

Synthesis and Primary Activity Assay of Novel Benitrobenrazide and Benserazide Derivatives

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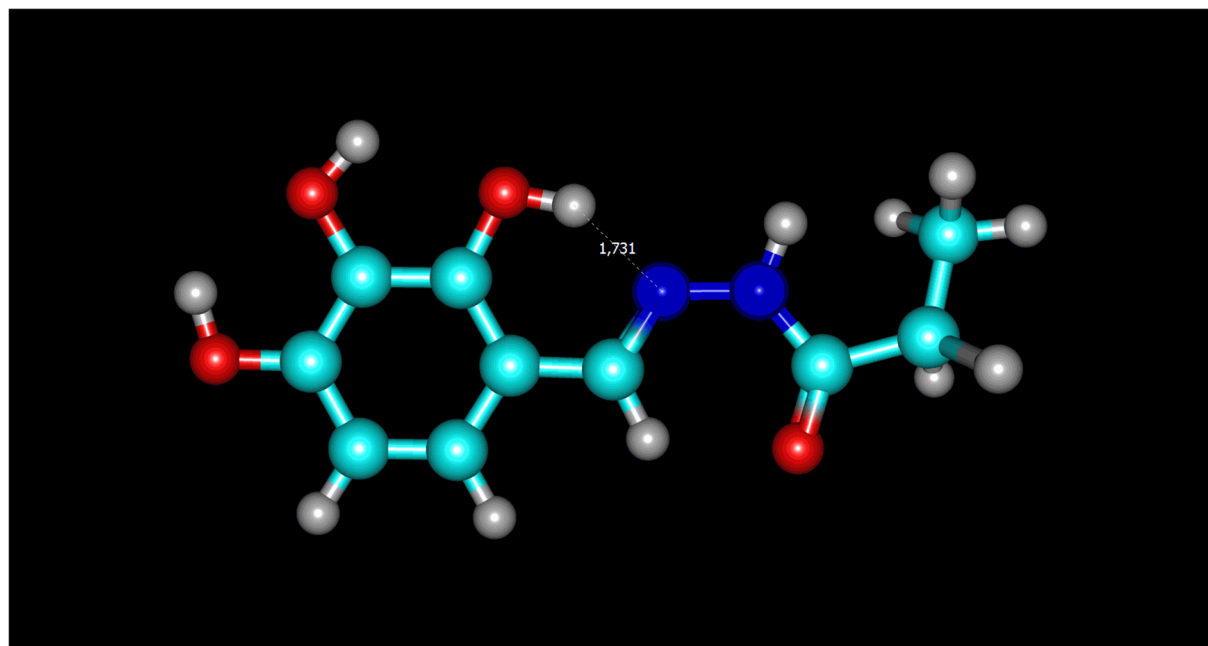
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Supporting Information

1. Hydrogen bonding interaction in compound **4a**S1
2. NMR spectra of compounds evaluated for inhibition of HK2.S2–S27

Figure S1: Hydrogen bonding interaction in compound **4a**



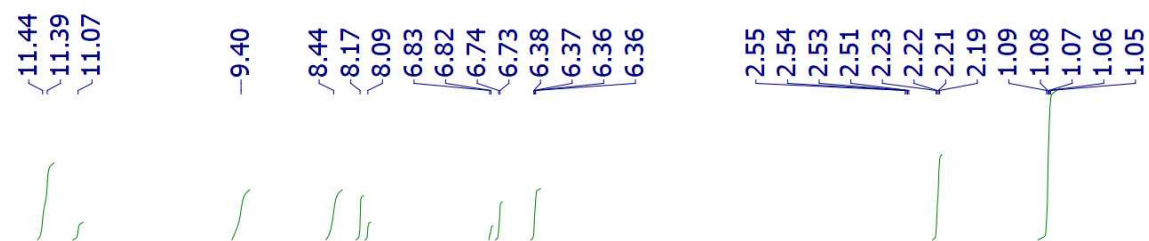


Figure S2: ^1H NMR spectrum of **4a** (DMSO, 600 MHz)

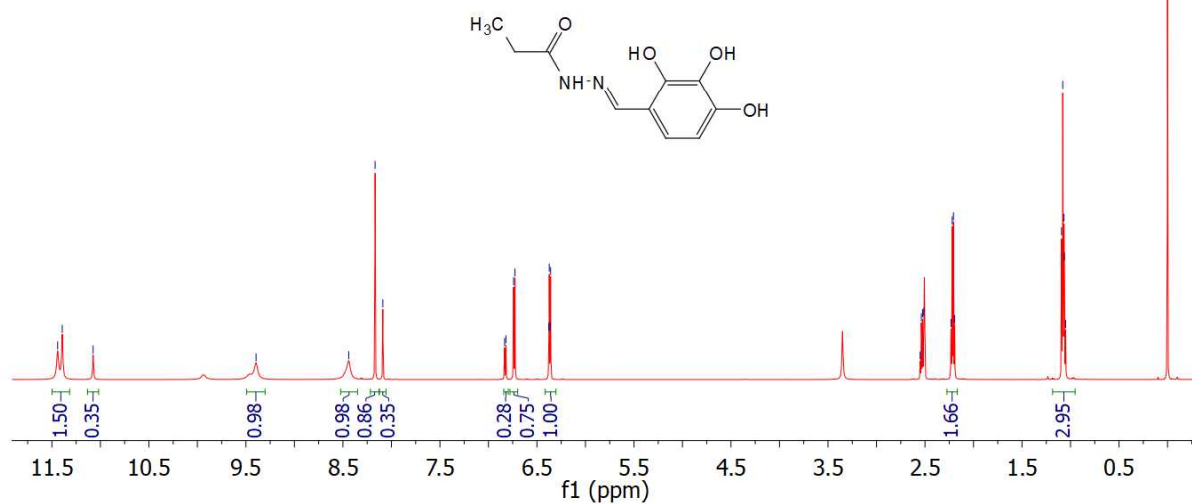
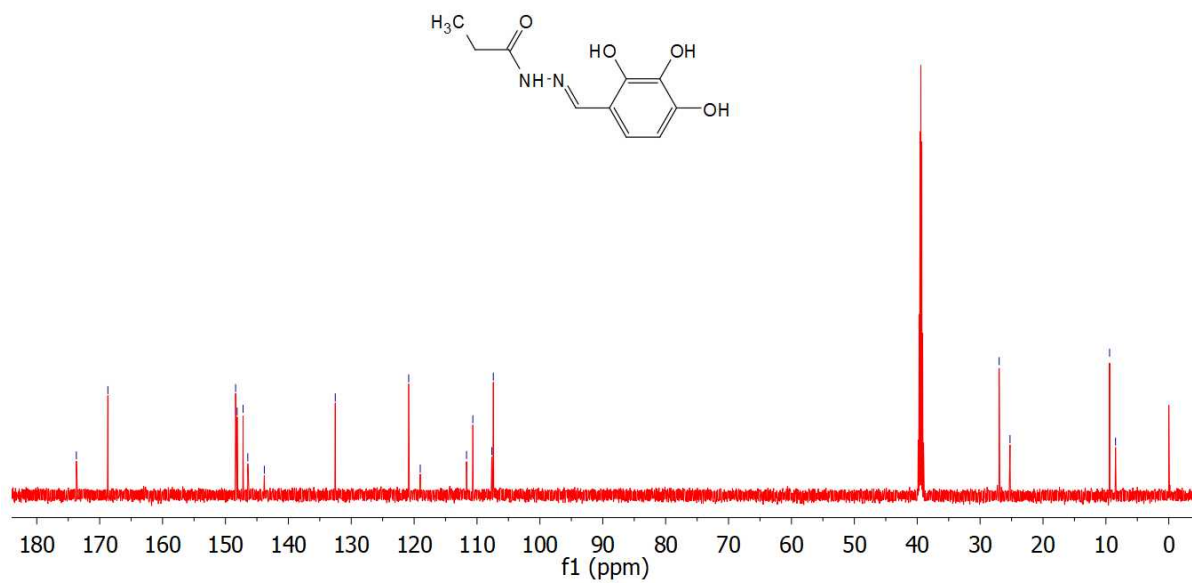


Figure S3: ^{13}C NMR spectrum of **4a** (DMSO, 600 MHz)



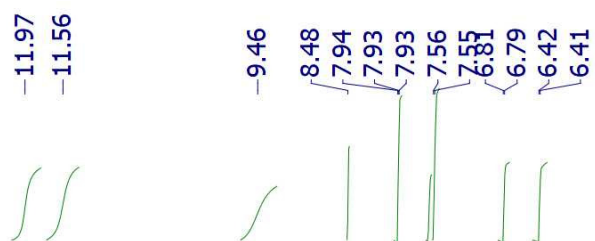


Figure S4: ¹H NMR spectrum of **4b** (DMSO, 600MHz)

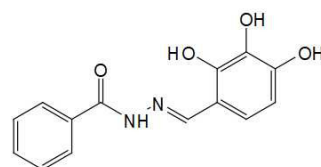
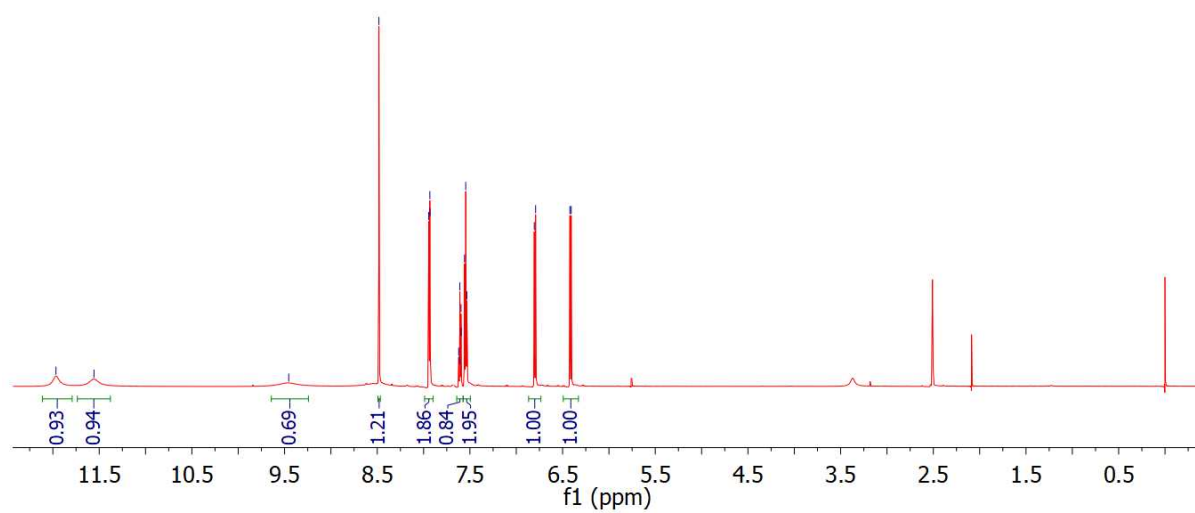
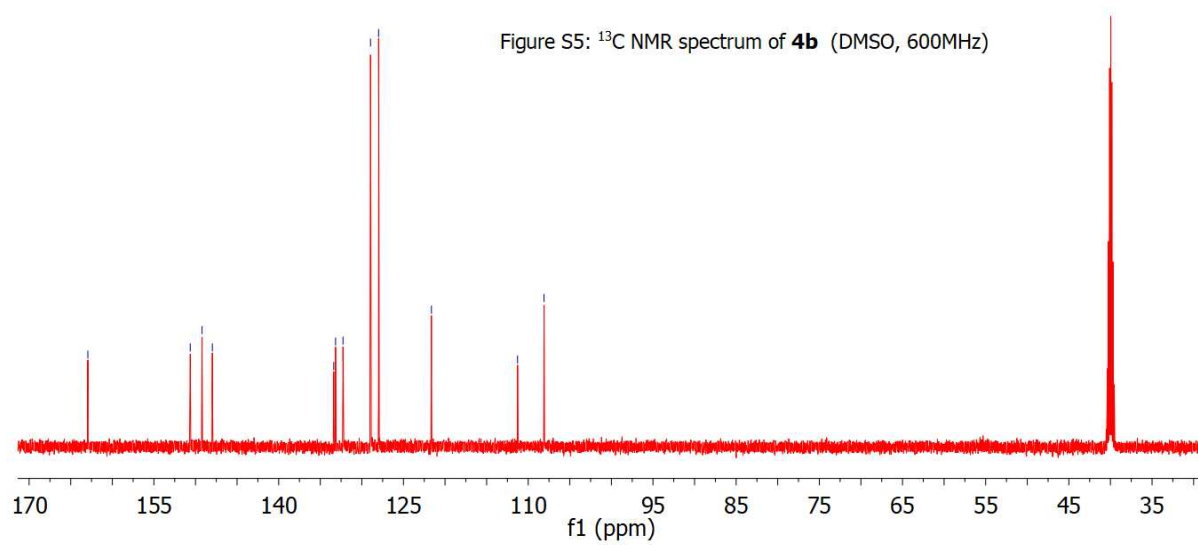
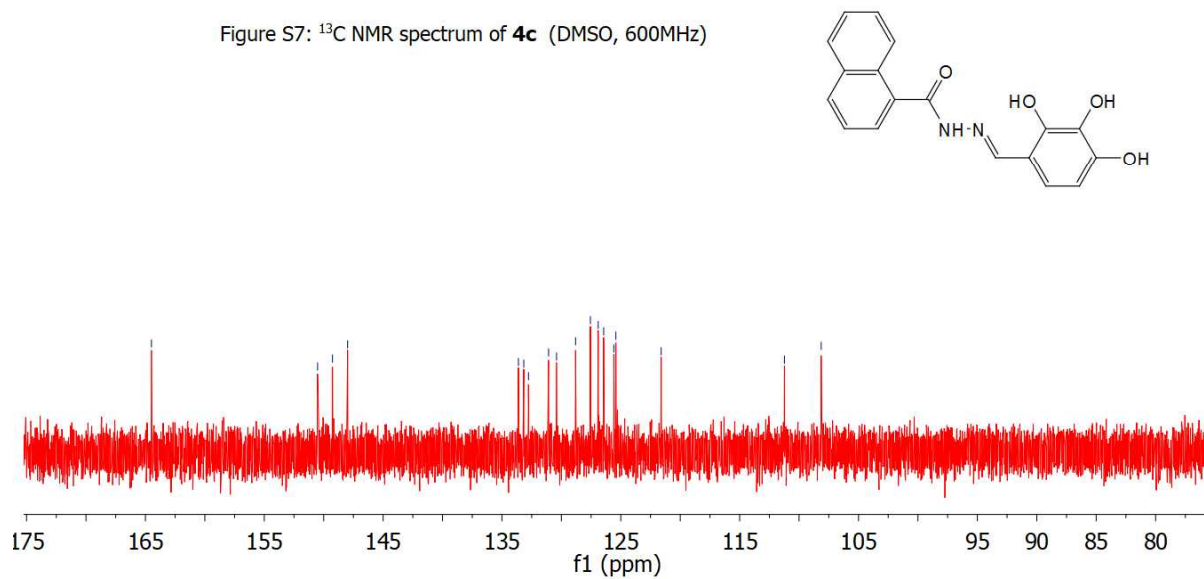
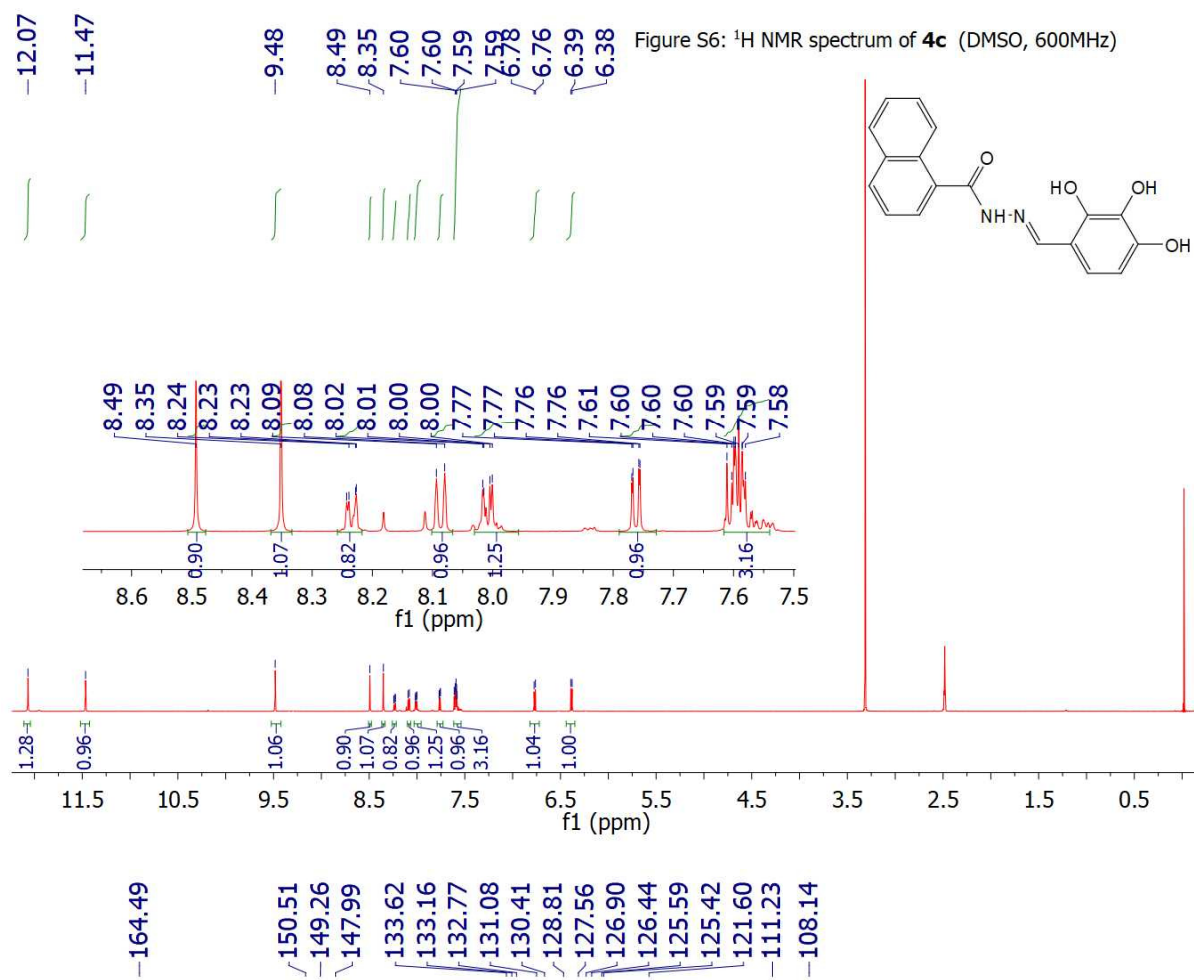
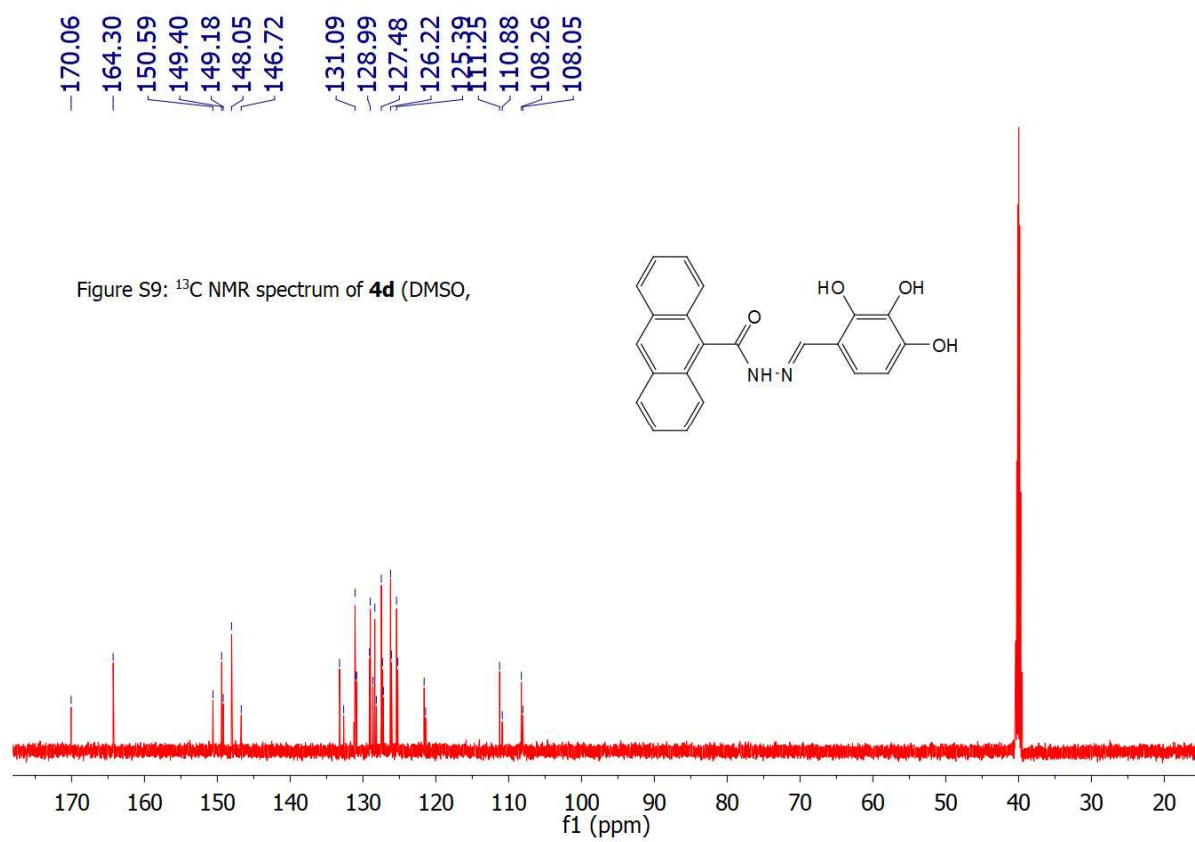
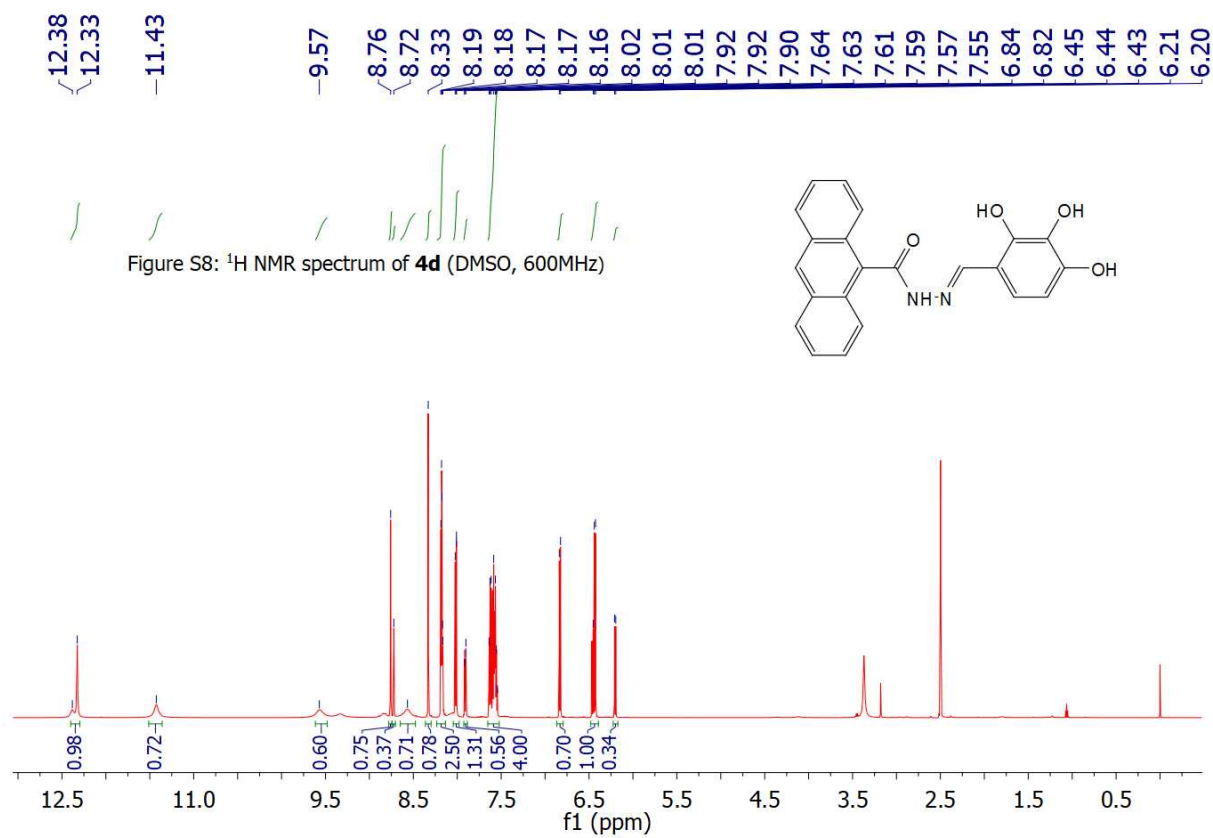


Figure S5: ¹³C NMR spectrum of **4b** (DMSO, 600MHz)







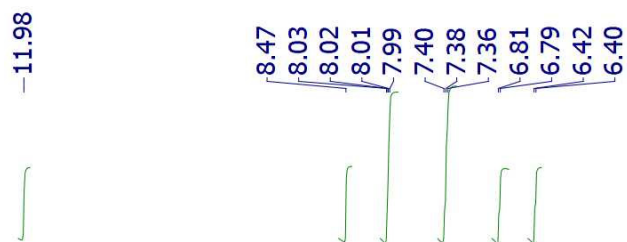


Figure S10: ^1H NMR spectrum of **4e** (DMSO, 600 MHz)

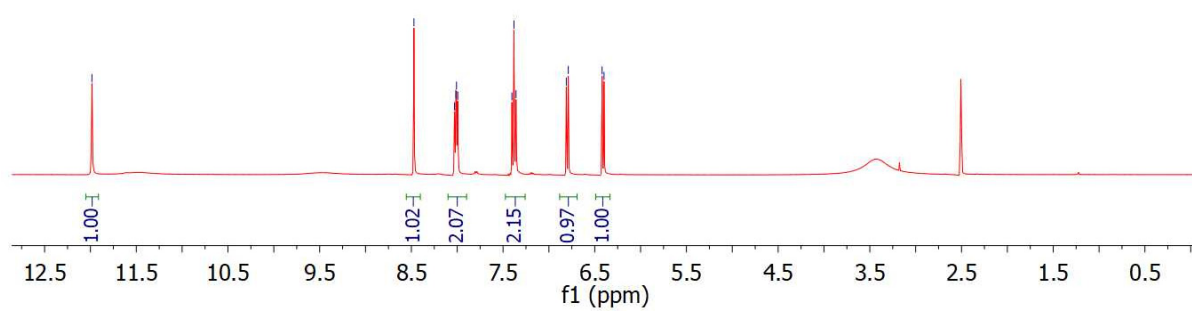
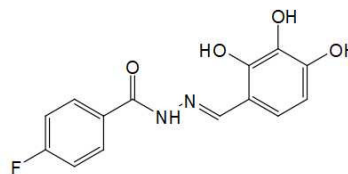
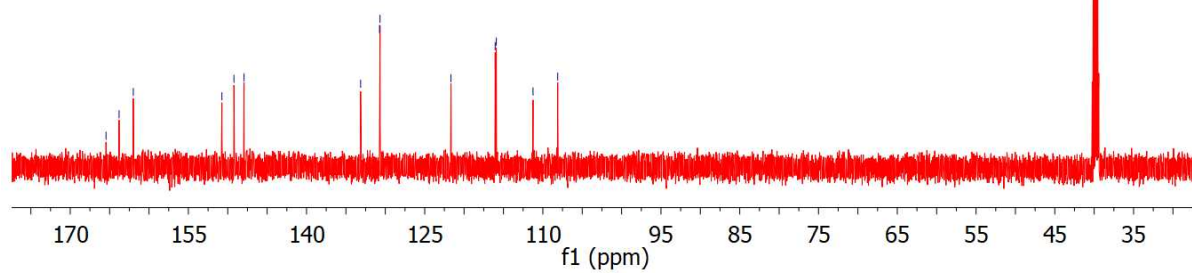
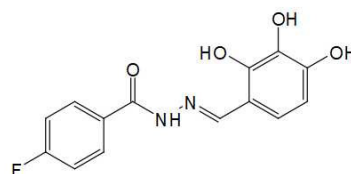


Figure S11: ^{13}C NMR spectrum of **4e** (DMSO, 600 MHz)



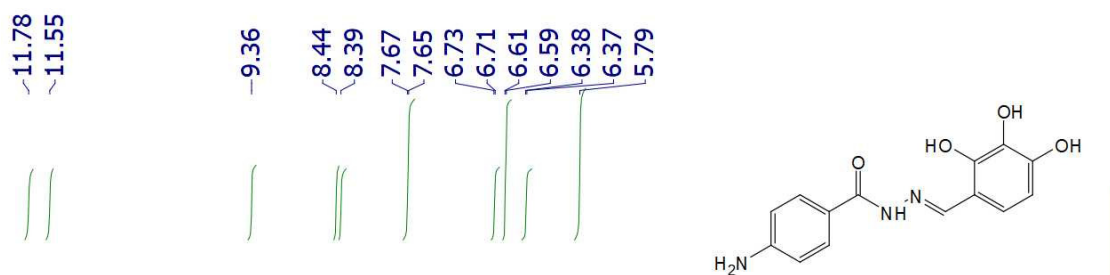


Figure S12: ¹H NMR spectrum of **4f** (DMSO, 600 MHz)

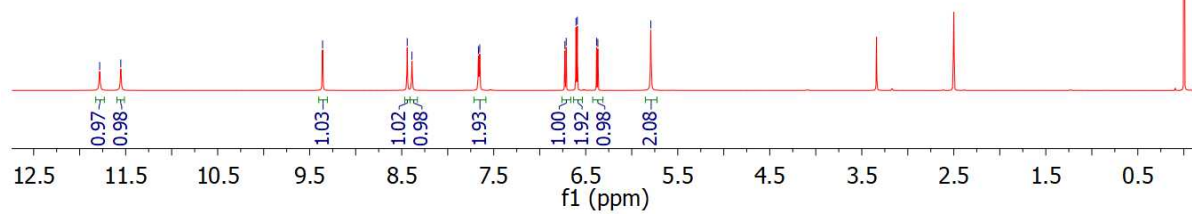
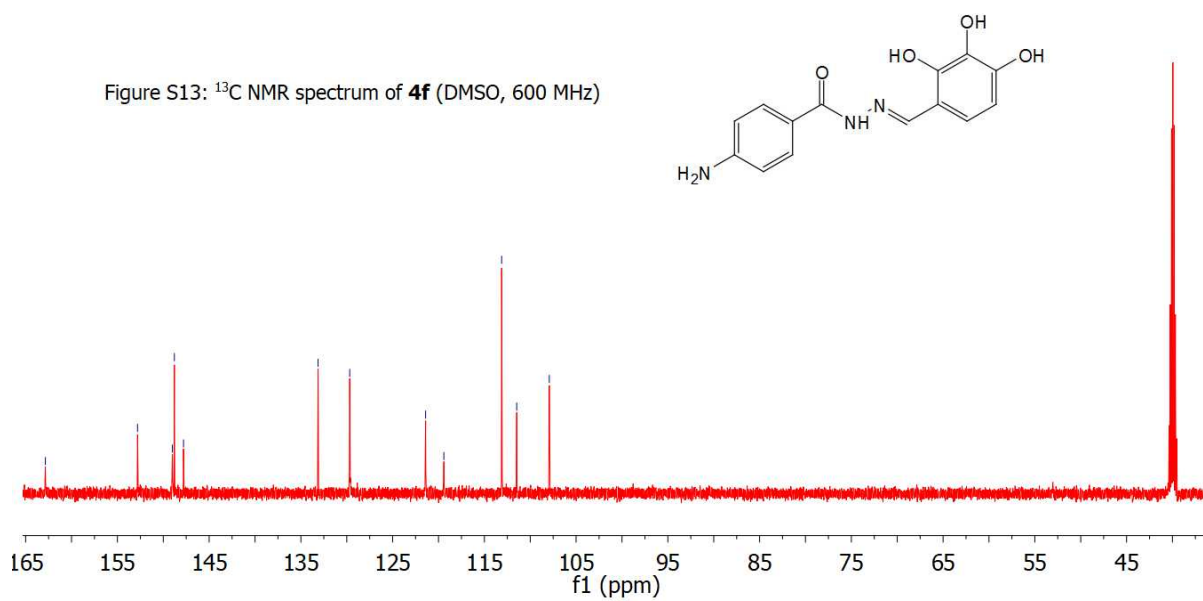


Figure S13: ¹³C NMR spectrum of **4f** (DMSO, 600 MHz)



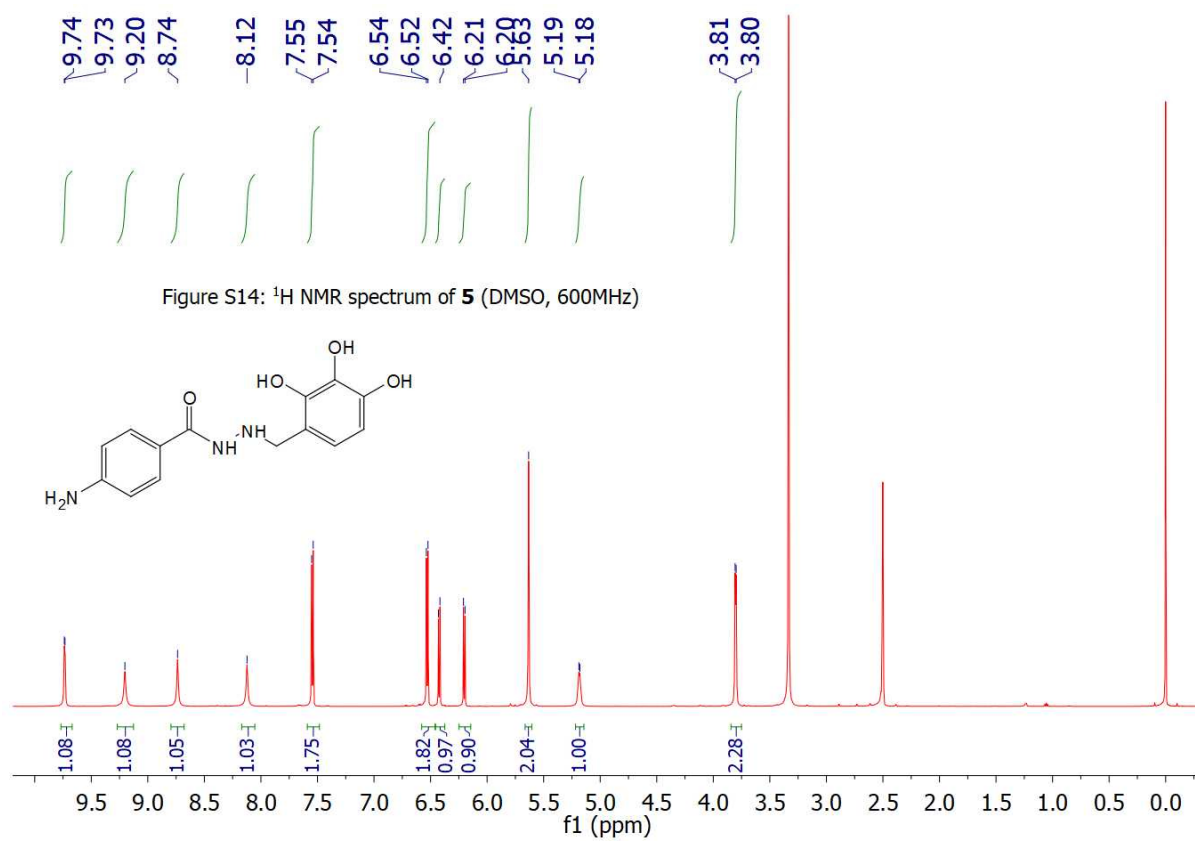


Figure S14: ¹H NMR spectrum of **5** (DMSO, 600MHz)

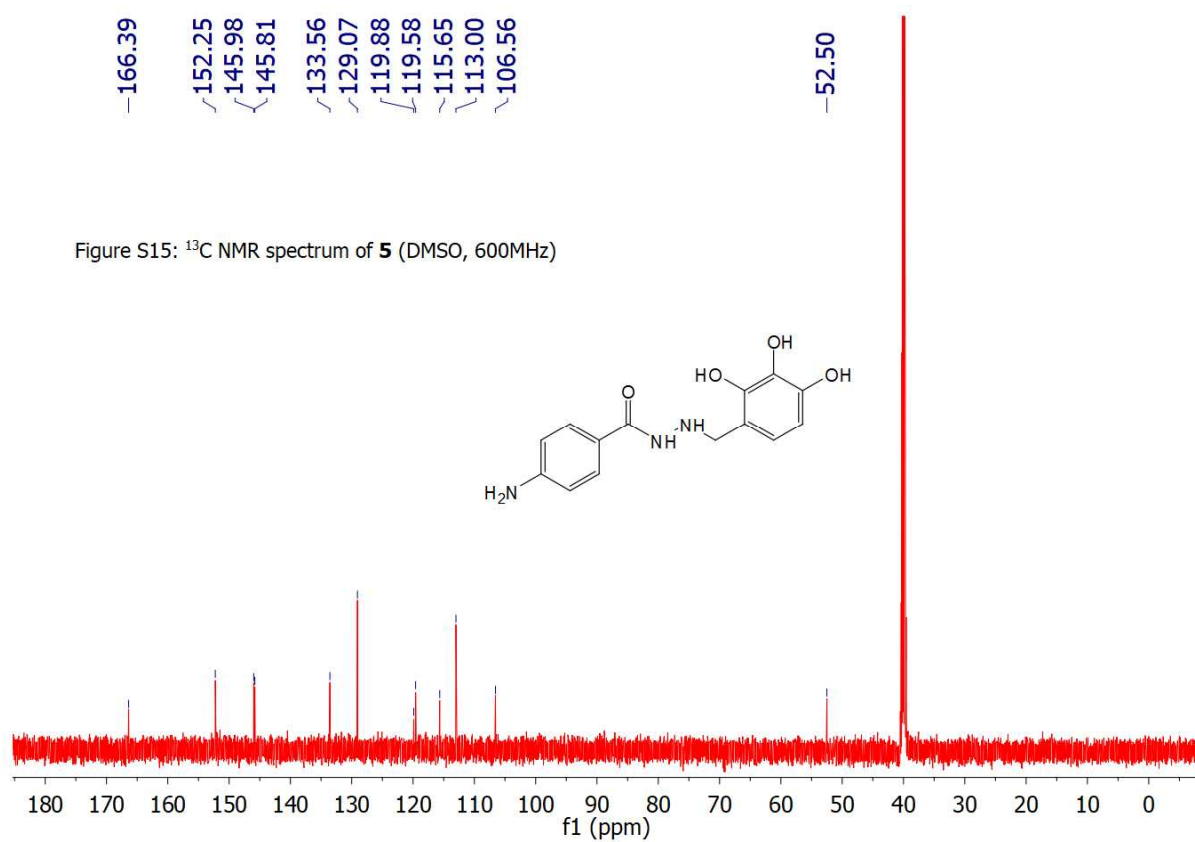
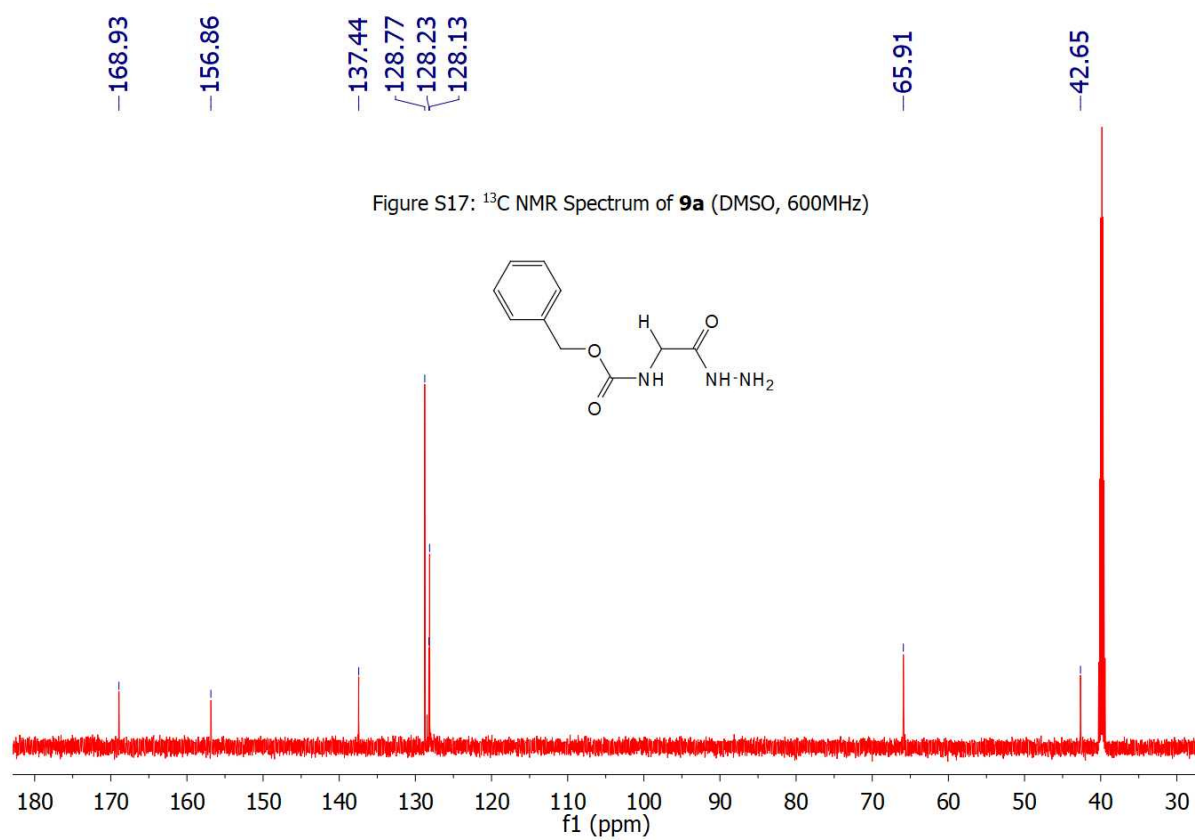
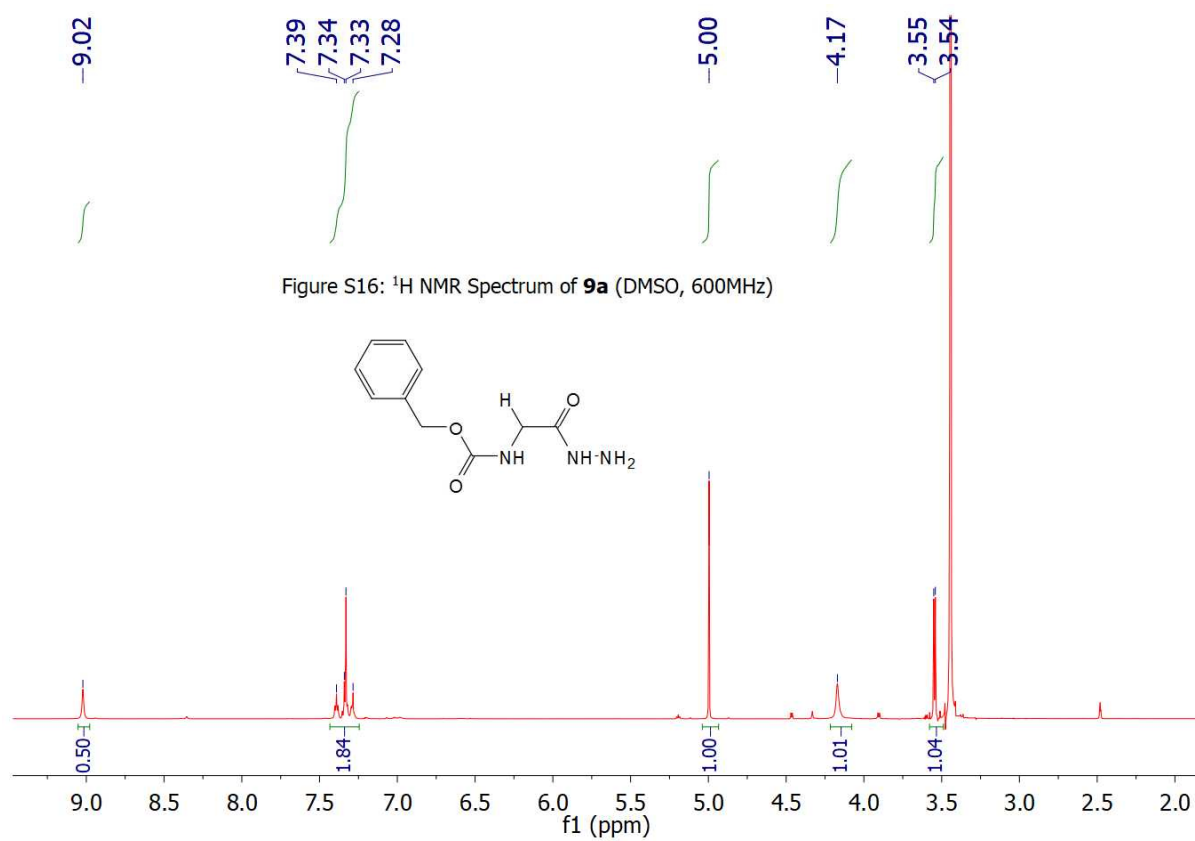
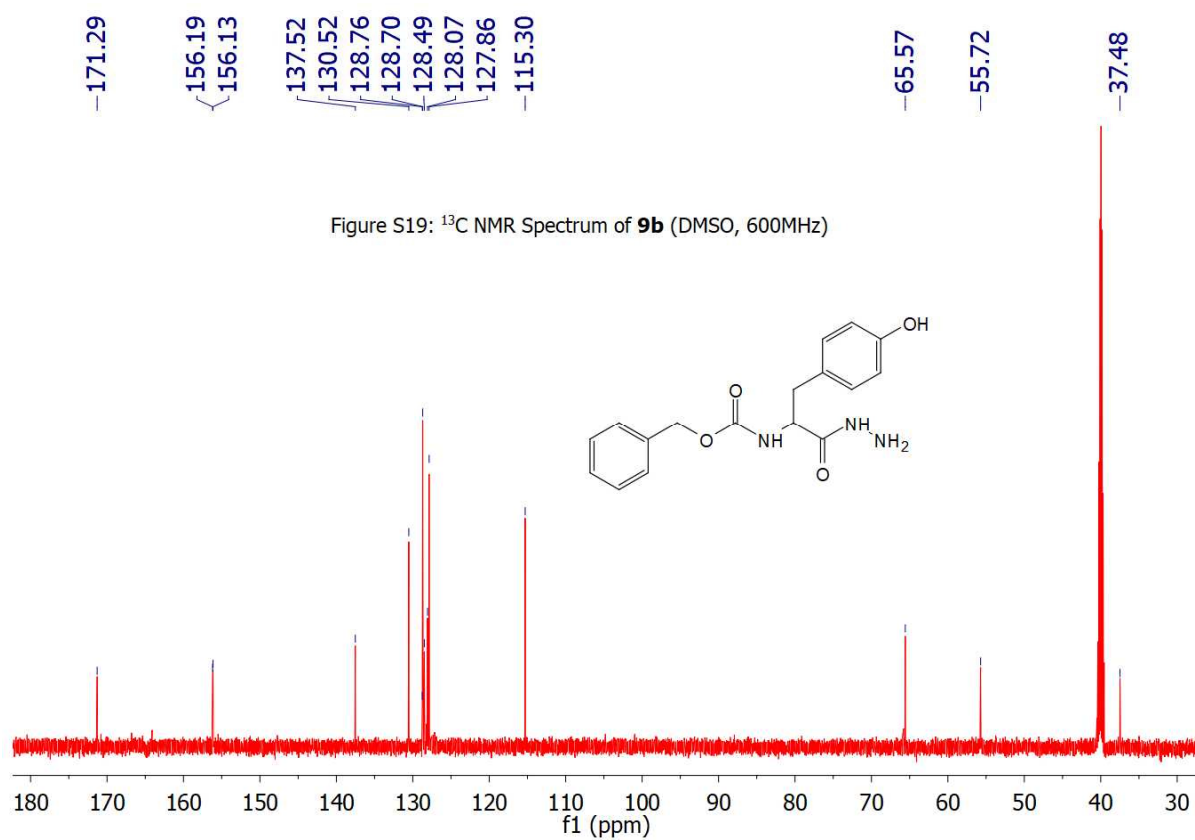
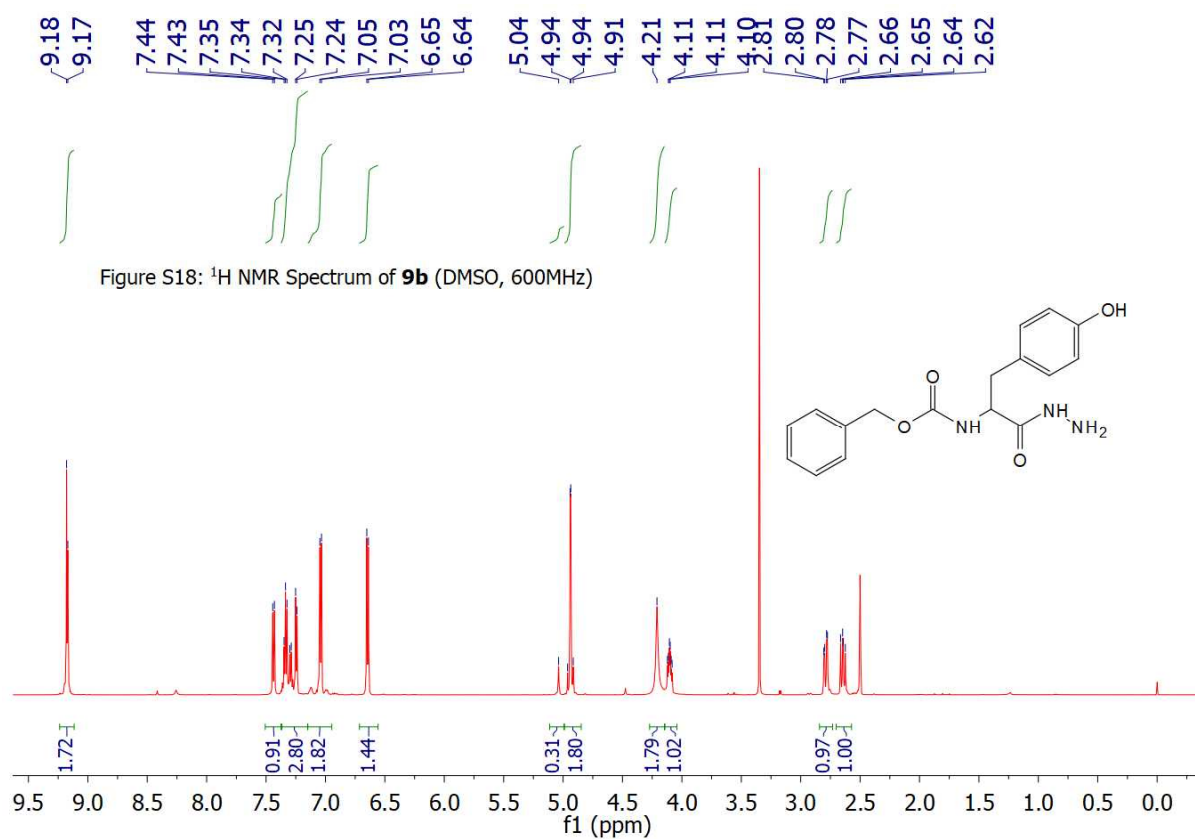
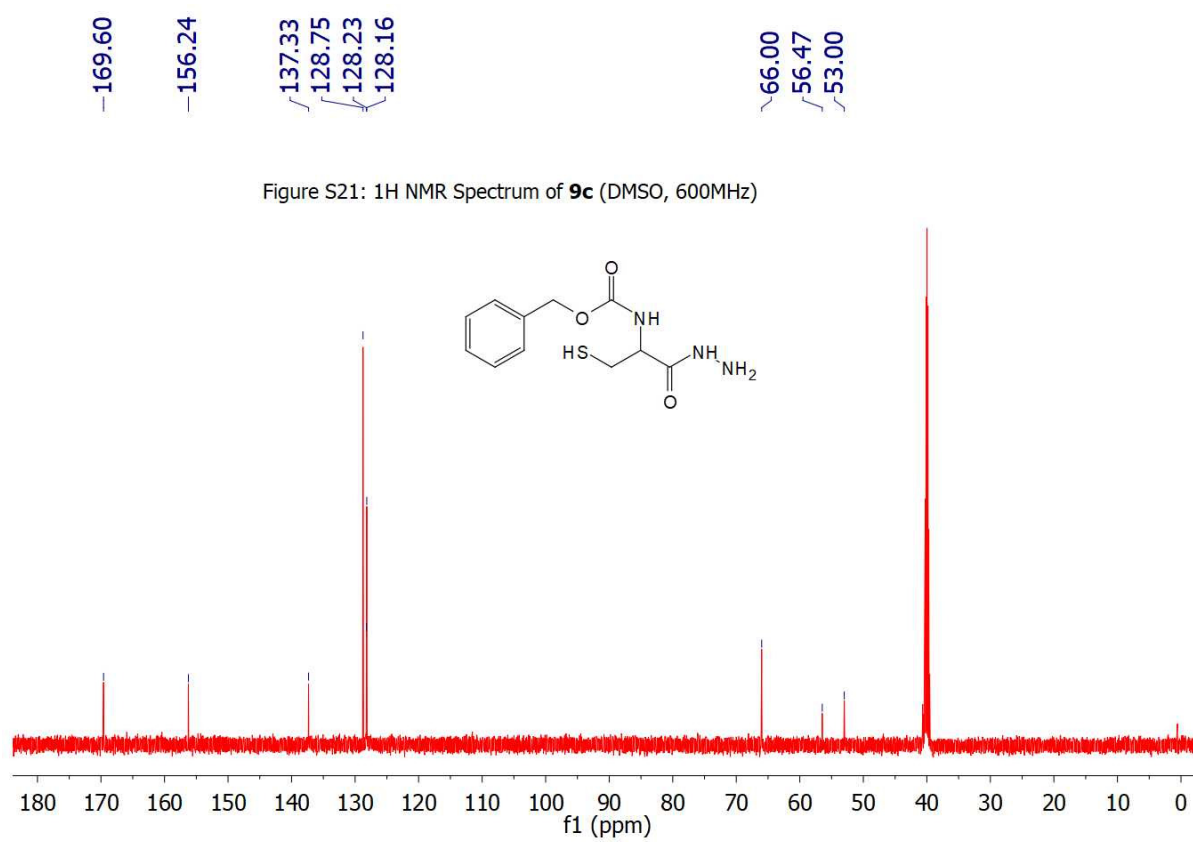
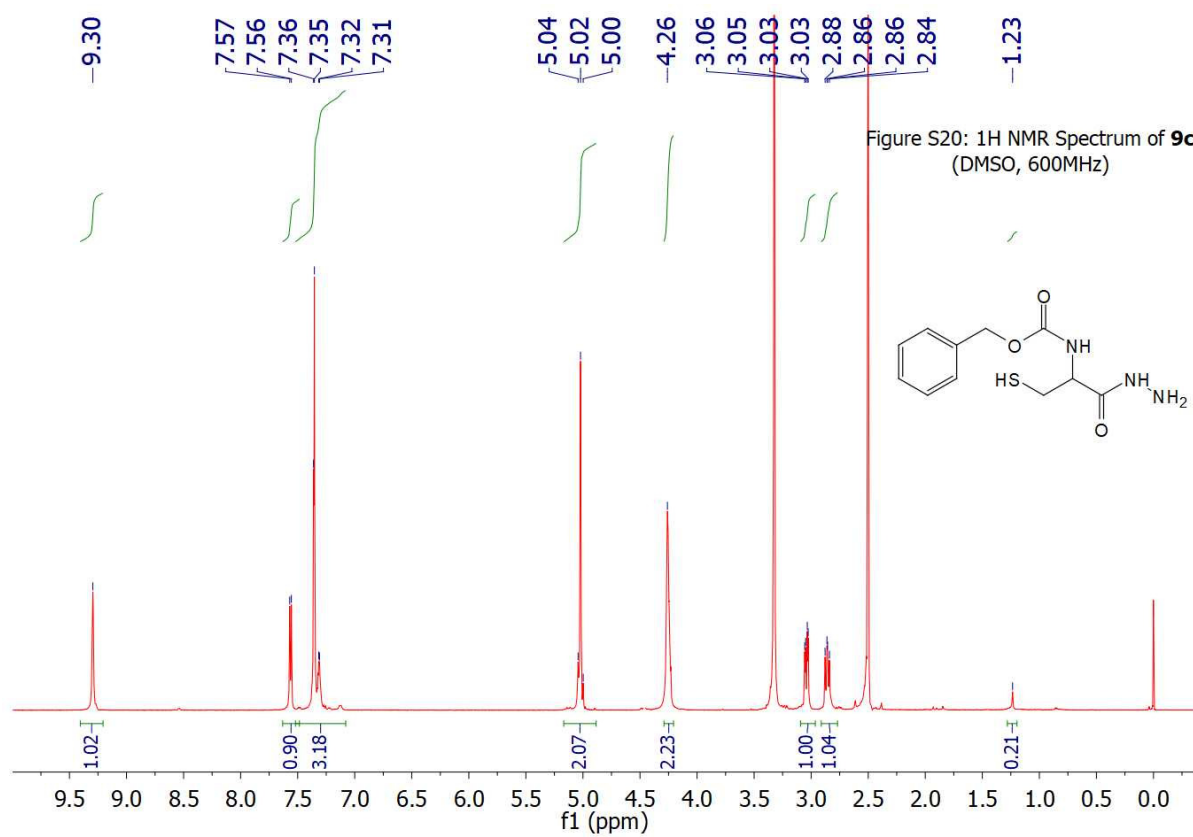


Figure S15: ¹³C NMR spectrum of **5** (DMSO, 600MHz)







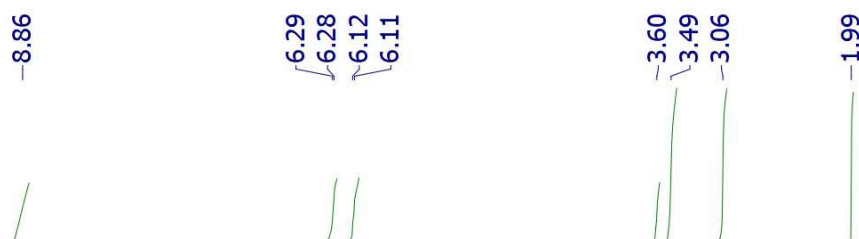


Figure S22: ^1H NMR spectrum of **11** (DMSO, 600MHz)

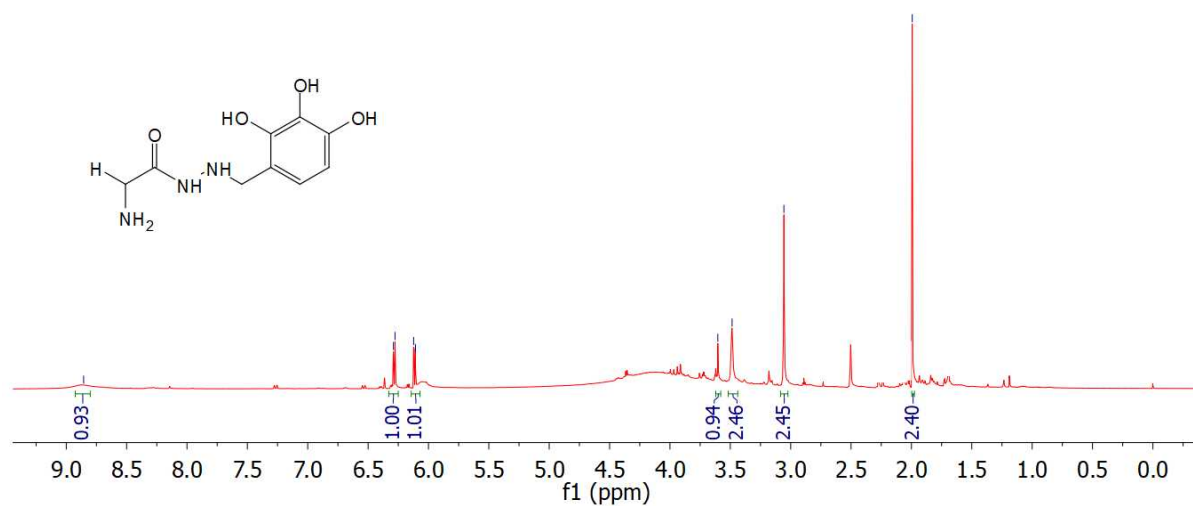
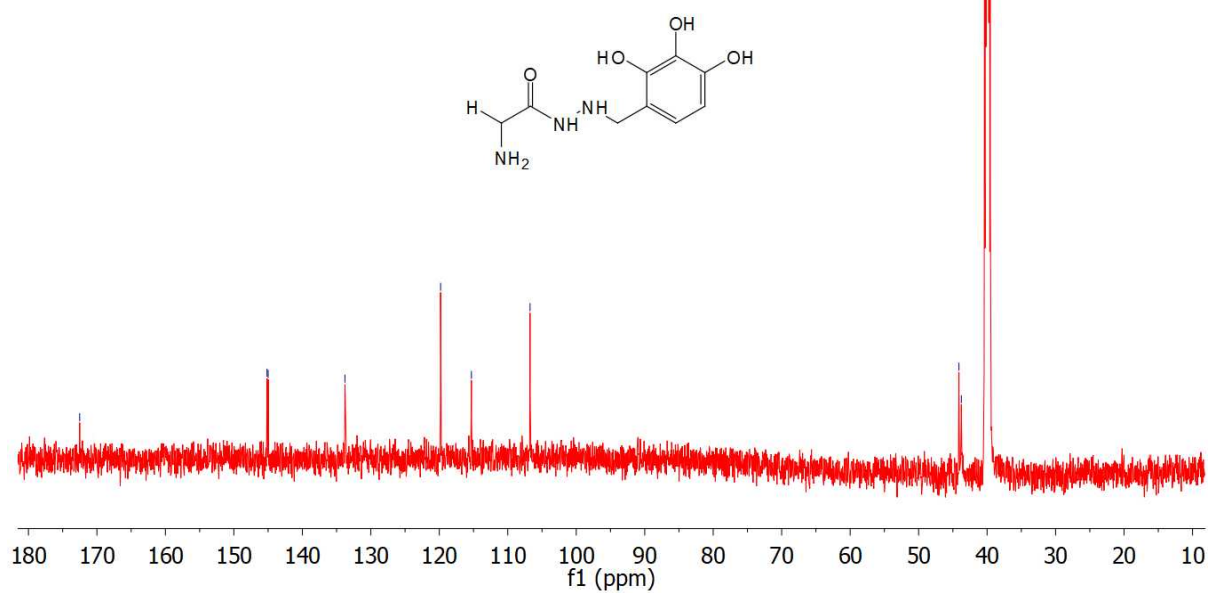


Figure S23: ^{13}C NMR spectrum of **11** (DMSO, 600MHz)



* According to TLC (Thin Layer Chromatography) the compound **11** is pure but probably contains undetectable residual palladium catalyst and water.

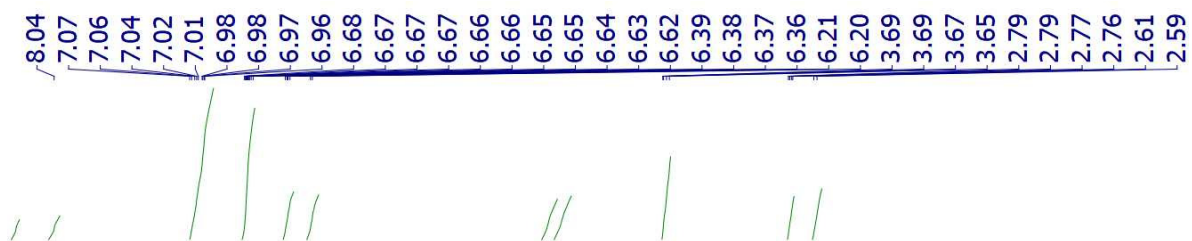
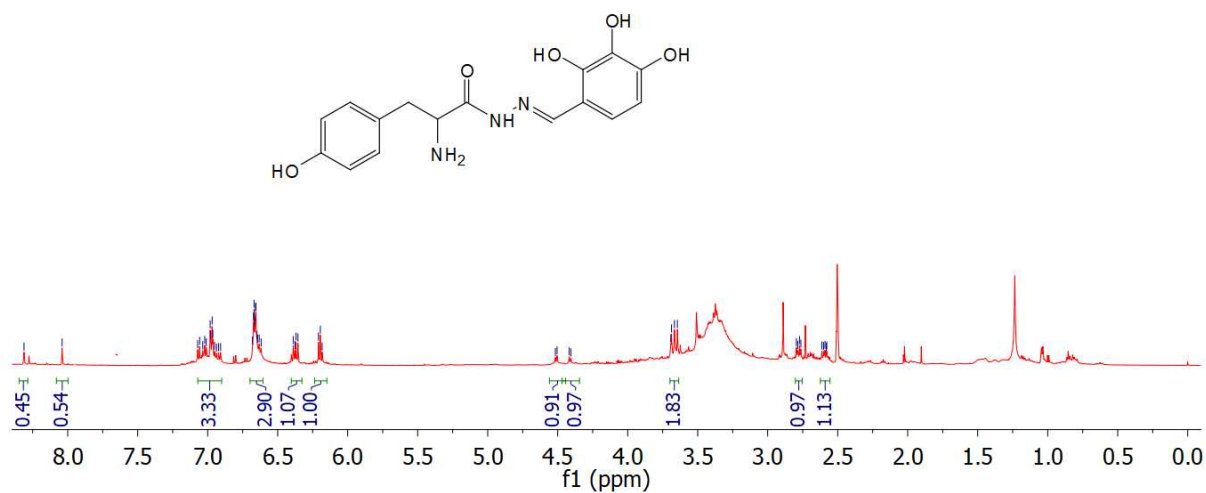


Figure S24: ^1H NMR spectrum of **12** (DMSO, 600MHz)



* According to TLC (Thin Layer Chromatography) the compound **12** is pure but probably contains undetectable residual palladium catalyst and water.

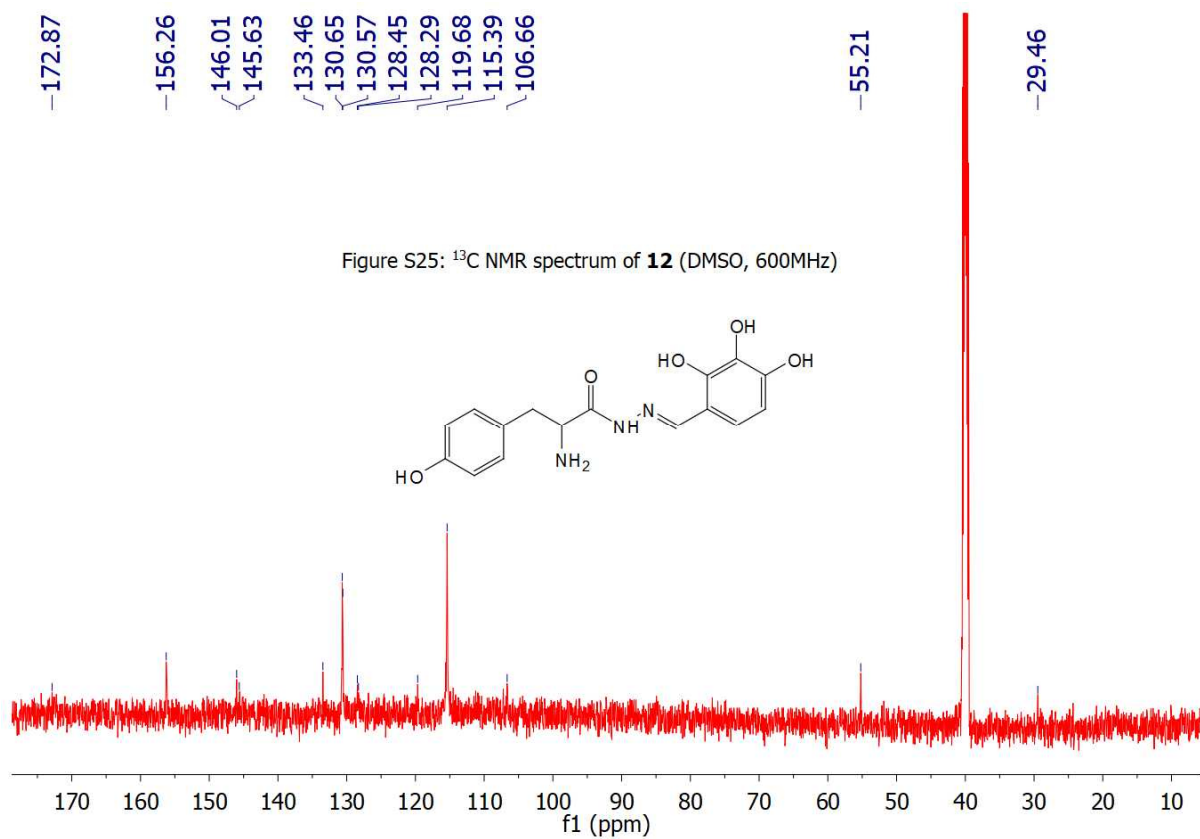


Figure S25: ^{13}C NMR spectrum of **12** (DMSO, 600MHz)

