

Supporting Information for

Facile construction of diverse polyheterocyclic scaffolds via gold-catalysed dearomative spirocyclization/1,6-addition cascade

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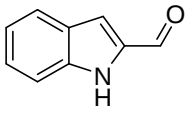
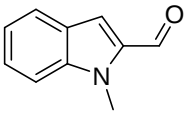
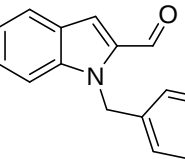
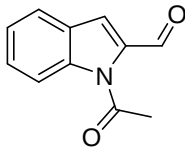
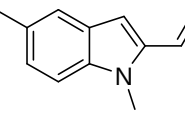
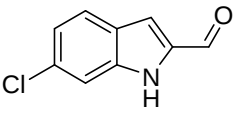
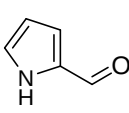
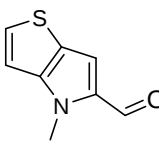
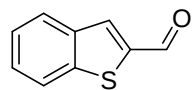
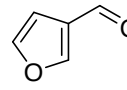
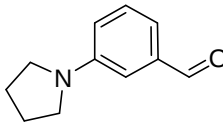
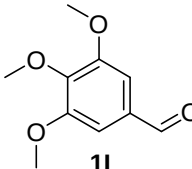
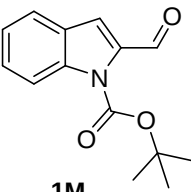
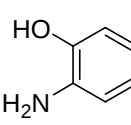
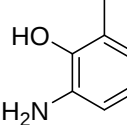
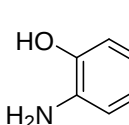
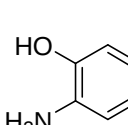
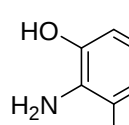
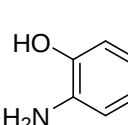
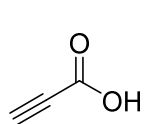
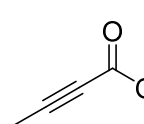
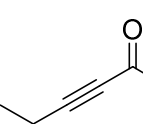
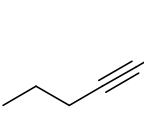
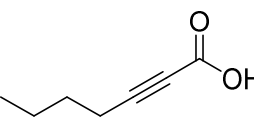
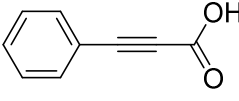
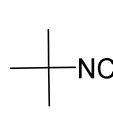
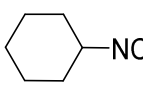
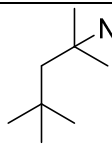
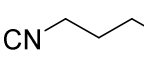
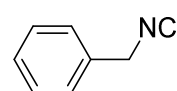
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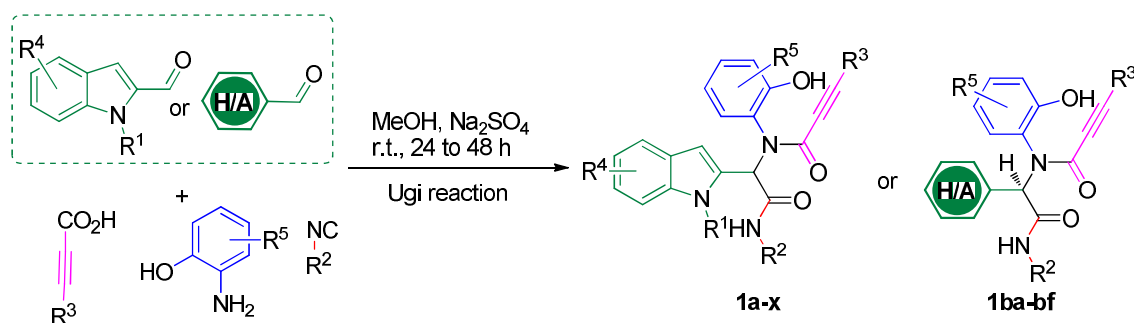
General Methods

NMR spectra were recorded on a 300, 400 or 600 MHz instrument using CDCl_3 or $\text{DMSO-}d_6$ as solvent. For Ugi adducts, the mixture of CDCl_3 and $\text{DMSO-}d_6$ was applied as solvent wherever is necessary. The ^1H and ^{13}C chemical shifts are reported in parts per million relative to tetramethylsilane as an internal standard. Spectra were acquired on a quadrupole orthogonal acceleration time-of-flight mass spectrometer (Synapt G2 HDMS, Waters, Milford, MA). Samples were infused at 3 $\mu\text{L}/\text{min}$ and spectra were obtained in positive (or: negative) ionization mode with a resolution of 15000 (FWHM) using leucine enkephalin as lock mass. For chromatography, analytical TLC plates and 70-230 mesh silica gel were used. All the solvents and chemicals were purchased and used as available. Data for ^1H NMR are recorded as follows: chemical shift (δ , ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant (s) in Hz, integration). Data for ^{13}C NMR are reported in terms of chemical shift (δ , ppm).

General procedure for the synthesis of Ugi products

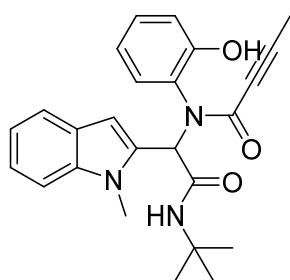
Table S1: Starting materials for Ugi reaction

Aldehydes	 1A  1B  1C  1D  1E
	 1F  1G  1H  1I  1J
	 1K  1L  1M
Amines	 2A  2B  2C  2D  2E  2F
Acids	 3A  3B  3C  3D  3E  3F
Isonitriles	 4A  4B  4C  4D  4E  4F



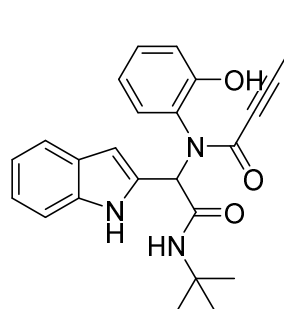
A screw-cap vial equipped with a magnetic stir bar was charged with aldehyde (0.8 mmol, 1.0 equiv.), amine (0.88 mmol, 1.1 equiv.), alkynoic acid (0.88 mmol, 1.1 equiv.), isocyanide (0.88 mmol, 1.1 equiv.), Na₂SO₄ (0.2 g) and methanol (3 mL). The reaction mixture was stirred at room temperature for 24-48 h. The reaction solution was diluted with water (25 mL) and extracted with EtOAc (50 mL). The organic layer was washed with brine (25 mL), dried over MgSO₄ and then concentrated under reduced pressure. The obtained residue was purified by column chromatography on silica gel with EtOAc/Heptane (v/v, 1/2) to provide the desired Ugi products **1a-x** and **1ba-bf** as solid.

N-(2-(*tert*-butylamino)-1-(1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxyphenyl)but-2-ynamide (**1a**)



Pale yellow solid, Yield 68%, Melting point: 137-138 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ = 11.62 (s, 1H), 8.56 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.12 – 7.03 (m, 1H), 6.97 – 6.78 (m, 3H), 6.65 (d, *J* = 8.1 Hz, 1H), 6.43 (t, *J* = 7.5 Hz, 1H), 6.19 (s, 1H), 6.18 (s, 1H), 3.75 (s, 3H), 1.68 (s, 3H), 1.33 (s, 9H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ = 171.4, 156.2, 155.0, 137.4, 132.5, 131.2, 130.7, 126.8, 125.7, 122.2, 120.9, 119.7, 118.7, 117.1, 110.2, 102.6, 90.5, 74.1, 60.2, 57.6, 51.8, 30.4, 28.8, 28.5, 28.4, 21.2, 14.6, 3.7, 3.6. HRMS (ESI) calculated for C₂₅H₂₈N₃O₃ [M+H]⁺: 418.2131, found 418.2122.

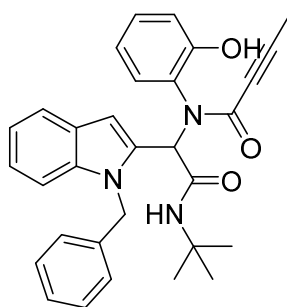
N-(2-(*tert*-butylamino)-1-(1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxyphenyl)but-2-ynamide (**1b**)



Pale yellow solid, Yield 77%, Melting point: 175-177 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ = 11.57 (s, 1H), 11.22 (s, 1H), 8.64 (s, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.03 (dd, *J* = 7.9, 1.6 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.94 – 6.89 (m, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.63 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.44 (t, *J* = 7.5 Hz, 1H), 6.07 (s, 2H), 1.68 (s, 3H), 1.33 (s, 9H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ = 171.3, 156.2, 154.8, 136.6, 132.3, 131.5, 130.4, 127.5, 125.9, 122.0, 120.7, 119.3, 118.4,

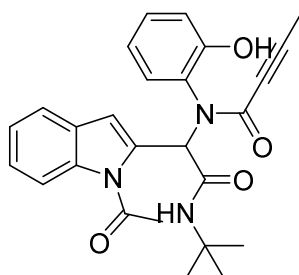
116.9, 111.4, 102.2, 90.1, 74.2, 59.7, 51.8, 28.5, 3.6. **HRMS (ESI)** calculated for $C_{24}H_{26}N_3O_3$ $[M+H]^+$: 404.1974, found 404.1966.

N-(1-(1-benzyl-1*H*-indol-2-yl)-2-(*tert*-butylamino)-2-oxoethyl)-*N*-(2-hydroxyphenyl)but-2-ynamide (**1c**)



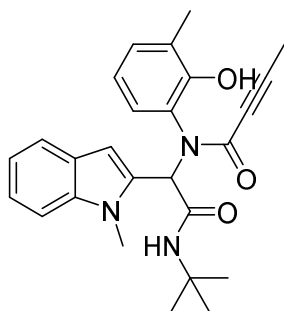
Pale yellow solid, Yield 35%, Melting point: 164-165 °C. **1H NMR (300 MHz, DMSO- d_6)** δ = 11.63 (s, 1H), 8.59 (s, 1H), 7.42 – 7.29 (m, 5H), 7.24 – 7.16 (m, 2H), 7.09 – 7.00 (m, 1H), 6.95 – 6.82 (m, 2H), 6.65 (dd, J = 8.2, 1.4 Hz, 1H), 6.26 (s, 1H), 6.23 – 6.15 (m, 2H), 5.70 (dd, J = 7.9, 1.7 Hz, 1H), 5.56 (d, J = 16.7 Hz, 1H), 5.46 (d, J = 16.7 Hz, 1H), 1.63 (s, 3H), 1.30 (s, 9H). **^{13}C NMR (151 MHz, DMSO- d_6)** δ = 171.2, 156.1, 155.0, 138.2, 137.3, 132.3, 131.6, 130.5, 129.0, 128.1, 128.0, 127.0, 125.5, 122.6, 121.0, 120.0, 118.5, 116.9, 111.1, 103.8, 90.3, 74.1, 60.2, 57.8, 51.9, 47.0, 28.7, 28.5, 28.4, 21.2, 14.6, 3.6. **HRMS (ESI)** calculated for $C_{31}H_{32}N_3O_3$ $[M+H]^+$: 494.2444, found 494.2458.

N-(1-(1-acetyl-1*H*-indol-2-yl)-2-(*tert*-butylamino)-2-oxoethyl)-*N*-(2-hydroxyphenyl)but-2-ynamide (**1d**)



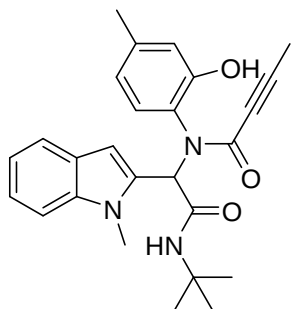
Pale yellow solid, Yield 57%, Melting point: 185-187 °C. **1H NMR (300 MHz, DMSO- d_6)** δ = 11.47 (s, 1H), 11.24 (s, 1H), 8.62 (s, 1H), 7.35 (d, J = 7.9 Hz, 1H), 7.24 (dd, J = 8.0, 1.0 Hz, 1H), 7.00 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 6.95 – 6.79 (m, 2H), 6.48 – 6.40 (m, 1H), 6.31 – 6.19 (m, 1H), 6.07 (s, 1H), 6.05 (s, 1H), 2.03 (s, 3H), 1.69 (s, 3H), 1.33 (s, 9H). **^{13}C NMR (101 MHz, DMSO- d_6)** δ = 171.8, 169.4, 156.0, 155.0, 135.1, 132.2, 130.5, 129.4, 127.4, 125.8, 125.5, 123.8, 119.7, 118.5, 117.0, 116.0, 115.1, 90.0, 74.2, 57.1, 51.8, 28.8, 28.5, 28.5, 24.2, 3.6. **HRMS (ESI)** calculated for $C_{26}H_{38}N_3O_4$ $[M+H]^+$: 446.2080, found 446.2083

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-3-methylphenyl) but-2-ynamide (**1e**)



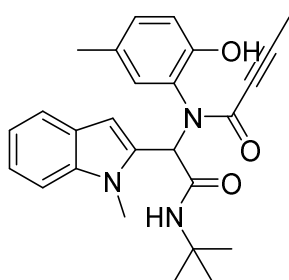
Yellow solid, Yield 65% (Mixture of rotamers $\approx$ 1: 2), Melting point: 196-197 °C. **^1H NMR (400 MHz, DMSO- d_6)** δ = 9.26 (s, 1H), 7.87 (s, 0.39H), 7.75 (d, J = 8.7 Hz, 0.54H), 7.63 (s, 1H), 7.42 (t, J = 8.0 Hz, 0.60H), 7.35 (dd, J = 8.1, 4.5 Hz, 1.22H), 7.16 – 7.10 (m, 0.40H), 7.10 – 7.04 (m, 0.64H), 6.97 (t, J = 7.4 Hz, 0.39H), 6.92 (t, J = 7.5 Hz, 0.63H), 6.51 (d, J = 2.6 Hz, 0.36H), 6.47 (dd, J = 8.7, 2.8 Hz, 0.56H), 6.33 (s, 0.35H), 6.29 (s, 0.52H), 6.27 – 6.23 (m, 1H), 6.12 (dd, J = 8.6, 2.6 Hz, 0.38H), 6.08 (d, J = 8.6 Hz, 0.46H), 6.03 (s, 0.57H), 3.68 (s, 1.32H), 3.66 (s, 1.61H), 1.74 (s, 1.07H), 1.70 (s, 2.02H), 1.25 (s, 9H), 1.20 (s, 3H). **^{13}C NMR (101 MHz, DMSO- d_6)** δ = 168.0, 166.4, 156.9, 156.8, 154.9, 154.8, 140.4, 138.3, 137.6, 137.2, 135.0, 133.5, 133.0, 130.3, 129.6, 129.3, 127.1, 126.9, 121.9, 120.8, 119.6, 117.0, 116.3, 113.0, 112.5, 110.3, 110.1, 104.7, 103.7, 89.3, 79.6, 74.8, 56.5, 56.0, 51.0, 50.8, 30.6, 30.3, 28.8, 28.7, 28.6, 18.9, 17.7, 3.6. **HRMS (ESI)** calculated for $\text{C}_{26}\text{H}_{30}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 432.2287, found 432.2290.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl) but-2-ynamide (**1f**)



Pale yellow solid, Yield 57%, Melting point: 209-210 °C. **^1H NMR (400 MHz, DMSO- d_6)** δ = 11.51 (s, 1H), 8.52 (s, 1H), 7.44 – 7.25 (m, 2H), 7.11 – 7.03 (m, 1H), 6.95 – 6.88 (m, 1H), 6.74 (d, J = 8.0 Hz, 1H), 6.48 – 6.43 (m, 1H), 6.24 (dd, J = 8.1, 2.0 Hz, 1H), 6.16 (s, 2H), 3.73 (s, 3H), 2.02 (s, 3H), 1.69 (s, 3H), 1.31 (s, 9H). **^{13}C NMR (101 MHz, DMSO- d_6)** δ = 171.4, 155.8, 155.2, 140.0, 137.5, 132.6, 130.8, 126.8, 123.2, 122.2, 121.0, 119.7, 119.6, 117.7, 110.2, 102.6, 90.5, 79.7, 74.2, 57.5, 51.8, 30.4, 28.5, 21.2, 3.71. **HRMS (ESI)** calculated for $\text{C}_{26}\text{H}_{30}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 432.2287, found 432.2274.

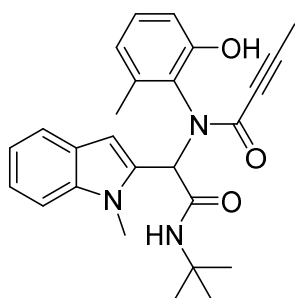
N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-5-methylphenyl) but-2-ynamide (**1g**)



Pale yellow solid, Yield 77%, Melting point: 137-138 °C. **^1H NMR (400 MHz, DMSO- d_6)** δ = 11.29 (s, 1H), 8.51 (s, 1H), 7.36 (d, J = 7.8 Hz, 2H), 7.11 – 7.03 (m, 1H), 6.91 (t, J = 7.5 Hz, 1H), 6.71 (dd, J = 8.3, 2.1 Hz, 1H), 6.66 (s, 1H), 6.52 (d, J = 8.2 Hz, 1H), 6.15 (s, 2H), 3.73 (s, 3H), 1.88 (s, 3H), 1.69 (s, 3H), 1.31 (s, 9H). **^{13}C NMR**

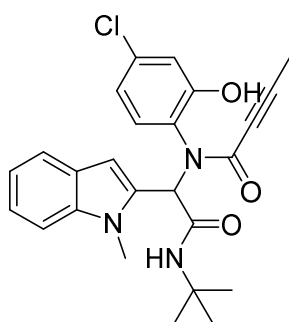
(151 MHz, DMSO-*d*₆) δ = 171.3, 154.9, 153.8, 137.5, 132.6, 131.2, 127.1, 126.8, 125.3, 122.2, 120.9, 119.7, 116.7, 110.1, 102.7, 90.3, 79.6, 74.2, 57.6, 51.8, 30.5, 28.8, 28.5, 20.0, 3.6. **HRMS (ESI)** calculated for C₂₆H₃₀N₃O₃ [M+H]⁺: 432.2287, found 432.2283.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-6-methylphenyl) but-2-ynamide (**1h**)



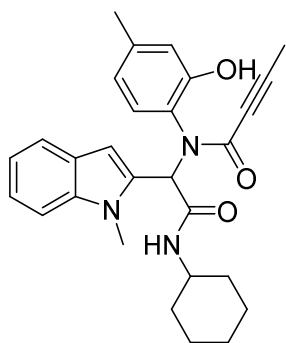
Pale yellow solid, Yield 37%, Melting point: 182-183 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.69 (s, 1H), 8.51 (s, 1H), 7.35 (dd, *J* = 8.0, 2.9 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.86 (t, *J* = 7.8 Hz, 1H), 6.56 (d, *J* = 8.0 Hz, 1H), 6.37 (d, *J* = 7.4 Hz, 1H), 6.28 (s, 1H), 6.12 (s, 1H), 3.74 (s, 3H), 1.98 (s, 3H), 1.68 (s, 3H), 1.26 (s, 9H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.6, 156.7, 155.3, 138.3, 137.6, 131.4, 130.1, 126.8, 124.9, 122.3, 120.9, 120.3, 119.9, 114.5, 110.6, 103.8, 88.9, 79.6, 73.9, 57.5, 51.8, 30.9, 28.4, 18.2, 3.6. **HRMS (ESI)** calculated for C₂₆H₃₀N₃O₃ [M+H]⁺: 432.2287, found 432.2279.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(4-chloro-2-hydroxyphenyl)but-2-ynamide (**1i**)



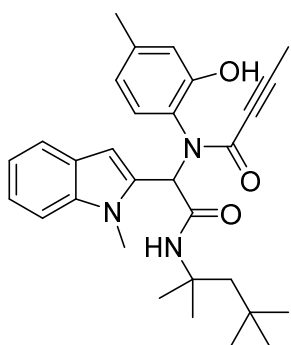
Yellow solid, Yield 47%, Melting point: 226-228 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 12.16 (s, 1H), 8.63 (s, 1H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.95 (t, *J* = 7.8 Hz, 2H), 6.71 (d, *J* = 2.4 Hz, 1H), 6.49 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.17 (s, 2H), 3.74 (s, 3H), 1.73 (s, 3H), 1.31 (s, 9H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.4, 157.3, 154.7, 137.5, 134.3, 132.7, 132.1, 126.7, 125.0, 122.4, 121.0, 119.8, 118.8, 117.0, 110.2, 102.6, 91.0, 79.6, 74.0, 57.5, 52.0, 30.4, 28.8, 28.4, 3.6. **HRMS (ESI)** calculated for C₂₅H₂₇ClN₃O₃ [M+H]⁺: 452.1741, found 452.1735.

N-(2-(cyclohexylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl) but-2-ynamide (**1j**)



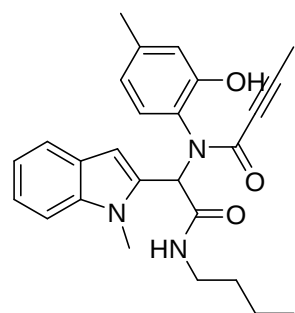
Pale yellow solid, Yield 39%, Melting point: 162-163 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.48 (s, 1H), 8.73 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.08 (t, *J* = 7.7 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.48 (s, 1H), 6.24 (d, *J* = 8.3 Hz, 1H), 6.18 (s, 1H), 6.14 (s, 1H), 3.74 (s, 3H), 3.71 – 3.60 (m, 1H), 2.02 (s, 3H), 1.85 – 1.71 (m, 3H), 1.69 (s, 3H), 1.65 – 1.49 (m, 2H), 1.36 – 1.18 (m, 3H), 1.17 – 0.98 (m, 2H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.0, 155.8, 155.2, 140.1, 137.5, 132.4, 130.8, 126.8, 123.1, 122.2, 121.0, 119.7, 117.7, 110.2, 102.8, 90.5, 79.7, 74.2, 57.1, 49.2, 32.3, 32.1, 30.4, 25.5, 24.8, 24.7, 21.2, 3.7. **HRMS (ESI)** calculated for C₂₈H₃₂N₃O₃ [M+H]⁺: 458.2444, found 458.2450.

N-(2-hydroxy-4-methylphenyl)-*N*-(1-(1-methyl-1*H*-indol-2-yl)-2-oxo-2-((2,4,4-trimethylpentan-2-yl)amino)ethyl)but-2-ynamide (**1k**)



Pale yellow solid, Yield 87%, Melting point: 149-150 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.52 (s, 1H), 8.36 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 6.47 (s, 1H), 6.23 (dd, *J* = 8.1, 1.9 Hz, 1H), 6.19 (s, 1H), 6.15 (s, 1H), 3.73 (s, 3H), 2.01 (s, 3H), 1.94 (d, *J* = 14.7 Hz, 1H), 1.69 (s, 3H), 1.56 (d, *J* = 14.7 Hz, 1H), 1.38 (s, 3H), 1.31 (s, 3H), 0.94 (s, 9H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.0, 155.8, 155.1, 140.0, 137.4, 132.6, 130.8, 126.8, 123.3, 122.1, 120.9, 119.6, 117.7, 110.2, 102.8, 90.4, 79.7, 74.3, 57.6, 55.9, 51.0, 31.8, 31.7, 31.5, 30.4, 29.0, 28.6, 21.2, 3.7. **HRMS (ESI)** calculated for C₃₀H₃₈N₃O₃ [M+H]⁺: 488.2913, found 488.2911.

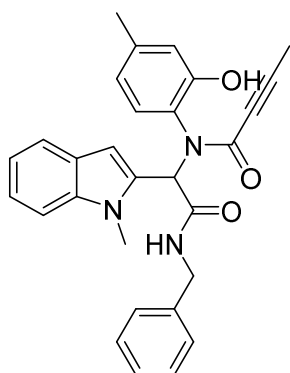
N-(2-(butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1l**)



Pale yellow solid, Yield 52%, Melting point: 172-173 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.46 (s, 1H), 8.84 (t, *J* = 5.7 Hz, 1H), 7.39 – 7.27 (m, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.49 (s, 1H), 6.24 (d, *J* = 7.4 Hz, 1H), 6.19 (s, 1H), 6.14 (s, 1H), 3.74 (s, 3H), 3.20 (q, *J* = 6.5 Hz, 2H), 2.02 (s, 3H), 1.69 (s, 3H), 1.45 – 1.35 (m, 2H), 1.31 – 1.18 (m, 2H), 0.85 (t, *J* = 7.3 Hz, 3H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ = 172.0, 155.8, 155.2, 140.1, 137.5, 132.3,

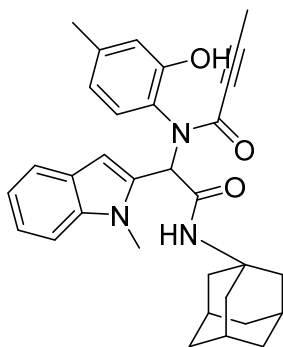
130.8, 126.8, 123.1, 122.3, 120.9, 119.7, 117.7, 110.3, 102.9, 90.5, 74.2, 57.1, 31.0, 30.4, 21.2, 19.8, 14.0, 3.7. **HRMS (ESI)** calculated for $C_{26}H_{30}N_3O_3$ $[M+H]^+$: 432.2287, found 432.2279.

N-(2-(benzylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1m**)



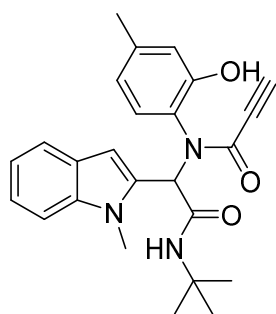
Pale yellow solid, Yield 55%, Melting point: 196-197 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.31 (s, 1H), 9.36 (t, *J* = 5.9 Hz, 1H), 7.50 – 7.19 (m, 8H), 7.08 (t, *J* = 7.9 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.75 (d, *J* = 7.9 Hz, 1H), 6.50 (s, 1H), 6.27 (s, 1H), 6.16 (s, 1H), 4.52 (dd, *J* = 15.1, 6.1 Hz, 1H), 4.38 (dd, *J* = 15.1, 5.3 Hz, 1H), 3.75 (s, 3H), 2.03 (s, 3H), 1.70 (s, 3H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 172.3, 155.7, 155.2, 140.2, 138.4, 137.5, 132.0, 130.9, 128.8, 128.6, 127.9, 127.9, 127.7, 127.6, 126.7, 123.1, 122.3, 120.9, 119.9, 119.8, 117.7, 110.3, 103.1, 90.7, 74.1, 57.2, 43.4, 30.3, 21.2, 3.7. **HRMS (ESI)** calculated for $C_{29}H_{28}N_3O_3$ $[M+H]^+$: 466.2131, found 466.2128.

N-(2-((3*s*,5*s*,7*s*)-adamantan-1-ylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1n**)



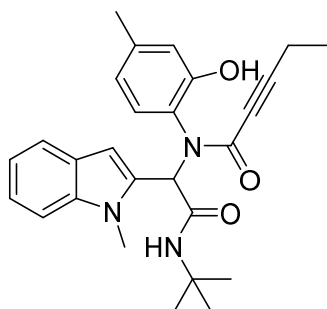
Light red solid, Yield 67%, Melting point: 162-163 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.49 (s, 1H), 8.40 (s, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.08 (t, *J* = 7.7 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 7.9 Hz, 1H), 6.46 (s, 1H), 6.24 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.16 (s, 1H), 6.15 (s, 1H), 3.72 (s, 3H), 2.06 – 2.02 (m, 3H), 2.01 (s, 2H), 1.98 – 1.90 (m, 6H), 1.69 (s, 2H), 1.64 (s, 6H), 1.25 (s, 1H), 0.86 (t, *J* = 6.6 Hz, 1H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.2, 155.8, 155.1, 140.0, 137.5, 132.7, 130.8, 126.8, 123.2, 122.2, 121.0, 119.7, 119.6, 117.7, 110.2, 102.6, 90.4, 74.2, 57.6, 52.5, 40.9, 36.3, 31.7, 30.4, 29.3, 29.2, 28.8, 22.6, 21.2, 14.4, 3.7. **HRMS (ESI)** calculated for $C_{32}H_{36}N_3O_3$ $[M+H]^+$: 510.2757, found 510.2755.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)propiolamide (**1o**)



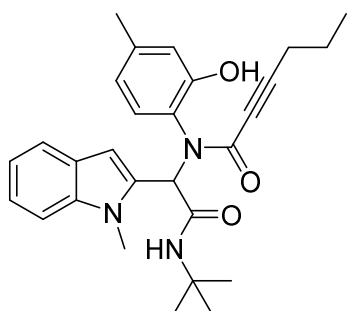
Yellow solid, Yield 77%, Melting point: 209-211 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.50 (s, 1H), 8.56 (s, 1H), 7.41 – 7.33 (m, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.48 (s, 1H), 6.28 – 6.22 (m, 1H), 6.17 (s, 1H), 6.17 (s, 1H), 4.19 (s, 1H), 3.75 (s, 3H), 2.02 (s, 3H), 1.31 (s, 9H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.2, 155.9, 154.4, 140.5, 137.5, 132.3, 130.8, 126.8, 122.8, 122.3, 121.0, 119.8, 119.7, 117.8, 110.3, 102.7, 83.1, 76.6, 57.7, 51.9, 30.4, 28.8, 28.5, 21.2. **HRMS (ESI)** calculated for C₂₅H₂₈N₃O₃ [M+H]⁺: 418.2131, found 418.2128.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)pent-2-ynamide (**1p**)



Pale yellow solid, Yield 83%, Melting point: 235-237 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.50 (s, 1H), 8.53 (s, 1H), 7.37 (dd, *J* = 8.1, 3.6 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 6.47 (s, 1H), 6.25 (dd, *J* = 8.1, 1.9 Hz, 1H), 6.17 (s, 1H), 6.16 (s, 1H), 3.74 (s, 3H), 2.04 (q, *J* = 7.4 Hz, 2H), 2.02 (s, 3H), 1.31 (s, 9H), 0.71 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.5, 155.9, 155.2, 140.1, 137.5, 132.7, 130.9, 126.8, 123.4, 122.2, 121.0, 119.7, 119.6, 117.5, 110.2, 102.5, 95.2, 79.6, 74.5, 57.4, 51.8, 30.4, 28.8, 28.5, 21.2, 12.9, 11.9. **HRMS (ESI)** calculated for C₂₇H₃₂N₃O₃ [M+H]⁺: 446.2444, found 446.2438.

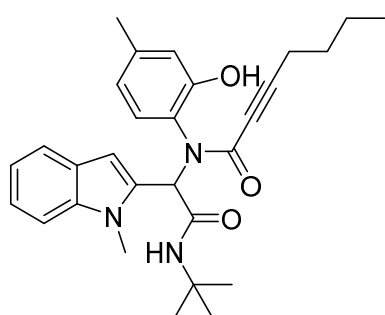
N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)hex-2-ynamide (**1q**)



Pale yellow solid, Yield 88%, Melting point: 203-204 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.50 (s, 1H), 8.53 (s, 1H), 7.44 – 7.26 (m, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 6.46 (s, 1H), 6.24 (dd, *J* = 8.1, 1.9 Hz, 1H), 6.16 (s, 2H), 3.74 (s, 3H), 2.05 (t, *J* = 6.7 Hz, 2H), 2.01 (s, 3H), 1.31 (s, 9H), 1.17 – 0.95 (m, 2H), 0.59 (t, *J* = 7.3 Hz, 3H). **¹³C NMR (151 MHz, DMSO-*d*₆)** δ = 171.5, 156.0, 155.2, 140.1, 137.5, 132.7, 130.9, 126.8, 123.3, 122.2, 121.0, 119.7, 119.6, 117.6, 110.2, 102.5, 93.9, 75.2, 57.4, 51.8, 30.4,

28.5, 21.1, 21.0, 20.1, 13.1. **HRMS (ESI)** calculated for $C_{28}H_{34}N_3O_3$ $[M+H]^+$: 460.2600, found 460.2594.

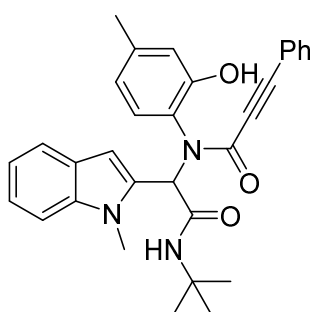
N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)hept-2-ynamide (**1r**)



White solid, Yield 63%, Melting point: 206-207 °C. **1H NMR (400 MHz, DMSO- d_6)** δ = 11.49 (s, 1H), 8.52 (s, 1H), 7.50 – 7.20 (m, 2H), 7.08 (t, J = 7.6 Hz, 1H), 6.91 (t, J = 7.5 Hz, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.47 (s, 1H), 6.24 (dd, J = 8.1, 1.9 Hz, 1H), 6.16 (s, 2H), 3.74 (s, 3H), 2.08 (t, J = 6.4 Hz, 2H), 2.02 (s, 3H), 1.31 (s, 9H), 1.09 – 0.88 (m, 4H), 0.68 (t, J = 7.1

Hz, 3H). **^{13}C NMR (101 MHz, DMSO- d_6)** δ = 171.5, 156.0, 155.2, 140.1, 137.5, 132.7, 130.8, 126.8, 123.3, 122.2, 121.0, 119.7, 119.6, 117.6, 110.2, 102.5, 94.0, 79.7, 75.1, 57.4, 51.8, 30.4, 29.5, 28.5, 21.2, 17.9, 13.8. **HRMS (ESI)** calculated for $C_{29}H_{36}N_3O_3$ $[M+H]^+$: 474.2757, found 474.2745.

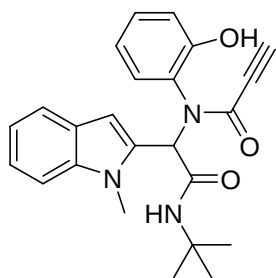
N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)-3-phenylpropiolamide (**1s**)



Yellow solid, Yield 19%, Melting point: 219-220 °C. **1H NMR (600 MHz, DMSO- d_6)** δ = 11.63 (s, 1H), 8.62 (s, 1H), 7.47 – 7.38 (m, 3H), 7.35 (t, J = 7.8 Hz, 2H), 7.11 (t, J = 7.8 Hz, 1H), 7.06 (d, J = 7.6 Hz, 2H), 6.94 (t, J = 7.6 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.55 (s, 1H), 6.34 (d, J = 7.8 Hz, 1H), 6.25 (s, 1H), 6.23 (s, 1H), 3.80 (s, 3H), 2.09 (s, 3H), 1.34 (s, 9H). **^{13}C NMR (151 MHz,**

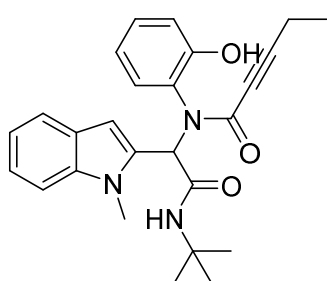
DMSO- d_6) δ = 171.3, 170.8, 156.2, 155.1, 140.6, 137.5, 132.7, 132.5, 132.5, 131.2, 131.1, 129.3, 129.3, 126.8, 123.3, 122.3, 121.0, 119.7, 119.7, 119.7, 117.6, 110.3, 102.6, 90.3, 82.7, 60.2, 57.5, 51.9, 30.5, 28.8, 28.5, 21.2, 21.2, 14.6. **HRMS (ESI)** calculated for $C_{31}H_{32}N_3O_3$ $[M+H]^+$: 494.2444, found 494.2439.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxyphenyl)propiolamide (**1t**)



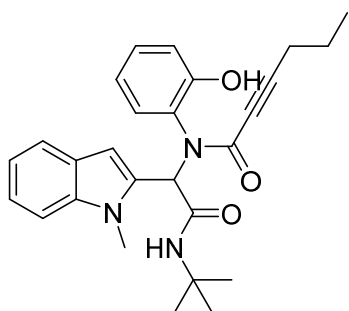
Pale yellow solid, Yield 33%, Melting point: 221-223 °C. **¹H NMR (300 MHz, DMSO-*d*₆)** δ = 11.65 (s, 1H), 8.64 (s, 1H), 7.50 – 7.25 (m, 2H), 7.10 (t, *J* = 7.9 Hz, 1H), 6.94 (q, *J* = 7.9, 7.4 Hz, 3H), 6.68 (d, *J* = 8.2 Hz, 1H), 6.46 (t, *J* = 7.8 Hz, 1H), 6.22 (s, 2H), 4.22 (s, 1H), 3.78 (s, 3H), 1.34 (s, 9H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ = 170.6, 155.8, 153.7, 137.0, 131.6, 130.7, 130.5, 126.2, 124.9, 121.8, 119.2, 118.4, 116.8, 109.7, 102.2, 76.1, 76.0, 57.2, 51.4, 50.5, 29.9, 27.9. **HRMS (ESI)** calculated for C₂₄H₂₆N₃O₃ [M+H]⁺: 404.1974, found 404.1962.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxyphenyl)pent-2-ynamide (**1u**)



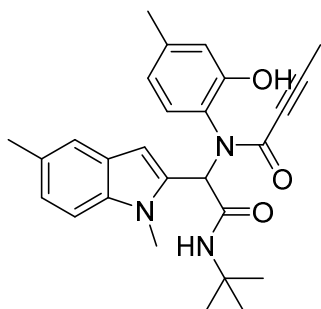
Pale yellow solid, Yield 90%, Melting point: 180-181 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.61 (s, 1H), 8.56 (s, 1H), 7.35 (d, *J* = 8.8 Hz, 2H), 7.11 – 7.01 (m, 1H), 6.96 – 6.81 (m, 3H), 6.64 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.42 (td, *J* = 7.6, 1.5 Hz, 1H), 6.18 (s, 1H), 6.17 (s, 1H), 3.75 (s, 3H), 2.03 (q, *J* = 7.4 Hz, 2H), 1.31 (s, 9H), 0.70 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ = 171.4, 156.3, 155.0, 137.5, 132.5, 131.2, 130.6, 126.8, 125.9, 122.2, 120.9, 119.7, 118.7, 117.1, 110.2, 102.6, 95.3, 74.4, 57.5, 51.8, 30.4, 28.8, 28.5, 12.9, 11.8. **HRMS (ESI)** calculated for C₂₆H₃₀N₃O₃ [M+H]⁺: 432.2287, found 432.2297.

N-(2-(*tert*-butylamino)-1-(1-methyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxyphenyl)hex-2-ynamide (**1v**)



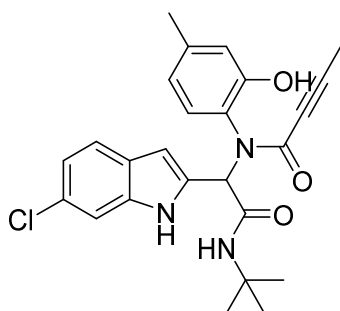
Pale yellow solid, Yield 61%, Melting point: 185-187 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.60 (s, 1H), 8.56 (s, 1H), 7.35 (d, *J* = 8.7 Hz, 2H), 7.13 – 7.02 (m, 1H), 6.96 – 6.76 (m, 3H), 6.64 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.42 (td, *J* = 7.6, 1.5 Hz, 1H), 6.18 (s, 1H), 6.17 (s, 1H), 3.75 (s, 3H), 2.04 (t, *J* = 6.7 Hz, 2H), 1.31 (s, 9H), 1.15 – 1.01 (m, 2H), 0.60 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ = 171.4, 156.3, 155.0, 137.4, 132.5, 131.2, 130.6, 126.8, 125.9, 122.2, 120.9, 119.7, 118.7, 117.1, 110.2, 102.6, 94.0, 79.6, 75.2, 57.5, 51.8, 30.4, 28.5, 21.0, 20.1, 13.3. **HRMS (ESI)** calculated for C₂₇H₃₂N₃O₃ [M+H]⁺: 446.2444, found 446.2454.

N-(2-(*tert*-butylamino)-1-(1,5-dimethyl-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1w**)



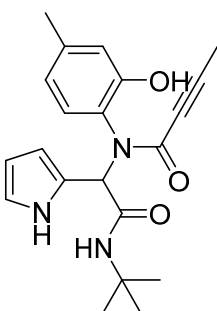
Pale yellow solid, Yield 70%, Melting point: 177-179 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ = 11.50 (s, 1H), 8.50 (s, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.14 (s, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 6.46 (s, 1H), 6.24 (d, *J* = 7.8 Hz, 1H), 6.12 (s, 1H), 6.06 (s, 1H), 3.70 (s, 3H), 2.27 (s, 3H), 2.02 (s, 3H), 1.69 (s, 3H), 1.30 (s, 9H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ = 171.5, 155.8, 155.2, 140.0, 136.0, 132.5, 130.8, 128.2, 127.0, 123.8, 123.2, 120.5, 119.6, 117.6, 109.9, 102.0, 90.4, 79.7, 74.2, 57.6, 51.8, 30.4, 28.5, 21.4, 21.2, 3.7. HRMS (ESI) calculated for C₂₇H₃₂N₃O₃ [M+H]⁺: 446.2444, found 446.2444.

N-(2-(*tert*-butylamino)-1-(6-chloro-1*H*-indol-2-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1x**)



Pale yellow solid, Yield 25%, Melting point: 175-176 °C. ¹H NMR (400 MHz, CDCl₃) δ = 10.48 (s, 1H), 9.77 (s, 1H), 7.50 (d, *J* = 8.5 Hz, 1H), 7.43 (s, 1H), 7.12 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.88 (s, 1H), 6.73 (d, *J* = 7.9 Hz, 1H), 6.56 (dd, *J* = 8.2, 1.7 Hz, 1H), 6.46 – 6.43 (m, 1H), 5.51 (s, 1H), 4.86 (s, 1H), 2.32 (s, 3H), 1.75 (s, 3H), 1.30 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ = 168.3, 157.3, 153.8, 141.4, 137.3, 132.2, 129.3, 128.9, 126.6, 125.6, 121.7, 121.2, 120.3, 118.6, 111.8, 106.1, 92.3, 73.1, 65.4, 52.8, 28.4, 28.3, 21.4, 4.1. HRMS (ESI) calculated for C₂₅H₂₇ClN₃O₃ [M+H]⁺: 452.1741, found 452.1728.

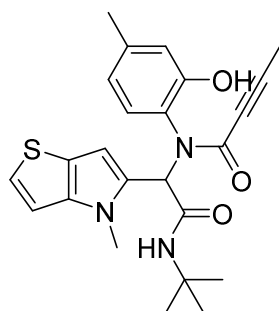
N-(2-(*tert*-butylamino)-2-oxo-1-(1*H*-pyrrol-2-yl)ethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1ba**)



Yellow solid, Yield 47%, Melting point: 162-174 °C. ¹H NMR (600 MHz, CDCl₃) δ = 10.62 (s, 1H), 9.76 (s, 1H), 6.88 – 6.82 (m, 2H), 6.79 (d, *J* = 7.9 Hz, 1H), 6.57 (d, *J* = 7.4 Hz, 1H), 6.15 (q, *J* = 2.9 Hz, 1H), 6.13 (s, 1H), 5.44 (s, 1H), 4.70 (s, 1H), 2.31 (s, 3H), 1.74 (s, 3H), 1.29 (s, 9H). ¹³C NMR (151 MHz, CDCl₃) δ = 169.6, 156.9, 153.9, 141.0, 128.9, 126.9,

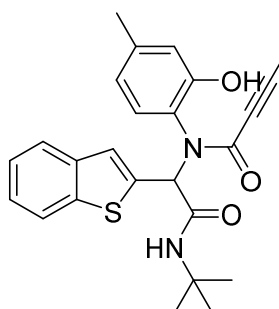
124.6, 120.4, 120.1, 118.5, 117.8, 111.9, 108.6, 108.1, 91.4, 73.3, 65.0, 52.4, 28.4, 28.4, 21.4, 4.0. **HRMS (ESI)** calculated for $C_{21}H_{26}N_3O_3^+$ ($[M+H]^+$): 368.1974, found 368.1966.

N-(2-(*tert*-butylamino)-1-(4-methyl-4*H*-thieno[3,2-*b*]pyrrol-5-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1bb**)



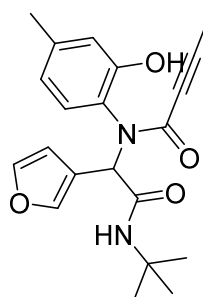
Pale yellow solid, Yield 50%, Melting point: 194-196 °C. **¹H NMR (600 MHz, CDCl₃)** δ = 10.68 (s, 1H), 7.09 (d, J = 5.3 Hz, 1H), 6.84 (d, J = 5.6 Hz, 1H), 6.71 (s, 1H), 6.40 (s, 1H), 6.27 (s, 1H), 6.26 (s, 1H), 6.17 (d, J = 8.0 Hz, 1H), 5.84 (s, 1H), 3.69 – 3.36 (m, 3H), 2.17 (s, 3H), 1.69 (s, 3H), 1.36 (s, 9H). **¹³C NMR (151 MHz, CDCl₃)** δ = 170.1, 156.1, 155.5, 140.7, 129.9, 128.8, 124.6, 122.6, 122.0, 120.0, 118.5, 118.3, 109.9, 103.9, 90.6, 73.2, 57.5, 52.8, 32.2, 28.4, 21.3, 4.0. **HRMS (ESI)** calculated for $C_{24}H_{28}N_3O_3S$ $[M+H]^+$: 438.1851, found 438.1855.

N-(1-(benzo[*b*]thiophen-2-yl)-2-(*tert*-butylamino)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1bc**)



Pale yellow solid, Yield 75%, Melting point: 182-185 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.20 (s, 1H), 8.64 (s, 1H), 7.87 – 7.66 (m, 2H), 7.37 – 7.17 (m, 3H), 6.74 (d, J = 7.9 Hz, 1H), 6.56 (s, 1H), 6.29 (d, J = 7.8 Hz, 1H), 6.17 (s, 1H), 2.07 (s, 3H), 1.69 (s, 3H), 1.28 (s, 9H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ = 171.2, 156.0, 155.0, 140.5, 140.1, 138.9, 136.7, 132.5, 126.9, 125.2, 124.8, 124.4, 122.9, 122.8, 122.6, 119.7, 117.5, 90.2, 79.6, 74.2, 61.0, 51.8, 51.0, 28.8, 28.5, 21.3, 3.7. **HRMS (ESI)** calculated for $C_{25}H_{27}N_2O_3S$ $[M+H]^+$: 435.1742, found 435.1730.

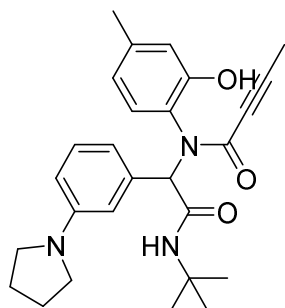
N-(2-(*tert*-butylamino)-1-(furan-3-yl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**1bd**)



Pale yellow solid, Yield 37%, Melting point: 167-168 °C. **¹H NMR (400 MHz, DMSO-*d*₆)** δ = 11.27 (s, 1H), 8.46 (s, 1H), 7.44 (s, 1H), 7.39 (s, 1H), 6.74 (d, J = 7.9 Hz, 1H), 6.57 (d, J = 1.8 Hz, 1H), 6.42 (dd, J = 8.0, 1.9 Hz, 1H), 6.09 (d, J = 1.7 Hz, 1H), 5.74 (s, 1H), 2.16 (s, 3H), 1.70 (s, 3H), 1.27 (s, 9H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ = 172.2, 155.7, 154.9, 143.9, 142.9, 139.9, 132.6, 123.4, 119.7, 118.9, 117.5, 111.1, 89.9, 79.6, 74.4, 57.2, 51.6,

28.5, 21.3, 3.7. **HRMS (ESI)** calculated for $C_{21}H_{25}N_2O_4$ $[M+H]^+$: 369.1814, found 369.1816.

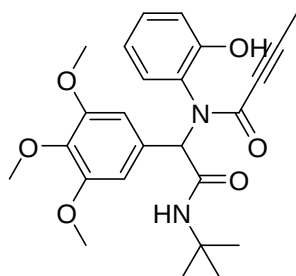
N-(2-(*tert*-butylamino)-2-oxo-1-(3-(pyrrolidin-1-yl)phenyl)ethyl)-*N*-(2-hydroxy-4-methylphenyl) but-2-ynamide (**1be**)



Pale yellow solid, Yield 57%, Melting point: 166-168 °C. **1H NMR (600 MHz, DMSO- d_6)** δ = 11.43 (s, 1H), 8.41 (s, 1H), 6.90 (t, J = 7.8 Hz, 1H), 6.54 (d, J = 8.0 Hz, 1H), 6.49 (s, 1H), 6.36 – 6.22 (m, 4H), 5.75 (s, 1H), 3.07 (s, 4H), 2.09 (s, 3H), 1.94 – 1.80 (m, 4H), 1.67 (s, 3H), 1.27 (s, 9H). **^{13}C NMR (151 MHz, DMSO- d_6)** δ = 172.7, 156.0, 155.1, 147.8, 139.5, 134.4, 132.7, 129.1, 123.4, 119.4, 117.3, 117.0, 113.6, 112.0, 89.6, 79.6, 74.5, 65.5, 51.6, 47.6, 47.6, 28.6, 25.3, 21.3, 3.7.

HRMS (ESI) calculated for $C_{27}H_{34}N_3O_3$ $[M+H]^+$: 448.2600, found 448.2595.

N-(2-(*tert*-butylamino)-2-oxo-1-(3,4,5-trimethoxyphenyl)ethyl)-*N*-(2-hydroxyphenyl)but-2-ynamide (**1bf**)



Pale yellow solid, Yield 68%, Melting point: 155-157 °C. **1H NMR (400 MHz, DMSO- d_6)** δ = 11.44 (s, 1H), 8.54 (s, 1H), 7.01 (t, J = 7.6 Hz, 1H), 6.76 (d, J = 7.7 Hz, 1H), 6.70 (d, J = 8.0 Hz, 1H), 6.53 – 6.42 (m, 3H), 5.78 (s, 1H), 3.60 (s, 6H), 3.52 (s, 3H), 1.67 (s, 3H), 1.30 (s, 9H). **^{13}C NMR (151 MHz, DMSO- d_6)** δ = 172.2, 170.8, 156.2, 154.8, 152.7, 152.7, 137.8, 133.1, 130.3, 129.3, 125.9, 118.6,

116.7, 107.8, 89.7, 74.4, 65.3, 60.4, 60.2, 56.2, 56.1, 51.7, 28.9, 28.5, 28.5, 21.2, 14.6, 3.6.

HRMS (ESI) calculated for $C_{25}H_{31}N_2O_6$ $[M+H]^+$: 455.2182, found 455.2179.

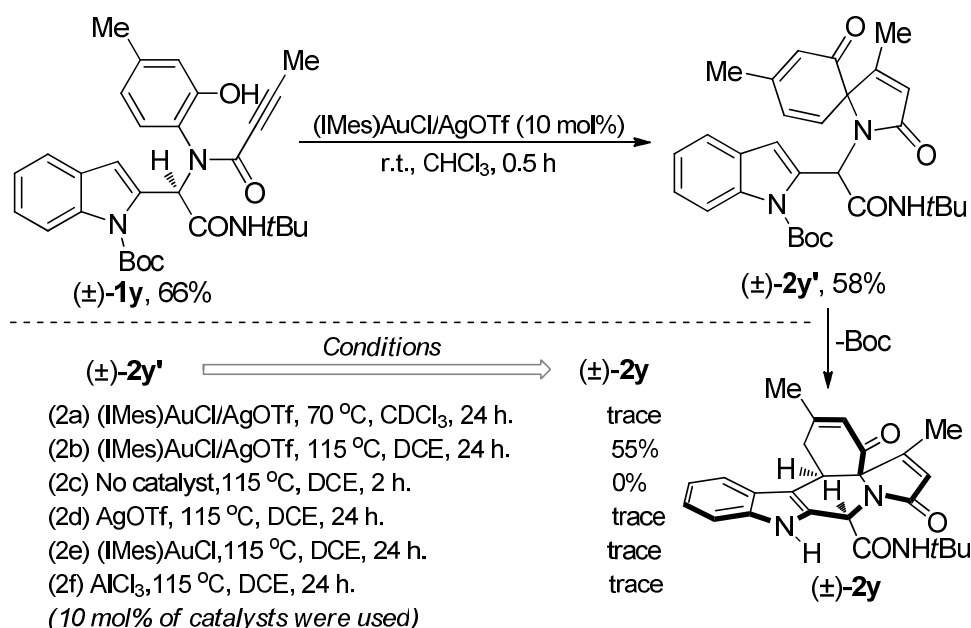
Capture of spirocarbocyclic intermediates and their further reactions

1) Synthesis of spiro intermediate **2y'**.

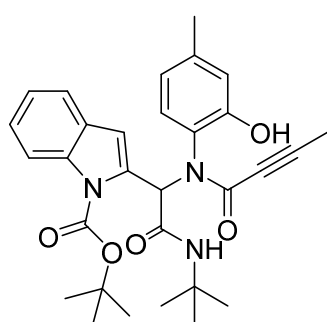
To a glass vial (IMes)AuCl (10 mol%) and AgOTf (10 mol%) were loaded along with chloroform (2 mL) to stir for 1 minute to generate cationic gold catalyst *in situ* without filtration. Ugi products **1y** (100mg, 0.19 mmol) was added and reaction mixture was stirred at room temperature in a screw capped vial for 0.5h. After completion, the reaction mixture was diluted with dichloromethane and evaporated under reduced pressure. The residue obtained was purified by silica gel column chromatography (EtOAc/Heptane = 1: 2) to afford the dearomative spiro intermediate **2y'** in 58% yield (58mg, 0.11 mmol).

2) Transformation of spirocarbocyclic Indole 2y'.

To a glass vial (IMes)AuCl (10 mol%) and AgOTf (10 mol%) were loaded along with chloroform (2 mL) to stir for 1 minute to generate cationic gold catalyst *in situ* without filtration. the dearomative spiro intermediate **2y'** (40mg, 0.075 mmol) was added and reaction mixture was stirred at 115°C in a screw capped vial for 24h. After completion, the reaction mixture was diluted with dichloromethane and evaporated under reduced pressure. The residue obtained was purified by silica gel column chromatography (EtOAc/Heptane = 1: 2) to afford the Boc deprotected **2y** in 55% yield (20mg, 0.04 mmol).



tert-butyl 2-(2-(*tert*-butylamino)-1-(*N*-(2-hydroxy-4-methylphenyl)but-2-ynamido)-2-oxoethyl)-1*H*-indole-1-carboxylate (**1y**)

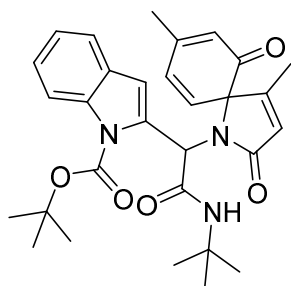


Yellow solid, Yield 66%, Melting point: 205-207 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ = 11.57 (s, 1H), 8.64 (s, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.31 – 7.20 (m, 1H), 7.13 (t, *J* = 7.4 Hz, 1H), 6.81 (d, *J* = 7.9 Hz, 1H), 6.48 (s, 1H), 6.47 (s, 1H), 6.44 (s, 1H), 6.37 – 6.25 (m, 1H), 2.03 (s, 3H), 1.72 (s, 9H), 1.71 (s, 3H), 1.32 (s, 9H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ =

171.7, 155.9, 154.8, 149.9, 140.2, 136.2, 133.4, 130.4, 128.1, 125.3, 123.4, 123.3, 121.5, 119.6, 117.6, 115.9, 111.4, 90.2, 85.4, 74.2, 60.2, 60.1, 51.8, 28.5, 28.3, 21.2, 21.2, 14.6, 3.7.

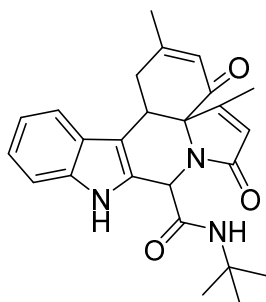
HRMS (ESI) calculated for C₃₀H₃₆N₃O₅ [M+H]⁺: 518.2655, found 518.2665.

tert-butyl 2-(2-(*tert*-butylamino)-1-(4,8-dimethyl-2,10-dioxo-1-azaspiro[4.5]deca-3,6,8-trien-1-yl)-2-oxoethyl)-1*H*-indole-1-carboxylate (**2y'**)



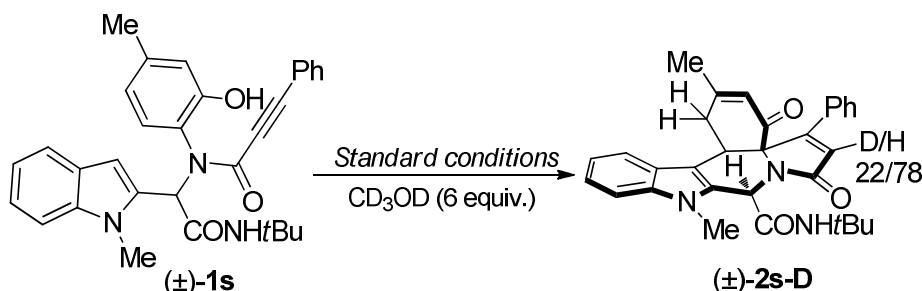
Yellow solid, Yield 58%, Melting point: 161-162 °C. ¹H NMR (400 MHz, CDCl₃) δ = 8.06 (d, *J* = 8.4 Hz, 1H), 7.98 (s, 1H), 7.36 (d, *J* = 7.7 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 6.32 (s, 1H), 6.27 (s, 1H), 6.07 (q, *J* = 1.6 Hz, 1H), 5.87 (s, 1H), 5.71 (d, *J* = 9.5 Hz, 1H), 5.46 (dd, *J* = 9.5, 1.4 Hz, 1H), 1.66 (s, 9H), 1.65 (s, 3H), 1.48 (s, 9H), 1.37 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ = 196.4, 171.5, 167.6, 157.0, 156.8, 149.7, 137.9, 135.9, 134.9, 128.1, 126.2, 125.3, 124.7, 124.2, 123.1, 121.0, 116.2, 113.3, 85.2, 56.7, 51.4, 34.1, 28.6, 28.4, 28.4, 28.3, 22.4, 22.3, 14.1, 12.1. HRMS (ESI) calculated for C₃₀H₃₆N₃O₅ [M+H]⁺: 518.2655, found 518.2659.

tert-butyl 9-(*tert*-butylcarbamoyl)-2,5-dimethyl-4,7-dioxo-1,7,9,14c-tetrahydroindolo[2,3-*c*]pyrrolo[2,1-*j*]quinoline-10(4*H*)-carboxylate (**2y**)



Yellow solid, Yield 55%, Melting point: 175-177 °C. ¹H NMR (300 MHz, CDCl₃) δ = 9.44 (s, 1H), 7.75 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.17 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.08 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 6.07 (q, *J* = 1.5 Hz, 1H), 5.97 (q, *J* = 2.5, 1.4 Hz, 1H), 5.53 (d, *J* = 2.2 Hz, 1H), 3.87 – 3.67 (m, 2H), 3.37 – 3.19 (m, 1H), 2.24 (d, *J* = 1.5 Hz, 3H), 2.10 (t, *J* = 1.2 Hz, 3H), 1.39 (s, 9H). ¹³C NMR (151 MHz, CDCl₃) δ = 193.0, 171.8, 167.2, 161.8, 159.2, 137.0, 130.3, 126.5, 125.3, 124.6, 122.0, 119.8, 119.2, 112.1, 106.1, 74.8, 52.9, 51.5, 39.1, 32.7, 31.9, 29.7, 28.4, 24.6, 22.7, 15.4, 14.1. HRMS (ESI) calculated for C₂₅H₂₈N₃O₃ [M+H]⁺: 418.2131, found 418.2135.

General procedure for the deuterium exchange experiments for compounds **2s**



The cationic gold catalyst (IMes)AuOTf was first generated *in situ* by mixing of (IMes)AuCl (10 mol%) and AgOTf (10 mol%) along with chloroform (2 mL) in a screw-cap vial under

stirring for 5 mins and used without filtration. To this vial with gold catalyst Ugi products **1s** (0.10 mmol) and 6 equivalents of methanol- d_4 were subsequently added. After stirring at 70 °C for 2 h, the reaction mixture was diluted with dichloromethane and evaporated under reduced pressure. The obtained residue was purified by silica gel column chromatography (EtOAc/Heptane = 1: 2) to afford the fused indole alkaloid mimics **2s-D**.

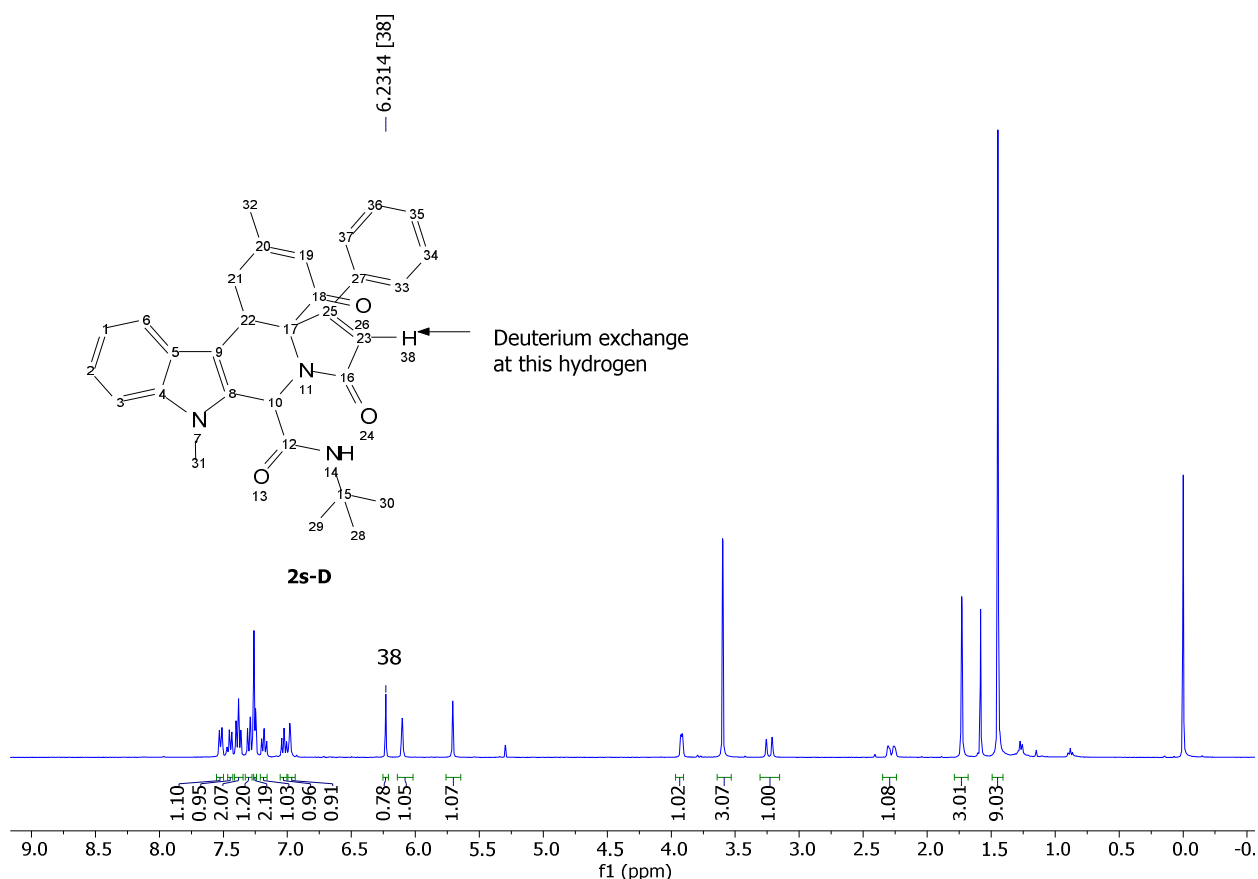
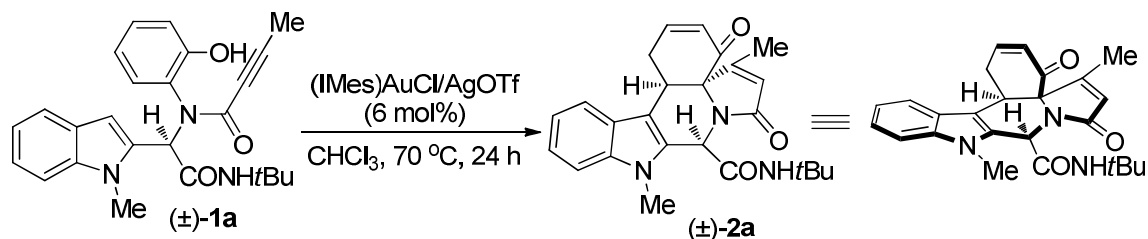


Figure S1. ^1H NMR spectra of compound **2s-D**

Scale-up synthesis of heterocycles **2a**

1) Scale-up synthesis of heterocycles **2a**

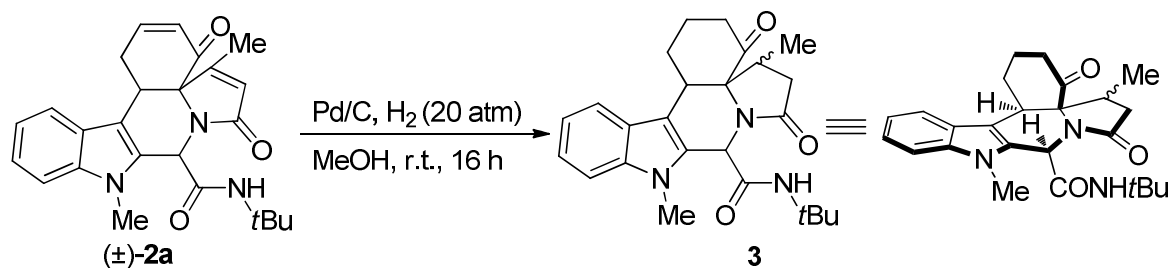


To a glass vial (IMes)AuCl (6 mol%) and AgOTf (6 mol%) were loaded along with chloroform (6 mL) to stir for 1 minute to generate cationic gold catalyst *in situ* without filtration. Ugi products **1a** (0.8g, 1.90 mmol) was added and reaction mixture was stirred at 70 °C in a screw capped vial for 24h. After completion, the reaction mixture was diluted

with dichloromethane and evaporated under reduced pressure. The residue obtained was purified by silica gel column chromatography (EtOAc/Heptane = 1: 1) to afford the fused indole alkaloid mimic **2a** in 53% yield (0.42 g, 0.99 mmol).

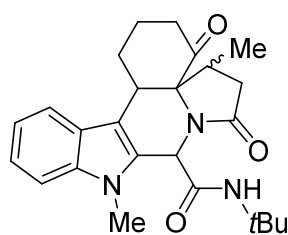
Transformations of heterocycles **2a**

1) Synthesis of compound **3**



A 10 mL stainless autoclave equipped with a magnetic stirring bar was charged with **2a** (50 mg, 0.120 mmol), MeOH (1.0 mL) and 20% mol Pd/C (5 wt. %, 51 mg), and then hydrogen gas (20 atm) was introduced. After the mixture was stirred at room temperature for 16 h, the mixture was filtered and the filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/Heptane = 3: 1) to afford compound **3** (49 mg, 98 % yield).

N-(*tert*-butyl)-5,10-dimethyl-4,7-dioxo-1,2,3,4,5,6,7,9,10,14c-decahydroindolo[2,3-*c*]pyrrolo[2,1-*j*]quinoline-9-carboxamide **3**



White solid, Yield 98% (d.r. = 10: 1), Melting point: 191-193 °C.

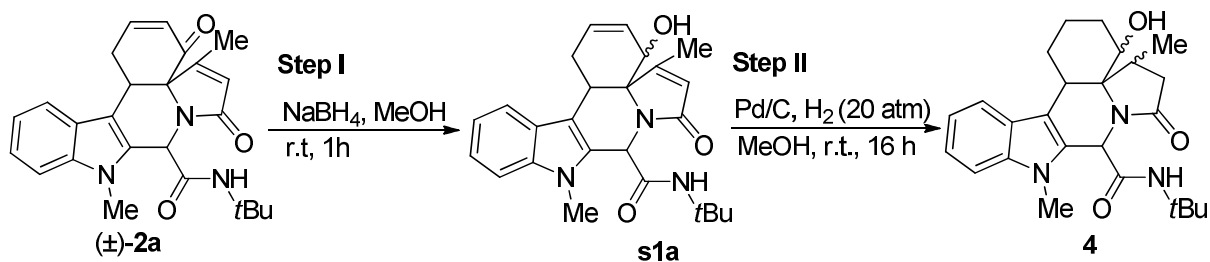
The NMR data of major diastereomer is as follows: **¹H NMR (400 MHz, CDCl₃)** δ = 7.64 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.12 – 6.99 (m, 2H), 5.58 (s, 1H), 3.73 (t, *J* = 3.5 Hz, 1H), 3.56 (s, 3H), 2.97 (dt, *J* = 14.3, 3.2 Hz, 1H), 2.69 –

2.54 (m, 3H), 2.35 – 2.15 (m, 3H), 1.82 – 1.69 (m, 2H), 1.41 (s, 9H), 1.25 (d, *J* = 6.4 Hz, 3H).

¹³C NMR (151 MHz, CDCl₃) δ = 207.4, 175.7, 166.0, 138.4, 131.2, 124.7, 121.7, 119.3, 119.2, 109.4, 108.3, 72.5, 52.2, 51.4, 43.8, 41.4, 40.6, 38.2, 29.9, 28.6, 26.2, 18.8, 17.9.

HRMS (ESI) calculated for C₂₅H₃₂N₃O₃ [M+H]⁺: 422.2444, found 422.2446.

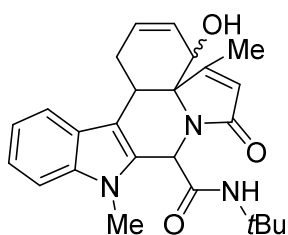
2) Synthesis of compound **4**



Step I: To a glass vial of **2a** (100 mg, 0.240 mmol) in MeOH (2 mL) was slowly added NaBH_4 (54.4 mg, 1.437 mmol) at r.t. and the resulting mixture was stirred for 1 h at room temperature. After completion, the mixture was diluted with H_2O (20 mL) and extracted with EtOAc (4×15 mL). The combined organic layer was washed with brine (15 mL), dried over anhyd Na_2SO_4 and concd under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/Heptane = 2: 1) to afford compound **s1a** (94.5mg, 95 % yield).

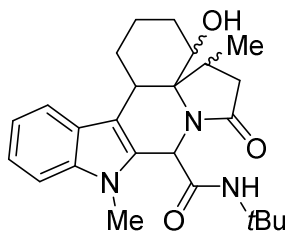
Step II: To a 10 mL stainless autoclave equipped with a magnetic stirring bar were added **s1a** (30 mg, 0.072 mmol), MeOH (1.0 mL) and 20% mol Pd/C (5 wt. %, 31.50 mg). Then hydrogen gas (20 atm) was introduced. The mixture was stirred at room temperature for 16 h. After completion, the mixture was filtered and the filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/Heptane = 2: 1) to afford compound **4** (28 mg, 95 % yield).

N-(*tert*-butyl)-4-hydroxy-5,10-dimethyl-7-oxo-3,4,7,9,10,14c-hexahydroindolo[2,3-*c*]pyrrolo[2,1-*j*]quinoline-9-carboxamide **s1a**



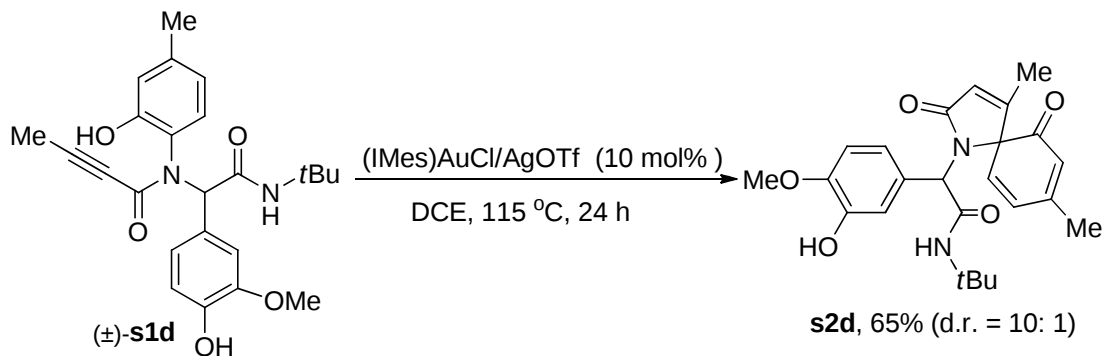
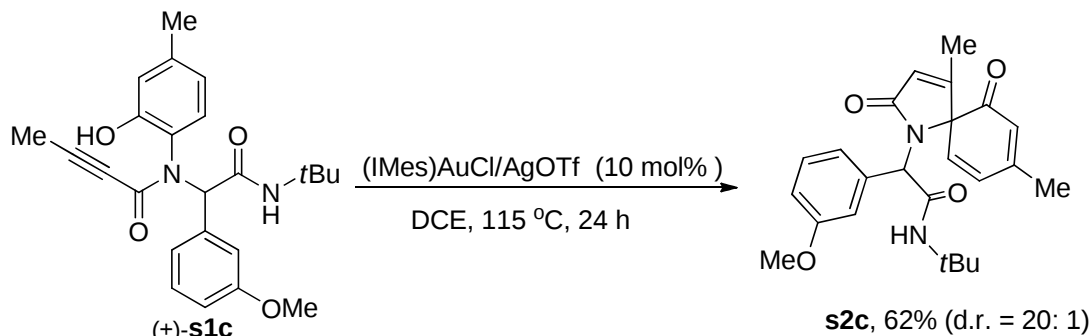
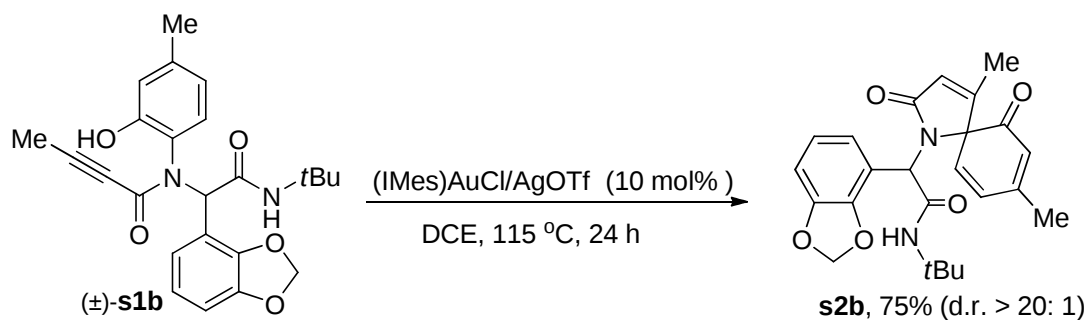
White solid, Yield 98% (d.r. = 9: 1), Melting point: 132-133 °C. The NMR data of major diastereomer is as follows: **^1H NMR (400 MHz, CDCl_3)** δ = 7.61 (d, J = 8.1 Hz, 1H), 7.32 (d, J = 8.3 Hz, 1H), 7.23 (t, J = 7.7 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 7.03 (s, 1H), 6.61 (ddd, J = 10.2, 4.9, 2.3 Hz, 1H), 6.02 (s, 1H), 5.85 – 5.77 (m, 1H), 5.74 (s, 1H), 4.65 – 4.54 (m, 1H), 3.78 (d, J = 5.2 Hz, 1H), 3.65 (s, 3H), 2.59 (dt, J = 18.7, 5.8 Hz, 1H), 2.44 – 2.33 (m, 1H), 2.26 (s, 3H), 1.39 (s, 9H). **^{13}C NMR (101 MHz, CDCl_3)** δ = 170.8, 168.1, 162.8, 138.4, 127.7, 126.6, 126.0, 125.2, 123.8, 122.0, 120.2, 119.5, 111.4, 109.4, 71.1, 65.0, 51.9, 51.5, 39.3, 32.2, 31.9, 30.4, 28.5, 28.5, 22.7, 16.1, 14.1. **HRMS (ESI)** calculated for $\text{C}_{25}\text{H}_{30}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 420.2287, found 420.2279.

N-(*tert*-butyl)-4-hydroxy-5,10-dimethyl-7-oxo-1,2,3,4,5,6,7,9,10,14c-decahydroindolo[2,3-*c*]pyrrolo[2,1-*j*]quinoline-9-carboxamide **4**

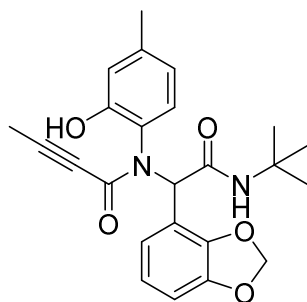


White solid, Yield 95% (d.r. = 9: 1), Melting point: 202-203 °C. The NMR data of major diastereomer is as follows: **¹H NMR (300 MHz, CDCl₃)** δ = 7.67 (d, J = 8.0 Hz, 1H), 7.57 (s, 1H), 7.32 (d, J = 8.2 Hz, 1H), 7.21 (ddd, J = 8.2, 7.0, 1.1 Hz, 3H), 7.07 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 5.66 (d, J = 1.7 Hz, 1H), 4.42 (dt, J = 11.6, 5.4 Hz, 1H), 3.60 (s, 3H), 3.33 (s, 1H), 2.82 (dt, J = 14.4, 2.5 Hz, 1H), 2.62 – 2.46 (m, 3H), 1.81 – 1.65 (m, 2H), 1.57 – 1.44 (m, 2H), 1.38 (s, 9H), 1.35 (s, 3H). **¹³C NMR (151 MHz, CDCl₃)** δ = 175.6, 168.0, 138.2, 129.2, 125.2, 121.5, 119.8, 119.2, 110.0, 109.3, 70.7, 69.0, 68.9, 52.6, 51.6, 51.4, 46.2, 45.9, 41.2, 41.0, 31.1, 31.0, 30.2, 30.1, 28.5, 28.5, 25.1, 24.8, 23.8, 23.8, 22.7, 22.0, 19.8, 19.7, 19.6. **HRMS (ESI)** calculated for C₂₅H₃₄N₃O₃ [M+H]⁺: 424.2600, found 424.2595.

Examples that only form the spirocarbocyclic products

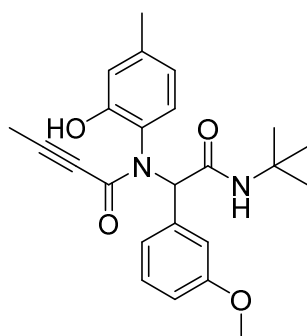


N-(1-(benzo[*d*][1,3]dioxol-4-yl)-2-(*tert*-butylamino)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl) but-2-ynamide (**s1b**)



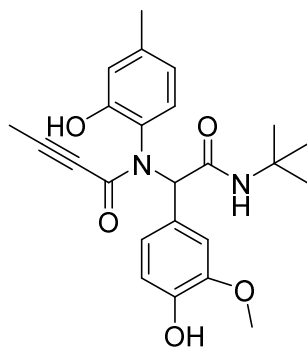
Yellow solid, Yield 55%, Melting point: 181-183 °C. ^1H NMR (400 MHz, DMSO- d_6) δ = 11.30 (s, 1H), 8.45 (s, 1H), 6.70 (d, J = 8.0 Hz, 1H), 6.67 (s, 1H), 6.64 – 6.55 (m, 2H), 6.52 (s, 1H), 6.32 (d, J = 7.8 Hz, 1H), 5.92 (s, 1H), 5.90 (s, 1H), 5.76 (s, 1H), 2.12 (s, 3H), 1.68 (s, 3H), 1.26 (s, 9H). ^{13}C NMR (101 MHz, DMSO- d_6) δ = 172.5, 155.8, 155.0, 147.4, 147.3, 139.7, 132.6, 127.6, 123.7, 123.3, 119.7, 117.3, 110.4, 108.4, 101.5, 89.6, 74.5, 64.7, 51.6, 28.5, 21.3, 3.7. HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{27}\text{N}_2\text{O}_5$ $[\text{M}+\text{H}]^+$: 423.1920, found 423.1926.

N-(2-(*tert*-butylamino)-1-(3-methoxyphenyl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**s1c**)



Pale yellow solid, Yield 69%, Melting point: 201-203 °C. ^1H NMR (600 MHz, DMSO- d_6) δ = 11.34 (s, 1H), 8.48 (s, 1H), 7.05 (t, J = 7.9 Hz, 1H), 6.79 – 6.62 (m, 3H), 6.57 (d, J = 7.9 Hz, 1H), 6.50 (s, 1H), 6.27 (dd, J = 8.0, 2.0 Hz, 1H), 5.81 (s, 1H), 3.62 (s, 3H), 2.09 (s, 3H), 1.68 (s, 3H), 1.27 (s, 9H). ^{13}C NMR (151 MHz, DMSO- d_6) δ = 172.3, 159.2, 155.8, 155.0, 139.7, 135.4, 132.7, 129.6, 123.2, 122.2, 119.5, 117.3, 115.8, 114.5, 89.7, 74.4, 65.0, 55.4, 51.6, 28.9, 28.5, 28.5, 21.3, 3.7. HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{29}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$: 409.2127, found 409.2126.

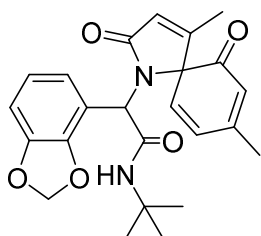
N-(2-(*tert*-butylamino)-1-(4-hydroxy-3-methoxyphenyl)-2-oxoethyl)-*N*-(2-hydroxy-4-methylphenyl)but-2-ynamide (**s1d**)



Pale yellow solid, Yield 89%, Melting point: 133-135 °C. ^1H NMR (600 MHz, DMSO- d_6) δ = 11.38 (s, 1H), 8.97 (s, 1H), 8.41 (s, 1H), 6.66 (s, 1H), 6.56 (d, J = 7.9 Hz, 1H), 6.52 (s, 2H), 6.50 – 6.49 (m, 1H), 6.29 (dd, J = 8.0, 2.0 Hz, 1H), 5.73 (s, 1H), 3.58 (s, 3H), 2.10 (s, 3H), 1.68 (s, 3H), 1.27 (s, 9H). ^{13}C NMR (151 MHz, DMSO- d_6) δ = 172.8, 155.9, 155.0, 147.4, 146.8, 139.5, 132.7, 124.6, 123.5, 122.8, 119.5, 117.2, 115.5, 114.3, 89.5, 79.6, 74.6, 64.9,

55.9, 51.6, 28.6, 21.3, 3.7. **HRMS (ESI)** calculated for $C_{24}H_{29}N_2O_5$ $[M+H]^+$: 425.2076, found 425.2086.

2-(benzo[*d*][1,3]dioxol-4-yl)-*N*-(*tert*-butyl)-2-(4,8-dimethyl-2,10-dioxo-1-azaspiro[4.5]deca-3,6,8-trien-1-yl)acetamide (**s2b**)

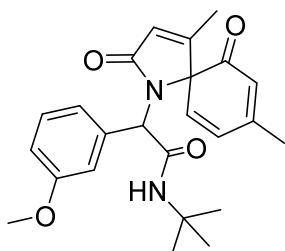


Pale yellow solid, Yield 75% (d.r. > 20: 1), Melting point: 161-163 °C.

1H NMR (400 MHz, $CDCl_3$) δ = 6.94 (s, 1H), 6.87 (s, 1H), 6.73 – 6.64 (m, 2H), 6.28 (d, J = 9.5 Hz, 1H), 6.09 (d, J = 9.5 Hz, 1H), 6.03 (s, 1H), 5.98 (s, 1H), 5.91 (s, 2H), 4.57 (s, 1H), 2.12 (s, 3H), 1.75 (s, 3H), 1.37 (s, 9H). **^{13}C NMR (151 MHz, $CDCl_3$)** δ = 195.5, 171.6,

167.4, 156.1, 155.9, 147.4, 147.3, 139.1, 129.1, 128.9, 124.9, 124.6, 124.1, 110.5, 107.7, 101.1, 77.6, 62.5, 51.4, 28.5, 23.3, 12.3. **HRMS (ESI)** calculated for $C_{24}H_{27}N_2O_5$ $[M+H]^+$: 423.1920, found 423.1930.

N-(*tert*-butyl)-2-(4,8-dimethyl-2,10-dioxo-1-azaspiro[4.5]deca-3,6,8-trien-1-yl)-2-(3-methoxyphenyl)acetamide (**s2c**)

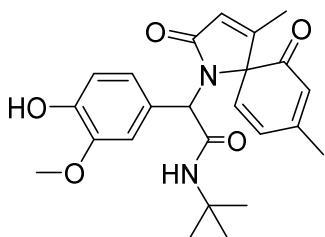


Pale yellow solid, Yield 62% (d.r. = 20: 1), Melting point: 179-181

°C. **1H NMR (600 MHz, $CDCl_3$)** δ = 7.90 (s, 1H), 7.06 (t, J = 7.8 Hz, 1H), 6.83 – 6.75 (m, 2H), 6.65 (s, 1H), 6.04 (s, 1H), 6.01 (s, 1H), 5.62 (d, J = 9.2 Hz, 1H), 5.50 (d, J = 9.5 Hz, 1H), 5.21 (s, 1H), 3.71 (s, 3H), 1.97 (s, 3H), 1.70 (s, 3H), 1.44 (s, 9H). **^{13}C NMR (151**

MHz, $CDCl_3$) δ = 196.2, 172.3, 168.4, 159.3, 157.5, 156.9, 139.4, 136.8, 129.4, 125.6, 124.3, 124.3, 123.1, 115.0, 114.7, 64.1, 55.0, 51.3, 28.5, 23.2, 12.0. **HRMS (ESI)** calculated for $C_{24}H_{29}N_2O_4$ $[M+H]^+$: 409.2127, found 409.2126.

N-(*tert*-butyl)-2-(4,8-dimethyl-2,10-dioxo-1-azaspiro[4.5]deca-3,6,8-trien-1-yl)-2-(4-hydroxy-3-methoxyphenyl)acetamide (**s2d**)



Pale yellow solid, Yield 65% (d.r. = 10: 1), Melting point: 196-198

°C. **1H NMR (600 MHz, $CDCl_3$)** δ = 7.99 (s, 1H), 6.61 – 6.58 (m, 1H), 6.57 – 6.53 (m, 2H), 6.03 (s, 1H), 5.95 (s, 1H), 5.61 (d, J = 9.4 Hz, 1H), 5.46 (d, J = 9.4 Hz, 1H), 5.18 (s, 1H), 3.75 (s, 3H), 1.97 (s, 3H), 1.69 (s, 3H), 1.45 (s, 9H). **^{13}C NMR (151 MHz,**

$CDCl_3$) δ = 196.5, 172.2, 168.9, 158.2, 156.9, 146.9, 146.2, 139.8, 126.9, 125.1, 124.4,

124.2, 124.2, 114.4, 112.1, 63.7, 55.5, 51.3, 28.5, 23.2, 12.0. **HRMS (ESI)** calculated for $C_{24}H_{29}N_2O_5$ $[M+H]^+$: 425.2076, found 425.2082.

Crystallographic data for compound **2o** and **2q**

Single crystals suitable for X-ray diffraction were obtained by slow evaporation at room temperature from a d1-chloroform-heptane mixture (1:2 v/v) for **2o**, and an ethyl acetate and heptane mixture (1:3 v/v) for **2q**. X-ray intensity data were collected at 150K for **2o** and **2q** on a Rigaku Ultra 18S generator (Xenocs mirrors, Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å) using a MAR345 image plate. The images were interpreted and integrated with CrysAlisPRO^[9] and the implemented absorption correction was applied. The structures were solved using Olex2^[10] with the ShelXS^[11] structure solution program by Direct Methods and refined with the ShelXL^[12] refinement package using full-matrix least-squares minimization on F^2 . Non-hydrogen atoms were refined anisotropically and hydrogen atoms in the riding mode with isotropic temperature factors fixed at 1.2 times U_{eq} of the parent atoms (1.5 for methyl groups). CCDC 1858541 (**2o**) and 1858542 (**2q**) contain the supplementary crystallographic data for this paper and can be obtained free of charge via <http://www.ccdc.cam.ac.uk/getstructures> or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44-1223-336033; deposit@ccdc.cam.ac.uk).

Table S2: Crystal data and structure refinement details for compound **2o**

Compound reference	2o
Empirical formula	$C_{25}H_{27}N_3O_3$
Formula weight	417.49
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.69310(18)
b/Å	24.9324(6)
c/Å	9.8261(2)
$\alpha/^\circ$	90
$\beta/^\circ$	90.438(2)
$\gamma/^\circ$	90
Volume/Å ³	2129.64(8)
Temperature/K	150(2)
Z	4
ρ_{calc}/cm^3	1.302
Crystal size/mm ³	$0.40 \times 0.35 \times 0.22$

Radiation	MoK α (λ = 0.71073 Å)
Absorption coefficient/mm ⁻¹	0.087
<i>F</i> (000)	888.0
Reflections collected	14631
Independent reflections	3992 [<i>R</i> _{int} = 0.0250, <i>R</i> _{sigma} = 0.0185]
Data/restraints/parameters	3992/0/285
Final <i>R</i> indexes [<i>I</i> ≥ 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0396, <i>wR</i> ₂ = 0.0970
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0419, <i>wR</i> ₂ = 0.0986
Goodness-of-fit	1.084
Largest diff. peak/hole	0.27/-0.25 e.Å ⁻³
CCDC	1858541

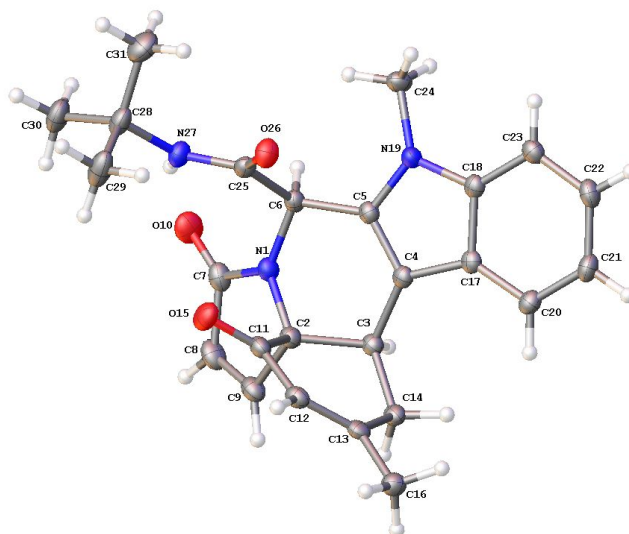


Figure S2. Crystal structure of compound **2o**. Thermal ellipsoids are drawn at the 50% probability level.

Table S3: Crystal data and structure refinement details for compound 2q

Compound reference	2q
Empirical formula	C ₂₈ H ₃₃ N ₃ O ₃
Formula weight	459.57
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> /Å	9.2977(8)
<i>b</i> /Å	9.9446(11)
<i>c</i> /Å	13.8192(11)
α /°	83.641(8)
β /°	73.868(7)
γ /°	74.132(9)
Volume/Å ³	1179.8(2)
Temperature/K	150(2)
<i>Z</i>	2
ρ _{calc} /cm ³	1.294
Crystal size/mm ³	0.50 × 0.35 × 0.25

Radiation	MoK α (λ = 0.71073 Å)
Absorption coefficient/mm ⁻¹	0.085
<i>F</i> (000)	492.0
Reflections collected	17279
Independent reflections	4450 [<i>R</i> _{int} = 0.0264, <i>R</i> _{sigma} = 0.0194]
Data/restraints/parameters	4450/0/313
Final <i>R</i> indexes [<i>I</i> ≥ 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0380, <i>wR</i> ₂ = 0.0927
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0401, <i>wR</i> ₂ = 0.0943
Goodness-of-fit	1.061
Largest diff. peak/hole	0.32/-0.19 e.Å ⁻³
CCDC	1858542

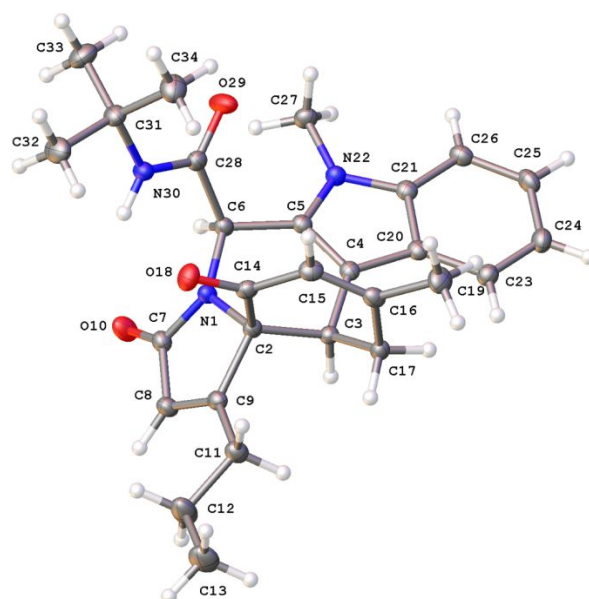


Figure S3. Crystal structure of compound **2q**. Thermal ellipsoids are drawn at the 50% probability level.

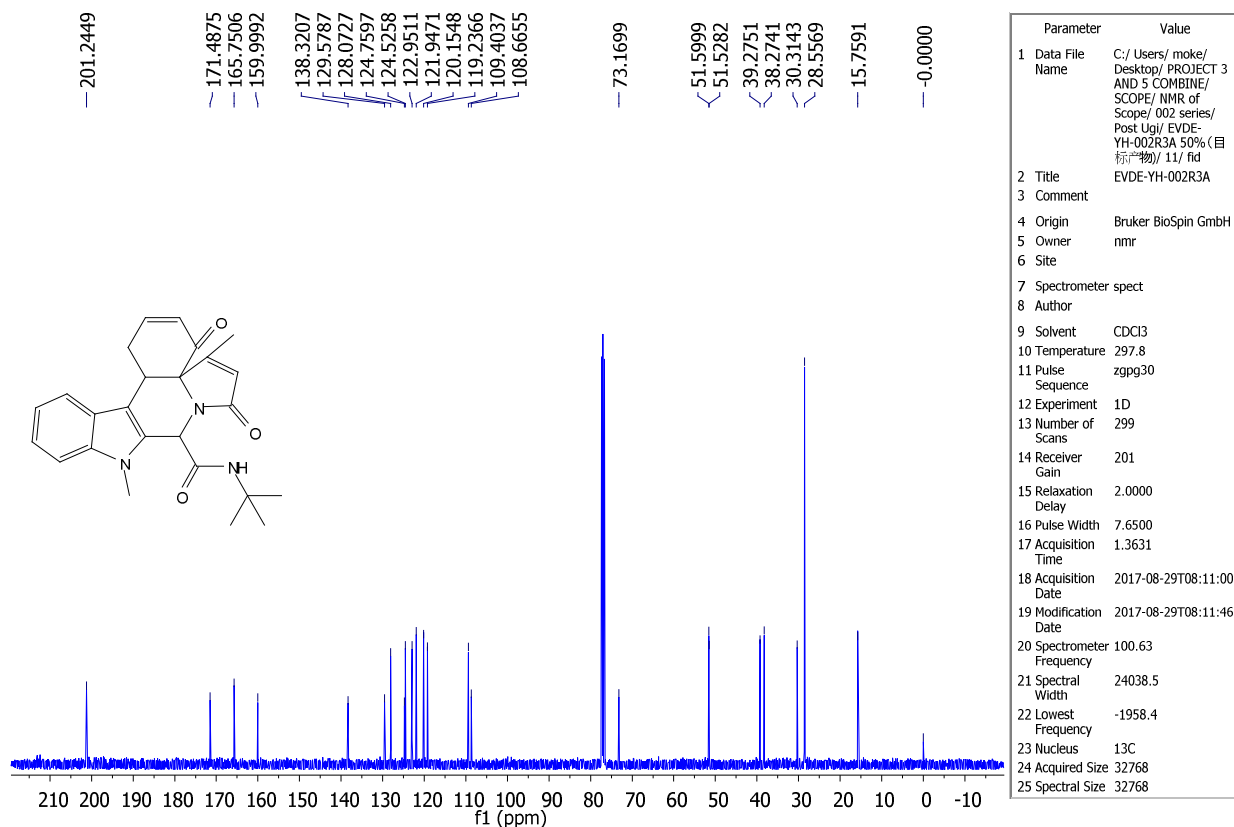
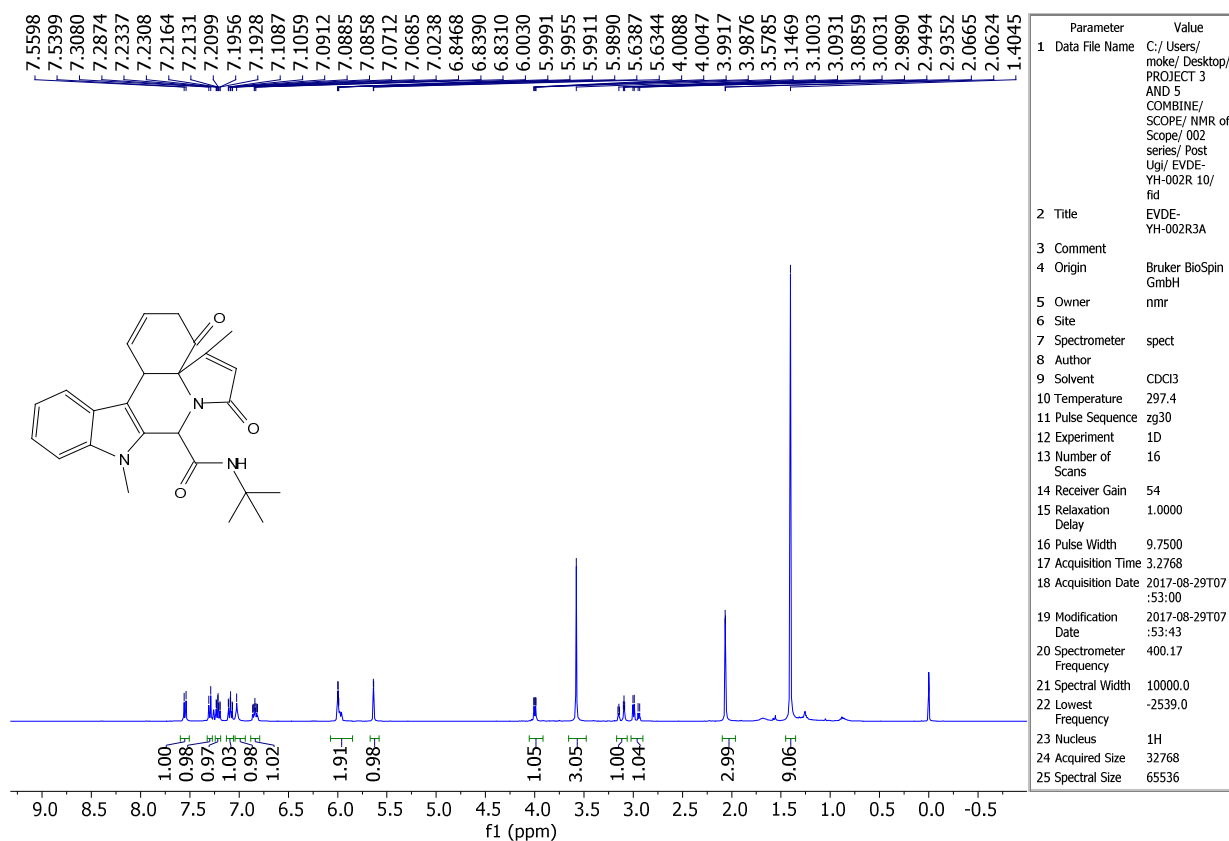
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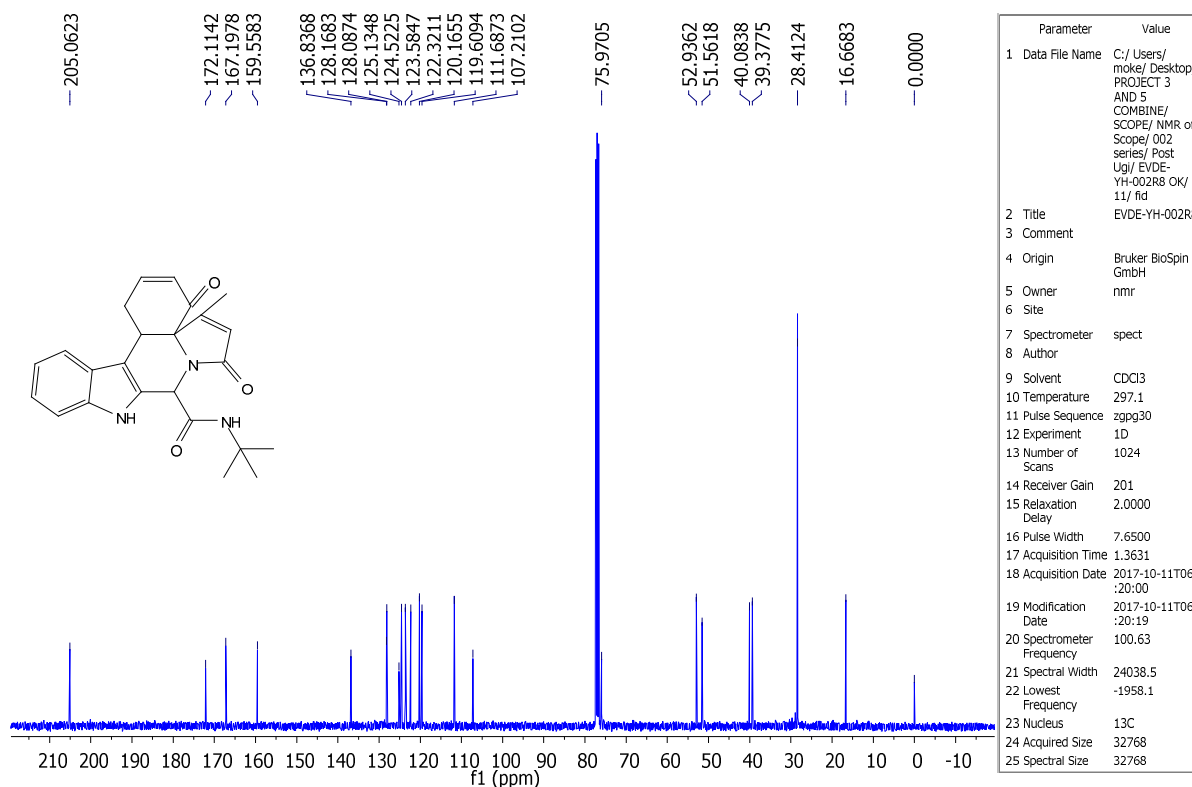
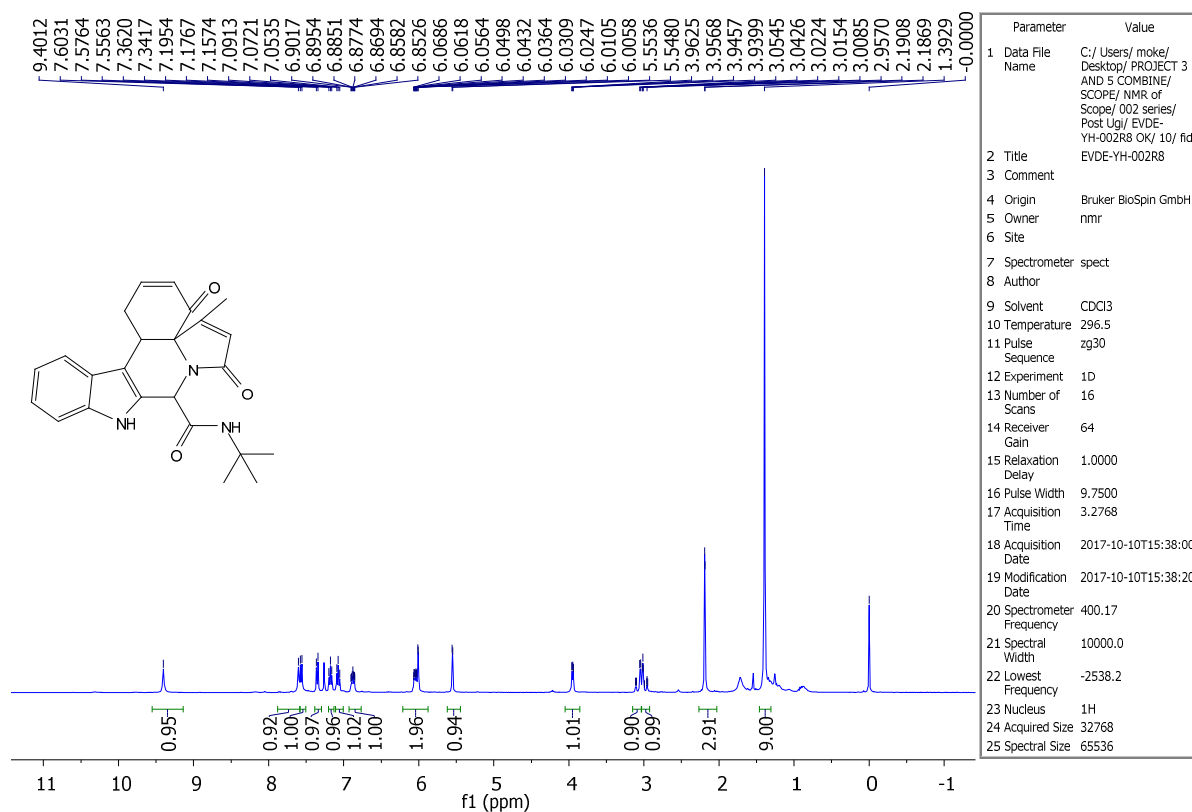
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Copies of NMR spectra (Post-Ugi products)

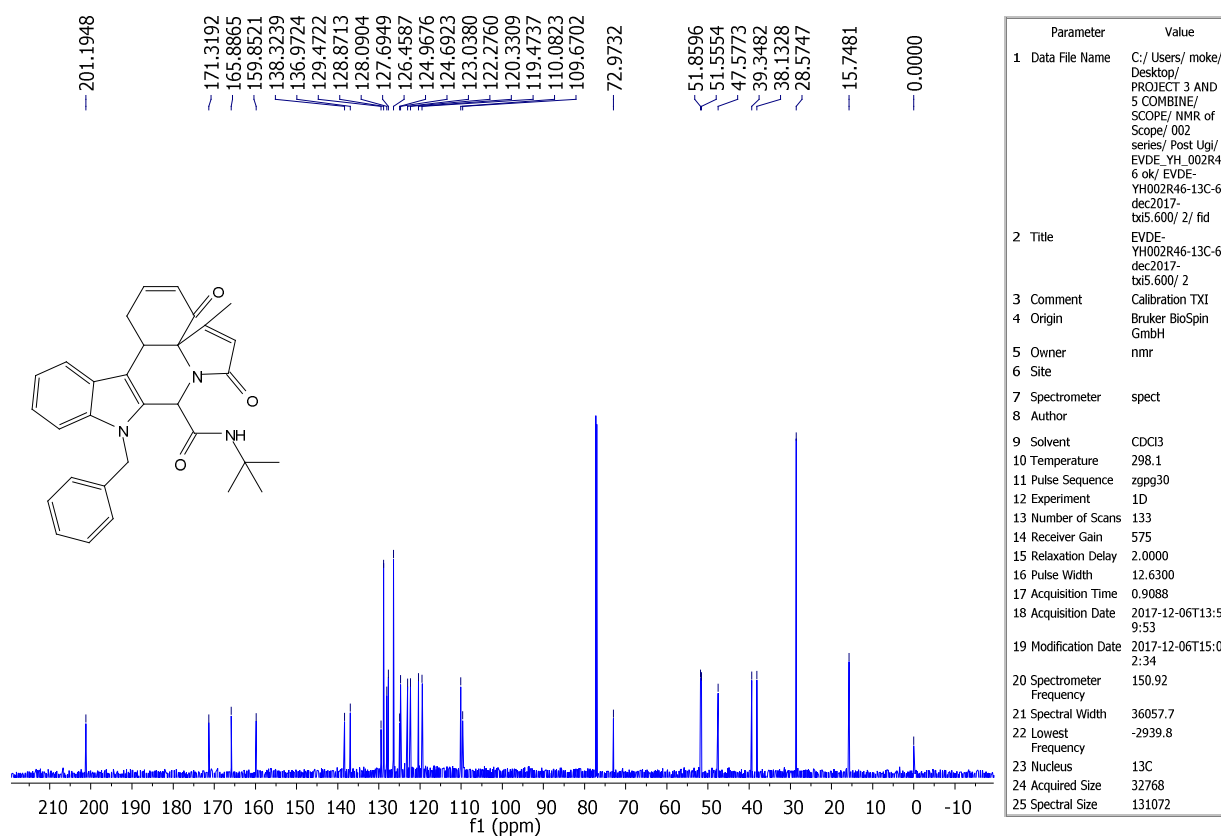
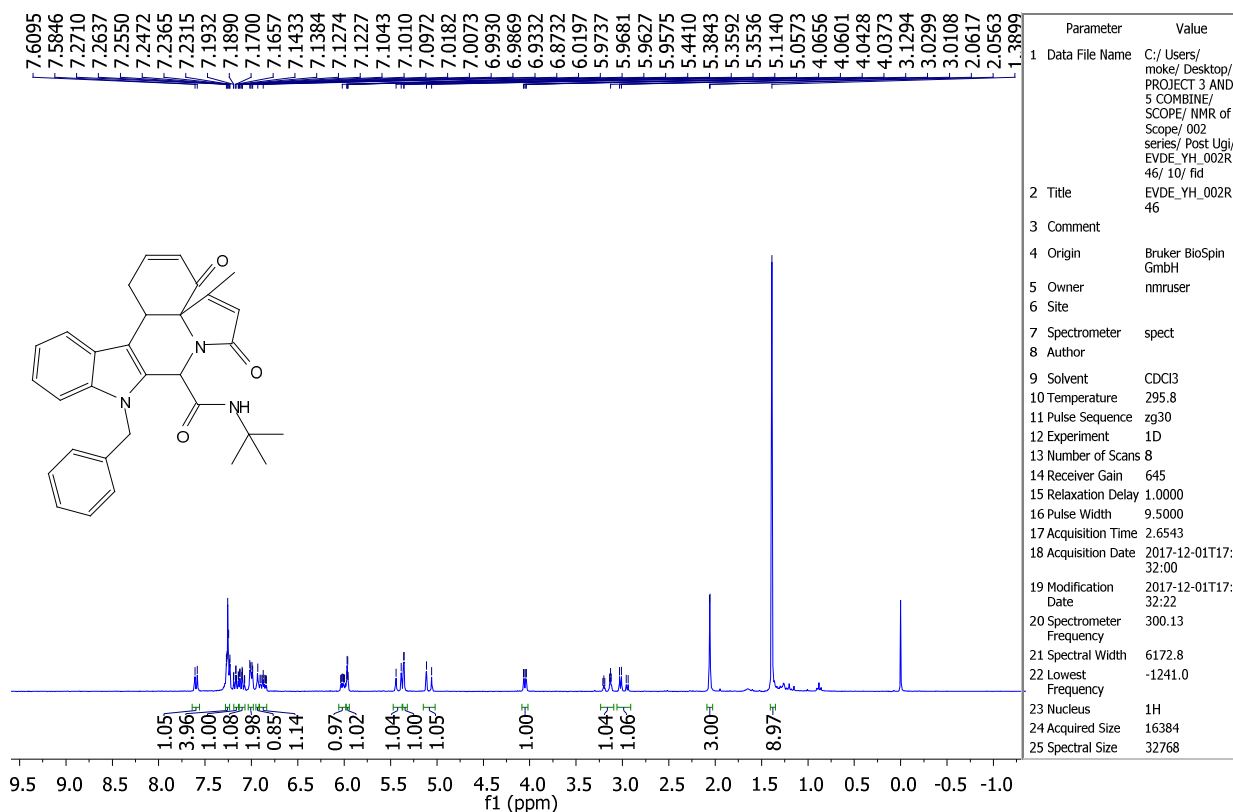
¹H and ¹³C NMR spectra of compound 2a



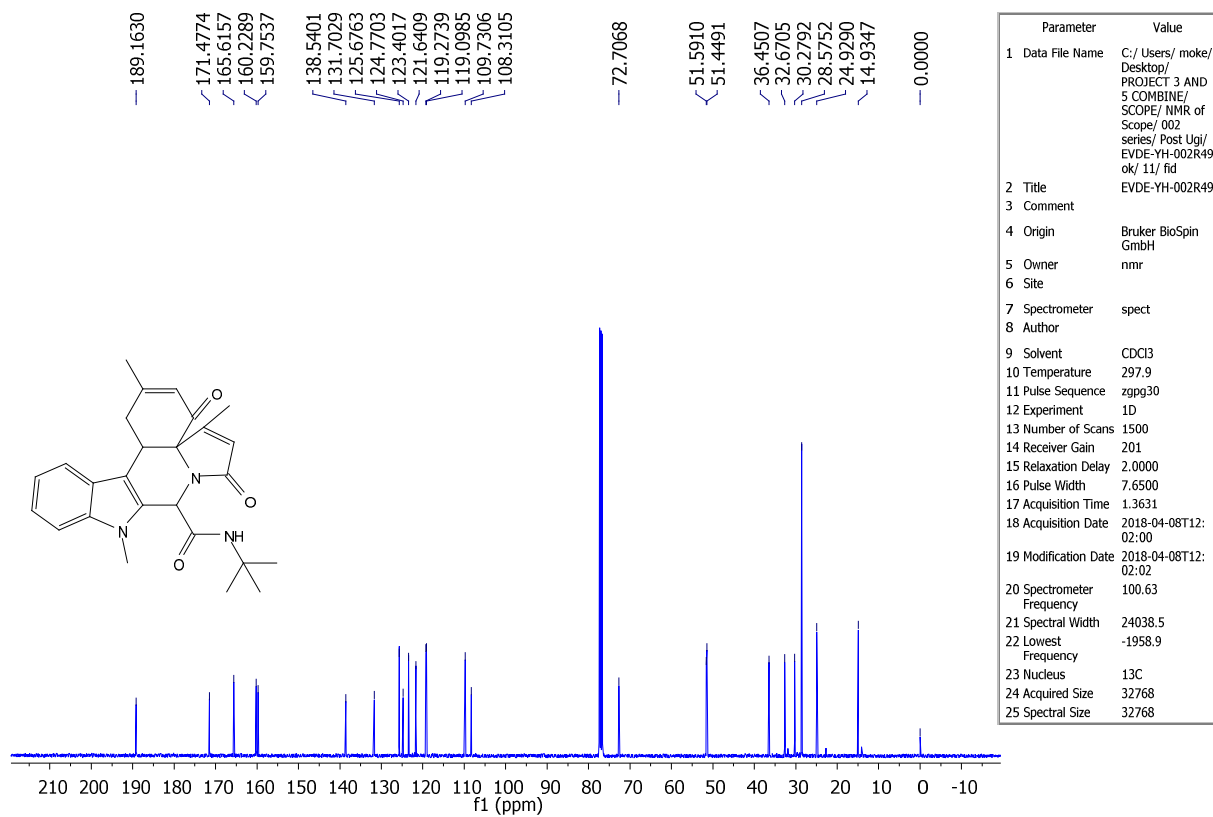
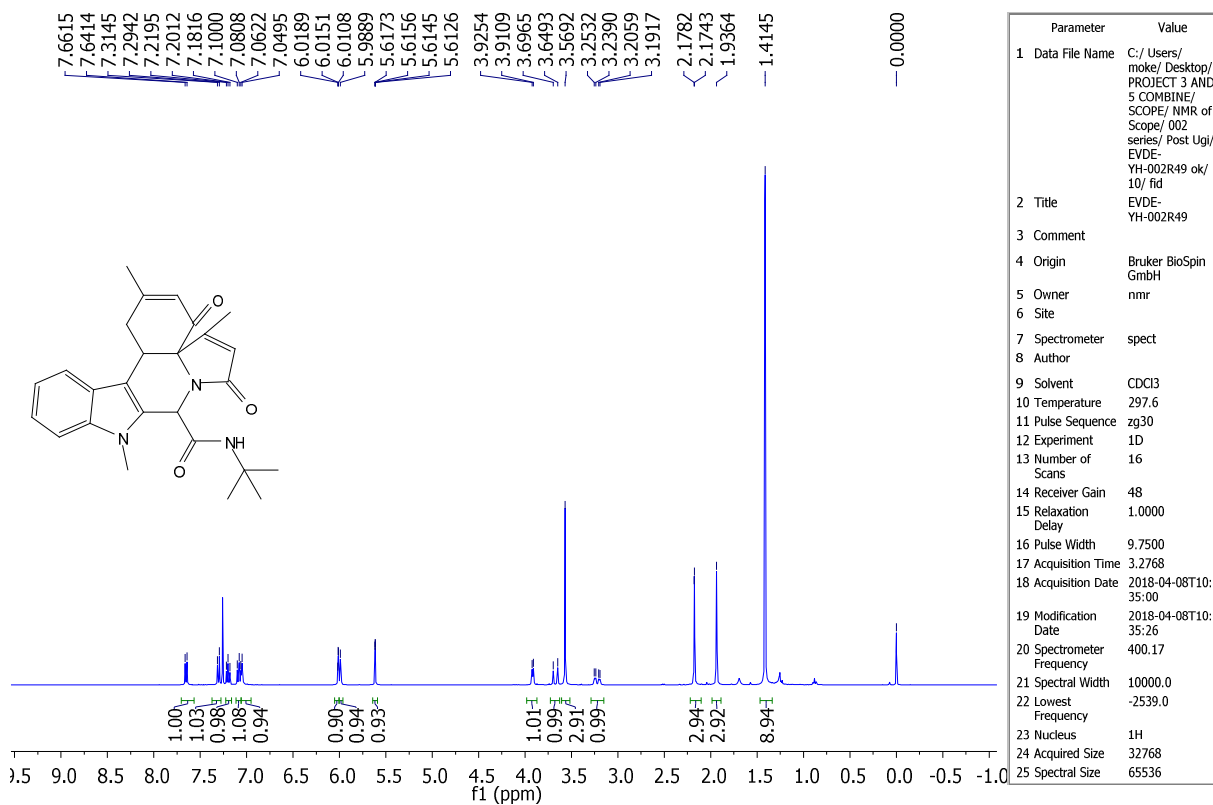
¹H and ¹³C NMR spectra of compound 2b



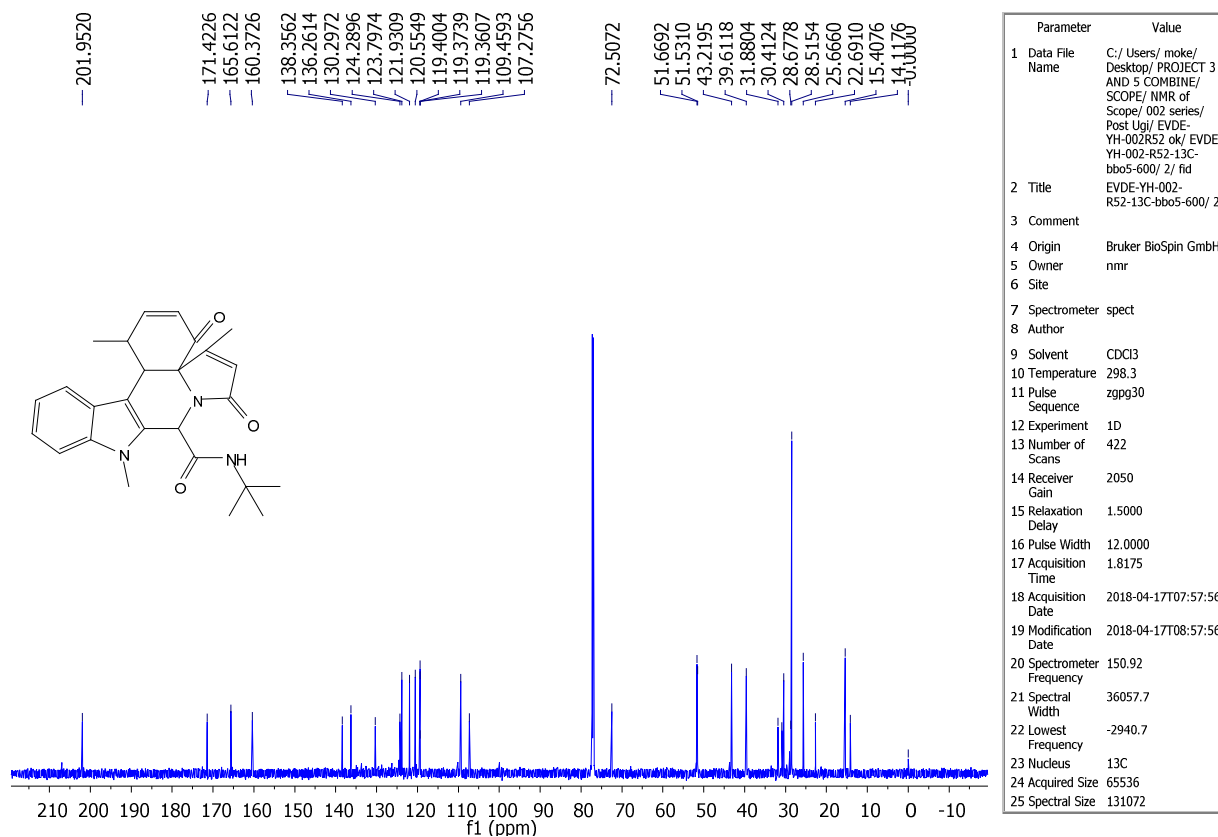
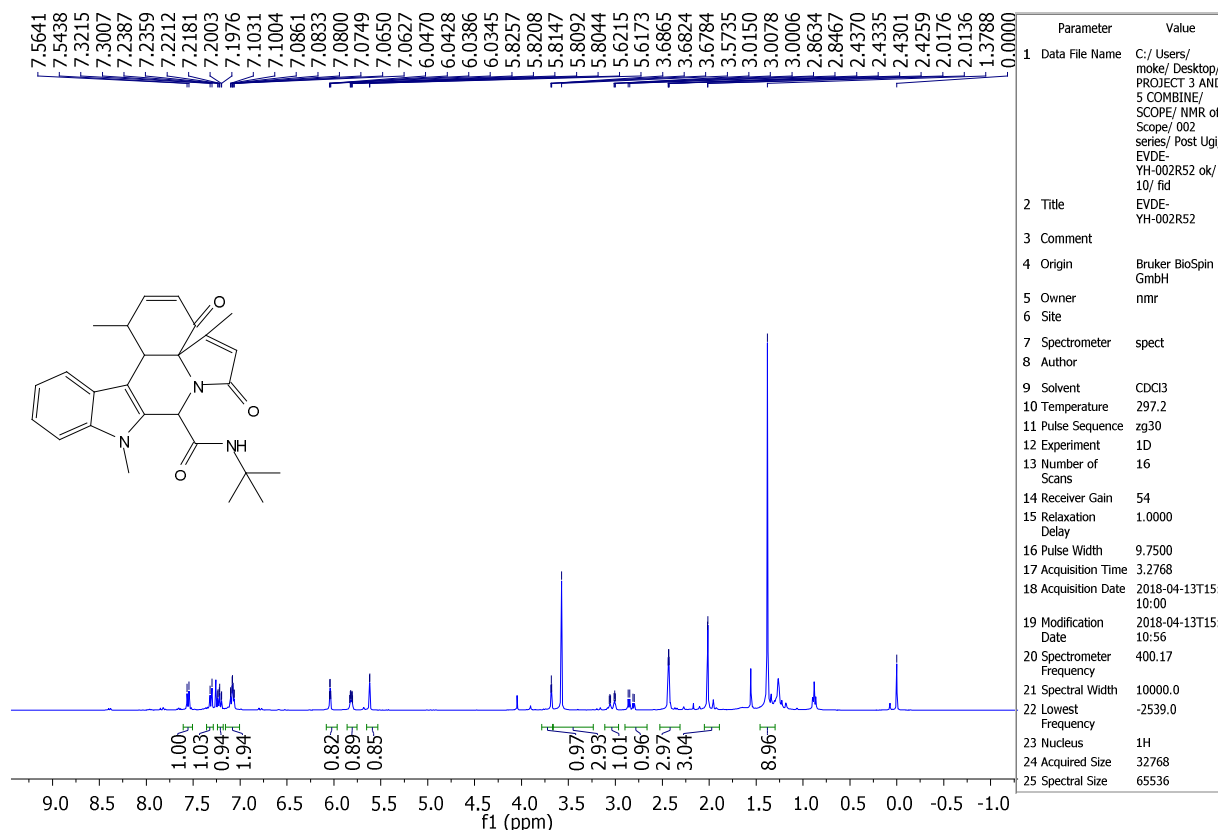
¹H and ¹³C NMR spectra of compound 2c



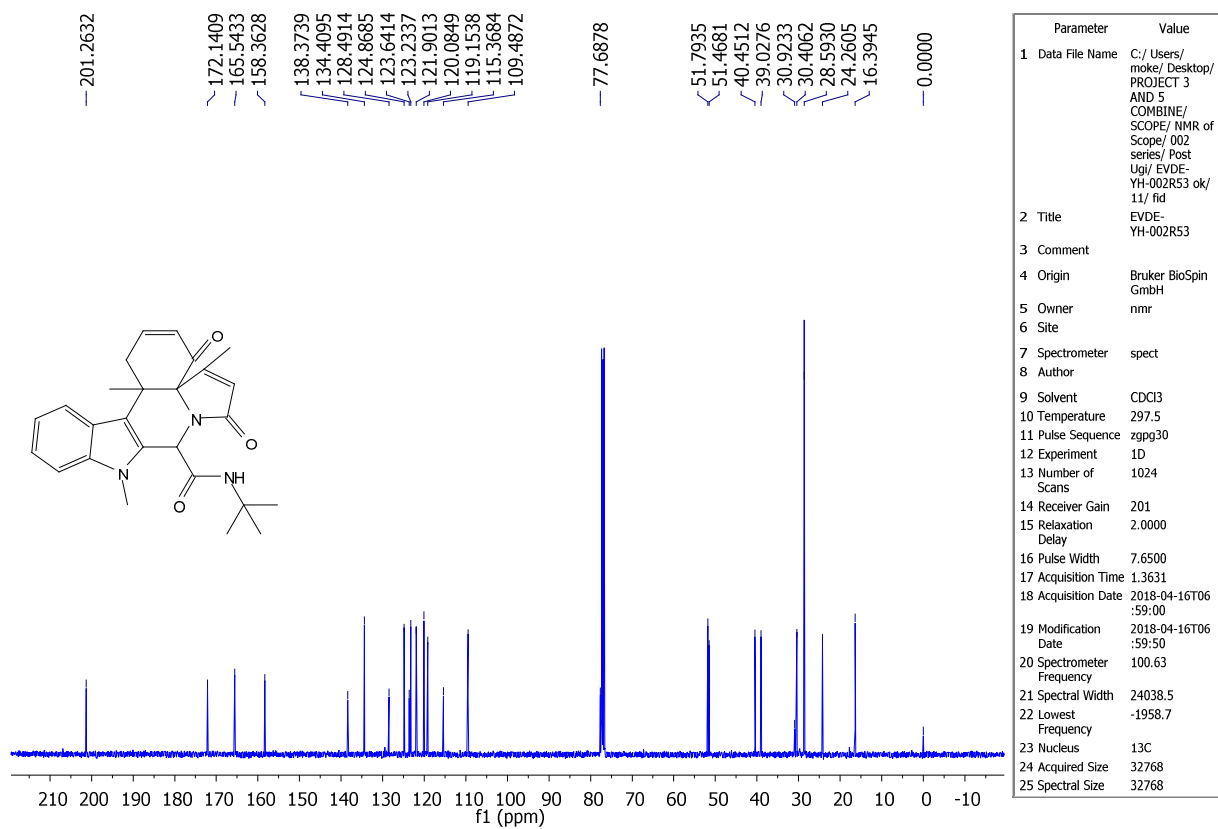
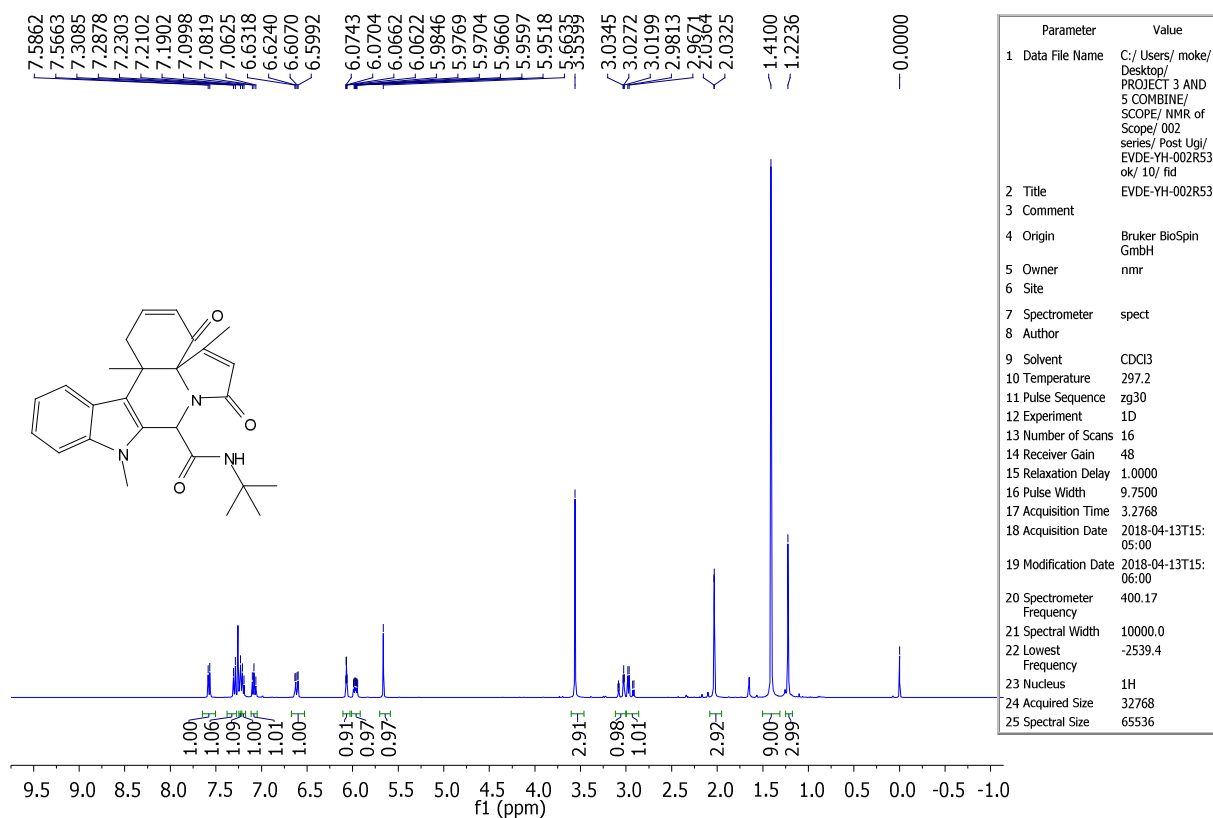
¹H and ¹³C NMR spectra of compound 2f



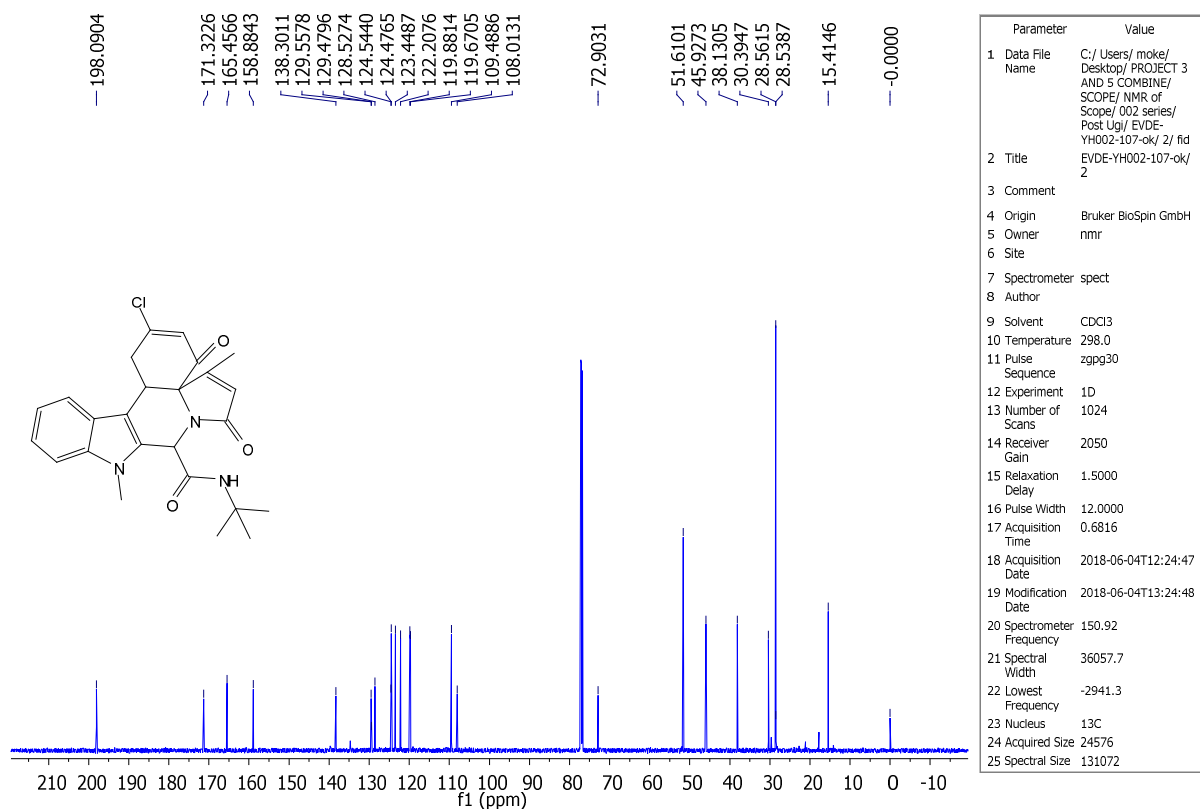
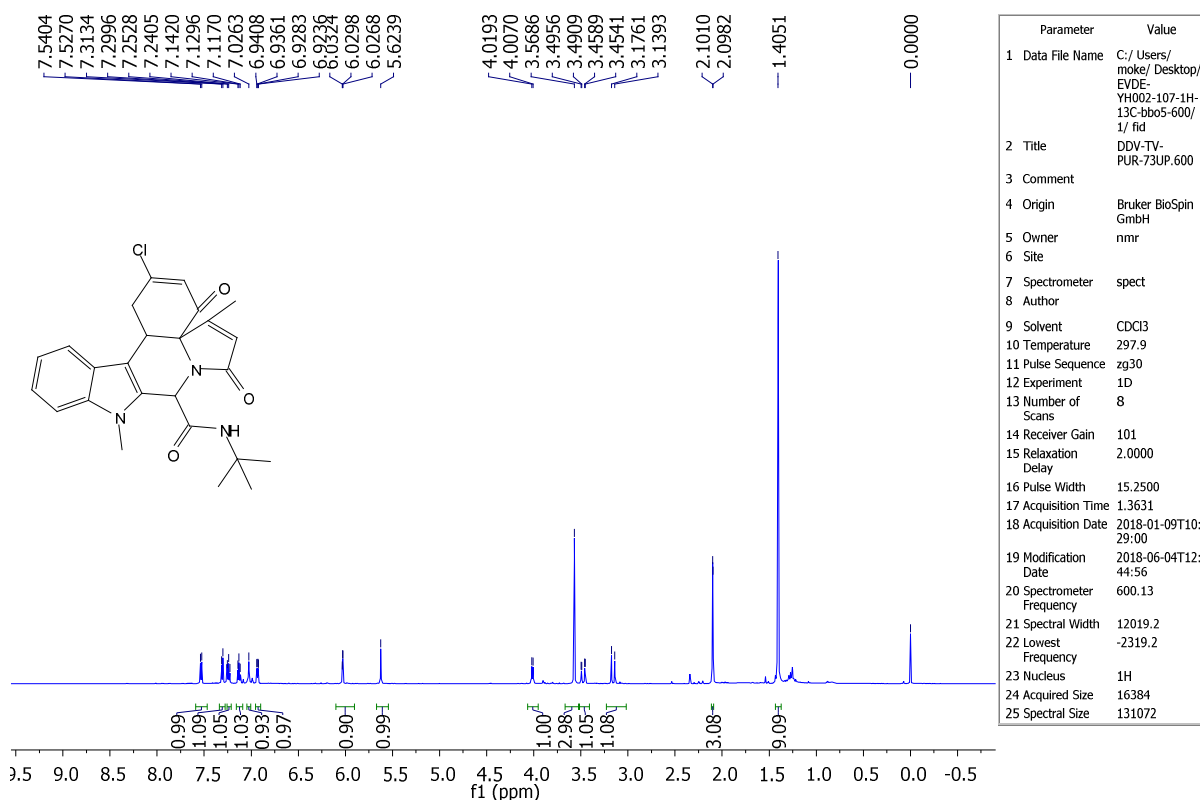
¹H and ¹³C NMR spectra of compound 2g



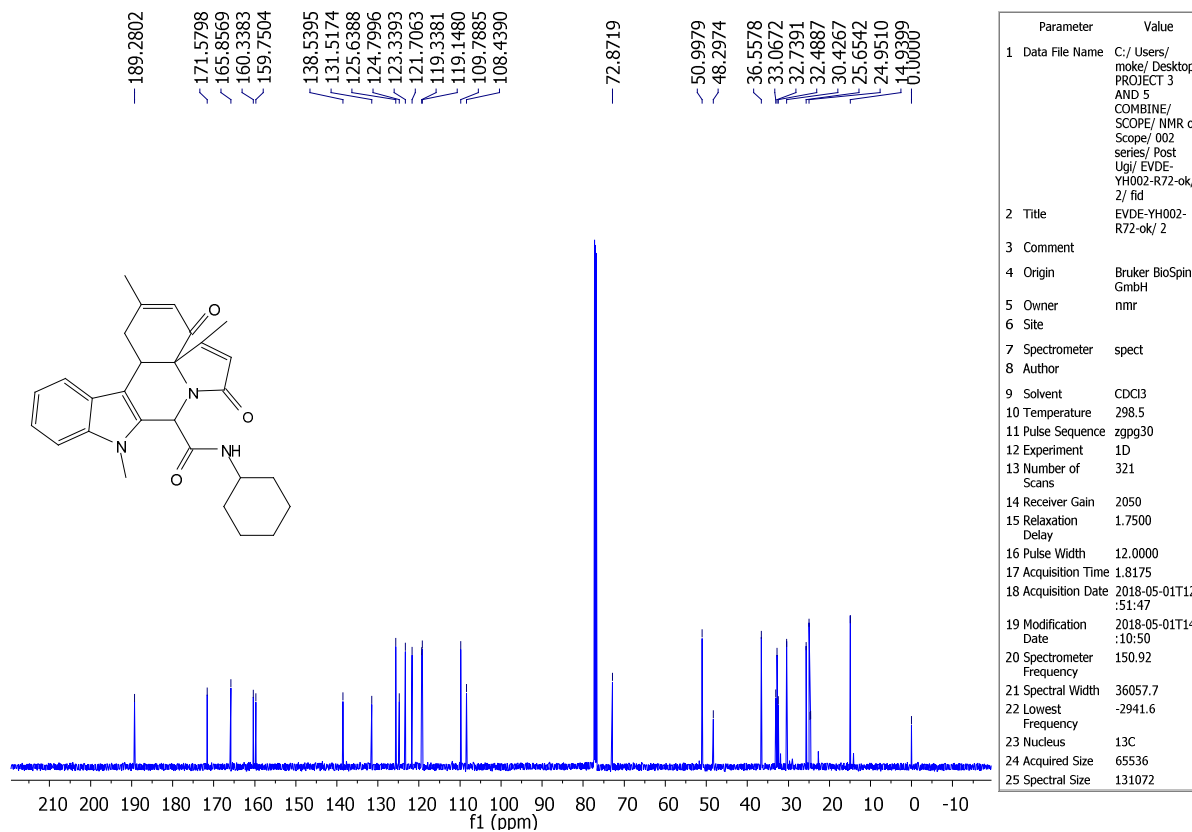
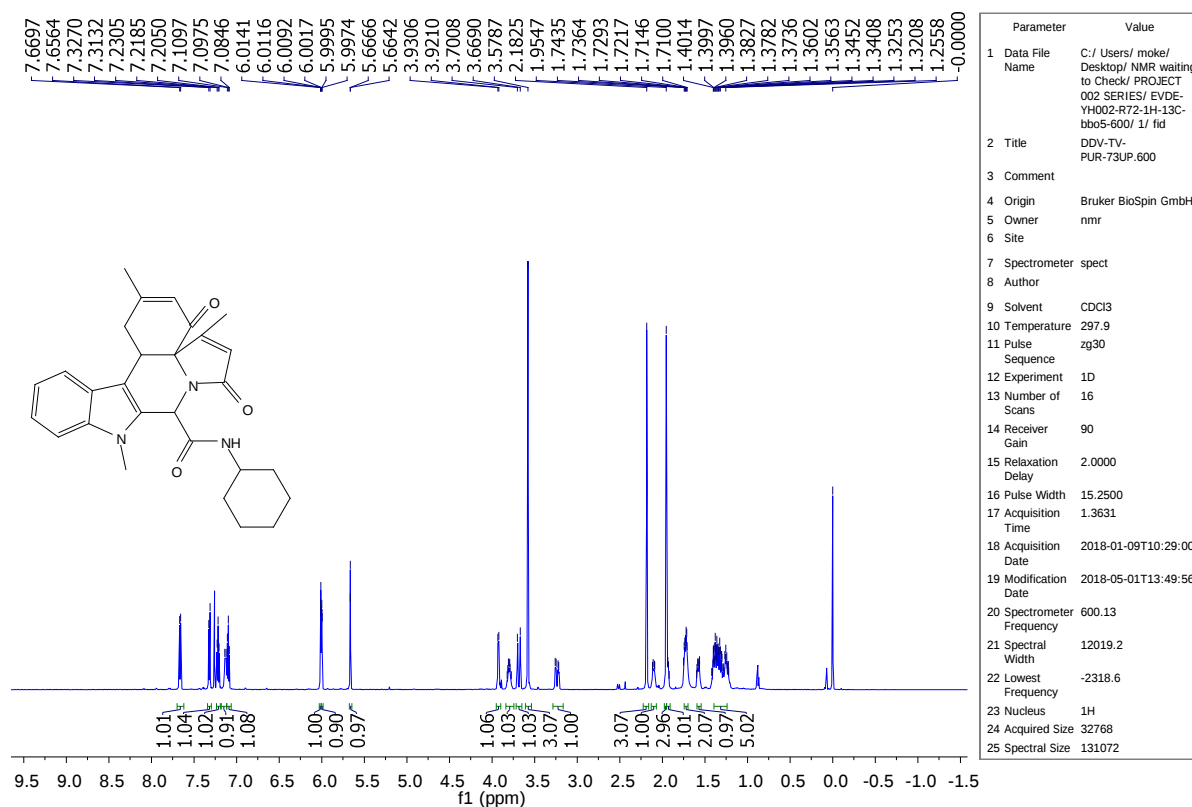
¹H and ¹³C NMR spectra of compound 2h



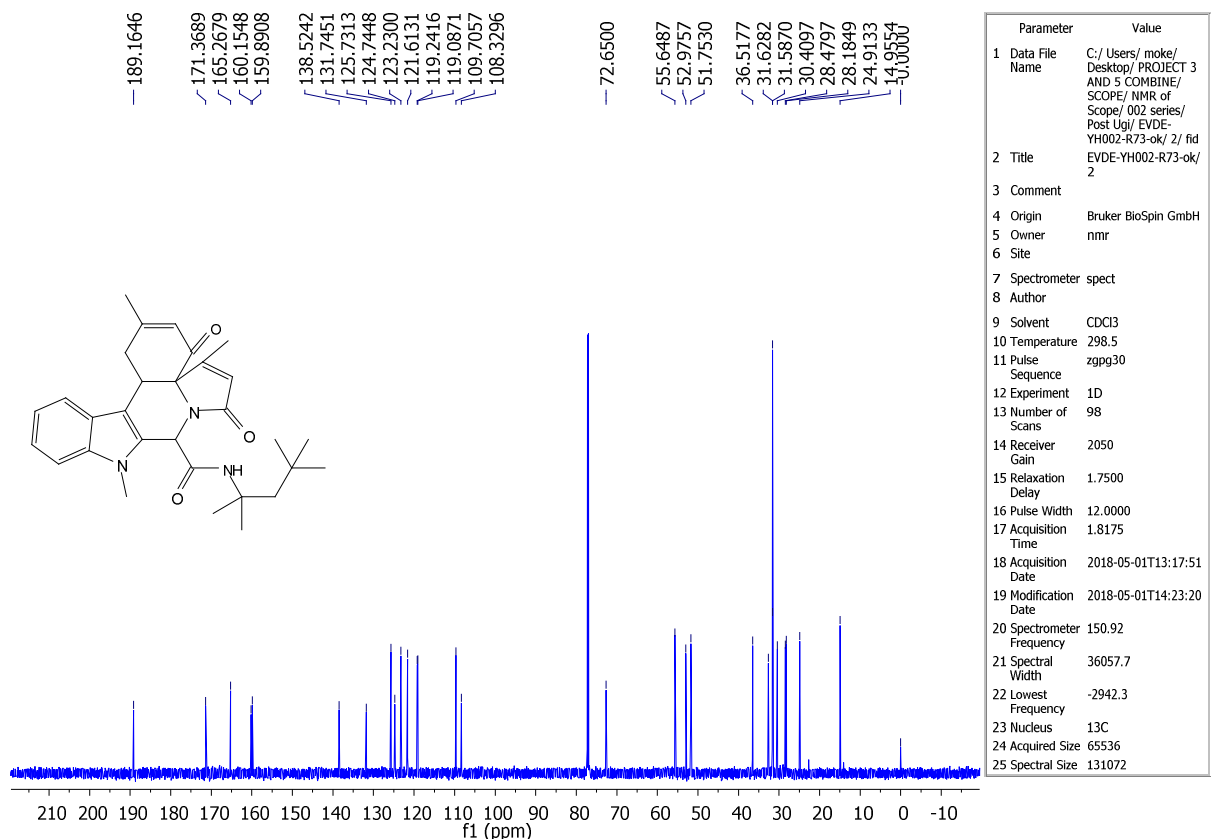
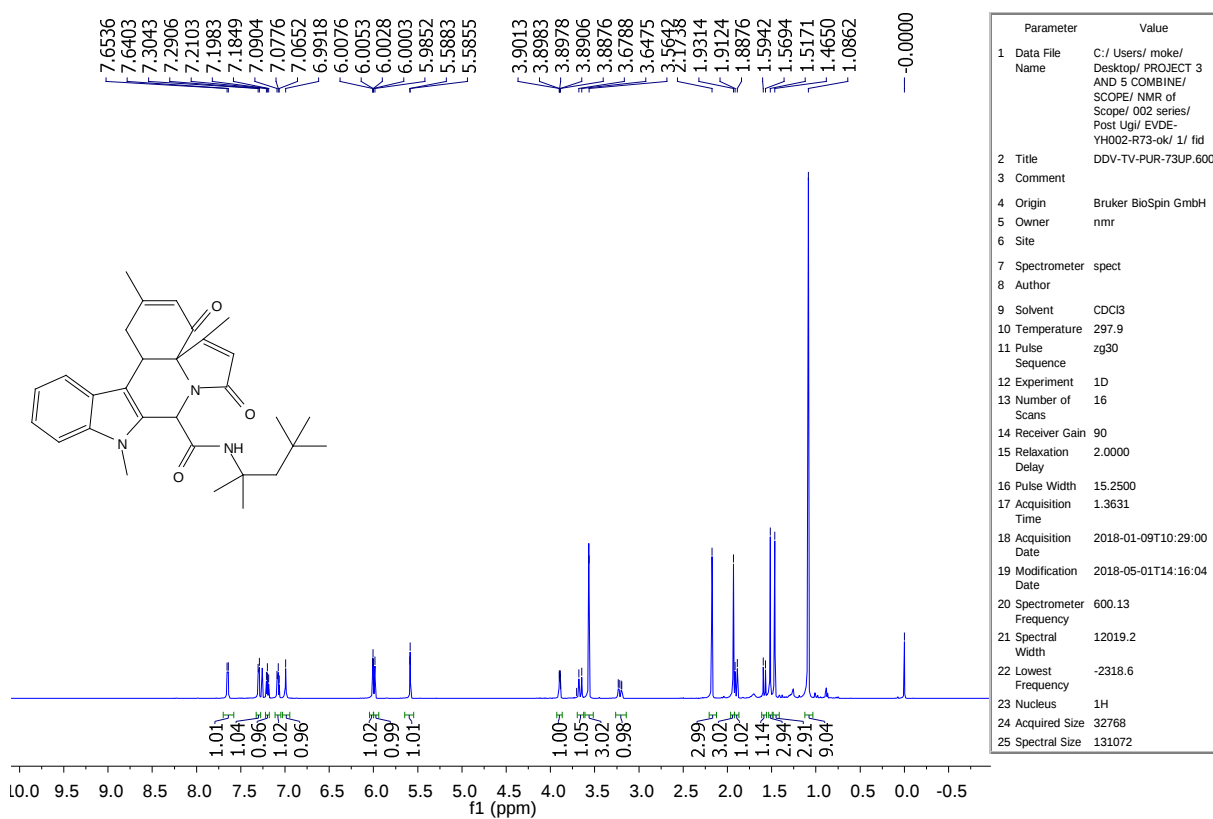
¹H and ¹³C NMR spectra of compound 2i



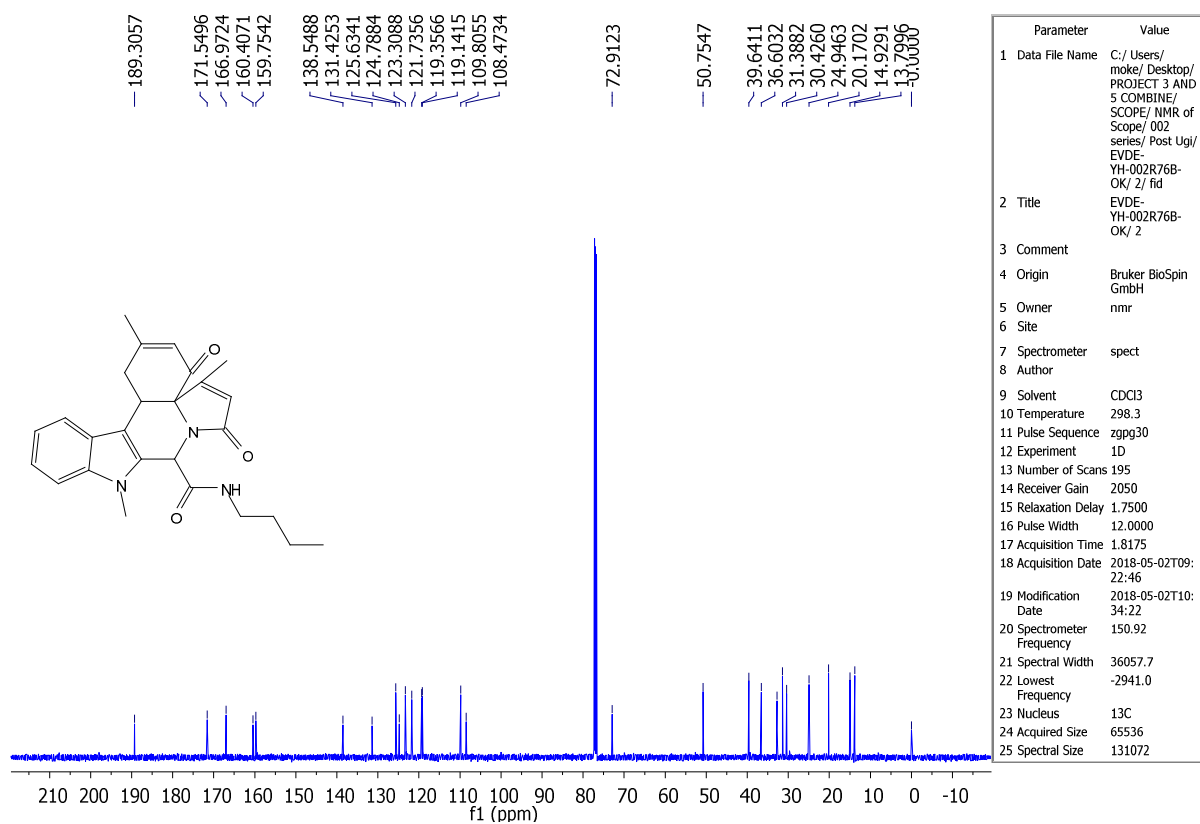
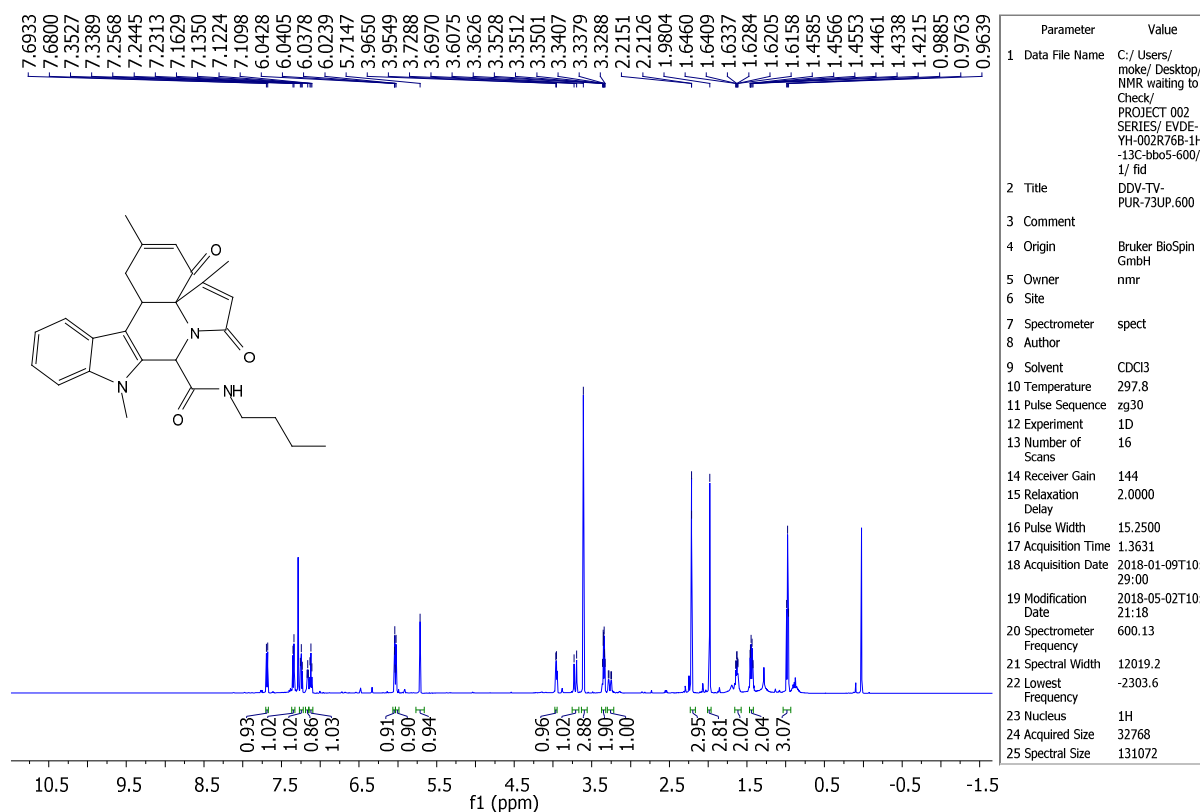
¹H and ¹³C NMR spectra of compound 2j



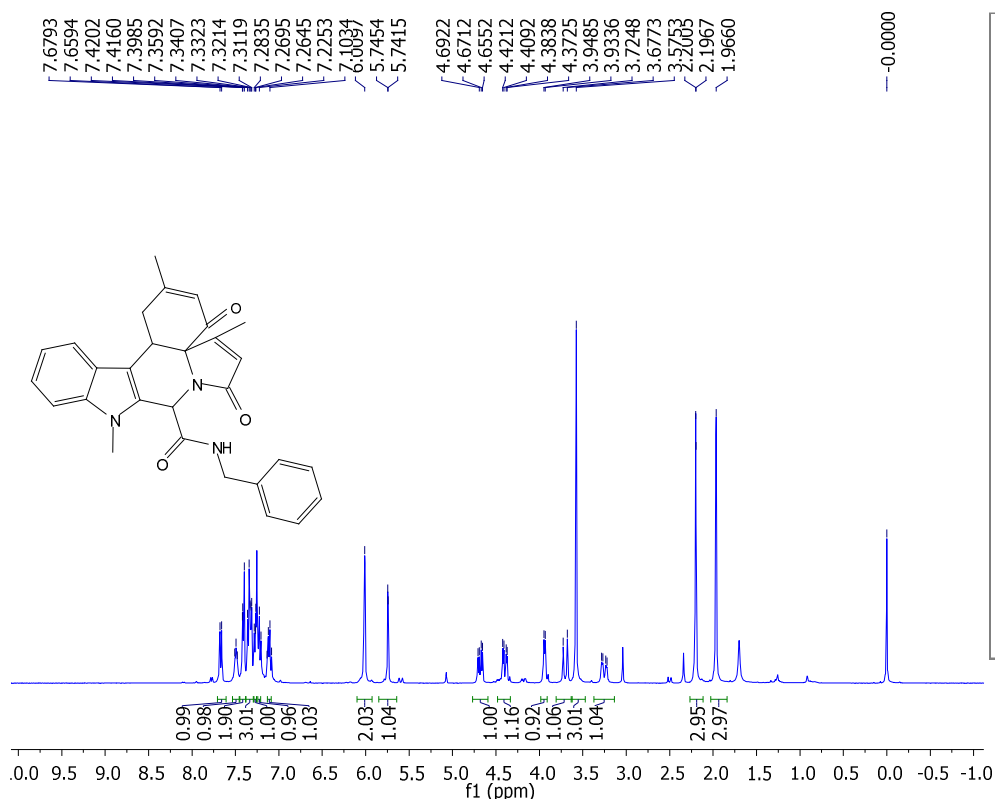
¹H and ¹³C NMR spectra of compound 2k



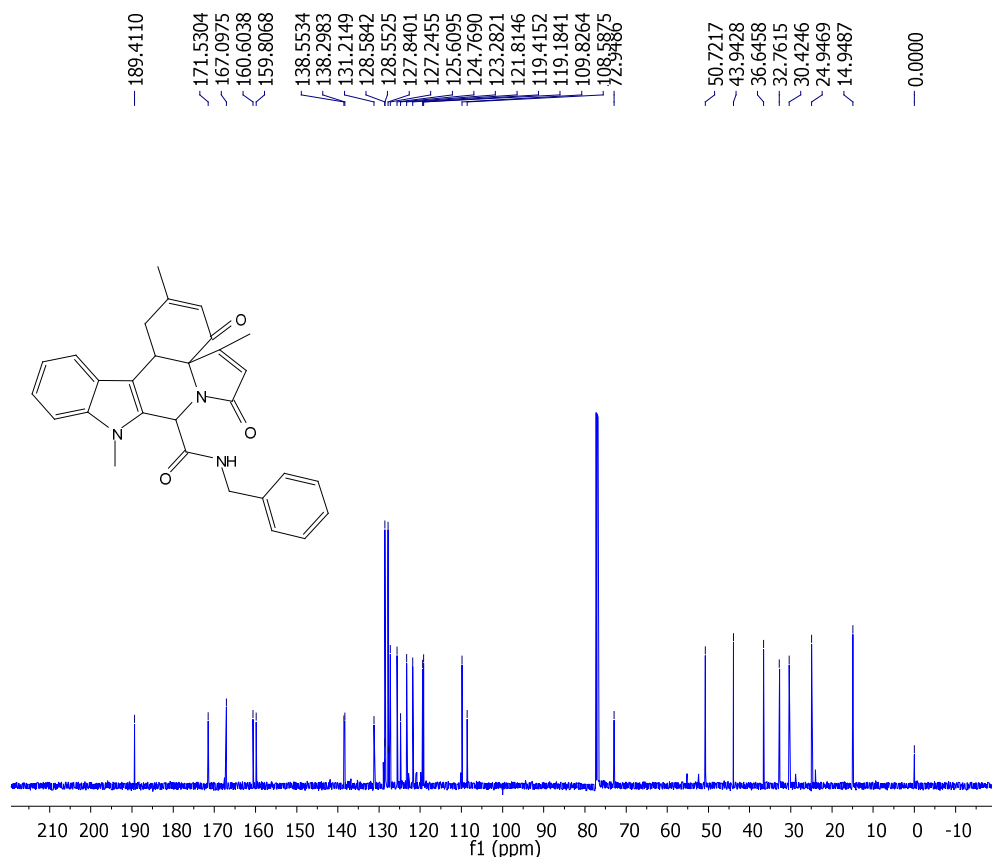
¹H and ¹³C NMR spectra of compound 2I



¹H and ¹³C NMR spectra of compound 2m

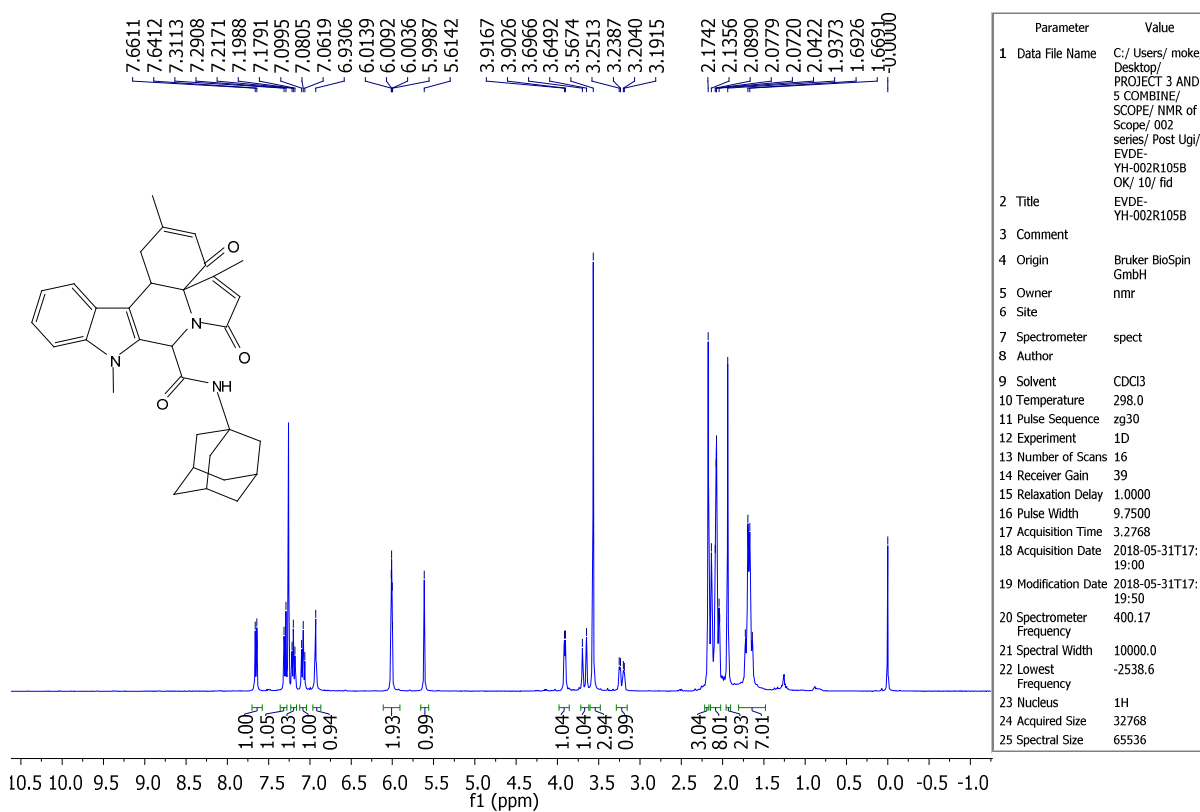


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4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
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12 Experiment	1D
13 Number of Scans	16
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16 Pulse Width	9.7500
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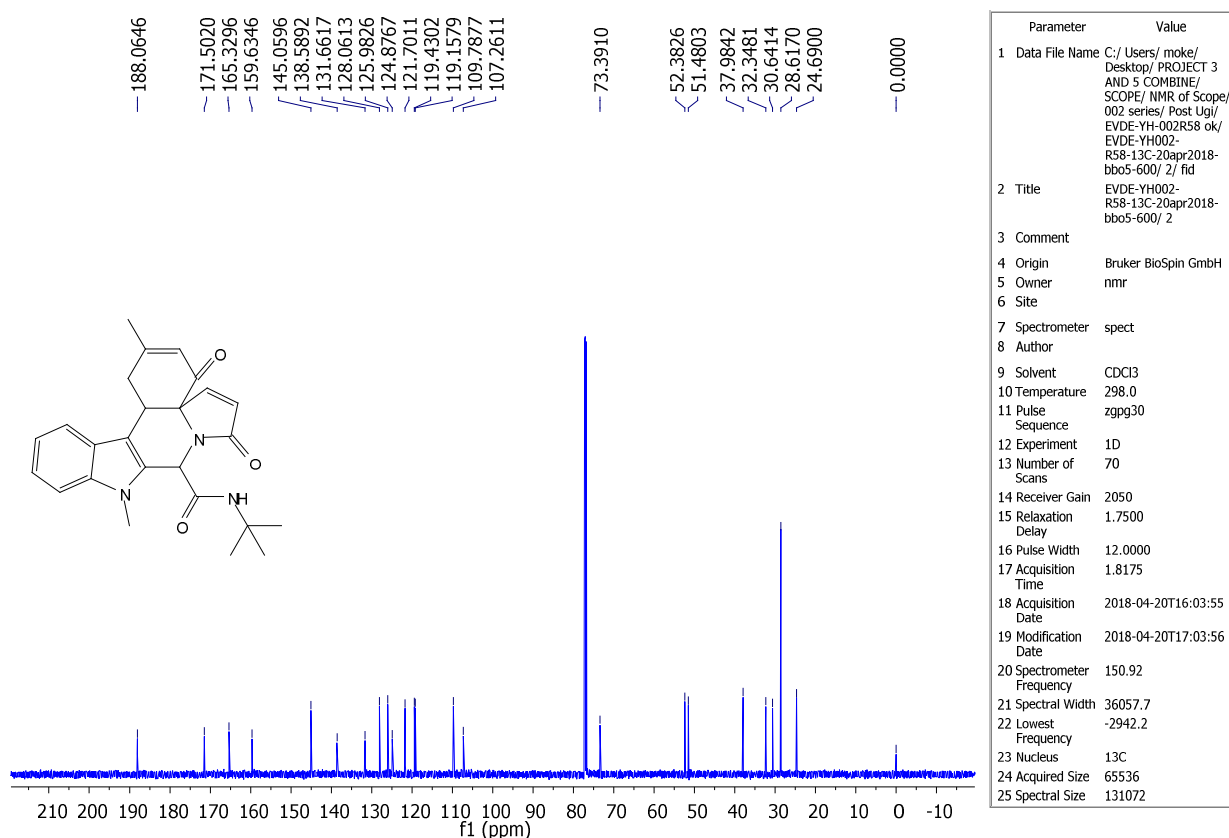
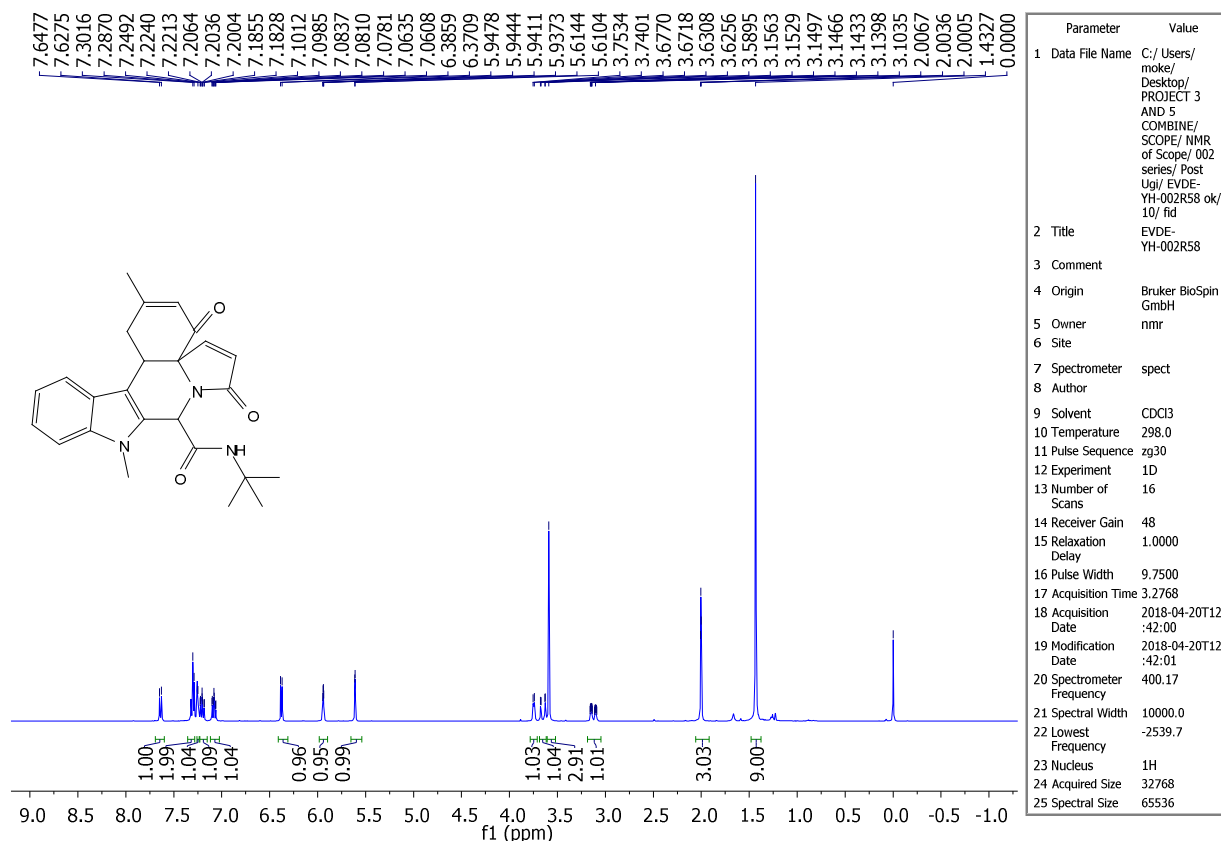


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5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
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12 Experiment	1D
13 Number of Scans	339
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23 Nucleus	13C
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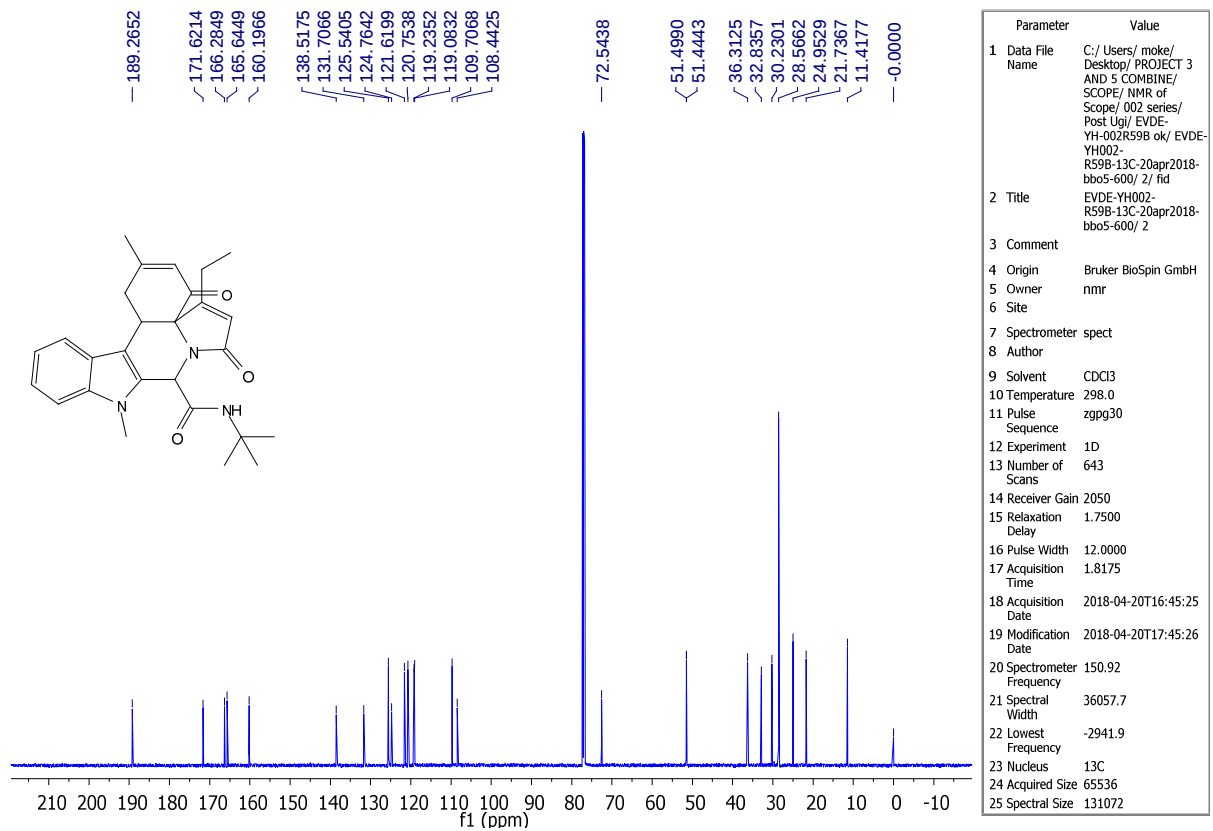
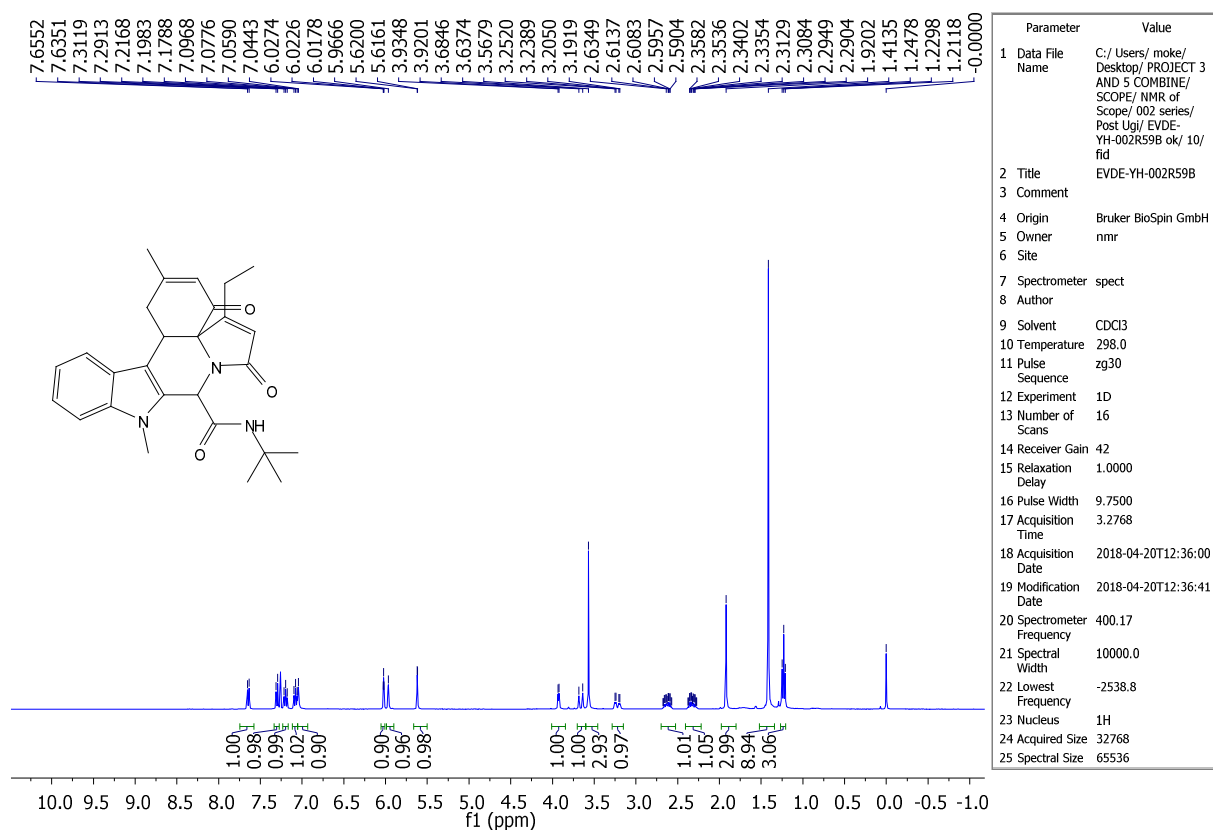
¹H and ¹³C NMR spectra of compound 2n



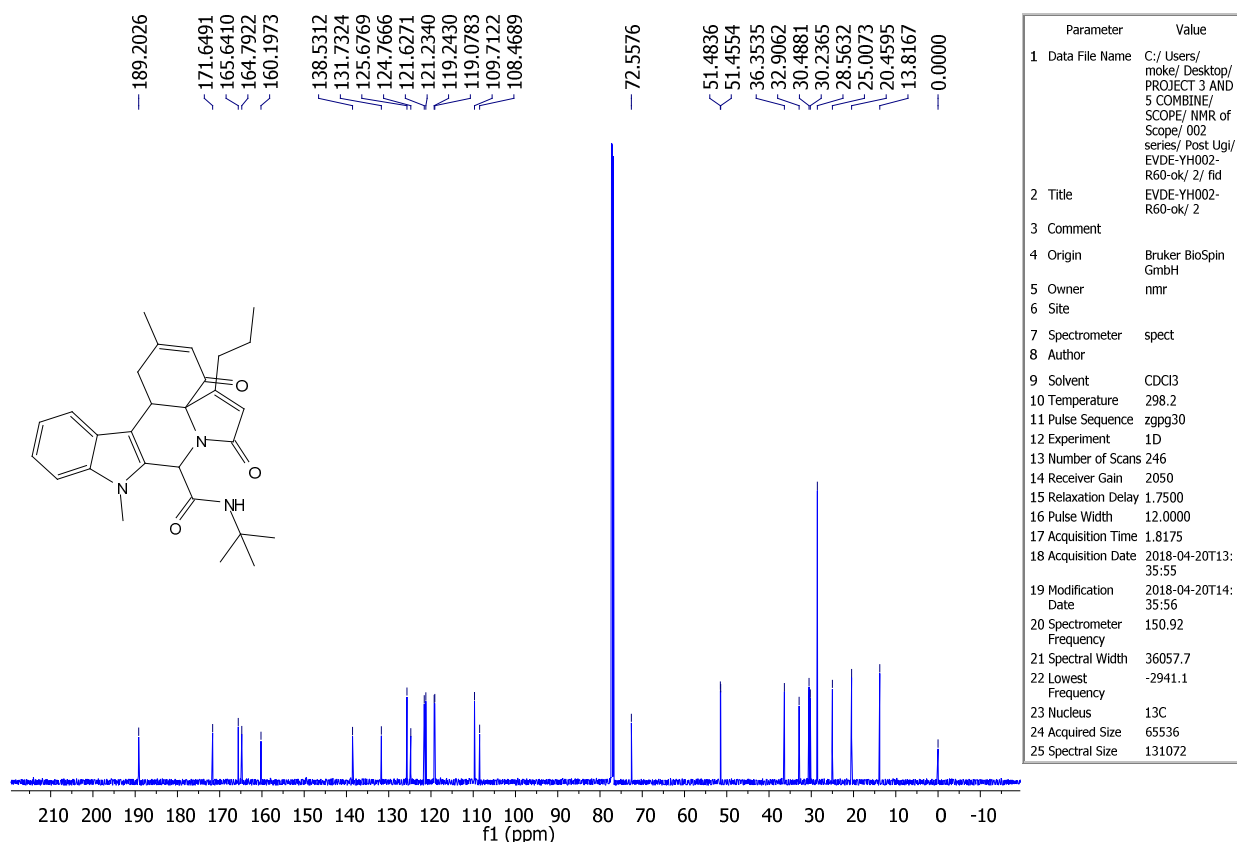
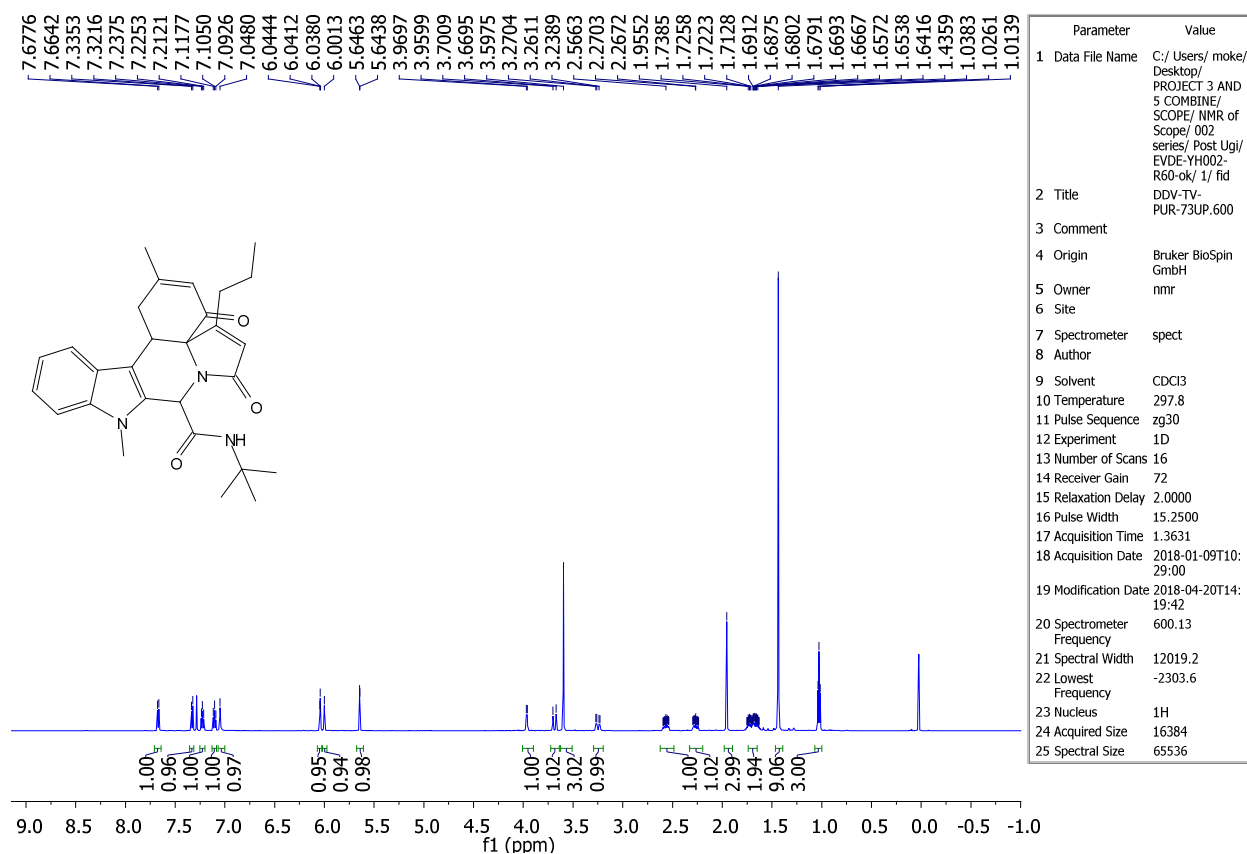
¹H and ¹³C NMR spectra of compound 2o



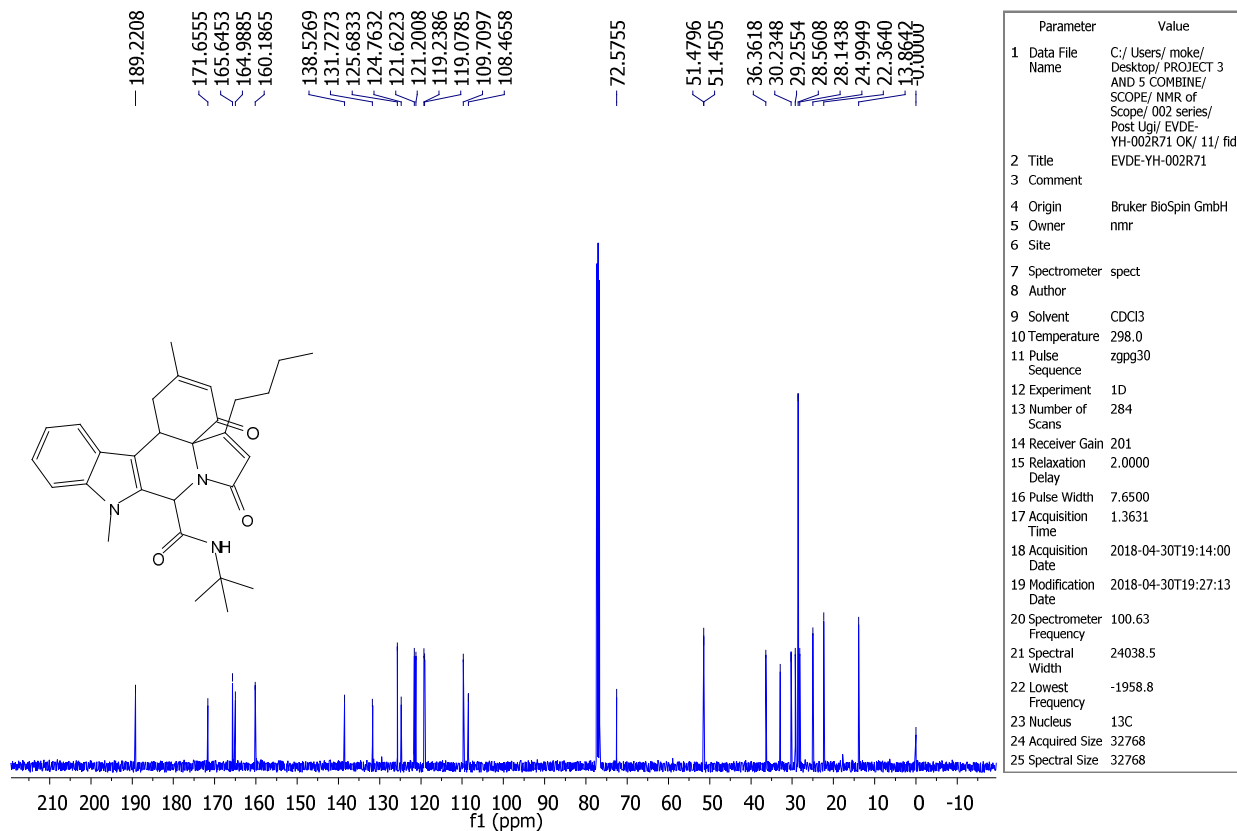
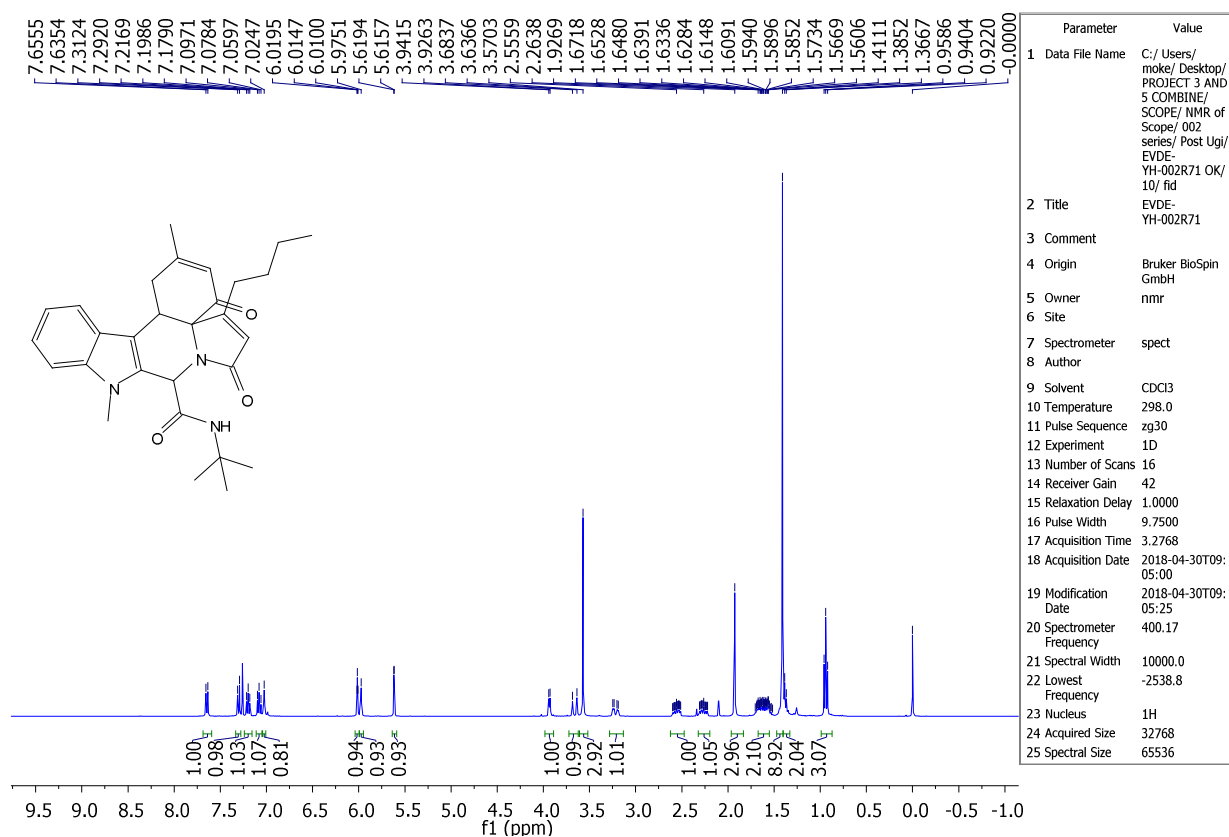
¹H and ¹³C NMR spectra of compound 2p



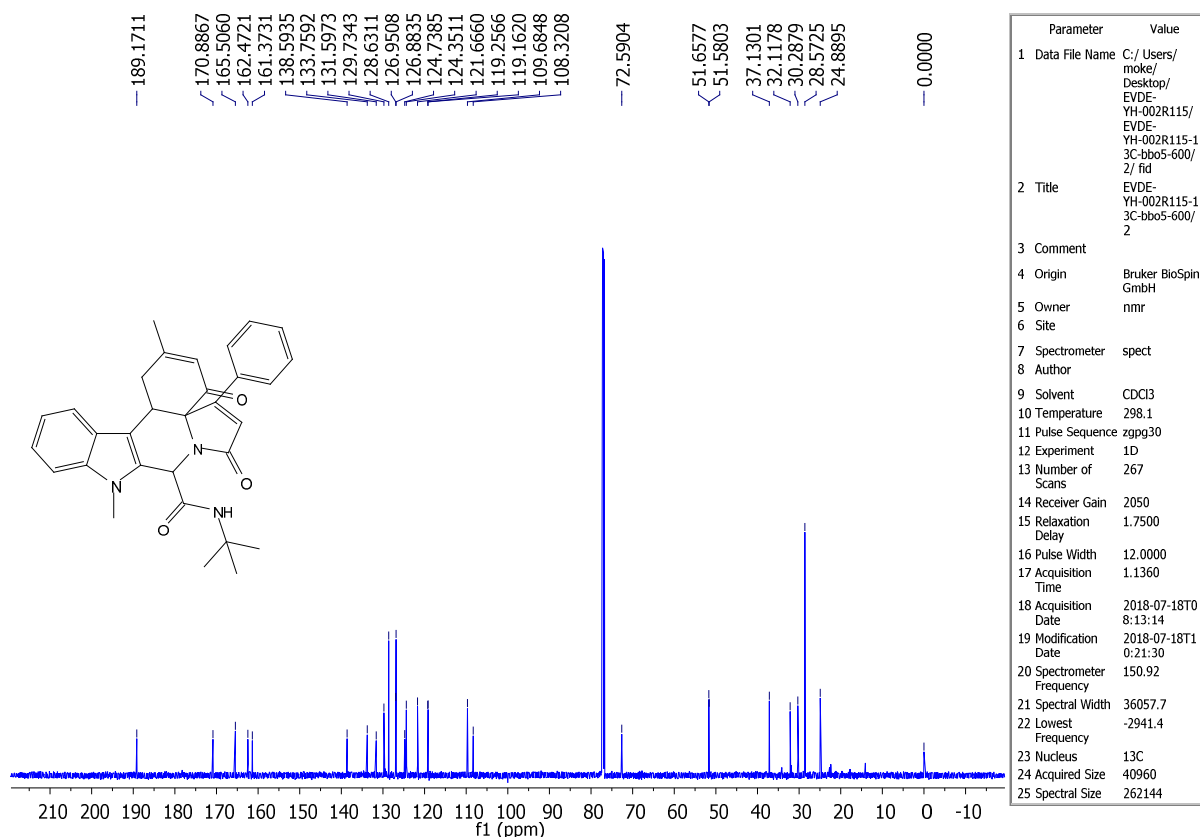
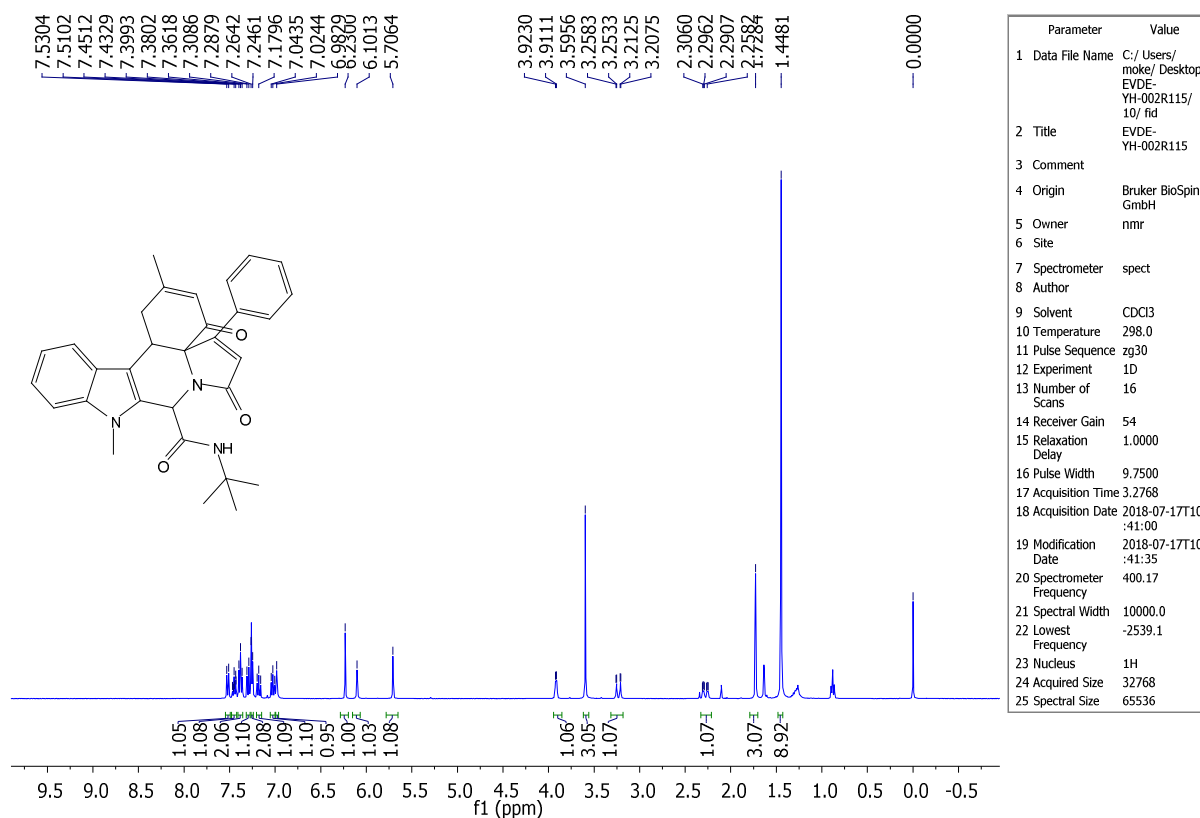
¹H and ¹³C NMR spectra of compound 2q



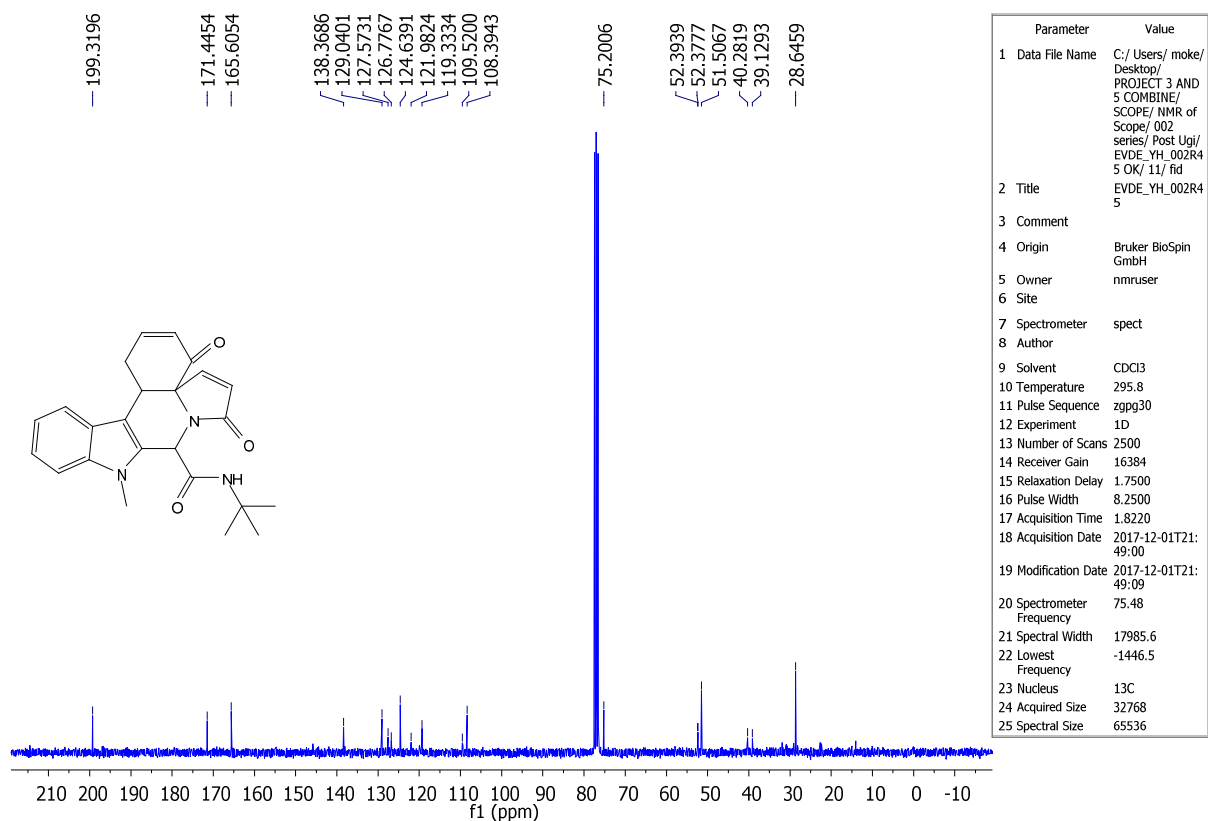
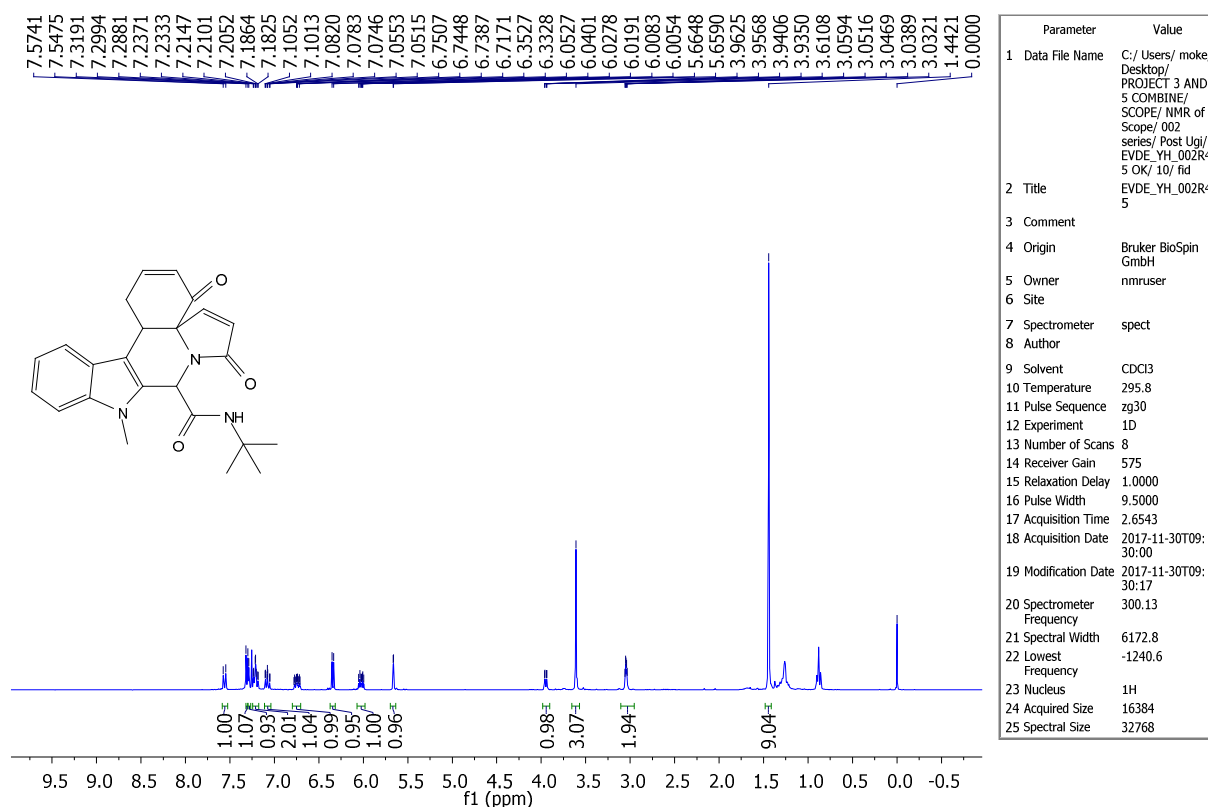
¹H and ¹³C NMR spectra of compound 2r



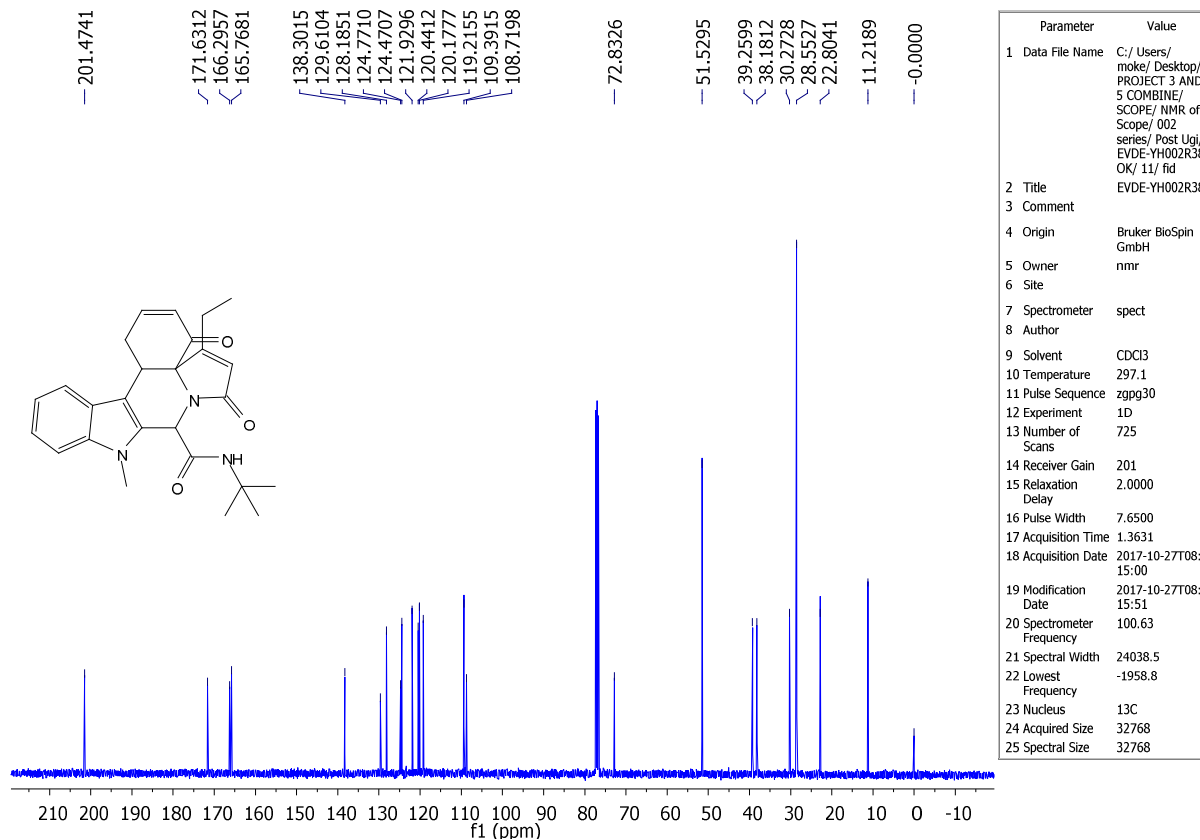
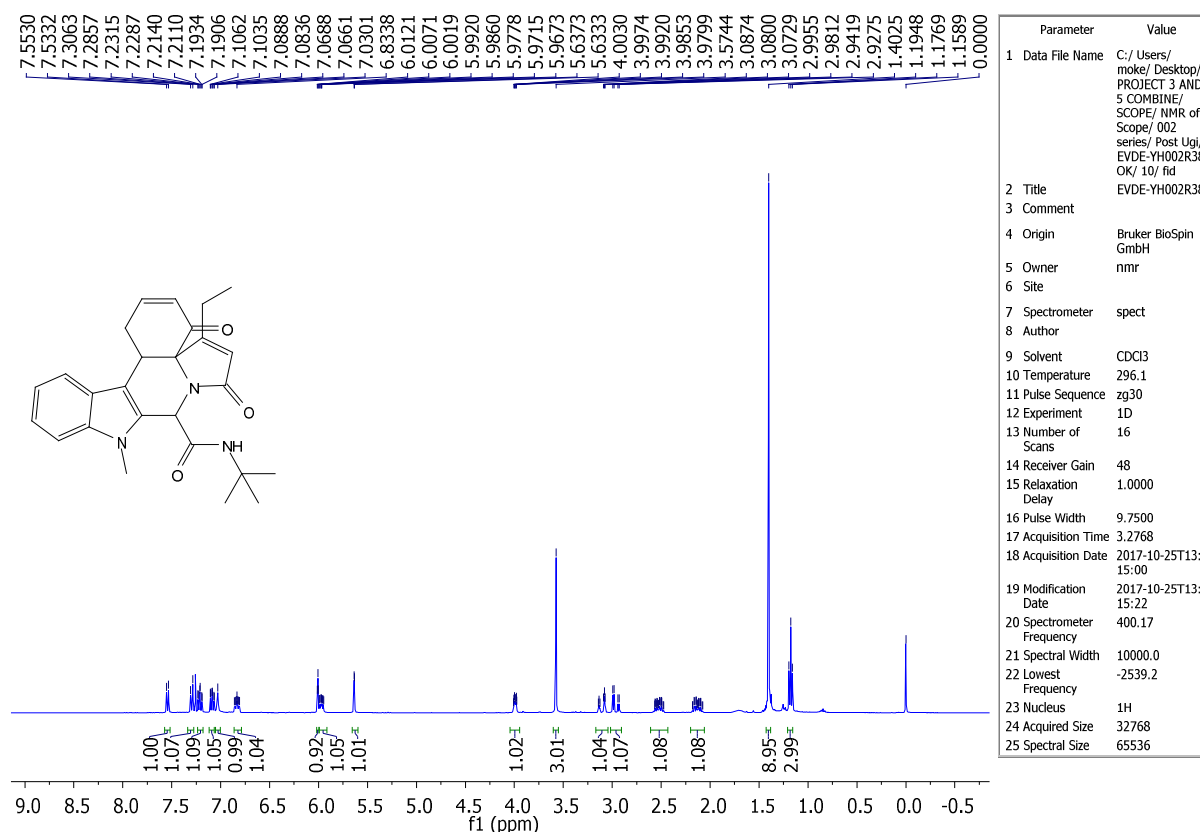
¹H and ¹³C NMR spectra of compound 2s



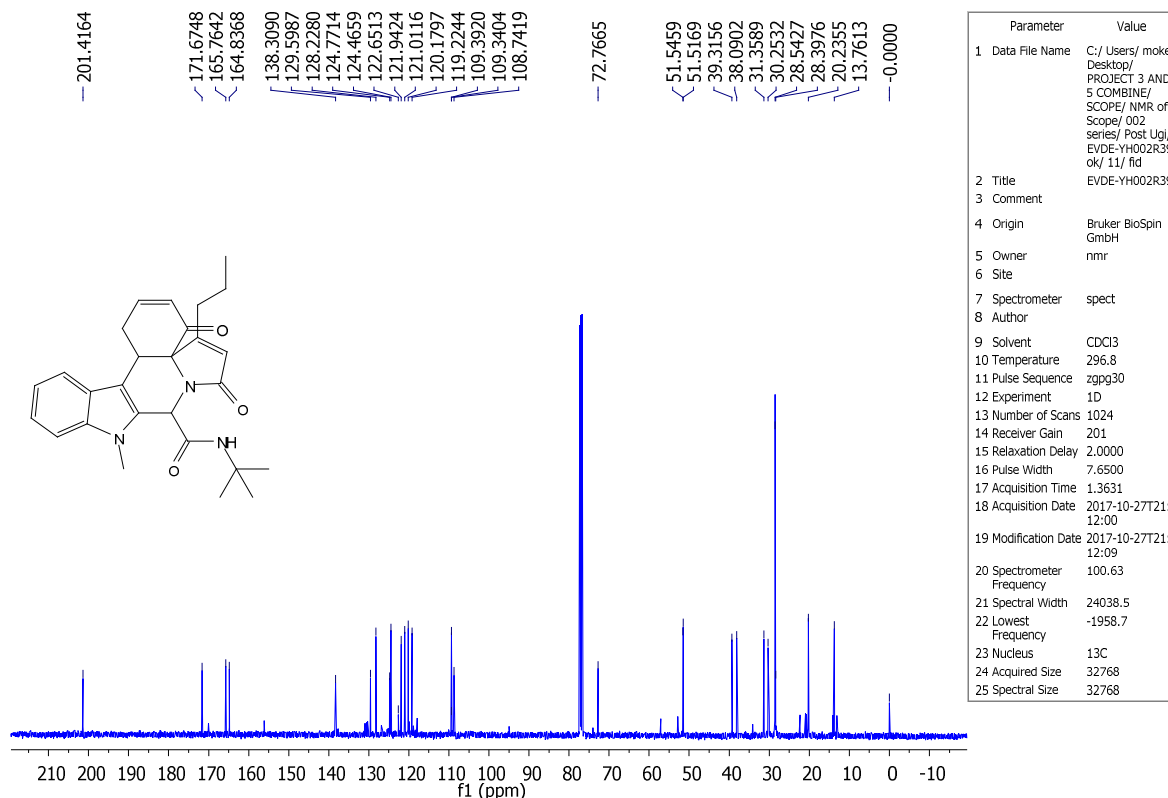
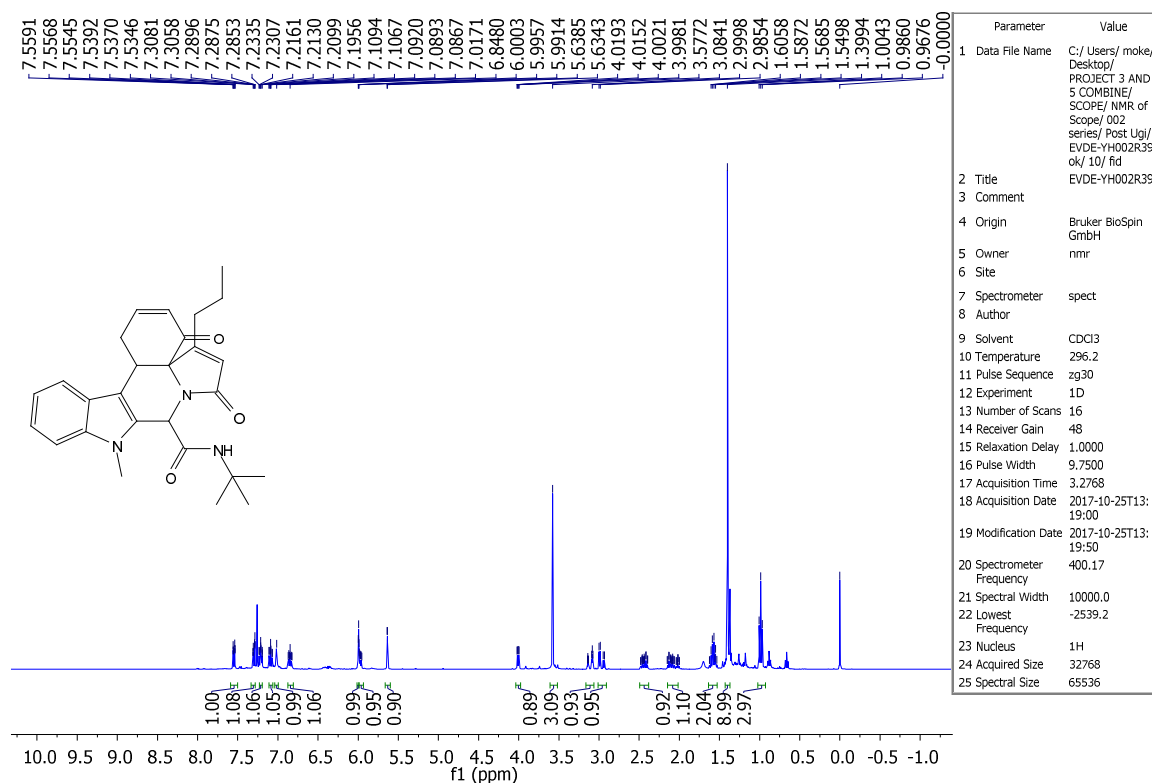
¹H and ¹³C NMR spectra of compound 2t



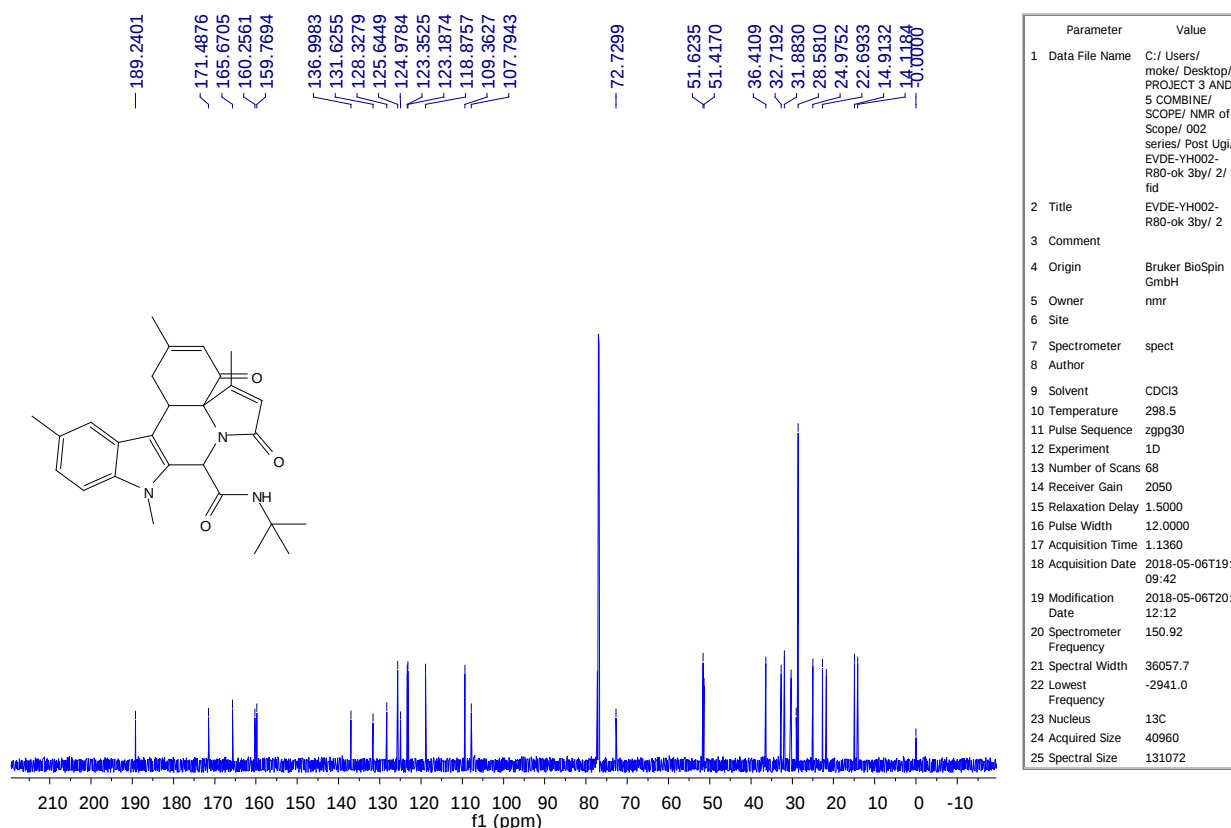
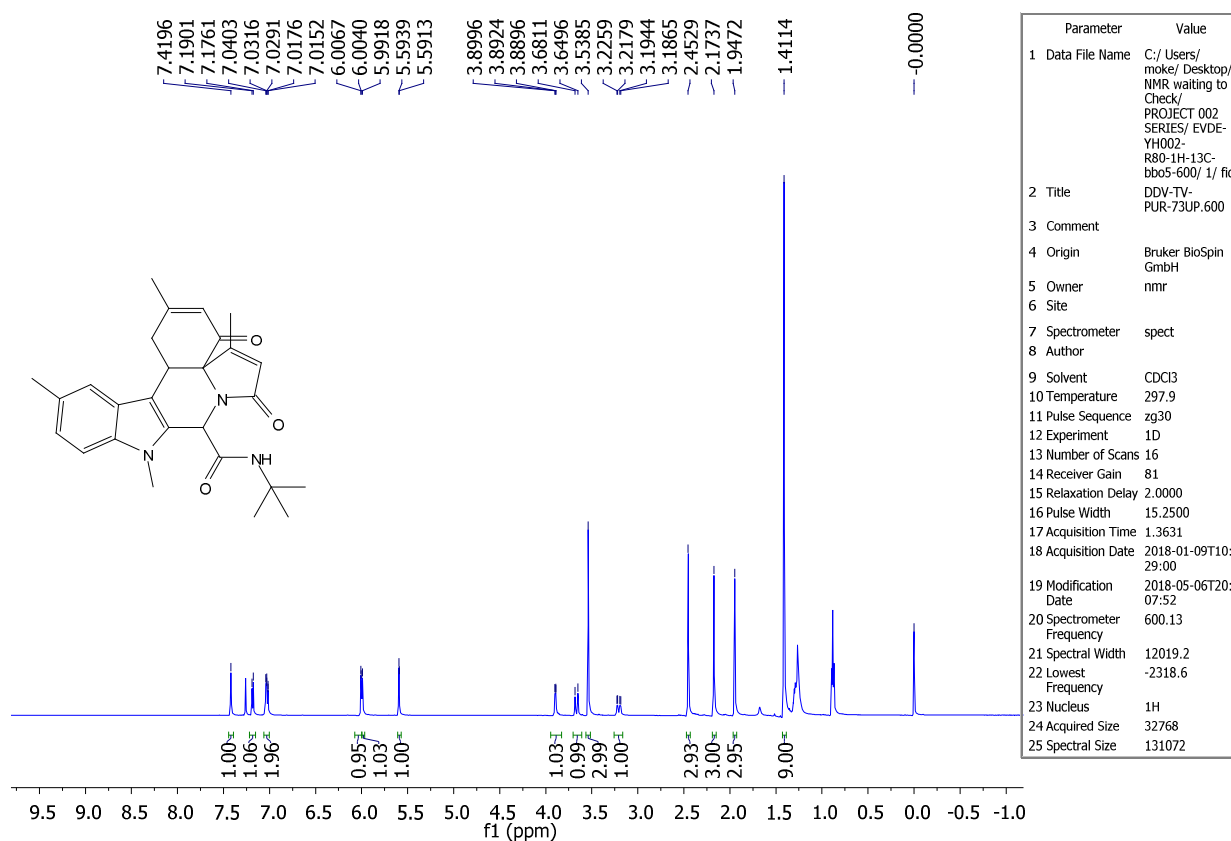
¹H and ¹³C NMR spectra of compound 2u



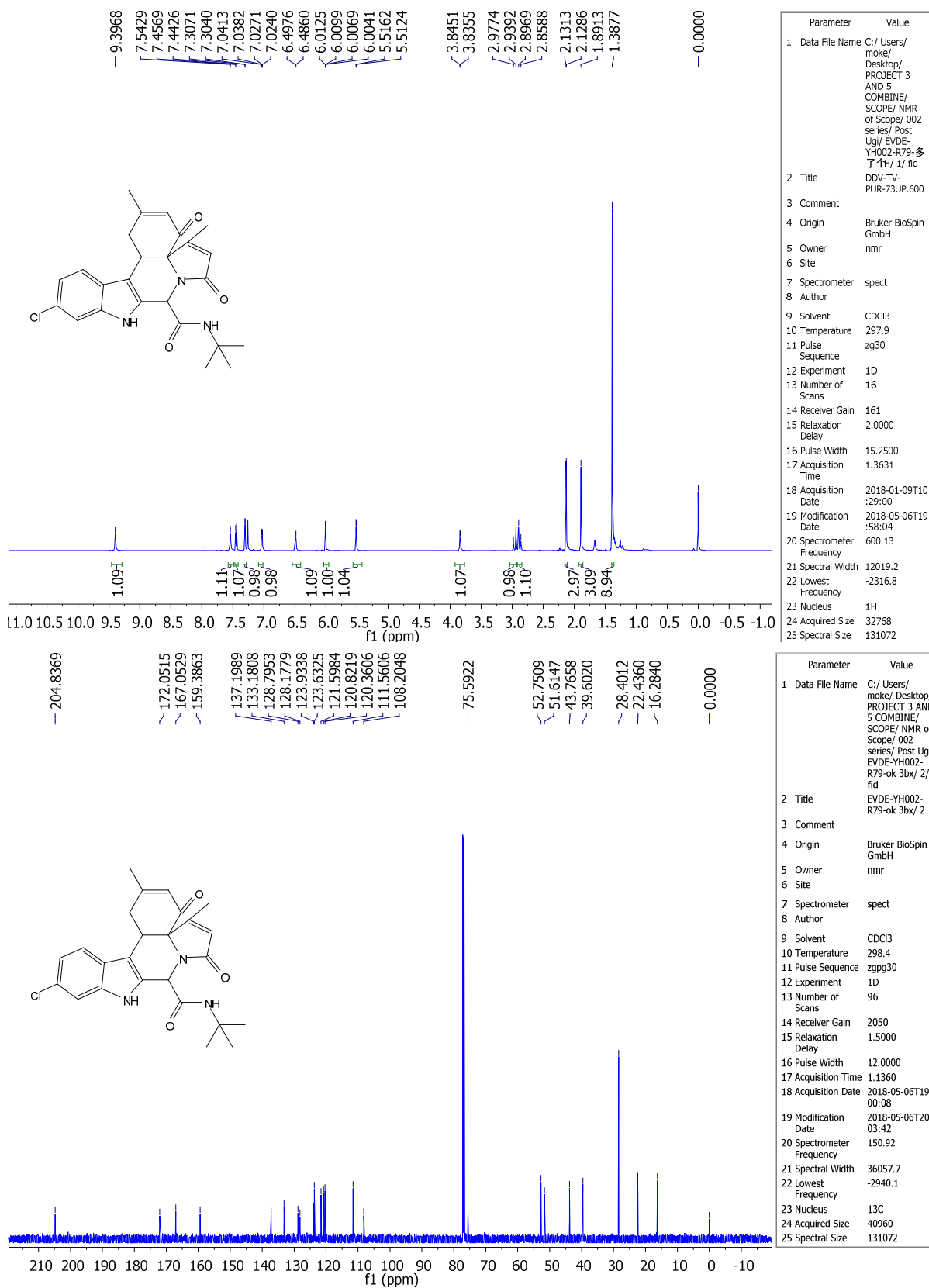
¹H and ¹³C NMR spectra of compound 2v



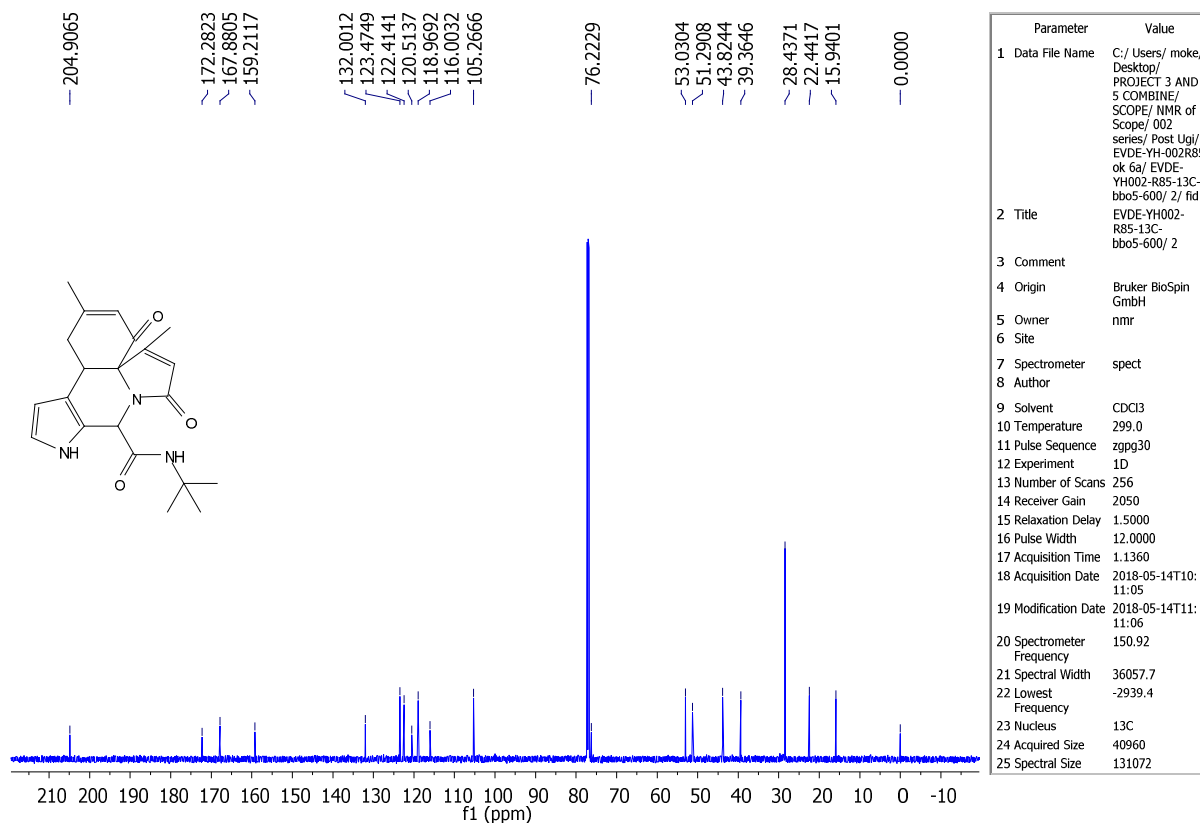
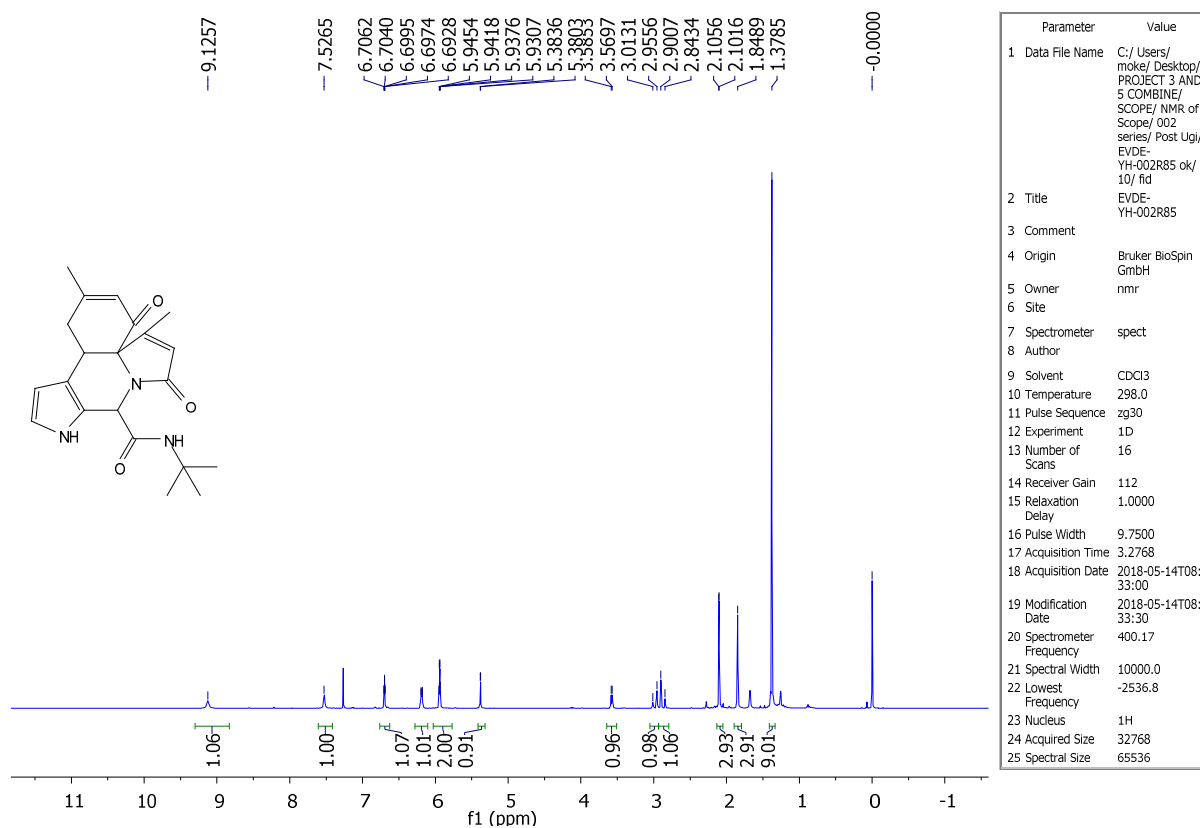
¹H and ¹³C NMR spectra of compound 2w



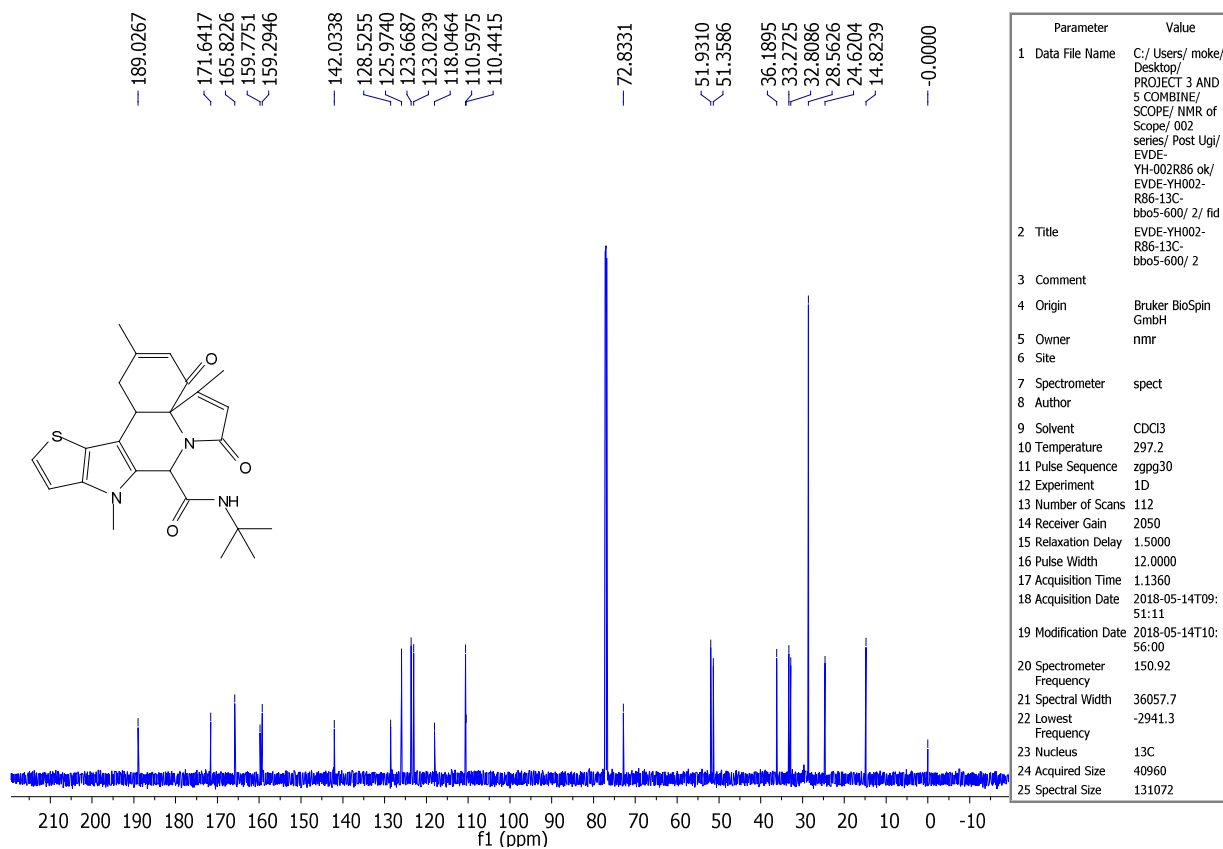
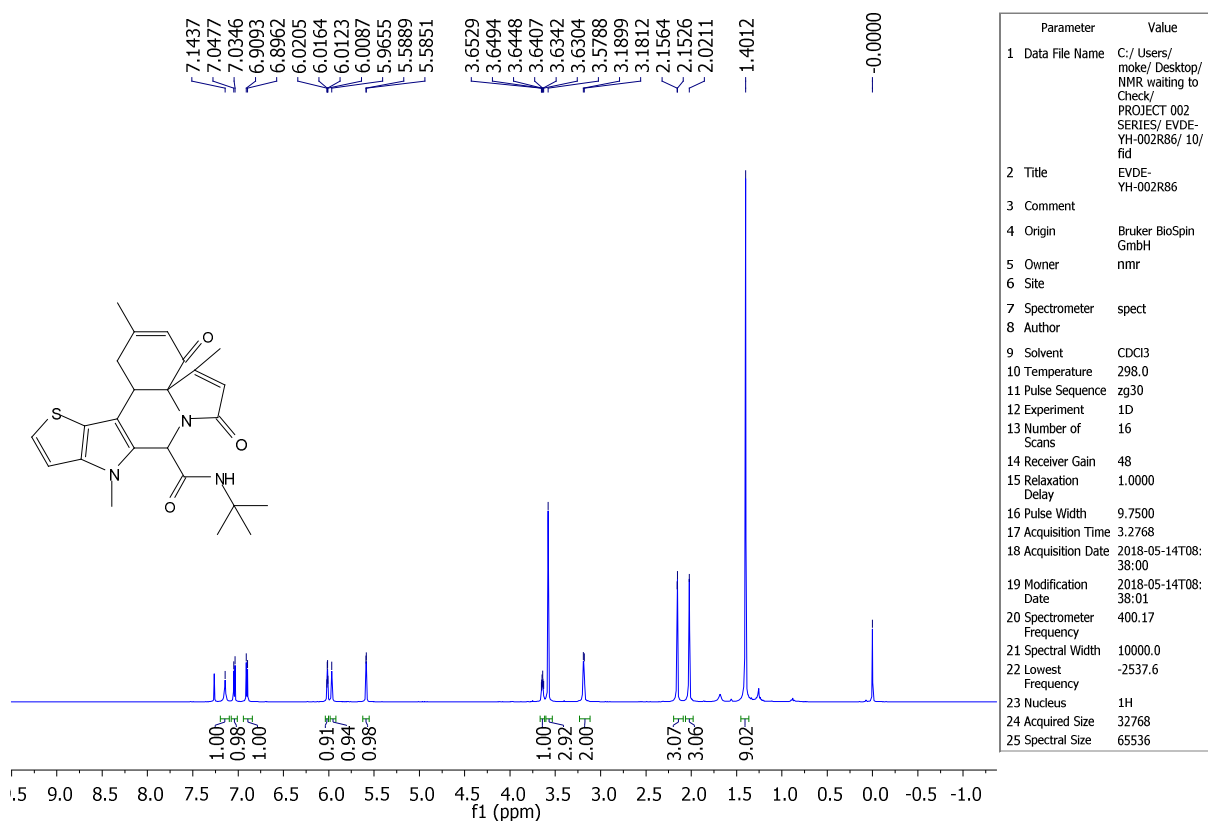
¹H and ¹³C NMR spectra of compound 2x



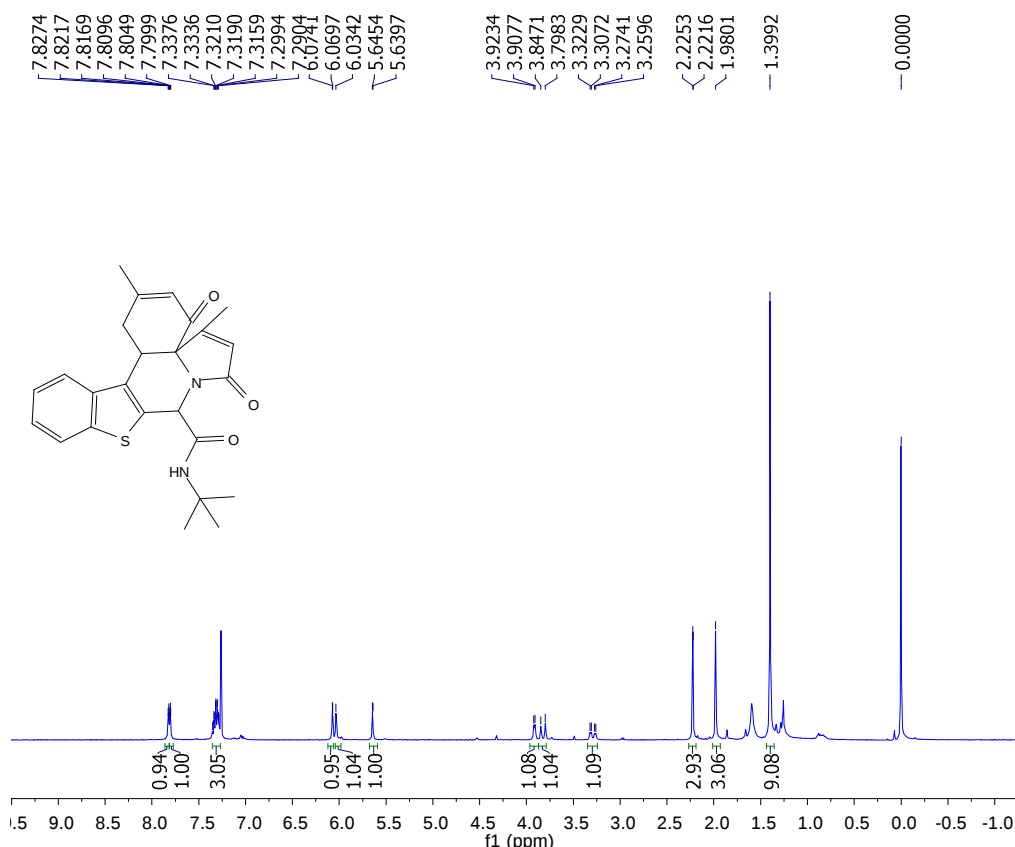
^1H and ^{13}C NMR spectra of compound **2ba**



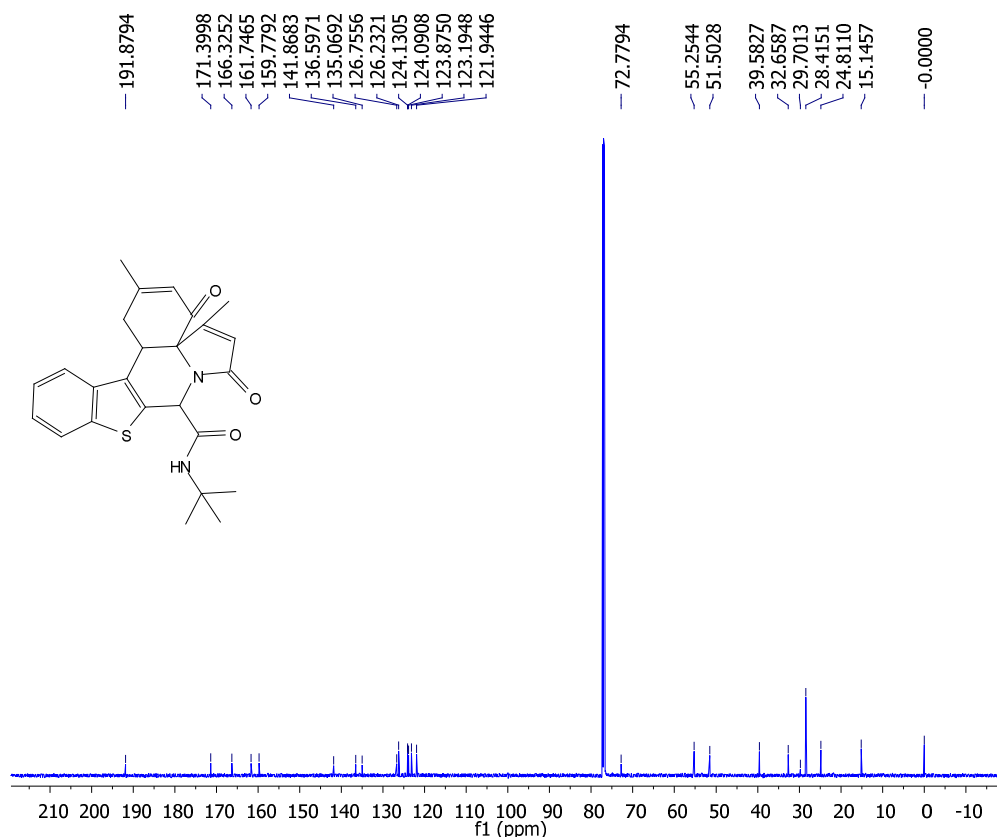
¹H and ¹³C NMR spectra of compound **2bb**



¹H and ¹³C NMR spectra of compound 2bc

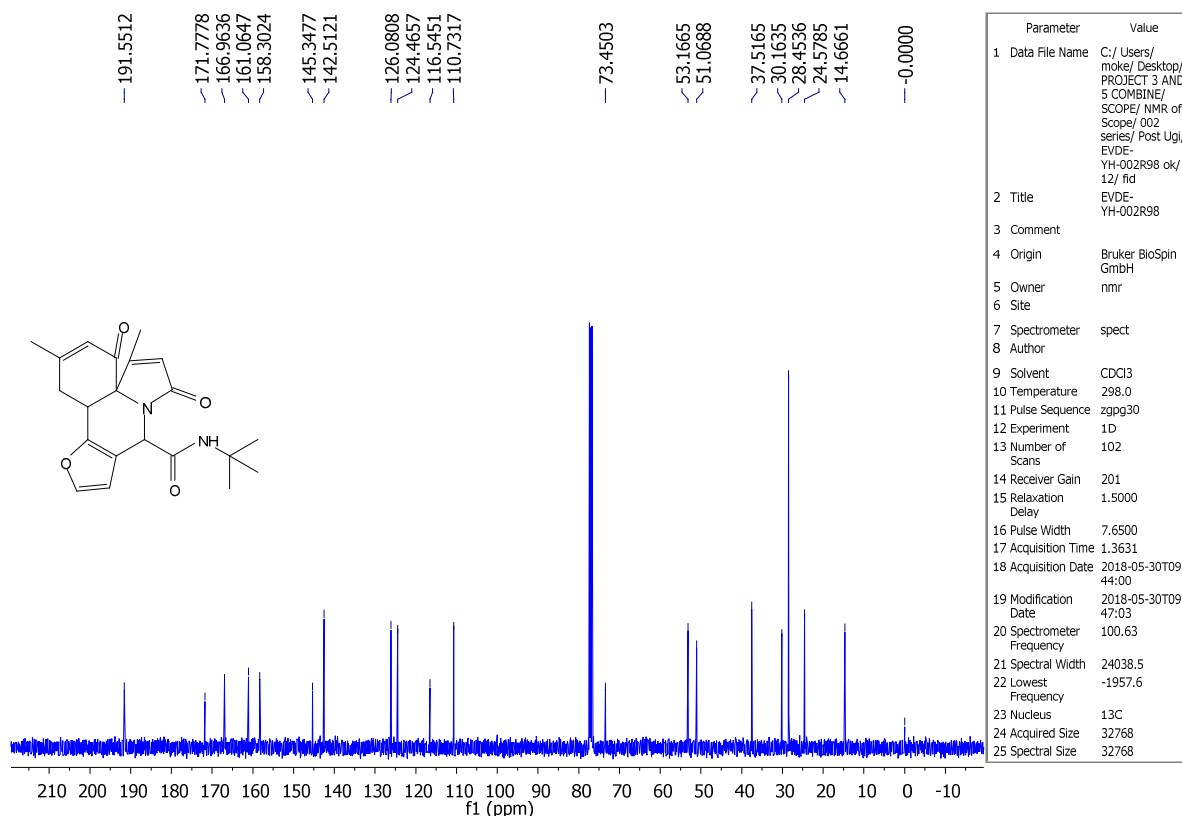
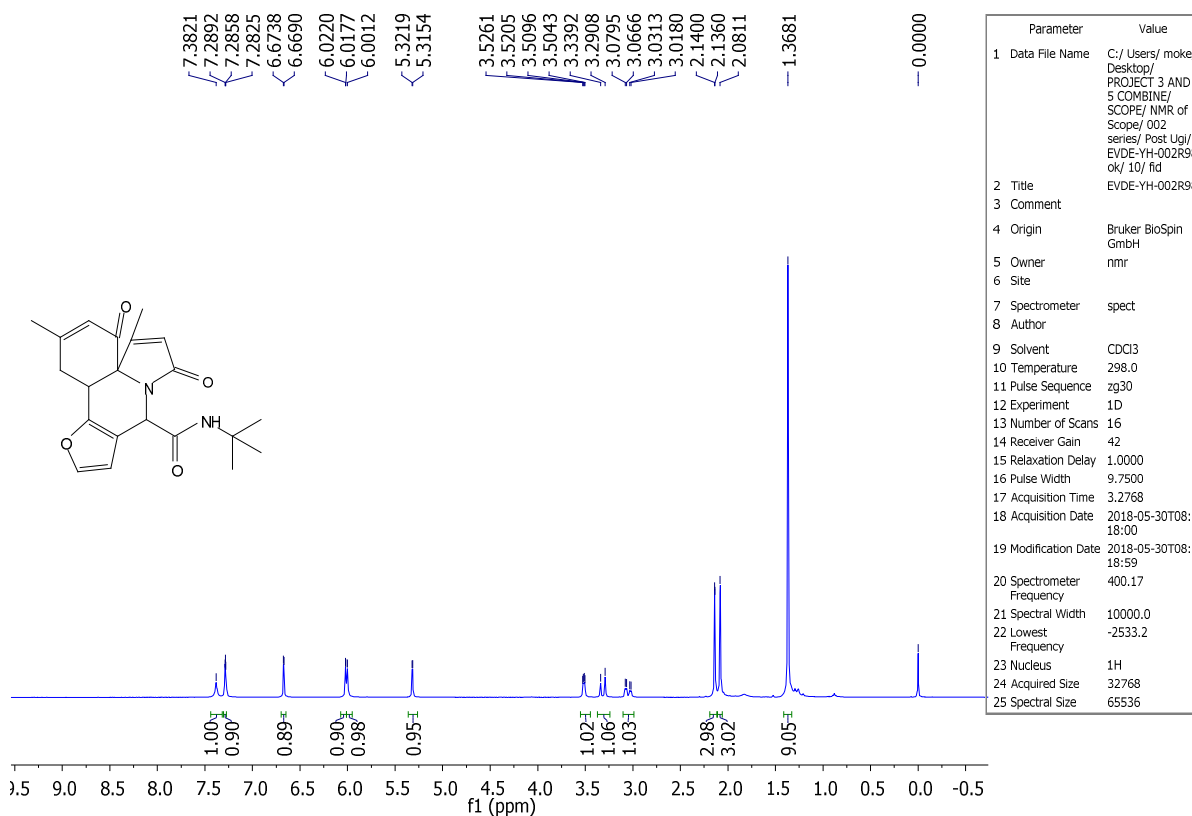


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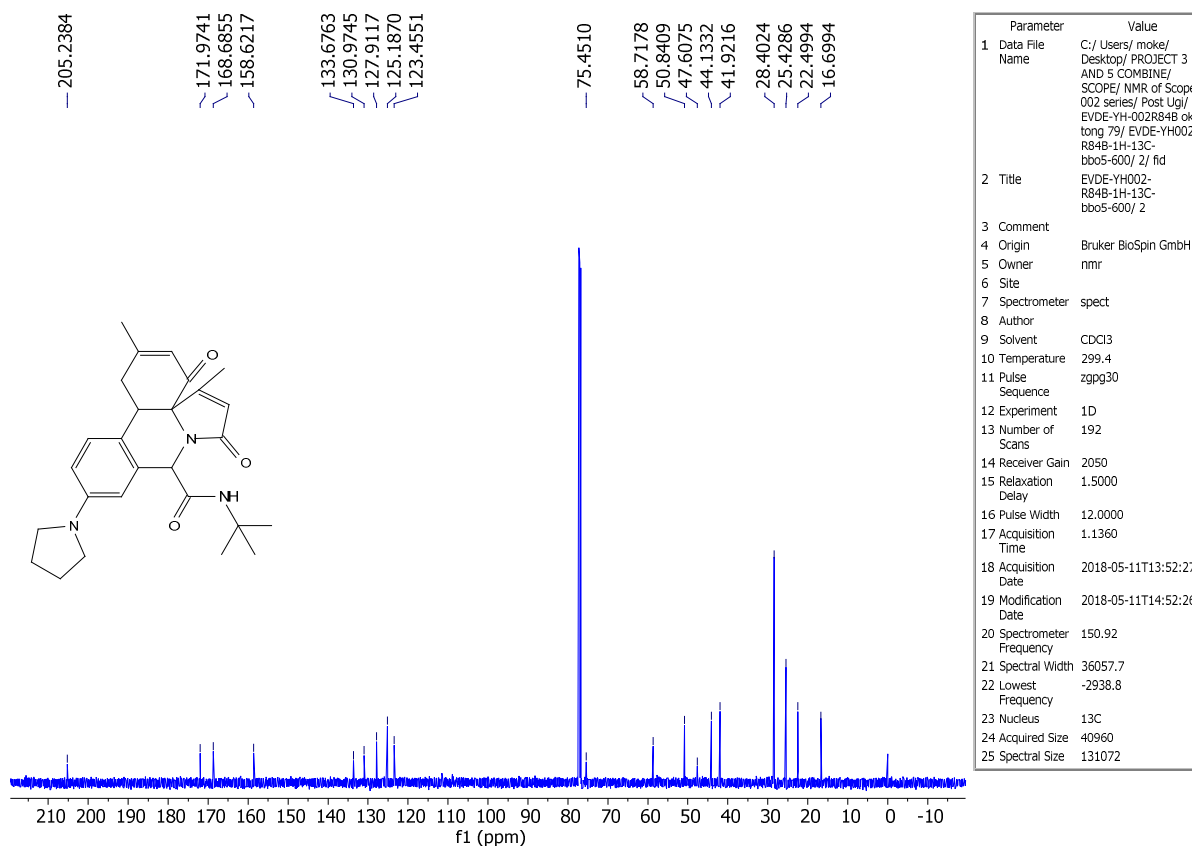
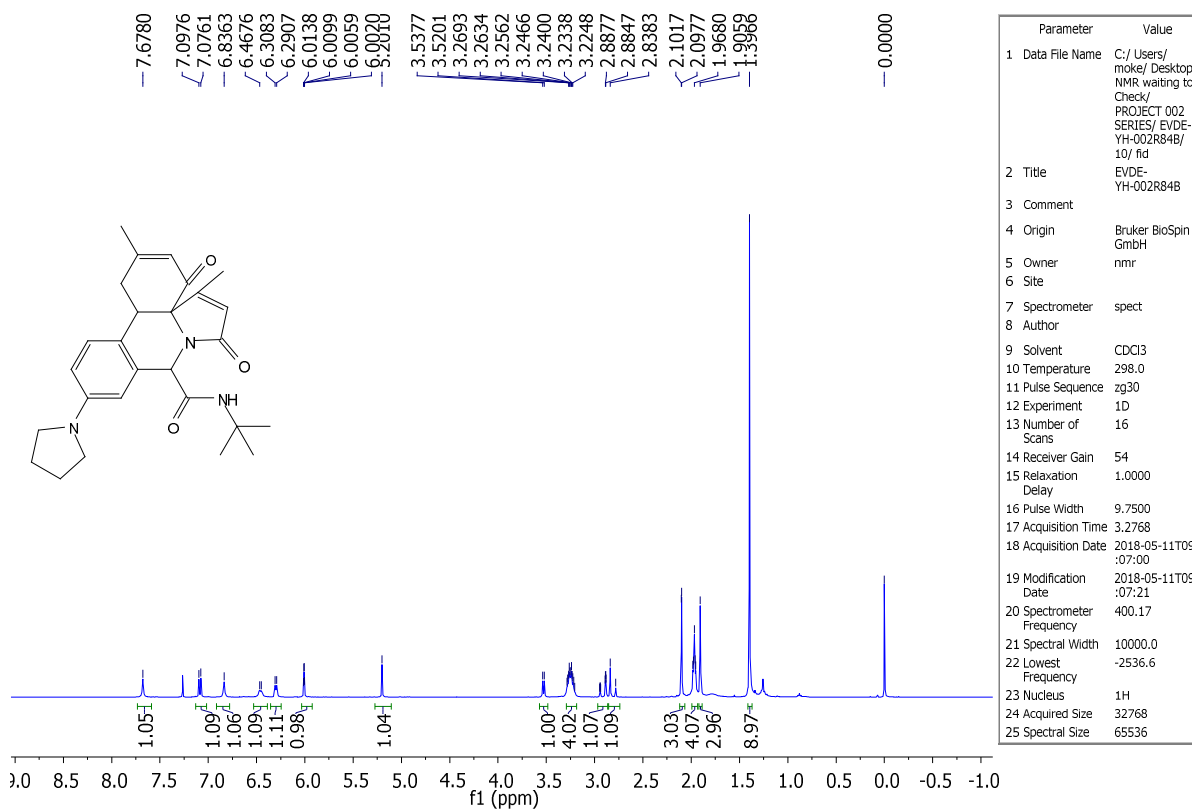


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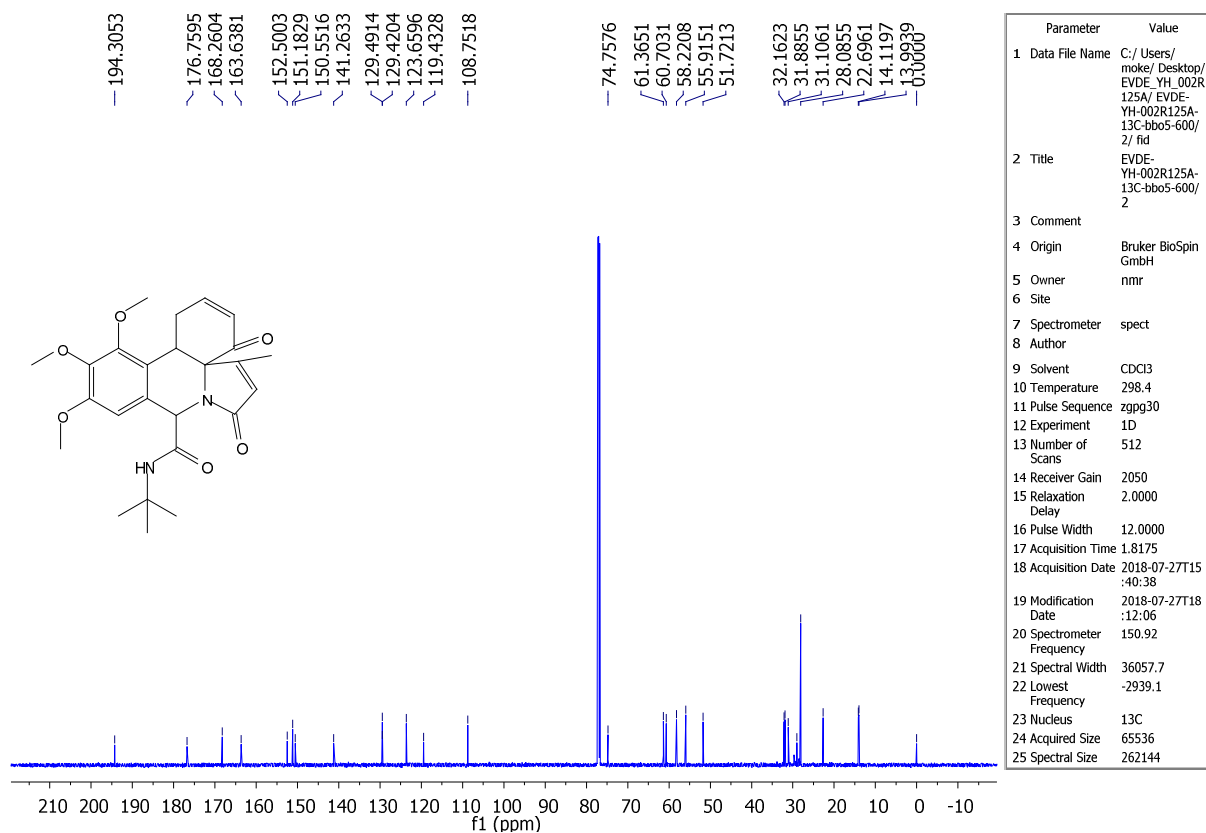
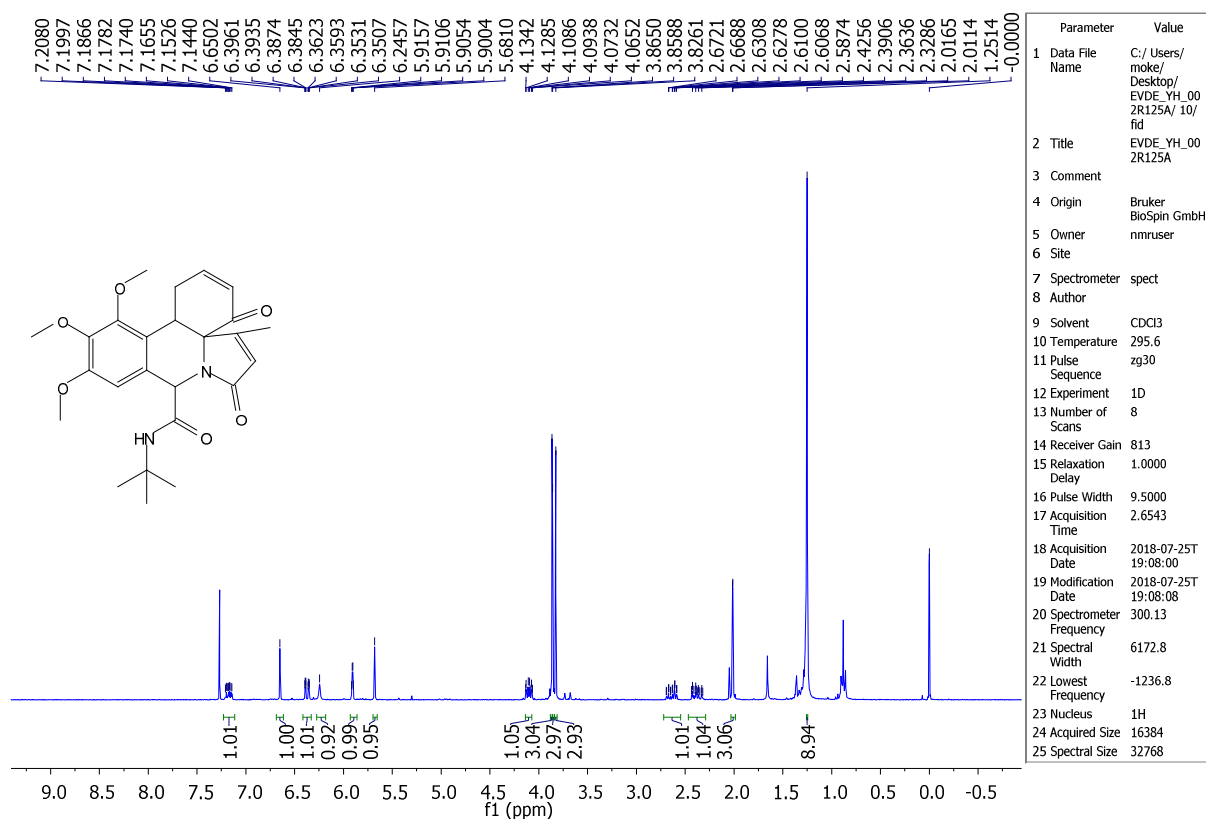
¹H and ¹³C NMR spectra of compound **2bd**



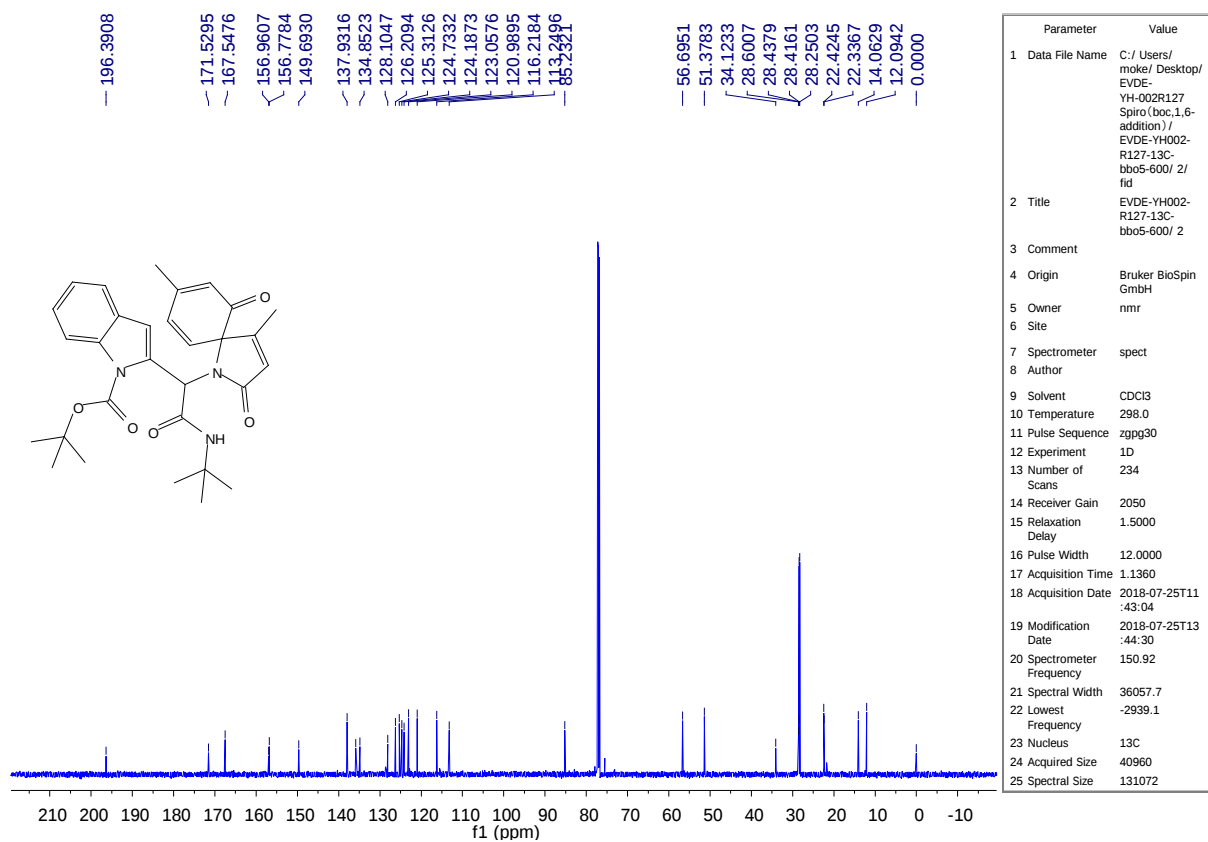
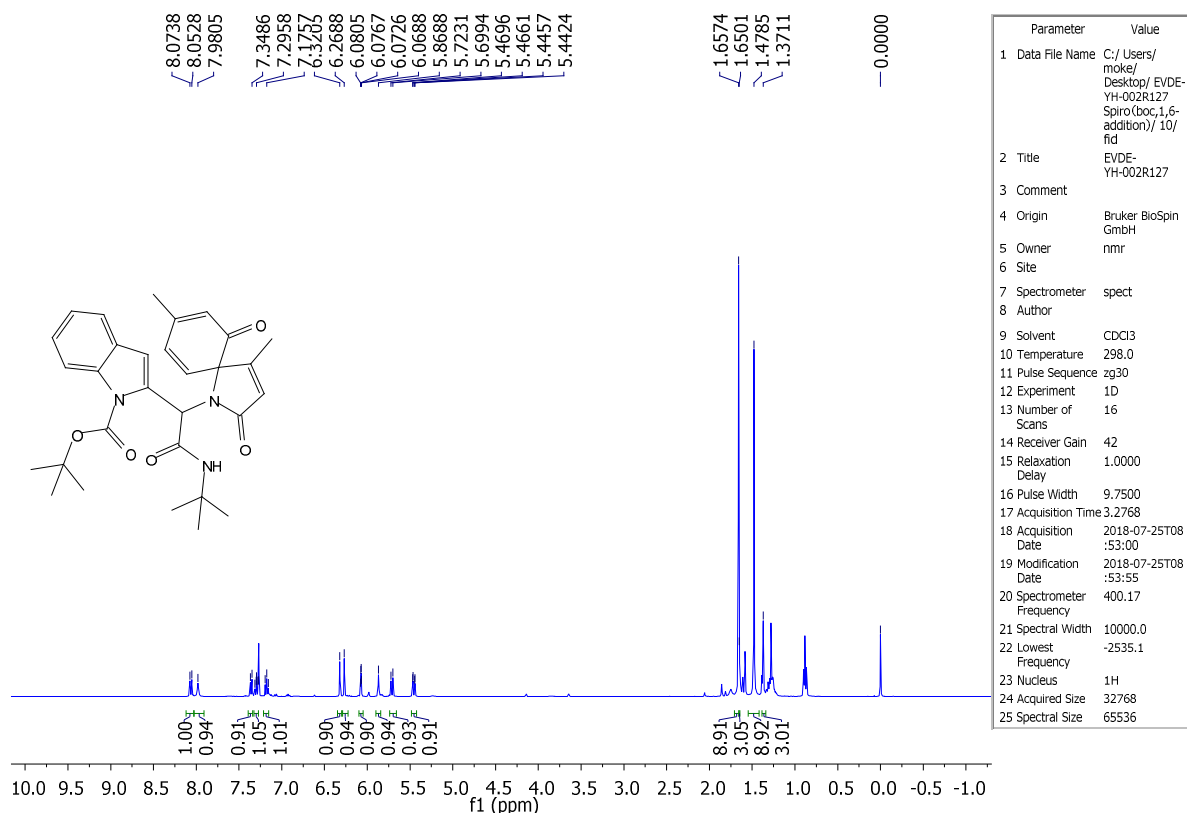
¹H and ¹³C NMR spectra of compound 2be



¹H and ¹³C NMR spectra of compound 2bf



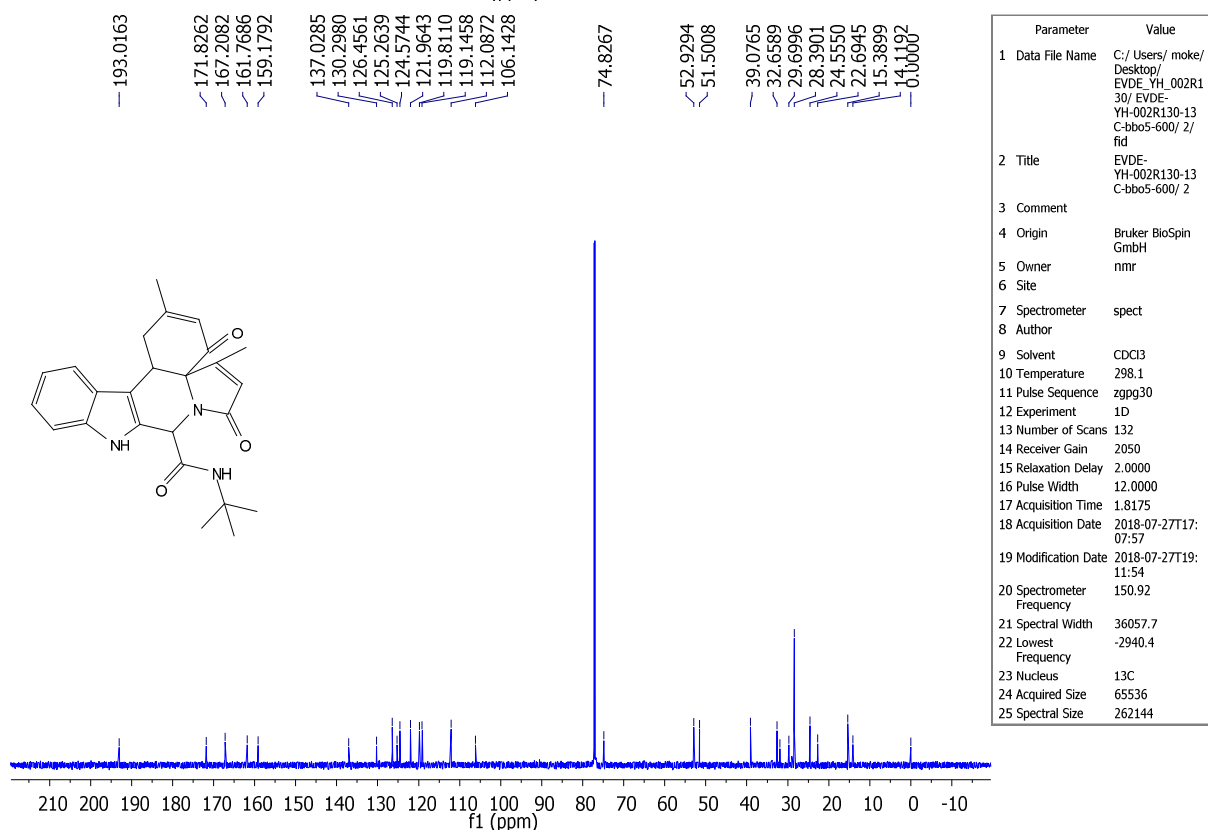
^1H and ^{13}C NMR spectra of compound **2y'**



Chemical structure of compound 1 is shown as an inset. The structure is a complex polycyclic molecule with a benzene ring fused to a pyrrole ring, which is further fused to a six-membered ring containing a nitrogen atom. The nitrogen atom is part of a five-membered ring containing a carbonyl group. The molecule has a tert-butyl group attached to the nitrogen atom.

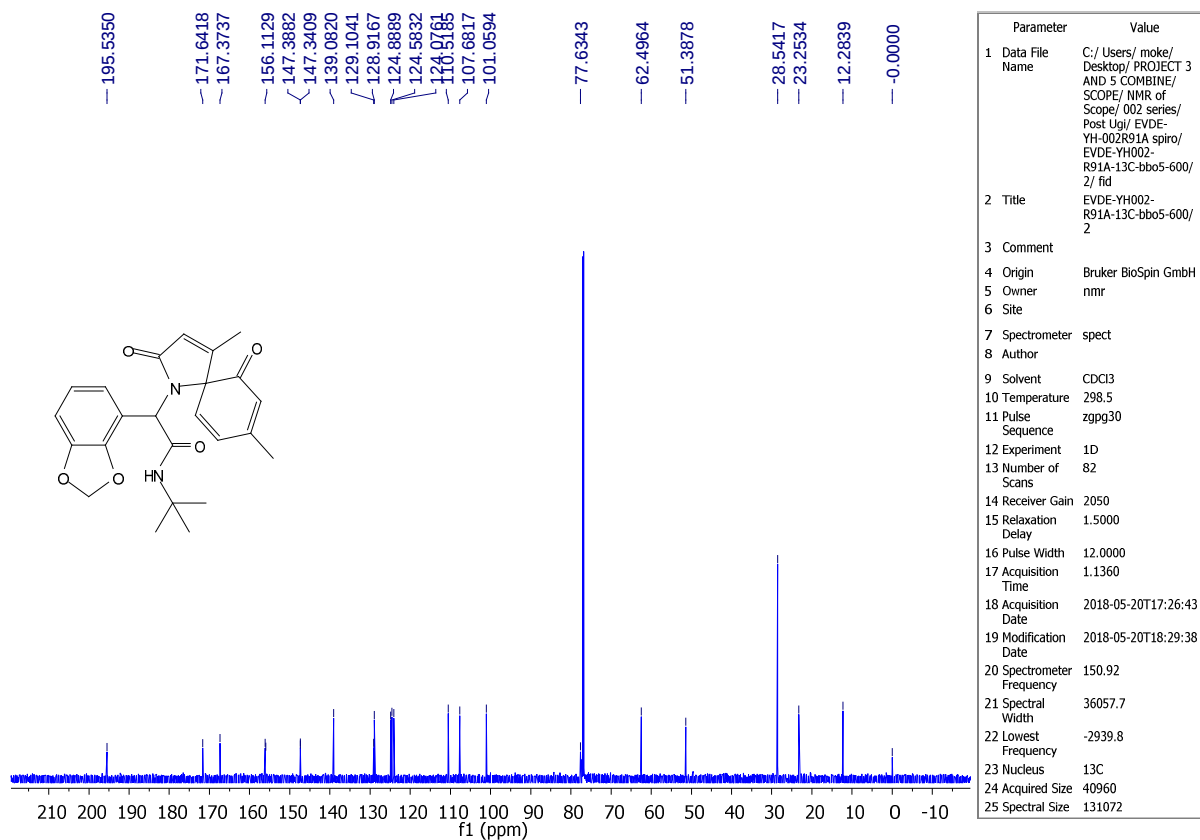
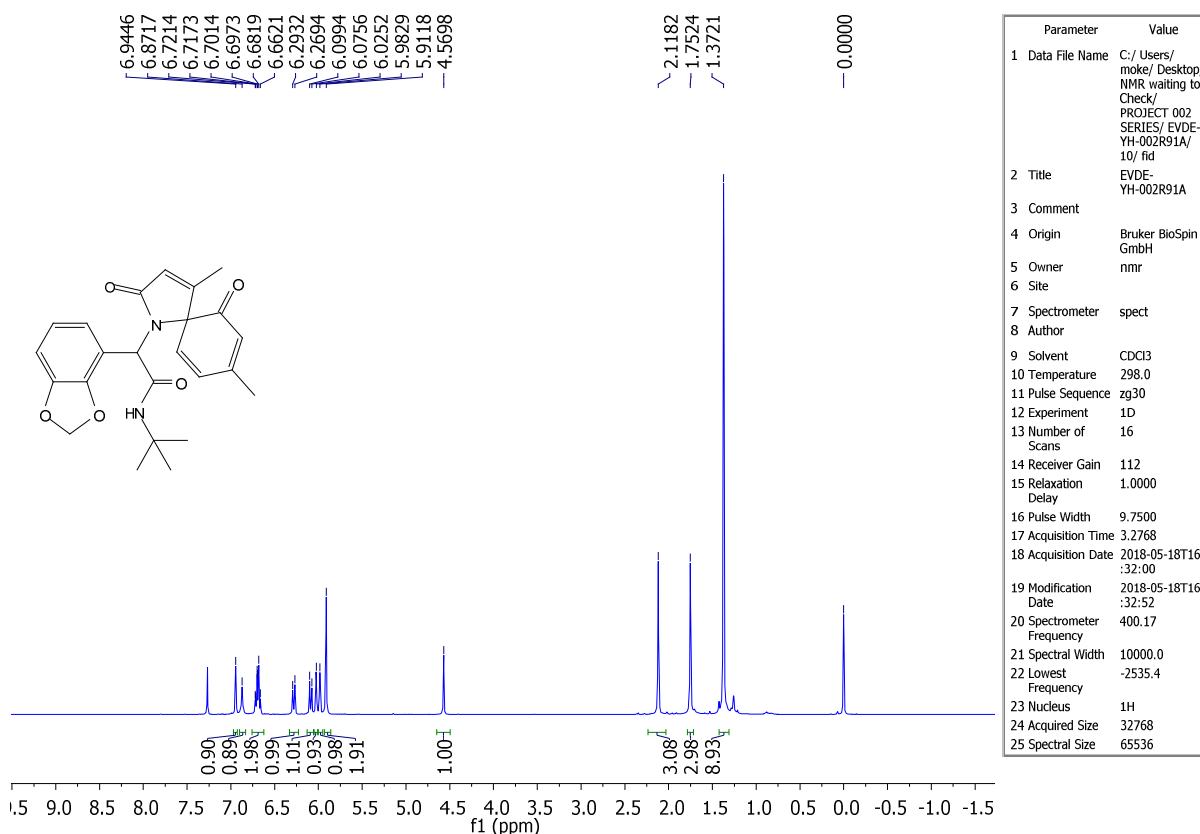
¹H NMR spectrum (CDCl₃) of compound 1. The x-axis represents the chemical shift in ppm, ranging from 0.000 to 9.4407. The spectrum shows several peaks, with the most prominent ones at 9.4407, 7.7490, 7.6602, 7.6333, 7.3804, 7.3537, 7.2011, 7.1974, 7.1771, 7.1737, 7.1702, 7.1504, 7.1466, 7.1107, 7.1064, 7.0869, 7.0832, 7.0795, 7.0600, 7.0561, 6.0815, 6.0764, 6.0710, 6.0658, 5.9762, 5.9718, 5.9679, 5.9633, 5.5333, 5.5261, 3.8482, 3.8419, 3.8220, 3.8151, 3.8093, 3.8026, 3.7962, 3.7835, 3.7773, 2.2439, 2.2386, 2.1064, 2.1027, 2.0987, 1.3884, and 0.0000 ppm. The peaks are assigned to the protons in the molecule. The integration values are 1.00, 0.95, 1.02, 1.07, 0.96, 0.99, 0.92, 0.94, 0.93, 1.92, 0.99, 3.01, 2.97, and 9.02.

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7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	1024
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
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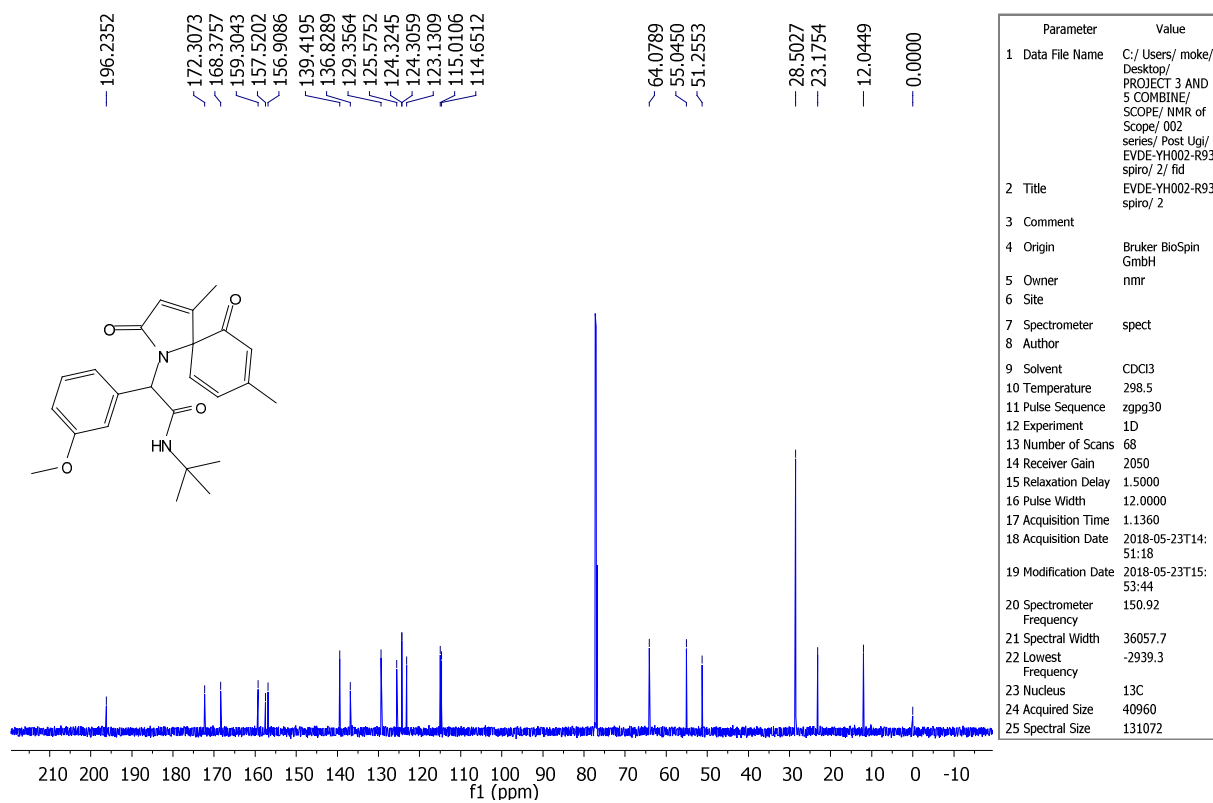
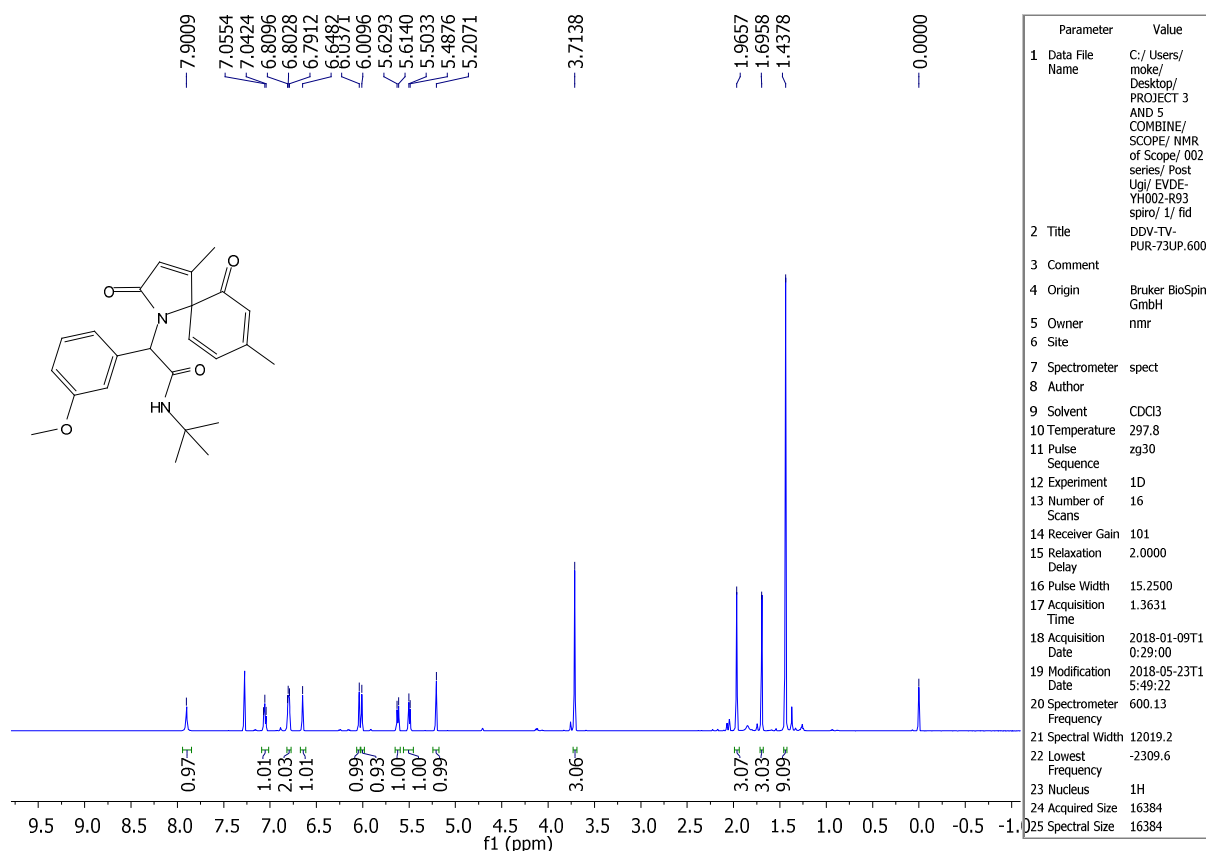


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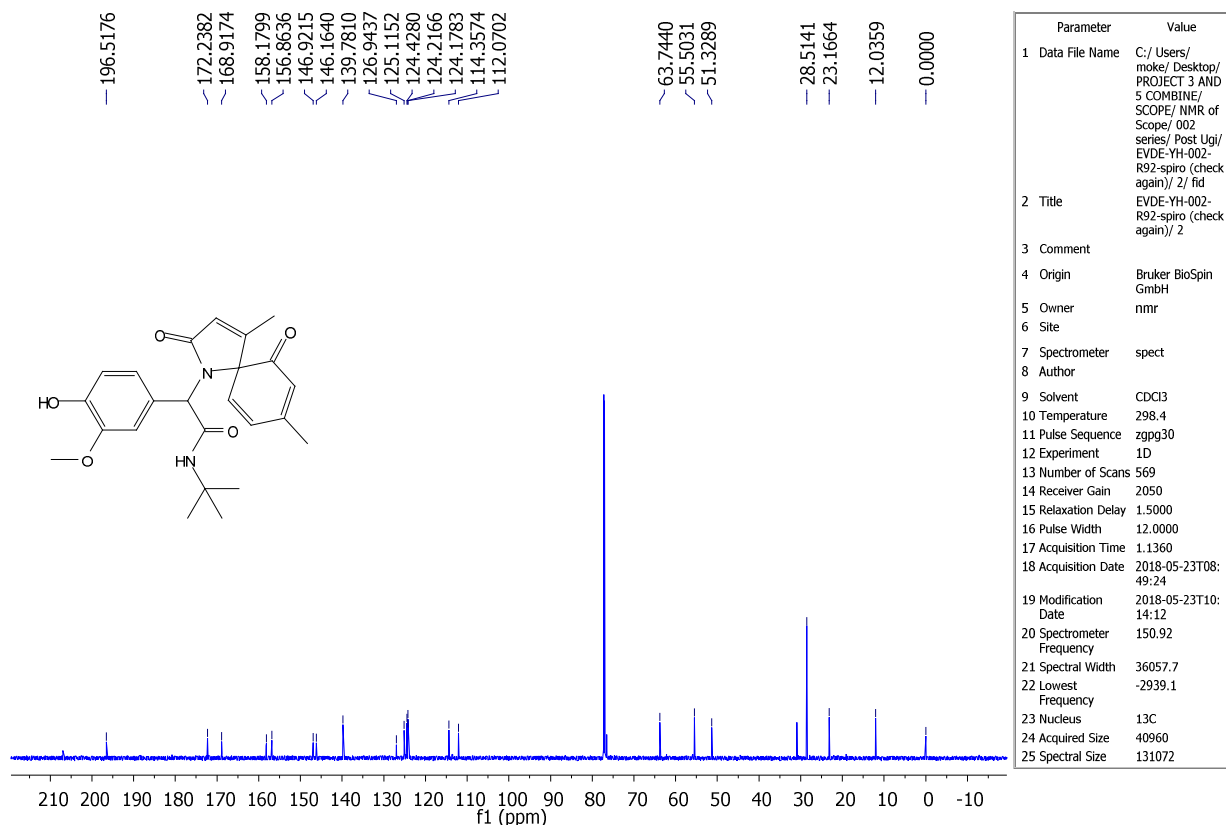
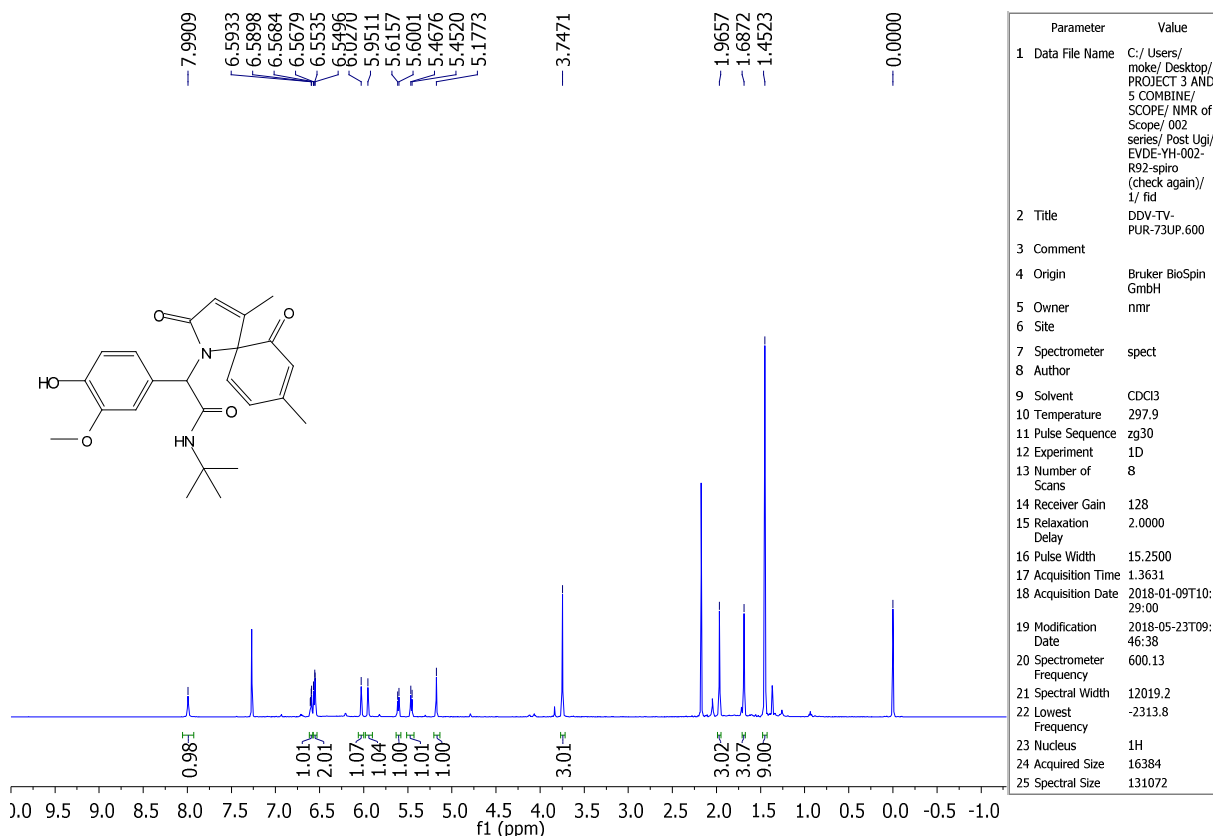
¹H and ¹³C NMR spectra of compound **s2b**



^1H and ^{13}C NMR spectra of compound s2c

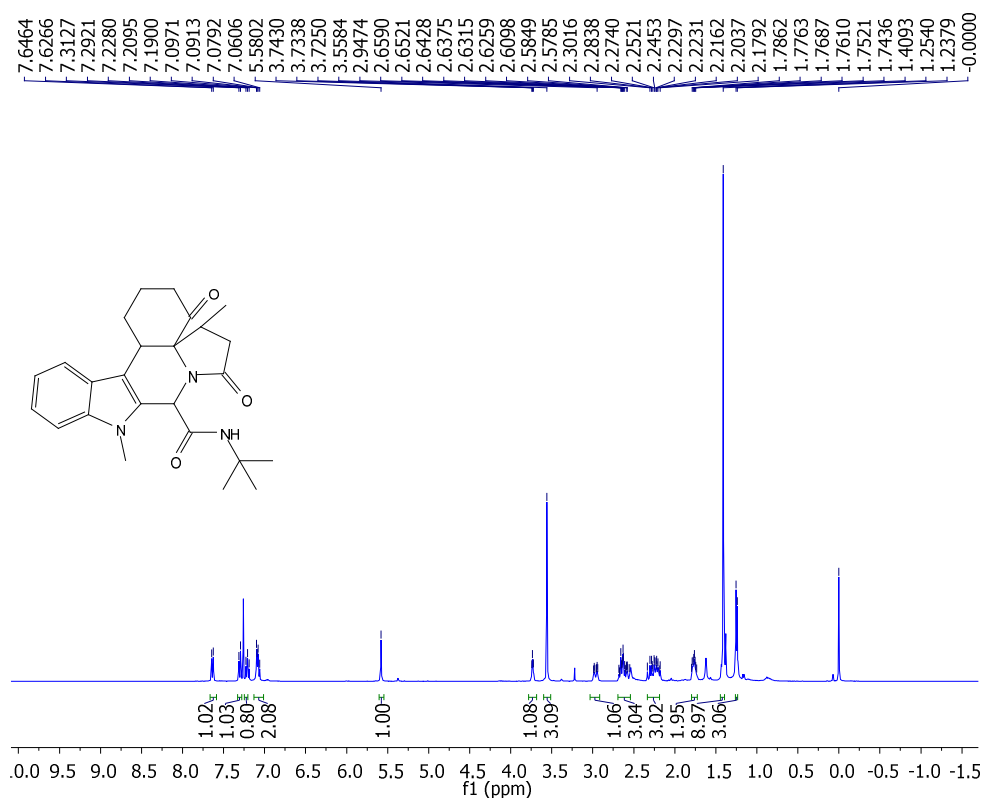


¹H and ¹³C NMR spectra of compound **s2d**

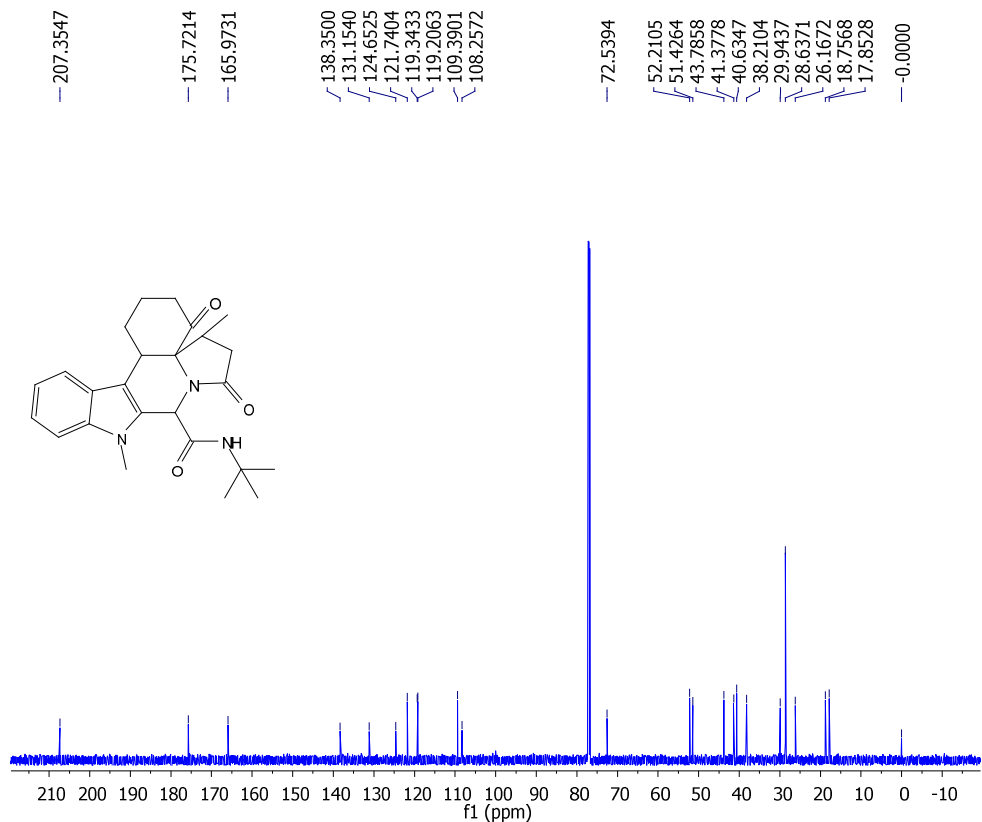


Copies of NMR spectra (transformation products of 2a)

¹H and ¹³C NMR spectra of compound 3

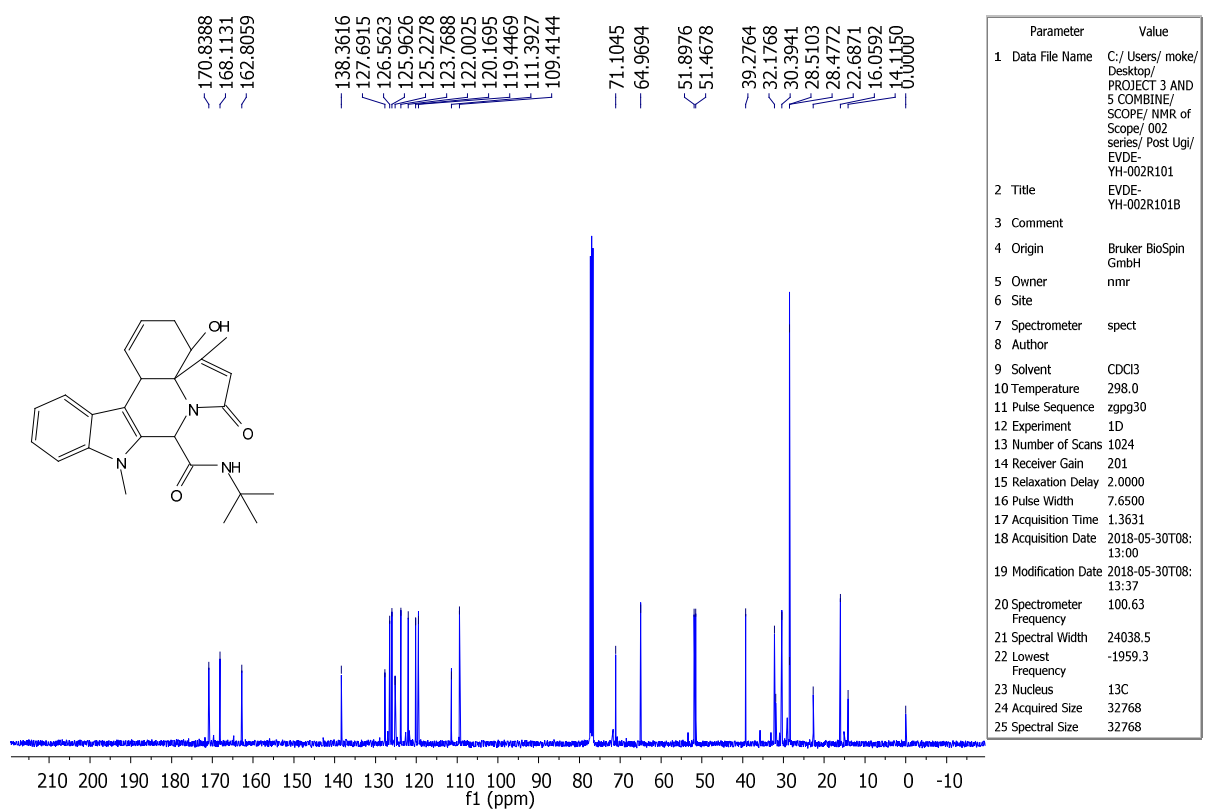
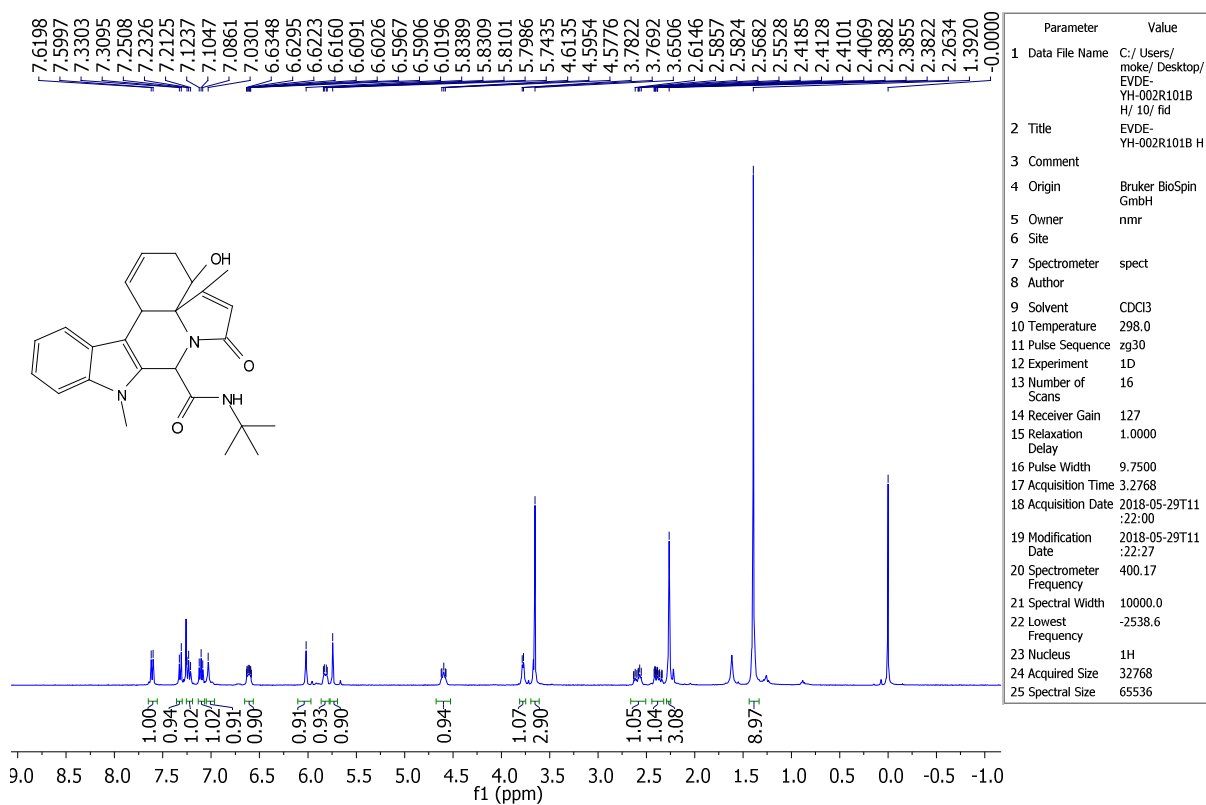


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7 Spectrometer	spect
8 Author	
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12 Experiment	1D
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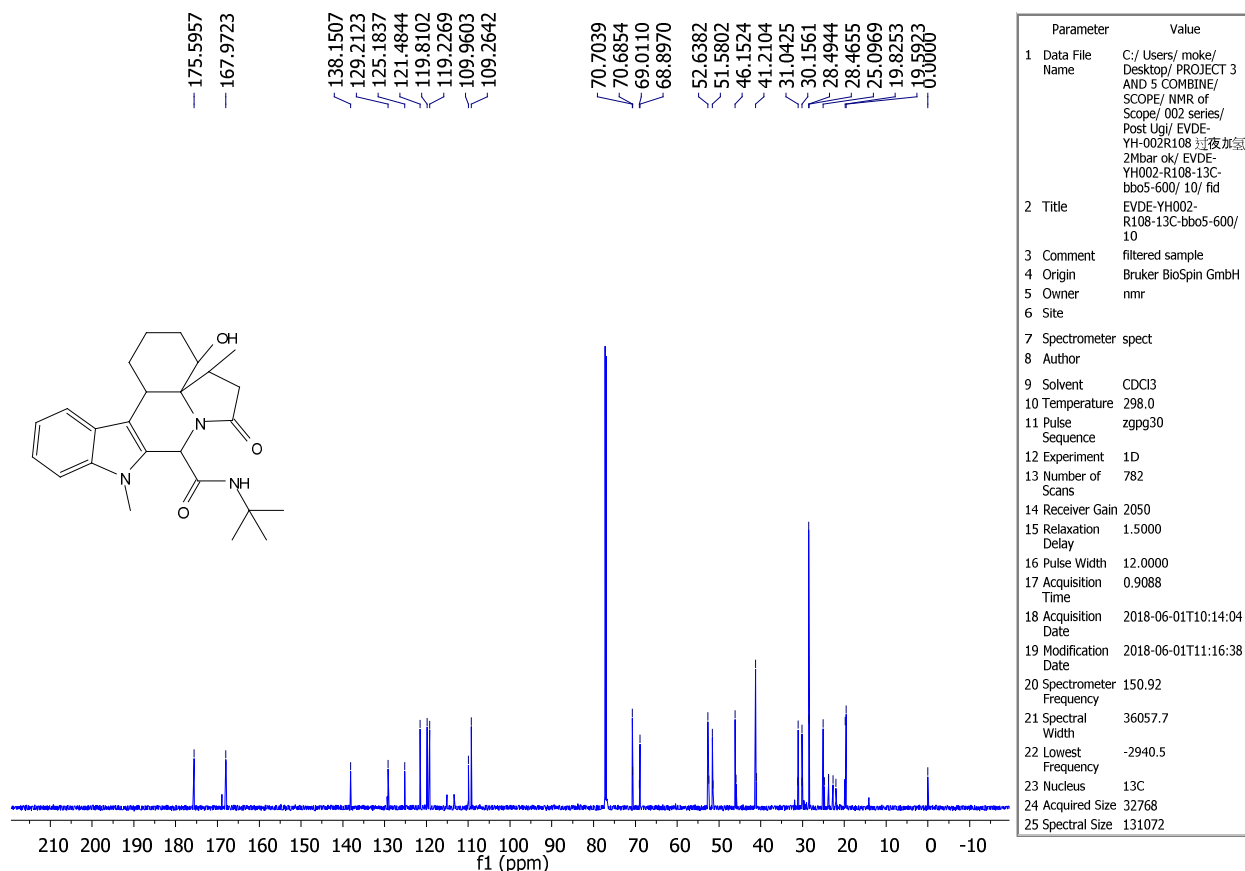
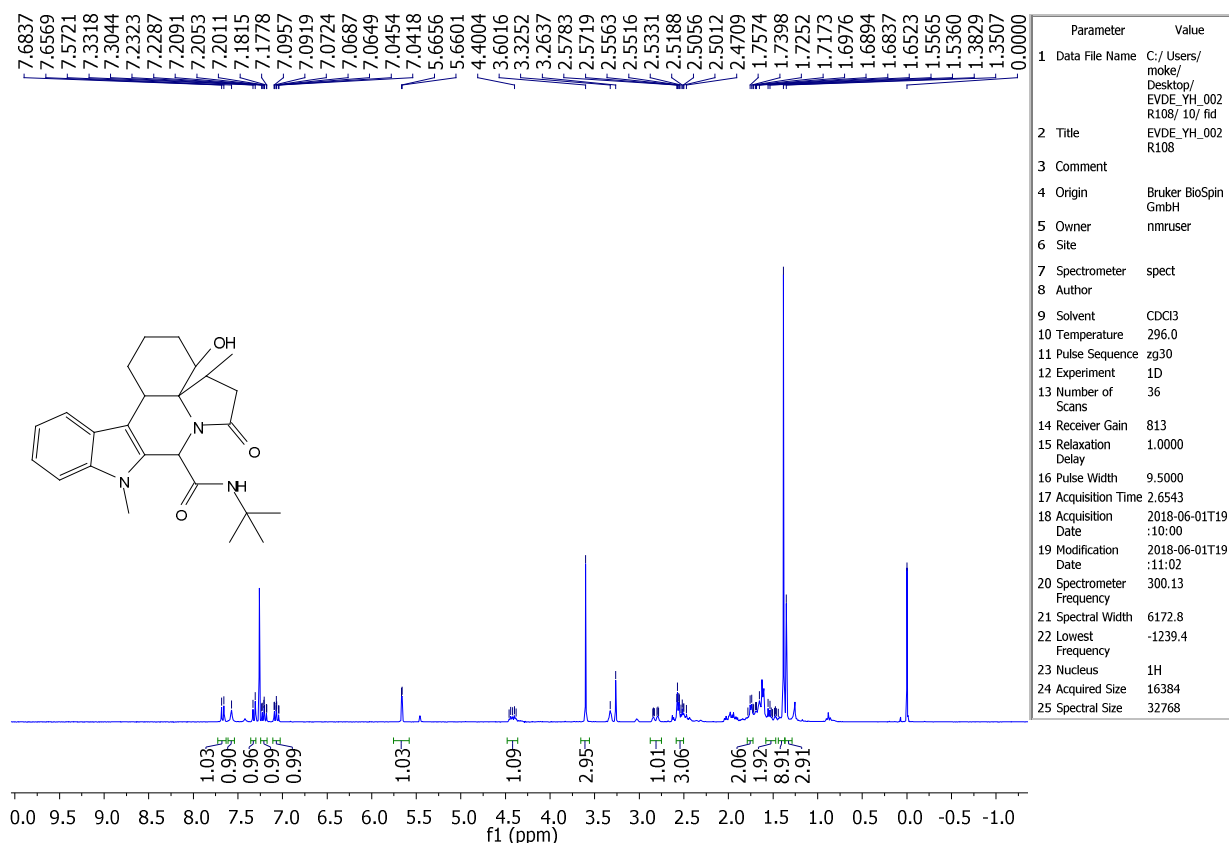


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Post Ugl/ EVDE-YH002- R110-13C- bbo5-600/ 2/ fid
2 Title	EVDE-YH002- R110-13C- bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	80
14 Receiver Gain	2050
15 Relaxation Delay	1.7500
16 Pulse Width	12.0000
17 Acquisition Time	1.1360
18 Acquisition Date	2018-06-07T09:22:36
19 Modification Date	2018-06-07T10:23:20
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2940.8
23 Nucleus	13C
24 Acquired Size	40960
25 Spectral Size	131072

^1H and ^{13}C NMR spectra of compound **s1a**

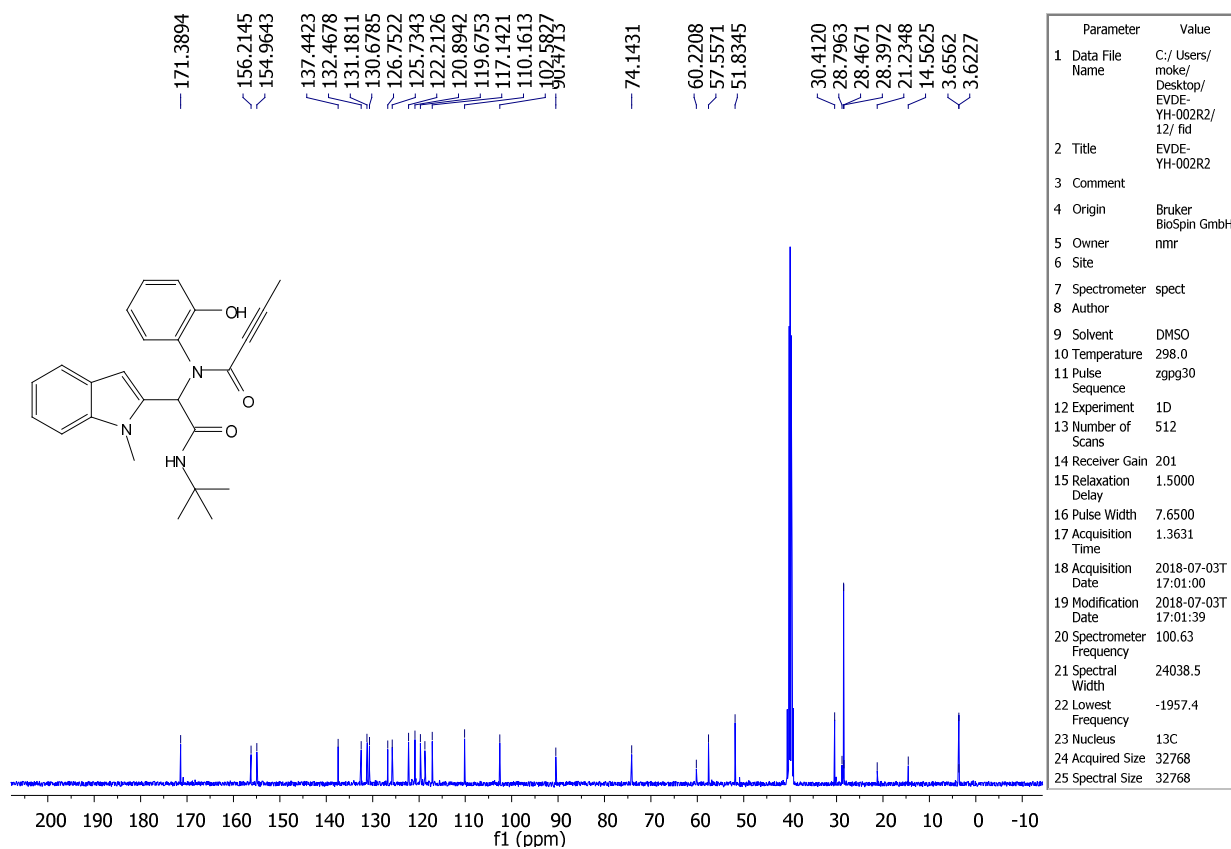
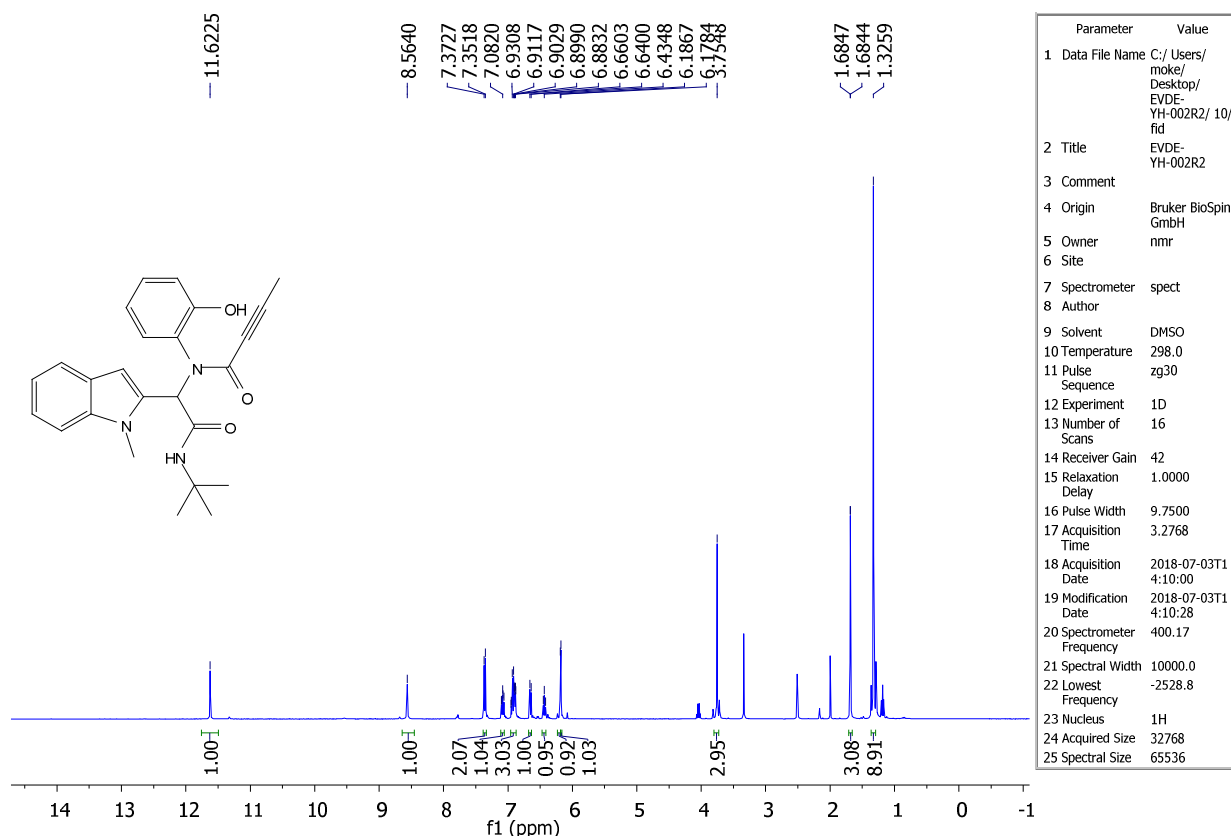


¹H and ¹³C NMR spectra of compound 4

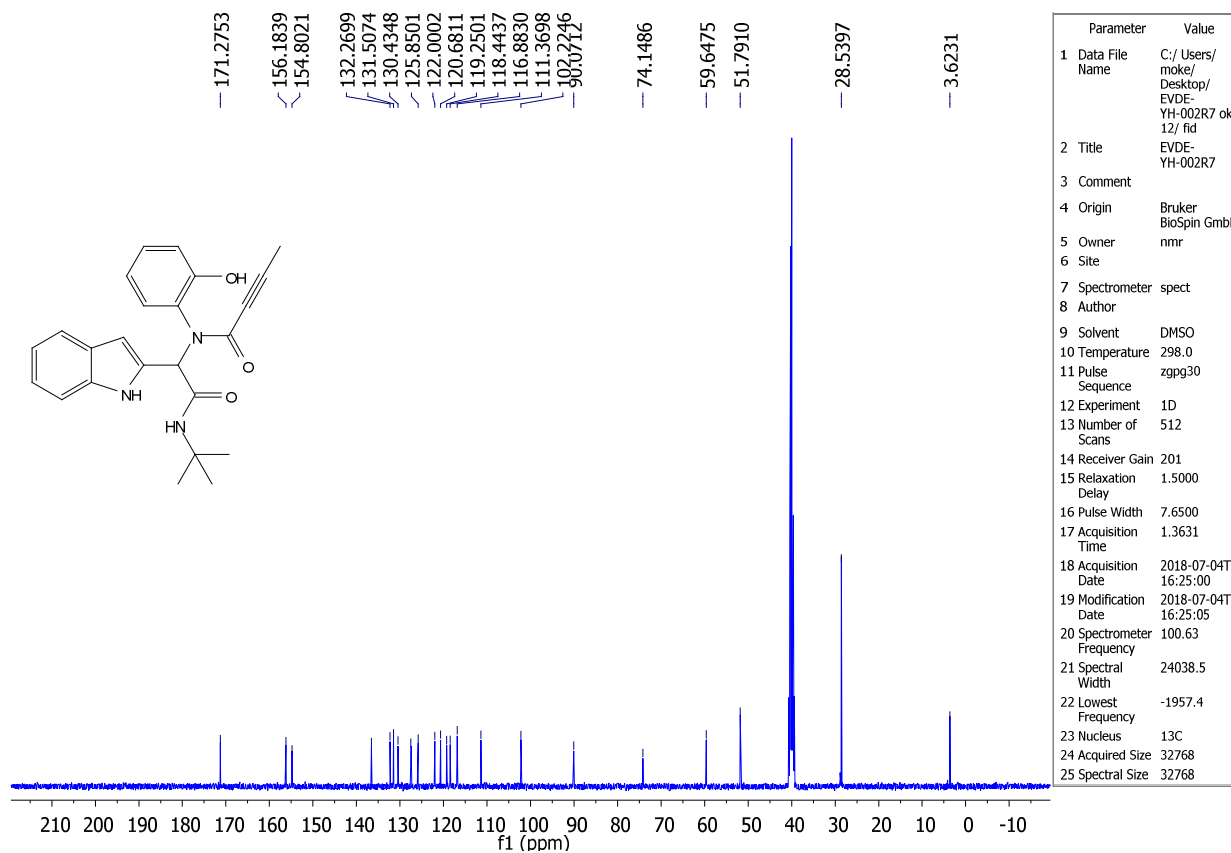
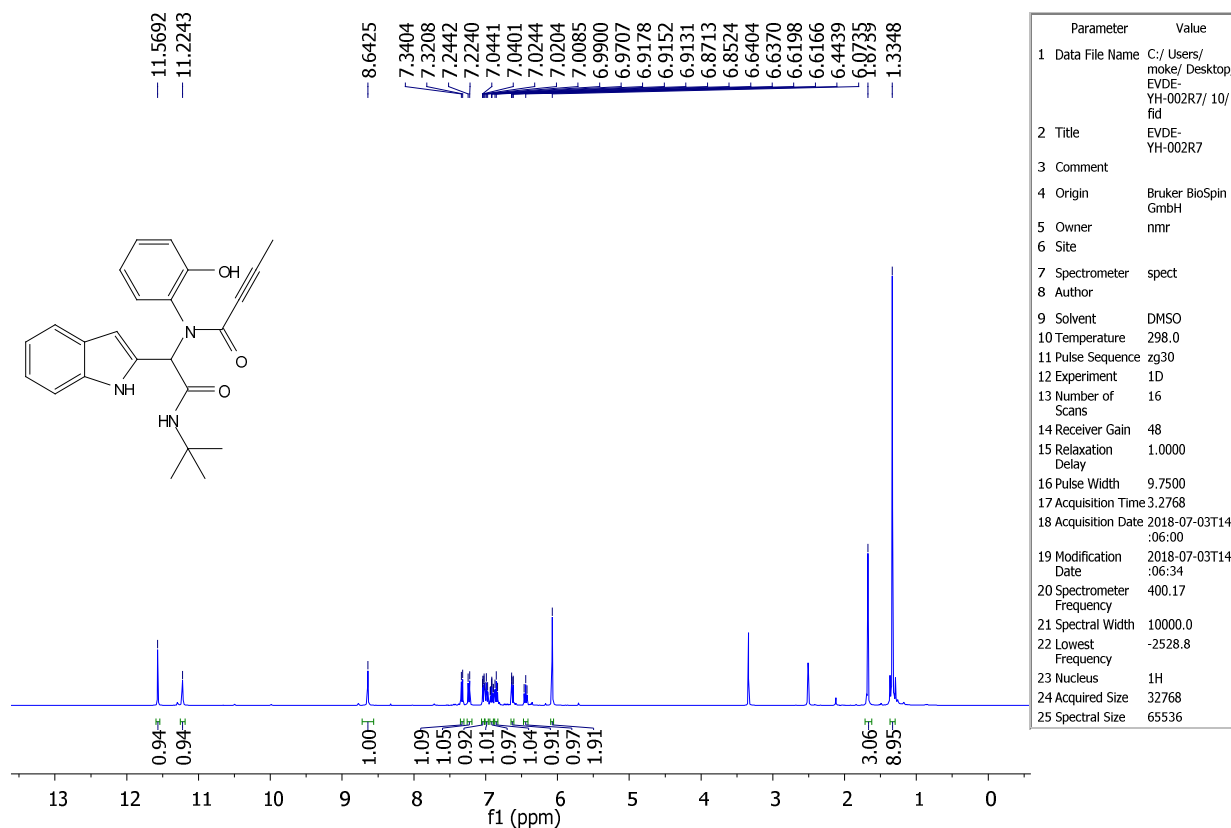


Copies of NMR spectra (Ugi products)

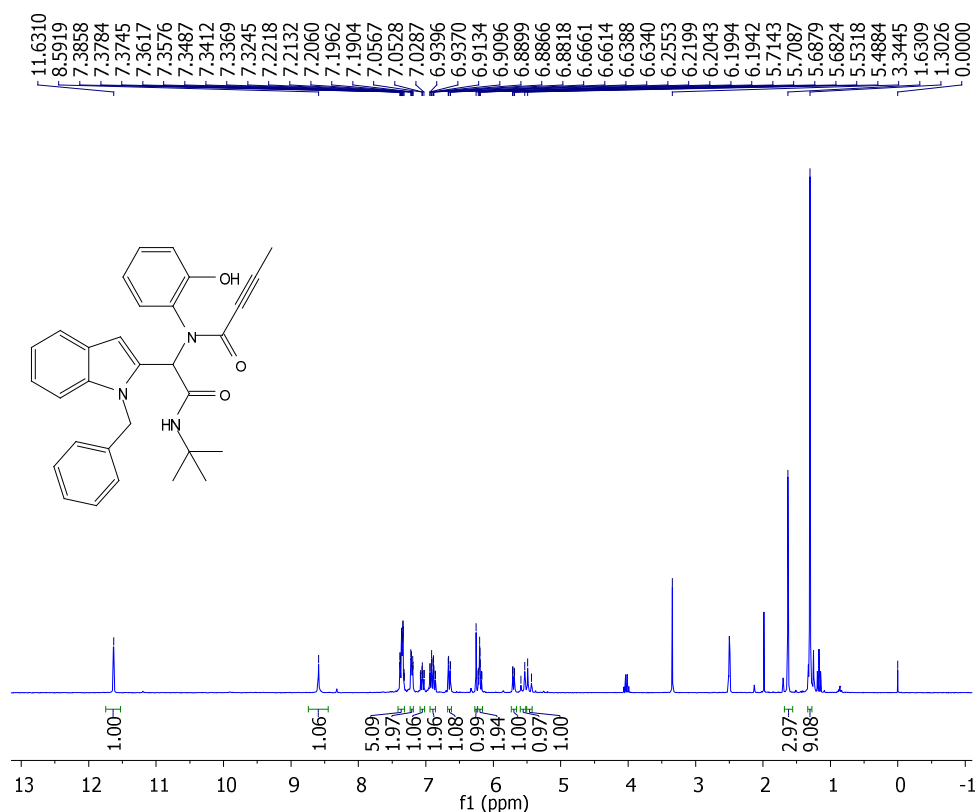
¹H and ¹³C NMR spectra of compound 1a



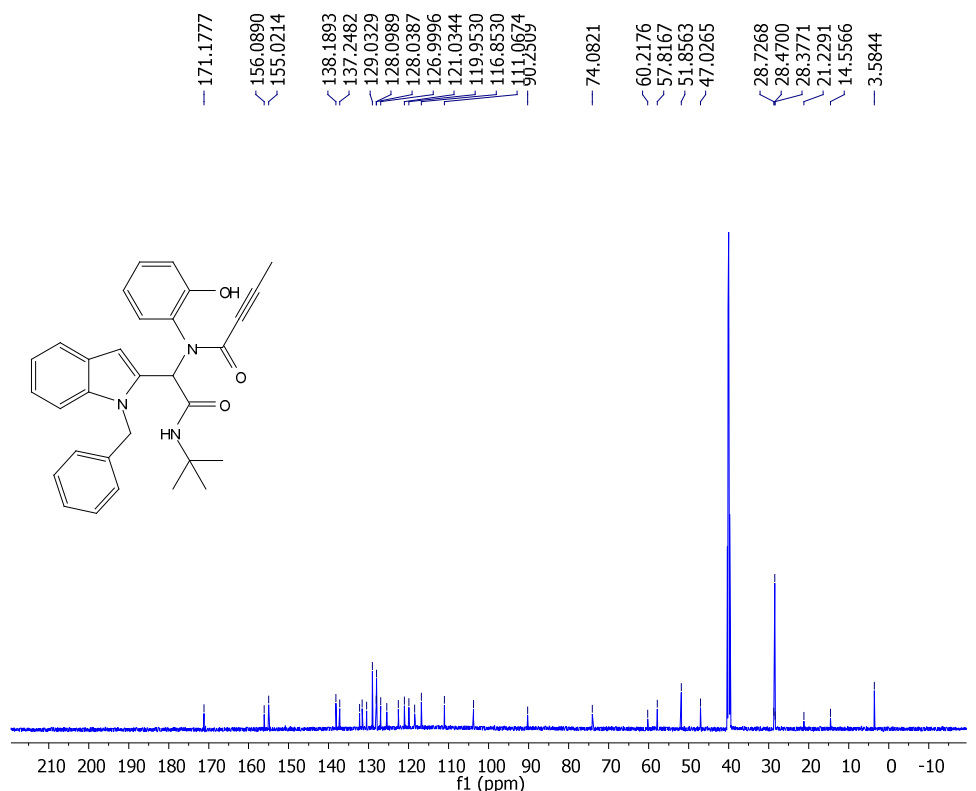
^1H and ^{13}C NMR spectra of compound **1b**



¹H and ¹³C NMR spectra of compound 1c

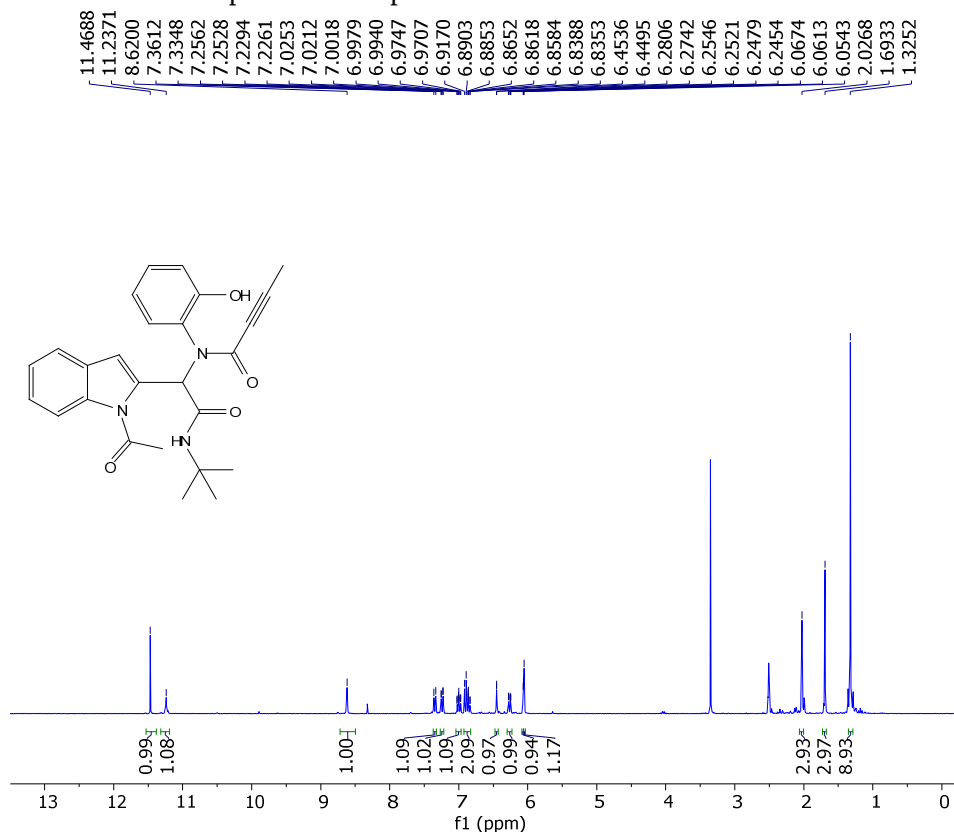


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ug/ EVDE_YH_002R43/ 10/ fid
2 Title	EVDE_YH_002R43
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmruser
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	295.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	512
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	2.6543
18 Acquisition Date	2017-11-30T16:57:00
19 Modification Date	2017-11-30T16:57:58
20 Spectrometer Frequency	300.13
21 Spectral Width	6172.8
22 Lowest Frequency	-1235.5
23 Nucleus	1H
24 Acquired Size	16384
25 Spectral Size	32768

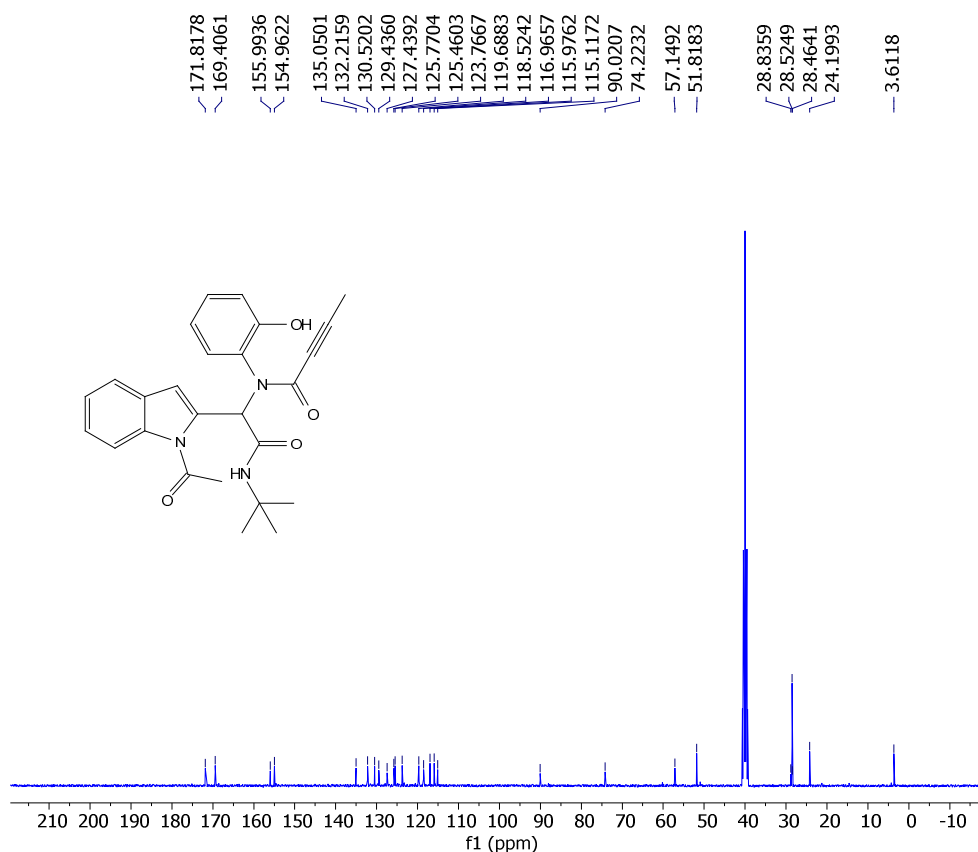


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ug/ EVDE_YH_002R43/ EVDE-YH002R43-13C-6dec2017-bi5.600/ 2/ fid
2 Title	EVDE-YH002R43-13C-6dec2017-bi5.600/ 2
3 Comment	Calibration TX1
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	477
14 Receiver Gain	575
15 Relaxation Delay	2.0000
16 Pulse Width	12.6300
17 Acquisition Time	0.9088
18 Acquisition Date	2017-12-06T12:02:37
19 Modification Date	2017-12-06T13:17:02
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2938.6
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	131072

¹H and ¹³C NMR spectra of compound **1d**

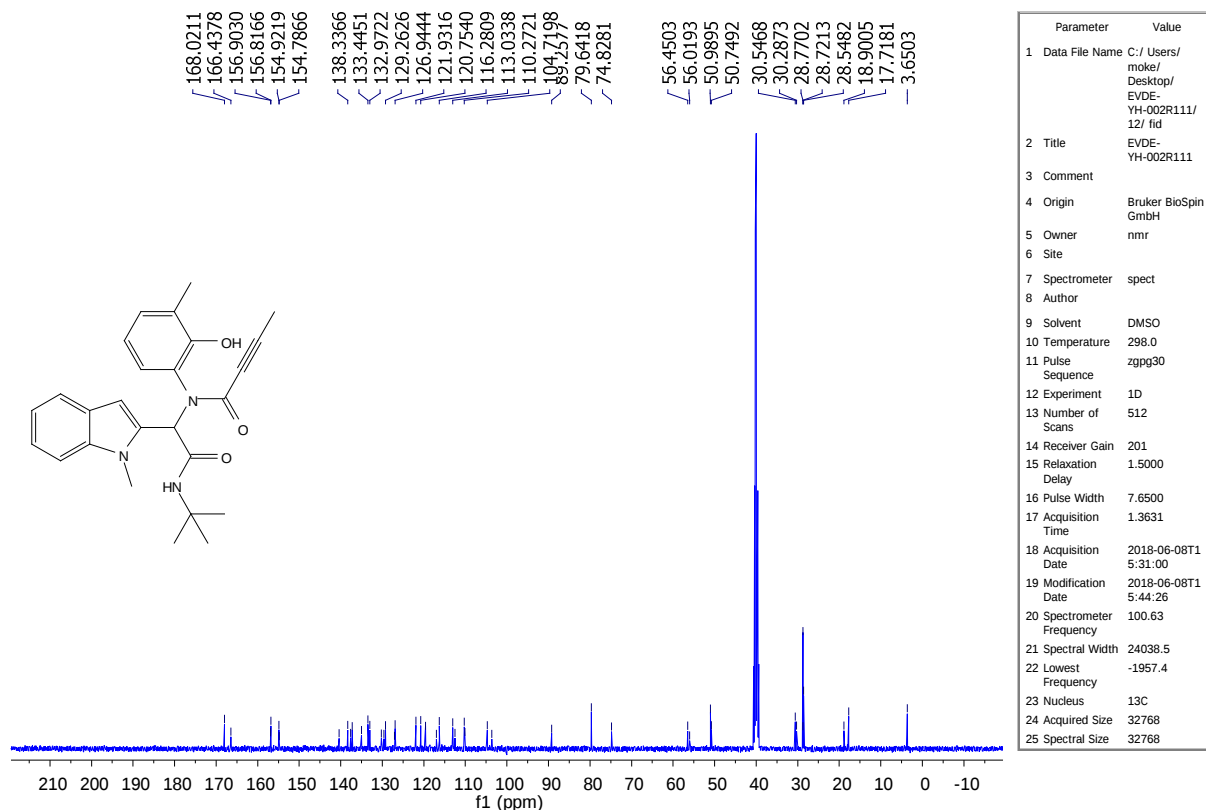
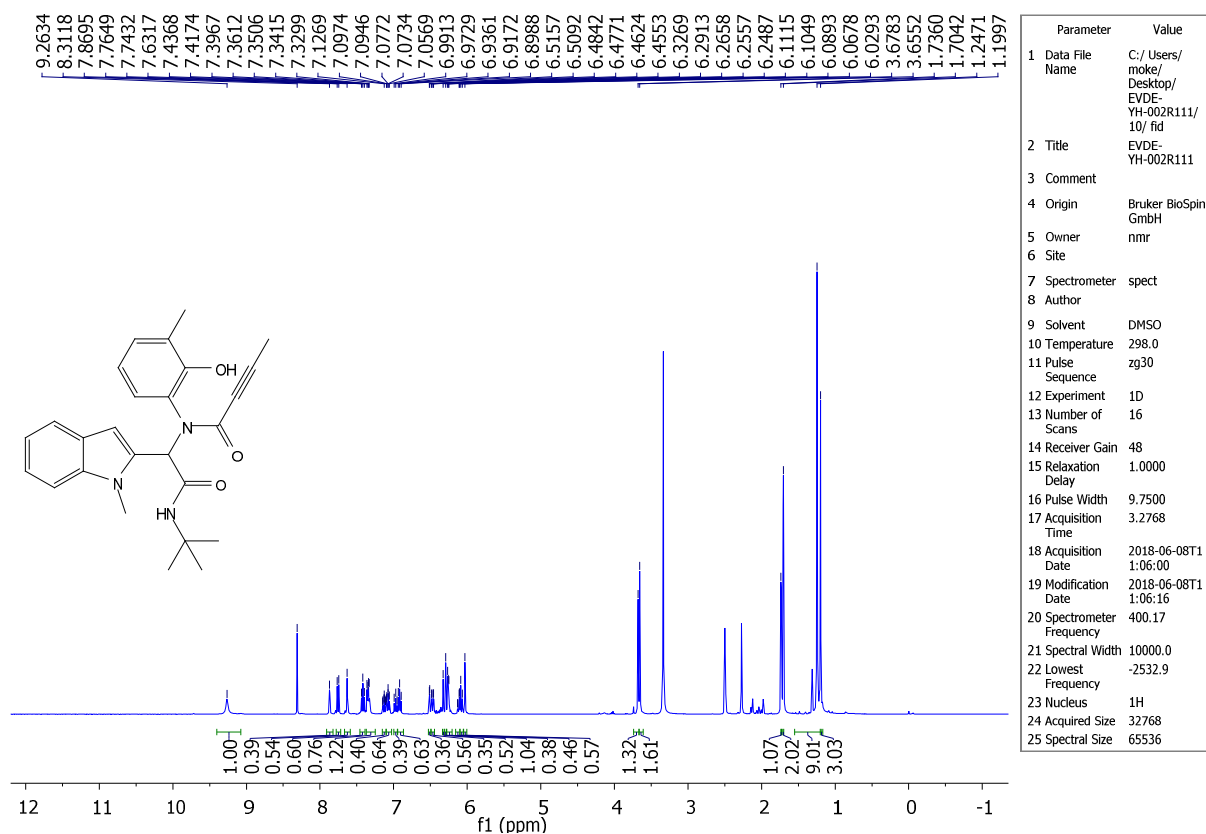


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/EVDE_YH_002R132(Ac)/10/ fid
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3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmruser
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	DMSO
10 Temperature	296.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm BBO BB-1H Z-GRD Z8284015/ 1
14 Number of Scans	8
15 Receiver Gain	812.7
16 Relaxation Delay	1.0000
17 Pulse Width	9.5000
18 Presaturation Frequency	
19 Acquisition Time	2.6543
20 Acquisition Date	2018-08-09T16:27:00
21 Modification Date	2018-08-09T16:27:26
22 Class	
23 Spectrometer Frequency	300.13
24 Spectral Width	6172.8
25 Lowest Frequency	-1233.0
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

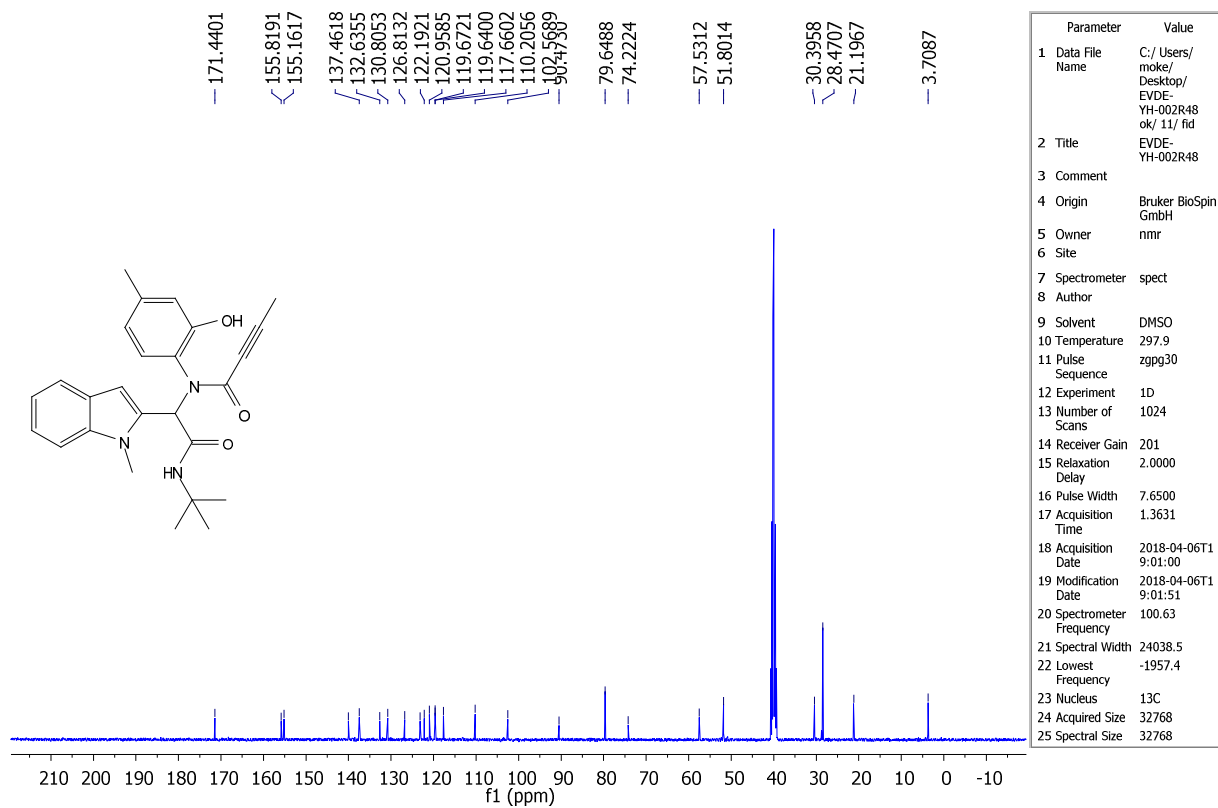
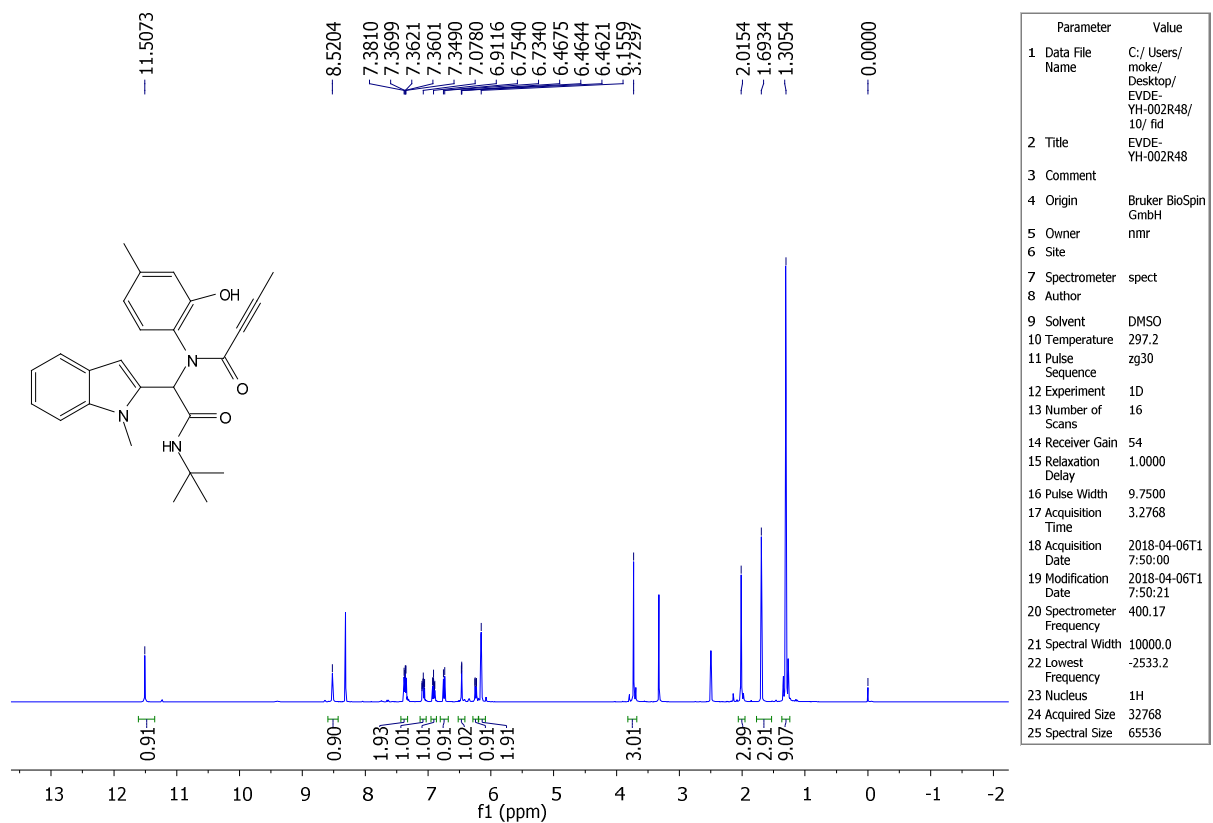


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/ SCOPE/ NMR of Scope/ 002 series/ EVDE_YH_002R132(Ac)/ EVDE-YH-002R132/ 10/ fid
2 Title	
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0435
14 Number of Scans	2048
15 Receiver Gain	201.3
16 Relaxation Delay	2.0000
17 Pulse Width	7.6500
18 Presaturation Frequency	
19 Acquisition Time	1.3631
20 Acquisition Date	2018-10-09T21:04:00
21 Modification Date	2018-10-09T21:04:53
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	24038.5
25 Lowest Frequency	-1957.4
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536

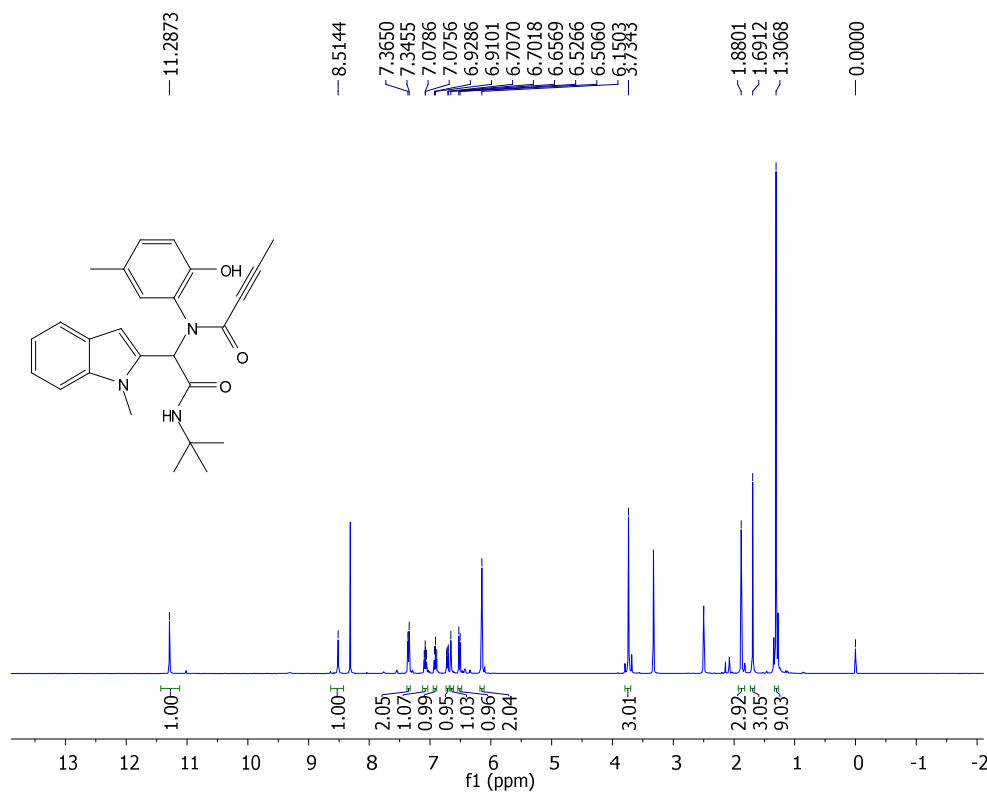
¹H and ¹³C NMR spectra of compound **1e**



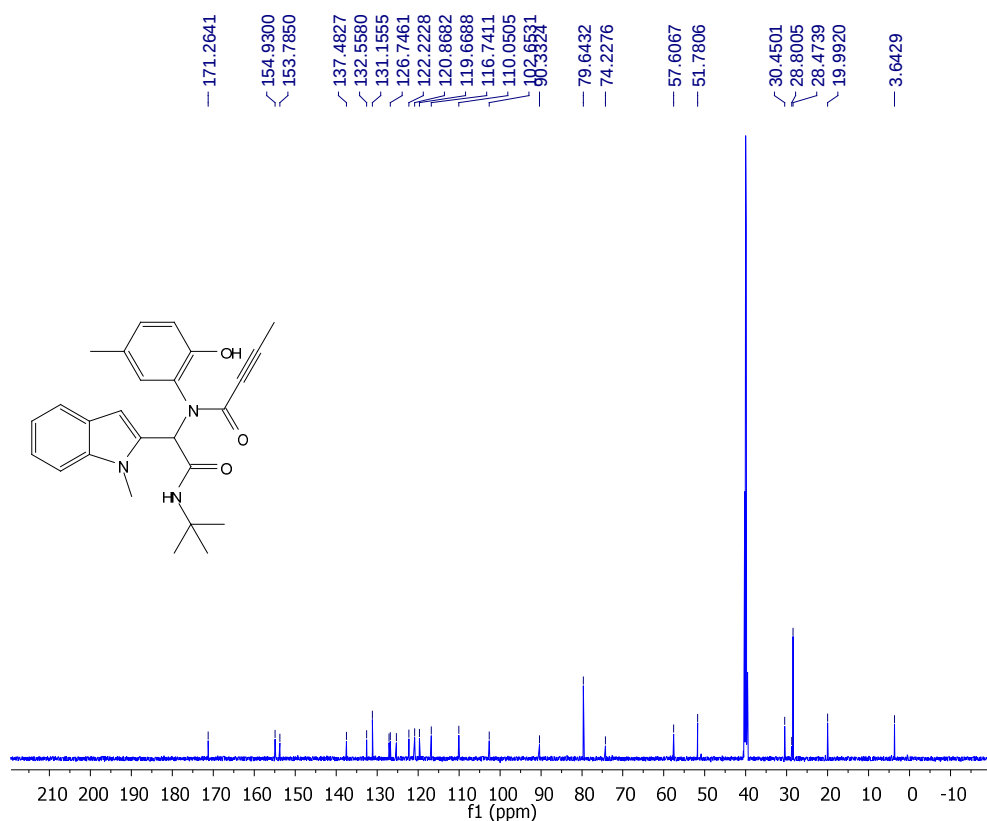
¹H and ¹³C NMR spectra of compound **1f**



¹H and ¹³C NMR spectra of compound **1g**

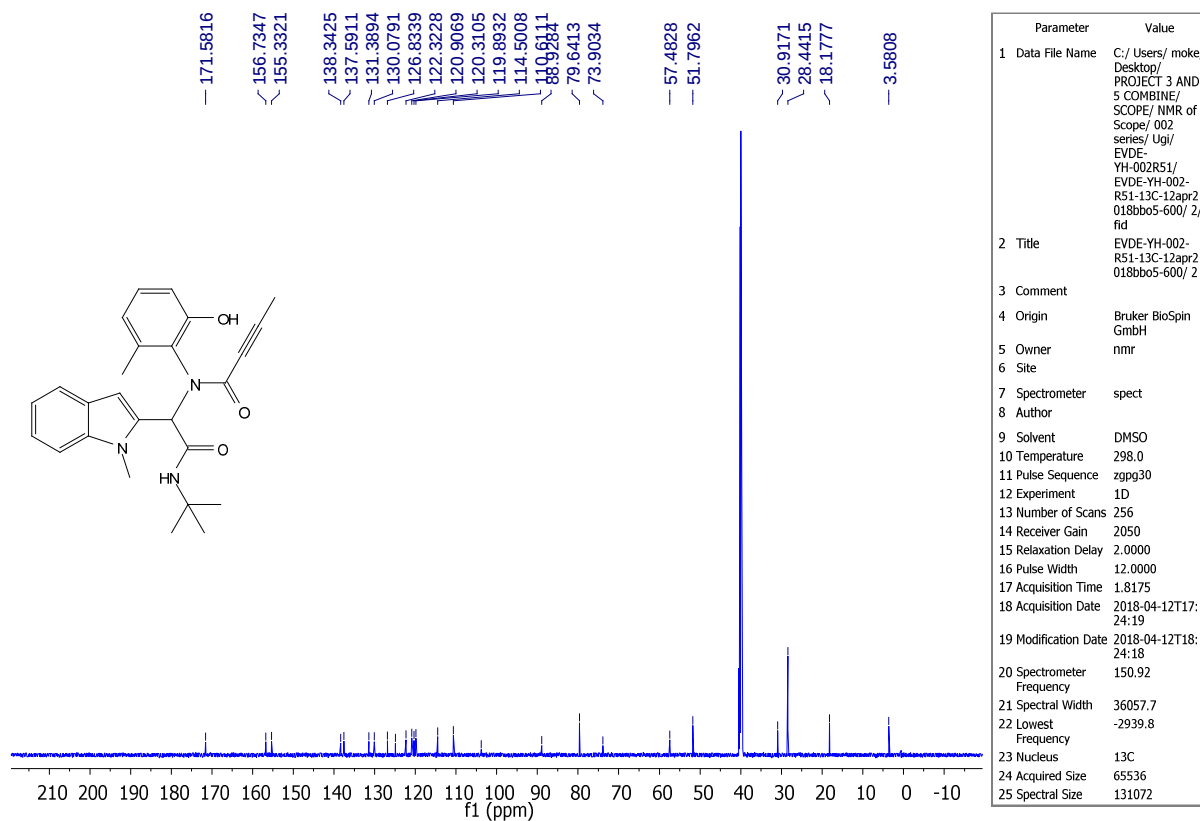
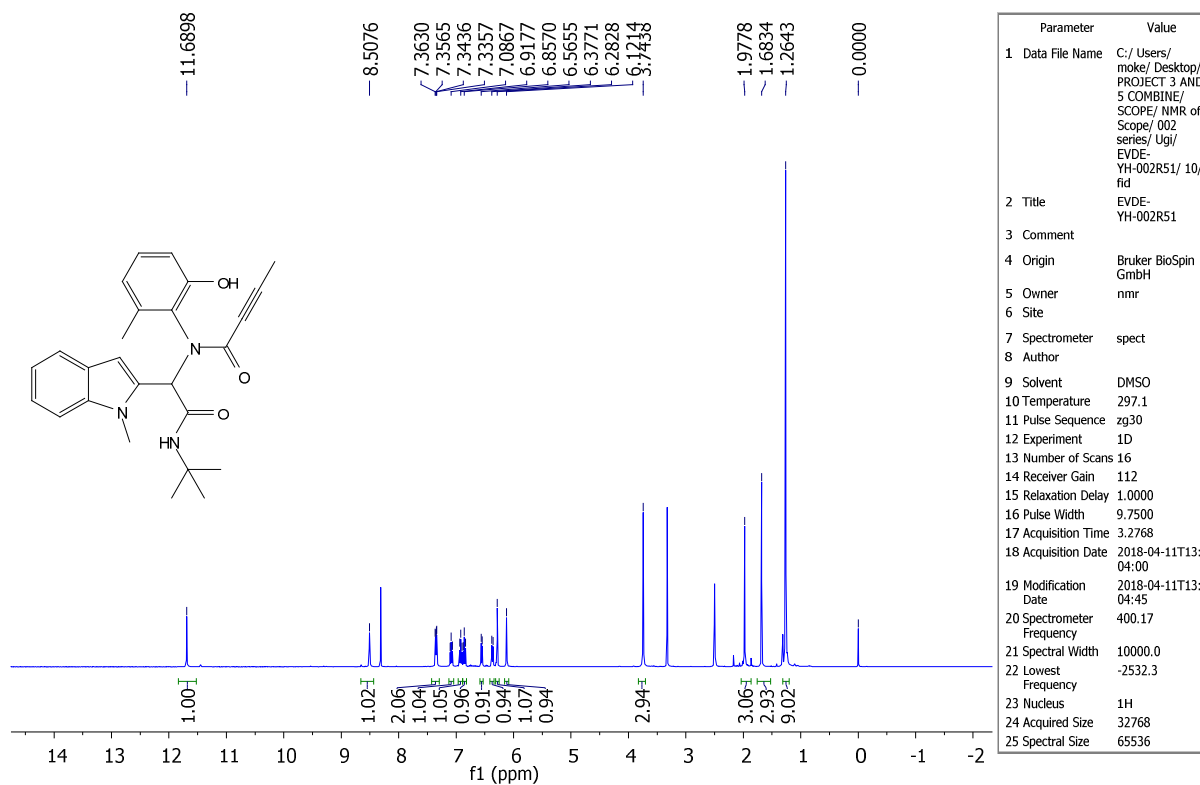


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R50/ 10/ fid
2 Title	EVDE- YH-002R50
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	297.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	54
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-04-11T13:01:00
19 Modification Date	2018-04-11T13:01:07
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2532.9
23 Nucleus	¹ H
24 Acquired Size	32768
25 Spectral Size	65536

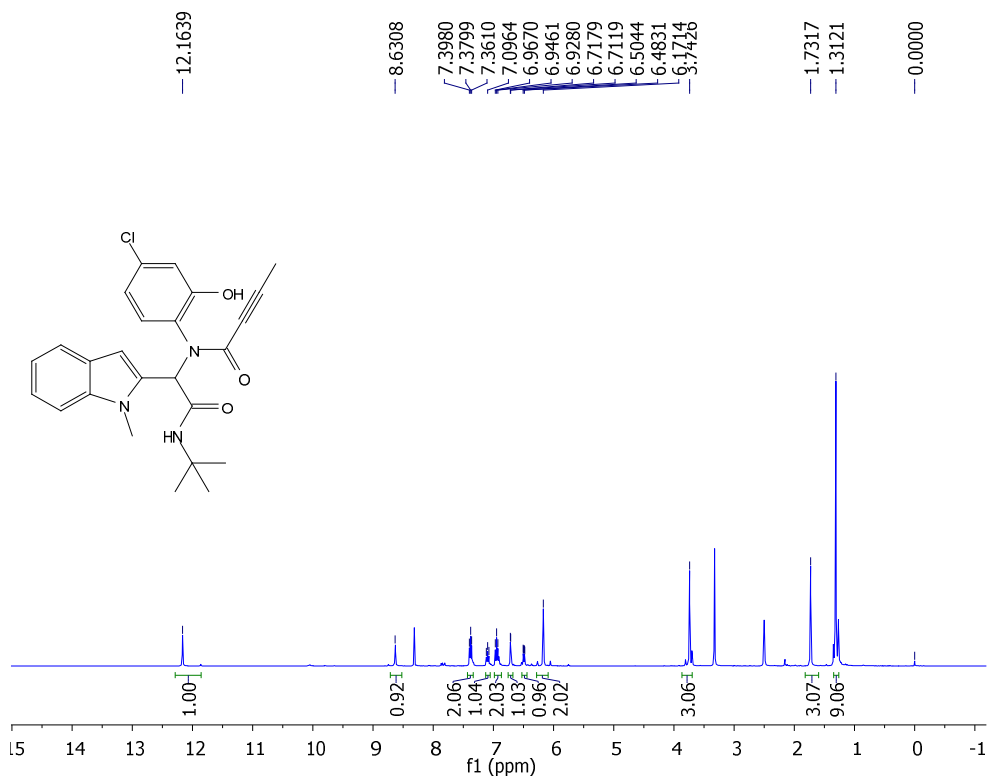


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R50/ EVDE-YH-002-R50-13c---13a pr2018bbo5-60 0/ 2/ fid
2 Title	EVDE-YH-002-R50-13c---13a pr2018bbo5-60 0/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	2050
15 Relaxation Delay	2.0000
16 Pulse Width	12.0000
17 Acquisition Time	1.8175
18 Acquisition Date	2018-04-13T09:19:25
19 Modification Date	2018-04-13T11:02:38
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	¹³ C
24 Acquired Size	65536
25 Spectral Size	131072

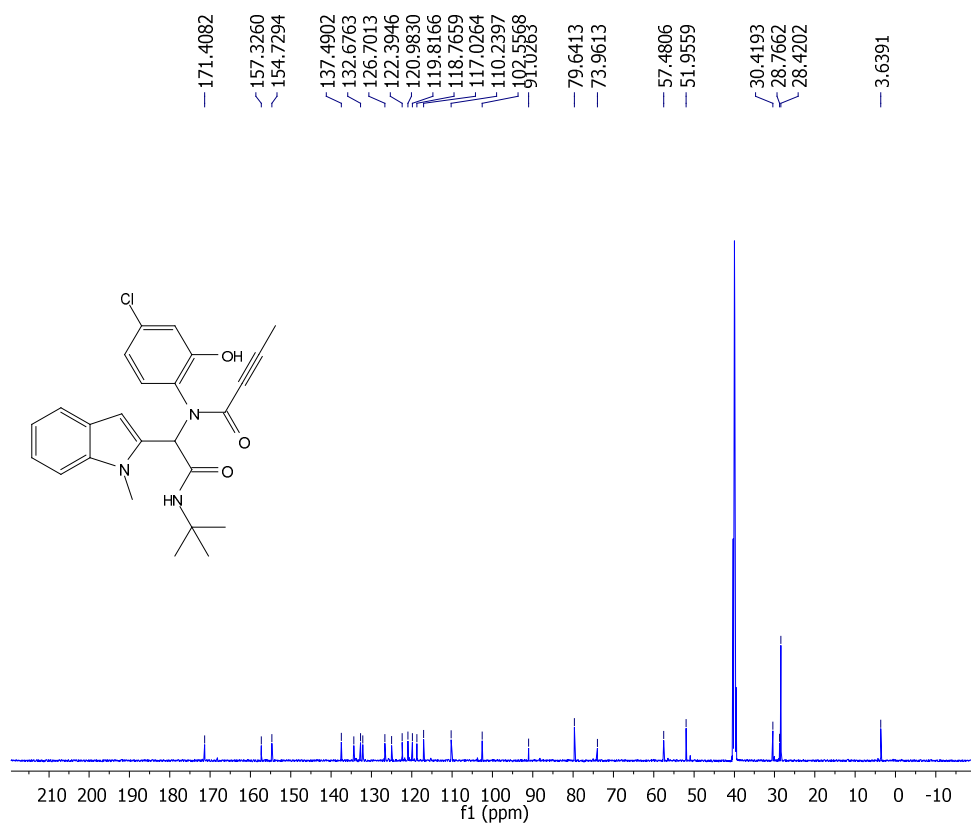
^1H and ^{13}C NMR spectra of compound **1h**



¹H and ¹³C NMR spectra of compound **1i**

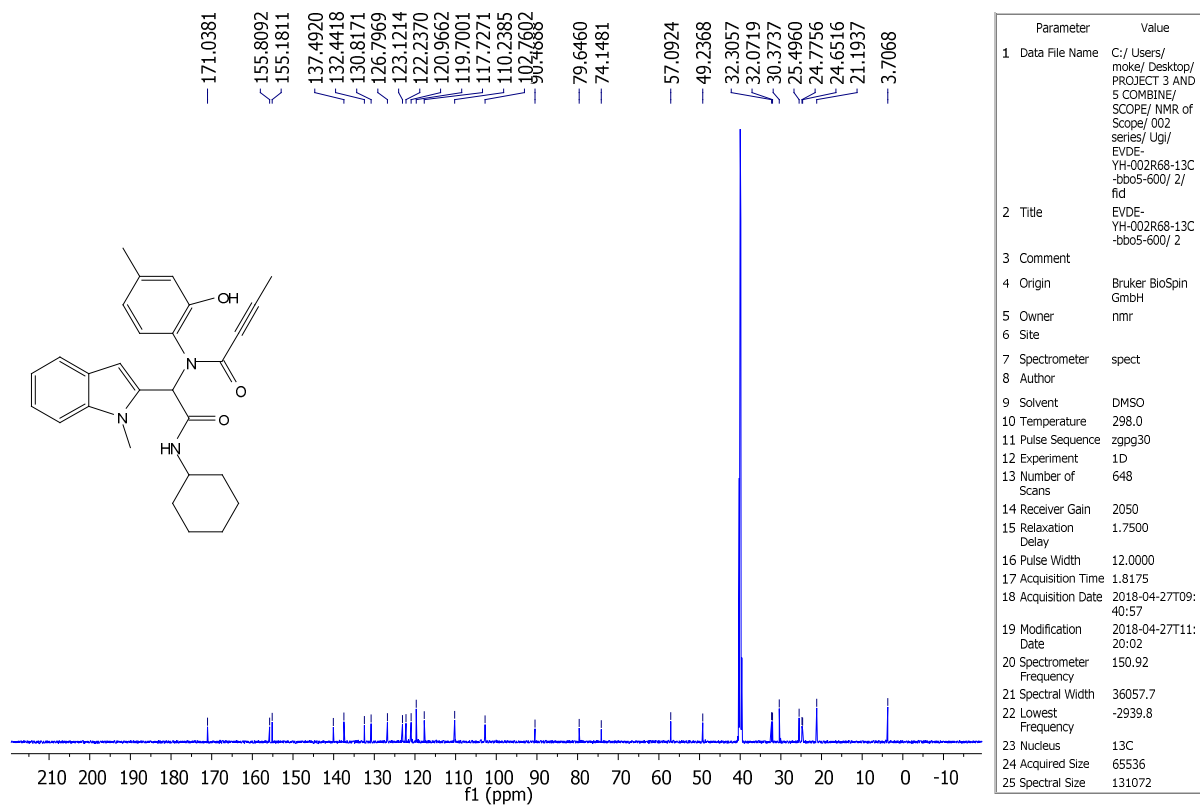
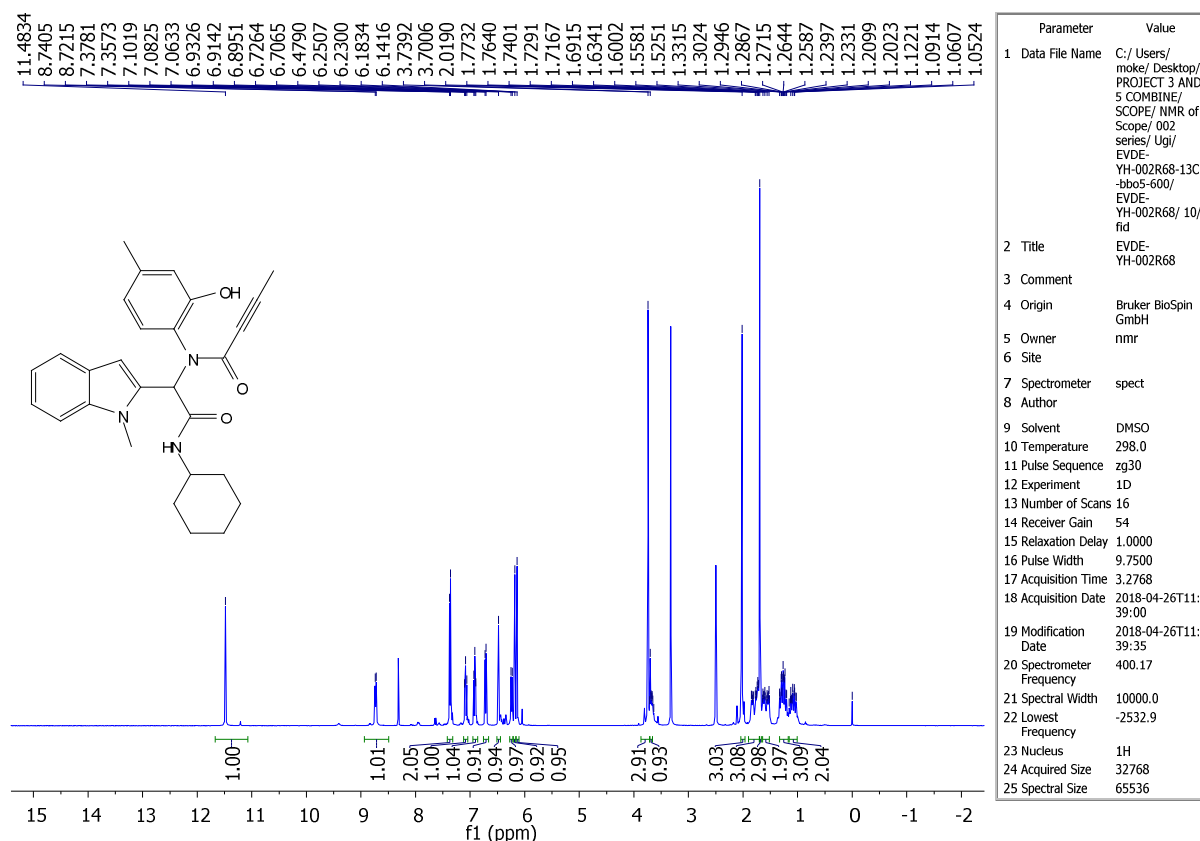


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2 Title	EVDE-YH-002R104
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	89
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-05-31T13:21:00
19 Modification Date	2018-05-31T13:21:18
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2532.1
23 Nucleus	¹ H
24 Acquired Size	32768
25 Spectral Size	65536

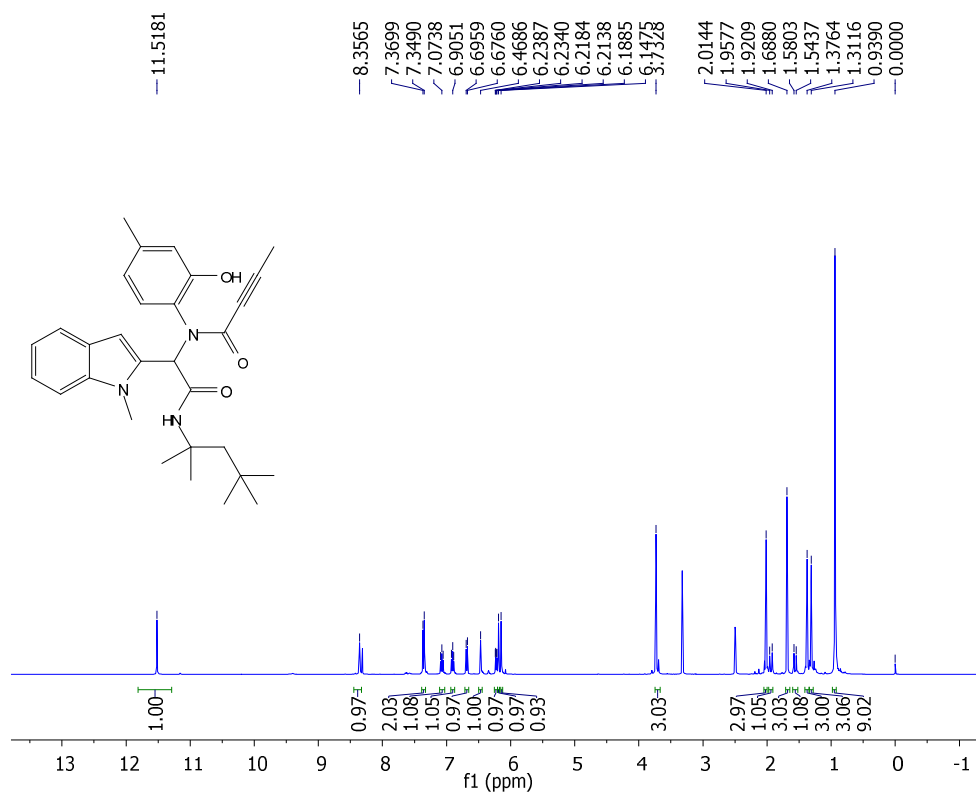


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/Ugi/ EVDE-YH-002R104 ok/ EVDE-YH002-R104-13C-bbo5-600/2/ fid
2 Title	EVDE-YH002-R104-13C-bbo5-600/2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1331
14 Receiver Gain	2050
15 Relaxation Delay	1.5000
16 Pulse Width	12.0000
17 Acquisition Time	0.9088
18 Acquisition Date	2018-05-31T15:49:10
19 Modification Date	2018-05-31T16:49:56
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	¹³ C
24 Acquired Size	32768
25 Spectral Size	131072

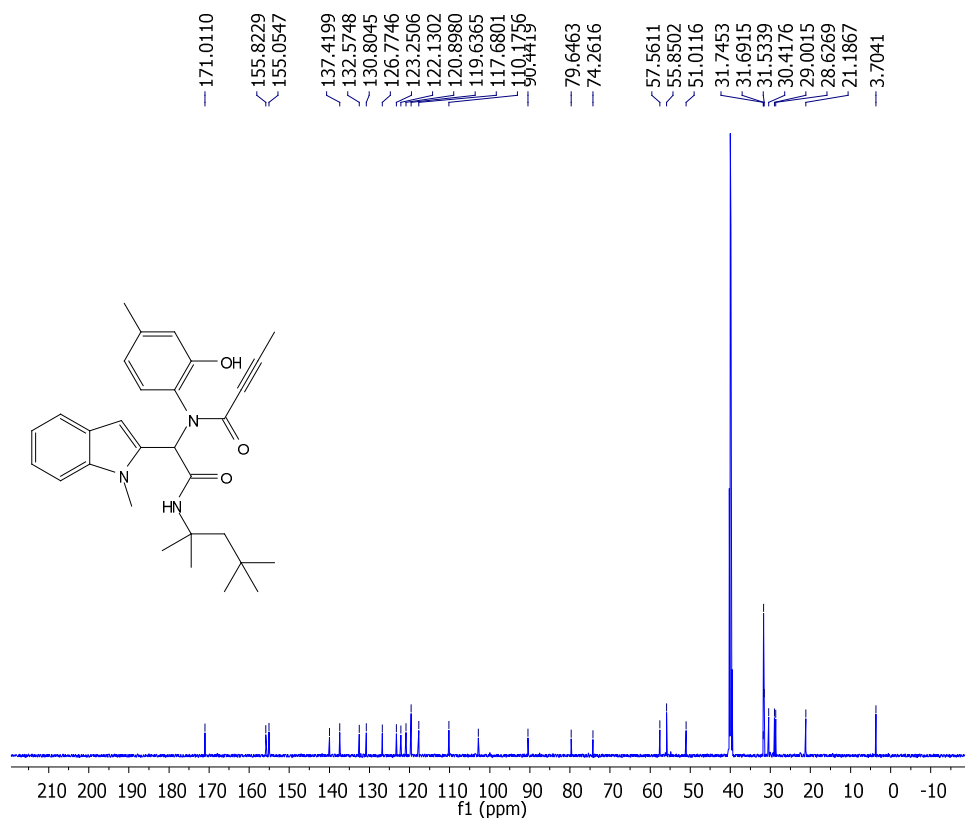
¹H and ¹³C NMR spectra of compound 1j



¹H and ¹³C NMR spectra of compound **1k**

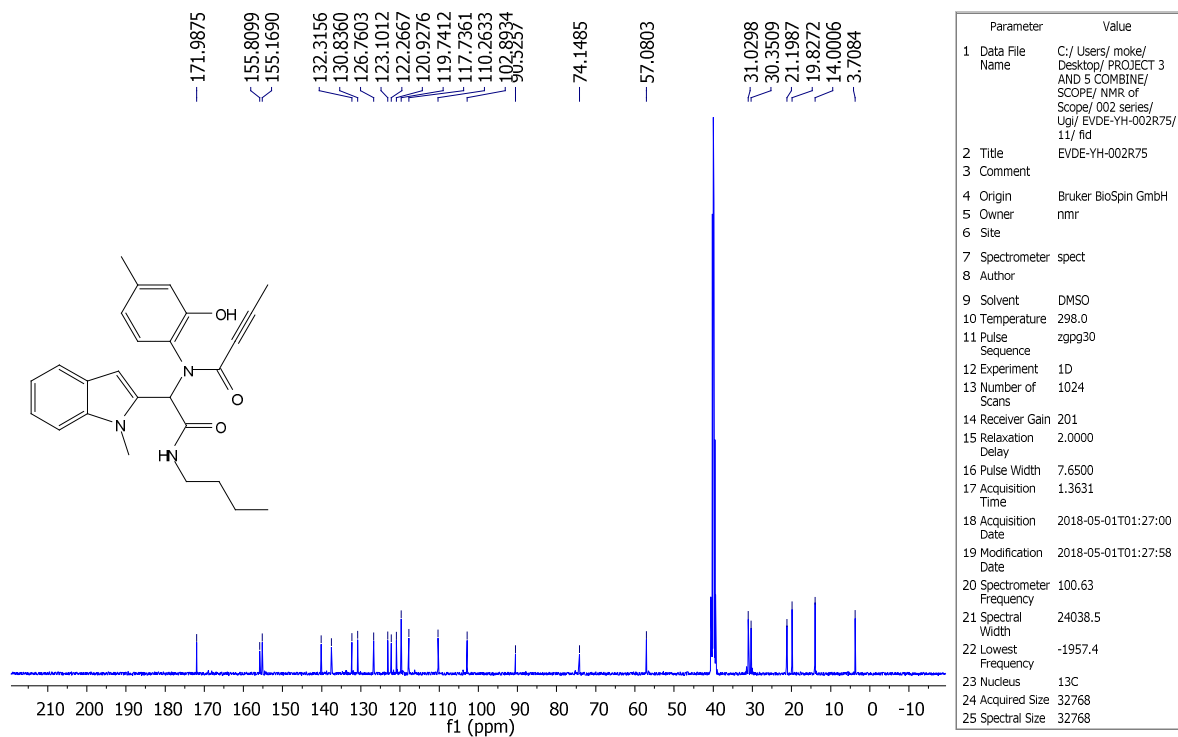
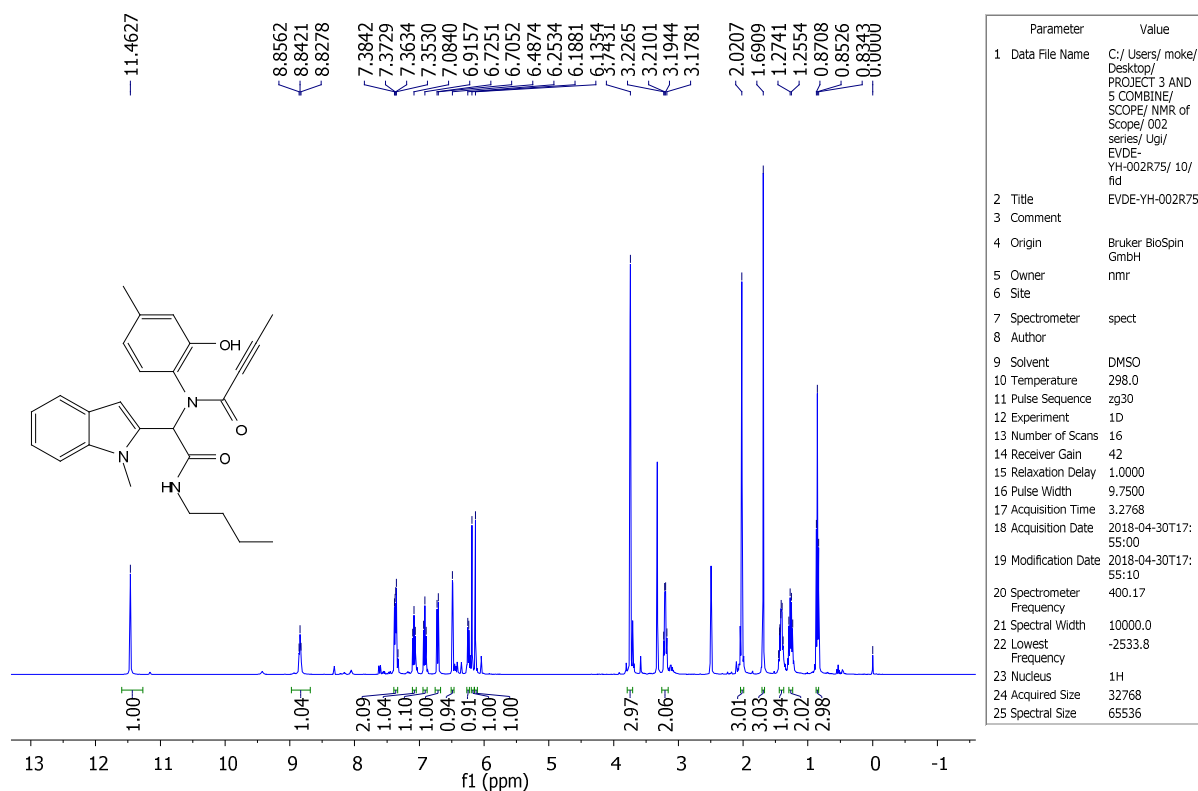


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2 Title	evde-yh-002r69
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	48
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-04-26T11:43:00
19 Modification Date	2018-04-26T11:43:14
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2533.3
23 Nucleus	¹ H
24 Acquired Size	32768
25 Spectral Size	65536

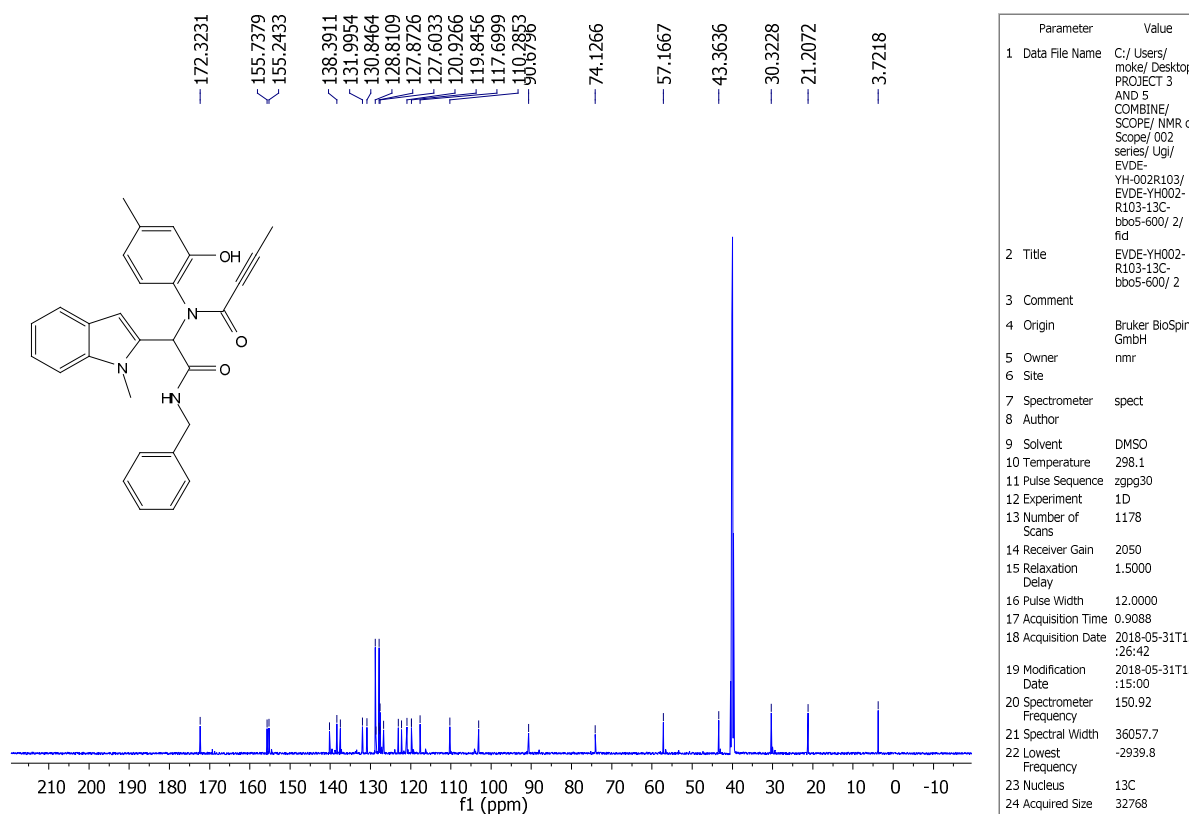
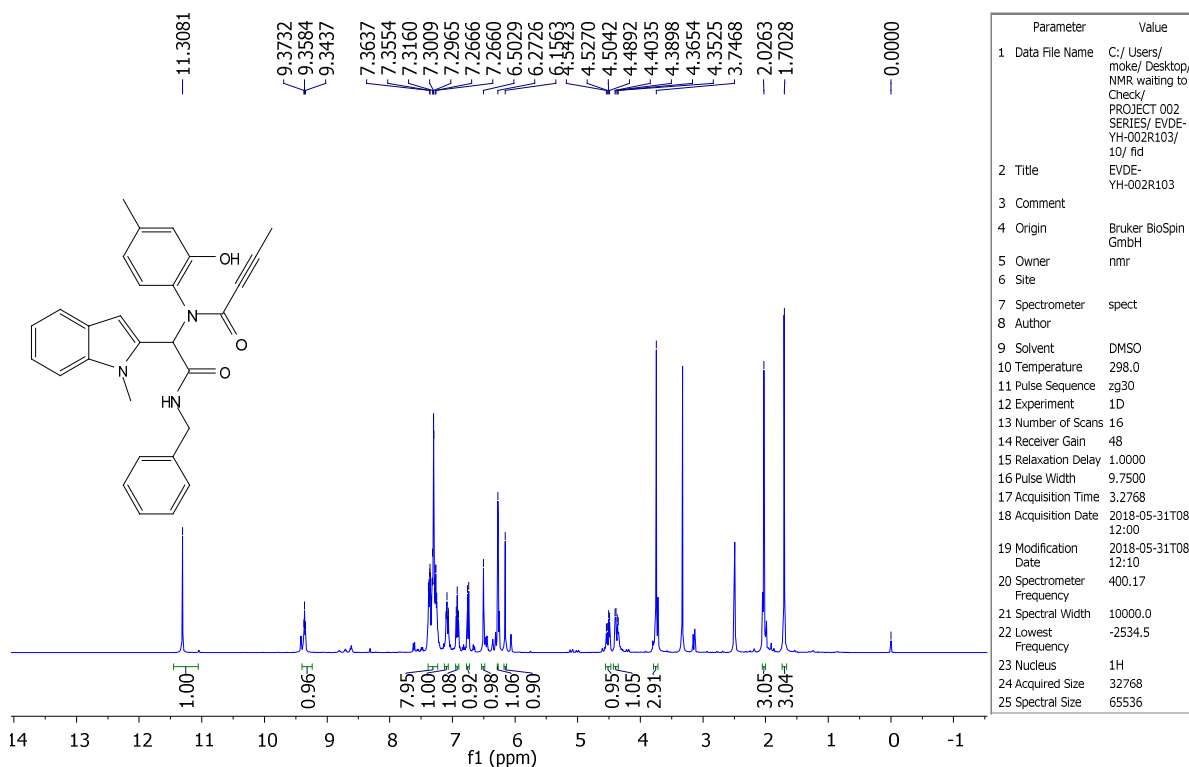


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2 Title	EVDE- YH-002R69-13C- bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	572
14 Receiver Gain	2050
15 Relaxation Delay	1.7500
16 Pulse Width	12.0000
17 Acquisition Time	1.8175
18 Acquisition Date	2018-04-27T10:22:56
19 Modification Date	2018-04-27T11:57:00
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	¹³ C
24 Acquired Size	65536
25 Spectral Size	131072

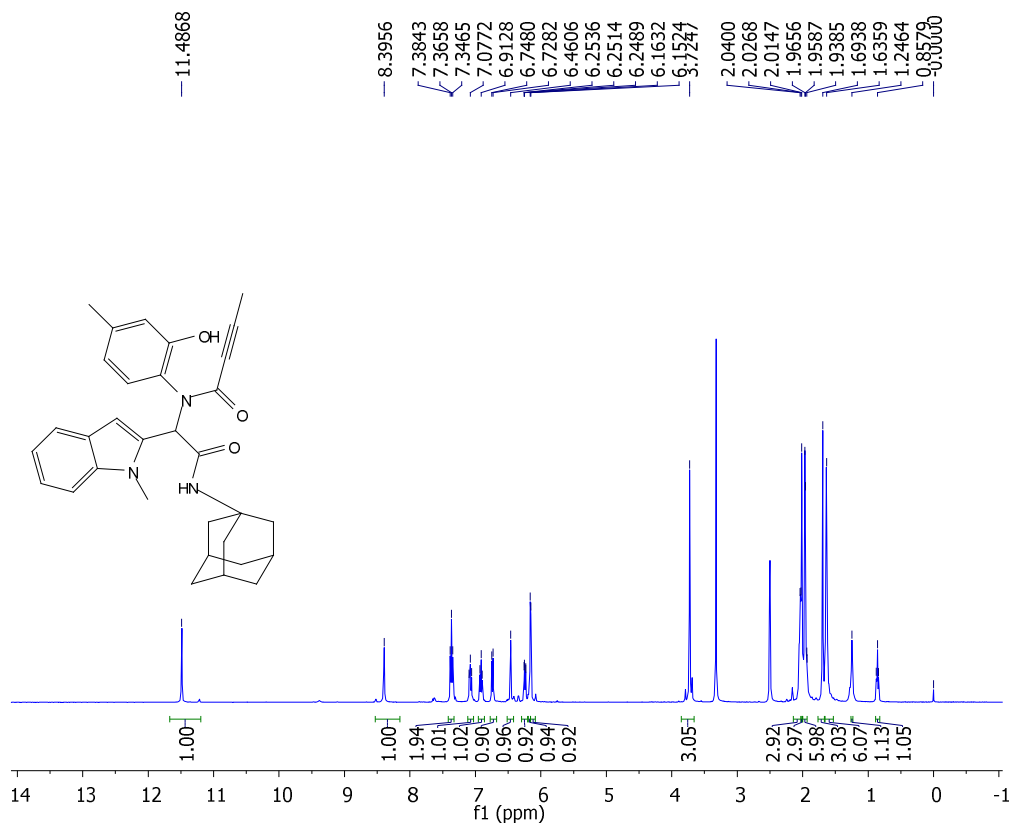
¹H and ¹³C NMR spectra of compound **11**



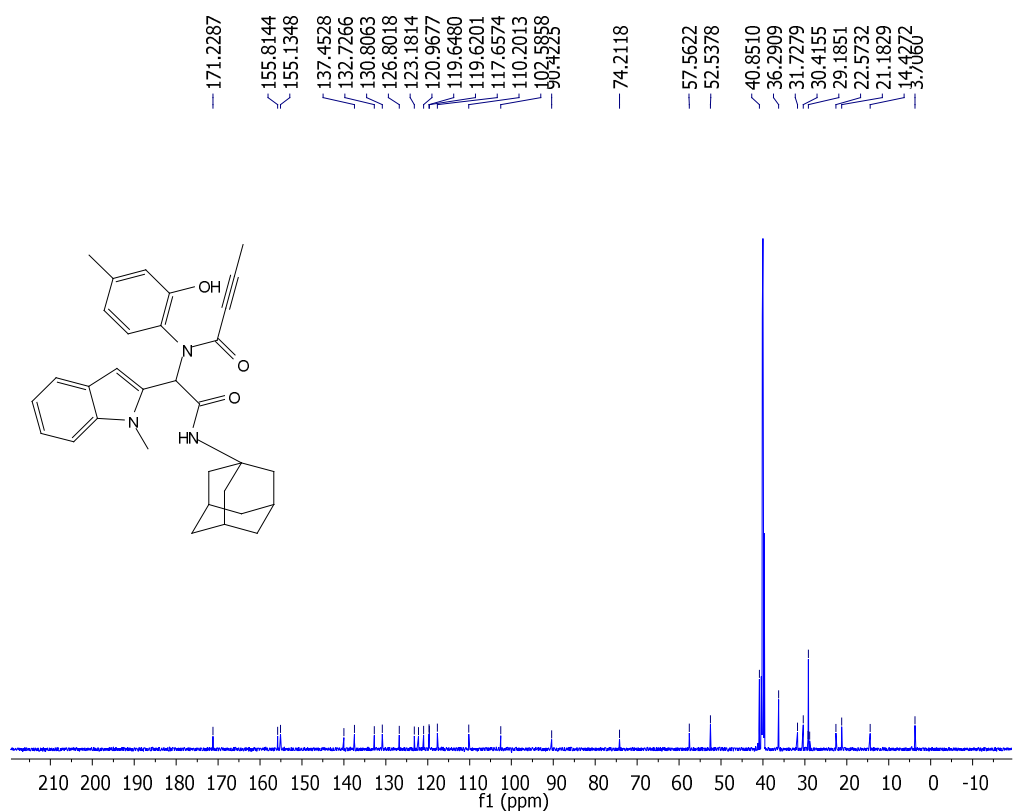
^1H and ^{13}C NMR spectra of compound **1m**



^1H and ^{13}C NMR spectra of compound **1n**

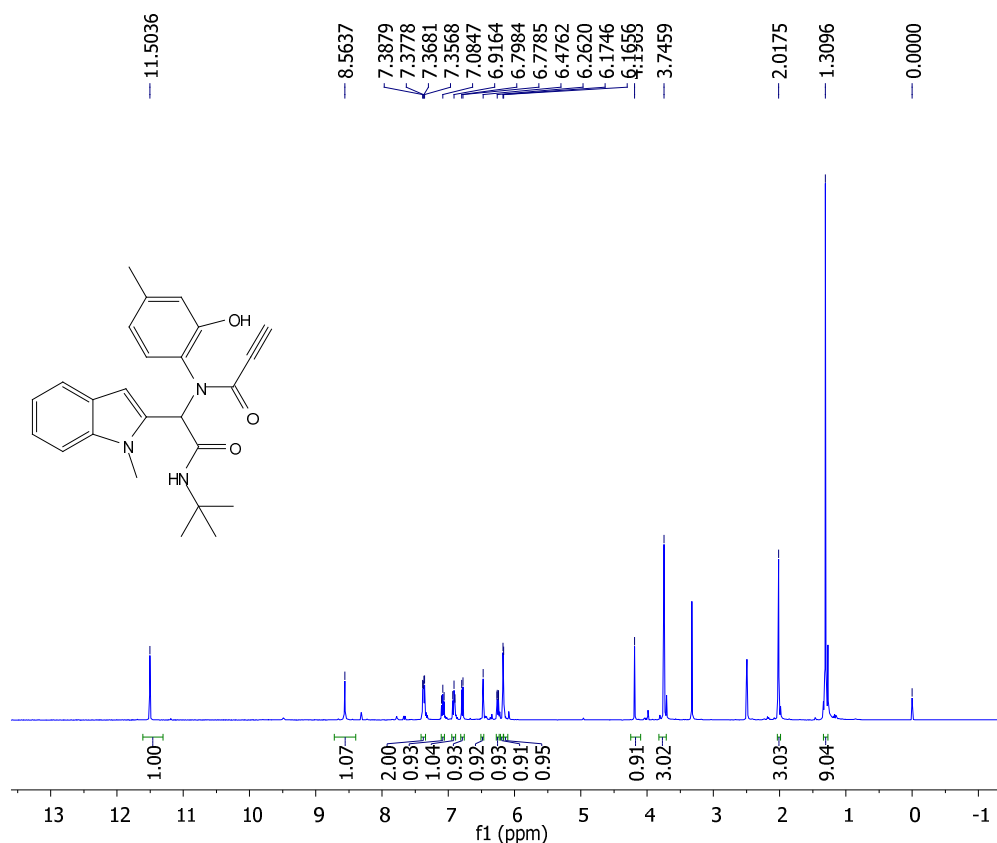


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2 Title	EVDE- YH-002R102
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	54
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-05-31T08:08:00
19 Modification Date	2018-05-31T08:08:24
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2532.5
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536

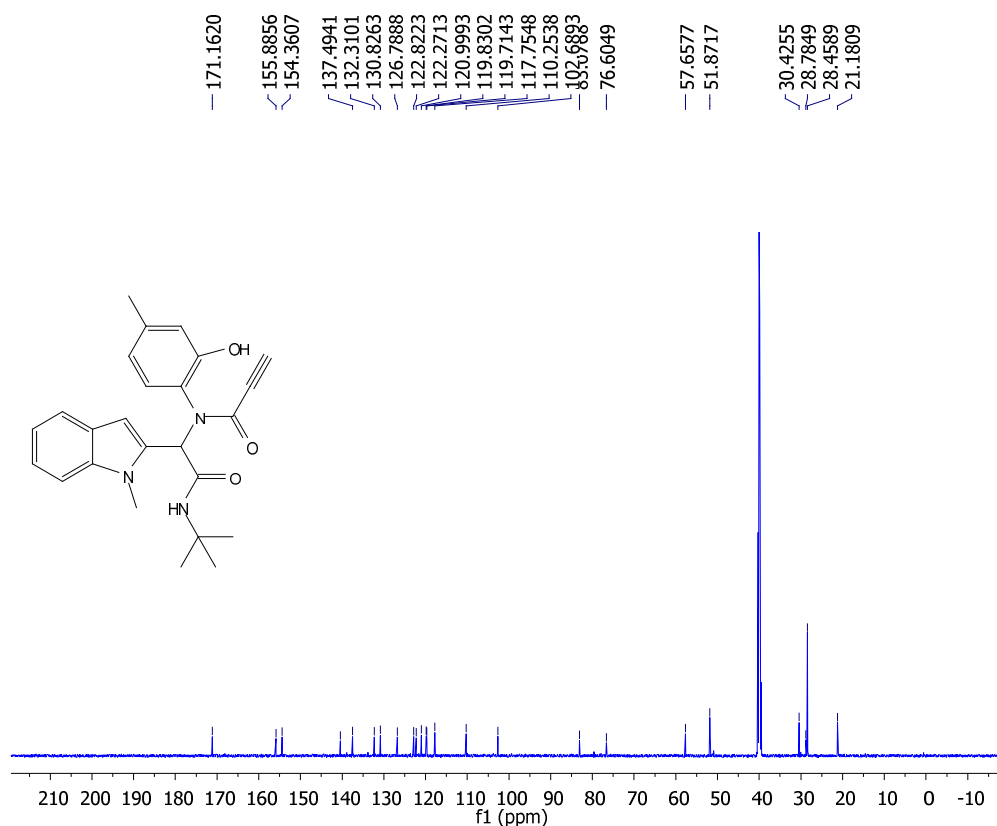


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R102/ EVDE-YH002-R102-13C-bbo5-600/ 2/ fid
2 Title	EVDE-YH002-R102-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	431
14 Receiver Gain	2050
15 Relaxation Delay	1.5000
16 Pulse Width	12.0000
17 Acquisition Time	0.9088
18 Acquisition Date	2018-05-31T13:05:46
19 Modification Date	2018-05-31T14:23:24
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	^{13}C
24 Acquired Size	32768
25 Spectral Size	131072

^1H and ^{13}C NMR spectra of compound **10**

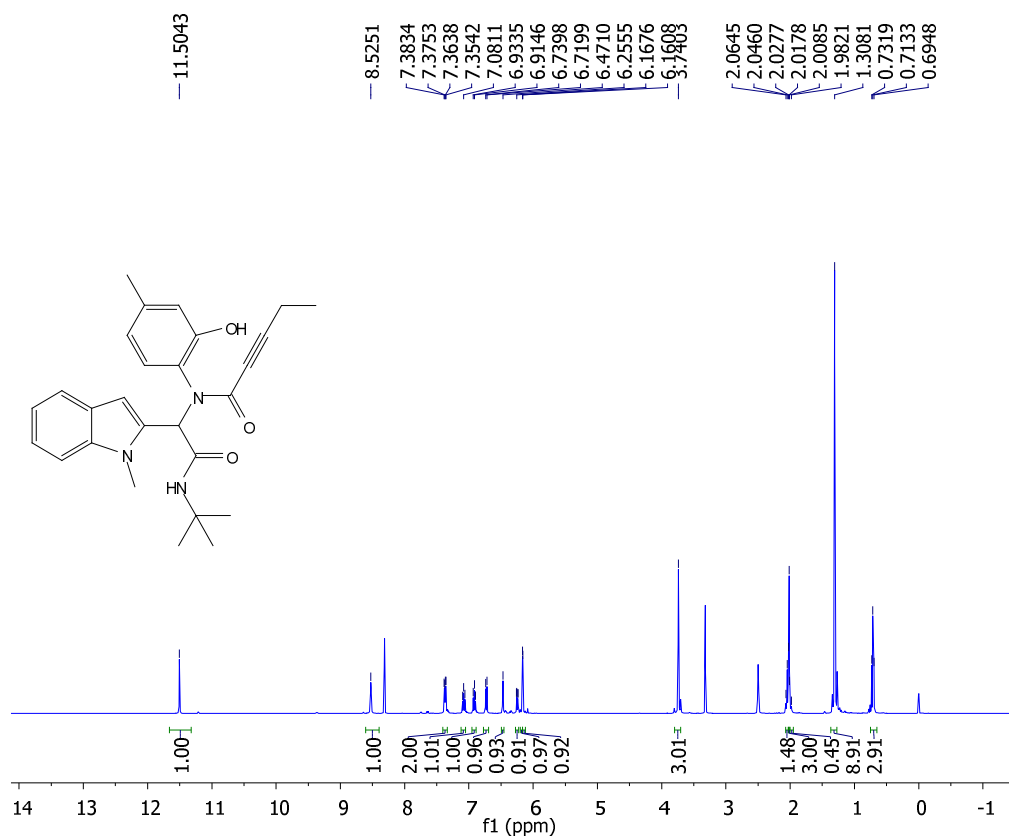


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R55/ 10/ fid
2 Title	EVDE-YH-002R55
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	54
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-04-19T11:13:00
19 Modification Date	2018-04-19T11:13:21
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2533.7
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536

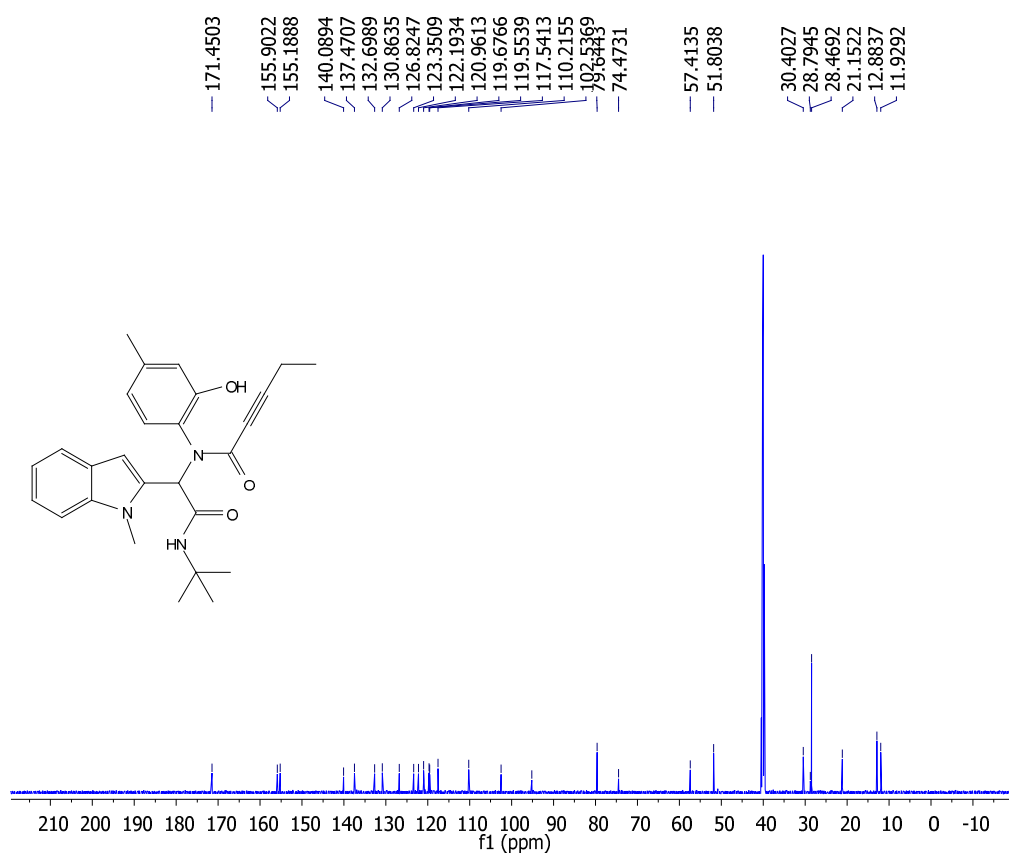


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2 Title	EVDE- YH002R55-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer spect	
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	366
14 Receiver Gain	2050
15 Relaxation Delay	1.7500
16 Pulse Width	12.0000
17 Acquisition Time	1.8175
18 Acquisition Date	2018-04-19T17:08:15
19 Modification Date	2018-04-19T18:08:16
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	^{13}C
24 Acquired Size	65536
25 Spectral Size	131072

^1H and ^{13}C NMR spectra of compound **1p**

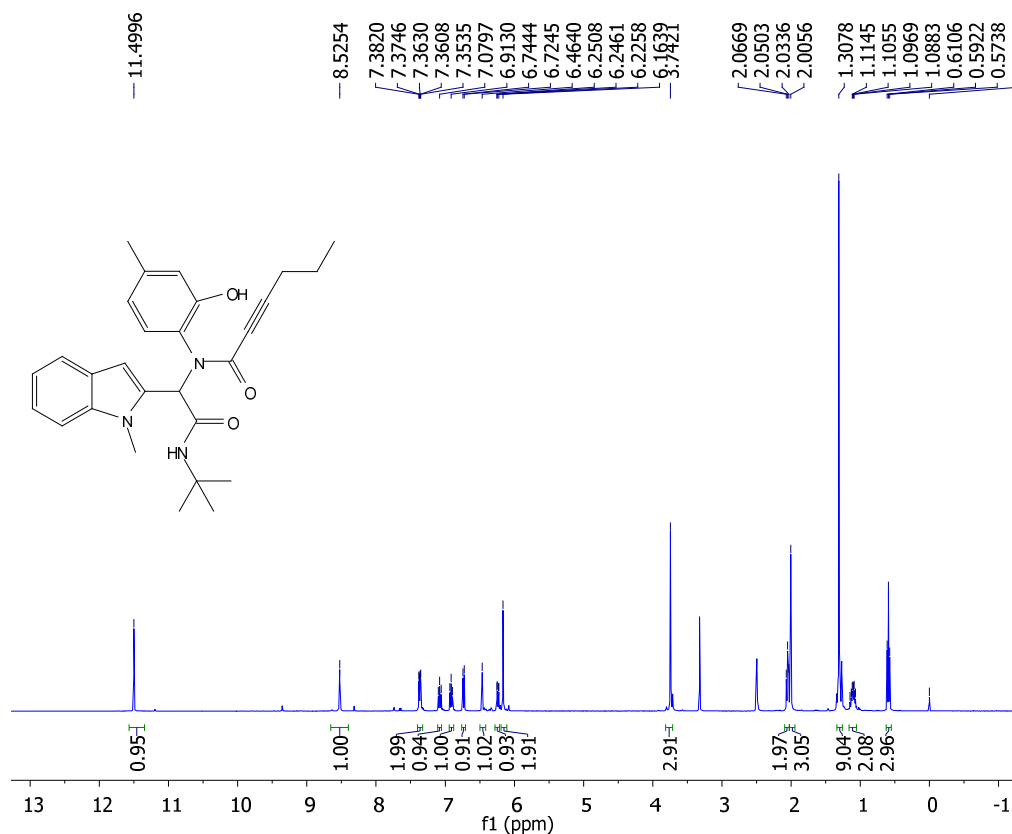


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2 Title	EVDE- YH-002R56
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	48
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-04-19T11:16:00
19 Modification Date	2018-04-19T11:16:57
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2533.1
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536

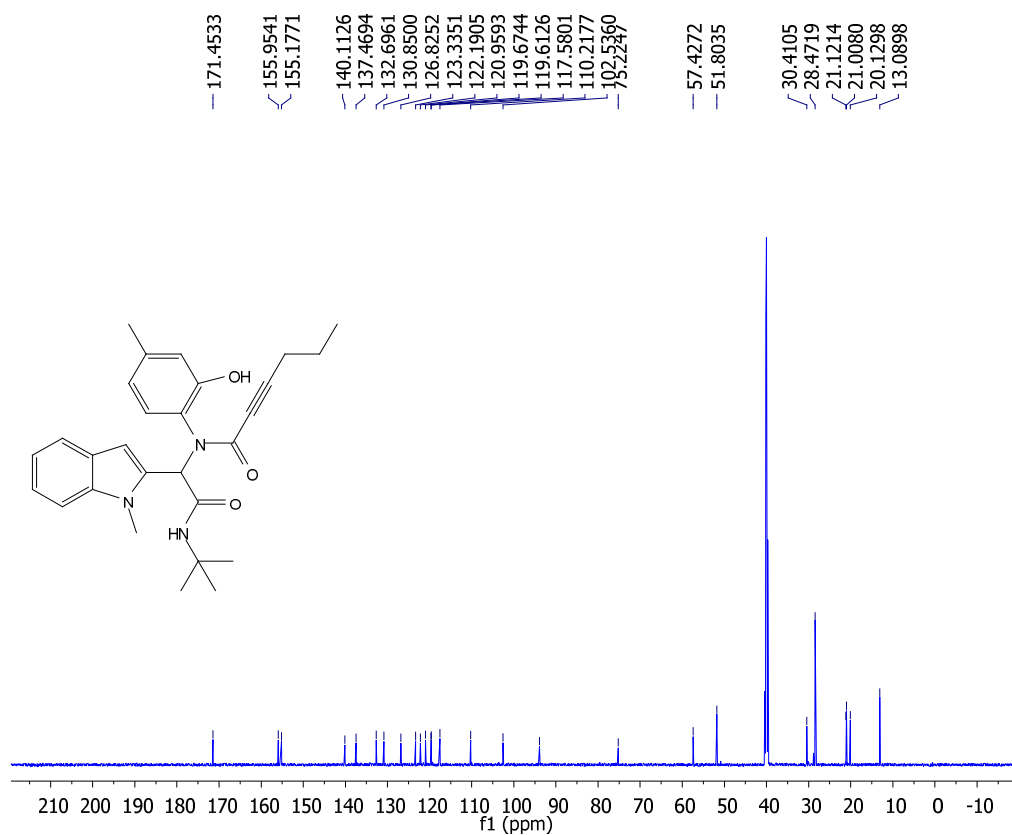


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R56/ EVDE- YH002R56-13C-bbo5-600/ 2/ f1d
2 Title	EVDE- YH002R56-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	194
14 Receiver Gain	2050
15 Relaxation Delay	1.7500
16 Pulse Width	12.0000
17 Acquisition Time	1.8175
18 Acquisition Date	2018-04-19T17:22:25
19 Modification Date	2018-04-19T18:22:26
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	^{13}C
24 Acquired Size	65536
25 Spectral Size	131072

^1H and ^{13}C NMR spectra of compound **1q**

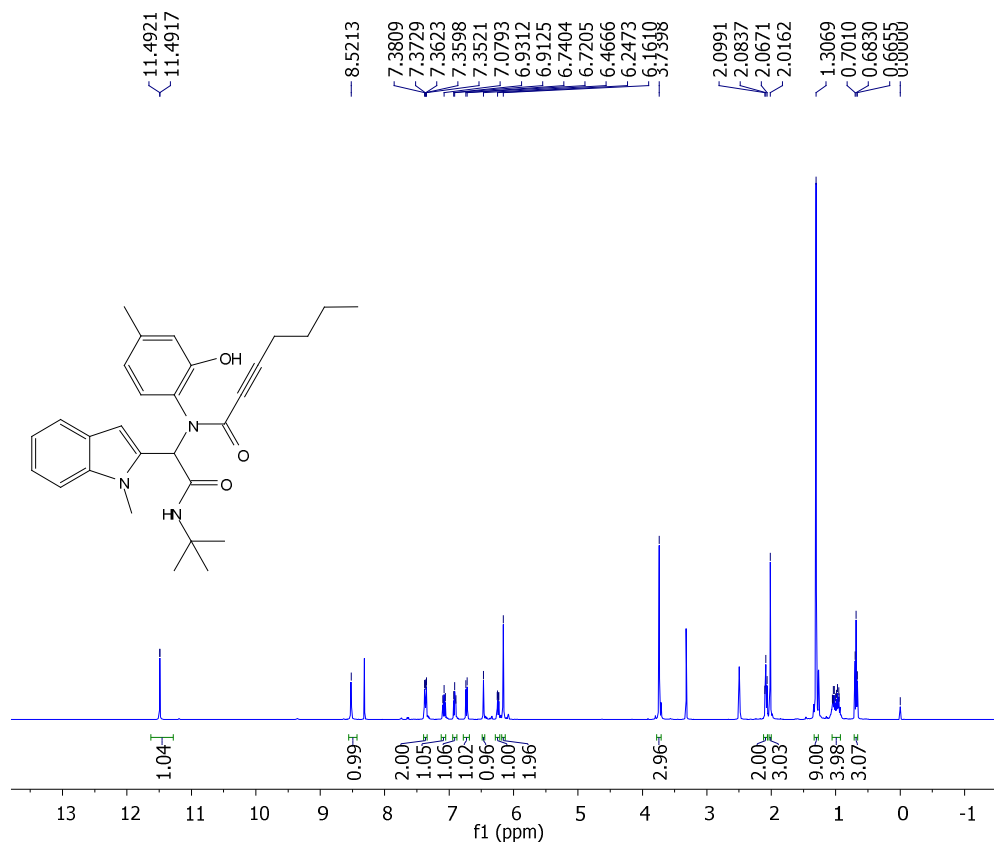


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R57/ 10/ fid
2 Title	EVDE- YH-002R57
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	48
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-04-19T11:20:00
19 Modification Date	2018-04-19T11:20:33
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2533.5
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536

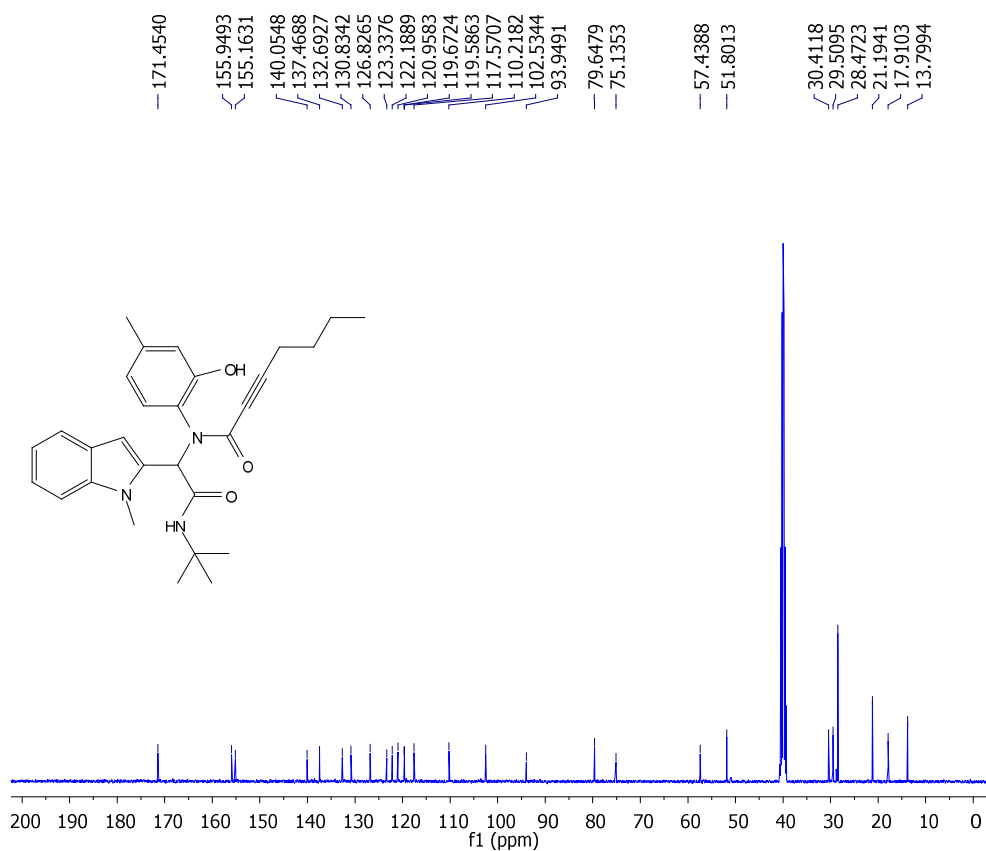


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R57/ EVDE- YH002R57-13C-bbo5-600/ 2/ fid
2 Title	EVDE- YH002R57-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	404
14 Receiver Gain	2050
15 Relaxation Delay	1.7500
16 Pulse Width	12.0000
17 Acquisition Time	1.8175
18 Acquisition Date	2018-04-19T17:49:33
19 Modification Date	2018-04-19T18:49:34
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	^{13}C
24 Acquired Size	65536
25 Spectral Size	131072

^1H and ^{13}C NMR spectra of compound **1r**

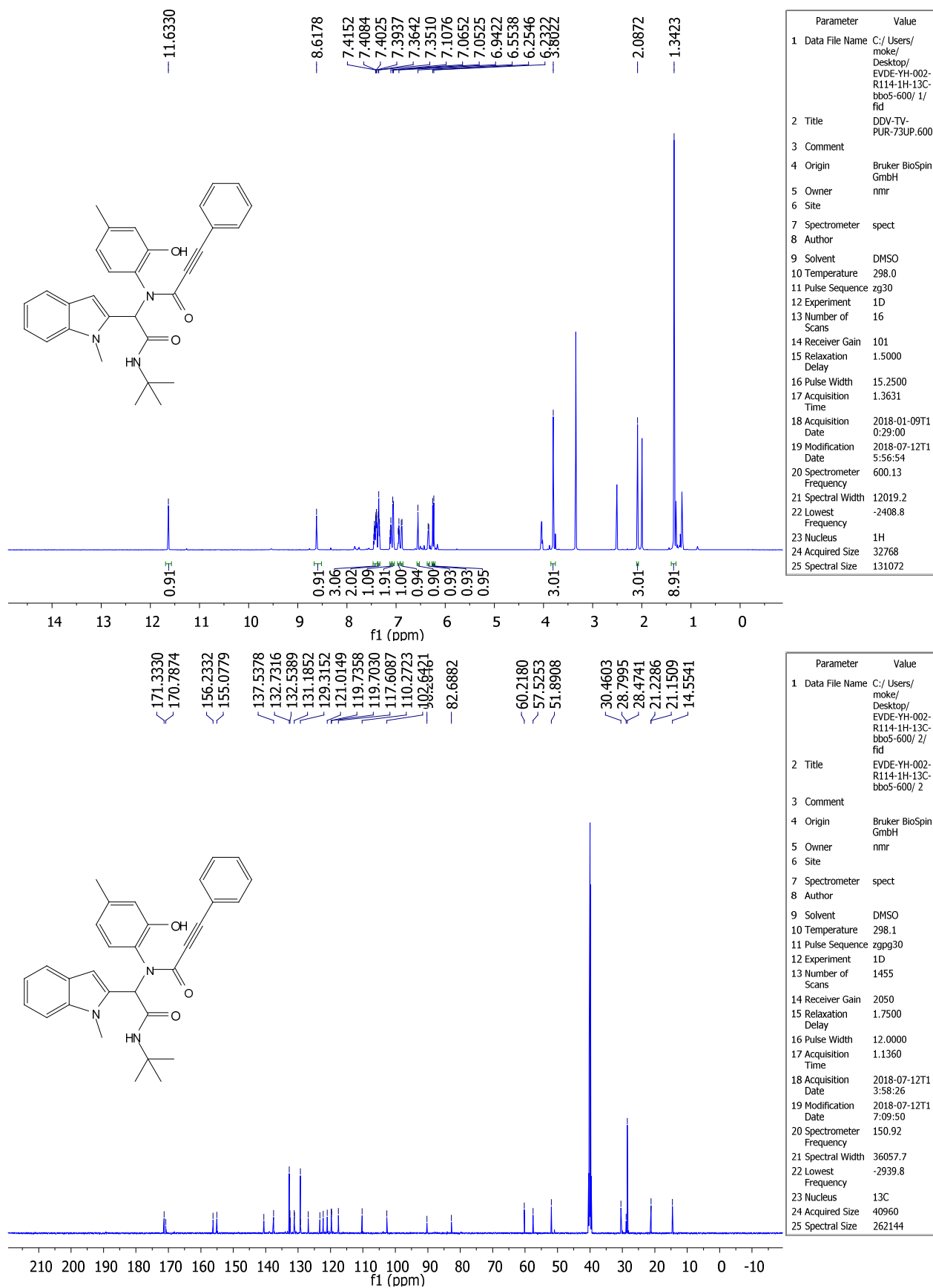


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2 Title	ECDE- YH-002R67
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	48
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-04-26T1 1:35:00
19 Modification Date	2018-04-26T1 1:35:53
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2533.3
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536

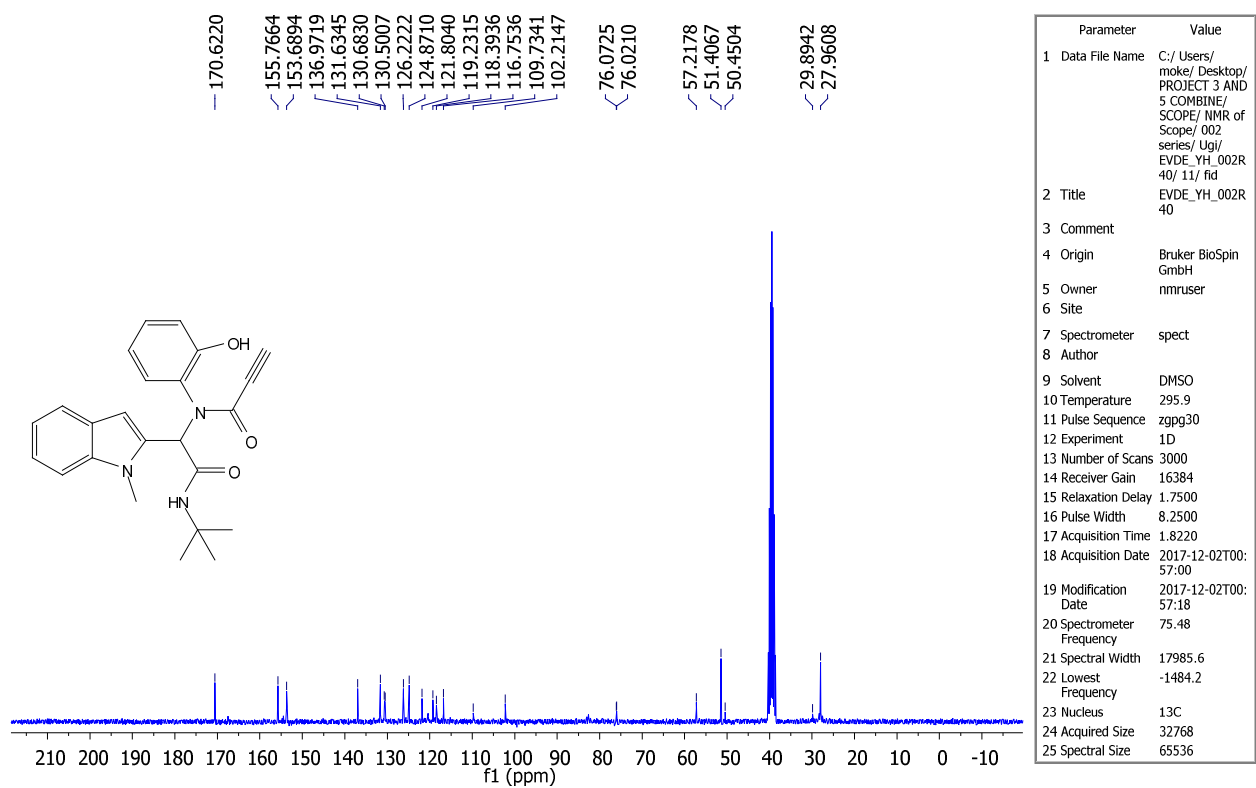
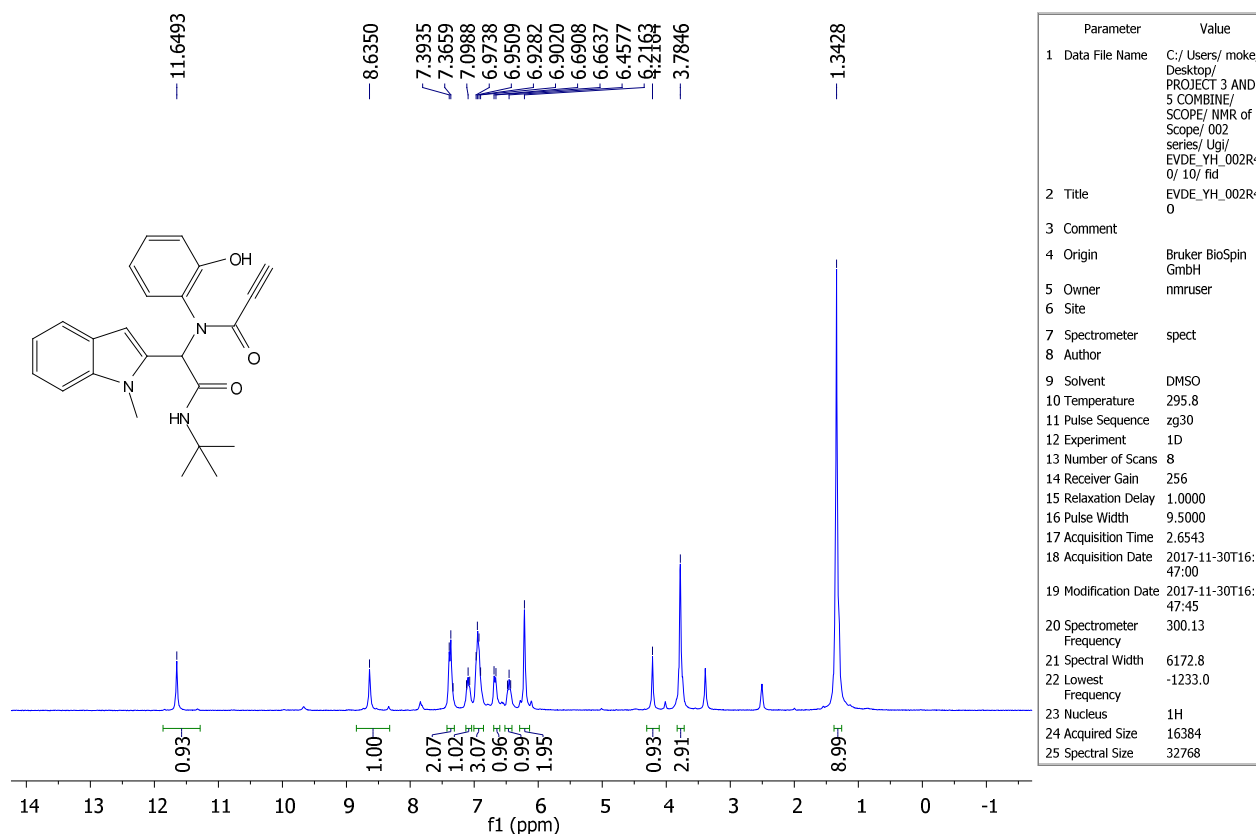


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE- YH-002R67/ 11/ fid
2 Title	ECDE- YH-002R67
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1024
14 Receiver Gain	201
15 Relaxation Delay	2.0000
16 Pulse Width	7.6500
17 Acquisition Time	1.3631
18 Acquisition Date	2018-04-28T12 :19:00
19 Modification Date	2018-04-28T12 :19:59
20 Spectrometer Frequency	100.63
21 Spectral Width	24038.5
22 Lowest Frequency	-1957.4
23 Nucleus	^{13}C
24 Acquired Size	32768
25 Spectral Size	32768

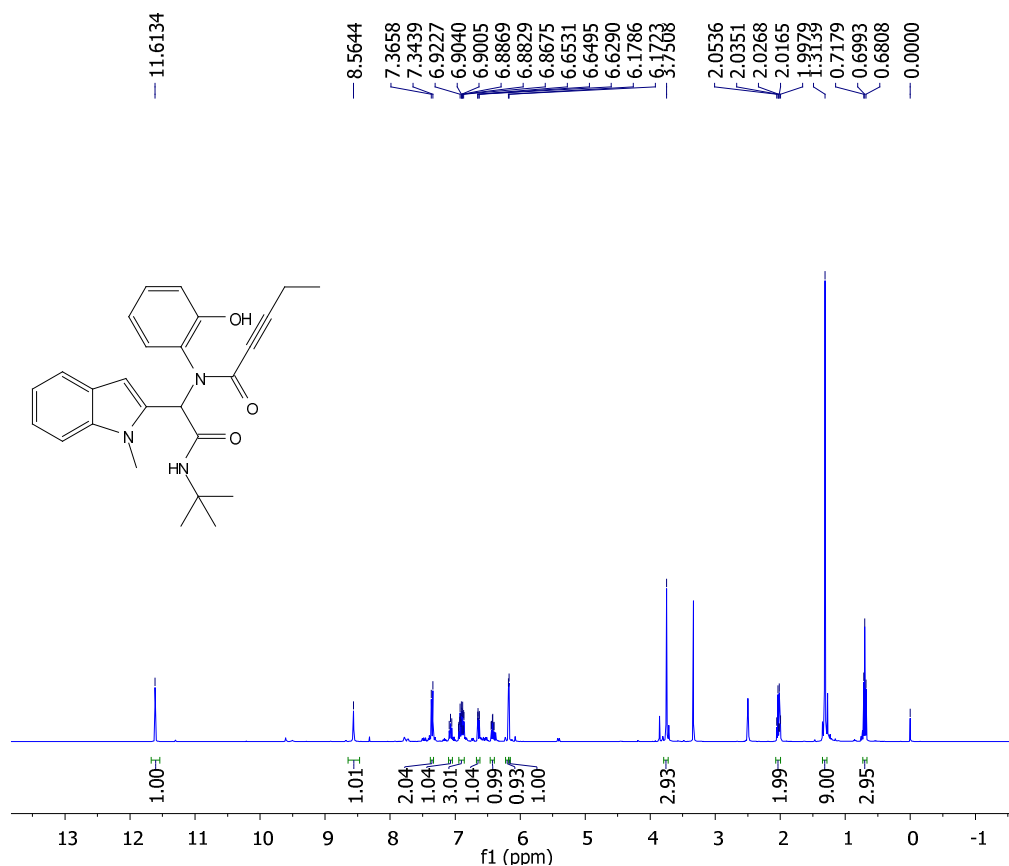
^1H and ^{13}C NMR spectra of compound **1s**



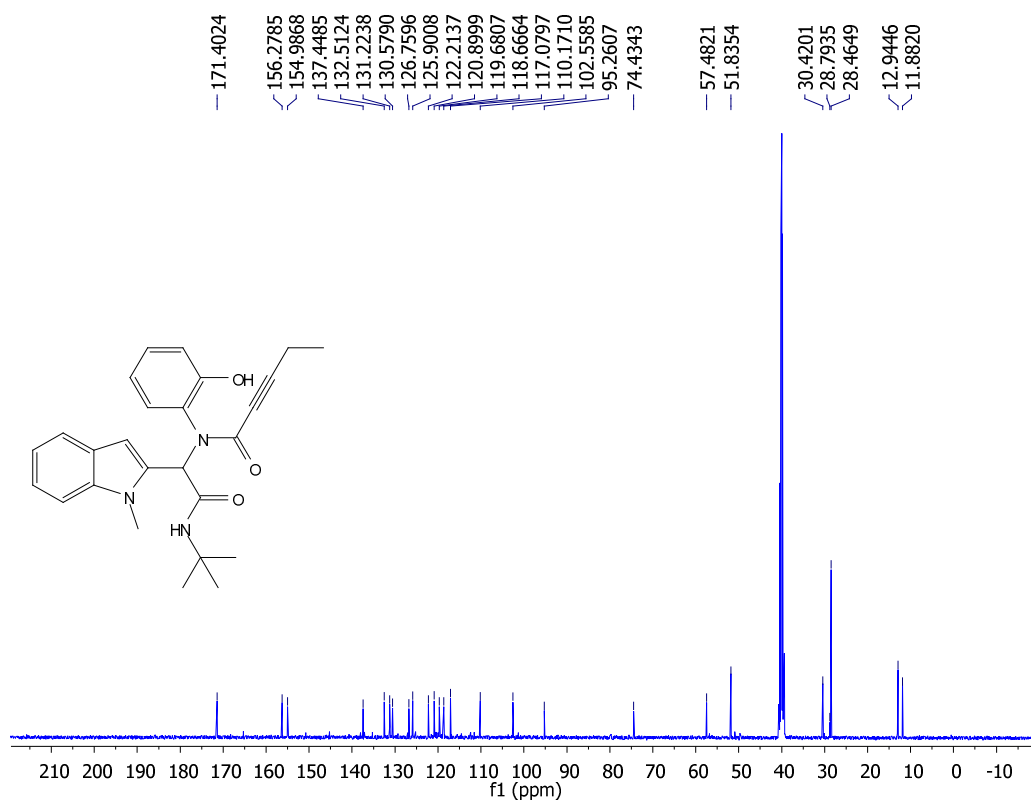
^1H and ^{13}C NMR spectra of compound **1t**



^1H and ^{13}C NMR spectra of compound **1u**

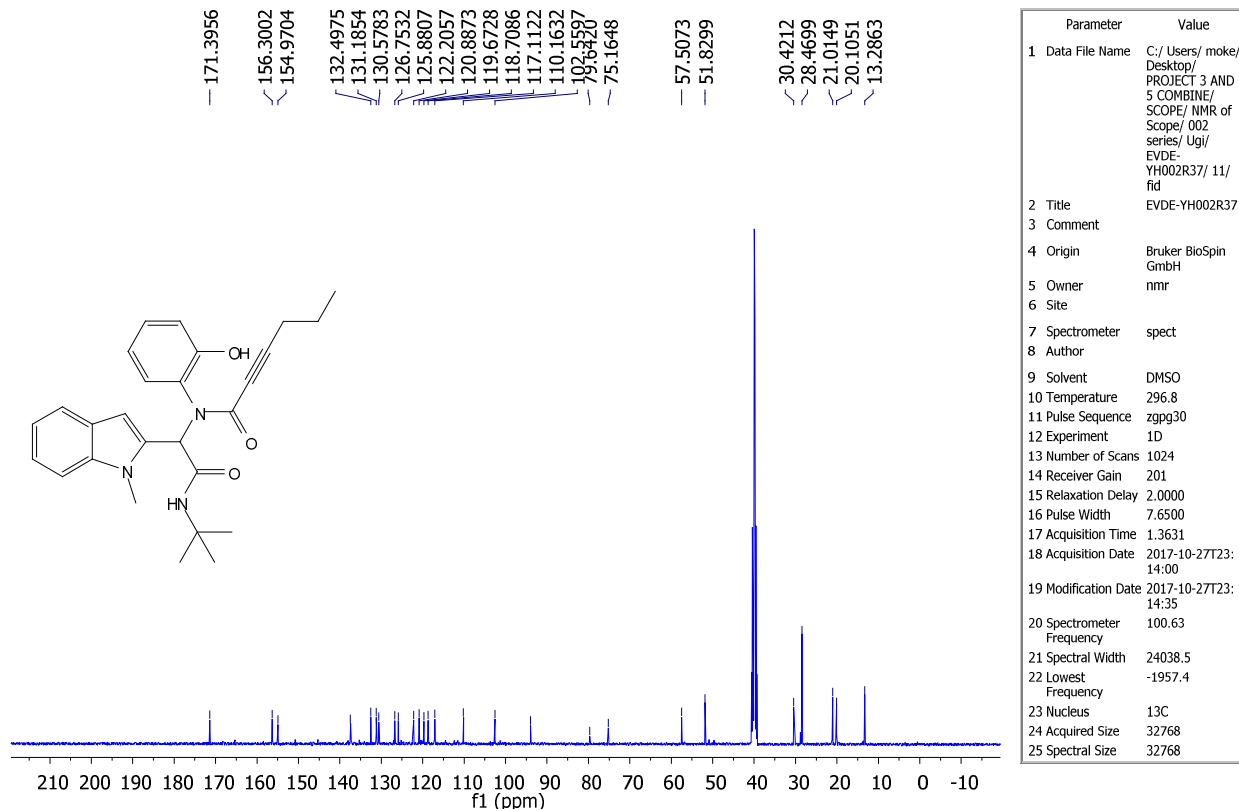
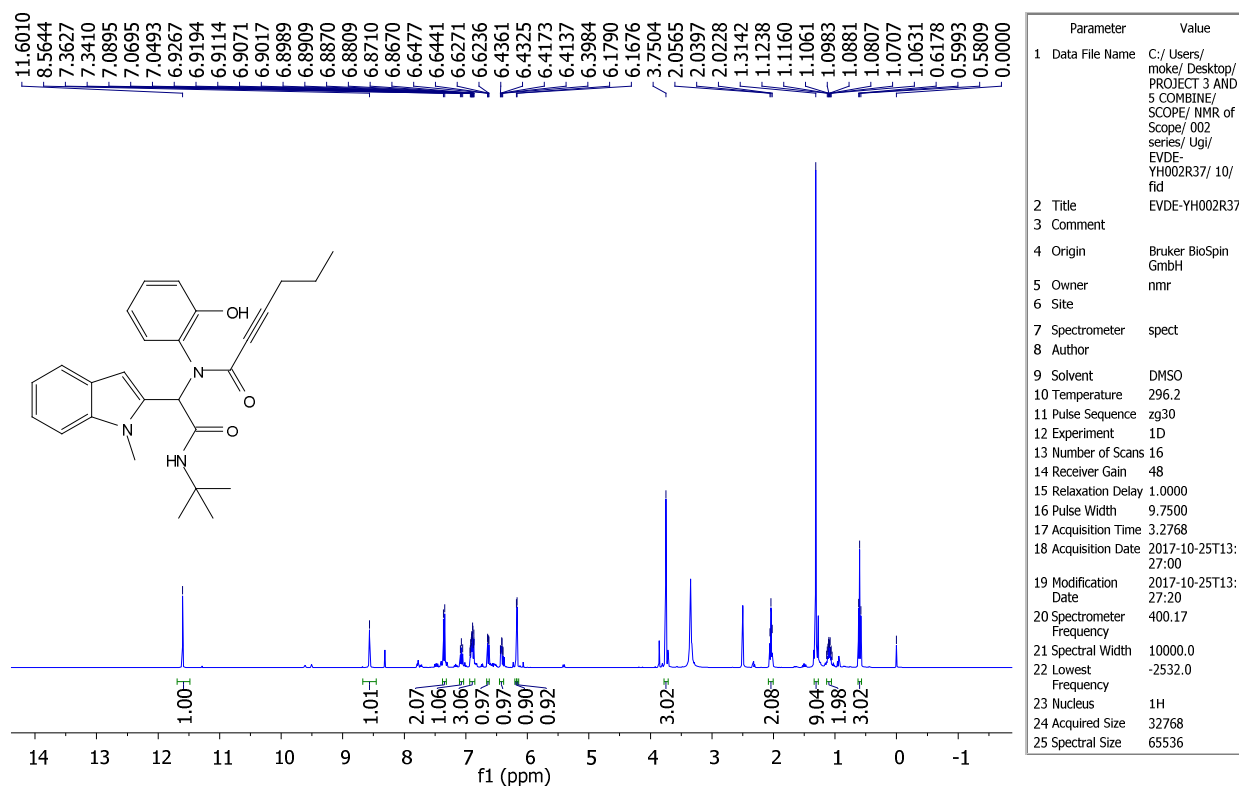


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of series/ Ugi/ EVDE- YH002R36/ 10/ fid
2 Title	EVDE- YH002R36
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	296.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	54
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2017-10-25T13:23:00
19 Modification Date	2017-10-25T13:23:29
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2532.7
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536

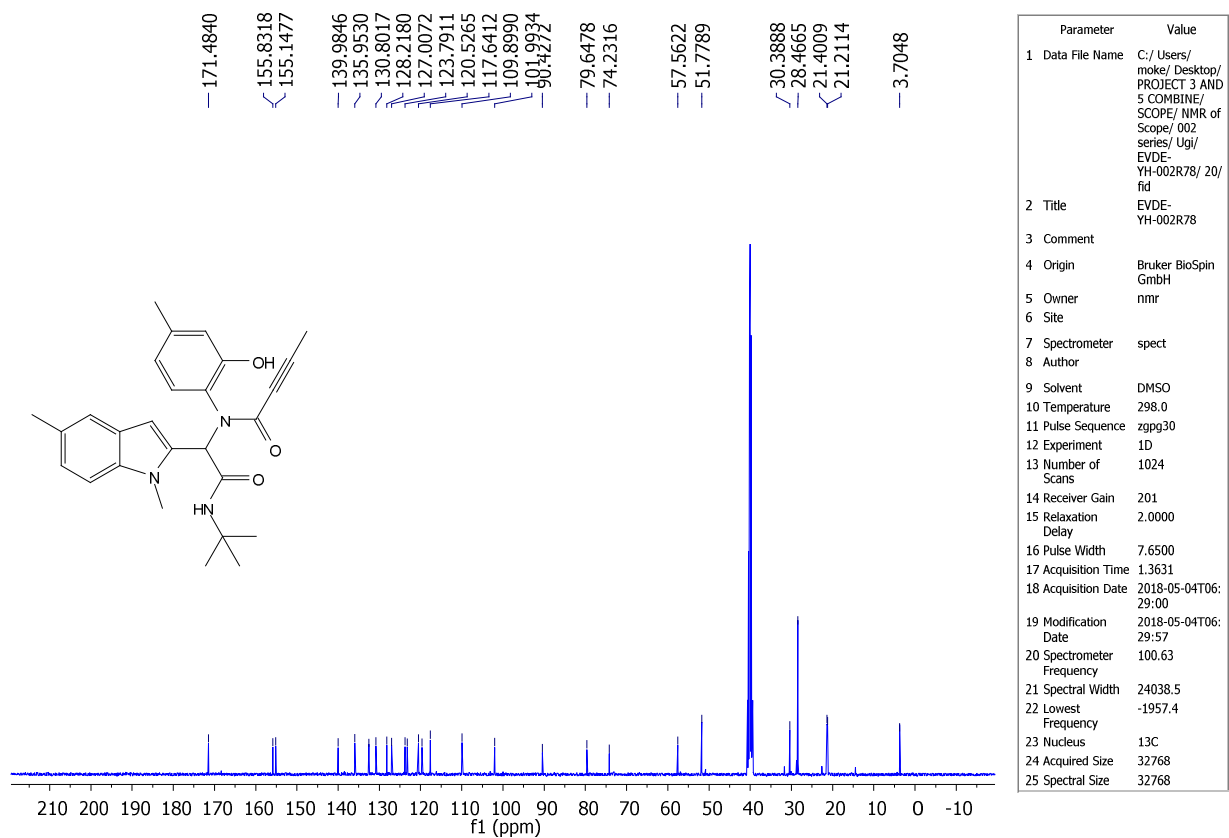
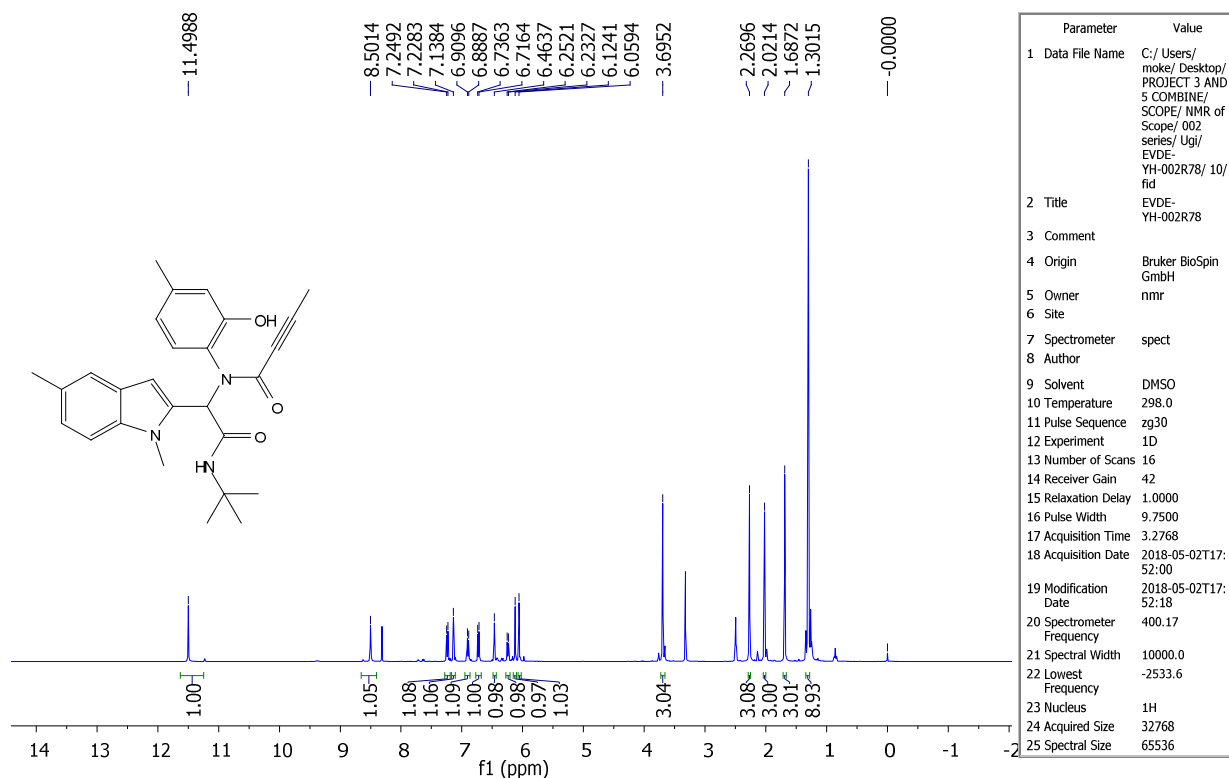


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of series/ Ugi/ EVDE- YH002R36/ 11/ fid
2 Title	EVDE-YH002R36
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	296.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1024
14 Receiver Gain	201
15 Relaxation Delay	2.0000
16 Pulse Width	7.6500
17 Acquisition Time	1.3631
18 Acquisition Date	2017-10-27T22:13:00
19 Modification Date	2017-10-27T22:13:16
20 Spectrometer Frequency	100.63
21 Spectral Width	24038.5
22 Lowest Frequency	-1957.4
23 Nucleus	^{13}C
24 Acquired Size	32768
25 Spectral Size	32768

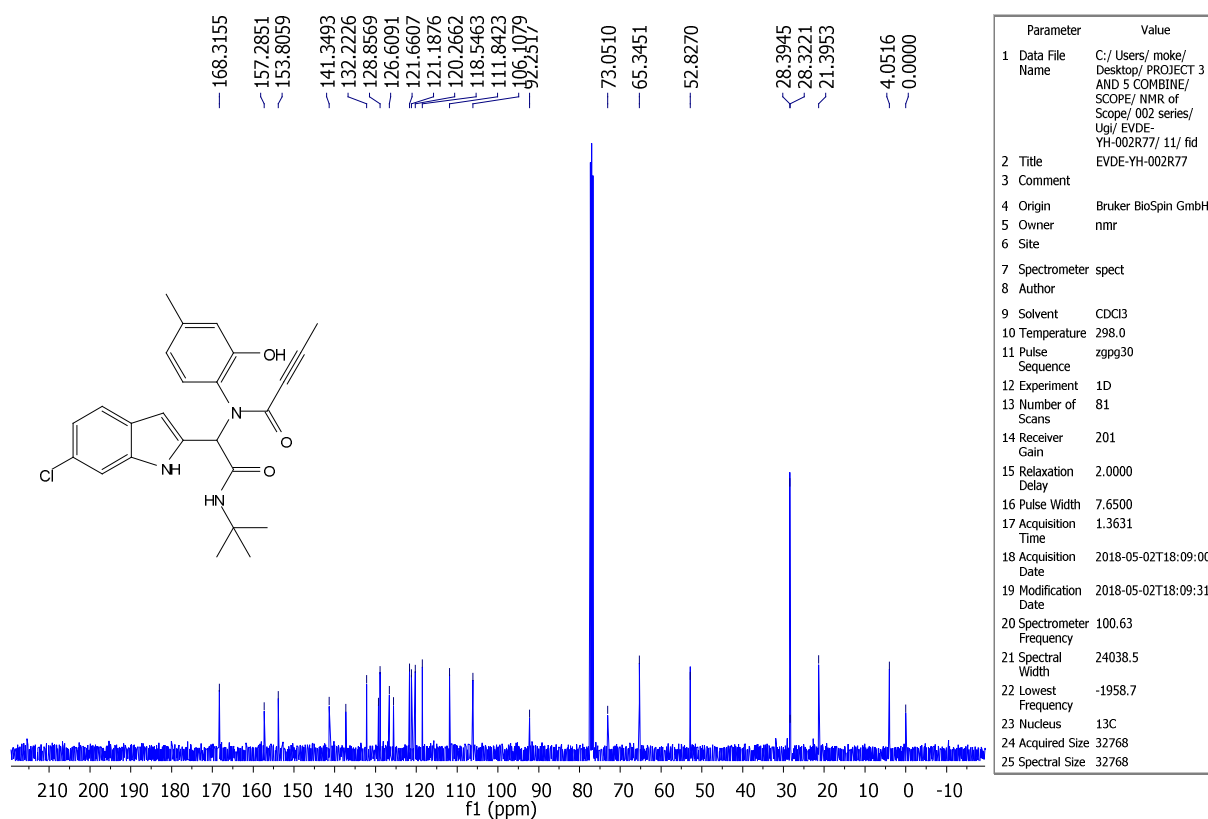
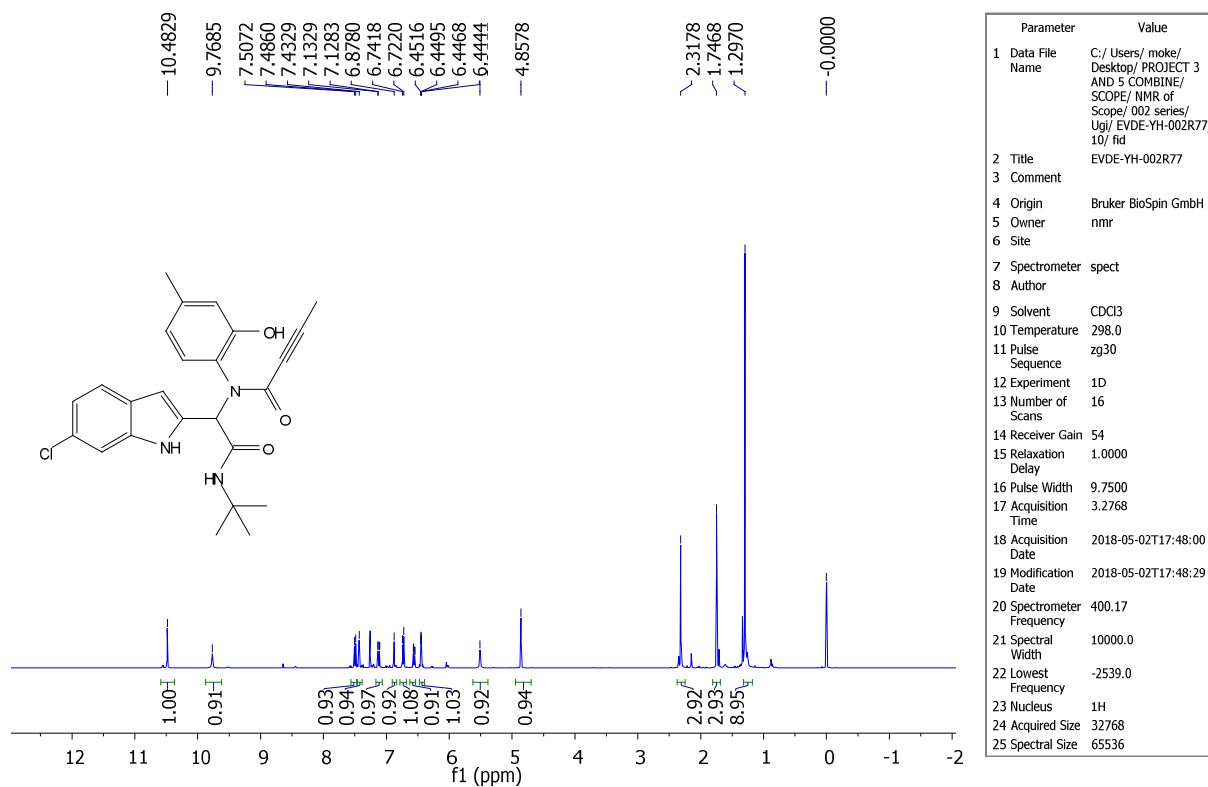
^1H and ^{13}C NMR spectra of compound **1v**



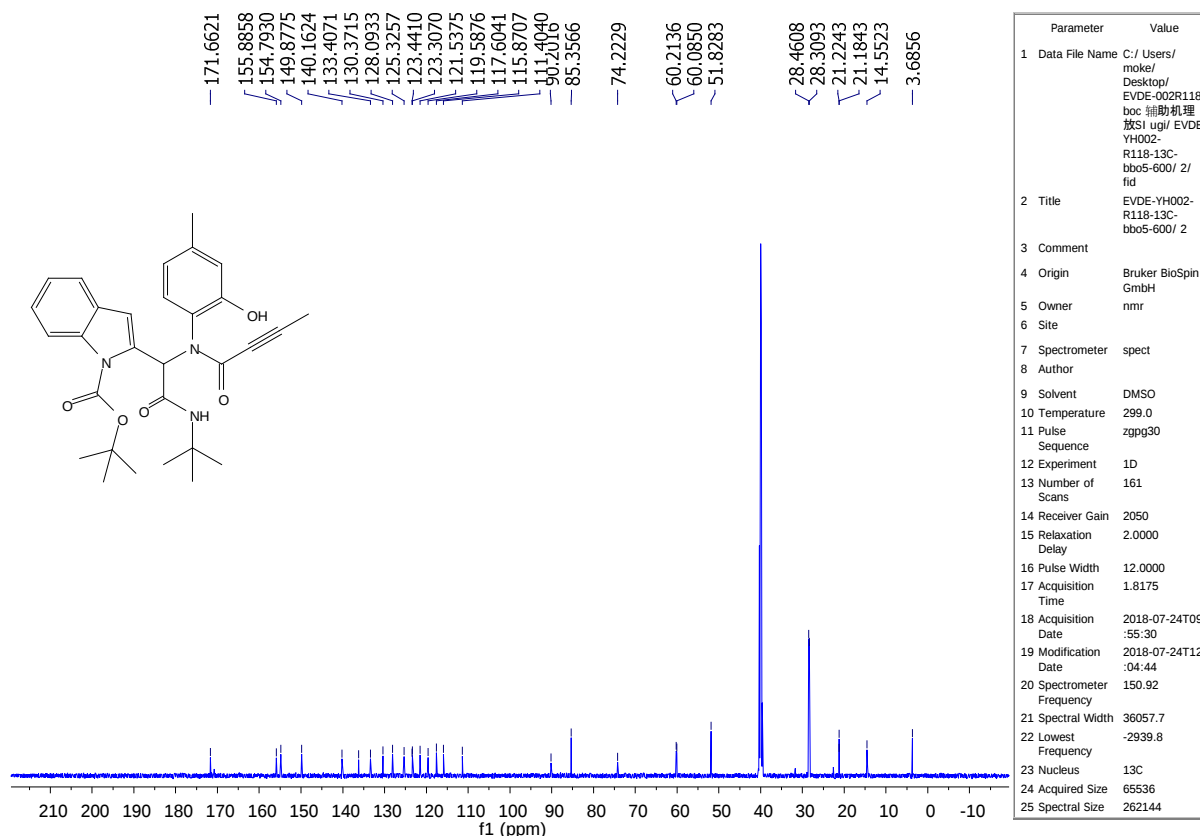
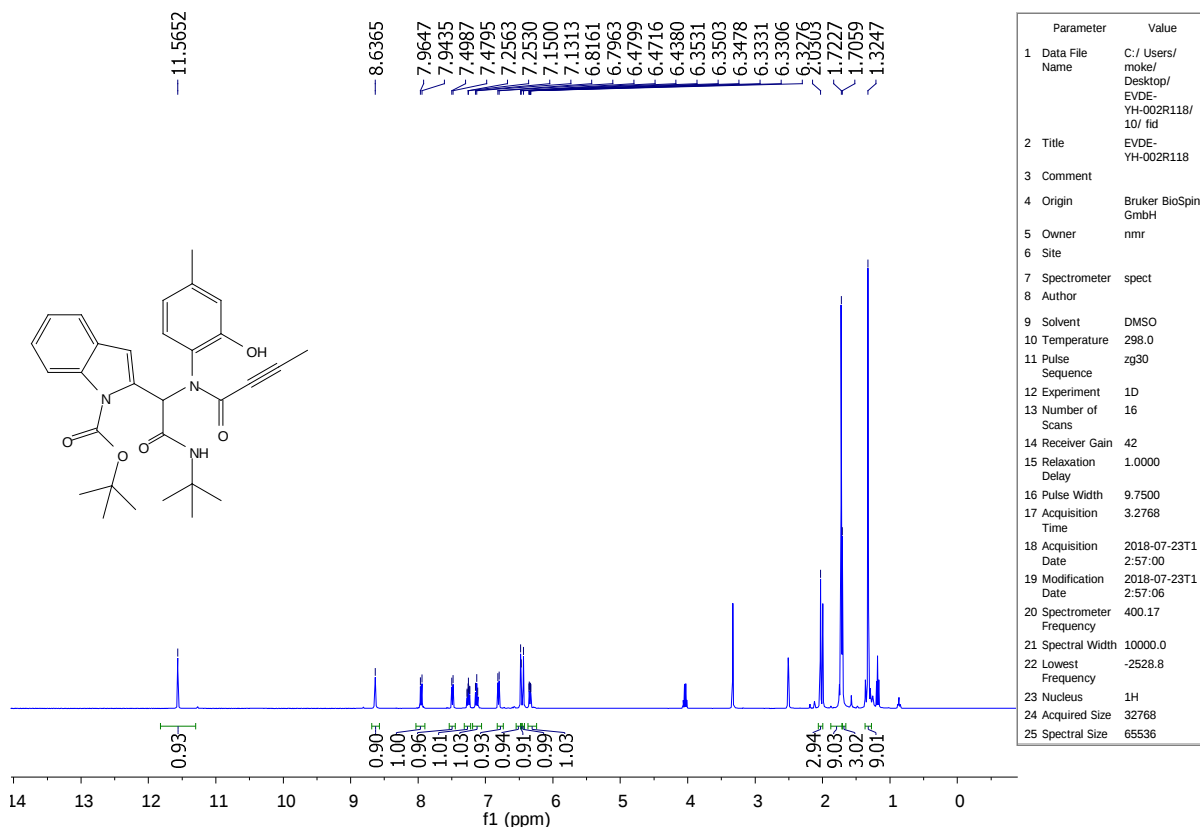
^1H and ^{13}C NMR spectra of compound **1w**



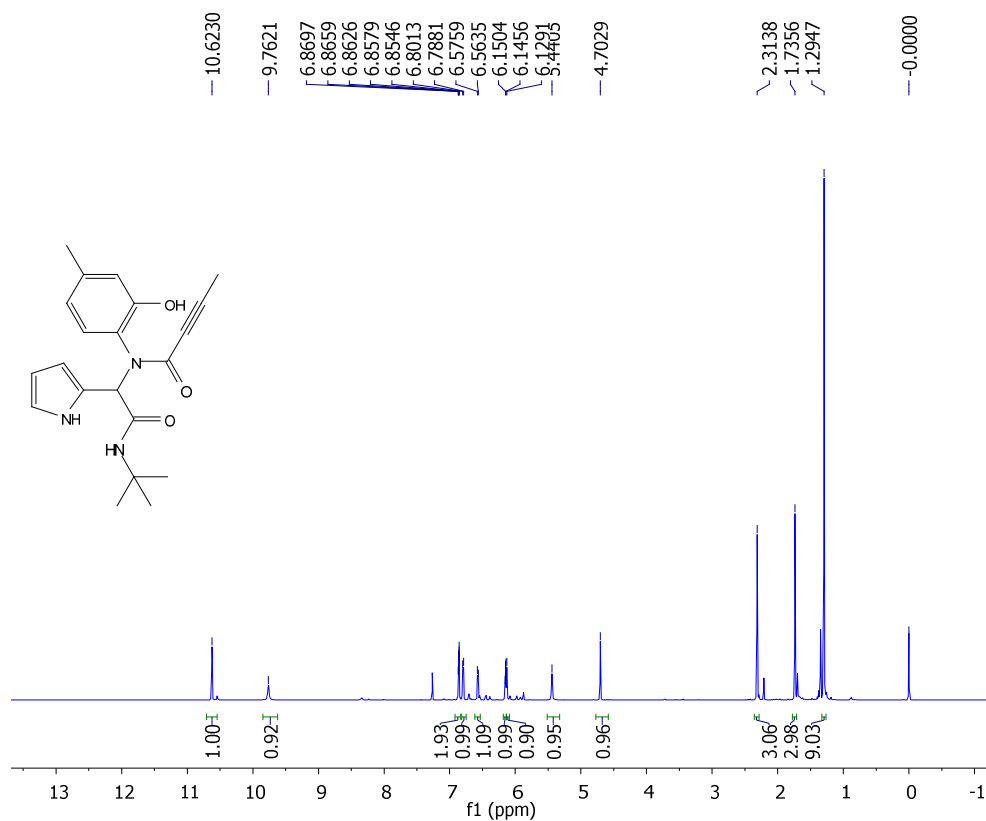
^1H and ^{13}C NMR spectra of compound **1x**



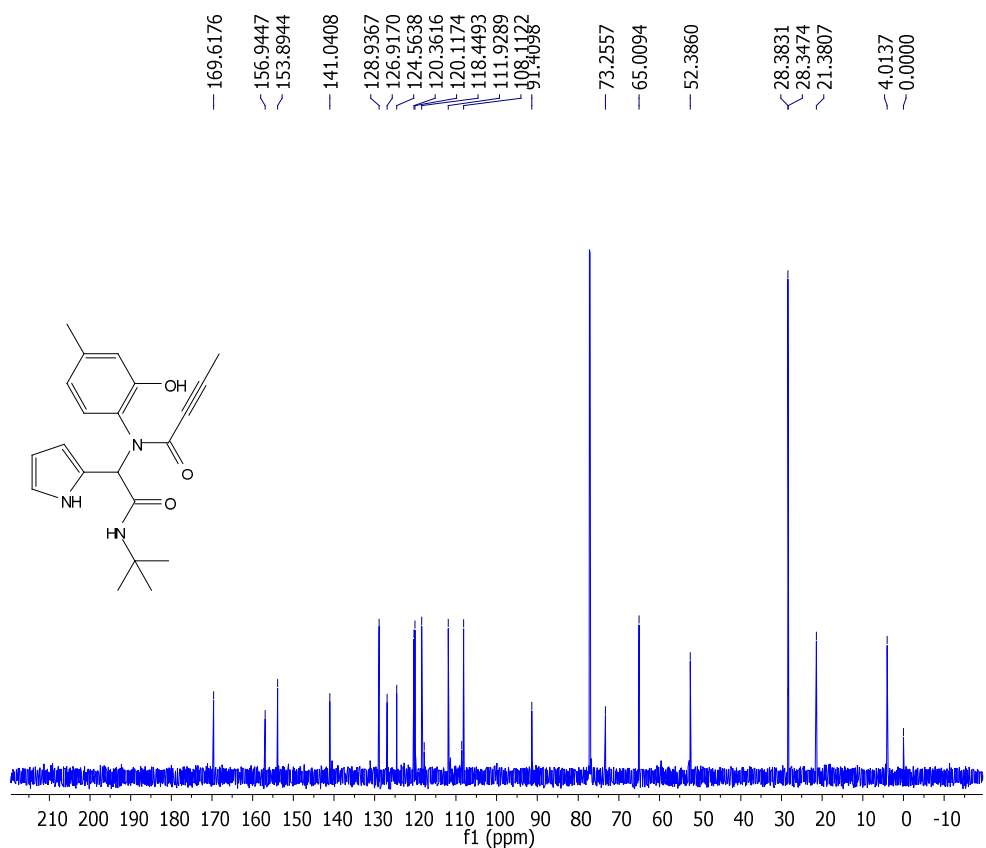
^1H and ^{13}C NMR spectra of compound **1y**



^1H and ^{13}C NMR spectra of compound **1ba**

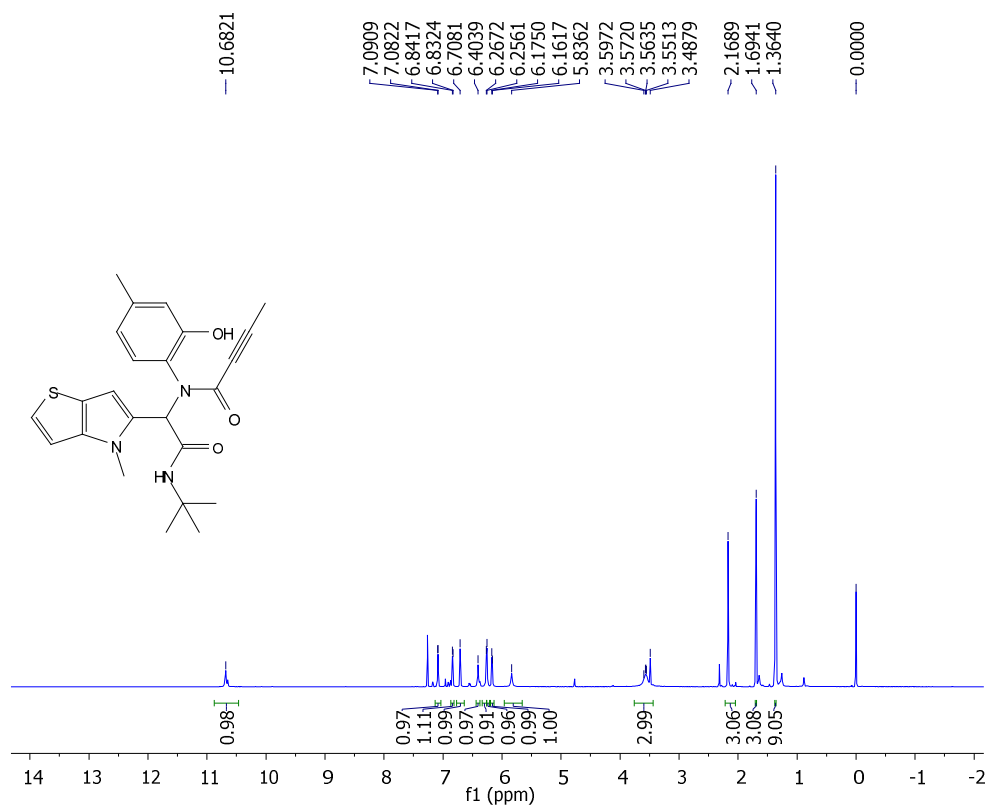


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1 Data File Name	C:/Users/moke/Desktop/NMR waiting to Check/PROJECT 002 SERIES/ EVDE-YH002-R81-1H-13C-bbo5-600/ 1/ fid
2 Title	DDV-TV-PUR-73UP.600
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	81
15 Relaxation Delay	2.0000
16 Pulse Width	15.2500
17 Acquisition Time	1.3631
18 Acquisition Date	2018-01-09T10:29:00
19 Modification Date	2018-05-11T11:56:42
20 Spectrometer Frequency	600.13
21 Spectral Width	12019.2
22 Lowest Frequency	-2316.2
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	131072

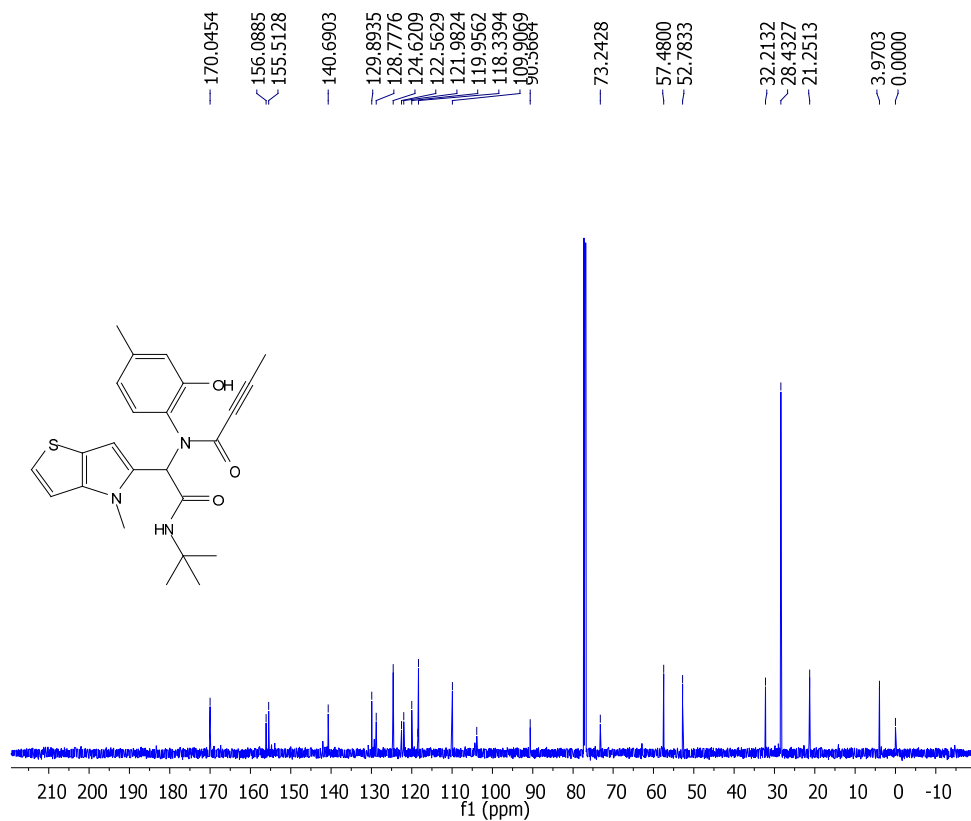


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/Scope/ 002 series/ Ugi/ EVDE-YH002-R81-1H-13C-bbo5-600/ 2/ fid
2 Title	EVDE-YH002-R81-1H-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	64
14 Receiver Gain	2050
15 Relaxation Delay	1.5000
16 Pulse Width	12.0000
17 Acquisition Time	1.1360
18 Acquisition Date	2018-05-11T11:30:07
19 Modification Date	2018-05-11T12:32:12
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.4
23 Nucleus	^{13}C
24 Acquired Size	40960
25 Spectral Size	131072

^1H and ^{13}C NMR spectra of compound **1bb**

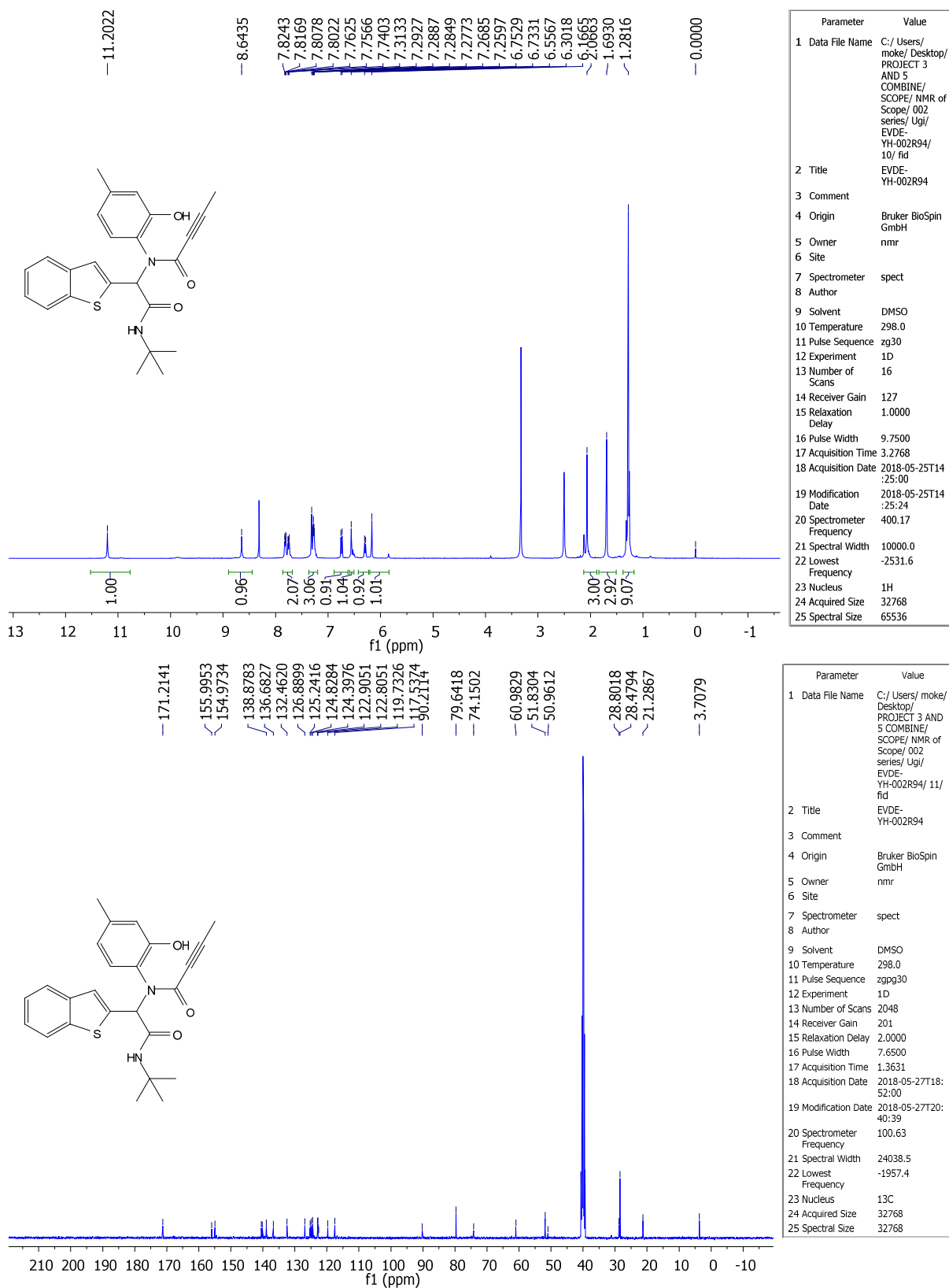


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1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ugi/ EVDE-YH002-R82-1H-13C-bbo5-600/ 1/ fid
2 Title	DDV-TV-PUR-73UP.600
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	81
15 Relaxation Delay	2.0000
16 Pulse Width	15.2500
17 Acquisition Time	1.3631
18 Acquisition Date	2018-01-09T10:29:00
19 Modification Date	2018-05-11T12:36:38
20 Spectrometer Frequency	600.13
21 Spectral Width	12019.2
22 Lowest Frequency	-2303.6
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	131072

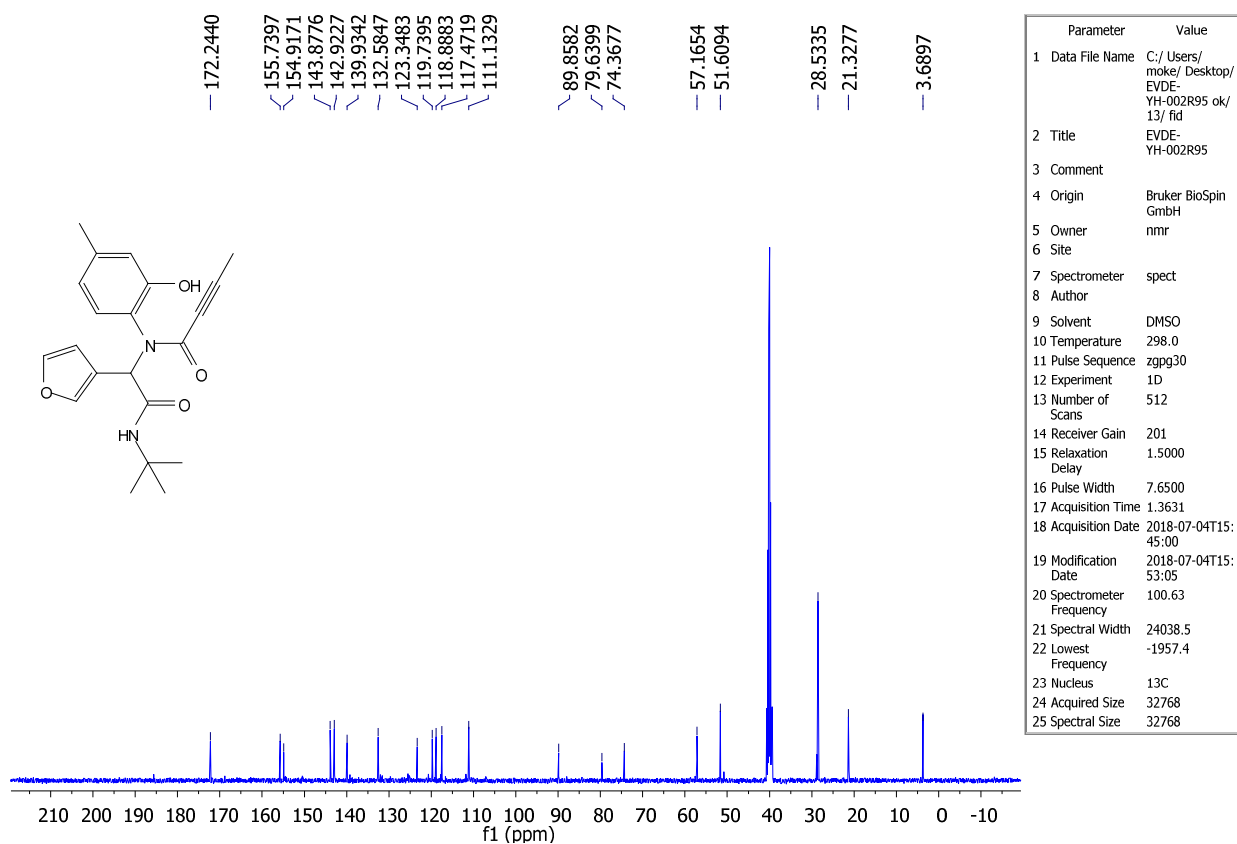
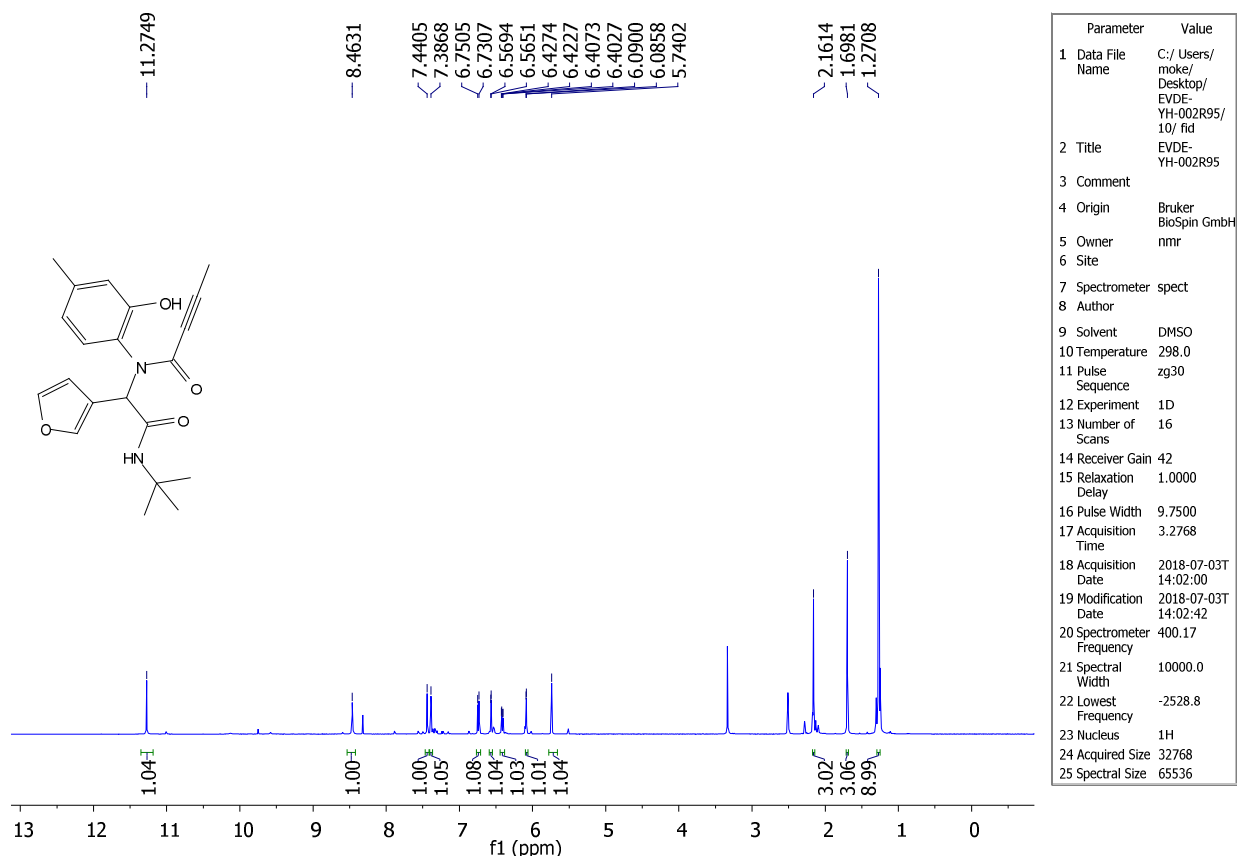


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2 Title	EVDE-YH002-R82-1H-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	192
14 Receiver Gain	2050
15 Relaxation Delay	1.5000
16 Pulse Width	12.0000
17 Acquisition Time	1.1360
18 Acquisition Date	2018-05-11T11:51:31
19 Modification Date	2018-05-11T12:55:30
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2940.5
23 Nucleus	^{13}C
24 Acquired Size	40960
25 Spectral Size	131072

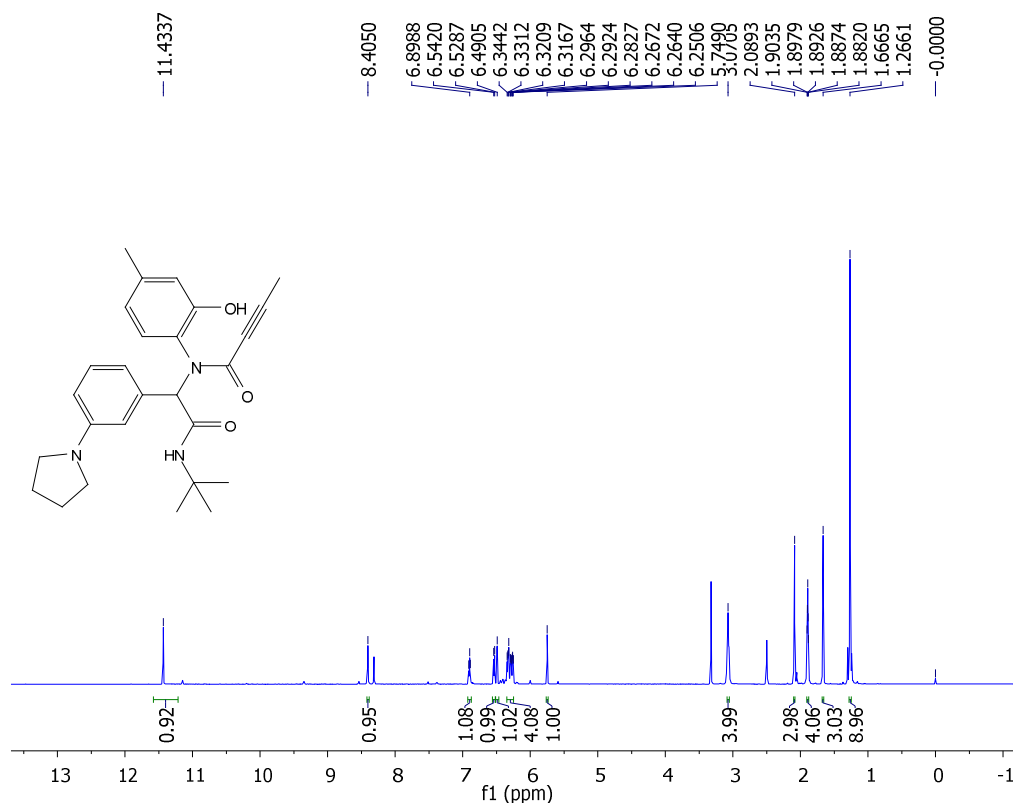
¹H and ¹³C NMR spectra of compound **1bc**



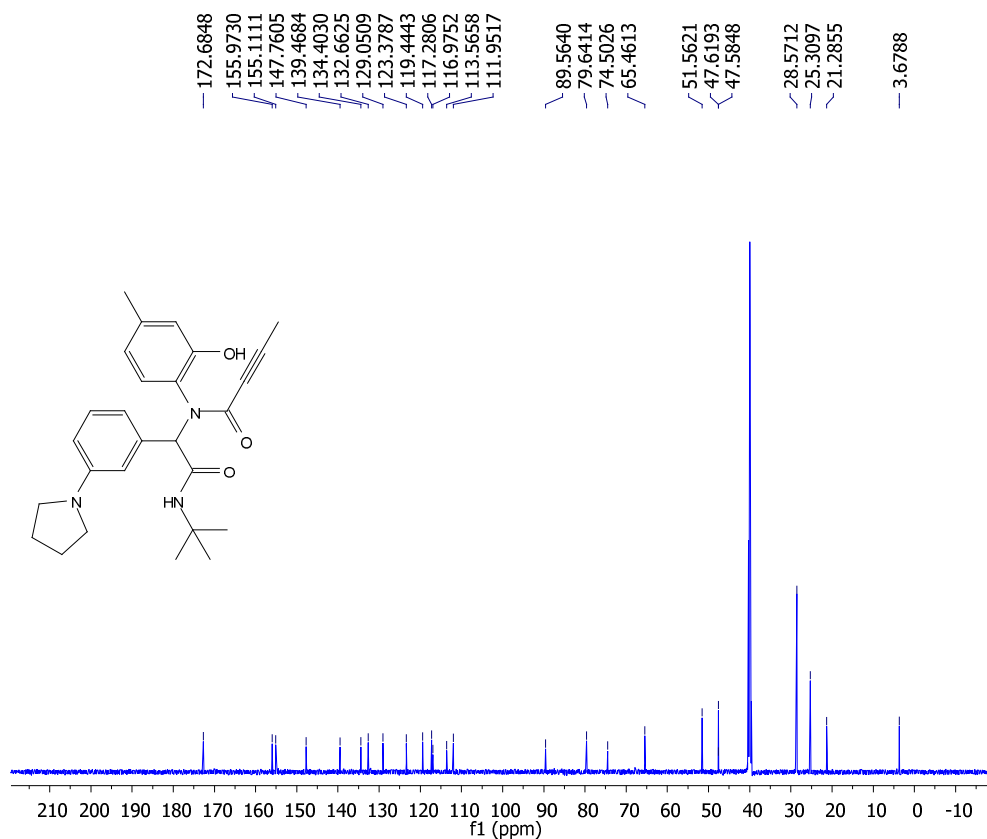
^1H and ^{13}C NMR spectra of compound **1bd**



^1H and ^{13}C NMR spectra of compound **1be**

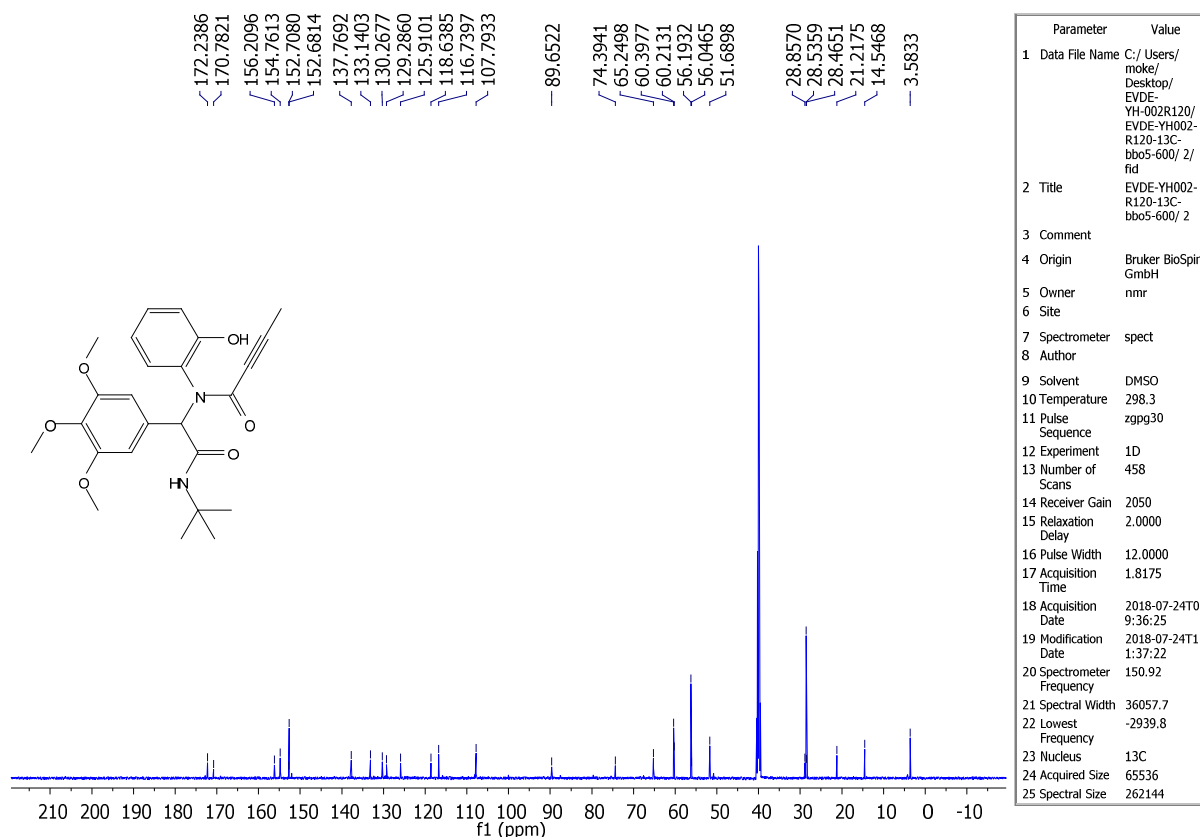
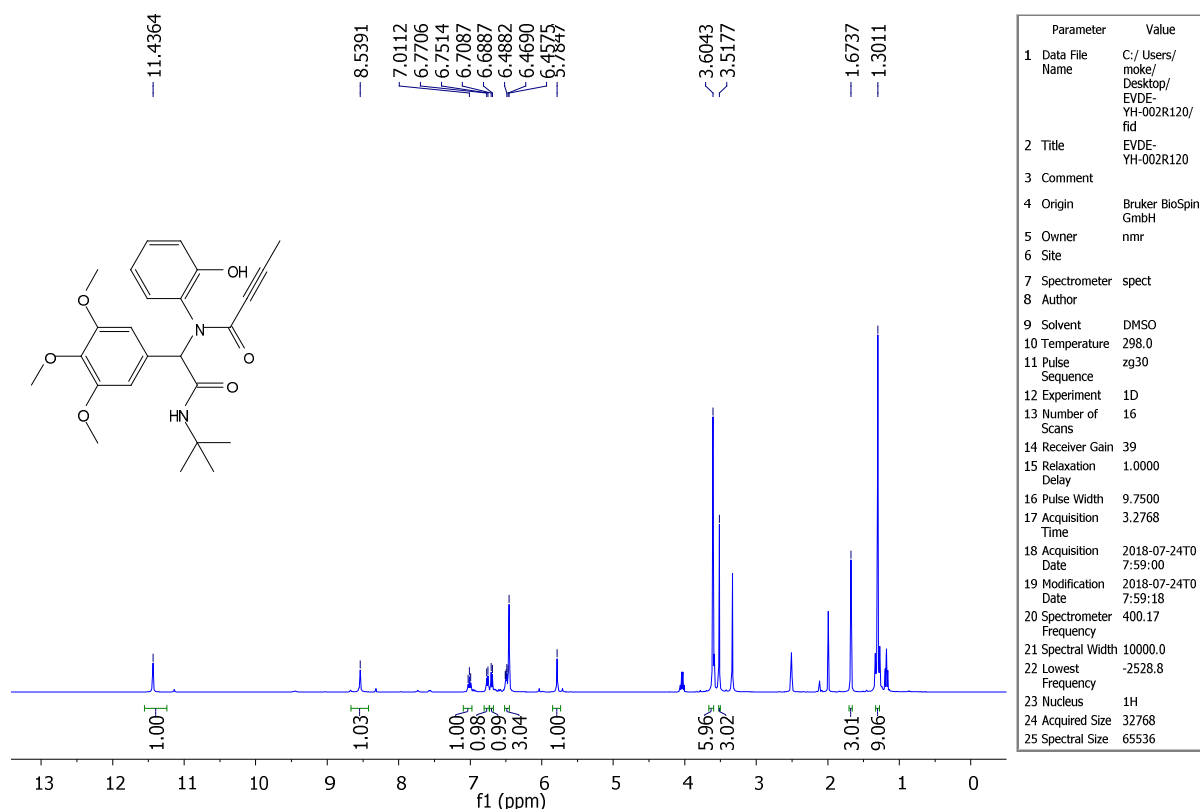


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ug/ EVDE-YH002-R83-1H-13C-bbo5-600/ 1/ fid
2 Title	DDV-TV-PUR-73UP.600
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	90
15 Relaxation Delay	2.0000
16 Pulse Width	15.2500
17 Acquisition Time	1.3631
18 Acquisition Date	2018-01-09T10:29:00
19 Modification Date	2018-05-11T17:29:04
20 Spectrometer Frequency	600.13
21 Spectral Width	12019.2
22 Lowest Frequency	-2309.0
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	131072

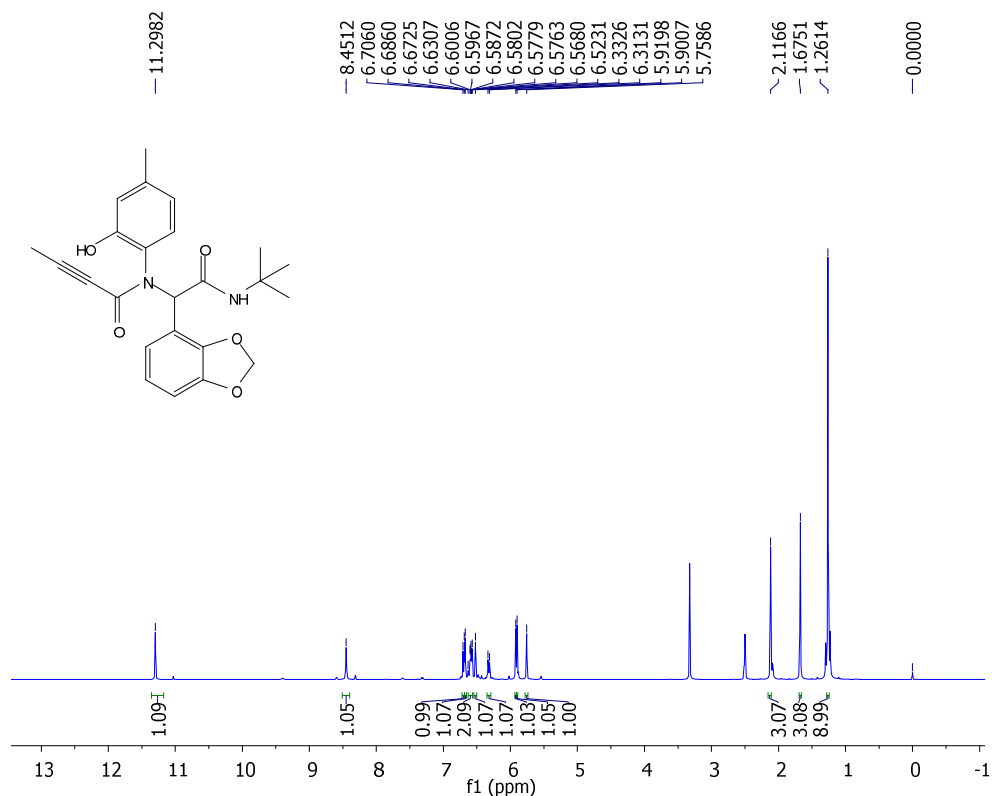


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/ Ug/ EVDE-YH002-R83-1H-13C-bbo5-600/ 2/ fid
2 Title	EVDE-YH002-R83-1H-13C-bbo5-600/ 2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	2050
15 Relaxation Delay	1.5000
16 Pulse Width	12.0000
17 Acquisition Time	1.1360
18 Acquisition Date	2018-05-11T16:30:52
19 Modification Date	2018-05-11T17:41:52
20 Spectrometer Frequency	150.92
21 Spectral Width	36057.7
22 Lowest Frequency	-2939.8
23 Nucleus	^{13}C
24 Acquired Size	40960
25 Spectral Size	131072

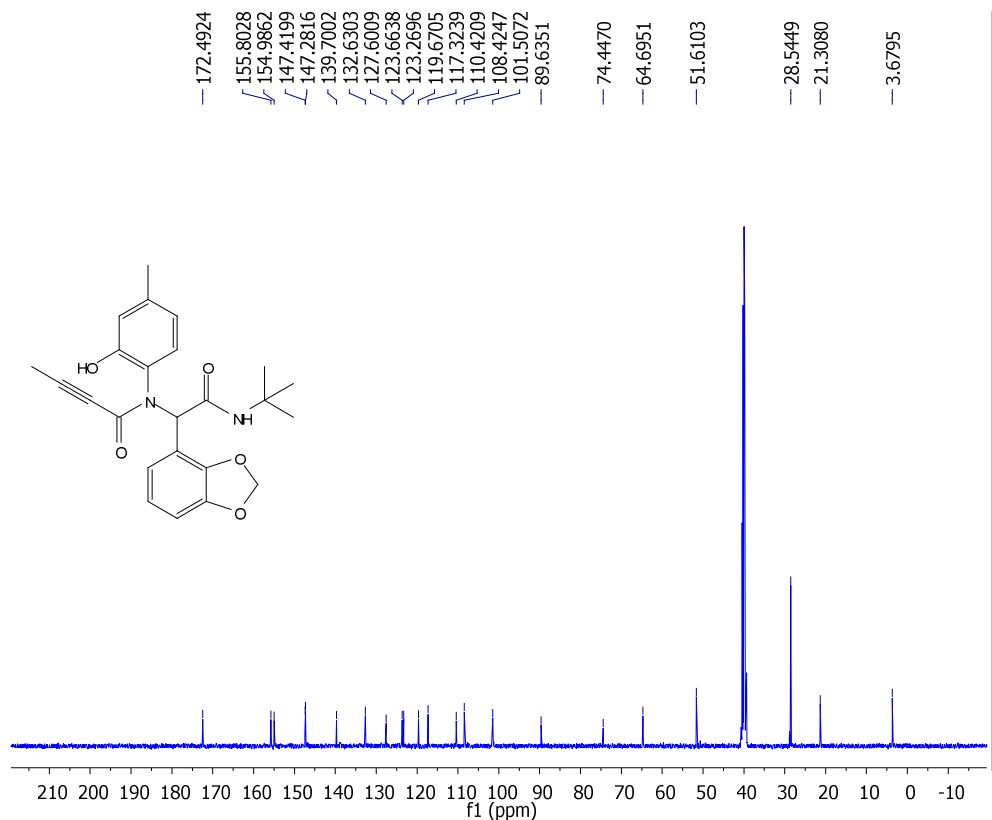
^1H and ^{13}C NMR spectra of compound **1bf**



^1H and ^{13}C NMR spectra of compound **s1b**

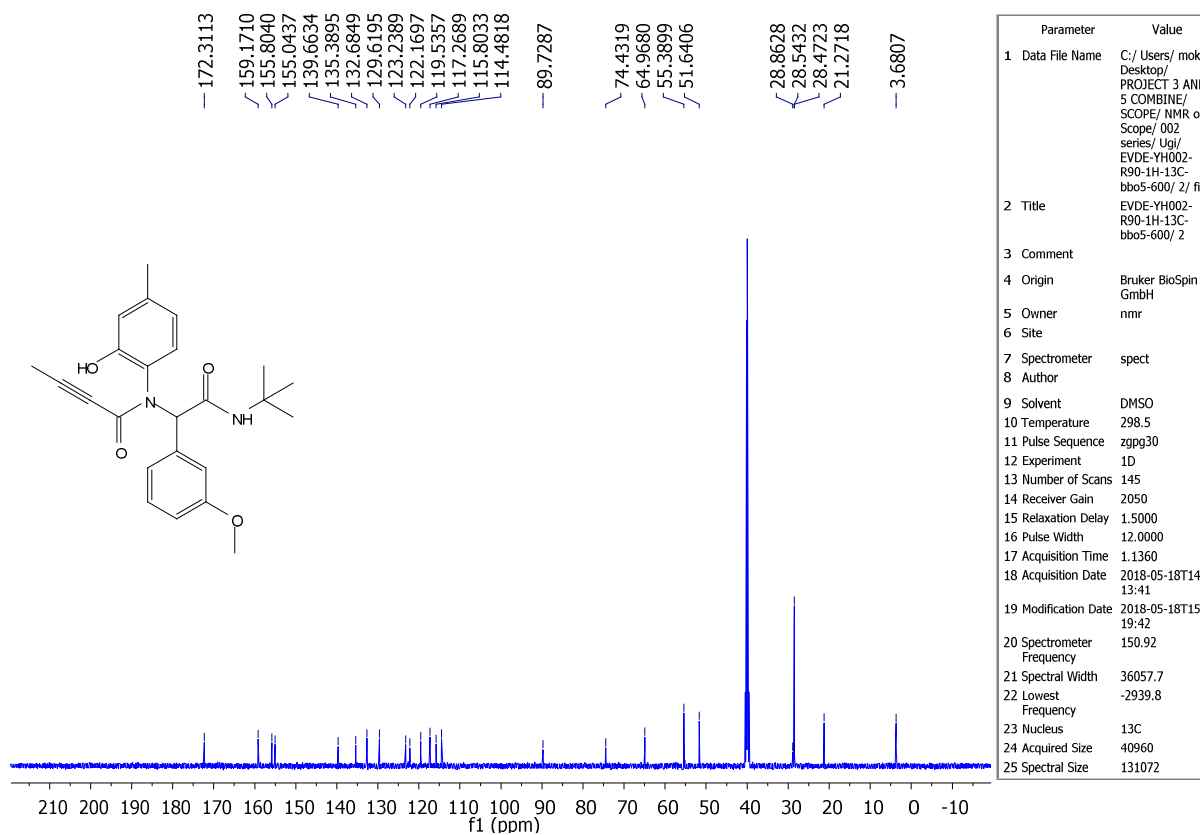
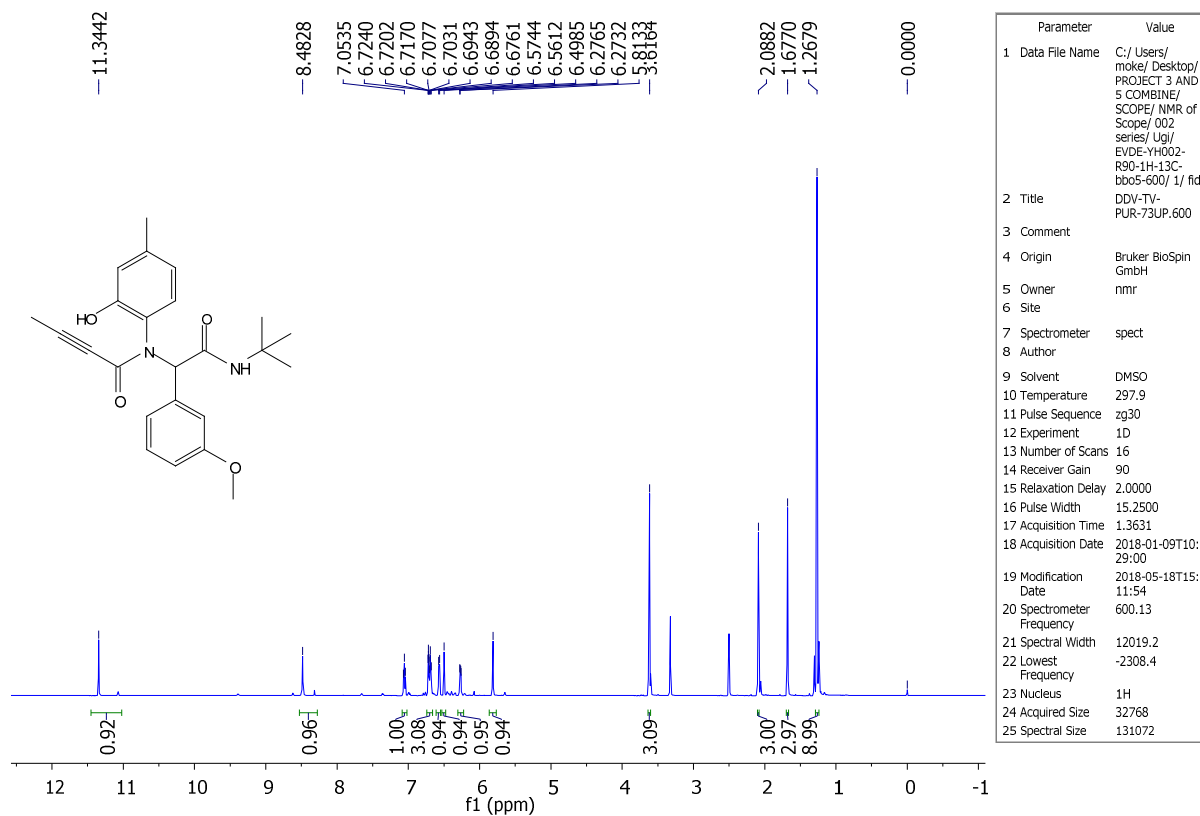


Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/EVDE-YH-002R88B/10/ fid
2 Title	EVDE-YH-002R88B
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	48
15 Relaxation Delay	1.0000
16 Pulse Width	9.7500
17 Acquisition Time	3.2768
18 Acquisition Date	2018-05-16T11:32:00
19 Modification Date	2018-05-16T11:32:08
20 Spectrometer Frequency	400.17
21 Spectral Width	10000.0
22 Lowest Frequency	-2532.0
23 Nucleus	^1H
24 Acquired Size	32768
25 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/Users/moke/Desktop/PROJECT 3 AND 5 COMBINE/SCOPE/ NMR of Scope/ 002 series/Ugi/ EVDE-YH-002R88B/ 12/ fid
2 Title	EVDE-YH-002R88B
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	512
14 Receiver Gain	201
15 Relaxation Delay	1.5000
16 Pulse Width	7.6500
17 Acquisition Time	1.3631
18 Acquisition Date	2018-05-16T17:35:00
19 Modification Date	2018-05-16T17:35:47
20 Spectrometer Frequency	100.63
21 Spectral Width	24038.5
22 Lowest Frequency	-1957.4
23 Nucleus	^{13}C
24 Acquired Size	32768
25 Spectral Size	32768

^1H and ^{13}C NMR spectra of compound **s1c**



¹H and ¹³C NMR spectra of compound **s1d**

