SUPPORTING INFORMATION

Ultrasound-Assisted Diastereoselective Green Synthesis of Spiro-Fused-γ-Lactams Functionalized with Amide Bond Heterocyclic Bioisostere via Ugi Azide/Domino Process Coupled Strategy

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1. General Experimental Methods

^{1}H and ^{13}C NMR spectra were acquired on a 500 MHz spectrometer. The solvent for the NMR samples was $CDCl_3$. Chemical shifts are reported in parts per million (δ/ppm). The internal reference for the NMR spectra is tetramethylsilane at 0.00 ppm. Coupling constants are reported in hertz (*J*/Hz). Multiplicities of the signals are reported using standard abbreviations: singlet (s), doublet (d), triplet (t), quartet (q), and multiplet (m). IR spectra were recorded by the attenuated total reflection (ATR) method, using neat compounds. The wavelengths are reported in reciprocal centimeters (ν_{max}/cm^{-1}). High-resolution mass spectrometry (HRMS) spectra were acquired via electrospray ionization ESI (+) and recorded via the time-of-flight (TOF) method. US irradiated reactions were performed in sealed vials placed in a Ultrasonic Bath of a sonicator Bransonic CPX1800H at frequencies of 40 KHz ± 6%. The reaction progress was monitored by TLC, and the spots were visualized under UV light (254 or 365 nm). Flash column chromatography was performed using silica gel (230−400 mesh) and mixtures in different proportions of hexanes, with ethyl acetate as mobile phase. Melting points were determined on a Fisher−Johns apparatus and were uncorrected. The purity degree was documented qualitatively for each product, with copies of all ^{1}H and ^{13}C NMR spectra. Commercially available reagents were used without further purification. The solvents were distilled and dried according to standard procedures.

2. General experimental procedures

2.1 General procedure (i) for synthesize of products 7a−l (RT)

In a round-bottomed flask (10 mL) containing a solution of 2-furaldehyde (0.5 mmol, 1.0 equiv) in anhydrous MeOH [1.0 M] under a nitrogen atmosphere were added sequentially the corresponding amine (0.5 mmol, 1.0 equiv), isocyanide (0.5 mmol, 1.0 equiv), and azidotrimethylsilane (0.5 mmol, 1.0 equiv). The flask was closed, and the reaction mixture was stirred for 24 h at rt. Then, the solvent was removed until dryness and the crude was purified by silica-gel column chromatography using a mixture of hexane with AcOEt (4/1; *v/v*) to afford the Ugi-azide products **7a-l**.

2.2 General procedure (ii) for synthesize of products 7a–l (USI)

In a round-bottomed flask (10 mL) containing a solution of 2-furaldehyde (0.5 mmol, 1.0 equiv) in anhydrous MeOH [1.0 M] under a nitrogen atmosphere were added sequentially the corresponding amine (0.5 mmol, 1.0 equiv), isocyanide (0.5 mmol, 1.0 equiv), and azidotrimethylsilane (0.5 mmol, 1.0 equiv). The flask was closed, and the reaction mixture was then sonicated in an ultrasonic cleaner water bath at room temperature for 2 hours. Then, the solvent was removed until dryness and the crude was purified by silica-gel column chromatography using a mixture of hexane with AcOEt (4/1; *v/v*) to afford the Ugi-azide products **7a-l**.

2.3 General procedure (iii) for synthesize of products 13a–j (RT)

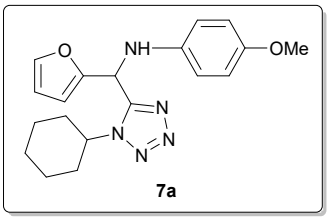
In a round bottomed flask (10 mL) containing a solution of compound **7a-l** (0.5 mmol, 1.0 equiv) in anhydrous PhMe [0.5 M] under a nitrogen atmosphere was added maleic anhydride (2.0 equiv). The flask was closed and the reaction mixture was stirred for 2 h at rt. The precipitate formed was filtered off, washed with the minimum of toluene and dichloromethane and dried to constant weight to afford the corresponding products **13a**−**j.**

2.4 General procedure (iv) for synthesize of products 13a–j (USI)

In a round bottomed flask (10 mL) containing a solution of compound **7a-l** (0.5 mmol, 1.0 equiv) in anhydrous PhMe [0.5 M] under a nitrogen atmosphere was added maleic anhydride (2.0 equiv). The flask was closed and the reaction mixture was then sonicated in an ultrasonic cleaner water bath at room temperature for 1 h. The precipitate formed was filtered off, washed with the minimum of toluene and dichloromethane and dried to constant weight to afford the corresponding products **13a**−**j.**

3. Experimental data of products 7a−l, products 13a−k and intermediates 13k and 13l.

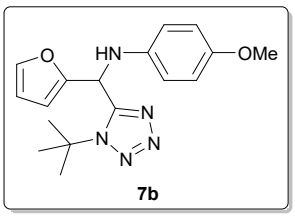
3.1 *N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)-4-methoxyaniline (7a).



7a

White solid (99.0 mg, 70%, RT); (120.2 mg, 85%, USI); mp=86 - 88 °C; R_f = 0.20 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz; $CDCl_3$) δ 7.40 – 7.39 (m, 1H), 6.75 (d, J = 8.83 Hz, 2H), 6.67 (d, J = 8.86 Hz, 1H), 6.37 – 6.35 (m, 1H), 6.32 – 6.29 (m, 1H), 6.00 (d, J = 4.5 Hz, 1H), 4.56 – 4.46 (m, 2H), 3.72 (s, 3H), 2.04 – 1.99 (m, 1H), 1.96 – 1.82 (m, 4H), 1.74 – 1.68 (m, 1H), 1.66 – 1.64 (m, 1H), 1.39 – 1.23 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.9, 153.0, 150.2, 143.1, 139.4, 116.2, 115.1, 111.2, 108.8, 58.8, 55.8, 49.8, 33.1, 32.9, 25.6, 25.5, 25.0; FT-IR (ATR) ν_{max}/cm^{-1} 3344 (N-H), 1237 (N-N=N); HRMS (ESI-TOF) m/z [M + H]$^+$ Calcd for $C_{19}H_{24}N_5O_2$ 354.1924, found 354.1926.

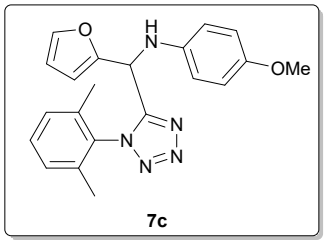
3.2 *N*-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)-4-methoxyaniline (7b).



7b

Light-brown powder (167.1 mg, 90%, RT); (167.1 mg, 90% USI); mp = 152 - 154°C; R_f = 0.40 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (s, 1H), 6.77 – 6.72 (m, 4H), 6.33 – 6.31 (m, 1H), 6.22 (d, J = 2.8 Hz, 1H), 6.12 (d, J = 4.5 Hz, 1H), 4.62 (s, 1H), 3.72 (s, 3H), 1.69 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.0, 151.3, 142.9, 139.5, 117.3, 115.0, 110.9, 108.9, 61.9, 55.7, 50.9, 30.1; FT-IR (ATR) ν_{max}/cm^{-1} 3303 (N-H), 1291 (N-N=N); HRMS (ESI-TOF) m/z [M + H]$^+$ Calcd for $C_{17}H_{22}N_5O_2$ 328.1768, found 328.1769.

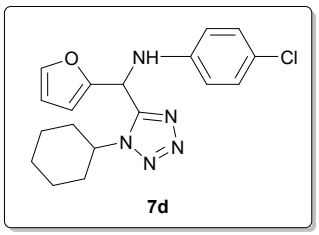
3.3 *N*-((1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)-4-methoxyaniline (7c).



7c

Light-brown solid (100.1 mg, 70%, RT); (94.4 mg, 66%, USI); mp = 83 - 85 °C; R_f = 0.30 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 - 7.38 (m, 1H), 7.29 (s, 1H), 7.21 - 7.17 (m, 2H), 6.70 (d, J = 8.8 Hz, 2H), 6.57 (d, J = 8.9 Hz, 2H), 6.28 – 6.24 (m, 1H), 6.20 – 6.16 (m, 1H), 5.51 (d, J = 9.8 Hz, 1H), 4.54 (d, J = 9.9 Hz, 1H), 3.71 (s, 3H), 1.76 (s, 3H), 1.68 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 154.0, 149.9, 143.1, 139.2, 136.7, 136.1, 131.5, 131.3, 129.0, 129.0, 128.9, 117.0, 114.9, 110.8, 108.9, 55.7, 49.1, 17.1; FT-IR (ATR) ν_{max}/cm^{-1} 3355 (N-H), 1237 (N-N=N); HRMS (ESI-TOF) m/z [M + H]$^+$ Calcd for $C_{21}H_{22}N_5O_2$ 376.1768, found 376.1750.

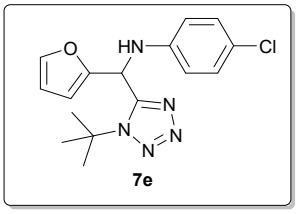
3.4 4-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)aniline (7d).



7d

Ambar solid (128.8 mg, 90% RT); (118.8 mg, 83%, USI); mp = 108 - 110 °C; R_f = 0.20 (Hex-AcOEt= 9:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.15 – 7.10 (m, 2H,), 6.64 (d, *J* = 8.5 Hz, 2H), 6.37 (s, 1H), 6.34 – 6.30 (m, 1H), 6.02 (d, *J* = 5.8 Hz, 1H), 5.00 – 4.93 (m, 1H), 4.47 – 4.42 (m, 1H), 2.07 – 2.02 (m, 1H), 1.97 – 1.93 (m, 2H), 1.88 – 1.84 (m, 2H), 1.75 – 1.72 (m, 1H), 1.62 – 1.59 (m, 1H), 1.34 - 1.27 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5, 149.6, 144.1, 143.3, 129.5, 124.5, 115.3, 111.3, 109.1, 58.9, 48.5, 33.1, 32.9, 25.5, 25.4, 24.9; FT-IR (ATR) ν_{max}/cm^{-1} 3386 (N-H), 1295 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{18}H_{21}ClN_5O$ 358.1429, found 358.1426.

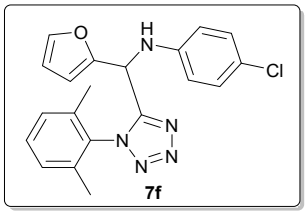
3.5 *N*-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)-4-chloroaniline (7e).



7e

White powder (175.0 mg, 93%, RT); (171.2 mg, 91%, USI); mp= 118 - 120 °C; R_f = 0.30 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (s, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.68 (d, *J* = 8.1 Hz, 2H), 6.33 (s, 1H), 6.24 (s, 1H), 6.19 (d, *J* = 9.6 Hz, 1H), 5.03 (d, *J* = 8.2 Hz, 1H), 1.72 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 150.6, 144.1, 143.1, 129.4, 124.4, 115.7, 111.0, 109.2, 62.1, 49.0, 30.0; FT-IR (ATR) ν_{max}/cm^{-1} 3280 (N-H) 1290 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{16}H_{19}ClN_5O$ 332.1273, found 332.1268.

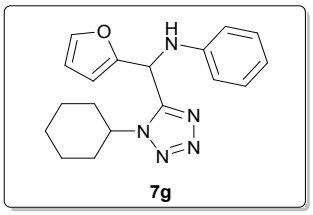
3.6 4-chloro-*N*-((1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)aniline (7f).



7f

Light-brown solid (123.0 mg, 85%, RT); (86.8 mg, 60%, USI); mp= 94 – 96°C; R_f = 0.30 (Hex-AcOEt= 95:5; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.35 (m, 1H), 7.25 – 7.23 (m, 1H), 7.20 – 7.15 (m, 2H), 7.06 – 7.00 (m, 2H), 6.55 (s, 1H), 6.53 (s, 1H); 6.24 – 6.20 (m, 2H), 5.65 (d, *J* = 9.0 Hz, 1H), 5.25 (s, 1H), 1.81 (s, 3H), 1.67 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 148.9, 143.8, 143.0, 136.3, 135.6, 131.2, 131.1, 129.0, 128.8, 128.8, 123.9, 115.2, 110.7, 109.0, 47.2, 16.9, 16.8; FT-IR (ATR) ν_{max}/cm^{-1} 3362 (N-H), 1276 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{20}H_{19}ClN_5O$ 380.1273, found 380.1269.

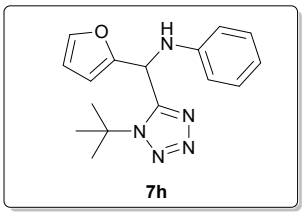
3.7 *N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)aniline (7g).



7g

Yellow-red solid (124.2 mg, 96% RT); (103.5 mg, 80%, USI); mp=108 – 110°C; R_f = 0.50 (Hex-AcOEt= 9:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.20 – 7.16 (m, 2H), 6.82 – 6.79 (m, 1H), 6.70 (d, *J* = 8.1 Hz, 2H), 6.38 – 6.36 (m, 1H), 6.34 – 6.32 (m, 1H), 6.08 (d, *J* = 5.9 Hz, 1H), 4.85 (d, *J* = 5.7 Hz, 1H), 4.53 – 4.47 (m, 1H), 2.07 – 2.01 (m, 1H), 1.96 – 1.92 (m, 2H), 1.89 – 1.83 (m, 2H), 1.75 – 1.71 (m, 1H), 1.64 – 1.60 (m, 1H), 1.37 – 1.26 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.8, 150.0, 145.5, 143.2, 129.6, 119.8, 114.1, 111.3, 108.9, 58.9, 48.6, 33.1, 32.9, 25.6, 25.5, 24.9; FT-IR (ATR) ν_{max}/cm^{-1} 3306 (N-H), 1286 (N-N=N); HRMS (ESI-TOF) *m/z* $[M + H]^+$ Calcd for $C_{18}H_{22}N_5O$ 324.1819, found 324.1831.

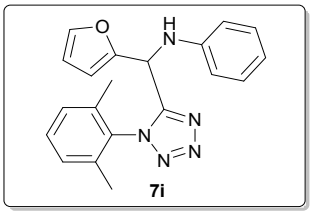
3.8 *N*-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)aniline (7h).



7h

Yellow solid (156.8 mg, 93%, RT); (118.0 mg, 70%, USI); mp = 112 - 114°C; R_f = 0.25 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (s, 1H), 7.22 – 7.16 (m, 2H), 6.89 – 6.77 (m, 3H), 6.31 (s, 1H), 6.27 (s, 2H), 5.22 (s, 1H), 1.72 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.7, 151.0, 145.5, 142.9, 129.5, 119.7, 114.6, 111.0, 109.0, 62.0, 48.9, 30.0; FT-IR (ATR) ν_{max}/cm^{-1} 3307 (N-H), 1286 (N-N=N); HRMS (ESI-TOF) *m/z* $[M + H]^+$ Calcd for $C_{16}H_{20}N_5O$ 298.1662, found 298.1656.

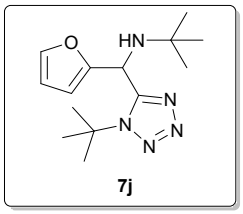
3.9 *N*-((1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)aniline (7i).



7i

Light-brown oil (121.1 mg, 92%, RT); (113.2 mg, 86%, USI); R_f = 0.30 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 - 7.37 (m, 1H), 7.27 – 7.25 (m, 1H), 7.20 – 7.17 (m, 2H), 7.12 – 7.09 (m, 2H), 6.77 – 6.73 (m, 1H), 6.58 (s, 1H), 6.57 (s, 1H), 6.27 – 6.23 (m, 1H), 6.21 – 6.18 (m, 1H), 5.67 (s, 1H), 4.91 (s, 1H), 1.79 (s, 3H), 1.68 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 149.5, 145.2, 143.0, 136.6, 135.9, 131.3, 131.2, 129.4, 128.9, 128.9, 119.6, 114.3, 110.8, 108.9, 47.4, 17.1, 17.0; FT-IR (ATR) ν_{max}/cm^{-1} 3362 (N-H), 1276 (N-N=N). HRMS (ESI-TOF) *m/z* $[M + H]^+$ Calcd for $C_{20}H_{20}N_5O$ 346.1662, found 346.1659.

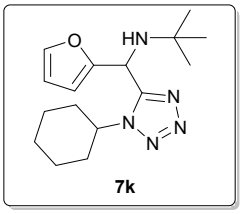
3.10 *N*-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)(furan-3-yl)methyl)-2-methylpropan-2-amine (7j).



7j

Ambar oil (130.5 mg, 83%, RT) (119.5 mg, 76%, USI); R_f = 0.40 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (s, 1H), 6.28 – 6.24 (m, 1H), 6.00 – 5.97 (m, 1H), 5.50 (s, 1H), 2.43 (s, 1H), 1.66 (s, 9H), 1.04 (s, 9H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 153.5, 142.3, 110.9, 108.0, 61.7, 51.5, 47.7, 30.0, 29.7; FT-IR (ATR) ν_{max}/cm^{-1} 3339 (N-H), 1279 (N-N=N). HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{14}H_{24}N_5O$ 278.1975, found 278.1977.

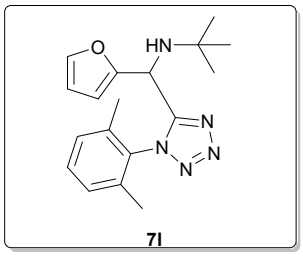
3.11 *N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)-2-methylpropan-2-amine (7k).



7k

Ambar solid (109.2 mg, 90%, RT) (100.7 mg, 83%, USI); mp=86 - 88°C; R_f = 0.50 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (s, 1H), 6.34 – 6.29 (m, 1H), 6.13 – 6.09 (m, 1H), 5.61 (s, 1H), 4.76 – 4.65 (m, 1H), 2.00 – 1.85 (m, 5H), 1.83 – 1.80 (m, 1H), 1.76 – 1.72 (m, 1H), 1.37 – 1.30 (m, 3H), 1.07 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 152.2, 142.6, 110.9, 107.5, 58.4, 51.9, 47.2, 32.9, 32.7, 29.4, 25.5, 25.5, 25.0; FT-IR (ATR)ν_{max}/cm^{-1} 3303 (N-H), 1244 (N-N=N). HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{16}H_{26}N_5O$ 304.2132, found 304.2132.

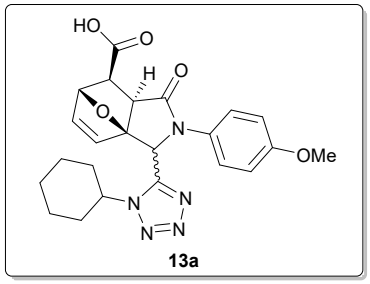
3.12 *N*-((1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)(furan-3-yl)methyl)-2-methylpropan-2-amine (7l).



7l

Light-brown oil (99.2 mg, 90%, RT), (85.5 mg, 69%, USI); R_f = 0.40 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (t, *J* = 5.7 Hz, 1H), 7.29 – 7.27 (m, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 6.25 – 6.22 (m, 1H), 6.04 (d, *J* = 3.2 Hz, 1H), 4.96 (s, 1H), 2.03 (s, 1H), 1.92 (s, 3H), 1.69 (s, 3H), 0.85 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.4, 152.2, 142.3, 136.2, 136.2, 132.0, 131.0, 128.7, 128.7, 110.8, 107.7, 51.4, 45.8, 29.3, 17.5, 17.2; FT-IR (ATR) ν_{max}/cm^{-1} 3386 (N-H), 1273 (N-N=N). HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{18}H_{24}N_5O$ 326.1975, found 326.1977.

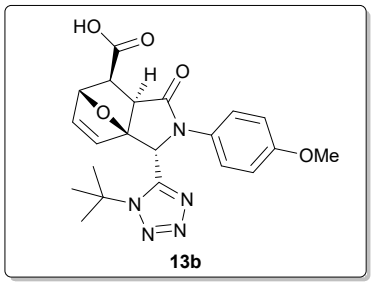
3.13 3-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-(4-methoxyphenyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13a).



13a

White powder (57.5 mg, 90%, RT); (58.8 mg, 92%, USI) mp= 222 – 224 °C; R_f = 0.30 (Hex-AcOEt= 1:4; v/v) as a mixture of diastereoisomers 75:25, signals of the major and minor isomers indicated as Q and q whenever possible; ^{1}H NMR (500 MHz, DMSO) δ 12.44 (s, 2H, Q + q), 7.28 (d, *J* = 9.0 Hz, 2H, Q), 7.25 (d, *J* = 9.0 Hz, 2H, q), 6.96- 6.88 (m, 4H, Q + q), 6.77 (d, *J* = 5.7 Hz, 1H, Q), 6.55 (d, *J* = 7.1 Hz, 1H, q), 6.45 (d, *J* = 5.7 Hz, 1H, Q), 6.10 (d, *J* = 5.8 Hz, 1H, q), 5.20 (s, 1H, q), 5.13 (s, 1H, Q), 4.62 (m, 1H, q), 4.47 (m, 1H, Q), 3.71 (s, 3H, q), 3.68 (s, 3H, Q), 3.35 (d, *J* = 9.2 Hz, 1H, q), 3.17 (d, *J* = 8.9 Hz, 1H, Q), 2.77 (d, *J* = 8.9 Hz, 1H, Q), 2.72 (d, *J* = 9.2 Hz, 1H, q),2.50 (s, 1H, Q), 2.30 (s, 1H, q), 1.98 (m, 2H, Q + q), 1.80 (m, 3H, Q + q), 1.62 (m, 7H, Q + q),1.42 (m, 3H, Q + q), 1.39 (m, 2H, Q + q), 1.14 (m, 3H, Q + q); ^{13}C NMR (126 MHz, DMSO) δ 172.5, 172.3, 170.0, 169.7, 157.4, 156.4, 151.3, 148.9, 138.1, 136.9, 135.1, 133.0, 129.7, 129.5, 128.8, 128.1, 125.4, 122.3, 114.2, 113.8, 89.7, 88.9, 81.8, 81.7, 58.3, 56.9, 55.3, 55.2, 54.5, 53.9, 51.2, 49.9, 45.1, 33.0, 32.9, 32.9, 32.6, 24.7, 24.5, 24.4, 24.3; FT-IR (ATR) ν_{max}/cm^{-1} 3000 (O-H), 1744 (C=O), 1714 (C=O), 1252 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{23}H_{26}N_5O_5$ 452.1928, found 452.1921; FT-IR (ATR) ν_{max}/cm^{-1} 3000 (O-H), 1744 (C=O), 1714 (C=O), 1252 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{23}H_{26}N_5O_5$ 452.1928, found 452.1921.

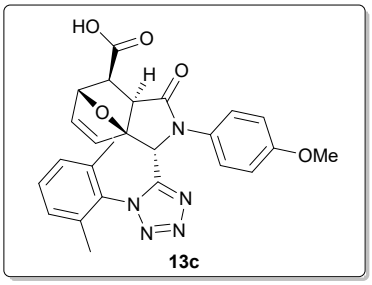
3.14 3-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-2-(4-methoxyphenyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13b).



13b

White powder (45.5mg, 70%, RT); (50.7 mg 78%, USI); mp =206 – 208 °C; R_f = 0.20 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.47 (s, 1H), 7.05 (d, *J* = 9.0 Hz, 2H), 6.80 (d, *J* = 8.9 Hz, 2H), 6.47 – 6.41 (ml, 1H), 5.88 (s, 1H), 5.83 (d, *J* = 5.8 Hz, 1H), 5.37 (s, 1H), 3.74 (s, 3H), 3.58 (d, *J* = 9.2 Hz, 1H), 2.91 (d, *J* = 9.2 Hz, 1H), 1.58 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 174.0, 172.2, 159.5, 151.7, 137.6, 133.5, 129.0, 128.3, 114.9, 91.2, 82.9, 62.1, 58.9, 55.6, 50.0, 45.8, 30.4; FT-IR (ATR) ν_{max}/cm^{-1} 3000 (O-H), 1714 (C=O), 1632 (C=O), 1252 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{21}H_{24}N_5O_5$ 426.1772, found 426.1762.

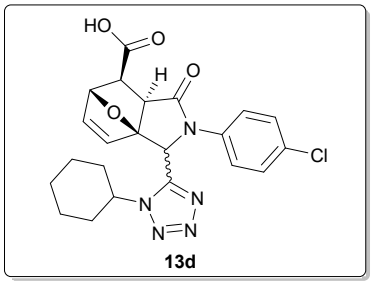
3.15 3-(1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)-2-(4-methoxyphenyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13c).



13c

White powder (40.4 mg, 64%, RT); (56.7 mg, 90%, USI); mp= 224 - 226 °C; R_f = 0.45 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 – 7.35 (m, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6. 89 (d, *J* = 9.0 Hz, 2H), 6.72 (d, *J* = 9.0 Hz, 2H), 6.48 (dd, *J* = 5.8, 1.7 Hz, 1H), 6.19 (d, *J* = 5.8 Hz, 1H), 5.34 (d, *J* = 1.6 Hz, 1H), 5.22 (s, 1H), 3.75 (s, 3H), 3.70 (d, *J* = 9.2 Hz, 1H), 2.93 (d, *J* = 9.2 Hz, 1H), 1.92 (s, 3H), 1.02 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 173.7, 171.4, 159.5, 153.1, 137.5, 137.1, 134.8, 133.8, 131.6, 130.6, 129.2, 129.0, 128.5, 127.6, 114.9, 90.8, 82.9, 55.8, 55.7, 50.5, 46.1, 17.9, 16.1; FT-IR (ATR) ν_{max}/cm^{-1} 2970 (O-H); 1746 (C=O), 1688 (C=O), 1298 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{25}H_{24}N_5O_5$ 474.1772, found 474.1762.

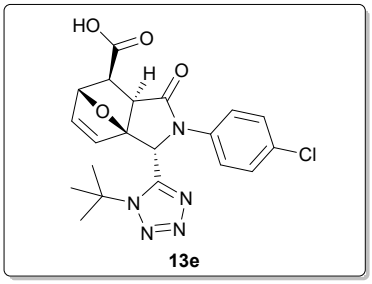
3.16 2-(4-chlorophenyl)-3-(1-cyclohexyl-1*H*-tetrazol-5-yl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13d).



13d

White powder (63.7 mg, 60%, USI); mp =140 – 142 °C; R_f = 0.37 (Hex-AcOEt= 1:4; v/v); mixture of diastereoisomers 50:50; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.9 Hz, 2H), 7.18 (d, *J* = 8.7 Hz, 2H), 7.11 (d, *J* = 8.8 Hz, 2H), 7.08 (d, *J* = 8.7 Hz, 2H), 6.87 (s, 1H), 6.76 (d, *J* = 5.8 Hz, 1H), 6.46 (dd, *J* = 5.8, 1.4 Hz, 1H), 6.35 (s, 1H), 6.30 (dd, *J* = 5.7, 1.4 Hz, 1H), 6.04 (d, *J* = 5.8 Hz, 1H), 5.65 (s, 1H), 5.09 (s, 1H), 4.24 (m, 1H), 4.00 (m, 1H), 3.55 (d, *J* = 9.1 Hz, 1H), 3.04 (d, *J* = 8.8 Hz, 1H), 2.89 (d, *J* = 9.1 Hz, 1H), 2.85 (d, *J* = 8.8 Hz, 1H), 1.94 – 1.82 (m, 4H), 1.78 – 1.63 (m, 6H), 1.55 – 1.42 (m, 4H), 1.32 – 1.27 (m, 2H), 1.13 – 1.05 (m, 2H), 0.90 – 0.80 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.4, 174.3, 171.1, 170.4, 150.3, 148.1, 137.7, 136.5, 136.5, 135.3, 134.9, 134.5, 133.7, 133.4, 131.4, 129.7, 129.2, 126.8, 122.5, 90.6, 89.4, 82.4, 82.2, 60.5, 60.0, 58.9, 56.0, 55.1, 52.0, 50.6, 45.8, 45.5, 33.3, 33.2, 33.1, 25.2, 25.1, 25.1, 24.8, 24.5, 21.0; FT-IR (ATR) ν_{max}/cm^{-1} 2938 (O-H), 1704 (C=O), 1266 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{22}H_{23}ClN_5O_4$ 456.1433, found 456.1424.

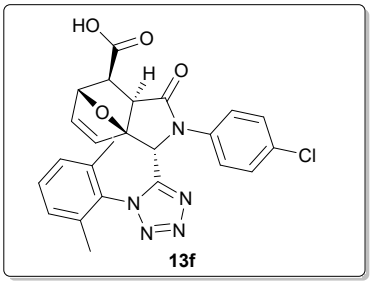
3.17 3-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-2-(4-chlorophenyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13e).



13e

White powder (36.2 mg, 56%, RT); (56.3 mg, 87%, USI); mp =207 – 209 °C; R_f = 0.40 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.29 (d, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 6.47 (d, *J* = 5.1 Hz, 1H), 5.98 (s, 1H), 5.82 (d, *J* = 5.6 Hz, 1H), 5.36 (s, 1H), 3.58 (d, *J* = 9.1 Hz, 1H), 2.92 (d, *J* = 9.1 Hz, 1H), 1.66 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 174.4, 171.6, 151.5, 137.5, 135.1, 134.0, 133.4, 129.8, 127.8, 91.1, 82.8, 62.3, 58.4, 50.2, 45.4, 30.5; FT-IR (ATR) ν_{max}/cm^{-1} 3232 (O-H), 1743 (C=O), 1703 (C=O), 1248 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{20}H_{21}ClN_5O_4$ 430.1277, found 430.1286.

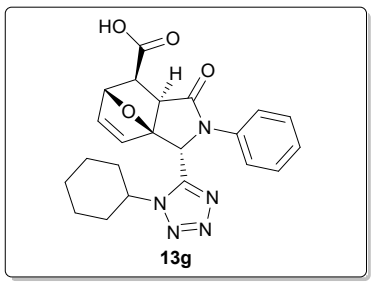
3.18 2-(4-chlorophenyl)-3-(1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)-1-oxo-1,2,3,6,7,7a–hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13f).



13f

White powder, (45.9 mg, 73%, RT); (44.0 mg, 70%, USI); mp= 205 – 207 °C; R_f = 0.25 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.20 (s, 1H), 7.41 – 7.37 (m, 1H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.48 (d, *J* = 5.4 Hz, 1H), 6.20 (d, *J* = 5.7 Hz, 1H), 5.31 – 5.24 (m, 2H), 3.73 (d, *J* = 9.1 Hz, 1H), 2.91 (d, *J* = 9.1 Hz, 1H), 1.93 (s, 3H), 1.05 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 174.9, 170.8, 152.9, 137.6, 137.0, 134.6, 134.4, 133.7, 133.7, 131.7, 130.5, 129.7, 129.3, 129.2, 127.1, 90.6, 82.6, 55.1, 51.0, 45.6, 17.9, 16.3; FT-IR (ATR) ν_{max}/cm^{-1} 3240 (O-H), 1735 (C=O), 1714 (C=O), 1271 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{24}H_{21}ClN_5O_4$ 478.1277, found 478.1282.

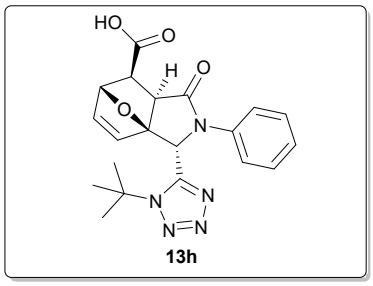
3.19 3-(1-cyclohexyl-1*H*-tetrazol-5-yl)-1-oxo-2-phenyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13g).



13g

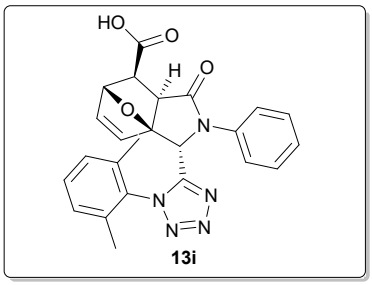
White powder (28.0 mg, 43%, RT); (33.9 mg, 52%, USI); mp =229 – 231 °C; R_f = 0.47 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$ + drops of DMSO) δ 12.85 (s, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.58 (m, 2H), 7.35 (m, 2H), 7.02 (d, *J* = 5.7 Hz, 1H), 6.71 (m, 1H), 6.55 (d, *J* = 12.0 Hz, 1H), 5.39 (s, 1H), 4.68 (m, 1H), 3.45 (d, *J* = 8.9 Hz, 1H), 3.04 (d, *J* = 8.9 Hz, 1H), 2.22 (m, 1H), 1.84 (m, 6H), 1.55 (m, 1H), 1.33 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.5, 169.7, 148.1, 136.7, 136.1, 134.8, 128.7, 125.4, 120.7, 88.9, 82.1, 59.3, 55.2, 51.6, 45.7, 33.1, 32.9, 25.1, 24.8, 24.7; FT-IR (ATR) ν_{max}/cm^{-1} 2938 (O-H); 1704 (C=O), 1266 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{22}H_{24}N_5O_4$ 422.1823, found 422.1815.

3.20 3-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-1-oxo-2-phenyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13h).



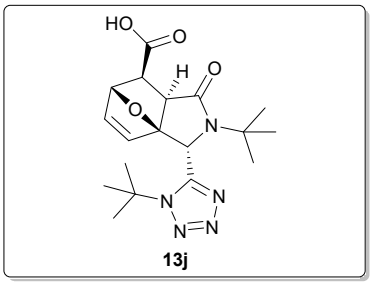
White powder (56.5 mg, 85%, RT); (49.9 mg, 75%, USI); mp =193 – 195 °C; R_f = 0.42 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (s, 1H), 7.33 – 7.20 (m, 3H), 7.20 – 7.13 (m, 2H), 6.44 (d, *J* = 4.9 Hz, 1H), 5.96 (s, 1H), 5.81 (d, *J* = 5.6 Hz, 1H), 5.35 (s, 1H), 3.60 (d, *J* = 9.1 Hz, 1H), 2.90 (d, *J* = 9.1 Hz, 1H), 1.60 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 174.1, 171.8, 151.7, 137.6, 136.5, 133.4, 129.6, 128.4, 126.6, 91.2, 82.9, 62.2, 58.6, 50.2, 45.7, 30.4; FT-IR (ATR) ν_{max}/cm^{-1} 2940 (O-H), 1724 (C=O), 1702 (C=O), 1268 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{20}H_{22}N_5O_4$ 396.1666, found 396.1656.

3.21 3-(1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)-1-oxo-2-phenyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13i).



Ambar oil (56.5 mg, 88%, RT); (48.8 mg, 76%, USI); R_f = 0.45 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 1H), 7.15 - 7.09 (m, 4H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 6.9 Hz, 2H), 6.41 (d, *J* = 5.1 Hz, 1H), 6.11 (d, *J* = 5.8 Hz, 1H), 5.25 – 5.21 (m, 2H), 3.67 (d, *J* = 9.2 Hz, 1H), 2.85 (d, *J* = 9.2 Hz, 1H), 1.86 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 174.4, 171.1, 153.1, 137.6, 137.2, 135.9, 134.7, 133.7, 131.6, 130.6, 129.6, 129.3, 129.0, 128.1, 125.9, 90.8, 82.7, 55.3, 50.9, 45.9, 17.9, 16.1; FT-IR (ATR) ν_{max}/cm^{-1} 2880 (O-H), 1706 (C=O), 1264 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{24}H_{22}N_5O_4$ 444.1666, found 444.1661.

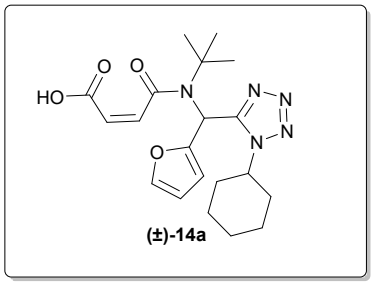
3.22 2-(*tert*-butyl)-3-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (13j).



13j

Ambar oil, (52.8 mg, 78%, RT); (58.2 mg, 86% USI); R_f = 0.25 (Hex-AcOEt= 4:1; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.91 (s, 1H), 5.69 (s, 1H), 5.51 (d, J = 5.8 Hz, 1H), 5.31 (d, J = 1.4 Hz, 1H), 3.12 (d, J = 9.2 Hz, 1H), 2.75 (d, J = 9.2 Hz, 1H), 2.35 (s, 1H), 1.67 (s, 9H), 1.05 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 173.8, 172.77, 152.9, 136.8, 132.9, 90.4, 82.6, 63.1, 56.1, 55.4, 50.0, 45.8, 30.6, 27.8; FT-IR (ATR) ν_{max}/cm^{-1} 2995 (O-H); 1740 (C=O), 1690 (C=O), 1276 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{18}H_{26}N_5O_4$ 376.1979, found 376.1975.

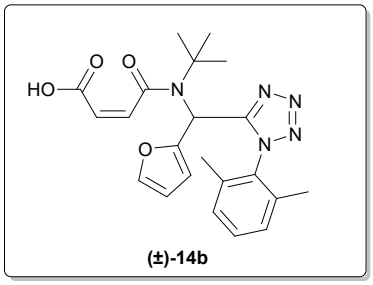
3.23 (*Z*)-4-(*tert*-butyl((1-cyclohexyl-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)amino)-4-oxobut-2-enoic acid (14a).



(±)-14a

White powder, (58.2 mg, 88%, RT); (56.9 mg, 86%, USI); mp =145 – 147 °C; R_f = 0.40 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.95 (s, 1H), 7.49 (s, 1H), 6.71 – 6.75 (m, 1H), 6.47 – 6.42 (m, 1H), 6.32 – 6.20 (m, 3H), 4.41 – 4.34 (m, 1H), 2.04 – 1.98 (m, 2H), 1.94 – 1.88 (m, 1H), 1.81 – 1.75 (m, 1H), 1.71 – 1.60 (m, 2H), 1.45 – 1.29 (m, 11H), 1.28 – 1.21 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 169.0, 144.4, 135.3, 112.1, 58.8, 46.8, 33.1, 32.2, 27.3, 25.3, 24.9; FT-IR (ATR) ν_{max}/cm^{-1} 2934 (O-H),1700 (C=O), 1232 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{20}H_{28}N_5O_4$ 402.2136, found 402.2118.

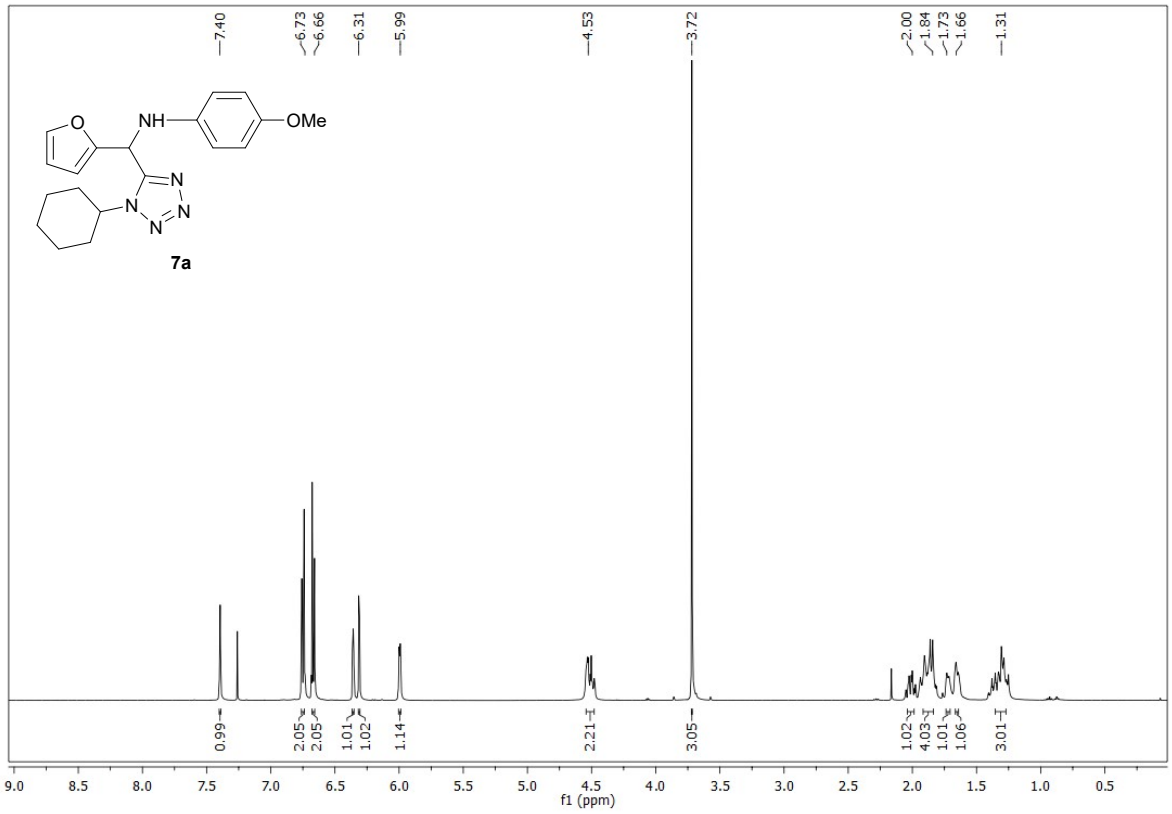
3.24 (*Z*)-4-(*tert*-butyl((1-(2,6-dimethylphenyl)-1*H*-tetrazol-5-yl)(furan-2-yl)methyl)amino)-4-oxobut-2-enoic acid (14b).



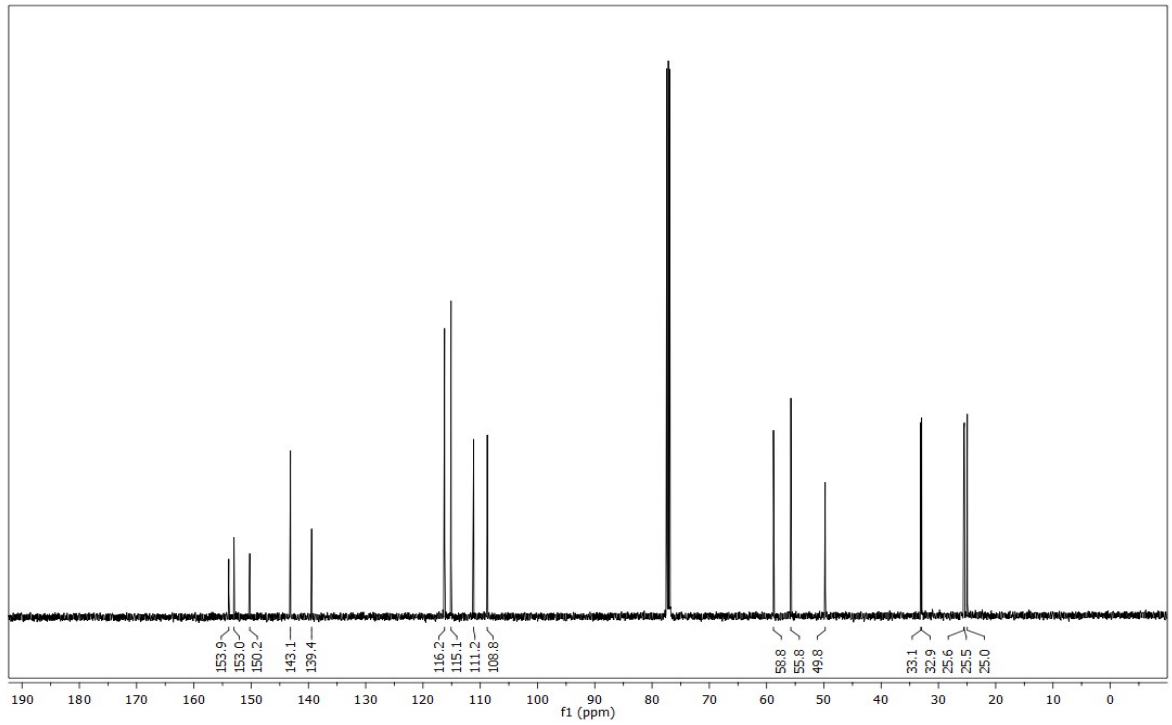
(±)-14b

White powder, (60.5 mg, 93%, RT); (59,8 mg, 92%, USI); mp =223 – 225 °C; R_f = 0.20 (Hex-AcOEt= 1:4; v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.29 (s, 1H), 7.39 – 7.35 (m, 2H), 7.25 (d, J = 7.7 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 6.37 (s, 2H), 6.34 – 6.31 (m, 1H), 6.25 (d, J = 3.3 Hz, 1H), 5.39 (s, 1H), 2.04 (s, 3H), 1.47 (s, 3H), 1.20 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 169.0, 151.5, 144.9, 142.6, 136.6, 135.4, 135.1, 131.7, 130.4, 129.2, 129.1, 114.0, 112.2, 60.2, 46.6, 26.6, 17.4, 16.5; FT-IR (ATR) ν_{max}/cm^{-1} 2930 (O-H), 1714 (C=O), 1256 (N-N=N); HRMS (ESI-TOF) *m/z* [M + H]$^+$ Calcd for $C_{22}H_{26}N_5O_4$ 424.1979, found 424.1981.

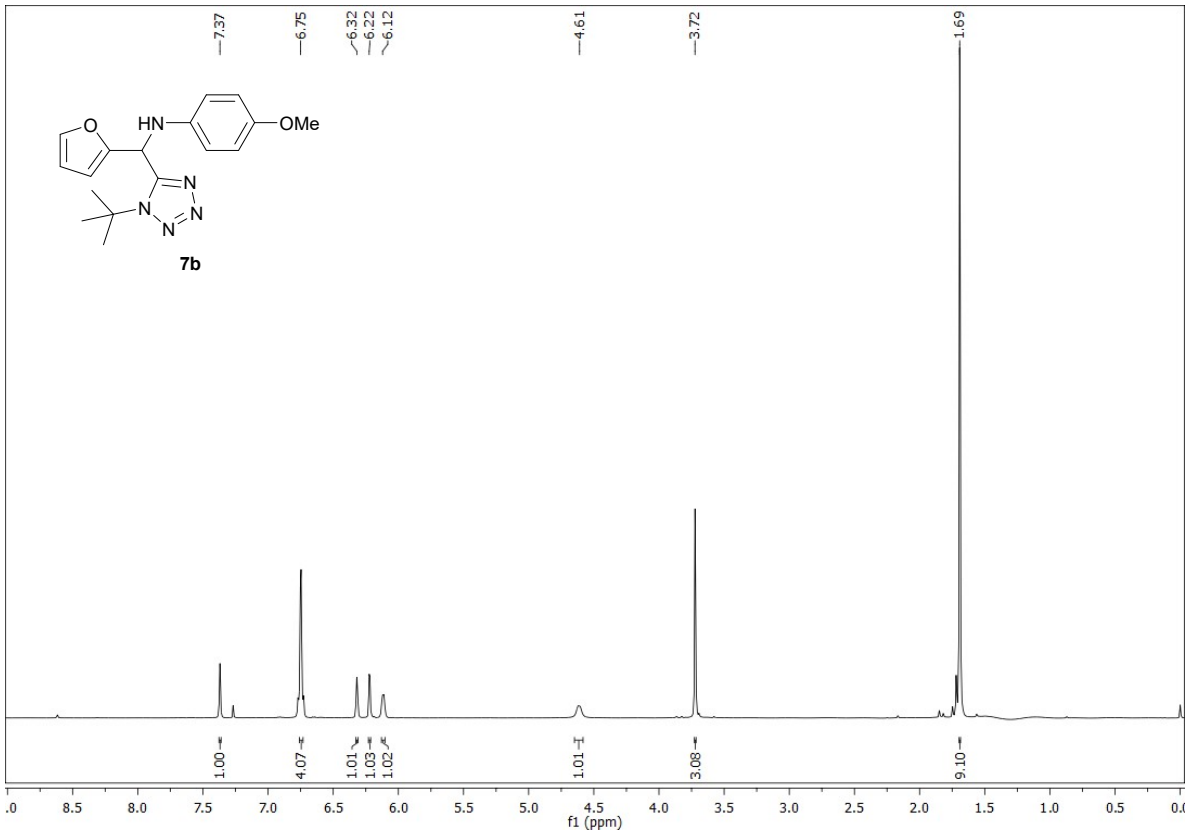
4. ^{1}H NMR and ^{13}C NMR spectra of products 7a–l, products 13a–j and intermediates 14a y 14b.



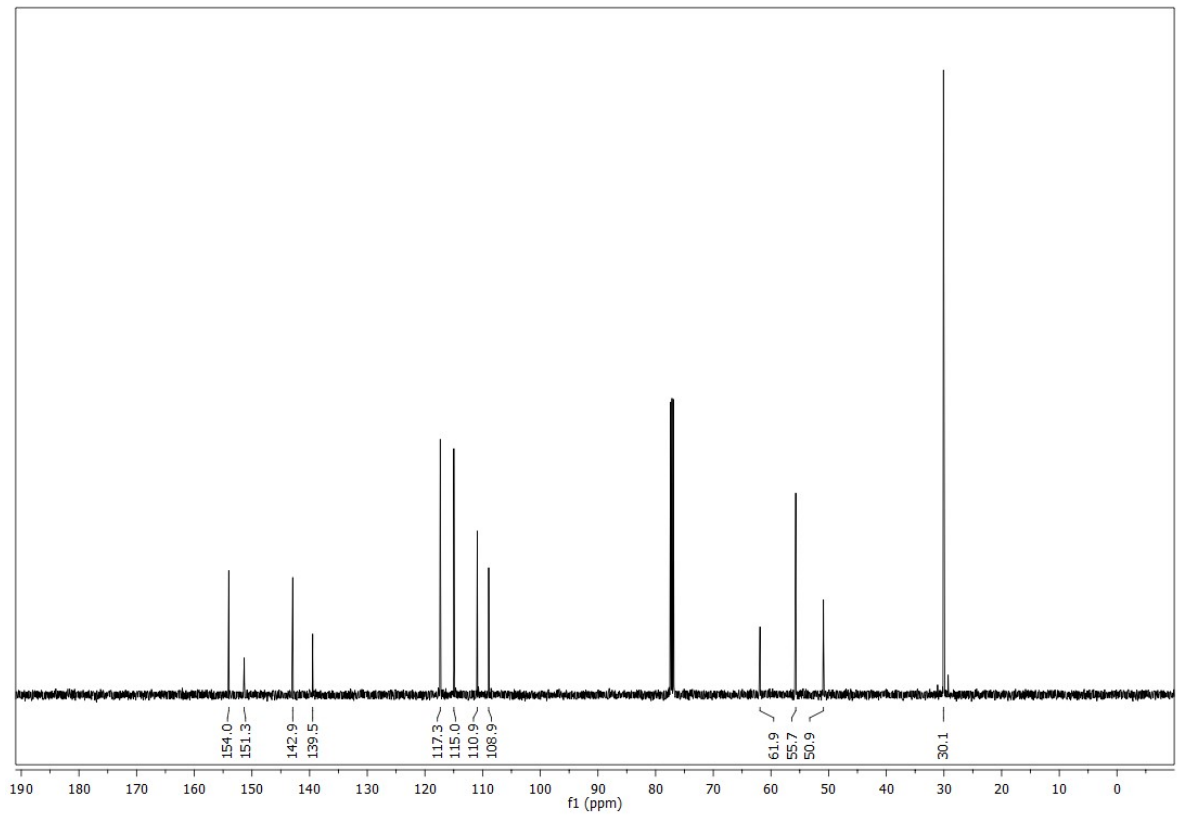
^{1}H NMR spectra of the compound **7a**



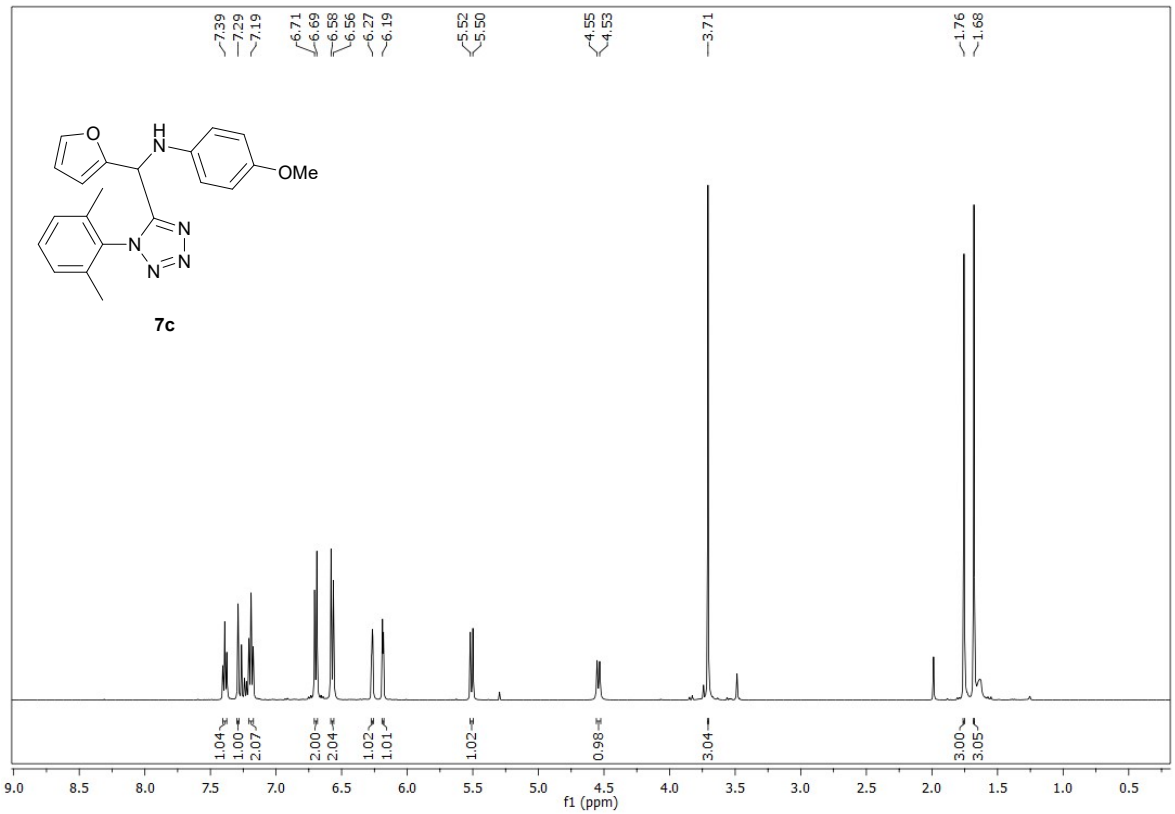
^{13}C NMR spectra of the compound **7a**



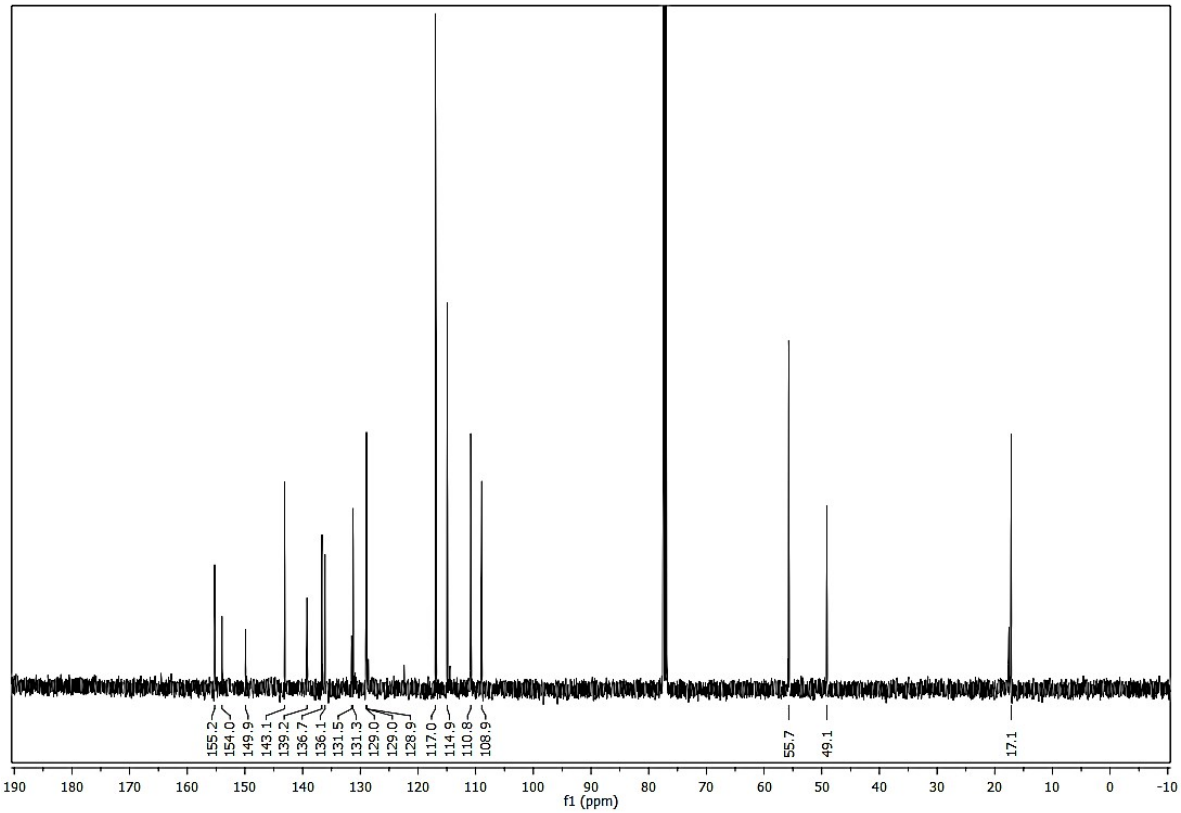
^{1}H NMR spectra of the compound **7b**



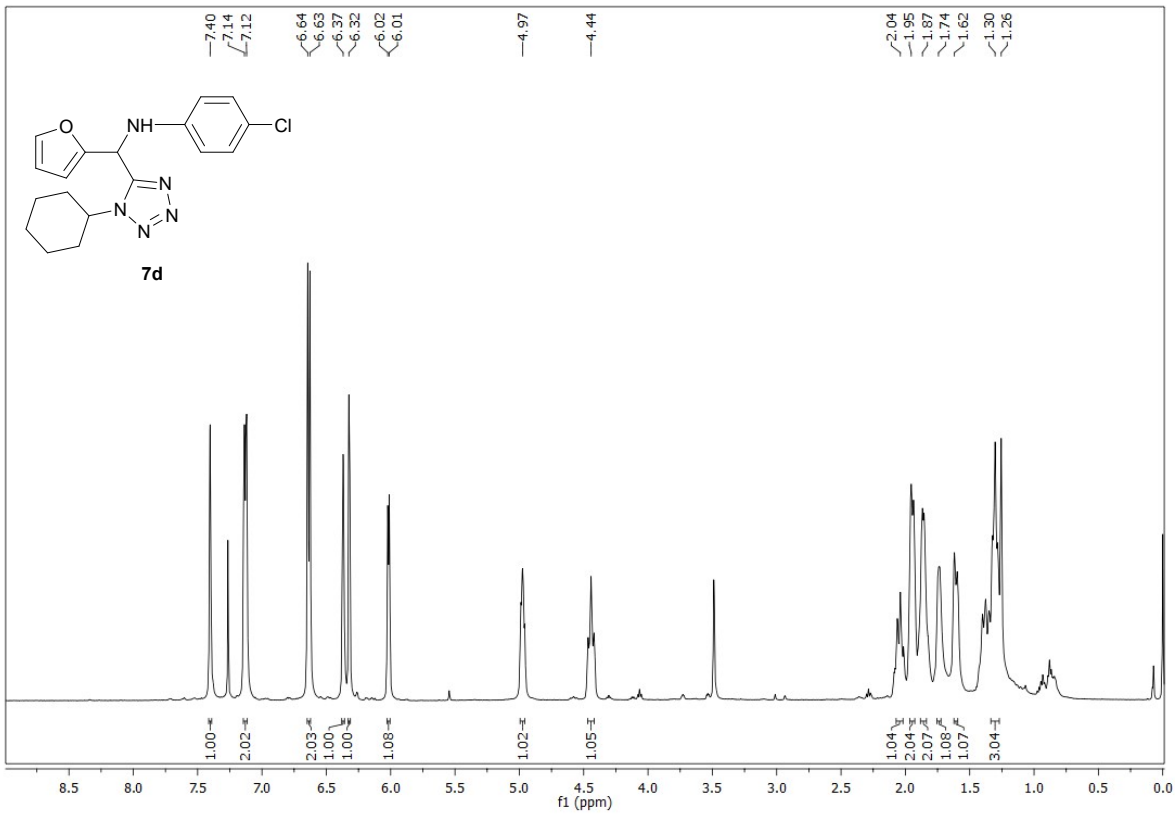
^{13}C NMR spectra of the compound **7b**



^{1}H NMR spectra of the compound **7c**

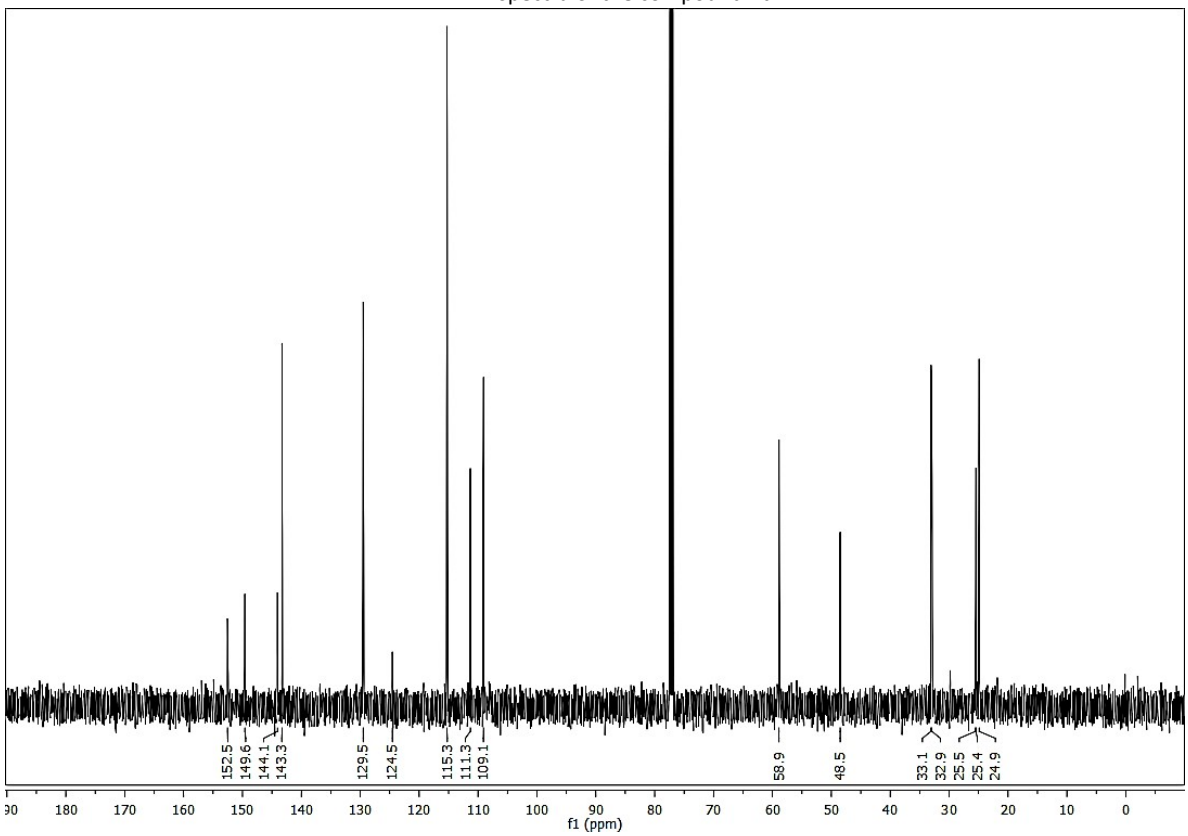


^{13}C NMR spectra of the compound **7c**

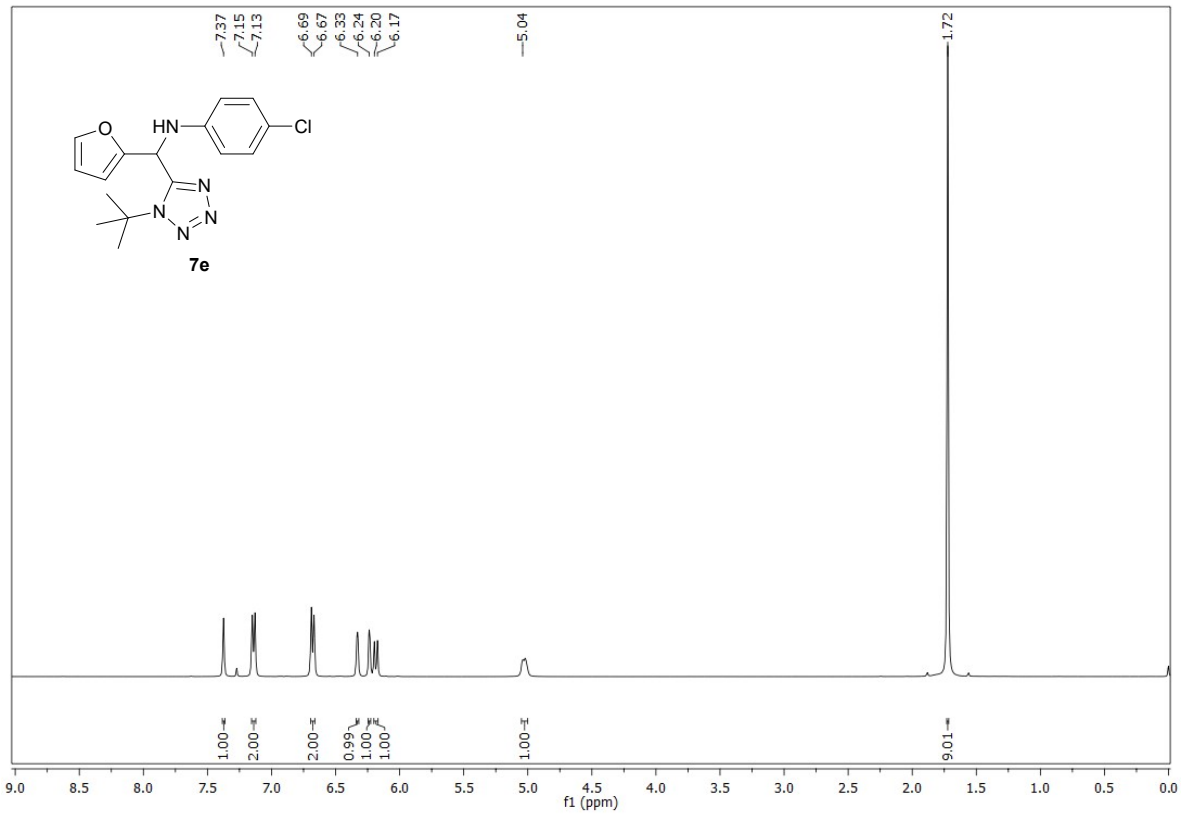


7d

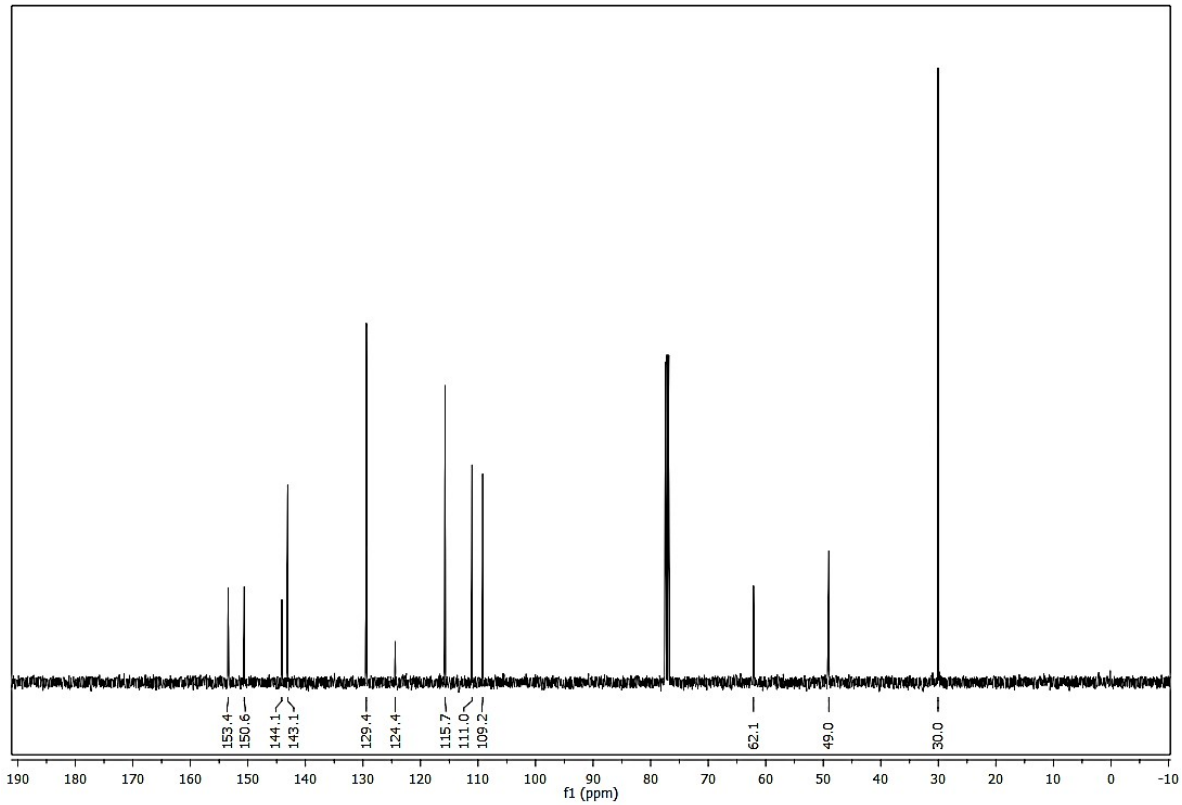
^{1}H NMR spectra of the compound **7d**



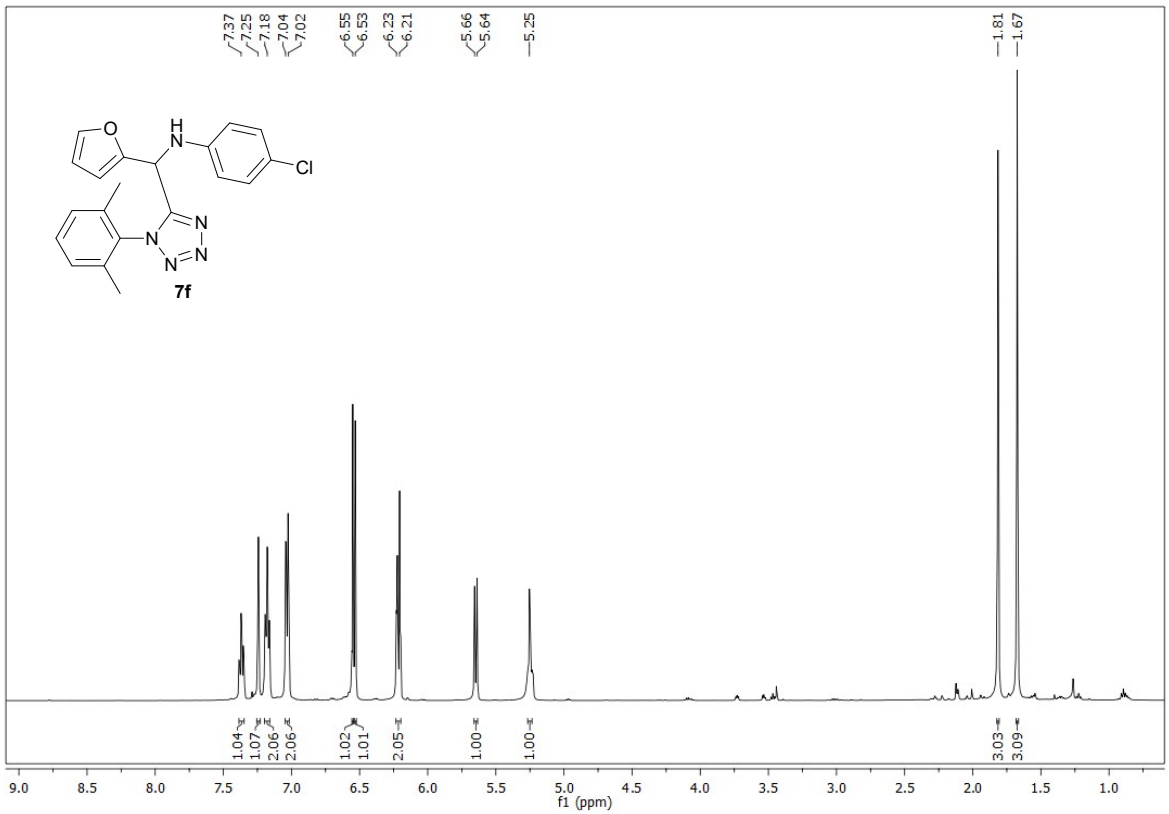
^{13}C NMR spectra of the compound **7d**



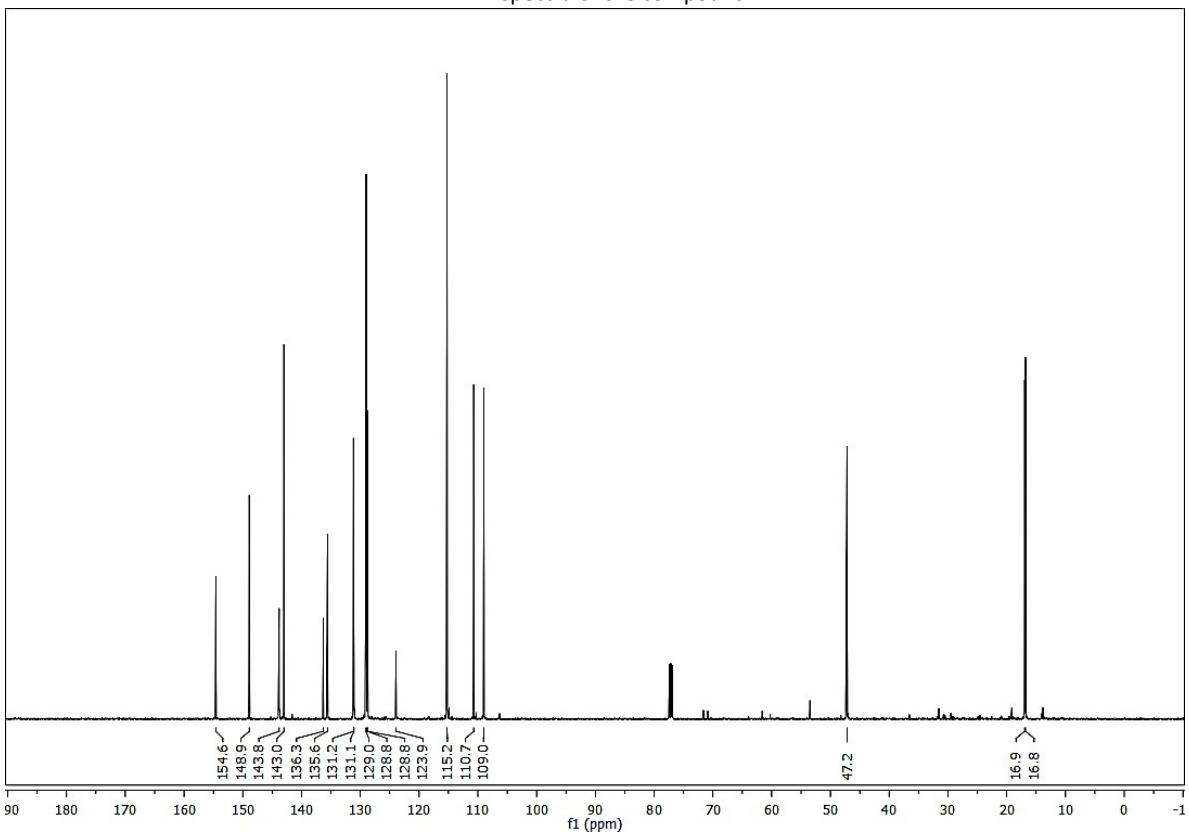
^{1}H NMR spectra of the compound **7e**



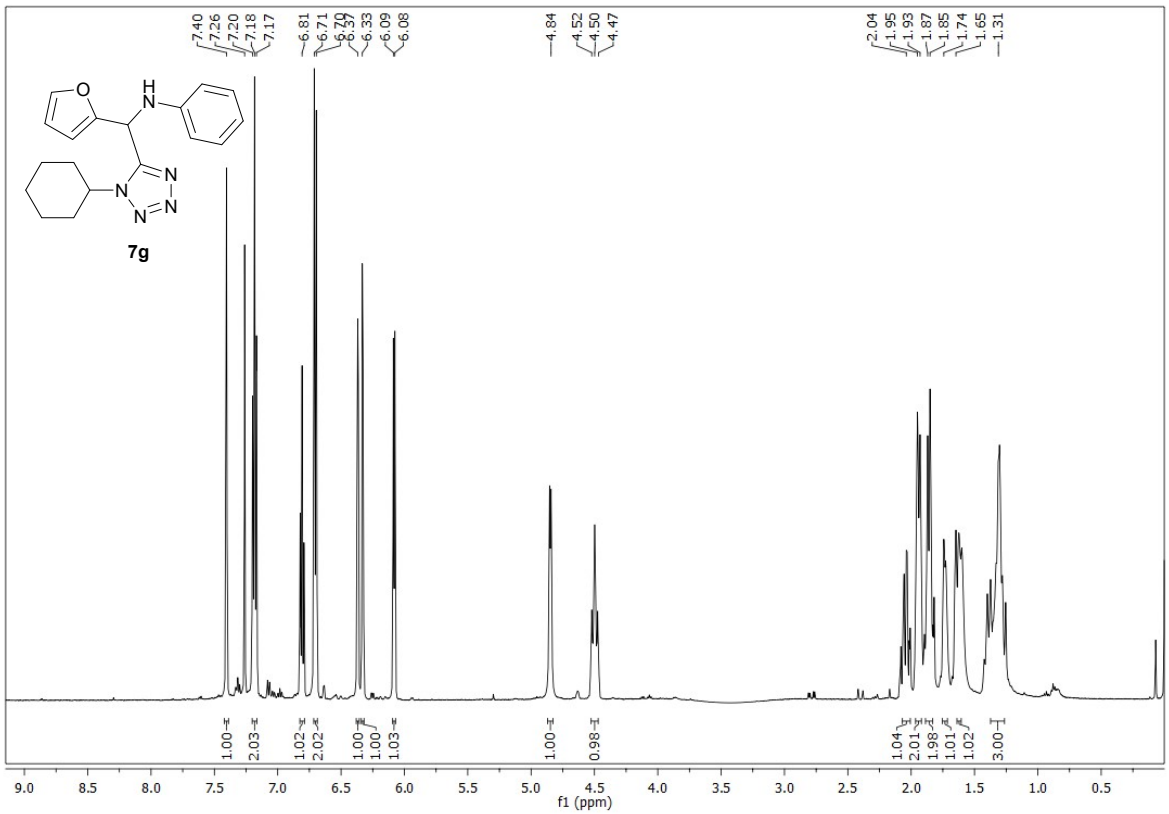
^{13}C NMR spectra of the compound **7e**



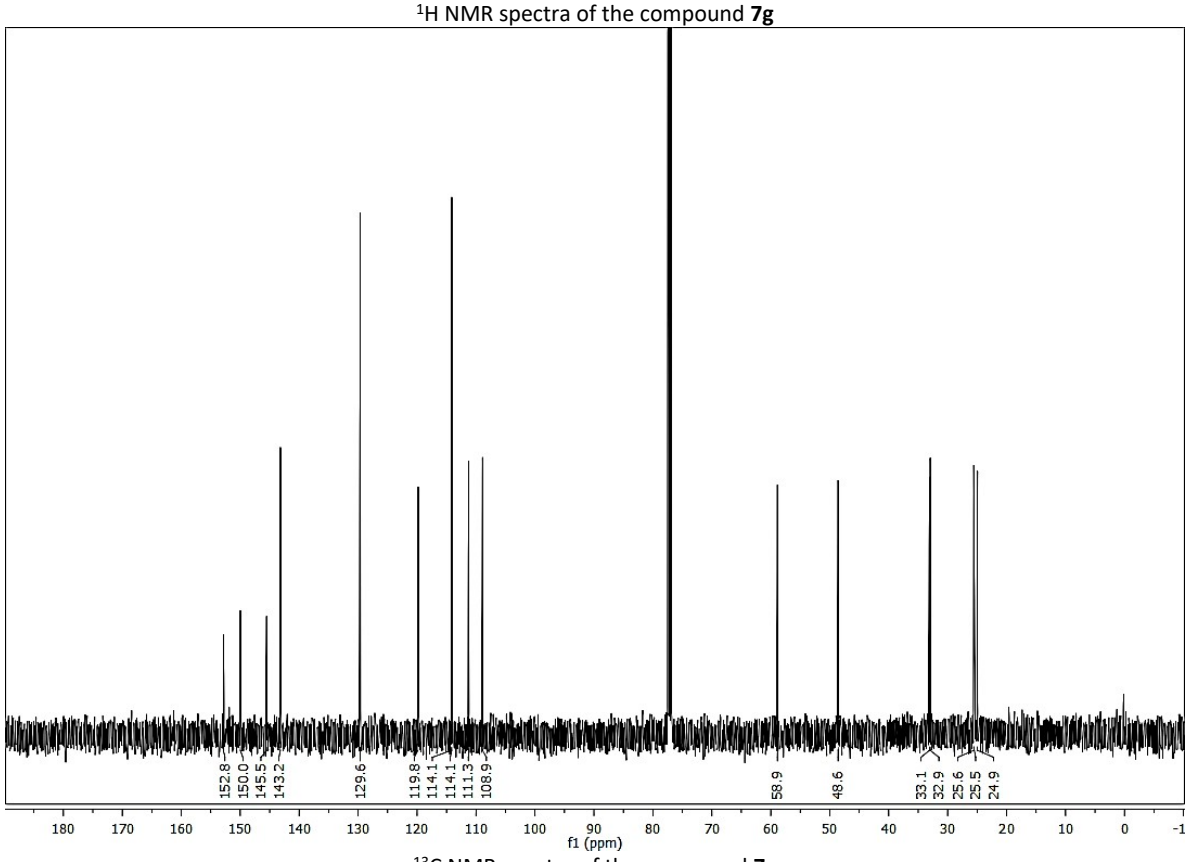
^{1}H NMR spectra of the compound **7f**



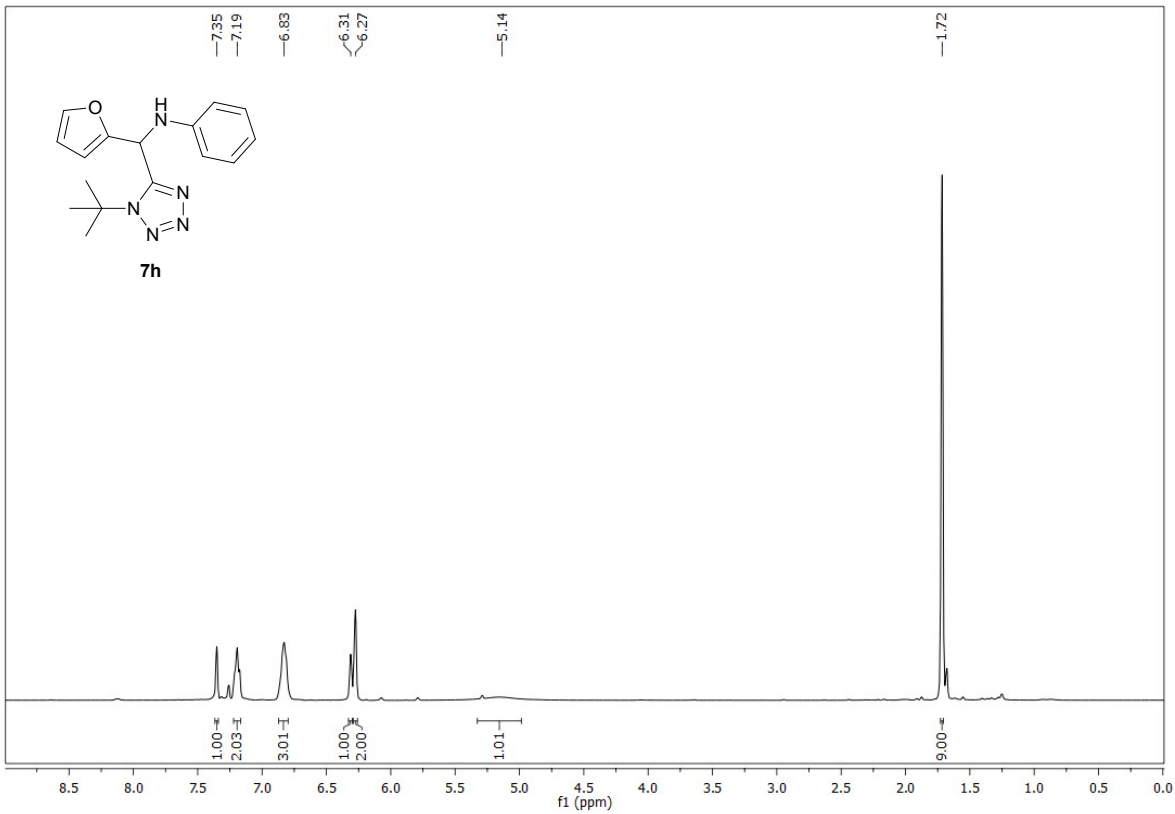
^{13}C NMR spectra of the compound **7f**



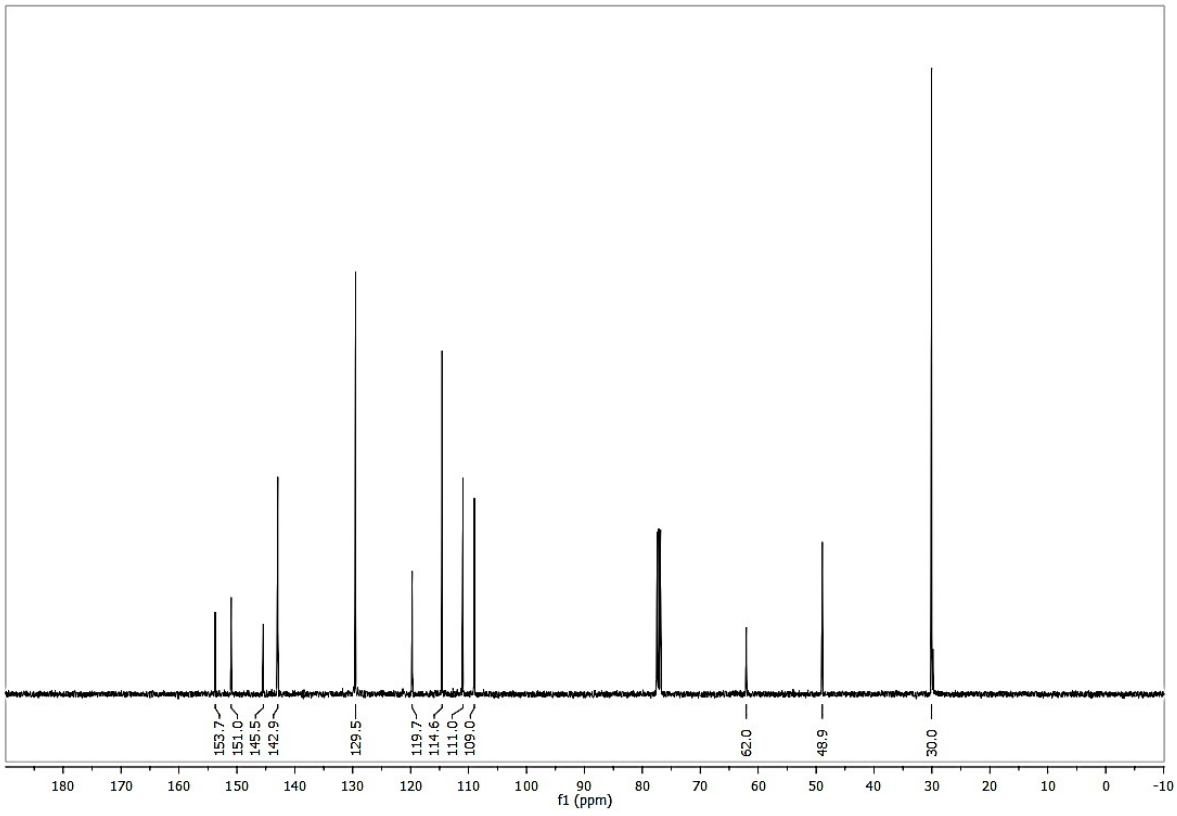
^{1}H NMR spectra of the compound **7g**



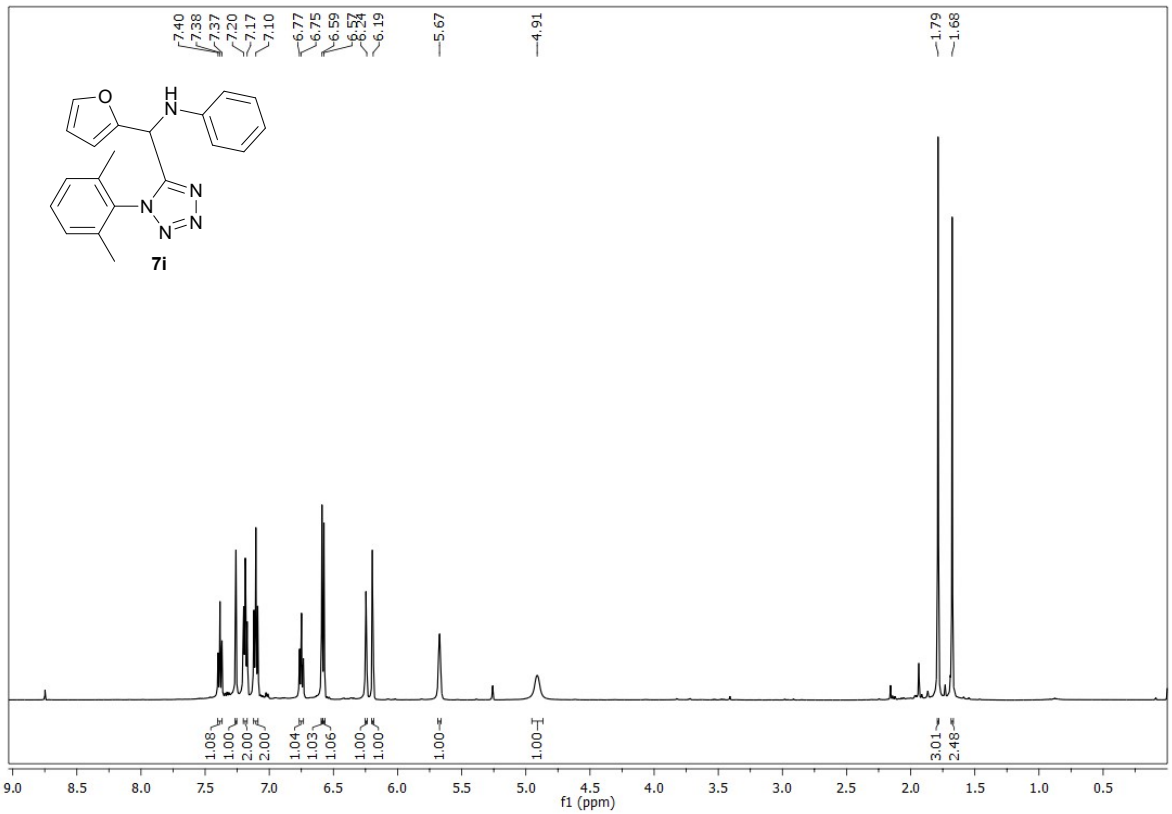
^{13}C NMR spectra of the compound **7g**



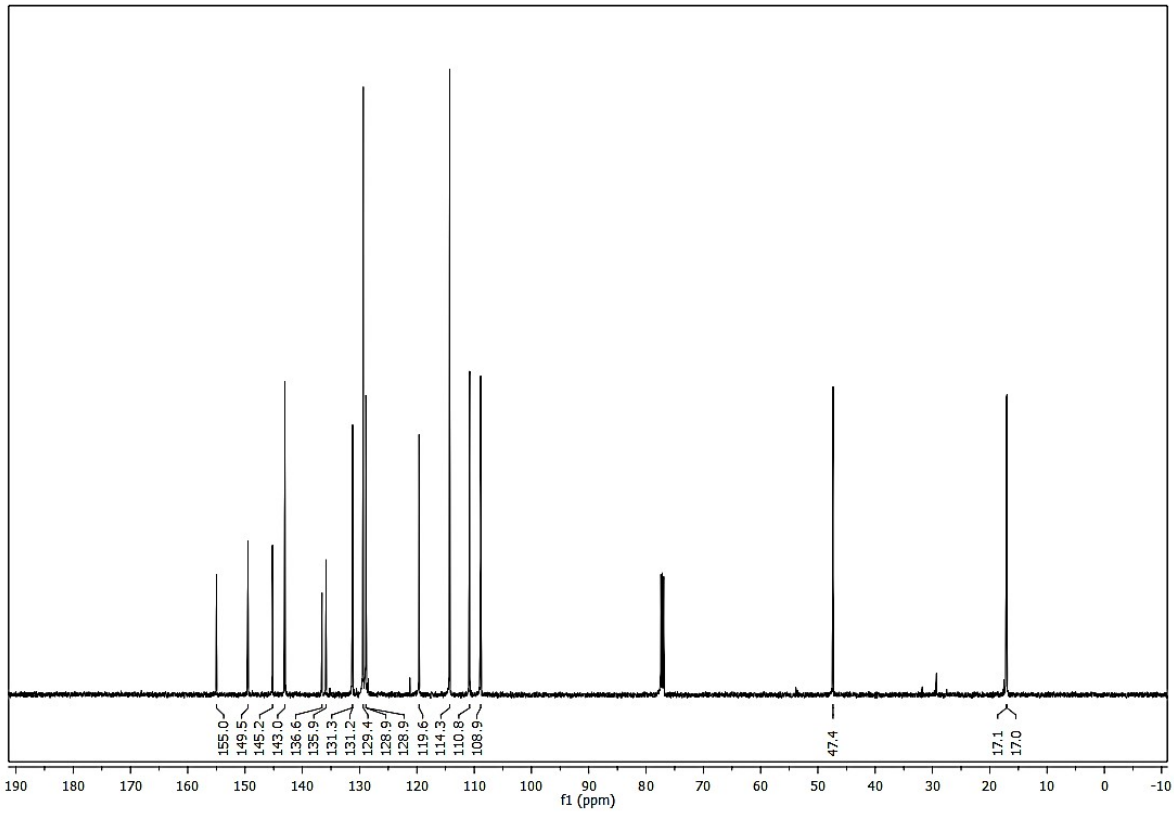
^{1}H NMR spectra of the compound **7h**



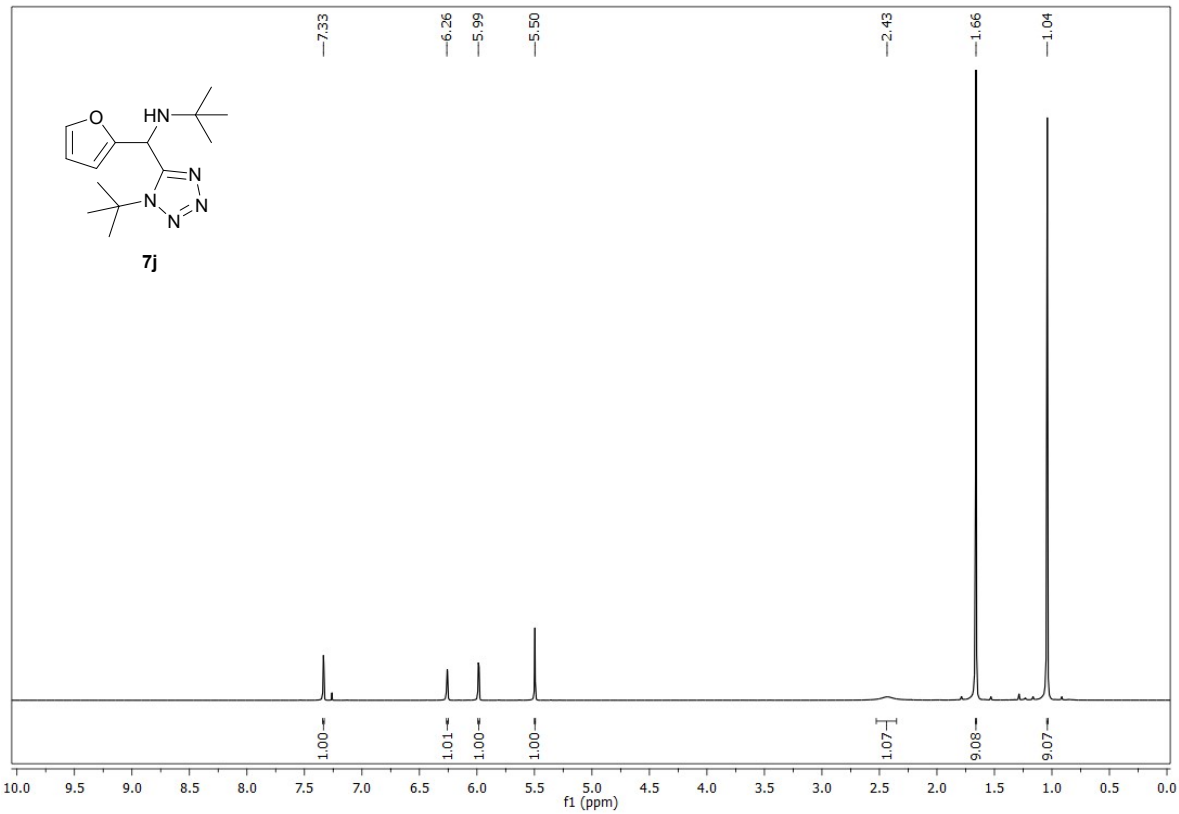
^{13}C NMR spectra of the compound **7h**



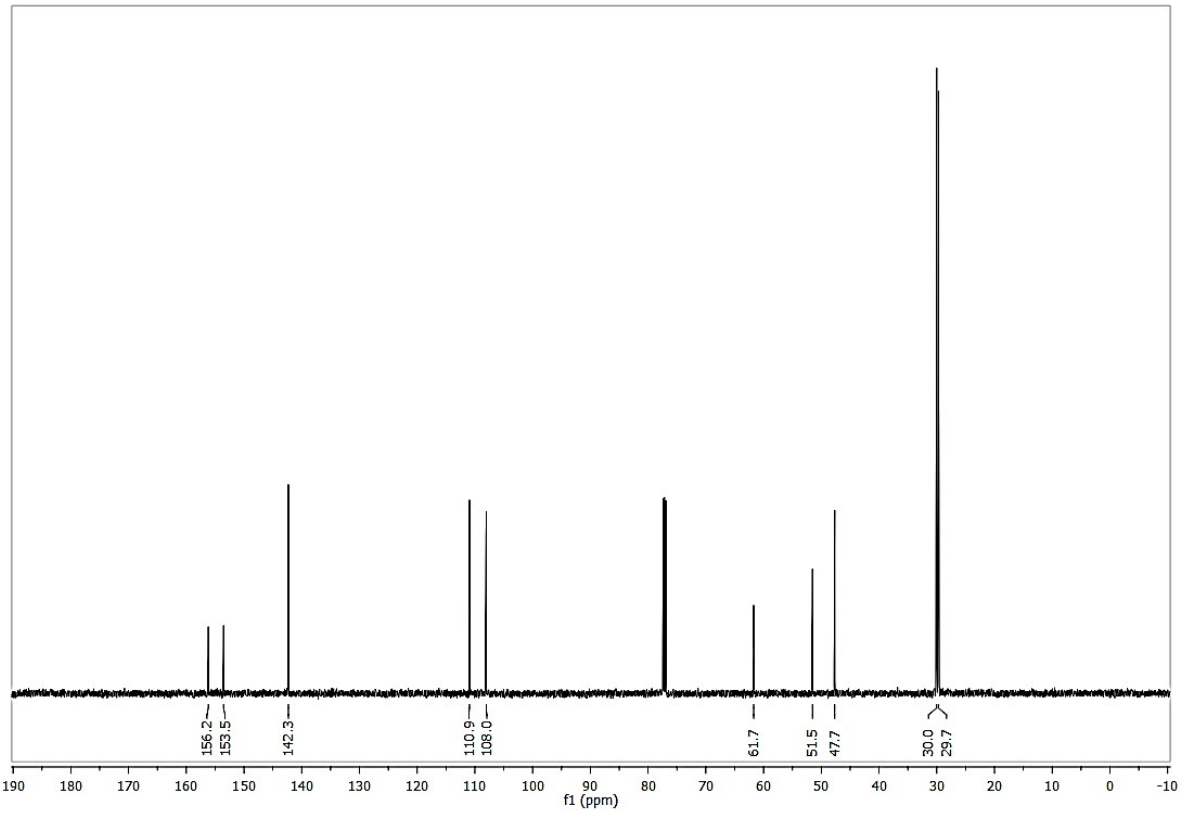
^{1}H NMR spectra of the compound **7i**



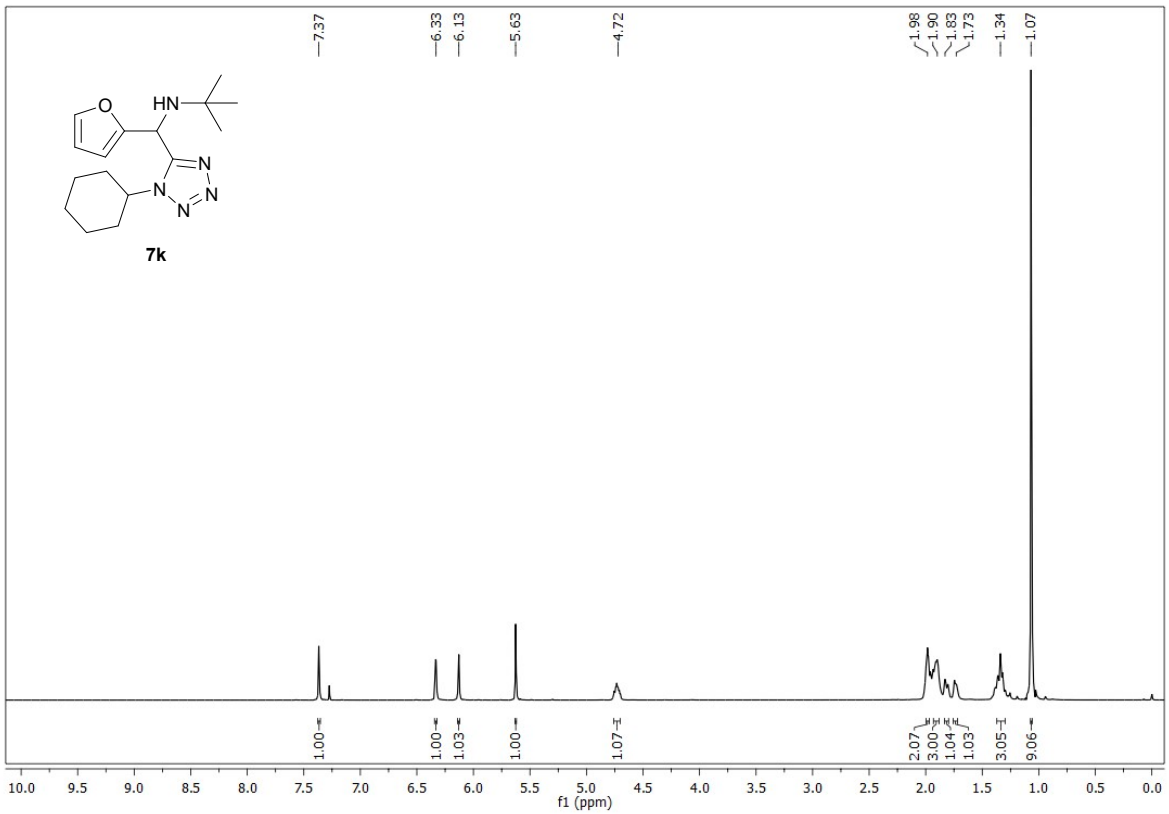
^{13}C NMR spectra of the compound **7i**



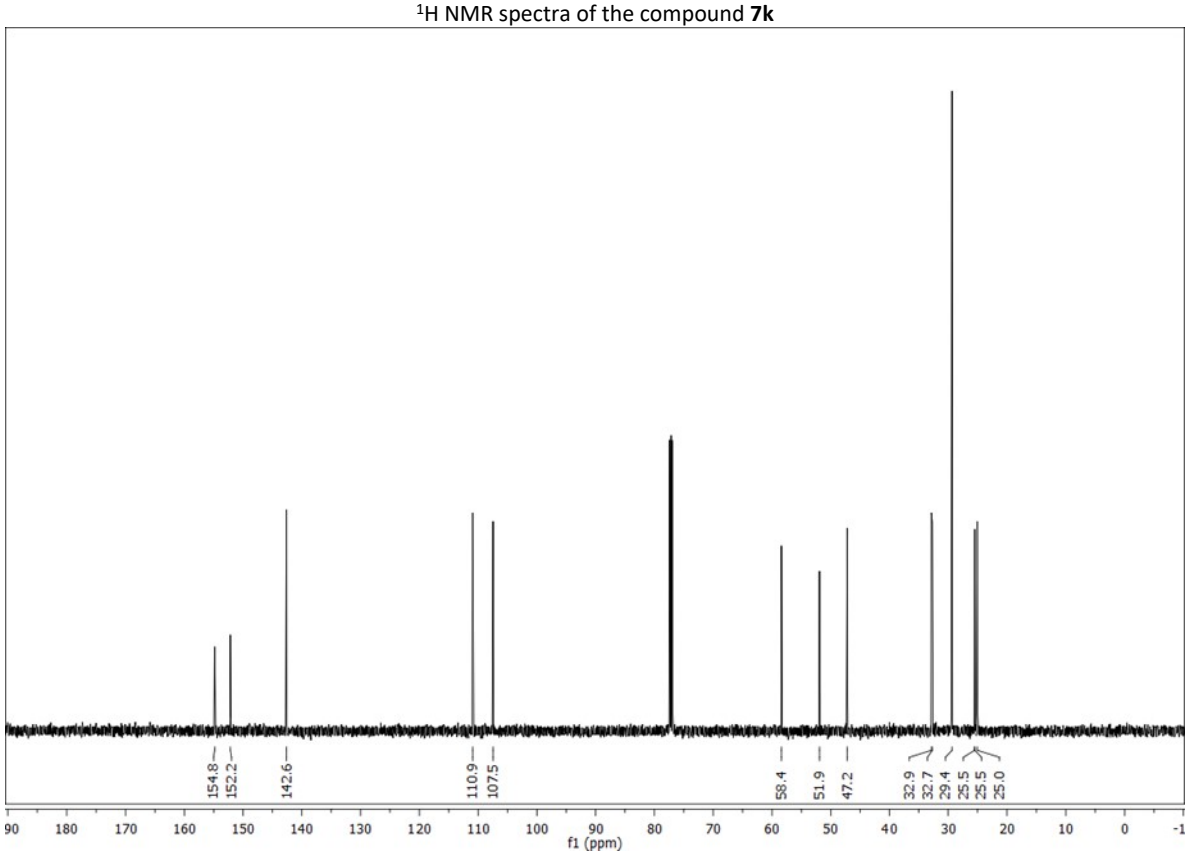
^{1}H NMR spectra of the compound **7j**



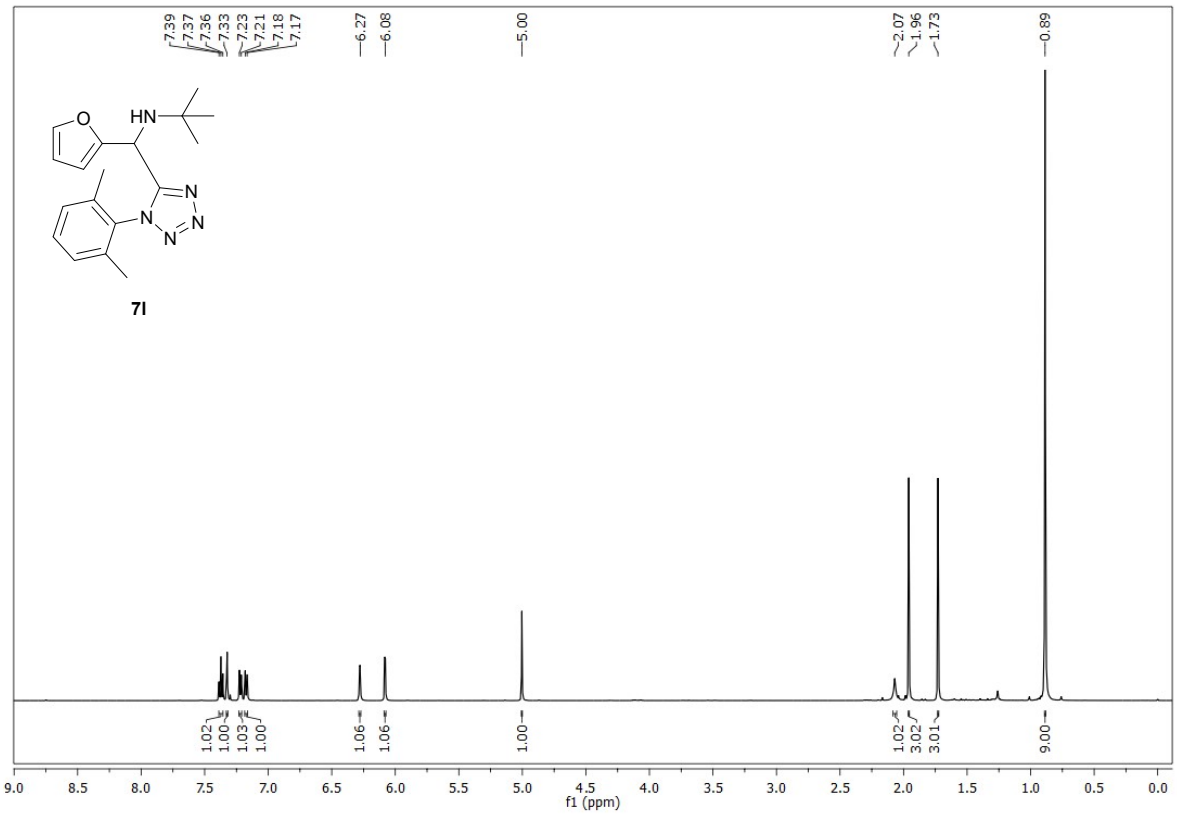
^{13}C NMR spectra of the compound **7j**



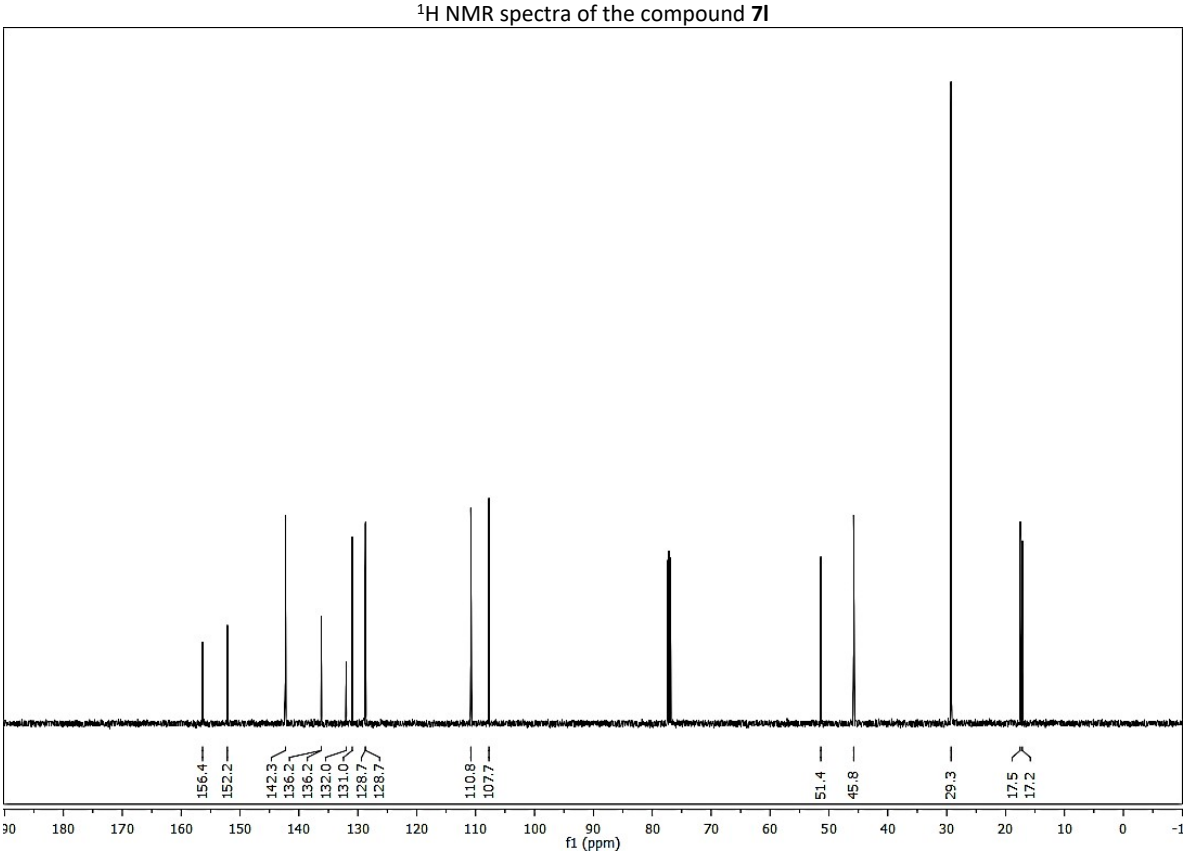
^{1}H NMR spectra of the compound **7k**



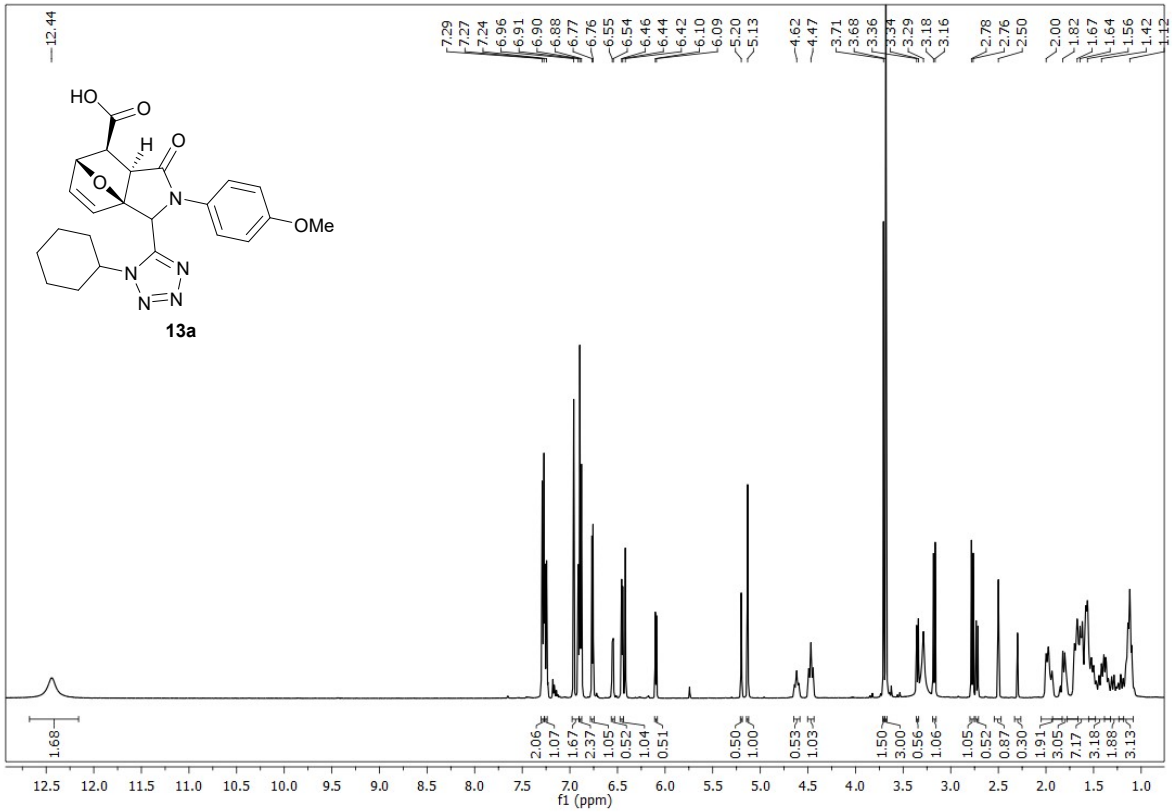
^{13}C NMR spectra of the compound **7k**



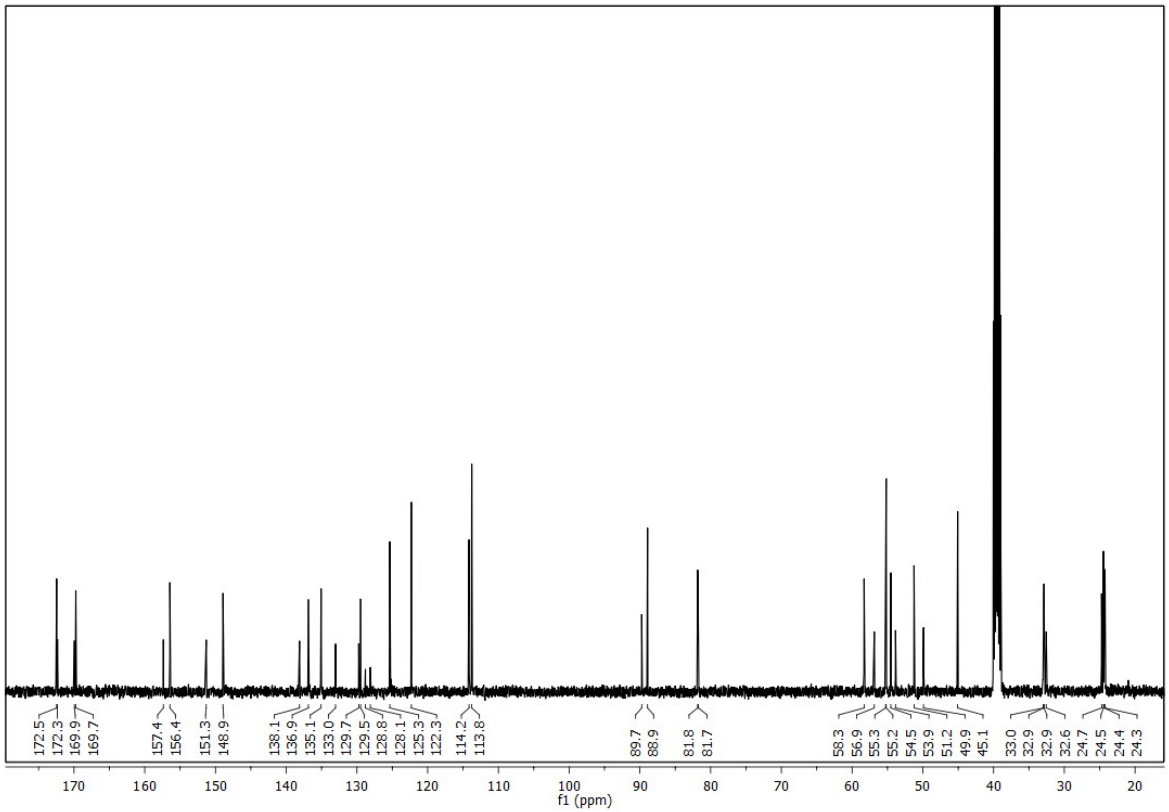
^{1}H NMR spectra of the compound **7l**



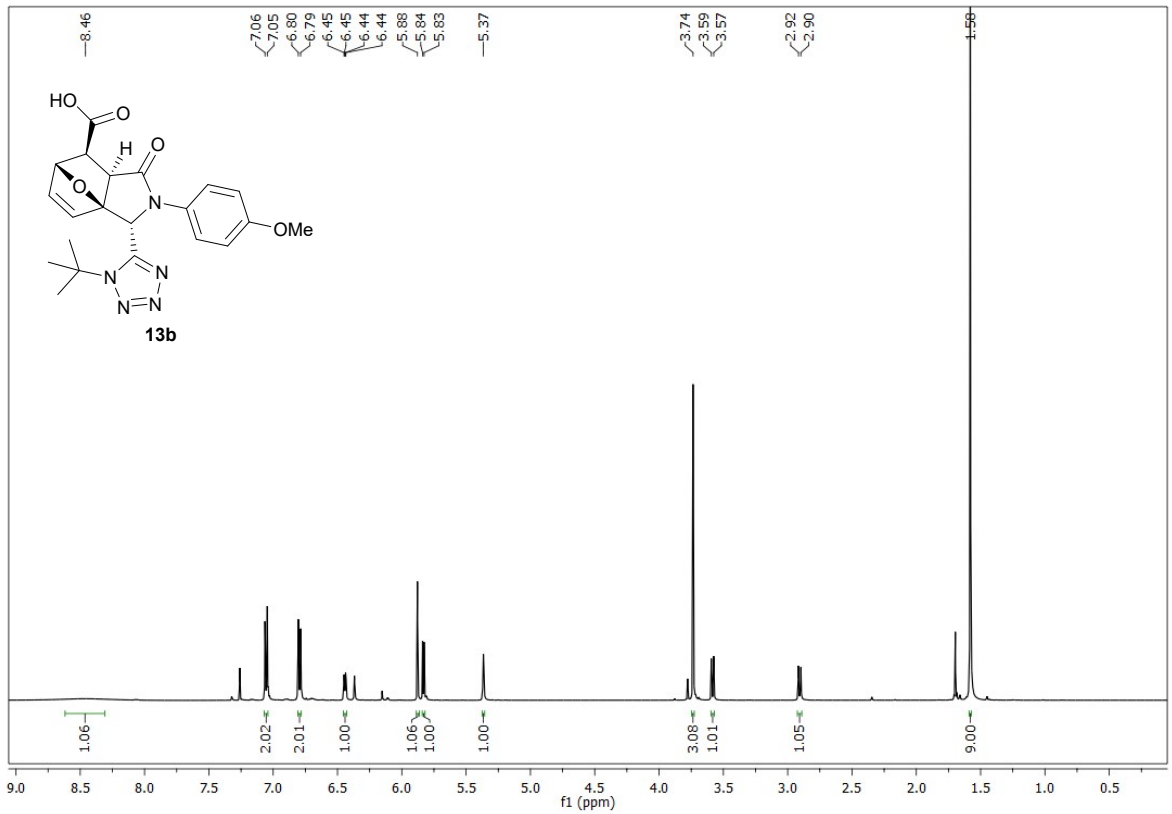
^{13}C NMR spectra of the compound **7l**



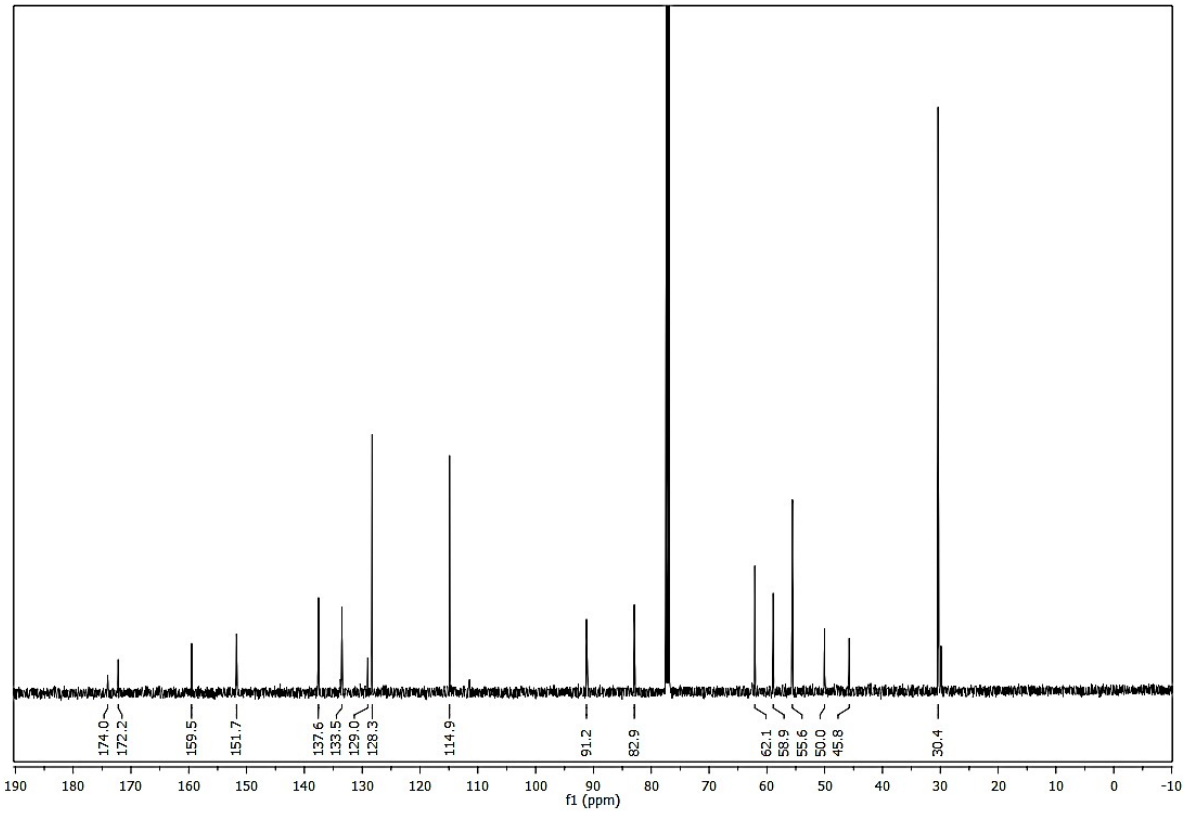
^{1}H NMR spectra of the compound **13a**



^{13}C NMR spectra of the compound **13a**



^{1}H NMR spectra of the compound **13b**



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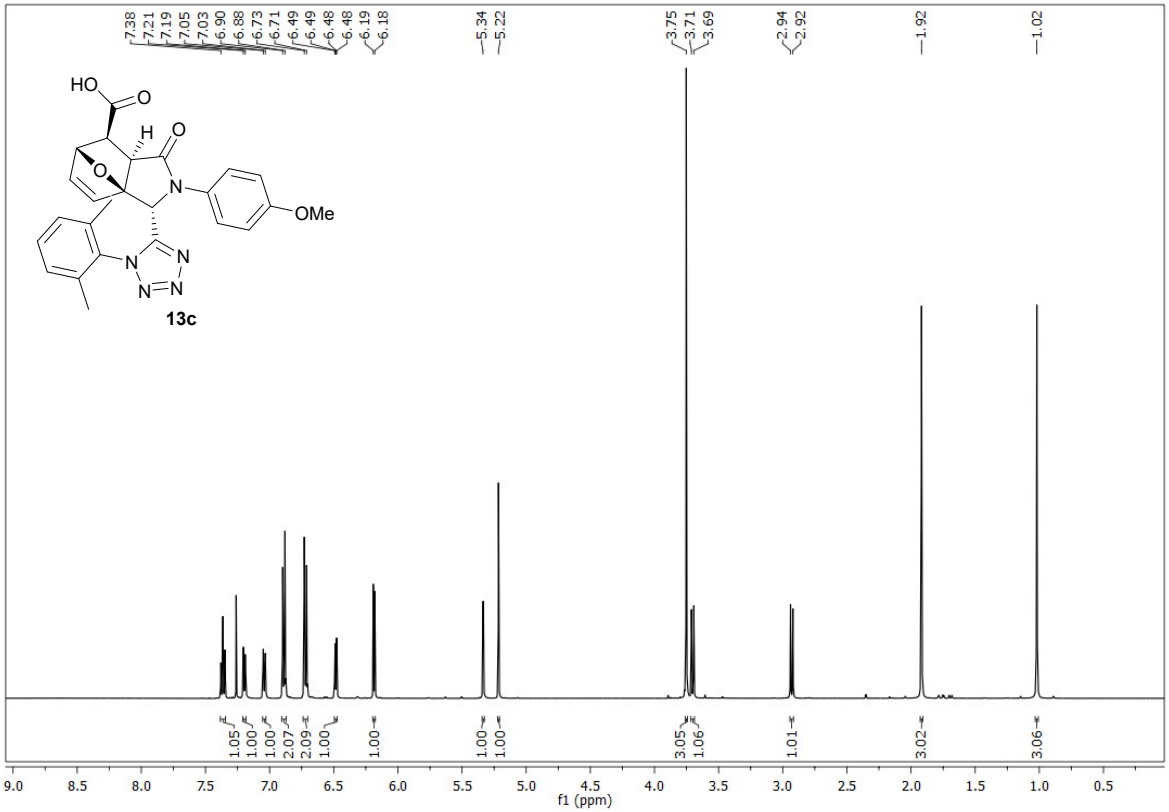
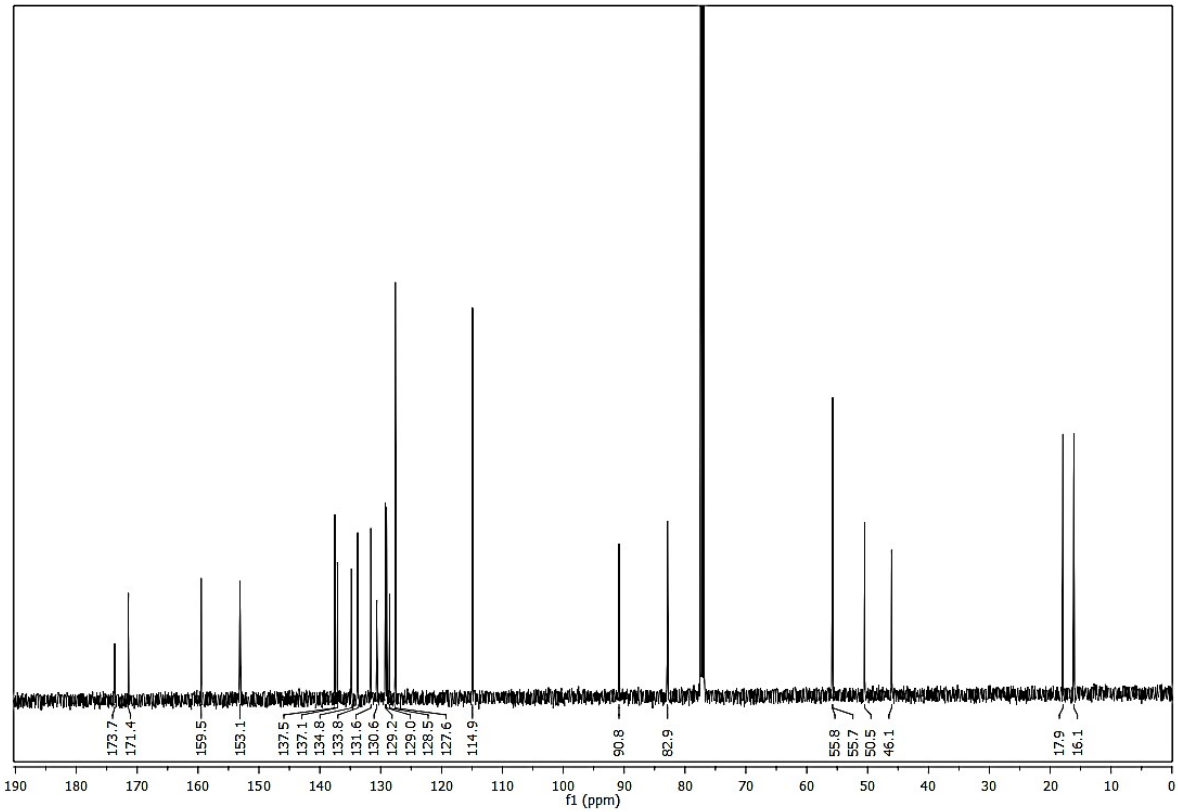
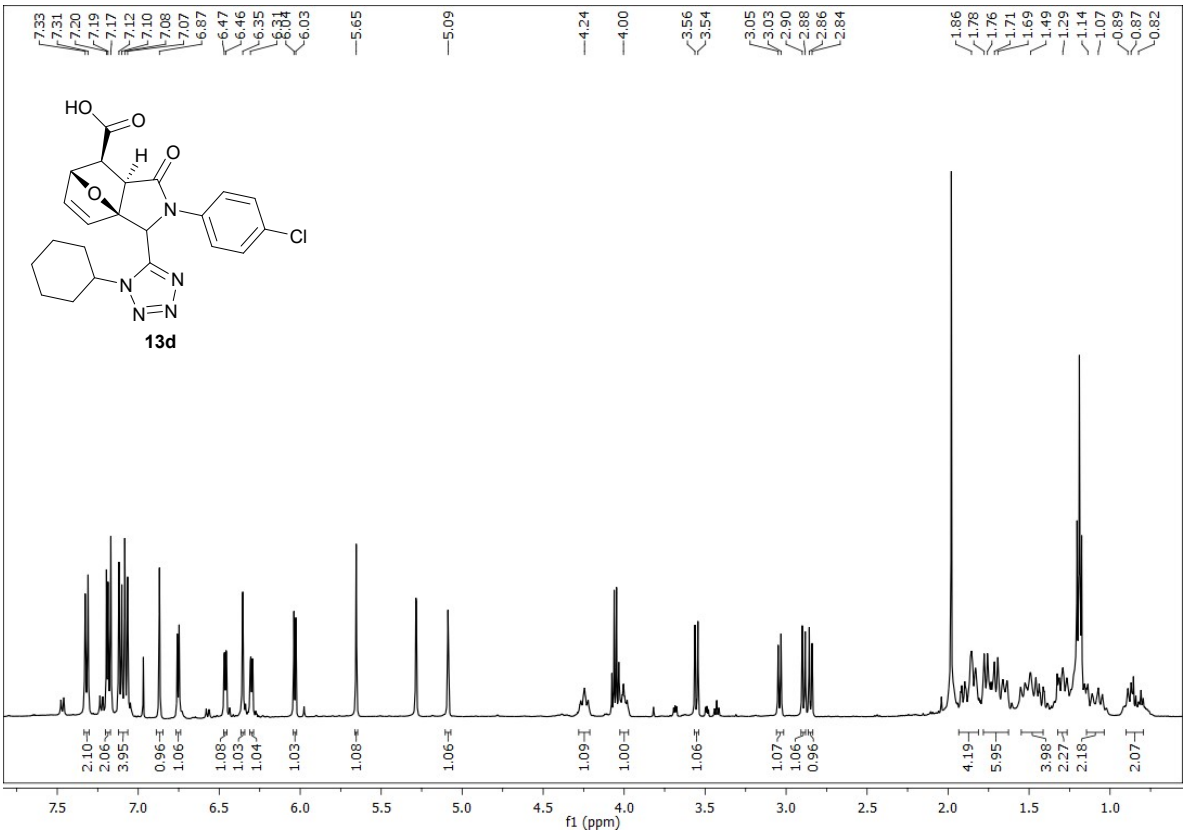


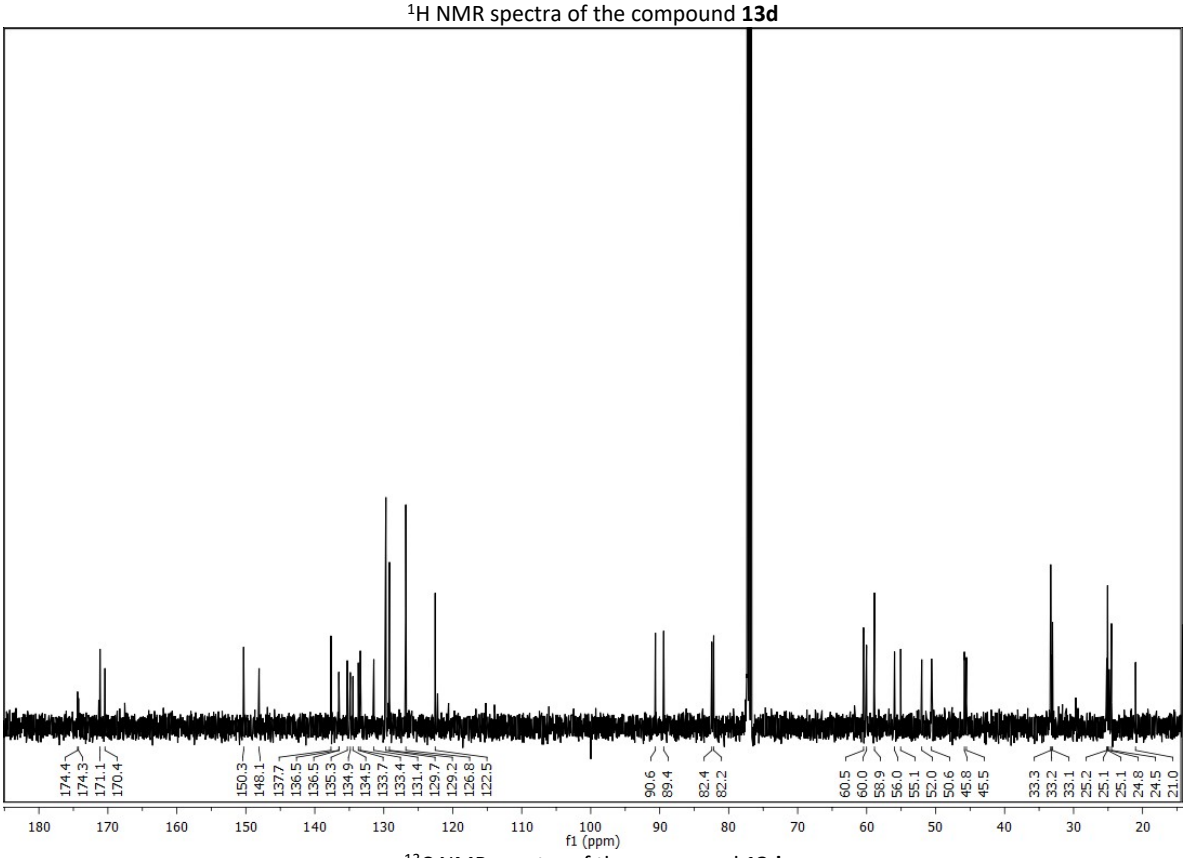
^{1}H NMR spectra of the compound **13c**



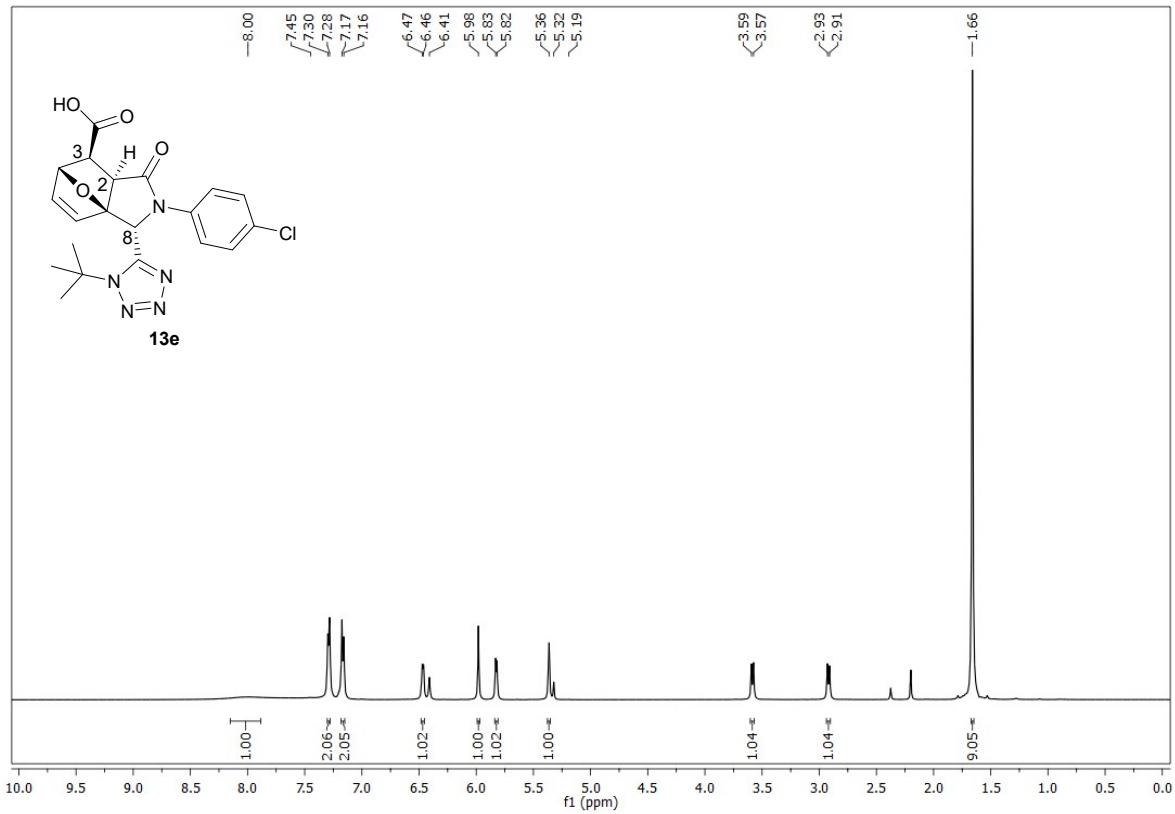
^{13}C NMR spectra of the compound **13c**



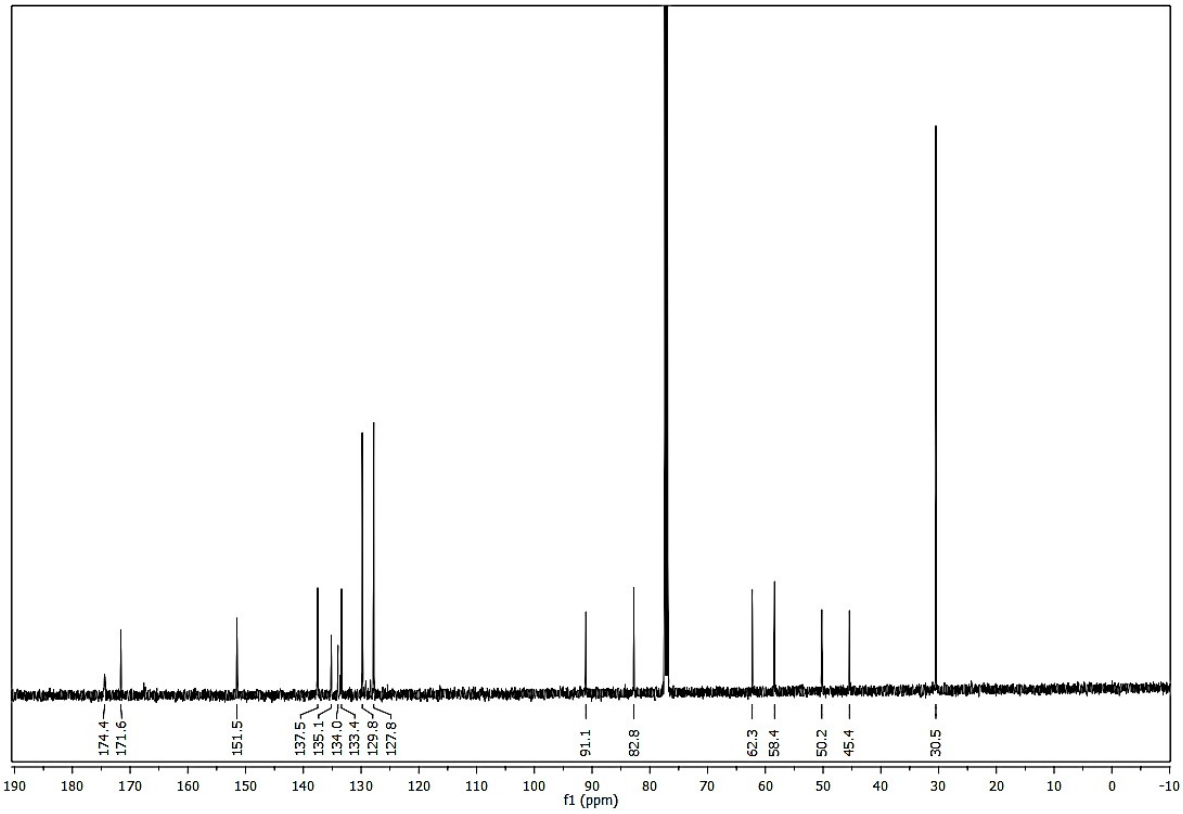
^{1}H NMR spectra of the compound **13d**



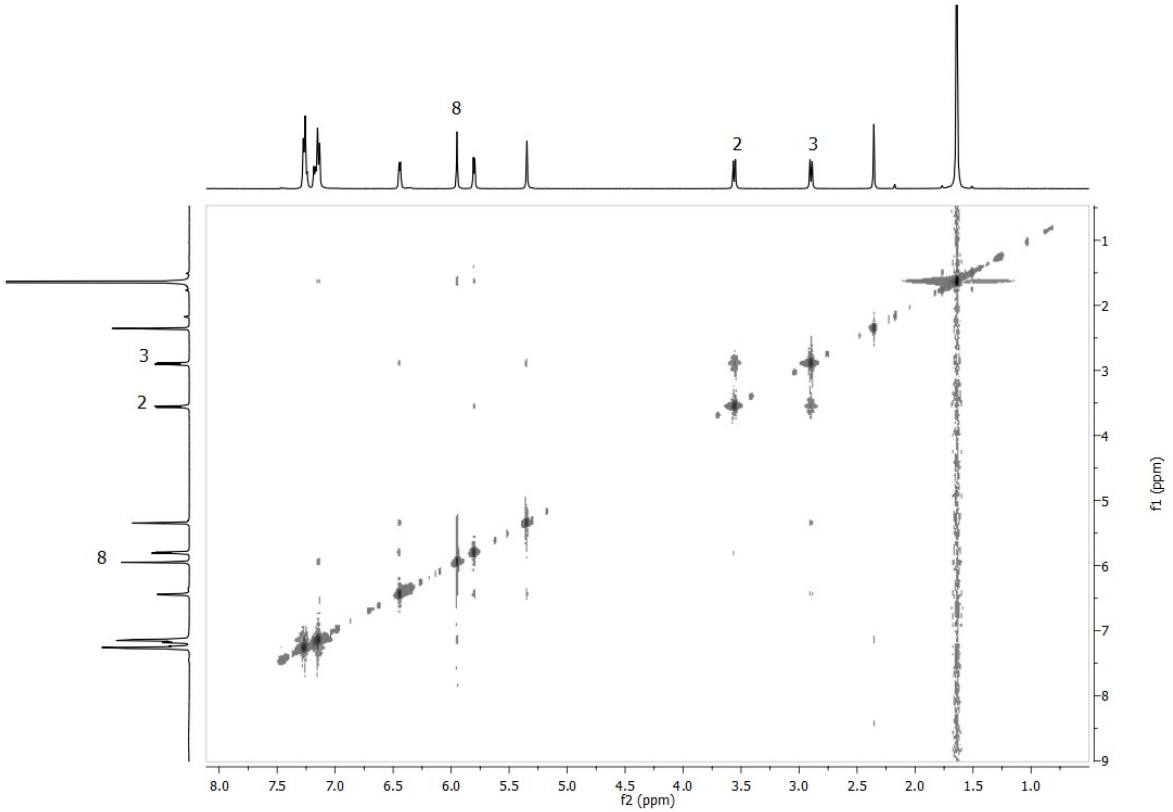
^{13}C NMR spectra of the compound **13d**



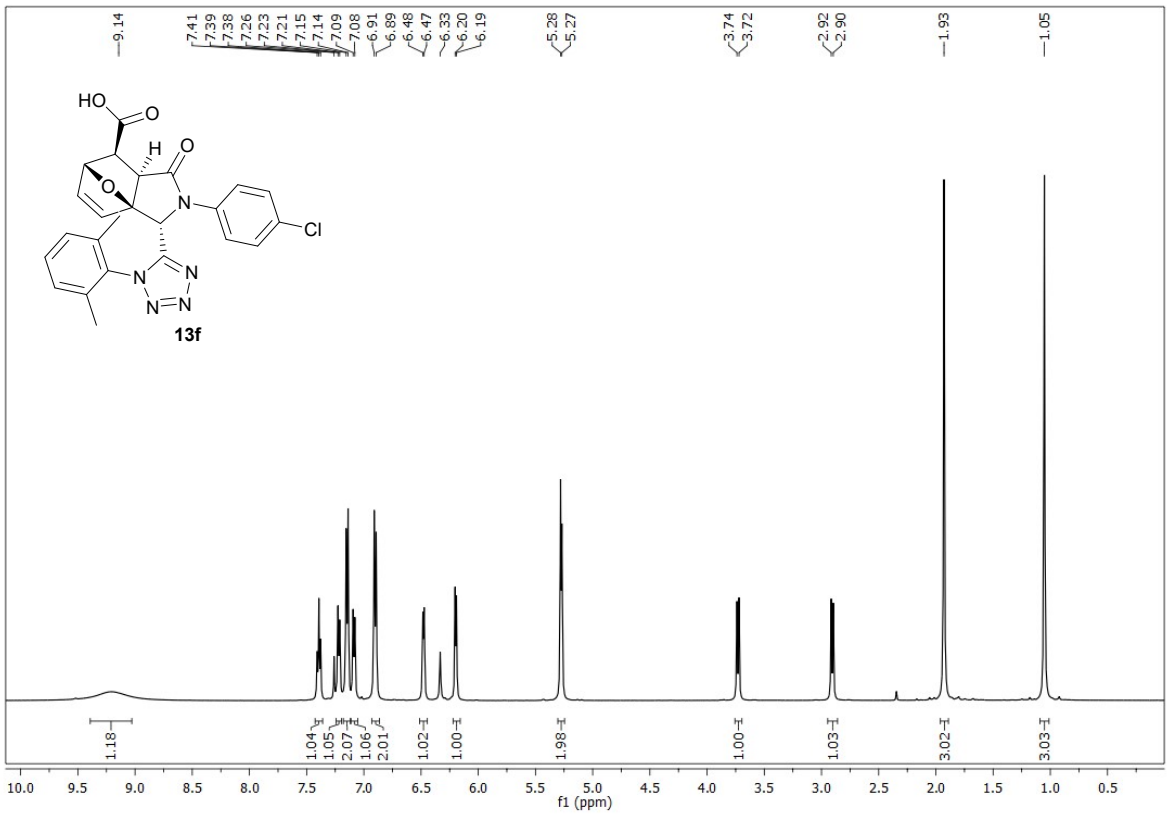
^{1}H NMR spectra of the compound **13e**



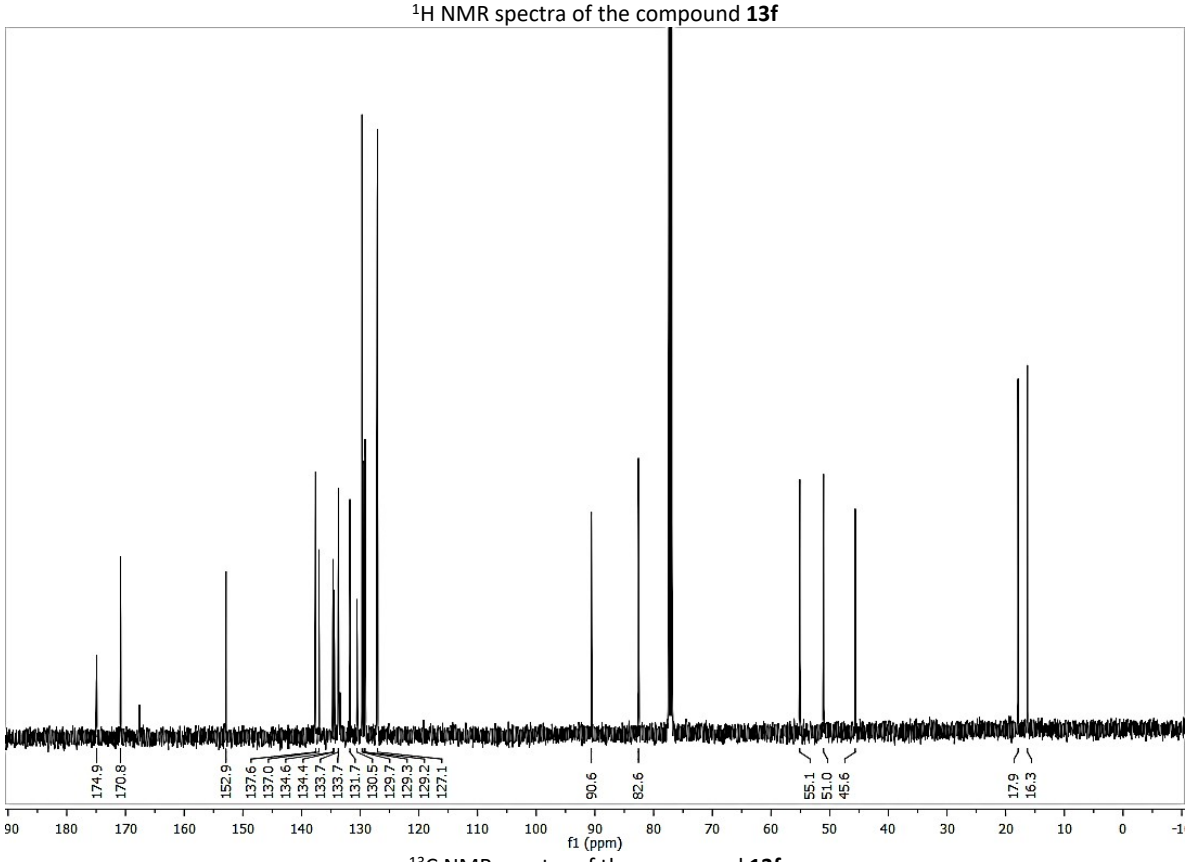
^{13}C NMR spectra of the compound **13e**



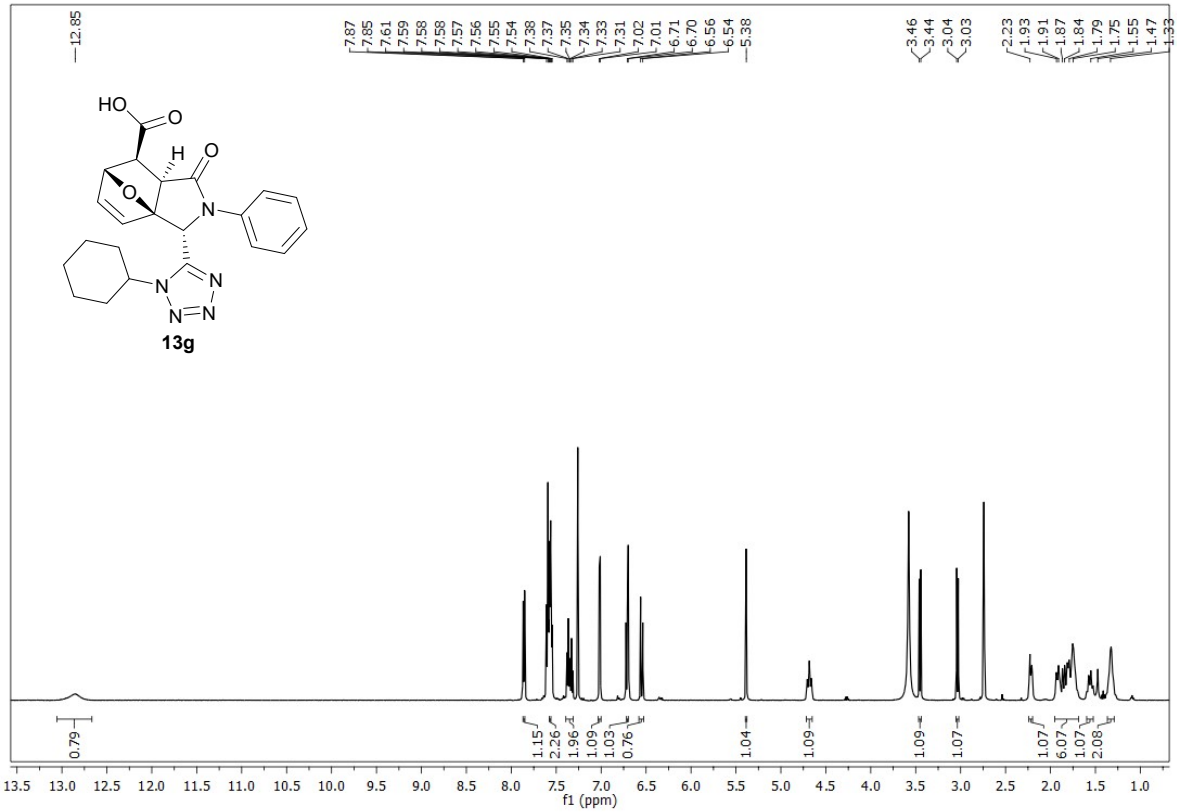
NOESY spectra of the compound **13e**



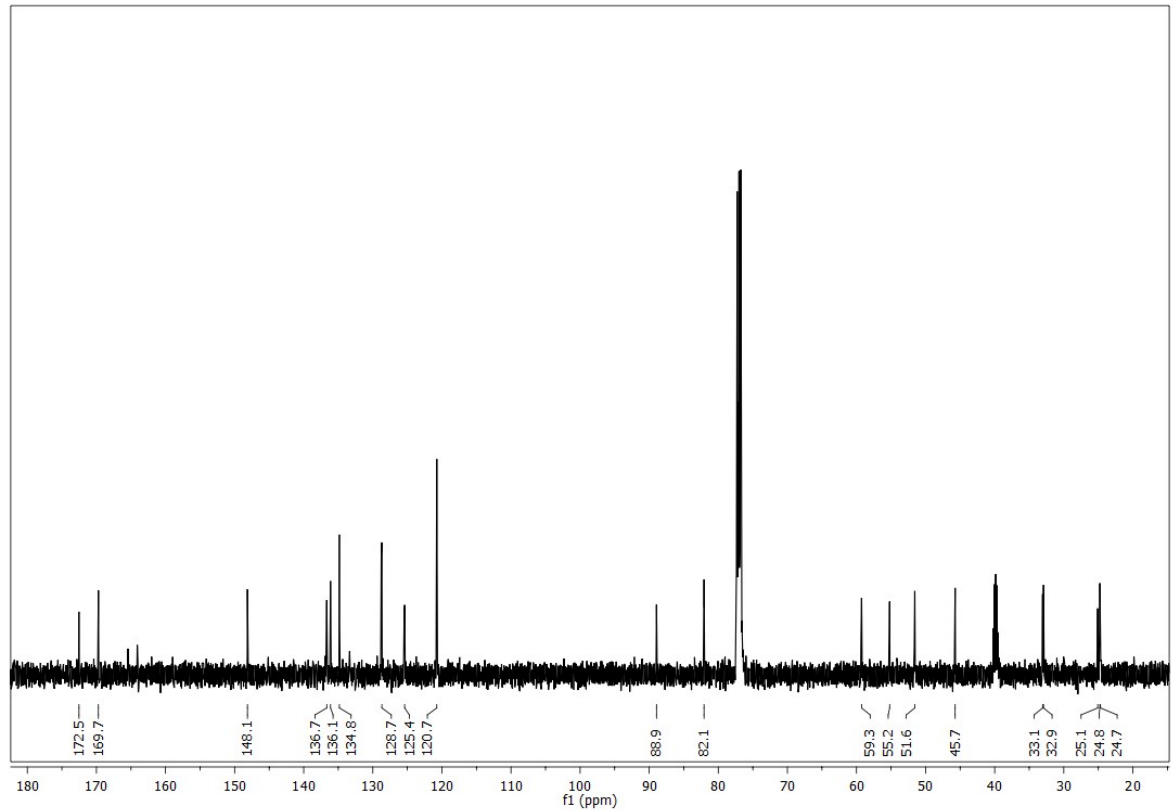
^{1}H NMR spectra of the compound **13f**



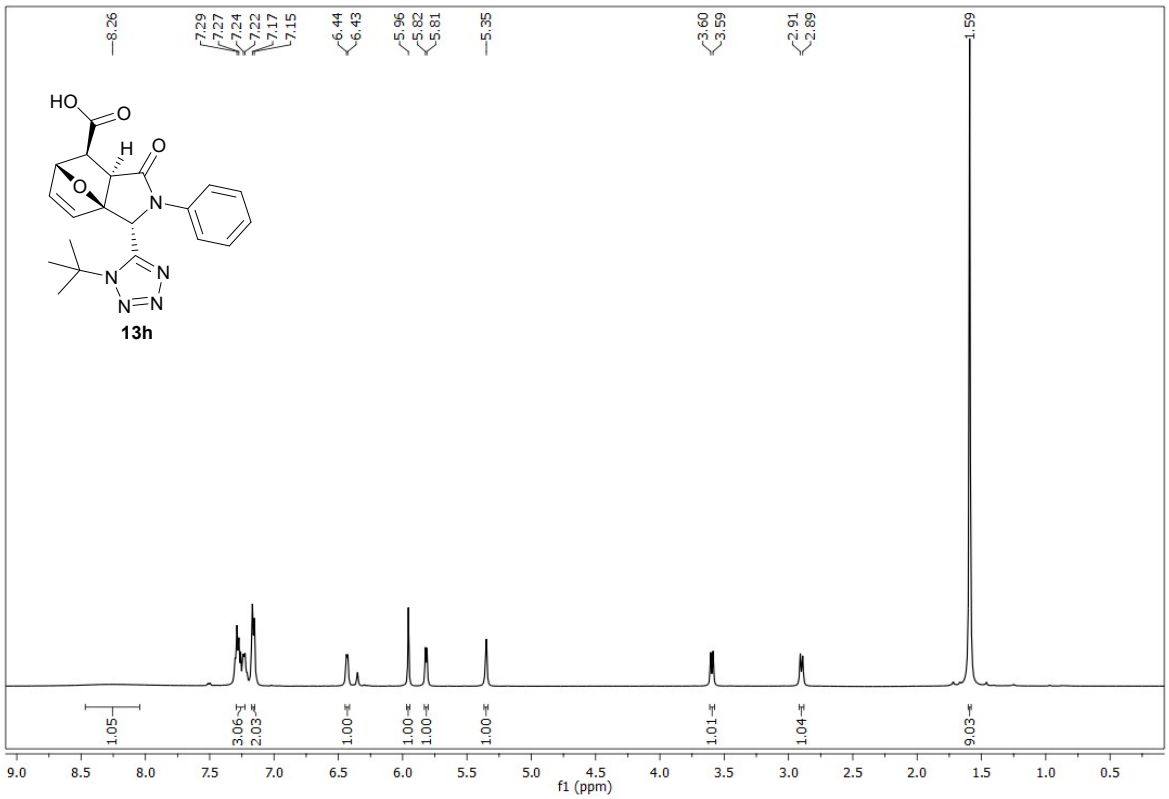
^{13}C NMR spectra of the compound **13f**



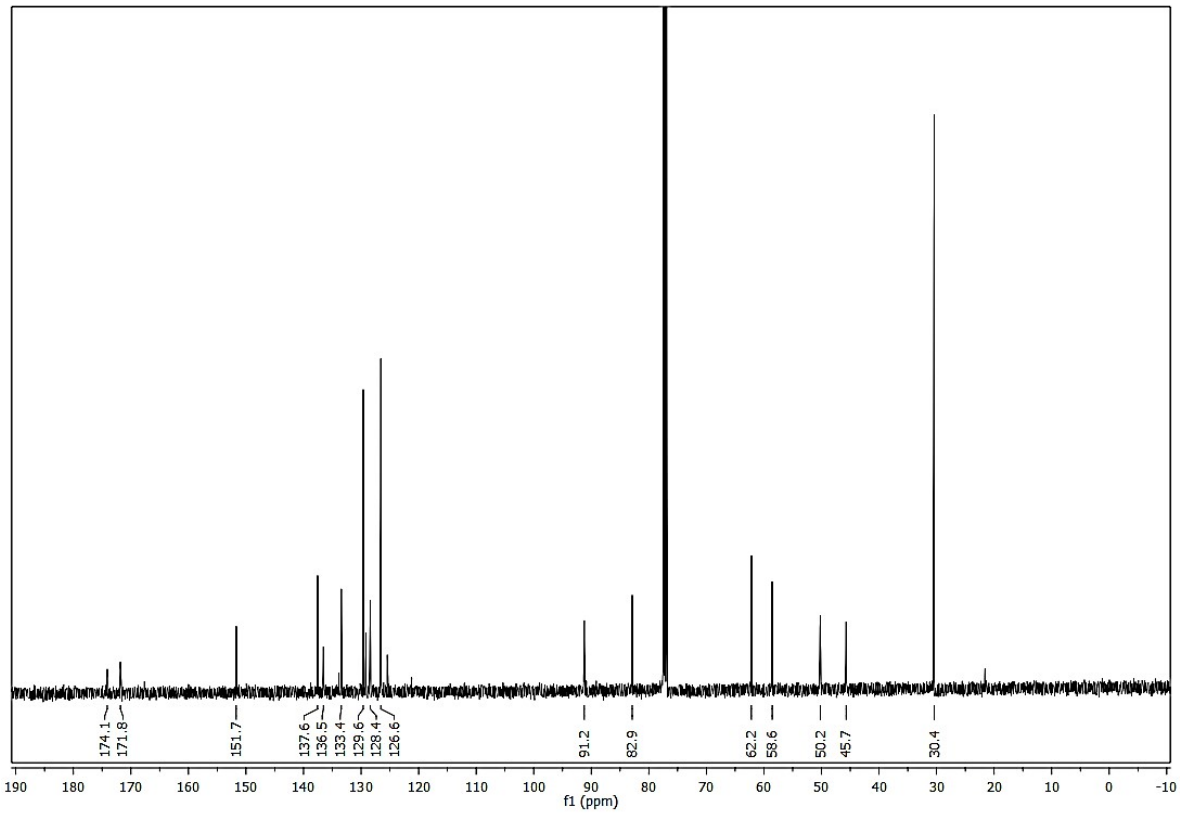
^{1}H NMR spectra of the compound **13g**



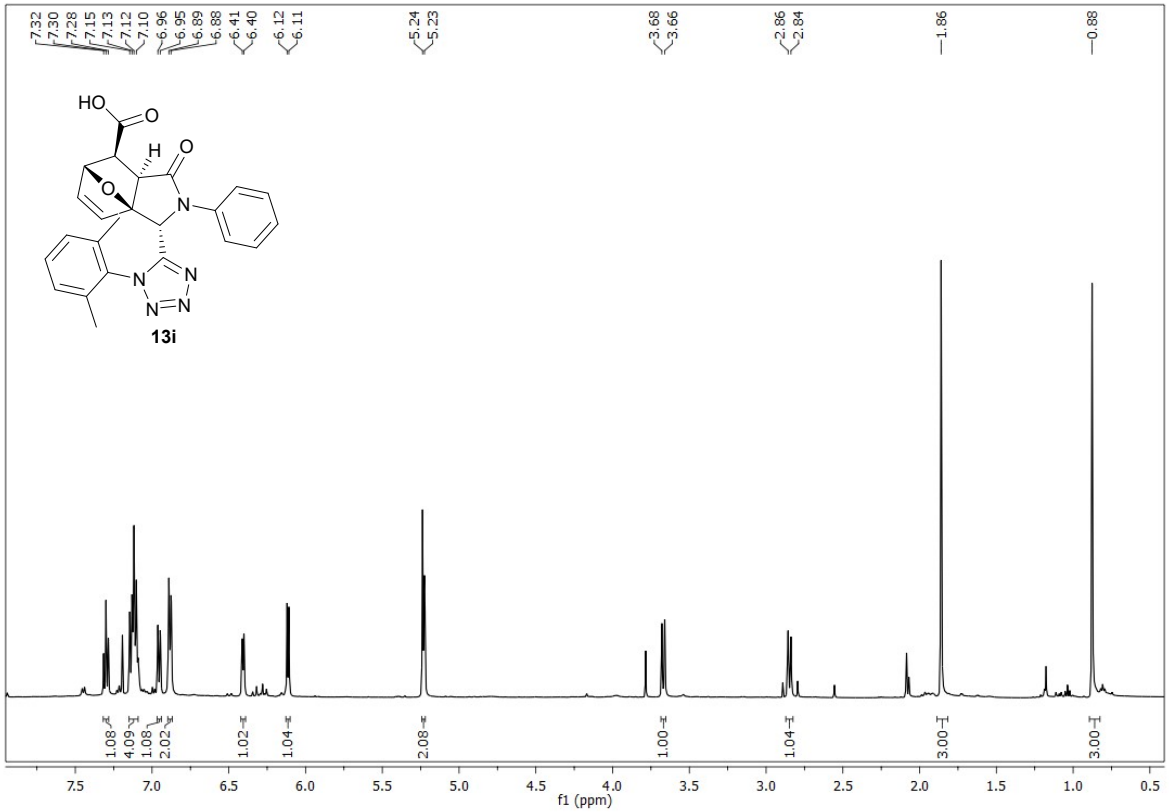
^{13}C NMR spectra of the compound **13g**



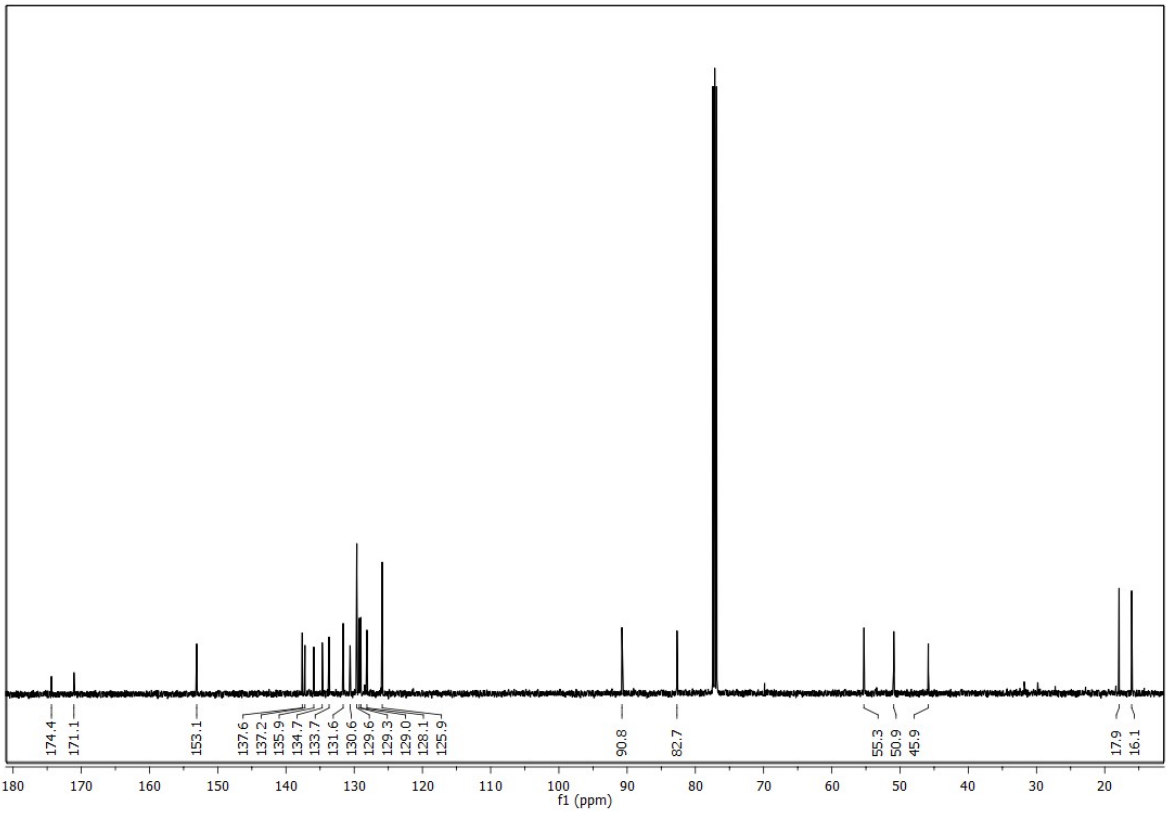
^{1}H NMR spectra of the compound **13h**



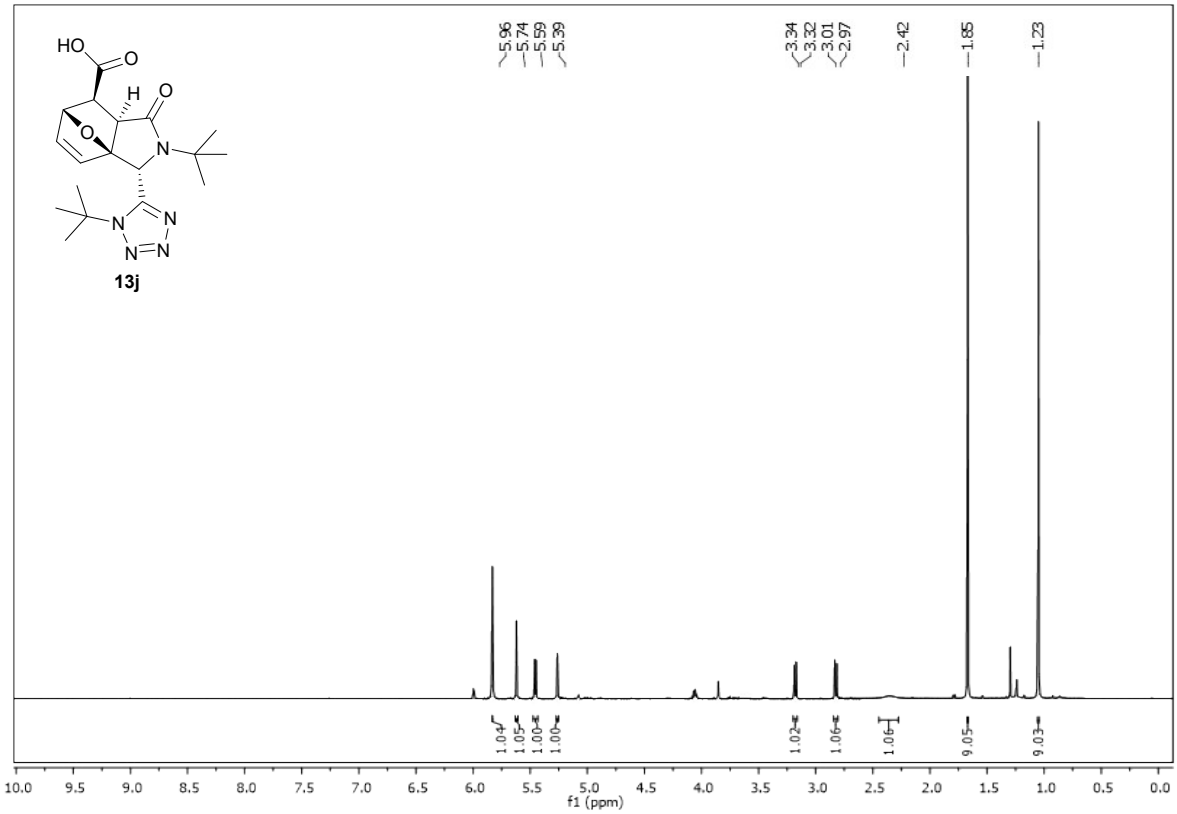
^{13}C NMR spectra of the compound **13h**



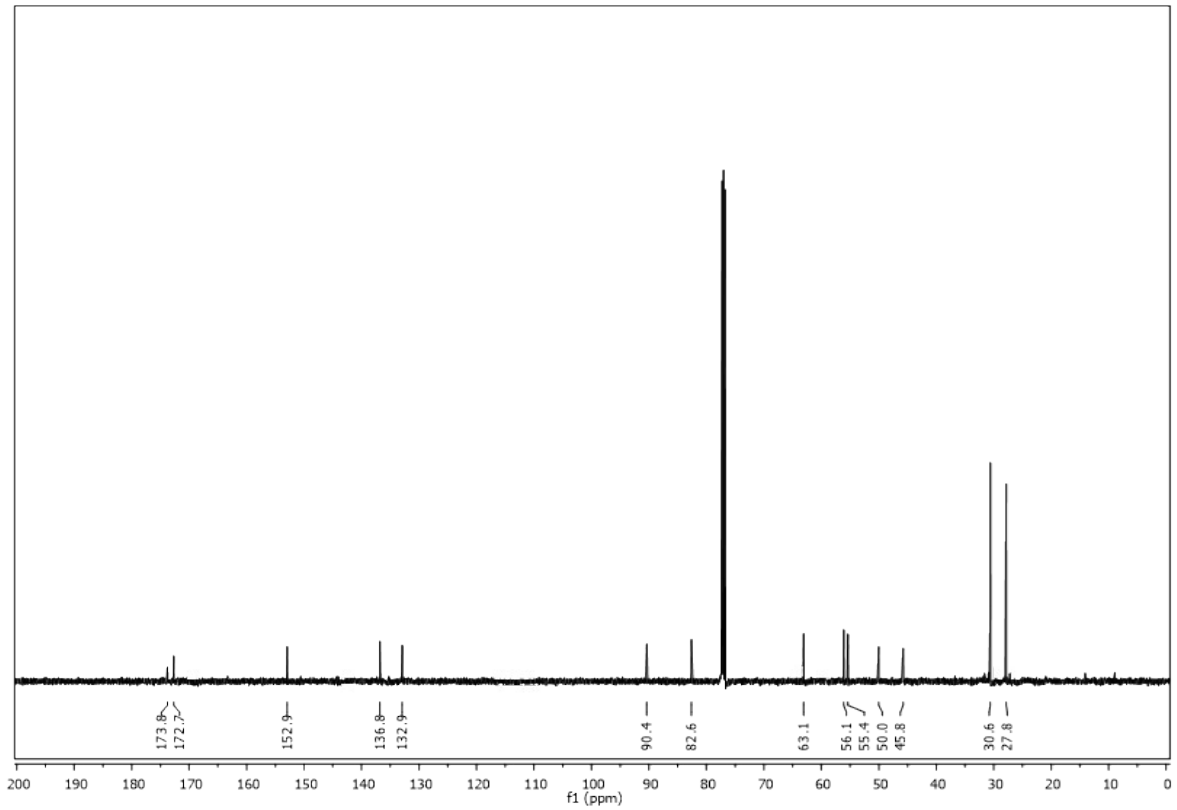
^{1}H NMR spectra of the compound **13i**



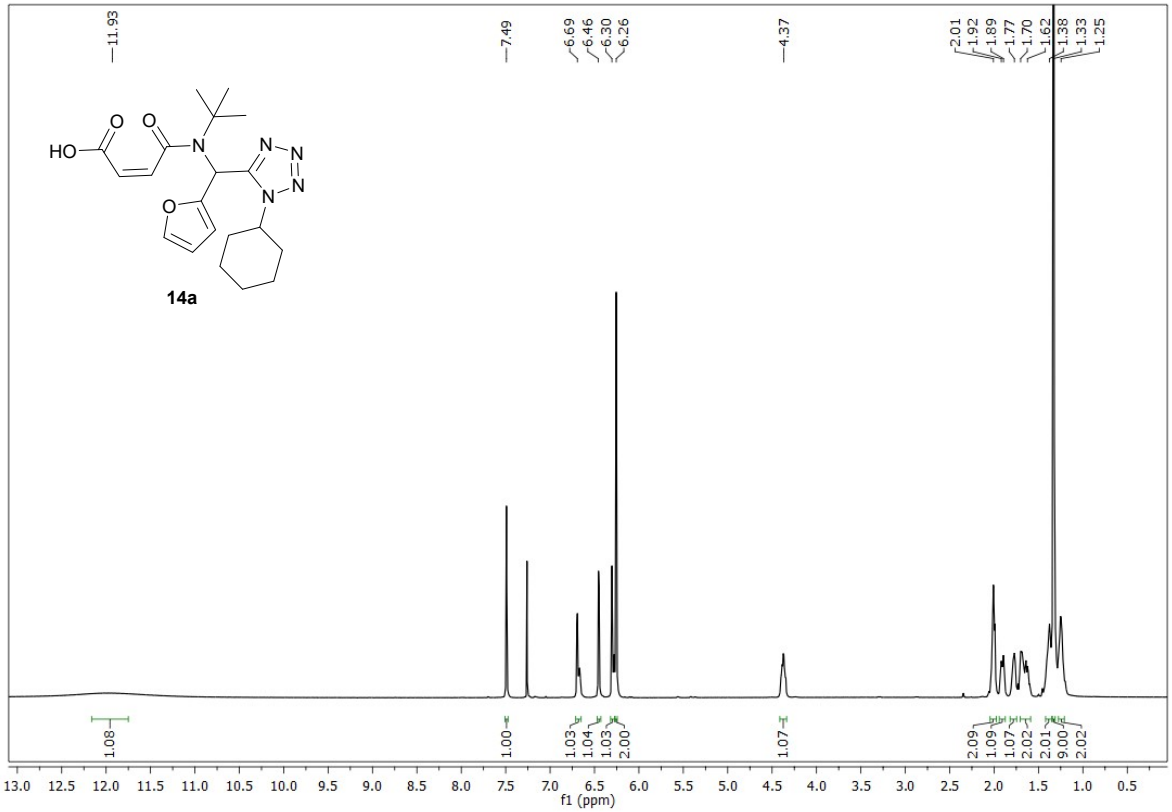
^{13}C NMR spectra of the compound **13i**



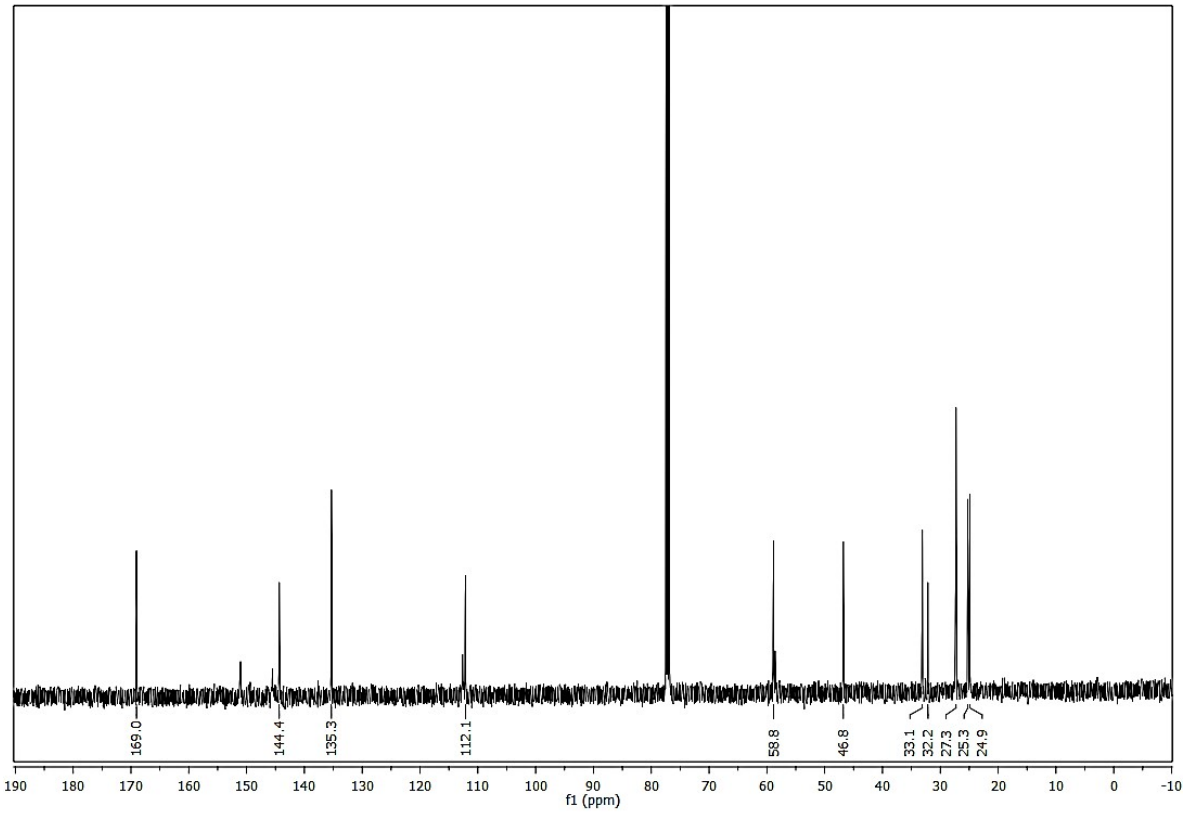
^{1}H NMR spectra of the compound **13j**



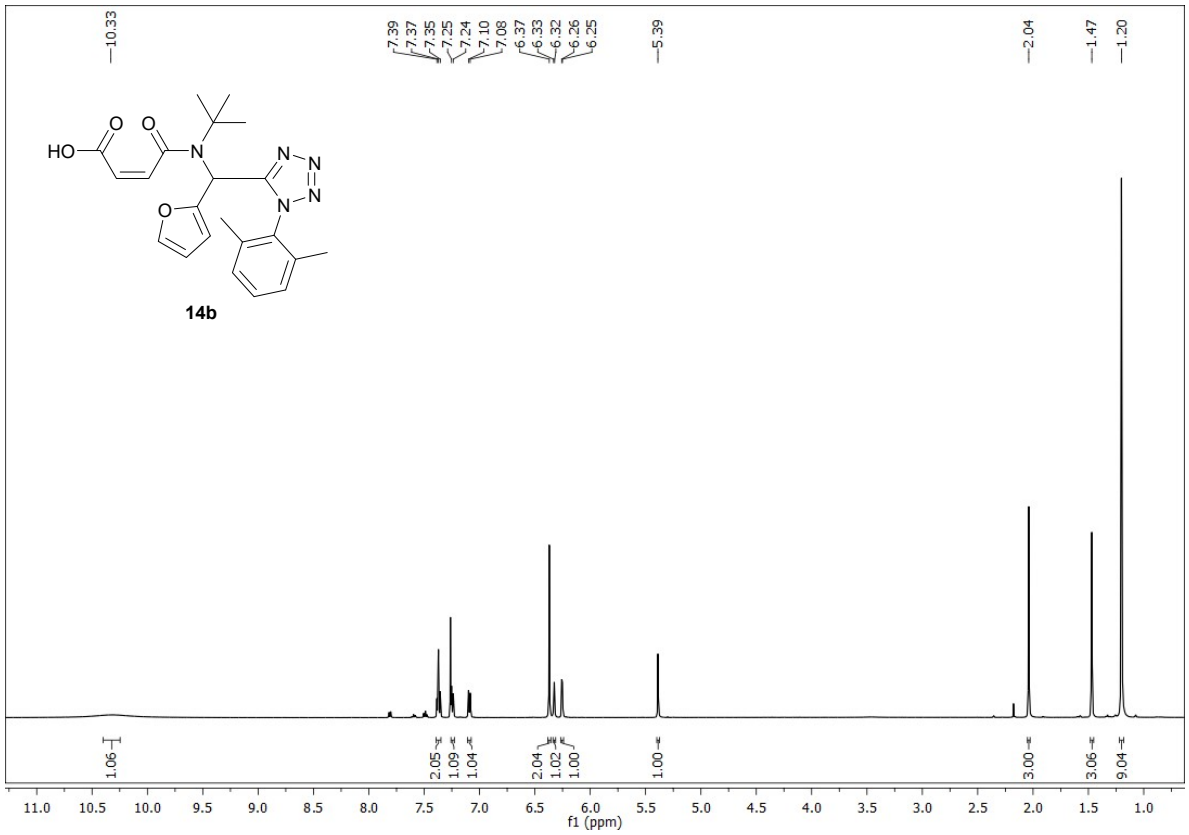
^{13}C NMR spectra of the compound **13j**



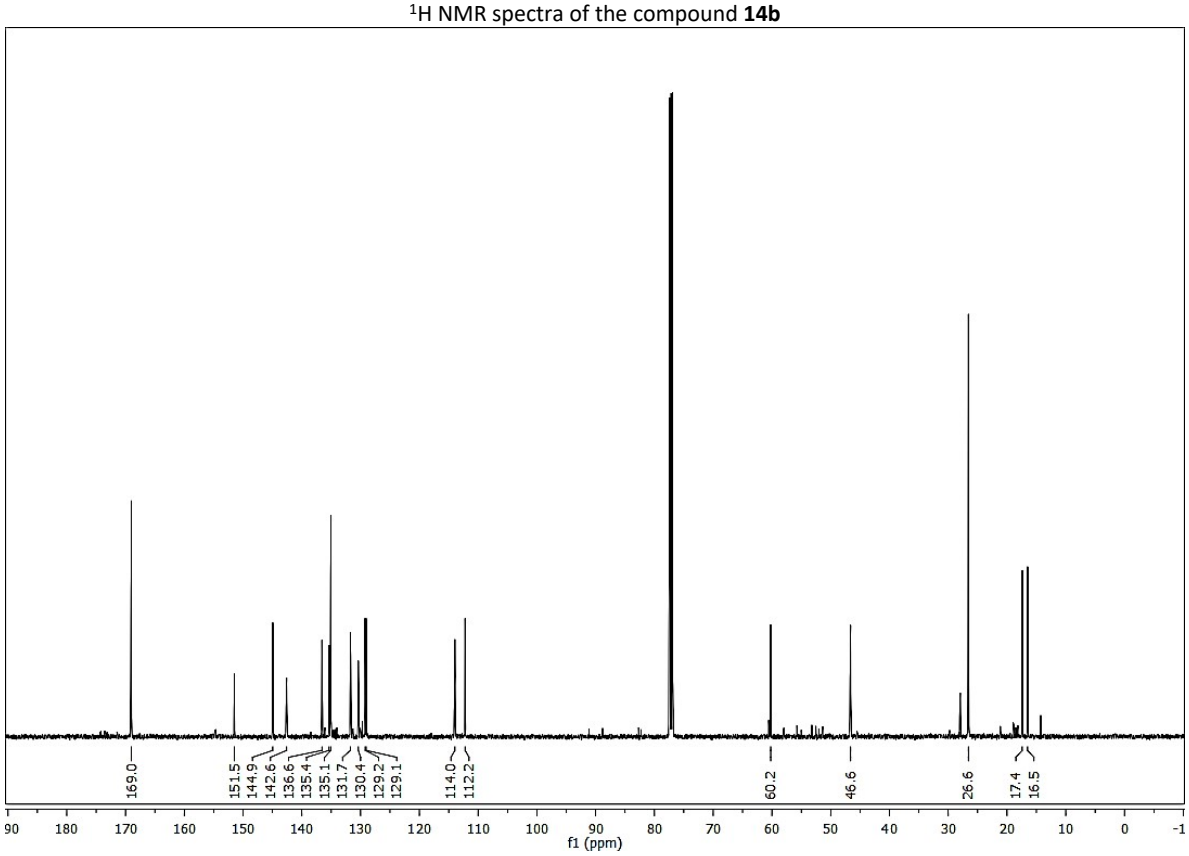
^{1}H NMR spectra of the compound **14a**



^{13}C NMR spectra of the compound **14a**



^{1}H NMR spectra of the compound **14b**



^{13}C NMR spectra of the compound **14b**

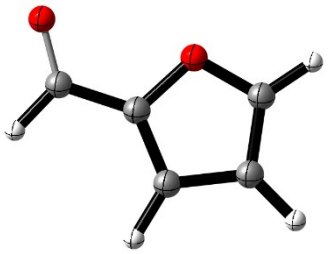
5. Computational study

Our theoretical calculations were carried out in Gaussian09 series of programs.[1] We have run geometry optimizations in solvent-phase with the default options set up in the program. We have chosen the hybrid *meta* M06-2x exchange-correlation density-functional as our DFT methodology as it has shown to reproduce empirically very well dispersion effects.[2] Therefore, our level of theory for optimizations was established as M06-2x/6-31+G(d,p) since we were exploring reaction mechanisms containing ionic species along the paths. For the reaction field calculation, we have used the Truhlar and coworkers' SMD solvation model[3] and the default options for methanol as the solvent (ε=32.613). Then, as a second step, we calculated harmonic frequencies of each optimized species, presumed critical point on the potential energy surface, for a twofold reason: first, depending on the number of negative eigenvalues, it is possible to classify each optimized structure as minimum (zero) or transition state (one and only one); second, in order to get the thermal and entropic corrections for expressing the total energy, according to the classical thermodynamics, as Gibbs free energy. Since the entropic contribution calculated within the ideal gas approximation at P = 1 atm is likely exaggerating the energy values for the addition upon each reaction component in the condensed phase,[4] all the thermochemical analysis was done at P = 1354 atm and T = 298.15 K, as suggested by Martin *et. al.*[5] Later, we executed single-point calculations in the same solvent-phase with the same density-functional but with a bigger basis set, Def2-TZVPD, with the aim of improving the numerical values reported herein for all of the structures calculated in the reaction routes. Therefore, our final reported energy values are in solvent-phase and the level of theory becomes SMD(MeOH)[M06–2X/Def2-TZVPD//M06–2X/6–31+G(d,p)].

Table S1. Cartesian coordinates (xyz format) of all the structures involved in each reaction mechanism studied calculated at M06-2X/6-31+G(d,p) level.

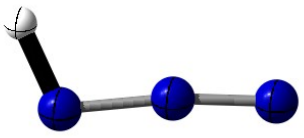
3
E(scf) = -343.234410610 a.u.
ν_{min} = 130.03 cm^{-1}

C	1.577090	-0.902223	0.000315	H	-1.999303	1.539454	0.000537
C	1.977358	0.403170	0.000050				
C	0.782623	1.176444	0.000097				
C	-0.253611	0.280267	0.000053				
O	0.231365	-0.994597	-0.000040				
H	2.116987	-1.838566	0.000435				
H	2.997116	0.759670	0.000016				
H	0.686766	2.254082	0.000088				
C	-1.685228	0.483777	0.000006				
O	-2.505234	-0.425810	-0.000485				



HN_3
E(scf) = -164.723686113 a.u.
ν_{min} = 550.55 cm^{-1}

N	1.118746	-0.138807	0.000071
N	-1.235547	0.015025	0.000097
N	-0.108381	0.012621	-0.000182
H	1.576272	0.778132	0.000096



N_3^-

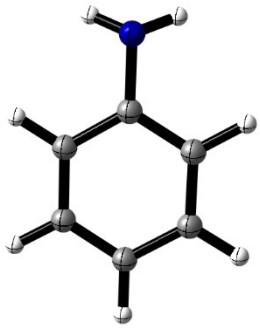
E(scf) = -164.265244287 a.u.
ν_{min} = 652.12 cm^{-1}

N	0.000000	0.000000	1.176903
N	0.000000	0.000000	-1.176902
N	0.000000	0.000000	-0.000001

4

E(scf) = -287.506318551 a.u.
ν_{min} = 222.37 cm^{-1}

C	1.879839	-0.000059	0.007759
C	1.169895	-1.202327	0.003696
C	-0.222645	-1.207948	-0.005861
C	-0.937686	0.000096	-0.009306
C	-0.222602	1.208055	-0.005617
C	1.169972	1.202230	0.003435
H	2.965351	0.000020	0.015896
H	1.703961	-2.148854	0.009224
H	-0.768888	-2.148217	-0.010440
H	-0.768680	2.148416	-0.009666
H	1.704218	2.148659	0.008812
N	-2.330399	-0.000079	-0.077300
H	-2.771880	-0.838500	0.281769
H	-2.771925	0.838739	0.280867



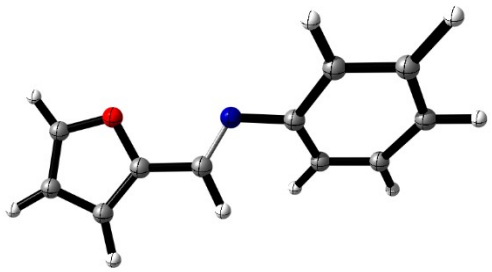
H_2O
E(scf) = -76.4095351099 a.u.
ν_{min} = 1576.07 cm^{-1}

O	0.000000	0.000000	0.117517
H	0.000000	0.766512	-0.470066
H	0.000000	-0.766512	-0.470066

11
E(scf) = -554.336509539 a.u.

ν_{min} = 35.58 cm^{-1}

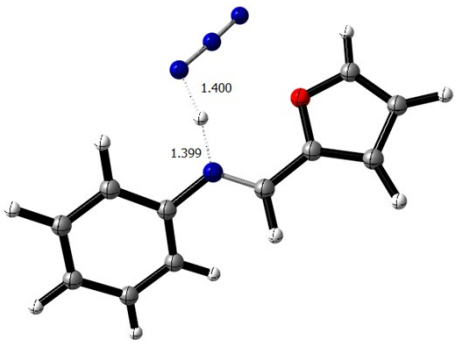
N	0.106063	-0.490352	0.155178
C	1.489186	-0.213404	0.082163
C	-0.713198	0.413662	-0.231191
H	-0.388789	1.365272	-0.667458
C	2.347905	-1.258766	-0.280017
H	1.923462	-2.232645	-0.508248
C	2.027951	1.038880	0.409253
H	1.372637	1.839705	0.741091
C	4.256044	0.208627	-0.045757
H	5.328381	0.372623	-0.093137
C	3.405067	1.243270	0.344166
H	3.814113	2.214065	0.609897
C	3.721139	-1.042830	-0.358044
H	4.376076	-1.857258	-0.654099
C	-2.146443	0.245801	-0.140885
C	-3.998982	-0.793892	0.380817
C	-4.380278	0.385028	-0.184471
H	-4.544740	-1.631168	0.791789
H	-5.394888	0.724357	-0.336206
O	-2.648000	-0.893775	0.414428
C	-3.171809	1.065704	-0.524871
H	-3.064193	2.035232	-0.992279



$TS_{11\rightarrow12}$
E(scf) = -719.059297942 a.u.

ν_{min} = -1638.51 cm^{-1}

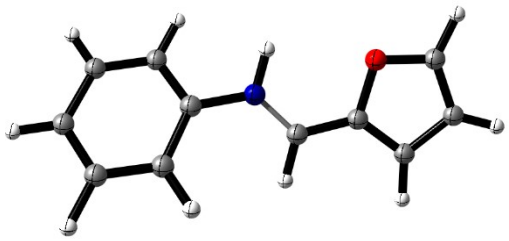
N	-0.505884	2.430824	-0.038152	H	-4.326965	0.521035	0.061115
N	-2.749164	2.868315	0.525363	H	-4.866793	-2.164249	-0.190740
N	-1.658355	2.630101	0.253350	O	-2.351142	-0.076364	-0.014623
N	0.422720	-0.197153	-0.079556	C	-2.617202	-2.289010	-0.221447
H	-0.162888	1.073049	-0.034206	H	-2.384759	-3.340381	-0.323234
C	1.839437	-0.205198	-0.032934				
C	-0.275688	-1.277276	-0.142573				
H	0.204528	-2.254448	-0.224939				
C	2.510353	0.875170	-0.615430				
H	1.941418	1.665242	-1.096055				
C	2.552582	-1.226136	0.604846				
H	2.027108	-2.036030	1.100636				
C	4.621661	-0.111264	0.027986				
H	5.706773	-0.076518	0.051910				
C	3.944305	-1.176594	0.625870				
H	4.497856	-1.966363	1.122477				
C	3.902115	0.913332	-0.588430				
H	4.421624	1.747305	-1.050460				
C	-1.705437	-1.268798	-0.132815				
C	-3.673526	-0.336917	-0.026570				
C	-3.900932	-1.677696	-0.152929				



12

E(scf) = -554.786748874 a.u.
ν_{min} = 47.60 cm^{-1}

N	0.115667	-0.323148	0.064692
H	-0.195712	-1.282644	0.232451
C	1.526122	-0.133633	0.042631
C	-0.796806	0.584645	-0.130835
H	-0.491205	1.601737	-0.359893
C	2.313306	-1.266373	-0.163752
H	1.841549	-2.235859	-0.299676
C	2.098548	1.124371	0.233283
H	1.488501	1.997669	0.441705
C	4.286119	0.120090	-0.034660
H	5.366258	0.223020	-0.065067
C	3.484775	1.241483	0.184922
H	3.939731	2.215620	0.333987
C	3.697969	-1.133317	-0.202790
H	4.314268	-2.011359	-0.368397
C	-2.178357	0.313850	-0.072753
C	-3.946552	-0.922278	0.204057
C	-4.410925	0.331629	-0.095270
H	-4.442937	-1.858260	0.420614
H	-5.446823	0.627561	-0.171593
O	-2.603098	-0.950214	0.221198
C	-3.264142	1.138739	-0.275426
H	-3.218853	2.191023	-0.522990

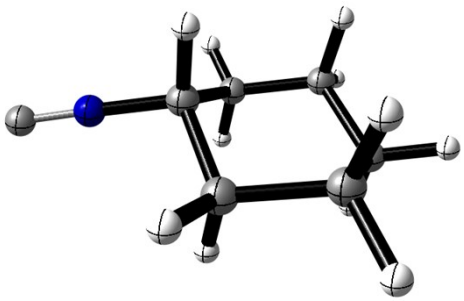


5

E(scf) = -327.967636946 a.u.

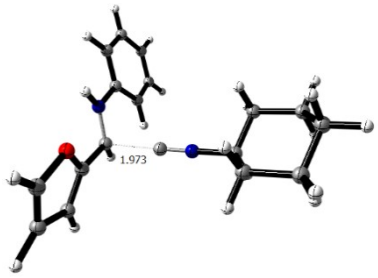
ν_{min} = 123.74 cm^{-1}

C	2.111094	-0.000019	-0.340520
C	1.425031	1.261429	0.188181
C	-0.067463	1.267435	-0.150039
C	-0.731917	0.000030	0.395619
C	-0.067509	-1.267419	-0.150003
C	1.424999	-1.261458	0.188158
H	-0.560716	2.149540	0.270725
H	1.547991	1.313515	1.278721
H	1.894667	2.158345	-0.229116
H	2.071543	-0.000007	-1.438751
H	3.169608	-0.000045	-0.058261
H	-0.673437	0.000044	1.490711
H	-0.560760	-2.149487	0.270842
H	-0.207046	-1.290886	-1.238681
H	1.548004	-1.313603	1.278689
H	1.894588	-2.158368	-0.229207
H	-0.206945	1.290846	-1.238727
N	-2.131388	0.000051	0.063062
C	-3.260533	-0.000041	-0.231126



$TS_{12\rightarrow 8}$
E(scf) = -882.743591474 a.u.
ν_{min} = -306.04 cm^{-1}

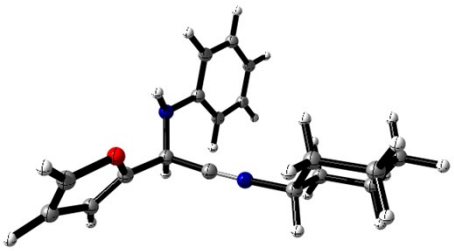
N	-1.263672	-0.076990	-0.790010				
N	2.226923	0.430945	0.352216	H	-2.962799	-0.678208	-1.732041
H	2.136036	0.757208	1.312835	C	-4.081096	-2.406998	0.140898
C	-0.175915	0.307000	-0.836049	H	-2.204549	-1.775432	1.021197
C	2.662549	-0.898083	0.183989	H	-2.020270	-2.622657	-0.527383
C	1.595748	1.141618	-0.597442	C	-4.921364	-0.026526	0.132360
H	1.892240	0.976484	-1.628322	H	-3.061965	0.667616	1.010608
C	3.281740	-1.521083	1.277166	H	-3.450407	1.434954	-0.539844
H	3.414138	-0.972719	2.202004	C	-4.969786	-1.377358	0.844607
C	2.482494	-1.590661	-1.014872	H	-4.089025	-3.359085	0.677418
H	2.004225	-1.130551	-1.872702	H	-4.479358	-2.599743	-0.865944
C	3.563819	-3.531578	-0.038623	H	-5.523496	0.713372	0.666804
H	3.911640	-4.553543	-0.127698	H	-5.350716	-0.129292	-0.871533
C	2.942646	-2.906354	-1.120027	H	-6.002036	-1.741275	0.891013
H	2.800136	-3.438510	-2.051466	H	-4.622858	-1.252749	1.883114
C	3.727772	-2.831874	1.156952	O	0.959429	2.807560	1.013070
H	4.211621	-3.308024	2.006063	C	1.118515	3.631088	-1.061590
C	1.239832	2.519291	-0.284231	H	1.282648	3.681041	-2.132113
C	0.658854	4.132097	1.063520				
C	0.740318	4.687280	-0.177431				
H	0.417281	4.522439	2.040485				
H	0.560305	5.720518	-0.429277				
C	-2.623451	-0.554325	-0.700063				
C	-2.637851	-1.906590	0.020161				
C	-3.484987	0.491387	0.015138				



8

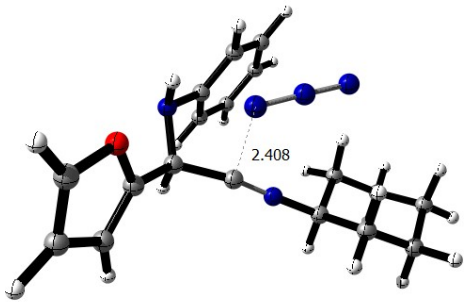
E(scf) = -882.760659336 a.u.
ν_{min} = 21.32 cm^{-1}

N	0.473574	-1.079932	-0.576788	C	2.814671	-0.670944	-1.026066
N	-1.814251	1.259993	0.305978	C	2.064025	-2.063392	0.969754
H	-1.967800	0.943652	1.260345	H	1.747979	-2.562179	-1.121396
C	-0.544831	-0.561909	-0.638941	C	4.213474	-1.281984	-0.911630
C	-0.799593	2.233830	0.207433	H	2.752369	0.248637	-0.430023
C	-1.855611	0.174079	-0.640082	H	2.575919	-0.423044	-2.064552
H	-1.993277	0.532093	-1.665823	C	3.469683	-2.661921	1.065458
C	-0.472096	2.970505	1.355470	H	1.994706	-1.162651	1.592066
H	-0.986645	2.756202	2.289061	H	1.307612	-2.776146	1.310700
C	-0.138647	2.506729	-0.996007	C	4.526161	-1.694567	0.527979
H	-0.373909	1.964850	-1.906877	H	4.947976	-0.556527	-1.274789
C	1.161538	4.238869	0.097606	H	4.277193	-2.160839	-1.567116
H	1.921496	5.012804	0.054267	H	3.676311	-2.917081	2.109470
C	0.835791	3.506054	-1.040313	H	3.502622	-3.597795	0.491751
H	1.340628	3.705682	-1.981199	H	5.517663	-2.156423	0.579030
C	0.497730	3.964073	1.296324	H	4.553840	-0.799067	1.163549
H	0.739551	4.524629	2.194743	O	-2.936645	-1.369059	0.884125
C	-2.951329	-0.794117	-0.348078	C	-4.004873	-1.243257	-1.076205
C	-4.012441	-2.199791	0.944276	H	-4.252592	-0.953333	-2.087884
C	-4.702467	-2.163881	-0.225266				
H	-4.145332	-2.731610	1.874955				
H	-5.598298	-2.721142	-0.458630				
C	1.788799	-1.671489	-0.484875				



$TS_{8\rightarrow 9}$
E(scf) = -1047.04025610 a.u.
ν_{min} = -125.84 cm^{-1}

N	-1.048956	-0.594020	1.877967	H	1.885888	-1.652938	-1.924525
N	0.482404	-0.901608	-0.668161	C	4.233349	-0.657076	-0.794087
N	1.182581	-0.343533	2.576840	H	2.630440	0.162320	0.419473
N	0.069765	-0.469463	2.247246	H	2.550404	0.634034	-1.290366
N	-1.950606	1.463412	-0.033224	C	3.574780	-3.011799	-0.175825
H	-2.157231	1.228216	0.937416	H	1.957245	-2.276806	1.067070
C	-0.584976	-0.506982	-0.483639	H	1.429177	-3.379875	-0.221189
C	-0.775467	2.267209	-0.086976	C	4.547308	-1.861836	0.095208
C	-1.874758	0.228445	-0.781851	H	4.907856	0.175265	-0.568370
H	-1.783613	0.427949	-1.856309	H	4.397361	-0.926380	-1.846380
C	-0.118361	2.618089	1.096855	H	3.784198	-3.857481	0.487119
H	-0.508500	2.268028	2.050078	H	3.709787	-3.370108	-1.205636
C	-0.269689	2.707868	-1.315469	H	5.578061	-2.192973	-0.071028
H	-0.785480	2.457251	-2.238758	H	4.469446	-1.563031	1.149843
C	1.546166	3.832746	-0.172640	O	-3.701570	-0.594976	0.610518
H	2.448145	4.436073	-0.206535	C	-3.714737	-1.497373	-1.429656
C	0.888635	3.481593	-1.352797	H	-3.437427	-1.717758	-2.451457
H	1.272859	3.818397	-2.311374				
C	1.032658	3.403689	1.050955				
H	1.534985	3.667878	1.977216				
C	-3.077789	-0.635409	-0.593280				
C	-4.757373	-1.447774	0.543734				
C	-4.813437	-2.034457	-0.680629				
H	-5.364086	-1.515065	1.434786				
H	-5.548062	-2.752062	-1.016985				
C	1.834260	-1.360592	-0.868960				
C	2.788547	-0.188973	-0.608130				
C	2.123352	-2.569808	0.023370				

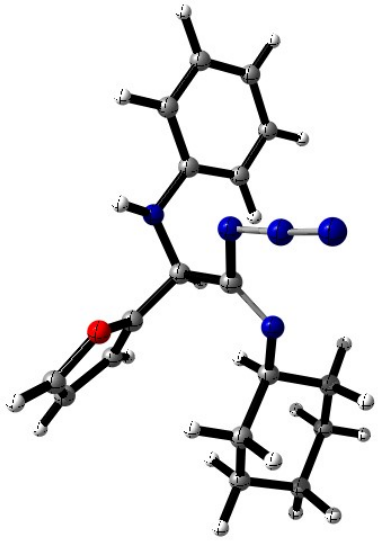


9

E(scf) = -1047.09304008 a.u.

ν_{min} = 21.37 cm^{-1}

N	1.198618	-0.111498	1.744023	H	-2.777995	0.795752	0.694745
N	-0.804114	-0.990901	0.913623	C	-4.680643	-1.742093	-0.739647
N	0.879513	-1.487407	3.638586	H	-3.789305	-3.602413	-1.416011
N	0.995937	-0.847572	2.723755	H	-3.193926	-2.166900	-2.245388
N	1.820575	1.235044	-0.487835	H	-5.115484	0.263358	-0.030132
H	2.003259	1.947724	0.212849	H	-3.999061	0.202085	-1.394181
C	0.183795	-0.216628	0.746723	H	-5.505216	-1.768089	-1.461036
C	2.890295	0.347956	-0.650551	H	-5.051988	-2.199994	0.188247
C	0.461598	0.731777	-0.436015	O	-0.634032	2.537168	0.773347
H	0.258163	0.180587	-1.358523	C	-1.365209	2.382870	-1.328960
C	4.175541	0.764733	-0.262842	H	-1.488510	2.033367	-2.345131
H	4.299109	1.746538	0.188739				
C	2.737009	-0.924445	-1.221930				
H	1.760099	-1.285183	-1.528367				
C	5.124152	-1.328157	-1.028168				
H	5.983672	-1.974895	-1.173910				
C	3.850640	-1.745338	-1.408200				
H	3.710335	-2.726342	-1.854045				
C	5.274919	-0.063446	-0.451448				
H	6.257693	0.280670	-0.140964				
C	-0.514885	1.863682	-0.405606				
C	-1.579465	3.500983	0.594406				
C	-2.061708	3.454832	-0.674701				
H	-1.787954	4.124642	1.451315				
H	-2.819909	4.100575	-1.094775				
C	-1.895999	-1.037201	-0.052413				
C	-2.302023	-2.489152	-0.306784				
C	-3.082540	-0.241708	0.507460				
H	-1.613151	-0.591986	-1.017680				
C	-3.495633	-2.557906	-1.263257				
H	-2.563692	-2.952736	0.654774				
H	-1.448034	-3.042761	-0.714883				
C	-4.272440	-0.295221	-0.451988				
H	-3.363975	-0.678217	1.476051				

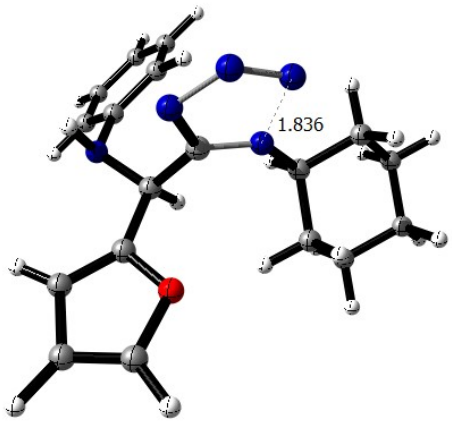


$TS_{9\rightarrow 7g}$

E(scf) = -1047.07524618 a.u.

ν_{min} = -386.55 cm^{-1}

N	0.301087	1.011269	2.287646	H	-1.871957	0.679024	-1.351256
N	-1.044853	-0.288947	1.034326	C	-4.138972	-1.965716	-1.419083
N	-1.407288	-0.318493	2.834198	H	-3.976242	-3.656087	-0.053872
N	-0.535243	0.456647	3.159909	H	-2.584519	-3.437555	-1.124564
N	2.203058	0.828386	0.022807	H	-3.835013	-0.179035	-2.627846
H	2.507241	1.228747	0.917906	H	-2.491332	-1.326112	-2.670452
C	-0.051294	0.527227	1.064551	H	-4.619386	-2.538687	-2.217825
C	2.716219	-0.506827	-0.141376	H	-4.944493	-1.494396	-0.833935
C	0.768519	0.985300	-0.139913	O	-0.846459	2.812190	-0.265349
H	0.463639	0.380395	-1.005675	C	1.215982	3.494253	-0.795395
C	3.741345	-0.700683	-1.080692	H	2.278798	3.486742	-0.980593
H	4.113068	0.162824	-1.637208				
C	2.239498	-1.607337	0.585436				
H	1.456828	-1.477334	1.333948				
C	3.802452	-3.058368	-0.564748				
H	4.222001	-4.046091	-0.727964				
C	2.774835	-2.876200	0.364252				
H	2.390581	-3.718369	0.936468				
C	4.289463	-1.967300	-1.284850				
H	5.090478	-2.096747	-2.012413				
C	0.457919	2.428966	-0.405578				
C	-0.914590	4.136222	-0.570310				
C	0.308770	4.607306	-0.902816				
H	-1.900870	4.580261	-0.502922				
H	0.552269	5.625887	-1.193610				
C	-1.712896	-1.030106	-0.028026				
C	-2.601923	-2.119552	0.589400				
C	-2.526776	-0.083411	-0.913592				
H	-0.922107	-1.508824	-0.625720				
C	-3.323456	-2.894462	-0.513785				
H	-3.337452	-1.633142	1.245649				
H	-1.992355	-2.787034	1.202819				
C	-3.242212	-0.869830	-2.016604				
H	-3.262133	0.439081	-0.281570				

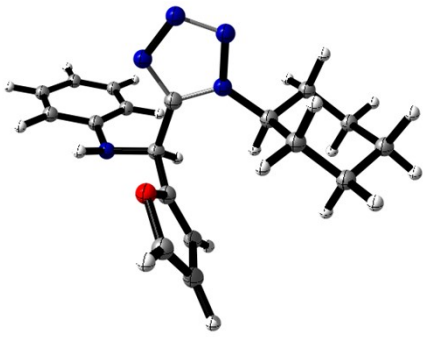


7g

E(scf) = -1047.14140203 a.u.

ν_{min} = 18.51 cm^{-1}

N	1.041527	-0.579333	1.798046
N	-0.821285	-0.991708	0.793666
N	-0.799373	-1.720241	1.912313
N	0.318259	-1.469505	2.499555
N	2.049142	1.184704	-0.224587
H	2.171203	1.822658	0.556532
C	0.318802	-0.282691	0.733361
C	3.124822	0.302391	-0.385567
C	0.686175	0.709671	-0.351599
H	0.564073	0.221295	-1.324536
C	4.385426	0.689091	0.100149
H	4.482282	1.637473	0.623759
C	3.005629	-0.923818	-1.055288
H	2.046445	-1.261762	-1.435057
C	5.378857	-1.344989	-0.760431
H	6.246432	-1.981144	-0.905185
C	4.129034	-1.731449	-1.238901
H	4.014635	-2.678503	-1.759257
C	5.495167	-0.125900	-0.086547
H	6.459178	0.194990	0.298544
C	-0.273600	1.857988	-0.340243
C	-1.361663	3.483320	0.650931
C	-1.767012	3.491662	-0.645473
H	-1.608260	4.081695	1.515630
H	-2.485370	4.168305	-1.086329
C	-1.997382	-0.959162	-0.090696
C	-2.541395	-2.364420	-0.338014
C	-3.065731	-0.031541	0.490307
H	-1.633802	-0.548560	-1.039439
C	-3.731154	-2.284868	-1.299286
H	-2.864973	-2.799590	0.615210
H	-1.749546	-3.001853	-0.746059
C	-4.255307	0.044439	-0.468734
H	-3.387077	-0.435039	1.460006
H	-2.641270	0.963539	0.668403
C	-4.817811	-1.348293	-0.764966
H	-4.137216	-3.288980	-1.459056
H	-3.383468	-1.920601	-2.275856
H	-5.029533	0.690022	-0.041138
H	-3.928920	0.514860	-1.407527
H	-5.639705	-1.276212	-1.485542
H	-5.235702	-1.770977	0.159206
O	-0.449680	2.492390	0.852146
C	-1.055871	2.426081	-1.294591
H	-1.121764	2.116769	-2.328910

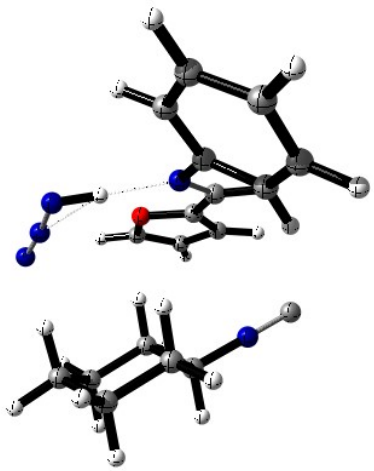


10+5

E(scf) = -1047.05374229 a.u.

ν_{min} = 29.77 cm^{-1}

N	-0.208936	0.037208	2.666269	H	0.929206	-2.811289	-1.606268
N	-2.557371	-0.110529	2.764939	C	-2.586666	-2.320575	0.129387
N	-1.434204	-0.010283	2.668745	H	-1.525370	-0.441402	-0.091109
N	1.019825	1.200640	0.392495	H	-2.802002	-0.685655	-1.298769
H	0.154351	0.526860	1.801883	C	-1.479970	-3.041837	0.903597
C	2.366902	0.788724	0.276732	H	0.426928	-4.012523	0.537183
C	0.455479	1.830265	-0.570389	H	-0.799762	-4.337324	-0.686107
C	3.138919	0.769518	1.444679	H	-3.336733	-1.917005	0.816961
H	2.690323	1.095155	2.379785	H	-3.101927	-3.039035	-0.523165
C	2.921674	0.344986	-0.931604	H	-1.902946	-3.873890	1.477142
H	2.311847	0.306688	-1.830693	H	-1.029801	-2.349378	1.628342
C	5.027300	-0.069149	0.189561				
H	6.060251	-0.401995	0.154655				
C	4.248648	-0.077767	-0.968992				
H	4.671223	-0.426890	-1.906782				
C	4.467089	0.354079	1.396051				
H	5.063243	0.354957	2.303822				
C	-0.942011	2.186357	-0.516807				
C	-2.929954	2.249366	0.391567				
C	-3.075736	2.761562	-0.862994				
H	-3.617245	2.087667	1.210231				
H	-3.994225	3.120900	-1.304348				
O	-1.641523	1.899959	0.617406				
C	-1.778193	2.722813	-1.457327				
H	-1.491715	3.032889	-2.453423				
H	0.987238	2.128823	-1.479084				
C	-0.040274	0.103090	-3.243925				
N	-0.451396	-0.738024	-2.547107				
C	-0.964139	-1.766649	-1.683982				
C	0.177475	-2.429139	-0.907973				
C	-2.013808	-1.190730	-0.729571				
H	-1.436162	-2.507528	-2.340830				
C	-0.385686	-3.554331	-0.036041				
H	0.657751	-1.666276	-0.277878				

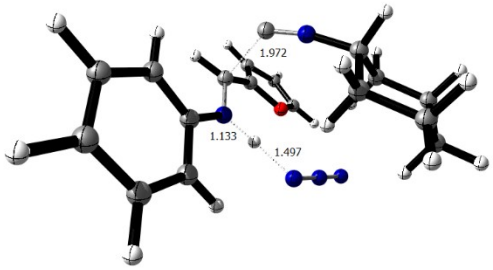


$TS_{10+5\rightarrow 8+N3^-}$

E(scf) = -1047.02659973 a.u.

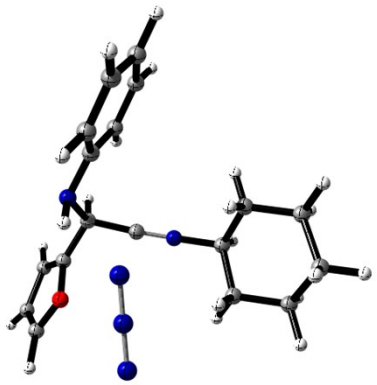
ν_{min} = -343.99 cm^{-1}

N	-0.269503	-0.412952	1.964128
N	-2.575388	-0.198914	2.372918
N	-1.437636	-0.295732	2.186529
N	1.136113	1.150862	0.411099
H	0.438623	0.584929	1.101517
C	2.425194	0.593078	0.318922
C	0.648459	1.972348	-0.501362
C	2.837206	-0.234174	1.373831
H	2.152274	-0.412616	2.197785
C	3.268350	0.805429	-0.778252
H	2.953775	1.413454	-1.620031
C	4.949680	-0.596050	0.252639
H	5.933059	-1.054183	0.228092
C	4.529482	0.212422	-0.799913
H	5.181615	0.382206	-1.650891
C	4.095751	-0.819139	1.334803
H	4.411218	-1.455710	2.155237
C	-0.675969	2.539508	-0.292059
C	-2.678870	2.515789	0.565637
C	-2.606796	3.648696	-0.192759
H	-3.432914	2.060041	1.191704
H	-3.386450	4.383134	-0.324373
O	-1.514113	1.841099	0.504255
C	-1.297047	3.662570	-0.761357
H	-0.870430	4.401596	-1.424221
H	1.330758	2.593215	-1.073219
C	0.243437	0.724199	-1.973255
N	-0.309409	-0.300502	-1.970880
C	-0.977415	-1.544861	-1.686709
C	-0.048193	-2.409943	-0.824473
C	-2.306304	-1.231814	-0.985666
H	-1.165019	-2.036130	-2.649616
C	-0.770894	-3.690758	-0.400679
H	0.221532	-1.834518	0.070465
H	0.866443	-2.631577	-1.385068
C	-2.996166	-2.521231	-0.536328
H	-2.098360	-0.607575	-0.110373
H	-2.946133	-0.653334	-1.661384
C	-2.068501	-3.363291	0.341504
H	-0.103513	-4.282232	0.233641
H	-0.996524	-4.303736	-1.285811
H	-3.904808	-2.258001	0.013003
H	-3.302718	-3.106396	-1.415725
H	-2.574351	-4.285305	0.646404
H	-1.832843	-2.802050	1.255117



8+N_3^-
E(scf) = -1047.04181866 a.u.
ν_{min} = 15.85 cm^{-1}

N	0.276535	0.507093	1.973634	H	-1.542473	2.283924	0.715835
N	0.819568	2.785835	2.192504	H	-1.103460	3.238061	-0.716105
N	0.550637	1.649043	2.087851	C	-4.280283	2.153397	0.217848
N	1.605193	-1.534853	0.280898	H	-4.966562	0.130106	-0.177307
H	1.551554	-0.990036	1.145831	H	-4.570912	1.059347	-1.622845
C	0.561894	-2.488487	0.240109	H	-3.237911	4.057627	0.302260
C	1.740131	-0.635584	-0.841833	H	-3.509330	3.450147	-1.330730
C	0.054870	-2.963244	1.459144	H	-5.280527	2.597987	0.182418
H	0.452704	-2.566246	2.389756	H	-4.062484	1.928575	1.270715
C	0.042811	-2.991662	-0.959239				
H	0.413001	-2.647796	-1.920318				
C	-1.463256	-4.434382	0.279366				
H	-2.247117	-5.185487	0.294242				
C	-0.962416	-3.960240	-0.930351				
H	-1.353367	-4.341074	-1.869563				
C	-0.945403	-3.928300	1.474650				
H	-1.326367	-4.283690	2.427812				
C	2.883770	0.311956	-0.706367				
C	3.984924	1.925409	0.267657				
C	4.728658	1.556647	-0.808176				
H	4.107855	2.666354	1.044127				
H	5.674718	1.981735	-1.111577				
O	2.855457	1.173835	0.341728				
C	4.003767	0.499268	-1.451609				
H	4.275699	-0.049384	-2.342670				
H	1.888673	-1.181928	-1.778722				
C	0.465494	0.135066	-1.023354				
N	-0.547136	0.656879	-1.132132				
C	-1.859196	1.257134	-1.143910				
C	-2.860758	0.228320	-0.607025				
C	-1.840383	2.539742	-0.308232				
H	-2.068507	1.486316	-2.194446				
C	-4.257263	0.854157	-0.590332				
H	-2.553656	-0.054047	0.408582				
H	-2.837672	-0.670187	-1.231469				
C	-3.244210	3.149309	-0.308169				



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