Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

An Efficient Passerini Tetrazole Reaction (PT-3CR)

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Contents

General Information

Reagents were available from commercial suppliers (Sigma Aldrich, ABCR, Acros and AK Scientific) and used without any purification unless otherwise noted. 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). All ultrasonic irradiation reactions were carried out in a Sonicor "SC" Ultrasonic Table Top Cleaner with 220/240V, frequency of 50/60 Hz and 25 Amps. Nuclear magnetic resonance spectra were recorded on a Bruker Avance 500 spectrometer. Chemical shifts for ^{1}H NMR were reported relative to TMS (δ 0 ppm) and coupling constants were in hertz (Hz). The following abbreviations were used for spin multiplicity: s = singlet, d = doublet, t = triplet, dt = double triplet, ddd = doublet of double doublet, and m = multiplet. Chemical shifts for ^{13}C NMR reported in ppm relative to the solvent peak ($CDCl_3$ δ 77.23 ppm). Mass spectra were measured on a Waters Investigator Supercritical Fluid Chromatograph with a 3100 MS Detector (ESI) using a solvent system of methanol and CO_2 on a Viridis silica gel column (4.6 × 250 mm, 5 μm particle size) and reported as (m/z).

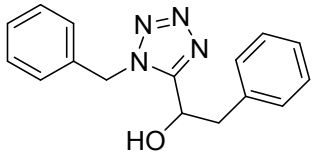
Experimental Procedures and Spectral Data

General procedure for the synthesis of tetrazole:

A 10 ml tube was charged with aldehyde/ketone (1.0 mmol) and isocyanide (1.0 mmol) and trimethylsilyl azide (1 mmol) in methanol:water (1:1) (1 ml). The mixture was sonicated in the water bath of an ultrasonic cleaner (220/240V, 25 Amps and frequency of 50/60 Hz) at room temperature till completion of the reaction (monitored by TLC). The solvent was removed under reduced pressure and the residue was purified by silica gel flash chromatography using EtOAc–hexane as eluent.

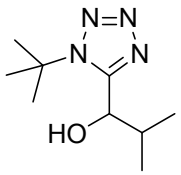
Spectral Data

1-(1-benzyl-1*H*-tetrazol-5-yl)-2-phenylethanol (3a)



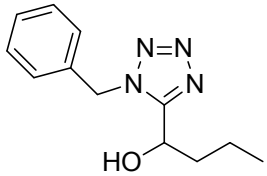
Colourless liquid, mp 79-80 °C, yield: 268 mg (96%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 3H), 7.29 – 7.23 (m, 3H), 7.18 (dd, *J* = 6.6, 2.9, 2H), 7.11 – 7.04 (m, 2H), 5.49 (d, *J* = 15.1, 1H), 5.37 (d, *J* = 15.1, 1H), 5.25 – 5.09 (m, 1H), 3.39 (s, 1H), 3.19 (dd, *J* = 13.8, 5.4, 1H), 3.07 (dd, *J* = 13.8, 8.3, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.9, 135.8, 133.8, 129.6, 129.0, 128.8, 128.7, 128.0, 127.2, 66.2, 51.3, 42.3. MS (ESI) m/z calculated $[M+H]^+$: 281.13; found $[M+H]^+$: 281.16.

1-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-2-methylpropan-1-ol (3b)



White solid, mp 126-127 °C, yield: 195 mg (98%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.71 (dd, *J* = 10.2, 8.5, 1H), 3.23 (d, *J* = 10.1, 1H), 2.53 – 2.39 (m, 1H), 1.78 (s, 9H), 1.18 (d, *J* = 6.6, 3H), 0.85 (d, *J* = 6.7, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 70.8, 61.6, 34.1, 30.3, 19.5, 18.2. MS (ESI) m/z calculated $[M+Na]^+$: 221.14; found $[M+Na]^+$: 221.18.

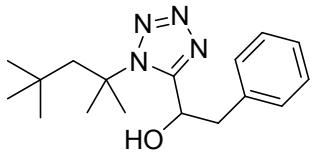
1-(1-benzyl-1*H*-tetrazol-5-yl)butan-1-ol (3c)



Colourless liquid, yield: 186 mg (80%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.31 (m, 3H), 7.31 – 7.24 (m, 2H), 5.72 (q, *J* = 15.1, 2H), 4.99 (t, *J* = 6.4, 1H), 3.98 (s, 1H), 1.92 – 1.78 (m, 1H), 1.77 – 1.67

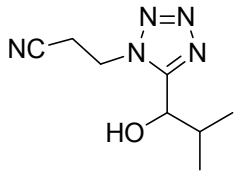
(m, 1H), 1.49 – 1.36 (m, 1H), 1.30 – 1.24 (m, 1H), 0.84 (t, J = 7.4, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 133.9, 129.0, 128.7, 127.9, 64.7, 51.5, 37.6, 18.4, 13.5. MS (ESI) m/z calculated $[M+Na]^+$: 255.12; found $[M+Na]^+$: 255.08.

2-phenyl-1-(1-(2,4,4-trimethylpentan-2-yl)-1*H*-tetrazol-5-yl)ethanol (3d)



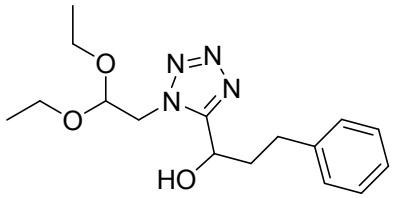
White solid, mp 135-136 °C, yield: 232 mg (77%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 – 7.22 (m, 2H), 7.21 – 7.16 (m, 3H), 5.38 – 5.20 (m, 1H), 4.09 (d, J = 9.6, 1H), 3.48 (qd, J = 13.4, 7.2, 2H), 1.96 (d, J = 15.2, 1H), 1.81 (d, J = 17.6, 4H), 1.57 (s, 3H), 0.68 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 136.2, 129.7, 128.7, 127.1, 67.1, 65.3, 53.8, 43.2, 31.6, 30.5, 30.3, 30.2. MS (ESI) m/z calculated $[M+Na]^+$: 325.20; found $[M+Na]^+$: 325.20.

3-(5-(1-hydroxy-2-methylpropyl)-1*H*-tetrazol-1-yl)propanenitrile (3e)



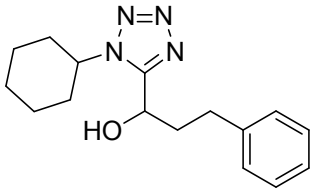
Colorless liquid, yield: 140 mg (72%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.92 (dt, J = 13.9, 6.9, 2H), 4.77 (dt, J = 13.7, 6.8, 1H), 4.30 (s, 1H), 3.12 (t, J = 6.9, 2H), 2.29 – 2.16 (m, 1H), 1.08 (d, J = 6.7, 3H), 0.91 (d, J = 6.8, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 116.3, 70.9, 43.7, 33.8, 18.7, 18.6, 17.8. MS (ESI) m/z calculated $[M+Na]^+$: 218.10; found $[M+Na]^+$: 218.09.

1-(1-(2,2-diethoxyethyl)-1*H*-tetrazol-5-yl)-3-phenylpropan-1-ol (3f)



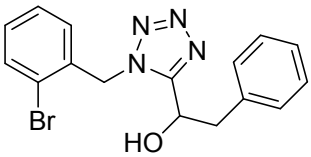
Colorless liquid, yield: 170 mg (53%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.24 (m, 2H), 7.23 – 7.12 (m, 3H), 5.04 (dd, J = 12.8, 6.4, 1H), 4.82 (t, J = 5.5, 1H), 4.63 (dd, J = 14.2, 5.6, 1H), 4.52 (dd, J = 14.2, 5.4, 1H), 4.08 (d, J = 5.8, 1H), 3.85 – 3.66 (m, 2H), 3.59 – 3.38 (m, 2H), 2.93 – 2.72 (m, 2H), 2.44 – 2.24 (m, 2H), 1.12 (dt, J = 14.3, 7.0, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 140.7, 128.5, 128.5, 126.1, 100.5, 64.3, 64.2, 64.0, 50.0, 36.9, 31.2, 15.0, 15.0. MS (ESI) m/z calculated $[M+H]^+$: 321.18; found $[M+H]^+$: 321.05.

1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-3-phenylpropan-1-ol (3g)



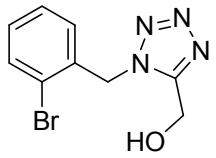
White solid, mp 104-105 °C, yield: 217 mg (76%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.23 (m, 2H), 7.21 – 7.14 (m, 3H), 5.08 – 4.93 (m, 2H), 4.57 – 4.39 (m, 1H), 2.92 – 2.80 (m, 1H), 2.79 – 2.68 (m, 1H), 2.41 – 2.26 (m, 1H), 2.26 – 2.10 (m, 1H), 2.05 – 1.82 (m, 6H), 1.71 (d, *J* = 12.4, 1H), 1.48 – 1.17 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.6, 140.7, 128.6, 128.5, 126.2, 63.7, 58.4, 37.4, 33.0, 31.5, 25.3, 25.2, 24.9. MS (ESI) m/z calculated $[M+H]^+$: 287.18; found $[M+H]^+$: 287.21.

1-(1-(2-bromobenzyl)-1*H*-tetrazol-5-yl)-2-phenylethanol (3h)



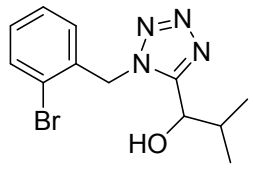
White solid, mp 94-95 °C, yield: 275 mg (77%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 7.5, 1.6, 1H), 7.29 – 7.21 (m, 3H), 7.17 (td, *J* = 7.1, 1.8, 2H), 7.09 (dd, *J* = 7.5, 1.6, 2H), 6.72 (dd, *J* = 7.3, 1.9, 1H), 5.49 (d, *J* = 16.0, 1H), 5.41 (d, *J* = 16.0, 1H), 5.26 (t, *J* = 6.7, 1H), 4.05 (s, 1H), 3.26 (dd, *J* = 13.7, 5.9, 1H), 3.19 (dd, *J* = 13.7, 7.7, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 135.6, 133.3, 133.1, 130.1, 129.6, 129.1, 128.8, 128.1, 127.3, 122.7, 66.2, 51.1, 42.5. MS (ESI) m/z calculated $[M+H]^+$: 359.04; found $[M+H]^+$: 359.04.

(1-(2-bromobenzyl)-1*H*-tetrazol-5-yl)methanol (3i)



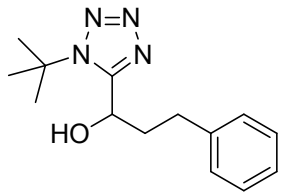
White solid, mp 64-65 °C, yield: 112 mg (42%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 7.9, 1.1, 1H), 7.28 (td, *J* = 7.3, 1.1, 1H), 7.21 (td, *J* = 7.7, 1.6, 1H), 7.04 (dd, *J* = 7.7, 1.5, 1H), 5.73 (s, 2H), 5.13 (s, 1H), 4.94 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.5, 133.3, 132.7, 130.5, 129.9, 128.2, 123.2, 53.6, 51.4. MS (ESI) m/z calculated $[M+H]^+$: 269.00; found $[M+H]^+$: 269.00.

1-(1-(2-bromobenzyl)-1*H*-tetrazol-5-yl)-2-methylpropan-1-ol (3j)



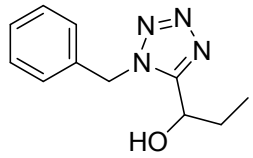
White solid, mp 86-87 °C, yield: 249 mg (80%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 7.8, 0.9, 1H), 7.24 (dt, *J* = 7.6, 3.8, 1H), 7.19 (td, *J* = 7.7, 1.5, 1H), 6.88 (dd, *J* = 7.6, 1.1, 1H), 5.79 (s, 2H), 4.89 – 4.73 (m, 1H), 4.67 (d, *J* = 6.2, 1H), 2.11 (dq, *J* = 13.6, 6.8, 1H), 1.03 (d, *J* = 6.7, 3H), 0.77 (d, *J* = 6.8, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 133.5, 133.1, 130.1, 129.2, 128.0, 122.8, 70.3, 51.4, 33.4, 18.7, 18.0. MS (ESI) m/z calculated $[M+H]^+$: 311.04; found $[M+H]^+$: 311.09.

1-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-3-phenylpropan-1-ol (3k)



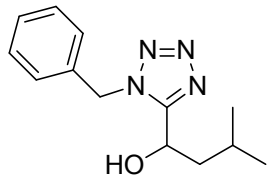
White solid, mp 102-103 °C, yield: 228 mg (88%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 2H), 7.20 (d, *J* = 7.3, 3H), 5.00 (td, *J* = 9.3, 4.8, 1H), 3.96 (d, *J* = 9.9, 1H), 3.01 – 2.78 (m, 2H), 2.55 – 2.40 (m, 1H), 2.34 – 2.19 (m, 1H), 1.63 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 140.6, 128.6, 128.5, 126.2, 63.9, 61.7, 38.2, 31.6, 29.9. MS (ESI) m/z calculated $[M+H]^+$: 283.15; found $[M+H]^+$: 283.06.

1-(1-benzyl-1*H*-tetrazol-5-yl)propan-1-ol (3l)



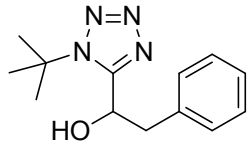
White solid, mp 77-78 °C, yield: 198 mg (91%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.22 (m, 5H), 5.73 (d, *J* = 15.1, 1H), 5.68 (d, *J* = 15.1, 1H), 4.94 (dd, *J* = 13.3, 6.3, 1H), 4.84 (d, *J* = 6.2, 1H), 1.94 – 1.73 (m, 2H), 0.87 (t, *J* = 7.4, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 134.0, 129.0, 128.7, 127.9, 66.3, 51.5, 28.9, 9.6. MS (ESI) m/z calculated $[M+H]^+$: 219.12; found $[M+H]^+$: 219.10.

1-(1-benzyl-1*H*-tetrazol-5-yl)-3-methylbutan-1-ol (3m)



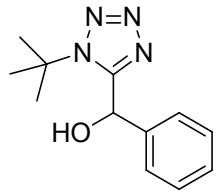
White solid, mp 85-86 °C, yield: 226 mg (92%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 3H), 7.28 – 7.23 (m, 2H), 5.74 (d, *J* = 15.2, 1H), 5.67 (d, *J* = 15.1, 1H), 5.15 – 4.95 (m, 1H), 4.55 (d, *J* = 6.4, 1H), 1.81 – 1.60 (m, 2H), 1.54 – 1.42 (m, 1H), 0.82 (d, *J* = 6.6, 3H), 0.77 (d, *J* = 6.5, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 133.9, 129.0, 128.7, 127.9, 63.2, 51.5, 44.3, 24.2, 22.8, 21.6. MS (ESI) m/z calculated $[M+Na]^+$: 269.14; found $[M+Na]^+$: 269.13.

1-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-2-phenylethanol (3n)



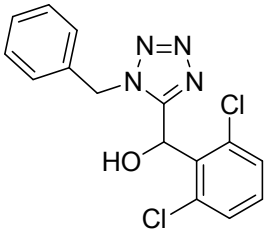
White solid, mp 160-161 °C, yield: 239 mg (97%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 3H), 7.28 – 7.23 (m, 2H), 5.74 (d, *J* = 15.2, 1H), 5.67 (d, *J* = 15.1, 1H), 5.15 – 4.95 (m, 1H), 4.55 (d, *J* = 6.4, 1H), 1.81 – 1.60 (m, 2H), 1.54 – 1.42 (m, 1H), 0.82 (d, *J* = 6.6, 3H), 0.77 (d, *J* = 6.5, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 133.9, 129.0, 128.7, 127.9, 63.2, 51.5, 44.3, 24.2, 22.8, 21.6. MS (ESI) m/z calculated $[M+Na]^+$: 269.14; found $[M+Na]^+$: 269.19.

(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)(phenyl)methanol (3o)



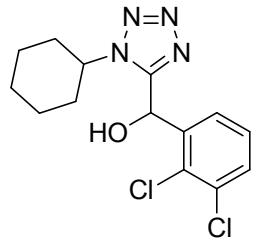
White solid, mp 122-123 °C, yield: 95 mg (41%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (t, *J* = 5.8, 3H), 7.33 – 7.25 (m, 2H), 6.30 (d, *J* = 7.3, 1H), 4.29 (s, 1H), 1.63 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 139.2, 129.0, 128.9, 127.2, 68.5, 62.1, 29.9. MS (ESI) m/z calculated $[M+Na]^+$: 255.12; found $[M+Na]^+$: 255.08.

(1-benzyl-1*H*-tetrazol-5-yl)(2,6-dichlorophenyl)methanol (3p)



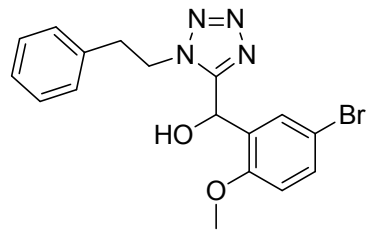
White solid, mp 144-145 °C, yield: 237 mg (71%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 4H), 7.29 (s, 1H), 7.24 (dd, *J* = 13.1, 6.0, 1H), 7.18 (dd, *J* = 6.5, 2.8, 2H), 6.63 (d, *J* = 9.3, 1H), 5.70 (d, *J* = 4.5, 2H), 3.94 (d, *J* = 9.4, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.0, 135.2, 133.4, 132.9, 130.9, 129.4, 129.0, 128.7, 127.5, 65.2, 51.8. MS (ESI) m/z calculated $[M+H]^+$: 335.04; found $[M+H]^+$: 335.10.

(1-cyclohexyl-1*H*-tetrazol-5-yl)(2,3-dichlorophenyl)methanol (3q)



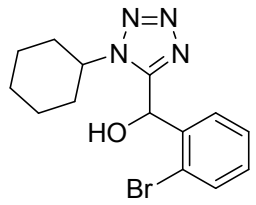
White soild, mp 156-157 °C, yield: 238 mg (73%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.9, 1.3, 1H), 7.50 (dd, *J* = 8.0, 1.5, 1H), 7.33 (t, *J* = 7.9, 1H), 6.49 (d, *J* = 6.2, 1H), 4.72 (d, *J* = 6.3, 1H), 4.29 (tt, *J* = 11.4, 3.8, 1H), 1.99 – 1.77 (m, 6H), 1.75 – 1.70 (m, 1H), 1.41 – 1.20 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.9, 138.3, 133.6, 130.9, 130.6, 127.9, 126.4, 64.2, 58.6, 32.8, 32.7, 25.3, 25.3, 24.8. MS (ESI) m/z calculated $[M+H]^+$: 327.07; found $[M+H]^+$: 327.03.

(5-bromo-2-methoxyphenyl)(1-phenethyl-1*H*-tetrazol-5-yl)methanol (3r)



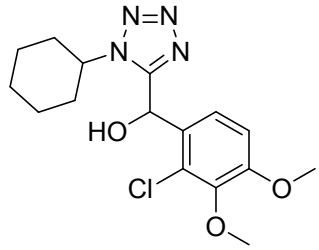
White soild, mp 133-134 °C, yield: 178 mg (46%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.40 (m, 2H), 7.35 – 7.27 (m, 3H), 7.04 (dd, *J* = 7.6, 1.4, 2H), 6.76 (d, *J* = 9.4, 1H), 5.85 (d, *J* = 7.0, 1H), 4.56 (t, *J* = 7.5, 2H), 3.86 (d, *J* = 7.0, 1H), 3.70 (s, 3H), 3.18 – 3.01 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.6, 155.3, 136.5, 132.9, 130.5, 129.0, 128.8, 128.1, 127.3, 113.5, 112.8, 63.1, 55.9, 49.2, 36.2. MS (ESI) m/z calculated $[M+H]^+$: 389.03; found $[M+H]^+$: 389.03.

(2-bromophenyl)(1-cyclohexyl-1*H*-tetrazol-5-yl)methanol (3s)



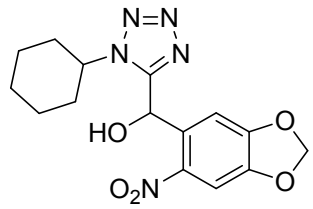
White soild, mp 141-142 °C, yield: 201 mg (60%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.8, 1.4, 1H), 7.57 (dd, *J* = 8.0, 0.8, 1H), 7.40 (t, *J* = 7.6, 1H), 7.24 (td, *J* = 7.8, 1.6, 1H), 6.48 (d, *J* = 6.0, 1H), 4.90 (d, *J* = 6.0, 1H), 4.25 (tt, *J* = 11.3, 3.8, 1H), 1.92 – 1.79 (m, 5H), 1.78 – 1.63 (m, 2H), 1.35 – 1.18 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.4, 137.5, 133.1, 130.5, 128.8, 128.2, 122.3, 66.0, 58.5, 32.7, 32.7, 25.3, 24.8. MS (ESI) m/z calculated $[M+H]^+$: 337.06; found $[M+H]^+$: 337.05.

(2-chloro-3,4-dimethoxyphenyl)(1-cyclohexyl-1*H*-tetrazol-5-yl)methanol (3t)



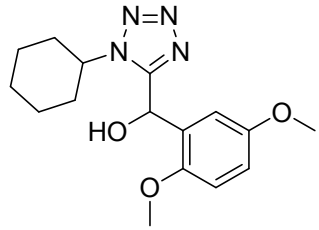
White soild, mp 167-168 °C, yield: 147 mg (42%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.7, 1H), 6.89 (d, *J* = 8.8, 1H), 6.46 (d, *J* = 6.0, 1H), 4.62 (d, *J* = 6.1, 1H), 4.25 (tt, *J* = 11.5, 3.8, 1H), 3.88 (s, 3H), 3.85 (s, 3H), 1.91 – 1.81 (m, 4H), 1.76 – 1.64 (m, 2H), 1.38 – 1.15 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.7, 154.01, 145.5, 128.8, 127.1, 123.5, 110.9, 63.8, 60.7, 58.4, 56.1, 32.7, 32.7, 25.3, 24.8. MS (ESI) m/z calculated $[M+H]^+$: 353.13; found $[M+H]^+$: 353.05.

(1-cyclohexyl-1*H*-tetrazol-5-yl)(6-nitrobenzo[*d*][1,3]dioxol-5-yl)methanol (3u)



Yellow soild, mp 198-199 °C, yield: 135 mg (39%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (s, 1H), 7.45 (s, 1H), 6.67 (d, *J* = 5.9, 1H), 6.19 (d, *J* = 11.5, 2H), 4.60 (t, *J* = 11.6, 1H), 4.06 (d, *J* = 5.7, 1H), 2.22 (d, *J* = 12.3, 1H), 2.15 – 1.94 (m, 5H), 1.78 (d, *J* = 12.1, 1H), 1.49 – 1.32 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.2, 132.7, 129.8, 108.0, 106.6, 105.9, 105.9, 103.5, 58.5, 33.1, 32.7, 25.3, 24.9. MS (ESI) m/z calculated $[M+H]^+$: 348.12; found $[M+H]^+$: 348.27.

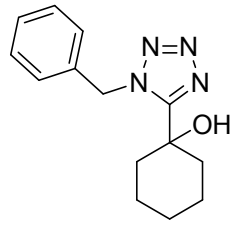
(1-cyclohexyl-1*H*-tetrazol-5-yl)(2,5-dimethoxyphenyl)methanol (3v)



White soild, mp 189-190 °C, yield: 152 mg (48%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.93 (d, *J* = 2.2, 1H), 6.86 (d, *J* = 3.1, 2H), 6.34 (d, *J* = 6.5, 1H), 4.35 (tt, *J* = 11.3, 3.7, 1H), 3.98 (d, *J* = 6.7, 1H),

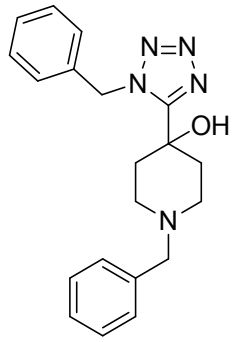
3.75 (s, 6H), 1.94 – 1.83 (m, 4H), 1.80 – 1.67 (m, 2H), 1.40 – 1.19 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 154.0, 150.5, 127.4, 114.89, 113.4, 112.15, 63.4, 58.23, 56.1, 55.8, 32.8, 32.7, 25.4, 24.9. MS (ESI) m/z calculated $[M+H]^+$: 319.17; found $[M+H]^+$: 319.22.

1-(1-benzyl-1*H*-tetrazol-5-yl)cyclohexanol (3w)



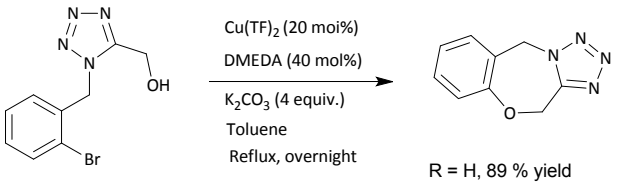
Colorless liquid, yield: 216 mg (84%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 3H), 7.25 – 7.21 (m, 2H), 5.83 (s, 2H), 3.84 (s, 1H), 1.98 – 1.87 (m, 2H), 1.85 – 1.76 (m, 2H), 1.76 – 1.53 (m, 5H), 1.36 – 1.21 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 134.9, 128.8, 128.3, 127.8, 70.45, 52.2, 37.0, 24.9, 21.1. MS (ESI) m/z calculated $[M+H]^+$: 259.15; found $[M+NH]^+$: 259.17.

1-benzyl-4-(1-benzyl-1*H*-tetrazol-5-yl)piperidin-4-ol (3x)



Colourless liquid, yield: 160 mg (46%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 7H), 7.25 – 7.18 (m, 3H), 5.82 (s, 2H), 3.52 (s, 2H), 3.40 (s, 1H), 2.79 – 2.59 (m, 2H), 2.43 (td, J = 11.6, 2.1, 2H), 2.31 – 2.11 (m, 2H), 1.77 (d, J = 12.8, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.8, 138.3, 134.8, 129.0, 128.9, 128.5, 128., 127.6, 127., 68.70, 62., 52., 48., 36.6. MS (ESI) m/z calculated $[M+H]^+$: 350.19; found $[M+H]^+$: 350.22.

Procedure for the synthesis of 5,11-dihydrobenzo[*f*]tetrazolo[5,1-*c*][1,4]oxazepine



DMEDA = N,N'-Dimethylethylenediamine

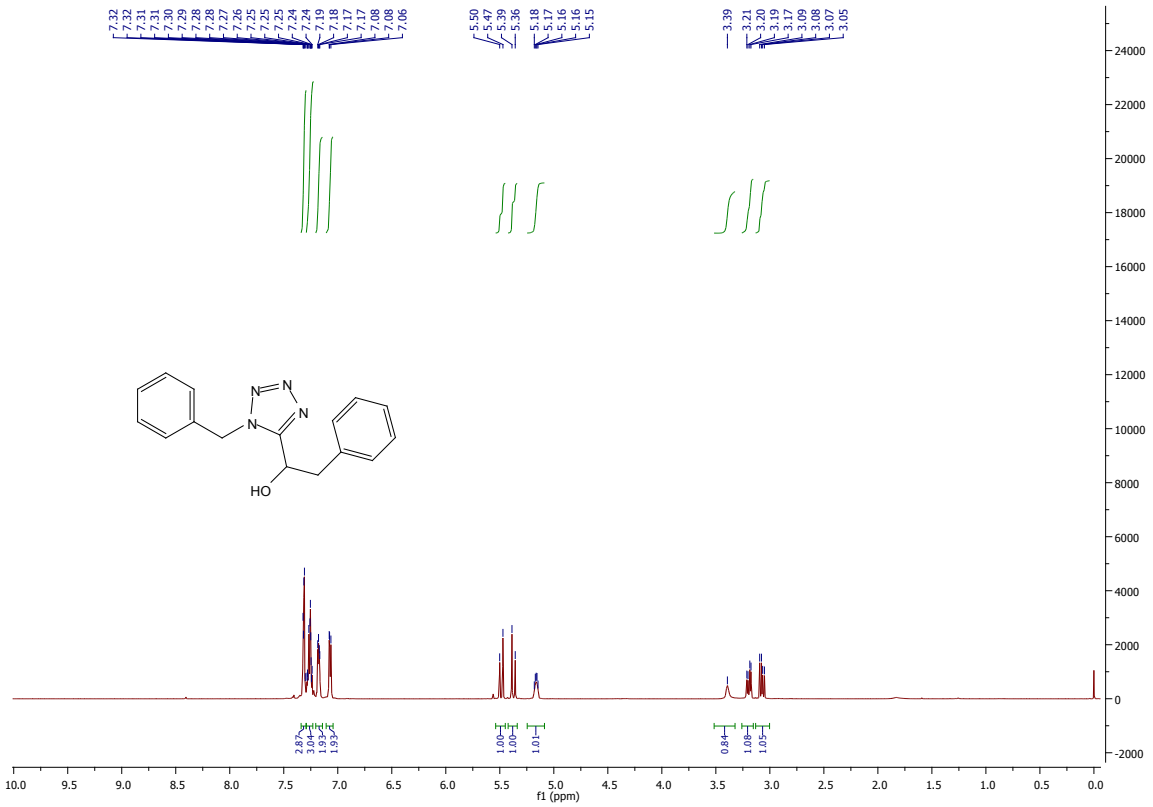
A 10 ml RBF equipped with a magnetic stirring bar was charged with (1-(2-bromobenzyl)-1H-tetrazol-5-yl)methanol (0.5 mmol, 134 mg), Copper triflate (20 mol%, 36 mg), N,N'Dimethylethylenediamine (40 mol%, 21µl), K_2CO_3 (4 equivalent, 276 mg) in toluene (2ml) and refluxed overnight. Then the reaction mixture was added to a 25 ml saturated $NaHCO_3$ solution and extracted in ethyl acetate. The solvent was removed under reduced pressure and the mixture was purified by flash chromatography on silica gel (eluent: hexane/EtOAc) to afford the titled compound as a white solid.

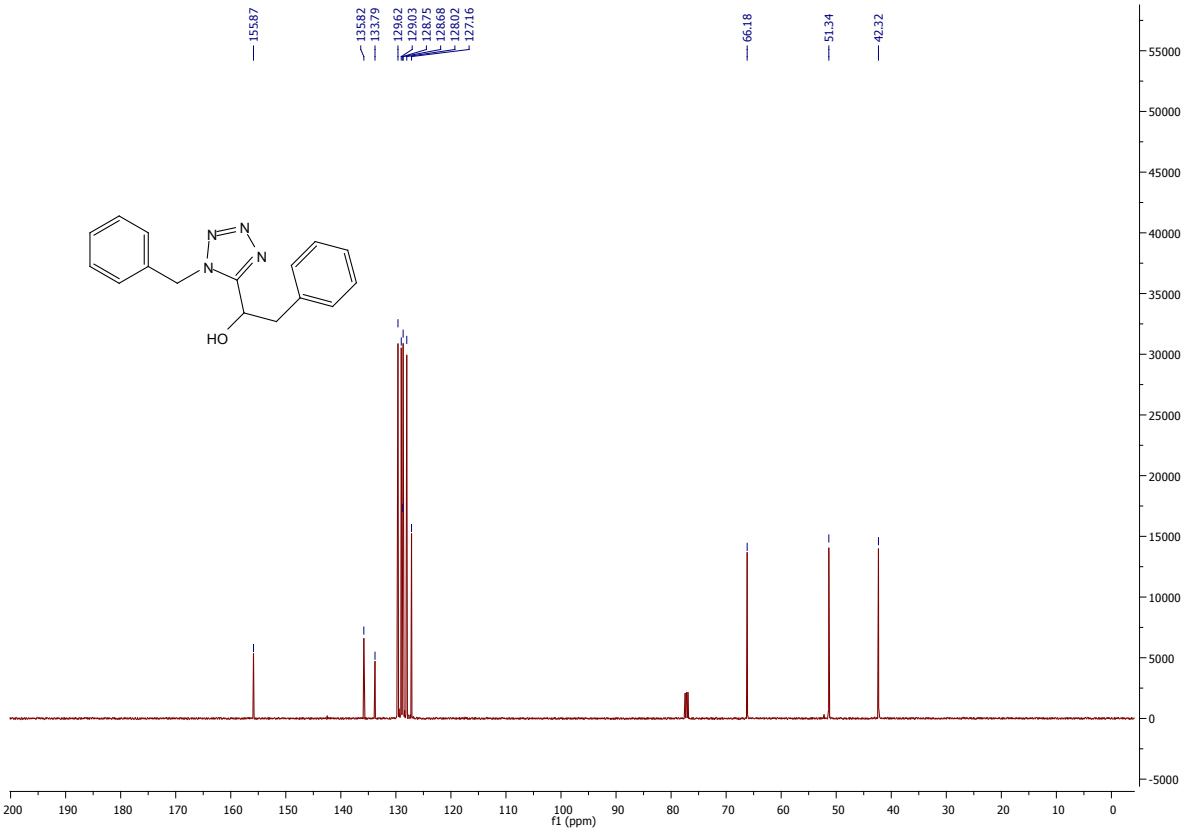
5,11-dihydrobenzo[*f*]tetrazolo[5,1-*c*][1,4]oxazepine (4)

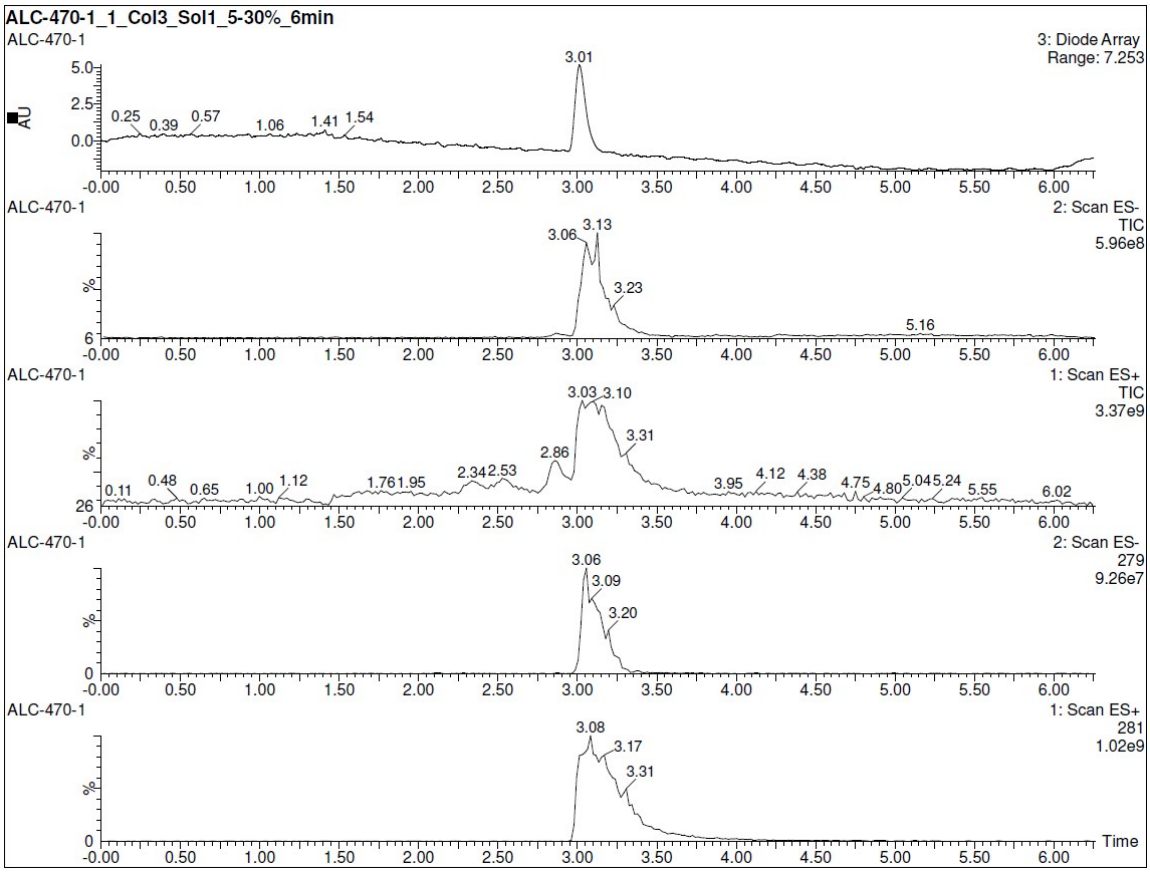
White solid, yield: 83 mg (89%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (td, *J* = 7.9, 1.4, 1H), 7.43 – 7.38 (m, 1H), 7.30 (d, *J* = 8.0, 1H), 7.25 (t, *J* = 7.5, 1H), 5.65 (s, 2H), 5.48 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 152.1, 131.7, 129.3, 127.8, 126.1, 122.2, 67.6, 49.5. MS (ESI) m/z calculated $[M+H]^+$: 189.07; found $[M+Na]^+$: 189.10.

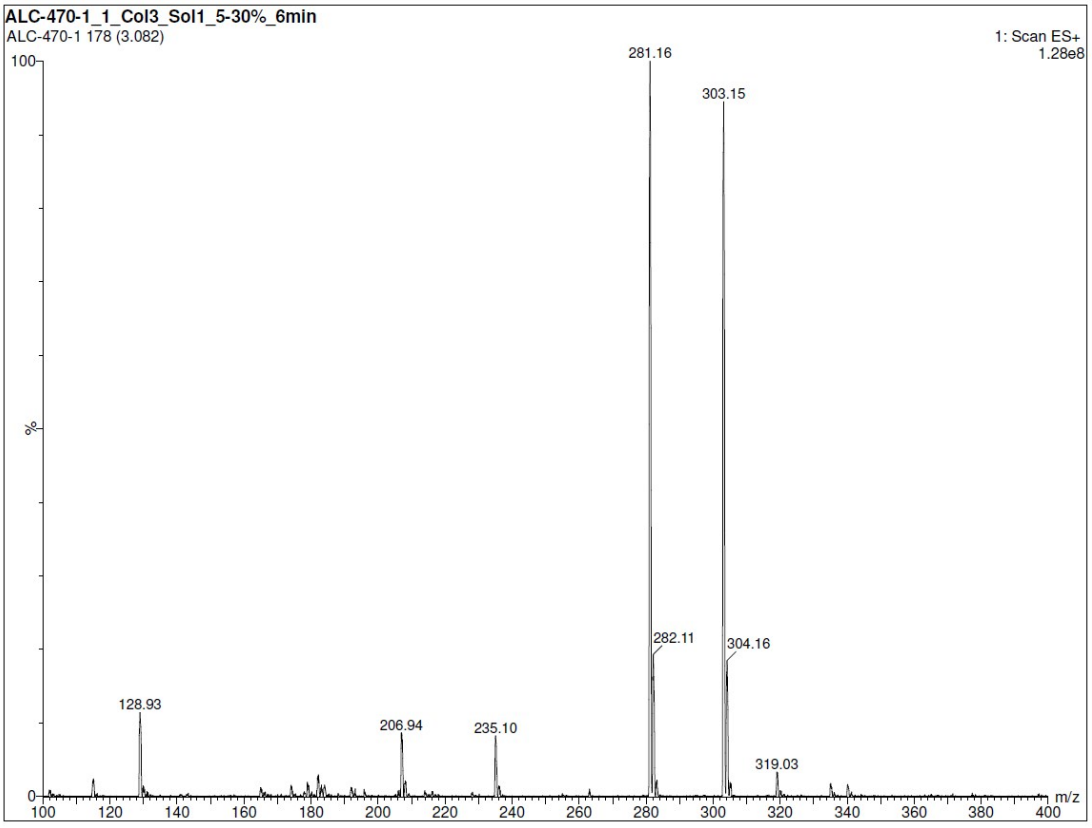
NMR spectra and SFC-MS Chromatograms

1-(1-benzyl-1*H*-tetrazol-5-yl)-2-phenylethanol (3a)

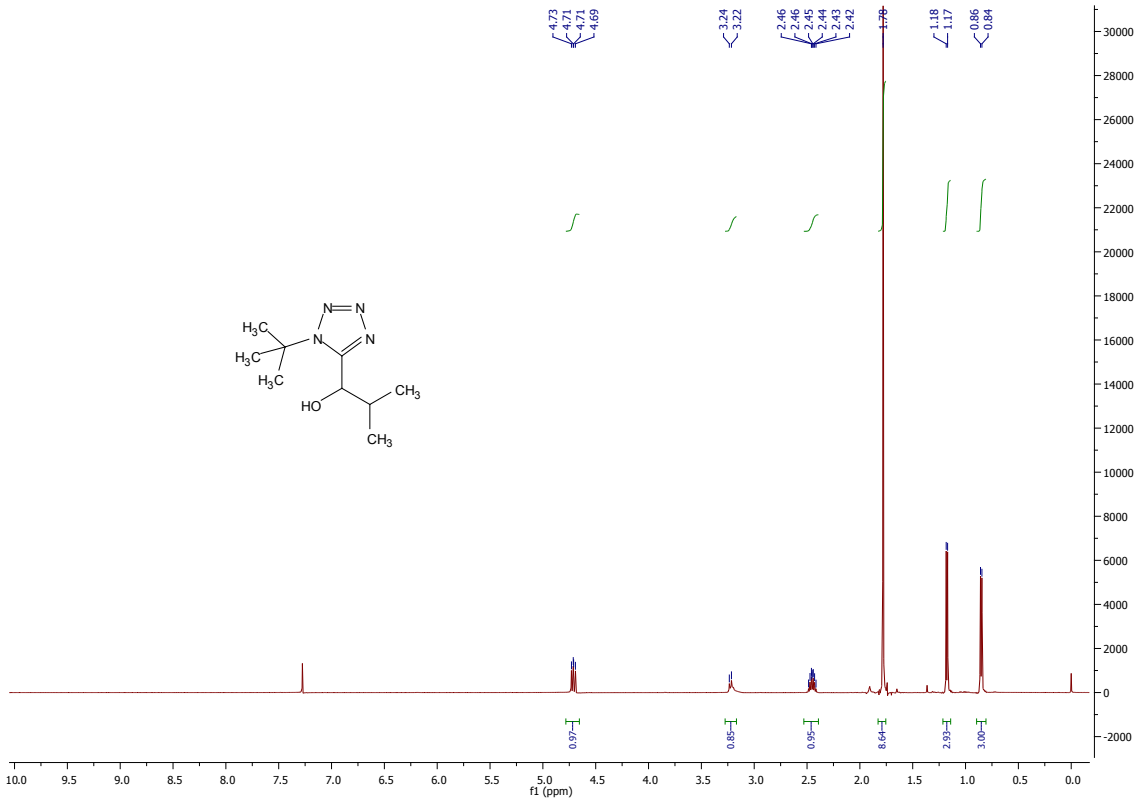


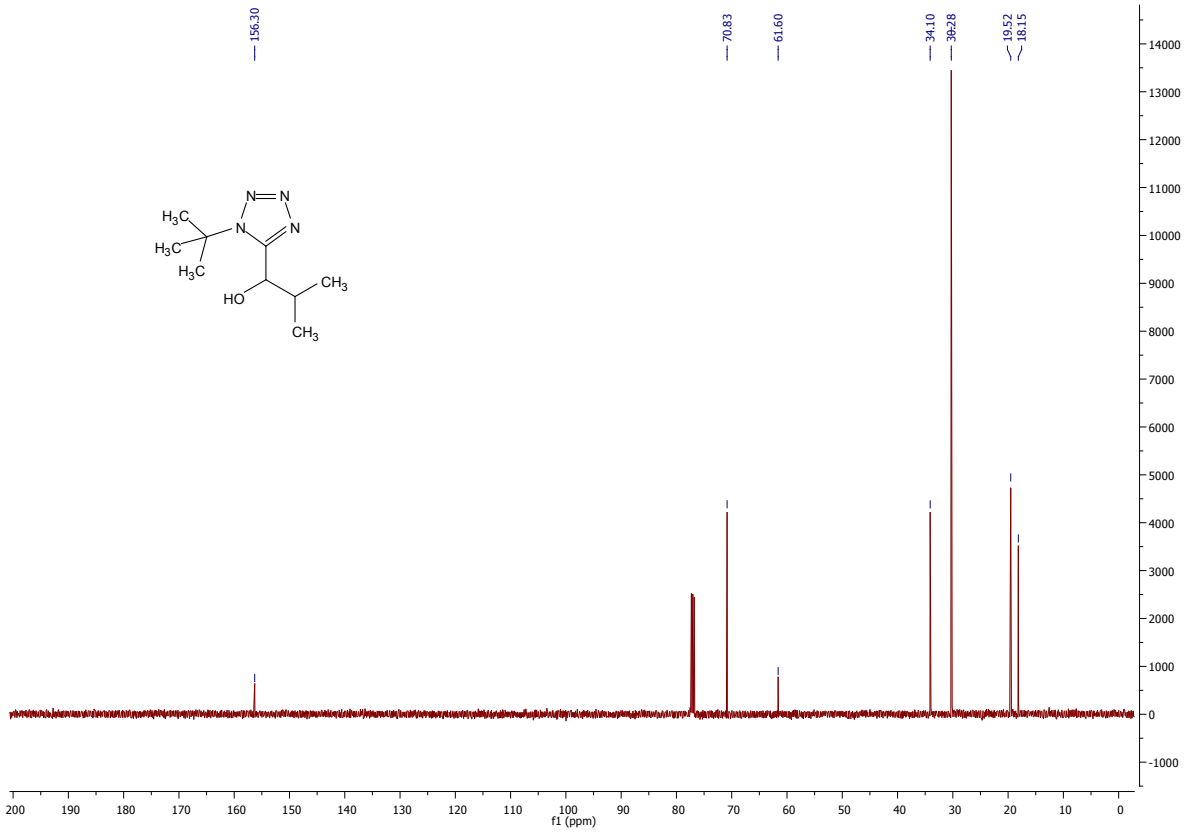

155.87
135.82
133.79
129.62
129.03
128.75
128.68
128.02
127.16
66.18
51.34
42.32
HO
f1 (ppm)

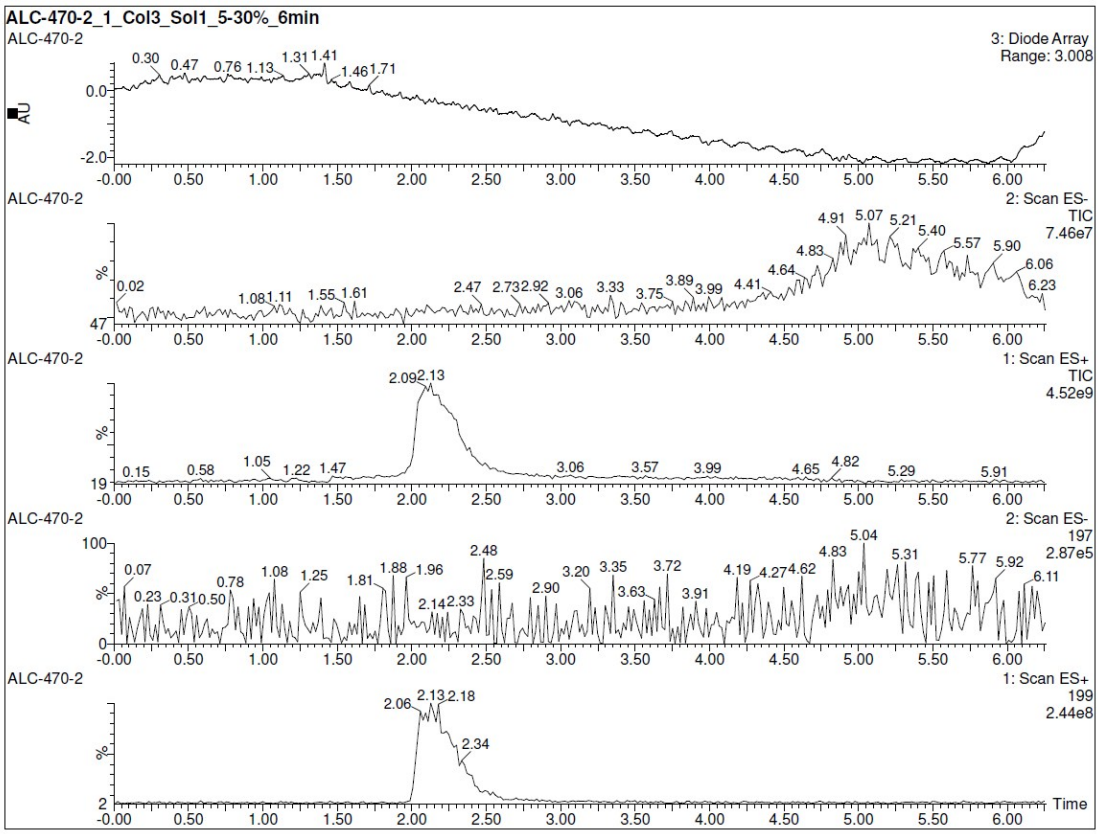

ALC-470-1_1_Col3_Sol1_5-30%_6min
ALC-470-1
3: Diode Array
Range: 7.253
AU
3.01
0.25
0.39
0.57
1.06
1.41
1.54
ALC-470-1
2: Scan ES-
TIC
5.96e8
3.06
3.13
3.23
5.16
ALC-470-1
1: Scan ES+
TIC
3.37e9
3.03
3.10
3.31
2.86
0.11
0.48
0.65
1.00
1.12
1.76
1.95
2.34
2.53
3.95
4.12
4.38
4.75
4.80
5.04
5.24
5.55
6.02
ALC-470-1
2: Scan ES-
279
9.26e7
3.06
3.09
3.20
ALC-470-1
1: Scan ES+
281
1.02e9
3.08
3.17
3.31
Time

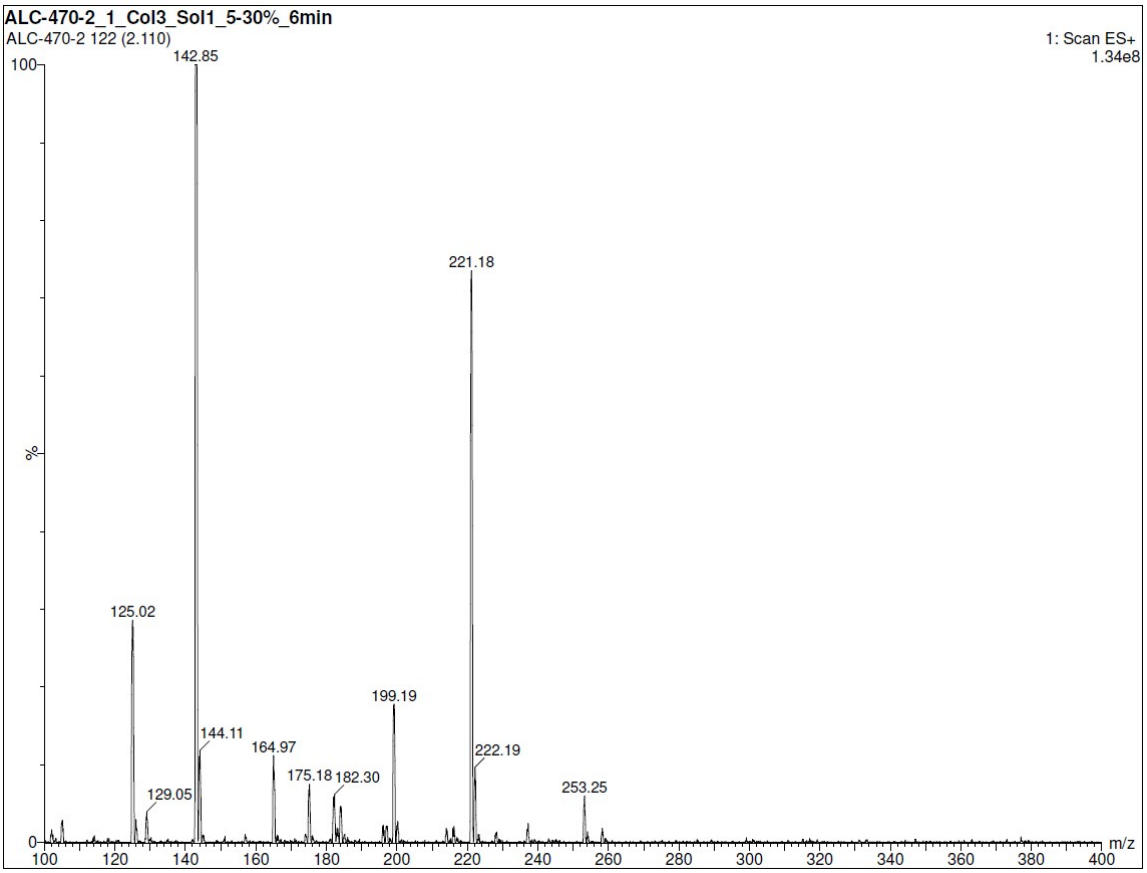

ALC-470-1_1_Col3_Sol1_5-30%_6min
ALC-470-1 178 (3.082)
1: Scan ES+
1.28e8
281.16
303.15
282.11
304.16
128.93
206.94
235.10
319.03
m/z

1-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-2-methylpropan-1-ol (3b)

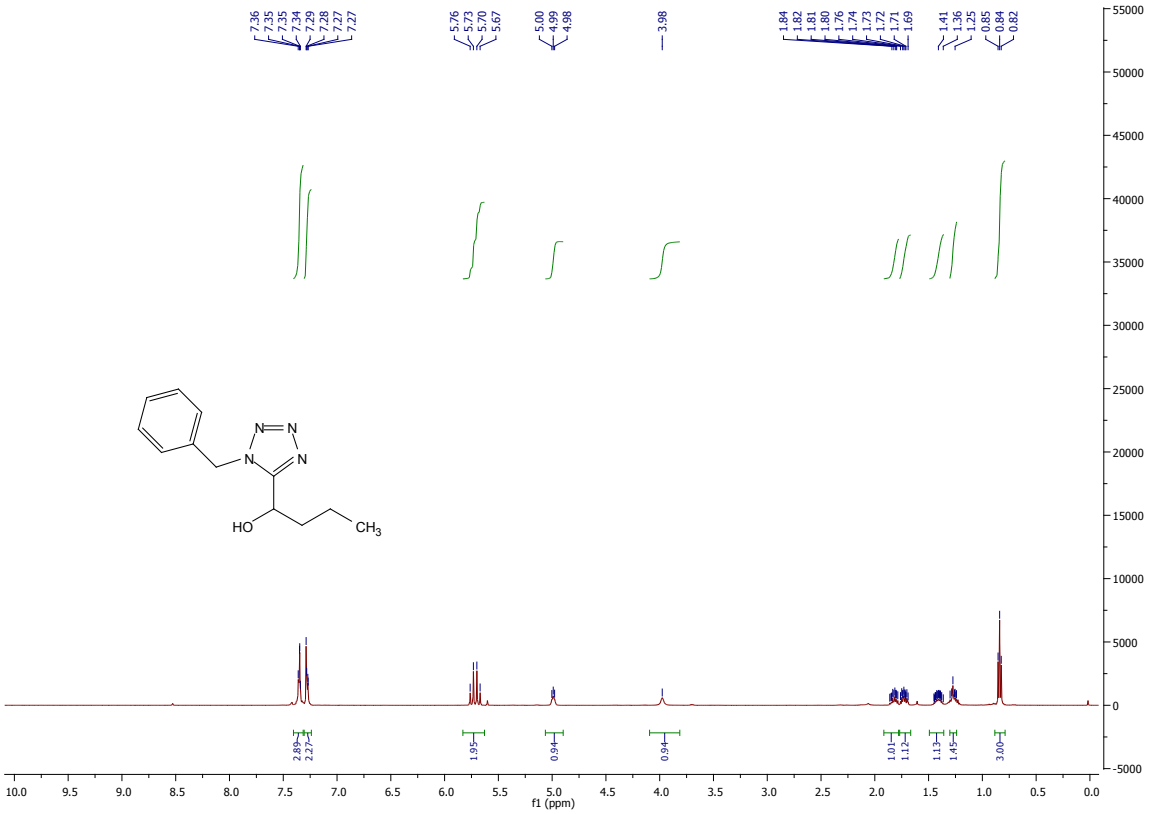


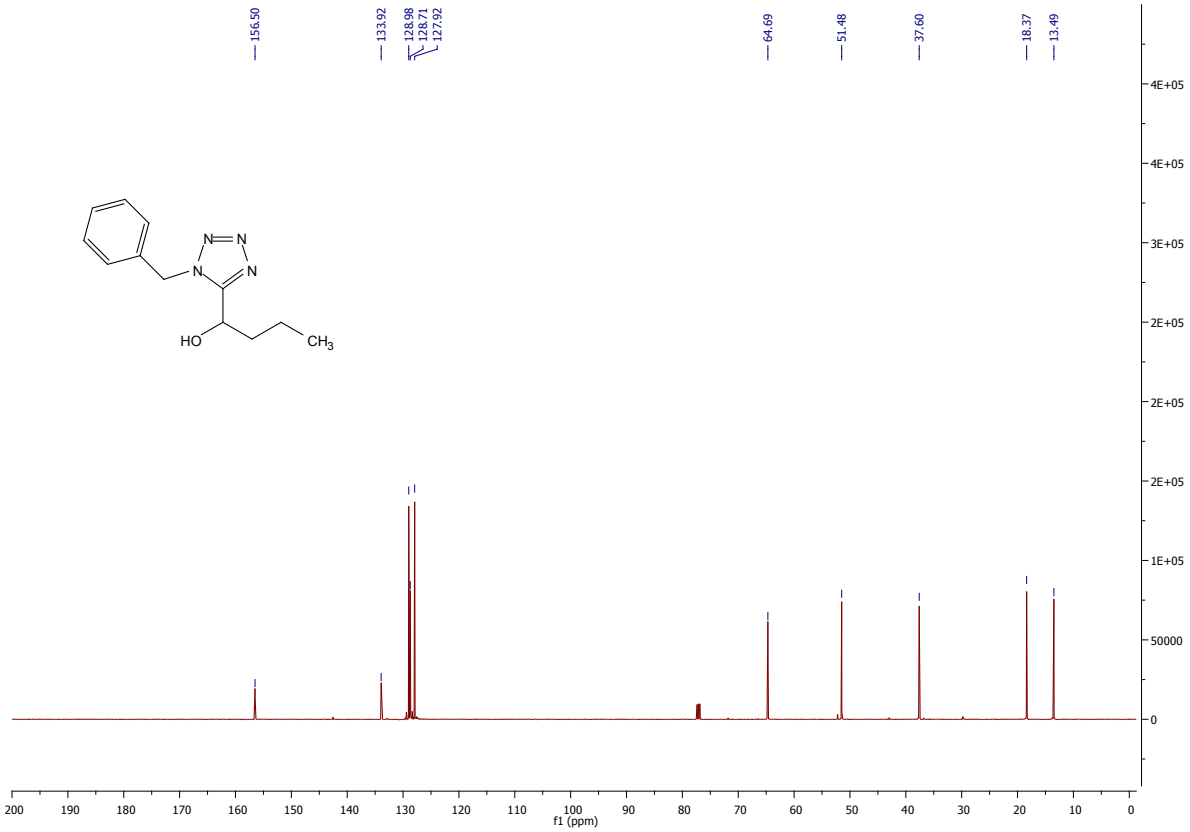


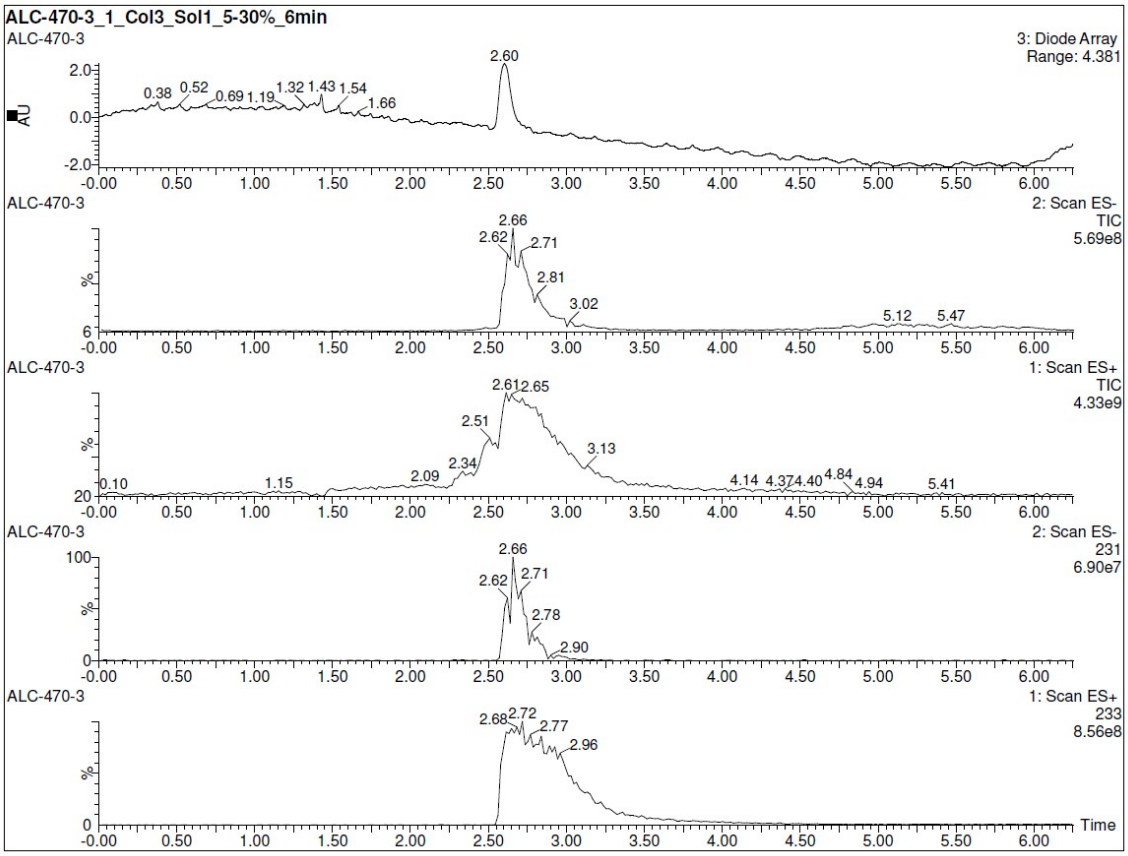

ALC-470-2_1_Col3_Sol1_5-30%_6min
ALC-470-2
3: Diode Array
Range: 3.008
AU
ALC-470-2
2: Scan ES-
TIC
7.46e7
ALC-470-2
1: Scan ES+
TIC
4.52e9
ALC-470-2
2: Scan ES-
197
2.87e5
ALC-470-2
1: Scan ES+
199
2.44e8
Time

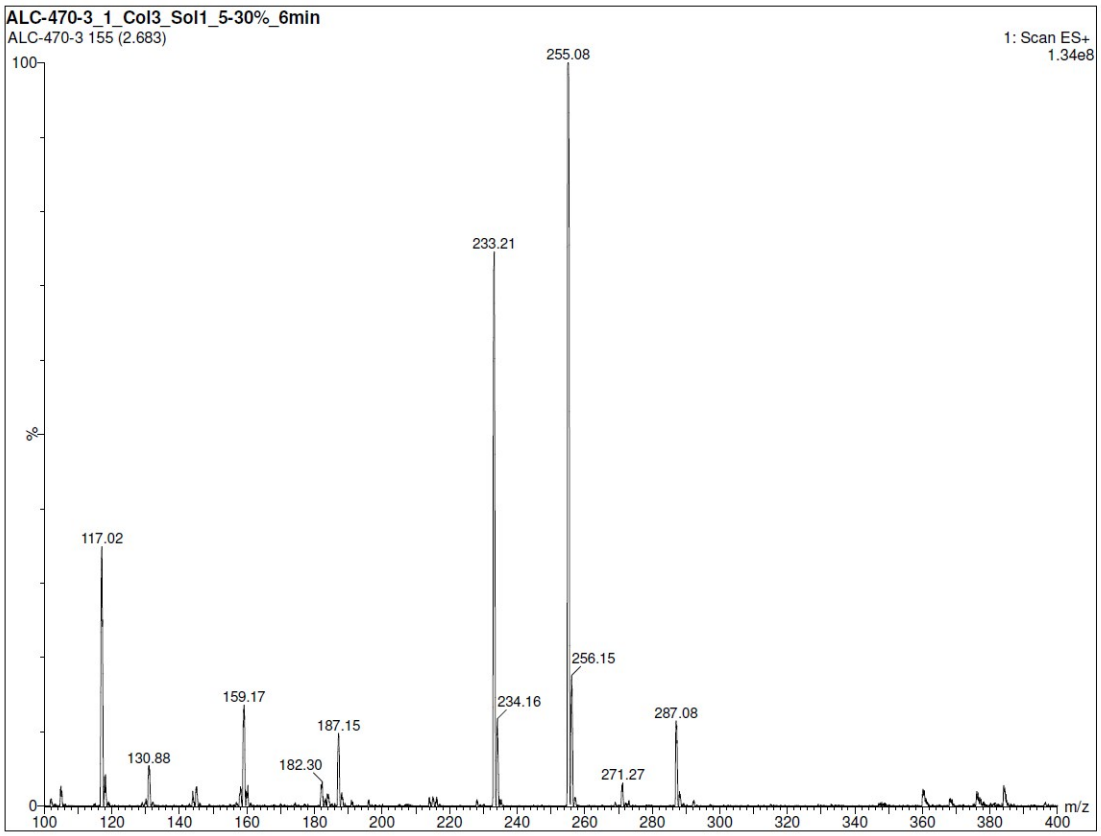

ALC-470-2_1_Col3_Sol1_5-30%_6min
ALC-470-2 122 (2.110)
1: Scan ES+
1.34e8
142.85
221.18
125.02
199.19
144.11
164.97
222.19
175.18
182.30
253.25
129.05
m/z

1-(1-benzyl-1*H*-tetrazol-5-yl)butan-1-ol (3c)

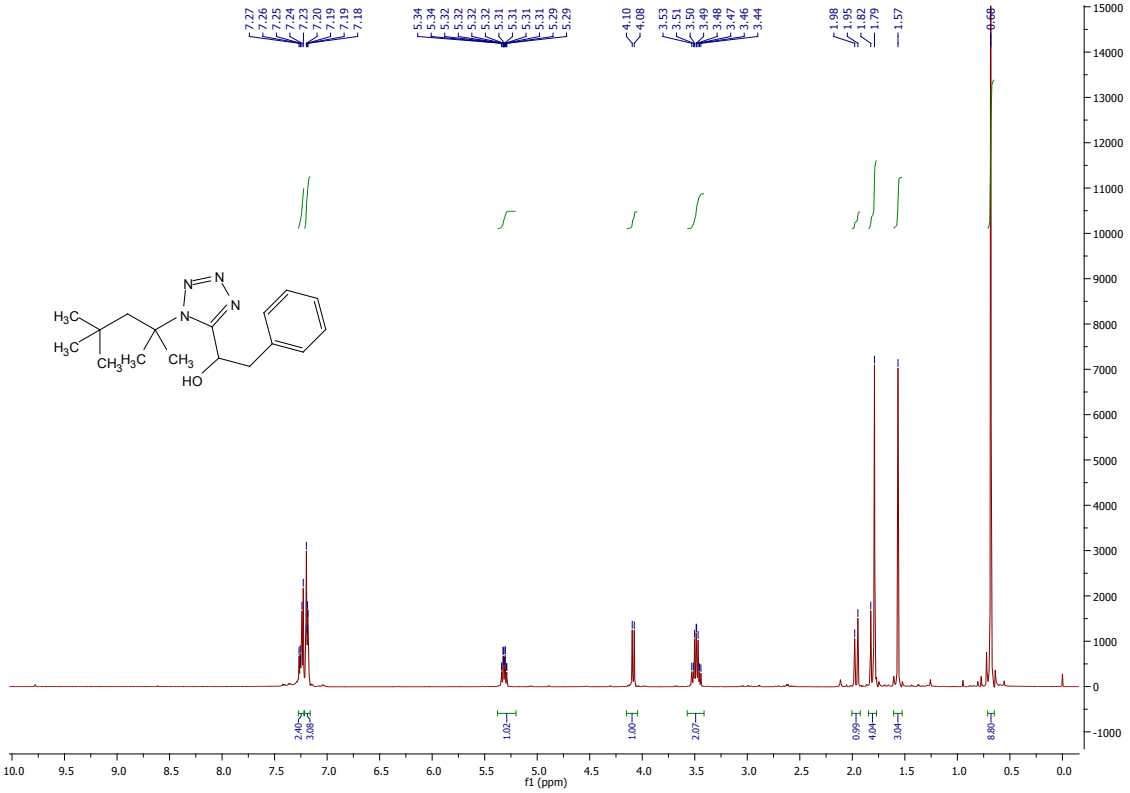


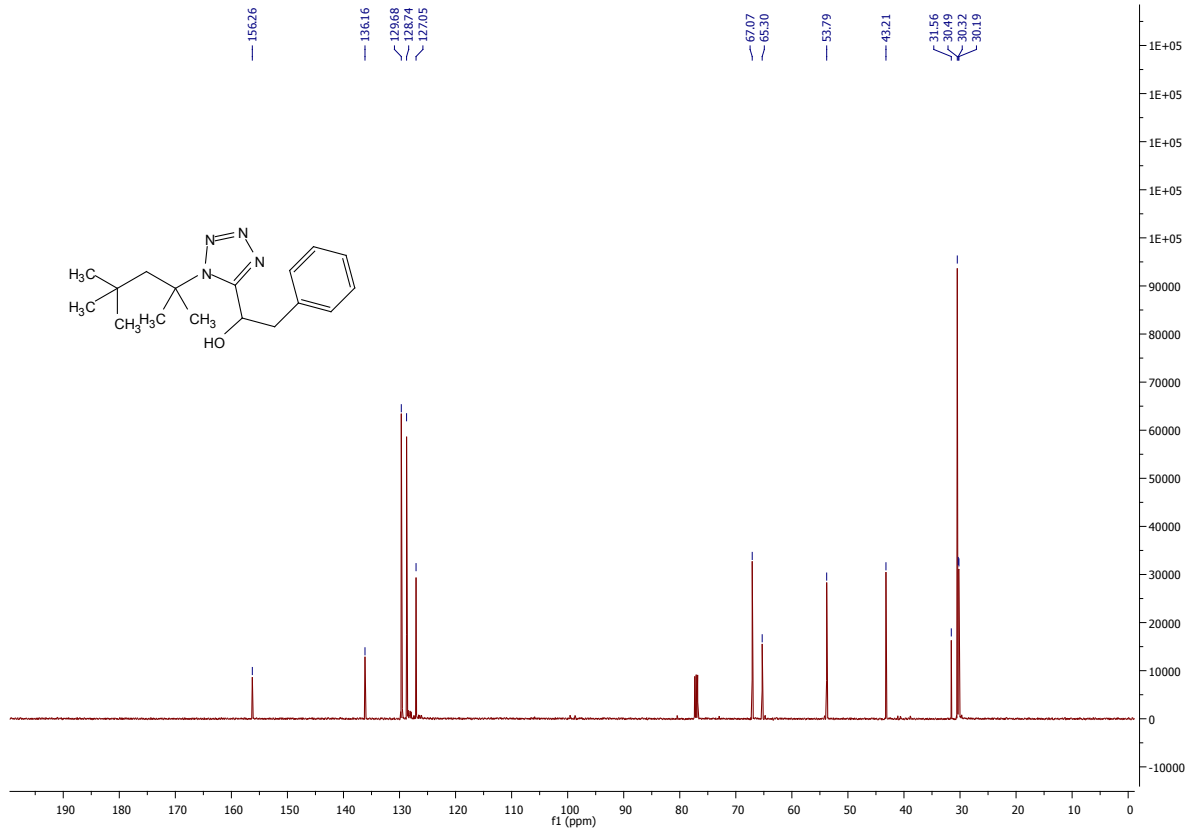


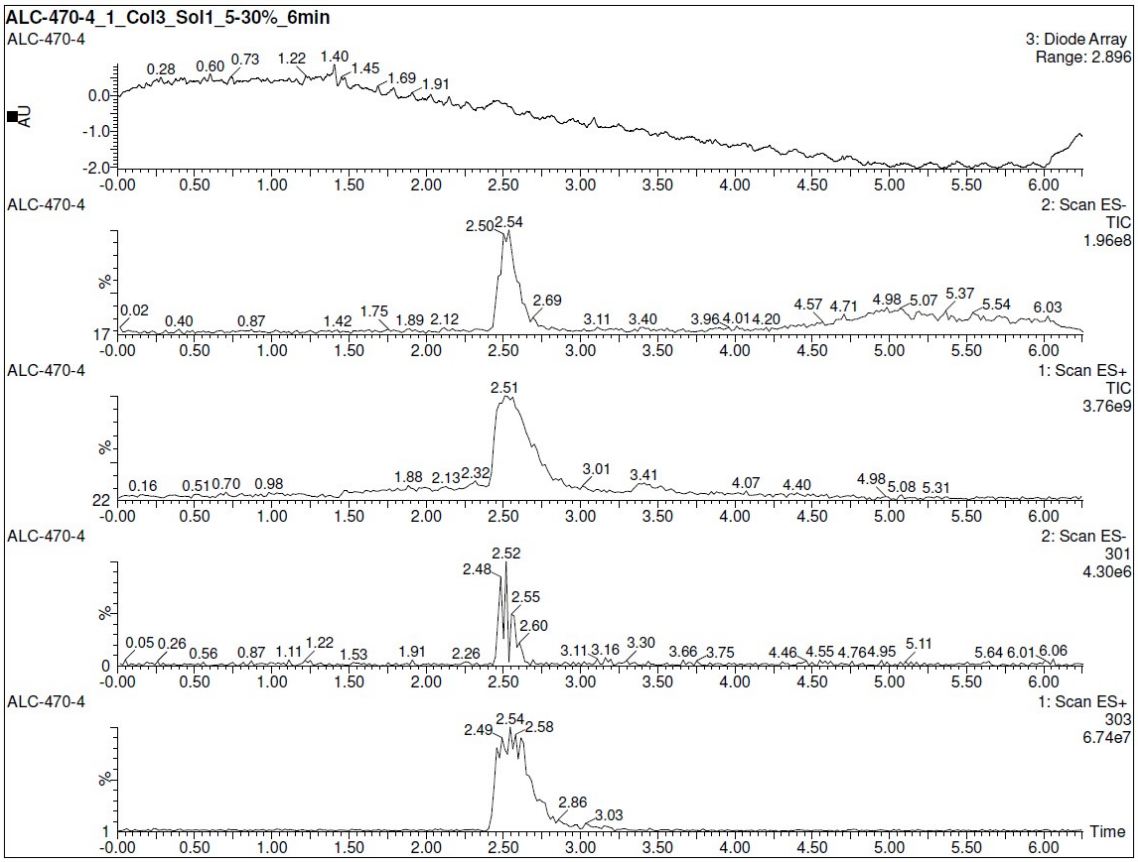

ALC-470-3_1_Col3_Sol1_5-30%_6min
ALC-470-3
3: Diode Array
Range: 4.381
AU
2.60
0.38 0.52 0.69 1.19 1.32 1.43 1.54 1.66
ALC-470-3
2: Scan ES-
TIC
5.69e8
2.66 2.62 2.71 2.81 3.02 5.12 5.47
ALC-470-3
1: Scan ES+
TIC
4.33e9
2.61 2.65 2.51 3.13 2.34 2.09 0.10 1.15 4.14 4.37 4.40 4.84 4.94 5.41
ALC-470-3
2: Scan ES-
231
6.90e7
2.66 2.62 2.71 2.78 2.90
ALC-470-3
1: Scan ES+
233
8.56e8
2.68 2.72 2.77 2.96
%
Time

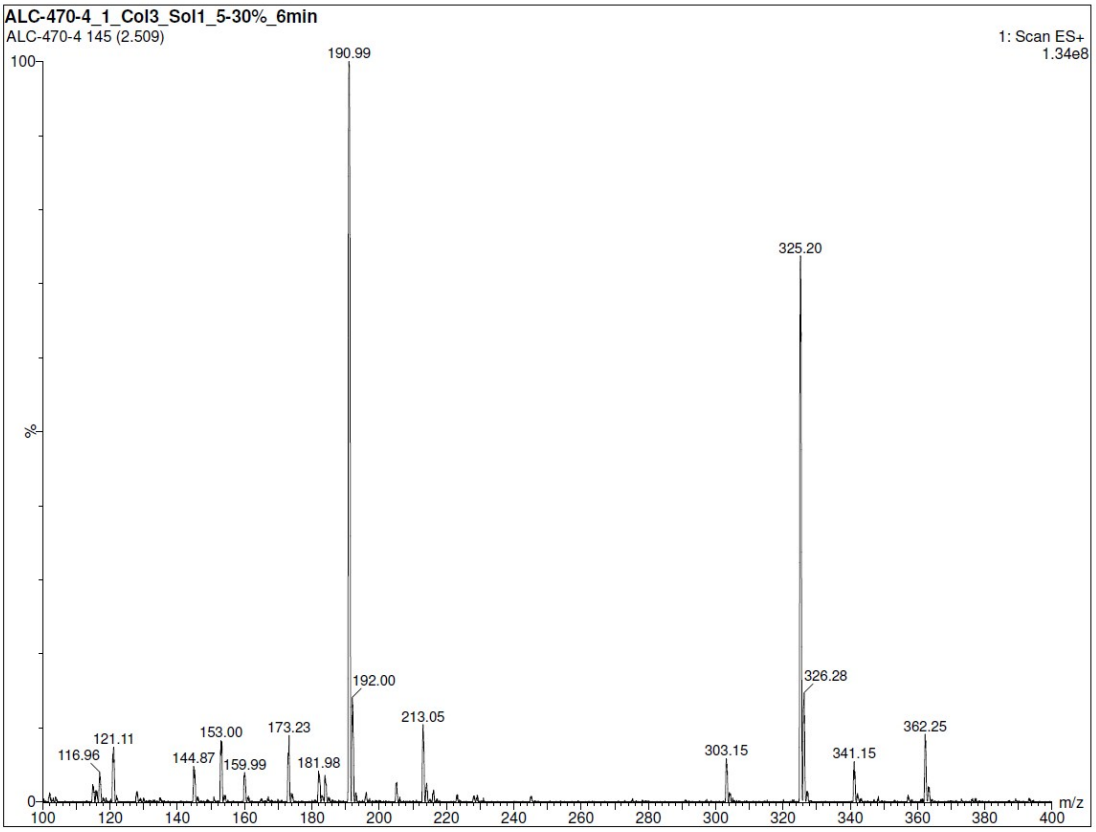

ALC-470-3_1_Col3_Sol1_5-30%_6min
ALC-470-3 155 (2.683)
1: Scan ES+
1.34e8
255.08
233.21
117.02
256.15
159.17
234.16
187.15
287.08
130.88
182.30
271.27
%
m/z

2-phenyl-1-(1-(2,4,4-trimethylpentan-2-yl)-1*H*-tetrazol-5-yl)ethanol (3d)

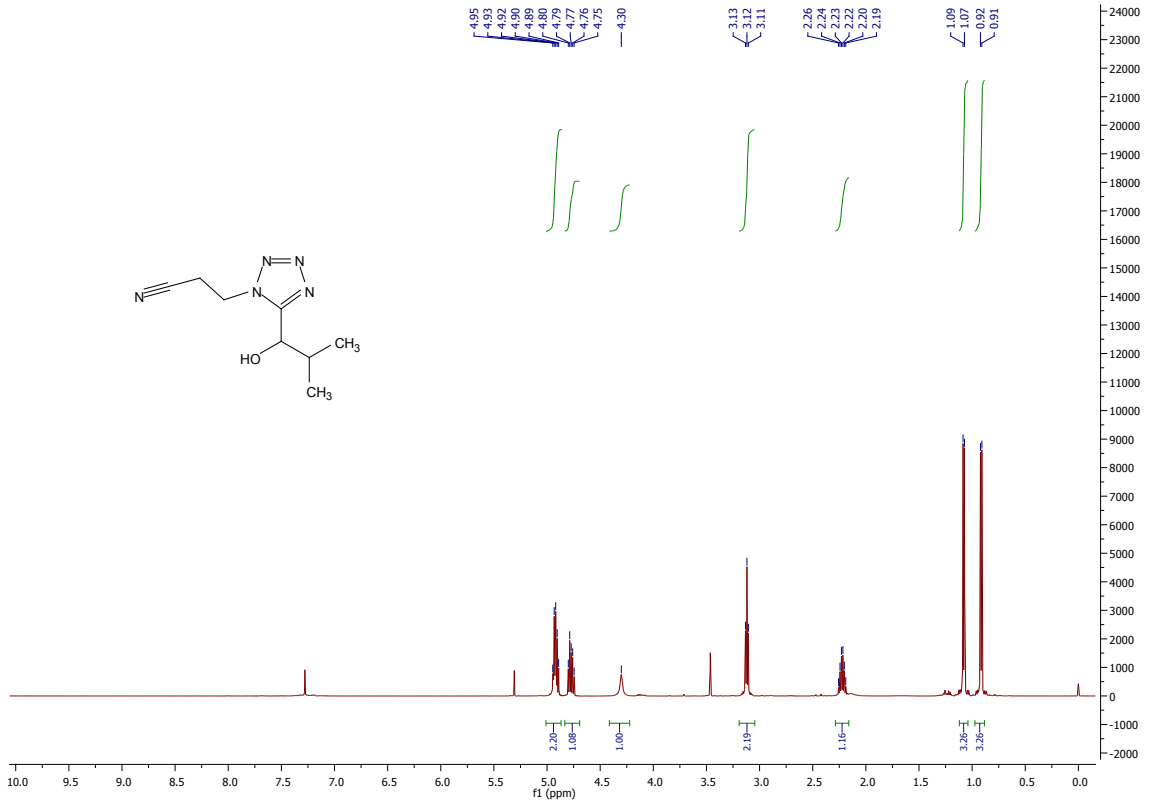


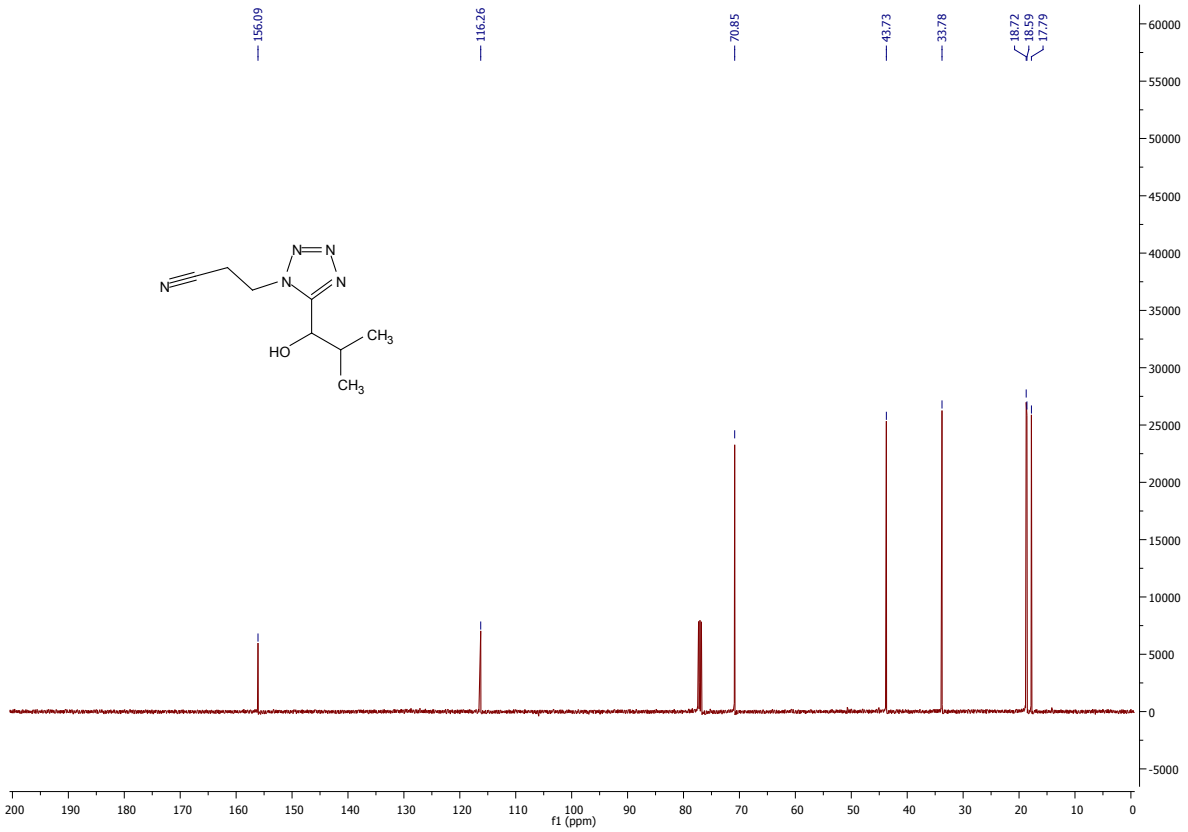


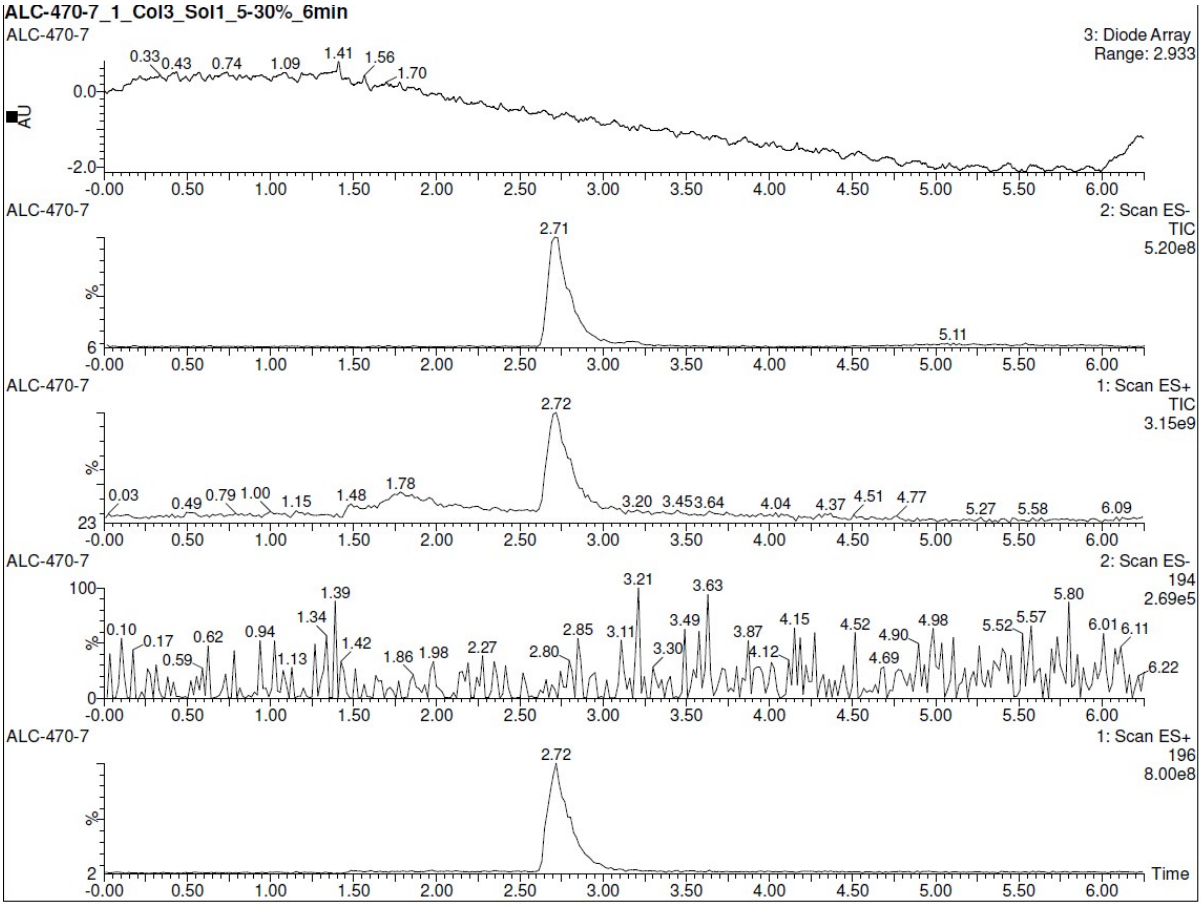

ALC-470-4_1_Col3_Sol1_5-30%_6min
ALC-470-4
3: Diode Array
Range: 2.896
AU
ALC-470-4
2: Scan ES-
TIC
1.96e8
ALC-470-4
1: Scan ES+
TIC
3.76e9
ALC-470-4
2: Scan ES-
301
4.30e6
ALC-470-4
1: Scan ES+
303
6.74e7
Time

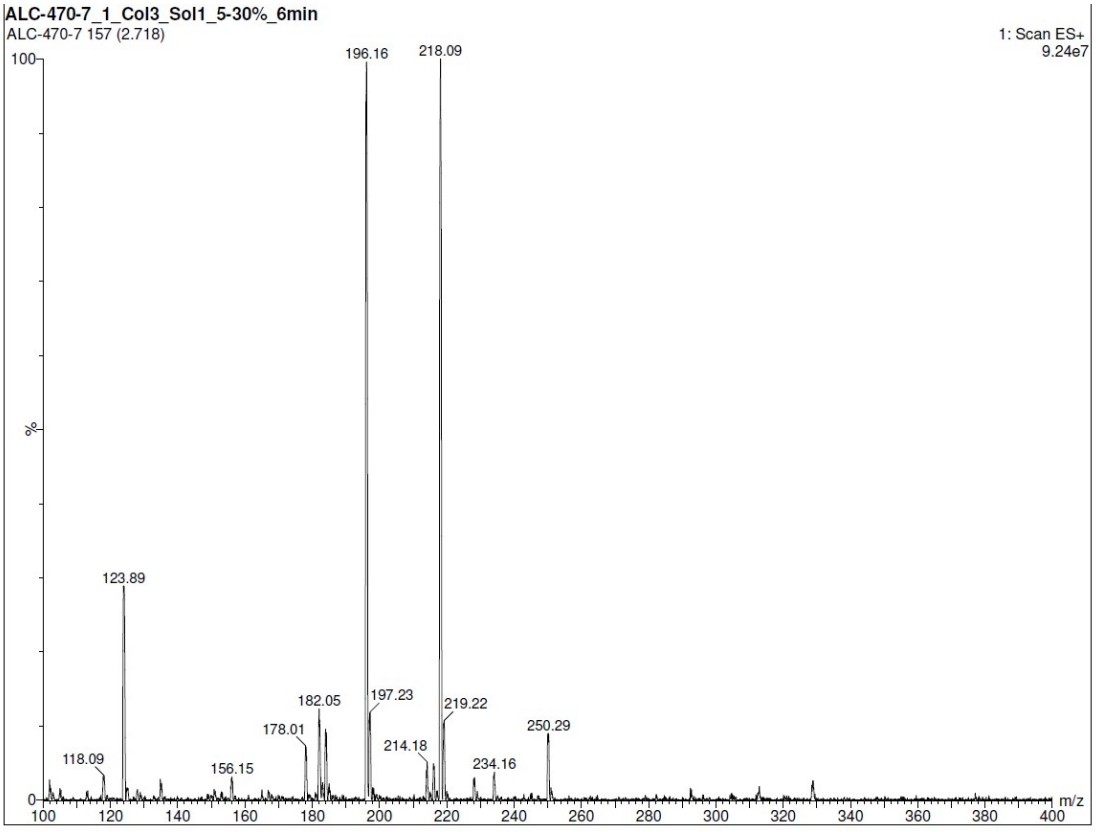

ALC-470-4_1_Col3_Sol1_5-30%_6min
ALC-470-4 145 (2.509)
1: Scan ES+
1.34e8
m/z

3-(5-(1-hydroxy-2-methylpropyl)-1*H*-tetrazol-1-yl)propanenitrile (3e)

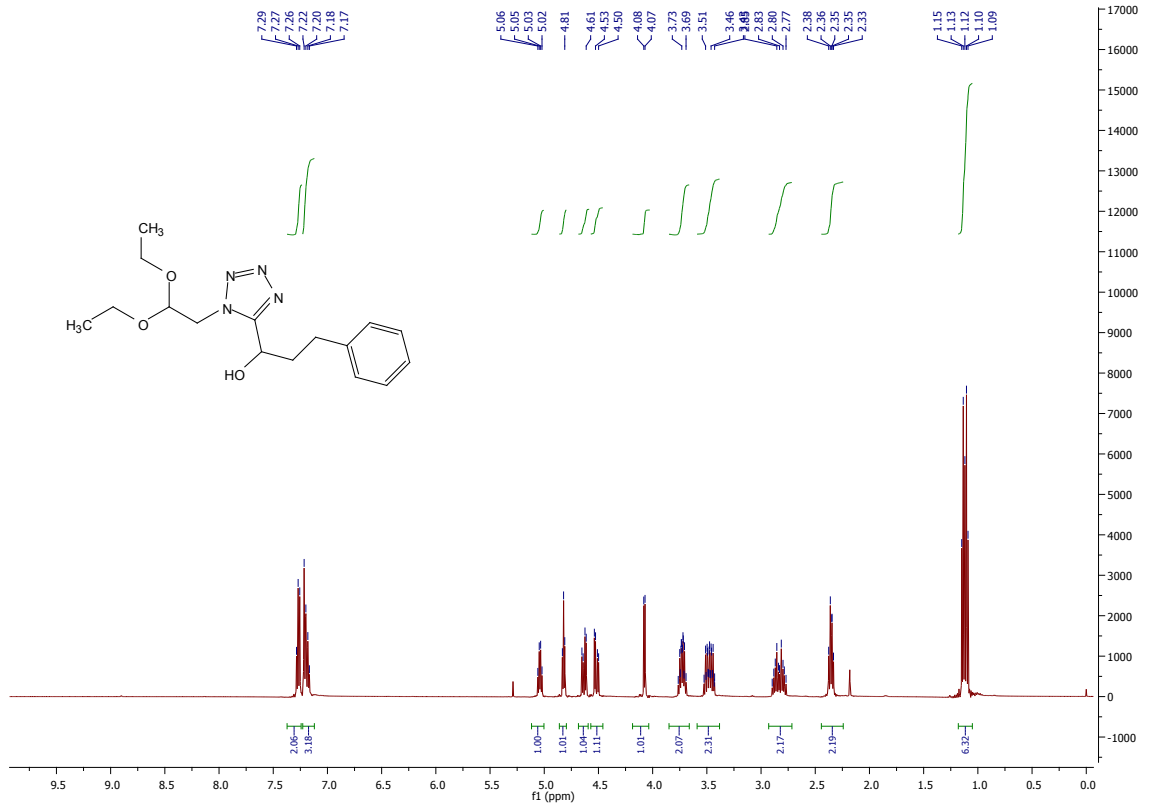


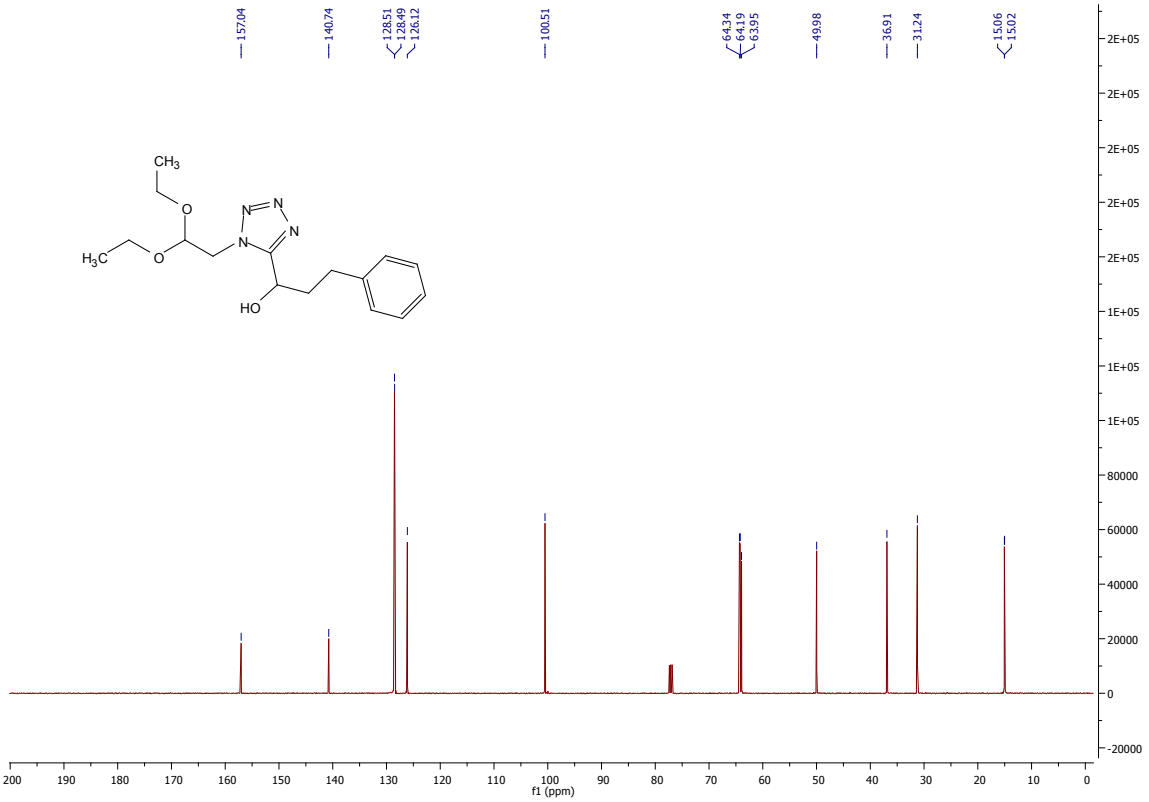


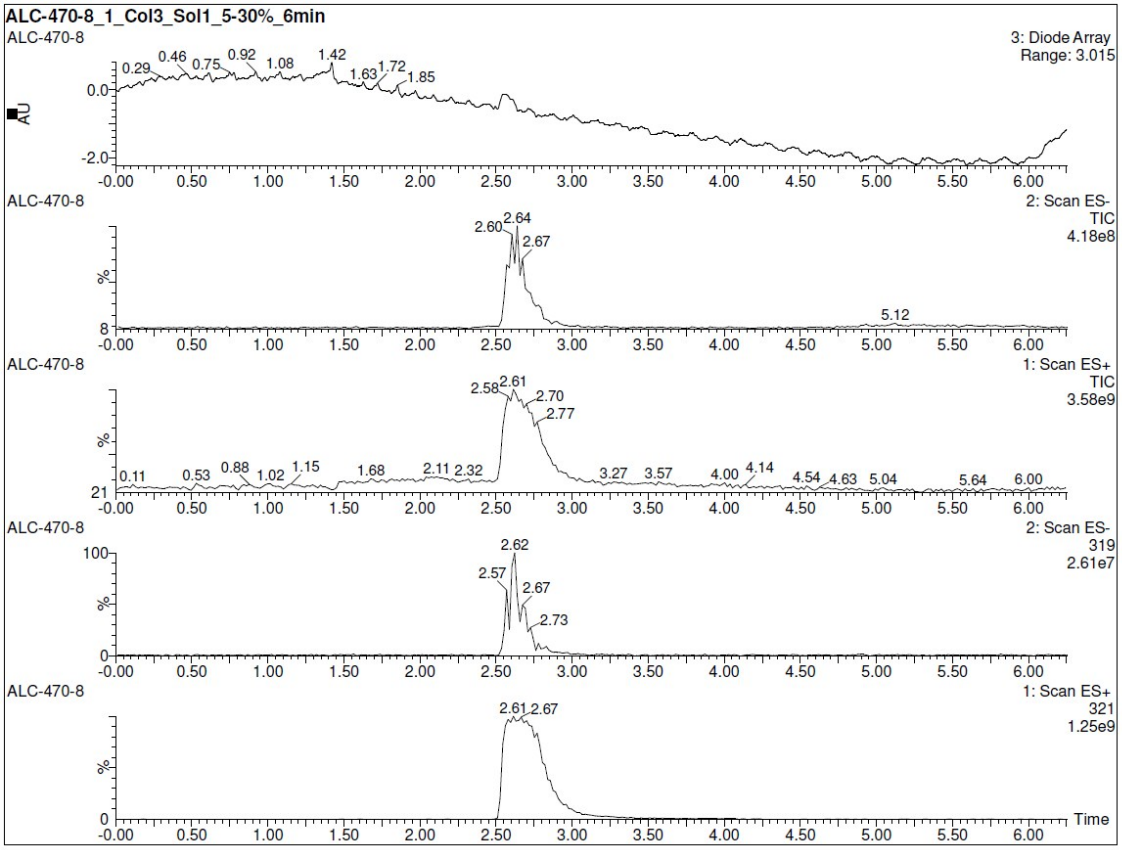

ALC-470-7_1_Col3_Sol1_5-30%_6min
ALC-470-7
3: Diode Array
Range: 2.933
AU
ALC-470-7
2: Scan ES-
TIC
5.20e8
ALC-470-7
1: Scan ES+
TIC
3.15e9
ALC-470-7
2: Scan ES-
194
2.69e5
ALC-470-7
1: Scan ES+
196
8.00e8
Time

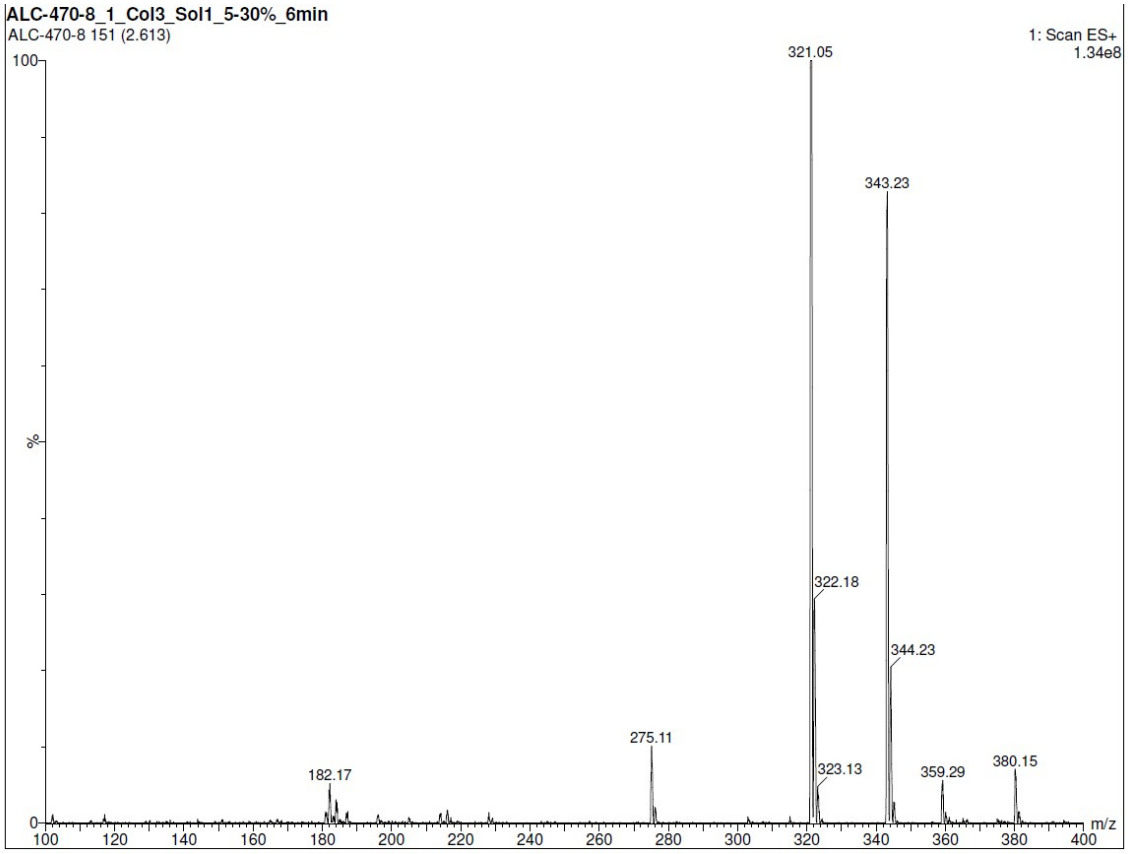

ALC-470-7_1_Col3_Sol1_5-30%_6min
ALC-470-7 157 (2.718)
1: Scan ES+
9.24e7
m/z

1-(1-(2,2-diethoxyethyl)-1*H*-tetrazol-5-yl)-3-phenylpropan-1-ol (3f)

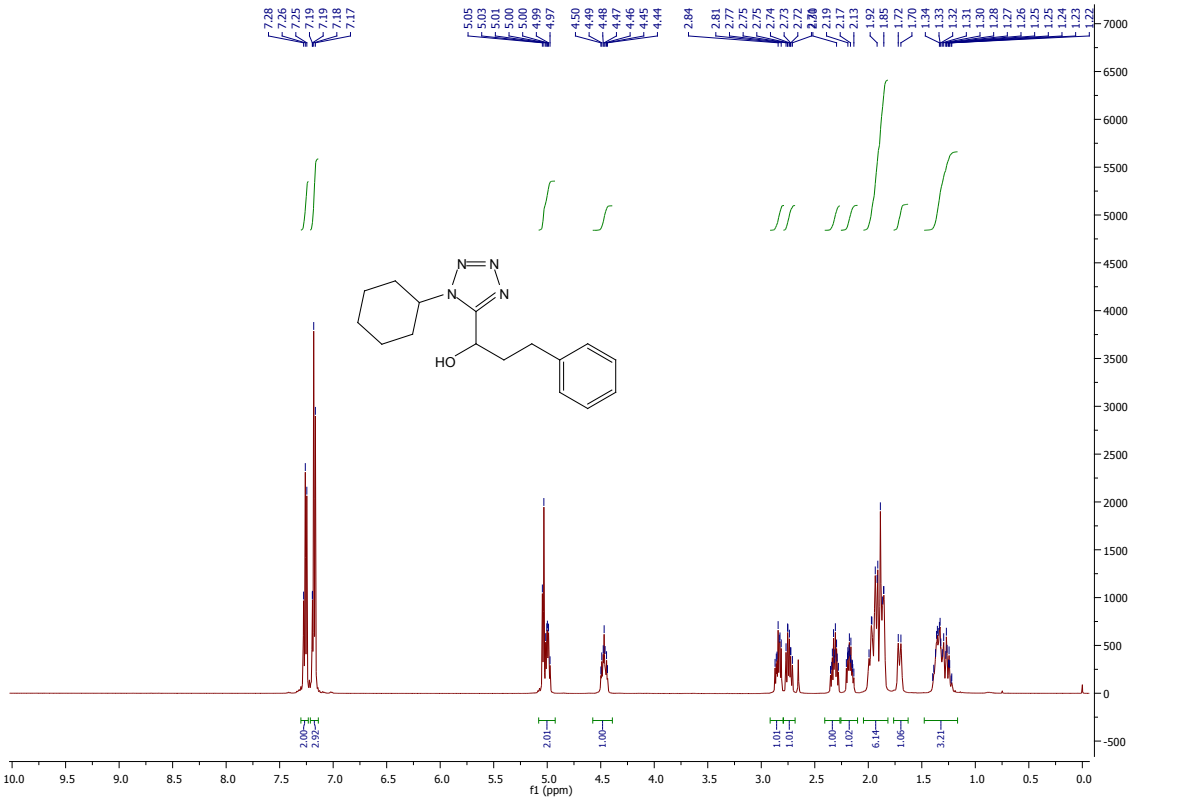


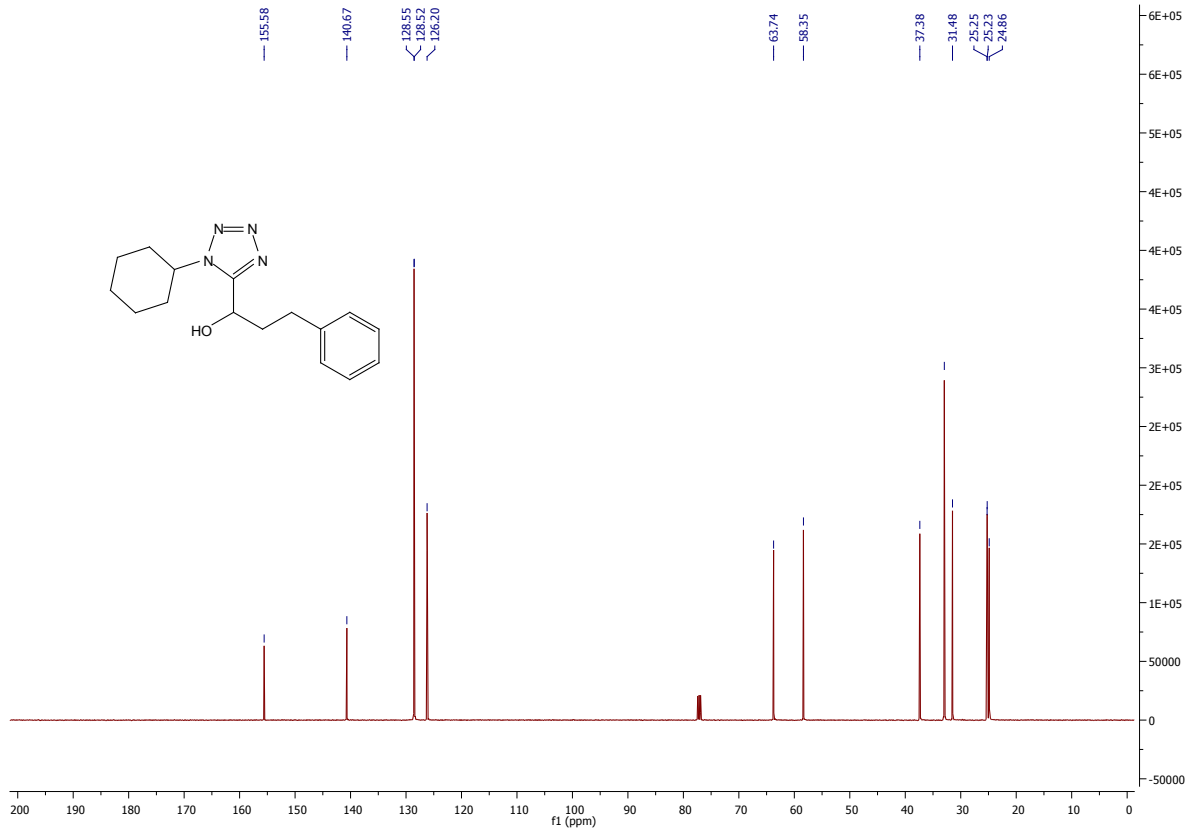


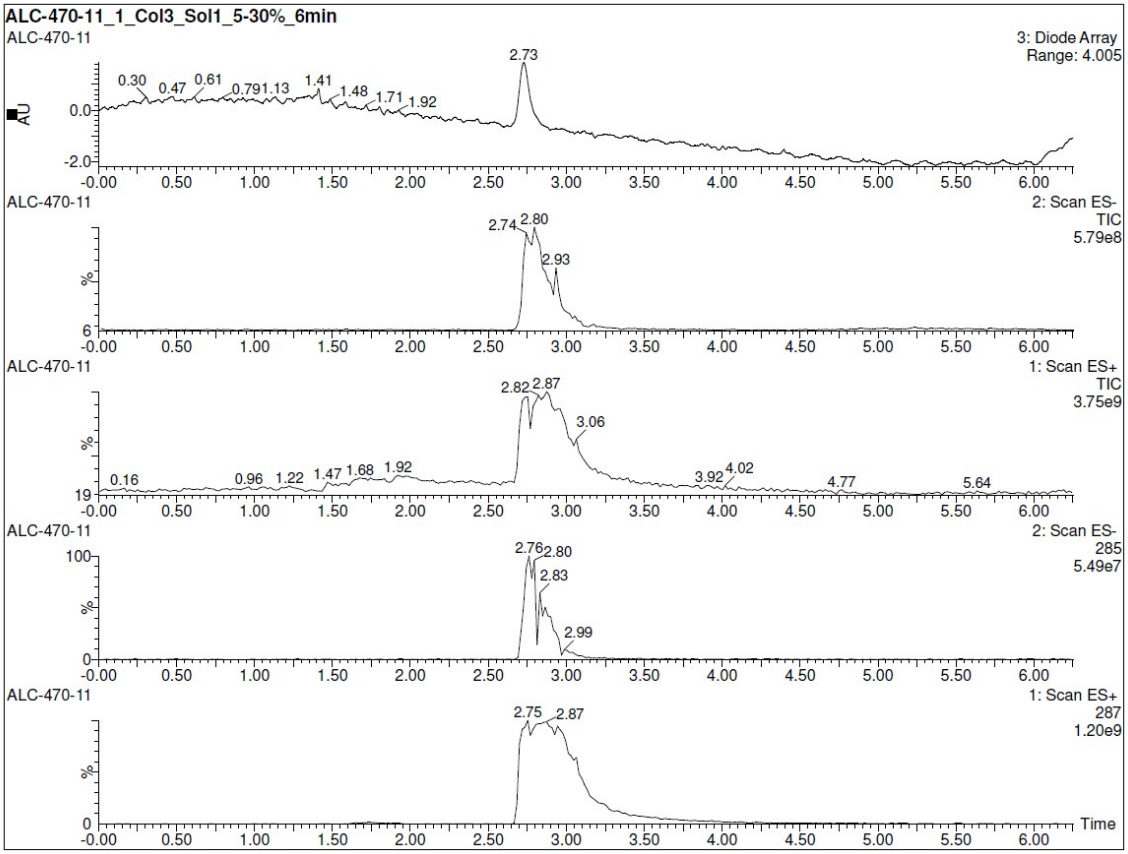

ALC-470-8_1_Col3_Sol1_5-30%_6min
ALC-470-8
3: Diode Array
Range: 3.015
AU
0.29
0.46
0.75
0.92
1.08
1.42
1.63
1.72
1.85
ALC-470-8
2: Scan ES-
TIC
4.18e8
2.60
2.64
2.67
5.12
ALC-470-8
1: Scan ES+
TIC
3.58e9
2.58
2.61
2.70
2.77
0.11
0.53
0.88
1.02
1.15
1.68
2.11
2.32
3.27
3.57
4.00
4.14
4.54
4.63
5.04
5.64
6.00
ALC-470-8
2: Scan ES-
319
2.61e7
2.57
2.62
2.67
2.73
ALC-470-8
1: Scan ES+
321
1.25e9
2.61
2.67
Time

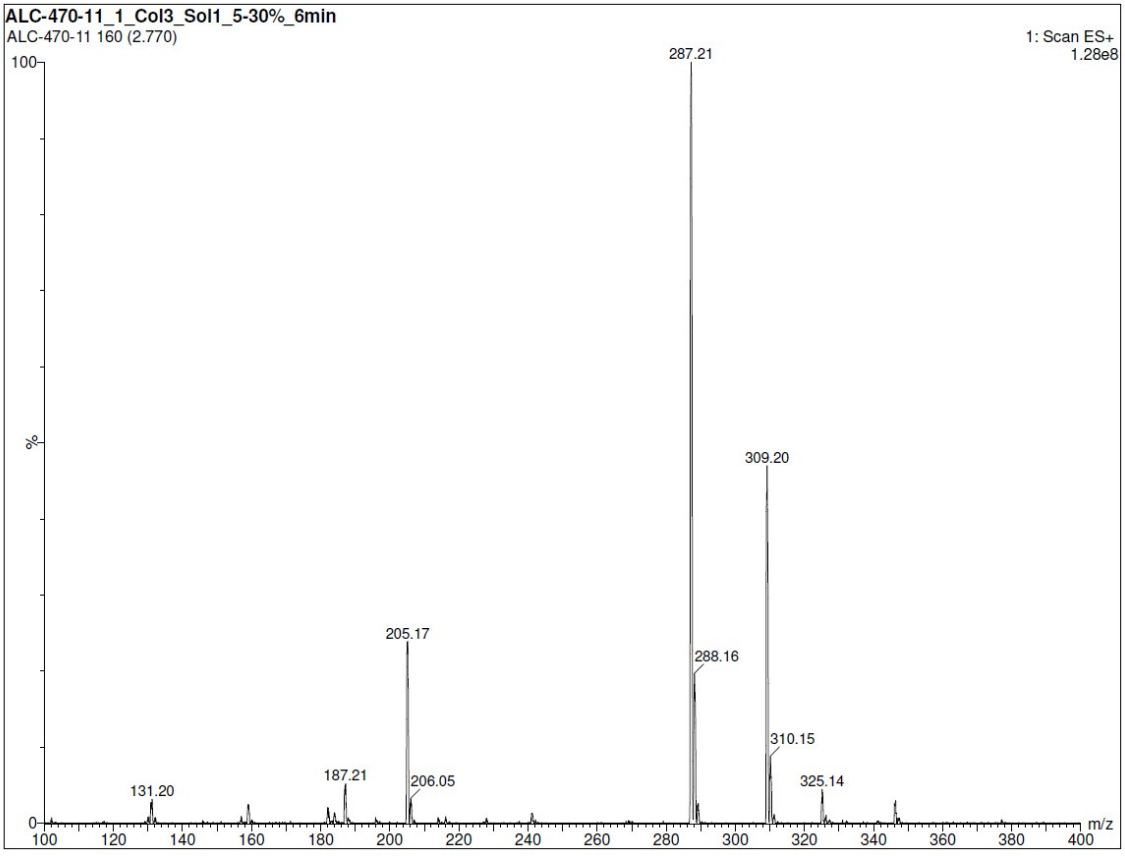

ALC-470-8_1_Col3_Sol1_5-30%_6min
ALC-470-8 151 (2.613)
1: Scan ES+
1.34e8
321.05
343.23
322.18
344.23
275.11
182.17
323.13
359.29
380.15
%
m/z

1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-3-phenylpropan-1-ol (3g)

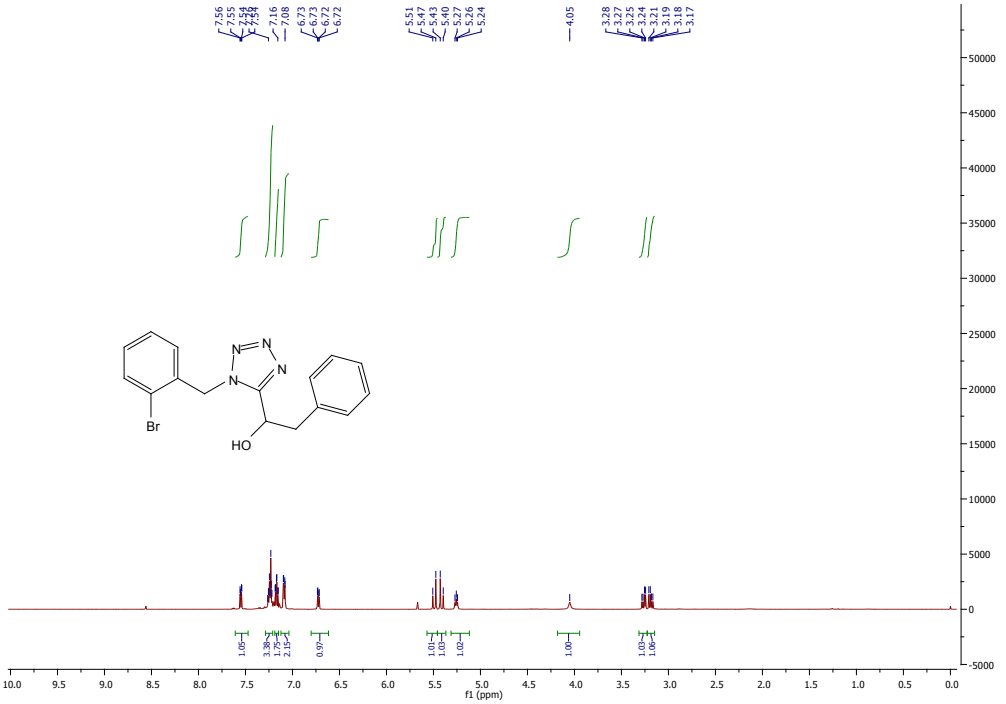


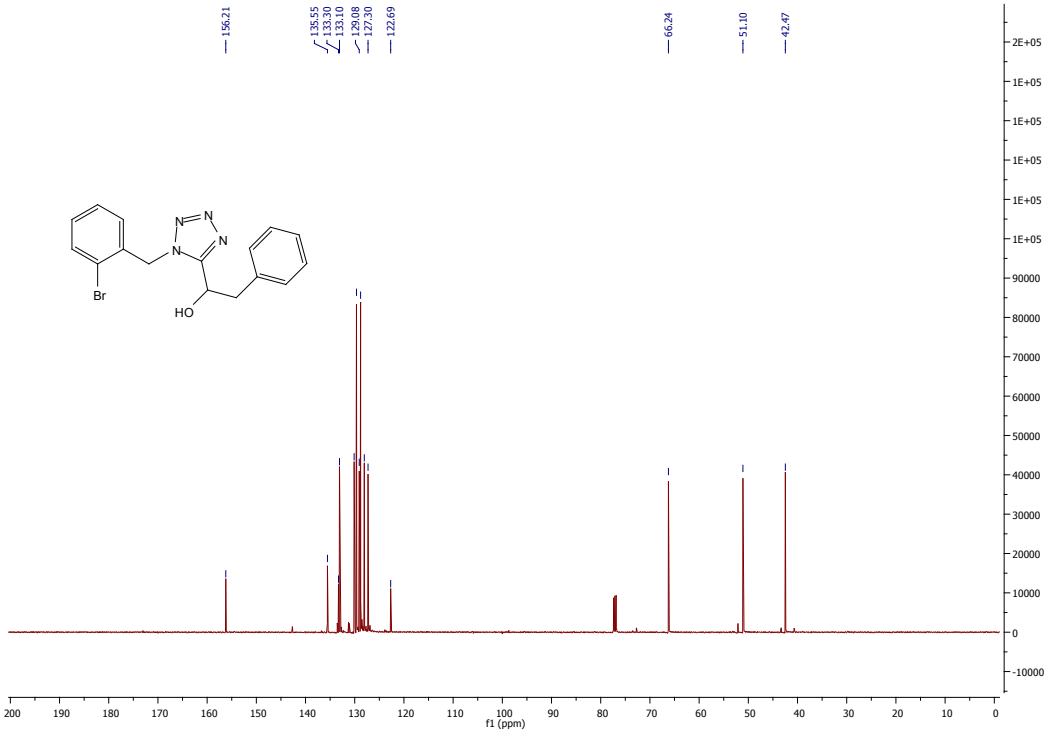


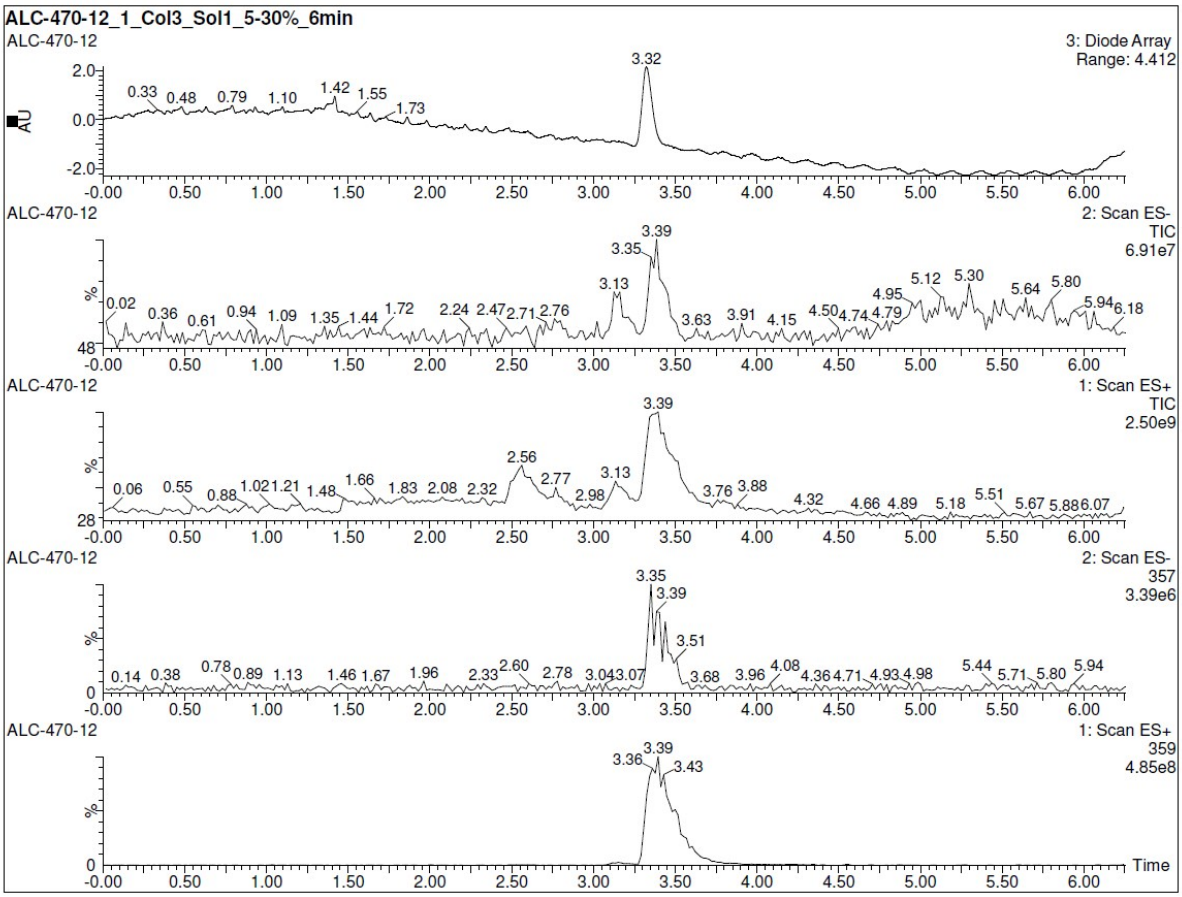

ALC-470-11_1_Col3_Sol1_5-30%_6min
ALC-470-11
3: Diode Array
Range: 4.005
AU
2.73
0.30 0.47 0.61 0.79 1.13 1.41 1.48 1.71 1.92
ALC-470-11
2: Scan ES-
TIC
5.79e8
2.74 2.80 2.93
ALC-470-11
1: Scan ES+
TIC
3.75e9
2.82 2.87 3.06
0.16 0.96 1.22 1.47 1.68 1.92 3.92 4.02 4.77 5.64
ALC-470-11
2: Scan ES-
285
5.49e7
2.76 2.80 2.83 2.99
ALC-470-11
1: Scan ES+
287
1.20e9
2.75 2.87
%
Time

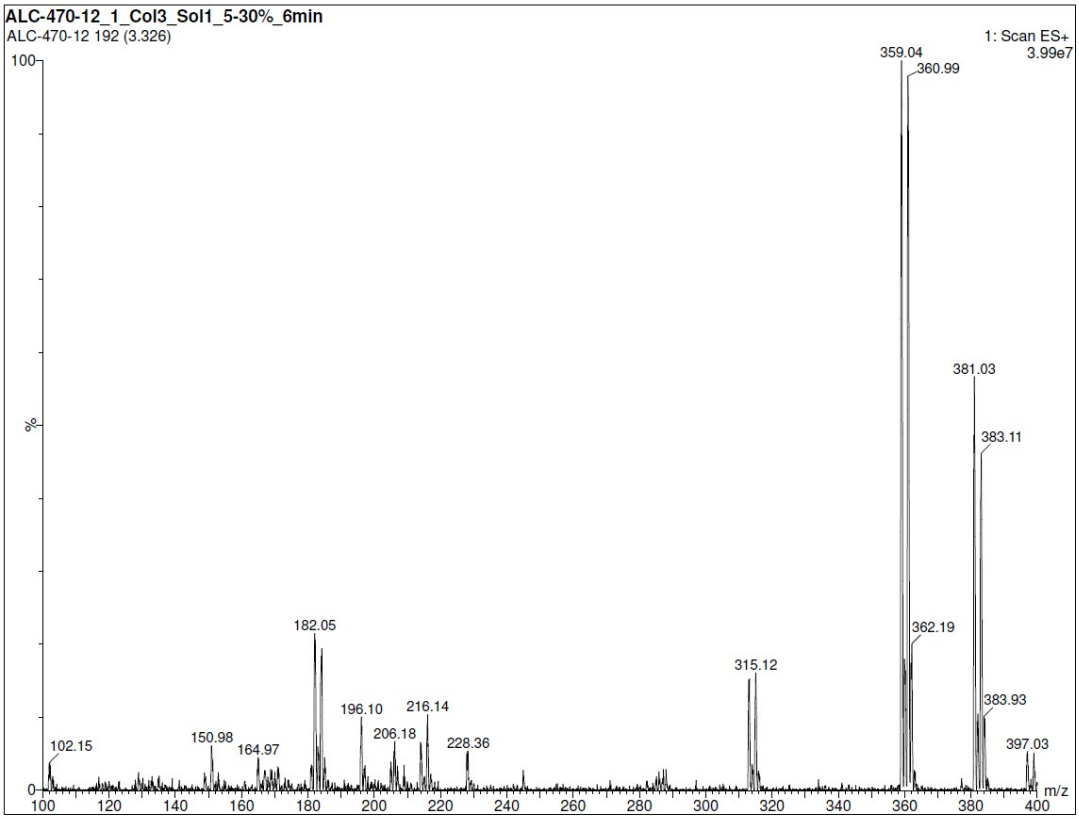

ALC-470-11_1_Col3_Sol1_5-30%_6min
ALC-470-11 160 (2.770)
1: Scan ES+
1.28e8
287.21
309.20
205.17
288.16
310.15
187.21
206.05
131.20
325.14
%
m/z

1-(1-(2-bromobenzyl)-1*H*-tetrazol-5-yl)-2-phenylethanol (3h)

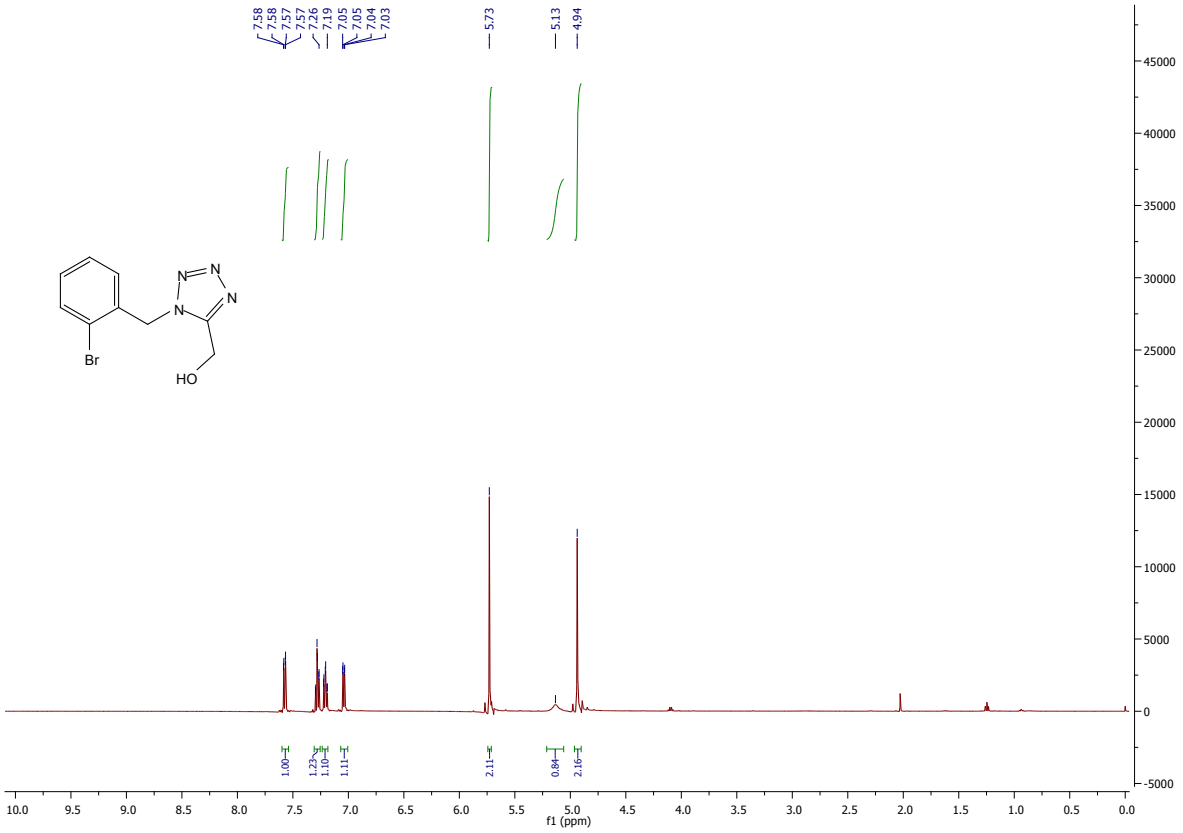


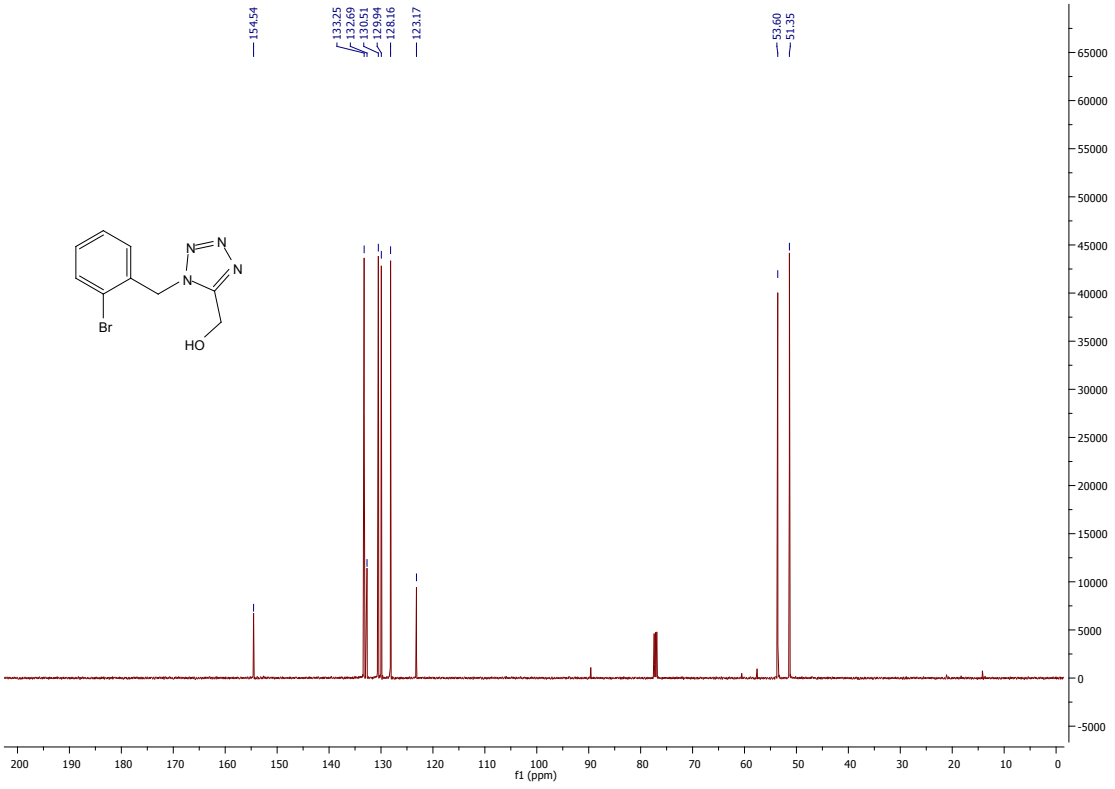


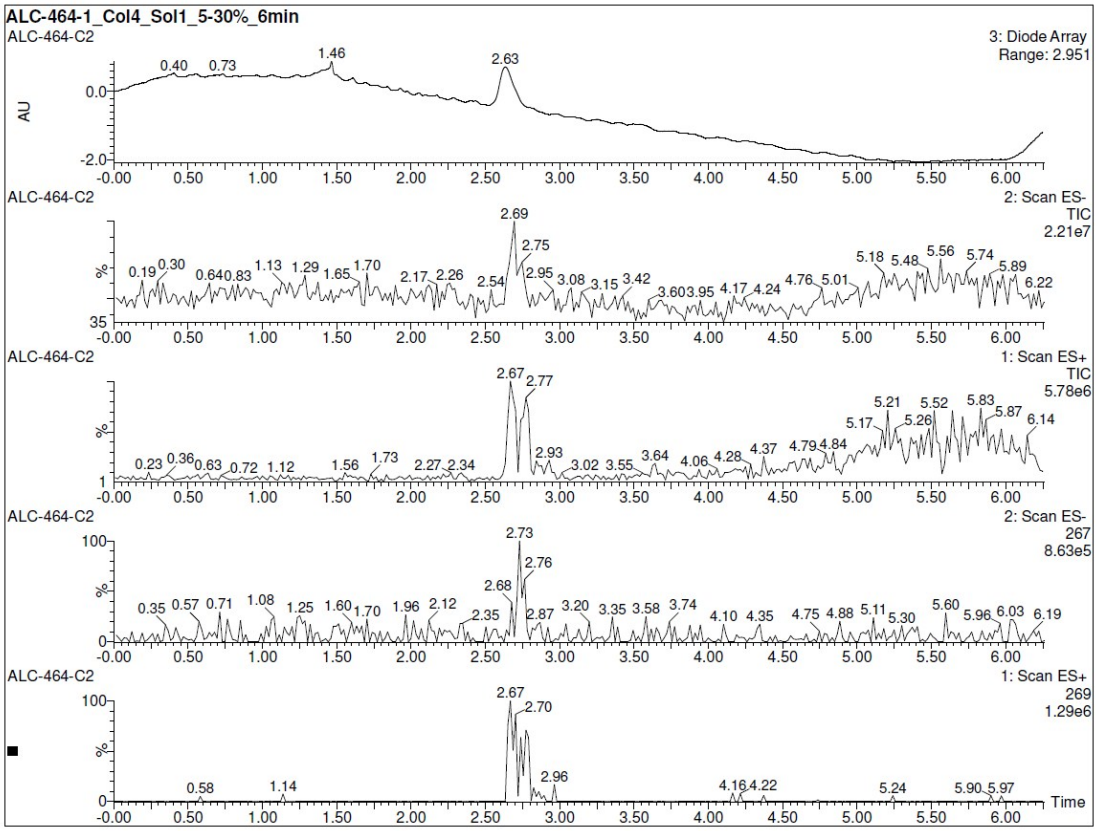

ALC-470-12_1_Col3_Sol1_5-30%_6min
ALC-470-12
3: Diode Array
Range: 4.412
AU
2: Scan ES-
TIC
6.91e7
1: Scan ES+
TIC
2.50e9
2: Scan ES-
357
3.39e6
1: Scan ES+
359
4.85e8
Time

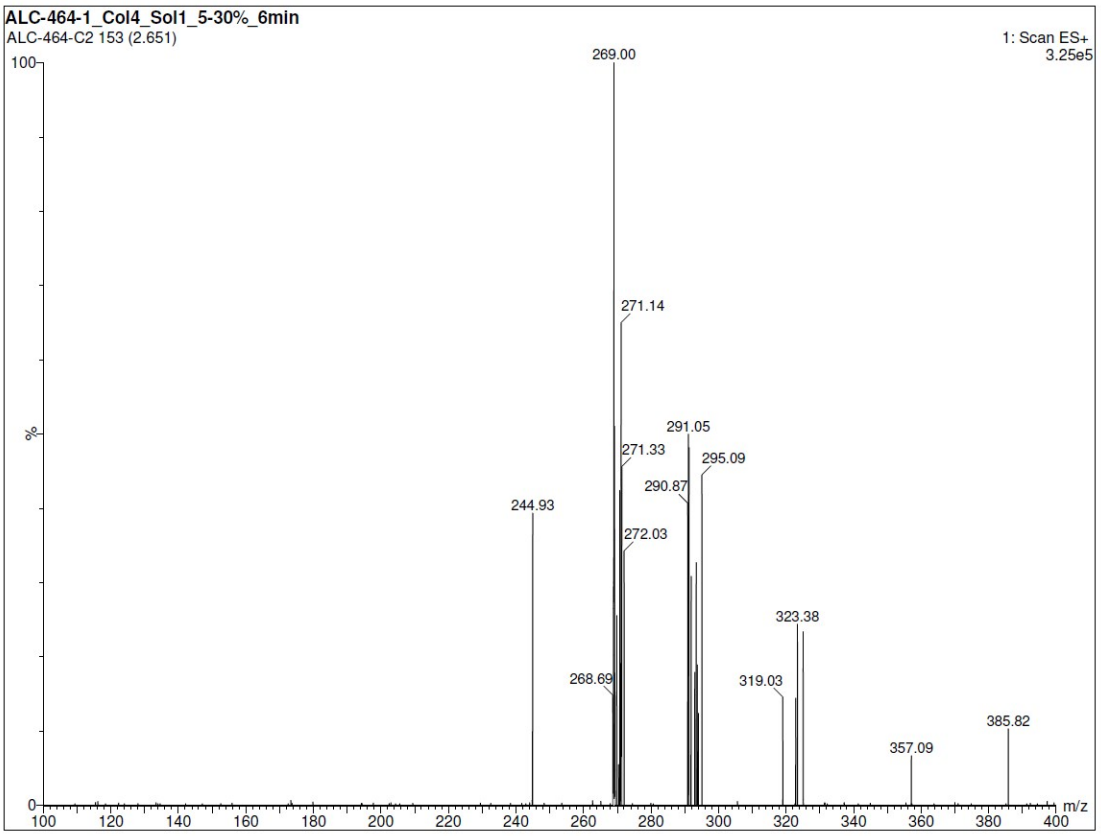

ALC-470-12_1_Col3_Sol1_5-30%_6min
ALC-470-12 192 (3.326)
1: Scan ES+
3.99e7
m/z

(1-(2-bromobenzyl)-1*H*-tetrazol-5-yl)methanol (3i)

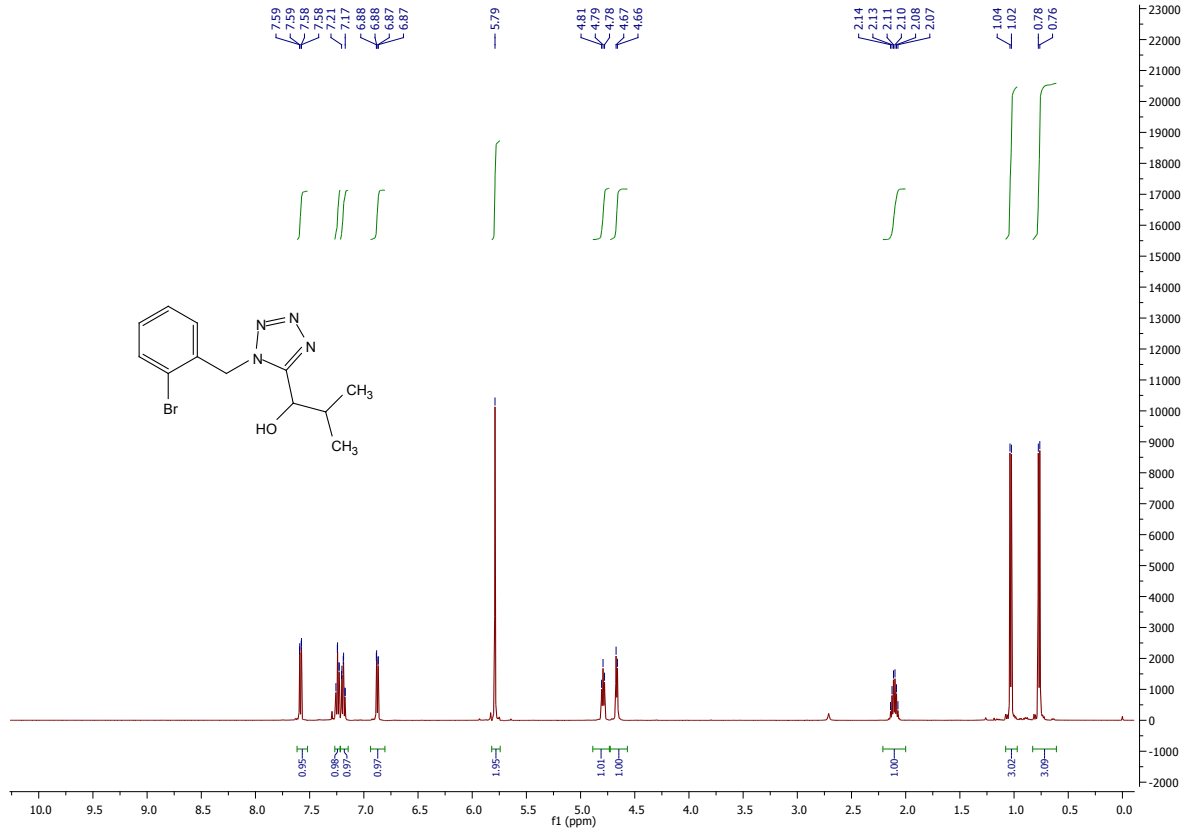


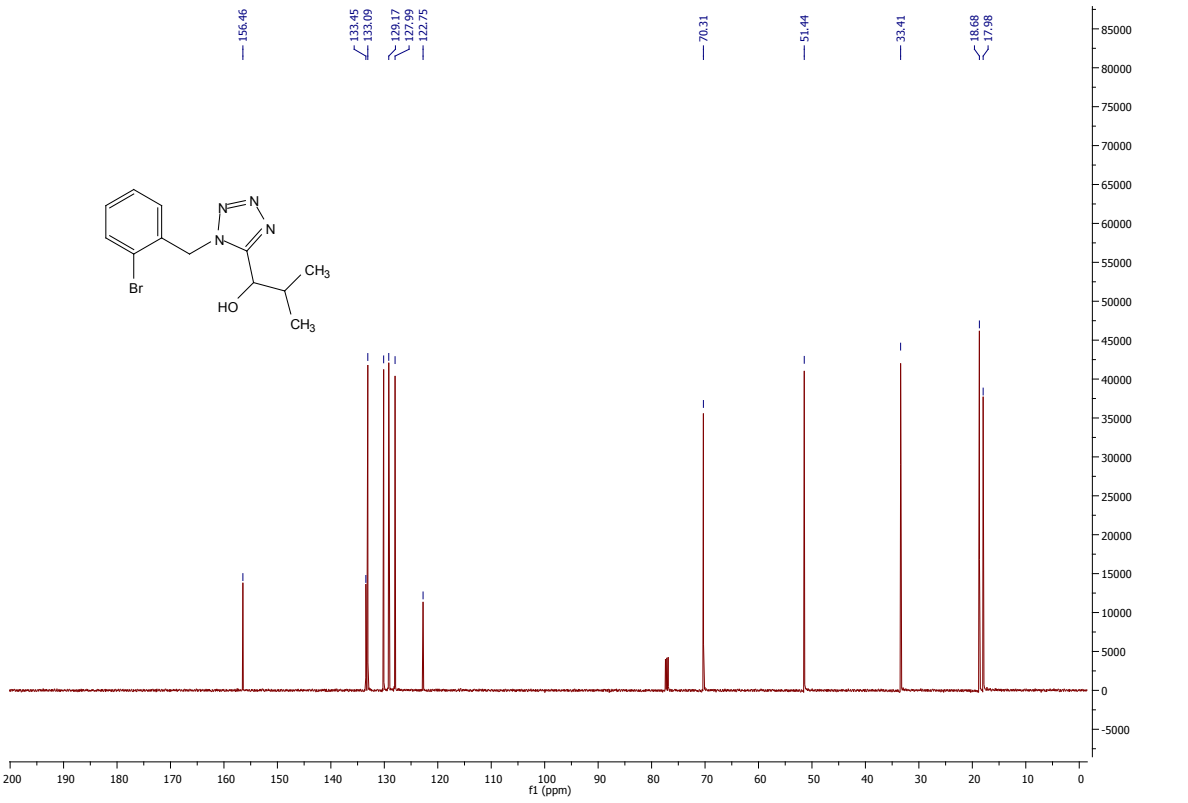


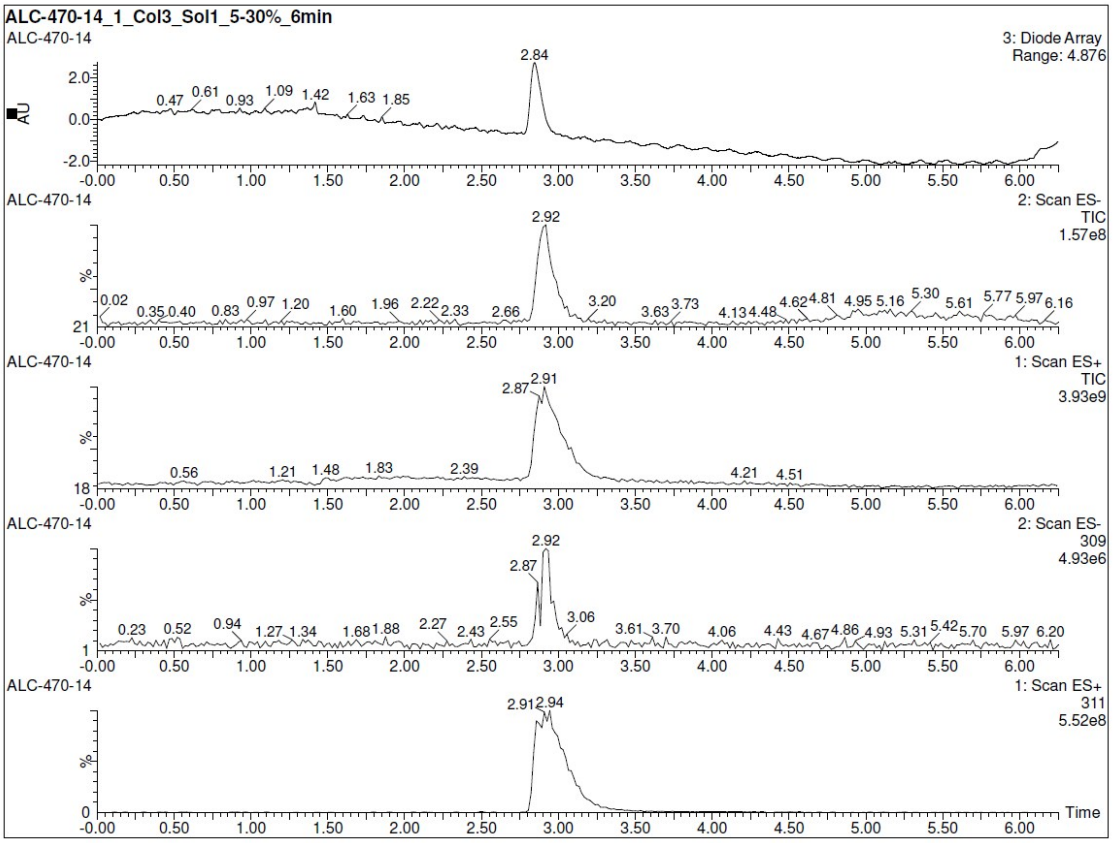

ALC-464-1_Col4_Sol1_5-30%_6min
ALC-464-C2
3: Diode Array
Range: 2.951
AU
ALC-464-C2
2: Scan ES-
TIC
2.21e7
ALC-464-C2
1: Scan ES+
TIC
5.78e6
ALC-464-C2
2: Scan ES-
267
8.63e5
ALC-464-C2
1: Scan ES+
269
1.29e6
Time

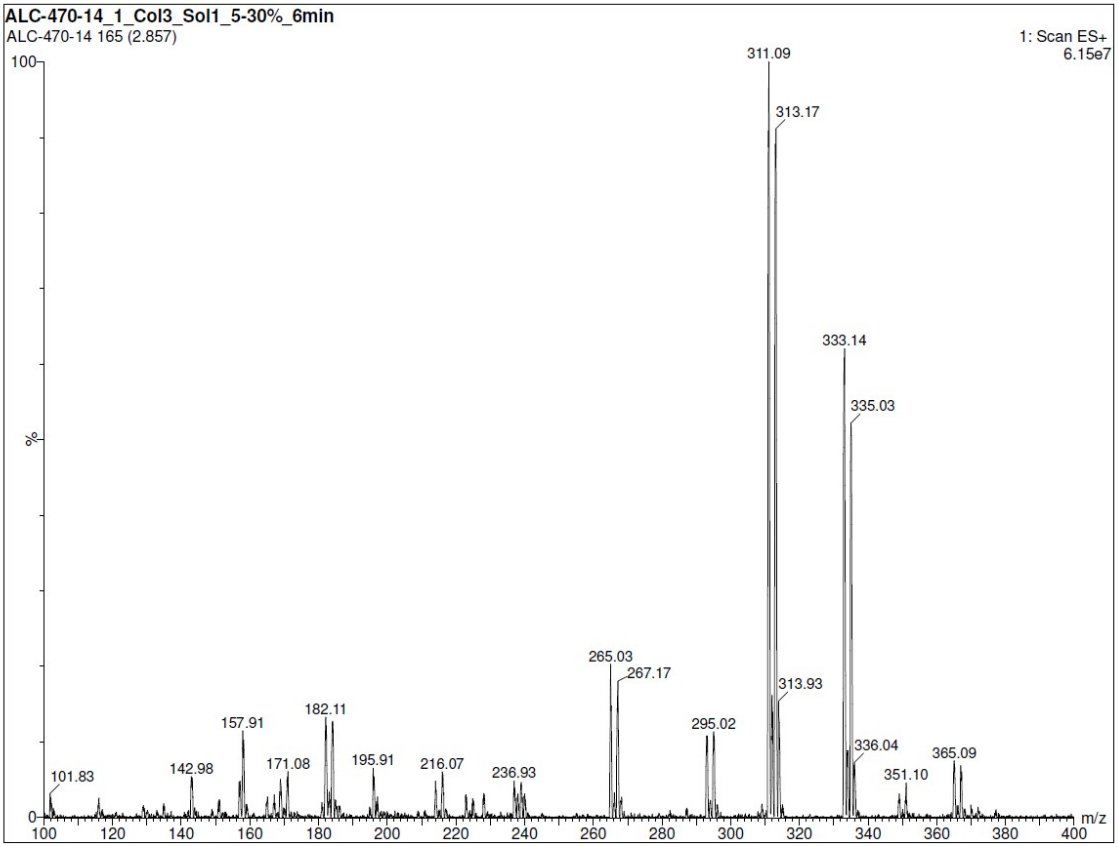

ALC-464-1_Col4_Sol1_5-30%_6min
ALC-464-C2 153 (2.651)
1: Scan ES+
3.25e5
269.00
271.14
291.05
271.33
295.09
290.87
244.93
272.03
323.38
268.69
319.03
385.82
357.09
m/z

1-(1-(2-bromobenzyl)-1*H*-tetrazol-5-yl)-2-methylpropan-1-ol (3j)

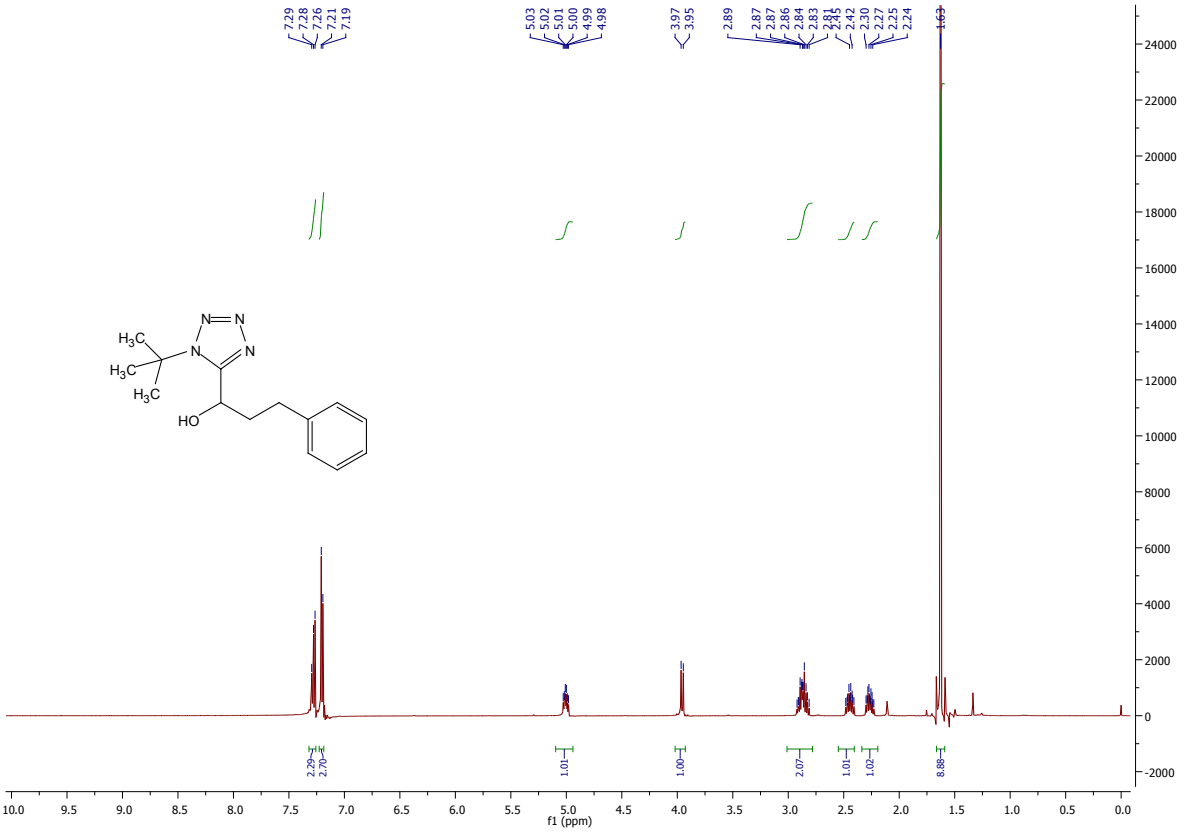


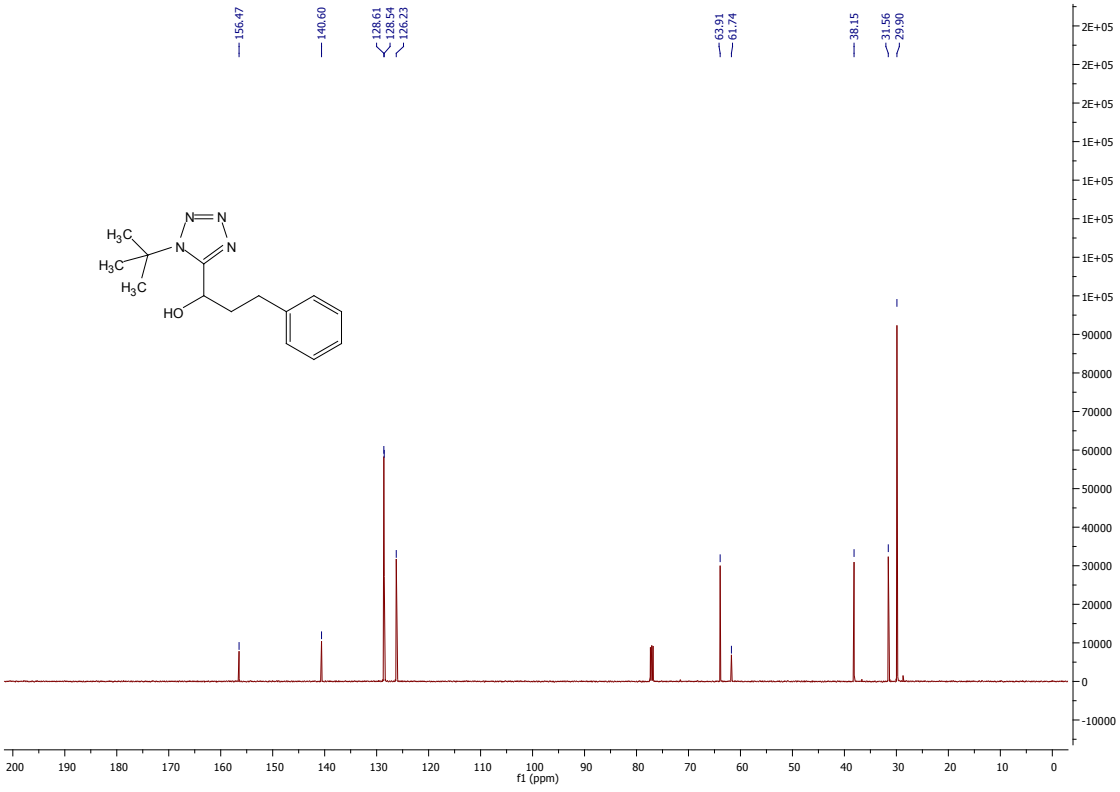


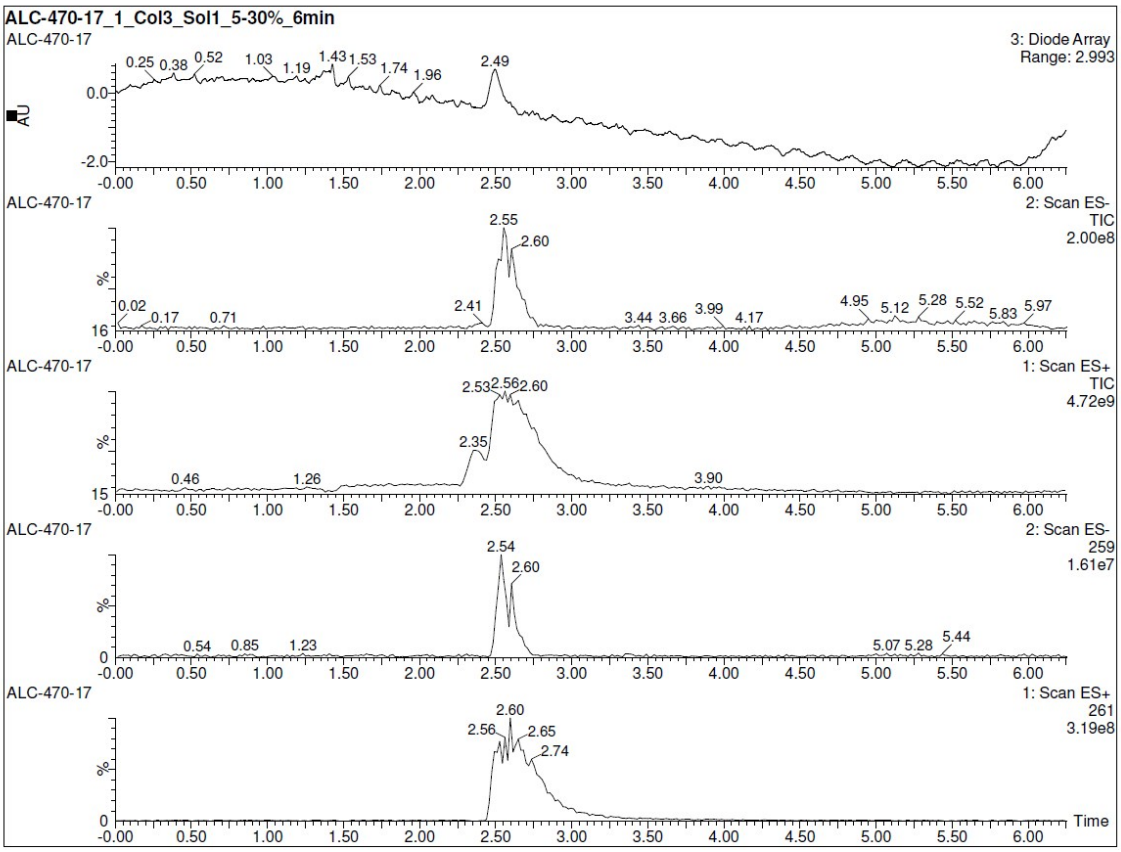

ALC-470-14_1_Col3_Sol1_5-30%_6min
ALC-470-14
3: Diode Array
Range: 4.876
2.84
0.47 0.61 0.93 1.09 1.42 1.63 1.85
AU
2.0
0.0
-2.0
ALC-470-14
2: Scan ES-
TIC
1.57e8
2.92
0.02 0.35 0.40 0.83 0.97 1.20 1.60 1.96 2.22 2.33 2.66 3.20 3.63 3.73 4.13 4.48 4.62 4.81 4.95 5.16 5.30 5.61 5.77 5.97 6.16
%
21
ALC-470-14
1: Scan ES+
TIC
3.93e9
2.87 2.91
0.56 1.21 1.48 1.83 2.39 4.21 4.51
%
18
ALC-470-14
2: Scan ES-
309
4.93e6
2.92
2.87
0.23 0.52 0.94 1.27 1.34 1.68 1.88 2.27 2.43 2.55 3.06 3.61 3.70 4.06 4.43 4.67 4.86 4.93 5.31 5.42 5.70 5.97 6.20
%
1
ALC-470-14
1: Scan ES+
311
5.52e8
2.91 2.94
%
0
Time
-0.00 0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00

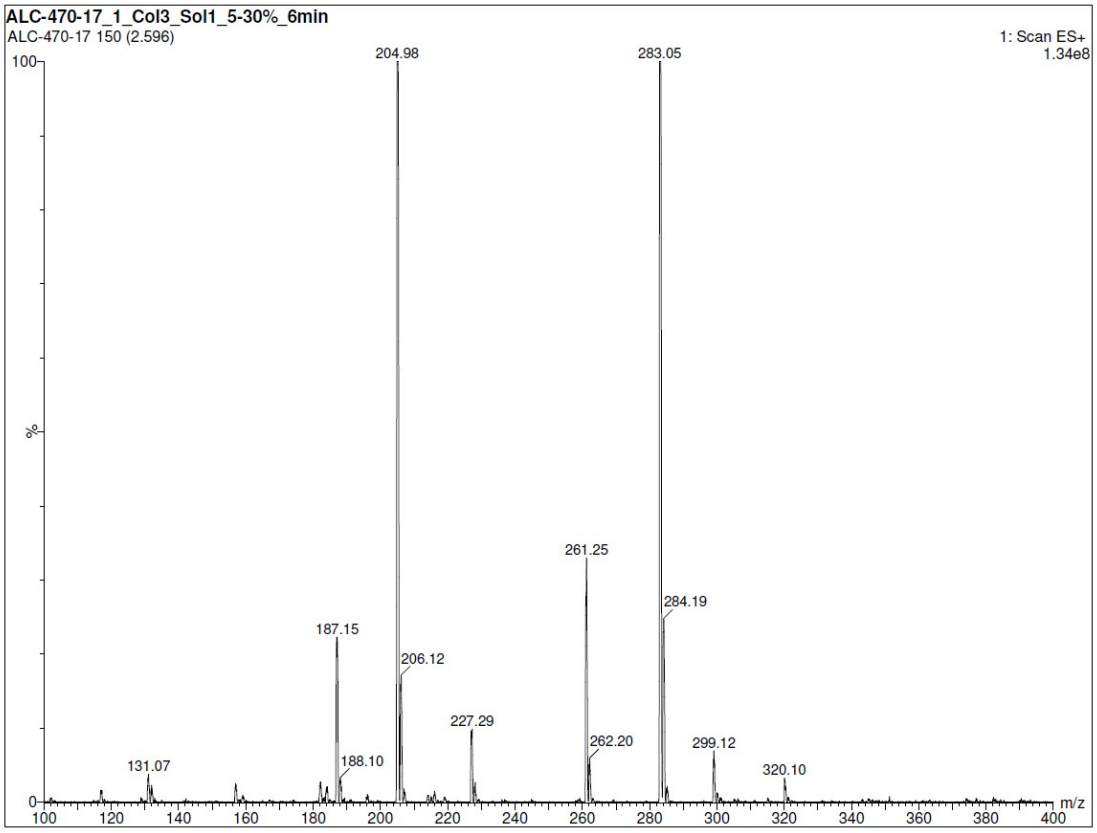

ALC-470-14_1_Col3_Sol1_5-30%_6min
ALC-470-14 165 (2.857)
1: Scan ES+
6.15e7
100
%
0
311.09
313.17
333.14
335.03
265.03
267.17
313.93
295.02
336.04
365.09
351.10
157.91
182.11
171.08
195.91
216.07
236.93
142.98
101.83
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400
m/z

1-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-3-phenylpropan-1-ol (3k)

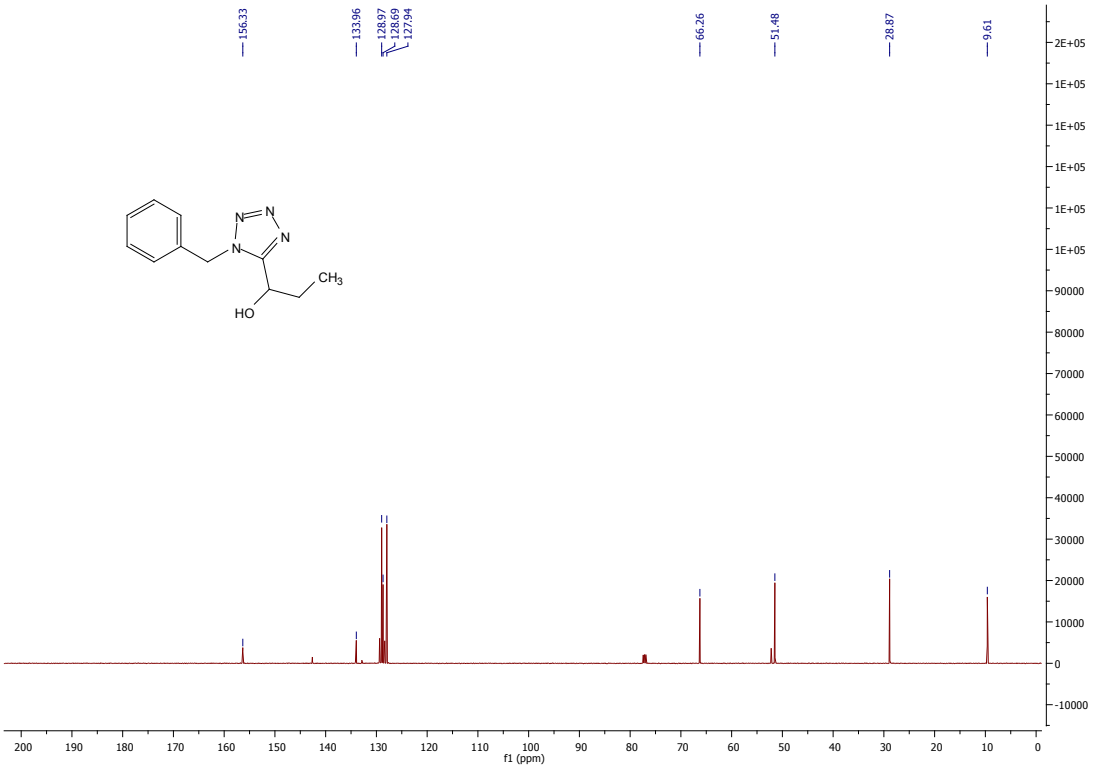


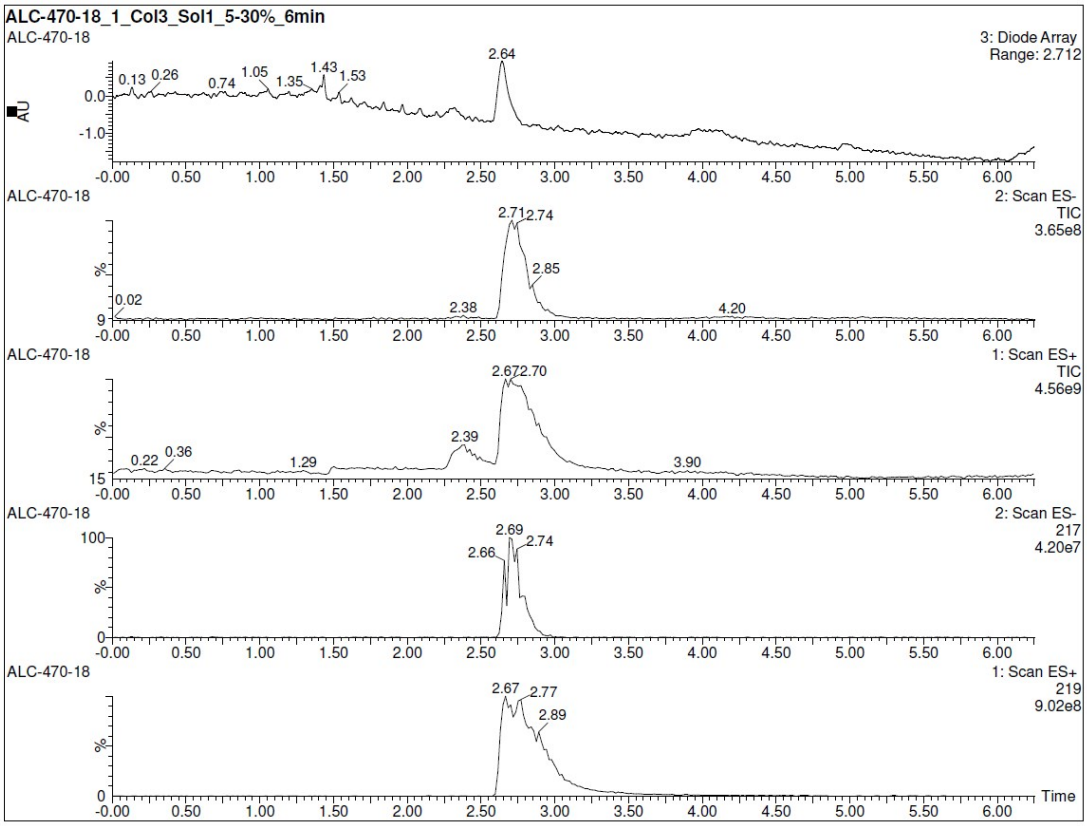


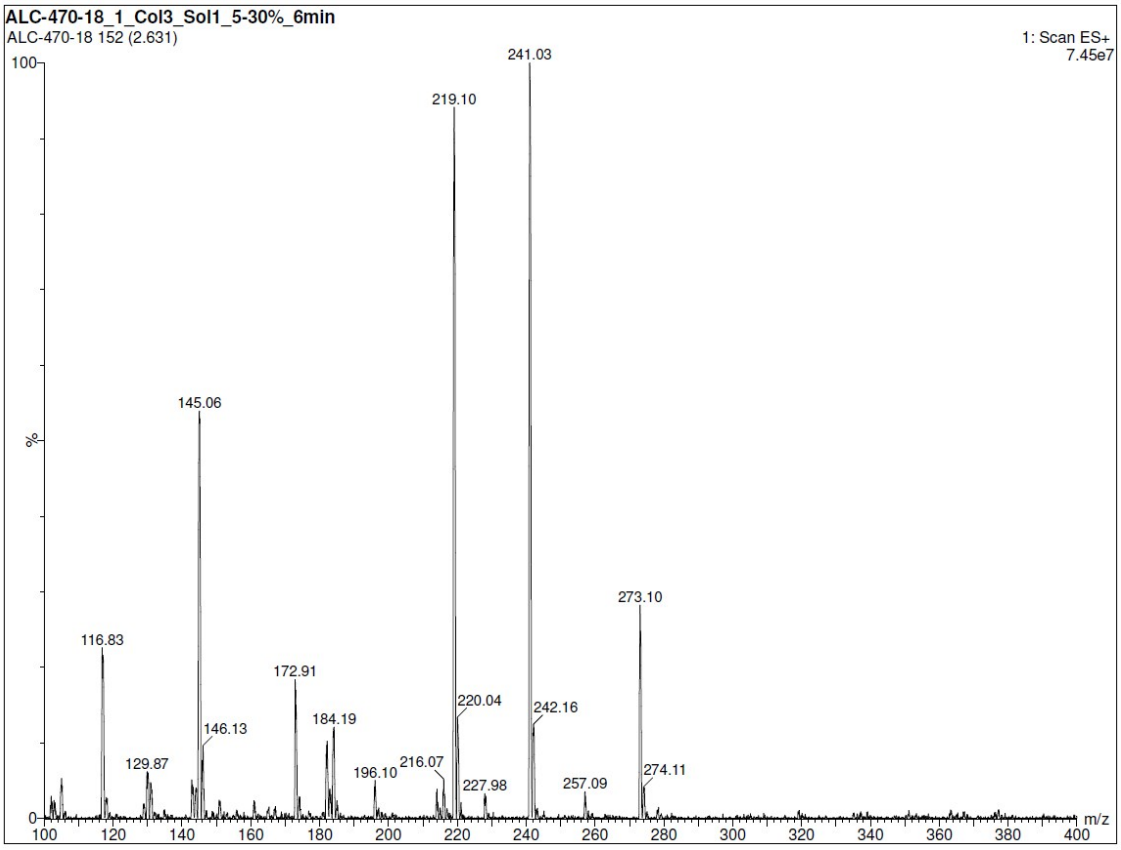

ALC-470-17_1_Col3_Sol1_5-30%_6min
ALC-470-17
3: Diode Array
Range: 2.993
AU
0.25 0.38 0.52 1.03 1.19 1.43 1.53 1.74 1.96 2.49
ALC-470-17
2: Scan ES-
TIC
2.00e8
2.55 2.60
0.02 0.17 0.71 2.41 3.44 3.66 3.99 4.17 4.95 5.12 5.28 5.52 5.83 5.97
ALC-470-17
1: Scan ES+
TIC
4.72e9
2.53 2.56 2.60 2.35
0.46 1.26 3.90
ALC-470-17
2: Scan ES-
259
1.61e7
2.54 2.60
0.54 0.85 1.23 5.07 5.28 5.44
ALC-470-17
1: Scan ES+
261
3.19e8
2.60 2.56 2.65 2.74
Time


ALC-470-17_1_Col3_Sol1_5-30%_6min
ALC-470-17 150 (2.596)
1: Scan ES+
1.34e8
204.98
283.05
261.25
284.19
187.15
206.12
227.29
262.20
299.12
320.10
188.10
131.07
m/z

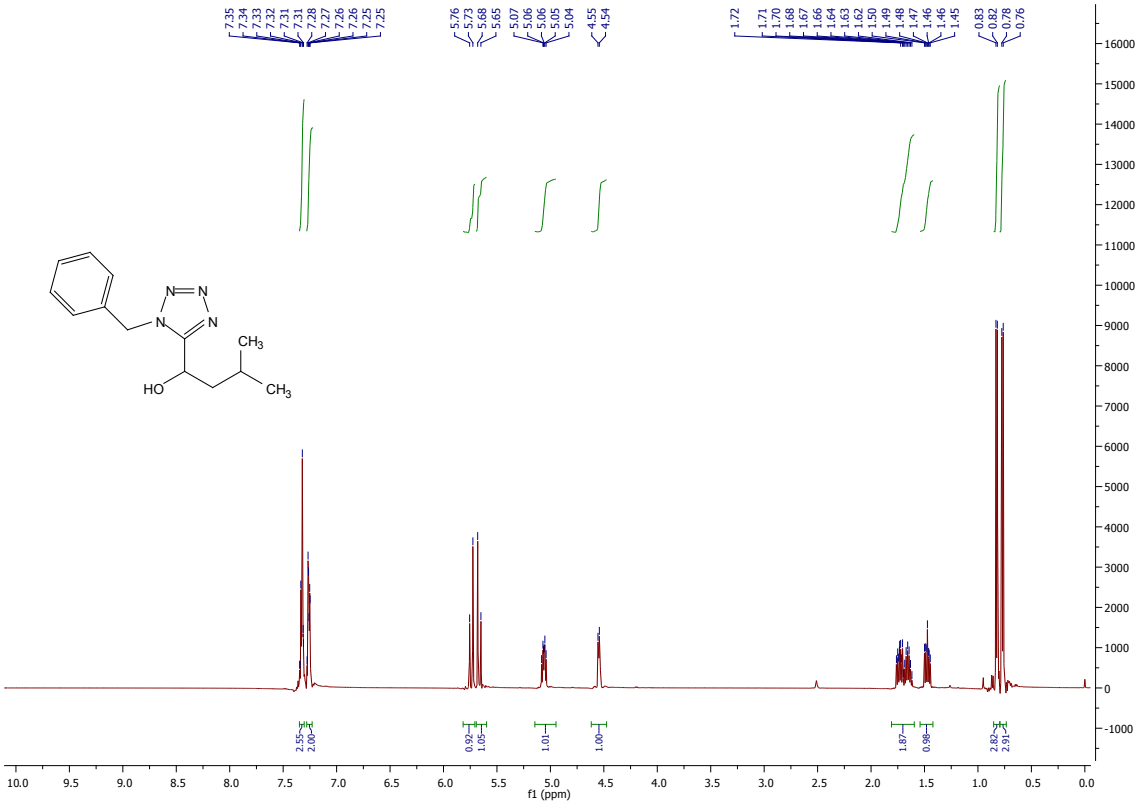
1-(1-benzyl-1*H*-tetrazol-5-yl)propan-1-ol (3l)

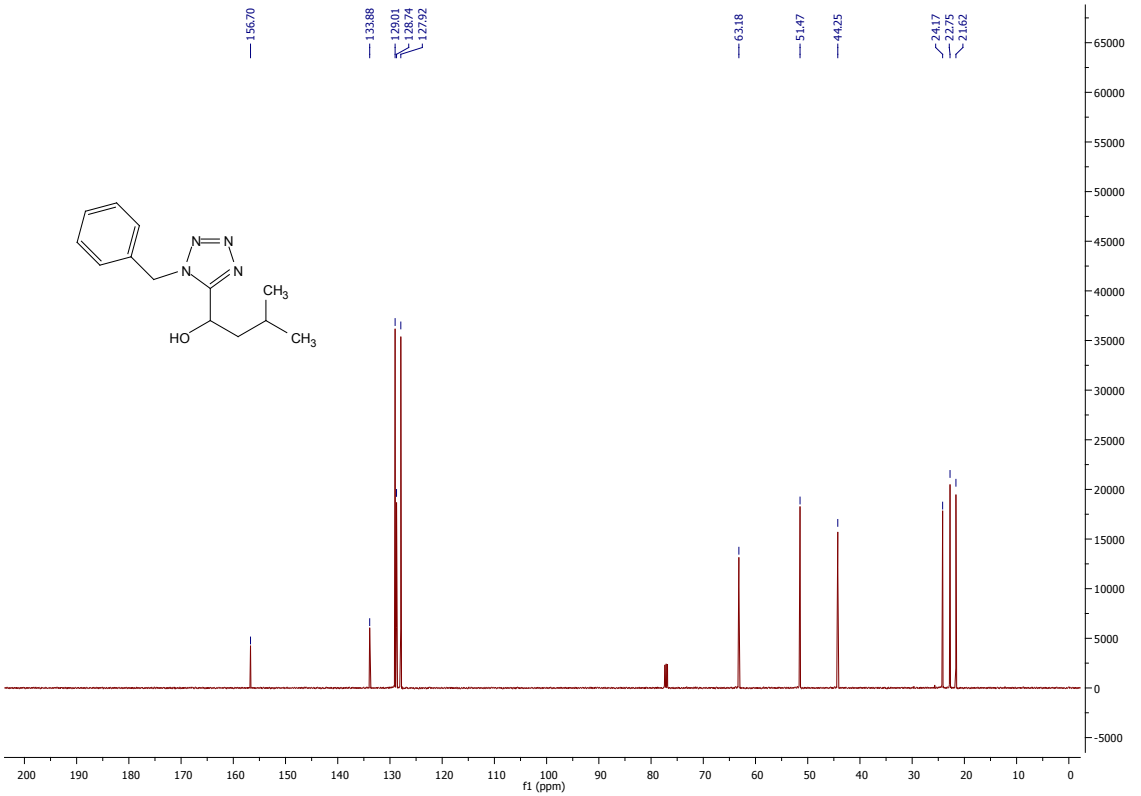


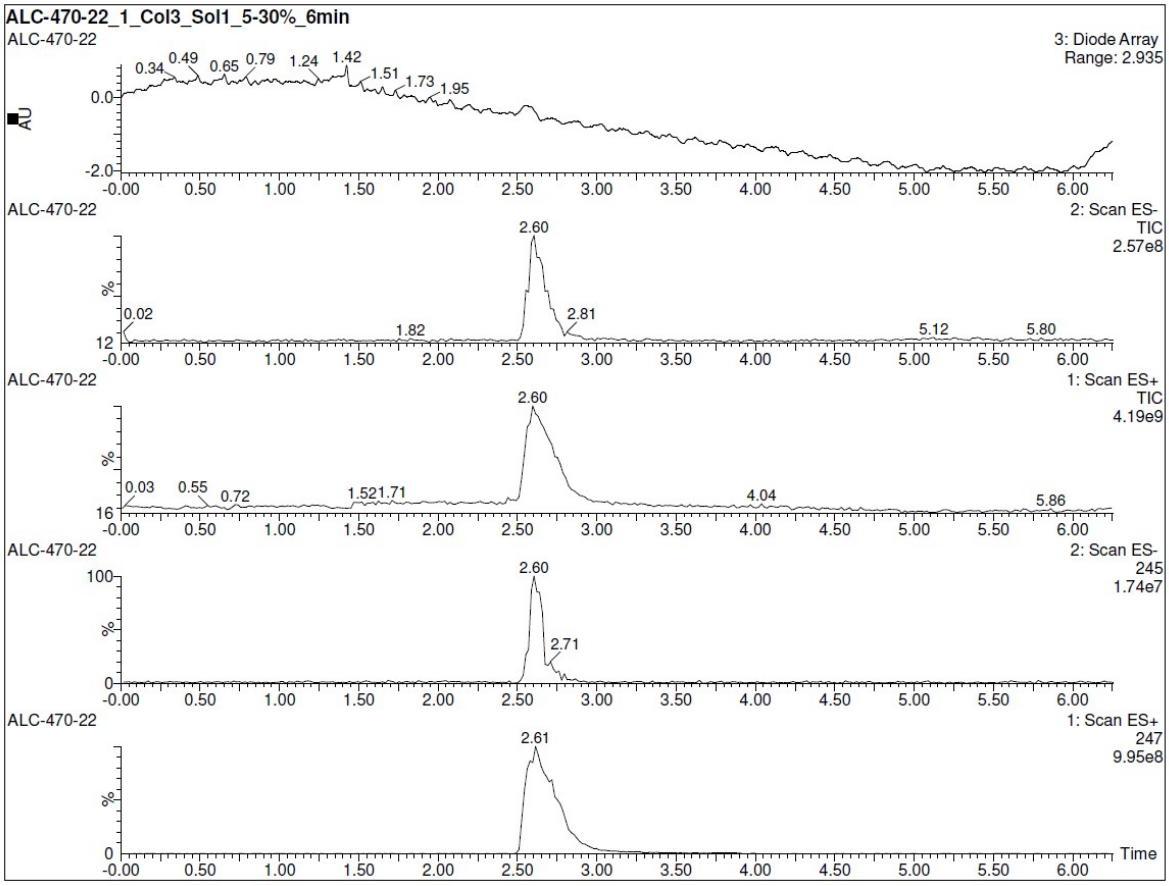


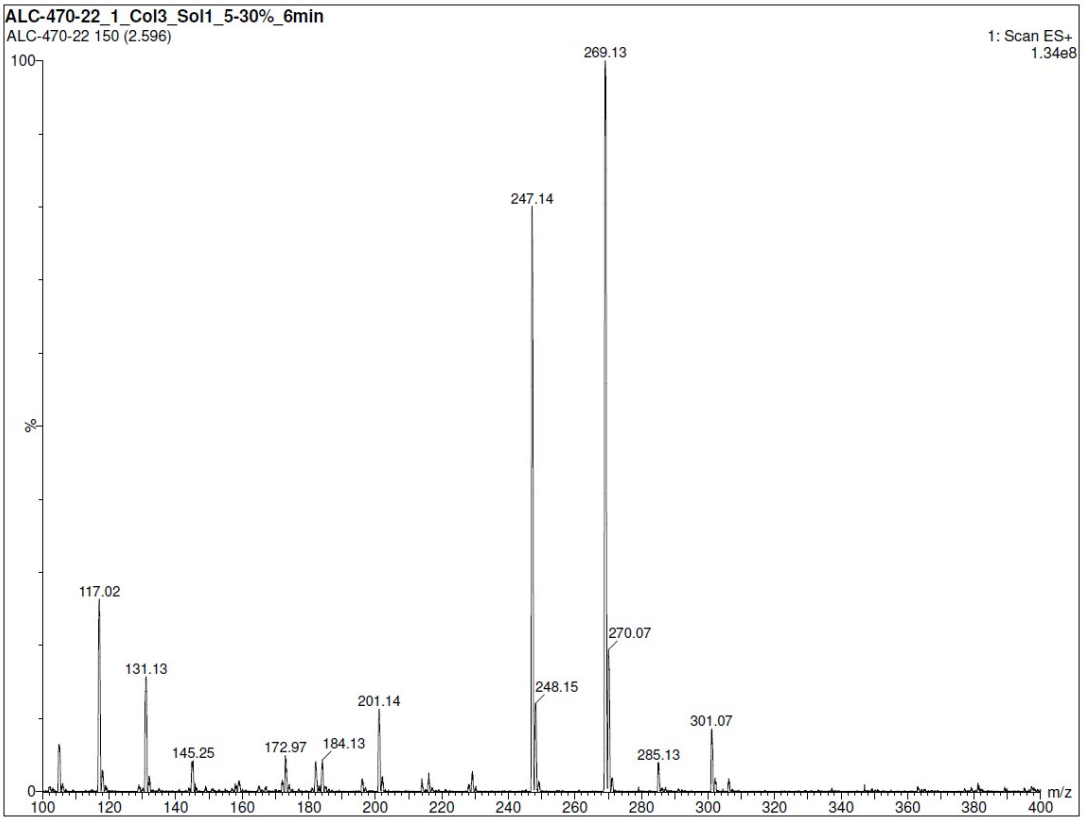


1-(1-benzyl-1*H*-tetrazol-5-yl)-3-methylbutan-1-ol (3m)

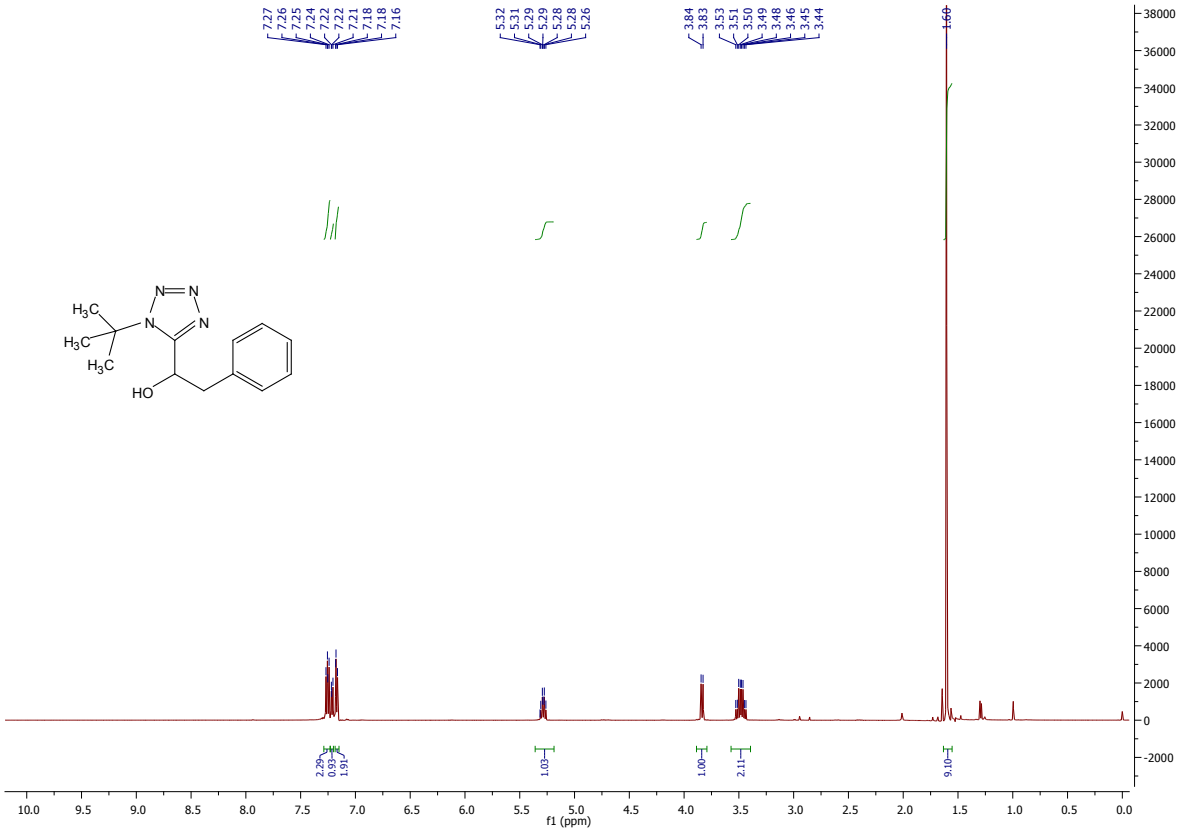

7.35
7.34
7.33
7.32
7.31
7.31
7.28
7.27
7.26
7.26
7.25
7.25
5.76
5.73
5.68
5.65
5.07
5.06
5.06
5.05
5.04
4.55
4.54
1.72
1.71
1.70
1.68
1.67
1.66
1.64
1.63
1.62
1.50
1.49
1.48
1.47
1.46
1.46
1.45
0.83
0.82
0.78
0.76
N
N
N
N
CH3
HO
CH3
2.55
2.00
0.92
1.05
1.01
1.00
1.87
0.98
2.82
2.91
f1 (ppm)

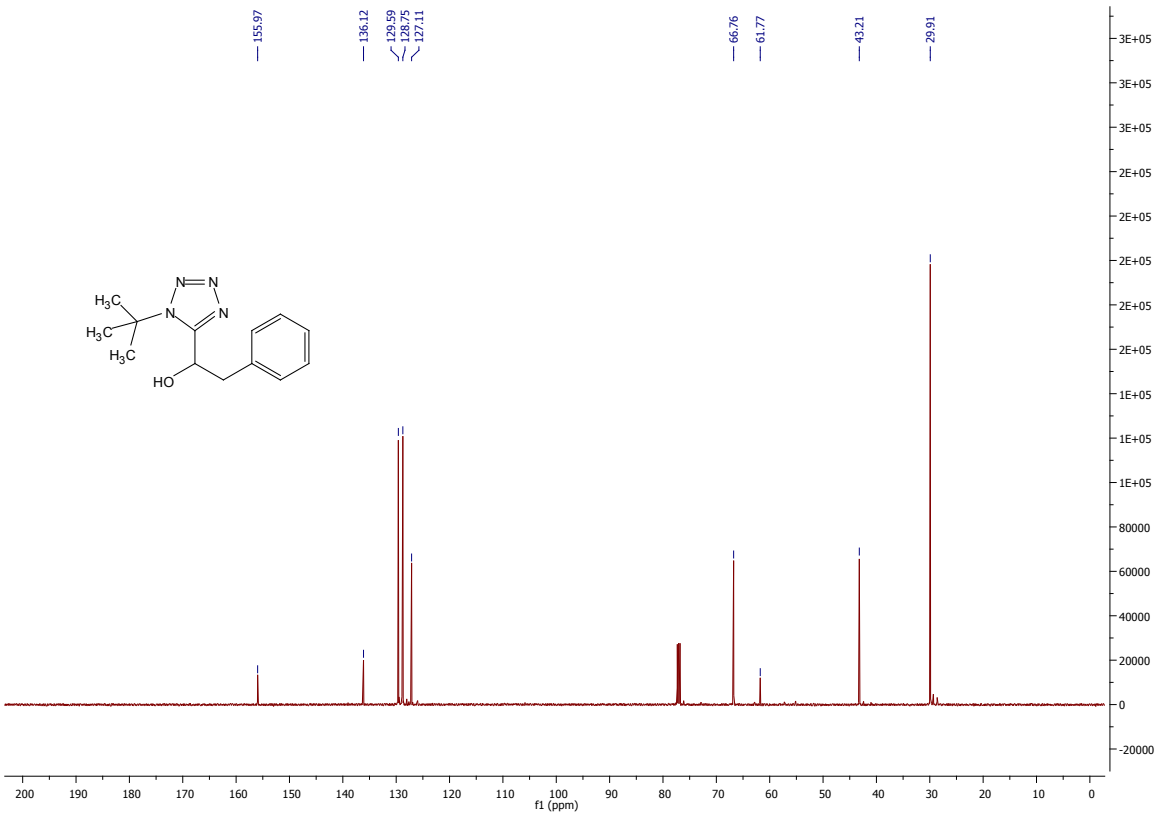

156.70
133.88
129.01
128.74
127.92
63.18
51.47
44.25
24.17
22.75
21.62
N
N
N
N
CH3
HO
CH3
f1 (ppm)

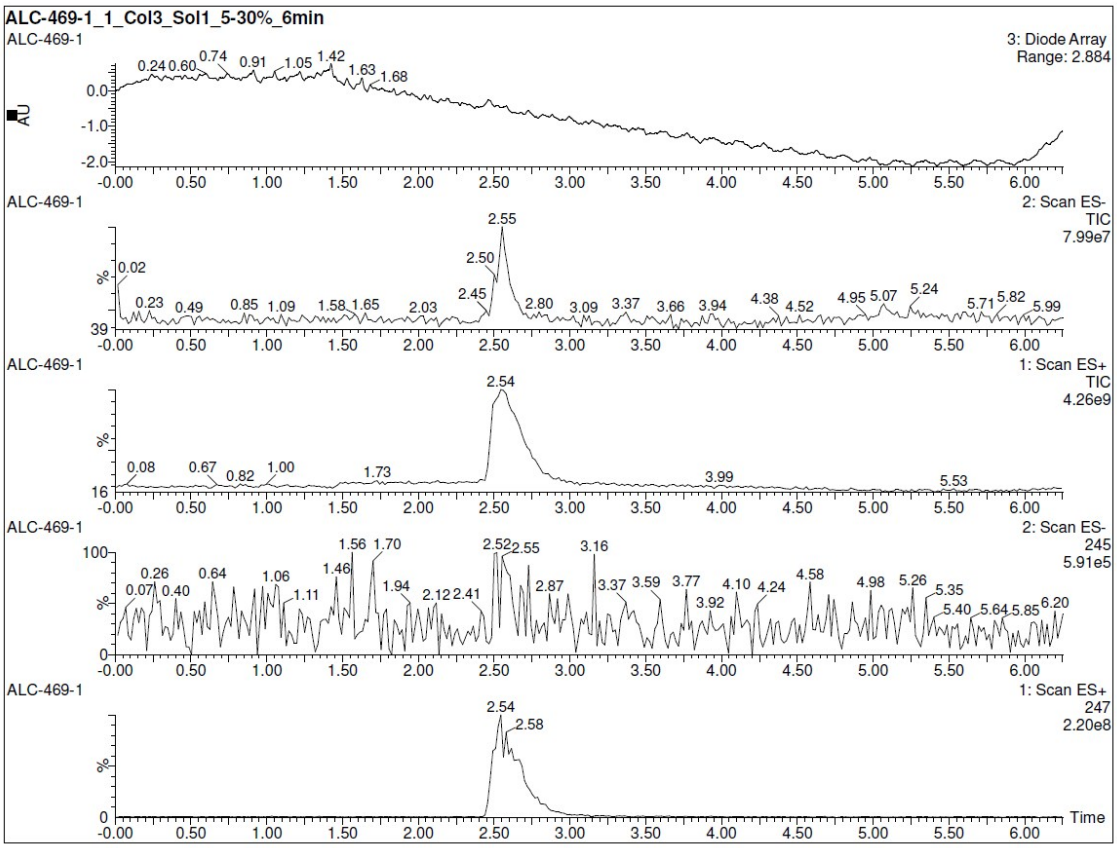

ALC-470-22_1_Col3_Sol1_5-30%_6min
ALC-470-22
3: Diode Array
Range: 2.935
AU
0.34 0.49 0.65 0.79 1.24 1.42 1.51 1.73 1.95
ALC-470-22
2: Scan ES-
TIC
2.57e8
2.60
0.02 1.82 2.81 5.12 5.80
ALC-470-22
1: Scan ES+
TIC
4.19e9
2.60
0.03 0.55 0.72 1.521.71 4.04 5.86
ALC-470-22
2: Scan ES-
245
1.74e7
2.60
2.71
ALC-470-22
1: Scan ES+
247
9.95e8
2.61
Time

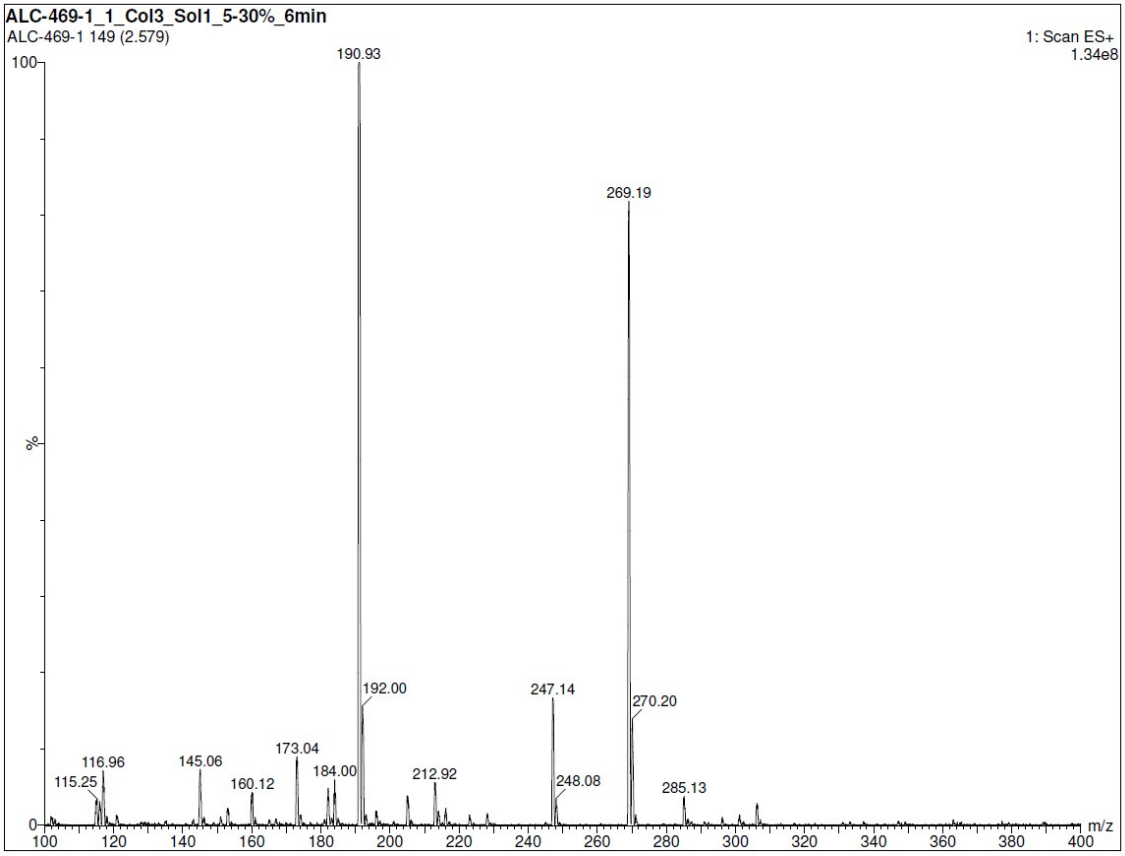

ALC-470-22_1_Col3_Sol1_5-30%_6min
ALC-470-22 150 (2.596)
1: Scan ES+
1.34e8
269.13
247.14
117.02
131.13
270.07
248.15
201.14
301.07
145.25
172.97
184.13
285.13
m/z

1-(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)-2-phenylethanol (3n)

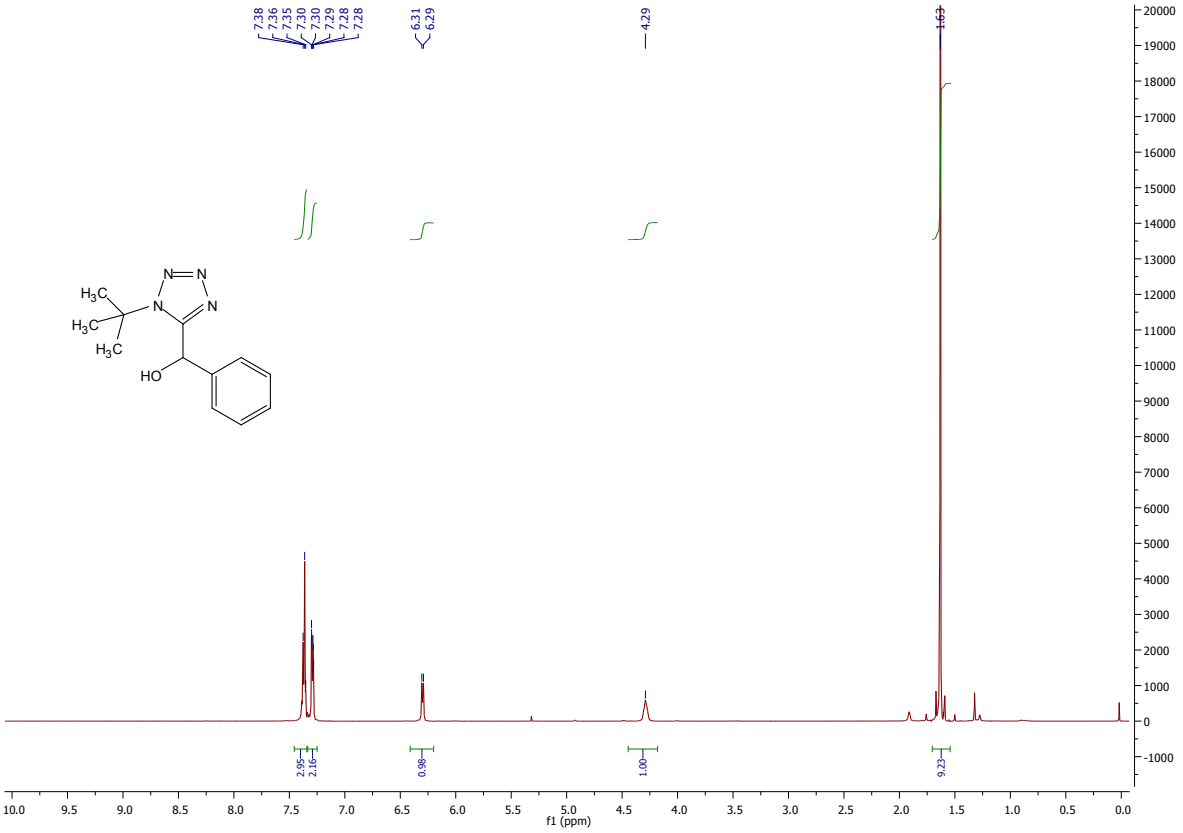


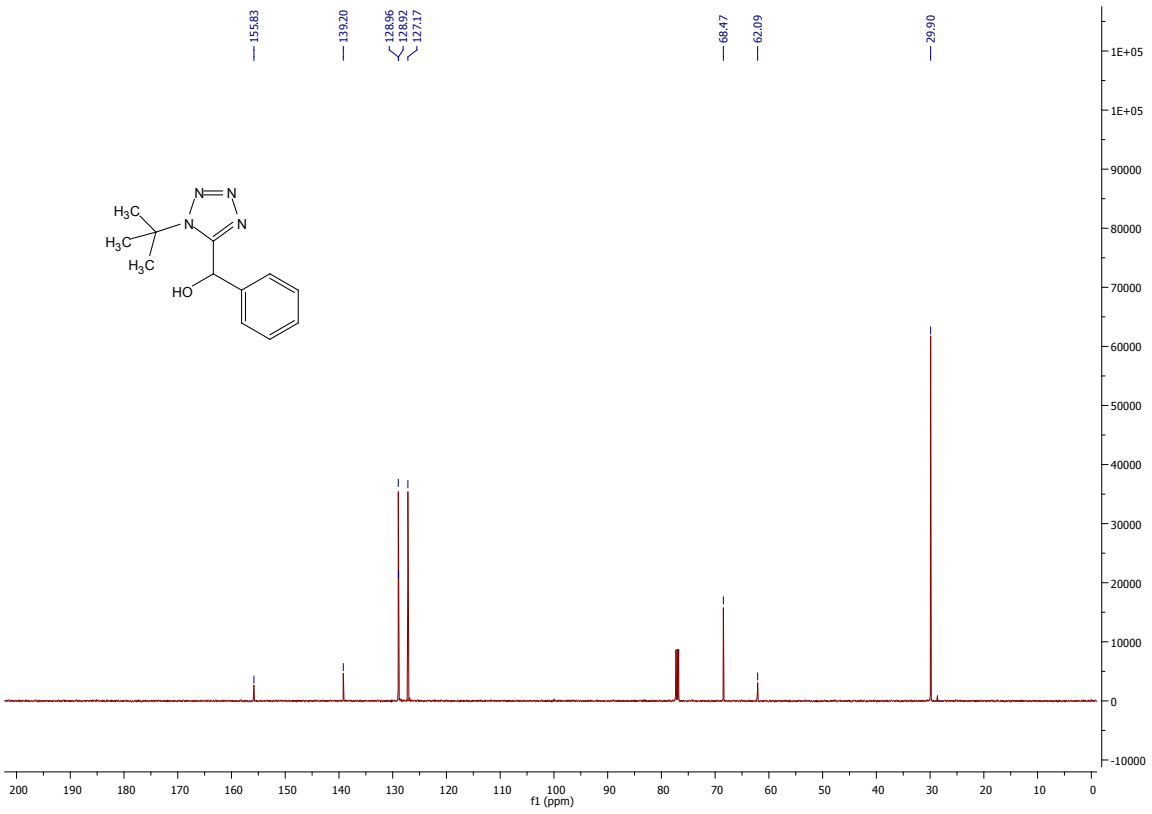


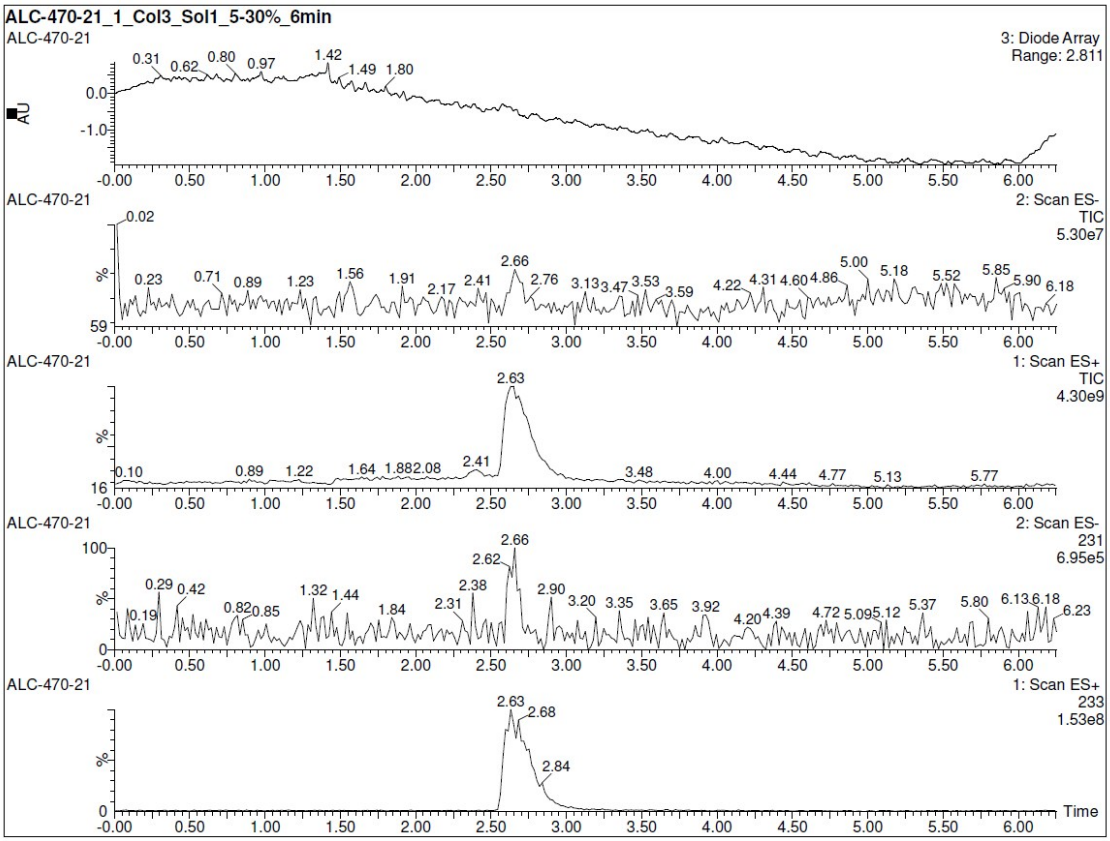

ALC-469-1_1_Col3_Sol1_5-30%_6min
ALC-469-1
3: Diode Array
Range: 2.884
AU
ALC-469-1
2: Scan ES-
TIC
7.99e7
ALC-469-1
1: Scan ES+
TIC
4.26e9
ALC-469-1
2: Scan ES-
245
5.91e5
ALC-469-1
1: Scan ES+
247
2.20e8
Time

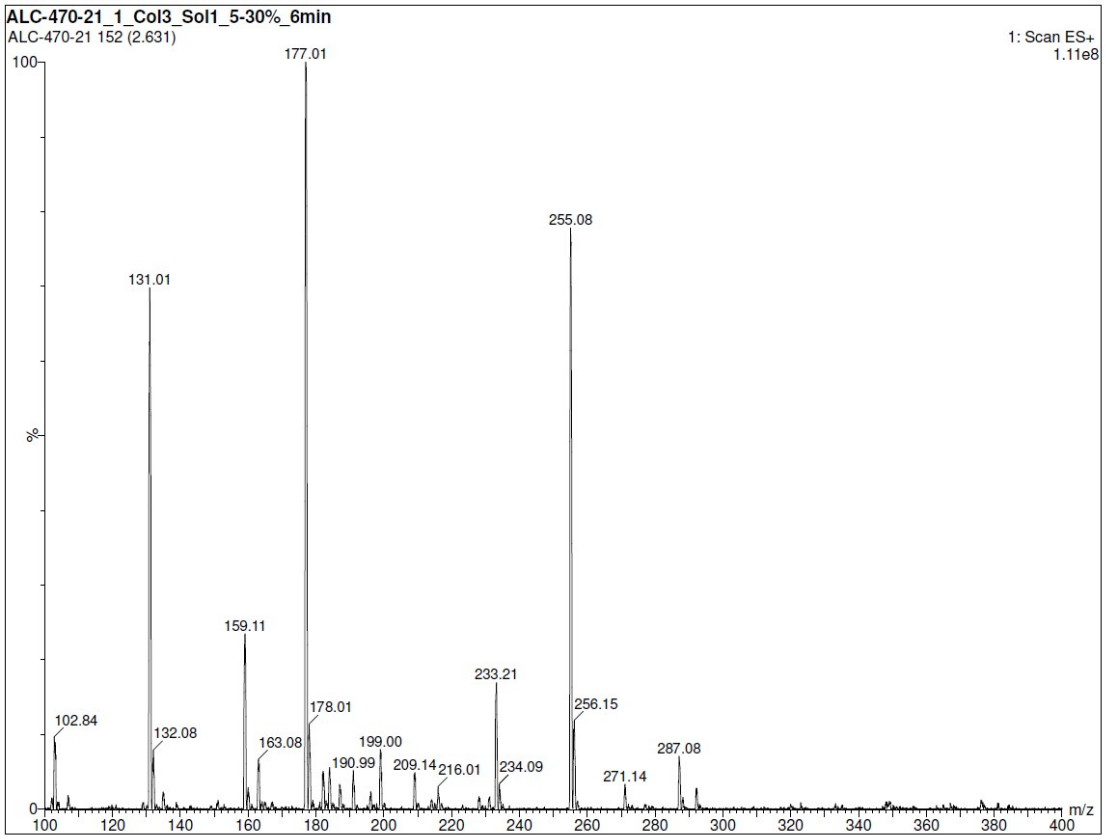

ALC-469-1_1_Col3_Sol1_5-30%_6min
ALC-469-1 149 (2.579)
1: Scan ES+
1.34e8
190.93
269.19
192.00
247.14
270.20
173.04
116.96
145.06
115.25
160.12
184.00
212.92
248.08
285.13
m/z

(1-(*tert*-butyl)-1*H*-tetrazol-5-yl)(phenyl)methanol (3o)

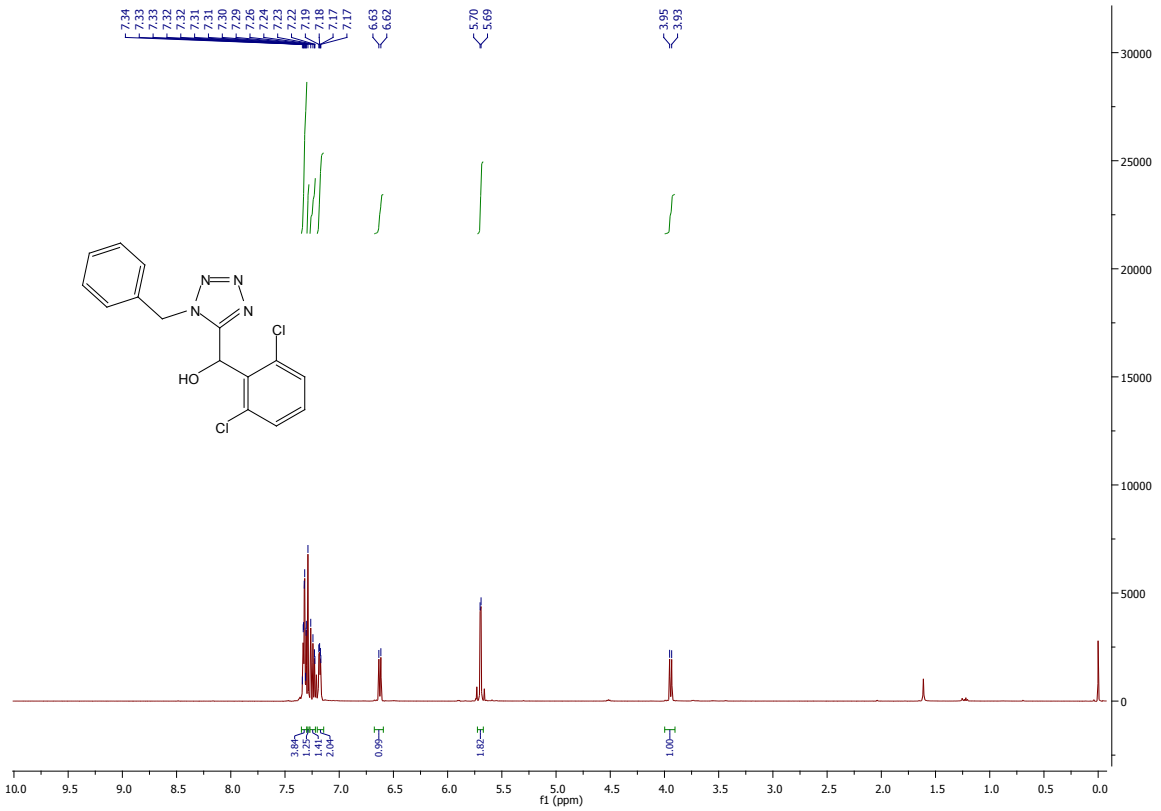


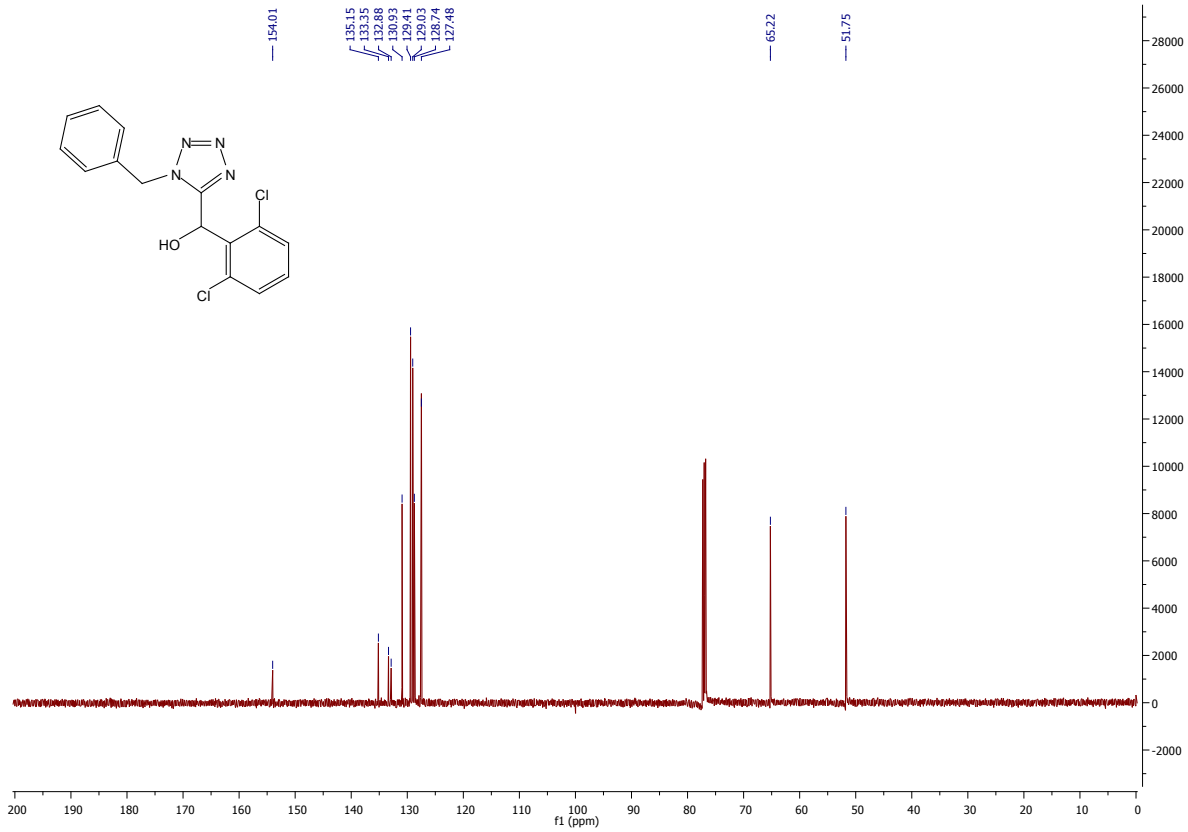


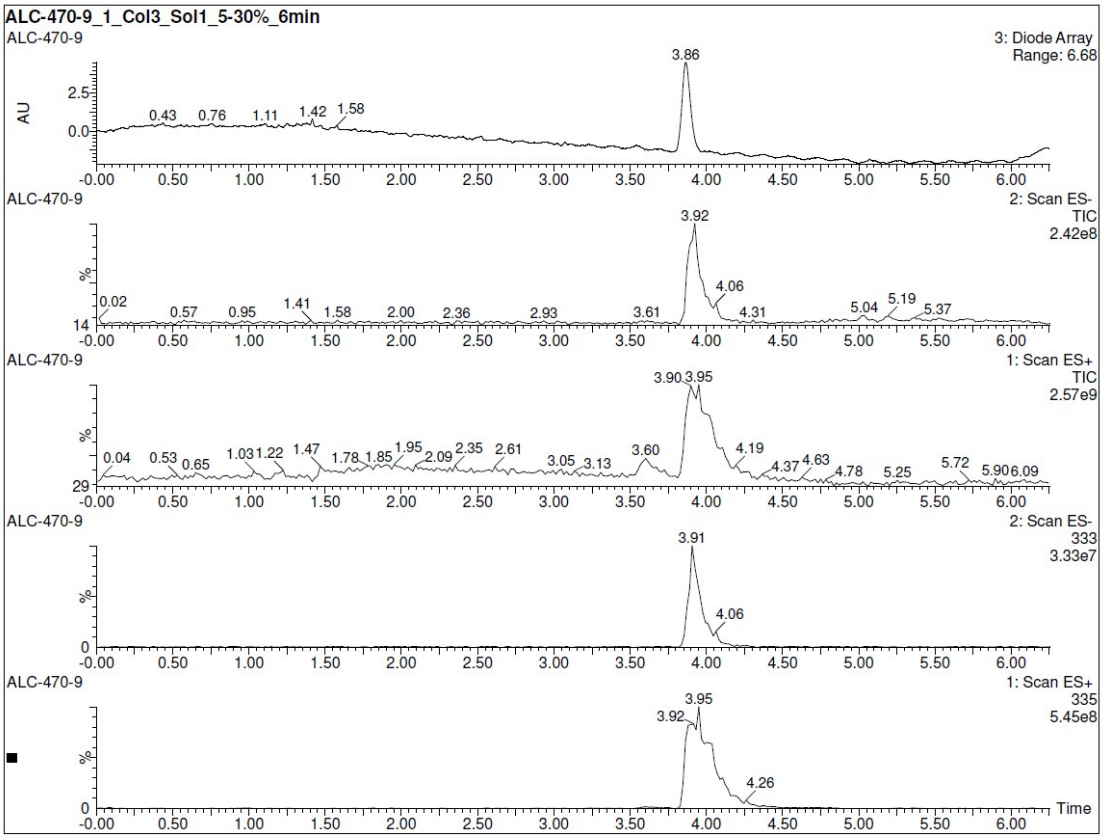

ALC-470-21_1_Col3_Sol1_5-30%_6min
ALC-470-21
3: Diode Array
Range: 2.811
AU
ALC-470-21
2: Scan ES-
TIC
5.30e7
ALC-470-21
1: Scan ES+
TIC
4.30e9
ALC-470-21
2: Scan ES-
231
6.95e5
ALC-470-21
1: Scan ES+
233
1.53e8
Time

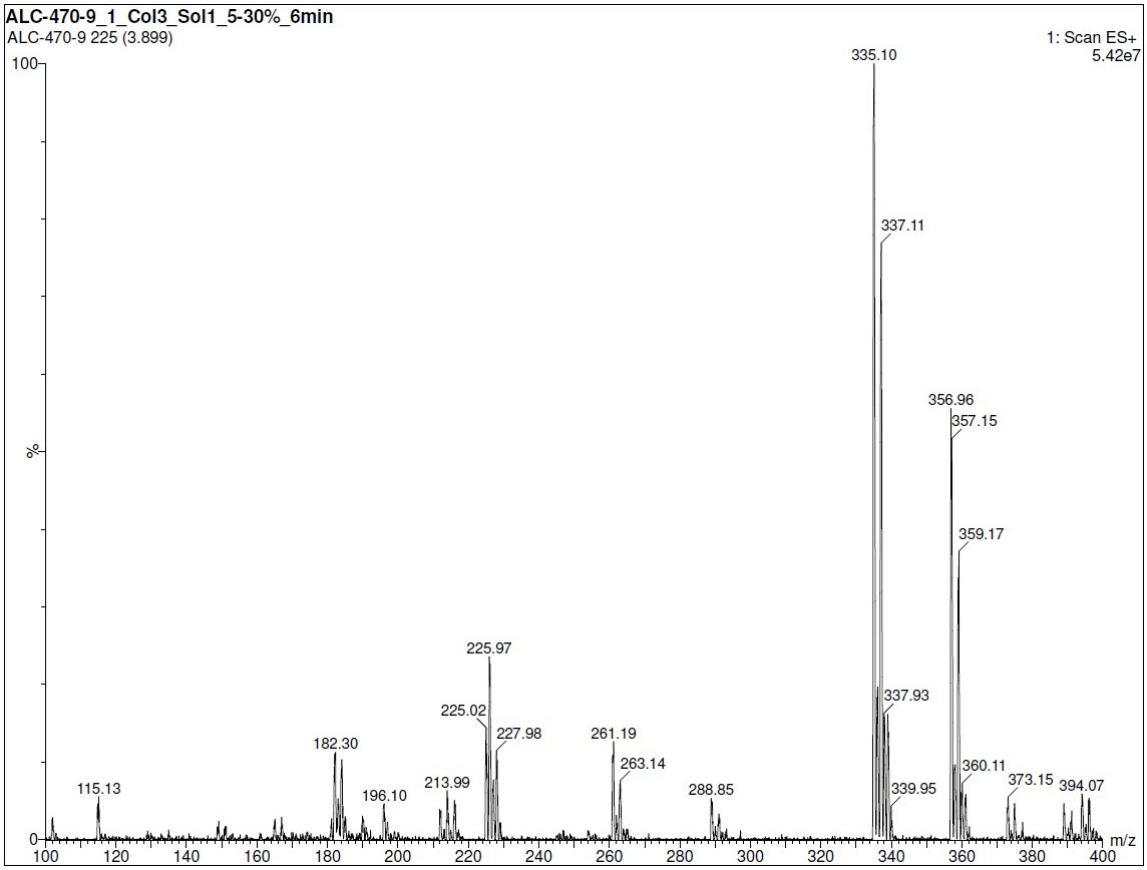

ALC-470-21_1_Col3_Sol1_5-30%_6min
ALC-470-21 152 (2.631)
1: Scan ES+
1.11e8
177.01
255.08
131.01
159.11
233.21
178.01
256.15
102.84
132.08
163.08
199.00
190.99
209.14
216.01
234.09
287.08
271.14
m/z

(1-benzyl-1*H*-tetrazol-5-yl)(2,6-dichlorophenyl)methanol (3p)

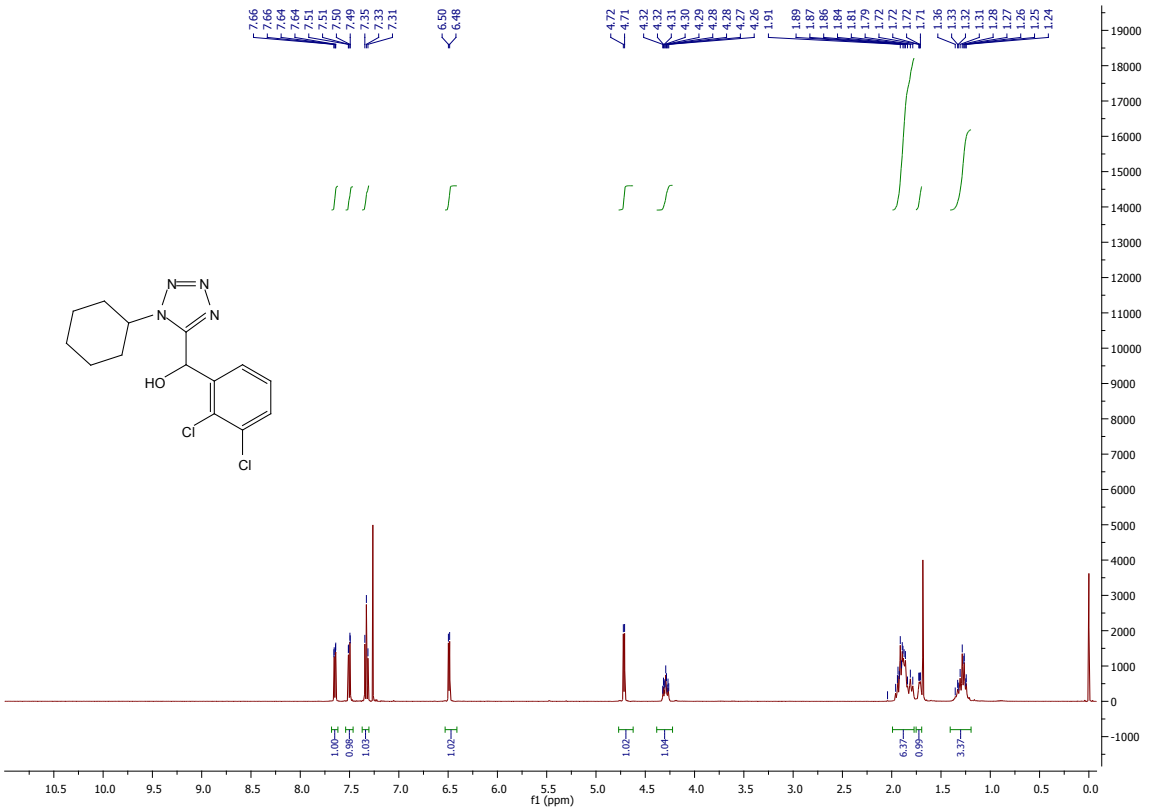


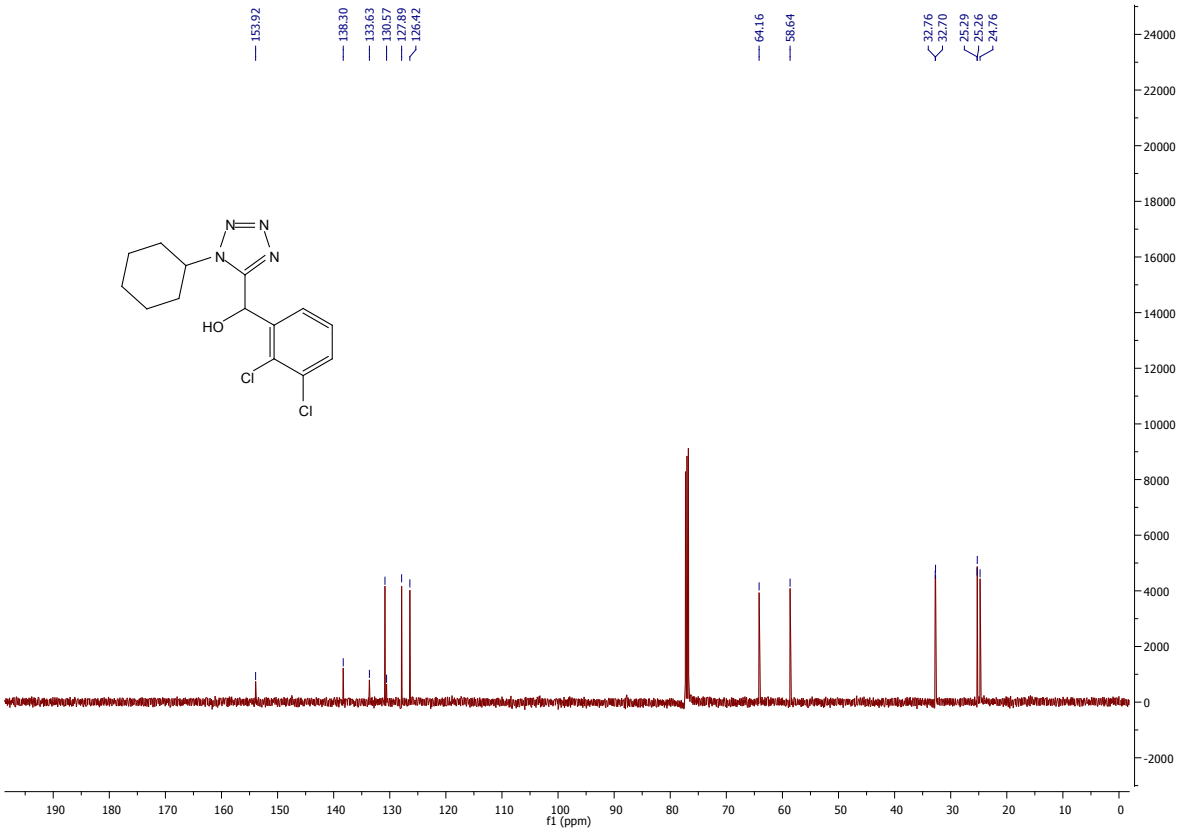


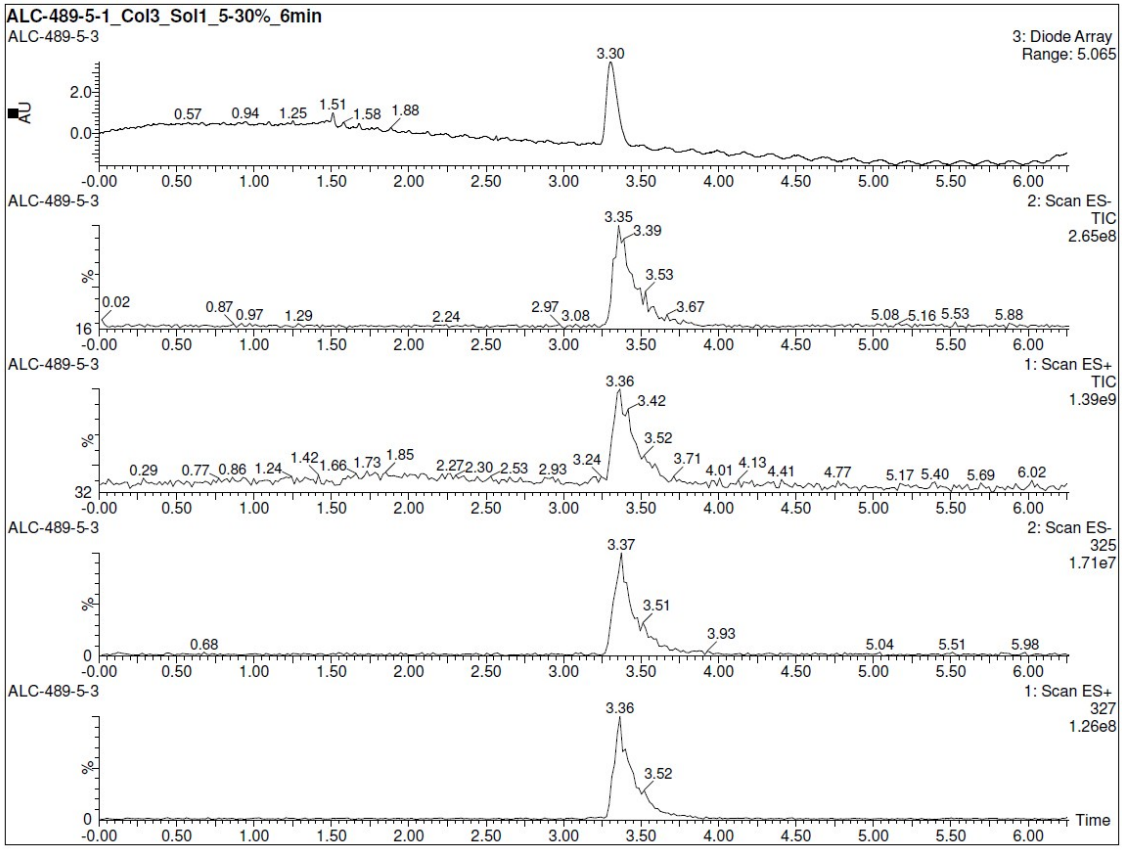

ALC-470-9_1_Col3_Sol1_5-30%_6min
ALC-470-9
3: Diode Array
Range: 6.68
AU
2: Scan ES-
TIC
2.42e8
1: Scan ES+
TIC
2.57e9
2: Scan ES-
333
3.33e7
1: Scan ES+
335
5.45e8
Time

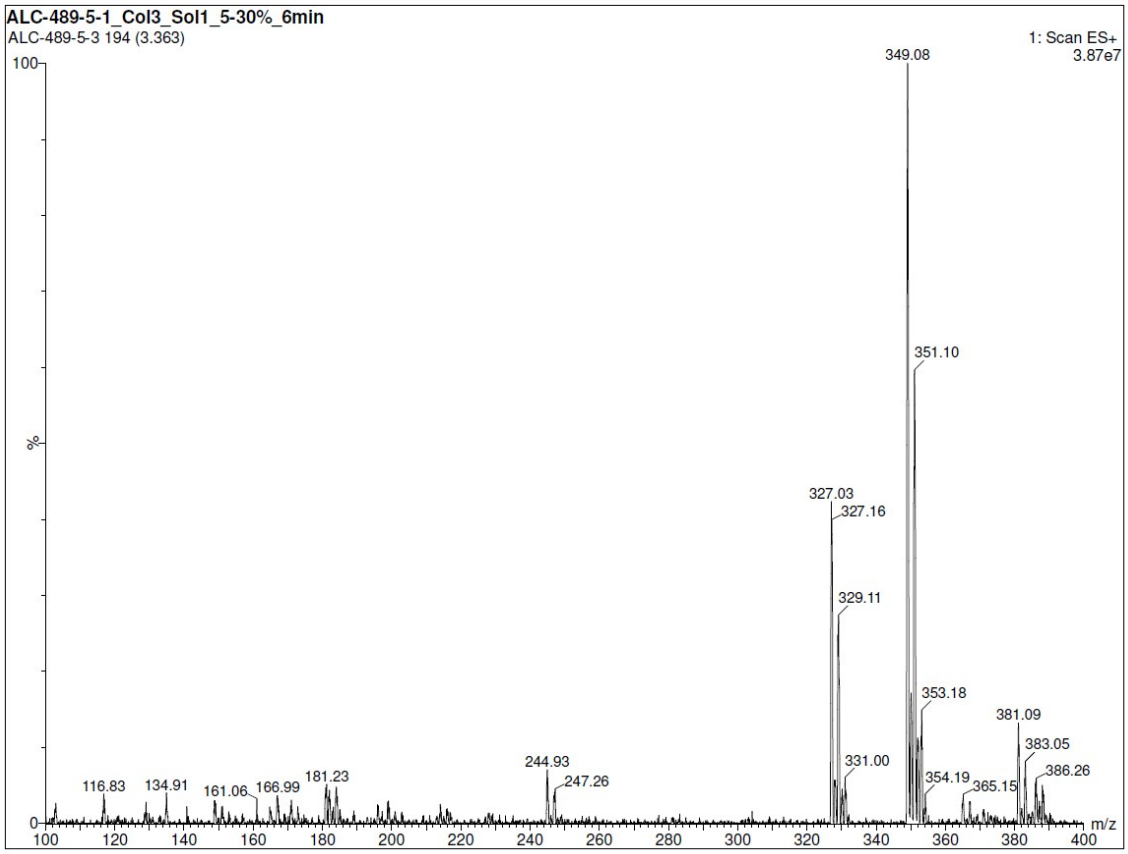

ALC-470-9_1_Col3_Sol1_5-30%_6min
ALC-470-9 225 (3.899)
1: Scan ES+
5.42e7
%
m/z

(1-cyclohexyl-1*H*-tetrazol-5-yl)(2,3-dichlorophenyl)methanol (3q)

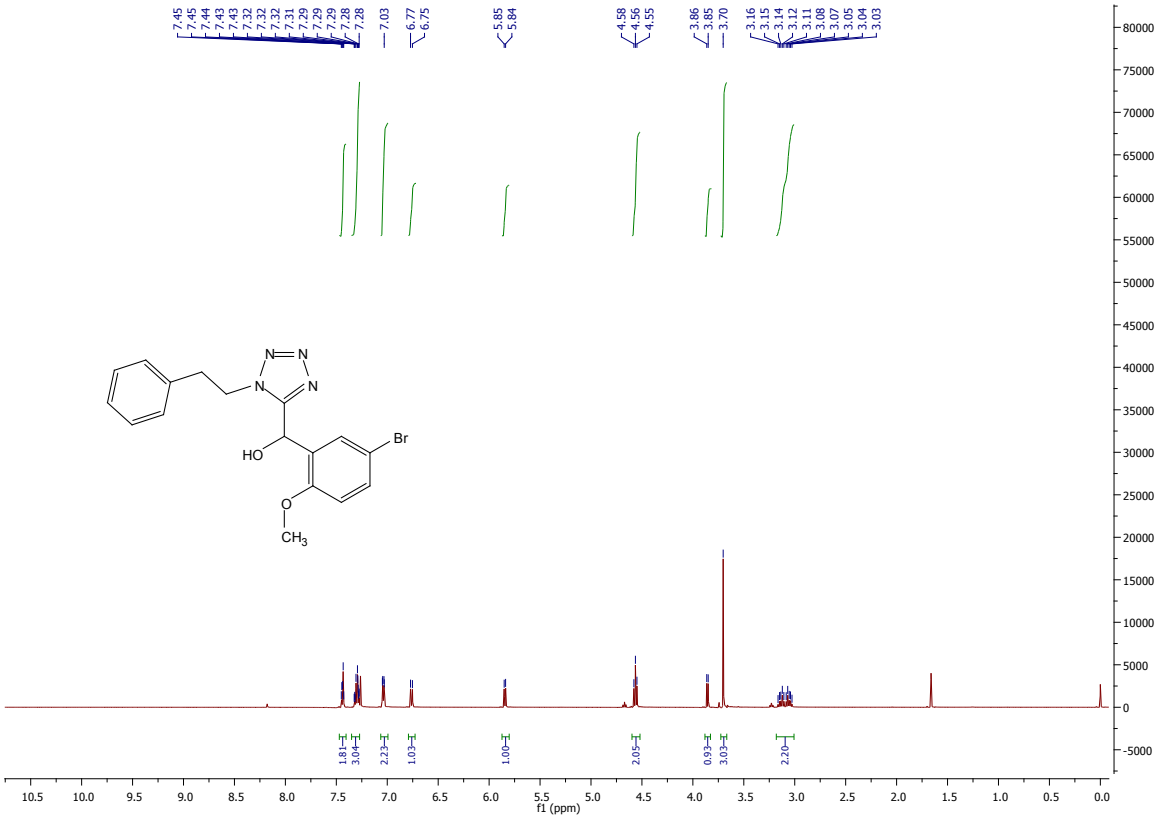


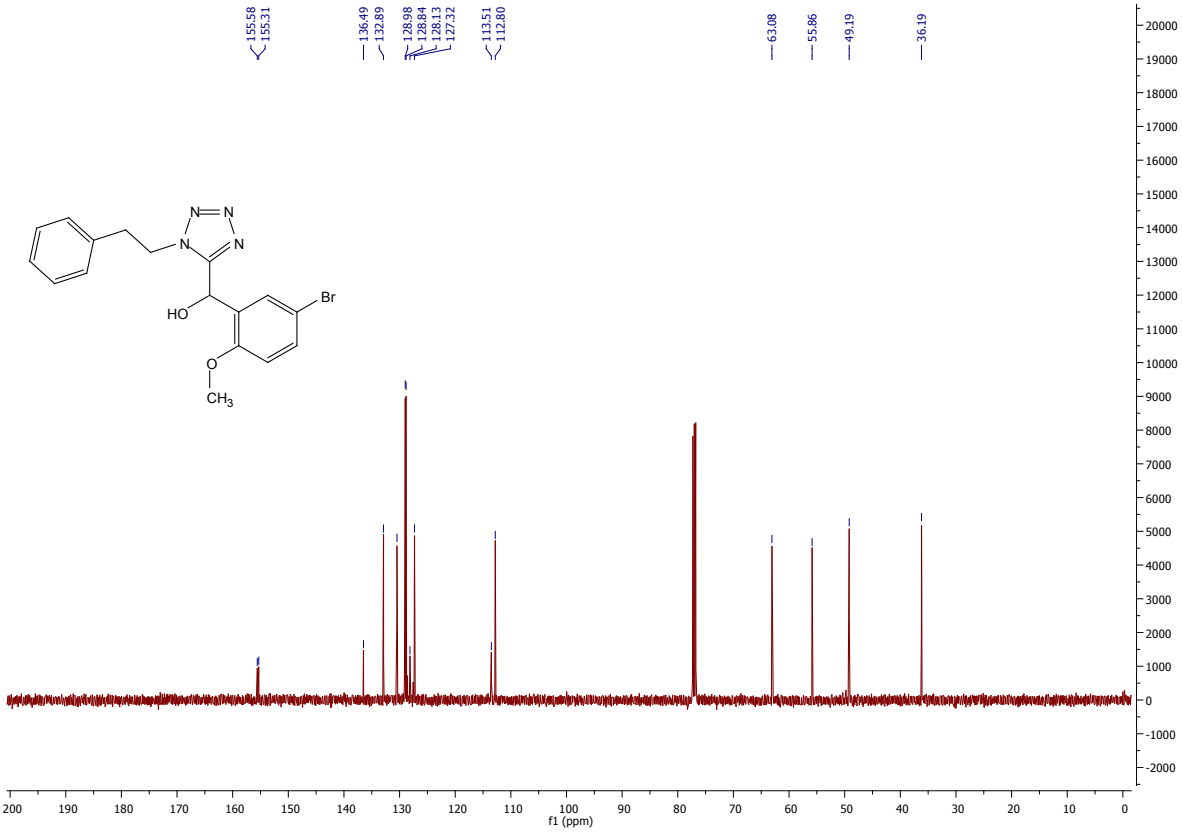


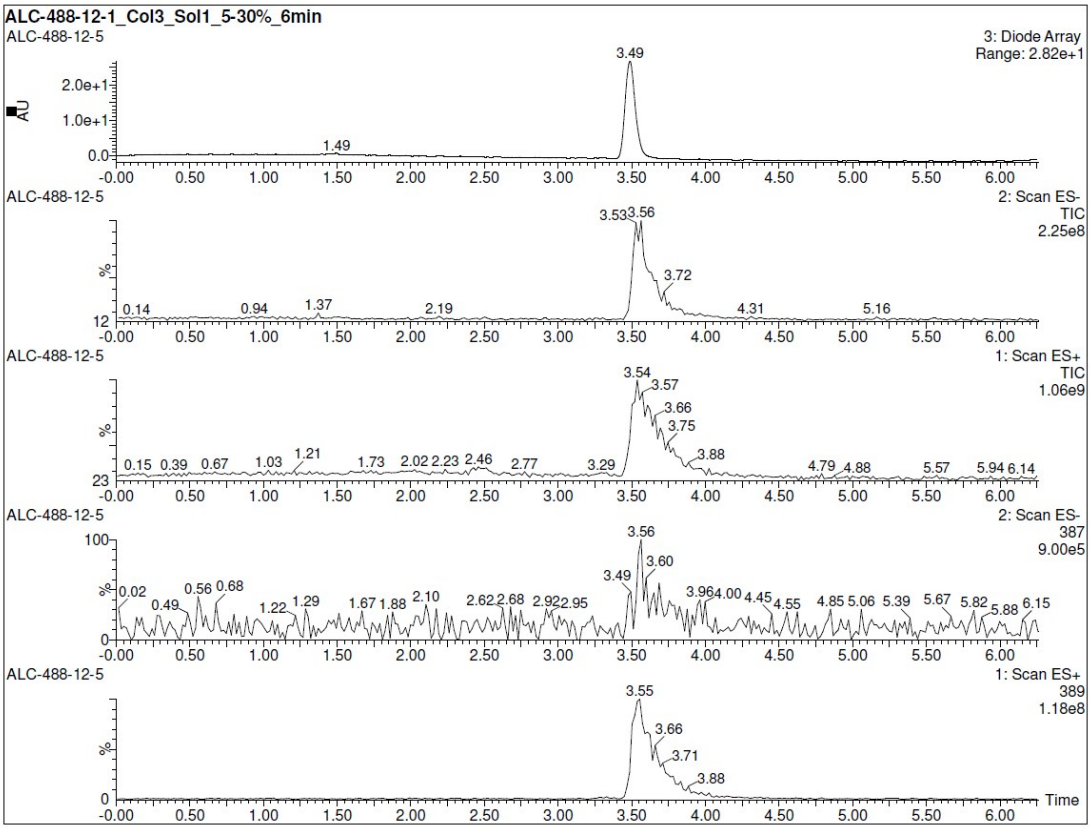

ALC-489-5-1_Col3_Sol1_5-30%_6min
ALC-489-5-3
3: Diode Array
Range: 5.065
AU
2: Scan ES-
TIC
2.65e8
1: Scan ES+
TIC
1.39e9
2: Scan ES-
325
1.71e7
1: Scan ES+
327
1.26e8
%
Time

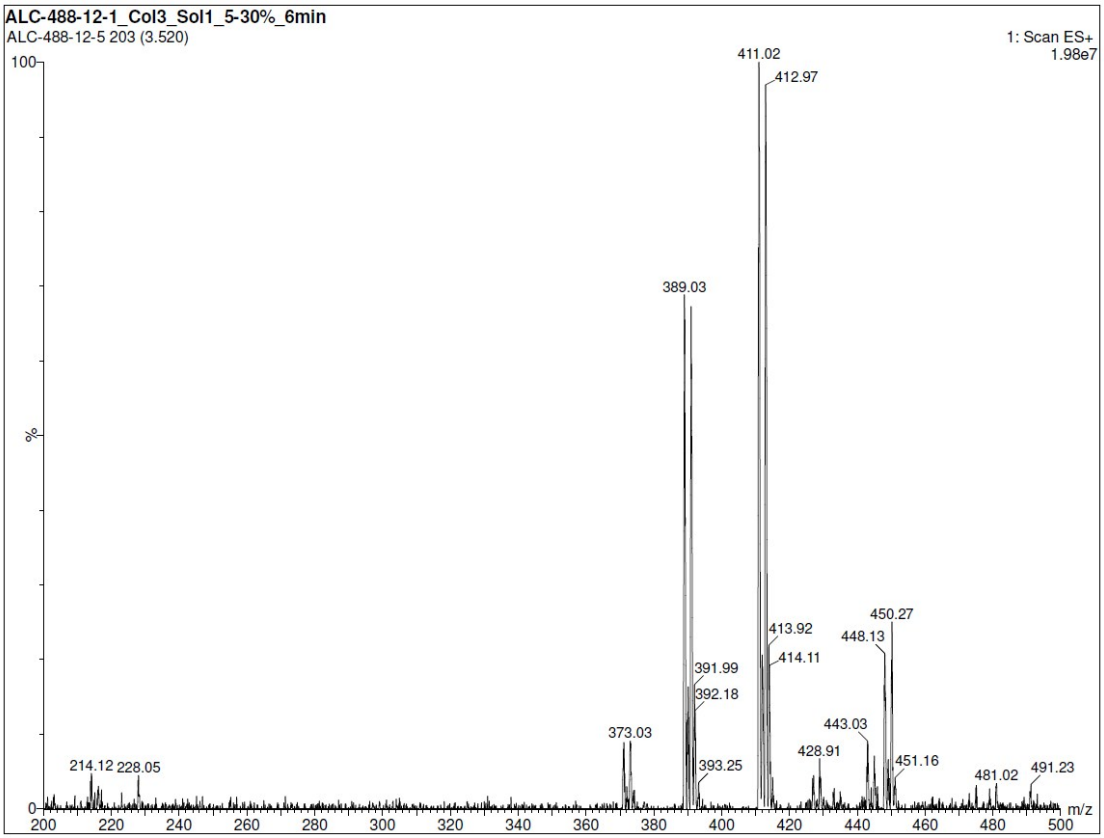

ALC-489-5-1_Col3_Sol1_5-30%_6min
ALC-489-5-3 194 (3.363)
1: Scan ES+
3.87e7
%
m/z

(5-bromo-2-methoxyphenyl)(1-phenethyl-1*H*-tetrazol-5-yl)methanol (3r)

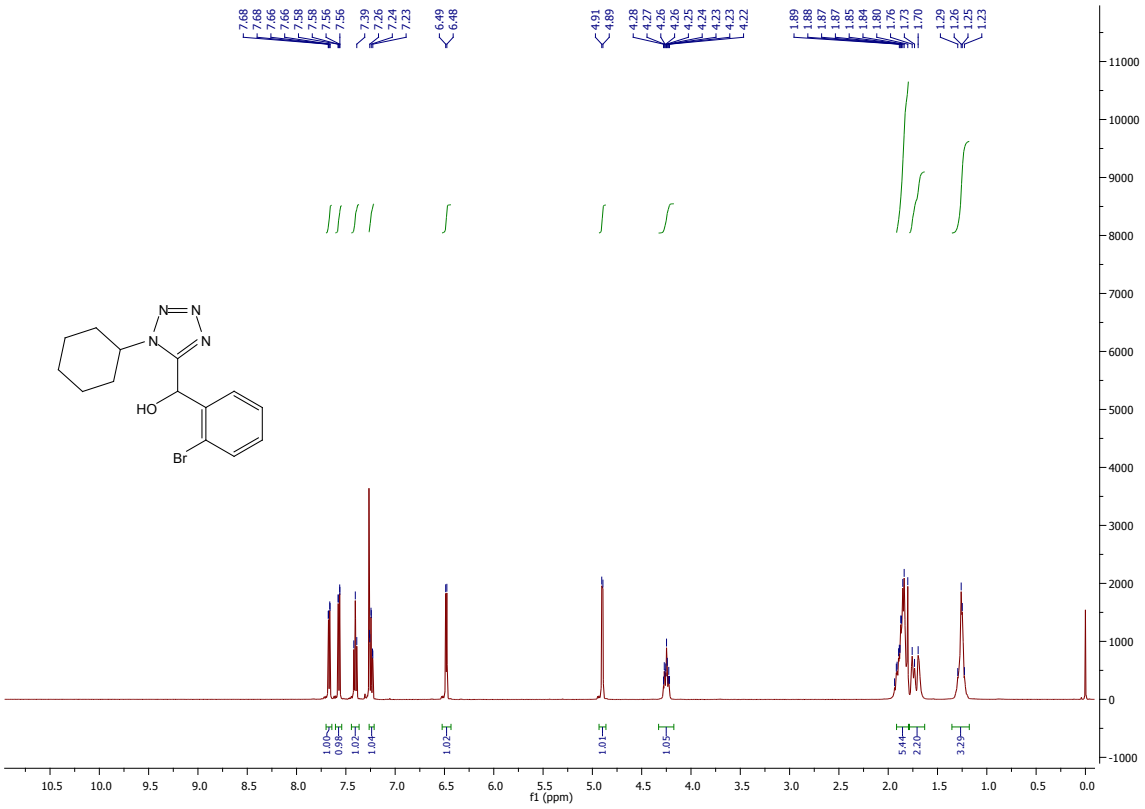


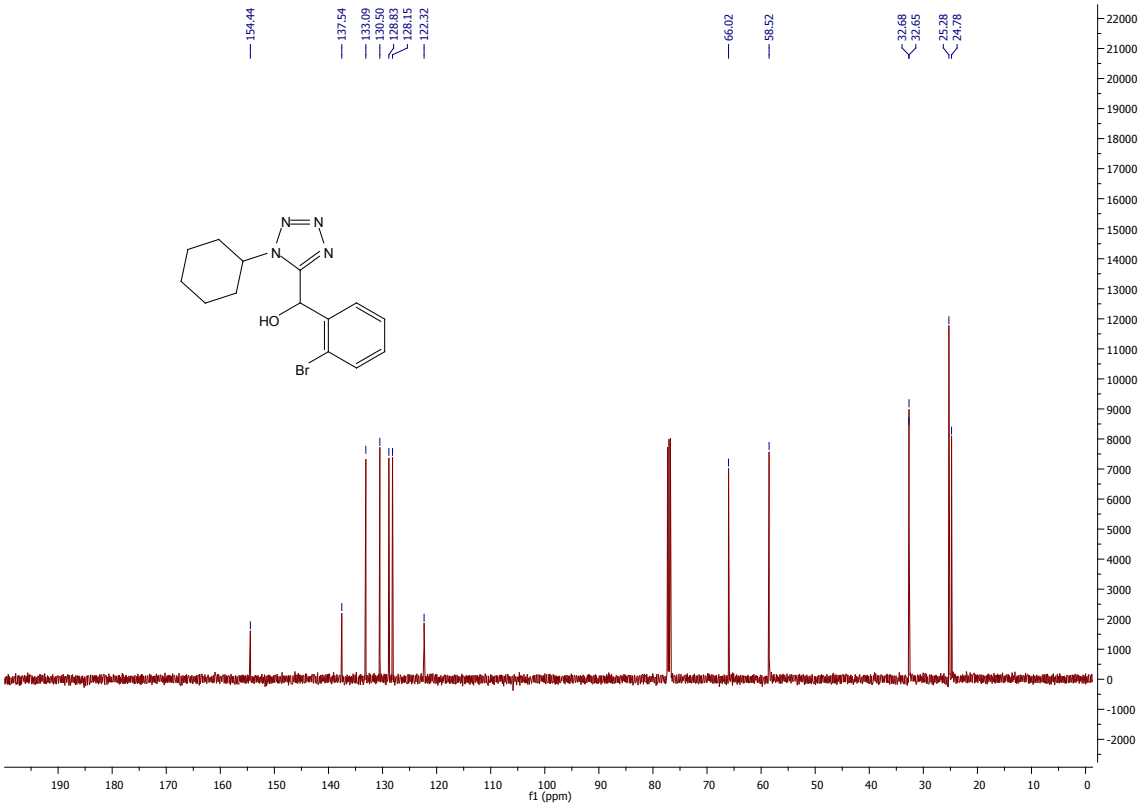


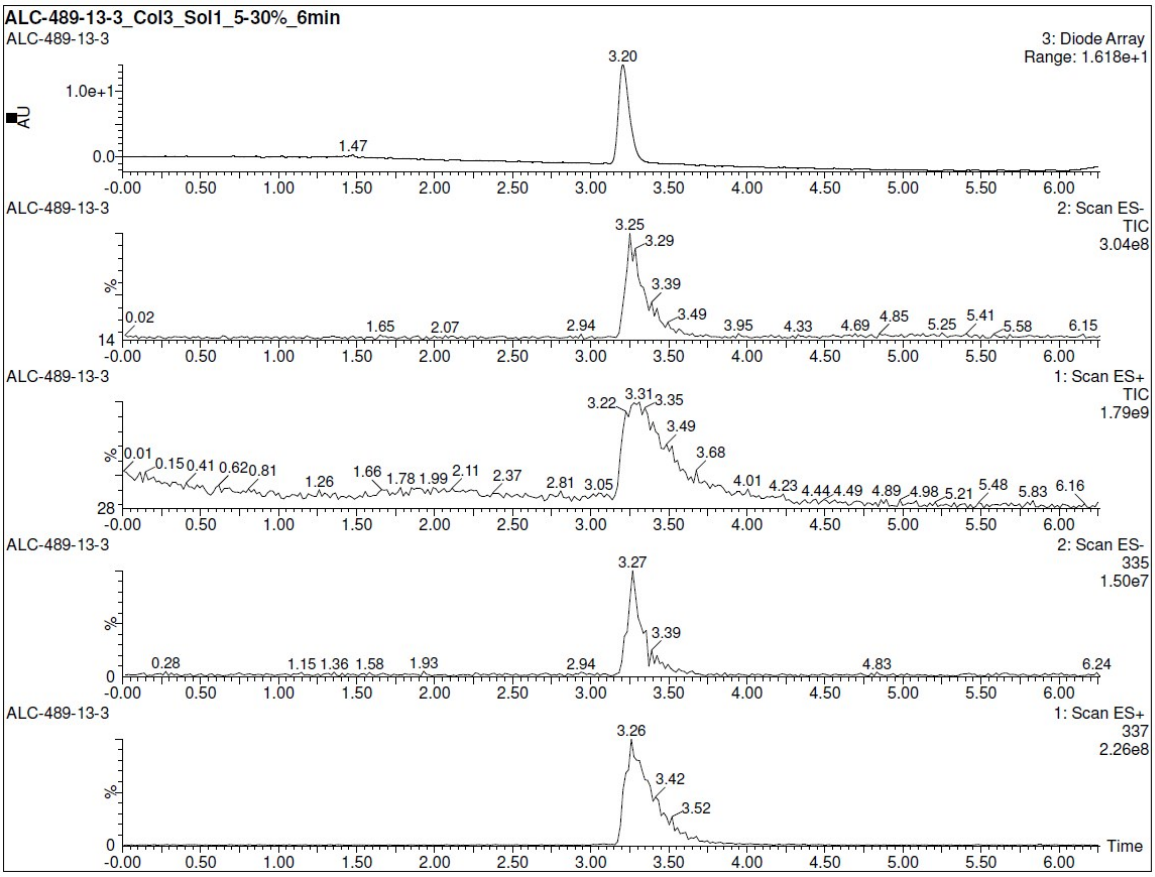

ALC-488-12-1_Col3_Sol1_5-30%_6min
ALC-488-12-5
3: Diode Array
Range: 2.82e+1
AU
2: Scan ES-
TIC
2.25e8
1: Scan ES+
TIC
1.06e9
2: Scan ES-
387
9.00e5
1: Scan ES+
389
1.18e8
Time

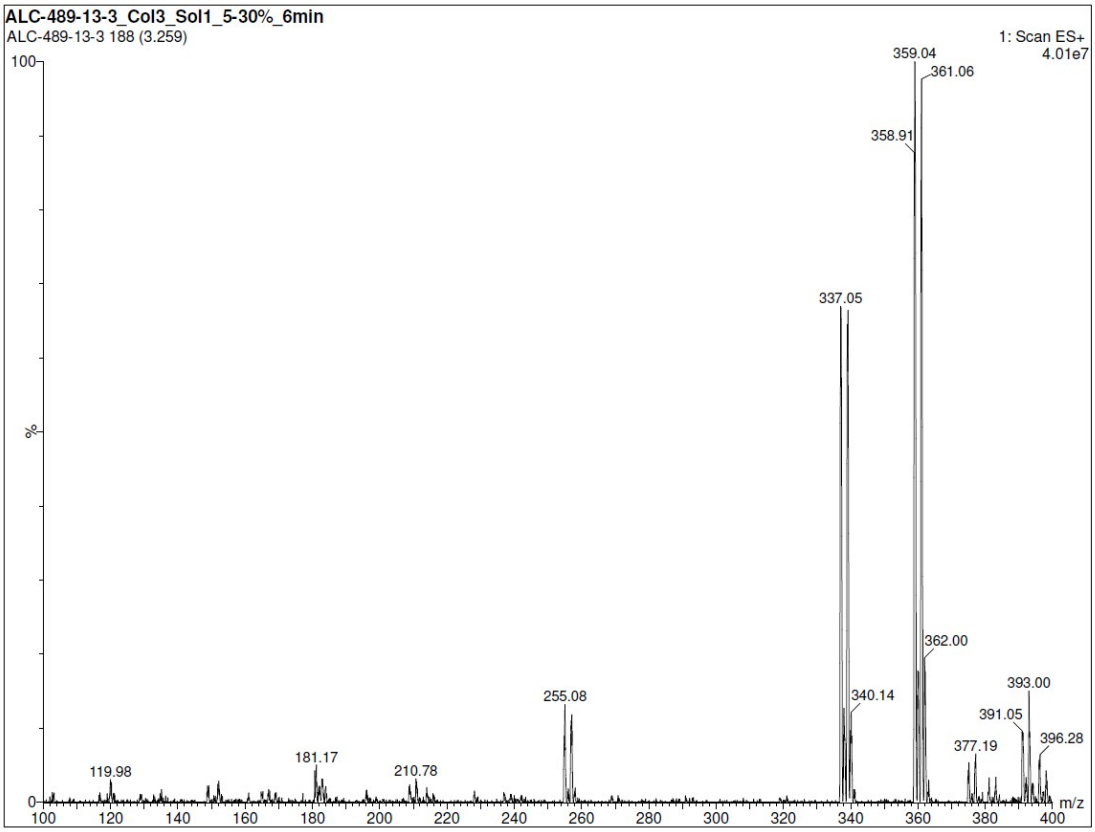

ALC-488-12-1_Col3_Sol1_5-30%_6min
ALC-488-12-5 203 (3.520)
1: Scan ES+
1.98e7
m/z

(2-bromophenyl)(1-cyclohexyl-1*H*-tetrazol-5-yl)methanol (3s)

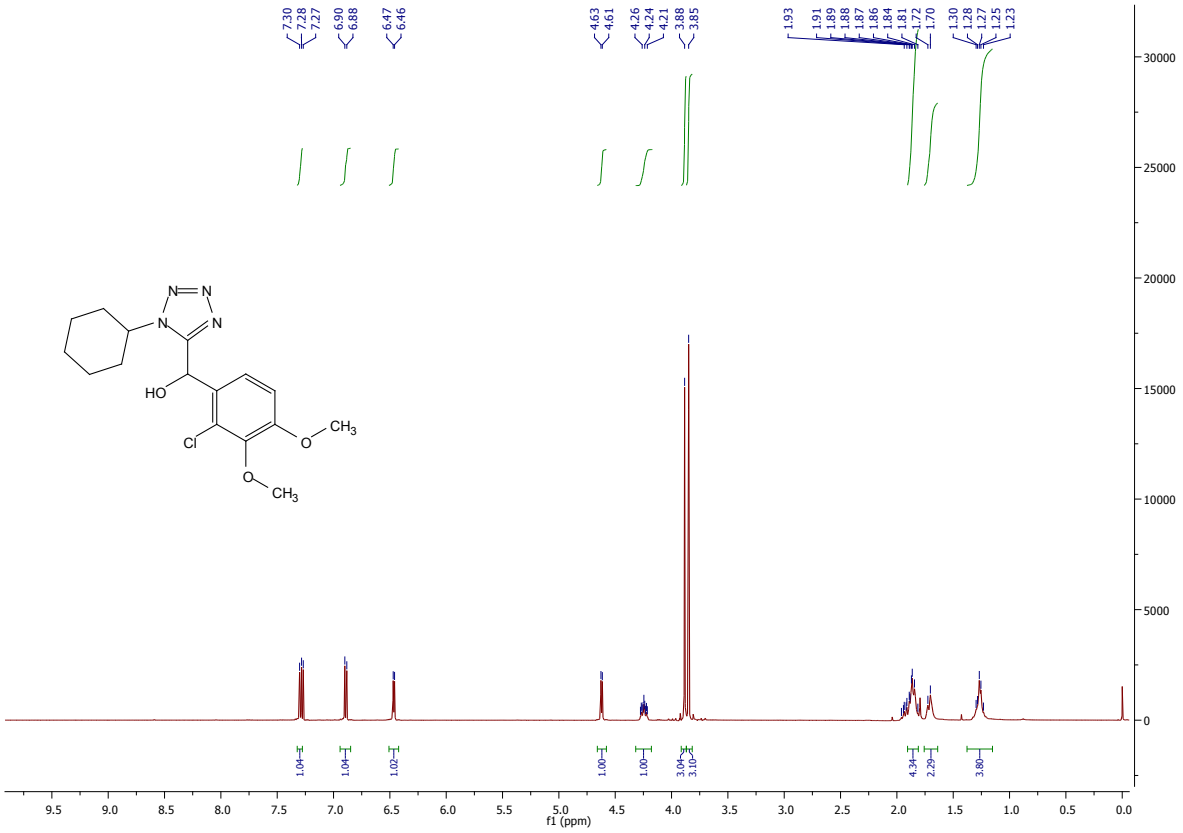


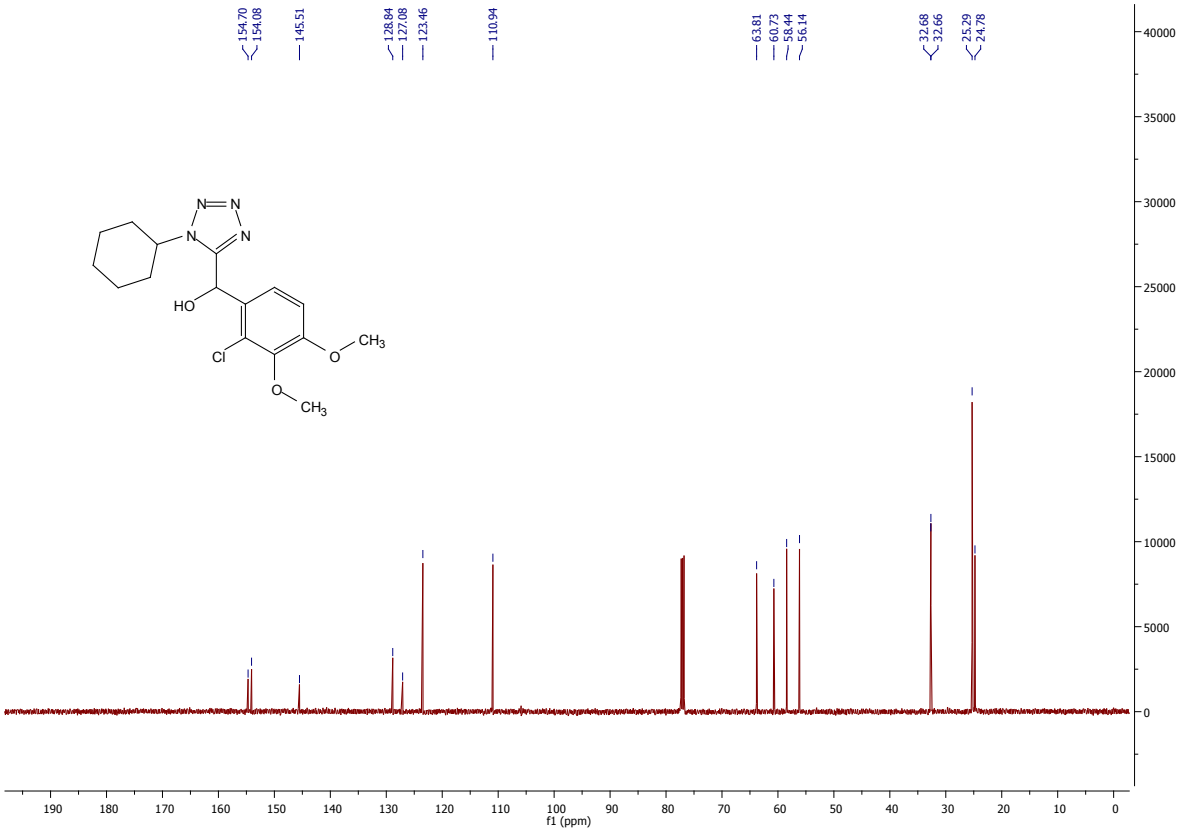


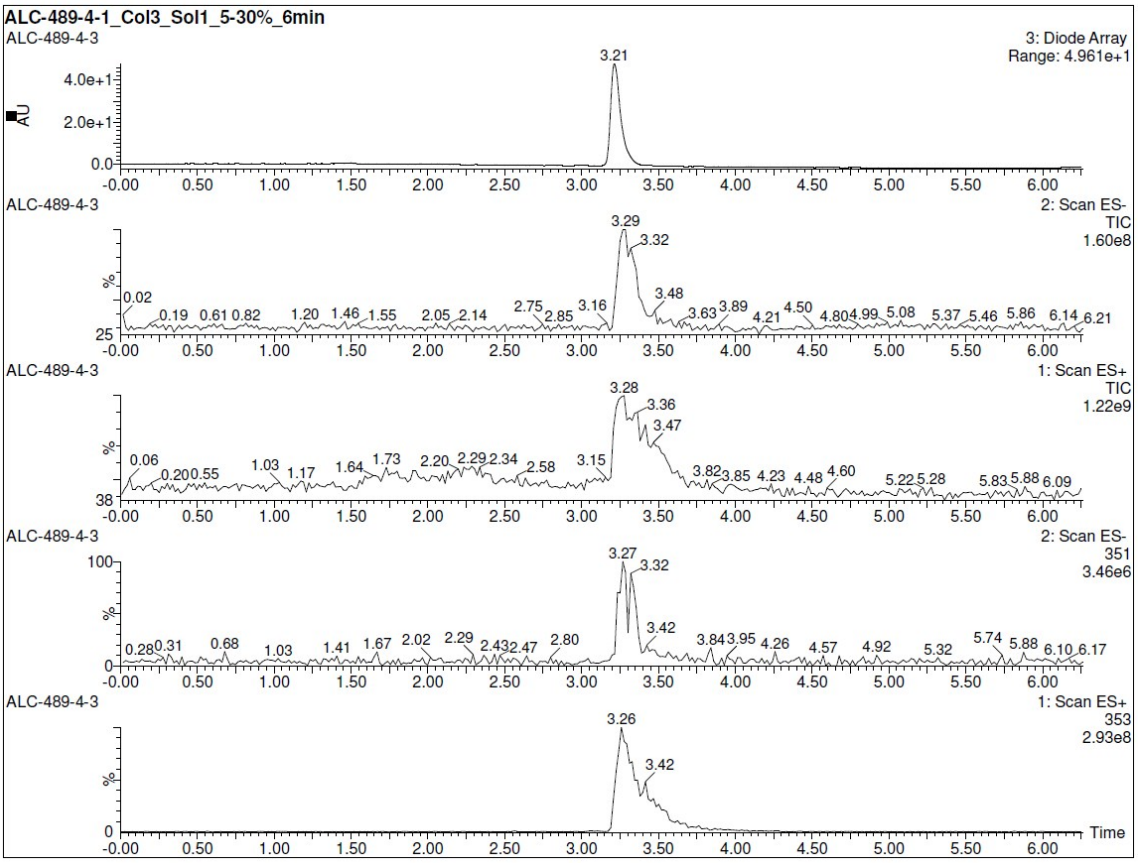

ALC-489-13-3_Col3_Sol1_5-30%_6min
ALC-489-13-3
3: Diode Array
Range: 1.618e+1
AU
1.0e+1
0.0
3.20
1.47
2: Scan ES-
TIC
3.04e8
3.25
3.29
3.39
3.49
1: Scan ES+
TIC
1.79e9
3.22
3.31
3.35
3.49
3.68
2: Scan ES-
335
1.50e7
3.27
3.39
1: Scan ES+
337
2.26e8
3.26
3.42
3.52
Time

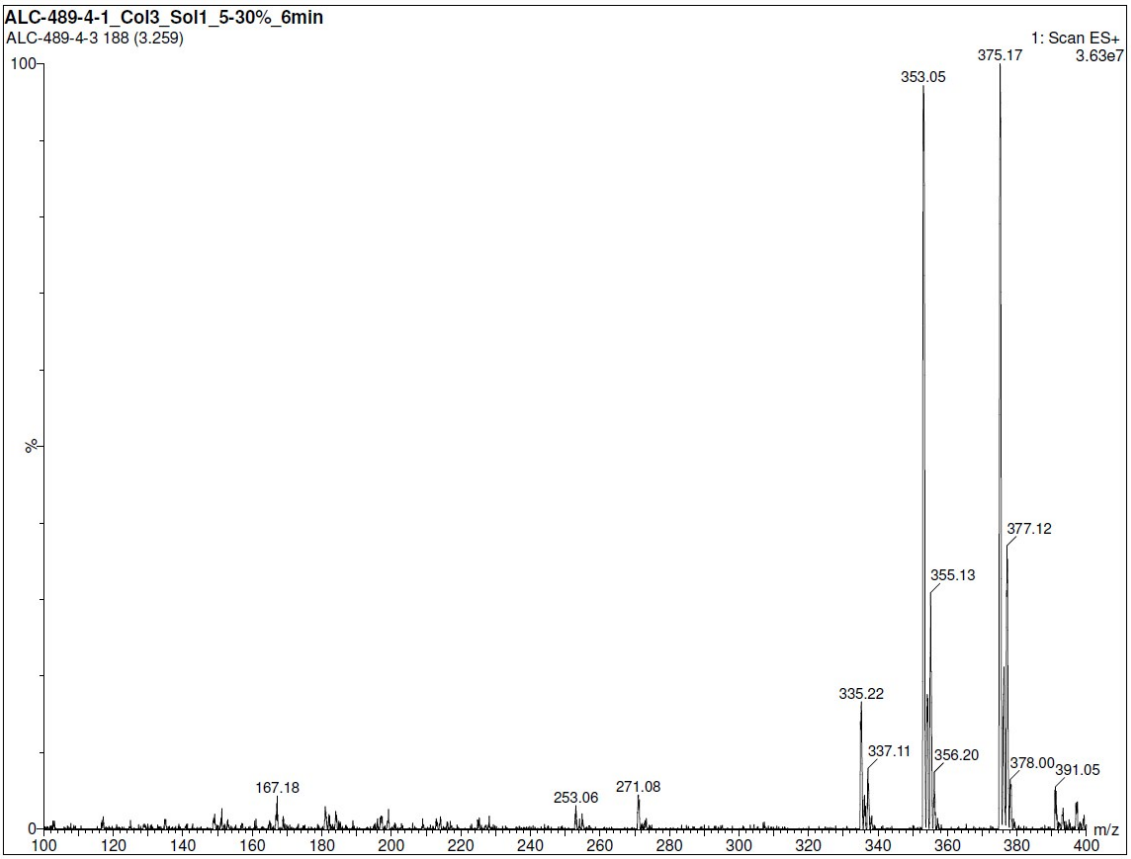

ALC-489-13-3_Col3_Sol1_5-30%_6min
ALC-489-13-3 188 (3.259)
1: Scan ES+
4.01e7
359.04
361.06
358.91
337.05
362.00
340.14
393.00
391.05
396.28
377.19
255.08
181.17
119.98
210.78
m/z

(2-chloro-3,4-dimethoxyphenyl)(1-cyclohexyl-1*H*-tetrazol-5-yl)methanol (3t)

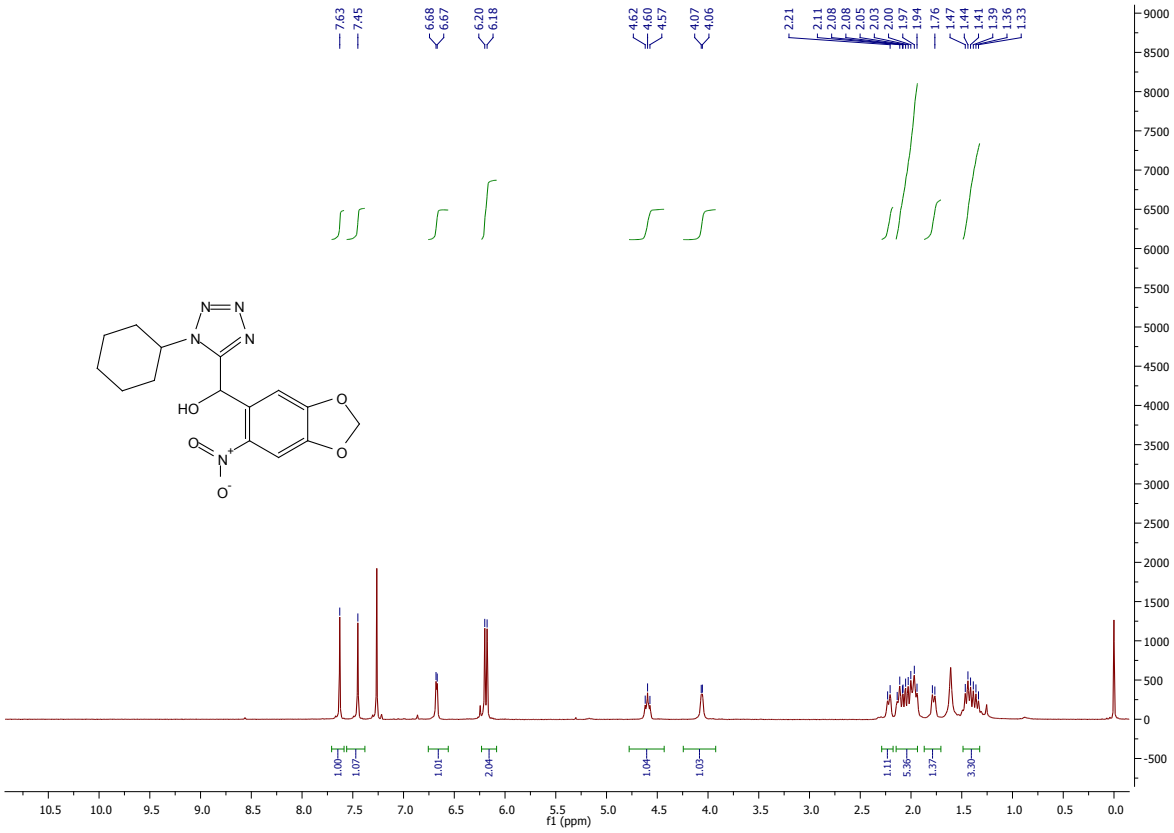


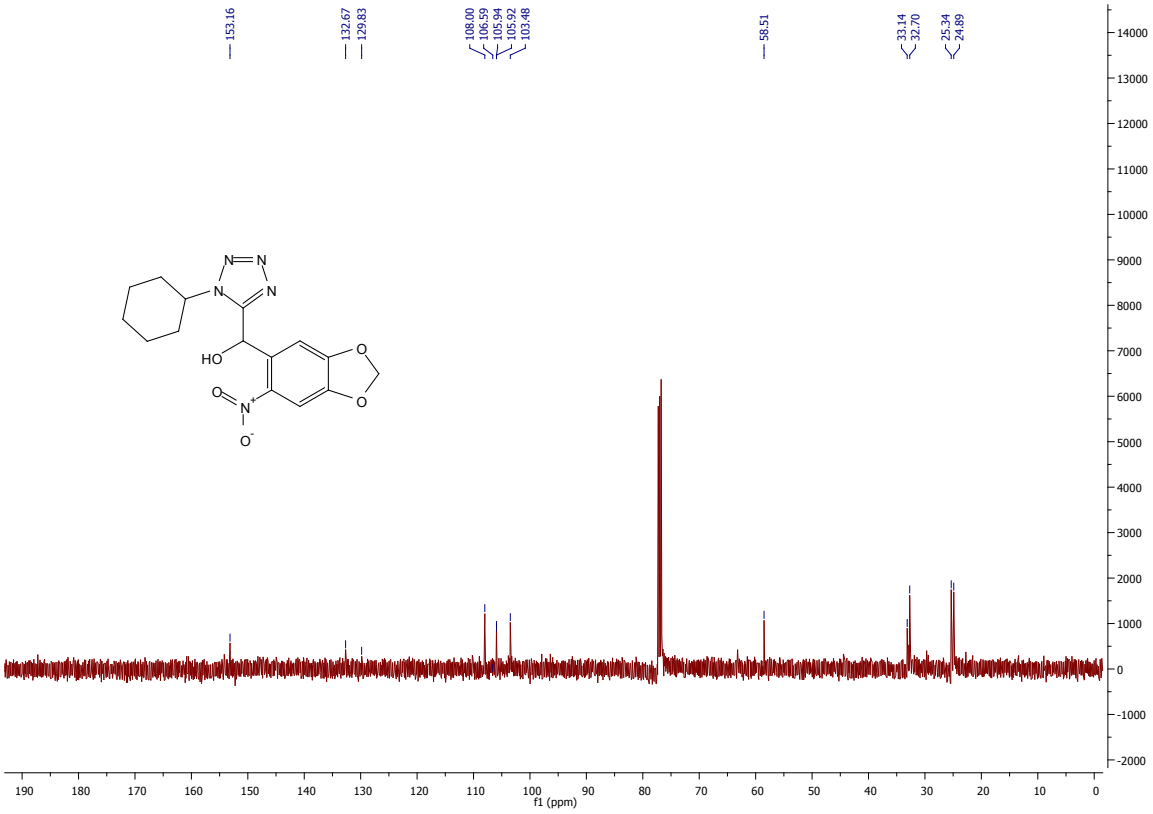


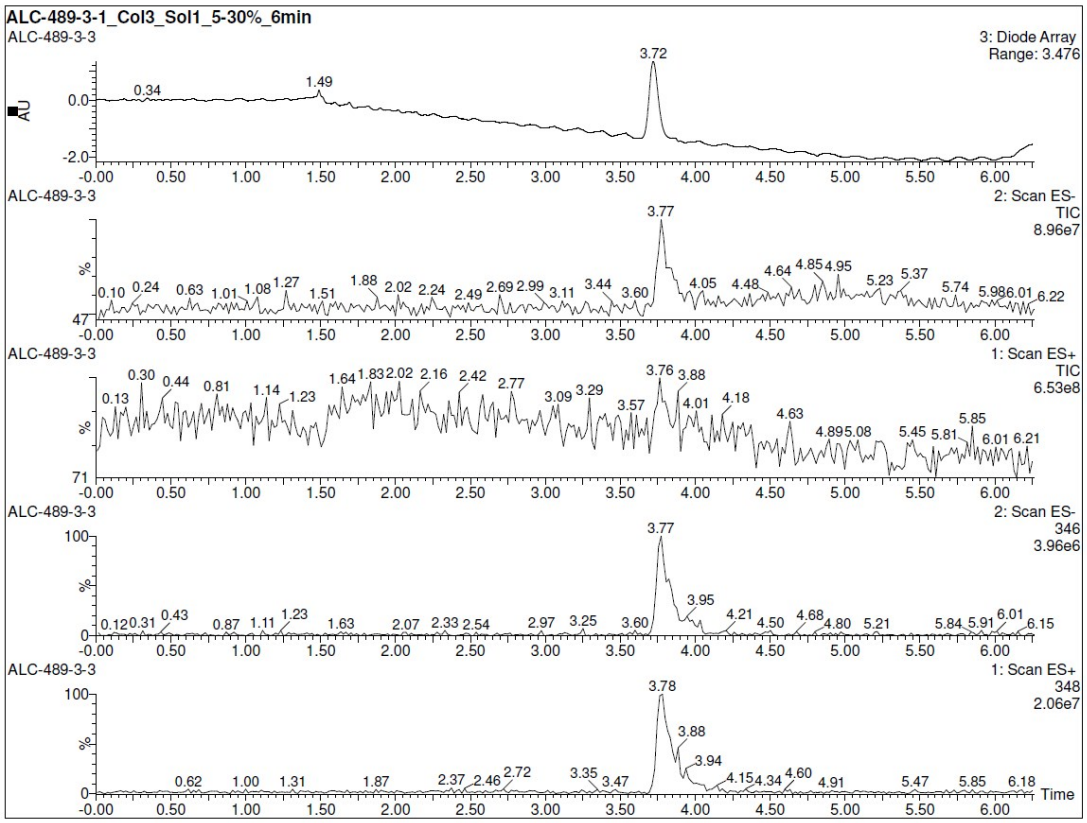

ALC-489-4-1_Col3_Sol1_5-30%_6min
ALC-489-4-3
3: Diode Array
Range: 4.961e+1
AU
2: Scan ES-
TIC
1.60e8
1: Scan ES+
TIC
1.22e9
2: Scan ES-
351
3.46e6
1: Scan ES+
353
2.93e8
Time

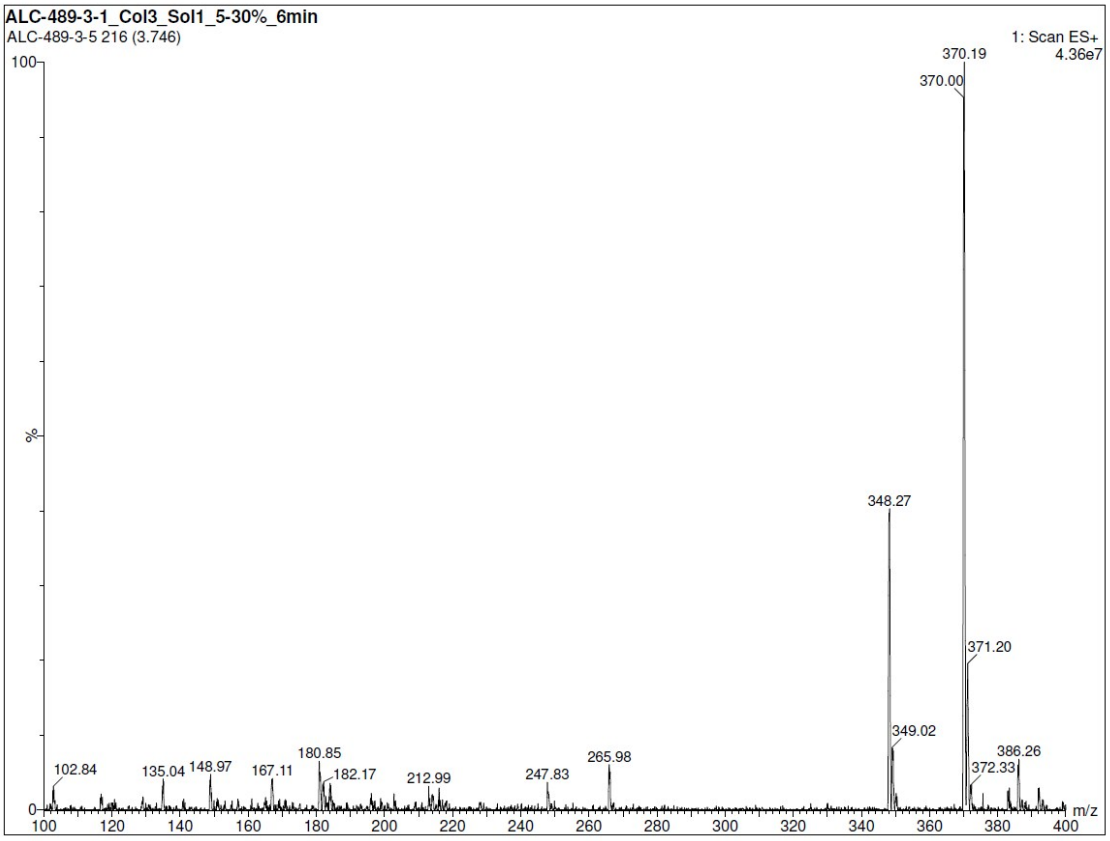

ALC-489-4-1_Col3_Sol1_5-30%_6min
ALC-489-4-3 188 (3.259)
1: Scan ES+
3.63e7
m/z

(1-cyclohexyl-1*H*-tetrazol-5-yl)(6-nitrobenzo[*d*][1,3]dioxol-5-yl)methanol (3u)

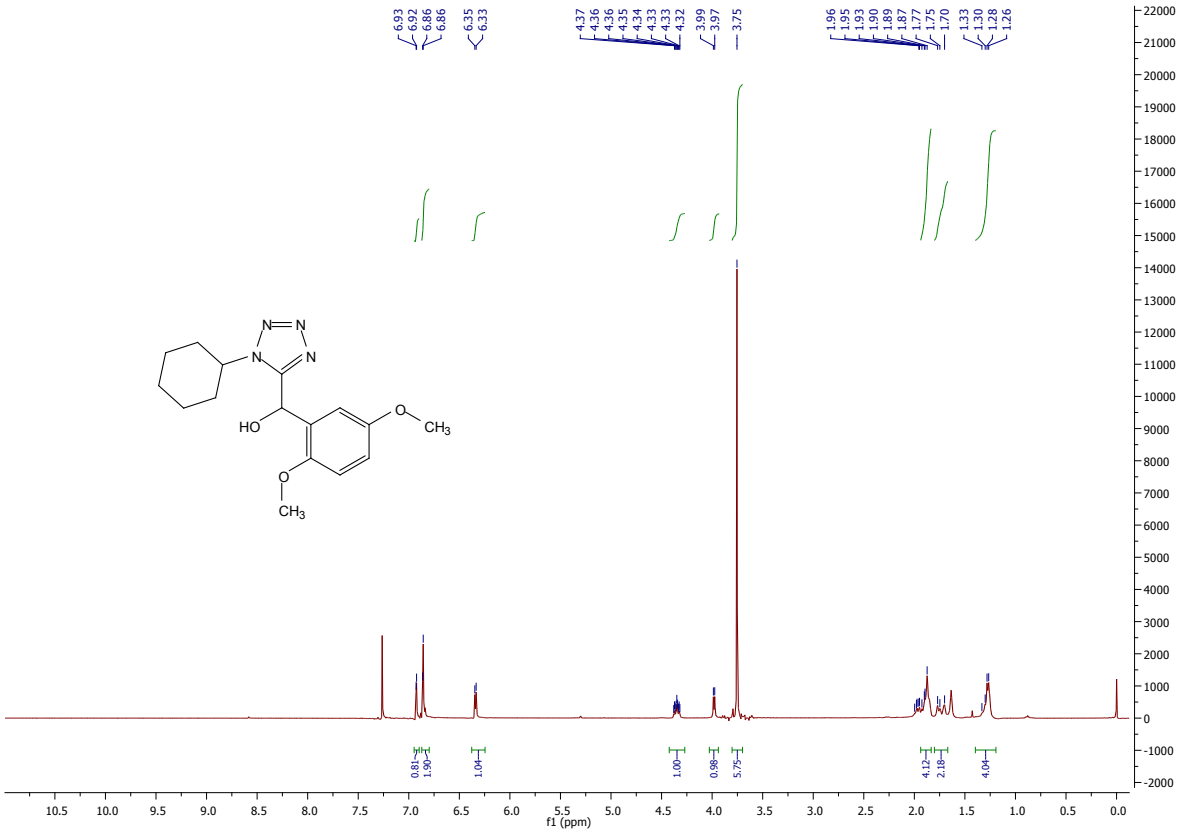


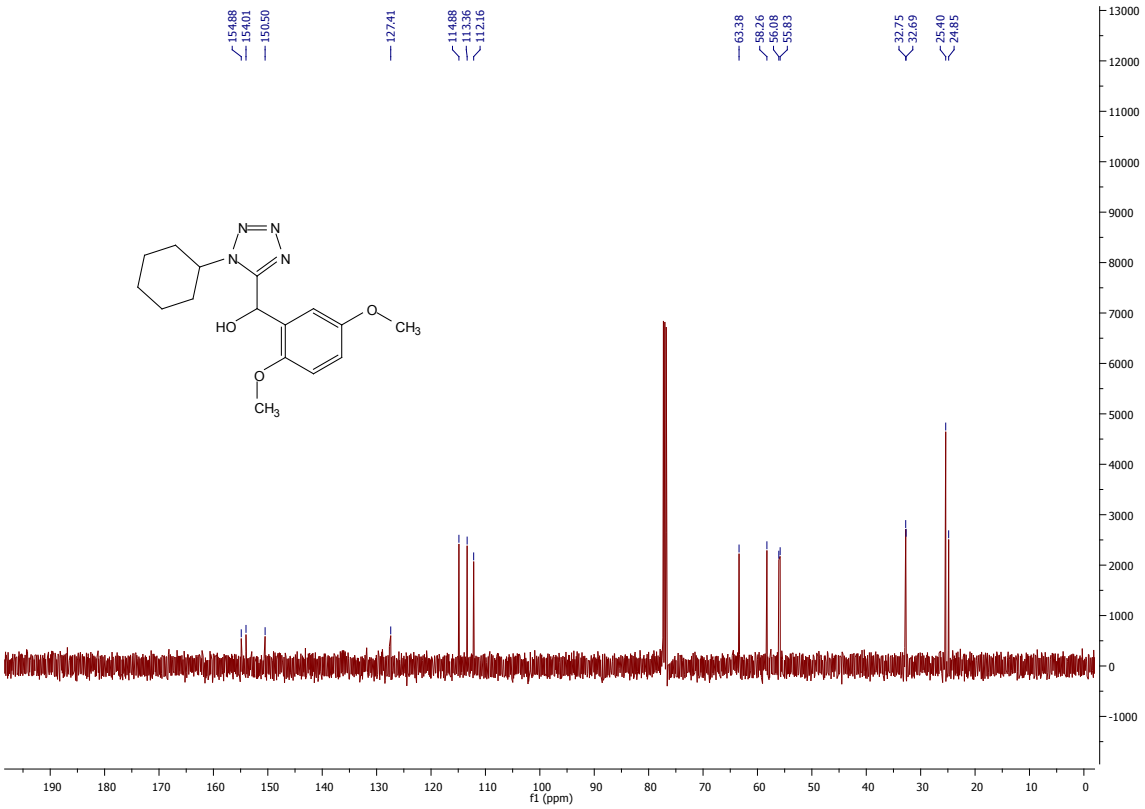


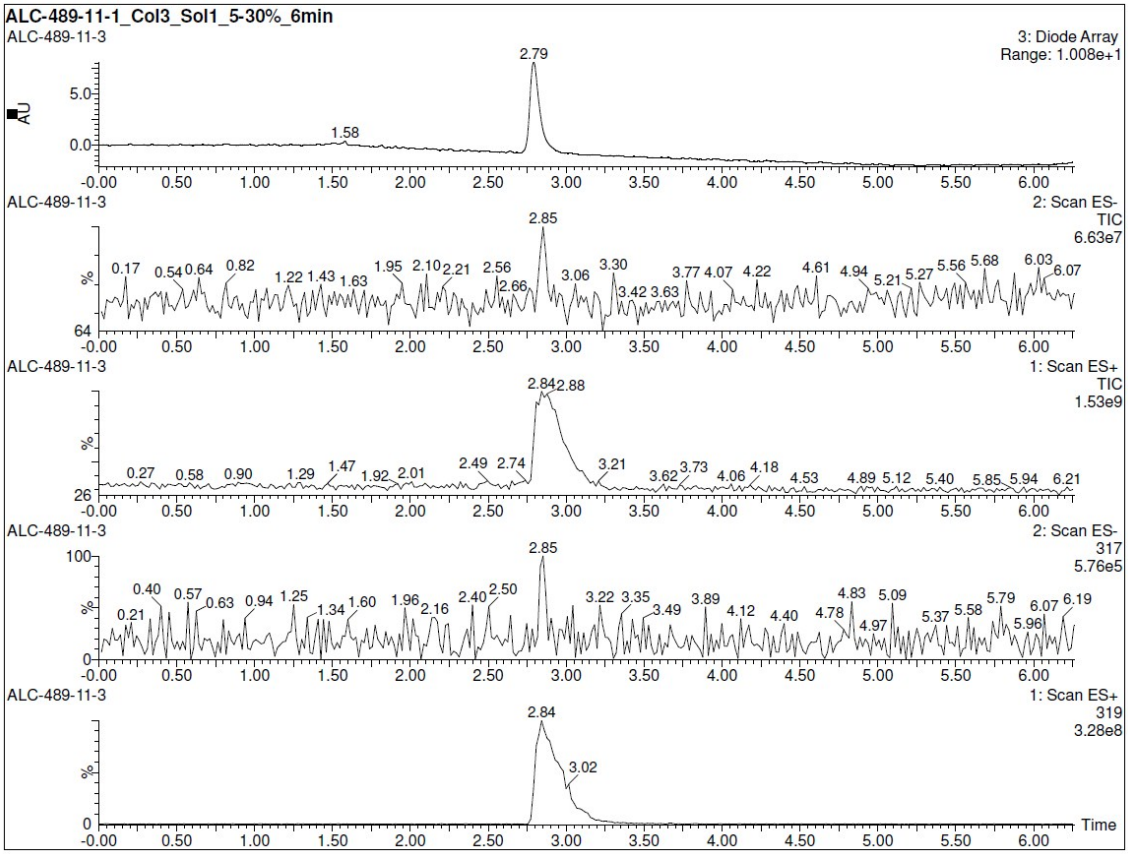

ALC-489-3-1_Col3_Sol1_5-30%_6min
ALC-489-3-3
3: Diode Array
Range: 3.476
AU
2: Scan ES-
TIC
8.96e7
1: Scan ES+
TIC
6.53e8
2: Scan ES-
346
3.96e6
1: Scan ES+
348
2.06e7
Time

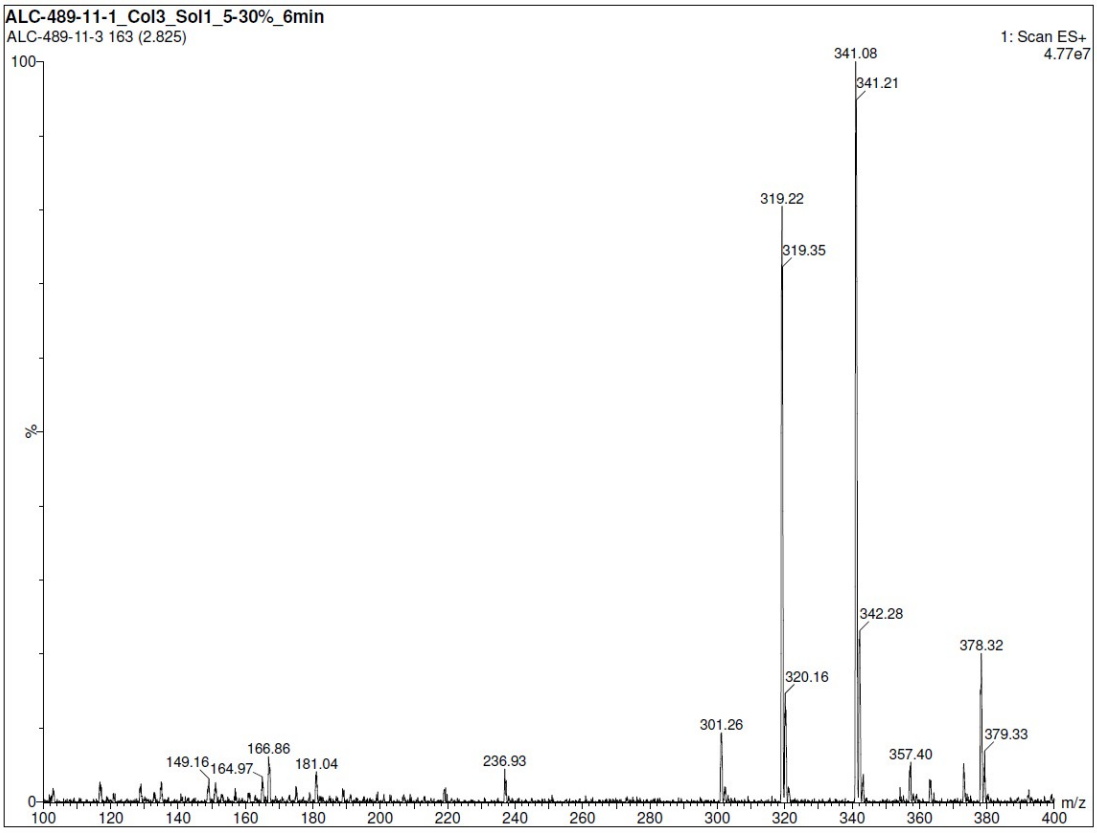

ALC-489-3-1_Col3_Sol1_5-30%_6min
ALC-489-3-5 216 (3.746)
1: Scan ES+
4.36e7
370.19
370.00
348.27
371.20
349.02
386.26
372.33
265.98
180.85
102.84
135.04
148.97
167.11
182.17
212.99
247.83
m/z

(1-cyclohexyl-1*H*-tetrazol-5-yl)(2,5-dimethoxyphenyl)methanol (3v)

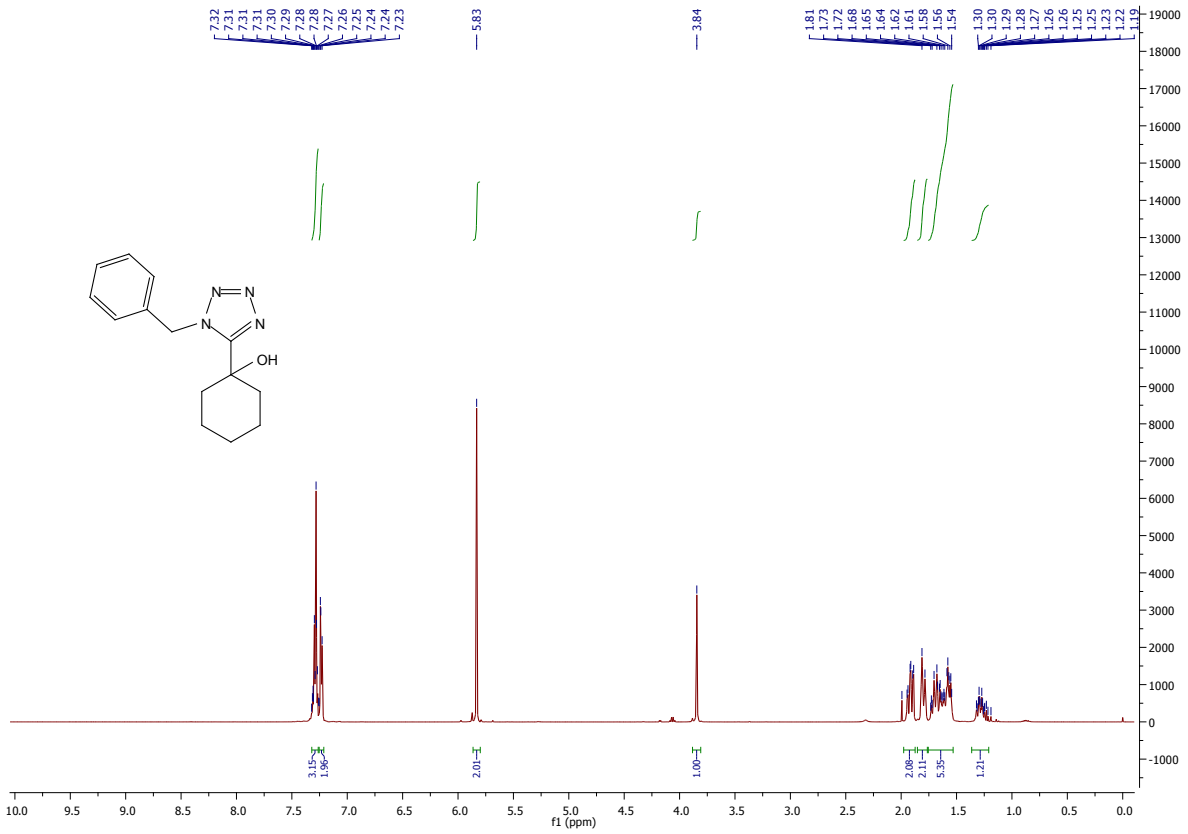


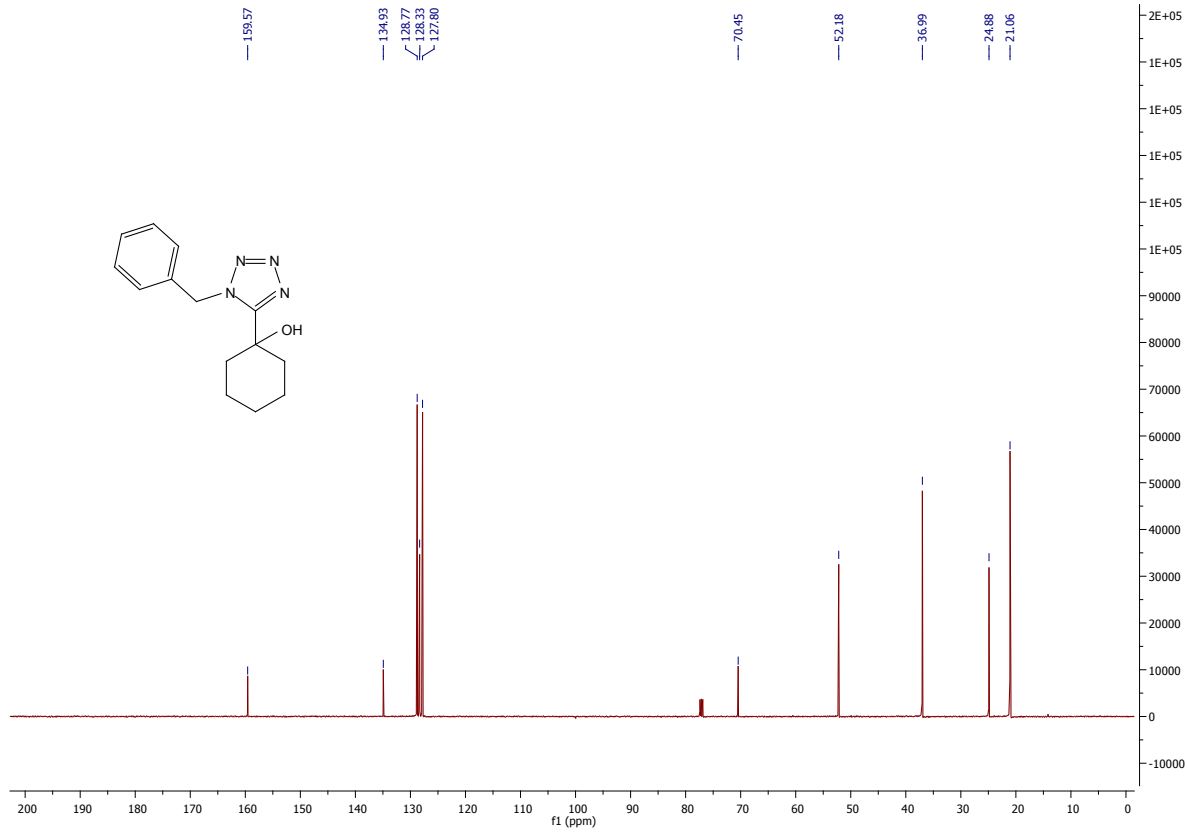


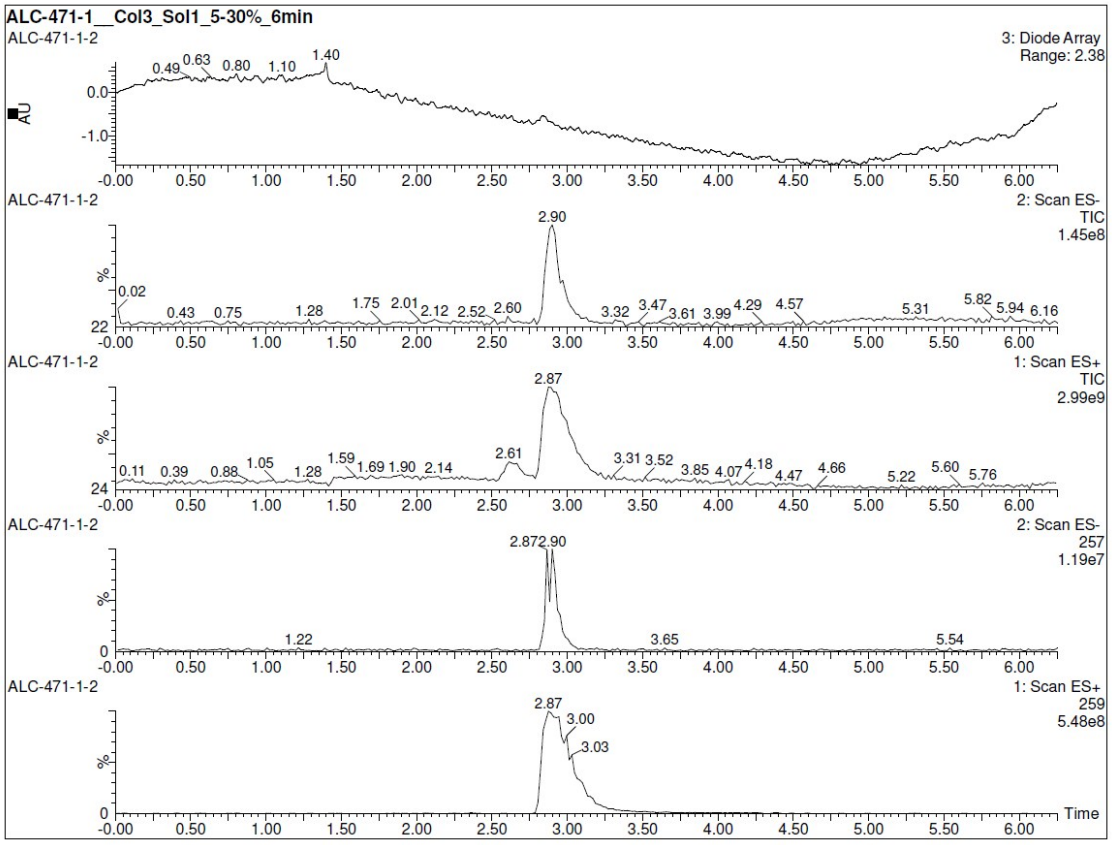

ALC-489-11-1_Col3_Sol1_5-30%_6min
ALC-489-11-3
3: Diode Array
Range: 1.008e+1
AU
2.79
1.58
ALC-489-11-3
2: Scan ES-
TIC
6.63e7
2.85
ALC-489-11-3
1: Scan ES+
TIC
1.53e9
2.84 2.88
ALC-489-11-3
2: Scan ES-
317
5.76e5
2.85
ALC-489-11-3
1: Scan ES+
319
3.28e8
2.84
3.02
Time

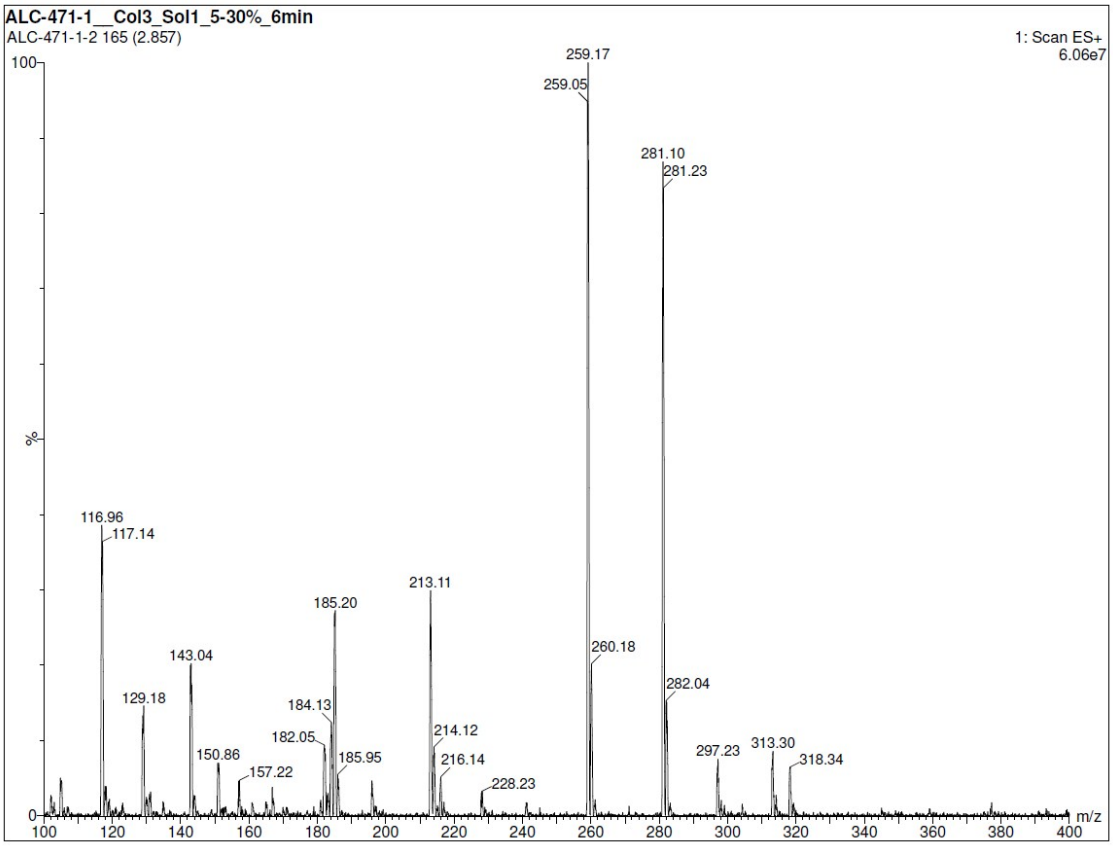

ALC-489-11-1_Col3_Sol1_5-30%_6min
ALC-489-11-3 163 (2.825)
1: Scan ES+
4.77e7
341.08
341.21
319.22
319.35
342.28
378.32
320.16
301.26
379.33
357.40
166.86
149.16
164.97
181.04
236.93
m/z

1-(1-benzyl-1*H*-tetrazol-5-yl)cyclohexanol (3w)

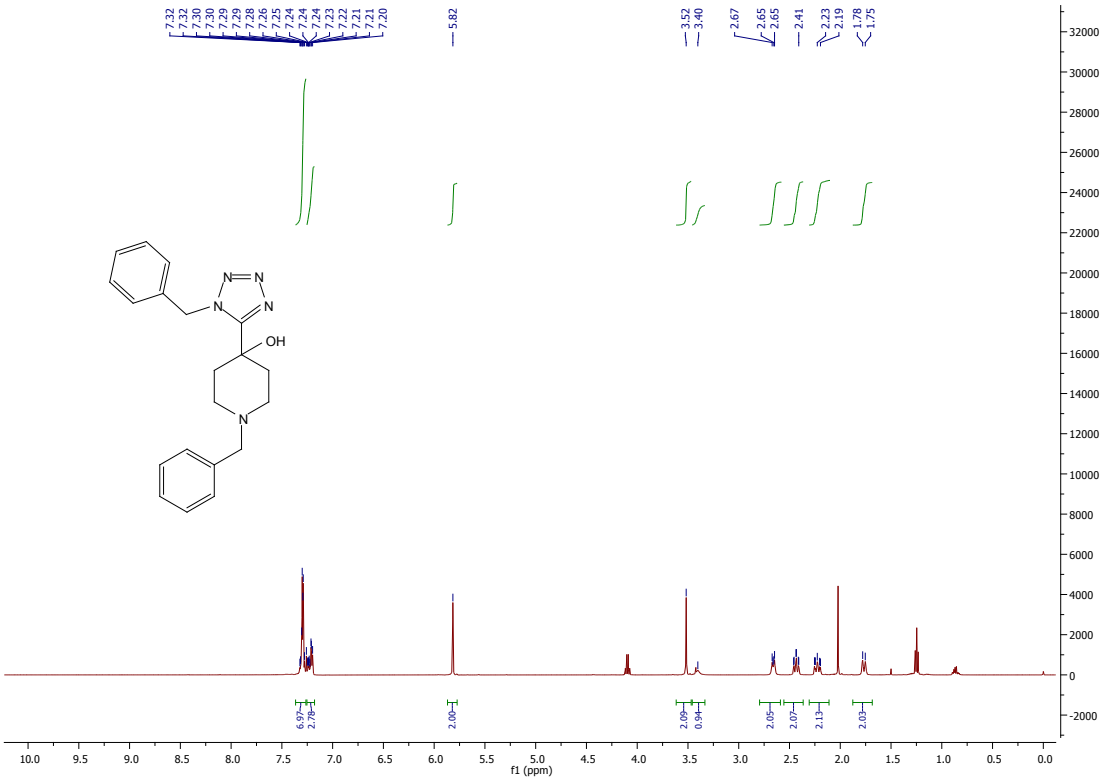


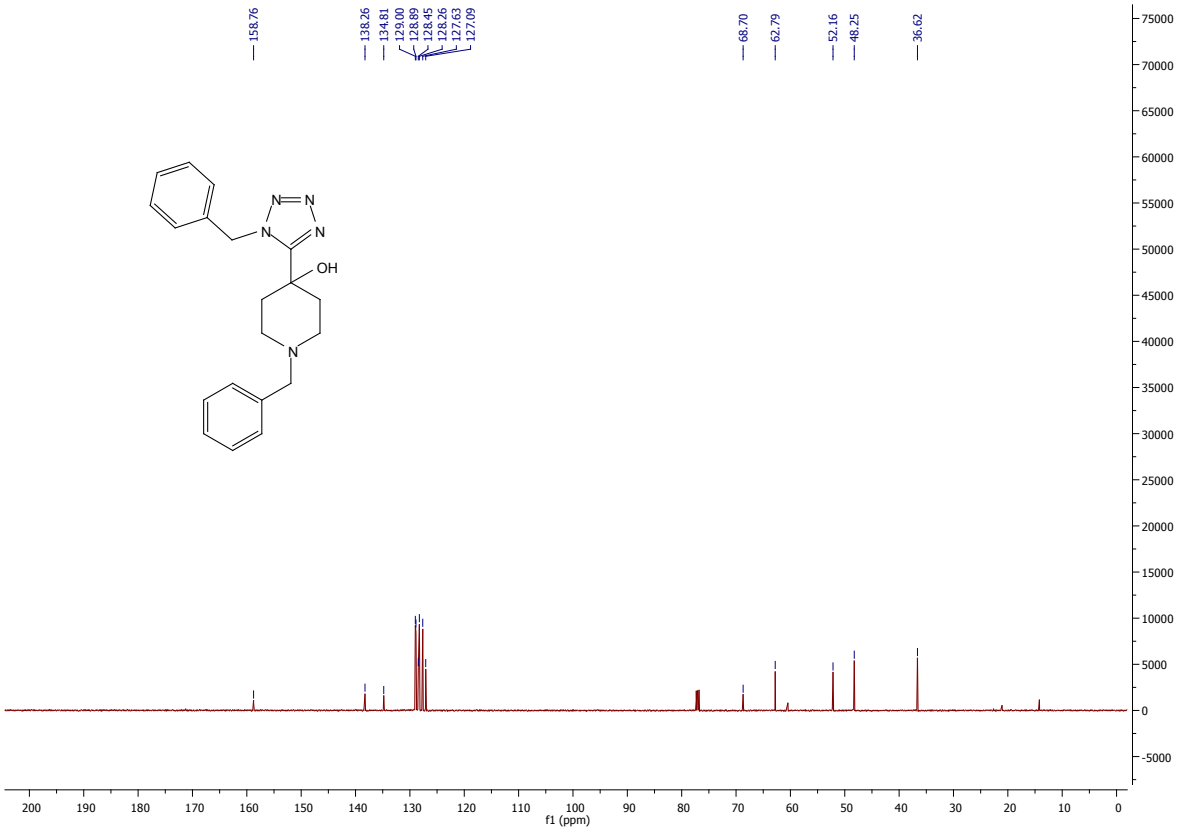


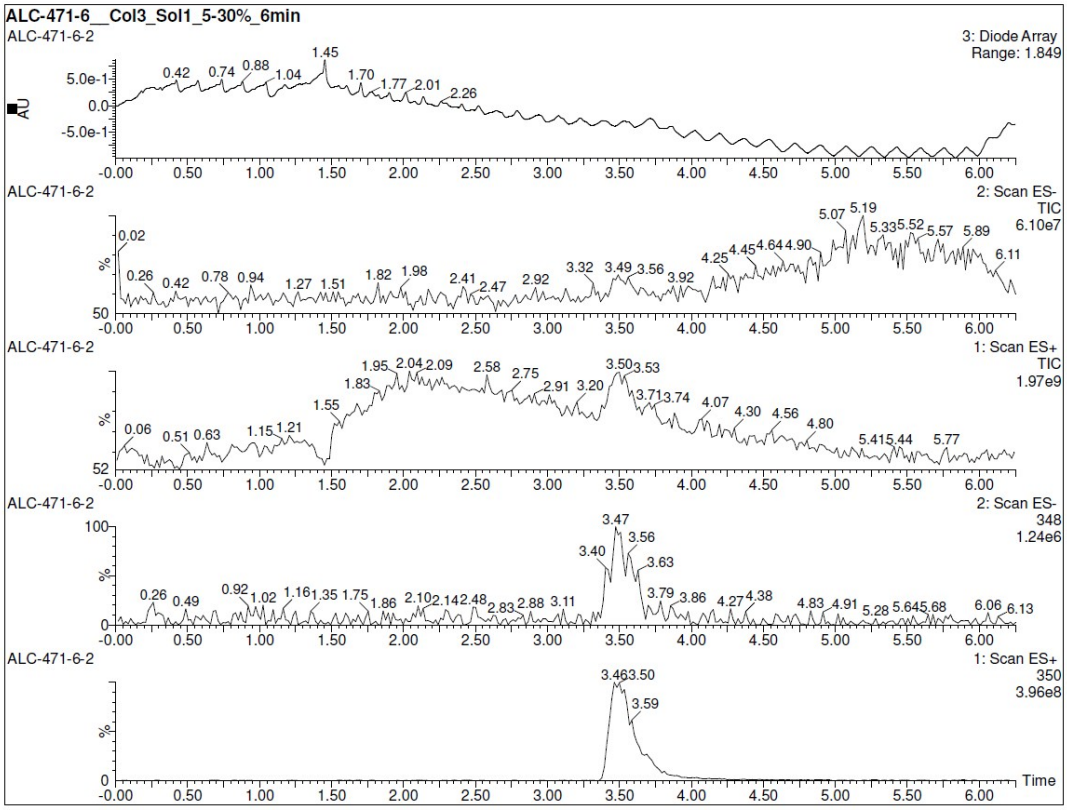

ALC-471-1__Col3_Sol1_5-30%_6min
ALC-471-1-2
3: Diode Array
Range: 2.38
AU
0.49 0.63 0.80 1.10 1.40
ALC-471-1-2
2: Scan ES-
TIC
1.45e8
2.90
ALC-471-1-2
1: Scan ES+
TIC
2.99e9
2.87
ALC-471-1-2
2: Scan ES-
257
1.19e7
2.87 2.90
ALC-471-1-2
1: Scan ES+
259
5.48e8
2.87 3.00 3.03
Time

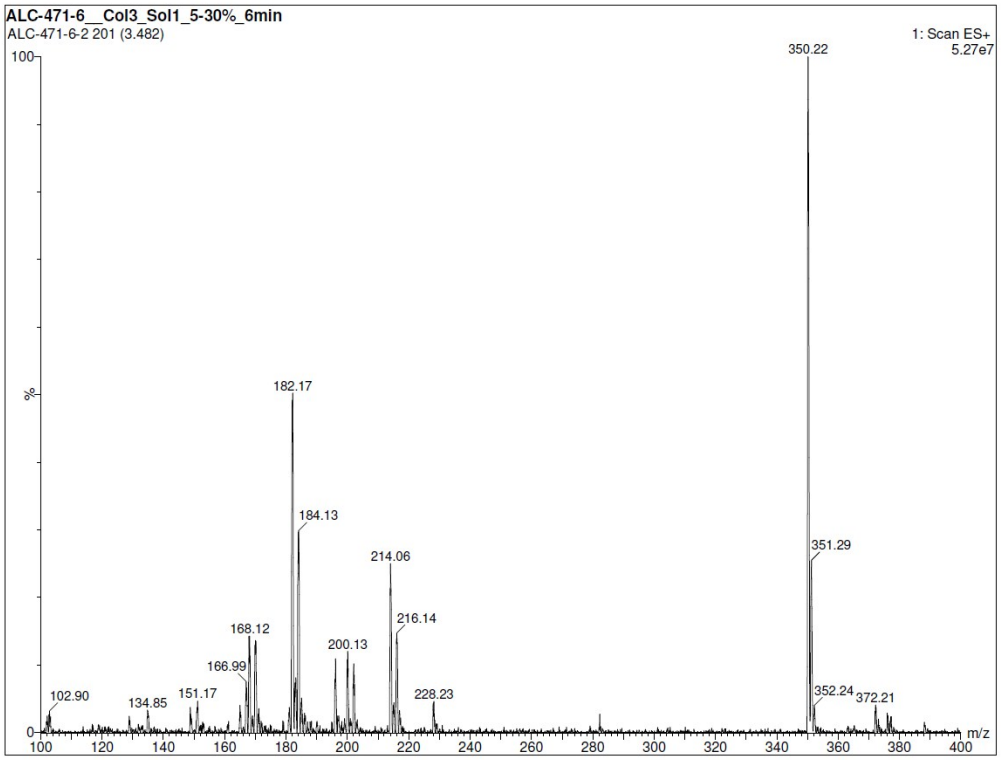

ALC-471-1__Col3_Sol1_5-30%_6min
ALC-471-1-2 165 (2.857)
1: Scan ES+
6.06e7
259.17
259.05
281.10
281.23
116.96
117.14
213.11
185.20
143.04
260.18
129.18
282.04
184.13
214.12
182.05
150.86
185.95
216.14
157.22
228.23
297.23
313.30
318.34
m/z

1-benzyl-4-(1-benzyl-1*H*-tetrazol-5-yl)piperidin-4-ol (3x)

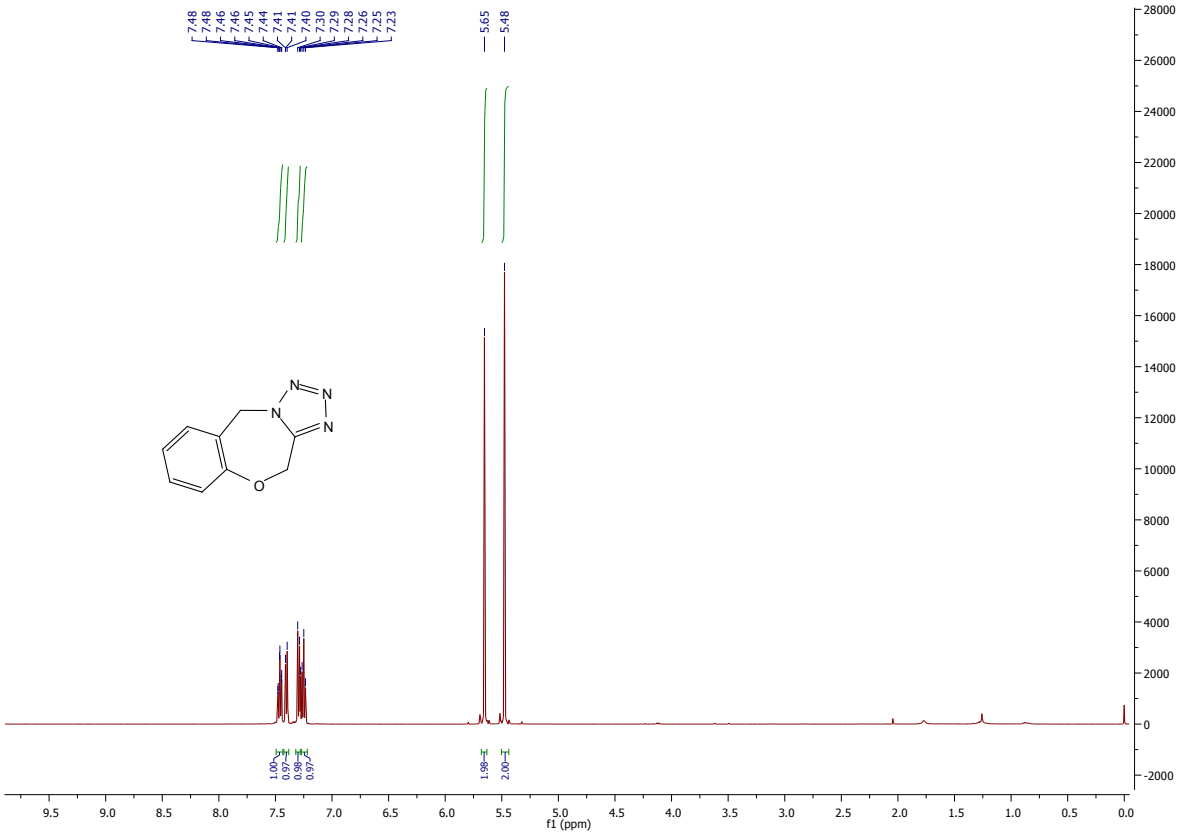


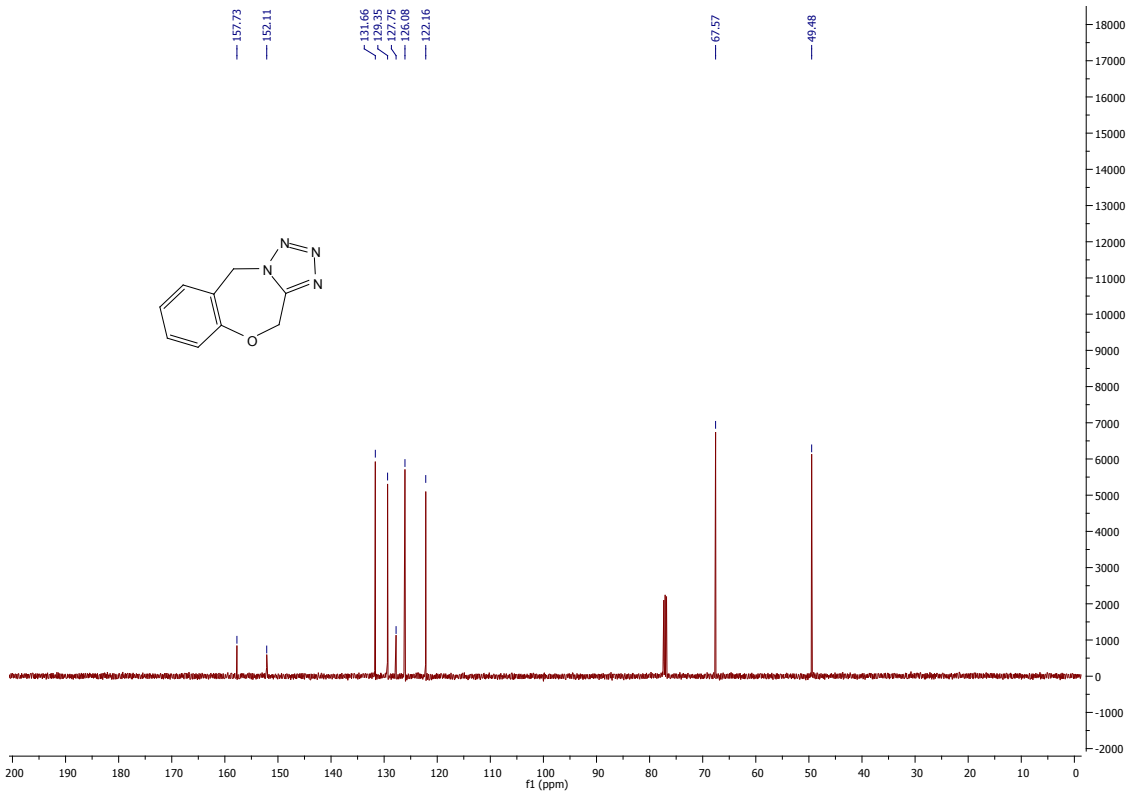


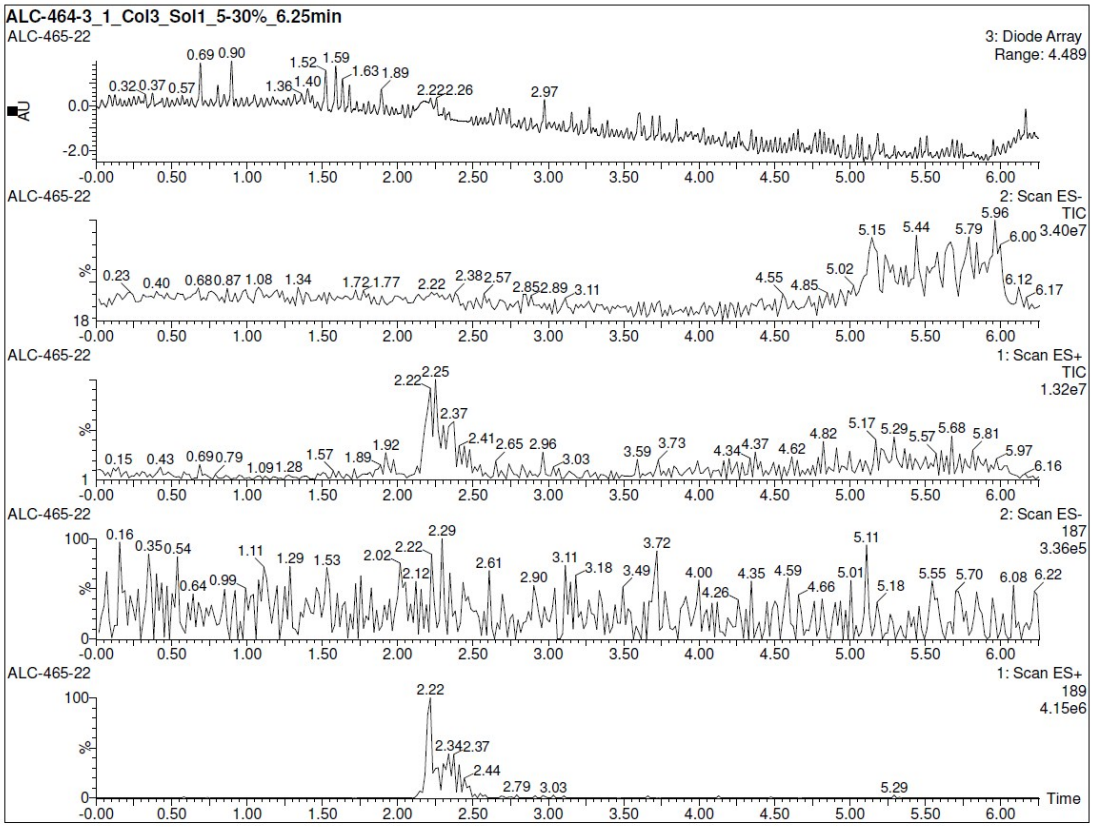

ALC-471-6__Col3_Sol1_5-30%_6min
ALC-471-6-2
3: Diode Array
Range: 1.849
AU
ALC-471-6-2
2: Scan ES-
TIC
6.10e7
ALC-471-6-2
1: Scan ES+
TIC
1.97e9
ALC-471-6-2
2: Scan ES-
348
1.24e6
ALC-471-6-2
1: Scan ES+
350
3.96e8
Time

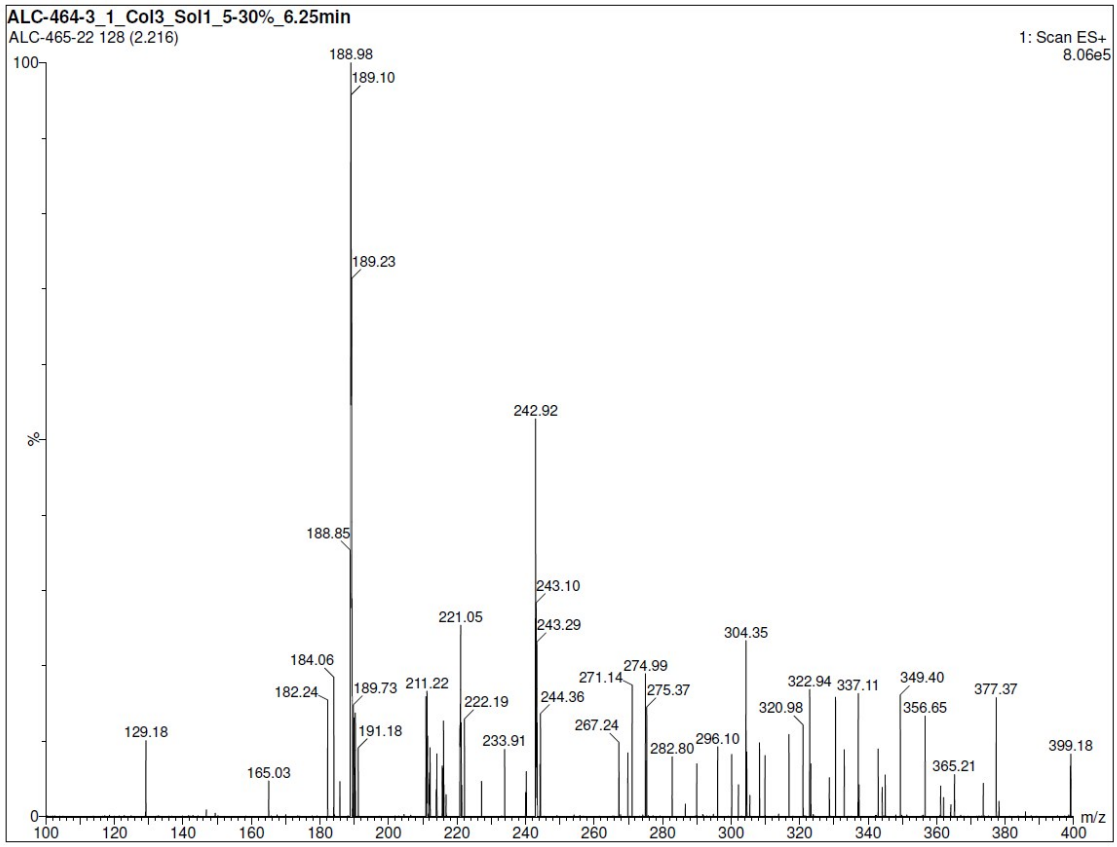

ALC-471-6__Col3_Sol1_5-30%_6min
ALC-471-6-2 201 (3.482)
1: Scan ES+
5.27e7
%
m/z

5,11-dihydrobenzo[*f*]tetrazolo[5,1-*c*][1,4]oxazepine (4)






ALC-464-3_1_Col3_Sol1_5-30%_6.25min
ALC-465-22
3: Diode Array
Range: 4.489
AU
ALC-465-22
2: Scan ES-
TIC
3.40e7
ALC-465-22
1: Scan ES+
TIC
1.32e7
ALC-465-22
2: Scan ES-
187
3.36e5
ALC-465-22
1: Scan ES+
189
4.15e6
Time


ALC-464-3_1_Col3_Sol1_5-30%_6.25min
ALC-465-22 128 (2.216)
1: Scan ES+
8.06e5
%
m/z