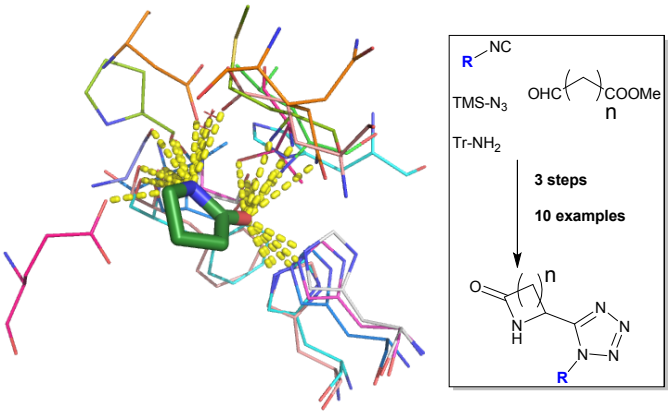
Supporting Information



Ugi 4-CR Synthesis of γ- and δ-Lactams

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General

All isonitriles were made in house by either performing the Hoffman or Ugi procedure. Other reagents were purchased from Sigma Aldrich, ABCR, Acros and AK Scientific and were used without further purification. All microwave irradiation reactions were carried out in a Biotage Initiator™ Microwave Synthesizer. The Ugi tetrazoles were purified by flash chromatography, on a Teledyne ISCO Rf 200, using RediSep Rf Normal-phase Silica Flash Columns (Silica Gel 60 Å, 230 - 400 mesh) unless otherwise noted. Column chromatography was performed with MP Ecochrom Silica Gel 32–63, 60 Å. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR spectra were recorded on a Bruker Avance DRX 500. Chemical shift values are reported as part per million (δ) relative to residual solvent peaks ($CDCl_3$, ^{1}H δ = 7.26, ^{13}C δ = 77.16 or TMS ^{1}H δ = 0.00 ppm). The coupling constants (J) are reported in Hertz (Hz). Electrospray ionization mass spectra were measured on an API 3000 triple-quadrupole mass spectrometer (Applied Biosystems/MDS Sciex) via a TurboIonSpray source. Data collected and analyzed by the Analyst 1.5 data acquisition software (Applied Biosystems/MDS Sciex).

Crystallographic data were collected on an X-ray single crystal diffractometer equipped with a CCD detector (Bruker APEX II, κ–CCD), a fine focus sealed tube (Bruker AXS, D8) with MoK_α radiation (λ = 0.71073 Å), and a graphite monochromator by using the SMART software package. [1] The measurements were performed on single crystals coated with perfluorinated ether. The crystals were fixed on the top of a cactus prickle (Opuntia ficus-india) with perfluorinated ether and transferred to the diffractometer. The crystals were frozen under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using SAINT. [2] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS. [2] Space group assignments were based upon systematic absences, *E* statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps, and were refined against all data using WinGX [7] based on SIR-92. [3] If not mentioned otherwise, non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms could be located in the difference Fourier maps and were allowed to refine freely. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2-F_c^2)^2$ with SHELXL-97 [5] weighting scheme. Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from *International Tables for Crystallography*. [4] Images of the crystal structures were generated by PLATON. [6] CCDC 961190 (**6b**), CCDC 961191 (**6e**), CCDC 961188 (**6f**),and CCDC 961189 (**6j**) contains the supplementary crystallographic data for this compound. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif or via https://www.ccdc.cam.ac.uk/services/structure_deposit/

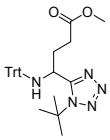
Synthetic Procedures and characterization data for compounds 5a-j and 6a-j

Synthetic procedure 1

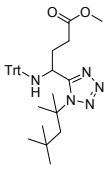
Aldehyde (1 mmol), tritylamine (1 mmol) were mixed in methanol (1 mL) and subjected to microwave irradiation for 15 minutes. Subsequently azidotrimethylsilane (1 mmol) and isonitrile (1mmol) were added and the mixture was again subjected to microwave irradiation for 15 minutes at 100°C. The solvent was evaporated under reduced pressure and the residue was purified using flash chromatography to obtain the product.

Synthetic procedure 2

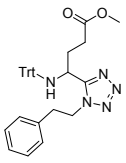
To a solution of Ugi tetrazole (0.5-1.0 mmol) in 3 mL CH_2Cl_2 was added TFA (150 µL, 2 mmol). After 1 minute the mixture was filtered through a silica bed washing with 50 mL Heptane:EtOAc 1:1 (v/v) to remove the trityl cation impurity. The amine was collected by washing the silica bed with 50 mL CH_2Cl_2:MeOH 1:1 (v/v). The mixture was concentrated under reduced pressure and redissolved in dry THF (3 mL). Sodium hydride (5 mmol) was washed with heptanes prior to addition. After 4 hours of stirring, EtOH was added to quench the reaction. The solvents were removed under reduced pressure, and the residue was purified by column chromatography using CH_2Cl_2:MeOH 20:1 (v/v) to afford the lactam.



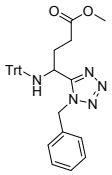
Methyl 4-(1-(tert-butyl)-1H-tetrazol-5-yl)-4-(tritylamino)butanoate (5a): The product was obtained using procedure 1 starting from *t*-butylisocyanide and **3a** as a white solid (354 mg, 73%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500MHz, $CDCl_3$): δ 7.40 (d, *J* = 7.5, 6H), 7.19 (t, *J* = 7.5, 9H), 7.13 (t, *J* = 7.2, 3H), 4.41 (s, 1H), 3.63 (s, 3H), 3.49 (s, 1H), 2.80 – 2.67 (m, 1H), 2.49 – 2.34 (m, 1H), 2.28 – 2.22 (m, 1H), 1.87 – 1.80 (m, 1H), 1.42 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.7, 156.8, 145.6, 128.9, 127.9, 126.7, 71.7, 61.8, 51.8, 48.4, 32.3, 29.9, 28.3 ppm. HRMS (ESI): *m/z,* calcd. for $C_{26}H_{37}O_2N_5Na$ [M + Na^+]: 506.2527, found 506.2529.



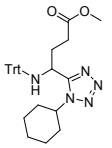
Methyl 4-(1-(2,4,4-trimethylpentan-2-yl)-1H-tetrazol-5-yl)-4-(tritylamino)butanoate (5b): The product was obtained using procedure starting from *t*-octylisocyanide and **3a** as a white solid (269 mg, 50%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.5, 6H), 7.19 (t, *J* = 7.5, 6H), 7.14 (t, *J* = 7.2, 3H), 4.50 – 4.40 (m, 1H), 3.62 (s, 3H), 3.54 (d, *J* = 9.0, 1H), 2.74 – 2.60 (m, 1H), 2.35 – 2.25 (m, 1H), 2.20 – 2.13 (m, 1H), 1.90 – 1.83 (m, 1H), 1.73 (q, *J* = 14.8, 2H), 1.52 (s, 3H), 1.43 (s, 3H), 0.81 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.6, 157.0, 145.7, 129.0, 127.9, 126.8, 71.7, 66.1, 55.2, 51.7, 48.6, 32.2, 31.6, 31.1, 29.9, 28.5, 28.4 ppm. HRMS (ESI): *m/z,* calcd. for $C_{33}H_{41}O_2N_5Na$ [M + Na^+]: 562.3153, found 562.3154.



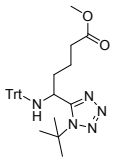
Methyl 4-(1-phenethyl-1H-tetrazol-5-yl)-4-(tritylamino)butanoate (5c): The product was obtained using procedure 1 starting from phenethylisocyanide and **3a** as a white solid (398 mg, 75%): R_f 0.31 (EtOAc:Hept 1:2).). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.5, 6H), 7.27 – 7.09 (m, 13H), 7.00 (d, *J* = 7.2, 2H), 4.02 – 3.84 (m, 2H), 3.81 – 3.71 (m, 1H), 3.64 (s, 3H), 3.15 – 2.96 (m, 3H), 2.56 – 2.40 (m, 1H), 2.18 – 2.02 (m, 1H), 1.93 – 1.87 (m, 1H), 1.43 – 1.37 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.33, 157.14, 145.15, 136.69, 128.96, 128.81, 128.62, 127.98, 127.32, 126.84, 71.59, 51.76, 48.56, 47.01, 35.43, 31.76, 29.01 ppm. HRMS (ESI): *m/z,* calcd. for $C_{33}H_{33}O_2N_5Na$ [M + Na^+]: 554.2527, found 554.2528.



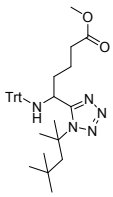
Methyl 4-(1-benzyl-1H-tetrazol-5-yl)-4-(tritylamino)butanoate (5d): The product was obtained using procedure 1 starting from benzylisocyanide and **3a** as a white solid (290 mg, 56%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.1, 6H), 7.24 – 7.27 (m, 3H), 7.20 – 7.11 (m, 9H), 7.05 (d, *J* = 6.7, 2H), 5.21 (d, *J* = 15.3, 1H), 4.76 (d, *J* = 15.3, 1H), 4.14 – 4.10 (m, 1H), 3.58 (s, 3H), 3.00 (d, *J* = 9.2, 1H), 2.47 – 2.41 (m, 1H), 2.20 – 2.07 (m, 1H), 1.96 – 1.89 (m, 1H), 1.59 – 1.53 (m, 1H), 1.33 – 1.24 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.31, 157.08, 145.21, 133.28, 129.14, 128.92, 128.58, 128.03, 128.00, 126.83, 71.49, 51.73, 50.82, 47.06, 31.50, 28.86 ppm. HRMS (ESI): *m/z,* calcd. for $C_{32}H_{31}O_2N_5Na$ [M + Na^+]: 540.2372, found 540.2372.



Methyl 4-(1-cyclohexyl-1H-tetrazol-5-yl)-4-(tritylamino)butanoate (5e): The product was obtained using procedure 1 starting from cyclohexylisocyanide and **3a** as a white solid (203 mg, 40%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.1, 6H), 7.20 (t, *J* = 7.5, 6H), 7.15 (t, *J* = 6.8, 3H), 4.16 – 4.02 (m, 1H), 3.78 – 3.68 (m, 1H), 3.61 (s, 3H), 3.12 (d, *J* = 8.3, 1H), 2.68 – 2.49 (m, 1H), 2.34 – 2.13 (m, 2H), 1.96 – 1.76 (m, 4H), 1.76 – 1.57 (m, 4H), 1.37 – 1.18 (m, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.33, 156.11, 145.39, 128.74, 127.97, 126.85, 71.80, 57.45, 51.77, 47.09, 33.59, 32.02, 31.99, 28.88, 25.34, 25.29, 24.80 ppm. HRMS (ESI): *m/z,* calcd. for $C_{31}H_{35}O_2N_5Na$ [M + Na^+]: 532.2683, found 532.2685.

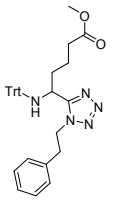


Methyl 5-(1-(tert-butyl)-1H-tetrazol-5-yl)-5-(tritylamino)pentanoate (5f): The product was obtained using procedure 1 starting from *t*-butylisocyanide and **3b** as a white solid (389 mg, 78%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.0, 6H), 7.20 (t, *J* = 7.5, 6H), 7.13 (t, *J* = 7.0, 3H), 4.34 – 4.25 (m, 1H), 3.62 (s, 3H), 3.40 (d, *J* = 9.3, 1H), 2.25 (t, *J* = 6.9, 2H), 1.94 – 1.70 (m, 2H), 1.64 – 1.48 (m, 2H), 1.41 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.47, 157.18, 145.78, 128.95, 127.91, 126.69, 71.75, 61.64, 51.57, 49.33, 37.13, 33.91, 30.02, 19.88 ppm. HRMS (ESI): *m/z,* calcd. for $C_{30}H_{35}O_2N_5Na$ [M + Na^+]: 520.2683, found 520.2686.

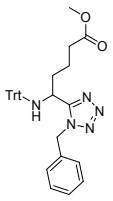


Methyl 5-(1-(2,4,4-trimethylpentan-2-yl)-1H-tetrazol-5-yl)-5-(tritylamino)pentanoate (5g): The product was obtained using procedure 1 starting from *t*-octylisocyanide and **3b** as a white solid (343 mg, 62%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.5, 6H), 7.21 (t, *J* = 7.5, 6H), 7.14 (t, *J* = 7.2, 3H), 4.42 – 4.25 (m, 1H), 3.61 (s, 2H), 3.39 (d, *J* = 8.9, 1H), 2.29 – 2.08 (m, 2H), 1.82 – 1.65 (m, 4H), 1.64 – 1.53 (m, 1H), 1.52 – 1.41 (m, 7H), 0.81 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.4, 157.2, 145.9, 129.0,

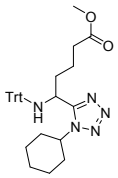
127.9, 126.7, 71.7, 66.0, 55.2, 51.6, 49.6, 36.6, 33.9, 31.6, 31.1, 30.0, 28.5, 19.9 ppm. HRMS (ESI): *m/z,* calcd. for $C_{34}H_{43}O_2N_5Na$ [M + Na^+]: 576.3309, found 576.3310.



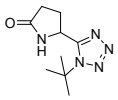
Methyl 5-(1-phenethyl-1H-tetrazol-5-yl)-5-(tritylamino)pentanoate (5h): The product was obtained using procedure 1 starting from phenethylisocyanide and **3b** as a white solid (235 mg, 43%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.6, 6H), 7.29 – 7.21 (m, 3H), 7.19 (t, *J* = 7.4, 6H), 7.16 – 7.10 (m, 3H), 7.00 (d, *J* = 6.5, 2H), 4.04 – 3.92 (m, 1H), 3.85 – 3.69 (m, 2H), 3.65 (s, 3H), 3.13 – 2.99 (m, 2H), 2.93 (d, *J* = 8.3, 1H), 2.19 – 2.01 (m, 2H), 1.62 – 1.48 (m, 1H), 1.42 – 1.30 (m, 2H), 1.25 – 1.14 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.3, 157.4, 145.2, 136.8, 129.0, 128.8, 128.6, 128.0, 127.3, 126.8, 71.7, 51.6, 48.7, 48.0, 36.4, 35.5, 33.6, 20.3 ppm. HRMS (ESI): *m/z,* calcd. for $C_{34}H_{35}O_2N_5Na$ [M + Na^+]: 568.2683, found 568.2685.



Methyl 5-(1-benzyl-1H-tetrazol-5-yl)-5-(tritylamino)pentanoate (5i): The product was obtained using procedure 1 starting from benzylisocyanide and **3b** as a white solid (364 mg, 68%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.4, 6H), 7.31 – 7.24 (m, 3H), 7.21 (t, *J* = 7.3, 6H), 7.19 – 7.13 (m, 3H), 7.01 (d, *J* = 5.5, 2H), 5.29 (d, *J* = 15.4, 1H), 4.68 (d, *J* = 15.4, 1H), 4.02 – 3.91 (m, 1H), 3.58 (s, 3H), 2.87 (d, *J* = 8.3, 1H), 1.96 (t, *J* = 6.9, 2H), 1.54 – 1.43 (m, 1H), 1.32 – 1.16 (m, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.1, 157.3, 145.3, 133.6, 129.1, 128.9, 128.6, 128.0, 127.7, 126.9, 71.6, 51.5, 50.9, 48.0, 36.1, 33.6, 20.2 ppm. HRMS (ESI): *m/z,* calcd. for $C_{33}H_{33}O_2N_5Na$ [M + Na^+]: 554.2527, found 554.2527.

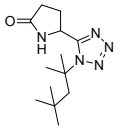


Methyl 5-(1-cyclohexyl-1H-tetrazol-5-yl)-5-(tritylamino)pentanoate (5j): The product was obtained using procedure 1 starting from cyclohexylisocyanide and **3b** as a white solid (214 mg, 41%): R_f 0.50 (EtOAc:Hept 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5, 6H), 7.21 (t, *J* = 7.5, 6H), 7.15 (t, *J* = 7.2, 3H), 4.07 – 3.95 (m, 1H), 3.89 – 3.75 (m, 1H), 3.60 (s, 3H), 2.90 (d, *J* = 7.3, 1H), 2.22 – 2.06 (m, 2H), 1.96 – 1.62 (m, 8H), 1.58 – 1.45 (m, 1H), 1.43 – 1.19 (m, 5H)ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.3, 156.3, 145.5, 128.8, 128.0, 126.9, 72.0, 57.6, 51.6, 48.1 36.4, 33.6, 33.6, 32.3, 25.4, 24.9, 20.3 ppm. HRMS (ESI): *m/z,* calcd. for $C_{32}H_{37}O_2N_5Na$ [M + Na^+]: 546.2840, found 546.2841.

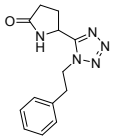


5-(1-(tert-butyl)-1H-tetrazol-5-yl)pyrrolidin-2-one (6a): The product was obtained using procedure 2 starting

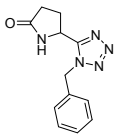
from **5a** as a white solid (74 mg, 55%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (s, 1H), 5.40 – 5.13 (m, 1H), 2.75 – 2.57 (m, 2H), 2.43 – 2.31 (m, 2H), 1.80 – 1.75 (m, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.7, 155.8, 61.6, 49.1, 30.3, 29.3, 28.1 ppm. HRMS (ESI): *m/z,* calcd. for $C_9H_{16}O_1N_5$ [M + H$^+$]: 210.1349, found 210.1350.



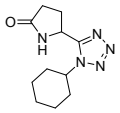
5-(1-(2,4,4-trimethylpentan-2-yl)-1H-tetrazol-5-yl)pyrrolidin-2-one (6b): The product was obtained using procedure 2 starting from **5b** as a white solid (154 mg, 89%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (s, 1H), 5.35 – 5.20 (m, 1H), 2.78 – 2.56 (m, 2H), 2.46 – 2.31 (m, 2H), 1.97 (q, *J* = 15.3, 2H), 1.86 (d, *J* = 3.4, 6H), 0.79 (s, 9H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.7, 156.3, 65.0, 54.3, 49.3, 31.8, 30.8, 30.5, 29.4, 28.2 ppm. HRMS (ESI): *m/z,* calcd. for $C_{13}H_{24}O_1N_5$ [M + H$^+$]: 266.1975, found 266.1977.



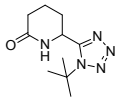
5-(1-phenethyl-1H-tetrazol-5-yl)pyrrolidin-2-one (6c): The product was obtained using procedure 2 starting from **5c** as a white solid (60 mg, 32%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 4.2, 3H), 7.06 – 6.91 (m, 2H), 6.82 (s, 1H), 4.71 – 4.46 (m, 2H), 4.44 – 4.25 (m, 1H), 3.37 – 3.11 (m, 2H), 2.54 – 2.37 (m, 1H), 2.33 – 2.08 (m, 2H), 2.08 – 1.87 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.3, 155.8, 136.6, 129.3, 129.0, 127.8, 49.3, 47.2, 36.4, 29.3, 26.5 ppm. MS (ESI) (m/z) 258.1 [M+H]$^+$. HRMS (ESI): *m/z,* calcd. for $C_{13}H_{16}O_1N_5$ [M + H$^+$]: 258.1349, found 258.1348.



5-(1-benzyl-1H-tetrazol-5-yl)pyrrolidin-2-one (6d): The product was obtained using procedure 2 starting from **5d** as a white solid (98 mg, 72%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.37 (d, *J* = 6.3, 3H), 7.28 – 7.17 (m, 2H), 5.67 (dd, *J* = 47.8, 15.6, 2H), 5.02 – 4.88 (m, 1H), 2.44 – 2.33 (m, 1H), 2.33 – 2.18 (m, 2H), 2.05 – 1.90 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.7, 155.5, 133.3, 129.4, 129.2, 127.7, 51.3, 47.9, 29.2, 26.3 ppm. HRMS (ESI): *m/z,* calcd. for $C_{12}H_{14}O_1N_5$ [M + H$^+$]: 244.1193, found 244.1192.

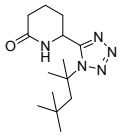


5-(1-cyclohexyl-1H-tetrazol-5-yl)pyrrolidin-2-one (6e): The product was obtained using procedure 2 starting from **5e** as a white solid (110 mg, 95%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 26.2, 1H), 5.18 – 4.93 (m, 1H), 4.37 – 4.14 (m, 1H), 2.74 – 2.55 (m, 2H), 2.53 – 2.33 (m, 2H), 2.13 – 1.91 (m, 6H), 1.78 (d, *J* = 12.7, 1H), 1.53 – 1.40 (m, 3H), 1.39 – 1.26 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.7, 154.5, 58.2, 47.7, 33.5, 32.7, 29.5, 26.8, 25.2, 25.1, 24.8 ppm. HRMS (ESI): *m/z,* calcd. for $C_{11}H_{18}O_1N_5$ [M + H$^+$]: 236.1506, found 236.1506.

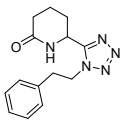


6-(1-(tert-butyl)-1H-tetrazol-5-yl)piperidin-2-one (6f): The product was obtained using procedure 2 starting

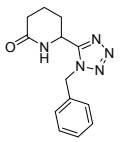
from **5f** as a white solid (120 mg, 76%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (s, 1H), 5.22 – 5.09 (m, 1H), 2.46 – 2.37 (m, 1H), 2.36 – 2.27 (m, 1H), 2.20 – 2.08 (m, 2H), 2.07 – 1.98 (m, 1H), 1.77 (s, 10H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.1, 155.4, 61.6, 47.9, 30.9, 30.2, 28.0, 18.6 ppm. $[M+H]^+$. HRMS (ESI): *m/z,* calcd. for $C_{10}H_{18}O_1N_5$ $[M + H^+]$: 224.1506, found 224.1507.



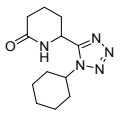
6-(1-(2,4,4-trimethylpentan-2-yl)-1H-tetrazol-5-yl)piperidin-2-one (6g): The product was obtained using procedure 2 starting from **5g** as a white solid (50 mg, 42%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.58 (d, J = 25.2, 1H), 5.15 (t, J = 6.1, 1H), 2.59 – 2.39 (m, 2H), 2.28 – 2.10 (m, 3H), 1.94 (q, J = 15.3, 2H), 1.86 (d, J = 12.9, 7H), 1.83 – 1.71 (m, 1H), 0.79 (s, 9H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.8, 155.6, 65.2, 54.5, 48.6, 31.9, 31.1, 30.8, 30.7, 30.7, 28.4, 19.0 ppm. HRMS (ESI): *m/z,* calcd. for $C_{14}H_{26}O_1N_5$ $[M + H^+]$: 280.2132, found 280.2131.



6-(1-phenethyl-1H-tetrazol-5-yl)piperidin-2-one (6h): The product was obtained using procedure 2 starting from **5h** as a white solid (43 mg, 40%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, J = 6.7, 3H), 7.06 – 6.91 (m, 3H), 4.65 – 4.46 (m, 2H), 4.28 (t, J = 5.8, 1H), 3.31 – 3.16 (m, 2H), 2.28 – 2.19 (m, 2H), 1.94 – 1.81 (m, 1H), 1.67 – 1.44 (m, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.1, 155.4, 136.6, 129.2, 128.9, 127.7, 49.4, 46.7, 36.3, 31.0, 26.9, 18.8 ppm. HRMS (ESI): *m/z,* calcd. for $C_{14}H_{18}O_1N_5$ $[M + H^+]$: 272.1506, found 272.1506.



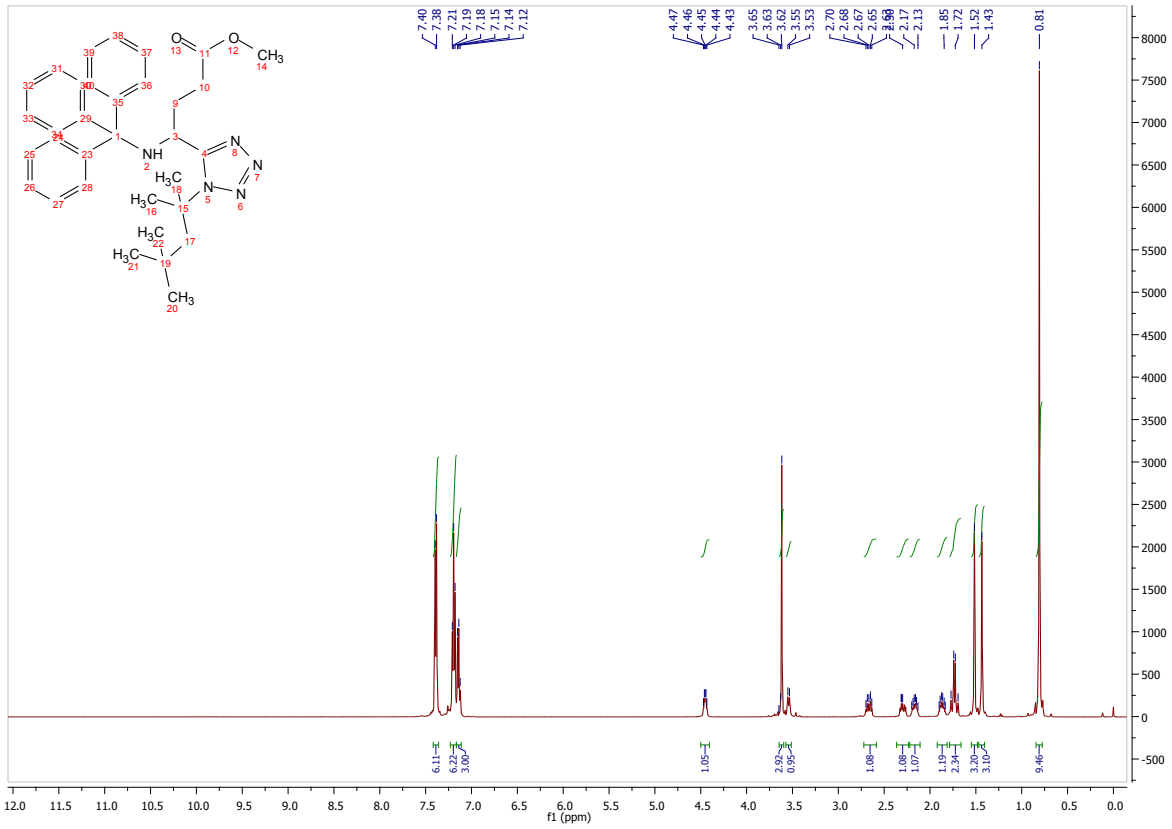
6-(1-benzyl-1H-tetrazol-5-yl)piperidin-2-one (6i): The product was obtained using procedure 2 starting from **5i** as a white solid (78 mg, 99%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.33 (m, 3H), 7.24 (s, 1H), 7.23 – 7.17 (m, 2H), 5.66 (s, 2H), 4.91 – 4.81 (m, 1H), 2.37 – 2.21 (m, 2H), 1.98 – 1.82 (m, 2H), 1.77 – 1.59 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.5, 155.1, 133.6, 129.5, 129.2, 127.7, 51.6, 47.4, 31.1, 25.0, 18.8 ppm. HRMS (ESI): *m/z,* calcd. for $C_{13}H_{16}O_1N_5$ $[M + H^+]$: 258.1349, found 258.1349.



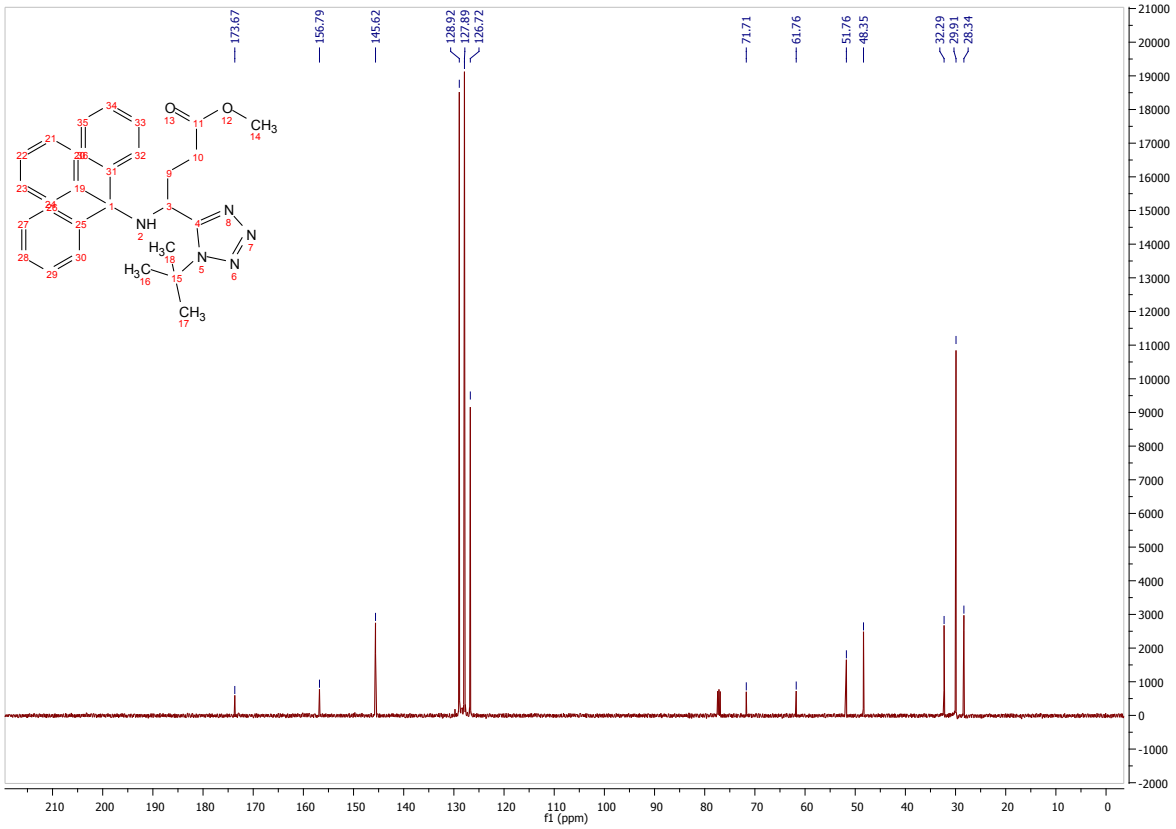
6-(1-cyclohexyl-1H-tetrazol-5-yl)piperidin-2-one (6j): The product was obtained using procedure 2 starting from **5j** as a white solid (75 mg, 79%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (s, 1H), 4.95 (t, J = 5.6, 1H), 4.38 – 4.19 (m, 1H), 2.48 – 2.32 (m, 2H), 2.23 – 1.91 (m, 10H), 1.91 – 1.82 (m, 1H), 1.82 – 1.70 (m, 1H), 1.51 – 1.39 (m, 2H), 1.39 – 1.31 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.4, 154.1, 58.3, 46.9, 33.6, 32.9, 31.1, 27.5, 25.3, 25.3, 24.8, 18.9 ppm. HRMS (ESI): *m/z,* calcd. for $C_{12}H_{20}O_1N_5$ $[M + H^+]$: 250.1662, found 250.1662.

^{1}H NMR and ^{13}C NMR spectra of compounds 5a-j and 6a-j

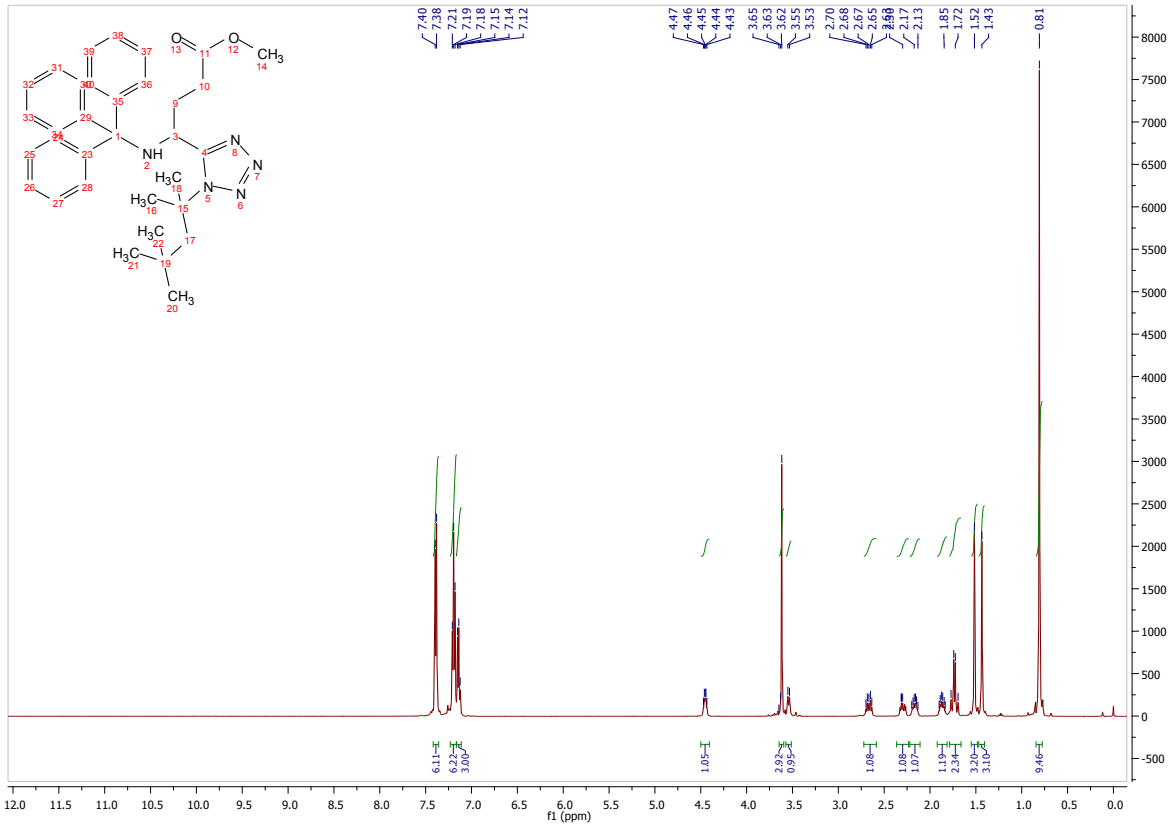
Compound **5a** ^{1}H NMR



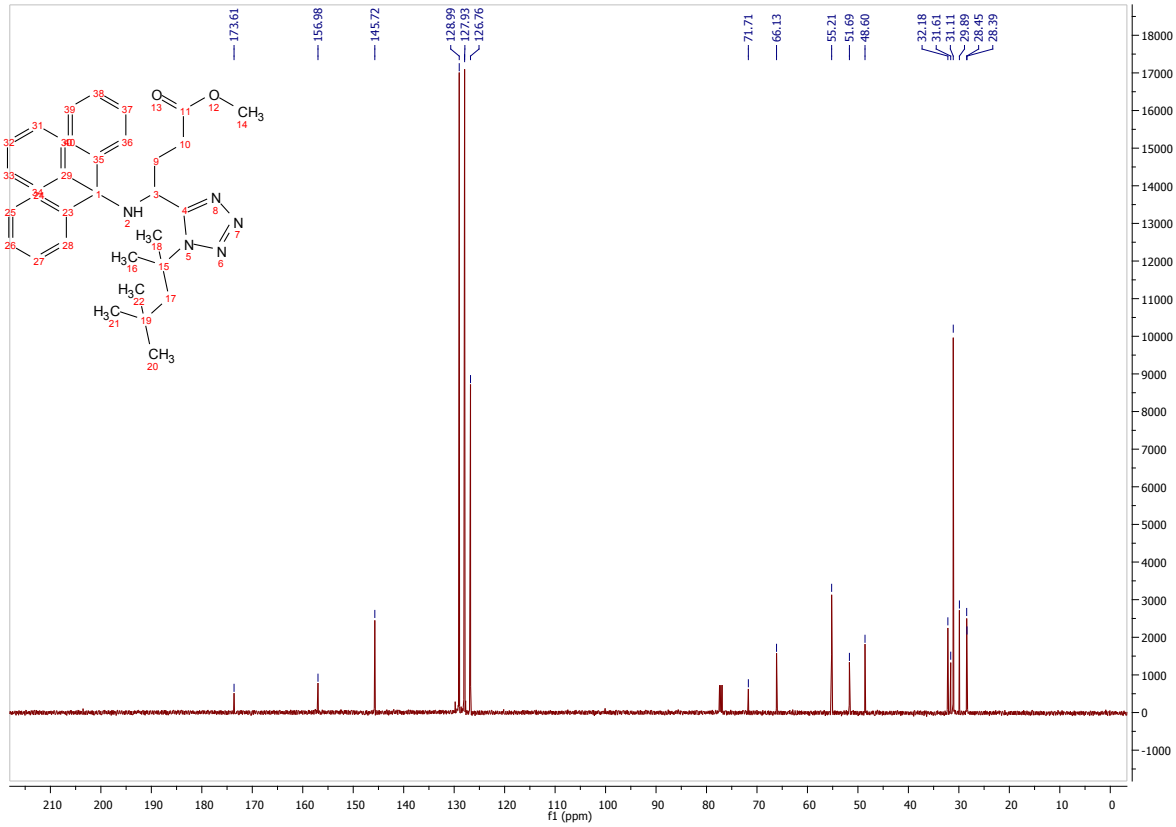
Compound **5a** ^{13}C NMR



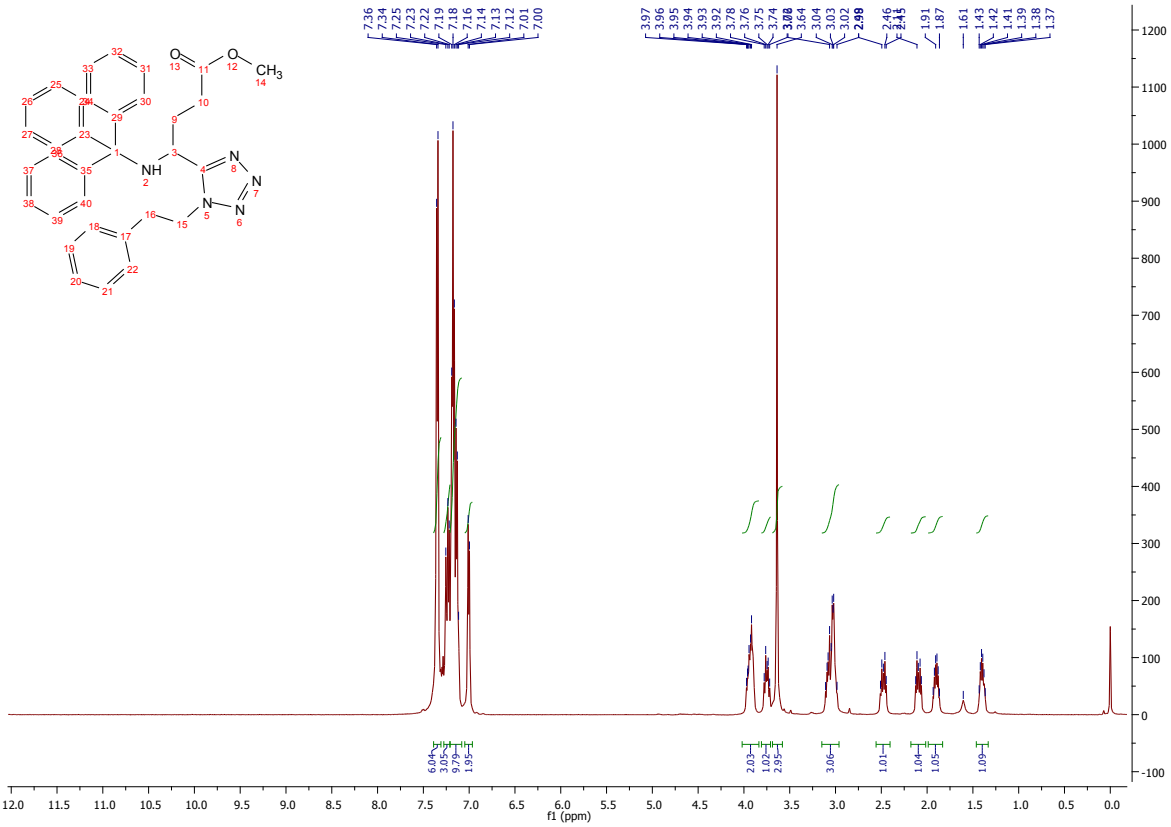
Compound **5b** ^{1}H NMR



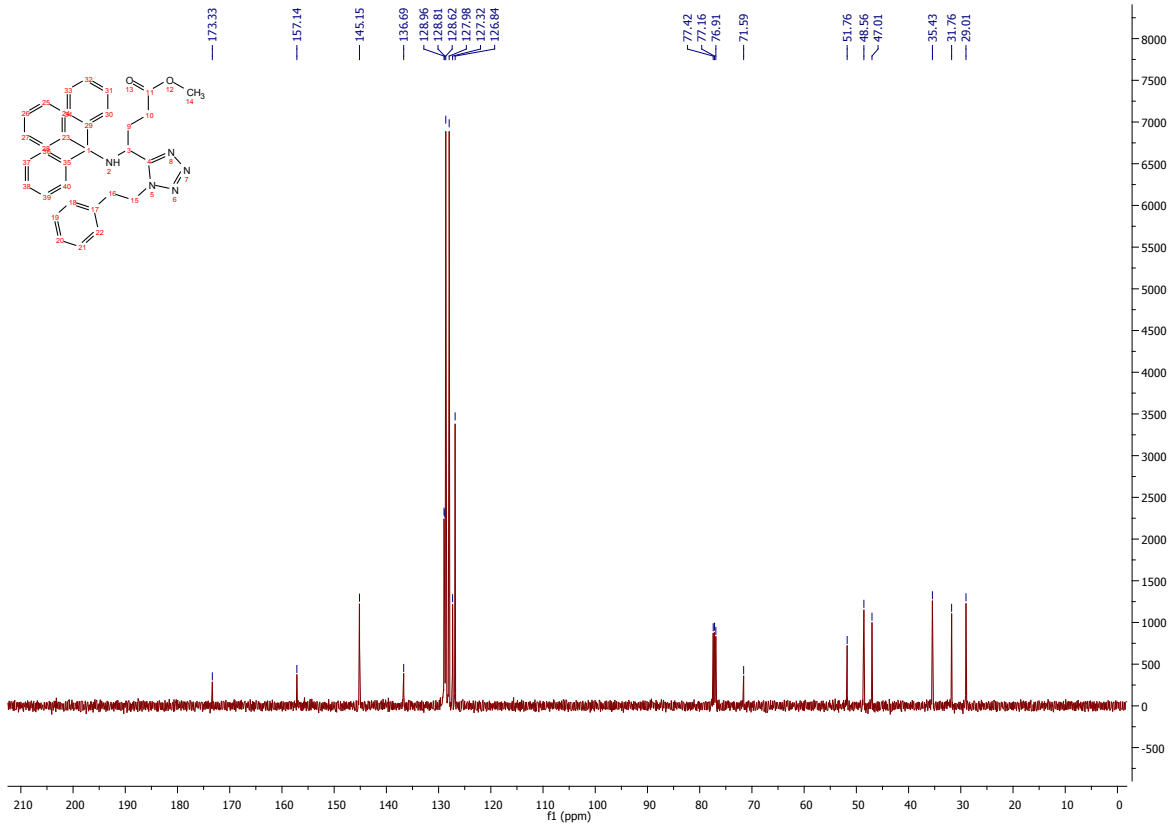
Compound **5b** ^{13}C NMR



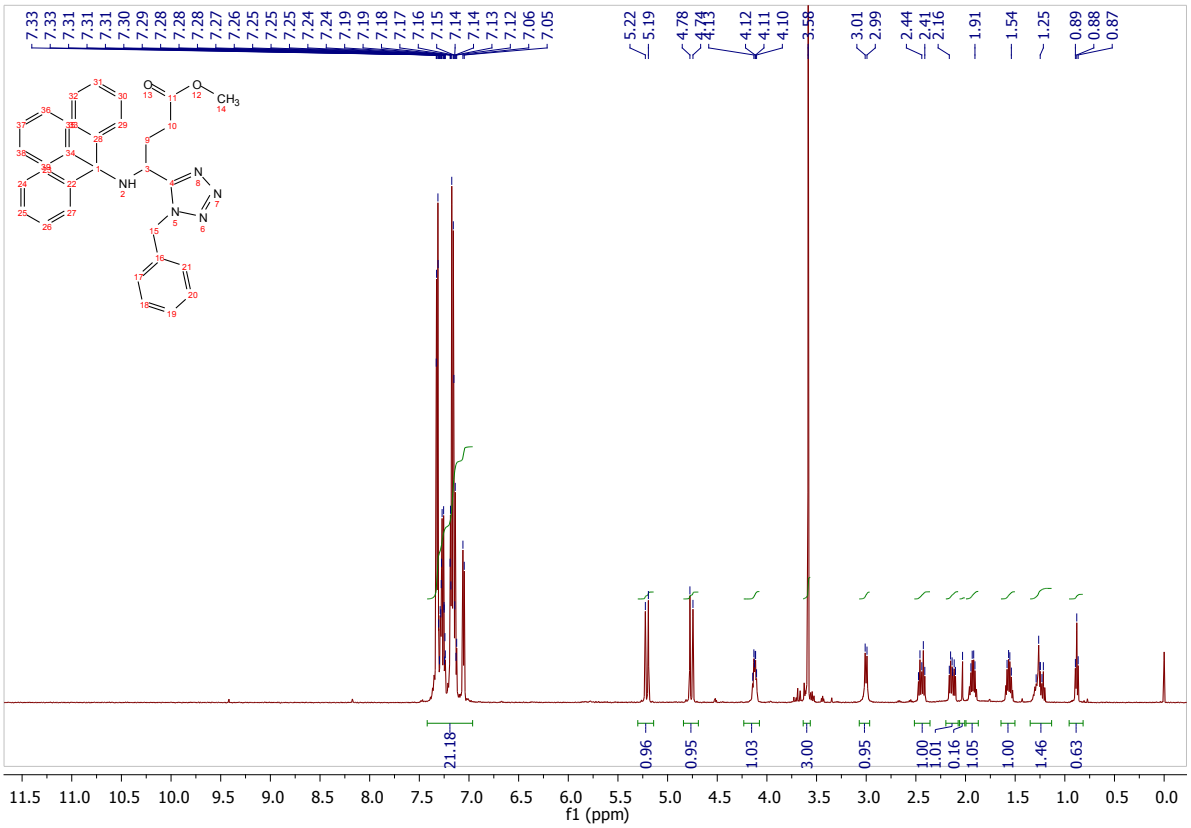
Compound **5c** 1H NMR



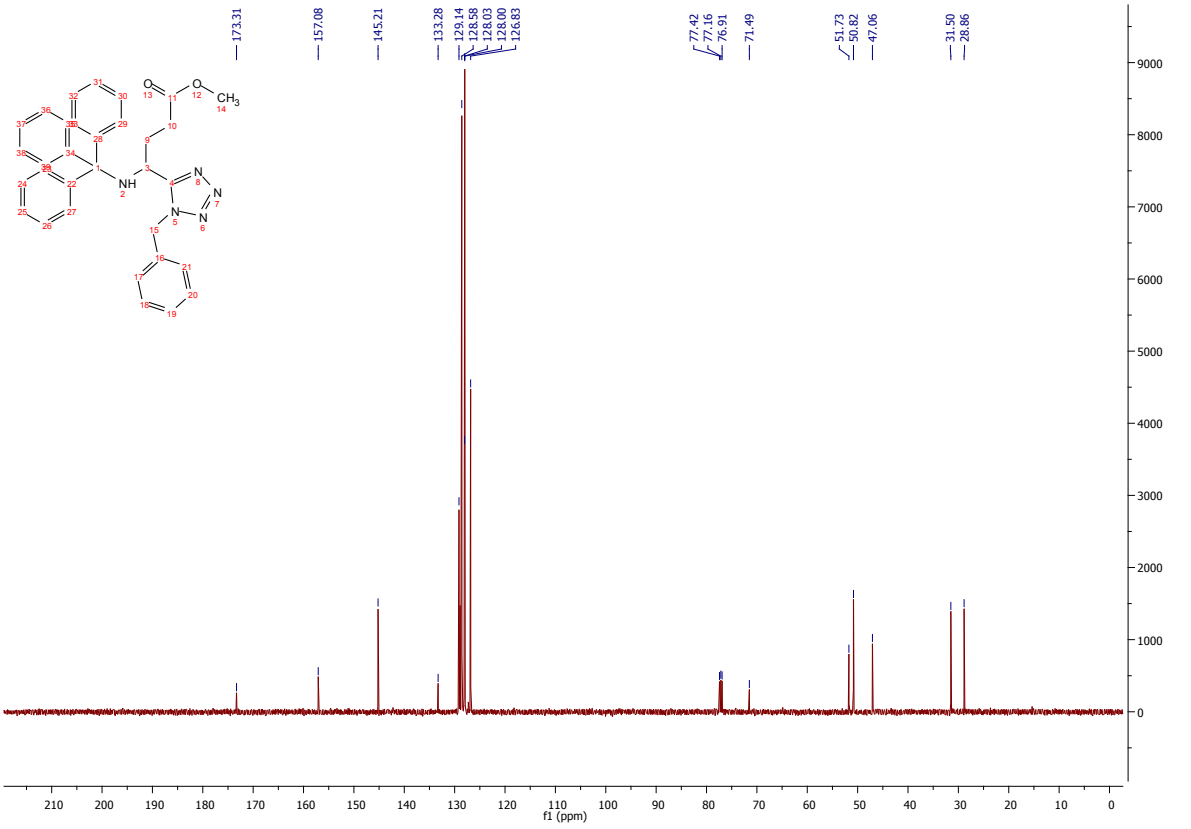
Compound **5c** ^{13}C NMR



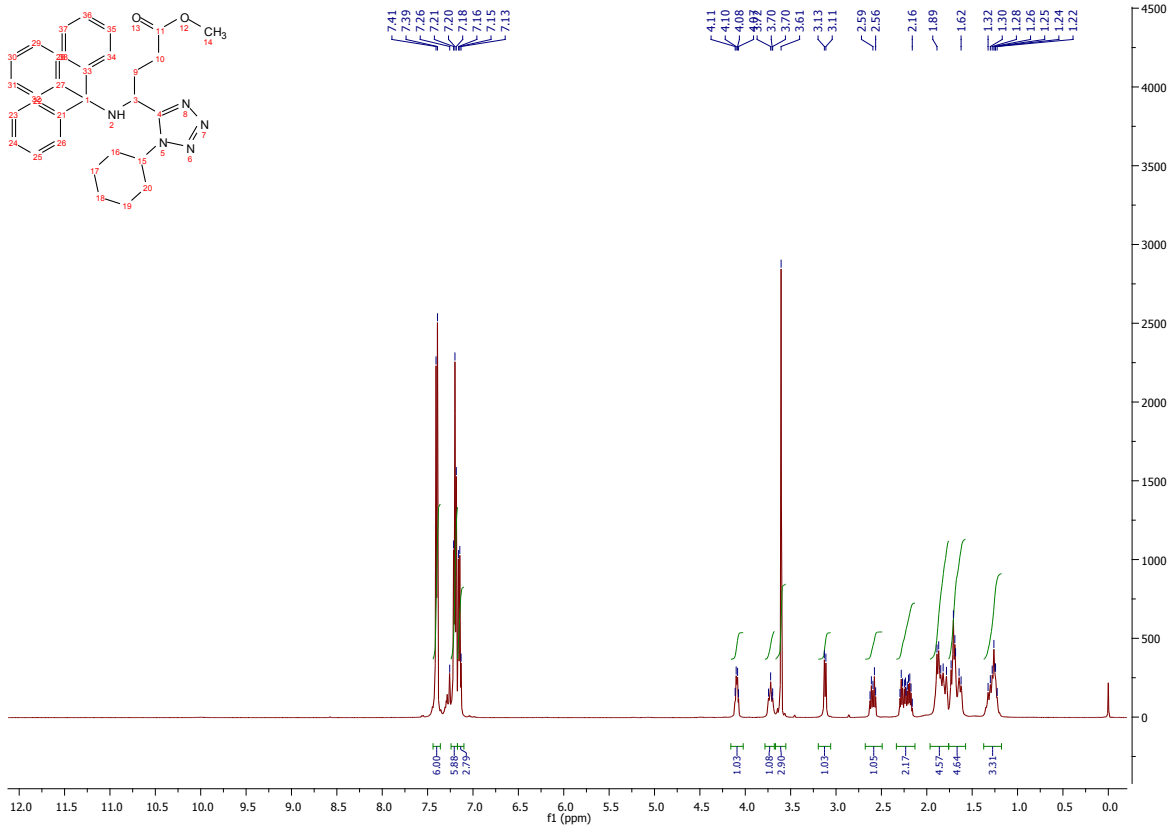
Compound **5d** ^{1}H NMR



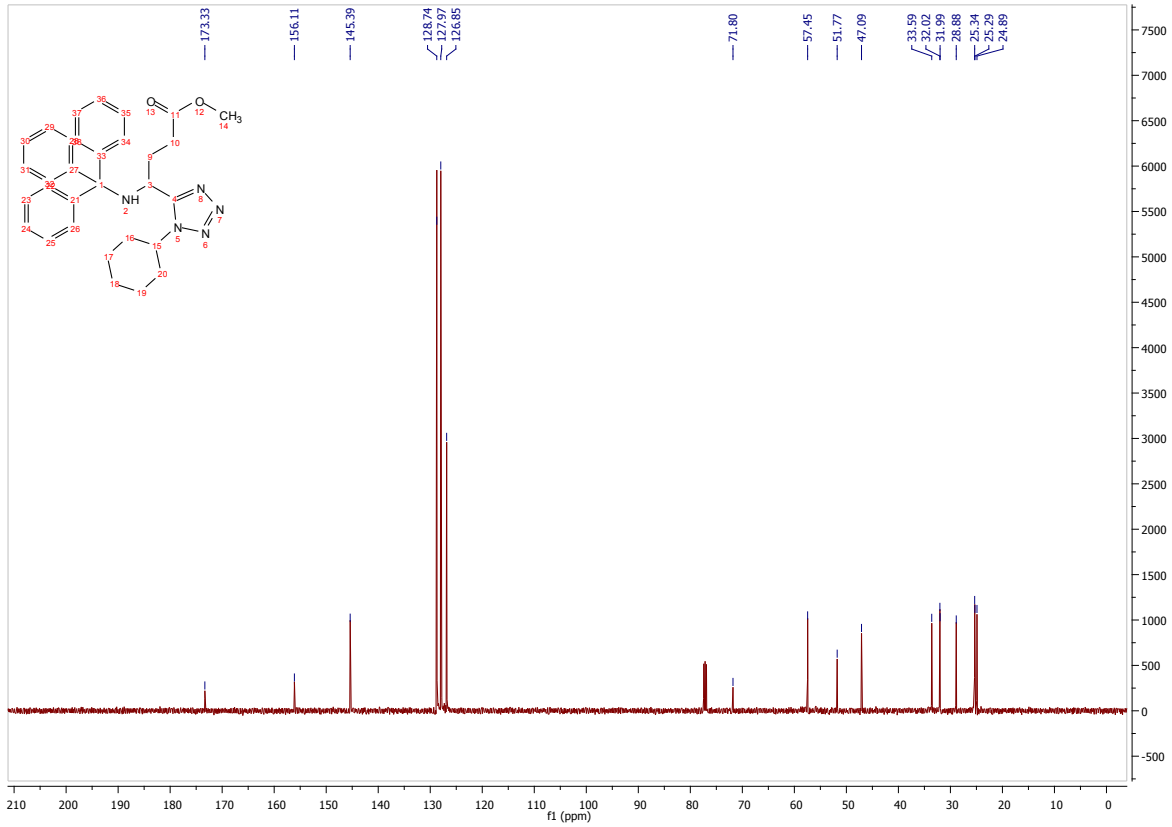
Compound **5d** ^{13}C NMR



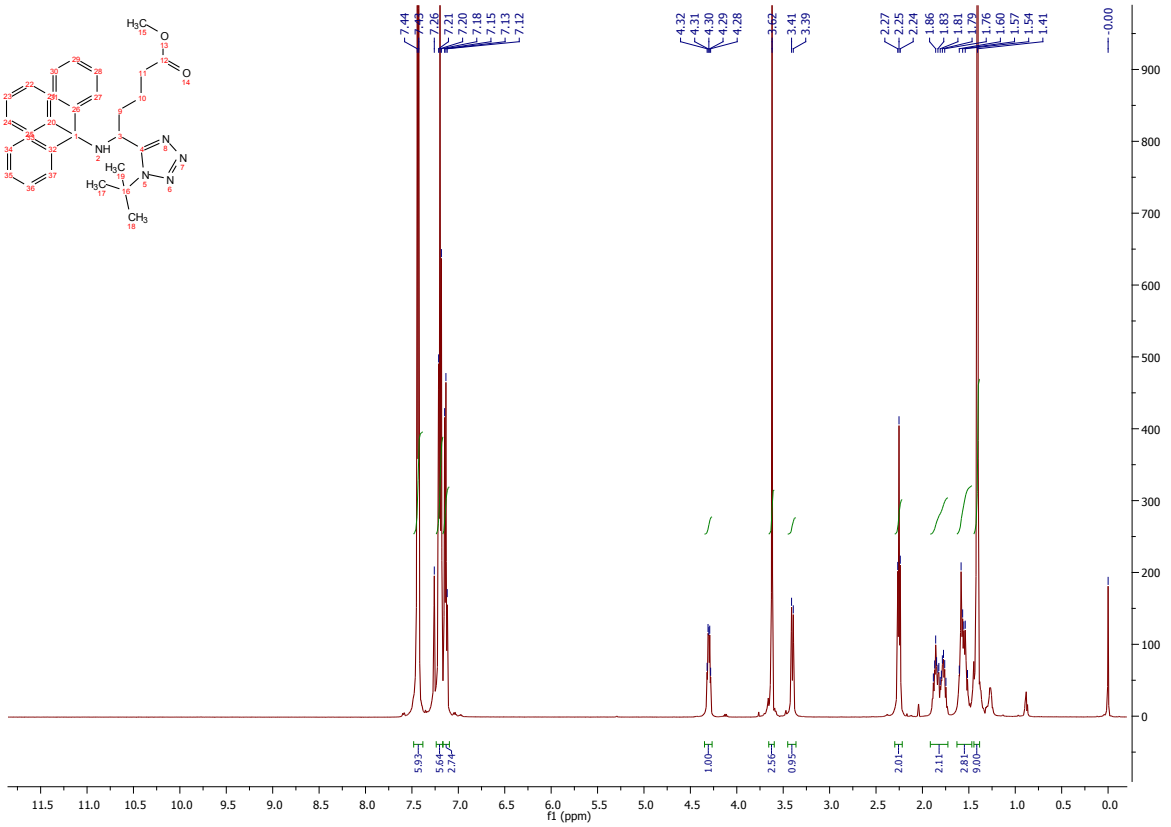
Compound **5e** ^{1}H NMR



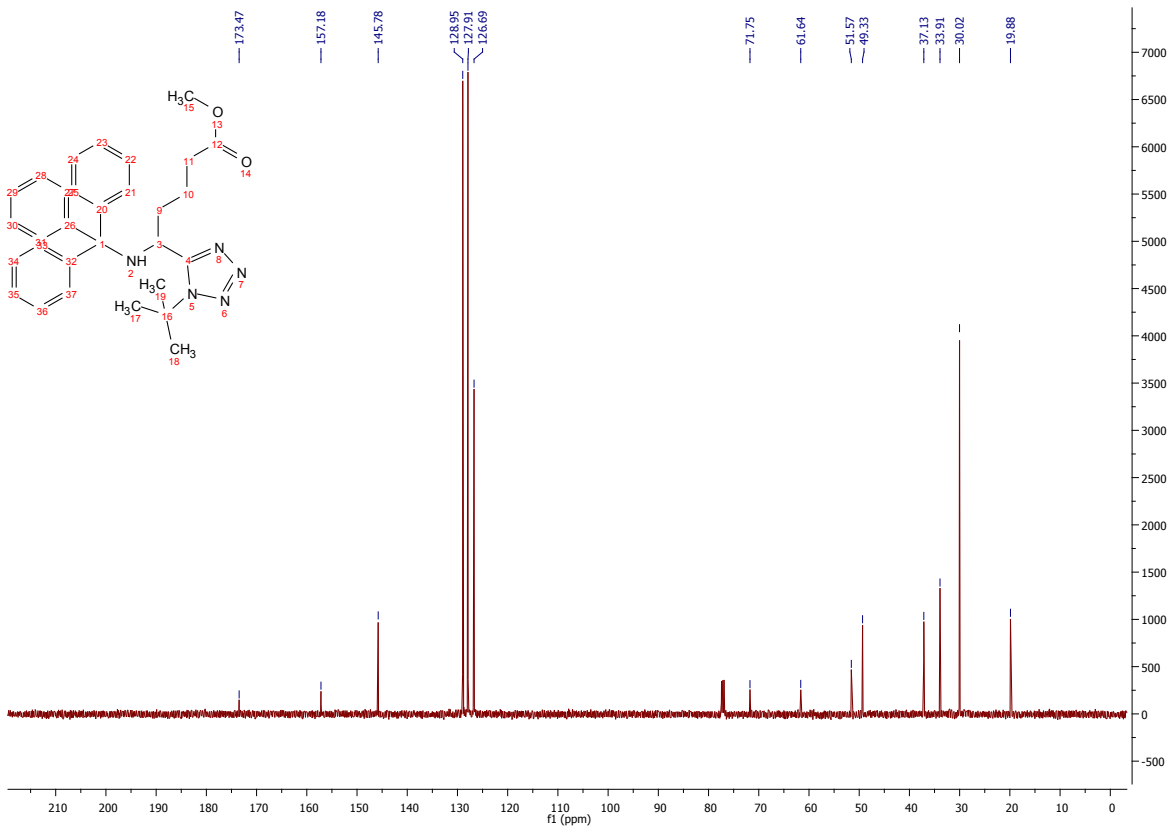
Compound **5e** ^{13}C NMR



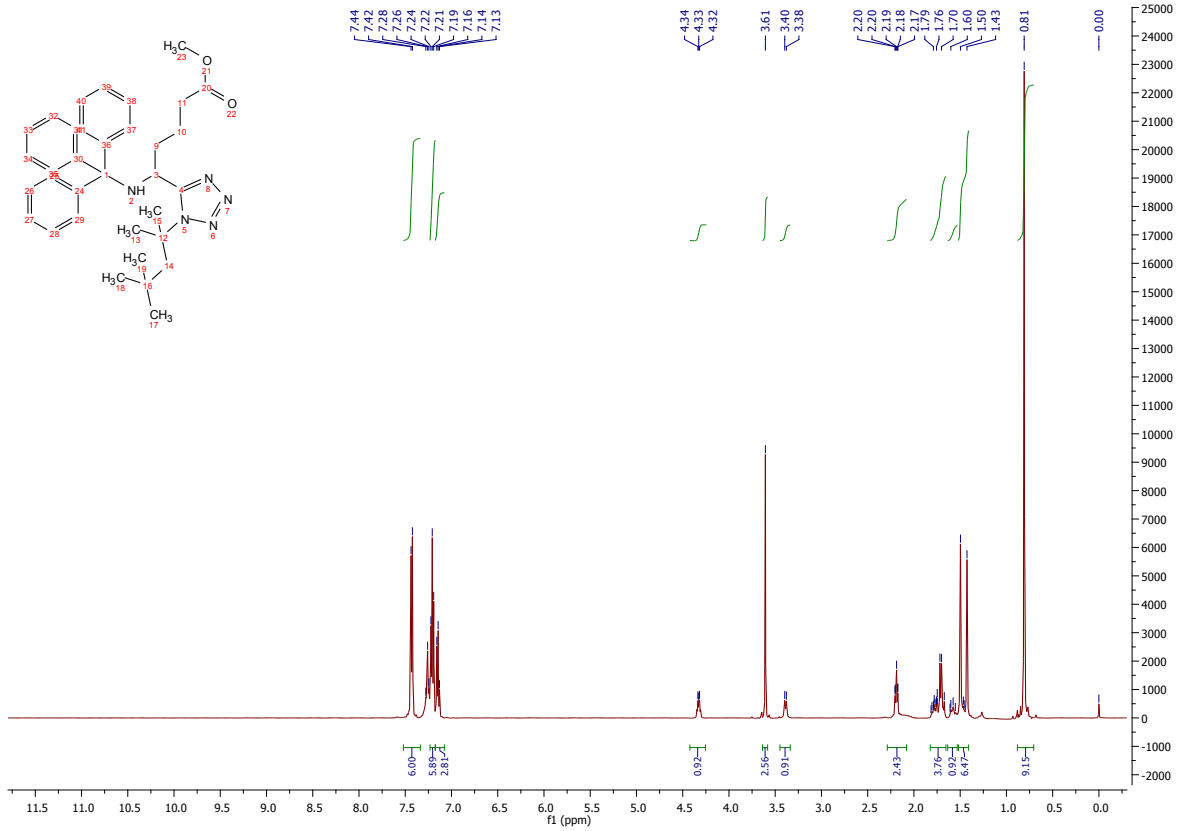
Compound **5f** ^{1}H NMR



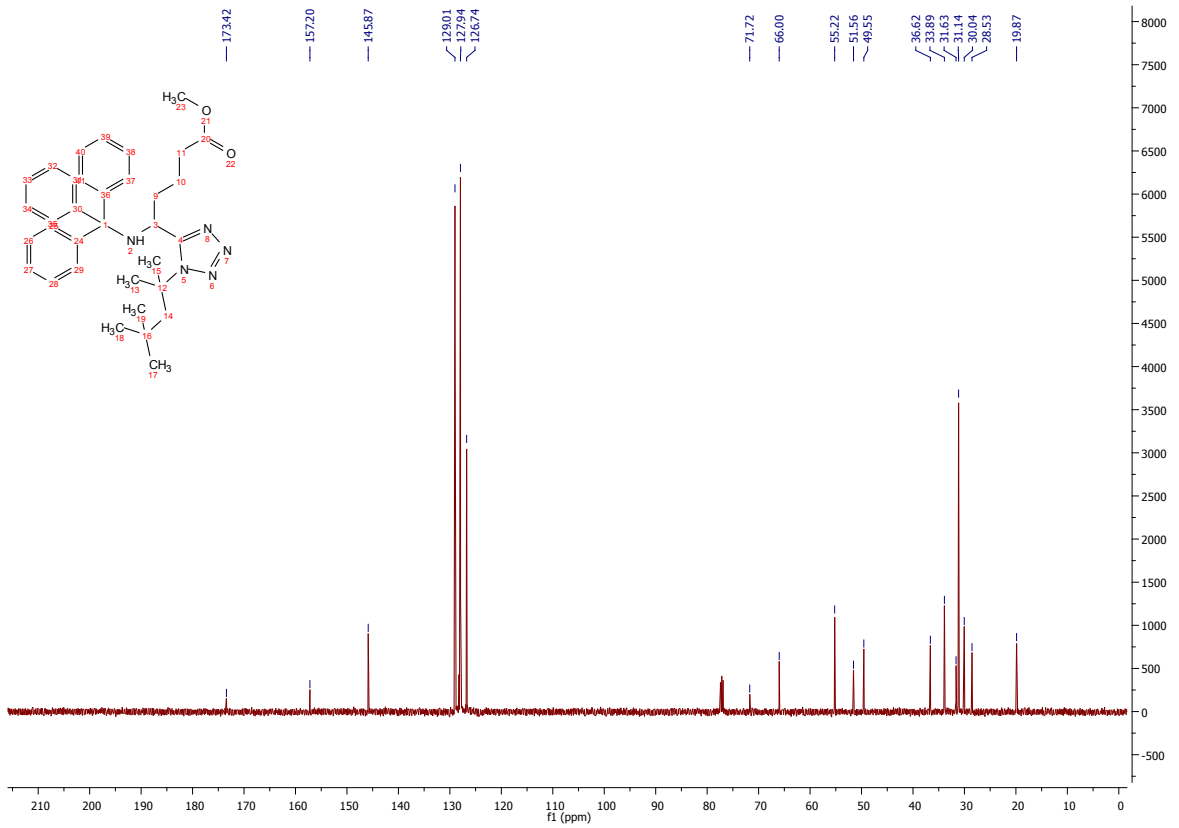
Compound **5f** ^{13}C NMR



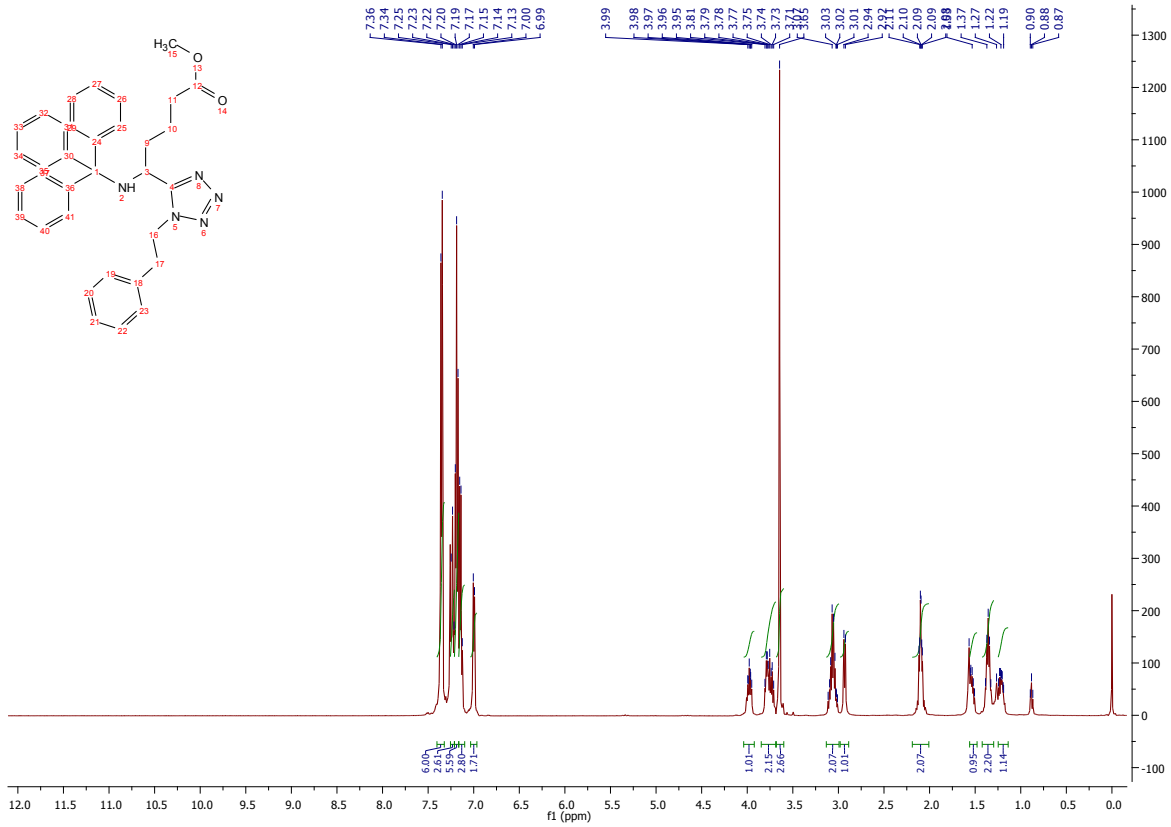
Compound **5g** ^{1}H NMR



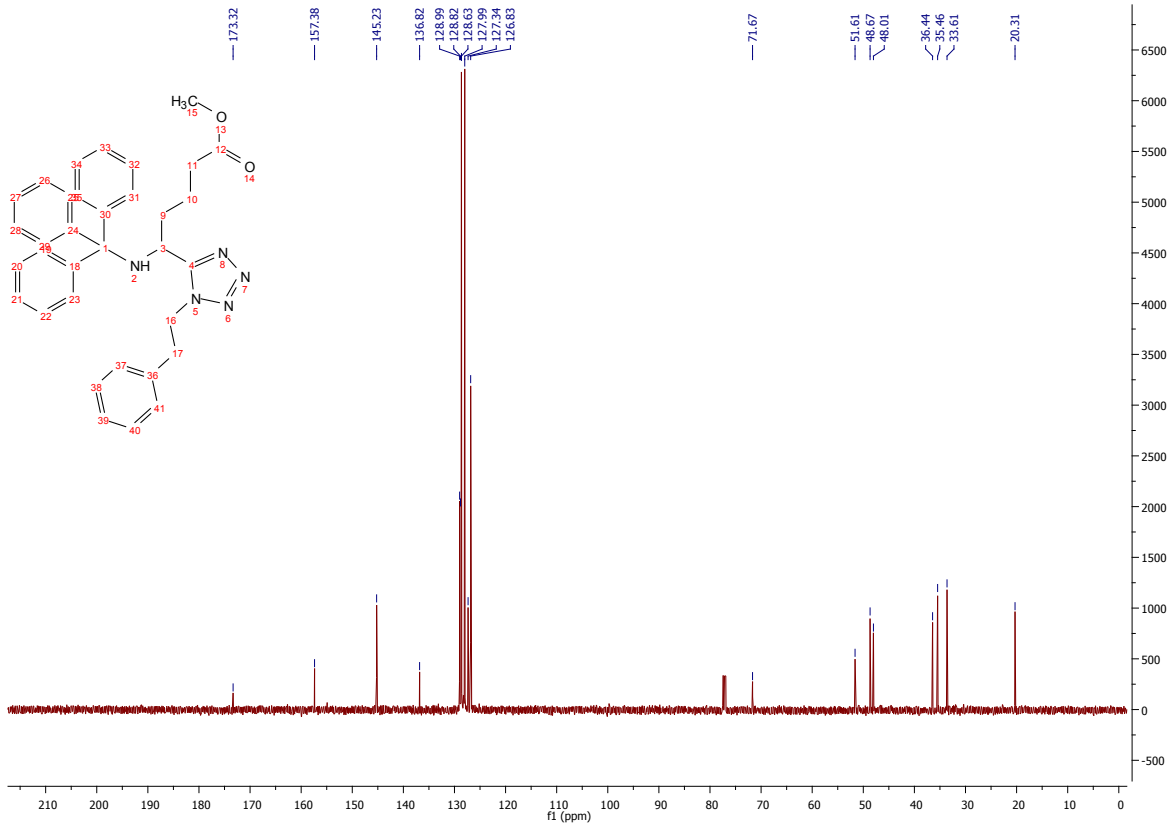
Compound **5g** ^{13}C NMR



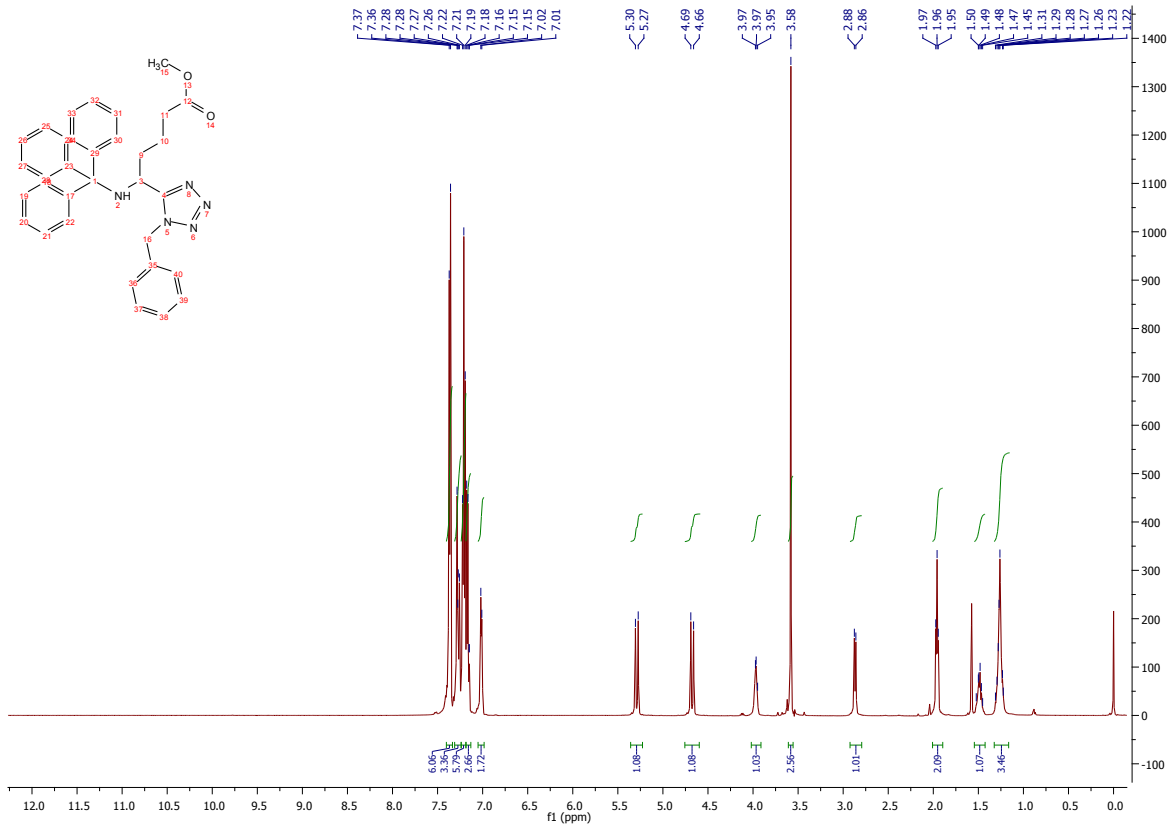
Compound **5h** ^{1}H NMR



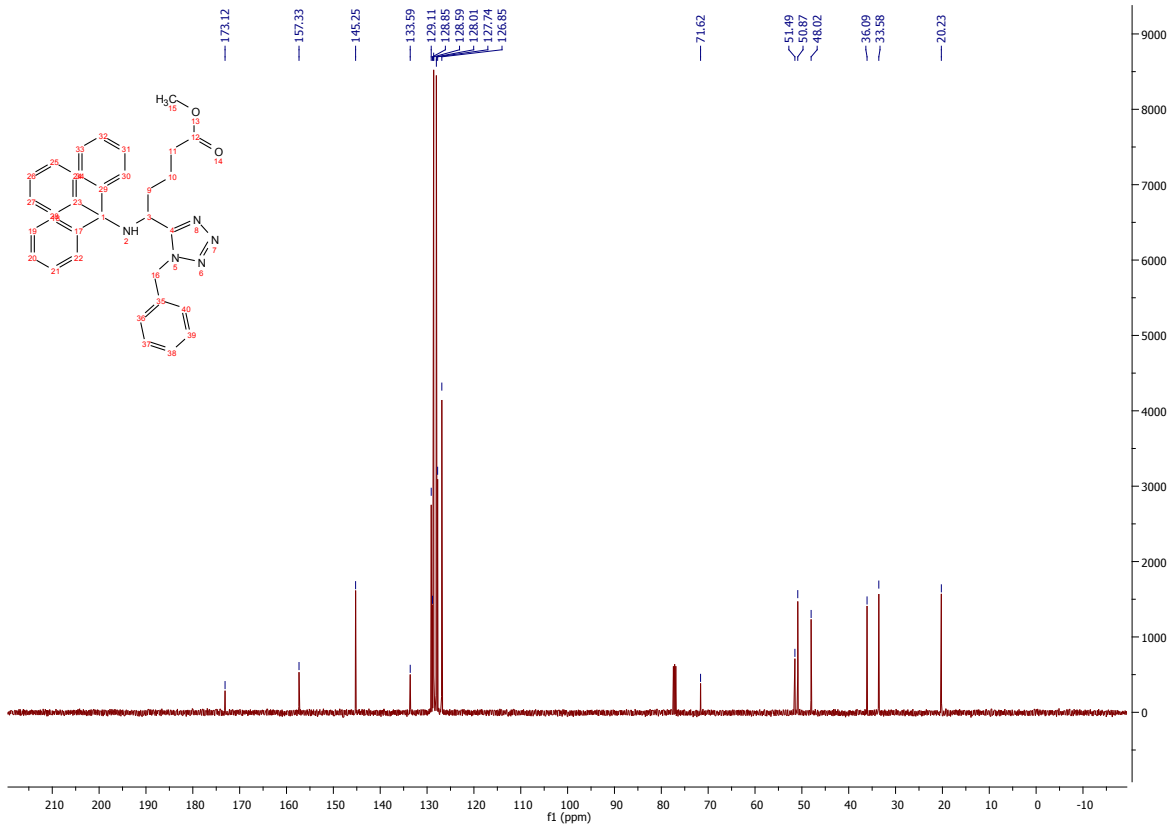
Compound **5h** ^{13}C NMR



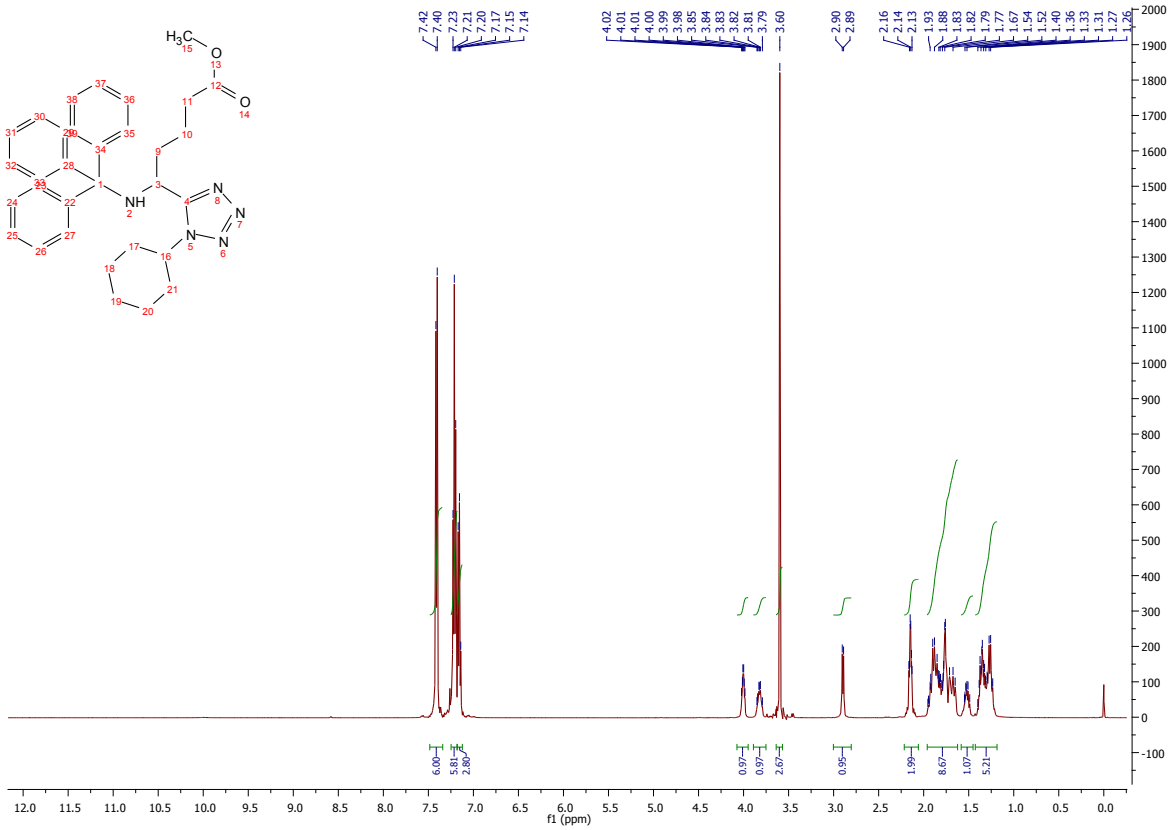
Compound **5i** ^{1}H NMR



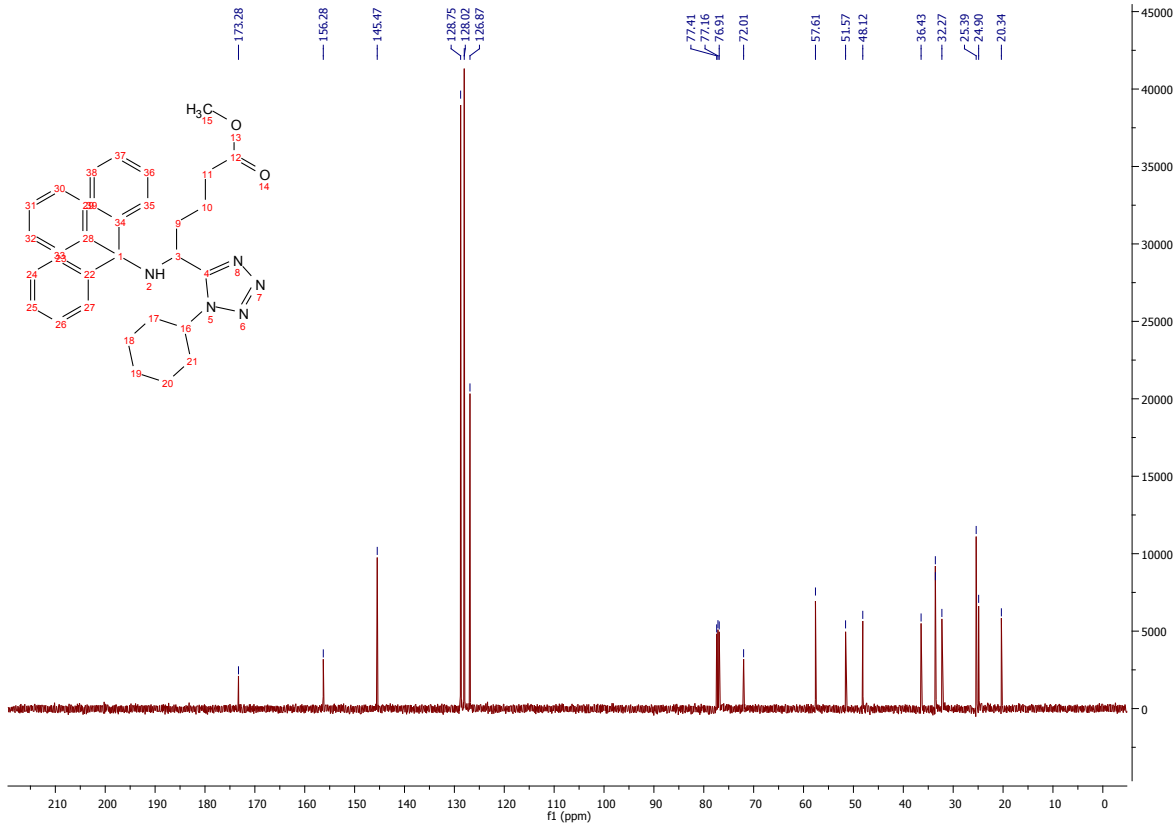
Compound **5i** ^{13}C NMR



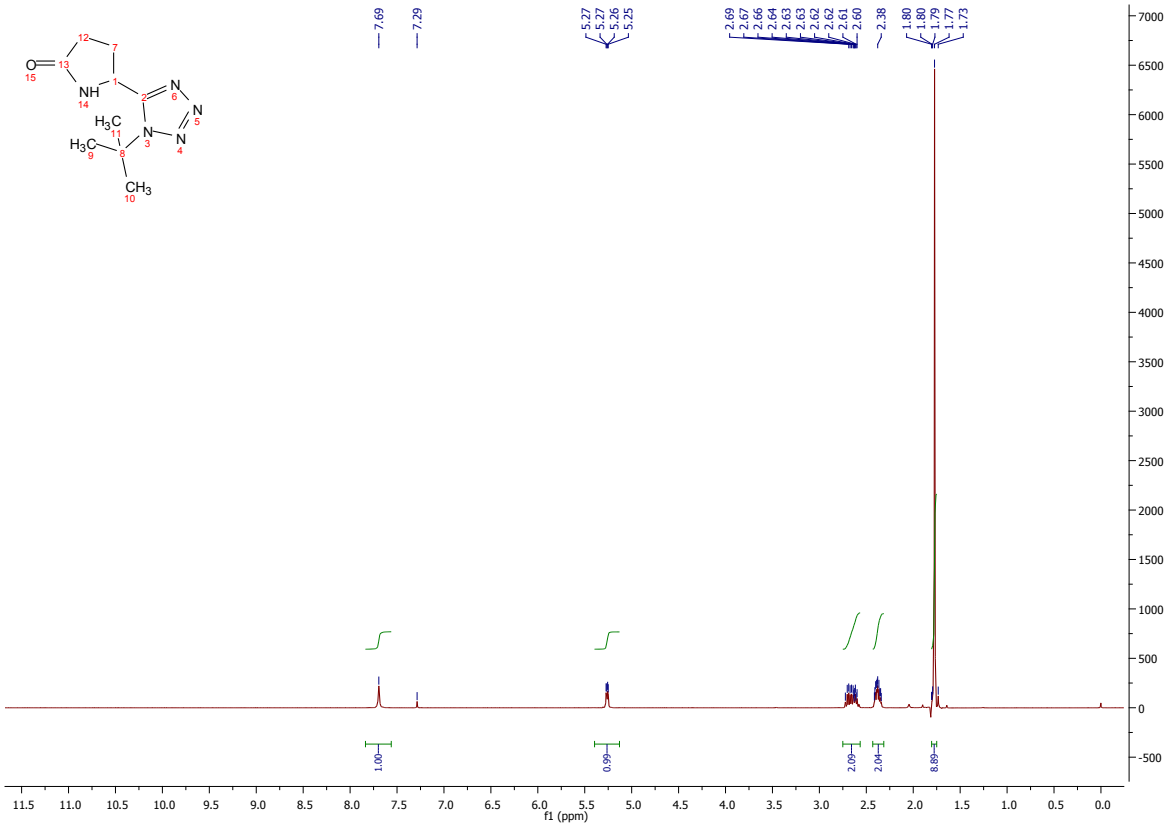
Compound **5j** ^{1}H NMR



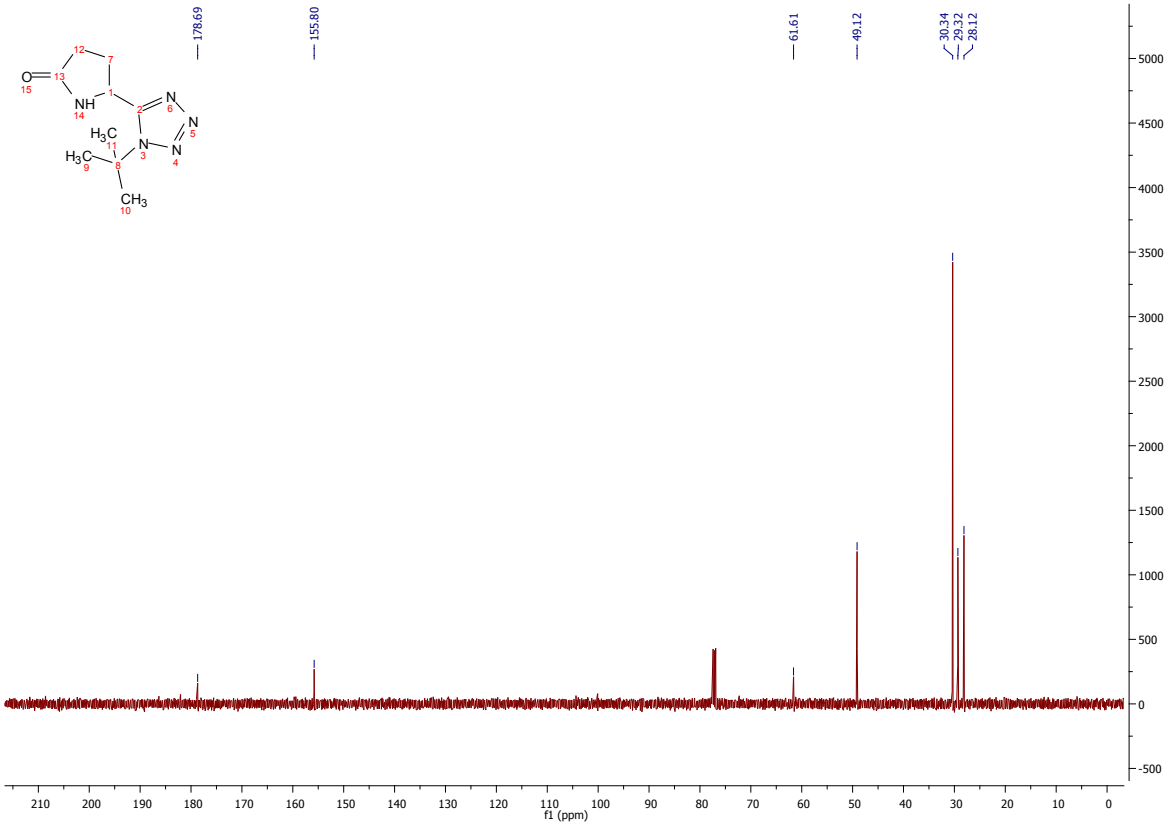
Compound **5j** ^{13}C NMR



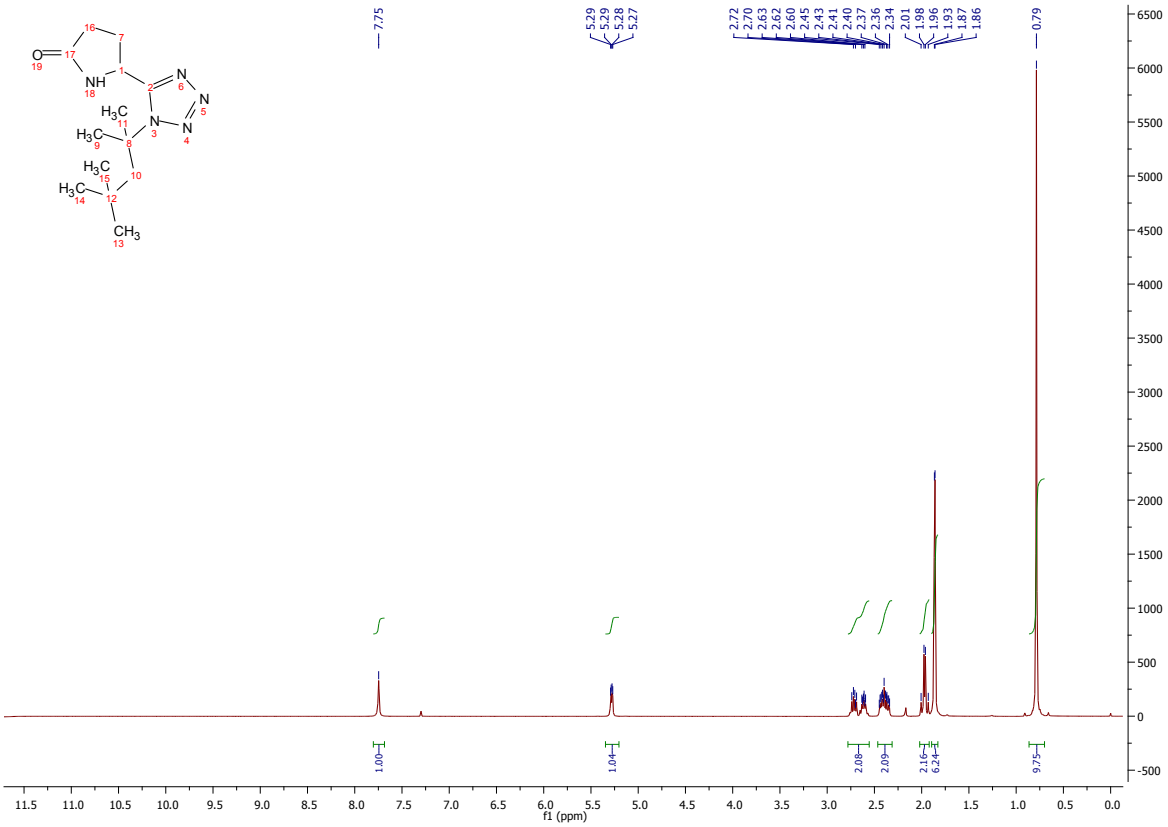
Compound **6a** ^{1}H NMR



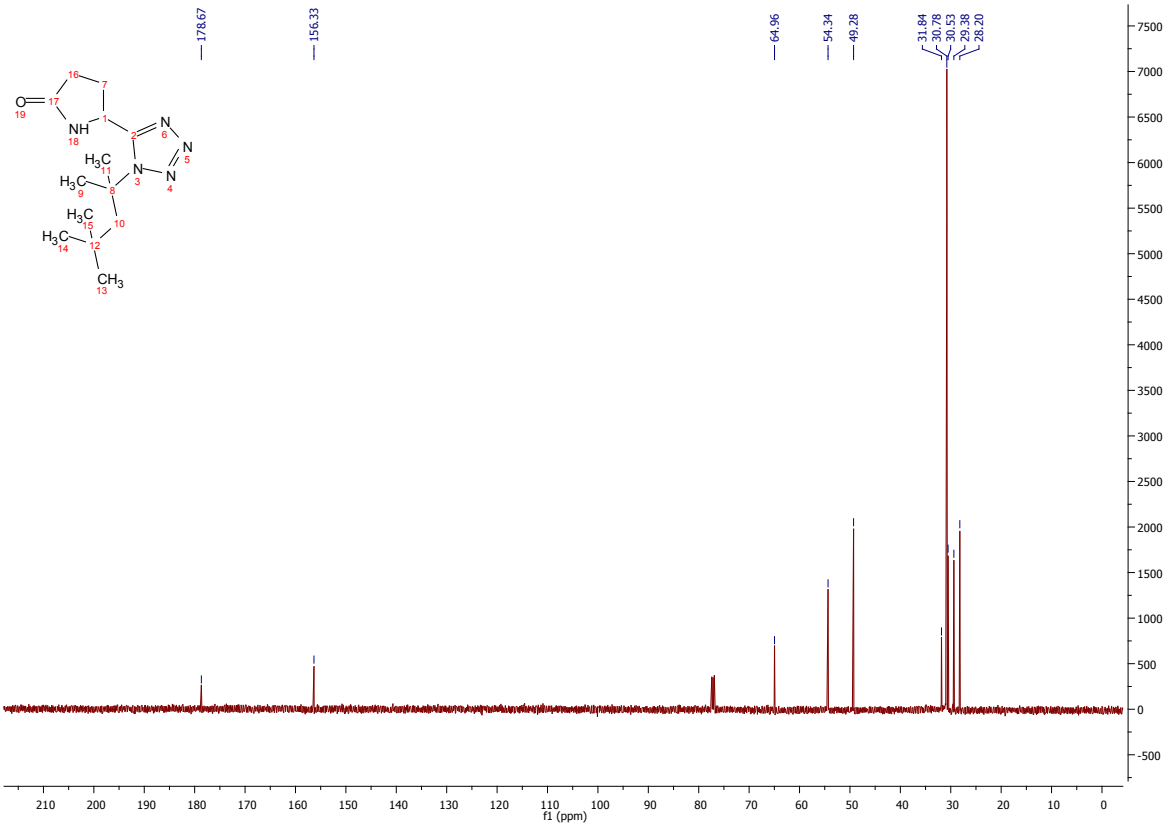
Compound **6a** 13C NMR



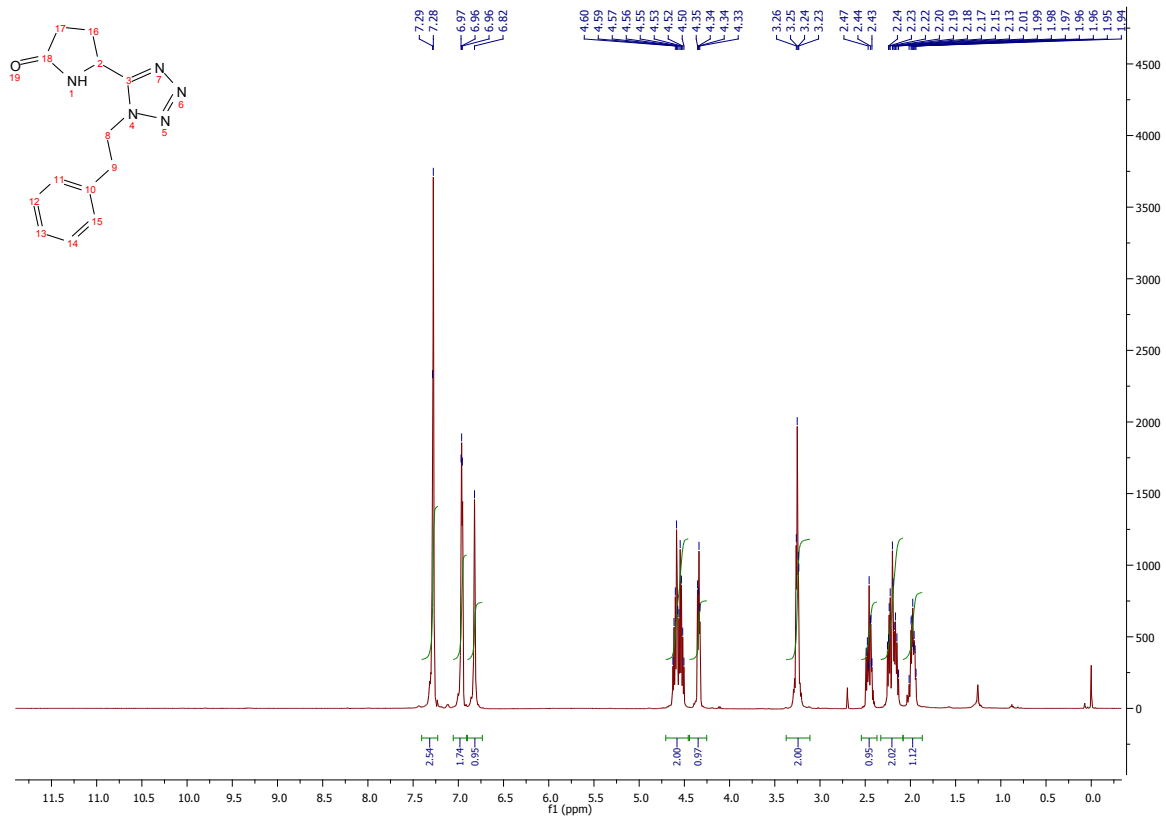
Compound **6b** ^{1}H NMR



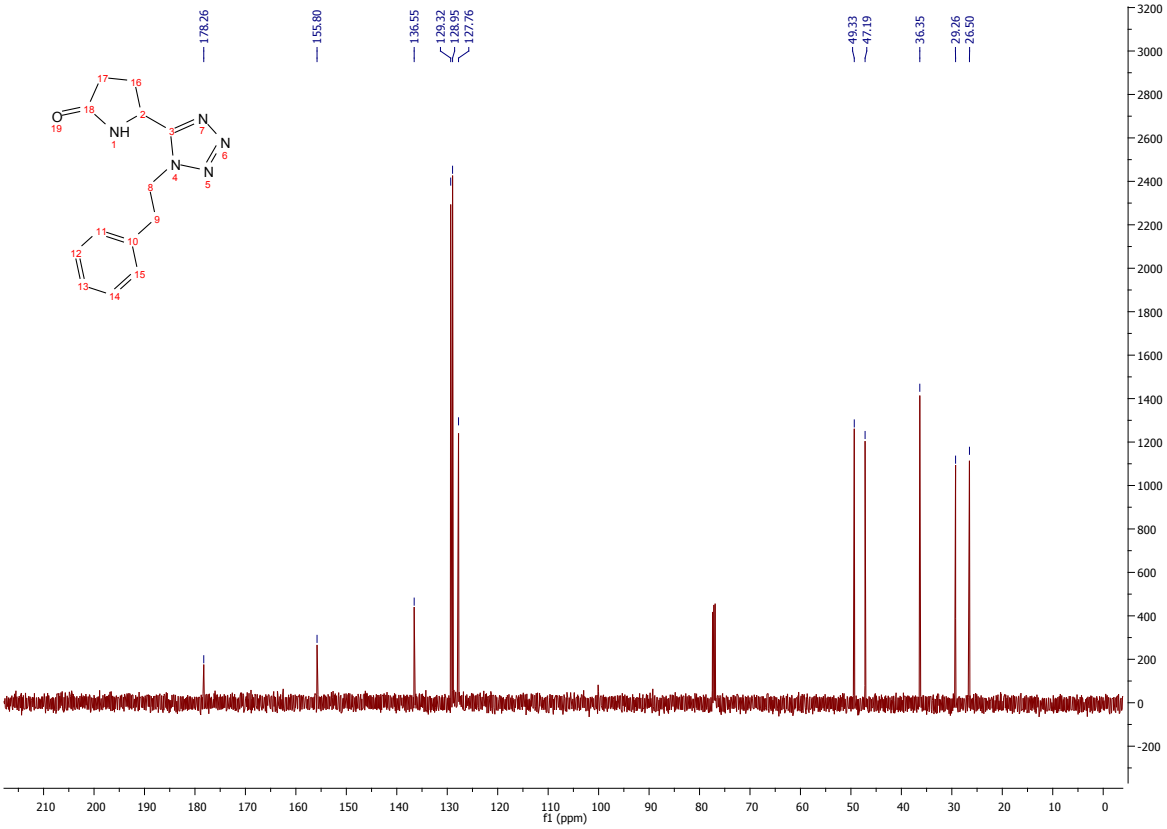
Compound **6b** ^{13}C NMR



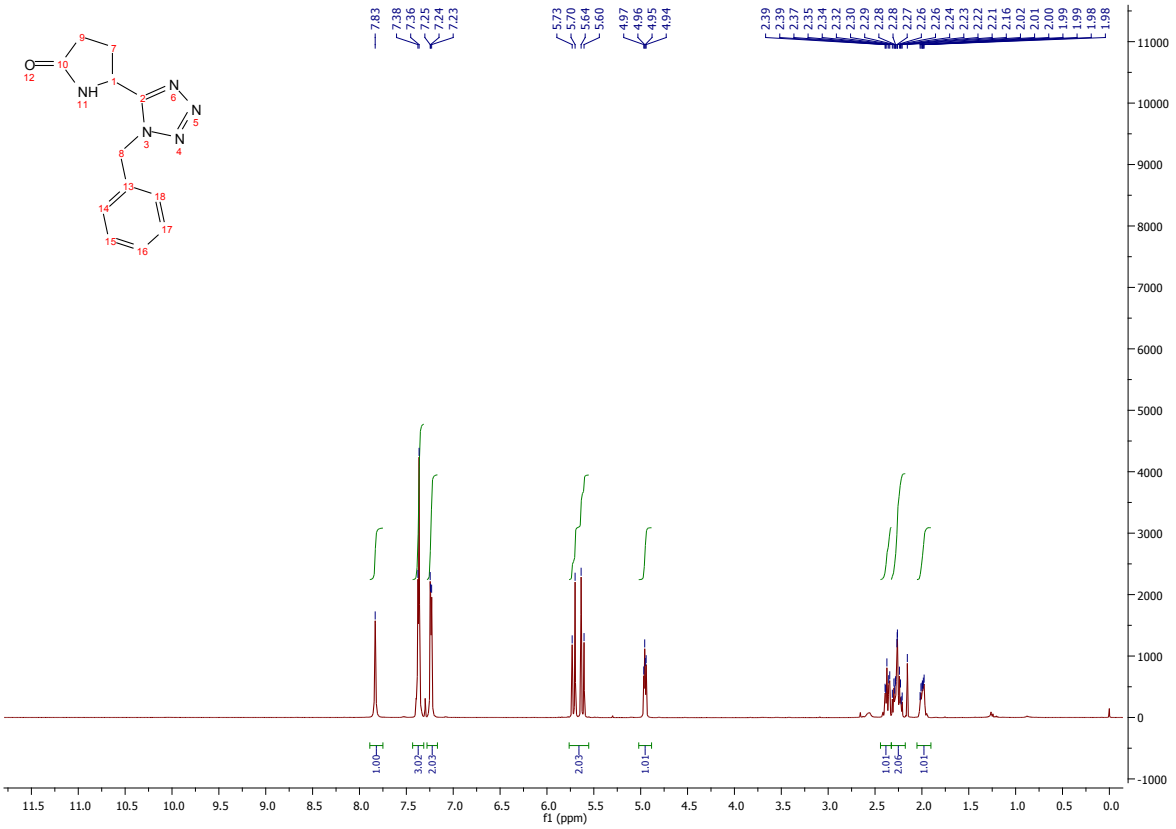
Compound **6c** ^{1}H NMR



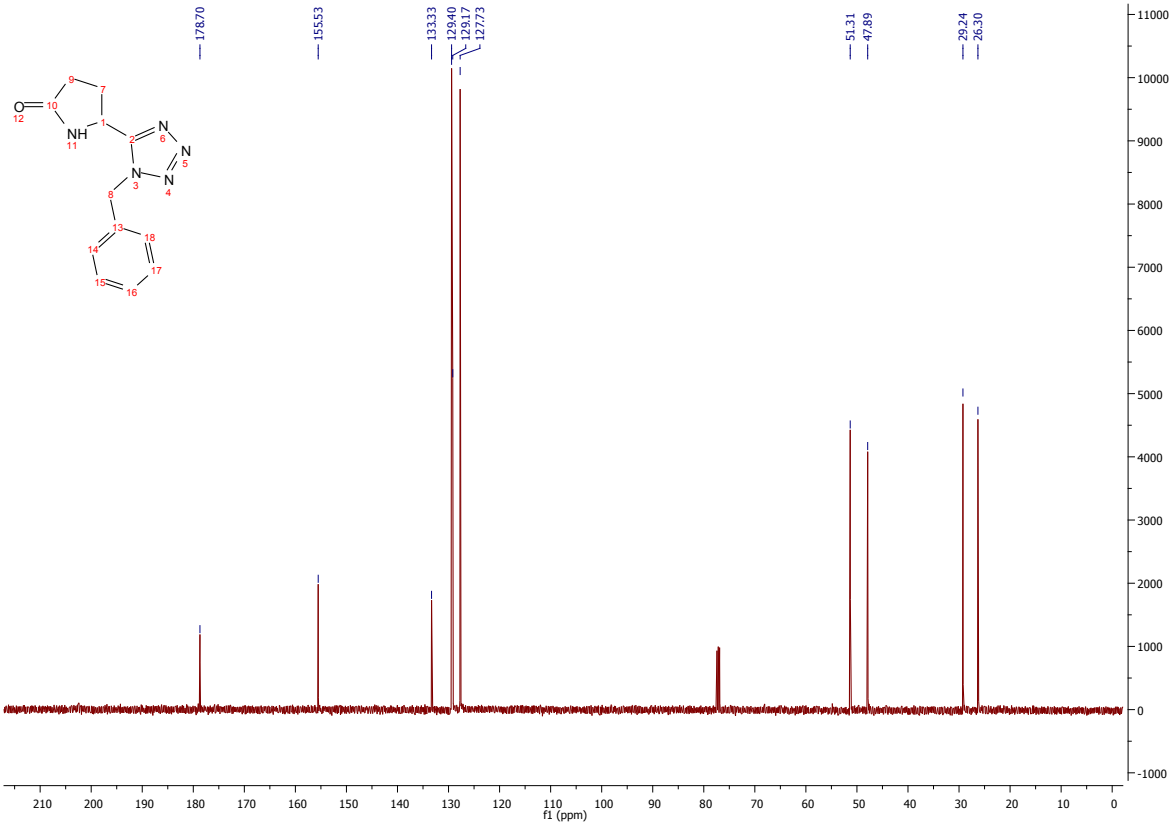
Compound **6c** ^{13}C NMR



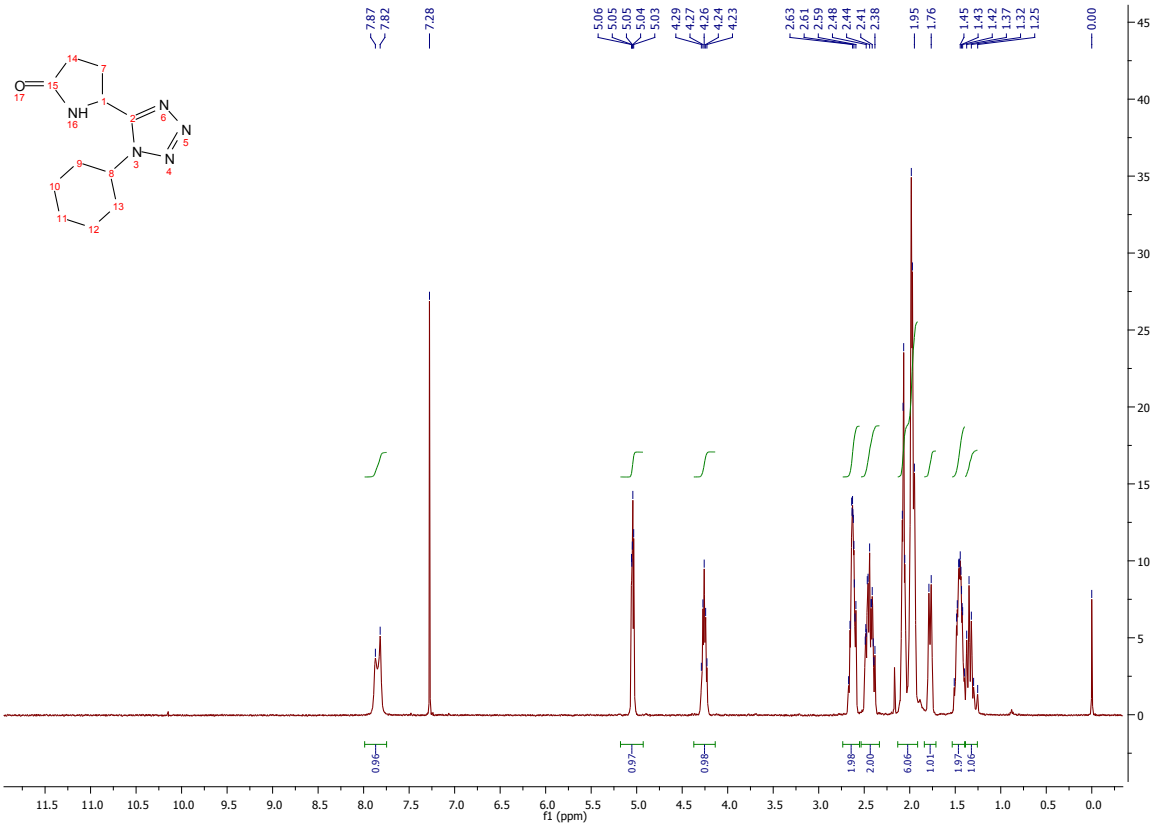
Compound **6d** ^{1}H NMR



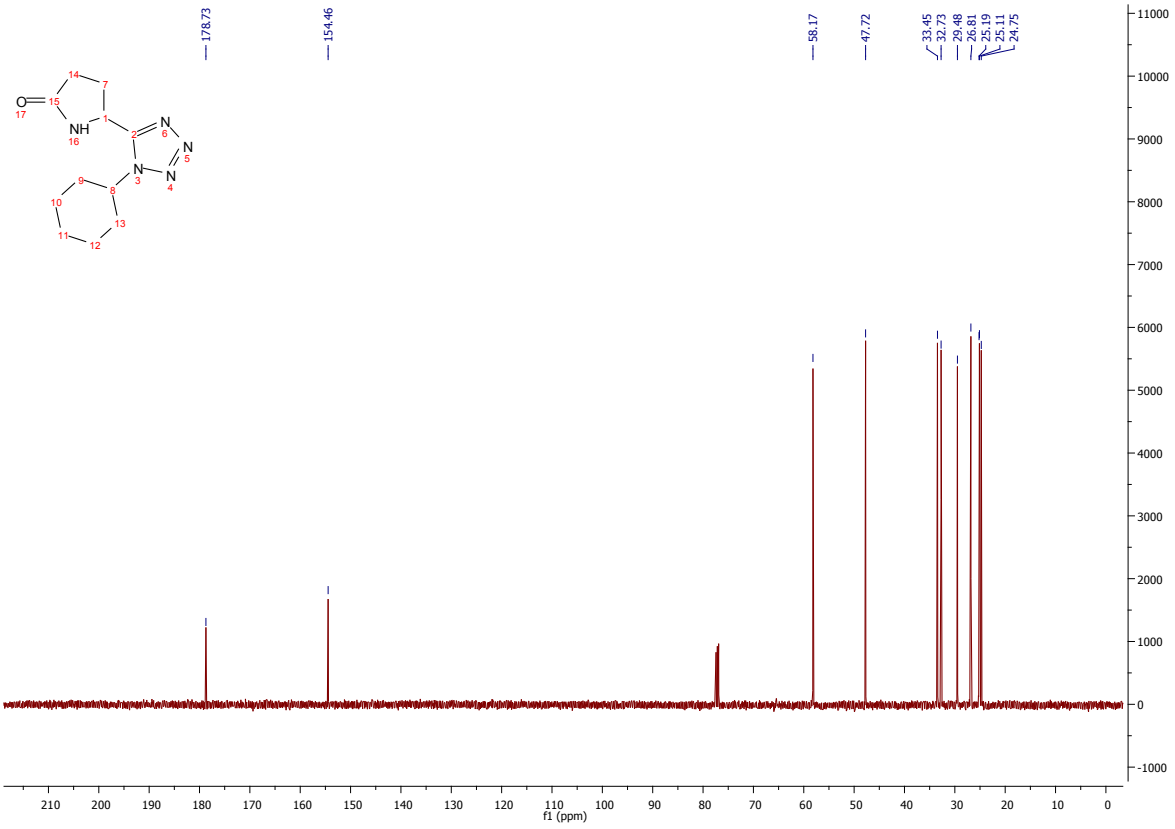
Compound **6d** ^{13}C NMR



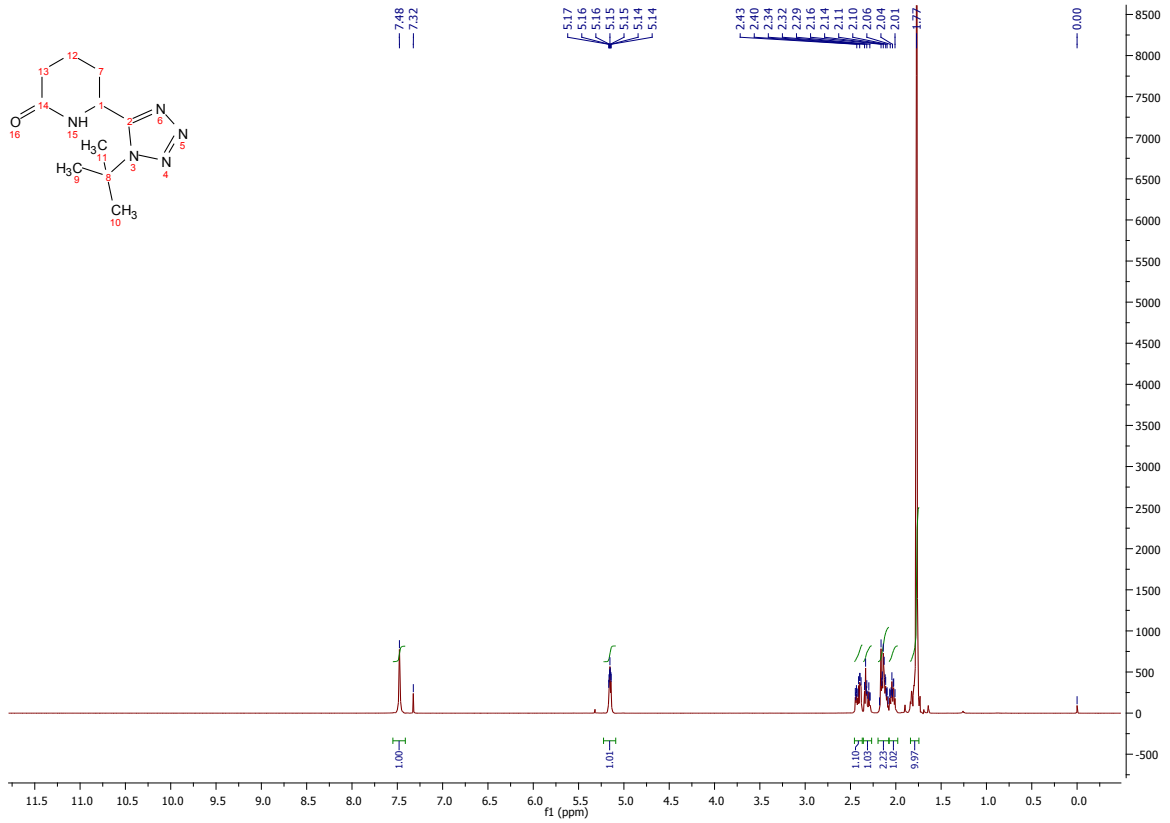
Compound **6e** ^{1}H NMR



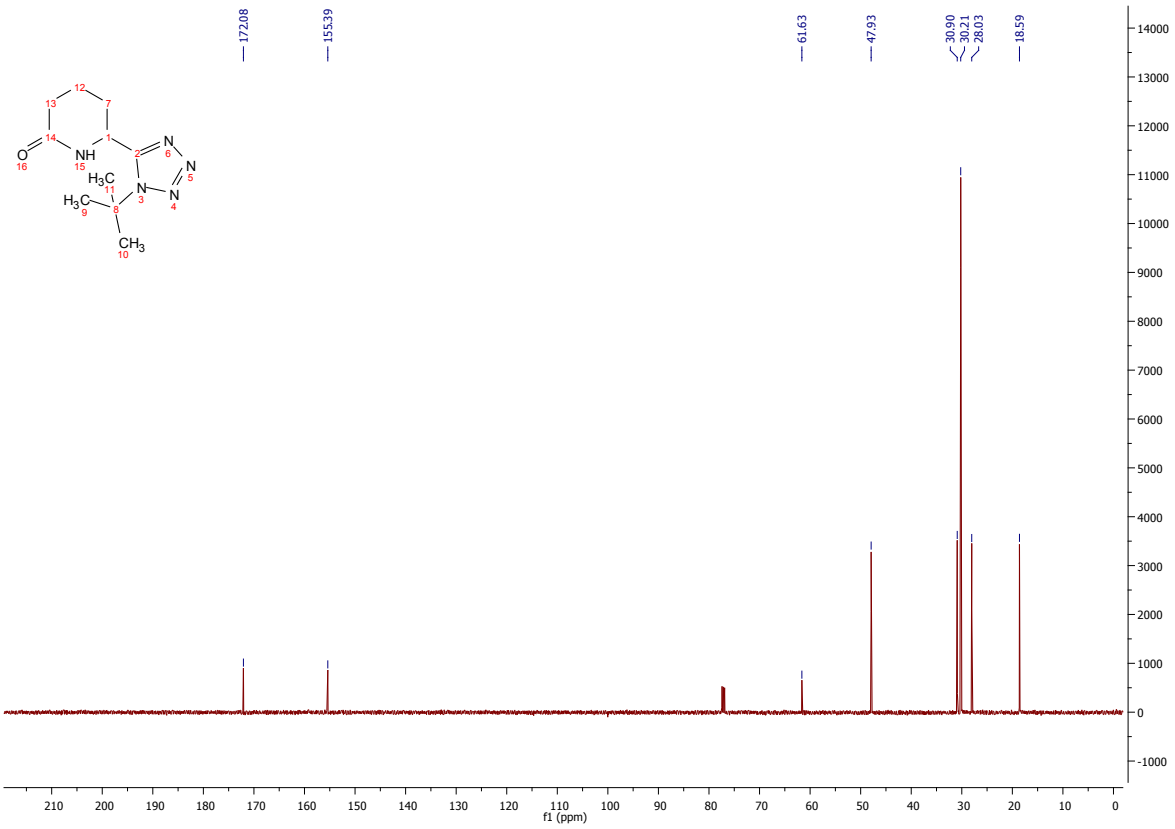
Compound **6e** ^{13}C NMR



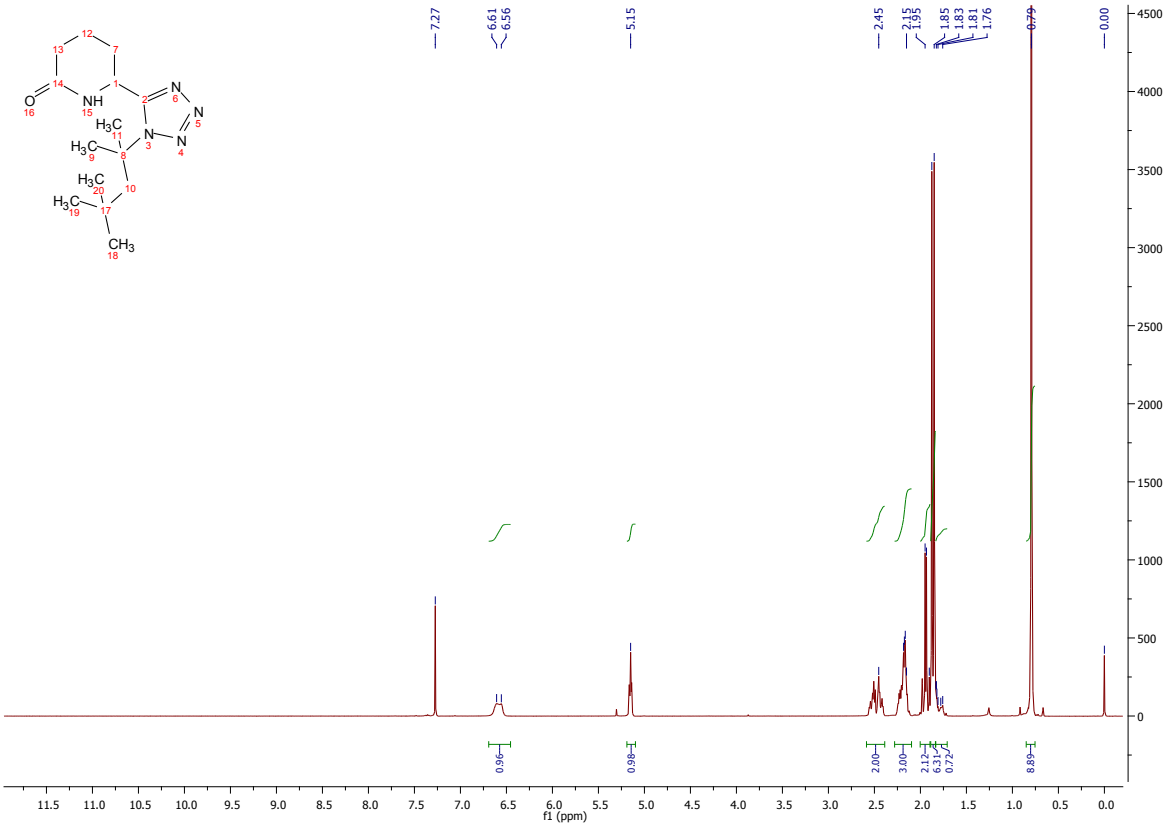
Compound **6f** ^{1}H NMR



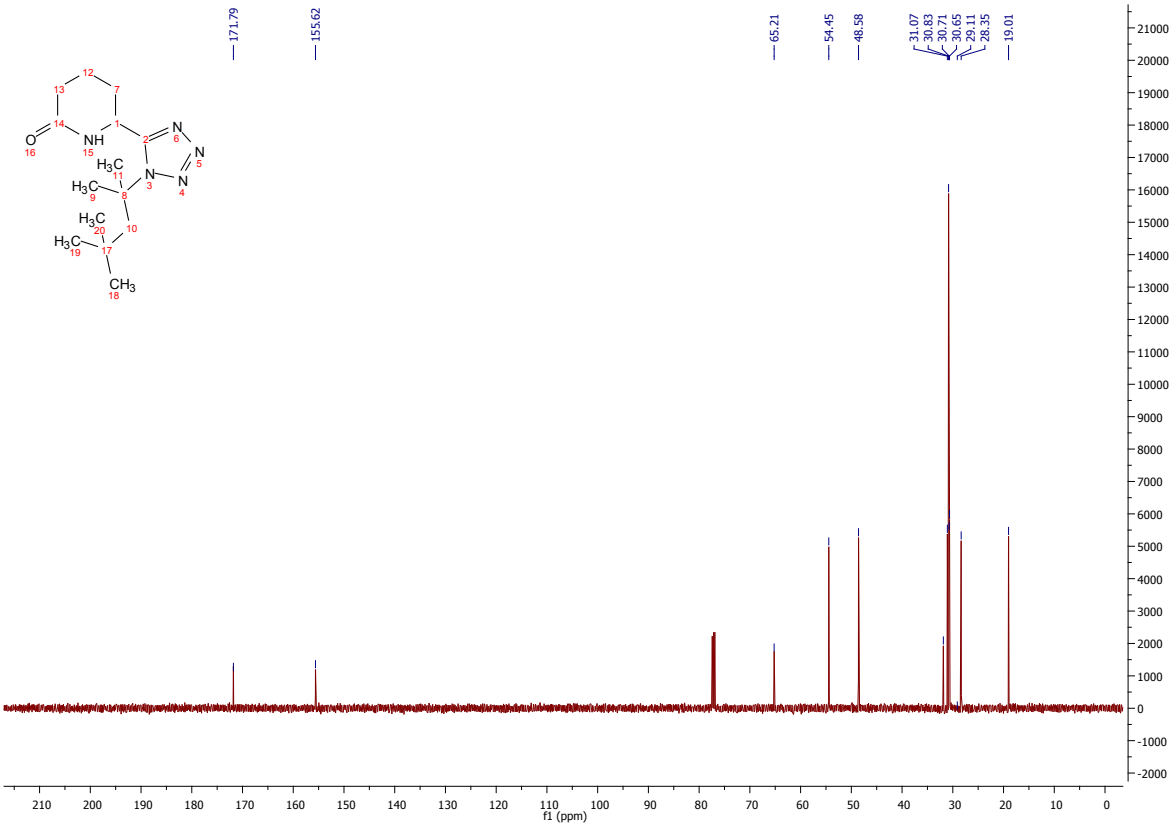
Compound **6f** ^{13}C NMR



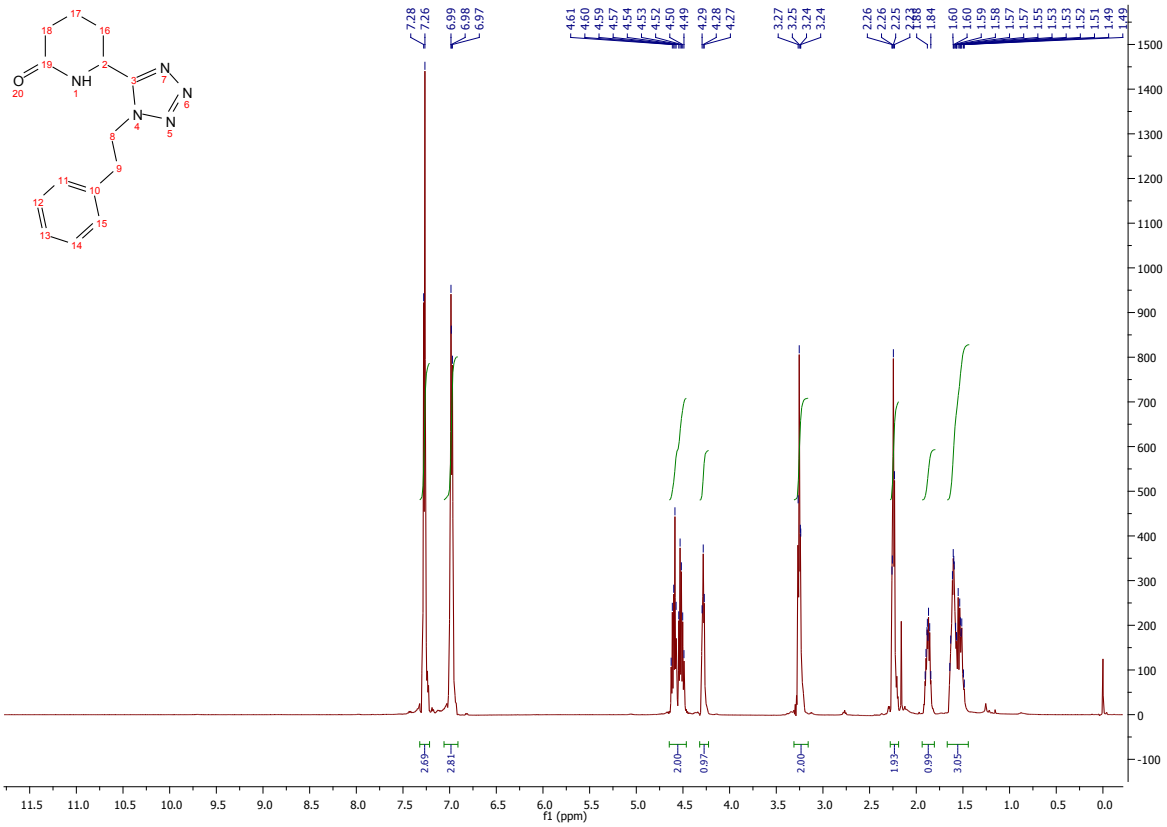
Compound **6g** ^{1}H NMR



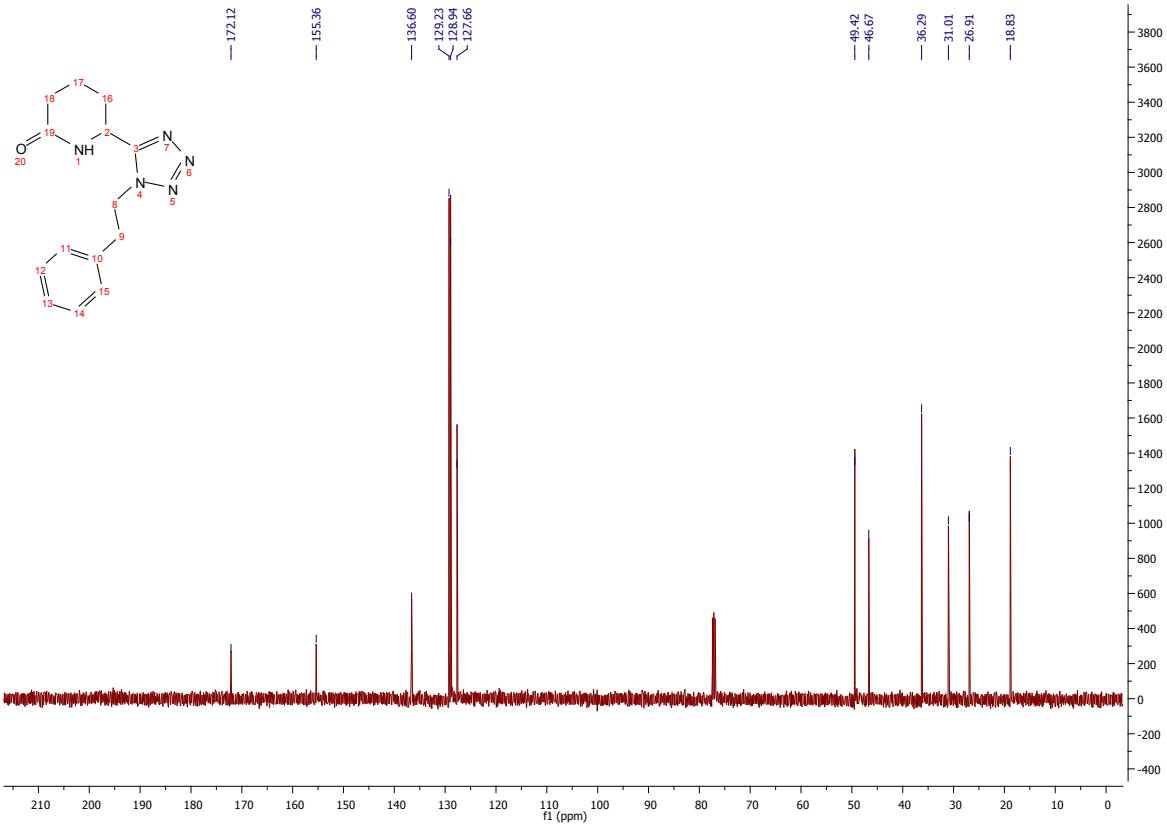
Compound **6g** ^{13}C NMR



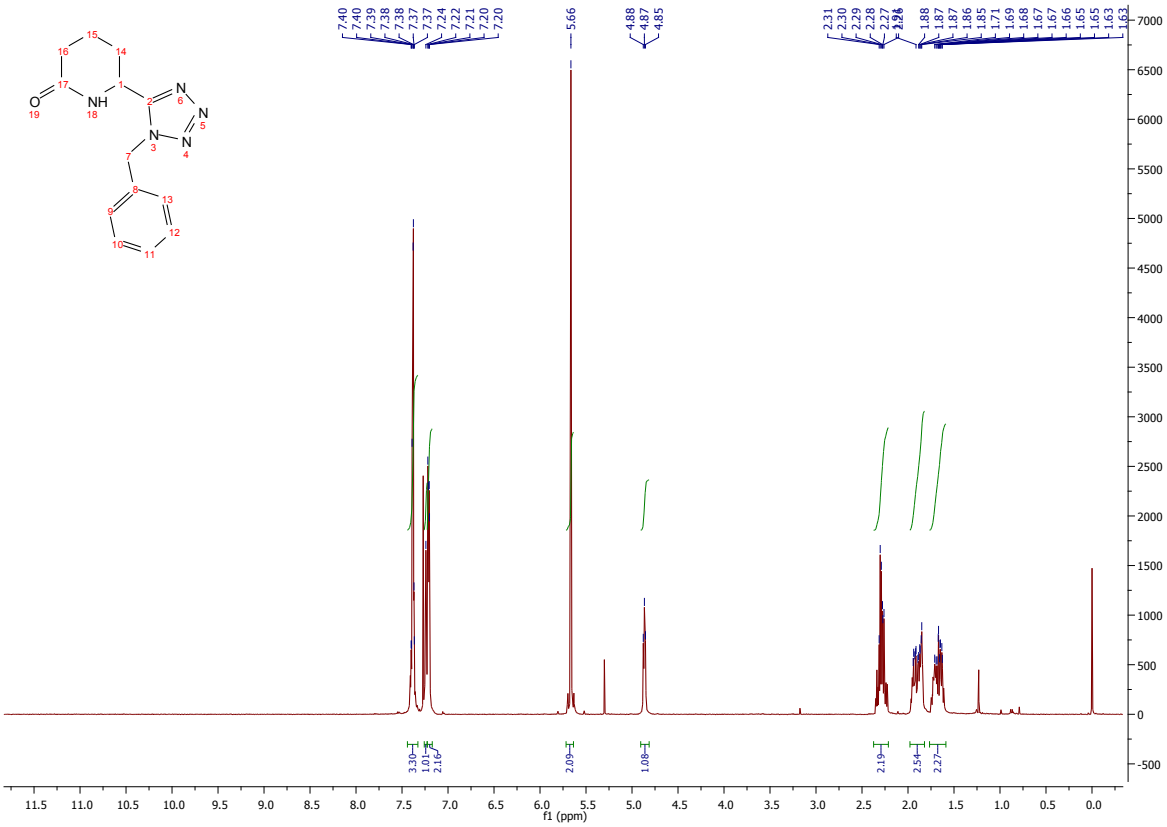
Compound **6h** ^{1}H NMR



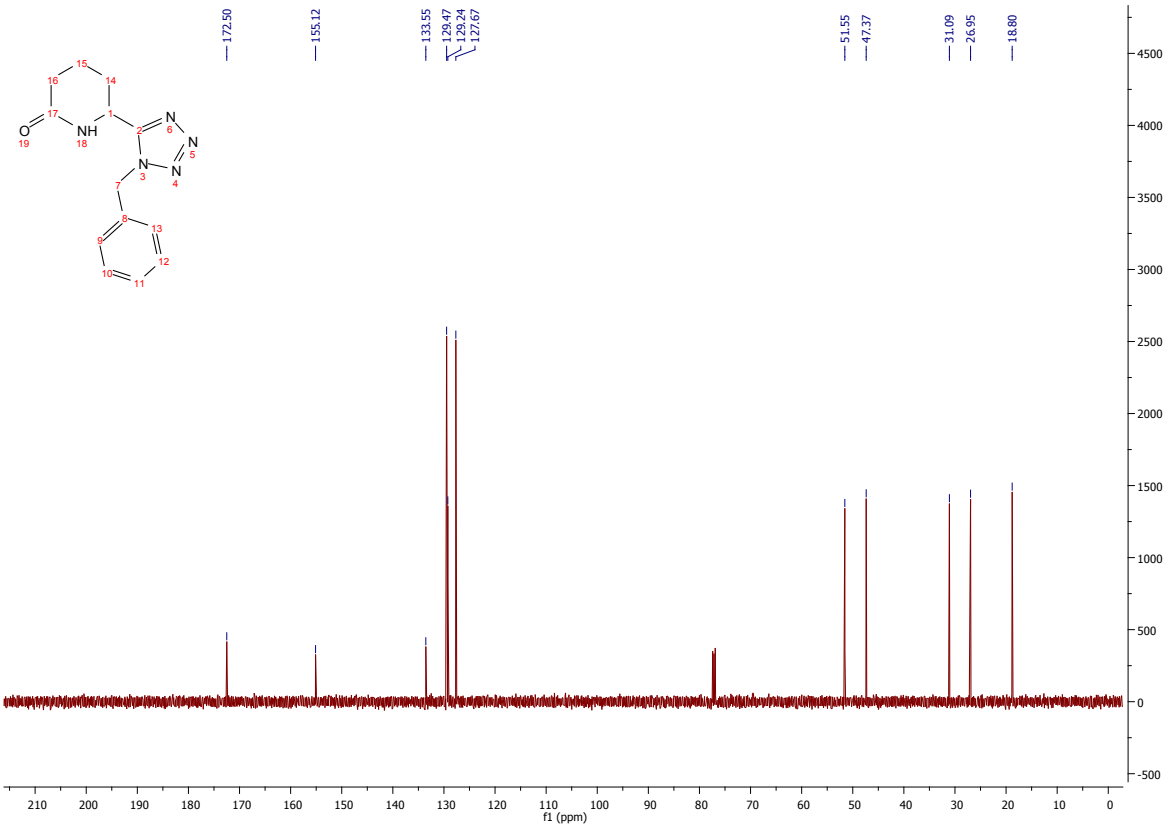
Compound **6h** ^{13}C NMR



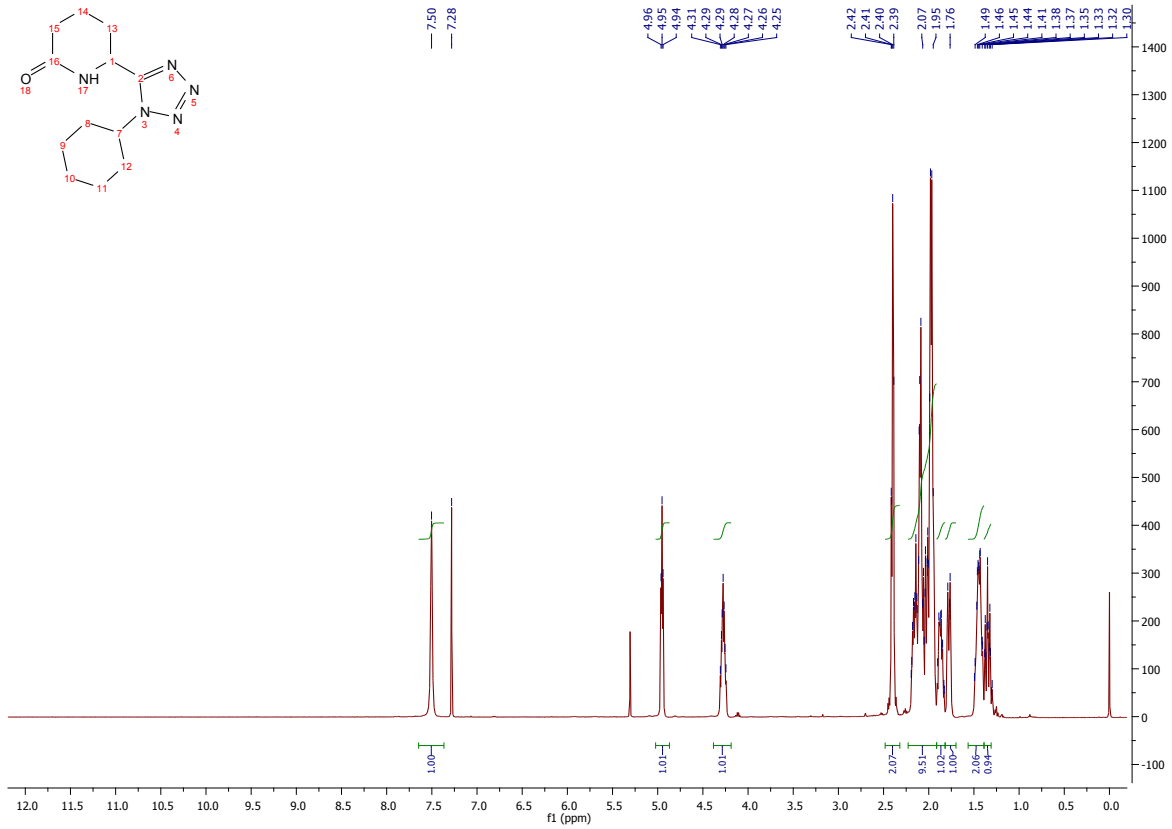
Compound **6i** ^{1}H NMR



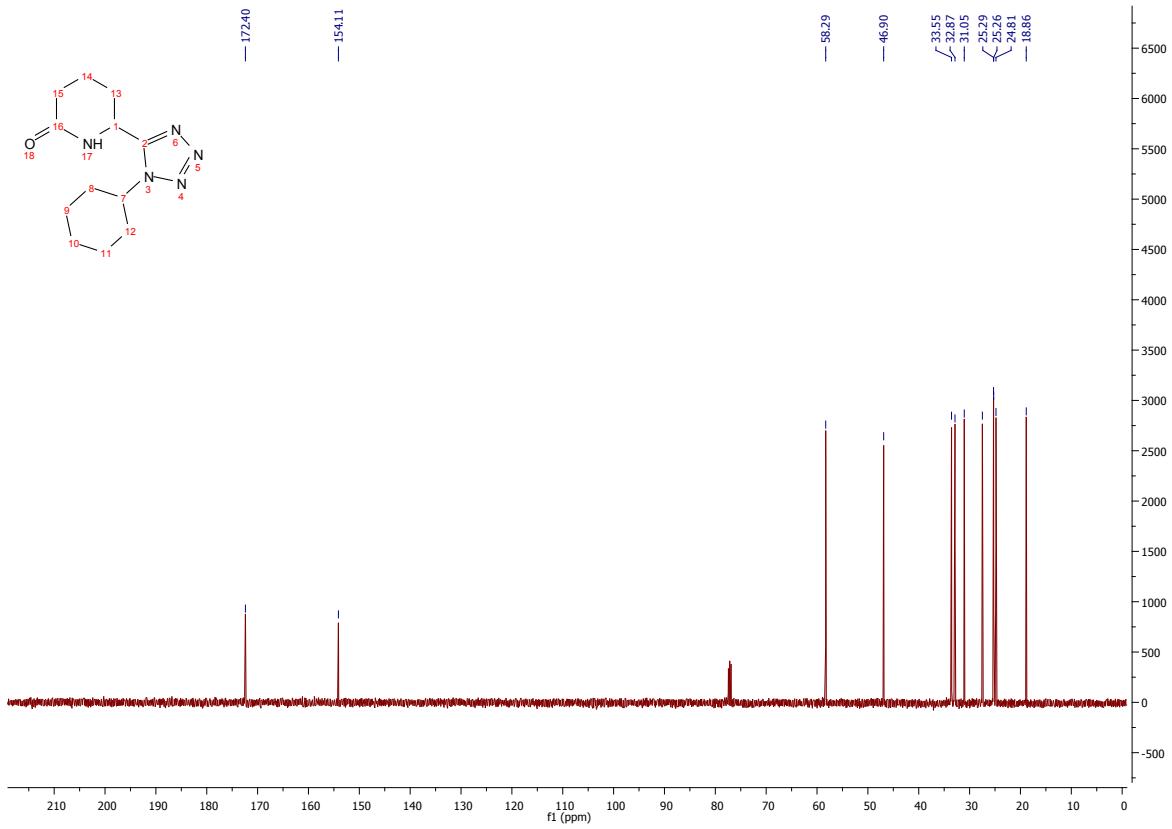
Compound **6i** ^{13}C NMR



Compound **6j** ^{1}H NMR



Compound 6j ^{13}C NMR



Single Crystal X-Ray Structure Determination of Compounds 6b, 6e, 6f, and 6j

6b: correction for extinction effects

Compound 6b

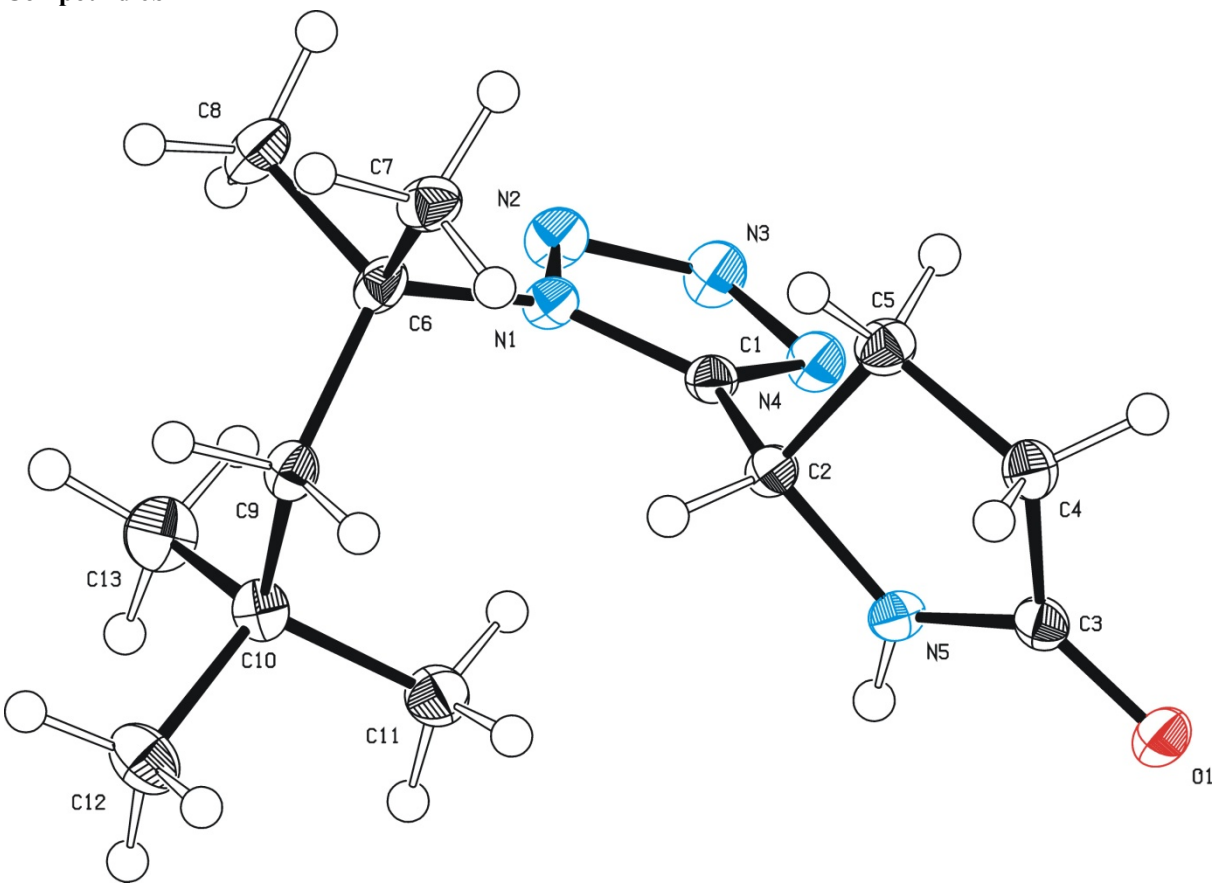


Figure F1 – Ortep drawing drawing of compound **6b** with 50% ellipsoids. [6]

Colorless fragment	
Crystal Size	Operator: *** Herdtweck ***
Molecular Formula:	$C_{13}H_{23}N_5O$
Crystal Color / Shape	Approximate size of crystal fragment used for data collection: 0.20 × 0.25 × 0.43 mm
Molecular Weight:	265.36 a.m.u.
F_{000}:	576
Systematic Absences:	h0l: l≠2n; 0k0: k≠2n
Space Group:	Monoclinic $P\,2_1/c$ (I.T.-No.: 14)
Cell Constants:	Least-squares refinement of 9399 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 2.28° < θ < 25.46°; Mo(K$\overline{\alpha}$); λ = 71.073 pm a = 907.24(2) pm b = 1147.13(3) pm β = 100.6508(13)° c = 1399.04(3) pm V = 1430.93(6)· 10^6 pm^3; Z = 4; D_{calc} = 1.232 g cm^{-3}; Mos. = 0.65
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); sealed tube; graphite monochromator; 50 kV; 30 mA; λ = 71.073 pm; Mo(K$\overline{\alpha}$)
Temperature:	(-173±1) °C; (100±1) K
Measurement Range:	2.28° < θ < 25.46°; h: -10/10, k: -13/13, l: -16/16

Measurement Time:	2 × 15 s per film	
Measurement Mode:	measured: 11 runs; 4743 films / scaled: 11 runs; 4743 films	
	φ– and ω–movement; Increment: $\Delta\varphi/\Delta\omega = 0.50°$; dx = 40.0 mm	
LP - Correction:	Yes [2]	
Intensity Correction	No/Yes; during scaling [2]	
Absorption Correction:	Multi-scan; during scaling; $\mu = 0.082$ mm^{-1} [2]	
	Correction Factors: T_{min} = 0.7079 T_{max} = 0.7452	
Reflection Data:	48744	reflections were integrated and scaled
	1510	reflections systematic absent and rejected
	47234	reflections to be merged
	2636	independent reflections
	0.020	R_{int}: (basis F_o^2)
	2636	independent reflections (all) were used in refinements
	2468	independent reflections with $I_o > 2\sigma(I_o)$
	100.0 %	completeness of the data set
	265	parameter full-matrix refinement
	9.9	reflections per parameter
Solution:	Direct Methods [3, 7]; Difference Fourier syntheses	
Refinement Parameters:	In the asymmetric unit:	
	19	Non-hydrogen atoms with anisotropic displacement parameters
	23	Hydrogen atoms with isotropic displacement parameters
Hydrogen Atoms:	All hydrogen atom positions were found in the difference map calculated from the model containing all non-hydrogen atoms. The hydrogen positions were refined with individual isotropic displacement parameters.	
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4, 5, 7]	
Extinction Correction:	F_c (korr) = k$F_c[1+ 0.001 \cdot \varepsilon \cdot F_c^2 \cdot \lambda^3/\sin(2\Theta)]^{-1/4}$	
	SHELXL-97 [5, 7] ε refined to $\varepsilon = 0.0054(9)$	
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$	
	with a: 0.0362; b: 0.5542; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3	
Shift/Err:	Less than 0.001 in the last cycle of refinement:	
Resid. Electron Density:	+0.28 e**Error!**/Å^3; -0.17 e**Error!**/Å^3	
R1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$	
[$F_o > 4\sigma(F_o)$; N=2468]:		= 0.0302
[all reflctns; N=2636]:		= 0.0320
wR2:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	
[$F_o > 4\sigma(F_o)$; N=2468]:		= 0.0748
[all reflctns; N=2636]:		= 0.0764
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$	= 1.033
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$	

Compound 6e

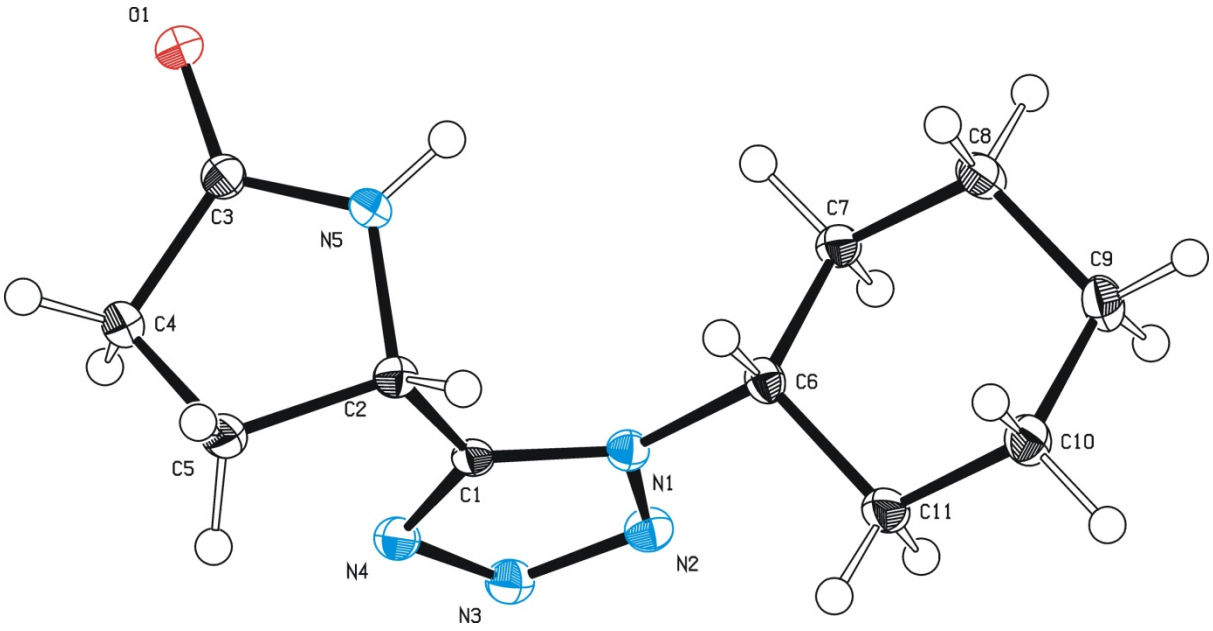


Figure F2 – Ortep drawing drawing of compound **6e** with 50% ellipsoids. [6]

Operator:	*** Herdtweck ***
Molecular Formula:	C_{11} H_{17} N_5 O
Crystal Color / Shape	Colorless fragment
Crystal Size	Approximate size of crystal fragment used for data collection: 0.28 × 0.41 × 0.51 mm
Molecular Weight:	235.30 a.m.u.
F_{000}:	252
Systematic Absences:	none
Space Group:	Triclinic $P\bar{1}$ (I.T.-No.: 2)
Cell Constants:	Least-squares refinement of 9939 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 2.14° < θ < 25.38°; Mo(K$\bar{\alpha}$); λ = 71.073 pm
	a = 654.62(2) pm α = 65.9412(10)°
	b = 925.70(2) pm β = 81.5752(11)°
	c = 1055.29(3) pm γ = 89.9391(11)°
	V = 576.41(3)· 10^6 pm^3; Z = 2; D_{calc} = 1.356 g cm^{-3}; Mos. = 0.64
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); sealed tube; graphite monochromator; 50 kV; 30 mA; λ = 71.073 pm; Mo(K$\bar{\alpha}$)
Temperature:	(-173±1) °C; (100±1) K
Measurement Range:	2.14 < θ < 25.38°; h: -7/7, k: -11/11, l: -12/12
Measurement Time:	2 × 15 s per film
Measurement Mode:	measured: 14 runs; 5785 films / scaled: 14 runs; 5785 films
	φ– and ω–movement; Increment: $\Delta\varphi/\Delta\omega$ = 0.50°; dx = 35.0 mm
LP - Correction:	Yes [2]
Intensity Correction	No/Yes; during scaling [2]
Absorption Correction:	Multi-scan; during scaling; μ = 0.093 mm^{-1} [2]
	Correction Factors: T_{min} = 0.6876 T_{max} = 0.7452
Reflection Data:	19536 reflections were integrated and scaled
	19536 reflections to be merged
	2111 independent reflections

0.016	R_{int}: (basis F_o^2)	
2111	independent reflections (all) were used in refinements	
2033	independent reflections with $I_o > 2\sigma(I_o)$	
99.9 %	completeness of the data set	
222	parameter full-matrix refinement	
9.5	reflections per parameter	

Solution: Direct Methods [3, 7]; Difference Fourier syntheses

Refinement Parameters: In the asymmetric unit:

17	Non-hydrogen atoms with anisotropic displacement parameters
17	Hydrogen atoms with isotropic displacement parameters

Hydrogen Atoms: All hydrogen atom positions were found in the difference map calculated from the model containing all non-hydrogen atoms. The hydrogen positions were refined with individual isotropic displacement parameters.

Atomic Form Factors: For neutral atoms and anomalous dispersion [4, 5, 7]

Extinction Correction: no

Weighting Scheme: $w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$

with a: 0.0400; b: 0.2260; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3

Shift/Err: Less than 0.001 in the last cycle of refinement:

Resid. Electron Density: +0.26 e**Error!**/Å^3; -0.23 e**Error!**/Å^3

R1: $\Sigma(||F_o|-|F_c||)/\Sigma|F_o|$

[$F_o > 4\sigma(F_o)$;	N=2033]:	= 0.0303
[all reflctns;	N=2111]:	= 0.0312

wR2: $[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

[$F_o > 4\sigma(F_o)$;	N=2033]:	= 0.0765
[all reflctns;	N=2111]:	= 0.0774

Goodness of fit: $[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$ = 1.050

Remarks: Refinement expression $\Sigma w(F_o^2-F_c^2)^2$

Compound 6f

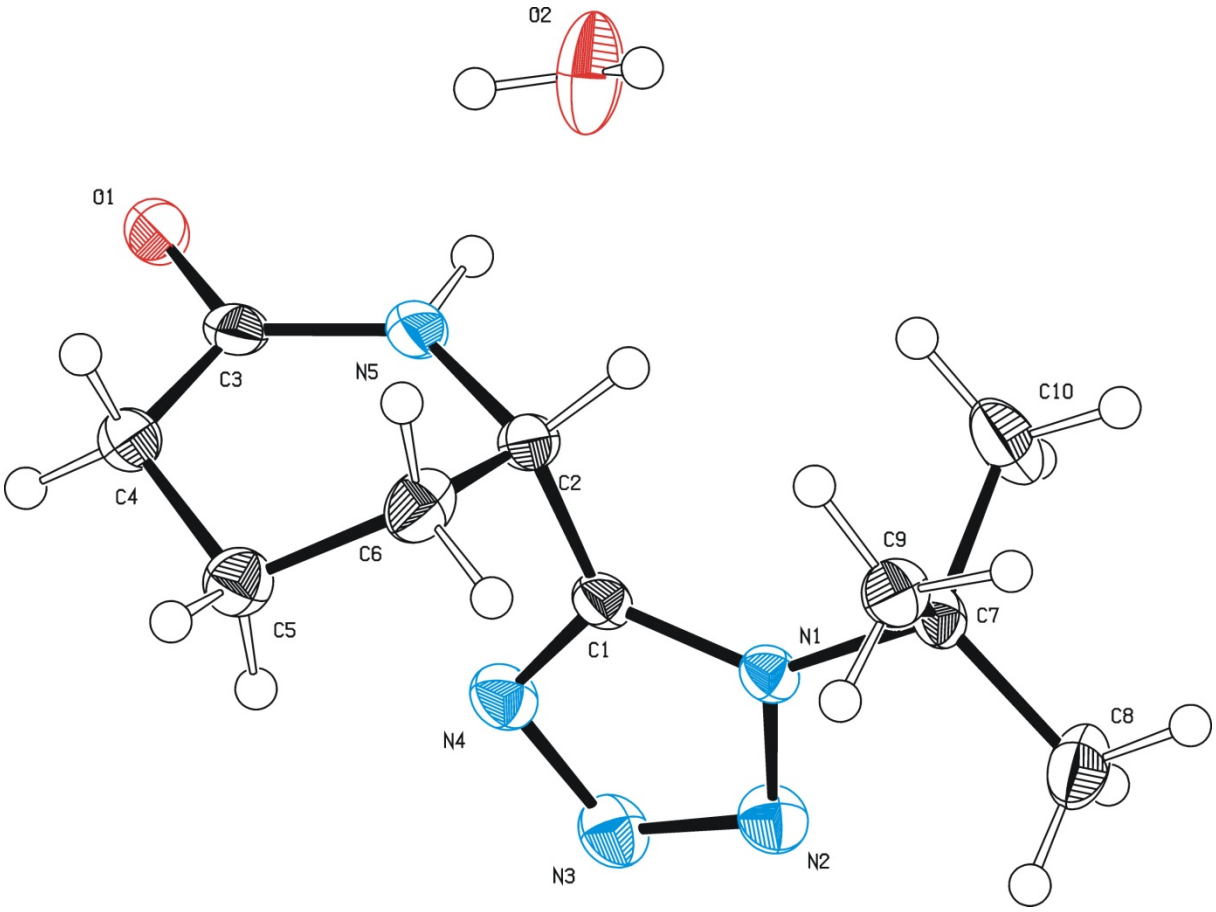


Figure F3 – Ortep drawing drawing of compound **6f** with 50% ellipsoids. [6]

Operator:	*** Herdtweck ***
Molecular Formula:	$C_{20}\ H_{36}\ N_{10}\ O_3$ $2(C_{10}\ H_{17}\ N_5\ O),\ (H_2\ O)$
Crystal Color / Shape	Colourless fragment
Crystal Size	Approximate size of crystal fragment used for data collection: 0.10 × 0.30 × 0.36 mm
Molecular Weight:	464.59 a.m.u.
F_{000}:	1000
Systematic Absences:	hkl: h+k≠2n; h0l: l≠2n
Space Group:	Monoclinic *C* 2/*c* (I.T.-No.: 15)
Cell Constants:	Least-squares refinement of 9875 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 1.63° < θ < 25.55°; Mo(K$\overline{\alpha}$); λ = 71.073 pm *a* = 2660.36(6) pm *b* = 630.28(1) pm β = 109.7809(9)° *c* = 1546.66(3) pm *V* = 2440.37(8)· 10^6 pm^3; *Z* = 4; D_{calc} = 1.265 g cm^{-3}; Mos. = 0.60
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); sealed tube; graphite monochromator; 50 kV; 30 mA; λ = 71.073 pm; Mo(K$\overline{\alpha}$)
Temperature:	(-150±1) °C; (123±1) K
Measurement Range:	1.63° < θ < 25.55°; h: -32/32, k: -7/7, l: -18/18
Measurement Time:	2 × 15 s per film

Measurement Mode:	measured: 7 runs; 3306 films / scaled: 7 runs; 3306 films φ– and ω–movement; Increment: $\Delta\varphi/\Delta\omega = 0.50°$; dx = 40.0 mm
LP - Correction:	Yes [2]
Intensity Correction	No/Yes; during scaling [2]
Absorption Correction:	Multi-scan; during scaling; $\mu = 0.089$ mm^{-1} [2] Correction Factors: $T_{min} = 0.6993$ $T_{max} = 0.7452$
Removing solvent molecules	Besides the solvent molecule, well located in the difference Fourier maps, unresolved solvent molecules remained and had to be removed with the SQUEEZE procedure. [6]
Reflection Data:	35663 reflections were integrated and scaled 2031 reflections systematic absent and rejected 33632 reflections to be merged 2264 independent reflections 0.026 R_{int}: (basis F_o^2) 2264 independent reflections (all) were used in refinements 2037 independent reflections with $I_o > 2\sigma(I_o)$ 98.7 % completeness of the data set 222 parameter full-matrix refinement 10.2 reflections per parameter
Solution:	Direct Methods [3, 7]; Difference Fourier syntheses
Refinement Parameters:	In the asymmetric unit: 17 Non-hydrogen atoms with anisotropic displacement parameters 18 Hydrogen atoms with isotropic displacement parameters
Hydrogen Atoms:	All hydrogen atom positions were found in the difference map calculated from the model containing all non-hydrogen atoms. The hydrogen positions were refined with individual isotropic displacement parameters.
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4, 5, 7]
Extinction Correction:	no
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$ with a: 0.0466; b: 1.7210; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3
Shift/Err:	Less than 0.001 in the last cycle of refinement:
Resid. Electron Density:	+0.19 e**Error!**/Å^3; -0.18 e**Error!**/Å^3
R1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$
[$F_o > 4\sigma(F_o)$; N=2037]:	= 0.0348
[all reflctns; N=2264]:	= 0.0385
wR2:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$
[$F_o > 4\sigma(F_o)$; N=2037]:	= 0.0887
[all reflctns; N=2264]:	= 0.0911
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$ = 1.049
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$

Compound 6j

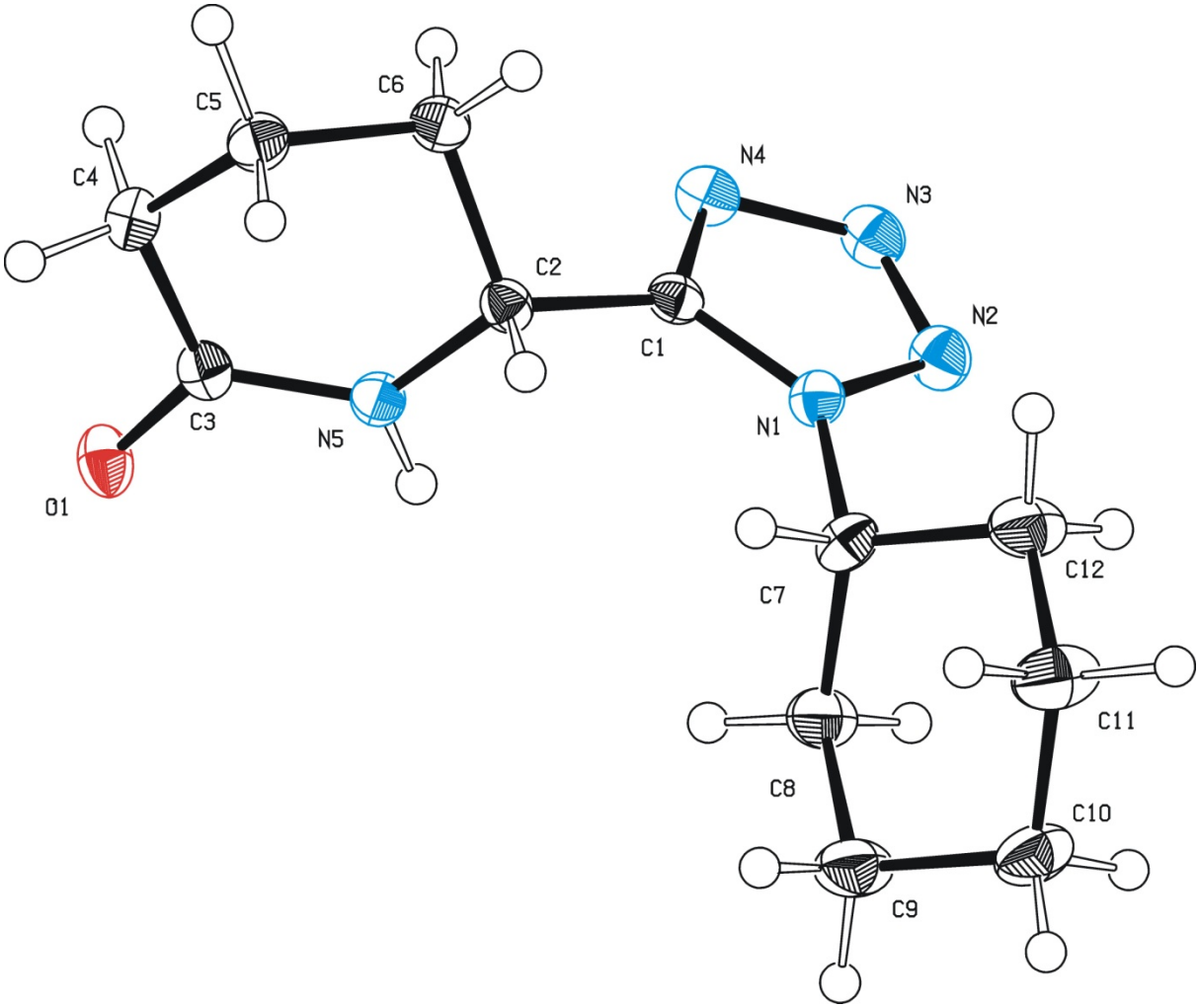


Figure F4 – Ortep drawing drawing of compound **6j** with 50% ellipsoids. [6]

Operator:	*** Herdtweck ***
Molecular Formula:	C_{12} H_{19} N_5 O
Crystal Color / Shape	Colorless fragment
Crystal Size	Approximate size of crystal fragment used for data collection: 0.25 × 0.25 × 0.28 mm
Molecular Weight:	249.32 a.m.u.
F_{000}:	1072
Systematic Absences:	0kl: k≠2n; h0l: l≠2n; hk0: h≠2n
Space Group:	Orthorhombic *P bca* (I.T.-No.: 61)
Cell Constants:	Least-squares refinement of 9968 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 2.79° < θ < 25.40°; Mo(K$\overline{\alpha}$); λ = 71.073 pm *a* = 991.62(3) pm *b* = 1193.89(3) pm *c* = 2152.52(7) pm *V* = 2548.34(13)· 10^6 pm^3; *Z* = 8; D_{calc} = 1.300 g cm^{-3}; Mos. = 0.67
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); sealed tube; graphite monochromator; 50 kV; 30 mA; λ = 71.073 pm; Mo(K$\overline{\alpha}$)
Temperature:	(-150±1) °C; (123±1) K
Measurement Range:	2.79° < θ < 25.40°; h: -11/11, k: -14/14, l: -25/25
Measurement Time:	2 × 10 s per film

Measurement Mode:	measured: 6 runs; 3381 films / scaled: 6 runs; 3381 films	
	φ– and ω–movement; Increment: $\Delta\varphi/\Delta\omega = 0.50°$; dx = 60.0 mm	
LP - Correction:	Yes [2]	
Intensity Correction	No/Yes; during scaling [2]	
Absorption Correction:	Multi-scan; during scaling; $\mu = 0.088$ mm^{-1} [2]	
	Correction Factors: T_{min} = 0.7060 T_{max} = 0.7452	
Reflection Data:	34576	reflections were integrated and scaled
	3008	reflections systematic absent and rejected
	2	obvious wrong intensity and rejected (one hkl)
	31566	reflections to be merged
	2338	independent reflections
	0.028	R_{int}: (basis F_o^2)
	2338	independent reflections (all) were used in refinements
	2085	independent reflections with $I_o > 2\sigma(I_o)$
	99.9 %	completeness of the data set
	239	parameter full-matrix refinement
	9.8	reflections per parameter
Solution:	Direct Methods [3, 7]; Difference Fourier syntheses	
Refinement Parameters:	In the asymmetric unit:	
	18	Non-hydrogen atoms with anisotropic displacement parameters
	19	Hydrogen atoms with isotropic displacement parameters
Hydrogen Atoms:	All hydrogen atom positions were found in the difference map calculated from the model containing all non-hydrogen atoms. The hydrogen positions were refined with individual isotropic displacement parameters.	
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4, 5, 7]	
Extinction Correction:	no	
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$	
	with a: 0.0491; b: 1.2420; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3	
Shift/Err:	Less than 0.001 in the last cycle of refinement:	
Resid. Electron Density:	+0.24 e**Error!**/Å^3; -0.24 e**Error!**/Å^3	
R1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$	
[$F_o > 4\sigma(F_o)$; N=2085]:		= 0.0359
[all reflctns; N=2338]:		= 0.0407
wR2:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	
[$F_o > 4\sigma(F_o)$; N=2085]:		= 0.0959
[all reflctns; N=2338]:		= 0.0994
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$	= 1.082
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$	

References:

[1] APEX suite of crystallographic software. APEX 2 Version 2008.4. Bruker AXS Inc., Madison, Wisconsin, USA (2008).

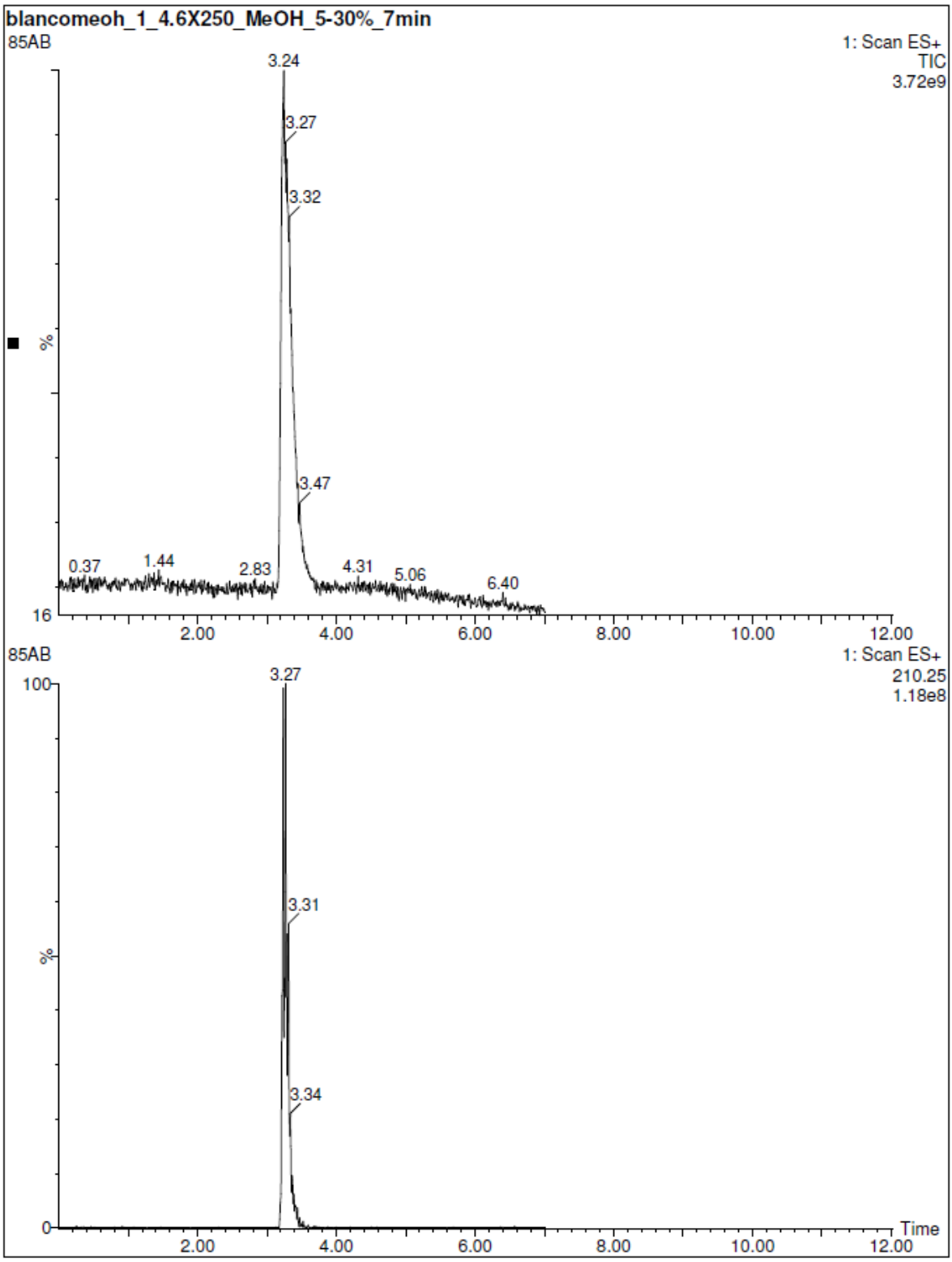
[2] SAINT, Version 7.56a and SADABS Version 2008/1. Bruker AXS Inc., Madison, Wisconsin, USA (2008).

[3] Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Burla, M. C.; Polidori, G.; Camalli M. "**SIR92**", *J. Appl. Cryst.* **1994**, *27*, 435-436.

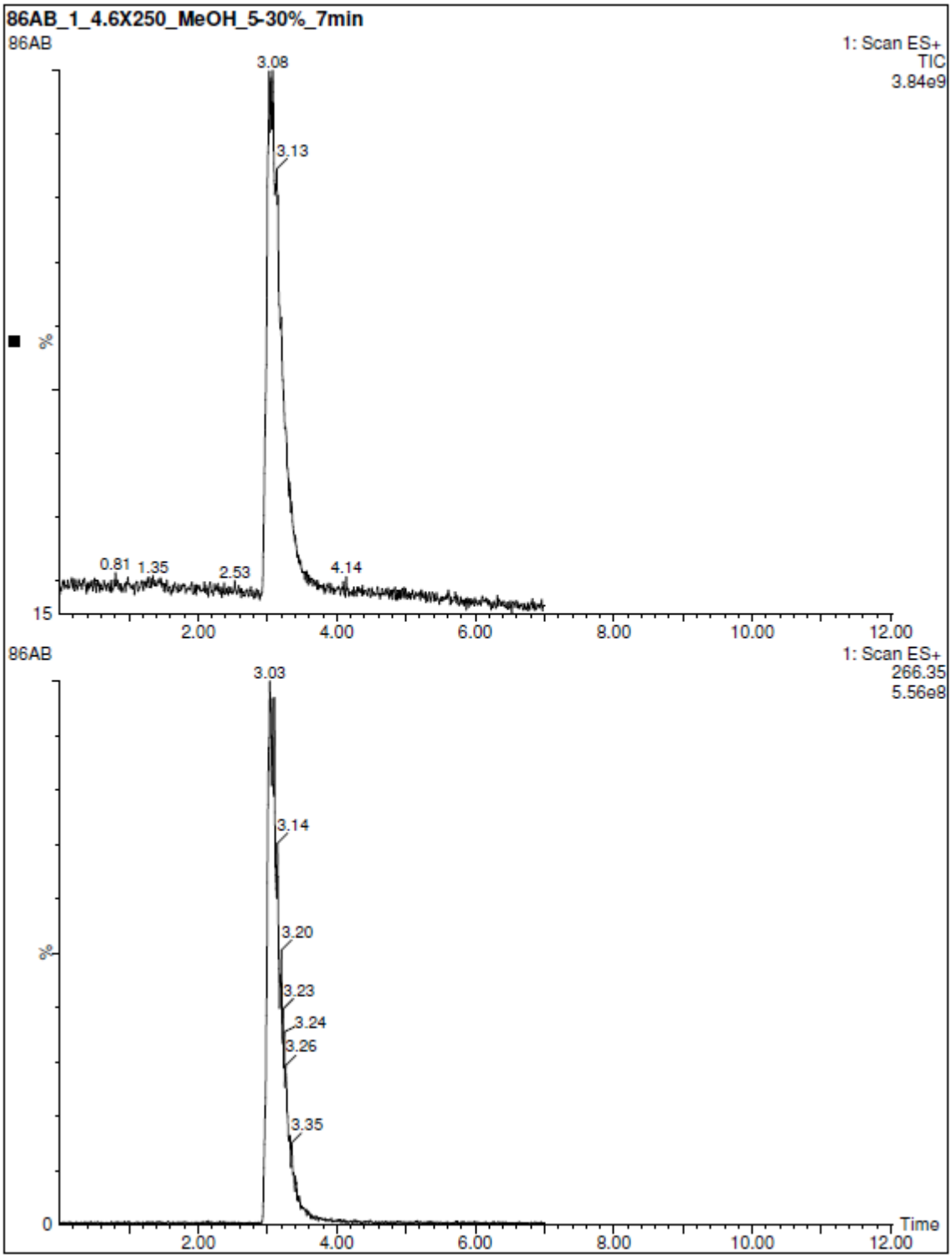
[4] International Tables for Crystallography, Vol. C, Tables 6.1.1.4 (pp. 500-502), 4.2.6.8 (pp. 219-222), and 4.2.4.2 (pp. 193-199), Wilson, A. J. C., Ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1992.
[5] Sheldrick, G. M. "**SHELXL-97**", University of Göttingen, Göttingen, Germany, (1998).
[6] Spek, A. L. "**PLATON**", A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, (2010).
[7] L. J. Farrugia, "**WinGX** (Version 1.70.01 January 2005) ", *J. Appl. Cryst.* **1999**, *32*, 837-838.

SFC-MS Chromatograms of compounds 6a-j

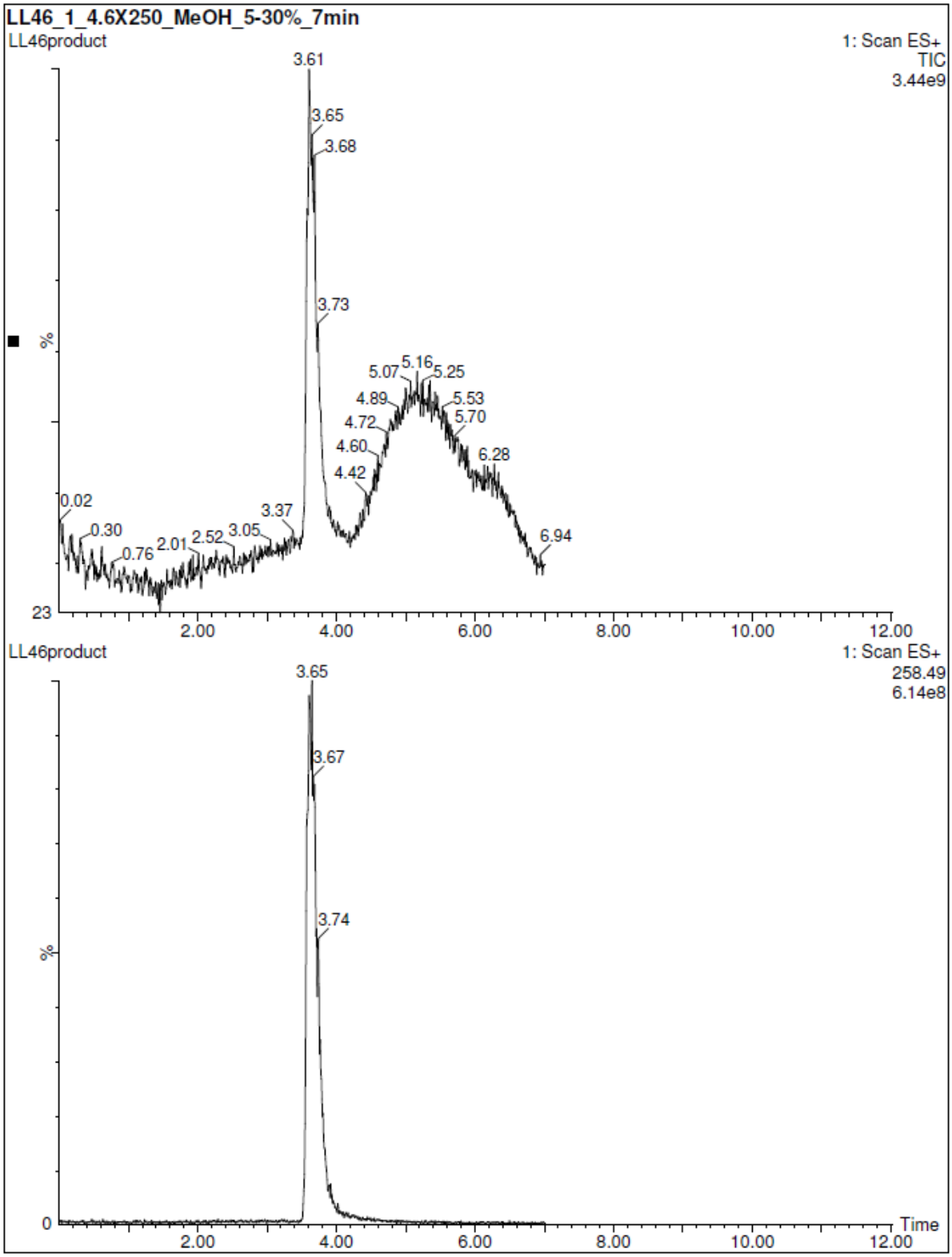
Compound **6a** SFC-MS



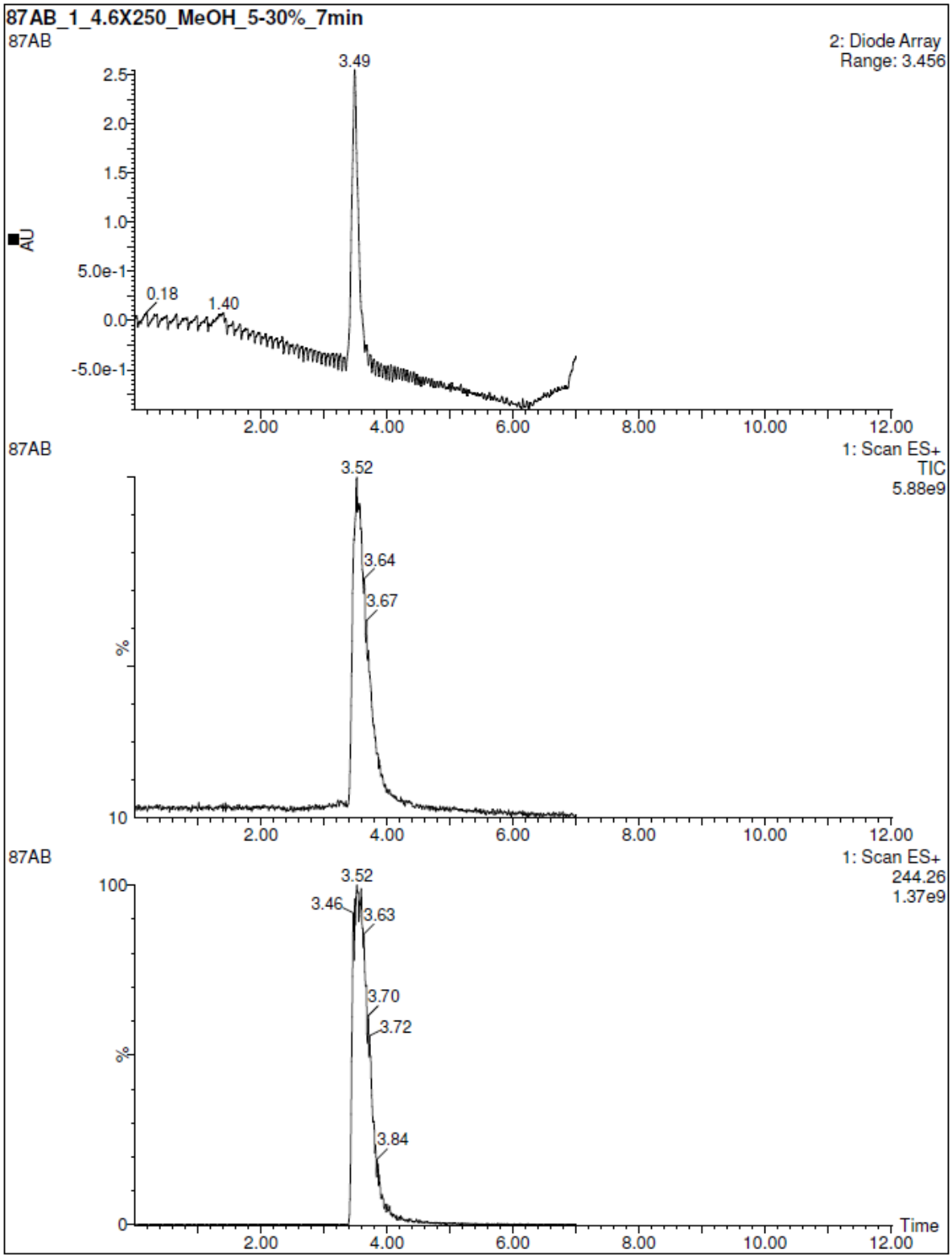
Compound **6b** SFC-MS



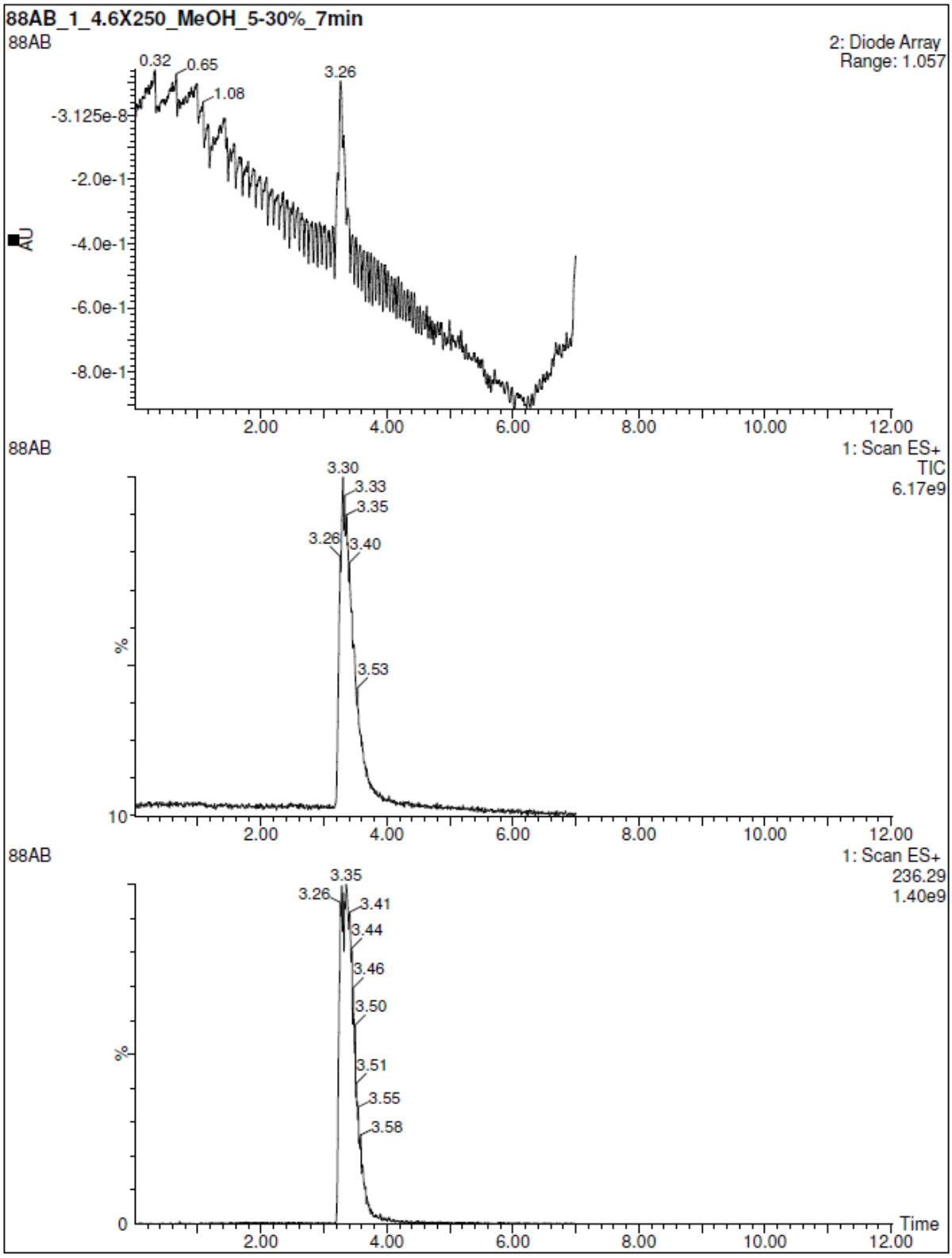
Compound **6c** SFC-MS



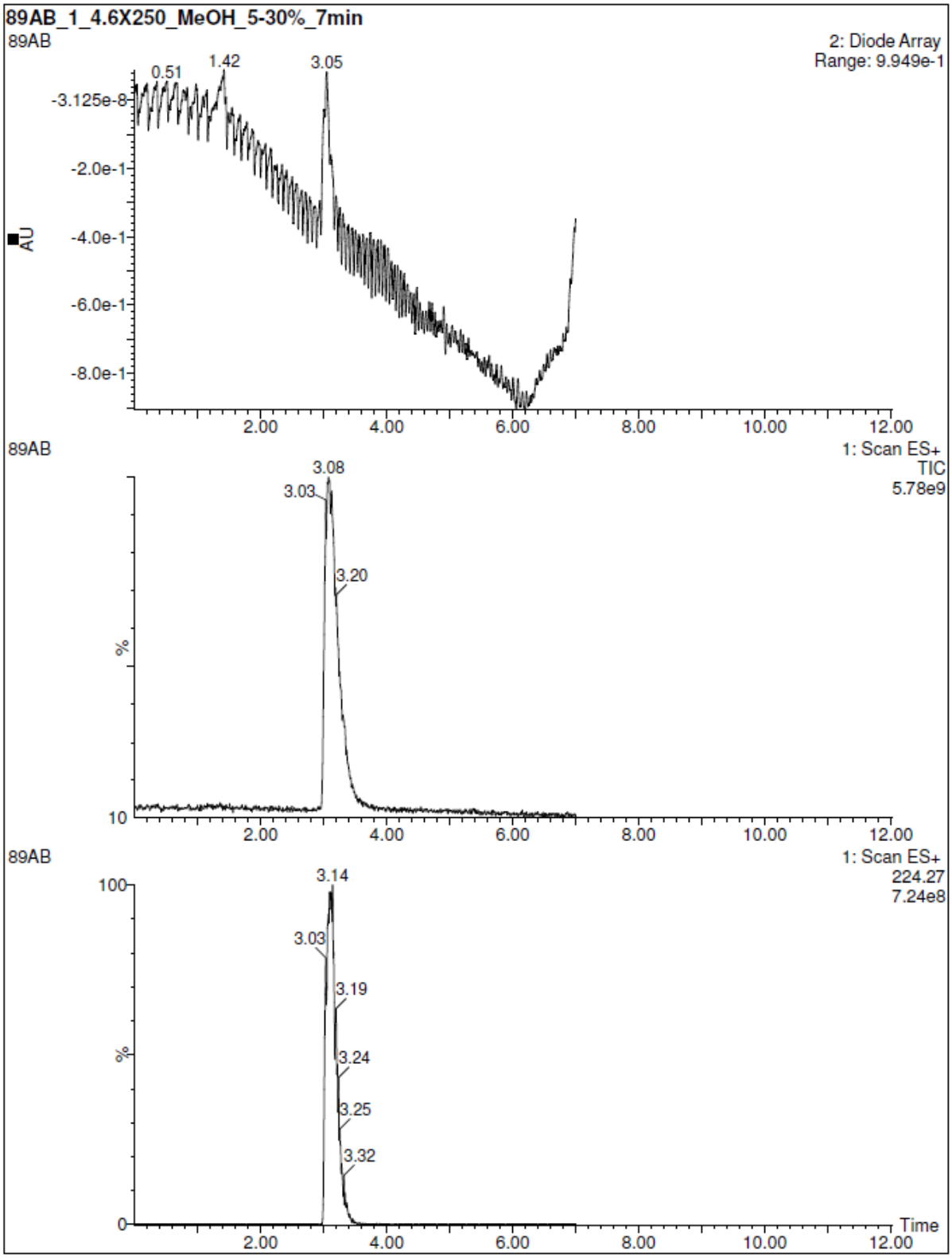
Compound **6d** SFC-MS



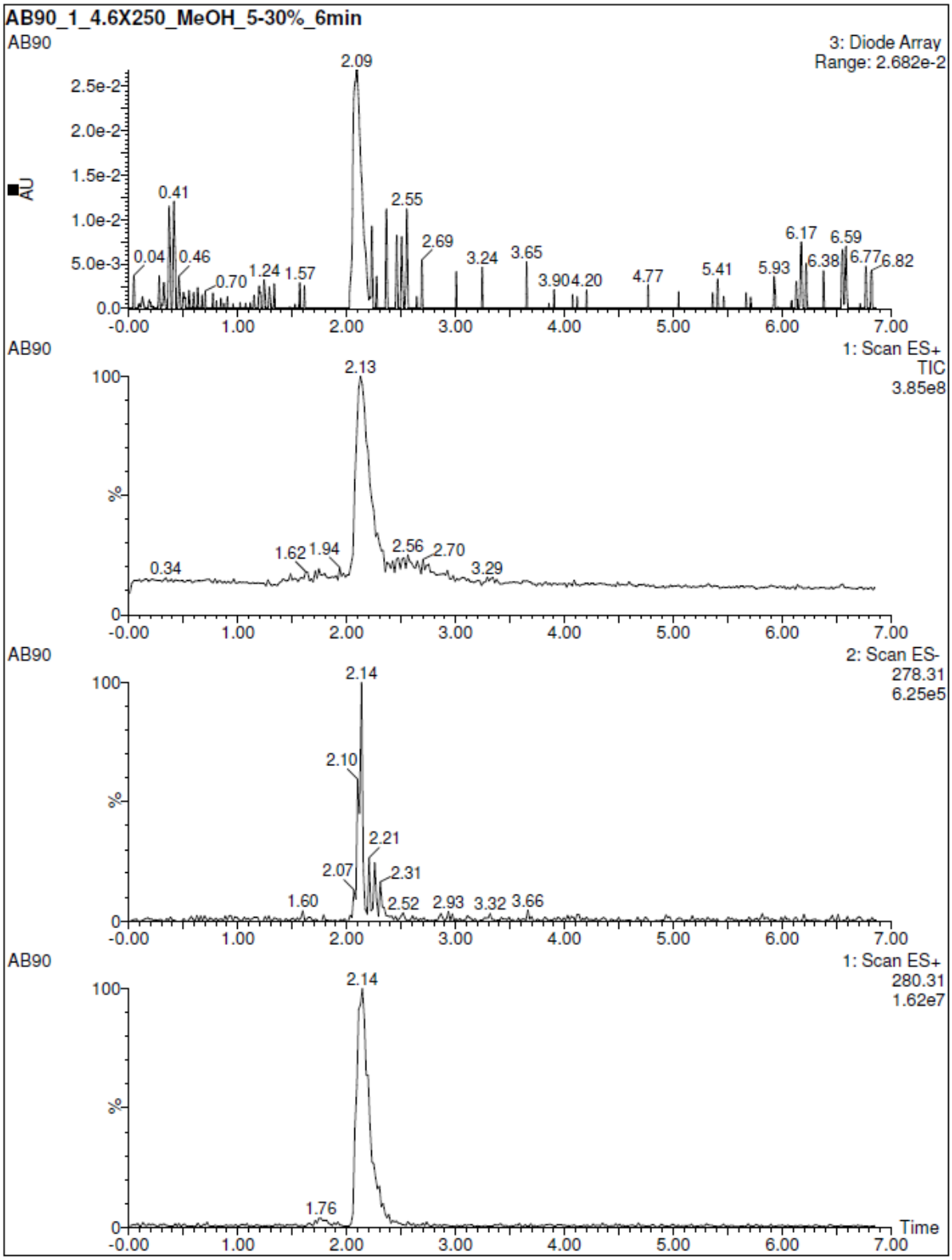
Compound **6e** SFC-MS



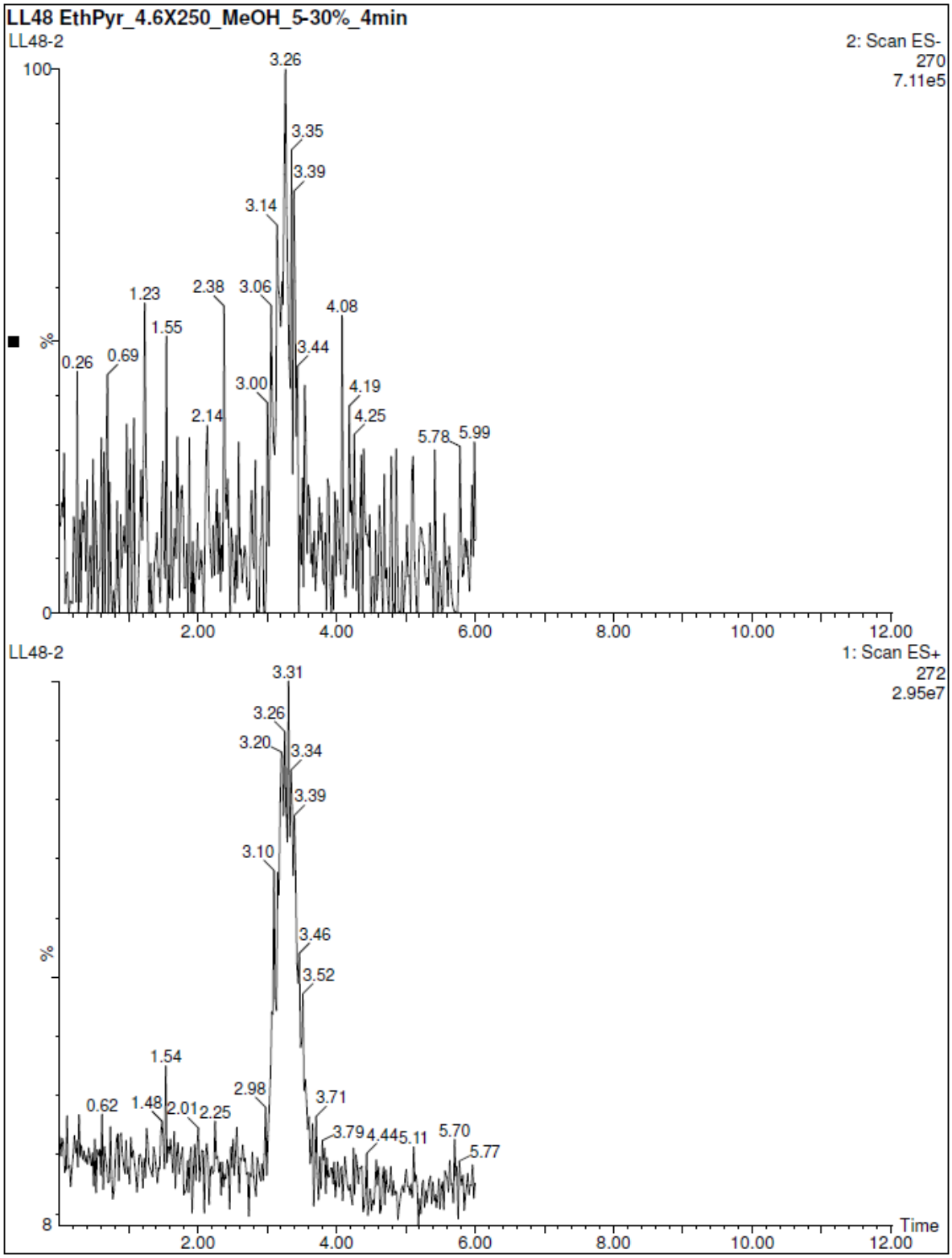
Compound **6f** SFC-MS



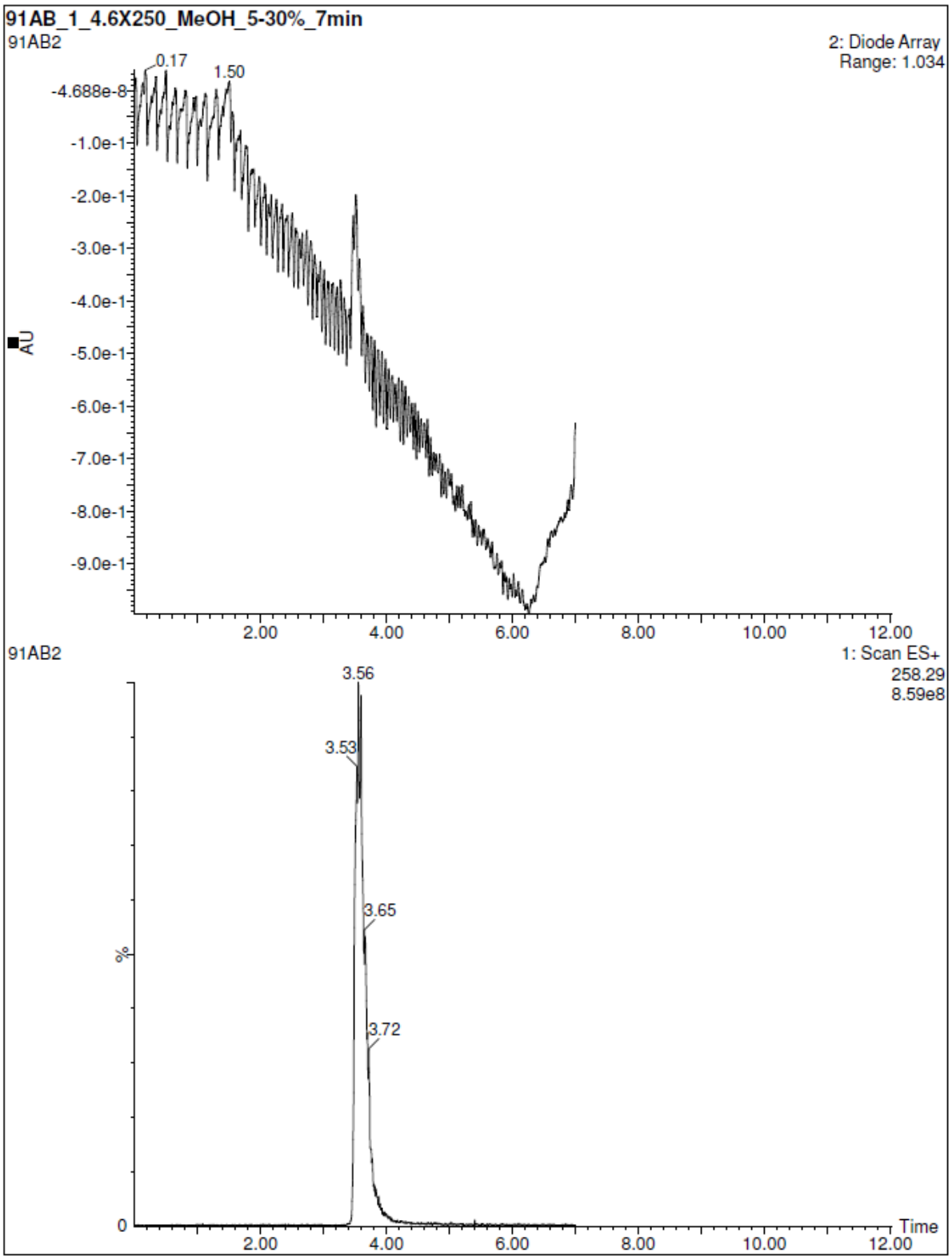
Compound **6g** SFC-MS



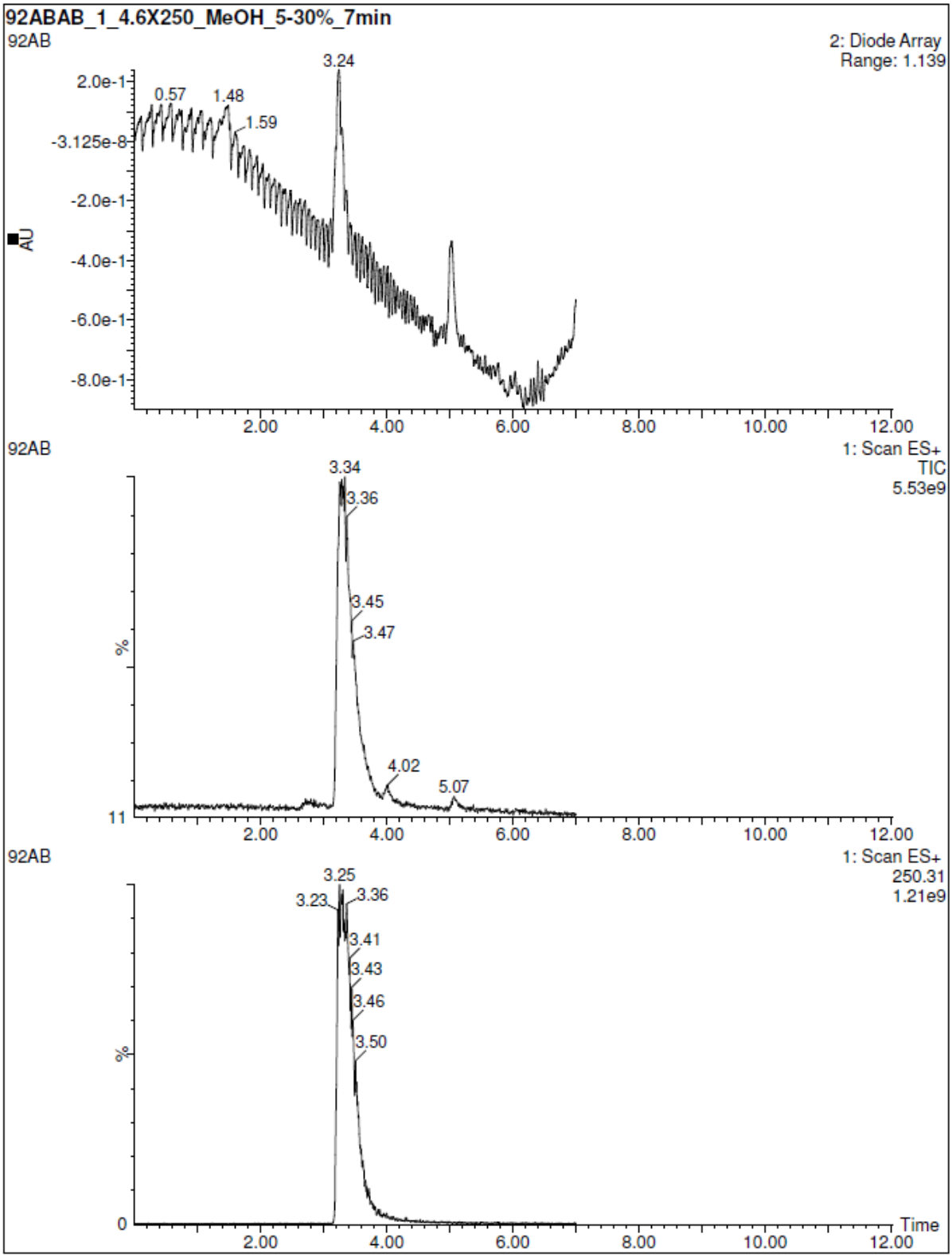
Compound **6h** SFC-MS



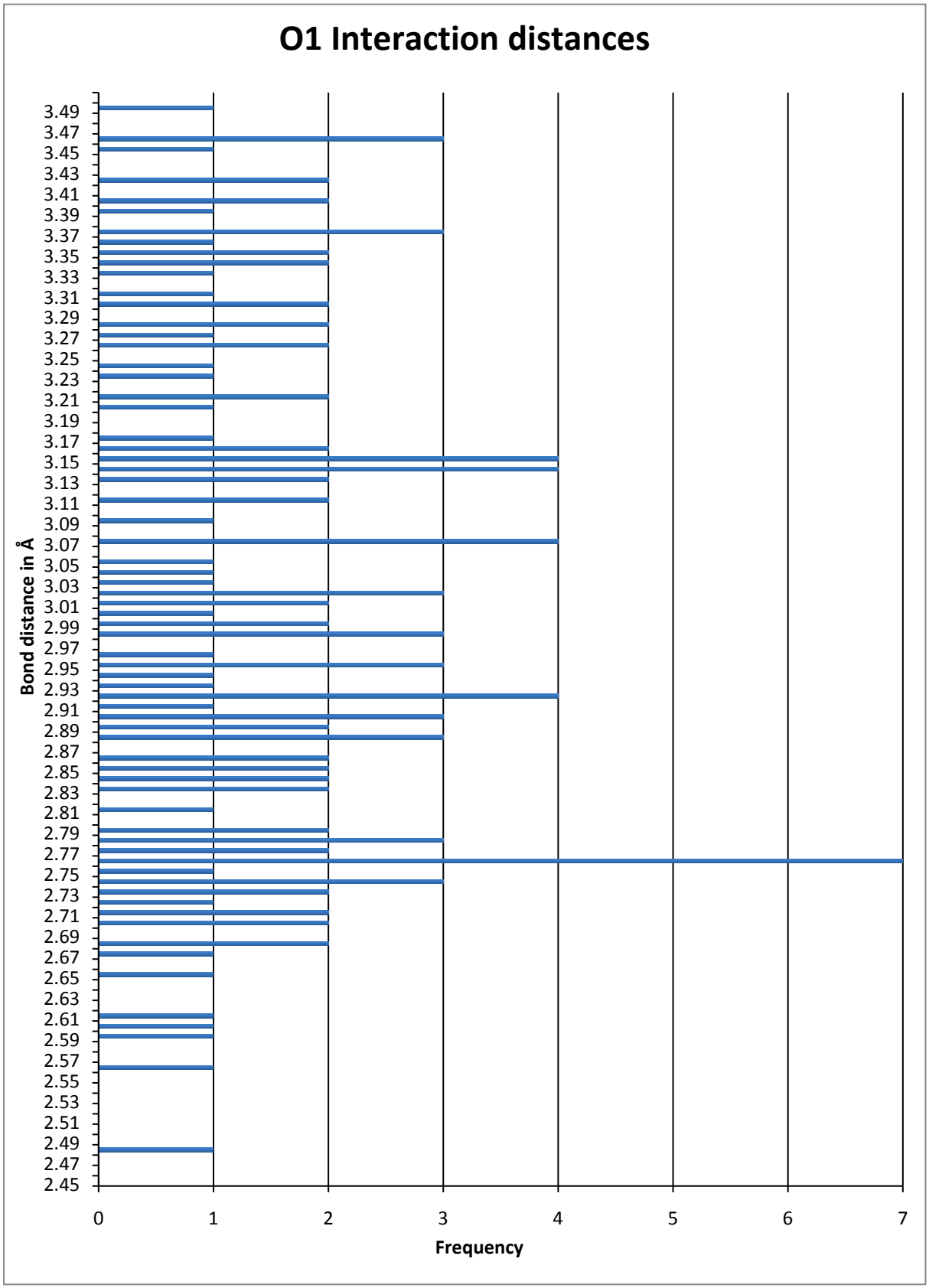
Compound **6i** SFC-MS

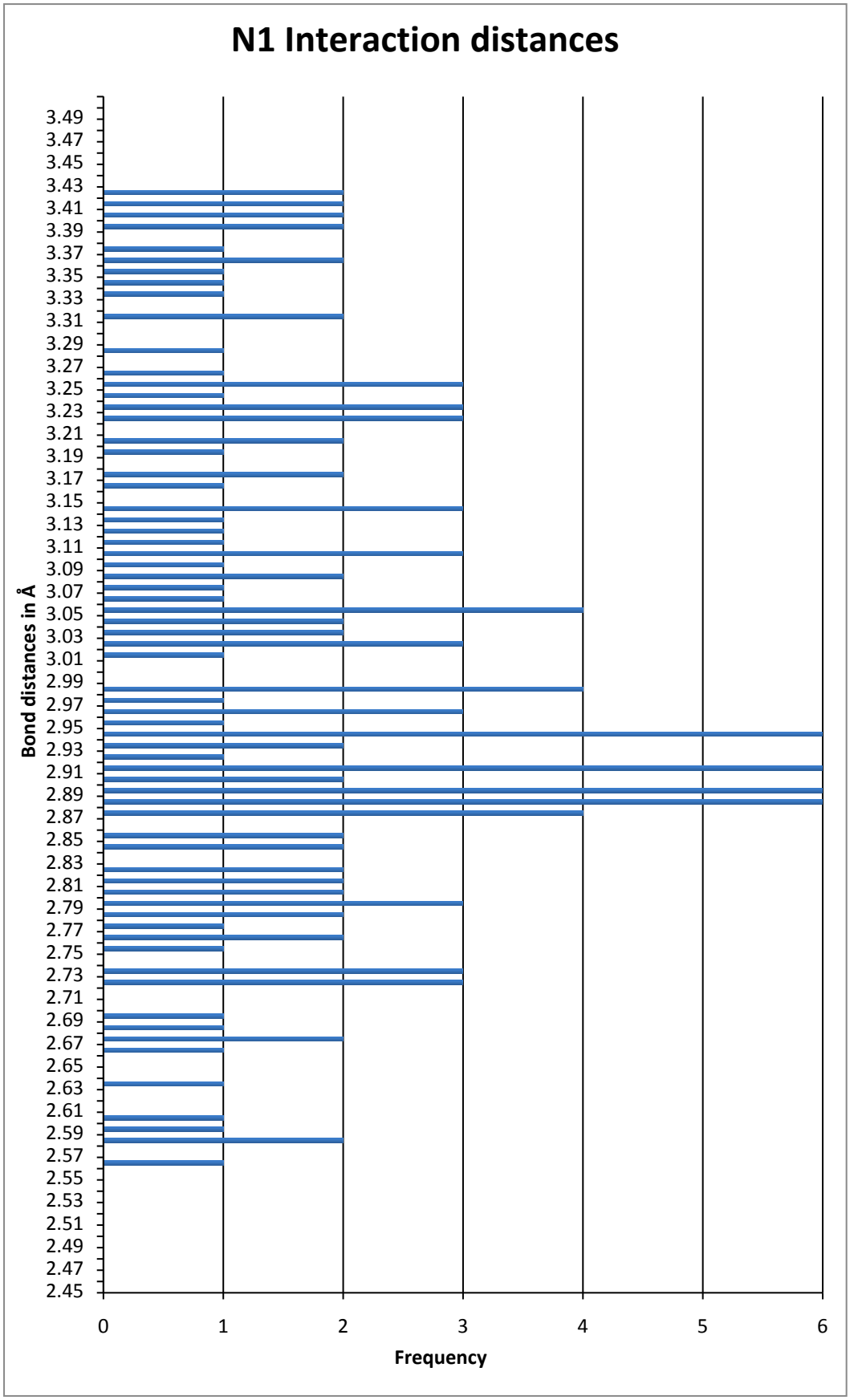


Compound **6j** SFC-MS



PDB Analysis – Interaction distances of gamma lactams found in the PDB database




N1 Interaction distances
Bond distances in Å
3.49
3.47
3.45
3.43
3.41
3.39
3.37
3.35
3.33
3.31
3.29
3.27
3.25
3.23
3.21
3.19
3.17
3.15
3.13
3.11
3.09
3.07
3.05
3.03
3.01
2.99
2.97
2.95
2.93
2.91
2.89
2.87
2.85
2.83
2.81
2.79
2.77
2.75
2.73
2.71
2.69
2.67
2.65
2.63
2.61
2.59
2.57
2.55
2.53
2.51
2.49
2.47
2.45
0
1
2
3
4
5
6
Frequency