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Supporting Information

$RuCl_2(PPh_3)_3$-Catalyzed Chemoselective Hydrogenation of β, δ-Diketo Acid Derivatives at the β-Carbonyls

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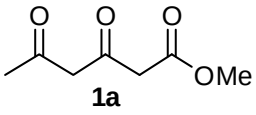
General and Materials

General: All reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques unless otherwise noted. ^{1}H NMR, ^{13}C NMR, ^{19}F spectra were obtained on a 400 MHz NMR spectrometer. The chemical shifts for ^{1}H NMR were recorded in ppm downfield from tetramethylsilane (TMS) with the solvent resonance as the internal standard. The chemical shifts for ^{13}C NMR were recorded in ppm downfield using the central peak of $CDCl_3$ (77.00 ppm) as the internal standard. Coupling constants (*J*) are reported in Hz and refer to apparent peak multiplications. Flash column chromatography was performed on silica gel (300-400 mesh).

Materials: Commercially available reagents were used throughout without further purification other than those detailed below. The solvents used in catalyst preparation and hydrogenation reactions were pretreated by the following procedures: THF was distilled over sodium benzopheneone ketyl under nitrogen.

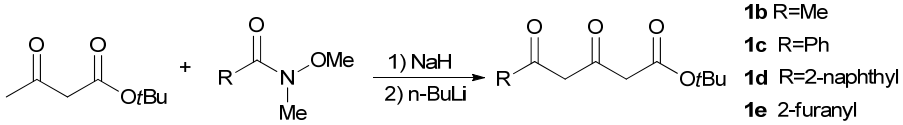
1. Preparation of 1a-t



1a

Methyl 3, 5-dioxohexanoate

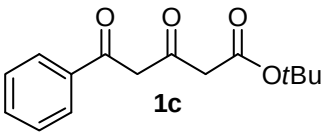
1a was prepared according to the literature[1]. Mixture of enol and keto forms: ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.61 (s, 0.69H), 3.74 (s, 3H), 3.57(s, 0.16H), 3.34 (s, 1.58H), 2.27(s, 0.14), 2.26 (s, 0.28H), 2.08 (s, 2.23H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 187.0, 167.9, 100.4, 57.1, 52.3, 49.0, 44.7, 24.2.



1b R=Me
1c R=Ph
1d R=2-naphthyl
1e 2-furanyl

tert-Butyl 3, 5-dioxohexanoate (1b)[2]: tert-Butyl acetoacetate (20 g, 126.4 mmol) was added dropwise to a suspension of NaH (60% dispersion in mineral oil, 5.6 g, 139.1 mmol) in 200 mL of anhydrous THF at 0 °C. The mixture was stirred for an additional 10 min. The clear solution was cooled to -10 °C, and *n*-BuLi (58 mL, 2.4 M in hexane) was added dropwise. After stirring for an additional 30 min at this temperature, *N*-methoxy-*N*-methylacetamide (14.4 g, 139.1 mmol) was added dropwise at -40°C. Then the mixture was warmed to room temperature within 2 h and quenched with 10% aqueous HCl to pH=3-4. The solvent was roto-evaporated for the sake of better extraction. The residue and aqueous phase was combined and extracted with EtOAc three times, washed with aq. $NaHCO_3$, brine and dried over Na_2SO_4. Flash column chromatography (PE/EA=15/1) to give **1b** (24.1 g, 95% yield) as colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.60 (s, 0.73H), 3.74-3.71 (m, 0.26H), 3.47-3.44 (m, 1H), 3.24 (s, 2H), 2.25 (s, 1H), 2.07 (s, 2H), 1.47 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 187.5, 166.6, 100.3, 81.7, 57.1, 50.6, 46.1, 27.8, 24.2.

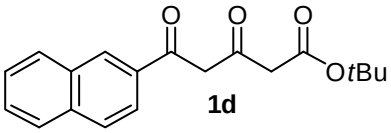
1c-d were prepared by the same procedure as **1b** with the corresponding *N*-methoxy-*N*-methyl-2-naphthamide[3] and *N*-methoxy-*N*-methylfuran-2-carboxamide[4].



1c

***tert*-butyl 3, 5-dioxo-5-phenylpentanoate**[5]

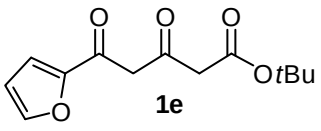
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (ddd, *J* = 7.0, 2.4, 1.0 Hz, 2H), 7.60-7.40 (m, 3H), 6.28 (s, 0.92H), 4.29-4.24 (m, 0.12H), 3.57-3.54 (m, 0.13H), 3.39 (s, 2.07H), 1.51-1.46 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 182.3, 166.6, 134.0, 132.4, 128.6, 128.5, 128.4, 126.9, 96.5, 81.8, 52.9, 50.4, 47.0, 27.8.



1d

***tert*-butyl-(naphthalen-2-yl)-3, 5-dioxopentanoate**

Thick oil, solidified upon cooling. ^{1}H NMR (400 MHz, $CDCl_3$) 8.40 (s, 1H), 7.95-7.72 (m, 4H), 7.60-7.40 (m, 2H), 6.40 (s, 1H), 3.41 (s, 2H), 1.49 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.6, 182.2, 166.7, 135.8, 132.5, 131.3, 129.2, 128.3, 128.2, 128.1, 127.6, 126.7, 122.8, 96.9, 81.9, 47.1, 27.9. HRMS Calculated for $C_{19}H_{20}O_4$ (M+Na): 355.1259, found: 355.1266.



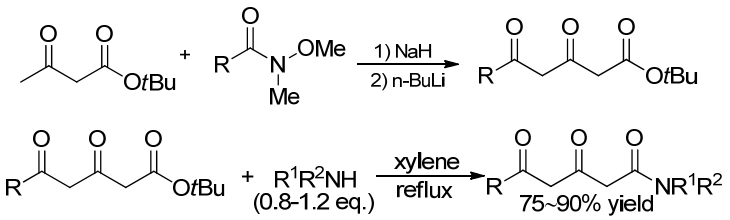
1e

***tert*-butyl 5-(furan-2-yl)-3,5-dioxopentanoate**

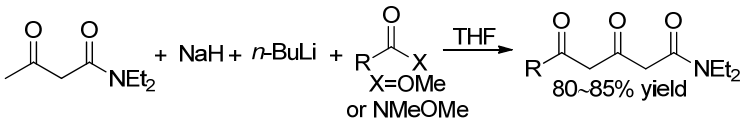
Light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 1.7, 0.7 Hz, 1H), 7.17 (dd, *J* = 3.6, 0.7 Hz, 1H), 6.55 (dd, *J* = 3.6, 1.7 Hz, 1H), 6.18 (s, 1H), 4.11 (s, 1H), 3.54 (s, 1H), 3.33 (d, *J* = 1.0 Hz, 2H), 1.48 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.6, 175.0, 166.6, 149.8, 147.1, 146.2, 118.6, 116.0, 112.7, 112.5, 96.2, 81.9, 52.8, 50.6, 45.8, 27.8. HRMS Calculated for $C_{13}H_{16}O_5$ (M+Na): 275.0895, found: 275.0898.

1f-s were prepared by either of the following route. The 3, 5-diketo tert-butyl esters were prepared by the same procedure as **1b-c**. The Weinreb amides were prepared according to the literature.[3-4, 6] The amminolysis was carried out according to the procedure in the literature.[7]

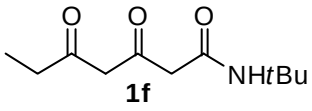
Route A:



Route B:



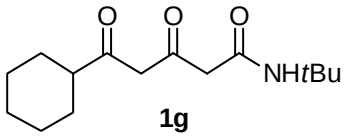
1f: R=Et, R^1=H, R^2=*t*Bu
1g:R=Cy, R^1 =H, R^2=*t*Bu
1h:R=Me R^1, R^2=-$(CH_2)_2O(CH_2)_2$-
1i: R=*t*Bu, R^1, R^2=-$(CH_2)_2O(CH_2)_2$-
1j: R=Et, R^1, R^2=-$(CH_2)_2O(CH_2)_2$-
1k: R=Me, R^1= R^2=Bn
1l: R=Ph$(CH_2)_2$, R^1= R^2=Et
1m: R=Ph, R^1= R^2=Et
1n: R=2-MeC_6H_5, R^1= R^2=Et
1o:R=3-ClC_6H_5, R^1= R^2=Et
1p:R=4-MeOC_6H_5, R^1= R^2=Et
1q:R=4-$CF_3C_6H_5$, R^1= R^2=Et
1r:R=1-Naphthyl, R^1= R^2=Et
1s:R=2-Thienyl, R^1= R^2=Et



1f

***N*-(tert-butyl)-3, 5-dioxoheptanamide**

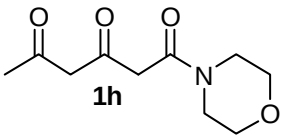
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.42 (s, 1H), 5.60 (s, 0.73H), 3.72 (s, 0.29H), 3.38 (s, 0.28H), 3.18 (s, 1.69H), 2.54 (q, *J* = 7.3 Hz, 0.31H), 2.34 (q, *J* = 7.5 Hz, 1.62H), 1.34 (s, 9H), 1.14 (t, *J* = 7.5 Hz, 2.37H), 1.07 (t, *J* = 7.3 Hz, 0.59H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 193.7, 190.0, 165.1, 99.3, 56.1, 51.4, 51.1, 47.4, 36.8, 30.5, 28.6, 28.3, 9.40, 7.2. HRMS Calculated for $C_{11}H_{19}NO_3$ (M+Na): 236.1263, found: 236.1272.



1g

***N*-(tert-butyl)-5-cyclohexyl-3, 5-dioxopentanamide**

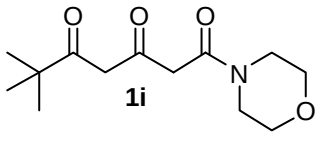
Yellow oil, solidified upon cooling. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.49 (s, 1H), 5.58 (s, 0.9H), 3.75 (s, 0.19H), 3.37 (s, 0.21H), 3.19 (s, 1.65H), 2.25 – 2.08 (m, 1H), 1.96 – 1.65 (m, 5H), 1.35 (s, 9H), 1.45 – 1.12 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 195.3, 191.5, 165.2, 98.1, 54.4, 51.4, 51.0, 47.6, 45.4, 29.2, 28.3, 27.8, 25.5, 25.4, 25.2. HRMS Calculated for $C_{15}H_{25}NO_3$ (M+Na): 290.1732, found: 290.1736.



1h

1-morpholinohexane-1, 3, 5-trione

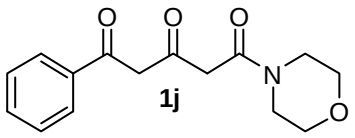
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.65 (s, 0.66H), 3.64-3.58 (m, 6H), 3.50-3.41 (m, 2H), 3.41 (s, 2.25H), 2.26 (s, 0.77H), 2.04 (s, 2.22H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.2, 198.1, 189.4, 188.4, 165.0, 164.7, 99.8, 88.0, 66.2, 66.12, 56.7, 50.4, 48.6, 46.4, 46.2, 44.7, 41.9, 41.7, 30.4, 23.4. HRMS Calculated for $C_{10}H_{15}NO_4$ (M+Na): 236.0899, found: 236.0893.



1i

6, 6-dimethyl-1-morpholinoheptane-1,3,5-trione

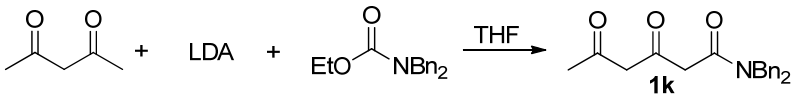
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.72 (s, 1H), 3.81 (s, 0.37H), 3.61-3.70 (m, 6H), 3.55 – 3.50 (m, 2H), 3.47 (s, 2H), 1.17 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.90, 198.1, 190.2, 165.1, 95.3, 66.2, 66.2, 50.5, 49.0, 46.5, 46.3, 45.0, 41.9, 41.7, 38.2, 26.8, 25.7, 25.6. HRMS Calculated for $C_{13}H_{21}NO_4$ (M+H): 256.1549, found: 256.1535.



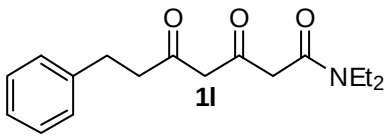
1-morpholino-5-phenylpentane-1, 3, 5-trione

Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.84 (m, 2H), 7.57-7.42 (m, 3H), 6.33 (s, 0.91H), 4.29 (s, 0.20H), 3.75 (s, 0.21H), 3.72-3.65 (m, 6H), 3.59 (s, 1.85H), 3.59-3.54 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 181.2, 165.1, 133.8, 133.4, 132.4, 128.6, 128.4, 128.2, 126.8, 96.2, 66.4, 66.3, 52.6, 48.9, 46.6, 46.4, 45.8, 42.1, 41.8. HRMS Calculated for $C_{15}H_{17}NO_4$ (M+H): 276.1236, found: 276.1237.

1k was prepared by the procedure reported in the literature[8]

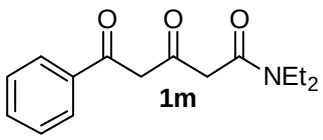


2, 4-Pentadione (5.1 g, 50 mmol) was added dropwise to a solution of LDA (100 mmol) (prepared from 10.6 g of $^{i}Pr_2NH$ and 42 mL of 2.4 M *n*-BuLi) in 80 mL of THF at -78°C during half an hour. Then warmed to -20°C, ethyl dibenzylcarbamate[9] (13.5 g, 50 mmol) was added dropwise. The mixture was warmed to room temperature and stirred overnight. The solvent was evaporated. The residue was dissolved in 30 mL water and washed with 20 mL Et_2O to remove the remained 2, 4-pentadione. The water phase was acidified with cold 10% HCl to pH=2-3 and extracted with EtOAc, washed with brine and dried over Na_2SO_4. Flash column chromatography (PE/EA=4/1) to give **1k** (10.5 g, 65% yield) as thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.12 (m, 10H), 5.65 (s, 0.7H), 5.30-5.27 (m, 0.19H), 4.63 (s, 2H), 4.49 (s, 2H), 3.78 (s, 0.29H), 3.71 (s, 0.30H), 3.51 (s, 1.59H), 3.24 (s, 0.25H), 2.24 (d, J = 2.0 Hz, 0.77H), 2.05 (s, 2.23H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 202.2, 198.4, 189.4, 188.8, 172.0, 170.9, 167.5, 167.2, 136.6, 135.8, 128.8, 128.4, 128.0, 127.9, 127.6, 127.3, 126.4, 126.2, 100.2, 89.0, 57.1, 50.8, 50.4, 49.6, 48.8, 48.2, 48.1, 47.7, 45.0, 30.6, 29.5, 23.8. HRMS Calculated for $C_{20}H_{21}NO_3$ (M+Na): 346.1419, found: 346.1423.



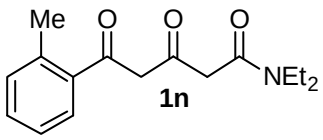
***N*, *N*-diethyl-3, 5-dioxo-7-phenylheptanamide**

Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.08 (m, 5H), 5.65 (s, 0.55H), 5.11 (s, 0.13H), 3.76 (s, 0.35H), 3.38 (s, 1.79H), 3.41-3.23 (m, 4H), 2.96-2.84 (m, 2H), 2.62-2.58 (m, 1.43H), 2.28 (s, 0.31H), 1.20-1.08 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 203.3, 198.5, 190.8, 189.3, 169.7, 165.5, 140.0, 128.0, 127.8, 125.8, 125.7, 99.5, 88.8, 56.1, 49.9, 48.4, 44.5, 43.4, 42.2, 39.8, 38.8, 31.1, 29.0, 28.9, 13.8, 12.4. HRMS Calculated for $C_{17}H_{23}NO_3$ (M+Na): 312.1576, found: 312.1577.



***N*, *N*-diethyl-3, 5-dioxo-5-phenylpentanamide**

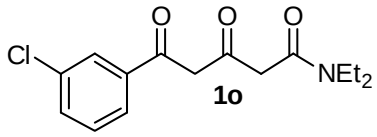
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.83 (m, 2H), 7.61-7.39 (m, 3H), 6.37 (s, 1H), 4.34 (s, 1H), 3.68 (s, 1H), 3.54 (s, 1H), 3.46-3.26 (m, 4H), 2.28 (s, 1H), 1.24-1.08 (m, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 181.5, 165.9, 133.9, 132.4, 128.6, 128.5, 128.4, 126.9, 96.4, 52.9, 49.8, 48.8, 46.0, 42.6, 42.5, 40.2, 40.1, 14.1, 12.8. HRMS Calculated for $C_{15}H_{19}NO_3$ (M+Na): 284.1263, found: 284.1233.



1n

***N*, *N*-diethyl-3, 5-dioxo-5-(o-tolyl)pentanamide**

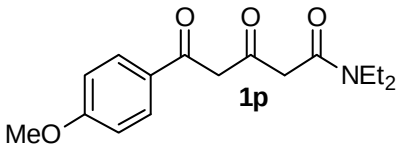
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.45 (m, 1H), 7.34 (d, *J* = 6.5 Hz, 1H), 7.31-7.17 (m, 2H), 6.03 (s, 0.78H), 4.30 (s, 0.18H), 3.68 (s, 0.19H), 3.52 (s, 1.93H), 3.49-3.29 (m, 4H), 2.50 (s, 3H), 1.18 (dt, *J* = 22.8, 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.7, 196.7, 190.6, 185.3, 170.3, 165.1, 136.3, 134.1, 131.3, 130.6, 130.1, 129.0, 127.7, 125.1, 125.0, 100.0, 88.5, 54.5, 48.1, 47.6, 44.6, 41.9, 41.8, 41.2, 39.5, 39.3, 20.7, 20.0, 13.4, 12.1. HRMS Calculated for $C_{16}H_{21}NO_3$ (M+H): 276.1600, found: 276.1584.



1o

5-(3-chlorophenyl)-*N*, *N*-diethyl-3, 5-dioxopentanamide

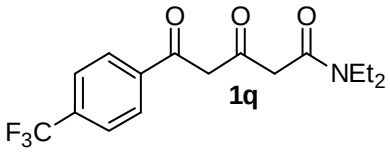
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (t, *J* = 1.9 Hz, 1H), 7.74 (ddd, *J* = 7.8, 1.6, 1.1 Hz, 1H), 7.47 (dd, *J* = 2.1, 1.1 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 6.34 (s, 1H), 3.81 (s, 1H), 3.66 (s, 1H), 3.54 (s, 2H), 3.40 (dd, *J* = 17.0, 7.2 Hz, 4H), 1.18 (dt, *J* = 19.2, 7.1 Hz, 6H). ^{13}C NMR (100MHz, $CDCl_3$) δ 198.6, 191.9, 179.0, 165.2, 135.2, 134.0, 131.6, 129.5, 129.3, 126.2, 124.4, 96.5, 88.8, 52.4, 48.0, 45.0, 42.1, 39.7, 13.6, 12.3. HRMS Calculated for $C_{15}H_{18}NO_3Cl$ (M+H): 296.1053, found: 296.1054.



1p

***N*, *N*-diethyl-5-(4-methoxyphenyl)-3, 5-dioxopentanamide**

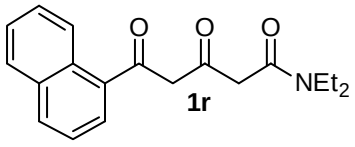
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.83 (m, 2H), 6.97-6.87 (m, 2H), 6.29 (s, 0.73H), 5.20 (s, 0.08H), 4.28 (s, 0.35H), 3.86 (s, 2.82H), 3.79-3.77 (m, 0.17H), 3.67 (s, 0.36H), 3.50 (s, 1.53H), 3.44-3.36 (m, 4H), 1.27-1.06 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 192.4, 189.5, 181.9, 170.7, 165.6, 162.7, 130.4, 130.3, 128.6, 125.9, 113.4, 95.1, 88.5, 54.8, 52.3, 48.2, 44.7, 42.1, 42.0, 39.7, 39.6, 13.6, 12.3. HRMS Calculated for $C_{16}H_{21}NO_4$ (M+H): 292.1549, found: 292.1540.



1q

***N*, *N*-diethyl-3, 5-dioxo-5-(4-(trifluoromethyl)phenyl)pentanemide.**

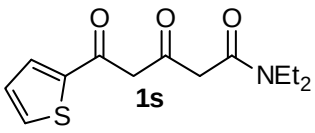
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 8.3 Hz, 2H), 6.41 (s, 0.82H), 4.38 (s, 0.11H), 3.65 (s, 0.11H), 3.56 (s, 1.70H), 3.40 (dd, *J* = 16.1, 7.2 Hz, 4H), 1.18 (dt, *J* = 21.5, 7.1 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3, 178.8, 165.6, 137.2, 133.7, 133.3, 129.0, 128.9, 127.2, 125.5, 125.4, 124.9, 122.1, 97.3, 89.2, 53.2, 48.4, 46.1, 42.6, 40.3, 14.1, 12.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.61, -63.78. HRMS Calculated for $C_{16}H_{18}NO_4F_3$ (M+H): 330.1317, found: 330.1310.



1r

***N*, *N*-diethyl-5-(naphthalen-1-yl)-3, 5-dioxopentanamide**

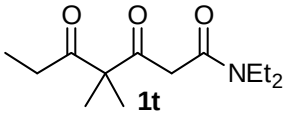
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (dd, *J* = 8.3, 1.0 Hz, 1H), 8.04-7.85 (m, 2H), 7.74 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.58-7.48 (m, 3H), 6.21 (s, 1H), 4.46 (s, 0.16H), 3.55 (s, 1.78H), 3.47-3.35 (m, 4H), 1.19 (dt, *J* = 28.2, 7.1 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 186.2, 165.7, 133.6, 133.5, 133.0, 131.7, 129.8, 128.3, 128.1, 127.2, 127.0, 126.3, 126.1, 125.5, 125.2, 124.5, 124.2, 101.46, 55.6, 48.8, 45.1, 42.5, 40.2, 14.0, 12.7. HRMS Calculated for $C_{19}H_{21}NO_3$ (M+H): 312.1600, found: 312.1584.



1s

***N*, *N*-diethyl-3, 5-dioxo-5-(thiophen-2-yl)pentanamide**

Light brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.58 (m, 2H), 7.15 (d, *J* = 4.1 Hz, 1H), 6.19 (s, 0.55H), 5.26 (s, 0.11H), 4.27 (s, 0.40H), 3.75 (s, 0.21H), 3.67 (s, 0.41H), 3.48 (s, 1.29H), 3.46-3.19 (m, 4H), 1.11-1.22 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 186.4, 185.1, 180.0, 169.9, 165.6, 165.4, 143.0, 140.2, 134.7, 134.3, 133.6, 133.2, 132.4, 130.3, 128.1, 128.0, 96.3, 88.8, 53.3, 49.3, 48.2, 46.3, 43.3, 42.3, 42.2, 41.7, 39.9, 39.8, 13.8, 13.7, 12.5. HRMS Calculated for $C_{13}H_{17}NO_3S$ (M+Na): 290.0827, found: 290.0825.



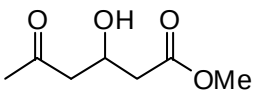
1t

***N*, *N*-diethyl-4, 4-dimethyl-3, 5-dioxoheptanamide**

1t was prepared by amminolysis[7] of tert-butyl 4, 4-dimethyl-3, 5-dioxoheptanoate, which was prepared according to the literature[10]. Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.16 (s,0.53H), 3.55 (s, 0.94H), 3.36 (dd, *J* = 14.3, 7.1 Hz, 4H), 3.32 – 3.21 (m, 2H), 2.55 (qd, *J* = 7.2, 3.4 Hz, 2H), 1.40 (s, 3H), 1.32 (s, 3H), 1.15 (dt, *J* = 20.1, 7.2 Hz, 6H), 1.05-1.01 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.7, 204.0, 179.3, 170.9, 165.7, 84.8, 61.8, 53.5, 44.2, 42.4, 41.9, 40.1, 39.9, 31.4, 30.5, 22.1, 21.3, 13.9, 13.0, 12.6, 7.9, 7.6. HRMS Calculated for $C_{13}H_{23}NO_3$ (M+Na): 264.1576, found: 264.1577.

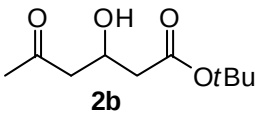
2. Procedure for the preparation of 2a-t

To a 50 mL dried Schlenk tube were added $RuCl_2(PPh_3)_3$ (24 mg, 0.025 mmol) (prepared according to the literature[11]) and 25 mL degassed THF and then the solution was equally divided into 5 vials which contained 1 mmol of substrates. Then the vials were taken into an autoclave. The autoclave was purged three times with H_2 and the required pressure of H_2 was set. Then the autoclave was stirred under specified reaction conditions. After being cooled to ambient temperature and careful release of the hydrogen, the autoclave was opened and the solvent was evaporated. Passing the crude samples through a short pad of silica gel eluted with petroleum ether and ethyl acetate.



Methyl 3-hydroxy-5-oxohexanoate[12]

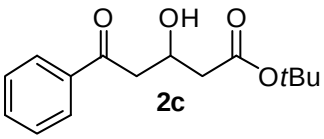
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.52 – 4.41 (m, 1H), 3.70 (s, 3H), 3.45 – 3.37 (m, 1H), 2.69– 2.67 (m, 2H), 2.54 – 2.49 (m, 2H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.1, 172.0, 51.55, 48.93, 40.34, 30.47.



2b

tert-butyl 3-hydroxy-5-oxohexanoate

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.47 – 4.35 (m, 1H), 3.48 (s, 1H), 2.65 (dd, *J* = 8.3, 6.2 Hz, 2H), 2.42 (d, *J* = 6.4 Hz, 2H), 2.19 (s, 3H), 1.44 (d, *J* = 5.2 Hz, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.1, 171.0, 80.9, 64.2, 49.1, 41.6, 30.5, 27.8. HRMS Calculated for $C_{10}H_{18}O_4$ (M+Na): 225.1103, found: 225.1126.

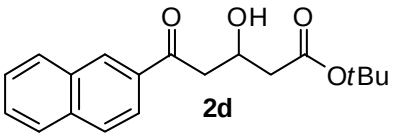


2c

tert-butyl 3-hydroxy-5-oxo-5-phenylpentanoate

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.92 (m, 2H), 7.61-7.57 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 3.63 (s, 1H), 3.22 (dd, *J* = 13.4, 5.3 Hz, 2H), 2.54 (dd, *J* = 6.3, 4.7 Hz, 2H), 1.47 (s, 9H). ^{13}C

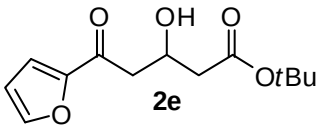
NMR (100 MHz, $CDCl_3$) δ 199.3, 171.3, 136.5, 133.5, 128.6, 128.0, 81.2, 64.8, 44.2, 41.8, 28.0, 27.9. HRMS Calculated for $C_{15}H_{20}O_4$ (M+Na): 287.1259, found: 287.1269.



2d

tert-butyl 3-hydroxy-5-(naphthalen-2-yl)-5-oxopentanoate

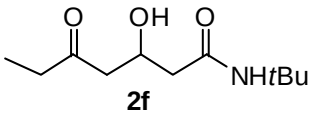
Light yellow oil. H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.06-7.84 (m, 4H), 7.64-7.53 (m, 2H), 4.71-4.64(m, 1H), 3.70 (d, *J* = 3.6 Hz, 1H), 3.41-3.28 (m, 2H), 2.67-2.50 (m, 2H), 1.47 (s, 9H).^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 171.2, 135.5, 133.8, 132.2, 129.9, 129.5, 128.5, 128.3, 127.59, 126.7, 123.4, 81.0, 64.8, 44.3, 41.8, 27.9. HRMS Calculated for $C_{19}H_{22}O_4$ (M+Na): 337.1416, found: 337.1414.



2e

tert-butyl 5-(furan-2-yl)-3-hydroxy-5-oxopentanoate

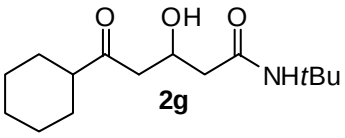
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.58(m, 1H), 7.24-7.21 (m, 1H), 6.55-6.52 (m, 1H), 4.61-4.51 (m, 1H), 3.56 (s, 1H), 3.13-2.94 (m, 2H), 2.50 (dd, *J* = 4.2, 3.0 Hz, 2H), 1.45 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.5, 170.9, 152.1, 146.6, 117.7, 112.1, 80.8, 64.4, 44.0, 41.7, 27.7. HRMS Calculated for $C_{13}H_{18}O_5$ (M+Na): 277.1052, found: 277.1050.



2f

***N*-(tert-butyl)-3-hydroxy-5-oxoheptanamide**

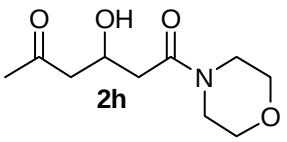
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.88 (s, 1H), 4.36 (dd, *J* = 7.9, 3.9 Hz, 1H), 4.19 (d, *J* = 3.1 Hz, 1H), 2.64-2.44 (m, 4H), 2.33-2.22 (qd, *J* = 15.1, 5.8 Hz, 2H), 1.33 (s, 9H), 1.05 (t, *J* = 7.3 Hz, 3H).^{13}C NMR (100MHz, $CDCl_3$) δ 210.8, 170.8, 64.8, 50.7, 48.0, 42.5, 36.4, 28.3, 7.1. HRMS Calculated for $C_{11}H_{21}NO_3$ (M+H): 216.1600, found: 216.1606.



2g

***N*-(tert-butyl)-5-cyclohexyl-3-hydroxy-5-oxopentanamide**

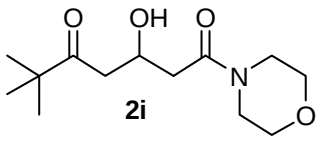
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.92 (s, 1H), 4.37 – 4.29 (m, 1H), 4.17 (d, *J* = 3.2 Hz, 1H), 2.66 (dd, *J* = 6.2, 2.0 Hz, 2H), 2.39-2.18 (m, 3H), 1.89-1.72 (m, 4H), 1.68 (s, 2H), 1.37-1.32 (m, 9H), 1.32-1.14 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.8, 170.7, 64.9, 50.9, 46.1, 42.6, 28.4, 27.9, 25.5, 25.2. HRMS Calculated for $C_{15}H_{27}NO_3$ (M+Na): 292.1889, found: 292.1887.



2h

3-hydroxy-1-morpholinohexane-1, 5-dione

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.45 (s, 1H), 4.14 (s, 1H), 3.70-3.64 (m, 4H), 3.64-3.58 (m, 2H), 3.50-3.41 (m, 2H), 2.71 (dd, *J* = 12.6, 6.3 Hz, 2H), 2.50 (ddd, *J* = 24.2, 16.0, 6.0 Hz, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.9, 170.09, 66.4, 66.2, 64.4, 49.3, 45.6, 41.5, 38.4, 30.6. HRMS Calculated for $C_{10}H_{17}NO_4$ (M+Na): 238.1055, found: 238.1050.

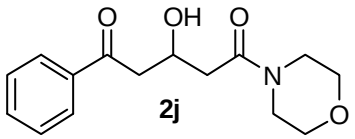


2i

3-hydroxy-6, 6-dimethyl-1-morpholinoheptane-1, 5-dione

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.47-4.37 (m, 1H), 4.16 (d, *J* = 3.5 Hz, 1H), 3.69-3.65 (m, 4H), 3.65-3.59 (m, 2H), 3.49-3.44 (m, 2H), 2.80 (ddd, *J* = 37.7, 17.7, 6.2 Hz,2H), 2.52 (ddd, *J* = 23.7, 15.8,

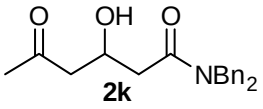
6.0 Hz,2H), 1.14 (s, 9H).^{13}C NMR (100 MHz, $CDCl_3$) δ 215.22, 170.06, 66.46, 66.26, 64.74, 45.66, 42.51, 41.50, 38.45, 25.91. HRMS Calculated for $C_{13}H_{21}NO_4$ (M+Na): 256.1549, found: 256.1535.



2j

3-hydroxy-1-morpholino-5-phenylpentane-1, 5-dione

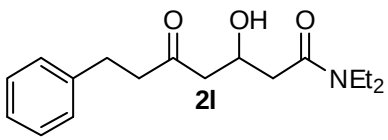
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.90 (m, 2H), 7.62 - 7.53 (m, 1H), 7.51-7.41 (m, 2H), 4.63 (s, 1H), 4.31 (d, *J* = 3.0 Hz, 1H), 3.72 – 3.57 (m, 6H), 3.46 (dd, *J* = 6.0, 3.7 Hz, 2H), 3.36–3.21 (m, 2H), 2.75–2.48 (m, 2H), 1.24 (dd, *J* = 7.9, 6.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 181.2, 165.1, 133.8, 133.4, 132.4, 128.6, 128.4, 128.2, 126.8, 96.3, 66.4, 66.3, 52.6, 48.9, 46.6, 46.4, 45.8, 42.1, 41.8. HRMS Calculated for $C_{15}H_{19}NO_4$ (M+Na): 300.1212, found: 300.1214.



2k

***N, N*-dibenzyl-3-hydroxy-5-oxohexanamide**

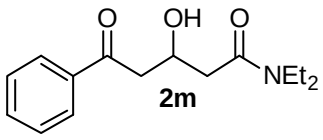
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.03 (m, 10H), 4.60 (q, *J* = 15.0 Hz, 2H), 4.51-4.56 (m, 1H), 4.44 (s, 2H), 4.36 (d, *J* = 3.3 Hz, 1H), 2.78-2.48 (m, 4H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.4, 172.0, 136.4, 135.5, 128.5, 128.2, 127.6, 127.2, 127.0, 126.0, 64.5, 49.4, 49.2, 47.6, 38.5, 30.2. ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.4, 172.0, 136.4, 135.5, 128.5, 128.2, 127.6, 127.2, 127.0, 126.0, 64.5, 49.4, 49.2, 47.6, 38.5, 30.2. HRMS Calculated for $C_{20}H_{23}NO_3$ (M+Na): 348.1576, found: 348.1574.



2l

***N, N*-diethyl-3-hydroxy-5-oxo-7-phenylheptanamide**

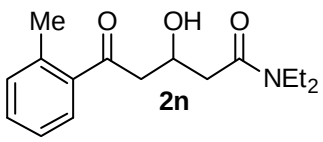
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16-7.29 (m, 5H), 4.58 (d, *J* = 3.3 Hz, 1H), 4.40-4.45 (m, 1H), 3.31 (dq, *J* = 21.9, 7.1 Hz, 4H), 2.92-2.70 (m, 4H), 2.62-2.53 (m, 2H), 2.34 (dd, *J* = 16.1, 8.4 Hz, 2H), 1.19-1.10 (m, 6H). ^{13}C NMR (100MHz, $CDCl_3$) δ 208.6, 170.7, 140.5, 128.0, 127.9, 125.6, 64.6, 48.7, 44.6, 41.6, 39.7, 38.0, 29.1, 22.0, 13.7, 12.6. HRMS Calculated for $C_{17}H_{25}NO_3$ (M+Na): 314.1732, found: 314.1725.



2m

***N, N*-diethyl-3-hydroxy-5-oxo-5-phenylpentanamide**

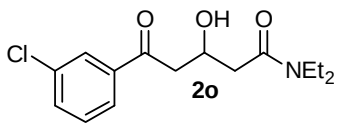
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.91 (m, 2H), 7.56 (d, *J* = 7.4 Hz, 1H), 7.47 (dd, *J* = 10.7, 4.5 Hz, 2H), 4.72 (d, *J* = 3.5 Hz, 1H), 4.66-4.55 (m, 1H), 3.43-3.16 (m, 6H), 2.77-2.44 (m, 2H), 1.15 (dt, *J* = 18.0, 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.7, 170.8, 136.5, 132.9, 128.2, 127.7, 65.0, 44.5, 41.6, 39.7, 38.2, 13.7, 12.6. HRMS Calculated for $C_{15}H_{21}NO_3$ (M+Na): 286.1419, found: 286.1411.



2n

***N, N* -diethyl-3-hydroxy-5-oxo-5-(o-tolyl)pentanamide**

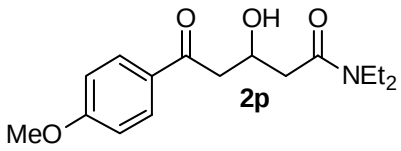
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.64 (m, 1H), 7.35 (td, *J* = 7.5, 1.3 Hz, 1H), 7.28-7.18 (m, 2H), 4.64 (s, 1H), 4.60-4.52 (m, 1H), 3.41-3.26 (m, 4H), 3.22-3.08 (m, 2H), 2.72-2.43 (m, 2H), 2.49 (s, 3H), 1.19-1.07 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 170.8, 137.7, 137.3, 131.6, 131.1, 128.4, 125.4, 65.2, 47.4, 41.7, 39.8, 38.2, 20.9, 13.7, 12.7. HRMS Calculated for $C_{16}H_{23}NO_3$ (M+H): 278.1756, found: 278.1739.



2o

5-(3-chlorophenyl)-*N*, *N* -diethyl-3-hydroxy-5-oxopentanamide

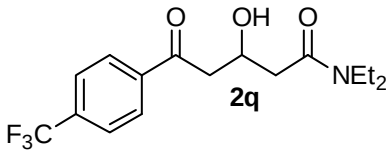
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 1.8 Hz, 1H), 7.85 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.57-7.51 (m, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 4.69 (d, = 3.5 Hz, 1H), 4.65-4.54 (m, 1H), 3.42-3.29 (m, 4H), 3.27-3.14 (m, 2H), 2.76-2.44 (m, 2H), 1.21-1.08 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 170.7, 138.1, 134.5, 132.7, 129.6, 127.8, 126.0, 64.9, 44.7, 41.7, 39.8, 38.1, 13.8, 12.7. HRMS Calculated for $C_{15}H_{20}NO_3Cl$ (M+H): 298.1210, found: 298.1196.



2p

***N*, *N* -diethyl-3-hydroxy-5-(4-methoxyphenyl)-5-oxopent-anamide**

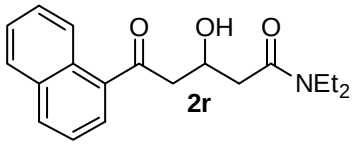
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 4.73 (d, *J* = 3.4 Hz, 1H), 4.65-4.53 (m, 1H), 3.87 (s, 3H), 3.41-3.28 (m, 4H), 3.77-3.44 (m, 2H), 2.77-2.44 (m, 2H), 1.14 (dt, *J* = 17.1, 7.1 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.2, 170.8, 163.2, 130.0, 129.6, 113.3, 65.1, 55.0, 44.1, 41.6, 39.7, 38.2, 13.7, 12.6. HRMS Calculated for $C_{16}H_{23}NO_4$ (M+Na): 316.1525, found: 316.1520.



2q

***N*, *N* -diethyl-3-hydroxy-5-oxo-5-(4-(trifluoromethyl)phenyl)-pentanamide**

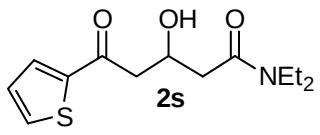
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 8.8, 0.7 Hz, 2H), 7.78-7.63 (m, 2H), 4.70 (s, 1H), 4.64-4.56 (m, 1H), 3.42-3.29 (m, 4H), 3.28-3.14 (m, 2H), 2.75-2.45 (m, 2H), 1.14 (dt, *J* = 21.4, 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 170.7, 139.3, 134.3, 134.0, 133.7, 133.3, 128.2, 125.2, 125.2, 64.9, 44.9, 41.6, 39.8, 38.2, 13.6, 12.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.67. HRMS Calculated for $C_{16}H_{20}NO_4F_3$ (M+H): 332.1474, found: 332.1456.



2r

***N*, *N*-diethyl-3-hydroxy-5-(naphthalen-1-yl)-5-oxopentanamide**

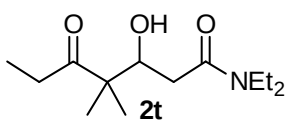
Thick yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68-8.61 (m, 1H), 8.03-7.86 (m, 3H), 7.64-7.48 (m, 3H), 4.71 (d, *J* = 3.5 Hz, 1H), 4.70-4.64 (m, 1H), 3.47-3.31 (m, 4H), 3.31-3.25 (m, 2H), 2.65 (ddd, *J* = 24.0, 16.0, 5.8 Hz, 2H), 1.15 (dt, *J* = 16.1, 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 170.9, 135.3, 133.6, 132.6, 129.8, 128.2, 128.0, 127.7, 126.2, 125.5, 124.1, 65.5, 48.0, 41.7, 39.8, 38.2, 13.8, 12.8. HRMS Calculated for $C_{19}H_{23}NO_3$ (M+H): 314.1756, found: 314.1762.



2s

***N*, *N*-diethyl-3-hydroxy-5-oxo-5-(thiophen-2-yl)pentanamide**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.65 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.14 (dd, *J* = 4.9, 3.8 Hz, 1H), 4.75 (d, *J* = 3.7 Hz, 1H), 4.63-4.50 (m, 1H), 3.42-3.28 (m, 4H), 3.27-3.10 (m, 2H), 2.76-2.44 (m, 2H), 1.19-1.07 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.2, 170.5, 143.8, 133.6, 132.3, 127.8, 65.0, 45.1, 41.5, 39.5, 38.0, 13.5, 12.5. HRMS Calculated for $C_{13}H_{17}NO_3S$ (M+Na): 290.0827, found: 290.0825.



2t

***N*, *N*-diethyl-3-hydroxy-4, 4-dimethyl-5-oxoheptanamide**

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.54 (d, *J* = 2.0 Hz, 1H), 4.16 (d, *J* = 10.4 Hz, 1H), 3.35-3.31(m, 4H), 2.67-2.51(m, 2H), 2.46-2.17 (m, 2H),

1.20-1.16(d, J = 2.3 Hz, 6H) 1.18-1.15 (m, 3H), 1.12 (t, J = 7.1 Hz, 3H), 1.02 (t, J = 7.2 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 215.3, 171.6, 72.7, 50.7, 41.8, 40.0, 33.6, 31.1, 20.7, 19.9, 13.8, 12.7, 7.6. HRMS Calculated for $C_{13}H_{25}NO_3$ (M+Na): 266.1732, found: 266.1726.

3. References

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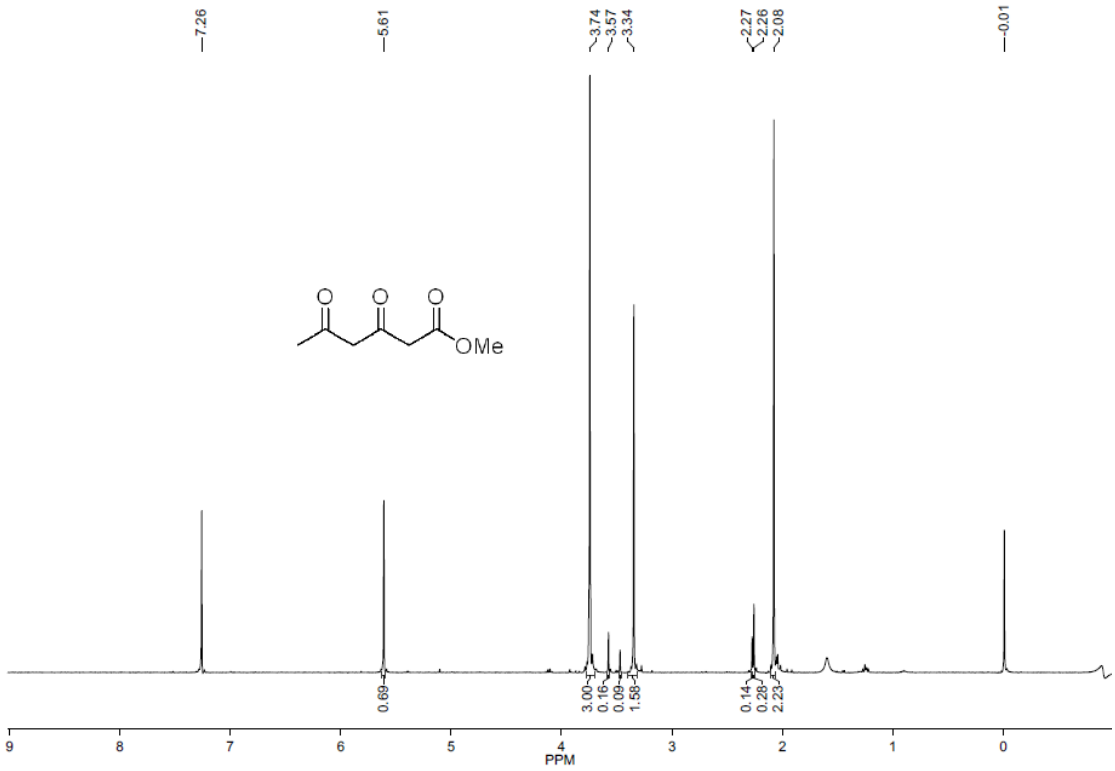
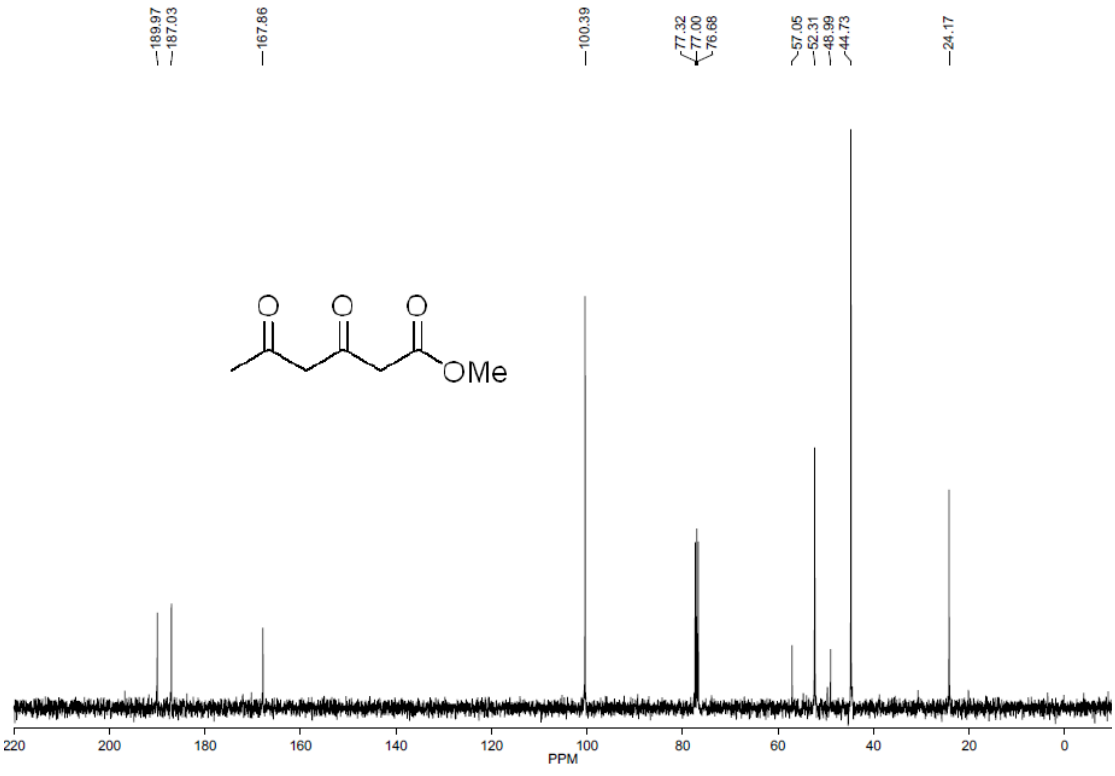
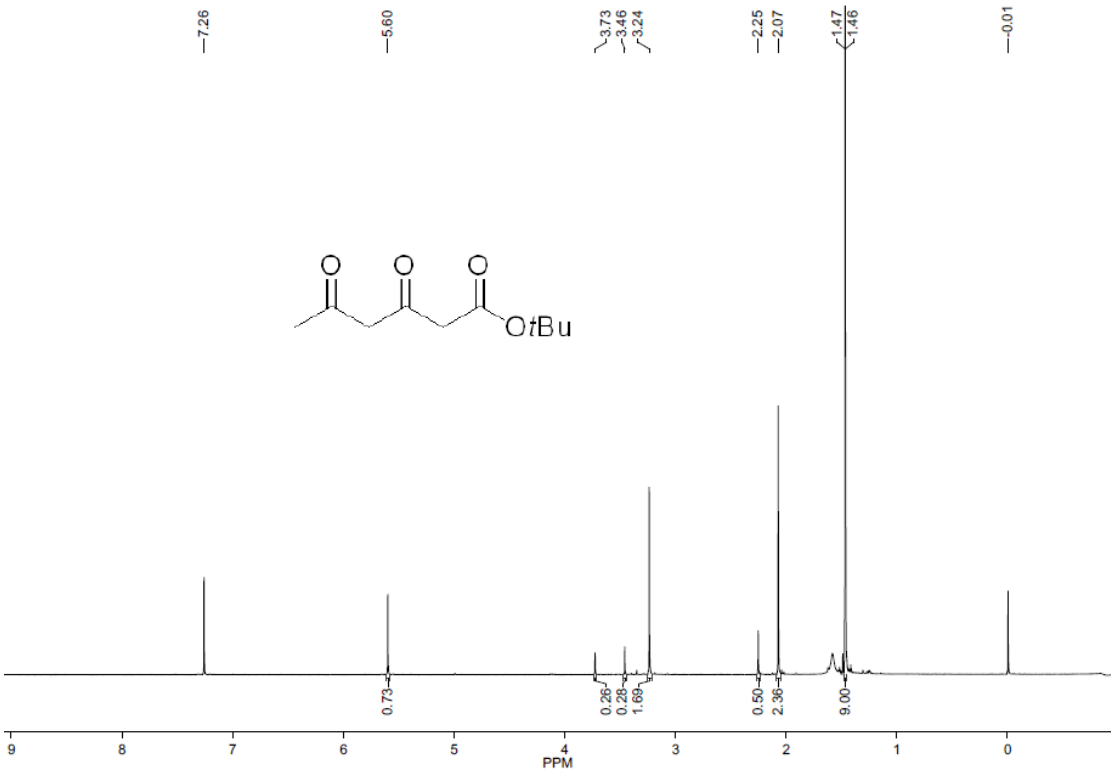
4. Copies of NMR Spectra and HRMS Reports

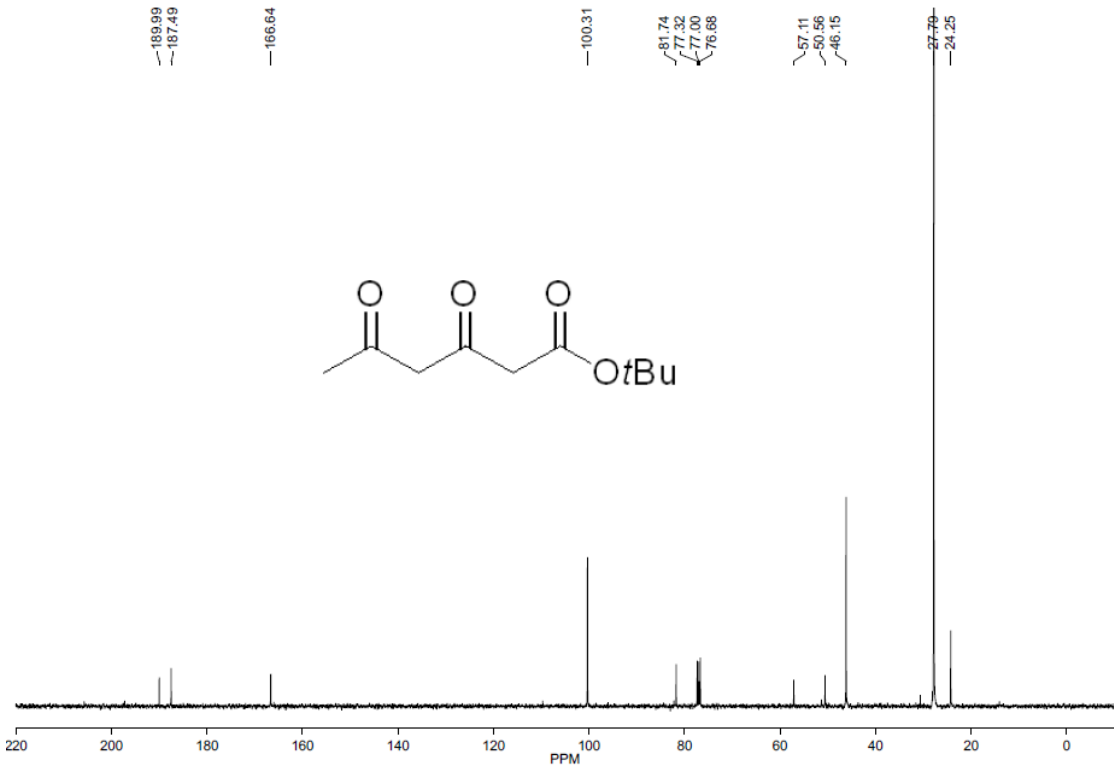
(1a) Methyl 3, 5-dioxohexanoate



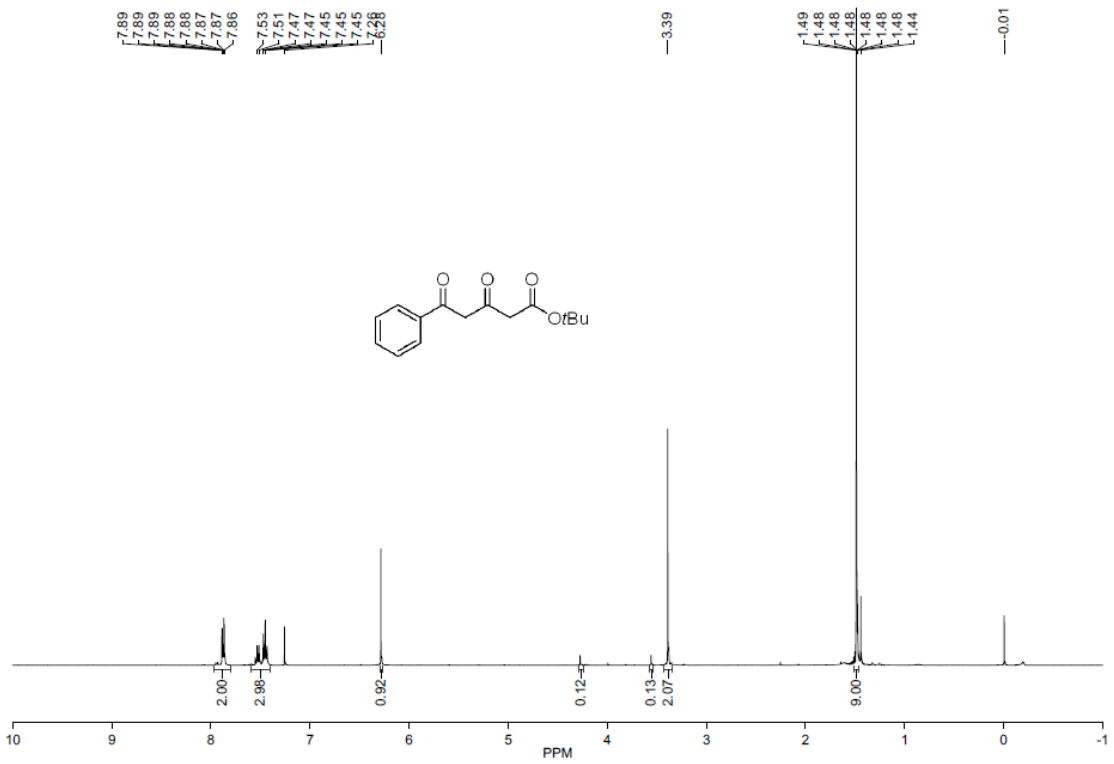


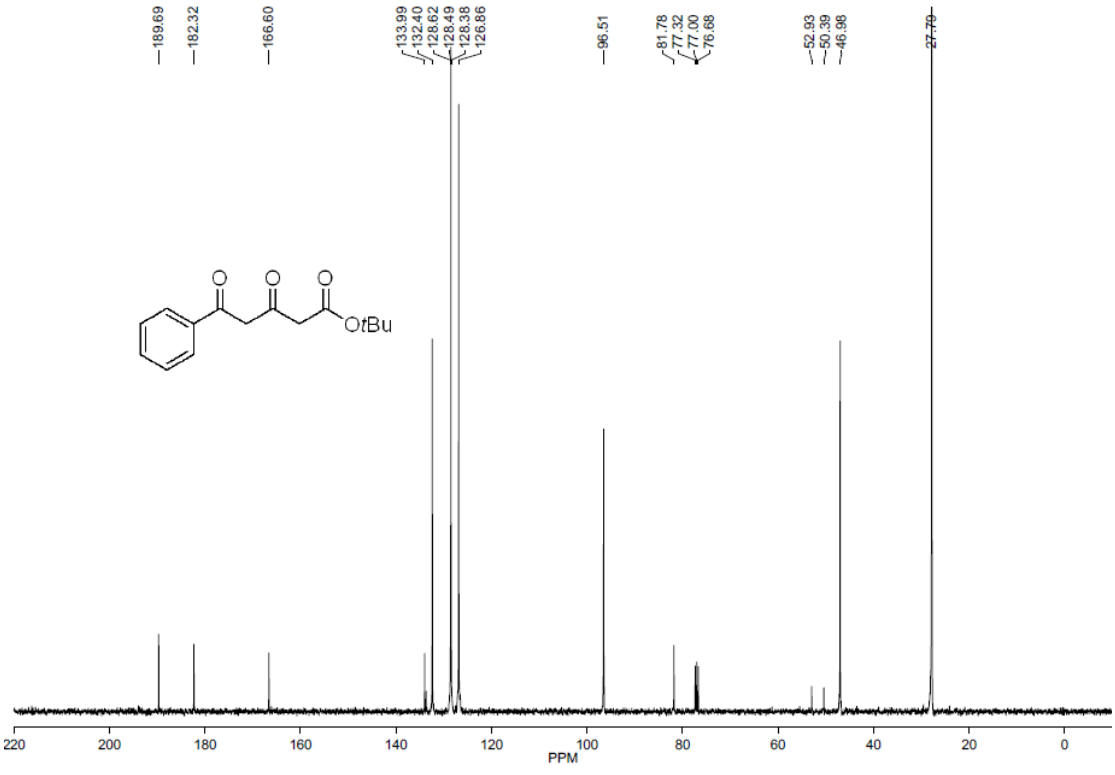
(1b) tert-butyl 3, 5-dioxohexanoate



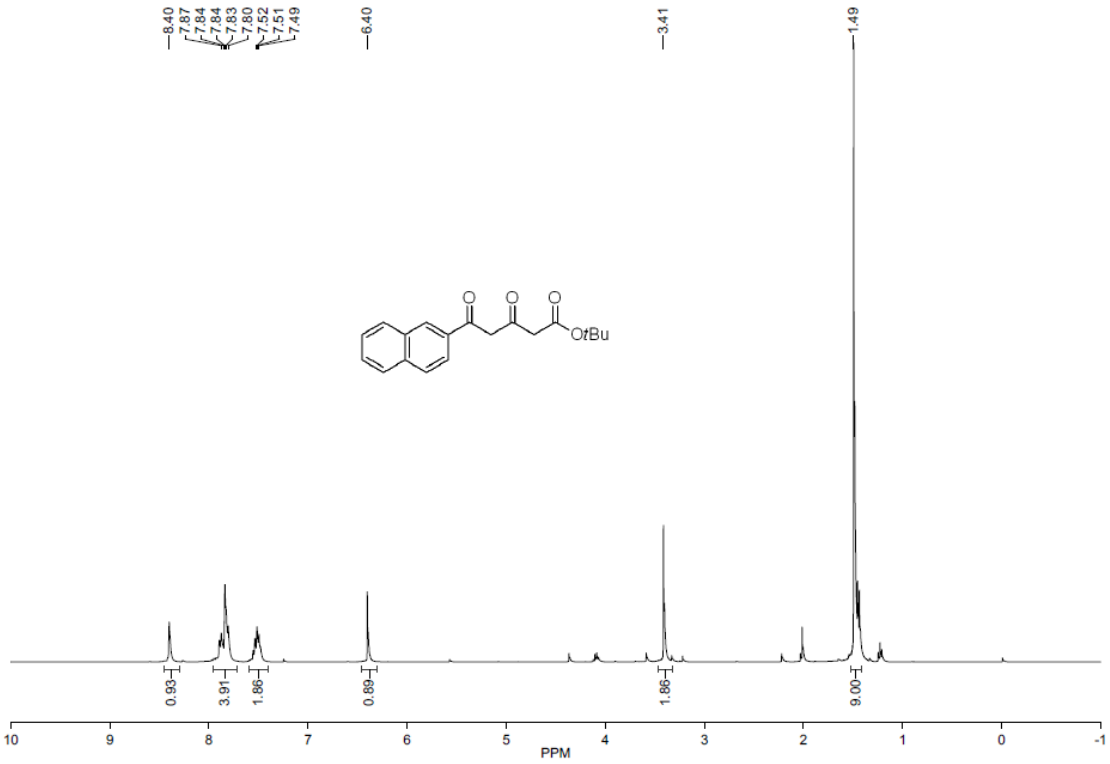


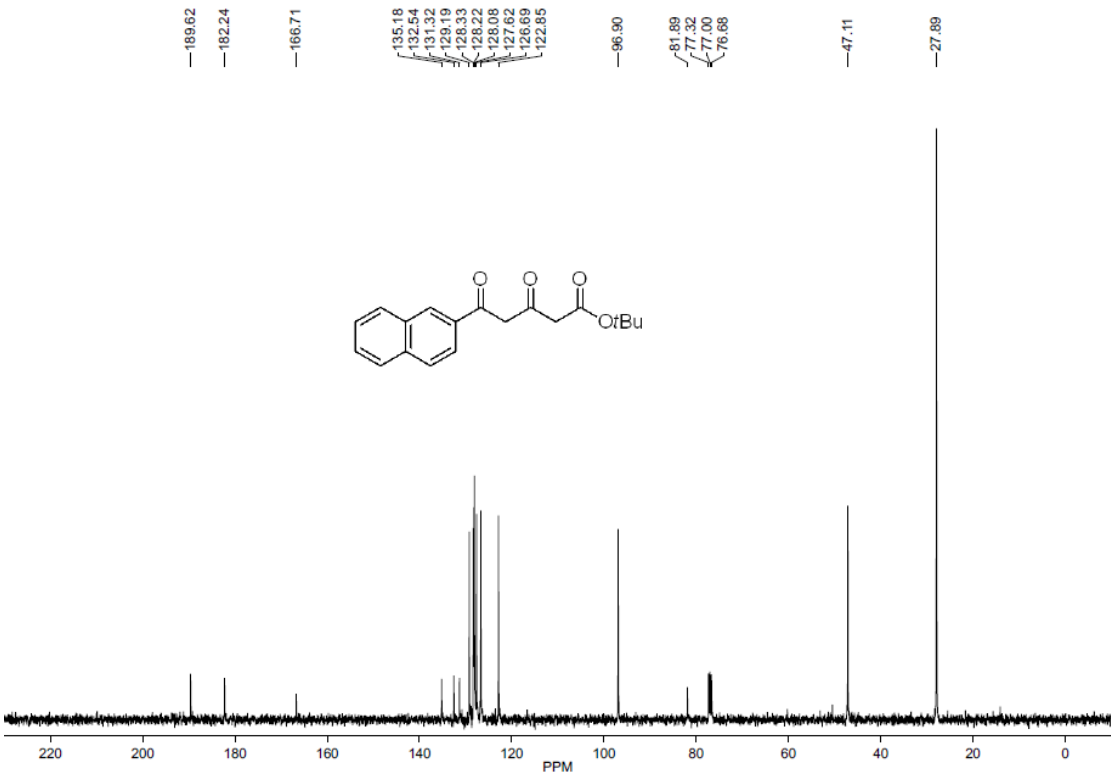
(1c) tert-butyl 3, 5-dioxo-5-phenylpentanoate





(1d) tert-butyl 5-(naphthalen-2-yl)-3, 5-dioxopentanoate





Elemental Composition Report

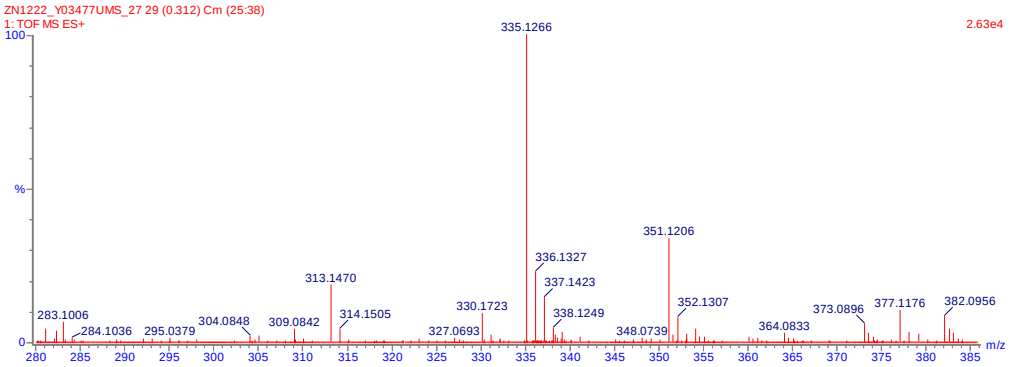
Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

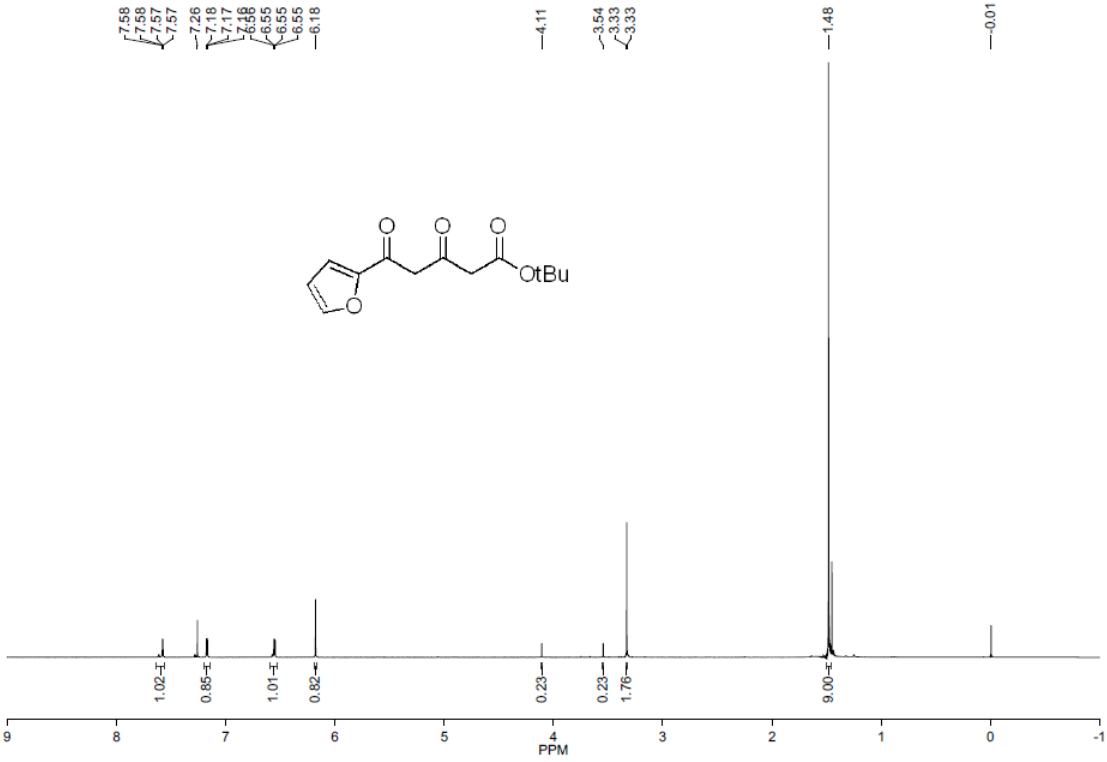
Elements Used: C: 10-20 H: 0-35 O: 0-5 Na: 0-1

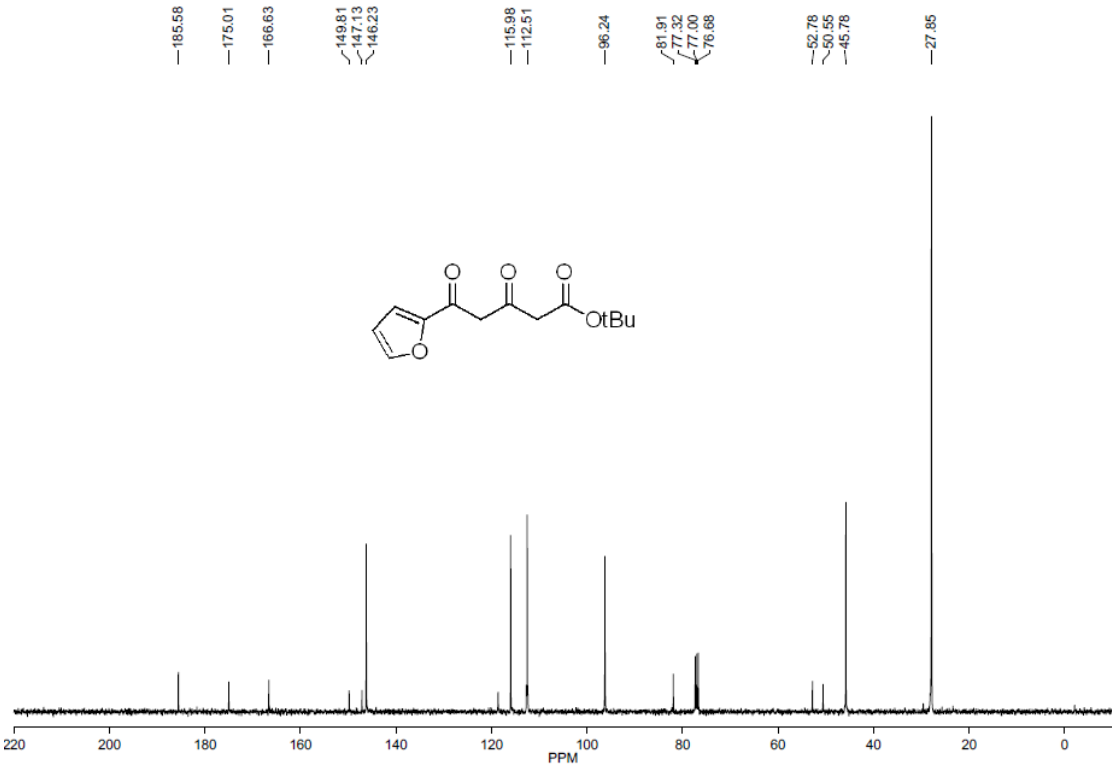


Minimum:				-1.5	
Maximum:		8.0	100.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
335.1266	335.1259	0.7	2.1	9.5	1202.6

Formula: $C_{19}H_{20}O_4Na$

(1e) tert-butyl 5-(furan-2-yl)-3, 5-dioxopentanoate





Elemental Composition Report

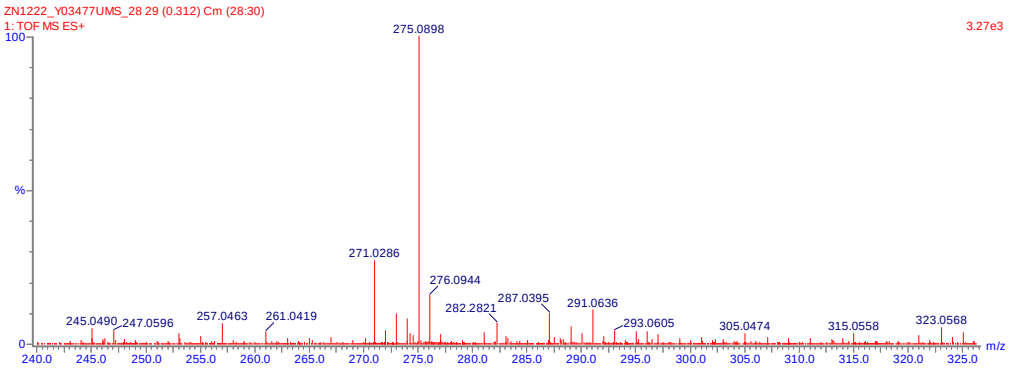
Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

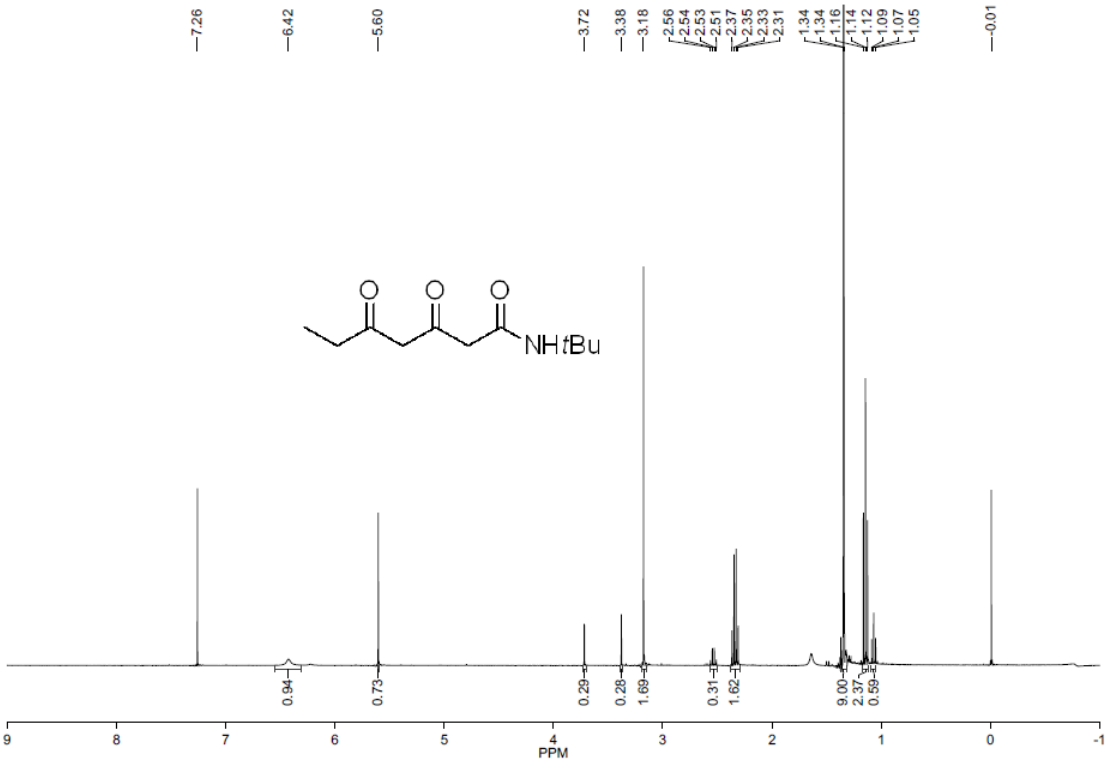
Elements Used: C: 10-20 H: 0-30 O: 4-5 Na: 0-1



Minimum:				-1.5	
Maximum:		8.0	100.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
275.0898	275.0895	0.3	1.1	5.5	5.3

Formula: $C_{13}H_{16}O_5Na$

(1f) *N*-(tert-butyl)-3, 5-dioxoheptanamide



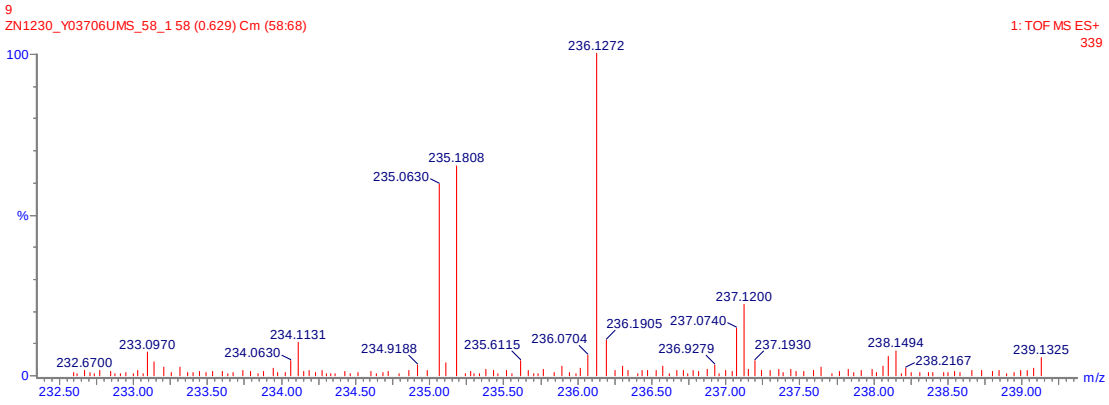
Elemental Composition Report

Single Mass Analysis Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 11-24 H: 6-21 N: 1-2 O: 2-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
236.1272	236.1263	0.9	3.8	2.5	14.4

Formula $C_{11}H_{19}NO_3Na$

(1g) *N*-(tert-butyl)-5-cyclohexyl-3, 5-dioxopentanamide

Elemental Composition Report

Single Mass Analysis

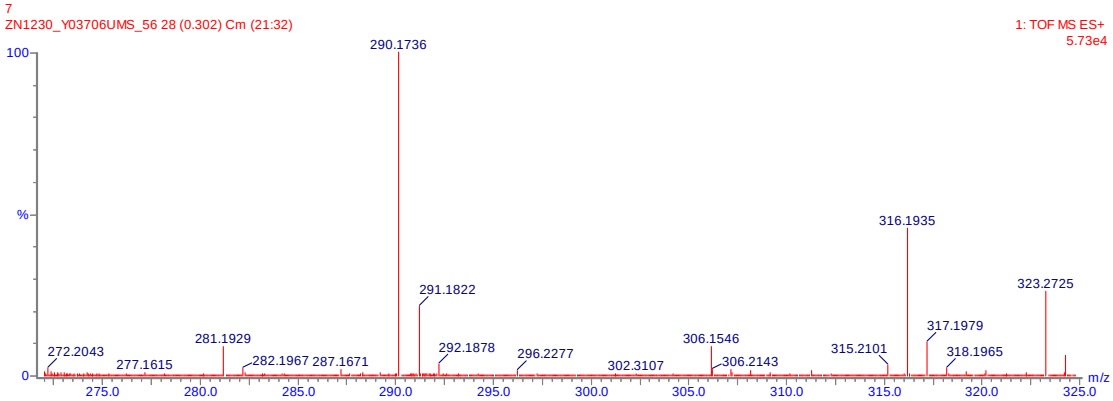
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

44 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each

mass)

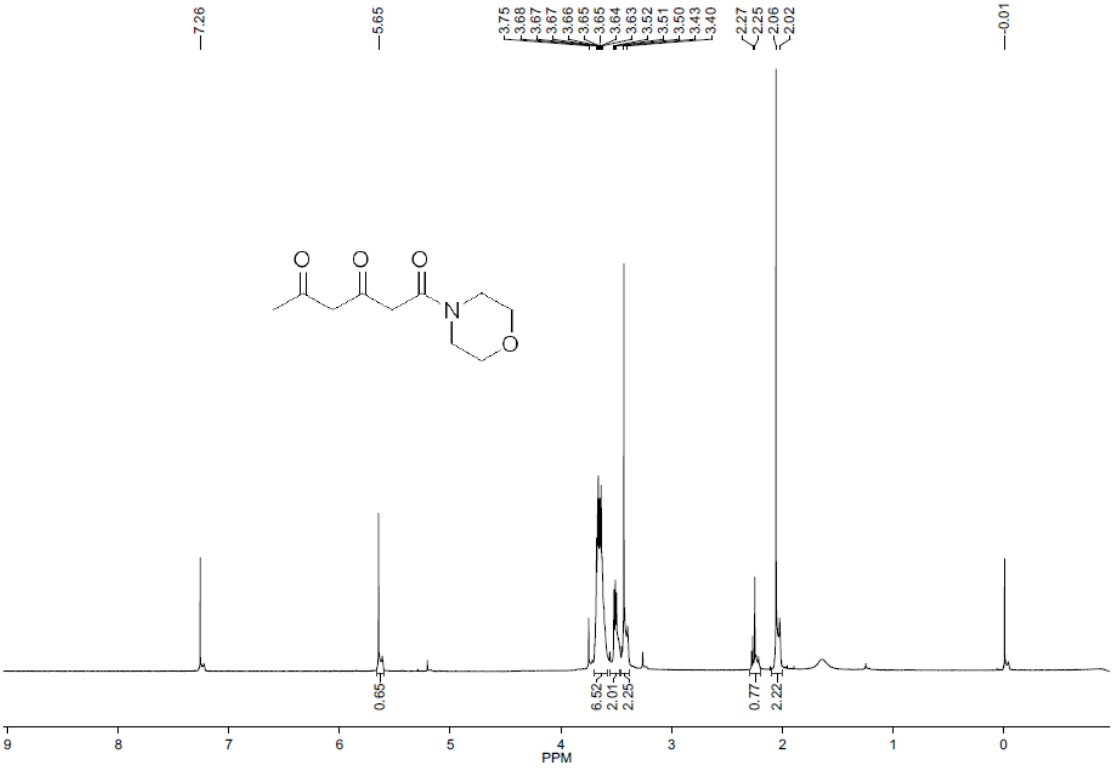
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1

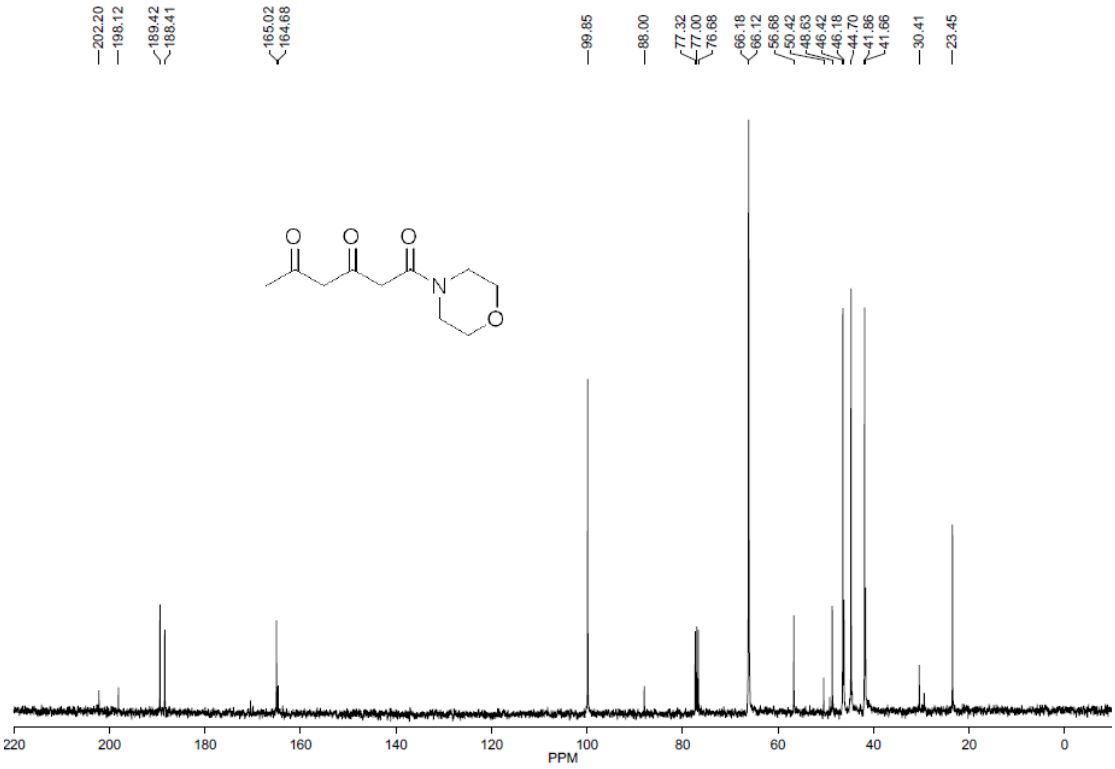


Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
290.1736	290.1732	0.4	1.4	3.5	301.9

Formula： $C_{15}H_{25}NO_3Na$

(1h) 1-morpholinohexane-1, 3, 5-trione





Elemental Composition Report

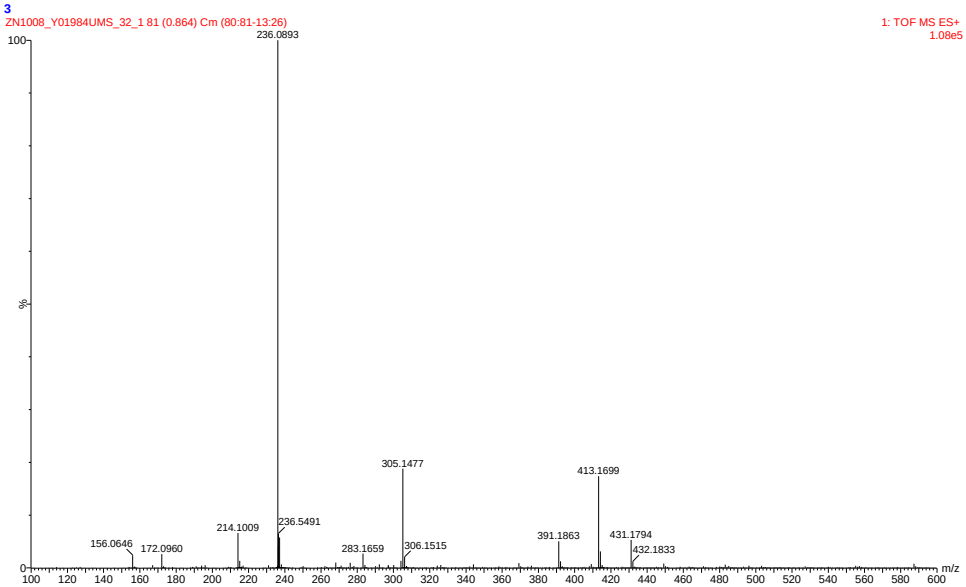
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

210 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 0-20 H: 0-40 N: 0-5 O: 0-5 Na: 0-1

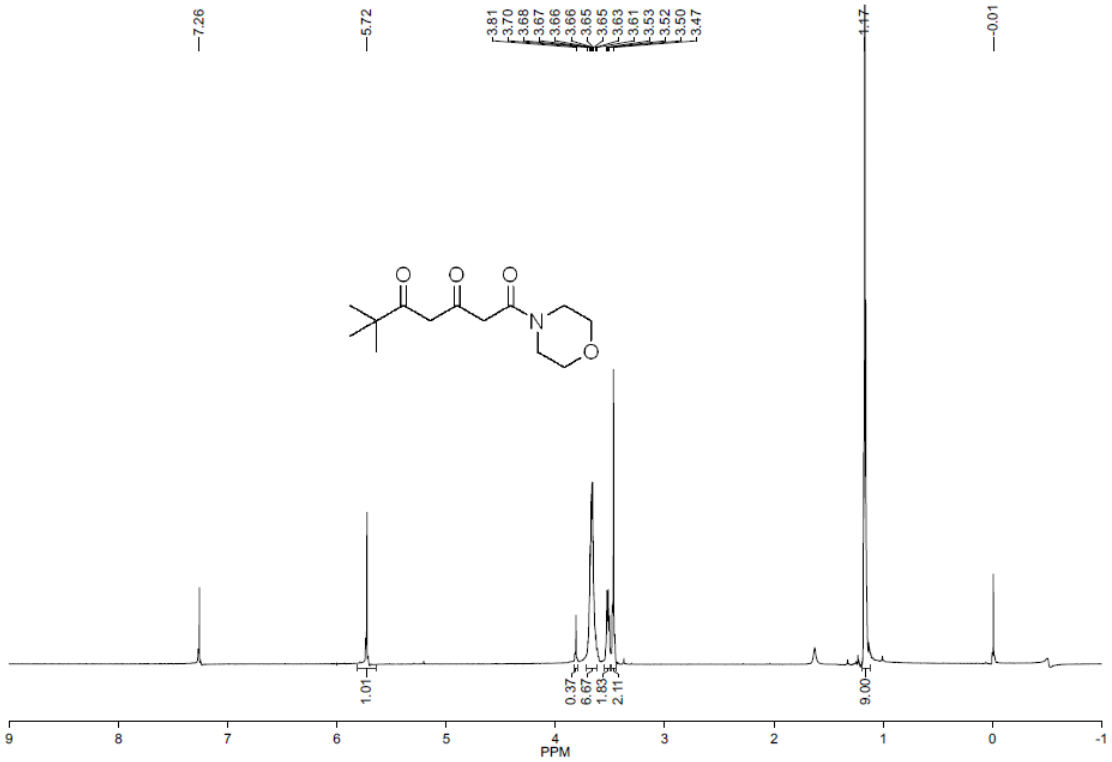


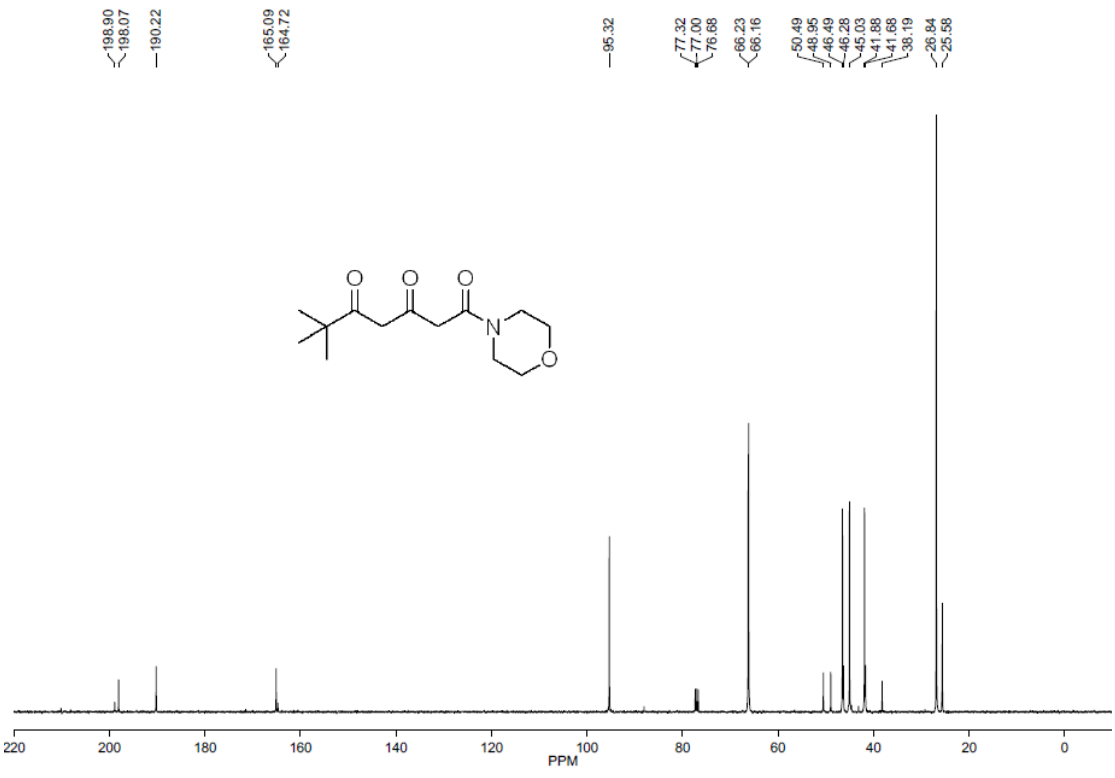
Minimum:	80.00				-1.5
Maximum:	100.00		50.0	5.0	50.0
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT

236.0893	236.0899	-0.6	-2.5	3.5	3227.3

Formula $C_{10}H_{15}NO_4Na$

(1i) 6, 6-dimethyl-1-morpholinoheptane-1, 3, 5-trione





Elemental Composition Report

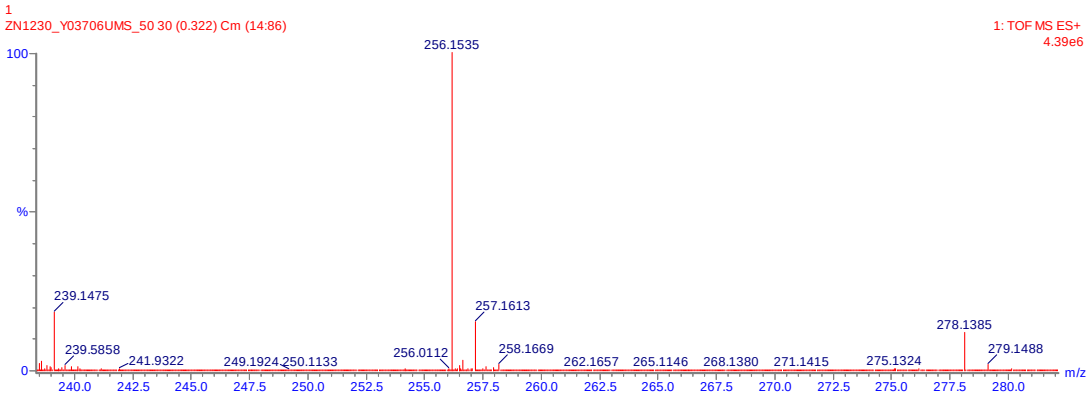
Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

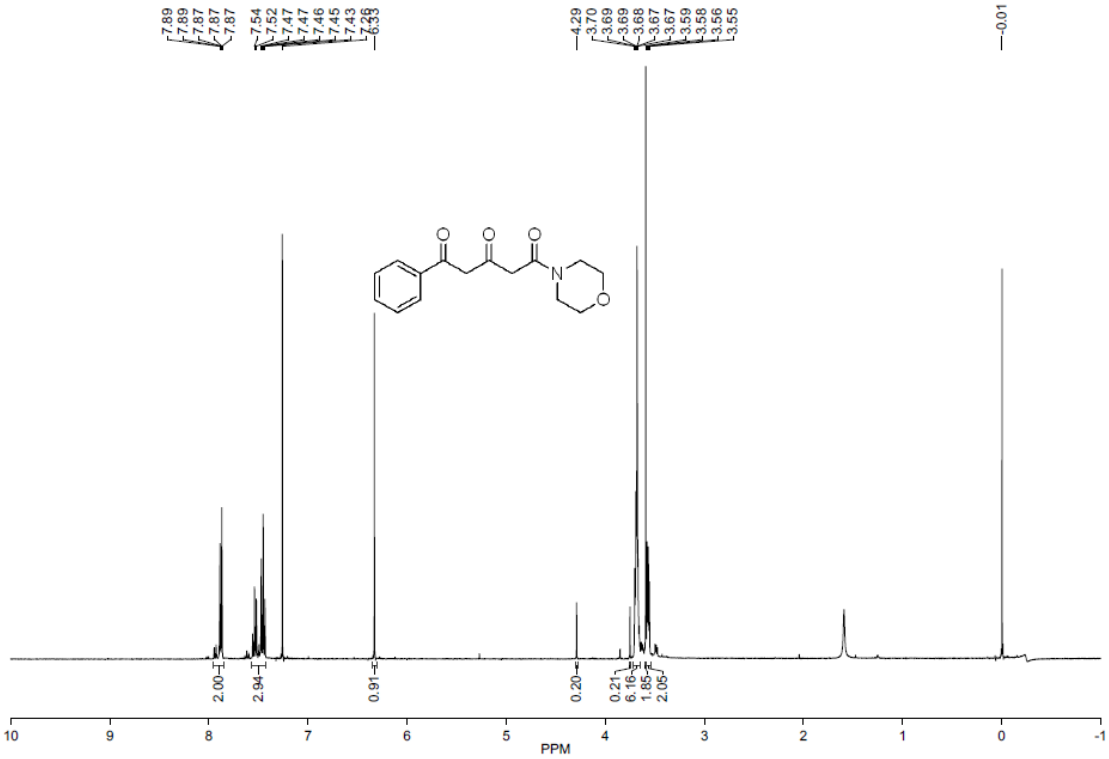
32 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

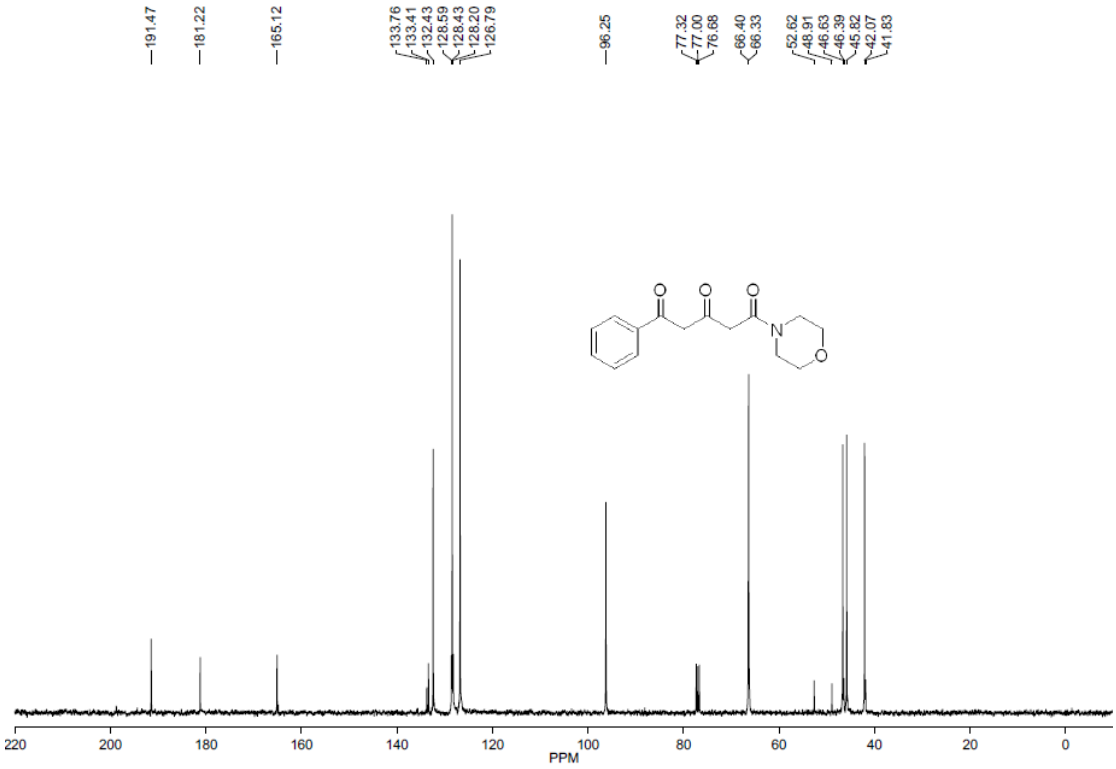
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	30.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
256.1535	256.1549	-1.4	-5.5	3.5	2249.1
Formula	$C_{13}H_{22}NO_4$				

(1j) 1-morpholino-5-phenylpentane-1, 3, 5-trione





Elemental Composition Report

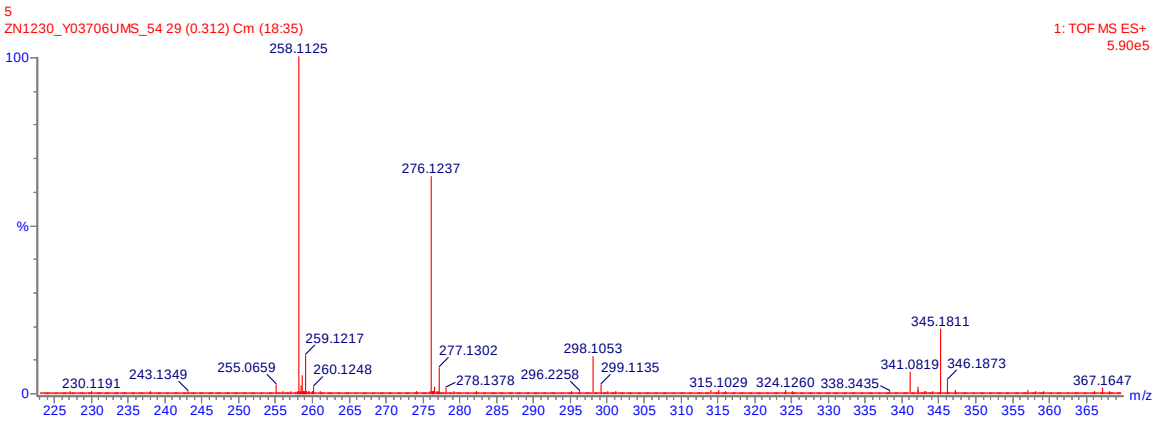
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

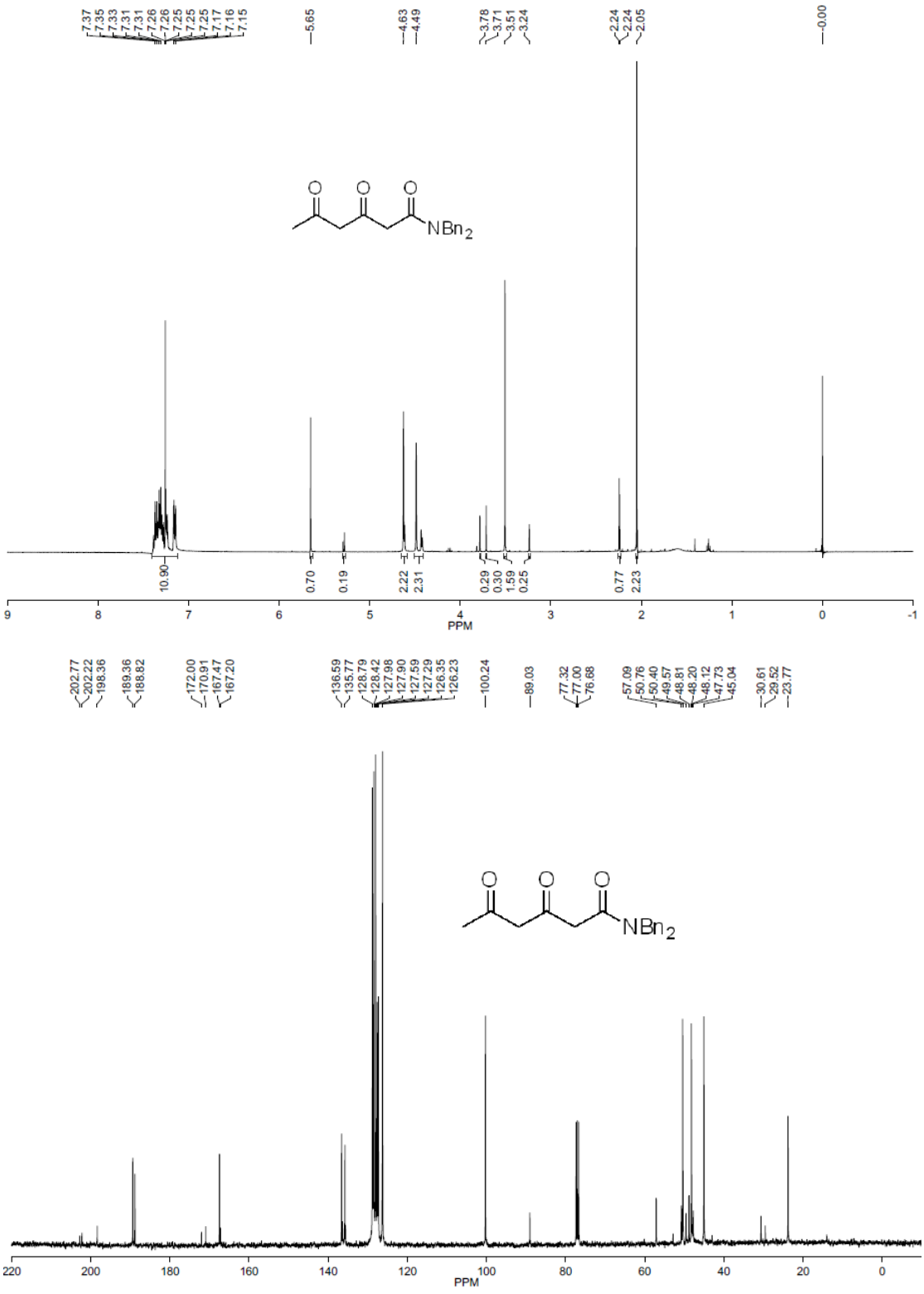
40 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
276.1237	276.1236	0.1	0.4	7.5	4315.1
Formula	$C_{15}H_{18}NO_4$				

(1k) *N*, *N*-dibenzyl-3, 5-dioxohexanamide



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

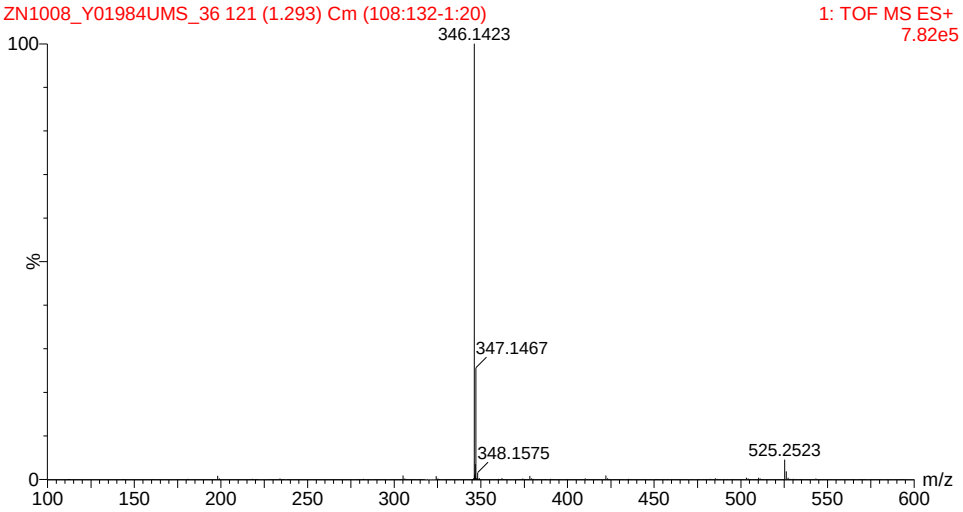
Selected filters: None Monoisotopic Mass, Even Electron Ions

32 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each

mass)

Elements Used: C: 0-20 H: 0-22 N: 0-2 O: 0-5 Na: 0-1

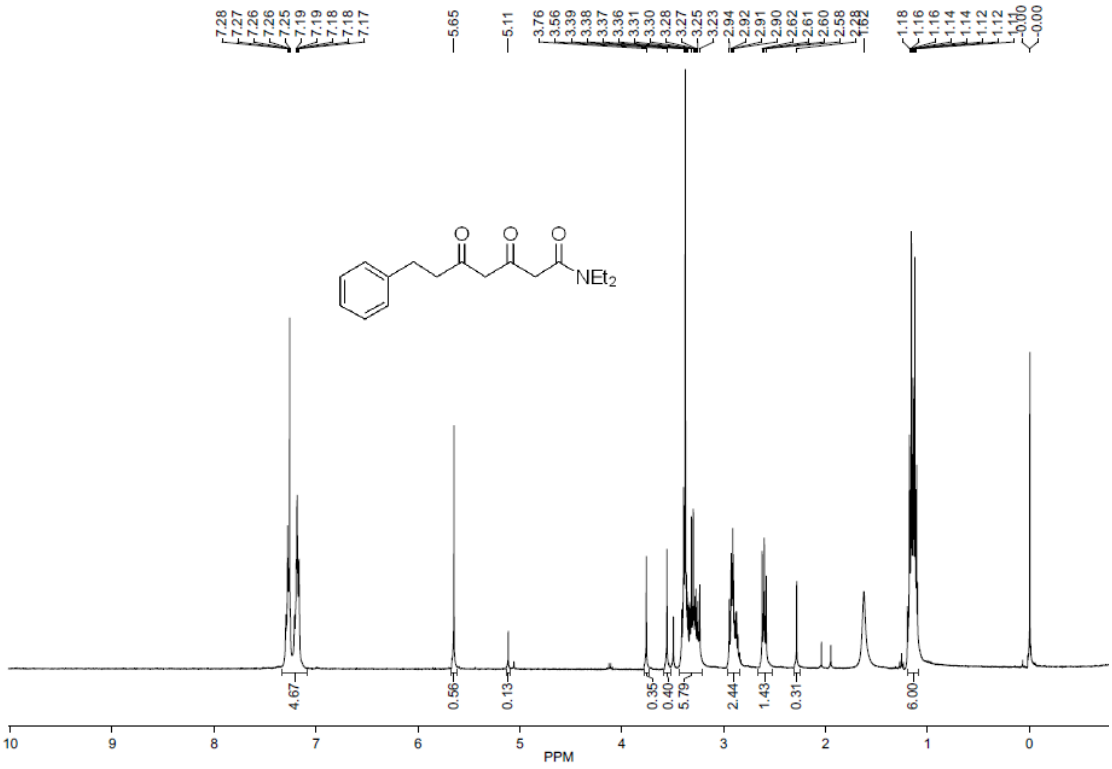
7

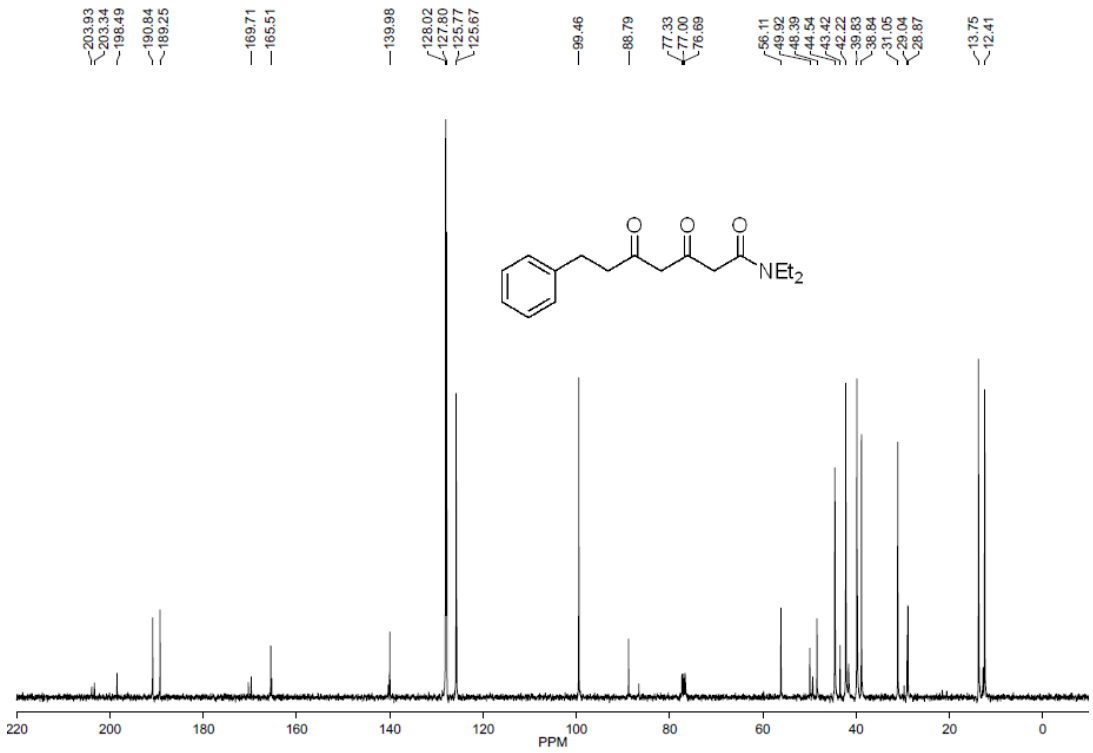


Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
346.1423	346.1419	0.4	1.2	10.5	8794.8

Formula $C_{20}H_{21}NO_3Na$

(1l) *N*, *N*-diethyl-3, 5-dioxo-7-phenylheptanamide





Elemental Composition Report

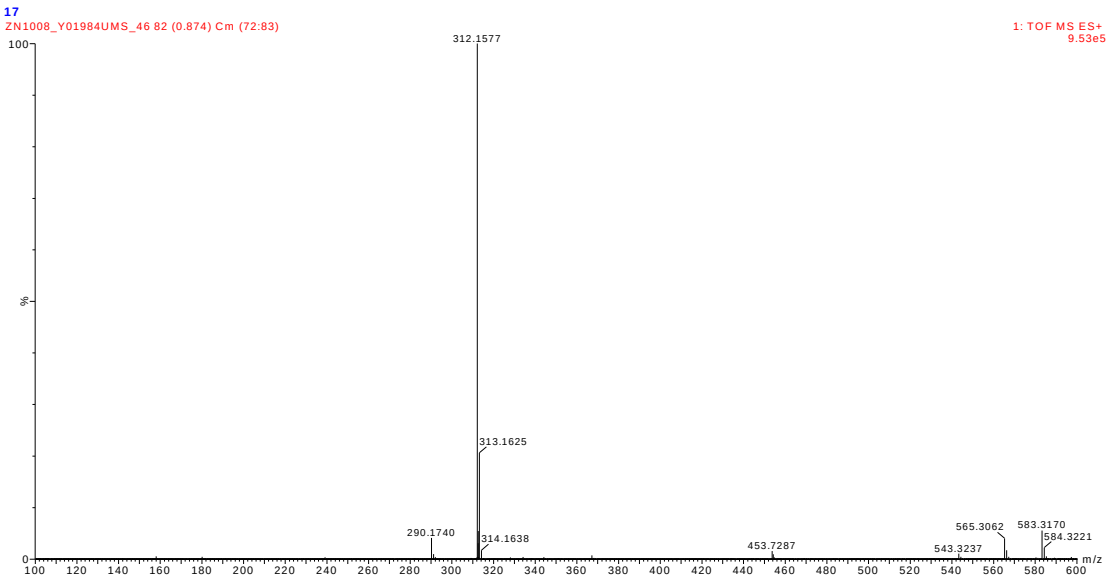
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

41 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

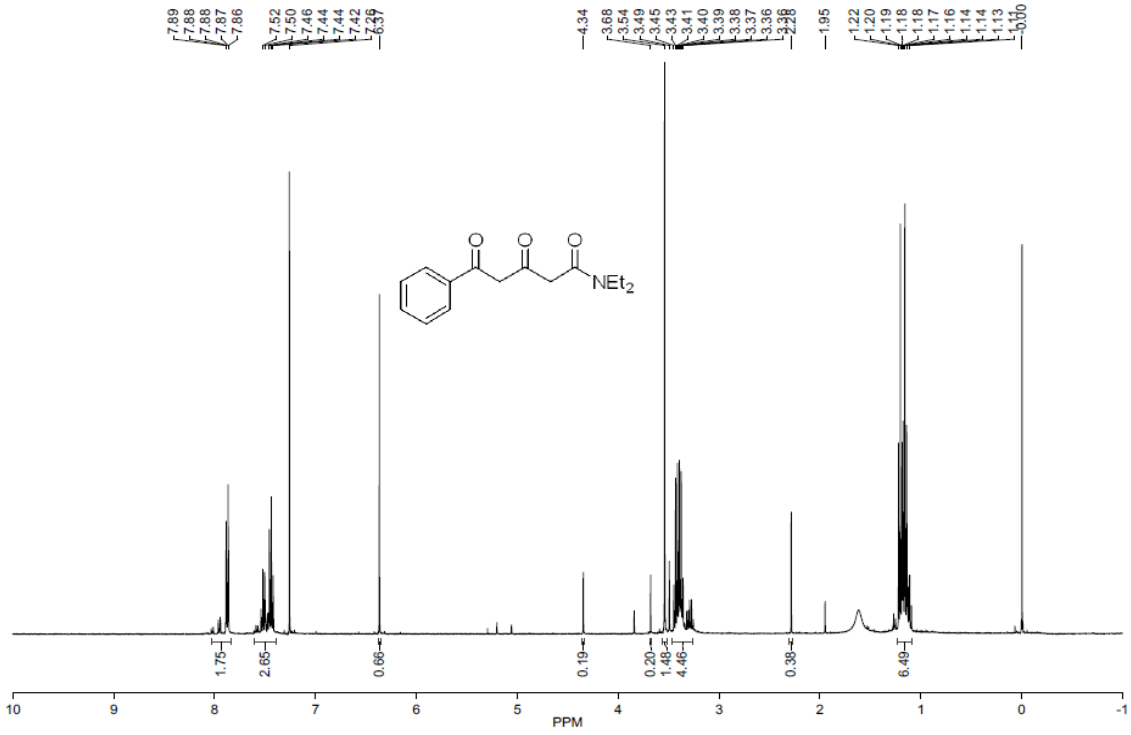
Elements Used: C: 0-18 H: 0-25 N: 0-2 O: 0-5 Na: 0-1

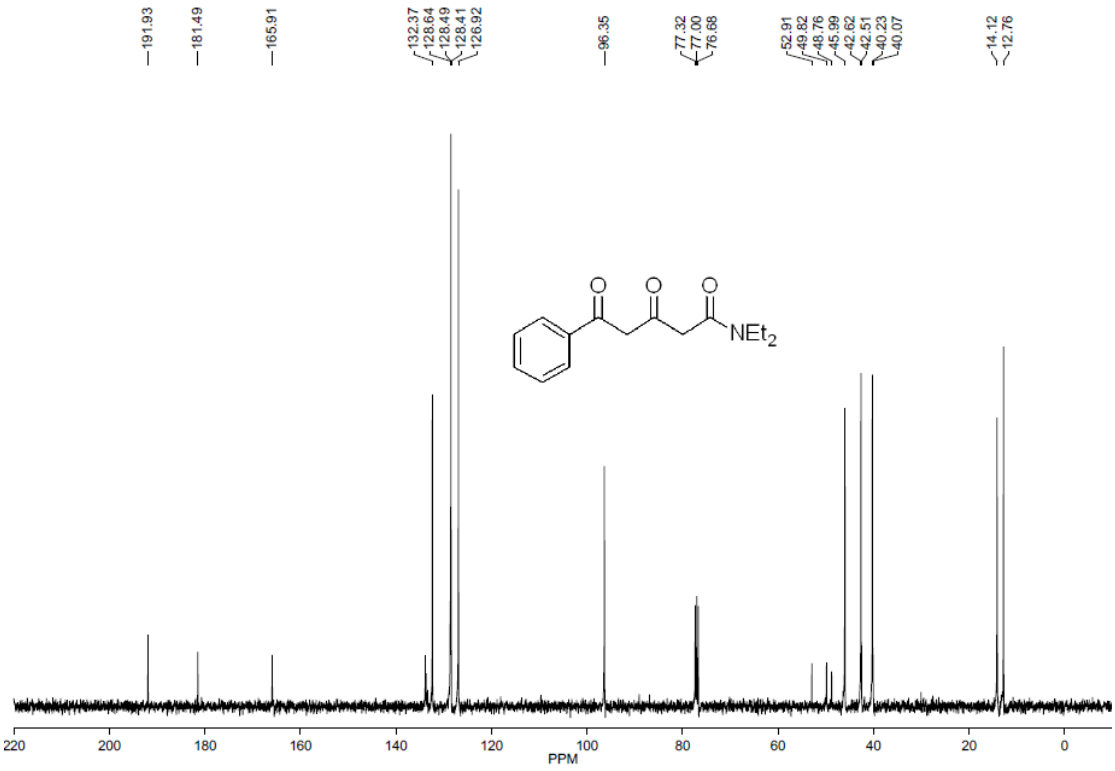


Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
312.1577	312.1576	0.1	0.3	6.5	1714.9

Formula $C_{17}H_{23}NO_3Na$

(1m) *N*, *N*-diethyl-3, 5-dioxo-5-phenylpentanamide





Elemental Composition Report

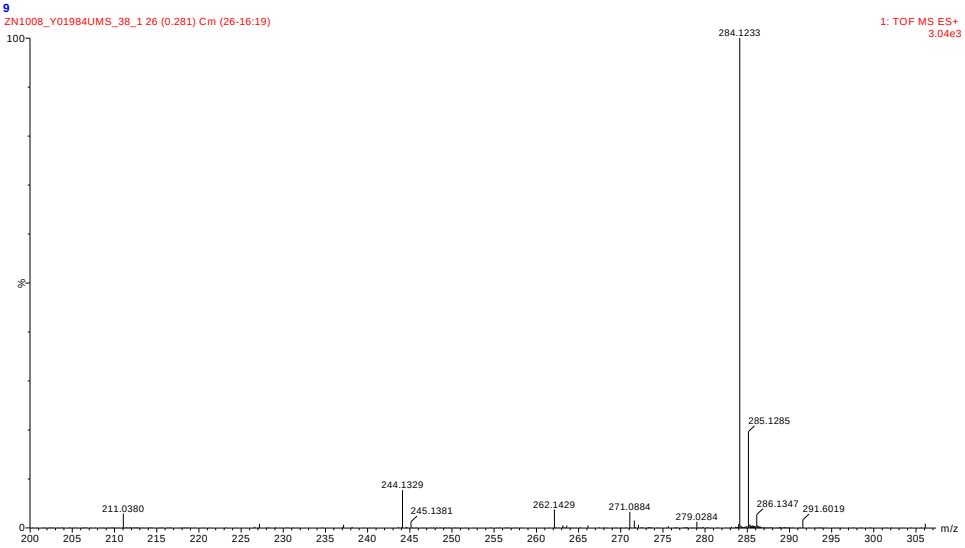
Single Mass Analysis

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

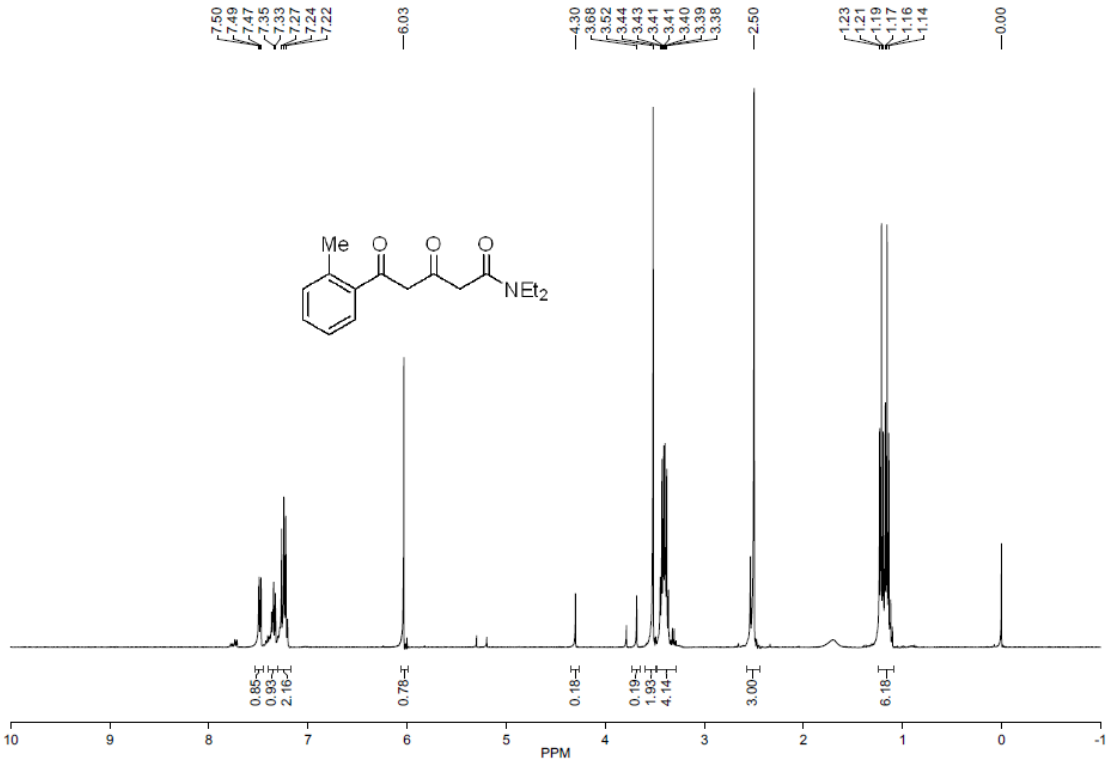
229 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

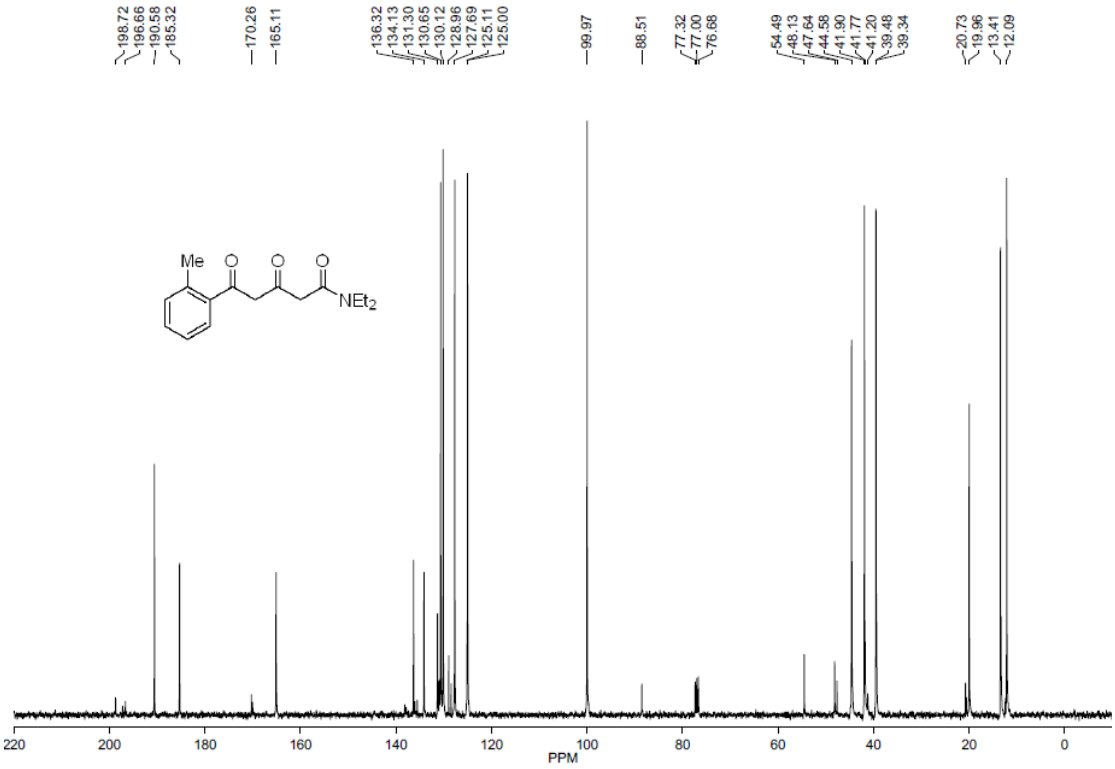
Elements Used: C: 0-20 H: 0-40 N: 0-5 O: 0-5 Na: 0-1



Minimum:				-1.5	
Maximum:		15.0	15.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
284.1233	284.1263	-3.0	-10.6	6.5	6.4
Formula	$C_{15}H_{19}NO_3Na$				

(1n) *N*, *N*-diethyl-3, 5-dioxo-5-(o-tolyl)pentanamide





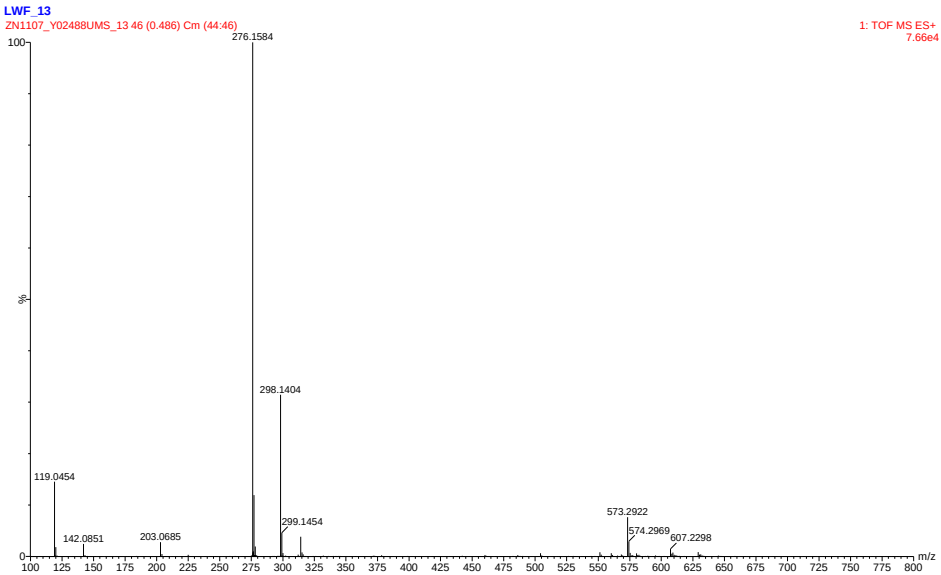
Elemental Composition Report

Single Mass Analysis Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

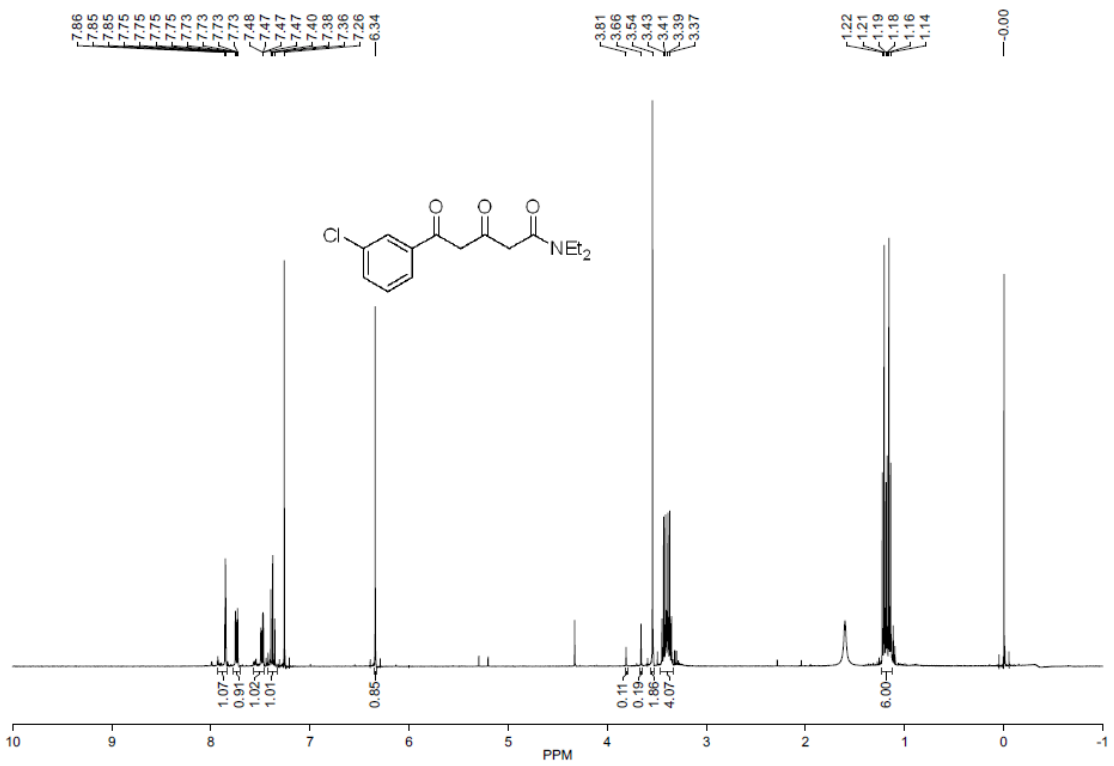
127 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

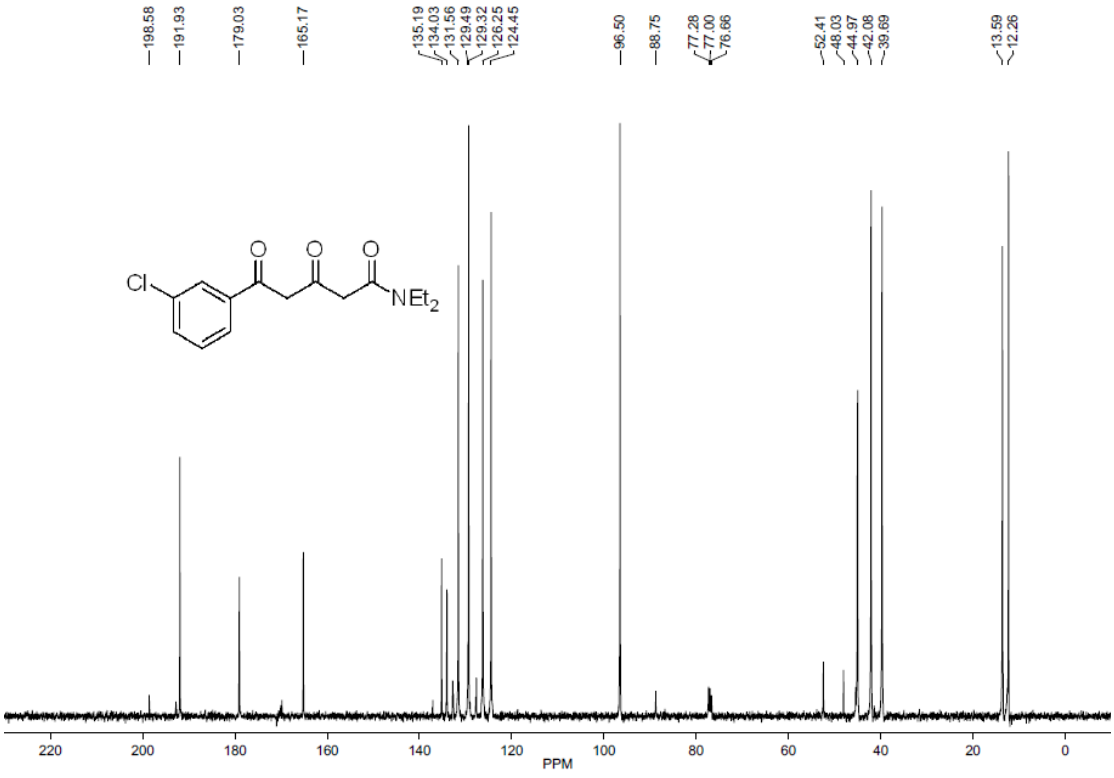
Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1 Br: 0-2



Minimum:				-1.5	
Maximum:		10.0	20.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
276.1584	276.1600	-1.6	-5.8	6.5	1130.2
Formula	$C_{16}H_{22}NO_3$				

(1o) 5-(3-chlorophenyl)-*N, N*-diethyl-3, 5-dioxopentanamide





Elemental Composition Report

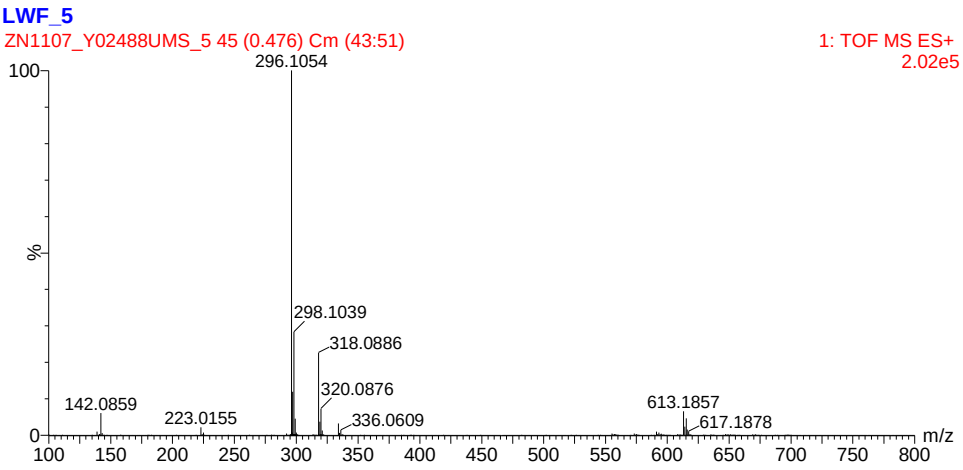
Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

144 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each

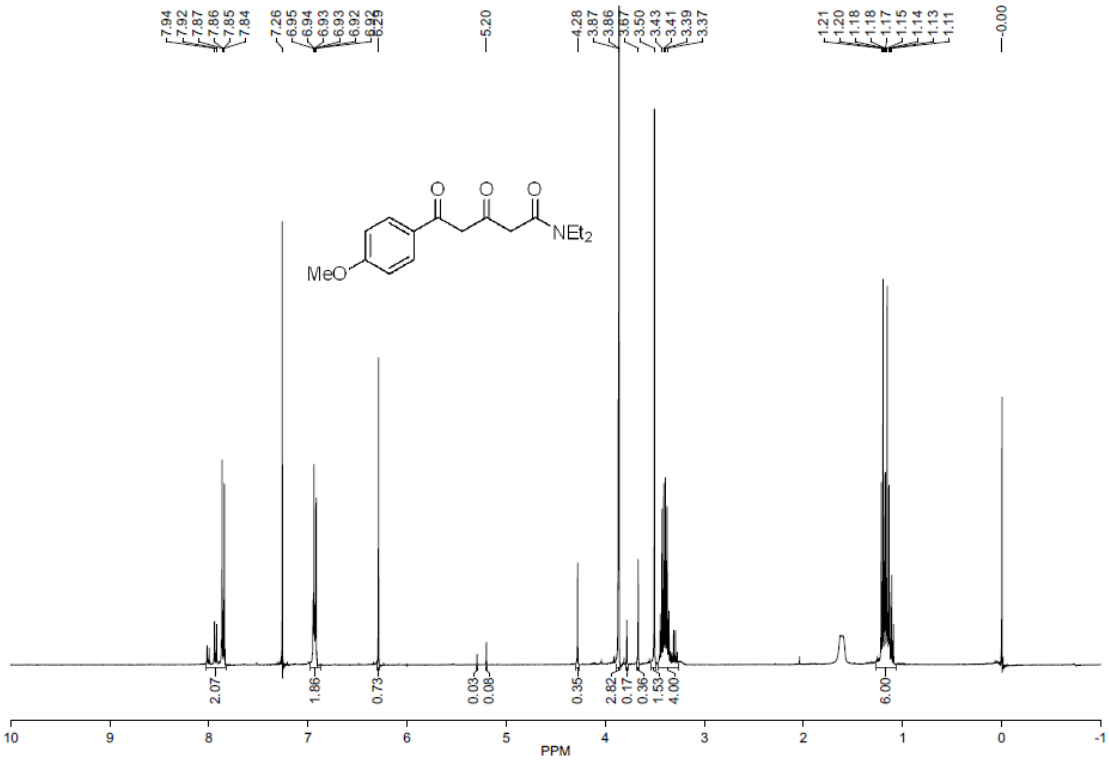
mass)

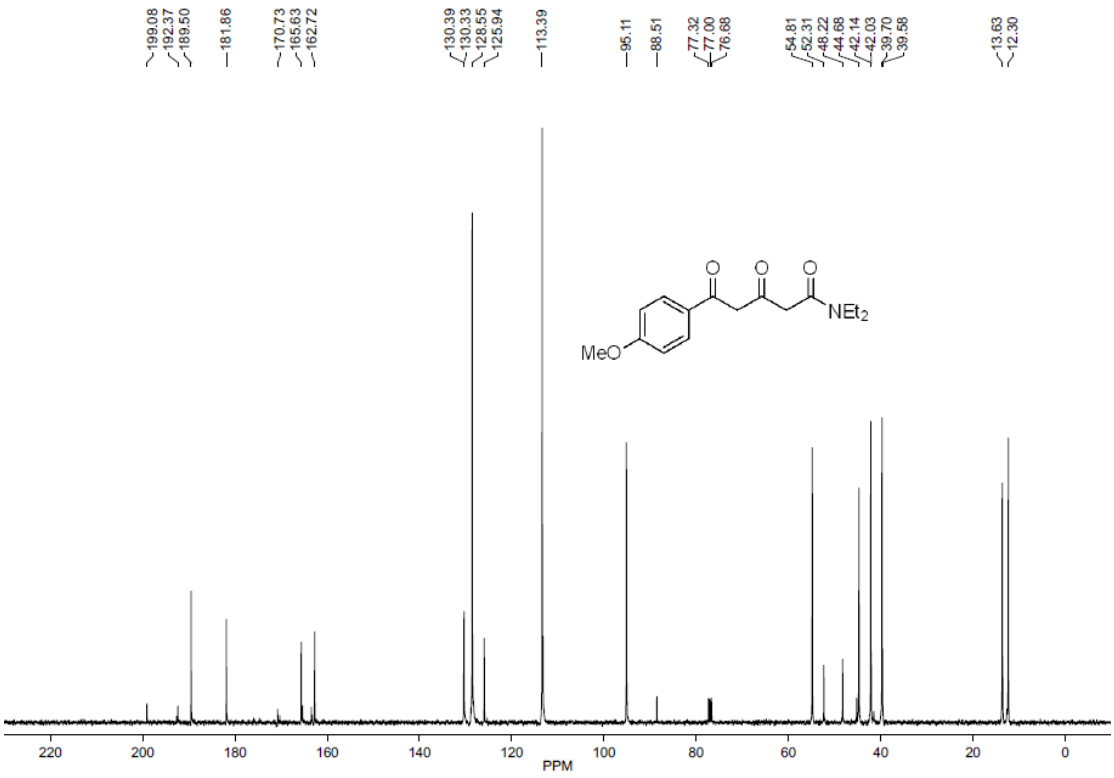
Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1 Cl: 0-2



Minimum:				-1.5	
Maximum:		10.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
296.1054	296.1053	-0.3	-1.0	6.5	356.8
Formula	$C_{15}H_{19}NO_3Cl$				

(1p) *N, N*-diethyl-5-(4-methoxyphenyl)-3, 5-dioxopentanamide





Elemental Composition Report

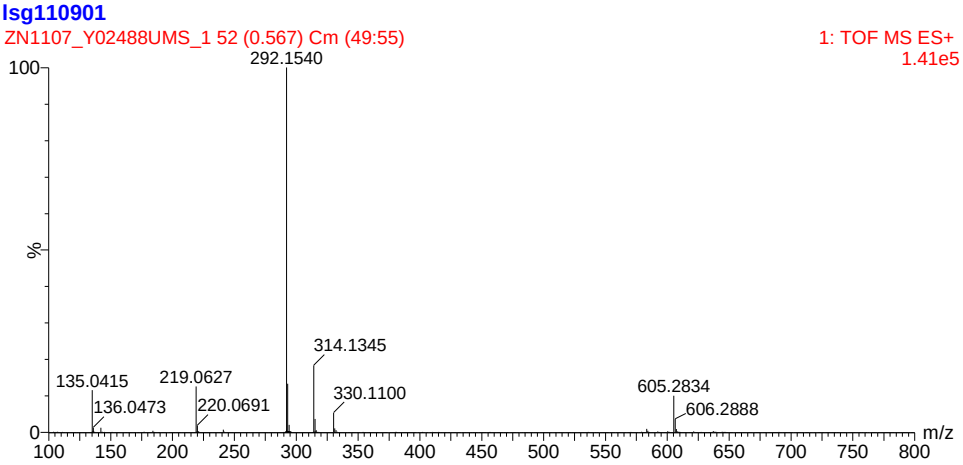
Single Mass Analysis Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

52 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

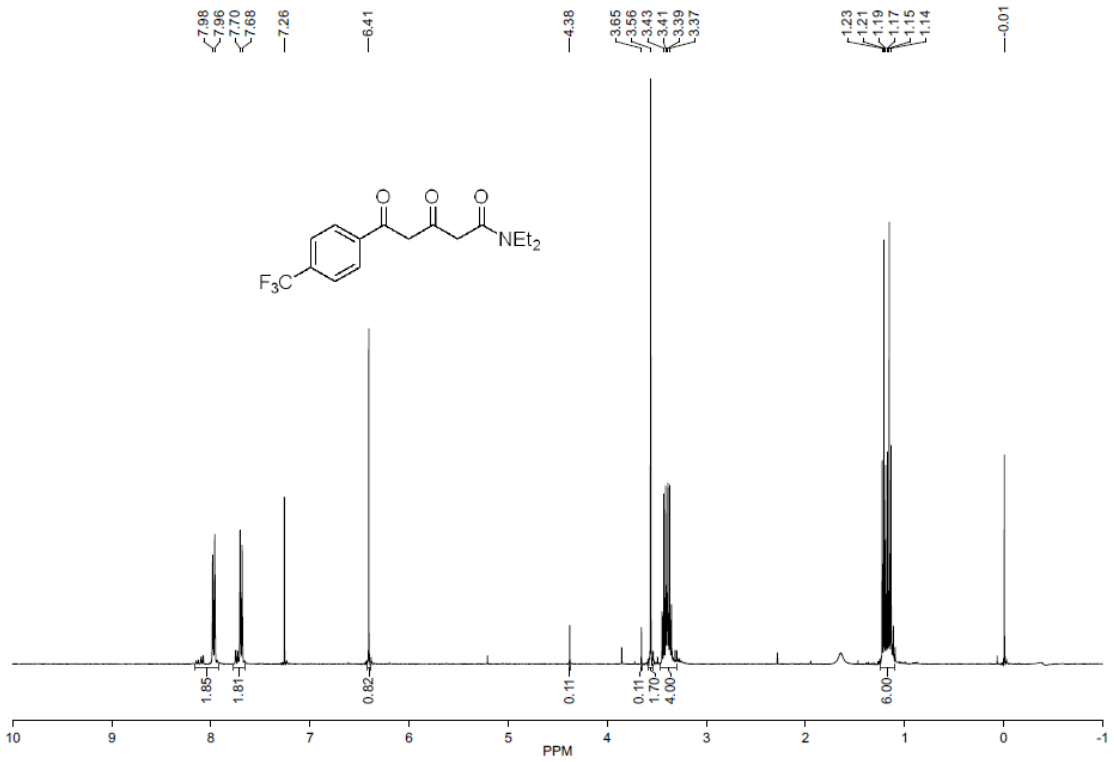
Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1

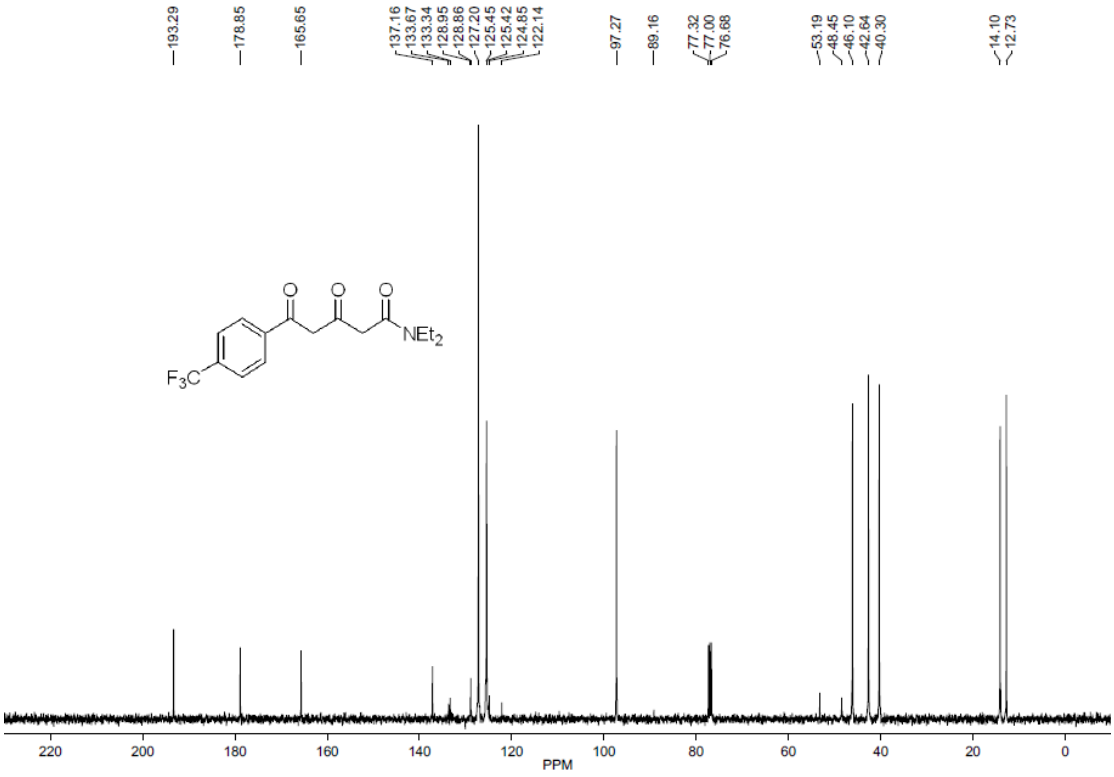
lsg110901



Minimum:				-1.5	
Maximum:		10.0	30.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
292.1540	292.1549	-0.9	-3.1	6.5	1257.8
Formula	$C_{16}H_{22}NO_4$				

(1q) *N, N*-diethyl-3, 5-dioxo-5-(4-(trifluoromethyl)phenyl)pentanamide





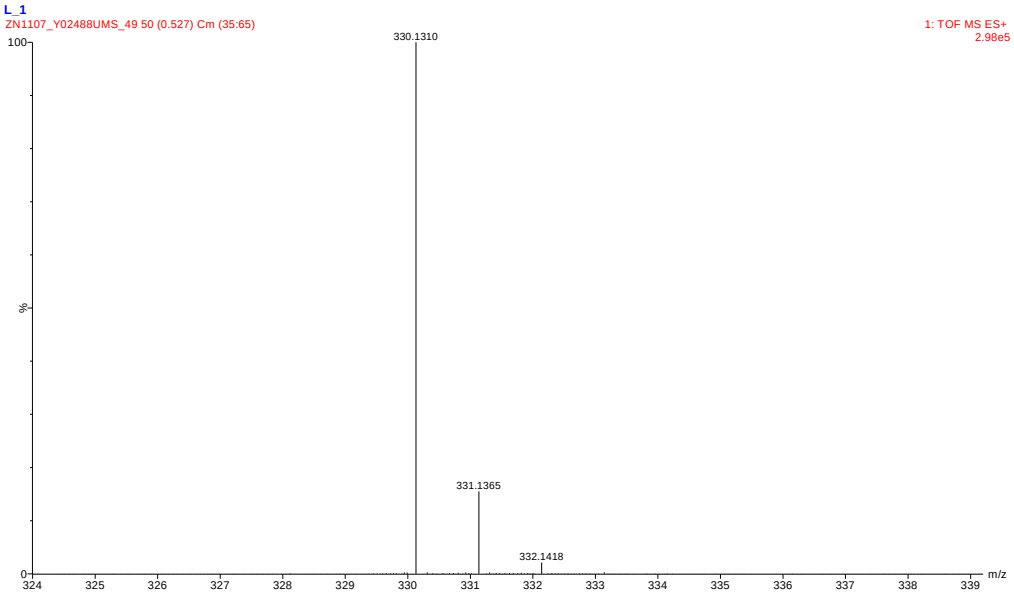
Elemental Composition Report

Single Mass Analysis Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

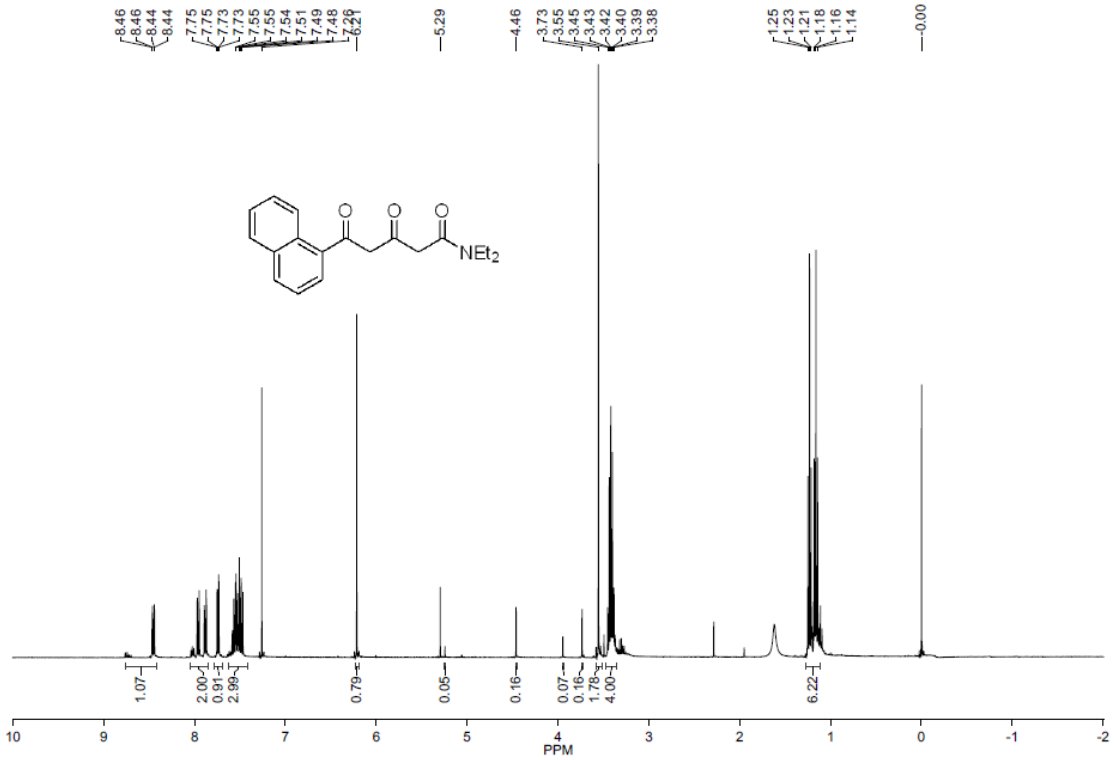
29 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

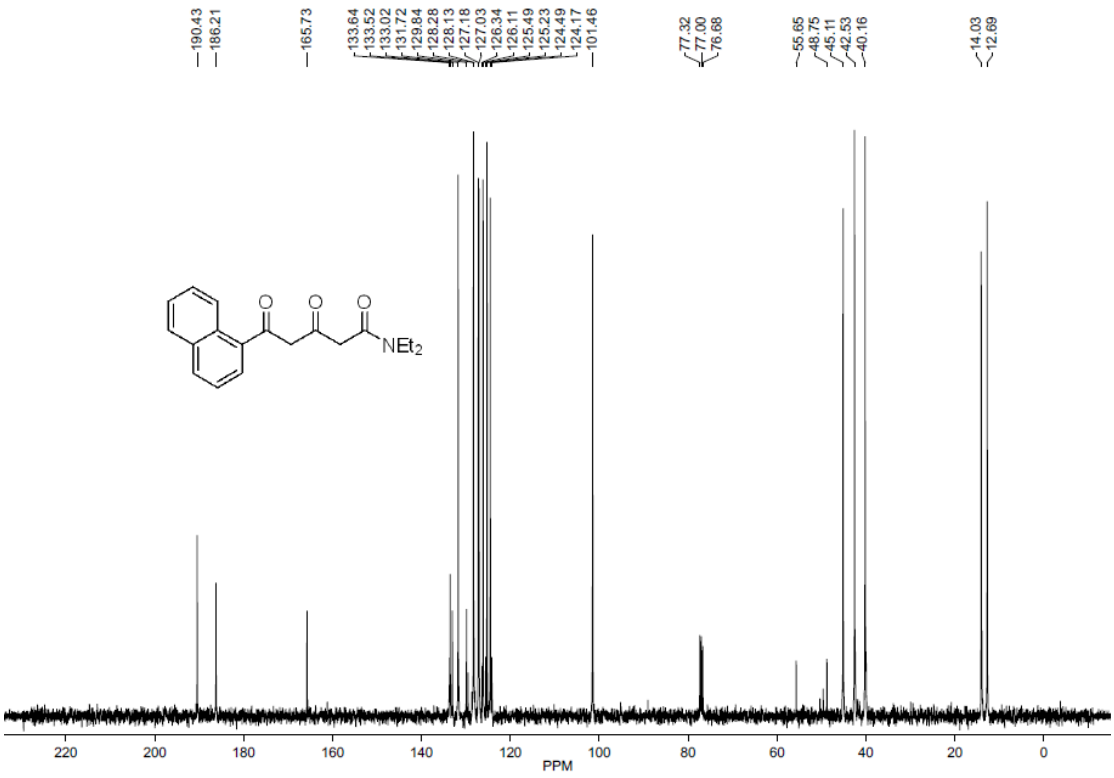
Elements Used: C: 16-20 H: 10-30 N: 0-2 O: 0-8 F: 3-3



Minimum:				-1.5	
Maximum:		10.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
330.1310	330.1317	-0.7	-2.1	6.5	750.7
Formula	$C_{16}H_{19}NO_3F_3$				

(1r) *N, N*-diethyl-5-(naphthalen-1-yl)-3, 5-dioxopentanamide





Elemental Composition Report

Single Mass Analysis

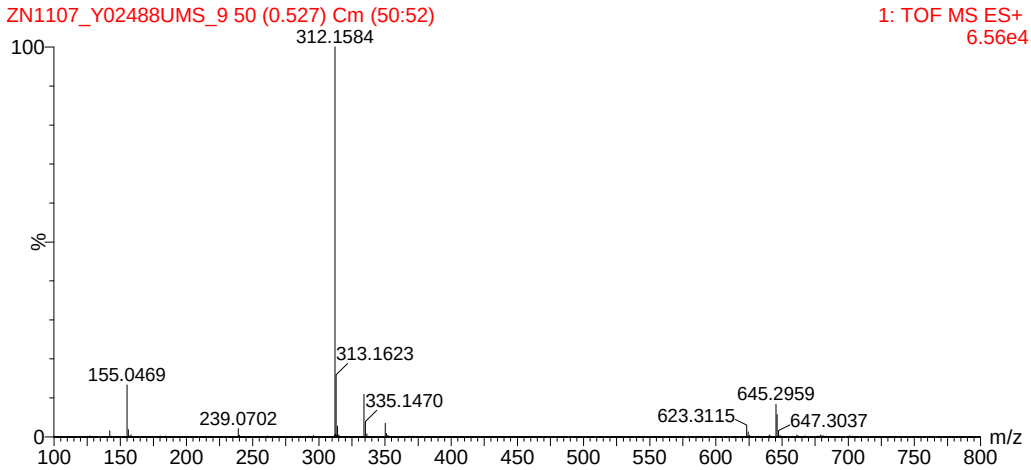
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

141 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1 Cl: 0-2

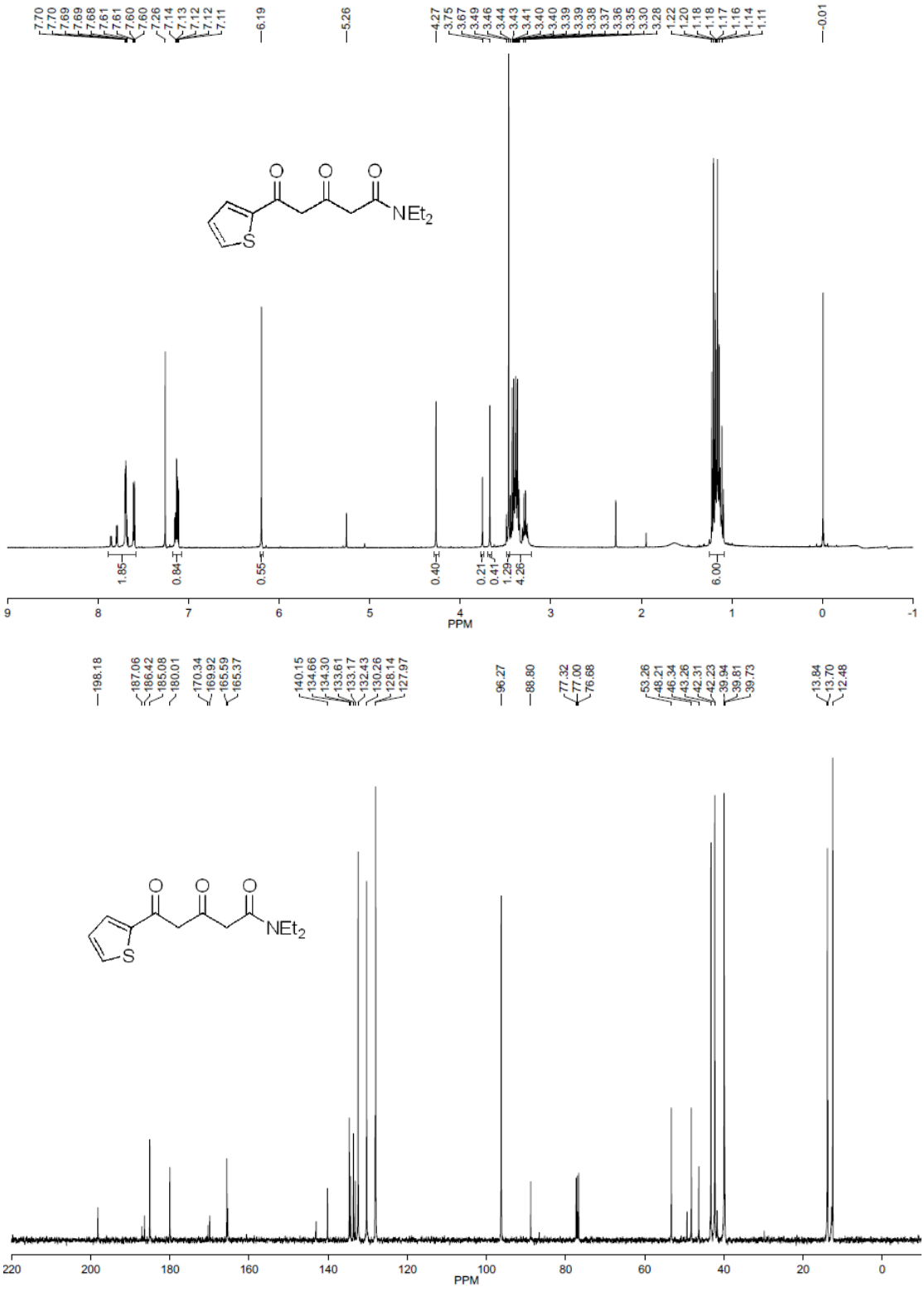
LWF_9



Minimum:				-1.5	
Maximum:		10.0	20.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
312.1584	312.1600	-1.6	-5.1	9.5	608.3

Formula $C_{19}H_{22}NO_3$

(1s) *N, N*-diethyl-3, 5-dioxo-5-(thiophen-2-yl)pentanamide



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

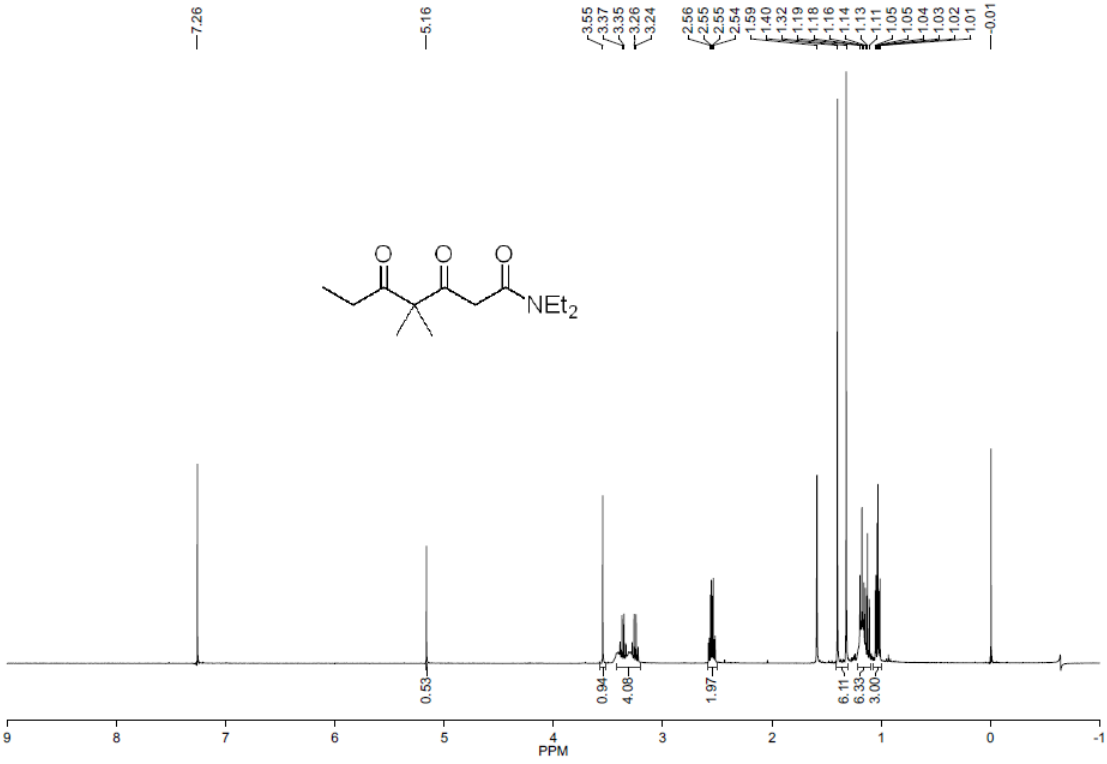
225 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each

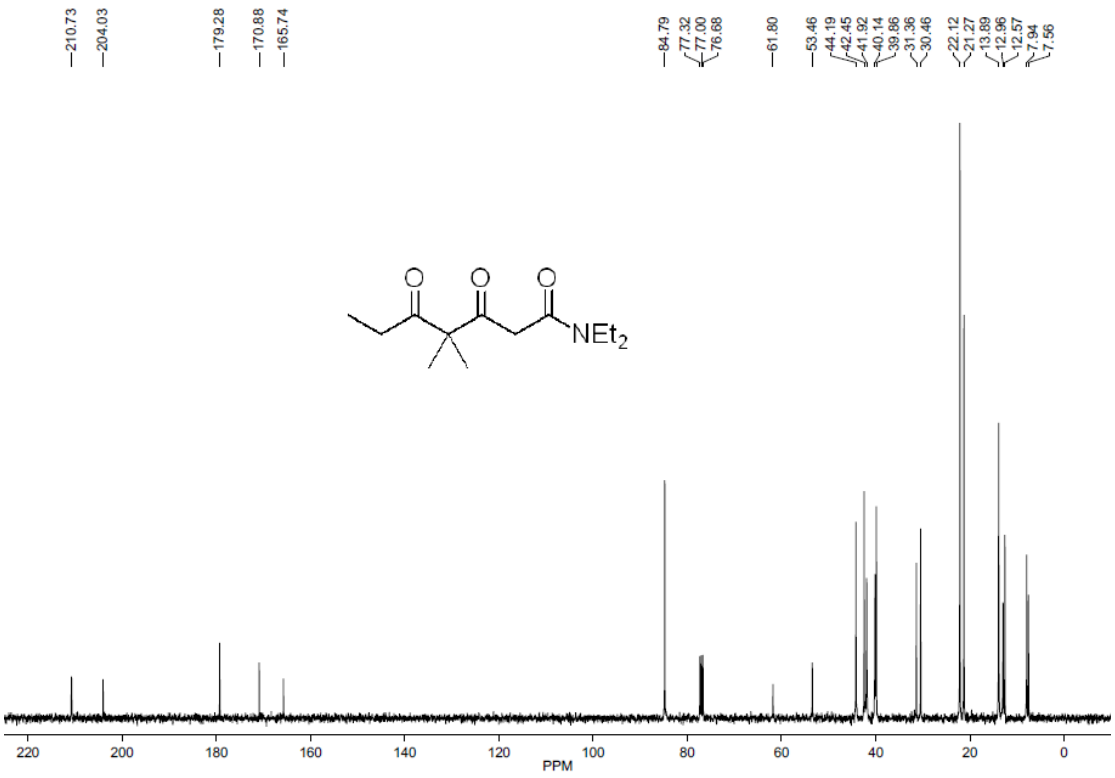
mass)

Elements Used: C: 0-20 H: 0-25 N: 0-2 O: 0-5 Na: 0-1 S: 0-2

Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
290.0825	290.0827	-0.2	-0.7	5.5	5379.4
Formula	$C_{13}H_{17}NO_3NaS$				

(1t) *N, N*-diethyl-4, 4-dimethyl-3, 5-dioxoheptanamide





Elemental Composition Report

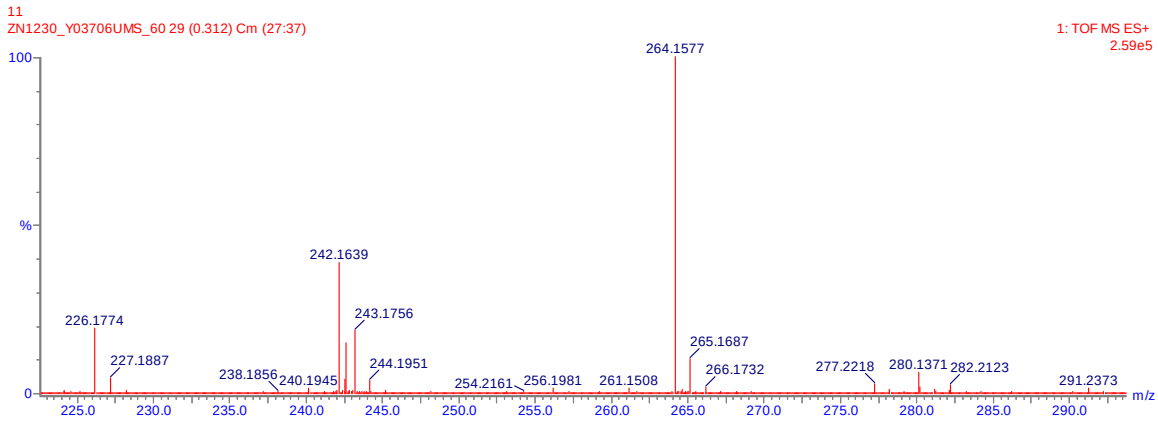
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

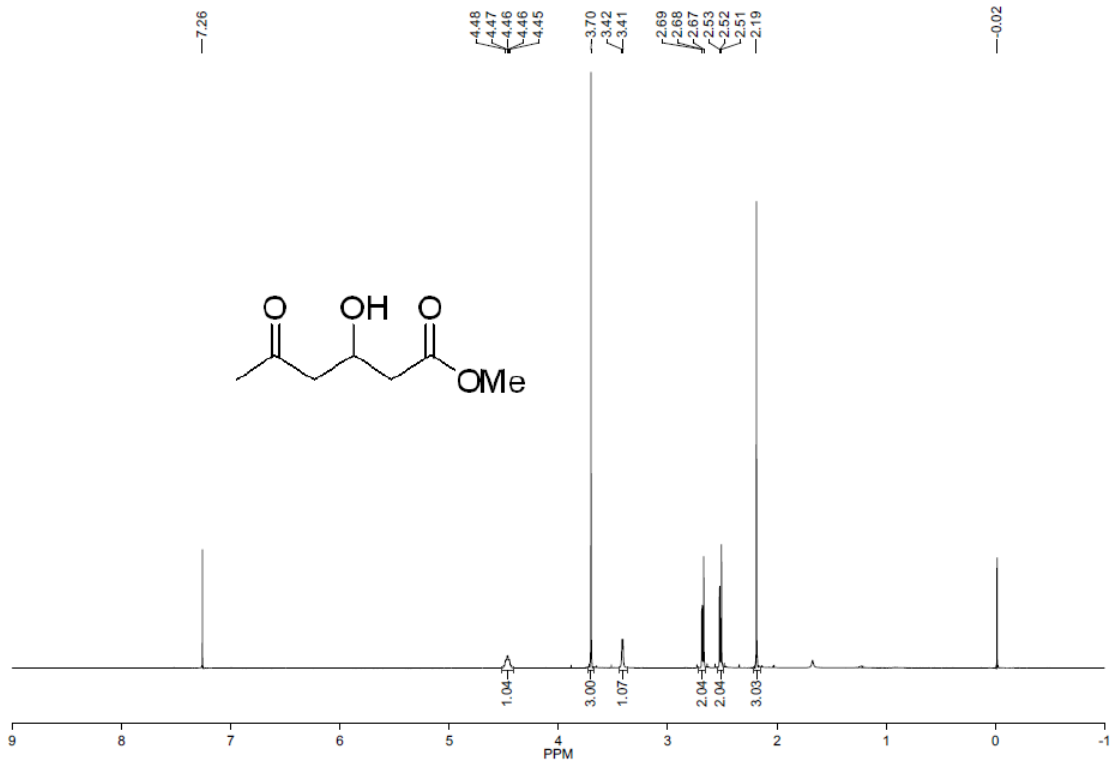
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1

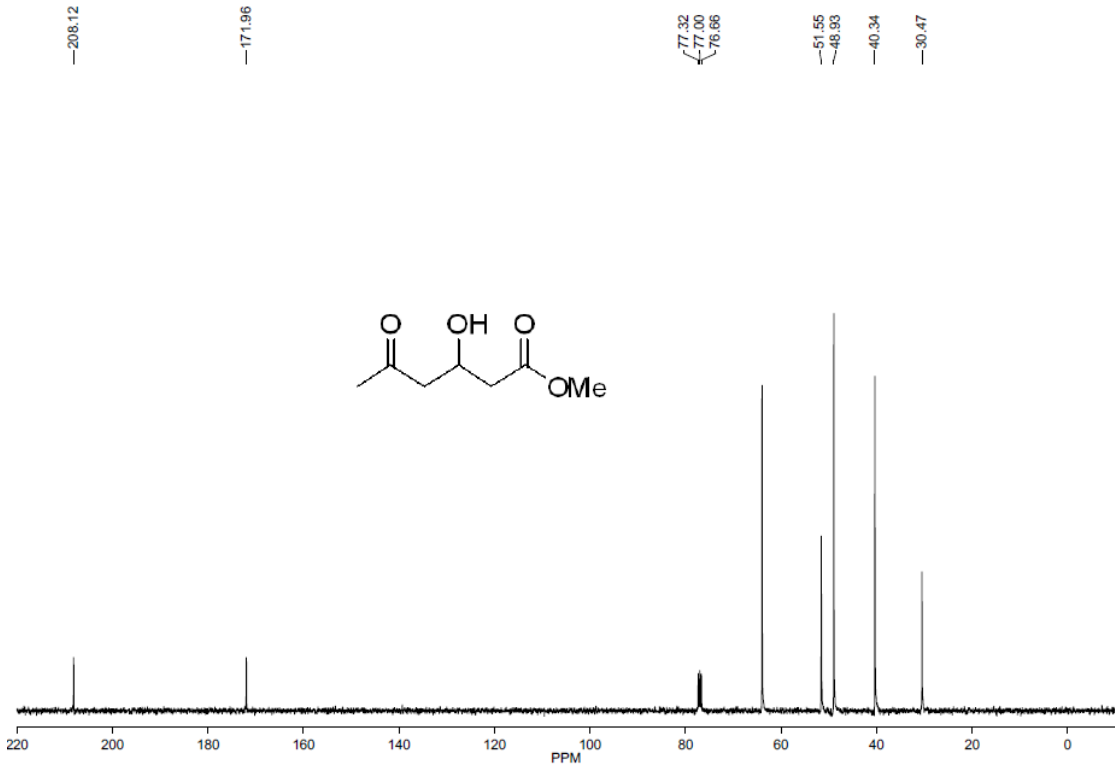


Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
264.1577	264.1576	0.1	0.4	2.5	2911.6

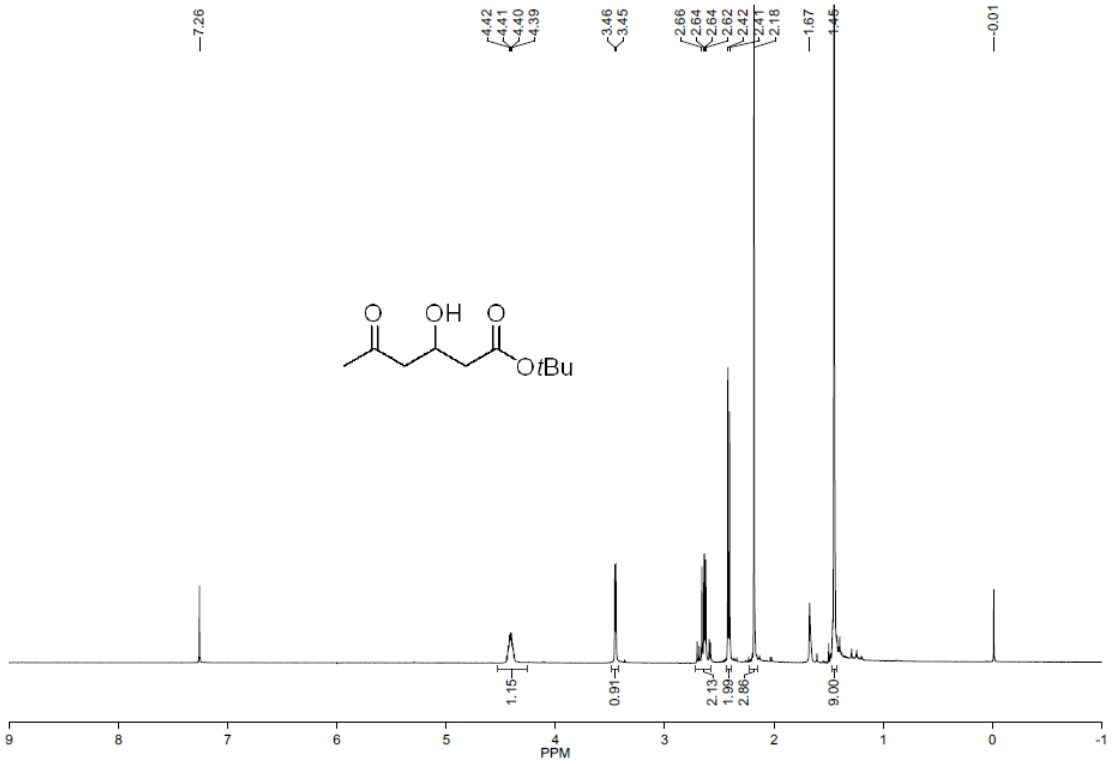
Formula $C_{13}H_{23}NO_3Na$

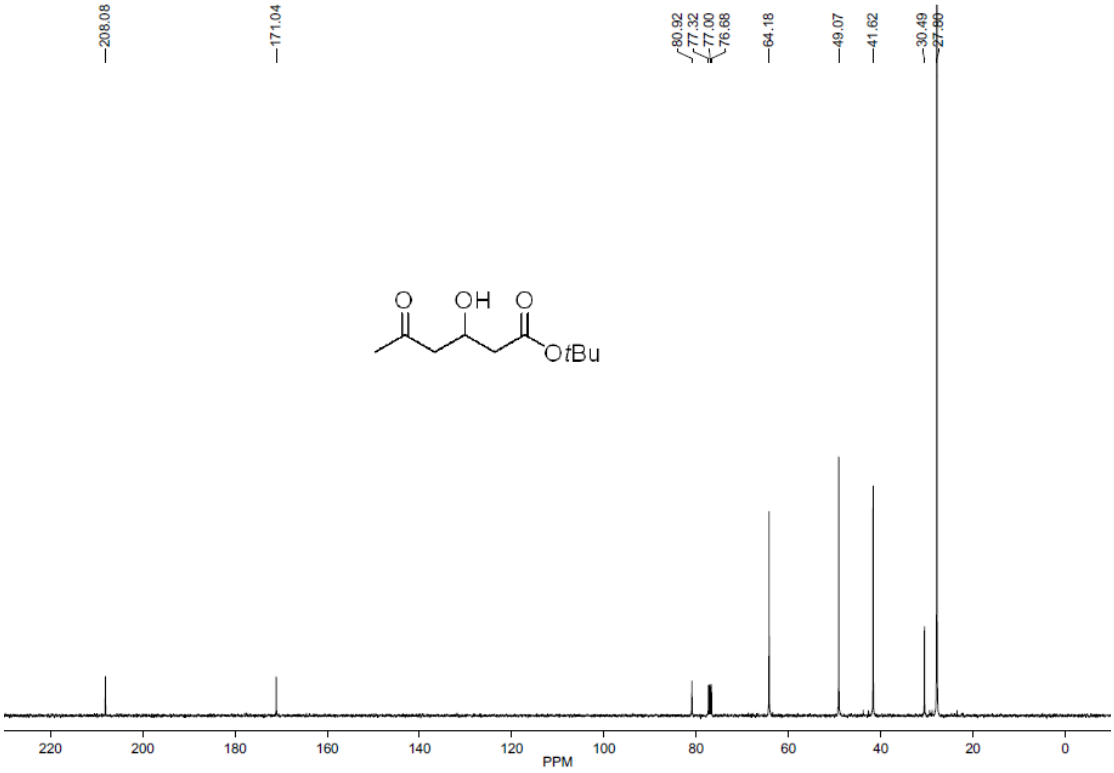
(2a) Methyl 3-hydroxy-5-oxohexanoate





(2b) tert-Butyl 3-hydroxy-5-oxohexanoate





Elemental Composition Report

Single Mass Analysis

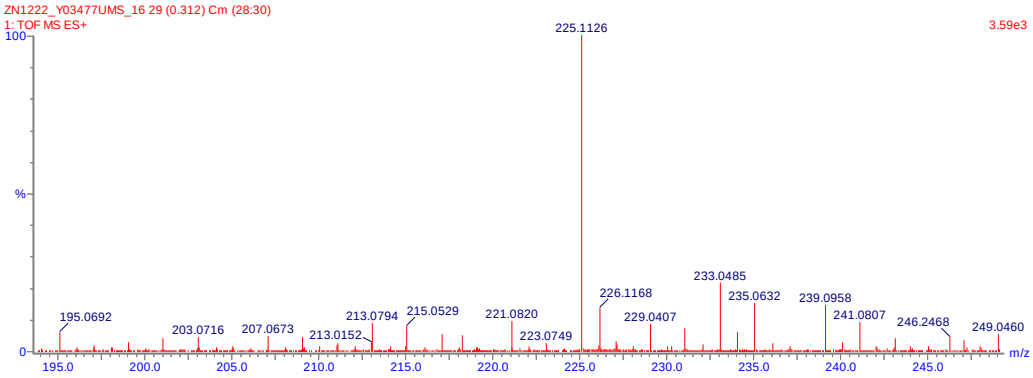
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

34 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each

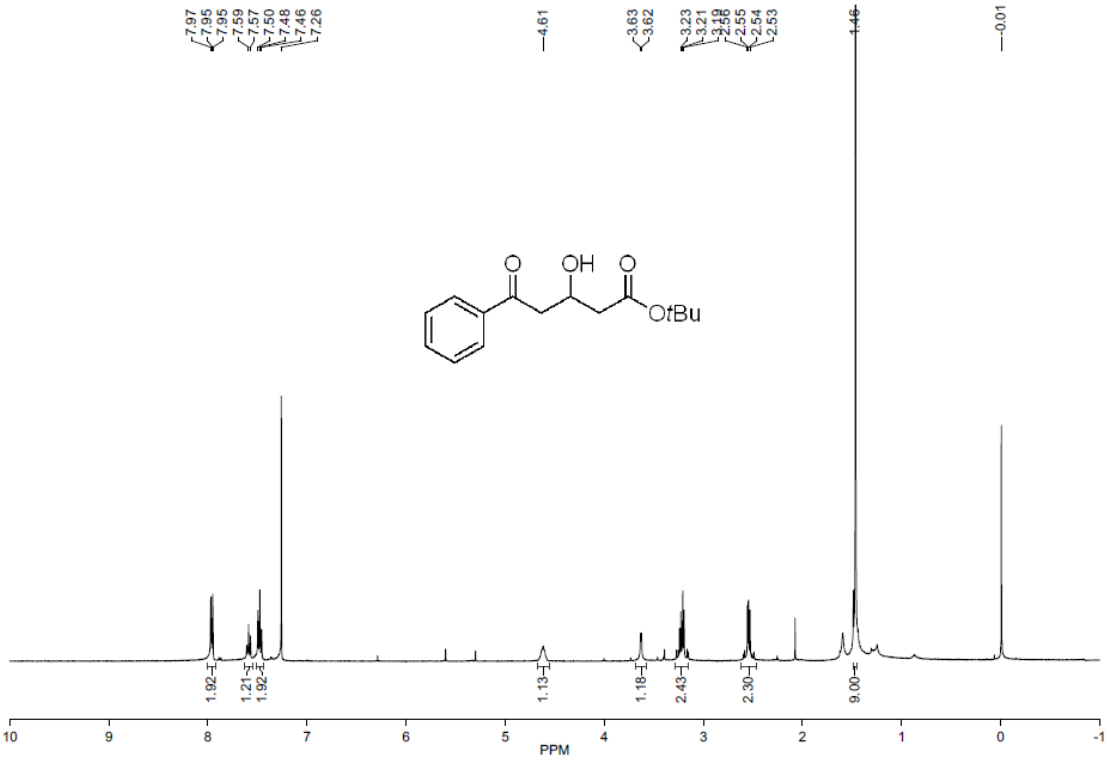
mass)

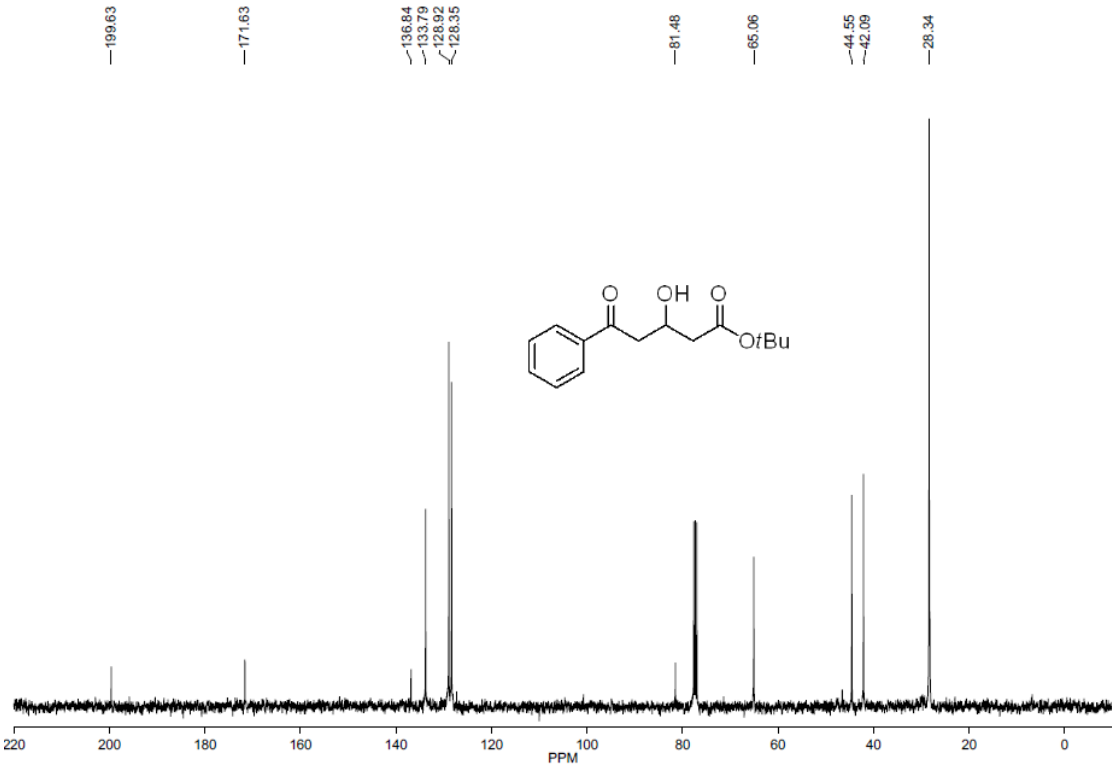
Elements Used: C: 0-20 H: 0-35 O: 0-5 Na: 0-1



Minimum:				-1.5	
Maximum:		8.0	100.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
225.1126	225.1103	2.3	10.2	1.5	7.7
Formula	$C_{10}H_{18}O_4Na$				

(2c) tert-Butyl 3-hydroxy-5-phenyl-5-oxopentanoate





Elemental Composition Report

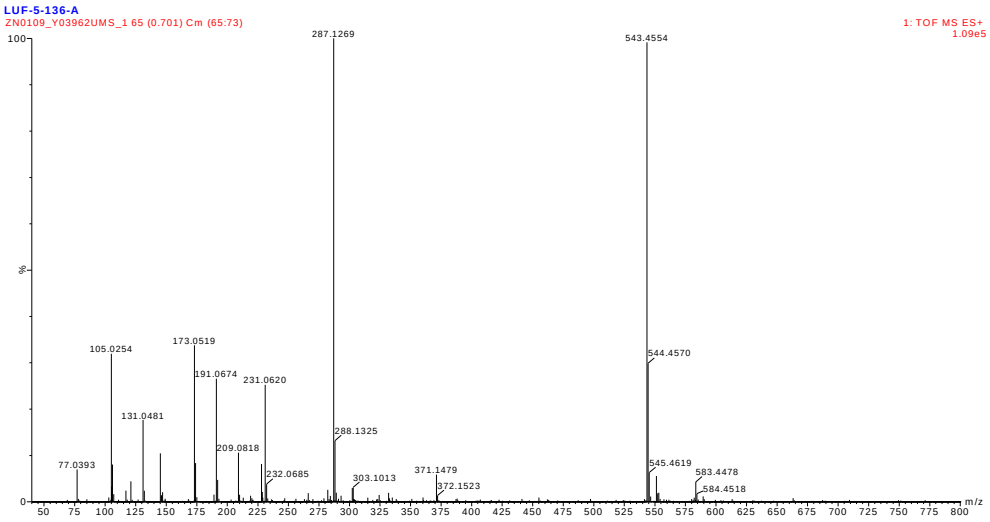
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

17 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

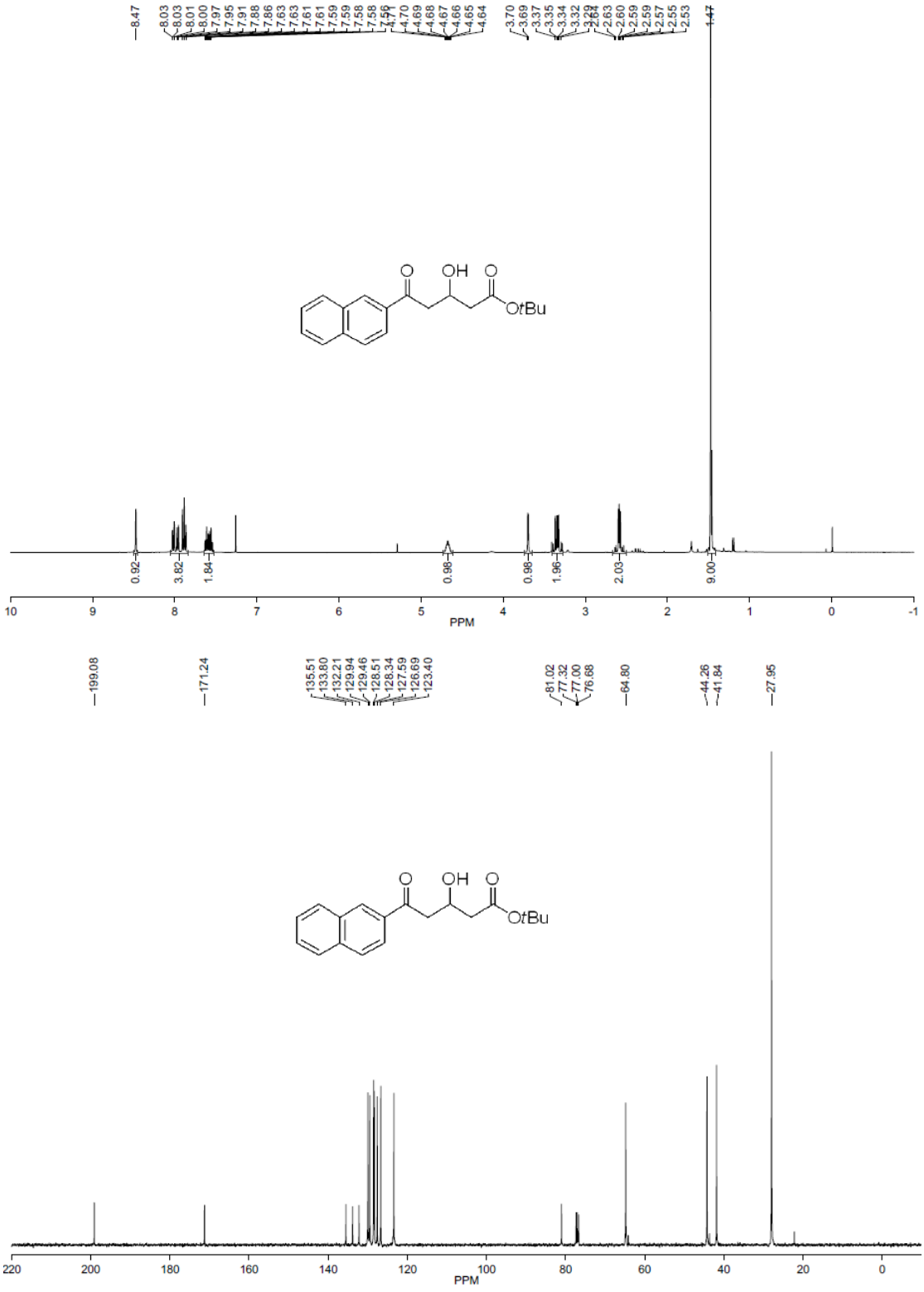
Elements Used: C: 0-20 H: 0-20 O: 0-5 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
287.1269	287.1259	1.0	3.5	5.5	552.2

Formula $C_{15}H_{20}O_4Na$

(2d) tert-Butyl 3-hydroxy-5-(naphthalen-2-yl)-5-oxopentanoate



Elemental Composition Report

Single Mass Analysis

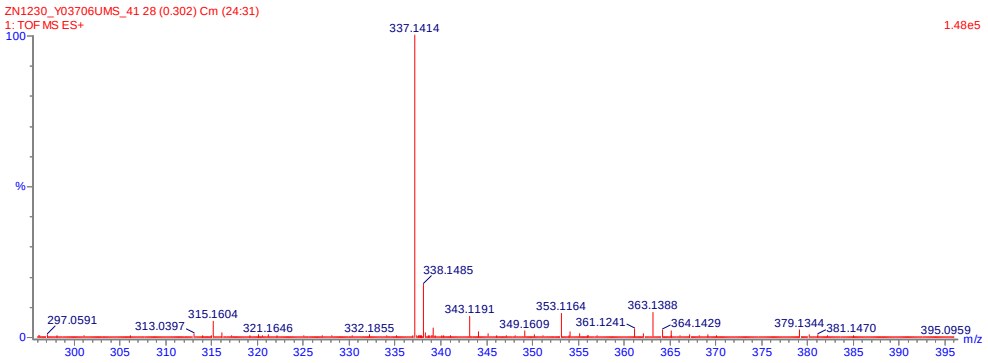
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each

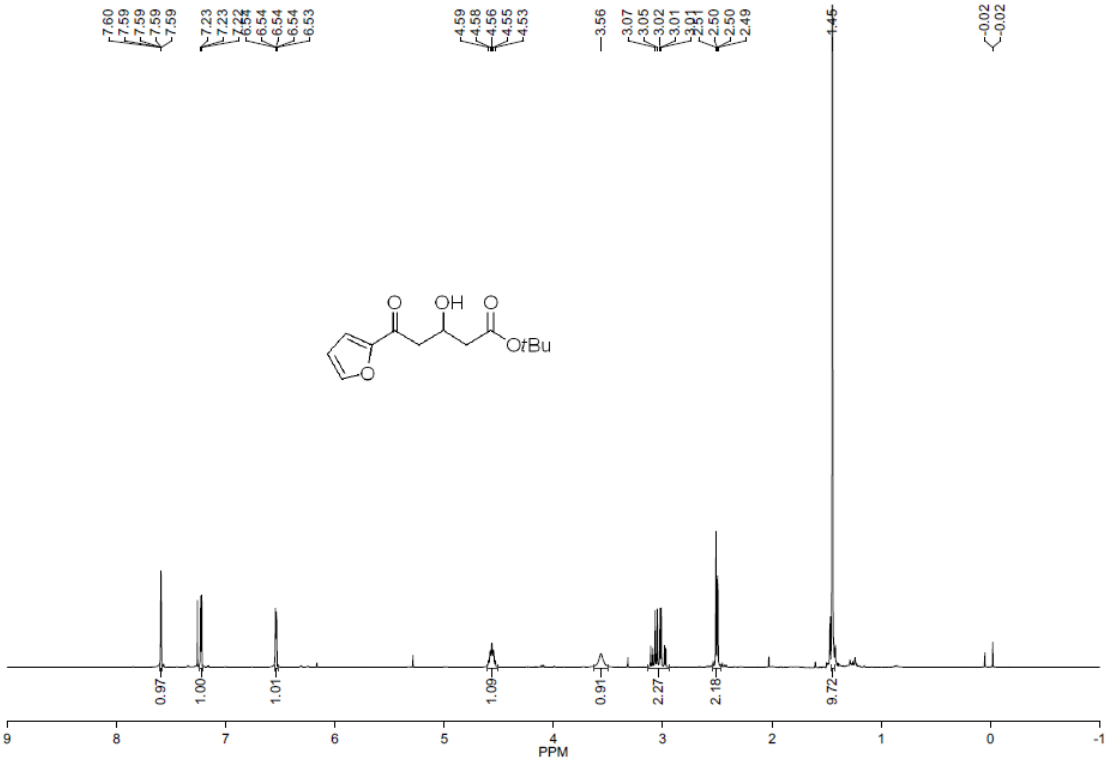
mass)

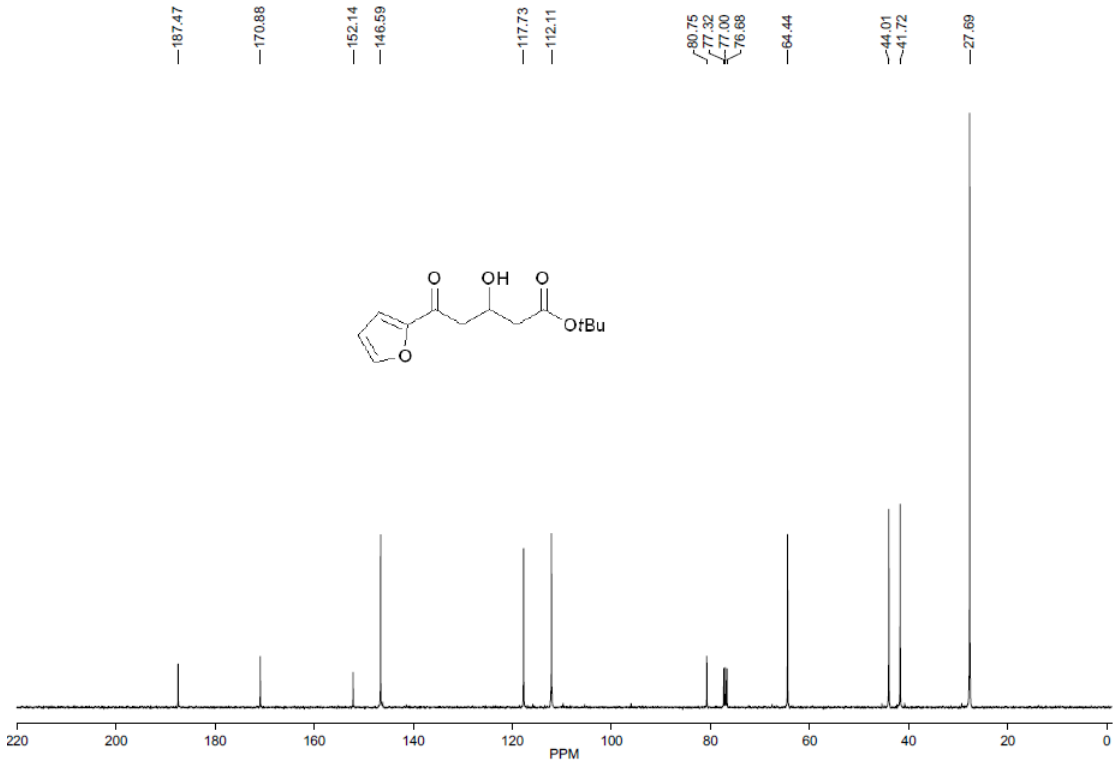
Elements Used: C: 2-20 H: 20-32 O: 3-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	30.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
337.1414	337.1416	-0.2	-0.6	8.5	613.6
Formula	$C_{19}H_{22}O_4Na$				

(2e) tert-butyl 5-(furan-2-yl)-3-hydroxy-5-oxopentanoate





Elemental Composition Report

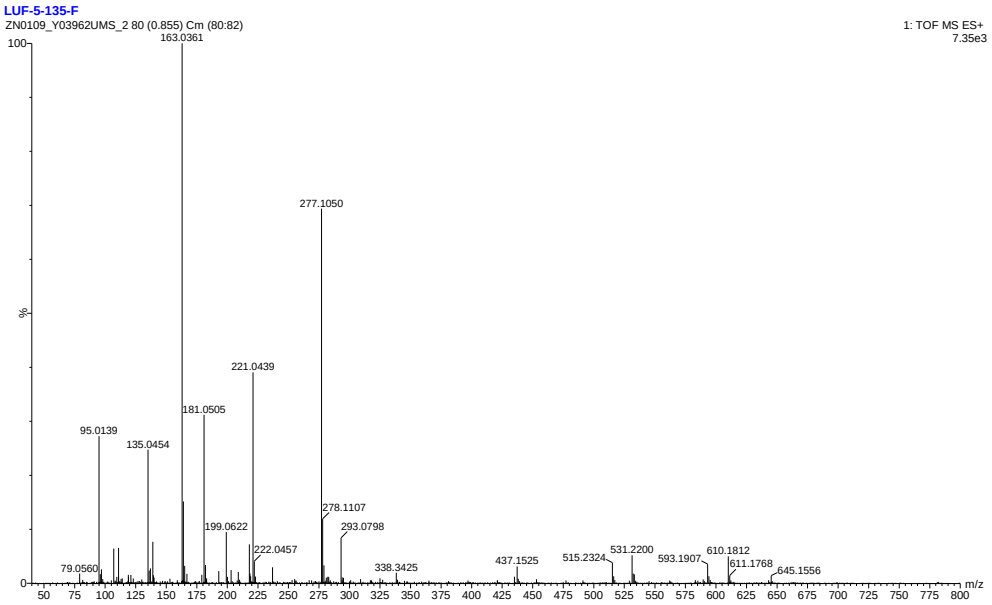
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 0-20 H: 0-20 O: 0-5 Na: 0-1

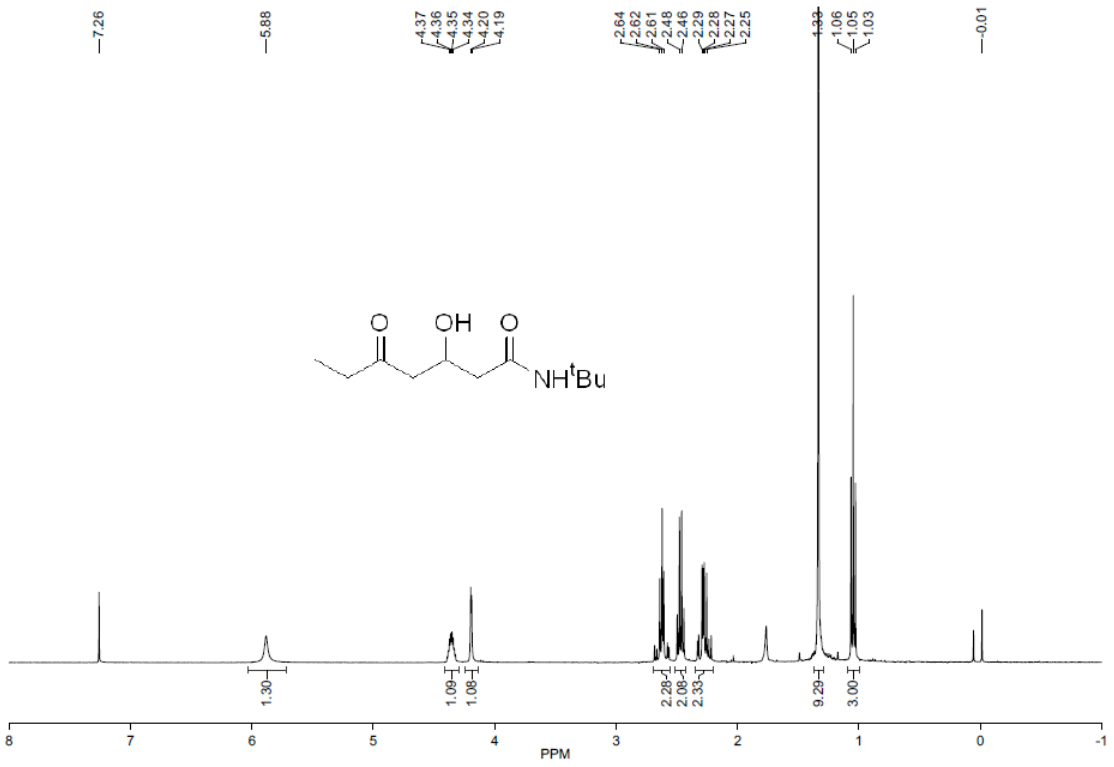


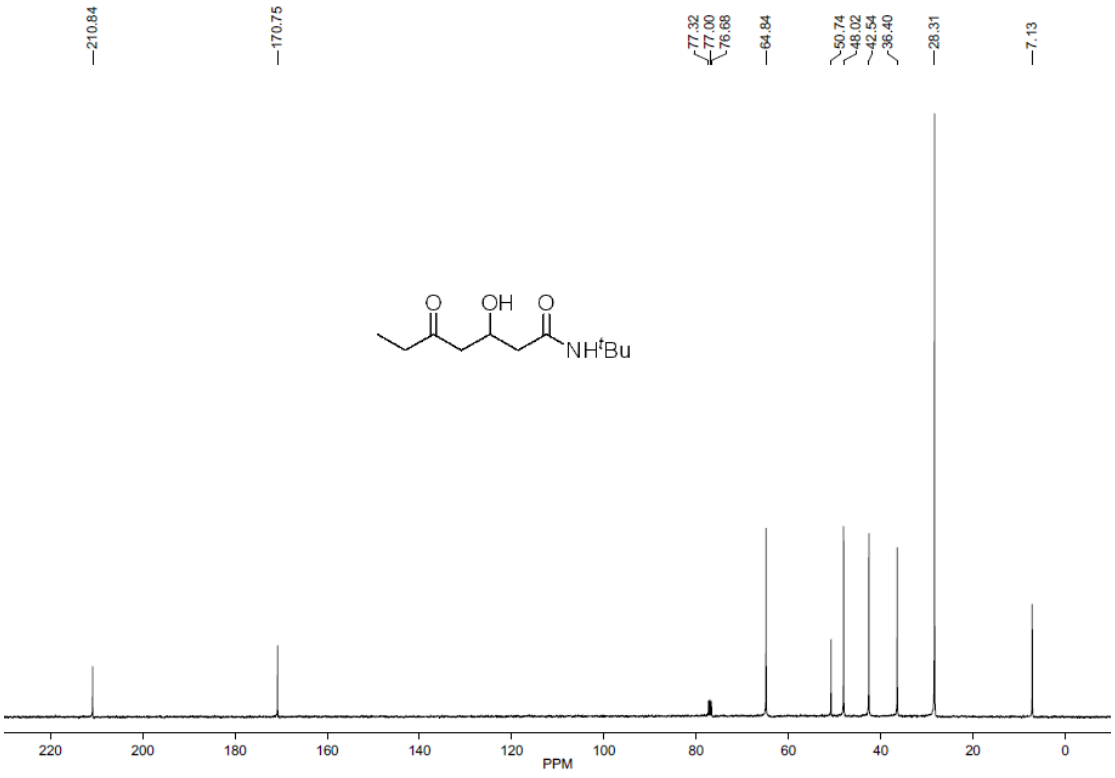
Minimum:				-1.5	
Maximum:		5.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT

277.1050	277.1052	-0.2	-0.7	4.5	45.1

Formula $C_{13}H_{18}O_5Na$

(2f) *N*-(tert-butyl)-3-hydroxy-5-oxoheptanamide





Elemental Composition Report

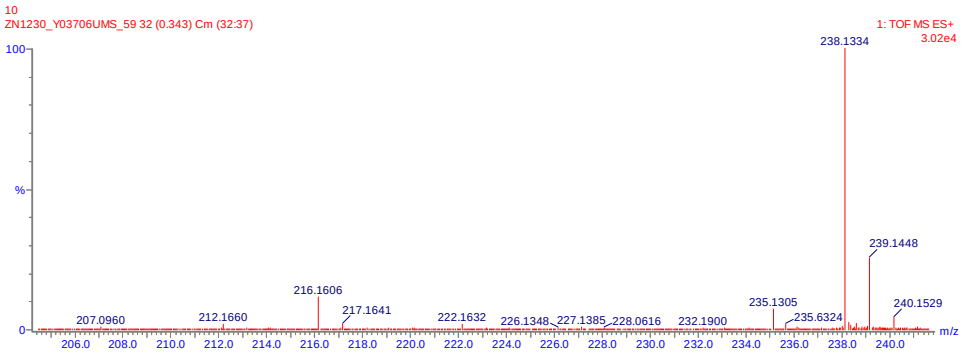
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

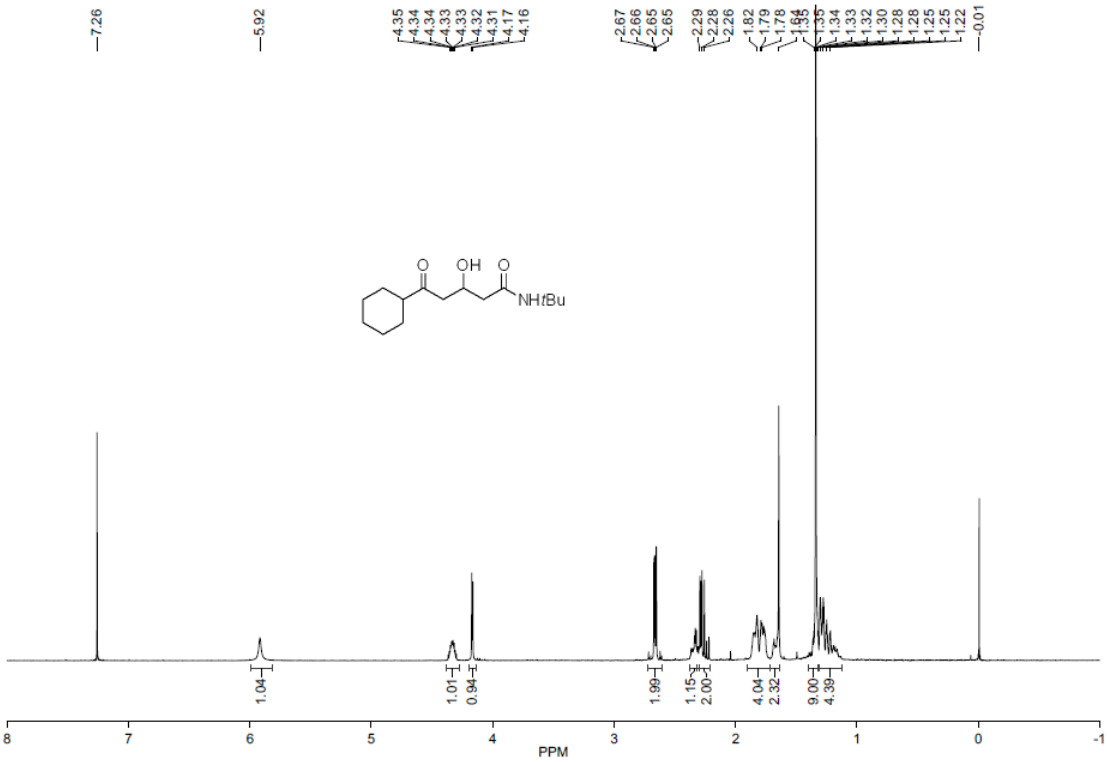
29 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

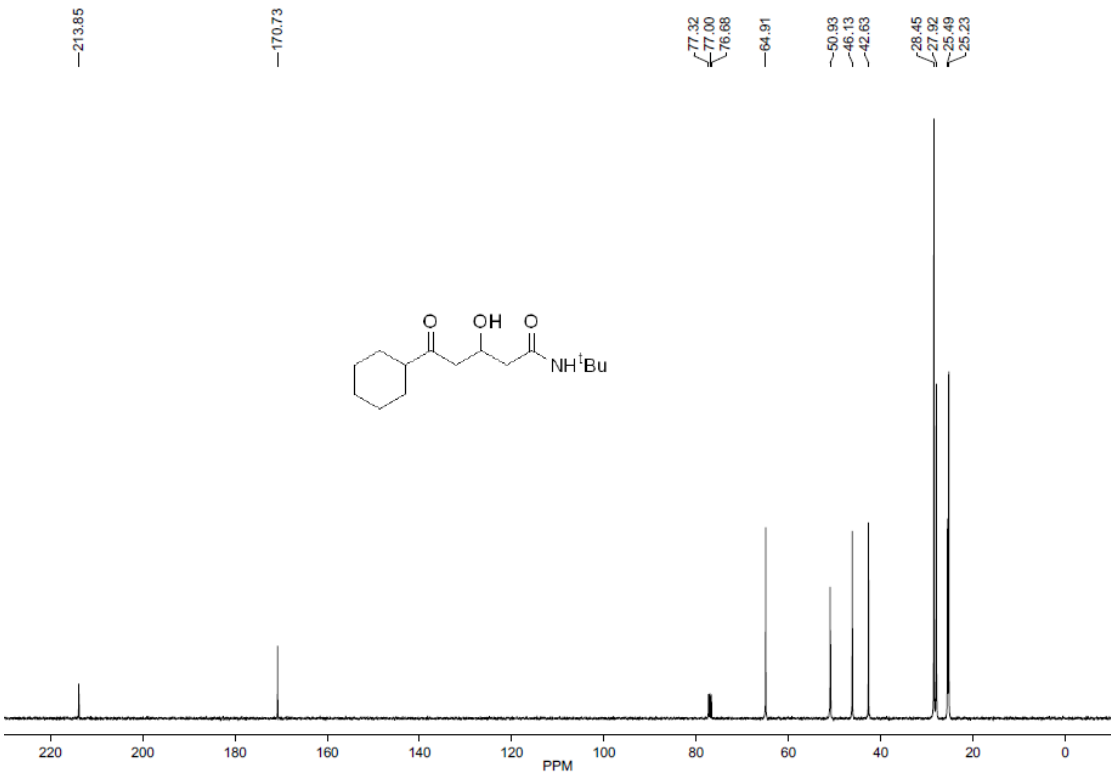
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 2-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
216.1606	216.1600	0.6	2.8	1.5	25.2
Formula	$C_{11}H_{22}NO_3$				

(2g) N-(tert-butyl)-5-cyclohexyl-3-hydroxy-5-oxopentanamide





Elemental Composition Report

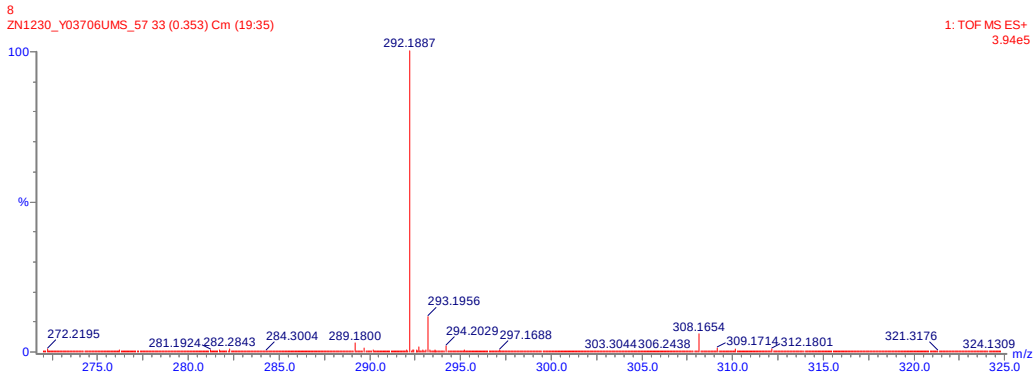
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

45 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

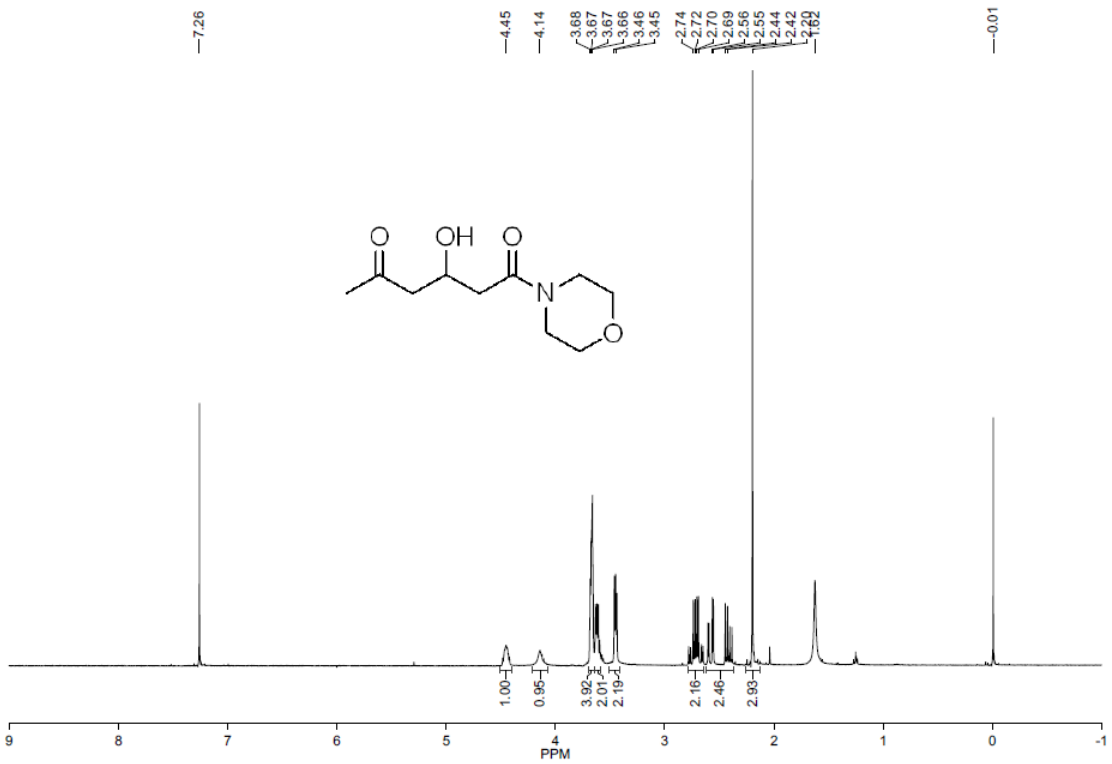
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1

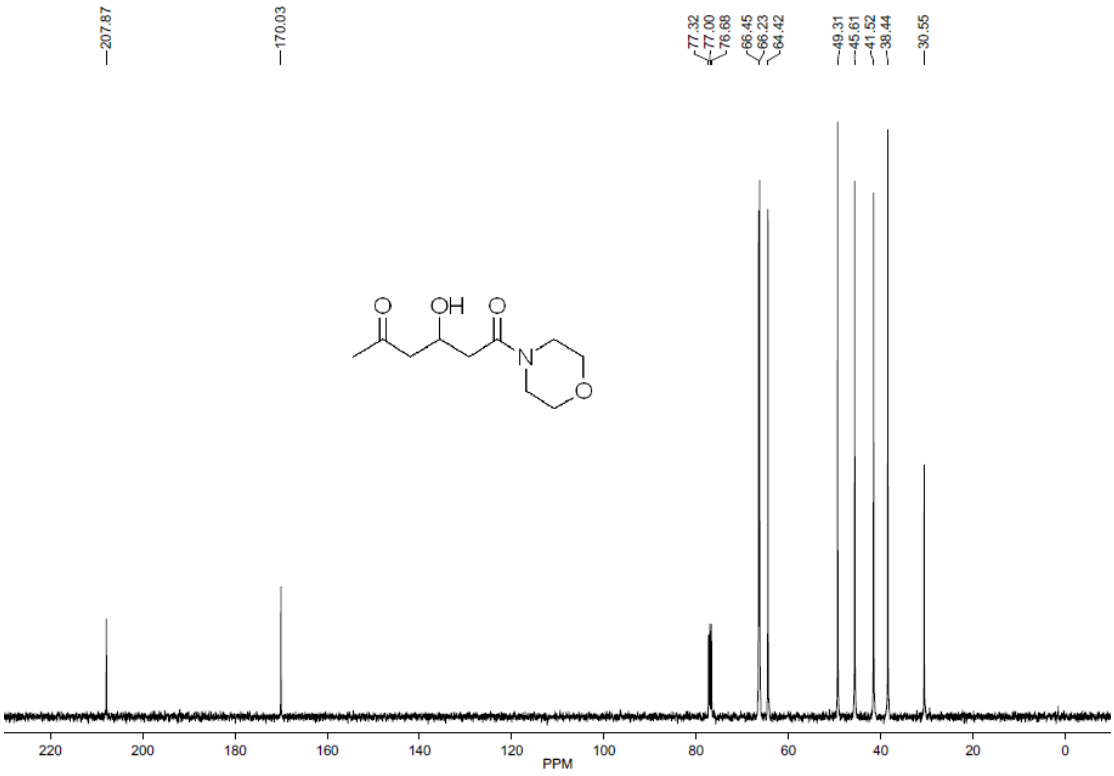


Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
292.1887	292.1889	-0.2	-0.7	2.5	5061.8

Formula $C_{15}H_{27}NO_3Na$

(2h) 3-hydroxy-1-morpholinohexane-1, 5-dione





Elemental Composition Report

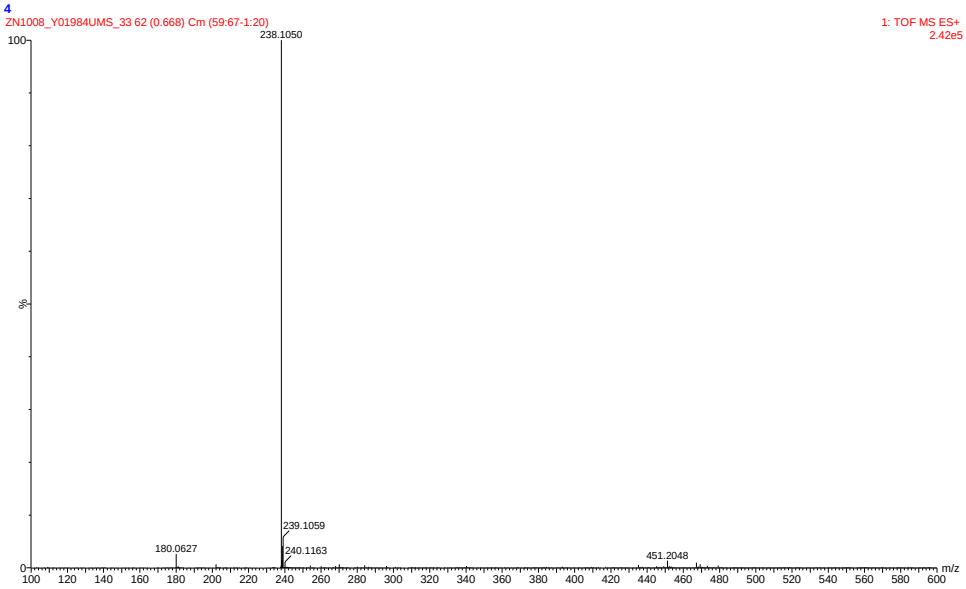
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

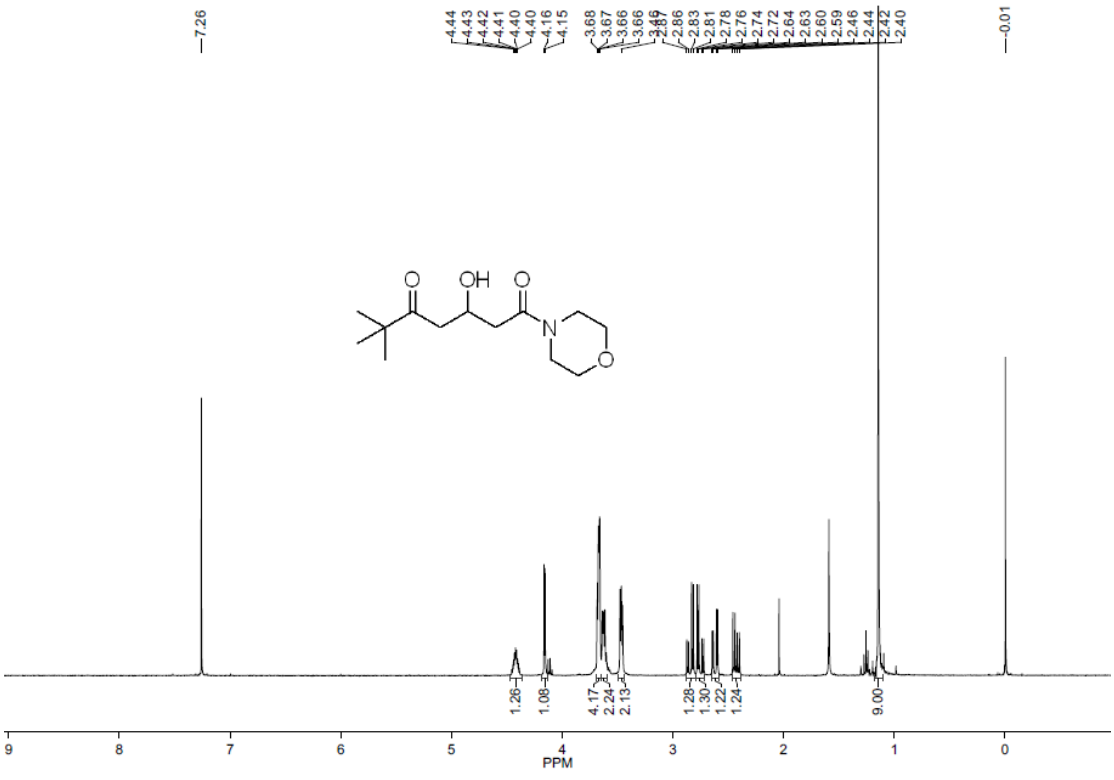
39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

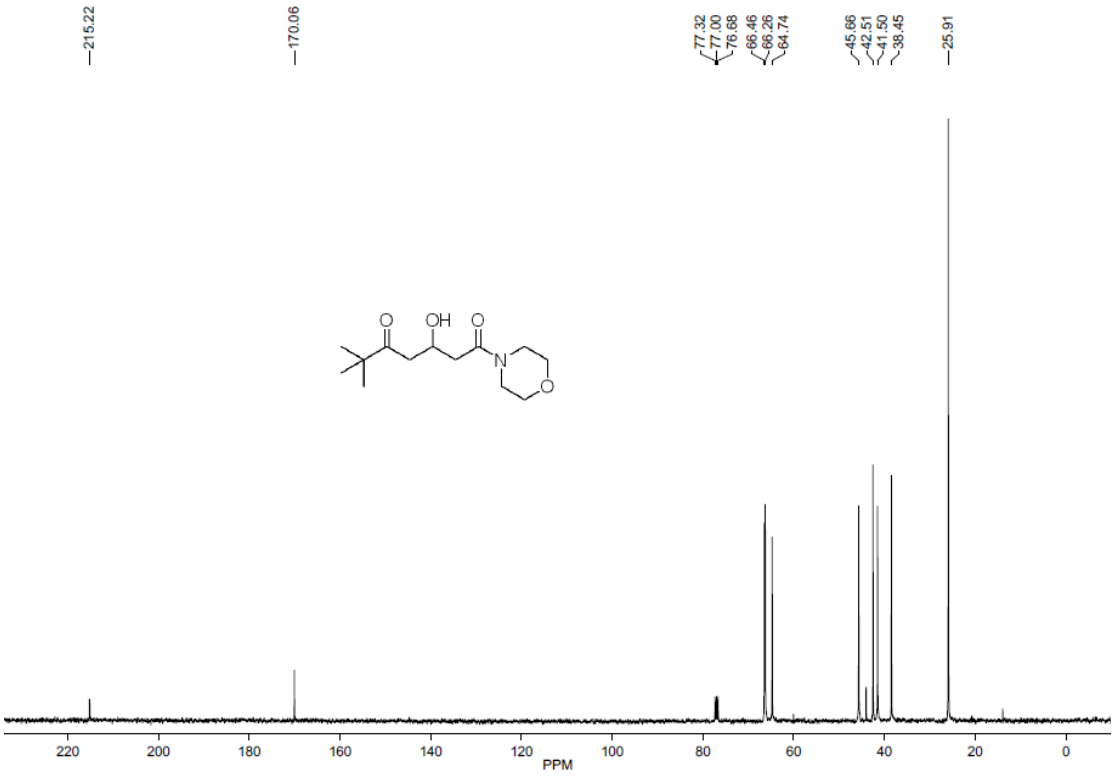
Elements Used: C: 0-12 H: 0-20 N: 0-2 O: 0-5 Na: 0-1



Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
238.1050	238.1055	-0.5	-2.1	2.5	6182.6
Formula	$C_{10}H_{17}NO_4Na$				

(2i) 3-hydroxy-6, 6-dimethyl-1-morpholinoheptane-1, 5-dione





Elemental Composition Report

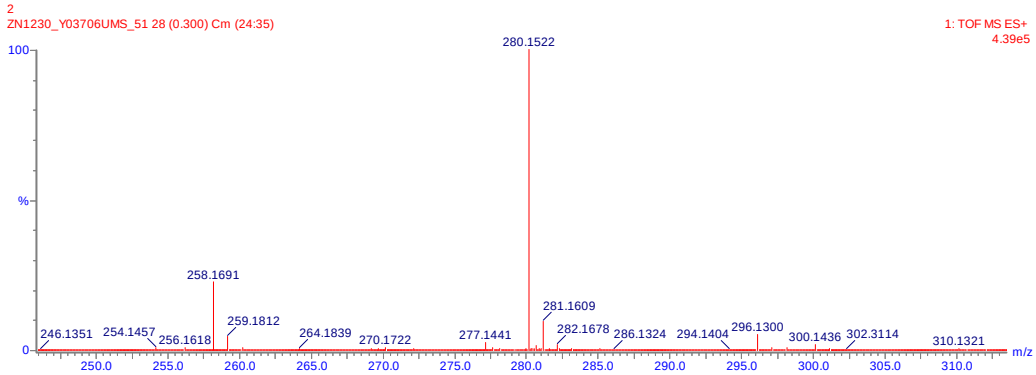
Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

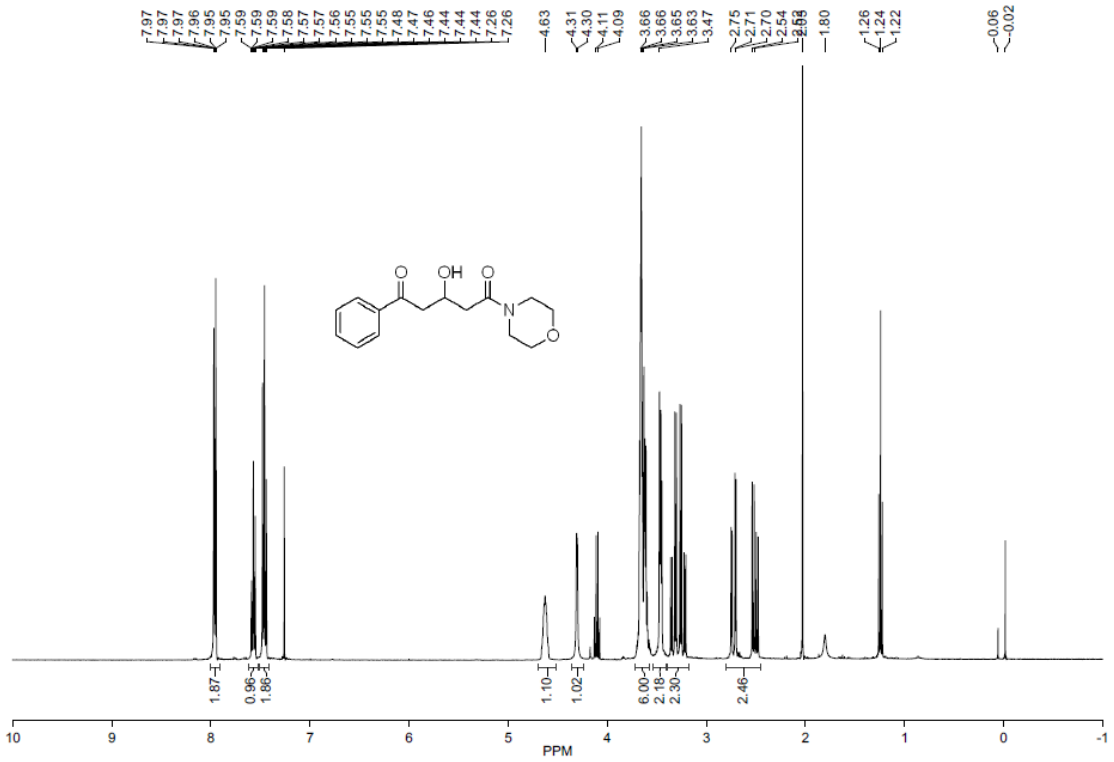
40 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

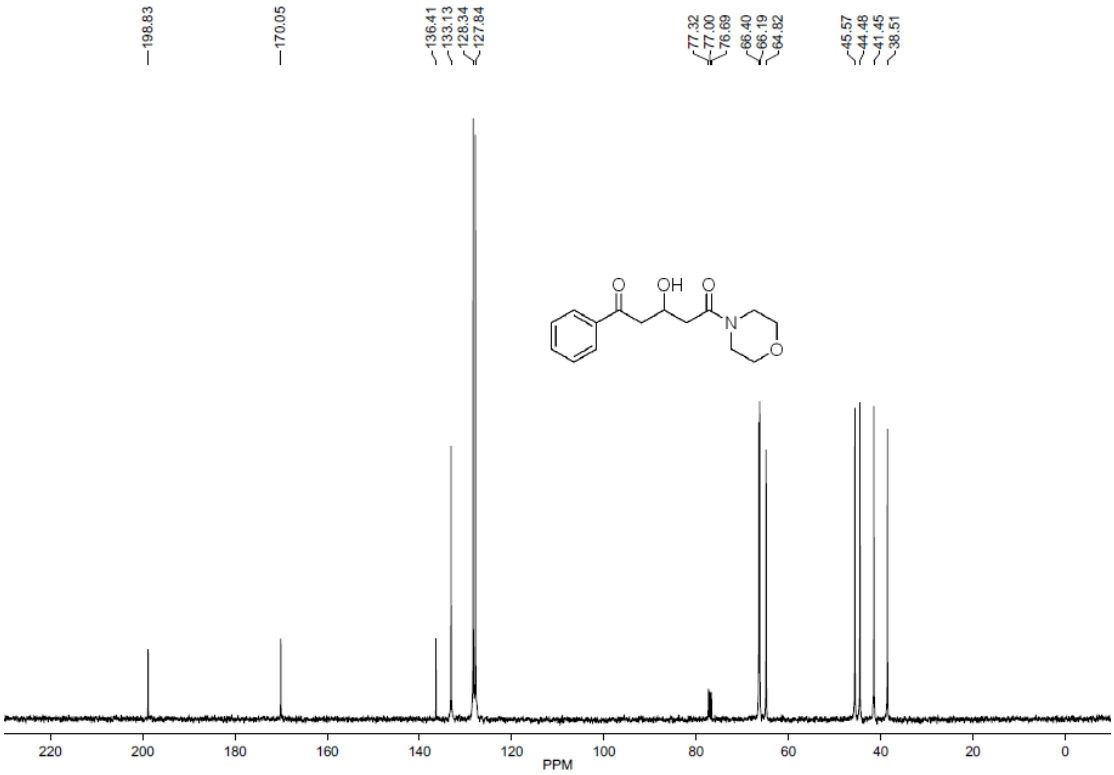
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	30.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
280.1522	280.1525	-0.3	-1.1	2.5	5066.5
Formula	$C_{13}H_{23}NO_4Na$				

(2j) 3-hydroxy-1-morpholino-5-phenylpentane-1, 5-dione





Elemental Composition Report

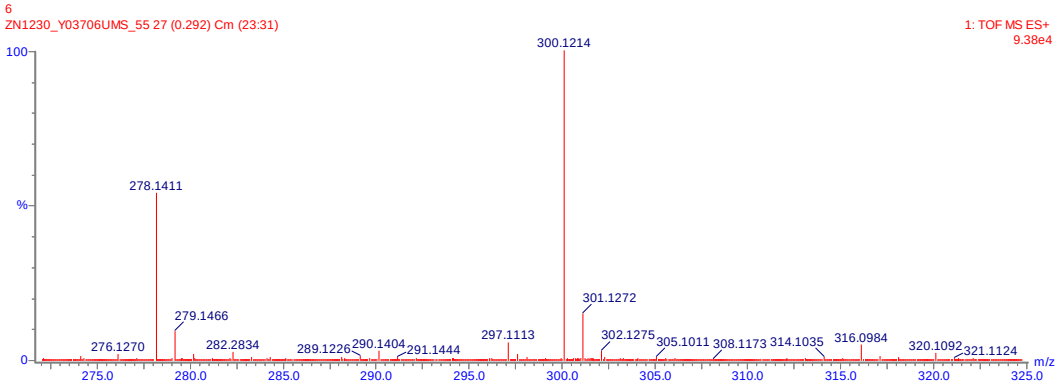
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

48 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

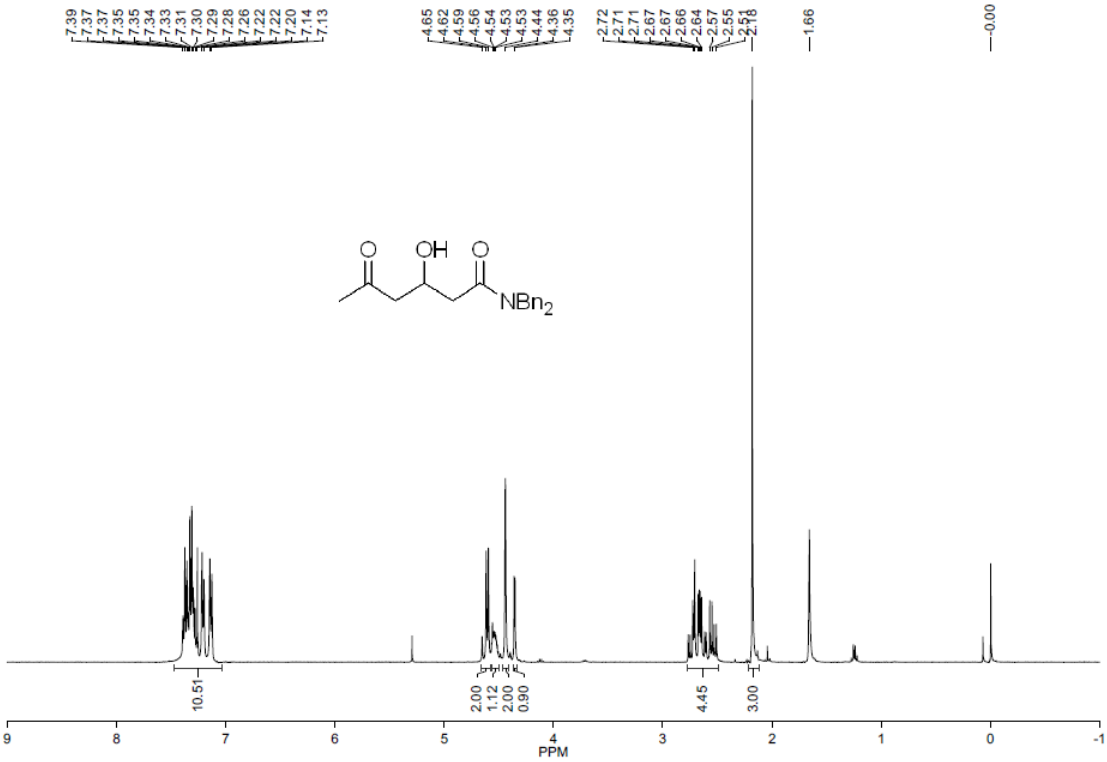
Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1

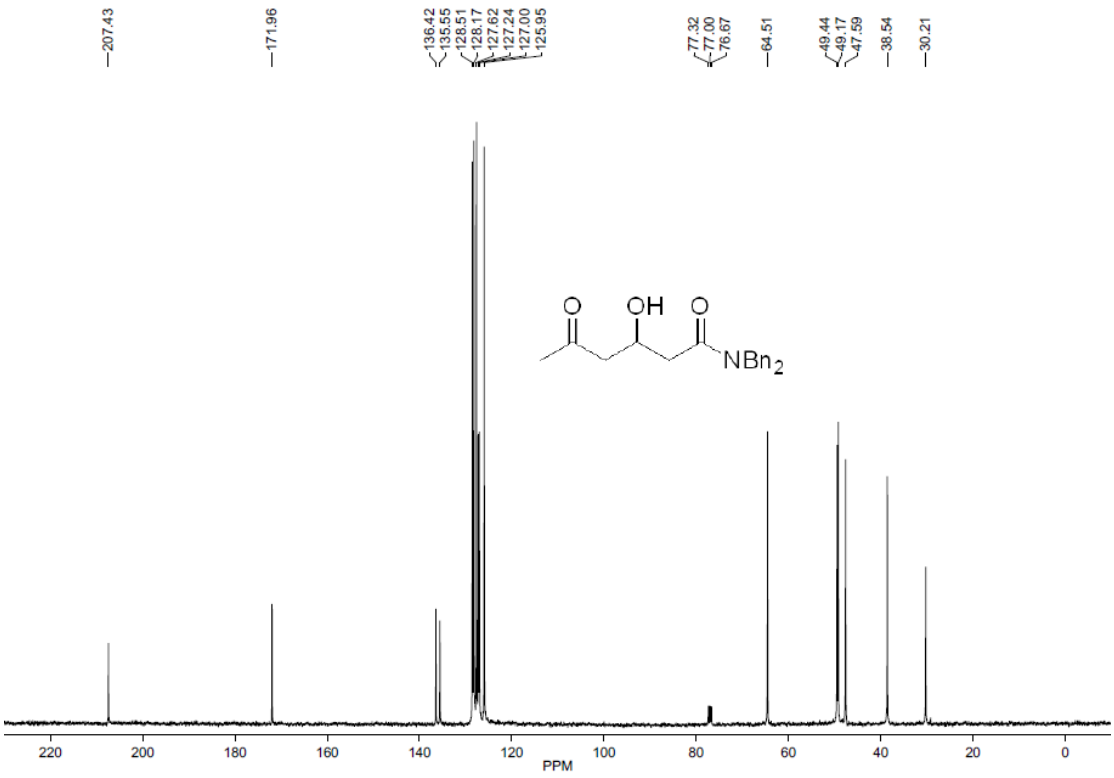


Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
300.1214	300.1212	0.2	0.7	6.5	246.2

Formula $C_{15}H_{19}NO_4Na$

(2k) *N, N*-dibenzyl-3-hydroxy-5-oxohexanamide





Elemental Composition Report

Single Mass Analysis

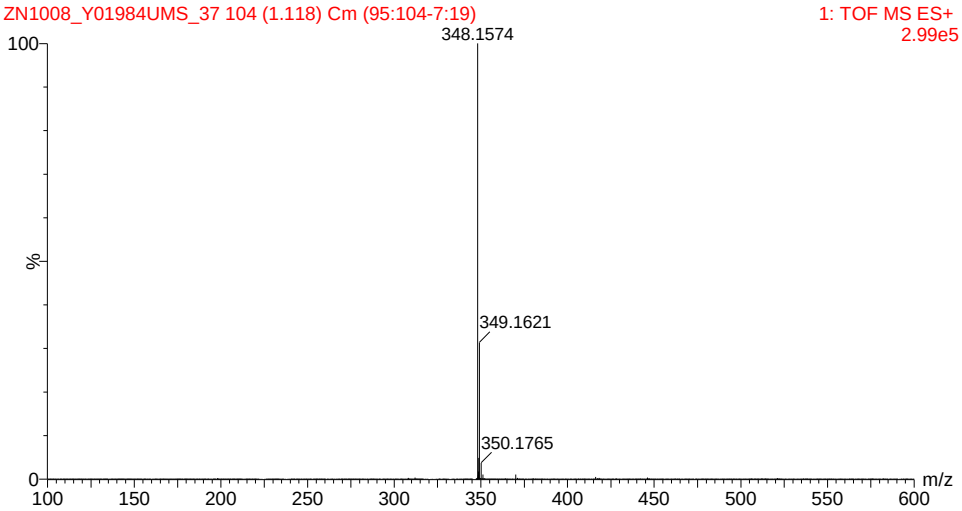
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

36 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 0-20 H: 0-25 N: 0-2 O: 0-5 Na: 0-1

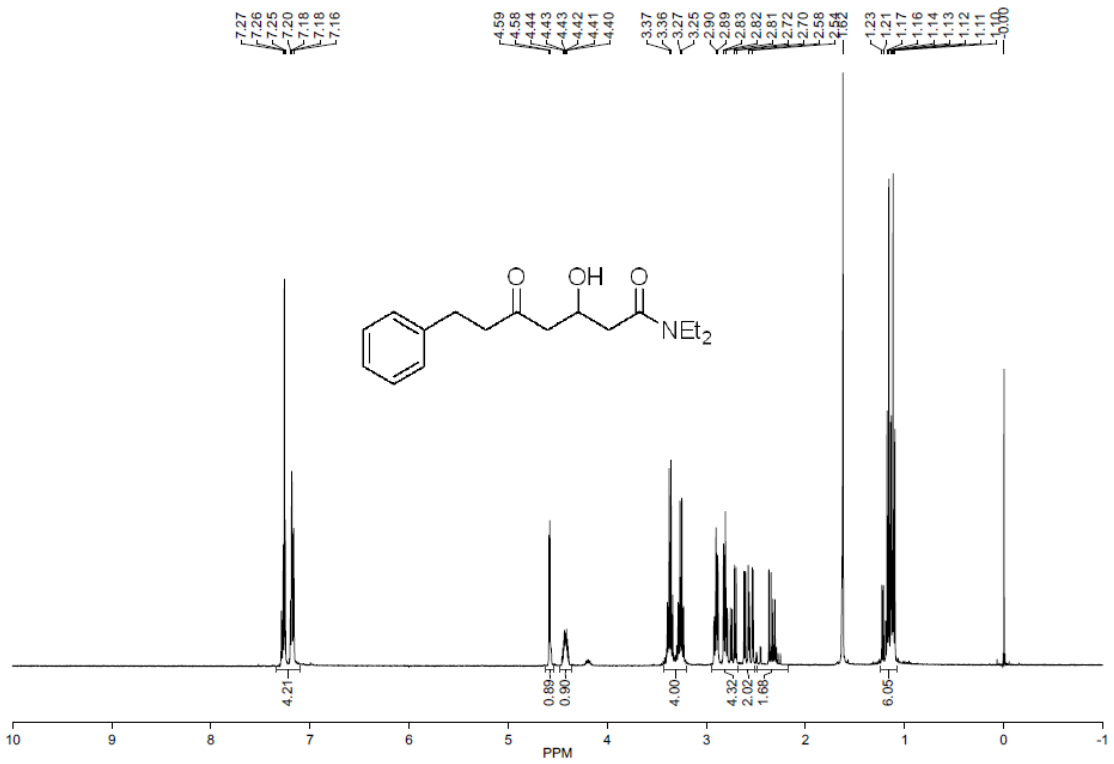
8

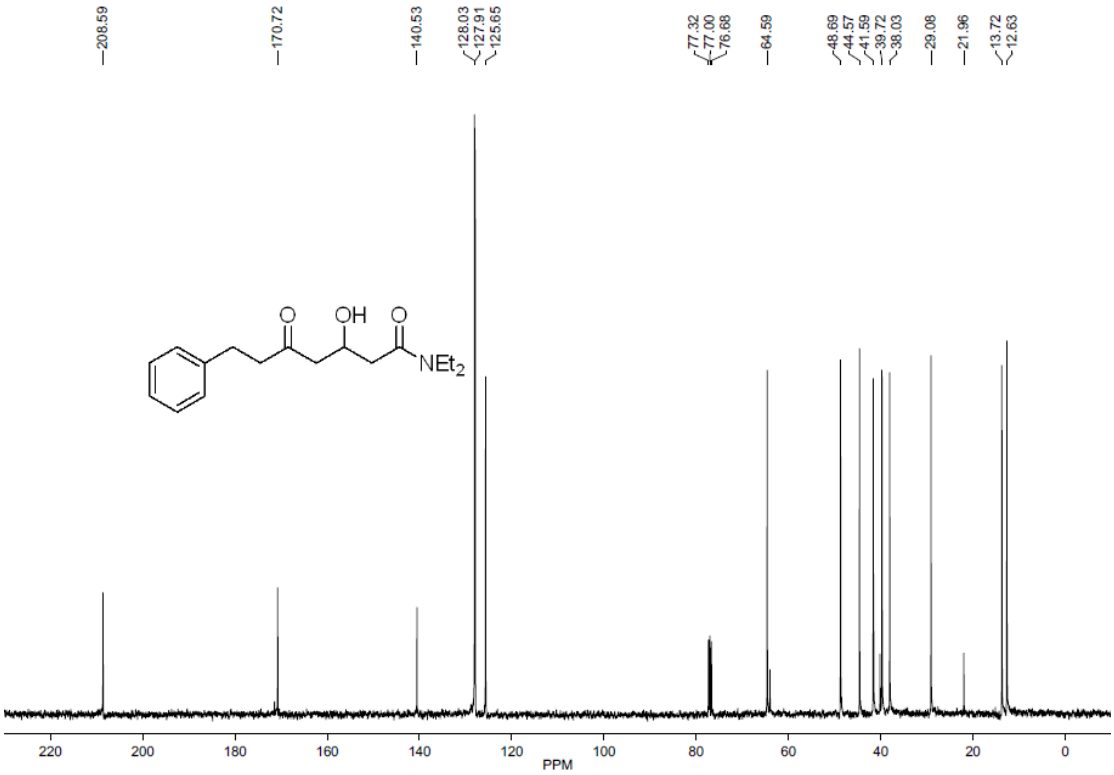


Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
348.1574	348.1576	-0.2	-0.6	9.5	2866.9

Formula $C_{20}H_{23}NO_3Na$

(2l) *N*, *N*-diethyl-3-hydroxy-5-oxo-7-phenylheptanamide





Elemental Composition Report

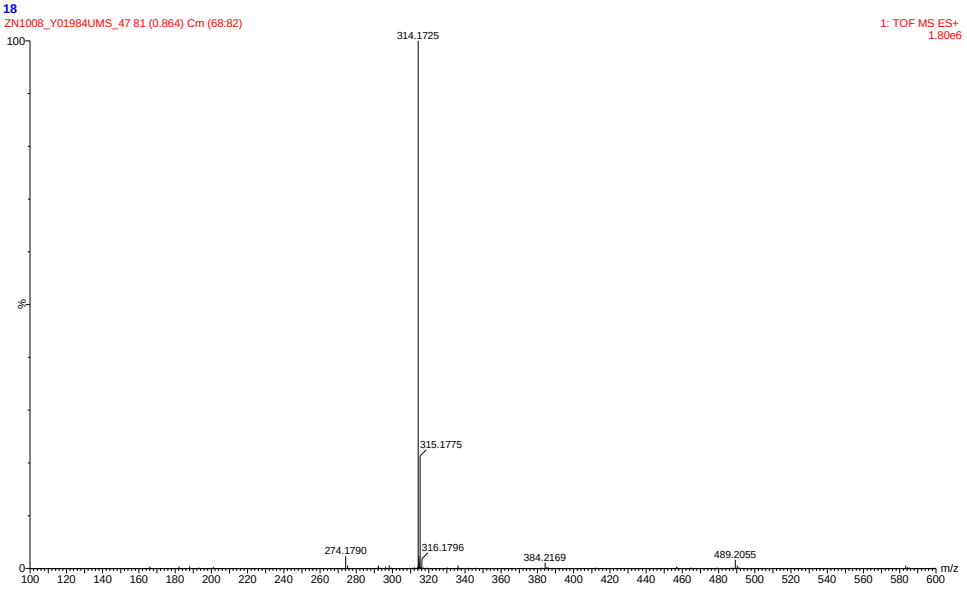
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

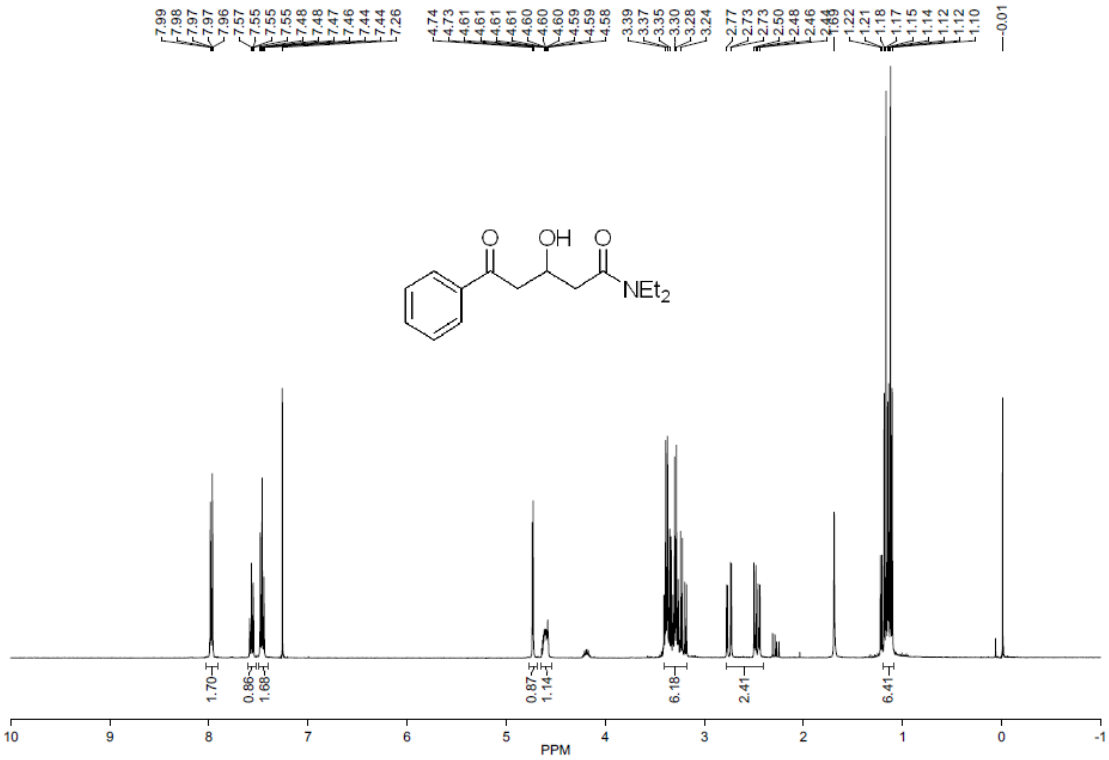
39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

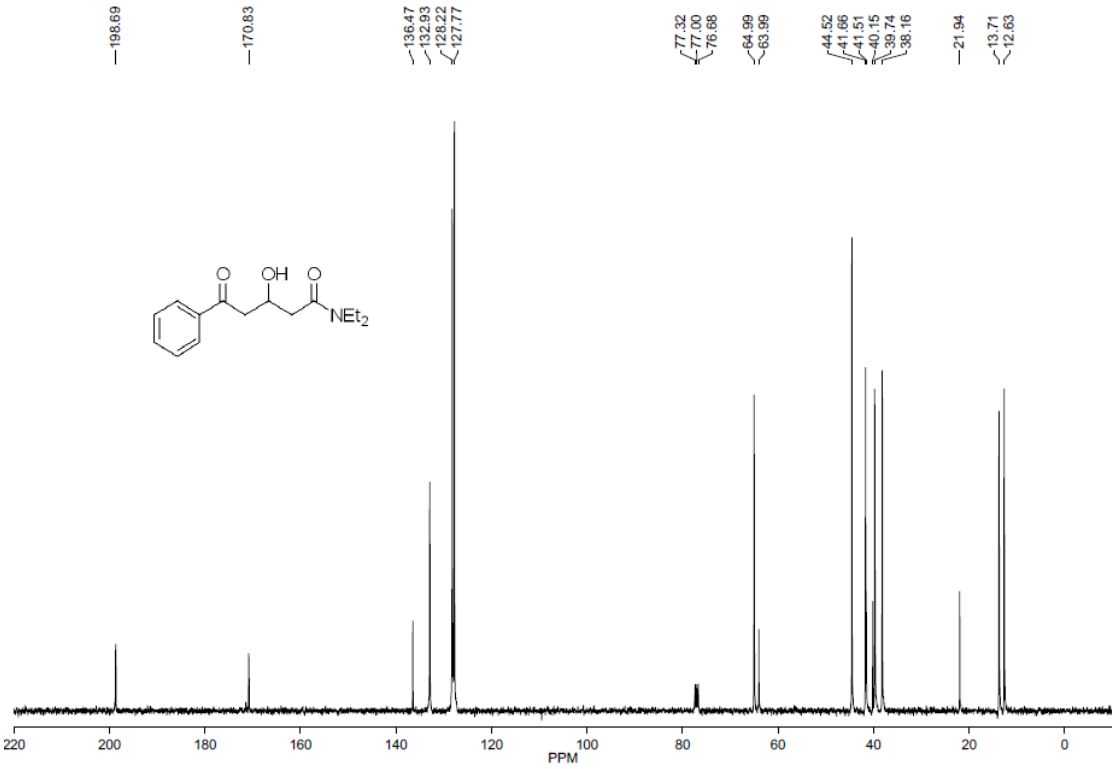
Elements Used: C: 0-18 H: 0-25 N: 0-2 O: 0-5 Na: 0-1



Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
314.1725	314.1732	-0.7	-2.2	5.5	3300.2
Formula	$C_{17}H_{25}NO_3Na$				

(2m) *N*, *N*-diethyl-3-hydroxy-5-oxo-5-phenylpentanamide





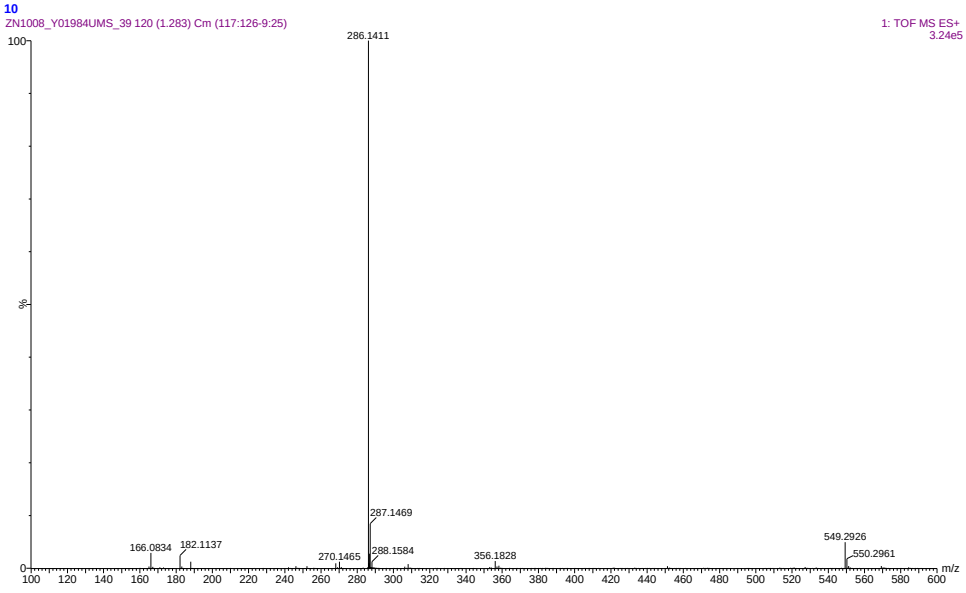
Elemental Composition Report

Single Mass Analysis Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

69 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

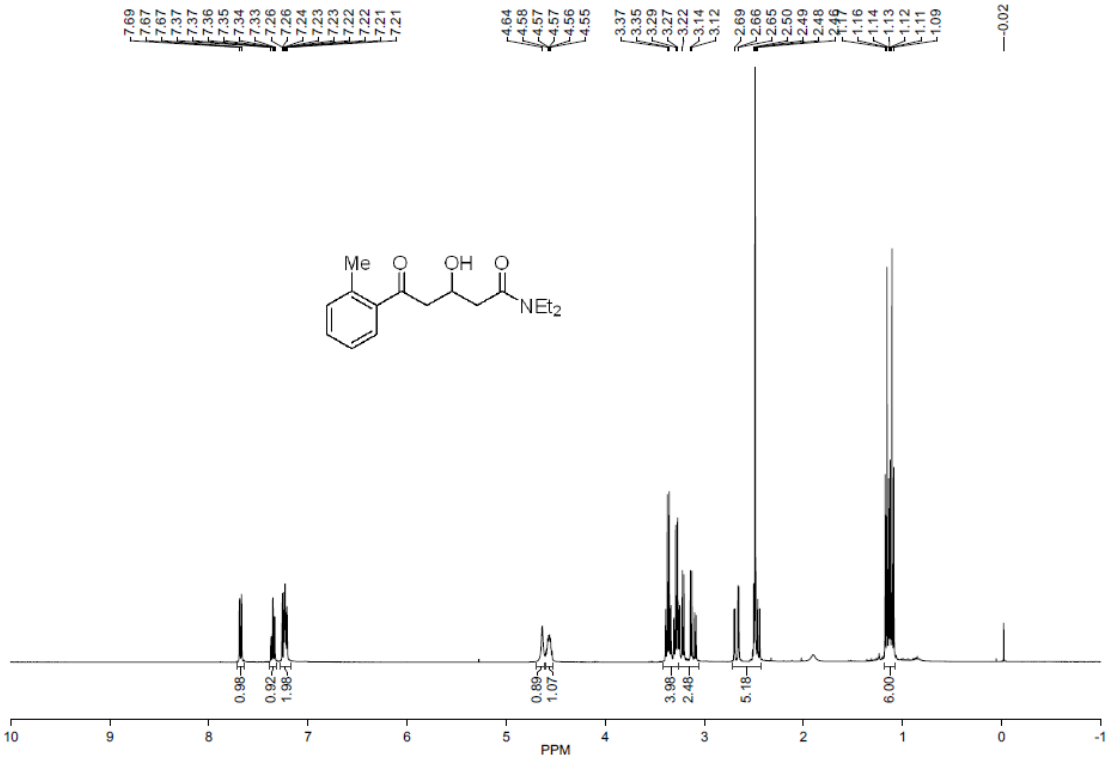
Elements Used: C: 0-20 H: 0-25 N: 0-2 O: 0-5 Na: 0-1

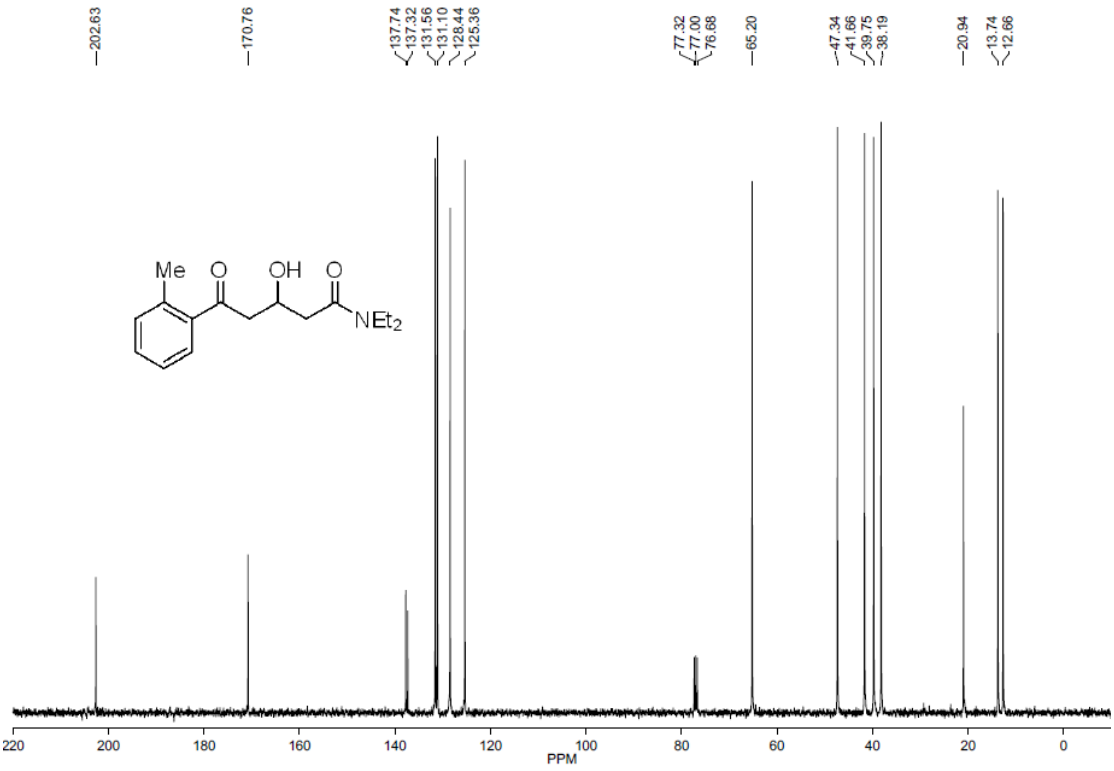


Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
286.1411	286.1419	-0.8	-2.8	5.5	11995.7

Formula $C_{15}H_{21}NO_3Na$

(2n) *N*, *N* -diethyl-3-hydroxy-5-oxo-5-(o-tolyl)pentanamide





Elemental Composition Report

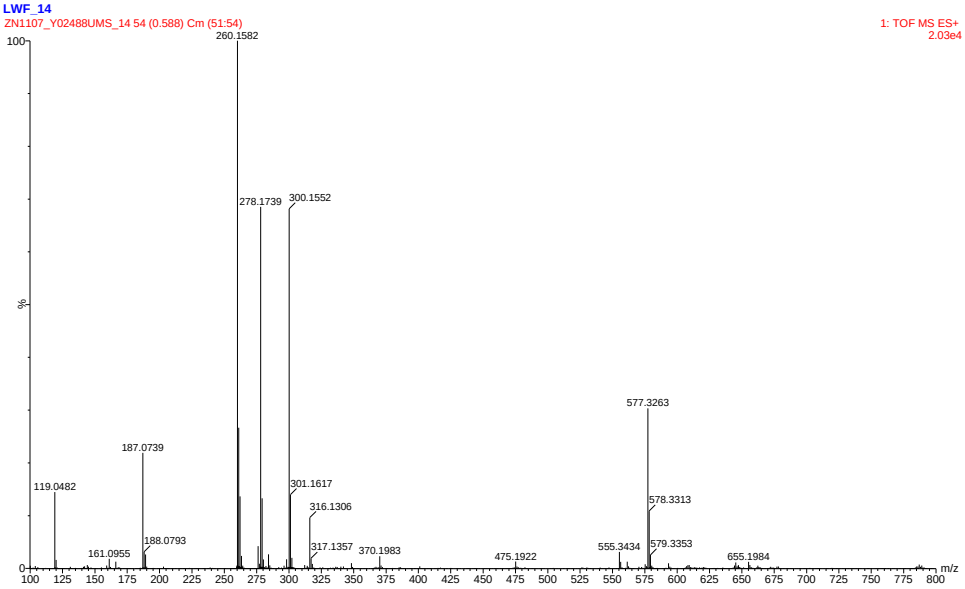
Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

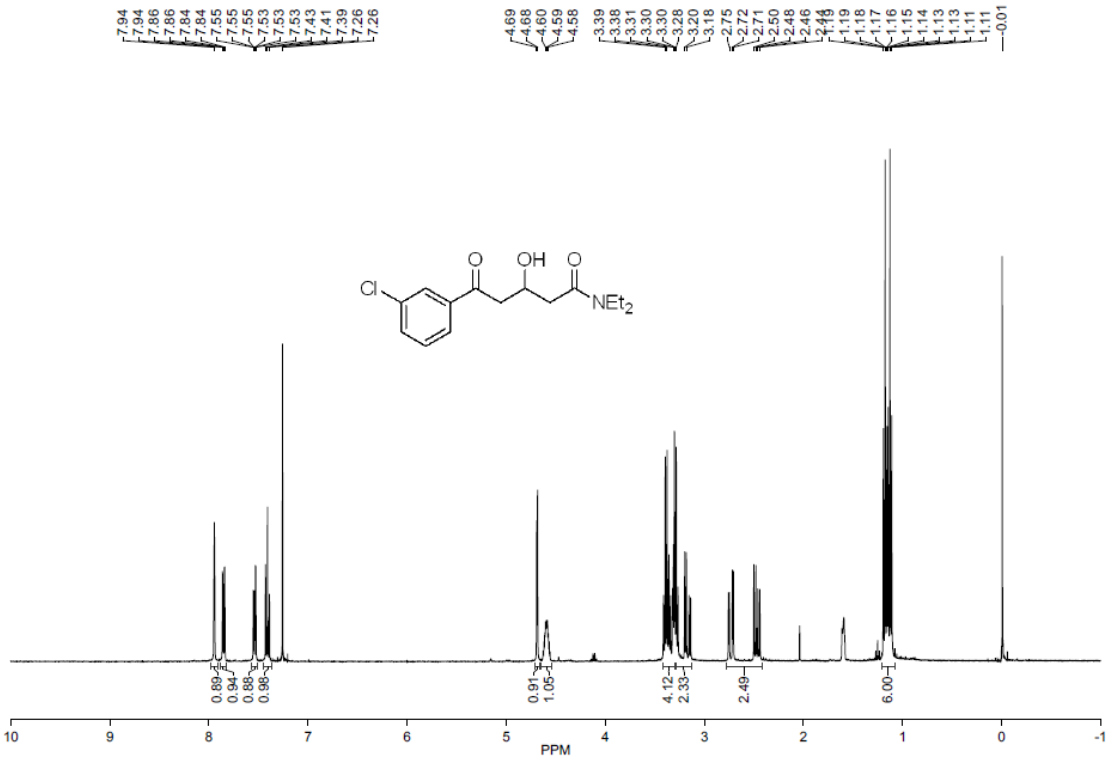
130 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

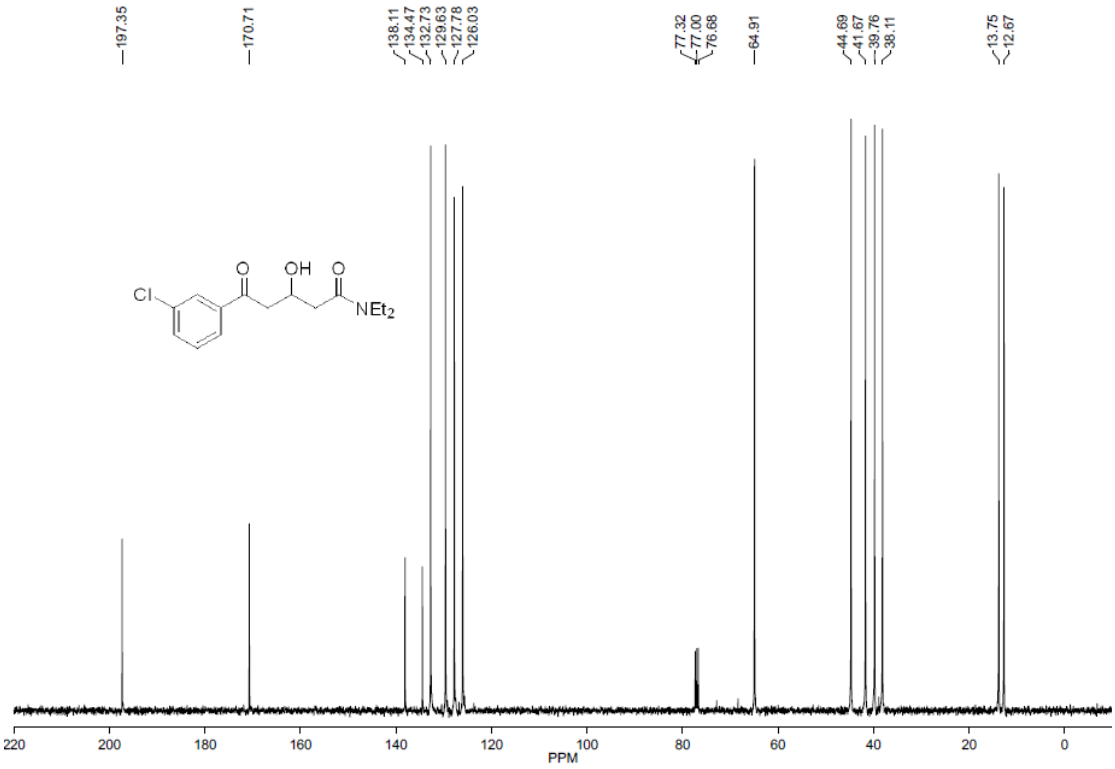
Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1 Br: 0-2



Minimum:				-1.5	
Maximum:		10.0	20.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
278.1739	278.1756	-1.7	-6.1	5.5	4.0
Formula	$C_{16}H_{24}NO_3$				

(2o) 5-(3-chlorophenyl)-*N*, *N* -diethyl-3-hydroxy-5-oxopentanamide





Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

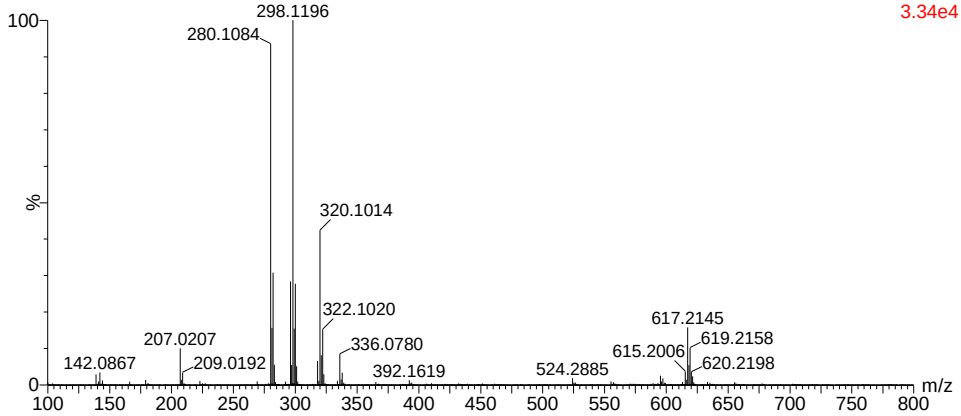
Selected filters: None Monoisotopic Mass, Even Electron Ions

142 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1 Cl: 0-2

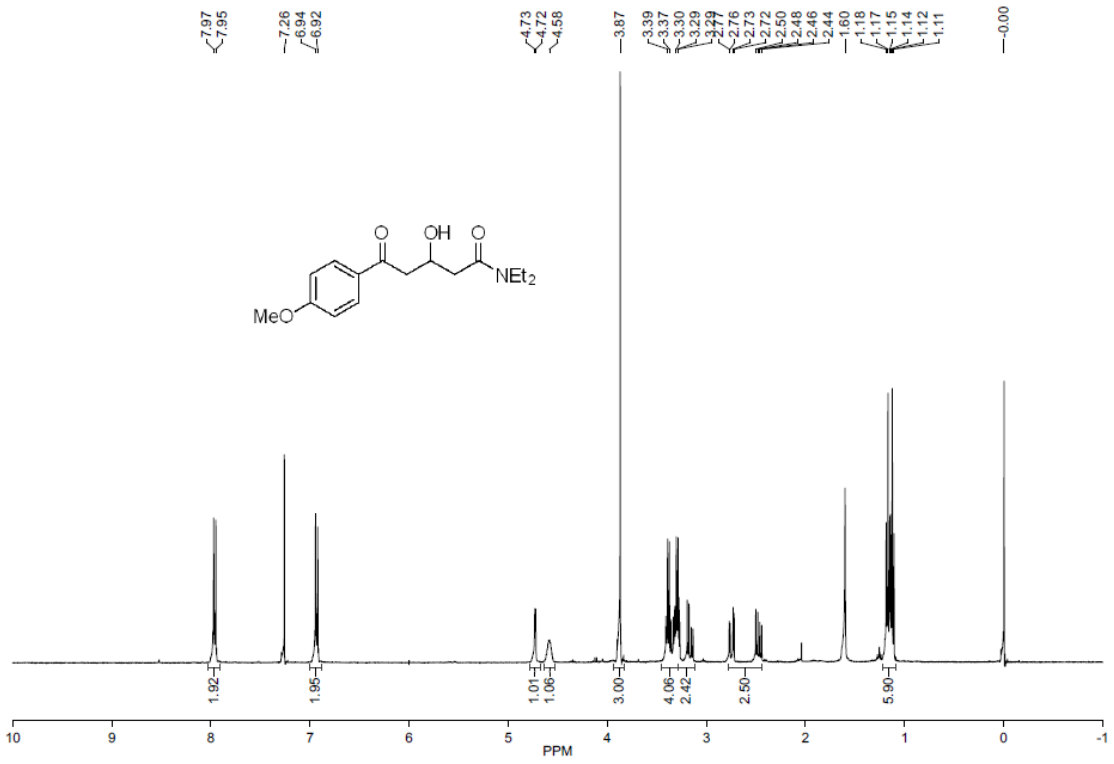
LWF_6

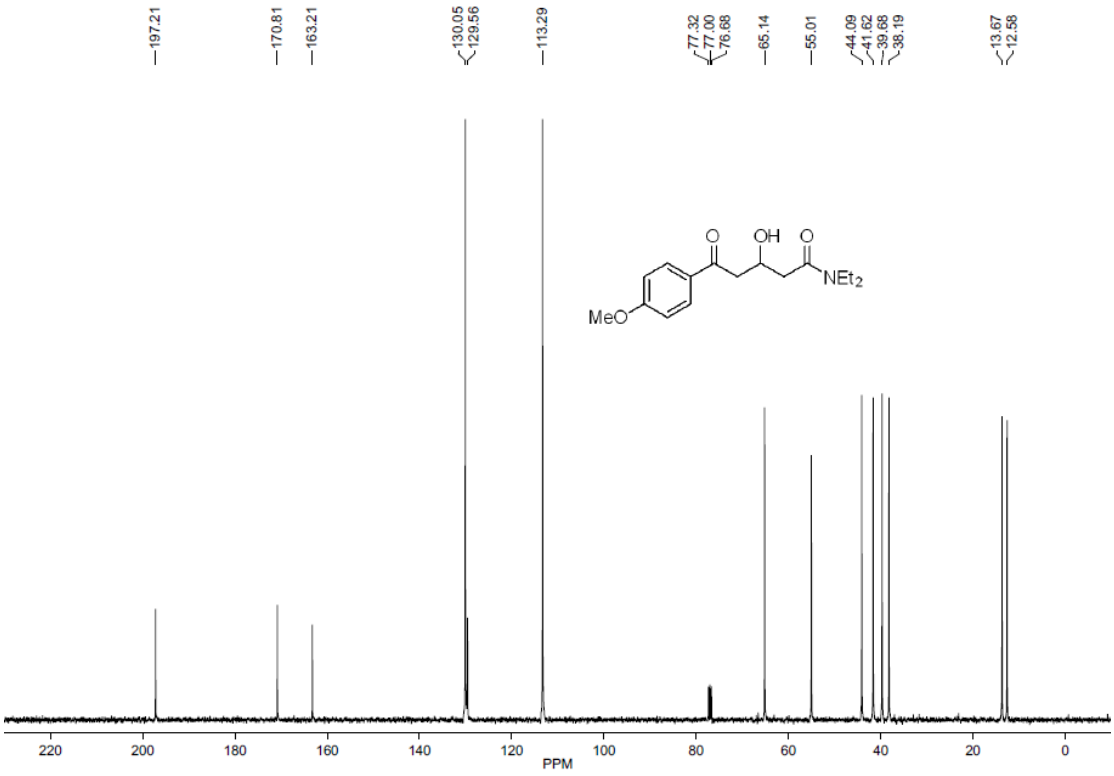
ZN1107_Y02488UMS_6 46 (0.486) Cm (44:47) 1: TOF MS ES+ 3.34e4



Minimum:				-1.5	
Maximum:		10.0	20.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
298.1196	298.1210	-1.4	-4.7	5.5	181.9
Formula	$C_{15}H_{21}NO_3Cl$				

(2p) *N*, *N* -diethyl-3-hydroxy-5-(4-methoxyphenyl)-5-oxopentanamide





Elemental Composition Report

Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0

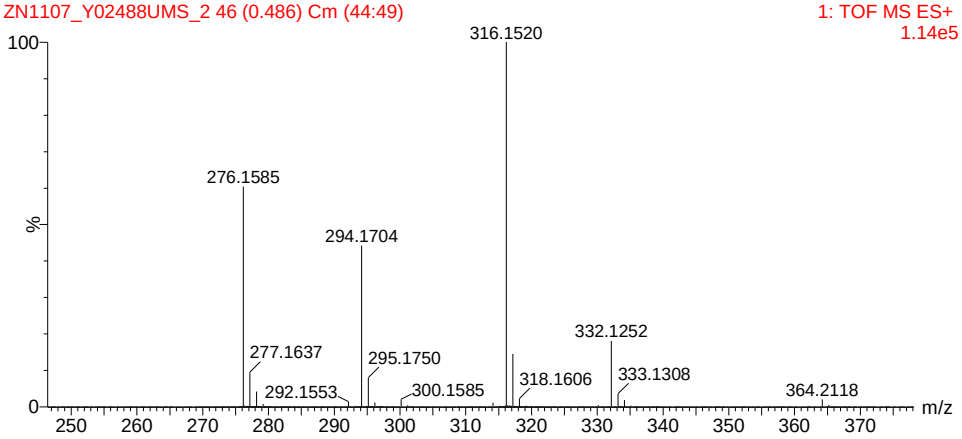
Selected filters: None Monoisotopic Mass, Even Electron Ions

43 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1

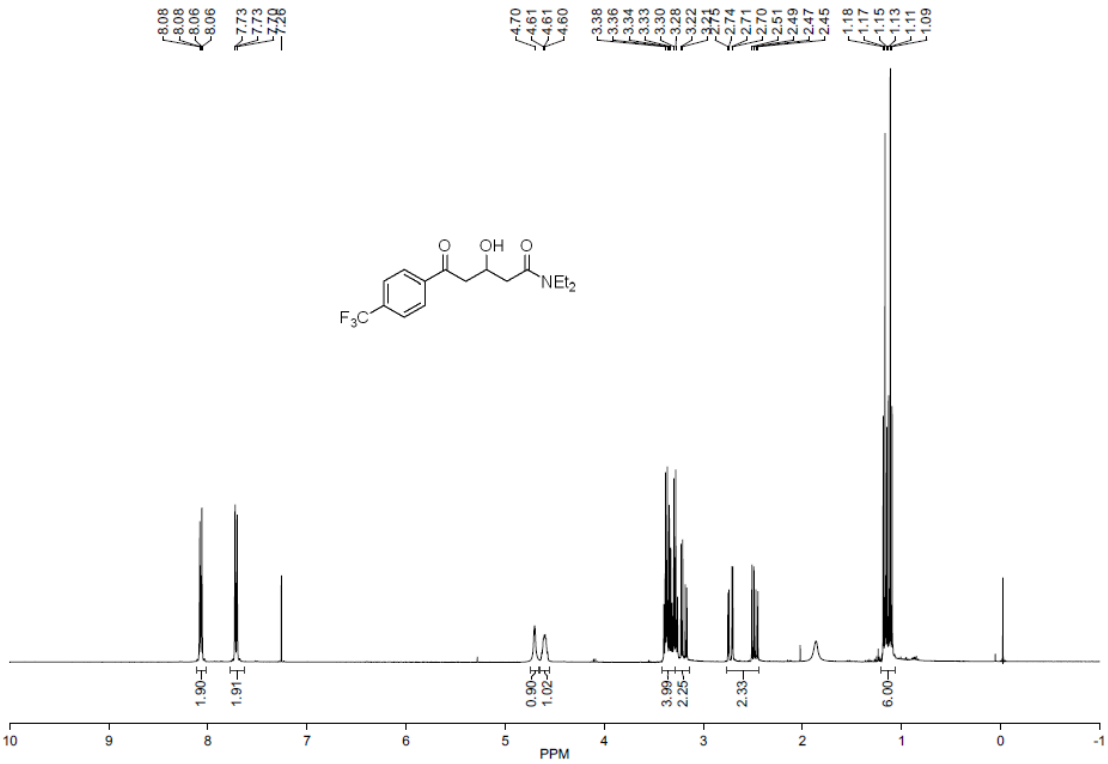
lsg110901

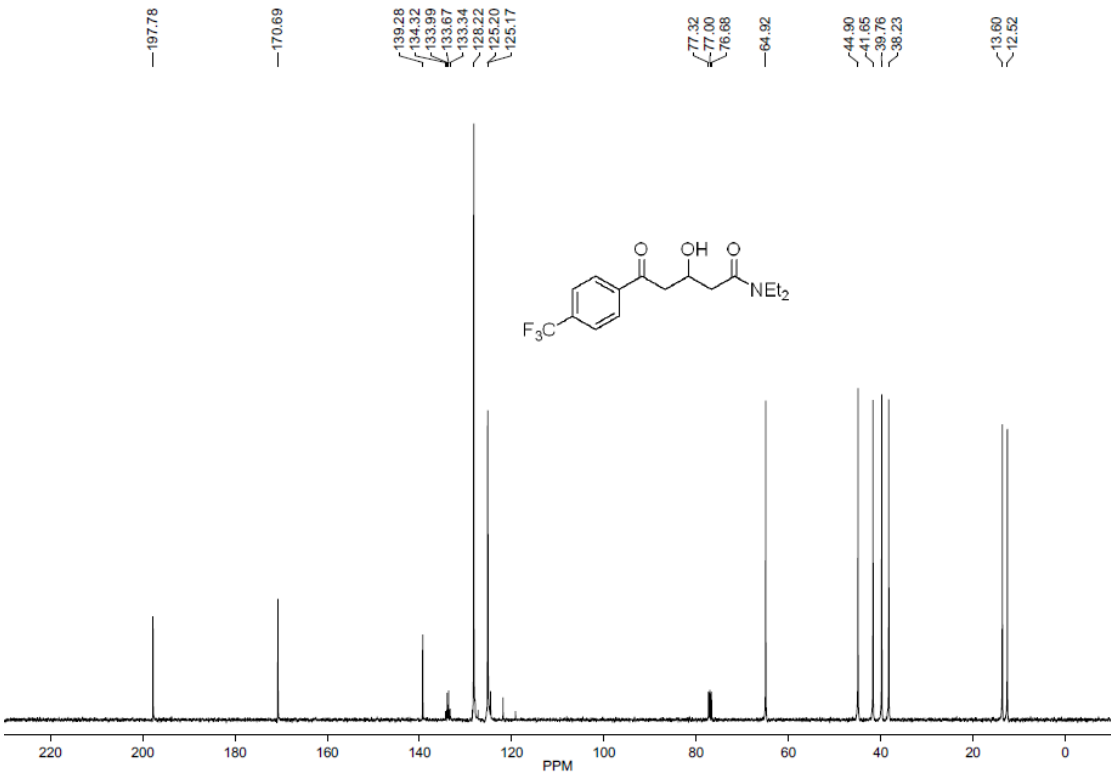
ZN1107_Y02488UMS_2 46 (0.486) Cm (44:49) 1: TOF MS ES+ 1.14e5



Minimum:				-1.5	
Maximum:		10.0	30.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
316.1520	316.1525	-0.5	-1.6	5.5	566.6
Formula	$C_{16}H_{23}NO_4Na$				

(2q) *N*, *N* -diethyl-3-hydroxy-5-oxo-5-(4-(trifluoromethyl)phenyl)-pentanamide





Elemental Composition Report

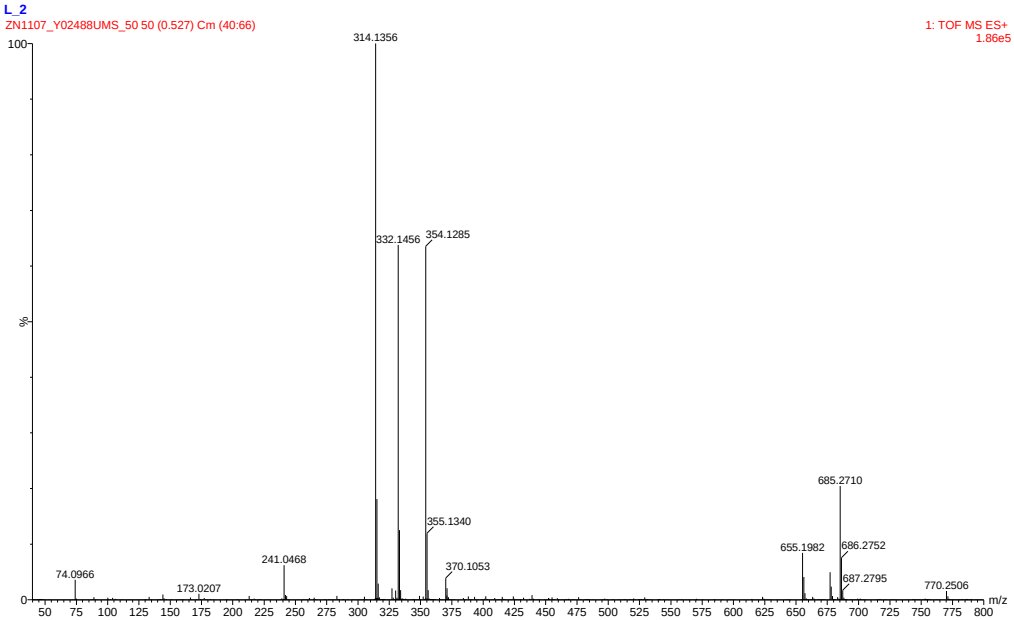
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 16-20 H: 10-30 N: 0-2 O: 0-8 F: 3-3

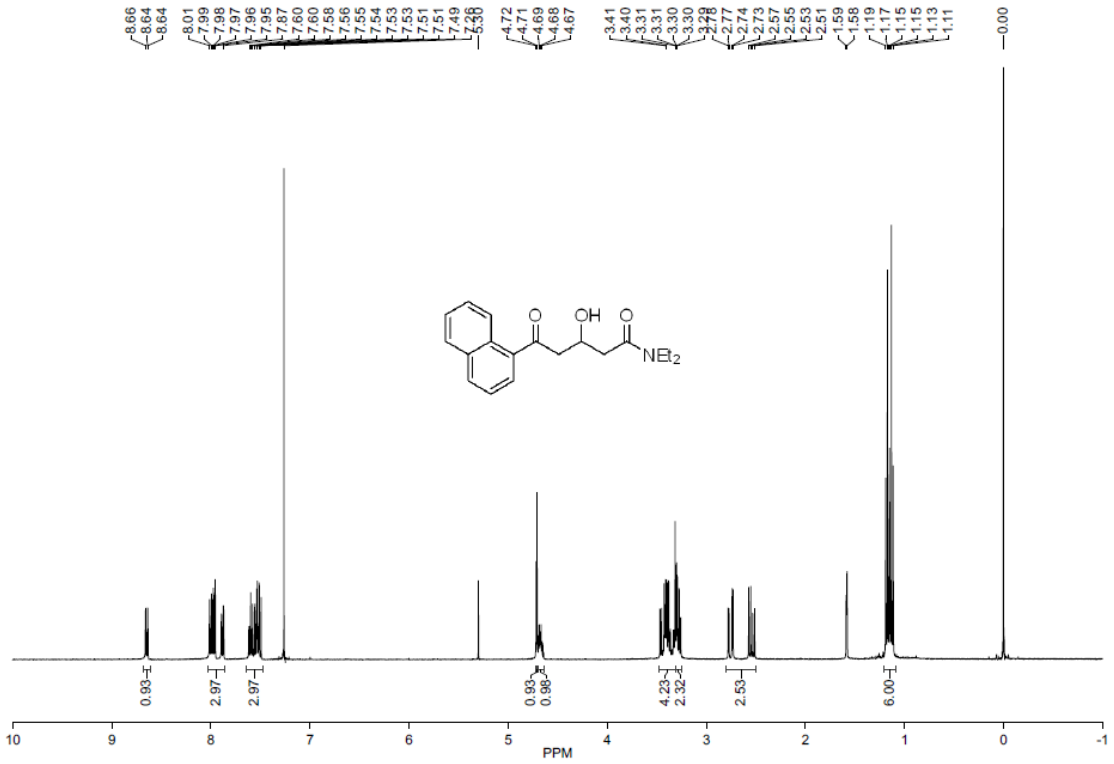


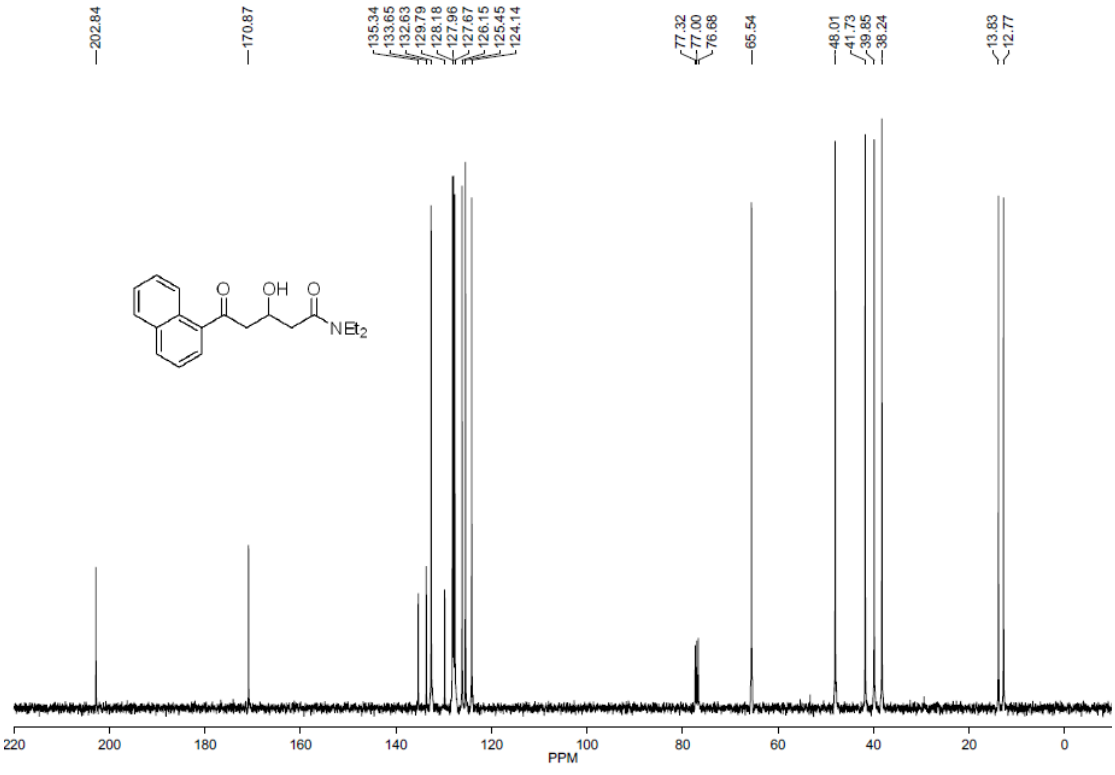
Minimum:				-1.5	
Maximum:		10.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT

332.1456	332.1474	-1.8	-5.4	5.5	75.2

Formula $C_{16}H_{21}NO_3F_3$

(2r) *N*, *N*-diethyl-3-hydroxy-5-(naphthalen-1-yl)-5-oxopentanamide





Elemental Composition Report

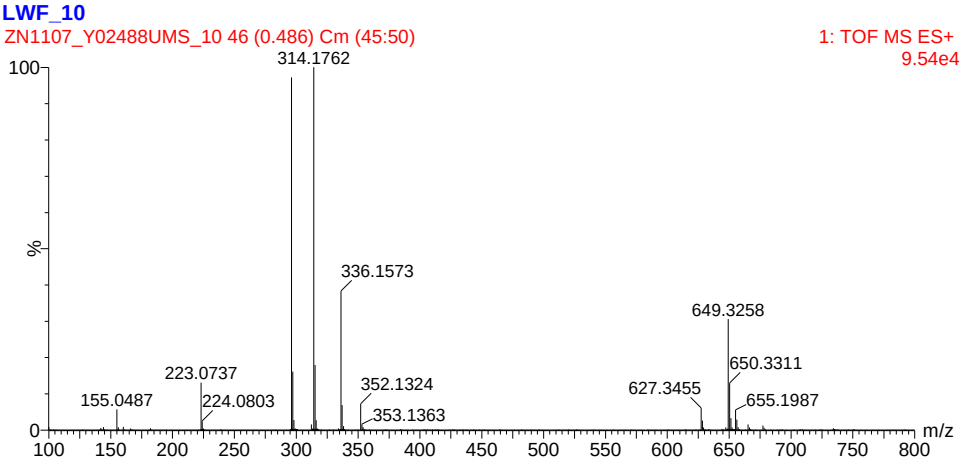
Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

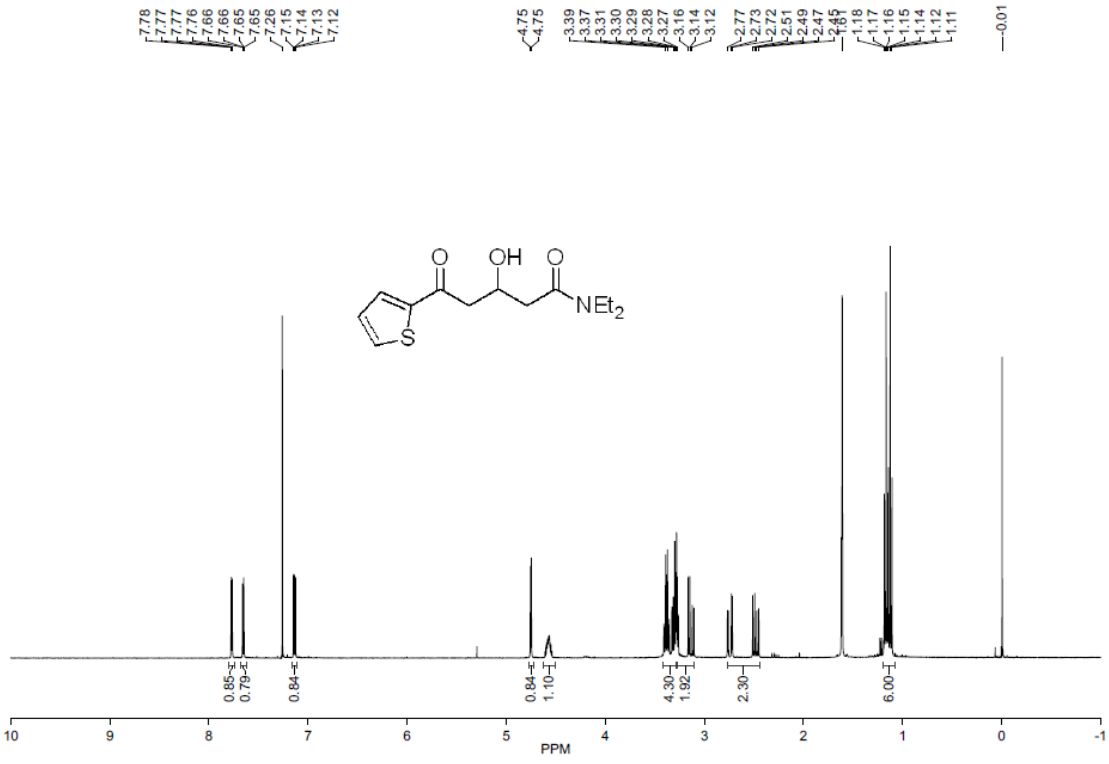
144 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

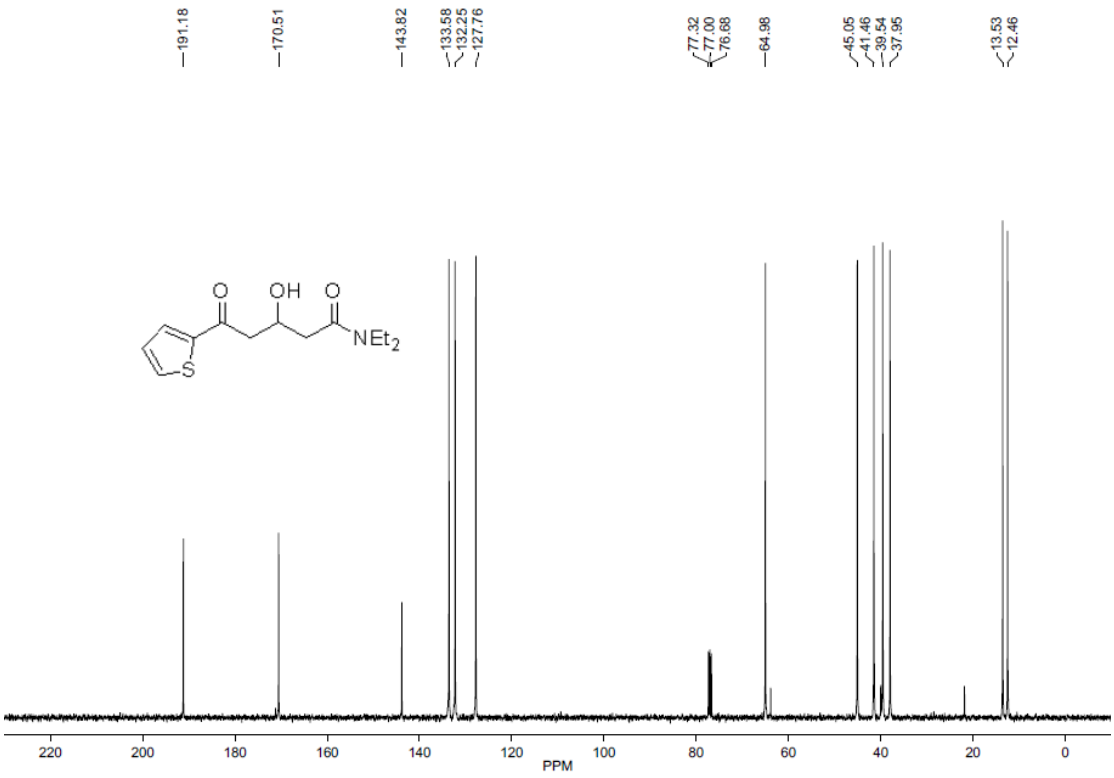
Elements Used: C: 10-20 H: 15-30 N: 0-2 O: 0-6 Na: 0-1



Minimum:				-1.5	
Maximum:		10.0	20.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
314.1762	314.1756	0.7	2.2	8.5	72.0
Formula	$C_{19}H_{24}NO_3$				

(2s) *N*, *N*-diethyl-3-hydroxy-5-oxo-5-(thiophen-2-yl)pentanamide





Elemental Composition Report

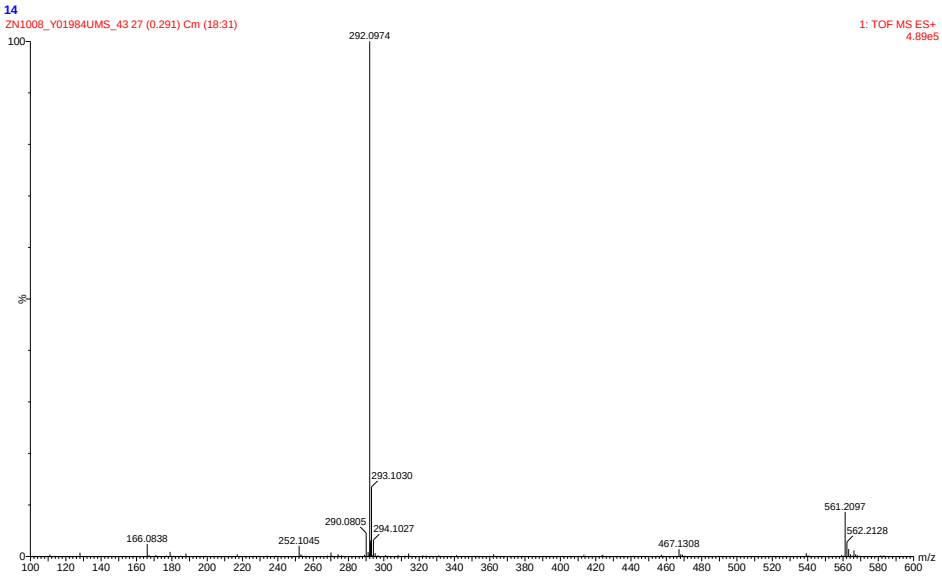
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

229 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

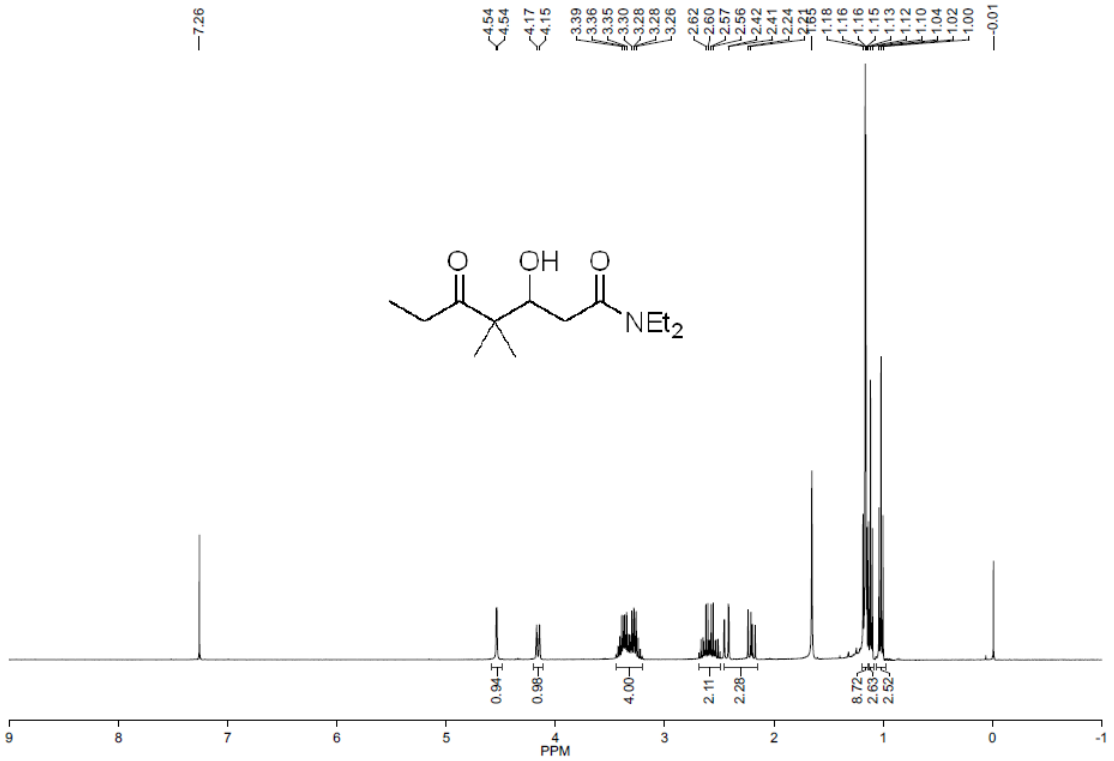
Elements Used: C: 0-20 H: 0-25 N: 0-2 O: 0-5 Na: 0-1 S: 0-2

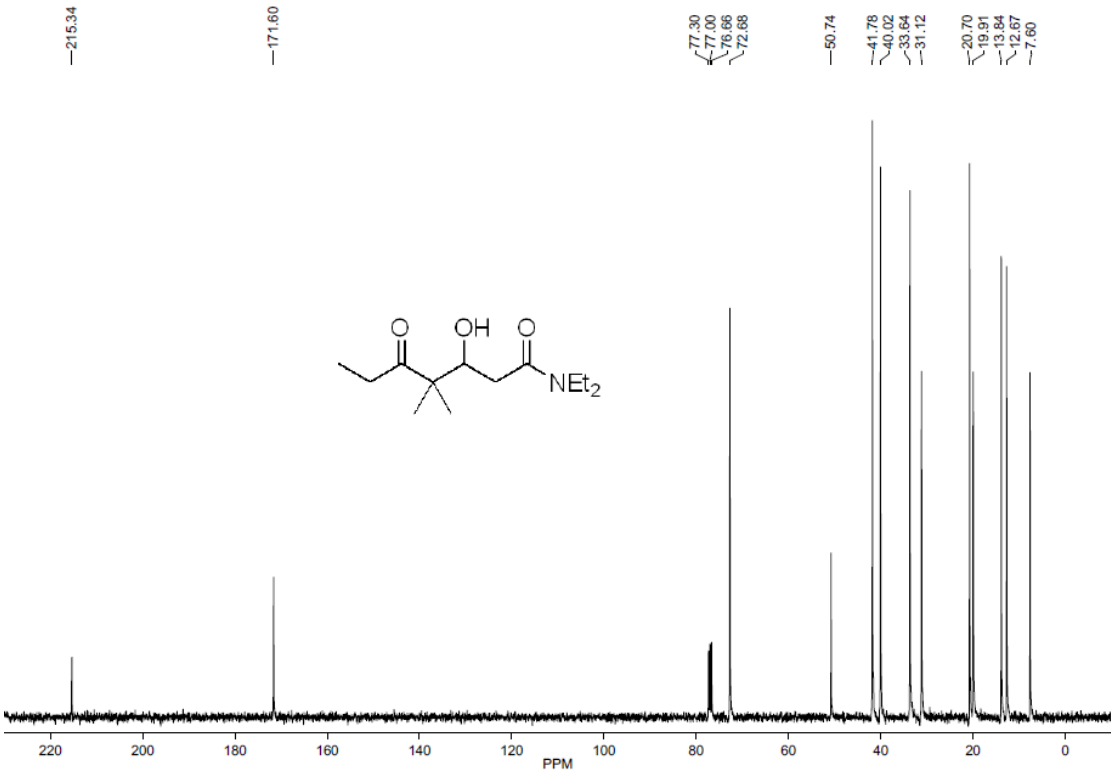


Minimum:				-1.5	
Maximum:		50.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
292.0974	292.0983	-0.9	-3.1	4.5	7157.3

Formula $C_{13}H_{19}NO_3SNa$

(2t) *N, N*-diethyl-3-hydroxy-4, 4-dimethyl-5-oxoheptanamide





Elemental Composition Report

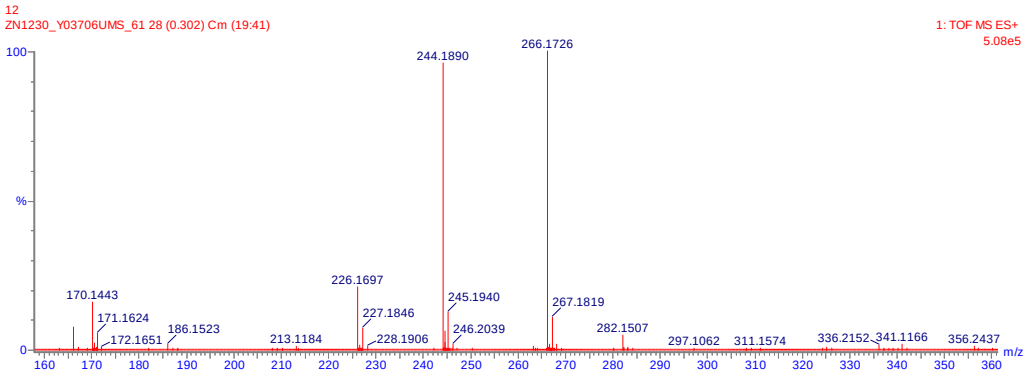
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used: C: 10-30 H: 10-35 N: 1-2 O: 3-8 Na: 0-1



Minimum:				-1.5	
Maximum:		5.0	50.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
266.1726	266.1732	-0.6	-2.3	1.5	4163.9
Formula	$C_{13}H_{25}NO_3Na$				