Concise Synthesis of Tetrazole Macrocycle

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Supporting Information

Contents

General methods

Nuclear magnetic resonance spectra were recorded on a Bruker Avance 500 spectrometer (^{1}H NMR (500 MHz), ^{13}C NMR (126 MHz)}. Chemical shifts for ^{1}H NMR were reported as δ values and coupling constants were in hertz (Hz); The following abbreviations were used for spin multiplicity: s = singlet, bs = broad singlet, d = doublet, t = triplet, q = quartet, quin = quintet, dd = double of doublets, ddd = double of doublet of doublets, m = multiplet. Chemical shifts for 13C NMR reported in ppm relative to the solvent peak. Thin layer chromatography was performed on Fluka precoated silica gel plates (0.20 mm thick, particle size 25 µm); Flash chromatography was performed on a Teledyne ISCO Combiflash Rf, using RediSep Rf Normal-phase Silica Flash Columns (Silica Gel 60 Å, 230 - 400 mesh) and on a Reveleris® X2 Flash Chromatography, using Grace® Reveleris Silica flash cartridges (12 grams); Reagents were available from commercial suppliers (Sigma Aldrich, ABCR, Acros and AK Scientific) and used without any purification unless otherwise noted. All microwave irradiation reactions were carried out in a Biotage Initiator™ Microwave Synthesizer. Electrospray ionization mass spectra (ESI-MS) were recorded on a Waters Investigator Semi-prep 15 SFC-MS instrument. High resolution mass spectra were recorded using a LTQ-Orbitrap-XL (Thermo) at a resolution of 60000@m/z400.

General Experimental Procedures:

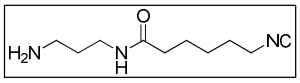
Procedure A: Procedure for synthesis of α-isocyano-ω-amine:

In a round bottom flask the diamine (1.2 eq.) and the α-isocyano-ω-methylester (1 eq.) were added to 1,4-dioxane (0.1M); The reaction mixture was stirred overnight at room temperature. The solvent was removed under reduced pressure and the residue was purified by column chromatography (manual column, 0-100 % AB; A 1:1 mixture of ethylacetate:dichloromethane B: methanol containing 10% conc. aq. ammonia. Silica particle size 60-200 µm).

Procedure B: Procedure for the macrocyclisation reactions:

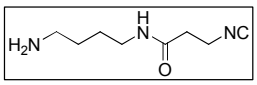
α-isocyano-ω-amine (1.0 mmol), aldehyde (1.2 mmol) and trimethylsilyl azide (1.2 mmol) were stirred at room temperature in MeOH (0.01 M, 100 mL) for 24 h. Under nitrogen, the solvent volume was reduced to 50 mL and the mixture was stirred for an additional 24 h. The solvent was removed under reduced pressure and the residue was purified using flash chromatography (DCM : MeOH 9:1).

N-(3-aminopropyl)-6-isocyanohexanamide 3a:



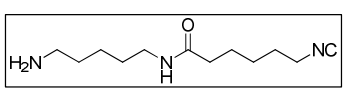
The product was obtained using procedure **A**, 60%, 0.118 g, as oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.62 (bs, 1H), 3.42 – 3.36 (m, 2H), 3.36 – 3.29 (m, 2H), 2.77 (t, *J* = 6.4 Hz, 2H), 2.18 (t, *J* = 7.5 Hz, 2H), 1.72 – 1.59 (m, 6H), 1.51 – 1.42 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.8, 155.6, 50.2, 41.5, 39.8, 37.7, 36.3, 32.2, 28.8, 25.9.

N-(4-aminobutyl)-3-isocyanopropanamide 3b:



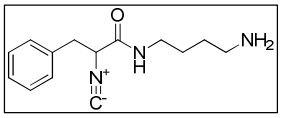
The product was obtained using procedure **A**, 55%, 0.093 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 3.78 (t, *J* = 6.3 Hz, 2H), 3.26 (t, *J* = 6.5 Hz, 2H), 2.73 (t, *J* = 6.5 Hz,, 2H), 2.66 – 2.51 (m, 2H), 1.64 – 1.51 (m, 4H); ^{13}C NMR (126 MHz, CD_3OD) δ 171.6, 156.8, 42.0, 40.3, 39.1, 36.7, 30.3, 27.9.

N-(5-aminopentyl)-6-isocyanohexanamide 3c:



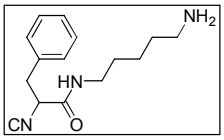
The product was obtained using procedure **A**, 65%, 0.146 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 5.81 (s, 1H), 3.45 – 3.37 (m, 2H), 3.25 (t, *J* = 7.1, 5.7 Hz, 2H), 2.70 (t, *J* = 6.9 Hz, 2H), 2.19 (t, *J* = 7.4 Hz, 2H), 1.75 – 1.63 (m, 4H), 1.55 – 1.44 (m, 6H), 1.41 – 1.32 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.5, 155.7, 41.9, 41.4, 39.4, 36.3, 33.1, 29.4, 28.8, 26.0, 24.7, 24.1.

N-(4-aminobutyl)-2-isocyano-3-phenylpropanamide 3d:



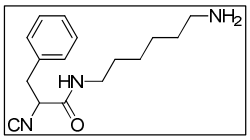
The product was obtained using procedure **A**, 42%, 0.103 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.38 – 7.34 (m, 2H), 7.33 – 7.29 (m, 3H), 3.26 – 3.12 (m, 5H), 2.62 (t, *J* = 7.1 Hz, 2H), 1.53 – 1.44 (m, 2H), 1.43 – 1.35 (m, 2H); ^{13}C NMR (126 MHz, CD_3OD) δ 166.4, 158.6, 135.2, 129.2, 128.3, 127.2, 58.9, 40.7, 39.2, 38.9, 29.5, 26.1.

N-(5-aminopentyl)-2-isocyano-3-phenylpropanamide 3e:



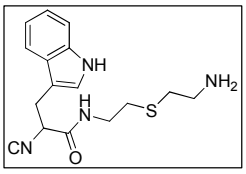
The product was obtained using procedure **A**, 48%, 0.124 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.46 – 7.18 (m, 5H), 3.38 (d, *J* = 1.3 Hz, 1H), 3.25 – 3.13 (m, 4H), 2.65 (t, *J* = 7.0 Hz, 2H), 1.55 – 1.41 (m, 4H), 1.34 – 1.21 (m, 2H);); ^{13}C NMR (126 MHz, CD_3OD) δ 166.3, 158.7, 135.1, 129.2, 128.3, 127.1, 58.5, 40.9, 39.3, 38.9, 31.7, 28.5, 23.7.

N-(6-aminohexyl)-2-isocyano-3-phenylpropanamide 3f:



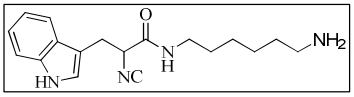
The product was obtained using procedure **A**, 56%, 0.153 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.42 – 7.23 (m, 5H), 3.34 (t, *J* = 1.7 Hz, 1H), 3.28 – 3.09 (m, 4H), 2.67 (t, *J* = 7.2 Hz, 2H), 1.57 – 1.41 (m, 4H), 1.40-1.31 (m, 2H), 1.30-1.23 (m, 2H); ^{13}C NMR (126 MHz, CD_3OD) δ 166.3, 158.7, 135.1, 129.1, 128.3, 127.1, 58.3, 40.9, 39.3, 38.9, 31.7, 28.7, 23.3.

N-(2-((2-aminoethyl)thio)ethyl)-3-(1H-indol-3-yl)-2-isocyanopropanamide 3g:



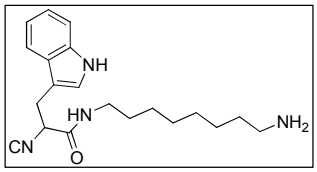
The product was obtained using procedure **A**, 49%, 0.155 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.58 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.20 (s, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 4.56 (t, *J* = 6.6 Hz, 1H), 3.40 – 3.35 (m, 2H), 3.32 (p, *J* = 1.6 Hz, 1H), 3.29 – 3.18 (m, 2H), 2.72 (t, *J* = 6.6 Hz, 2H), 2.51 (t, *J* = 6.6 Hz, 2H), 2.32 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (126 MHz, CD_3OD) δ 168.4, 159.8, 137.9, 128.5, 125.3, 122.6, 120.0, 119.9, 112.4, 109.1, 59.8, 41.5, 40.4, 35.0, 31.1, 30.8.

N-(6-aminohexyl)-3-(1H-indol-3-yl)-2-isocyanopropanamide 3h:



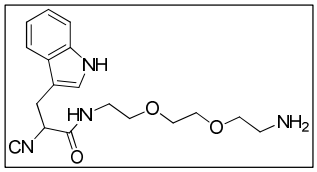
The product was obtained using procedure **A**, 56%, 0.175 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.59 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.18 (s, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 4.54 (t, *J* = 6.9 Hz, 1H), 3.45 – 3.30 (m, 3H), 3.16 – 3.00 (m, 2H), 2.59 (t, *J* = 7.3 Hz, 1H), 1.45 – 1.32 (m, 2H), 1.34 – 1.17 (m, 4H), 1.15 – 1.04 (m, 2H); ^{13}C NMR (126 MHz, CD_3OD) δ 168.7, 159.9, 138.5, 128.9, 125.8, 123.1, 120.5, 119.8, 112.9, 109.7, 59.8, 42.8, 41.2, 33.7, 31.4, 30.3, 28.0.

N-(8-aminooctyl)-3-(1H-indol-3-yl)-2-isocyanopropanamide 3i:



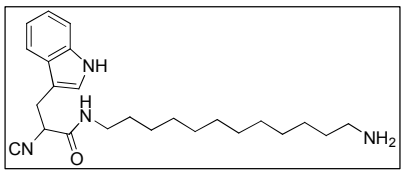
The product was obtained using procedure **A**, 56%, 0.190 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.58 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.17 (s, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 4.52 (t, *J* = 7.0 Hz, 1H), 3.45 – 3.28 (m, 2H), 3.18 – 2.98 (m, 2H), 2.60 (t, *J* = 7.3 Hz, 2H), 1.50 – 1.37 (m, 2H), 1.36 – 1.14 (m, 8H), 1.15 – 1.03 (m, 2H); ^{13}C NMR (126 MHz, CD_3OD) δ 168.2, 159.3, 137.9, 128.4, 125.1, 122.5, 120.0, 119.2, 112.4, 109.0, 59.5, 42.4, 40.7, 33.5, 30.9, 30.3, 30.2, 29.8, 27.8, 27.6.

N-(2-(2-(2-aminoethoxy)ethoxy)ethyl)-3-(1H-indol-3-yl)-2-isocyanopropanamide 3j:



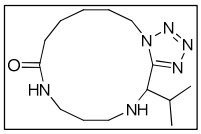
The product was obtained using procedure **A**, 54%, 0.186 g, as oil; ^{1}H NMR (500 MHz, CD_3OD) δ 7.59 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.19 (s, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 4.57 (t, *J* = 6.6 Hz, 1H), 3.52 – 3.48 (m, 2H), 3.45 (t, *J* = 5.3 Hz, 2H), 3.43 – 3.40 (m, 2H), 3.40 – 3.36 (m, 2H), 3.32 – 3.30 (m, 2H), 3.30 – 3.26 (m, 2H), 2.75 (t, *J* = 5.3 Hz, 2H); ^{13}C NMR (126 MHz, CD_3OD) δ 167.1, 158.2, 136.8, 127.1, 124.0, 121.2, 118.6, 117.9, 111.0, 107.8, 71.7, 69.8, 69.8, 68.7, 40.6, 39.3, 29.4.

N-(12-aminododecyl)-3-(1H-indol-3-yl)-2-isocyanopropanamide 3k:



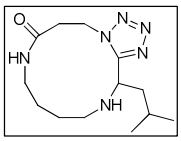
The product was obtained using procedure **A**, 54%, 0.214 g, as oil. ^{1}H NMR (500 MHz, CD_3OD) δ 7.61 (d, *J* = 8.0, 1.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.20 (s, 1H), 7.13 (t, *J* = 7.5 Hz , 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 4.55 (t, *J* = 7.0 Hz, 1H), 3.44 – 3.38 (m, 2H), 3.20 – 3.02 (m, 2H), 2.73 – 2.65 (m, 2H), 1.52 (t, *J* = 7.1 Hz, 2H), 1.39 – 1.21 (m, 16H), 1.20 – 1.07 (m, 2H);^{13}C NMR (126 MHz, CD_3OD) δ 165.3, 156.4, 135.0, 125.5, 122.3, 119.6, 117.1, 116.3, 109.4, 106.3, 64.9, 37.9, 28.0, 27.7, 27.6, 27.5, 27.4, 27.0, 24.8, 17.6, 14.2.

16-Isopropyl-6,7,8,9,11,12,13,14,15,16-decahydrotetrazolo[1,5-a][1,4,8]triazacyclo tetradecin-10(5H)-one 6a:



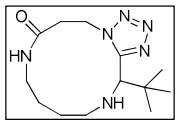
The product was obtained using procedure **B**, 40%, 0.117 g, as white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.38 (t, *J* = 6.1 Hz, 1H), 4.70 – 4.54 (m, 1H), 4.26 – 4.13 (m, 1H), 3.87 (d, *J* = 7.2 Hz, 1H), 3.57 – 3.40 (m, 1H), 3.22 – 3.06 (m, 1H), 2.66 – 2.55 (m, 1H), 2.54 – 2.44 (m, 1H), 2.29 – 2.18 (m, 1H), 2.12 – 1.94 (m, 5H), 1.83 – 1.71 (m, 2H), 1.71 – 1.59 (m, 2H), 1.26 – 1.10 (m, 2H), 1.01 (d, *J* = 6.7 Hz, 3H), 0.83 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.1, 156.4, 59.1, 47.8, 45.2, 37.5, 36.2, 32.5, 28.9, 28.9, 25.5, 24.5, 19.1, 18.9; HRMS calcd for $C_{14}H_{27}N_6O$ $[M+H]^+$: 295.22389, found $[M+H]^+$: 295.22379.

14-Isobutyl-5,6,9,10,11,12,13,14-octahydrotetrazolo[5,1-c][1,4,8]triazacyclododecin-7(8H)-one 6b:



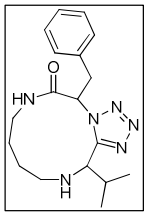
The product was obtained using procedure **B**, 51%, 0.143 g, as oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (s, 1H), 4.86 – 4.73 (m, 1H), 4.63 – 4.51 (m, 1H), 4.38 (t, *J* = 7.6 Hz, 1H), 3.41 – 3.31 (m, 1H), 3.30 – 3.19 (m, 1H), 3.18 – 3.09 (m, 1H), 3.06 – 2.95 (m, 1H), 2.90-2.74 (m, 1H), 2.72-2.60 (m, 1H), 2.52-2.41 (m, 1H), 1.91 – 1.81 (m, 1H), 1.83 – 1.74 (m, 1H), 1.67 – 1.55 (m, 3H), 1.57 – 1.45 (m, 2H), 0.99 (dd, *J* = 6.6, 1.8 Hz, 3H), 0.93 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.2, 155.9, 52.2, 46.6, 43.7, 42.6, 39.2, 36.4, 27.5, 25.4, 25.2, 22.5, 22.4; HRMS calcd for $C_{13}H_{25}N_6O$ $[M+H]^+$: 281.20844, found $[M+H]^+$: 281.20831.

14-(Tert-butyl)-5,6,9,10,11,12,13,14-octahydrotetrazolo[5,1-c][1,4,8]triazacyclododecin-7(8H)-one 6c:



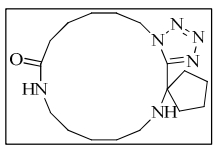
The product was obtained using procedure **B**, 30%, 0.084 g, as oil yellow. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.85 (bs, 1H), 4.95-4.82 (m, 1H), 4.66-4.55 (m, 1H), 4.10-3.92 (m, 1H), 3.72 (s, 1H), 2.91 – 2.81 (m, 2H), 2.77 – 2.63 (m, 1H), 2.51-2.35 (m, 1H), 1.93 (s, 1H), 1.52-1.42 (m, 1H), 1.41-1.25 (m, 3H), 0.95 (s, 9H);^{13}C NMR (126 MHz, $CDCl_3$) δ 170.0, 158.8, 60.7, 48.6, 44.9, 38.0, 37.8, 35.9, 26.3, 25.7, 24.8; HRMS calcd for $C_{13}H_{25}N_6O$ $[M+H]^+$: 281.20844, found $[M+H]^+$: 281.20816.

5-Benzyl-13-isopropyl-8,9,10,11,12,13-hexahydro-5H-tetrazolo[5,1-c][1,4,7]triaza cycloundecin-6(7H)-one 6d:



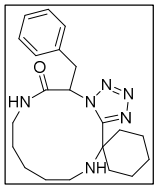
The product was obtained using procedure **B**, 25%, 0.086 g, as oil yellow. diastereomeric ratio: 3:2; ^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer) δ 8.37 (s, 1H), 7.22 -7.15 (m, 5H), 5.02 (dd, *J* = 10.0, 5.3 Hz, 1H), 3.92 – 3.83 (m, 2H), 3.48 – 3.43 (m, 2H), 3.26 – 3.20 (m, 1H), 3.04 – 2.98 (m, 1H), 2.70 – 2.62 (m, 1H 1.85 – 1.74 (m, 4H), 1.28 (s, 2H), 1.05 (d, *J* = 6.7 Hz, 3H), 0.75 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 166.1, 155.0, 136.5, 129.2, , 128.6, 127.0, 64.4, 58.2, 49.0, 39.6, 35.030.7, 28.5, 27.6, 20.5, 19.0, 14.2; HRMS calcd for $C_{18}H_{27}N_6O$ $[M+H]^+$: 343.22409, found $[M+H]^+$: 343.22403.

6',7',8',9',12',13',14',15',16',17'-decahydro-5'H-spiro[cyclopentane-1,18'-tetrazolo[1,5-a][1,4,10]triazacyclohexadecin]-10'(11'H)-one 6e:



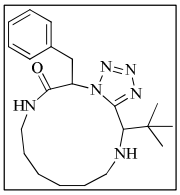
The product was obtained using procedure **B**, 66%, 0.220 g, as oil yellow. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.81 (t, *J* = 5.5 Hz, 1H), 4.55 (t, *J* = 7.1 Hz, 2H), 3.34 (q, *J* = 5.7 Hz, 2H), 2.33 – 2.26 (m, 4H), 2.26 – 2.21 (m, 2H), 2.14 – 2.06 (m, 2H), 2.06 – 1.99 (m, 2H), 1.81 – 1.68 (m, 6H), 1.60 – 1.53 (m, 3H), 1.41 – 1.28 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.9, 158.6, 63.6, 48.7, 44.2, 37.9, 36.6, 35.5, 29.2, 28.4, 27.3, 25.2, 25.0, 24.2, 23.7.

5'-Benzyl-8',9',10',11',12',13'-hexahydro-5'H-spiro[cyclohexane-1,14'-tetrazolo[5,1-c][1,4,7]triazacyclododecin]-6'(7'H)-one 6f:



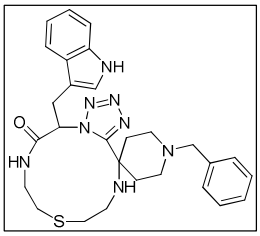
The product was obtained using procedure **B**, 23%, 0.088 g, as oil yellow. Mixture of rotamers is observed; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (bs, 1H), 7.24 – 7.19 (m, 3H), 7.05 – 7.00 (m, 2H), 6.19 – 6.06 (m, 1H), 4.04 – 3.91 (m, 1H), 3.73 – 3.59 (m, 1H), 3.58 – 3.44 (m, 1H), 3.30 (dd, *J* = 13.2, 6.4 Hz, 1H), 2.89 – 2.79 (m, 1H), 2.24 – 2.15 (m, 1H), 1.93 – 1.83 (m, 2H), 1.67 – 1.51 (m, 3H), 1.47 – 1.35 (m, 3H), 1.31 – 1.26 (m, 2H), 1.20 – 1.09 (m, 2H), 0.93 – 0.79 (m, 2H), 0.66 – 0.51 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 155.5, 135.9, 129.3, 128.8, 127.3, 65.9, 60.9, 55.4, 46.8, 44.242.5, 39.1, 36.5, 32.3, 29.9, 29.3, 27.3, 25.1, 24.1, 21.0; HRMS calcd for $C_{21}H_{31}N_6O$ $[M+H]^+$: 383.25539, found $[M+H]^+$: 383.25552.

5-Benzyl-15-(tert-butyl)-8,9,10,11,12,13,14,15-octahydro-5H-tetrazolo[5,1-c][1,4,7] triazacyclotridecin-6(7H)-one 6g:



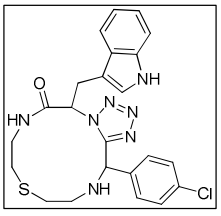
The product was obtained using procedure **B**, 28%, 0.107 g, as oil yellow, diastereomeric ratio: 19:1;^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer) δ 7.35 – 7.31 (m, 2H), 7.29 – 7.26 (m, 2H), 7.24 – 7.20 (m, 1H), 6.43 (d, *J* = 9.7 Hz, 1H), 6.01 – 5.93 (m, 1H), 4.50 – 4.40 (m, 1H), 4.22 – 4.14 (m, 1H), 3.72 – 3.62 (m, 1H), 3.46 – 3.36 (m, 1H), 2.87 – 2.70 (m, 1H), 2.45 – 2.34 (m, 1H), 2.25 – 2.13 (m, 1H), 2.07 – 1.96 (m, 1H), 1.70 – 1.61 (m, 3H), 1.52 – 1.41 (m, 2H), 1.33 – 1.23 (m, 3H), 0.83 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 174.7, 154.8, 135.8, 129.4, 128.7, 127.2, 70.7, 48.2, 45.5, 43.1, 39.4, 34.6, 28.0, 26.8, 26.4, 23.3, 22.7; HRMS calcd for $C_{21}H_{33}N_6O$ $[M+H]^+$: 385.27104, found $[M+H]^+$: 385.27109.

5'-((1H-indol-3-yl)methyl)-1-benzyl-8',9',12',13'-tetrahydro-5'H,11'H-spiro[piperidine-4,14'-tetrazolo[5,1-f][1]thia[4,7,10]triazacyclododecin]-6'(7'H)-one 6h:



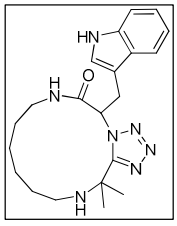
The product was obtained using procedure **B**, 53%, 0.281 g, as white solid.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 – 7.92 (m, 1H), 7.53 – 7.45 (m, 2H), 7.32 – 7.26 (m, 3H), 7.21 – 7.15 (m, 1H), 7.12 (d, *J* = 7.0 Hz, 2H), 7.09 – 7.03 (m, 2H), 6.74 (d, *J* = 2.3 Hz, 1H), 5.64 (dd, *J* = 11.9, 3.8 Hz, 1H), 4.03 (dd, *J* = 15.1, 11.9 Hz, 1H), 3.75 (dd, *J* = 15.1, 3.8 Hz, 1H), 3.72 – 3.58 (m, 1H), 3.28 – 3.15 (m, 2H), 3.11 – 3.01 (m, 2H), 2.99 – 2.89 (m, 1H), 2.88 – 2.79 (m, 2H), 2.63 – 2.51 (m, 1H), 2.48 – 2.29 (m, 2H), 2.20 – 2.08 (m, 1H), 1.80 – 1.72 (m, 1H), 1.67 – 1.53 (m, 2H), 1.43 – 1.23 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.5, 156.6, 137.8, 136.1, 129.1, 128.2, 127.1, 126.6, 123.9, 122.3, 119.9, 117.8, 111.5, 109.3, 63.2, 62.5, 54.3, 50.1, 48.0, 39.5, 39.4, 36.3, 33.8, 31.4, 27.0; HRMS calcd for $C_{28}H_{35}N_8OS$ $[M+H]^+$: 531.2649, found $[M+H]^+$: 531.26447.

5-((1H-indol-3-yl)methyl)-14-(4-chlorophenyl)-8,9,11,12,13,14-hexahydro-5H-tetrazolo [5,1-f][1]thia[4,7,10]triazacyclododecin-6(7H)-one 6i:



The product was obtained using procedure **B**, 27%, 0.129 g, as white solid, diastereomeric ratio: 25:1; ^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer) δ 7.87 (d, *J* = 10.5 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.34 – 7.27 (m, 3H), 7.23 – 7.16 (m, 3H), 5.26 (dd, *J* = 9.4, 2.9 Hz, 1H), 4.33 – 4.20 (m, 1H), 3.32 – 3.25 (m, 1H), 3.11 (s, 1H), 2.94 (dd, *J* = 14.3, 2.9 Hz, 1H), 2.86 – 2.72 (m, 2H), 2.70 – 2.63 (m, 1H), 2.55 – 2.45 (m, 1H), 2.35 – 2.22 (m, 2H), 2.25 – 2.13 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 178.8, 171.9, 156.3, 137.5, 136.9, 134.1, 129.4, 129.1, 127.1, 123.1, 121.8, 106.9, 75.7, 74.5, 58.9, 46.1, 36.6, 34.1, 33.7, 30.5; HRMS calcd for $C_{23}H_{25}N_7OClS$ $[M+H]^+$: 482.15243, found $[M+H]^+$: 482.1525.

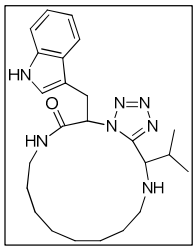
5-((1H-indol-3-yl)methyl)-15,15-dimethyl-8,9,10,11,12,13,14,15-octahydro-5H-tetrazolo[5,1-c][1,4,7]triazacyclotridecin-6(7H)-one 6j:



The product was obtained using procedure **B**, 21%, 0.083 g, as white solid.^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.9 Hz, 1H),

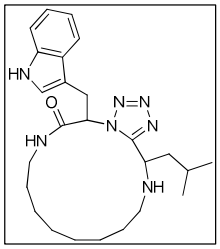
7.24 – 7.17 (m, 1H), 7.18 – 7.11 (m, 1H), 6.99 (d, *J* = 2.4 Hz, 1H), 6.01 – 5.84 (m, 1H), 4.13 – 3.98 (m, 1H), 3.98 – 3.85 (m, 1H), 3.64 – 3.49 (m, 2H), 2.73 – 2.57 (m, 1H), 2.32 – 2.20 (m, 1H), 2.18 – 2.04 (m, 1H), 2.00 – 1.88 (m, 1H), 1.33 (s, 3H), 1.31 – 1.24 (m, 2H), 1.20 (s, 5H), 1.18 – 1.07 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.2, 154.9, 136.0, 127.2, 123.3, 122.4, 120.0, 118.5, 111.2, 110.0, 59.3, 47.3, 44.4, 41.6, 29.8, 27.6, 24.5, 23.7, 22.2; HRMS calcd for $C_{21}H_{30}N_7O$ $[M+H]^+$: 396.25064, found $[M+H]^+$: 396.25037.

5-((1H-indol-3-yl)methyl)-17-isopropyl-8,9,10,11,12,13,14,15,16,17-decahydro-5H-tetrazolo[5,1-c][1,4,7]triazacyclopentadecin-6(7H)-one 6k:



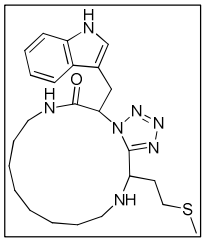
The product was obtained using procedure **B**, 29%, 0.127 g, as white solid; diastereomeric ratio: 25:1; ^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer) δ 8.23 (s, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.28 – 7.13 (m, 2H), 6.99 (bs, 1H), 6.84 (s, 1H), 5.99 – 5.83 (m, 1H), 3.87 – 3.74 (m, 1H), 3.74 – 3.59 (m, 2H), 3.46 (dd, *J* = 13.9, 10.2 Hz, 1H), 2.87 – 2.67 (m, 2H), 2.41 – 2.26 (m, 1H), 1.93 – 1.85 (m, 1H), 1.83 – 1.73 (m, 2H), 1.39 (q, *J* = 6.6 Hz, 2H), 1.35 – 1.27 (m, 2H), 1.23 – 1.15 (m, 4H), 1.12 – 1.05 (m, 3H), 1.01 (d, *J* = 6.7 Hz, 3H), 0.97 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 174.7, 155.3, 136.1, 126.8, 123.2, 122.5, 120.1, 118.3, 111.4, 109.6, 68.9, 47.93, 46.8, 44.0, 31.8, 28.3, 26.6, 26.4, 24.5, 24.2, 19.4, 18.9; HRMS calcd for $C_{24}H_{36}N_7O$ $[M+H]^+$: 438.29759, found $[M+H]^+$: 438.29721.

5-((1H-indol-3-yl)methyl)-17-isobutyl-8,9,10,11,12,13,14,15,16,17-decahydro-5H-tetrazolo[5,1-c][1,4,7]triazacyclopentadecin-6(7H)-one 6l:



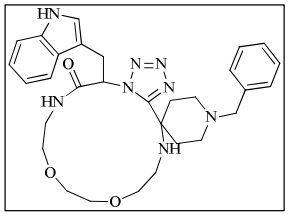
The product was obtained using procedure B, 32%, 0.144 g, as white solid; diastereomeric ratio: 25:1; ^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer)δ 8.04 (d, *J* = 3.3 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.41 – 7.34 (m, 1H), 7.27 – 7.16 (m, 2H), 6.92 (s, 1H), 6.84 (d, *J* = 2.3 Hz, 1H), 5.92 – 5.76 (m, 1H), 3.85 – 3.74 (m, 1H), 3.72 – 3.60 (m, 2H), 3.41 (dd, *J* = 13.9, 10.1 Hz, 1H), 3.11 (s, 1H), 2.64 – 2.55 (m, 1H), 2.38 – 2.24 (m, 2H), 1.85 – 1.74 (m, 2H), 1.72 – 1.65 (m, 1H), 1.51 – 1.43 (m, 2H), 1.38 – 1.28 (m, 3H), 1.21 – 1.07 (m, 5H), 1.03 (d, *J* = 6.6 Hz, 2H), 0.95 (d, *J* = 6.6 Hz, 3H), 0.92 (d, *J* = 6.5 Hz, 3H);^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 175.4, 155.3, 136.1, 126.9, 123.1, 122.5, 120.1, 118.3, 111.3, 109.6, 60.7, 46.9, 46.5, 44.2, 41.9, 31.4, 29.7, 28.126.3, 24.8, 24.2, 22.8, 22.5; HRMS calcd for $C_{25}H_{38}N_7O$ $[M+H]^+$: 452.31324, found $[M+H]^+$: 452.31351.

5-((1H-indol-3-yl)methyl)-17-(2-(methylthio)ethyl)-8,9,10,11,12,13,14,15,16,17-deca hydro-5H-tetrazolo[5,1-c][1,4,7]triazacyclopentadecin-6(7H)-one 6m:



The product was obtained using procedure **B**, 52%, 0.244 g, as white solid, diastereomeric ratio: 25:1; ^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer) δ 8.11 (bs, 1H), 7.98 (d, *J* = 7.3 Hz, 1H), 7.78 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.35 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.26 – 7.11 (m, 2H), 6.80 (d, *J* = 2.4 Hz, 1H), 5.60 – 5.48 (m, 1H), 3.97 – 3.87 (m, 1H), 3.86 – 3.70 (m, 1H), 3.64 – 3.51 (m, 1H), 3.39 (dd, *J* = 13.7, 10.1 Hz, 1H), 3.24 (dd, *J* = 7.6, 5.4 Hz, 1H), 2.80 – 2.66 (m, 1H), 2.68 – 2.50 (m, 2H), 2.41 (dt, *J* = 12.7, 6.4 Hz, 1H), 2.14 (s, 3H), 2.04 – 1.97 (m, 1H), 1.89 – 1.73 (m, 2H), 1.75 – 1.59 (m, 3H), 1.16 – 0.98 (m, 8H), 0.78-0.66 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 175.2, 155.1, 136.0, 127.0, 123.2, 122.4, 120.0, 118.7, 111.2, 110.0, 62.8, 48.0, 47.4, 45.2, 33.2, 31.1, 30.7, 28.3, 27.4, 26.0, 25.9, 24.6, 23.9, 15.5; HRMS calcd for $C_{24}H_{36}N_7OS$ $[M+H]^+$: 470.26966, found $[M+H]^+$: 470.26968.

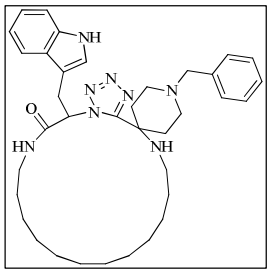
5'-((1H-indol-3-yl)methyl)-1-benzyl-8',9',11',12',15',16'-hexahydro-5'H,14'H-spiro[piperidine-4,17'-tetrazolo[5,1-i][1,4]dioxa[7,10,13]triazacyclopentadecin]-6'(7'H)-one 6n:



The product was obtained using procedure **B**, 36%, 0.201 g, as white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (bs, 1H), 8.00 (d, *J* = 7.1 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.40 – 7.33 (m, 5H), 7.25 –7.17 (m, 1H), 7.16 –7.13 (m, 1H), 6.84 (d, *J* = 2.3 Hz, 1H), 5.75 – 5.64 (m, 1H), 3.97 – 3.87 (m, 1H), 3.76 (dd, *J* = 14.1, 5.5 Hz, 1H), 3.69 – 3.62 (m, 3H), 3.60 – 3.55

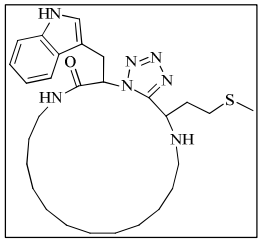
(m, 2H), 3.51 – 3.45 (m, 2H), 3.33 (dd, *J* = 13.9, 9.6 Hz, 1H), 3.30 – 3.20 (m, 3H), 3.20 – 3.13 (m, 1H), 2.86 – 2.76 (m, 1H), 2.76 – 2.69 (m, 1H), 2.66 – 2.56 (m, 2H), 2.40 – 2.30 (m, 2H), 2.13 – 2.00 (m, 1H), 1.86 – 1.77 (m, 1H), 1.75-156 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.5, 156.6, 136.0, 129.2, 128.3, 127.2, 123.1, 122.4, 120.0, 118.7, 118.0, 111.2, 110.4, 71.2, 70.9, 70.1, 68.7, 49.5, 49.2, 47.1, 45.7, 42.5, 31.2; HRMS calcd for $C_{30}H_{39}N_8O_3$ $[M+H]^+$: 559.31396, found $[M+H]^+$: 559.31409.

5'-((1H-indol-3-yl)methyl)-1-benzyl-7',8',9',10',11',12',13',14',15',16',17',18',19',20'-tetradecahydrospiro[piperidine-4,21'-tetrazolo[5,1-c][1,4,7]triazacyclononadecin]-6'(5'H)-one 6o:



The product was obtained using procedure **B**, 48%, 0.293 g, as white solid.^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.16 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.42 (s, 2H), 7.40 – 7.35 (m, 3H), 7.33 (d, *J* = 7.1 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 6.79 (s, 1H), 5.58 – 5.45 (m, 1H), 3.71 – 3.58 (m, 3H), 3.53-3.40 (m, 1H), 3.30-3.17 (m, 1H), 3.12 (dd, *J* = 13.7, 10.2 Hz, 1H), 3.00-2.85 (m, 1H), 2.78-2.67 (m, 1H), 2.50 – 2.32 (m, 3H), 2.12 – 2.01 (m, 2H), 1.52 – 1.38 (m, 3H), 1.30 (t, *J* = 7.1 Hz, 1H), 1.27 – 0.90 (m, 16H), 0.86 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.2, 155.5, 136.1, 128.4, 127.0, 123.1, 122.6, 120.3, 118.4, 111.3, 109.7, 49.4, 49.1, 46.8, 45.3, 42.9, 32.2, 31.0, 29.7, 28.2, 27.2, 26.8, 26.6, 26.4, 25.9, 25.3, 24.0; HRMS calcd for $C_{36}H_{51}N_8O$ $[M+H]^+$: 611.41803, found $[M+H]^+$: 611.41815.

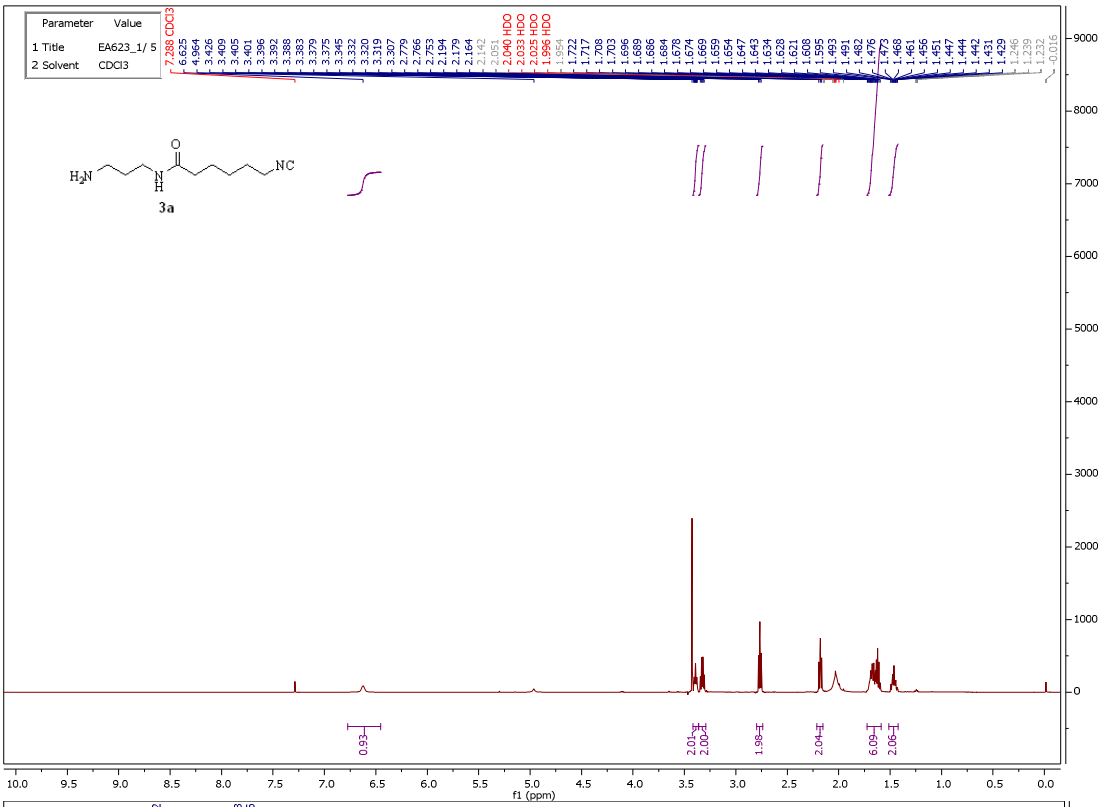
5-((1H-indol-3-yl)methyl)-21-(2-(methylthio)ethyl)-8,9,10,11,12,13,14,15,16,17,18, 19,20,21-tetradecahydro-5H-tetrazolo[5,1-c][1,4,7]triazacyclononadecin-6(7H)-one 6p:

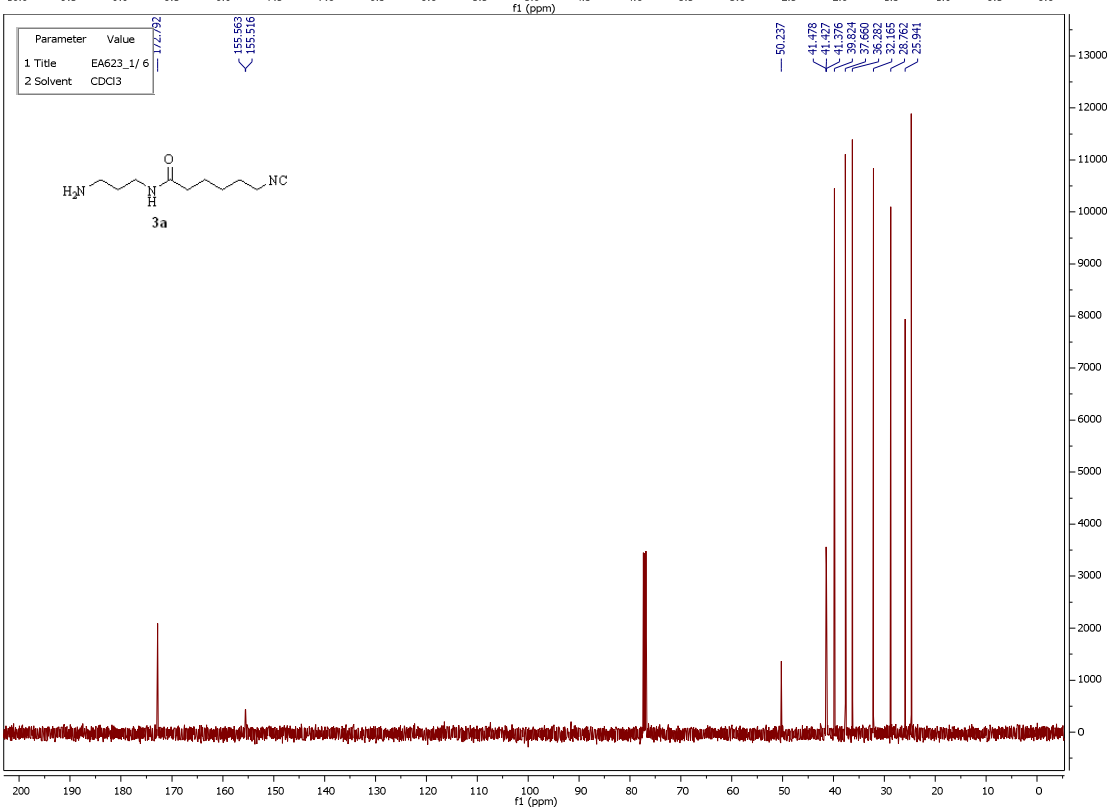


The product was obtained using procedure **B**, 26%, 0.136 g, as white solid, diastereomeric ratio: 3:2; ^{1}H NMR (500 MHz, $CDCl_3$) (Major isomer) δ 8.30 – 8.19 (m, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.34 (dd, *J* = 8.0, 4.4 Hz, 2H), 7.22 – 7.16 (m, 1H), 7.17 – 7.08 (m, 1H), 6.78 (dd, *J* = 5.9, 2.3 Hz, 1H), 5.66 – 5.57 (m, 1H), 3.67 – 3.52 (m, 2H), 3.45 – 3.19 (m, 3H), 2.64 – 2.49 (m, 2H), 2.49 – 2.33 (m, 2H), 2.16 – 2.11 (m, 1H), 2.10 (d, *J* = 1.7 Hz, 2H), 2.00 – 1.86 (m, 2H), 1.82 – 1.68 (m, 1H), 1.56 – 1.43 (m, 1H), 1.43 – 1.31 (m, 1H), 1.23 – 1.18 (m, 3H), 1.17 – 1.01 (m, 10H), 1.01 – 0.80 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) (Major isomer) δ 174.4, 155.4, 136.1, 126.9, 123.1, 120.3, 118.3, 111.4, 109.8, 105.9, 62.0, 48.3, 46.8, 44.9, 32.9, 32.5, 31.9, 30.8, 28.828.6, 27.8, 27.3, 27.0, 26.7, 26.2, 25.4, 24.7, 15.5; HRMS calcd for $C_{28}H_{44}N_7OS$ $[M+H]^+$: 526.33226, found $[M+H]^+$: 526.33179.

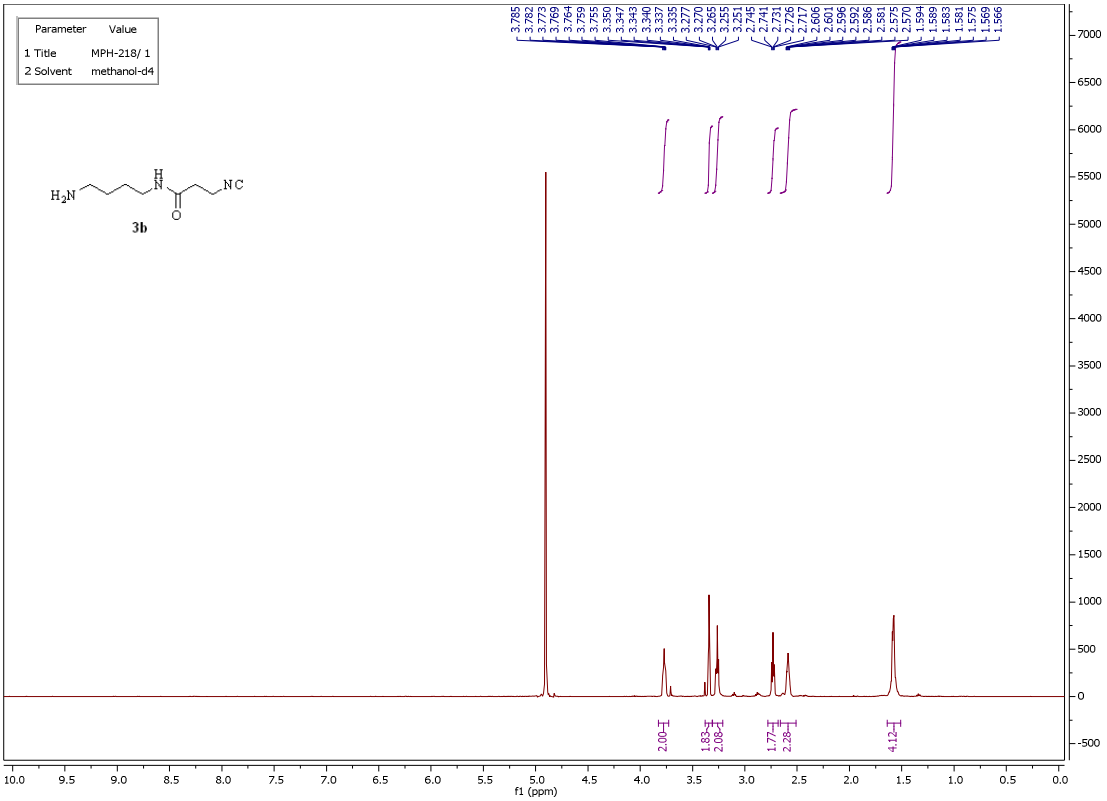
^{1}H, ^{13}C NMR, chromatograms and mass spectra of the novel synthesized compounds:

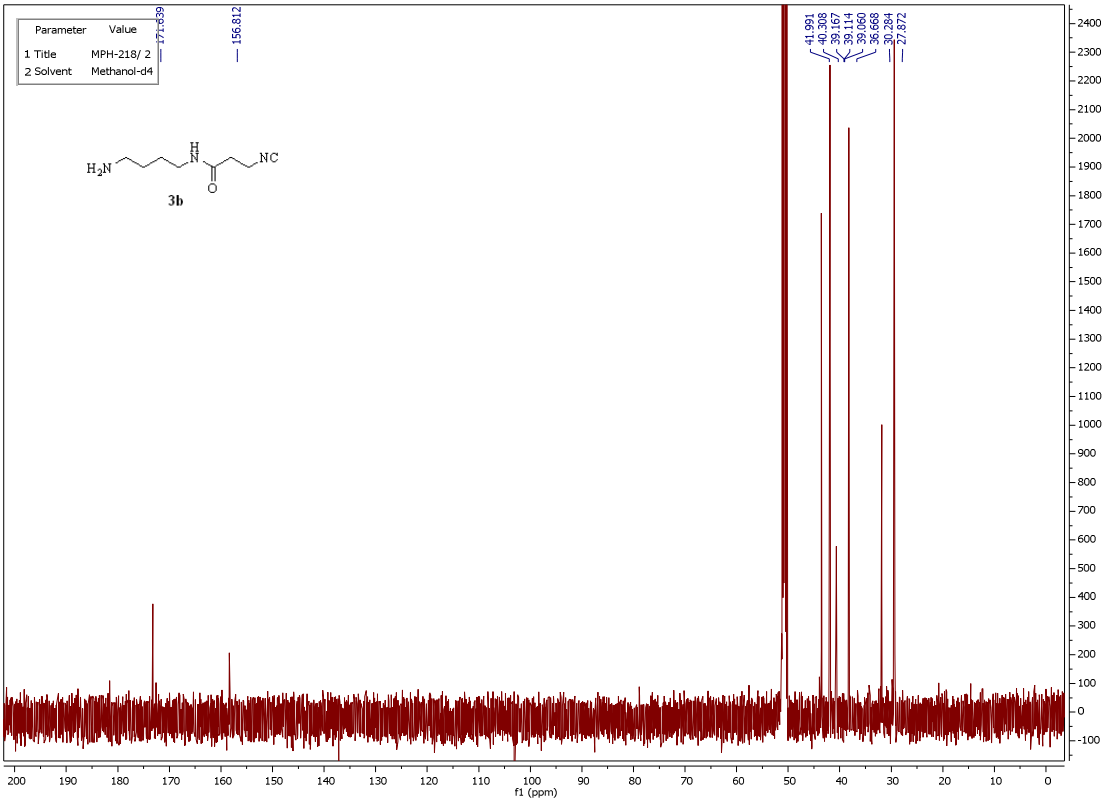
Compound3a:


Parameter Value
1 Title EA623_1/ 5
2 Solvent CDCl3
3a
f1 (ppm)

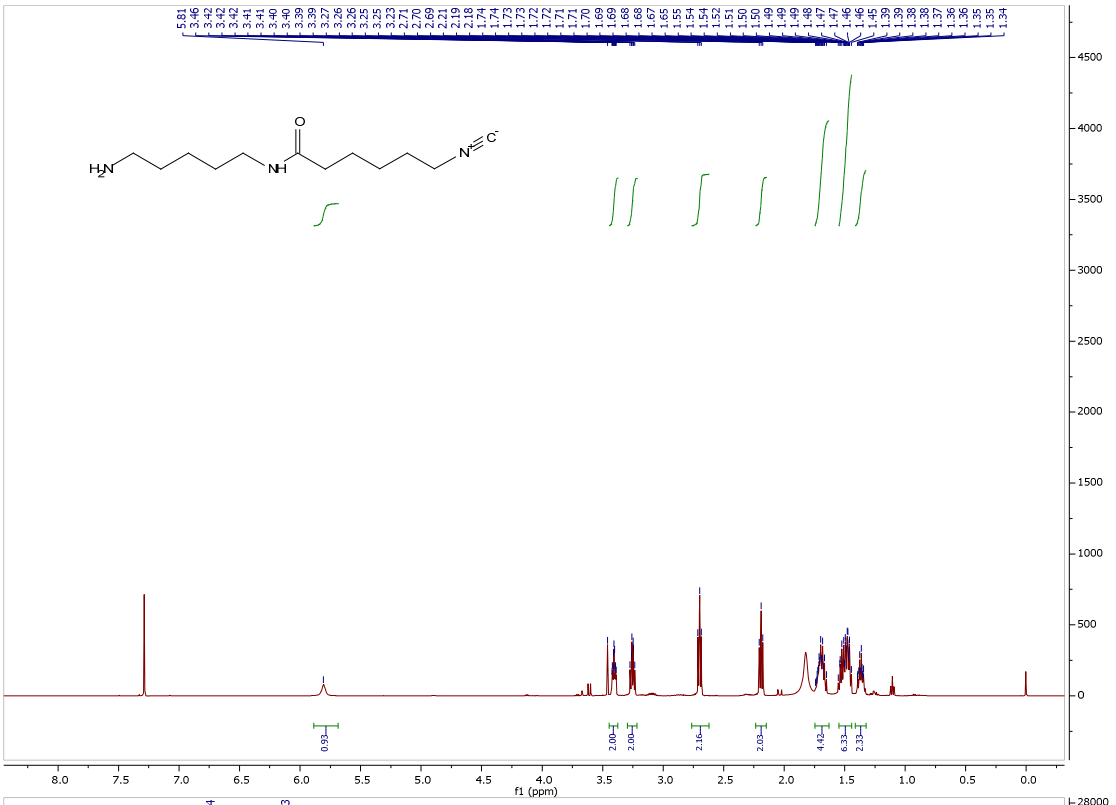

Parameter Value
1 Title EA623_1/ 6
2 Solvent CDCl3
3a
f1 (ppm)

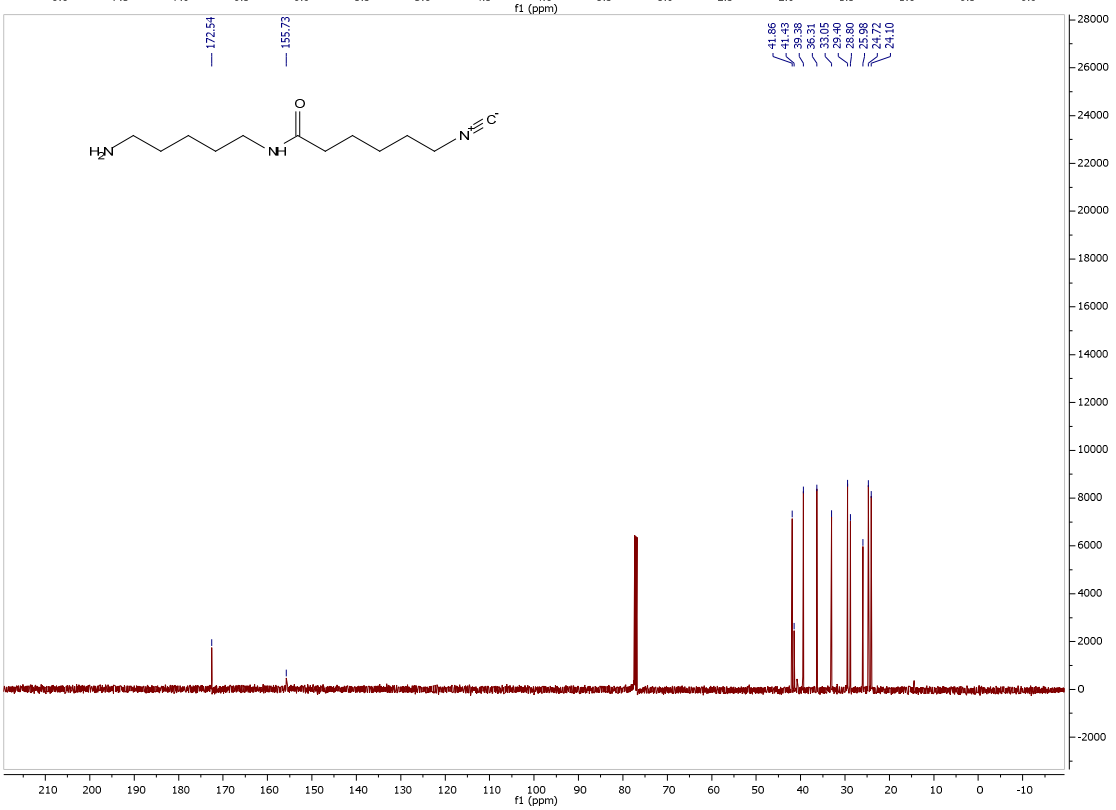
Compound 3b:


Parameter Value
1 Title MPH-218/ 1
2 Solvent methanol-d4
3b
f1 (ppm)

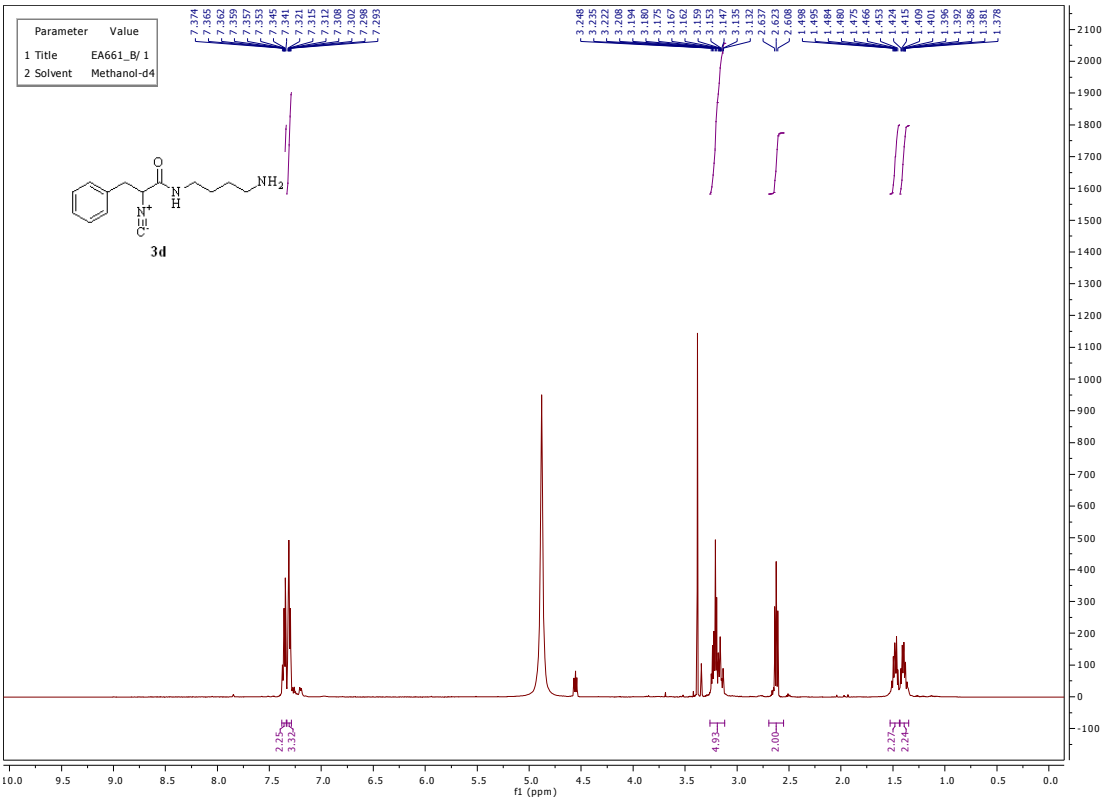

Parameter Value
1 Title MPH-218/ 2
2 Solvent Methanol-d4
171.639
156.812
41.991
40.308
39.167
39.114
39.060
36.668
30.284
27.872
3b
f1 (ppm)

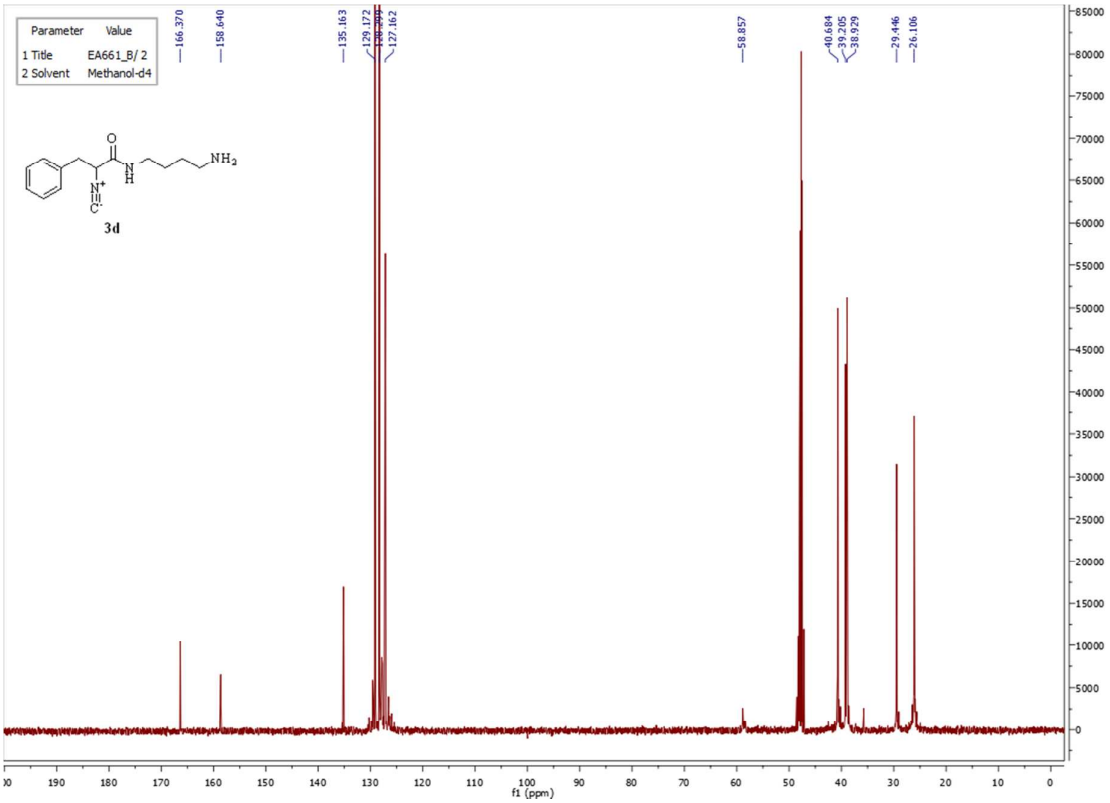
Compound 3c:


5.81
3.46
3.42
3.42
3.42
3.41
3.41
3.40
3.40
3.39
3.39
3.27
3.26
3.26
3.25
3.25
3.23
2.71
2.70
2.69
2.21
2.19
2.18
1.74
1.74
1.73
1.73
1.72
1.72
1.71
1.71
1.70
1.69
1.69
1.68
1.68
1.67
1.65
1.55
1.54
1.54
1.52
1.51
1.50
1.50
1.49
1.49
1.49
1.48
1.47
1.47
1.46
1.46
1.45
1.39
1.39
1.38
1.38
1.37
1.36
1.36
1.35
1.35
1.34
O
NH
N
C
0.93
2.00
2.00
2.16
2.03
4.42
6.33
2.33
f1 (ppm)

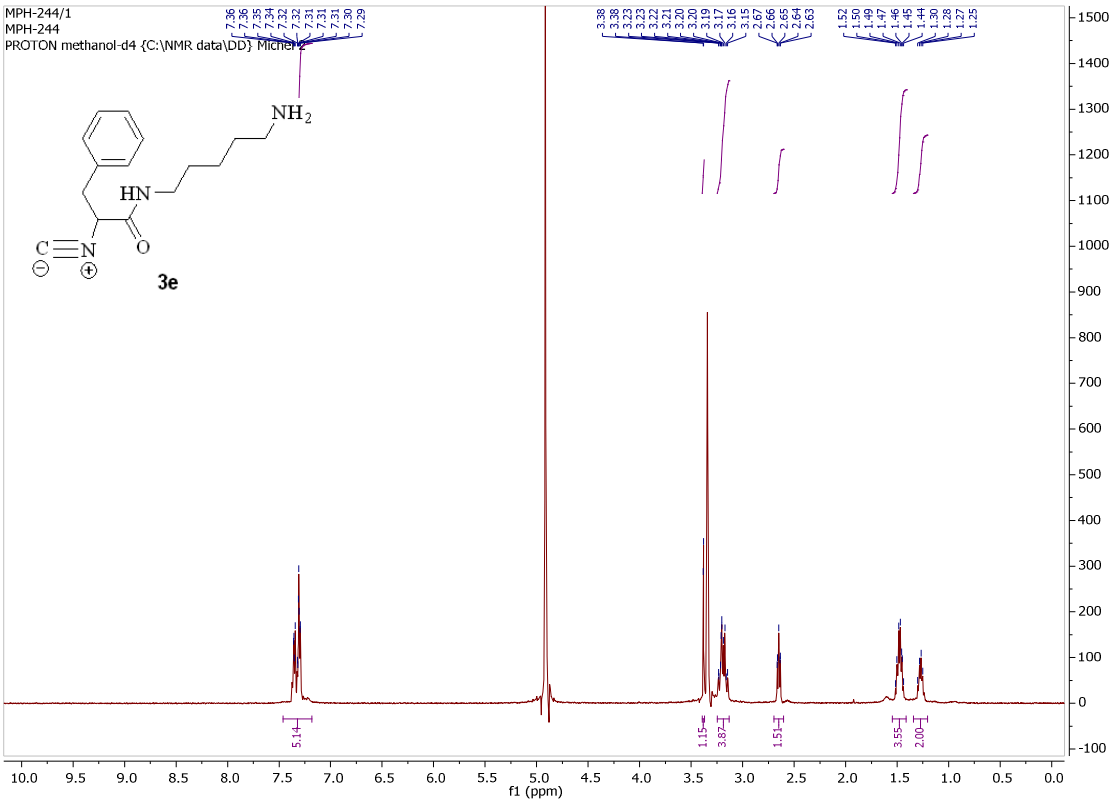

172.54
155.73
41.86
41.43
39.38
36.31
33.05
29.40
28.80
25.58
24.72
24.10
O
NH
N
C
f1 (ppm)

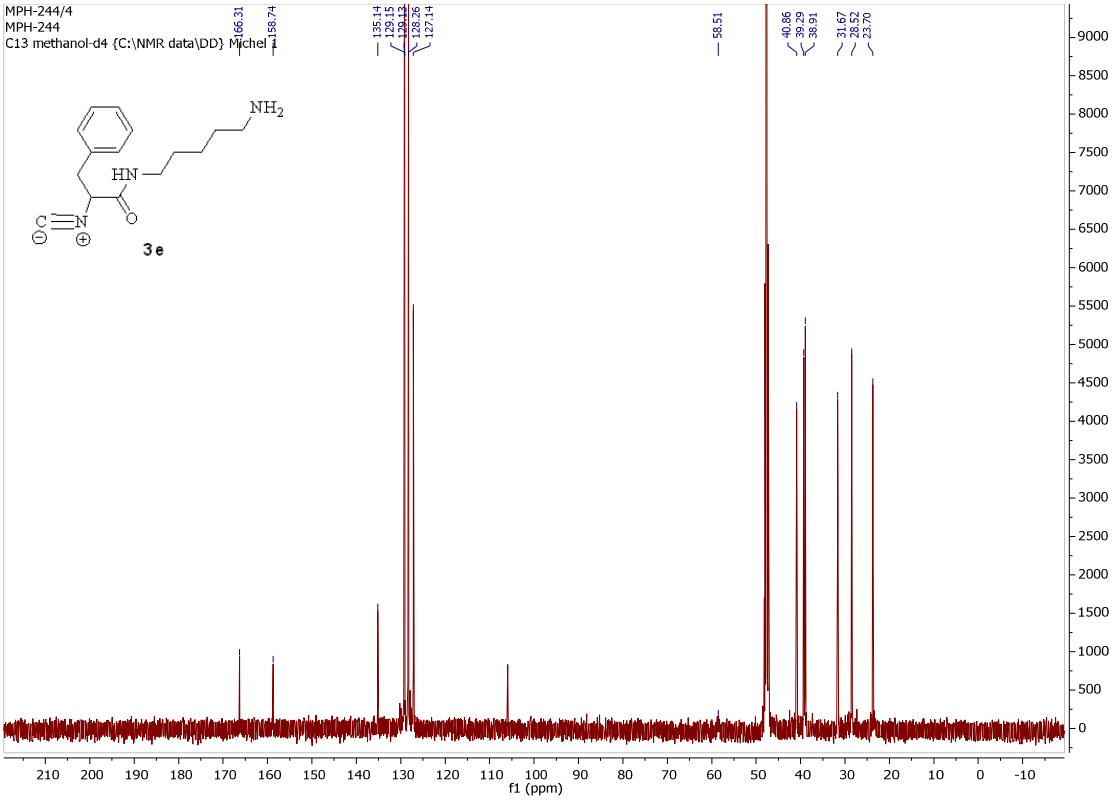
Compound 3d:


Parameter Value
1 Title EA661_B/ 1
2 Solvent Methanol-d4
3d
f1 (ppm)

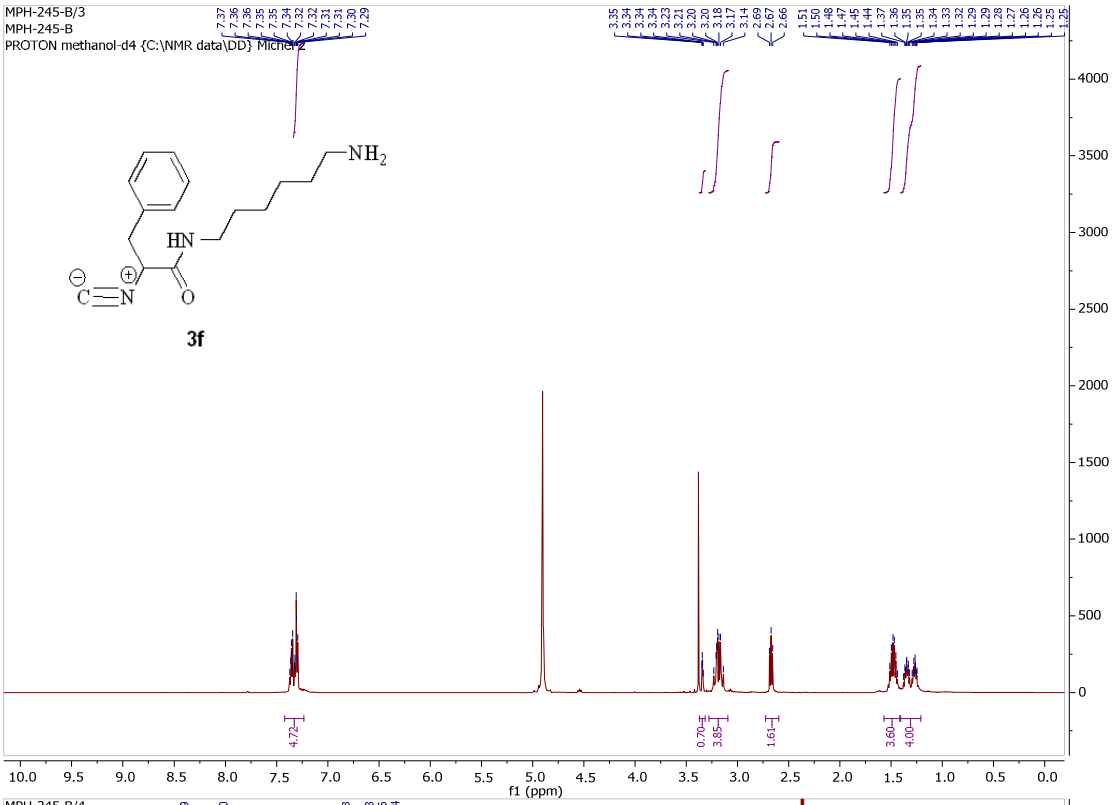

Parameter Value
1 Title EA661_B/ 2
2 Solvent Methanol-d4
3d
f1 (ppm)

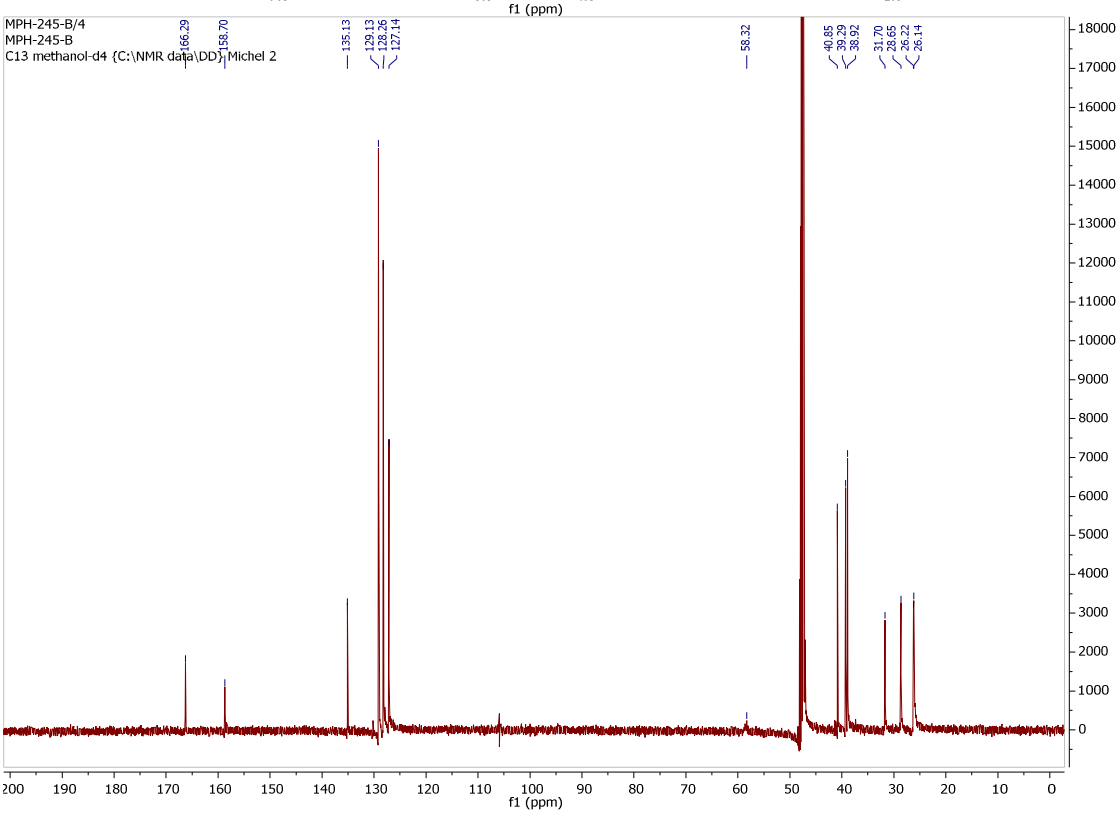
Compound 3e:


MPH-244/1
MPH-244
PROTON methanol-d4 {C:\NMR data\DD} Michel 1
NH2
HN
O
C
N
3e
f1 (ppm)

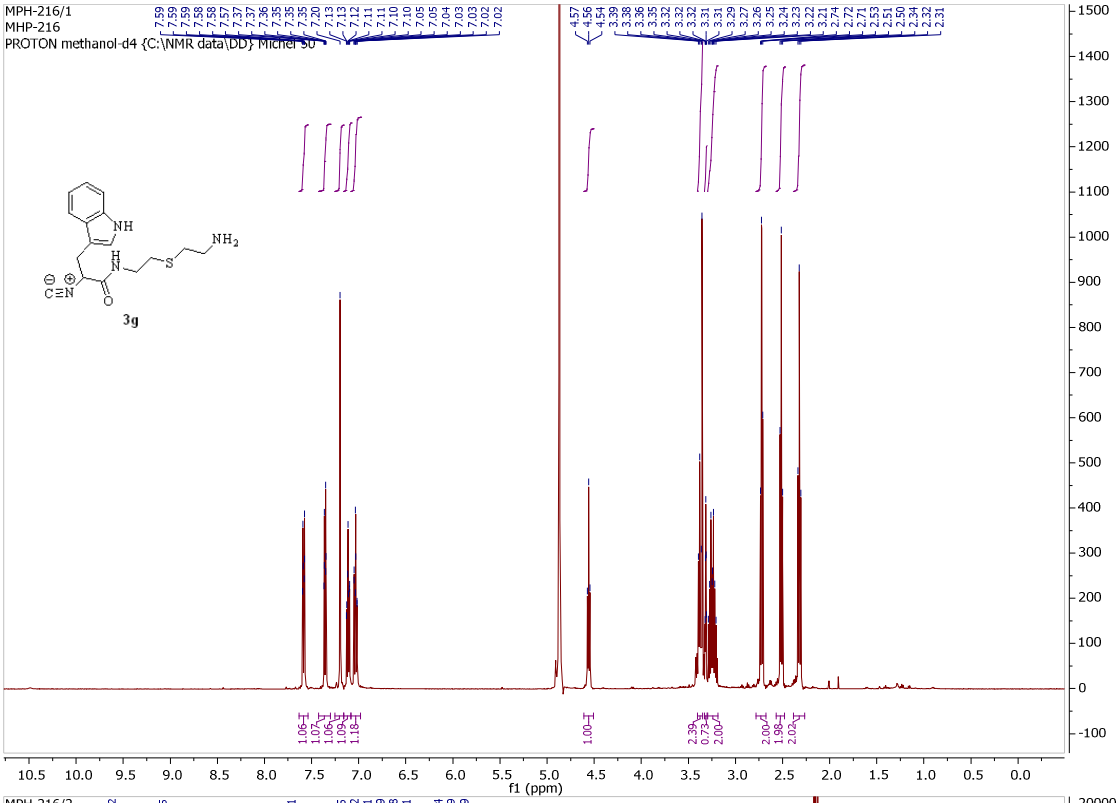

MPH-244/4
MPH-244
C13 methanol-d4 {C:\NMR data\DD} Michel 1
NH2
HN
O
C
N
3 e
f1 (ppm)

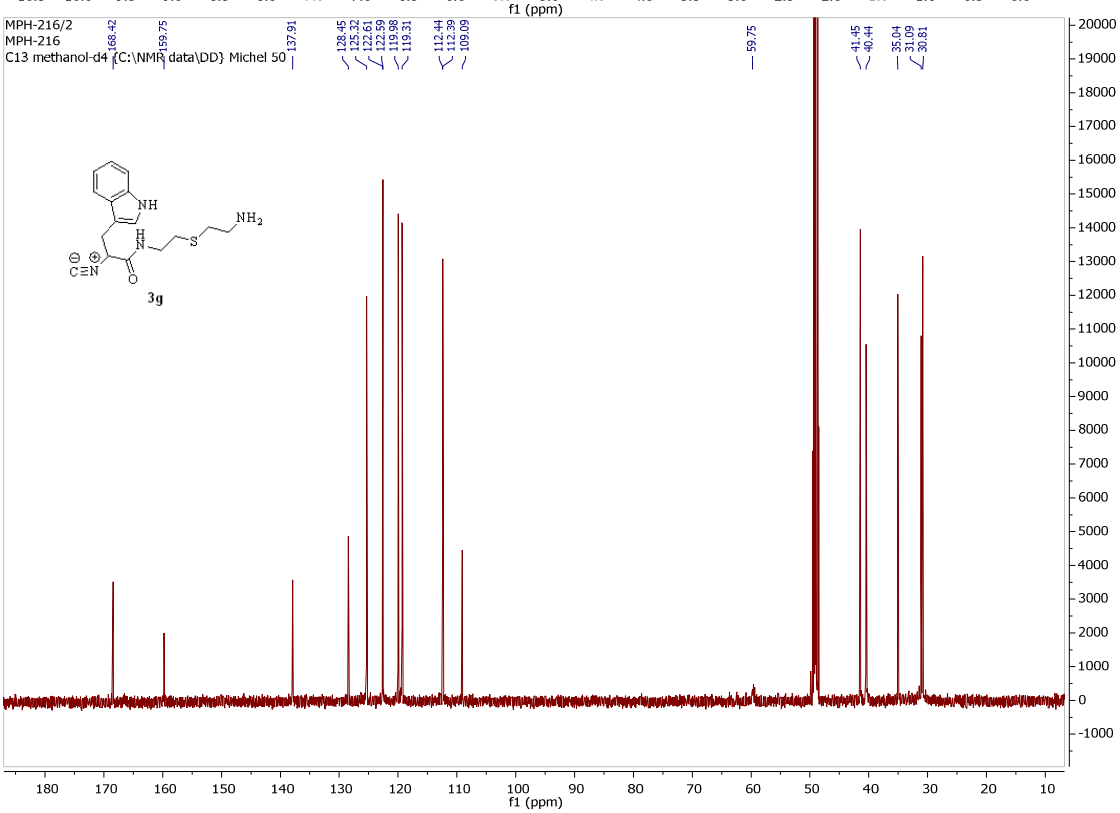
Compound 3f:


MPH-245-B/3
MPH-245-B
PROTON methanol-d4 {C:\NMR data\DD} Michel 2
NH2
HN
C≡N
O
3f
f1 (ppm)

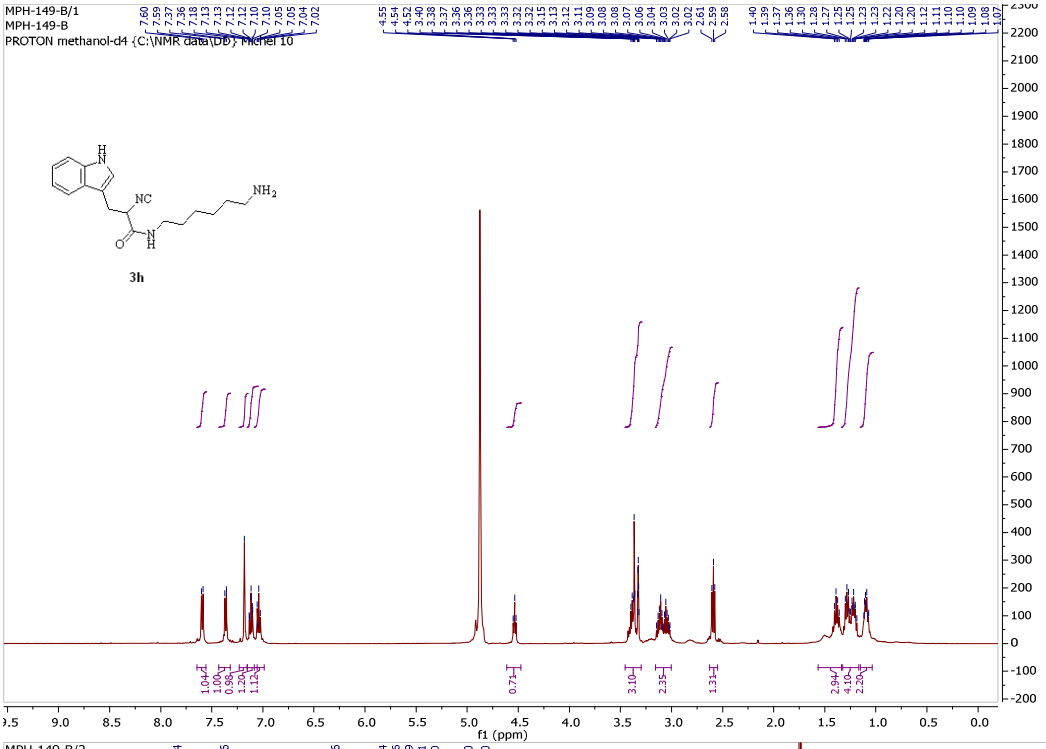

MPH-245-B/4
MPH-245-B
C13 methanol-d4 {C:\NMR data\DD} Michel 2
f1 (ppm)

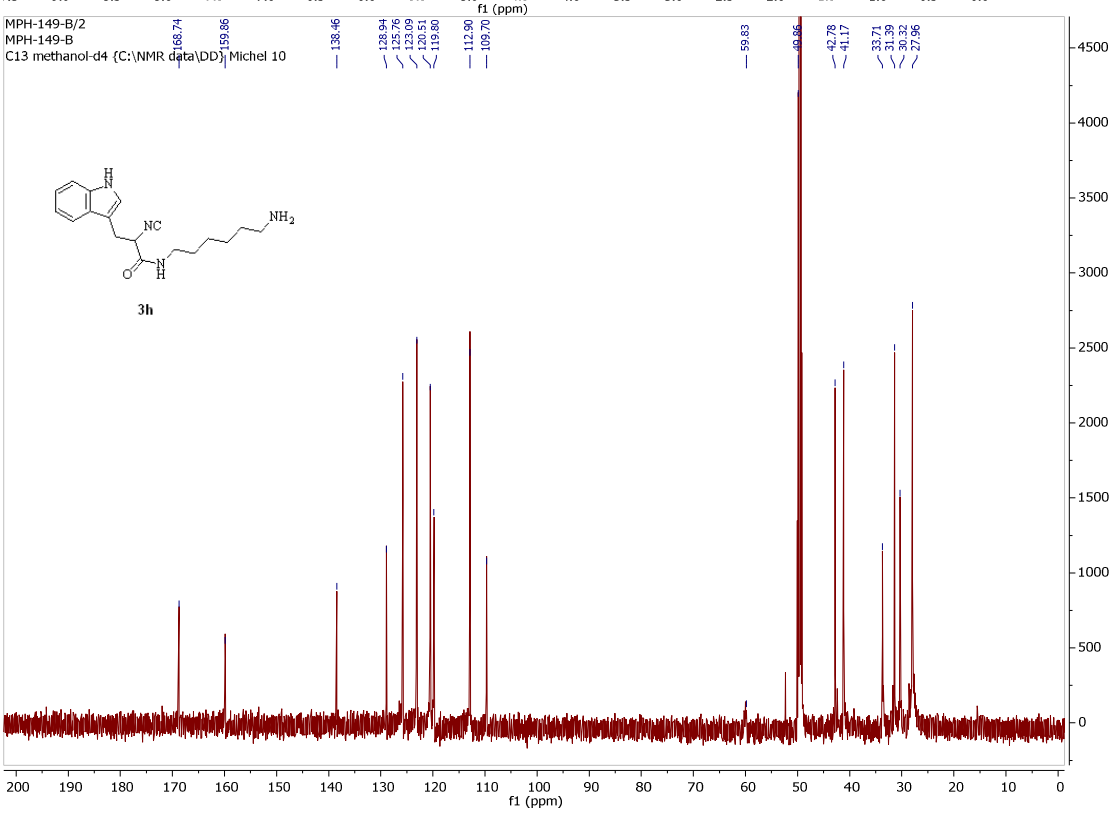
Compound 3g:


MPH-216/1
MHP-216
PROTON methanol-d4 {C:\NMR data\DD} Michel 50
3g
f1 (ppm)

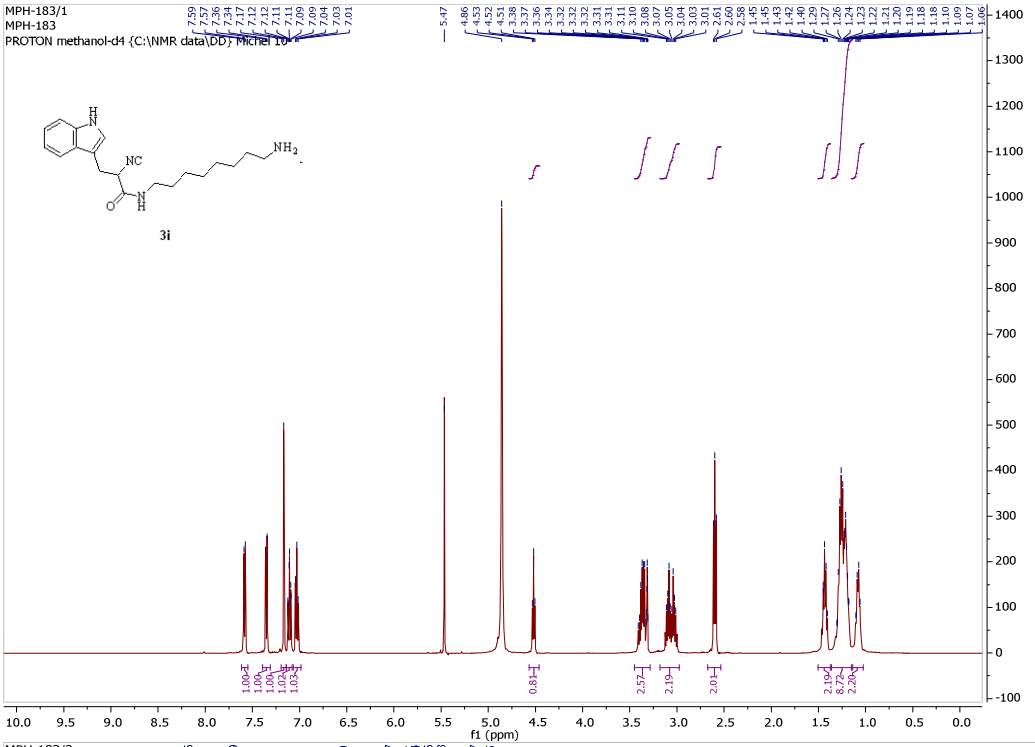

MPH-216/2
MPH-216
C13 methanol-d4 {C:\NMR data\DD} Michel 50
3g
f1 (ppm)

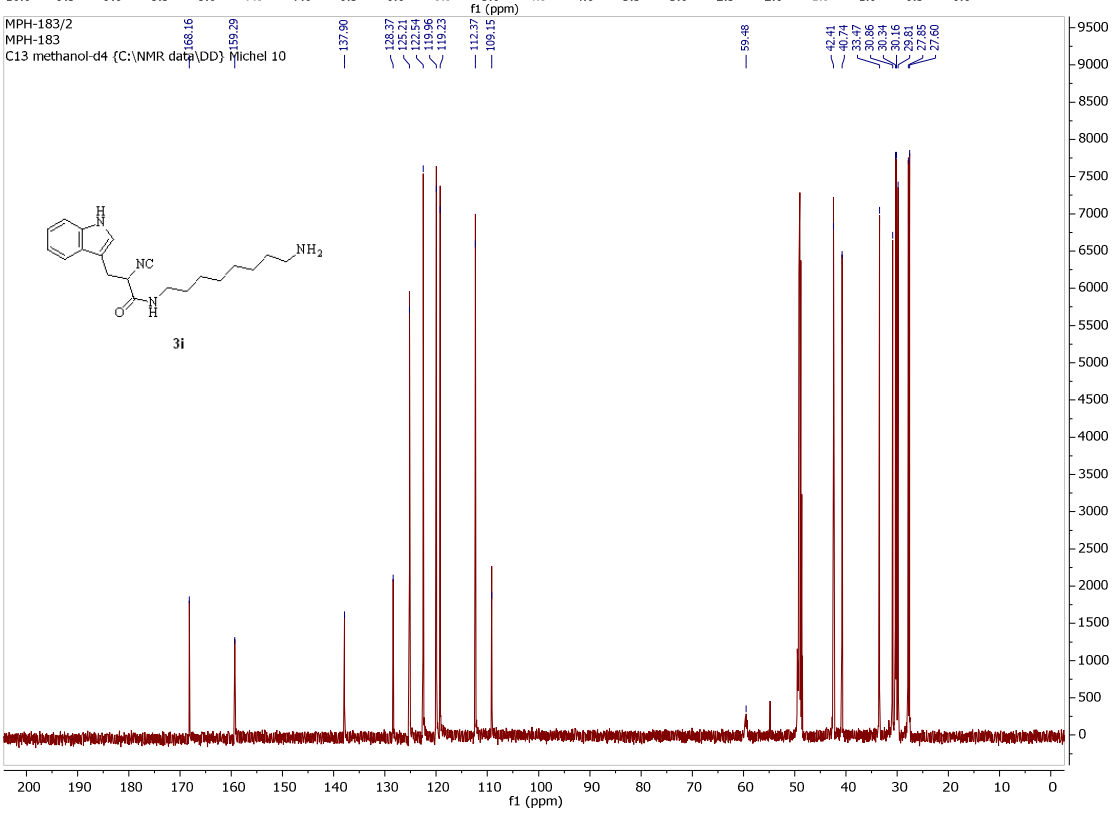
Compound3h:


MPH-149-B/1
MPH-149-B
PROTON methanol-d4 {C:\NMR data\DD} Michel 10
3h
f1 (ppm)

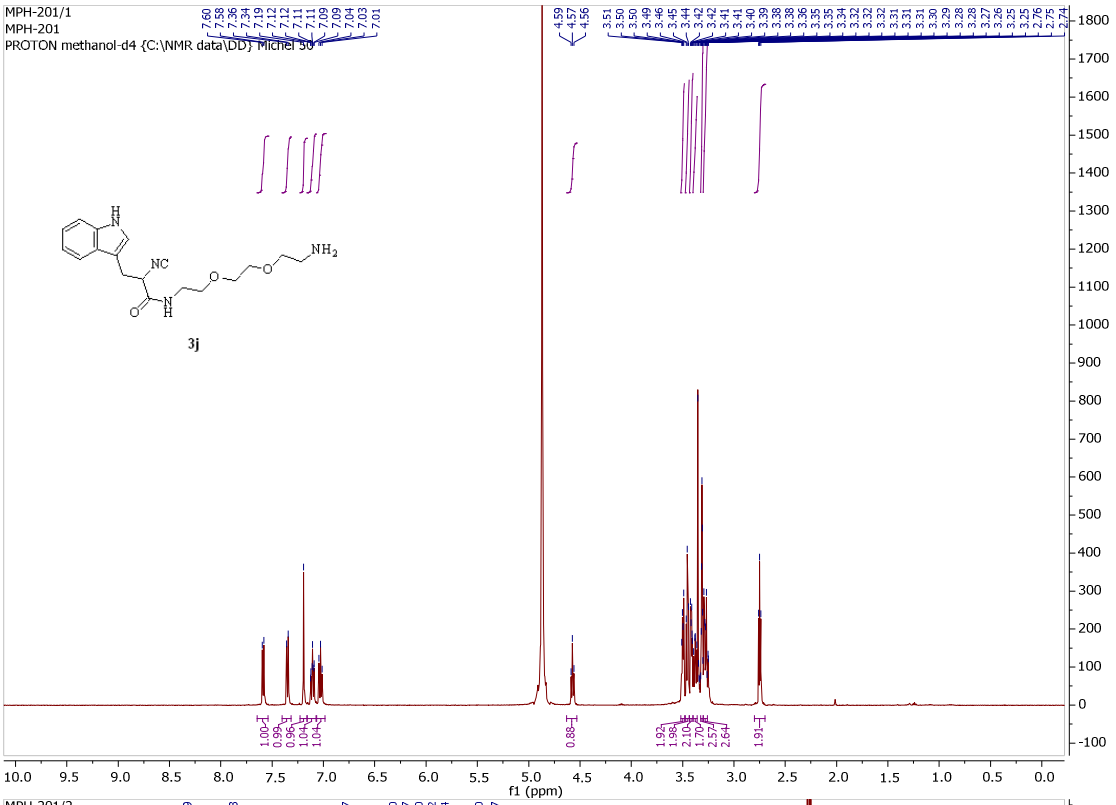

MPH-149-B/2
MPH-149-B
C13 methanol-d4 {C:\NMR data\DD} Michel 10
3h
f1 (ppm)

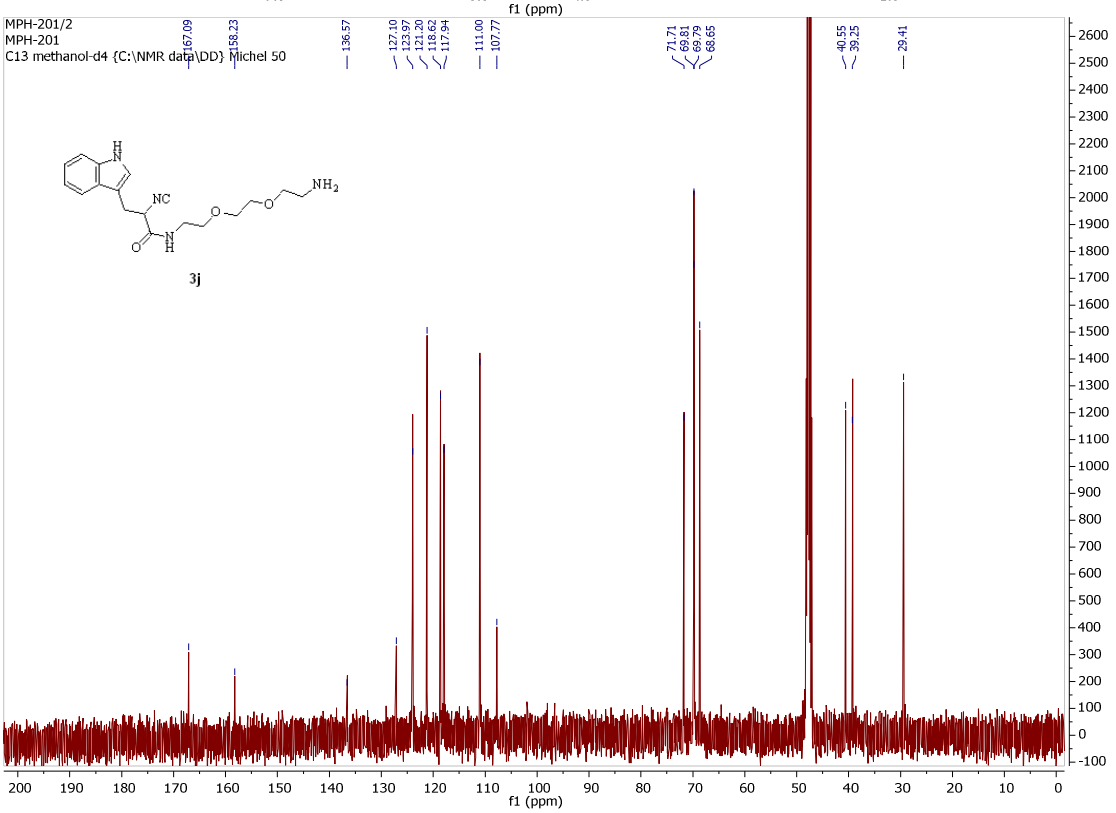
Compound 3i:


MPH-183/1
MPH-183
PROTON methanol-d4 {C:\NMR data\DD} Michel 10
3i
f1 (ppm)

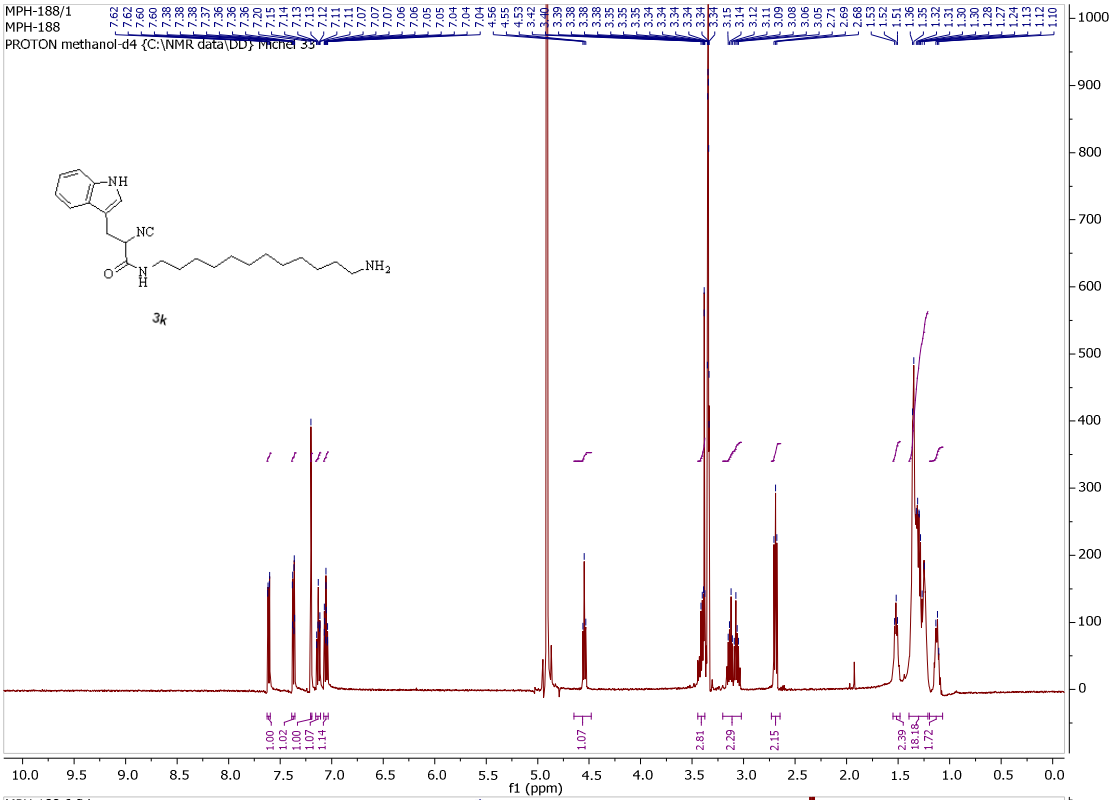

MPH-183/2
MPH-183
C13 methanol-d4 {C:\NMR data\DD} Michel 10
3i
f1 (ppm)

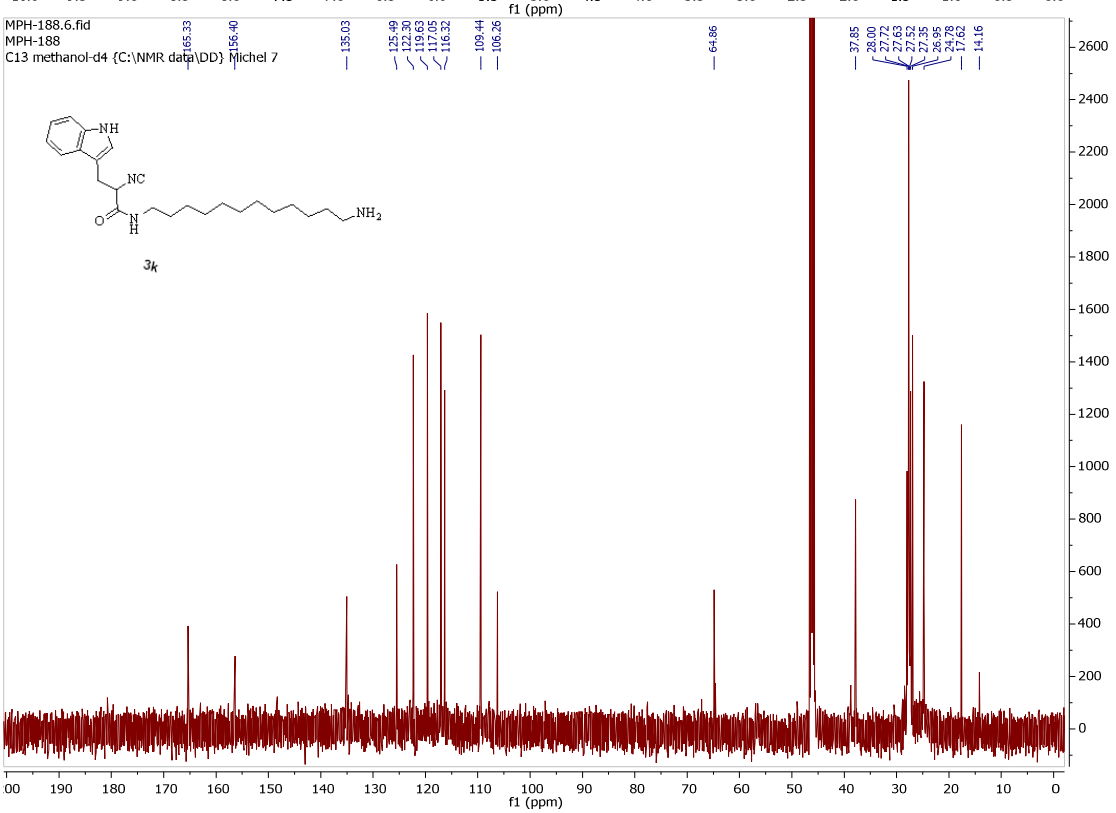
Compound 3j:


MPH-201/1
MPH-201
PROTON methanol-d4 {C:\NMR data\DD} Michel 50
3j
f1 (ppm)

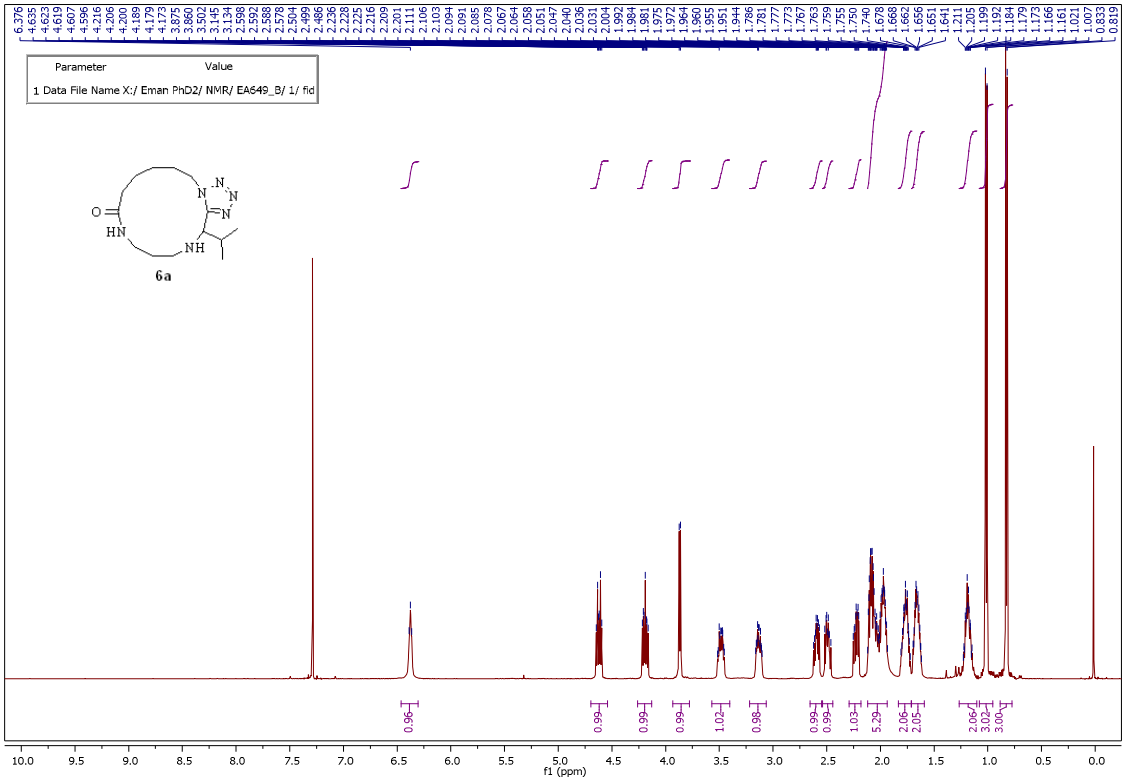

MPH-201/2
MPH-201
C13 methanol-d4 {C:\NMR data\DD} Michel 50
3j
f1 (ppm)

Compound 3k:


MPH-188/1
MPH-188
PROTON methanol-d4 {C:\NMR data\DD} Michel 33
NH
NC
O
N
H
NH2
3k
f1 (ppm)


MPH-188.6.fid
MPH-188
C13 methanol-d4 {C:\NMR data\DD} Michel 7
NH
NC
O
N
H
NH2
3k
f1 (ppm)

Compound 6a:


Parameter
Value
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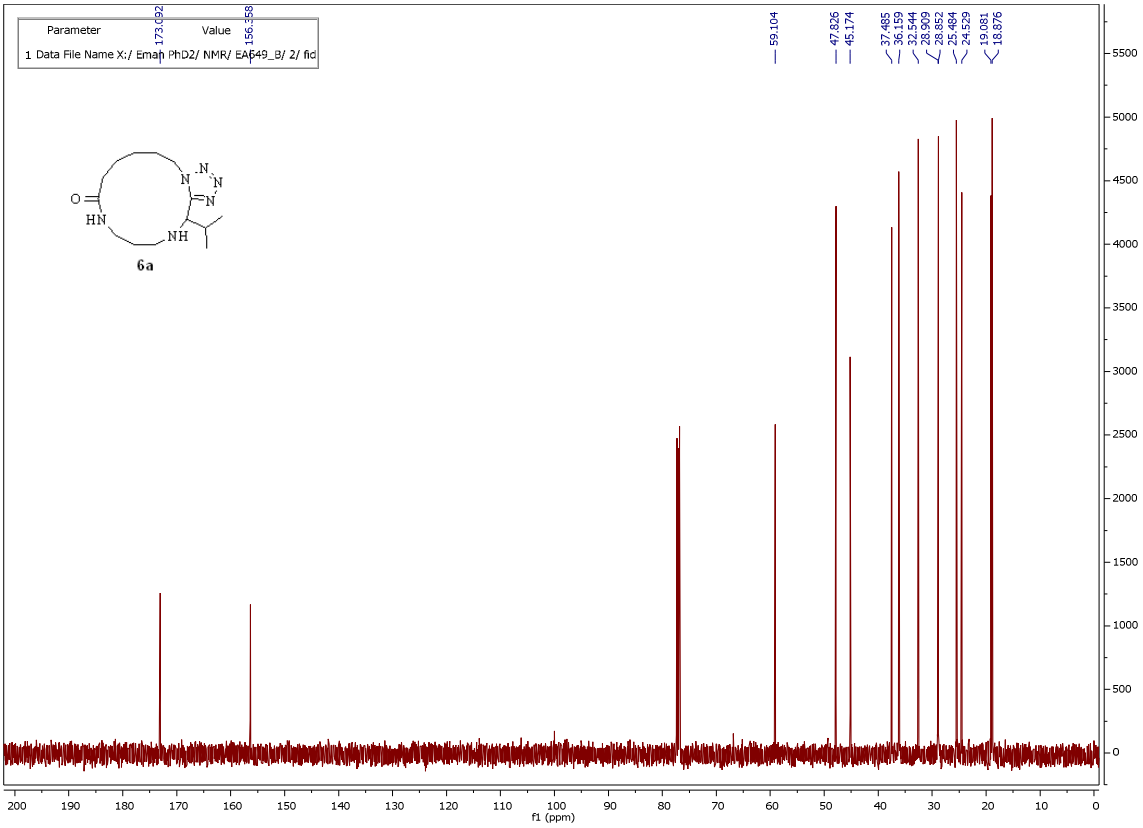
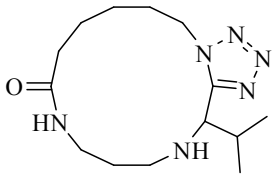
6a
f1 (ppm)

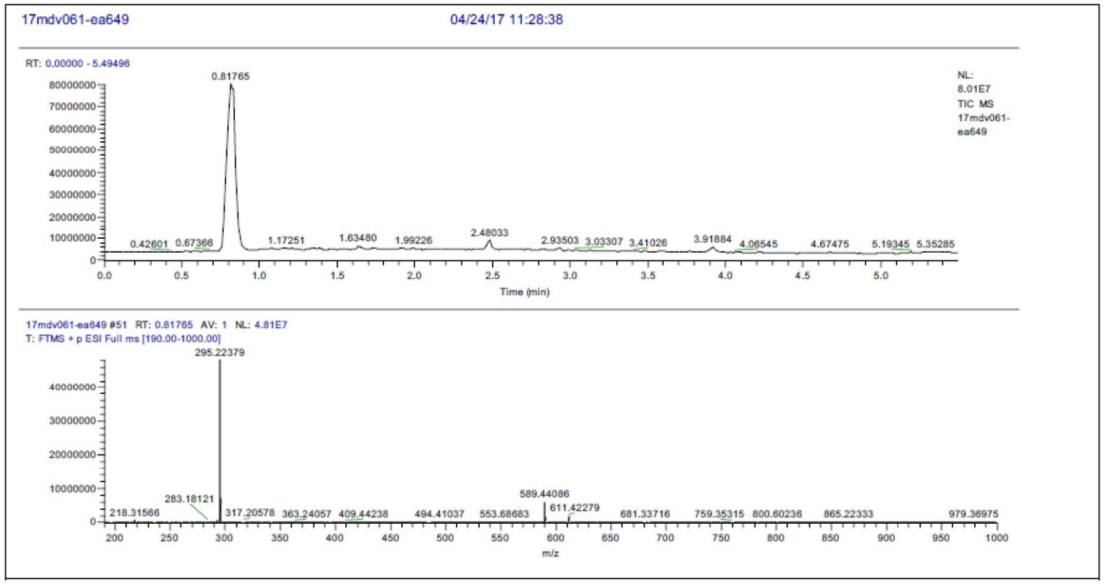

Parameter
Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA649_B/ 2/ fid
6a
f1 (ppm)



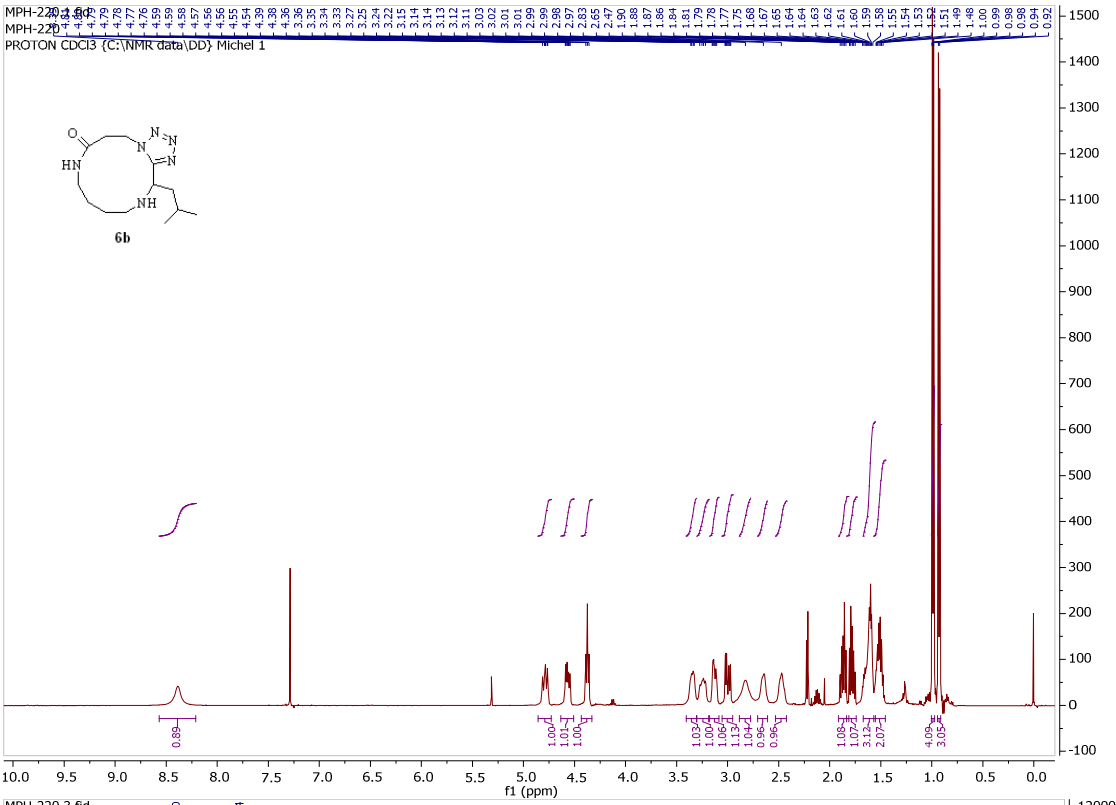
6a

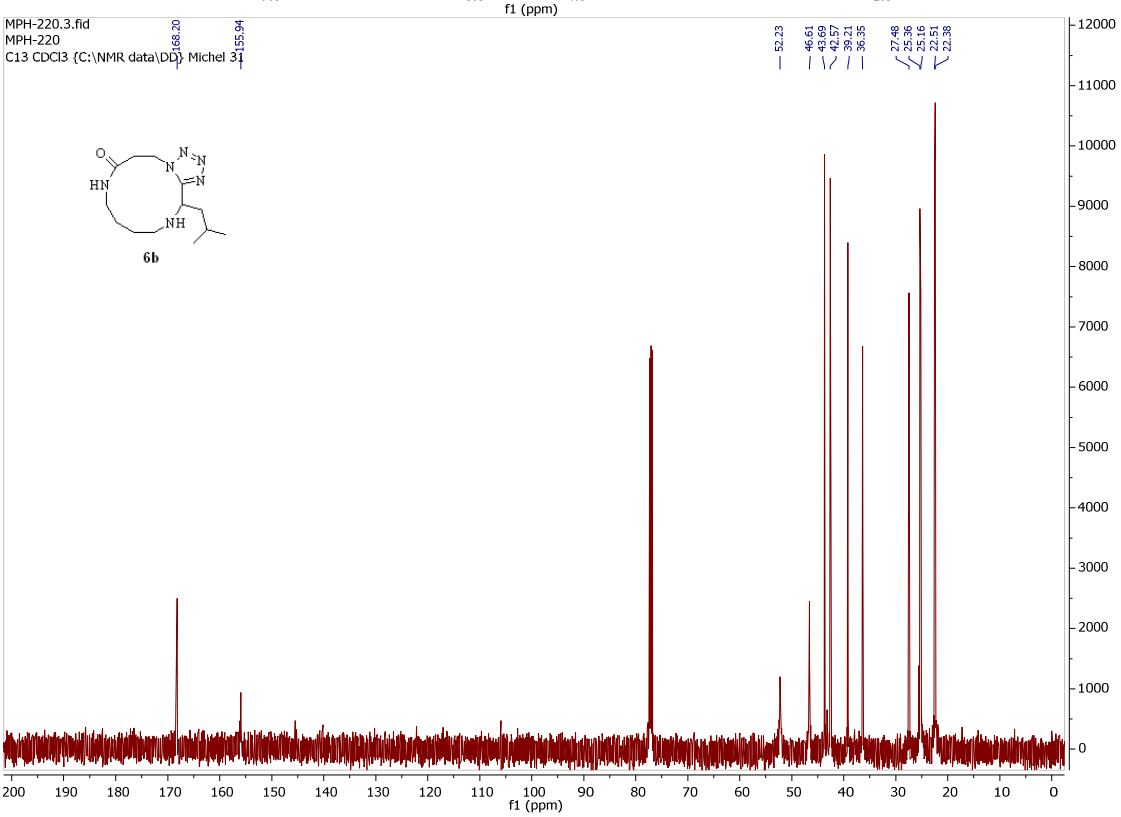
Chemical Formula: $C_{14}H_{26}N_6O$

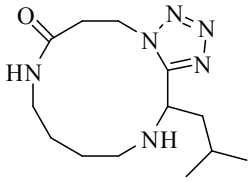
Exact Mass: 294.2168



Compound 6b:

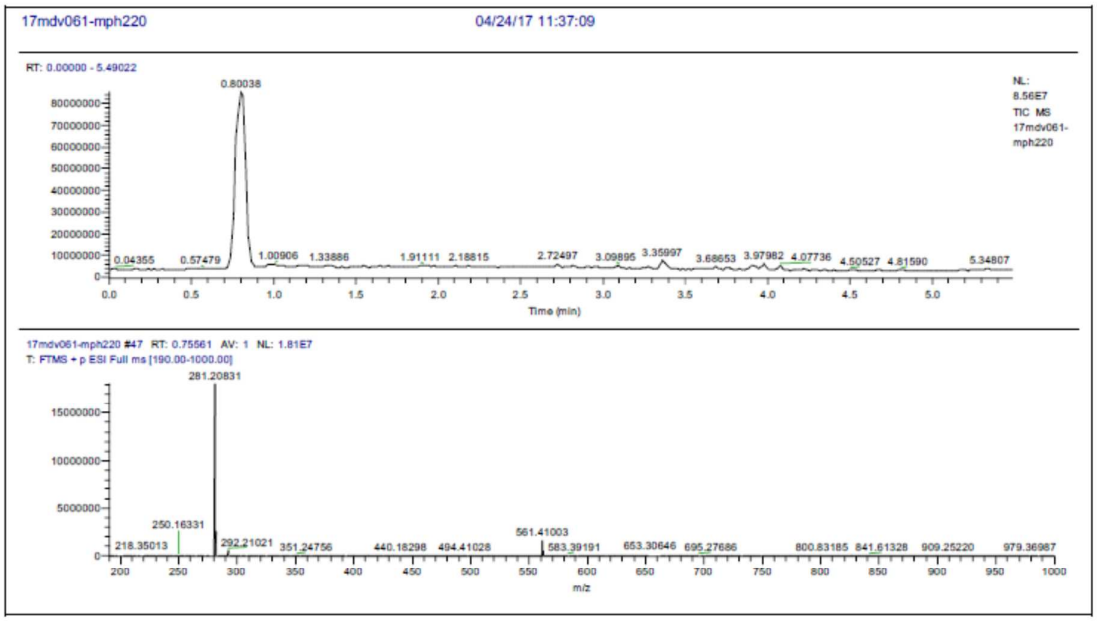

MPH-220.1.fid
MPH-220
PROTON CDCl3 {C:\NMR data\DD} Michel 1
6b
f1 (ppm)


MPH-220.3.fid
MPH-220
C13 CDCl3 {C:\NMR data\DD} Michel 3
168.20
155.94
52.23
46.61
45.69
45.57
39.21
36.35
27.48
25.36
25.16
22.51
22.38
6b
f1 (ppm)

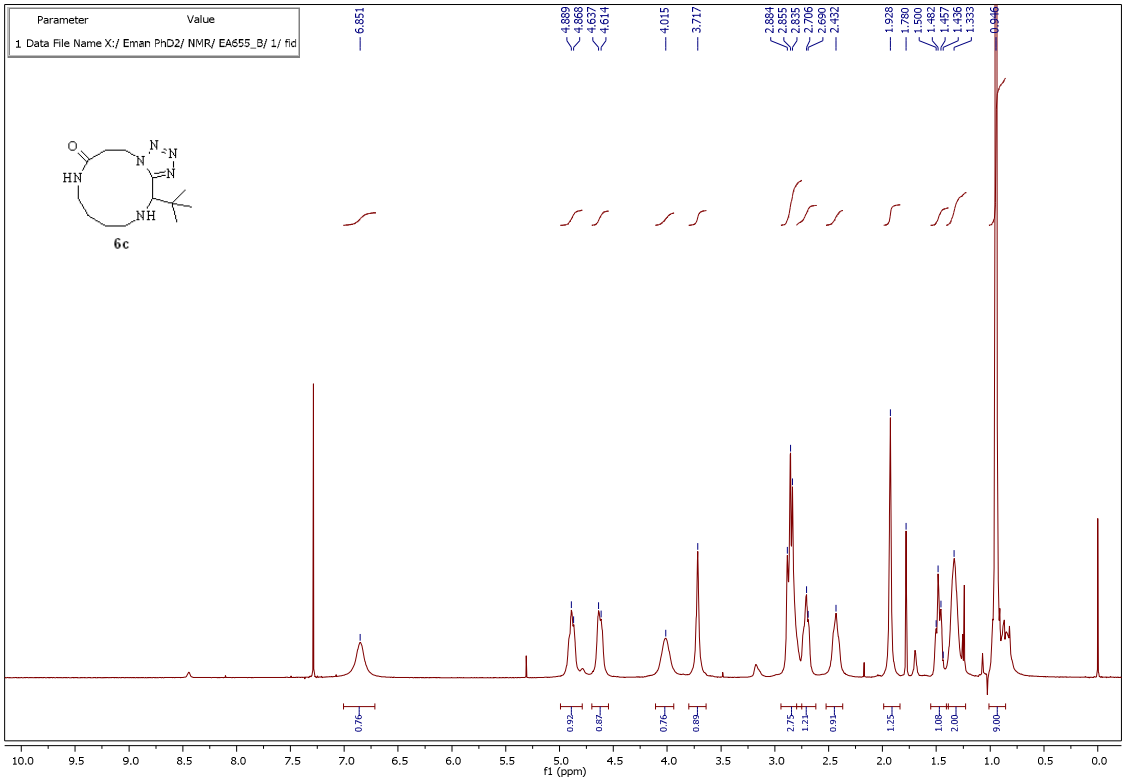


6b

Chemical Formula: $C_{13}H_{24}N_6O$
Exact Mass: 280.2012



Compound 6c:


Parameter
Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA655_B/ 1/ fid
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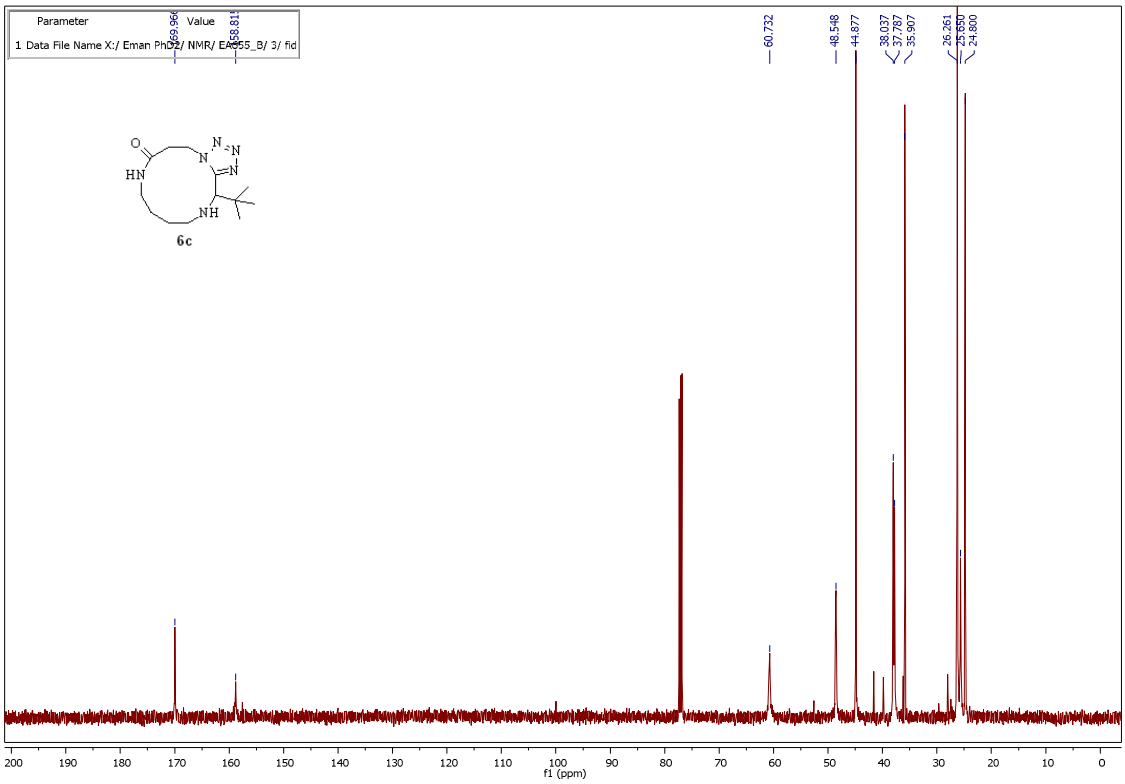
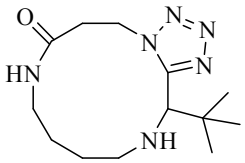
4.889
4.868
4.637
4.614
4.015
3.717
2.884
2.855
2.835
2.706
2.690
2.432
1.928
1.780
1.500
1.482
1.457
1.436
1.333
0.946
6c
f1 (ppm)

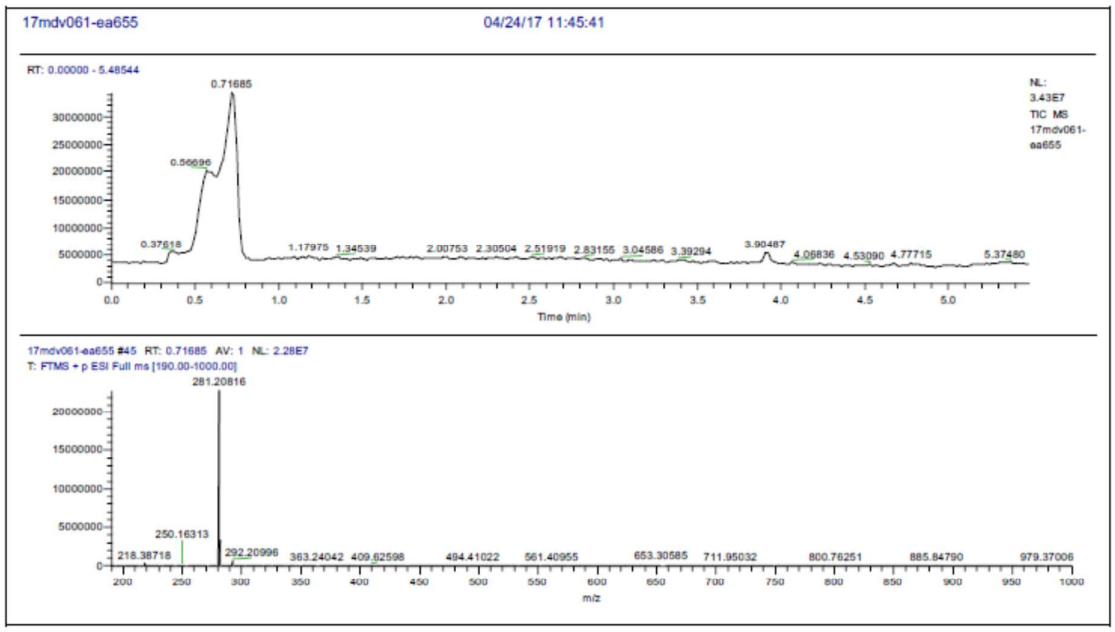

Parameter
Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA655_B/ 3/ fid
169.966
158.811
60.732
48.548
44.877
38.037
37.787
35.907
26.261
25.650
24.800
6c
f1 (ppm)



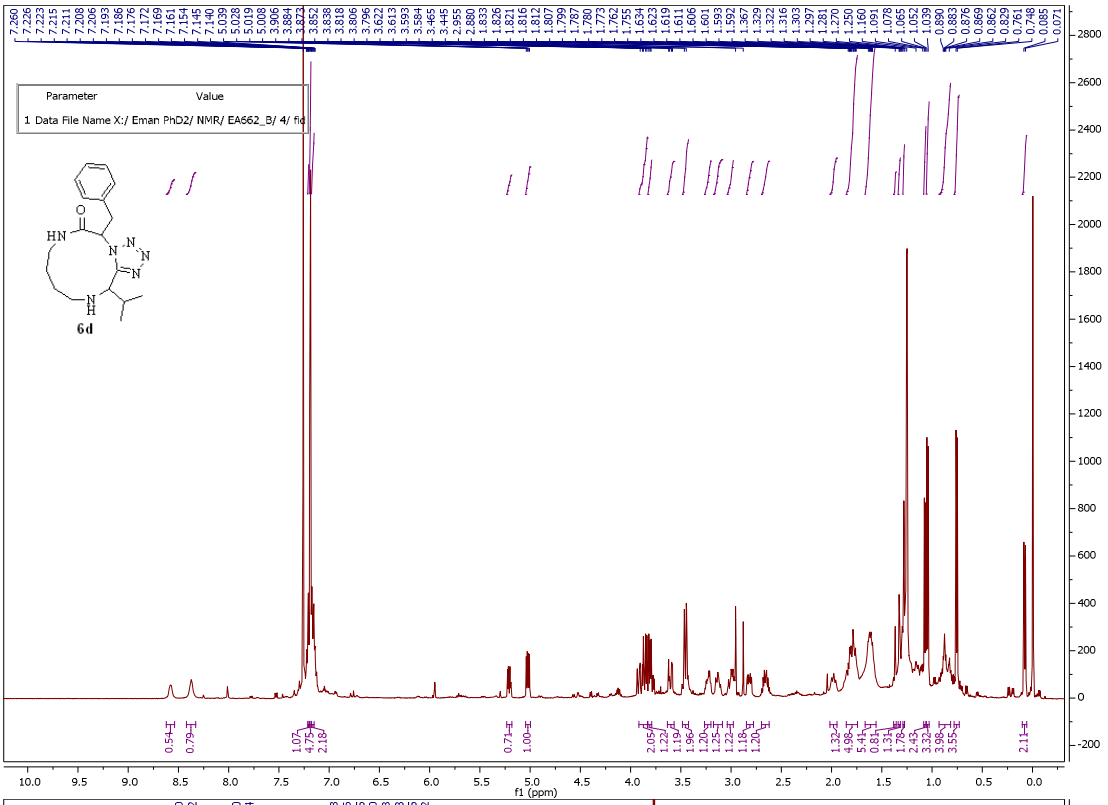
6c

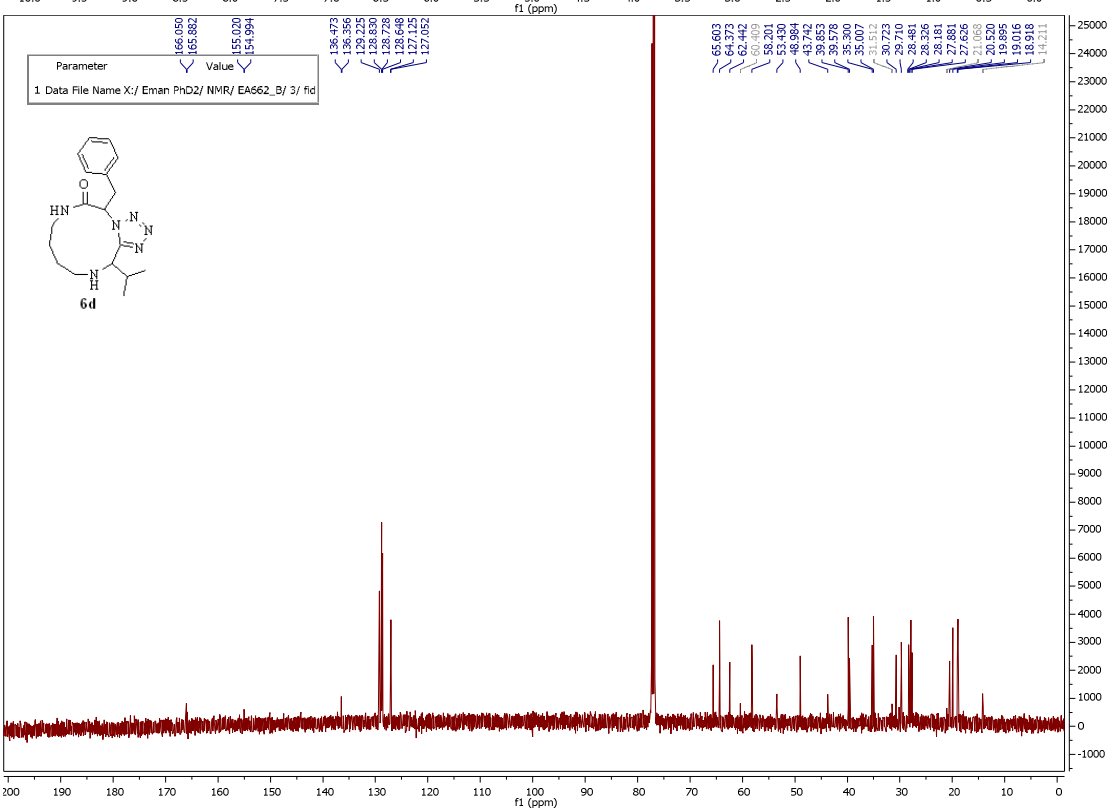
Chemical Formula: $C_{13}H_{24}N_6O$

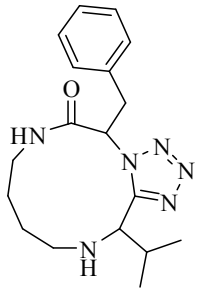
Exact Mass: 280.2012



Compound 6d:


Parameter Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA662_B/ 4/ fid
6d
f1 (ppm)

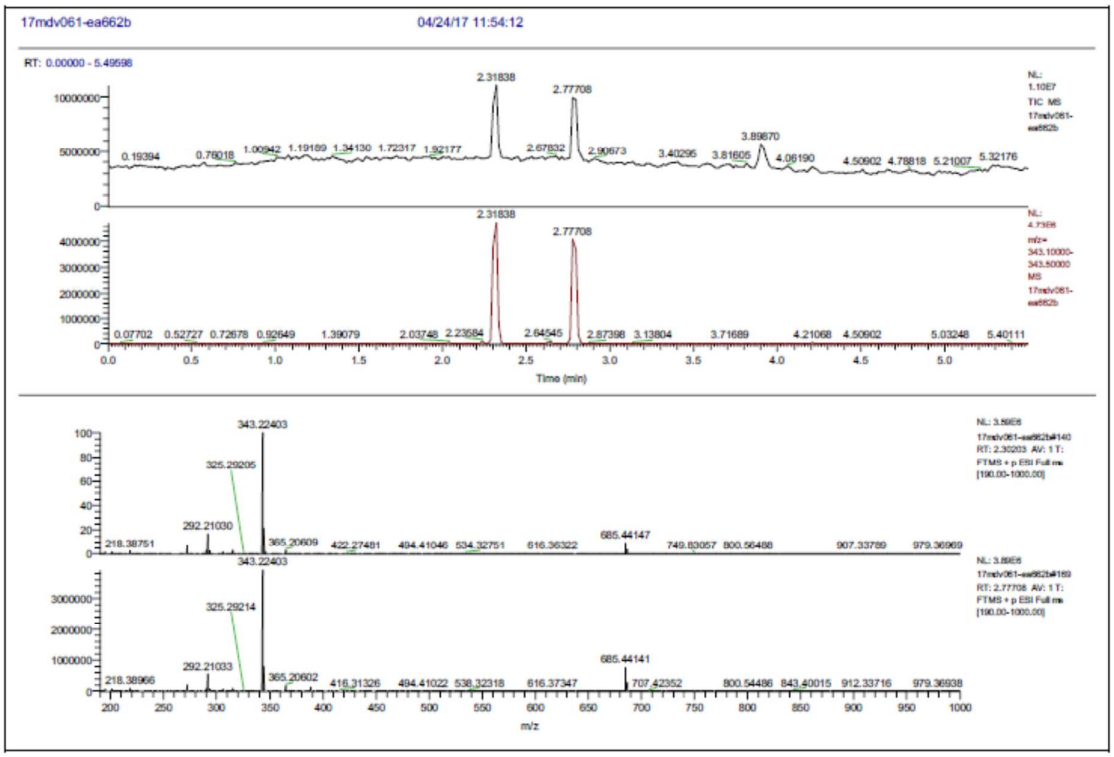

Parameter Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA662_B/ 3/ fid
6d
f1 (ppm)



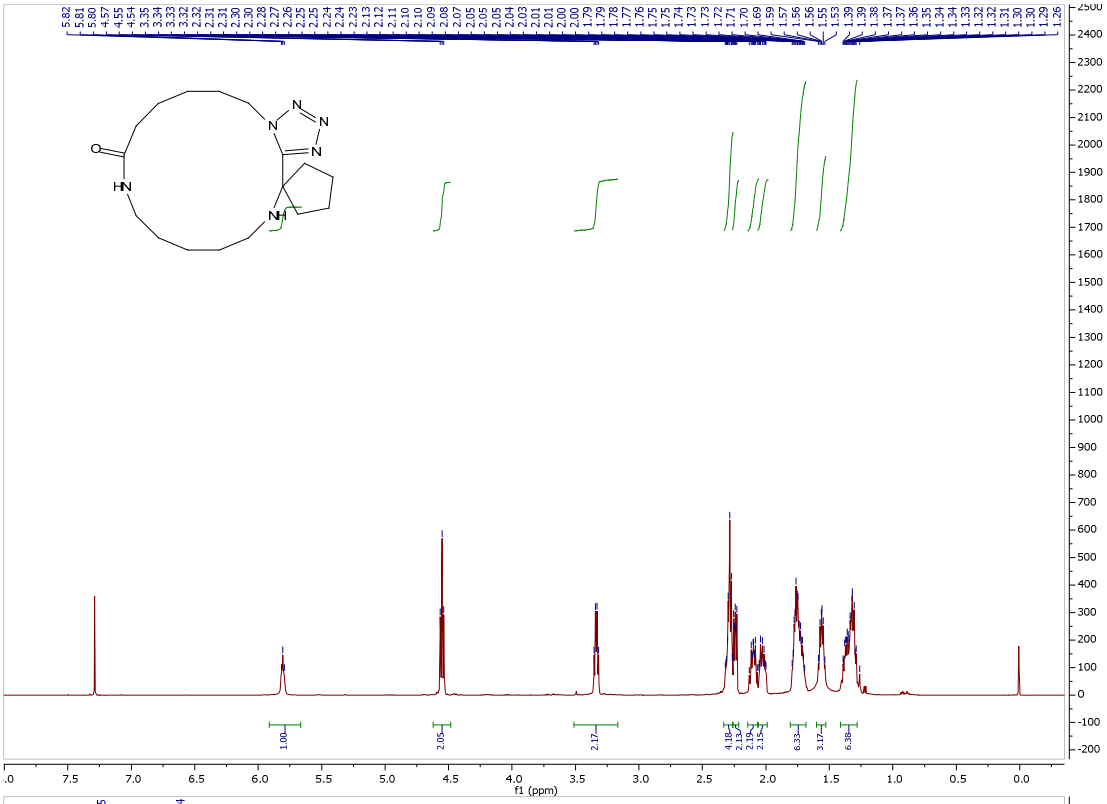
6d

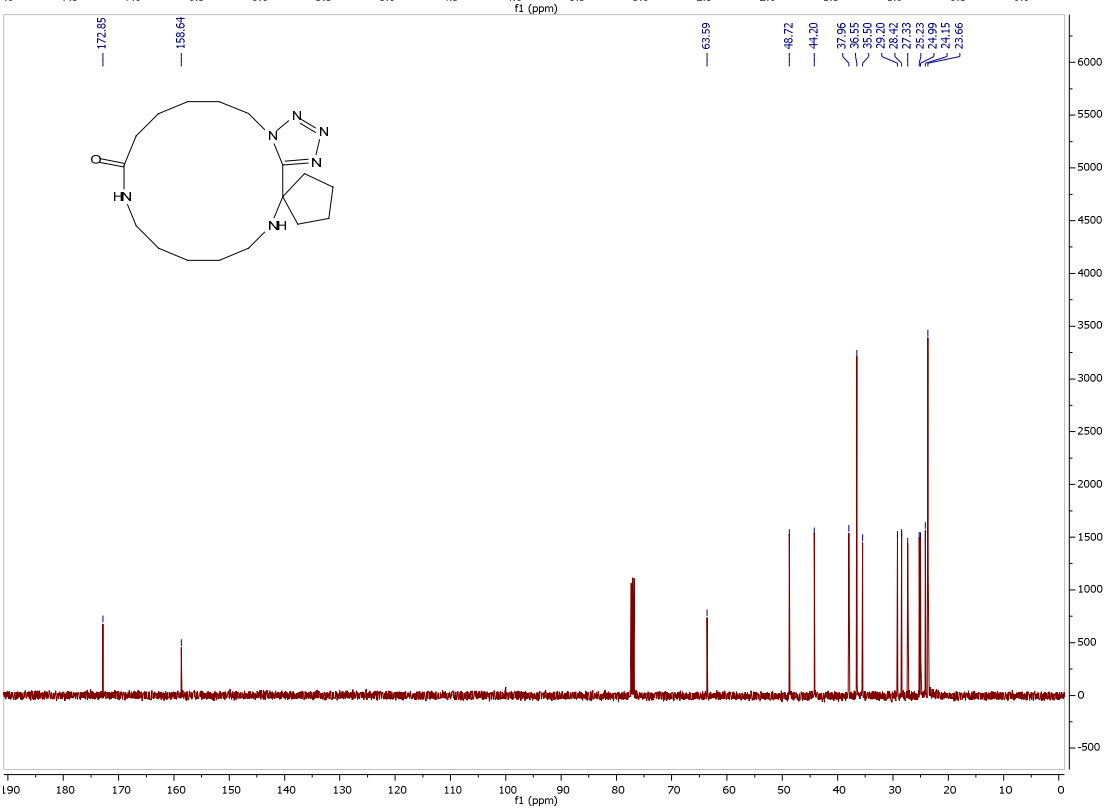
Chemical Formula: $C_{18}H_{26}N_6O$

Exact Mass: 342.2168

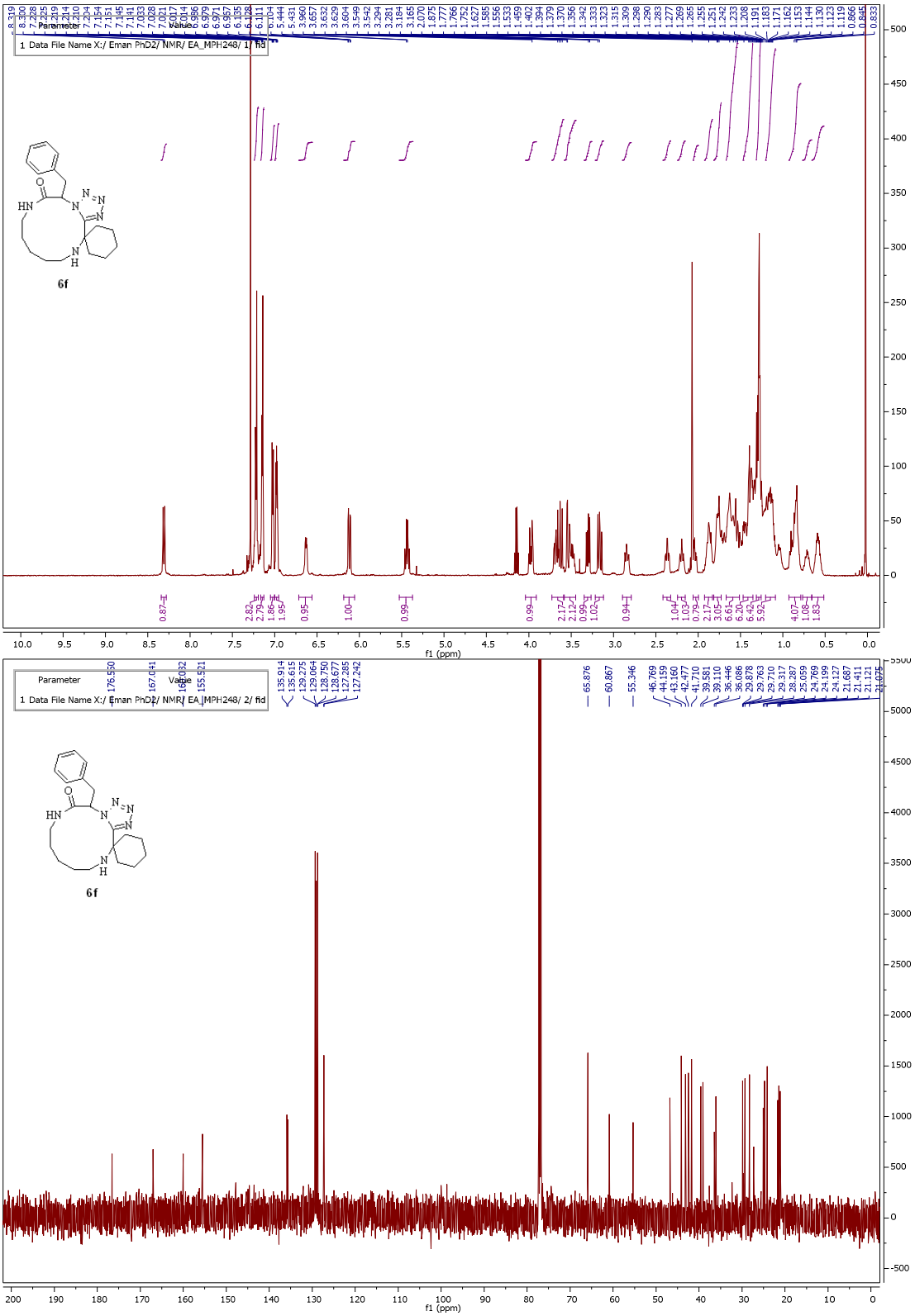


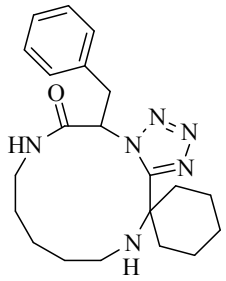
Compound 6e:


f1 (ppm)


172.85
158.64
63.59
48.72
44.20
37.96
36.55
35.50
29.20
28.42
27.33
25.23
24.89
24.15
23.66
f1 (ppm)

Compound6f:

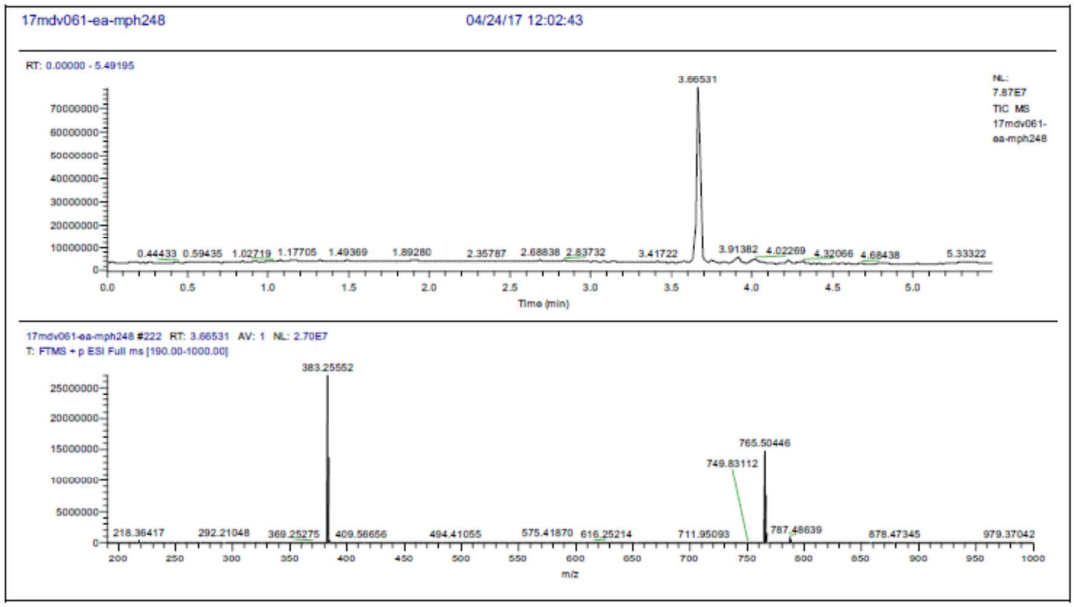

Parameter
Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA_MPH248/ 1/ fid
6f
f1 (ppm)
Parameter
Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA_MPH248/ 2/ fid
6f
f1 (ppm)



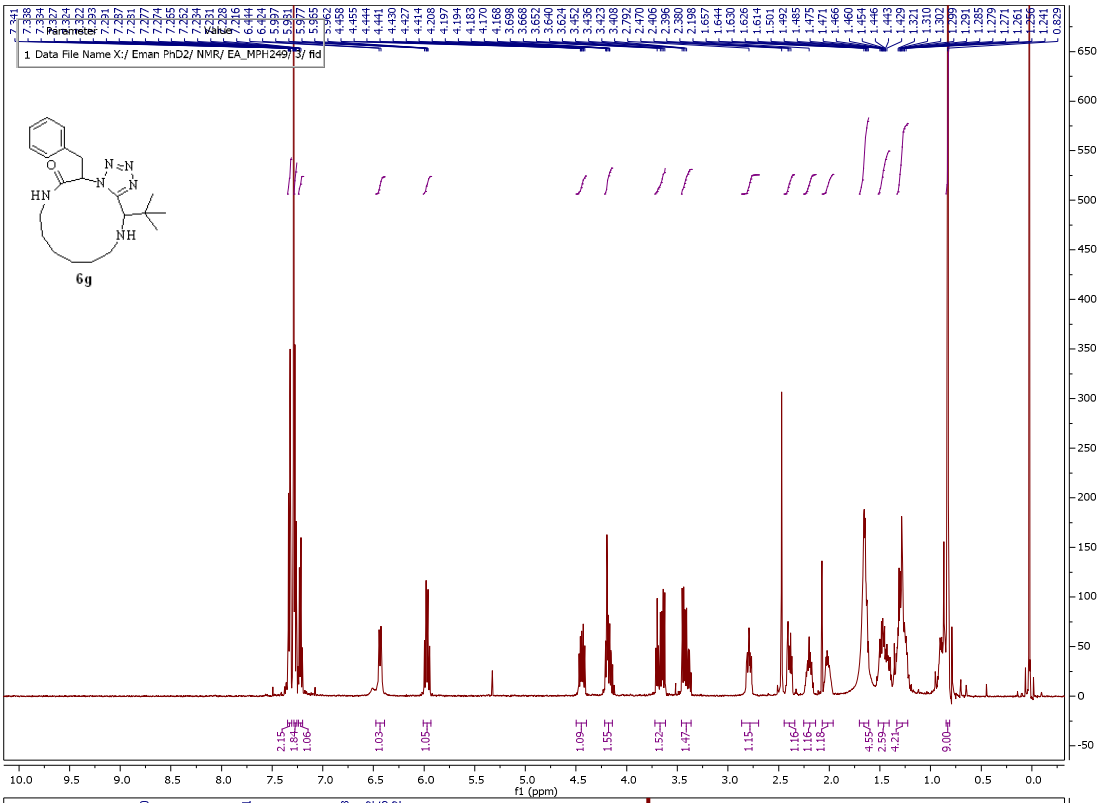
6f

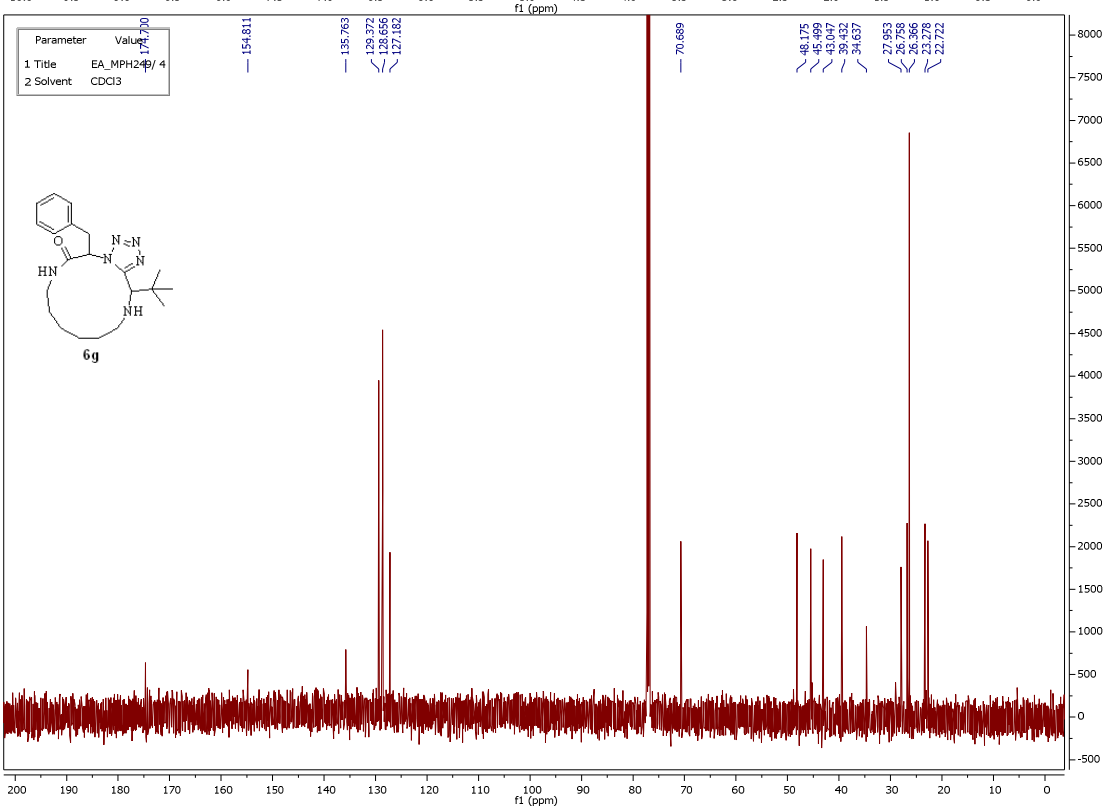
Chemical Formula: $C_{21}H_{30}N_6O$

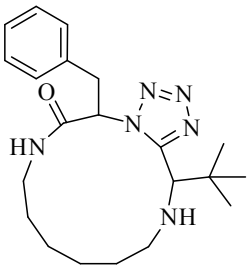
Exact Mass: 382.2481



Compound 6g:


Parameter Value
1 Data File Name X:/ Eman PhD2/ NMR/ EA_MPH249/ 3/ fid
6g
f1 (ppm)

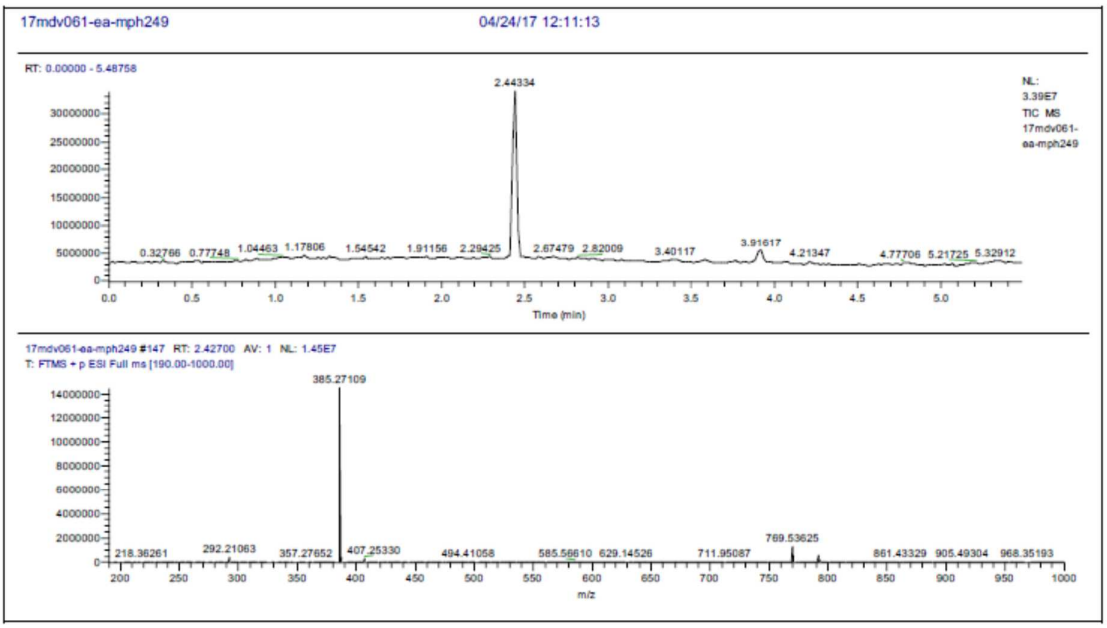

Parameter Value
1 Title EA_MPH249/ 4
2 Solvent CDCl3
6g
f1 (ppm)



6g

Chemical Formula: $C_{21}H_{32}N_6O$

Exact Mass: 384.2638



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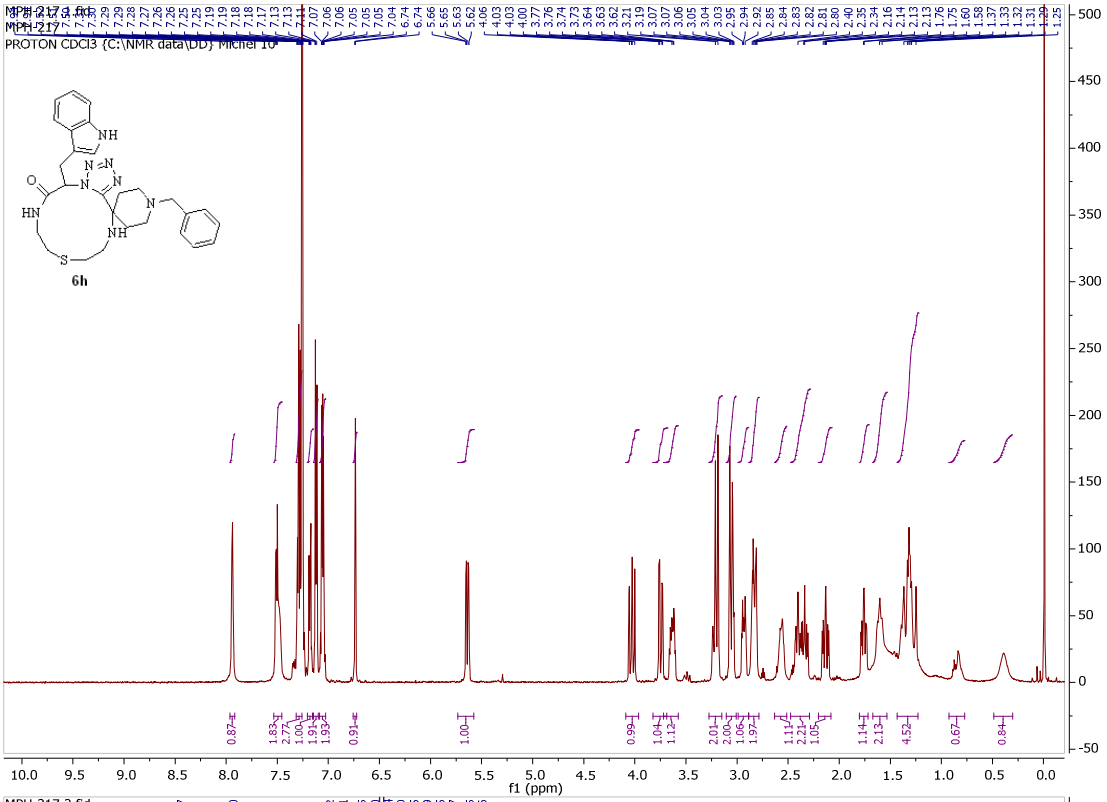
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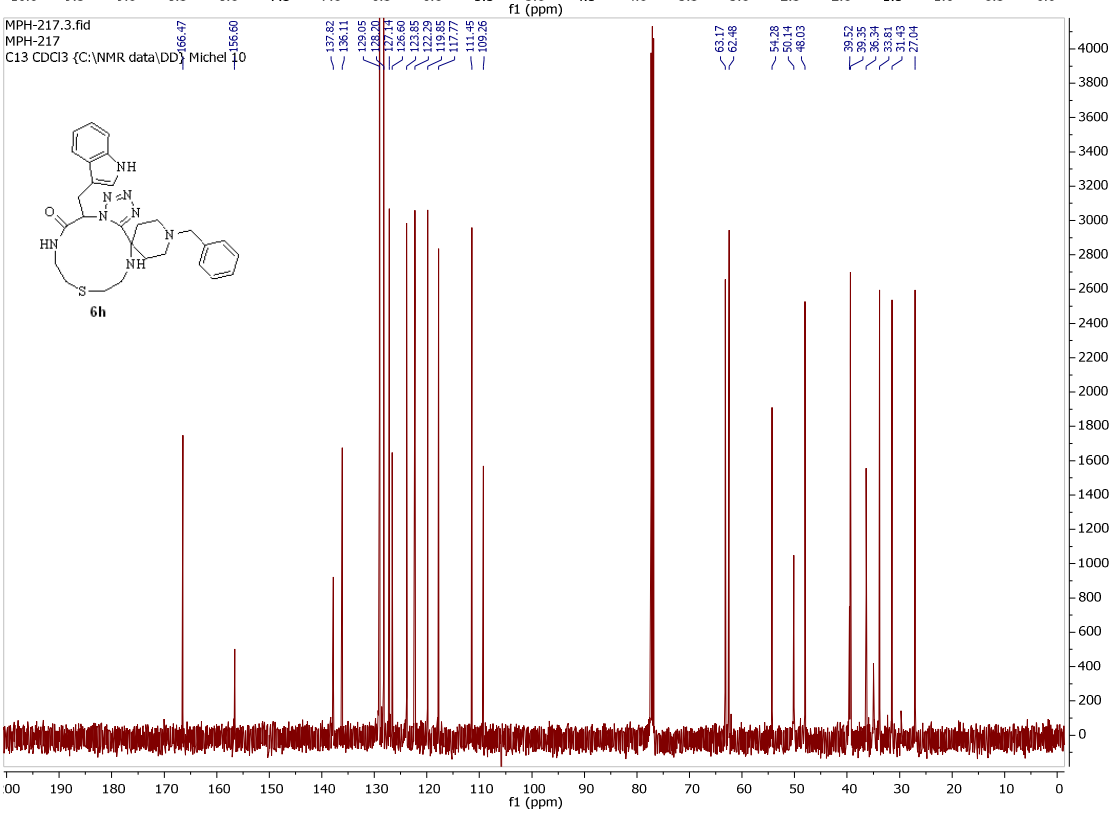
f1 (ppm)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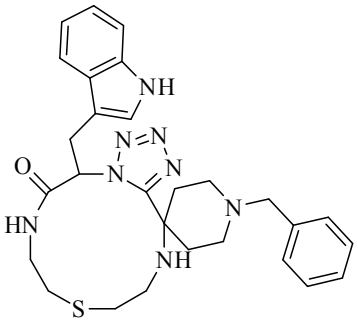
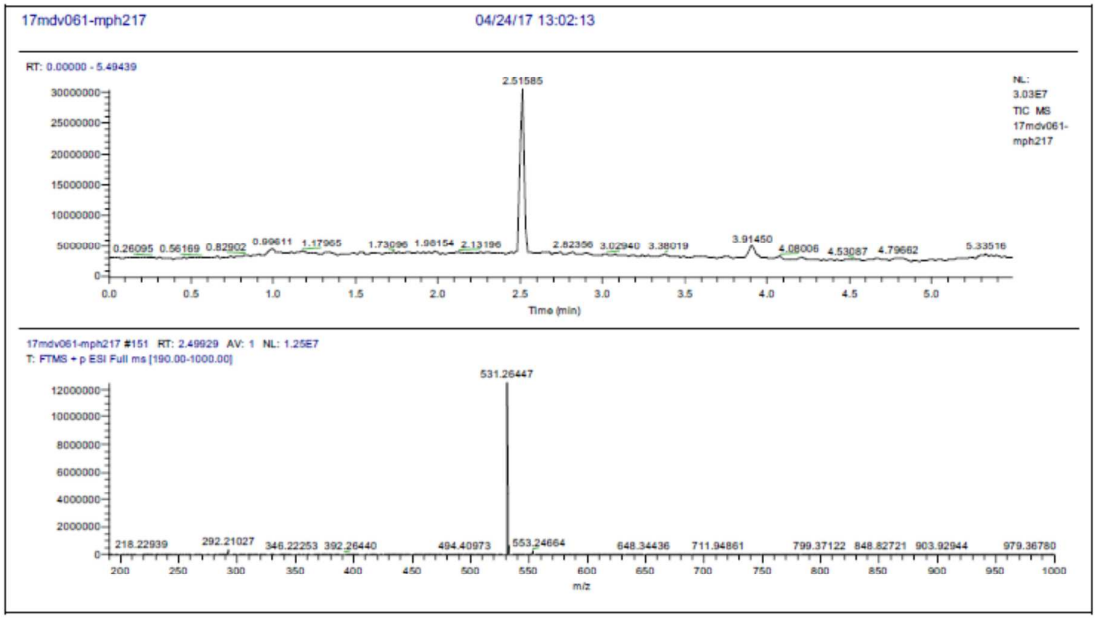
6h
f1 (ppm)



6h

Chemical Formula: $C_{28}H_{34}N_8OS$

Exact Mass: 530.2576



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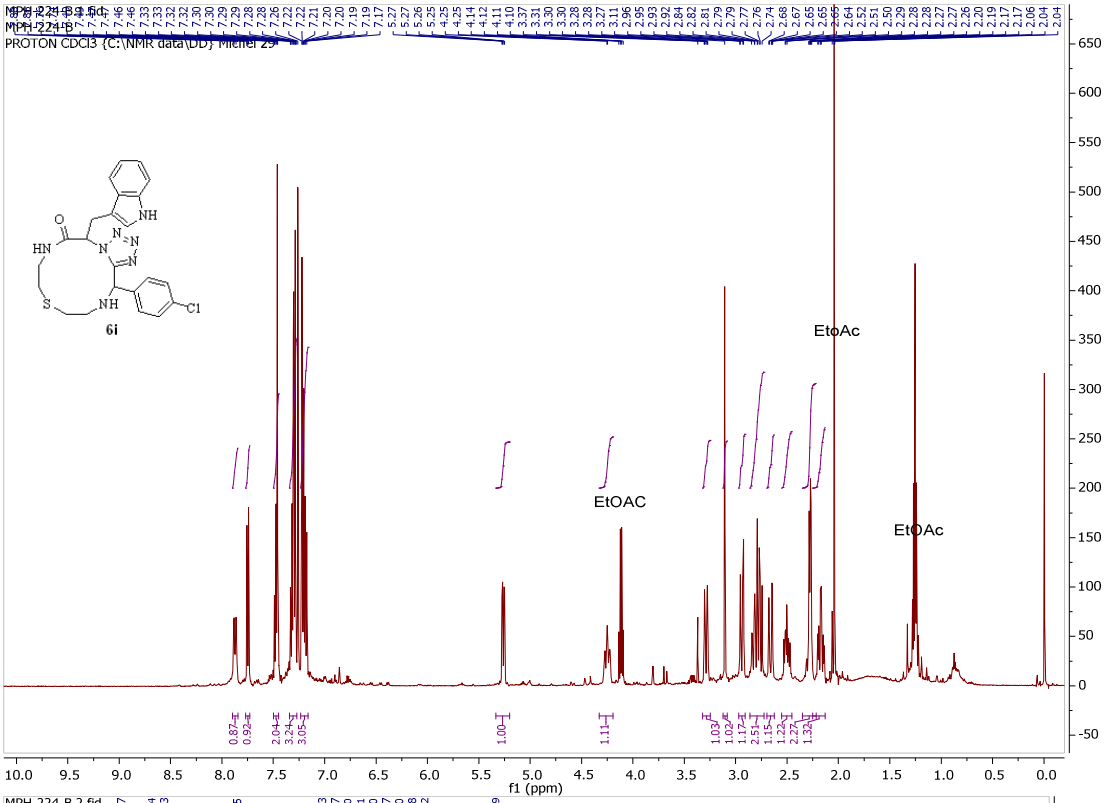
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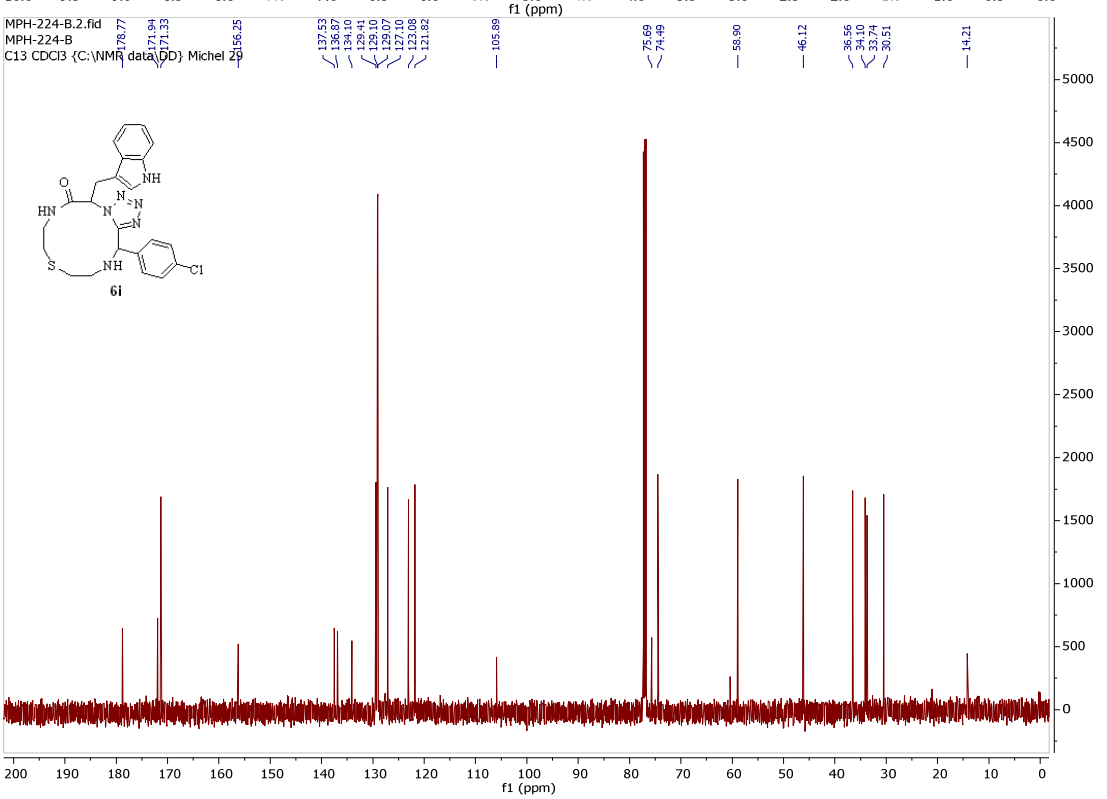
EtoAc
EtOAC
EtOAc
6i
f1 (ppm)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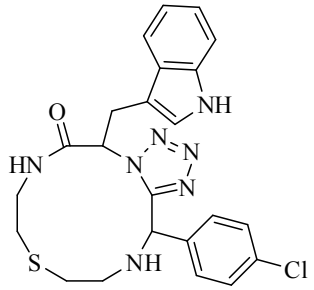
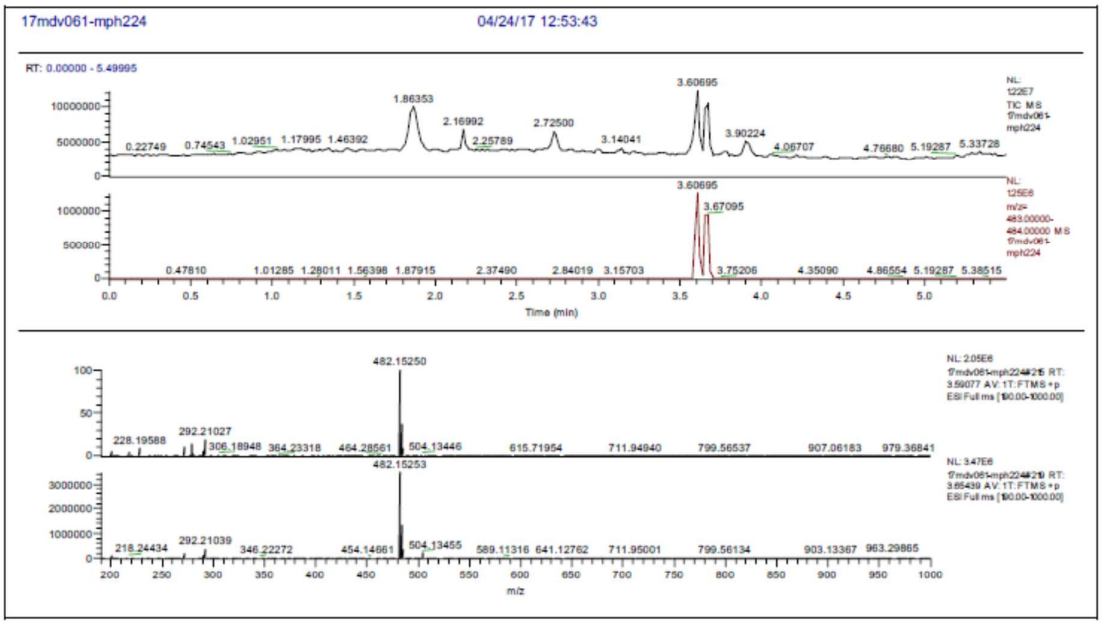
6i
f1 (ppm)



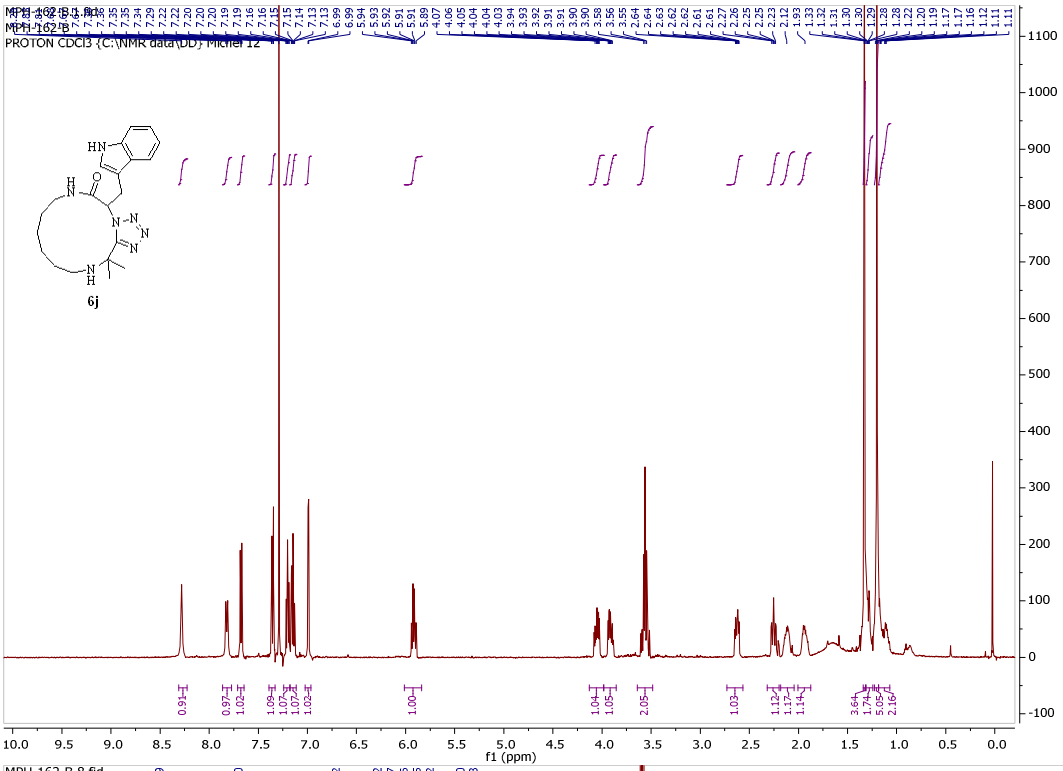
6i

Chemical Formula: $C_{23}H_{24}ClN_7OS$

Exact Mass: 481.1452



Compound 6j: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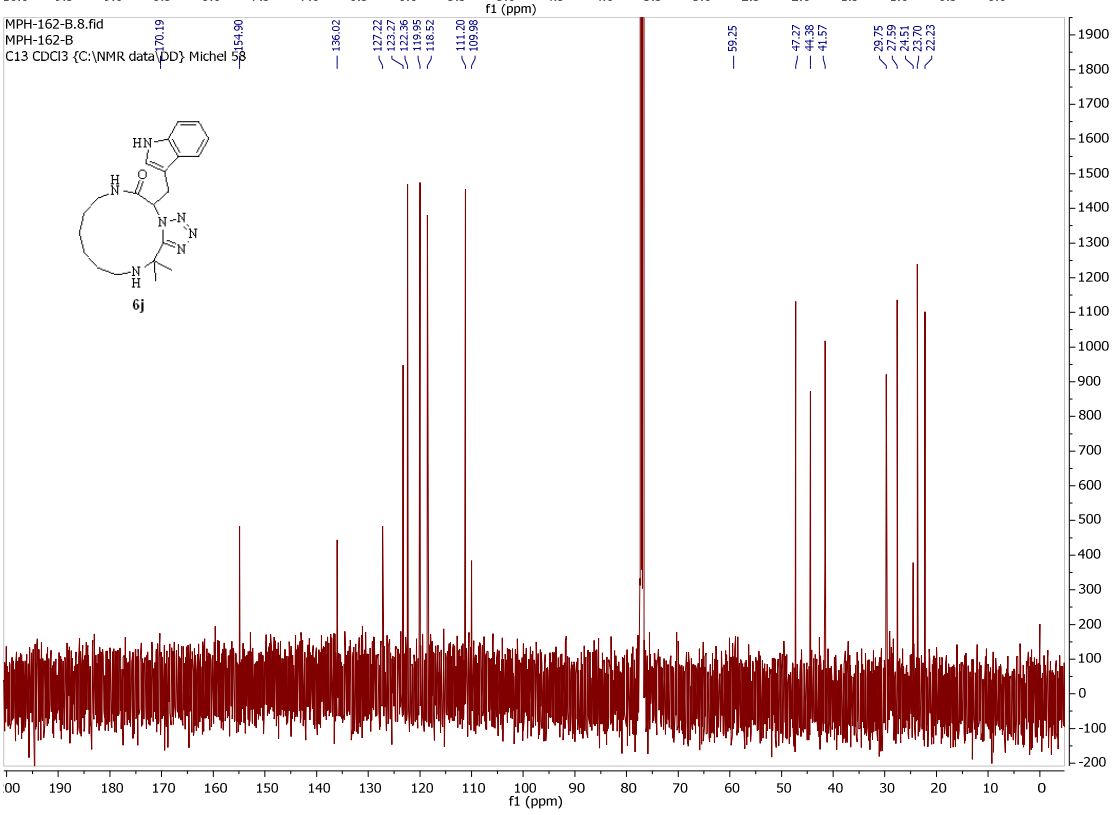
6j
f1 (ppm)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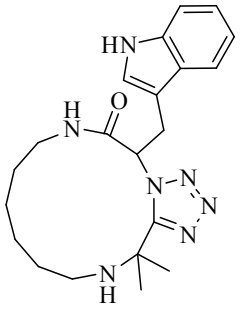
MPH-162-B
C13 CDCl3 {C:\NMR data\DD} Michel 58
6j
f1 (ppm)

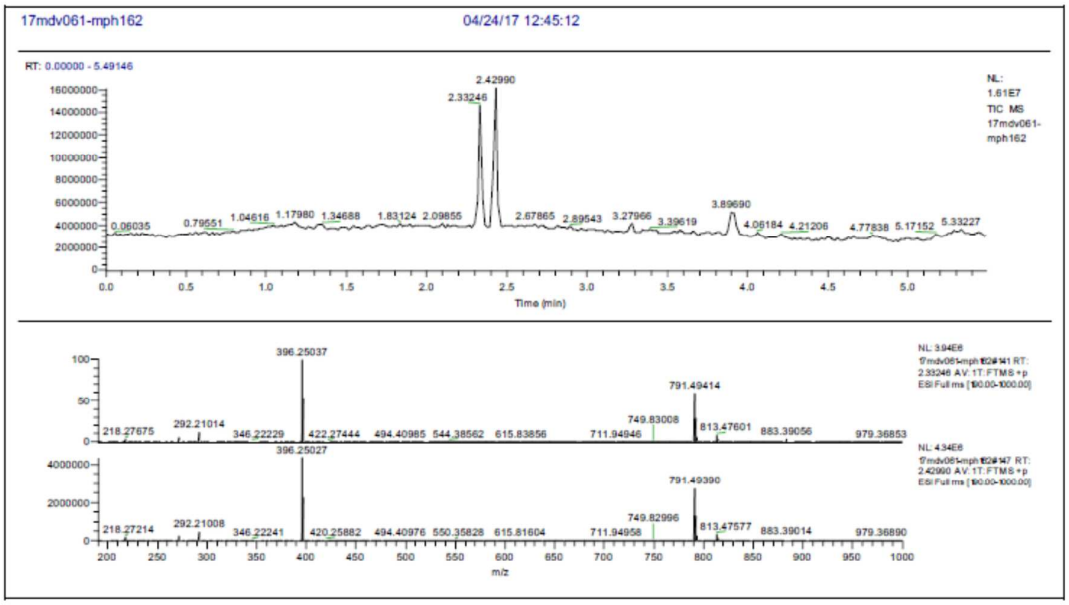


6j

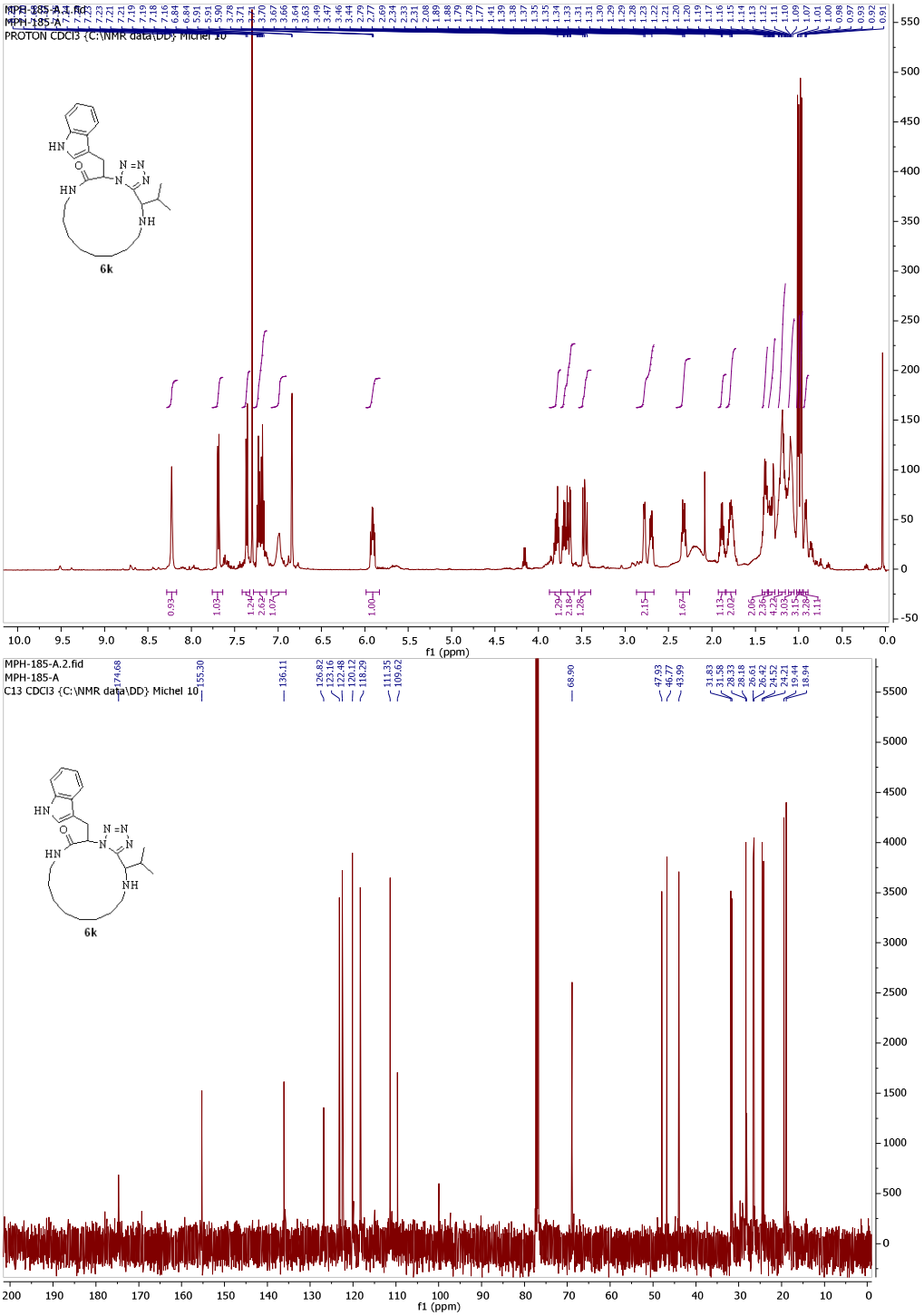
Chemical Formula:

$C_{21}H_{29}N_7O$

Exact Mass: 395.2434



Compound 6k: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f1 (ppm)
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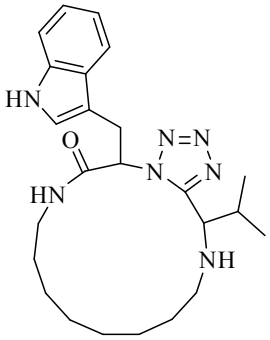
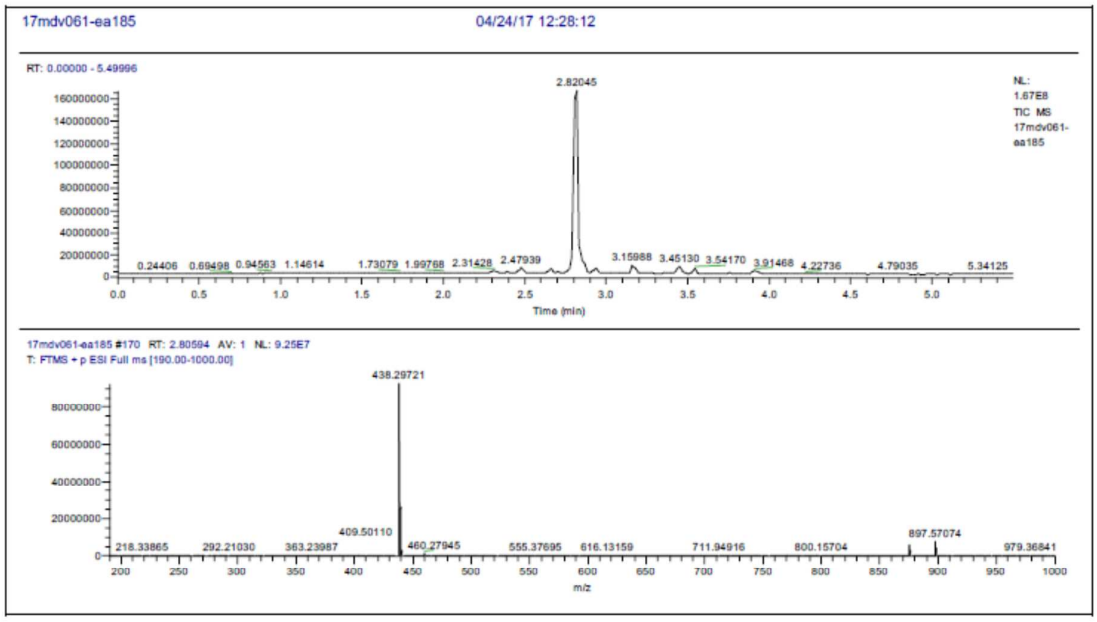
MPH-185-A
C13 CDCl3 {C:\NMR data\DD} Michel 10
f1 (ppm)



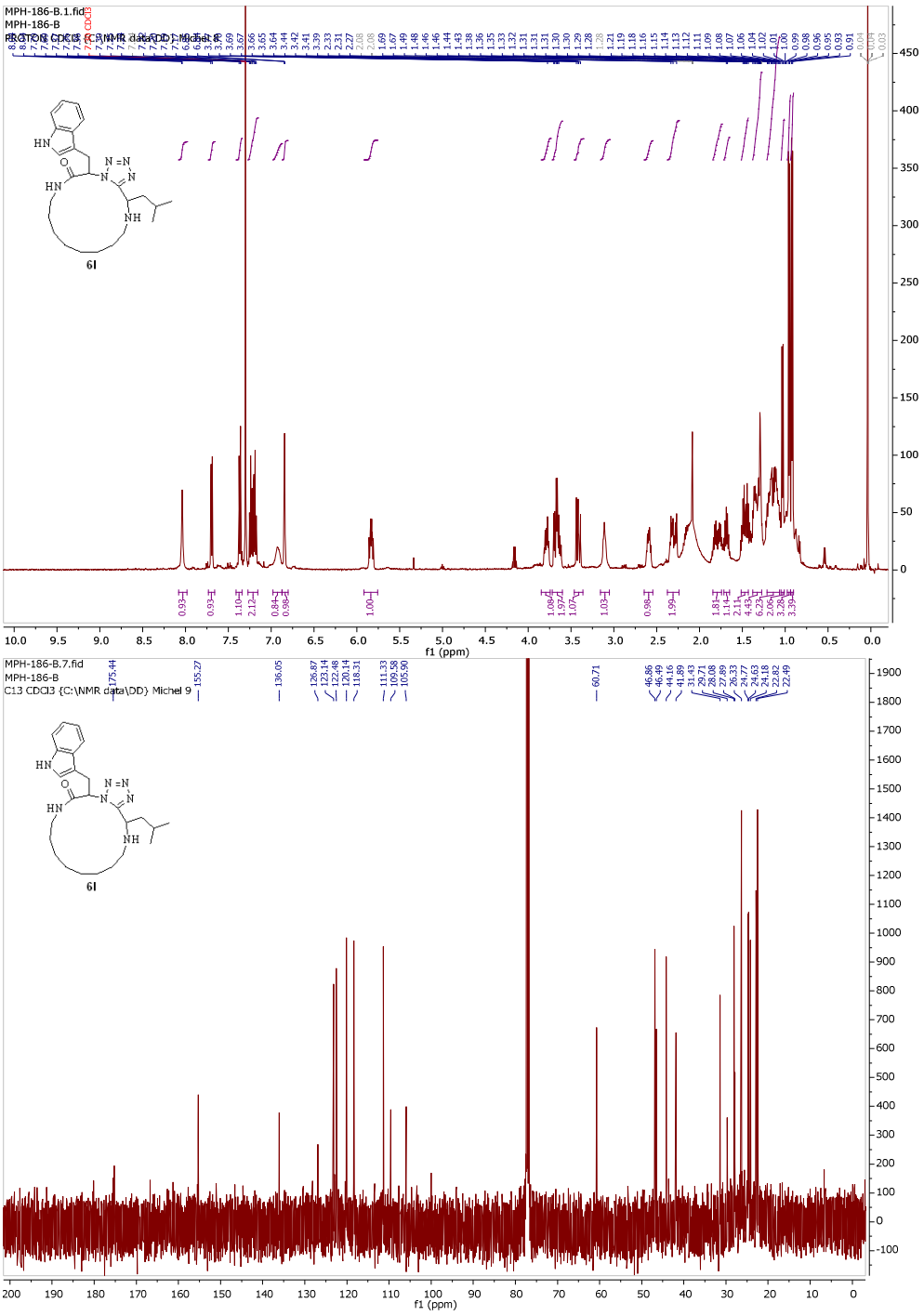
6k

Chemical Formula: $C_{24}H_{35}N_7O$

Exact Mass: 437.2903



Compound 6l: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6l
f1 (ppm)
MPH-186-B.7.fid
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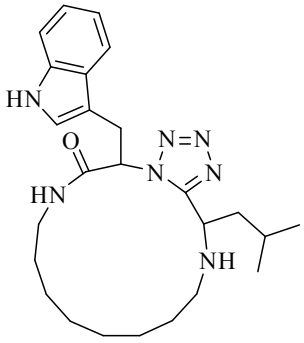
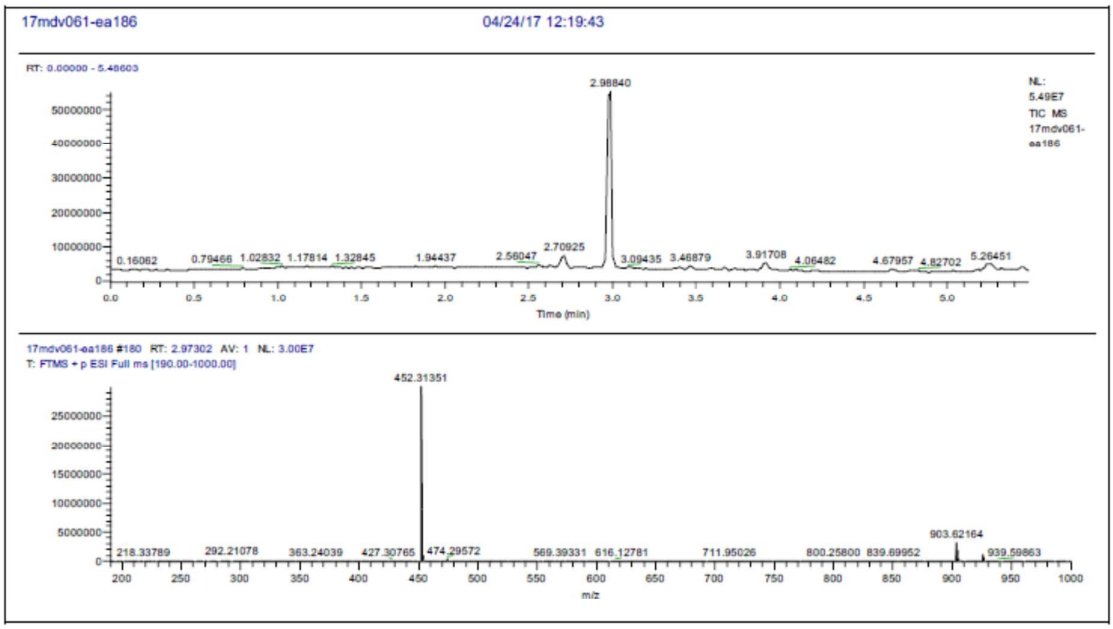
6l
f1 (ppm)



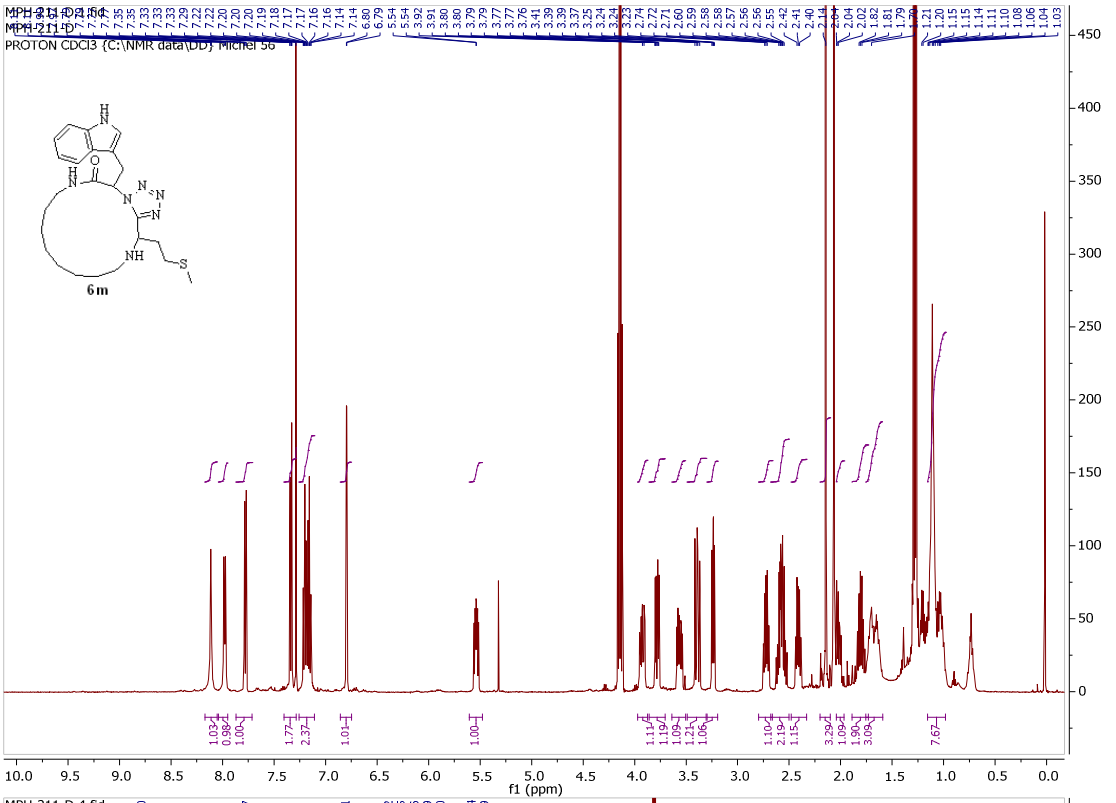
6l

Chemical Formula: $C_{25}H_{37}N_7O$

Exact Mass: 451.3060



Compound 6m: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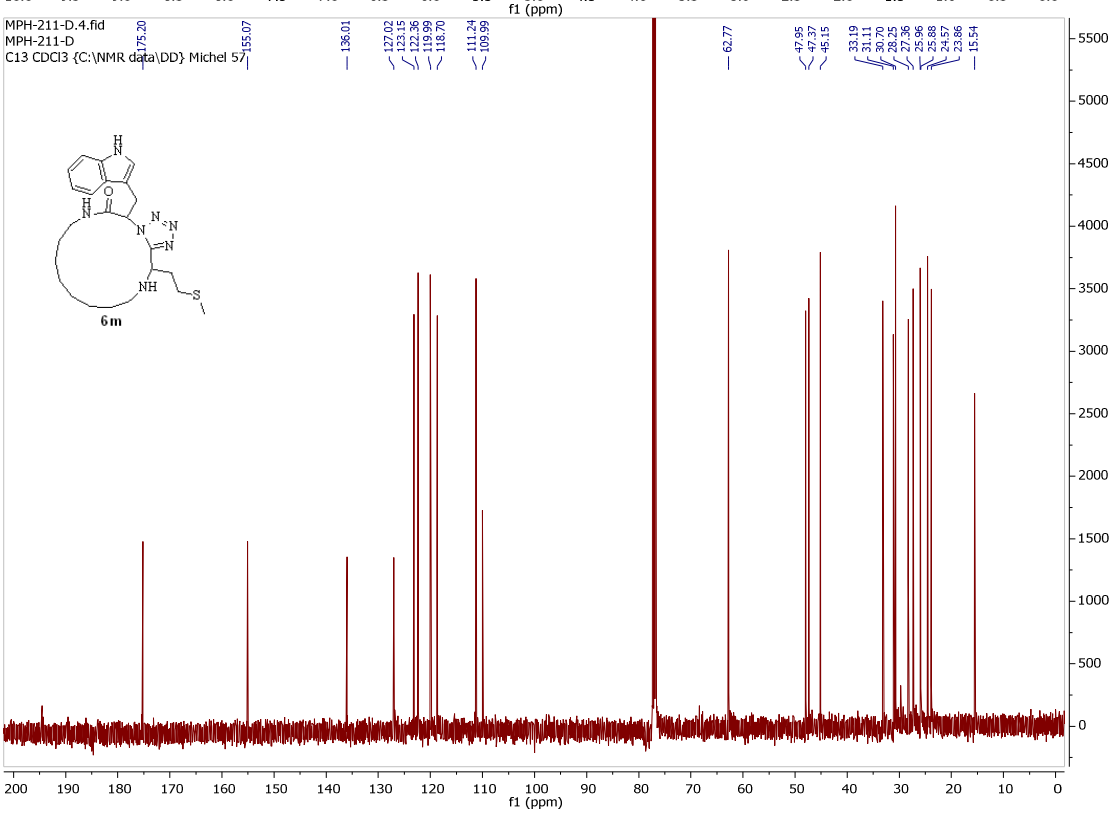
6m
f1 (ppm)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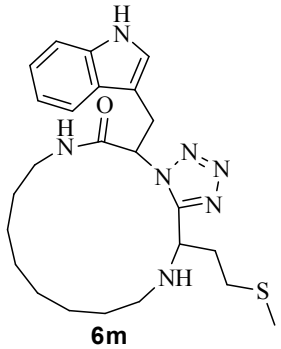
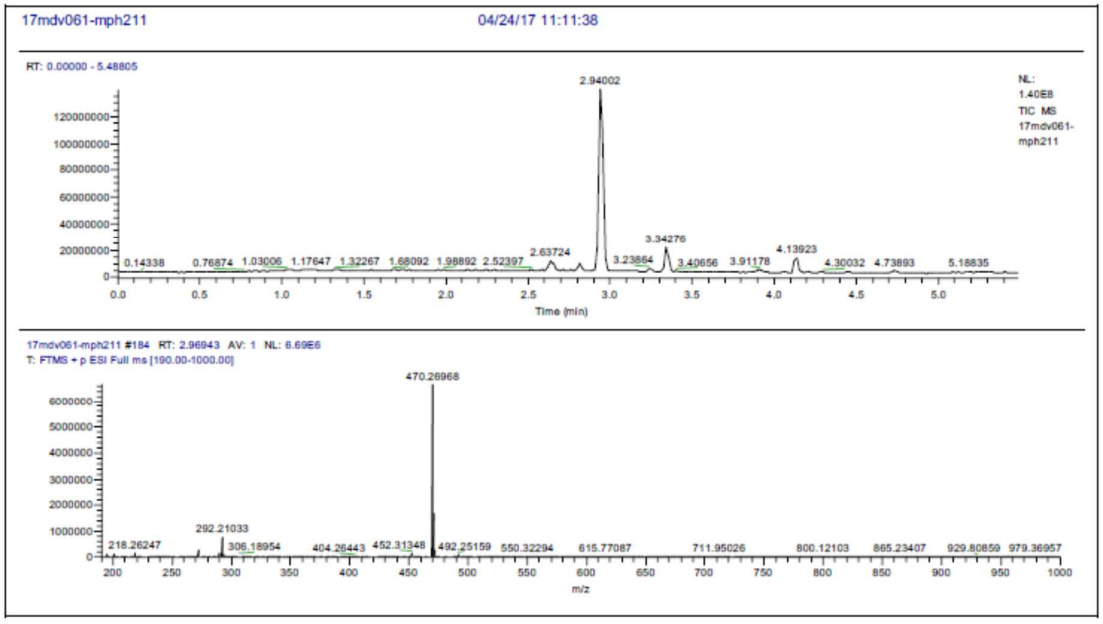
6m
f1 (ppm)



6m

Chemical Formula: $C_{24}H_{35}N_7OS$

Exact Mass: 469.2624



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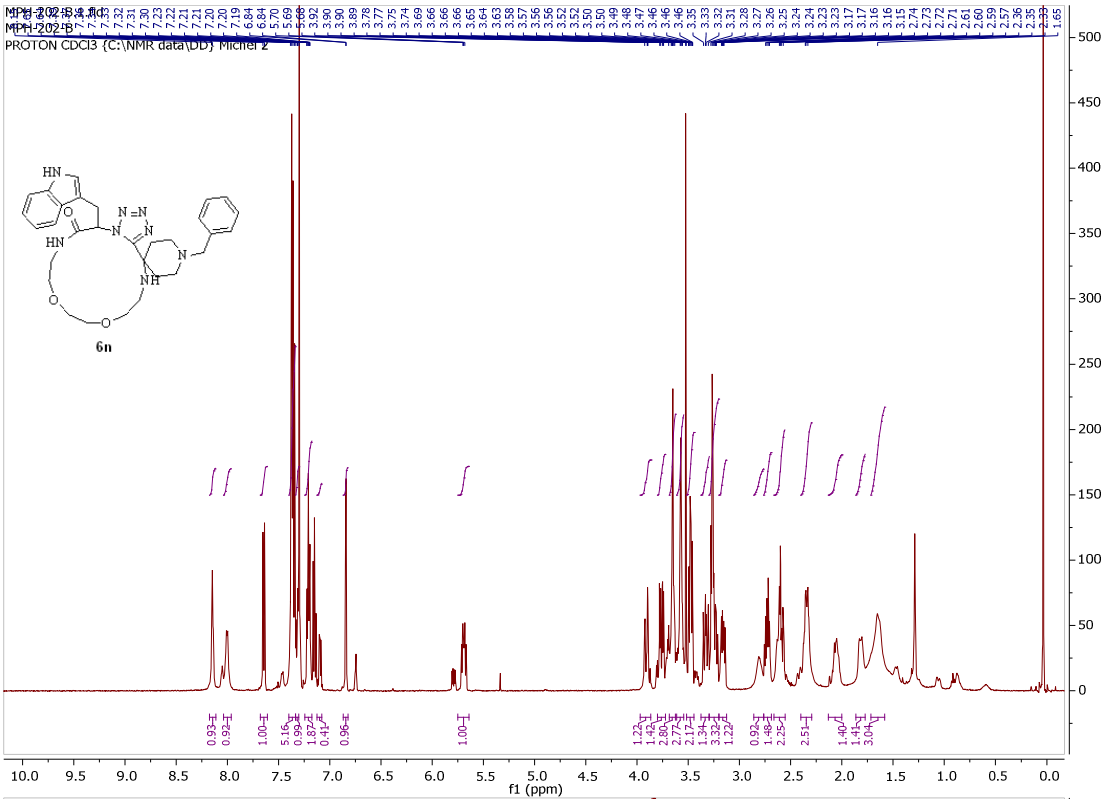
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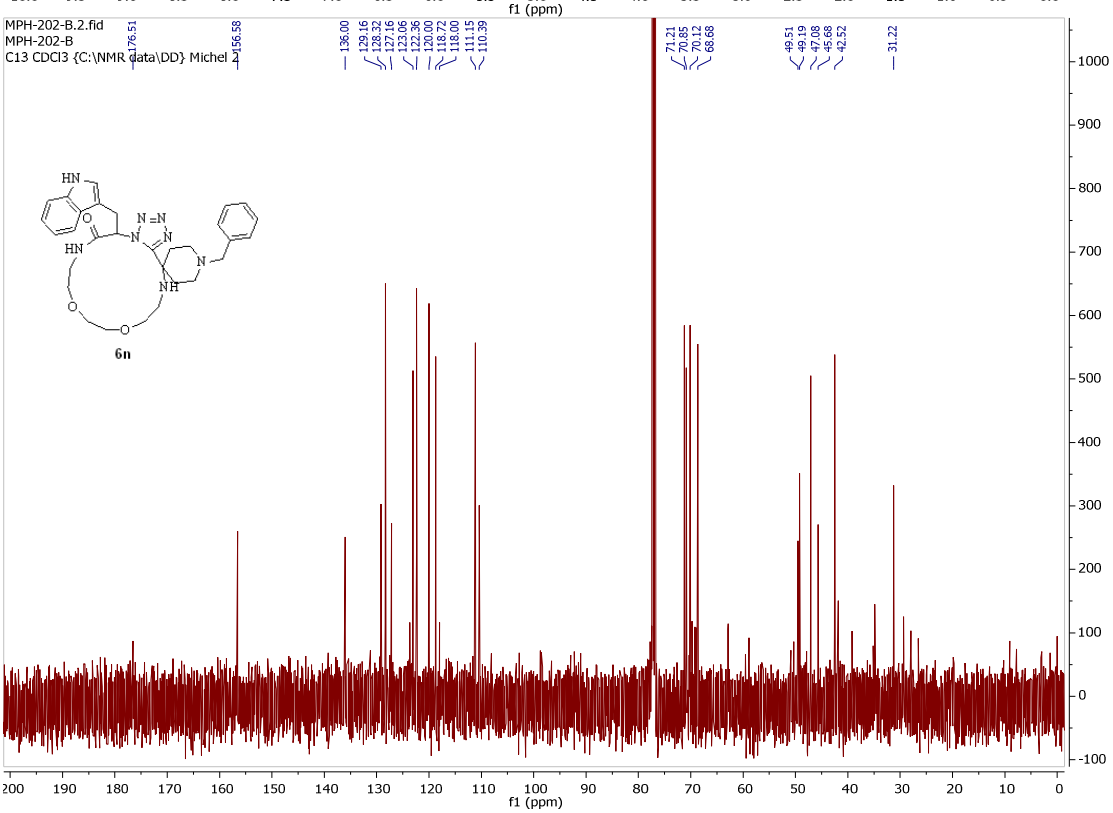
f1 (ppm)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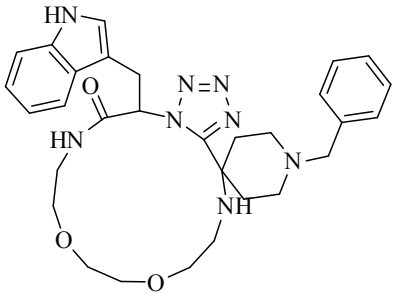
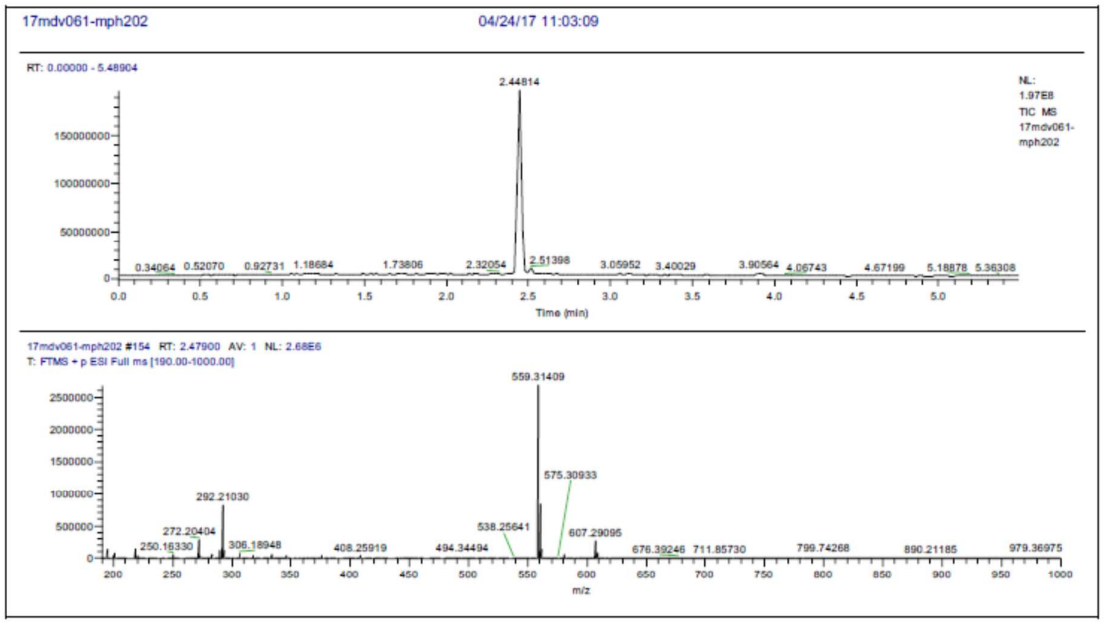
6n
f1 (ppm)



6n

Chemical Formula: $C_{30}H_{38}N_8O_3$

Exact Mass: 558.3067



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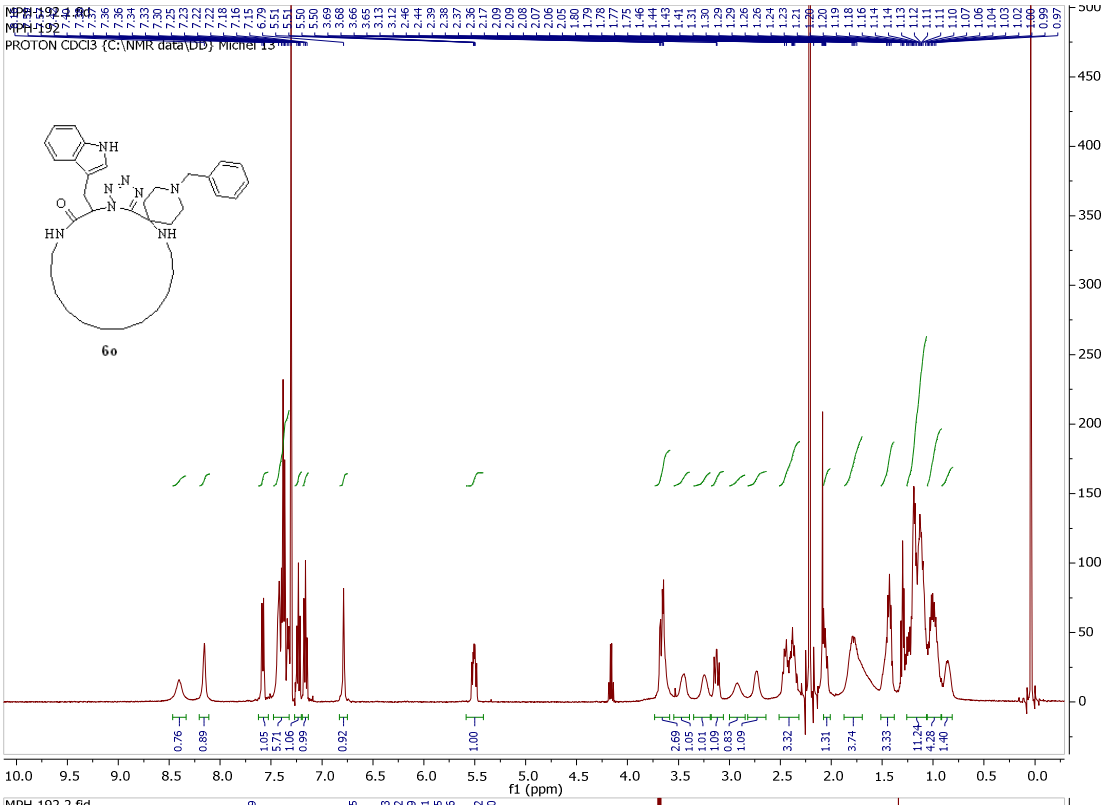
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MPH-192
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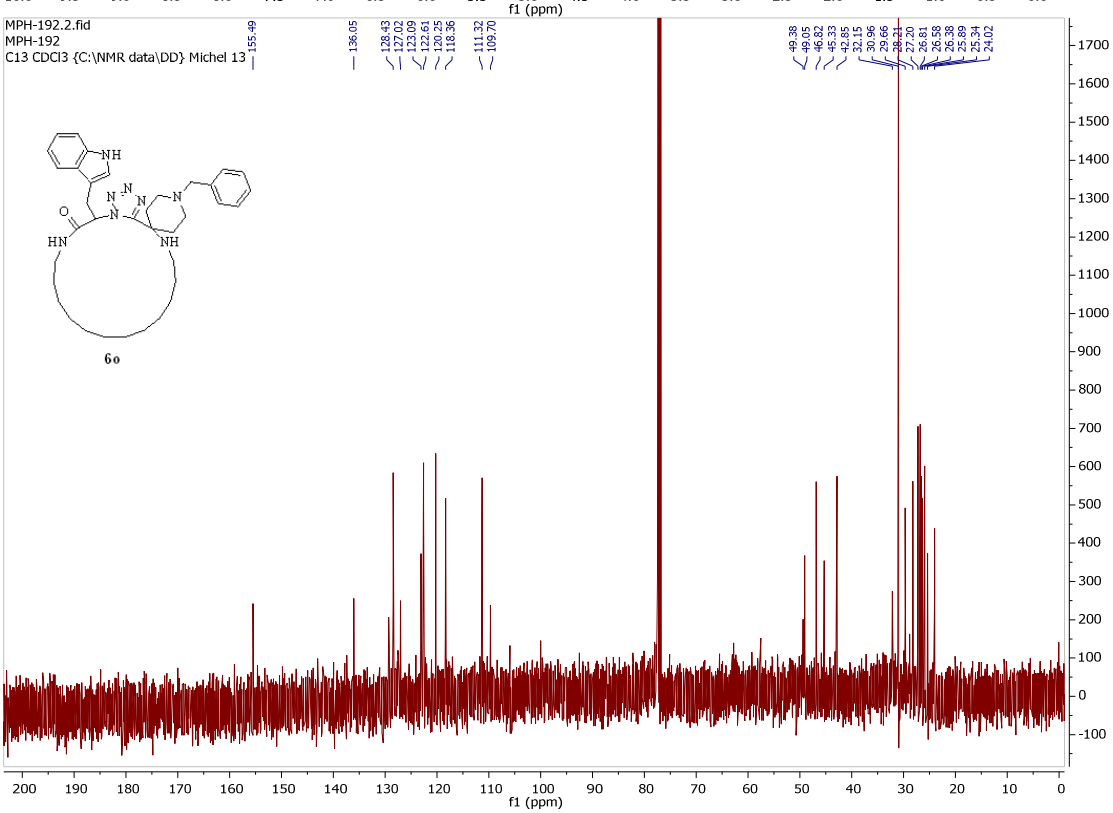
6o
f1 (ppm)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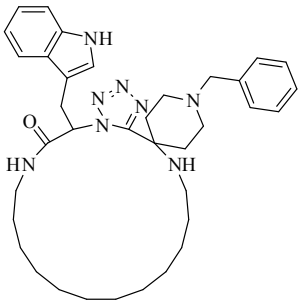
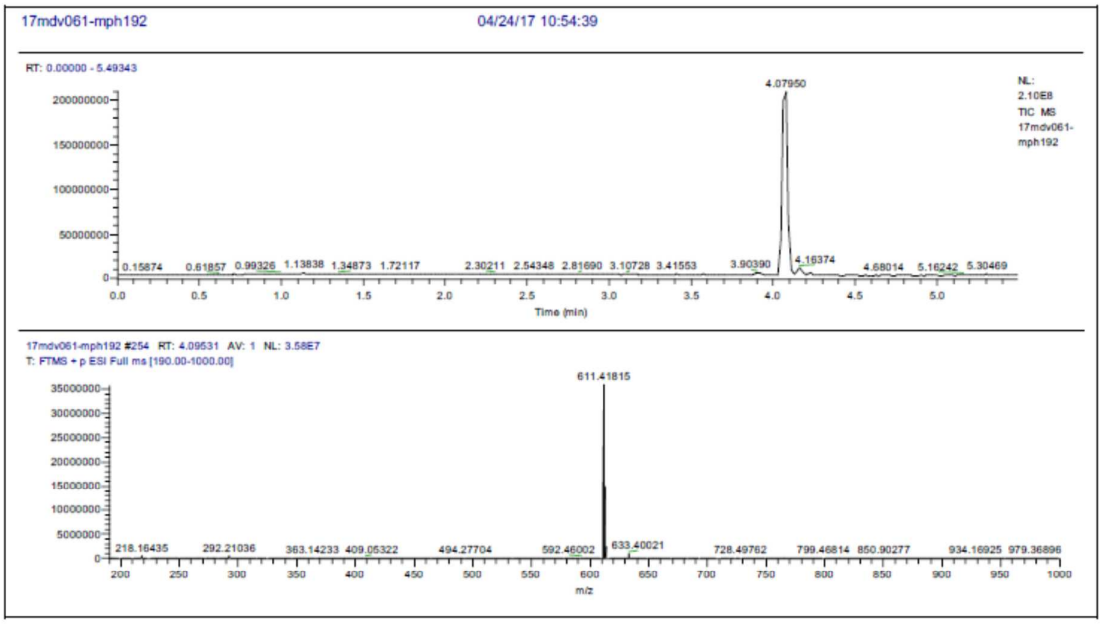
6o
f1 (ppm)



6o

Chemical Formula: $C_{36}H_{50}N_8O$
Exact Mass: 610.4108



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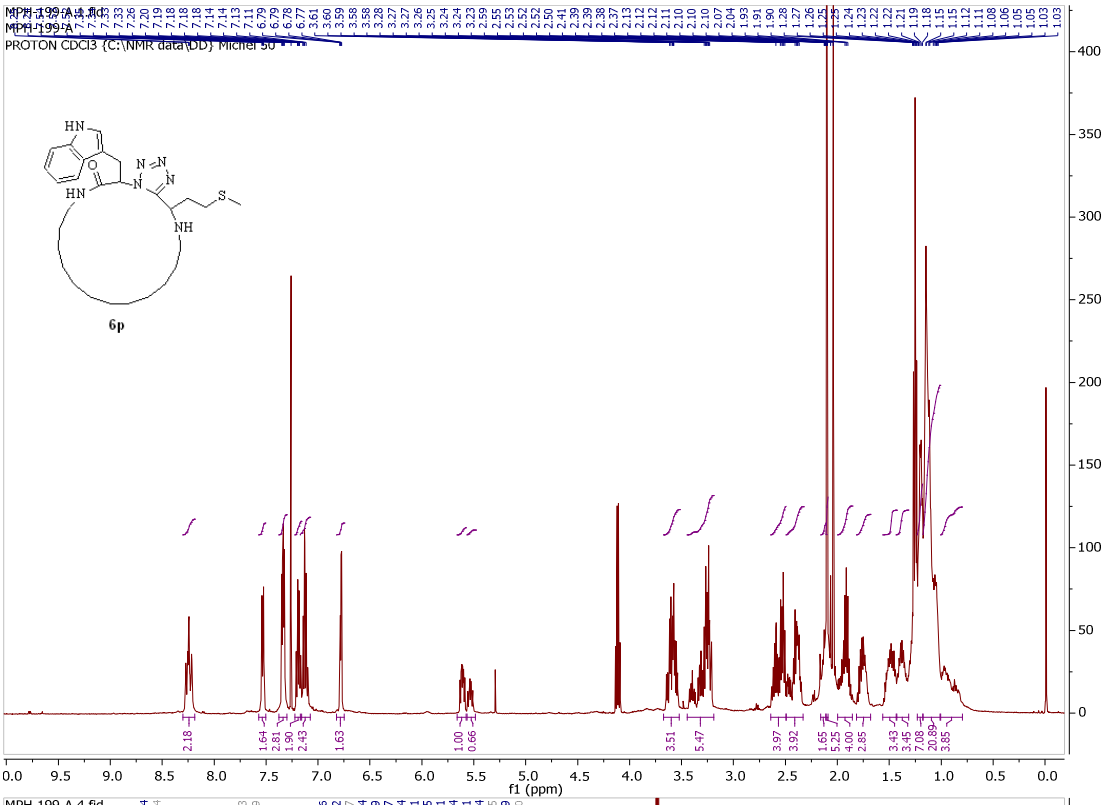
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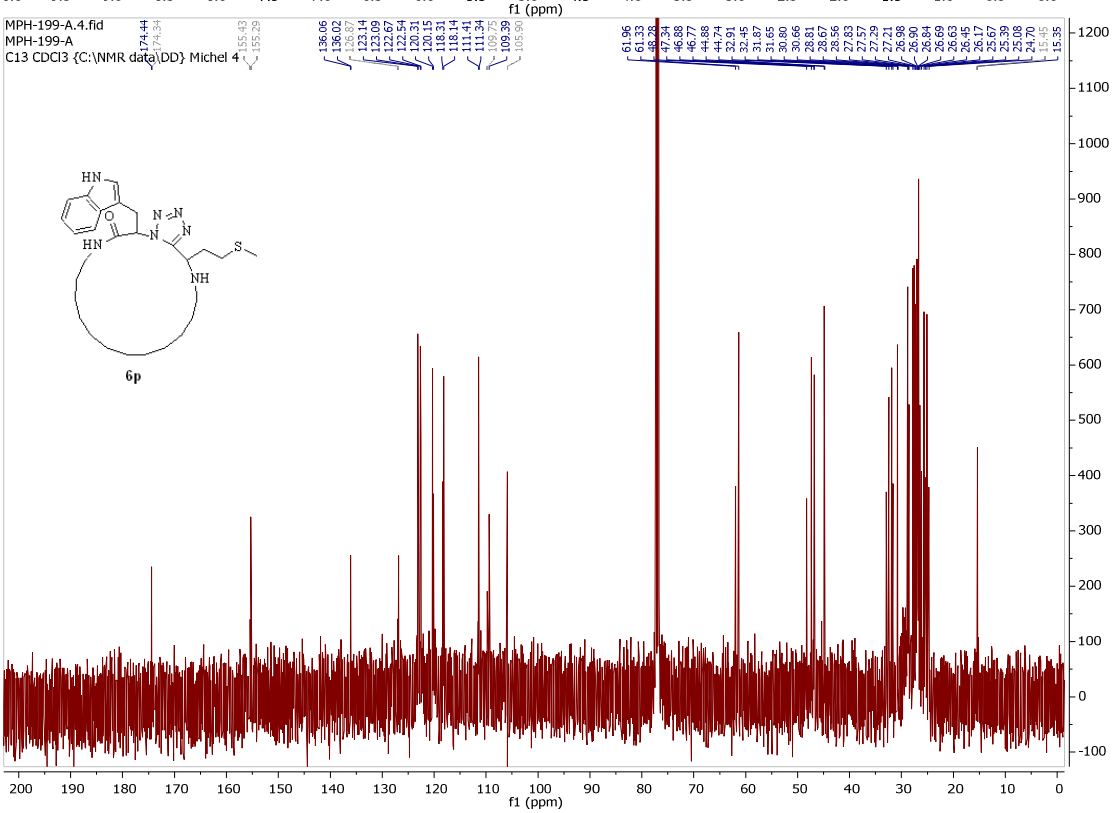
6p
f1 (ppm)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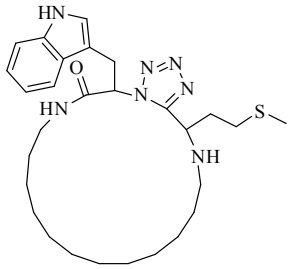
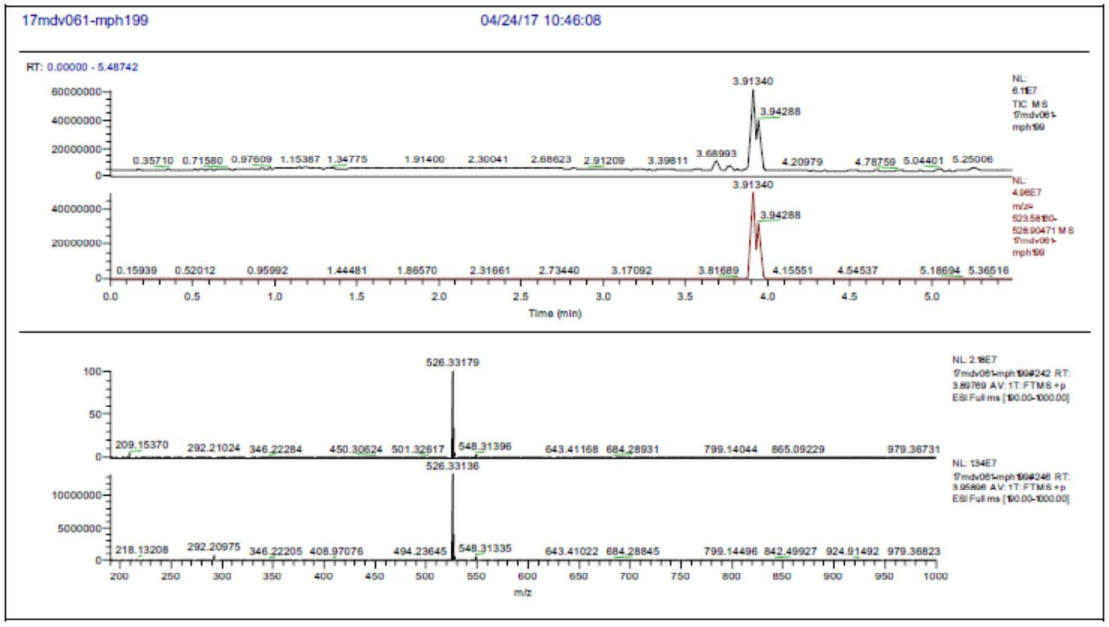
6p
f1 (ppm)



6p

Chemical Formula: $C_{28}H_{43}N_7OS$

Exact Mass: 525.3250



Crystal structure determination

X-ray diffraction data for single crystals of compounds **6a** and **6h** were collected using SuperNova (Rigaku - Oxford Diffraction) four circle diffractometer with a mirror monochromator and a microfocus MoKα radiation source (λ = 0.7107 Å). Single crystals were mounted on Micro MountsTM. Intensities were collected at 130 K. The obtained data sets were processed with CrysAlisPro software [S1]. The phase problem was solved by direct methods using SIR2002 [S2]. Parameters of obtained models were refined by full-matrix least-squares on F^2 using SHELXL-2014/6 [S3]. Calculations were performed using WinGX integrated system (ver. 2013.2) [S4]. Figures were prepared with Mercury 3.5 software [S5].

All non-hydrogen atoms were refined anisotropically to ensure the convergence of the refinement process. All hydrogen atoms attached to carbon atoms were positioned with the idealised geometry and refined with the riding model (isotropic displacement parameter U_{iso}[H] = 1.2 (or 1.5) U_{eq}[C]). The position of hydrogen atoms linked to the N atoms were found on the difference Fourier map. Crystal data and structure refinement results for compounds **6a and 6h** are shown in Table S1. Molecular geometry observed in the crystal structures **6a and 6h** are shown in Figure S1.

In the asymmetric unit of compound **6a** there is one molecule of the macrocyclic compound and one chloroform molecule. The solvent shows positional disorder with site occupancies 76% and 24% and additionally dynamic disorder refined with equal site occupancy. The disordered chloroform molecule interact with N10 of the macrocyclic system, leading to alternative conformations (different positions of N10 (N10A) and C6 (C6A)), refined with site occupancies 78% and 22%.

In the crystal structure of compound **6h** there are channels in [101] direction, occupied by a solvent molecule. (ethanol). Ethanol in the channel is highly disordered. This leads to complicated refinement procedures and many restrains applied in order to obtain more realistic and acceptable molecular geometry. In the proximity of solvent channels there are benzyl groups of the macrocyclic molecule. The disordered solvent leads in consequence to disorder within the mentioned aromatic fragment, which was refined in two alternative positions (site occupancies: 63% and 37%), with several restraints applied. The displacement ellipsoids indicate strongly dynamic character of the disorder, with several alternative positions involved.

Crystallographic data for structures presented in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC 1548701 (**6a**) and CCDC 1548704 (**6h**). Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-(0)1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

References:

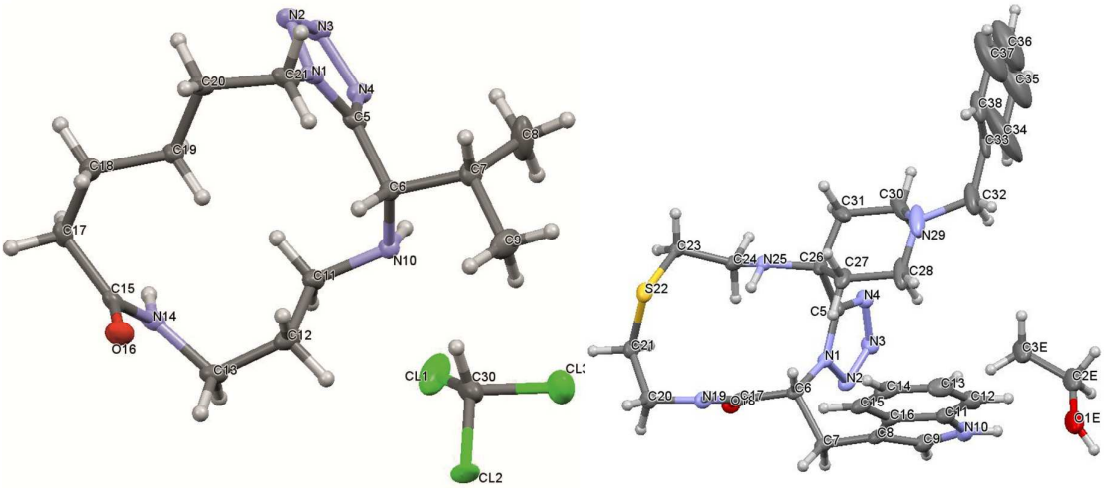
[S1] Oxford Diffraction (2006). CrysAlisPro Oxford Diffraction Ltd, Abingdon, England, Version 1.171.36.20 (release 27-06-2012 CrysAlis171.NET)

[S2] M. C. Burla, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, G. Polidori and R. Spagna, J. Appl. Crystallogr., 2003, 36, 1103.

[S3] Sheldrick, G. M. ActaCryst. 2008, A64, 112-122.

[S4] Farrugia, L., J. J. Appl. Cryst. 1999, 32, 837-838.

[S5] Macrae C. F., Edgington P.R., McCabe P., Pidcock E., Shields G.P., Taylor R., Towler M., & van de Streek J., J. Appl. Cryst. 2006, 39, 453-457.



6a **6h**

Figure S1. Molecular geometry observed in the crystal structures of compounds **6a** and **6h**, showing the atom labelling scheme. For structure **6a**, the more abundant conformer of the partially disordered macrocyclic molecule is shown. For the crystal structure of **6h** a disorder of the ethanol molecule is observed, which causes an additional disorder effect in the benzyl group of the macrocyclic molecule (only more abundant conformers are shown here). Displacement ellipsoids of non-hydrogen atoms are drawn at the 30% probability level. H atoms are presented as small spheres with an arbitrary radius.

Table S1. Crystal data and structure refinement results for compounds **6a and 6h**.

	6a	**6h**
Empirical moiety formula	C_{14} H_{26} N_6 O, $CHCl_3$	C_{28} H_{34} N_8 O S, C_2H_5OH
Formula weight [g/mol]	413.77	576.76
Crystal system	Monoclinic	Monoclinic
Space group	C2/*c*	$P2_1/c$
Unite cell dimensions	a = 22.9082(7) Å b = 8.4405(3) Å c = 21.5120(7) Å α = 90° β = 94.190(3)° γ = 90°	a = 9.3964(3) Å b = 39.1393(10) Å c = 9.7341(3) Å α = 90° β = 109.847(4)° γ = 90°
Volume [$Å^3$]	4148.4(2)	3367.26(19)
Z	8	4
D_{calc} [Mg/m^3]	1.325	1.138
μ [mm^{-1}]	0.458	0.133
F(000)	1744	1232
Crystal size [mm^3]	0.4 x 0.3 x 0.2	0.4 x 0.4 x 0.1
Θ range	3.16° to 28.60°	2.78° to 28.61°
Index ranges	$-27 \le h \le 29$, $-8 \le k \le 10$, $-24 \le l \le 28$	$-12 \le h \le 12$, $-50 \le k \le 51$, $-12 \le l \le 13$
Refl. collected	14349	32691
Independent reflections	4886 [R(int) = 0.0237]	7948 [R(int)=0.0372]
Completeness [%] (Θ 25.24°)	99.8	99.7
Absorption correction	Multi-scan	Multi-scan
Max. and min. transmission	0.897 and 1.000	0.839 and 1.000
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/ restraints/parameters	4886 / 5 / 302	948 / 57 / 454
GooF on F2	1.036	1.030
Final R indices [I>2sigma(I)]	R1= 0.0514, wR2= 0.1207	R1= 0.0902, wR2= 0.2449
R indices (all data)	R1= 0.0646, wR2= 0.1292	R1= 0.1143, wR2= 0.2685
$\Delta\rho_{max}$, $\Delta\rho_{min}$ [$e \cdot Å^{-3}$]	0.66 and -0.51	0.94 and -0.75

Virtual Library Synthesis

The virtual library of azido-Ugi-4CR was created using ChemAxon's REACTOR software (http://www.chemaxon. com). 13 isocyanide esters and 17 diamines making 221 α-Isocyano-ω-amine and 272 oxo compounds were used as reactants. Therefore, the theoretical chemical space of this virtual library is 221 × 272 = 60112 (stereoisomers are not included). To investigate such large chemical space, the program RandReactor was used to provide smaller random sublibrary (N=1000) as smiles file.[1] The smiles file was then uploaded into Instant JChem for calculating molecular weight and LogP. This data was exported as an excel file in order to draw MW vs cLogP plot.

(1) Huang, Y.; Wolf, S.; Bista, M.; Meireles, L.; Camacho, C.; Holak, T. A.; Dömling, A. *Chem. Biol. Drug Des.* **2010**, *76*, 116-129.

List of random 1000 product smiles:

[H]C1(C)NCCNC(=O)CN2N=NN=C12

O=C1N[C@@H]2CCCC[C@H]2NC2(CCN(CC3=CC=CC=C3)CC2)C2=NN=NN2[C@H]1CC1=CNC=N1

FC1=CC(F)=C(C=C1)C1NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NCCCNC1=O)C1=CC(C)=CC=C1

[H]C1(NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CO1

SCC1N2N=NN=C2C(CCl)NC2=CC=CC=C2NC1=O

[H]C1(CC)NCCCCCNC(=O)C(C)(C)N2N=NN=C12

CC1(C)NCCCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(C)NC(C(NC(=O)C(C(C)C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(C)N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(C)NCCCNC(=O)C(CC(C)C)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(CS)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(C)(C)N2N=NN=C12

O=C1N[C@@H]2CCCC[C@H]2NC2(CCN(CC3=CC=CC=C3)CC2)C2=NN=NN2C1CC1=CC=CC=C1

FC(F)(F)C1=CC=C(C=C1)C1NCCOCCOCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(NCCCCNC(=O)C(CS)N2N=NN=C12)C1=C(OC)C=CC=C1

CC1(C)N2N=NN=C2C(NCCCNC1=O)C1CCCCC1

CCC(C)C1NC2=CC=CC=C2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(CCC)NCCSCCNC(=O)C(C(C)C)N2N=NN=C12

[H]C1(CC)NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)NC2=CC=CC=C2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(C)NCCCCCNC(=O)C(CC(C)C)N2N=NN=C12

[H]C1(C)NCCOCCOCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)C(CS)N2N=NN=C12

[H]C1(C)NCCCNC(=O)C(C)(C)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(C)NCCNC(=O)C(C(C)C)N2N=NN=C12

OC1CNC(C2=NN=NN2CC(=O)NC1)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

CCC1(CC)NCCOCCOCCNC(=O)C(CC[Se]C)N2N=NN=C12

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1CC1

[H]C1(CC)NCCOCCOCCNC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(C)(C)NCCCCNC1=O

[H]C1(C)NCC(O)CNC(=O)CN2N=NN=C12

[H]C1(C)NCCSCCNC(=O)[C@H](CCSC)N2N=NN=C12

O=C1CN2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC2=CC=CC=C2N1

COC1CC(C(OC)O1)C1NCCOCCOCCNC(=O)C(C(C)C)N2N=NN=C12

FC1=CC(C2NCCSCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)=C(Cl)C=C1

[H]C1(NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(C)S1

O=C1NCCSCCNC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CN=C1

CC(C)(C)C1NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC(C)C1NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CC)NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1(C)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC2=CC=CC=C2NC1=O

FC1=CC(F)=C(C=C1)C1NCCSCCNC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCCCNC1=O)C1=CC(C)=CC=C1

O=C1NC(C(NC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC(OC2=CC=CC=C2)=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1

O=C1NC(C(NC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC2=C(NC=C2)C=C1)C1=CC=CC=C1)C1=CC=CC=C1

O=C1NC(C(NC(CC2=CC=CC=C2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CO1

ClCC1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(CC)NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC1(C)NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(C)NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(C)N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCC(O)CNC1=O

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(C=C1)C(F)(F)F

[H]C1(NCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=C(OC)C=CC=C1

SCC1N2N=NN=C2C(NCCCNC1=O)C1CCCCC1

[H]C1(NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC(Cl)=C1Cl

OC1=C(O)C=C(C=C1)C1NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CN1CCC2(CC1)NCC(O)CNC(=O)C(CC1=CNC3=C1C=CC=C3)N1N=NN=C21

[H]C1(NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C(O)CO

[H]C1(CCC)NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CC)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1(C)NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCCOCCOCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCC(C)(C)CNC1=O

FC1=CC(F)=C(C=C1)C1NCCOCCOCCNC(=O)CN2N=NN=C12

OC1CNC(C2=NN=NN2[C@@H](CC2=CNC=N2)C(=O)NC1)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC(OC)=C1O

FC1=C(C=CC=C1)C1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CSCCC1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CCC1(CC)NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

O=C1NC(C(NC(C2CC2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(CC)N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1(C)NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C(NCCCNC1=O)C1=CC=C(OC(F)(F)F)C=C1

CC(C)CC1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC=C(C=C1)C(F)(F)F

COC1CC(C(OC)O1)C1NC2=CC=CC=C2NC(=O)CN2N=NN=C12

CC(C)C1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=C2C=CC=CC2=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NC2=CC=CC=C2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NC(C(NC(=O)C(CS)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OC)C(O)=C1

[H]C1(NCC(O)CNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

C[Se]CCC1N2N=NN=C2C(NCCNC1=O)C(C)(C)C

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCNC1=O)C(C)C

[H]C1(CC)NC2=CC=CC=C2NC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(C)(C)NCCSCCNC1=O

CC1(C)N2N=NN=C2C(NCCCNC1=O)C1=CC=C(OC(F)(F)F)C=C1

FC1=CC(F)=C(C=C1)C1NC2=CC=CC=C2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C(NCCSCCNC1=O)C1=CC(C)=CC=C1

[H]C1(NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CO1

ClCC1NC2=CC=CC=C2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(CC)NCCCCCNC(=O)C(CC(C)C)N2N=NN=C12

CC1(C)NCCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(C)NC(C(NC(=O)C(CS)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

FC1=CC(F)=C(C=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1=CC=CC(=C1)C1NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(NCCCNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CO1

ClCC1NC2=CC=CC=C2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(CC)NCCCCCNC(=O)C(CS)N2N=NN=C12

CC(C)C1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=CC=C1OC(F)(F)F

FC(F)(F)C1=C(C=CC=C1)C1NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=C(OC)C=CC=C1

O=C1NCCSCCNC(C2CCCCC2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

CCC(C)C1NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CCC)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CC)NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1(C)NC2=CC=CC=C2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(OC(F)(F)F)C=C1

CC(C)CC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C(C=C1)C(F)(F)F

[H]C1(NCCOCCOCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=C(OC)C=CC=C1

SCC1N2N=NN=C2C(NCCCCNC1=O)C1CCCCC1

CCC(C)C1NCC(O)CNC(=O)C(C)(C)N2N=NN=C12

[H]C1(CCC)NCCSCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(NCC(O)CNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=C(Br)S1

CCOC(=O)C1CC1C1NCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=C(OCC2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1

[H]C1(NCCCCCCNC(=O)C(C)N2N=NN=C12)C1=CC=CC(O)=C1

[H]C1(NC(C(NC(=O)CN2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C(OC)OC

CCC1(CC)N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CCSC)N2N=NN=C12

FC(F)(F)OC1=CC=CC=C1C1NCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CCOC(=O)C1CC1C1NCCOCCOCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C(NCCCCNC1=O)C1=CC=C(OCC2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1

[H]C1(NCCCCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=CC(O)=C1

OC1=CC(C2NCCCCCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)=C(Br)C=C1

SCC1N2N=NN=C2C(NCCCNC1=O)C1=C(Cl)C=CC=C1Cl

CSCC[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CSC2=C1C=CC=C2

CC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC=C(F)C=C1Cl

ClCC1(CCl)NCCSCCNC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC=CN=C1

[H]C1(NCCCCNC(=O)CN2N=NN=C12)C1=CC=C(Br)S1

CC(C)C1N2N=NN=C2C(NCCNC1=O)C1=CC2=CC=CC=C2S1

OC1CNC(C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1)C1=C(Cl)C=CC(F)=C1

[H]C1(NCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(C)S1

O=C1NCCOCCOCCNC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CN=C1

CC(CC1=CC=C(C=C1)C(C)(C)C)C1NCCCCNC(=O)C(C)N2N=NN=C12

OC1CNC(C2=CNC3=C2C=CC=C3)C2=NN=NN2CC(=O)NC1

CSCC[C@@H]1N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C(C)C=C1

[H]C1(NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

O=C1NCCSCCNC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC2=C1C=CN2

CC1=CC=C(C=C1)C1NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

O=C1NCCNC2(CCCCC2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

[H]C1(NC2=CC=CC=C2NC(=O)C(C)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

O=C1CN2N=NN=C2C(NCCSCCN1)C1=CC=CC2=C1C=CN2

CSCC[C@@H]1N2N=NN=C2C(NCCCNC1=O)C1=CC=C(C)C=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

O=C1NCCCCNC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC2=C1C=CN2

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC(Br)=CC=C1

[H]C1(NCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=C(Cl)C=C1

CC1=C(C=CC=C1)C1NCCCNC(=O)C(CS)N2N=NN=C12

CC(C)C1N2N=NN=C2C(NCCNC1=O)C1=CC(OCC2=CC=CC=C2)=CC=C1

OC1CNC(C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1)C1=C(Cl)C(F)=CC=C1F

OC1=C(O)C=C(C=C1)C1NCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CN1CCC2(CC1)NCCCCCCNC(=O)C(CC1=CNC3=C1C=CC=C3)N1N=NN=C21

CC(C)CC1N2N=NN=C2C(NCCCNC1=O)C1=C(Cl)C(F)=CC=C1F

OC1=C(O)C=C(C=C1)C1NC2=CC=CC=C2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CN1CCC2(CC1)NCCCCCNC(=O)C(CS)N1N=NN=C21

FC1=CC=C(F)C(C2NCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)=C1Cl

COC1=CC(OC)=C(C=C1)C1NCC(C)(C)CNC(=O)C(CS)N2N=NN=C12

CC1(C)N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=C(C=C1)C#N

[H]C1(NCCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1O

[H]C1(NC(C(NC(=O)C(CS)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC2=C(OCO2)C=C1

[H]C1(NCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=C(OC)C=CC=C1O

[H]C1(NCCCCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=CC(OC)=C1O

[H]C1(NCCCCNC(=O)C(C)(C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCSCCNC(=O)C(CS)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCSCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

FC1=CC=C(C=C1)C1NCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

COC(=O)C1=C(C2NC3=CC=CC=C3NC(=O)[C@H](CCSC)N3N=NN=C23)C(OC)=CC(OC)=C1

CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CNC2=C1C=CC(Cl)=C2

[H]C1(NCCOCCOCCNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC(OC)=CC(OC)=C1

FC1=CC=CC(Cl)=C1C1NCCCCCCNC(=O)CN2N=NN=C12

CC(C)C1N2N=NN=C2C(NCCCCNC1=O)C1=CC=C2C=CC=CC2=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCCCCCNC(=O)C(CS)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NC2=CC=CC=C2NC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCOCCOCCNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCOCCOCCNC(=O)CN2N=NN=C12)C1=CC=C(OC)C(O)=C1

C[Se]CCC1N2N=NN=C2C(NCCCNC1=O)C1=CC=C(F)C=C1

COC(=O)C1=C(C2NC3=CC=CC=C3NC(=O)C(N3N=NN=C23)C2=CC=CC=C2)C(OC)=CC(OC)=C1

CC(C)C1N2N=NN=C2C(NCCSCCNC1=O)C1=C(C=CC=C1)C(O)=O

OC1=C(C=CC=C1)C1NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(CCCCC)NC2=CC=CC=C2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C2(CCCC2)NCCCCCNC1=O

O=C1NCCOCCOCCNC(C2CC2)C2=NN=NN2C1CC1=CC=CC=C1

[H]C1(CC)NCCCCNC(=O)C(CS)N2N=NN=C12

CC1(C)NCCCNC(=O)C(C)(C)N2N=NN=C12

[H]C1(C)NC2=CC=CC=C2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(C)NCCSCCNC(=O)C(C(C)C)N2N=NN=C12

[H]C1(C)NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(C)NCCNC(=O)C(CC(C)C)N2N=NN=C12

O=C1N[C@@H]2CCCC[C@H]2NC2(CCN(CC3=CC=CC=C3)CC2)C2=NN=NN2C1CC1=CC=CS1

COC1CC(C(OC)O1)C1NCCOCCOCCNC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(NCCCCNC1=O)C1=CC(=CC=C1)C#N

OC1CNC(C2=NN=NN2CC(=O)NC1)C1=CC=NC=C1

CSCC[C@@H]1N2N=NN=C2C(CC(C)C)NCCSCCNC1=O

C[Se]CCC1N2N=NN=C2C(C)(C)NCCOCCOCCNC1=O

[H]C1(C)NCC(C)(C)CNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

[H]C1(C)NCCOCCOCCNC(=O)C(CO)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)C(C)N2N=NN=C12

[H]C1(C)NCCCNC(=O)CN2N=NN=C12

[H]C1(C)NCCNC(=O)[C@H](CCSC)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NCCCCNC1=O)C1=C(F)C=C(F)C=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCCNC1=O)C1=CC(C)=CC=C1

SCC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC(OCC2=CC=CC=C2)=CC=C1

CC1(C)N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C2C=NNC2=C1

O=C1NCCCCCCNC(CC2=CC=CC=C2)C2=NN=NN2C1C1=CC=CC=C1

CC(C)C1N2N=NN=C2C2(CCCCC2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

O=C1N[C@@H]2CCCC[C@H]2NC2(CCCC2)C2=NN=NN2[C@H]1CC1=CNC=N1

O=C1NCCCCNC(C2CC2)C2=NN=NN2C1CC1=CC=CS1

[H]C1(CC)NCCCNC(=O)C(CC(C)C)N2N=NN=C12

CC1(C)NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(C)NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12

[H]C1(C)NCCSCCNC(=O)C(C)(C)N2N=NN=C12

[H]C1(C)NCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)CC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC2=CC=CC=C2NC1=O

FC(F)(F)C1=CC=C(C=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)CN2N=NN=C12

[H]C1(NCCCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=C(OC)C=CC=C1

CC(C)C1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OCC(O)=O)C=C1

ClC1=C(C=CC=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

COC(=O)CCC1NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NCCCNC1=O)C1=CC=CN1

ClCC1NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(CC)NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12

CC1(C)NCCCCCNC(=O)C(C)(C)N2N=NN=C12

[H]C1(C)NCCCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(C)N[C@@H]2CCCC[C@H]2NC(=O)C(C(C)C)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC2=CC=CC=C2NC1=O

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCSCCNC1=O)C1=C(F)C=C(F)C=C1

OC1CNC(C2=NN=NN2C(CS)C(=O)NC1)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

CSCC[C@@H]1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=C(Br)C=CC=C1

CC(C)(C)OC(=O)N1C=C(C2NCCSCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)C2=C1C=CC=C2

[H]C1(NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC(O)=C1

[H]C1(NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C(OC)OC

CCC1(CC)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

OC1CNC(C2CC2)C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1

[H]C1(CC)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1(C)NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NC2=CC=CC=C2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCCCCCNC1=O

CC(C)CC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC=C(C=C1)C(F)(F)F

COC1CC(C(OC)O1)C1N[C@@H]2CCCC[C@H]2NC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCCCCNC1=O)C1=CC(=CC=C1)C#N

CC(C)C1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CNC2=C1C=C(Cl)C=C2

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC(OC)=CC(OC)=C1

O=C1NC(C(NC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC(=CC=C1)C#N)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CSC=C1

CC(C)CC1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC(C)C1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(CC)NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC1(C)N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(C)NCC(C)(C)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCCCCCCNC1=O

FC1=CC(F)=C(C=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCCCCNC1=O)C1=CC(C)=CC=C1

CC(C)C1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(Cl)C(F)=CC=C1F

OC1=C(O)C=C(C=C1)C1NC(C(NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CN1CCC2(CC1)NC(C(NC(=O)C(CC1=CC=CS1)N1N=NN=C21)C1=CC=CC=C1)C1=CC=CC=C1

C[Se]CCC1N2N=NN=C2C2(CCCCC2)NCC(C)(C)CNC1=O

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCCC2)NCCOCCOCCNC1=O

OCC1N2N=NN=C2C(NCCCCNC1=O)C1CC1

[H]C1(CC)NCCCNC(=O)C(C)N2N=NN=C12

CC1(C)N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC=C(OC(F)(F)F)C=C1

C[Se]CCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=C(C=C1)C(F)(F)F

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=C(OC)C=CC=C1

CC1(C)OB(OC1(C)C)C1=CC(=CC=C1)C1NCC(C)(C)CNC(=O)C(CS)N2N=NN=C12

[H][C@@]12C[C@@]3([H])C[C@@]([H])(C1)C1(NCCCCCCNC(=O)C(C)(C)N4N=NN=C14)[C@@]([H])(C2)C3

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CS)N2N=NN=C12)C1=C(OC)C=CC=C1O

FC1=CC=CC(F)=C1C1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC1=C(C=CC=C1)C1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

O=C1NC(C(NC(C2=CC=CN2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC=C1)C1=CC=CC=C1

ClCC1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CC)NCC(C)(C)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=CC=C1OC(F)(F)F

CCOC(=O)C1CC1C1NCCCCNC(=O)CN2N=NN=C12

O=C1NCCNC(C2=NN=NN2[C@H]1CC1=CNC=N1)C1=CC=C(OCC2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1

CC1(C)CNC(C2=NN=NN2C(C)(C)C(=O)NC1)C1=C(Br)C=CC=C1

[H]C1(NC(C(NC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OC)C(OC)=C1

FC1=CC(=CC(F)=C1F)C1NCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

OCC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC=C2C=CC=CC2=C1

CC1N2N=NN=C2C(NCCSCCNC1=O)C1=C(C)C=CS1

OC(=O)C1=C(C=CC=C1)C1NC2=CC=CC=C2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C(NCCSCCNC1=O)C1=C(O)C=CC=C1

[H]C1(CCCCC)NCC(O)CNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

O=C1NCCCCCNC2(CCCC2)C2=NN=NN2C1CC1=CC=CS1

CSCC[C@@H]1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=C(Br)S1

CC1N2N=NN=C2C2(CCC(CC2)C2=CC=CC=C2)NCC(O)CNC1=O

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC2=CC=CC=C2S1

CC1(C)CNC(C2=NN=NN2C(CC2=CC=CC=C2)C(=O)NC1)C1=CC(=CC=C1)C#N

SCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=NC=C1

CC(C)CC1N[C@@H]2CCCC[C@H]2NC(=O)C(C)(C)N2N=NN=C12

CC(C)C1NCC(C)(C)CNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(CC)NCCCCCCNC(=O)C(C(C)C)N2N=NN=C12

OCC1N2N=NN=C2C(NCCCNC1=O)C1=C(C=CC=C1)C(F)(F)F

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1CC(OC)OC1OC

OCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC(=CC=C1)C#N

CC1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC=NC=C1

CC(C)CC1NCCOCCOCCNC(=O)CN2N=NN=C12

COC1=CC(=CC(OC)=C1OC)C1NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

O=C1NCCNC(C2=NN=NN2C1CC1=CC=CS1)C1=CC2=C(NC=C2)C=C1

CC(C)CC1N2N=NN=C2C(CC2=CC=CC=C2)NC2=CC=CC=C2NC1=O

BrCCC1=CC=C(C=C1)C1NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NCCCNC1=O)C1=CC=C(C=C1)C(C)C

[H]C1(CCCCC)NCCNC(=O)C(CS)N2N=NN=C12

CC1(C)N2N=NN=C2C2(CCCC2)NC2=CC=CC=C2NC1=O

CC1(C)CNC(C2=CC=C(Br)S2)C2=NN=NN2C(CC2=CC=CC=C2)C(=O)NC1

COC(=O)CCCCC1NCCOCCOCCNC(=O)C(CS)N2N=NN=C12

CC1(C)N2N=NN=C2C(CC2=CC=CC=C2)NCCCCNC1=O

BrCCC1=CC=C(C=C1)C1NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CC(C)C1=CC=C(C=C1)C1NCCNC(=O)C(CS)N2N=NN=C12

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1

FC1=CC=C(Cl)C(F)=C1C1NCCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CS)N2N=NN=C12)C1=CC=CC(O)=C1O

COC1=C(OCC2=CC=CC=C2)C=CC(=C1)C1NCC(C)(C)CNC(=O)C(C(C)C)N2N=NN=C12

O=C1NC(C(NC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)(C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1

ClC1=C(C=CC=C1)C1NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

COC(=O)CCC1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

O=C1NCCCCNC(C2=CC=CN2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

CC1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC(OC2=CC=CC=C2)=CC=C1

CC(C)CC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(Br)O1

[H]C1(NC(C(NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OC)C=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(C=C1)B1OC(C)(C)C(C)(C)O1

O=C1NCCOCCOCCNC(C2=NN=NN2C1C1=CC=CC=C1)(C1=CC=CC=C1)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=C(Cl)C=CC=C1

C[Se]CCC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=C(F)C=CC=C1F

O=C1NCCCCNC(C2=NN=NN2C1C1=CC=CC=C1)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

[H]C1(NC2=CC=CC=C2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CC(O)=C1

C[Se]CCC1N2N=NN=C2C(NCCCCNC1=O)C1=CC(NC(=O)OC(C)(C)C)=CC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC=C(C=C1)C(O)=O

CSCC[C@@H]1N2N=NN=C2C(NCCCCCNC1=O)C1=CC(Br)=CC=C1

CC(C)(C)OC(=O)N1C=C(C2NCCCCCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)C2=C1C=CC=C2

SCC1N2N=NN=C2C(NCCCNC1=O)C1=C(Br)C=CC=C1

[H]C1(NCC(C)(C)CNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1

CC1N2N=NN=C2C(NCCNC1=O)C1=CC(F)=C(F)C(F)=C1

COC(=O)CCCC1NC2=CC=CC=C2NC(=O)CN2N=NN=C12

CC1(C)N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CNC2=C1C=C(Cl)C=C2

[H]C1(NCCCCCCNC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC(OC)=CC(OC)=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC(=CC=C1)C#N

CC1(C)OB(OC1(C)C)C1=C(C=CC=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CS)N2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=C(OCC(O)=O)C=C1

[H]C1(NCCOCCOCCNC(=O)C(C)N2N=NN=C12)C1=CC(OC)=CC=C1OC

O=C1CN2N=NN=C2C(CCC2=CC=CC=C2)NCCCCN1

CC1(C)OB(OC1(C)C)C1=C(C=CC=C1)C1NC2=CC=CC=C2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(OCC(O)=O)C=C1

ClC1=C(C=CC=C1)C1NCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

COC(=O)CCC1NCCCNC(=O)C(C(C)C)N2N=NN=C12

O=C1NCCNC(C2=CC=CN2)C2=NN=NN2[C@H]1CC1=CNC=N1

C[Se]CCC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC(OC2=CC=CC=C2)=CC=C1

BrC1=CC=C(O1)C1NCCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(NC(C(NC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OC)C=C1

O=C1NC(C(NC(C2CCCCC2)C2=NN=NN2C1CC1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NCCCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC(Cl)=C1Cl

CC(C)C1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC(O)=C(O)C=C1

CN1CCC2(CC1)NCC(C)(C)CNC(=O)[C@H](CC1=CNC=N1)N1N=NN=C21

FC1=CC=C(F)C(C2NCCNC(=O)C(CC3=CC=CS3)N3N=NN=C23)=C1Cl

CC(C)CC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC(O)=C(O)C=C1

COC1=C(OCC2=CC=CC=C2)C=CC(=C1)C1NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(NCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC(O)=CC=C1

[H]C1(NCCCCCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=C(OC)C=CC(Br)=C1

OCC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(C=C1)C(O)=O

[H]C1(NCC(O)CNC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC(OC)=C1O

[H]C1(NCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCSCCNC(=O)C(CO)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)N[C@@H]2CCCC[C@H]2NC1=O

FC(F)(F)C1=CC=C(C=C1)C1NCCOCCOCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(NCCCCNC(=O)C(C(C)C)N2N=NN=C12)C1=C(OC)C=CC=C1

OCC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OCC(O)=O)C=C1

[H]C1(NCC(O)CNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC(OC)=CC=C1OC

CC(C)(C)OC(=O)NCC1N[C@@H]2CCCC[C@H]2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

O=C1NCCOCCOCCNC(C2=NN=NN2[C@H]1CC1=CNC=N1)C1=CN=C2C=CC=CC2=C1

CC1(C)N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=C2C=CC=CC2=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCSCCNC(=O)C(CC[Se]C)N2N=NN=C12

[H]C1(NCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CO)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCOCCOCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

OCC1N2N=NN=C2C(NCCCCNC1=O)C1=CC=C(F)C=C1

[H]C1(NCCCNC(=O)C(C)N2N=NN=C12)C1=CC=CC=C1

[H]C1(NC2=CC=CC=C2NC(=O)C(C)(C)N2N=NN=C12)C1=C(O)C=CC(Br)=C1

C[Se]CCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=C(Cl)C=CC=C1Cl

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=C(O)C=C(O)C=C1

CN1CCC2(CC1)NCCOCCOCCNC(=O)C(CO)N1N=NN=C21

[H]C1(NCCCCNC(=O)C(C)N2N=NN=C12)C(O)CO

[H]C1(CCC)NCC(O)CNC(=O)CN2N=NN=C12

[H]C1(CC)NCCSCCNC(=O)[C@H](CCSC)N2N=NN=C12

[H]C1(C)NCCOCCOCCNC(=O)C(CC[Se]C)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

[H]C1(C)NCCCNC(=O)C(CO)N2N=NN=C12

OCC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC2=CC=CC=C2NC1=O

CC1N2N=NN=C2C(NCCSCCNC1=O)C1=C(F)C=C(F)C=C1

CC1(C)N2N=NN=C2C(NCC(O)CNC1=O)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

[H]C1(NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC(OC)=C1O

FC1=C(C=CC=C1)C1NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12

CSCCC1NCCCCCNC(=O)C(C)(C)N2N=NN=C12

CCC1(CC)NCCCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1CC1

[H]C1(CC)N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(C)NCC(O)CNC(=O)C(CC(C)C)N2N=NN=C12

[H]C1(C)NCCSCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCC(O)CNC1=O

FC(F)(F)C1=CC=C(C=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

COC1CC(C(OC)O1)C1NCCOCCOCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)N2N=NN=C2C(NCCOCCOCCNC1=O)C1=C(Cl)C=CC(F)=C1

C[Se]CCC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C2C=CC=CC2=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NC2=CC=CC=C2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C(F)C=C1

[H]C1(NCCOCCOCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC=C1

CC(C)(C)C1NCCCCNC(=O)C(CS)N2N=NN=C12

CC(C)C1NCCCNC(=O)C(C)(C)N2N=NN=C12

[H]C1(CC)NC2=CC=CC=C2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C(C)(C)NCCSCCNC1=O

[H]C1(C)NCC(O)CNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(C)NCCSCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCC(O)CNC1=O

[H]C1(NCCNC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC=CO1

CC[C@H](C)[C@@H]1N2N=NN=C2C(CCl)NC2=CC=CC=C2NC1=O

[H]C1(CC)NCCCCCNC(=O)C(CO)N2N=NN=C12

OCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=CC=C1OC(F)(F)F

CCOC(=O)C1CC1C1NCCCCNC(=O)C(C)N2N=NN=C12

CC1=CC=CC(=C1)C1NCC(O)CNC(=O)CN2N=NN=C12

[H]C1(NCCSCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=CO1

C[Se]CCC1N2N=NN=C2C(C)(C)NCCCCCCNC1=O

[H]C1(C)NC(C(NC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

SCC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

CSCC[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC=C(C=C1)C(F)(F)F

CCC(C)C1NC2=CC=CC=C2NC(=O)C(CC[Se]C)N2N=NN=C12

[H]C1(CCC)NCCSCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

[H]C1(NCC(O)CNC(=O)C(CS)N2N=NN=C12)C1=CC=C(Br)S1

CSCC[C@@H]1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(C=CC=C1)C(F)(F)F

CCC(C)C1NCC(C)(C)CNC(=O)C(CC[Se]C)N2N=NN=C12

[H]C1(CCC)NCCOCCOCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

[H]C1(CC)NCCCCNC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(C)(C)NCC(O)CNC1=O

CC1(C)N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(OC(F)(F)F)C=C1

OC1CNC(C2=NN=NN2C(C2=CC=CC=C2)C(=O)NC1)C1=C(F)C=C(F)C=C1

CC(C)CC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

[H]C1(NCC(C)(C)CNC(=O)C(CS)N2N=NN=C12)C1=CC=CC(O)=C1

[H]C1(NCCCCCCNC(=O)C(C)(C)N2N=NN=C12)C(OC)OC

OC1=CC(C2NCCCCCCNC(=O)C(CC3=CC=CC=C3)N3N=NN=C23)=C(Br)C=C1

SCC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC2=C1C=CN2

FC1=CC=CC(=C1)C1NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CSCCC1NCCCNC(=O)C(CC(C)C)N2N=NN=C12

CCC1(CC)NC2=CC=CC=C2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

SCC1N2N=NN=C2C(NCCCCCNC1=O)C1CC1

CC(C)C1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=CC=C1OC(F)(F)F

FC(F)(F)C1=C(C=CC=C1)C1NC2=CC=CC=C2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

COC1CC(C(OC)O1)C1NC(C(NC(=O)C(CS)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CSCC[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=C(Cl)C=CC(F)=C1

CC(CC1=CC=C(C=C1)C(C)(C)C)C1NCCCCNC(=O)CN2N=NN=C12

COC1=CC(OC)=C(C=C1)C1NCCNC(=O)C(C(C)C)N2N=NN=C12

OC1CNC(C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1)C1=CC=C(F)C=C1Cl

ClCC1(CCl)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

OC1CNC(C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1)C1=CC=CN=C1

CC(C)(C)C1NCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC(C)C1NCCOCCOCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCCCCNC(=O)C(C)N2N=NN=C12)C1=CC=C(Br)S1

CCOC(=O)C1CC1C1NCC(O)CNC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCCCCCNC1=O)C1=CC(C)=CC=C1

[H]C1(NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

O=C1NCCNC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC2=C1C=CN2

CSCC[C@@H]1N2N=NN=C2C(NCCCNC1=O)C1=CC(F)=CC=C1

OC1=CC(C2NC(C(NC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)C2=CC=CC=C2)C2=CC=CC=C2)=C(Br)C=C1

O=C1NC(C(NC(C2=NN=NN2C1CC1=CNC2=C1C=CC=C2)C1=CC=CC2=C1C=CN2)C1=CC=CC=C1)C1=CC=CC=C1

CC1=CC=C(C=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

O=C1NCCCCNC2(CCCCC2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

[H]C1(NCC(O)CNC(=O)C(C)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC(Cl)=C(Cl)C=C1

OC1=CC(O)=C(C=C1)C1NCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CN1CCC2(CC1)NCCCNC(=O)C(CS)N1N=NN=C21

[H]C1(NCCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC(Cl)=C1Cl

COC1=CC(OC)=C(C=C1)C1NCC(O)CNC(=O)C(CS)N2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(F)C=C1Cl

CC(CC1=CC=C(C=C1)C(C)(C)C)C1NCCOCCOCCNC(=O)CN2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=C(O)C=C(O)C=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCN(C)CC2)N[C@@H]2CCCC[C@H]2NC1=O

CC1(C)N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=C2NN=CC2=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CC(OC)=C1O

CC1(C)CNC(C2=NN=NN2C(CC2=CC=CS2)C(=O)NC1)C1=C(F)C=CC=C1

CSCCC1NCCCCCCNC(=O)C(CC(C)C)N2N=NN=C12

[H]C1(NCCOCCOCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=C(O)C=CC(Br)=C1

CC(C)CC1N2N=NN=C2C(NCCCCNC1=O)C1=CNC2=C1C=CC=C2

[H]C1(NCCOCCOCCNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC(OC)=C1O

OCC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(C=C1)C(F)(F)F

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCSCCNC1=O)C1CC(OC)OC1OC

FC1=CC(C2NCCSCCNC(=O)C(N3N=NN=C23)C2=CC=CC=C2)=C(Cl)C=C1

O=C1NCCCCCNC(C2=NN=NN2[C@H]1CC1=CNC=N1)C1=CC=C2C=CC=CC2=C1

CC1=C(SC=C1)C1NCCOCCOCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(NCC(C)(C)CNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC=C1

[H]C1(NCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=C(O)C=CC(Br)=C1

OCC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CSC2=C1C=CC=C2

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC=C(F)C=C1Cl

O=C1N[C@@H]2CCCC[C@H]2NC(C2=NN=NN2C1C1=CC=CC=C1)C1=C2C=CC=CC2=CC=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCCNC(=O)C(C)(C)N2N=NN=C12

FC1=CC=C(C=C1)C1NC2=CC=CC=C2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(NCCSCCNC(=O)C(C(C)C)N2N=NN=C12)C1=CC=CC=C1

CC(C)(C)C1NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC(C)C1NCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(CC)NC2=CC=CC=C2NC(=O)C(CC(C)C)N2N=NN=C12

CC1(C)CNC(C2=NN=NN2C(CC2=CC=CS2)C(=O)NC1)C1=CC=C(OC(F)(F)F)C=C1

CC(C)CC1N2N=NN=C2C(NCCCCCCNC1=O)C1=C(F)C=C(F)C=C1

O=C1NCCCCCCNC(C2=NN=NN2C1CC1=CC=CS1)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

[H]C1(NCC(C)(C)CNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC(O)=C1

[H]C1(NCCCCCCNC(=O)C(CS)N2N=NN=C12)C(OC)OC

CCC1(CC)N[C@@H]2CCCC[C@H]2NC(=O)C(C)(C)N2N=NN=C12

CC1(C)CNC(C2CC2)C2=NN=NN2C(C2=CC=CC=C2)C(=O)NC1

[H]C1(CC)NCCOCCOCCNC(=O)C(C(C)C)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC(C)=CC=C1

[H]C1(NCCCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=CO1

OCC1N2N=NN=C2C(CCl)NCC(O)CNC1=O

OCC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(Br)S1

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCC(CC2)C2=CC=CC=C2)NCCSCCNC1=O

O=C1NCCSCCNC(C2=CC3=CC=CC=C3S2)C2=NN=NN2C1C1=CC=CC=C1

FC1=CC(C2NCCCCCNC(=O)[C@H](CC3=CNC=N3)N3N=NN=C23)=C(Cl)C=C1

[H]C1(NCCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC=C(C)S1

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=CN=C1

CC(C)(C)C1NCC(C)(C)CNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CC(C)C1NCCOCCOCCNC(=O)C(CS)N2N=NN=C12

[H]C1(CC)NCC(C)(C)CNC(=O)C(C)(C)N2N=NN=C12

FC(F)(F)OC1=CC=C(C=C1)C1NCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

FC(F)(F)C1=C(C=CC=C1)C1NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12)C1=C(OC)C=CC=C1

CC1(C)N2N=NN=C2C(NCCSCCNC1=O)C1CCCCC1

CCC(C)C1NCC(O)CNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

COC1=CC(=CC(OC)=C1OC)C1NCCCCCNC(=O)C(CC(C)C)N2N=NN=C12

O=C1NCCOCCOCCNC(C2=NN=NN2C1CC1=CC=CC=C1)C1=CC2=C(NC=C2)C=C1

CC1(C)CNC(CC2=CC=CC=C2)C2=NN=NN2C(CS)C(=O)NC1

[H]C1(NCCCCCCNC(=O)C(C)(C)N2N=NN=C12)C1=CC=CO1

[H]C1(NCCOCCOCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

SCC1N2N=NN=C2C(NCCCCNC1=O)C1=CC=CC2=C1C=CN2

CC1=CC=C(C=C1)C1NCCCNC(=O)C(C)(C)N2N=NN=C12

O=C1NCCNC2(CCCCC2)C2=NN=NN2C1C1=CC=CC=C1

CC(C)C1N2N=NN=C2C2(CCCC2)NCCNC1=O

OC1CNC(C2=NN=NN2CC(=O)NC1)C1=CC=C(OCC2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1

CC(C)(C)OC(=O)NC1=CC=CC(=C1)C1NCCOCCOCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

SCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=CNC2=C1C=CC(Cl)=C2

[H]C1(NC(C(NC(=O)C(C)(C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC(O)=C1O

CCCC1(CCC)N[C@@H]2CCCC[C@H]2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)CC1N2N=NN=C2C(NCCCCNC1=O)C1=CC=C(OCC2=CC=CC=C2)C=C1

FC1=CC=C(F)C(C2NCCSCCNC(=O)CN3N=NN=C23)=C1Cl

CSCC[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC(O)=C(O)C=C1

O=C1CN2N=NN=C2C(NCCCCN1)C1=CC(OC2=CC=CC=C2)=CC=C1

CC(C)C1N2N=NN=C2C(NCCNC1=O)C1=CSC2=C1C=CC=C2

FC1=CC=C(C2NCCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)C(Cl)=C1

ClCC1(CCl)NCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCCNC(=O)CN2N=NN=C12)C1=CC2=C(OCO2)C=C1

[H]C1(NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

FC1=CC=C(C=C1)C1NCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

COC(=O)C1=C(C2NC3=CC=CC=C3NC(=O)C(C)N3N=NN=C23)C(OC)=CC(OC)=C1

OC(=O)C1=C(C=CC=C1)C1NCCSCCNC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCCCNC1=O)C1=C(O)C=CC=C1

OC1=CC(C2NCCCCNC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)=C(Br)C=C1

SCC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC(Cl)=C(Cl)C=C1

CSCC[C@@H]1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CSC2=C1C=CC=C2

CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(F)C=C1Cl

CC(C)CC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=C2C=CC=CC2=CC=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCCCCCNC(=O)CN2N=NN=C12

[H]C1(NCC(C)(C)CNC(=O)C(C(C)C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

FC1=CC=C(C=C1)C1NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

COC(=O)C1=C(C2NCC(O)CNC(=O)C(C)N3N=NN=C23)C(OC)=CC(OC)=C1

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CNC2=C1C=CC(Cl)=C2

CN1C2CCC1CC1(C2)NCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CCCC1(CCC)NCC(O)CNC(=O)C(CS)N2N=NN=C12

CC(C)C1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(OCC2=CC=CC=C2)C=C1

O=C1NCCCNC(C2=NN=NN2[C@H]1CC1=CNC=N1)C1=CC=C2C=NNC2=C1

O=C1NC2=CC=CC=C2NC(CC2=CC=CC=C2)C2=NN=NN2C1CC1=CC=CS1

CC(C)CC1N2N=NN=C2C2(CCCCC2)NCCCCCNC1=O

O=C1NCCOCCOCCNC2(CCCC2)C2=NN=NN2C1CC1=CC=CC=C1

SCC1N2N=NN=C2C(NCCCCNC1=O)C1CC1

[H]C1(CC)NCCCNC(=O)C(C)(C)N2N=NN=C12

CC1(C)NCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(C)NC2=CC=CC=C2NC(=O)C(C(C)C)N2N=NN=C12

OCC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC=C(C=C1)C(F)(F)F

[H]C1(NCCSCCNC(=O)C(C)N2N=NN=C12)C1=C(OC)C=CC=C1

CC1(C)OB(OC1(C)C)C1=CC(=CC=C1)C1NCC(O)CNC(=O)C(C)(C)N2N=NN=C12

[H][C@@]12C[C@@]3([H])C[C@@]([H])(C1)C1(NCCCCCNC(=O)C(N4N=NN=C14)C1=CC=CC=C1)[C@@]([H])(C2)C3

[H]C1(NCC(O)CNC(=O)CN2N=NN=C12)C1=CC=C(Br)C=C1

CSCC[C@@H]1N2N=NN=C2C(NCCSCCNC1=O)C1=C(F)C=CC=C1F

C[Se]CCC1N2N=NN=C2C(CCl)NCCOCCOCCNC1=O

[H]C1(CC)NCC(C)(C)CNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

CC1(C)NCCCCCCNC(=O)C(CO)N2N=NN=C12

[H]C1(C)NC(C(NC(=O)C(C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC1(C)N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

FC1=CC(F)=C(C=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)CC1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

BrC1=C(C=CC=C1)C1NC2=CC=CC=C2NC(=O)CN2N=NN=C12

CC(C)C1N2N=NN=C2C(NCCCNC1=O)C1=CC(F)=C(F)C(F)=C1

COC(=O)CCCC1NC2=CC=CC=C2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(NCCOCCOCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC2=C(OCO2)C=C1

CC1(C)CNC(C2=NN=NN2C(CO)C(=O)NC1)C1=C(O)C=CC=C1

[H]C1(CCCCC)NCCCCCCNC(=O)C(C)N2N=NN=C12

O=C1CN2N=NN=C2C2(CCCC2)NC(C(N1)C1=CC=CC=C1)C1=CC=CC=C1

CSCC[C@@H]1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1CC1

FC(F)(F)OC1=CC=C(C=C1)C1NC2=CC=CC=C2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

FC(F)(F)C1=CC=C(C=C1)C1NC(C(NC(=O)C(CS)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

COC1CC(C(OC)O1)C1NCC(O)CNC(=O)[C@H](CCSC)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(CC(C)C)NCCSCCNC1=O

COC1=CC(=CC(OC)=C1OC)C1NCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

BrC1=CC=C(O1)C1NCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)N2N=NN=C2C(NCCCCCNC1=O)C1=CC2=CC=CC=C2S1

O=C1NCCCCCCNC(C2=NN=NN2C1C1=CC=CC=C1)C1=CC(=CC=C1)C#N

CC(C)C1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=NC=C1

CC(C)CC1N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC(C)C1NCC(C)(C)CNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(CC)NCCCCCCNC(=O)C(CC(C)C)N2N=NN=C12

FC(F)(F)OC1=CC=C(C=C1)C1NCCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(F)C=C(F)C=C1

CC1=CC=CC(=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC(OCC2=CC=CC=C2)=CC=C1

OCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=C2C=NNC2=C1

CC1N2N=NN=C2C(CC2=CC=CC=C2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(C)(C)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1

CC(C)C1=CC=C(C=C1)C1NCC(C)(C)CNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(CCCCC)NCCCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

OCC1N2N=NN=C2C2(CCCC2)NCC(O)CNC1=O

OCC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C(Br)S1

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCC(CC2)C2=CC=CC=C2)NC2=CC=CC=C2NC1=O

[H]C1(NCCSCCNC(=O)C(CO)N2N=NN=C12)C1=CC=C(OC)C=C1

CC1(C)OB(OC1(C)C)C1=CC=C(C=C1)C1NCCCNC(=O)C(CO)N2N=NN=C12

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCCCNC1=O)(C1=CC=CC=C1)C1=CC=CC=C1

OCC1N2N=NN=C2C(NCC(O)CNC1=O)C1=C(Cl)C=CC=C1

[H]C1(NCCCCCNC(=O)C(CO)N2N=NN=C12)C1=CC=C(OCC2=CC=CC=C2)C(OC)=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(NCCSCCNC(=O)C(CO)N2N=NN=C12)C1=CC=CC(Cl)=C1

CC(C)(C)OC(=O)N1C=C(C2NCCCNC(=O)C(CO)N3N=NN=C23)C2=C1C=CC=C2

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(NCCOCCOCCNC(=O)C(CO)N2N=NN=C12)C1=CC=CC(Cl)=C1

COC(=O)CCC1NCC(C)(C)CNC(=O)C(C)N2N=NN=C12

O=C1CN2N=NN=C2C(NCCOCCOCCN1)C1=CC=CN1

OC1CNC(C2=NN=NN2[C@@H](CC2=CNC=N2)C(=O)NC1)C1=CC(OC2=CC=CC=C2)=CC=C1

O=C1NCCCCCNC(C2=NN=NN2C1CC1=CC=CS1)C1=CC2=C(NC=C2)C=C1

CC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC(Br)=CC=C1

[H]C1(NCCCCNC(=O)CN2N=NN=C12)C1=CC=C(Cl)C=C1

CC(C)(C)OC(=O)N1C=C(C2NC3=CC=CC=C3NC(=O)[C@H](CC3=CNC=N3)N3N=NN=C23)C2=C1C=CC=C2

CC1(C)N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC(Cl)=C1

CC(C)CC1N2N=NN=C2C(NCCCCNC1=O)C1=CN(C(=O)OC(C)(C)C)C2=C1C=CC=C2

O=C1CN2N=NN=C2C(NCCCCCN1)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(NCCOCCOCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=CC(Cl)=C1

[H]C1(NCCSCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=CC(O)=C1

CC(C)(C)OC(=O)NC1=CC=CC(=C1)C1NCCCNC(=O)C(CS)N2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CNC2=C1C=CC(Cl)=C2

[H]C1(NCCNC(=O)C(C)N2N=NN=C12)C1=CC(OC)=CC(OC)=C1

O=C1CN2N=NN=C2C(NC2=CC=CC=C2N1)C1=CC(=CC=C1)C#N

CC1(C)OB(OC1(C)C)C1=C(C=CC=C1)C1NCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(OCC(O)=O)C=C1

ClC1=C(C=CC=C1)C1NCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(NC2=CC=CC=C2NC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=C(OCC2=CC=CC=C2)C(OC)=C1

O=C1CN2N=NN=C2C(N[C@@H]2CCCC[C@H]2N1)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(NCCCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=CC(Cl)=C1

CC(C)C1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1

CC1(C)CNC(CCC2=CC=CC=C2)C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1

CC1N2N=NN=C2C(NCCCCCCNC1=O)C1=C(C=CC=C1)B1OC(C)(C)C(C)(C)O1

[H][C@@]12C[C@@]3([H])C[C@@]([H])(C1)C1(N[C@@H]4CCCC[C@H]4NC(=O)CN4N=NN=C14)[C@@]([H])(C2)C3

[H]C1(NCCCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC(O)=CC=C1

CC(C)C1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CNC2=C1C=CC(Cl)=C2

[H]C1(NCC(C)(C)CNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CC(O)=C1O

COC1=C(OCC2=CC=CC=C2)C=CC(=C1)C1NCCCCCNC(=O)C(CC[Se]C)N2N=NN=C12

O=C1NCCNC(C2=NN=NN2C1CC1=CC=CS1)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(NCCNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC(Cl)=C1

[H]C1(NC(C(NC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OCC2=CC=CC=C2)C(OC)=C1

COC(=O)CCC1NCC(O)CNC(=O)C(CC[Se]C)N2N=NN=C12

O=C1NCCCCCNC(C2=NN=NN2C1C1=CC=CC=C1)C1=CC=C(OCC2=CC=CC=C2)C=C1

FC1=CC=C(F)C(C2NC3=CC=CC=C3NC(=O)[C@H](CC3=CNC=N3)N3N=NN=C23)=C1Cl

COC1=CC(OC)=C(C=C1)C1NC(C(NC(=O)C(C)(C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

O=C1NC(C(NC(C2=NN=NN2C1C1=CC=CC=C1)C1=CC=C(C=C1)C#N)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NC(C(NC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(Br)C=CC(OC)=C1O

[H]C1(NC(C(NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC2=C(OCO2)C=C1

[H]C1(NCCOCCOCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C1=CC=C(Br)C=C1

CC(C)C1N2N=NN=C2C(NCCCCNC1=O)C1=C(F)C=CC=C1F

OCC1N2N=NN=C2C(NCCCCNC1=O)C1=C(Br)C=CC=C1

[H]C1(NCC(O)CNC(=O)C(C)N2N=NN=C12)C1=CC=CC(Cl)=C1

CC(C)(C)OC(=O)N1C=C(C2NCCSCCNC(=O)C(C)(C)N3N=NN=C23)C2=C1C=CC=C2

[H]C1(NCCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=C(OC)C=CC=C1O

FC1=C(C=CC=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CS)N2N=NN=C12

COC(=O)C1=C(C2NCCCCNC(=O)C(C(C)C)N3N=NN=C23)C(OC)=CC(OC)=C1

ClC1=CC2=C(C=C1)C(=CN2)C1NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCCSCCNC(=O)C(CS)N2N=NN=C12)C1=CC(OC)=CC(OC)=C1

CSCC[C@@H]1N2N=NN=C2C(NCCCCCNC1=O)C1=C(Cl)C=CC=C1F

SCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CNC2=C1C=C(Cl)C=C2

CN1C2CCC1CC1(C2)NCC(C)(C)CNC(=O)C(C)(C)N2N=NN=C12

[H]C1(NCCSCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=C(OCC2=CC=CC=C2)C(OC)=C1

O=C1NCCSCCNC(C2=NN=NN2C1CC1=CC=CC=C1)C1=CC=C(C=C1)C1=CC=CC=C1

[H]C1(NCCSCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1

CC(C)(C)OC(=O)NCC1NCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

O=C1NC2=CC=CC=C2NC(C2=NN=NN2C1CC1=CC=CC=C1)C1=CN=C2C=CC=CC2=C1

[H]C1(NCCSCCNC(=O)C(CS)N2N=NN=C12)C1=CC=C(C)S1

OC(=O)C1=C(C=CC=C1)C1NCCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

OC1=C(C=CC=C1)C1NCCOCCOCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(CCCCC)NCC(C)(C)CNC(=O)C(CC(C)C)N2N=NN=C12

OC1=CC(C2NCCSCCNC(=O)C(CC3=CC=CS3)N3N=NN=C23)=C(Br)C=C1

CC1(C)OB(OC1(C)C)C1=CC=C(C=C1)C1NCC(C)(C)CNC(=O)CN2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=C(Cl)C=CC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(CCC(=O)OC)NCCOCCOCCNC1=O

OCC1N2N=NN=C2C(NCCCCNC1=O)C1=CC=CN1

CC1N2N=NN=C2C(CCl)NCCCNC1=O

CC1(C)N2N=NN=C2C(NCCNC1=O)C1=CC=C(Br)S1

C[Se]CCC1N2N=NN=C2C2(CCC(CC2)C2=CC=CC=C2)NCCCNC1=O

O=C1NCCCCNC(C2=CC3=CC=CC=C3S2)C2=NN=NN2C1CC1=CC=CS1

CC(C)CC1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC(=CC=C1)C#N

O=C1NCCCCCNC(C2=NN=NN2C1CC1=CC=CC=C1)C1=CC=NC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCCCCCNC1=O)C(C)CC1=CC=C(C=C1)C(C)(C)C

OCC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CNC2=C1C=CC=C2

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC(Br)=CC=C1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CO)N2N=NN=C12)C1=CC=C(Cl)C=C1

CC(C)(C)OC(=O)N1C=C(C2NCC(C)(C)CNC(=O)C(CO)N3N=NN=C23)C2=C1C=CC=C2

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)CN2N=NN=C12)C1=CC=CC(O)=C1

[H]C1(NCC(C)(C)CNC(=O)[C@H](CCSC)N2N=NN=C12)C(OC)OC

C[Se]CCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=CC=CC2=C1C=CN2

CC[C@H](C)[C@@H]1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(C)C=C1

CC1(C)CNC(C2=NN=NN2C(CS)C(=O)NC1)C1=CC=C(CCBr)C=C1

CC(C)C1=CC=C(C=C1)C1NCCOCCOCCNC(=O)C(C)(C)N2N=NN=C12

BrC1=CC=CC(=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CC(=O)OCC1=CC=C(O1)C1NCCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CS)N2N=NN=C12)C1=CC(OC)=CC=C1

CC(C)C1N2N=NN=C2C(NCCCCNC1=O)C1=CC=CC(=C1)B1OC(C)(C)C(C)(C)O1

CC1(C)CNC(C2=NN=NN2C(CC2=CNC3=C2C=CC=C3)C(=O)NC1)C1=CC=C(OCC(O)=O)C=C1

[H]C1(NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12)C1=CC(OC)=CC=C1OC

CC1(C)N2N=NN=C2C(CCC2=CC=CC=C2)NCCSCCNC1=O

[H]C1(NCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C1=CC=CS1

CC(C)CC1N2N=NN=C2C(CC2=CC=CC=C2)(CC2=CC=CC=C2)NC2=CC=CC=C2NC1=O

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)CN2N=NN=C12)C1=CC=CC(Cl)=C1Cl

CSCC[C@@H]1N2N=NN=C2C(NCCCCNC1=O)C1=CC(O)=C(O)C=C1

CC(C)C1N2N=NN=C2C(NCC(C)(C)CNC1=O)(C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC(OC)=CC=C1OC

O=C1N[C@@H]2CCCC[C@H]2NC(CCC2=CC=CC=C2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

[H]C1(NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CS1

CC1N2N=NN=C2C(CC2=CC=CC=C2)(CC2=CC=CC=C2)NCC(O)CNC1=O

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC(Cl)=C1Cl

OC1=C(O)C=C(C=C1)C1NCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

CN1CCC2(CC1)NCC(O)CNC(=O)C(CS)N1N=NN=C21

O=C1NCCCCCCNC(C2=NN=NN2[C@H]1CC1=CNC=N1)C1=CC=C2NN=CC2=C1

O=C1CN2N=NN=C2C(N[C@@H]2CCCC[C@H]2N1)C1=CC(OCC2=CC=CC=C2)=CC=C1

CSCC[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC=C2C=NNC2=C1

[H]C1(NC2=CC=CC=C2NC(=O)C(C(C)C)N2N=NN=C12)C1=CC=CC(OC)=C1O

OCC1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCCSCCNC1=O

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(C=C1)C(F)(F)F

COC1CC(C(OC)O1)C1NCCSCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

FC1=CC(C2NCCSCCNC(=O)[C@H](CC3=CNC=N3)N3N=NN=C23)=C(Cl)C=C1

[H]C1(NCC(O)CNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC=C(C)S1

[H]C1(NCCCNC(=O)C(CS)N2N=NN=C12)C1=CC=C(Br)C=C1

CSCC[C@@H]1N2N=NN=C2C(NCCCCNC1=O)C1=C(Cl)C(C)=CC=C1F

CC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC(F)=C(F)C(F)=C1

CC(C)CC1N2N=NN=C2C(NCCNC1=O)C1=C(Cl)C=CC(F)=C1

CC1(C)CNC(C2=NN=NN2CC(=O)NC1)C1=CC=C2C=CC=CC2=C1

C[Se]CCC1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC=C(F)C=C1

[H]C1(NCCOCCOCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=CC=C1

CC(C)(C)C1NCCCCNC(=O)C(CO)N2N=NN=C12

CC(C)C1NCCCNC(=O)C(C)N2N=NN=C12

[H]C1(NCCNC(=O)C(C)(C)N2N=NN=C12)C1=CC=C(Br)S1

C[Se]CCC1N2N=NN=C2C(NCC(O)CNC1=O)C1=C(C=CC=C1)C(F)(F)F

COC1CC(C(OC)O1)C1NC(C(NC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

C[Se]CCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=CN=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCC(C)(C)CNC1=O)C(C)(C)C

CC(C)C1NCCOCCOCCNC(=O)C(CO)N2N=NN=C12

[H]C1(CC)NCC(C)(C)CNC(=O)C(C)N2N=NN=C12

CC1(C)NCCOCCOCCNC(=O)CN2N=NN=C12

FC(F)(F)OC1=CC=C(C=C1)C1NCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

FC1=CC(F)=C(C=C1)C1NC2=CC=CC=C2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC(C)=CC=C1

[H]C1(NCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CO1

[H]C1(NCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

OCC1N2N=NN=C2C(NCCNC1=O)C1=CC=CC2=C1C=CN2

CC1N2N=NN=C2C(NCCNC1=O)C1=CC=C(C)C=C1

O=C1CN2N=NN=C2C2(CCCCC2)NCCN1

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1Cl

O=C1NCCCCNC(C2=NN=NN2C1CC1=CC=CS1)C1=CC=CC2=C1C=CN2

CC(C)CC1N2N=NN=C2C(NCCCNC1=O)C1=CC=C(C)C=C1

O=C1NCCNC2(CCCCC2)C2=NN=NN2C1CC1=CC=CC=C1

SCC1N2N=NN=C2C2(CCCC2)NCCNC1=O

CC1(C)N2N=NN=C2C(NCCNC1=O)C1CC1

FC(F)(F)OC1=CC=CC=C1C1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

FC(F)(F)C1=C(C=CC=C1)C1NCCOCCOCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(NCC(C)(C)CNC(=O)C(CS)N2N=NN=C12)C1=C(OC)C=CC=C1

CC1(C)N2N=NN=C2C(NCCOCCOCCNC1=O)C1CCCCC1

[H]C1(NCC(C)(C)CNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC(Cl)=C1Cl

OC1=C(O)C=C(C=C1)C1NCCOCCOCCNC(=O)C(CS)N2N=NN=C12

CN1CCC2(CC1)NCC(C)(C)CNC(=O)C(C)(C)N1N=NN=C21

FC1=CC=C(F)C(C2NCCNC(=O)C(CC3=CC=CC=C3)N3N=NN=C23)=C1Cl

OC1=C(O)C=C(C=C1)C1NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12

CN1CCC2(CC1)NCCCCCNC(=O)C(C)(C)N1N=NN=C21

[H]C1(NCCOCCOCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C(O)CO

[H]C1(CCC)NCC(C)(C)CNC(=O)C(C(C)C)N2N=NN=C12

O=C1CN2N=NN=C2C(N[C@@H]2CCCC[C@H]2N1)C1=CC=C(OCC2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1

[H]C1(NCCCNC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC=CC(OC)=C1O

[H]C1(NCCNC(=O)C(C(C)C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCSCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NC2=CC=CC=C2NC(=O)CN2N=NN=C12)C1=C(O)C=CC(Br)=C1

CC(C)C1N2N=NN=C2C(NCCCCCCNC1=O)C1=CSC2=C1C=CC=C2

FC1=CC=C(C2NC3=CC=CC=C3NC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)C(Cl)=C1

SCC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=C2C=CC=CC2=CC=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCCCCCNC(=O)[C@H](CCSC)N2N=NN=C12

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NCCCNC(=O)C(C)N2N=NN=C12

[H]C1(NCC(C)(C)CNC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NC2=CC=CC=C2NC(=O)CN2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCOCCOCCNC(=O)C(C(C)C)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

[H]C1(NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

FC1=CC=C(C=C1)C1NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1

[H]C1(NC2=CC=CC=C2NC(=O)C(C)N2N=NN=C12)C1=C(O)C=CC(Br)=C1

O=C1CN2N=NN=C2C(NCCSCCN1)C1=CNC2=C1C=CC=C2

CSCC[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC=C(C)C=C1

C[Se]CCC1N2N=NN=C2C(NCCNC1=O)C1CC1

[H]C1(CC)NCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12

CC1(C)NCCNC(=O)C(CO)N2N=NN=C12

[H]C1(C)NC2=CC=CC=C2NC(=O)C(C)N2N=NN=C12

[H]C1(C)NCCSCCNC(=O)CN2N=NN=C12

[H]C1(C)NCCCNC(=O)[C@H](CCSC)N2N=NN=C12

O=C1N[C@@H]2CCCC[C@H]2NC2(CCN(CC3=CC=CC=C3)CC2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

FC1=CC(F)=C(C=C1)C1NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

CC(C)CC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=C(Br)C=CC=C1

[H]C1(NCC(C)(C)CNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC(Cl)=C1

COC(=O)CCC1NCCCCCCNC(=O)C(CS)N2N=NN=C12

CC1(C)N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=CN1

ClCC1NCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(CC)NCC(O)CNC(=O)C(C(C)C)N2N=NN=C12

CC1(C)NCCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(C)NCCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(C)N[C@@H]2CCCC[C@H]2NC(=O)C(CC(C)C)N2N=NN=C12

[H]C1(C)NCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(C)NCCCNC(=O)C(CS)N2N=NN=C12

CC(C)C1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC2=CC=CC=C2NC1=O

FC(F)(F)C1=CC=C(C=C1)C1NCCOCCOCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

COC1CC(C(OC)O1)C1NCCOCCOCCNC(=O)C(CS)N2N=NN=C12

CC1(C)N2N=NN=C2C(NCCCCNC1=O)C1=CC(=CC=C1)C#N

[H]C1(NCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1O

[H]C1(NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12)C1=CC2=C(OCO2)C=C1

CC1(C)N2N=NN=C2C(NCCCCCNC1=O)C1=C(O)C=CC=C1

[H]C1(CCCCC)NCCCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C2(CCCC2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

O=C1N[C@@H]2CCCC[C@H]2NC(C2CC2)C2=NN=NN2[C@H]1CC1=CNC=N1

[H]C1(CC)NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(C)(C)NCCCNC1=O

[H]C1(C)NC2=CC=CC=C2NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12

[H]C1(C)NCCSCCNC(=O)C(CS)N2N=NN=C12

CC(C)C1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NCC(O)CNC1=O

FC1=CC(F)=C(C=C1)C1NCCSCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1=CC=CC(=C1)C1NCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC(OCC2=CC=CC=C2)=CC=C1

CC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(Cl)C(F)=CC=C1F

COC1=CC=CC(C2NCCCNC(=O)C(CC(C)C)N3N=NN=C23)=C1OC

O=C1NCCNC(C2=NN=NN2C1CC1=CC=CC=C1)C1=CC(=CC=C1)C#N

[H]C1(NC2=CC=CC=C2NC(=O)C(CS)N2N=NN=C12)C1=CSC=C1

CC(C)CC1NCCCCCNC(=O)C(C)(C)N2N=NN=C12

CC(C)C1NCCCCCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

[H]C1(CC)NC(C(NC(=O)C(C(C)C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC1(C)N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(C)NCC(C)(C)CNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(C)NCCOCCOCCNC(=O)C(CC(C)C)N2N=NN=C12

OC1CNC(=O)C(CC2=CC=CS2)N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)NC1

CC1(C)OB(OC1(C)C)C1=CC(=CC=C1)C1NCC(O)CNC(=O)CN2N=NN=C12

[H][C@@]12C[C@@]3([H])C[C@@]([H])(C1)C1(NCCCCCNC(=O)[C@H](CCSC)N4N=NN=C14)[C@@]([H])(C2)C3

[H]C1(NCC(O)CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=C(OC)C=CC(Br)=C1

OC(=O)C1=CC=C(C=C1)C1NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CCCCC)NCCSCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

OC1CNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C2C2(CCCC2)NC1

O=C1NCCSCCNC(C2CC2)C2=NN=NN2C1CC1=CNC2=C1C=CC=C2

[H]C1(CC)NCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1(C)NCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

CC1N2N=NN=C2C(NCCNC1=O)C1=CC=C(OC(F)(F)F)C=C1

FC1=CC(F)=C(C=C1)C1NC2=CC=CC=C2NC(=O)CN2N=NN=C12

CC1(C)CNC(C2=NN=NN2[C@@H](CC2=CNC=N2)C(=O)NC1)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

CC1(C)N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=C(Br)C=CC=C1

[H]C1(NCCCCCCNC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC=C(OC)C(OC)=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(CCC2=CC=CC=C2)NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1

CC1(C)OB(OC1(C)C)C1=C(C=CC=C1)C1NC(C(NC(=O)C(CS)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CSCC[C@@H]1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC=C(OCC(O)=O)C=C1

C[Se]CCC1N2N=NN=C2C(NCCNC1=O)C1=CC=CN1

CC[C@H](C)[C@@H]1N2N=NN=C2C(CCl)NCCNC1=O

[H]C1(CC)NC2=CC=CC=C2NC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(C)(C)NCCCCCNC1=O

CC1(C)N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CC=C(OC(F)(F)F)C=C1

C[Se]CCC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC=C(C=C1)C(F)(F)F

COC1CC(C(OC)O1)C1NC2=CC=CC=C2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

CC(C)CC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC(=CC=C1)C#N

OC1CNC(C2=NN=NN2C(CC2=CC=CC=C2)C(=O)NC1)C1=CC=NC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NCCCCCNC1=O)C(C)CC1=CC=C(C=C1)C(C)(C)C

[H]C1(NCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC(Cl)=C1Cl

CC(C)C1N2N=NN=C2C(NCCNC1=O)C1=CC(O)=C(O)C=C1

[H]C1(NCC(C)(C)CNC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC(O)=CC=C1

[H]C1(NCCOCCOCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C(OC)OC

CCC1(CC)NCCCCNC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(NCC(O)CNC1=O)C1CC1

CC1(C)N2N=NN=C2C(NCCCCCNC1=O)C1=CC=CC=C1OC(F)(F)F

CCOC(=O)C1CC1C1NCCOCCOCCNC(=O)C(N2N=NN=C12)C1=CC=CC=C1

CC(C)C1N2N=NN=C2C(NCC(C)(C)CNC1=O)C1=CC(C)=CC=C1

CC1=CC=C(F)C(C2NC(C(NC(=O)C(CC3=CNC4=C3C=CC=C4)N3N=NN=C23)C2=CC=CC=C2)C2=CC=CC=C2)=C1Cl

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC(OC)=CC=C1

[H]C1(NC(C(NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CS1

CCC(C)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(CCC)NCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12

[H]C1(NCC(O)CNC(=O)C(C)N2N=NN=C12)C1=CC=C(Br)S1

CC(C)CC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(C=CC=C1)C(F)(F)F

[H]C1(NC(C(NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(OC)C=CC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC(=C1)B1OC(C)(C)C(C)(C)O1

O=C1NCCCNC(C2=NN=NN2C1C1=CC=CC=C1)(C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NCC(C)(C)CNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC(OC)=CC=C1OC

CC(C)(C)OC(=O)NCC1NC2=CC=CC=C2NC(=O)C(C)(C)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=CN=C2C=CC=CC2=C1

[H]C1(NCCCCNC(=O)[C@H]([C@@H](C)CC)N2N=NN=C12)C1=CC=C(C)S1

OCC1N2N=NN=C2C(NCCCNC1=O)C1=CC=CN=C1

CC(CC1=CC=C(C=C1)C(C)(C)C)C1NCCNC(=O)C(CO)N2N=NN=C12

CC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CNC2=C1C=CC=C2

CC1=CC=C(C=C1)C1NCCCCCNC(=O)CN2N=NN=C12

CSCC[C@@H]1N2N=NN=C2C2(CCCCC2)NCCOCCOCCNC1=O

C[Se]CCC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=CC2=C1C=CN2

BrC1=CC=CC(=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

[H]C1(NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC=C(Cl)C=C1

CC(C)CC1N2N=NN=C2C(NCCCNC1=O)C1=C(C)C=CC=C1

O=C1NC2=CC=CC=C2NC(C2=CC=CN2)C2=NN=NN2C1CC1=CC=CC=C1

SCC1N2N=NN=C2C(CCl)NCCSCCNC1=O

CC(C)C1N2N=NN=C2C(NCCCNC1=O)C1=CC=C(Br)S1

COC(=O)CCCCC1NCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(N[C@@H]2CCCC[C@H]2NC1=O)C1=CC=C(OCC2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1

BrC1=C(C=CC=C1)C1NCCCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(NC(C(NC(=O)C(CC(C)C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC(Cl)=C1

COC(=O)CCC1NC(C(NC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C(OCC2=CC=CC=C2)C=C1

OC1CNC(C2=NN=NN2C(C2=CC=CC=C2)C(=O)NC1)C1=C(Cl)C(F)=CC=C1F

COC1=CC(OC)=C(C=C1)C1NC(C(NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

O=C1NC(C(NC(C2=NN=NN2C1CC1=CC=CS1)C1=CC=C(C=C1)C#N)C1=CC=CC=C1)C1=CC=CC=C1

[H]C1(NC(C(NC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(Br)C=CC(OC)=C1O

[H]C1(CCCCC)NC(C(NC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC=CC=C1)C1=CC=CC=C1

OC1=CC(C2N[C@@H]3CCCC[C@H]3NC(=O)C(N3N=NN=C23)C2=CC=CC=C2)=C(Br)C=C1

ClC1=C(Cl)C=C(C=C1)C1NCCCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

CC1(C)N2N=NN=C2C(NCC(O)CNC1=O)C1=CSC2=C1C=CC=C2

O=C1NCCSCCNC(C2=NN=NN2C1C1=CC=CC=C1)C1=CC=C(C=C1)C#N

[H]C1(NCC(O)CNC(=O)C(CC(C)C)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1O

[H]C1(NCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CC2=C(OCO2)C=C1

[H]C1(NCCCCNC(=O)C(CO)N2N=NN=C12)C1=C(OC)C=CC=C1O

CC1N2N=NN=C2C(NCCCNC1=O)C1=C(F)C=CC=C1

COC(=O)C1=C(C2NCCNC(=O)C(C)(C)N3N=NN=C23)C(OC)=CC(OC)=C1

C[Se]CCC1N2N=NN=C2C(NCCCNC1=O)C1=CNC2=C1C=CC(Cl)=C2

[H]C1(NCCCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC(OC)=CC(OC)=C1

CC(C)CC1N2N=NN=C2C(NCC(O)CNC1=O)C1=CC(=CC=C1)C#N

[H]C1(NCCCCCNC(=O)C(CC2=CC=CC=C2)N2N=NN=C12)C1=CSC=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(CC2=CC=CC=C2)(CC2=CC=CC=C2)NCCOCCOCCNC1=O

OCC1N2N=NN=C2C(NCCCCNC1=O)C1=CC=C2NN=CC2=C1

CC1N2N=NN=C2C(CC2=CC=CC=C2)NCCCNC1=O

[H]C1(NCCNC(=O)C(C)(C)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1

C[Se]CCC1N2N=NN=C2C(NCC(O)CNC1=O)C1=C(F)C(Cl)=CC=C1F

COC1=CC=CC(C2N[C@@H]3CCCC[C@H]3NC(=O)C(CC3=CC=CS3)N3N=NN=C23)=C1OC

OCC1N2N=NN=C2C(NCCCCCCNC1=O)C1=C2C=CC=CC2=CC=C1

CC1N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=C(C)C=CS1

CC1(C)CNC(C2=NN=NN2C(C2=CC=CC=C2)C(=O)NC1)C1=C(C=CC=C1)C(O)=O

CC(C)C1N2N=NN=C2C(NCCOCCOCCNC1=O)C1=C(O)C=CC=C1

[H]C1(NCCCCCNC(=O)C(CC[Se]C)N2N=NN=C12)C1=CC=C(Cl)C=C1

CC(C)(C)OC(=O)N1C=C(C2NCCCCCCNC(=O)C(N3N=NN=C23)C2=CC=CC=C2)C2=C1C=CC=C2

[H]C1(N[C@@H]2CCCC[C@H]2NC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12)C1=CC=CC(O)=C1

[H]C1(NCC(C)(C)CNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C(OC)OC

CCC1(CC)NCCOCCOCCNC(=O)C(CC(C)C)N2N=NN=C12

OCC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC2=CC=CC=C2S1

CC1N2N=NN=C2C(NCCCCCNC1=O)C1=CC(=CC=C1)C#N

[H]C1(NCCOCCOCCNC(=O)C(C)(C)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1O

C[Se]CCC1N2N=NN=C2C(NCCCCCNC1=O)C1=CNC2=C1C=C(Cl)C=C2

[H]C1(NCCNC(=O)C(CC2=CC=CS2)N2N=NN=C12)C1=CC(OC)=CC=C1OC

CC(C)CC1N2N=NN=C2C(CCC2=CC=CC=C2)NCCNC1=O

CC1(C)OB(OC1(C)C)C1=C(C=CC=C1)C1N[C@@H]2CCCC[C@H]2NC(=O)C(CC2=CC=CS2)N2N=NN=C12

[H]C1(NCCOCCOCCNC(=O)C(CO)N2N=NN=C12)C1=CC(OC)=CC=C1OC

CC1N2N=NN=C2C(CCC2=CC=CC=C2)NCCCCNC1=O

[H]C1(NCCCNC(=O)CN2N=NN=C12)C1=CC=CS1

CCC(C)C1NCCNC(=O)[C@H](CCSC)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NCCCCNC1=O)C1=CC2=C(NC=C2)C=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C(CC2=CC=CC=C2)NCC(O)CNC1=O

SCC1N2N=NN=C2C(NCCSCCNC1=O)C1=CC=C(CCBr)C=C1

CSCC[C@@H]1N2N=NN=C2C(NCCSCCNC1=O)C1=C(F)C(Cl)=CC=C1F

O=C1CN2N=NN=C2C(NCCN1)C1=CC=C(OCC2=CC=CC=C2)C=C1

C[Se]CCC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC(O)=C(O)C=C1

CC[C@H](C)[C@@H]1N2N=NN=C2C2(CCN(C)CC2)NCCCCCNC1=O

CC1(C)N2N=NN=C2C(NC(C(NC1=O)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=C2NN=CC2=C1

O=C1N[C@@H]2CCCC[C@H]2NC(CC2=CC=CC=C2)C2=NN=NN2C1C1=CC=CC=C1

[H]C1(NCCCCNC(=O)C(CC(C)C)N2N=NN=C12)C1=C(Br)C=CC(OC)=C1

FC1=CC=C(Cl)C(F)=C1C1NCCCCCNC(=O)CN2N=NN=C12

[H]C1(NCCOCCOCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=CC(O)=C1O

[H]C1(NCC(C)(C)CNC(=O)C(C(C)C)N2N=NN=C12)C1=C(OC)C=CC=C1O

[H]C1(NCCCCNC(=O)[C@H](CCSC)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

CC(C)C1N2N=NN=C2C2(CCN(CC3=CC=CC=C3)CC2)N[C@@H]2CCCC[C@H]2NC1=O

FC1=CC(F)=C(C=C1)C1NCCCCNC(=O)[C@H](CC2=CNC=N2)N2N=NN=C12

C[Se]CCC1N2N=NN=C2C(NC2=CC=CC=C2NC1=O)C1=CC(OCC2=CC=CC=C2)=CC(OCC2=CC=CC=C2)=C1

CC1N2N=NN=C2C(NCCCCCNC1=O)C1=C(Cl)C(C)=CC=C1F

COC1CC(C(OC)O1)C1NCCNC(=O)C(CC(C)C)N2N=NN=C12

FC1=CC(C2NCCCCNC(=O)CN3N=NN=C23)=C(Cl)C=C1

[H][C@]12CC[C@](C)(C1(C)C)C1(C2)NC2=CC=CC=C2NC(=O)C(C(C)C)N2N=NN=C12

[H]C1(NCCCCCCNC(=O)C(CC2=CNC3=C2C=CC=C3)N2N=NN=C12)C1=CC=C(OC)C(O)=C1

List of 13 isocyanide ester smiles:

O=C(C[N+]#[C-])OC

O=C(CC[N+]#[C-])OC

O=C(CCC[N+]#[C-])OC

O=C(CCCC[N+]#[C-])OC

O=C(CCCCC[N+]#[C-])OC

O=C(OC)C([N+]#[C-])CC1=CNC2=C1C=CC=C2

O=C(OC)C([N+]#[C-])CC1=CC=CC=C1

CC(C([N+]#[C-])C(OC)=O)C

O=C(OC)CC([N+]#[C-])C1=CC=C(OC)C=C1

CC(C)CC([N+]#[C-])C(OC)=O

O=C(CC([N+]#[C-])CC(C)C)OC

O=C(OC)CC([N+]#[C-])C1=CC=C(Cl)C=C1

O=C(OC)CC([N+]#[C-])C1=CC=CC=C1

List of 17 diamine smiles:

NCCN

NCCCN

NCCCCN

NCCSCCN

NCCOCCOCCN

N[C@H]1[C@H](N)CCCC1

NC1=CC=CC=C1N

NCC(O)CN

NCC(C)(C)CN

NCCCCCN

NCCCCCCN

NC(C1=CC=CC=C1)C(C2=CC=CC=C2)N

NCC1=CC(CN)=CC=C1

NCCCCCCCCN

NCCCCCCCCCCCCN

NCCCCCCCCCCN

NCC2=CC=C(CN)C=C2

List of 221 α-isocyano-ω-amine smiles:

NCCNC(=O)C[N+]#[C-]

CC(C)CC(CC(=O)NCCCCCCCCN)[N+]#[C-]

NC1=CC=CC=C1NC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

NC(C(NC(=O)CCC[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

N[C@@H]1CCCC[C@H]1NC(=O)CC[N+]#[C-]

CC(C)CC(CC(=O)NCC(C)(C)CN)[N+]#[C-]

NCC1=CC=CC(CNC(=O)CC([N+]#[C-])C2=CC=C(Cl)C=C2)=C1

NCCCCCCCCCCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

NCCCCCCCCCCNC(=O)CCC[N+]#[C-]

NCC(O)CNC(=O)CC[N+]#[C-]

CC(C)CC(CC(=O)NCCCCCN)[N+]#[C-]

NCCOCCOCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

NCCCCCCNC(=O)CCC[N+]#[C-]

CC(C)CC(CC(=O)NCCSCCN)[N+]#[C-]

NCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCCCCCN)[N+]#[C-]

NCCOCCOCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

NCCCCCCCCNC(=O)CCC[N+]#[C-]

NC1=CC=CC=C1NC(=O)CC[N+]#[C-]

NC(C(NC(=O)C[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

N[C@@H]1CCCC[C@H]1NC(=O)C[N+]#[C-]

NCCCCNC(=O)C[N+]#[C-]

CC(C)CC(CC(=O)NCCCCCCCCCCCCN)[N+]#[C-]

NC(C(NC(=O)C(CC1=CC=CC=C1)[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

N[C@@H]1CCCC[C@H]1NC(=O)CCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCCCCCN

NCCCCCCCCNC(=O)CCCCC[N+]#[C-]

NC1=CC=CC=C1NC(=O)CCC[N+]#[C-]

CC(C)CC(CC(=O)NCCCN)[N+]#[C-]

NCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

CC(C)(CN)CNC(=O)CCC[N+]#[C-]

CC(C)CC(CC(=O)NCCCCN)[N+]#[C-]

NCC1=CC=C(CNC(=O)C(CC2=CC=CC=C2)[N+]#[C-])C=C1

CC(C)C([N+]#[C-])C(=O)NC(C(N)C1=CC=CC=C1)C1=CC=CC=C1

CC(C)(CN)CNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCC1=CC=CC(CNC(=O)C(CC2=CNC3=C2C=CC=C3)[N+]#[C-])=C1

NCCCCCCCCCCCCNC(=O)CCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NC1=CC=CC=C1N

NC(C(NC(=O)CCCCC[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

N[C@@H]1CCCC[C@H]1NC(=O)CCC[N+]#[C-]

NCCCCNC(=O)CC[N+]#[C-]

NCCCCCNC(=O)C[N+]#[C-]

NCCOCCOCCNC(=O)C[N+]#[C-]

CC(C)CC(CC(=O)NCCCCCCCCCCN)[N+]#[C-]

NCC(O)CNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCCCCCCCN)[N+]#[C-]

NC1=CC=CC=C1NC(=O)CCCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCSCCN

CC(C)C([N+]#[C-])C(=O)NCCSCCN

CC(C)C([N+]#[C-])C(=O)NCCCCCCCCN

CC(C)C([N+]#[C-])C(=O)N[C@@H]1CCCC[C@H]1N

CC(C)C([N+]#[C-])C(=O)NCCCCCCCCCCCCN

NCCCCCCCCCCNC(=O)CCCC[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCC1=CC=C(CN)C=C1)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NCCCCN

NCCCCCNC(=O)CCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCC1=CC(CN)=CC=C1

NCCCCCCCCCCCCNC(=O)CCCCC[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCC(C)(C)CN)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NCCN

CC(C)(CN)CNC(=O)CCCC[N+]#[C-]

NCC1=CC=CC(CNC(=O)CC[N+]#[C-])=C1

NCCCCCCCCCCCCNC(=O)C[N+]#[C-]

NCCSCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCCCCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCC1=CC=C(CNC(=O)CC([N+]#[C-])C2=CC=CC=C2)C=C1

NCCCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCOCCOCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCOCCOCCN)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NCC(O)CN

CC(C)C([N+]#[C-])C(=O)NCCCCCCCCCCN

NCCCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NC1=CC=CC=C1NC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)N[C@@H]1CCCC[C@H]1N)[N+]#[C-]

NCCCCNC(=O)CCCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCCN

NC1=CC=CC=C1NC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NC(C(NC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

CC(C)C([N+]#[C-])C(=O)NCC1=CC=C(CN)C=C1

NCC1=CC=C(CNC(=O)CCCC[N+]#[C-])C=C1

NCC1=CC=C(CNC(=O)CC[N+]#[C-])C=C1

NCC1=CC=C(CNC(=O)C[N+]#[C-])C=C1

CC(C)CC(CC(=O)N[C@@H]1CCCC[C@H]1N)[N+]#[C-]

NCCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

NCCCCCNC(=O)CCC[N+]#[C-]

NCCOCCOCCNC(=O)CC[N+]#[C-]

NCCCCCCNC(=O)C[N+]#[C-]

NCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCC1=CC=CC(CNC(=O)C(CC2=CC=CC=C2)[N+]#[C-])=C1

CC(C)C([N+]#[C-])C(=O)NCCCCCN

CC(C)C([N+]#[C-])C(=O)NCCOCCOCCN

NCCCCCCNC(=O)CCCC[N+]#[C-]

NCCCCCCCCNC(=O)CC[N+]#[C-]

NCC1=CC=CC(CNC(=O)CC([N+]#[C-])CC(C)C)=C1

NCCCCCCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCCCCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCC(O)CNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NCCSCCNC(=O)CCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCCCCN

NCC1=CC=C(CNC(=O)CC([N+]#[C-])C2=CC=C(Cl)C=C2)C=C1

NCC1=CC=C(CNC(=O)C(CC2=CNC3=C2C=CC=C3)[N+]#[C-])C=C1

NCC1=CC=C(CNC(=O)CCC[N+]#[C-])C=C1

CC(C)CC([N+]#[C-])C(=O)NCC(O)CN

NCCCCCCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NC1=CC=CC=C1NC(=O)CCCC[N+]#[C-]

NC(C(NC(=O)CC[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

CC(C)CC(CC(=O)NC(C(N)C1=CC=CC=C1)C1=CC=CC=C1)[N+]#[C-]

N[C@@H]1CCCC[C@H]1NC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCC1=CC(CN)=CC=C1)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NCCCN

CC(C)C([N+]#[C-])C(=O)NCC1=CC(CN)=CC=C1

NCCCCCCCCCCCCCNC(=O)CCCC[N+]#[C-]

NCCCCCCCCCCCNC(=O)CC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCCCCCCCCCCCN

NCCCCCCCCCCNC(=O)CCCCC[N+]#[C-]

NCC(O)CNC(=O)CCC[N+]#[C-]

NCCSCCNC(=O)CC[N+]#[C-]

CC(C)CC(CC(=O)NCC(O)CN)[N+]#[C-]

NCCSCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NC(C(N)C1=CC=CC=C1)C1=CC=CC=C1)[N+]#[C-]

N[C@@H]1CCCC[C@H]1NC(=O)CCCCC[N+]#[C-]

NCCCCNC(=O)CCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCC1=CC=C(CN)C=C1

NCC1=CC=C(CNC(=O)CCCCC[N+]#[C-])C=C1

COC1=CC=C(C=C1)C(CC(=O)NCCCCCN)[N+]#[C-]

NCCOCCOCCNC(=O)CCCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCCCN

NCCCCCNC(=O)CCCCC[N+]#[C-]

NCCOCCOCCNC(=O)CCC[N+]#[C-]

CC(C)CC(CC(=O)NCCN)[N+]#[C-]

NCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCCCN)[N+]#[C-]

NCCCCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCN)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NC1=CC=CC=C1N

NC(C(NC(=O)CCCC[N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1

CC(C)CC([N+]#[C-])C(=O)NCCCCCCCCN

NCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

CC(C)(CN)CNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NC1=CC=CC=C1N)[N+]#[C-]

NC(C(NC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1)C1=CC=CC=C1)C1=CC=CC=C1

NCCCCCCCCCCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

CC(C)(CN)CNC(=O)CC([N+]#[C-])C1=CC=CC=C1

N[C@@H]1CCCC[C@H]1NC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCSCCN)[N+]#[C-]

NCCCNC(=O)CCCCC[N+]#[C-]

NCCNC(=O)CCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCCCCCCCCCN

NCCCCCCCCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NCC(O)CNC(=O)CCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NC(C(N)C1=CC=CC=C1)C1=CC=CC=C1

NCCCCCCCCCCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NCCCCCCN

NCCCCCCCCNC(=O)CCCC[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCCCCCCCCCN)[N+]#[C-]

NCC(O)CNC(=O)CCCCC[N+]#[C-]

NCCSCCNC(=O)CCC[N+]#[C-]

NCCCNC(=O)CC[N+]#[C-]

CC(C)CC(CC(=O)NC1=CC=CC=C1N)[N+]#[C-]

NCCCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NCCOCCOCCNC(=O)CCCC[N+]#[C-]

NCCCCCCNC(=O)CC[N+]#[C-]

NCCCCCCCCNC(=O)C[N+]#[C-]

NC1=CC=CC=C1NC(=O)C[N+]#[C-]

CC(C)CC(CC(=O)NCC1=CC=C(CN)C=C1)[N+]#[C-]

NCCCCCCCCCCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCCCCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCCN)[N+]#[C-]

NCCNC(=O)CCCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCN

CC(C)(CN)CNC(=O)CCCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCCOCCOCCN

NCCCCCCNC(=O)CCCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)N[C@@H]1CCCC[C@H]1N

NCC(O)CNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCC1=CC=CC(CNC(=O)CC([N+]#[C-])C2=CC=CC=C2)=C1

NCC(O)CNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCSCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NCCCNC(=O)CCCC[N+]#[C-]

CC(C)CC([N+]#[C-])C(=O)NCC(C)(C)CN

NCC1=CC=CC(CNC(=O)CCCCC[N+]#[C-])=C1

COC1=CC=C(C=C1)C(CC(=O)NCC(O)CN)[N+]#[C-]

NCCSCCNC(=O)CCCCC[N+]#[C-]

NCCCNC(=O)CCC[N+]#[C-]

NCCNC(=O)CC[N+]#[C-]

CC(C)(CN)CNC(=O)C[N+]#[C-]

NCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

CC(C)(CN)CNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

NCC1=CC=CC(CNC(=O)CCC[N+]#[C-])=C1

CC(C)CC(CC(=O)NCCOCCOCCN)[N+]#[C-]

NCCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCCCCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NC1=CC=CC=C1NC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCOCCOCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCSCCNC(=O)CC([N+]#[C-])C1=CC=CC=C1

NCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NCCNC(=O)CCCC[N+]#[C-]

CC(C)(CN)CNC(=O)CC[N+]#[C-]

NCC1=CC=CC(CNC(=O)C[N+]#[C-])=C1

NCCCCNC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NCCCCCNC(=O)C(CC1=CNC2=C1C=CC=C2)[N+]#[C-]

COC1=CC=C(C=C1)C(CC(=O)NCCCCCCCCCCCCN)[N+]#[C-]

N[C@@H]1CCCC[C@H]1NC(=O)CC([N+]#[C-])C1=CC=C(Cl)C=C1

NC(C(NC(=O)CC([N+]#[C-])C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1

N[C@@H]1CCCC[C@H]1NC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

NCCCCNC(=O)CCCC[N+]#[C-]

NCCCCCNC(=O)CC[N+]#[C-]

CC(C)CC(CC(=O)NCCCCCCN)[N+]#[C-]

NCCCCCCNC(=O)C(CC1=CC=CC=C1)[N+]#[C-]

CC(C)C([N+]#[C-])C(=O)NCC(C)(C)CN

NCC1=CC=CC(CNC(=O)CCCC[N+]#[C-])=C1

NCCCCCCCCCCCCCNC(=O)CC[N+]#[C-]

NCCCCCCCCCCCNC(=O)C[N+]#[C-]

NCC(O)CNC(=O)C[N+]#[C-]

NCCSCCNC(=O)C[N+]#[C-]

NCCCNC(=O)C[N+]#[C-]

List of 272 oxo compound smiles:

[H]C(C)=O

[H]C(=O)C=C

CC(C)=O

[H]C(=O)CC

CC(=O)C=C

O=C1CCC1

[H]C(=O)\C=C\C

[H]C(=O)C(C)=C

O=CC1CC1

CC(=O)C=O

CCC(C)=O

[H]C(=O)CCC

CC(C)C=O

[H]C(=O)C(O)=O

CC(=O)CO

ClCC=O

O=C1CCC=C1

O=C1CCCC1

C\C=C(/C)C=O

CC(C)C(C)=O

CCC(=O)CC

CCC(C)C=O

CC(C)CC=O

CC(C)(C)C=O

[H]C(=O)C(O)CO

CC(=O)CCl

O=CC1=CC=CN1

[H]C(=O)C1=CC=CO1

O=C1CCCC=C1

O=C1CCCCC1

CC(C)=CC(C)=O

CC(=O)CCC=C

O=C1CCOCC1

[H]C(=O)CCCC([H])=O

CC(C)CC(C)=O

[H]C(=O)CCCCC

CCOC(=O)C=O

[H]C(=O)C(OC)OC

CSCCC=O

[H]C(=O)C1=CC=CC=C1

O=CC1=CC=NC=C1

O=CC1=CC=CN=C1

CC1=CC(=O)CCC1

[H]C(=O)C1=CC=CS1

[H]C(=O)C1=CSC=C1

CC1(C)CCCC1=O

O=CC1CCCCC1

CN1CCC(=O)CC1

CCC(=O)C(=O)CC

CCCC(=O)CCC

COC(=O)CC(C)=O

COC(=O)CCC=O

COC(OC)C(C)=O

CC(=O)C1=CC=CC=C1

O=CCC1=CC=CC=C1

CC1=CC=C(C=O)C=C1

O=CCC1=CC=CC=C1

CC1=CC=CC(C=O)=C1

CC1=C(C=O)C=CC=C1

[H]C(=O)C1=CC=CC(O)=C1

[H]C(=O)C1=CC(O)=CC=C1

OC1=C(C=O)C=CC=C1

[H]C(=O)C1=CC=C(O)C=C1

NC1=C(C=O)C=CC=N1

NC1=C(C=O)C=NC=N1

FC1=CC=C(C=O)C=C1

FC1=C(C=O)C=CC=C1

FC1=CC=CC(C=O)=C1

[H]C(=O)C1=CC=C(C)S1

CC1=C(SC=C1)C=O

ClCC(=O)CCl

CCOC(=O)CC(C)=O

COC(=O)CCC(C)=O

COC(=O)CCC(C)=O

COC(=O)CCCC=O

O=CC1=CC(=CC=C1)C#N

O=CC1=CC=C(C=C1)C#N

O=CC1=CC(=CC=C1)C#N

O=C1CC2=CC=CC=C2C1

[H]C(=O)\C=C\C1=CC=CC=C1

ClC1CCCCC1=O

[H]C(=O)C1=CC=CC=C1C([H])=O

O=CC(=O)C1=CC=CC=C1

CC(=O)CC1=CC=CC=C1

CCC(=O)C1=CC=CC=C1

O=CCCC1=CC=CC=C1

OCC(=O)C1=CC=CC=C1

CC(=O)C1=C(O)C=CC=C1

[H]C(=O)C1=CC=C(OC)C=C1

[H]C(=O)C1=C(OC)C=CC=C1

[H]C(=O)C1=CC(OC)=CC=C1

[H]C(=O)C1=CC=CC(O)=C1O

OC1=C(O)C=C(C=O)C=C1

OC1=CC(O)=C(C=O)C=C1

CC(=O)C1=CC=CC(F)=C1

CN1C2CCC1CC(=O)C2

CCOC1=CC(=O)CCC1

CCC(=O)C1=CC=CS1

[H]C(=O)C1=CC=C(Cl)C=C1

[H]C(=O)C1=CC=CC(Cl)=C1

ClC1=C(C=O)C=CC=C1

CCCN1CCC(=O)CC1

FC1=CC(F)=C(C=O)C=C1

FC1=CC=CC(F)=C1C=O

CCOC(=O)C1CC1C=O

COC(=O)CCCC(C)=O

CCC(C(C)=O)C(=O)OC

COC(=O)CCCCC=O

O=CC1=CNC2=C1C=CC=C2

O=CC1=CC=CC2=C1C=CN2

O=CC1=CC2=C(NC=C2)C=C1

OC(=O)CC(=O)CC(O)=O

O=CC1=CC=C2C=NNC2=C1

O=CC1=CC=C2NN=CC2=C1

O=C1CCC2=CC=CC=C2C1

O=C1CCCC2=C1C=CC=C2

O=C(C1CC1)C1=CC=CC=C1

O=C1CCCC2=C1C=CC=N2

CCOC(=O)C(F)C(C)=O

O=C1CCOC2=CC=CC=C12

OC1=CC=CC2=C1C(=O)CC2

CC(=O)C1=C(C=O)C=CC=C1

CC(C)C1=CC=C(C=O)C=C1

[H]C(=O)C1=CC2=C(OCO2)C=C1

OC(=O)C1=C(C=O)C=CC=C1

OC(=O)C1=CC=C(C=O)C=C1

CCC(=O)C1=CC=C(O)C=C1

COC1=CC=CC=C1C(C)=O

CCC(=O)C1=C(O)C=CC=C1

O=CCOCC1=CC=CC=C1

CC(=C)C1CC=C(C)C(=O)C1

O=C1C2CC3CC(C2)CC1C3

COC(=O)CC(=O)CCl

[H]C(=O)C1=CC(=CC=C1)[N+]([O-])=O

[O-][N+](=O)C1=CC=C(C=O)C=C1

[H]C(=O)C1=CC=CC=C1[N+]([O-])=O

[O-][N+](=O)C1=C(C=O)C=CC=C1

[O-][N+](=O)C1=CC=CC=C1C=O

CC(=O)C1=CC(O)=CC(O)=C1

[H]C(=O)C1=CC=C(OC)C(O)=C1

[H]C(=O)C1=CC=CC(OC)=C1O

[H]C(=O)C1=C(OC)C=CC=C1O

CCC(=O)C1=CC=C(F)C=C1

CC1(C)C2CCC1(C)C(=O)C2

CC(C)=CCC\C(C)=C\C=O

CC(=O)C1=CC=C(Cl)C=C1

ClCC(=O)C1=CC=CC=C1

COC(=O)C1CCCCC1=O

CCOC(=O)C1CCCC1=O

O=CC1=C2C=CC=CC2=CC=C1

O=CC1=CC=C2C=CC=CC2=C1

O=CC1=CN=C2C=CC=CC2=C1

CCOC(=O)C(CC)C(C)=O

CCOC(=O)CC(=O)C(C)C

FC1=CC=CC(Cl)=C1C=O

FC1=CC=C(C=O)C(Cl)=C1

FC1=CC(C=O)=C(Cl)C=C1

CC(C)(C)OC(=O)NCC=O

FC1=CC(C=O)=CC(F)=C1F

COC1CC(C=O)C(OC)O1

CC1CCC2=CC=CC=C2C1=O

COC1=CC2=C(C=C1)C(=O)CC2

COC1=CC=C2CCC(=O)C2=C1

COC1=CC=CC2=C1C(=O)CC2

O=CC1=CSC2=C1C=CC=C2

O=CC1=CC2=CC=CC=C2S1

COC(=O)C(=O)C1=CC=CC=C1

COC1=CC=CC=C1CC(C)=O

COC1=CC=C(CC(C)=O)C=C1

COC1=CC(CC(C)=O)=CC=C1

O=C1CCSC2=C1C=CC=C2

CCOC(=O)CC(=O)CCl

CCOC(=O)C(Cl)C(C)=O

FC(F)(F)C(=O)C(F)(F)F

[H]C(=O)C1=CC=C(OC)C(OC)=C1

[H]C(=O)C1=CC(OC)=CC=C1OC

[H]C(=O)C1=CC(OC)=CC(OC)=C1

COC1=CC=CC(C=O)=C1OC

COC1=CC(OC)=C(C=O)C=C1

CC(=O)OCC1=CC=C(O1)C=O

CC1=C(\C=C/S)C(=O)CCC1

O=C1CCCCCCCCCC1

C=CCCCCCCCCC=O

ClCCC(=O)C1=CC=CC=C1

CCC(=O)C1=CC=C(Cl)C=C1

CCOC(=O)C1CCC(=O)CC1

CCOC(=O)C1CCCCC1=O

CC(=O)C1=CC=CC2=C1C=CC=C2

CCOC(=O)N1CCC(=O)CC1

CC1=CC=C(F)C(C=O)=C1Cl

FC(F)(F)C1=C(C=O)C=CC=C1

FC(F)(F)C1=CC=C(C=O)C=C1

O=C1CCC(CC1)C1=CC=CC=C1

BrC1=CC=C(O1)C=O

[H]C(=O)C1=CC=CC(Cl)=C1Cl

ClC1=CC=CC(Cl)=C1C=O

ClC1=C(Cl)C=C(C=O)C=C1

COC1=CC2=C(CCCC2=O)C=C1

COC1=CC=CC2=C1CCCC2=O

COC1=CC=C2C(=O)CCCC2=C1

FC1=CC=C(Cl)C(F)=C1C=O

FC1=CC=C(F)C(C=O)=C1Cl

ClC1=CC2=C(NC=C2C=O)C=C1

ClC1=CC2=C(C=C1)C(C=O)=CN2

ClC1=CC2=C(C=C1)C(C=O)=CN2

OC(=O)COC1=CC=C(C=O)C=C1

COC1=C(OC)C=C(C=C1)C(C)=O

CC1(C)C2CCC1(C(O)=O)C(=O)C2

O=C(C1=CC=CC=C1)C1=CC=CC=C1

O=CC1=CC=C(C=C1)C1=CC=CC=C1

ClCCCC(=O)C1=CC=CC=C1

CCCN(CC)C1CCC(=O)CC1

[H]C(=O)C1=CC=C(Br)C=C1

BrC1=CC=CC(C=O)=C1

BrC1=CC=CC(C=O)=C1

BrC1=C(C=O)C=CC=C1

[O-][N+](=O)C1=C(C=O)C=C(Cl)C=C1

ClCCCC(=O)C1=CC=CS1

CC(=O)C1=CC=C(Cl)C(Cl)=C1

O=C1CCCN(CC2=CC=CC=C2)C1

O=C1CCN(CC2=CC=CC=C2)CC1

FC(F)(F)OC1=CC=CC=C1C=O

FC(F)(F)OC1=CC=C(C=O)C=C1

BrC1=CC=C(S1)C=O

[H]C(=O)C1=CC=C(Br)S1

COC1=CC2=C(OCC(C)C2=O)C=C1

CC(=O)CC(=O)OCC1=CC=CC=C1

COC1=C(OC)C=C(CC(C)=O)C=C1

[O-][N+](=O)C1=CC2=C(OCO2)C=C1C=O

COC1=CC(C=O)=CC(OC)=C1OC

O=C(CC1=CC=CC=C1)C1=CC=CC=C1

O=CC1=CC(OC2=CC=CC=C2)=CC=C1

BrCC(=O)C1=CC=CC=C1

CC(C)(C)OC(=O)N1CCC(=O)CC1

[H]C(=O)C1=CC=C(OC)C(OC)=C1Cl

FC1=CC=C(C=C1)C(=O)CCCCl

[H]C(=O)C1=C(O)C=CC(Br)=C1

OC1=CC(C=O)=C(Br)C=C1

FC1=CC=C2C(NC=C2C(=O)CC#N)=C1

CCOC(=O)CC(=O)CC(=O)OCC

O=C1CCN(CCC2=CC=CC=C2)CC1

COC1=CC=CC(=C1)C1CCCCC1=O

CC(CC1=CC=C(C=C1)C(C)(C)C)C=O

CC(=O)C1=CC=C(Br)S1

O=C(CC1=CC=CC=C1)CC1=CC=CC=C1

COC1=C(OC)C=C(C(C=O)=C1)[N+]([O-])=O

O=CC1=CC(OCC2=CC=CC=C2)=CC=C1

O=CC1=CC=C(OCC2=CC=CC=C2)C=C1

BrCCC1=CC=C(C=O)C=C1

CC(=O)C1=C(O)C=CC(Br)=C1

[H]C(=O)C1=C(OC)C=CC(Br)=C1

[H]C(=O)C1=C(Br)C=CC(OC)=C1

FC1=CC(=CC=C1)C(=O)CBr

ClCCCC(=O)C1=CC=C(Cl)C=C1

CC(C)(C)OC(=O)NC1=CC=CC(C=O)=C1

O=C1CCC(C2=CC=CC=C2)C2=C1C=CC=C2

CC(=O)C1=CC=C(Cl)C(Cl)=C1Cl

COC(=O)C1=C(C=O)C(OC)=CC(OC)=C1

[O-][N+](=O)C1=C(Br)C=CC(C=O)=C1

[O-][N+](=O)C1=C(C=O)C=CC(Br)=C1

[H]C(=O)C1=C(Br)C=CC(OC)=C1O

CC1(C)OB(OC1(C)C)C1=CC=C(C=O)C=C1

CC1(C)OB(OC1(C)C)C1=CC(C=O)=CC=C1

CC1(C)OB(OC1(C)C)C1=C(C=O)C=CC=C1

O=C(OCC1=CC=CC=C1)N1CCC(=O)CC1

ClC1=CC=C(C=C1)C(=O)CBr

O=C1CCC(CC2=CC=CC=C2)C2=CC=CC=C12

[H]C(=O)C1=CC=C(OCC2=CC=CC=C2)C(OC)=C1

COC1=C(OCC2=CC=CC=C2)C=CC(C=O)=C1

CC(C)(C)OC(=O)N1C=C(C=O)C2=C1C=CC=C2

COC1=CC=CC=C1CC(=O)\C=C\C1=CC=CC=C1

CC(=O)C1=CC(=CC(=C1)C(F)(F)F)C(F)(F)F