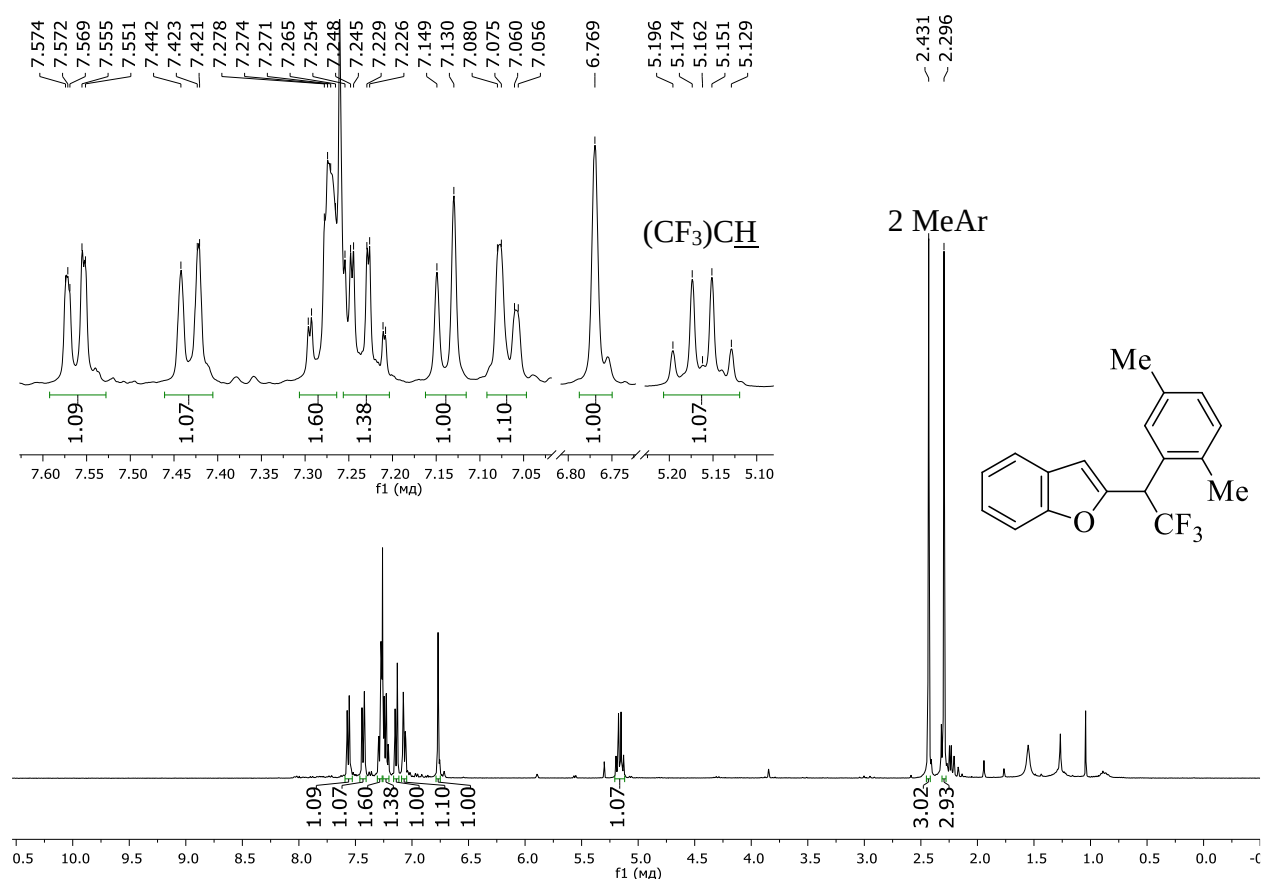


Fig. S30. ¹H NMR spectrum of the compound **2ac** (CDCl₃, 400 MHz).

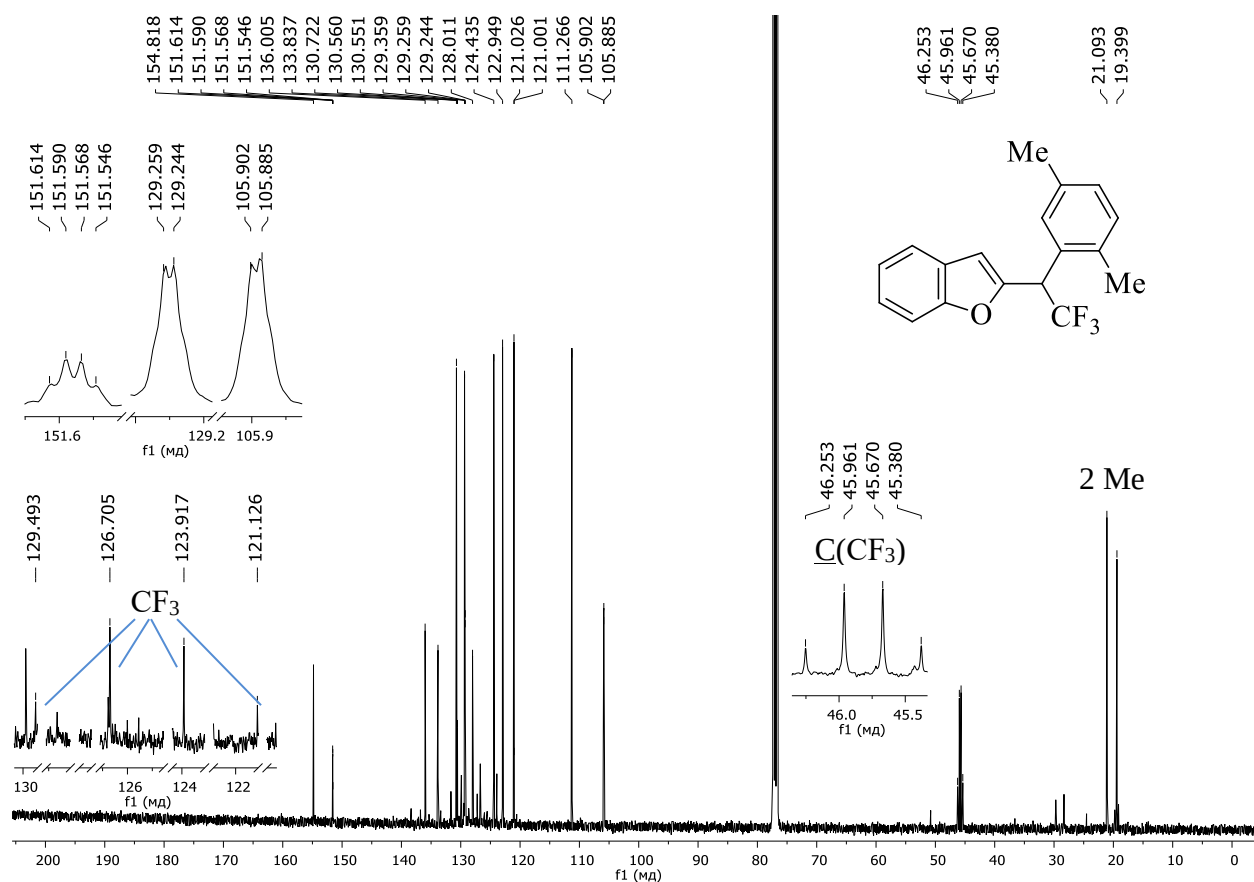


Fig. S31. ¹³C{¹H} NMR spectrum of the compound **2ac** (CDCl₃, 101 MHz).

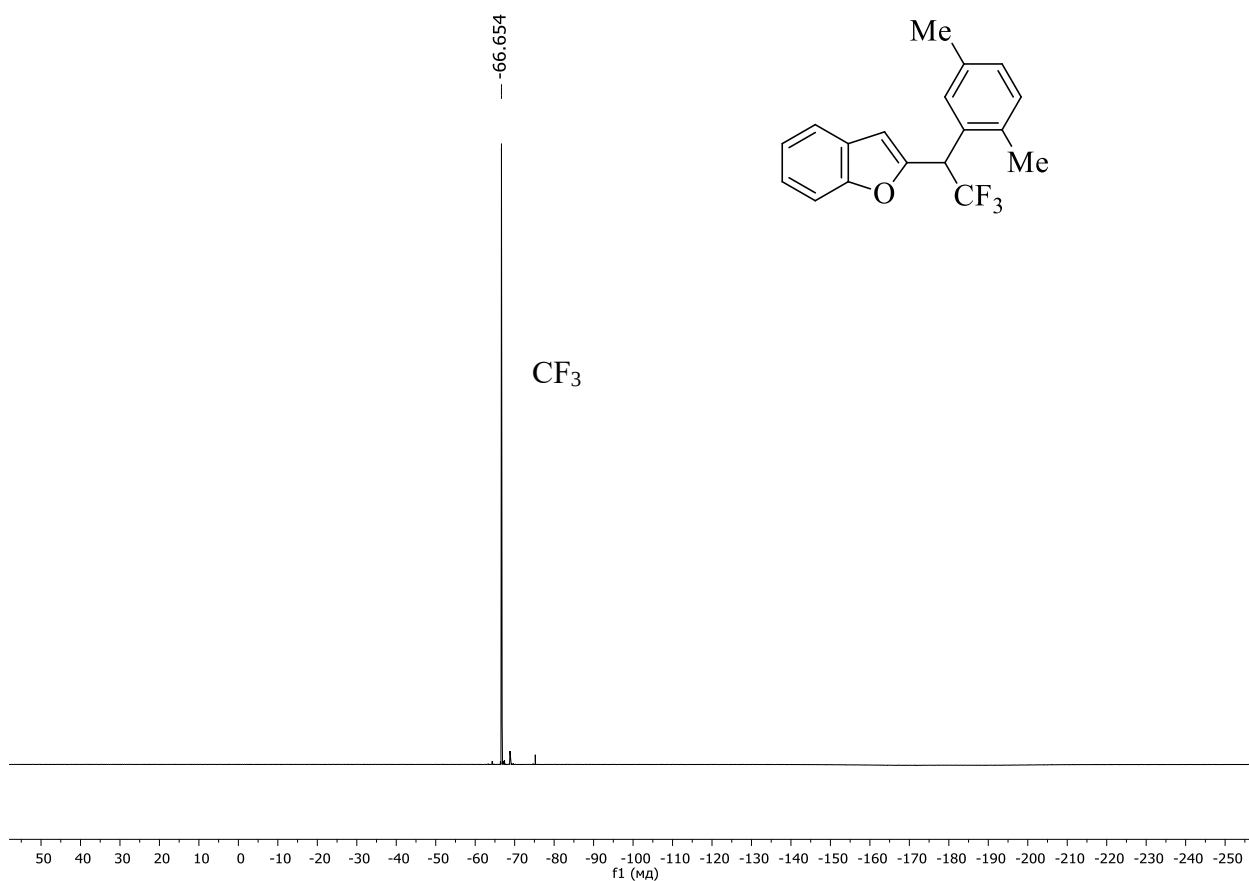


Fig. S32. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ac** (CDCl_3 , 376 MHz).

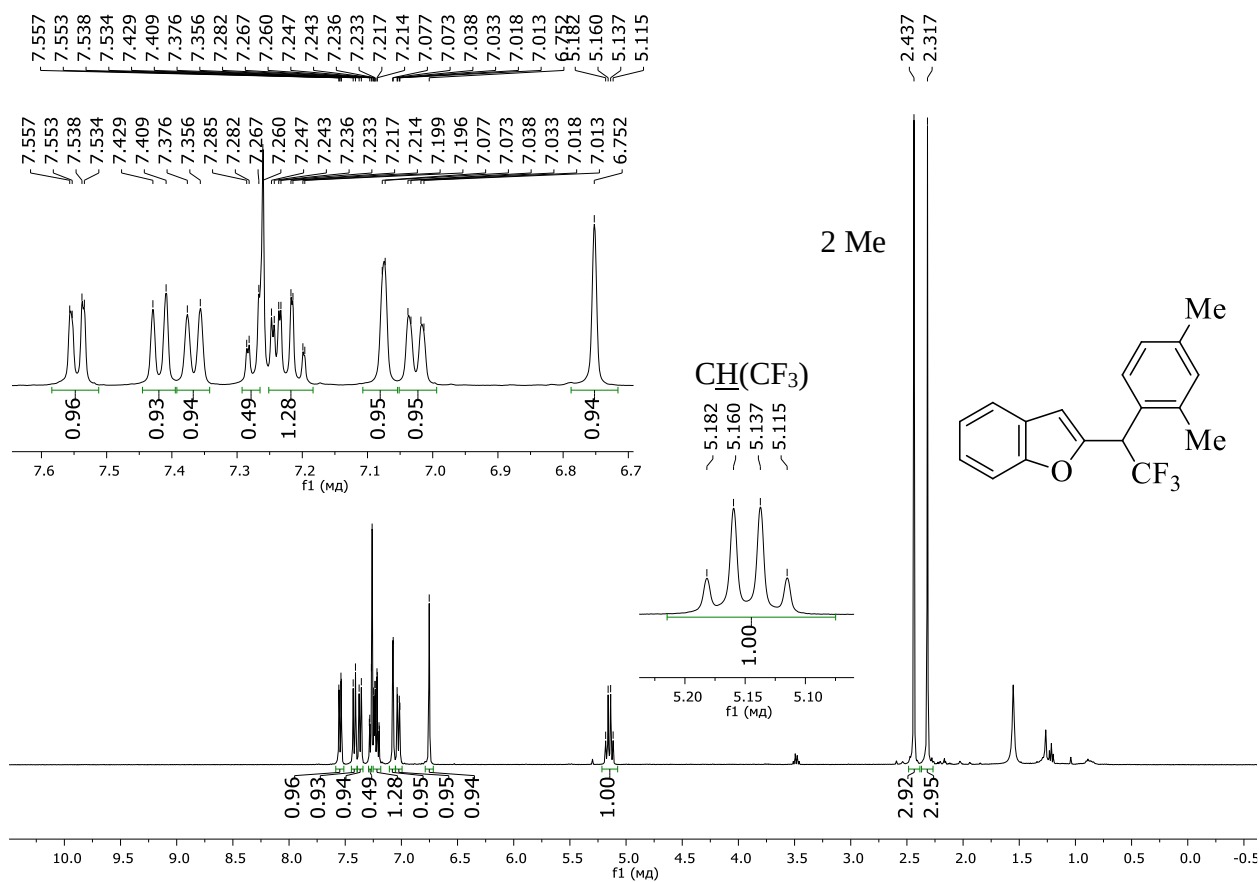


Fig. S33. ^1H NMR spectrum of the compound **2ad** (CDCl_3 , 400 MHz).

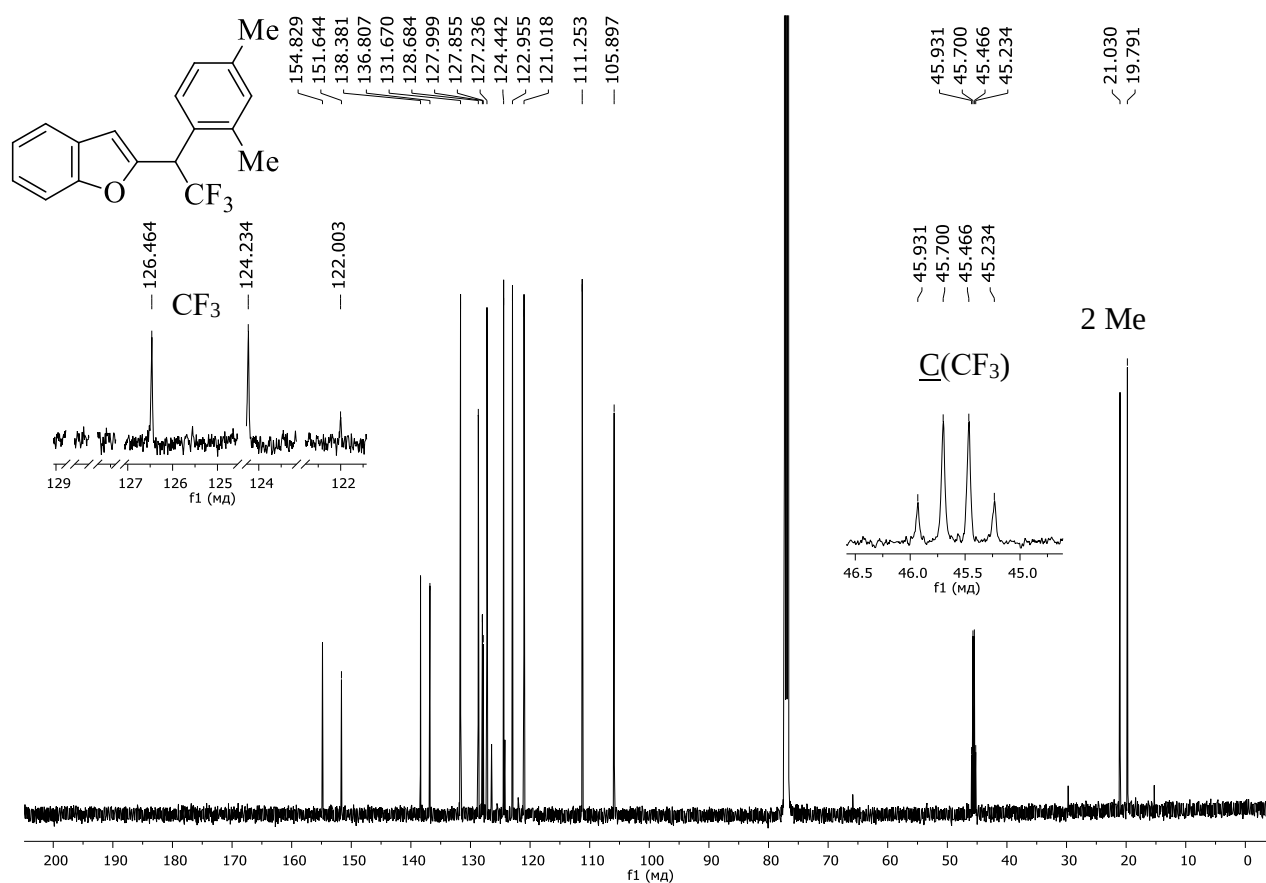


Fig. S34. ¹³C{¹H} NMR spectrum of the compound **2ad** (CDCl₃, 101 MHz).

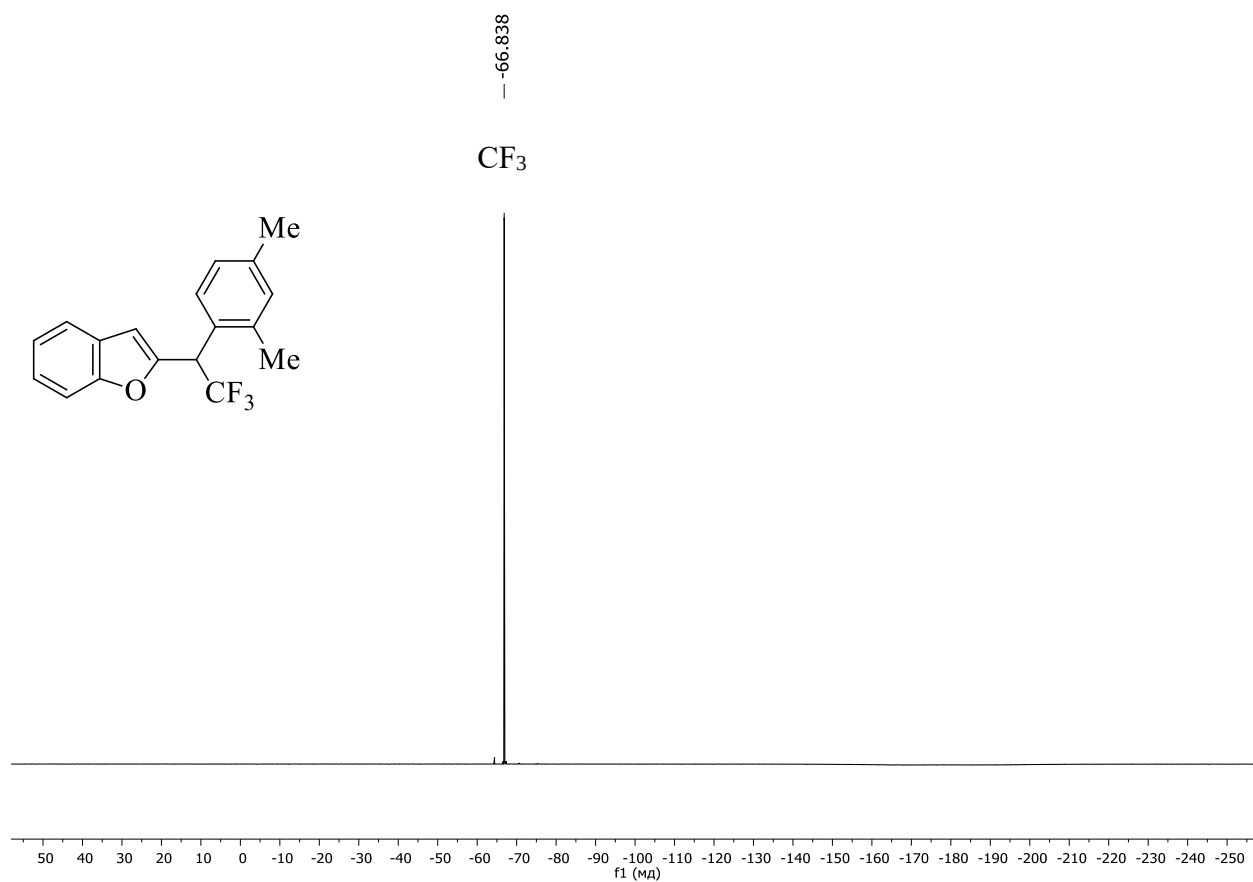


Fig. S35. ¹⁹F{¹H} NMR spectrum of the compound **2ad** (CDCl₃, 376 MHz).

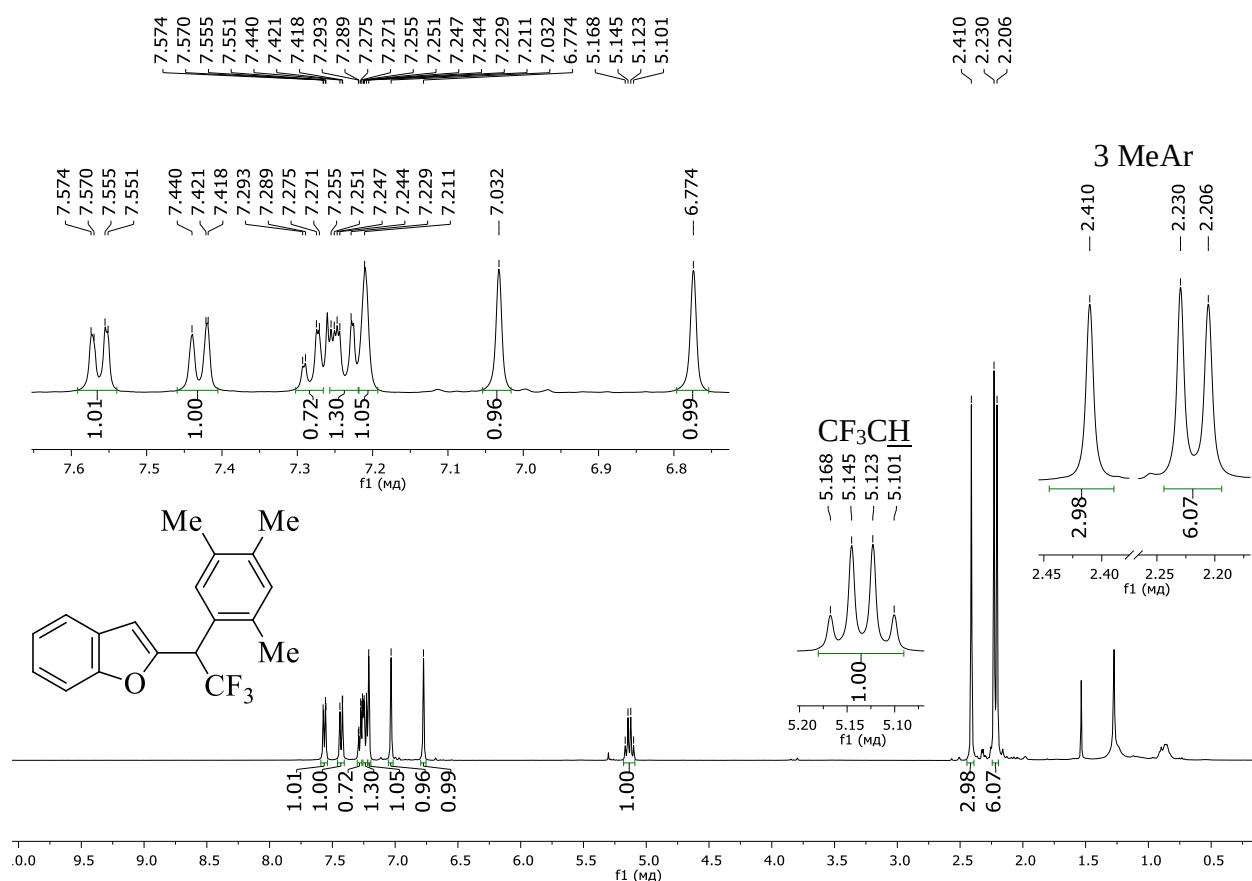


Fig. S36. ¹H NMR spectrum of the compound **2ae** (CDCl₃, 400 MHz).

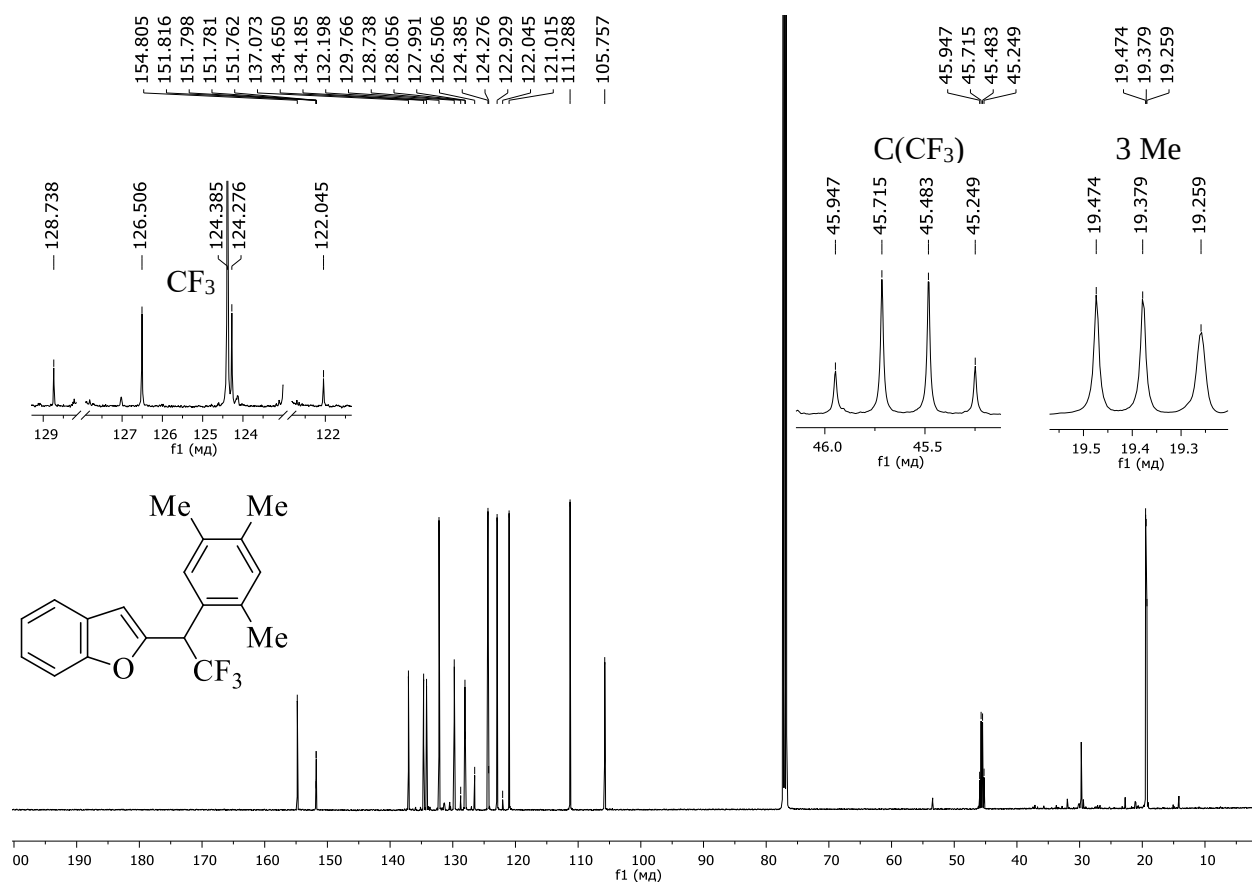


Fig. S37. ¹³C{¹H} NMR spectrum of the compound **2ae** (CDCl₃, 101 MHz).

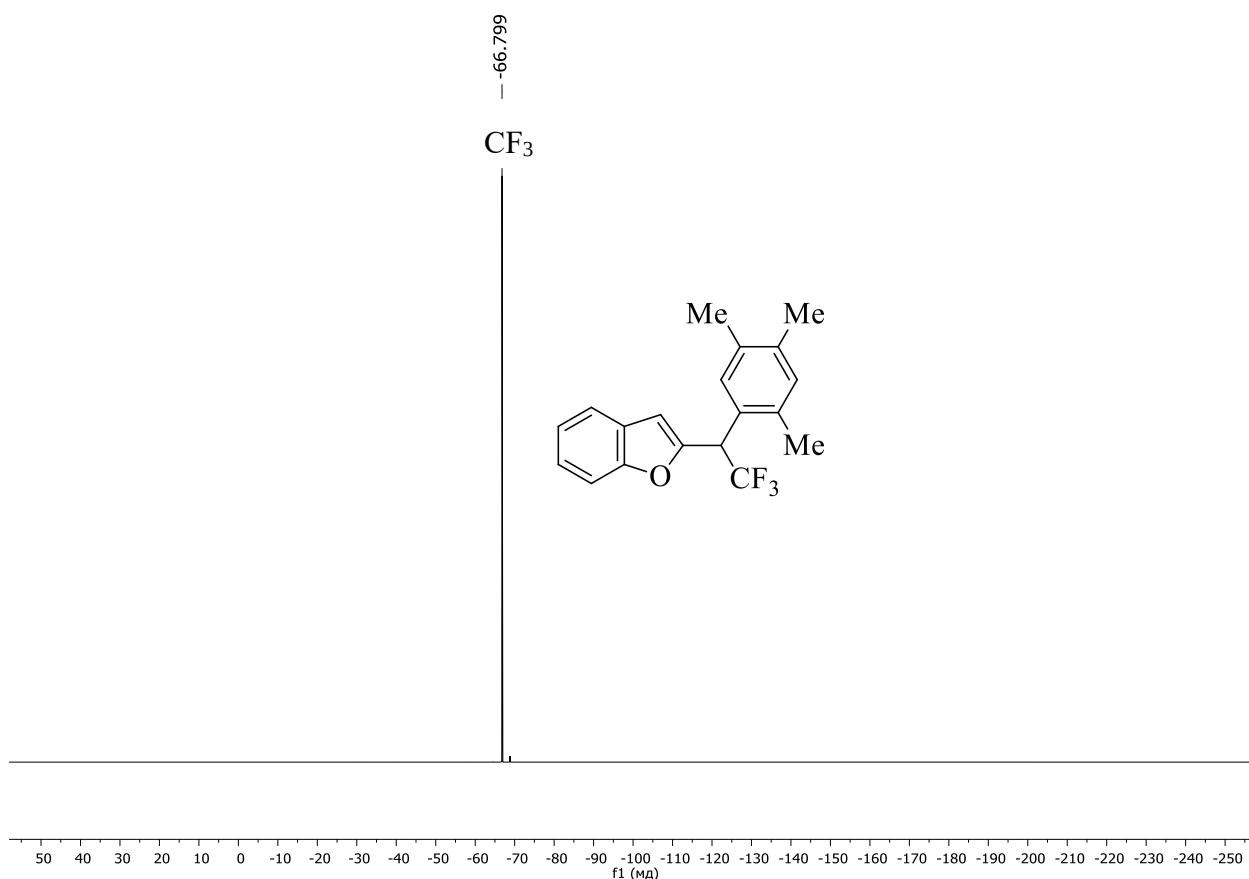


Fig. S38. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ae** (CDCl₃, 376 MHz).

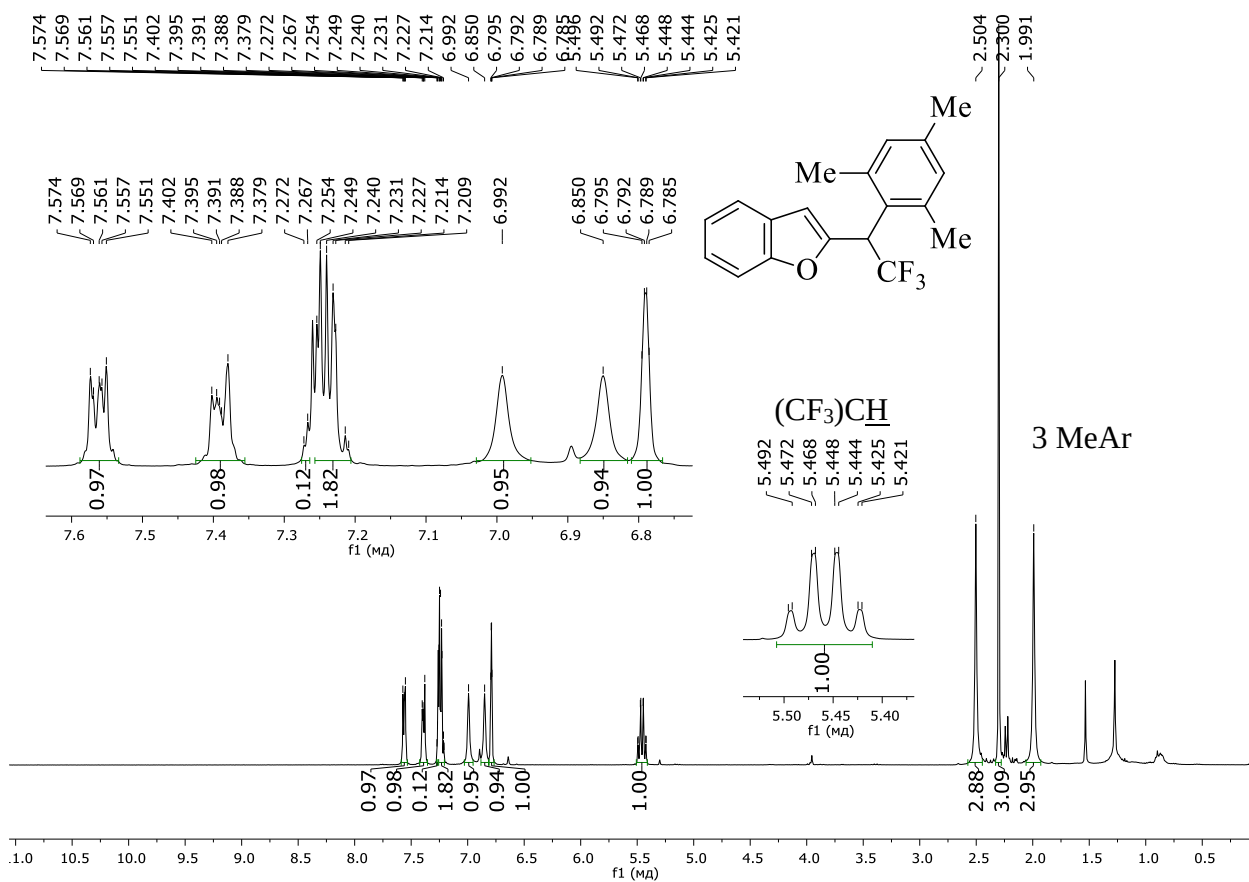


Fig. S39. ^1H NMR spectrum of the compound **2af** (CDCl₃, 400 MHz).

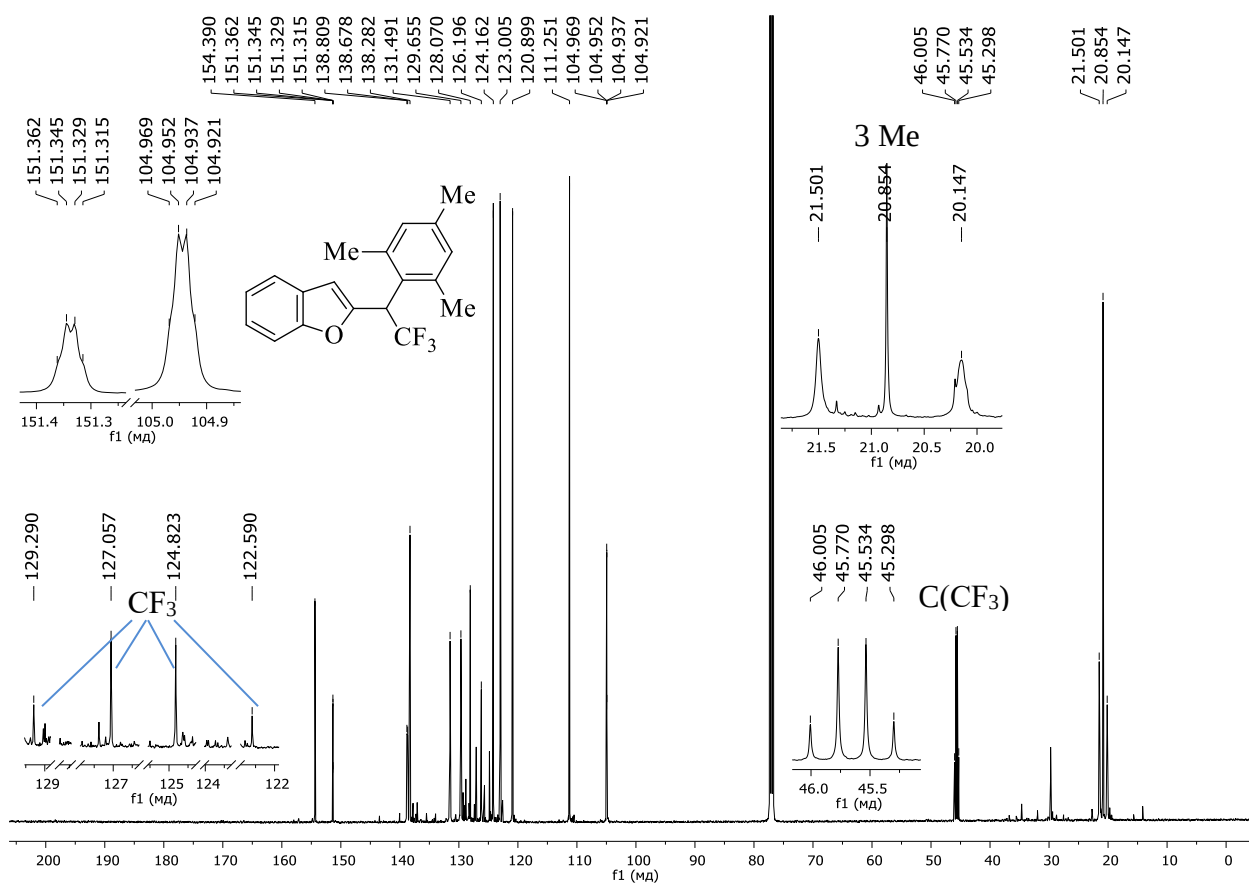


Fig. S40. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2af** (CDCl_3 , 101 MHz).

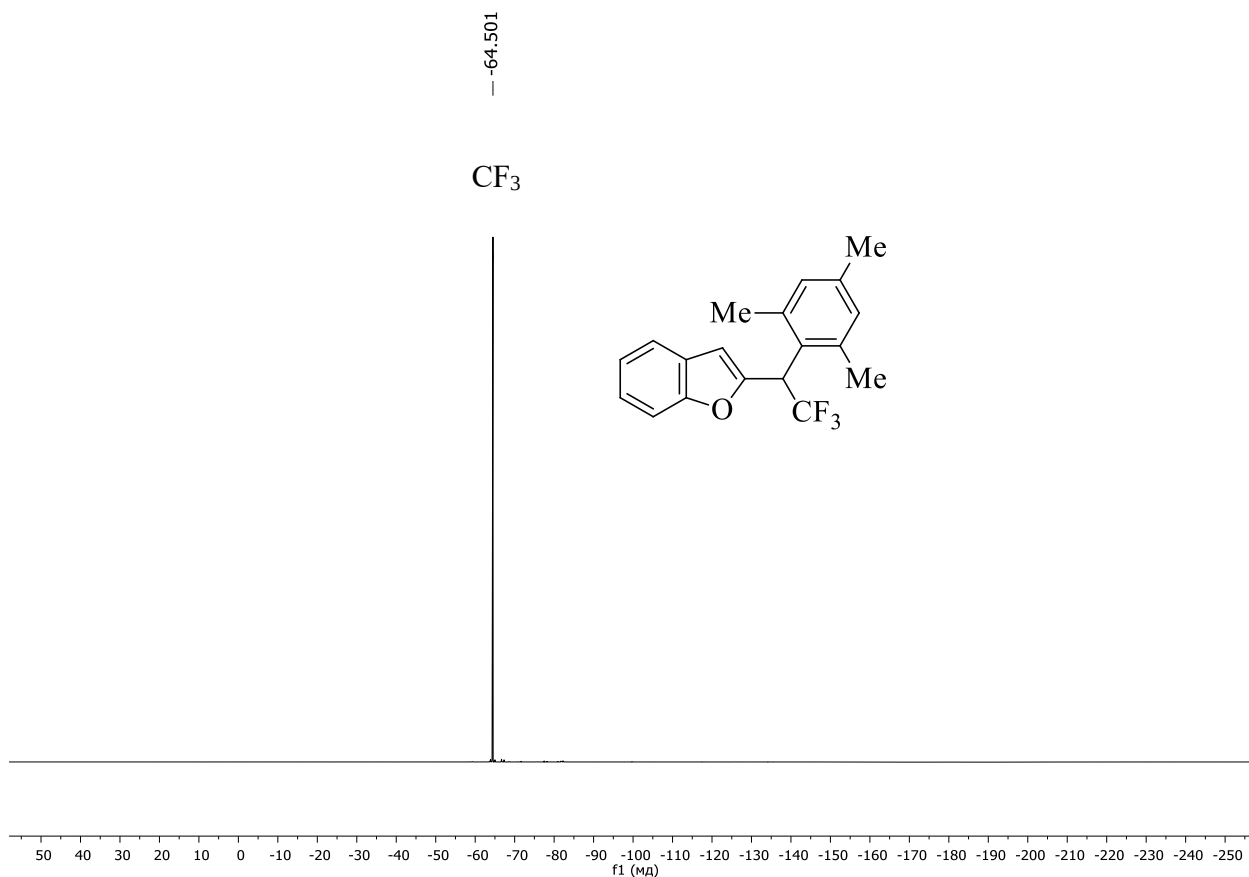


Fig. S41. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2af** (CDCl_3 , 376 MHz).

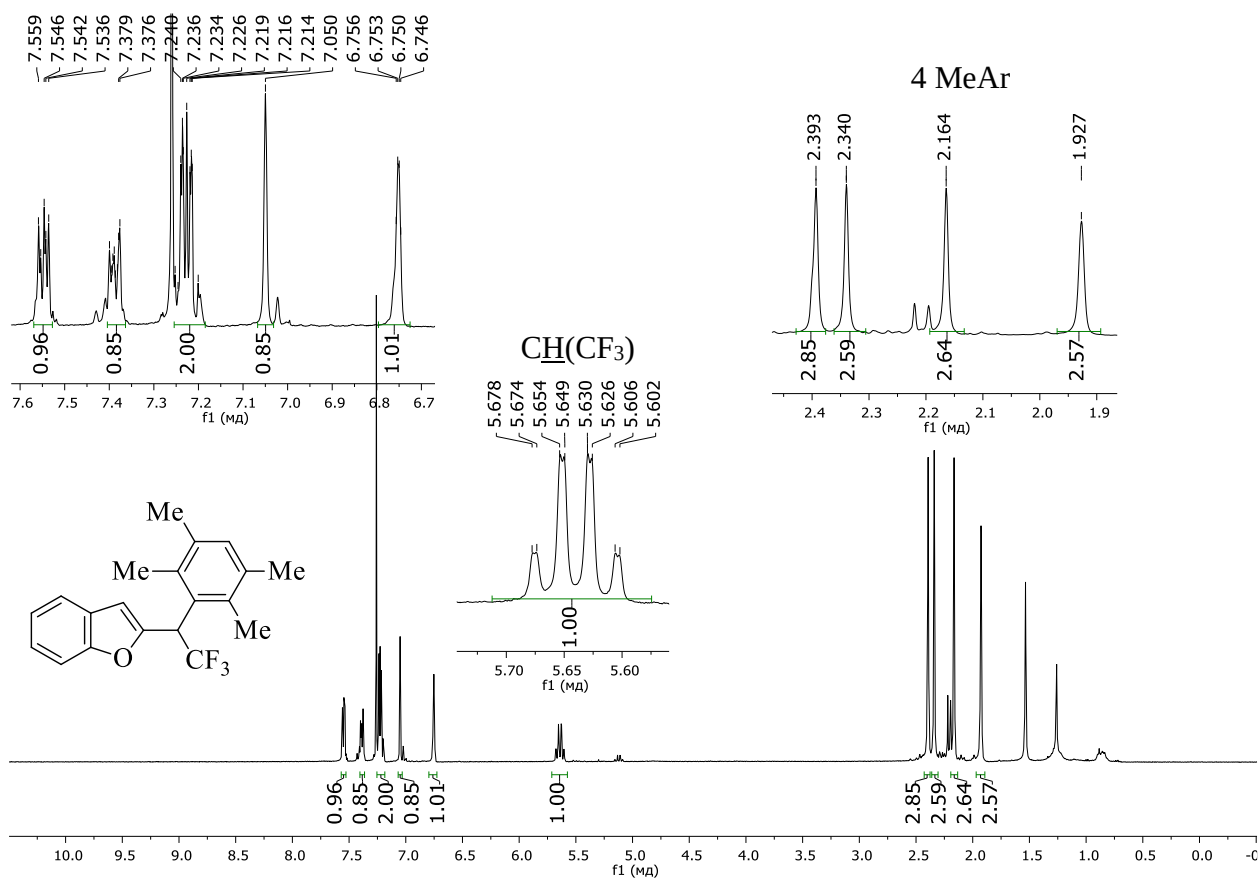


Fig. S42. ¹H NMR spectrum of the compound **2ag** (CDCl₃, 400 MHz).

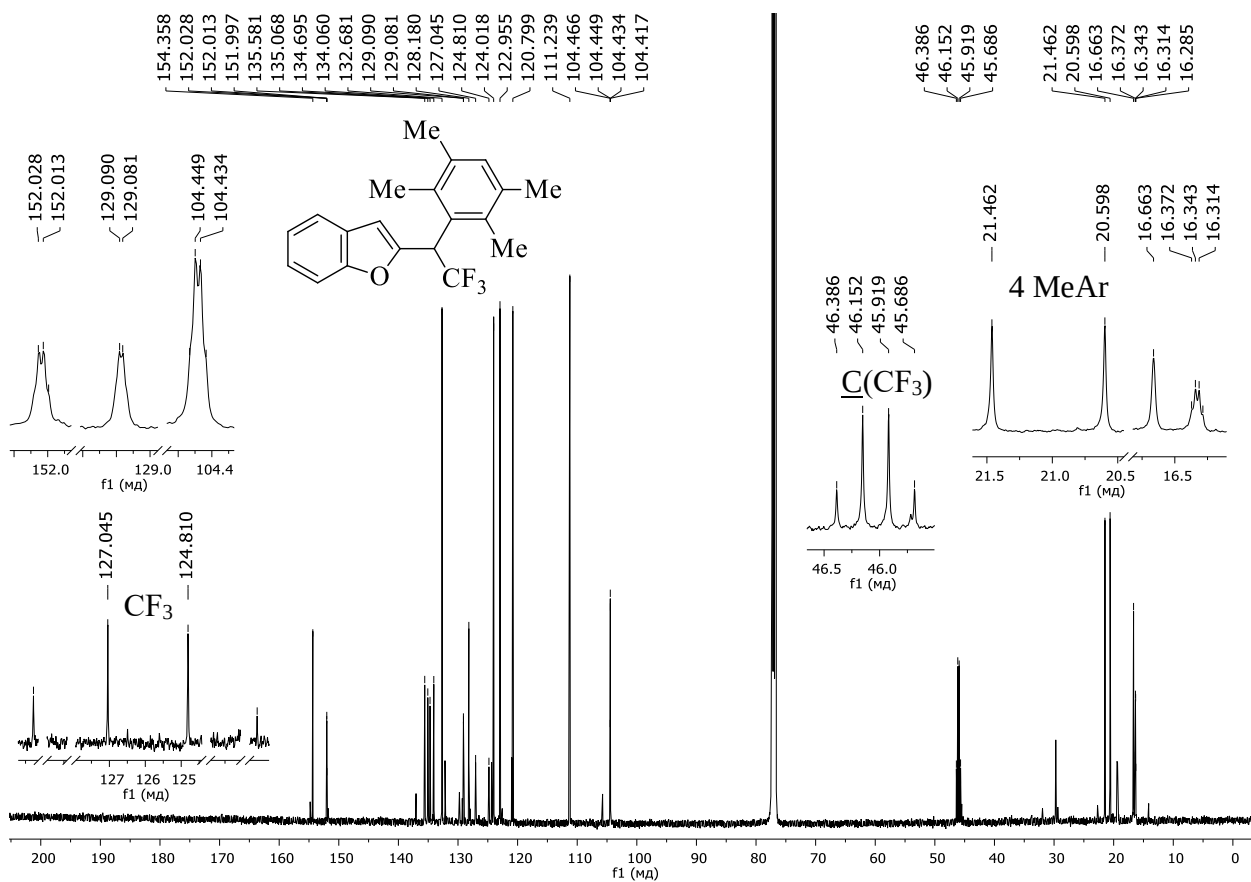


Fig. S43. ¹³C{¹H} NMR spectrum of the compound **2ag** (CDCl₃, 101 MHz).

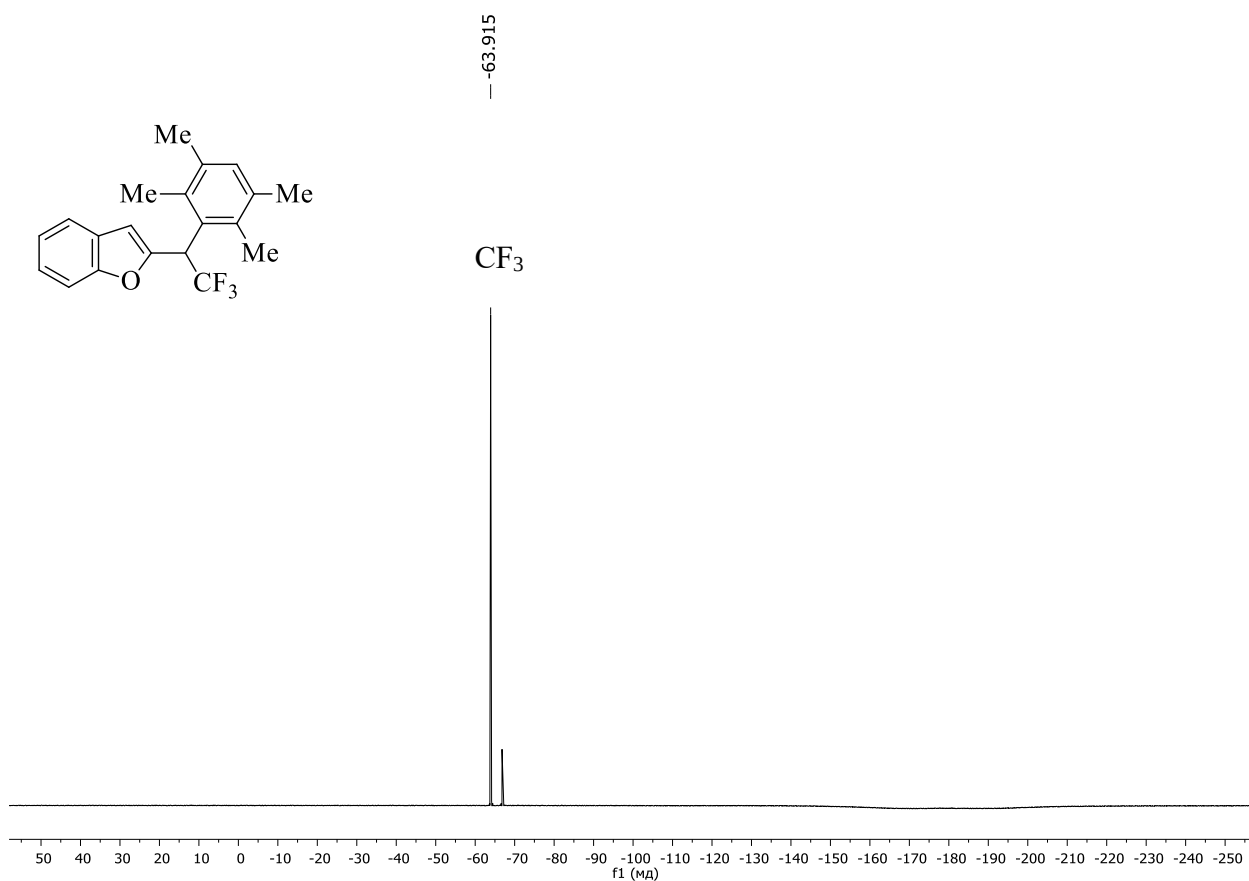


Fig. S44. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ag** (CDCl₃, 376 MHz).

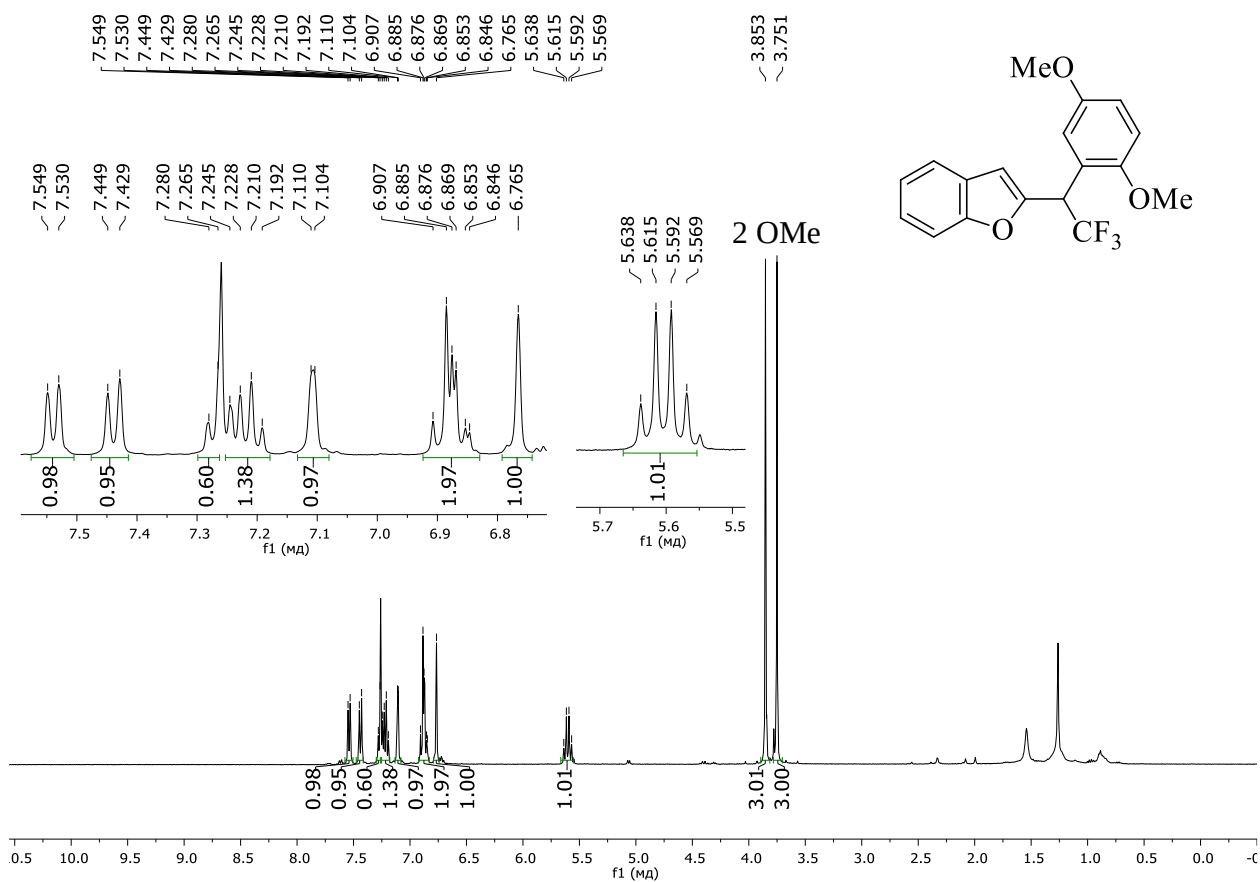


Fig. S45. ^1H NMR spectrum of the compound **2ah** (CDCl₃, 400 MHz).

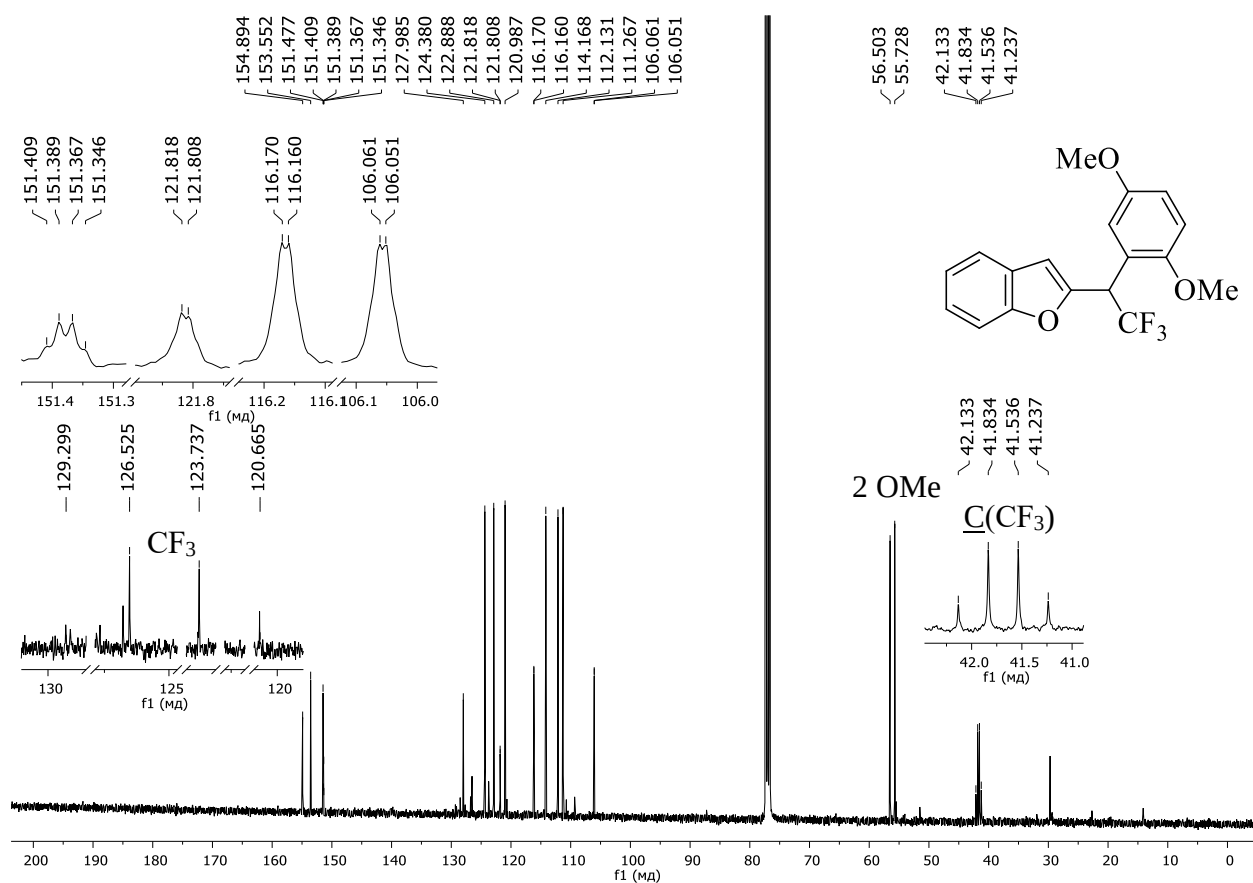


Fig. S46. ¹³C{¹H} NMR spectrum of the compound **2ah** (CDCl₃, 101 MHz).

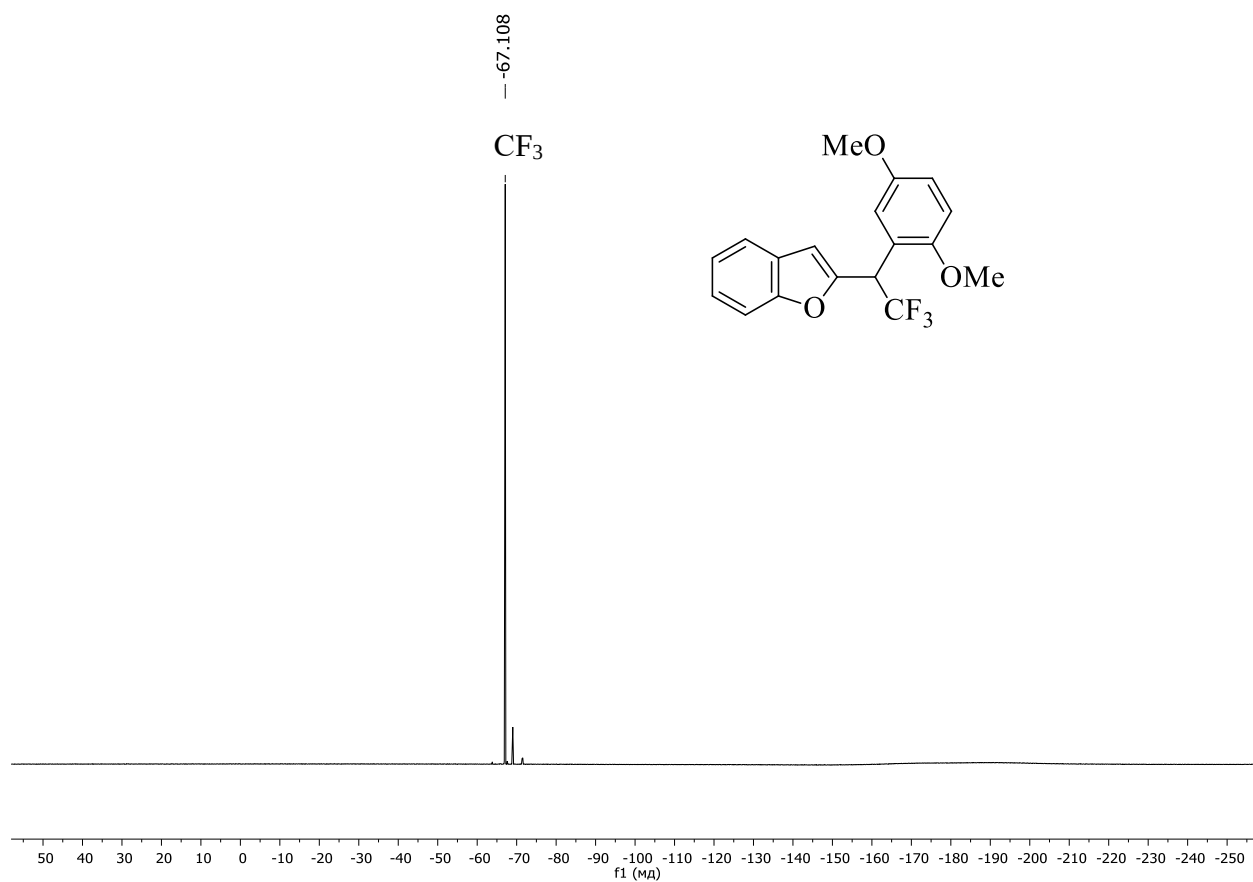


Fig. S47. ¹⁹F{¹H} NMR spectrum of the compound **2ah** (CDCl₃, 376 MHz).

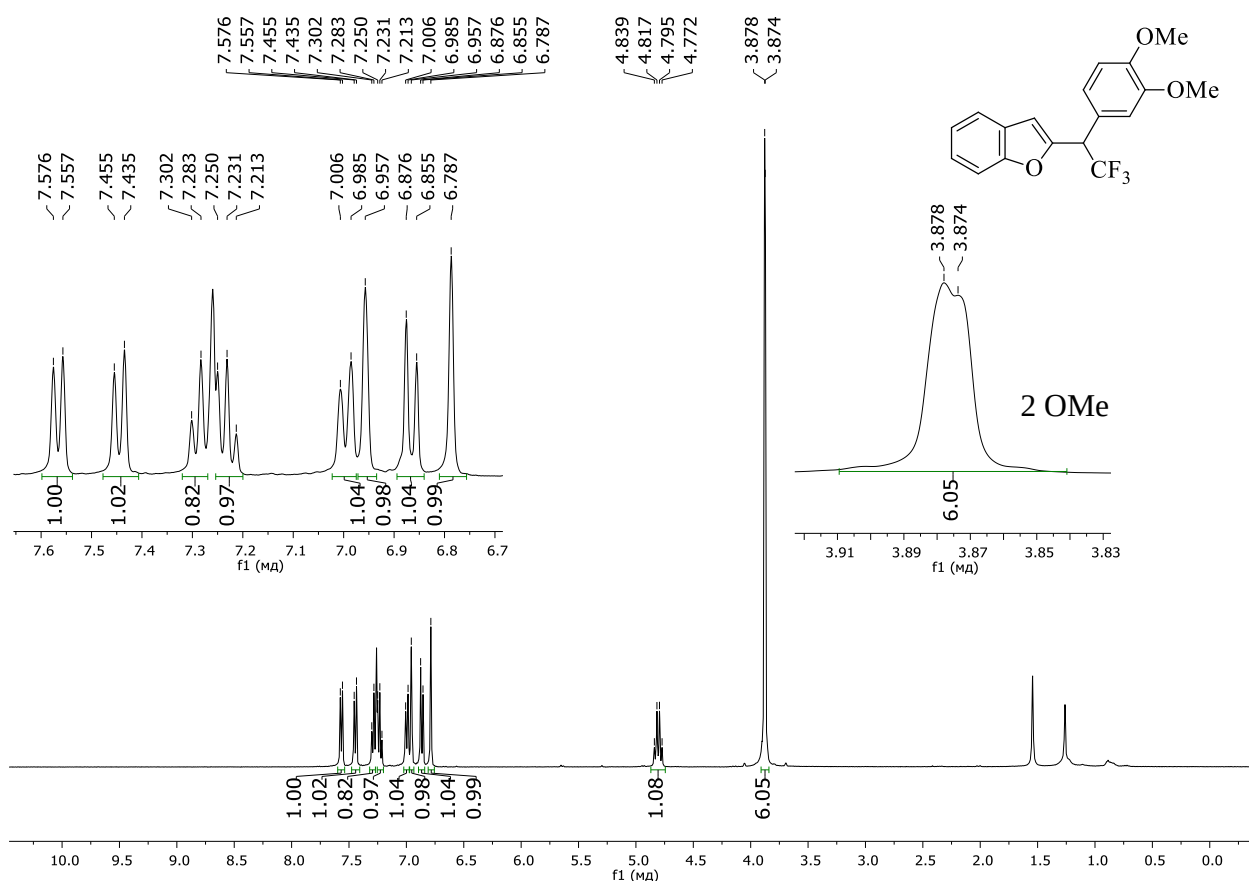


Fig. S48. ¹H NMR spectrum of the compound **2ai** (CDCl₃, 400 MHz).

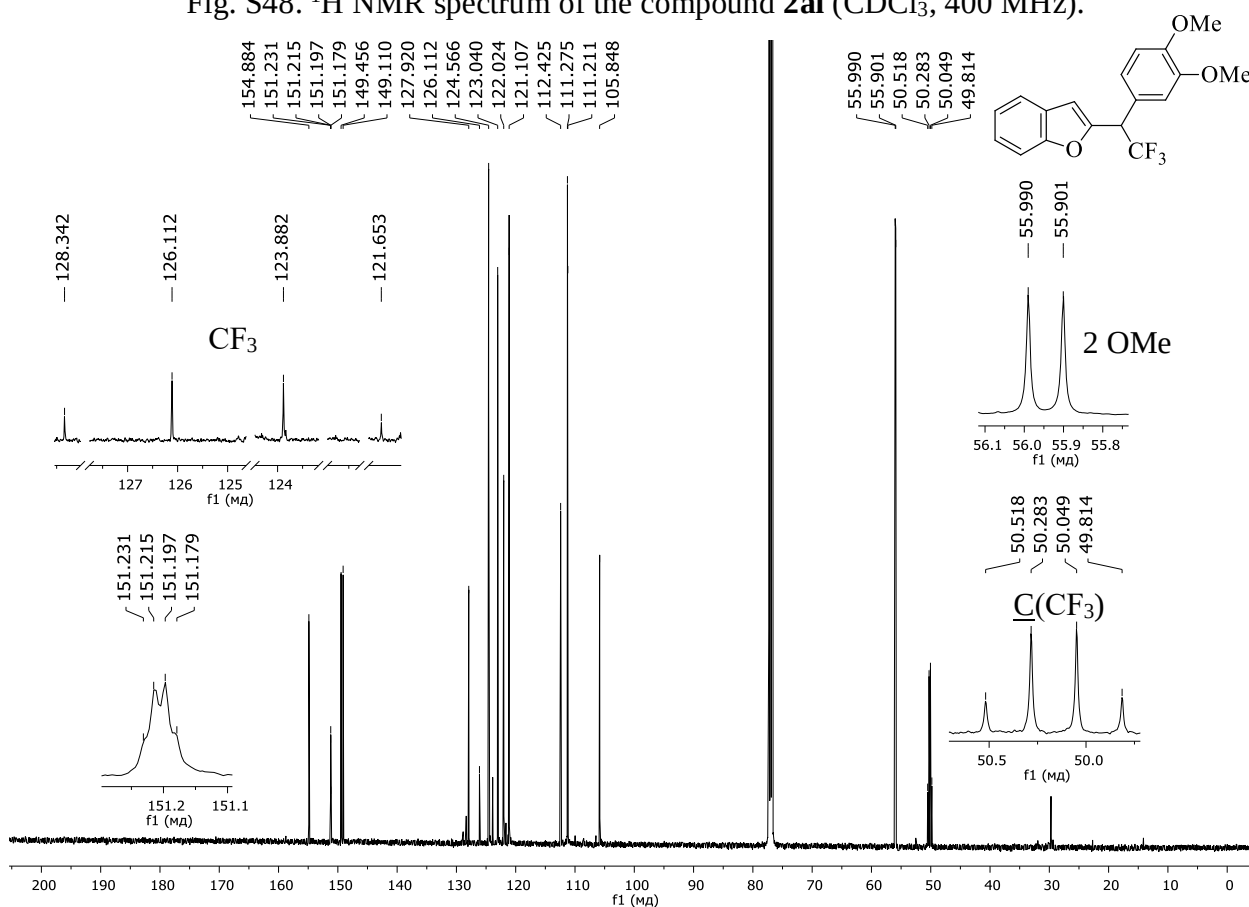


Fig. S49. ¹³C{¹H} NMR spectrum of the compound **2ai** (CDCl₃, 101 MHz).

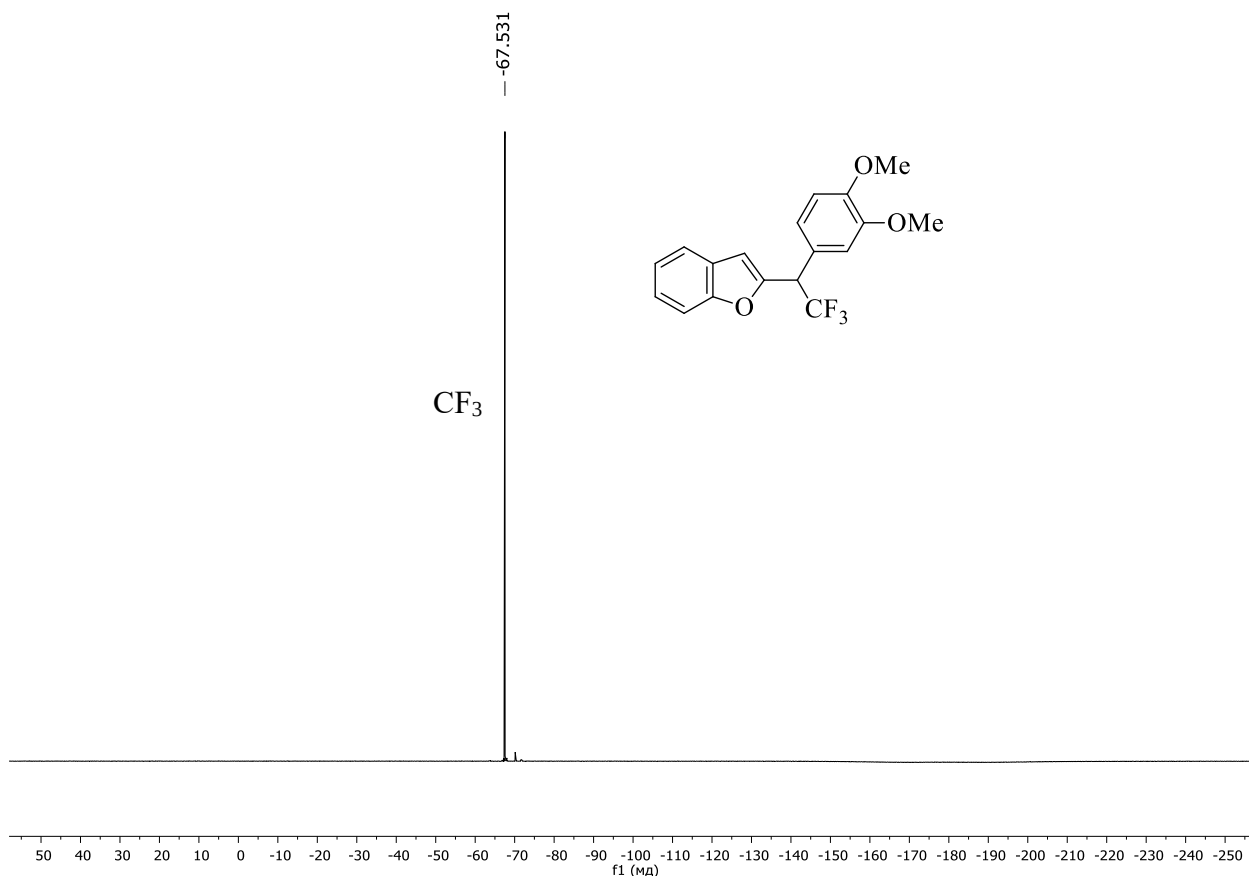


Fig. S50. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ai** (CDCl₃, 376 MHz).

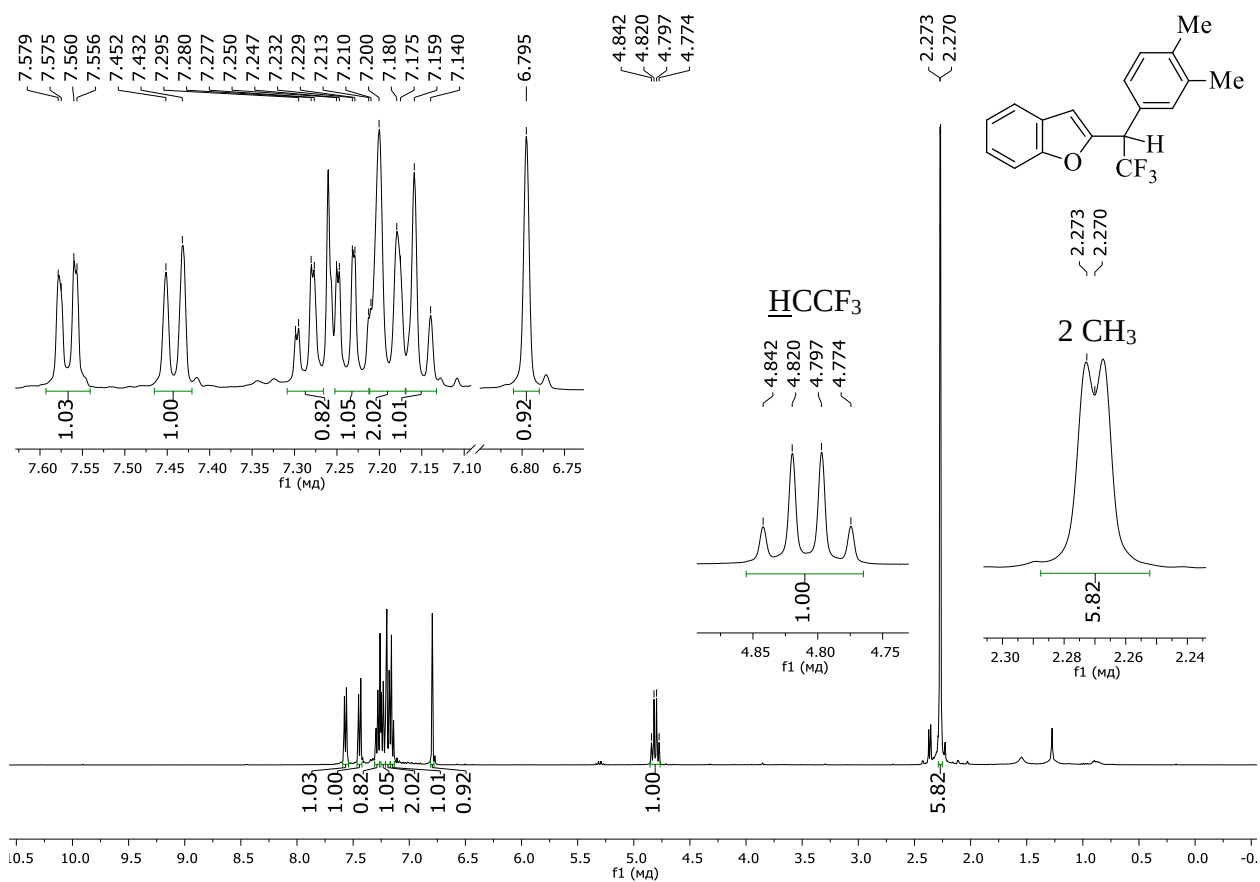


Fig. S51. ^1H NMR spectrum of the compound **2aj** (CDCl₃, 400 MHz).

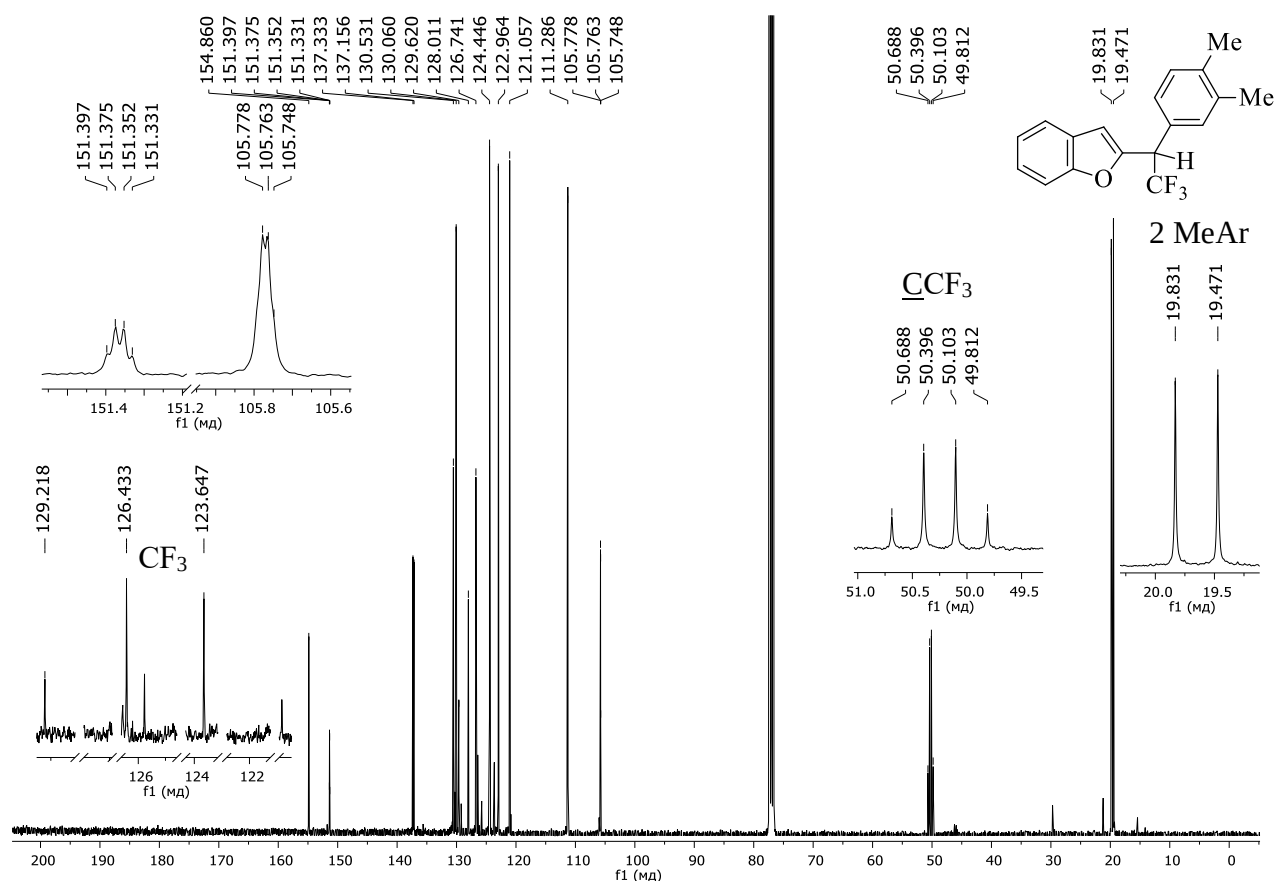


Fig. S52. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2aj** (CDCl_3 , 101 MHz).

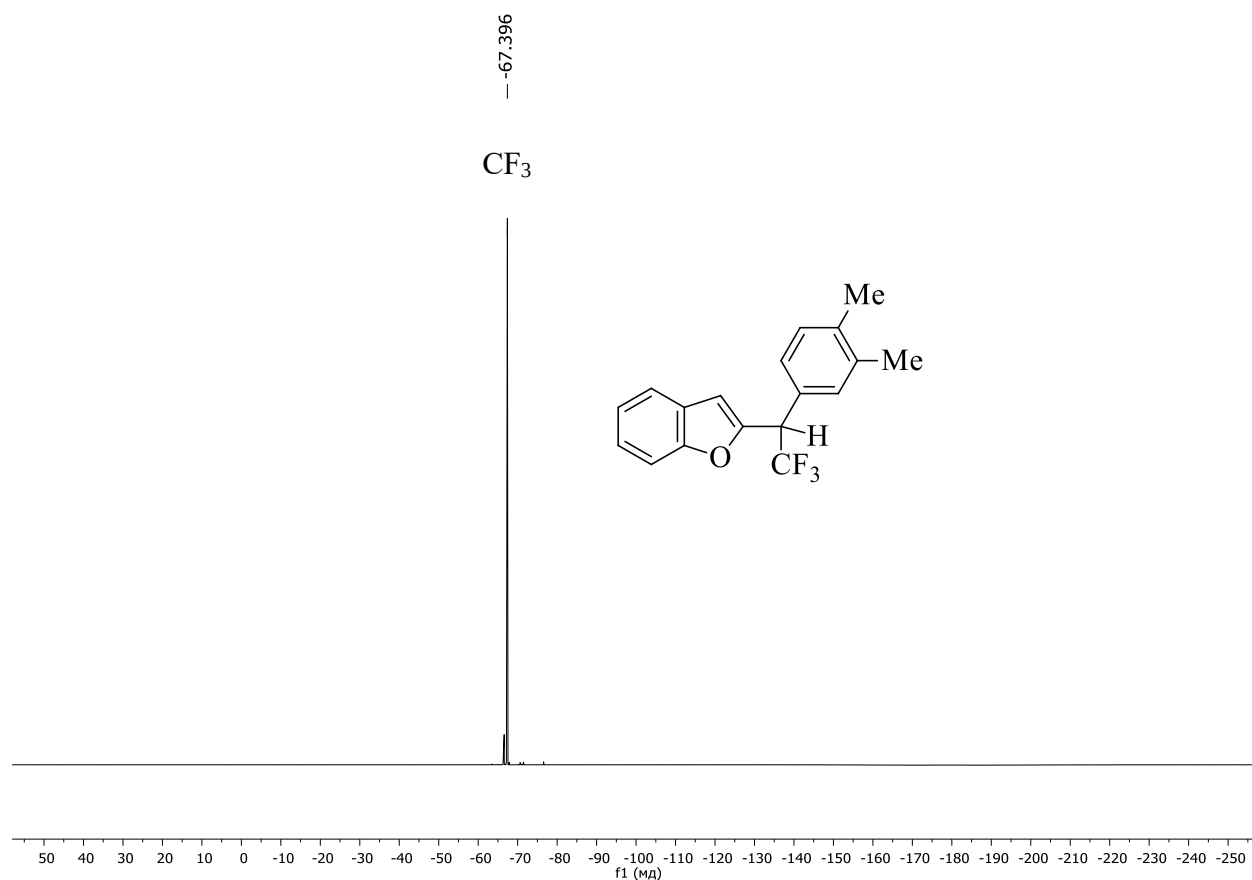


Fig. S53. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2aj** (CDCl_3 , 376 MHz).

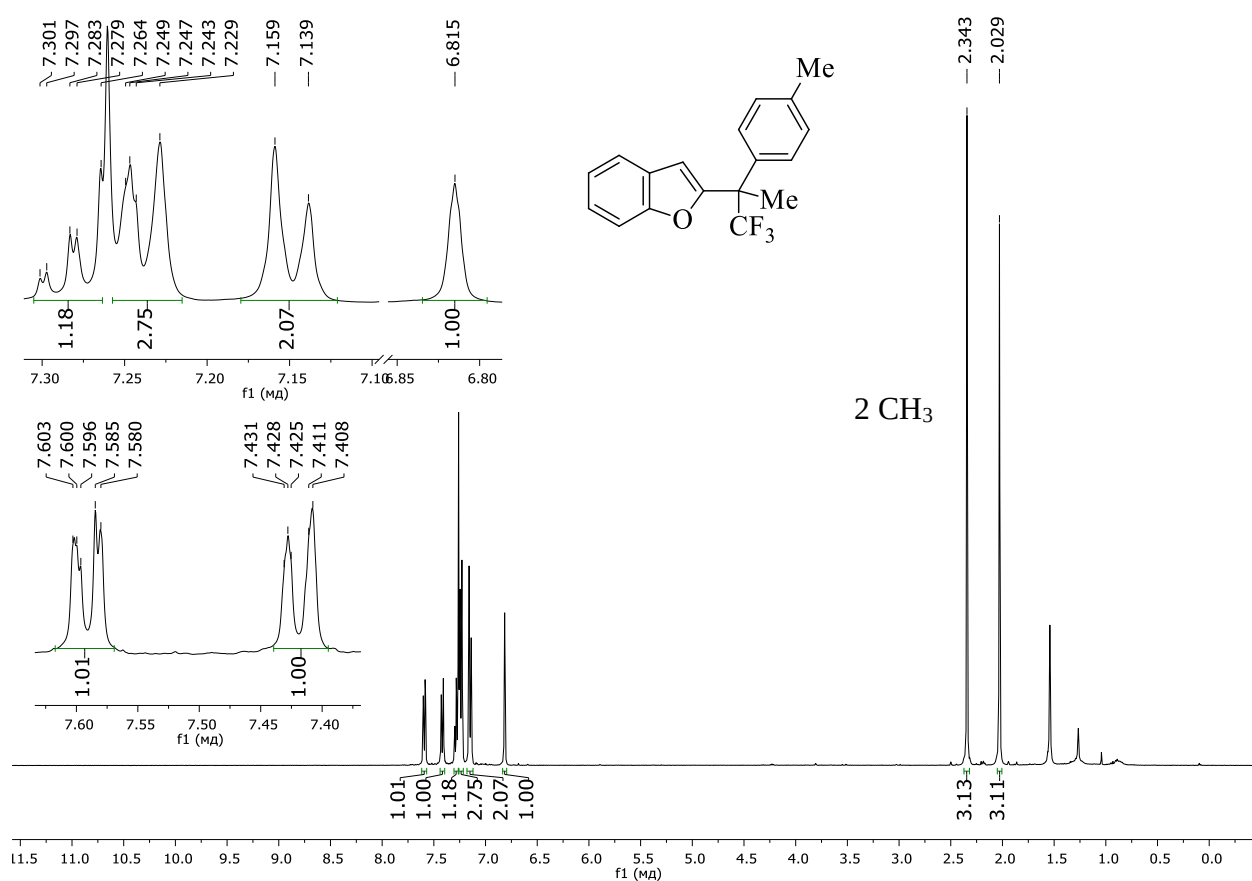


Fig. S54. ¹H NMR spectrum of the compound **2ba** (CDCl₃, 400 MHz).

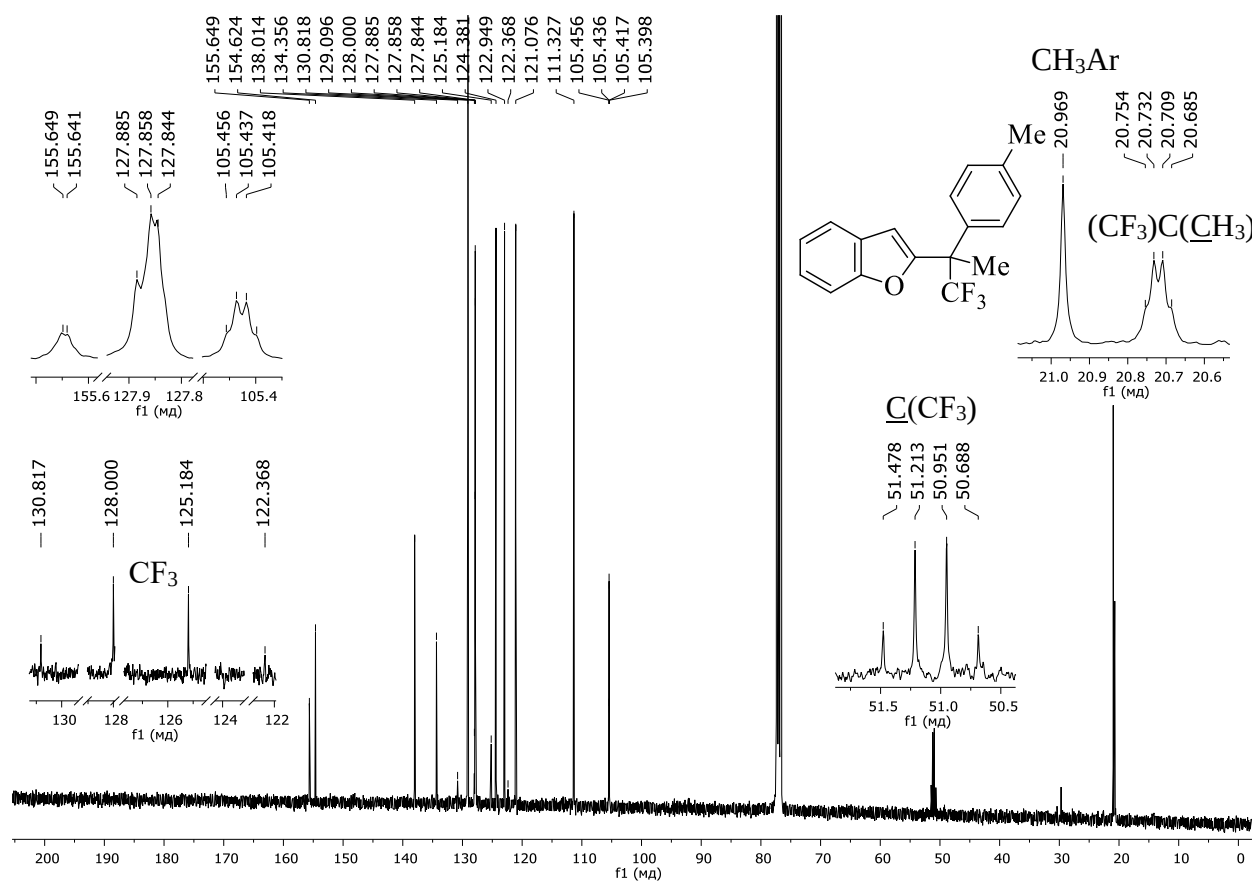


Fig. S55. ¹³C{¹H} NMR spectrum of the compound **2ba** (CDCl₃, 101 MHz).

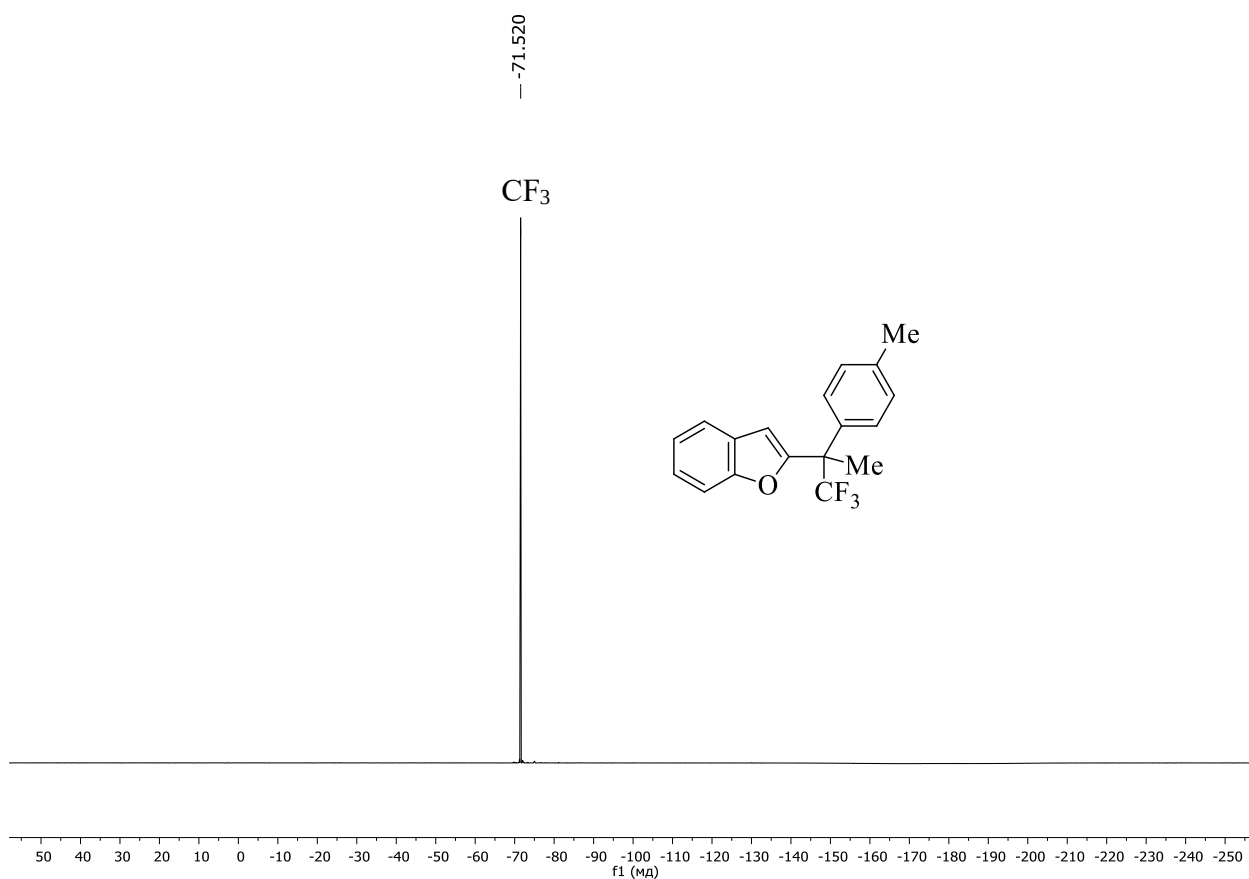


Fig. S56. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ba** (CDCl₃, 376 MHz).

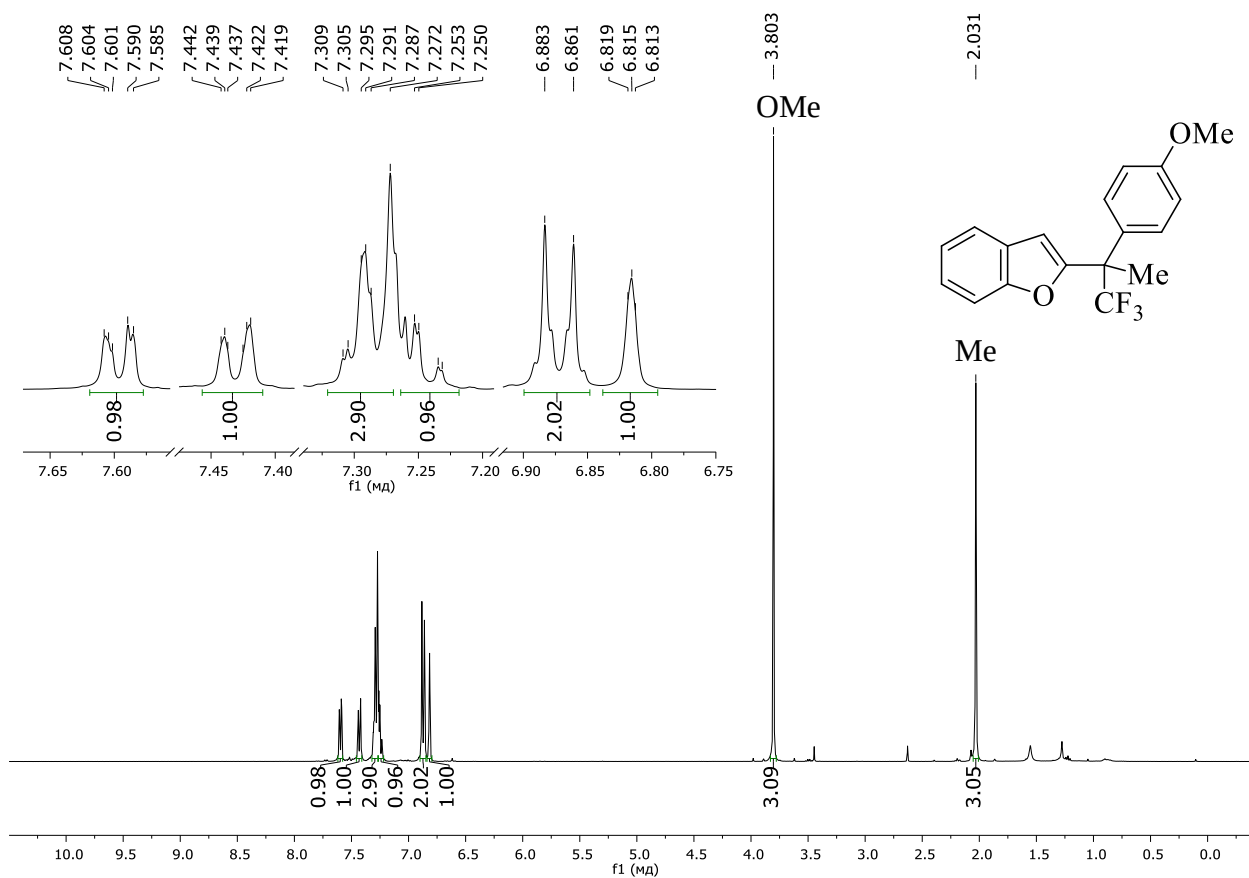


Fig. S57. ^1H NMR spectrum of the compound **2bb** (CDCl₃, 400 MHz).

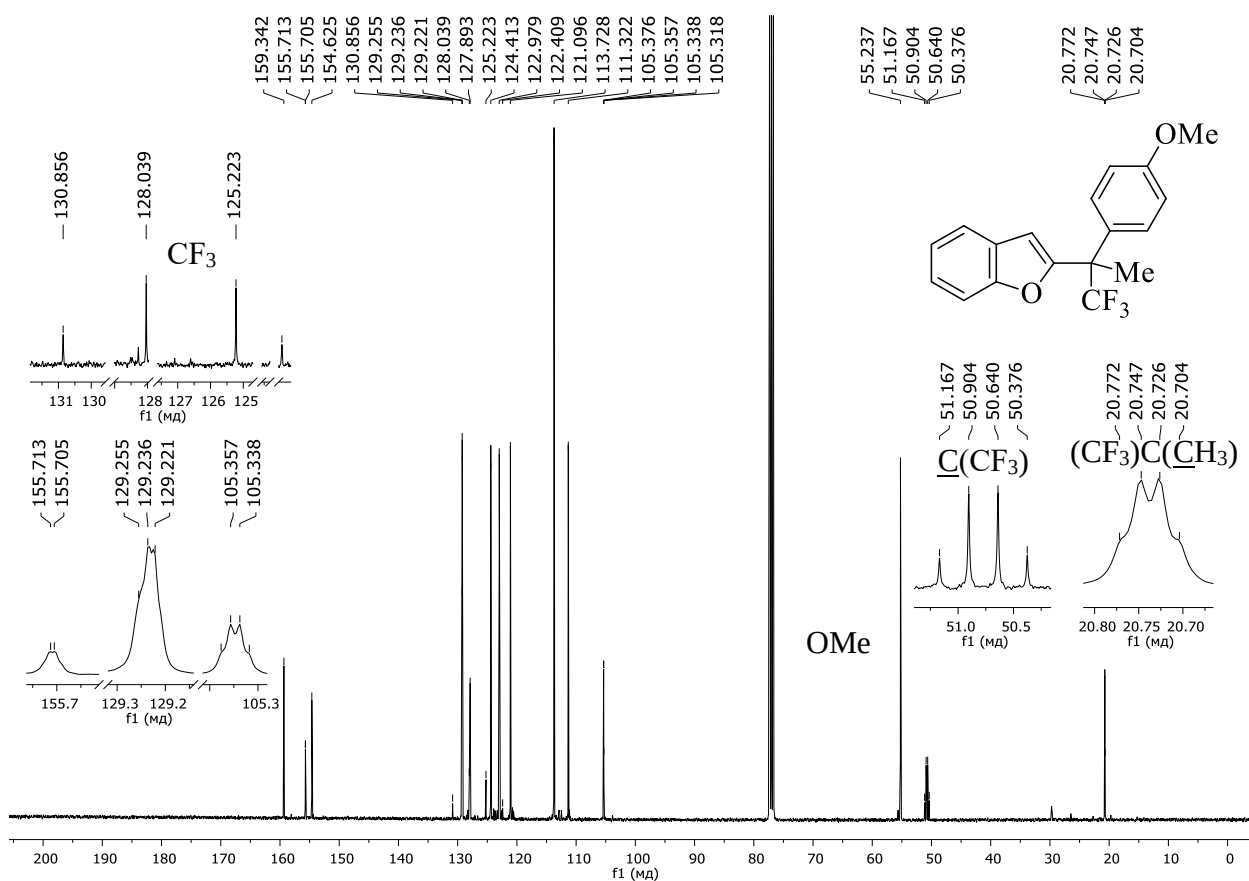


Fig. S58. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2bb** (CDCl_3 , 101 MHz).

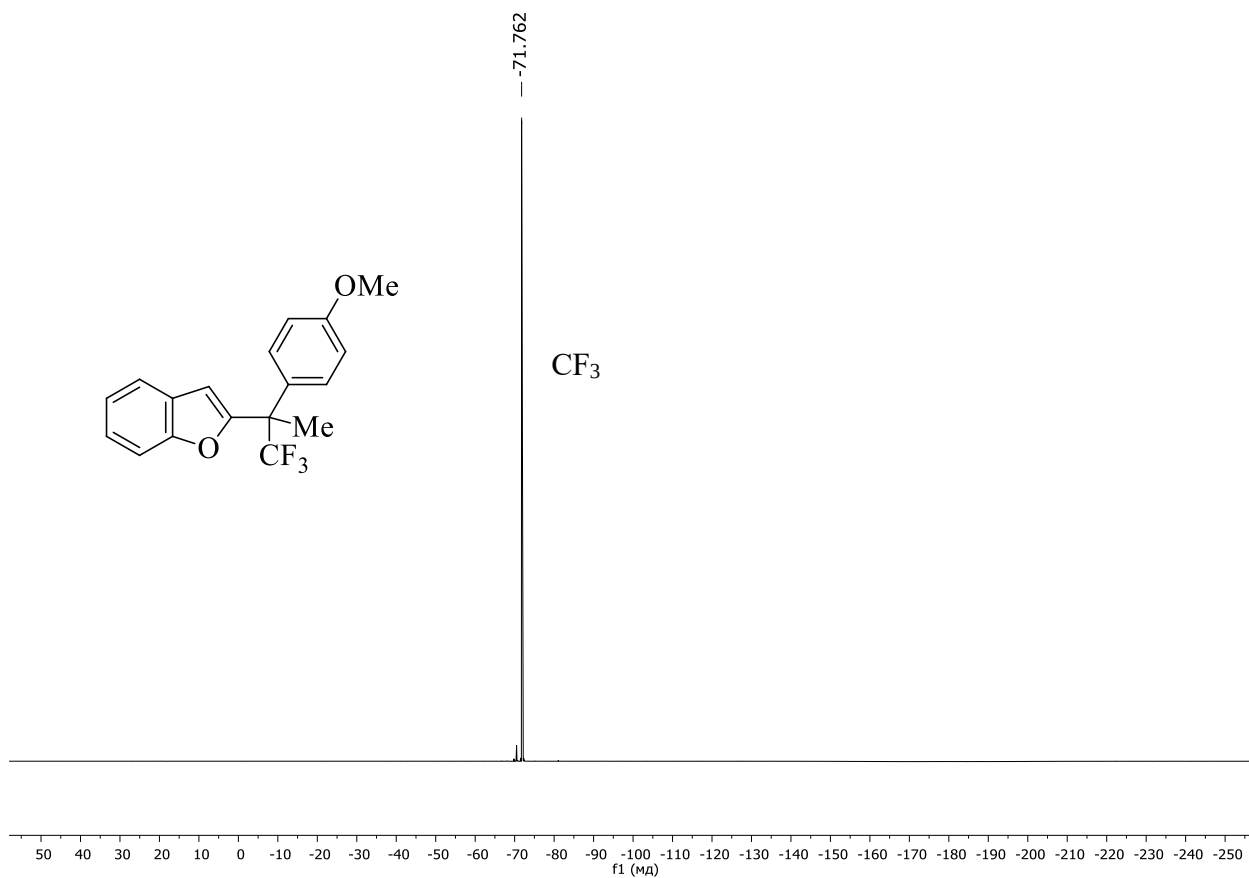


Fig. S59. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2bb** (CDCl_3 , 376 MHz).

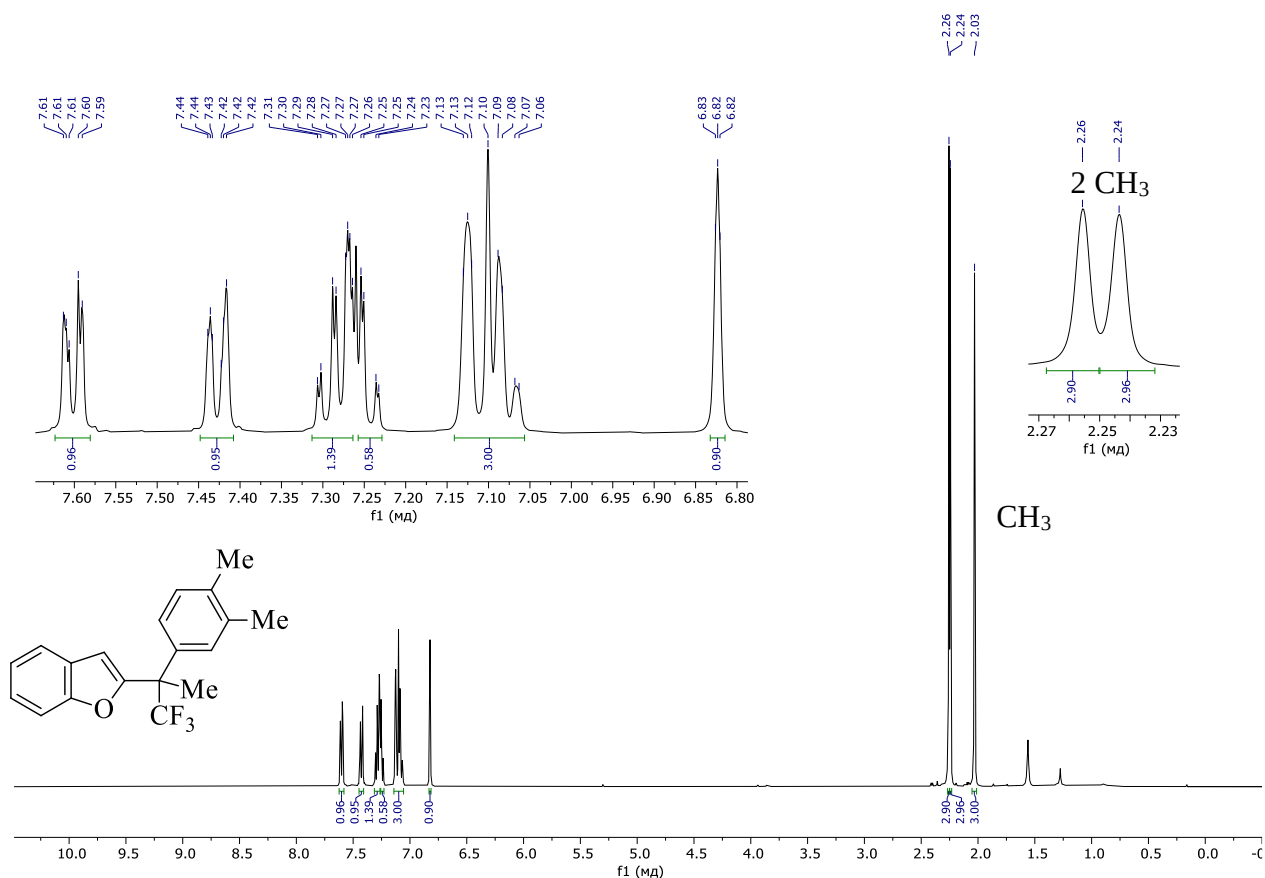


Fig. S60. ¹H NMR spectrum of the compound 2bc (CDCl₃, 400 MHz).

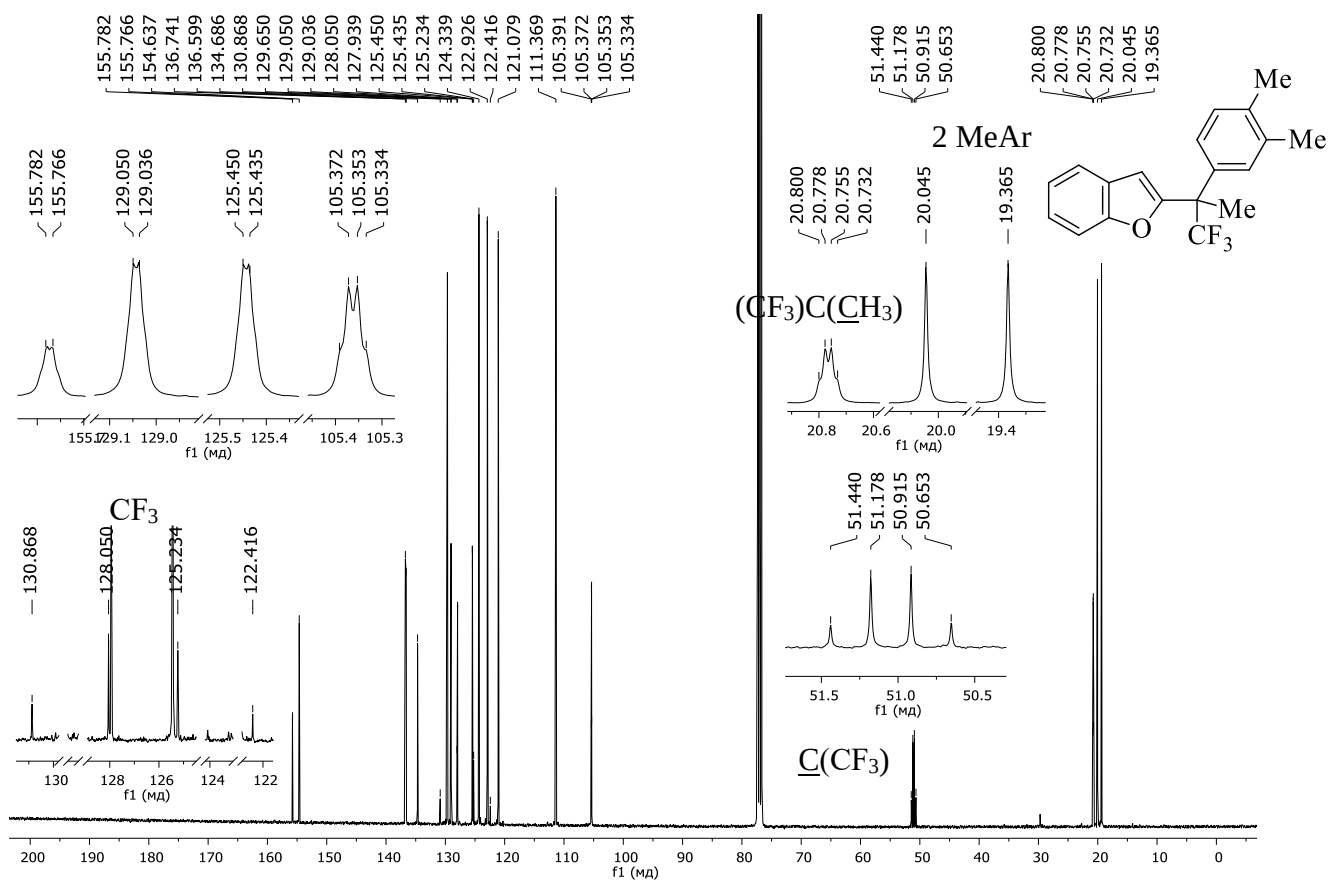


Fig. S61. ¹³C{¹H} NMR spectrum of the compound 2bc (CDCl₃, 101 MHz).

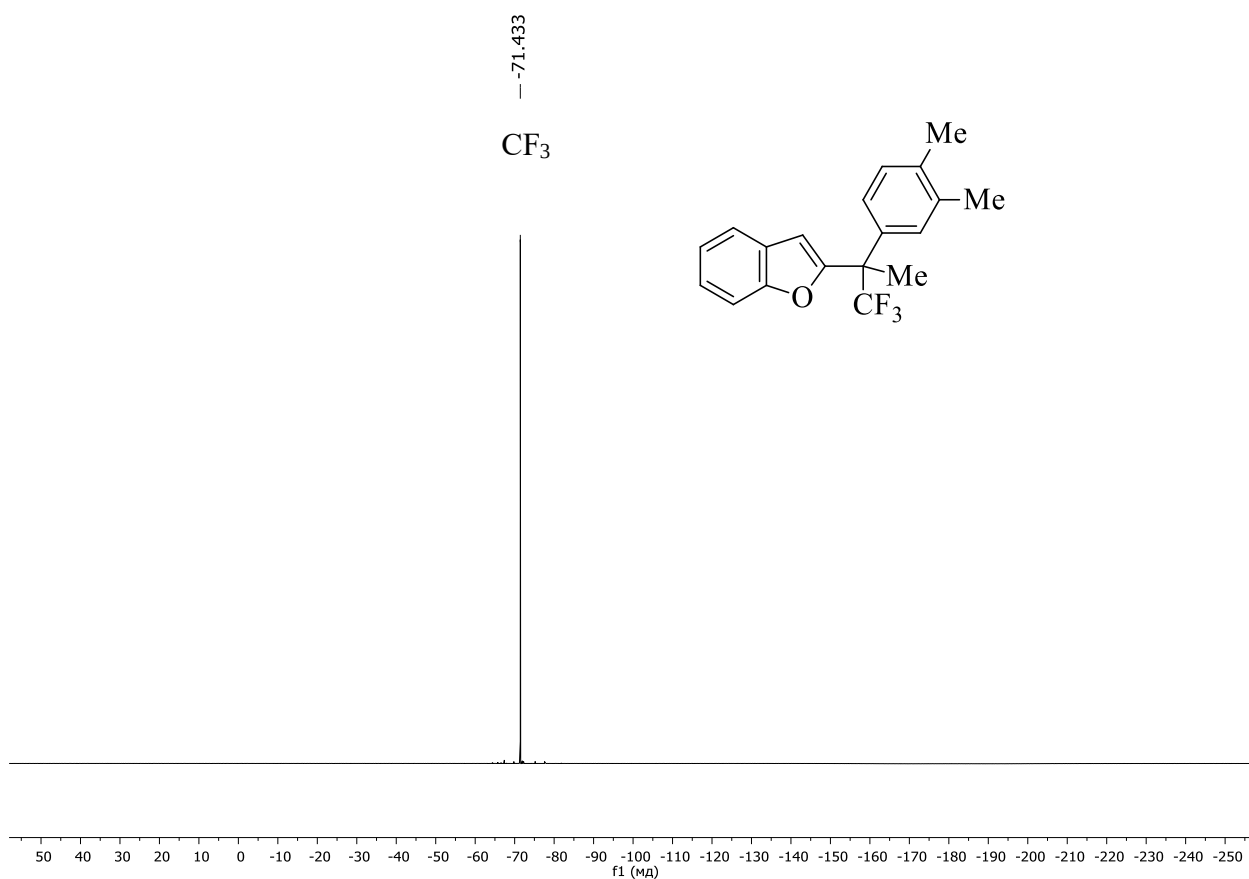


Fig. S62. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2bc** (CDCl₃, 376 MHz).

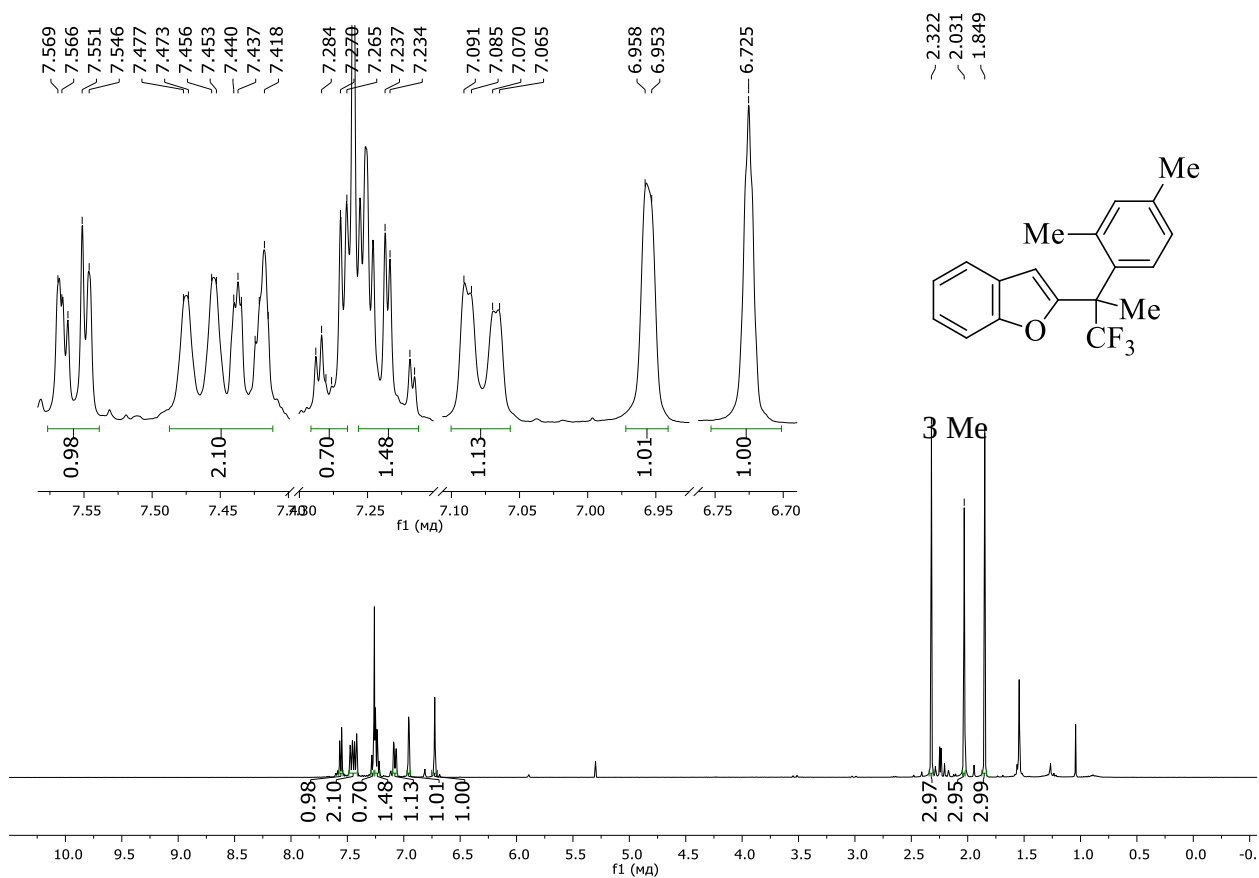


Fig. S63. ^1H NMR spectrum of the compound **2bd** (CDCl₃, 400 MHz).

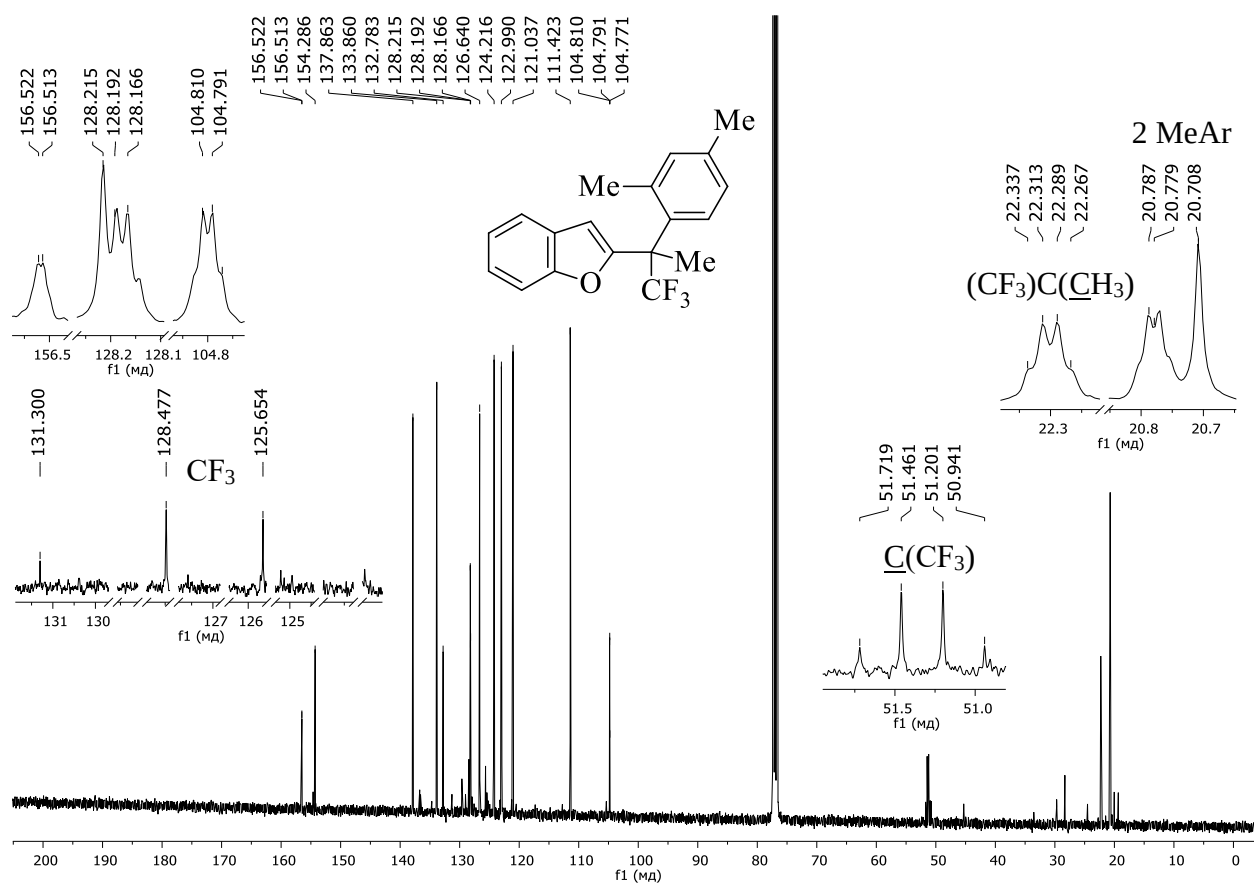


Fig. S64. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2bd** (CDCl_3 , 101 MHz).

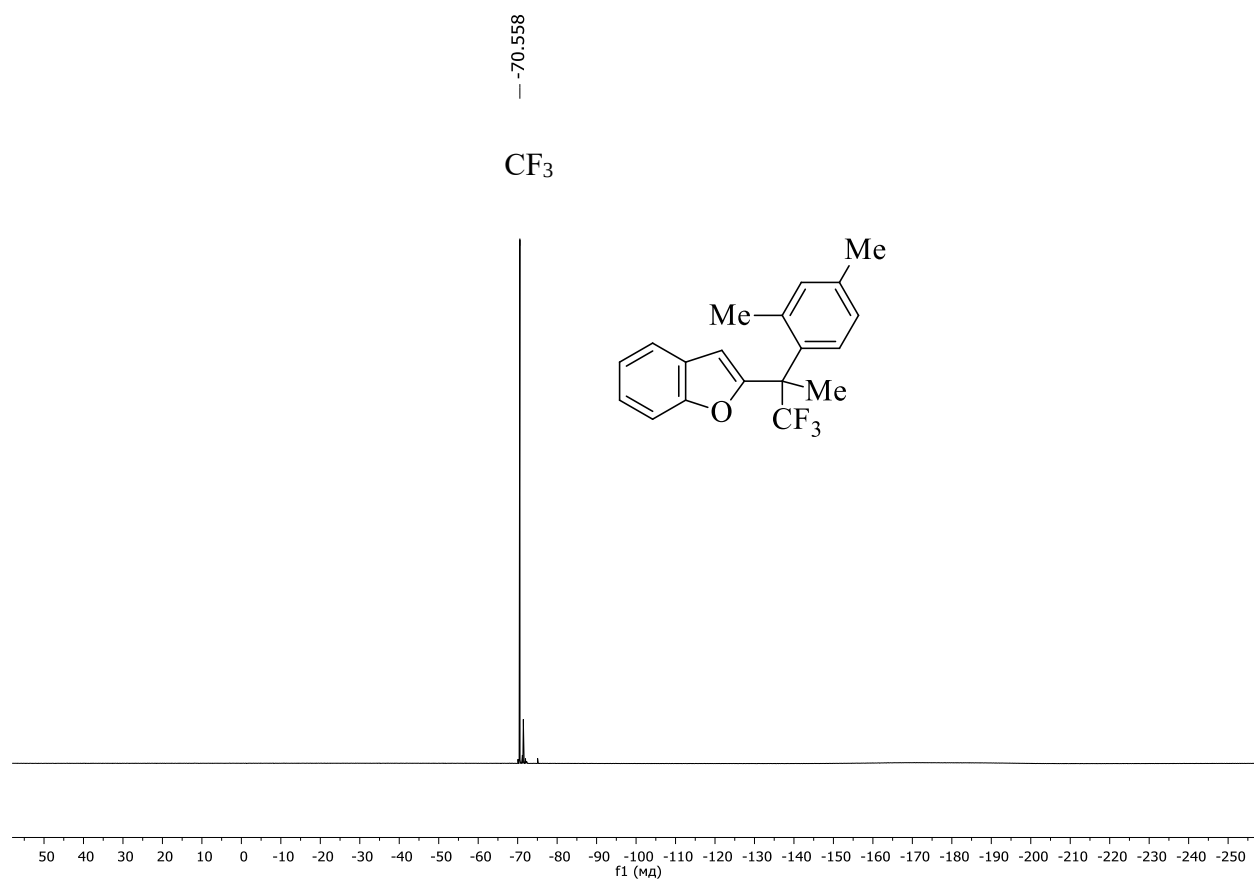


Fig. S65. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2bd** (CDCl_3 , 376 MHz).

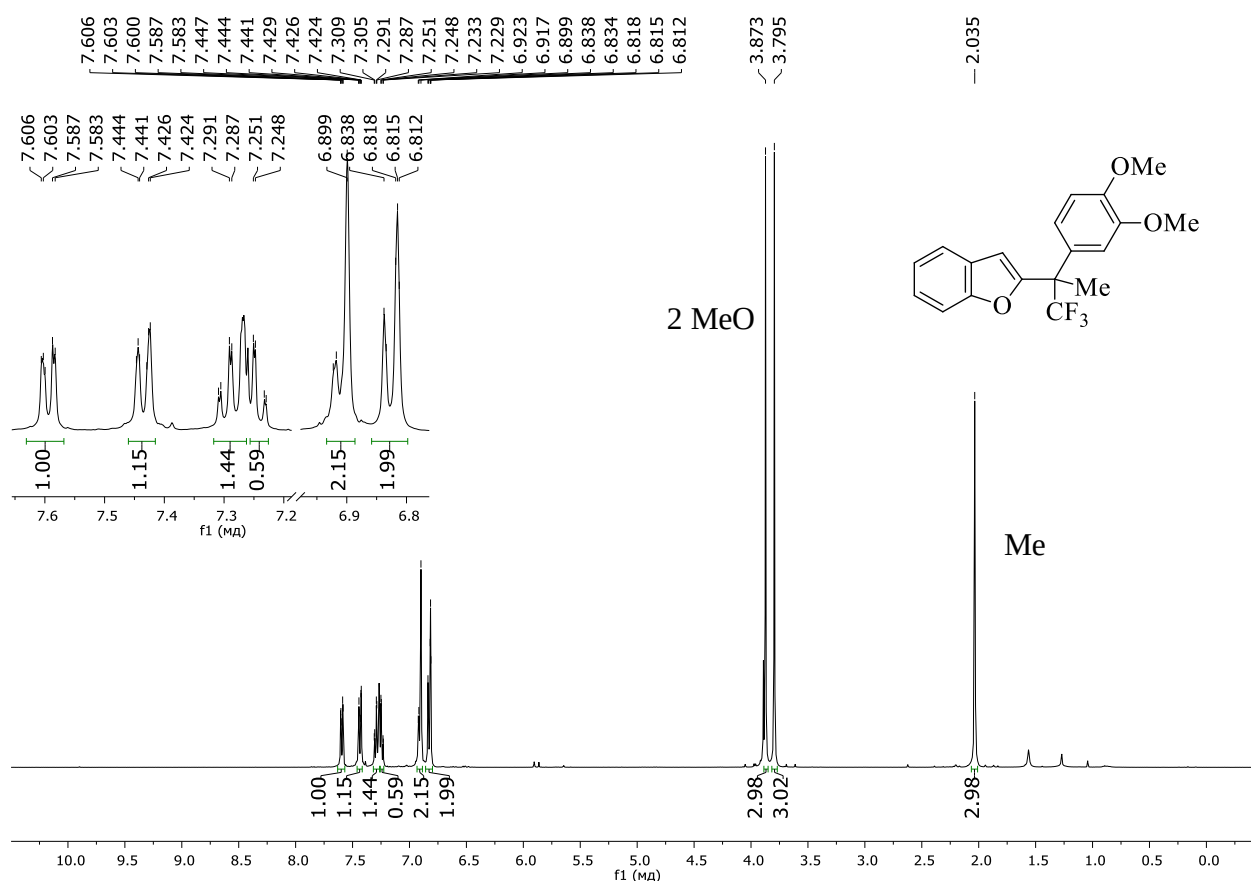


Fig. S66. ¹H NMR spectrum of the compound **2be** (CDCl₃, 400 MHz).

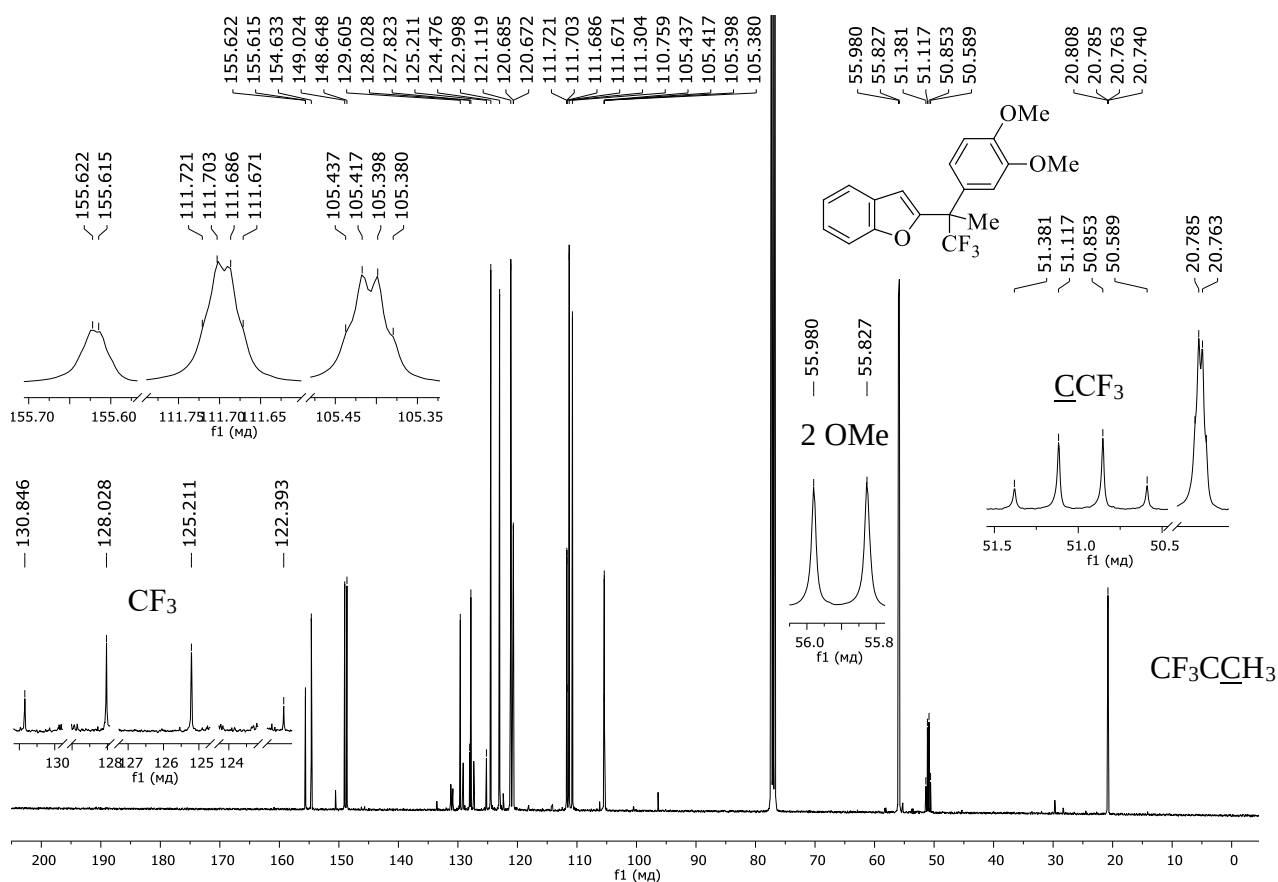


Fig. S67. ¹³C{¹H} NMR spectrum of the compound **2be** (CDCl₃, 101 MHz).

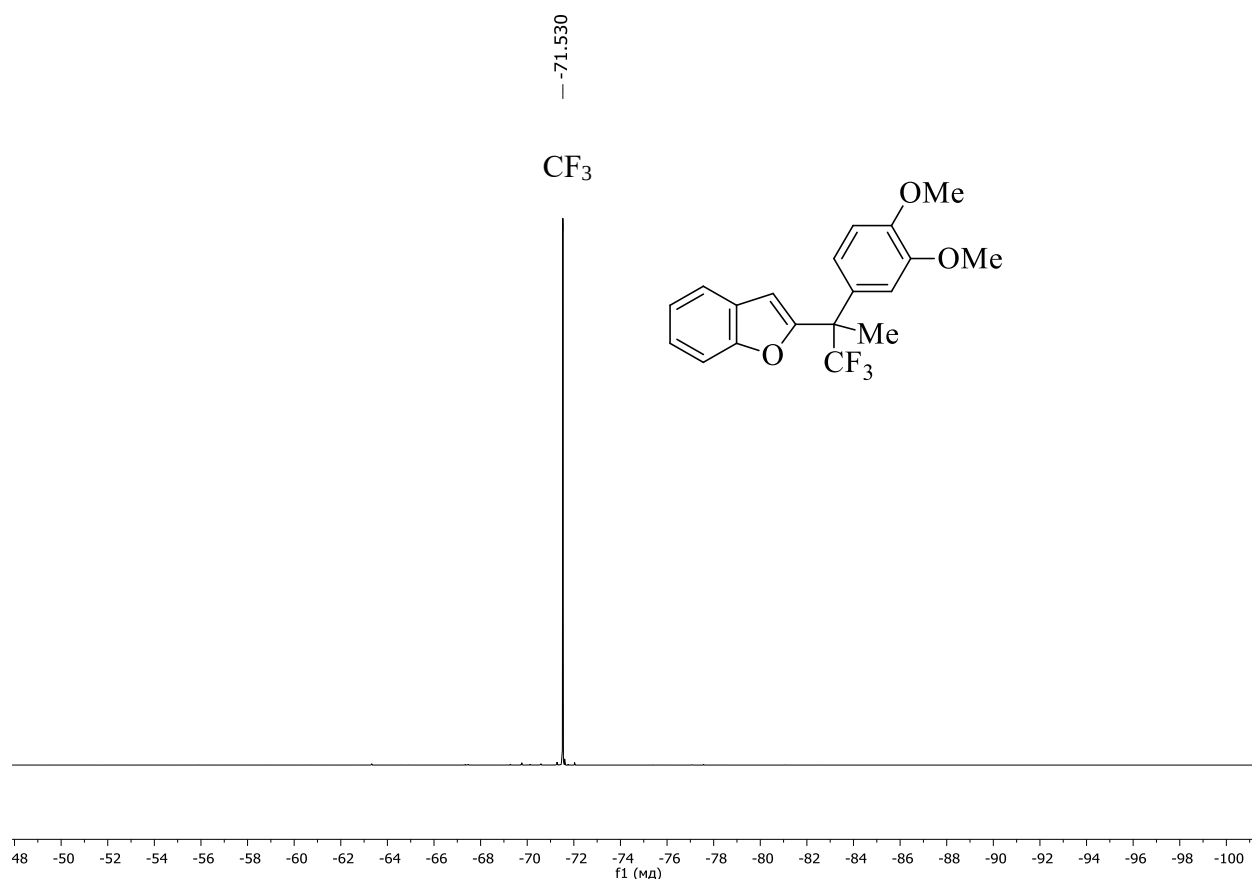


Fig. S68. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2be** (CDCl₃, 376 MHz).

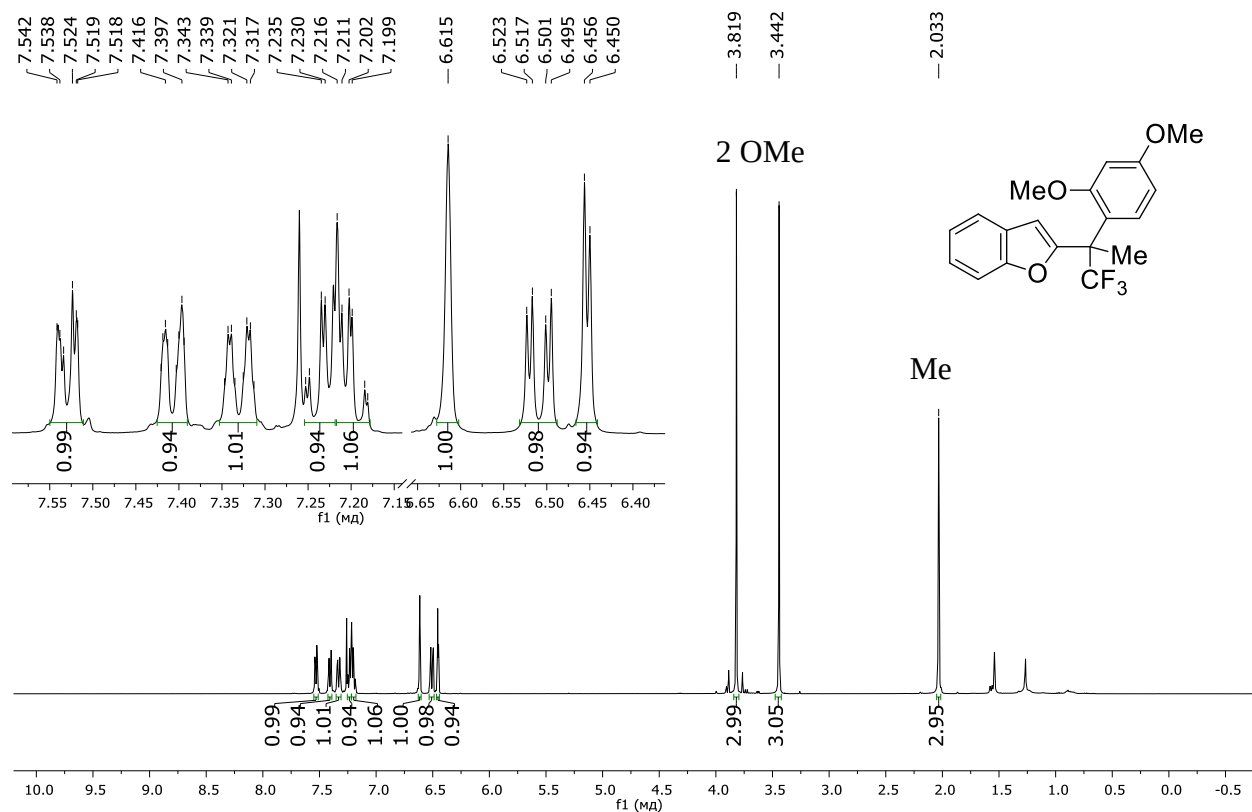


Fig. S69. ^1H NMR spectrum of the compound **2bf** (CDCl₃, 400 MHz).

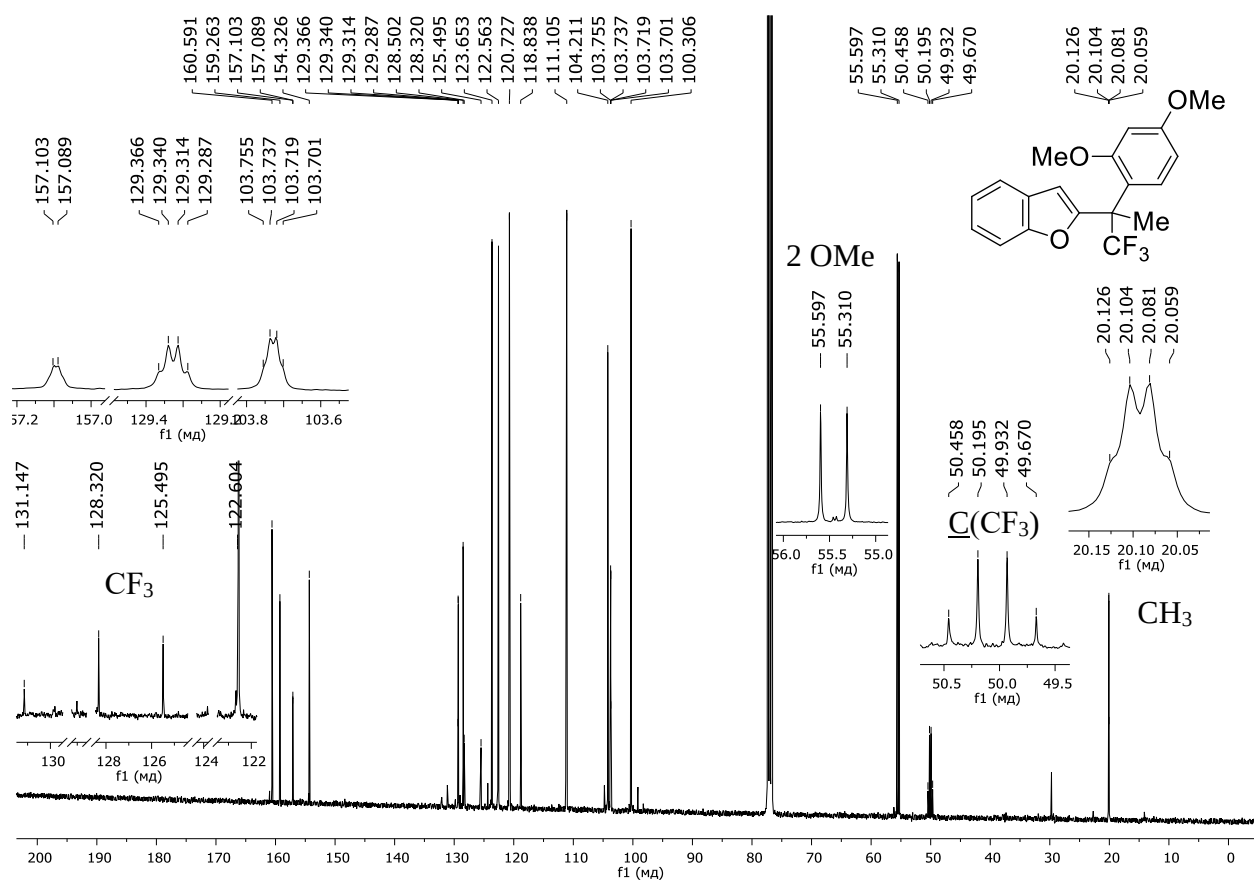


Fig. S70. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2bf** (CDCl_3 , 101 MHz).

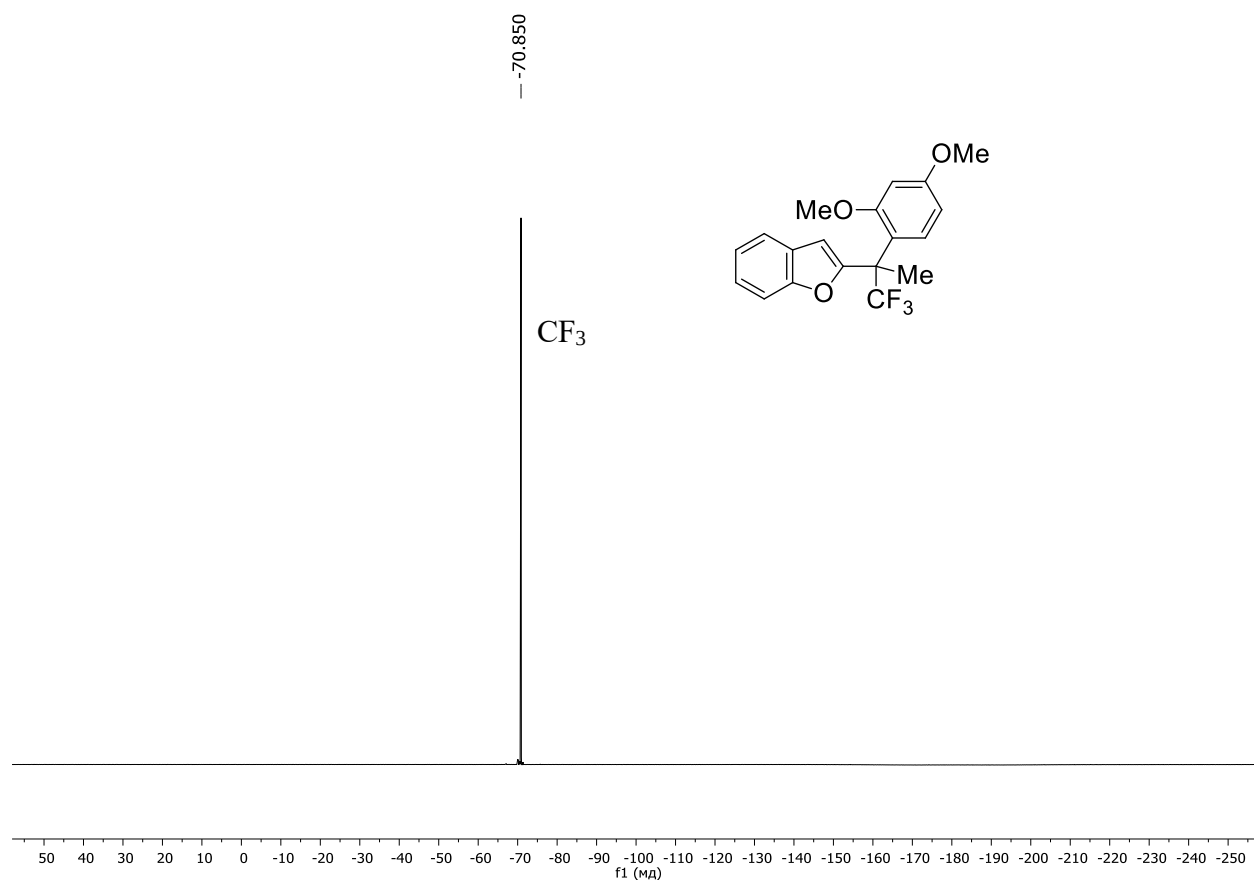


Fig. S71. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2bf** (CDCl_3 , 376 MHz).

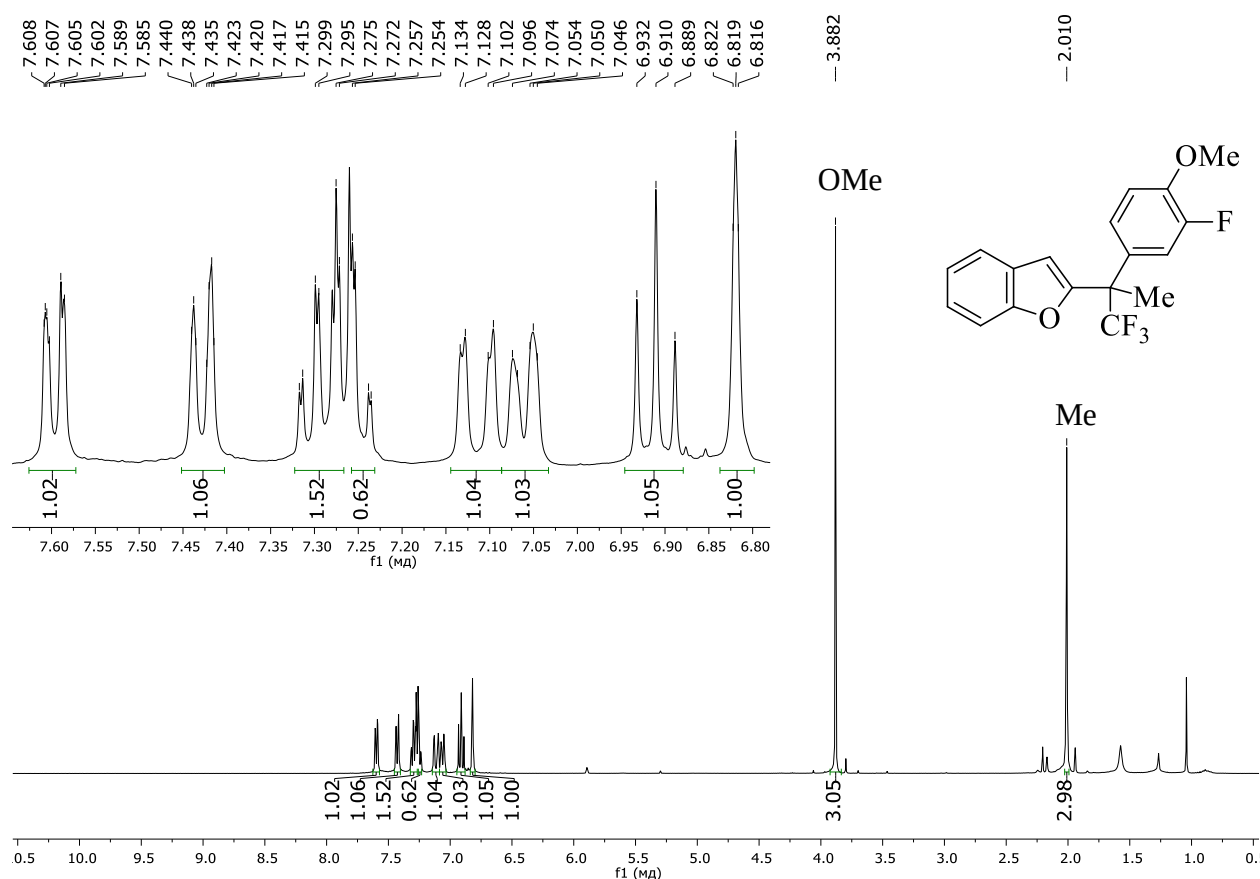


Fig. S72. ¹H NMR spectrum of the compound **2bg** (CDCl₃, 400 MHz).

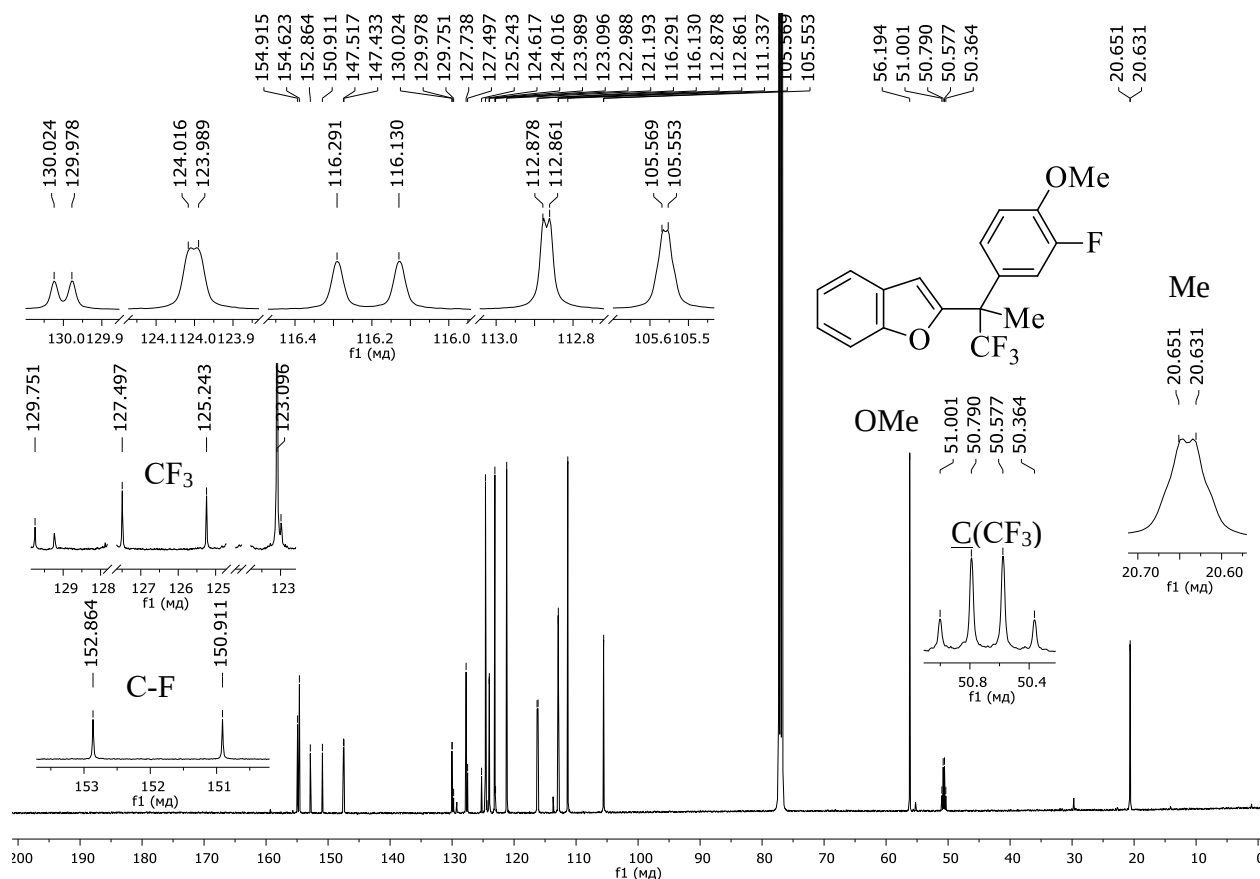


Fig. S73. ¹³C{¹H} NMR spectrum of the compound **2bg** (CDCl₃, 101 MHz).

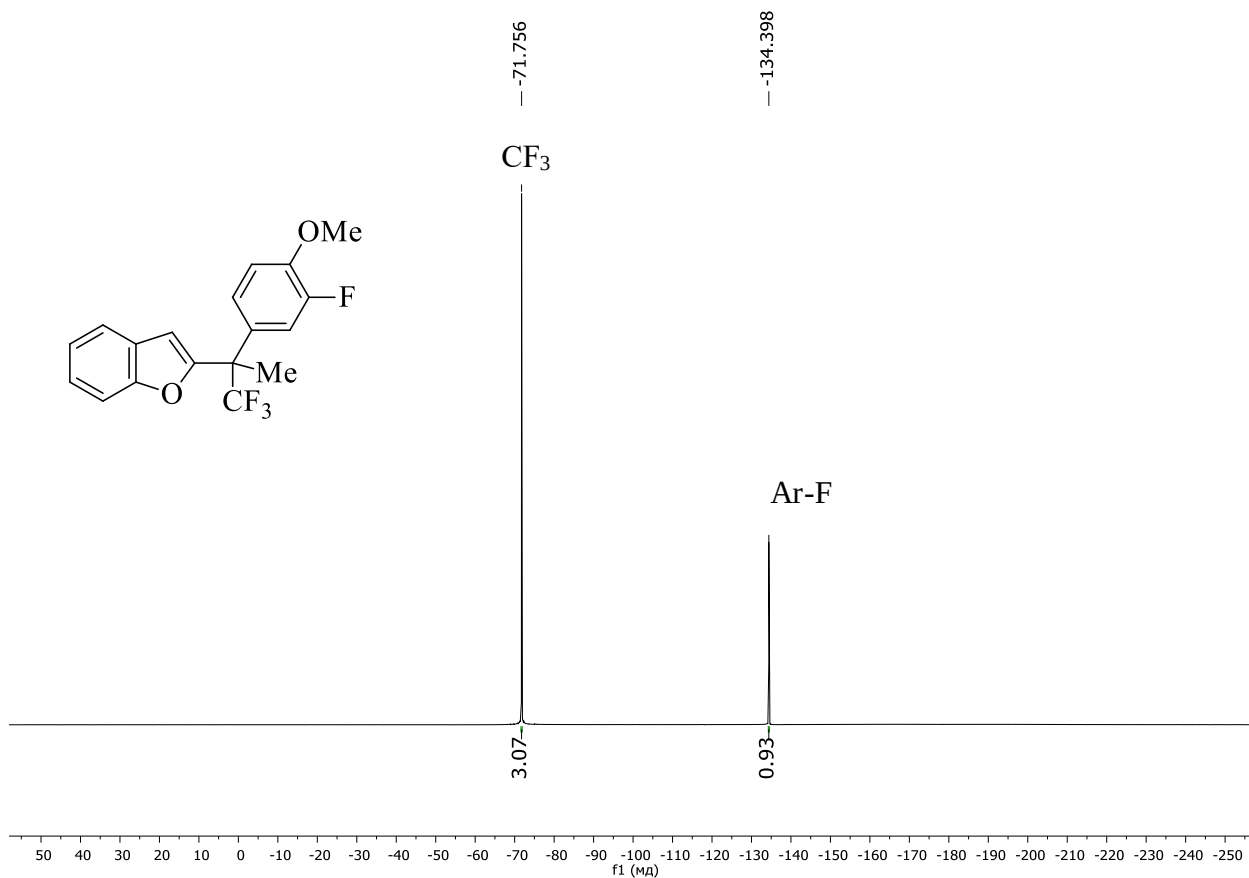


Fig. S74. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2bg** (CDCl₃, 376 MHz).

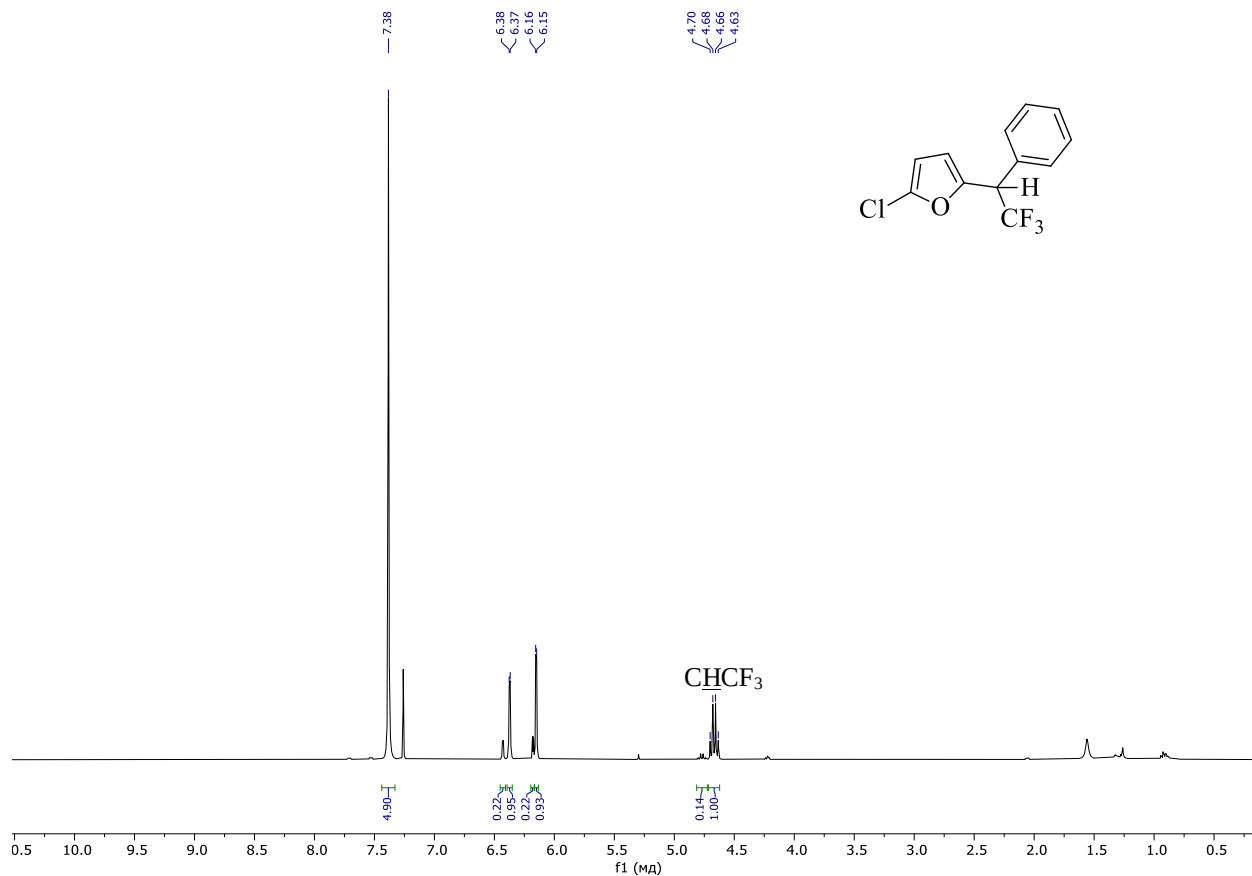


Fig. S75. ^1H NMR spectrum of the compound **2ca** (CDCl₃, 400 MHz).

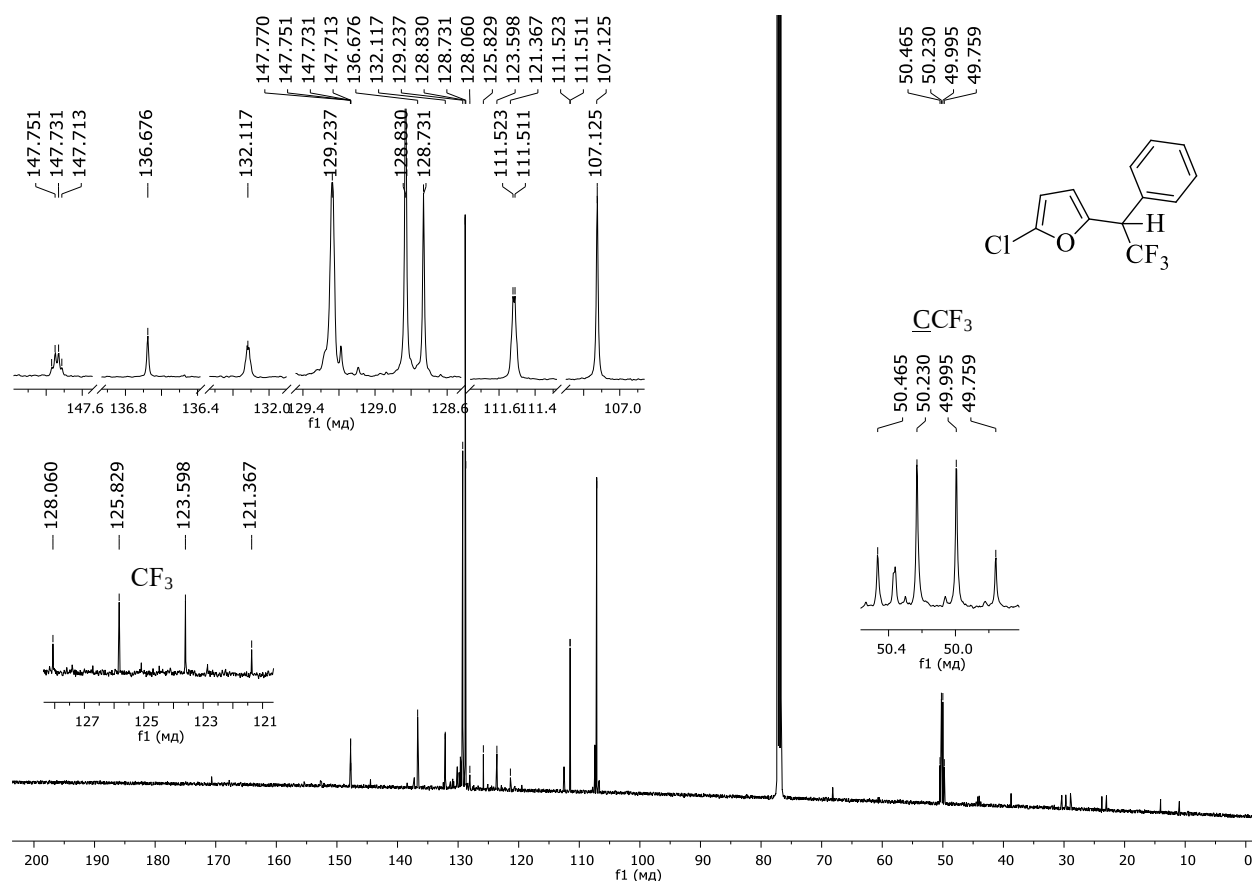


Fig. S76. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2ca** (CDCl_3 , 101 MHz).

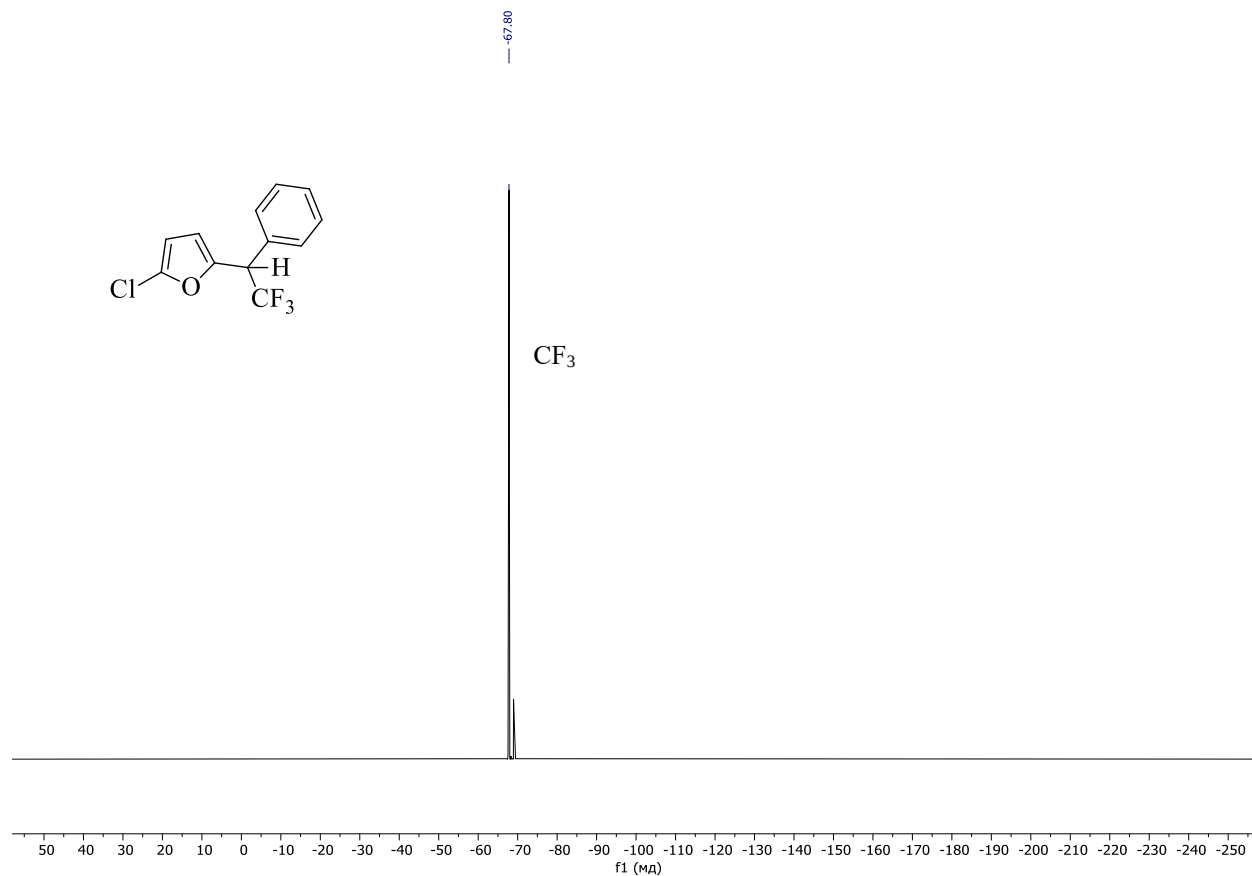


Fig. S77. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ca** (CDCl_3 , 376 MHz).

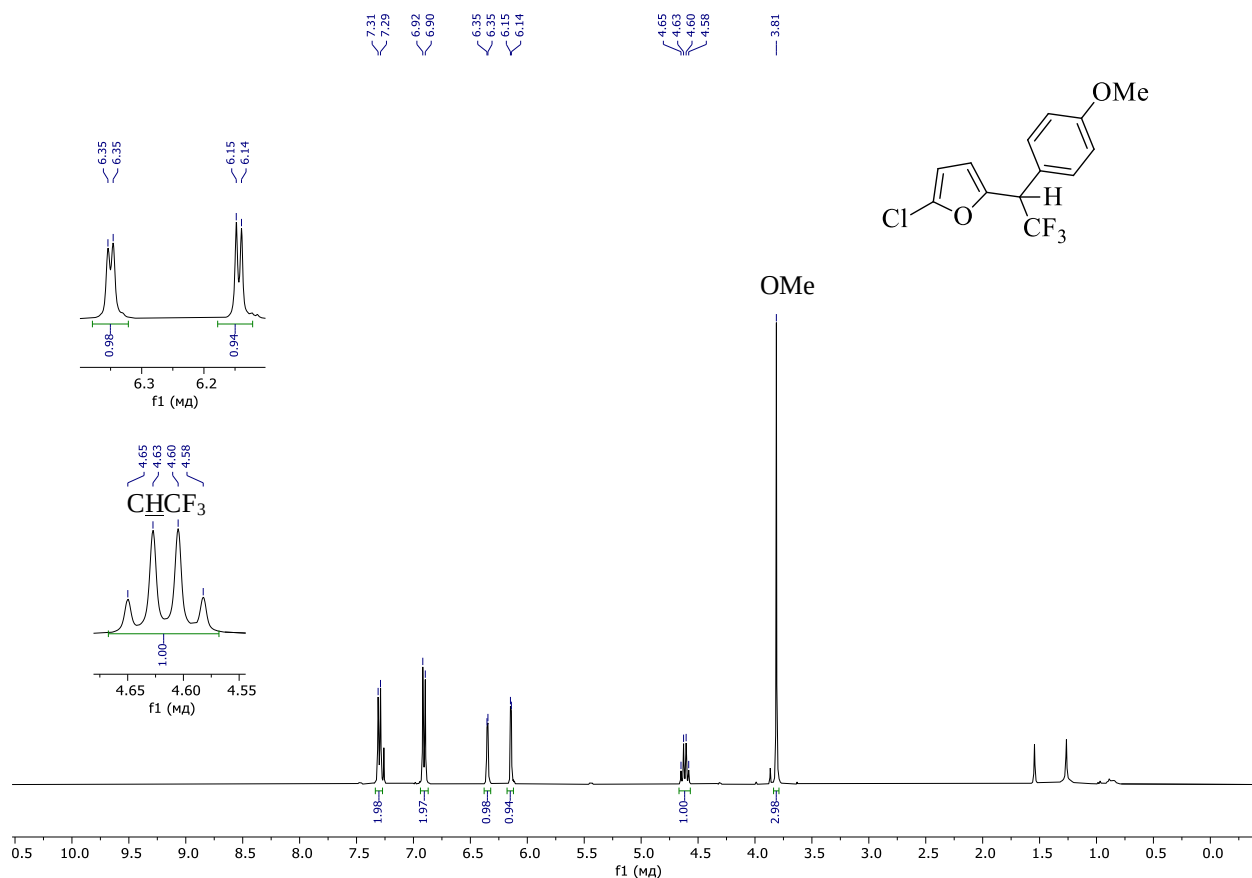


Fig. S78. ¹H NMR spectrum of the compound **2cb** (CDCl₃, 400 MHz).

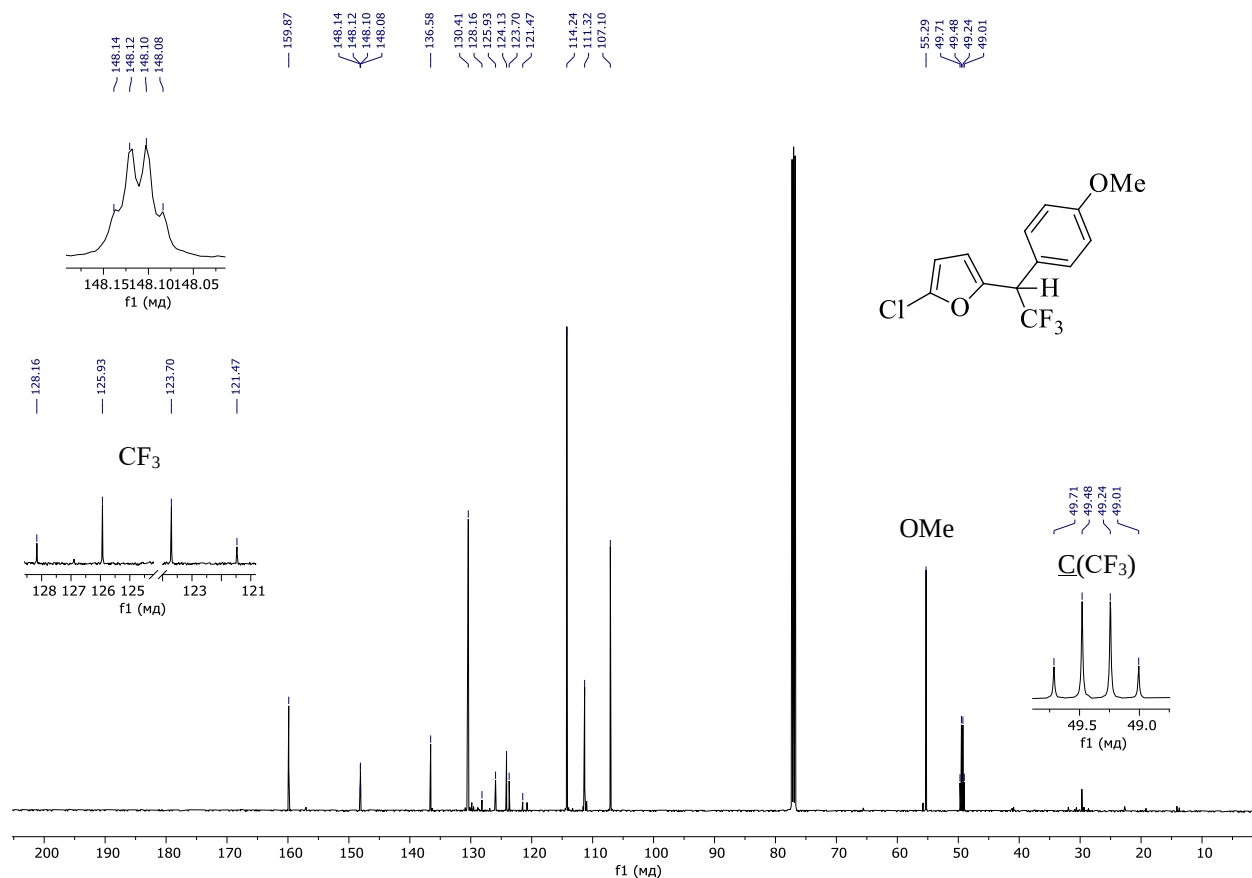


Fig. S79. ¹³C{¹H} NMR spectrum of the compound **2cb** (CDCl₃, 101 MHz).

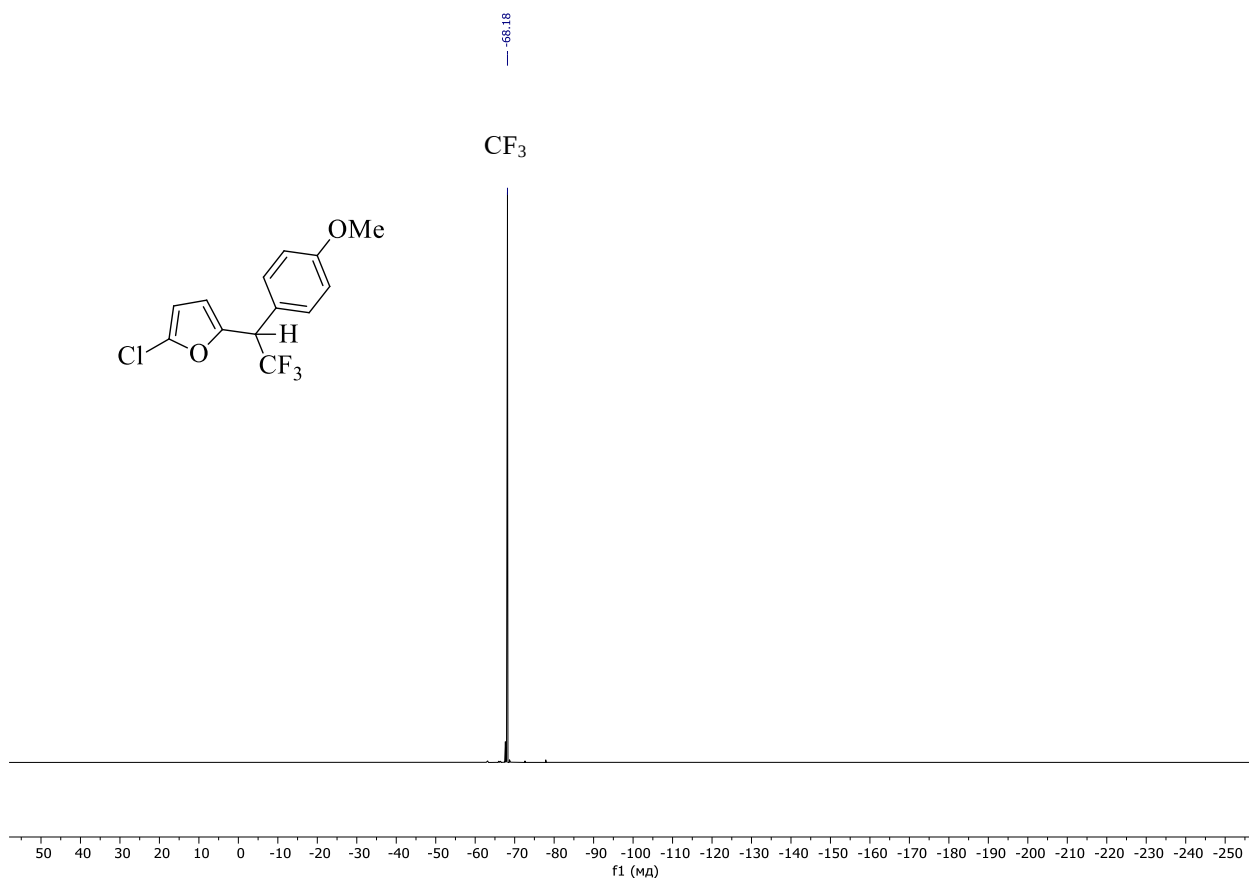


Fig. S80. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2cb** (CDCl_3 , 376 MHz).

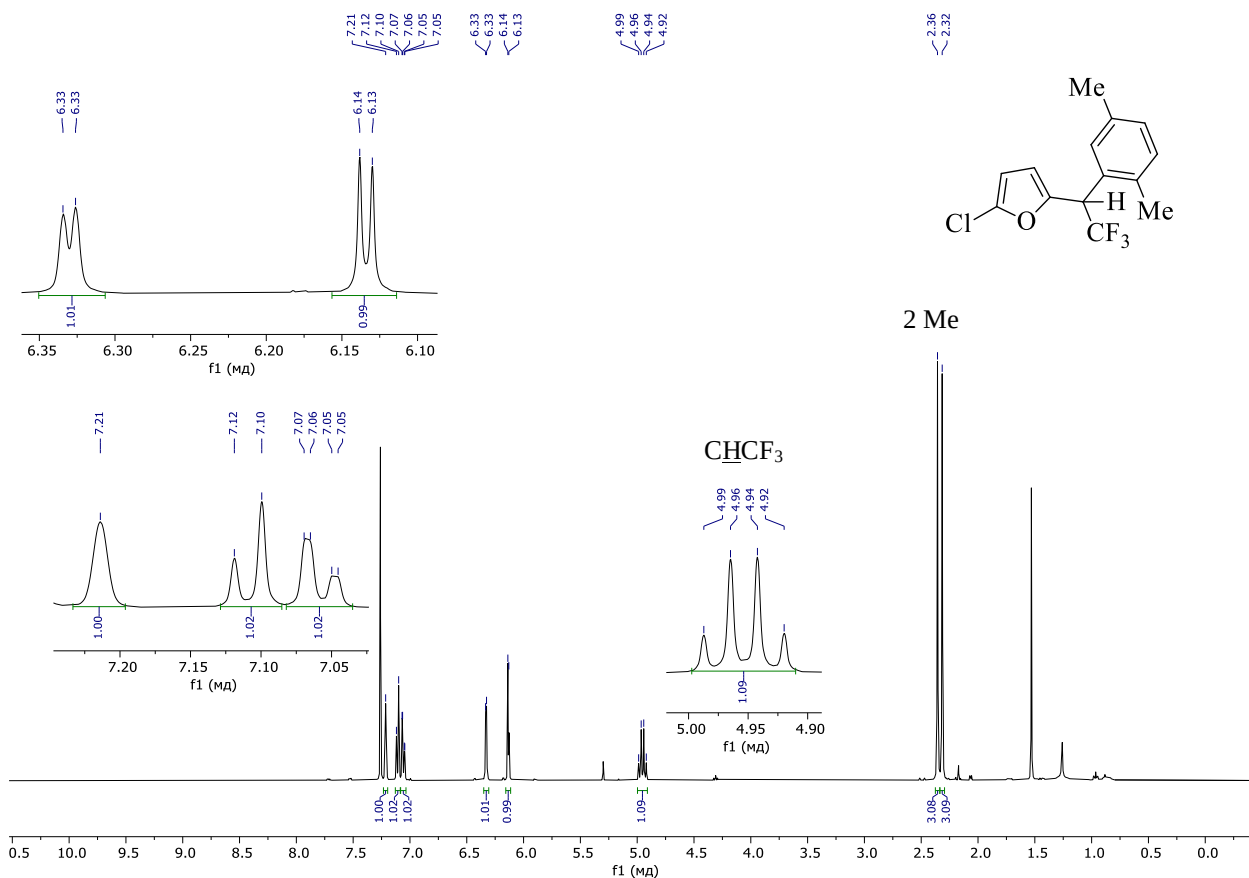
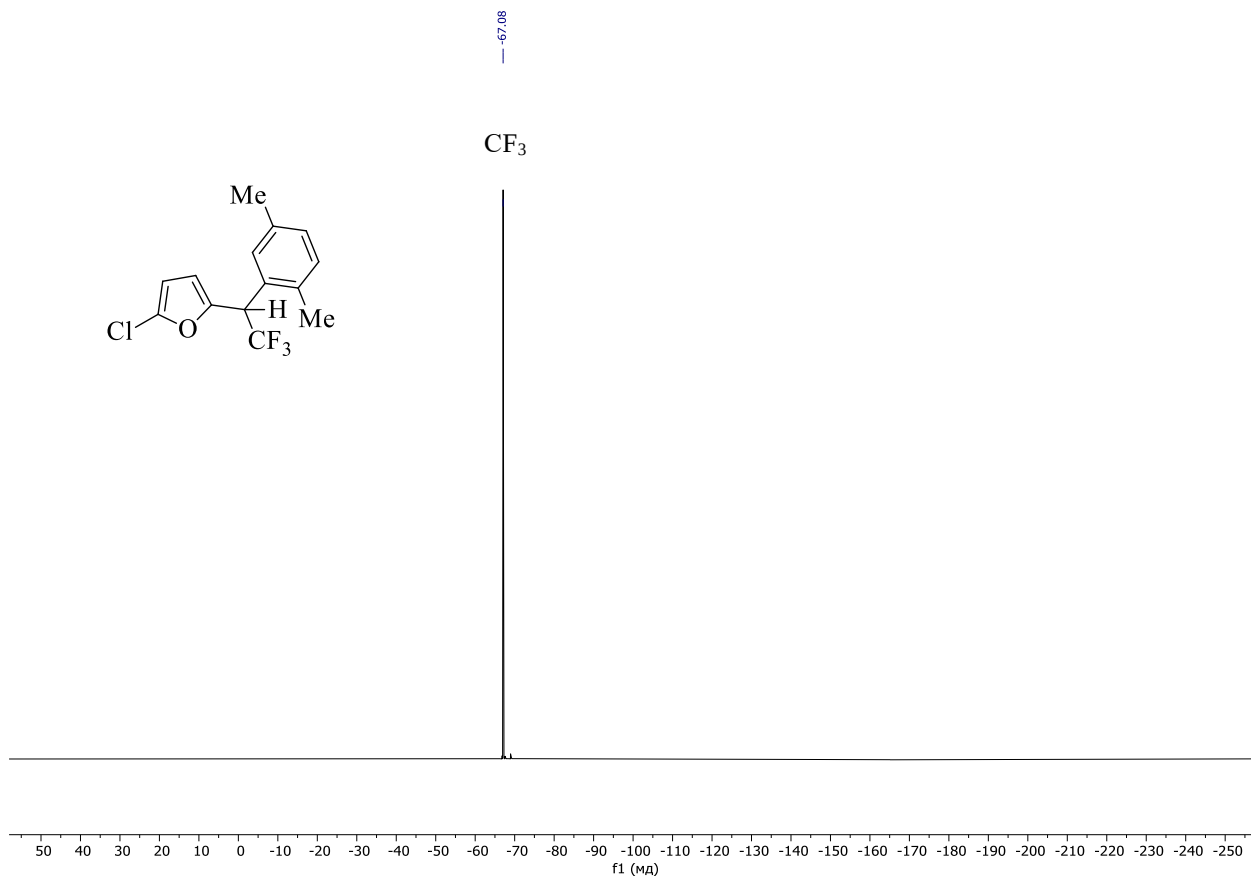
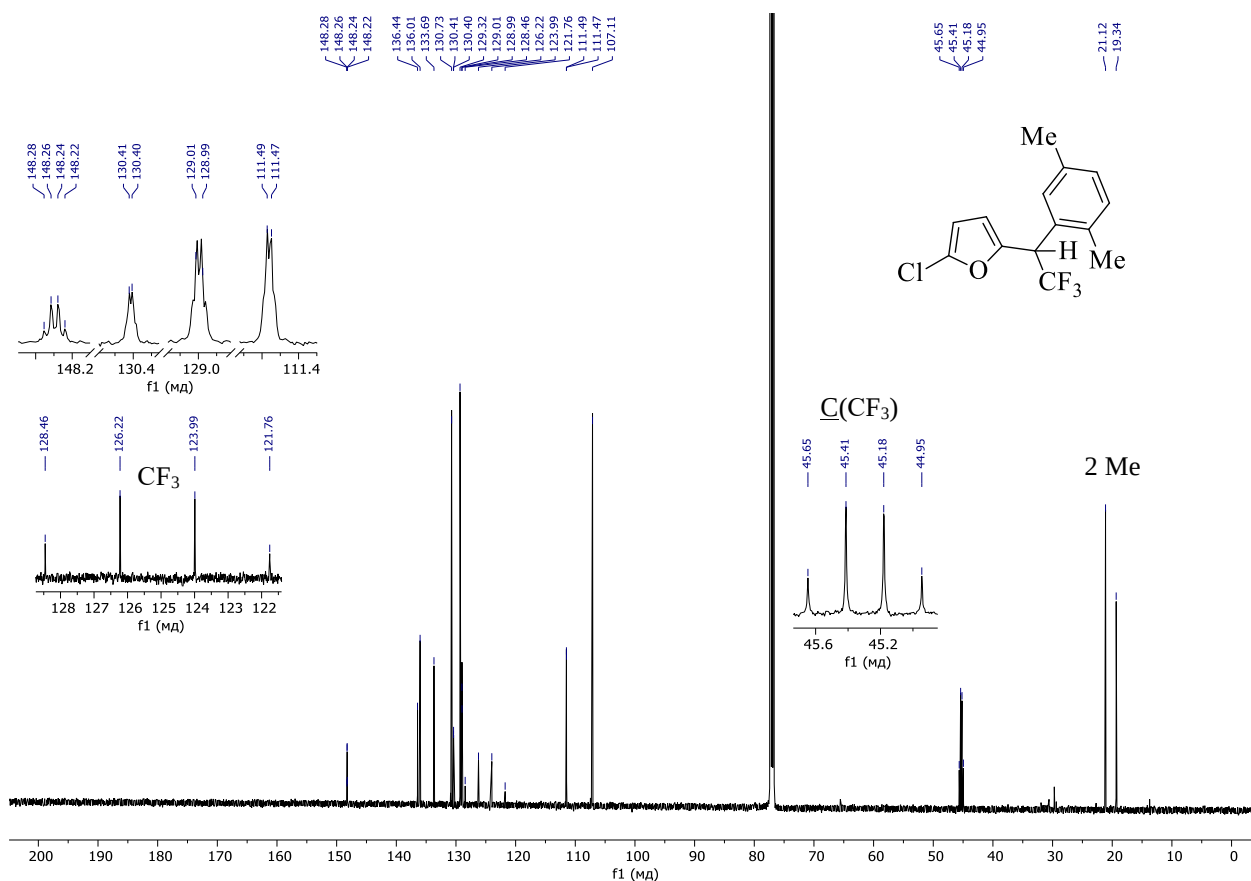


Fig. S81. ^1H NMR spectrum of the compound **2cc** (CDCl_3 , 400 MHz).



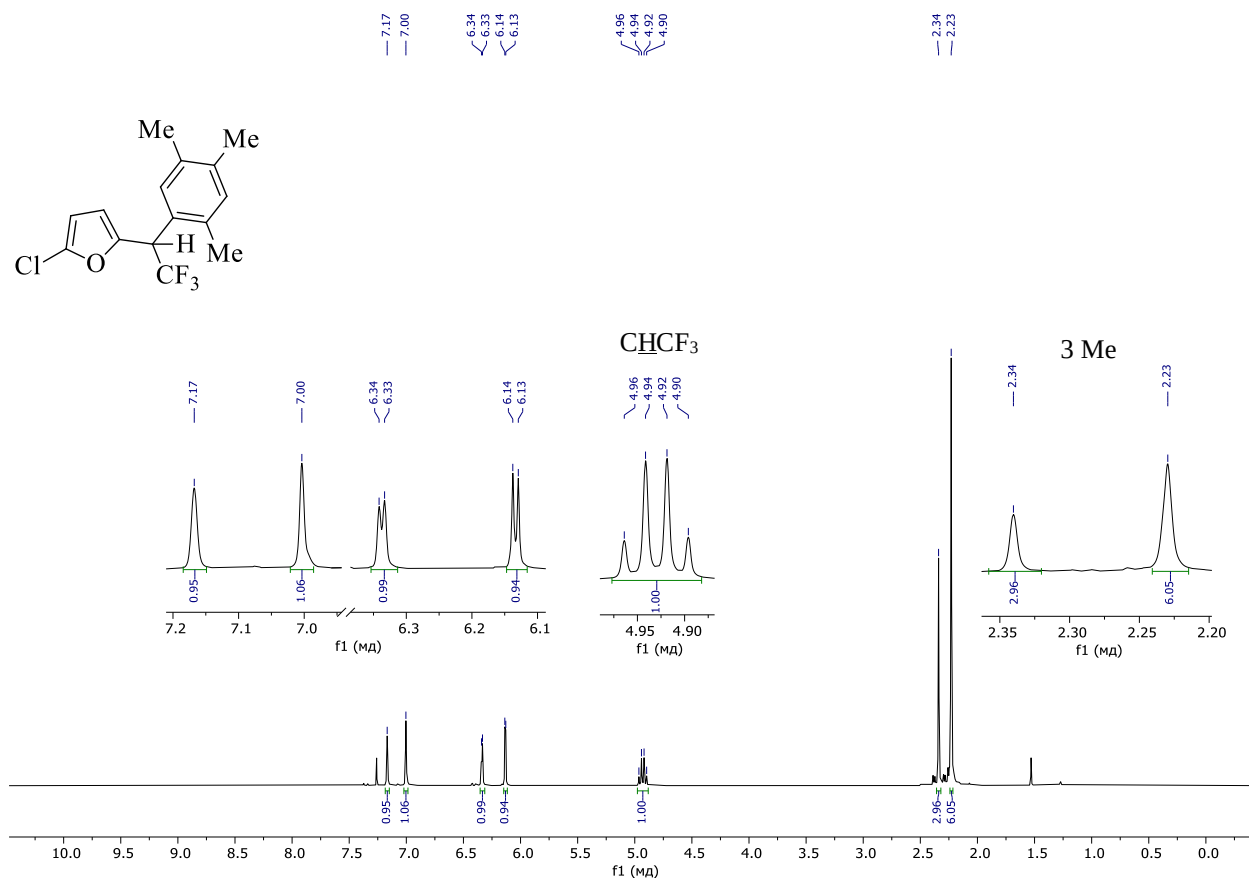


Fig. S84. ^1H NMR spectrum of the compound **2cd** (CDCl_3 , 400 MHz).

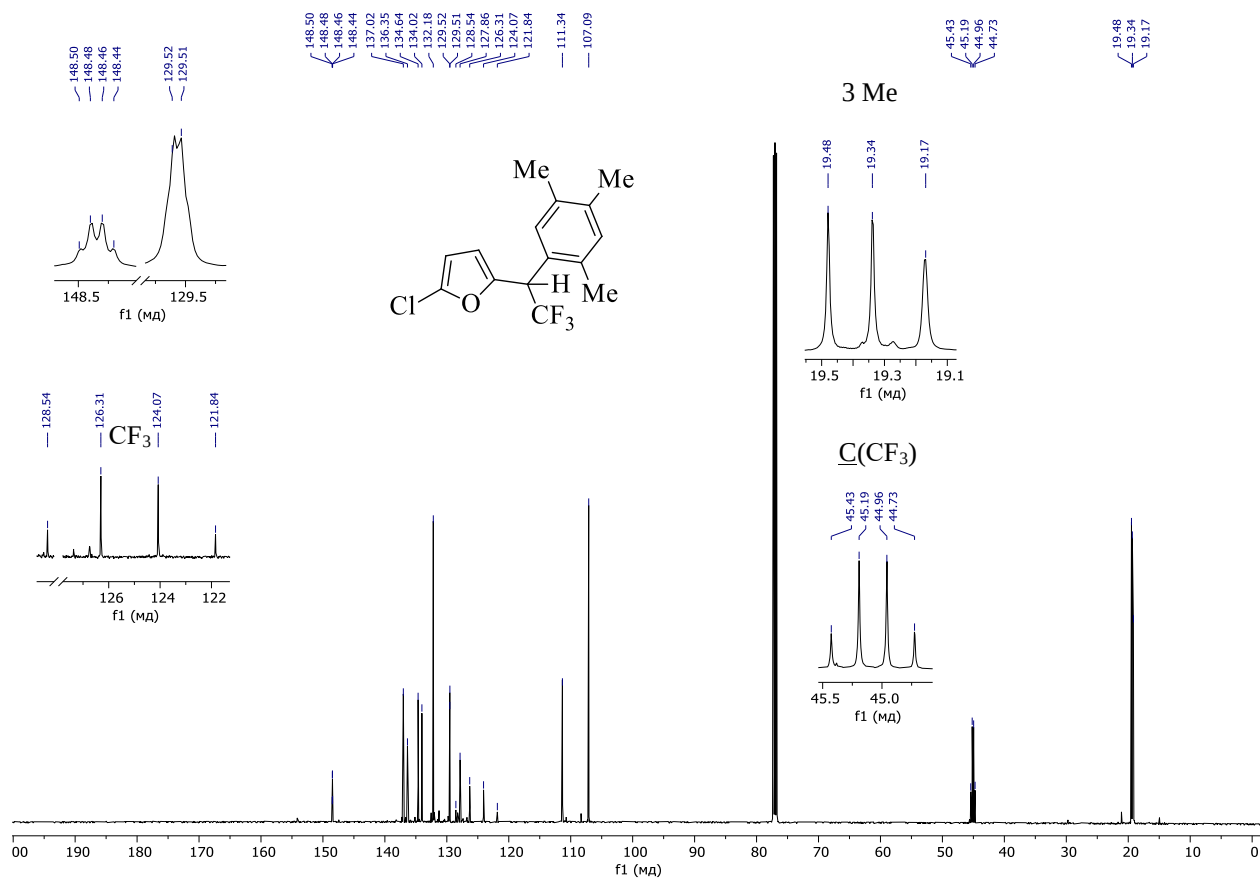


Fig. S85. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2cd** (CDCl_3 , 101 MHz).

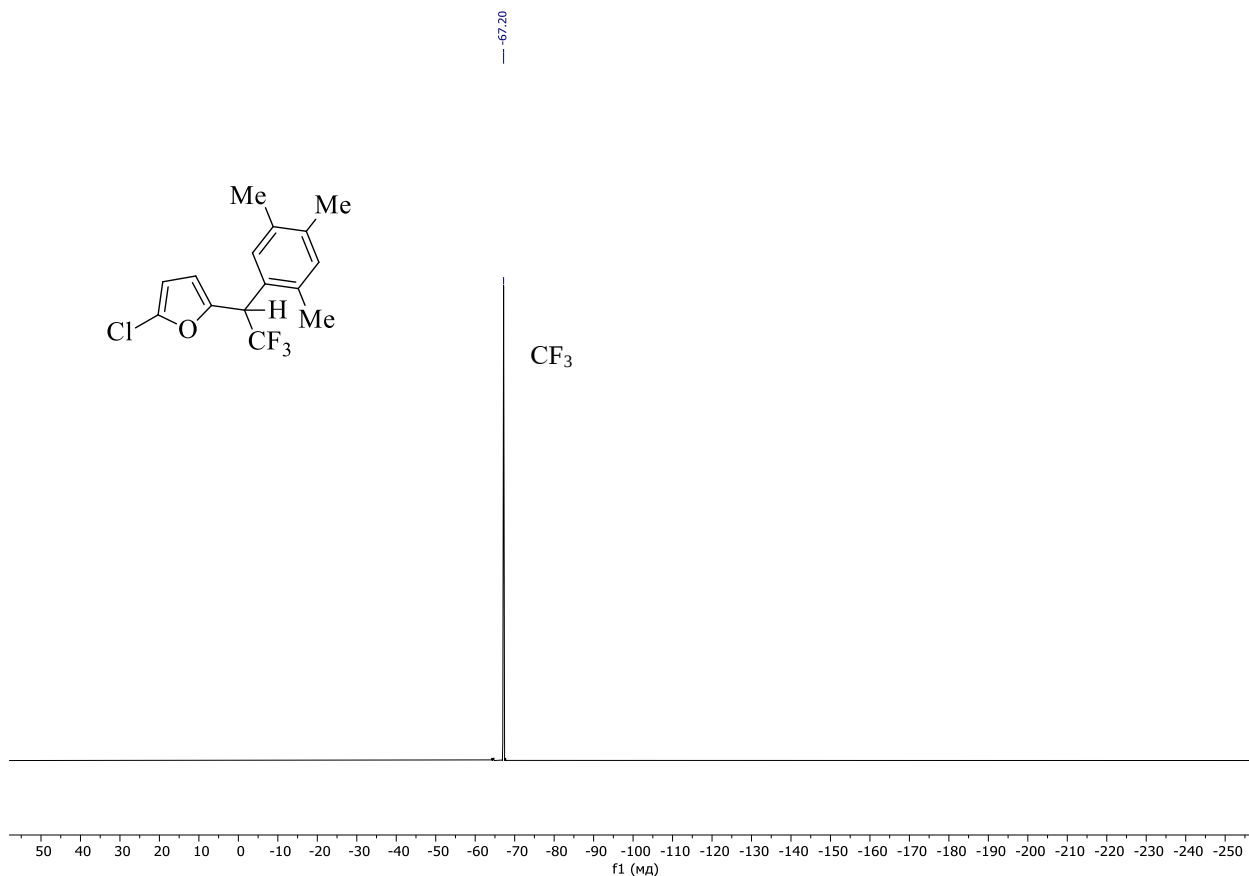


Fig. S86. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2cd** (CDCl_3 , 376 MHz).

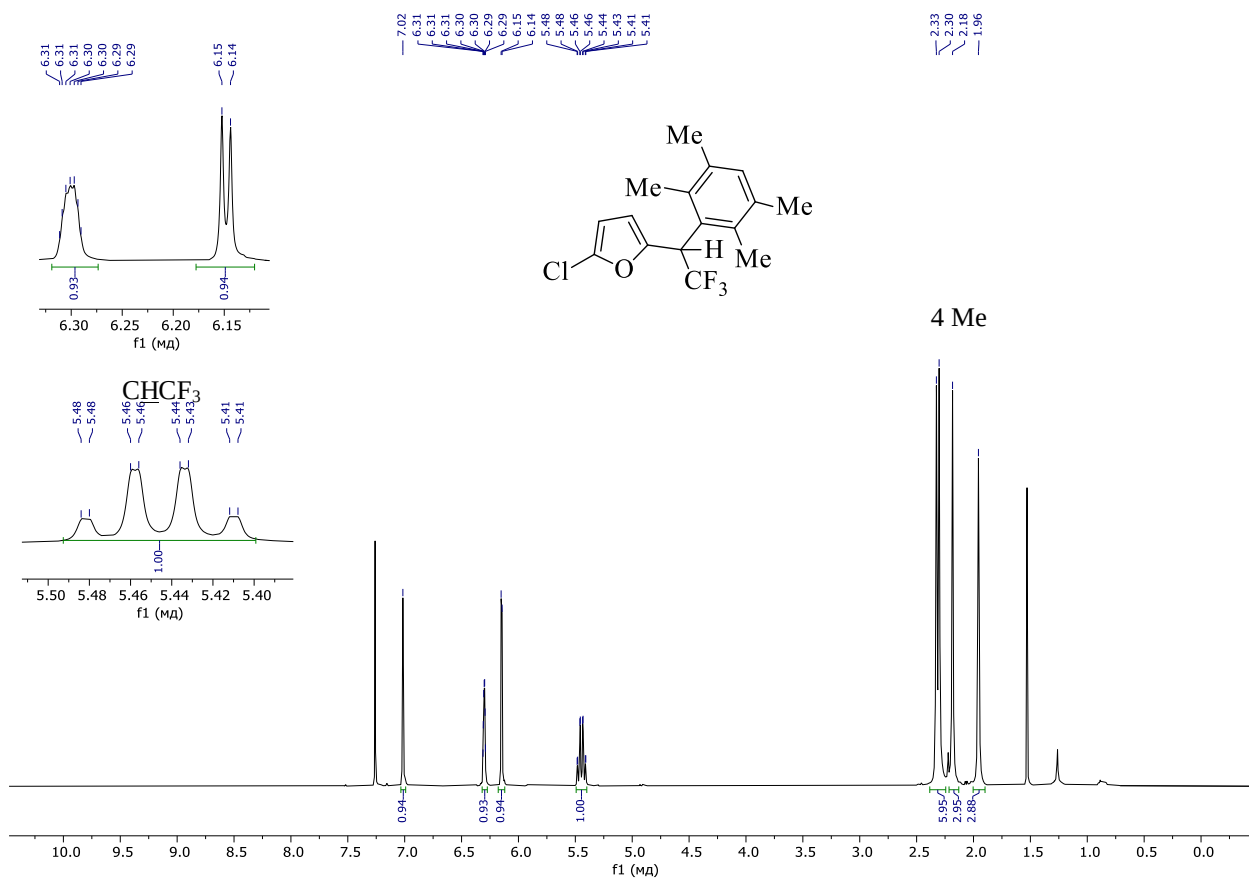


Fig. S87. ^1H NMR spectrum of the compound **2ce** (CDCl_3 , 400 MHz).

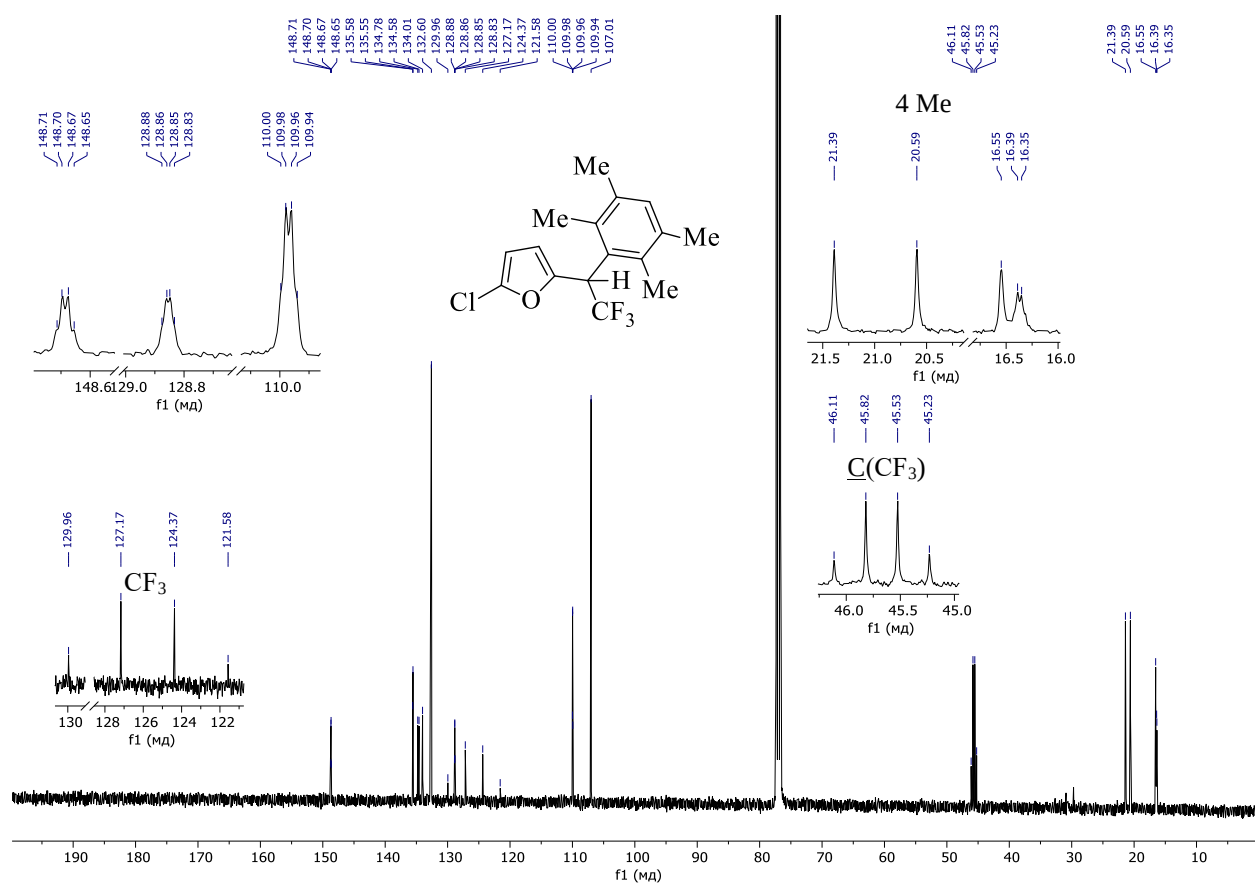


Fig. S88. ¹³C{¹H} NMR spectrum of the compound **2ce** (CDCl₃, 101 MHz).

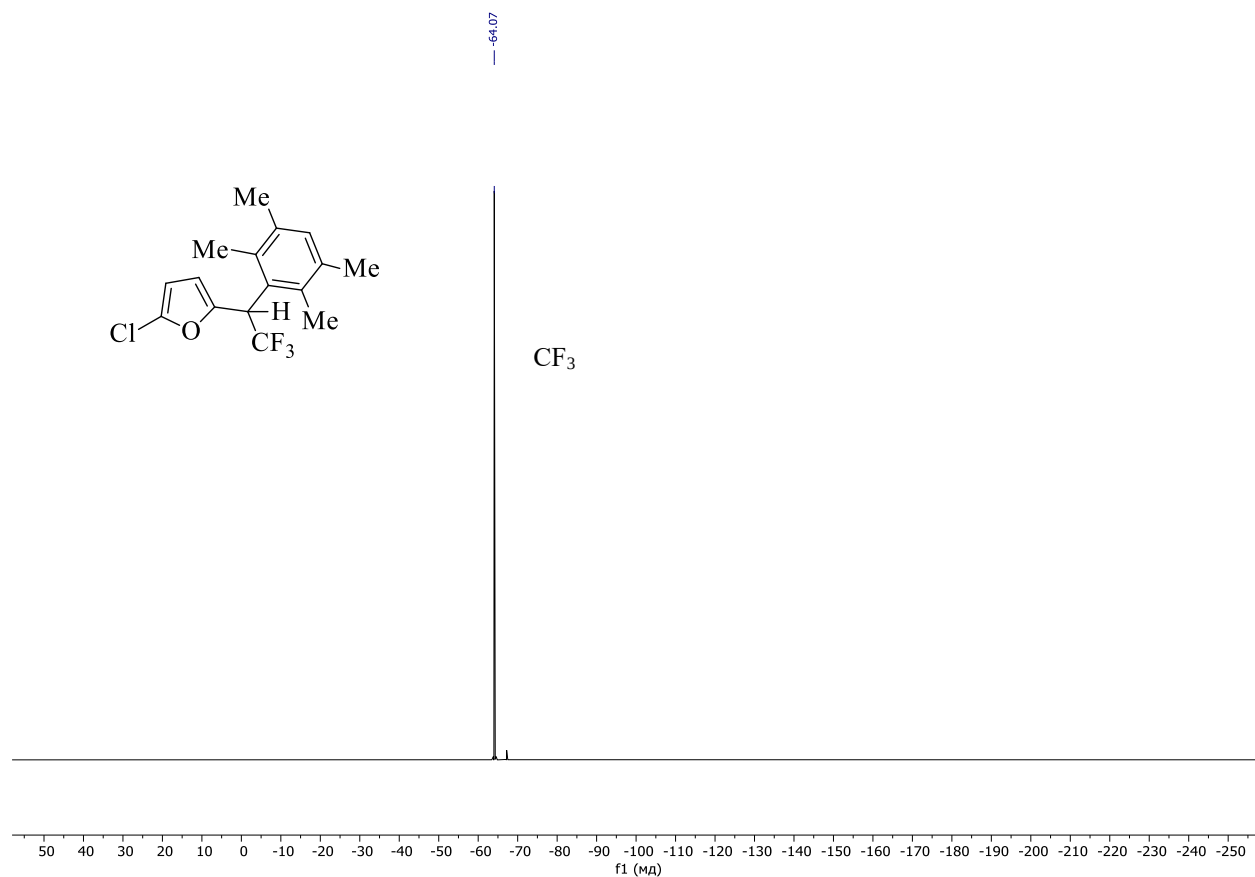


Fig. S89. ¹⁹F{¹H} NMR spectrum of the compound **2ce** (CDCl₃, 376 MHz).

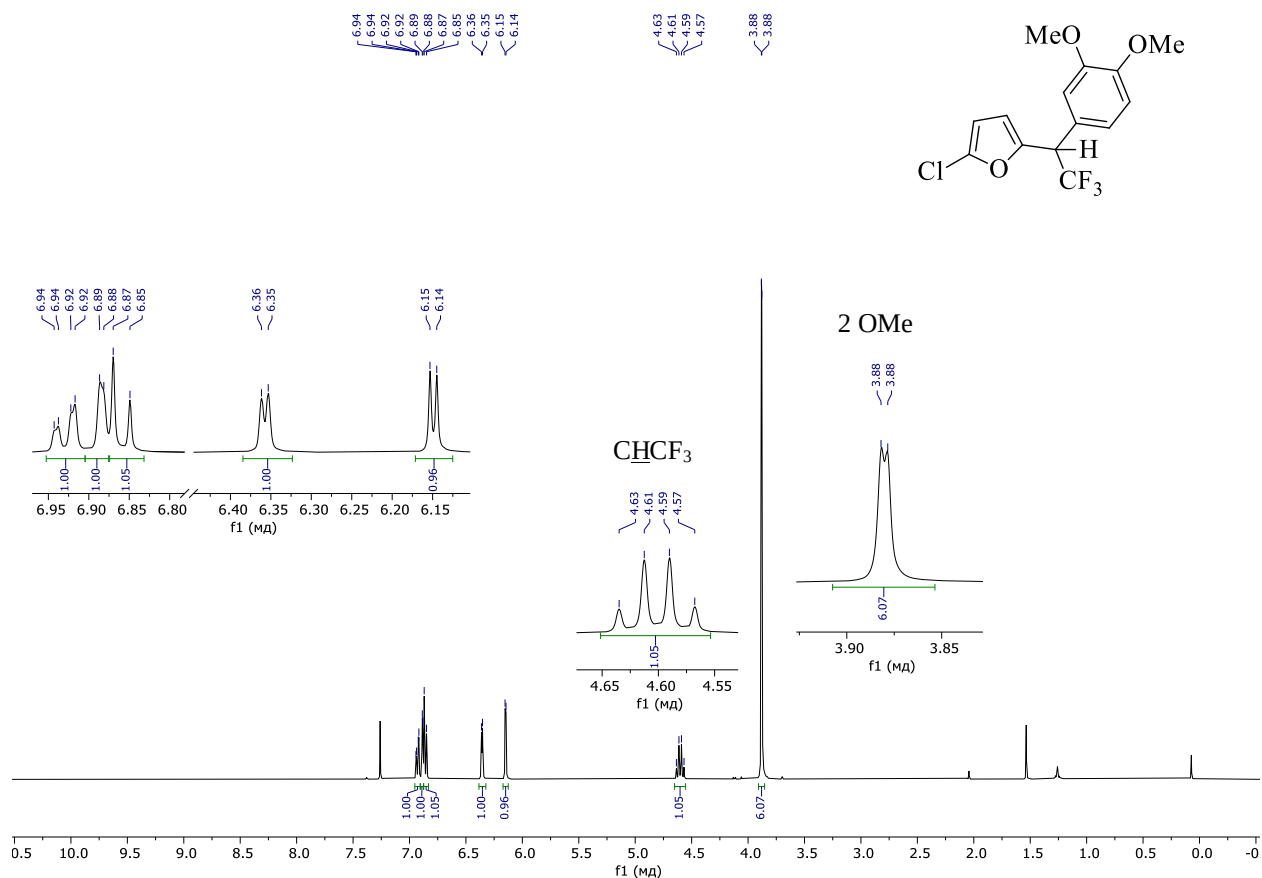


Fig. S90. ¹H NMR spectrum of the compound **2cf** (CDCl₃, 400 MHz).

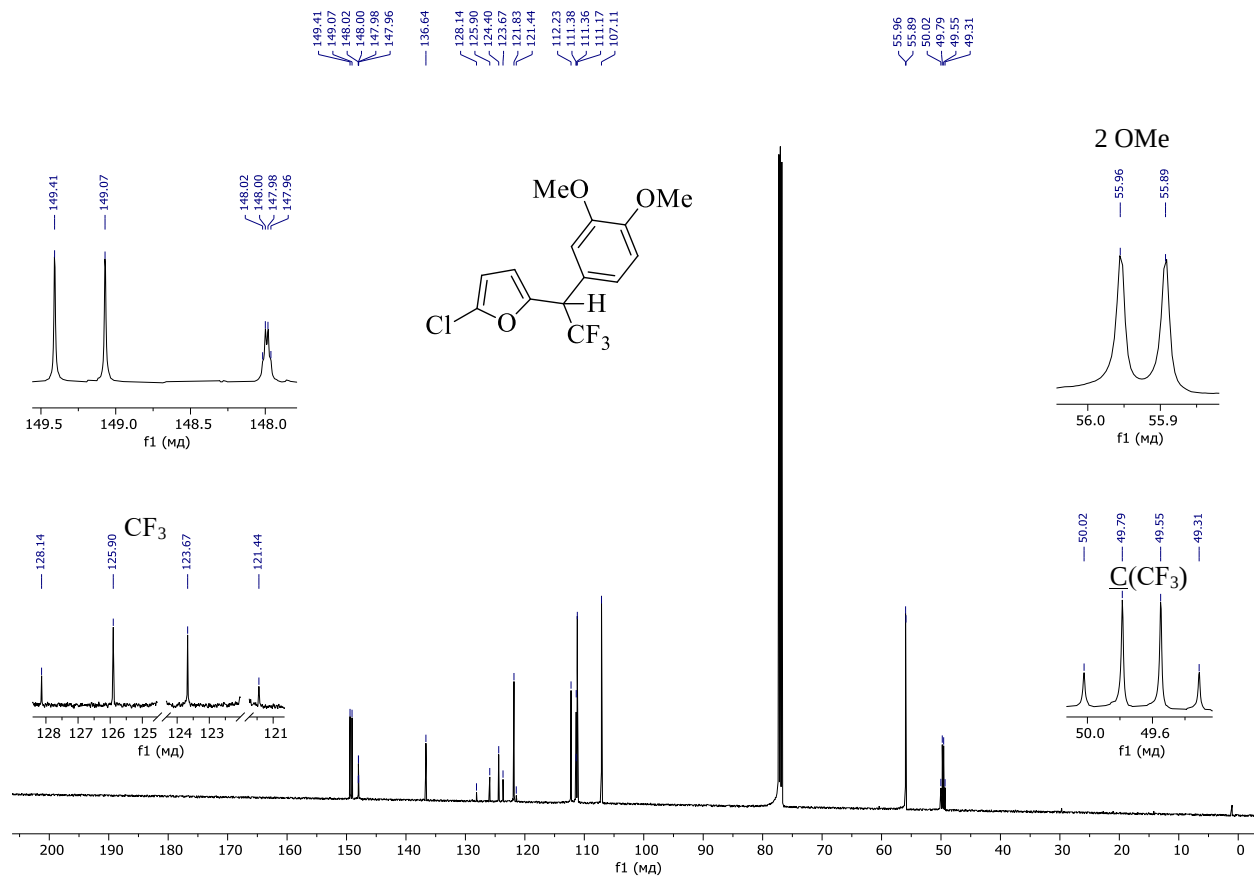


Fig. S91. ¹³C{¹H} NMR spectrum of the compound **2cf** (CDCl₃, 101 MHz).

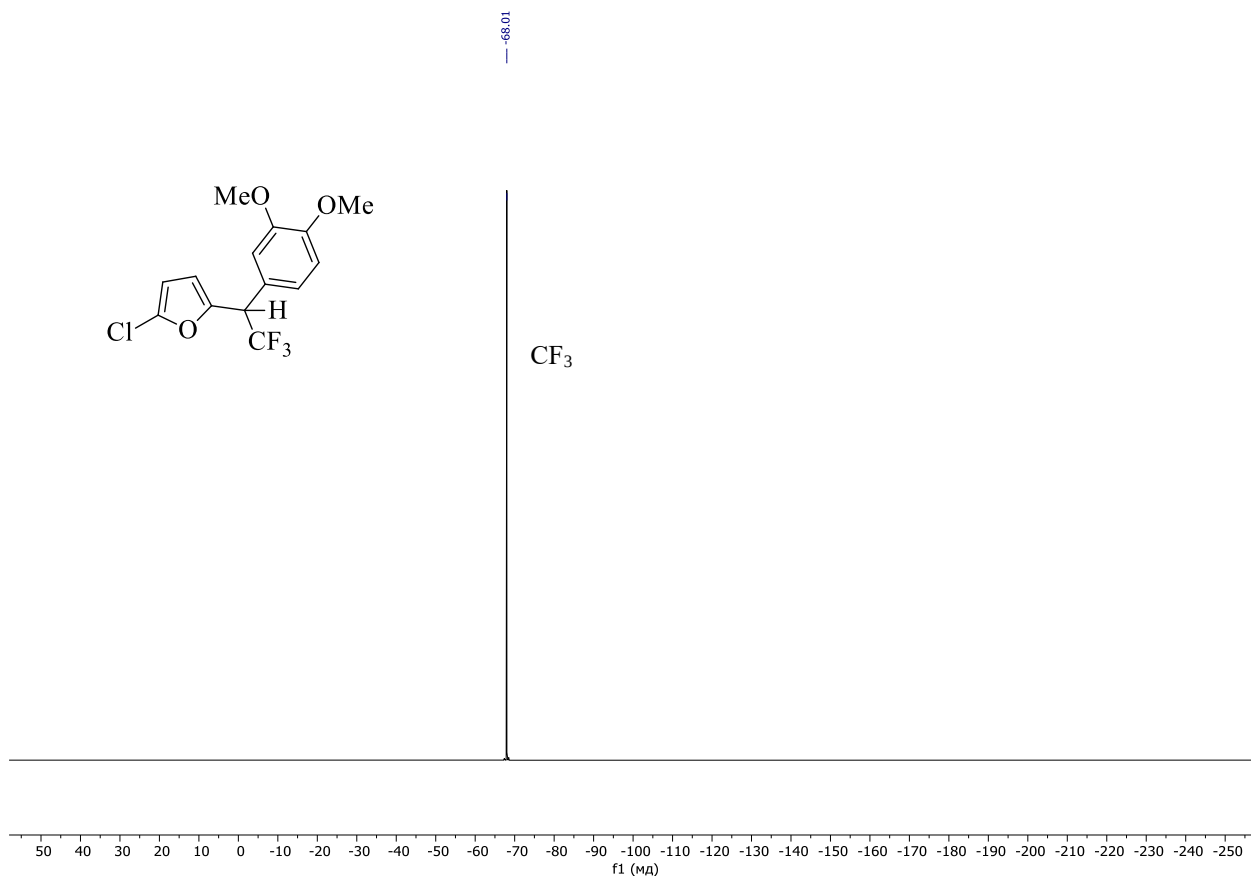


Fig. S92. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2cf** (CDCl₃, 376 MHz).

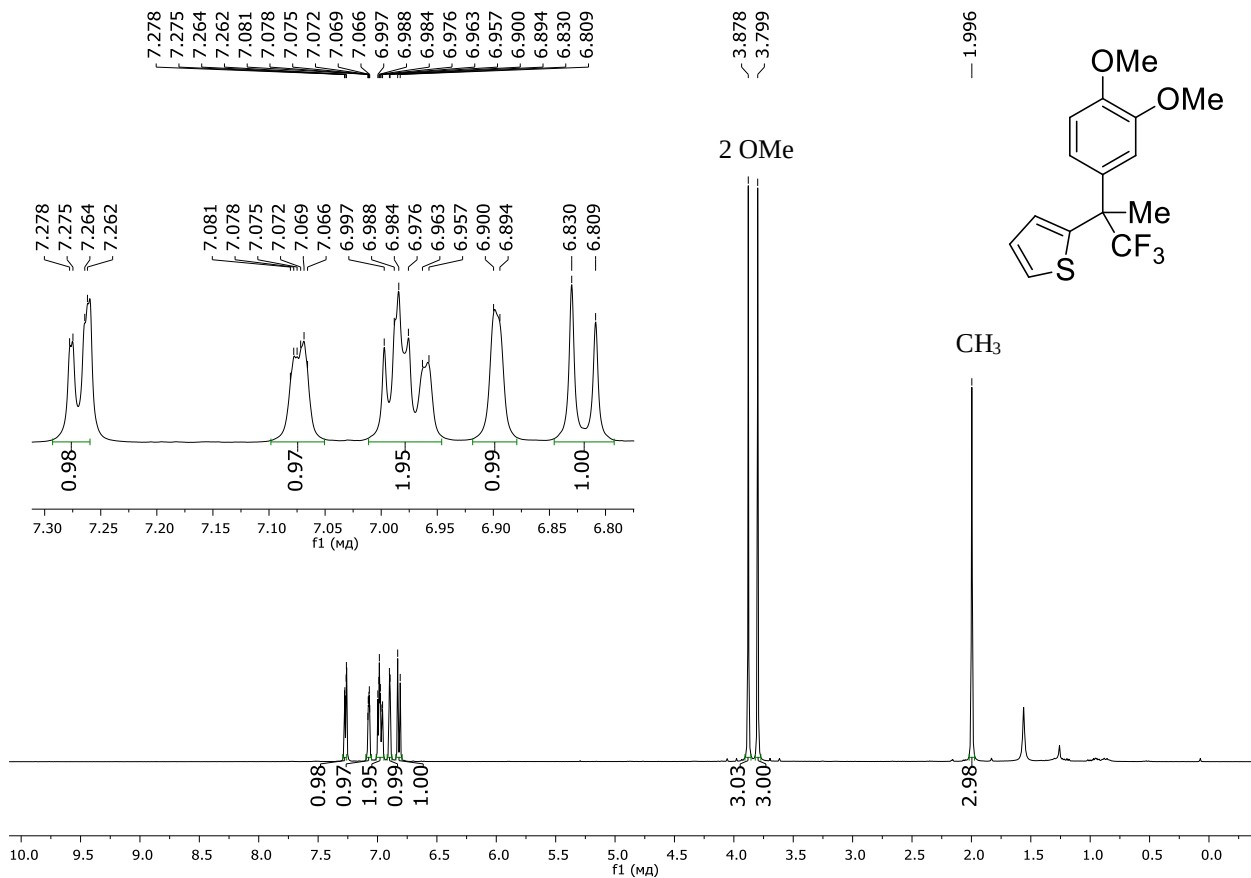


Fig. S93. ^1H NMR spectrum of the compound **2da** (CDCl₃, 400 MHz).

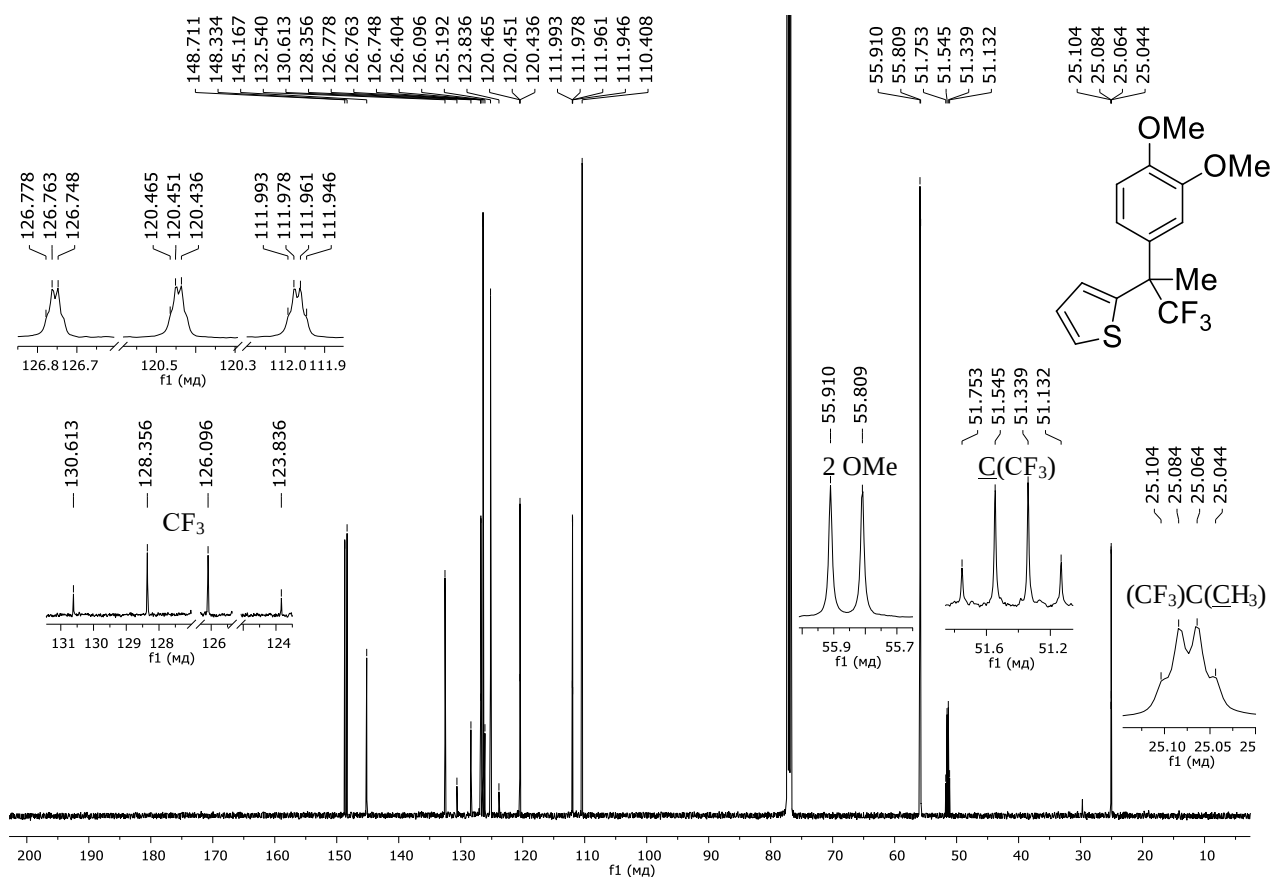


Fig. S94. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2da** (CDCl_3 , 101 MHz).

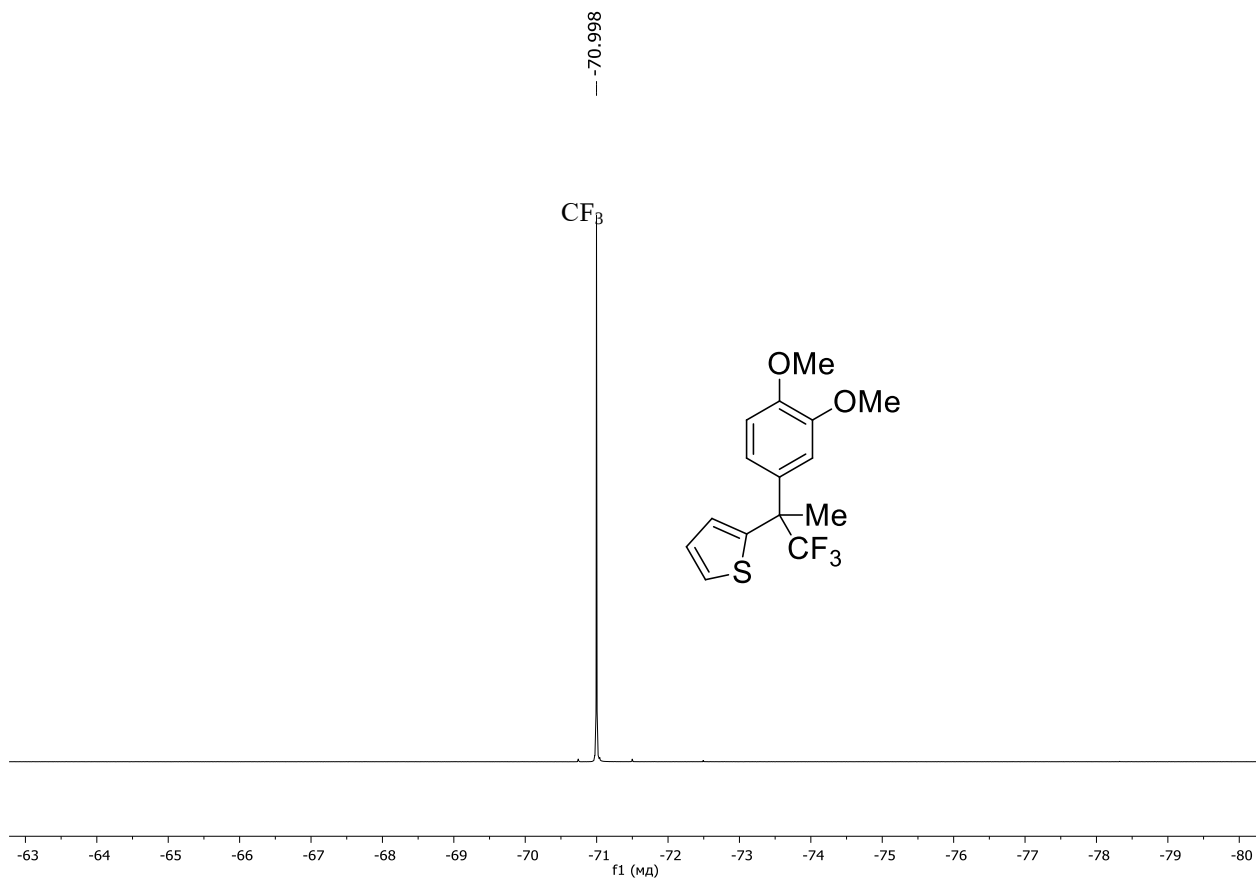


Fig. S95. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2da** (CDCl_3 , 376 MHz).

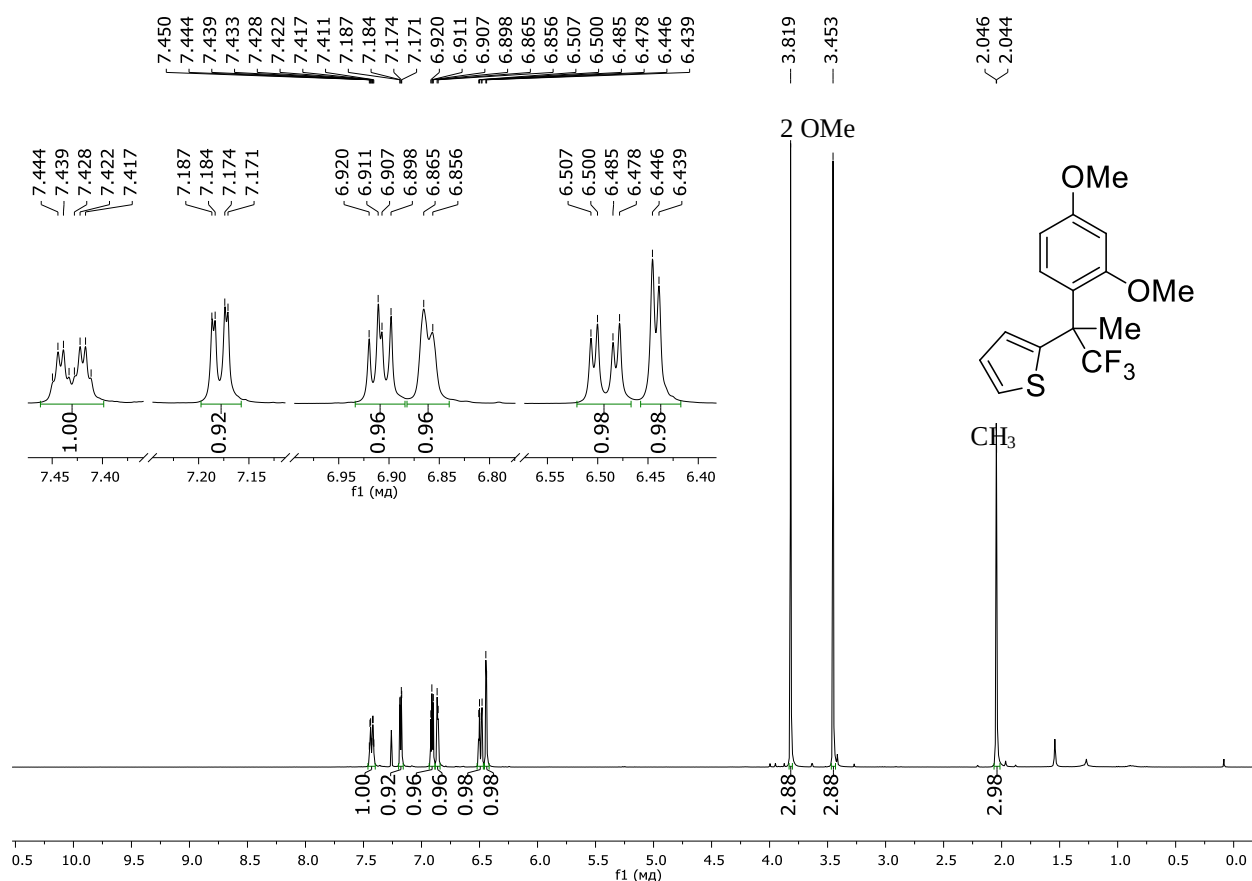


Fig. S96. ¹H NMR spectrum of the compound **2dc** (CDCl₃, 400 MHz).

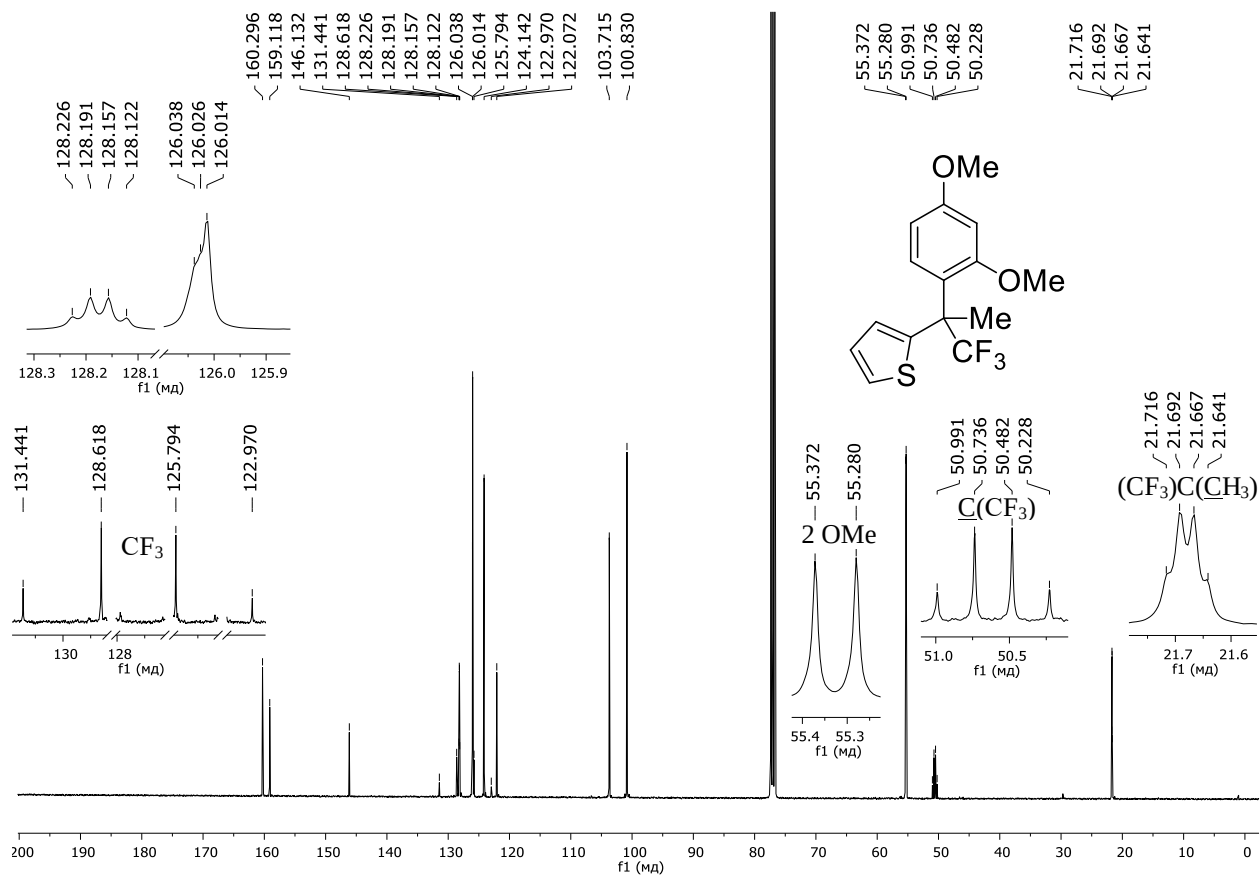


Fig. S97. ¹³C{¹H} NMR spectrum of the compound **2dc** (CDCl₃, 101 MHz).

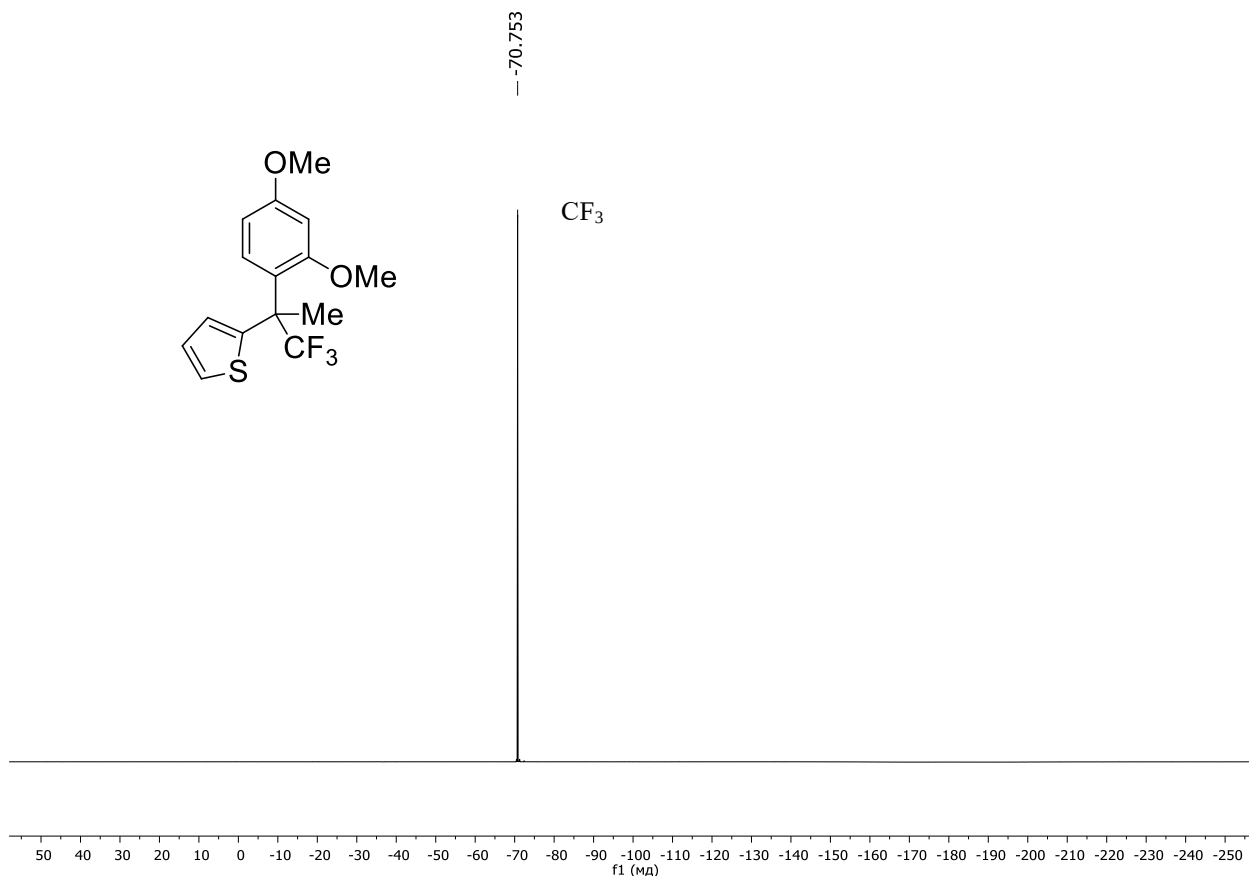


Fig. S98. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2dc** (CDCl_3 , 376 MHz).

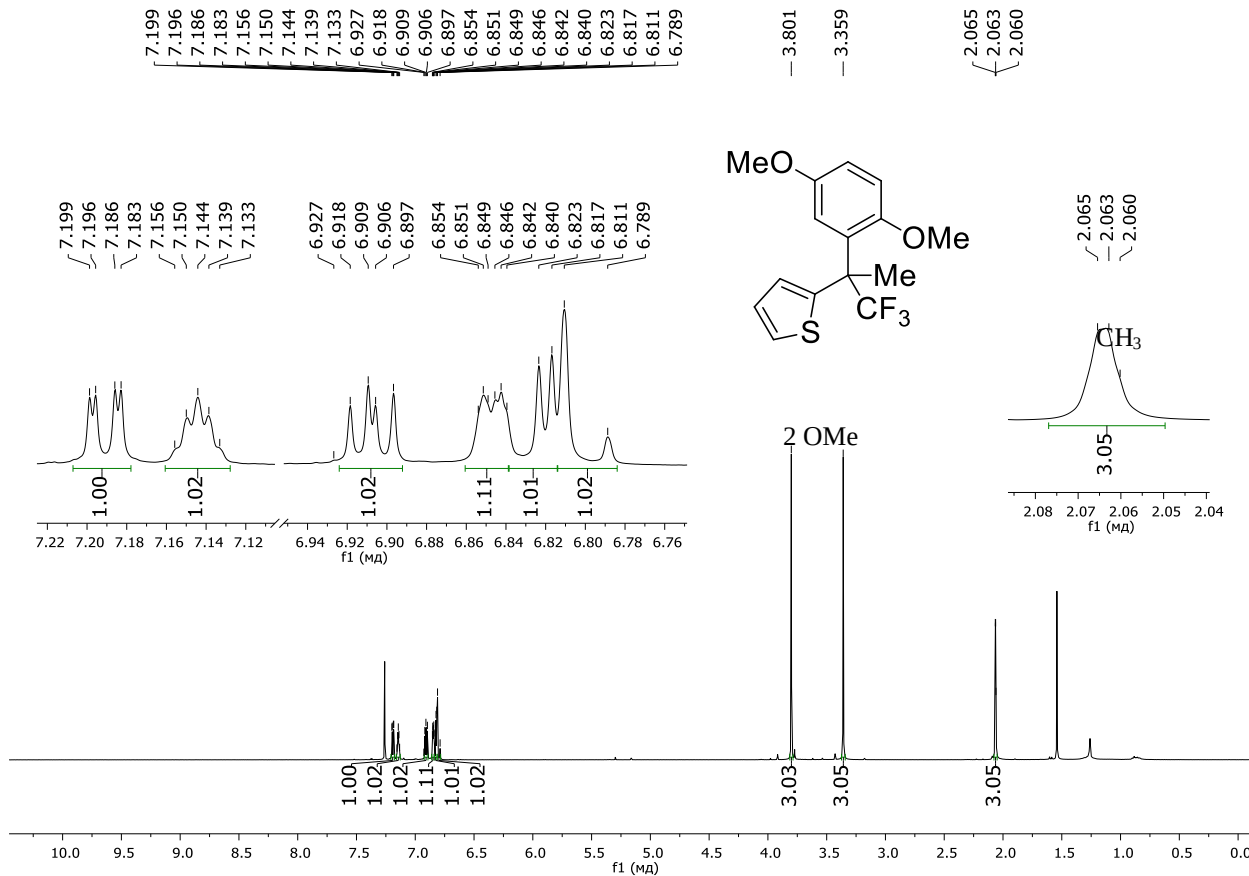
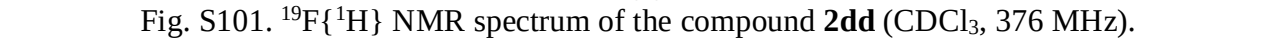
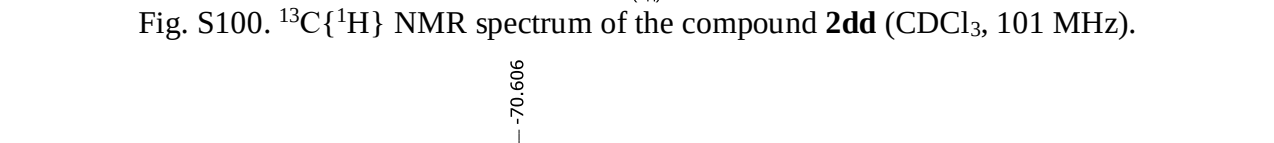


Fig. S99. ^1H NMR spectrum of the compound **2dd** (CDCl_3 , 400 MHz).



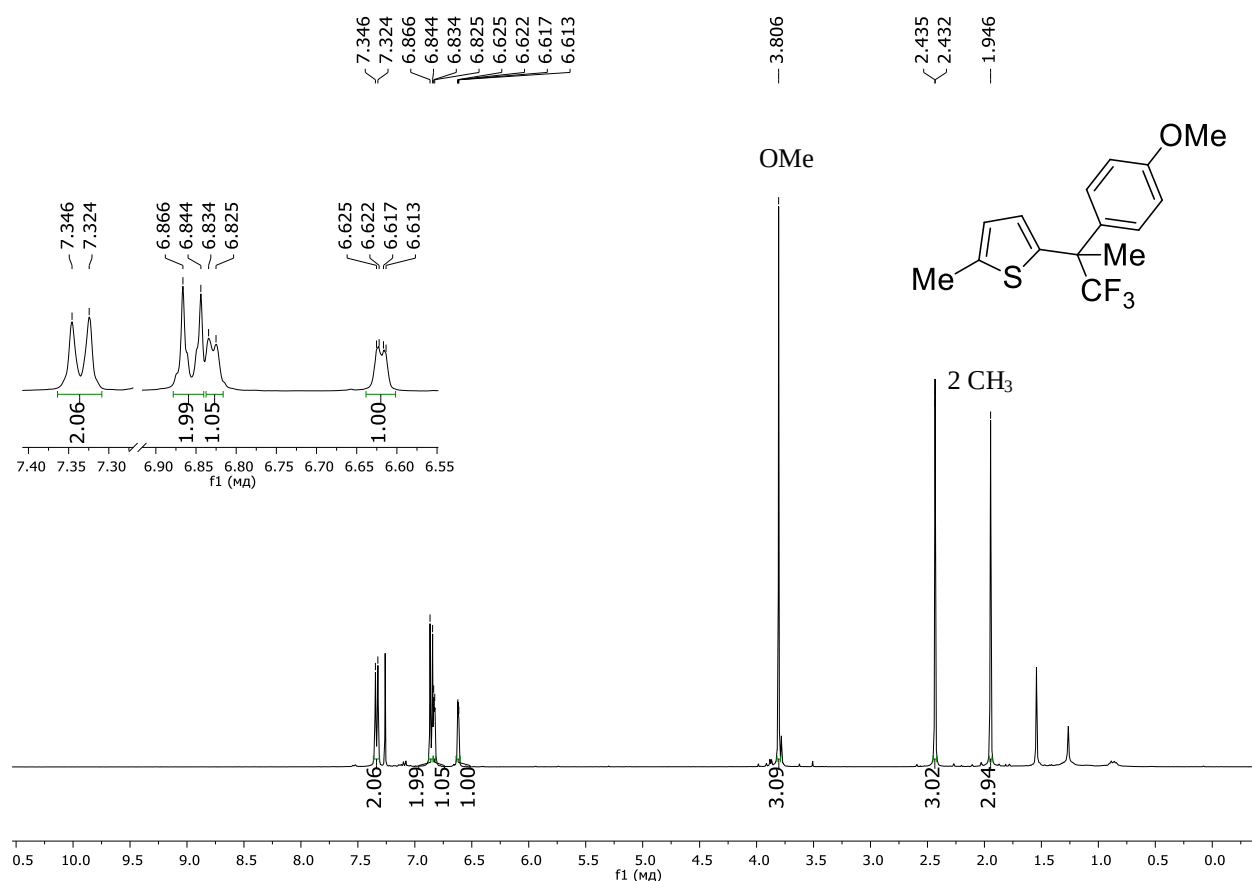


Fig. S102. ¹H NMR spectrum of the compound **2ea** (CDCl₃, 400 MHz).

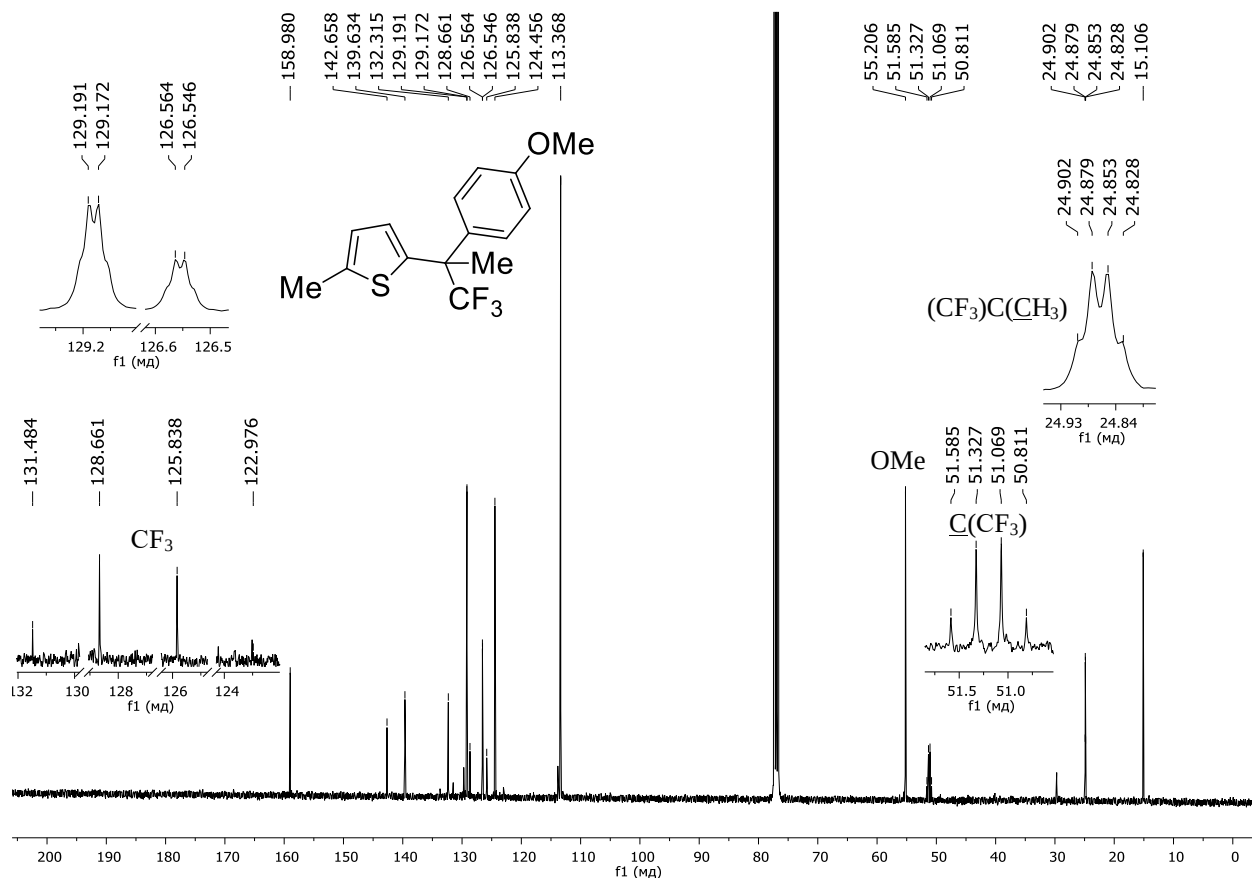


Fig. S103. ¹³C{¹H} NMR spectrum of the compound **2ea** (CDCl₃, 101 MHz).

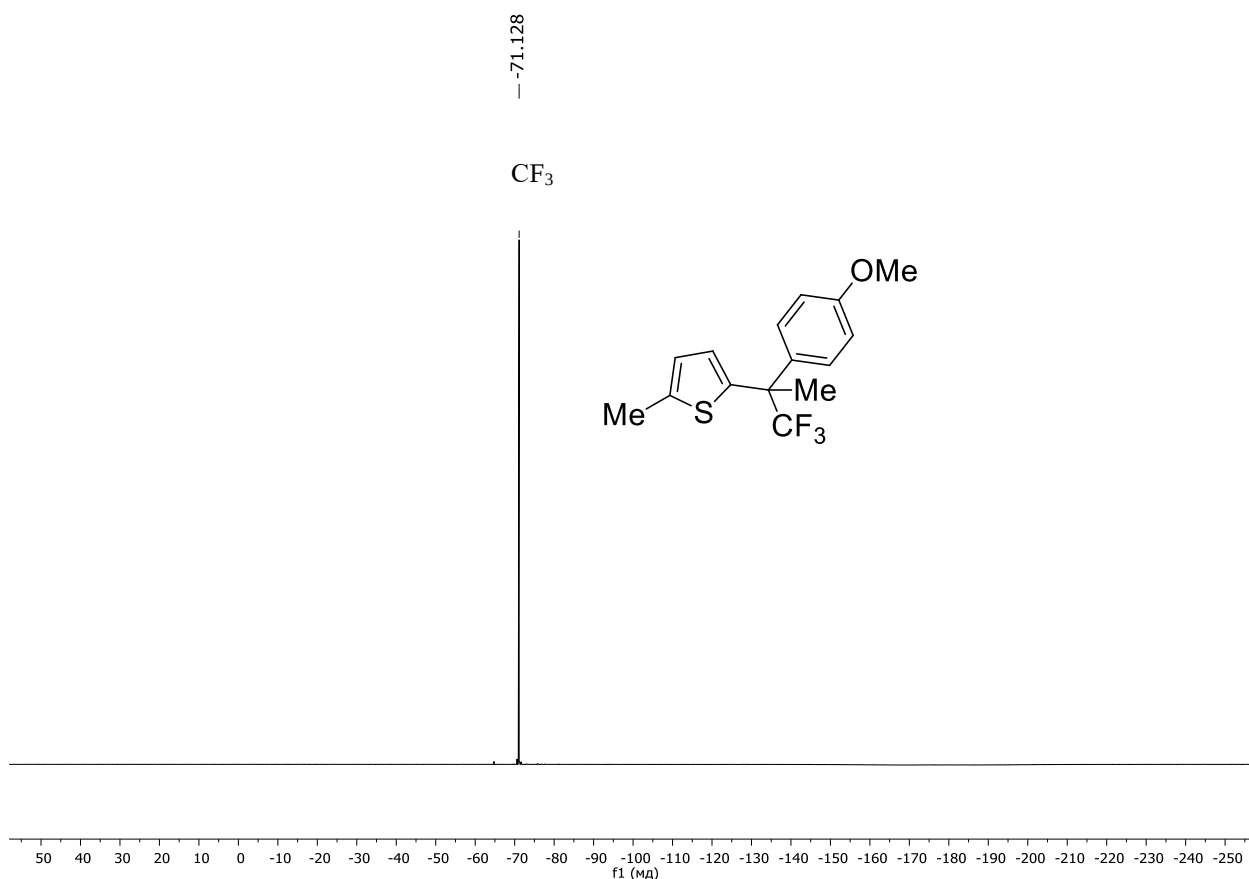


Fig. S104. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ea** (CDCl₃, 376 MHz).

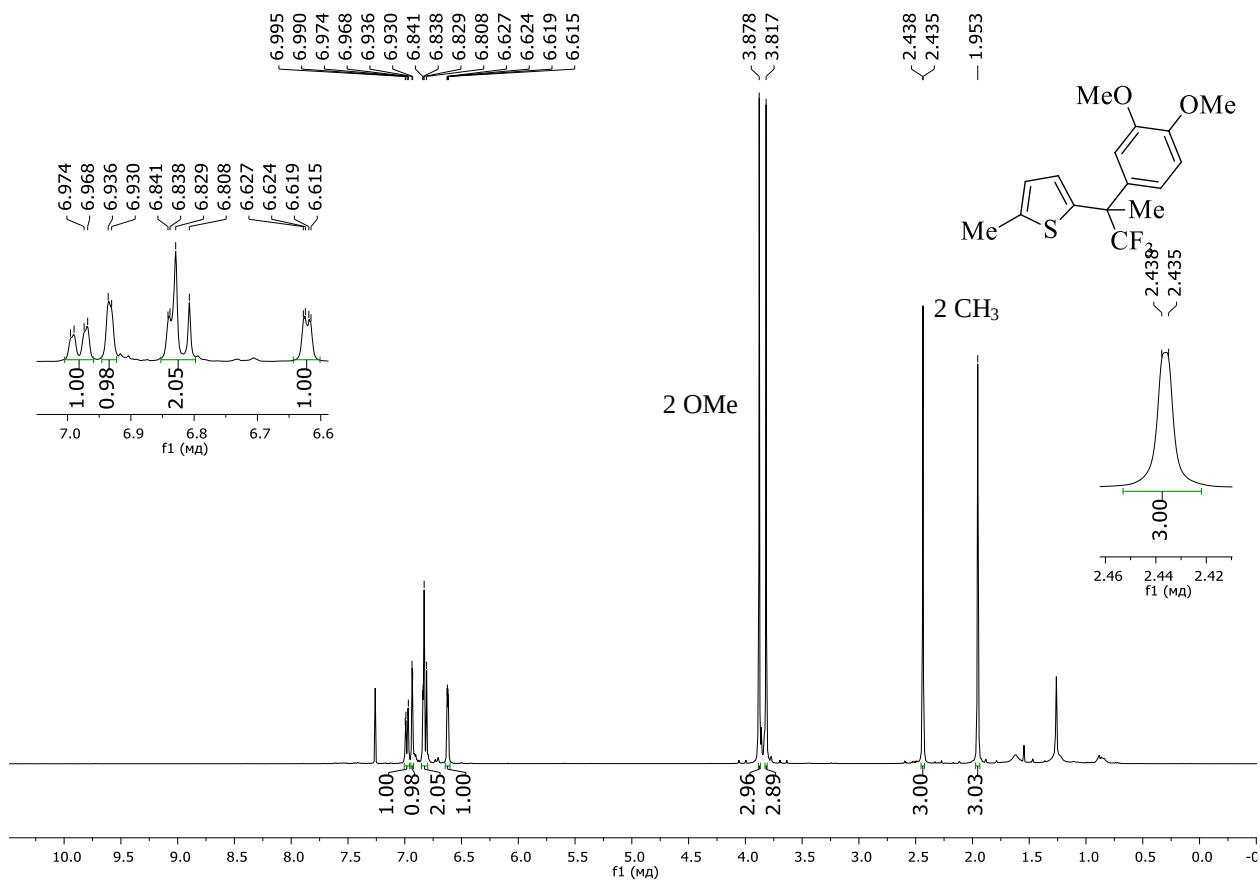


Fig. S105. ^1H NMR spectrum of the compound **2eb** (CDCl₃, 400 MHz).

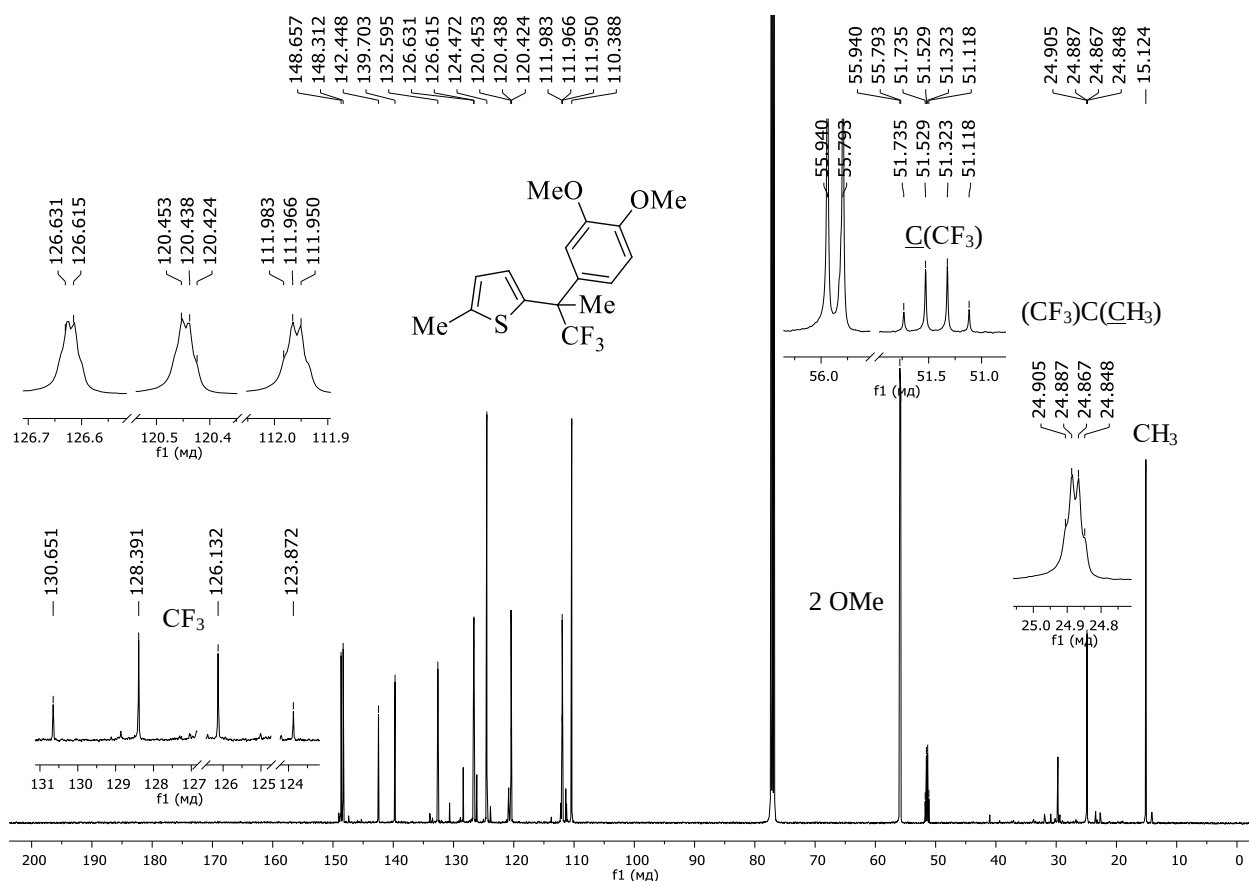


Fig. S106. ¹³C{¹H} NMR spectrum of the compound **2eb** (CDCl₃, 101 MHz).

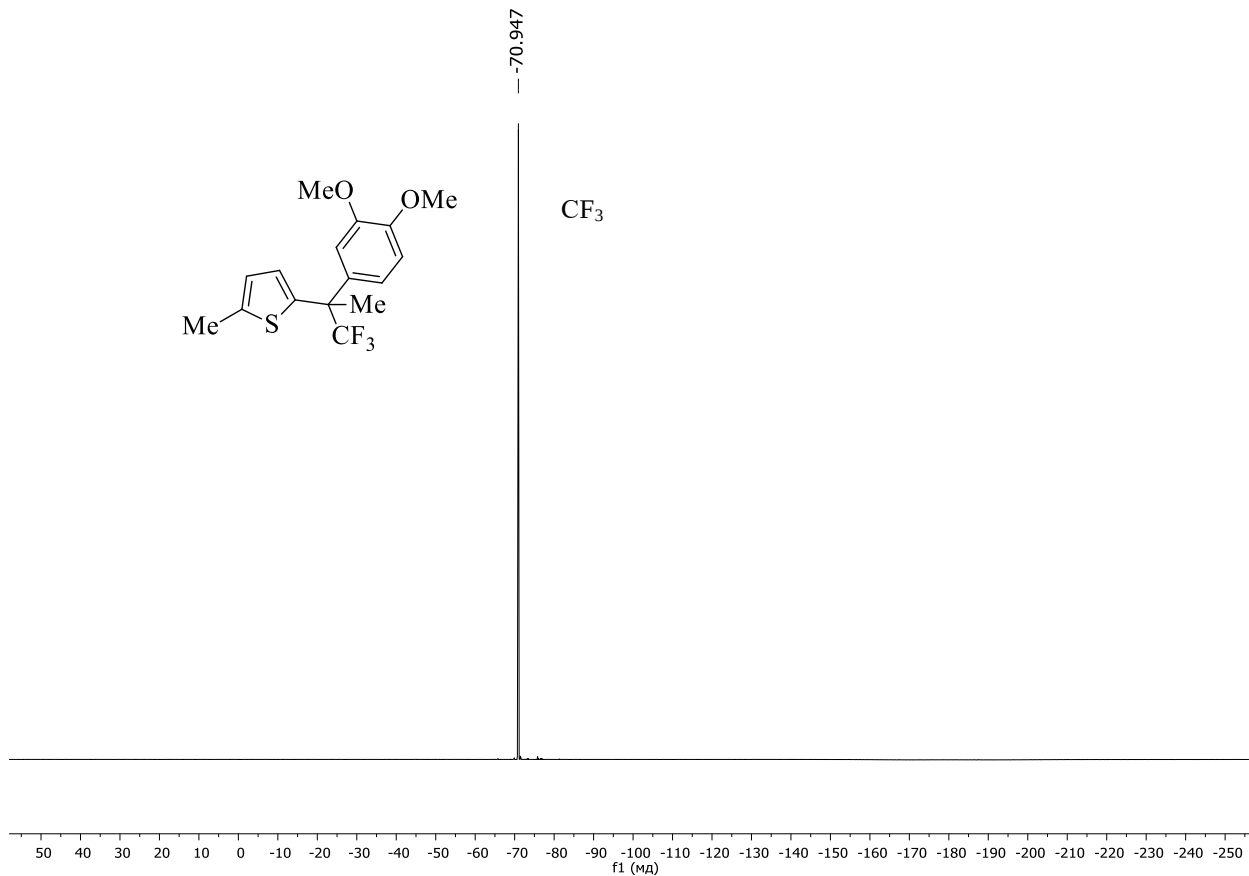


Fig. S107. ¹⁹F{¹H} NMR spectrum of the compound **2eb** (CDCl₃, 376 MHz).

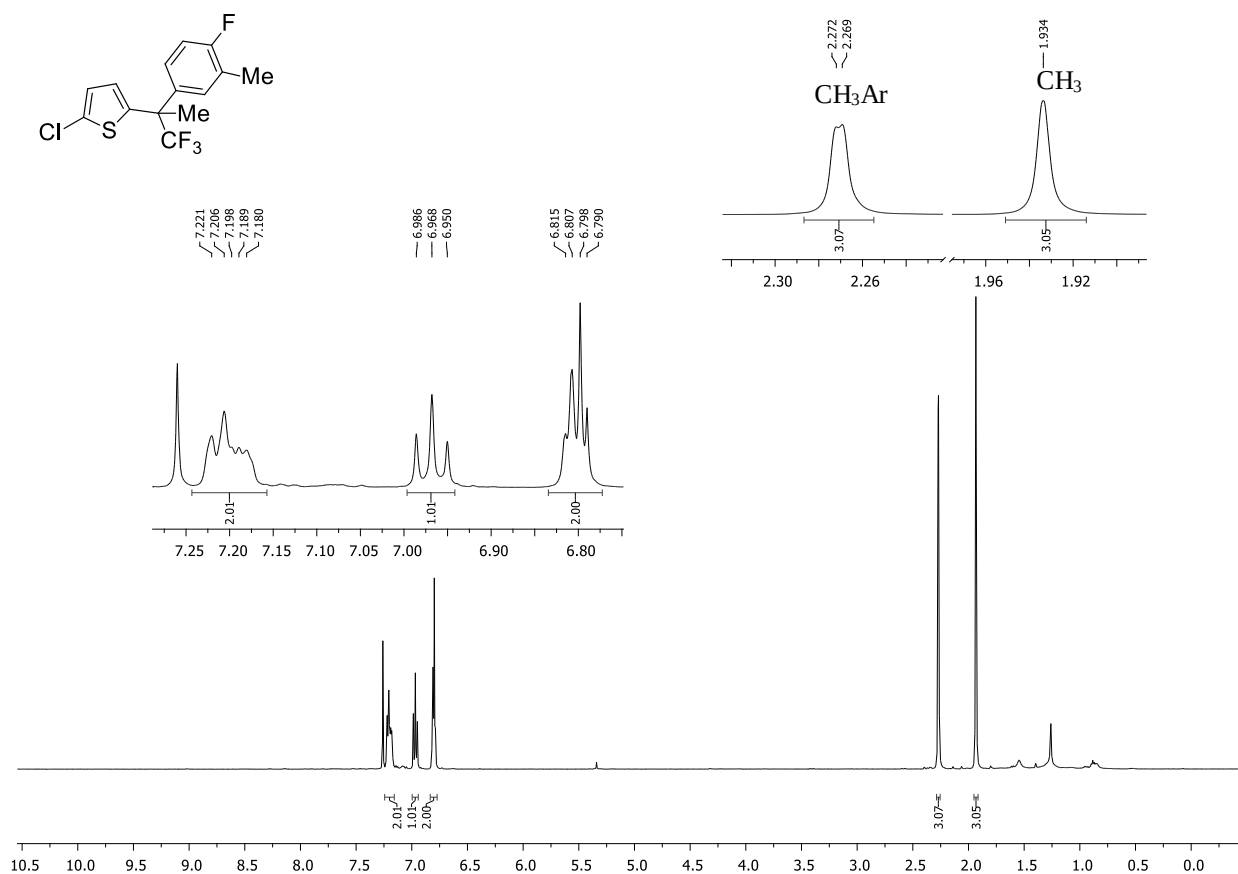


Fig. S108. ¹H NMR spectrum of the compound **2fa** (CDCl₃, 400 MHz).

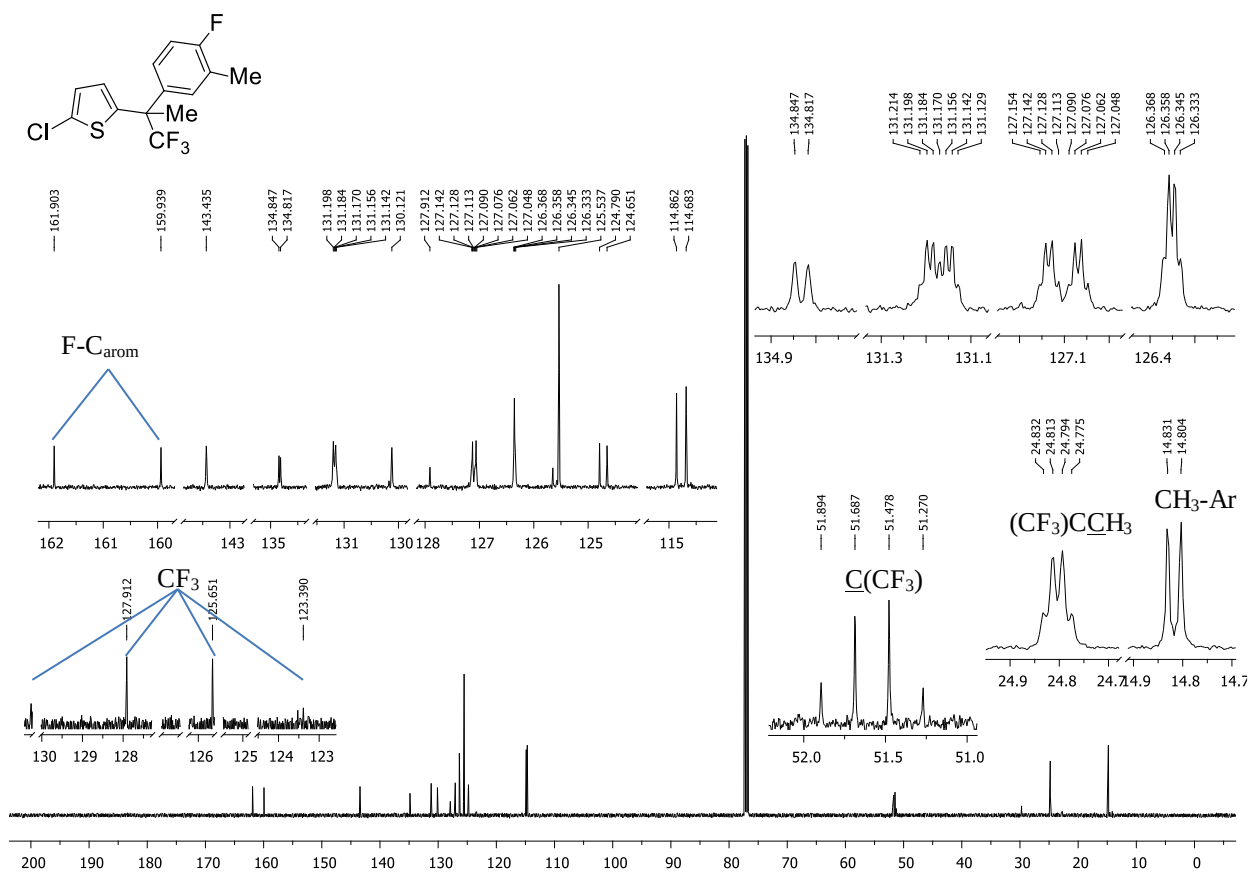


Fig. S109. ¹³C{¹H} NMR spectrum of the compound **2fa** (CDCl₃, 101 MHz).

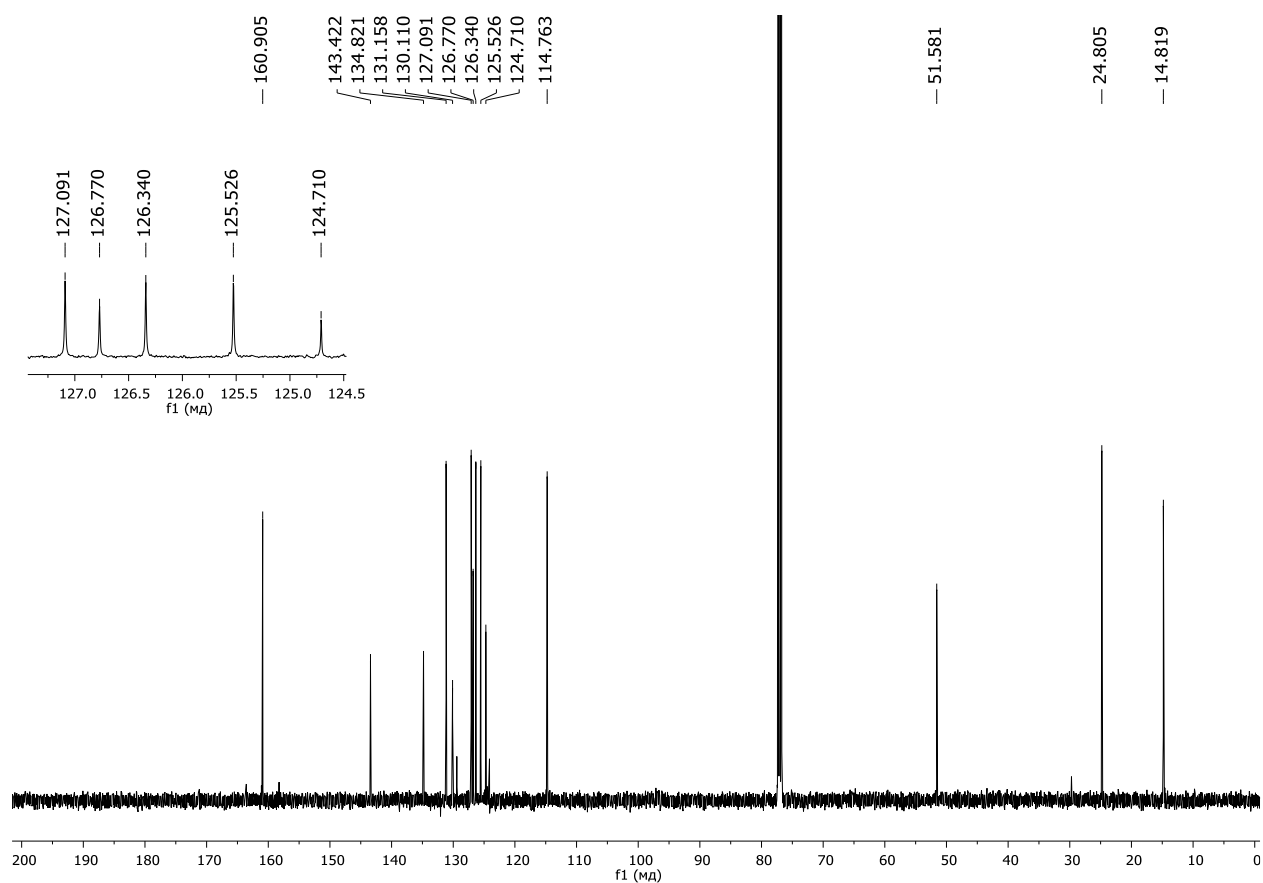


Fig. S110. $^{13}\text{C}\{^{19}\text{F}\}$ NMR spectrum of the compound **2fa** (CDCl_3 , 101 MHz).

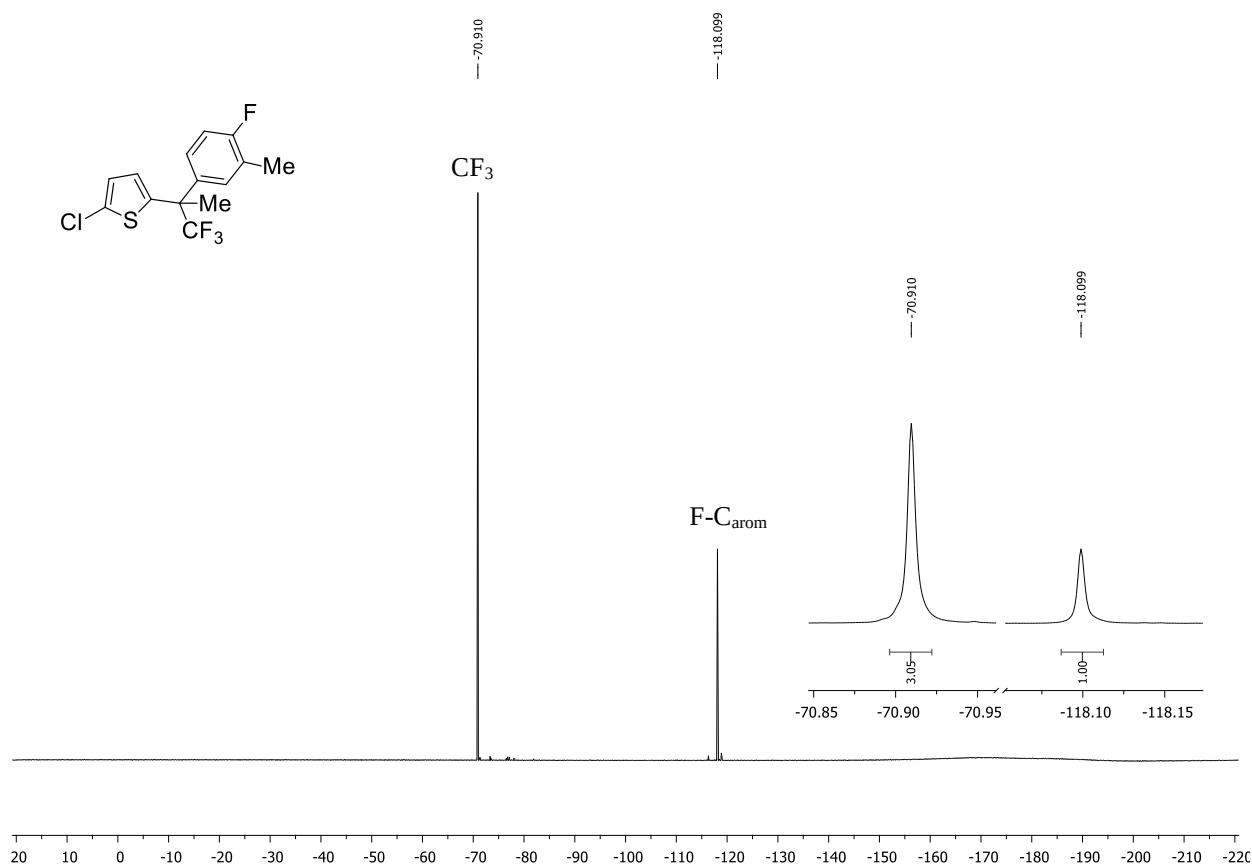


Fig. S111. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2fa** (CDCl_3 , 376 MHz).

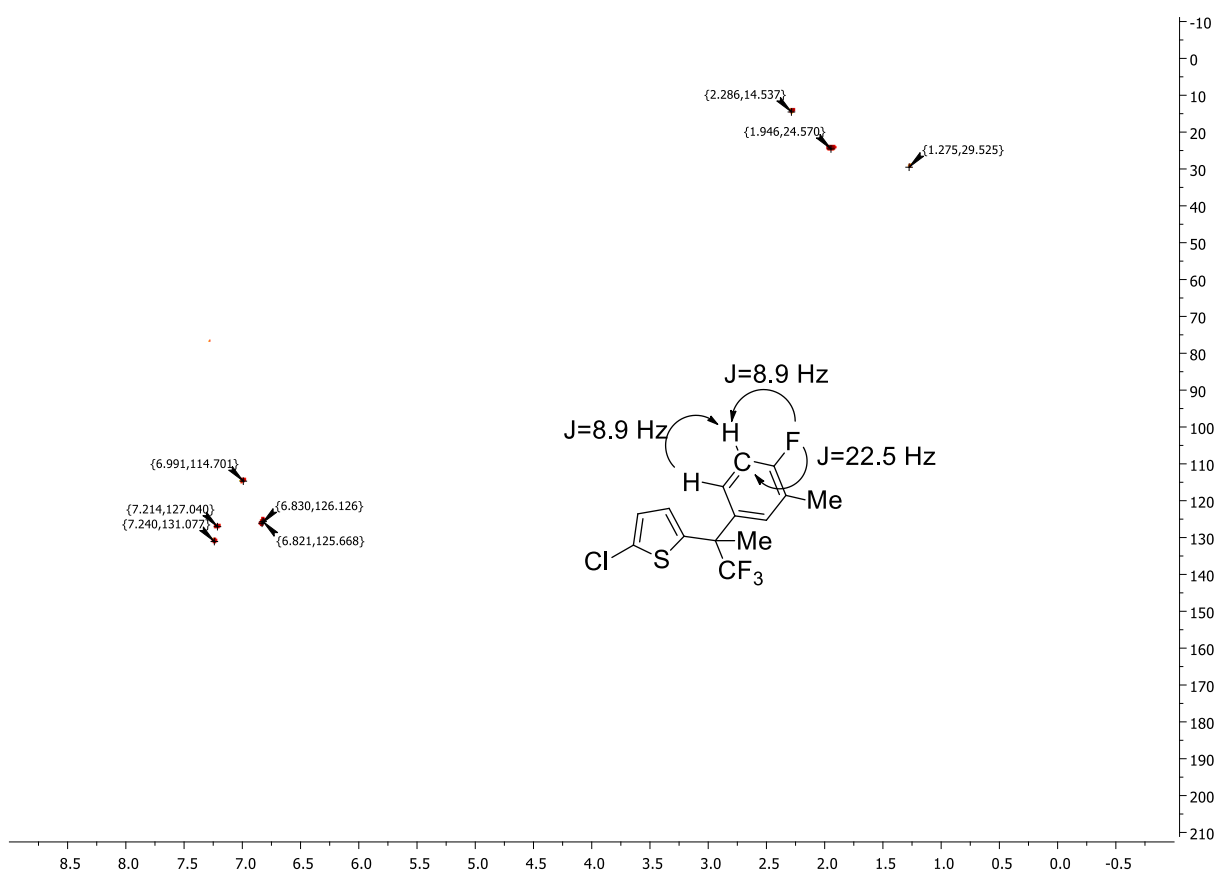


Fig. S112. HSQC NMR spectrum of the compound **2fa** (101-400 MHz, CDCl₃).

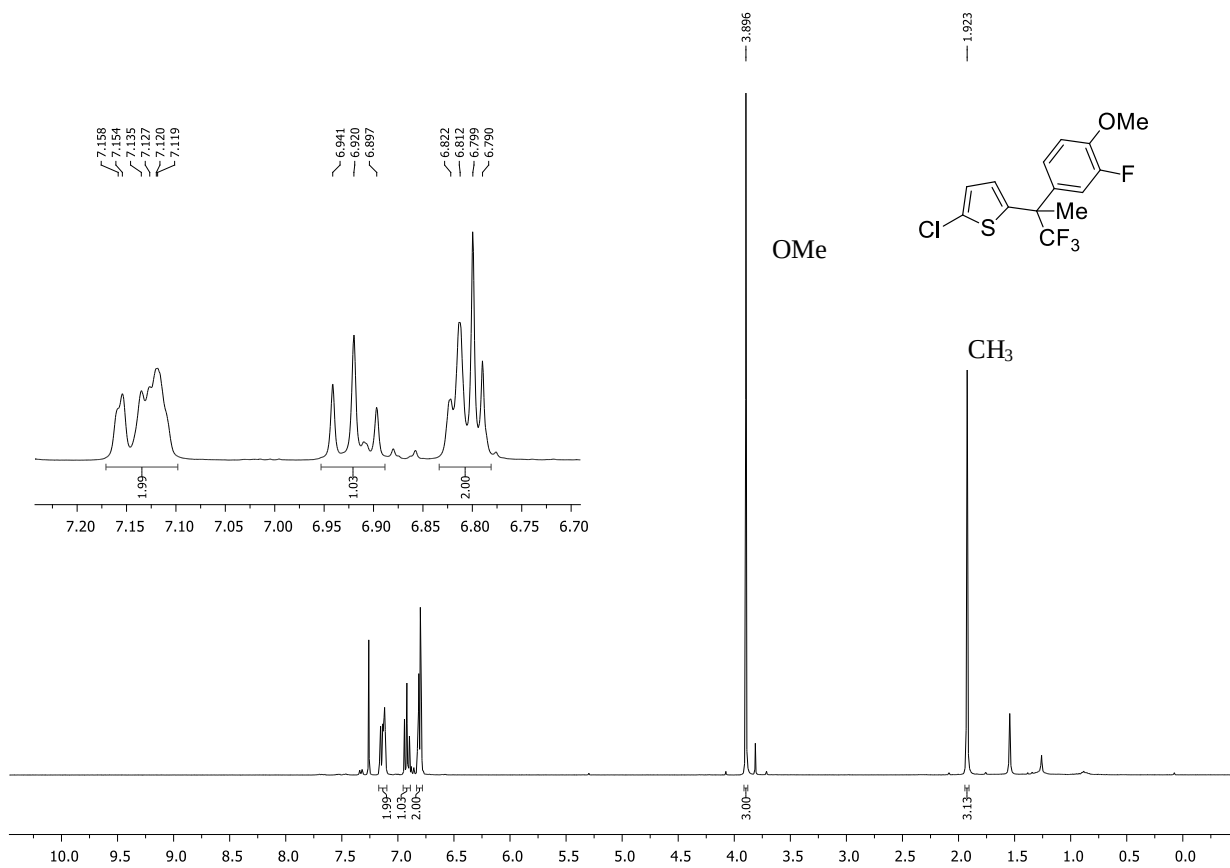


Fig. S113. ¹H NMR spectrum of the compound **2fb** (CDCl₃, 400 MHz).

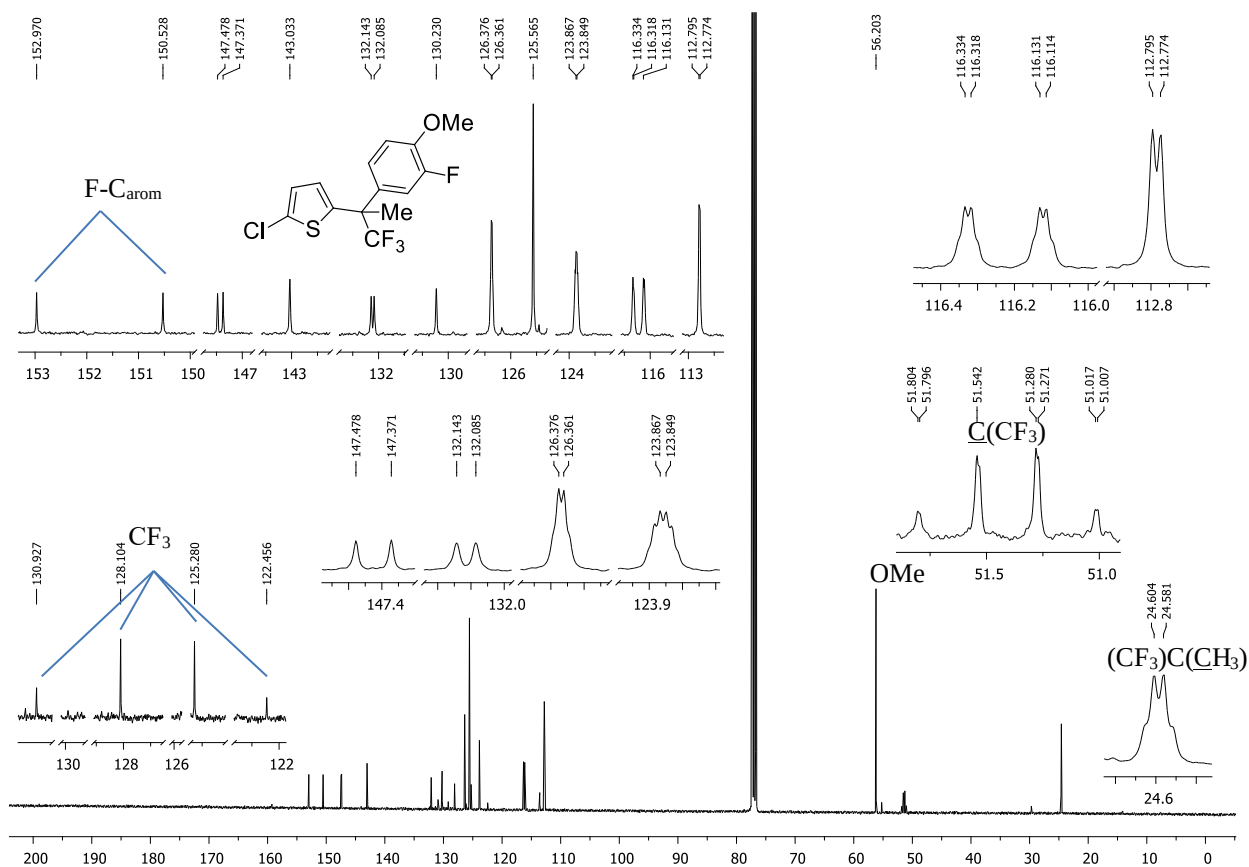


Fig. S114. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2fb** (CDCl₃, 101 MHz).

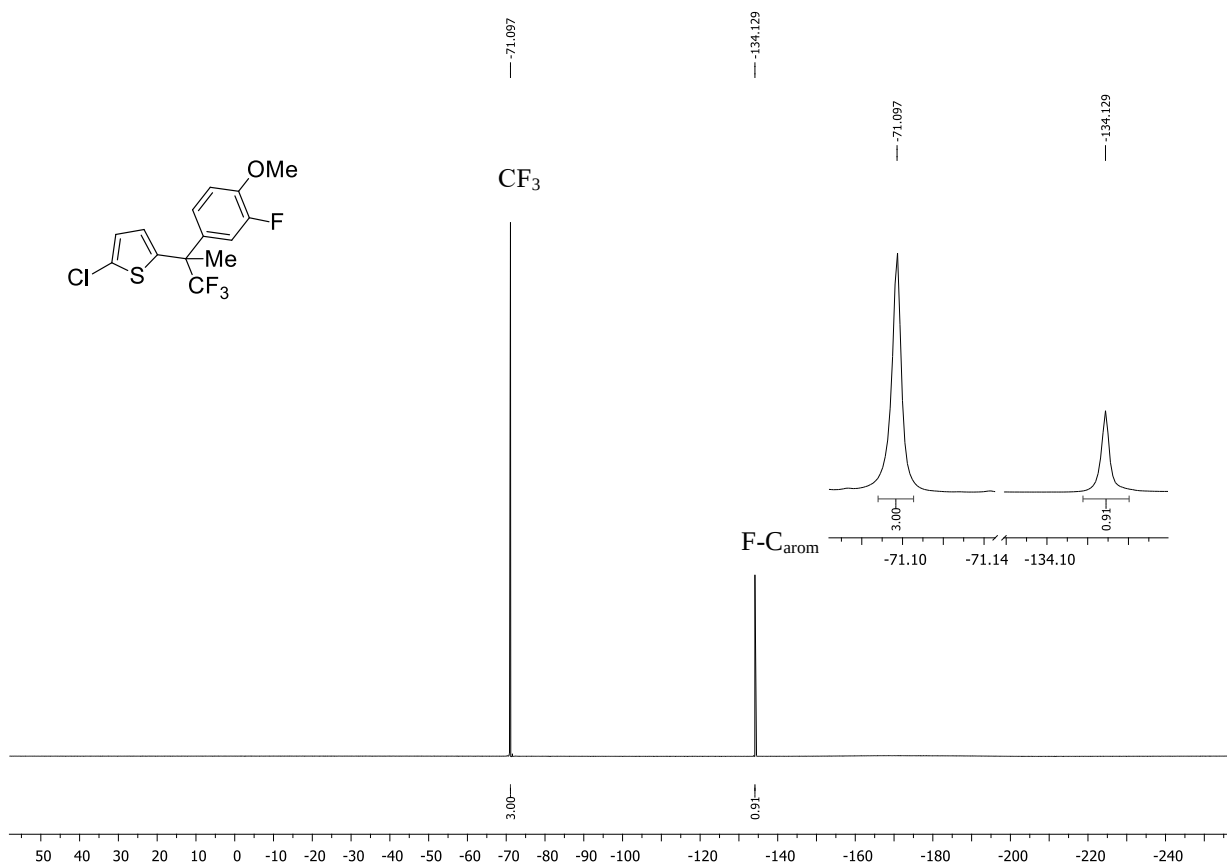


Fig. S115. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2fb** (CDCl₃, 376 MHz).

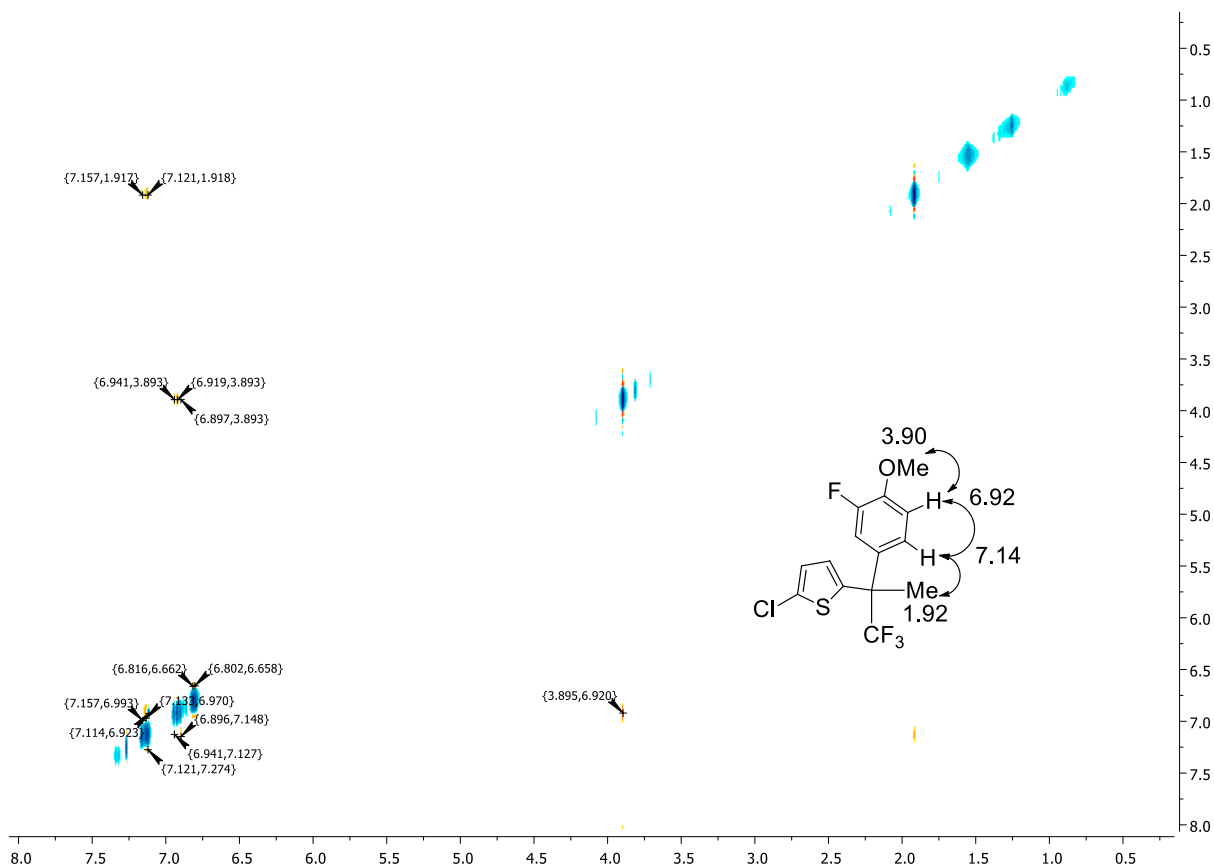


Fig. S116. NOESY H-H NMR spectrum of the compound **2fb** (400 MHz, CDCl₃).

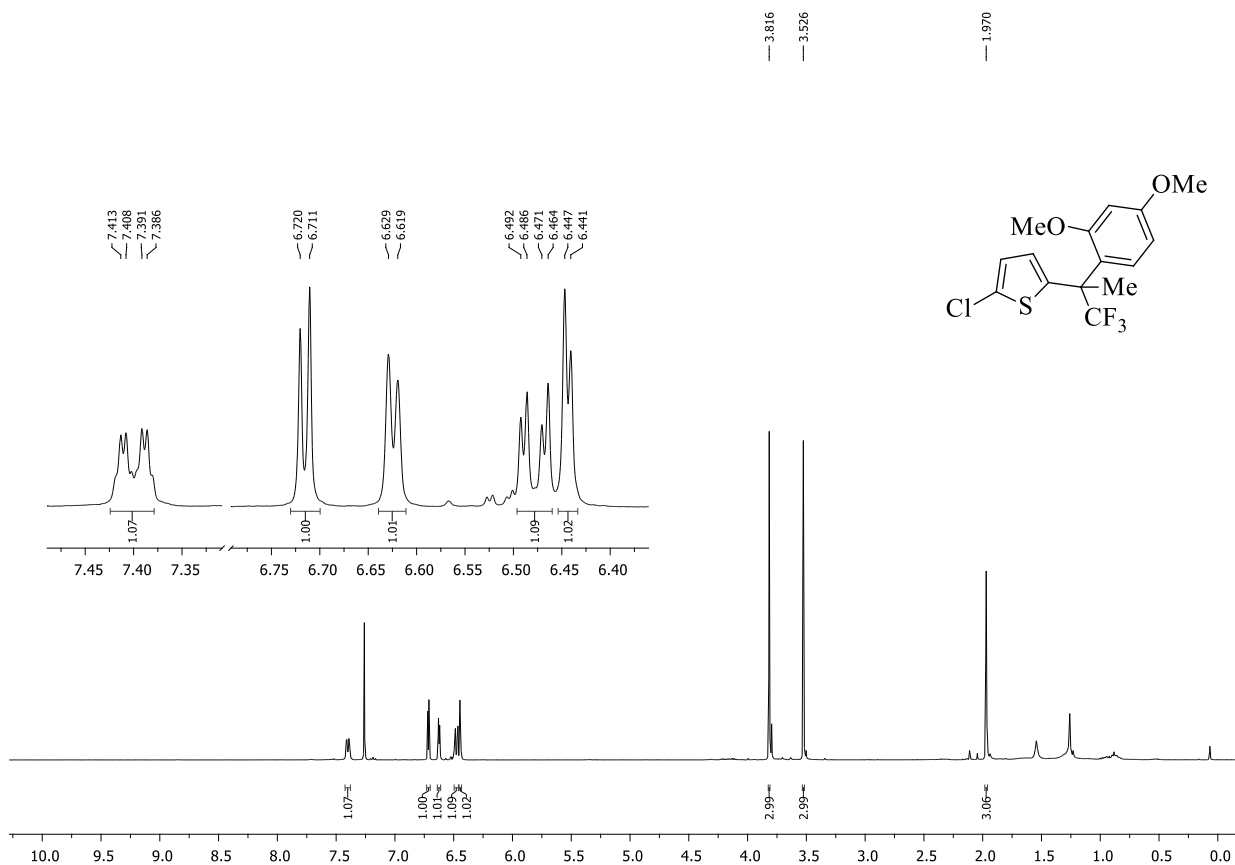


Fig. S117. ¹H NMR spectrum of the compound **2fc** (CDCl₃, 400 MHz).

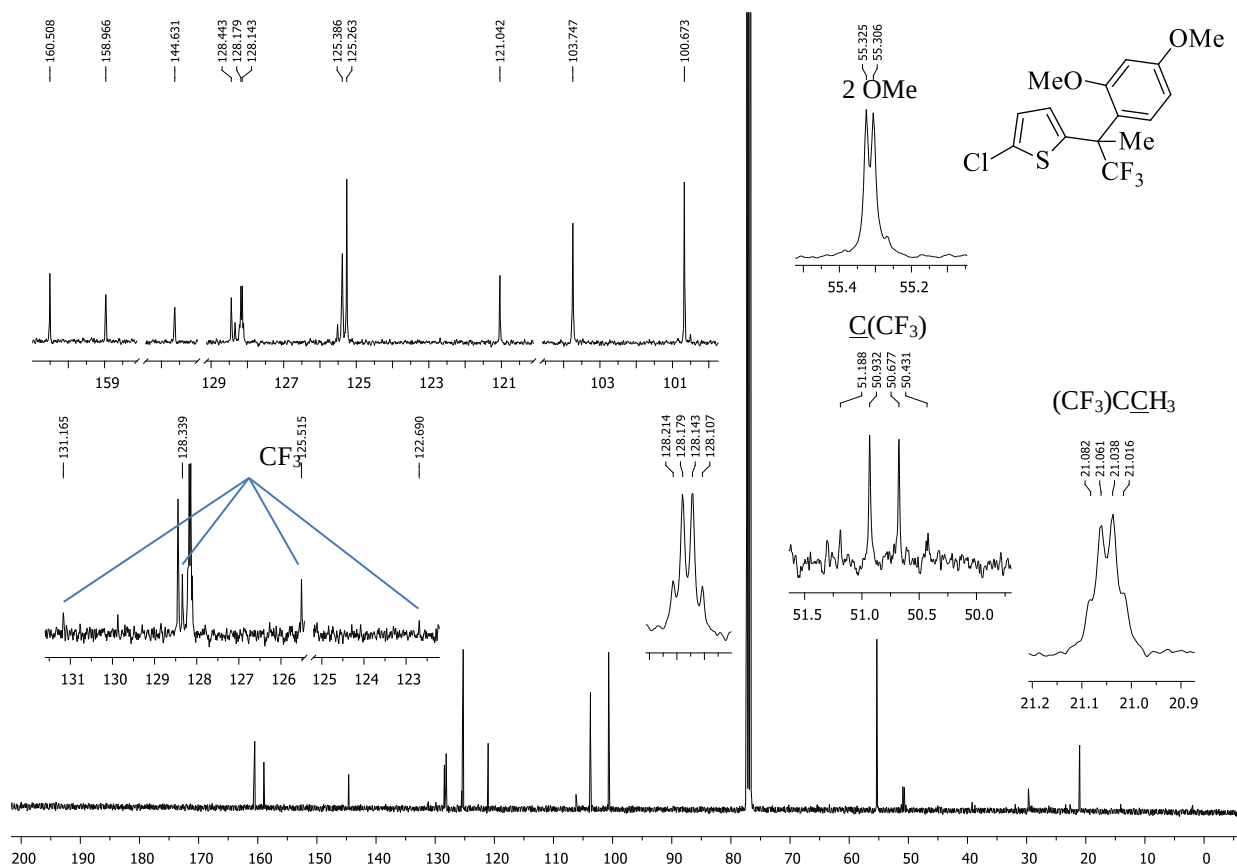


Fig. S118. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2fc** (CDCl_3 , 101 MHz).

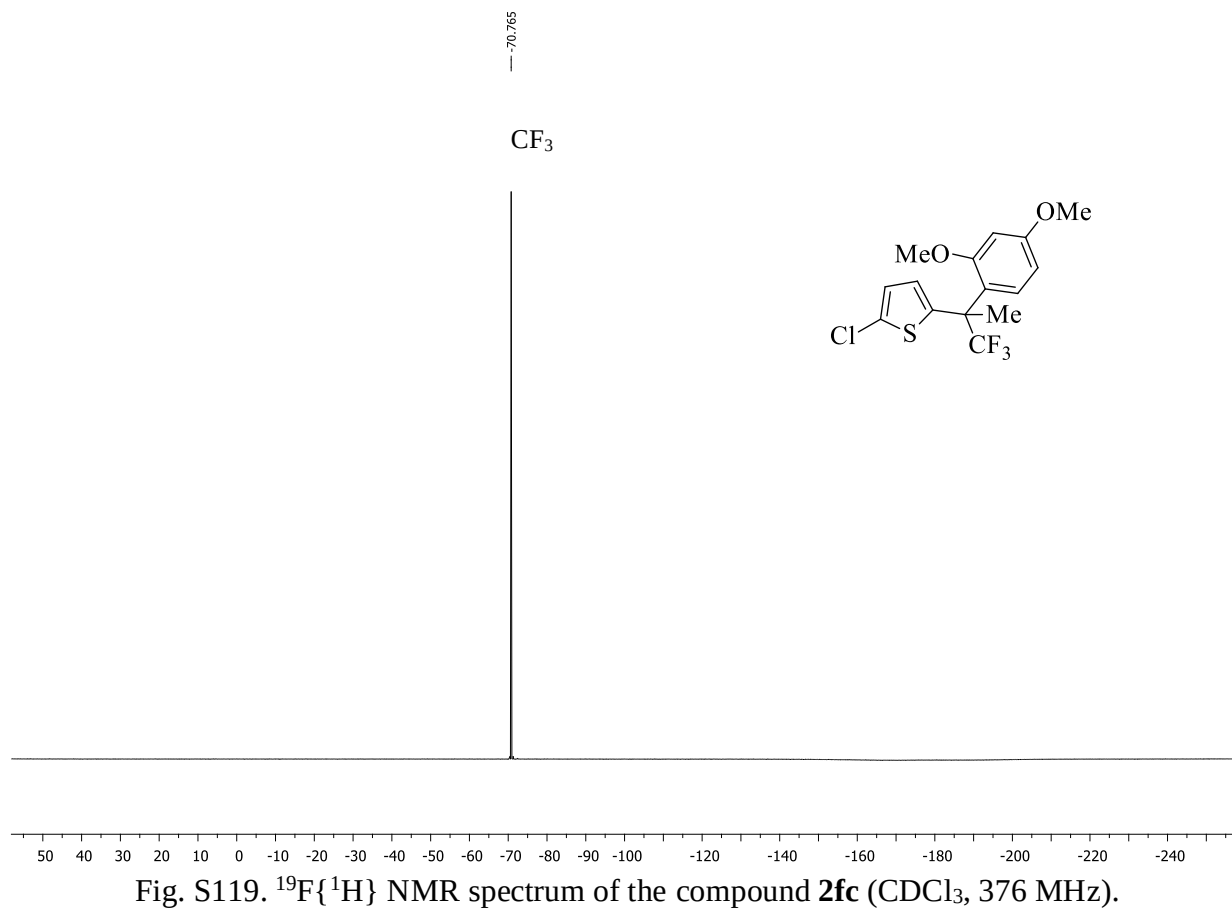


Fig. S119. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2fc** (CDCl_3 , 376 MHz).

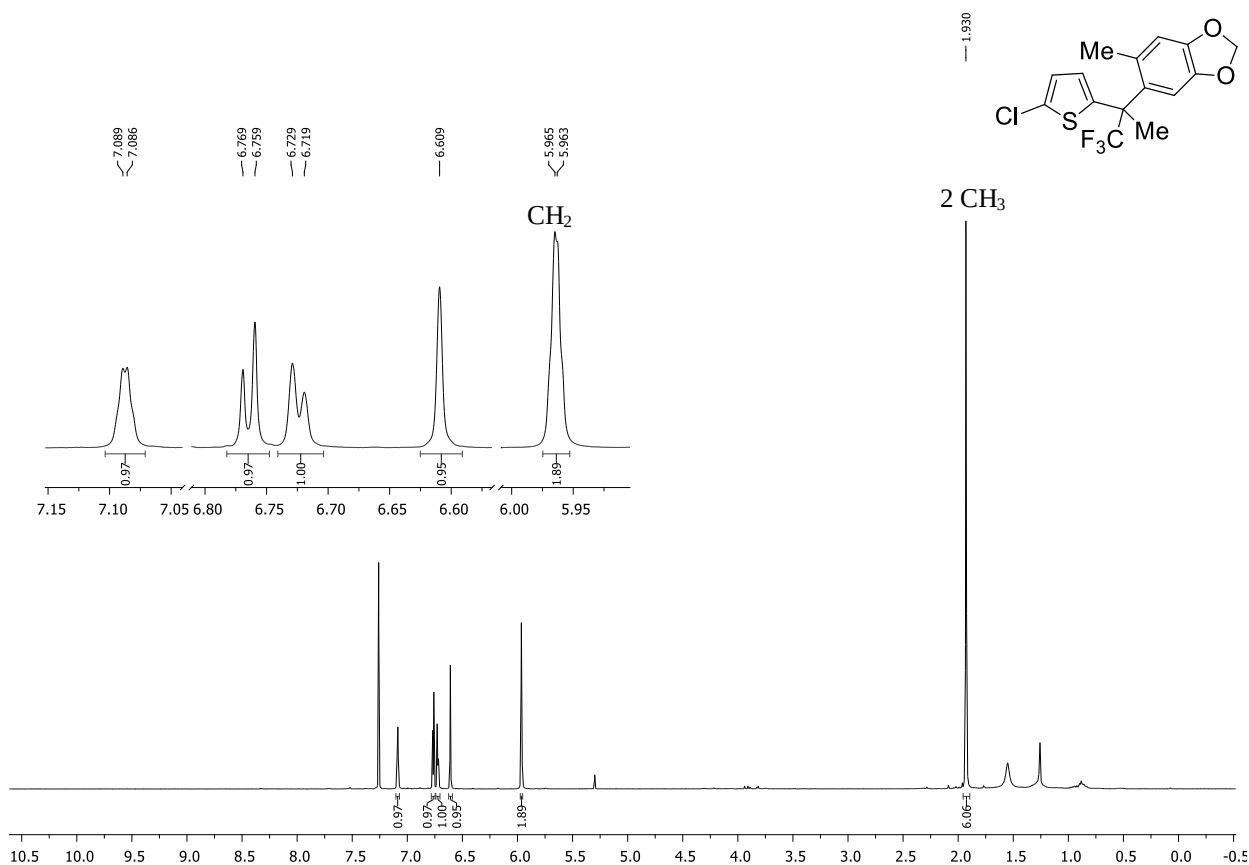


Fig. S120. ¹H NMR spectrum of the compound **2fd** (CDCl₃, 400 MHz).

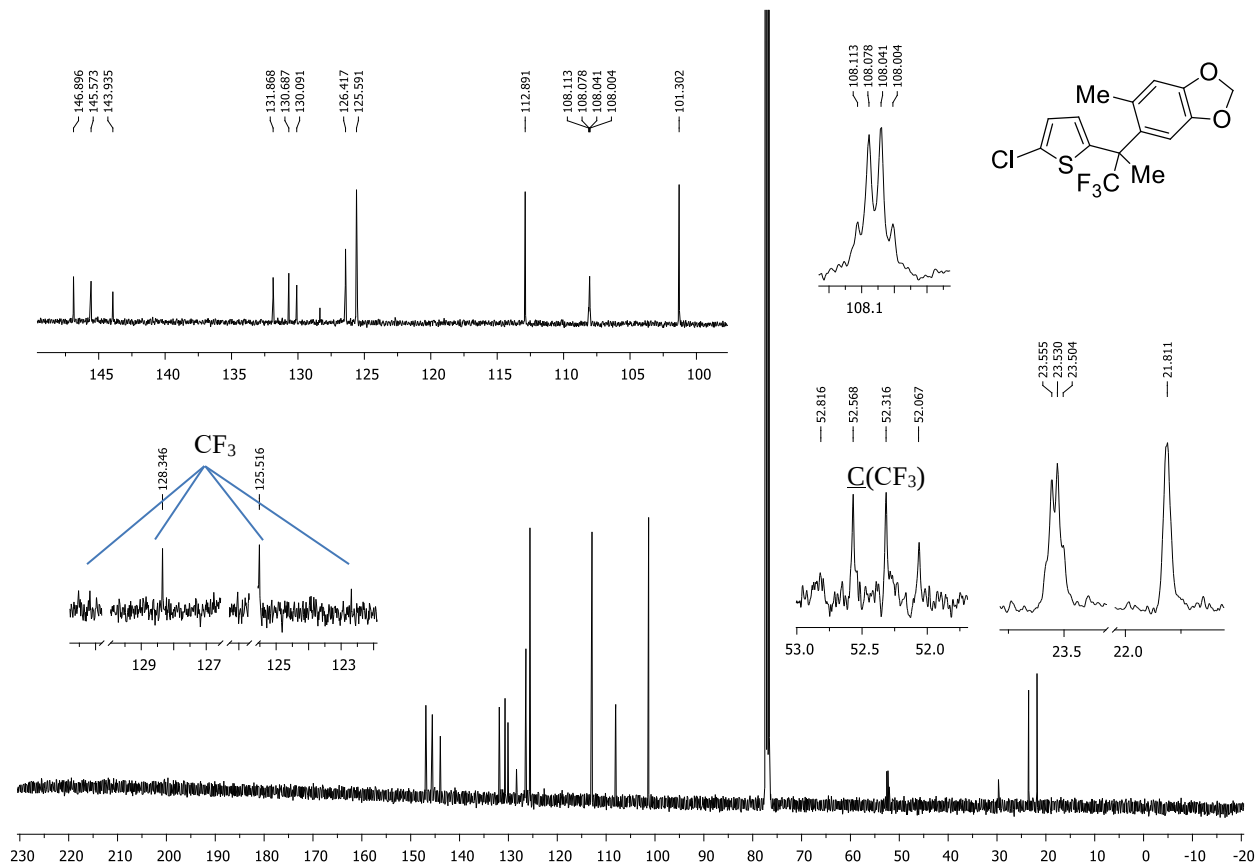


Fig. S121. ¹³C{¹H} NMR spectrum of the compound **2fd** (CDCl₃, 101 MHz).

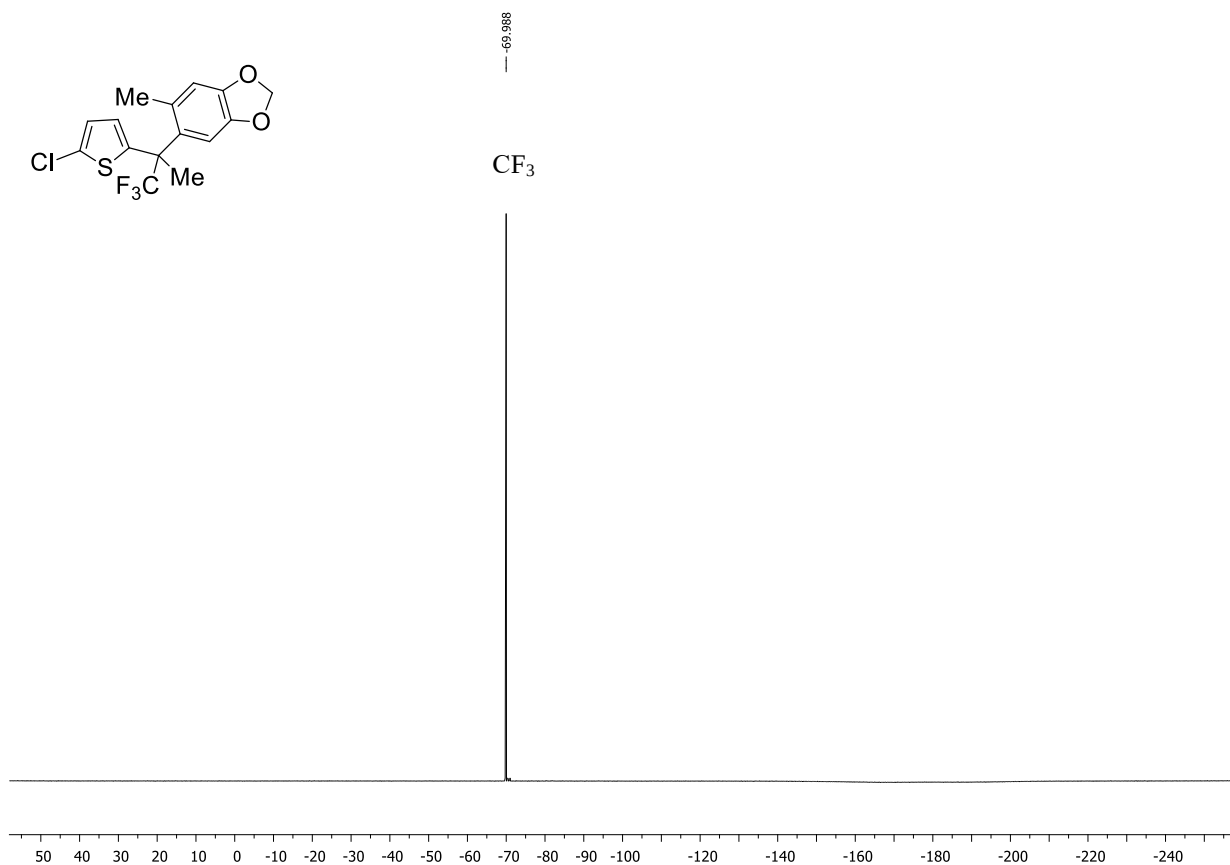


Fig. S122. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2fd** (CDCl₃, 376 MHz).

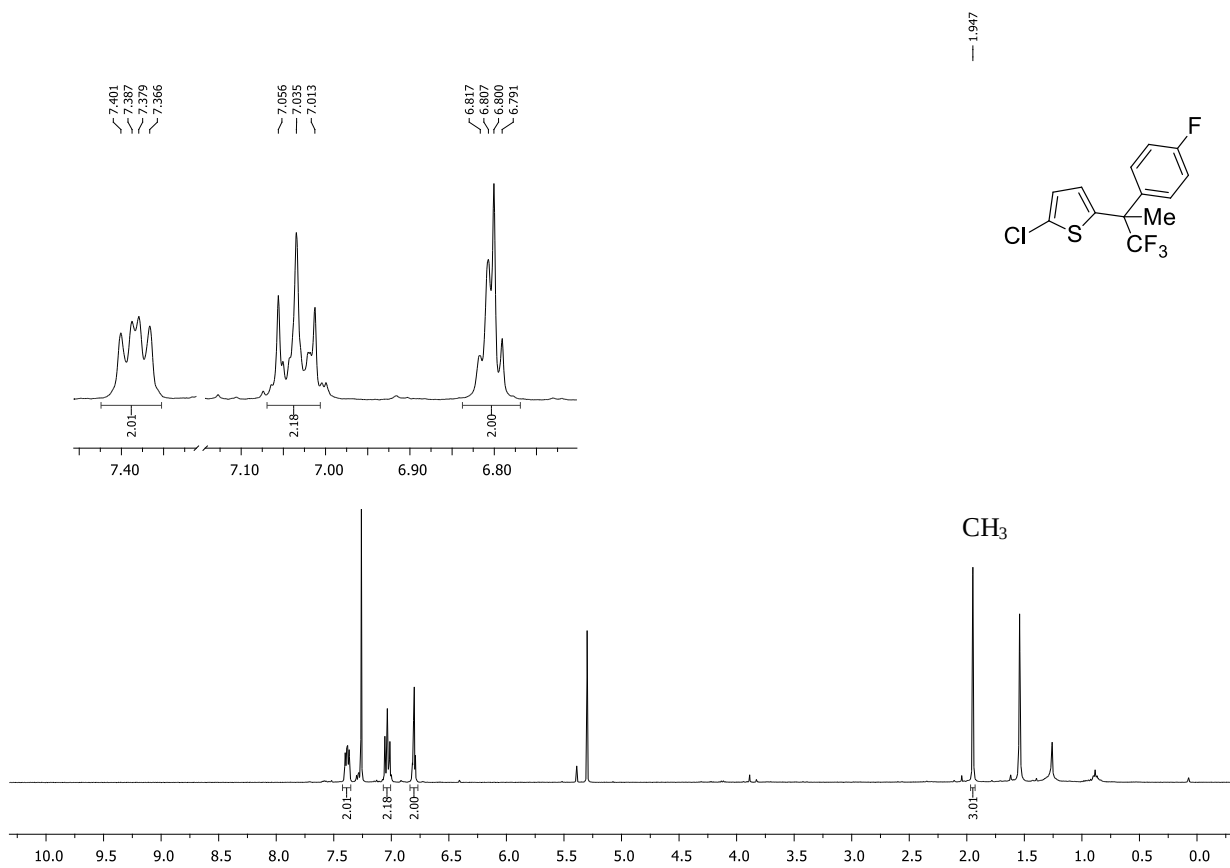


Fig. S123. ^1H NMR spectrum of the compound **2fe** (CDCl₃, 400 MHz).

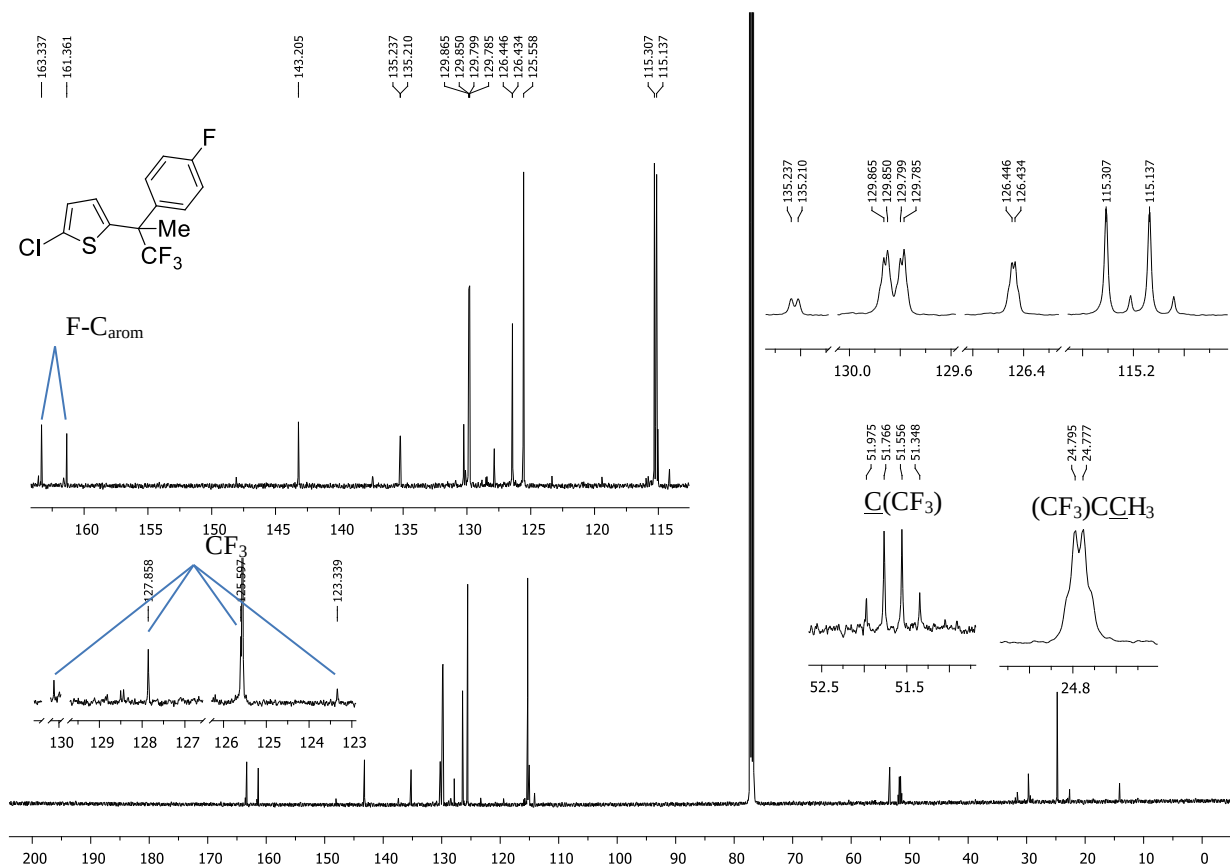


Fig. S124. ¹³C{¹H} NMR spectrum of the compound **2fe** (CDCl₃, 101 MHz).

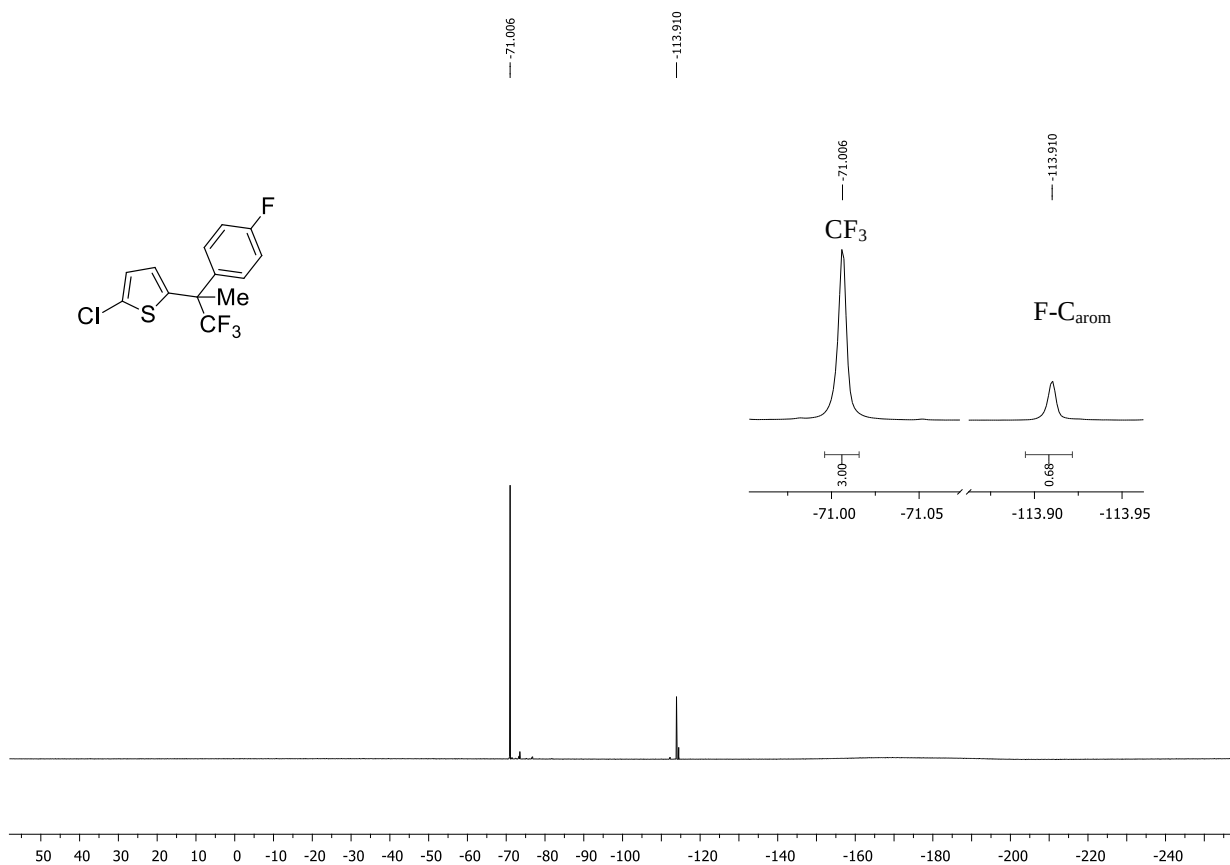


Fig. S125. ¹⁹F{¹H} NMR spectrum of the compound **2fe** (CDCl₃, 376 MHz).

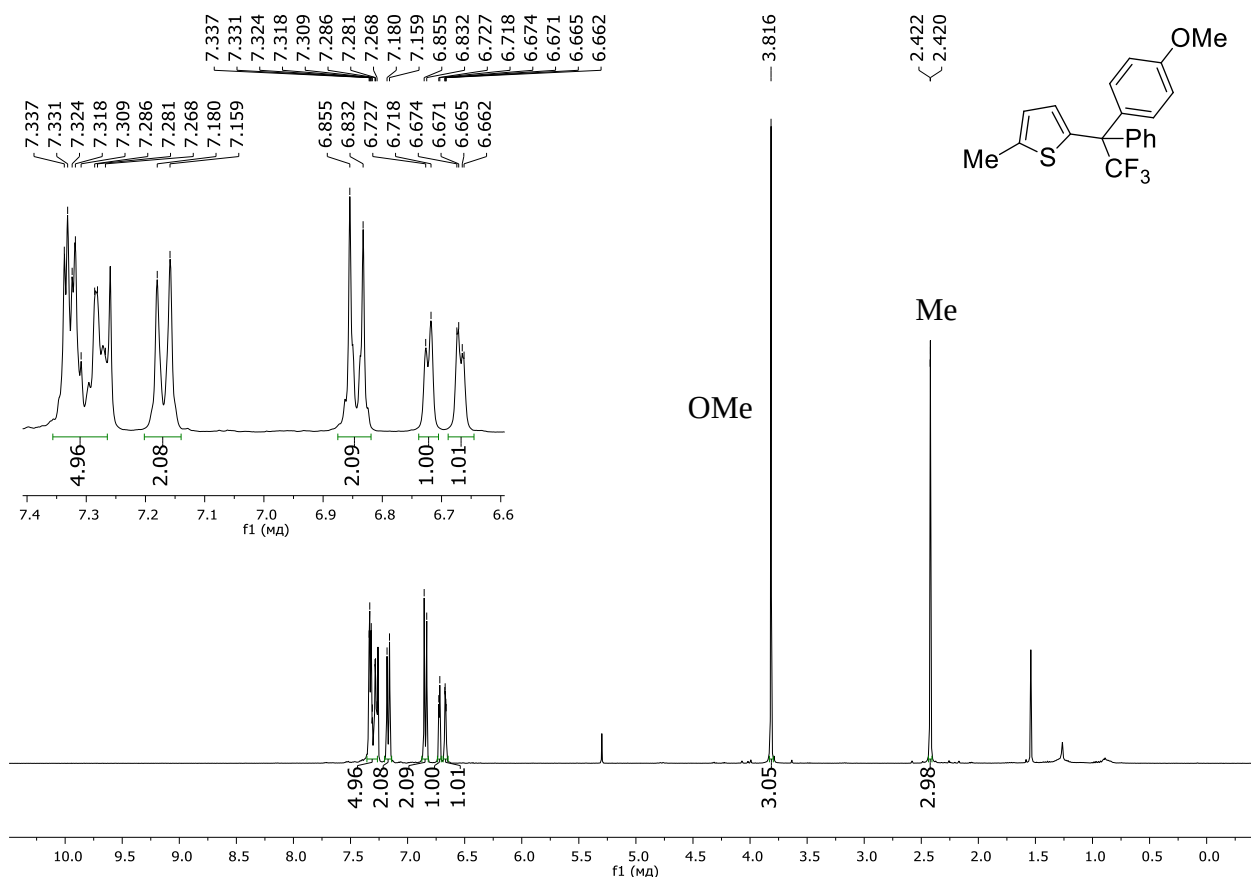


Fig. S126. ¹H NMR spectrum of the compound **2ha** (CDCl₃, 400 MHz).

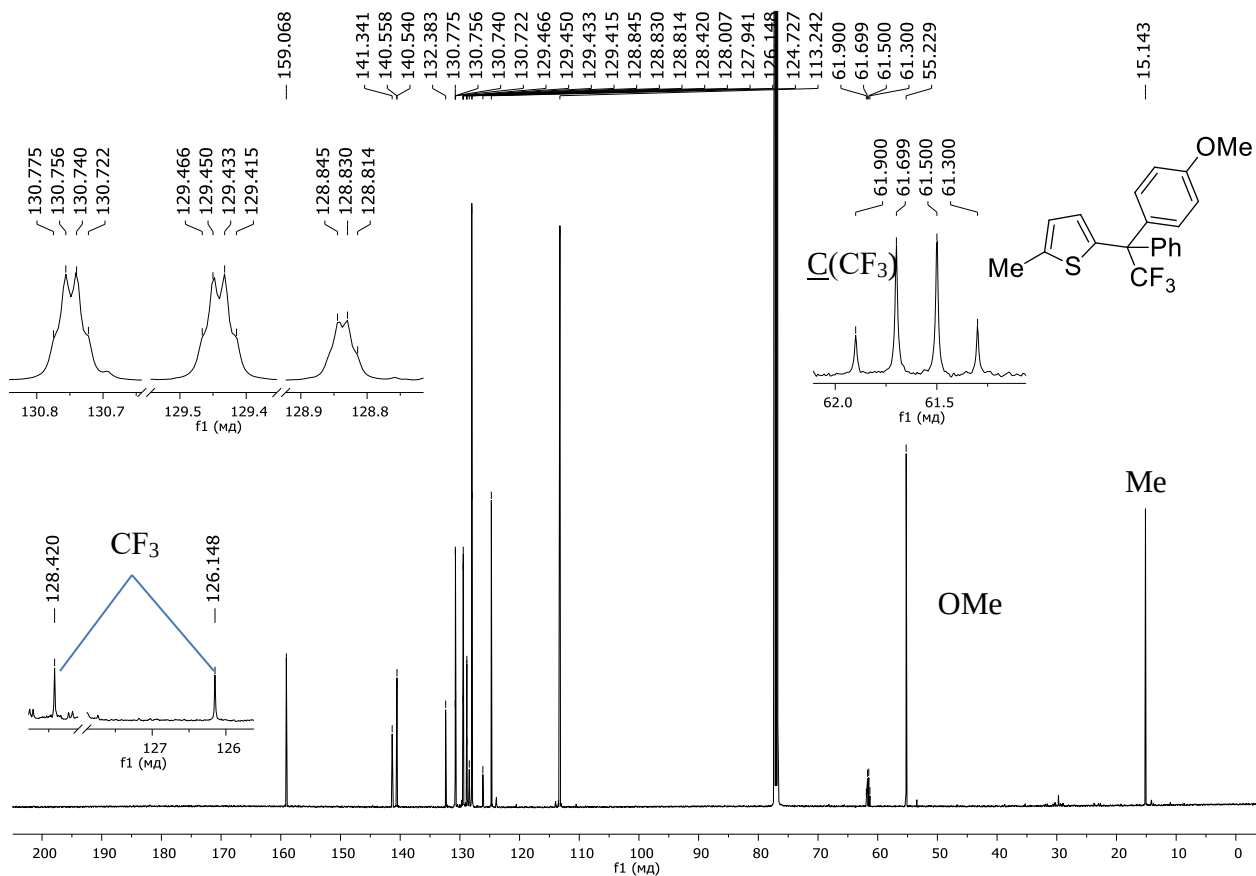
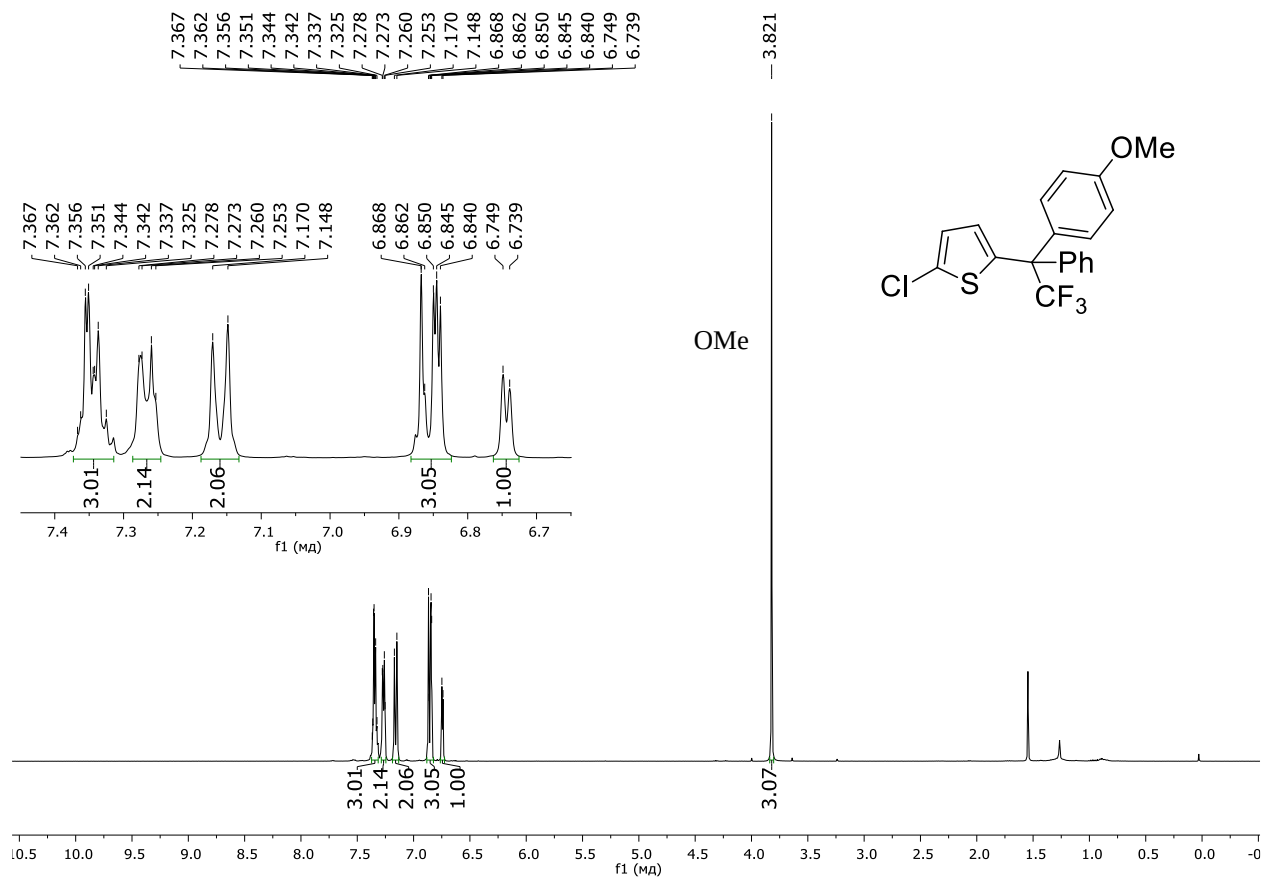
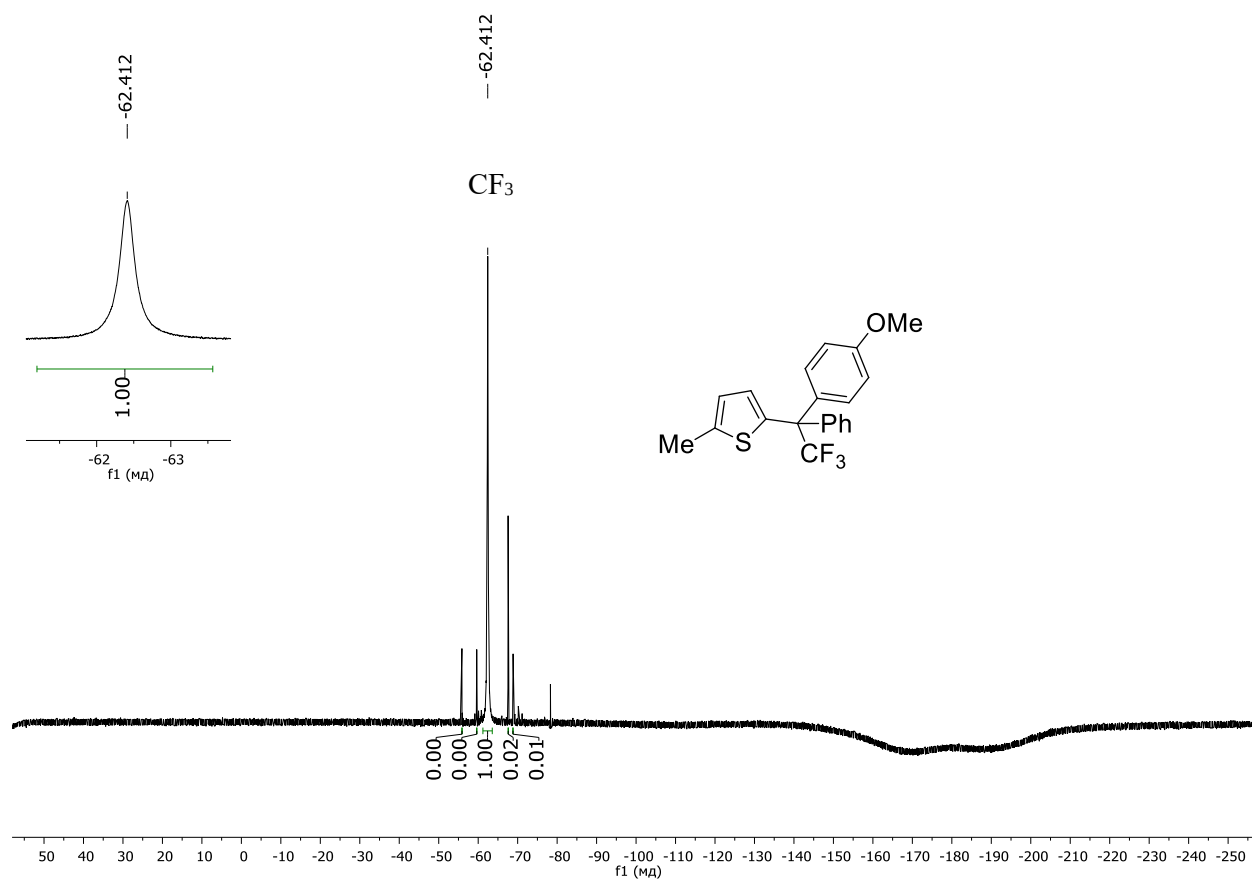


Fig. S127. ¹³C{¹H} NMR spectrum of the compound **2ha** (CDCl₃, 101 MHz).



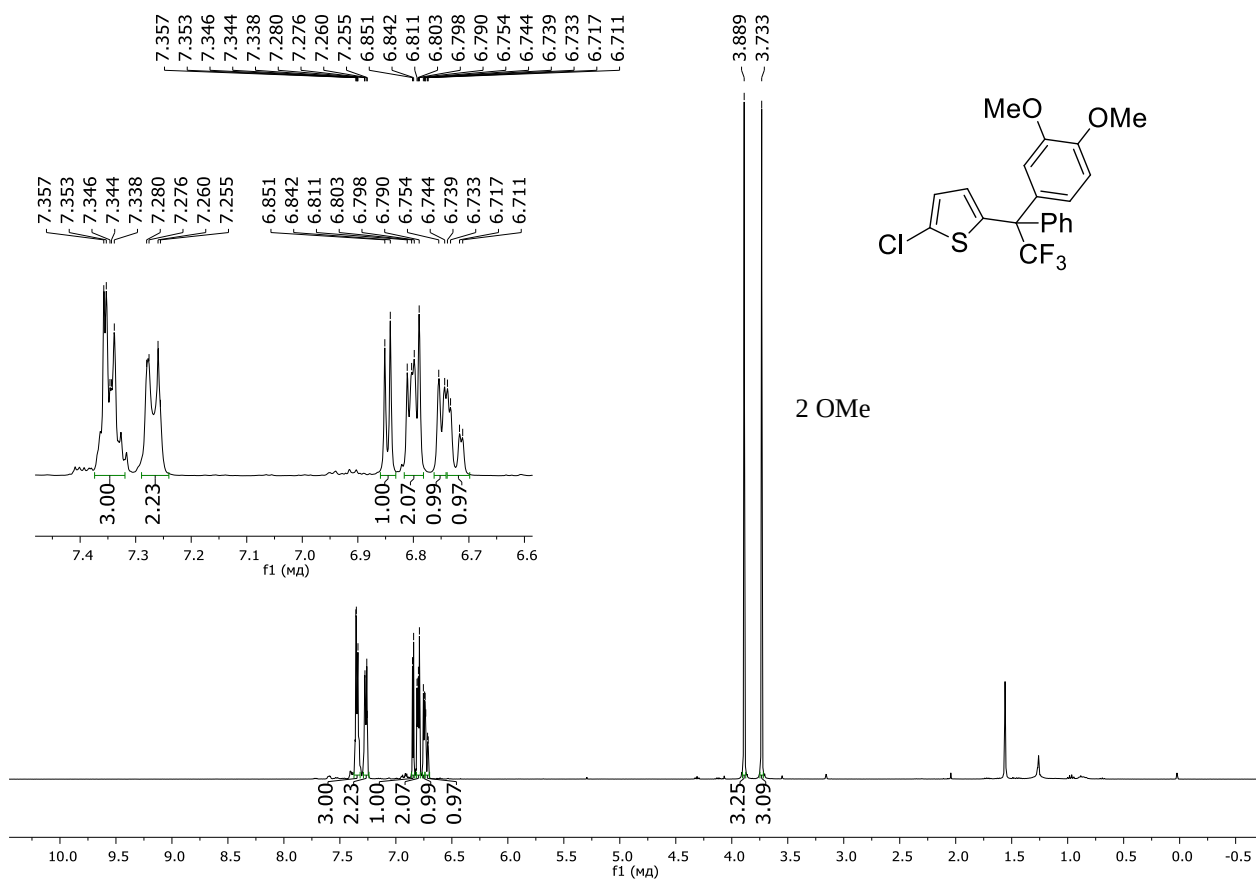


Fig. S132. ¹H NMR spectrum of the compound **2ib** (CDCl₃, 400 MHz).

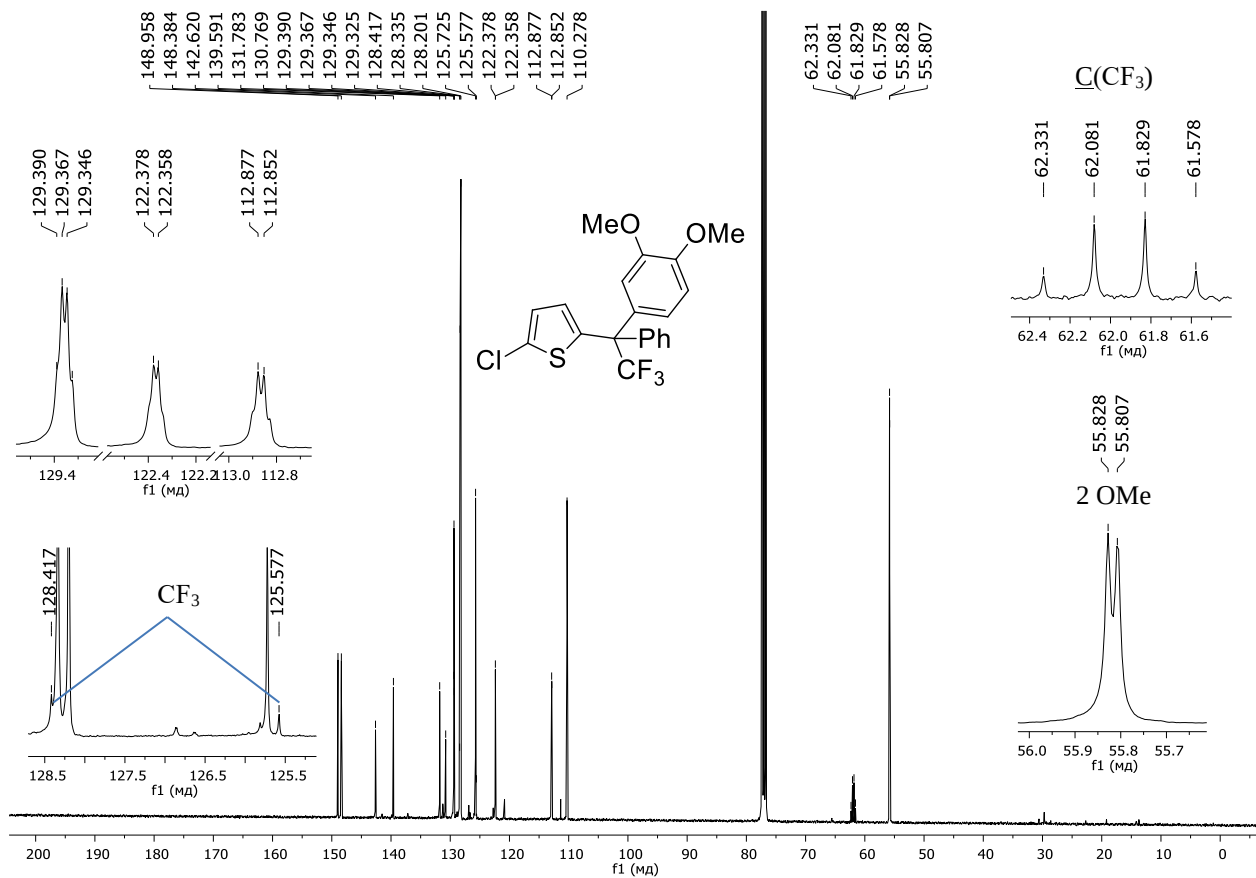


Fig. S133. ¹³C{¹H} NMR spectrum of the compound **2ib** (CDCl₃, 101 MHz).

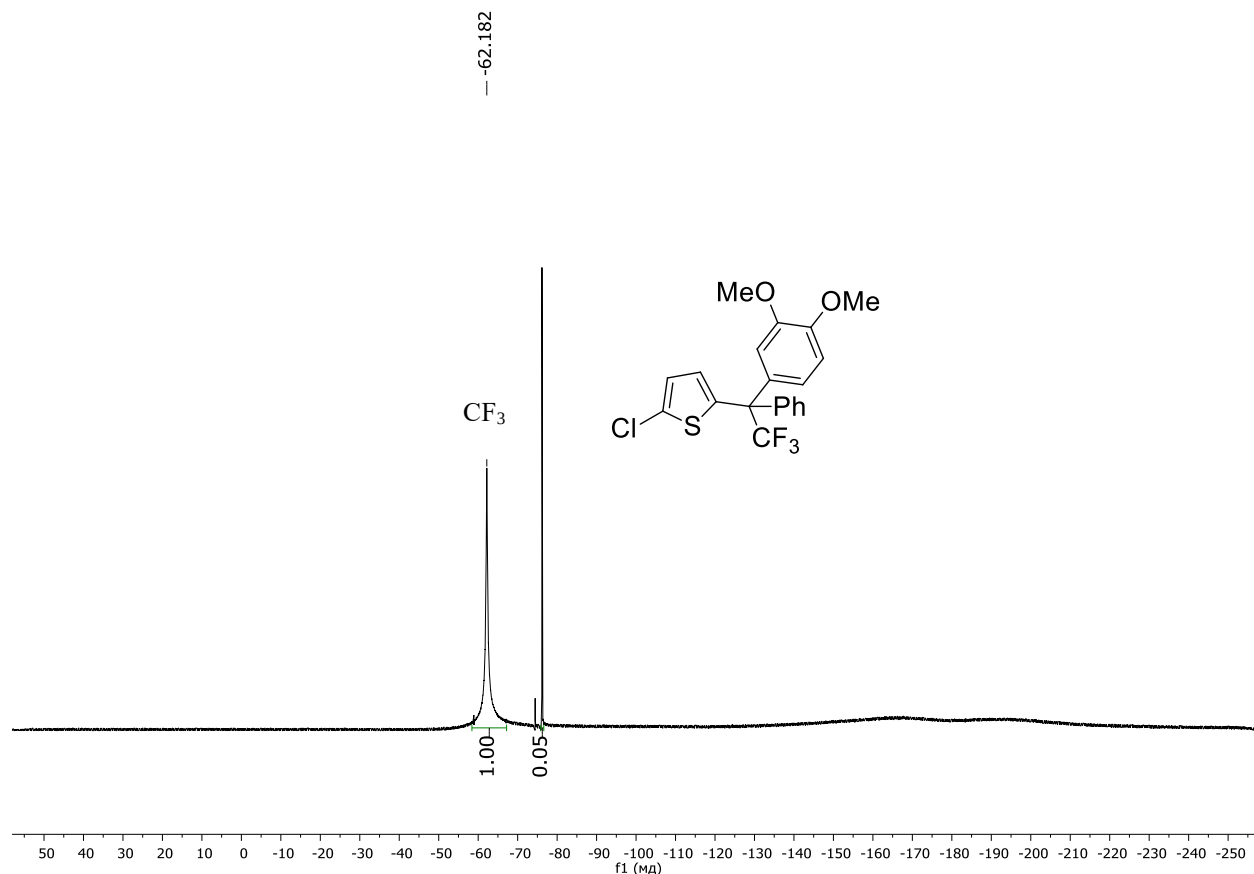


Fig. S134. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2ib** (CDCl_3 , 376 MHz).

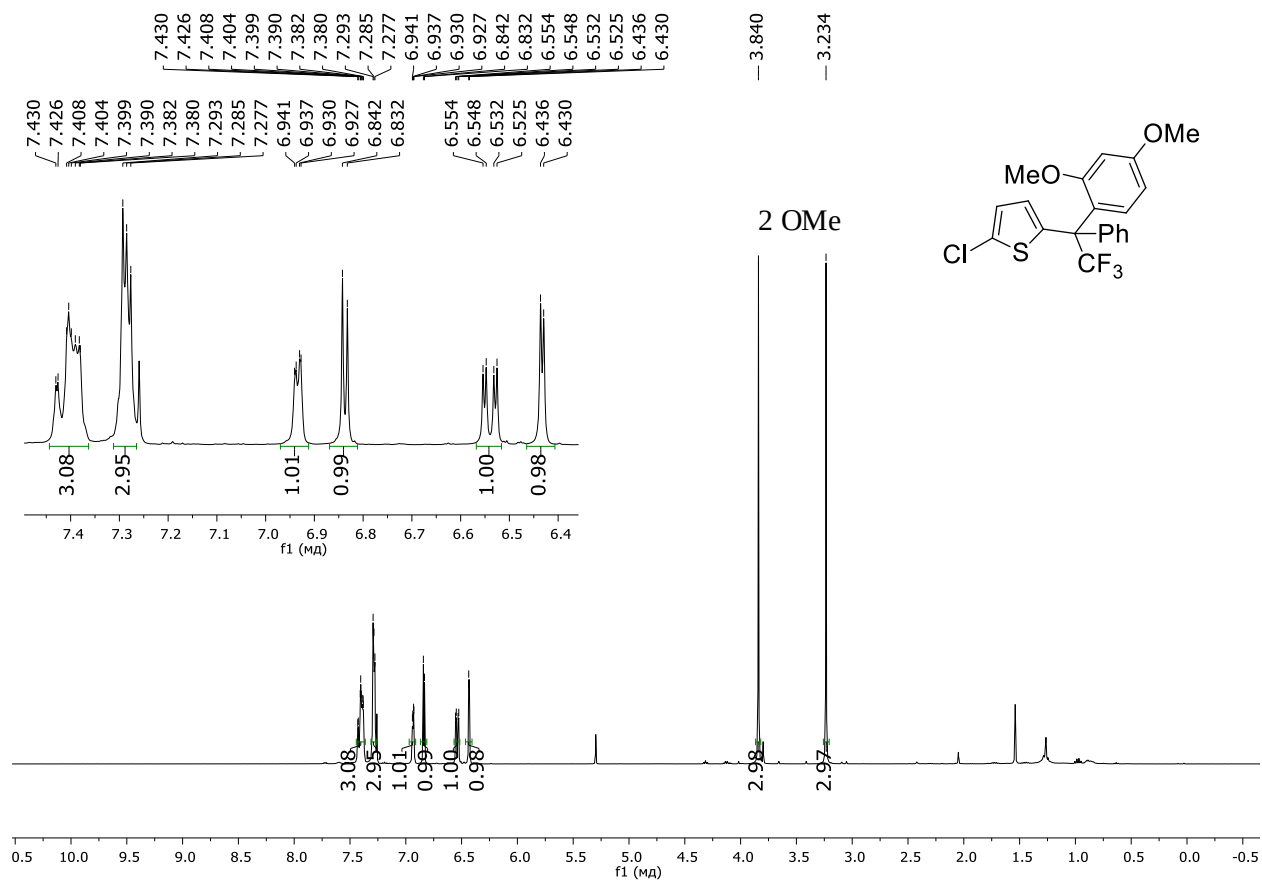


Fig. S135. ^1H NMR spectrum of the compound **2ic** (CDCl_3 , 400 MHz).

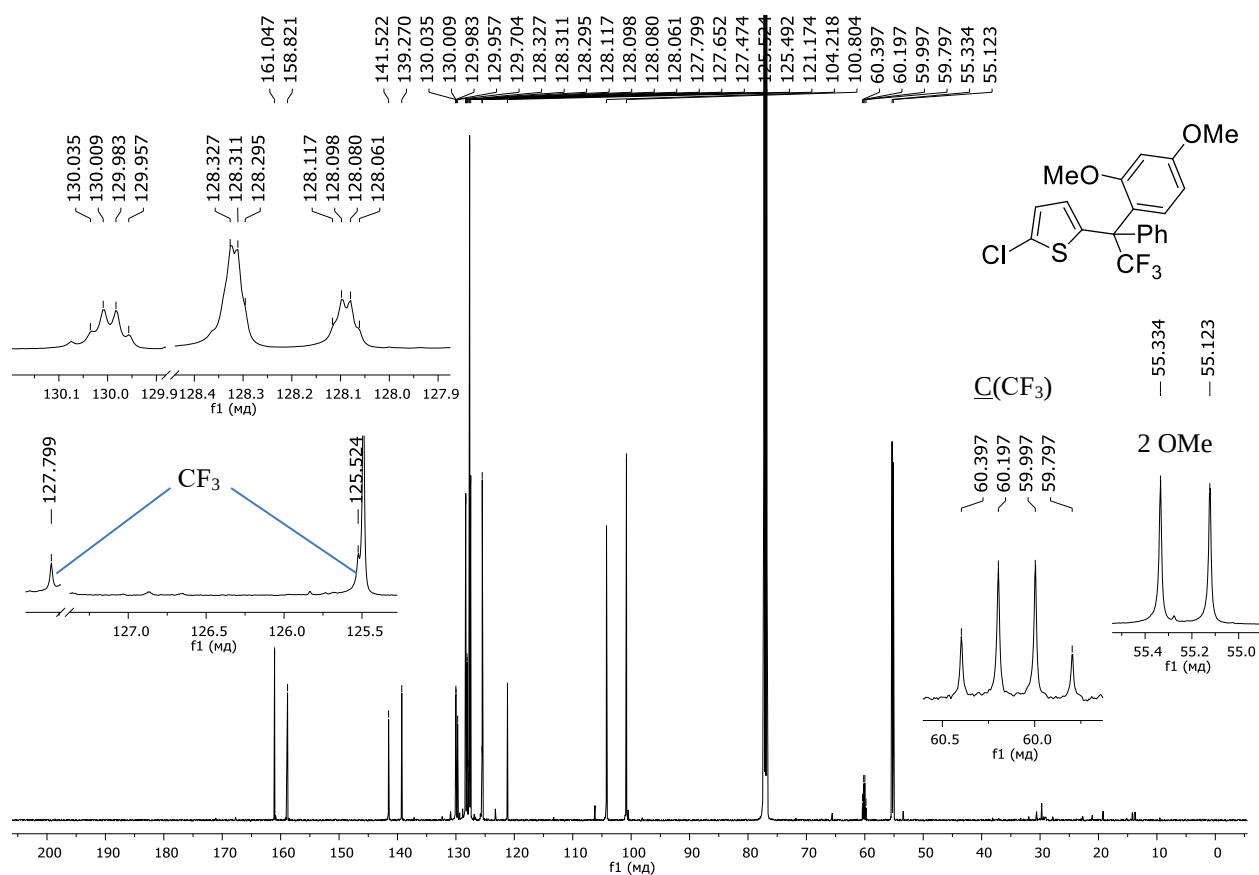


Fig. S136. ¹³C{¹H} NMR spectrum of the compound **2ic** (CDCl₃, 101 MHz).

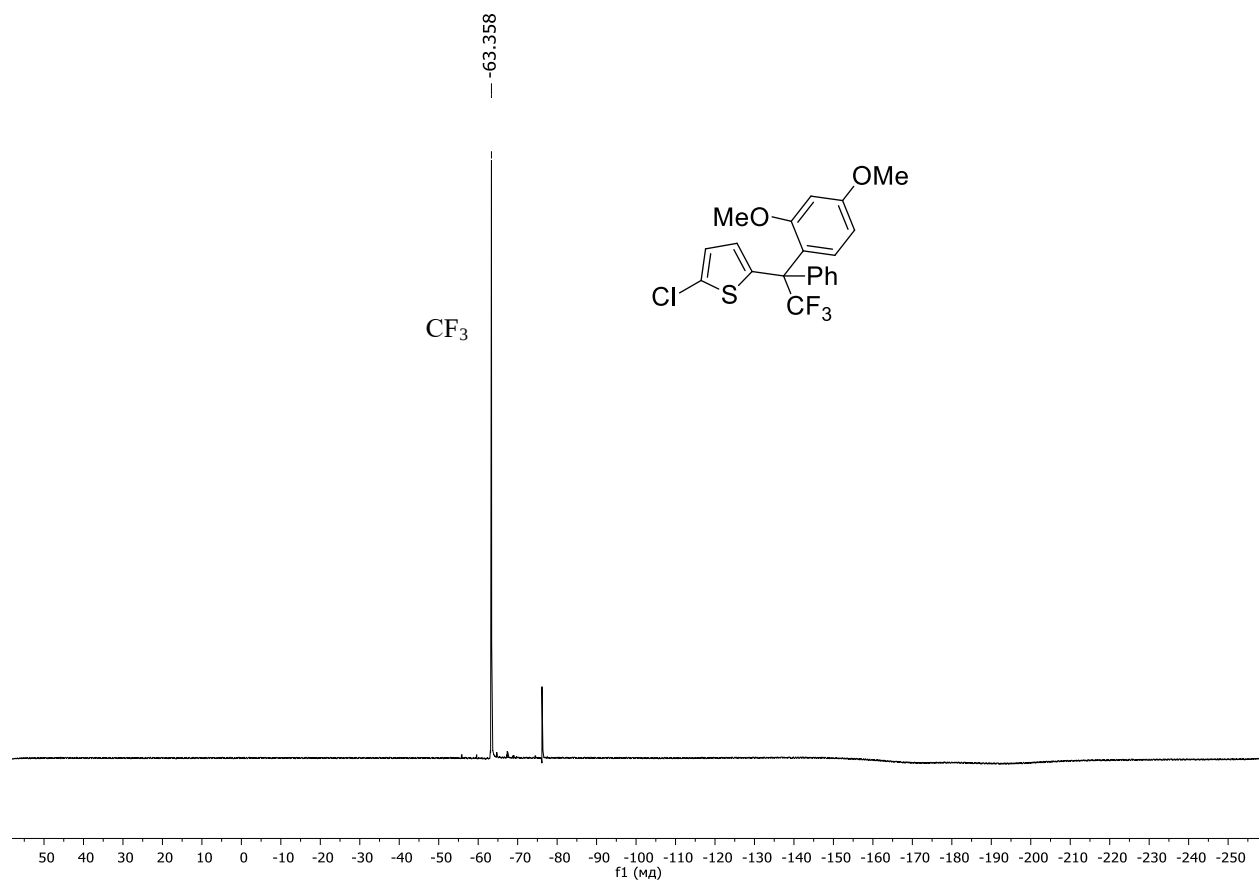


Fig. S137. ¹⁹F{¹H} NMR spectrum of the compound **2ic** (CDCl₃, 376 MHz).

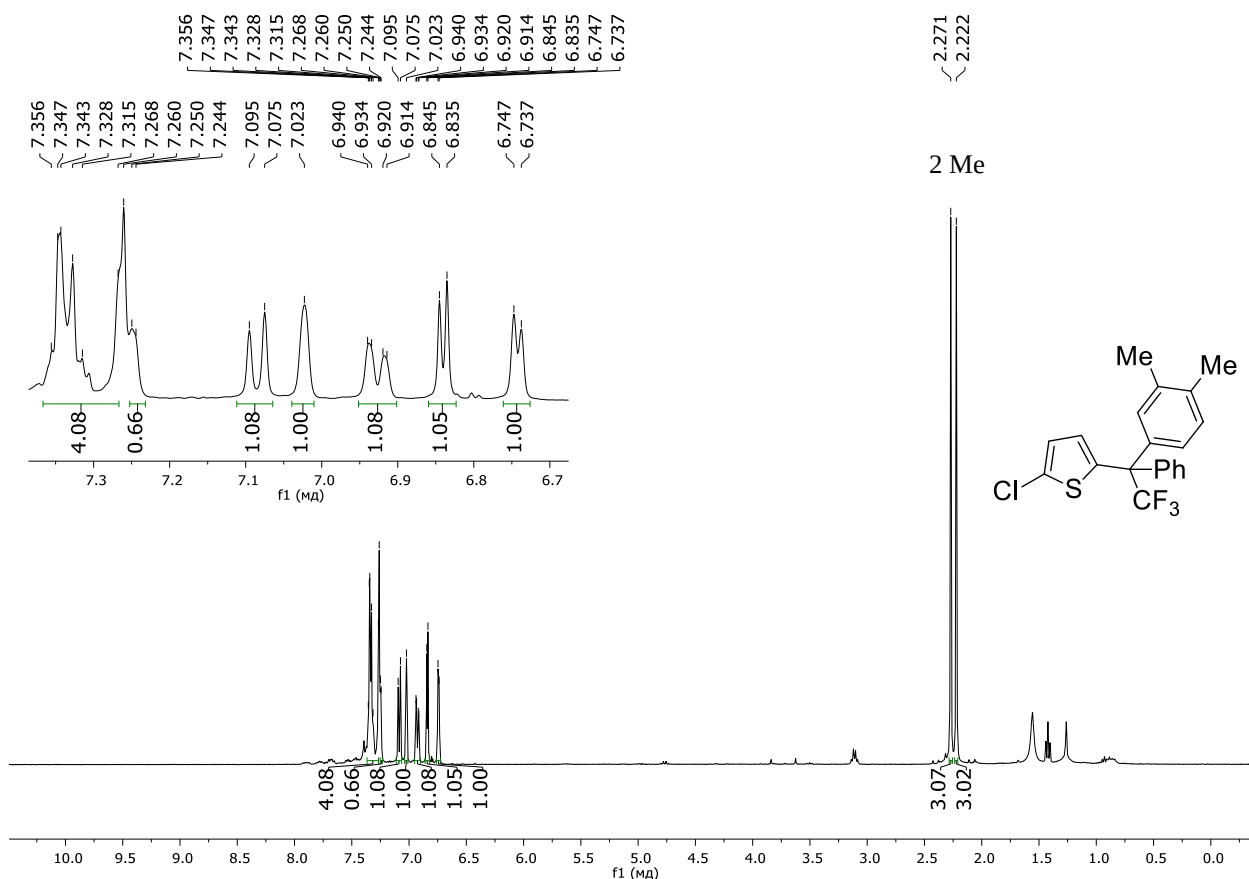


Fig. S138. ¹H NMR spectrum of the compound **2id** (CDCl₃, 400 MHz).

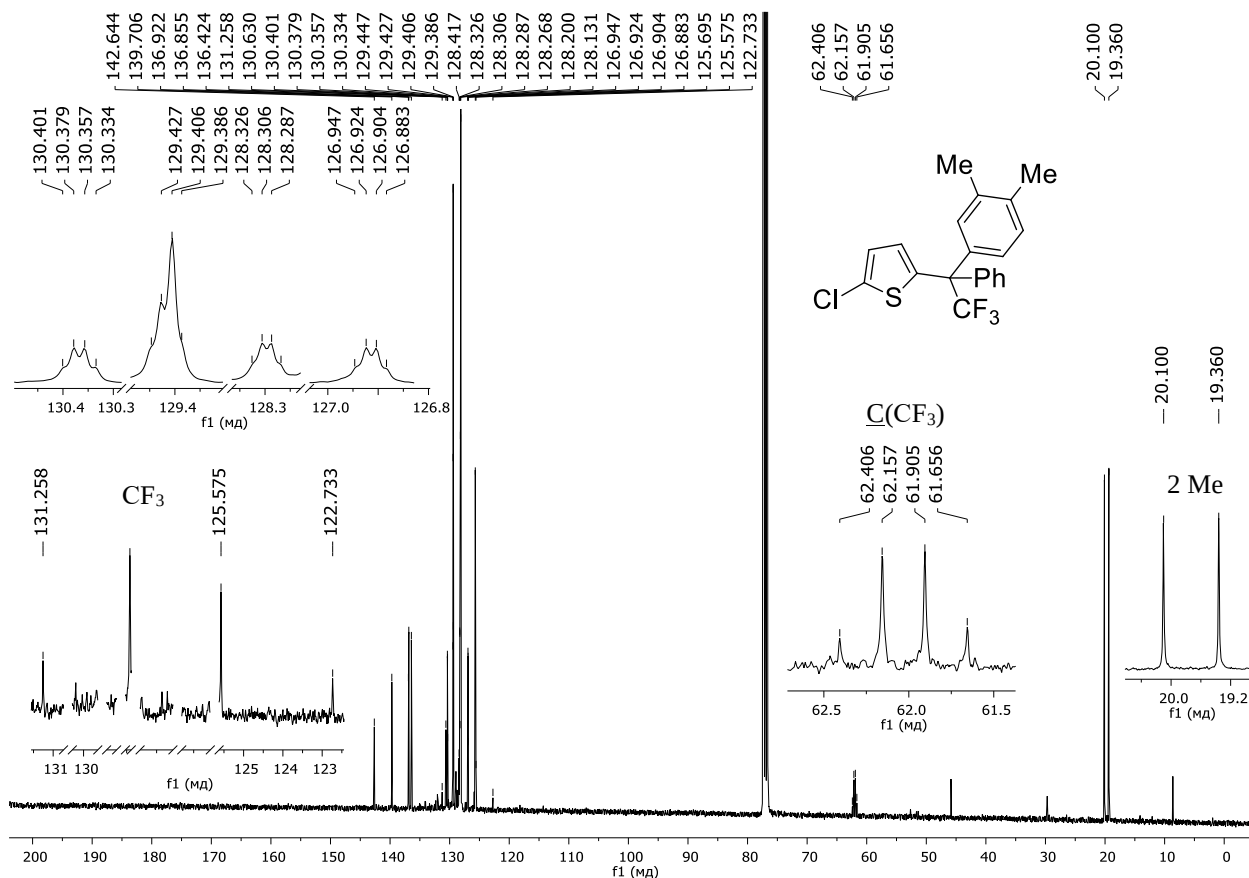


Fig. S139. ¹³C{¹H} NMR spectrum of the compound **2id** (CDCl₃, 101 MHz).

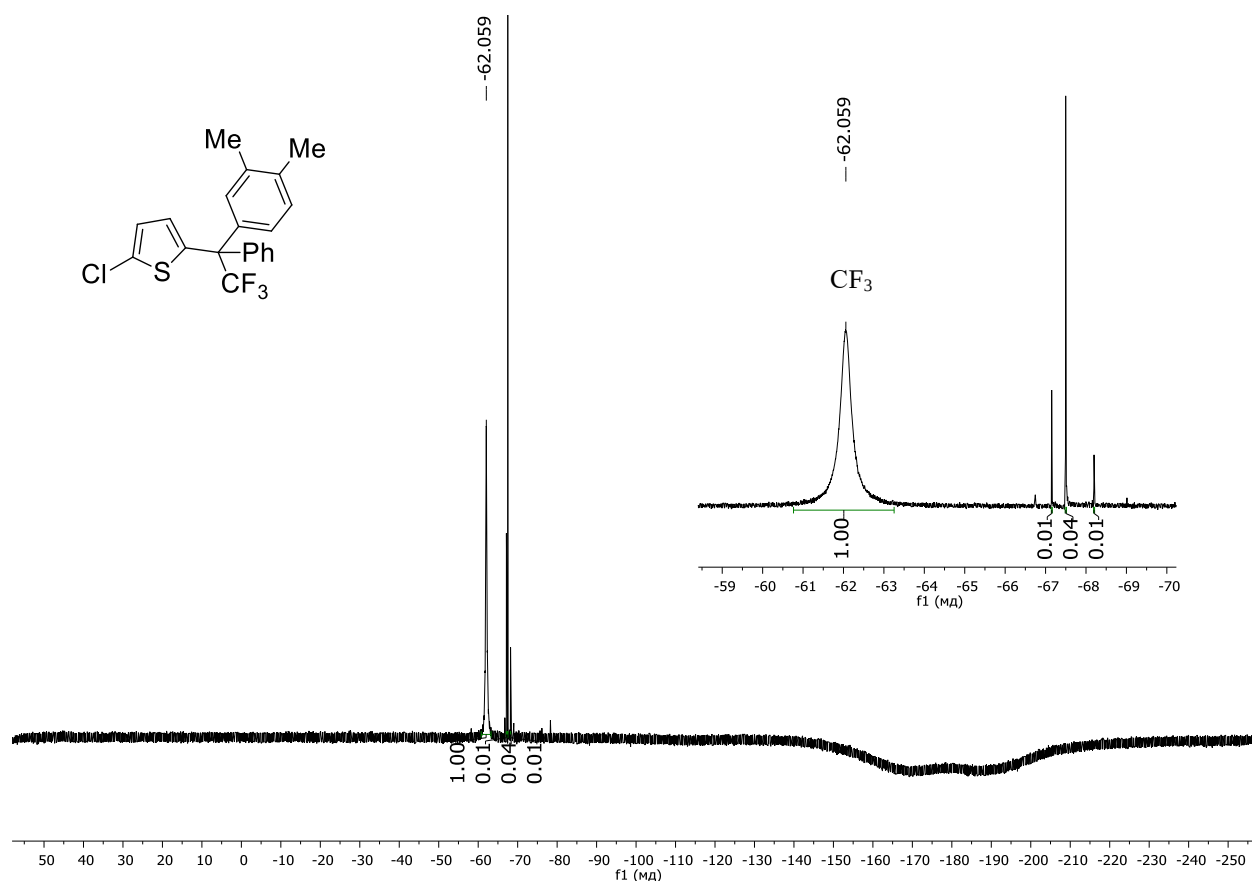


Fig. S140. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2id** (CDCl_3 , 376 MHz).

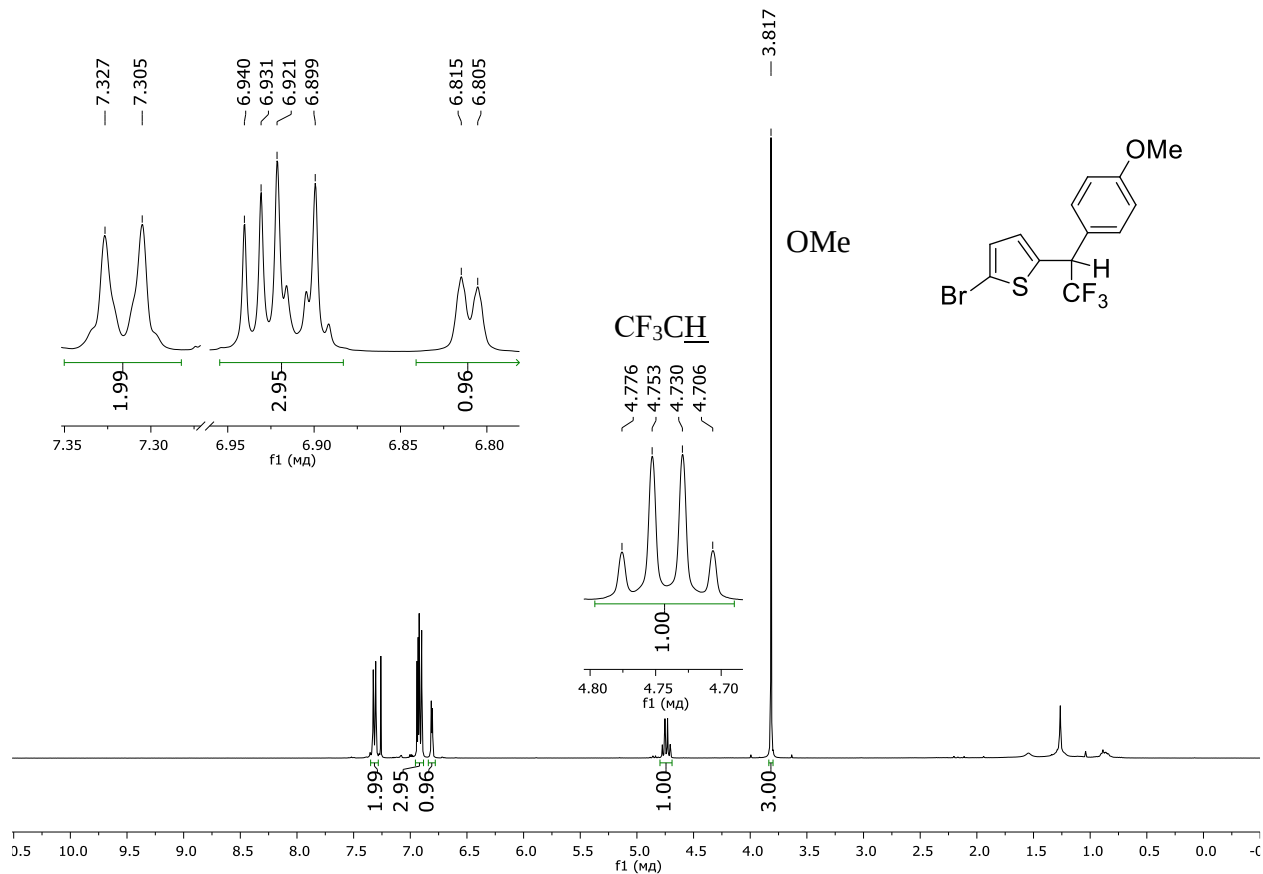


Fig. S141. ^1H NMR spectrum of the compound **2ja** (CDCl_3 , 400 MHz).

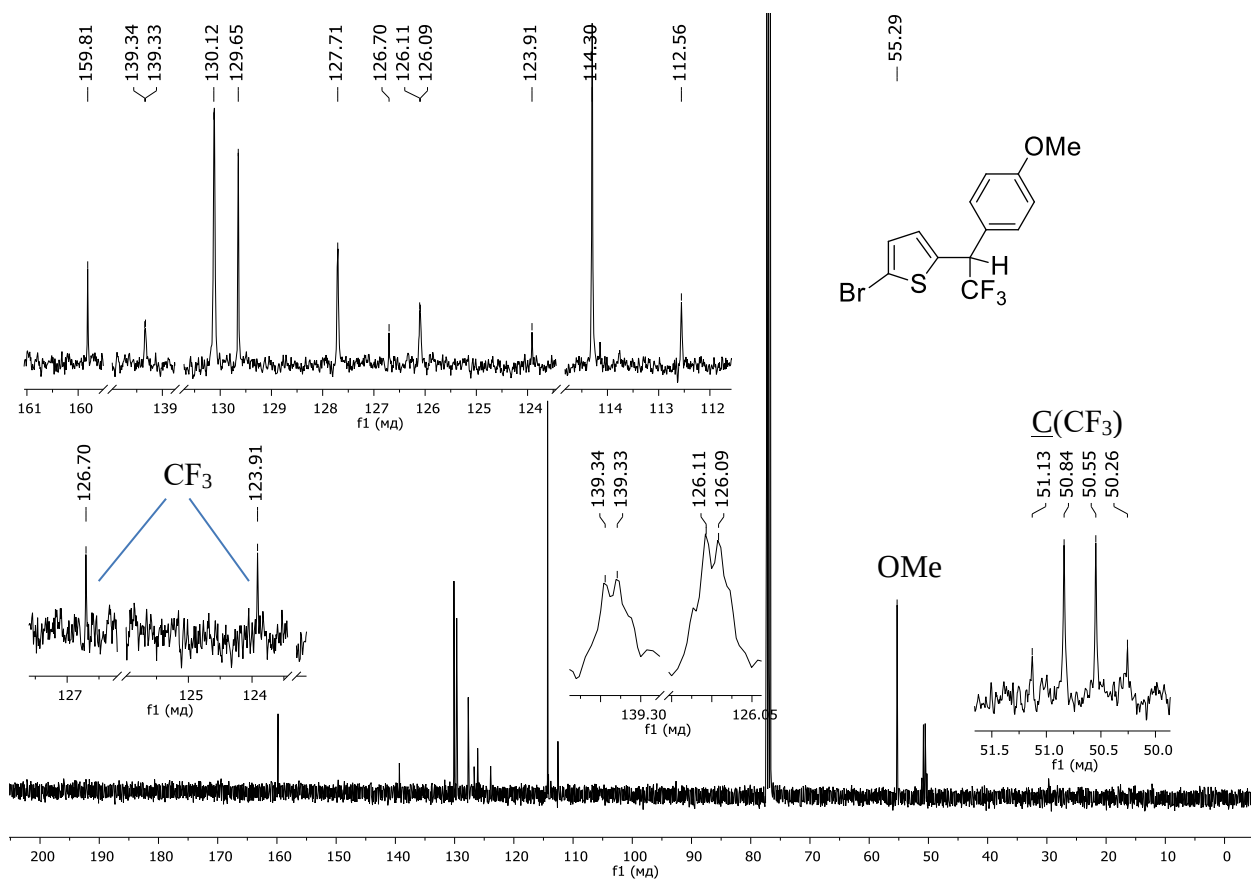


Fig. S142. ¹³C{¹H} NMR spectrum of the compound **2ja** (CDCl₃, 101 MHz).

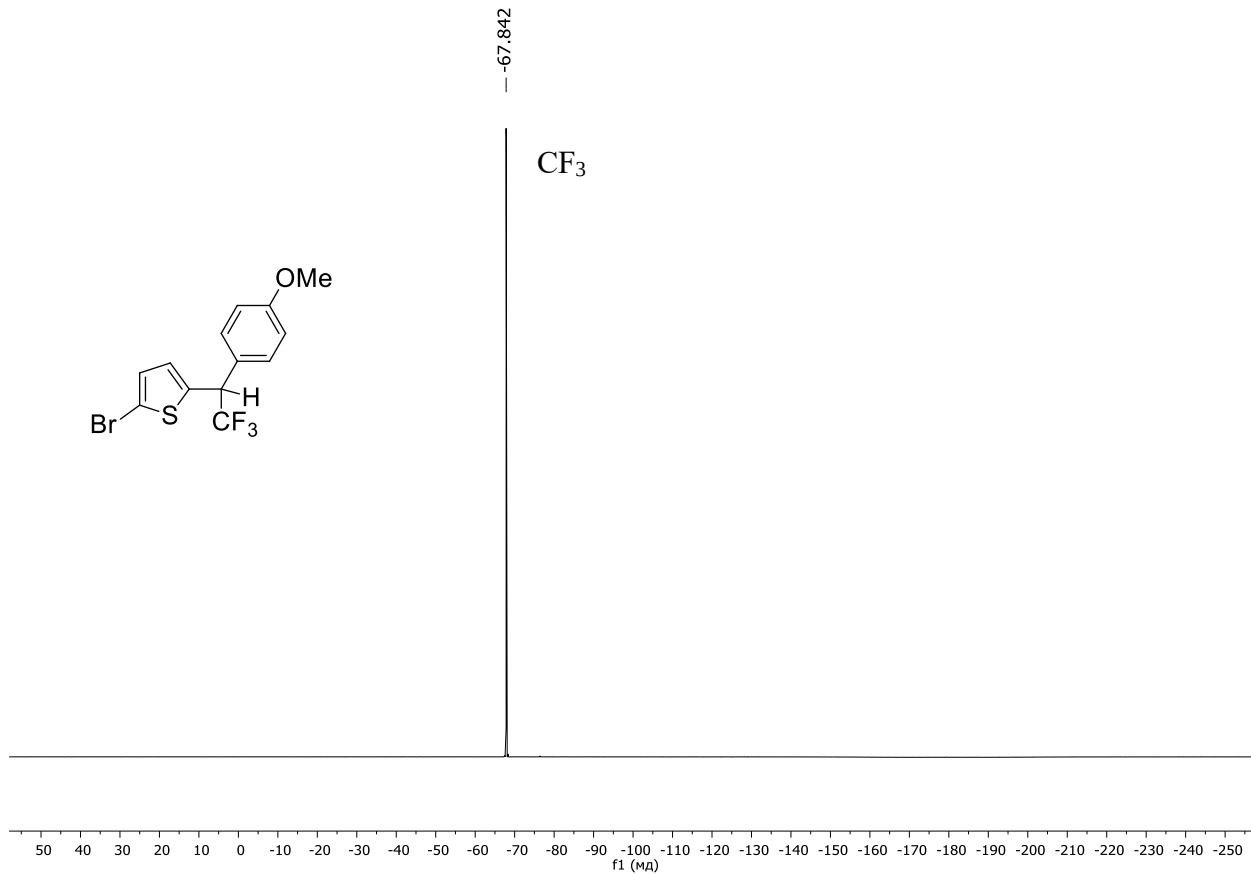


Fig. S143. ¹⁹F{¹H} NMR spectrum of the compound **2ja** (CDCl₃, 376 MHz).

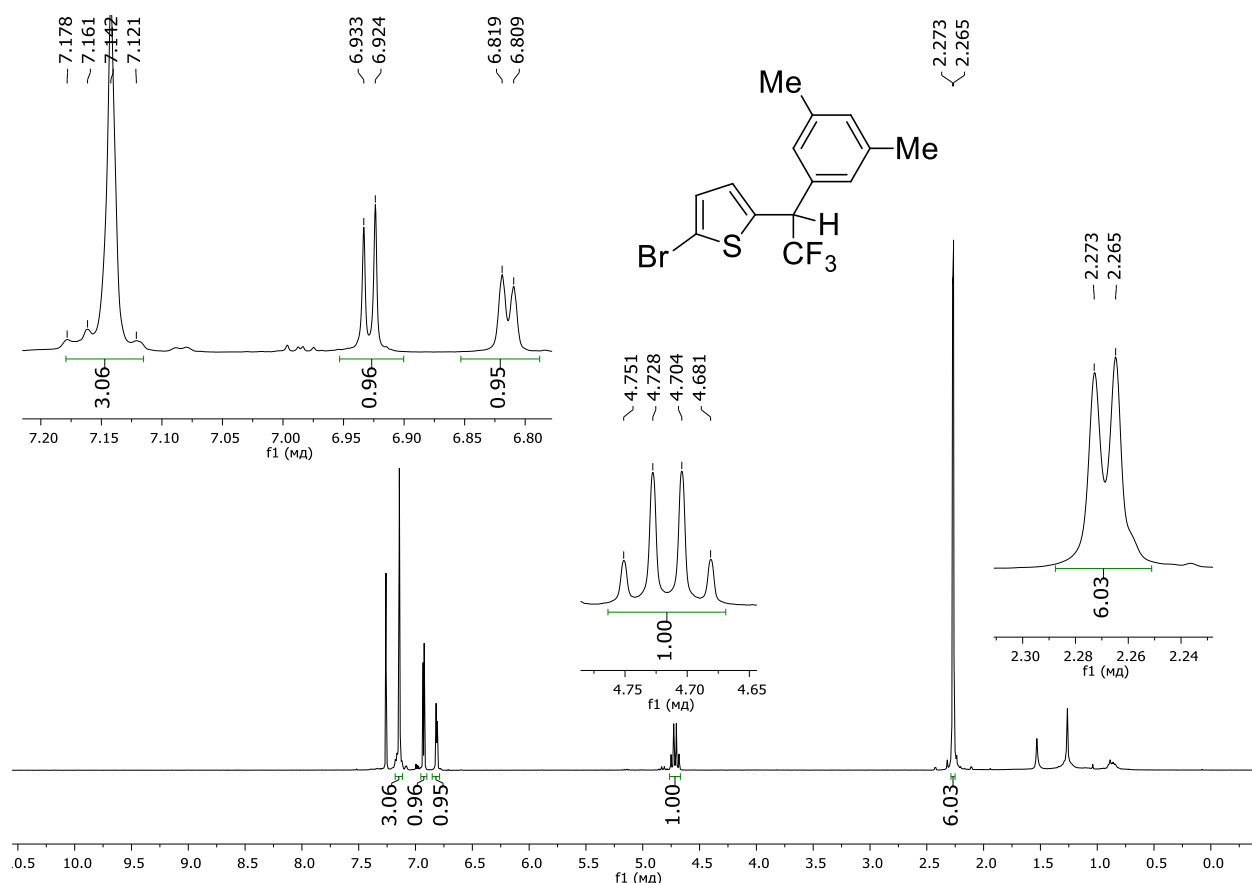


Fig. S144. ¹H NMR spectrum of the compound **2jb** (CDCl₃, 400 MHz).

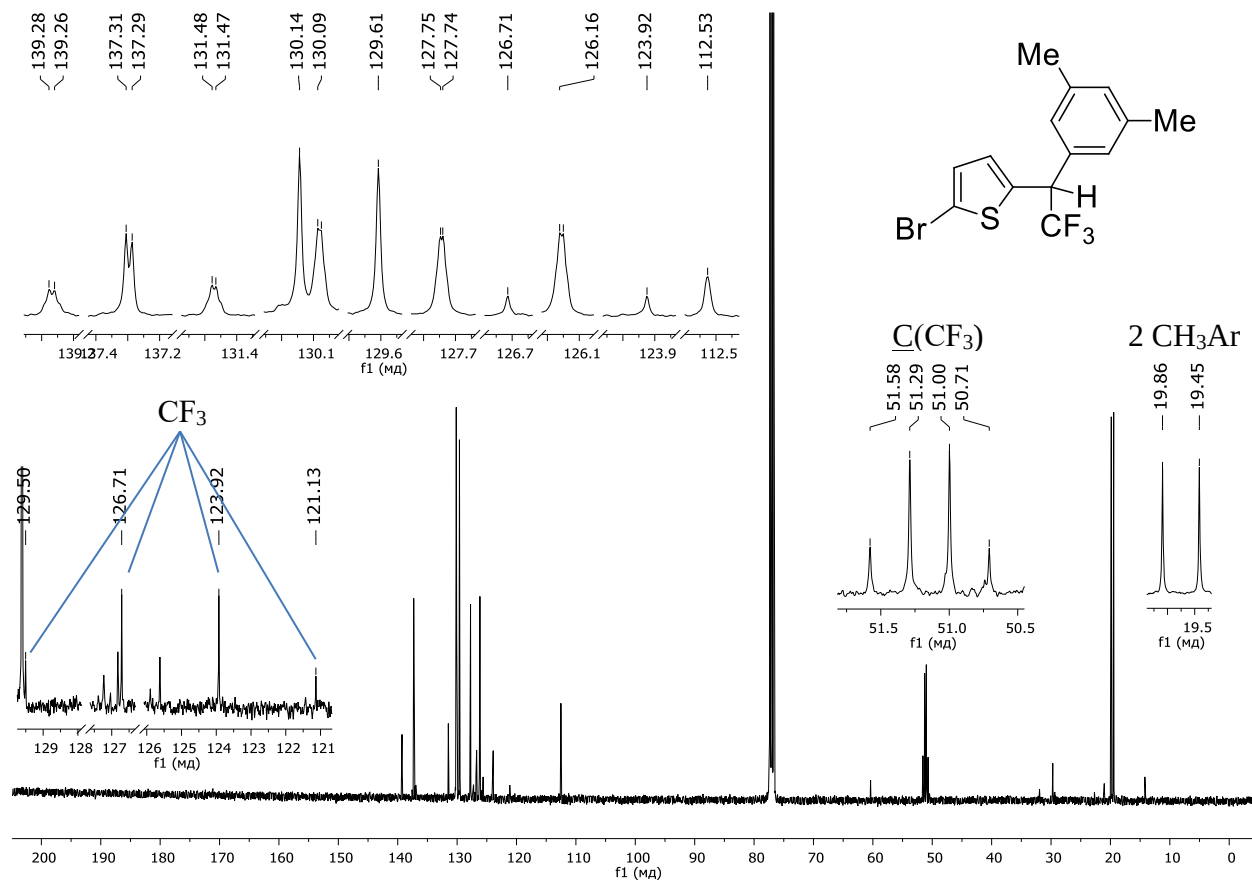


Fig. S145. ¹³C{¹H} NMR spectrum of the compound **2jb** (CDCl₃, 101 MHz).

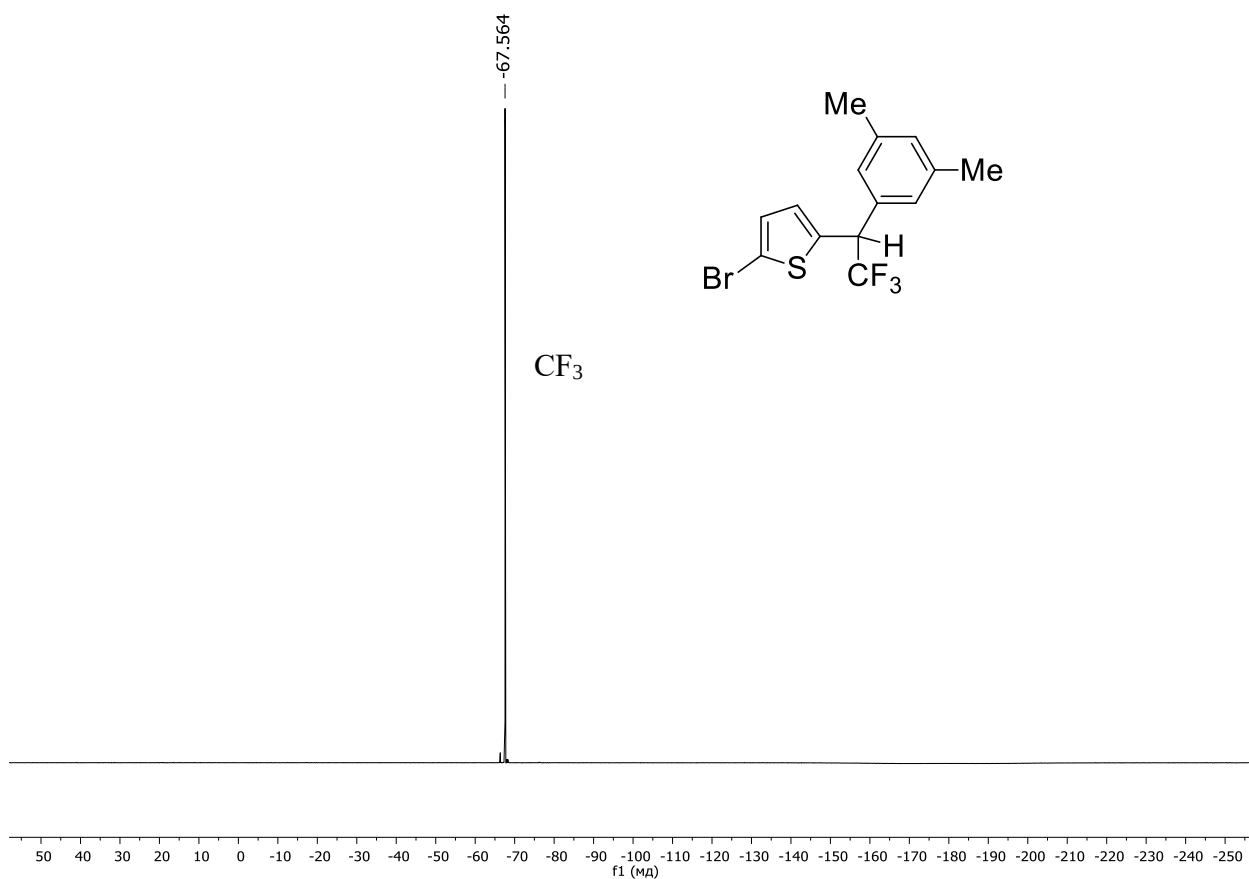


Fig. S146. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2jb** (CDCl₃, 376 MHz).

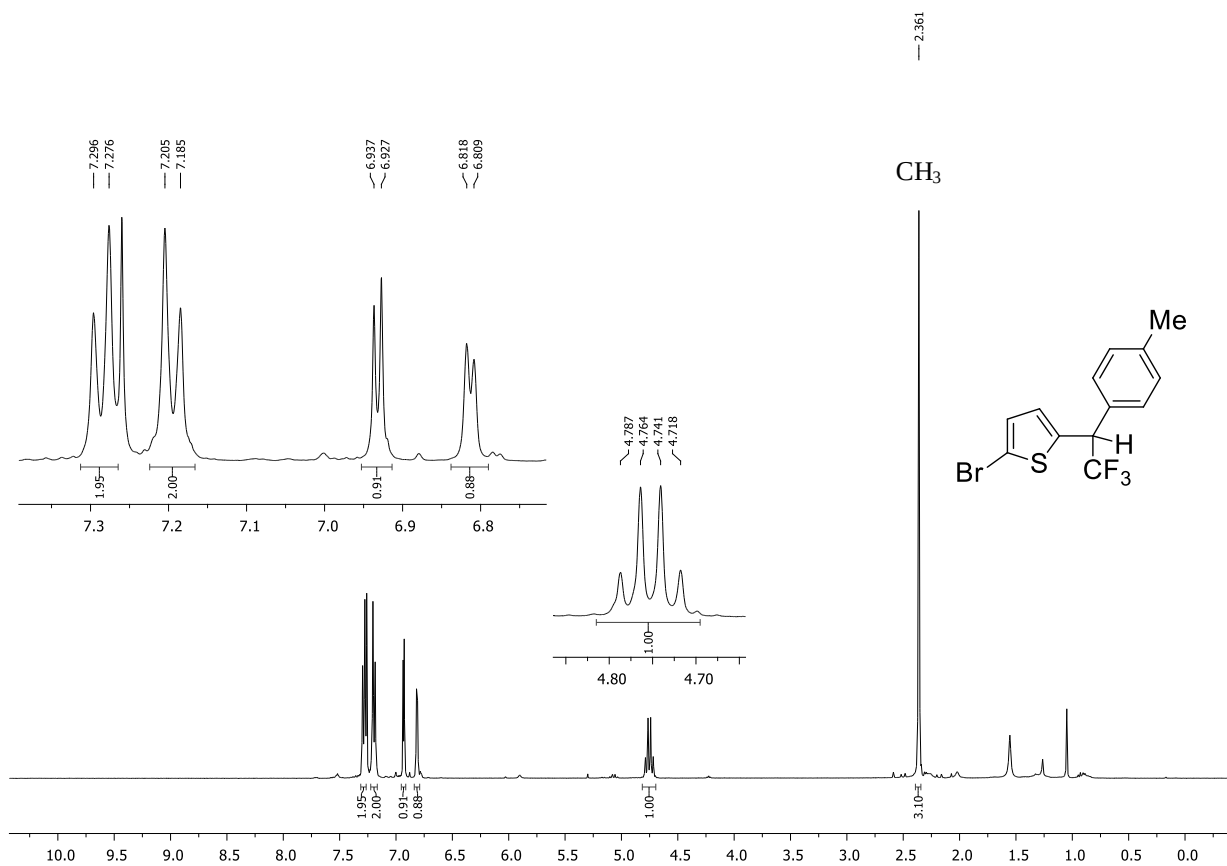


Fig. S147. ^1H NMR spectrum of the compound **2jc** (CDCl₃, 400 MHz).

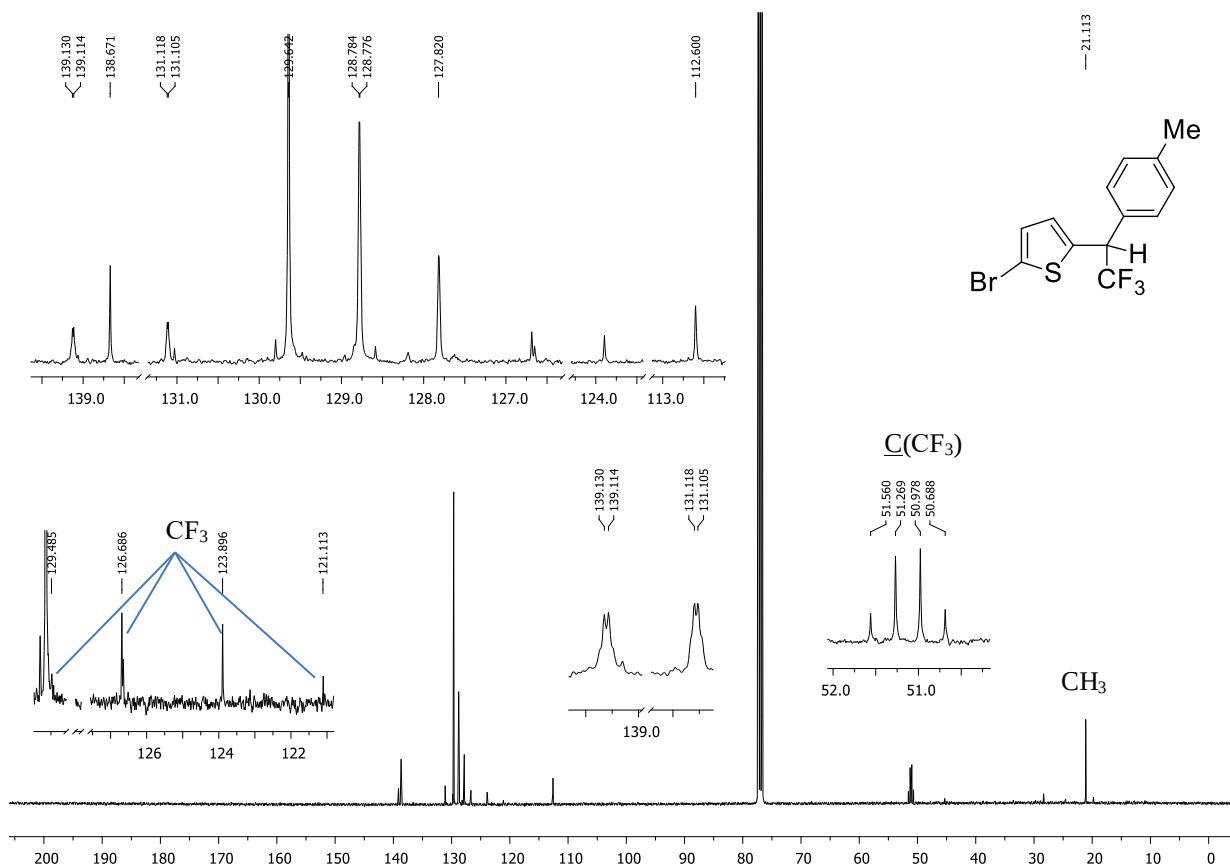


Fig. S148. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **2jc** (CDCl_3 , 101 MHz).

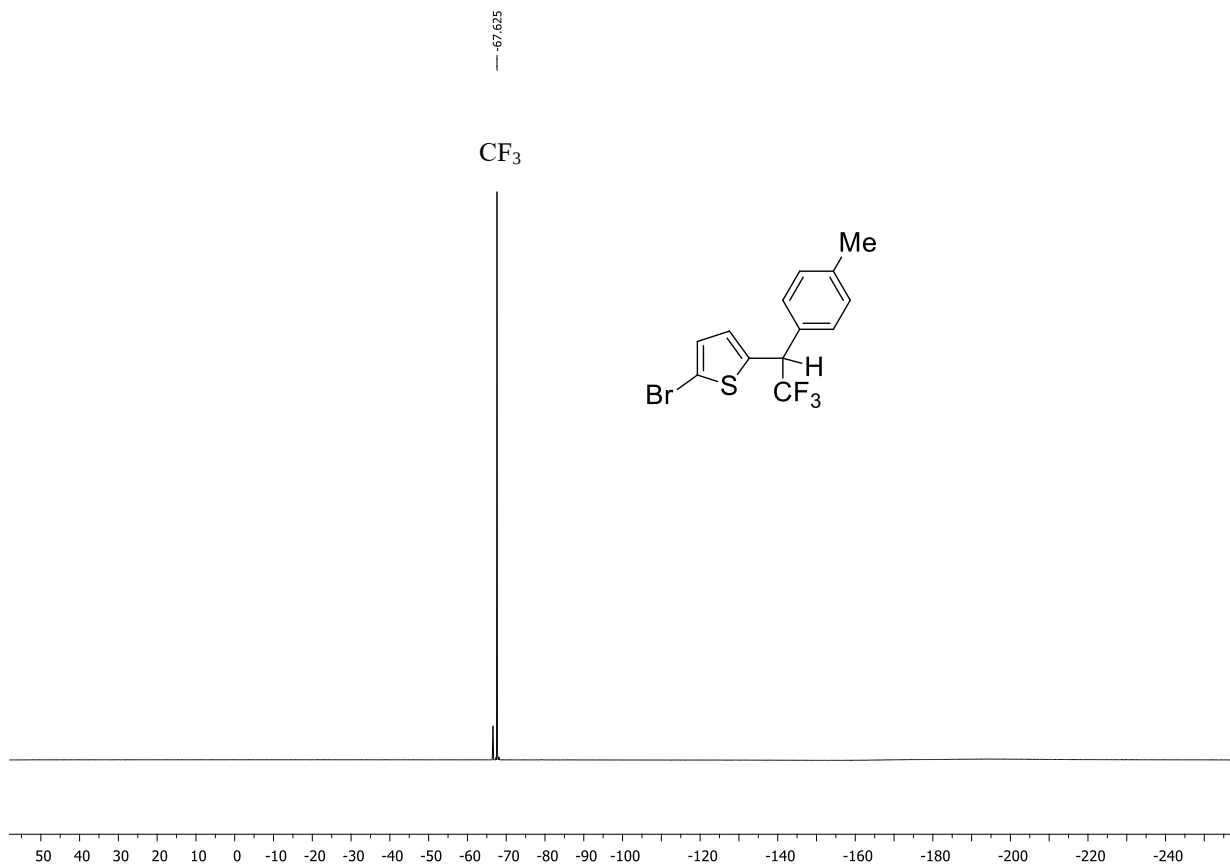


Fig. S149. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **2jc** (CDCl_3 , 376 MHz).

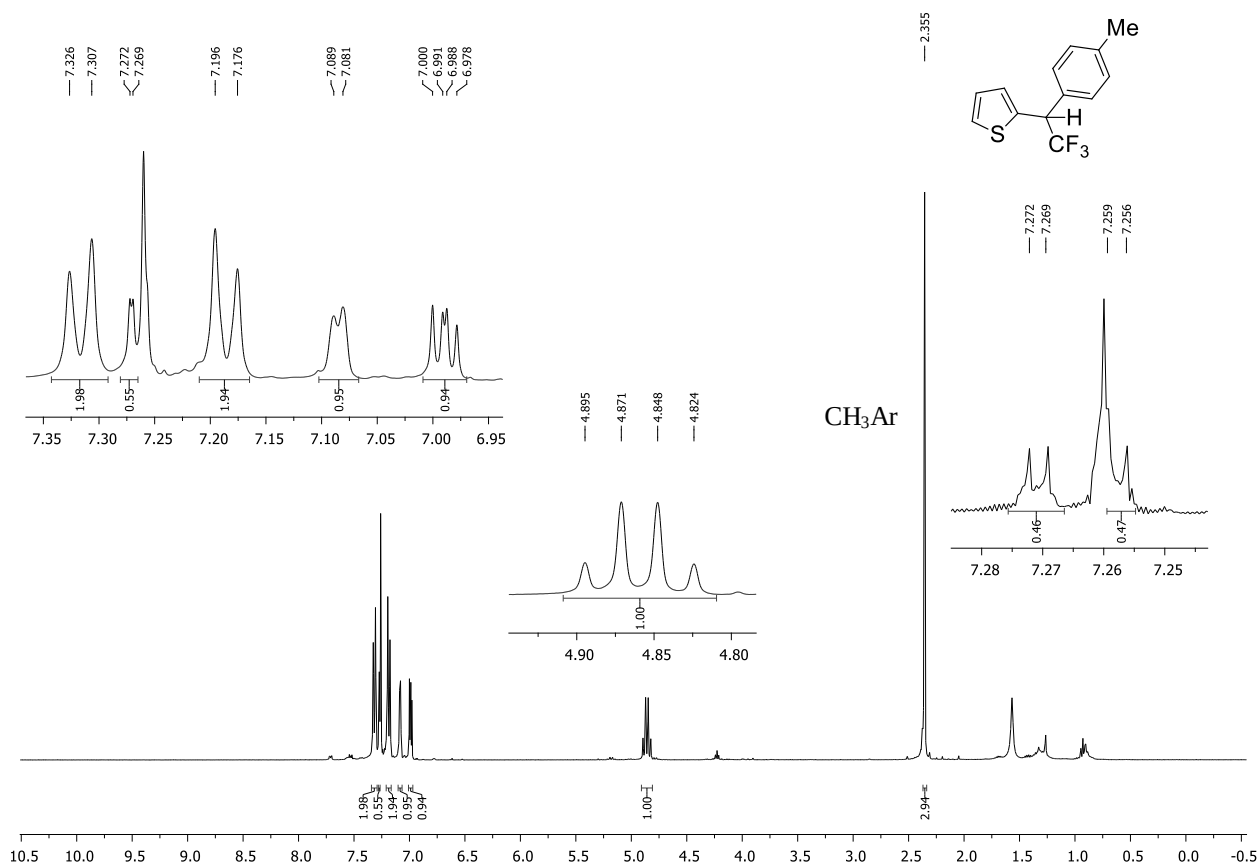


Fig. S150. ¹H NMR spectrum of the compound **3kb** (CDCl₃, 400 MHz).

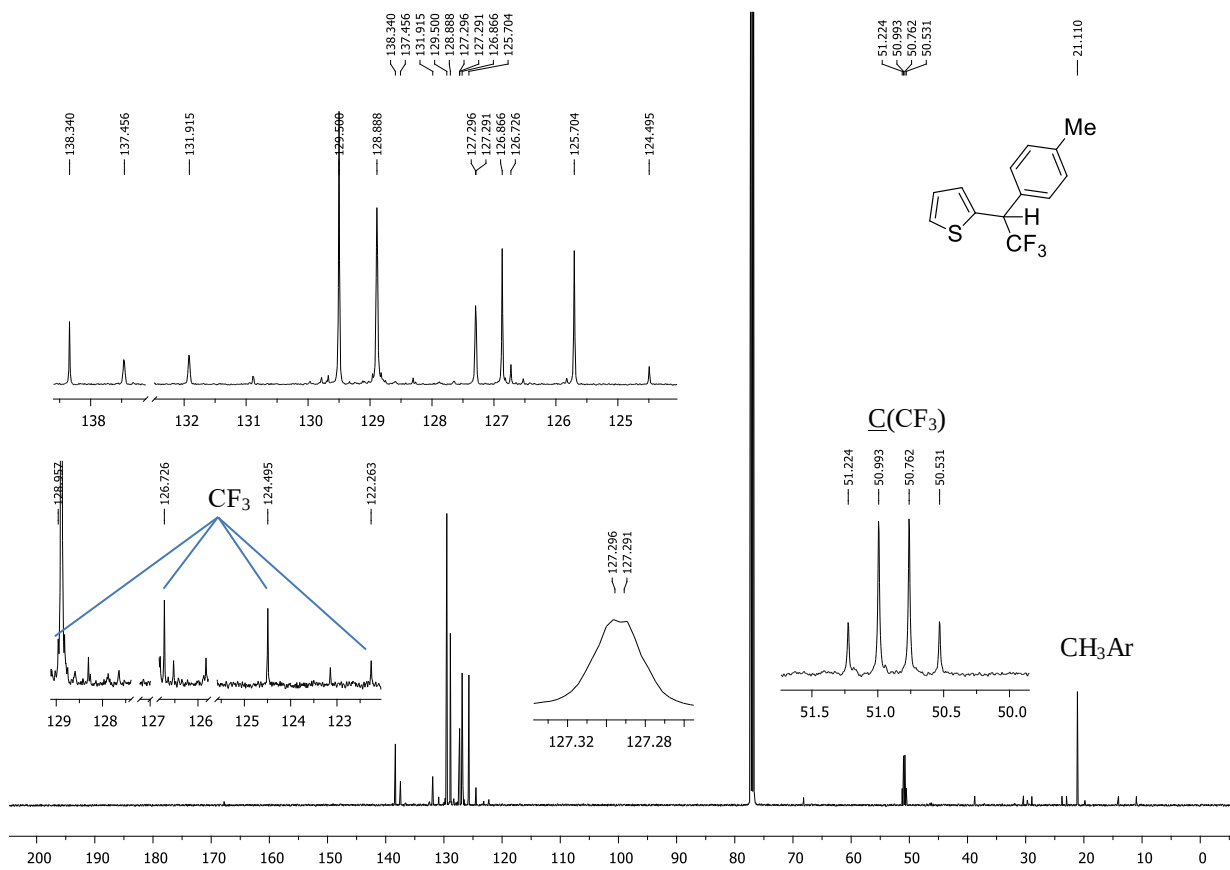


Fig. S151. ¹³C{¹H} NMR spectrum of the compound **3kb** (CDCl₃, 101 MHz).

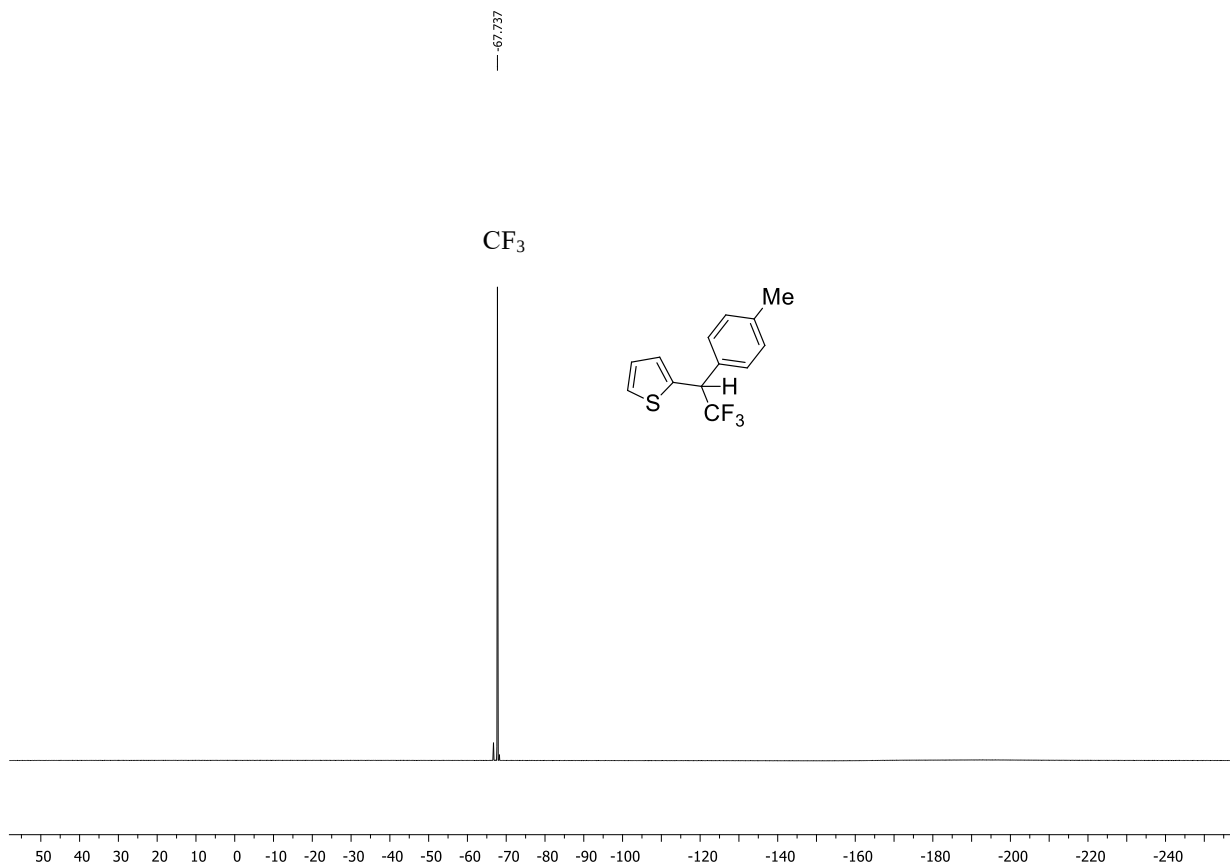


Fig. S152. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **3kb** (CDCl₃, 376 MHz).

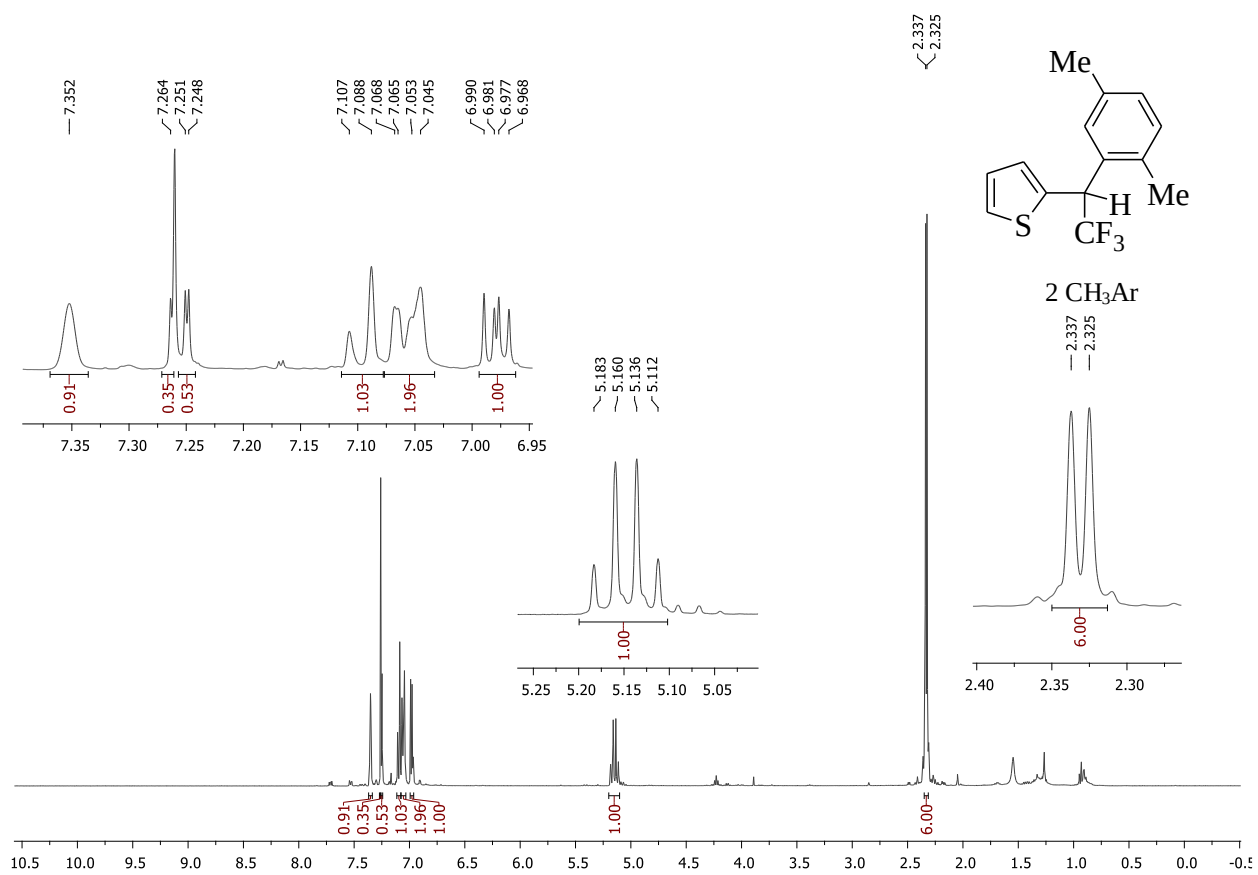


Fig. S153. ^1H NMR spectrum of the compound **3kc** (CDCl₃, 400 MHz).

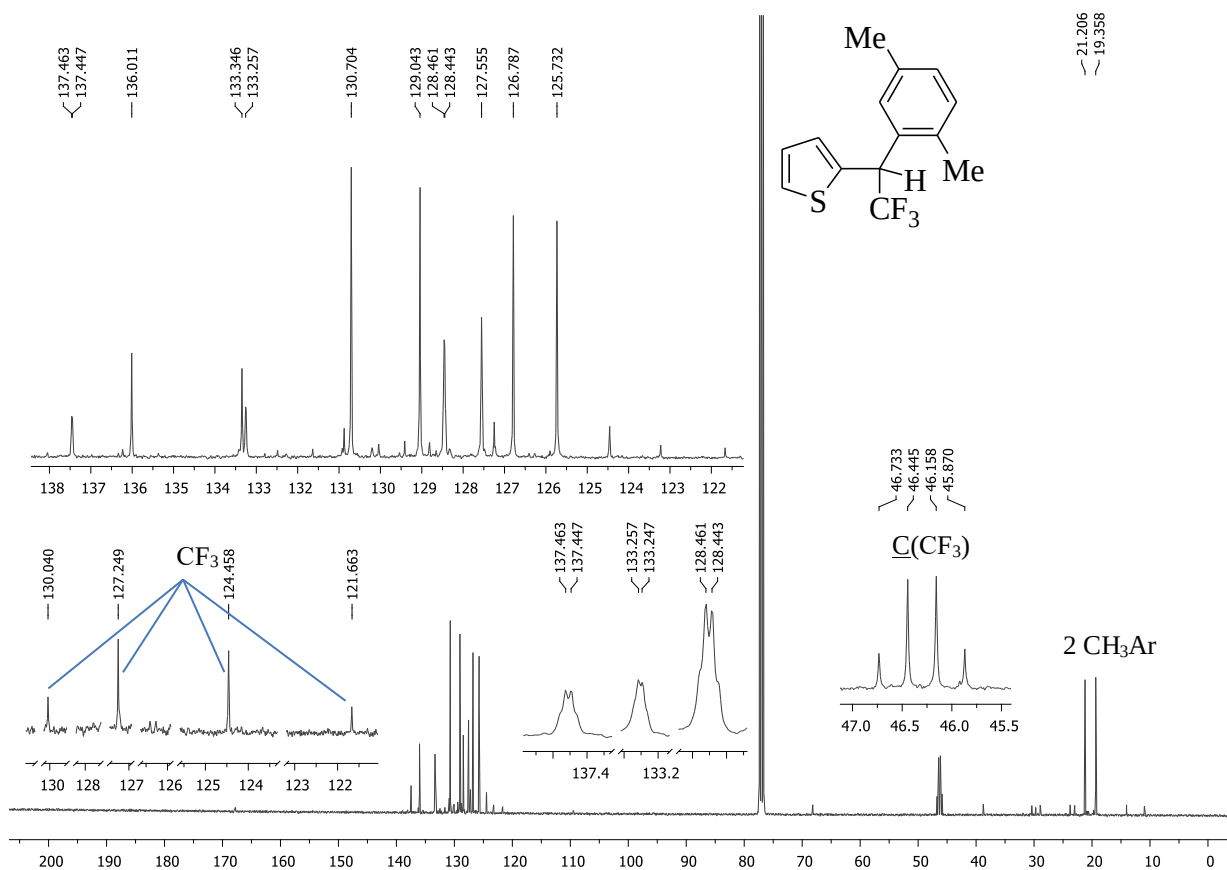


Fig. S154. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **3kc** (CDCl₃, 101 MHz).

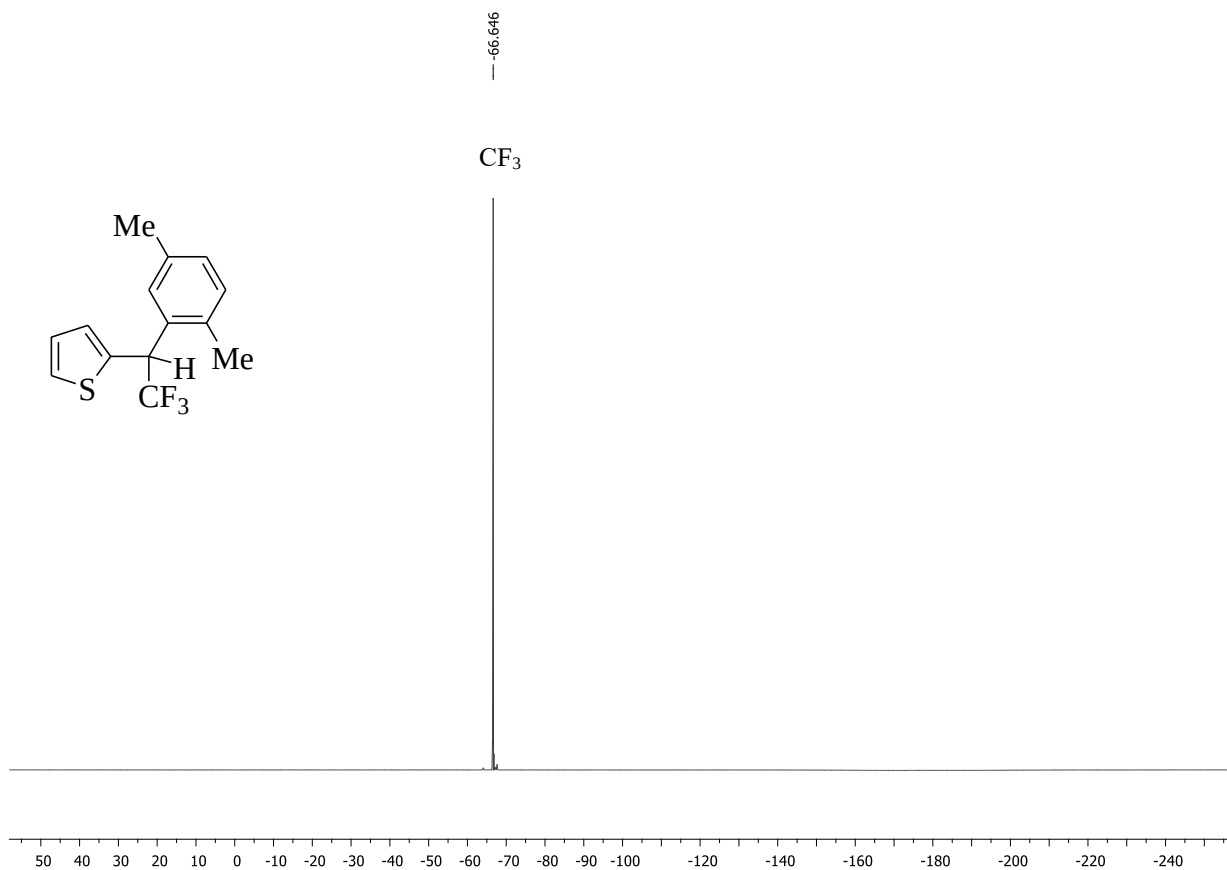


Fig. S155. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **3kc** (CDCl₃, 376 MHz).

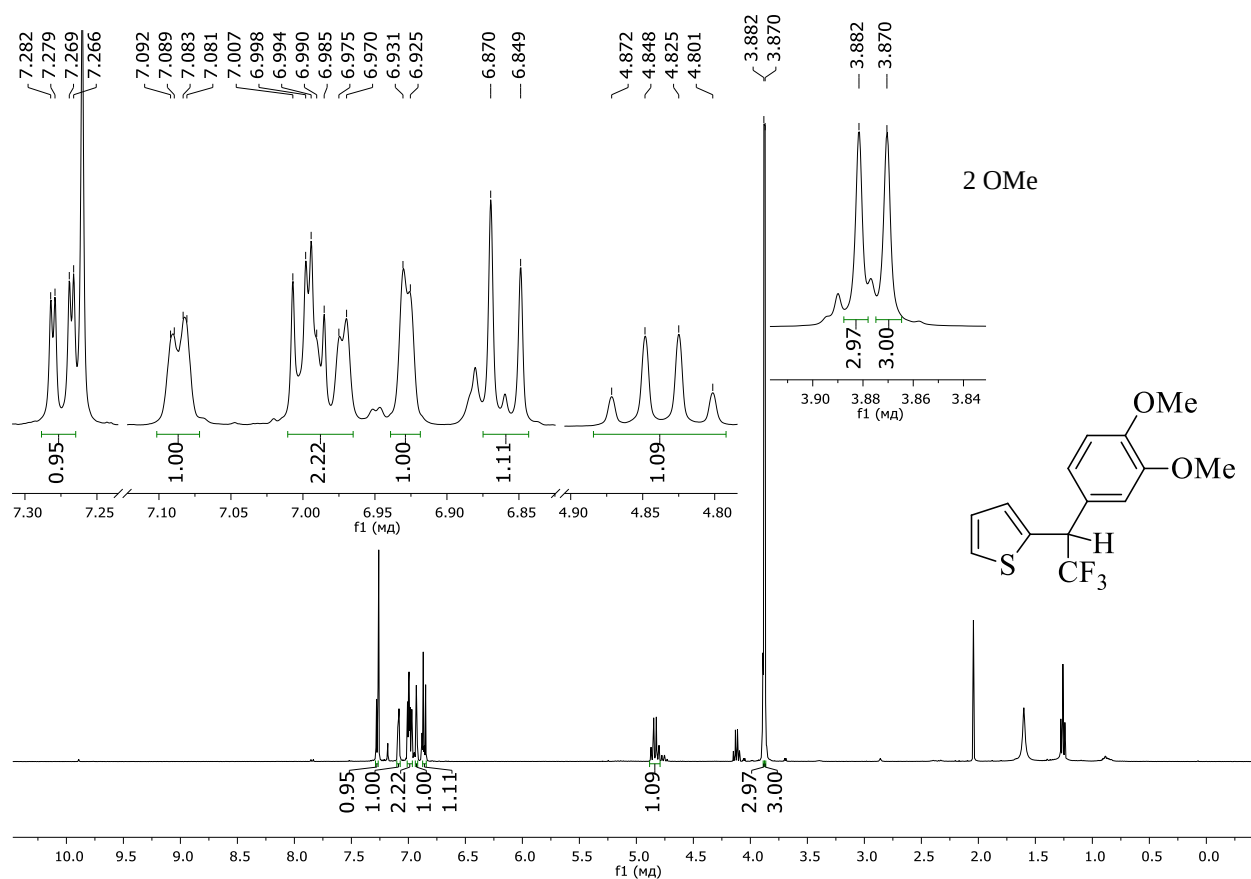


Fig. S156. ¹H NMR spectrum of the compound **3ja** (CDCl₃, 400 MHz).

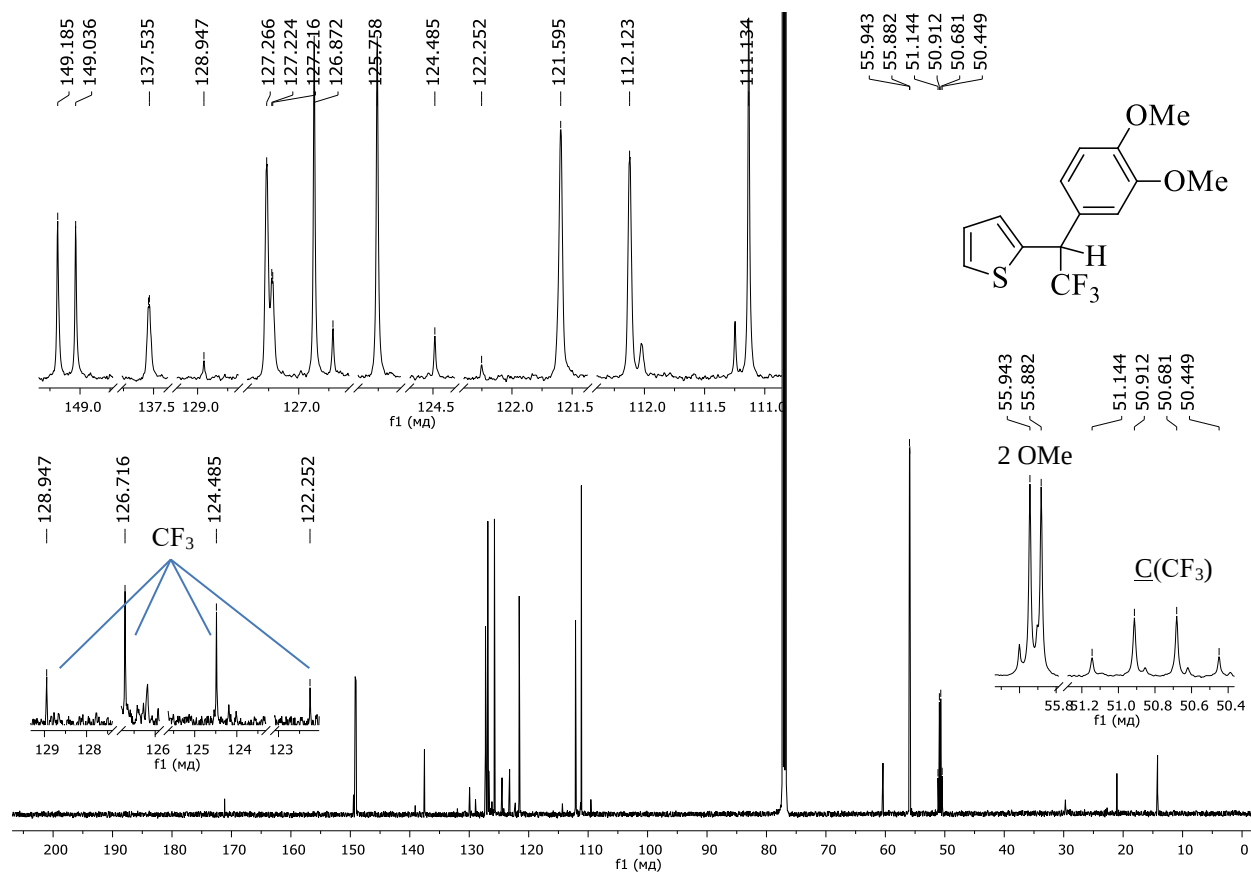


Fig. S157. ¹³C{¹H} NMR spectrum of the compound **3ja** (CDCl₃, 101 MHz).

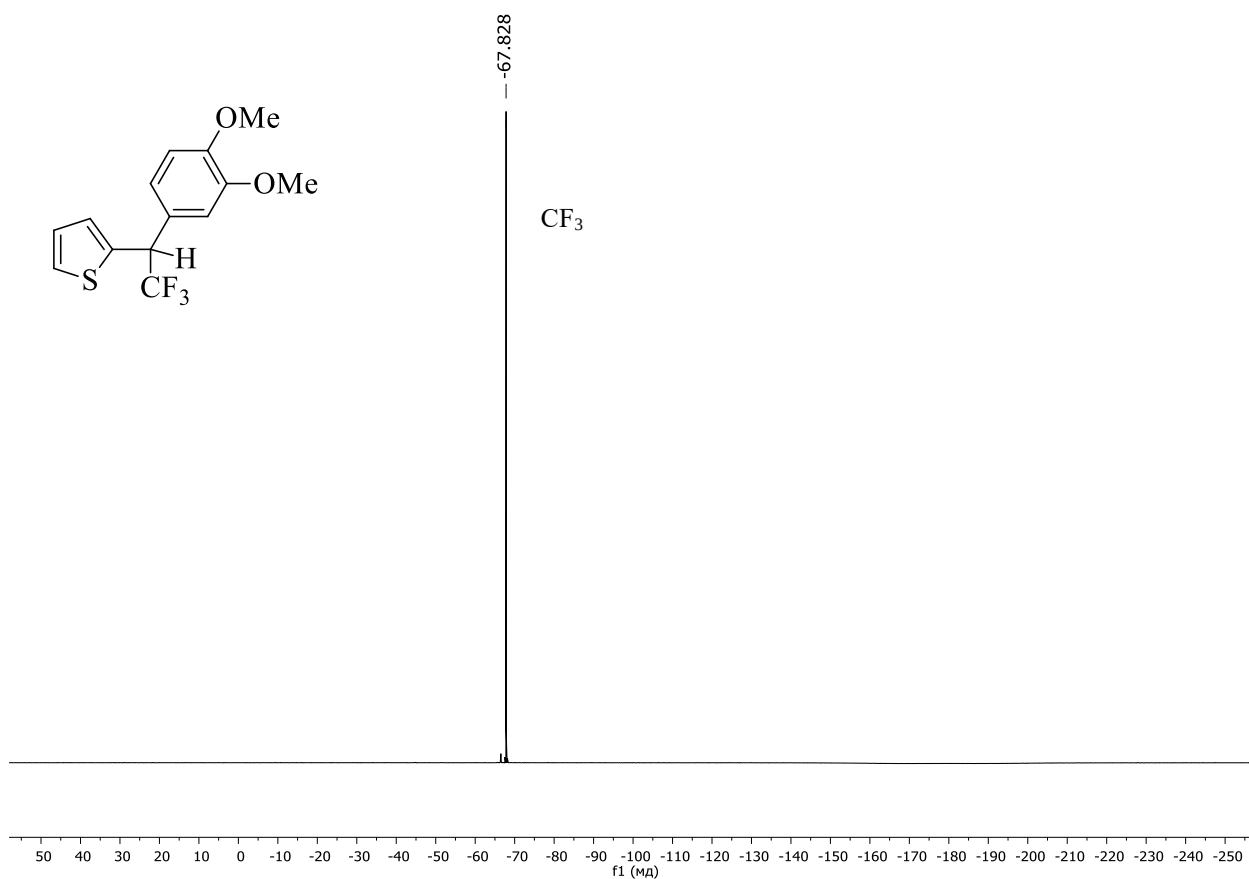


Fig. S158. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **3ja** (CDCl_3 , 376 MHz).

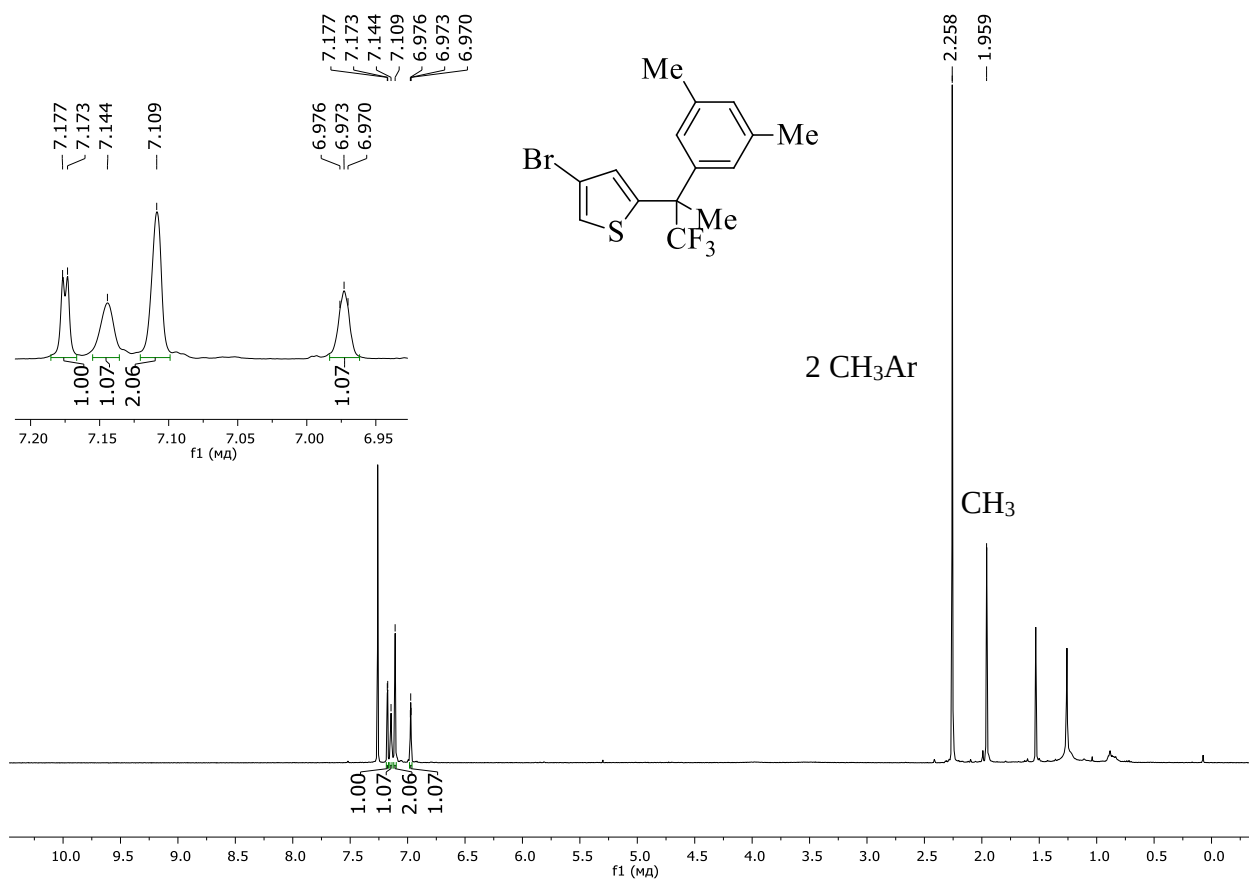


Fig. S159. ^1H NMR spectrum of the compound **4ga** (CDCl_3 , 400 MHz).

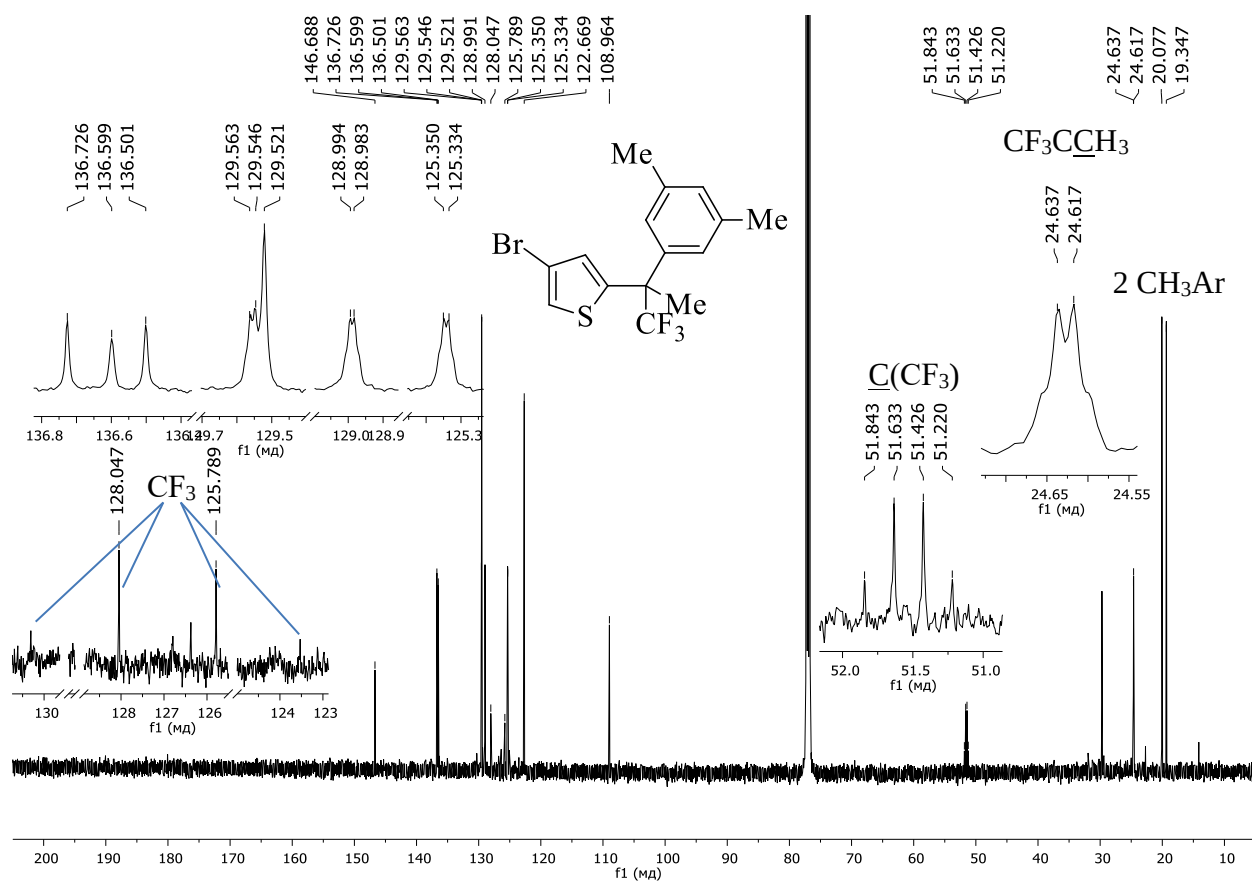


Fig. S160. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **4ga** (CDCl_3 , 101 MHz).

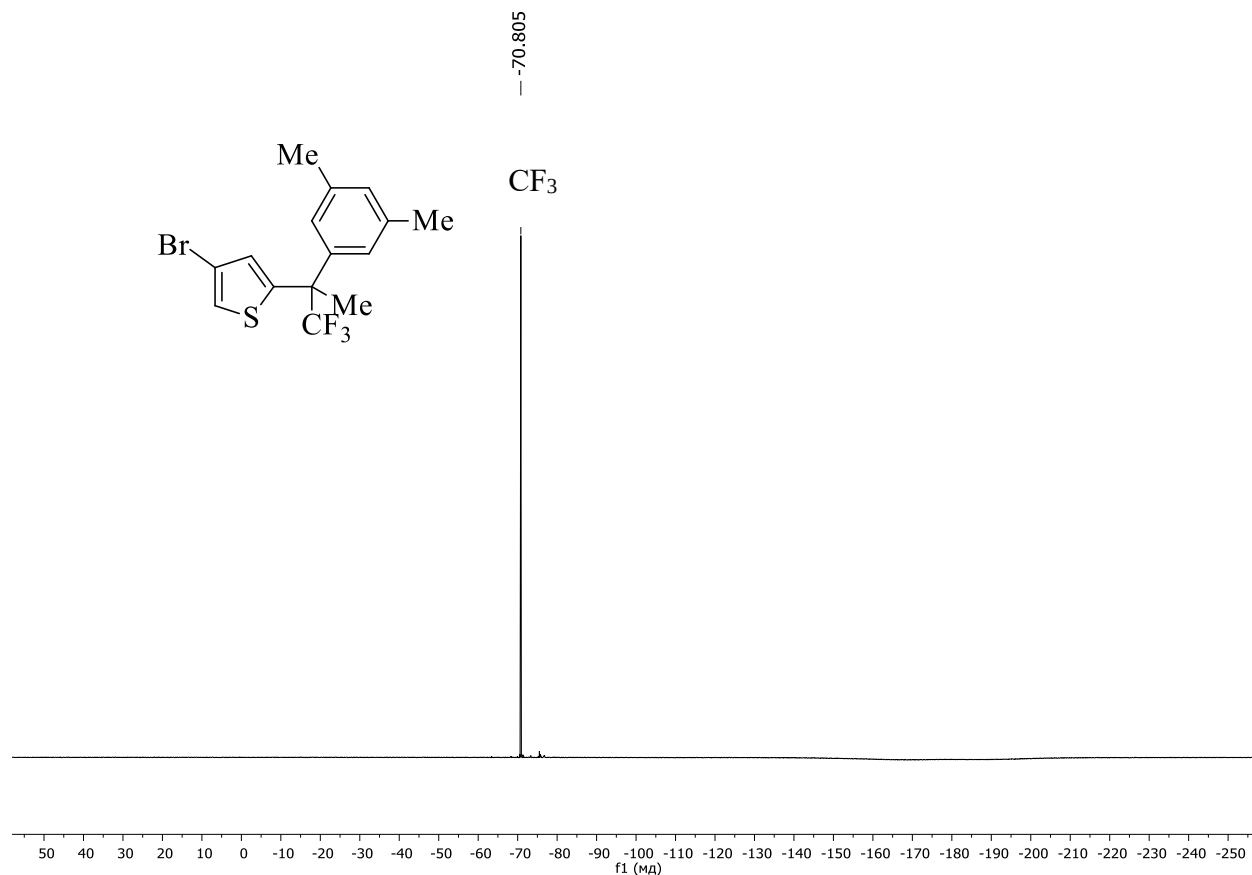


Fig. S161. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **4ga** (CDCl_3 , 376 MHz).

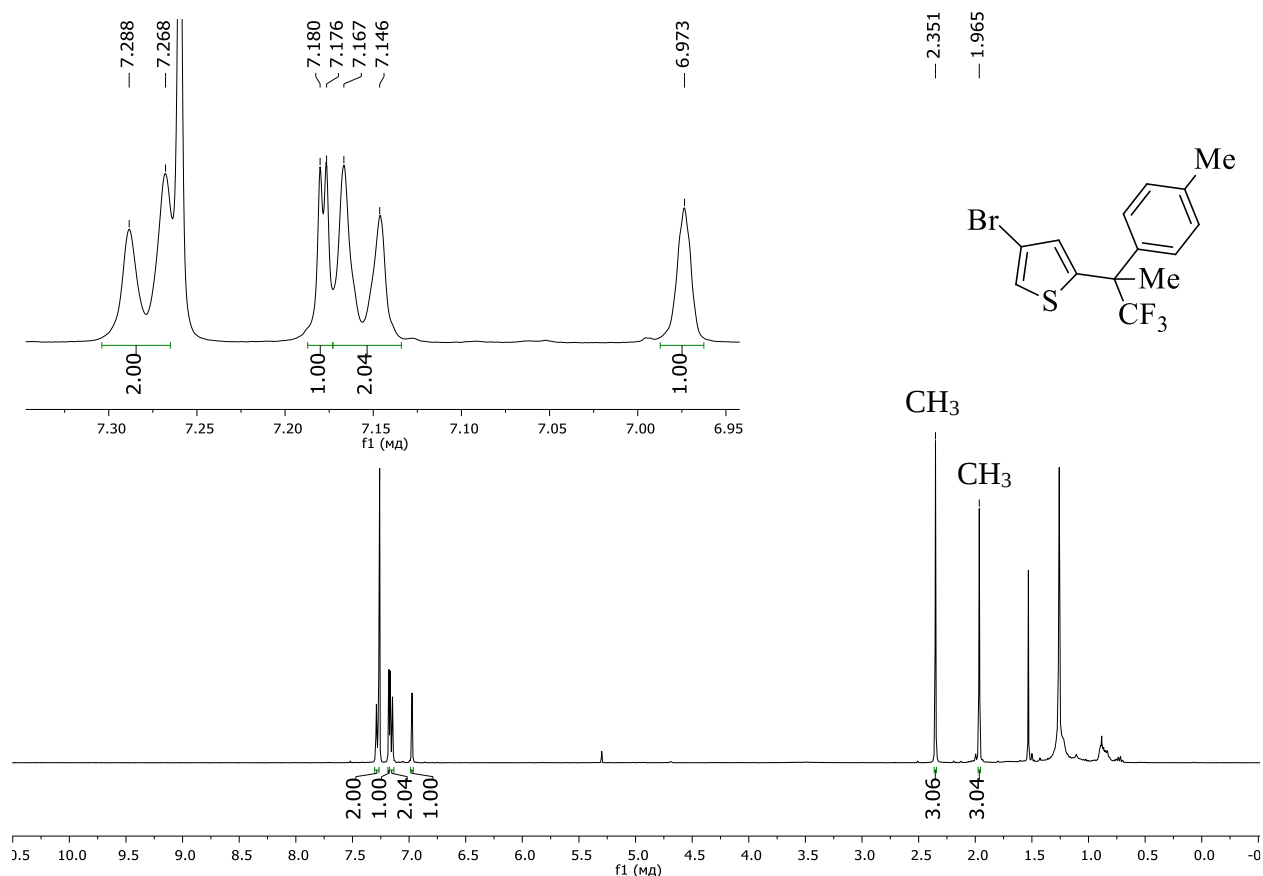


Fig. S162. ¹H NMR spectrum of the compound **4gb** (CDCl₃, 400 MHz).

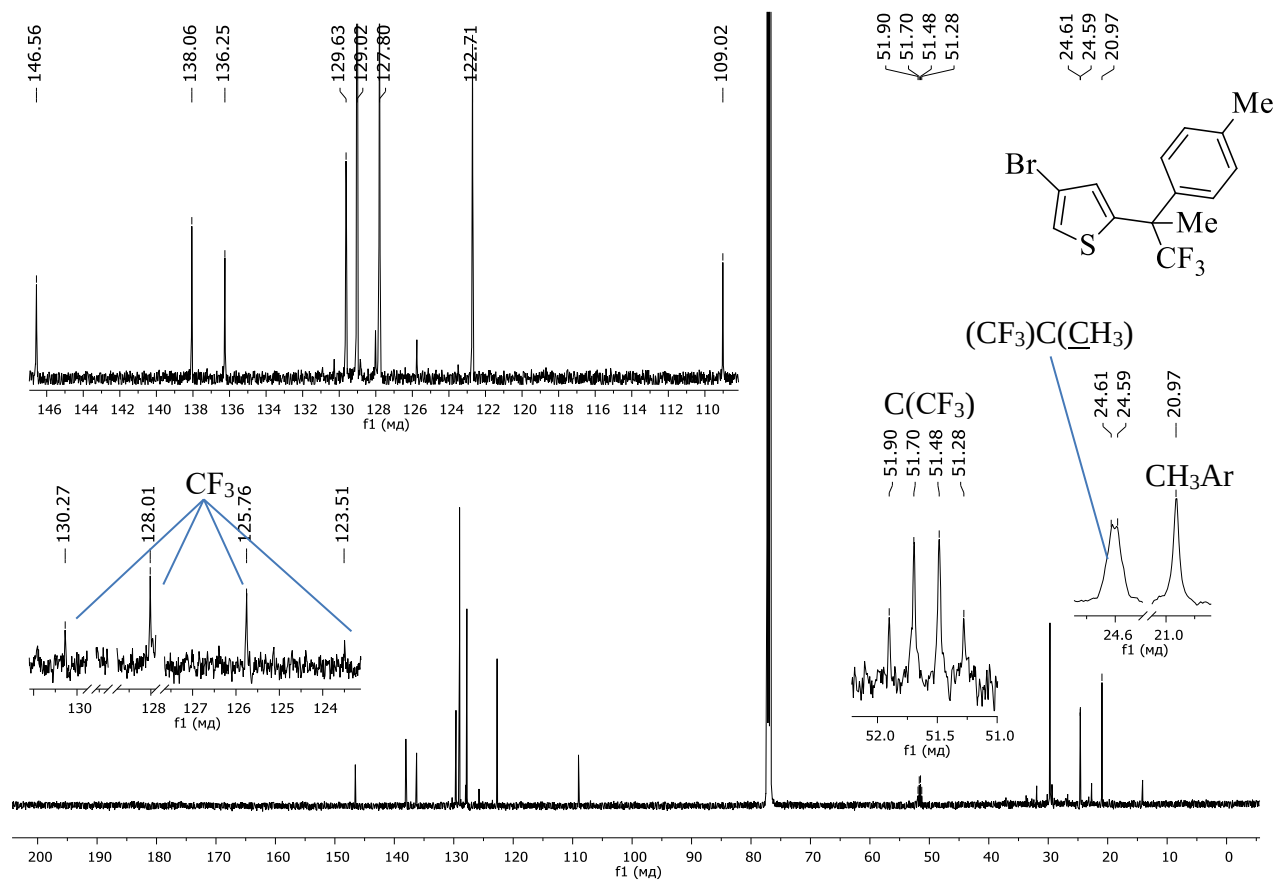


Fig. S163. ¹³C{¹H} NMR spectrum of the compound **4gb** (CDCl₃, 101 MHz).

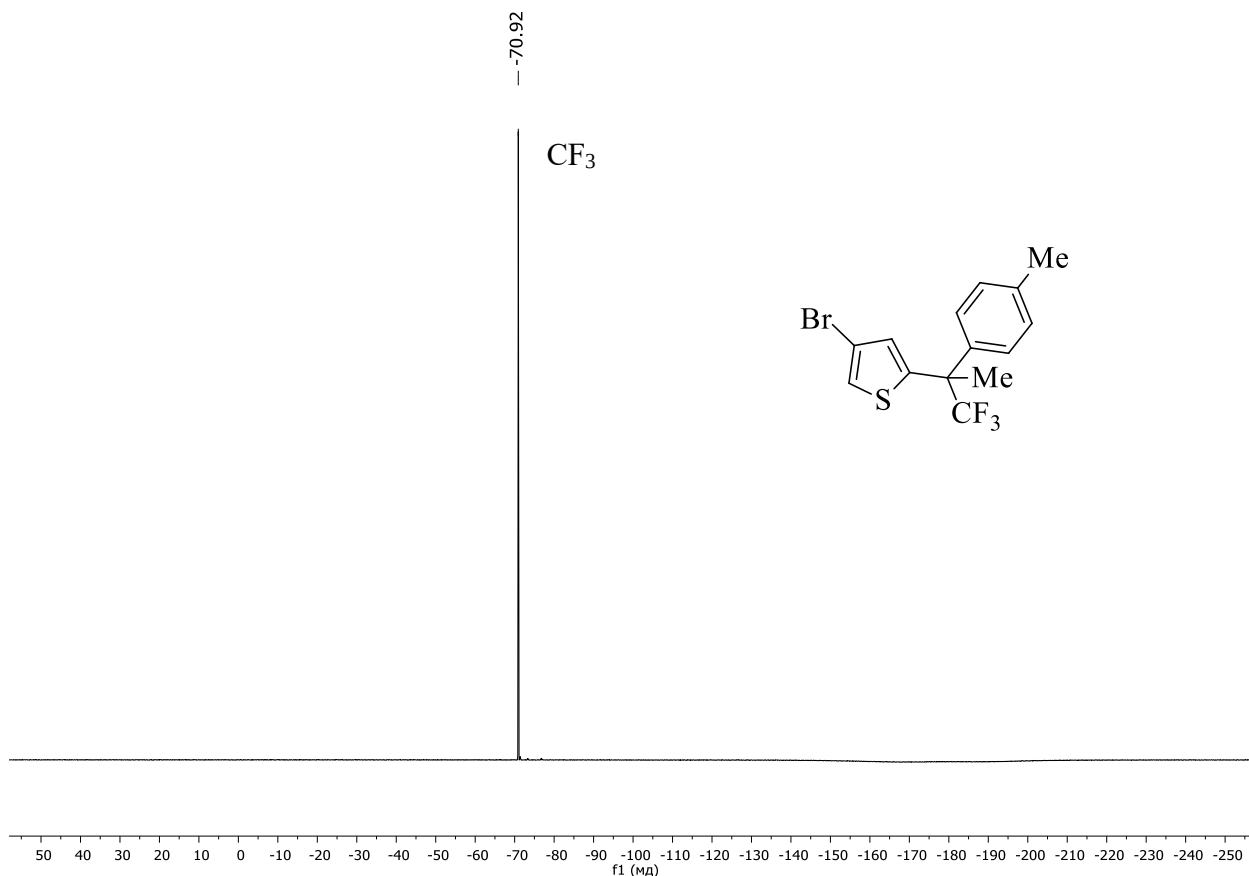


Fig. S164. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **4gb** (CDCl_3 , 376 MHz).

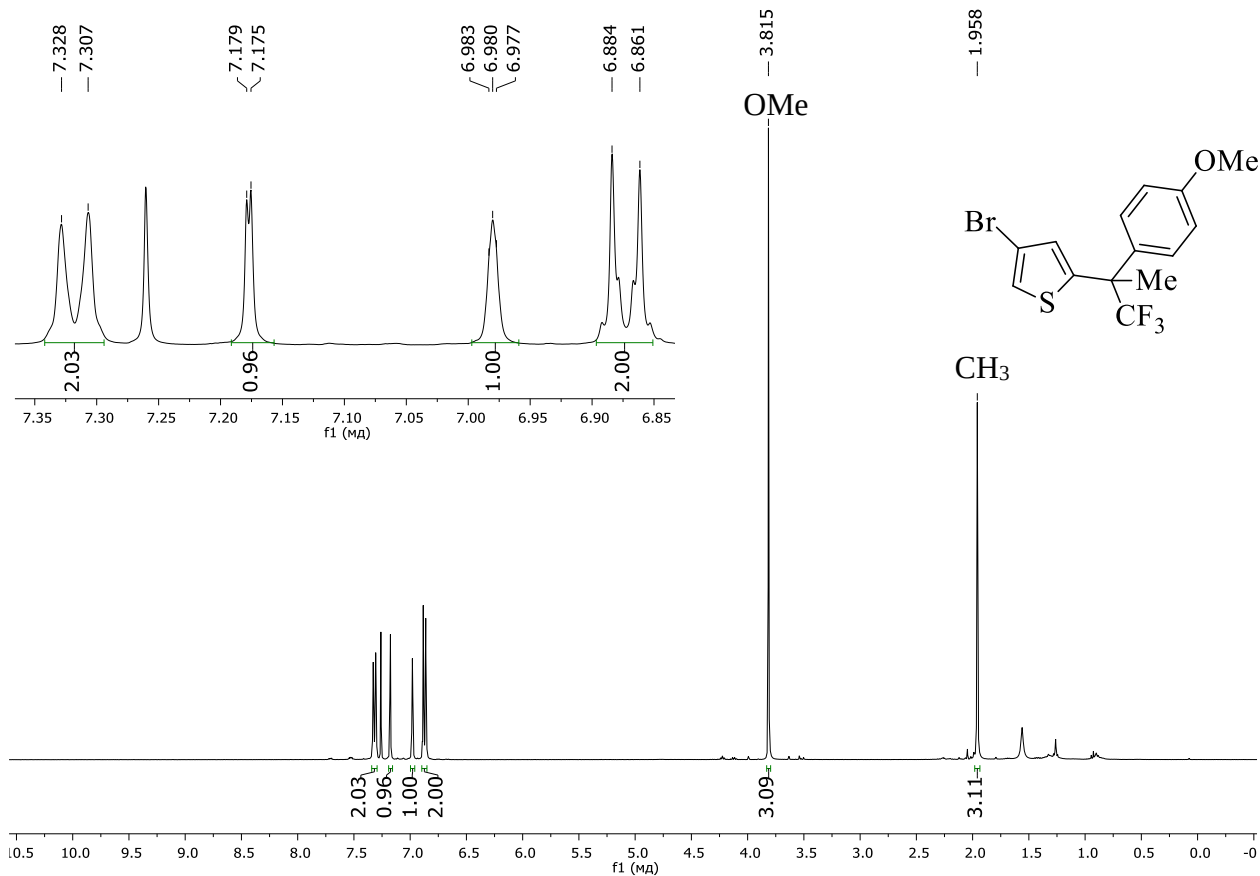


Fig. S165. ^1H NMR spectrum of the compound **4gc** (CDCl_3 , 400 MHz).

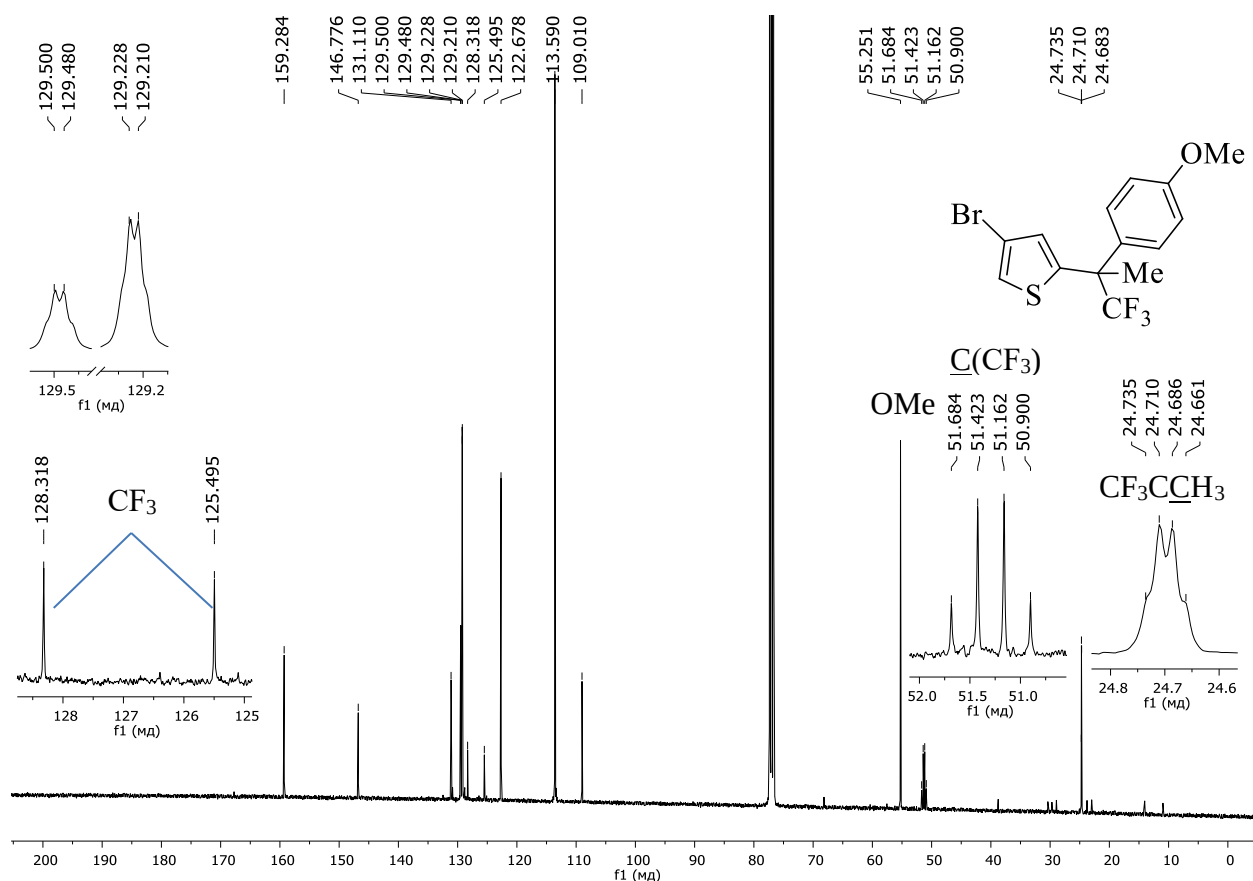


Fig. S166. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **4gc** (CDCl_3 , 101 MHz).

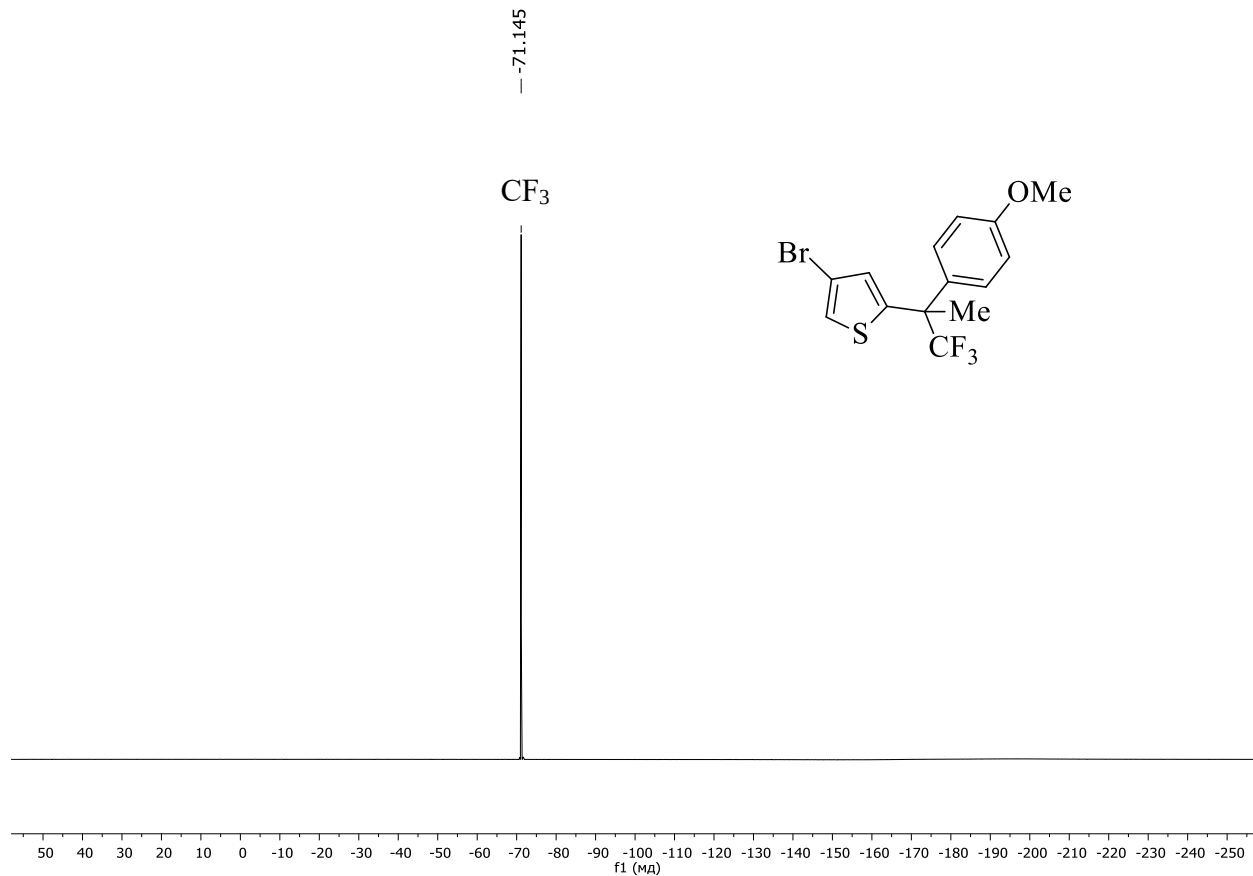


Fig. S167. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **4gc** (CDCl_3 , 376 MHz).

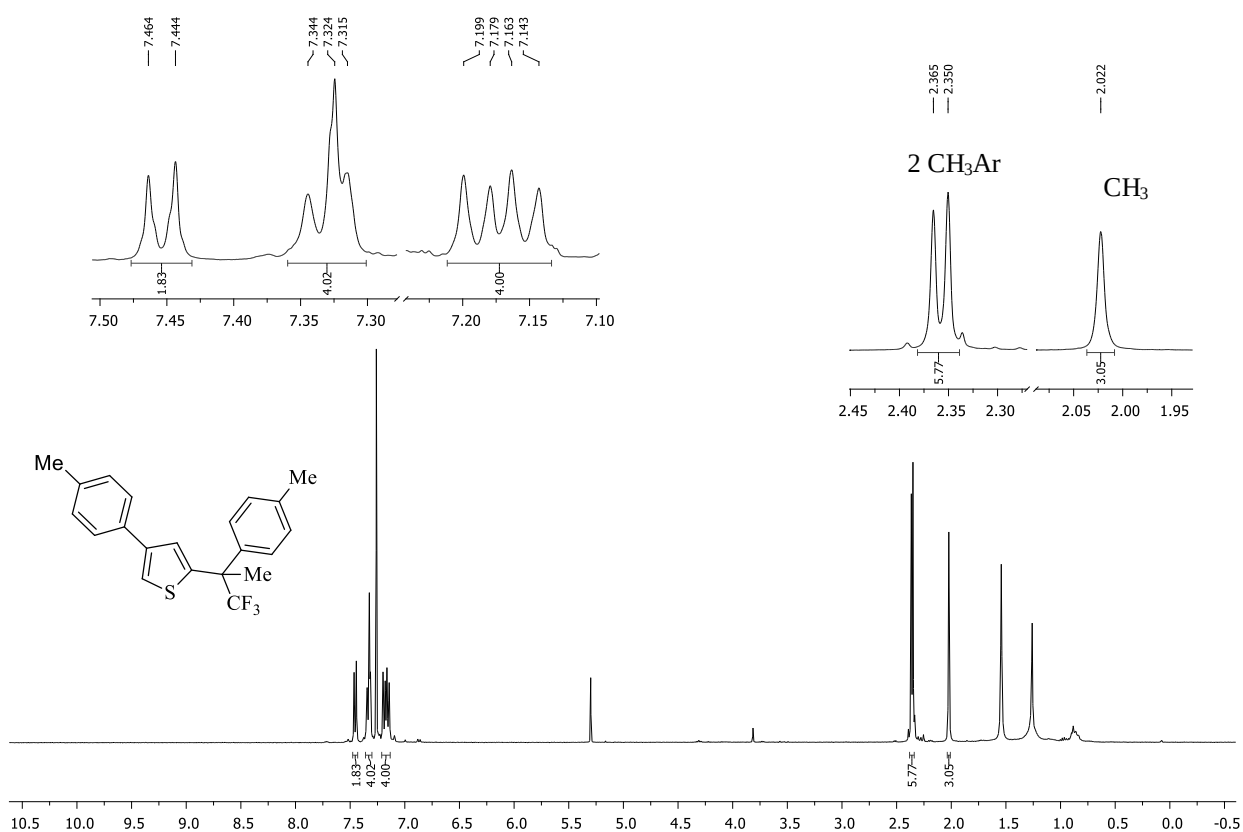


Fig. S168. ¹H NMR spectrum of the compound **5fa** (CDCl₃, 400 MHz).

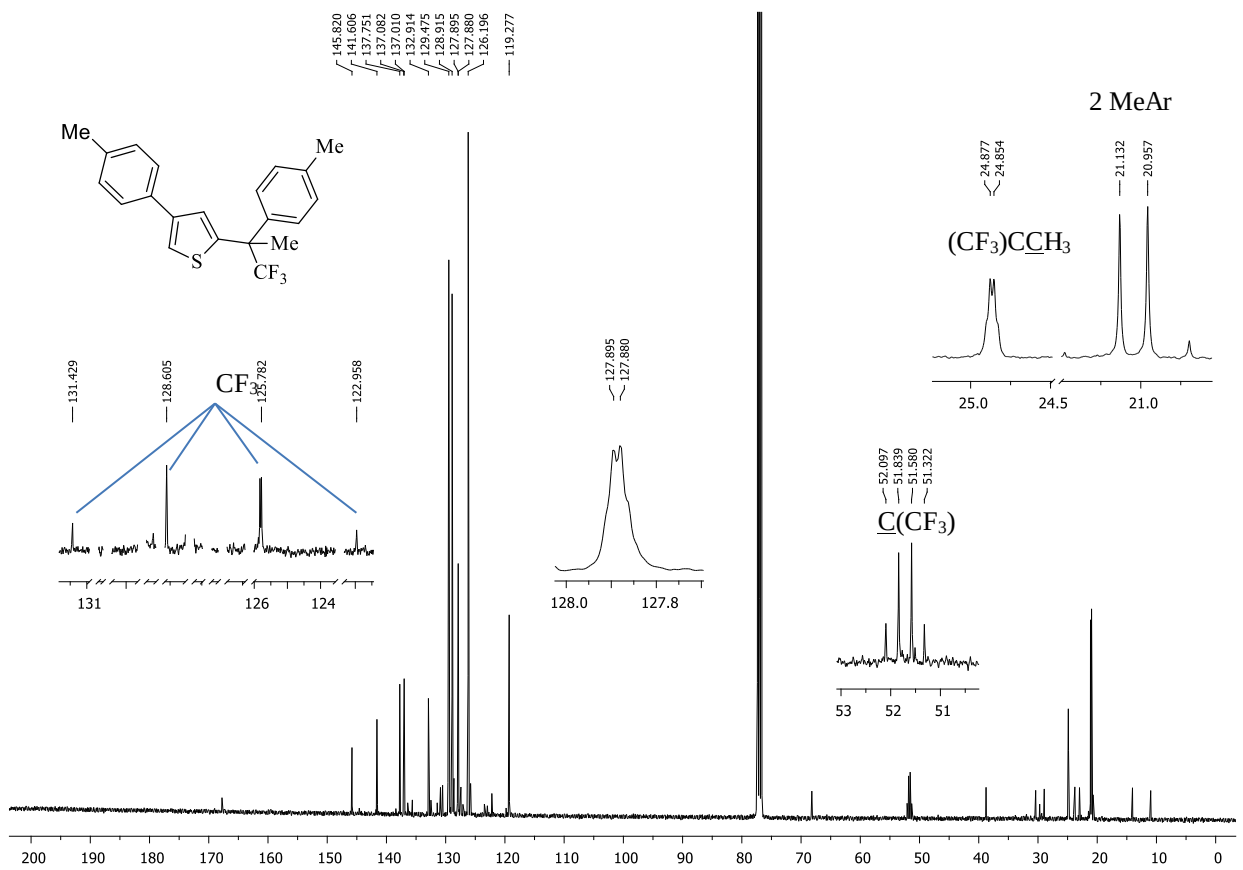


Fig. S169. ¹³C{¹H} NMR spectrum of the compound **5fa** (CDCl₃, 101 MHz).

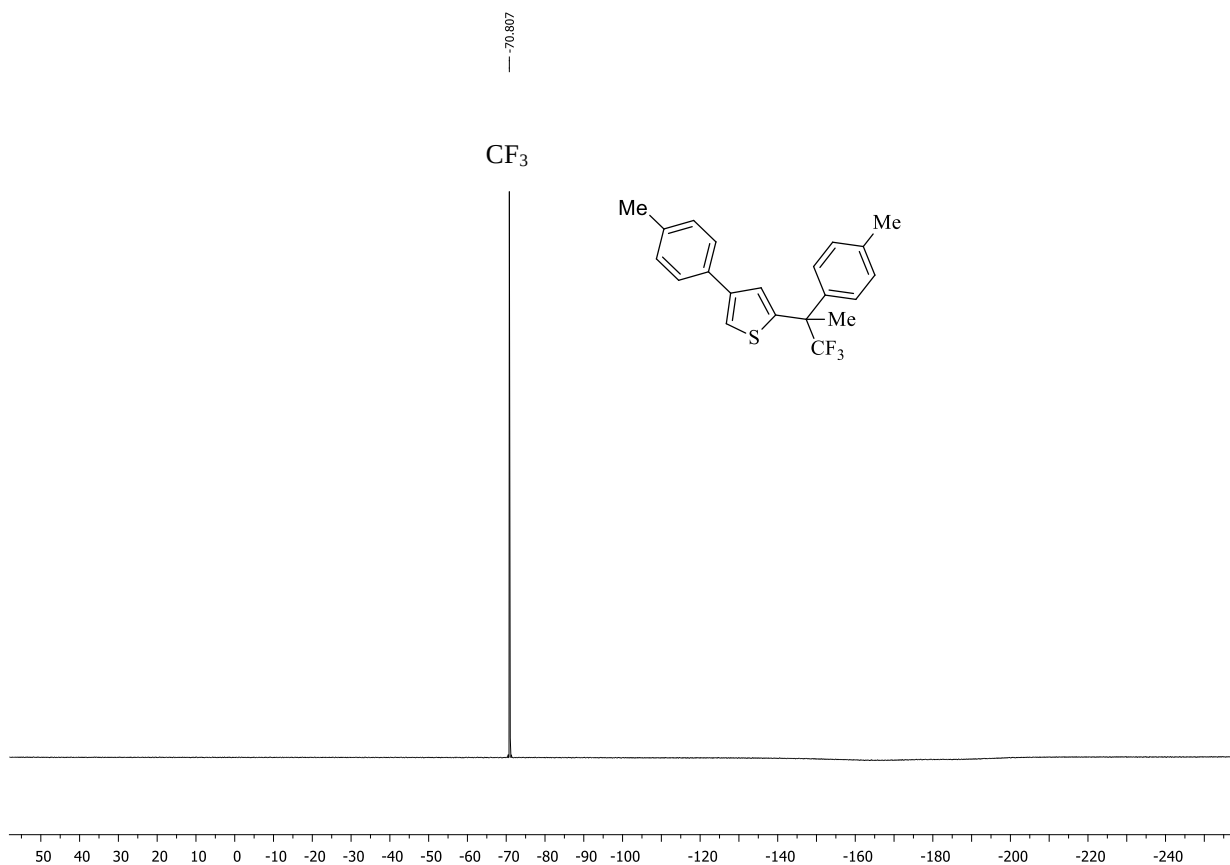


Fig. S170. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **5fa** (CDCl₃, 376 MHz).

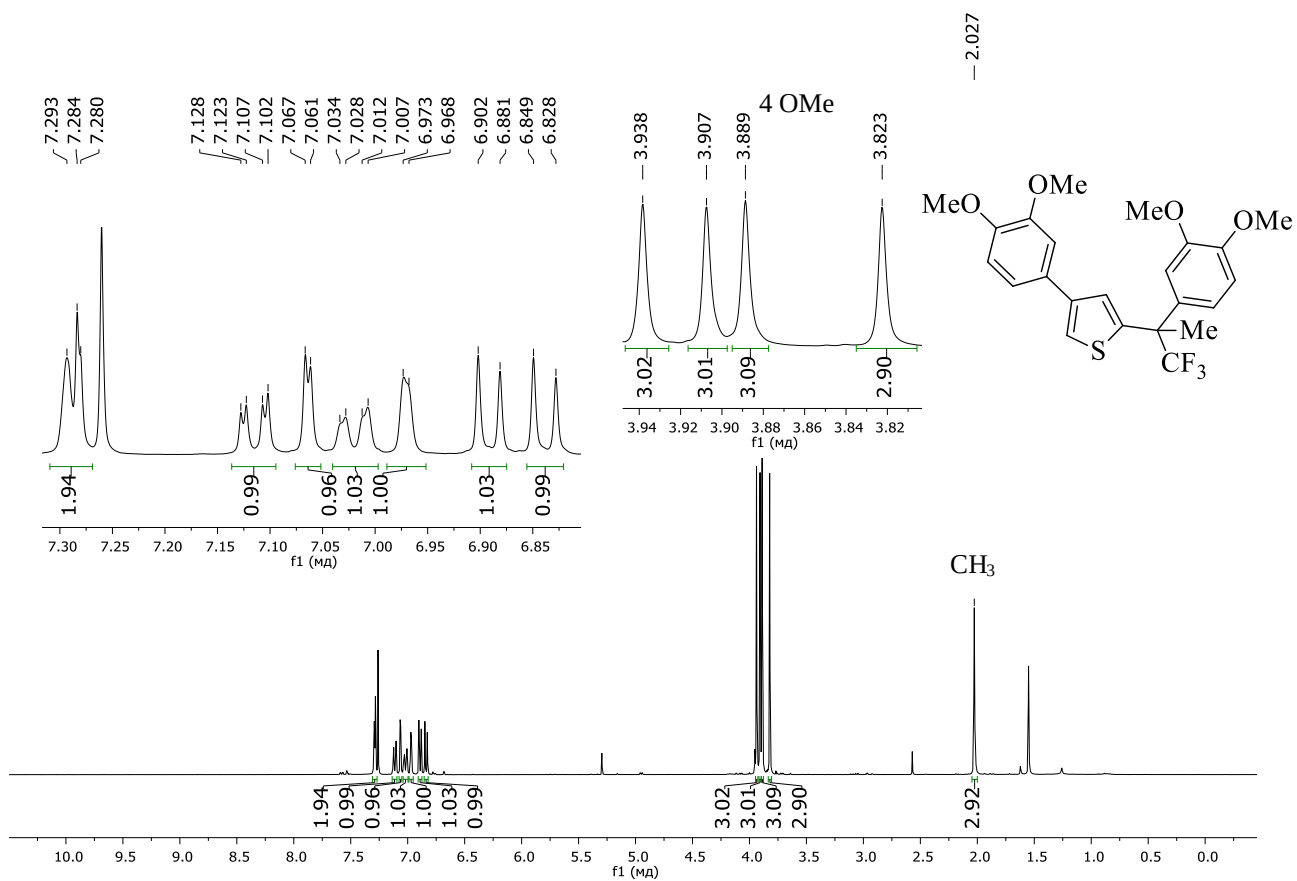


Fig. S171. ^1H NMR spectrum of the compound **5fb** (CDCl₃, 400 MHz).

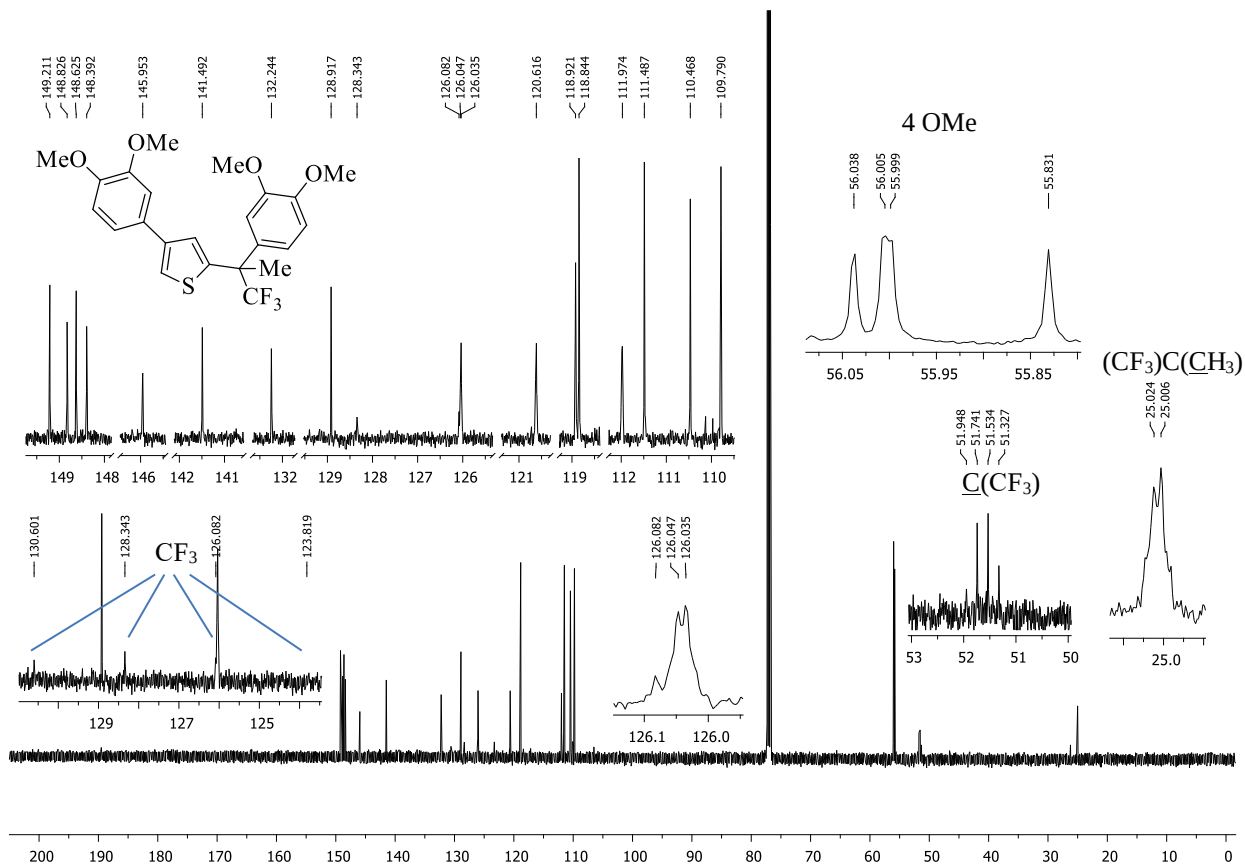


Fig. S172. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **5fb** (CDCl_3 , 101 MHz).

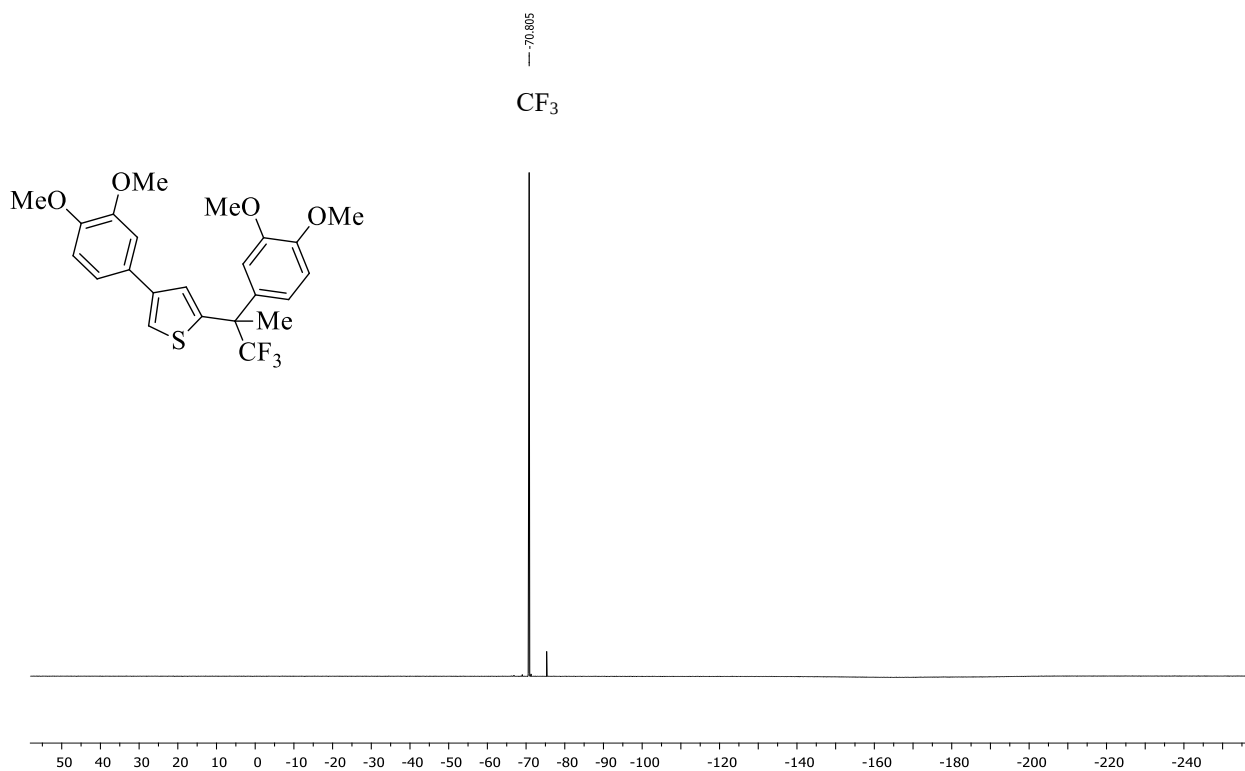


Fig. S173. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **5fb** (CDCl_3 , 376 MHz).

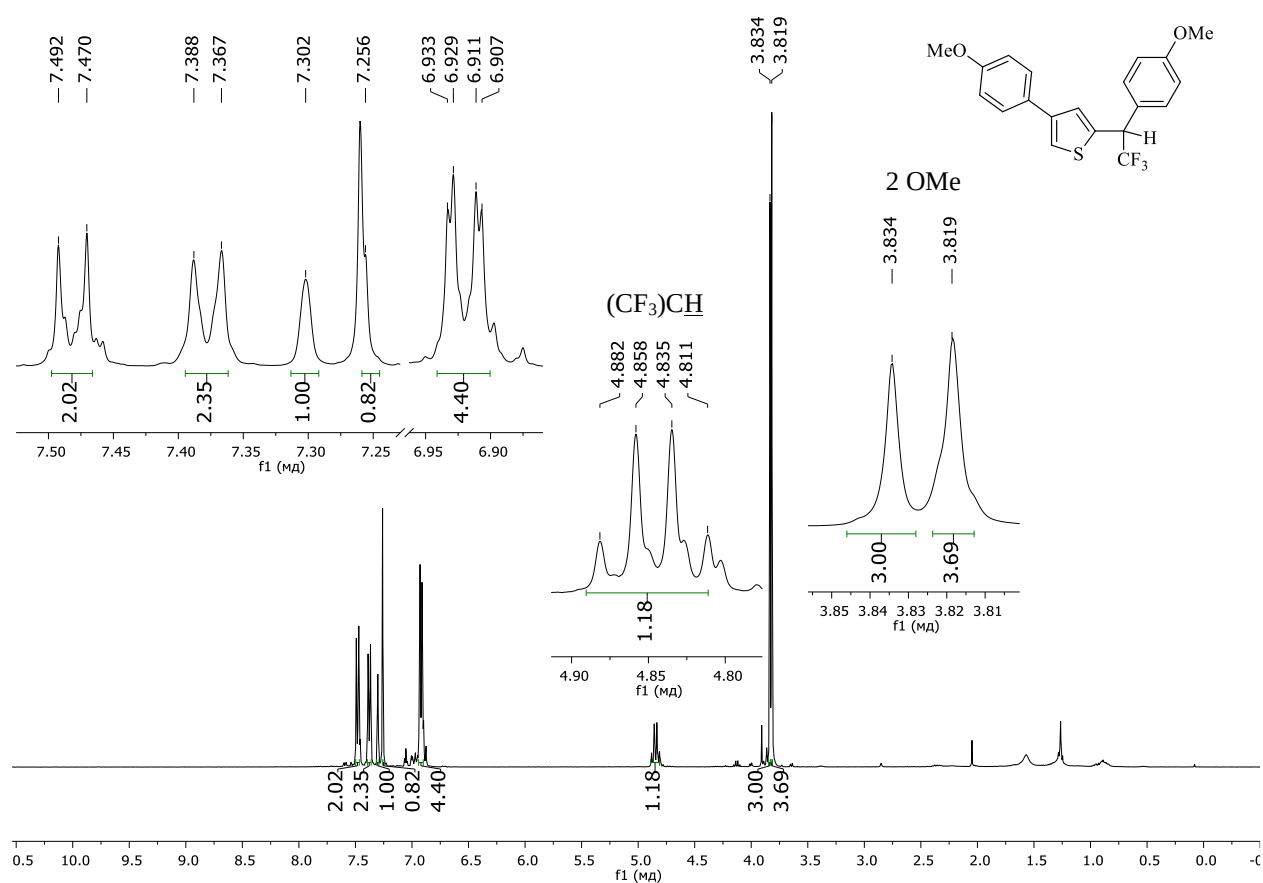


Fig. S174. ¹H NMR spectrum of the compound **5ja** (CDCl₃, 400 MHz).

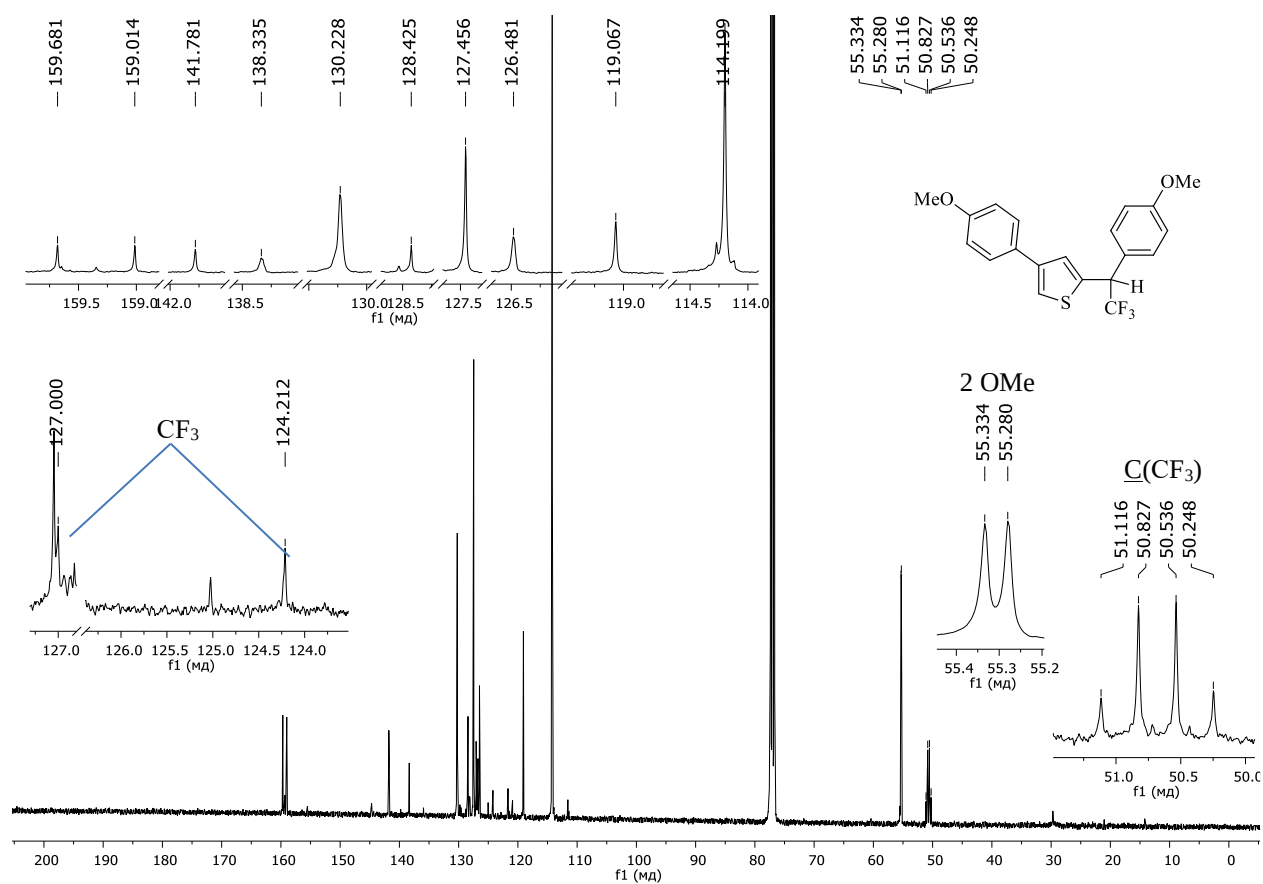


Fig. S175. ¹³C{¹H} NMR spectrum of the compound **5ja** (CDCl₃, 101 MHz).

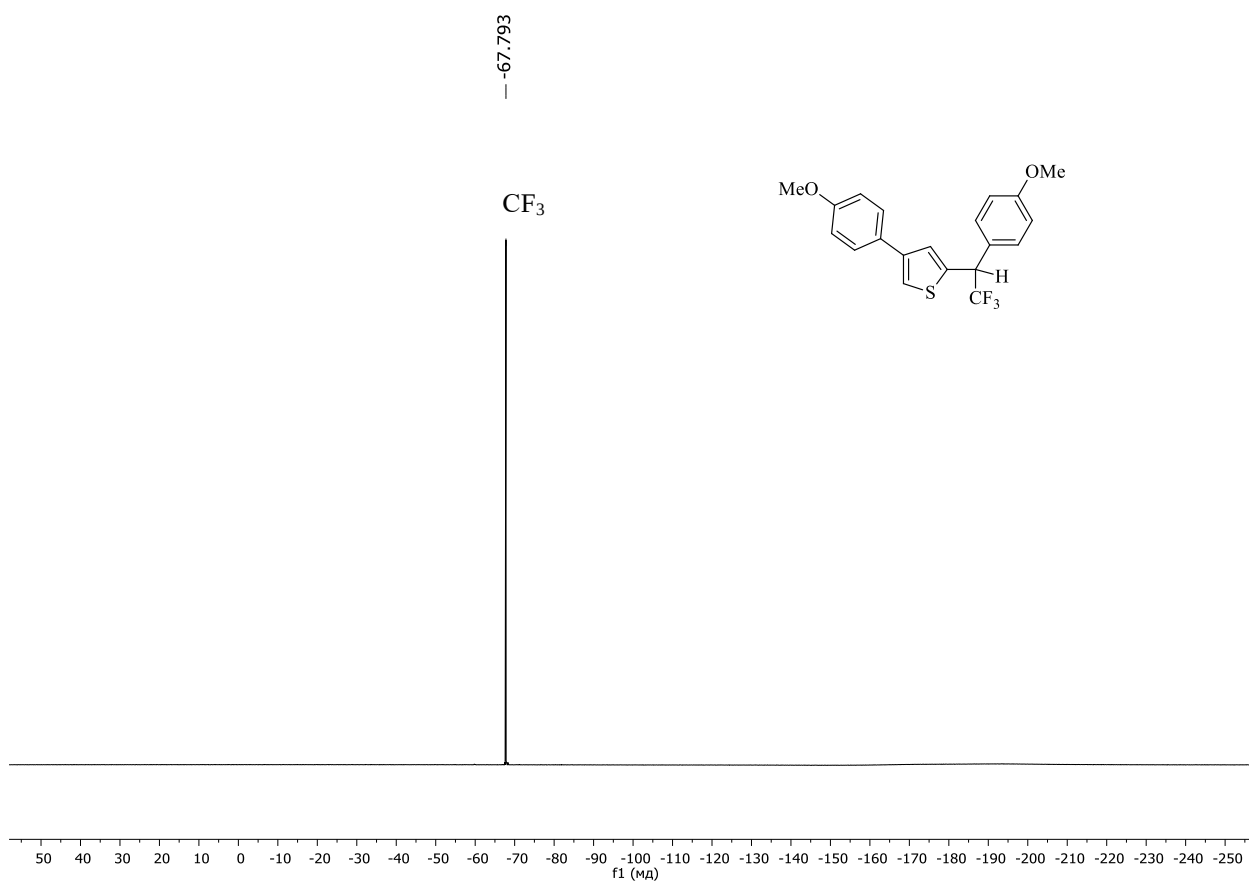


Fig. S176. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **5ja** (CDCl_3 , 376 MHz).

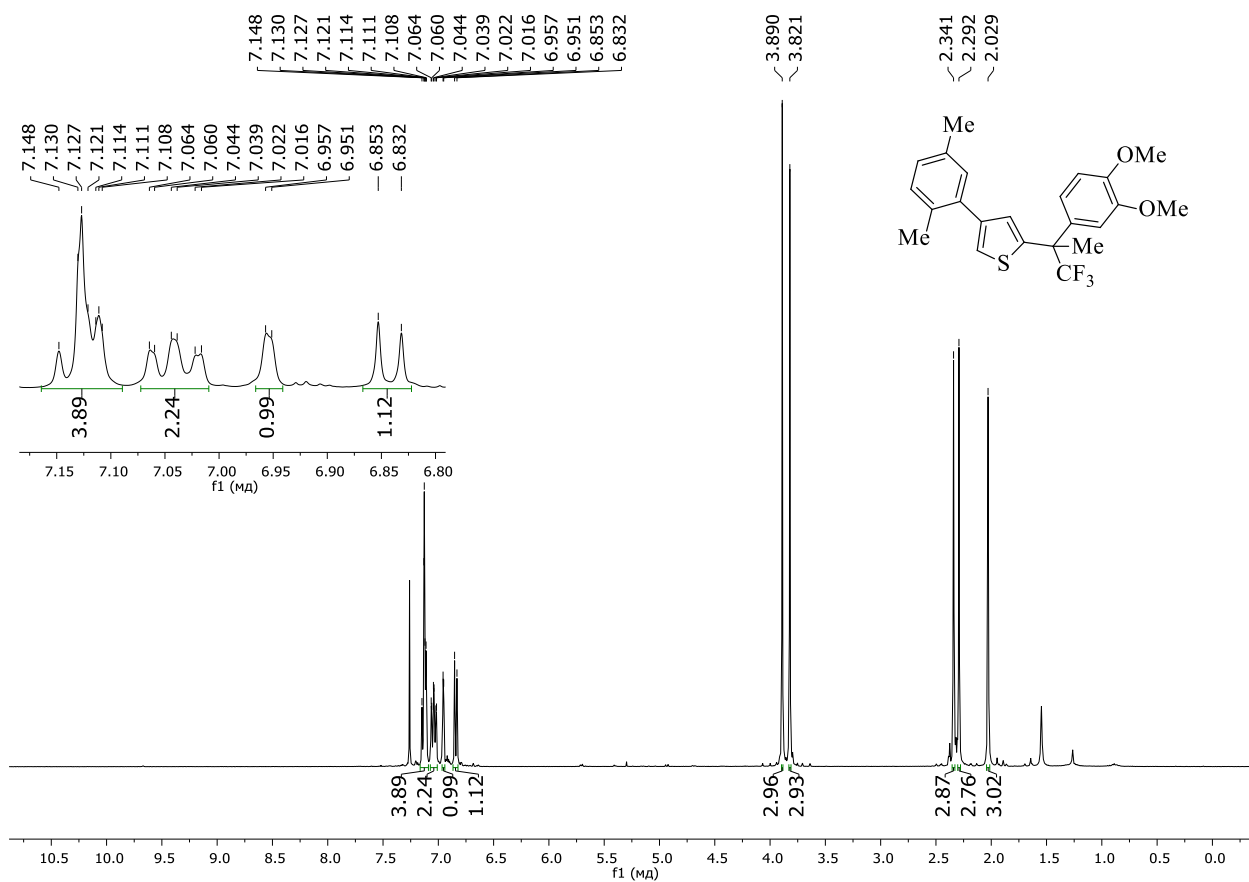


Fig. S177. ^1H NMR spectrum of the compound **6fa** (CDCl_3 , 400 MHz).

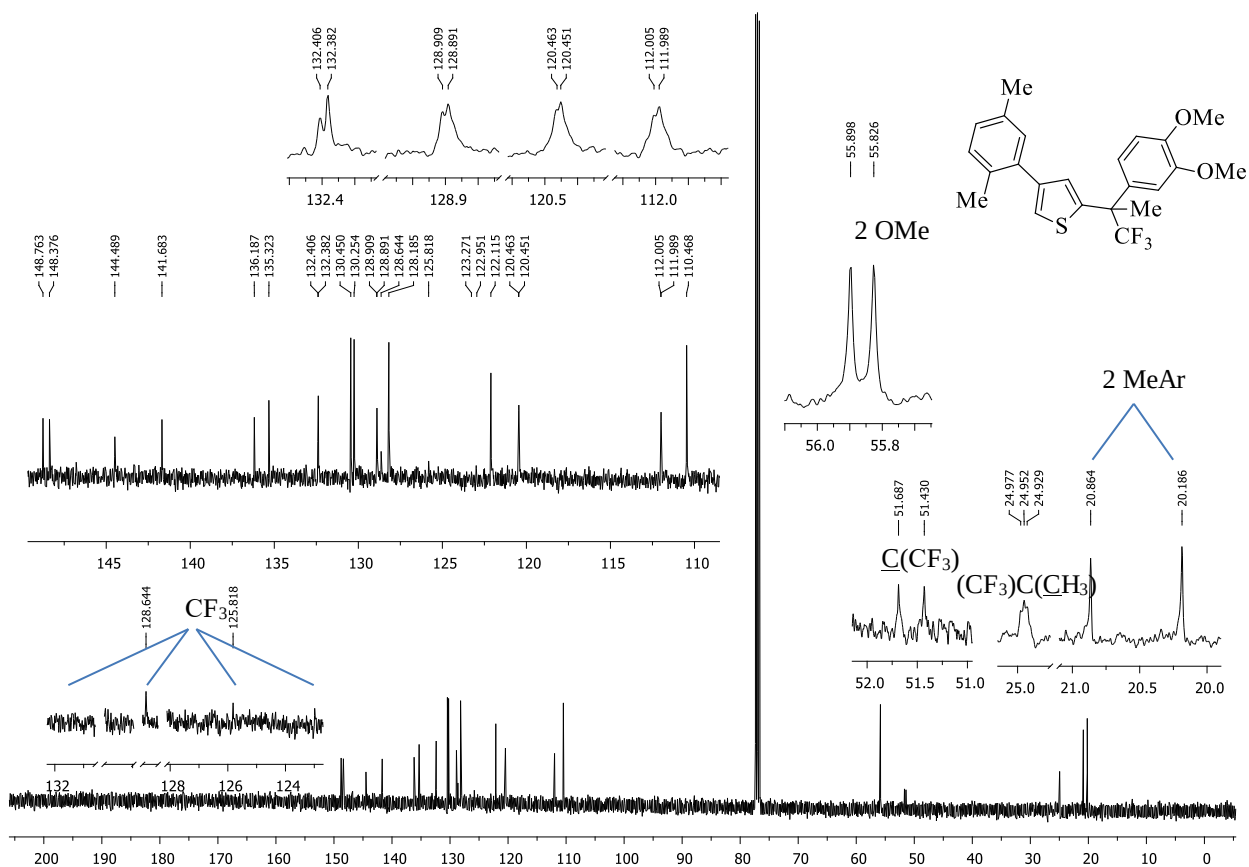


Fig. S178. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **6fa** (CDCl_3 , 101 MHz).

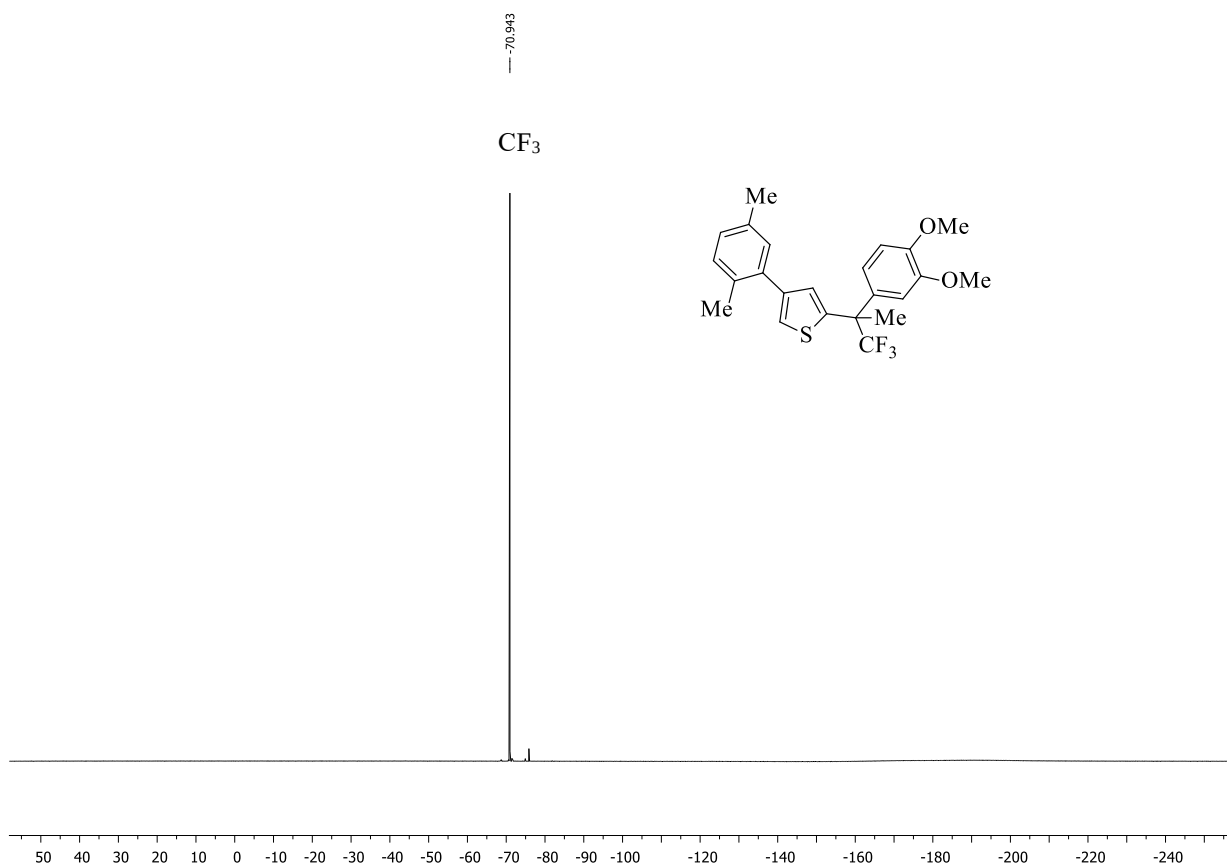


Fig. S179. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **6fa** (CDCl_3 , 376 MHz).

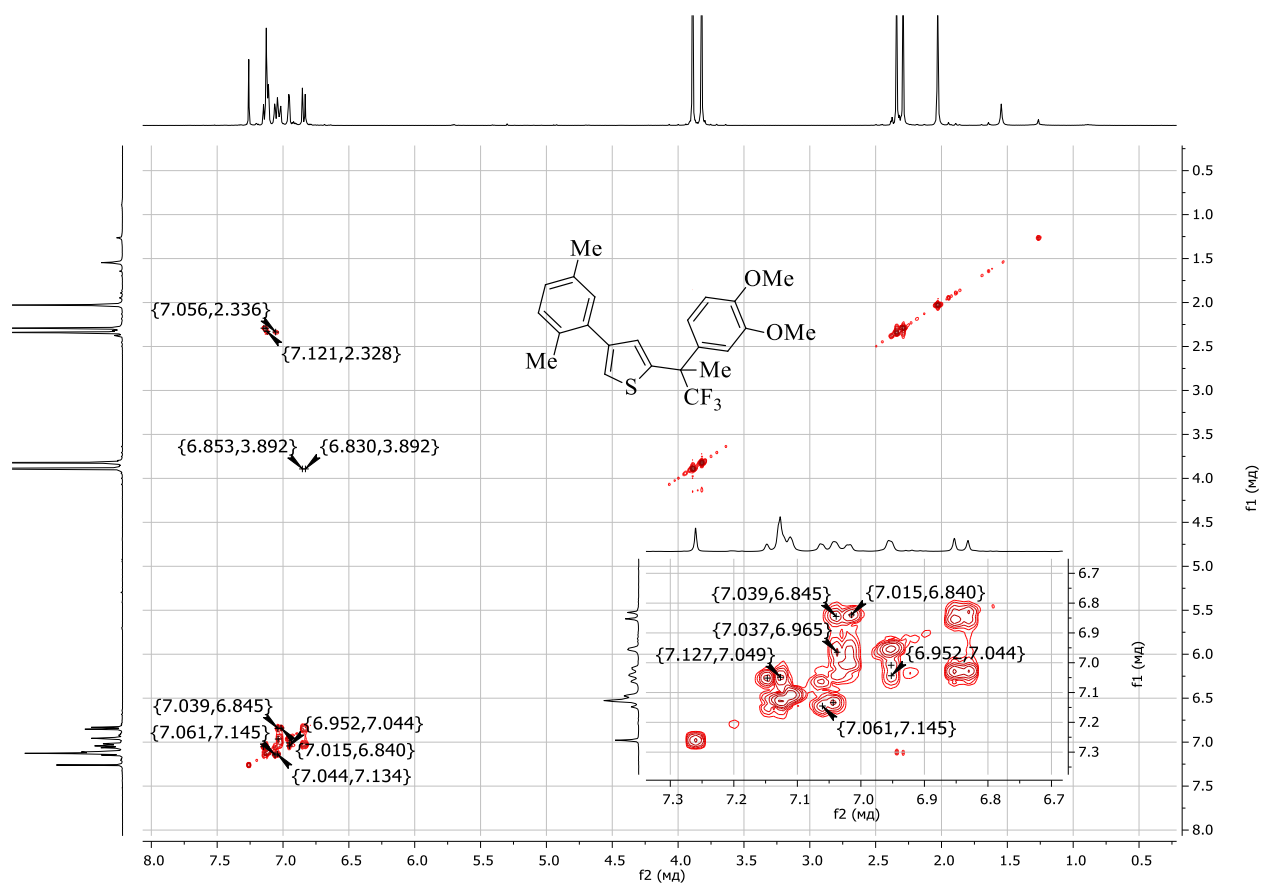


Fig. S180. COSY H-H NMR spectrum of the compound **6fa** (400 MHz, CDCl₃).

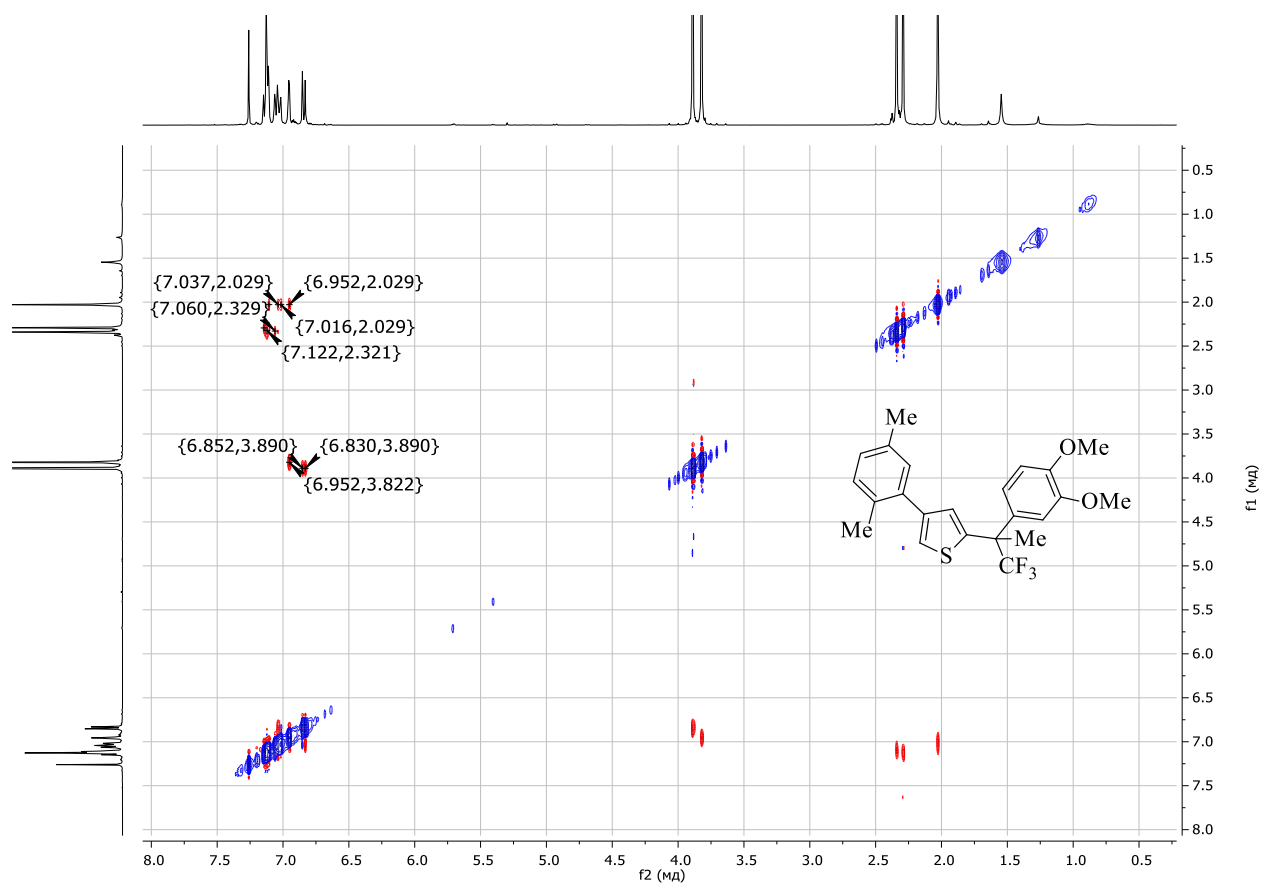


Fig. S181. NOESY H-H NMR spectrum of the compound **6fa** (400 MHz, CDCl₃).

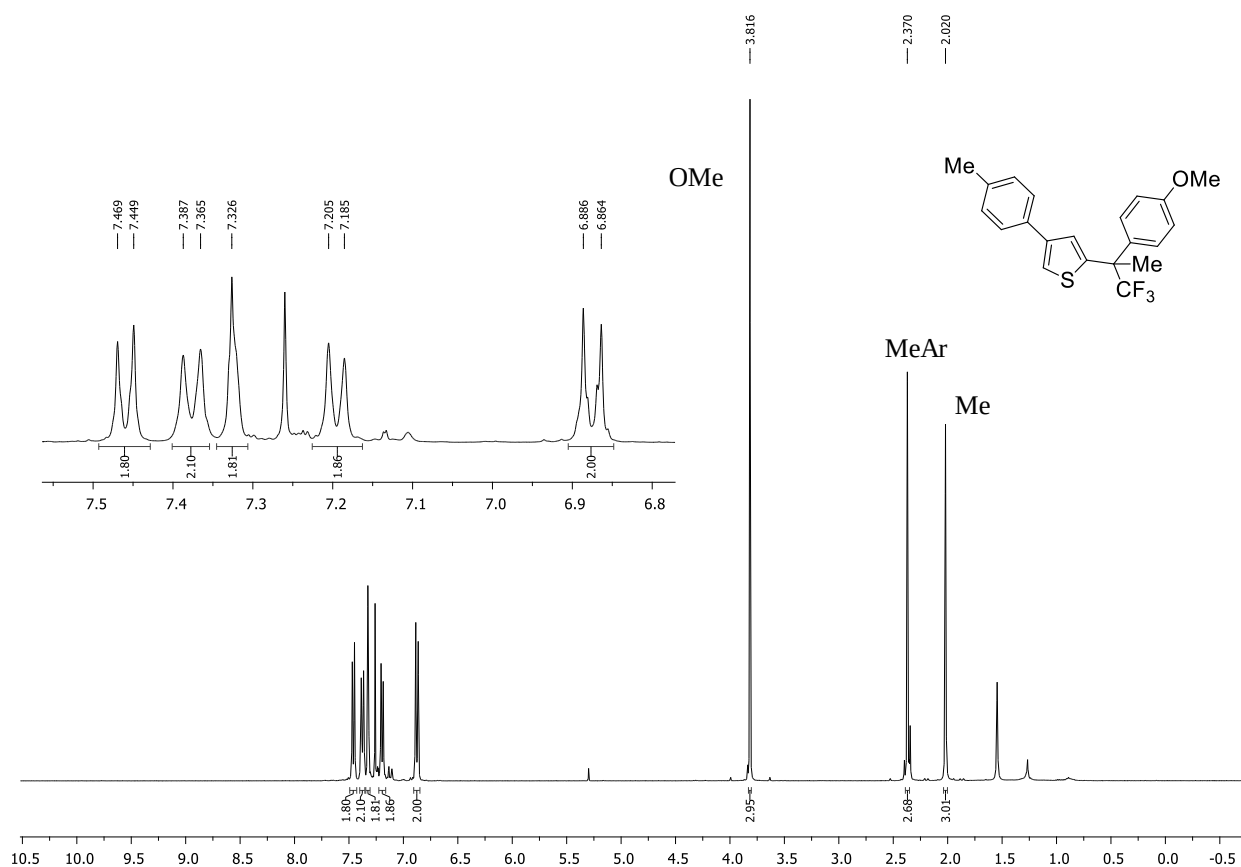


Fig. S182. ¹H NMR spectrum of the compound **6fb** (CDCl₃, 400 MHz).

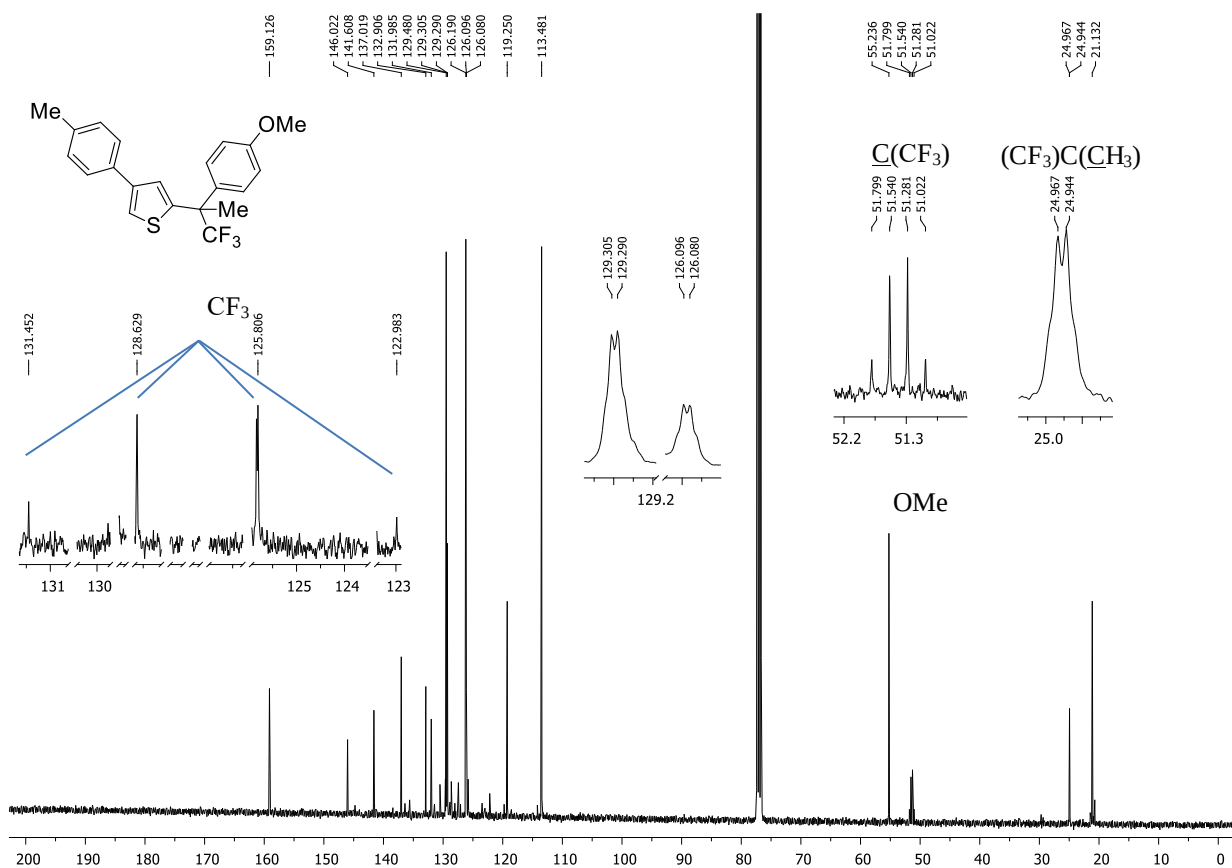


Fig. S183. ¹³C{¹H} NMR spectrum of the compound **6fb** (CDCl₃, 101 MHz).

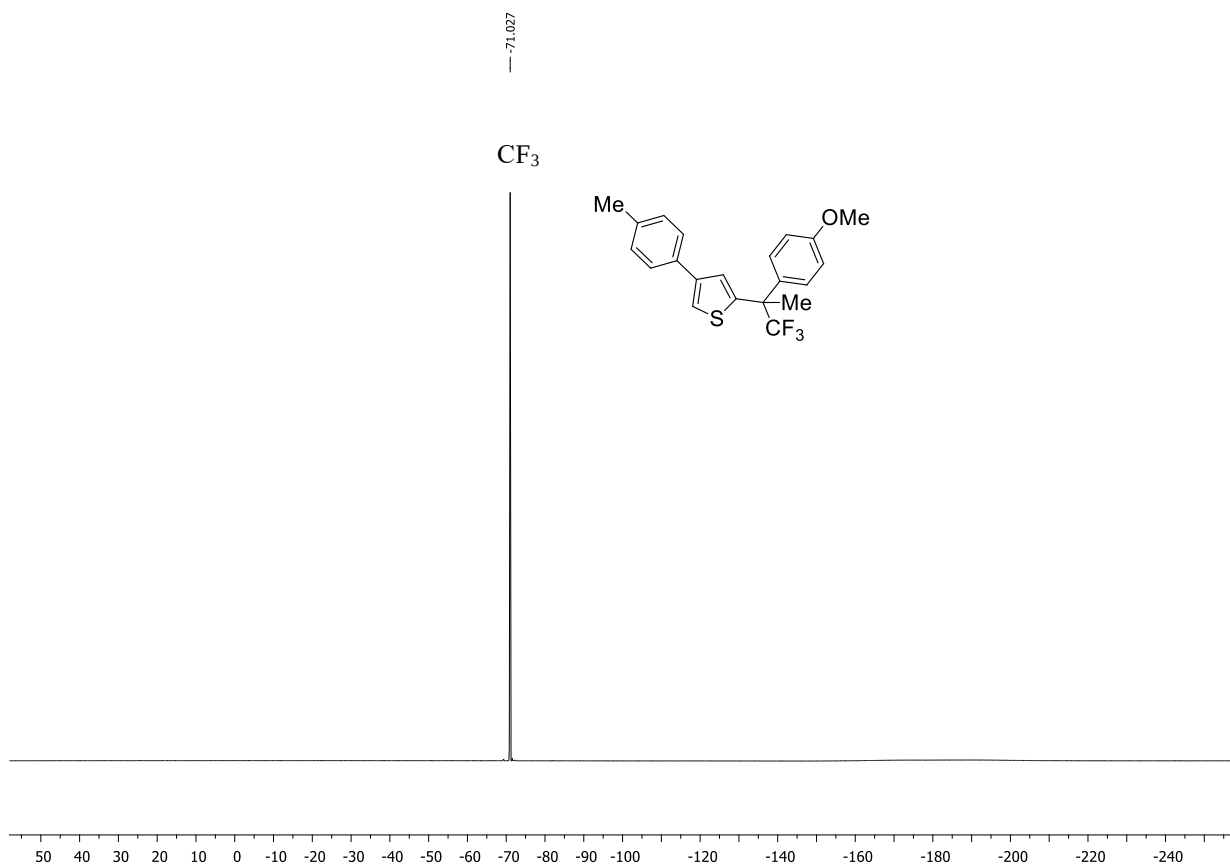


Fig. S184. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **6fb** (CDCl_3 , 376 MHz).

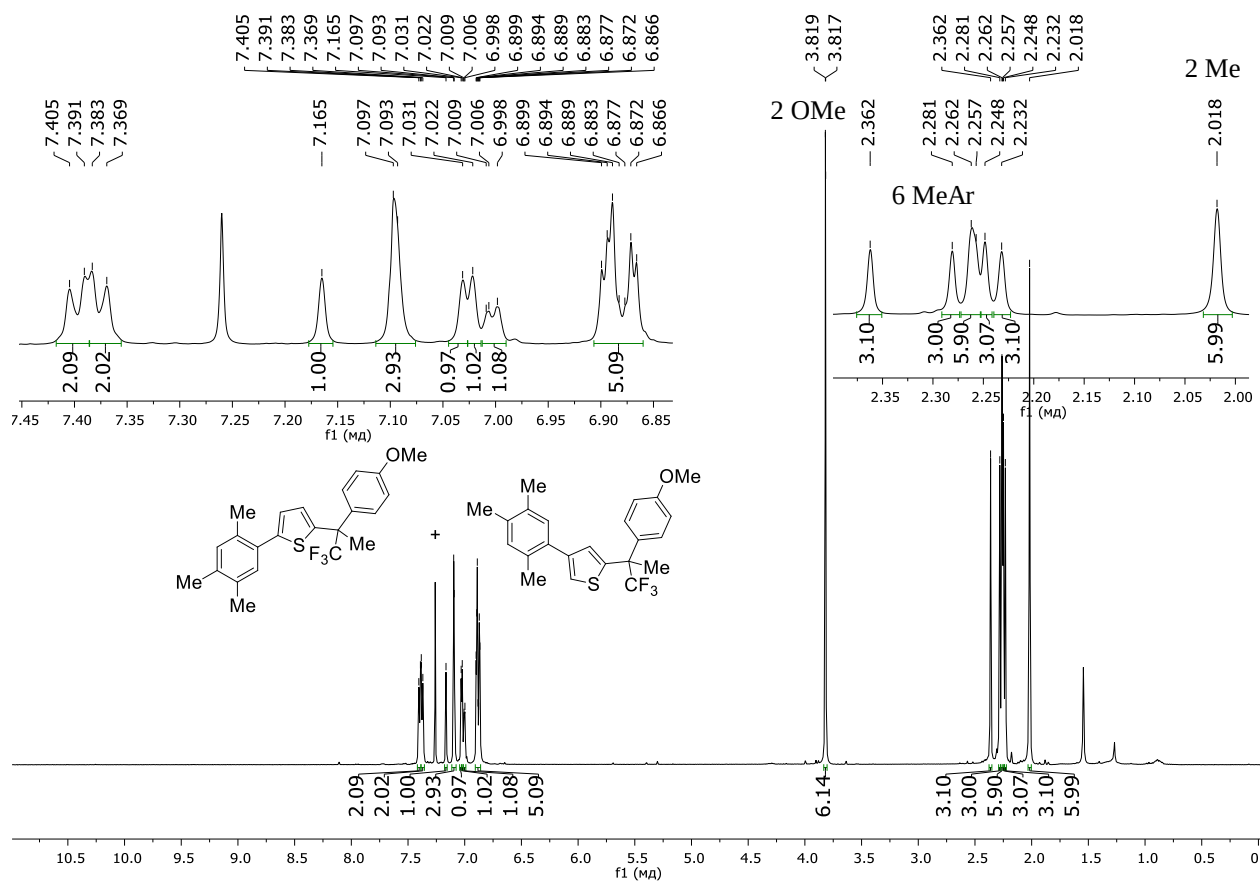


Fig. S185. ^1H NMR spectrum of the compounds **α-6fc** and **β-6fc** (CDCl_3 , 400 MHz).

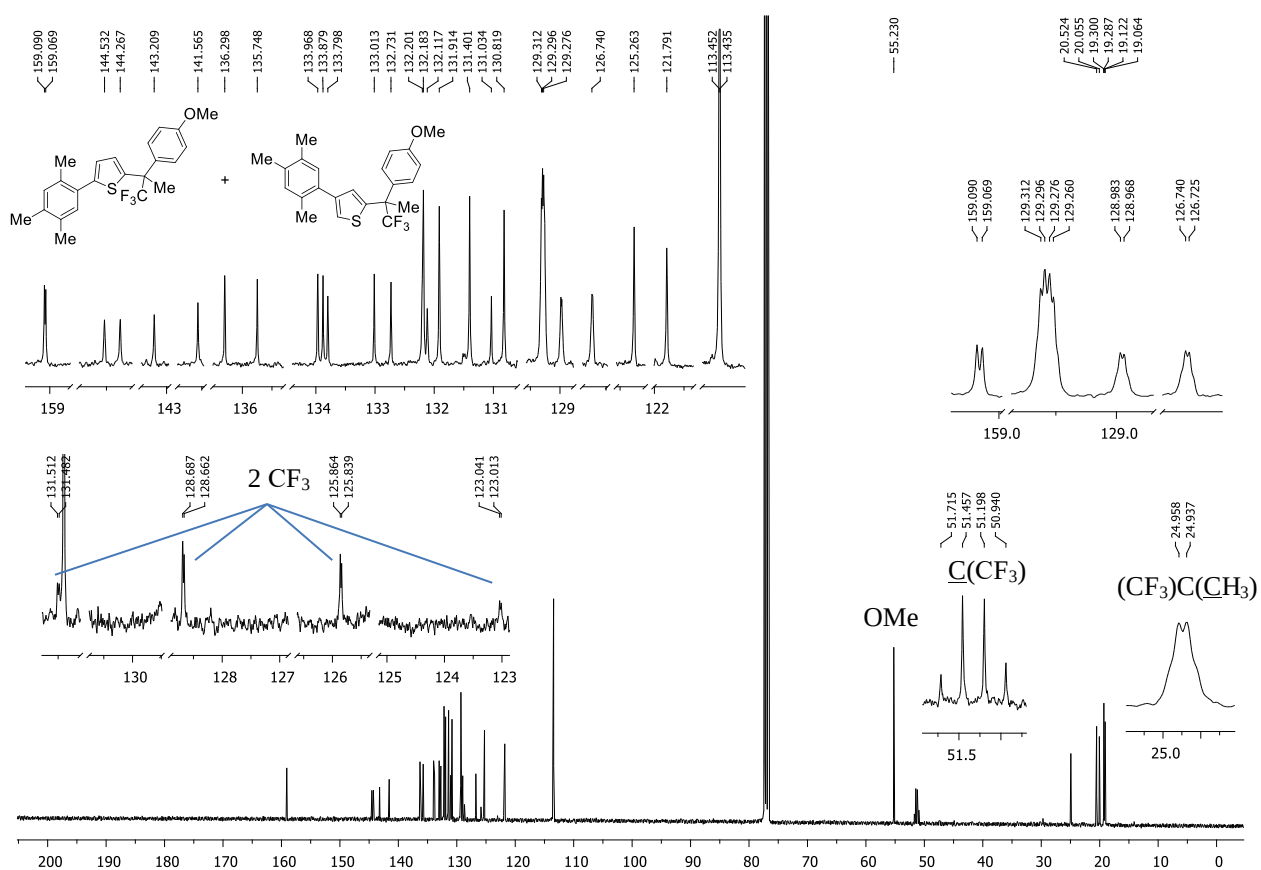


Fig. S186. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compounds α -6fc and β -6fc (CDCl₃, 101 MHz).

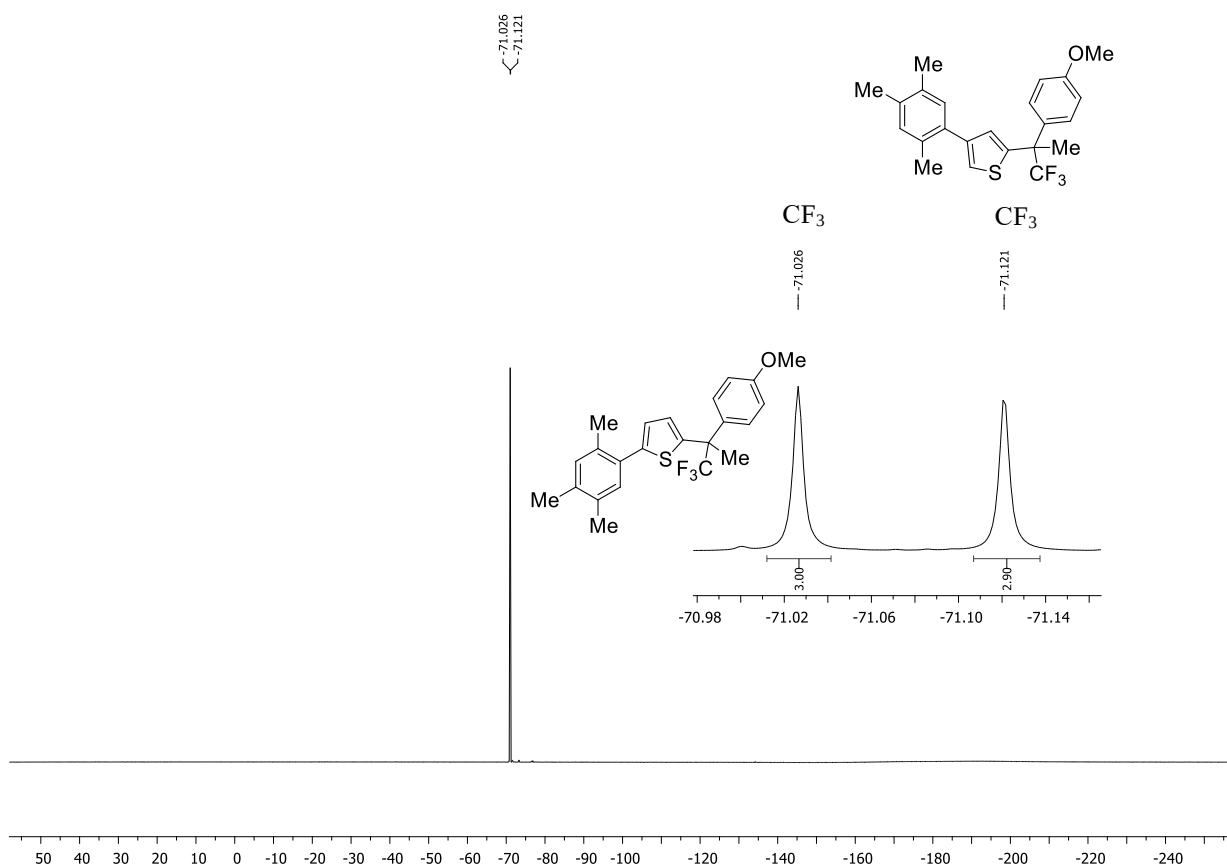


Fig. S187. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compounds α -6fc and β -6fc (CDCl₃, 376 MHz).

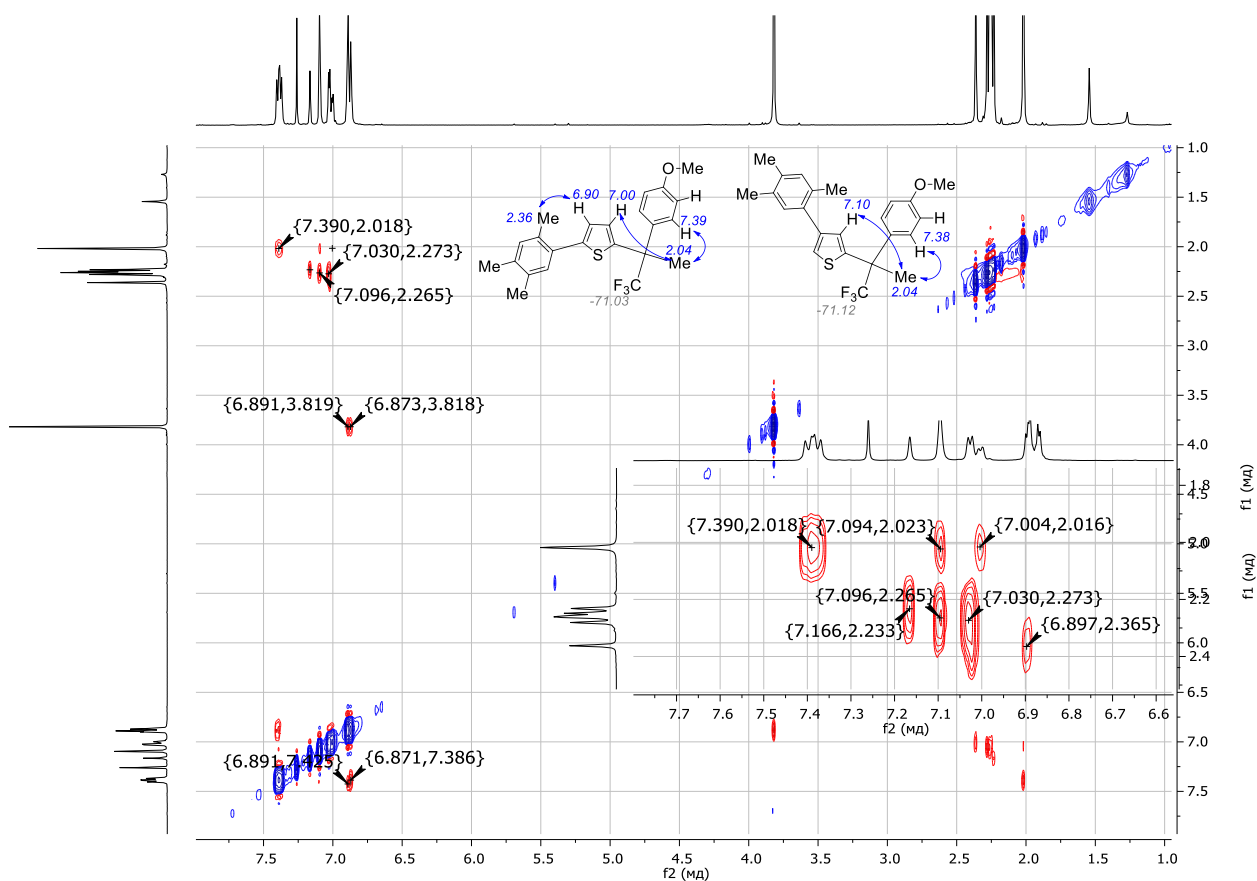


Fig. S188. NOESY H-H NMR spectrum of the compounds **α-6fc** and **β-6fc** (400 MHz, CDCl₃).

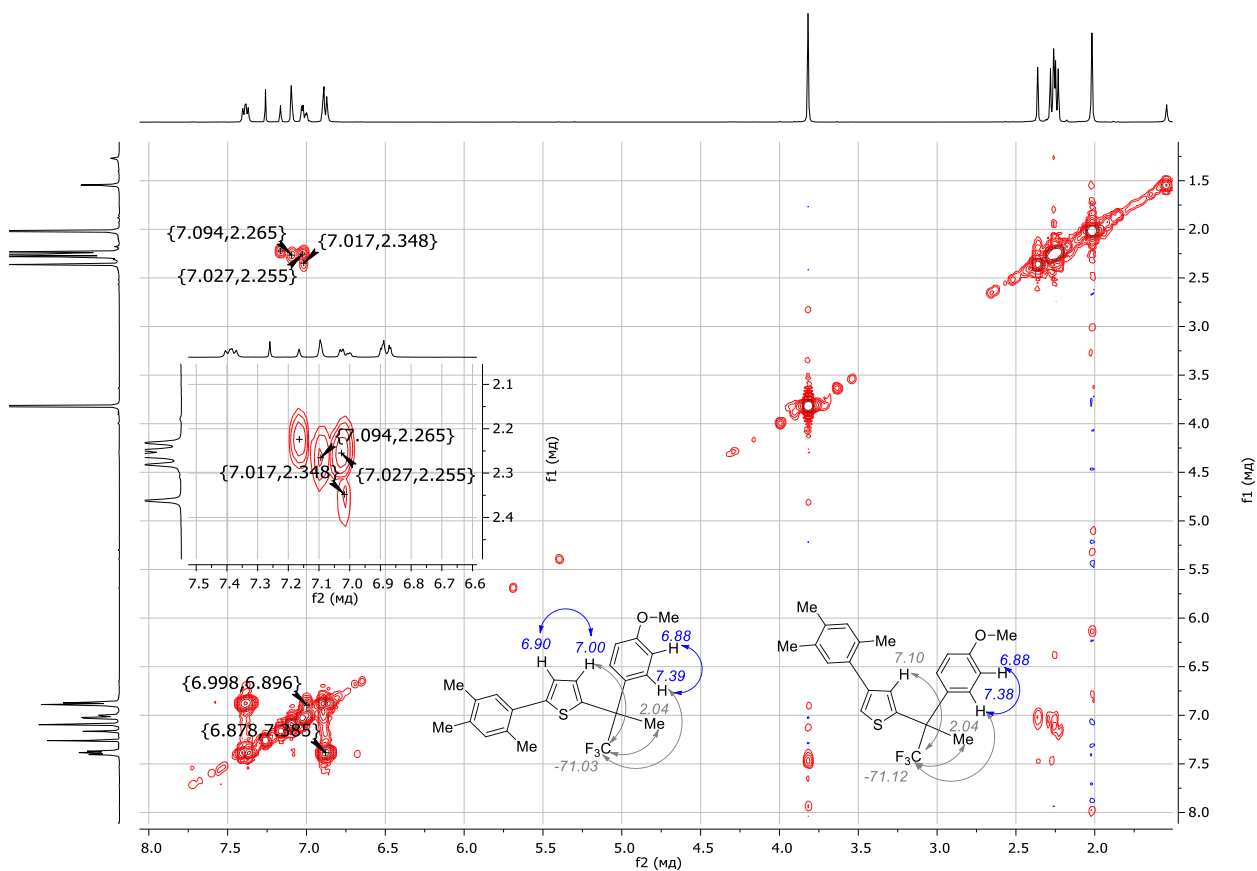


Fig. S189. COSY H-H NMR spectrum of the compounds **α-6fc** and **β-6fc** (400 MHz, CDCl₃).

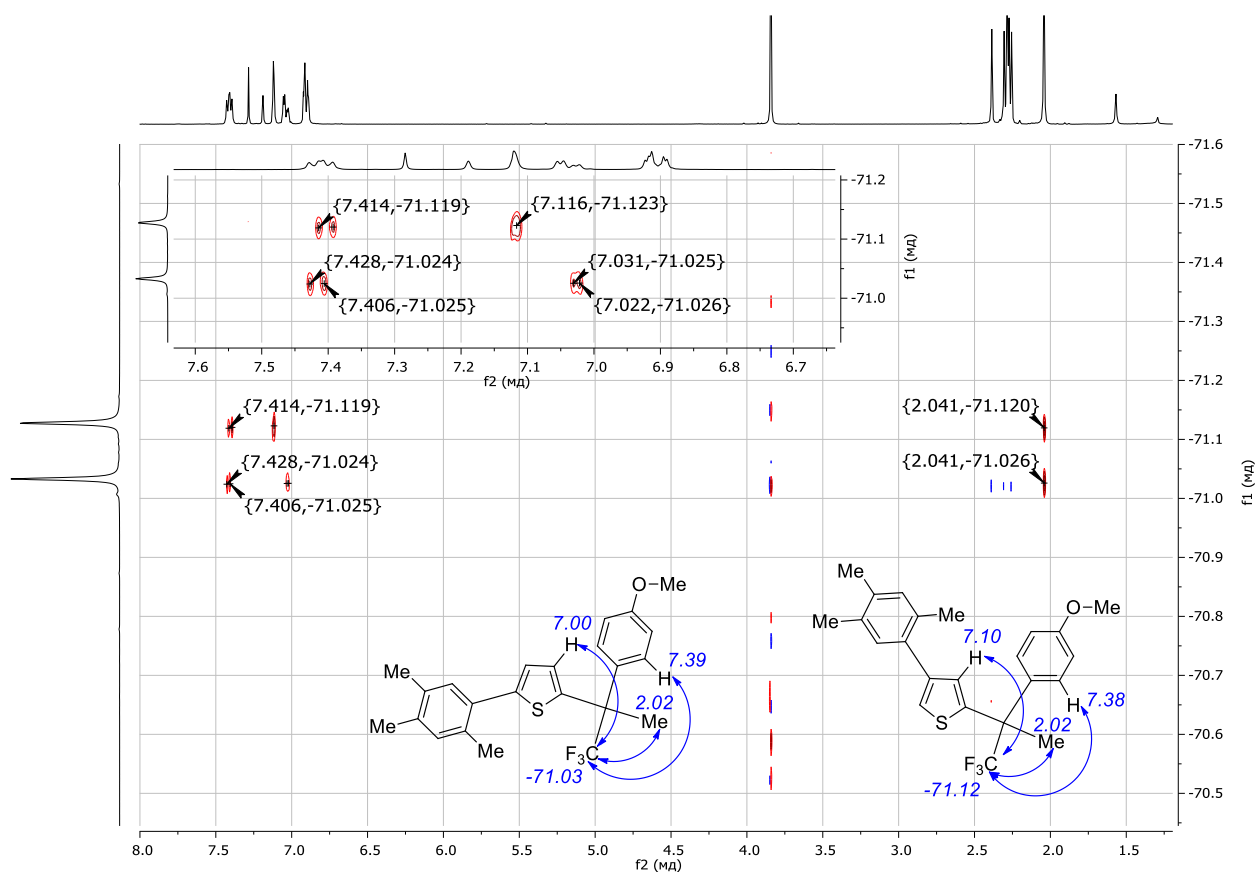


Fig. S190. HOESY H-F NMR spectrum of the compounds α -6fc and β -6fc (400 MHz, CDCl_3).

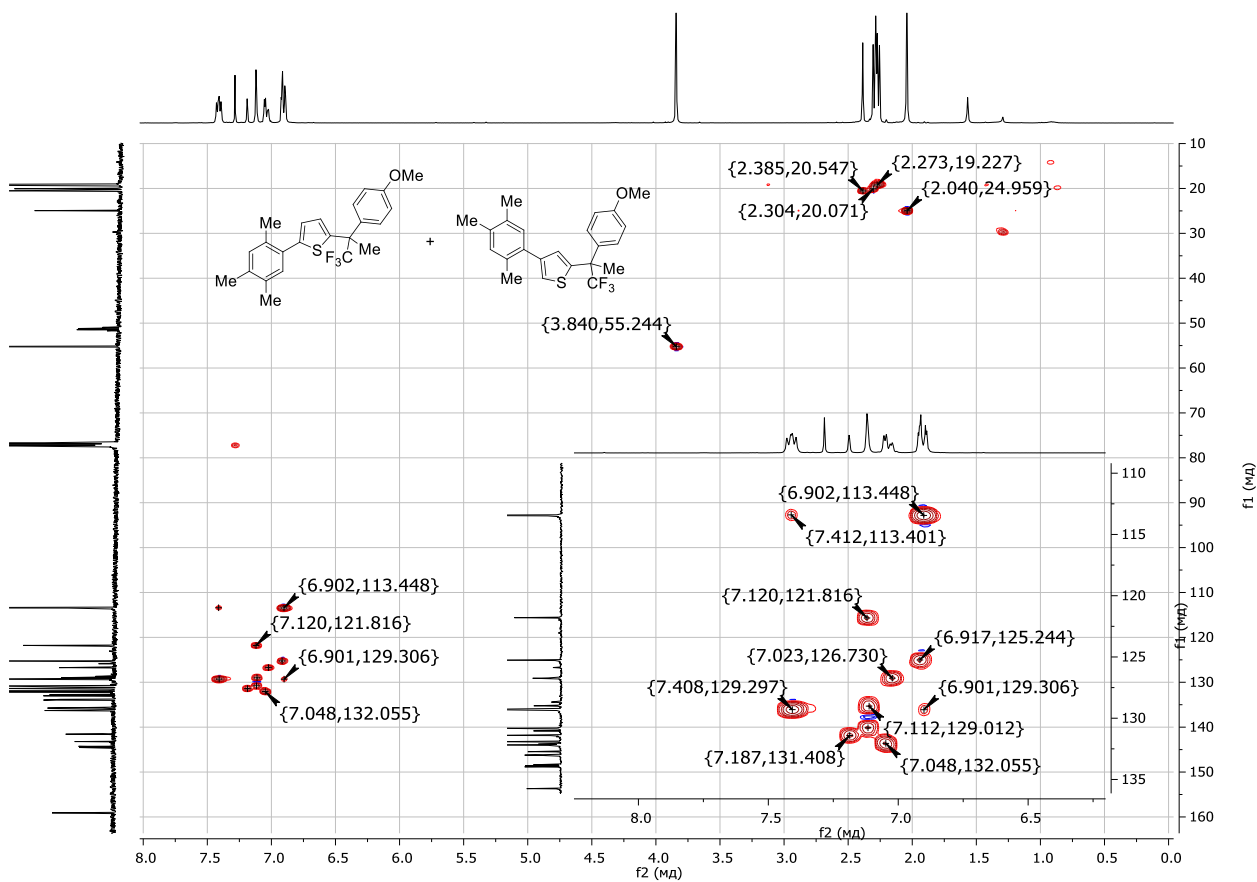


Fig. S191. HSQC C-H NMR spectrum of the compounds α -6fc and β -6fc (101-400 MHz, CDCl_3).

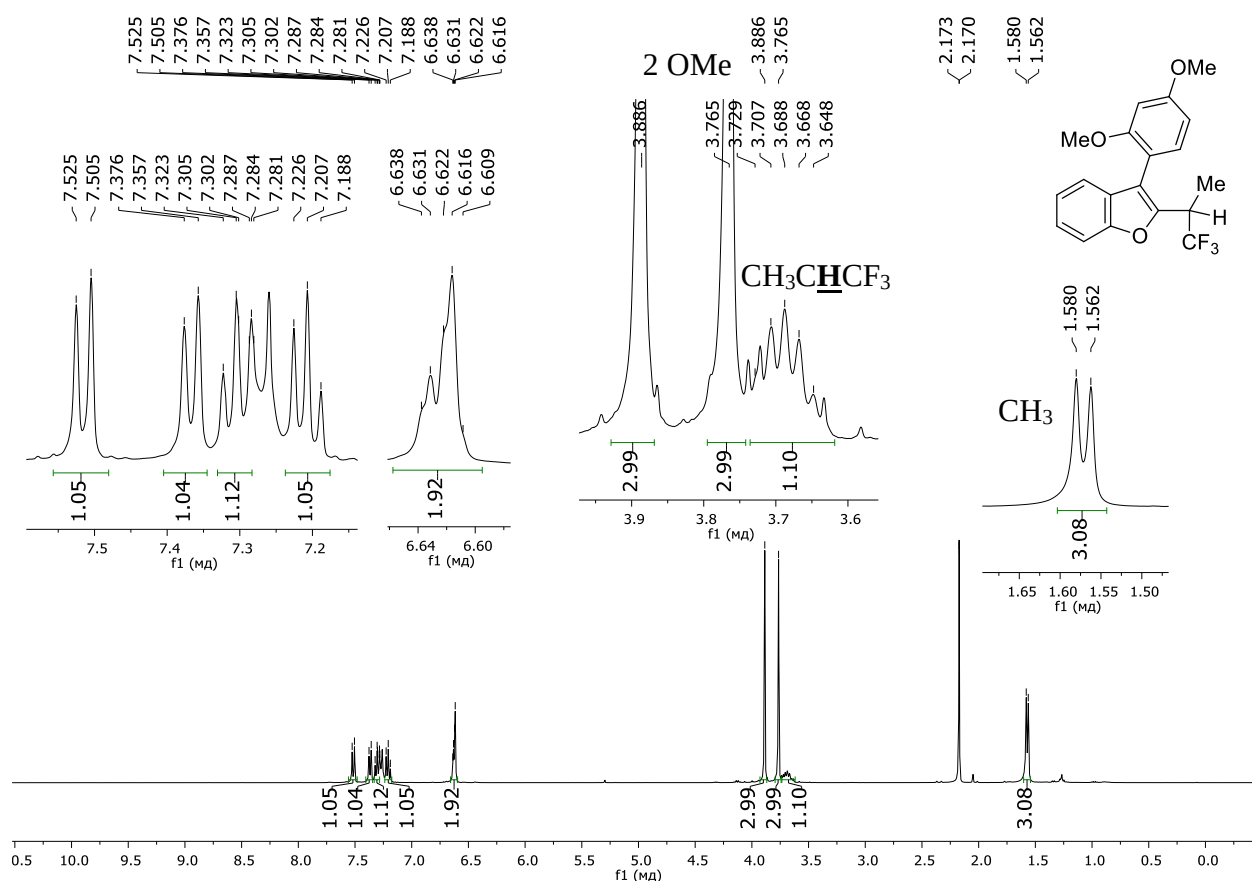


Fig. S192. ¹H NMR spectrum of the compound **7b** (CDCl₃, 400 MHz).

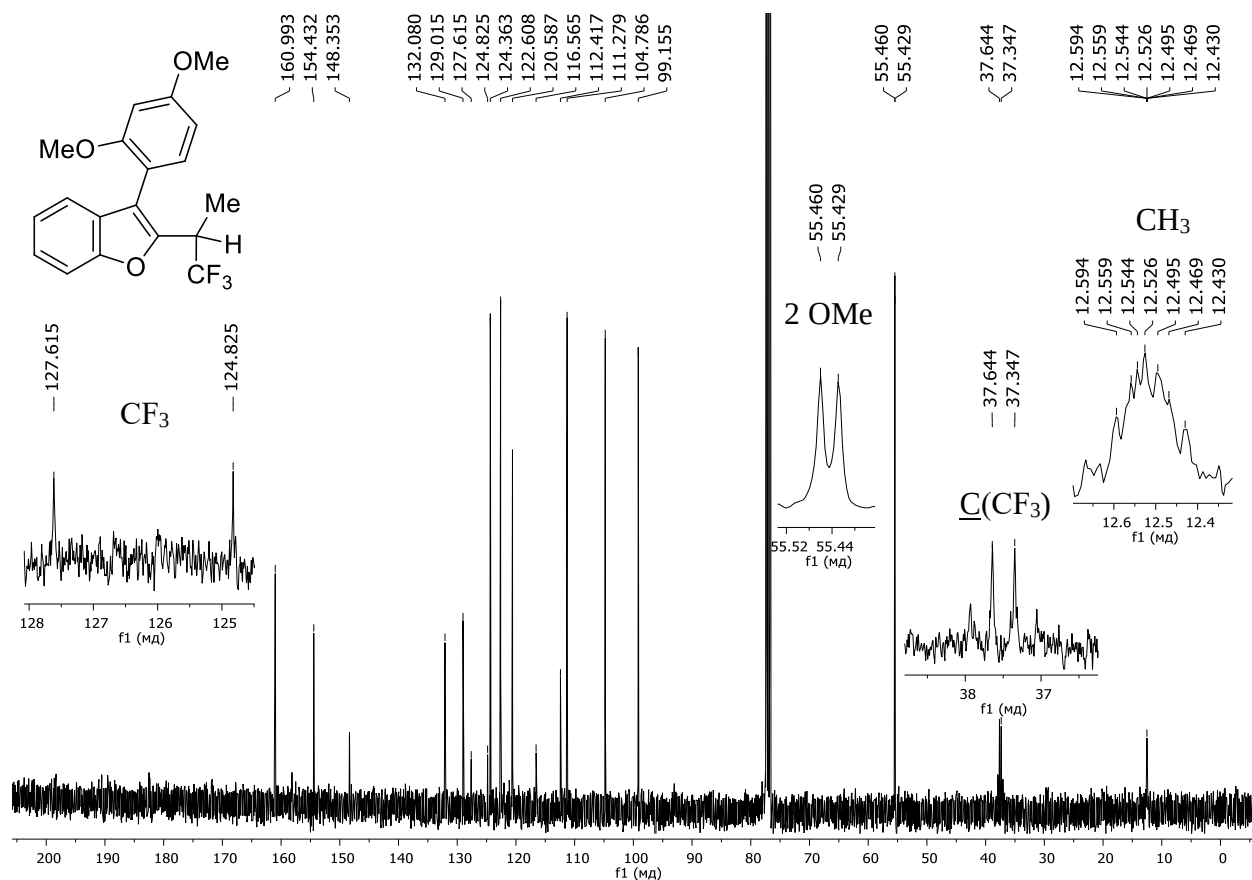


Fig. S193. ¹³C{¹H} NMR spectrum of the compound **7b** (CDCl₃, 101 MHz).

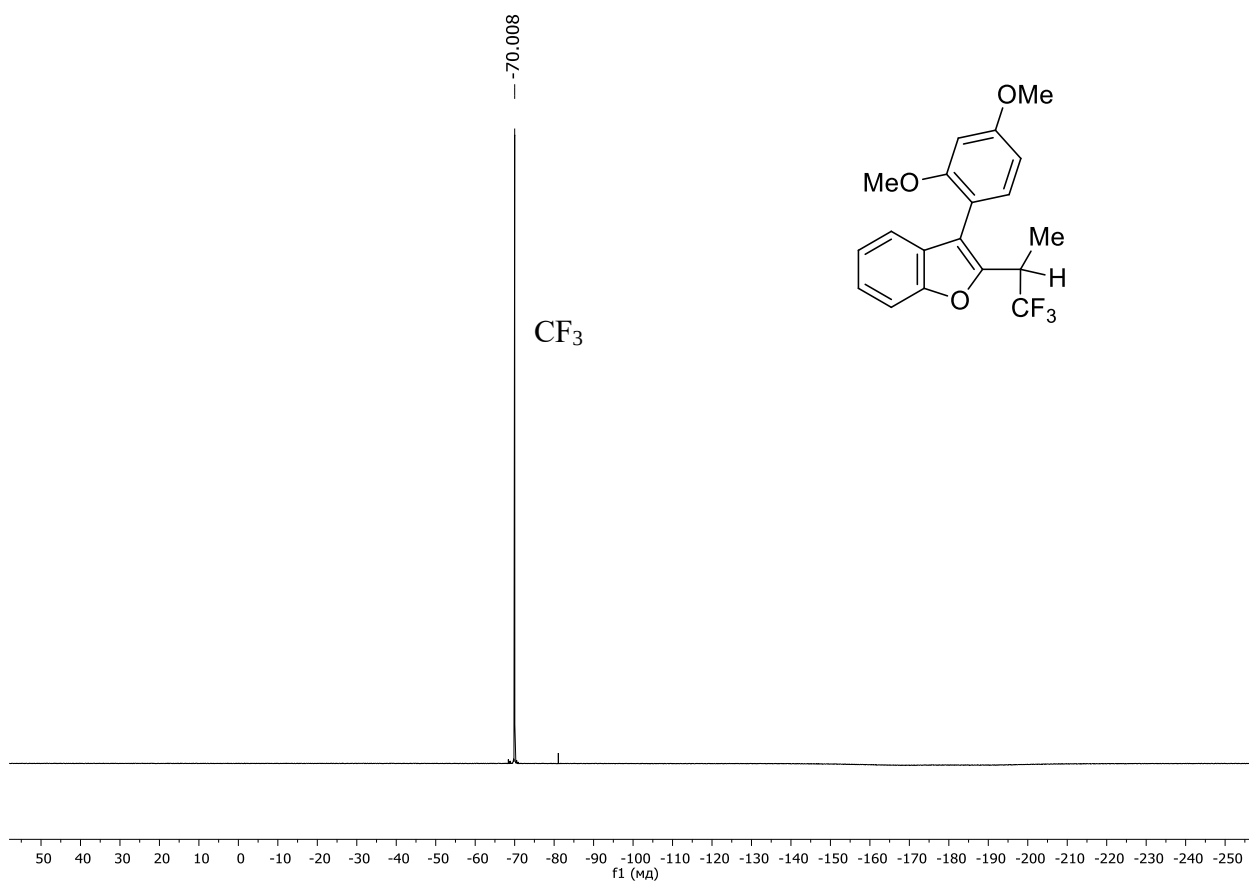


Fig. S194. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **7b** (CDCl_3 , 376 MHz).

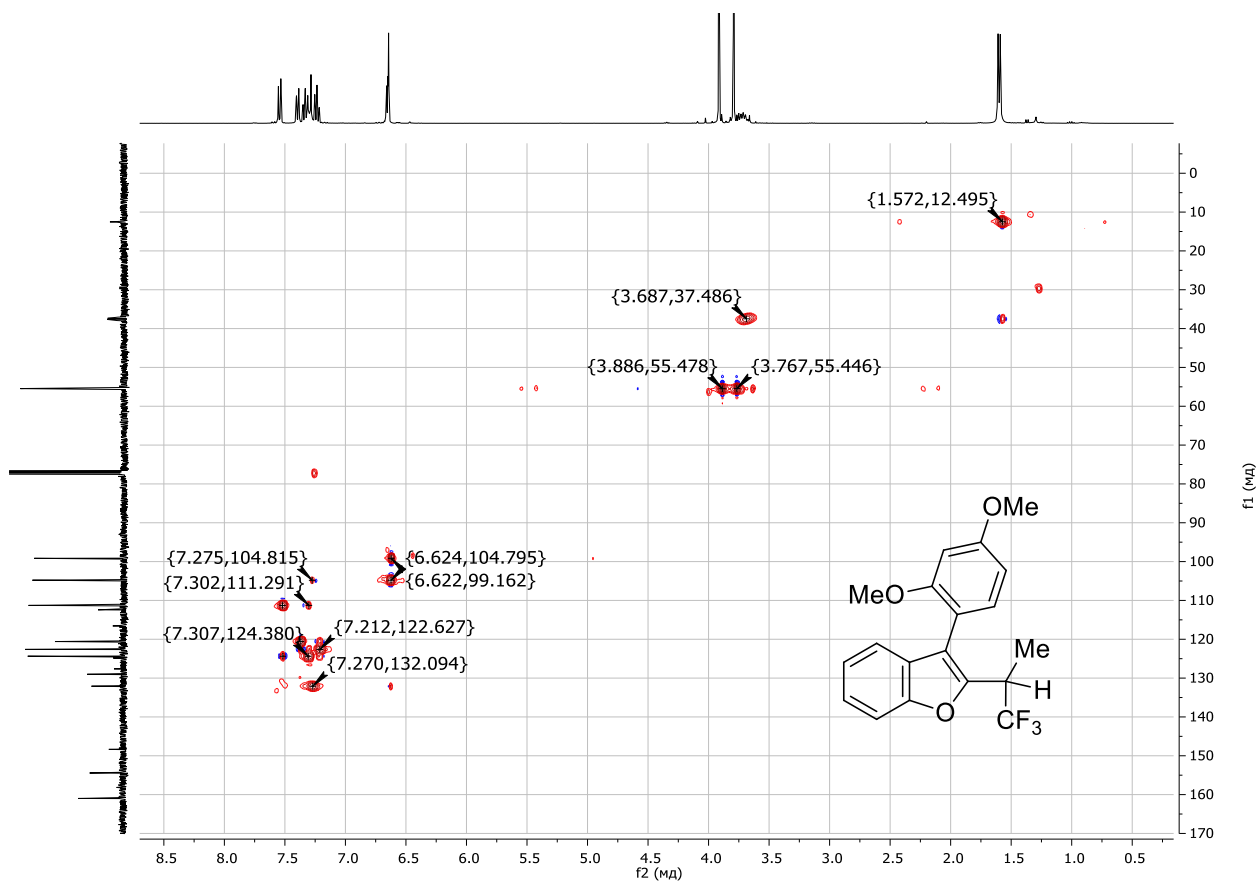


Fig. S195. HSQC C-H NMR spectrum of the compound **7b** (CDCl_3 , 101-400 MHz).

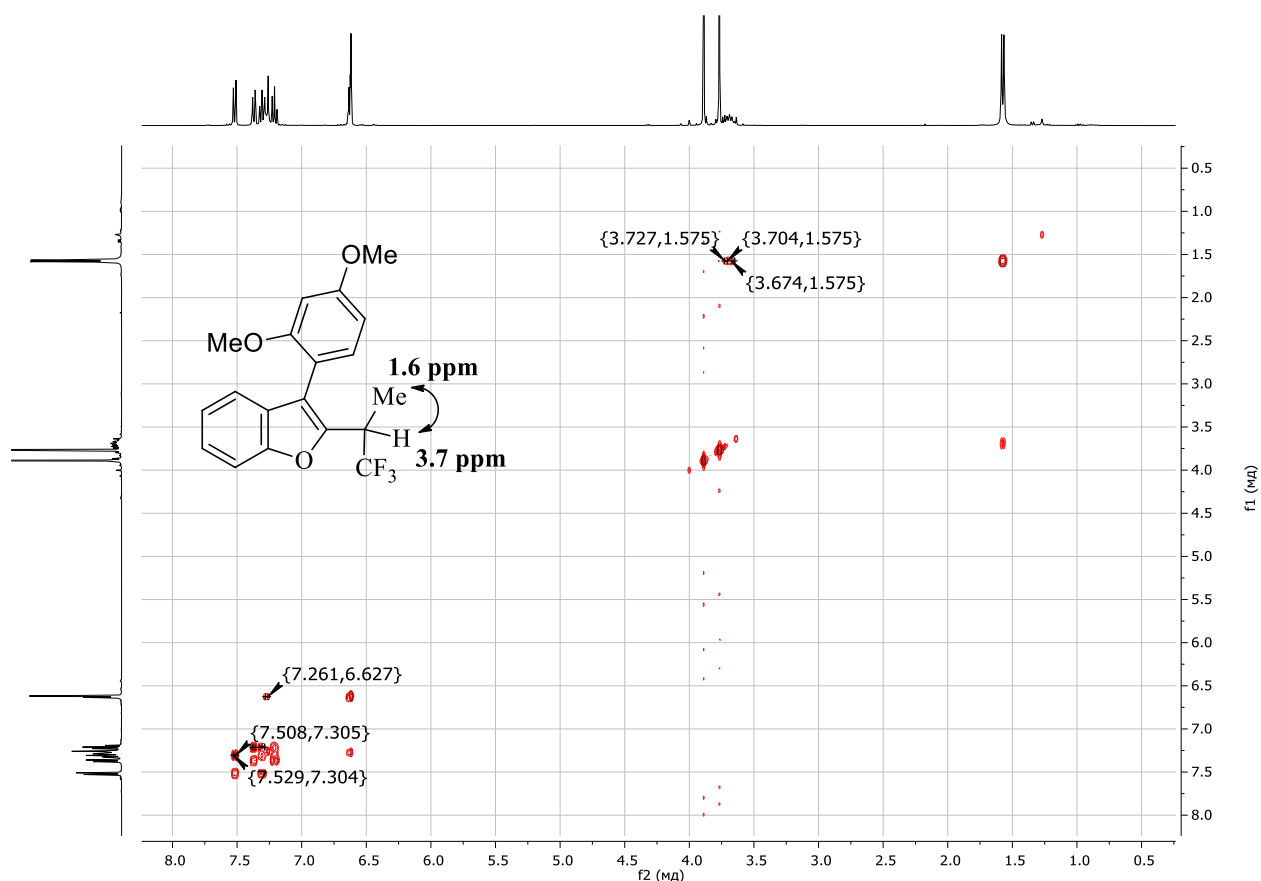


Fig. S196. COSY H-H spectrum of the compound **7b** (CDCl_3 , 400 MHz).

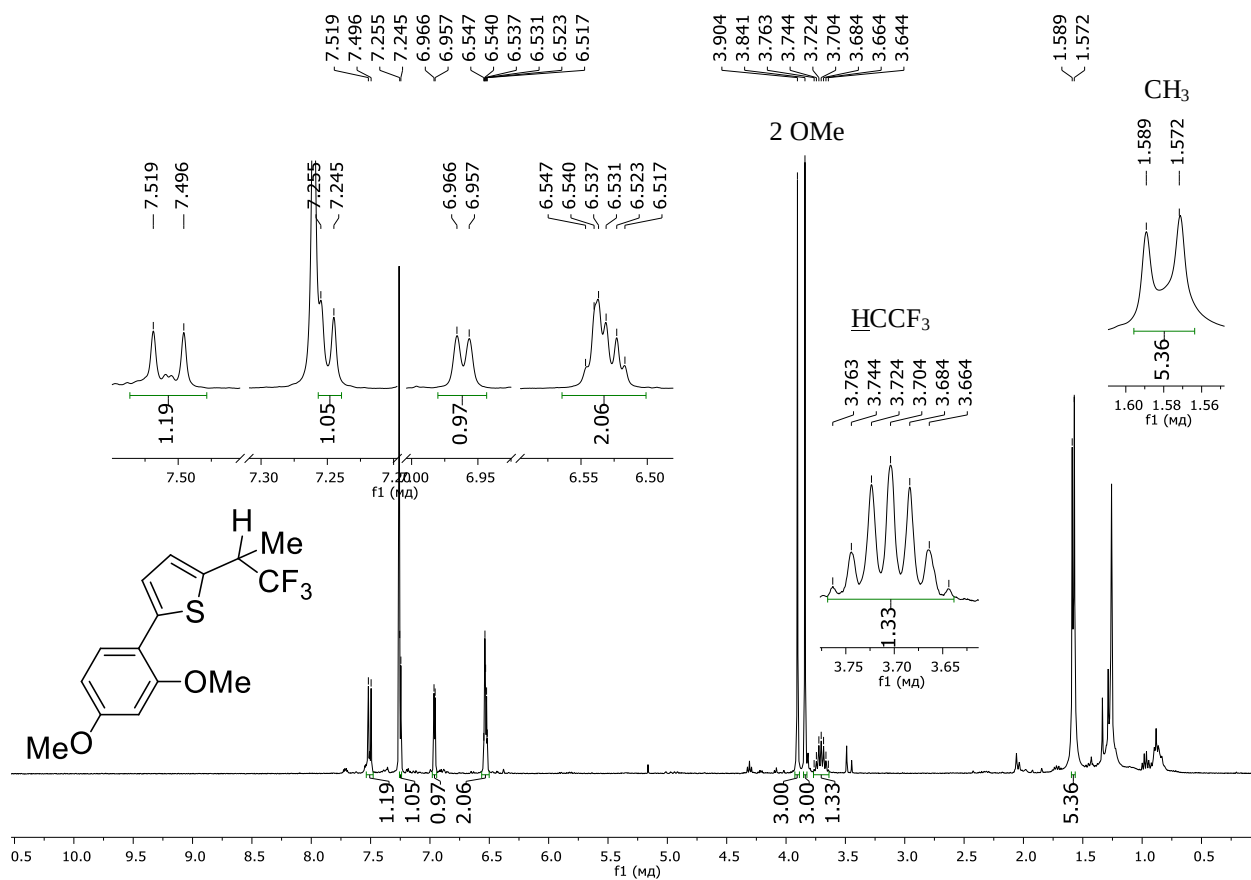


Fig. S197. ^1H NMR spectrum of the compound **7d** (CDCl_3 , 400 MHz).

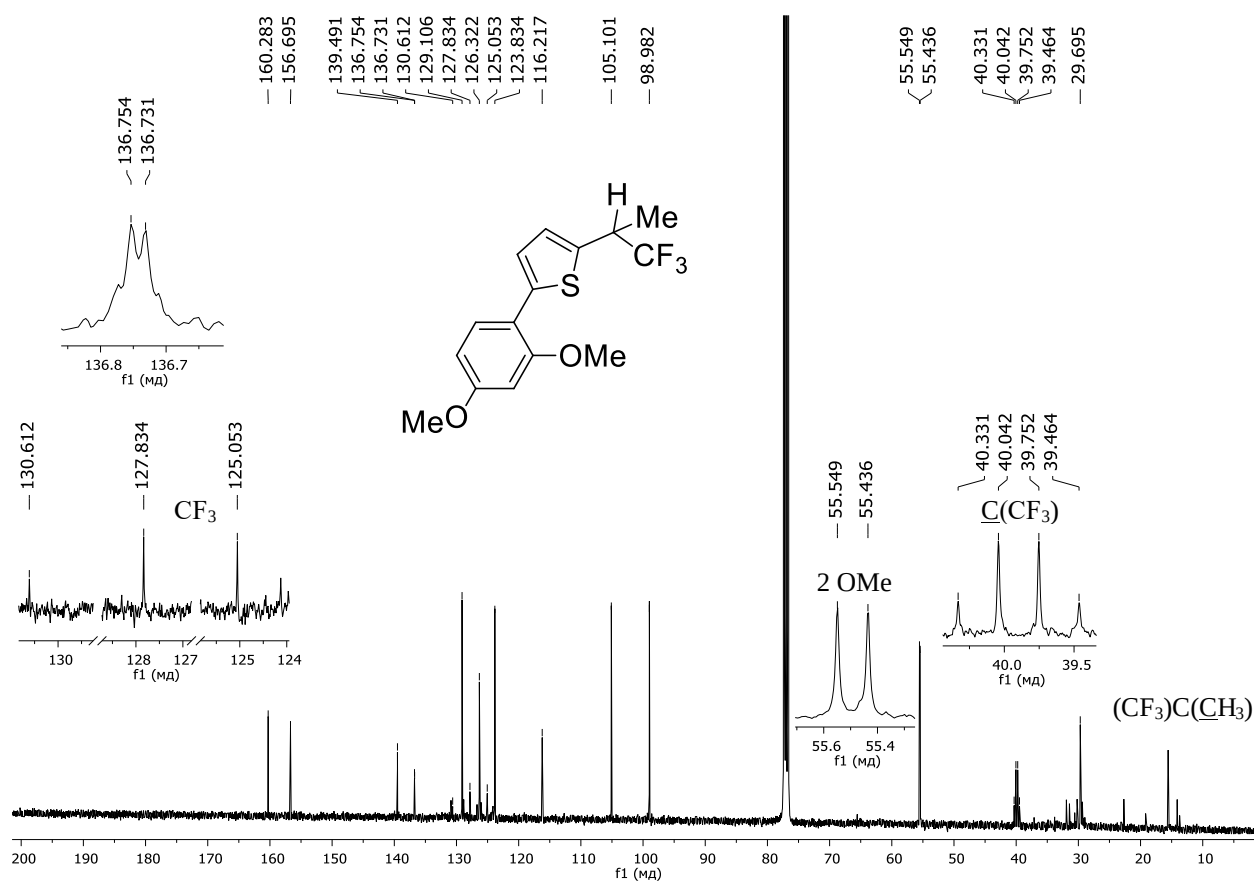


Fig. S198. ¹³C{¹H} NMR spectrum of the compound **7d** (CDCl₃, 101 MHz).

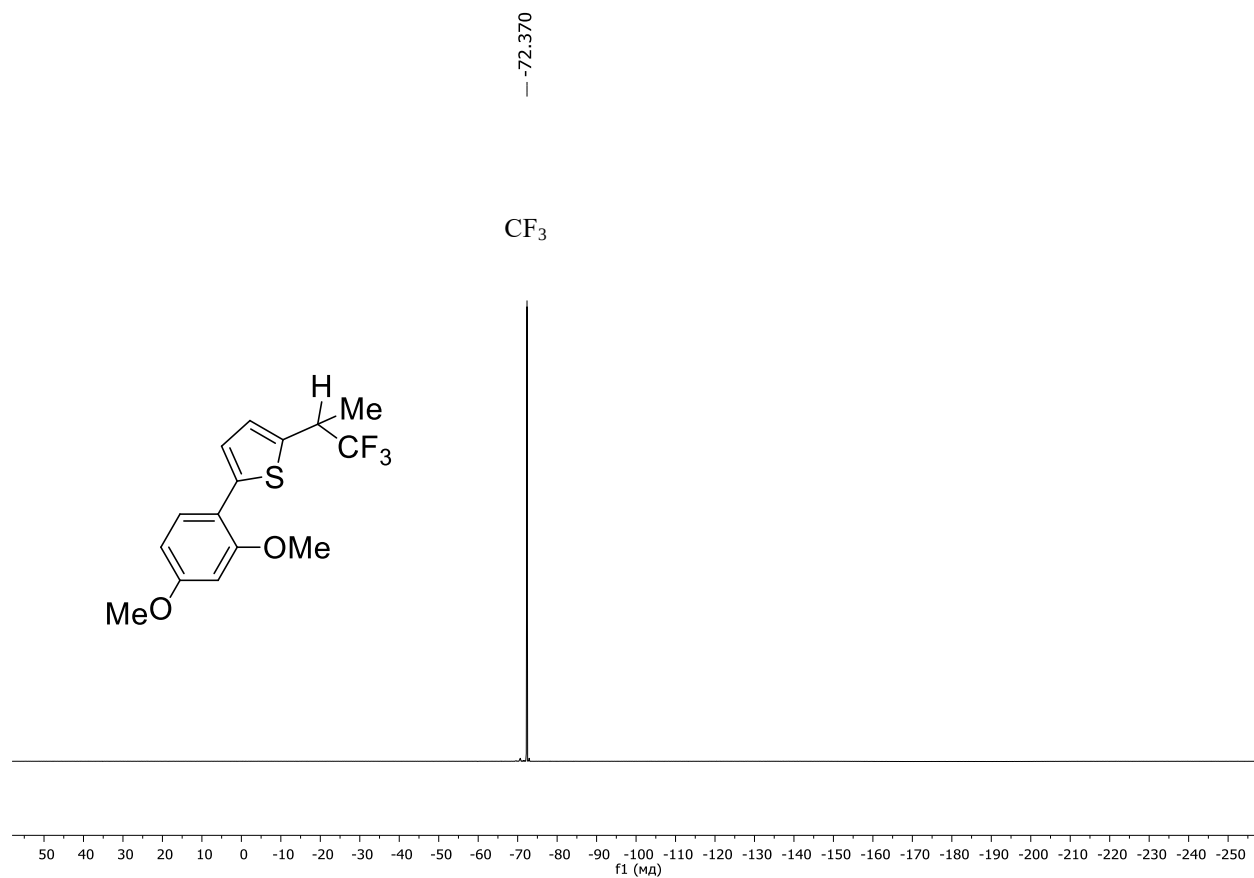
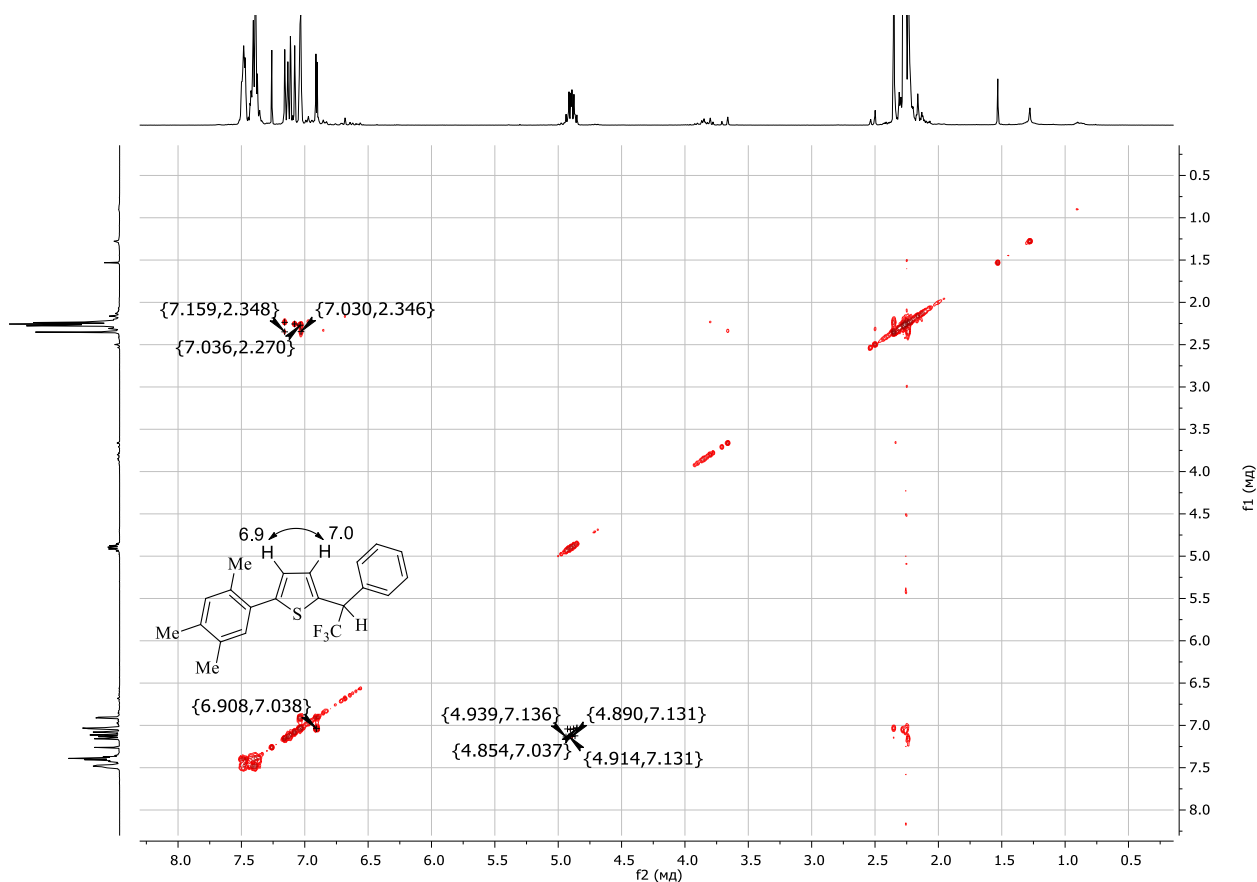
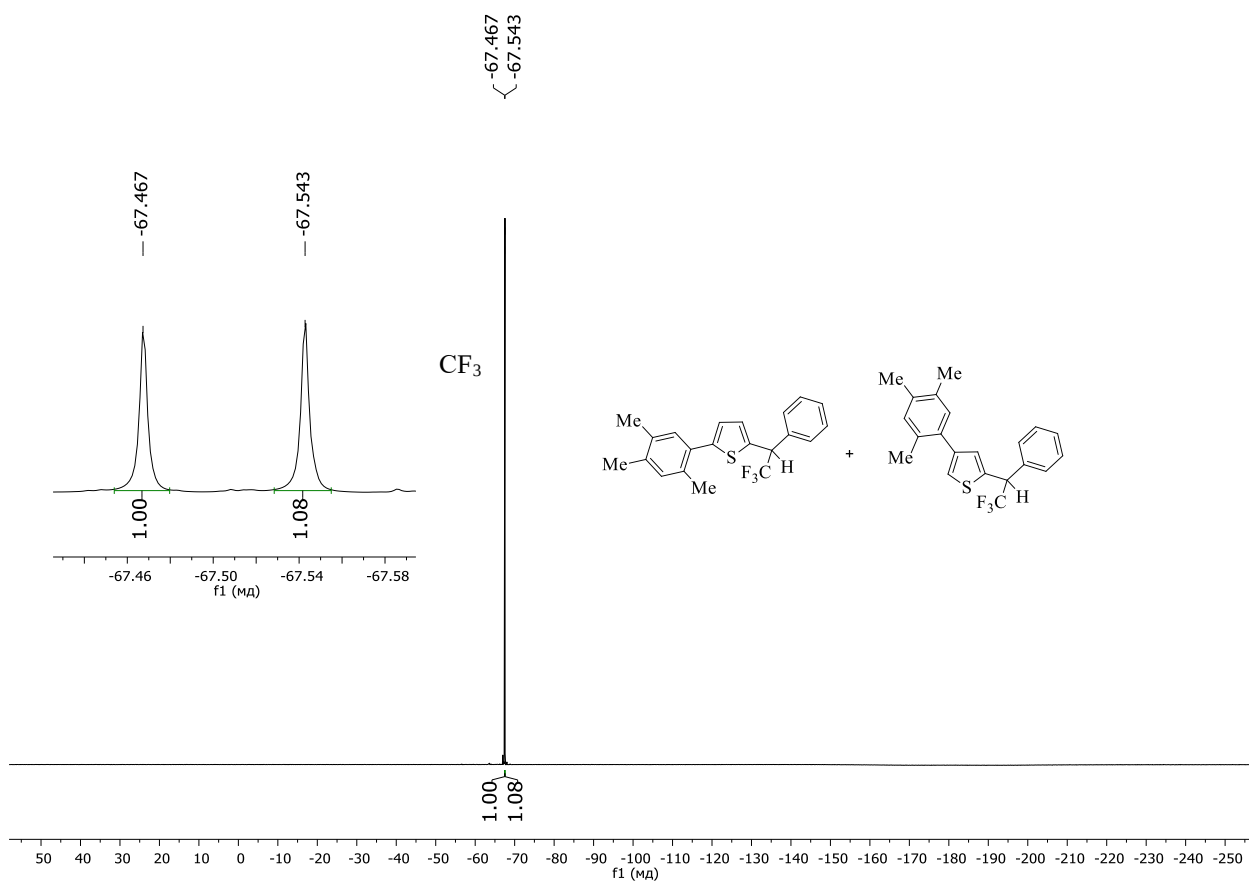


Fig. S199. ¹⁹F{¹H} NMR spectrum of the compound **7d** (CDCl₃, 376 MHz).



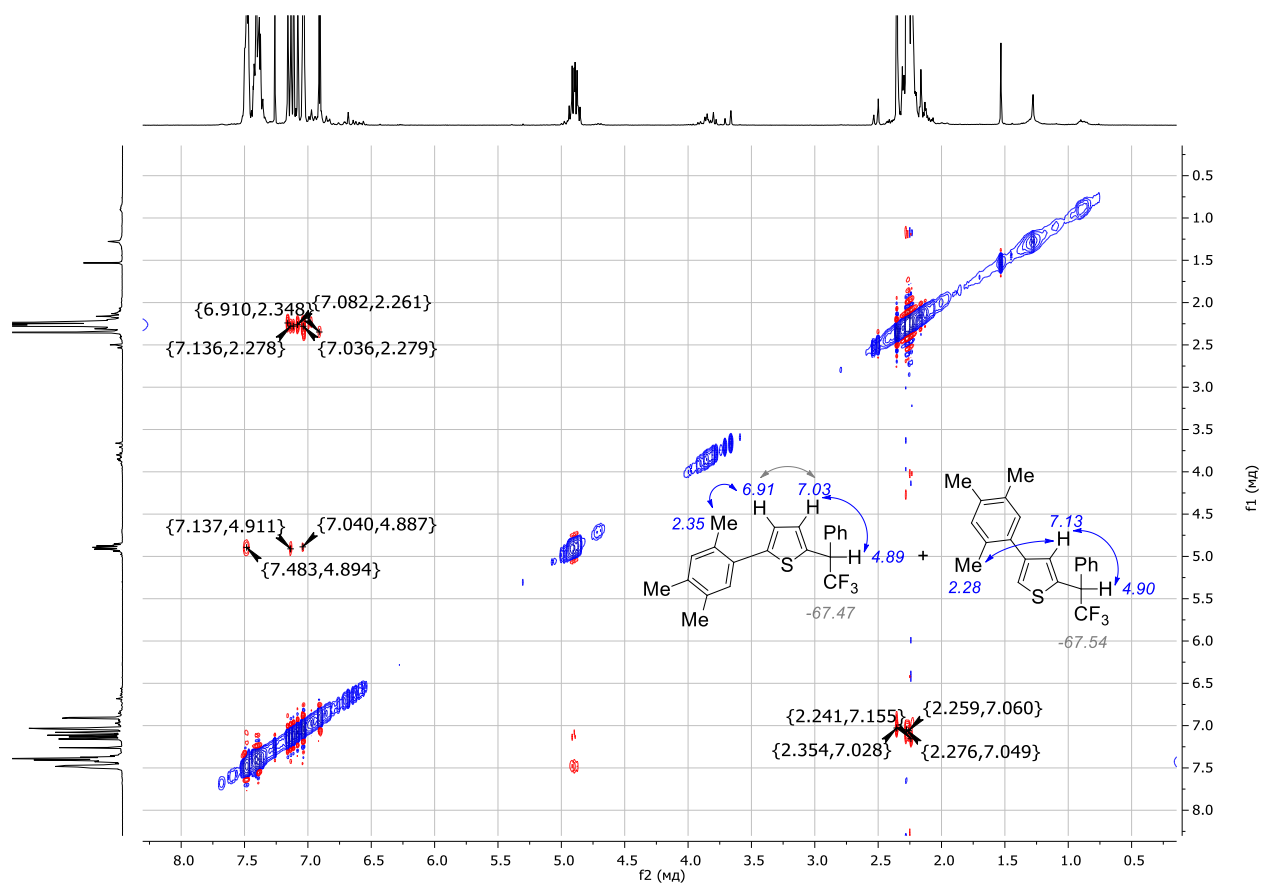


Fig. S204. NOESY H-H NMR spectrum of the mixture of α -7i and β -7i (CDCl_3 , 400 MHz).

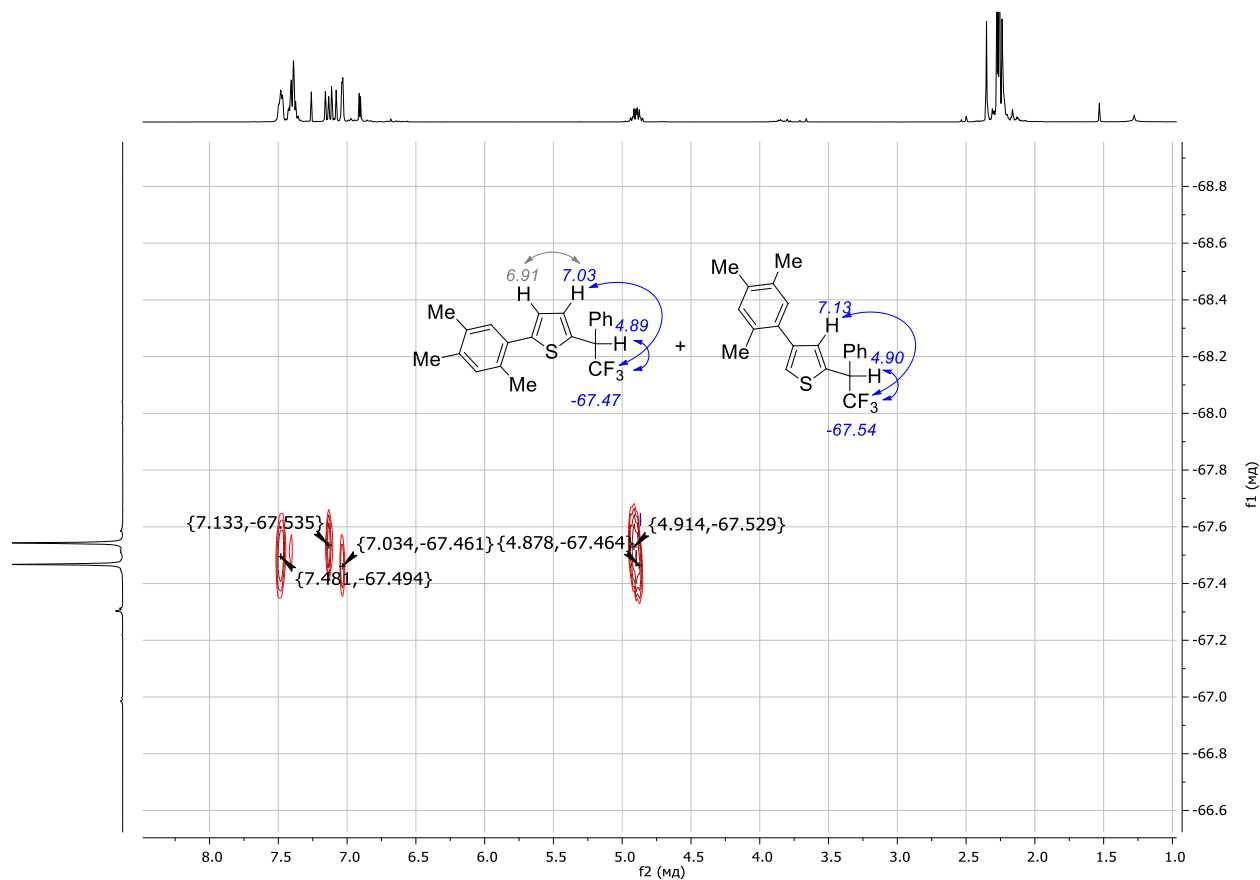


Fig. S205. HOESY F-H NMR spectrum of the mixture of α -7i and β -7i (CDCl_3 , 376-400 MHz).

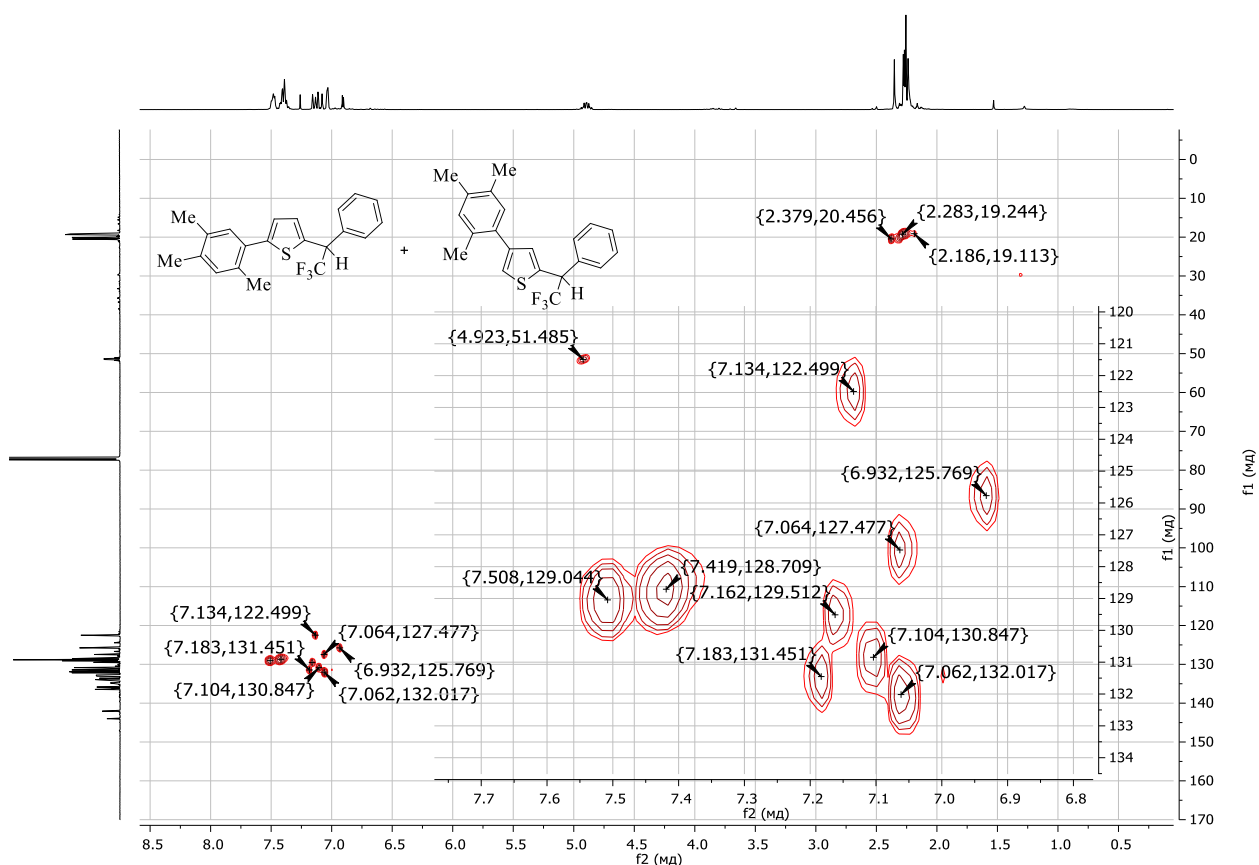


Fig. S206. HSQC C-H NMR spectrum of the mixture of α -7i and β -7i (CDCl_3 , 101-400 MHz).

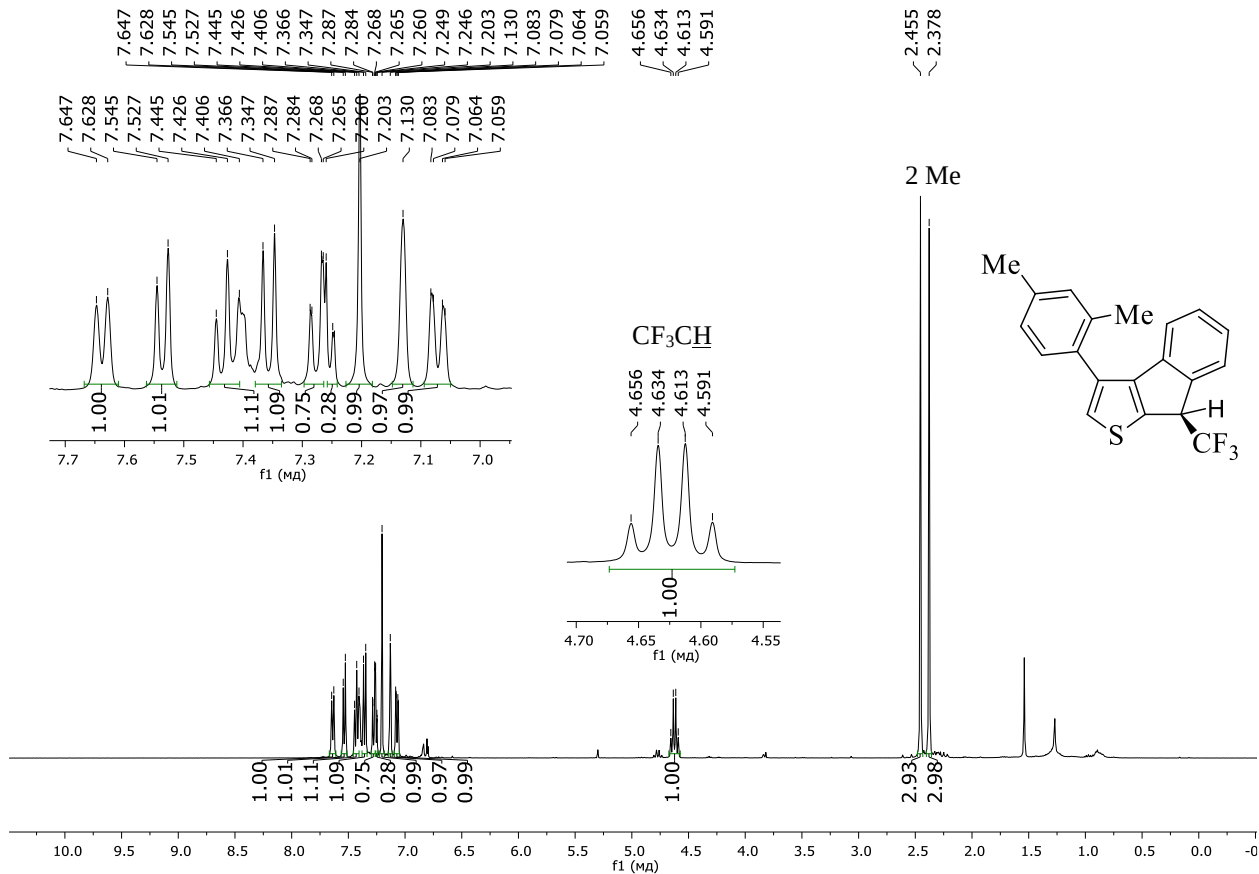


Fig. S207. ^1H NMR spectrum of the compound **8i** (CDCl_3 , 400 MHz).

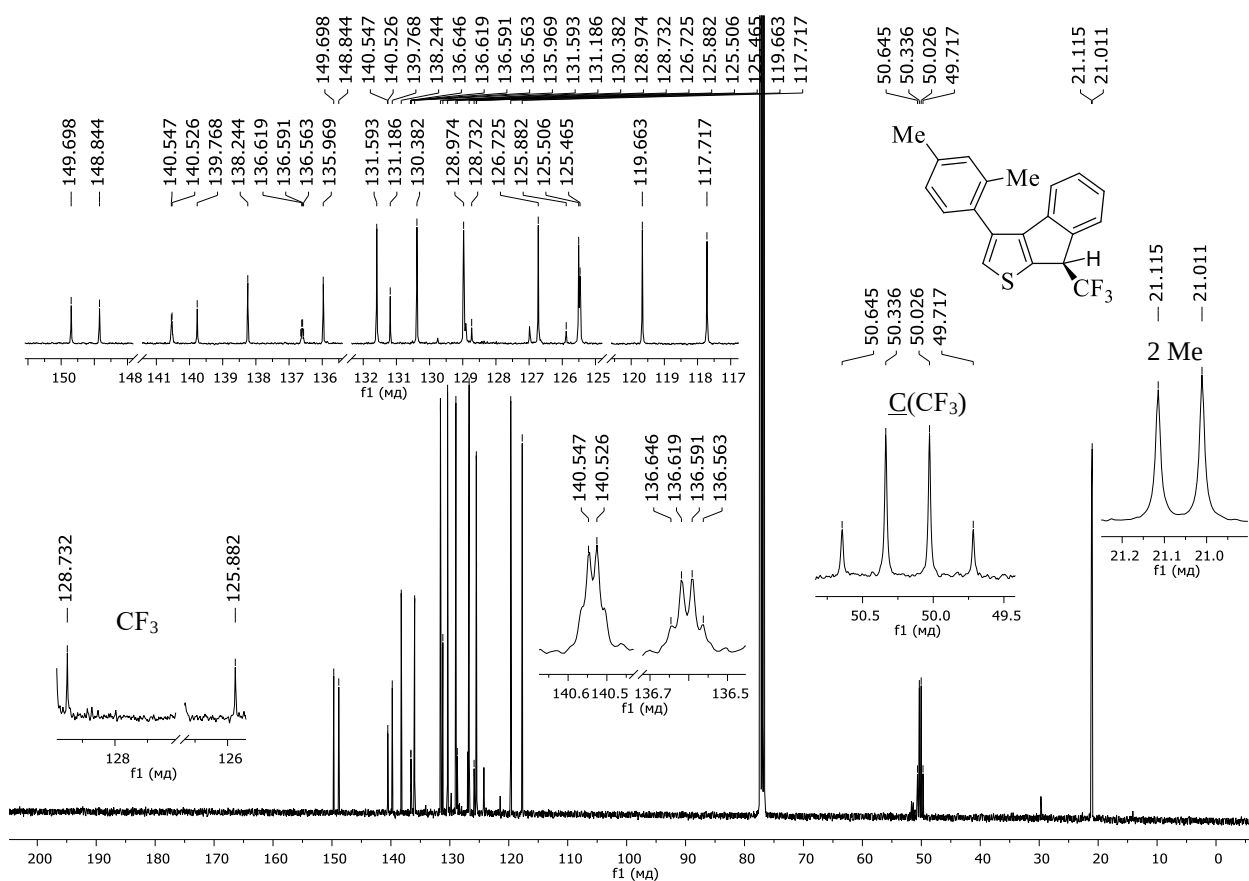


Fig. S208. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **8i** (CDCl_3 , 101 MHz).

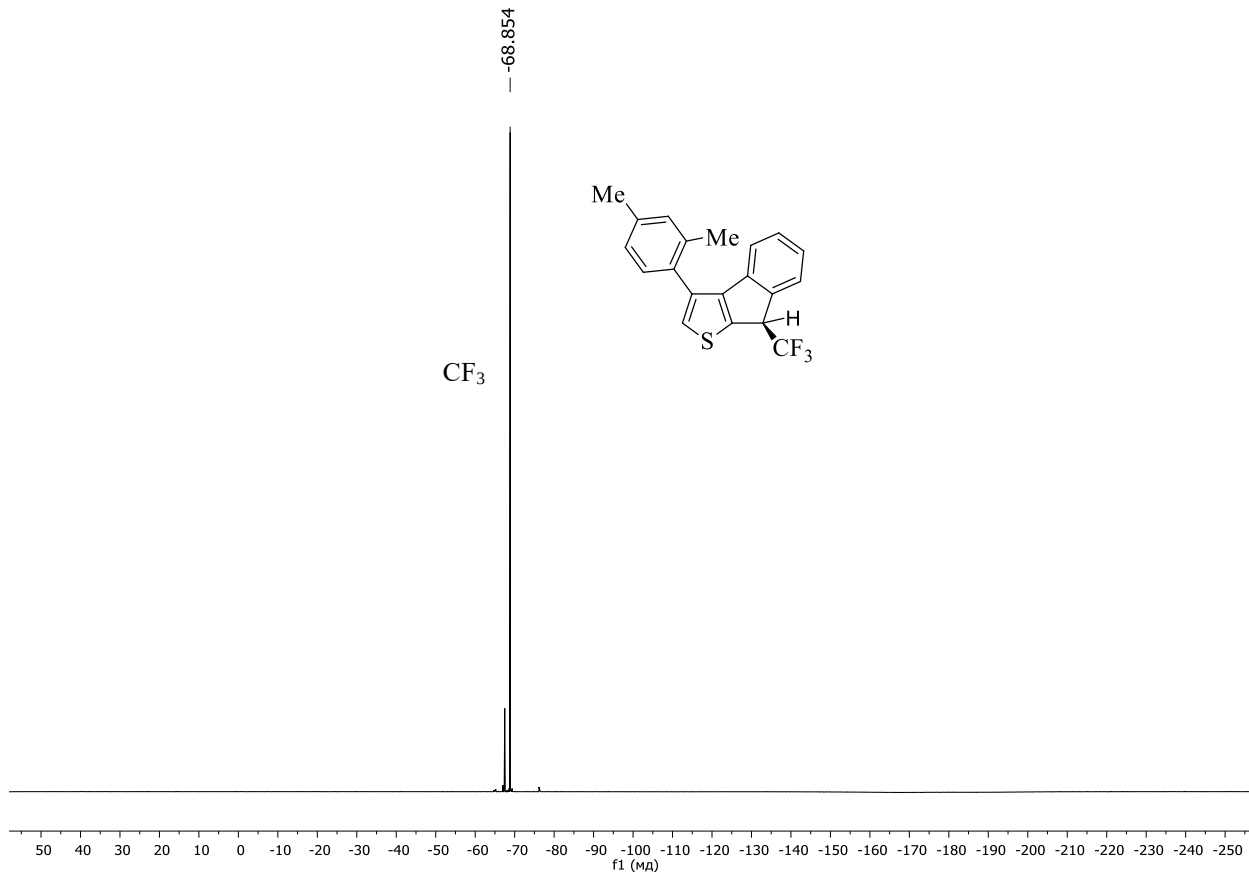


Fig. S209. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **8i** (CDCl_3 , 376 MHz).

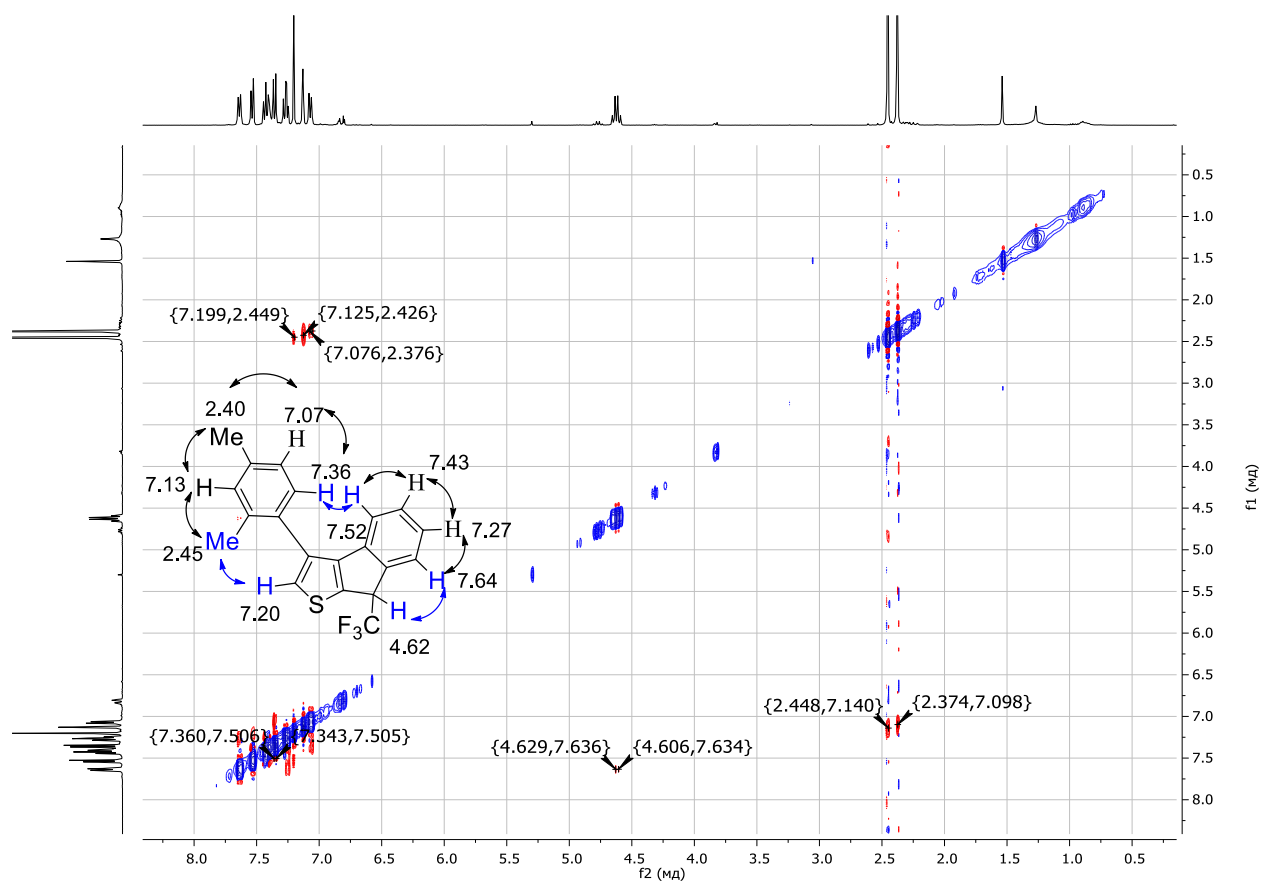


Fig. S210. NOESY H-H NMR spectrum of the compound **8i** (CDCl₃, 400 MHz).

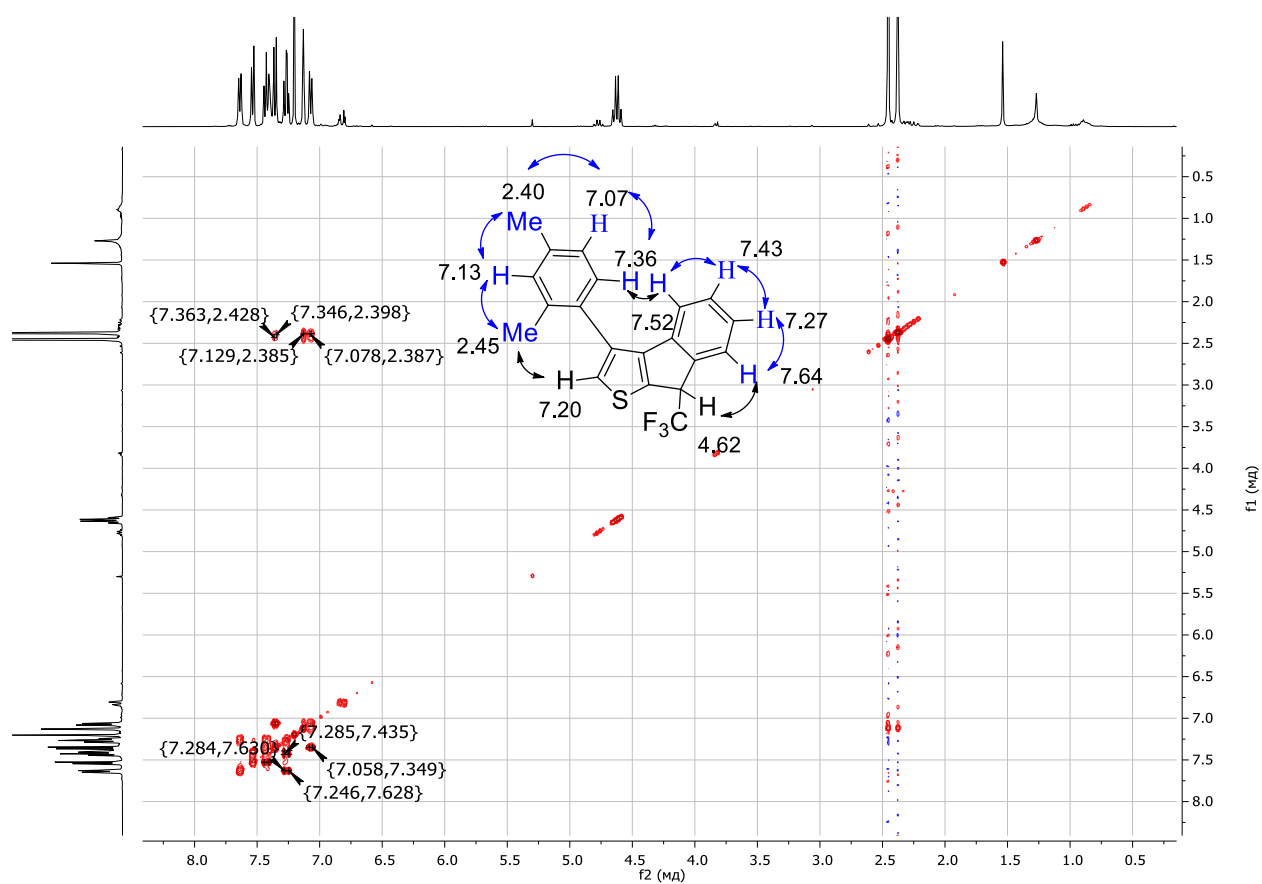


Fig. S211. COSY H-H spectrum of the compound **8i** (CDCl₃, 400 MHz).

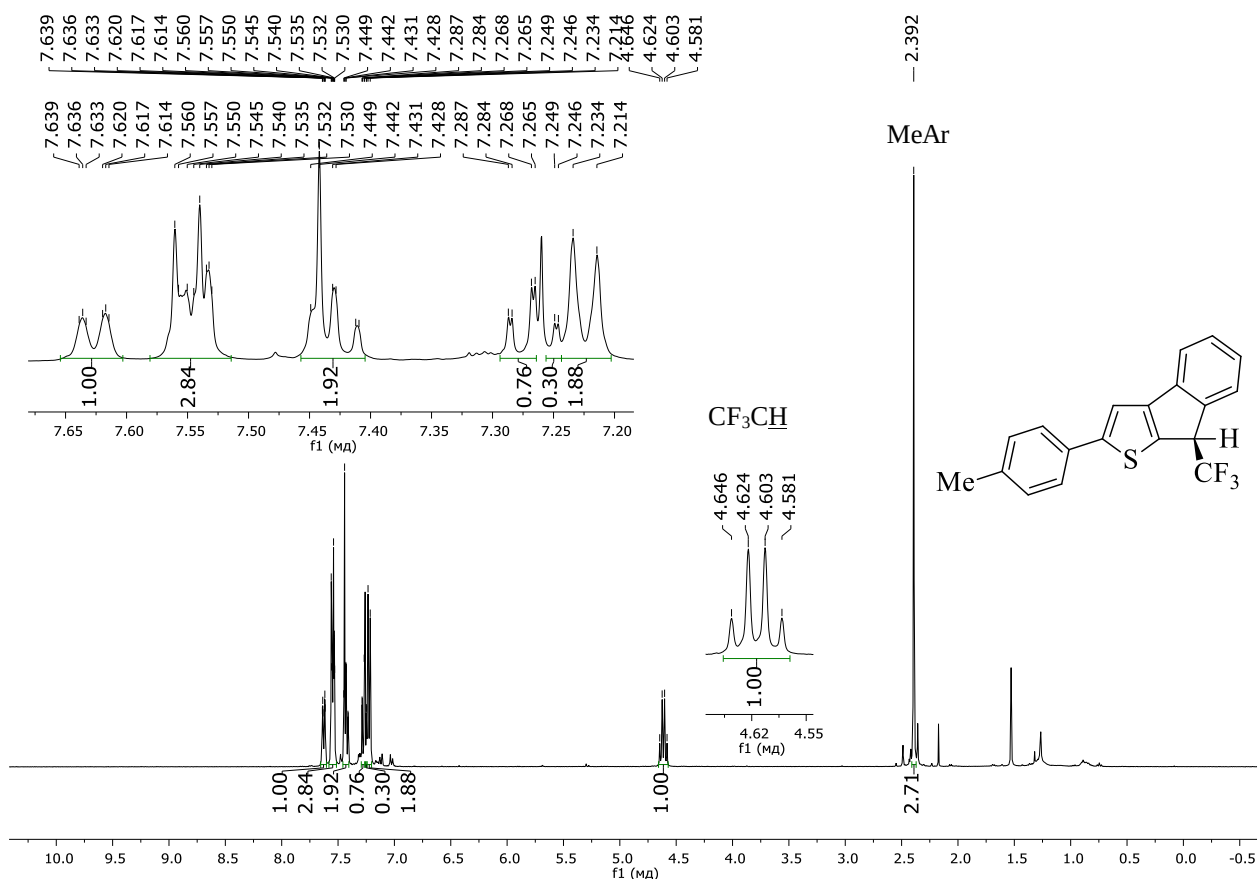


Fig. S212. ¹H NMR spectrum of the compound **9i** (CDCl₃, 400 MHz).

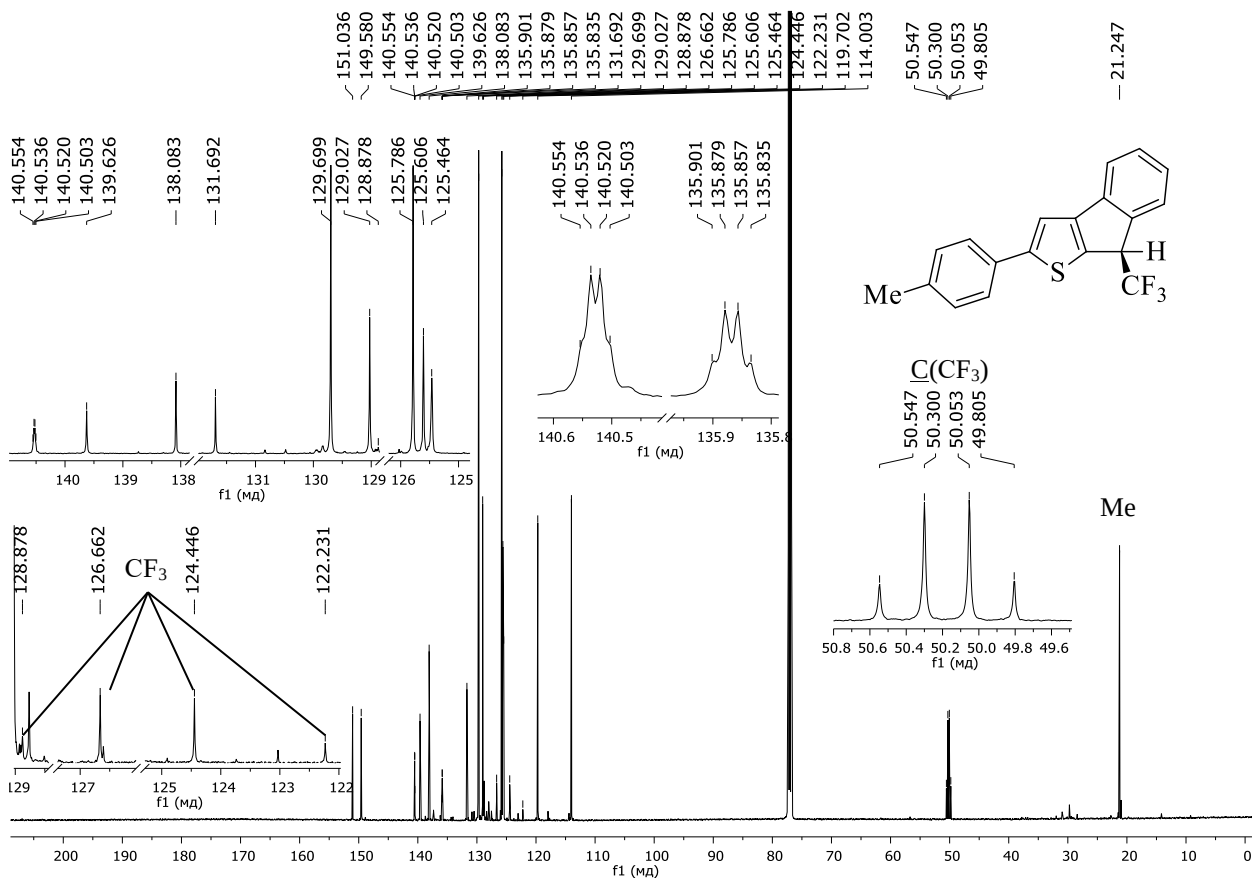


Fig. S213. ¹³C{¹H} NMR spectrum of the compound **9i** (CDCl₃, 101 MHz).

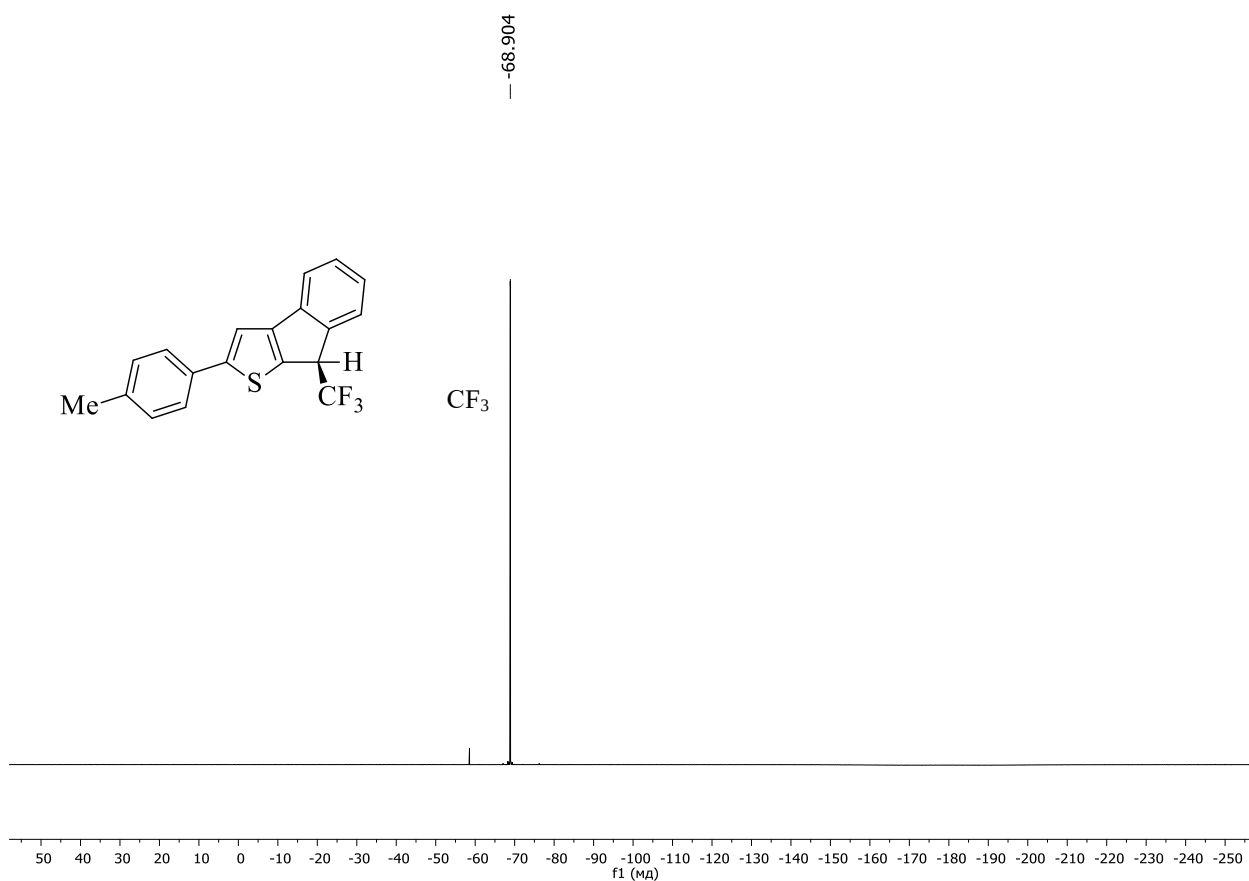


Fig. S214. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **9i** (CDCl₃, 376 MHz).

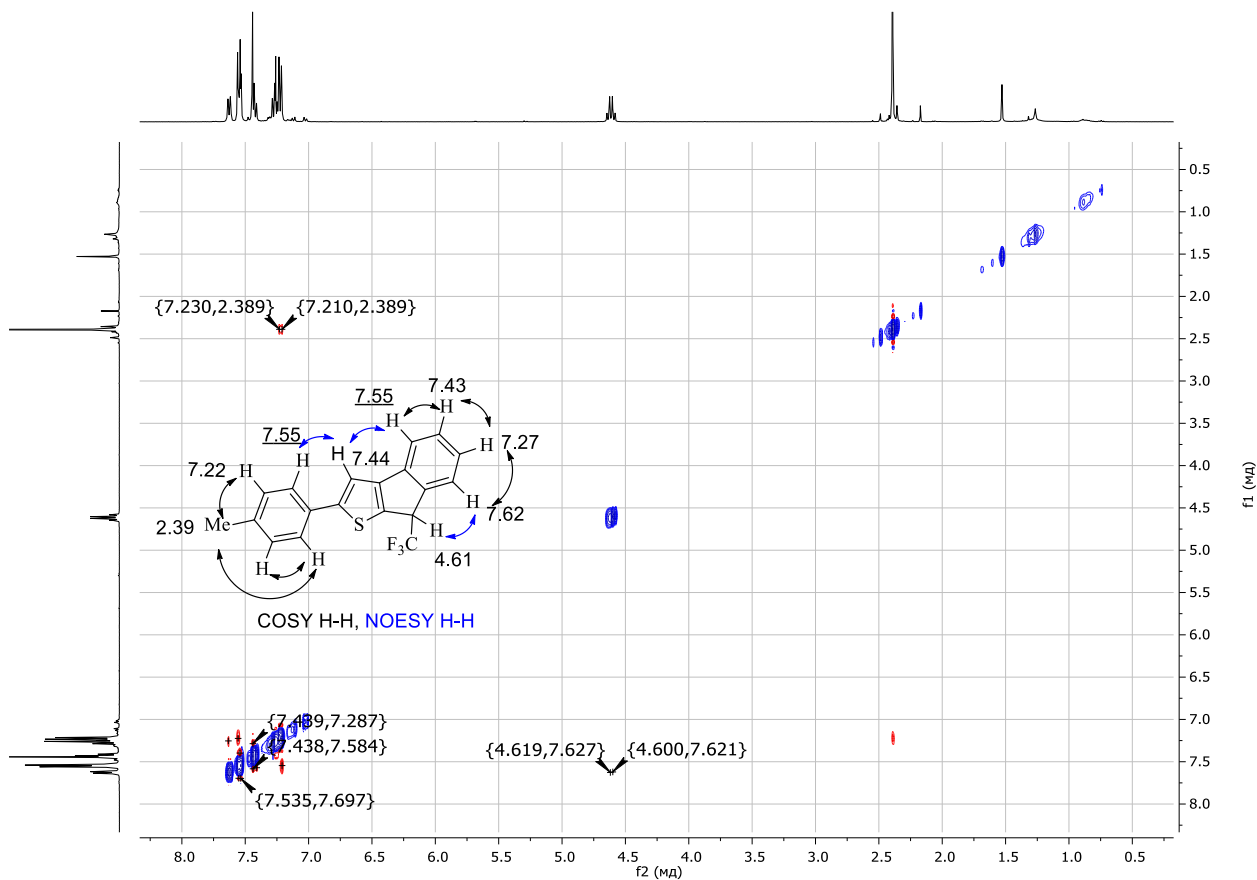


Fig. S215. NOESY H-H spectrum of the compound **9i** (CDCl₃, 400 MHz).

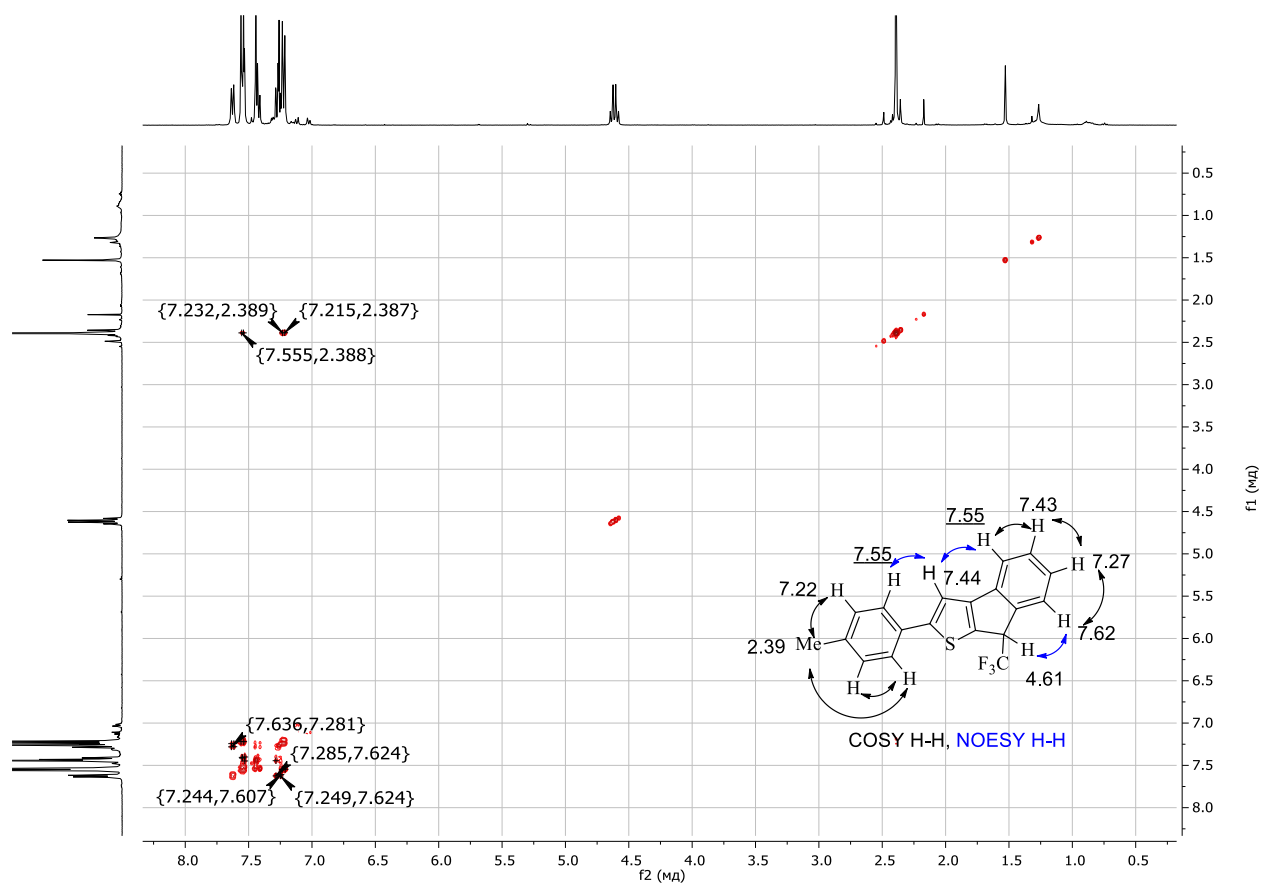


Fig. S216. COSY H-H spectrum of the compound **9i** (CDCl₃, 400 MHz).

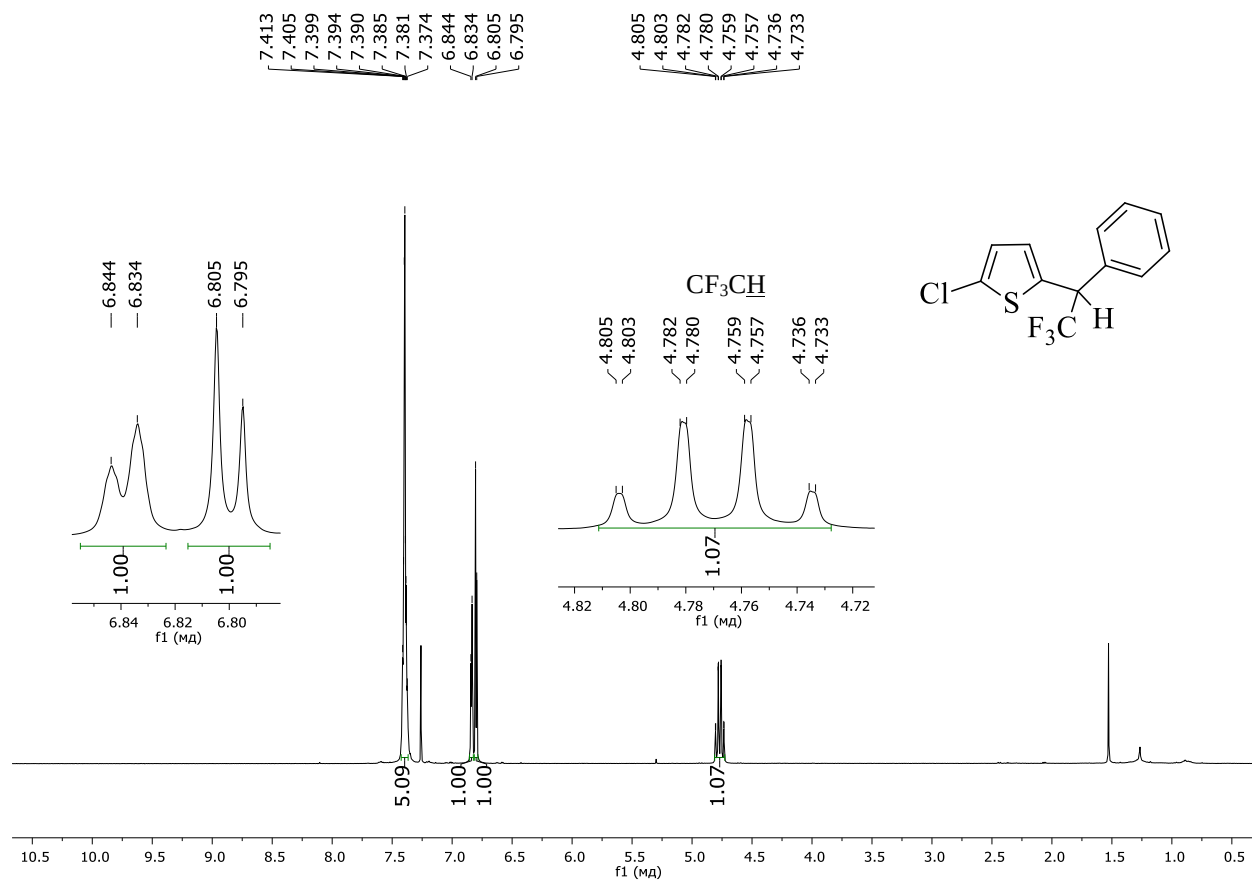


Fig. S217. ¹H NMR spectrum of the compound **10i** (CDCl₃, 400 MHz).

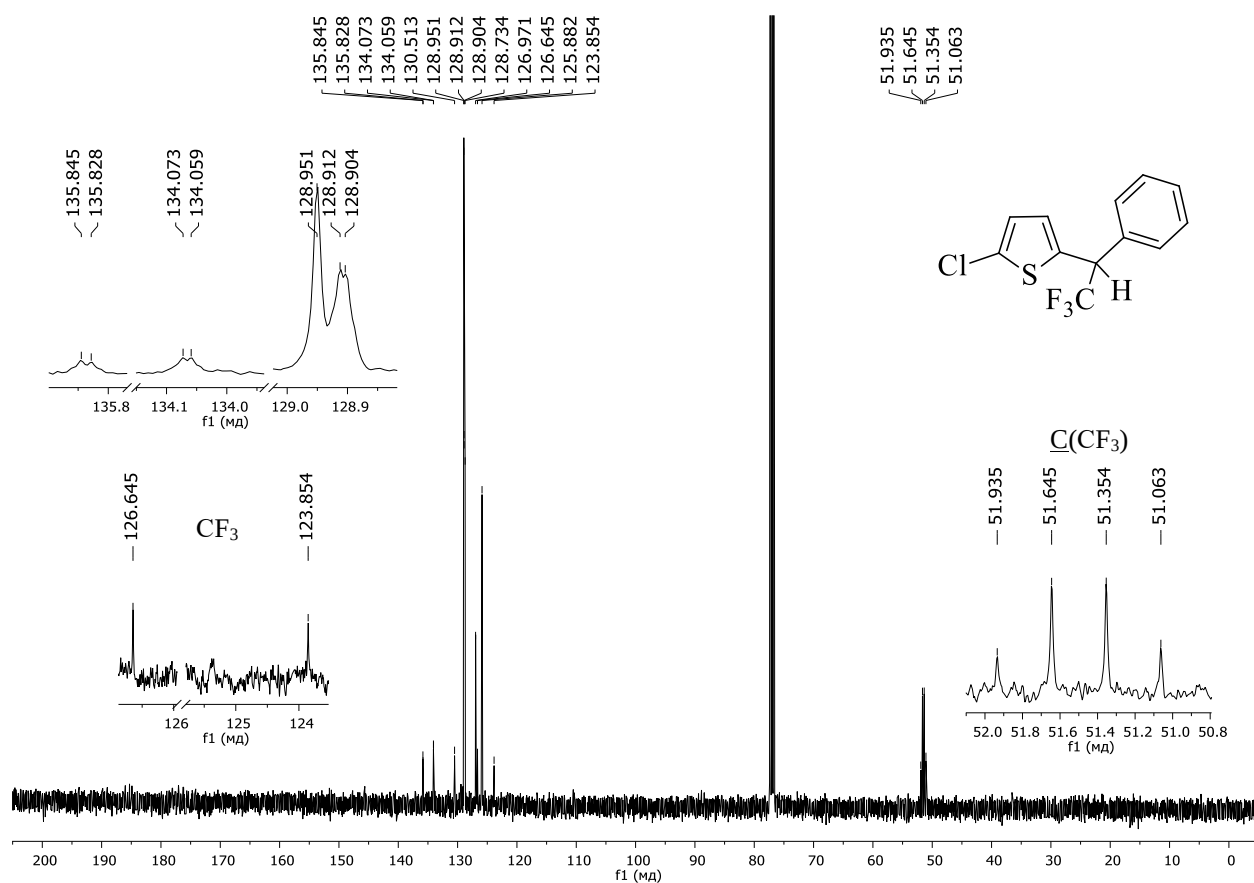


Fig. S218. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **10i** (CDCl_3 , 101 MHz).

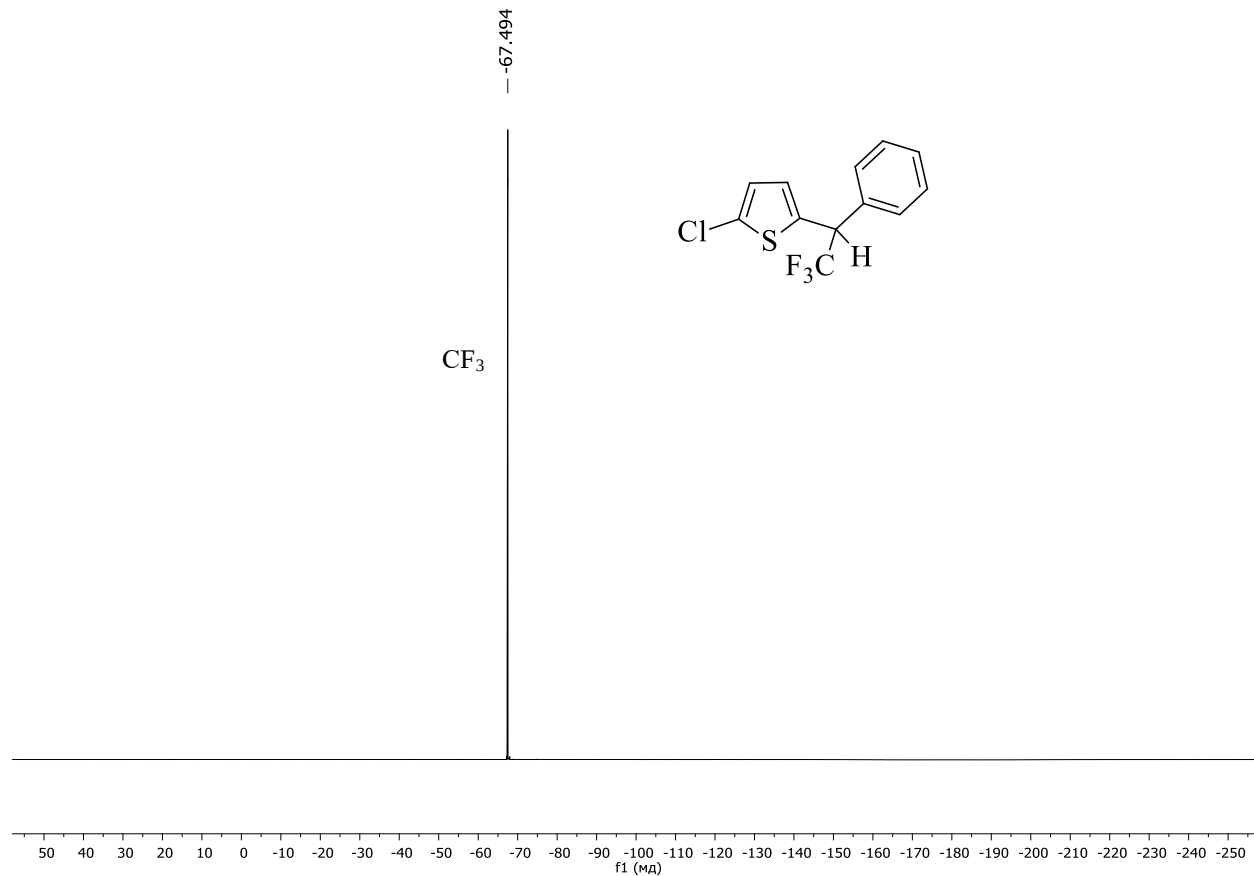


Fig. S219. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **10i** (CDCl_3 , 376 MHz).

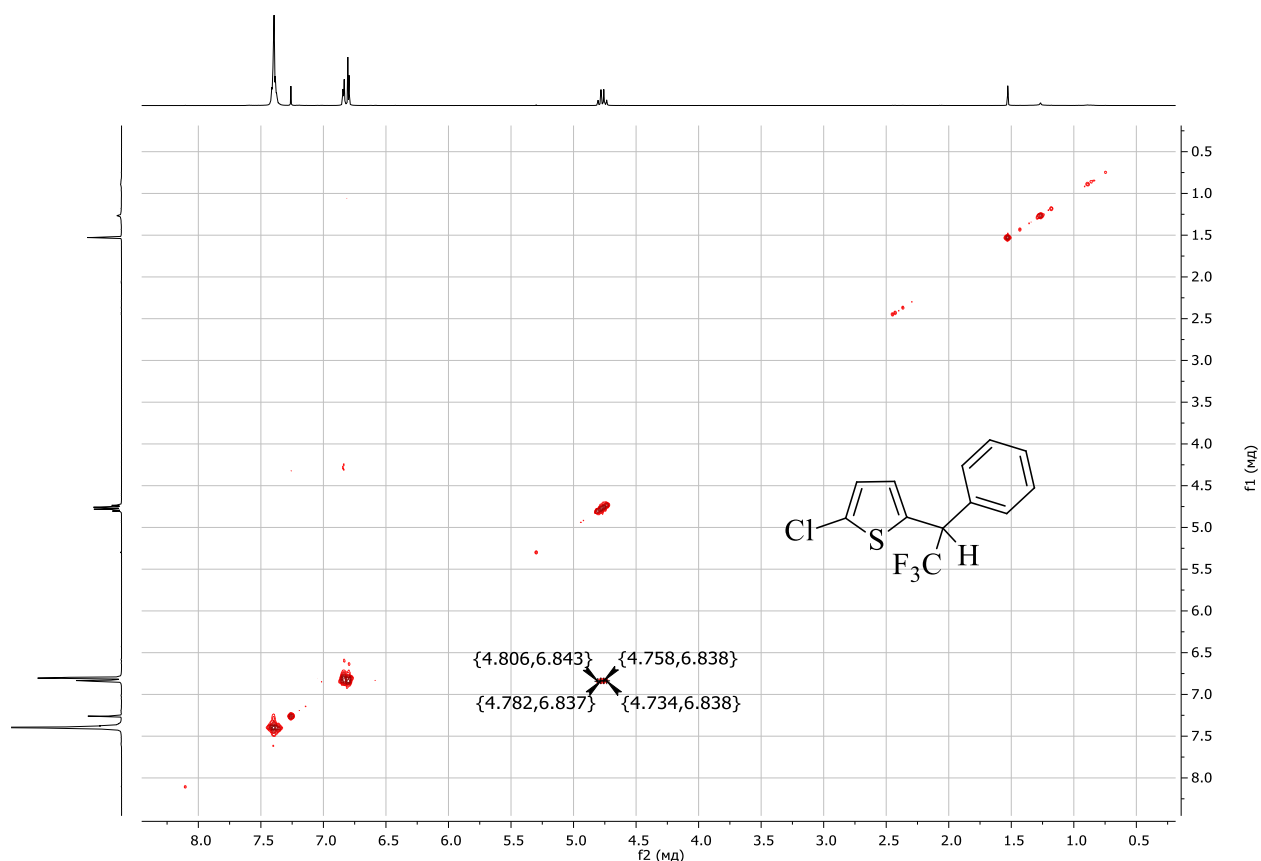


Fig. S220. COSY H-H NMR spectrum of the compound **10i** (CDCl_3 , 400 MHz)

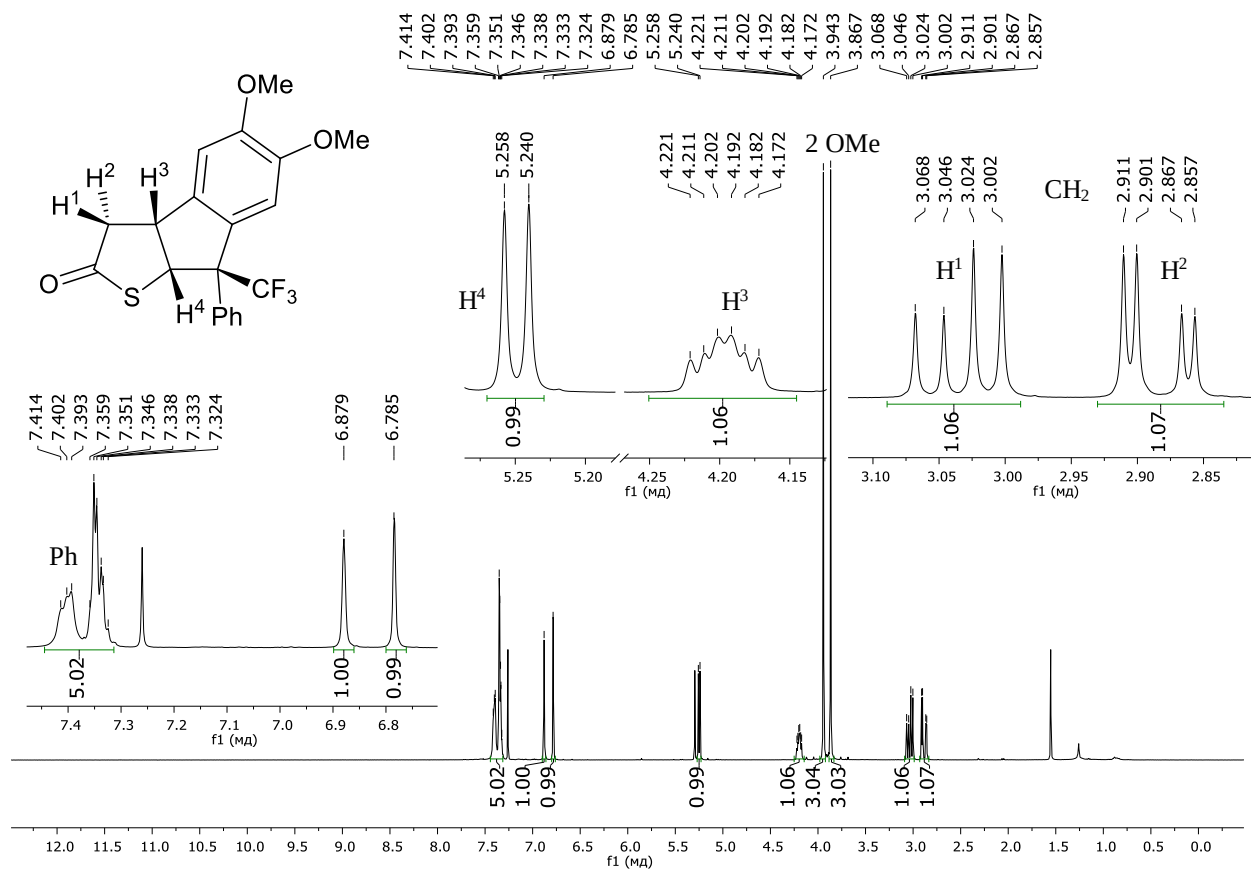


Fig. S221. ^1H NMR spectrum of the compound **11i** (CDCl_3 , 400 MHz).

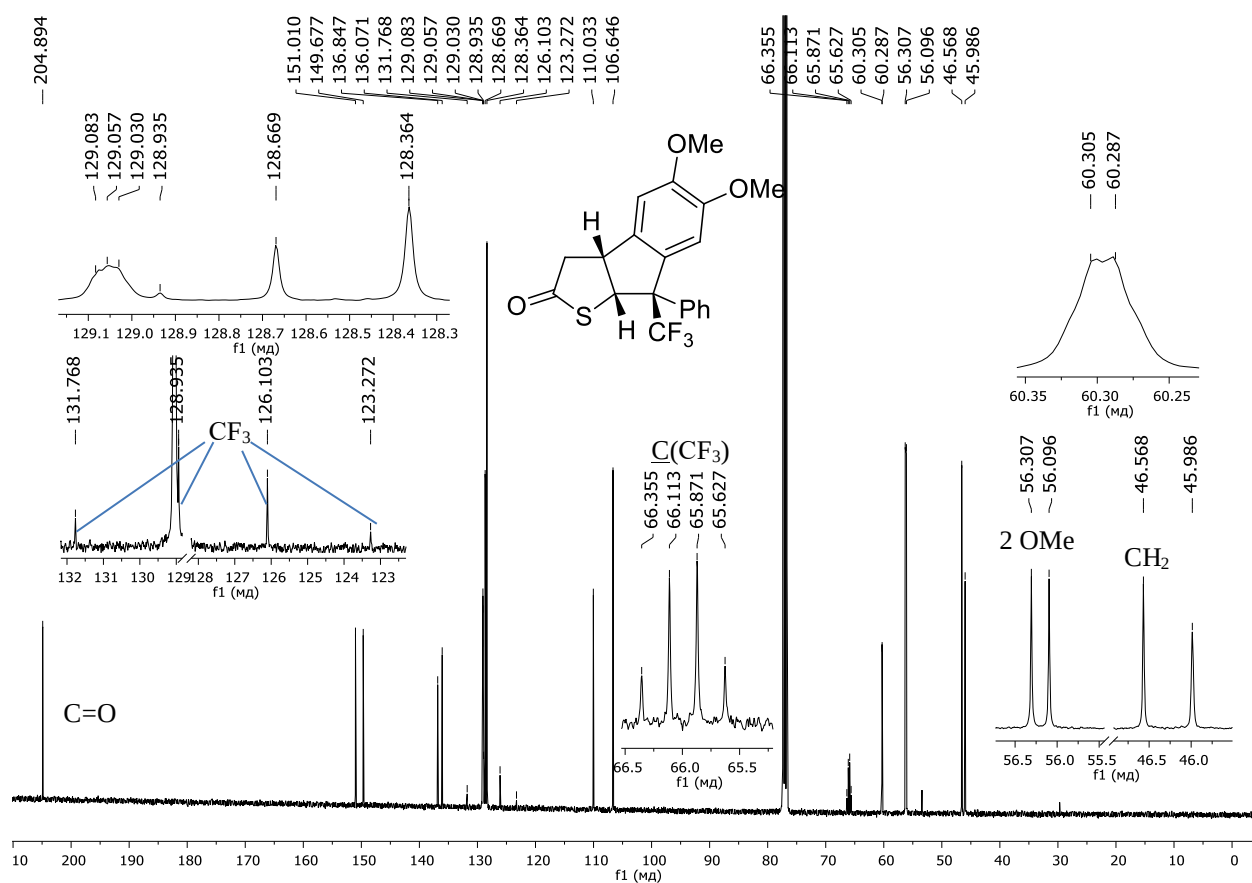


Fig. S222. ¹³C{¹H} NMR spectrum of the compound **11i** (CDCl₃, 101 MHz).

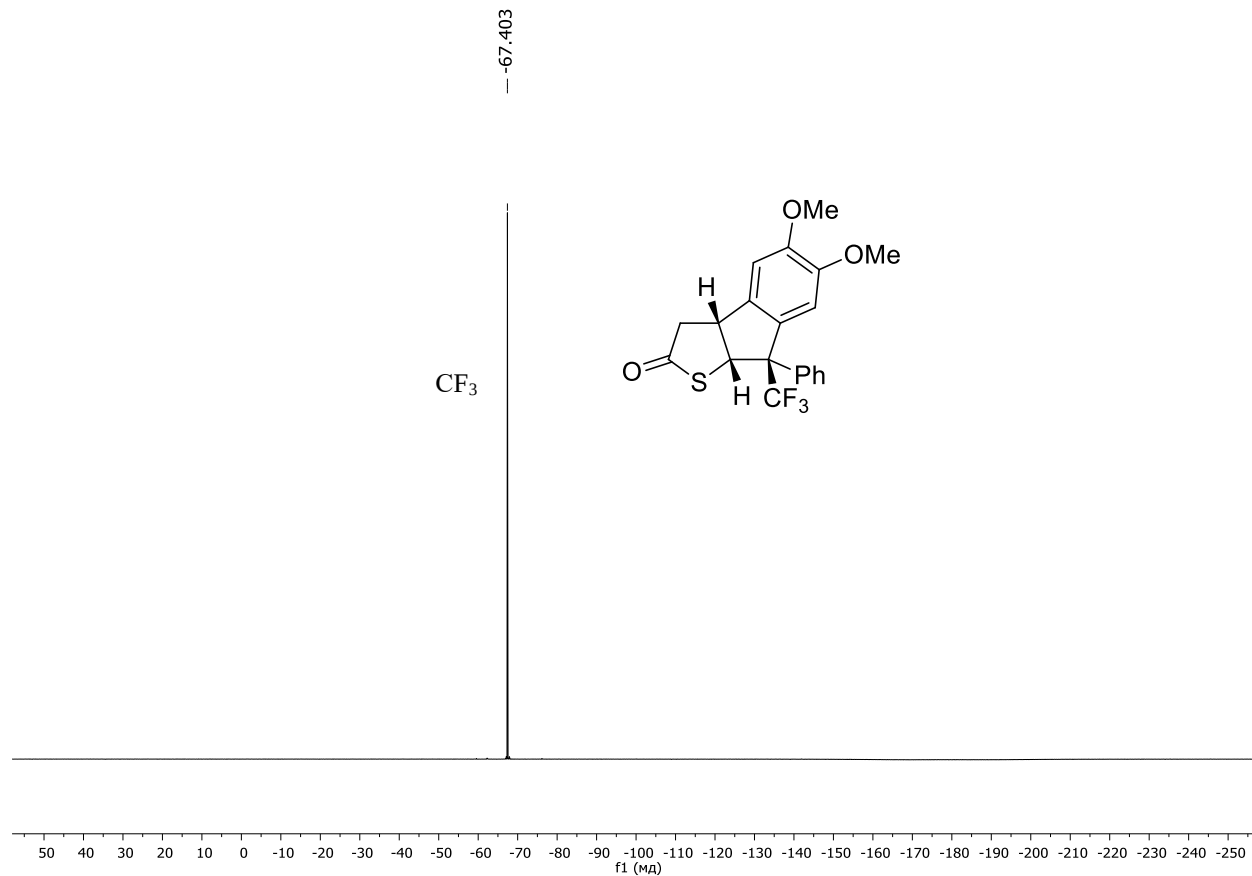


Fig. S223. ¹⁹F{¹H} NMR spectrum of the compound **11i** (CDCl₃, 376 MHz).

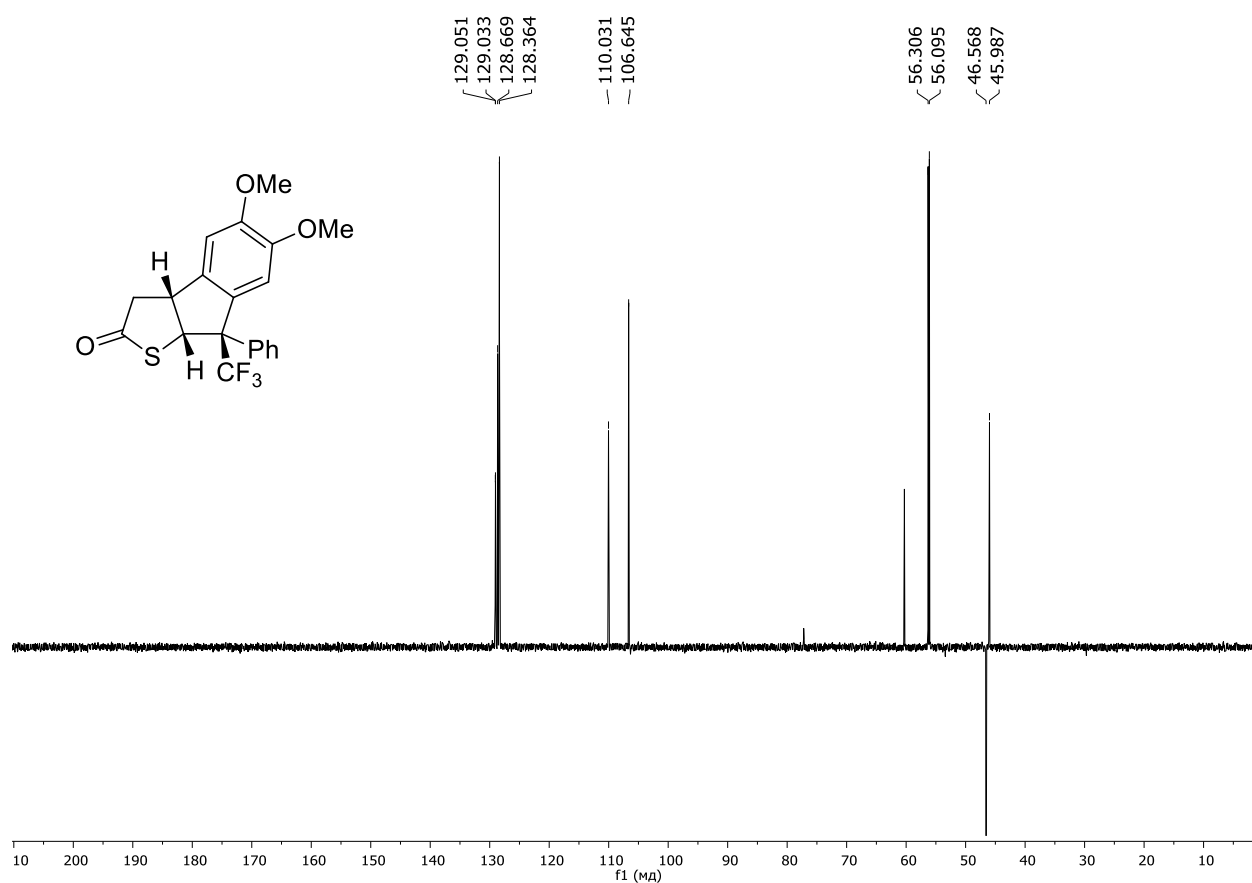


Fig. S224. DEPT NMR spectrum of the compound **11i** (CDCl₃, 101 MHz).

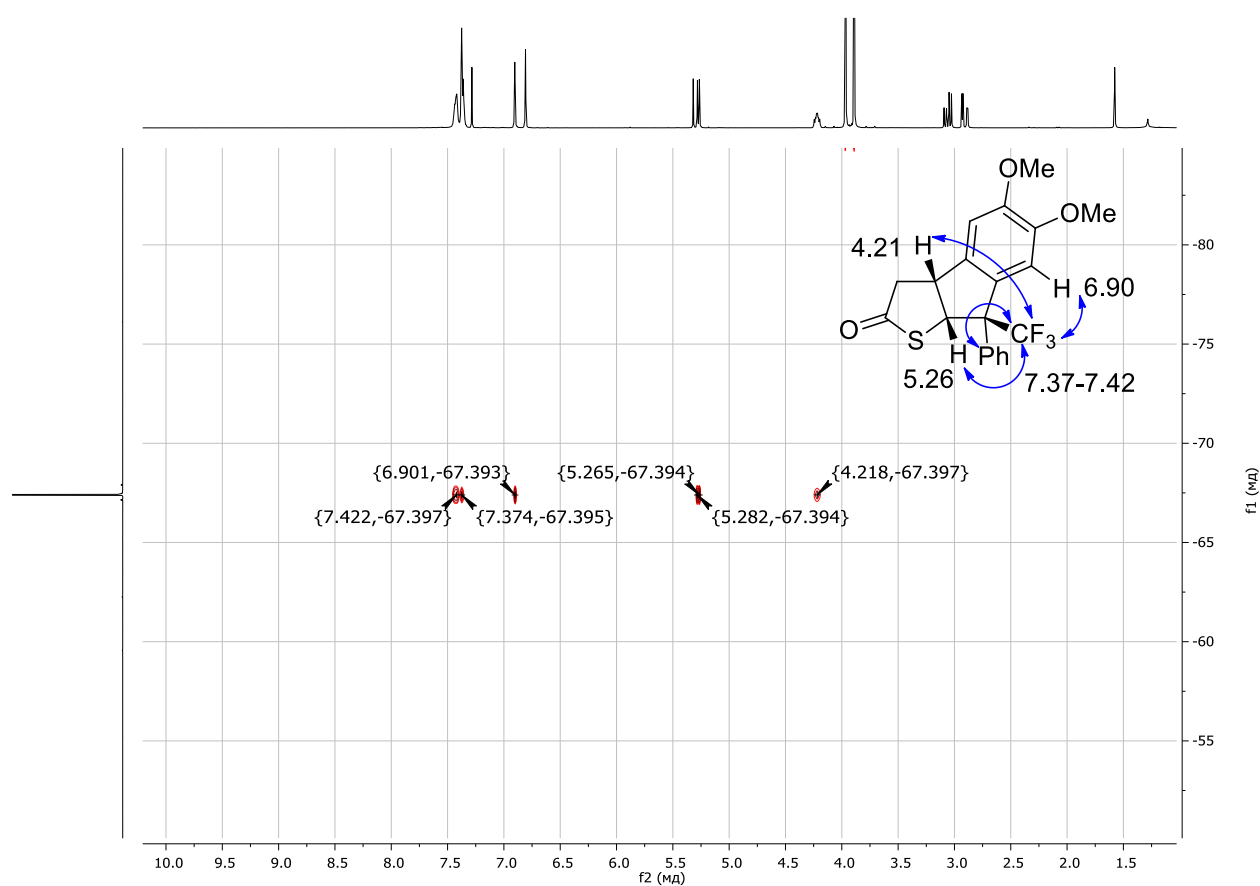


Fig. S225. HOESY H-F NMR spectrum of the compound **11i** (CDCl₃, 400-376 MHz).

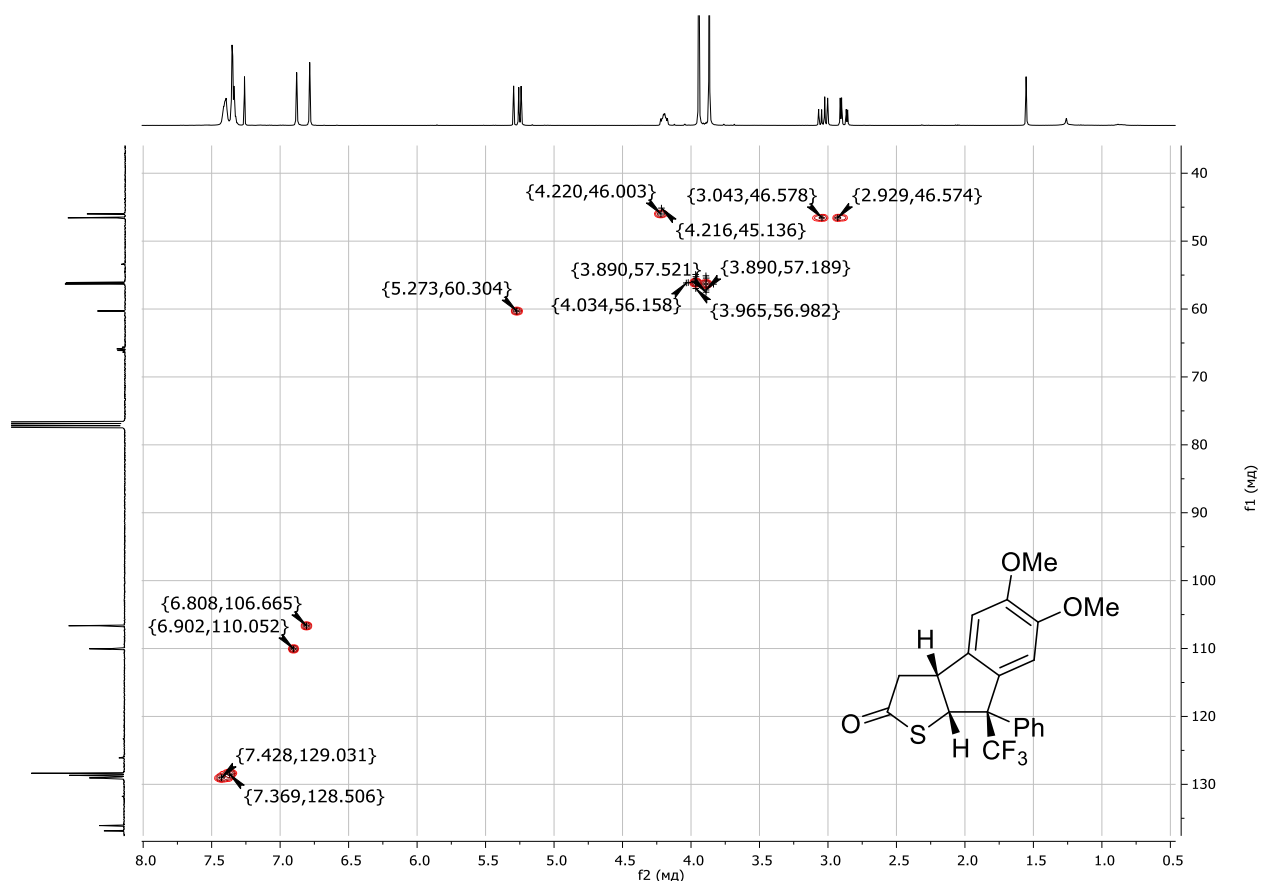


Fig. S226. HSQC C-H NMR spectrum of the compound **11i** (CDCl₃, 101-400 MHz).

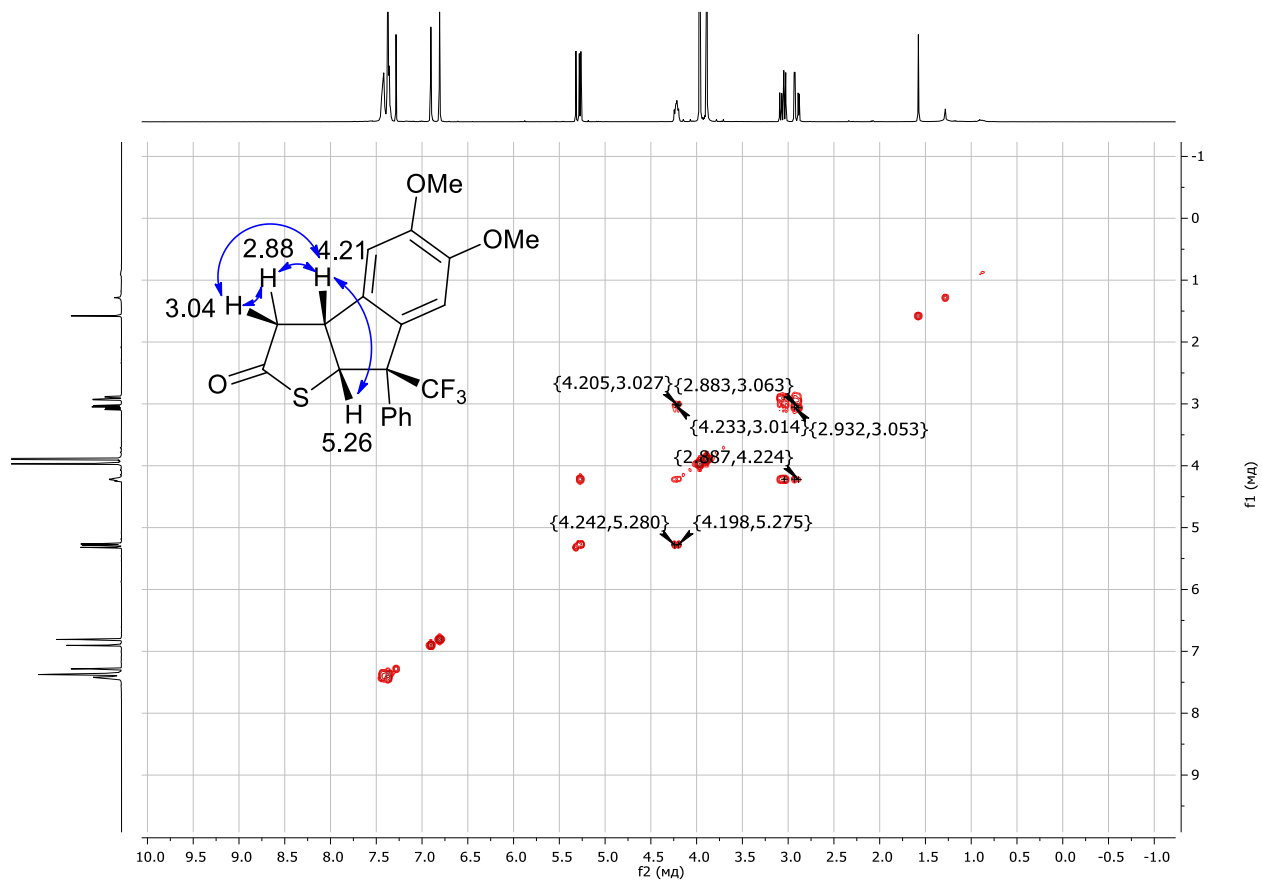


Fig. S227. COSY H-H NMR spectrum of the compound **11i** (CDCl₃, 400 MHz).

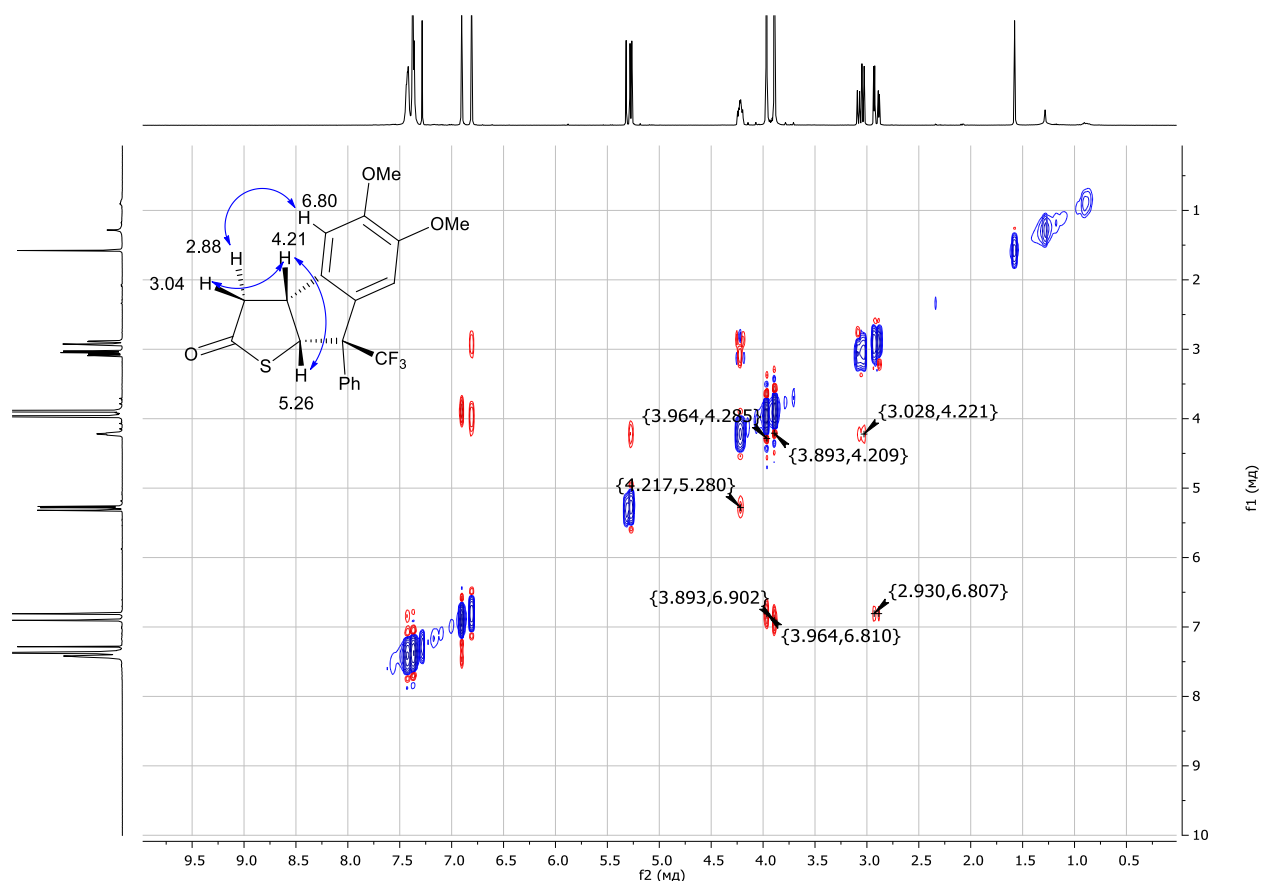


Fig. S228. NOESY H-H NMR spectrum of the compound **11i** (CDCl₃, 400 MHz).

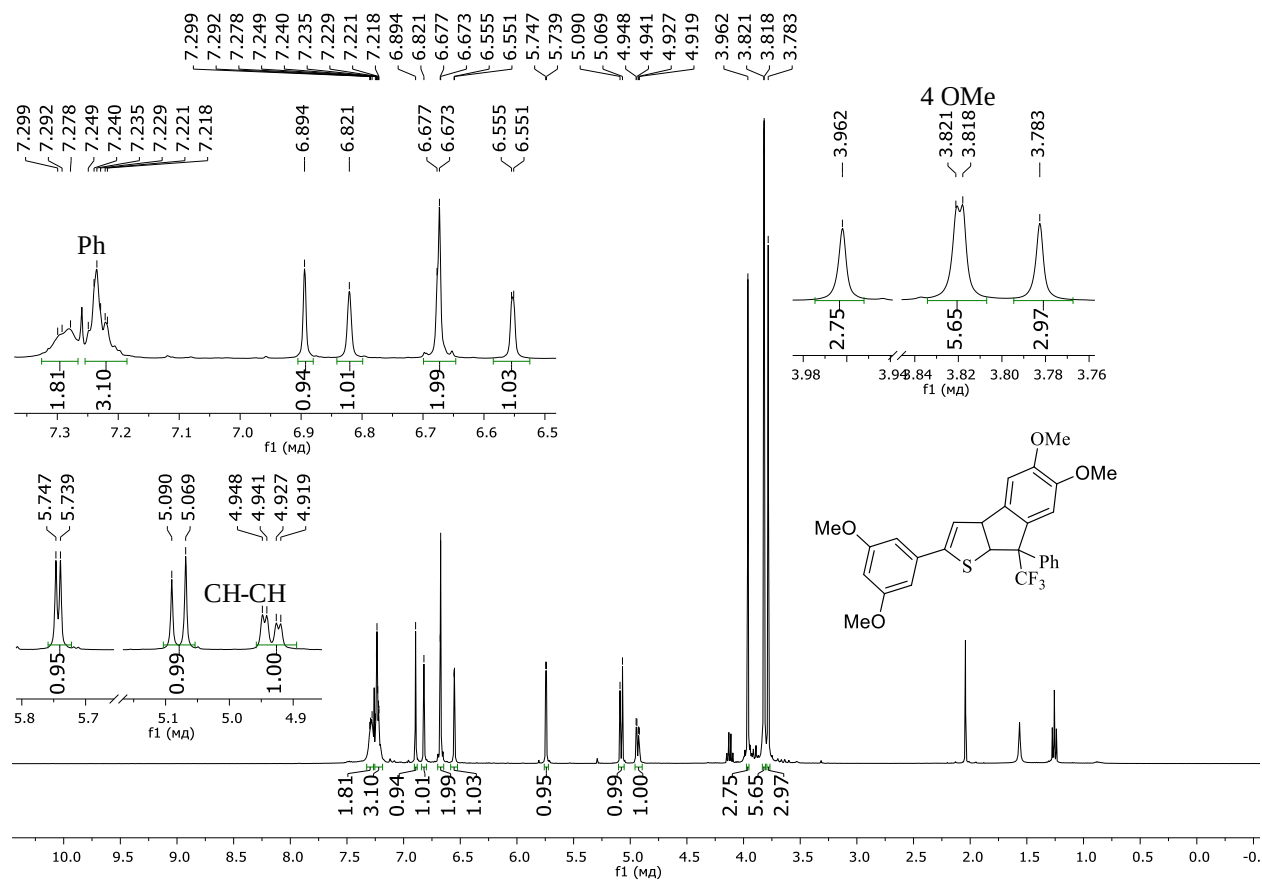


Fig. S229. ¹H NMR spectrum of the compound **12i** (CDCl₃, 400 MHz).

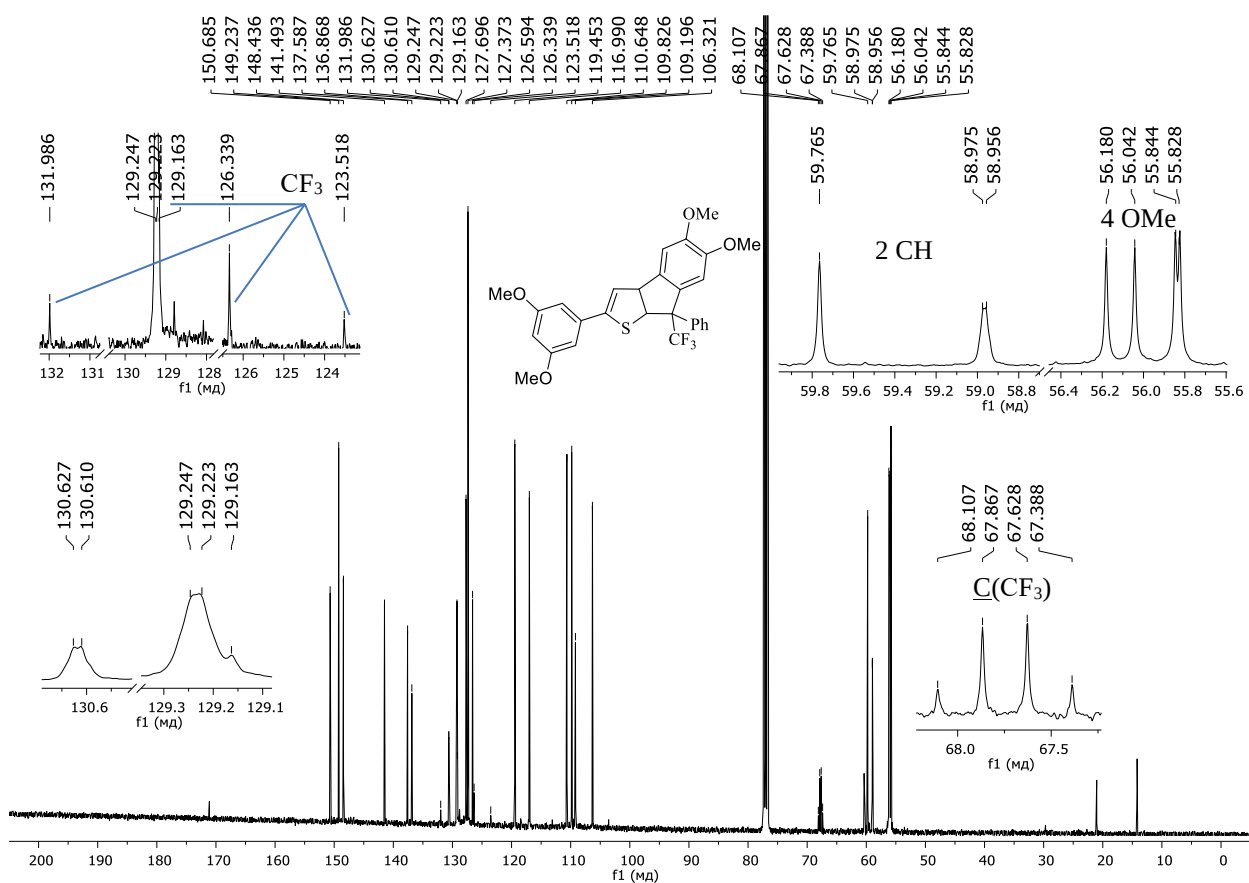


Fig. S230. ¹³C{¹H} NMR spectrum of the compound **12i** (CDCl₃, 101 MHz).

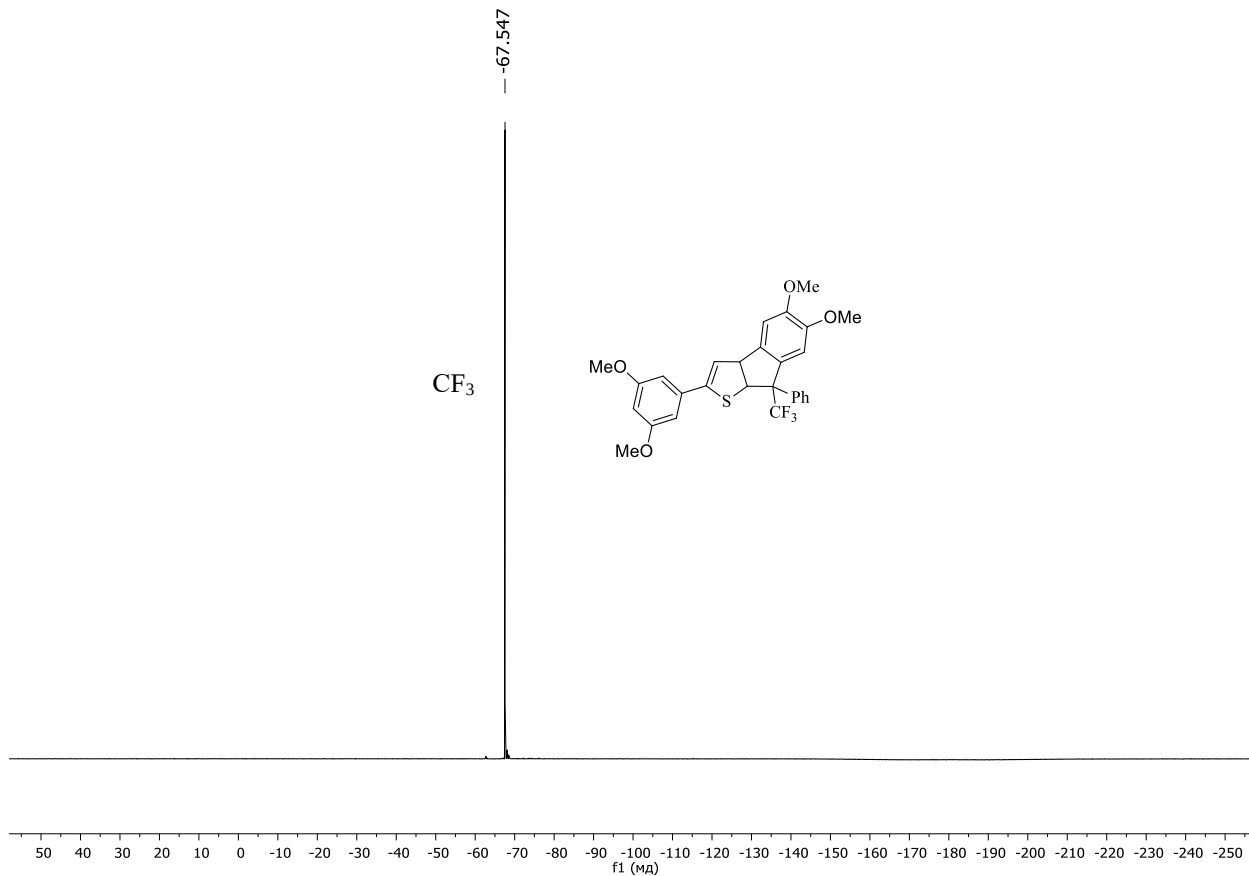


Fig. S231. ¹⁹F{¹H} NMR spectrum of the compound **12i** (CDCl₃, 376 MHz).

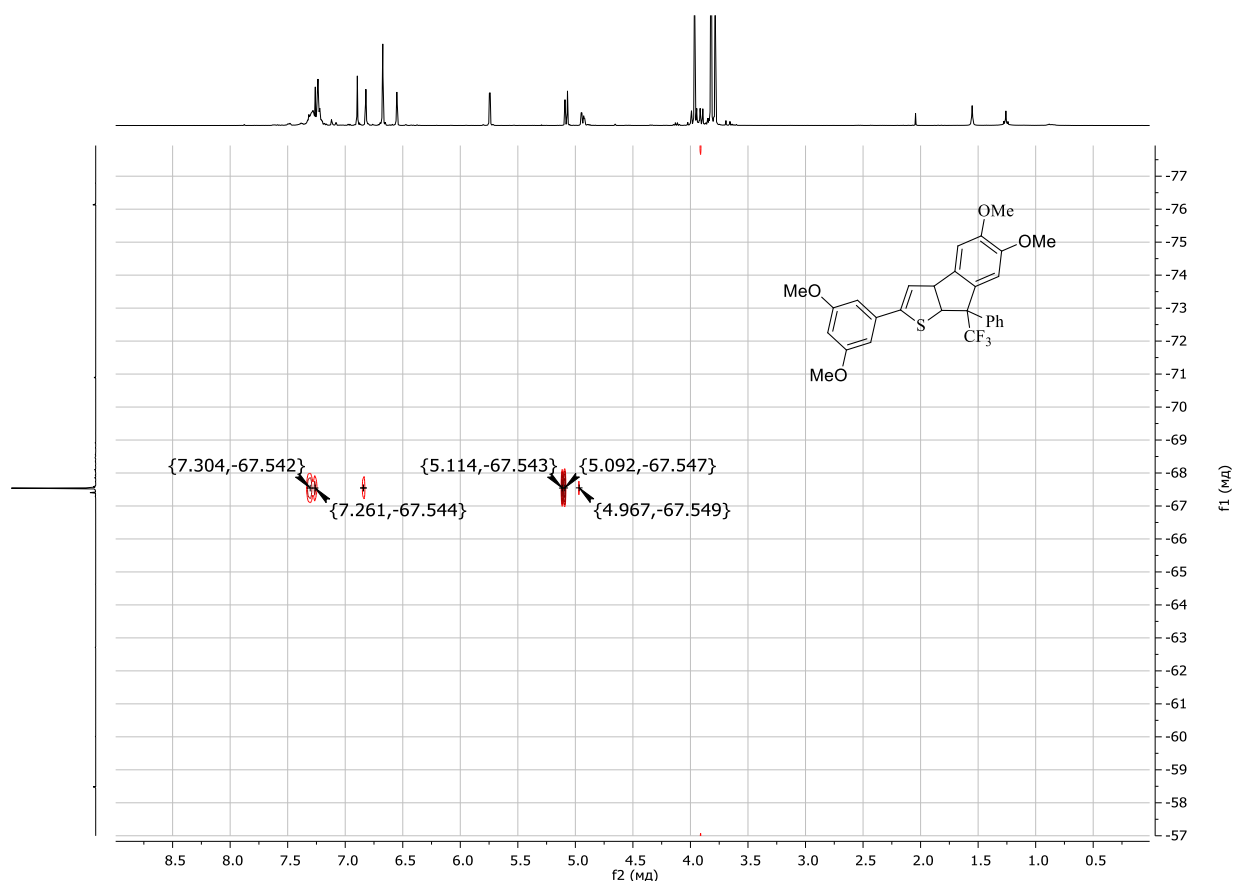


Fig. S232. HOESY H-F NMR spectrum of the compound **12i** (CDCl₃, 400 – 376 MHz).

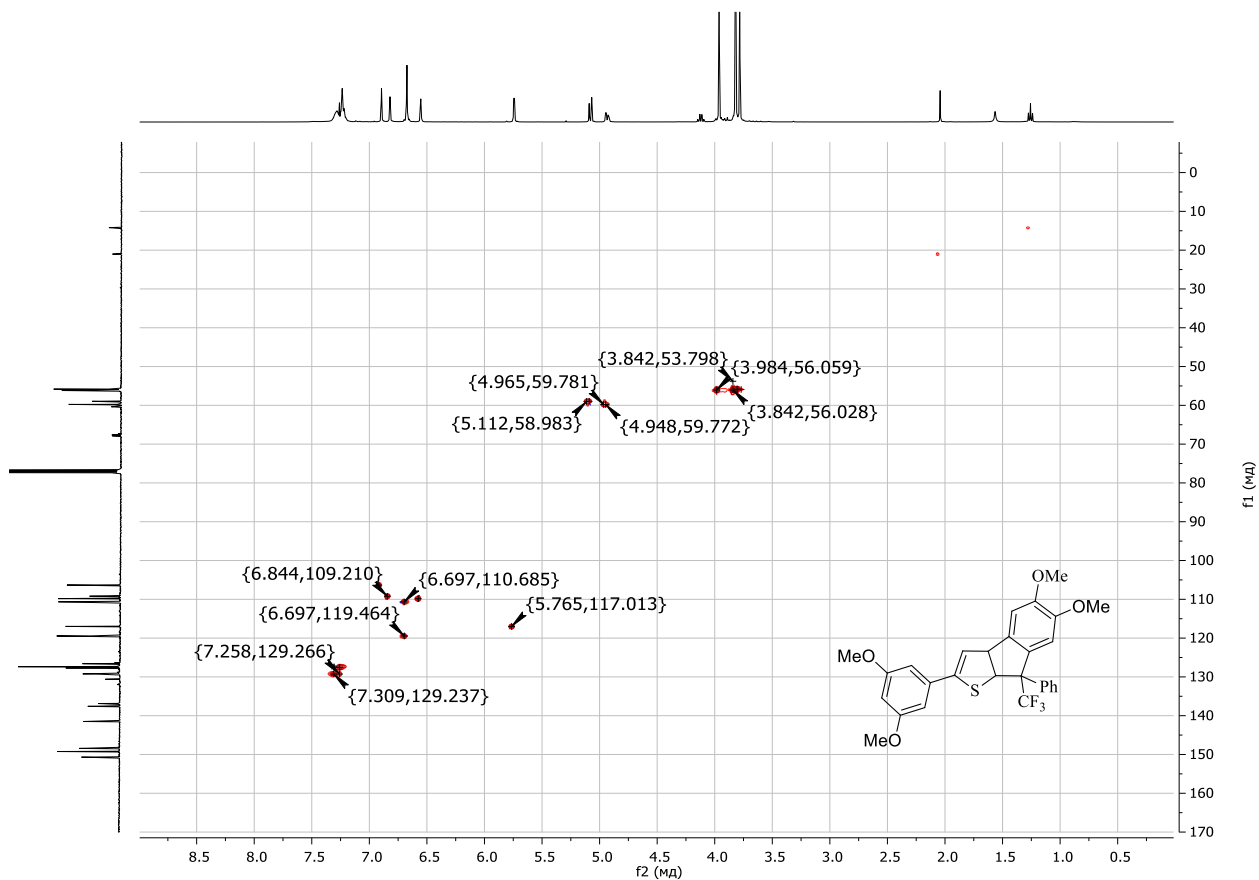


Fig. S233. HSQC C-H NMR spectrum of the compound **12i** (CDCl₃, 100 – 400 MHz).

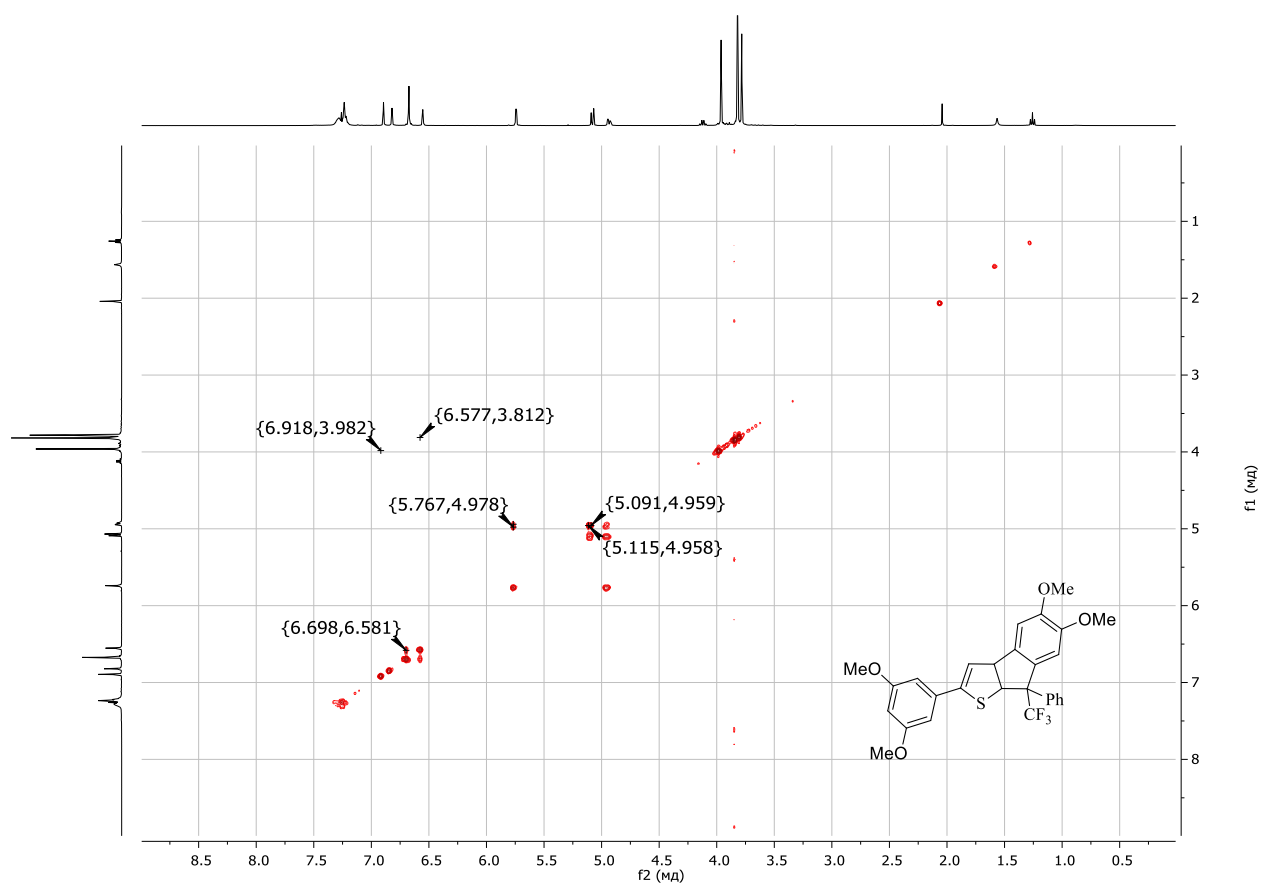


Fig. S234. COSY H-H NMR spectrum of the compound **12i** (CDCl₃, 400 MHz).

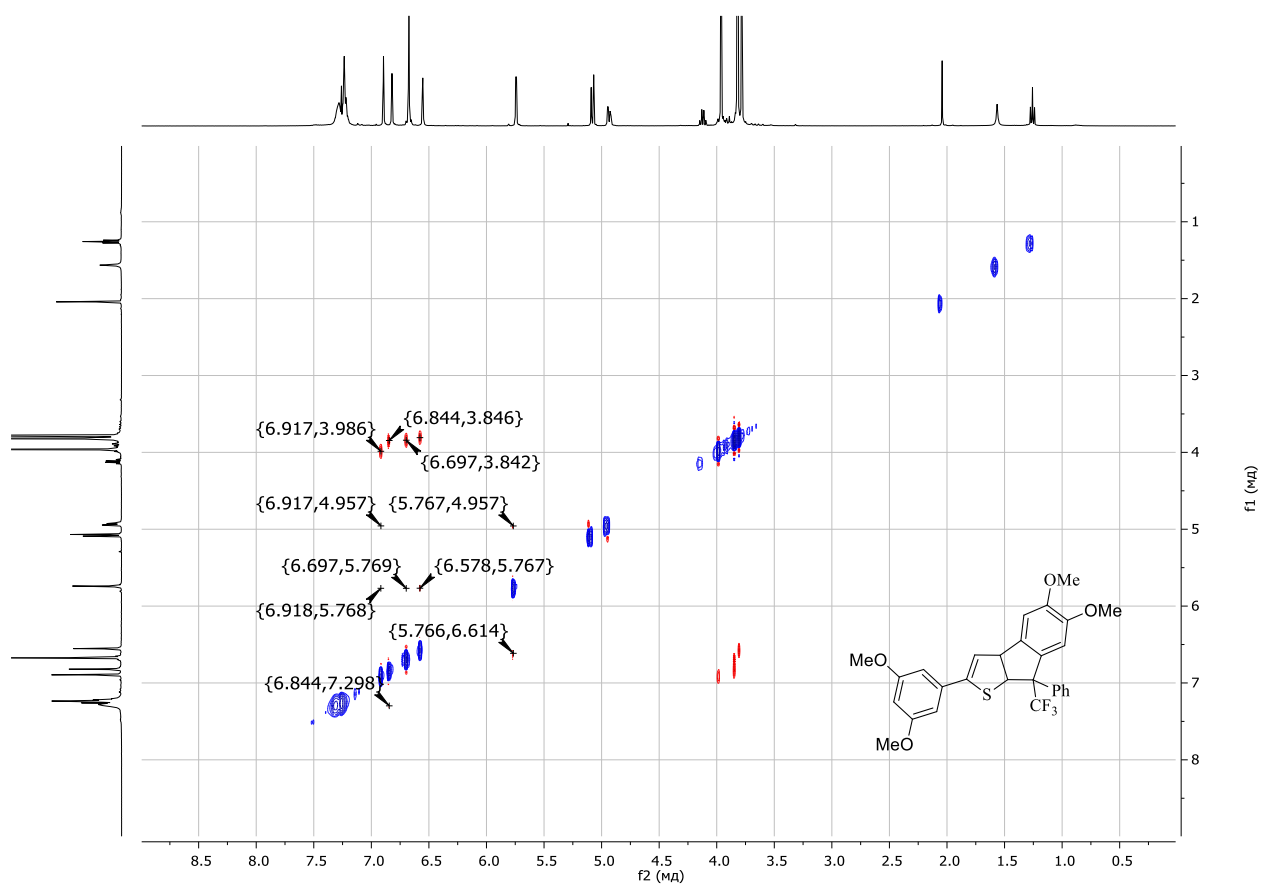


Fig. S235. NOESY H-H NMR spectrum of the compound **12i** (CDCl₃, 400 MHz).

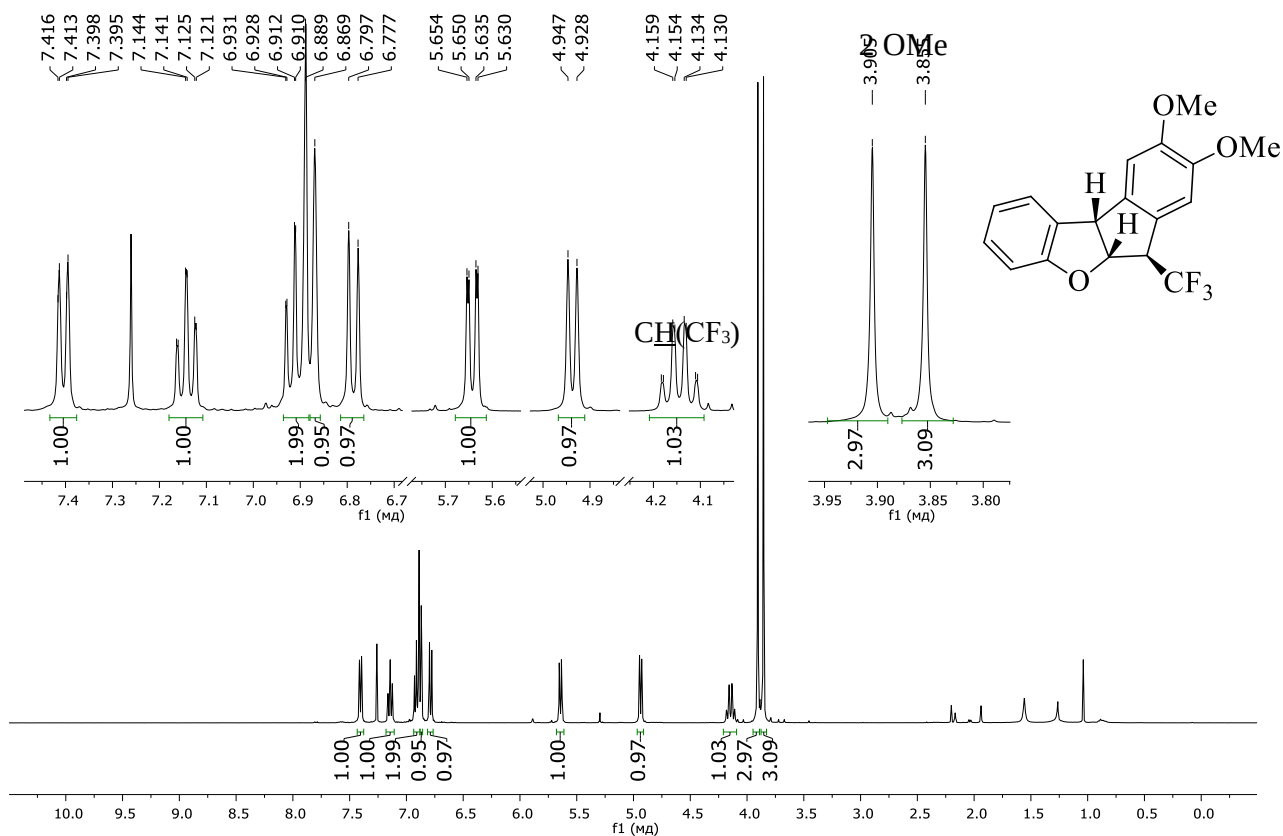


Fig. S236. ¹H NMR spectrum of the compound **13aa** (CDCl₃, 400 MHz).

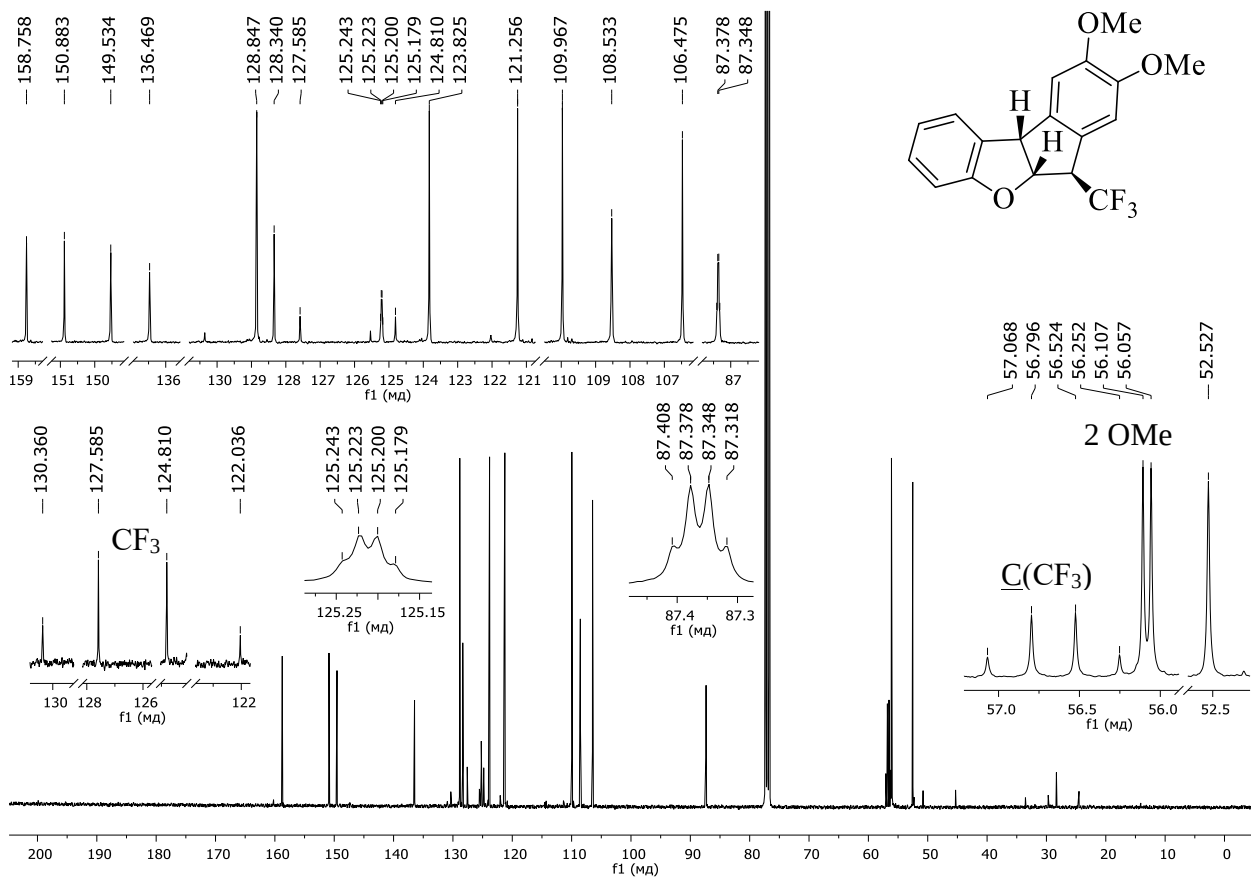


Fig. S237. ¹³C{¹H} NMR spectrum of the compound **13aa** (CDCl₃, 101 MHz).

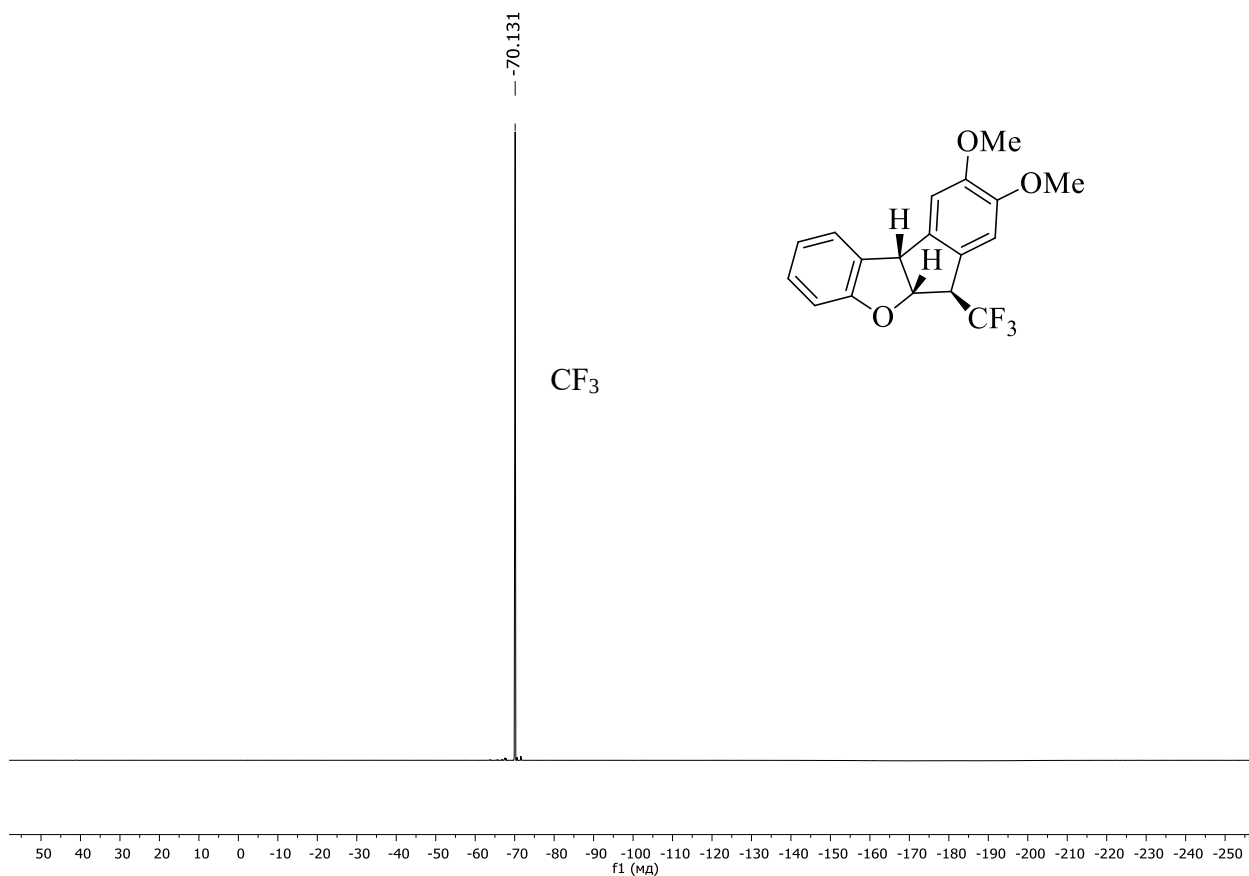


Fig. S238. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **13aa** (CDCl_3 , 376 MHz).

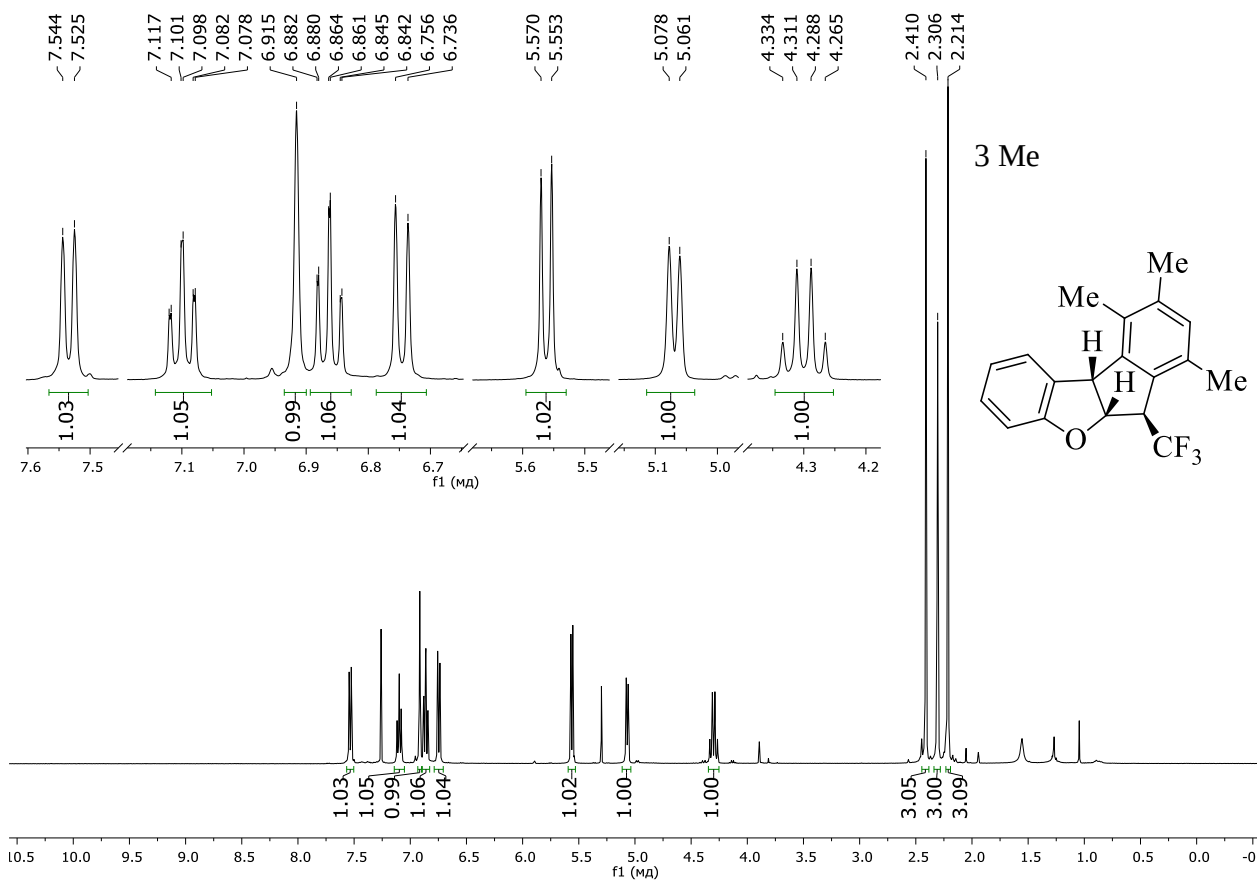


Fig. S239. ^1H NMR spectrum of the compound **13ab** (CDCl_3 , 400 MHz).

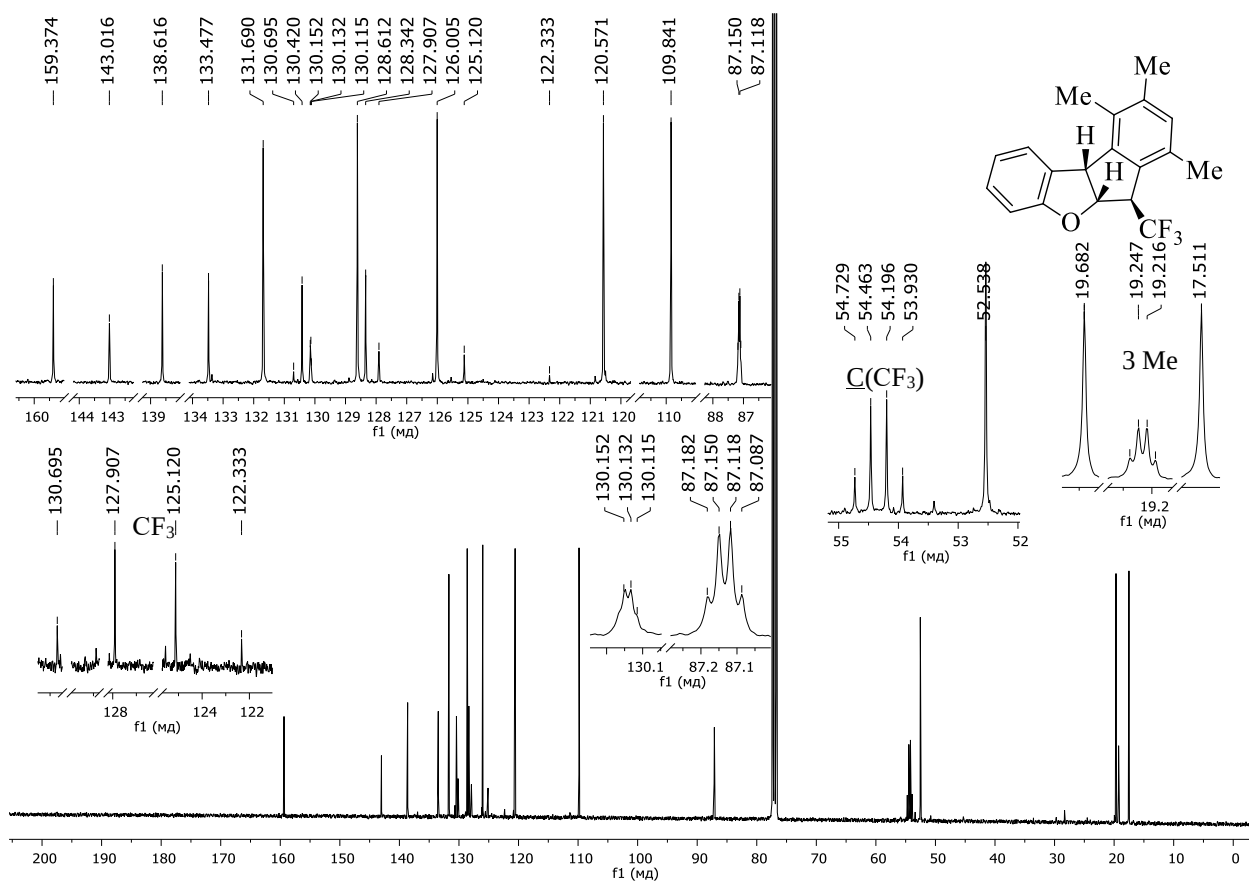


Fig. S240. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **13ab** (CDCl_3 , 101 MHz).

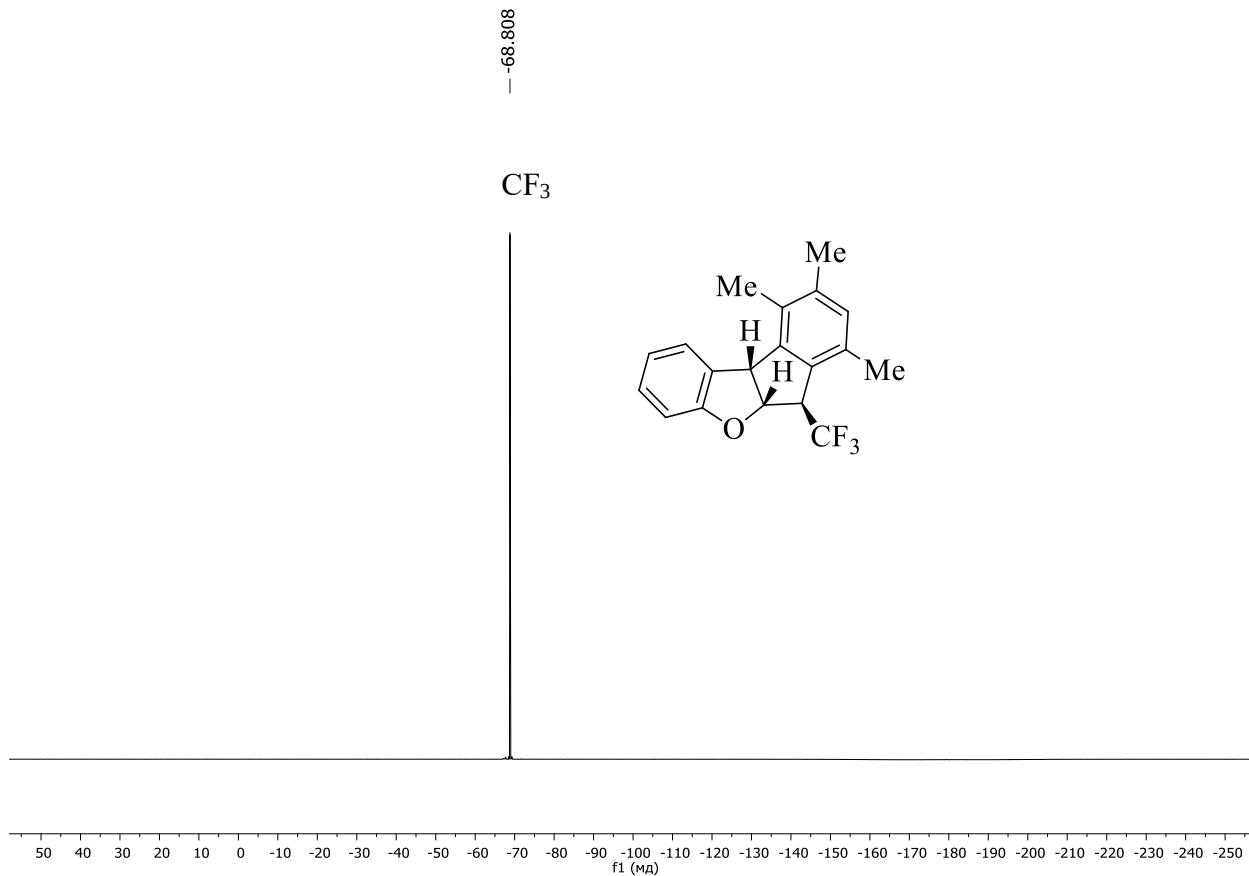


Fig. S241. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **13ab** (CDCl_3 , 376 MHz).

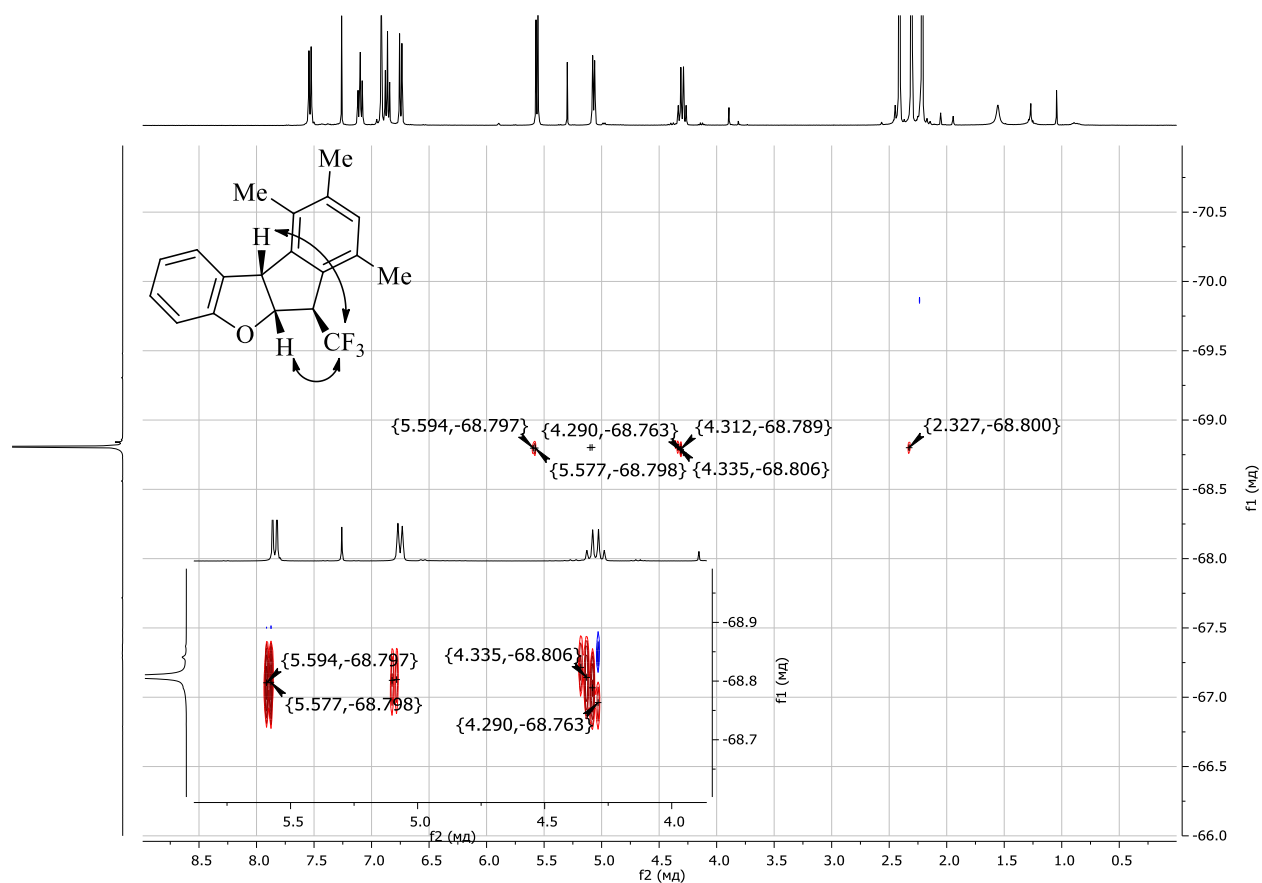


Fig. S242. HOESY F-H NMR spectrum of the compound **13ab** (CDCl₃, 376 – 400 MHz).

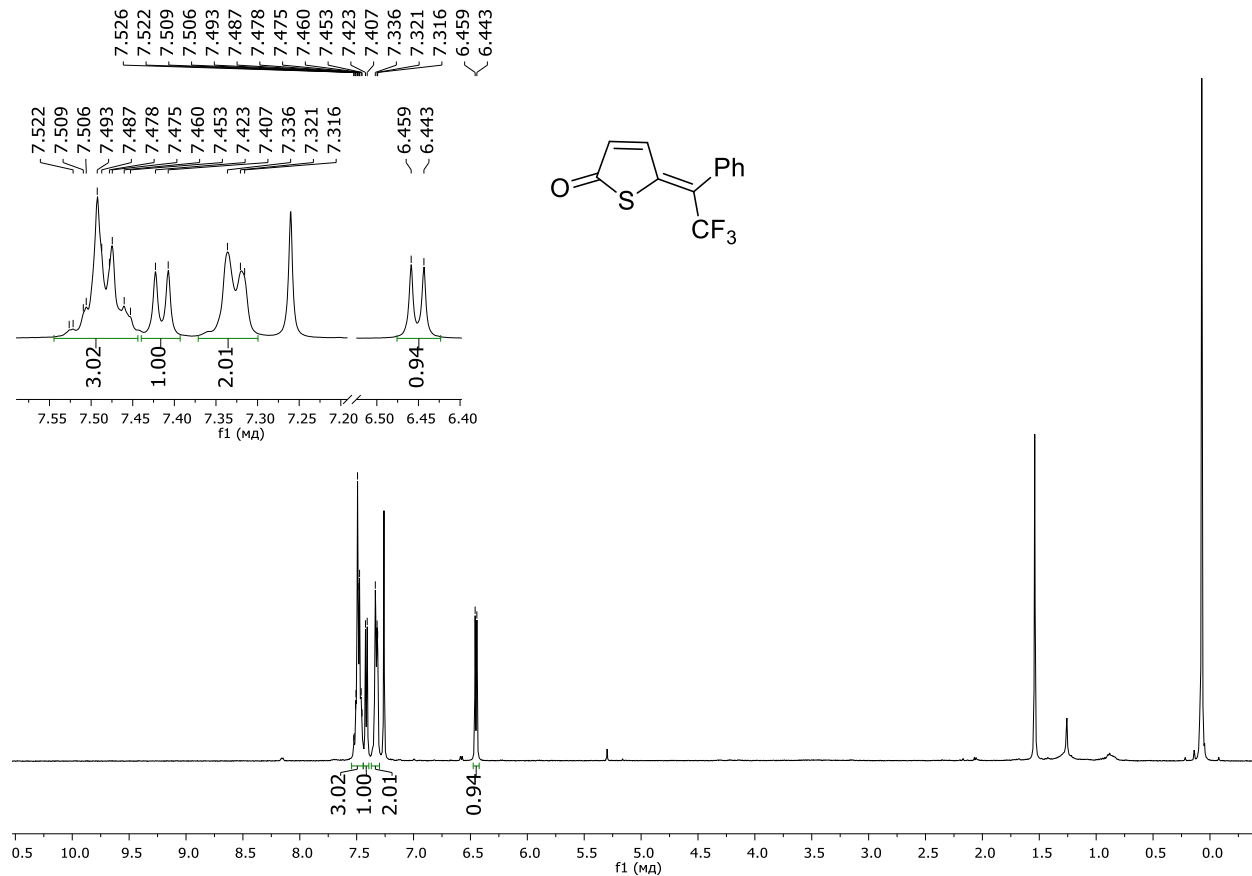


Fig. S243. ¹H NMR spectrum of the compound **Z-14i** (CDCl₃, 400 MHz).

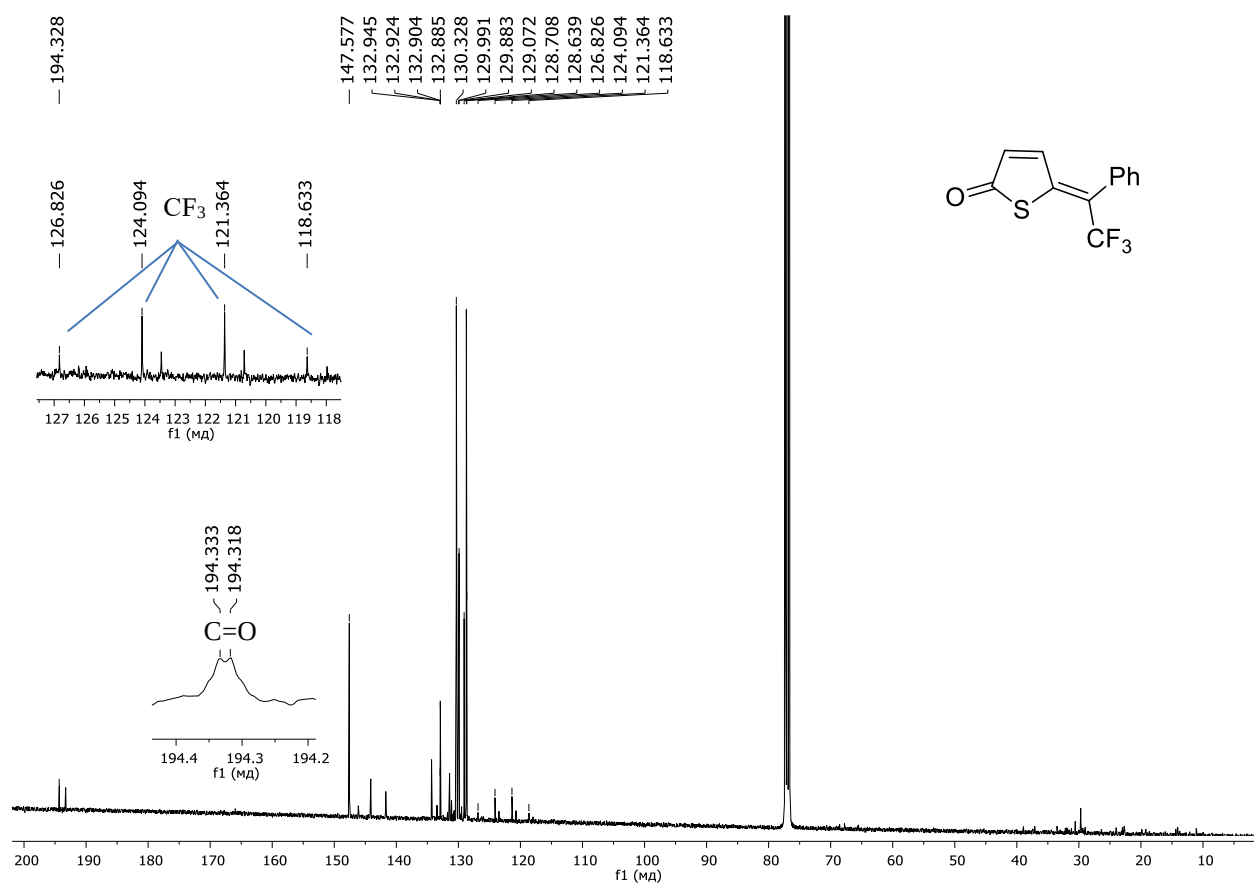


Fig. S244. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **Z-14i** (CDCl_3 , 101 MHz).

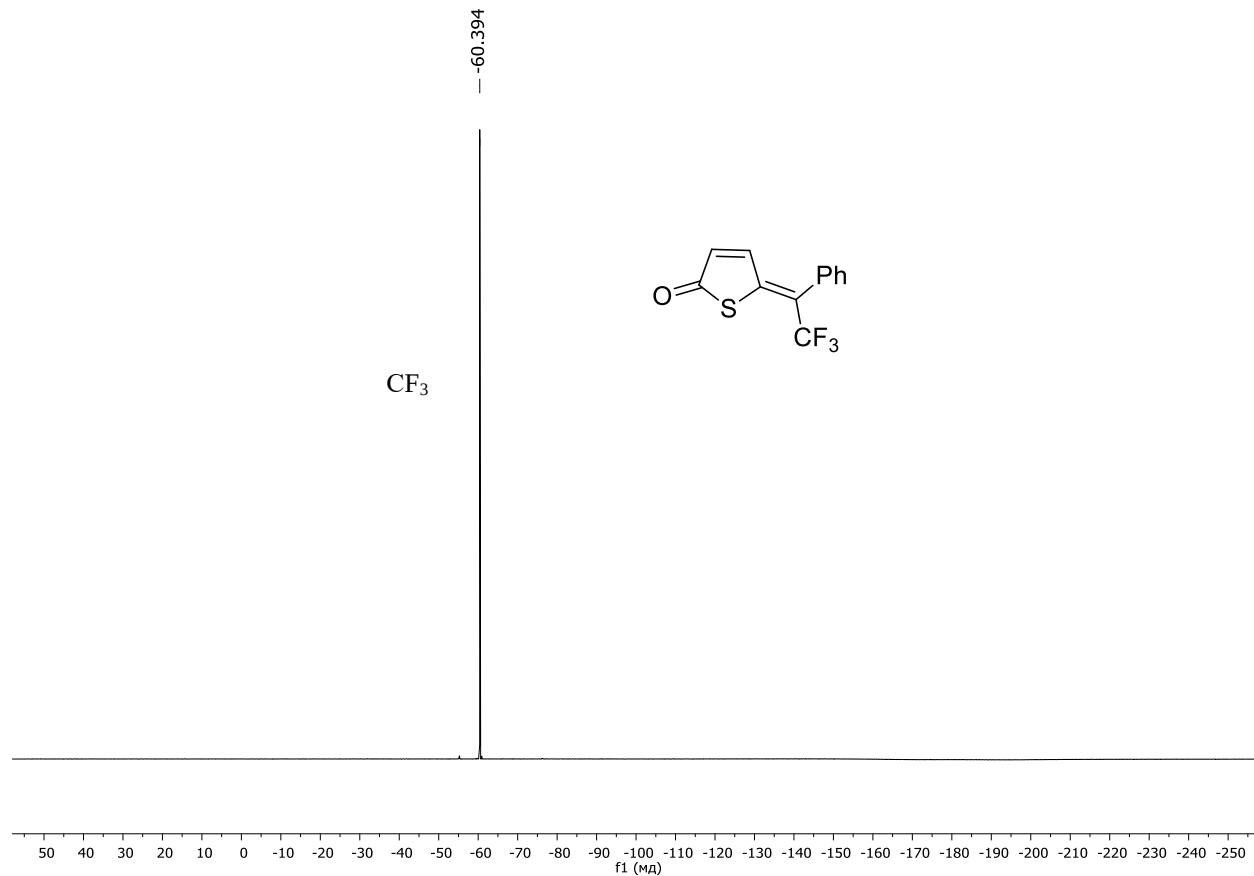


Fig. S245. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **Z-14i** (CDCl_3 , 376 MHz).

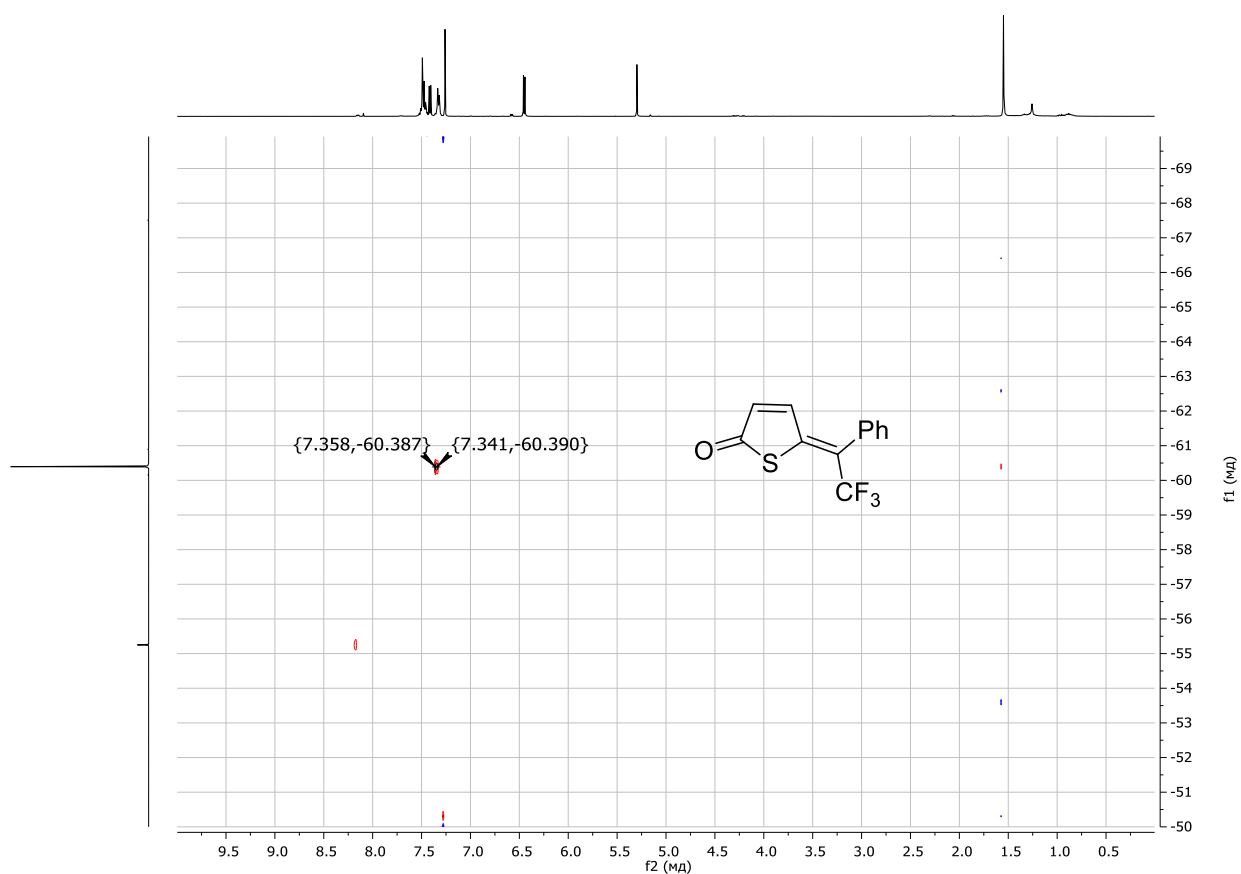


Fig. S246. HOESY H-F NMR spectrum of the compound **Z-14i** (CDCl_3 , 400-376 MHz).

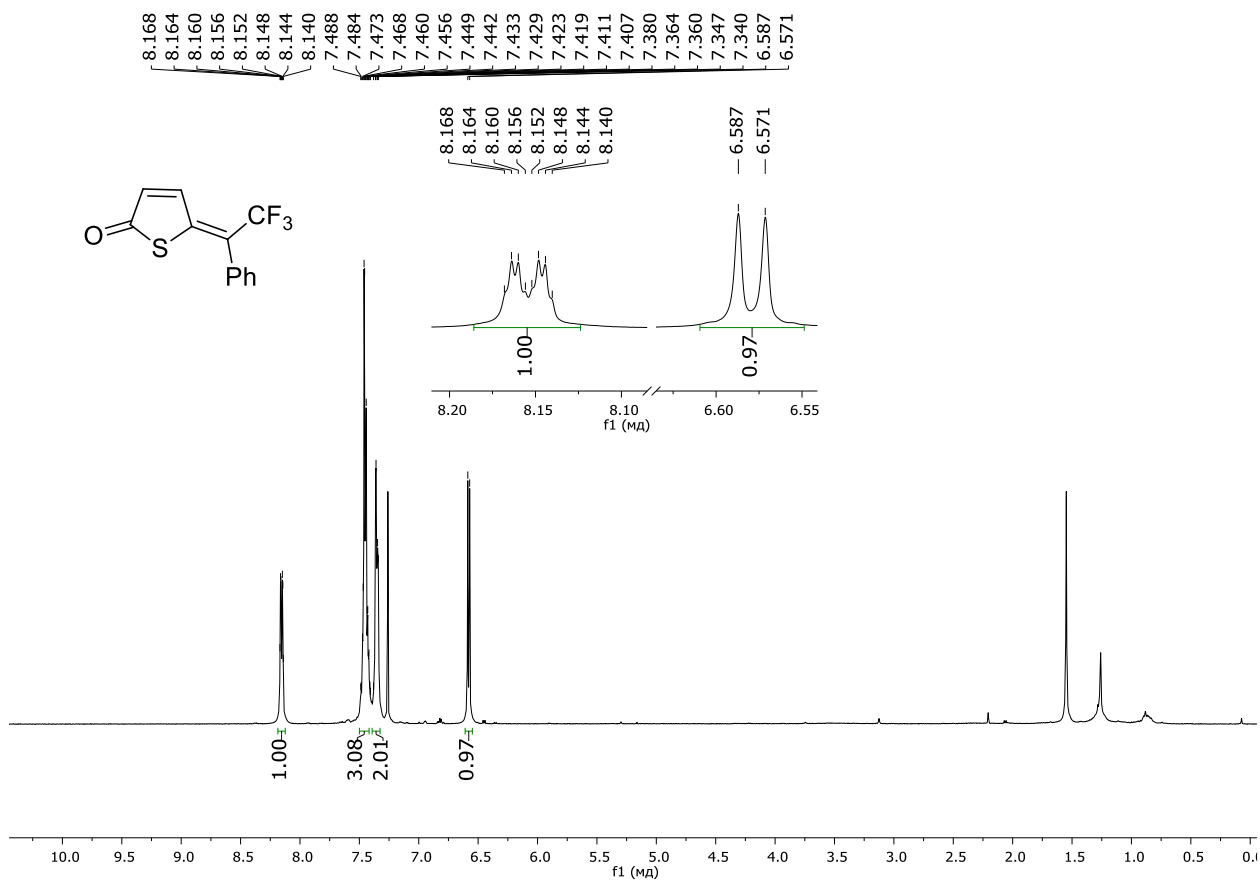


Fig. S247. ^1H NMR spectrum of the compound **E-14i** (CDCl_3 , 400 MHz).

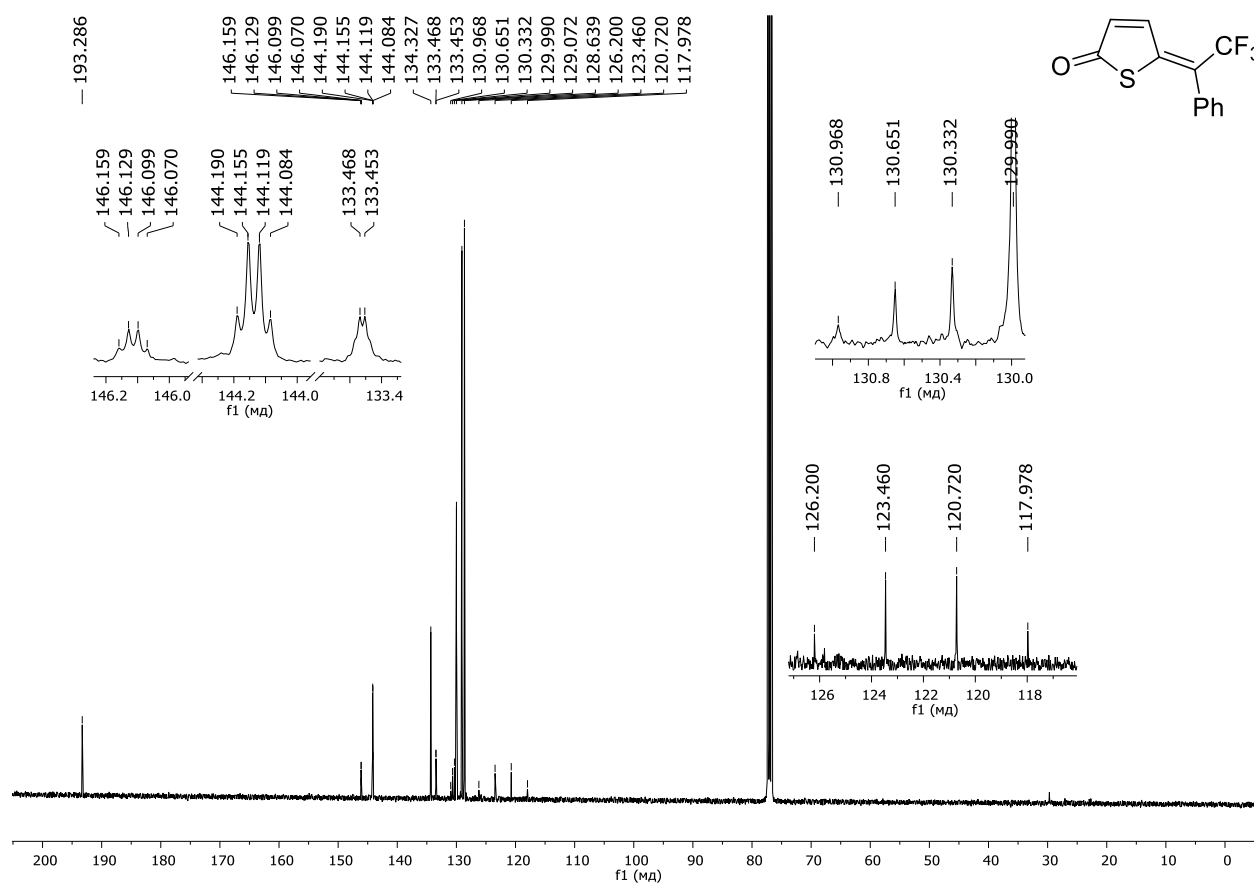


Fig. S248. ¹³C{¹H} NMR spectrum of the compound **E-14i** (CDCl₃, 101 MHz).

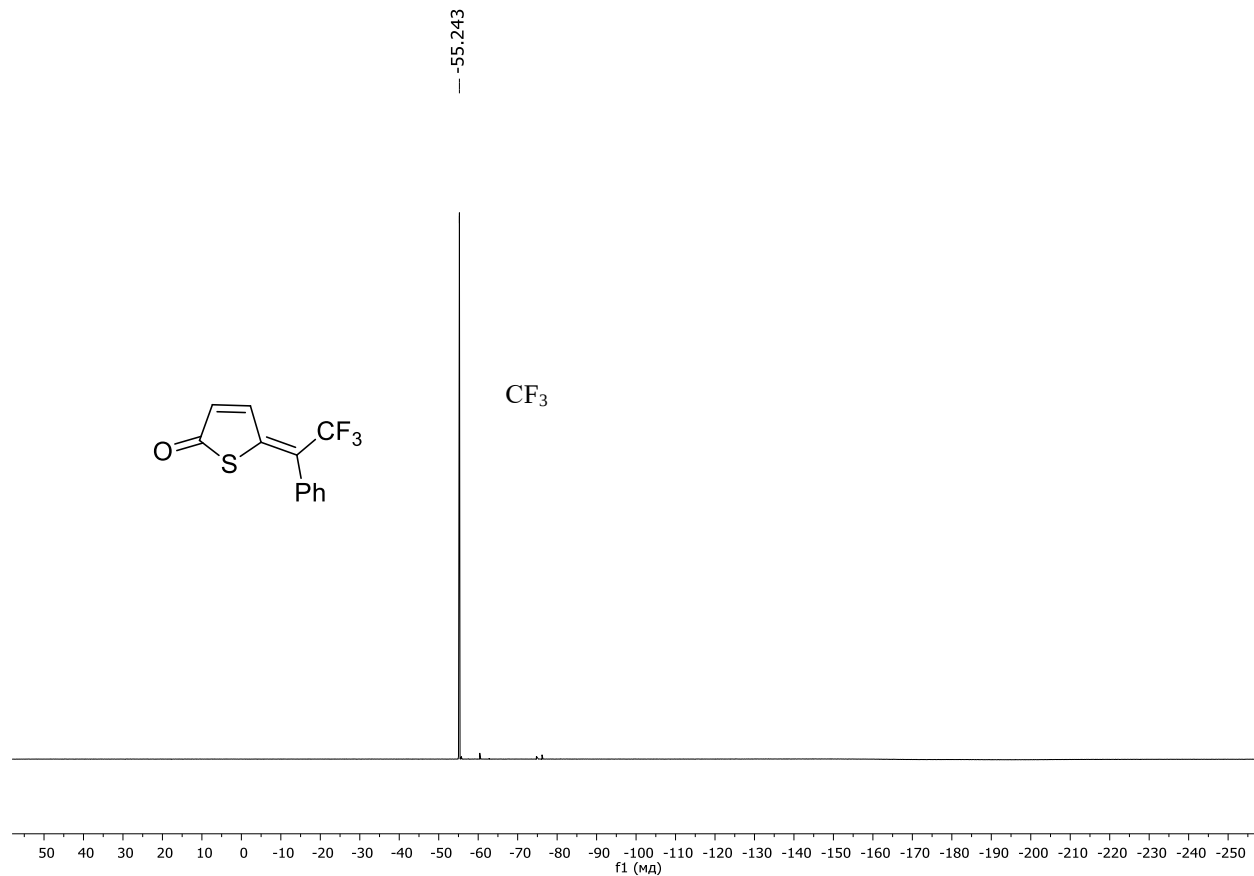


Fig. S249. ¹⁹F{¹H} NMR spectrum of the compound **E-14i** (CDCl₃, 376 MHz).

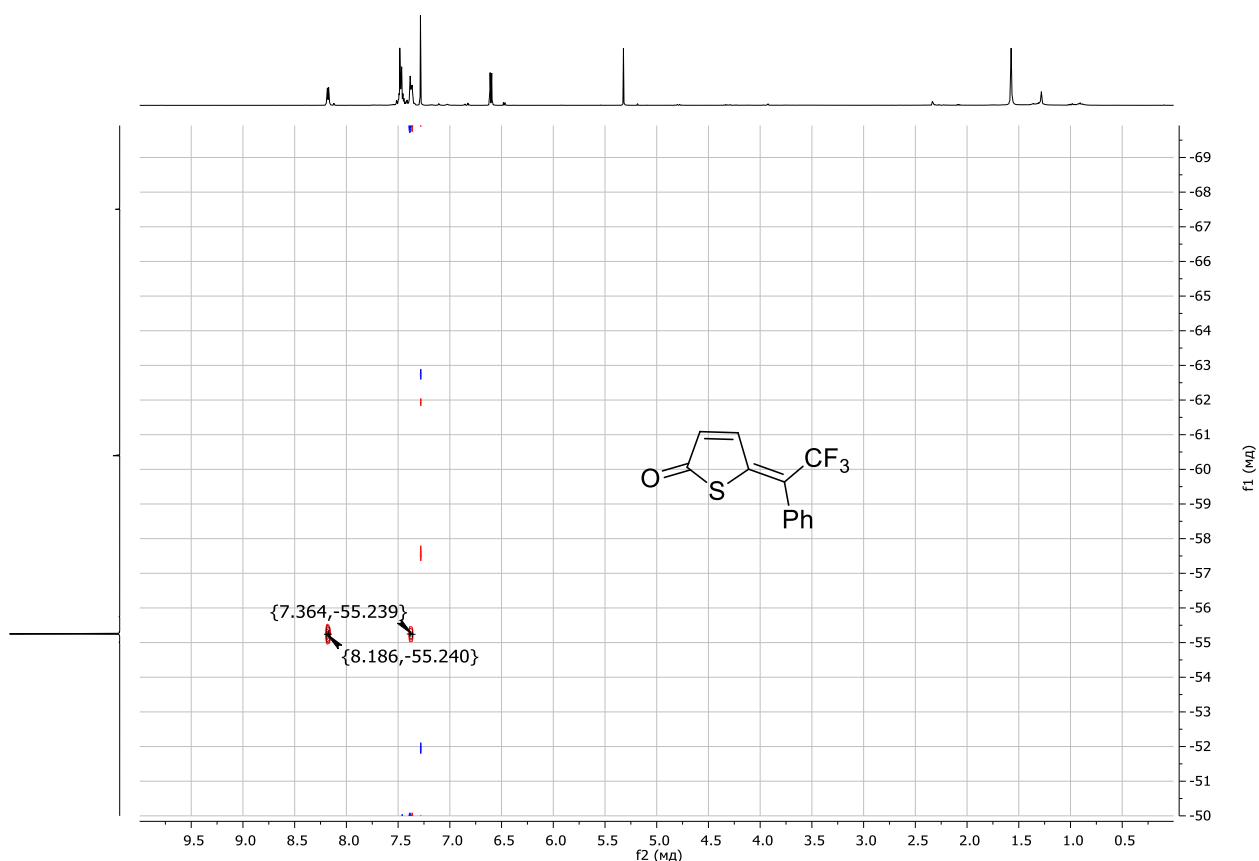


Fig. S250. HOESY H-F NMR spectrum of the compound **E-14i** (CDCl₃, 400-376 MHz).

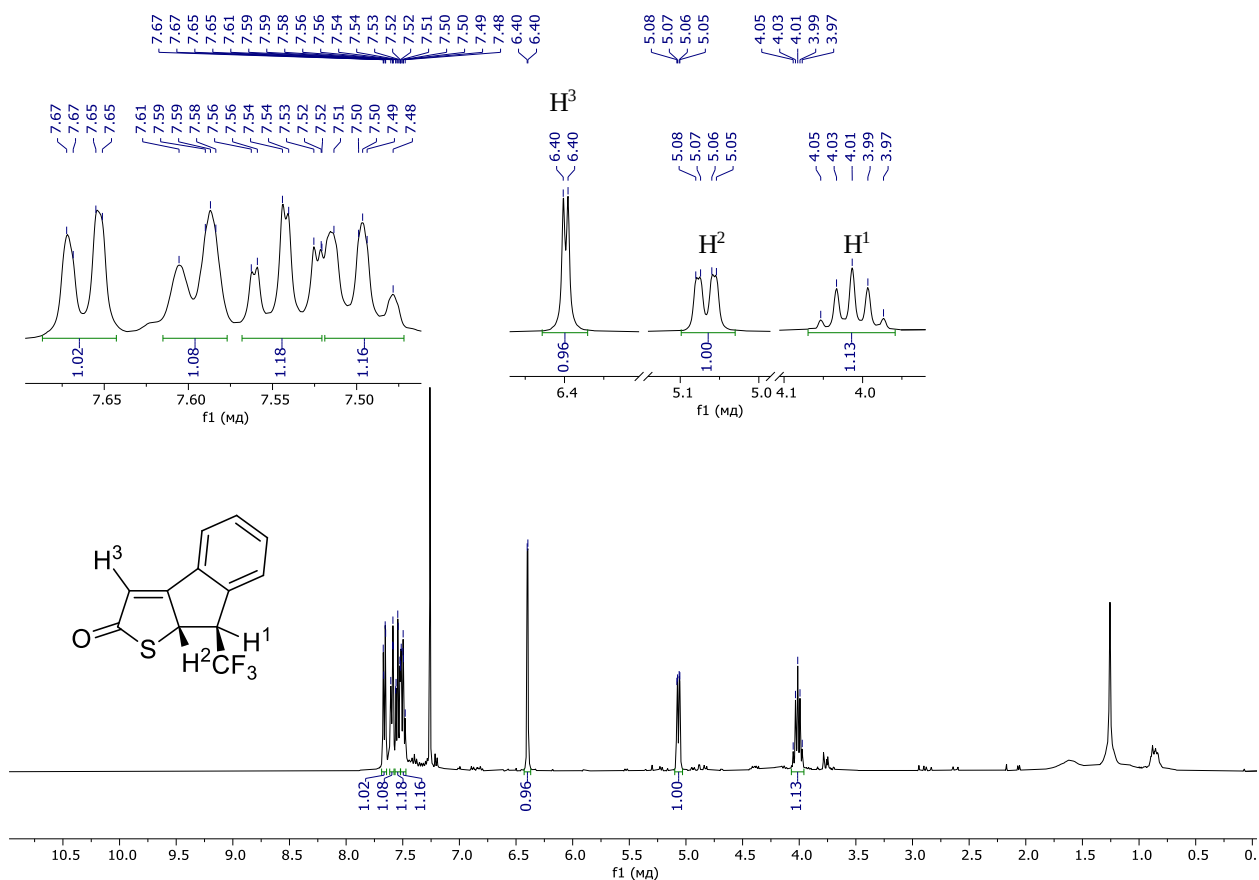


Fig. S251. ¹H NMR spectrum of the compound **15i** (CDCl₃, 400 MHz).

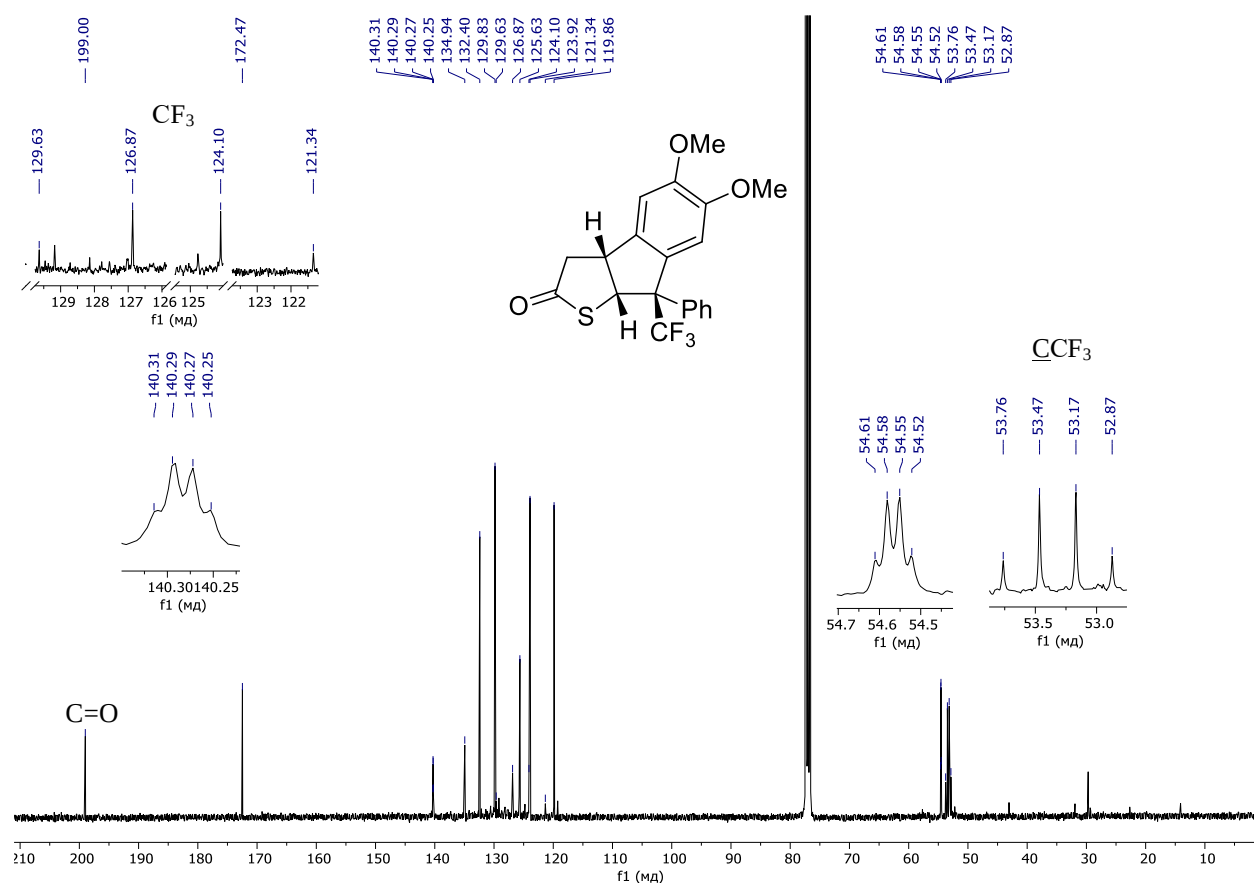


Fig. S252. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the compound **15i** (CDCl₃, 101 MHz).

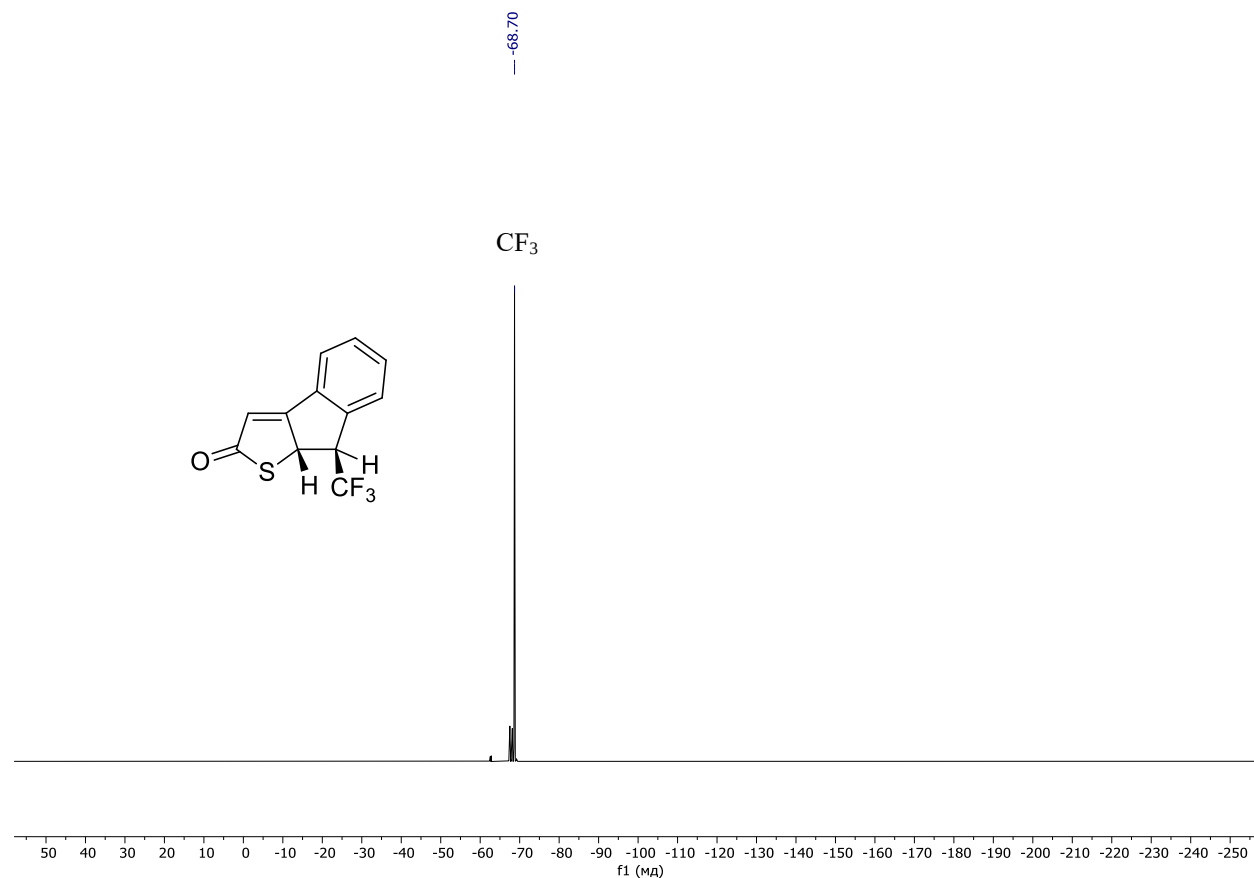


Fig. S253. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of the compound **15i** (CDCl₃, 376 MHz).

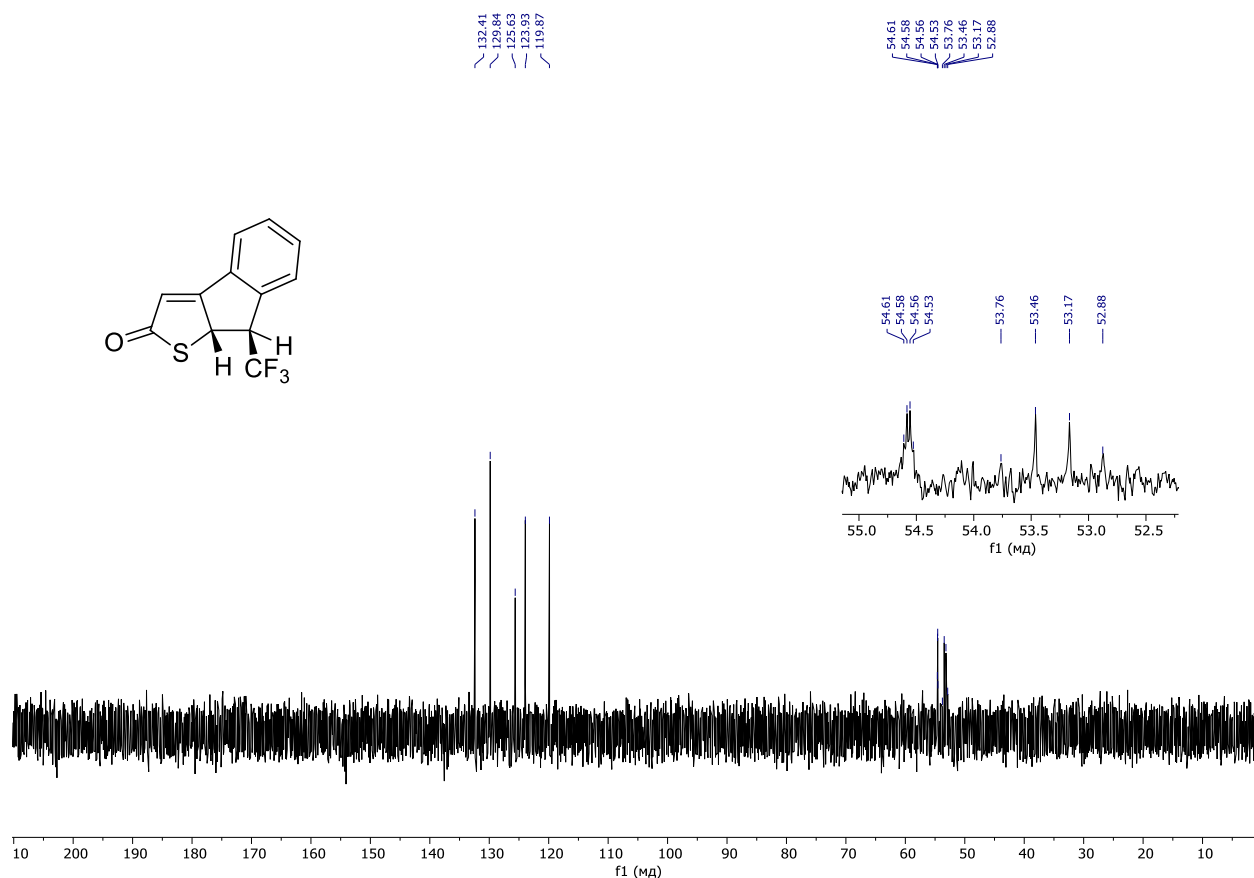


Fig. S254. DEPT NMR spectrum of the compound **15i** (CDCl_3 , 101 MHz).

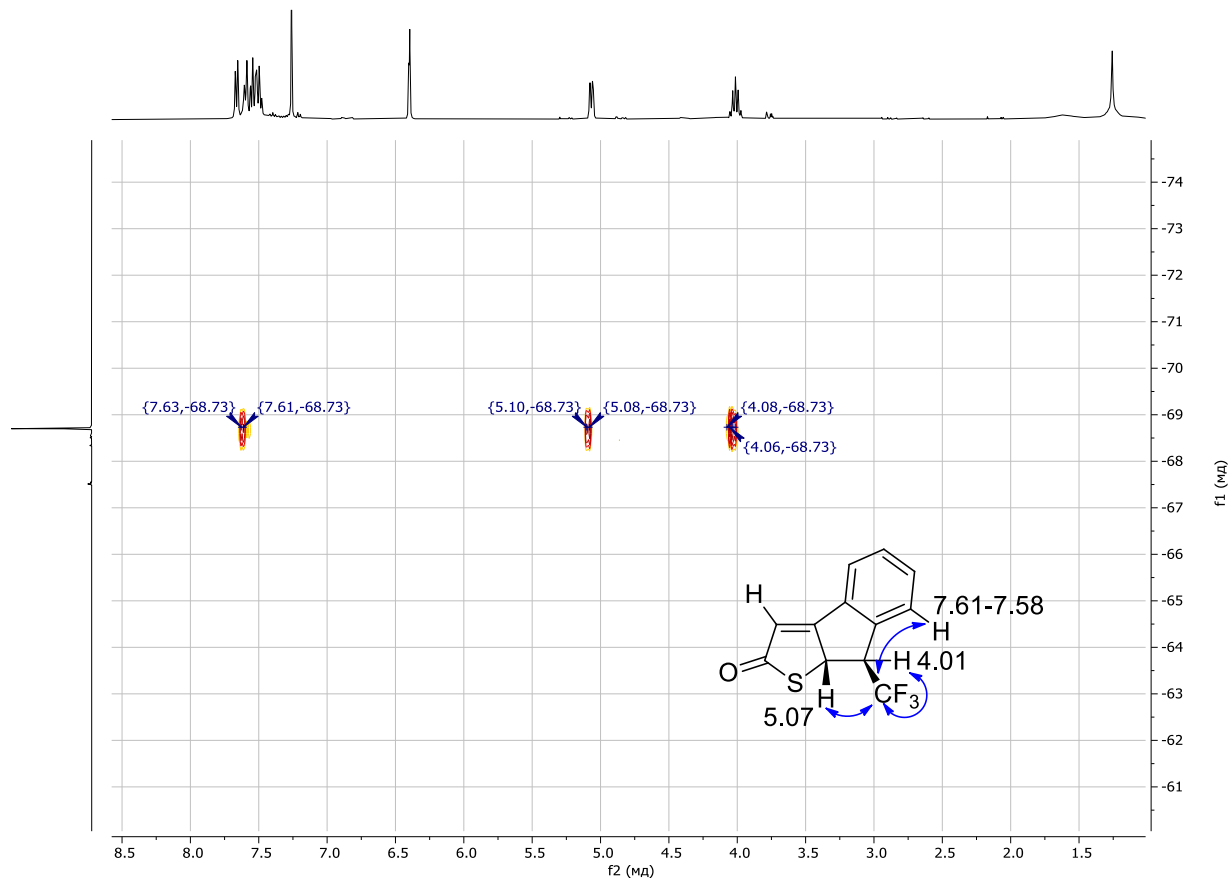


Fig. S255. HOESY H-F NMR spectrum of the compound **15i** (CDCl_3 , 400 – 376 MHz).

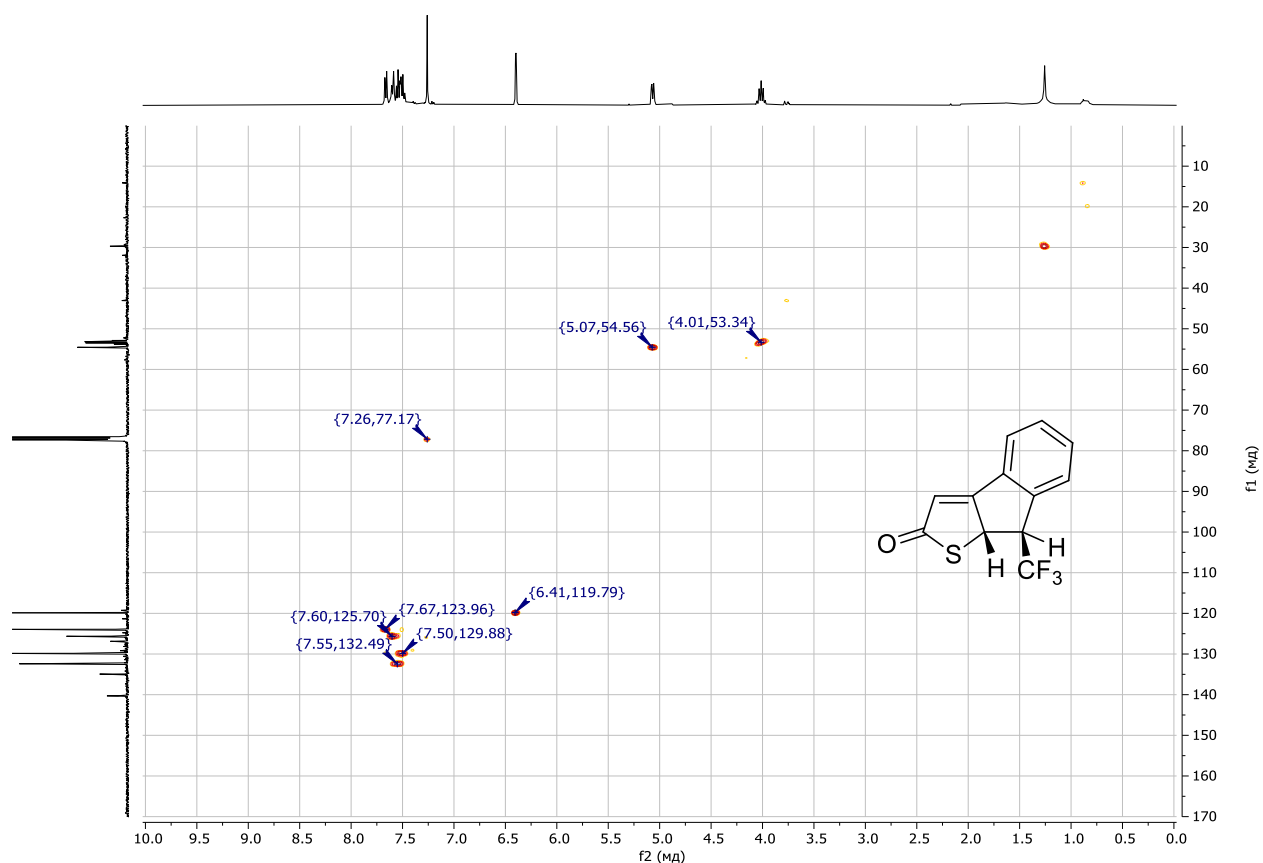


Fig. S256. HSQC C-H NMR spectrum of the compound **15i** (CDCl₃, 100 – 400 MHz).

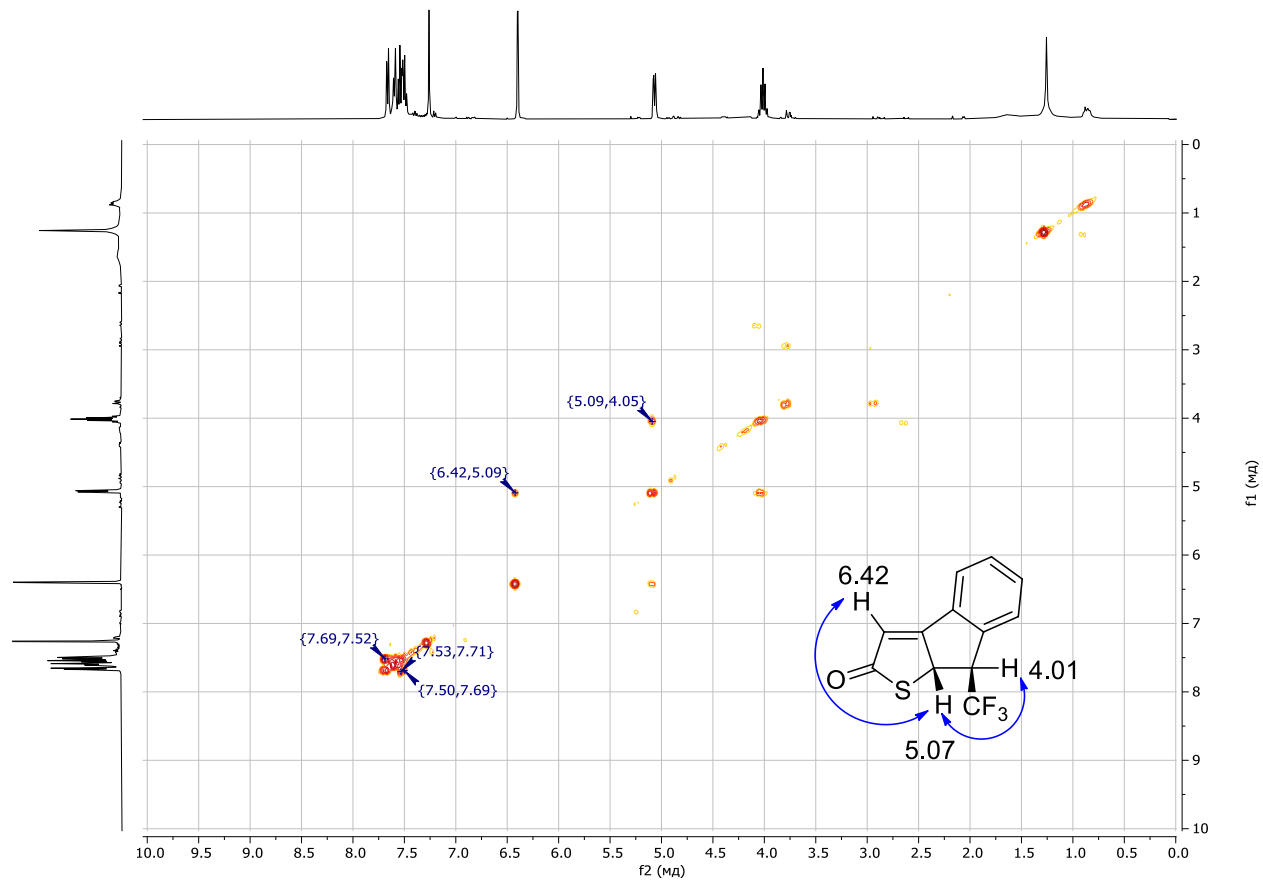


Fig. S257. COSY H-H NMR spectrum of the compound **15i** (CDCl₃, 400 MHz).

Copies of ^1H NMR Spectra of the compounds previously obtained by ourselves

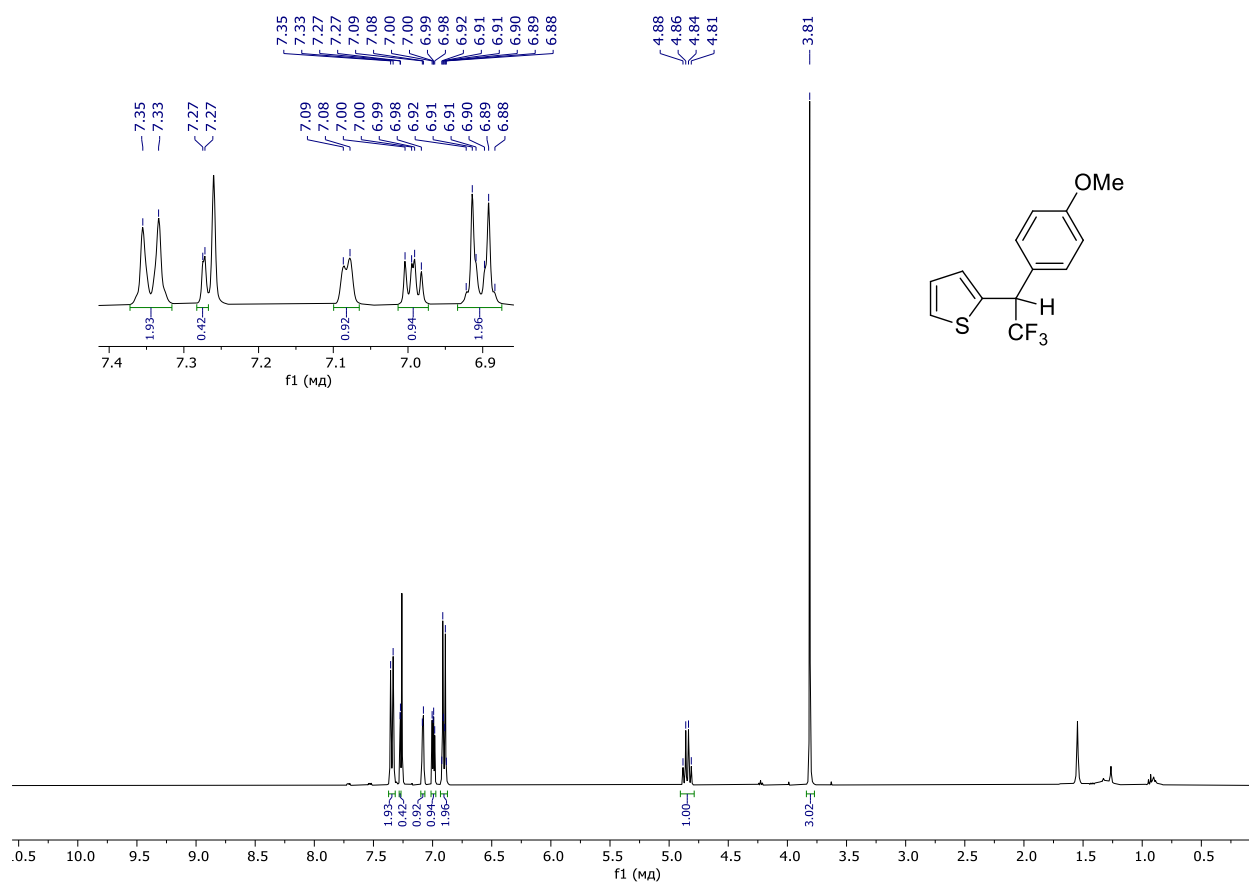


Fig. S258. ^1H NMR spectrum of the compound **3ka** (CDCl_3 , 400 MHz).

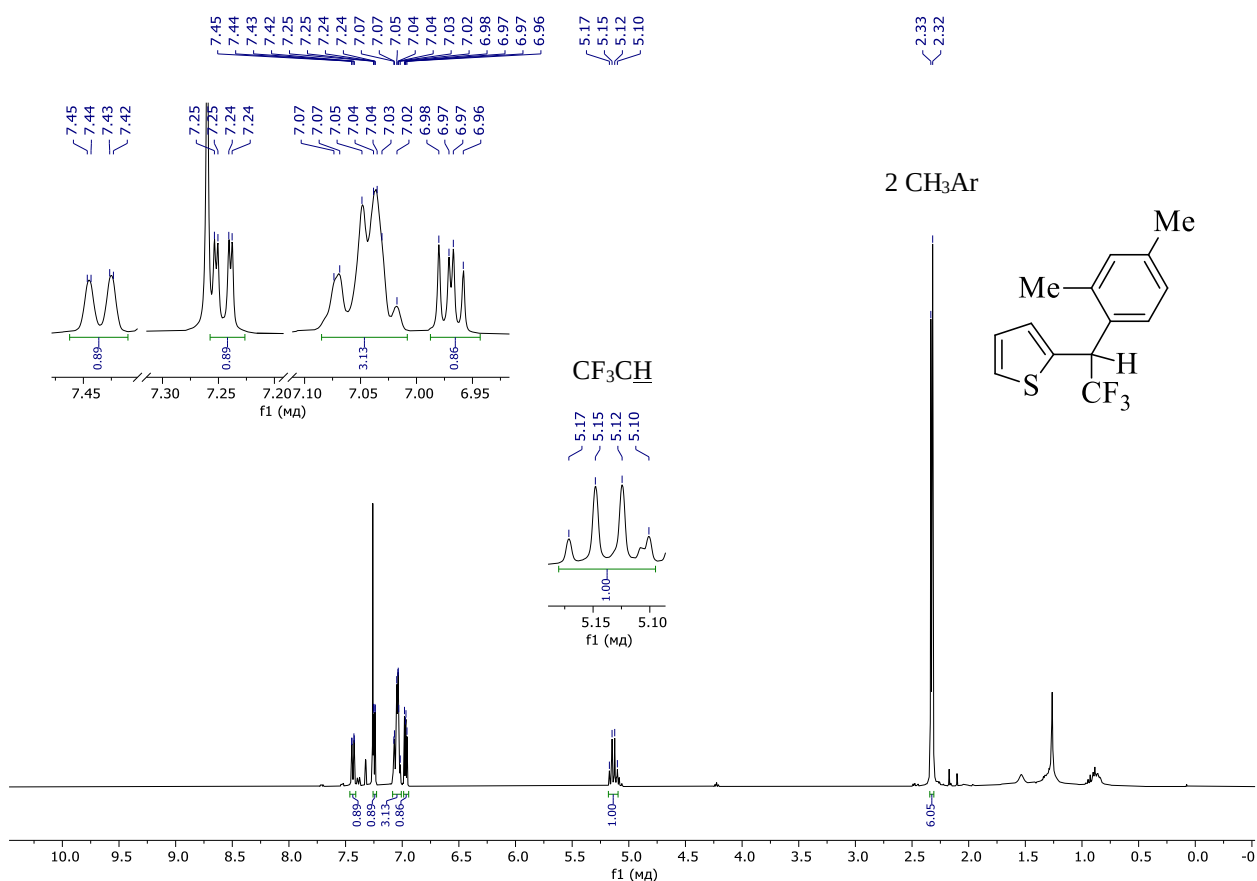


Fig. S259. ¹H NMR spectrum of the compound **3kd** (CDCl₃, 400 MHz).

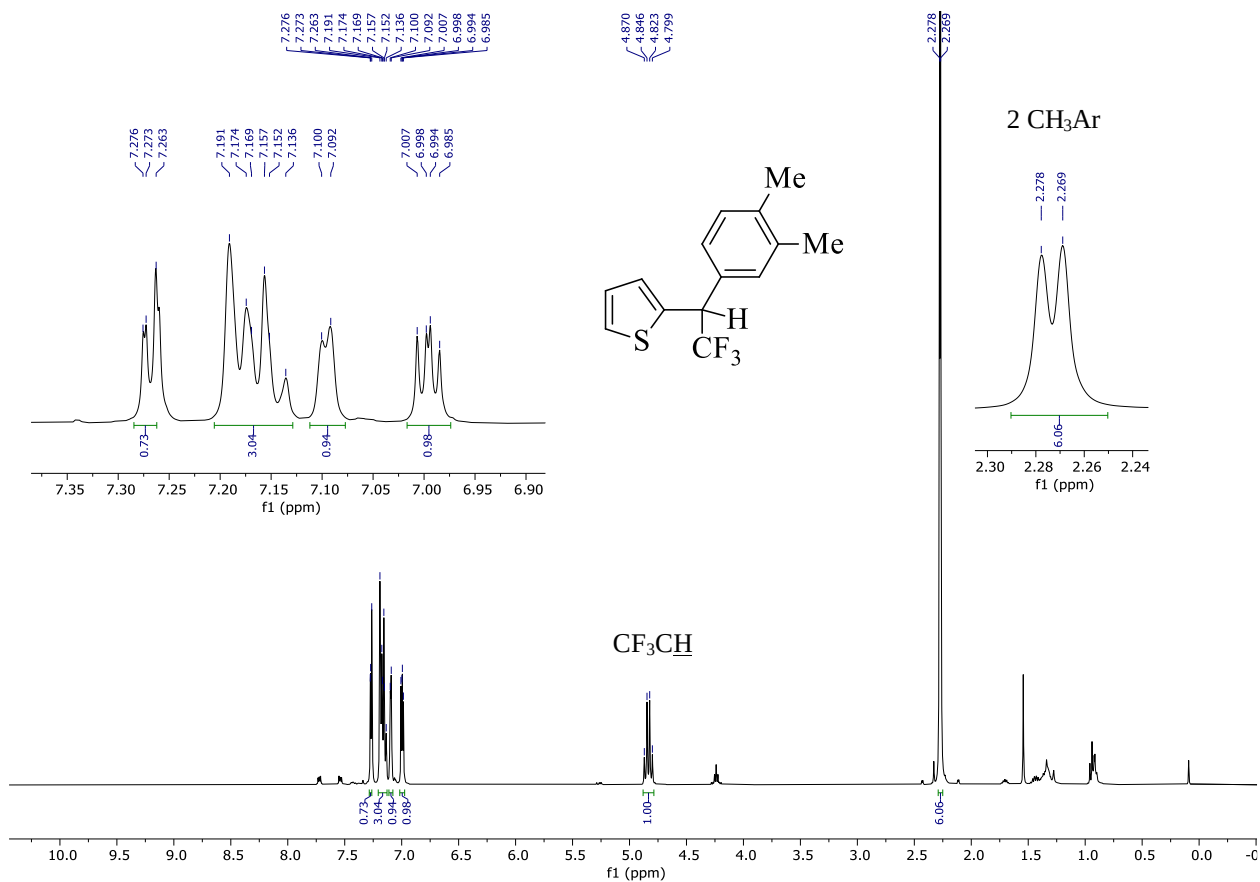


Fig. S260. ¹H NMR spectrum of the compound **3ke** (CDCl₃, 400 MHz).

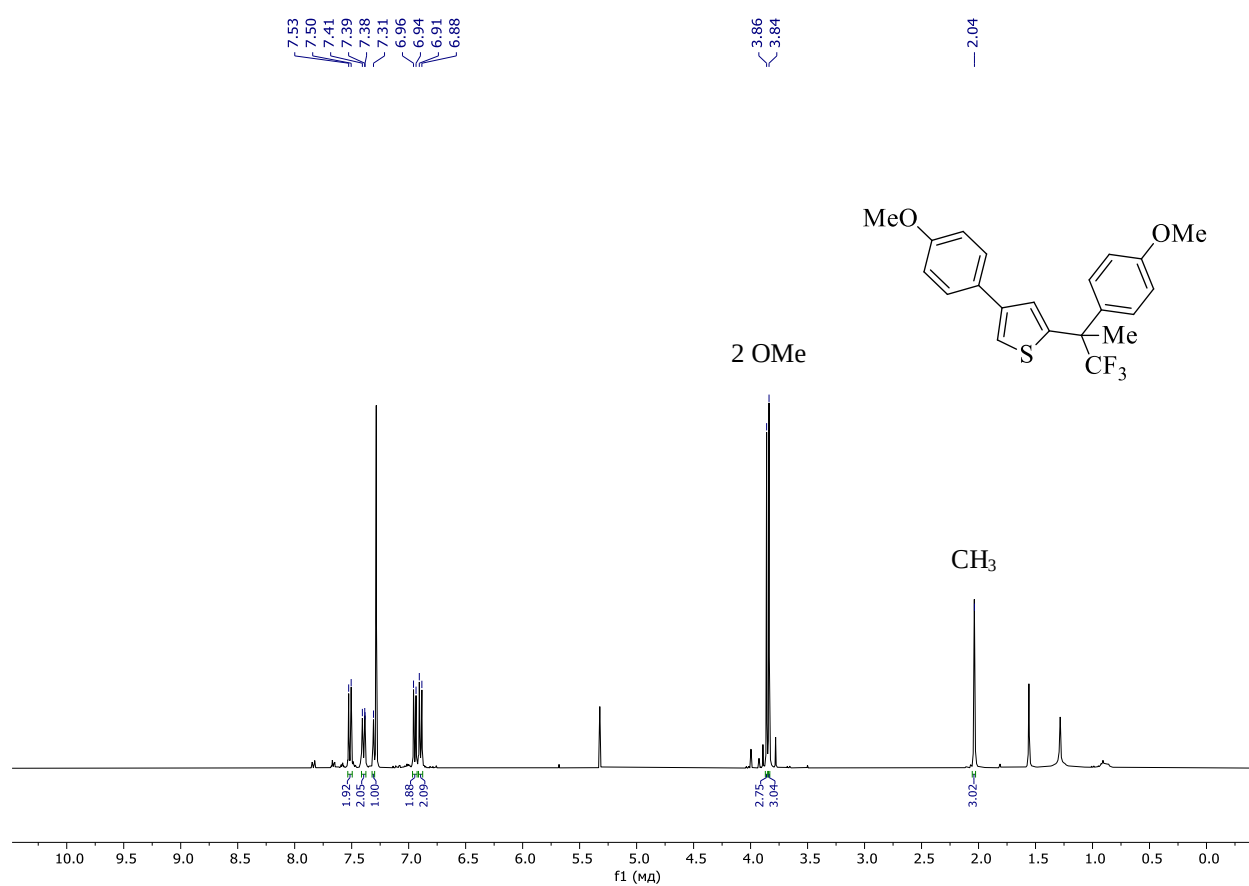


Fig. S261. ¹H NMR spectrum of the compound **5ga** (CDCl₃, 400 MHz).

X-RAY data

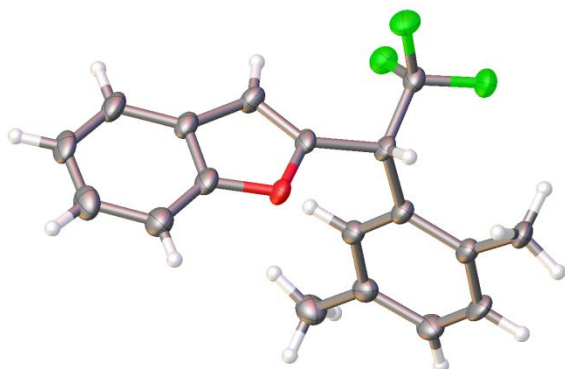


Fig. S262. Molecular structure of **2ac**, CCDC 2233369 (ellipsoid contour of probability levels is 50%).

Table S1. Crystal data and structure refinement for 2ac .	
Empirical formula	C ₁₈ H ₁₅ F ₃ O
Formula weight	304.30
Temperature/K	100(4)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	14.8404(12)
b/Å	5.1873(5)
c/Å	18.6784(10)
α/°	90
β/°	93.721(6)
γ/°	90
Volume/Å ³	1434.87(19)
Z	4
ρ _{calc} /g/cm ³	1.409
μ/mm ⁻¹	0.955
F(000)	632.0
Crystal size/mm ³	0.42 × 0.005 × 0.005
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	7.38 to 142.978
Index ranges	-17 ≤ h ≤ 18, -6 ≤ k ≤ 6, -22 ≤ l ≤ 22
Reflections collected	7791
Independent reflections	2710 [R _{int} = 0.0633, R _{sigma} = 0.0625]
Data/restraints/parameters	2710/0/201
Goodness-of-fit on F ²	1.081
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0917, wR ₂ = 0.2474
Final R indexes [all data]	R ₁ = 0.1219, wR ₂ = 0.2780
Largest diff. peak/hole / e Å ⁻³	0.46/-0.47
CCDC	2233369

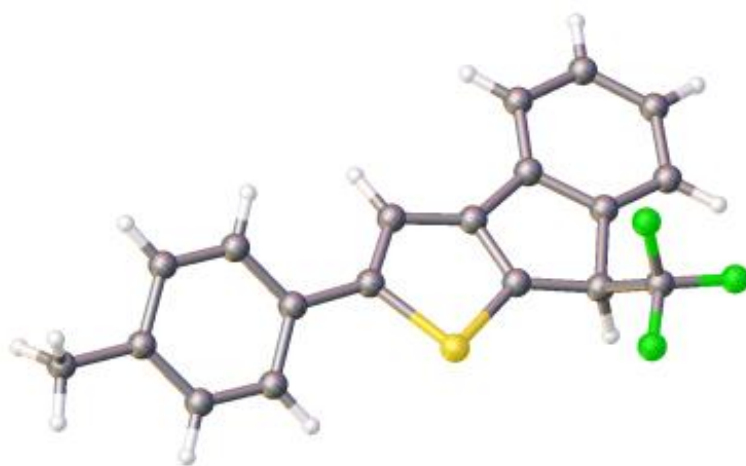


Fig. S263. Molecular structure of **9i**, CCDC 2248983 (ellipsoid contour of probability levels is 50%).

Table S2. Crystal data and structure refinement for 9i .	
Empirical formula	C ₁₉ H ₁₃ F ₃ S
Formula weight	330.35
Temperature/K	100.0(3)
Crystal system	monoclinic
Space group	C2/c
a/Å	44.8162(4)
b/Å	9.25160(10)
c/Å	29.8662(2)
α /°	90
β /°	101.3840(10)
γ /°	90
Volume/Å ³	12139.54(19)
Z	32
ρ_{calc} /g/cm ³	1.446
μ /mm ⁻¹	2.156
F(000)	5440.0
Crystal size/mm ³	0.48 × 0.1 × 0.06
Radiation	Cu K α (λ = 1.54184)
2 Θ range for data collection/°	6.038 to 139.986
Index ranges	-54 ≤ h ≤ 54, -10 ≤ k ≤ 11, -36 ≤ l ≤ 36
Reflections collected	77853
Independent reflections	11500 [R_{int} = 0.0324, R_{sigma} = 0.0177]
Data/restraints/parameters	11500/0/833
Goodness-of-fit on F ²	1.033
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0325, wR_2 = 0.0963
Final R indexes [all data]	R_1 = 0.0344, wR_2 = 0.0980
Largest diff. peak/hole / e Å ⁻³	0.28/-0.23
CCDC	2248983

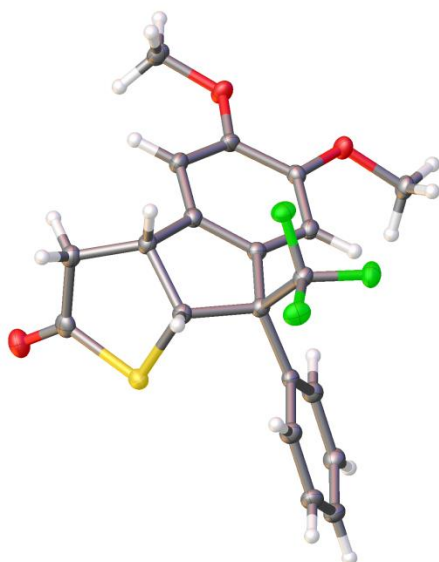


Fig. S264. Molecular structure of **11i**, CCDC 2233370 (ellipsoid contour of probability levels is 50%).

Table S3. Crystal data and structure refinement for 11i .	
Empirical formula	C ₂₀ H ₁₇ F ₃ O ₃ S
Formula weight	394.39
Temperature/K	100(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	13.4778(2)
b/Å	7.91980(10)
c/Å	17.0401(3)
α/°	90
β/°	108.952(2)
γ/°	90
Volume/Å ³	1720.29(5)
Z	4
ρ _{calc} /g/cm ³	1.523
μ/mm ⁻¹	2.136
F(000)	816.0
Crystal size/mm ³	0.09 × 0.07 × 0.05
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	6.934 to 159.69
Index ranges	-17 ≤ h ≤ 17, -10 ≤ k ≤ 7, -21 ≤ l ≤ 20
Reflections collected	12865
Independent reflections	3629 [R _{int} = 0.0310, R _{sigma} = 0.0289]
Data/restraints/parameters	3629/0/246
Goodness-of-fit on F ²	1.102
Final R indexes [I > 2σ (I)]	R ₁ = 0.0338, wR ₂ = 0.0920
Final R indexes [all data]	R ₁ = 0.0369, wR ₂ = 0.0938
Largest diff. peak/hole / e Å ⁻³	0.40/-0.31
CCDC	2233370

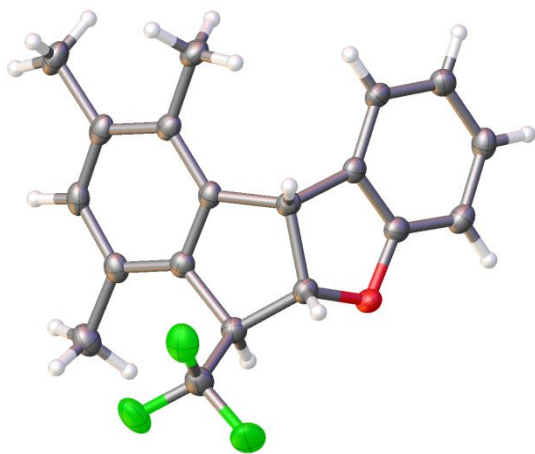


Fig. S265. Molecular structure of **13ab**, CCDC 2233371 (ellipsoid contour of probability levels is 50%).

Table S4. Crystal data and structure refinement for 13ab .	
Empirical formula	C ₁₉ H ₁₇ F ₃ O
Formula weight	318.32
Temperature/K	100(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	5.85016(9)
b/Å	11.07614(16)
c/Å	23.2374(3)
α/°	90
β/°	93.4883(14)
γ/°	90
Volume/Å ³	1502.93(4)
Z	4
ρ _{calc} /g/cm ³	1.407
μ/mm ⁻¹	0.936
F(000)	664.0
Crystal size/mm ³	0.25 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	7.624 to 140.888
Index ranges	-6 ≤ h ≤ 7, -13 ≤ k ≤ 13, -28 ≤ l ≤ 28
Reflections collected	15404
Independent reflections	2871 [R _{int} = 0.0476, R _{sigma} = 0.0314]
Data/restraints/parameters	2871/0/211
Goodness-of-fit on F ²	1.073
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0451, wR ₂ = 0.1112
Final R indexes [all data]	R ₁ = 0.0513, wR ₂ = 0.1155
Largest diff. peak/hole / e Å ⁻³	0.20/-0.28
CCDC	2233371

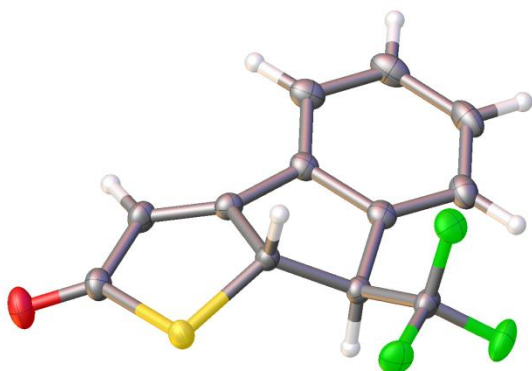


Fig. S266. Molecular structure of **15i**, CCDC 2233372 (ellipsoid contour of probability levels is 50%).

Table S5. Crystal data and structure refinement for 15i .	
Empirical formula	C ₁₂ H ₇ F ₃ OS
Formula weight	256.24
Temperature/K	100(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	4.7366(2)
b/Å	25.8695(8)
c/Å	8.5888(4)
α/°	90
β/°	97.737(4)
γ/°	90
Volume/Å ³	1042.83(7)
Z	4
ρ _{calc} /cm ³	1.632
μ/mm ⁻¹	3.012
F(000)	520.0
Crystal size/mm ³	0.12 × 0.09 × 0.04
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	6.834 to 152.446
Index ranges	-5 ≤ h ≤ 5, -18 ≤ k ≤ 32, -10 ≤ l ≤ 10
Reflections collected	4144
Independent reflections	2115 [R _{int} = 0.0331, R _{sigma} = 0.0468]
Data/restraints/parameters	2115/0/154
Goodness-of-fit on F ²	1.039
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0402, wR ₂ = 0.0944
Final R indexes [all data]	R ₁ = 0.0495, wR ₂ = 0.0999
Largest diff. peak/hole / e Å ⁻³	0.66/-0.26
CCDC	2233372

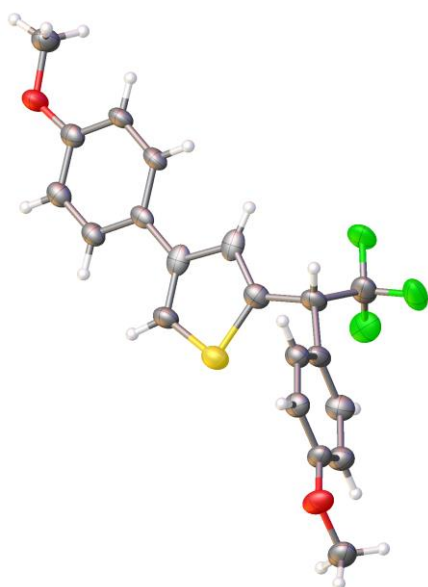


Fig. S267. Molecular structure of **5ja**, CCDC 2248301 (ellipsoid contour of probability levels is 50%).

Table S6. Crystal data and structure refinement for 5ja .	
Empirical formula	C ₂₀ H ₁₇ F ₃ O ₂ S
Formula weight	378.39
Temperature/K	100(2)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	9.3648(5)
b/Å	5.3613(3)
c/Å	17.6629(10)
α/°	90
β/°	100.307(6)
γ/°	90
Volume/Å ³	872.50(9)
Z	2
ρ _{calc} /g/cm ³	1.440
μ/mm ⁻¹	2.036
F(000)	392.0
Crystal size/mm ³	0.16 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	5.086 to 135.914
Index ranges	-10 ≤ h ≤ 11, -6 ≤ k ≤ 6, -20 ≤ l ≤ 21
Reflections collected	5999
Independent reflections	2820 [R _{int} = 0.0575, R _{sigma} = 0.0716]
Data/restraints/parameters	2820/1/232
Goodness-of-fit on F ²	1.058
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0693, wR ₂ = 0.1825
Final R indexes [all data]	R ₁ = 0.0774, wR ₂ = 0.1887
Largest diff. peak/hole / e Å ⁻³	1.04/-0.49
CCDC	2248301

Biological study data

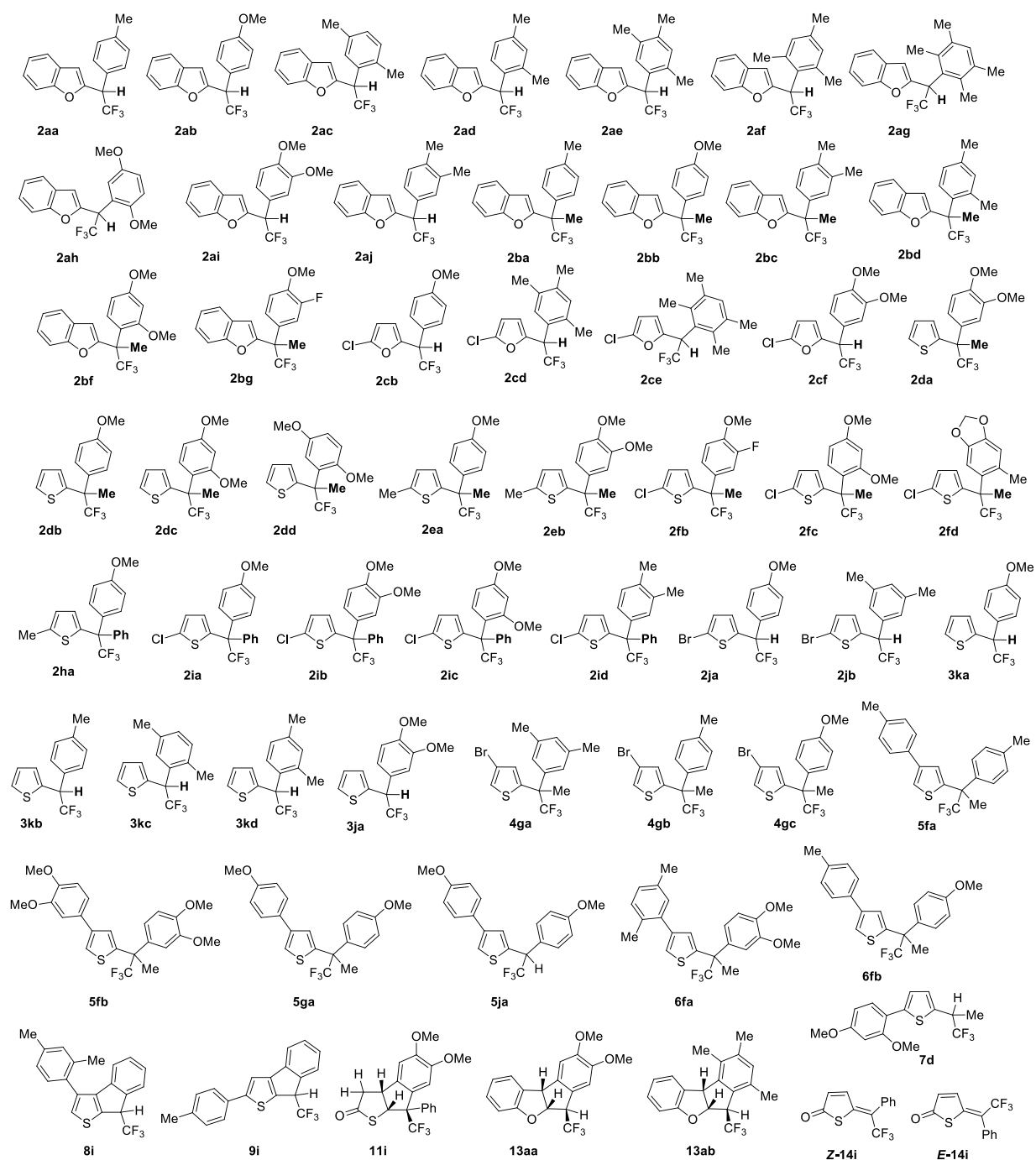


Fig. S268. Selected compounds from this study to evaluate biological activity.

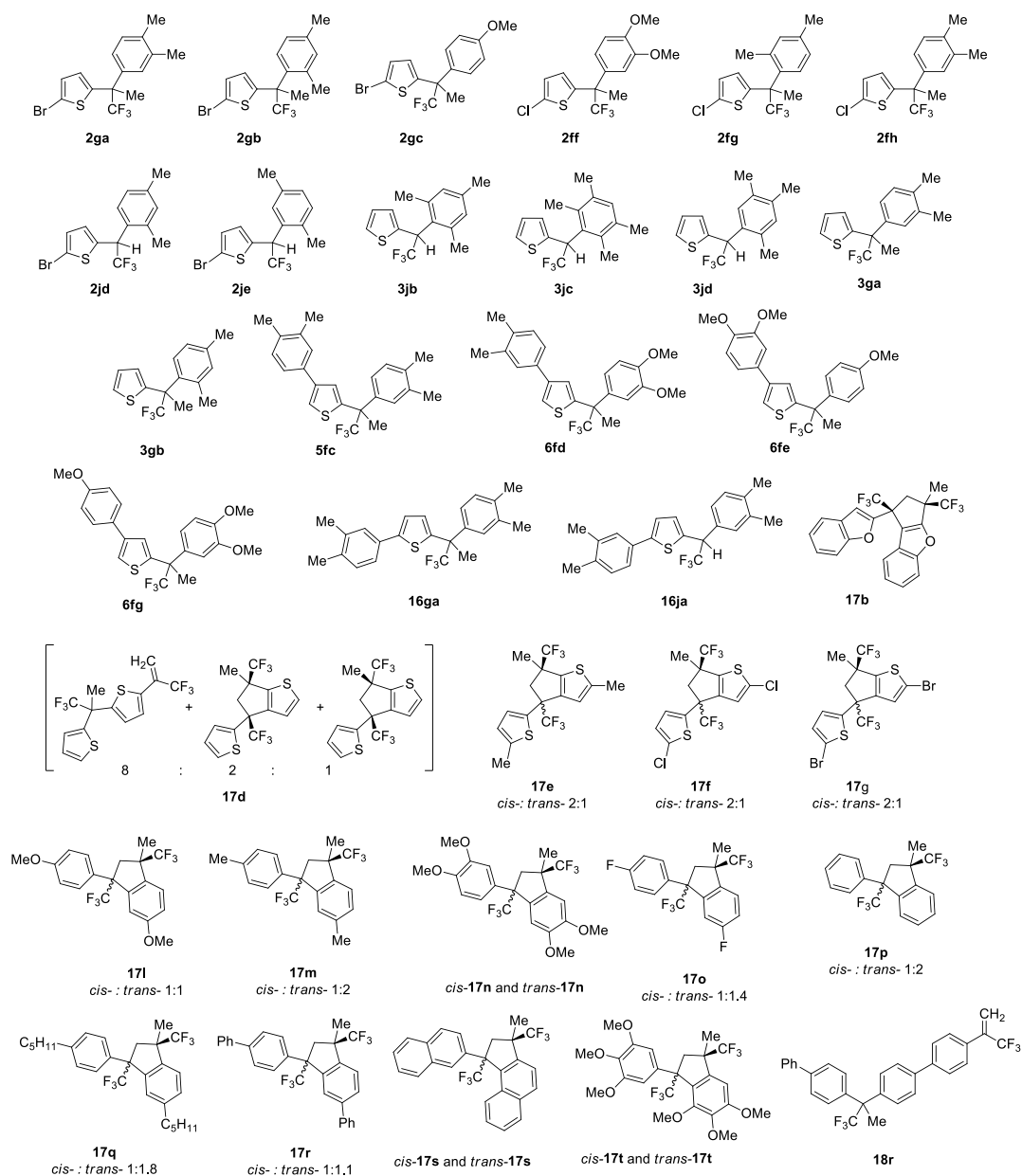


Fig. S269. Previously synthesized compounds subjected to biological activity evaluation [24,28].

Table S7. Preparation of common stock solutions of test objects.

Compound	Sample weight, mg	Solvent volume, mL	Concentration of common stock solution, $\mu\text{g/mL}$
17l	5.1	4.980	1024
17m	3.9	3.809	1024
<i>cis</i> - 17n	6.0	5.859	1024
<i>trans</i> - 17n	3.3	3.223	1024
17o	3.5	3.418	1024
17p	3.3	3.223	1024
17q	5.0	4.883	1024
17r	3.5	3.418	1024
<i>cis</i> - 17s	3.3	3.223	1024
<i>trans</i> - 17s	3.3	3.223	1024

cis-17t	3.2	3.125	1024
trans-17t	3.0	2.930	1024
18r	2.8	2.734	1024
17d	4.3	4.199	1024
17f	4.1	4.004	1024
17g	3.0	2.930	1024
17e	3.8	3.711	1024
17b	4.2	4.102	1024
2bf	2.7	2.637	1024
2bb	3.3	3.223	1024
2ba	3.5	3.418	1024
2bc	5.5	5.371	1024
2bd	4.8	4.688	1024
2bg	3.0	2.930	1024
2ae	2.5	2.441	1024
2ab	4.4	4.297	1024
2aj	4.1	4.004	1024
2ai	4.3	4.199	1024
2ah	3.4	3.320	1024
2ag	2.0	1.953	1024
2ac	4.0	3.906	1024
2ad	3.3	3.223	1024
2aa	2.1	2.051	1024
2af	3.0	2.930	1024
13ab	2.2	2.148	1024
13aa	2.3	2.246	1024
9i	3.7	3.613	1024
8i	4.0	3.906	1024
11i	3.1	3.027	1024
2ia	4.1	4.004	1024
2ic	2.0	1.953	1024
2ib	2.9	2.832	1024
2id	1.9	1.855	1024
2ha	4.0	3.906	1024
2ea	2.2	2.148	1024
2eb	1.9	1.855	1024
2cb	2.5	2.441	1024
2cf	4.4	4.297	1024
2cd	2.4	2.344	1024
2ce	3.8	3.711	1024
2dd	3.0	2.930	1024
2da	2.5	2.441	1024
2dc	2.4	2.344	1024
Z-14i	2.6	2.539	1024
E-14i	2.0	1.953	1024
3kb	1.9	1.855	1024
3jc	3.2	3.125	1024
3jb	4.3	4.199	1024
3kc	1.6	1.562	1024
3ja	3.5	3.417	1024

3jd	2.1	2.050	1024
3ka	3.0	2.929	1024
3kd	1.6	1.562	1024
2db	4.1	4.004	1024
3ga	1.4	1.367	1024
3gb	1.5	1.465	1024
2jd	1.5	1.465	1024
2je	2.2	2.148	1024
2jb	1.3	1.269	1024
2ja	3.0	2.929	1024
2ga	1.6	1.562	1024
2gb	1.2	1.171	1024
2gc	2.9	2.832	1024
4ga	3.0	2.929	1024
4gb	1.4	1.367	1024
4gc	2.0	1.953	1024
7d	2.0	1.953	1024
2fd	2.2	2.148	1024
2fb	2.3	2.246	1024
4ff	2.0	1.953	1024
2fg	3.1	3.027	1024
2fc	2.0	1.953	1024
2fh	2.3	2.246	1024
6fe	2.8	2.734	1024
6fg	4.8	4.687	1024
5ga	5.8	5.664	1024
5fb	3.5	3.417	1024
6fd	4.5	4.394	1024
5fa	2.8	2.734	1024
5fc	2.1	2.050	1024
16ga	1.3	1.269	1024
6fb	2.0	1.953	1024
6fa	2.4	2.343	1024
16ja	2.4	2.344	1024
5ja	4.2	4.102	1024

Table S8. Scheme for preparing working solutions of test objects for the microplate method.

Concentration of the test object in the stock solution, µg /mL	Volume of the stock solution, mL	Volume of nutrient broth, mL	Resulting concentration of the test object in the working solution, µg/mL	Final concentration of the test object in the wells of the plate with the addition of the test strain of the microorganism, µg/mL
1024	0,5	0,5	512	256
512	0,5	0,5	256	128
256	0,25	0,25	128	64
256	0,5	1,5	64	32
64	0,5	0,5	32	16
64	0,5	1,5	16	8

16	0,5	0,5	8	4
16	0,5	1,5	4	2
4	0,5	0,5	2	1

Table S9. Distribution of test objects solutions in the wells of the plate.

	1	2	3	4	5	6	7	8	9	10	11	12
				Test object №1								
A	K-	K+	-	256	128	64	32	16	8	4	2	1
B	K-	K+	-	256	128	64	32	16	8	4	2	1
C	K-	K+	-	256	128	64	32	16	8	4	2	1
D	K-	K+	-	256	128	64	32	16	8	4	2	1
				Test object №2								
E	K-	K+	-	256	128	64	32	16	8	4	2	1
F	K-	K+	-	256	128	64	32	16	8	4	2	1
G	K-	K+	-	256	128	64	32	16	8	4	2	1
H	K-	K+	-	256	128	64	32	16	8	4	2	1

Notes:

K- – Culture medium control

K+ – Growth control of the test microorganism

"-" – empty cells

256–1 – the final concentration of the test object in µg/mL.

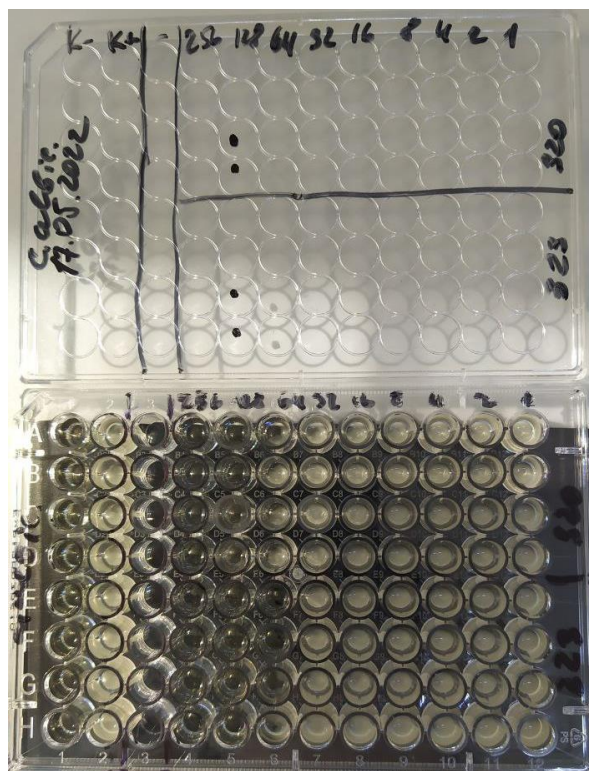


Fig. S270. Plate inoculated with *C. albicans* in the presence of test objects **3ka** (№320), **3kd** (№323).

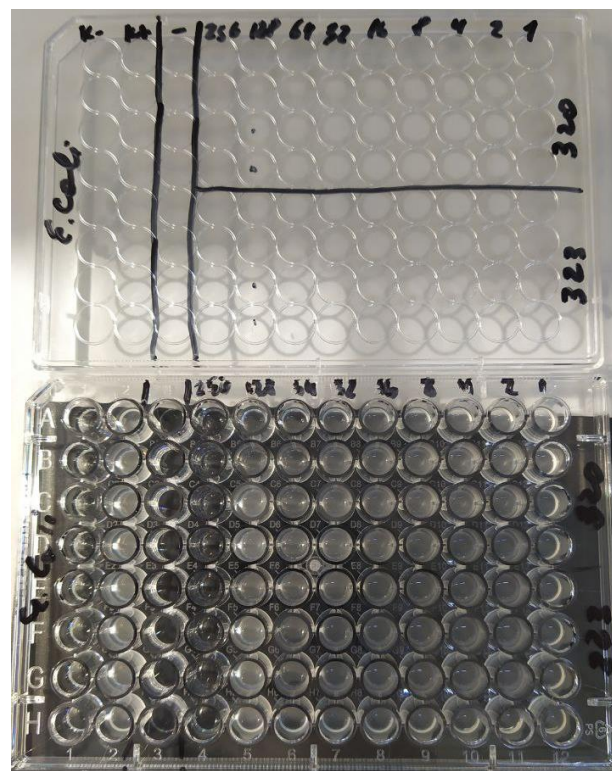


Fig. S271. Plate inoculated with *E. coli* in the presence of test objects **3ka** (№320), **3kd** (№323).

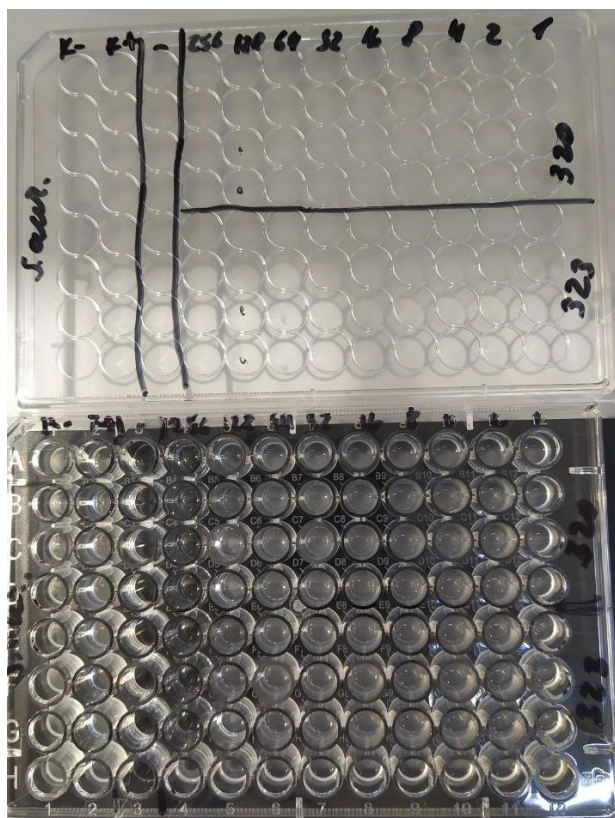


Fig. S272. Plate inoculated with *S. aureus* in the presence of test objects **3ka** (№320), **3kd** (№323).

Table S10. Evaluation of the antimicrobial activity of the test objects.

Compound	MIC, µg/mL		
	<i>S. aureus</i>	<i>E. coli</i>	<i>C. albicans</i>
2ae	256	128	128
2bd	256	128	128
2aa	256	128	128
2dd	128	128	128
9i	>256	>256	128
2ic	256	128	>256
2dc	256	128	128
2eb	256	128	128
2ce	256	128	128
2cb	256	128	128
2af	256	128	128
13aa	256	>256	128
11i	>256	>256	128
2ea	256	128	128
2bg	256	128	128
2ab	256	128	128
2ag	256	128	>256
2ad	256	128	128
2cf	256	128	64
2cd	256	128	128
8i	>256	>256	128
2ib	256	128	128
2ah	256	128	128

13ab	>256	>256	>256
2id	256	256	>256
2ha	256	128	>256
2aj	256	128	128
2ai	256	128	128
2da	256	128	128
2ac	256	128	128
2ia	256	128	256
2ga	256	128	128
7d	256	128	128
2gb	256	128	128
2fc	256	128	128
5ga	256	128	128
6fb	256	128	128
5fb	256	128	128
6fa	256	128	128
16ga	256	128	128
6fg	256	128	128
2gc	256	128	128
2fd	256	128	128
2fg	256	128	128
4ff	256	128	128
6fe	256	128	128
2fb	256	128	128
4ga	256	128	128
6fd	256	128	128
5fa	256	128	128
2ja	256	128	128
2fh	256	128	128
5fc	256	128	128
4gc	256	128	128
4gb	256	128	128
trans-17s	256	128	128
17d	256	128	128
2bc	256	128	128
17r	>256	>256	128
2bb	256	128	128
17e	256	128	128
17g	256	128	128
18r	>256	>256	128
16ja	>256	>256	>256
5ja	>256	>256	>256
17l	256	128	128
17m	256	128	128
trans-17n	256	128	128
17o	256	128	256
cis-17t	256	128	128
trans-17t	256	128	128
17f	256	128	128
17q	256	128	128
cis-17n	256	128	128
2ba	256	128	128
17b	256	128	128
2bf	256	128	128

<i>cis-17s</i>	256	128	128
17p	256	128	128
3kb	128	128	128
3jc	256	256	128
Z-14i	256	256	128
E-14i	256	256	128
3kc	256	256	128
3jb	256	256	128
3ja	256	128	128
3jd	256	256	128
2db	256	256	128
3ga	256	256	128
3ka	256	256	128
3kd	256	256	128
2jd	256	128	128
3gb	256	128	128
2jb	256	128	128
2je	256	256	128