

Supporting Information

Synthesis of novel pyrazoline based bis 1,2,3-triazole scaffolds via click chemistry

DONGAMANTI ASHOK^{1,*}, KOTHURI KIRAN^{1,2} BODDU ANANDA RAO¹ and ALAPATI
SRINIVAS RAO²

Corresponding author: Dongamanti Ashok, Green and Medidcinal Chemistry Laboratory,
Department of Chemistry, Osmania University, Hyderabad, 500 007, Telanagana, India.

E-mail: ashokdou@gmail.com

¹*Green and Medidcinal Chemistry Laboratory, Department of Chemistry, Osmania University,
Hyderabad, 500007, Telangana, India.*

²*Medidcinal Chemistry Laboratory, GVK Biosciences Private Limited, Plot No.28A, IDA,
Nacharam, Hyderabad, 500076, Telangana, India.*

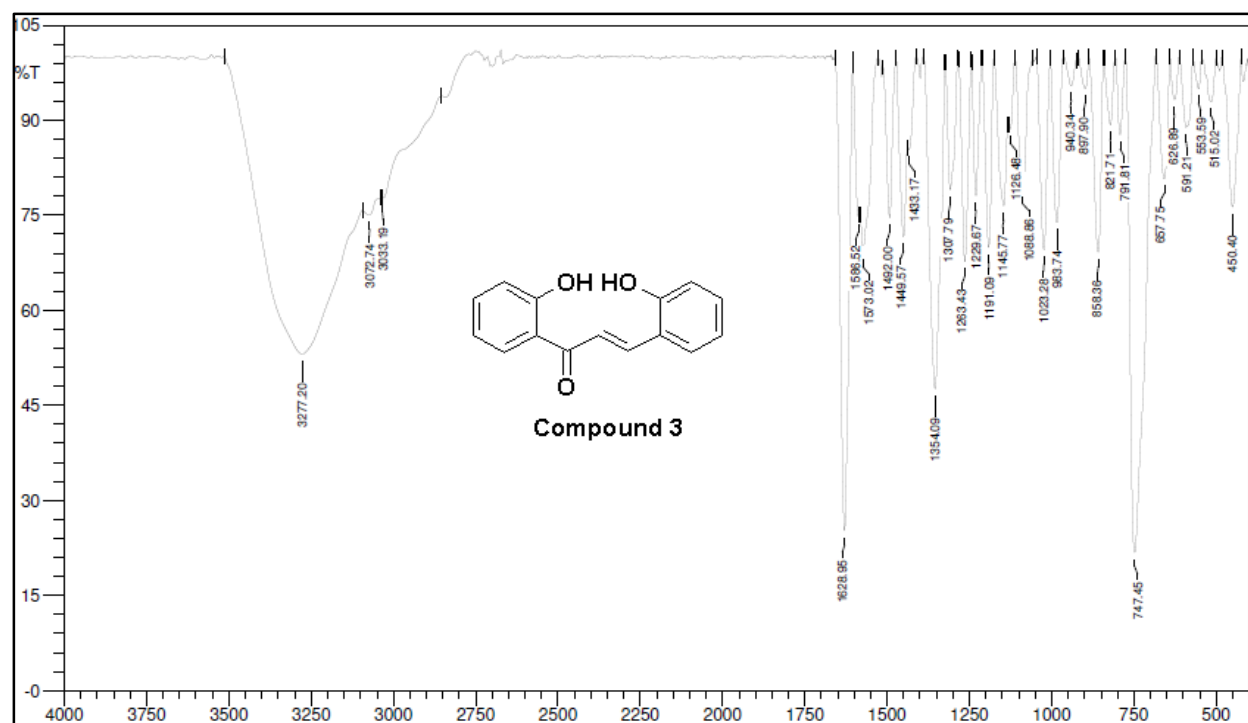


Figure S1: IR spectra of compound 3

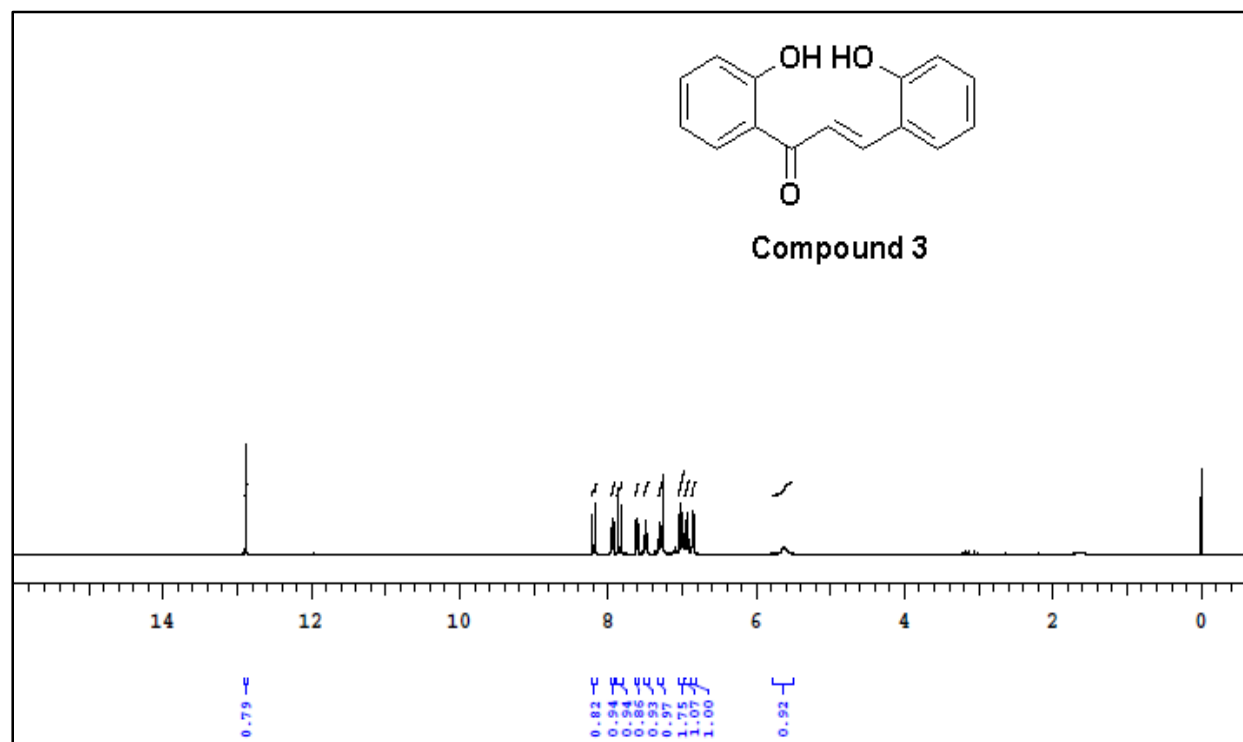


Figure S2: ¹H-NMR (400 MHz, CDCl₃) spectra of compound 3

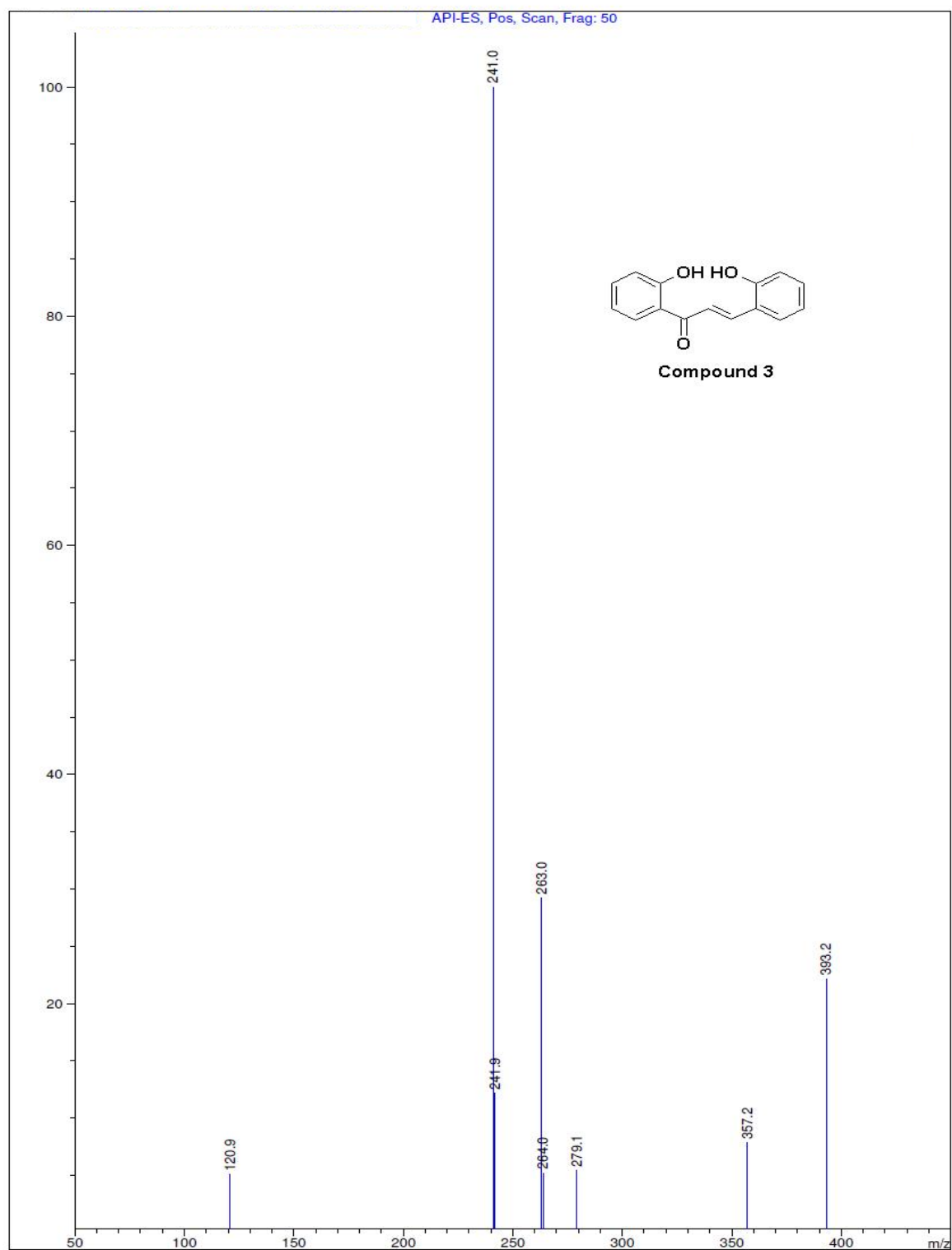


Figure S5: Mass spectra of compound 3

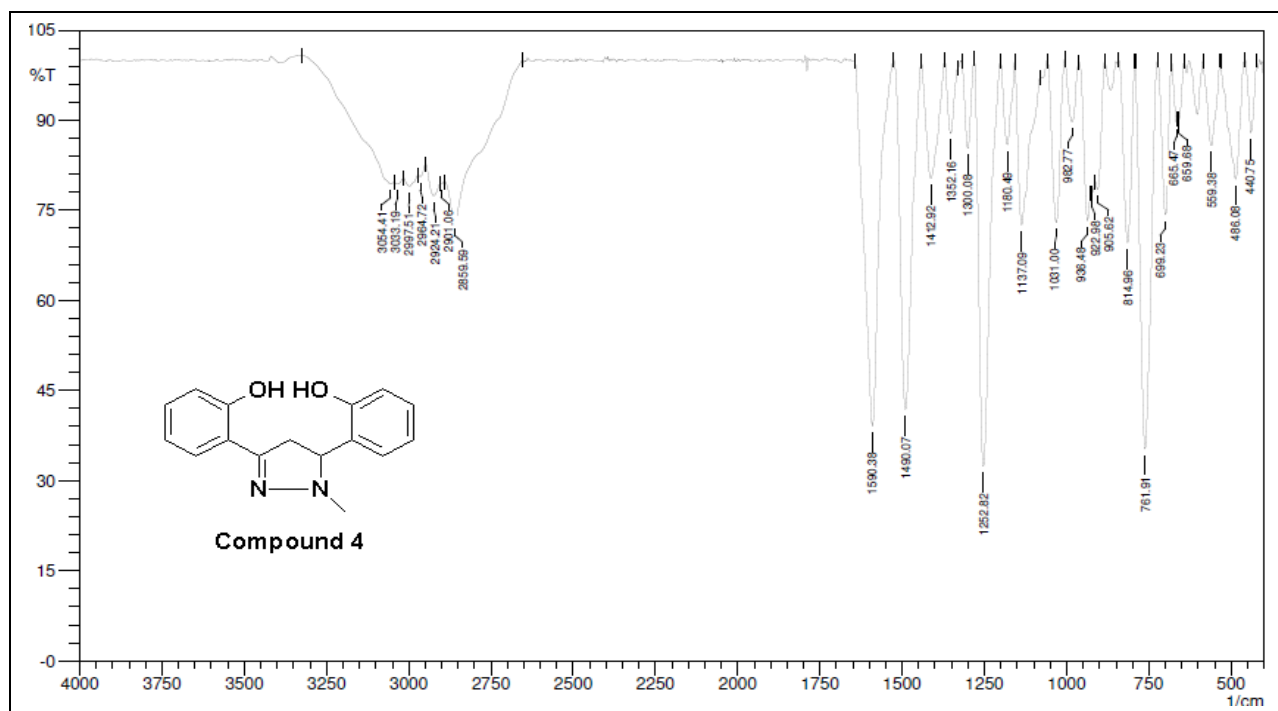


Figure S6: IR spectra of compound 4

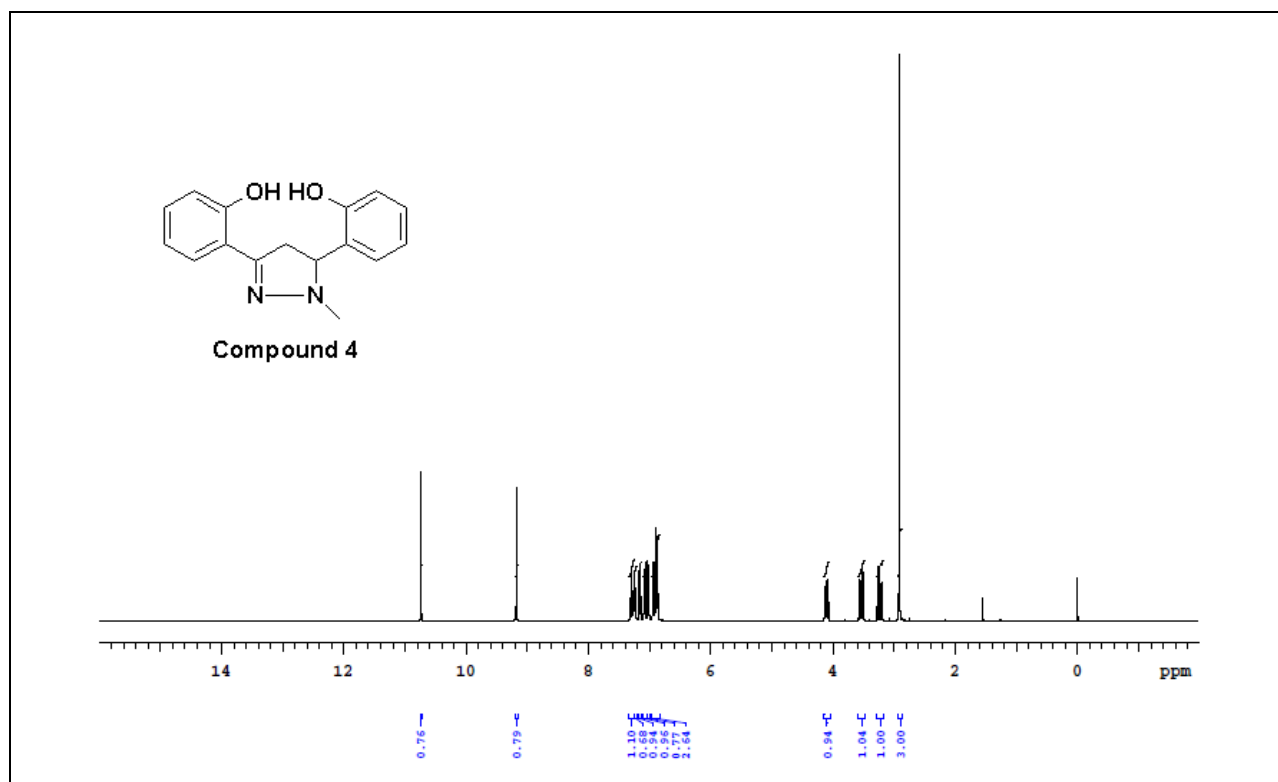


Figure S7: ¹H-NMR (400 MHz, CDCl₃) spectra of compound 4

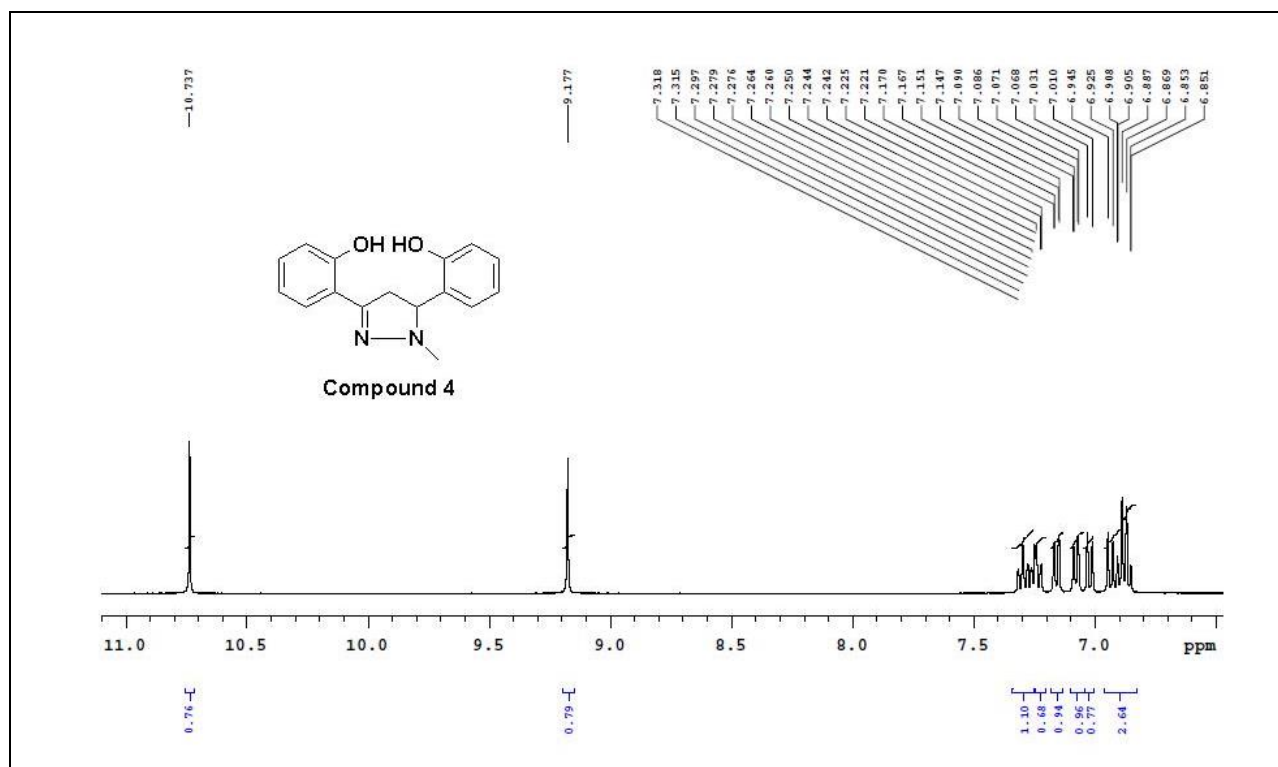


Figure S8: ¹H-NMR (400 MHz, CDCl₃) spectra of compound 4

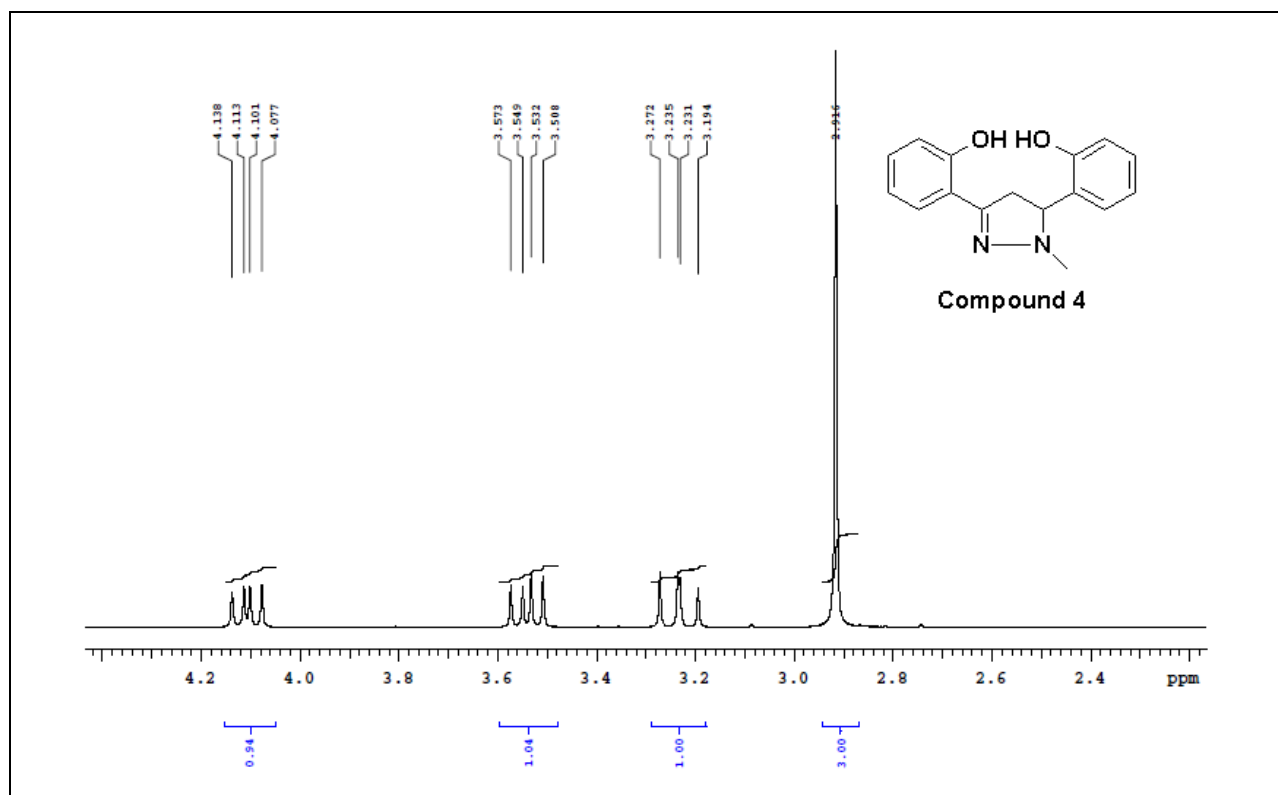


Figure S9: ¹H-NMR (400 MHz, CDCl₃) spectra of compound 4

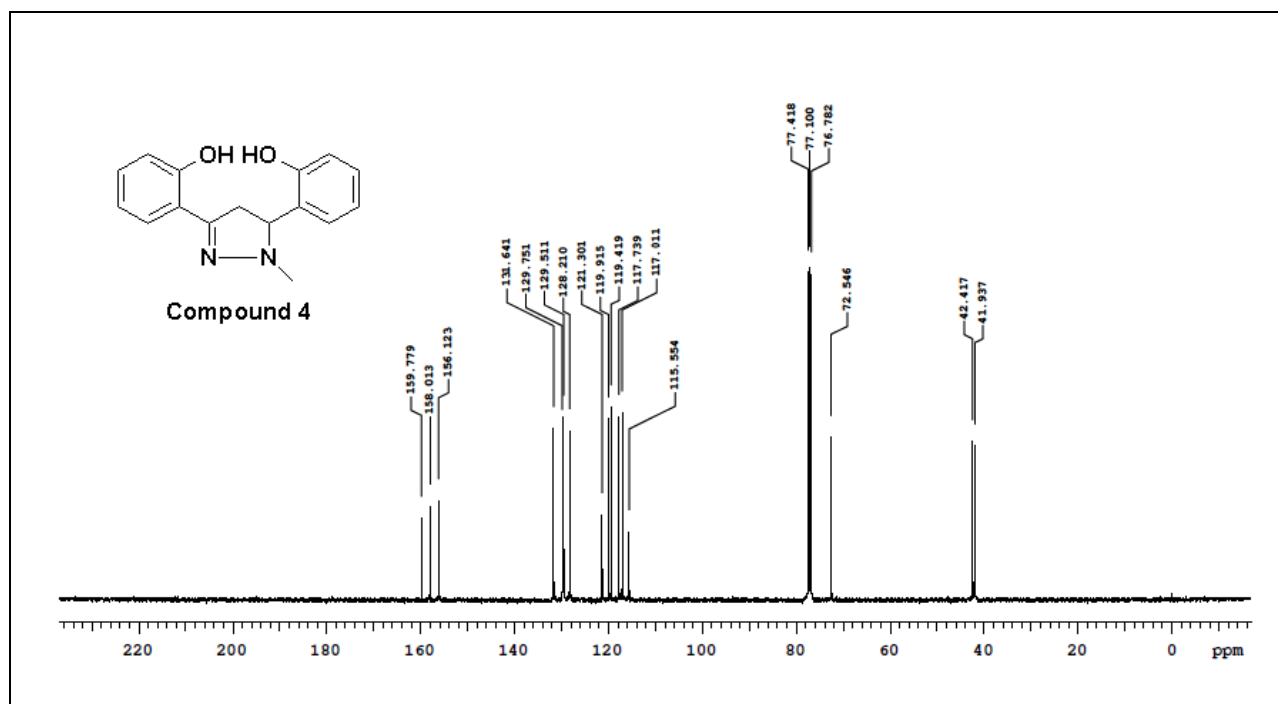


Figure S10: ¹³C NMR (100 MHz, CDCl₃) spectra of compound **4**

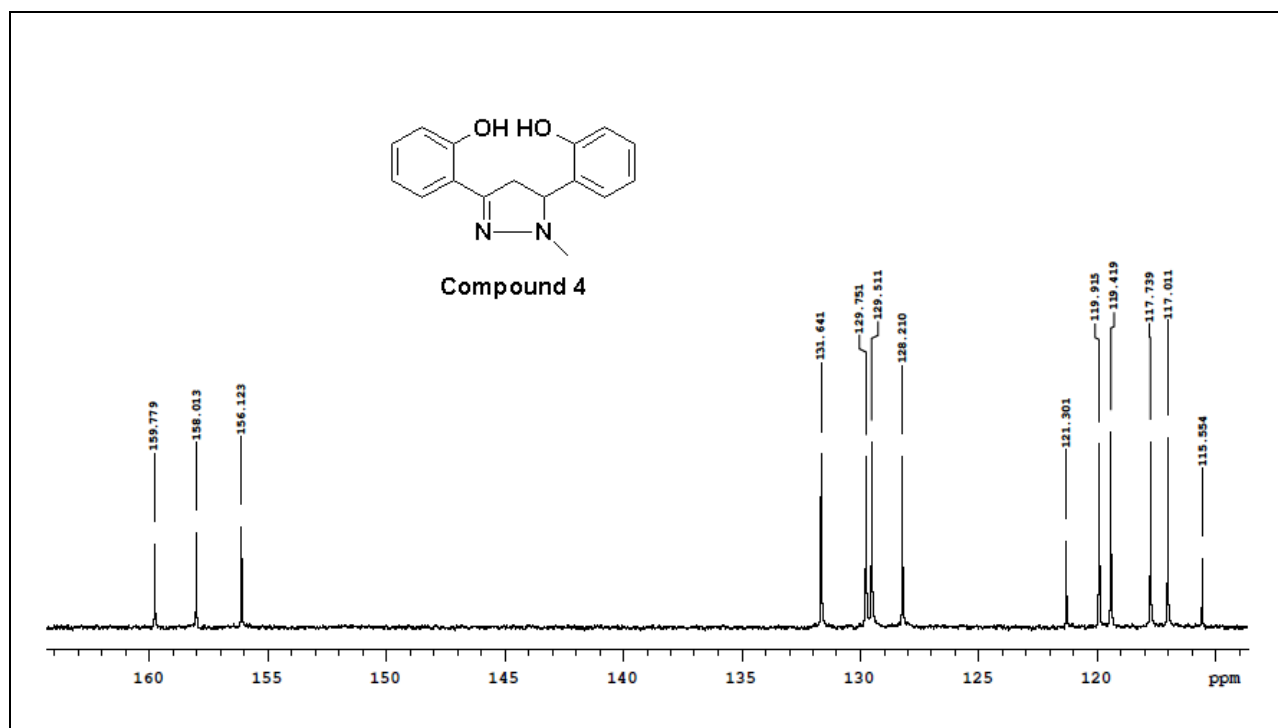


Figure S11: ¹³C NMR (100 MHz, CDCl₃) spectra of compound **4**

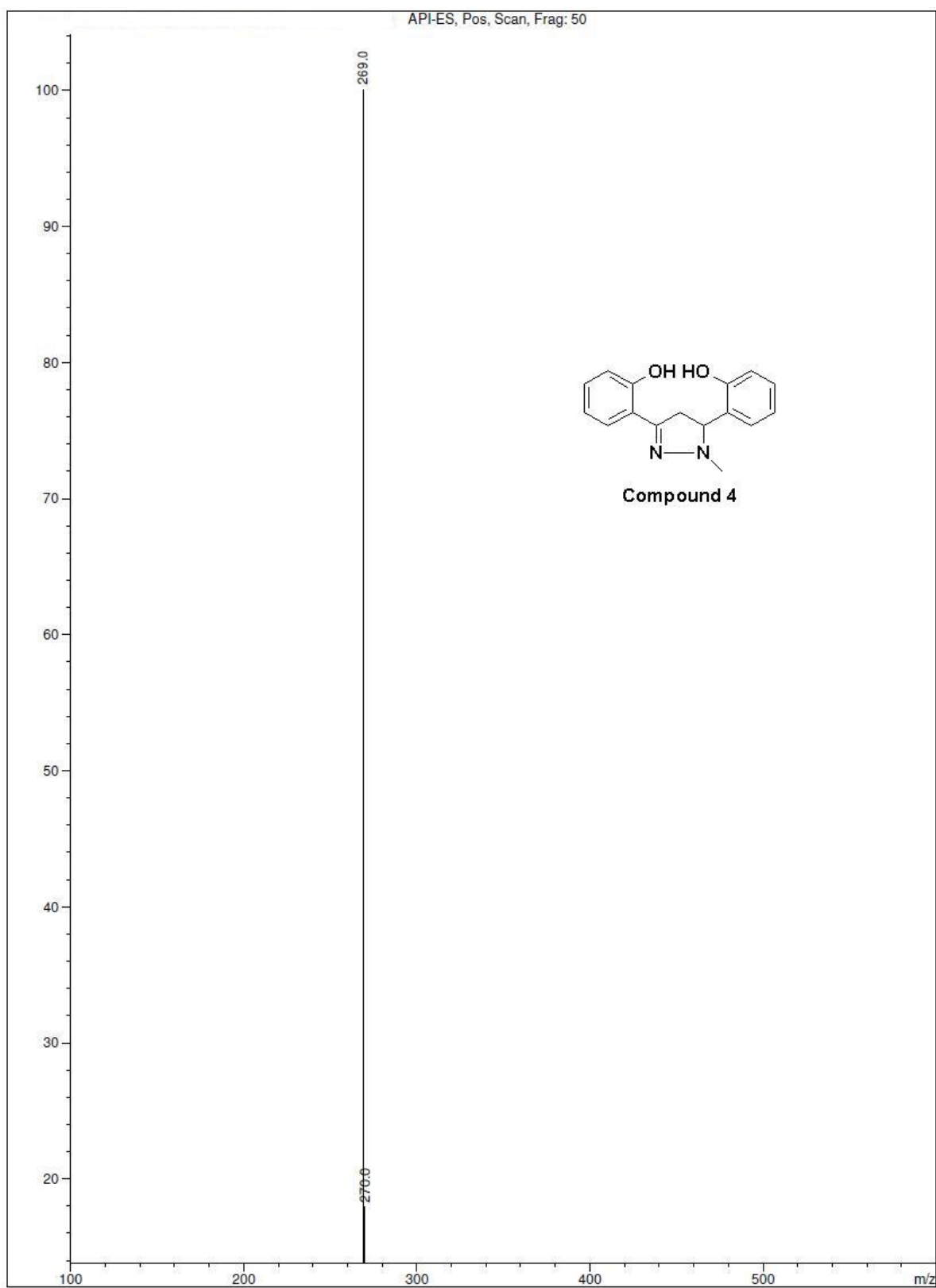


Figure S12: Mass spectra of compound 4

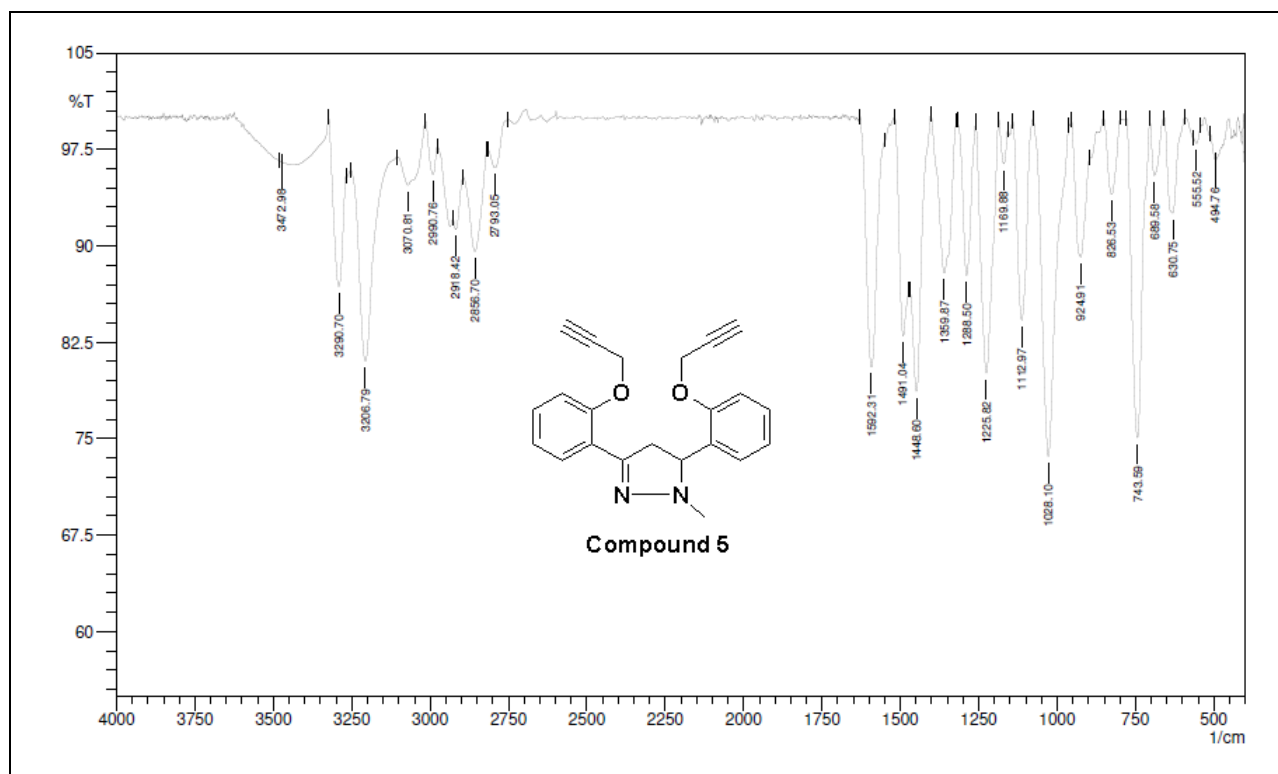


Figure S13: IR spectra of compound 5

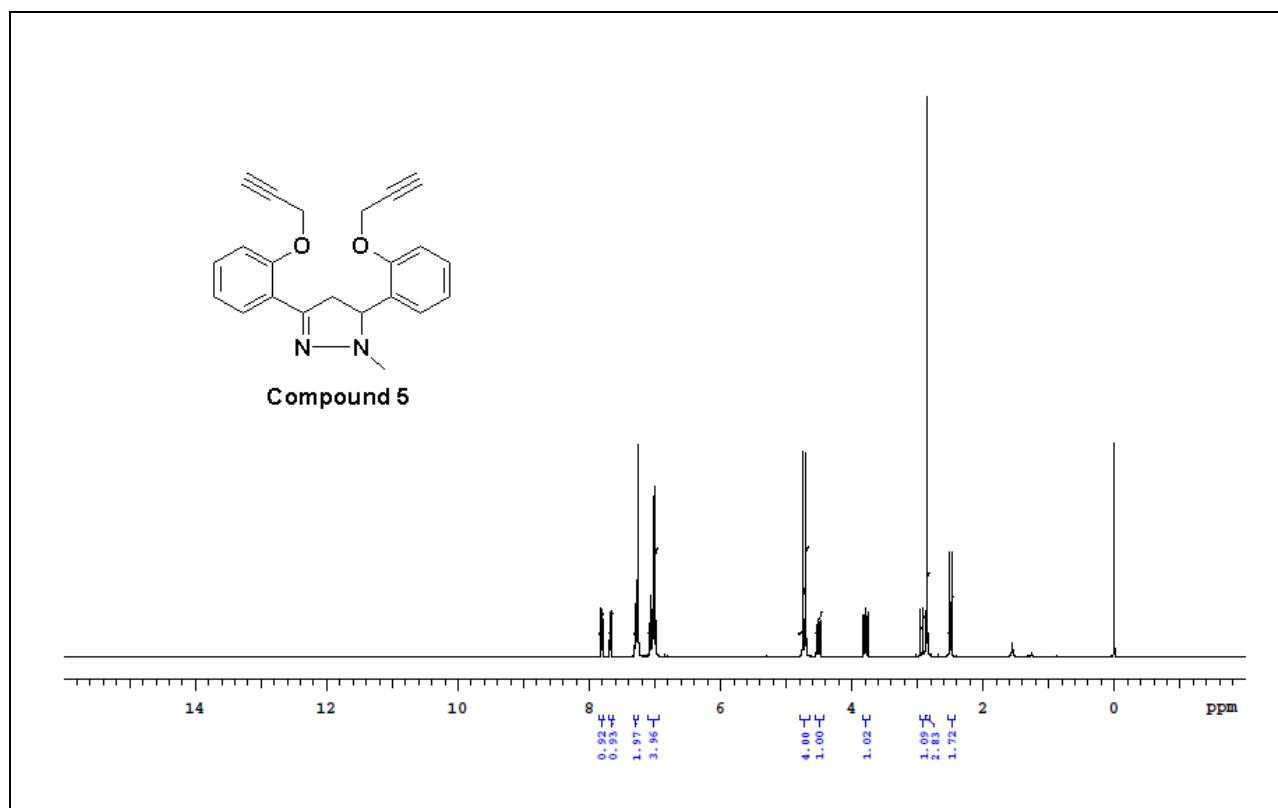


Figure S14: $^1\text{H-NMR}$ (400 MHz, CDCl_3) spectra of compound 5

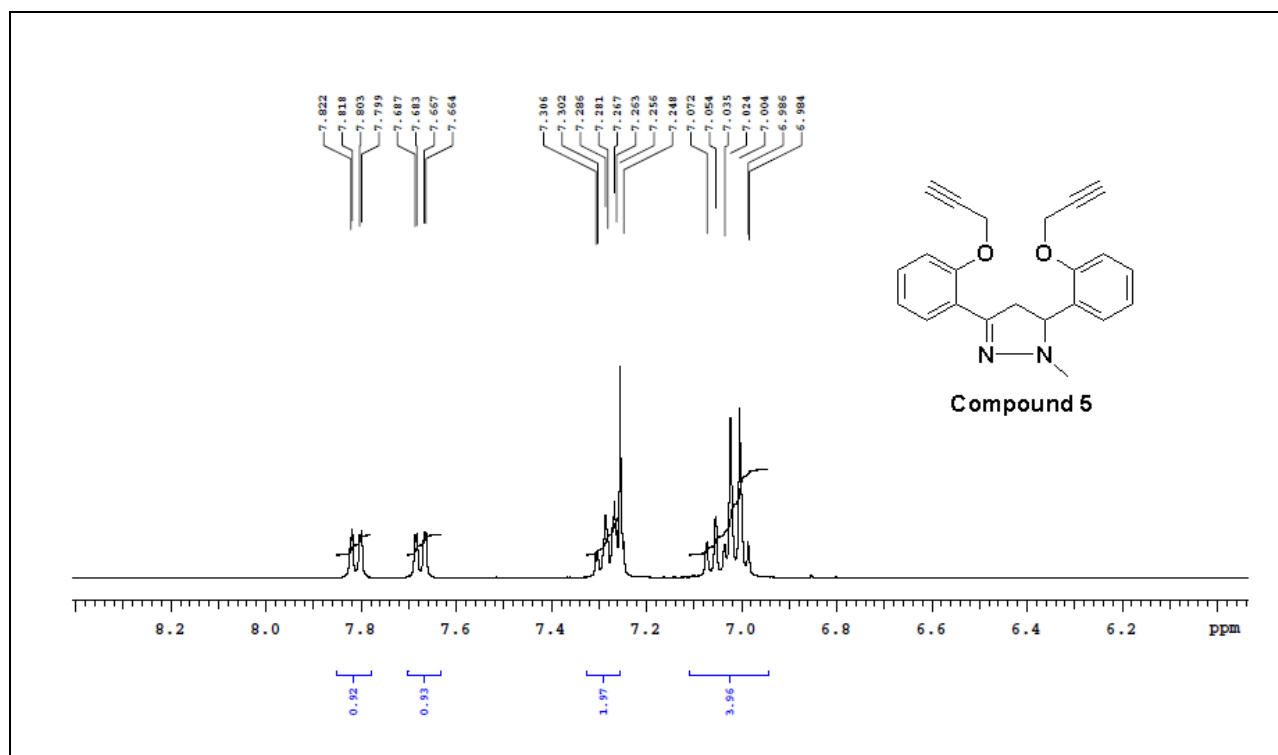


Figure S15: ^1H -NMR (400 MHz, CDCl_3) spectra of compound 5

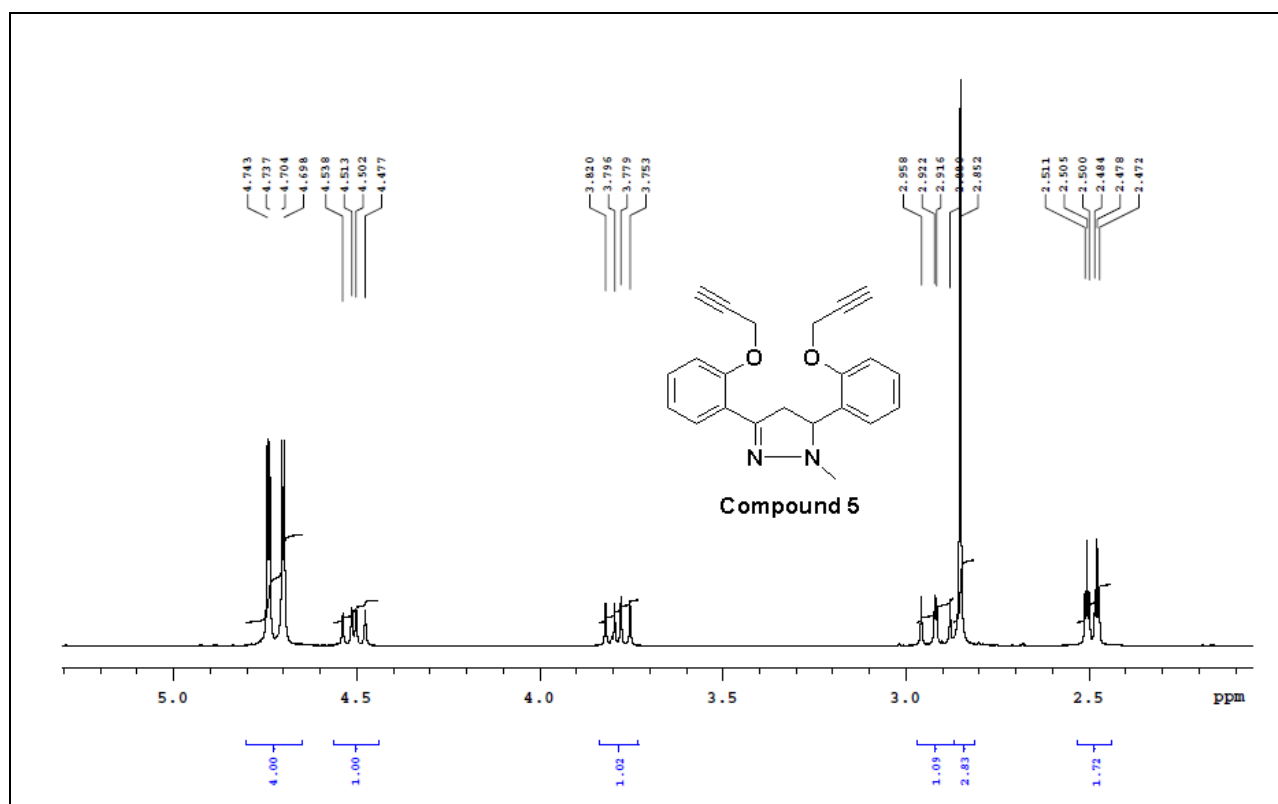


Figure S16: ^1H -NMR (400 MHz, CDCl_3) spectra of compound 5

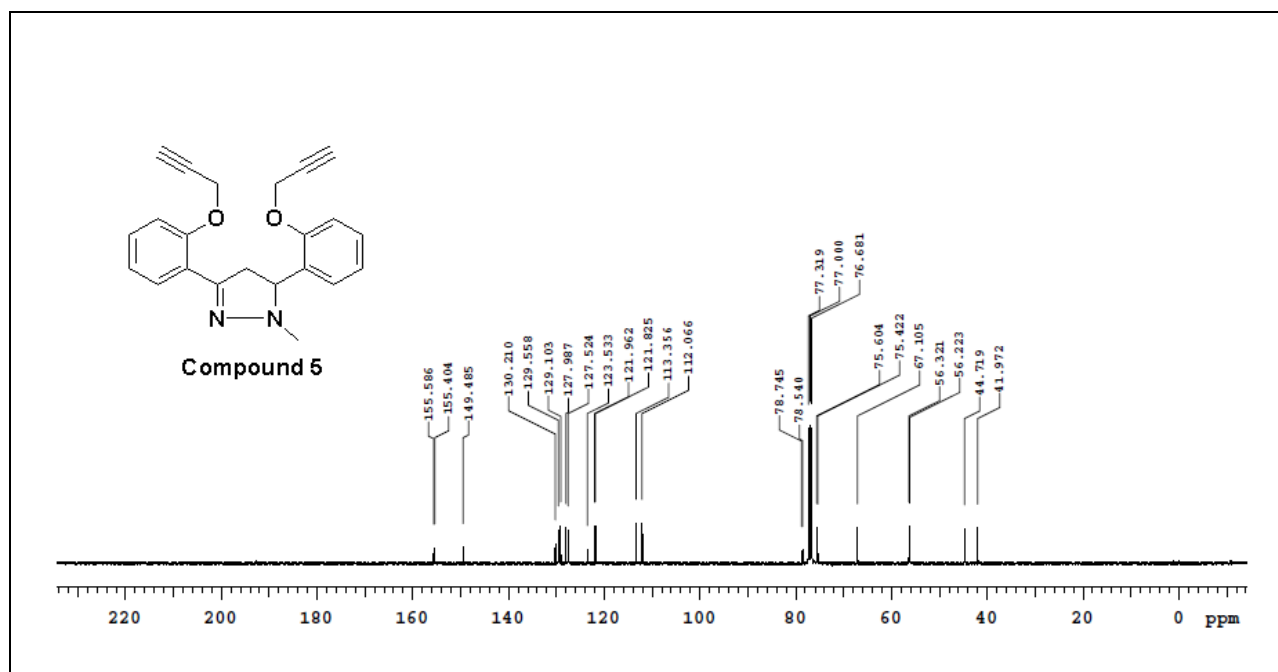


Figure S17: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 5

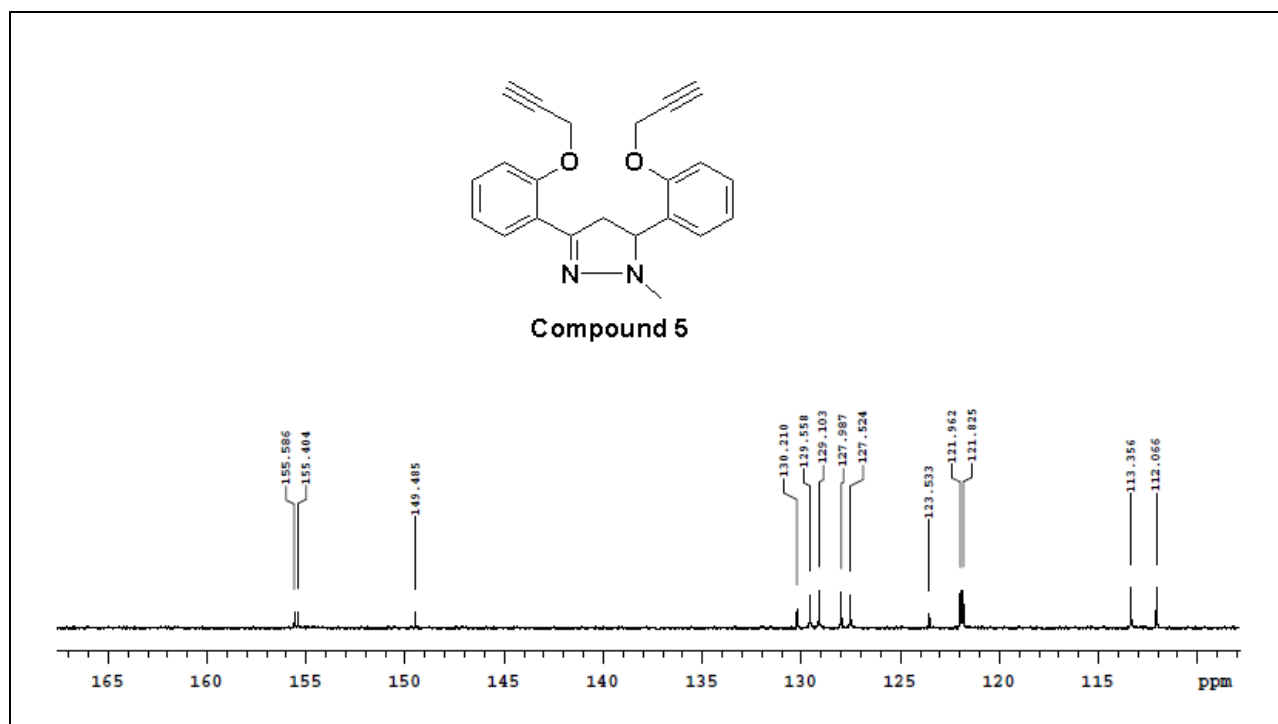


Figure S18: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 5

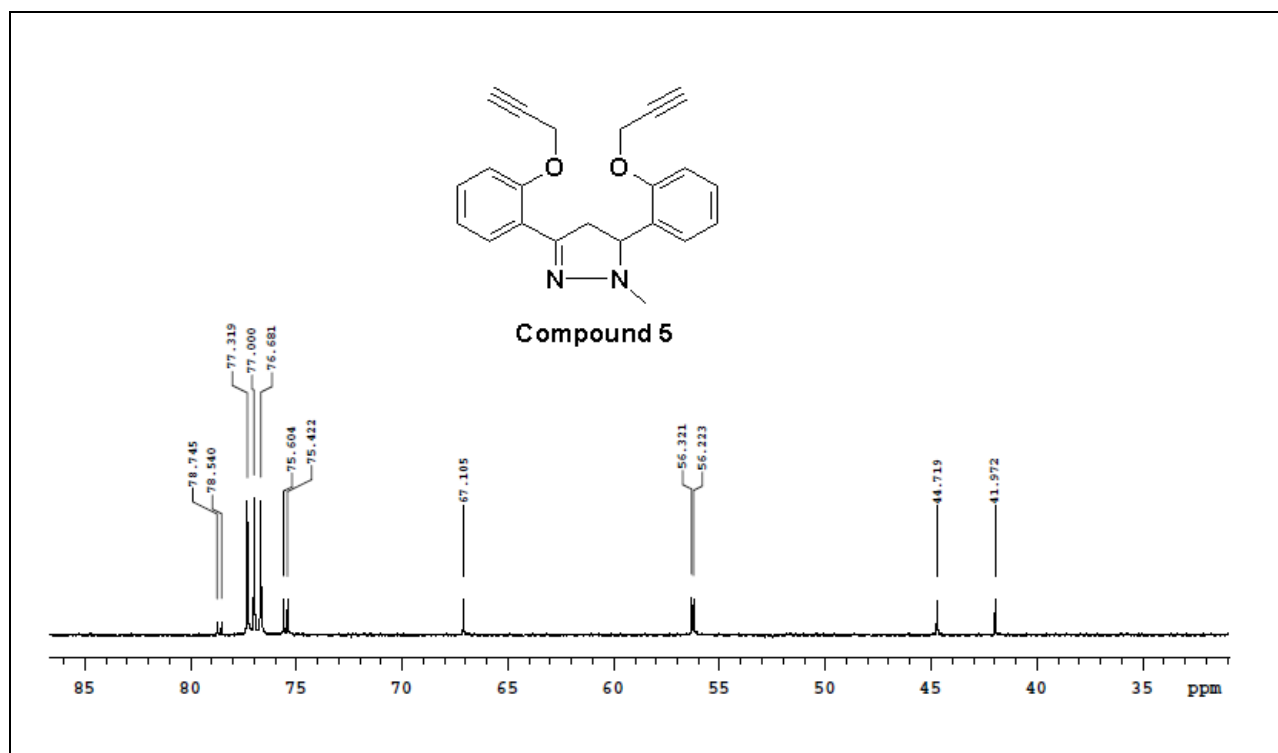


Figure S19: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 5

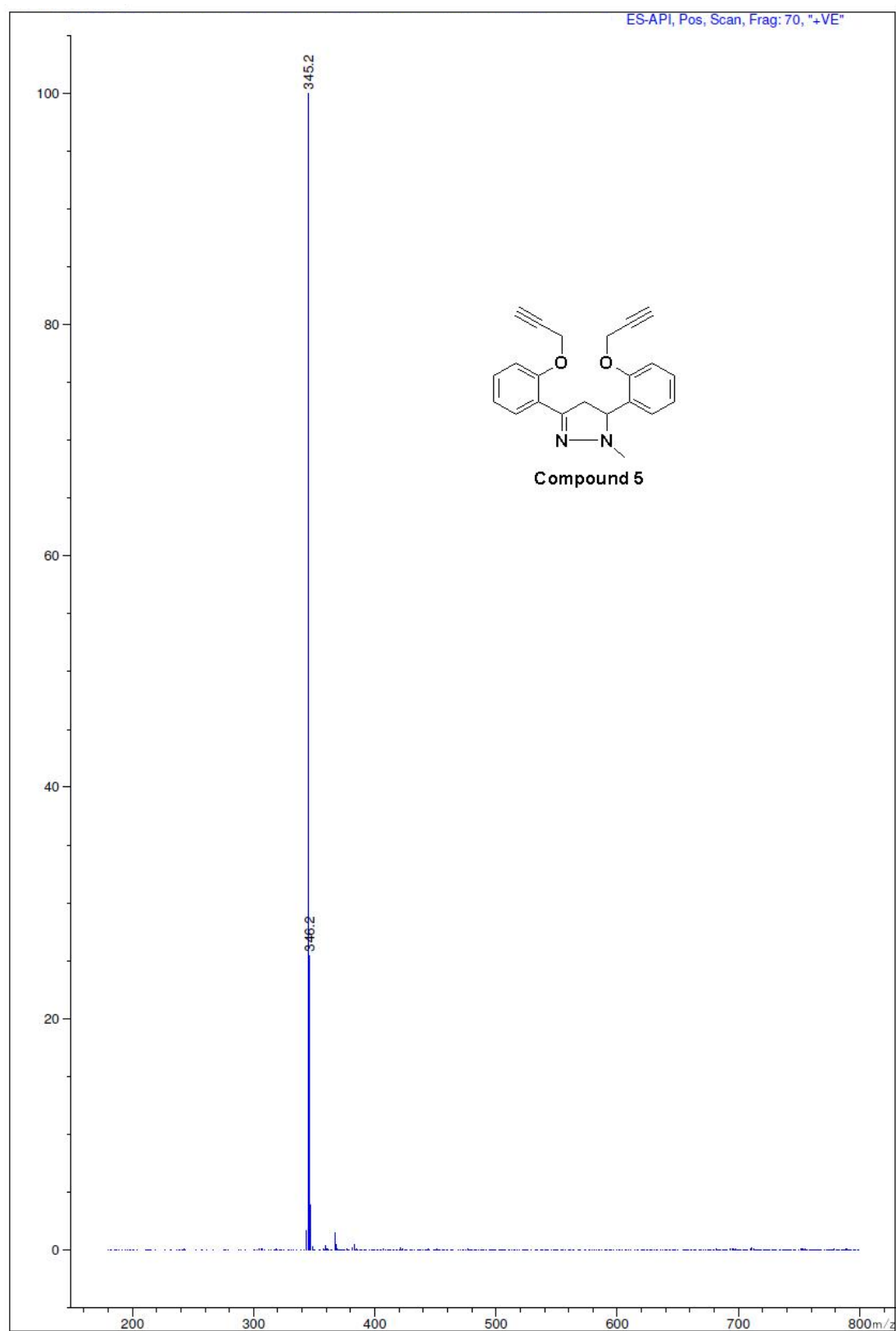


Figure S20: Mass spectra of compound 5

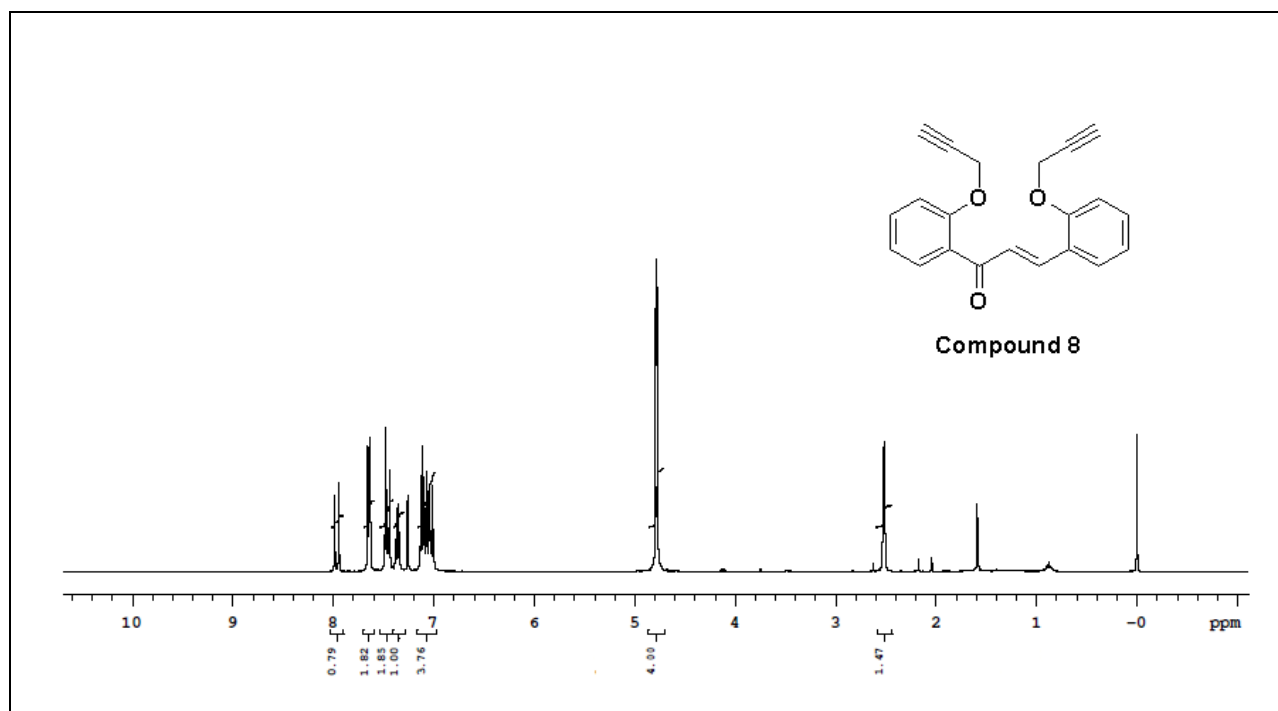


Figure S21: ¹H-NMR (400 MHz, CDCl₃) spectra of compound **8**

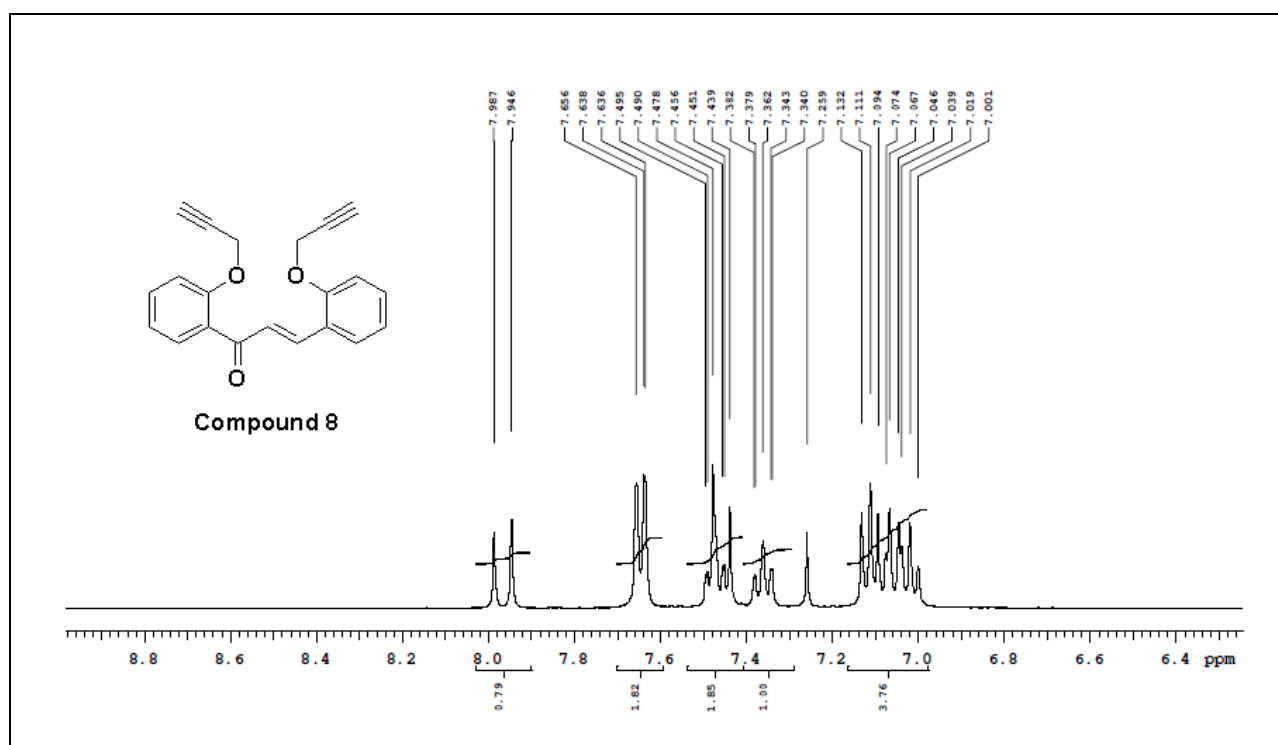


Figure S22: ¹H-NMR (400 MHz, CDCl₃) spectra of compound **8**

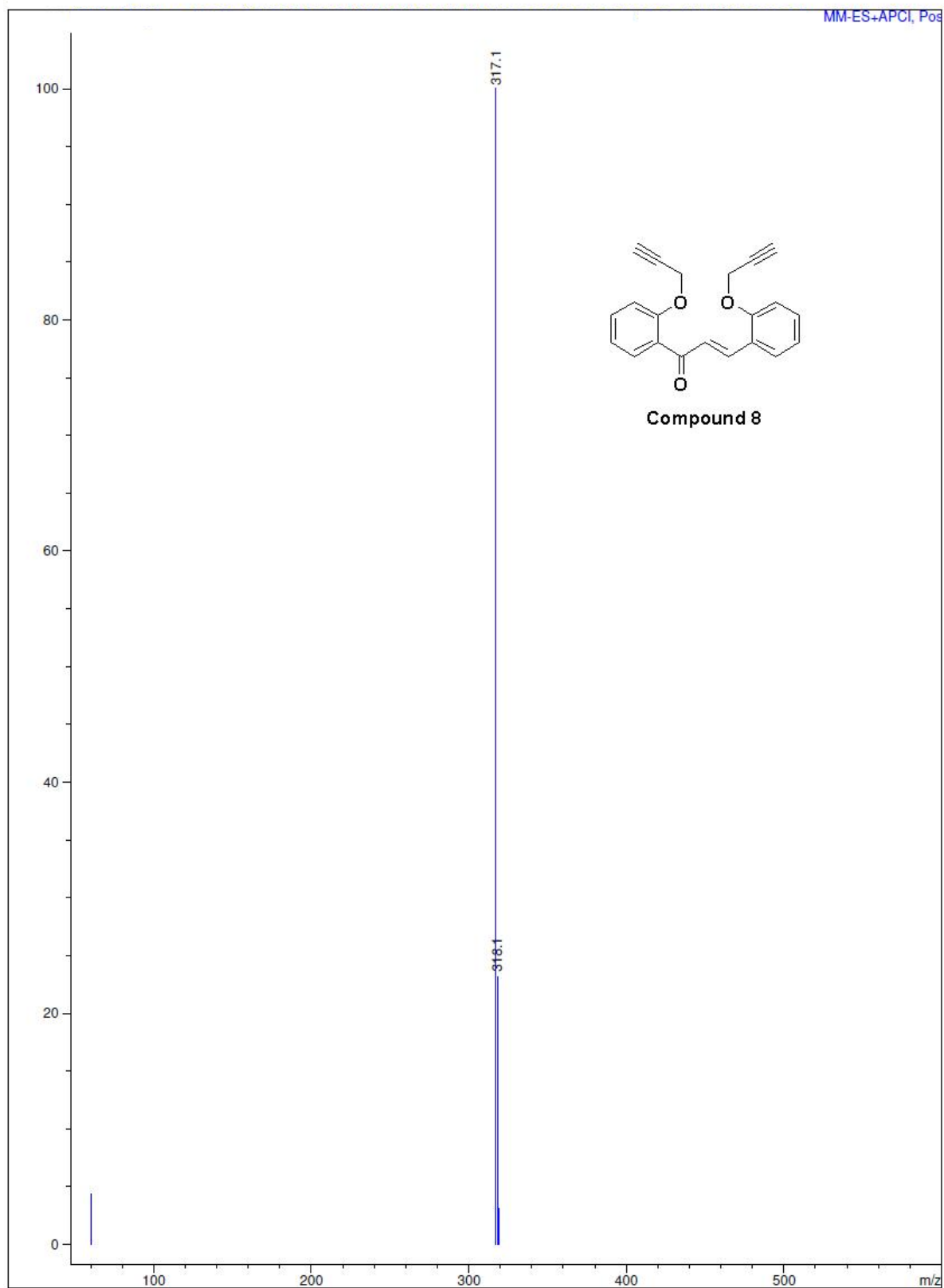


Figure S23: Mass spectra of compound **8**

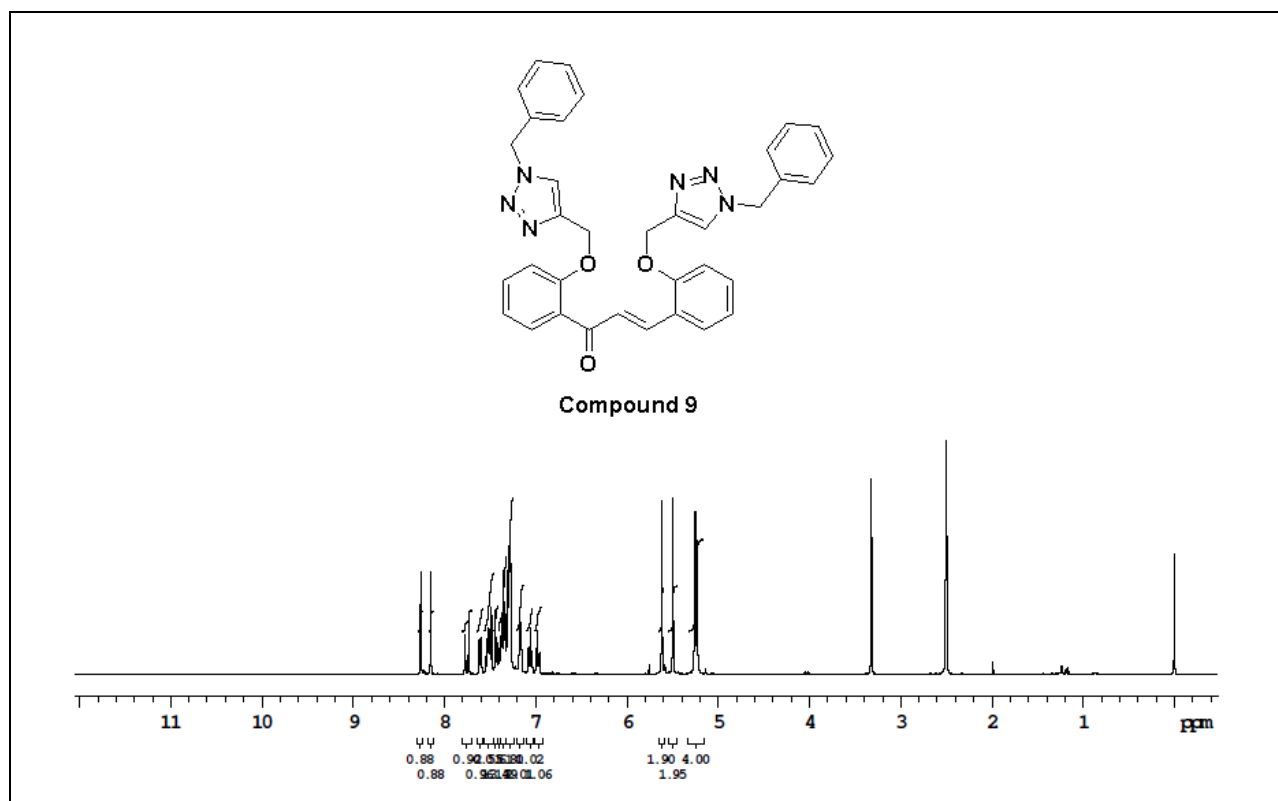


Figure S24: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 9

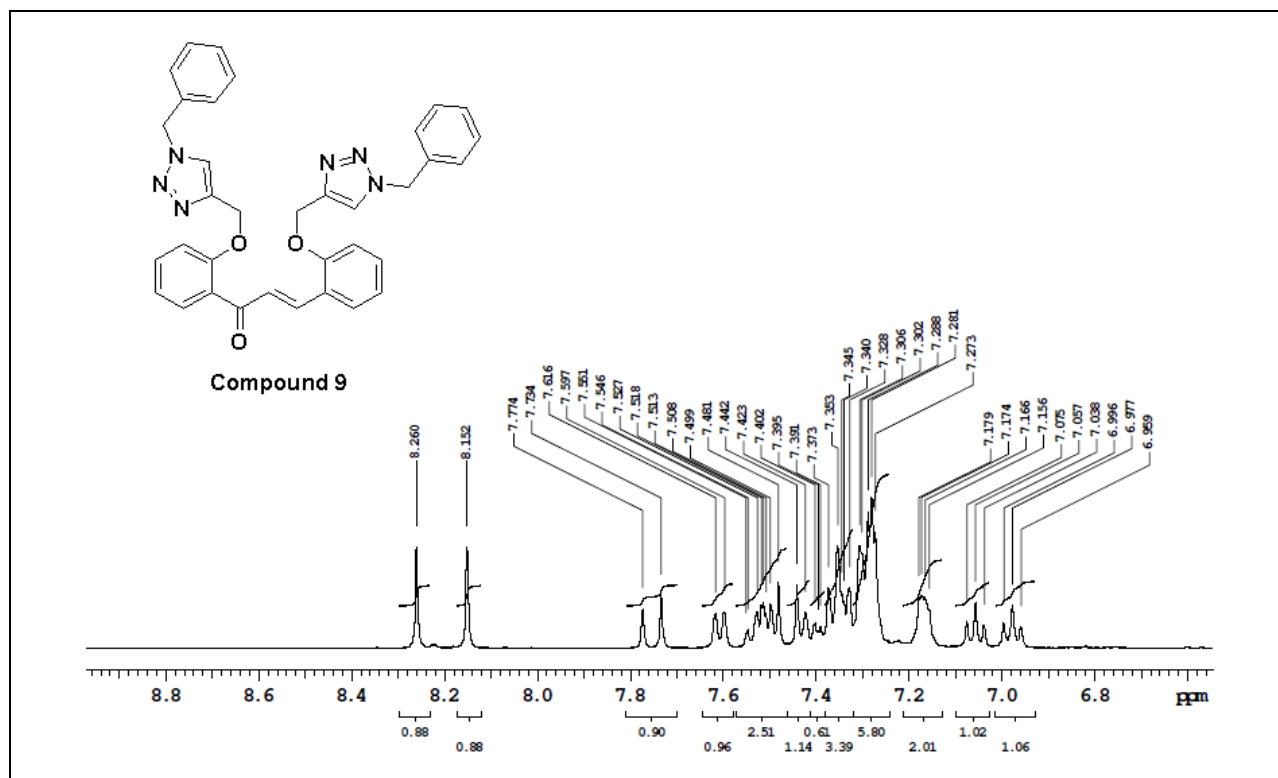


Figure S25: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 9

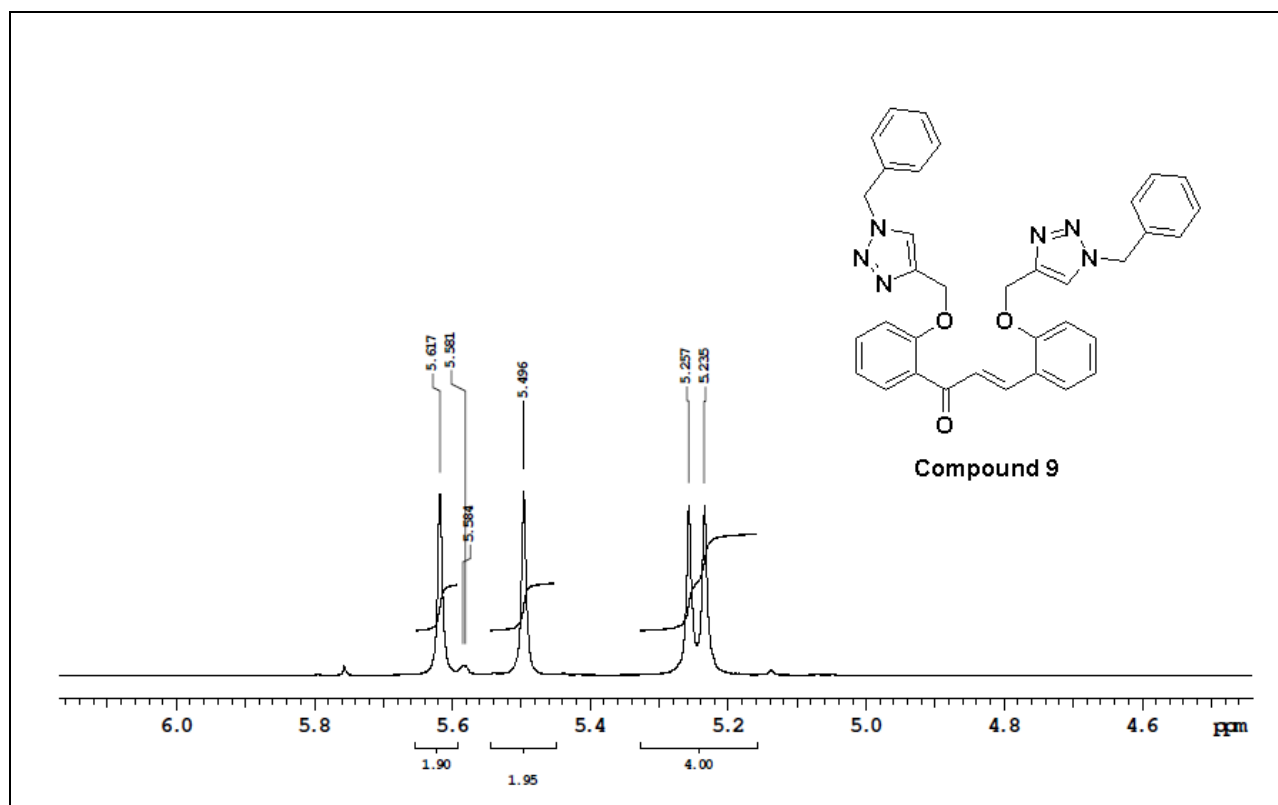


Figure S26: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound **9**

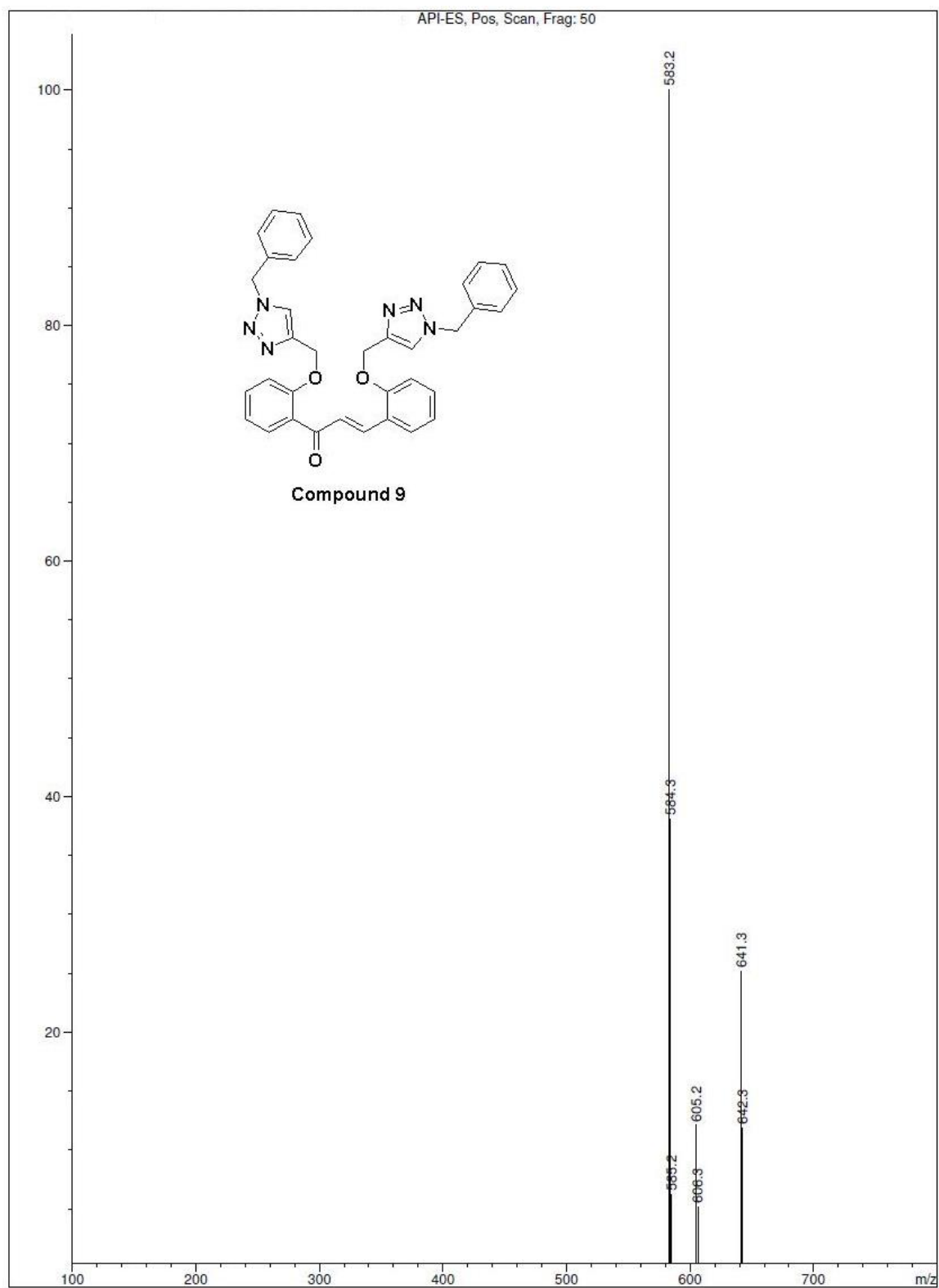


Figure S27: Mass spectra of compound 9

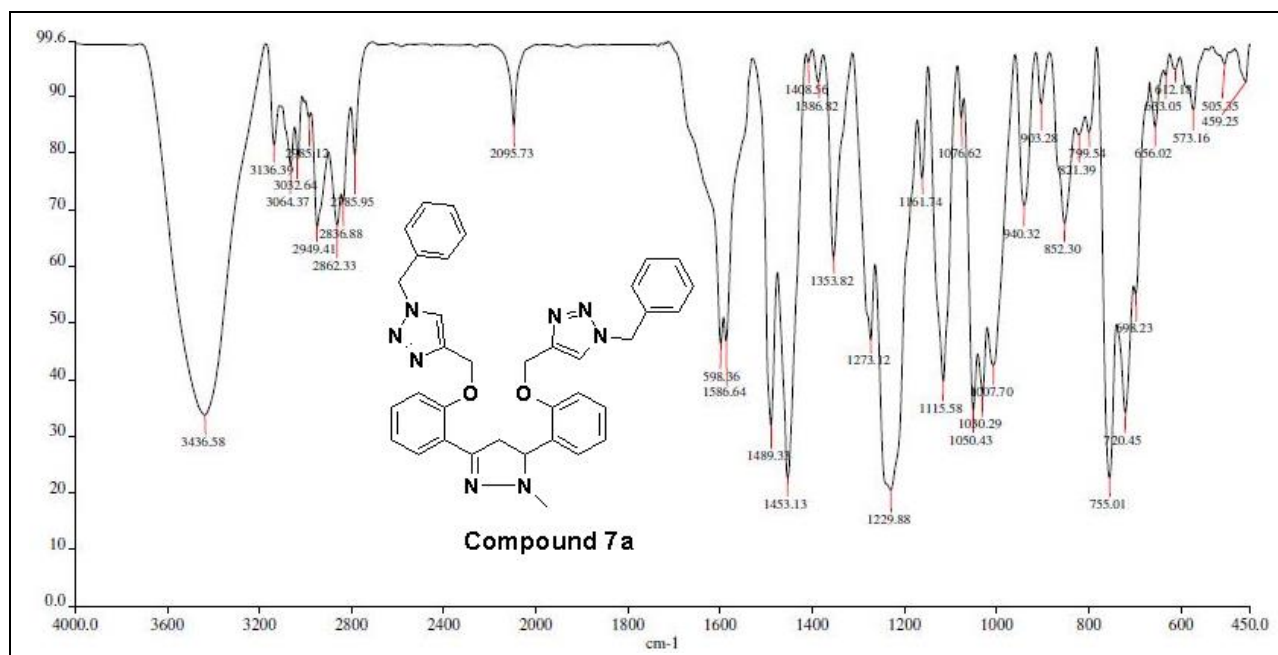


Figure S28: IR spectra of compound **7a**

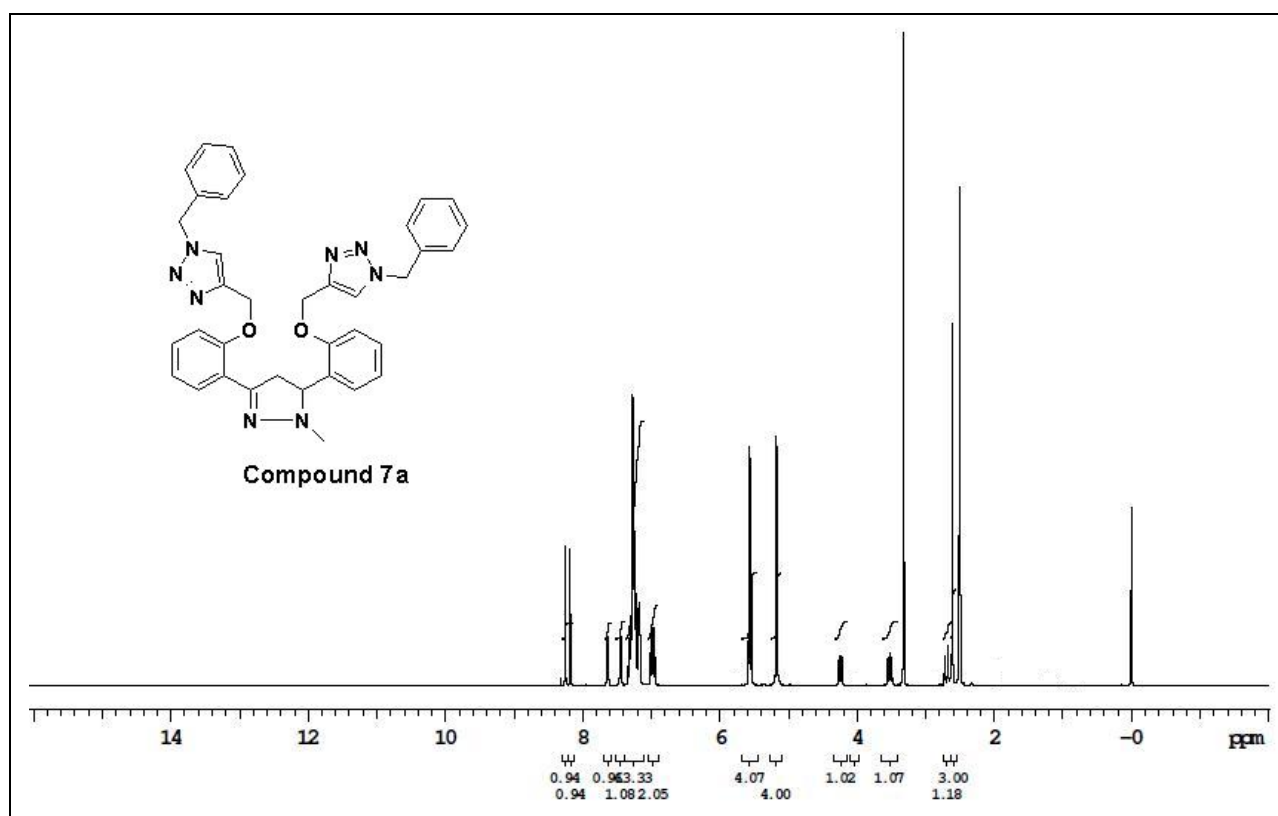


Figure S29: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7a**

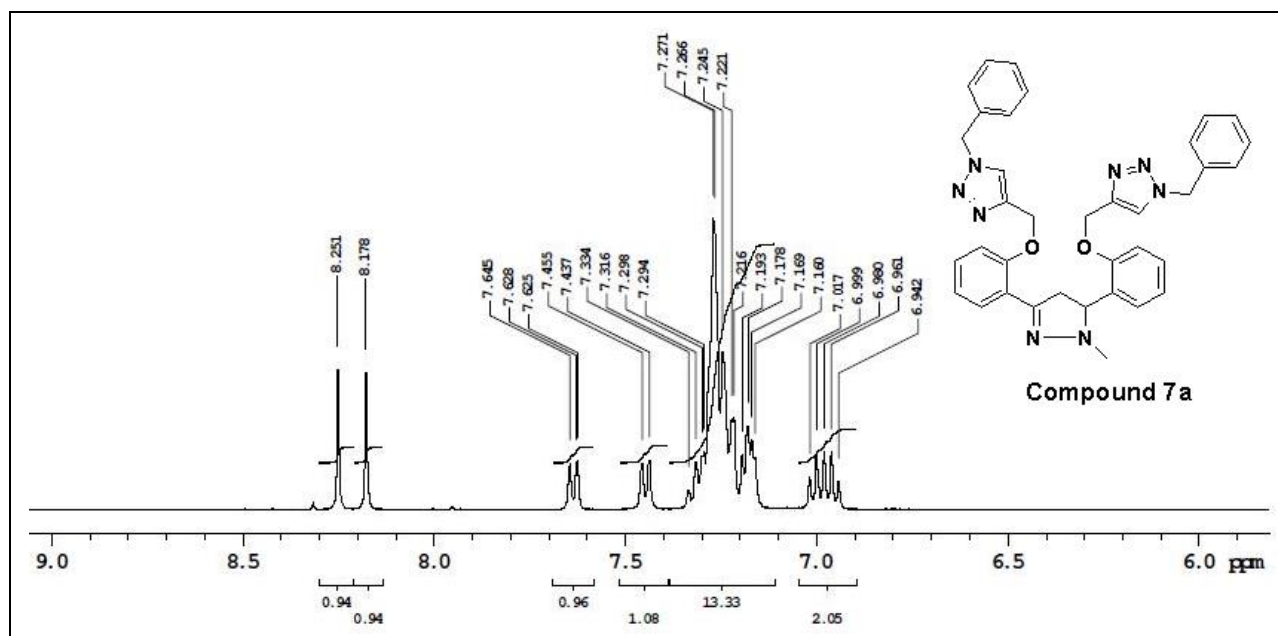


Figure S30: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7a

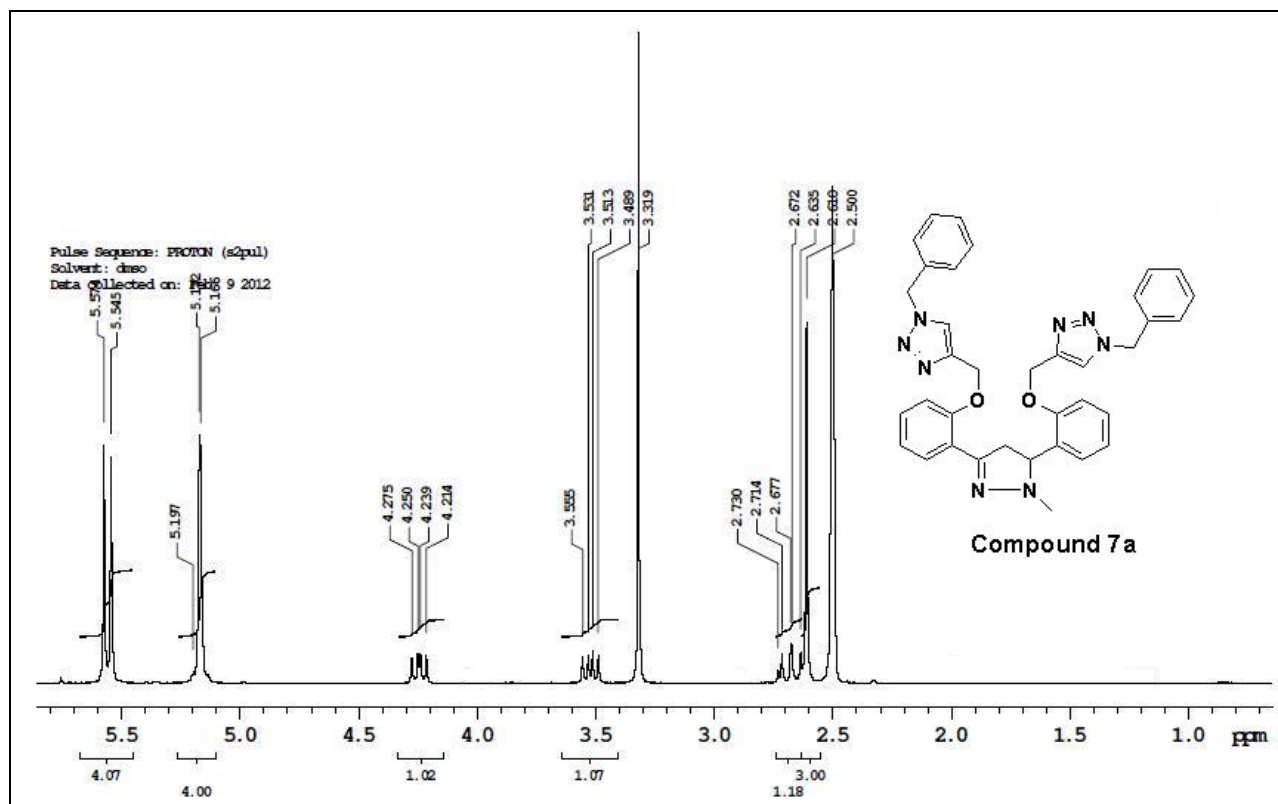


Figure S31: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7a

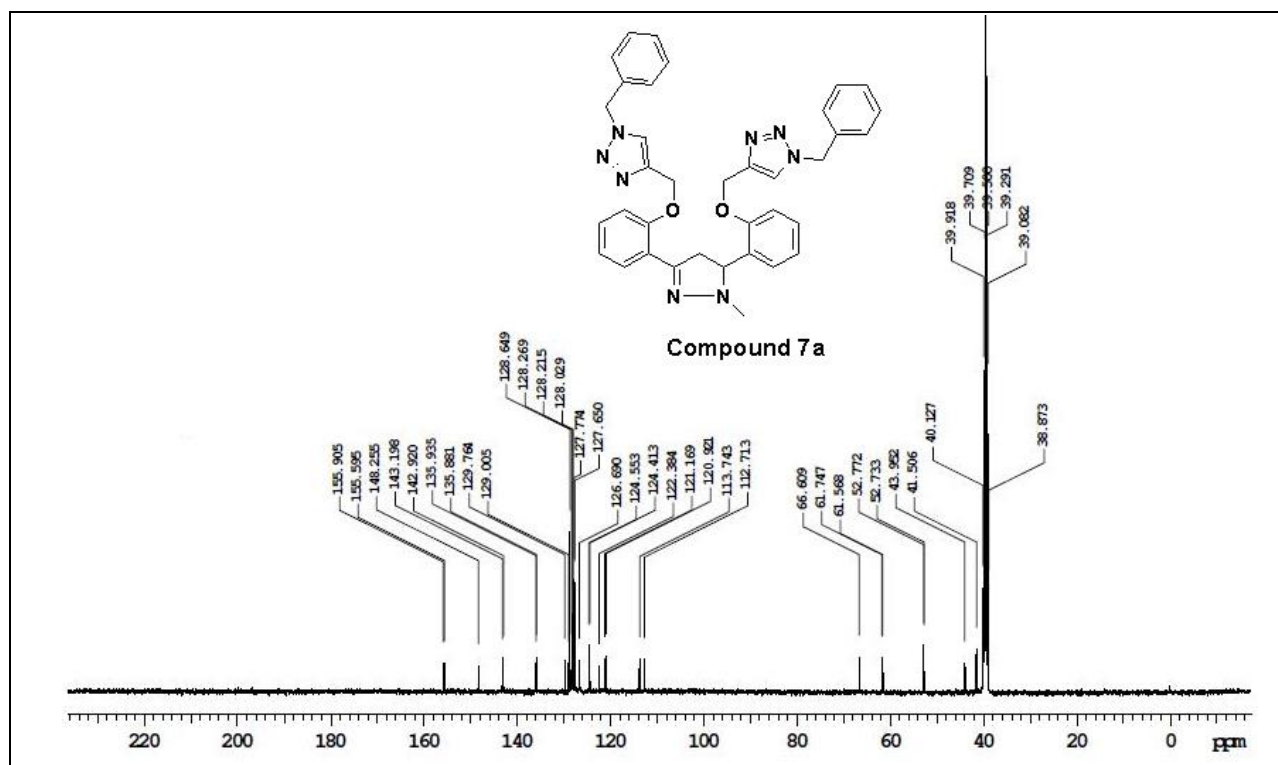


Figure S32: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7a**

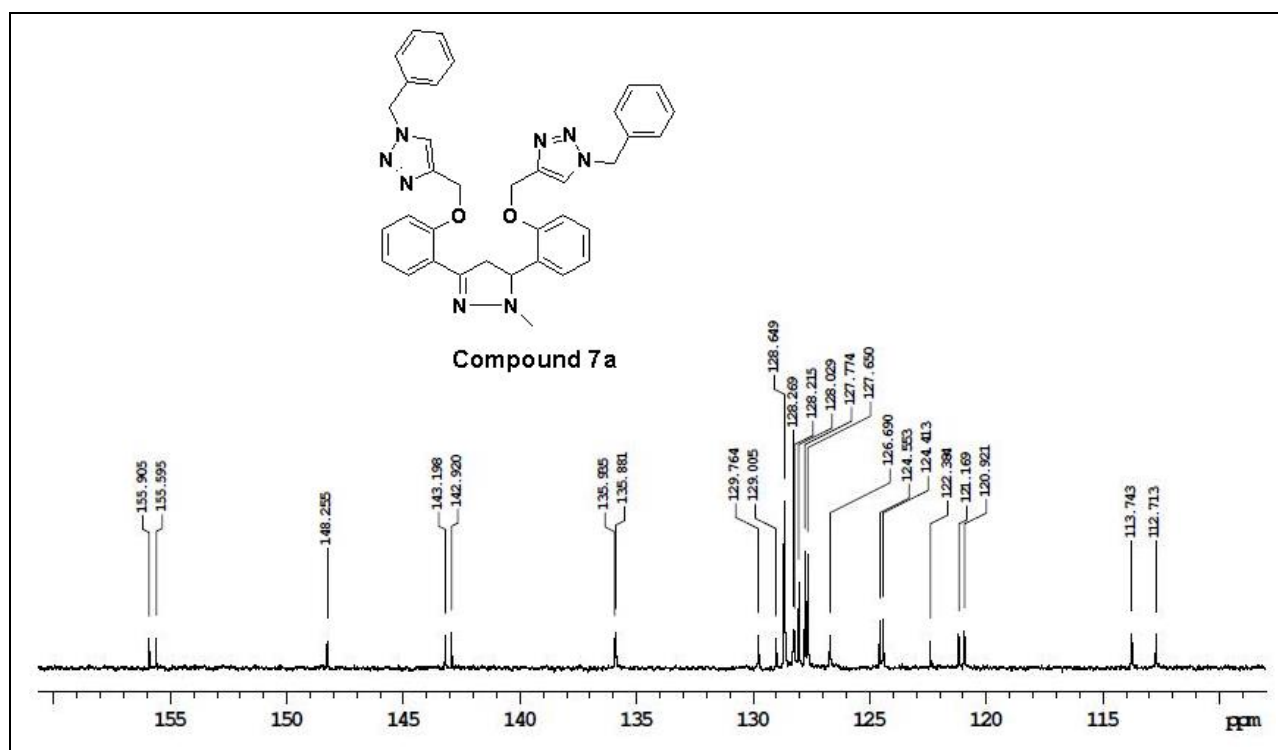
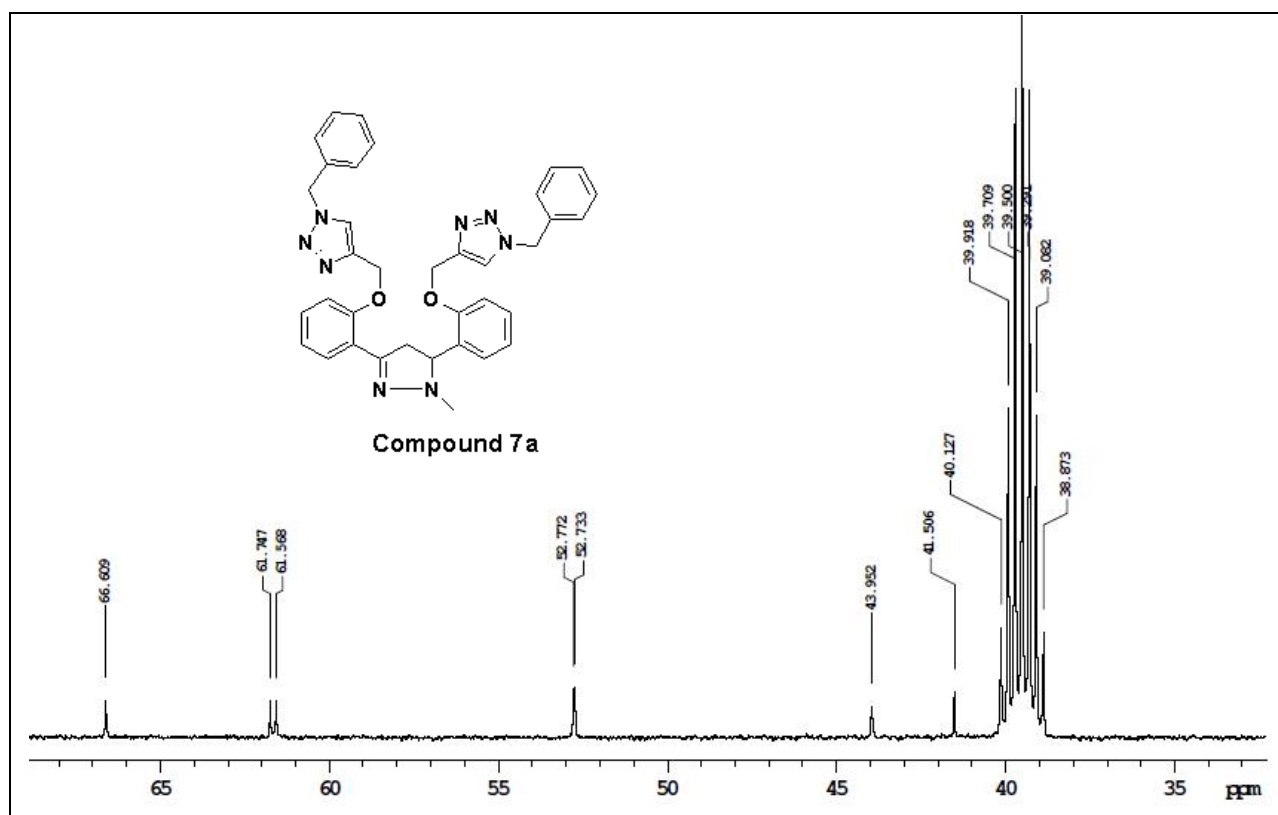


Figure S33: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7a**

126



127

128

Figure S34: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound 7a

129

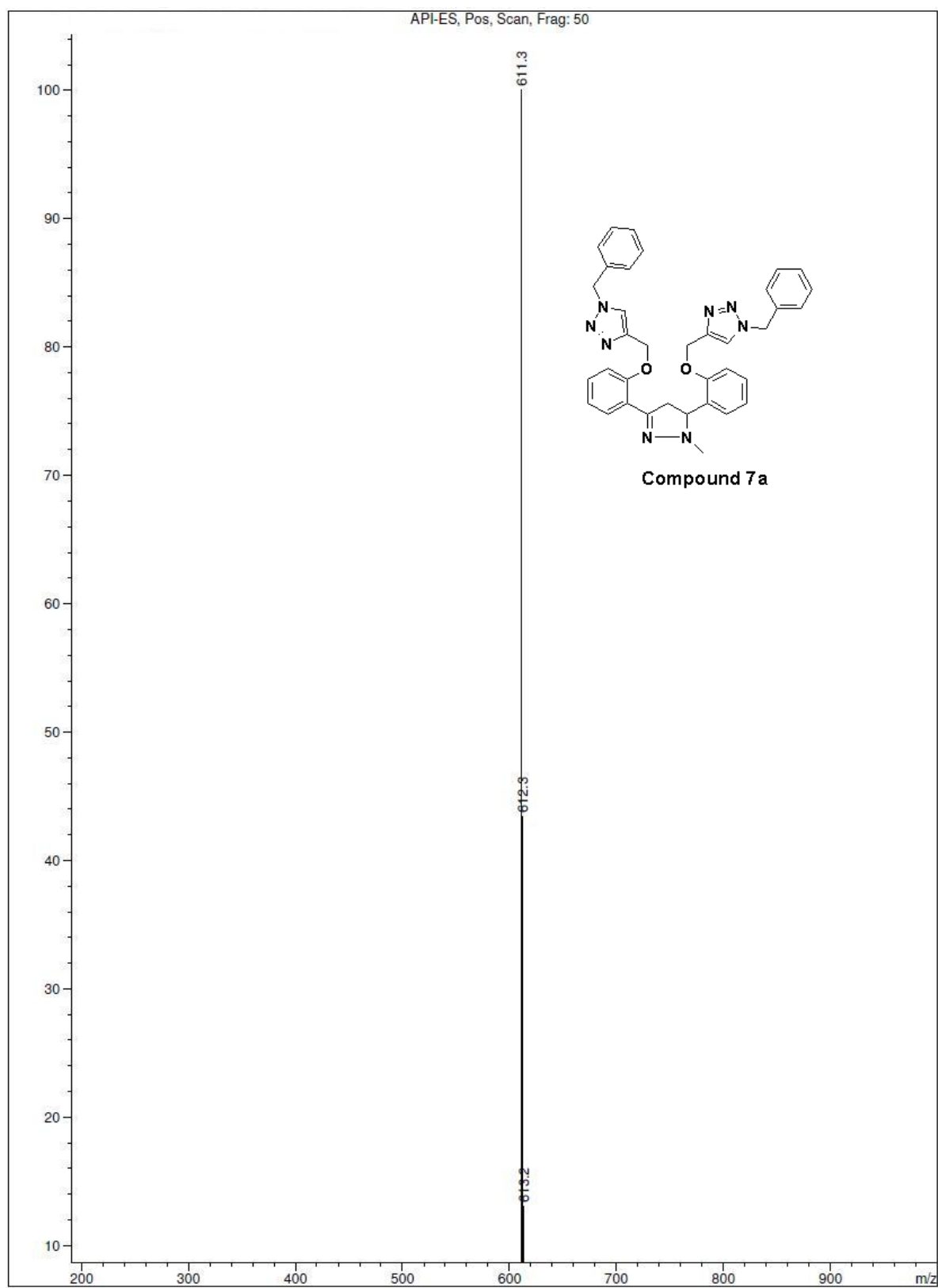


Figure S35: Mass spectra of compound **7a**

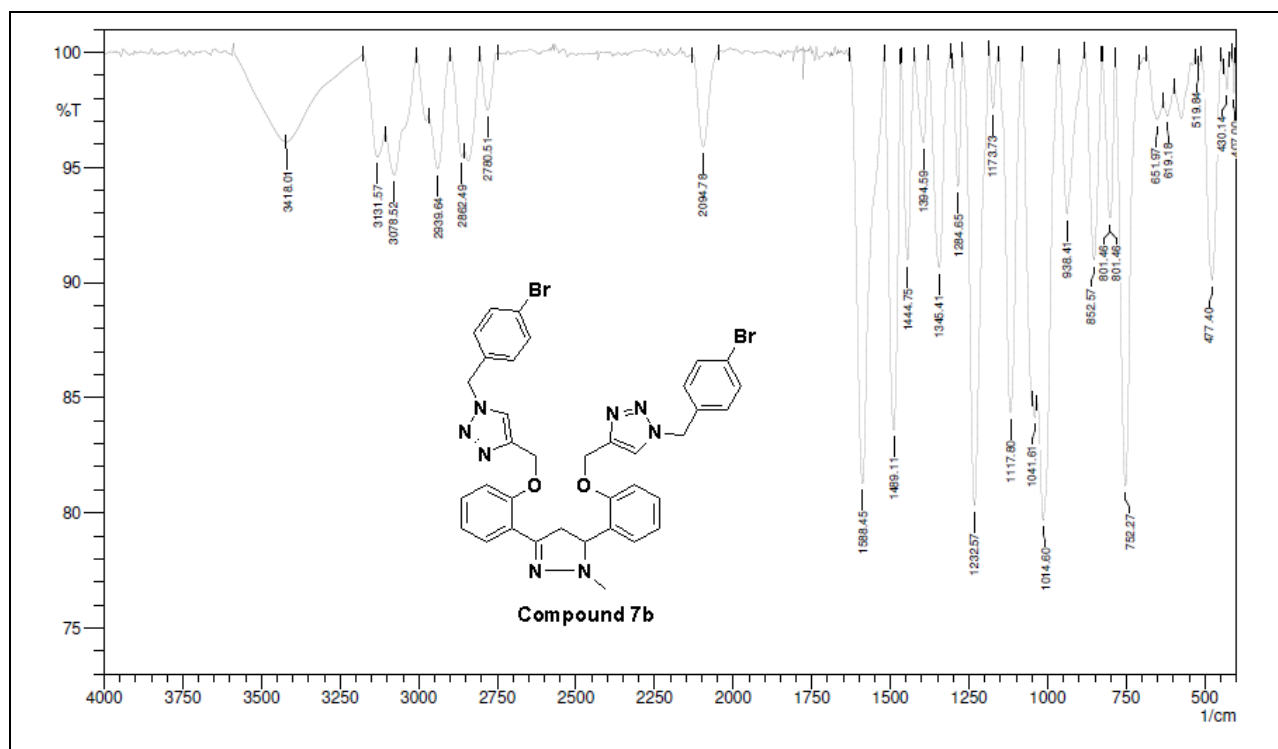


Figure S36: IR spectra of compound 7b

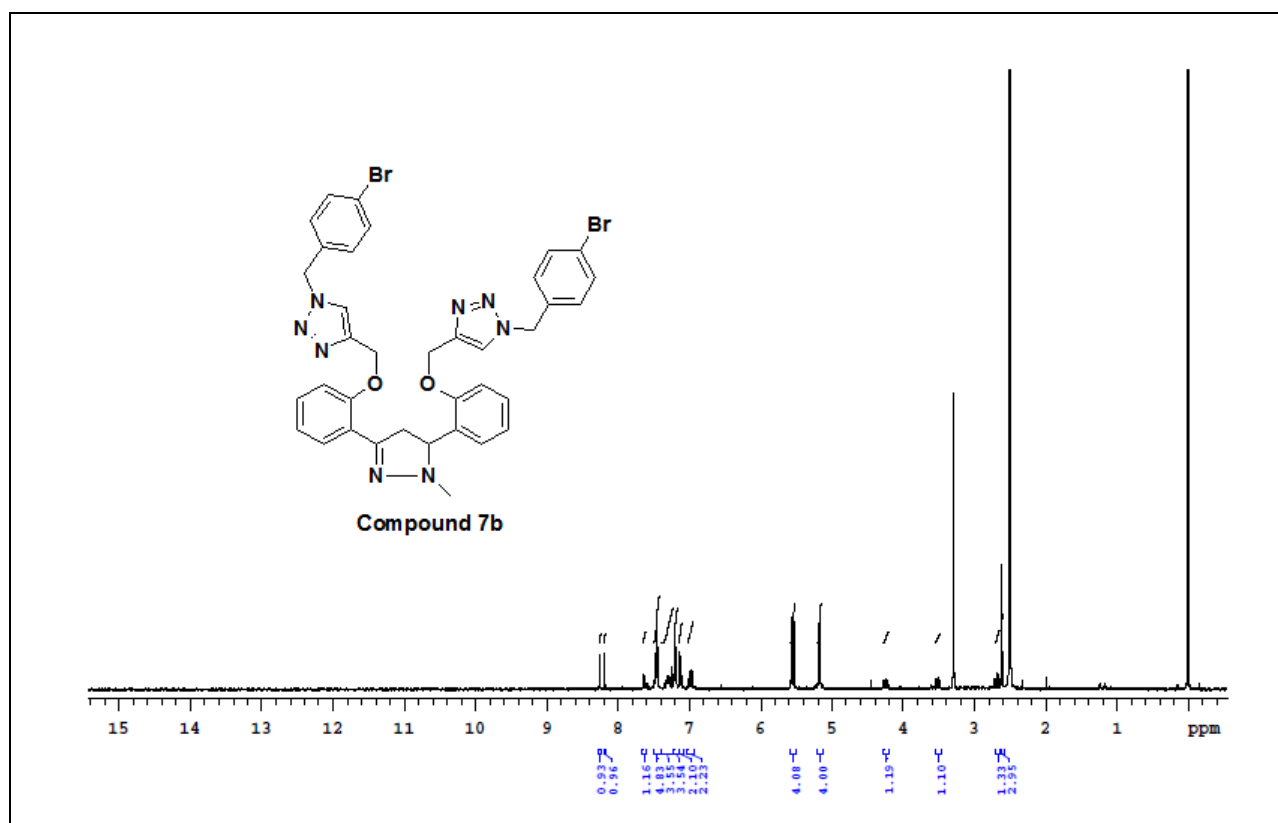


Figure S37: $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) spectra of compound 7b

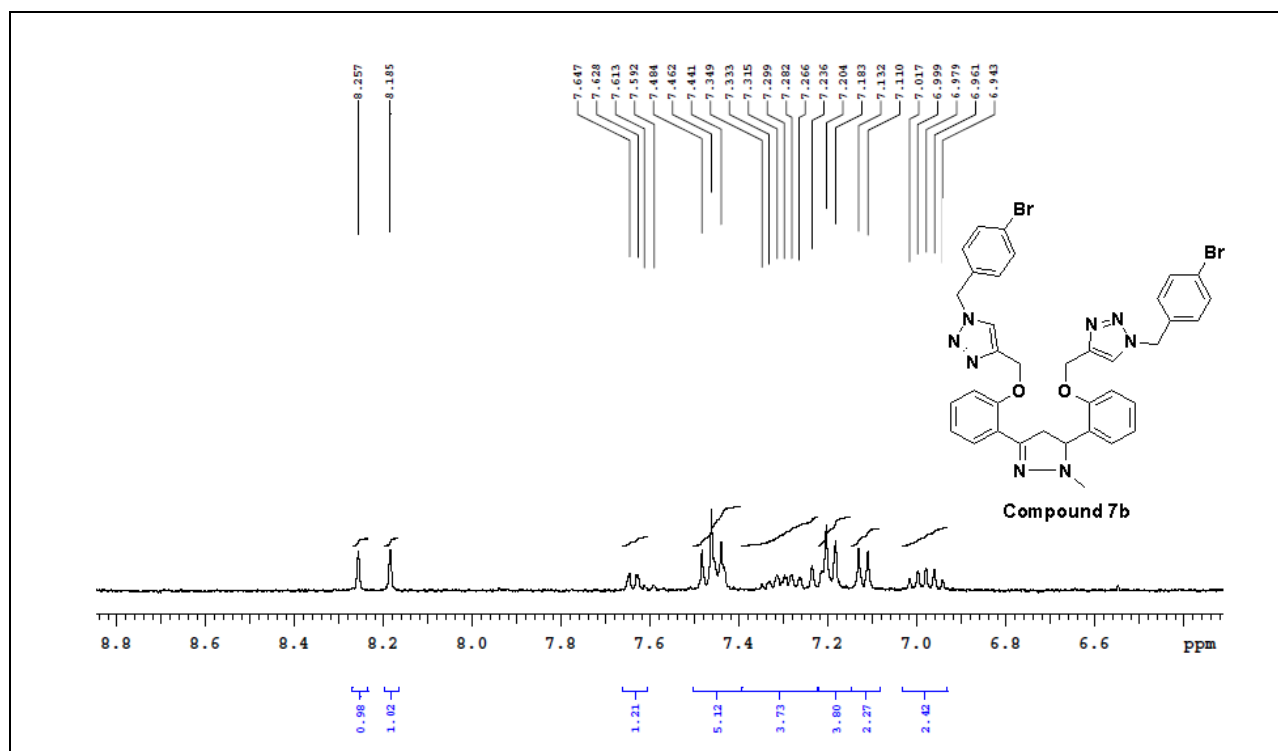


Figure S38: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7b

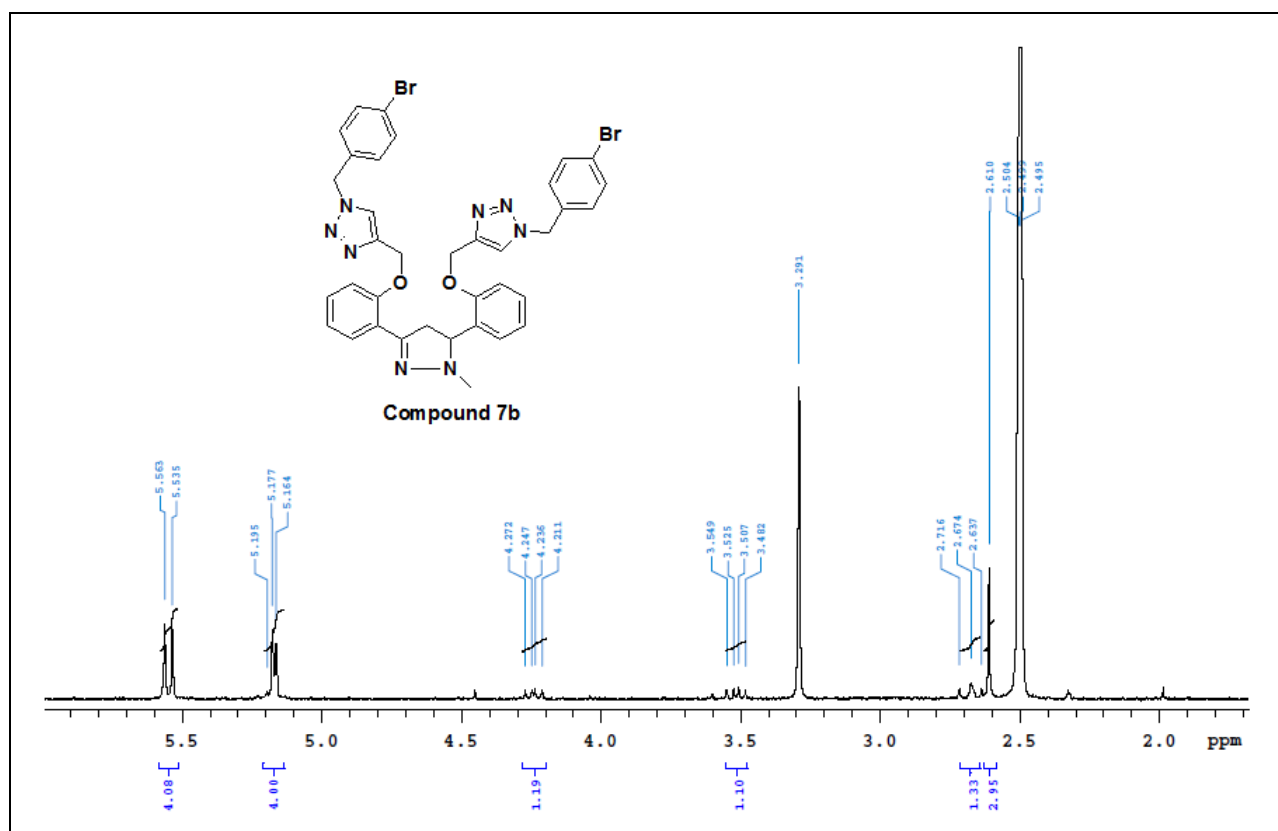


Figure S39: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7b

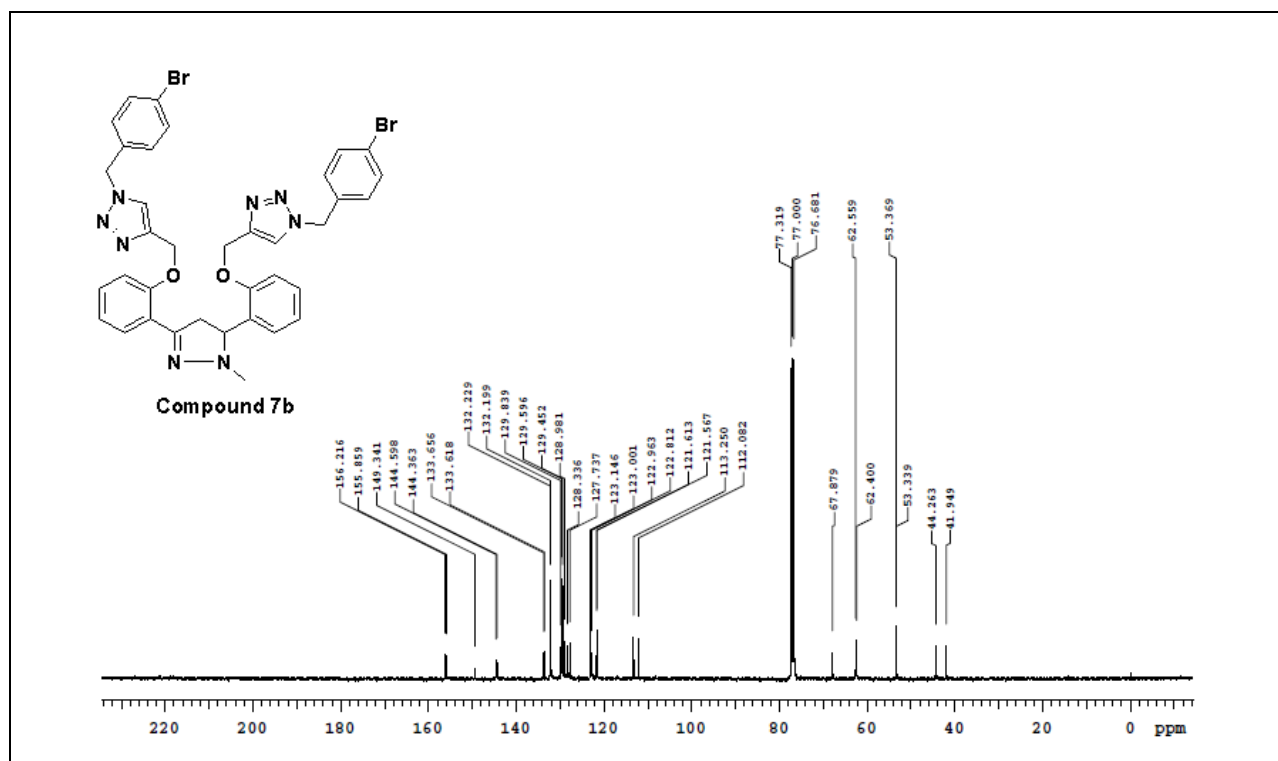


Figure S40: ^{13}C NMR (100 MHz, CDCl_3) spectra of compound 7b

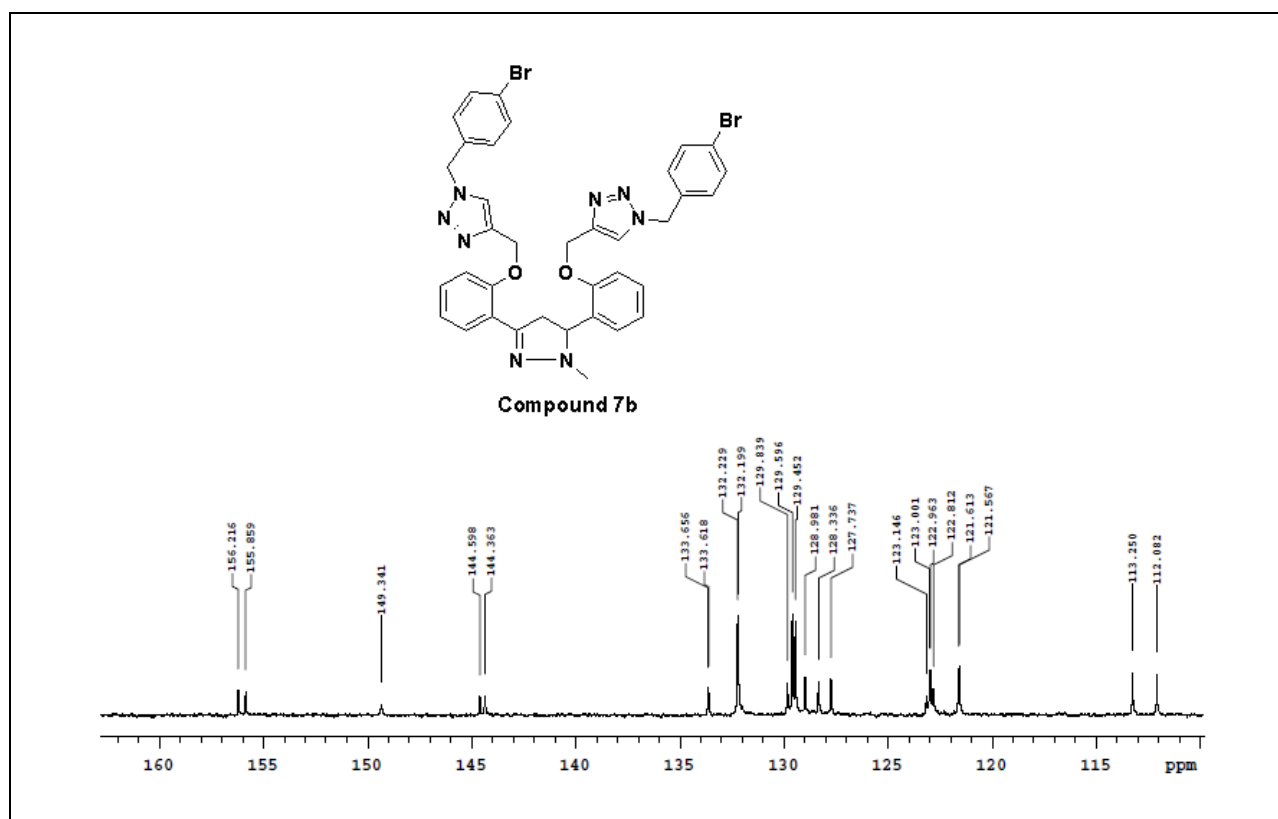


Figure S41: ^{13}C NMR (100 MHz, CDCl_3) spectra of compound 7b

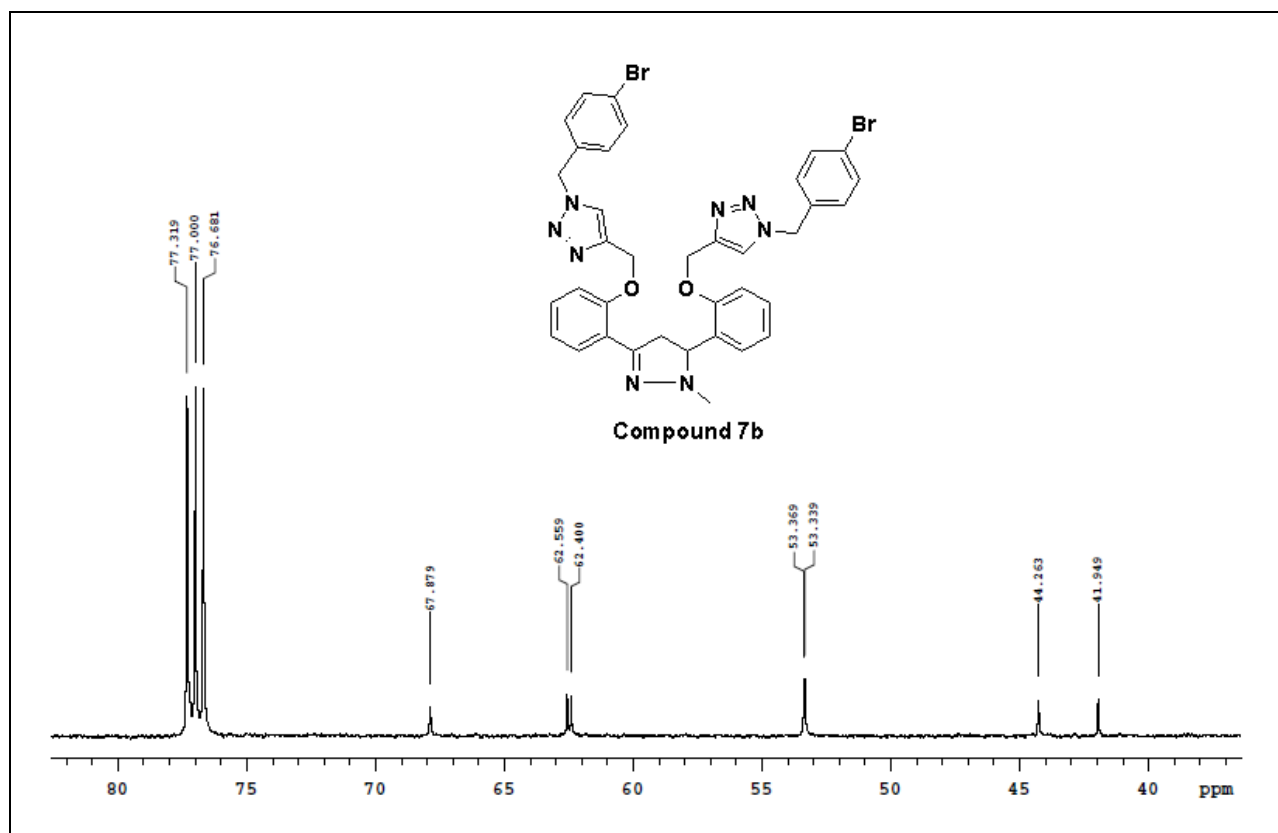


Figure S42: ^{13}C NMR (100 MHz, CDCl_3) spectra of compound 7b

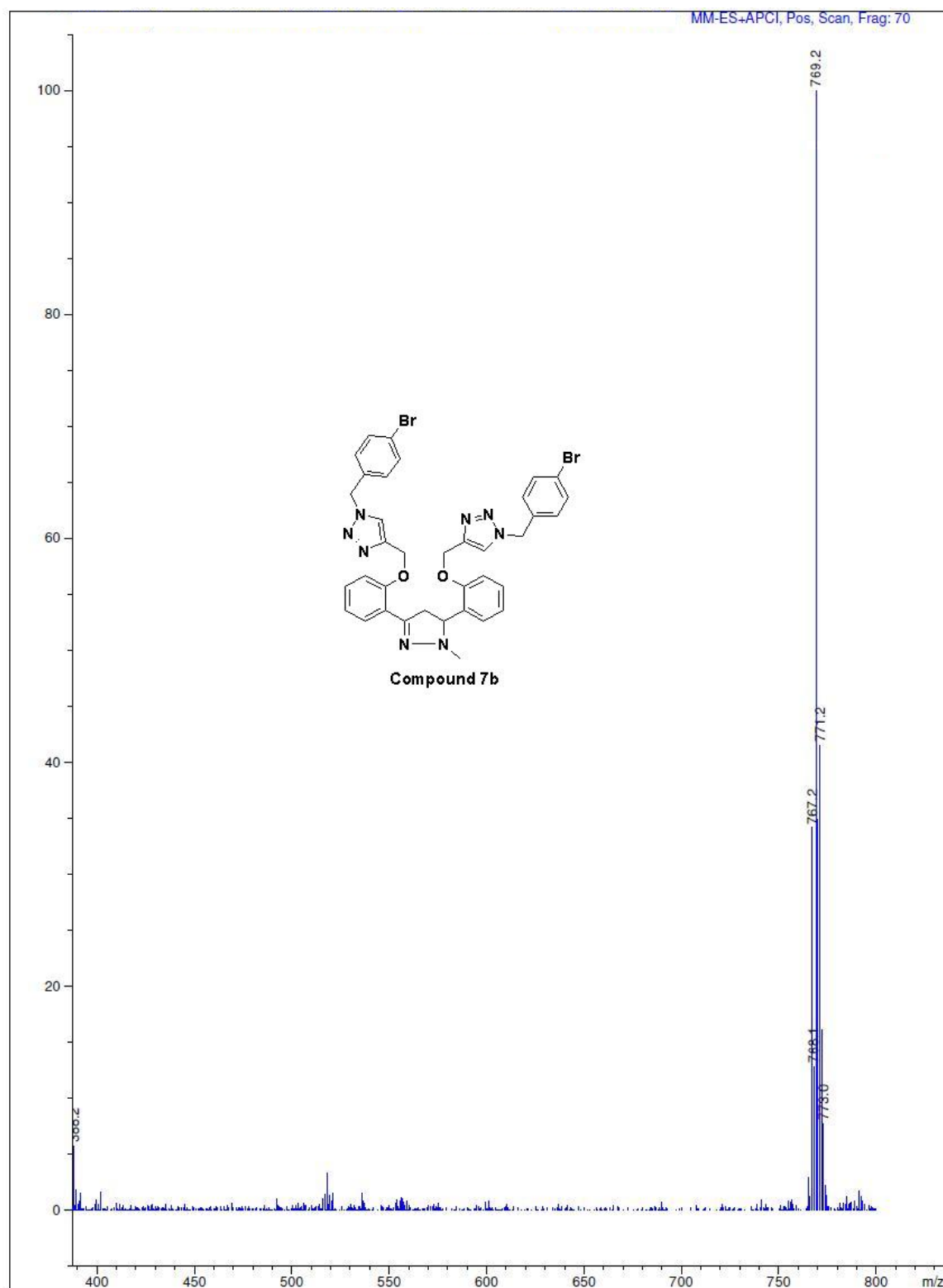


Figure S43: Mass spectra of compound 7b

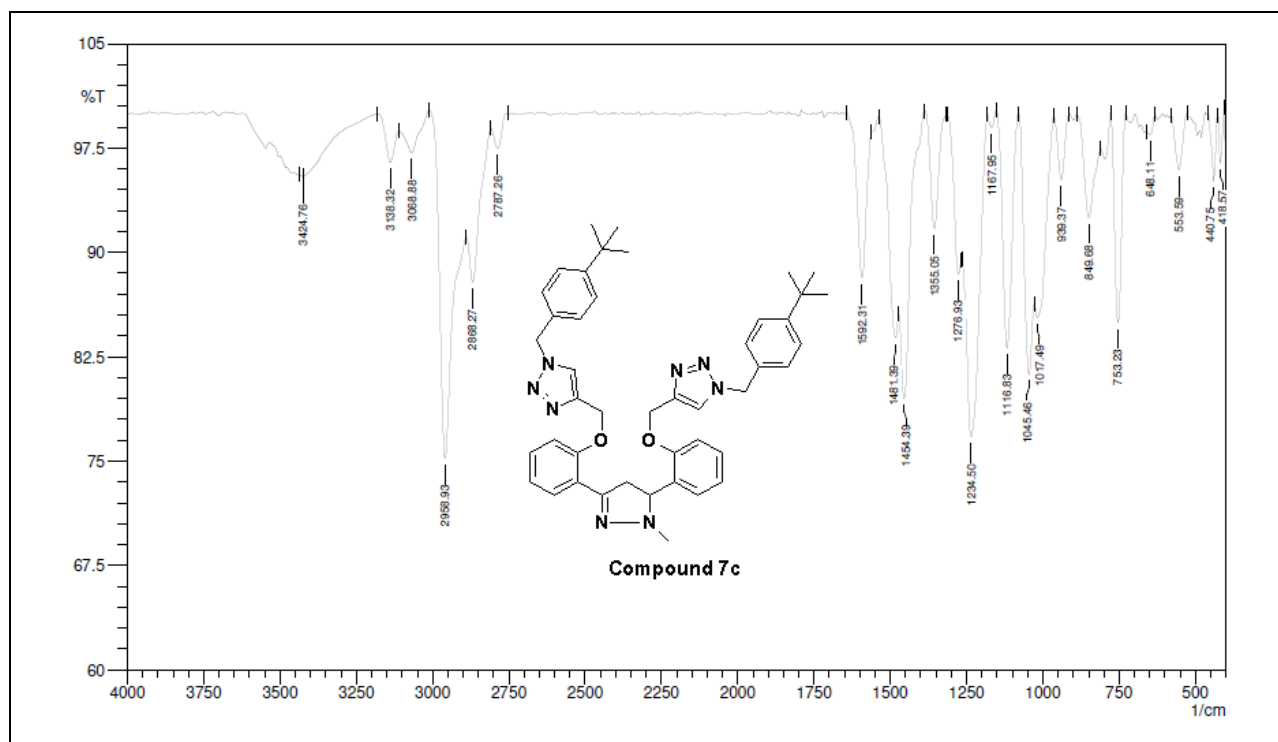


Figure S44: IR spectra of compound 7c

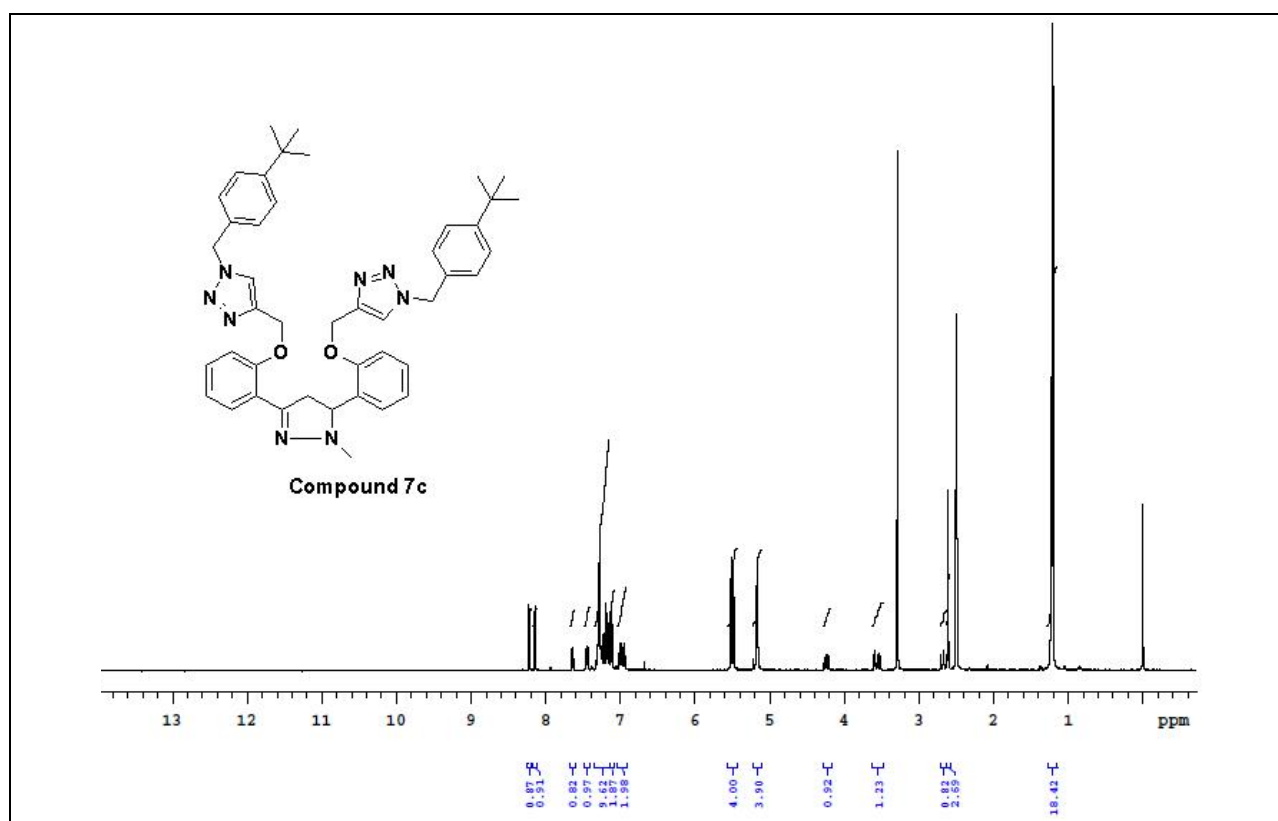


Figure S45: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7c

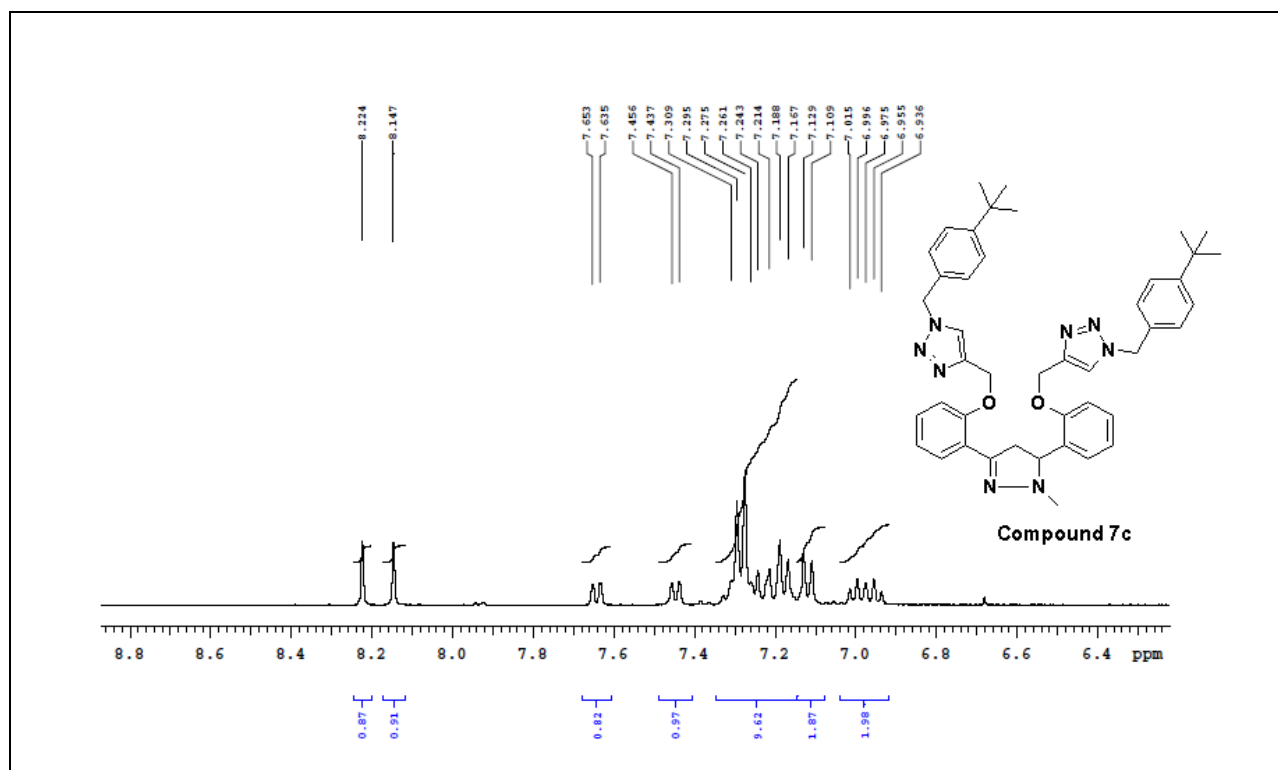


Figure S46: $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) spectra of compound 7c

169

170

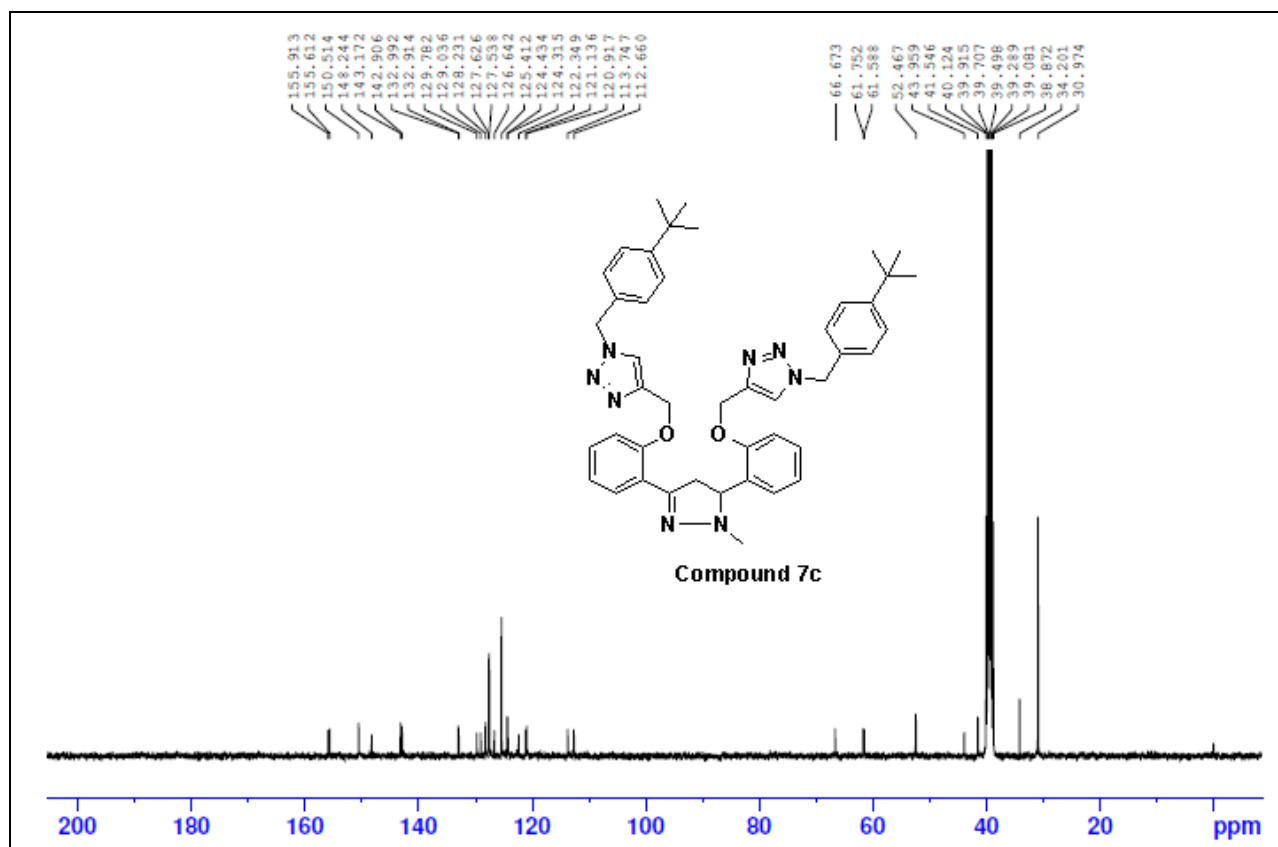


Figure S48: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound 7c

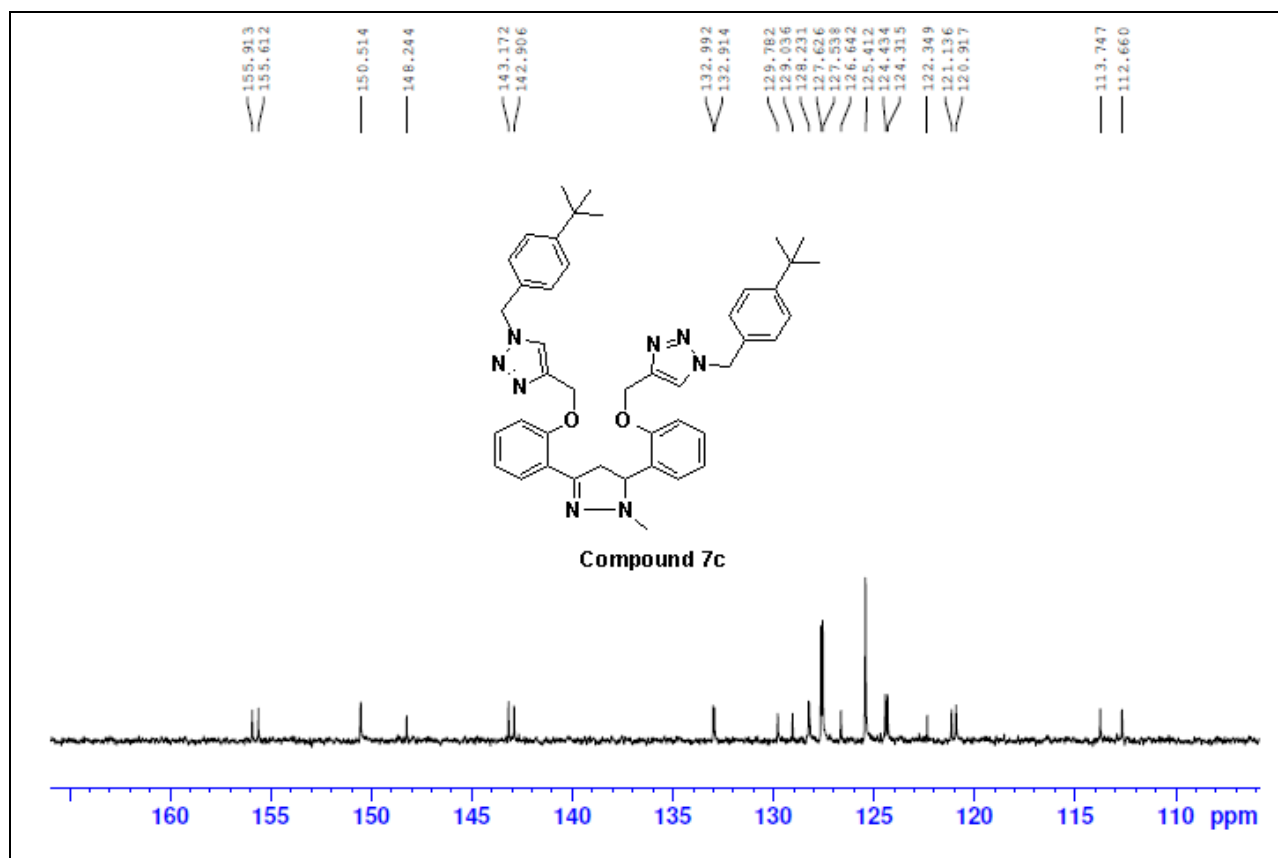


Figure S49: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound 7c

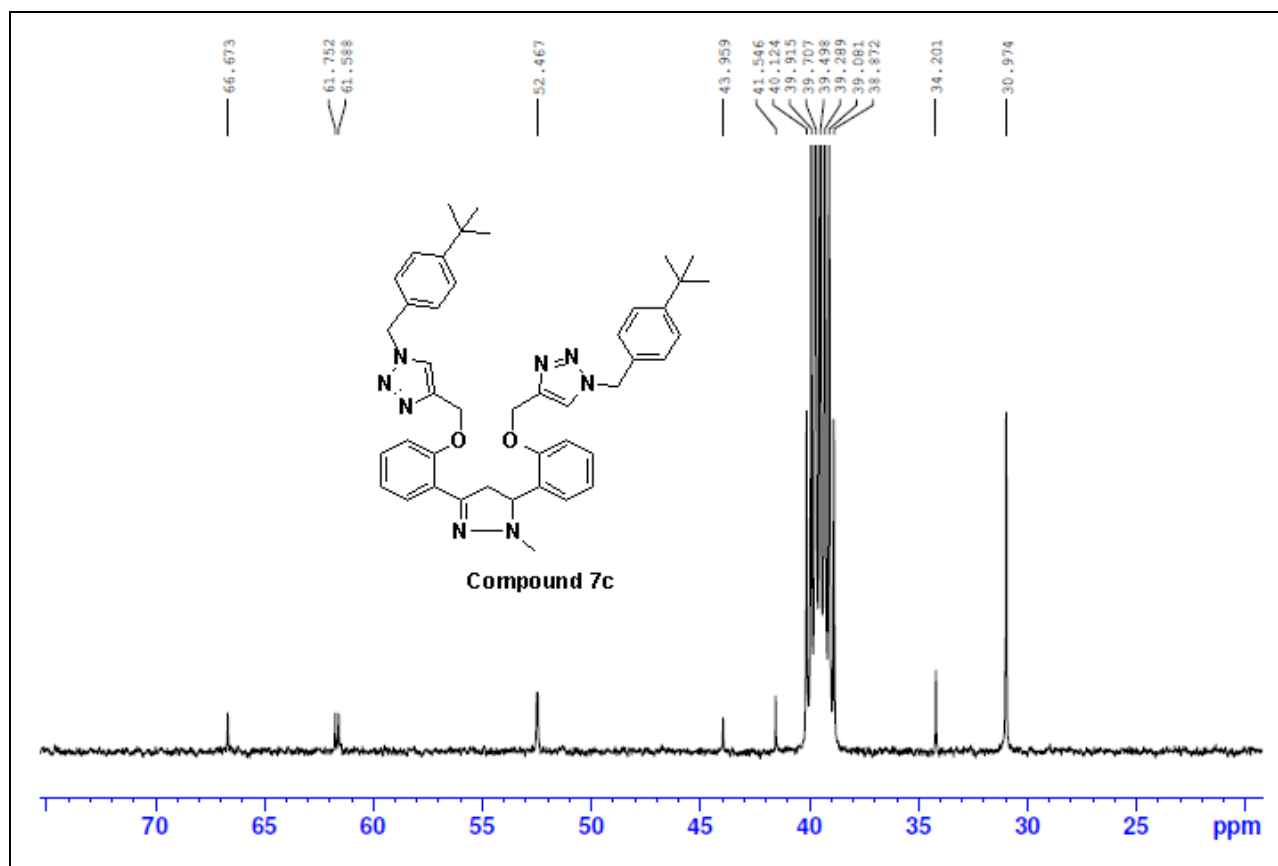
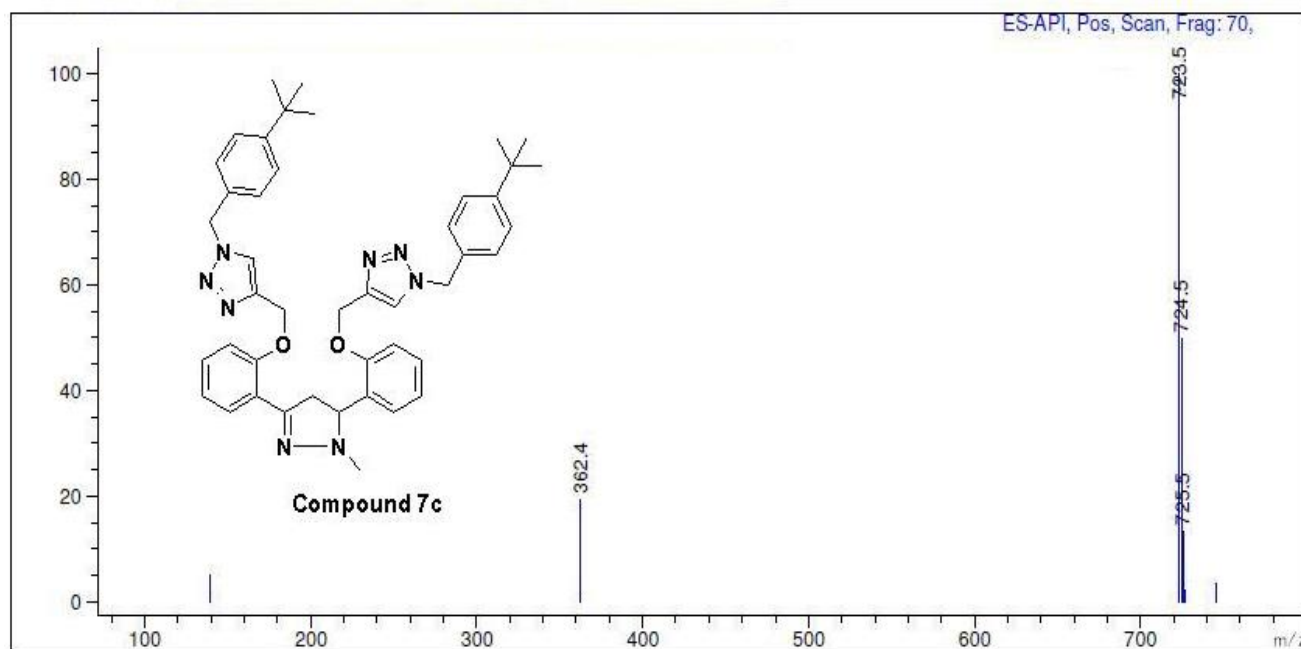


Figure S50: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound 7c

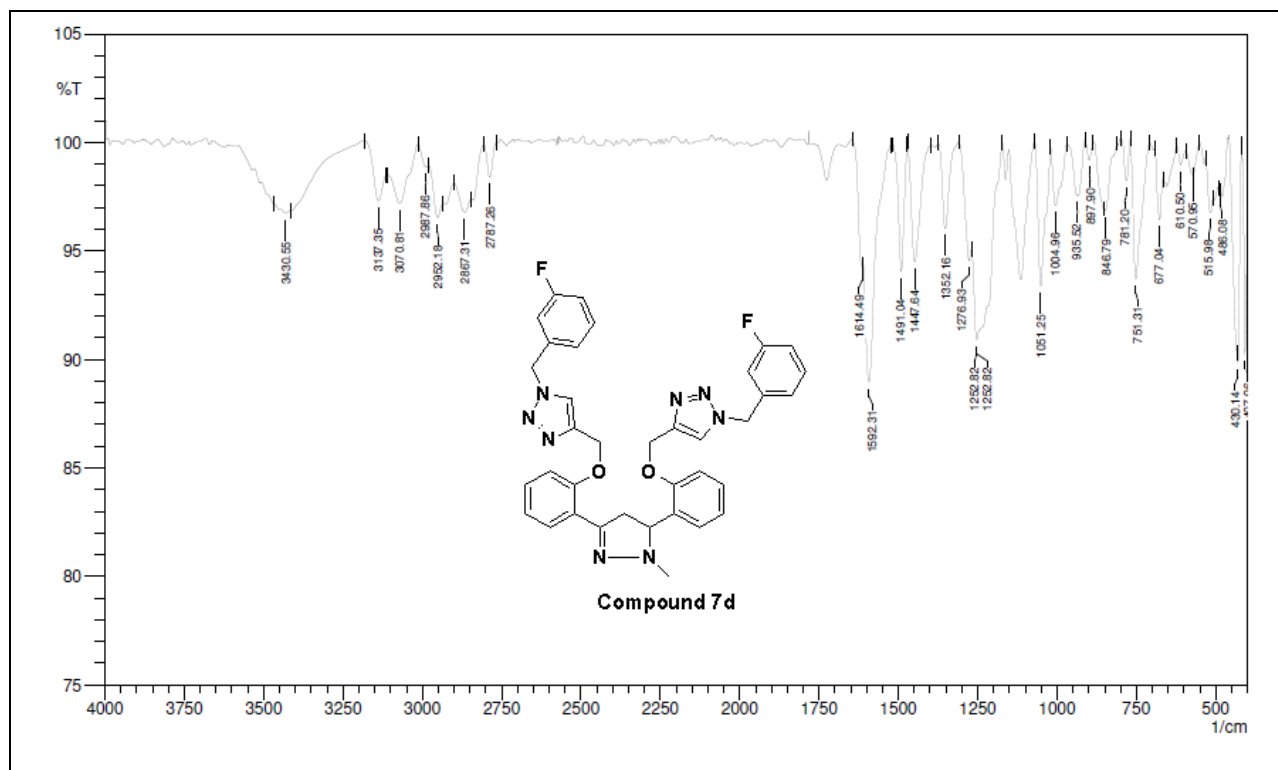
176



177

178

Figure S51: Mass spectra of compound 7c



179

180

Figure S52: IR spectra of compound 7d

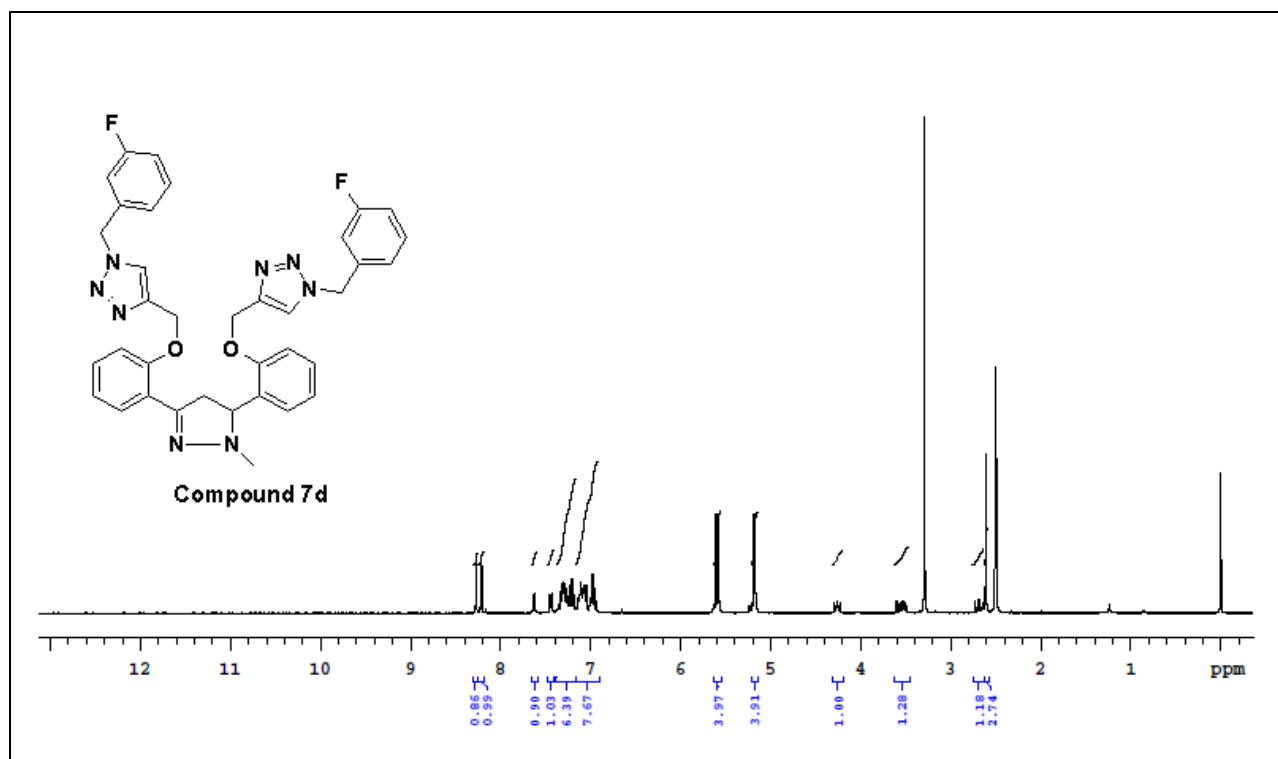


Figure S53: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7d

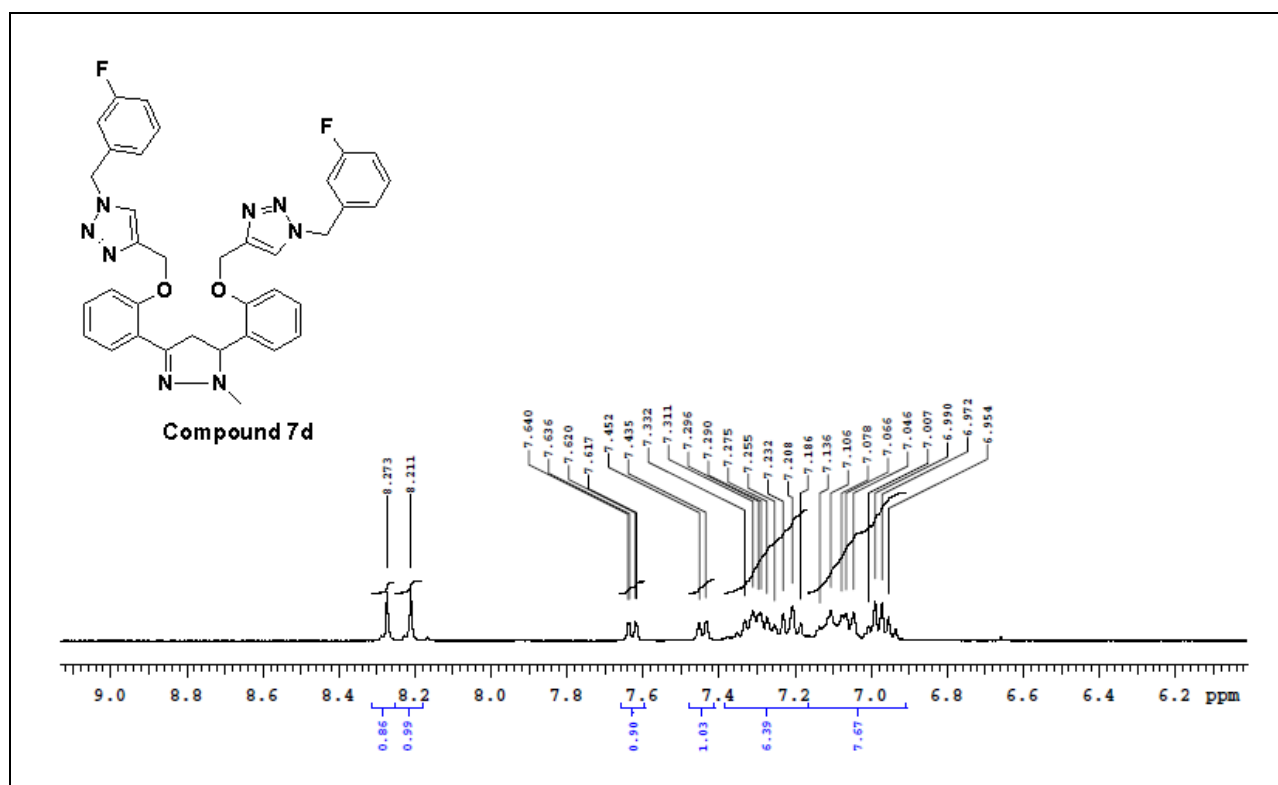


Figure S54: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7d

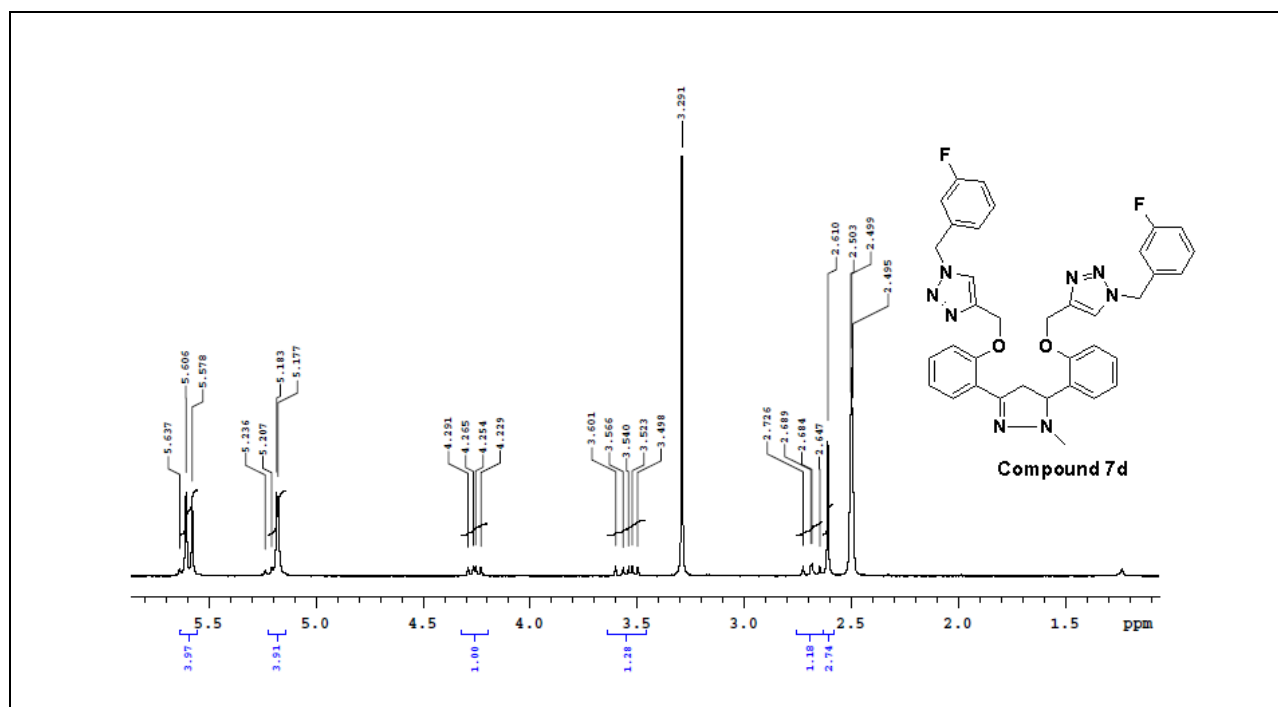


Figure S55: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7d

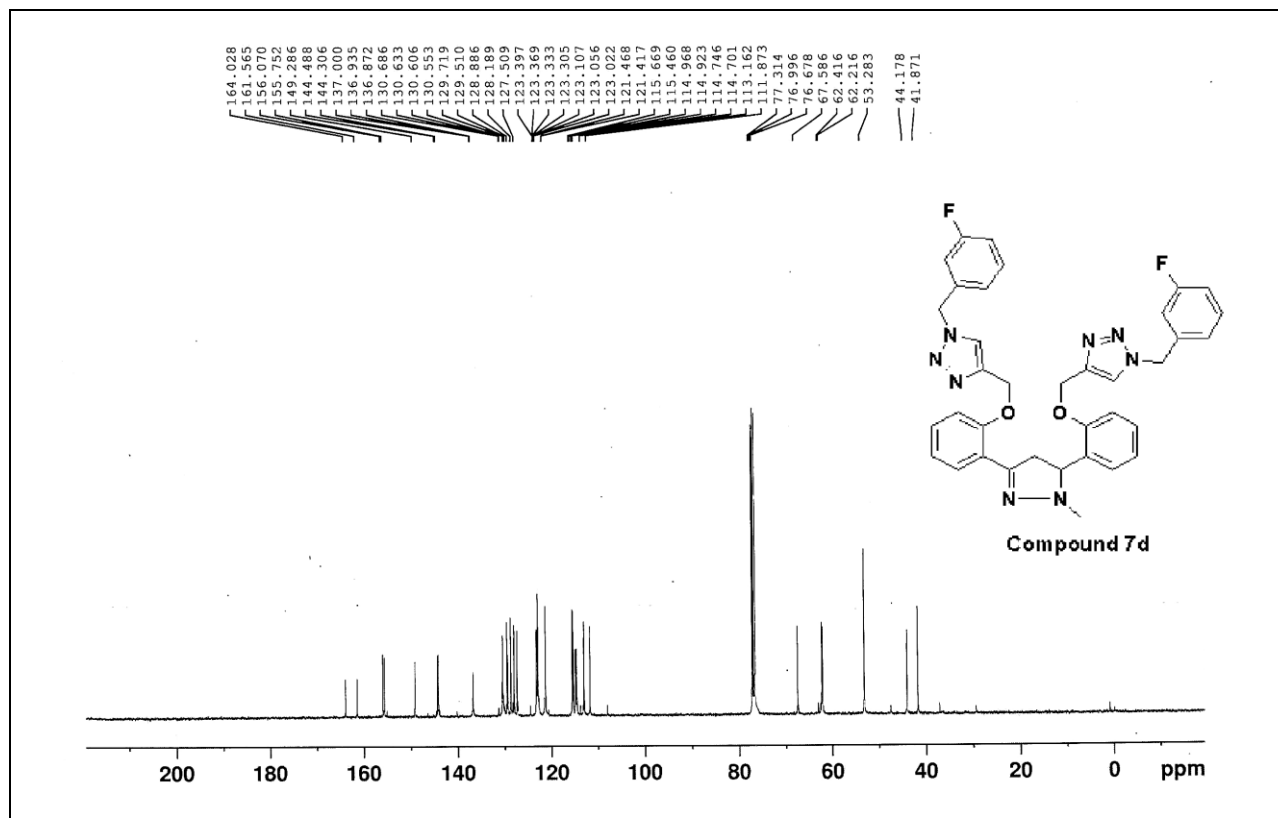
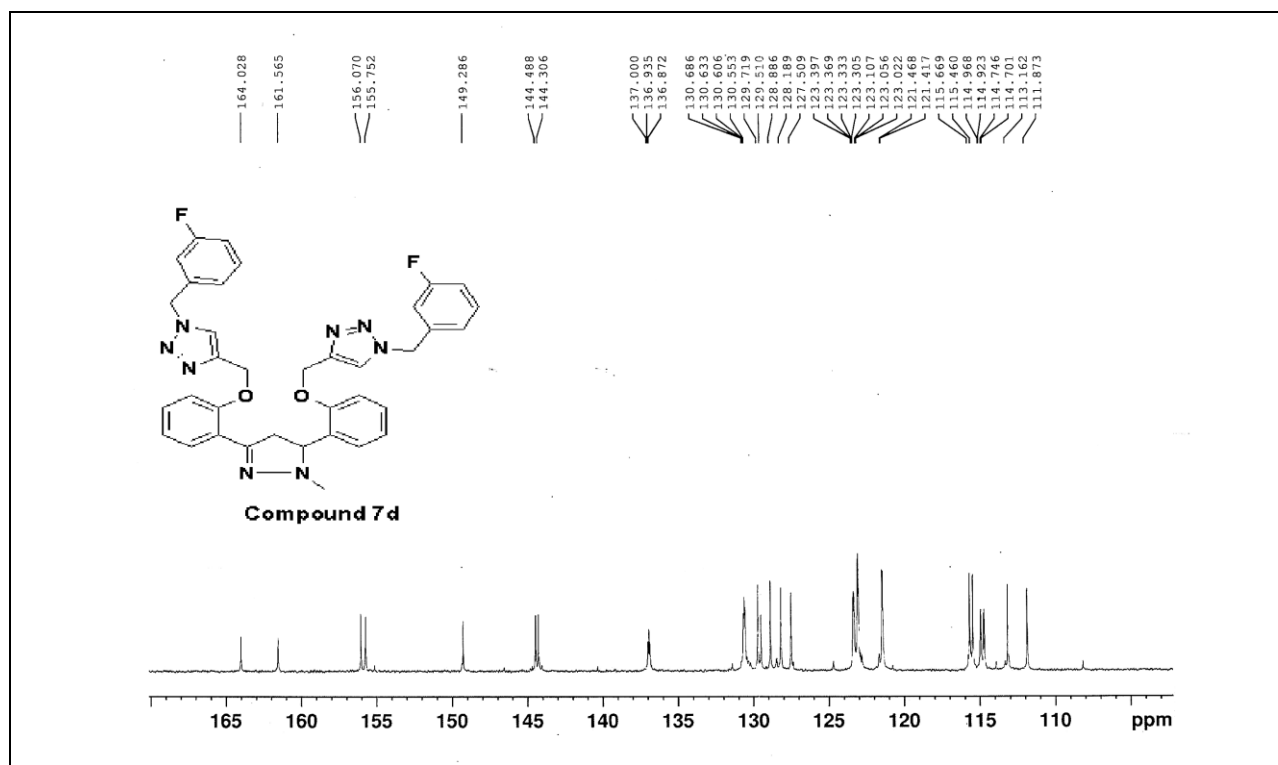


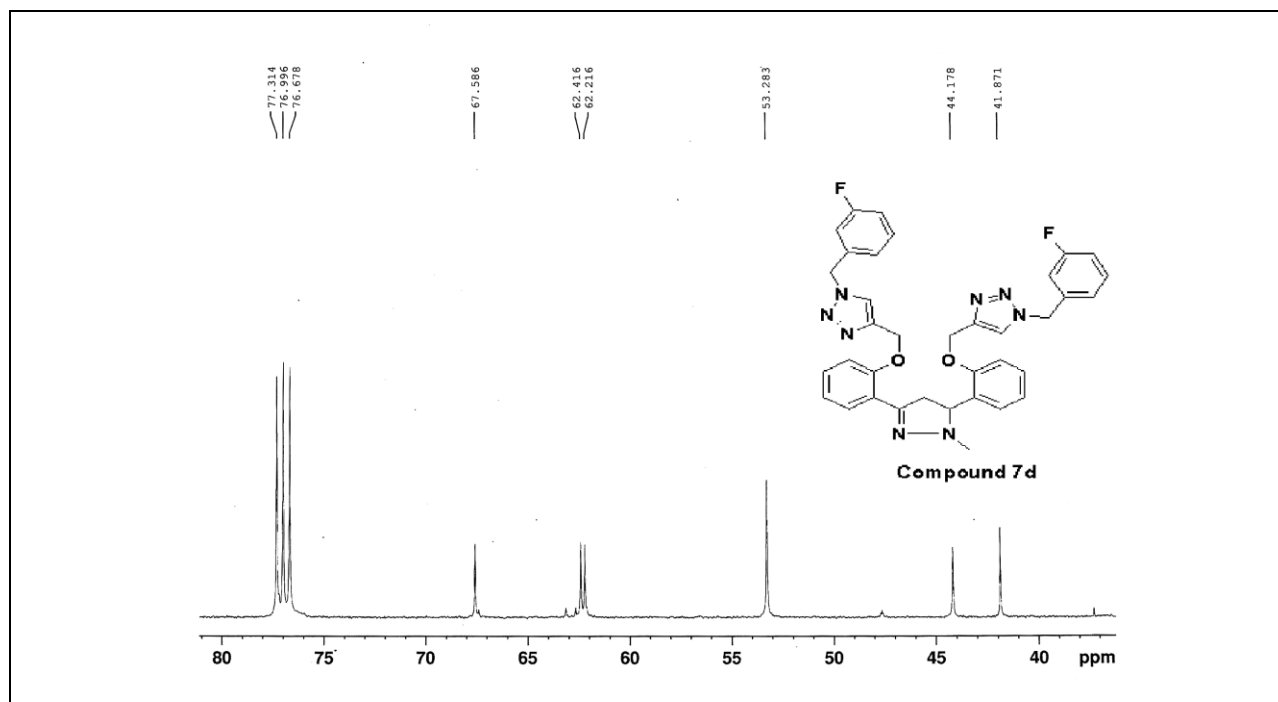
Figure S56: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 7d

189



190

191

Figure S57: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 7d

192

193

Figure S58: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 7d

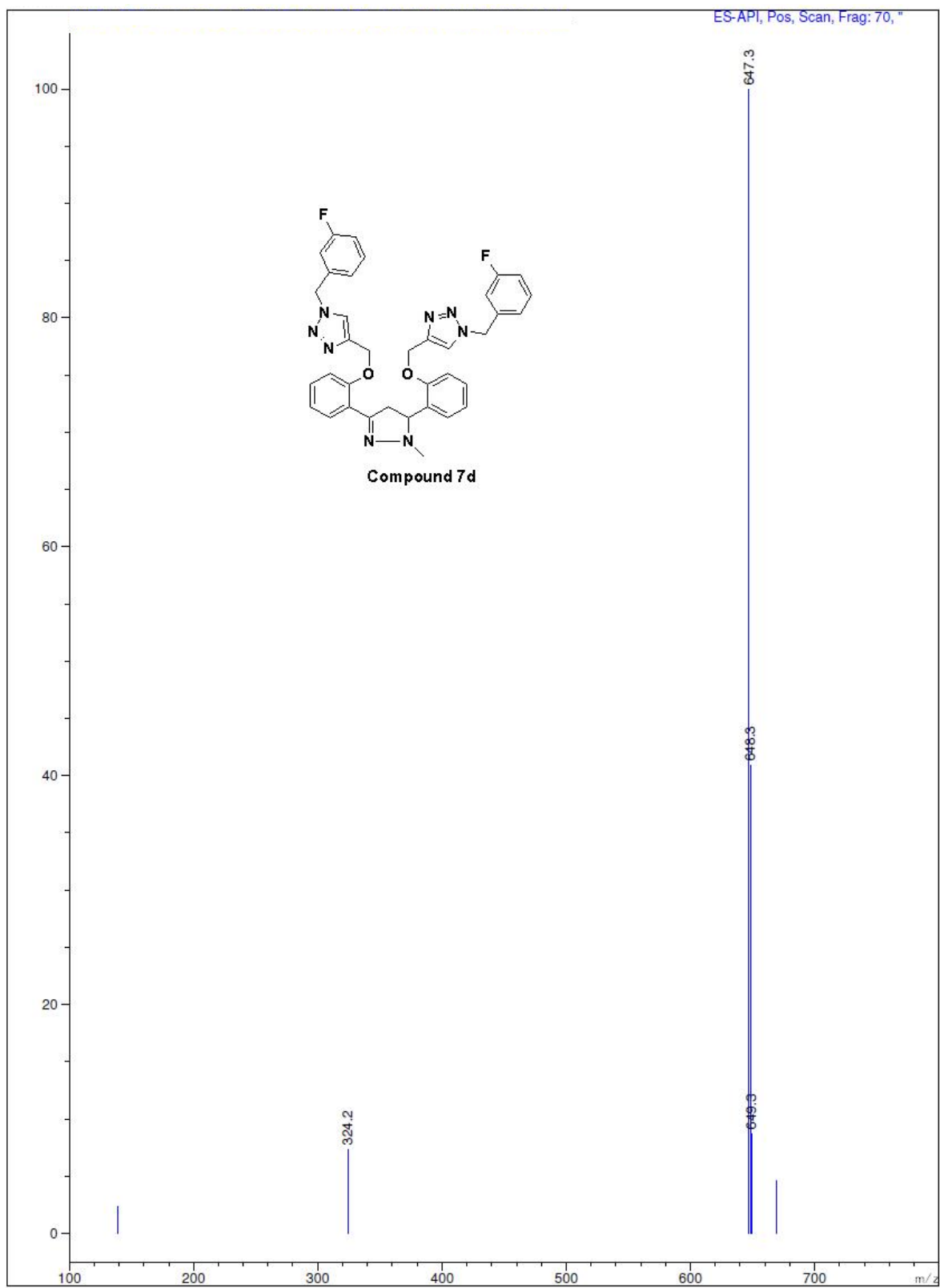


Figure S59: Mass spectra of compound **7d**

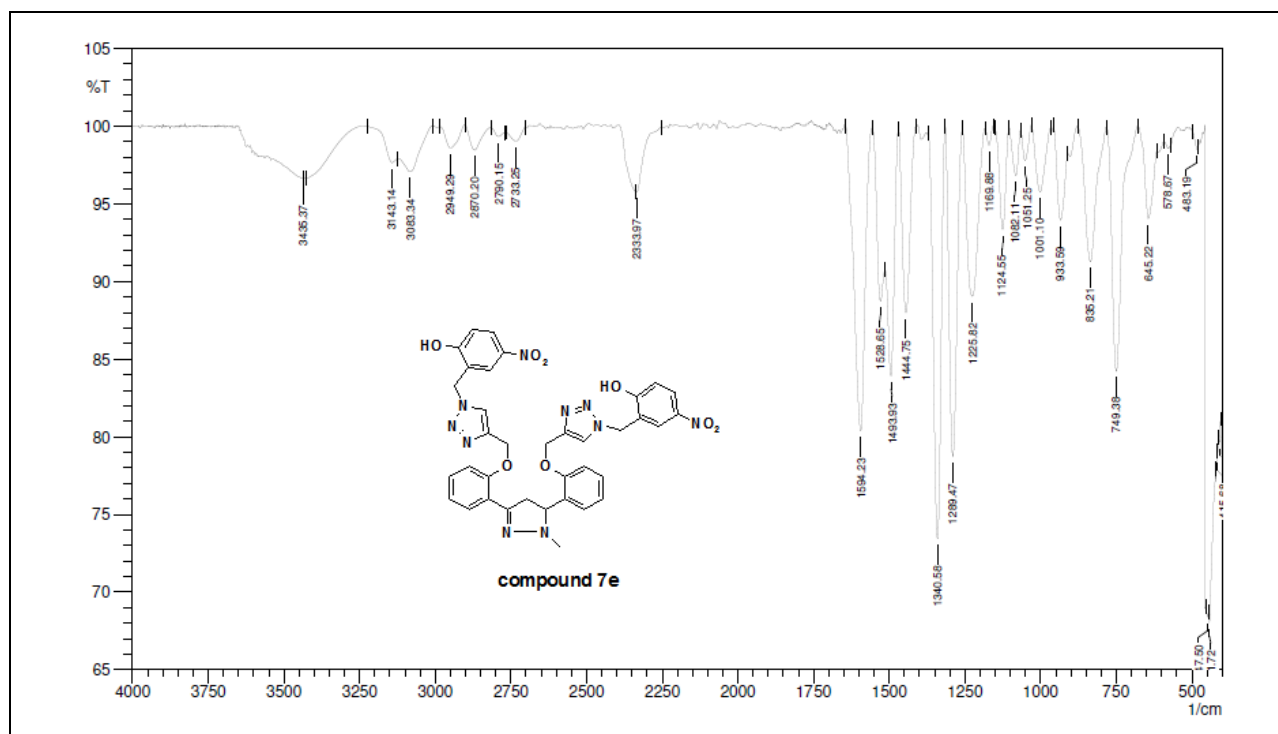


Figure S60: IR spectra of compound 7e

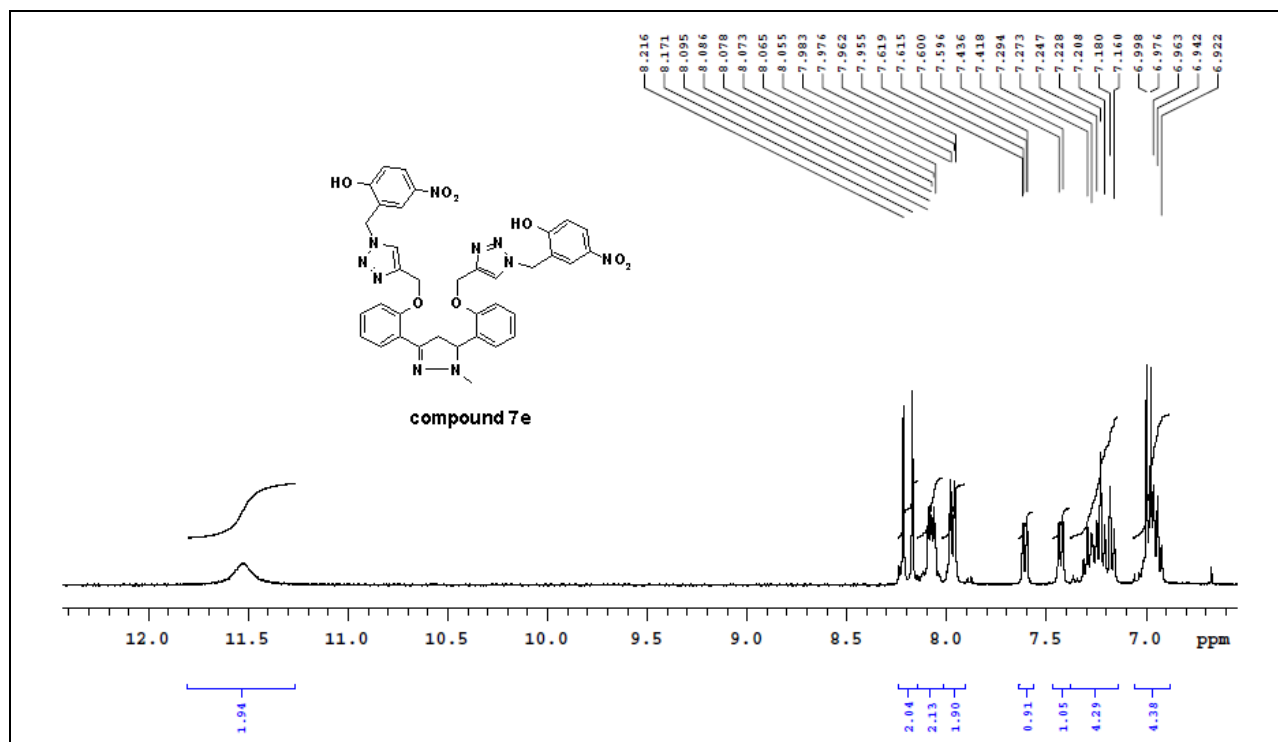


Figure S61: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7e

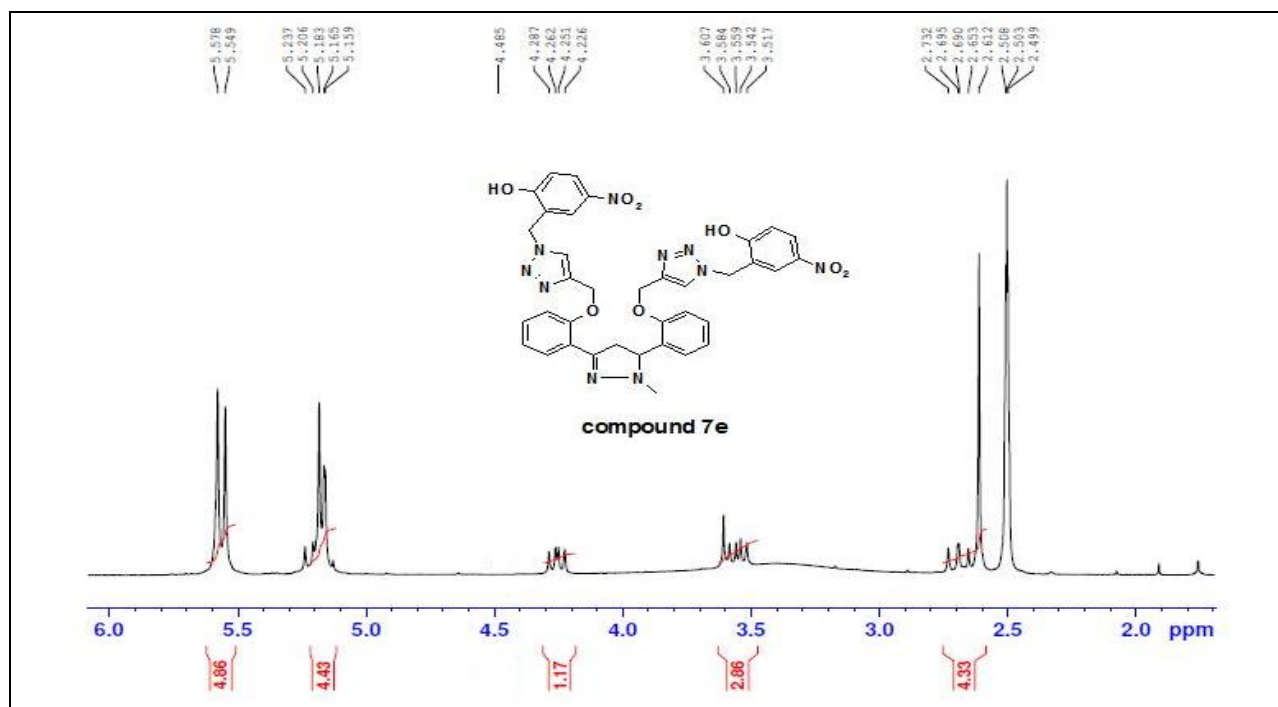


Figure S62: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7e

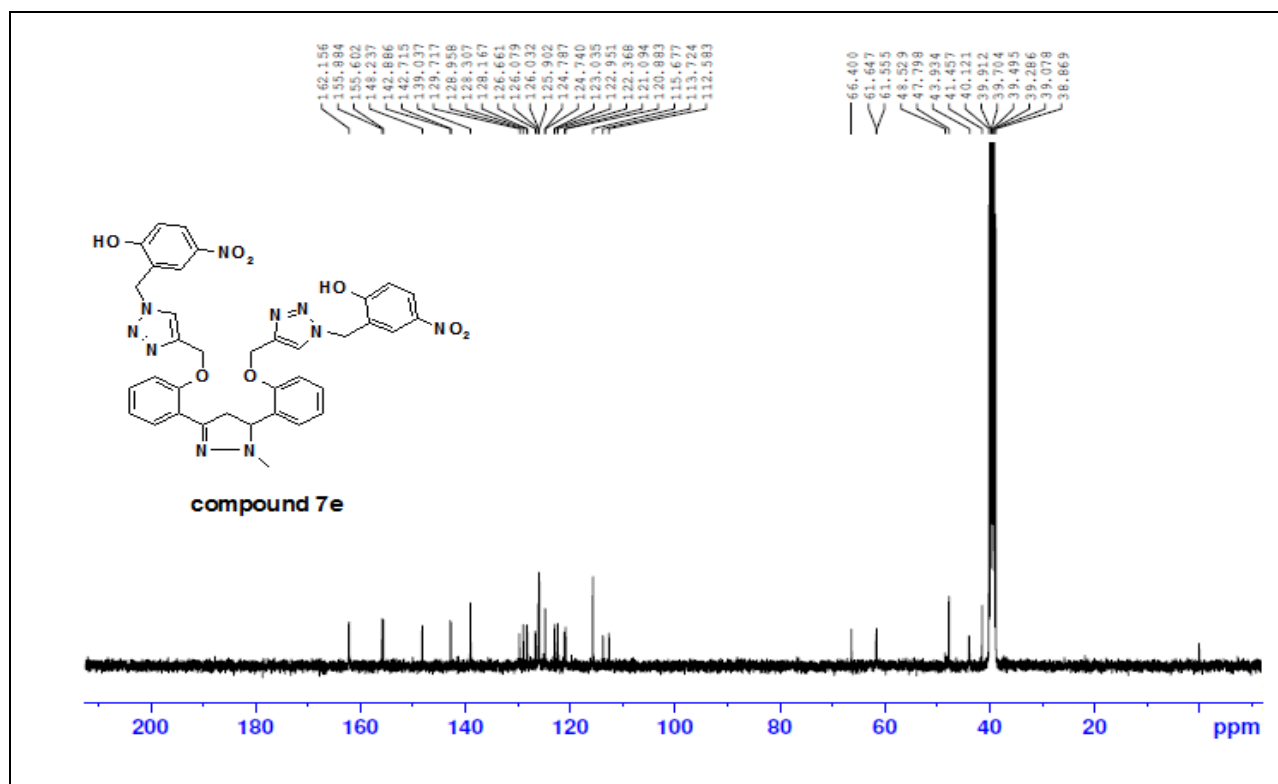


Figure S63: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound 7e

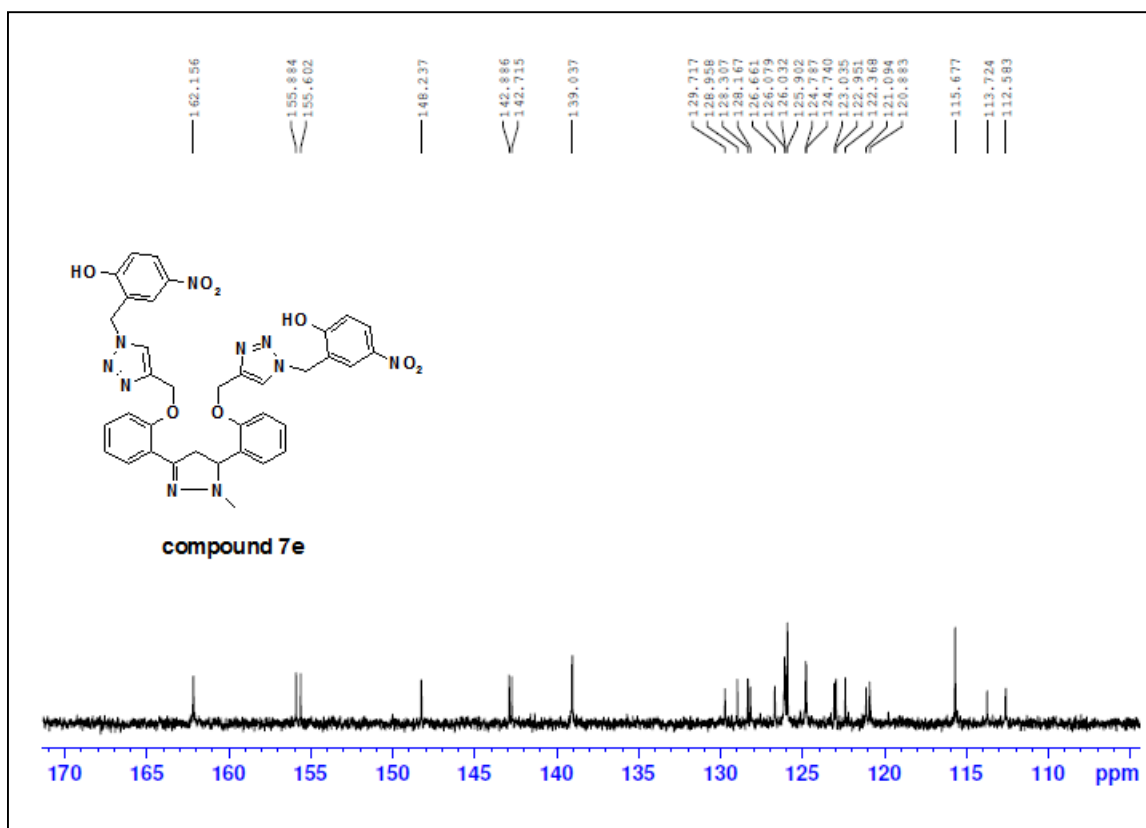


Figure S64: ^{13}C NMR (100 MHz, DMSO- d_6) spectra of compound 7e

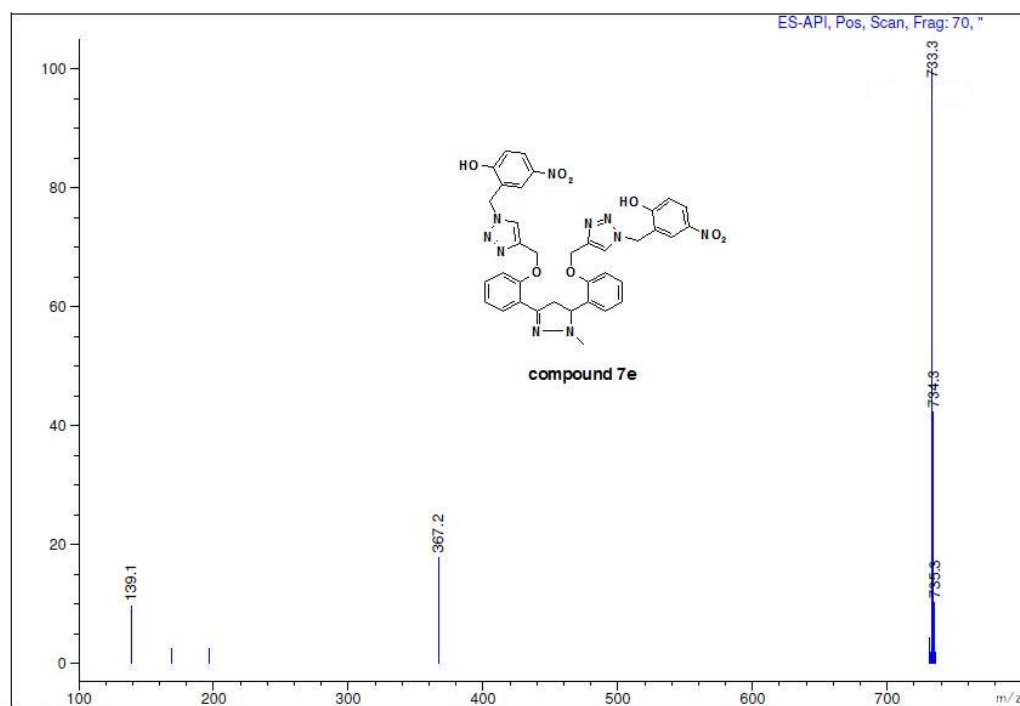


Figure S65: Mass spectra of compound 7e

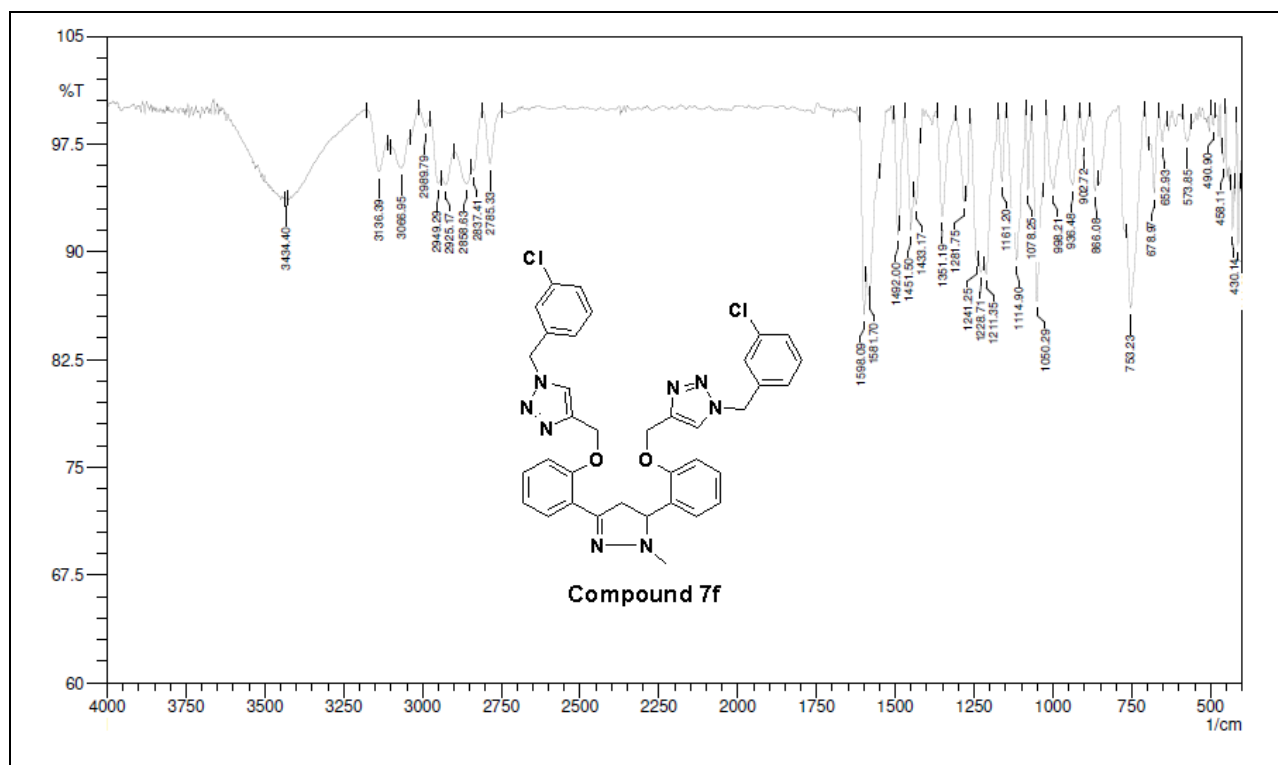


Figure S66: IR spectra of compound 7f

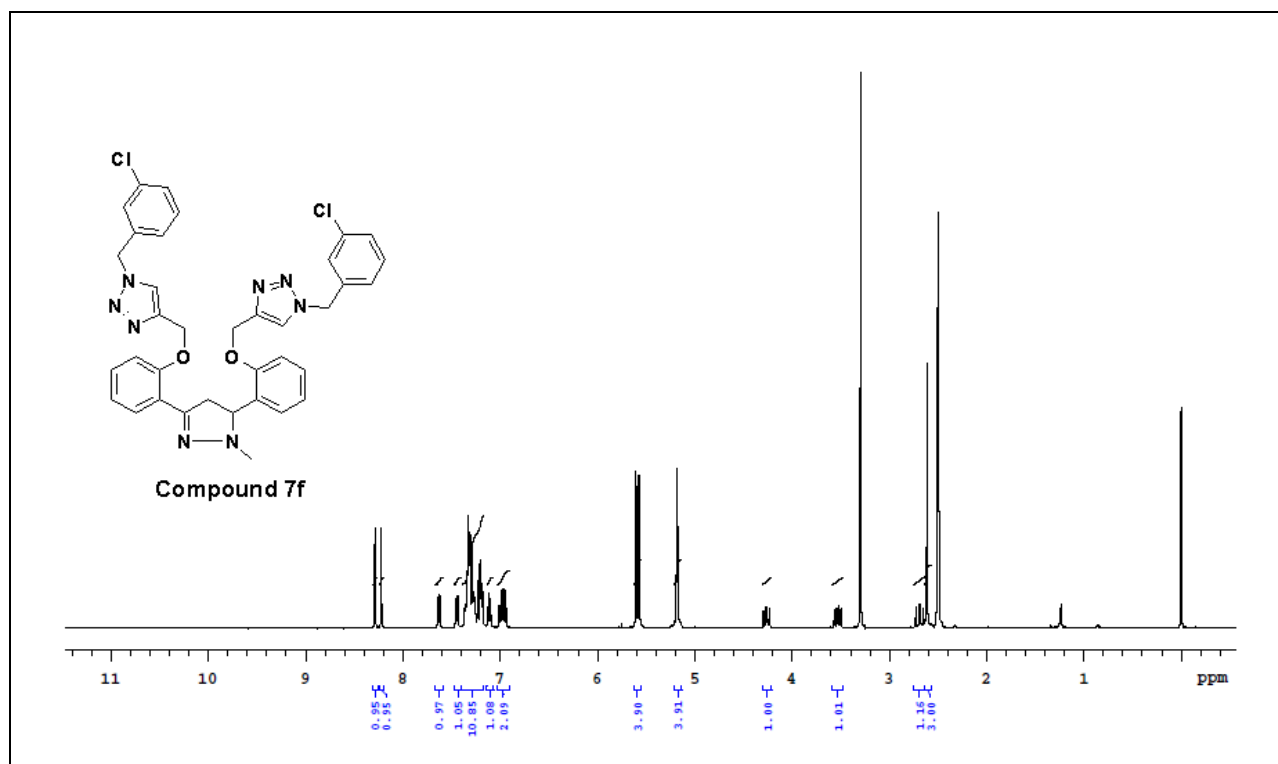


Figure S67: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7f

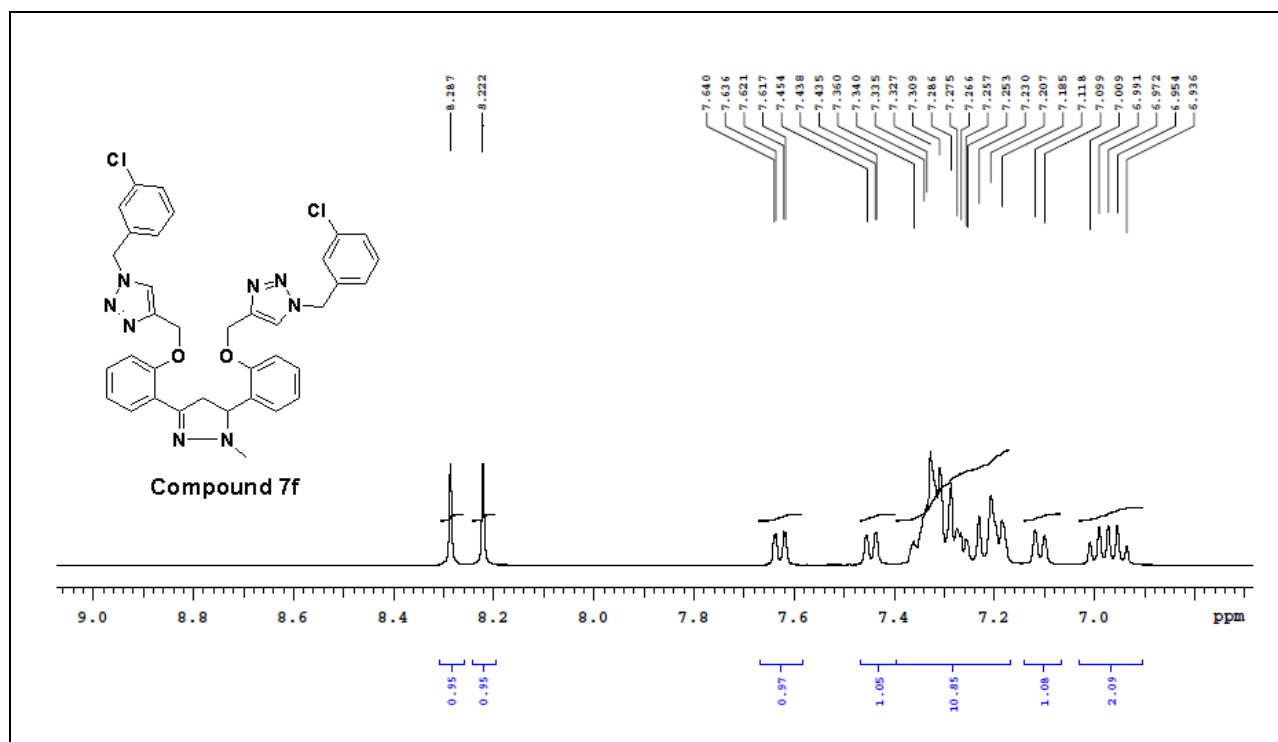


Figure S68: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7f

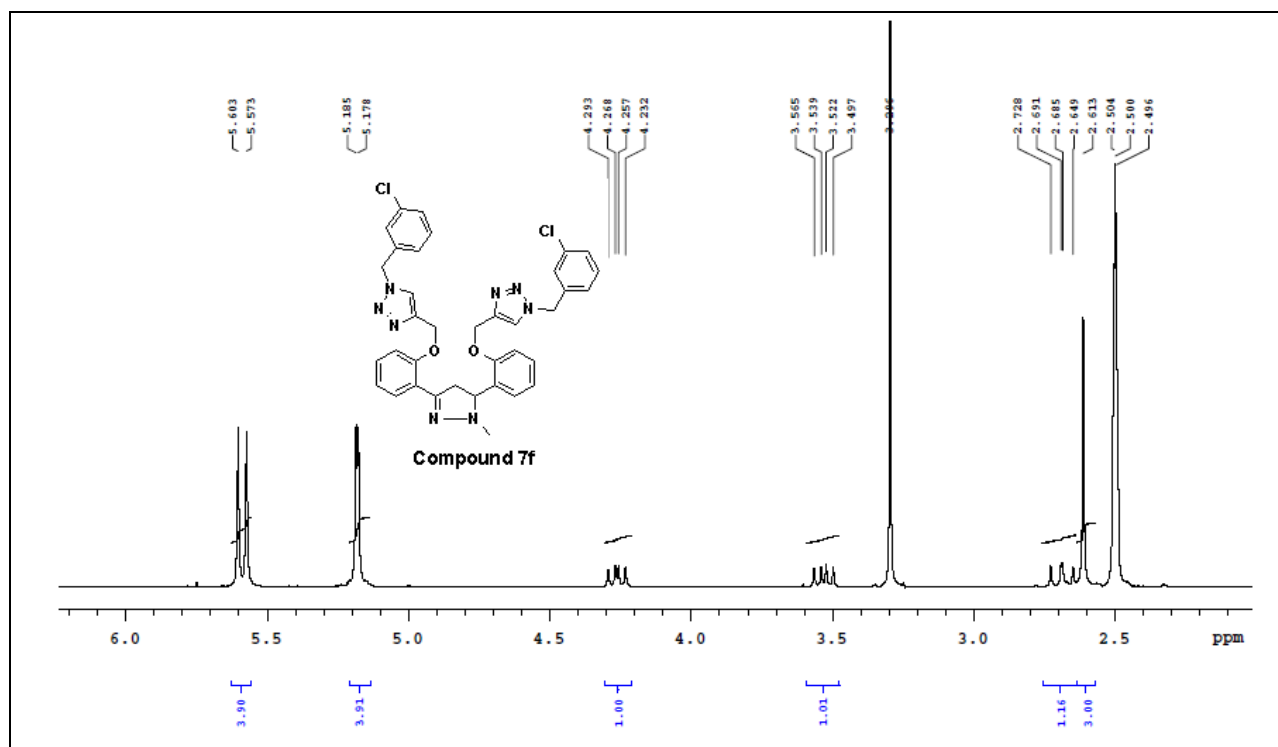


Figure S69: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7f

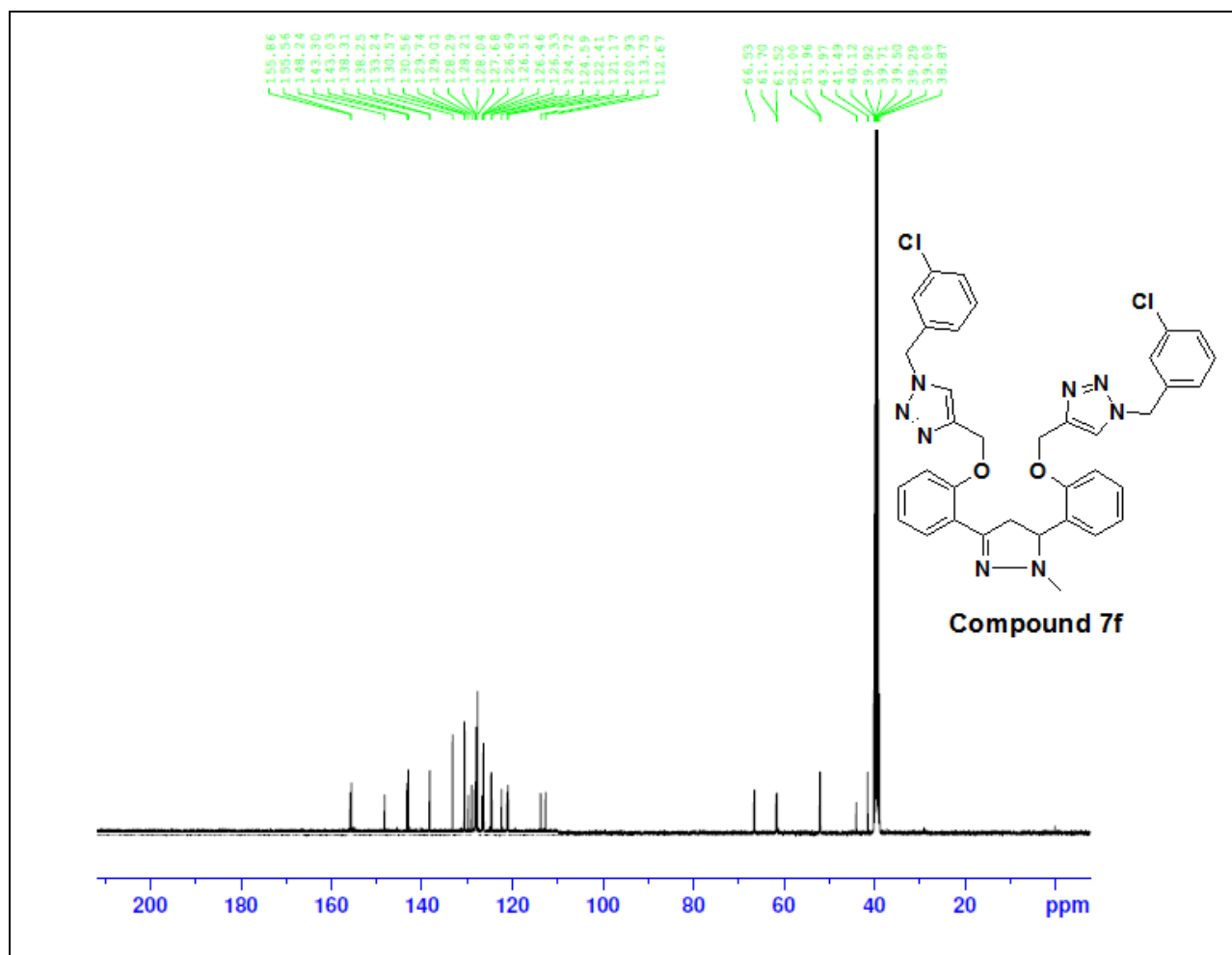


Figure S70: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound **7f**

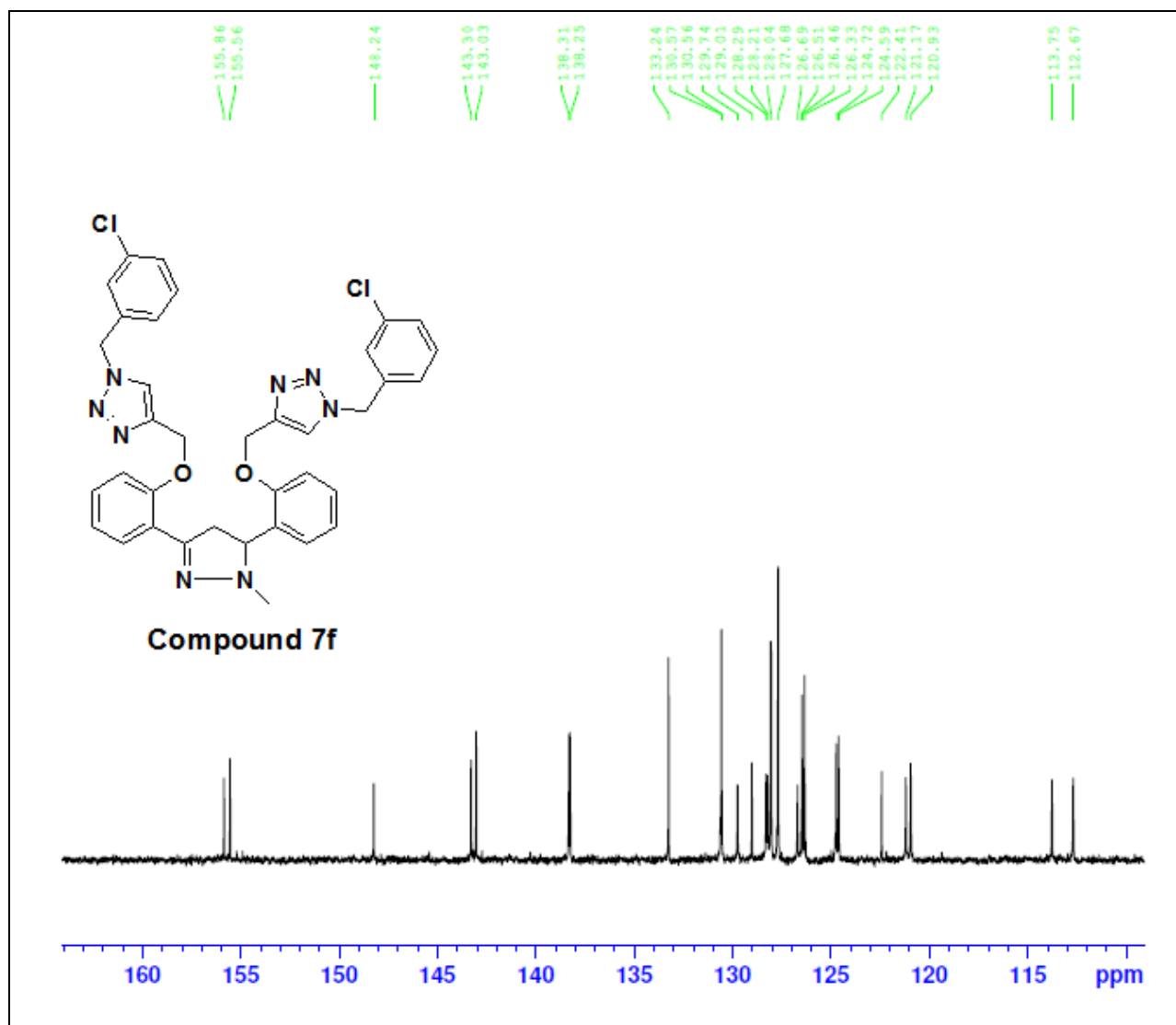


Figure S71: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound 7f

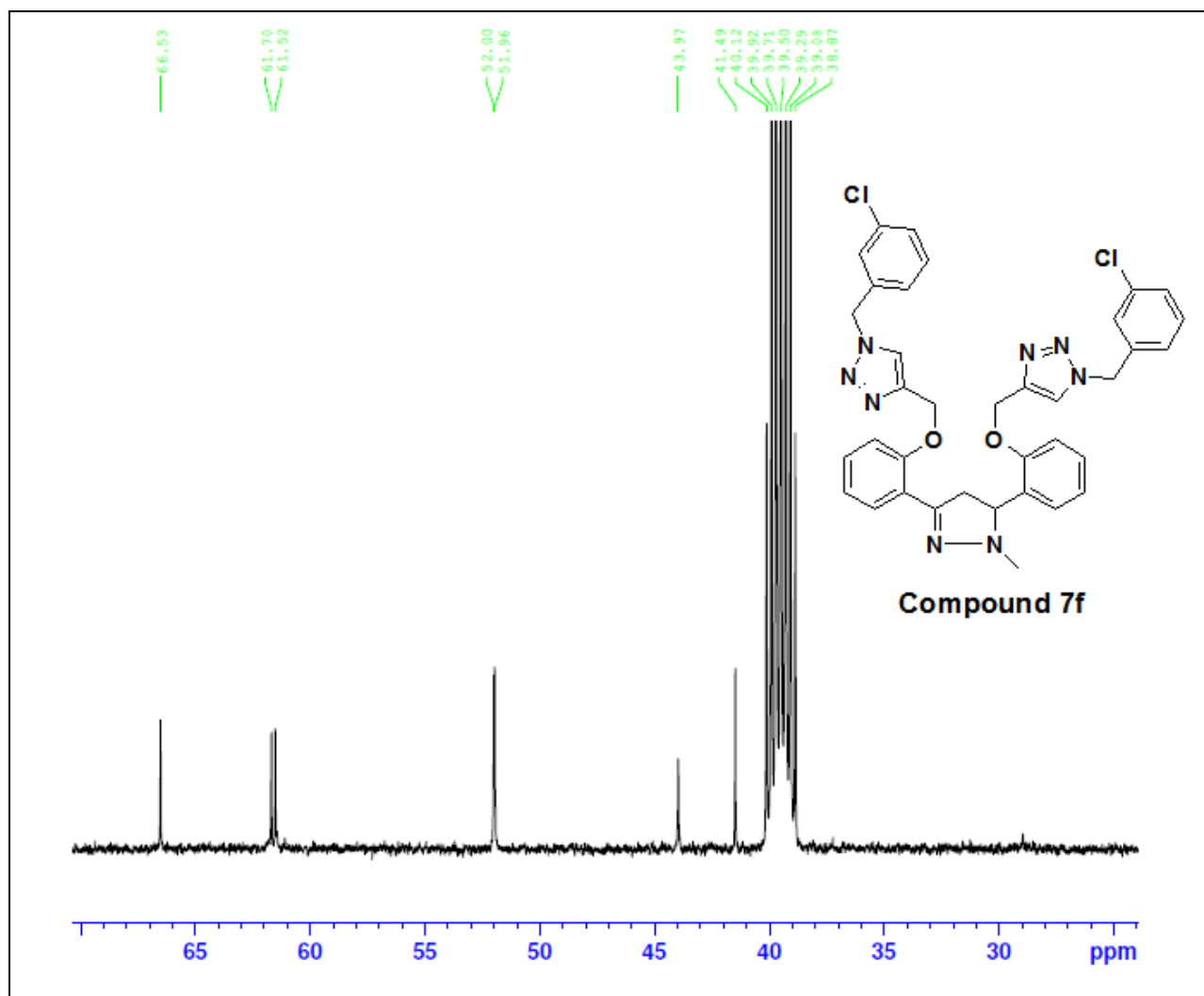


Figure S72: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound 7f

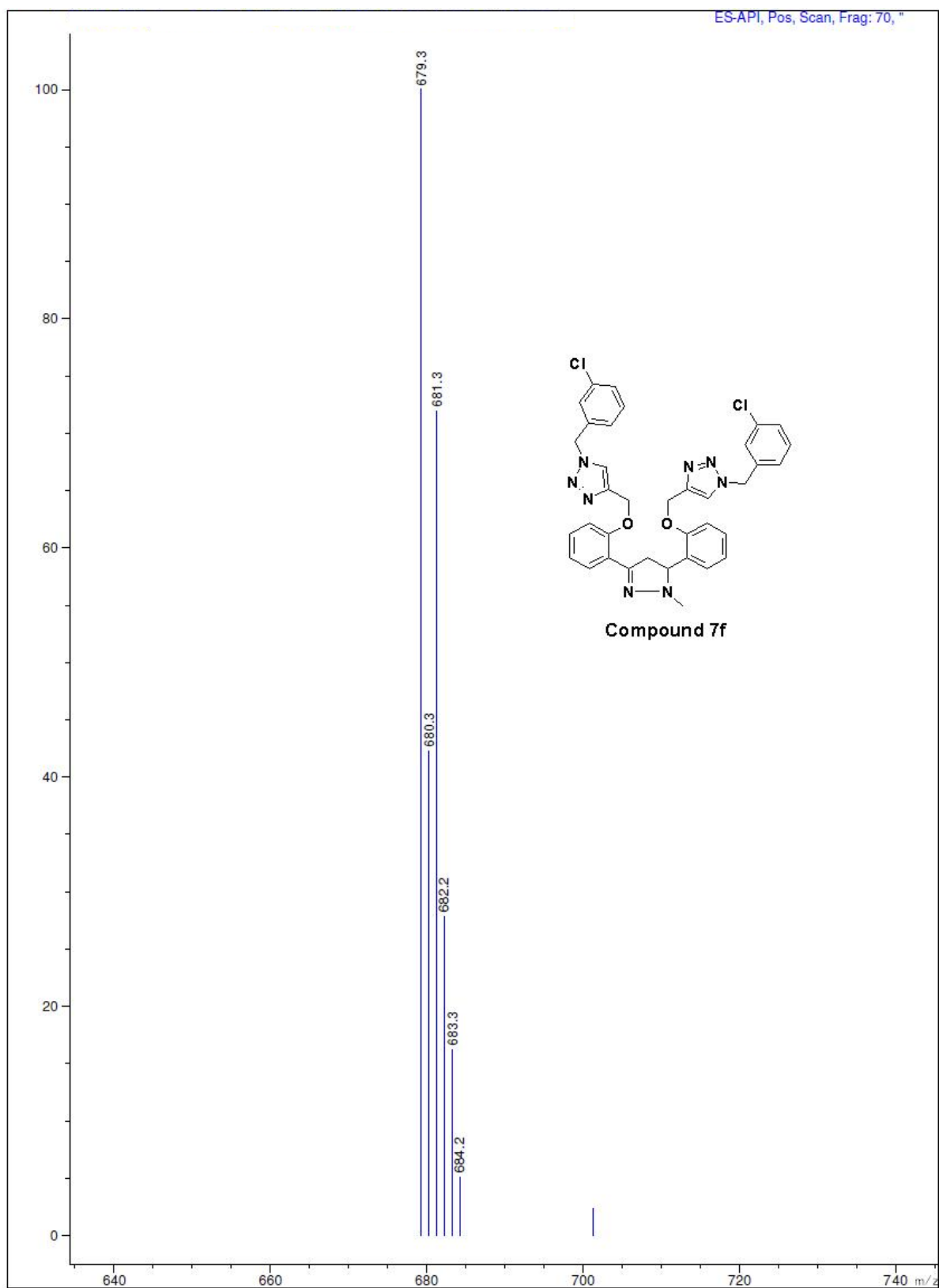


Figure S73: Mass spectra of compound 7f

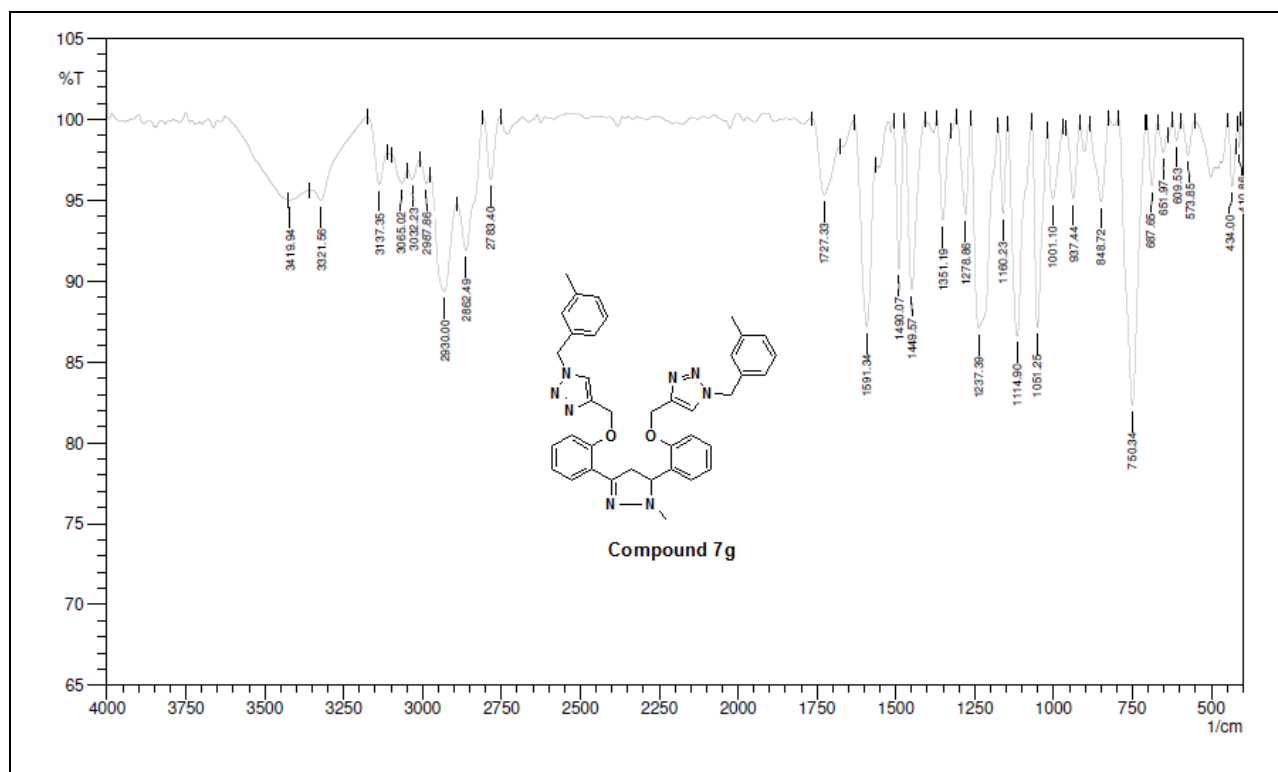


Figure S74: IR spectra of compound 7g

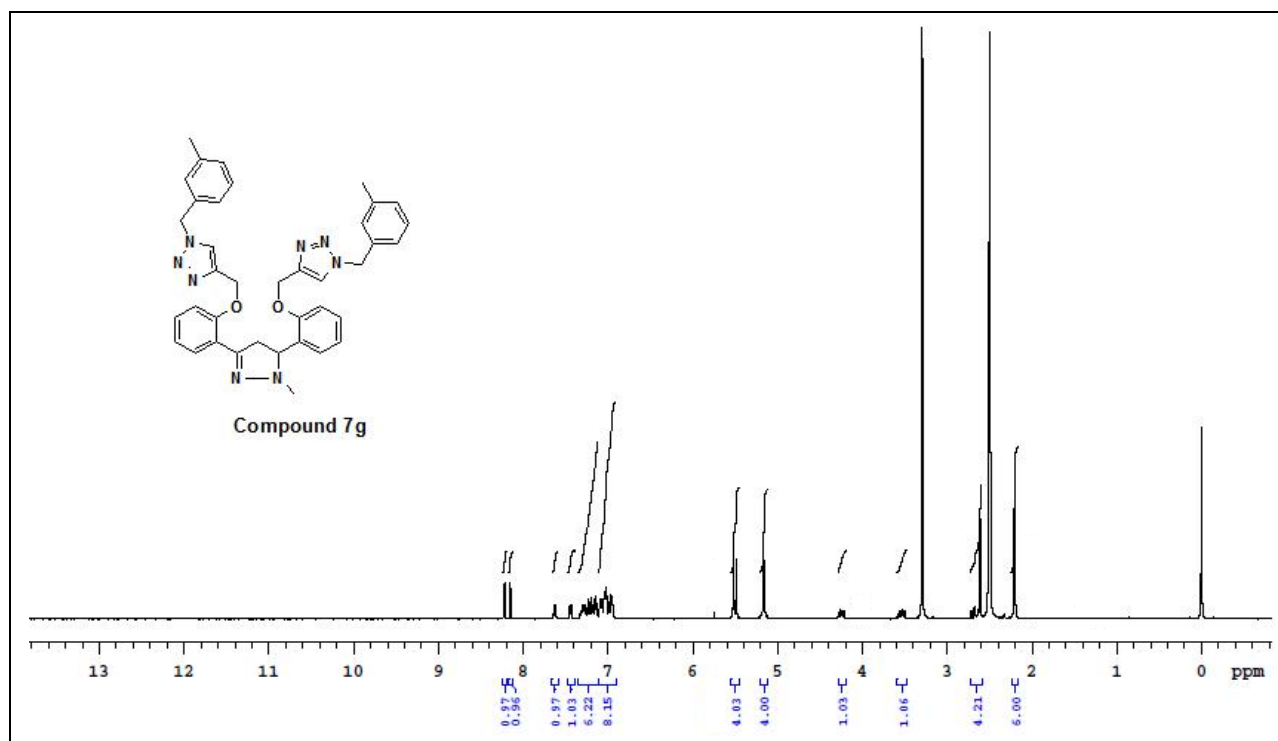


Figure S75: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7g

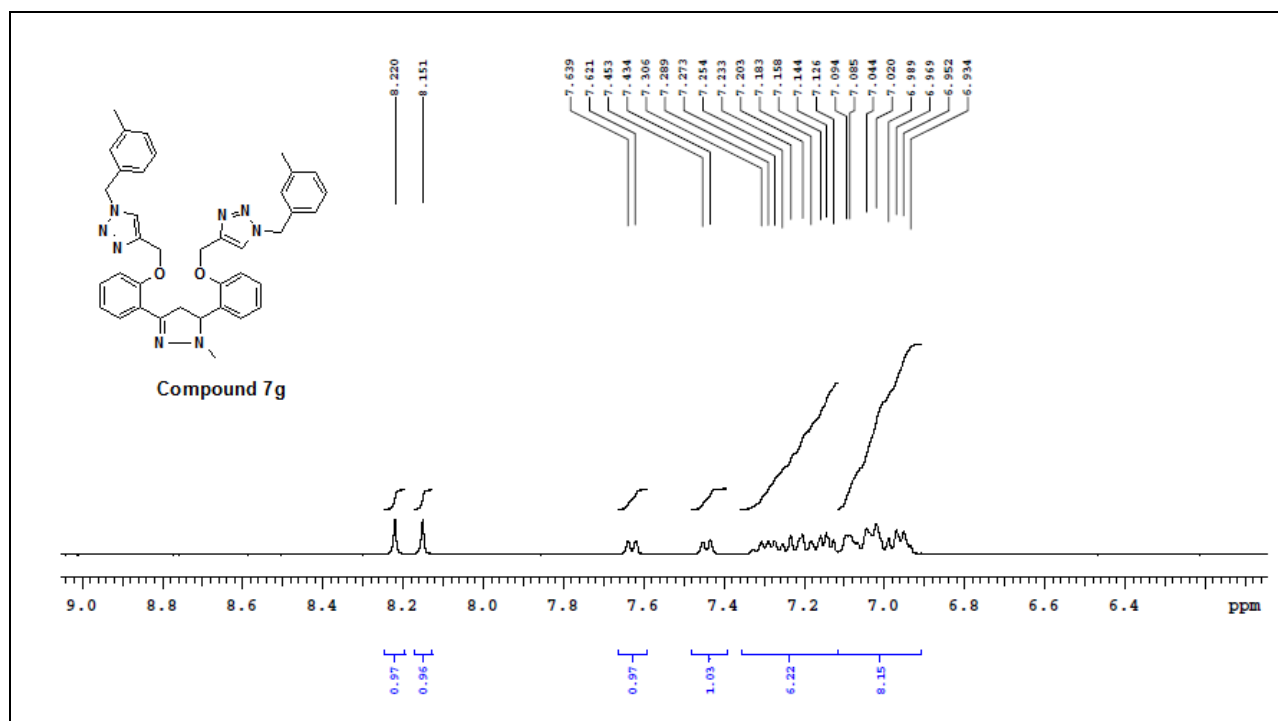


Figure S76: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7g

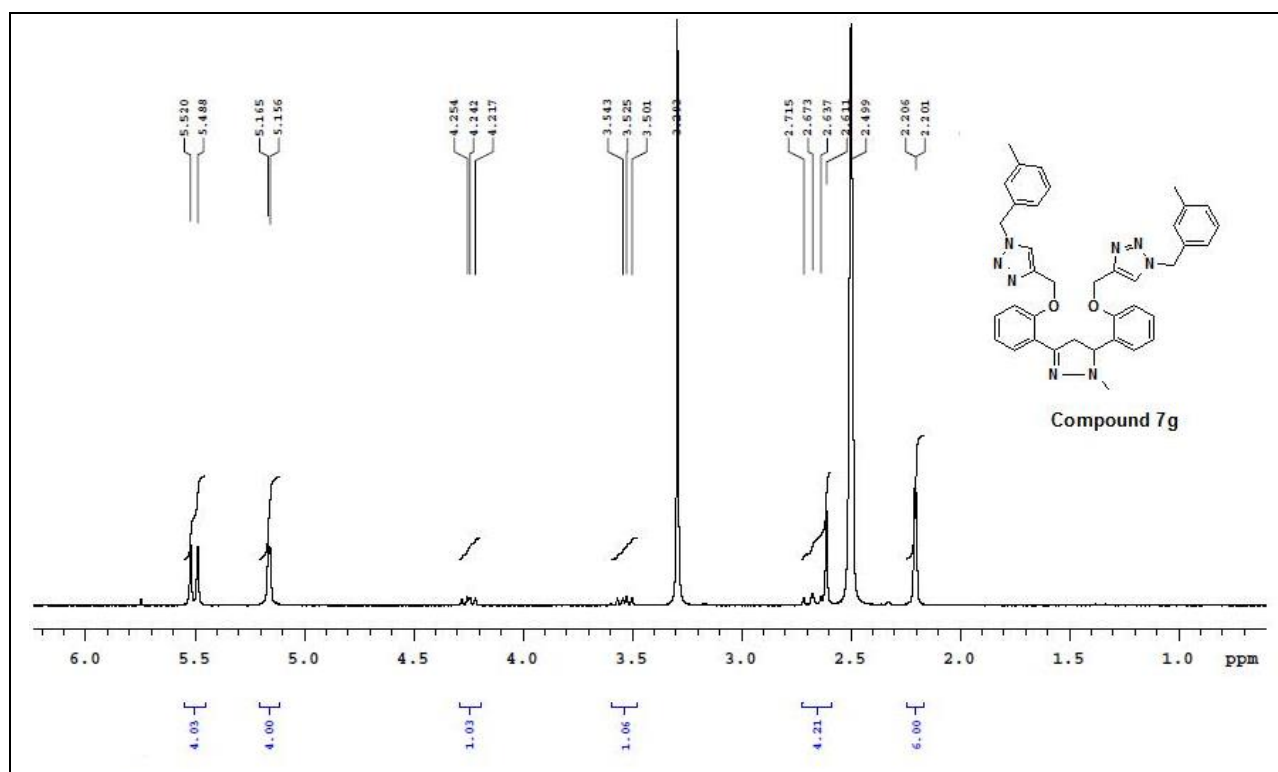


Figure S77: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7g

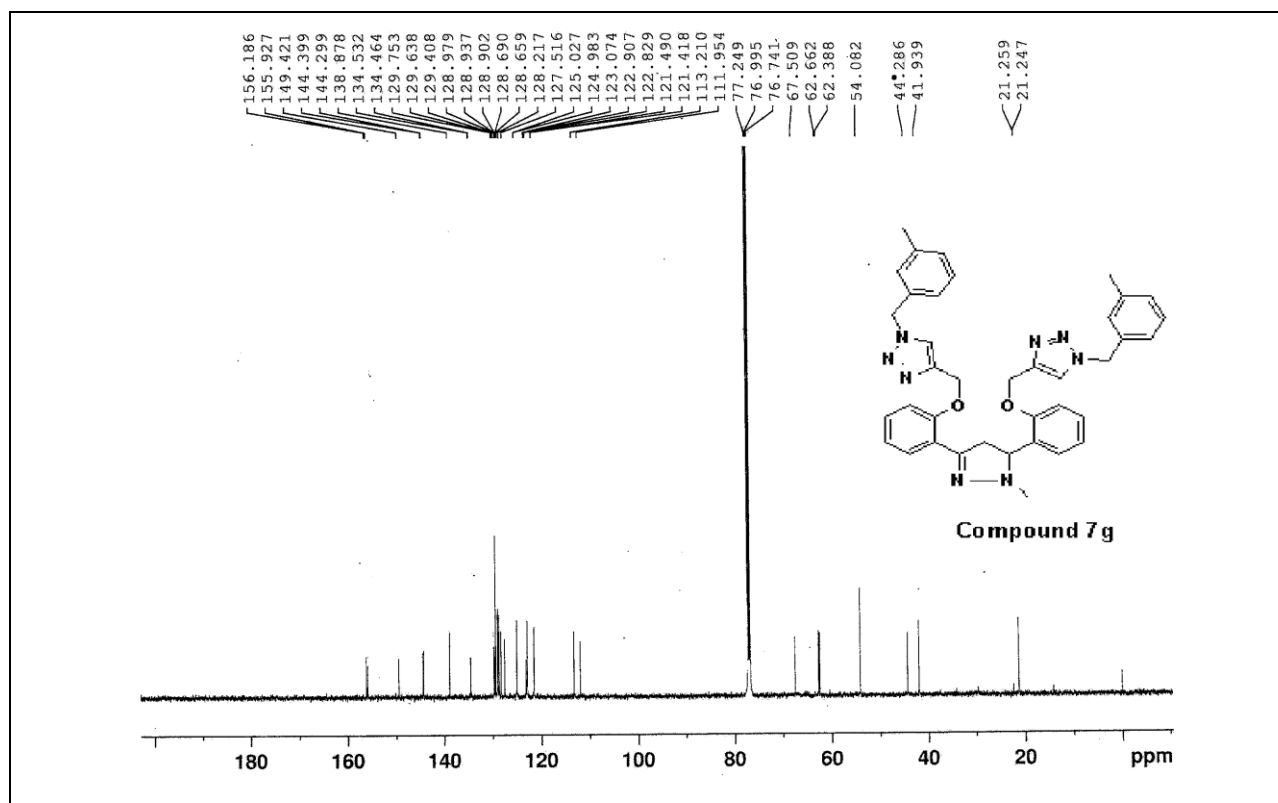


Figure S78: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound **7g**

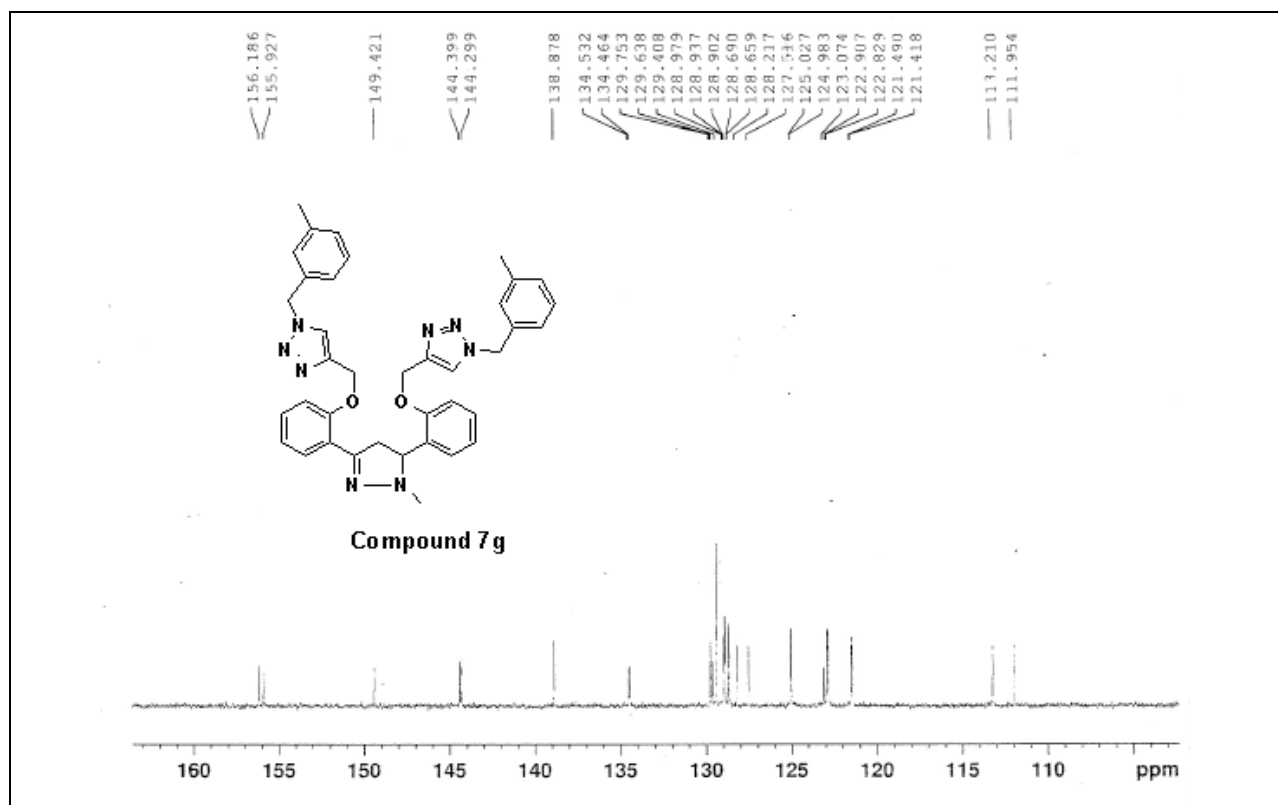


Figure S79: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound **7g**

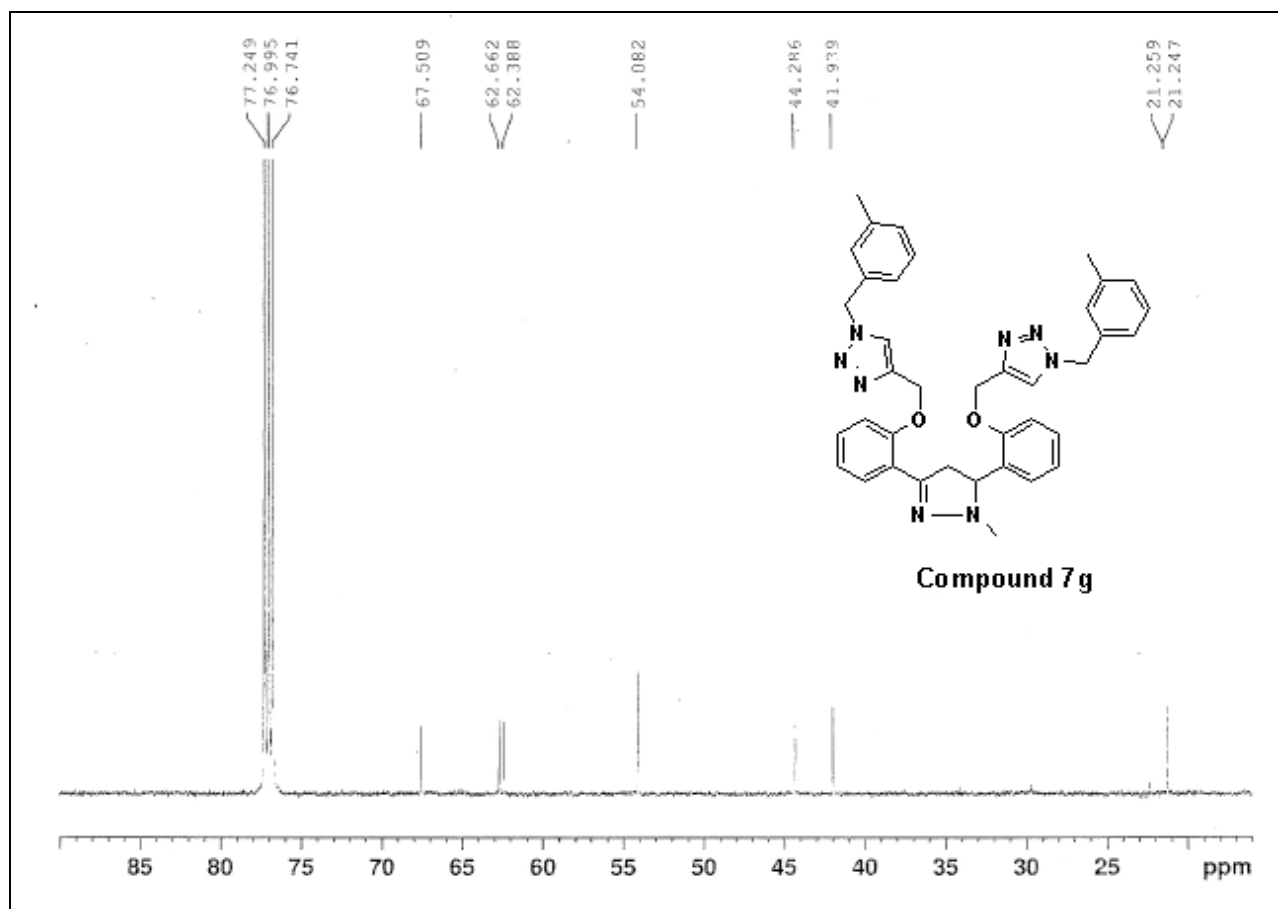


Figure S80: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound **7g**

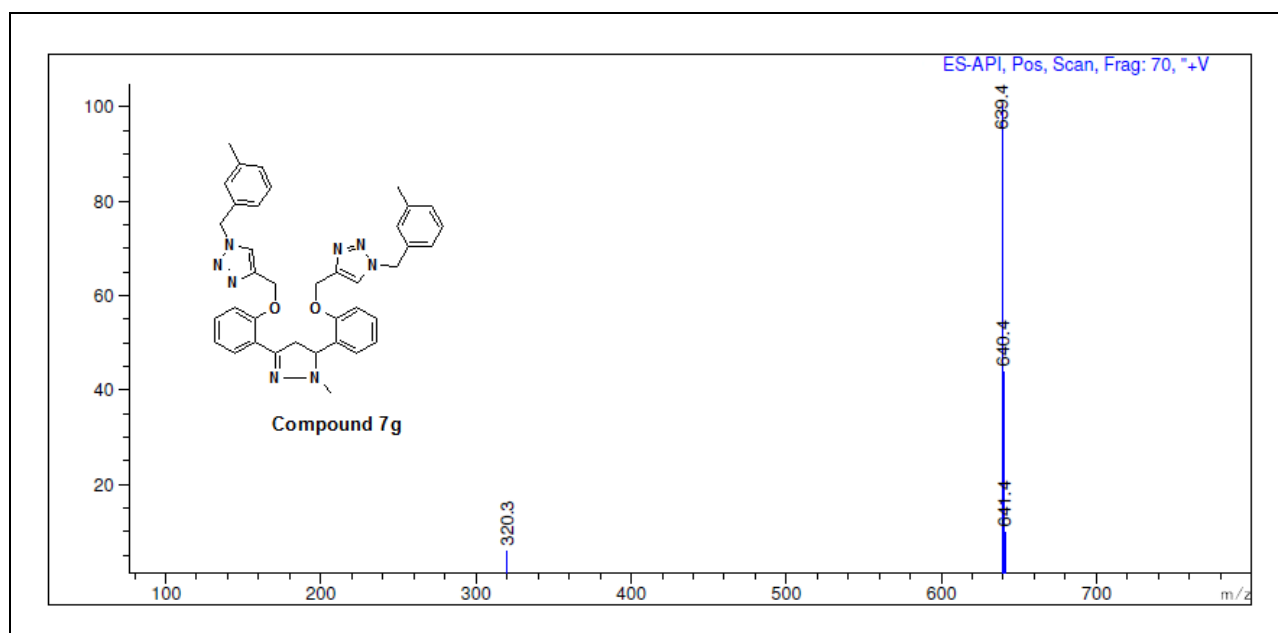


Figure S81: Mass spectra of compound **7g**

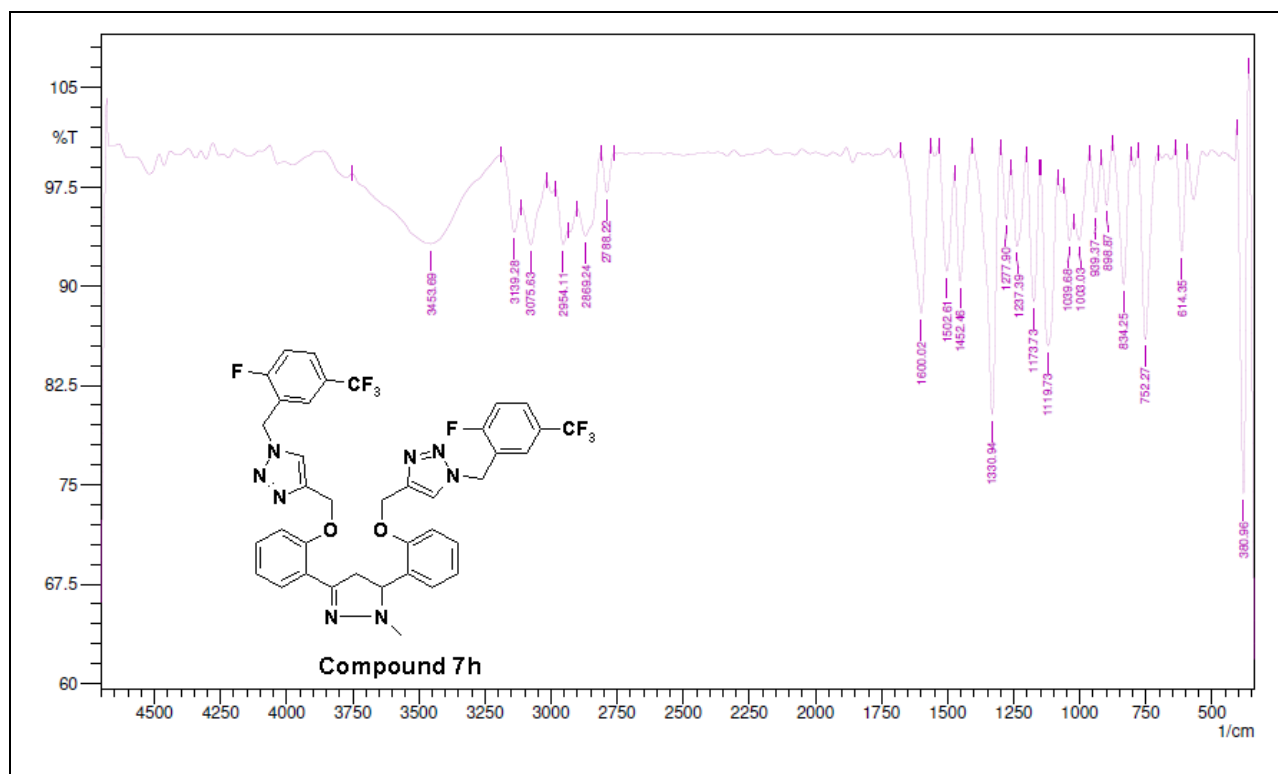


Figure S82: IR spectra of compound 7h

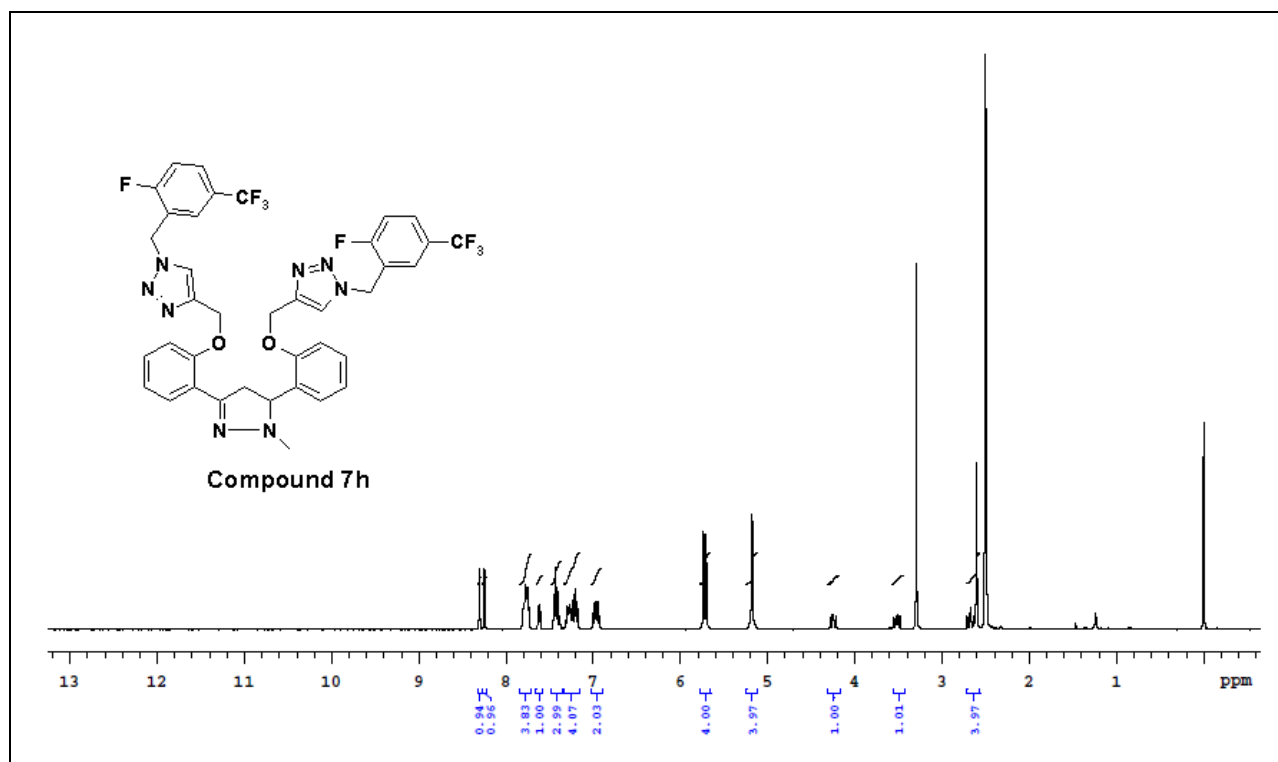


Figure S83: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7h

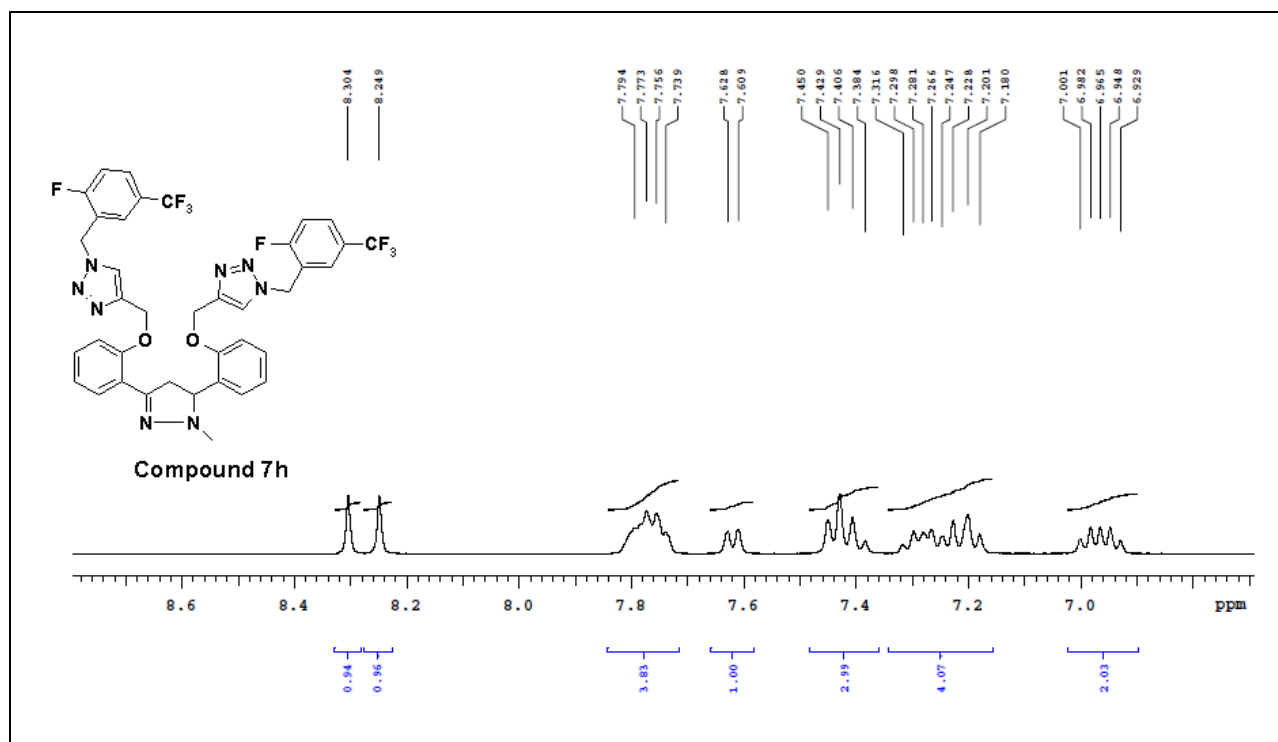


Figure S84: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7h**

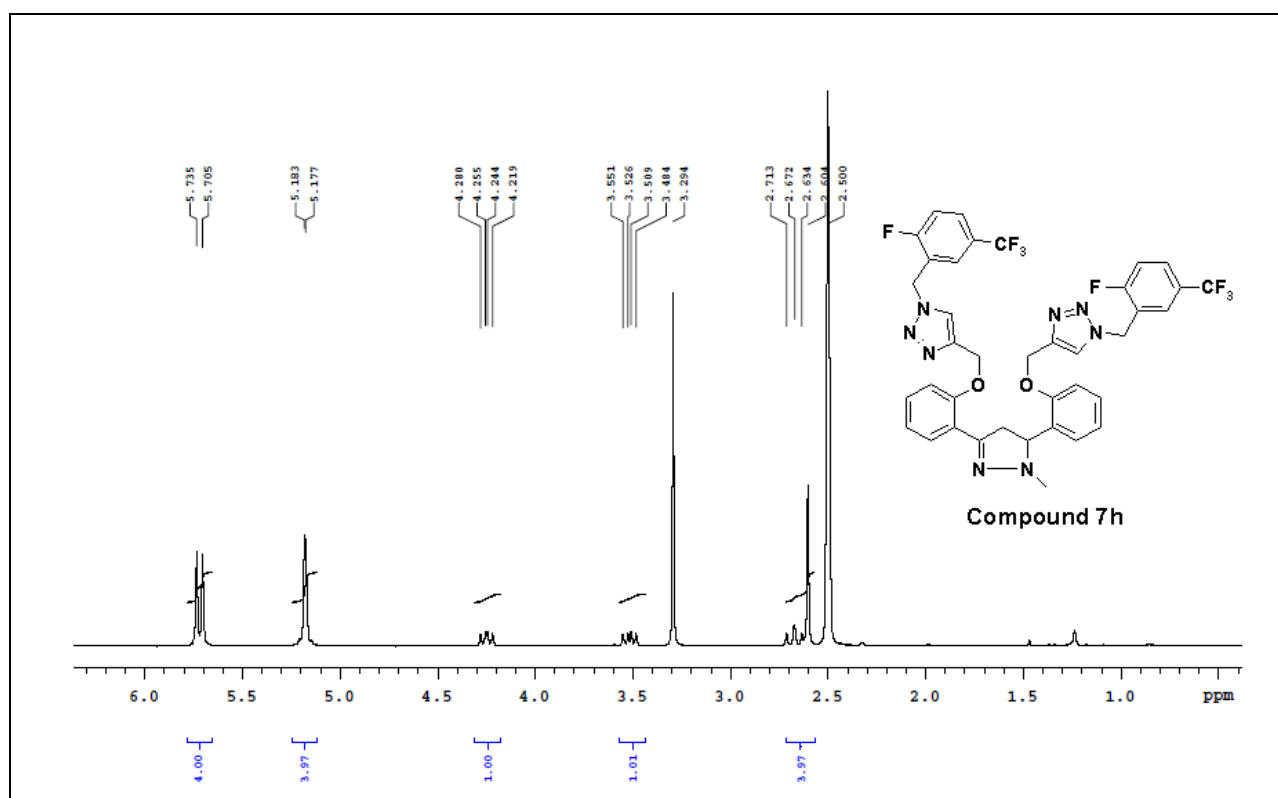


Figure S85: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7h**

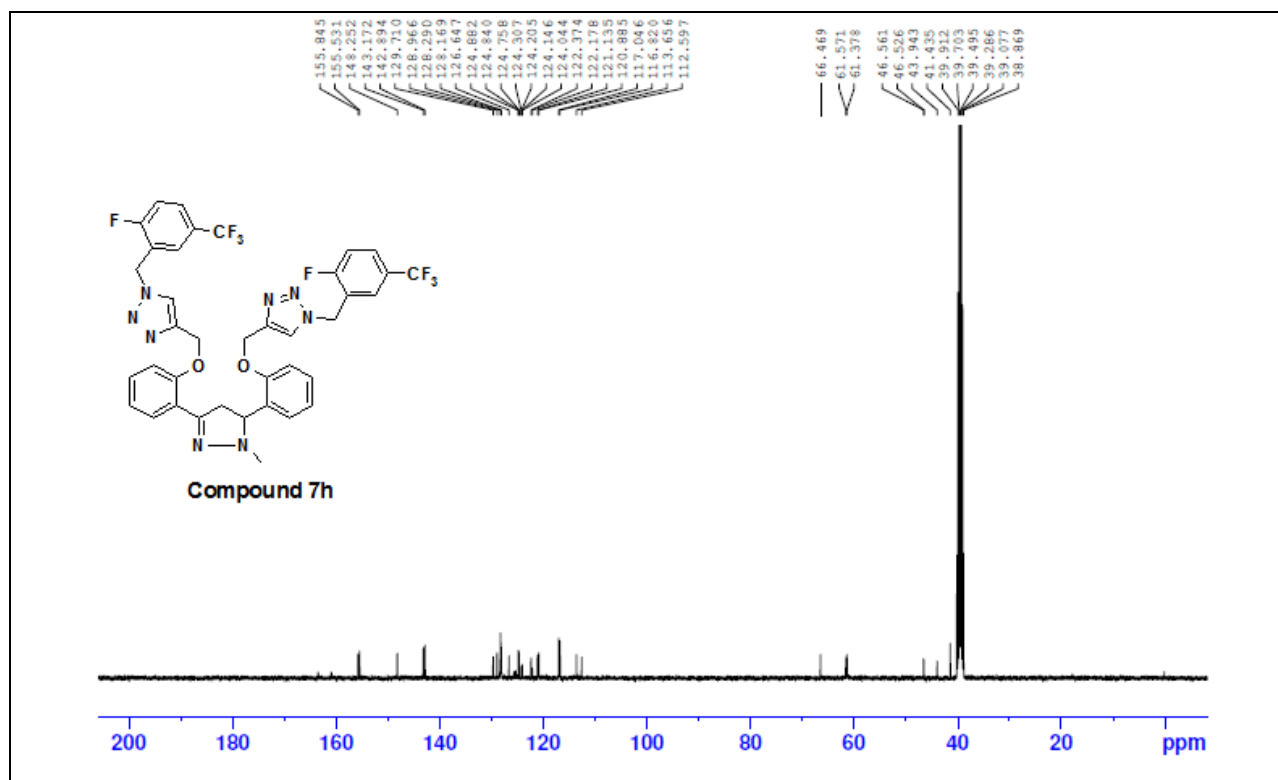


Figure S86: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound **7h**

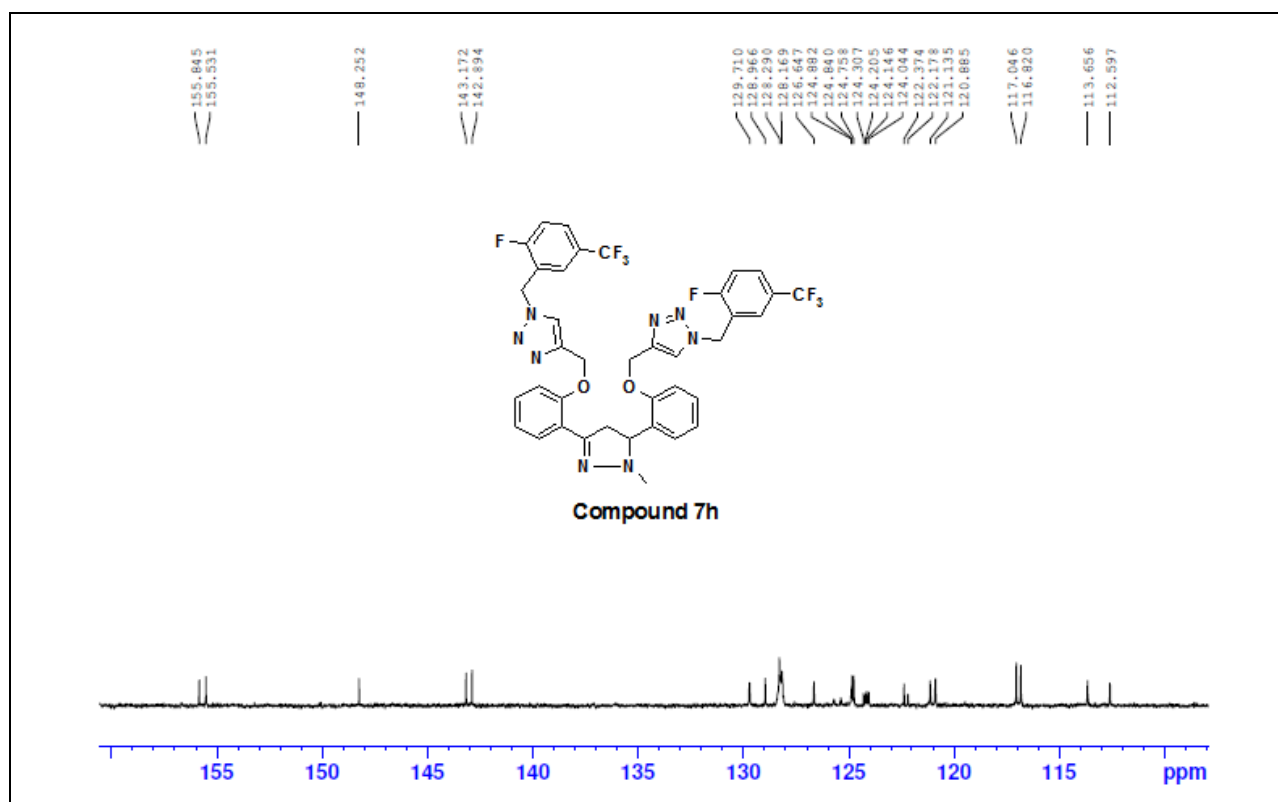


Figure S87: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound **7h**

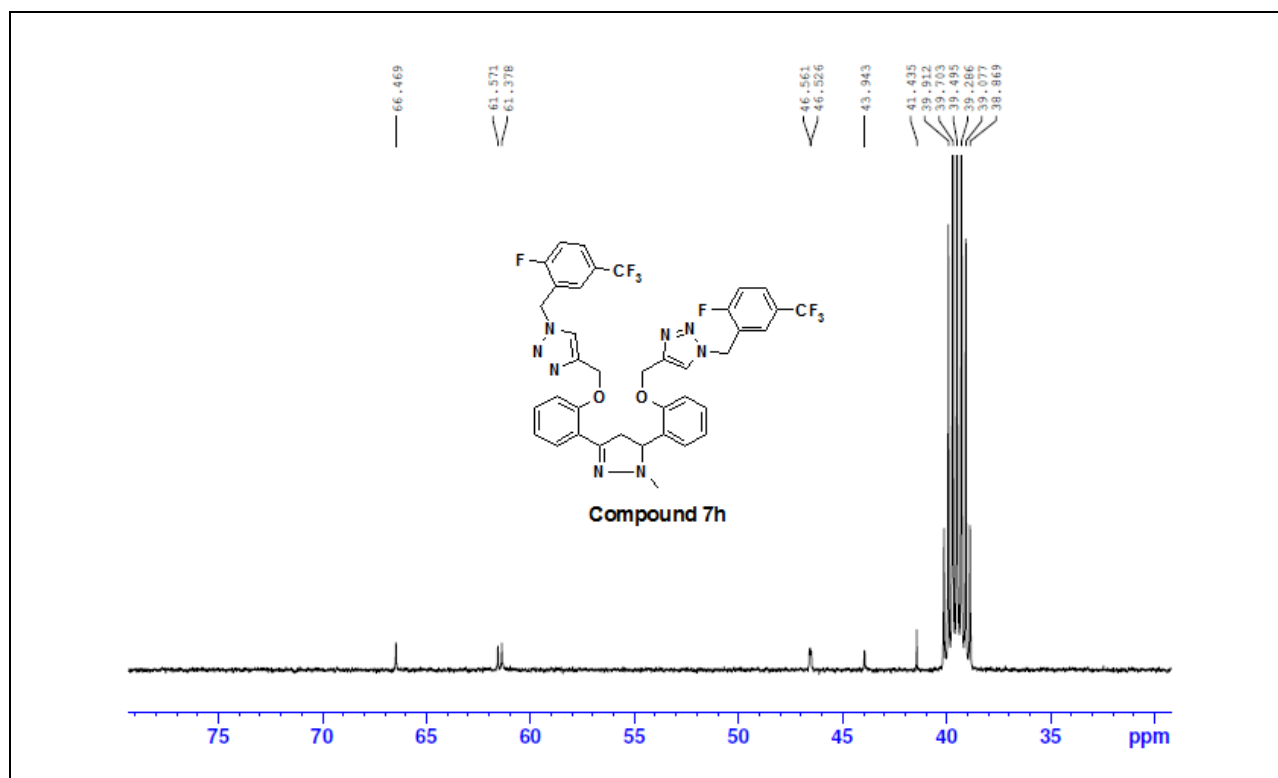


Figure S88: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound **7h**

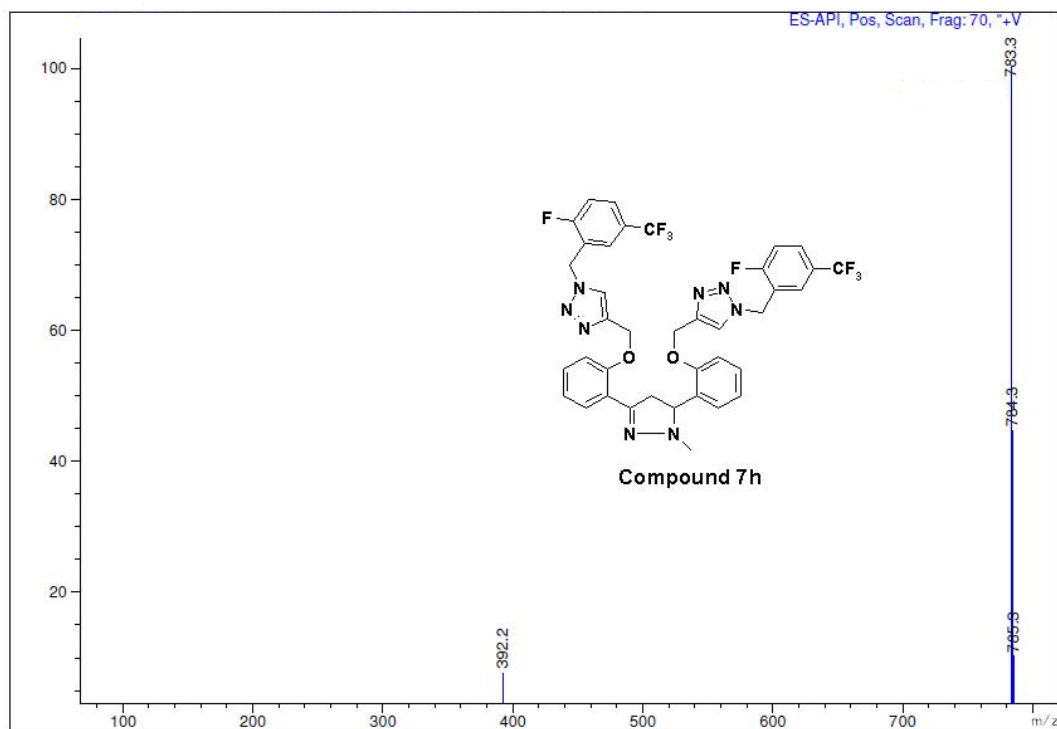


Figure S89: Mass spectra of compound **7h**

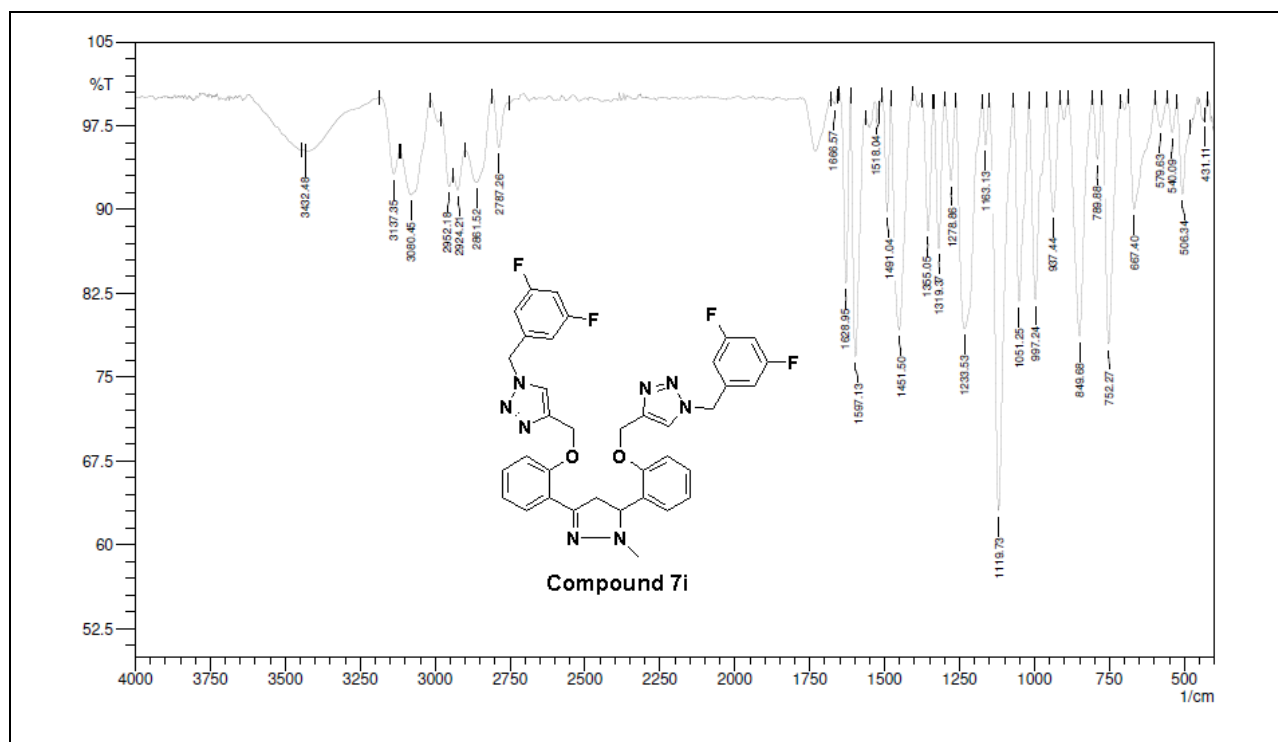


Figure S90: IR spectra of compound 7i

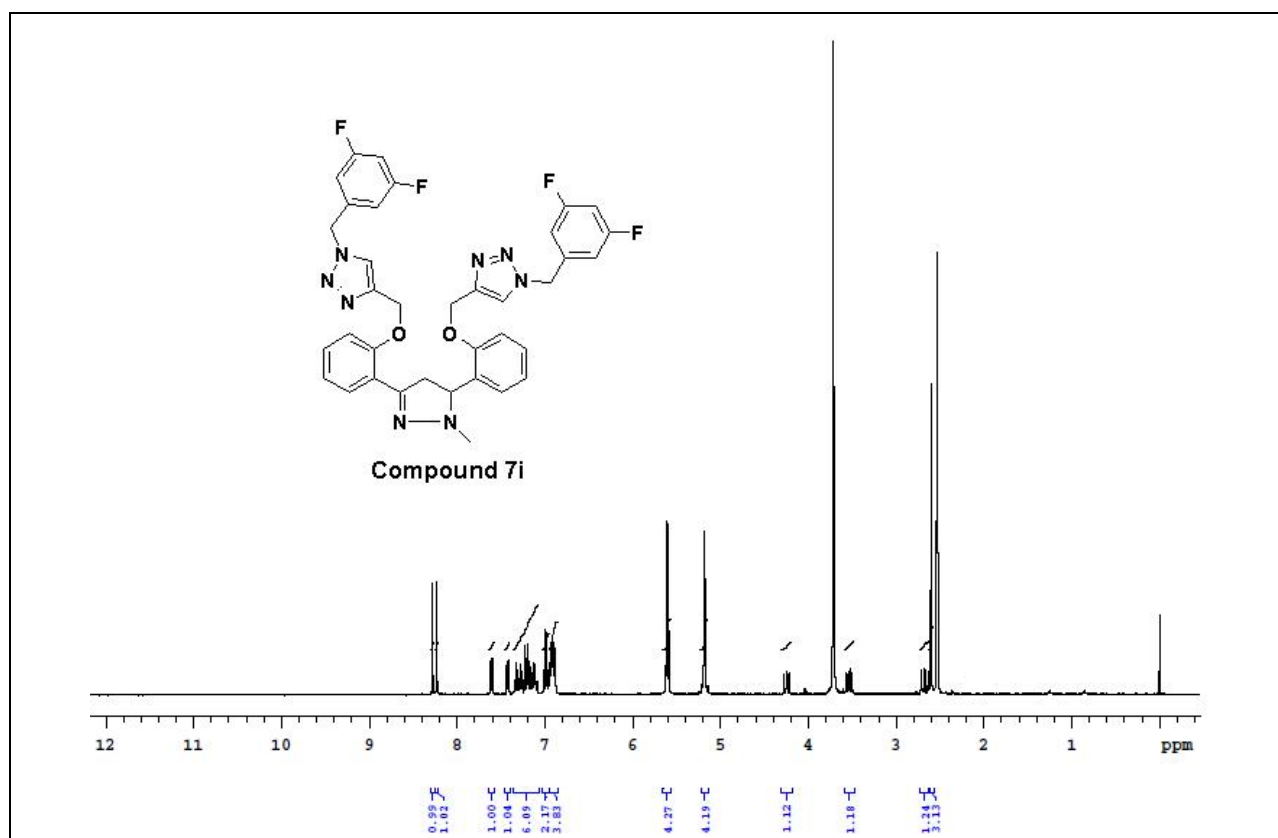


Figure S91: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7i

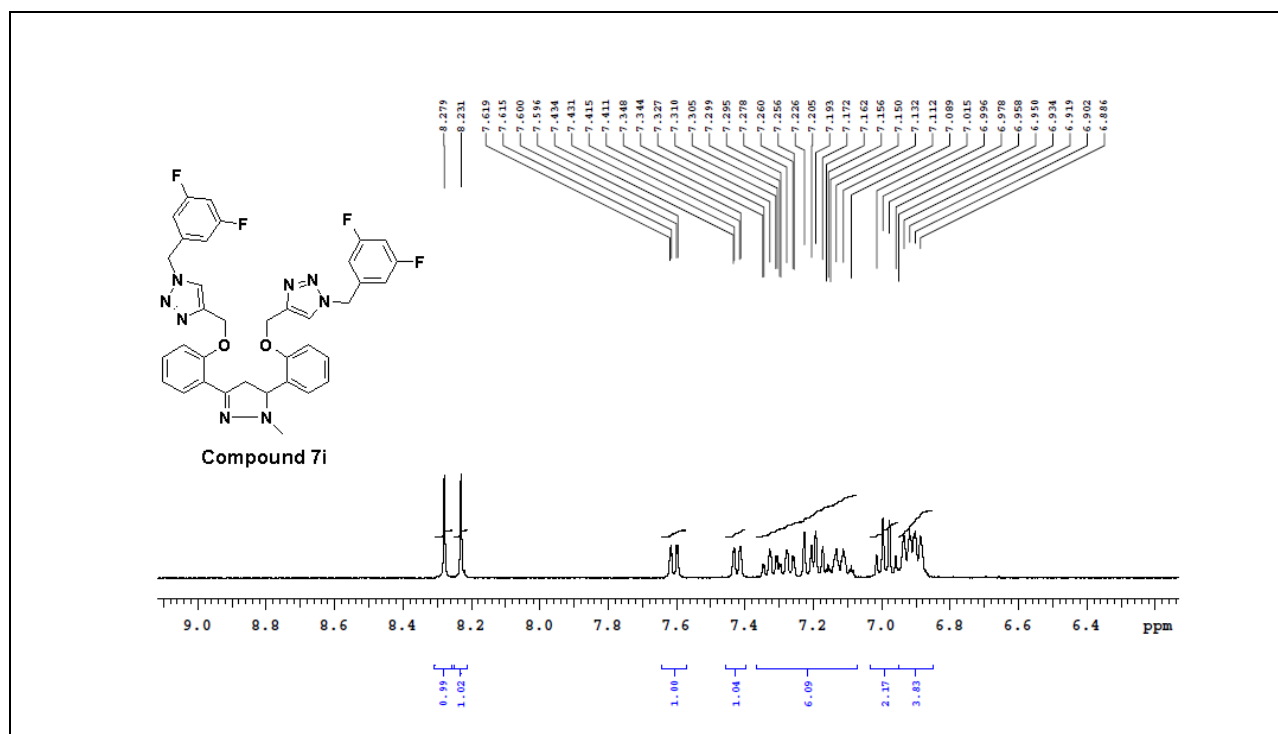


Figure S92: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7i

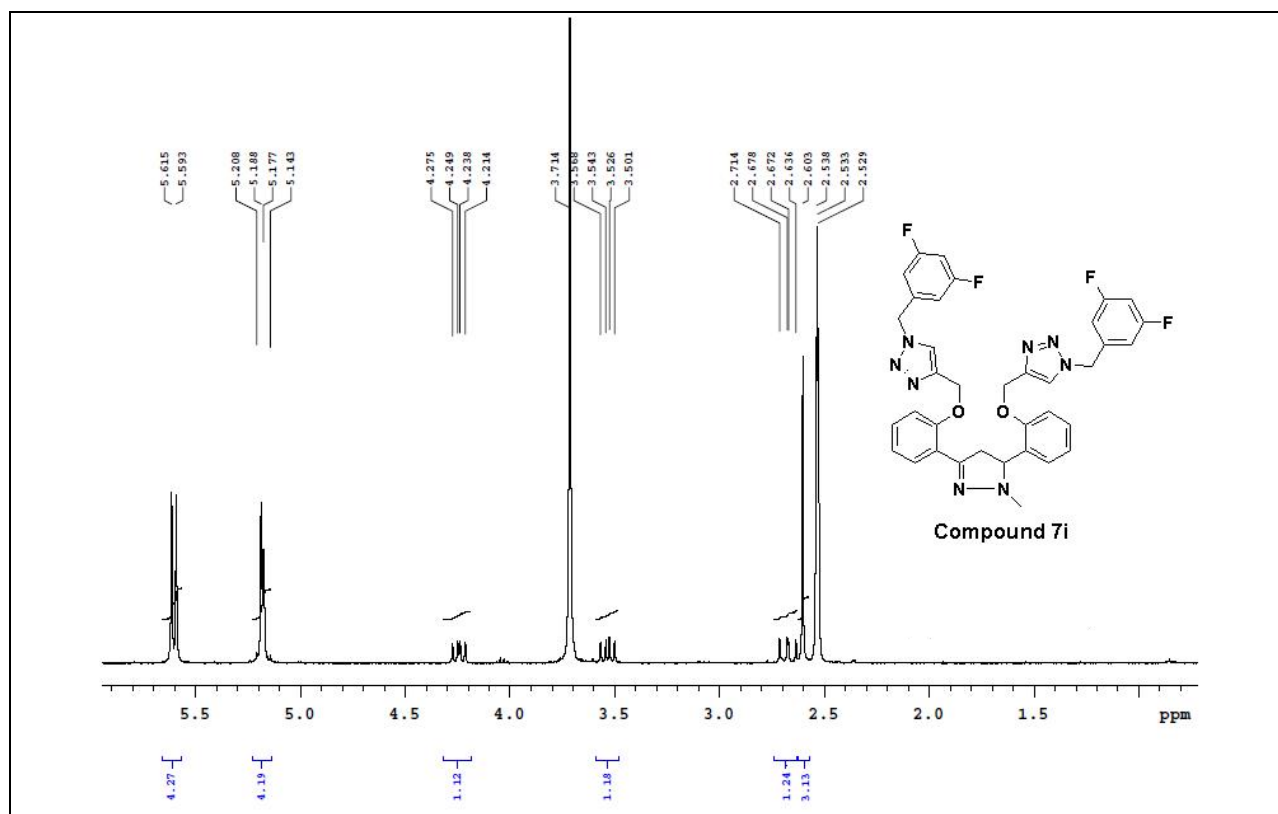


Figure S93: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7i

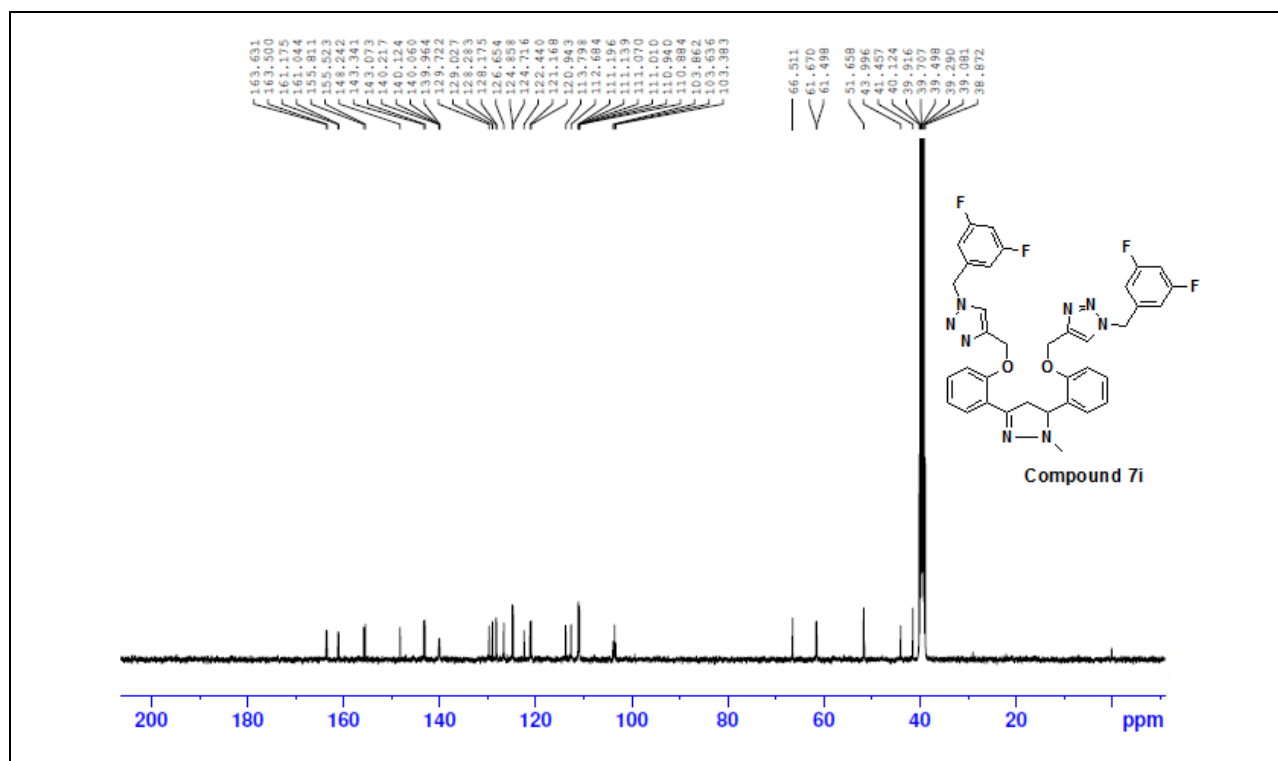


Figure S94: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound 7i

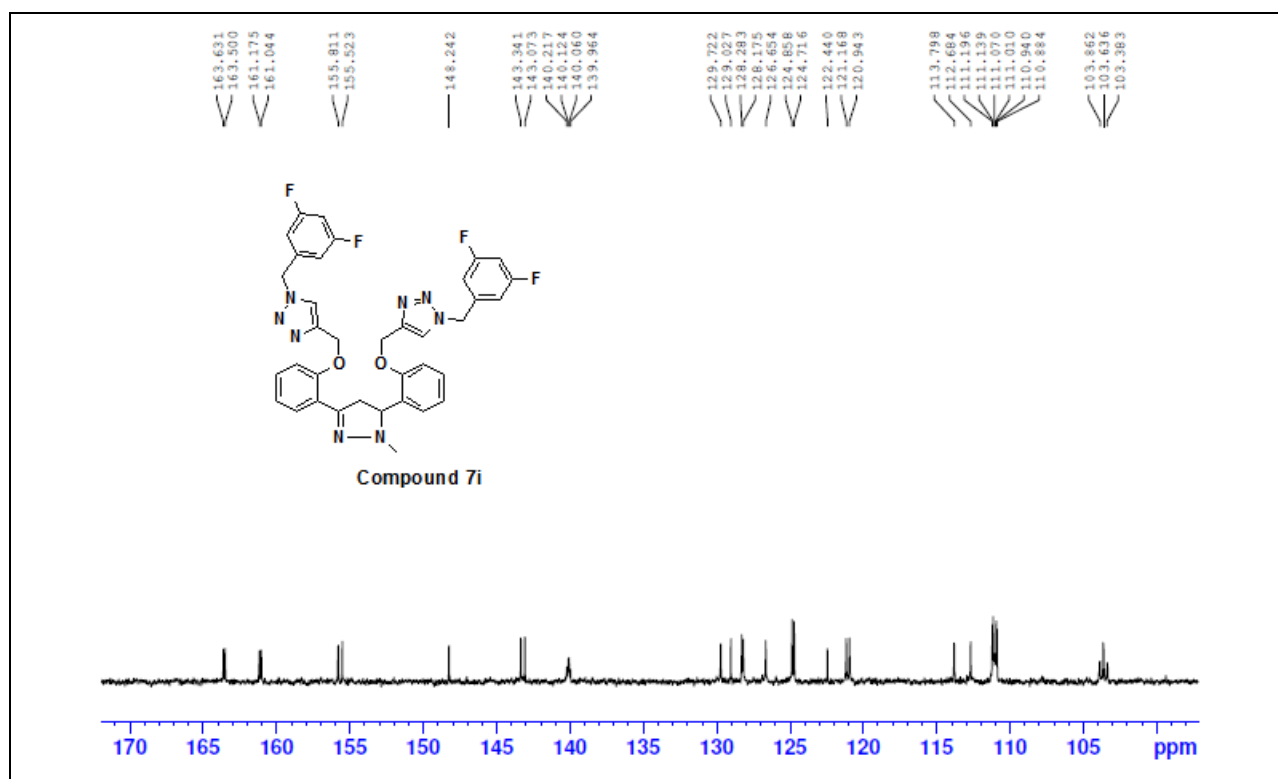


Figure S95: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound 7i

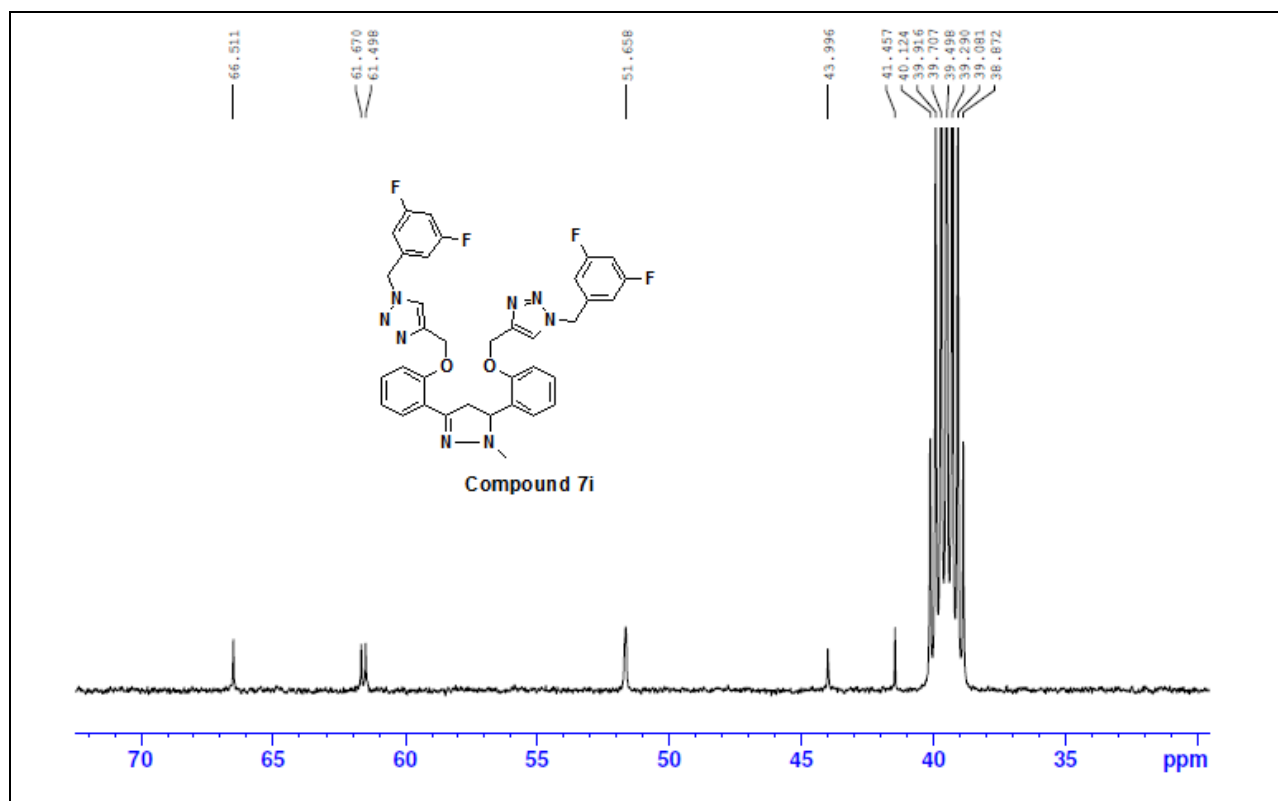


Figure S96: ¹³C NMR (100 MHz, DMSO-d₆) spectra of compound **7i**

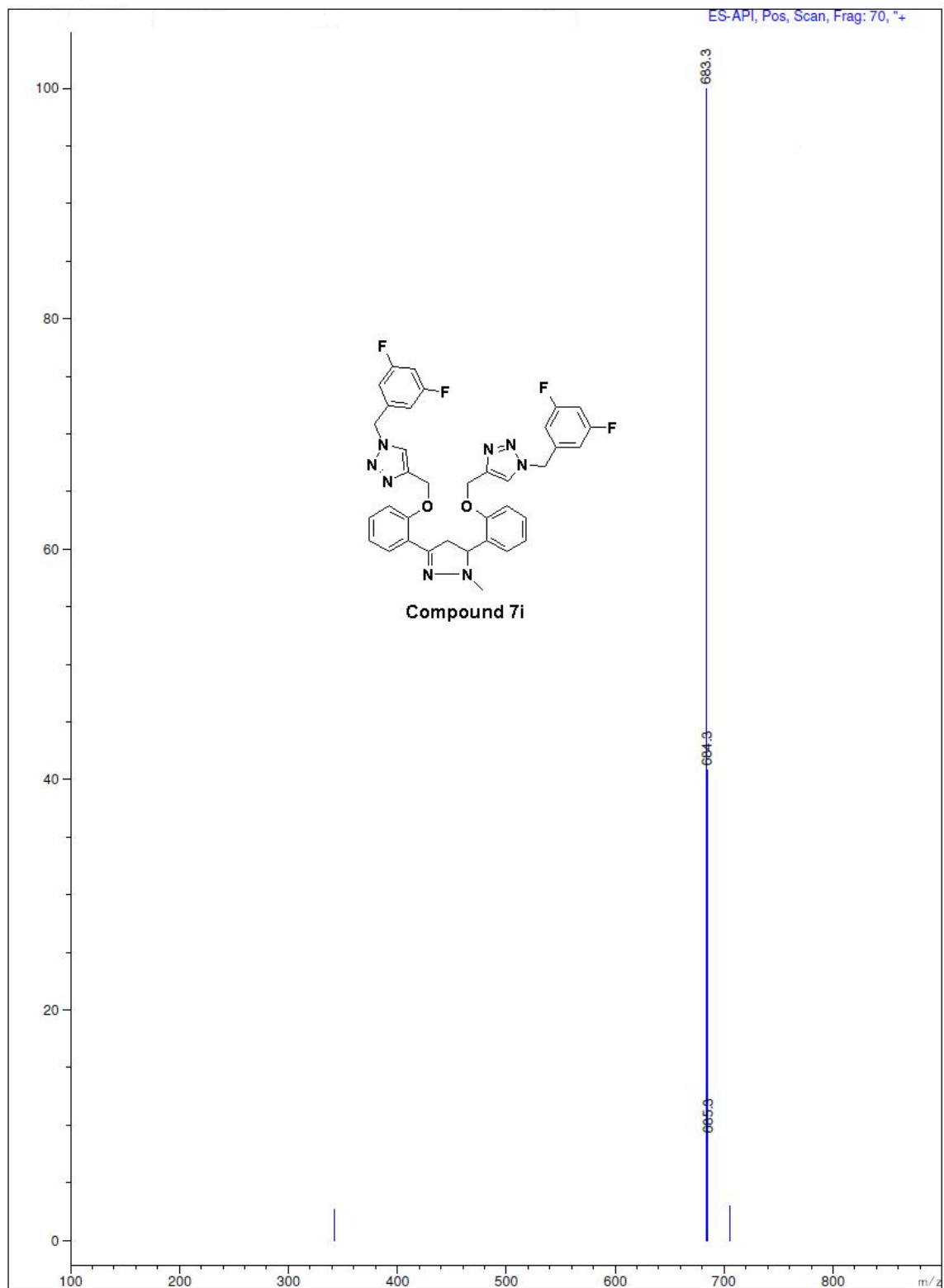


Figure S97: Mass spectra of compound 7i

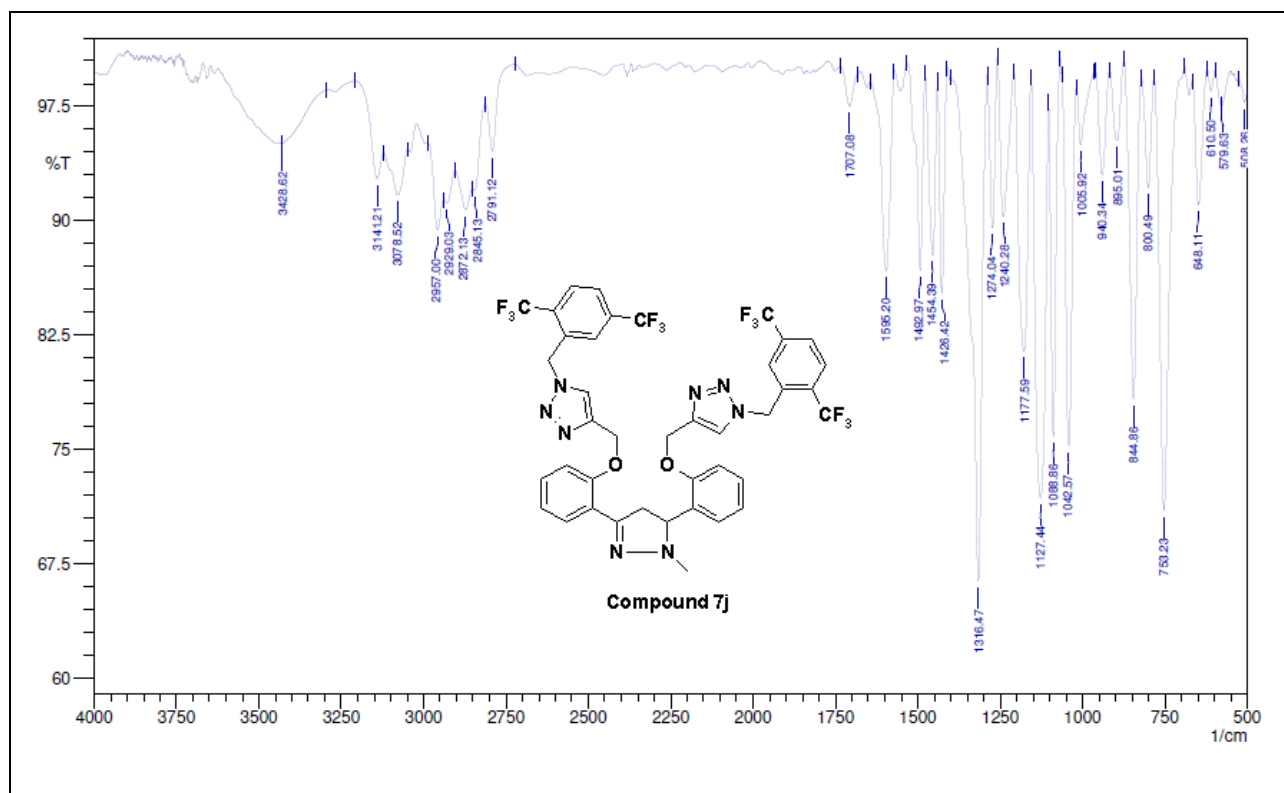


Figure S98: IR spectra of compound 7j

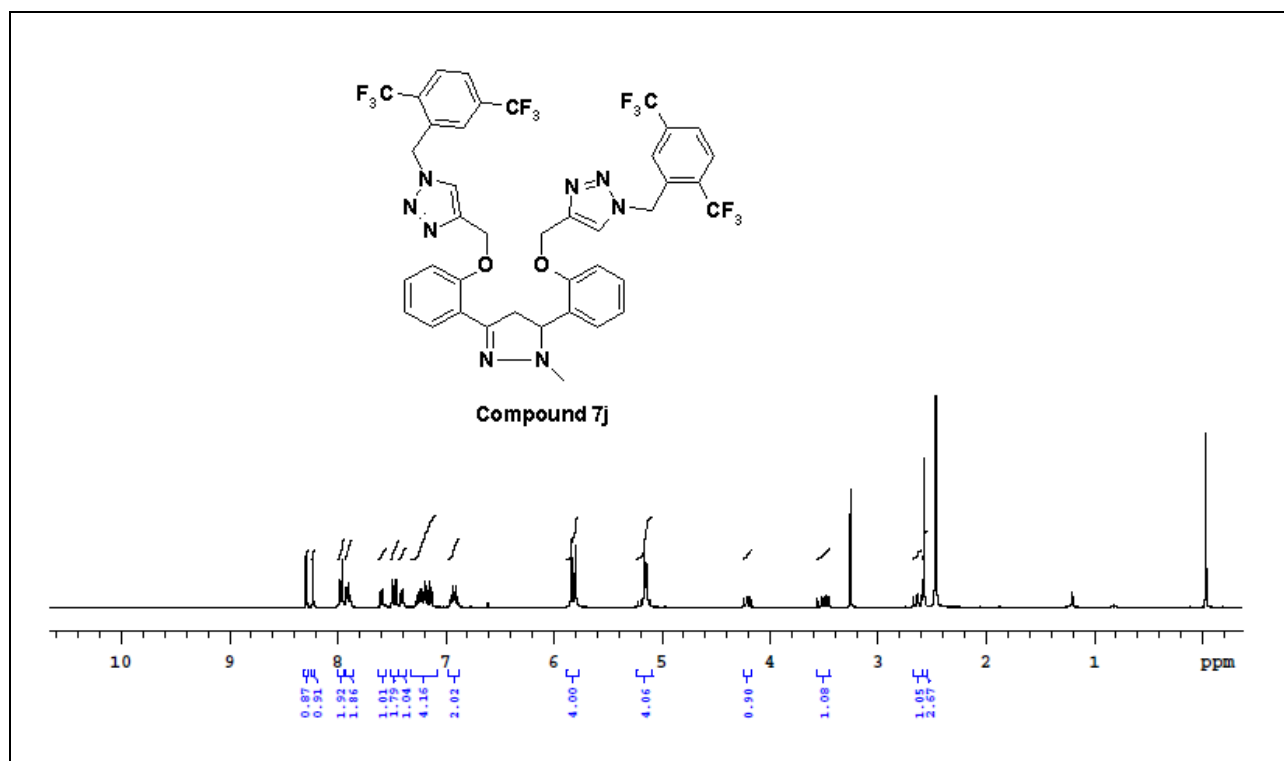


Figure S99: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound 7j

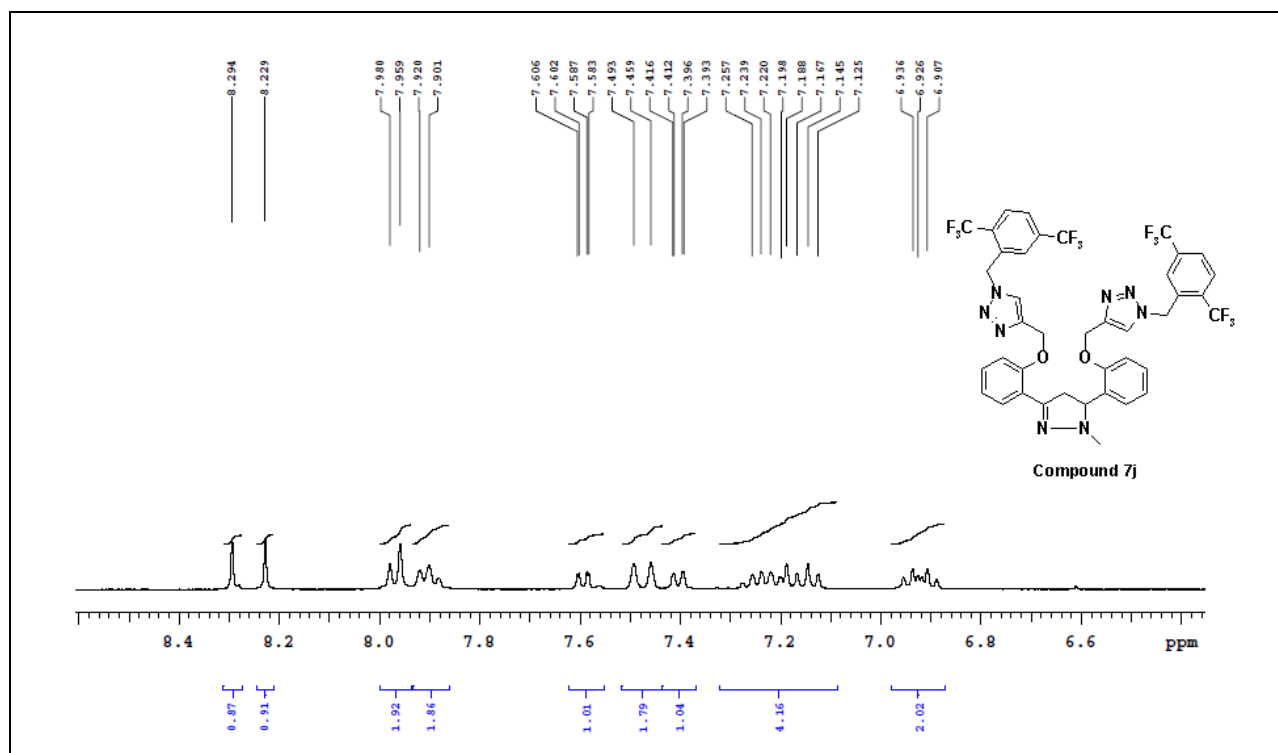


Figure S100: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7j

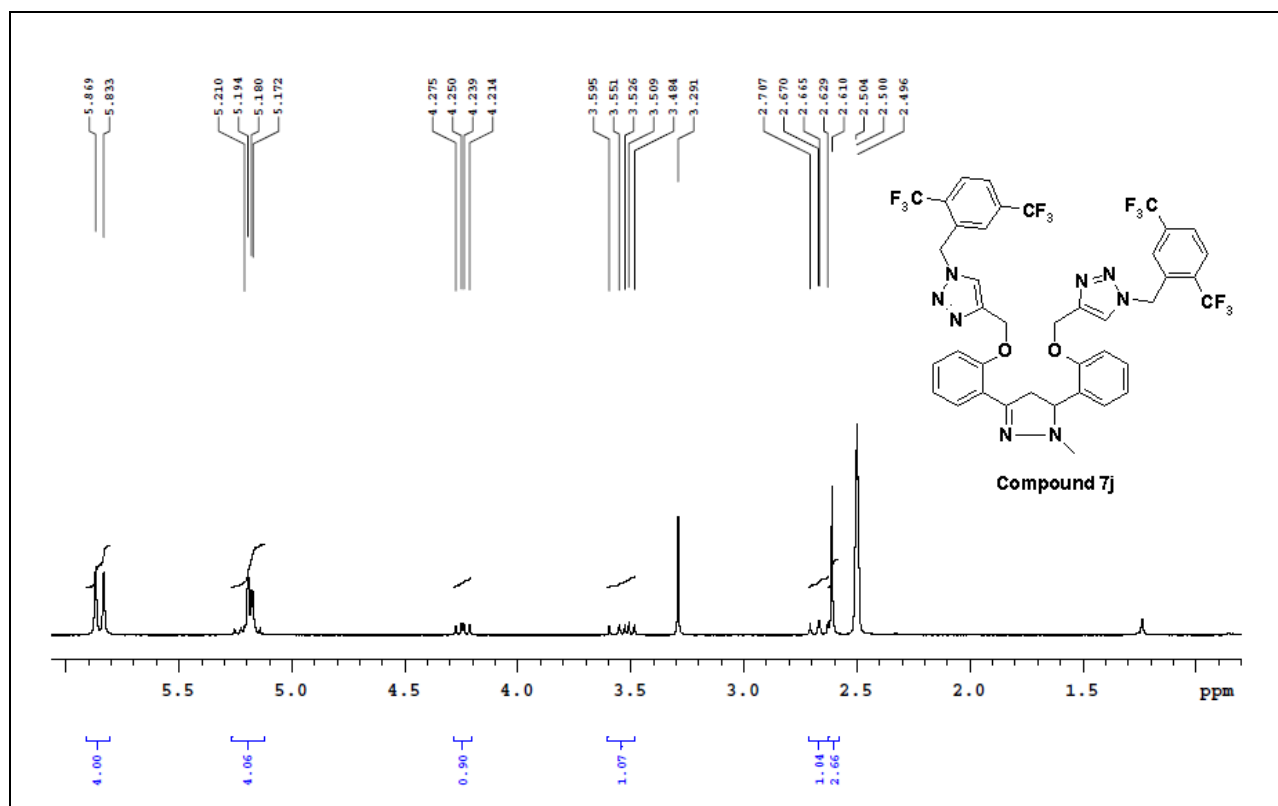


Figure S101: ¹H-NMR (400 MHz, DMSO-d₆) spectra of compound 7j

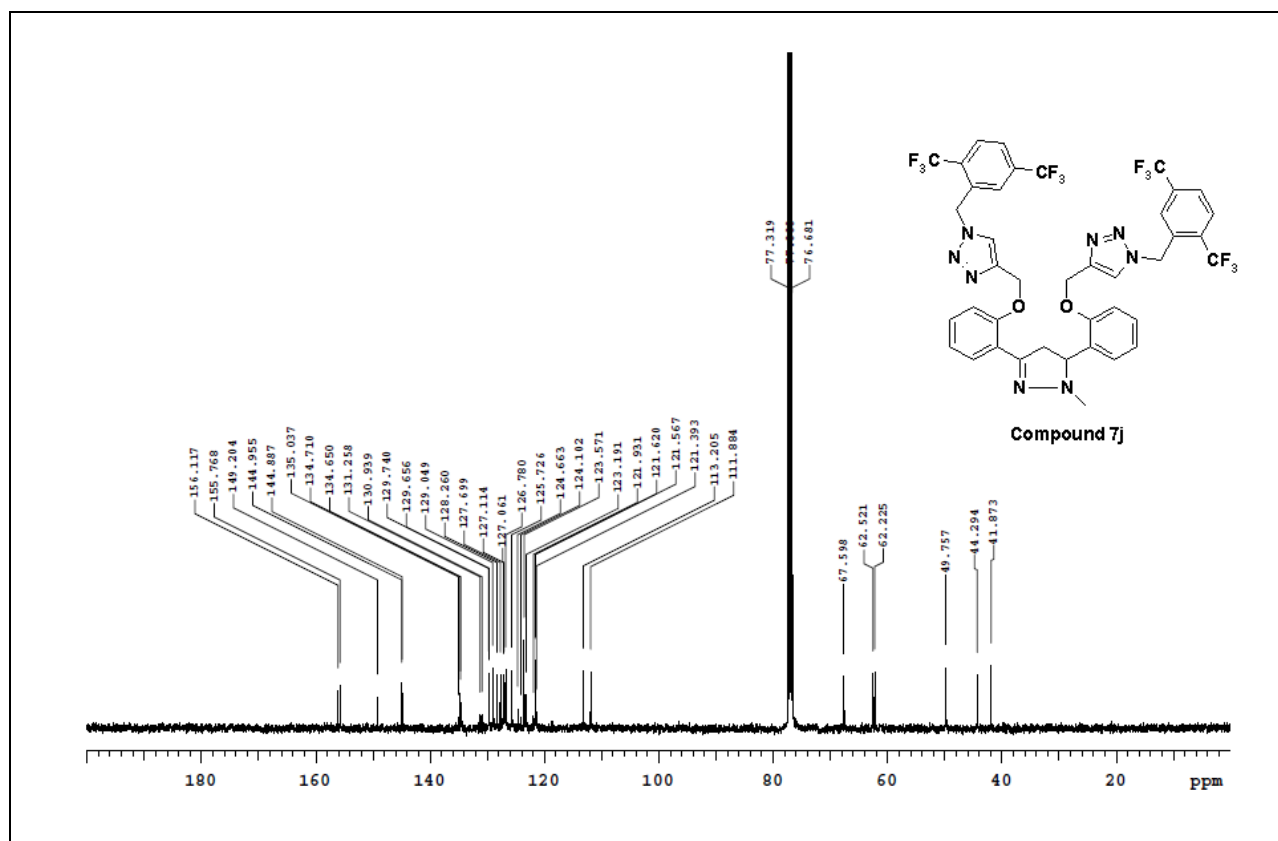


Figure S102: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 7j

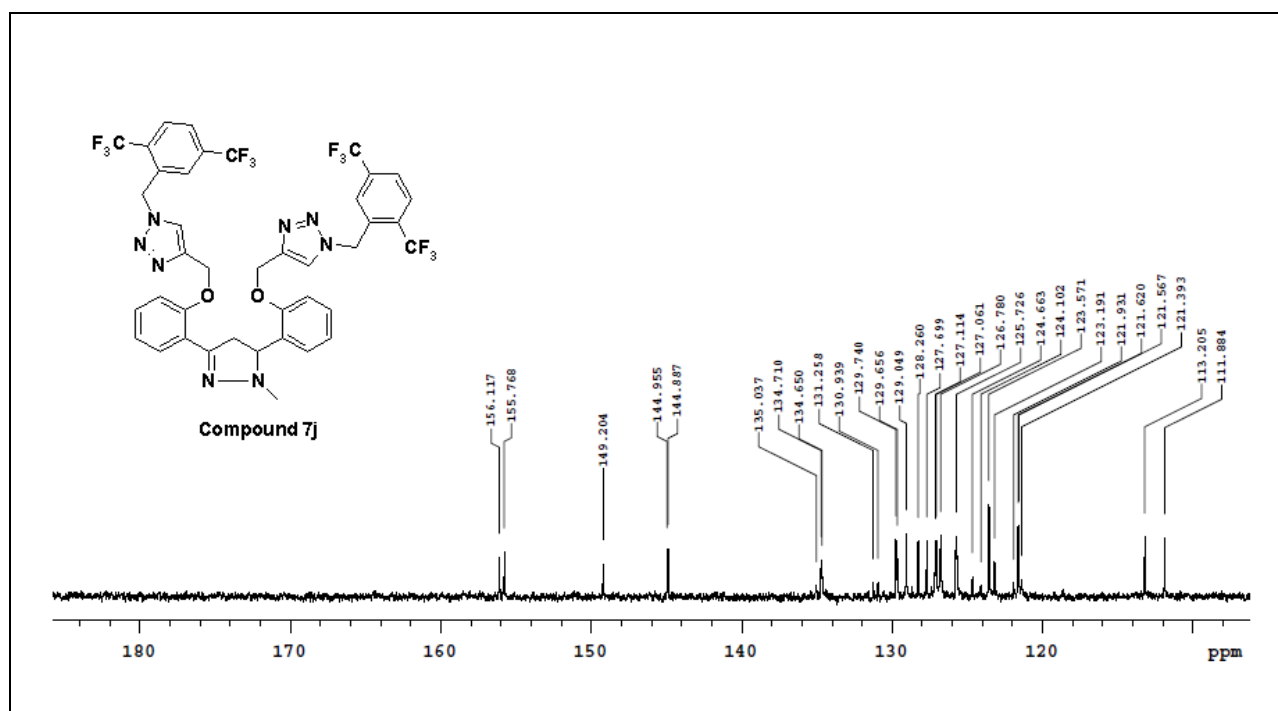


Figure S103: ¹³C NMR (100 MHz, CDCl₃) spectra of compound 7j

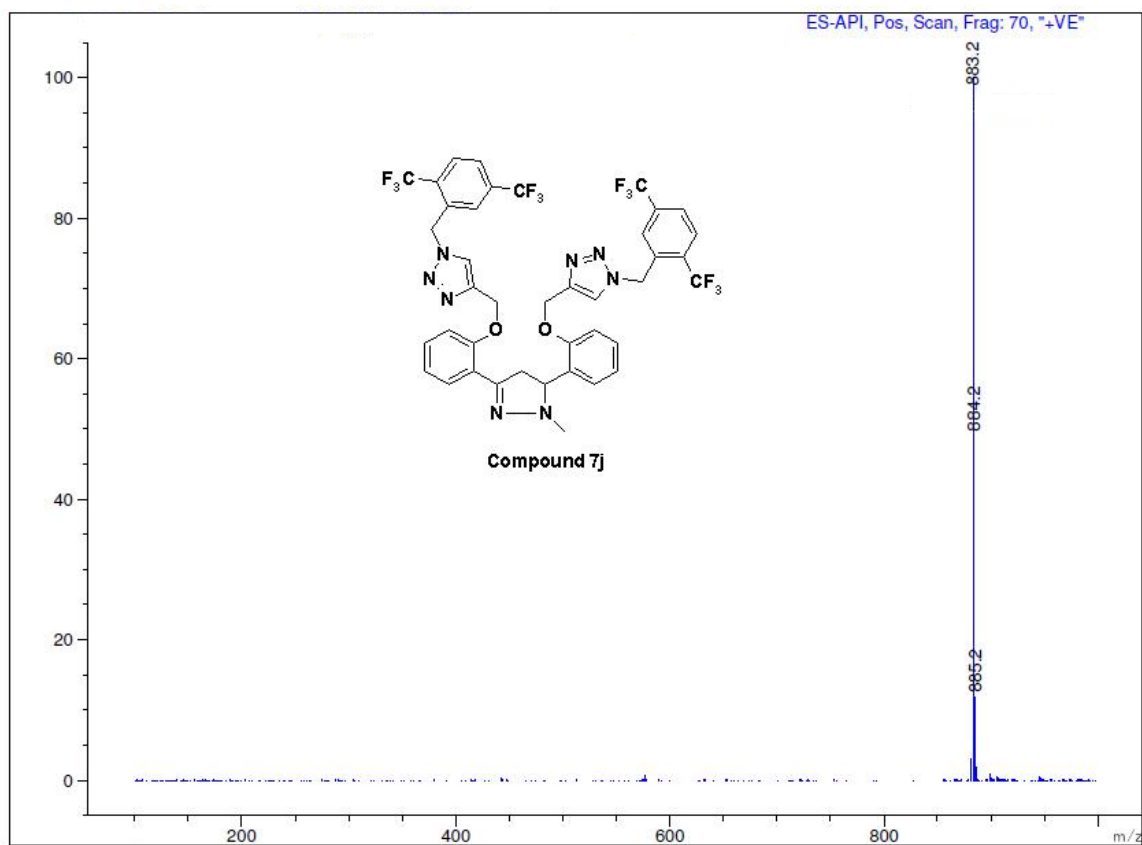


Figure S104: Mass spectra of compound 7j

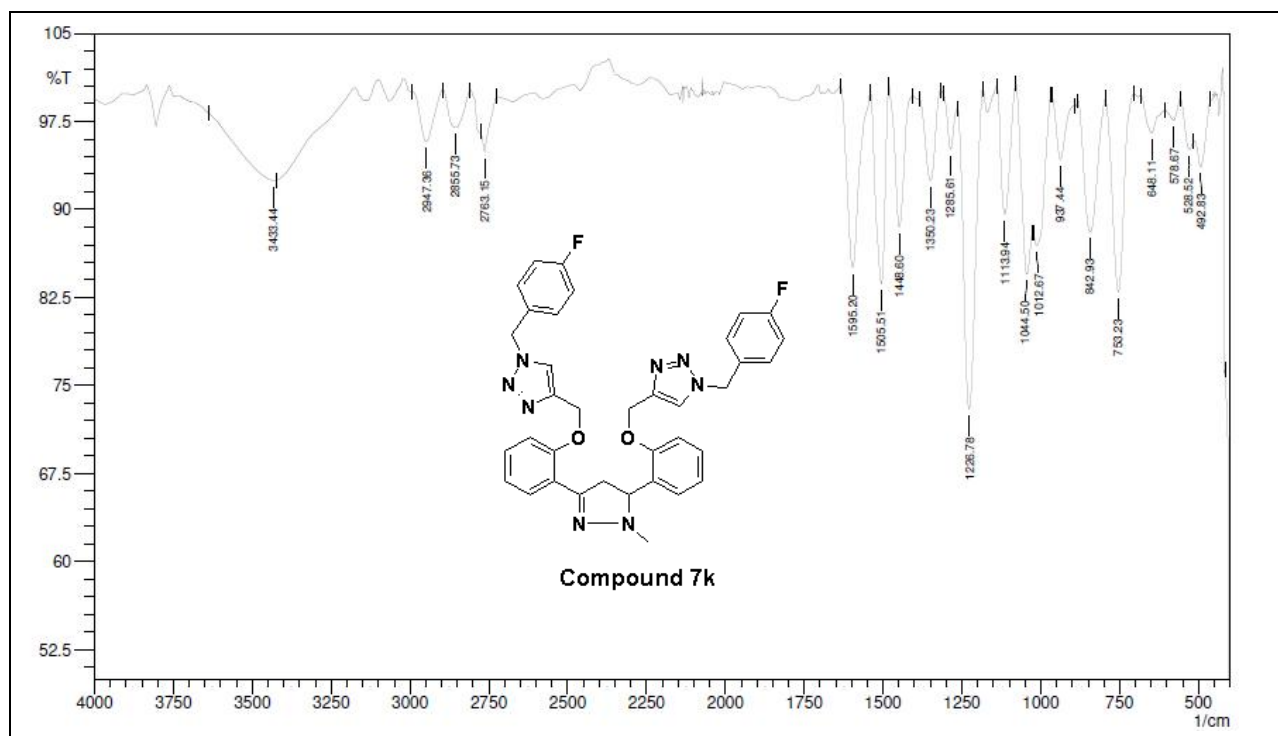


Figure S105: IR spectra of compound 7k

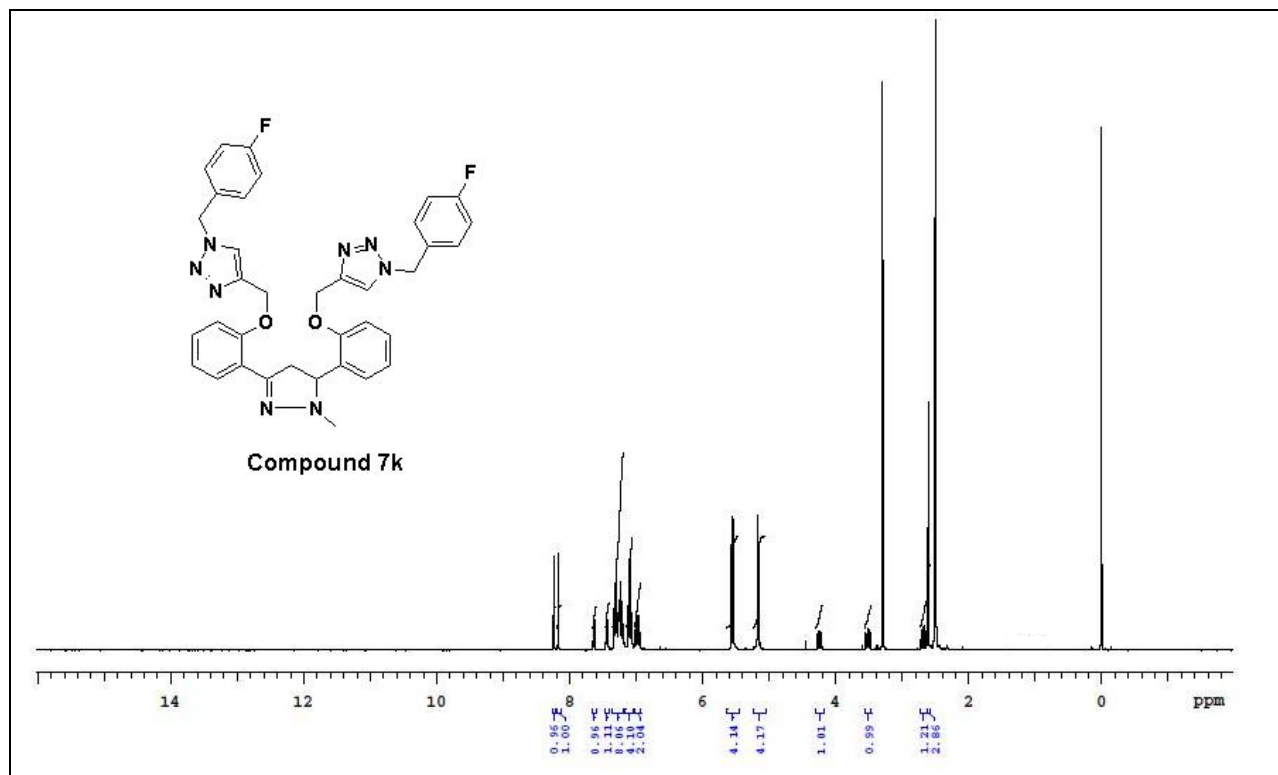


Figure S106: $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) spectra of compound 7k

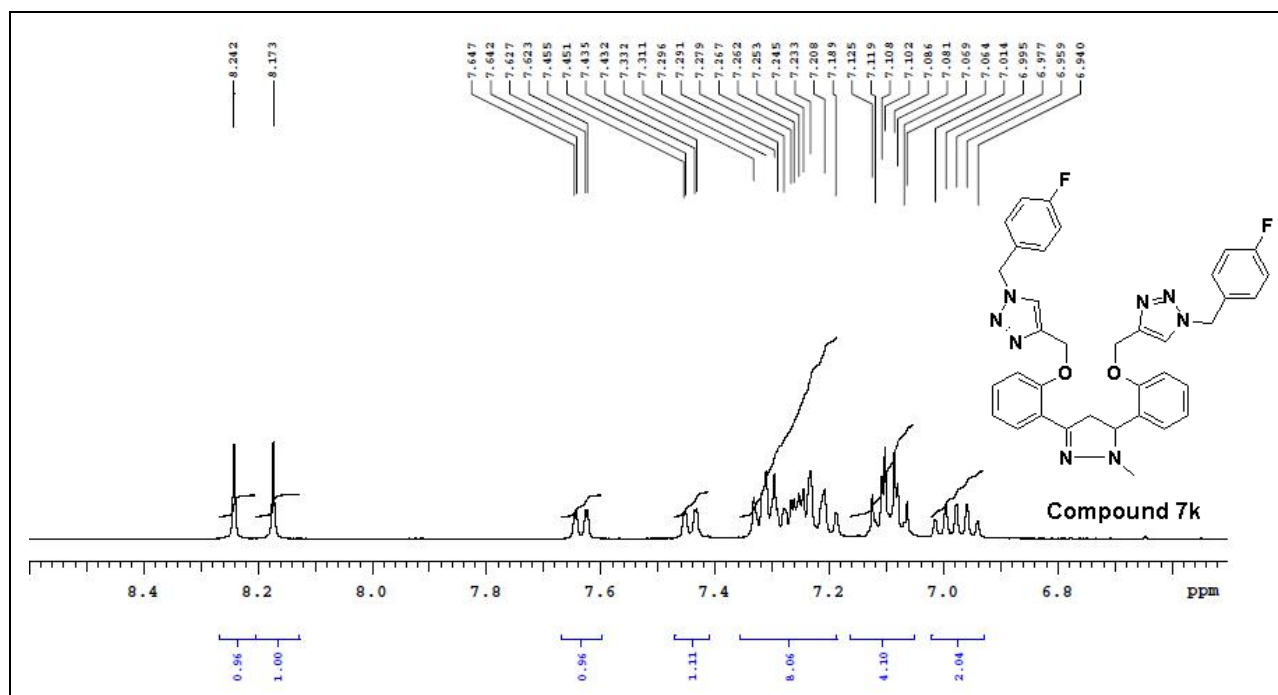


Figure S107: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7k**

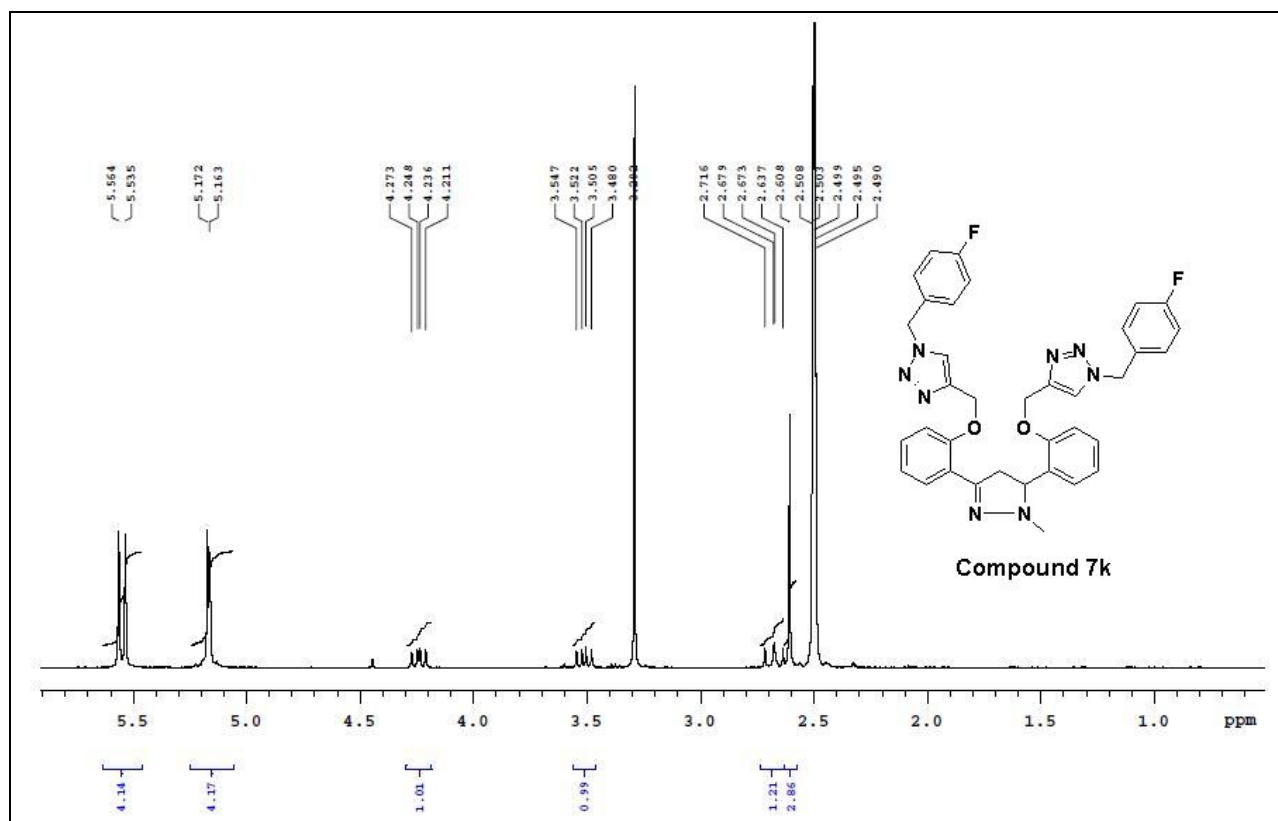


Figure S108: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7k**

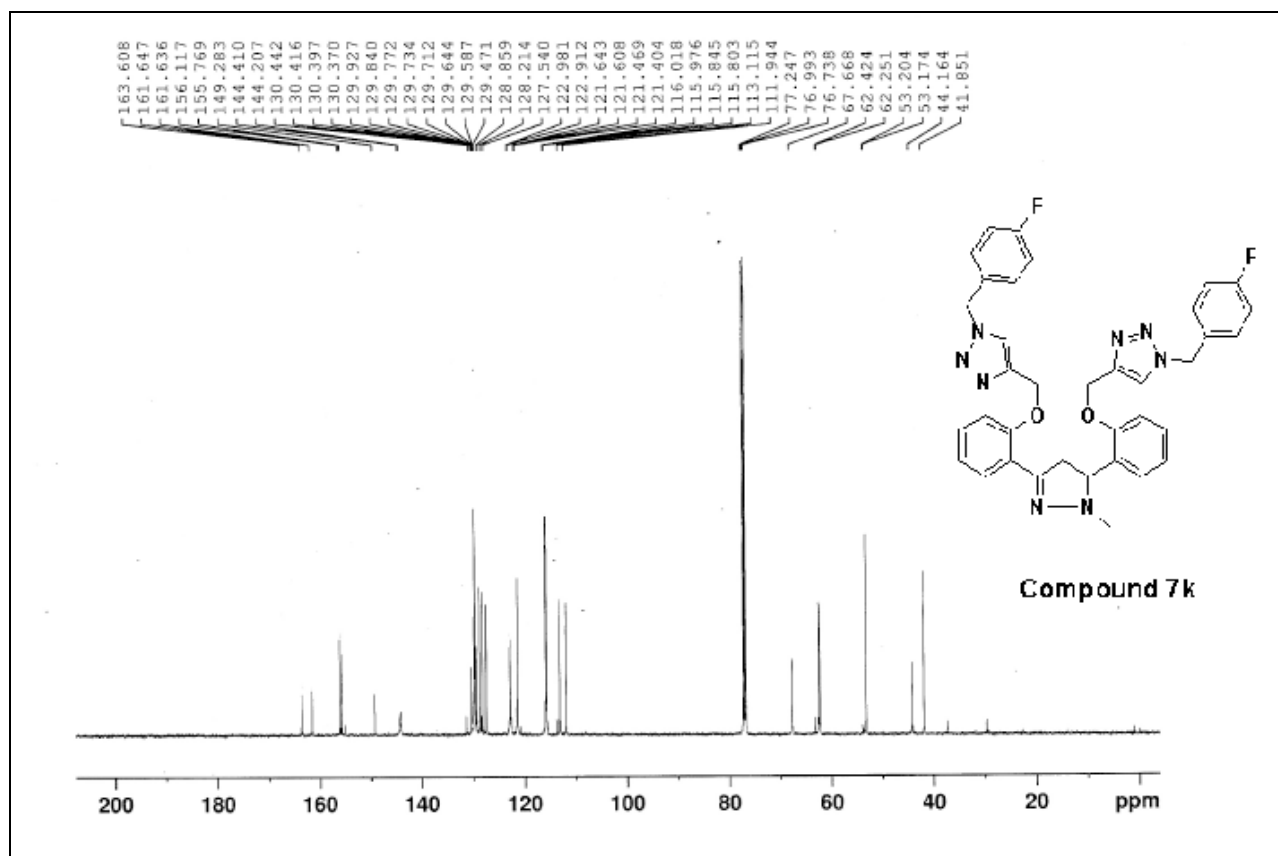


Figure S109: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound 7k

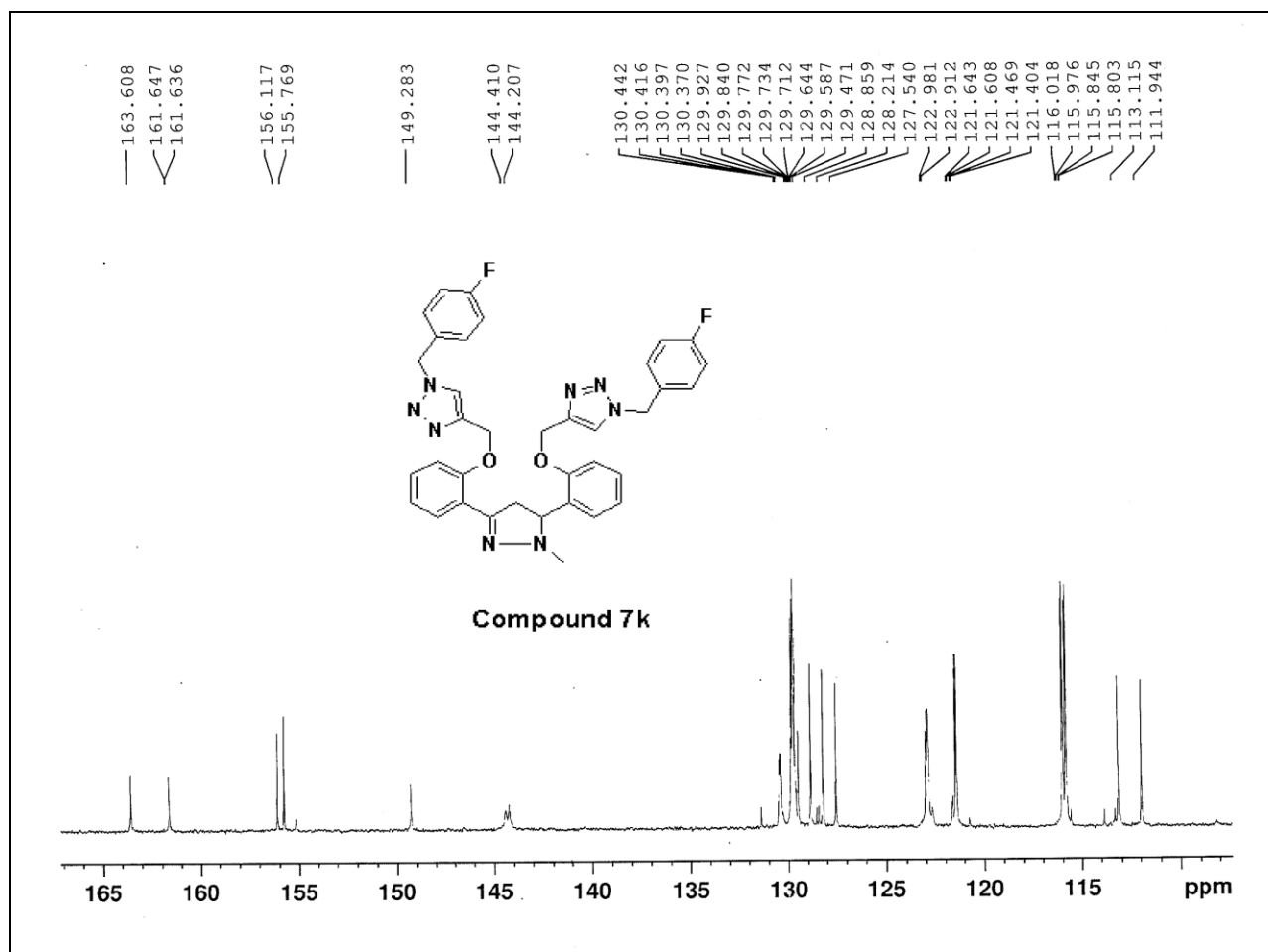


Figure S110: ¹³C NMR (125 MHz, CDCl₃) spectra of compound 7k

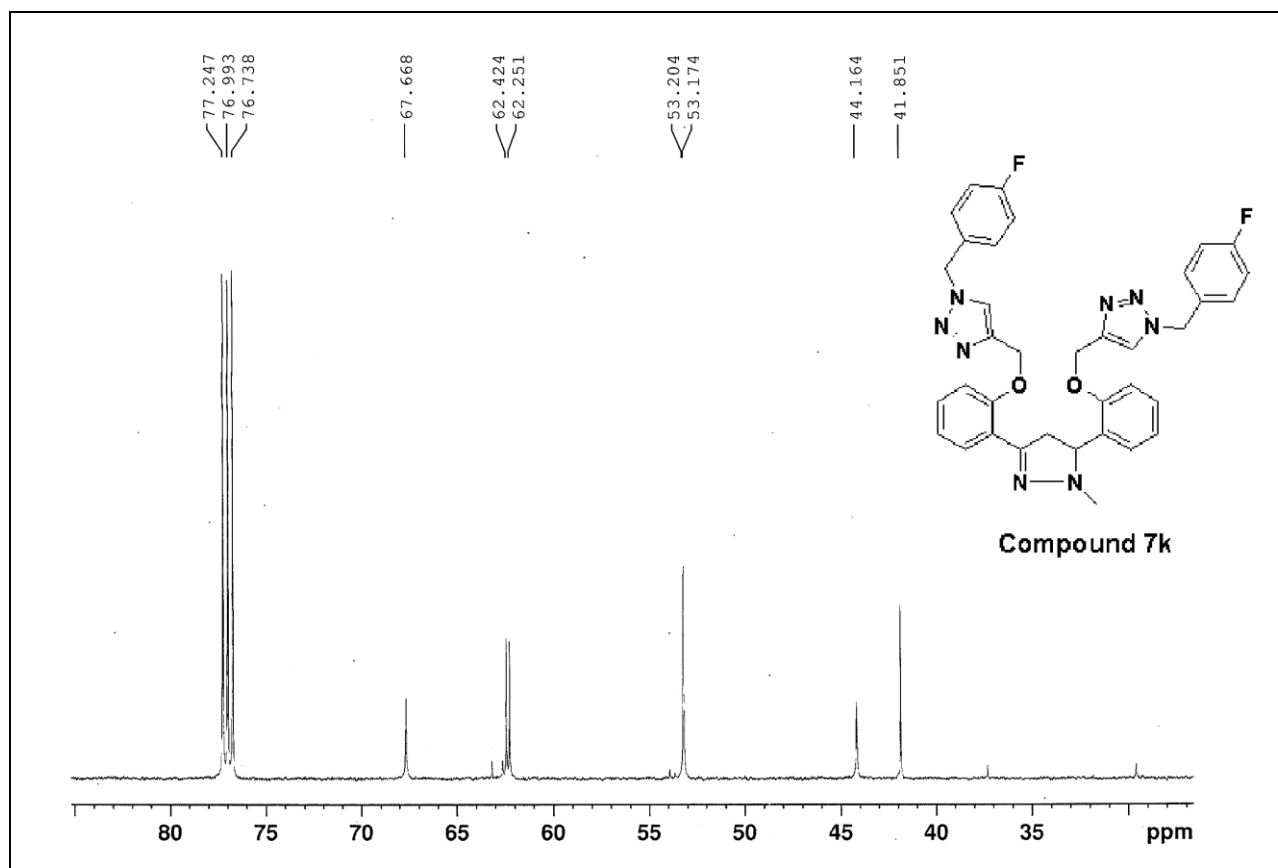


Figure S111: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound **7k**

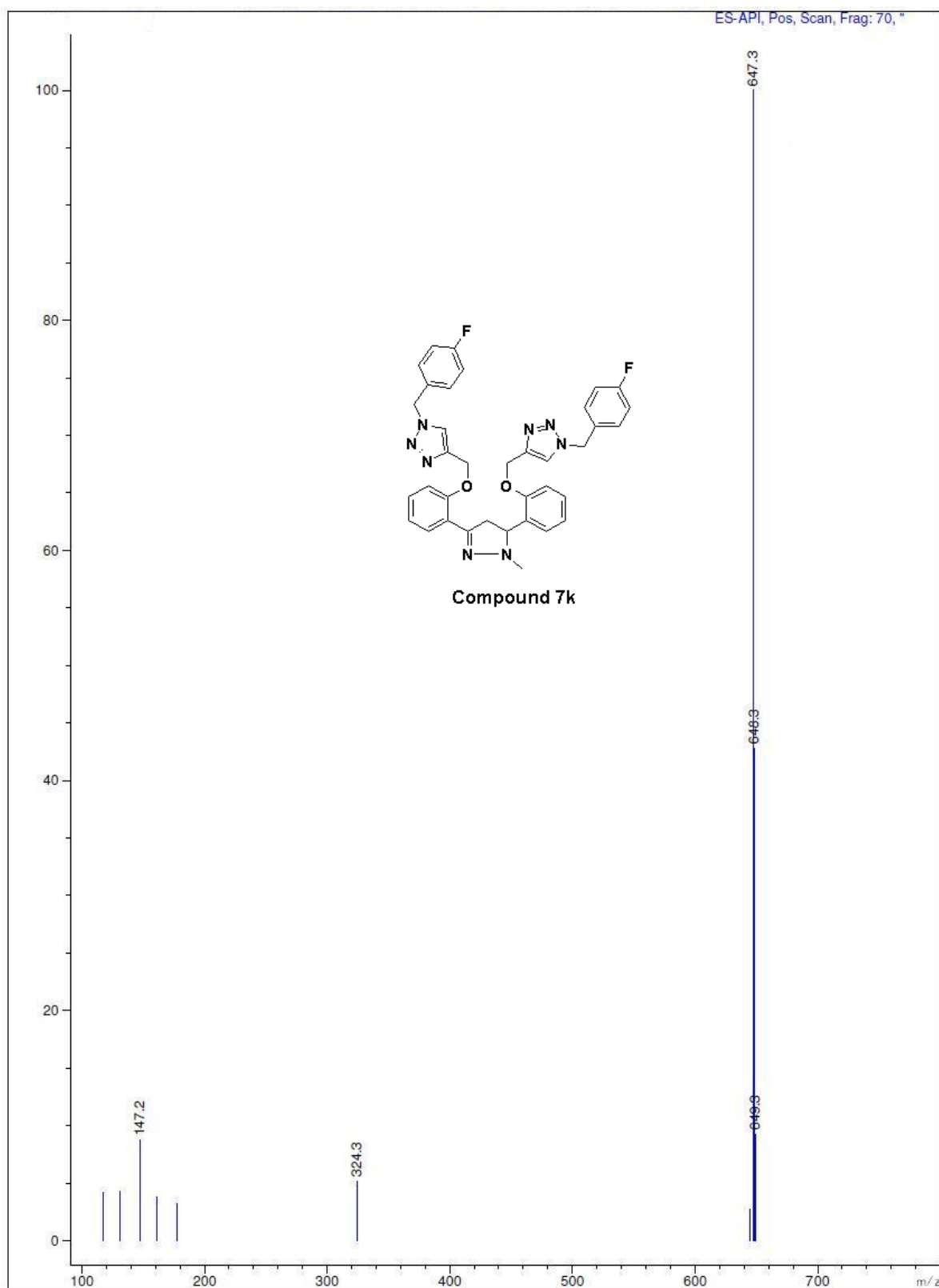


Figure S112: Mass spectra of compound 7k

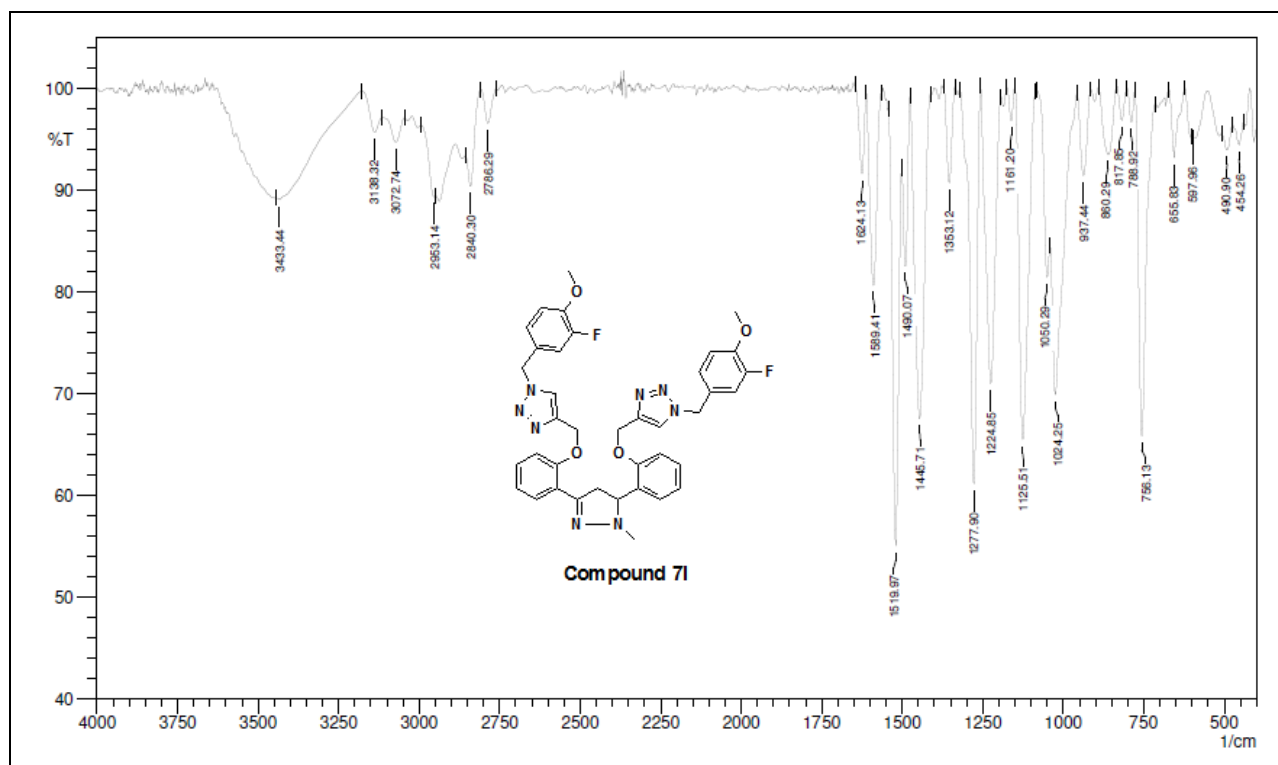


Figure S113: IR spectra of compound 7l

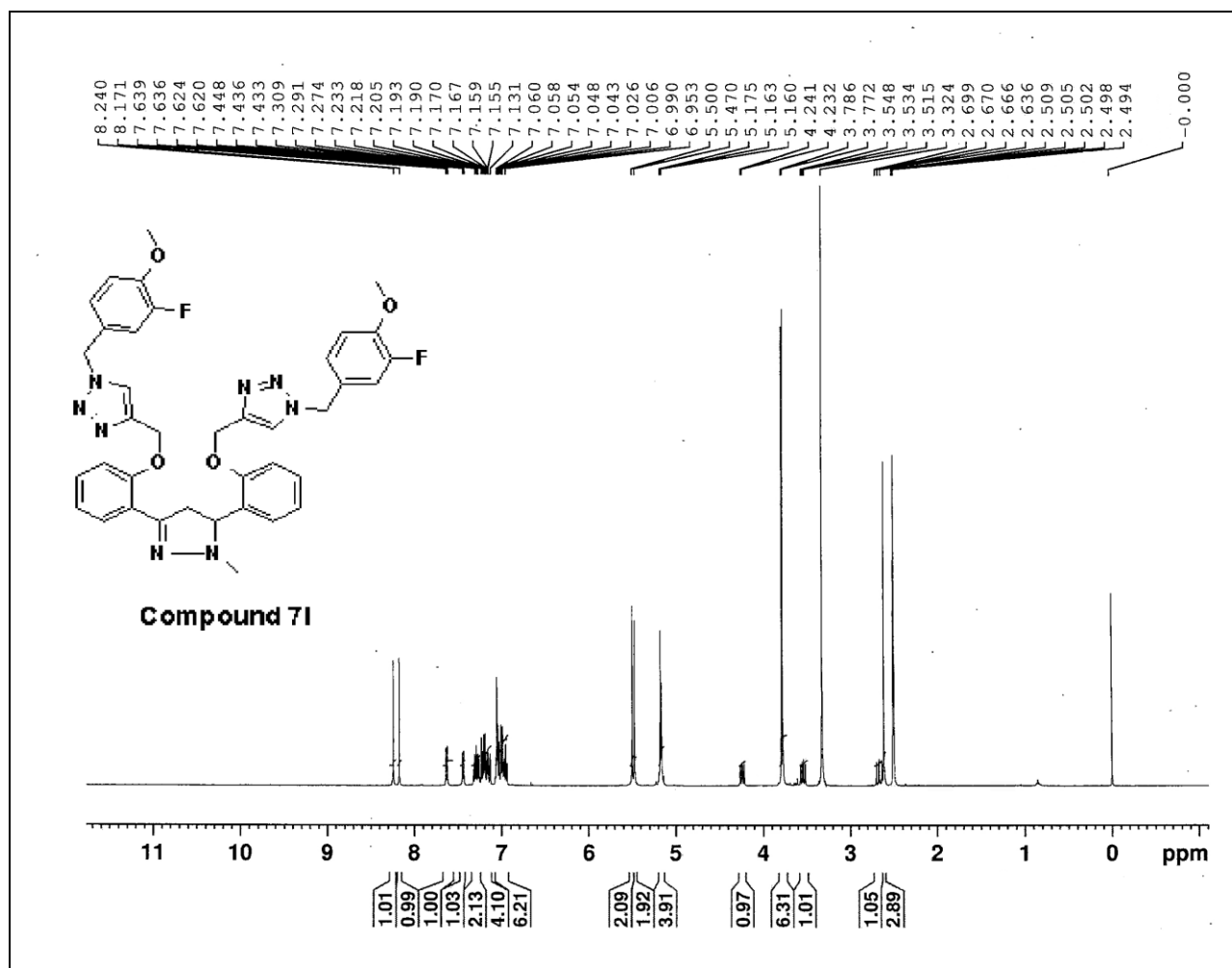


Figure S114: ¹H-NMR (500 MHz, DMSO-d₆) spectra of compound **71**

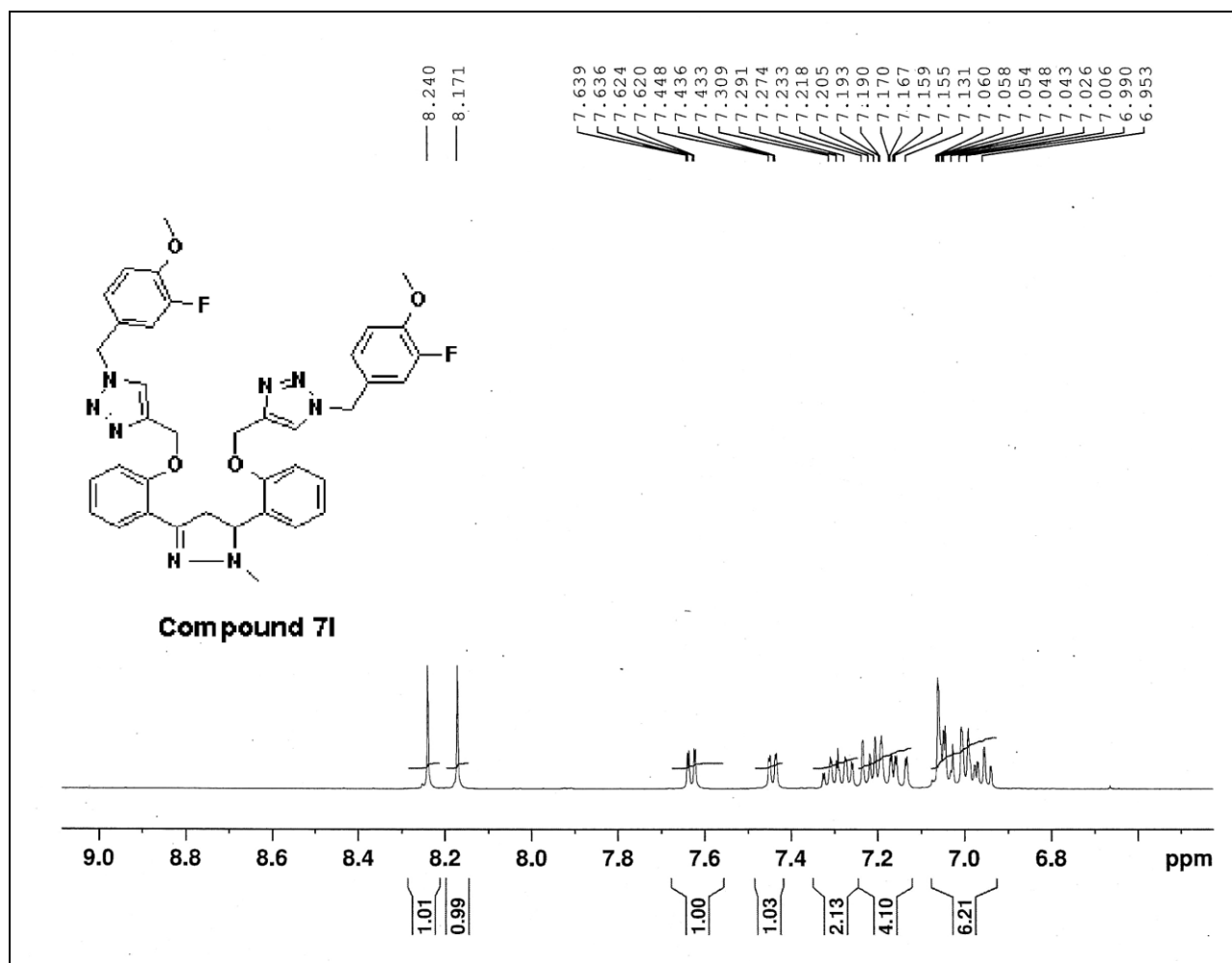


Figure S115: ¹H-NMR (500 MHz, DMSO-d₆) spectra of compound 7l

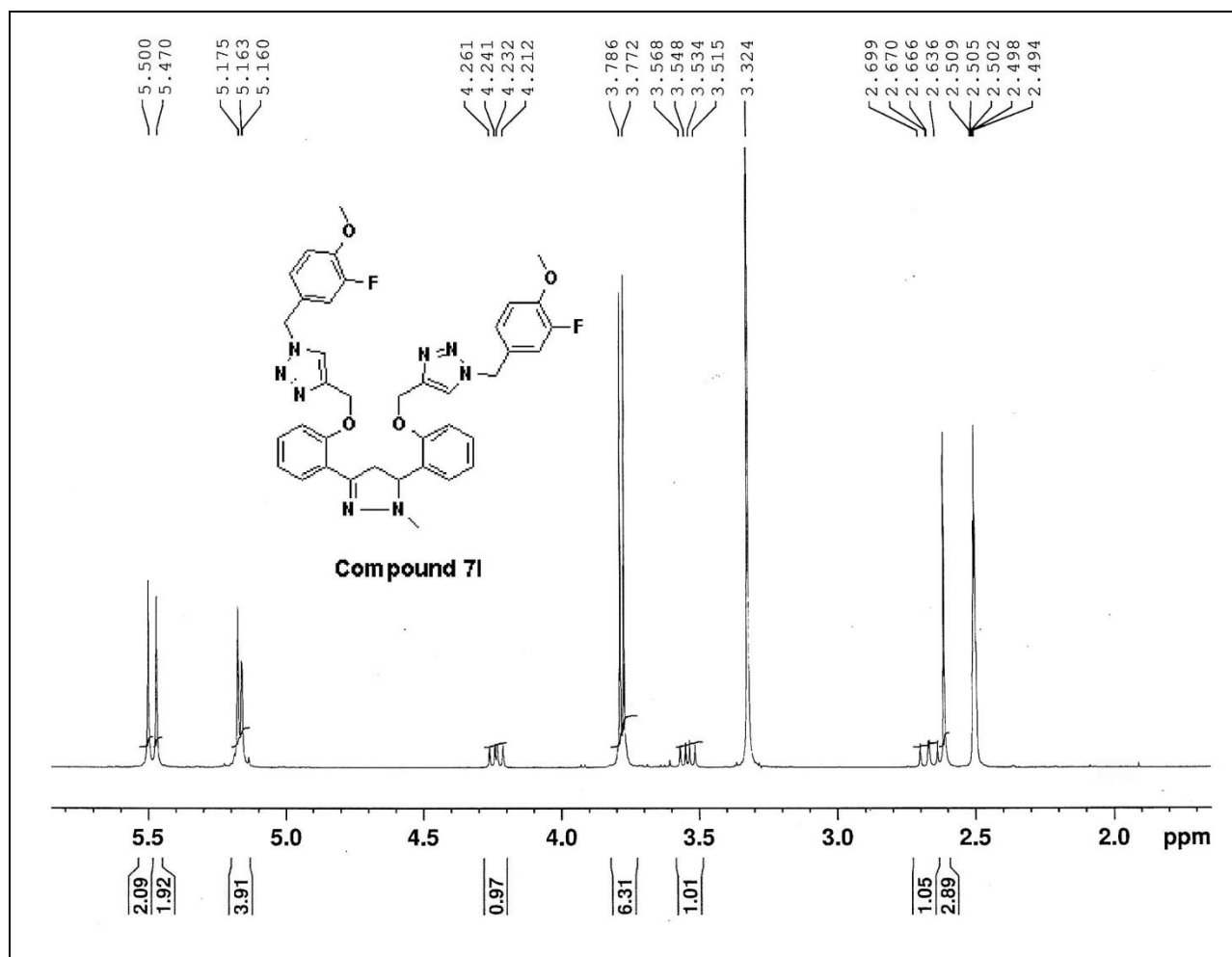


Figure S116: ^1H -NMR (500 MHz, DMSO-d_6) spectra of compound **71**

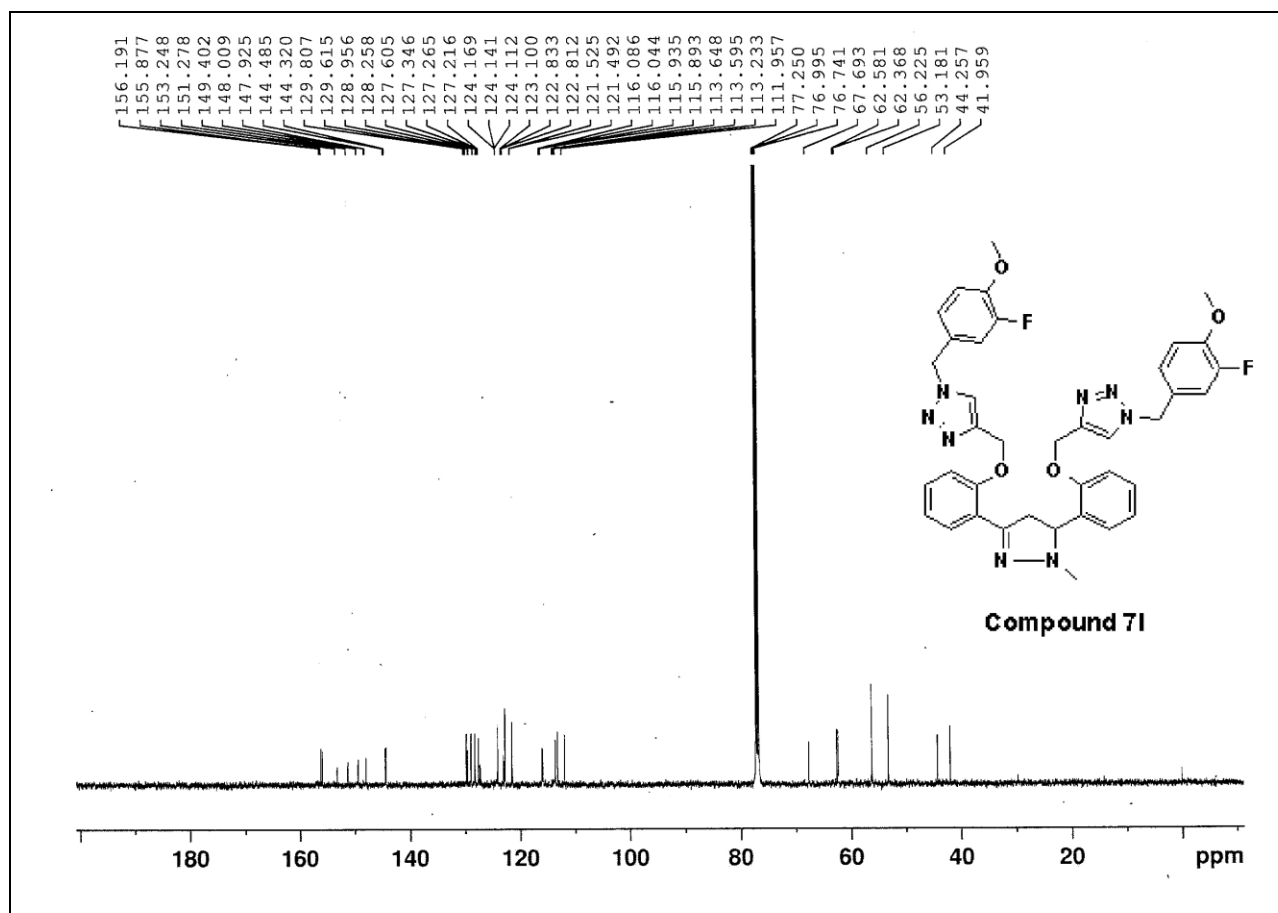


Figure S117: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound 71

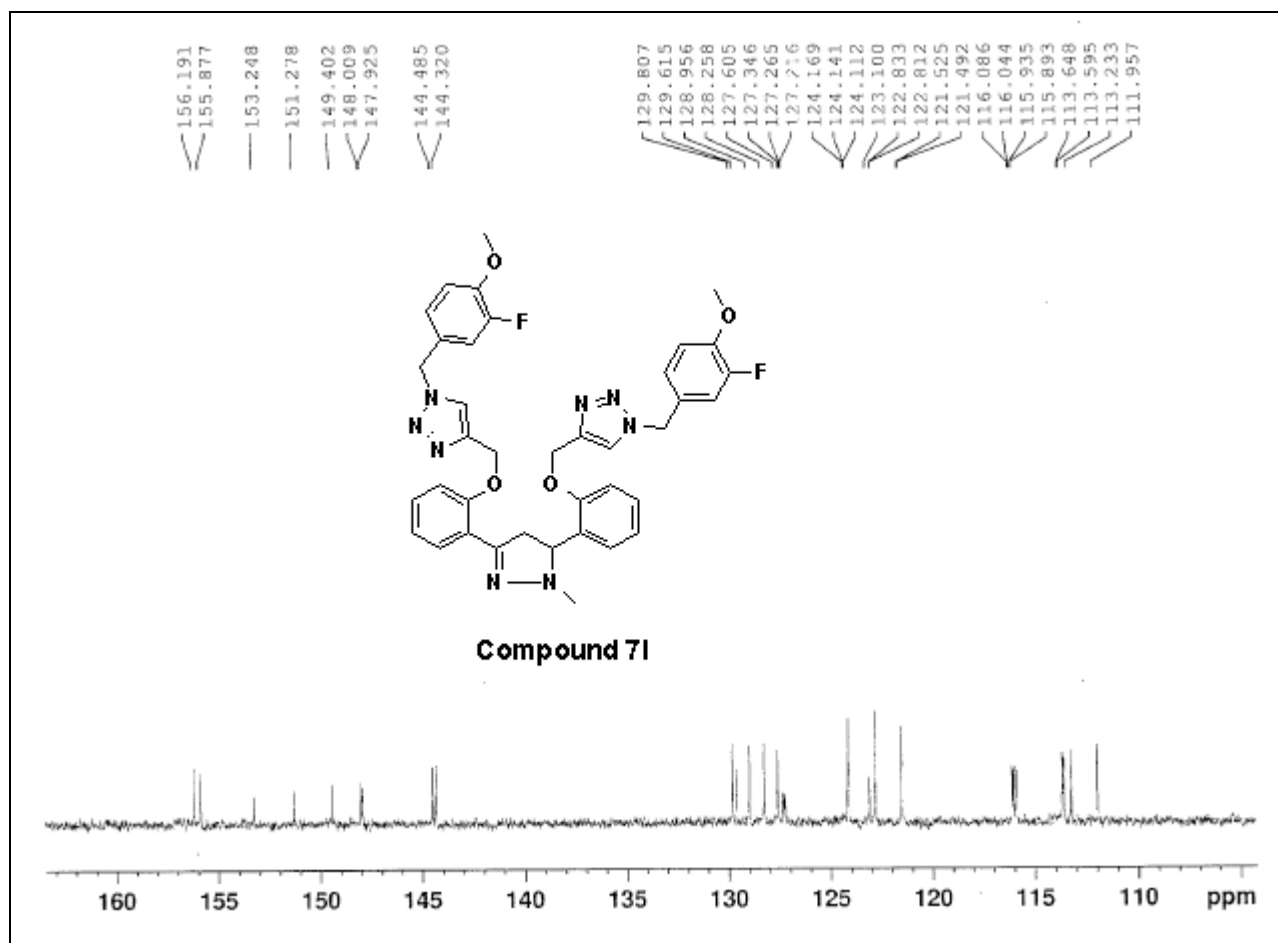


Figure S118: ¹³C NMR (125 MHz, CDCl₃) spectra of compound **71**

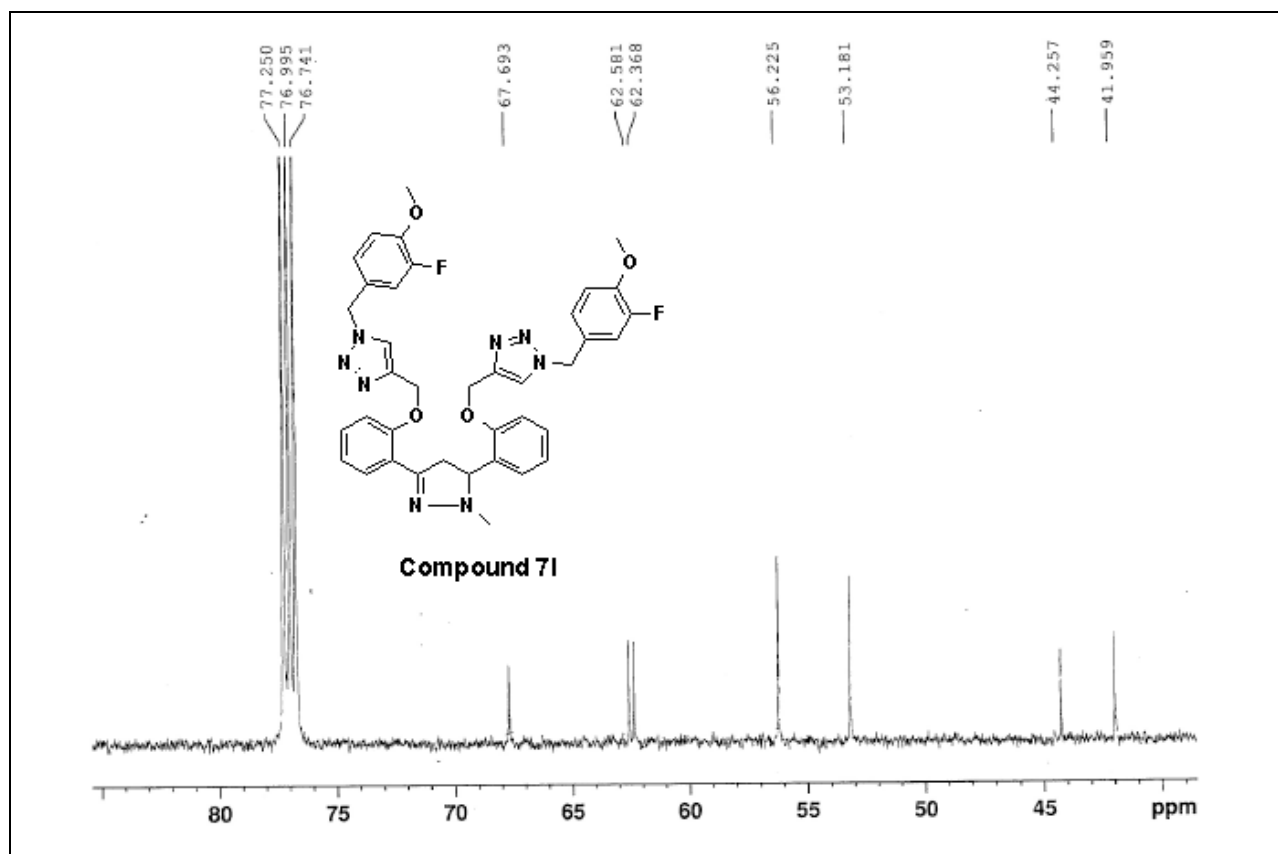


Figure S119: ^{13}C NMR (125 MHz, CDCl_3) spectra of compound **71**

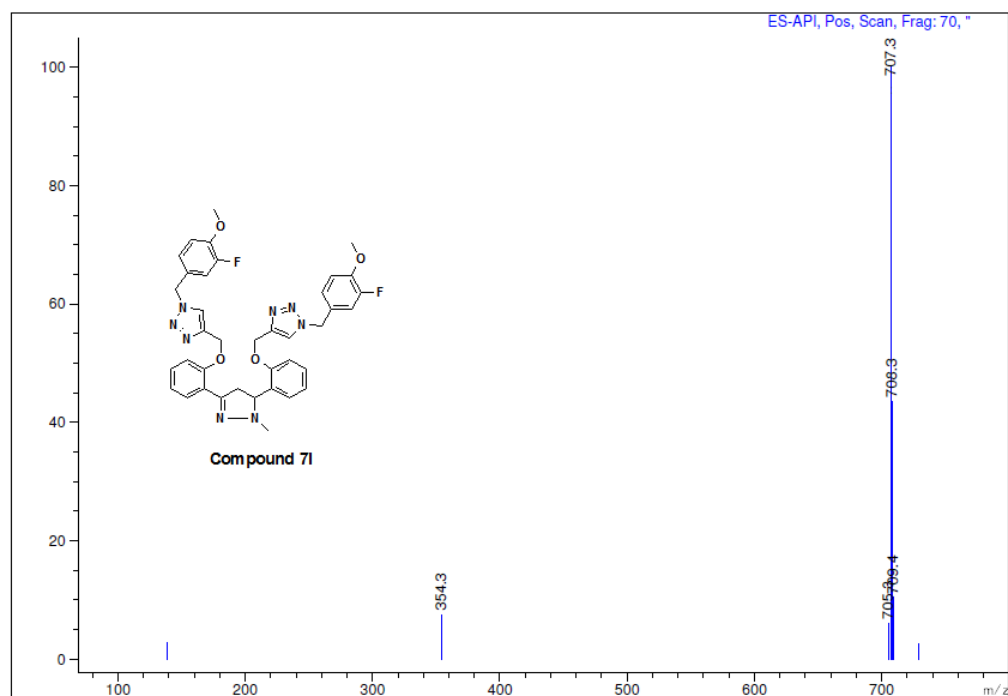


Figure S120: Mass spectra of compound **71**

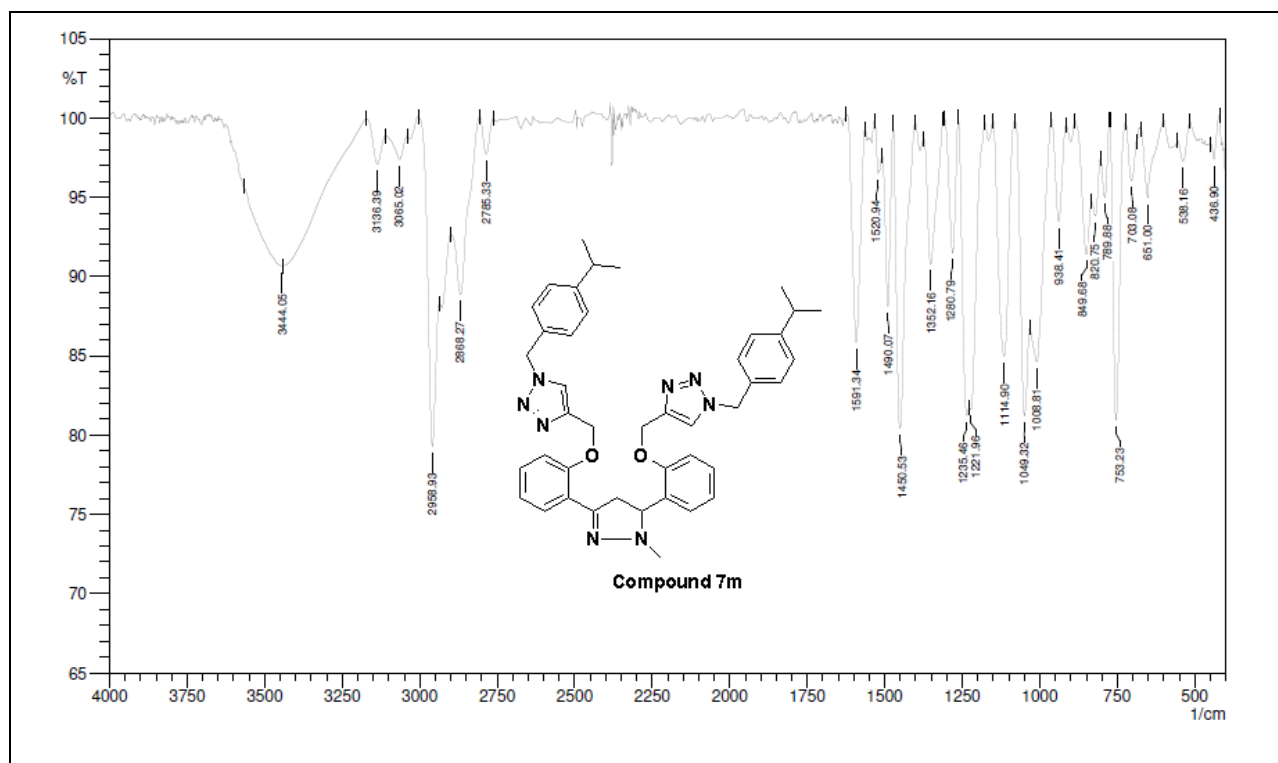


Figure S121: IR spectra of compound 7m

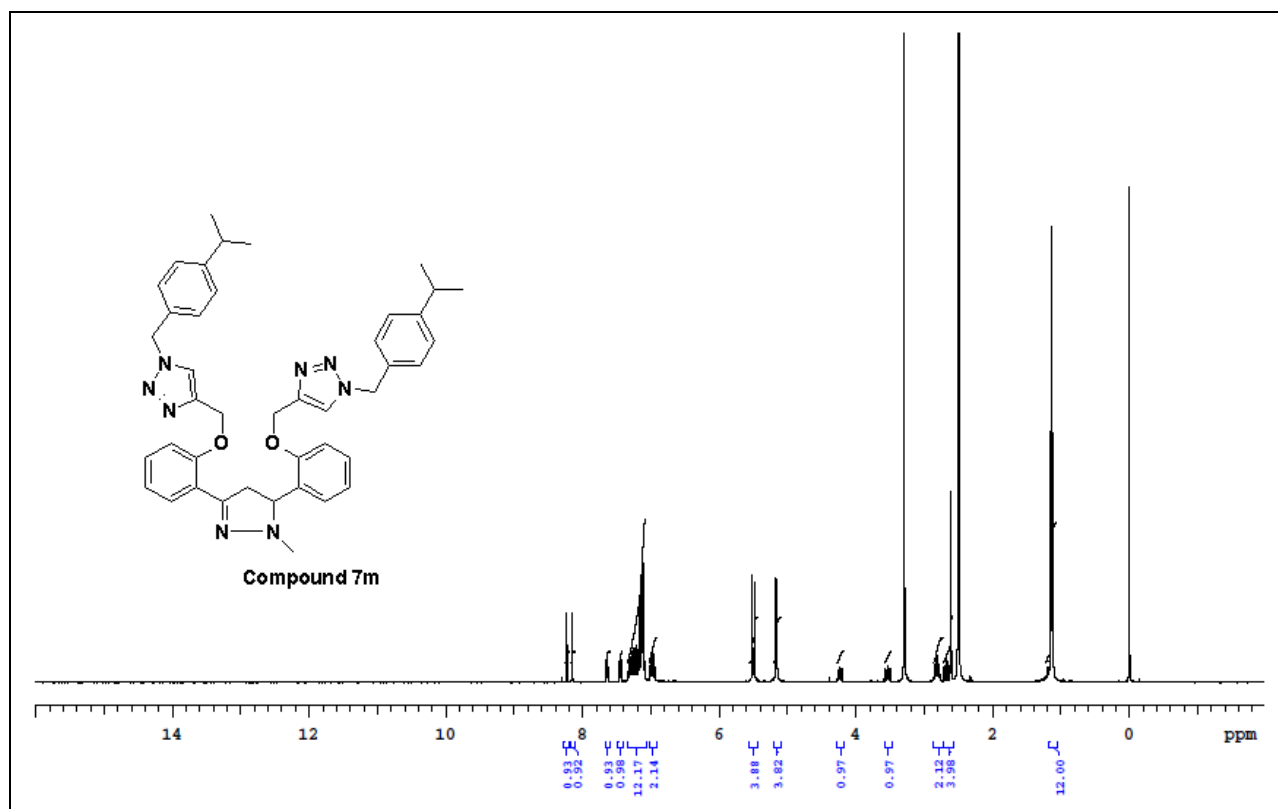


Figure S122: $^1\text{H-NMR}$ (400 MHz, DMSO-d_6) spectra of compound 7m

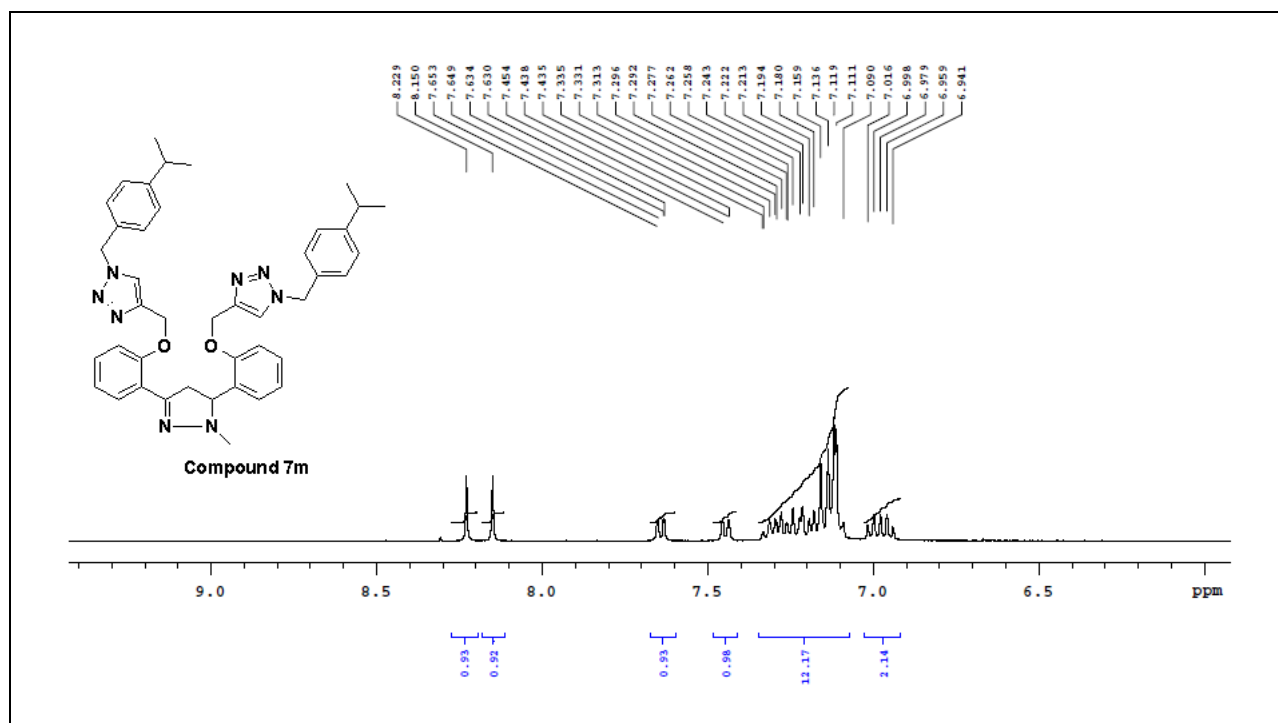


Figure S123: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7m**

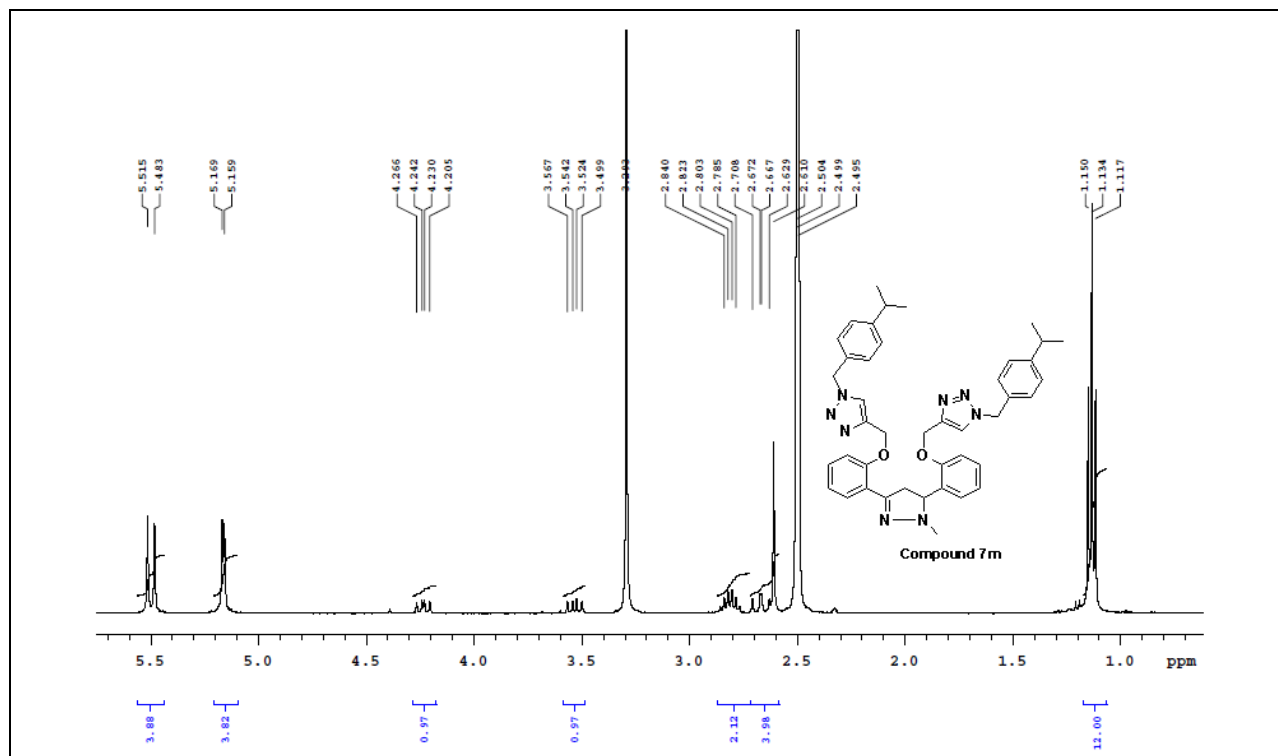
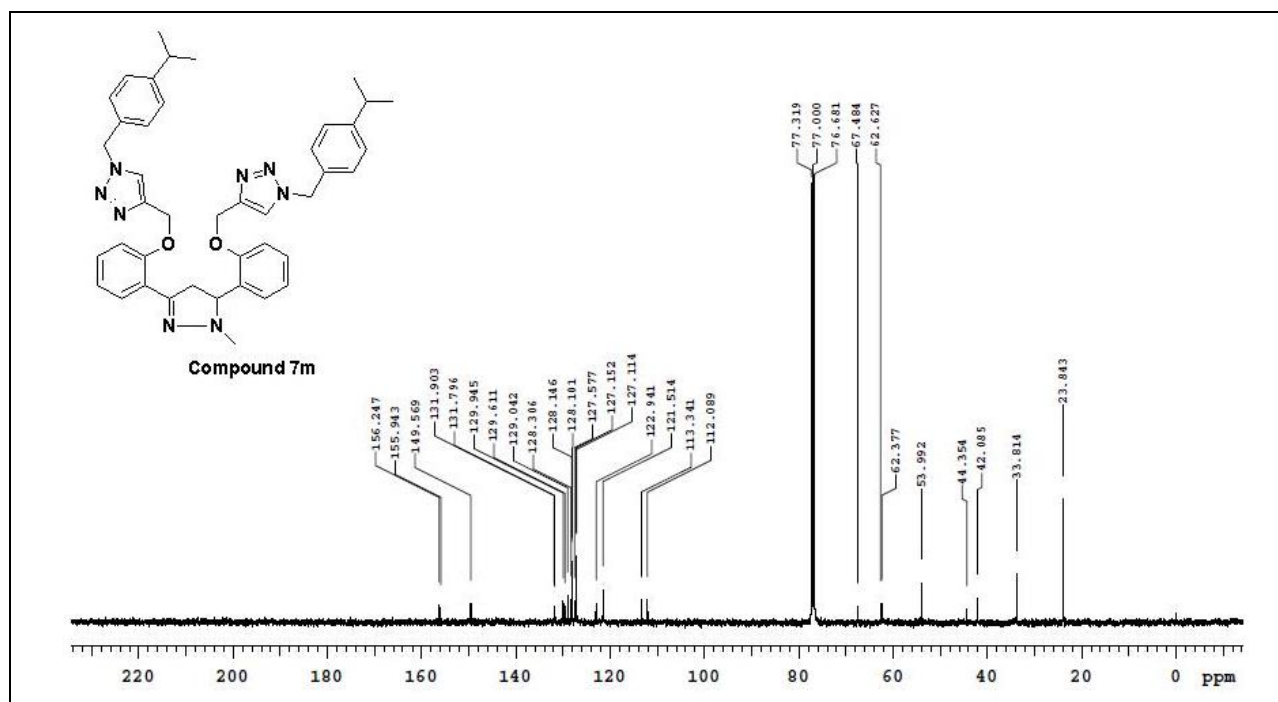


Figure S124: ^1H -NMR (400 MHz, DMSO-d_6) spectra of compound **7m**

371

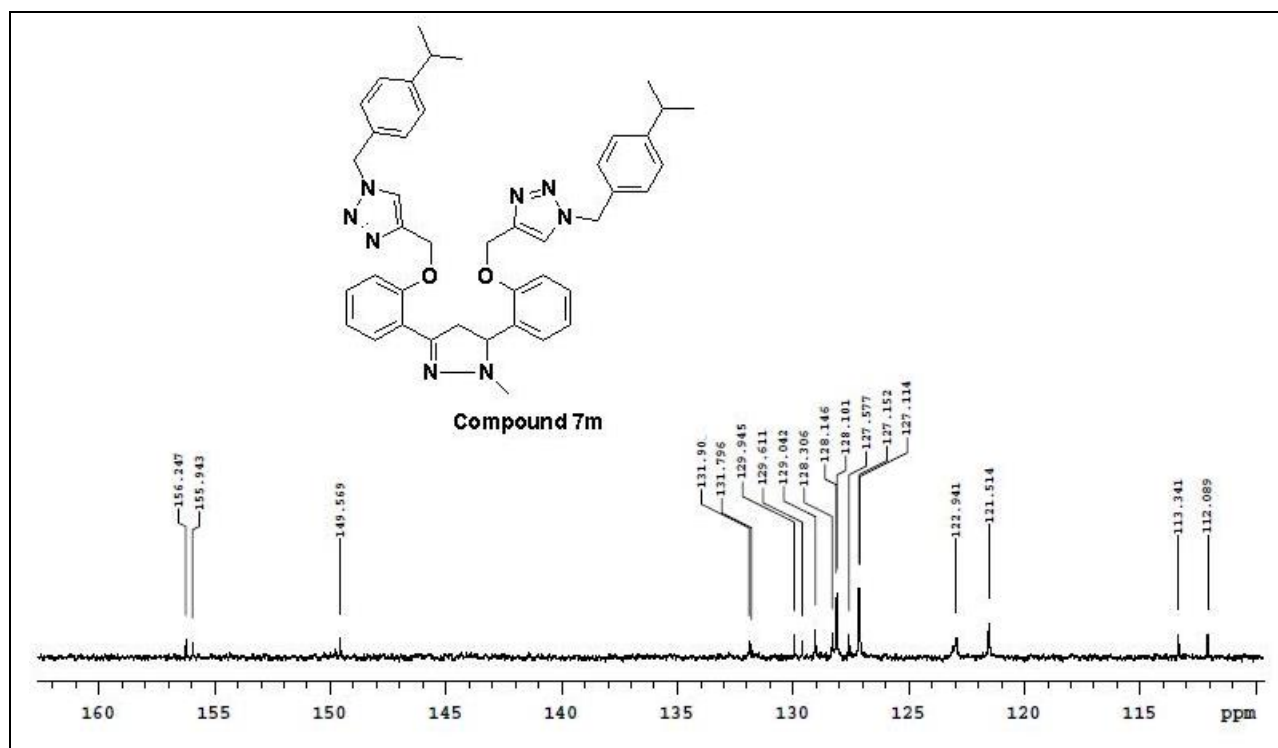


372

373

Figure S125: ^{13}C NMR (100 MHz, CDCl_3) spectra of compound 7m

374

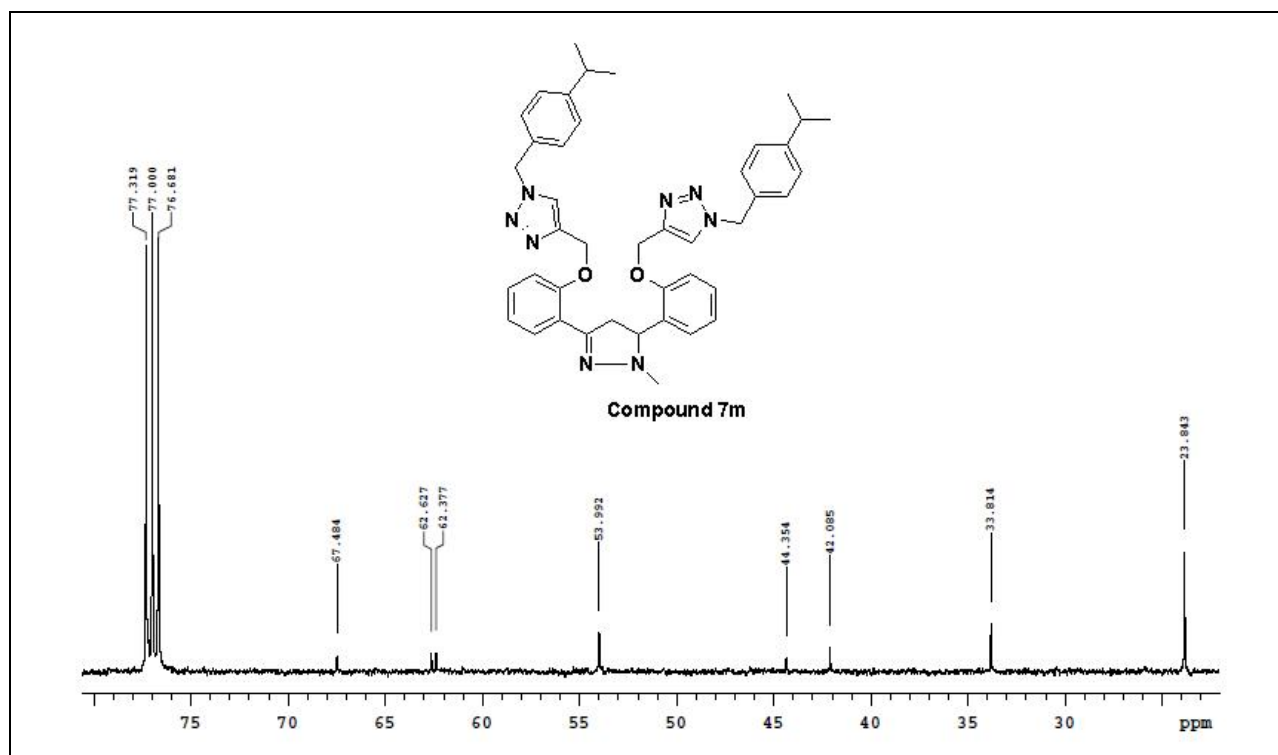


375

376

Figure S126: ^{13}C NMR (100 MHz, CDCl_3) spectra of compound 7m

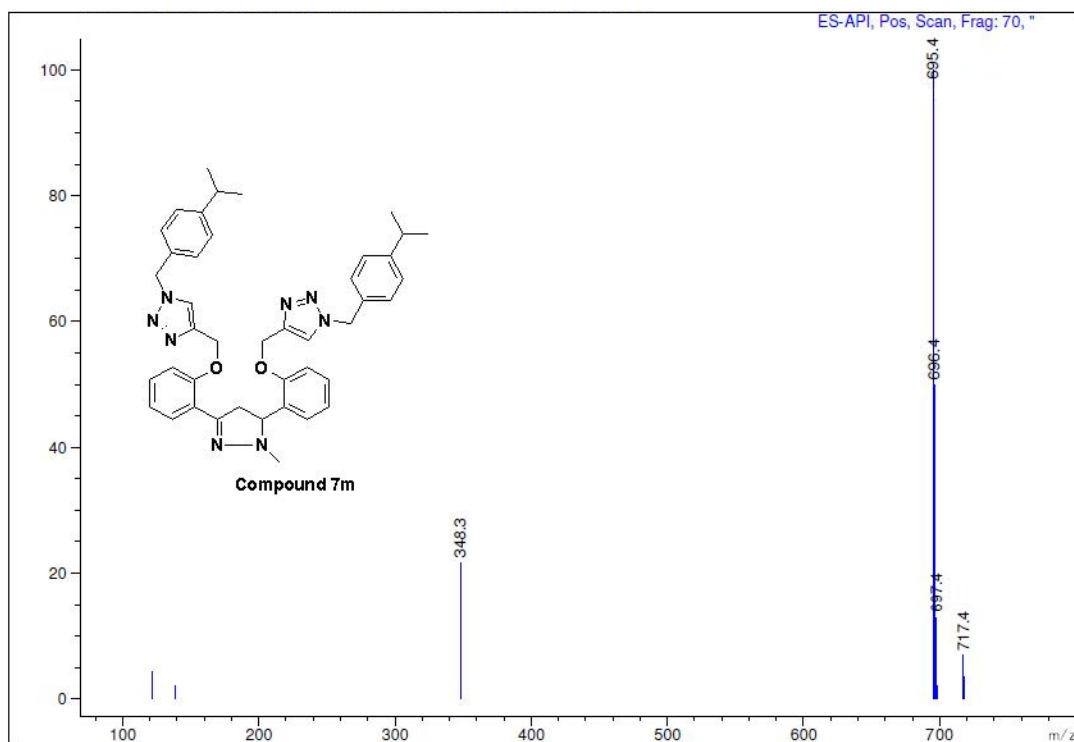
377



378

379

Figure S127: ¹³C NMR (100 MHz, CDCl₃) spectra of compound **7l**



380

381

Figure S128: Mass spectra of compound **7m**