

Electronic Supplementary Information (ESI)

A comparative study between Cu(INA)₂-MOF and [Cu(INA)₂(H₂O)₄] complex for a click reaction and the Biginelli reaction under solvent-free conditions

Julia C. Mansano Willig^a, Gustavo Granetto^a, Danielly Reginato^a, Felipe R. Dutra^a, Érica Fernanda Poruczinski^a, Isadora M. de Oliveira^b, Helio A. Stefani^b, Silvia D. de Campos^a, Élvio A. de Campos^a, Flávia Manarin^a and Giancarlo V. Botteselle^{a*}

^a*Centro de Engenharias e Ciências Exatas-CECE, Universidade Estadual do Oeste do Paraná, Toledo, 85903-000, PR-Brazil.*

^b*Departamento de Química Fundamental, Instituto de Química, Universidade de São Paulo, São Paulo, Brazil.*

^c*Departamento de Farmácia, Faculdade de Ciências Farmacêuticas, Universidade de São Paulo, São Paulo, 05508-000, SP-Brazil.*

*e-mail: giancarlo.botteselle@unioeste.br or gian.botteselle@gmail.com

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S1. Characterization of $\text{Cu}(\text{INA})_2\text{-MOF}$ and of $[\text{Cu}(\text{INA})_2(\text{H}_2\text{O})_4]$ complex

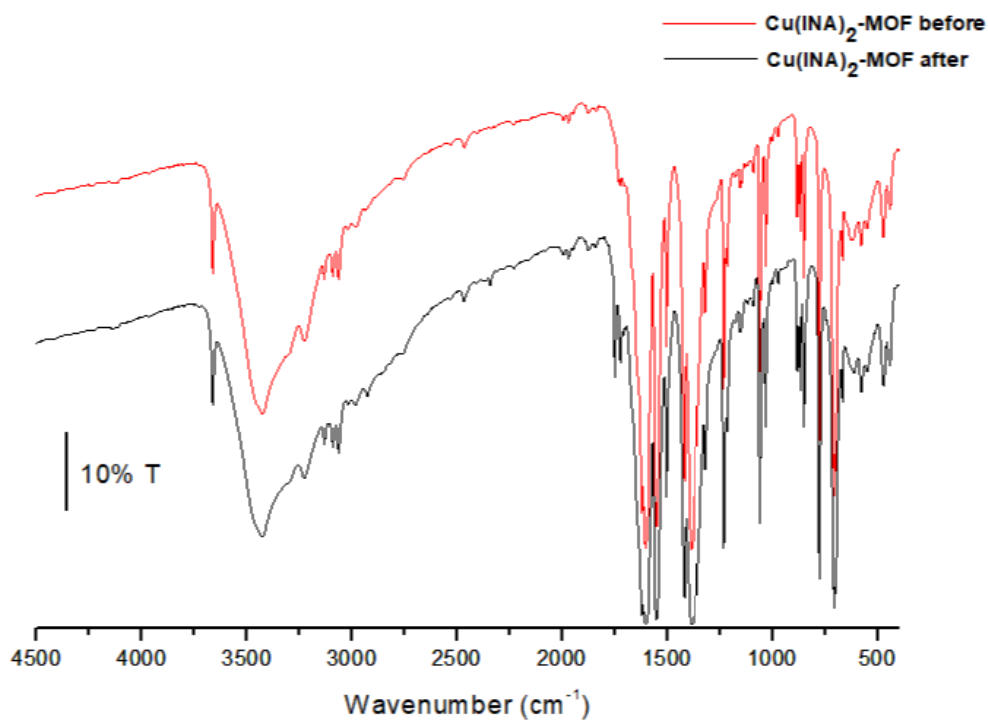


Figure S1. Infrared (IR) analysis of Cu-MOF before and after the reaction.

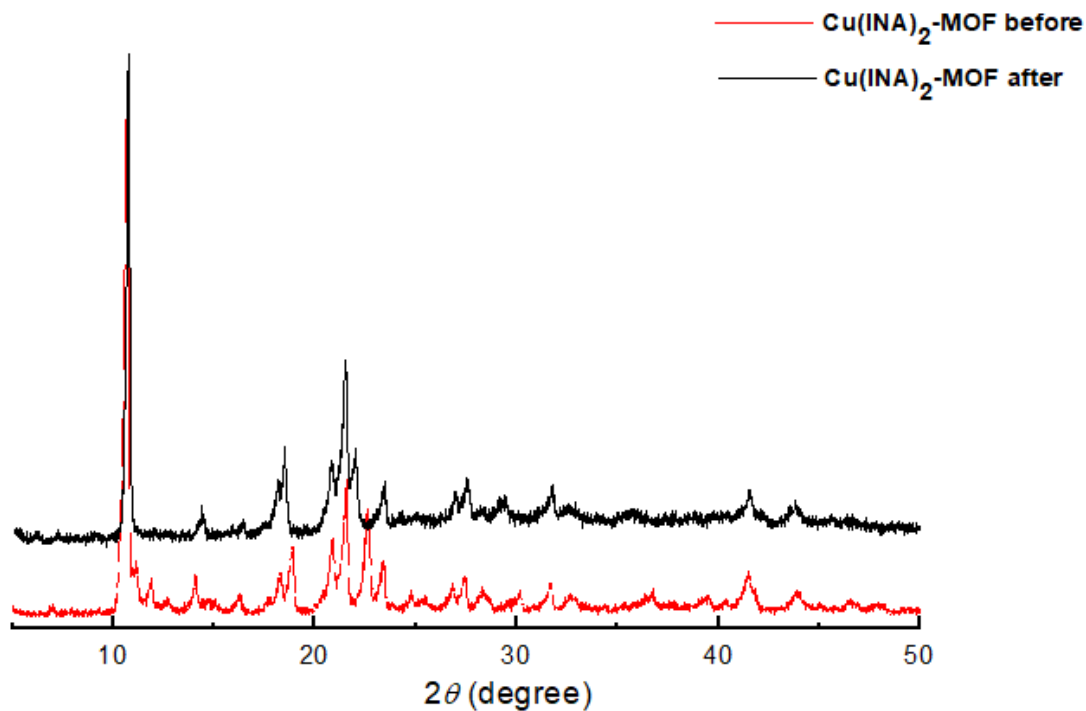


Figure S2. X-ray powder diffraction (XRD) analysis of Cu-MOF before and after the reaction.

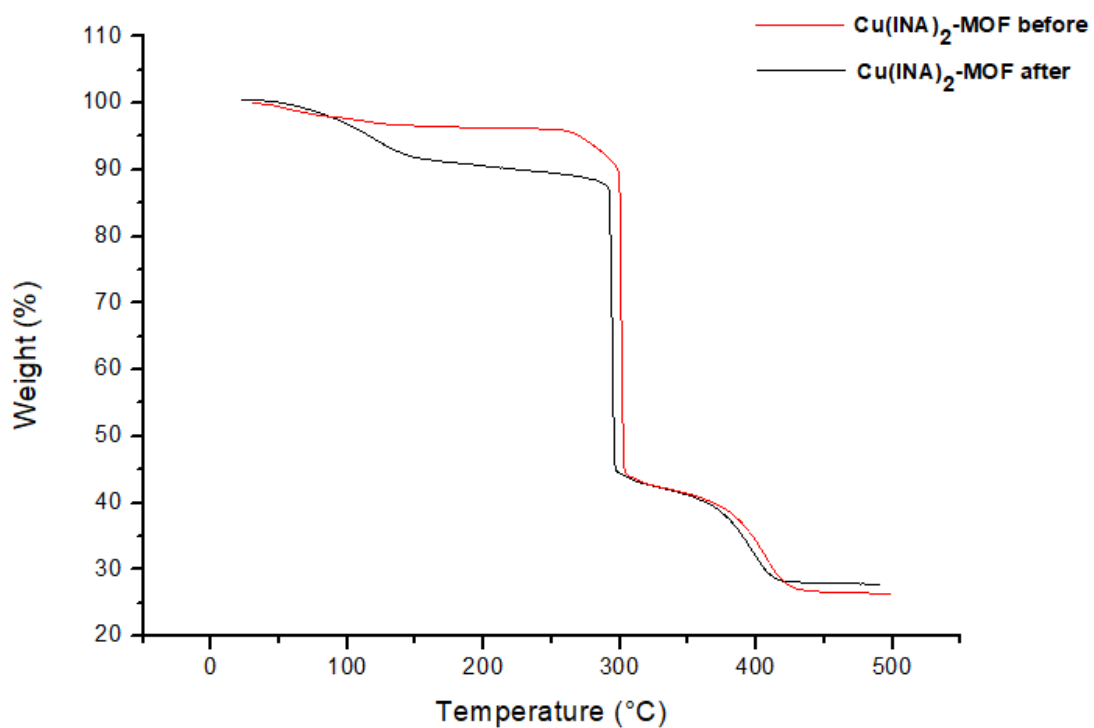


Figure S3. Thermogravimetric analysis (TGA) of Cu-MOF before and after the reaction.

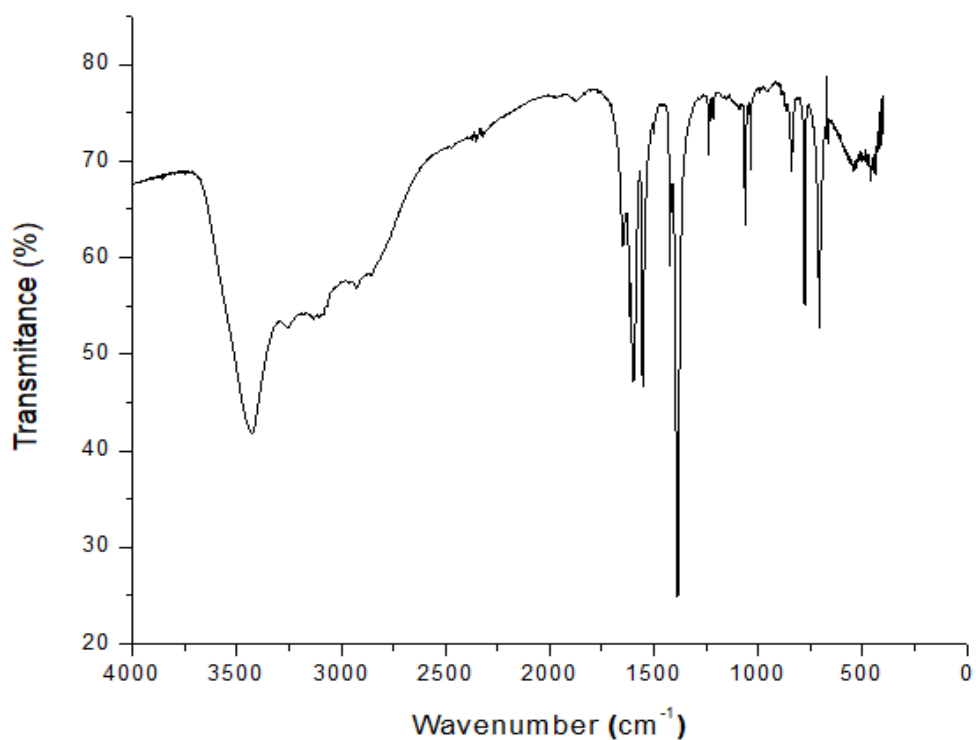


Figure S4. IR analysis of [Cu(INA)₂(H₂O)₄] complex after the reaction.

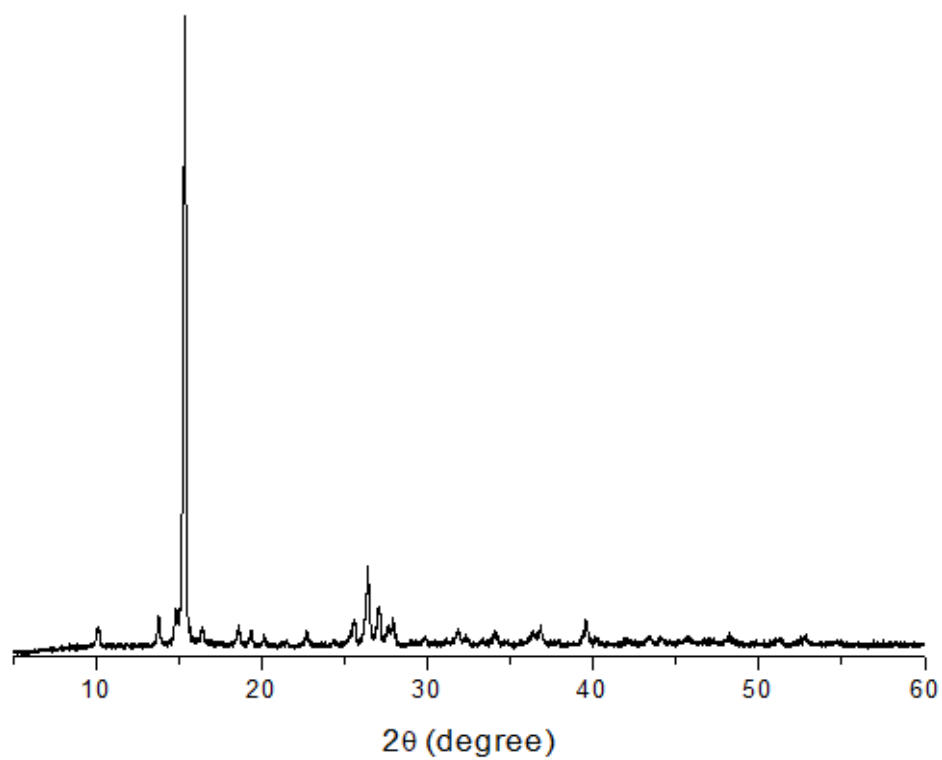


Figure S5. XRD analysis of $[\text{Cu}(\text{INA})_2(\text{H}_2\text{O})_4]$ complex after the reaction.

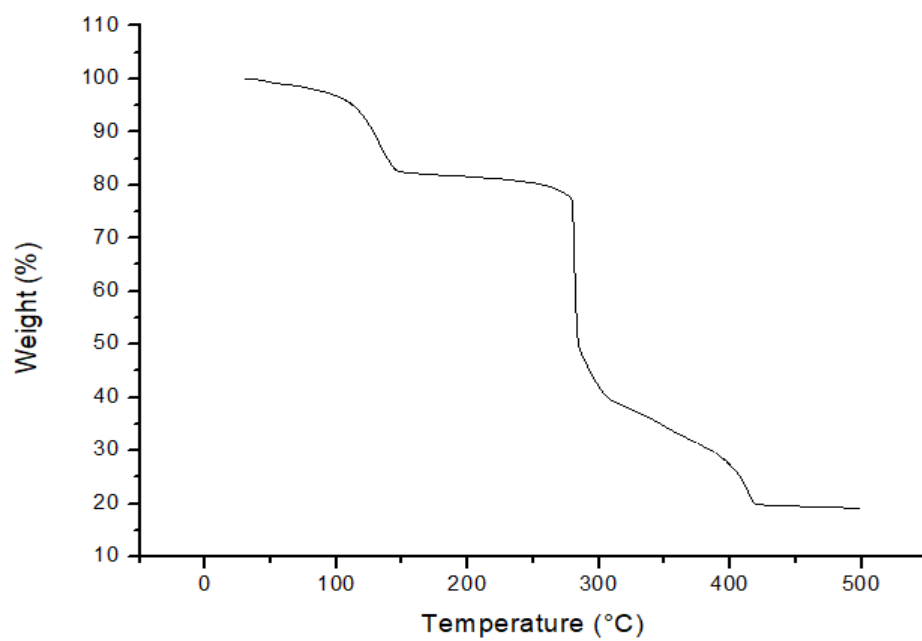
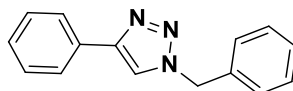


Figure S6. TGA of $[\text{Cu}(\text{INA})_2(\text{H}_2\text{O})_4]$ complex after the reaction.

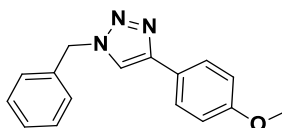
S2. NMR spectroscopic data

1-benzyl-4-phenyl-1*H*-1,2,3-triazole (3a)¹



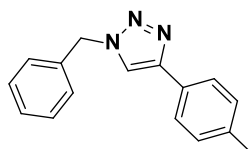
Purification by extraction with dichloromethane. m.p.: 129°C (Lit. 128-129 °C). ¹H NMR (CDCl₃, 300 MHz): δ = 7.78 (d, *J* = 7.8 Hz, 2H); 7.65 (s, 1H); 7.40-7.25 (m, 8H); 5.54 (s, 2H). ¹³C NMR (CDCl₃, 75 MHz): δ = 148.2, 134.7, 130.6, 129.1, 128.8, 128.8, 128.2, 128.0, 125.7, 119.5, 54.2.

1-benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3b)²



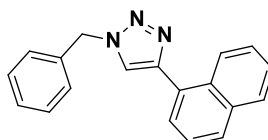
Purification by extraction with dichloromethane. m.p.: 144°C (Lit. 145 °C). ¹H NMR (CDCl₃, 300 MHz): δ = 7.64 (d, *J* = 8.4 Hz, 2H); 7.54 (s, 1H); 7.29-7.18 (m, 5H); 6.83 (d, *J* = 9.6 Hz, 2H); 5.46 (s, 2H); 3.72 (s, 3H). ¹³C NMR (CDCl₃, 75 MHz): δ = 159.8, 134.6, 129.1, 128.8, 128.1, 127.1, 122.9, 118.9, 114.3, 55.3, 54.3.

1-benzyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3c)³



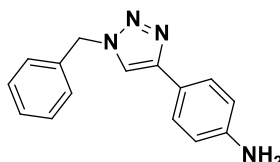
Purification by extraction with dichloromethane. m.p.: 154°C (Lit. 154-155 °C). ¹H NMR (CDCl₃, 300 MHz): δ = 7.6 (d, *J* = 8.1 Hz, 2H); 7.56 (s, 1H); 7.29-7.22 (m, 3H); 7.21-7.19 (m, 2H); 7.10 (d, *J* = 7.8 Hz, 2H); 5.45 (s, 2H); 2.26 (s, 3H). ¹³C NMR (CDCl₃, 75 MHz): δ = 138.1, 134.7, 129.5, 129.1, 128.8, 128.1, 127.6, 125.7, 119.4, 54.3, 21.7.

1-benzyl-4-(naphthalen-1-yl)-1*H*-1,2,3-triazole (3d)⁴



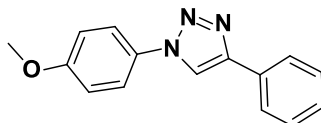
Purification by extraction with dichloromethane. m.p.: 190°C. ¹H NMR (CDCl₃, 300 MHz): δ = 7.85-7.80 (m, 2H); 7.61-7.53 (m, 4H); 7.37-7.27 (m, 7H); 5.52 (s, 2H). ¹³C NMR (CDCl₃, 75 MHz): δ = 141.2, 140.5, 134.4, 129.2, 129.0, 128.8, 128.2, 127.5, 127.5, 127.4, 127.0, 126.2, 119.7, 54.5.

4-(1-benzyl-1H-1,2,3-triazol-4-yl)aniline (3e)⁵



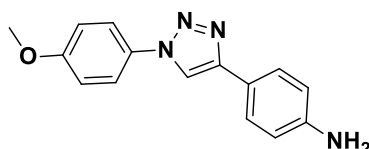
Purification by extraction with dichloromethane. m.p.: 161 °C (Lit. 160-161 °C). ¹H NMR (CDCl₃, 200 MHz): δ = 7.61 (s, 1H); 7.54 (d, *J* = 8.6 Hz, 2H); 7.35-7.26 (m, 5H); 6.70 (d, *J* = 8.4 Hz, 2H); 5.54 (s, 2H), 3.75 (br, 2H). ¹³C NMR (CDCl₃, 50 MHz): δ = 148.6, 146.5, 134.9, 129.1, 128.7, 128.0, 126.9, 121.1, 118.2, 115.2, 54.2.

1-(4-methoxyphenyl)-4-phenyl-1H-1,2,3-triazole (3f)⁶



Cu-MOF: Purification by extraction with dichloromethane. Cu-Complex: Purification by column chromatography, eluent: hexane/ethyl acetate 80:20. m.p.: 160 °C (Lit. 160-161 °C). ¹H NMR (CDCl₃, 300 MHz): δ = 8.05 (s, 2H); 7.82 (d, *J* = 7.8 Hz, 2H); 7.59 (d, *J* = 8.7 Hz, 2H); 7.39-7.25 (m, 3H); 6.94 (d, *J* = 8.7 Hz, 2H); 3.79 (s, 3H). ¹³C NMR (CDCl₃, 75 MHz): 159.9, 148.2, 130.6, 130.4, 128.9, 128.3, 125.8, 122.2, 117.8, 114.8, 55.6.

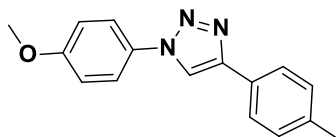
4-(1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)aniline (3g)⁷



Cu-MOF: Purification by extraction with dichloromethane. Cu-Complex: Purification by column chromatography, eluent: hexane/ethyl acetate 80:20. m.p.: 160 °C (Lit. 160-161 °C). ¹H NMR (CD₃OD, 300 MHz): δ = 8.55 (s, 1H); 7.77 (d, *J* = 8.7 Hz, 2H); 7.63 (d, *J* = 8.4 Hz, 2H); 7.12 (d, *J* = 9 Hz, 2H); 6.78 (d, *J* = 8.1 Hz, 2H); 3.88 (s, 3H).

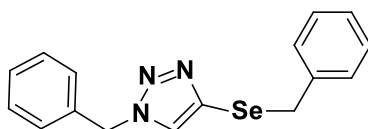
. ^{13}C NMR (CDCl_3 , 75 MHz): 159.9, 146.8, 146.4, 130.9, 129.9, 127.2, 122.3, 115.4, 114.9, 113.9, 55.8.

1-(4-methoxyphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3h)⁸



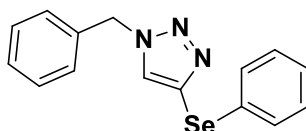
Purification by extraction with dichloromethane. m.p.: °C (Lit. °C). ^1H NMR (CDCl_3 , 400 MHz): δ = 8.07 (s, 1H); 7.78 (d, J = 8 Hz, 2H); 7.65 (d, J = 8.8 Hz, 2H); 7.24 (d, J = 7.6 Hz, 2H); 7.00 (d, J = 8.8 Hz, 2H); 3.85 (s, 3H); 2.38 (s, 3H). ^{13}C NMR (CDCl_3 , 75 MHz): 159.8, 138.2; 130.6, 129.6, 127.6, 125.7, 122.1, 117.6, 114.8, 55.6, 21.7.

1-benzyl-4-(benzylselanyl)-1*H*-1,2,3-triazole (3i)



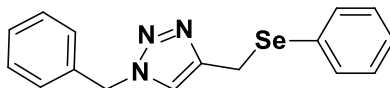
Cu-MOF: Purification by extraction with dichloromethane. Cu-Complex: Purification by column chromatography, eluent: hexane/ethyl acetate 80:20. m.p.: 180 °C. ^1H NMR (CDCl_3 , 300 MHz): δ = 7.42-7.40 (m, 2H); 7.37-7.34 (m, 3H); 7.22-7.16 (m, 5H); 7.07 (s, 1H); 5.42 (s, 2H); 4.13 (s, 2H). ^{13}C NMR (CDCl_3 , 75 MHz): 146.6, 145.9, 134.7, 134.6, 133.5, 129.6, 129.1, 128.7, 127.9, 121.7, 54.1, 20.7. HRMS (APCI-ESI-TOF, positive mode) m/z calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_3\text{NaSe}$ [$\text{M}+\text{Na}$]: 352,0329; found 352,0205.

1-benzyl-4-(phenylselanyl)-1*H*-1,2,3-triazole (3j)⁹



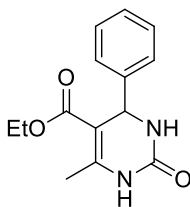
Cu-MOF: Purification by extraction with dichloromethane. Cu-Complex: Purification by column chromatography, eluent: hexane/ethyl acetate 80:20. m.p.: °C (Lit. 56-58 °C). ^1H NMR (CDCl_3 , 300 MHz): δ = 7.55 (s, 1H); 7.42-7.35 (m, 5H); 7.26-7.20 (m, 5H); 5.52 (s, 2H). ^{13}C NMR (CDCl_3 , 75 MHz): 134.2, 132.6, 131.4, 130.6, 129.3, 129.2, 128.9, 128.5, 128.1, 127.2, 54.3.

1-benzyl-4-((phenylselanyl)methyl)-1*H*-1,2,3-triazole (3k)⁹



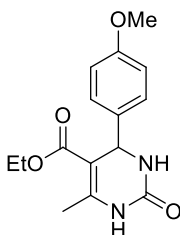
Cu-MOF: Purification by extraction with dichloromethane. Cu-Complex: Purification by column chromatography, eluent: hexane/ethyl acetate 80:20. m.p.: 50°C (Lit. 35-36 °C). ¹H NMR (CDCl₃, 300 MHz): δ = 7.38-7.21 (m, 3H); 7.19-7.06 (m, 8H); 5.45 (s, 2H); 4.06 (s, 2H). ¹³C NMR (CDCl₃, 75 MHz): 138.5, 134.4, 131.5, 129.1, 128.9, 128.8, 128.3, 128.1, 128.0, 126.9, 54.1, 32.0.

Ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7a)¹⁰



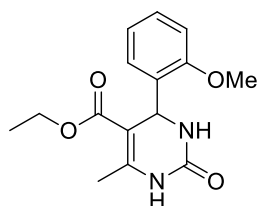
Purification by column chromatography, eluent: hexane/ethyl acetate 60:40. ¹H NMR (DMSO-d₆, 300 MHz): δ = 7.96 (br, 1H); 7.25-7.19 (m, 5H); 5.67 (br, 1H); 5.33 (s, 1H); 4.01 (q, *J* = 7.2 Hz, 2H); 2.27 (s, 3H); 1.09 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz): δ = 165.7, 153.3, 146.3, 143.8, 128.8, 128.1, 126.7, 101.5, 60.1, 55.9, 18.8, 14.2.

Ethyl-4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7b)¹⁰



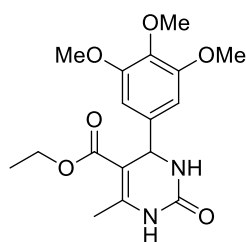
Purification by column chromatography, eluent: hexane/ethyl acetate 65:35. ¹H NMR (DMSO-d₆, 300 MHz): δ = 9.11 (sl, 1H); 7.63 (sl, 1H); 7.14 (d, *J* = 8.4 Hz, 2H); 6.87 (d, *J* = 8.7 Hz, 2H); 5.10 (s, 1H); 3.98 (q, *J* = 7.2 Hz, 2H); 3.72 (s, 3H); 2.24 (s, 3H); 1.10 (t, *J* = 7.2, Hz, 3H); ¹³C NMR (DMSO-d₆, 75 MHz): δ = 165.3, 158.4, 152.1, 147.9, 137.0, 127.4, 113.7, 99.6, 59.1, 55.0, 53.3, 17.7, 14.1.

Ethyl-4-(2-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7c)¹¹



Purification by column chromatography, eluent: hexane/ethyl acetate 65:35. ¹H NMR (DMSO-d₆, 300 MHz): δ = 9.15 (s, 1H); 7.59 (s, 1H); 7.19-7.11 (m, 4H); 5.41 (s, 1H); 3.88 (q, *J* = 6.9 Hz, 2H); 2.41 (s, 3H); 2.29 (s, 3H); 0.98 (t, *J* = 7.2 Hz, 3H). ¹³C NMR (DMSO-d₆, 75 MHz): δ = 165.8, 152.6, 148.6, 142.4, 136.8, 129.3, 126.6, 99.9, 59.6, 54.1, 21.1, 18.2, 14.6.

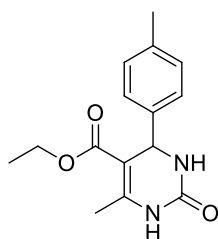
Ethyl-6-methyl-2-oxo-4-(3,4,5-trimethoxyphenyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7d)¹¹



Purification by column chromatography, eluent: hexane/ethyl acetate 60:40. ¹H NMR (DMSO-d₆, 300 MHz): δ = 9.15 (s, 1H); 7.68 (s, 1H); 6.54 (s, 2H); 5.13 (s, 1H); 4.03 (q, *J* = 7.2 Hz, 2H); 3.73 (s, 6H); 3.64 (s, 3H); 1.13 (t, *J* = 7.2, 3H); ¹³C NMR (DMSO-d₆, 75 MHz): δ = 165.9, 153.2, 152.7, 148.9, 140.9, 104.0, 99.6, 60.4, 59.7, 56.3, 54.4, 18.2, 14.6.

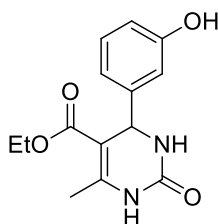
Ethyl-6-methyl-2-oxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7e)

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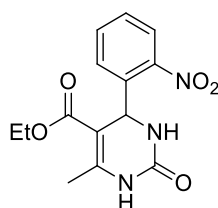
Purification by column chromatography, eluent: hexane/ethyl acetate 60:40. ¹H NMR (DMSO-d₆, 300 MHz): δ = 9.12 (s, 1H); 7.65 (s, 1H); 7.12 (s, 4H); 5.11 (s, 1H); 3.98 (q, *J* = 6.9 Hz, 2H); 2.26 (s, 3H); 2.24 (s, 3H); 1.10 (t, *J* = 6.9, 3H); ¹³C NMR (DMSO-d₆, 75 MHz): δ = 165.8, 152.6, 148.6, 142.4, 136.8, 129.3, 126.6, 99.9, 59.6, 54.1, 21.1, 18.2, 14.6.

Ethyl-4-(3-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7f)¹²



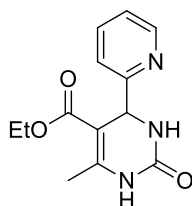
Purification by column chromatography, eluent: hexane/ethyl acetate 65:35. ¹H NMR (DMSO-d₆, 300 MHz): δ = 9.32 (s, 1H); 9.13 (s, 1H); 7.66 (s, 1H); 7.09 (t, *J* = 7.8 Hz, 1H); 6.65 (m, 3H); 5.43 (s, 1H); 5.08 (s, 1H); 4.00 (q, *J* = 7.2 Hz, 2H); 2.24 (s, 3H); 1.12 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (DMSO-d₆, 75 MHz): δ = 165.4, 157.3, 152.2, 148.0, 146.2, 129.2, 116.9, 114.1, 113.1, 99.4, 59.1, 53.8, 17.7, 14.0.

Ethyl-6-methyl-4-(2-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7g)¹³



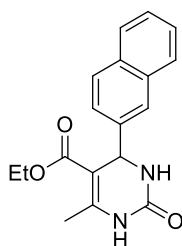
Purification by column chromatography, eluent: hexane/ethyl acetate 65:35. ¹H NMR (DMSO-d₆, 300 MHz): δ = 9.25 (s, 1H); 7.65 (s, 1H); 7.57 (d, *J* = 7.2 Hz, 1H); 7.37-7.29 (m, 2H); 7.18 (t, *J* = 7.2 Hz, 1H); 5.62 (s, 1H); 3.90 (q, *J* = 6.9 Hz, 2H); 2.31 (s, 3H); 0.99 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (DMSO-d₆, 75 MHz): δ = 164.9, 151.2, 149.1, 143.3, 133.7, 132.5, 128.7, 128.3, 122.2, 98.2, 58.9, 54.0, 17.6, 13.9.

Ethyl-6-methyl-2-oxo-4-(pyridin-2-yl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7h)¹⁴



Purification by column chromatography, eluent: hexane/ethyl acetate 65:35. ^1H NMR (DMSO- d_6 , 300 MHz): δ = 9.09 (s, 1H); 8.51 (s, 1H) 7.76-7.58 (m, 2H); 7.25-7.23 (m, 2H);); 5.21 (s, 1H); 3.97 (q, J = 6.9 Hz, 3H); 2.23 (s, 3H); 1.08 (t, J = 6.9 Hz, 3H); ^{13}C NMR (DMSO- d_6 , 75 MHz): δ = 165.3, 162.3, 152.3, 149.2, 148.9, 136.5, 122.5, 120.8, 98.04, 59.0, 55.7, 17.8, 14.0.

Ethyl-6-methyl-4-(naphthalen-2-yl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (7i)¹⁰



Purification by column chromatography, eluent: hexane/ethyl acetate 60:40. ^1H NMR (DMSO- d_6 , 300 MHz): δ = 9.21 (s, 1H); 8.31 (d, J = 8.1 Hz, 1H); 7.93 (d, J = 7.8 Hz, 1H); 7.84 (d, J = 9.0 Hz, 1H); 7.70 (s, 1H); 7.60-7.40 (m, 4H); 6.06 (s, 1H); 3.80 (q, J = 7.2 Hz, 2H); 2.36 (s, 3H); 0.81 (q, J = 7.2 Hz, 3H); ^{13}C NMR (DMSO- d_6 , 75 MHz): δ = 165.2, 151.6, 148.6, 140.4, 133.4, 130.0, 128.4, 127.8, 125.9, 125.6, 125.5, 124.1, 123.6, 99.1, 58.9, 49.8, 17.7, 13.7.

S3. ^1H NMR and ^{13}C NMR spectra for all compounds and HRMS for compound 3i

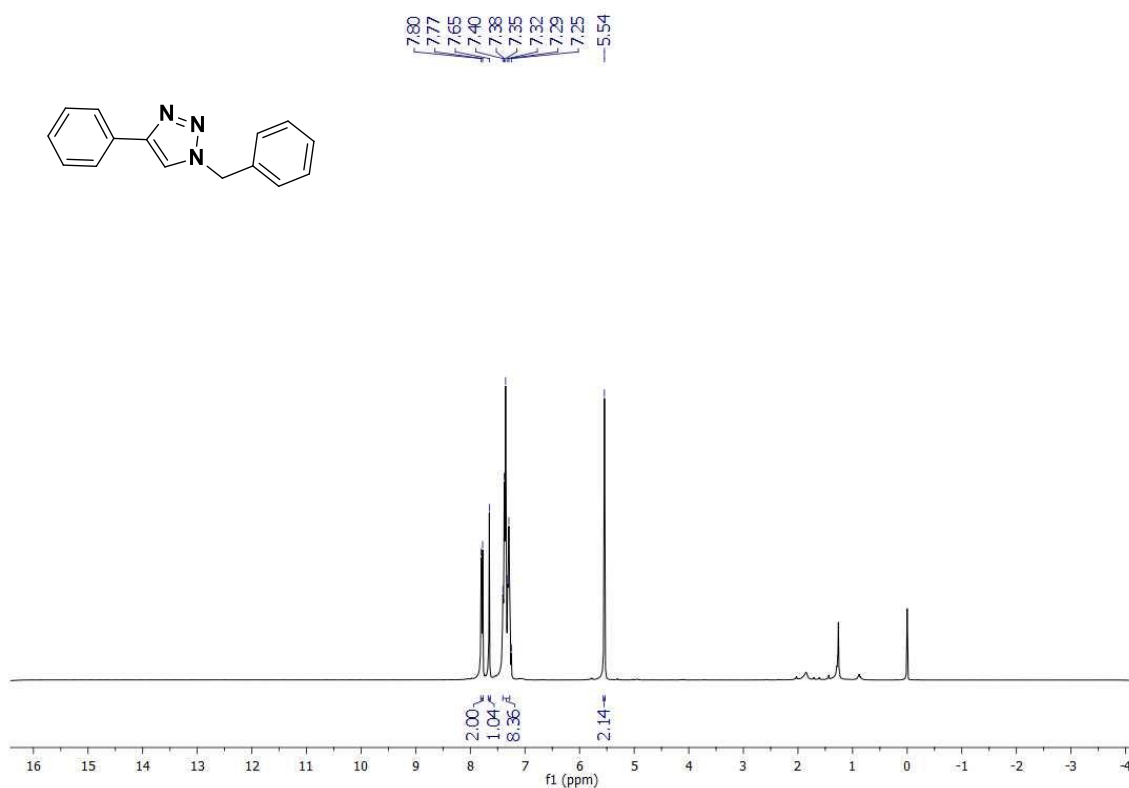


Figure S7. NMR ^1H spectrum (300 MHz, CDCl_3) of product 3a.

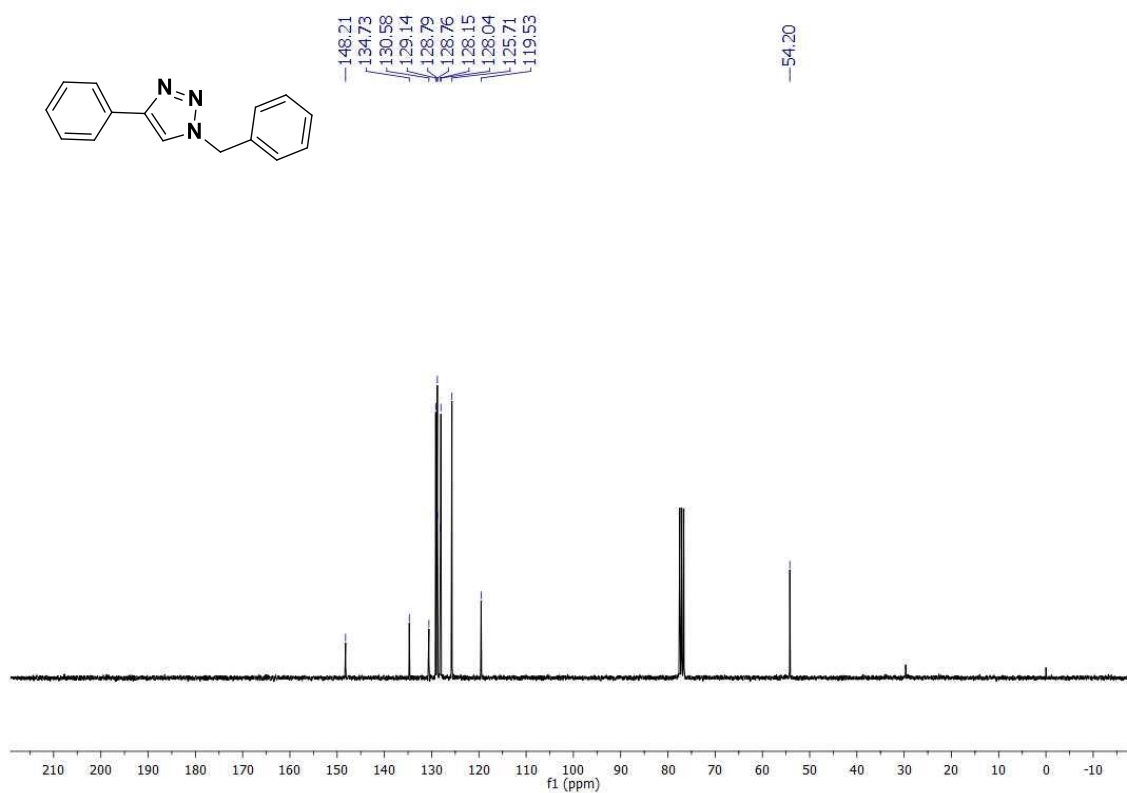


Figure S8. NMR ^{13}C spectrum (75 MHz, CDCl_3) of product 3a.

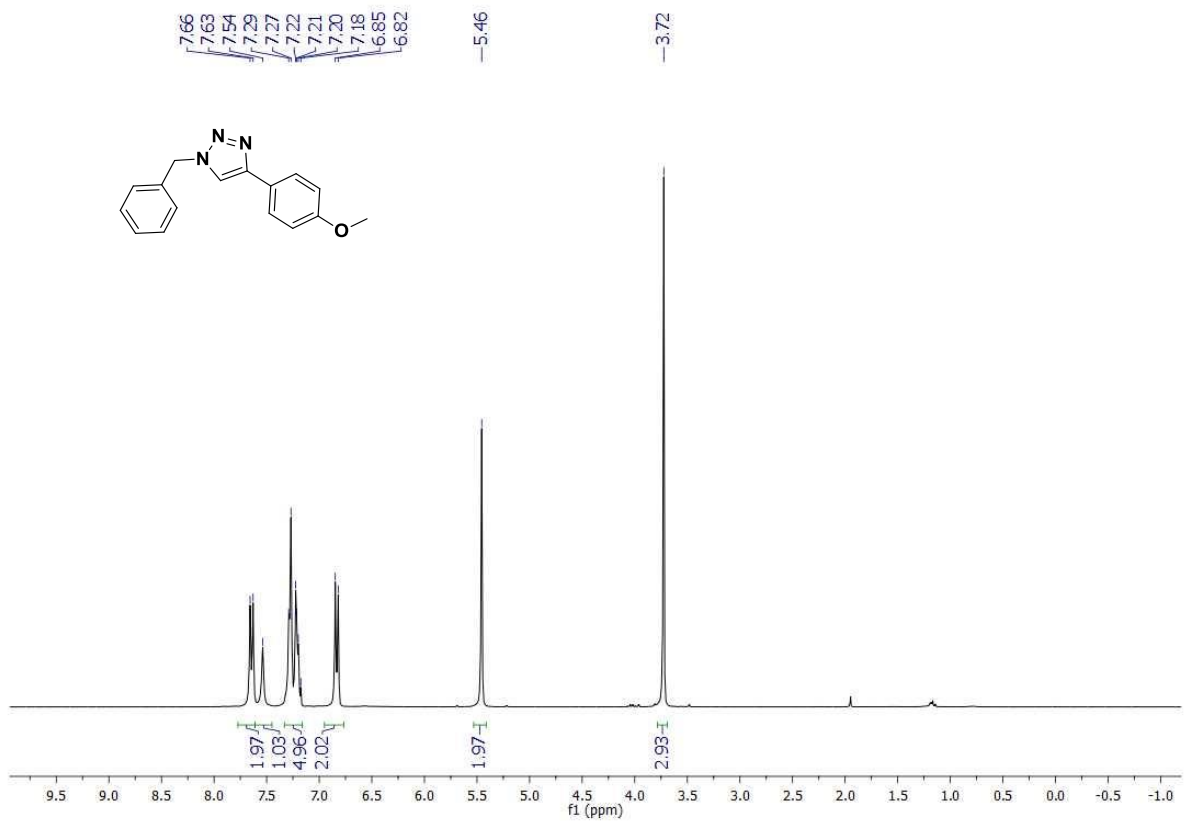


Figure S9. NMR ¹H spectrum (300 MHz, CDCl₃) of product **3b**.

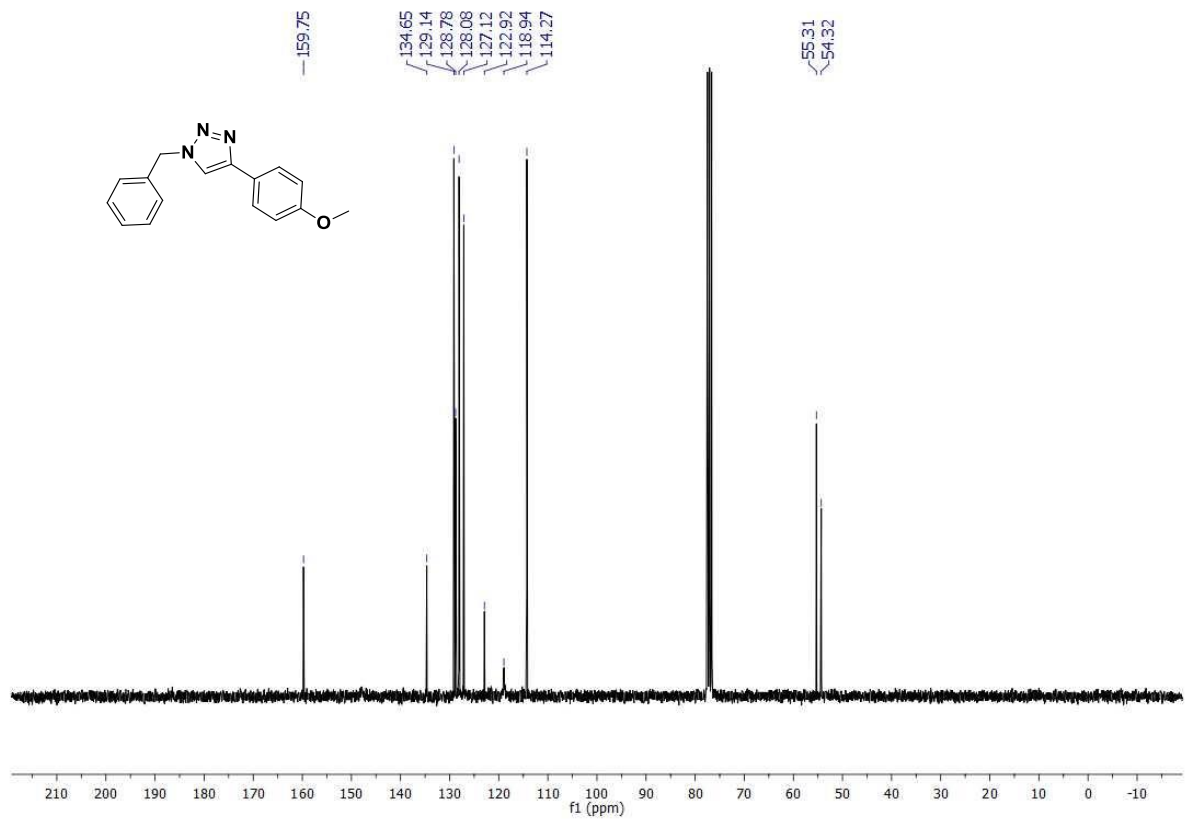


Figure S10. NMR ¹³C spectrum (75 MHz, CDCl₃) of product **3b**.

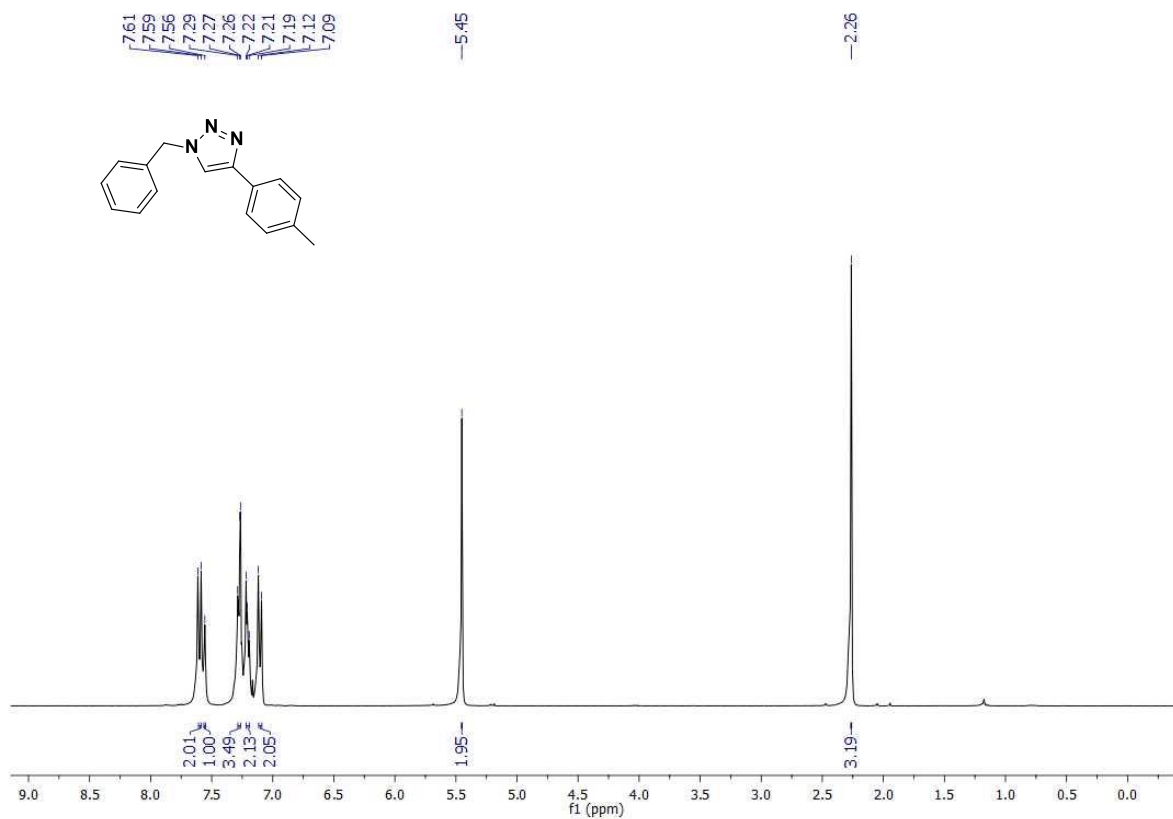
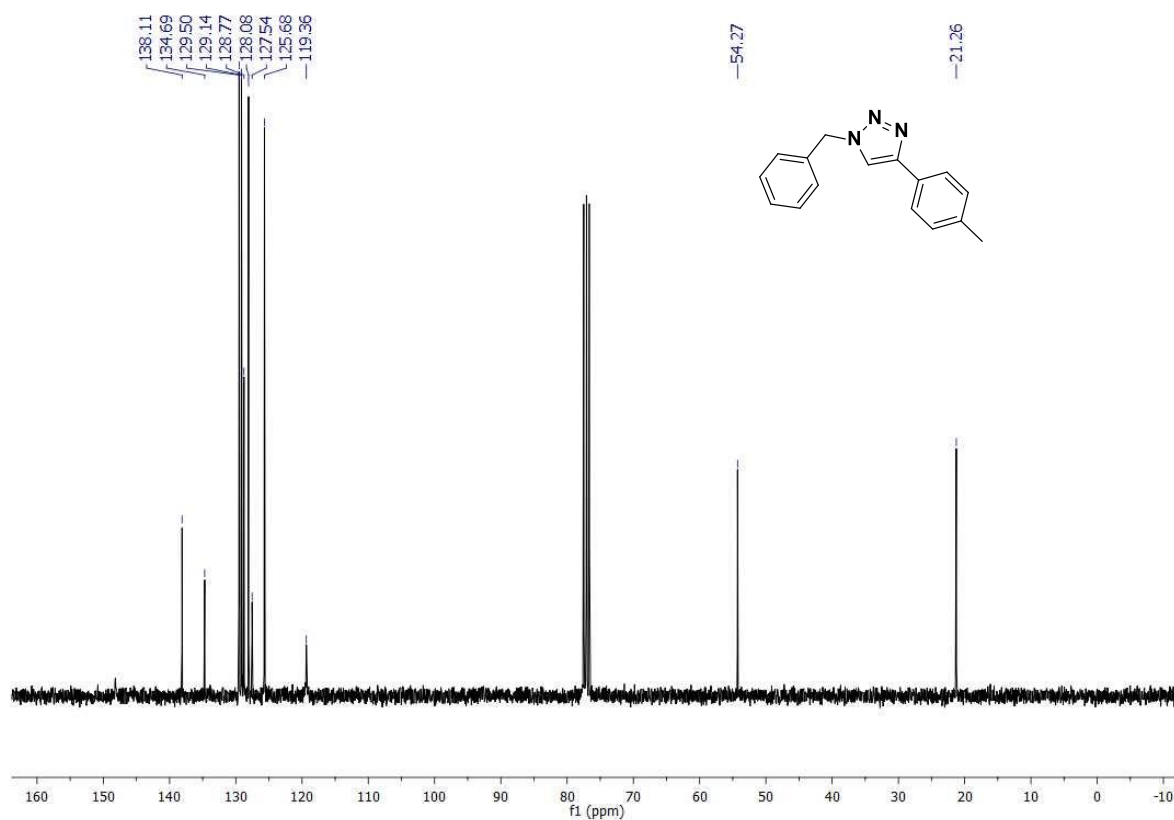


Figure S11. NMR ^1H spectrum (300 MHz, CDCl_3) of product **3c**.



FigureS12. NMR ^{13}C spectrum (75 MHz, CDCl_3) of product **3c**.

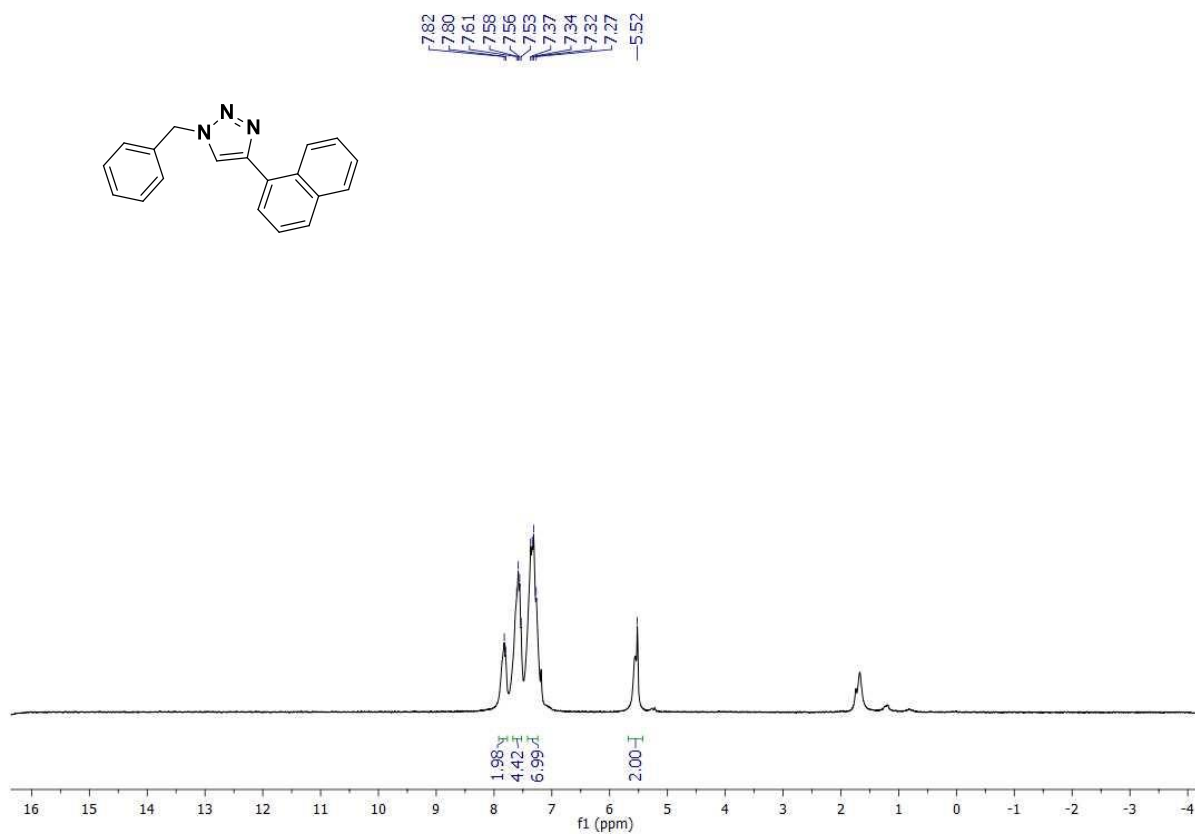


Figure S13. NMR ¹H spectrum (300 MHz, CDCl₃) of product 3d.

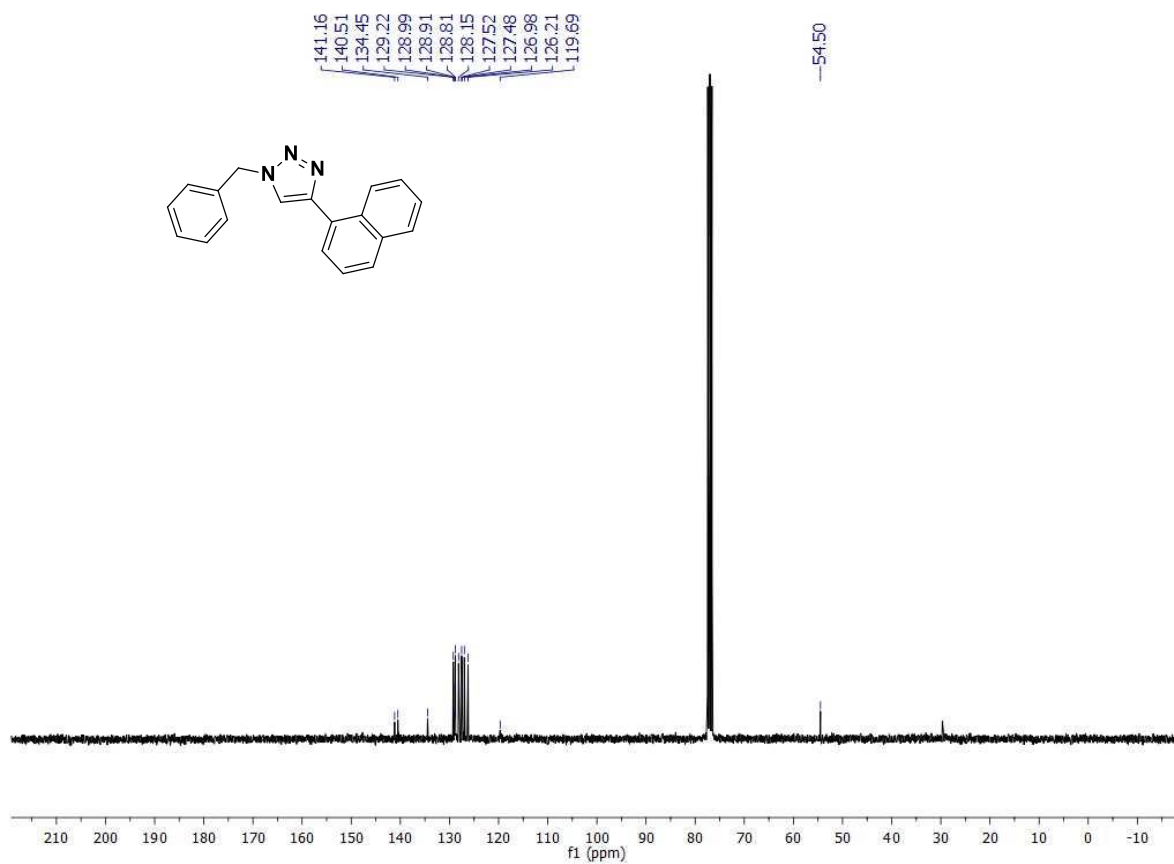


Figure S14. NMR ¹³C spectrum (75 MHz, CDCl₃) of product 3d.

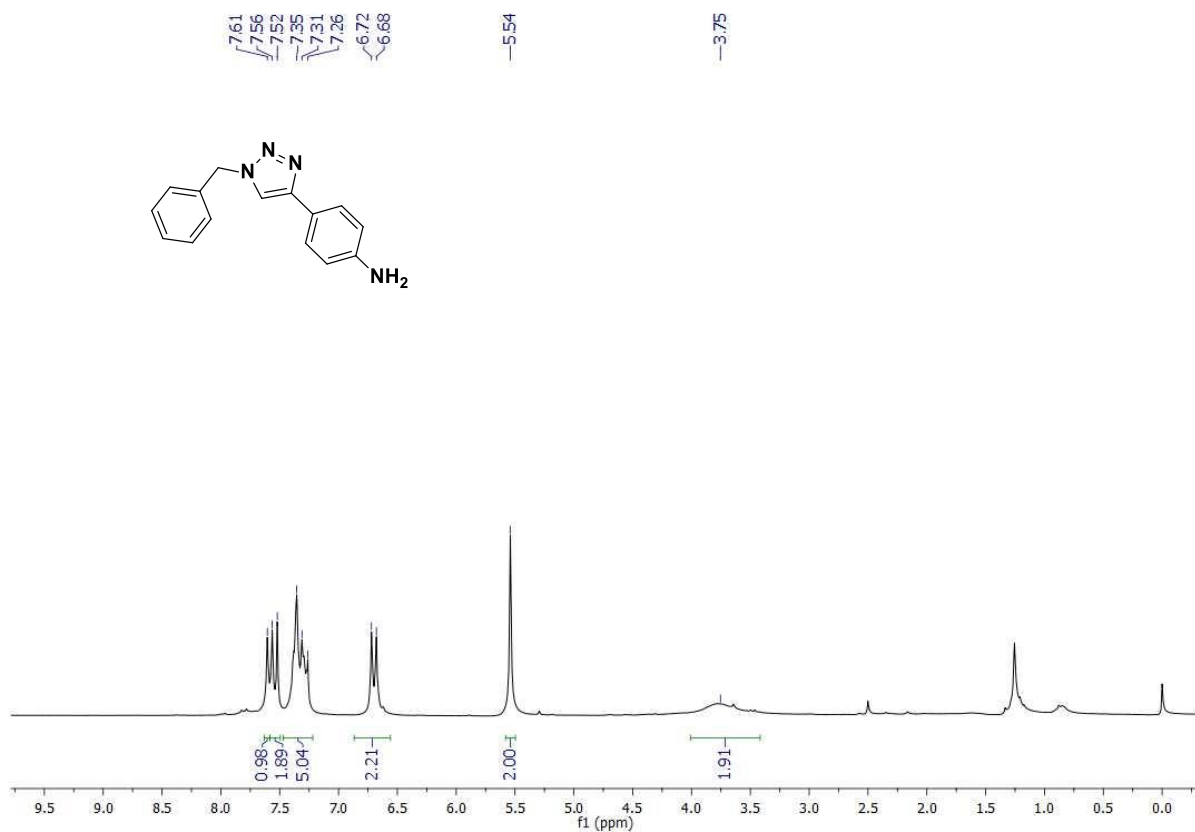


Figure S15. NMR ¹H spectrum (200 MHz, CDCl₃) of product 3e.

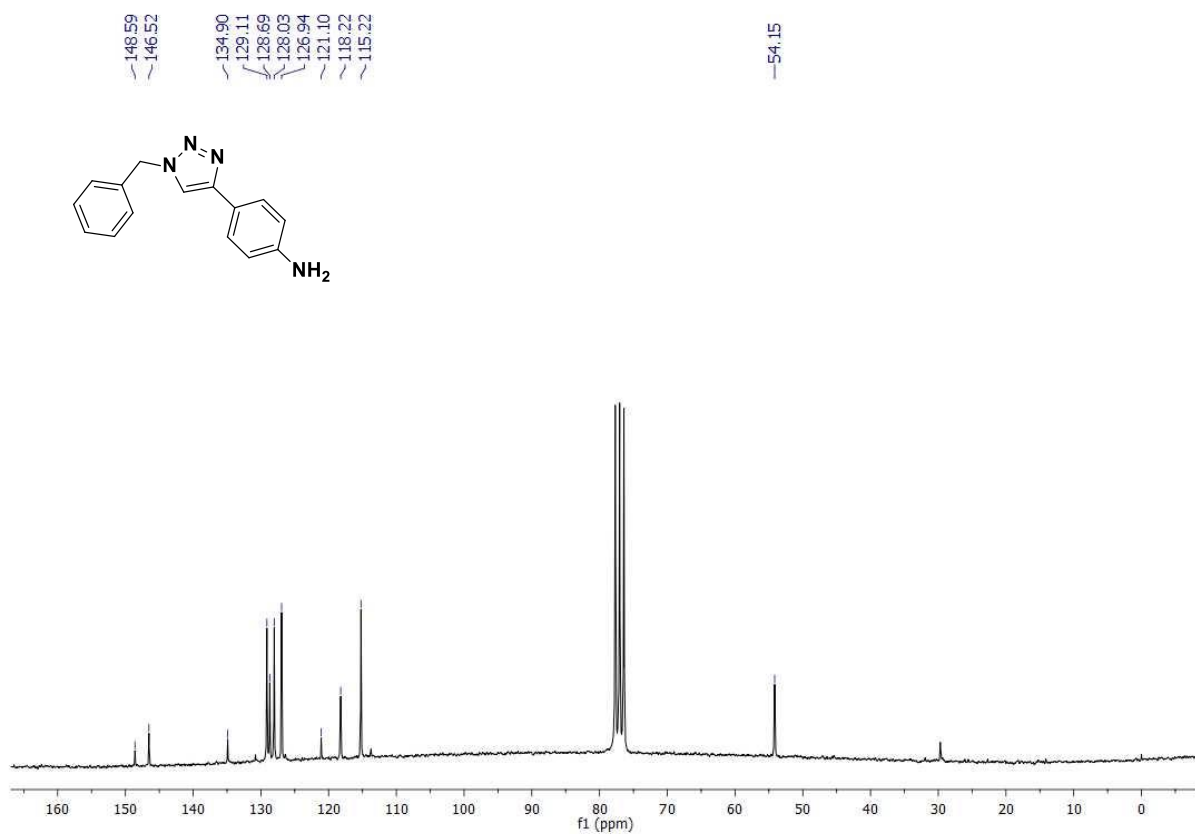


Figure S16. NMR ¹³C spectrum (50 MHz, CDCl₃) of product 3e.

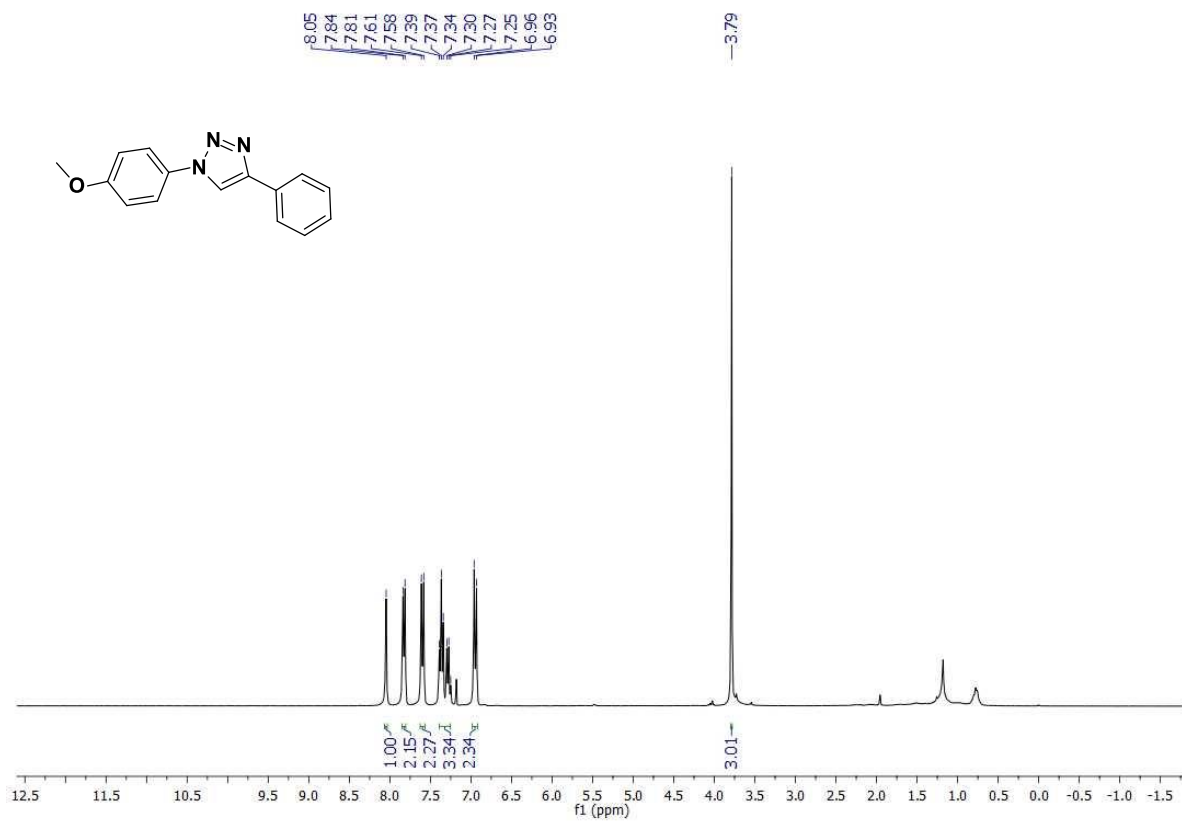


Figure S17. NMR ¹H spectrum (300 MHz, CDCl₃) of product 3f.

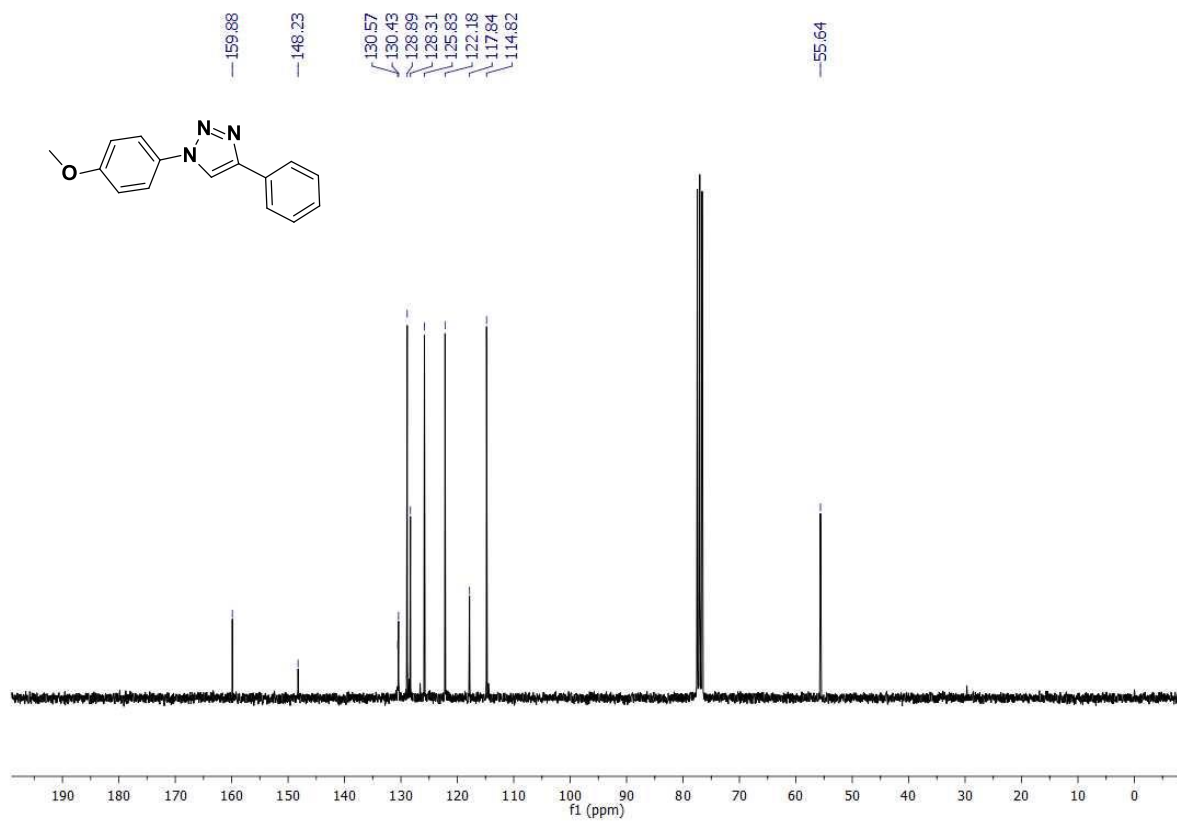


Figure S18. NMR ¹³C spectrum (75 MHz, CDCl₃) of product 3f.

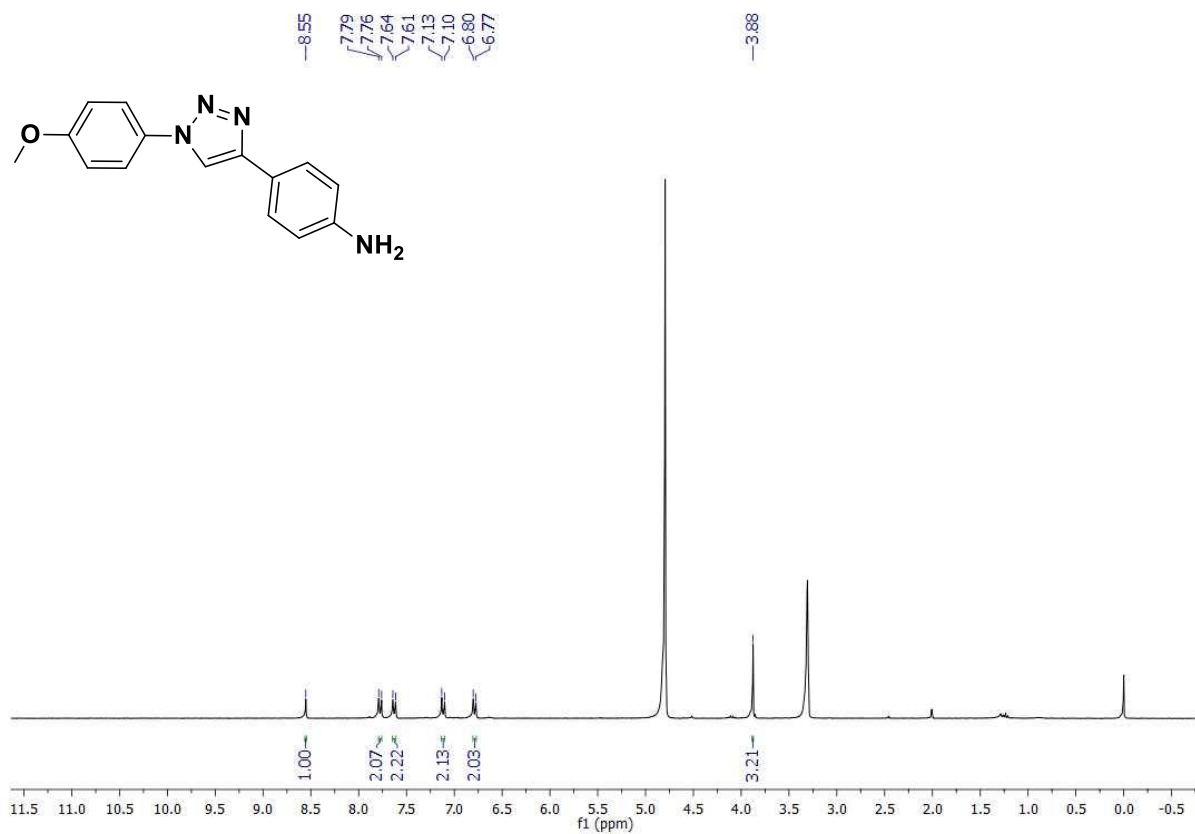


Figure S19. NMR ¹H spectrum (300 MHz, CD₃OD) of product **3g**.

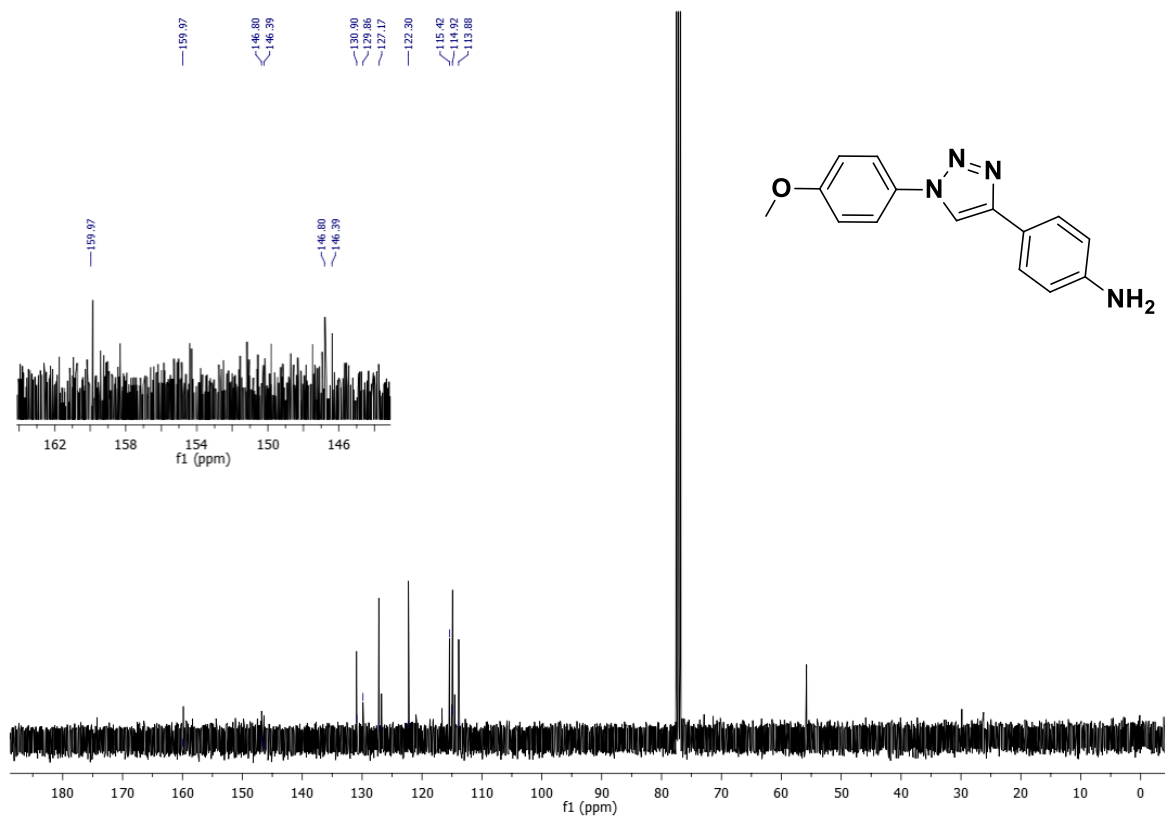


Figure S20. NMR ¹³C spectrum (75 MHz, CDCl₃) of product **3g**.

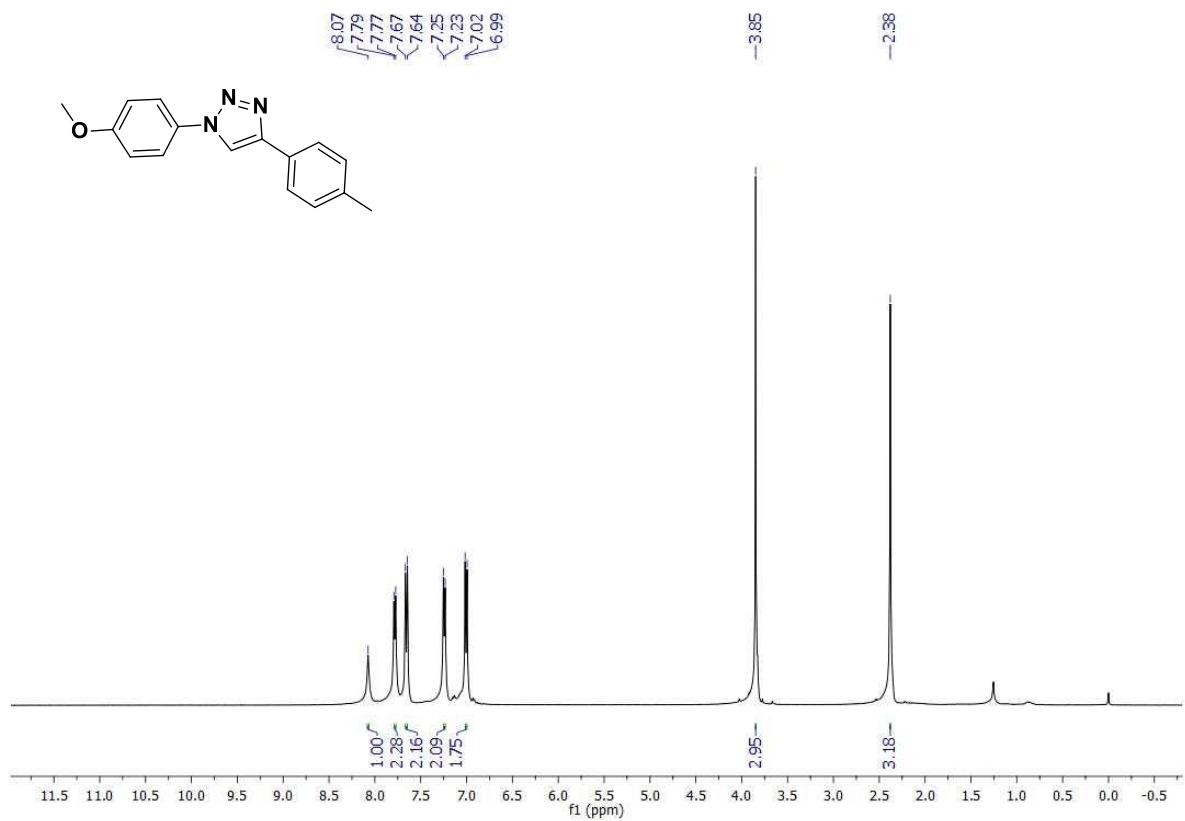


Figure S21. NMR ¹H spectrum (300 MHz, CDCl₃) of product 3h.

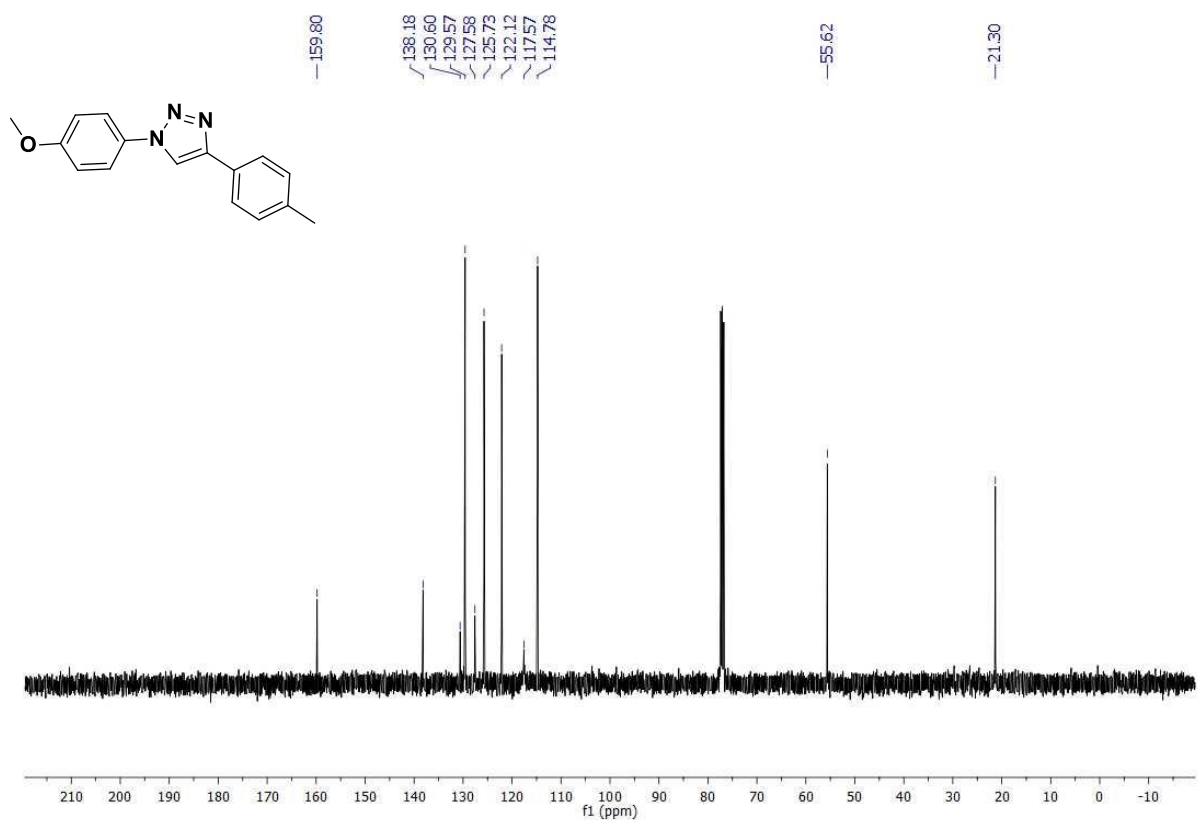


Figure S22. NMR ¹³C spectrum (75 MHz, CDCl₃) of product 3h.

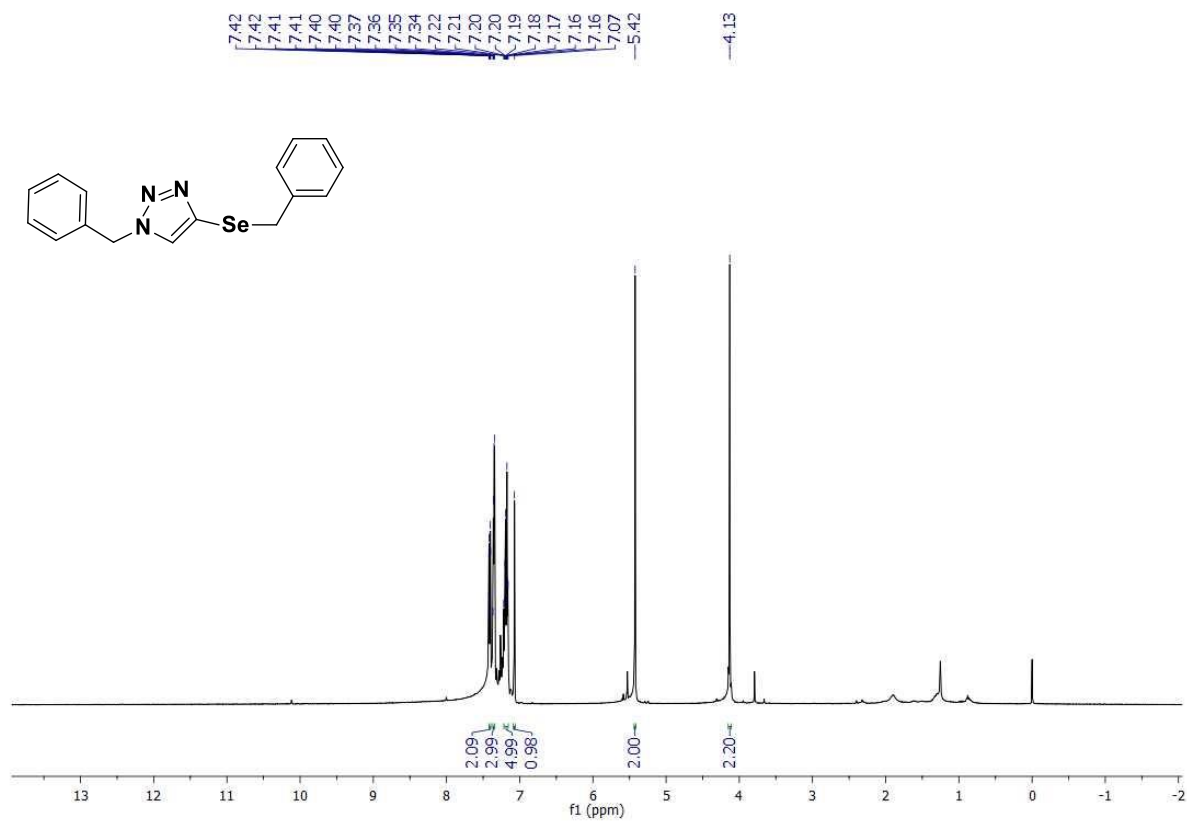


Figure S23. NMR ¹H spectrum (300 MHz, CDCl₃) of product **3i**.

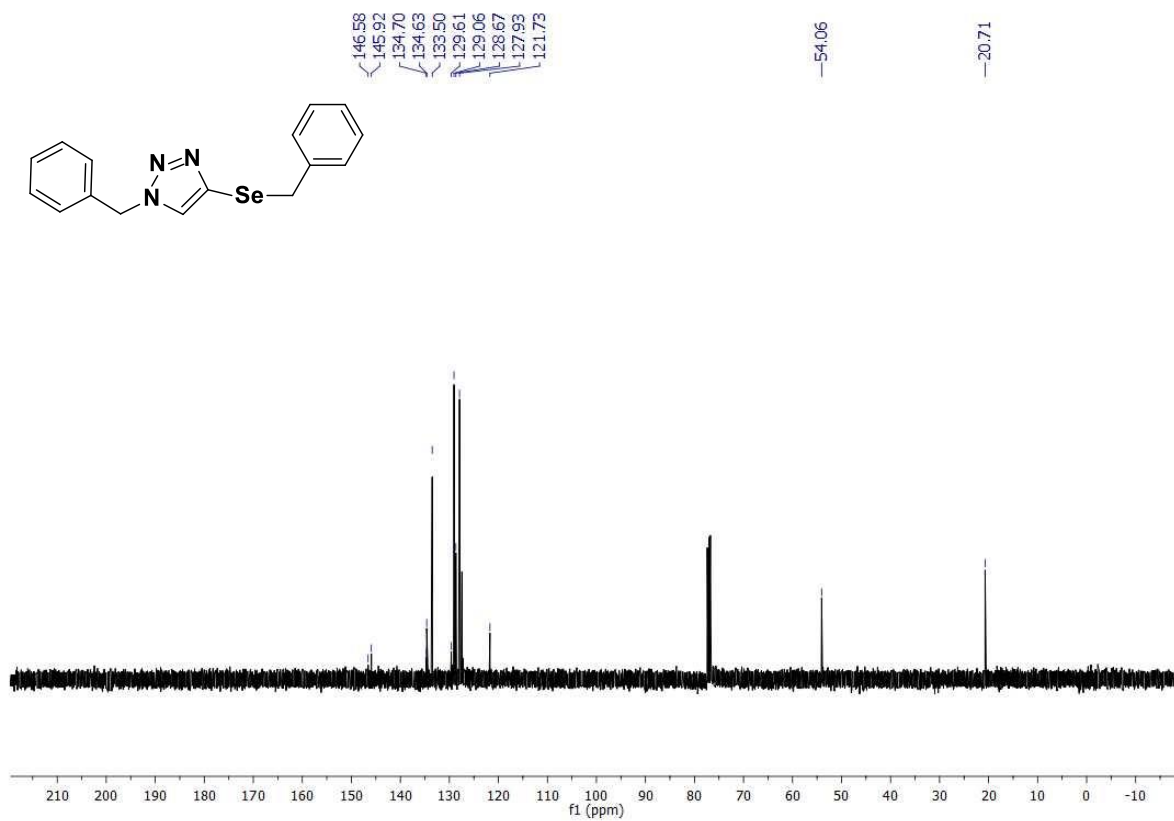


Figure S24. NMR ¹³C spectrum (75 MHz, CDCl₃) of product **3i**.

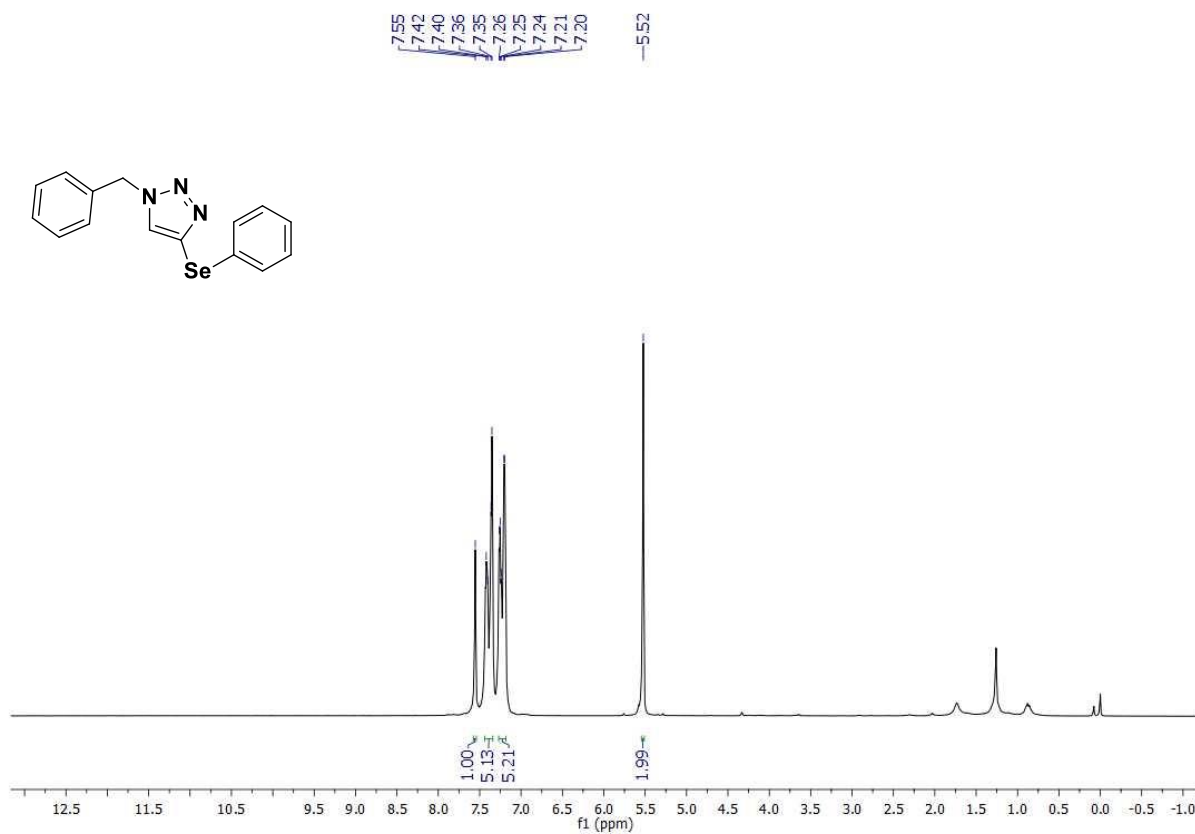


Figure S25. NMR ¹H spectrum (300 MHz, CDCl₃) of product **3j**.

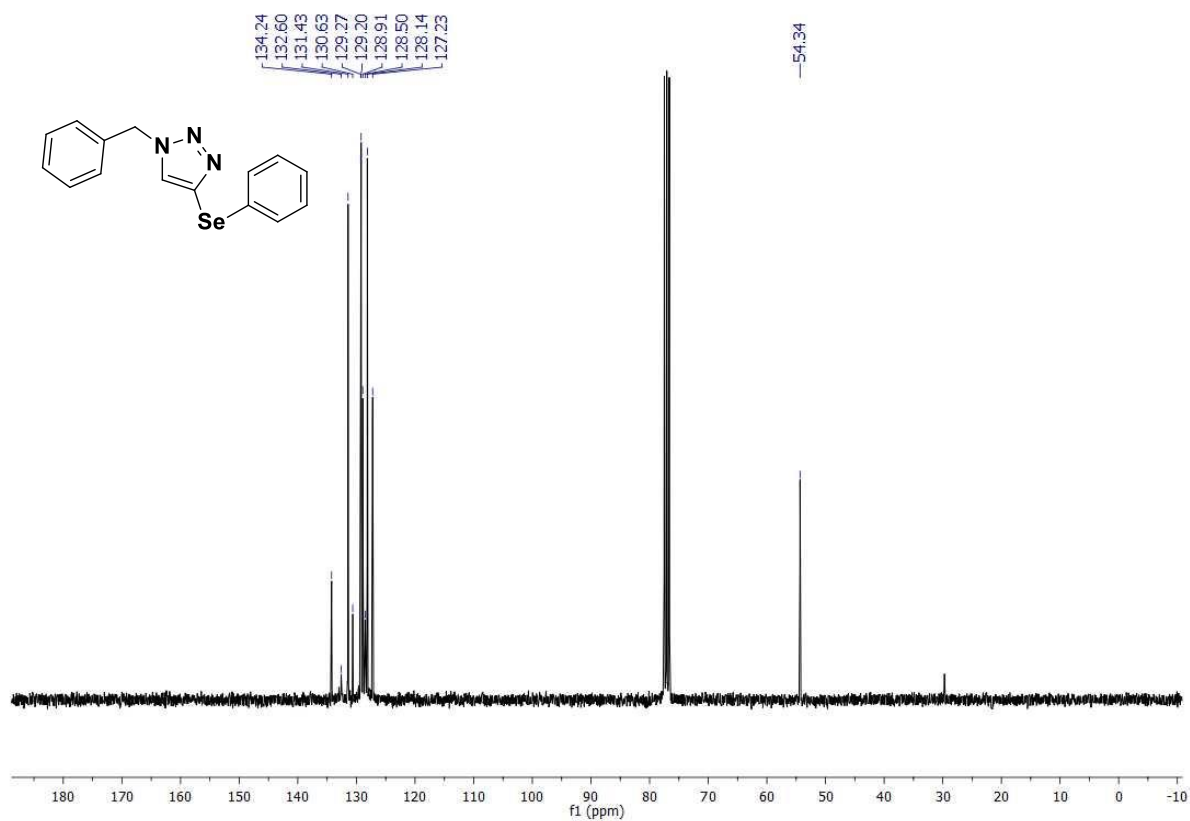


Figure S26. NMR ¹³C spectrum (75 MHz, CDCl₃) of product **3j**.

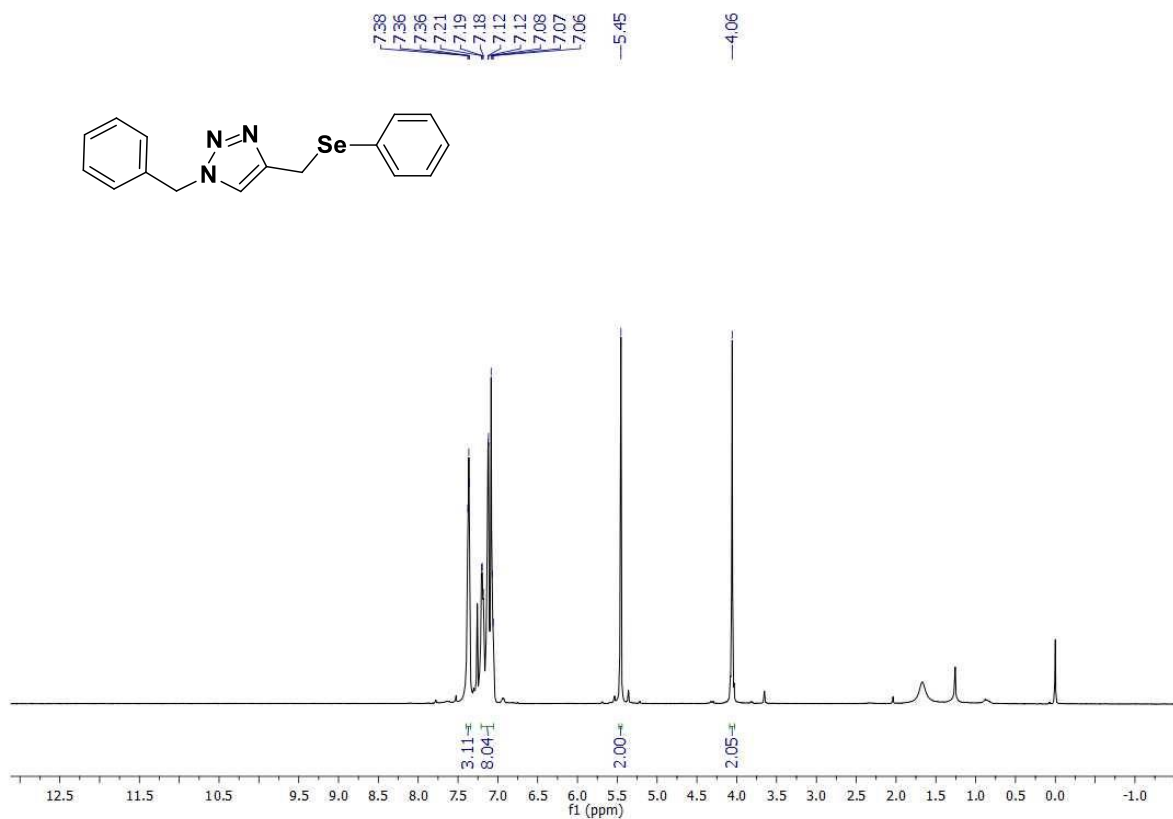


Figure S27. NMR ¹H spectrum (300 MHz, CDCl₃) of product **3k**.

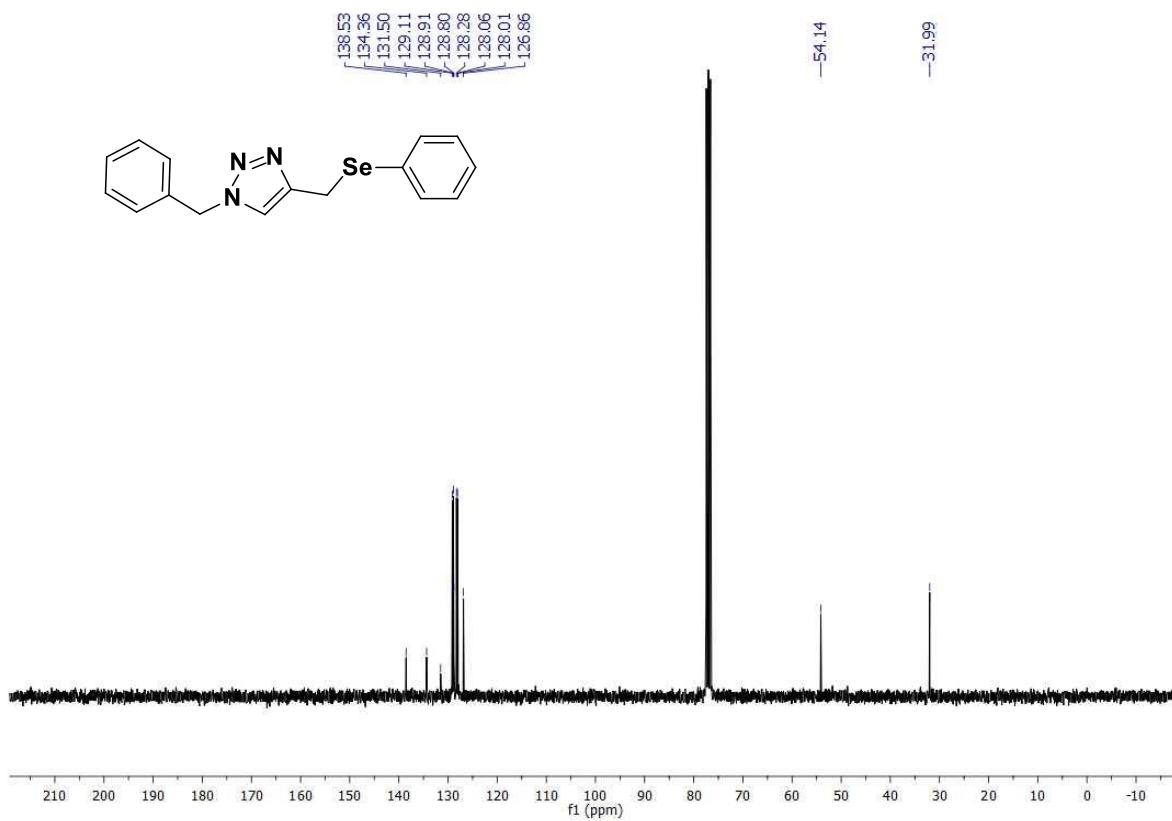


Figure S28. NMR ¹³C spectrum (75 MHz, CDCl₃) of product **3k**.

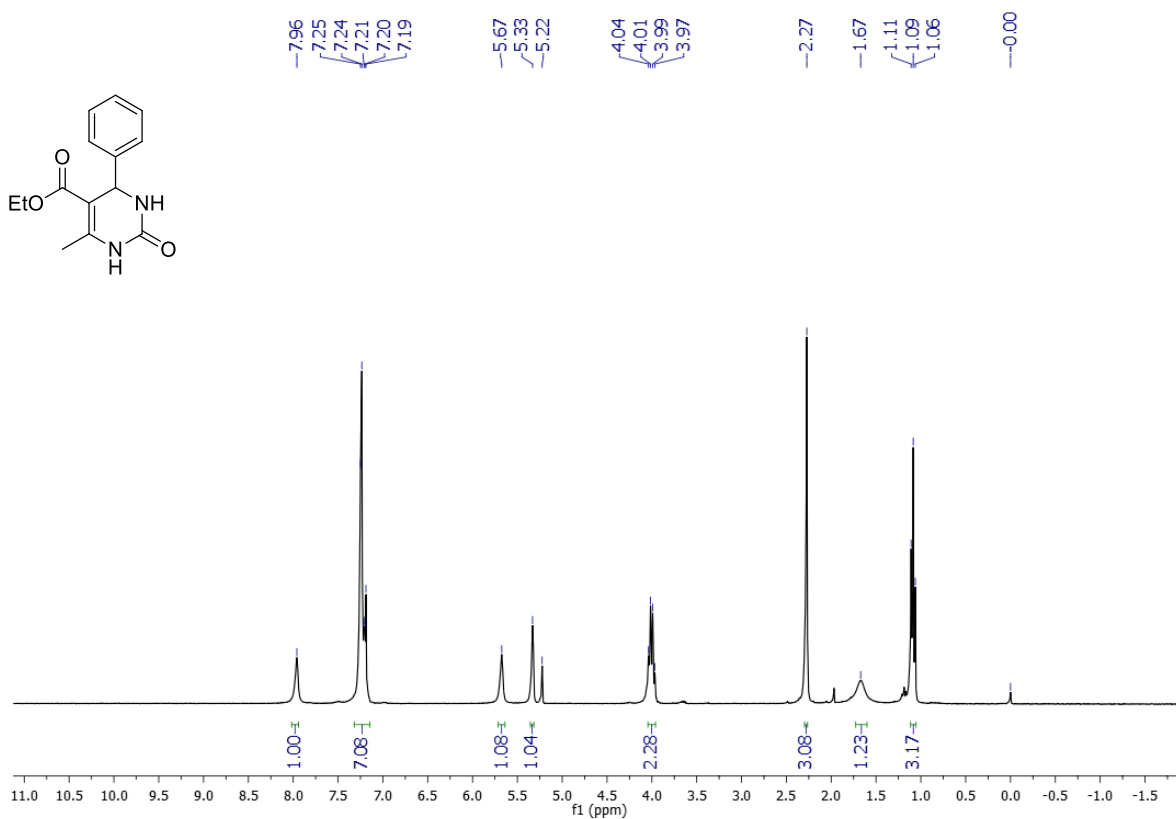


Figure S29. NMR ¹H spectrum (300 MHz, DMSO deuterated) of product 7a.

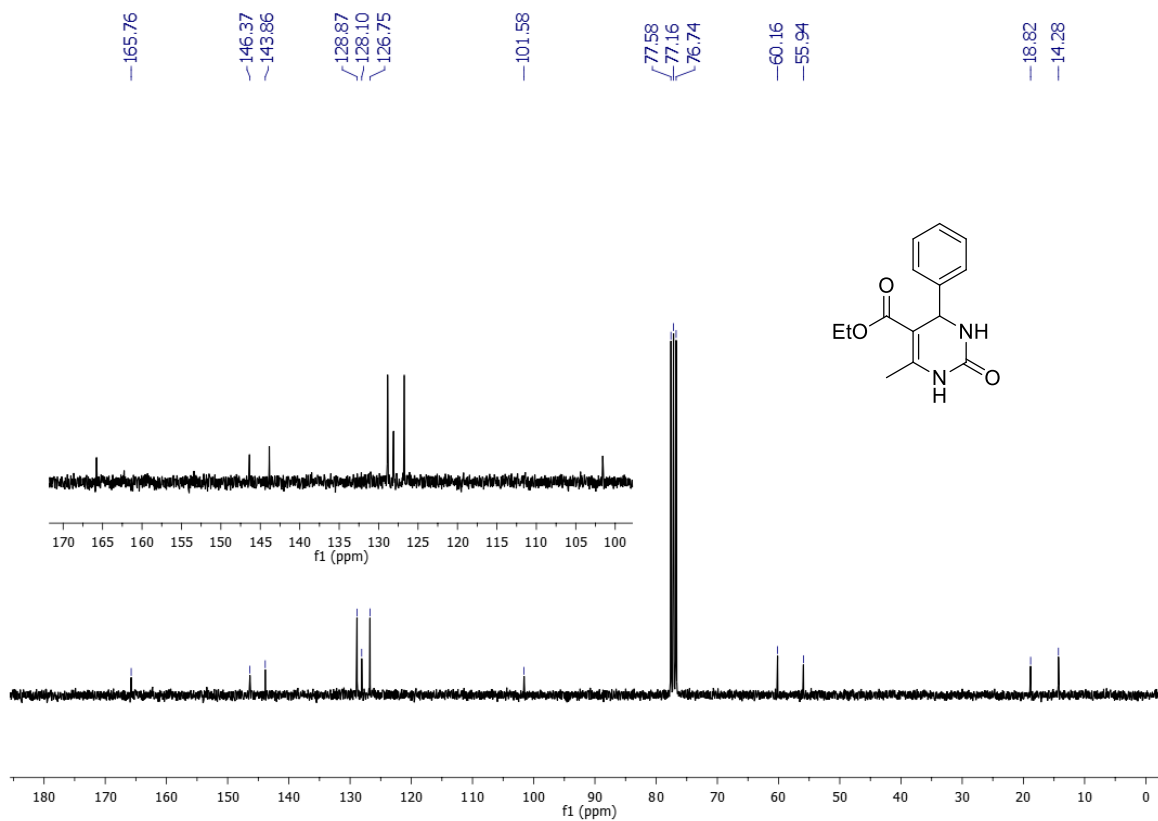


Figure S30. NMR ¹³C spectrum (75 MHz, CDCl₃) of product 7a.

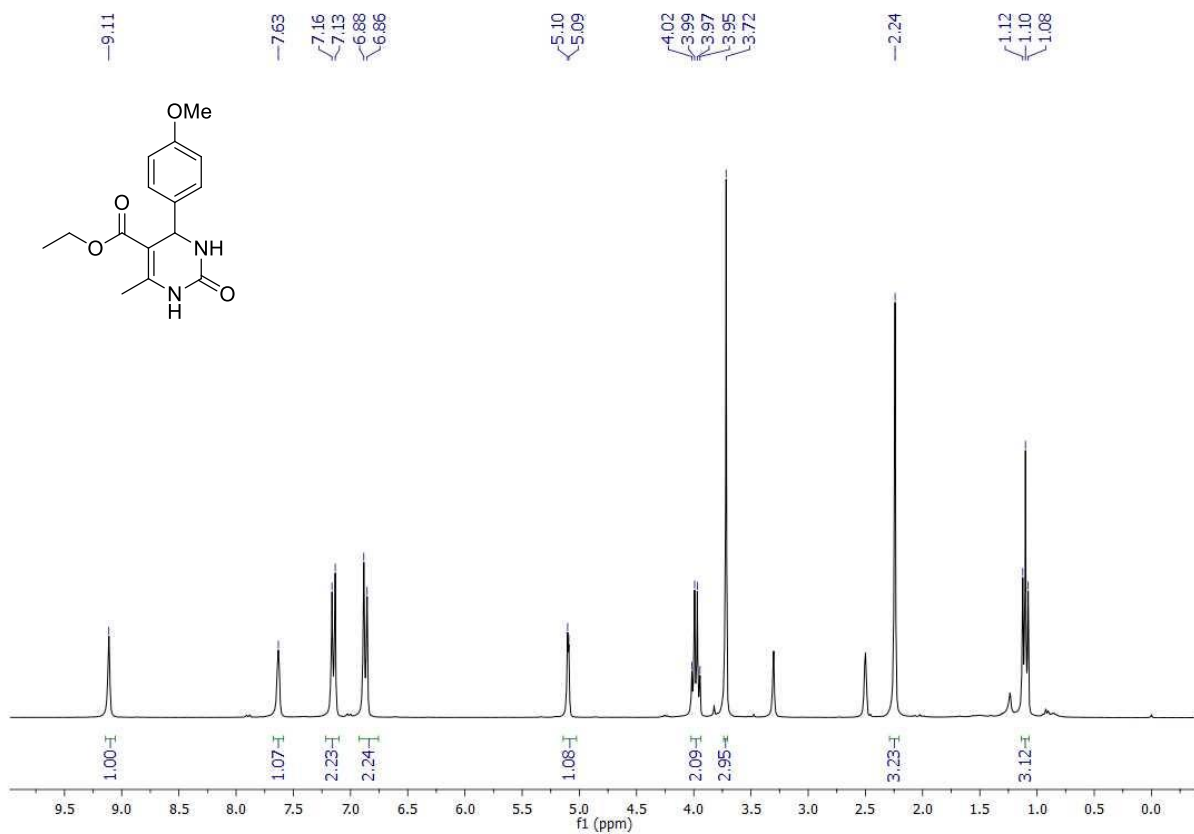


Figure S31. NMR ¹H spectrum (300 MHz, DMSO-d₆) of product **7b**.

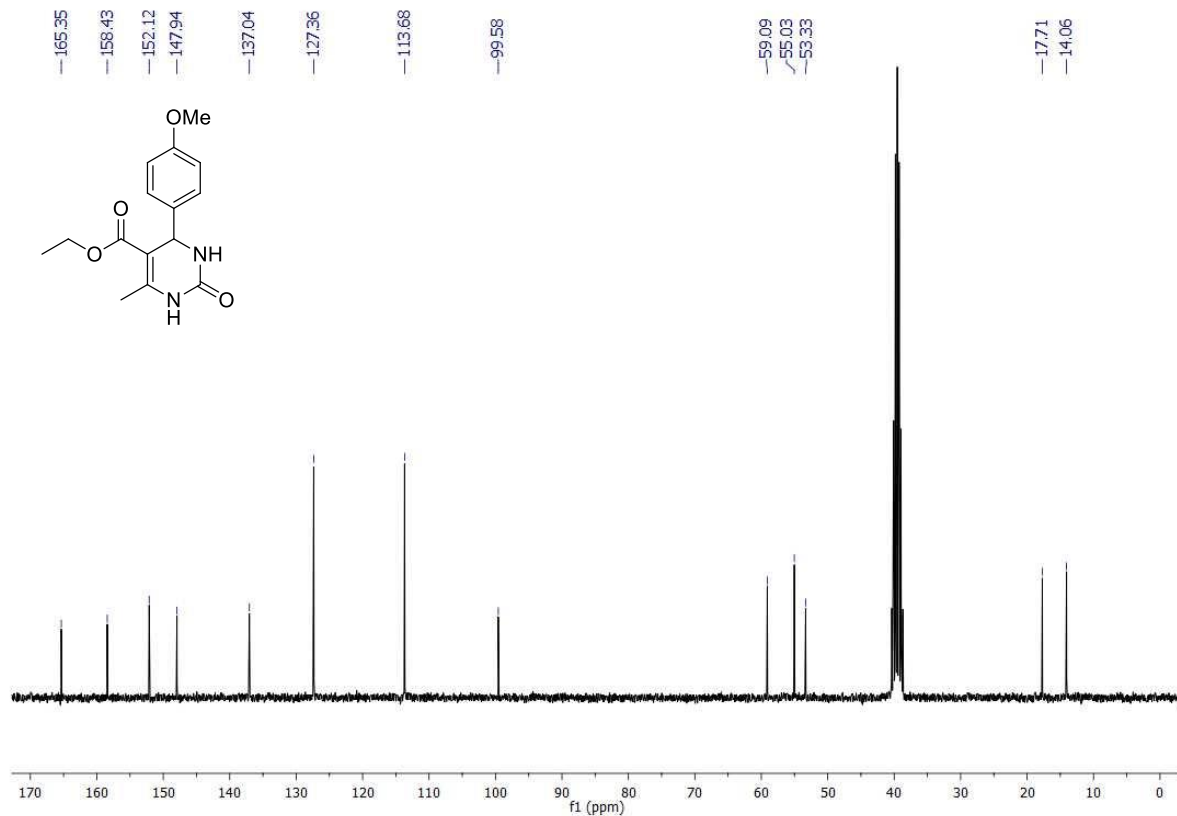


Figure S32. NMR ¹³C spectrum (75 MHz, DMSO-d₆) of product **7b**.

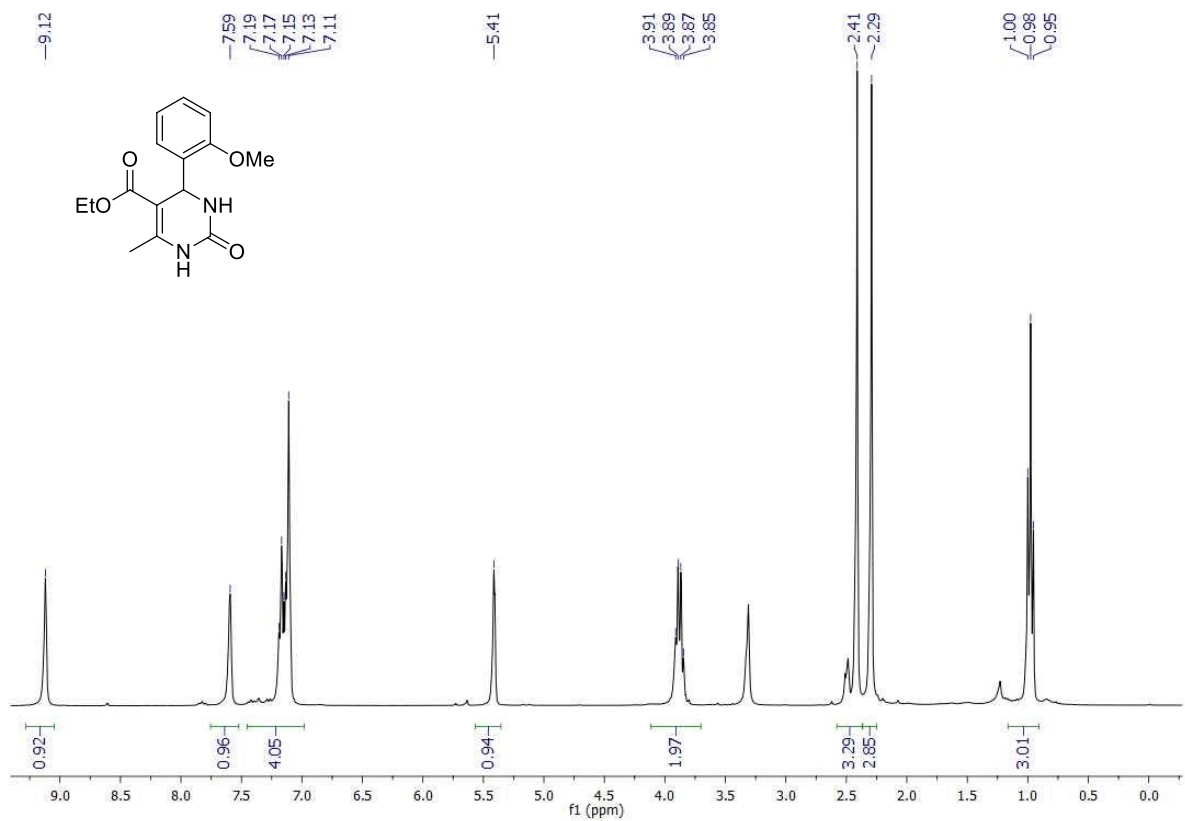


Figure S33. NMR ^1H spectrum (300 MHz, DMSO- d_6) of product **7c**.

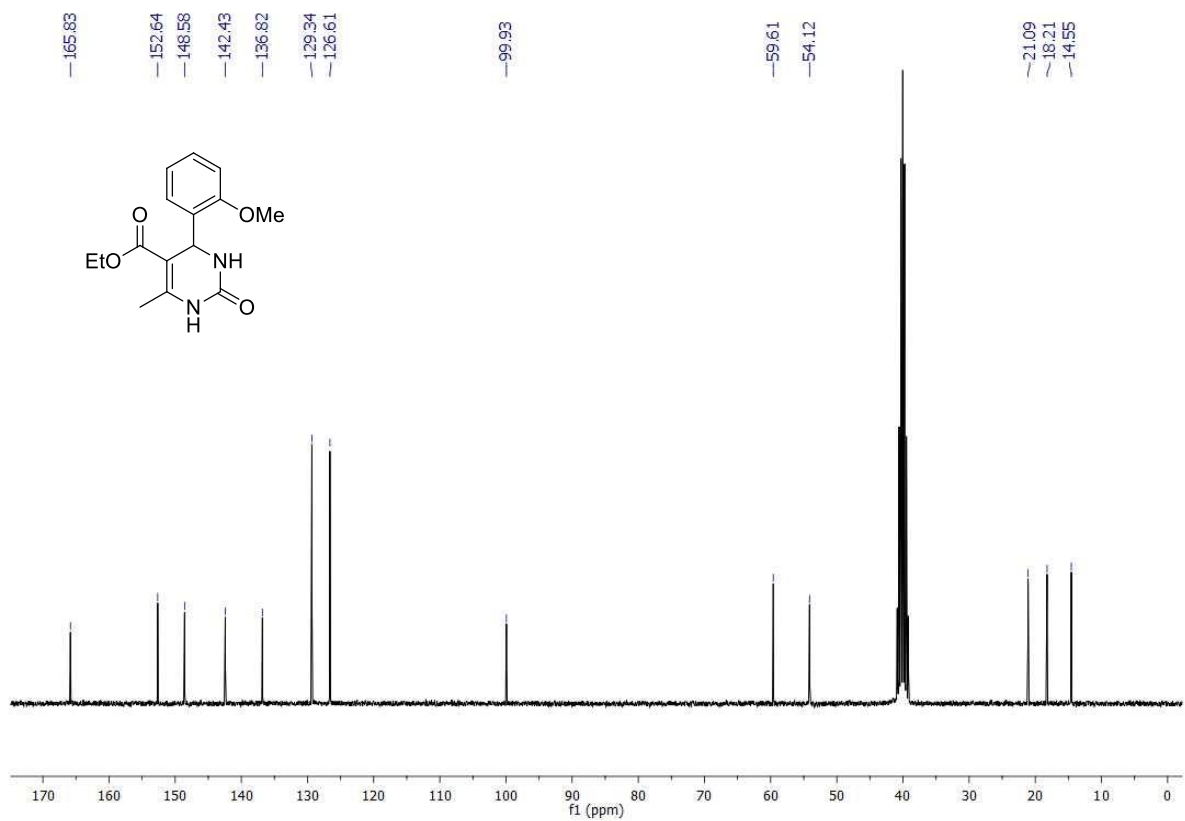


Figure S34. NMR ^{13}C spectrum (75 MHz, DMSO- d_6) of product **7c**.

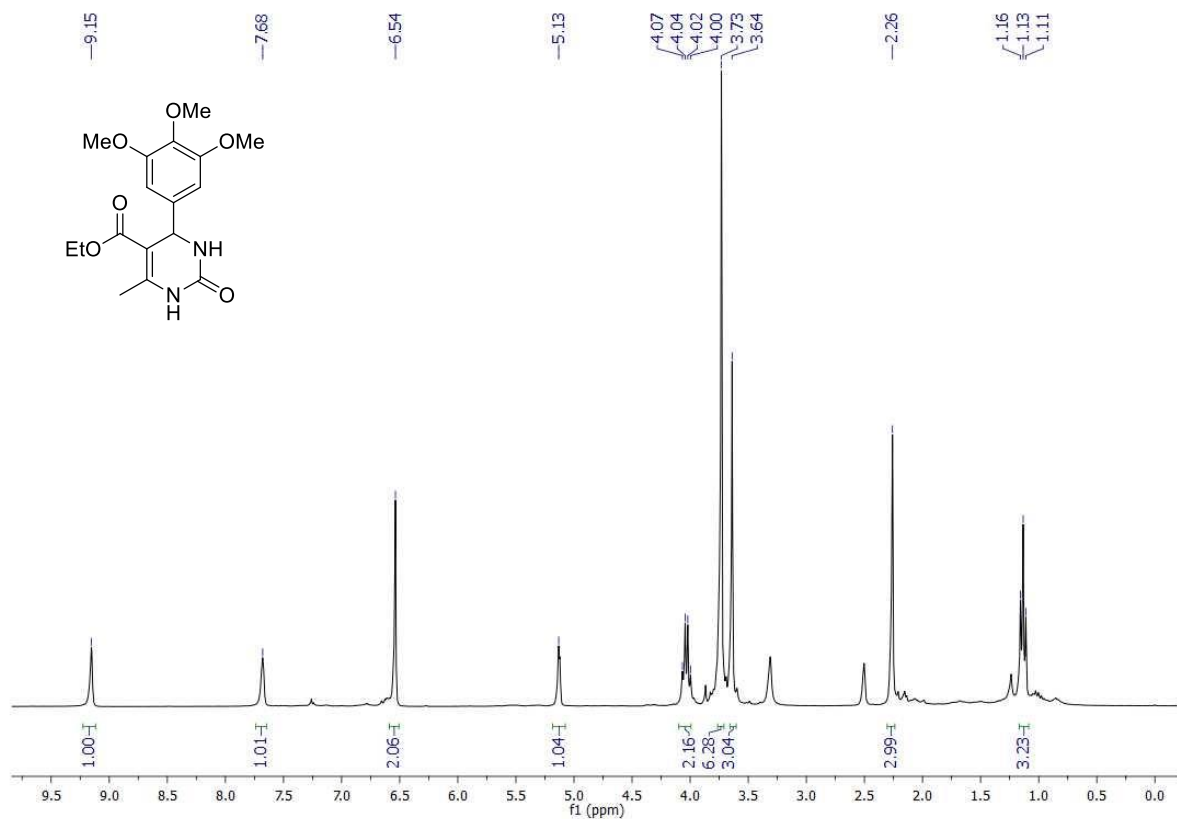


Figure S35. NMR ^1H spectrum (300 MHz, DMSO- d_6) of product 7d.

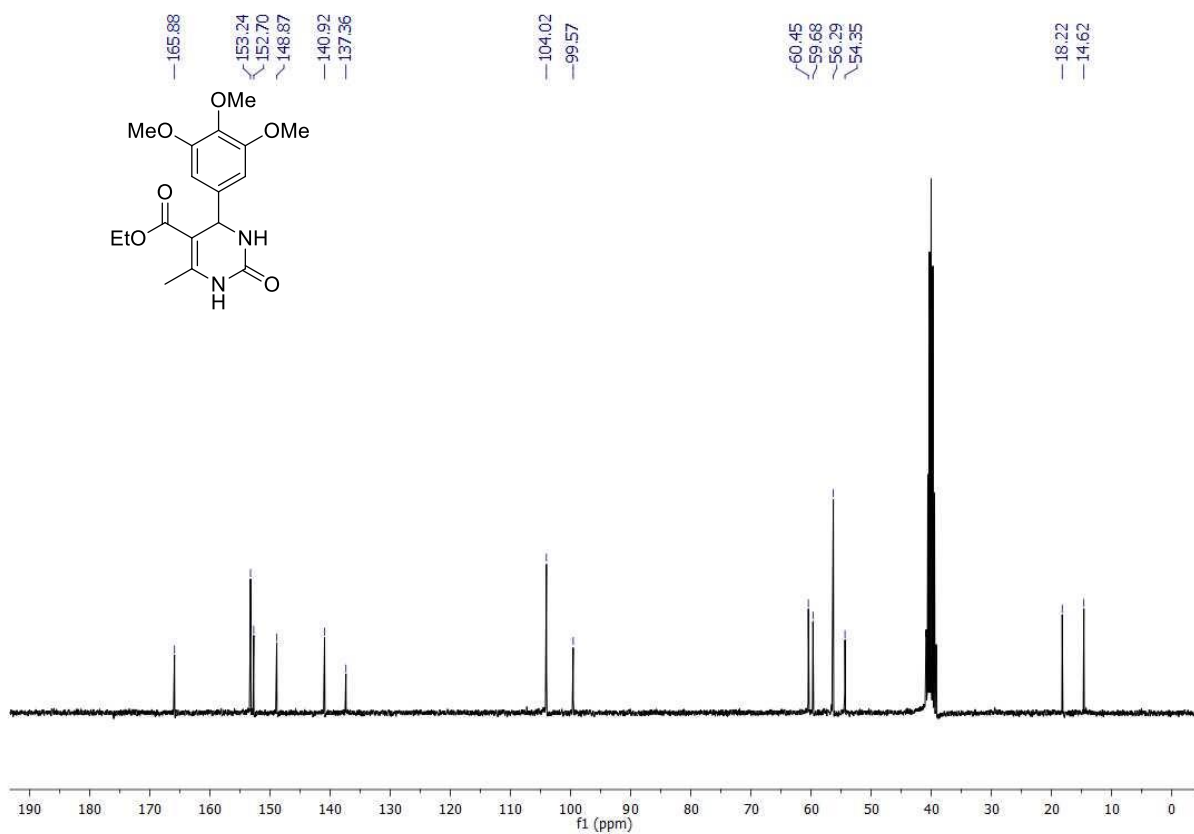


Figure S36. NMR ^{13}C spectrum (75 MHz, DMSO- d_6) of product 7d.

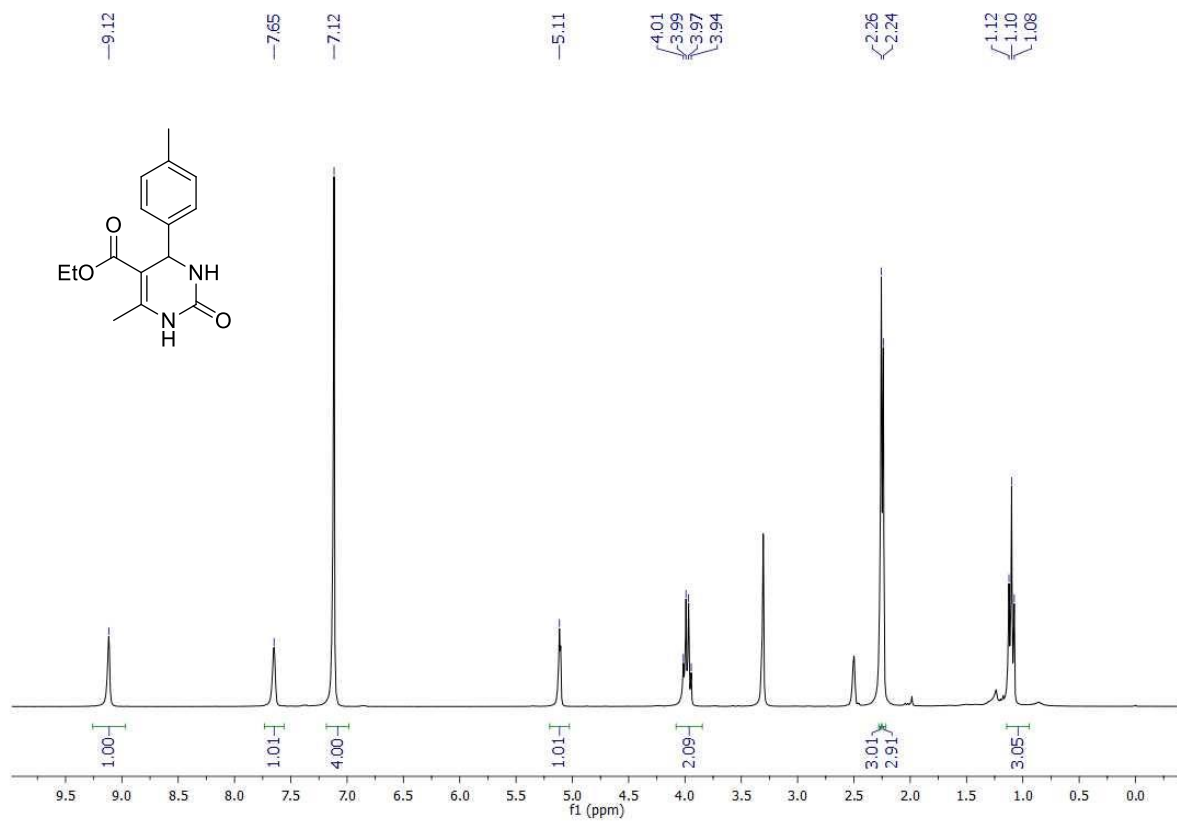


Figure S37. NMR ^1H spectrum (300 MHz, DMSO- d_6) of product 7e.

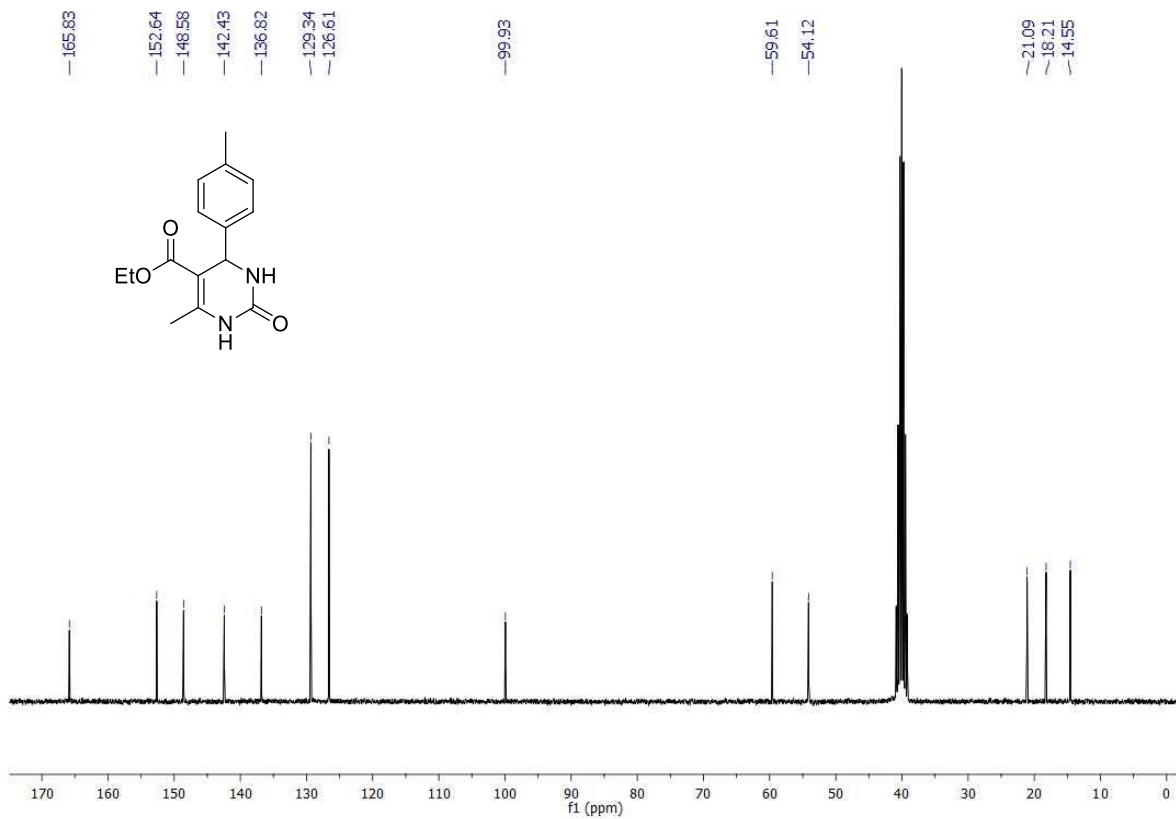


Figure S38. NMR ^{13}C spectrum (75 MHz, DMSO- d_6) of product 7e.

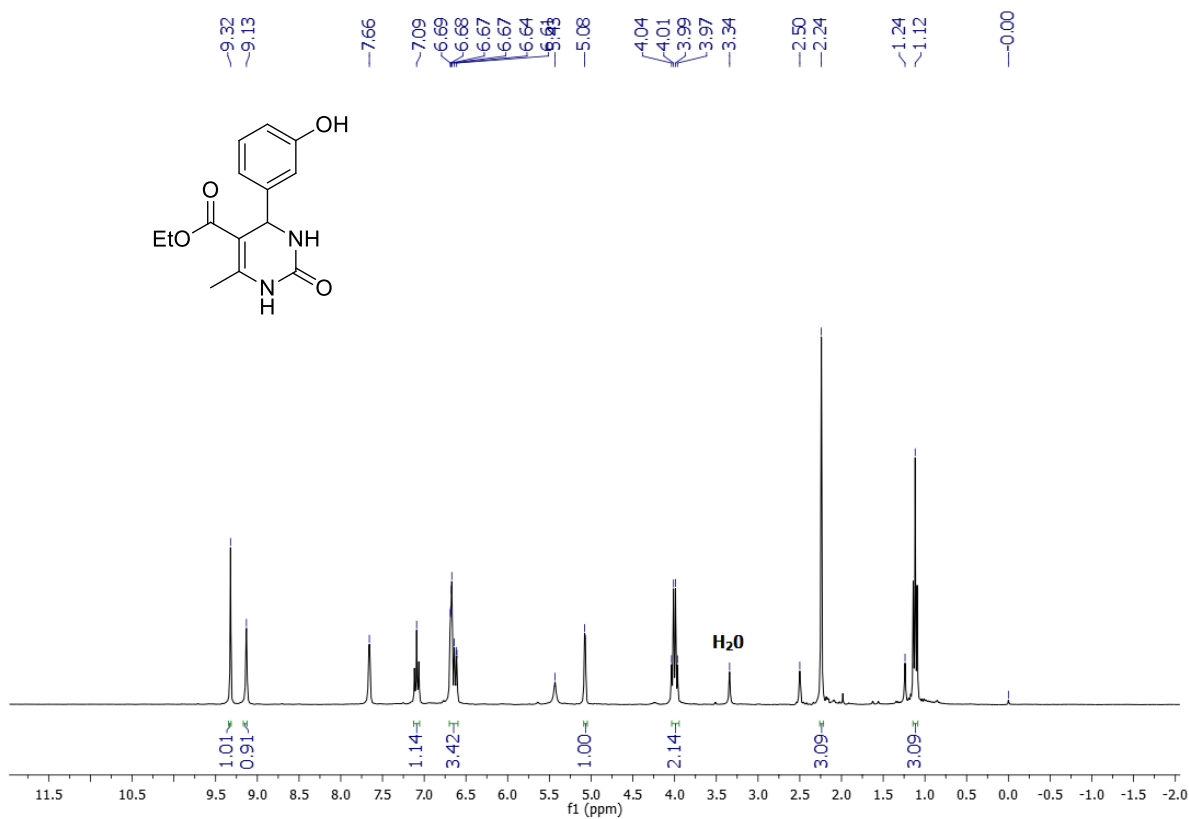


Figure S39. NMR ¹H spectrum (300 MHz, DMSO-d₆) of product 7f.

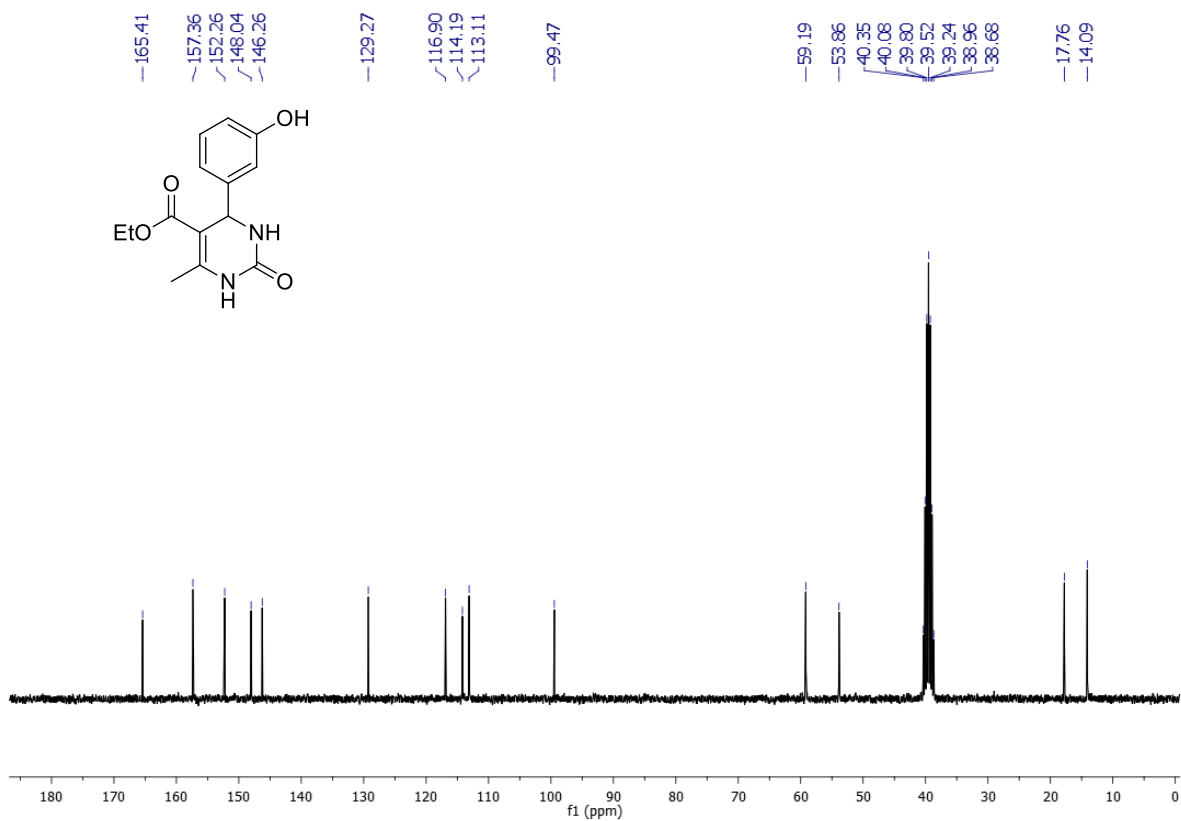


Figure S40. NMR ¹³C spectrum (75 MHz, DMSO-d₆) of product 7f.

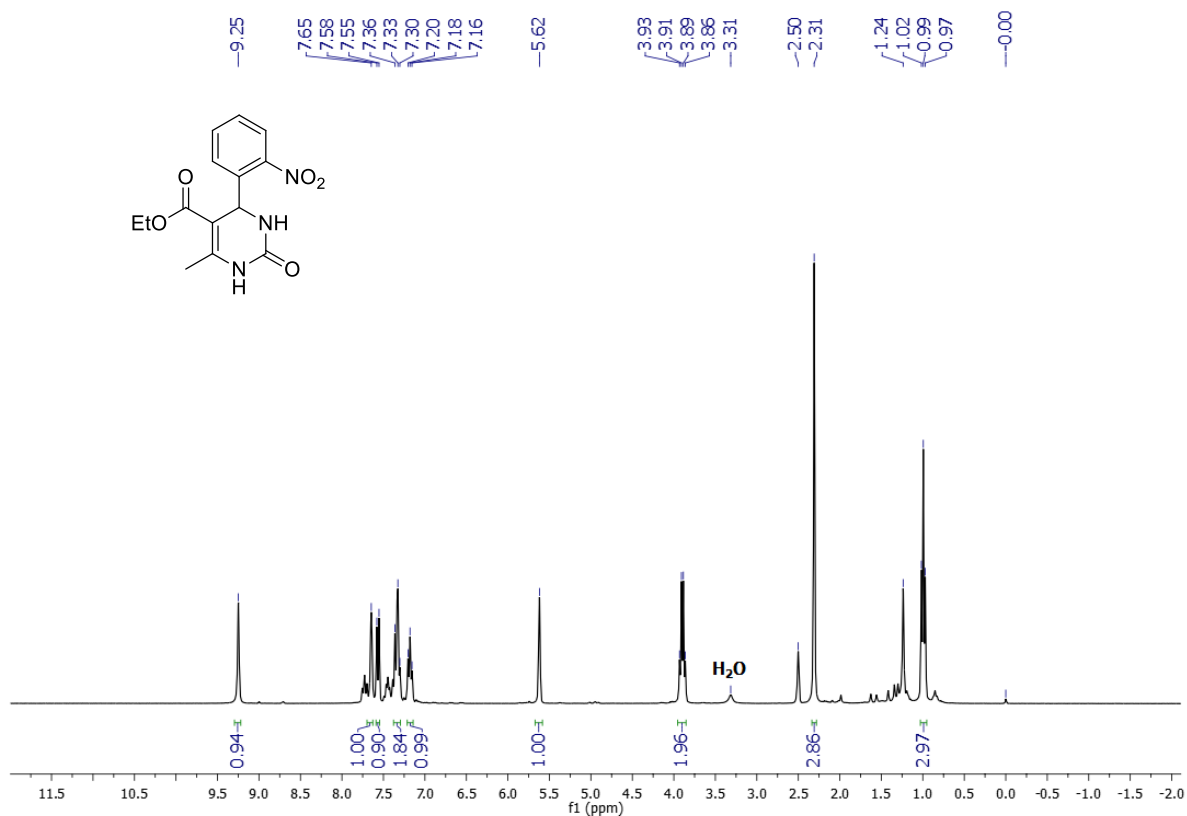


Figure S41. NMR ¹H spectrum (300 MHz, DMSO-d₆) of product **7g**.

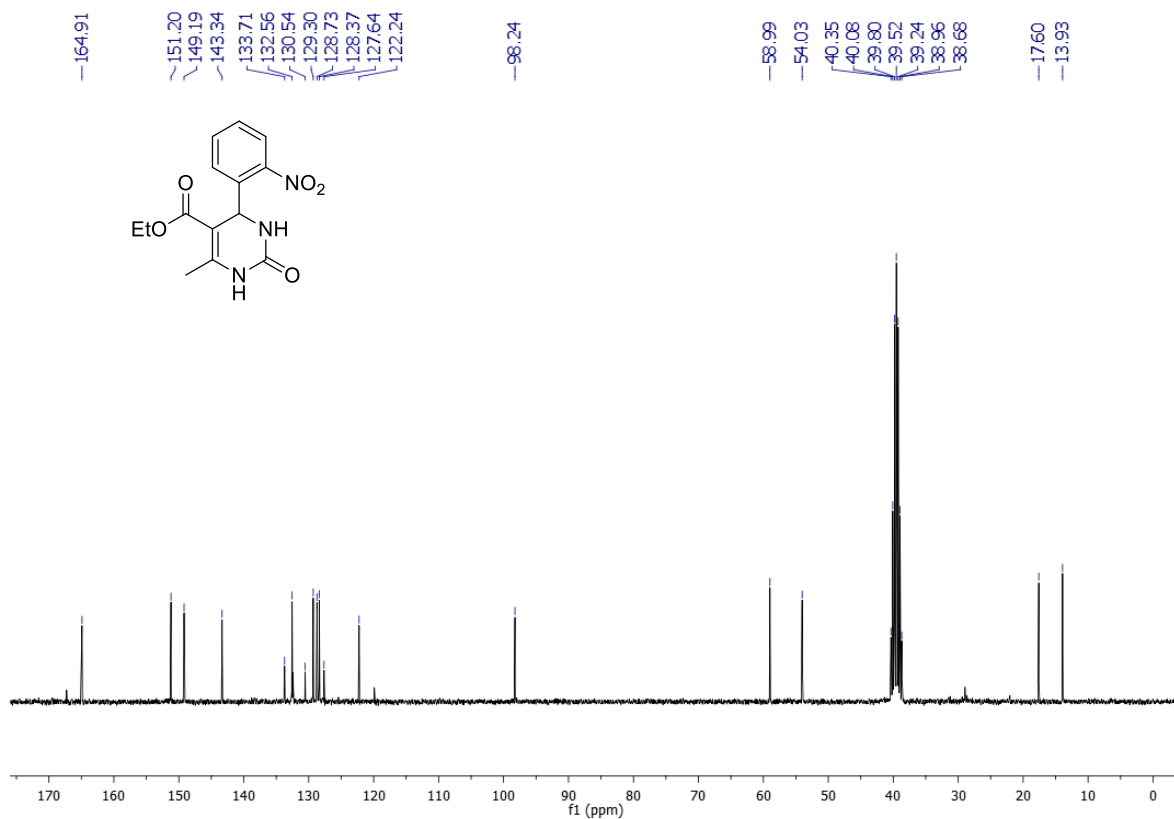


Figure S42. NMR ¹³C spectrum (75 MHz, DMSO-d₆) of product **7g**.

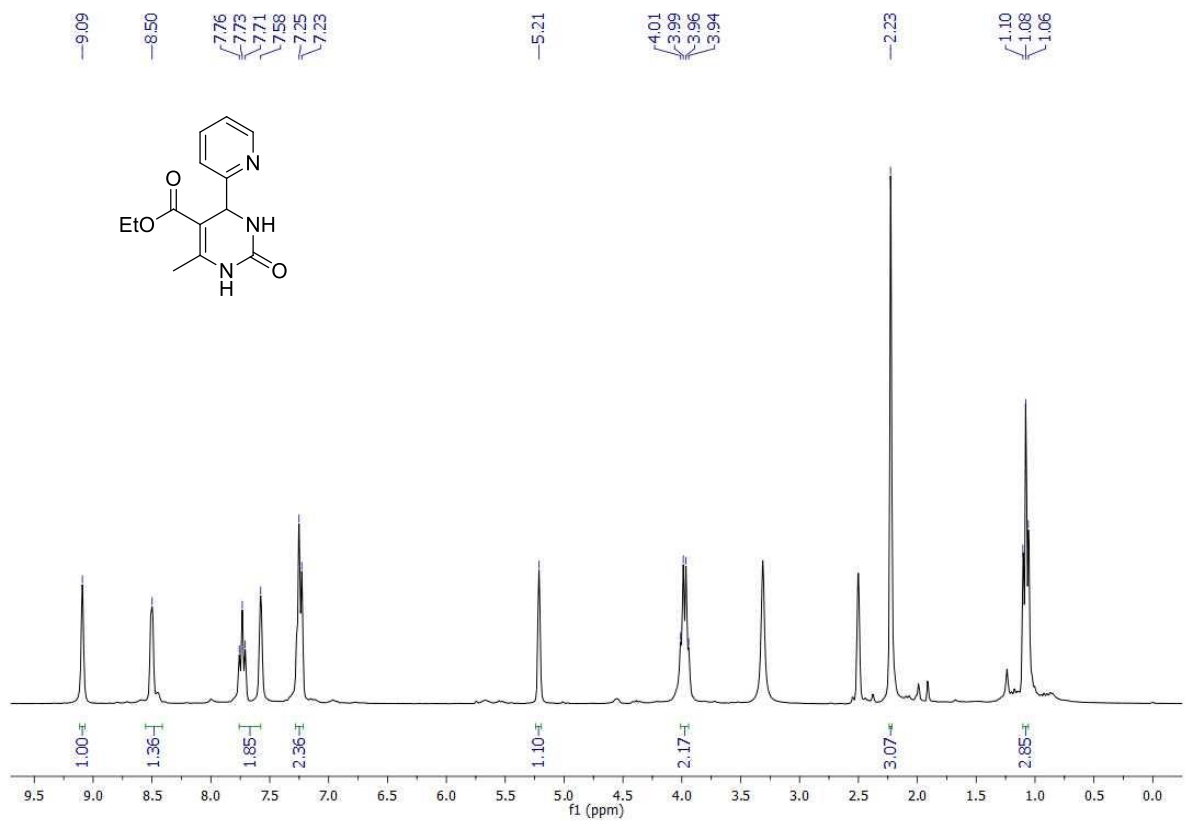


Figure S43. NMR ^1H spectrum (300 MHz, DMSO- d_6) of product **7h**.

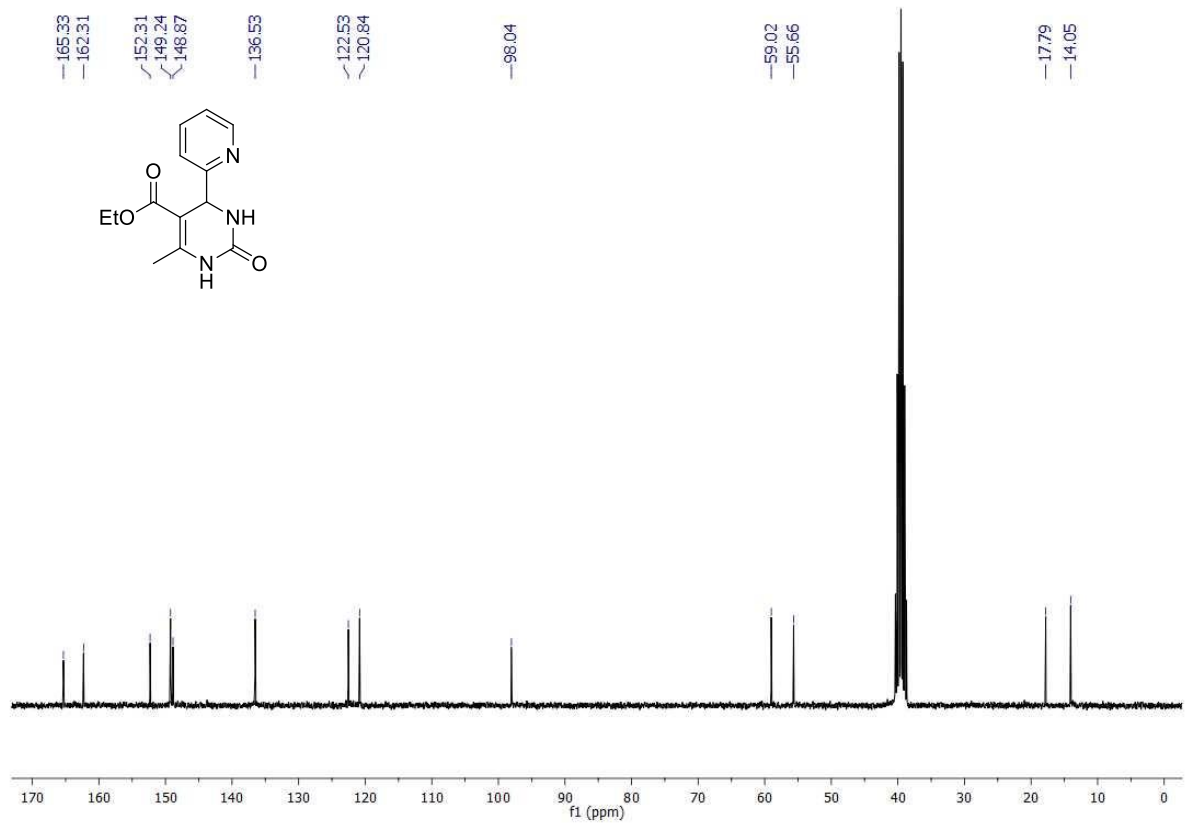


Figure S44. NMR ^{13}C spectrum (75 MHz, DMSO- d_6) of product **7h**.

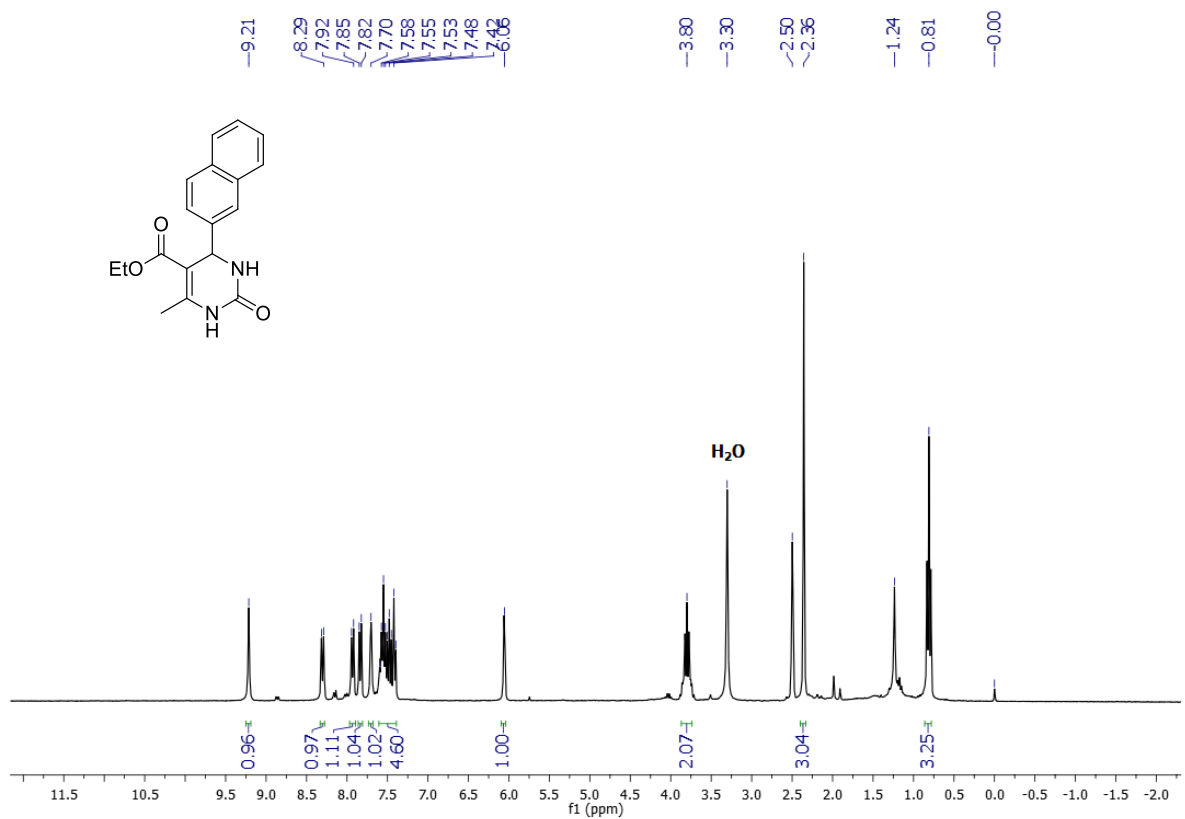


Figure S45. NMR ^1H spectrum (300 MHz, DMSO- d_6) of product 7i.

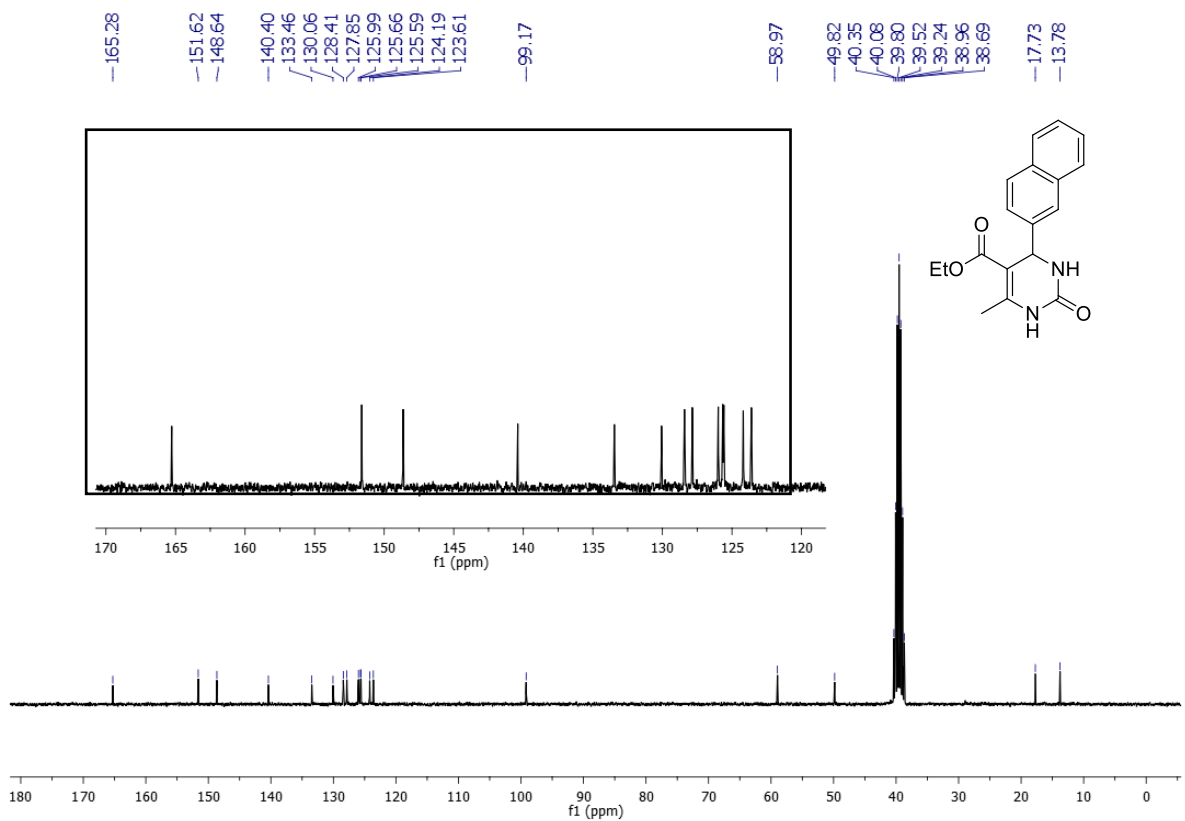


Figure S46. NMR ^{13}C spectrum (75 MHz, DMSO- d_6) of product 7i.

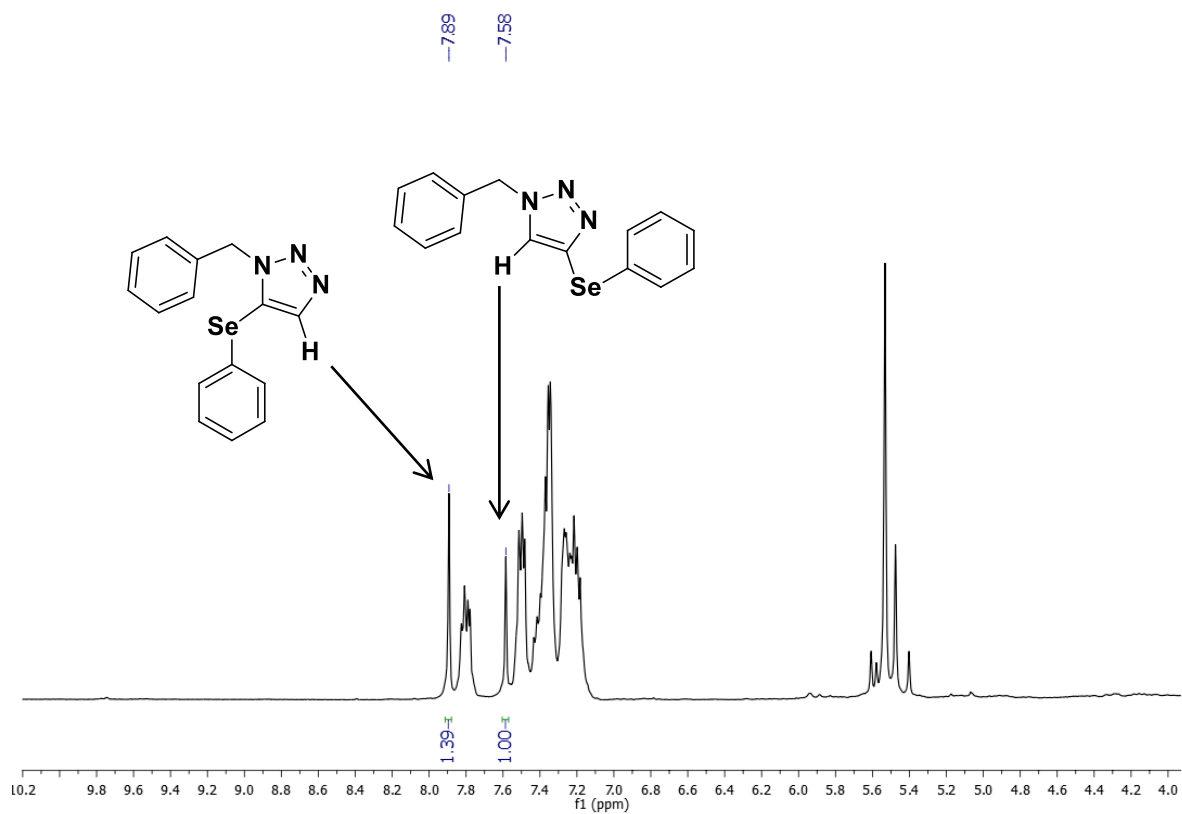


Figure S47. NMR ¹H spectrum (400 MHz, CDCl₃) of a mixture of 1,4- and 1,5-disubstituted (1:1.4) triazole (3j).

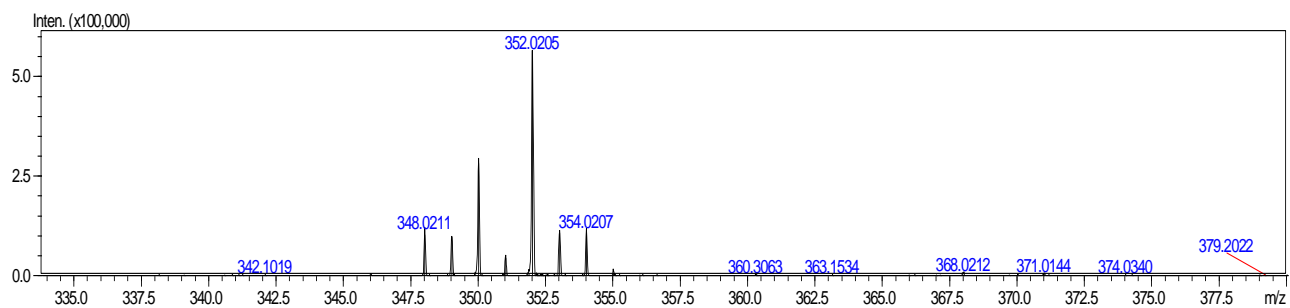


Figure S48. HRMS spectra of compound 3i.

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