Efficient Synthesis of Diverse Heterobifunctionalized Clickable Oligo(ethylene glycol) Linkers: Potential Applications in Bioconjugation and Targeted Drug Delivery

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SUPPLEMENTARY INFORMATION

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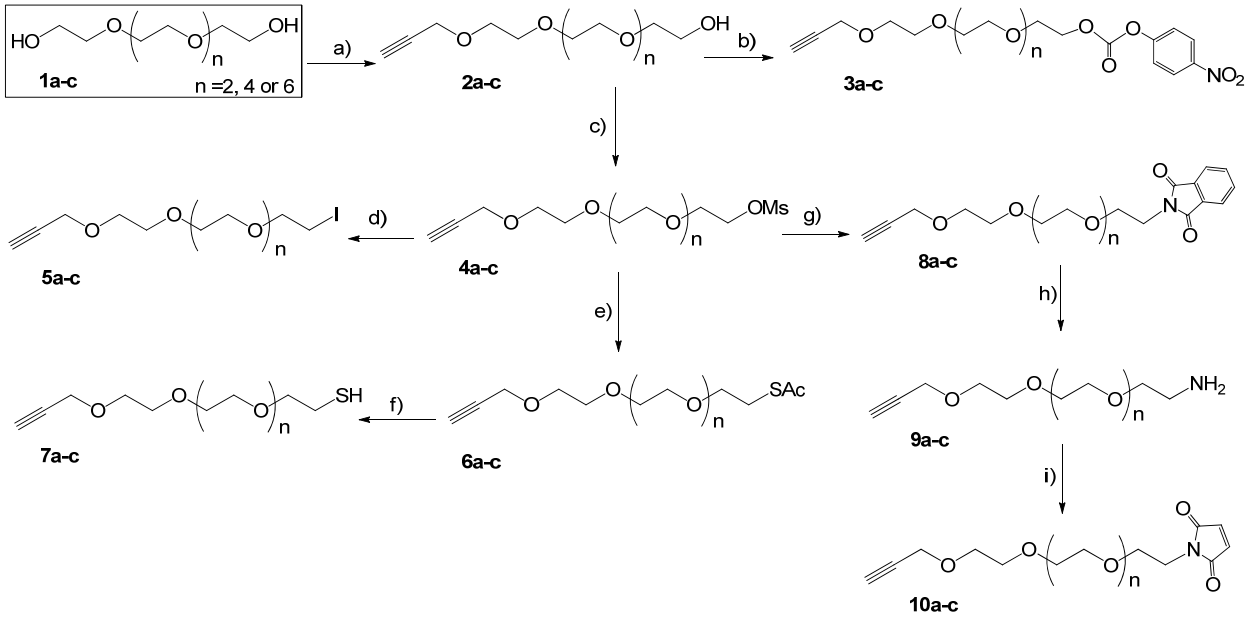
S1 – EXPERIMENTAL PROCEDURES AND CHARACTERIZATION

Abbreviations. Acetonitrile (MeCN), ammonium chloride (NH_4Cl), dichloromethane (DCM), diethyl ether (Et_2O), N,N-diisopropylethylamine (DIPEA), N,N'-dimethylformamide (DMF), hydrochloric acid (HCl), lithium aluminum hydride (LAH), methanesulfonyl chloride (MsCl), methanol (MeOH), oligoethylene glycol (OEG), potassium thioacetate (KSAc), sodium azide (NaN_3), sodium hydride (NaH), sodium iodide (NaI), sodium sulfate (Na_2SO_4), tetrahydrofuran (THF), triethylamine (Et_3N).



Scheme 1 Synthesis of alkyne terminated heterobifunctionalized OEG linkers. *Reagents and conditions*: (a) Propargyl bromide, NaH, THF, 0 °C-RT-60 °C, 15 h; (b) 4-nitrophenyl chloroformate, pyridine, MeCN, RT, 15 h; (c) MsCl, Et_3N, DCM, 0 °C-RT, 3.5 h; (d) NaI, acetone, 65 °C, 15 h; (e) KSAc, DMF, RT, 15 h; (f) LAH, THF, -10 °C-RT, 3 h; (g) Potassium phthalimide, DMF, 110 °C, 15 h; (h) Hydrazine, EtOH, 60 °C, 3 h; (i) N-methoxycarbonyl maleimide, Sat. aq $NaHCO_3$, 0 °C-RT, 2 h.

*Synthesis of **2a**.* By using the general procedure in the main article with OEG **1a** (5.20 g, 26.8 mmol), NaH (0.15 g, 18.7 mmol), and propargyl bromide (3.18 g, 26.8 mmol), the pure product was obtained as a colorless oil (3.61 g, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 3.88 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.42 (m, 1H, -CH_2CH_2O*H*), 3.42-3.33 (m, 14H, -OC*H*$_2$C*H*$_2$O-), 3.26 (t, *J* = 4.0 Hz, 2H, -CH_2C*H*$_2$OH), 2.37 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH_2O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.34 (1C), 75.77 (1C), 73.16 (1C), 71.04-70.79 (5C), 69.52 (1C), 61.86 (1C), 58.74 ppm (1C). HRMS (ESI): m/z calcd for $C_{11}H_{20}O_5$+Na^+ [*M*+Na]$^+$ 255.1208; found 255.1016.

*Synthesis of **2b.*** By using the general procedure in the main article OEG **1b** (5.27 g, 18.7 mmol), NaH (0.31 g, 13.10 mmol), and propargyl bromide (2.22 g, 18.7 mmol), the pure product was obtained as a colorless oil (2.22 g, 37%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.00 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.49-3.39 (m, 24H, -OC*H*$_2$C*H*$_2$O-), 2.39 ppm (m, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.37 (1C), 75.59 (1C), 73.26 (1C), 71.17-70.93 (9C), 69.67 (1C), 62.11 (1C), 58.94 ppm (1C). HRMS (ESI): m/z calcd for $C_{15}H_{28}O_7$+Na^+ [*M*+Na]$^+$ 343.1733; found 343.2077.

*Synthesis of **3a***. By using the general procedure in the main article with **2a** (0.24 g, 1.01 mmol), 4-nitrophenyl chloroformate (0.31 g, 1.52 mmol), and pyridine (0.16 g, 2.02 mmol), the pure product was obtained as a yellow oil (0.30 g, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.13 (d, *J* = 9.2 Hz, 2H, Ar-H-NO$_2$), 7.28 (d, *J* = 9.2 Hz, 2H, Ar-H-OCO-), 4.30 (m, 2H, -O-CH$_2$C*H*$_2$-OCO-), 4.12 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.67 (m, 2H, -O-C*H*$_2$CH$_2$-OCO-), 3.57-3.52 (m, 12H, -OC*H*$_2$C*H*$_2$O-), 2.38 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 156.25 (1C), 153.12 (1C), 146.02 (1C), 125.97 (2C), 122.59 (2C), 80.47 (1C), 75.48 (1C), 71.31-71.22 (4C), 71.01 (1C), 69.76 (1C), 69.26 (1C), 69.05 (1C), 59.98 ppm (1C). HRMS (ESI): m/z calcd for $C_{18}H_{23}NO_9$+Na^+ [*M*+Na]$^+$ 420.1271; found 420.0280.

*Synthesis of **3b***. By using the general procedure in the main article with **2b** (0.25 g, 0.78 mmol), 4-nitrophenyl chloroformate (0.24 g, 1.17 mmol), and pyridine (0.12 g, 1.56 mmol), the pure product was obtained as a yellow oil (0.27 g, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.21 (d, *J* = 9.2 Hz, 2H, Ar-H-NO$_2$), 7.34 (d, *J* = 9.2 Hz, 2H, Ar-H-OCO-), 4.38 (m, 2H, -O-CH$_2$C*H*$_2$-OCO-), 4.12 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.75 (m, 2H, -O-C*H*$_2$CH$_2$-OCO-), 3.64-3.59 (m, 20H, -OC*H*$_2$C*H*$_2$O-), 2.42 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 156.29 (1C), 153.20 (1C), 146.12 (1C), 126.03 (2C), 122.58 (2C), 80.48 (1C), 75.42 (1C), 71.43-71.29 (8C), 71.11 (1C), 69.83 (1C), 69.34 (1C), 69.08 (1C), 59.09 ppm (1C). HRMS (ESI): m/z calcd for $C_{22}H_{31}NO_{11}$+Na^+ [*M*+Na]$^+$ 508.1795; found 508.0996.

*Synthesis of **4a.*** By using the general procedure in the main article with **2a** (2.03 g, 8.75 mmol), MsCl (1.50 g, 13.1 mmol), and Et_3N (1.77 g, 17.5 mmol), the pure product was obtained as a pale yellow oil (2.69 g, 100%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.24 (m, 2H, HCCC*H*$_2$O-), 4.06 (d, *J* = 2.40 Hz, 2H, -OCH$_2$C*H*$_2$-SO$_2$CH$_3$), 3.64 (m, 2H, -OC*H*$_2$CH$_2$-SO$_2$CH$_3$), 3.57-3.51 (m, 12H, -O-C*H*$_2$C*H*$_2$-O-), 2.96 (s, 3H, -S-(C*H*$_3$), 2.42 ppm (t, *J* = 4.8 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.49 (1C), 75.59 (1C), 71.23-71.14 (4C), 70.99 (1C), 70.27 (1C), 69.76 (1C), 69.63 (1C), 58.98 (1C), 38.32 ppm (1C). HRMS (ESI): m/z calcd for $C_{12}H_{22}O_7S$+Na^+ [*M*+Na]$^+$ 333.0984; found 333.0419.

*Synthesis of **4b.*** By using the general procedure in the main article with **2b** (1.71 g, 5.34 mmol), MsCl (0.92 g, 8.01 mmol), and Et_3N (1.08 g, 10.7 mmol), the pure product was obtained as a pale yellow oil (2.11 g, 100%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.30 (m, 2H, HCCC*H*$_2$O-), 4.13 (d, *J* = 2.40 Hz, 2H, -OCH$_2$C*H*$_2$-SO$_2$CH$_3$), 3.70 (m, 2H, -OC*H*$_2$CH$_2$-SO$_2$CH$_3$), 3.63-3.57 (m, 20H, -O-C*H*$_2$C*H*$_2$-O-), 3.02 (s, 3H, -S-(C*H*$_3$), 2.42 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.48 (1C), 75.44 (1C), 71.34-71.22 (8C), 71.10 (1C), 70.17 (1C), 69.83 (1C), 69.72 (1C), 59.08 (1C), 38.43 ppm (1C). HRMS (ESI): m/z calcd for $C_{16}H_{30}O_9S$+Na^+ [*M*+Na]$^+$ 421.1508; found 421.1120; for $C_{16}H_{30}O_9S$+K^+ [*M*+K]$^+$ 437.1248; found 437.0769.

*Synthesis of **5a.*** By using the general procedure in the main article with **4a** (0.24 g, 7.67 mmol) and NaI (0.46 g, 3.07 mmol), the pure product was obtained as a pale yellow oil (0.19 g, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.15 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.70 (t, *J* = 6.8 Hz, -OC*H*$_2$CH$_2$I, 2H), 3.66-3.61 (m, 12H, -OC*H*$_2$C*H*$_2$-O), 3.22 (t, *J* = 6.8 Hz, 2H, -OCH$_2$C*H*$_2$I), 2.42 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.48 (1C), 75.43 (1C), 72.72 (1C), 71.41-71.34 (3C), 71.18 (1C), 70.98 (1C), 69.87 (1C), 59.16 (1C), 3.86 ppm (1C). HRMS (ESI): m/z calcd for $C_{11}H_{19}IO_4$+H^+ [*M*+H]$^+$ 343.0406; found 342.9579.

*Synthesis of **5b.*** By using the general procedure in the main article with **4b** (0.24 g, 0.60 mmol) and NaI (0.36 g, 2.38 mmol), the pure product was obtained as a pale yellow oil (0.20 g, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.13 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.69 (t, 2H, *J* = 6.8 Hz, -OC*H*$_2$CH$_2$I), 3.64-3.58 (m, 20H, -OC*H*$_2$C*H*$_2$-O), 3.19 (t, *J* = 6.8 Hz, 2H, -OCH$_2$C*H*$_2$I), 2.42 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.46 (1C), 75.46 (1C), 72.69 (1C), 71.41-71.31 (7C), 71.13 (1C), 70.96 (1C), 69.84 (1C), 59.13 (1C), 3.85 ppm (1C). HRMS (ESI): m/z calcd for $C_{15}H_{27}IO_6$+Na^+ [*M*+Na]$^+$ 453.0750; found 453.0149; for $C_{15}H_{27}IO_6$+K^+ [*M*+K]$^+$ 469.0489, found 469.0003.

*Synthesis of **6a.*** By using the general procedure in the main article with **4a** (0.20 g, 0.64 mmol) and KSAc (0.11 g, 9.66 mmol), the pure product was obtained as a colorless oil (0.19 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.18 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.69-3.56 (m, 14H, -OC*H*$_2$C*H*$_2$O-), 3.07 (t, *J* = 6.4 Hz, 2H, -OCH$_2$C*H*$_2$-SCOCH$_3$), 2.43 (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-), 2.31 ppm (s, 3H, -OCH$_2$CH$_2$-SCOC*H*$_3$). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 196.18 (1C), 80.47 (1C), 75.33 (1C), 71.39-71.09, (5C), 70.51 (1C), 69.88 (1C), 59.15 (1C), 31.32 (1C), 29.62 ppm (1C). HRMS (ESI): m/z calcd for $C_{13}H_{22}O_5S$+Na^+ [*M*+Na]$^+$ 313.1086; found 313.1276.

*Synthesis of **6b.*** By using the general procedure in the main article with **4b** (0.25 g, 0.63 mmol) and KSAc (0.11 g, 0.94 mmol), the pure product was obtained as a colorless oil (0.22 g, 97%). ^{1}H NMR (400 MHz,

$CDCl_3$) δ = 4.10 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.60-3.48 (m, 22H, -OC*H*$_2$C*H*$_2$O-), 2.98 (t, *J* = 6.4 Hz, 2H, -OCH$_2$C*H*$_2$-SCOCH$_3$), 2.40 (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-), 2.24 ppm (s, 3H, -OCH$_2$CH$_2$-SCOC*H*$_3$). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 196.00 (1C), 80.43 (1C), 75.44 (1C), 71.34-71.02, (8C), 71.09 (1C), 71.02 (1C), 70.44 (1C), 59.06 (1C), 31.26 (1C), 29.53 ppm (1C). HRMS (ESI): m/z calcd for $C_{17}H_{30}O_7S+Na^+$ [*M*+Na]$^+$ 401.1610; found 401.1097.

Synthesis of ***7a.*** By using the general procedure in the main article with **6a** (0.19 g, 0.64 mmol) and LAH (0.12 g, 3.18 mmol), the pure product was obtained as a pale yellow oil (0.15 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.18 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.69-3.56 (m, 14H, -OC*H*$_2$C*H*$_2$O-), 2.68 (m, 2H, -OCH$_2$C*H*$_2$SH), 2.43 (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-), 1.58 (t, *J* = 8.4 Hz, 1H, -OCH$_2$CH$_2$S*H*). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.46 (1C), 75.34 (1C), 73.65 (1C), 71.40-71.01 (5C), 69.89 (1C), 59.16 (1C), 25.04 ppm (1C). HRMS (ESI): m/z calcd for $C_{11}H_{20}O_4S+Na^+$ [*M*+Na]$^+$ 271.0980; found 271.0797.

Synthesis of ***7b.*** By using the general procedure in the main article with **6b** (0.03 g, 0.08 mmol) and LAH (0.01 g, 0.24 mmol), the pure product was obtained as a pale yellow oil (0.02 g, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 4.22 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.72-3.62 (m, 22H, -OC*H*$_2$C*H*$_2$O-), 2.72 (m, 2H, -OCH$_2$C*H*$_2$SH), 2.45 (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-), 1.61 ppm (t, *J* = 8.0 Hz, 1H, -OCH$_2$CH$_2$S*H*). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.49 (1C), 75.32 (1C), 73.71 (1C), 71.47-71.36 (7C), 71.23 (1C), 71.06 (1C), 69.94 (1C), 59.22 (1C), 25.08 (1C). HRMS (ESI): m/z calcd for $C_{15}H_{28}O_6S+Na^+$ [*M*+Na]$^+$ 359.1504; found 359.1524.

Synthesis of ***8a.*** By using the general procedure in the main article with **4a** (2.29 g, 7.36 mmol) and potassium phthalimide (2.04 g, 11.04 mmol), the pure product was obtained as a yellow oil (2.64 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.82 (m, 2H, Ar-H), 7.70 (m, 2H, Ar-H), 4.17 (m, 2H, HCCC*H*$_2$O-), 3.87 (t, *J* = 6.0 Hz, 2H, -OC*H*$_2$CH$_2$-NPhth), 3.71 (t, *J* = 3.2 Hz, 2H, -OCH$_2$C*H*$_2$-NPhth), 3.64-3.55 (m, 14H, -OCH$_2$CH$_2$O-), 2.43 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 169.06 (2C), 134.70 (2C), 132.91 (2C), 123.98 (2C), 80.49 (1C), 75.35 (1C), 71.35-71.32 (3C), 71.12 (1C), 70.87 (1C), 69.86 (1C), 68.66 (1C), 59.13 (1C), 38.06 ppm (1C). HRMS (ESI): m/z calcd for $C_{19}H_{23}NO_6+Na^+$ [*M*+Na]$^+$ 384.1423; found 384.0653.

Synthesis of 8b. By using the general procedure in the main article with **4b** (1.73 g, 4.34 mmol) and potassium phthalimide (1.21 g, 6.52 mmol), the pure product was obtained as a yellow oil (1.80 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.79 (m, 2H, Ar-H), 7.68 (m, 2H, Ar-H), 4.15 (d, *J* = 4.4 Hz, 2H, HCCC*H*$_2$O-), 3.85 (t, *J* = 5.6 Hz, 2H, -OC*H*$_2$CH$_2$-NPhth), 3.71-3.53 (m, 22H, -OCH$_2$CH$_2$O-), 2.43 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 169.96 (2C), 134.70 (2C), 132.88 (2C),

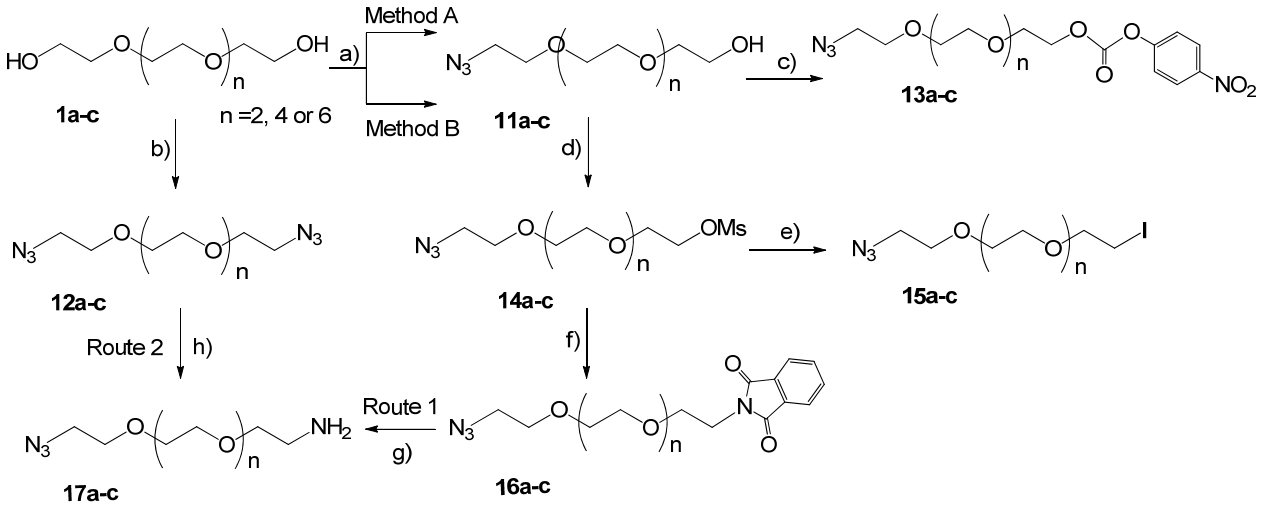
123.97 (2C), 80.47 (1C), 75.40 (1C), 71.34-71.28 (7C), 71.13 (1C), 70.84 (1C), 69.85 (1C), 68.64 (1C), 59.12 (1C), 38.03 ppm (1C). HRMS (ESI): m/z calcd for $C_{23}H_{31}NO_8$+Na^+ $[M+Na]^+$ 472.1942; found 472.1947.

Synthesis of ***9a.*** By using the general procedure in the main article with **8a** (2.63 g, 7.28 mmol) and hydrazine (2.60 g, 81.25 mmol), the pure product was obtained as a pale yellow oil (1.67 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 3.93 (m, 2H, HCCC*H*$_2$O-), 3.42-3.36 (m, 14H, -OC*H*$_2$C*H*$_2$O-), 3.22 (m, 2H, -OC*H*$_2$CH$_2$NH$_2$), 2.57 (m, 2H, -OCH$_2$C*H*$_2$NH$_2$), 2.32 ppm (m, 1H, -*H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.31 (1C), 75.47 (1C), 73.98 (1C), 71.12-71.01 (3C), 70.91 (1C), 70.80 (1C), 69.61 (1C), 58.86 (1C), 42.34 ppm (1C). HRMS (ESI): m/z calcd for $C_{11}H_{21}NO_4$+H^+ $[M+H]^+$ 232.1549; found 232.1547.

Synthesis of ***9b.*** By using the general procedure in the main article with **8b** (1.70 g, 3.78 mmol) and hydrazine (1.70 g, 63.8 mmol), the pure product was obtained as a pale yellow oil (1.20 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 3.98 (d, *J* = 2.4 Hz, 2H, HCCC*H*$_2$O-), 3.48-3.39 (m, 22H, -OC*H*$_2$C*H*$_2$O-), 3.28 (t, *J* = 5.2 Hz, 2H, -OC*H*$_2$CH$_2$NH$_2$), 2.63 (t, *J* = 5.2 Hz, 2H, -OCH$_2$C*H*$_2$NH$_2$), 2.34 ppm (t, *J* = 2.4 Hz, 1H, -*H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 80.33 (1C), 75.48 (1C), 74.02 (1C), 71.17-71.09 (7C), 70.96 (1C), 70.87 (1C), 69.66 (1C), 58.92 (1C), 42.39 ppm (1C). HRMS (ESI): m/z calcd for $C_{15}H_{29}NO_6$+H^+ $[M+H]^+$ 320.2073; found 320.1923.

Synthesis of ***10a.*** By using the general procedure in the main article with **9a** (0.21 g, 0.91 mmol) and N-methoxycarbonyl maleimide (0.14 g, 0.91 mmol), the pure product was obtained as a pale yellow oil (0.14 g, 49%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.67 (s, 2H, Mal-H), 4.14 (d, *J* = 2.4 Hz, 2H, -HCCC*H*$_2$O-), 3.67-3.54 (m, 16H, -OC*H*$_2$C*H*$_2$O-), 2.42 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 171.40 (2C), 134.93 (2C), 80.47 (1C), 75.40 (1C), 71.32-71.28 (3C), 71.11 (1C), 70.79 (1C), 69.84 (1C), 68.53 (1C), 59.10 (1C), 37.88 ppm (1C). HRMS (ESI): m/z calcd for $C_{15}H_{21}NO_6$+Na^+ $[M+Na]^+$ 334.1261; found 334.1267.

Synthesis of ***10b.*** By using the general procedure in the main article with **9b** (0.24 g, 0.75 mmol) and N-methoxycarbonyl maleimide (0.12 g, 0.75 mmol), the pure product was obtained as a pale yellow oil (0.18 g, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.64 (s, 2H, Mal-H), 4.10 (d, *J* = 2.4 Hz, 2H, -HCCC*H*$_2$O-), 3.64-3.49 (m, 24H, -OC*H*$_2$C*H*$_2$O-), 2.41 ppm (t, *J* = 2.4 Hz, 1H, *H*CCCH$_2$O-). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 171.37 (2C), 134.94 (2C), 80.45 (1C), 75.45 (1C), 71.30-71.23 (7C), 71.08 (1C), 70.76 (1C), 69.80 (1C), 68.48 (1C), 59.06 (1C), 37.84 ppm (1C). HRMS (ESI): m/z calcd for $C_{19}H_{29}NO_8$+Na^+ $[M+Na]^+$ 422.1791; found 422.1298.



Scheme 2 Sequential synthesis of azide terminated heterobifunctionalized OEG linkers. *Reagents and conditions*: (a) Method A: (i) MsCl, Et_3N, DCM, 0 °C-RT, 3 h; (ii) NaN_3, DMF, 65 °C, 15 h; Method B: (i) MsCl, Ag_2O, DCM, 0 °C-RT, 24 h; (ii) NaN_3, DMF, 65 °C, 15 h; (b) (i) MsCl, Et_3N, DCM, 0 °C-RT, 4 h; (ii) NaN_3, DMF, 65 °C, 15 h; (c) 4-nitrophenyl chloroformate, pyridine, MeCN, RT, 15 h; (d) MsCl, Et_3N, DCM, 0 °C-RT, 3.5 h; (e) NaI, acetone, 65 °C, 15 h; (f) Potassium phthalimide, DMF, 110 °C, 15 h; (g) Hydrazine, EtOH, 60 °C, 3 h; (h) Ph_3P, Et_2O-5% aq HCl, RT, 24 h.

*Synthesis of **11a***

By using the general procedure in the main article for Method A with OEG **1a** (5.19 g, 26.7 mmol), MsCl (2.76 g, 24.1 mmol), Et_3N (4.05 g, 40.1 mmol), and NaN_3 (8.69 g, 134 mmol), the pure product was obtained as a pale yellow oil (1.90 g, 36%). By using the general procedure in the main article for Method B with OEG **1a** (1.00 g, 5.15 mmol), Ag_2O (1.79 g, 7.72 mmol), and MsCl (651 mg, 5.66 mmol), the pure product was obtained as a pale yellow oil (774 mg, 69%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 3.62-3.58 (m, 12H, -OCH2CH2O-), 3.51 (m, 2H, -OCH_2CH_2OH), 3.30 (t, *J* = 4.8 Hz, 2H, $N_3CH_2CH_2$O-), 3.10 ppm (t, *J* = 6.0 Hz, -OCH_2CH_2OH). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 73.28 (1C), 71.37-71.13 (3C), 71.02 (1C), 70.72 (1C), 62.29 (1C), 51.35 ppm (1C). HRMS (ESI): m/z calcd for $C_8H_{17}N_3O_4$+Na^+ $[M+Na]^+$ 242.1111; found 242.0553.

*Synthesis of **11b***

By using the general procedure in the main article for Method A with OEG **1b** (5.25 g, 18.6 mmol), MsCl (1.92 g, 16.8 mmol), Et_3N (2.82 g, 27.9 mmol), and NaN_3 (6.04 g, 93.0 mmol), the pure product was obtained as a pale yellow oil (2.11 g, 37%). By using the general procedure in the main article for

Method B with OEG **1b** (500 mg, 1.77 mmol), Ag_2O (616 mg, 2.66 mmol), KI (59.0 mg, 0.35 mmol), and MsCl (223 mg, 1.95 mmol), the pure product was obtained as a pale yellow oil (293 mg, 54%): ^{1}H-NMR (500 MHz, $CDCl_3$) δ = 3.52-3.47 (m, 18H, -OC*H*$_2$C*H*$_2$O-), 3.40 (m, 4H, $N_3CH_2CH_2O$- & -OCH_2CH_2OH), 3.21 ppm (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2O$-). ^{13}C-NMR (125.8 MHz, $CDCl_3$) δ = 72.44 (1C), 70.33-70.25 (7C), 70.04 (1C), 69.77 (1C), 61.20 (1C), 50.38 ppm (1C). HRMS (ESI): m/z calcd for $C_{12}H_{25}N_3O_6$+Na^+ [*M*+Na]$^+$ 330.1636; found 330.1119; for $C_{12}H_{25}N_3O_6$+K^+ [*M*+K]$^+$ 346.1375; found 346.0851.

Synthesis of ***12a***

By using the general procedure in the main article with OEG **1a** (1.03 g, 5.30 mmol), MsCl (1.84 g, 15.9 mmol), Et_3N (1.61 g, 15.9 mmol), and NaN_3 (1.72 g, 26.5 mmol), the pure product was obtained as a pale yellow oil (1.30 g, 100%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 3.47 (m, 12H, -OC*H*$_2$C*H*$_2$O-), 3.25 ppm (t, *J* = 5.0 Hz, 4H, $N_3CH_2CH_2O$-). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 71.26-71.20 (4C), 70.60 (2C), 51.25 ppm (2C). HRMS (ESI): m/z calcd for $C_8H_{16}N_6O_3$+Na^+ [*M*+Na]$^+$ 267.1176; found 267.1507.

Synthesis of ***12b***

By using the general procedure in the main article with OEG **1b** (200 mg, 0.708 mmol), MsCl (244 mg, 2.13 mmol), Et_3N (215 mg, 2.13 mmol), and NaN_3 (230 mg, 3.54 mmol), the pure product was obtained as a pale yellow oil (235 mg, 100%): ^{1}H-NMR (500 MHz, $CDCl_3$) δ = 3.53 (m, 20H, -OC*H*$_2$C*H*$_2$O-), 3.25 ppm (t, *J* = 5.0 Hz, 4H, $N_3CH_2CH_2O$-). ^{13}C-NMR (125.8 MHz, $CDCl_3$) δ = 71.42-71.35 (8C), 69.81 (2C), 50.44 ppm (2C). HRMS (ESI): m/z calcd for $C_{12}H_{24}N_6O_5$+Na^+ [*M*+Na]$^+$ 355.1700; found 355.1082.

Synthesis of ***13a***

By using the general procedure in the main article with **11a** (253 mg, 1.15 mmol), 4-nitrophenyl chloroformate (349 mg, 1.73 mmol), and pyridine (183 mg, 2.13 mmol), the pure product was obtained as a pale yellow oil (417 mg, 94%): ^{1}H-NMR: (400 MHz, $CDCl_3$) δ = 8.24 (d, *J* = 5.2 Hz, 2H, Ar-H-NO_2), 7.36 (d, *J* = 5.2 Hz, 2H, Ar-H-OCO-), 4.41 (t, *J* = 1.6 Hz, 2H, -O-CH_2CH_2-OCO-), 3.79 (t, *J* = 1.6 Hz, 2H, -O-C*H*$_2$$CH_2$-OCO-), 3.66 (m, 10H, -OC*H*$_2$C*H*$_2$O-), 3.36 ppm (t, J = 4.8 Hz, 2H, $N_3CH_2CH_2O$-). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 156.33 (1C), 153.23 (1C), 146.14 (1C), 126.04 (2C), 122.58 (2C), 71.44 (4C), 70.79 (1C), 69.37 (1C), 69.11 (1C), 51.44 ppm (1C). HRMS (ESI): m/z calcd for $C_{15}H_{20}N_4O_8$+Na^+ [*M*+Na]$^+$ 407.1173; found 407.0414.

Synthesis of ***13b***

By using the general procedure in the main article with **11b** (100 mg, 0.33 mmol), 4-nitrophenyl chloroformate (98.3 mg, 0.49 mmol), and pyridine (51.5 mg, 0.65 mmol), the pure product was obtained as a pale yellow oil (134 mg, 87%): ^{1}H-NMR: (500 MHz, $CDCl_3$) δ = 8.32 (d, *J* = 5.0 Hz, 2H, Ar-H-NO_2), 7.44 (d, *J* = 5.0 Hz, 2H, Ar-H-OCO-), 4.49 (m, 2H, -O-CH_2CH_2-OCO-), 3.86 (m, 2H, -O-CH_2CH_2-OCO-), 3.71 (m, 18H, -OCH_2CH_2O-), 3.43 ppm (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2O$-). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 155.51 (1C), 152.45 (1C), 145.34 (1C), 125.27 (2C), 121.79 (2C), 70.67-70.55 (8C), 69.99 (1C), 68.58 (1C), 68.30 (1C), 50.64 ppm (1C). HRMS (ESI): m/z calcd for $C_{19}H_{28}N_4O_{10}$+Li^+ $[M+Li]^+$ 479.1960; found 479.1313; for $C_{19}H_{28}N_4O_{10}$+Na^+ $[M+Na]^+$ 495.1698; found 495.1131.

Synthesis of ***14a***

By using the general procedure in the main article with **11a** (1.15 g, 5.25 mmol), MsCl (901 mg, 7.86 mmol), and Et_3N (1.06 g, 10.5 mmol), the pure product was obtained as a pale yellow oil (1.54 g, 99%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 4.35 (m, 2H, -OCH_2CH_2OMs), 3.75 (m, 2H, $N_3CH_2CH_2O$-), 3.65 (m, 10H, -OCH_2CH_2O-), 3.37 (t, *J* = 4.8 Hz, 2H, $N_3CH_2CH_2O$-), 3.06 ppm (s, 3H, -OSO_2CH_3). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 71.44-71.37 (4C), 70.79 (1C), 70.17 (1C), 69.77 (1C), 51.45 (1C), 38.42 ppm (1C). HRMS: m/z calcd for $C_9H_{19}N_3O_6S$+Na^+ $[M+Na]^+$ 320.0887; found 320.0583.

Synthesis of ***14b***

By using the general procedure in the main article with **11b** (1.10 g, 3.59 mmol), MsCl (616 mg, 5.38 mmol), and Et_3N (724 mg, 7.17 mmol), the pure product was obtained as a pale yellow oil (1.37 g, 99%): ^{1}H-NMR (500 MHz, $CDCl_3$) δ = 4.41 (m, 2H, -OCH_2CH_2OMs), 3.80 (m, 2H, $N_3CH_2CH_2O$-), 3.69 (m, 18H, -OCH_2CH_2O-), 3.43 (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2O$-), 3.12 ppm (s, 3H, -OSO_2CH_3). ^{13}C-NMR (125.8 MHz, $CDCl_3$) δ = 71.61-71.52 (6C), 70.45 (1C), 69.96 (1C), 69.40 (1C), 68.95 (1C), 50.62 (1C), 37.67 (1C), 31.58 ppm (1C). HRMS (ESI): m/z calcd for $C_{13}H_{27}N_3O_8S$+Na^+ $[M+Na]^+$ 408.1411; found 408.0851; for $C_{13}H_{27}N_3O_8S$ +$C_6H_{16}N^+$ $[M+C_6H_{16}N]^+$ 487.2769; found 487.2290.

Synthesis of ***15a***

By using the general procedure in the main article with **14a** (200 mg, 0.67 mmol) and sodium iodide (403 mg, 2.69 mmol), the pure product was obtained as a pale yellow oil (213 mg, 96%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 3.73 (t, *J* = 6.8 Hz, 2H, -OCH_2CH_2I), 3.65 (m, 10H, -OCH_2CH_2O-), 3.37 (t, *J* = 4.8 Hz, 2H, $N_3CH_2CH_2O$-), 3.24 ppm (t, *J* = 6.8 Hz, 2H, -OCH_2CH_2I). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 72.73 (1C), 71.49-71.46 (3C), 71.01 (1C), 70.84 (1C), 51.48 (1C), 3.85 ppm (1C). HRMS (ESI): m/z calcd for $C_8H_{16}IN_3O_3$+Na^+ $[M+Na]^+$ 352.0129; found 351.9791.

*Synthesis of **15b***

By using the general procedure in the main article with **14b** (117 mg, 0.30 mmol) and sodium iodide (182 mg, 1.21 mmol), the pure product was obtained as a pale yellow oil (77.3 mg, 61%): ^{1}H-NMR (500 MHz, $CDCl_3$) δ = 3.81 (t, *J* = 10.0 Hz, 2H, -OC*H*$_2$CH$_2$I), 3.72 (m, 18H, -OC*H*$_2$C*H*$_2$O-), 3.44 (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2$O-), 3.31 ppm (t, *J* = 5.0 Hz, 2H, -OCH$_2$C*H*$_2$I). ^{13}C-NMR (125.8 MHz, $CDCl_3$) δ = 71.19 (1C), 71.68-71.57 (7C), 70.20 (1C), 70.02 (1C), 50.66 (1C), 3.01 ppm (1C). HRMS: m/z calcd for $C_{12}H_{24}IN_3O_5$+Na^+ [*M*+Na]$^+$ 440.0653; found 440.0297.

*Synthesis of **16a***

By using the general procedure in the main article with **14a** (850 mg, 2.86 mmol) and potassium phthalimide (688 mg, 3.72 mmol), the pure product was obtained as a yellow oil (956 mg, 96%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 7.78 (m, 2H, Ar-H), 7.67 (m, 2H, Ar-H), 3.85 (t, *J* = 5.6 Hz, 2H, -OC*H*$_2$CH$_2$NPhth), 3.70 (t, *J* = 6.0 Hz, 2H, -OCH$_2$C*H*$_2$NPhth), 3.58 (m, 10H, -OC*H*$_2$C*H*$_2$O-), 3.32 ppm (t, *J* = 4.8 Hz, 2H, $N_3CH_2CH_2$O-). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 168.95 (2C), 134.69 (2C), 132.89 (2C), 123.94 (2C), 71.41-71.36 (3C), 70.88 (1C), 70.73 (1C), 68.64 (1C), 51.41 (1C), 38.05 ppm (1C). HRMS (ESI): m/z calcd for $C_{16}H_{20}N_4O_5$+Na^+ [*M*+Na]$^+$ 371.1326; found 371.0903.

*Synthesis of **16b***

By using the general procedure in the main article with **14b** (1.16 g, 2.89 mmol) and potassium phthalimide (803 mg, 4.34 mmol), the pure product was obtained as a yellow oil (1.30 g, 99%): ^{1}H-NMR (500 MHz, $CDCl_3$) δ = 7.89 (m, 2H, Ar-H), 7.76 (m, 2H, Ar-H), 3.94 (t, *J* = 10.0 Hz, 2H, -OC*H*$_2$CH$_2$NPhth), 3.78 (t, *J* = 5.0 Hz, 2H, -OCH$_2$C*H*$_2$NPhth), 3.70 (m, 18H, -OC*H*$_2$C*H*$_2$O-), 3.43 ppm (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2$O-). ^{13}C-NMR (125.8 MHz, $CDCl_3$) δ = 168.19 (2C), 133.91 (2C), 132.09 (2C), 123.18 (2C), 70.64-70.48 (7C), 70.04 (1C), 69.98 (1C), 67.85 (1C), 50.64 (1C), 37.22 ppm (1C). HRMS (ESI): m/z calcd for $C_{20}H_{28}N_4O_7$+Na^+ [*M*+Na]$^+$ 459.1850; found 459.1211.

*Synthesis of **17a***

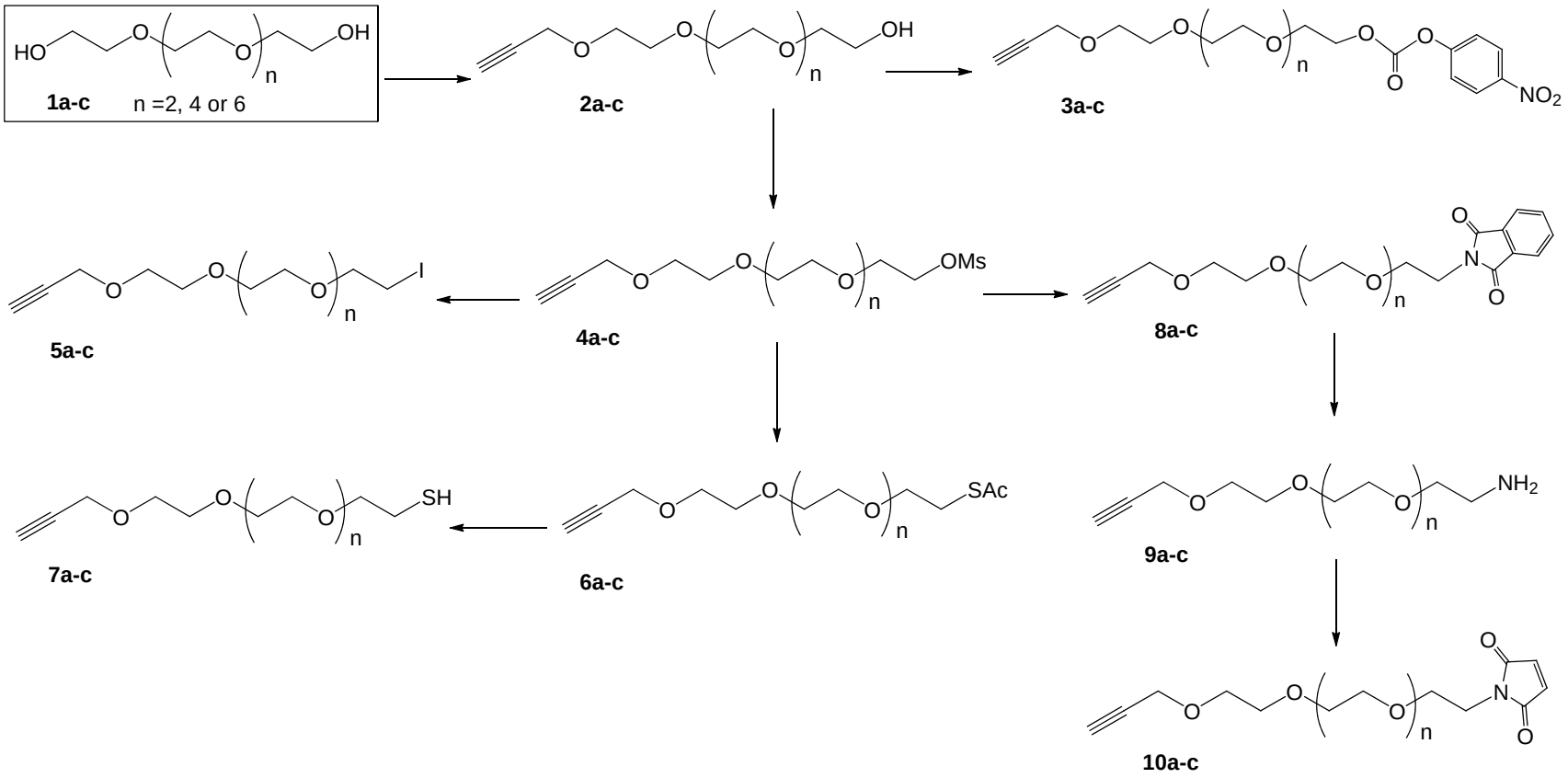
By using the general procedure in the main article for **Route 1** with **16a** (955 mg, 2.74 mmol) and hydrazine (1.02 g, 31.9 mmol), the pure product was obtained as a yellow oil (550 mg, 92%). By using the general procedure in the main article for **Route 2** with **12a** (500 mg, 2.05 mmol), triphenyl phosphine (483 mg, 1.84 mmol), 5% HCl (10 mL), and Et_2O (10 mL) , the pure product was obtained as a pale yellow oil (394 mg, 88%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 3.55 (m, 10H, -OC*H*$_2$C*H*$_2$O-), 3.41 (t, *J* = 5.2

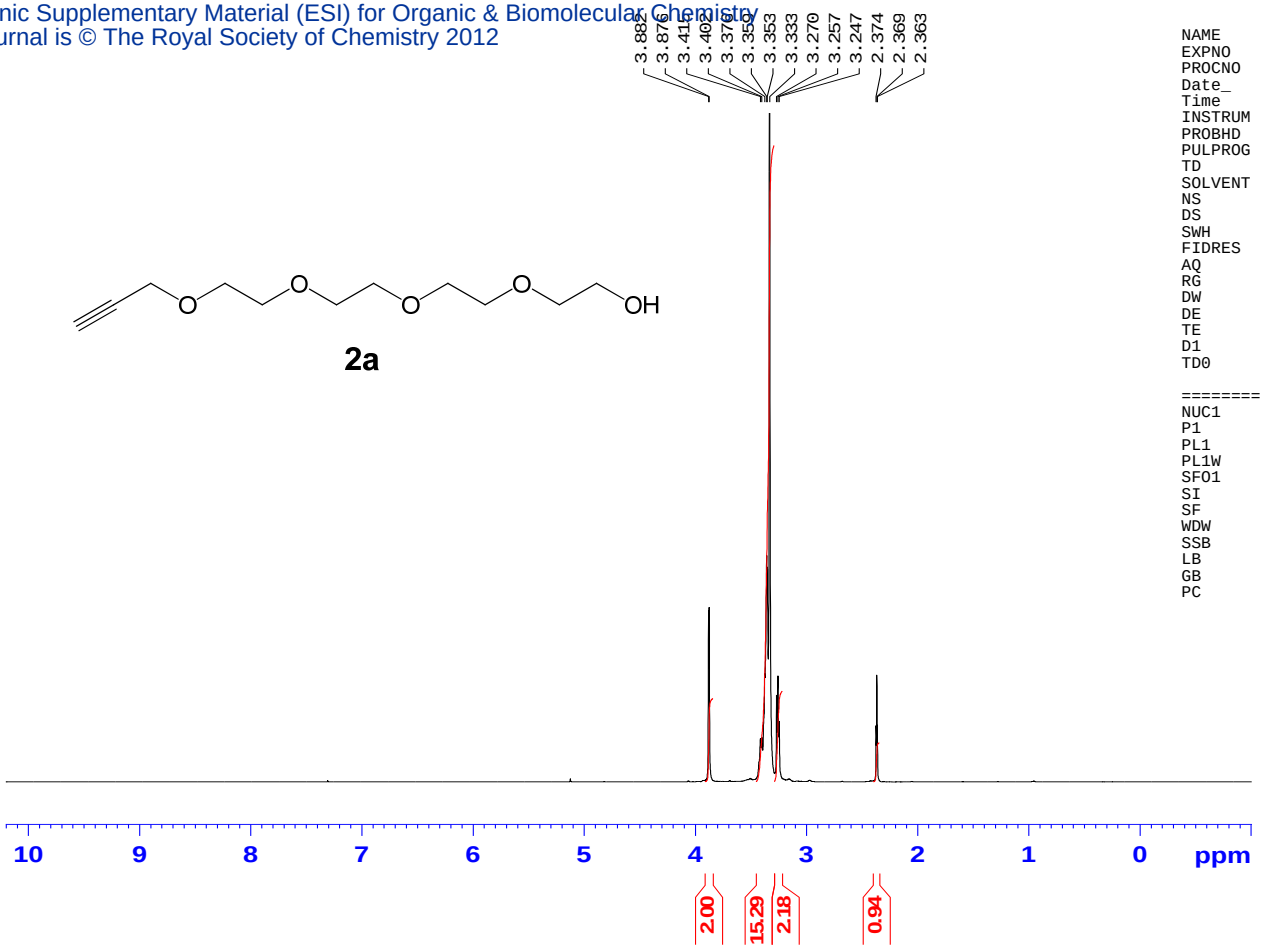
Hz, 2H, $N_3CH_2CH_2O$-), 3.30 (t, *J* = 4.8 Hz, 2H, -$OCH_2CH_2NH_2$), 2.76 (t, *J* = 5.2 Hz, 2H, $N_3CH_2CH_2O$-), 1.43 ppm (bs, 2H, -NH_2). ^{13}C-NMR (100.6 MHz, $CDCl_3$) δ = 74.19 (1C), 71.42-71.09 (3C), 71.01 (1C), 70.68 (1C), 51.39 (1C), 42.51 ppm (1C). HRMS (ESI): m/z calcd for $C_8H_{18}N_4O_3$+H^+ $[M+H]^+$ 219.1452; found 219.1202.

Synthesis of ***17b***

By using the general procedure in the main article for **Route 1** with **16b** (1.44 g, 3.31 mmol) and hydrazine (1.45 g, 45.3 mmol), the pure product was obtained as a yellow oil (940 mg, 93%). By using the general procedure in the main article for **Route 1** with **12b** (500 mg, 1.50 mmol), triphenyl phosphine (355 mg, 1.35 mmol), 5% HCl (10 mL), and Et_2O (10 mL) , the pure product was obtained as a pale yellow oil (398 mg, 86%): ^{1}H-NMR (500 MHz, $CDCl_3$) δ = 3.70 (m, 18H, -OCH_2CH_2O-), 3.54 (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2O$-), 3.42 (t, *J* = 5.0 Hz, 2H, -$OCH_2CH_2NH_2$), 2.89 ppm (t, *J* = 5.0 Hz, 2H, $N_3CH_2CH_2O$-). ^{13}C-NMR (125.8 MHz, $CDCl_3$) δ = 73.46 (1C), 70.65-70.52 (7C), 70.31 (1C), 69.98 (1C), 50.63 (1C), 41.78 ppm (1C). HRMS (ESI): m/z calcd for $C_{12}H_{26}N_4O_5$+H^+ $[M+H]^+$ 307.1976; found 307.1723.

S2 – COPIES OF ^{1}H NMR, ^{13}C NMR & HRMS



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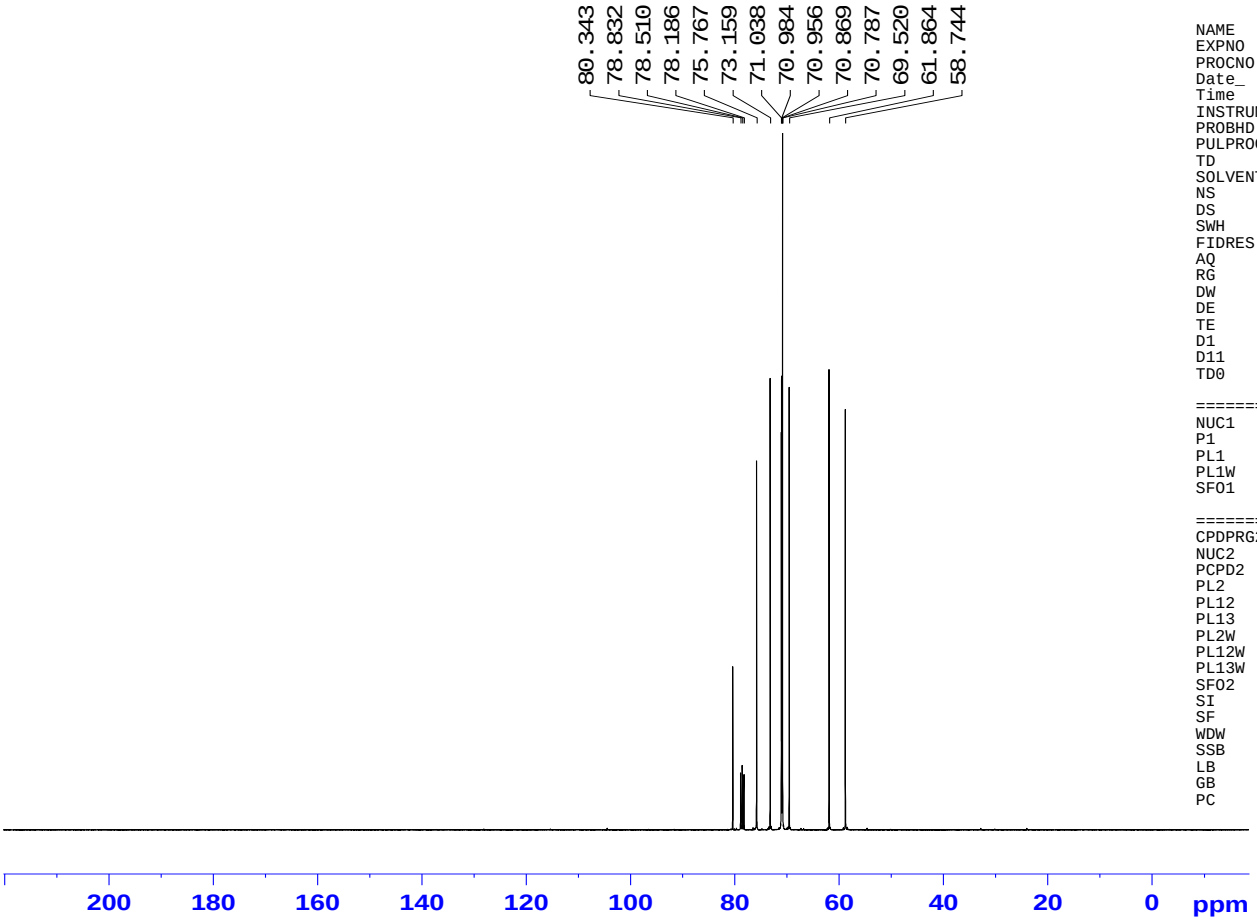


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TD0                         1

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Applied Biosystems Mariner System 5268

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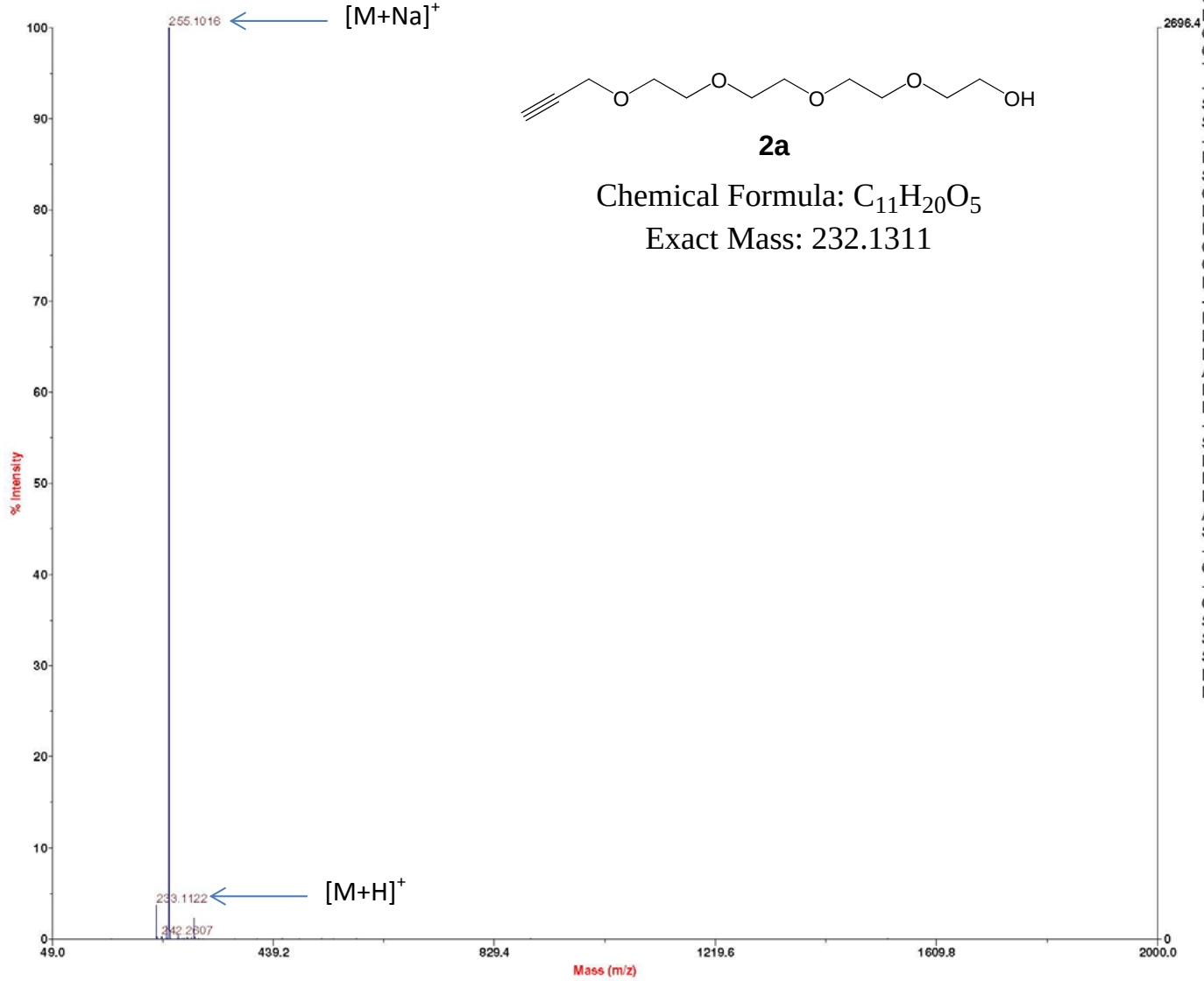

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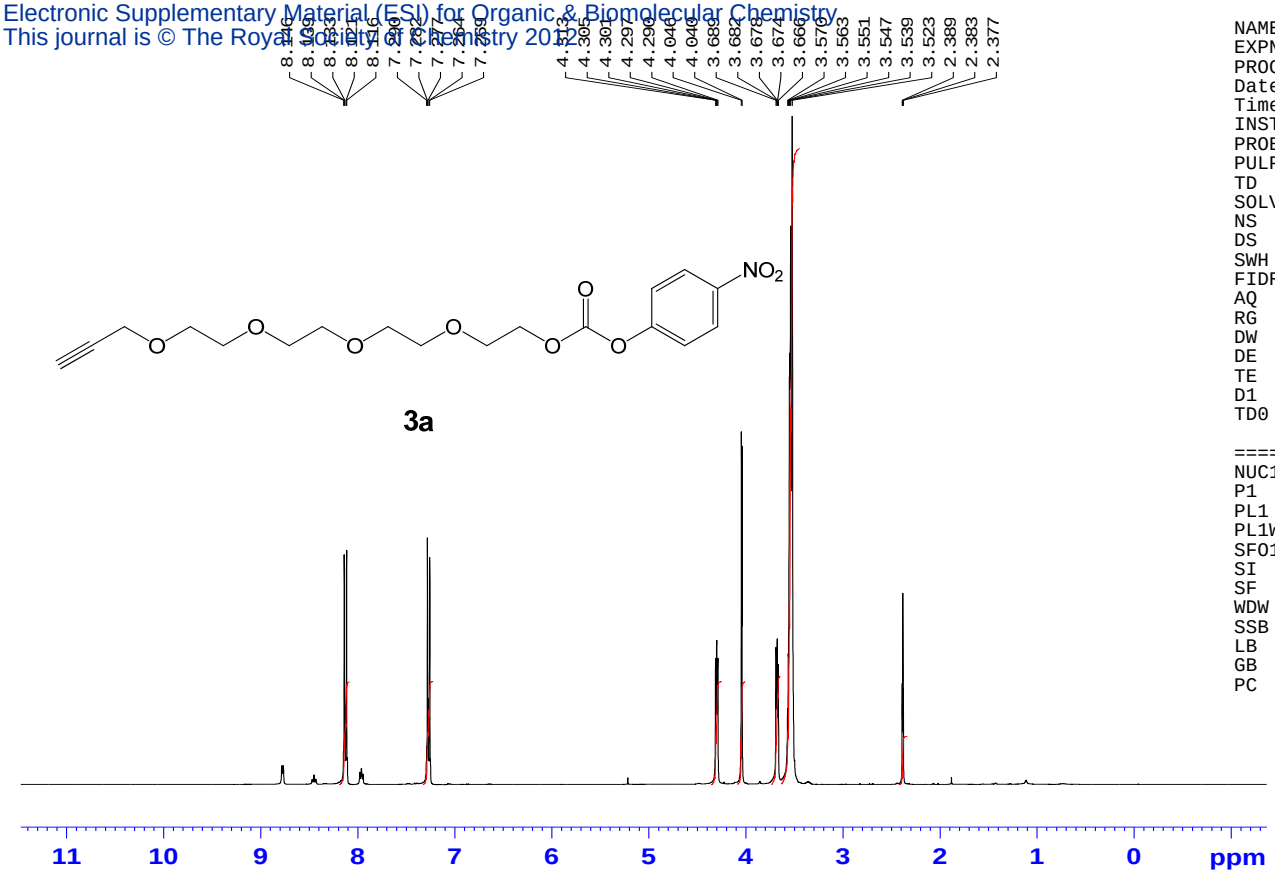


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AQ                       3.7224948 sec
RG                           14.2
DW                          56.800 usec
DE                           6.50 usec
TE                          292.6 K
D1                    1.00000000 sec
TD0                             1

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PL1                         -0.60 dB
PL1W                 13.81451130 W
SFO1                400.1320007 MHz
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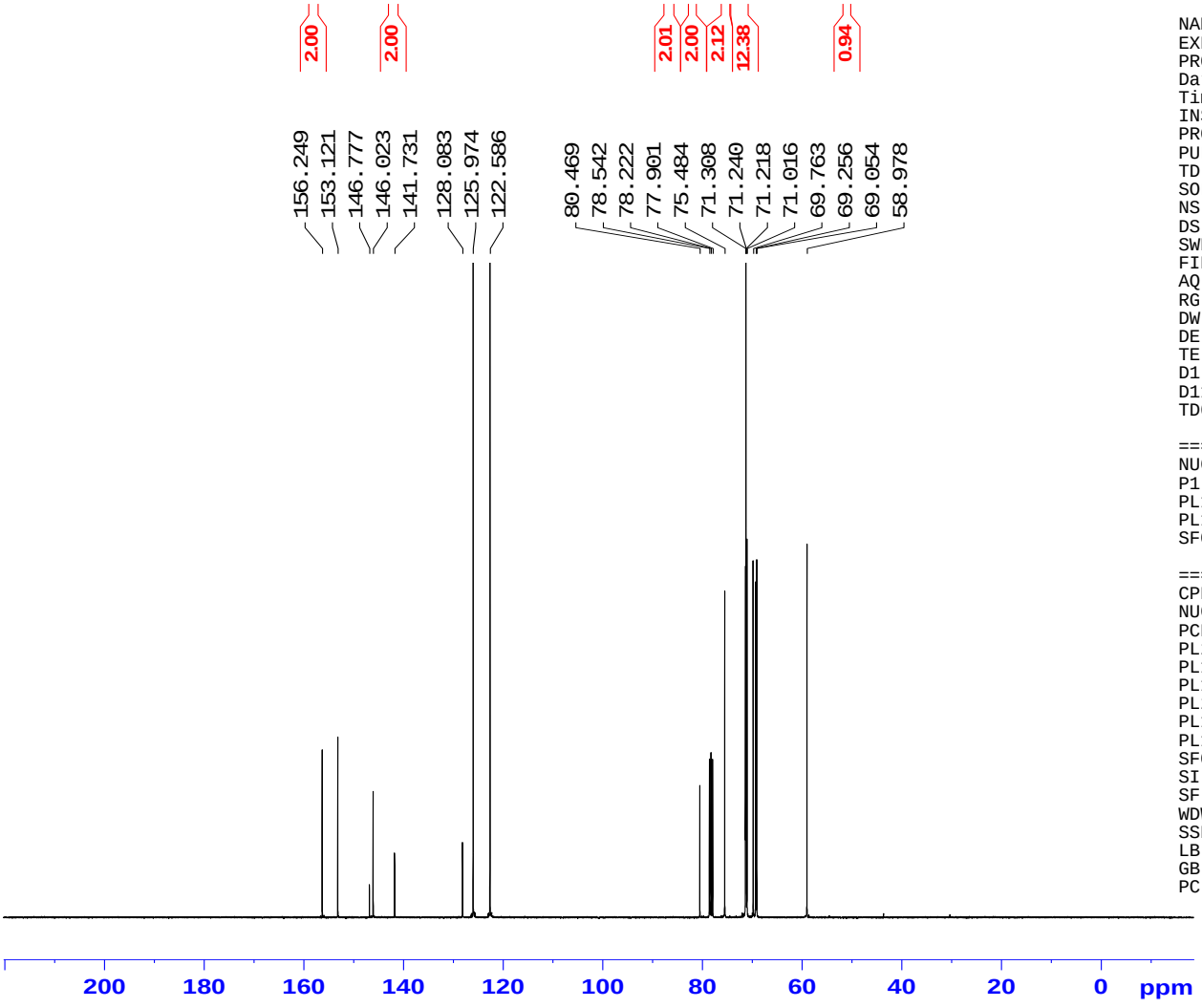


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D1                    2.00000000 sec
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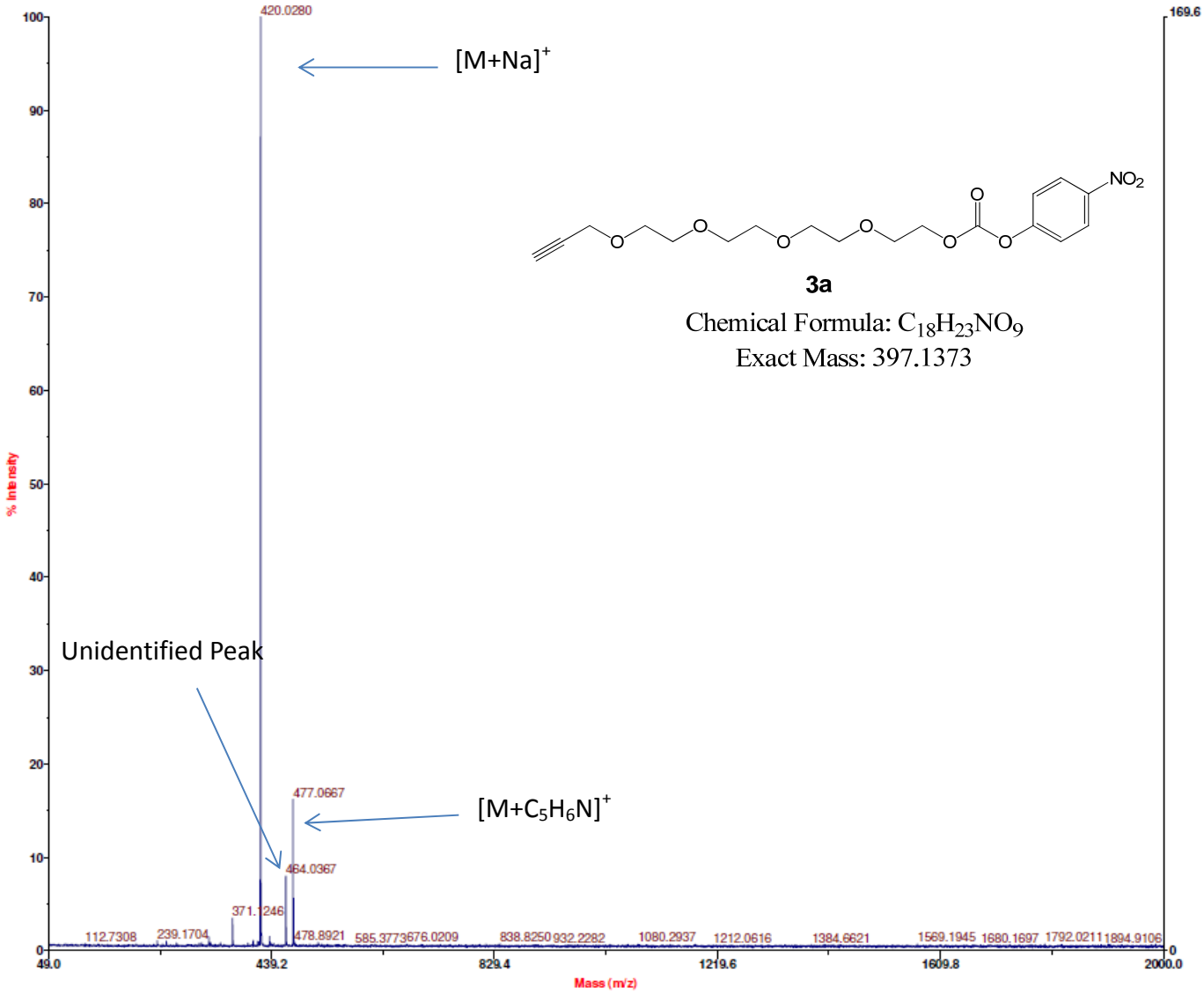
TD0                             1

======== CHANNEL f1 ========
NUC1                           13C
P1                           9.99 usec
PL1                         -3.00 dB
PL1W                73.67452240 W
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                       80.00 usec
PL2                         -0.65 dB
PL12                        13.40 dB
PL13                        13.40 dB
PL2W                13.97447491 W
PL12W                0.54996562 W
PL13W                0.54996562 W
SFO2                400.1316005 MHz
SI                          32768
SF                  100.6126885 MHz
WDW                            EM
SSB                             0
LB                           1.00 Hz
GB                              0
PC                           1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:28 (T /0.00:0.48) ASC[BP = 420.0, 170]



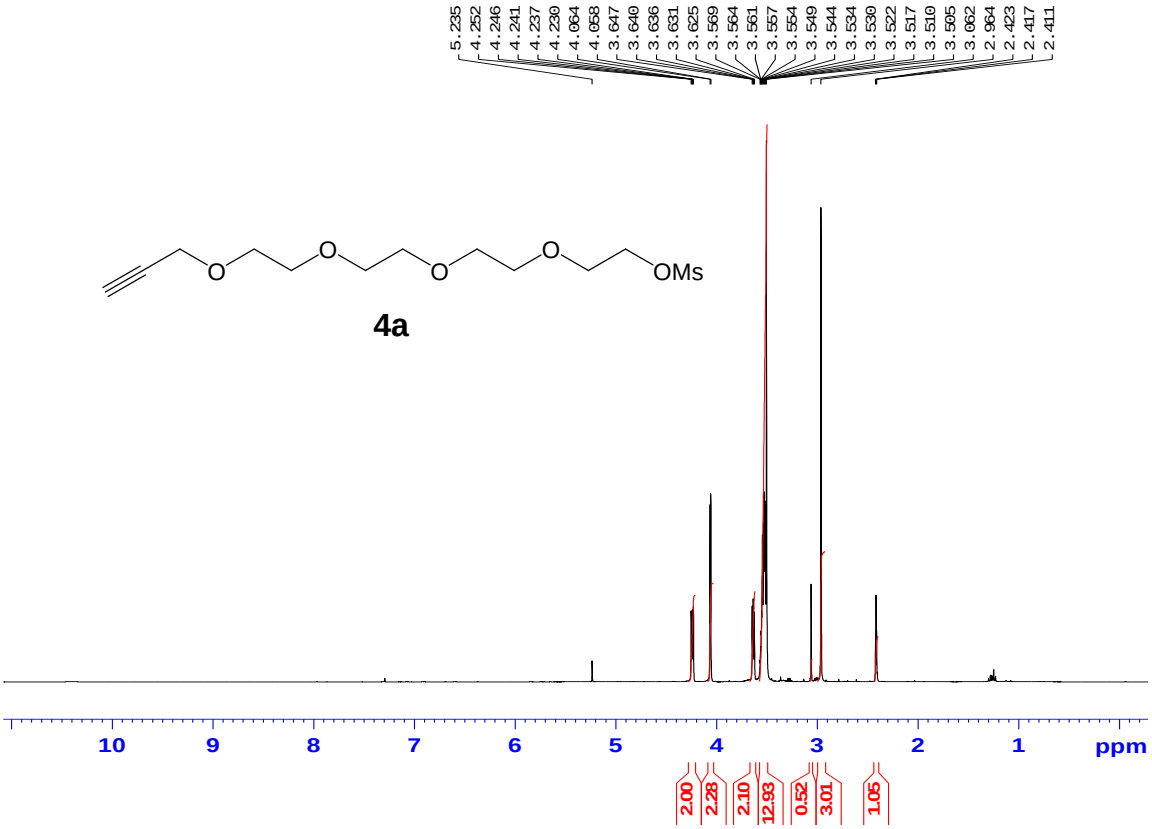
3a

Chemical Formula: $C_{18}H_{23}NO_9$
Exact Mass: 397.1373

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

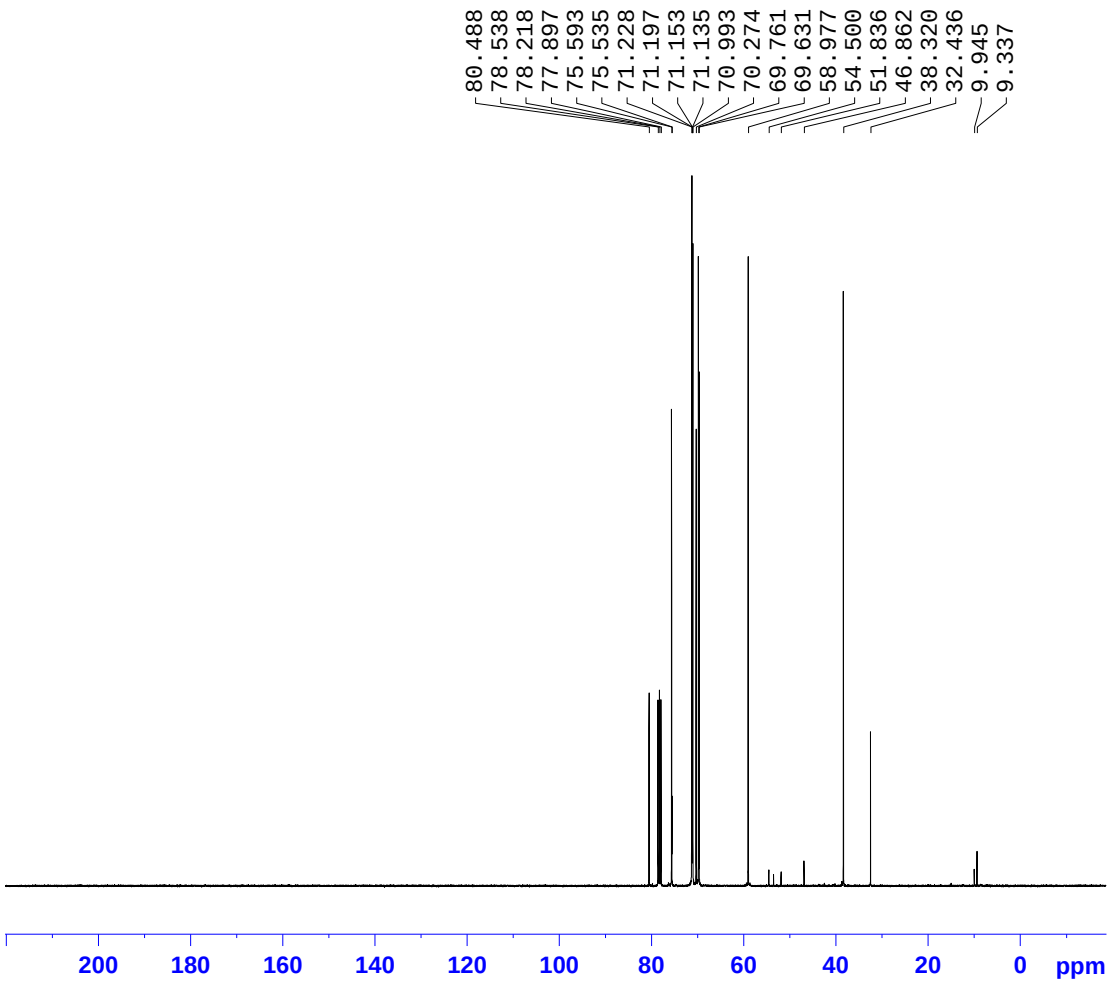
Acquired: Oct 18 14:38:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\18 Tues\ZH3-129001.dat

Printed: 14:39, October 18, 2011



NAME ZH3-128_Alk-P4-OMs
EXPNO 1
PROCNO 1
Date_ 20111017
Time 21.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224948 sec
RG 12.7
DW 56.800 usec
DE 6.50 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1

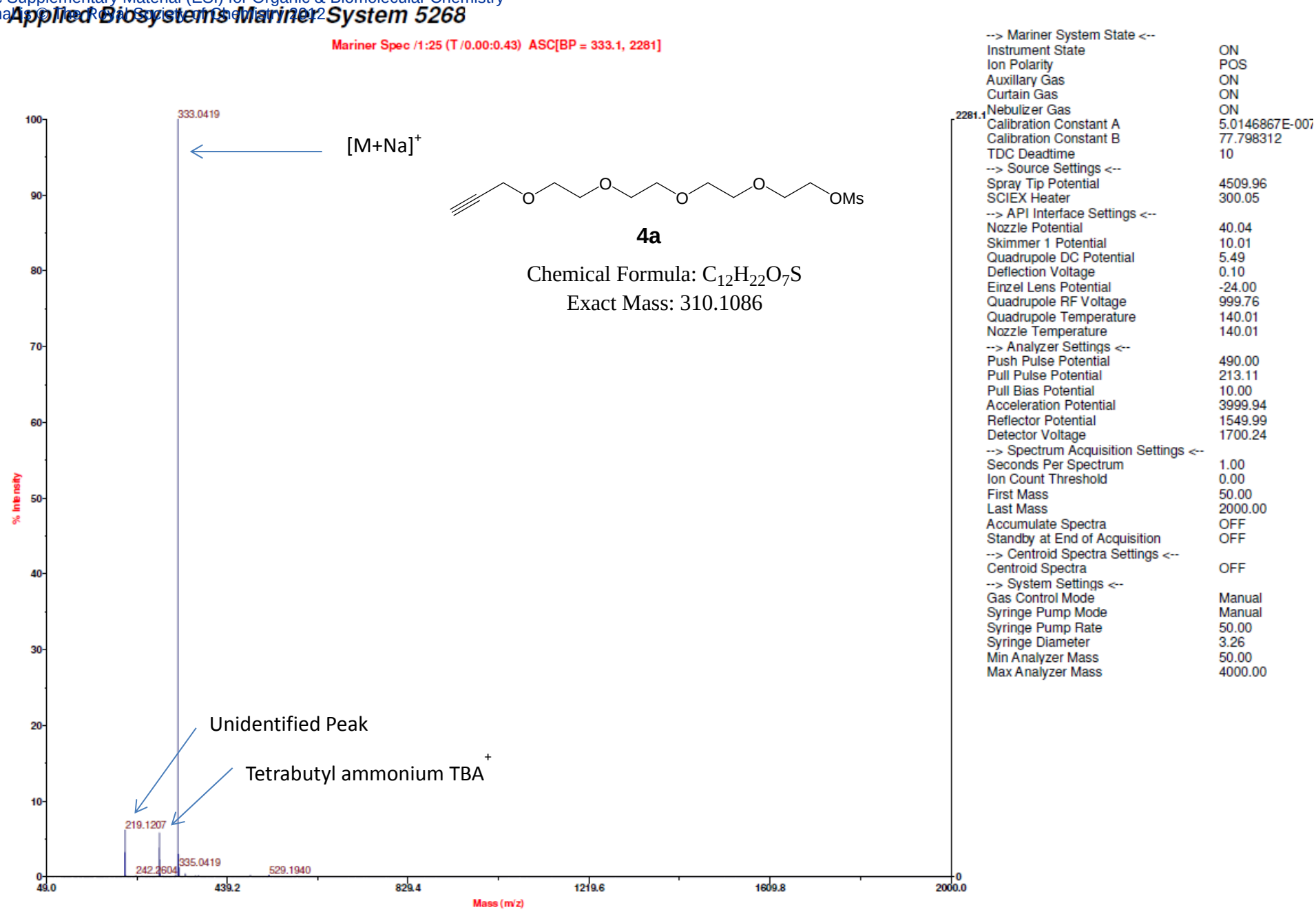
======== CHANNEL f1 ========
NUC1 1H
P1 14.85 usec
PL1 -0.60 dB
PL1W 13.81451130 W
SFO1 400.1320007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

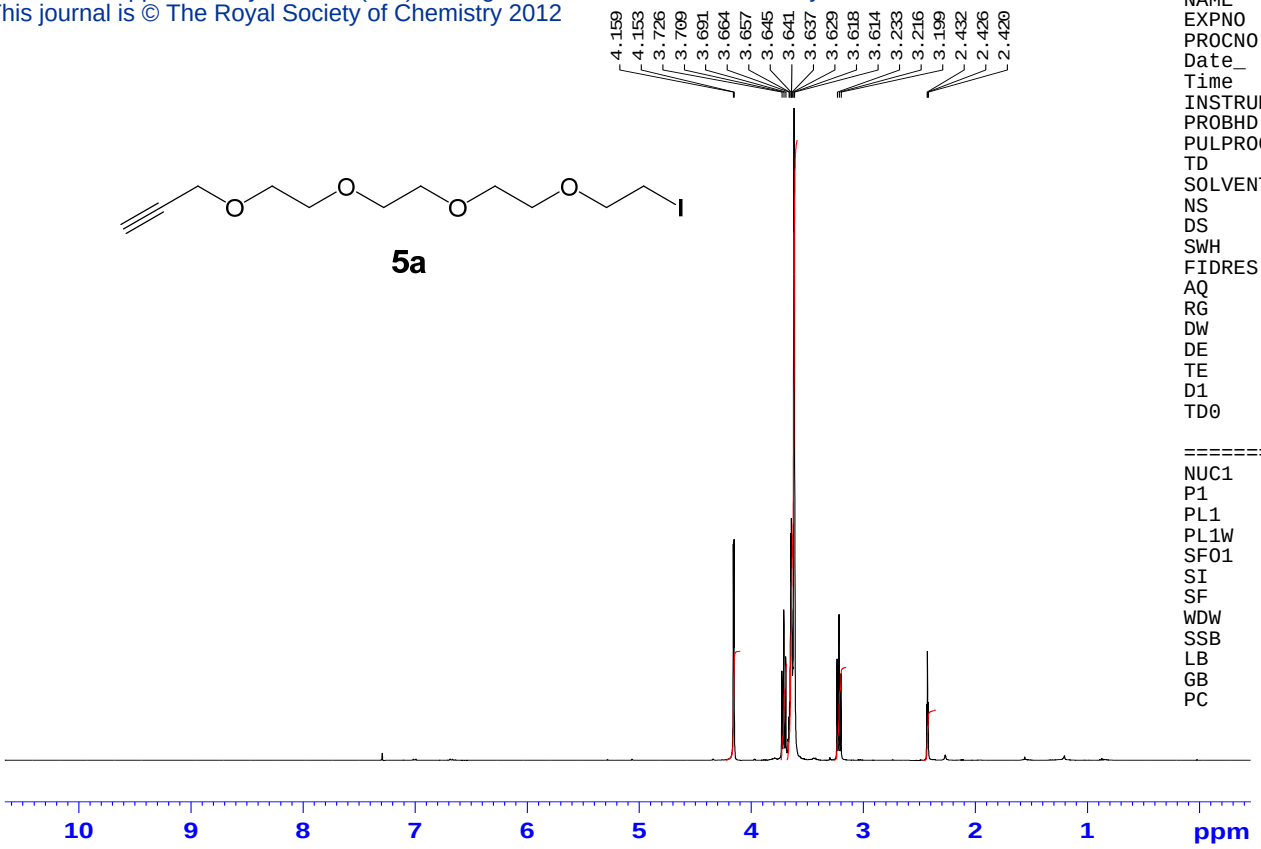


NAME ZH3-128_Alk-P4-OMs
EXPNO 2
PROCNO 1
Date_ 20111017
Time 22.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 1030
DW 20.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.99 usec
PL1 -3.00 dB
PL1W 73.67452240 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.65 dB
PL12 13.40 dB
PL13 13.40 dB
PL2W 13.97447491 W
PL12W 0.54996562 W
PL13W 0.54996562 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6126885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

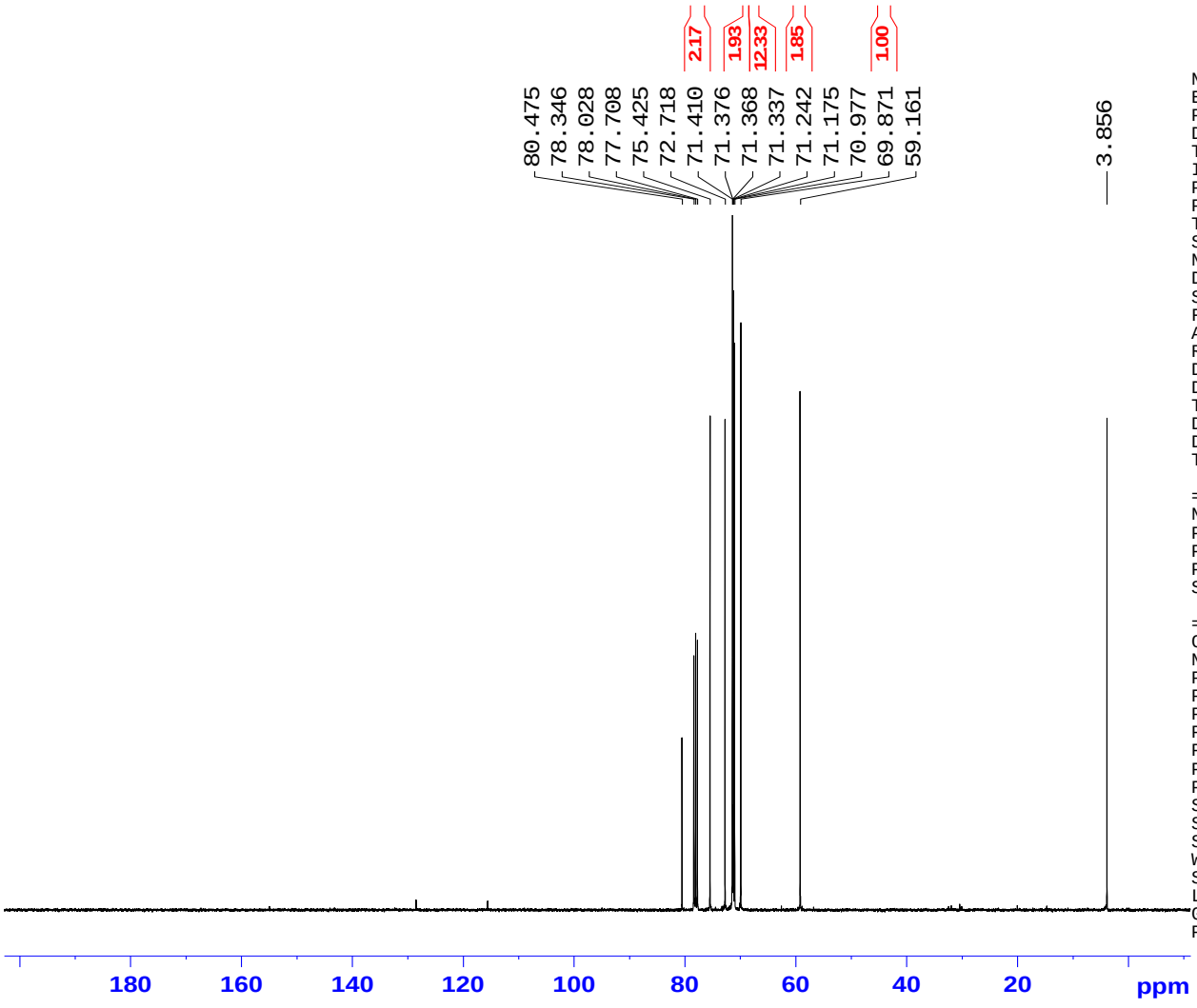

Applied Biosystems Mariner System 5268
Mariner Spec /1:25 (T /0.00:0.43) ASC[BP = 333.1, 2281]
333.0419
[M+Na]+
2281.1
100
90
80
70
60
50
40
30
20
10
0
% Intensity
O
O
O
O
OMs
4a
Chemical Formula: C12H22O7S
Exact Mass: 310.1086
Unidentified Peak
Tetrabutyl ammonium TBA+
219.1207
242.2604
335.0419
529.1940
49.0
439.2
829.4
1219.6
1609.8
2000.0
Mass (m/z)
--> Mariner System State <--
Instrument State ON
Ion Polarity POS
Auxillary Gas ON
Curtain Gas ON
Nebulizer Gas ON
Calibration Constant A 5.0146867E-007
Calibration Constant B 77.798312
TDC Deadtime 10
--> Source Settings <--
Spray Tip Potential 4509.96
SCIEX Heater 300.05
--> API Interface Settings <--
Nozzle Potential 40.04
Skimmer 1 Potential 10.01
Quadrupole DC Potential 5.49
Deflection Voltage 0.10
Einzel Lens Potential -24.00
Quadrupole RF Voltage 999.76
Quadrupole Temperature 140.01
Nozzle Temperature 140.01
--> Analyzer Settings <--
Push Pulse Potential 490.00
Pull Pulse Potential 213.11
Pull Bias Potential 10.00
Acceleration Potential 3999.94
Reflector Potential 1549.99
Detector Voltage 1700.24
--> Spectrum Acquisition Settings <--
Seconds Per Spectrum 1.00
Ion Count Threshold 0.00
First Mass 50.00
Last Mass 2000.00
Accumulate Spectra OFF
Standby at End of Acquisition OFF
--> Centroid Spectra Settings <--
Centroid Spectra OFF
--> System Settings <--
Gas Control Mode Manual
Syringe Pump Mode Manual
Syringe Pump Rate 50.00
Syringe Diameter 3.26
Min Analyzer Mass 50.00
Max Analyzer Mass 4000.00
Acquired: Oct 18 09:03:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\18 Tues\ZH3-128001.dat
Printed: 09:04, October 18, 2011



5a

```
NAME      ZH3-131_Alk-P4-I
EXPNO                   1
PROCNO                  1
Date_            20111018
Time                23.21
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                   22.6
DW                 56.800 usec
DE                  6.50 usec
TE                 292.5 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.85 usec
PL1                -0.60 dB
PL1W         13.81451130 W
SFO1         400.1320007 MHz
SI                  32768
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```



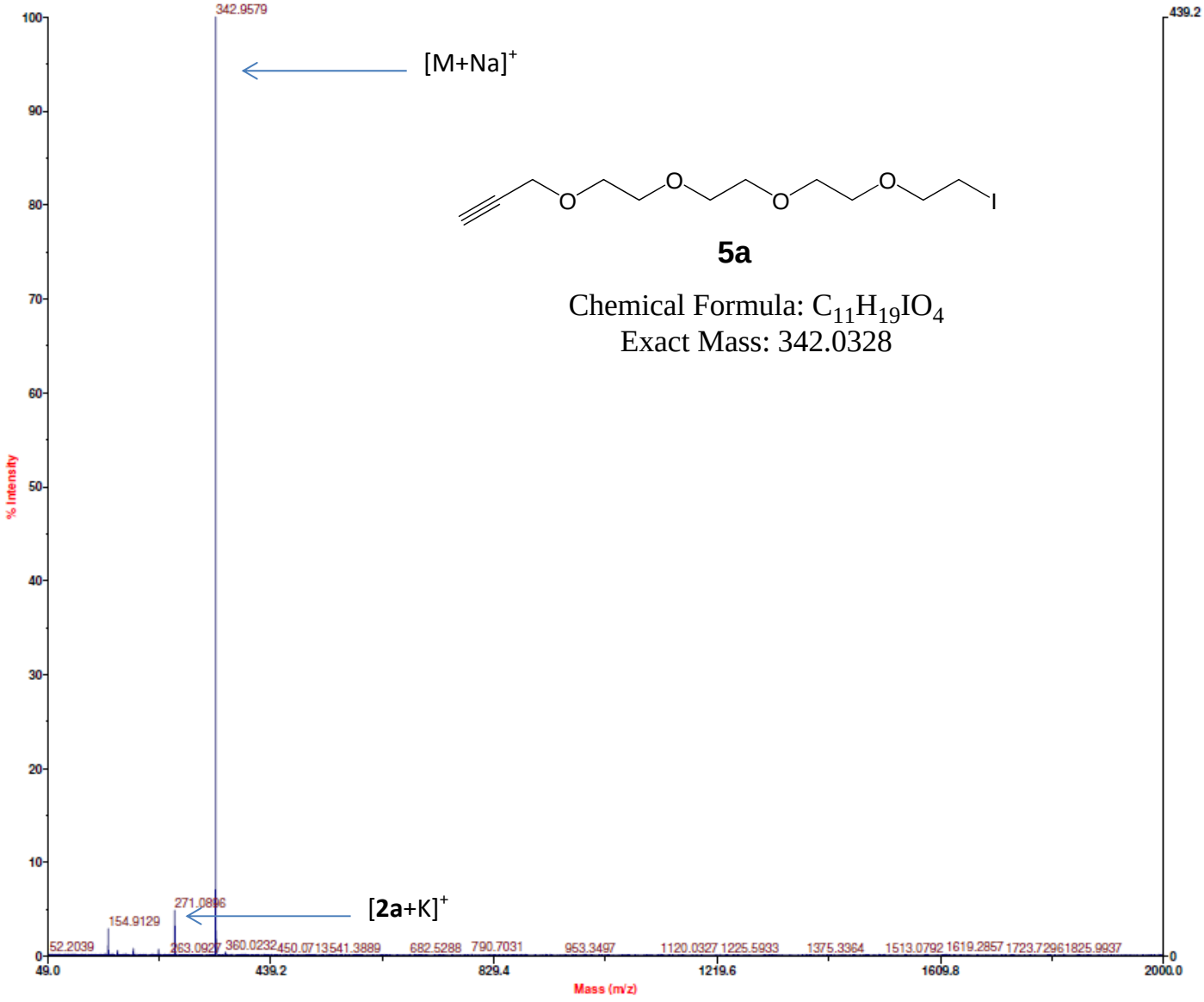

```
NAME      ZH3-131_Alk-P4-I
EXPNO                   2
PROCNO                  1
Date_            20111019
Time                 0.21
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    724
DW                 20.800 usec
DE                  6.50 usec
TE                 294.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.99 usec
PL1                -3.00 dB
PL1W         73.67452240 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -0.65 dB
PL12               13.40 dB
PL13               13.40 dB
PL2W         13.97447491 W
PL12W         0.54996562 W
PL13W         0.54996562 W
SFO2        400.1316005 MHz
SI                  32768
SF           100.6126885 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5219

Mariner Spec /1:39 (T /0.00:0.68) ASC[BP = 343.0, 439]



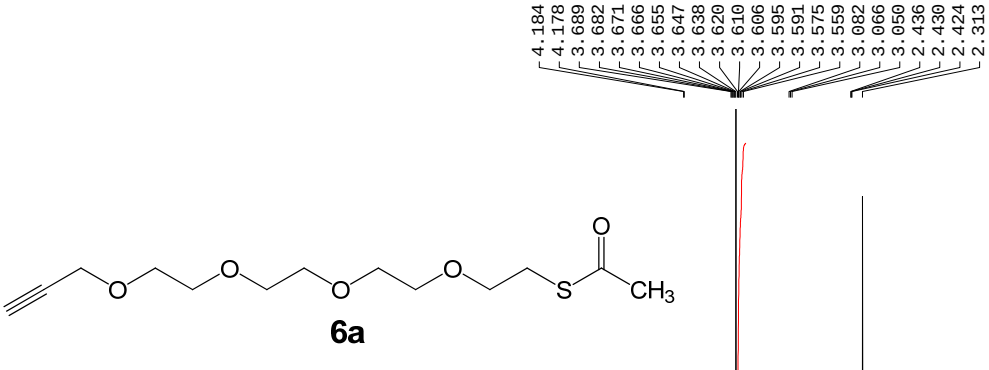
5a

Chemical Formula: $C_{11}H_{19}IO_4$
Exact Mass: 342.0328

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0149194E-007
Calibration Constant B	78.267402
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Jul 13 11:03:00 2012
Mariner Mass Spectrum
C:\Mariner\Data\2012\Jul\13 Fri\ZH3-131-APCI002.dat

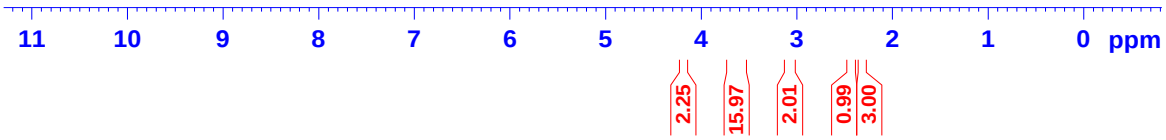
Printed: 11:05, July 13, 2012

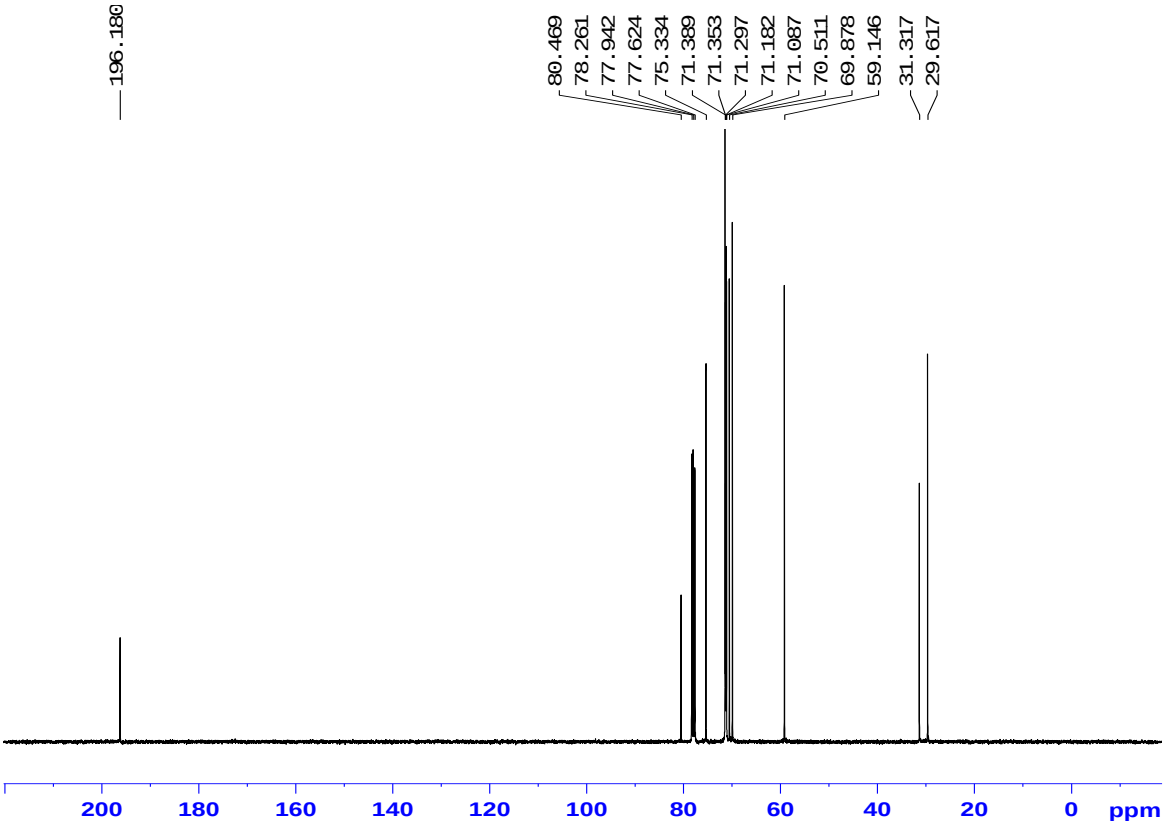


6a

```
NAME      LG-811B_Alkyne-P4-SAc
EXPNO                 1
PROCNO                1
Date_          20111020
Time              17.33
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8802.817 Hz
FIDRES         0.134320 Hz
AQ            3.7224948 sec
RG                 28.5
DW                56.800 usec
DE                 6.50 usec
TE                292.7 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.85 usec
PL1               -0.60 dB
PL1W        13.81451130 W
SFO1        400.1320007 MHz
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```





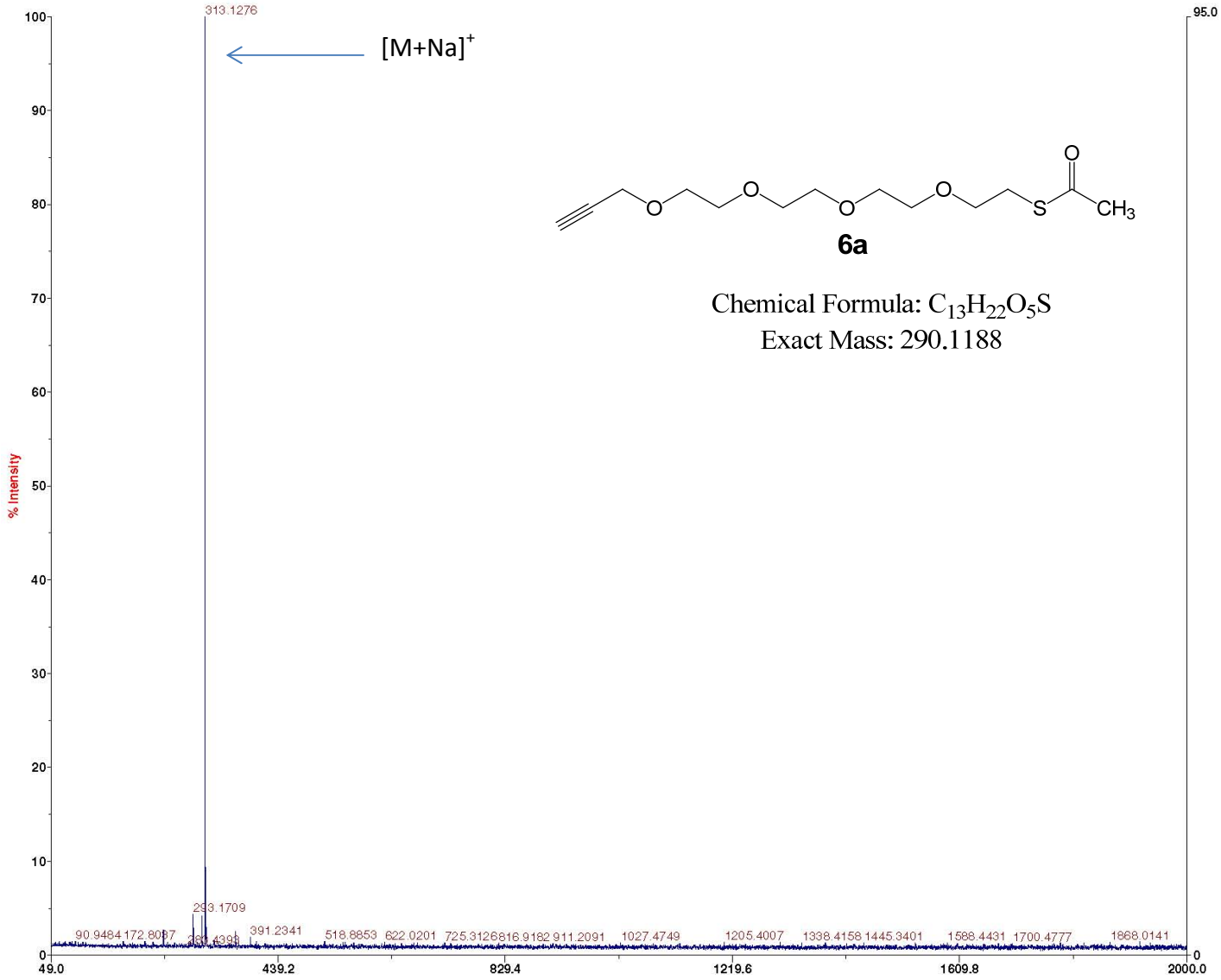

```
NAME      LG-811A_Alkyne-P4-SAc
EXPNO                 2
PROCNO                1
Date_          20111020
Time              18.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                  645
DW               20.800 usec
DE                 6.50 usec
TE                294.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.99 usec
PL1               -3.00 dB
PL1W        73.67452240 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               -0.65 dB
PL12              13.40 dB
PL13              13.40 dB
PL2W        13.97447491 W
PL12W        0.54996562 W
PL13W        0.54996562 W
SFO2       400.1316005 MHz
SI                32768
SF         100.6126885 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:23 (T /0.00:0.39) ASC[BP = 313.1, 95]



6a

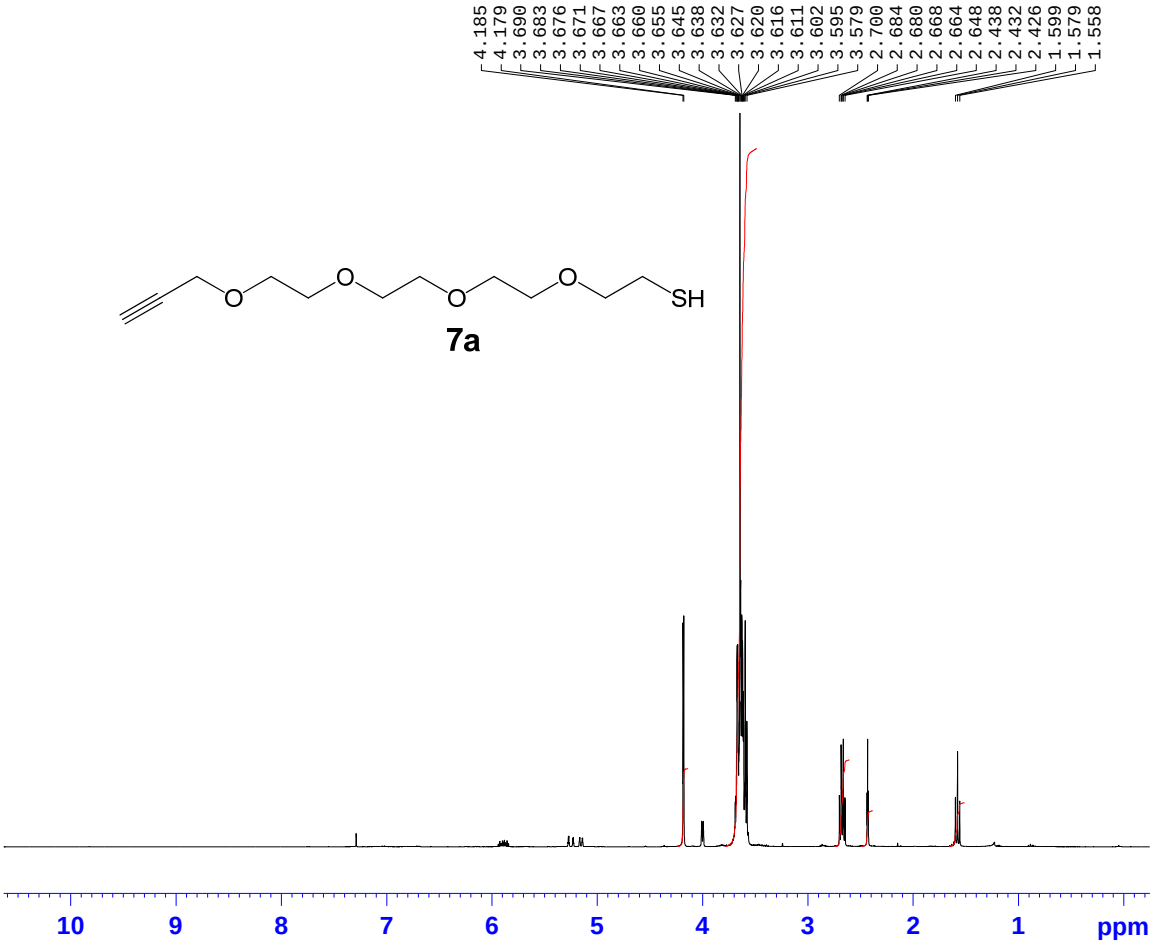
Chemical Formula: $C_{13}H_{22}O_5S$

Exact Mass: 290.1188

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

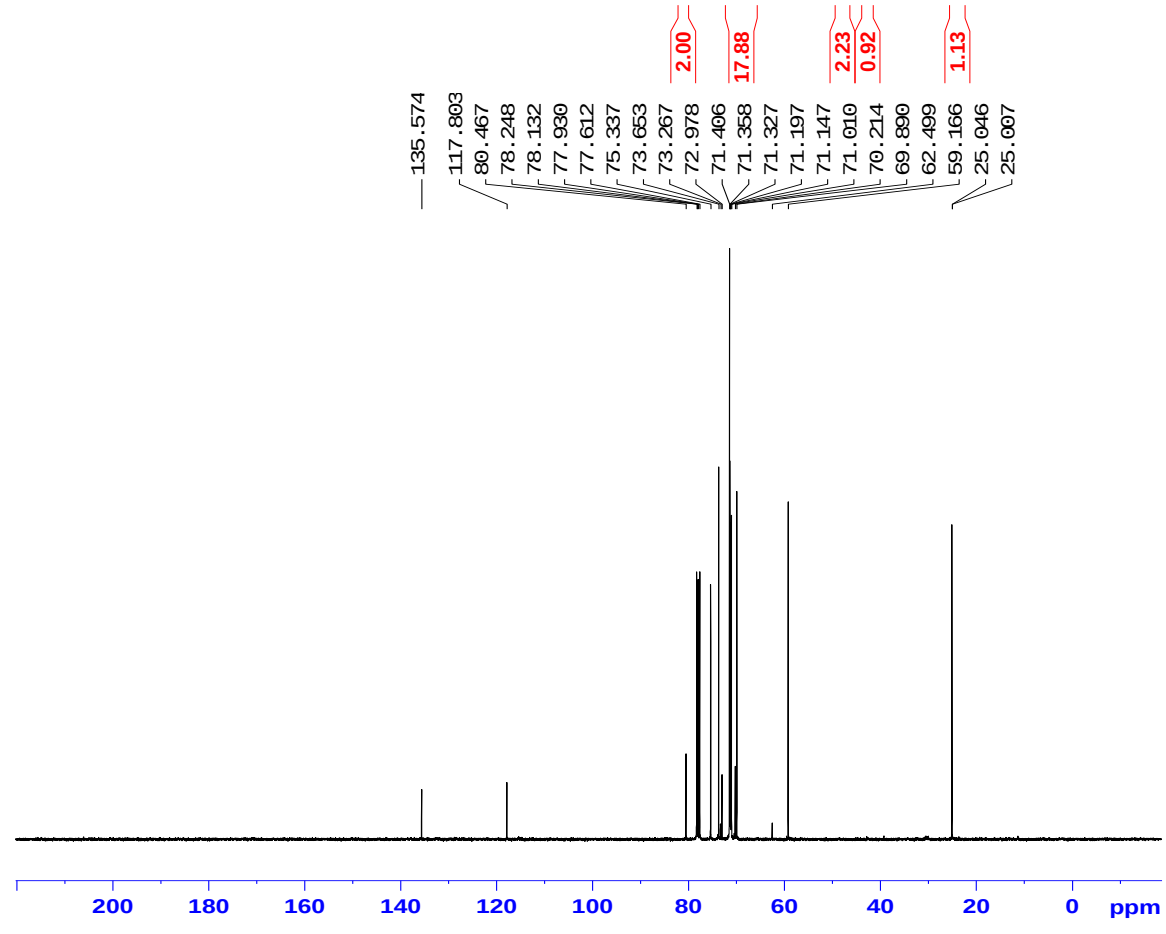
Acquired: Oct 24 08:47:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\24 Mon\LNG-811002.dat

Printed: 08:48, October 24, 2011




```
NAME      LG-813A_Alkyne-P4-SH
EXPNO                    1
PROCNO                   1
Date_             20111026
Time                 18.47
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                      28.5
DW                    56.800 usec
DE                     6.50 usec
TE                    292.4 K
D1                 1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.85 usec
PL1                   -0.60 dB
PL1W            13.81451130 W
SFO1            400.1320007 MHz
SI                    32768
SF              400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



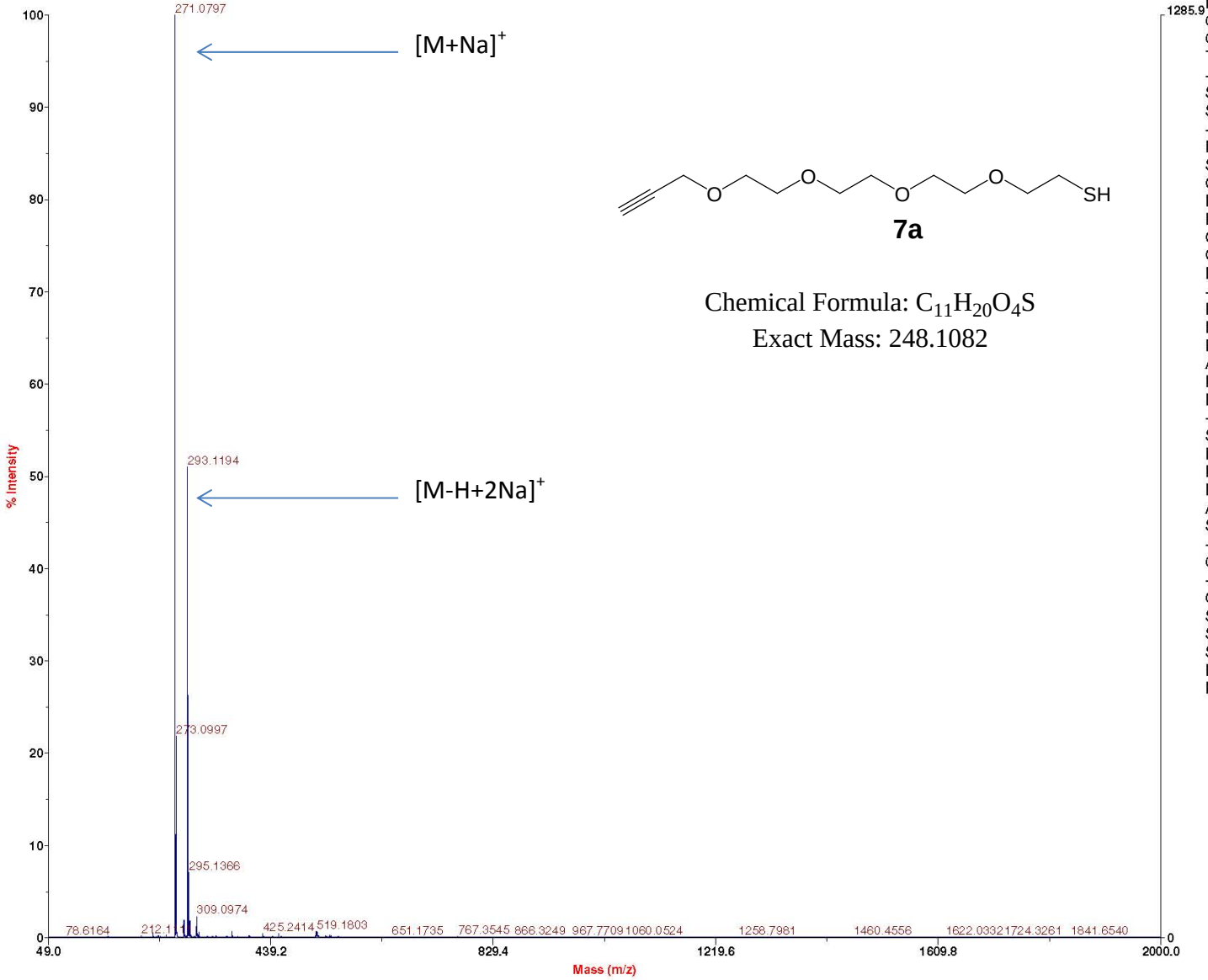

```
NAME      LG-813A_Alkyne-P4-SH
EXPNO                    2
PROCNO                   1
Date_             20111026
Time                 19.48
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      80.6
DW                    20.800 usec
DE                     6.50 usec
TE                    294.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W            73.67452240 W
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -0.65 dB
PL12                  13.40 dB
PL13                  13.40 dB
PL2W            13.97447491 W
PL12W            0.54996562 W
PL13W            0.54996562 W
SFO2            400.1316005 MHz
SI                    32768
SF              100.6126885 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:38 (T /0.00:0.66) ASC[BP = 271.1, 1286]



7a

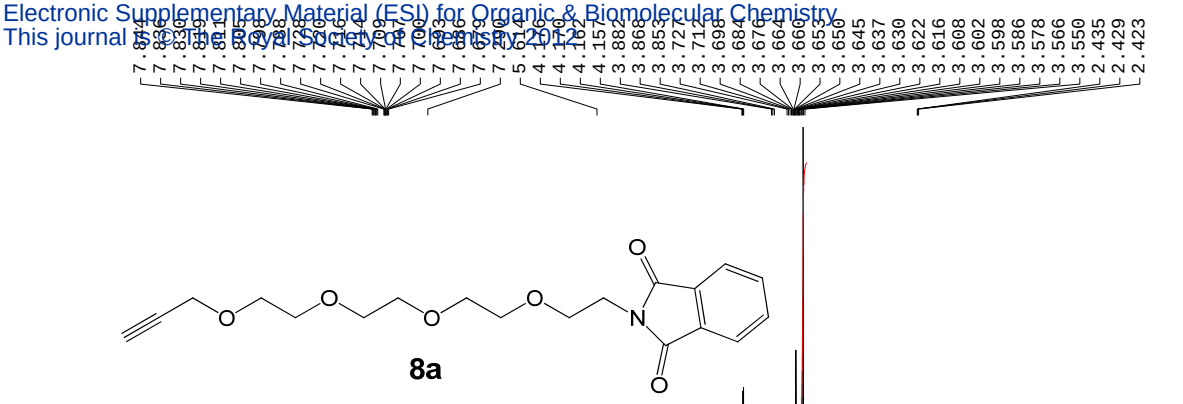
Chemical Formula: $C_{11}H_{20}O_4S$

Exact Mass: 248.1082

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	149.90
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

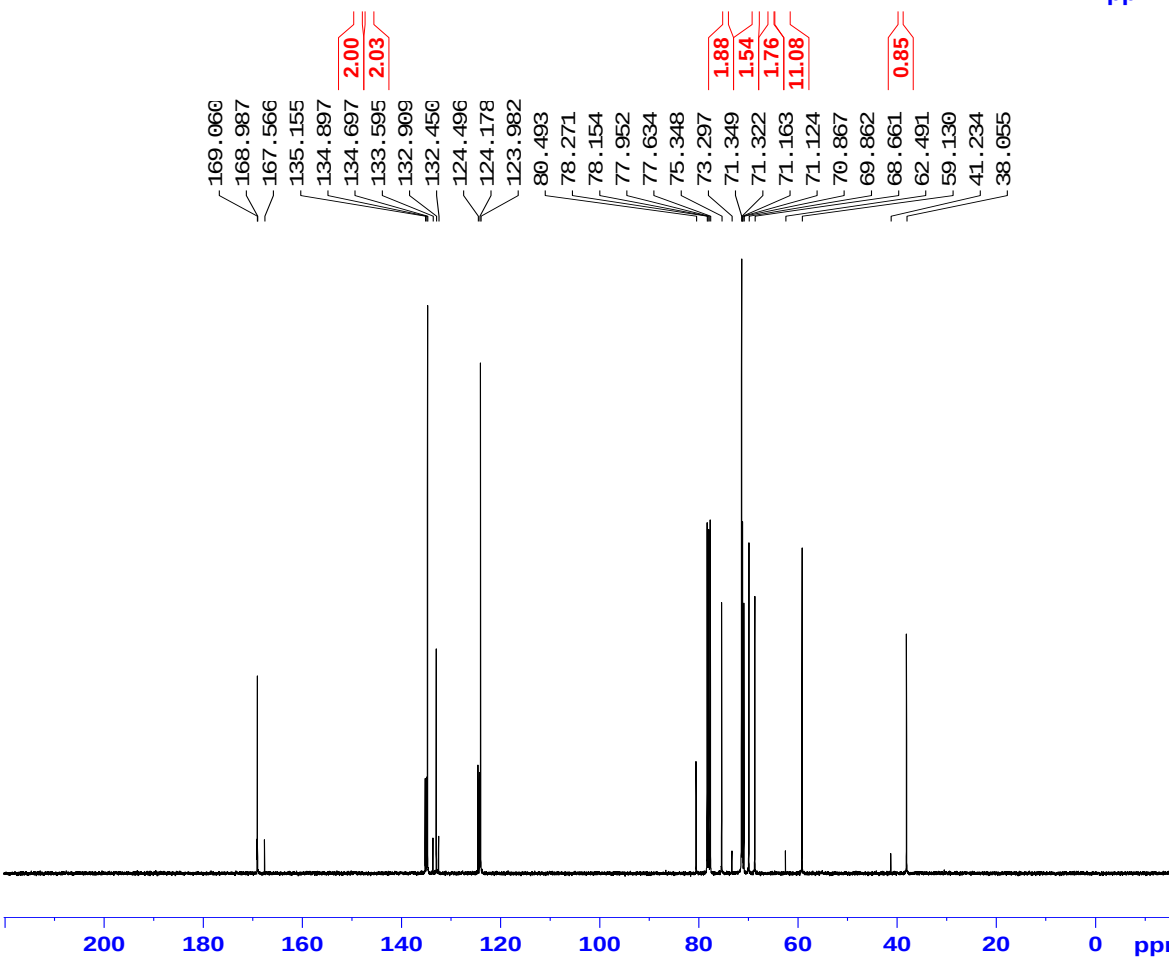
Acquired: Oct 27 10:18:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\27 Thur\LNG-813001.dat

Printed: 10:19, October 27, 2011




```
NAME      ZH3-130_Alk-P4-NPth
EXPNO                       1
PROCNO                      1
Date_            20111019
Time                    21.04
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8802.817 Hz
FIDRES              0.134320 Hz
AQ                  3.7224948 sec
RG                       28.5
DW                     56.800 usec
DE                      6.50 usec
TE                     292.4 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W             13.81451130 W
SFO1             400.1320007 MHz
SI                     32768
SF               400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



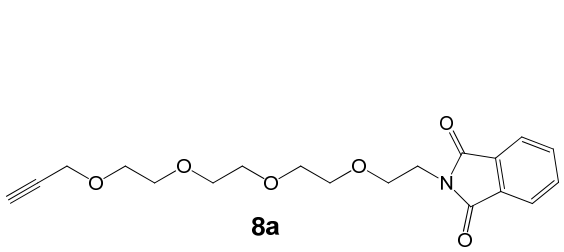
```
NAME      ZH3-130_Alk-P4-NPth
EXPNO                       3
PROCNO                      1
Date_            20111019
Time                    22.05
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       724
DW                     20.800 usec
DE                      6.50 usec
TE                     294.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.99 usec
PL1                    -3.00 dB
PL1W             73.67452240 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W             13.97447491 W
PL12W             0.54996562 W
PL13W             0.54996562 W
SFO2             400.1316005 MHz
SI                     32768
SF               100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:28 (T /0.00:0.48) ASC[BP = 384.1, 360]



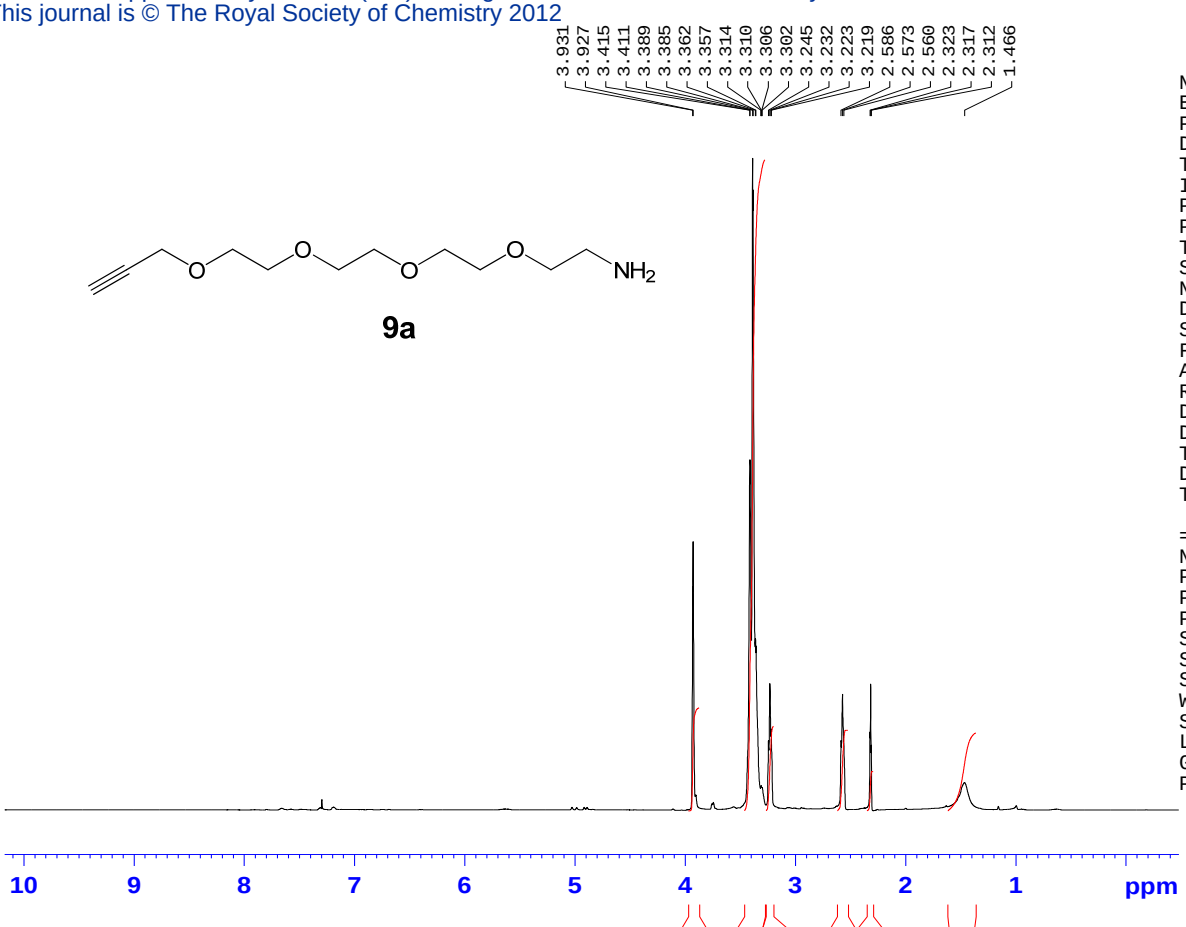
8a

Chemical Formula: $C_{19}H_{23}NO_6$
Exact Mass: 361.1525

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

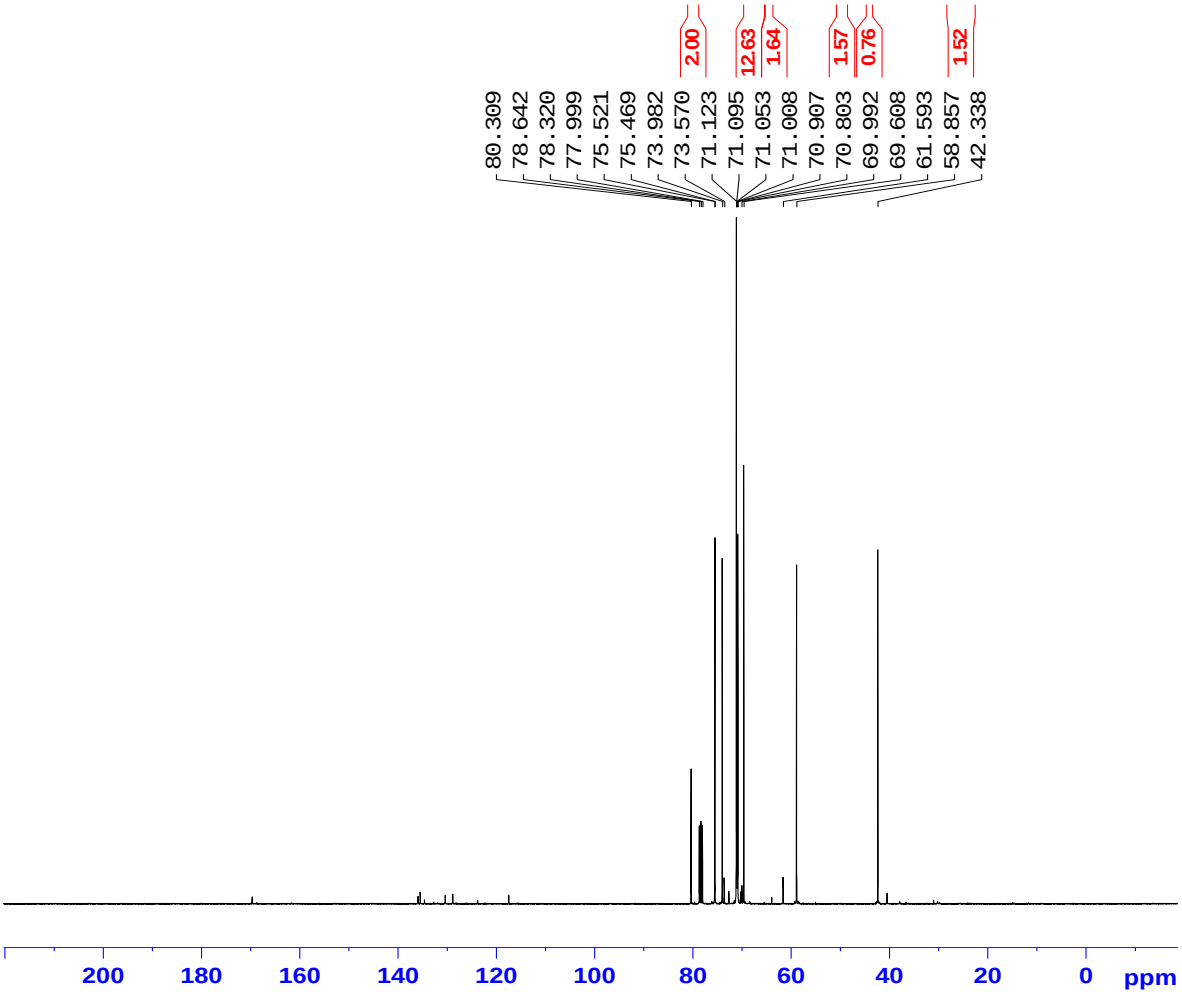
Acquired: Oct 18 14:52:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\18 Tues\ZH3-130001.dat

Printed: 14:53, October 18, 2011




```
NAME      ZH3-132_Alk-P4-NH2
EXPNO                      1
PROCNO                     1
Date_               20111019
Time                   23.09
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8802.817 Hz
FIDRES              0.134320 Hz
AQ                  3.7224948 sec
RG                        10
DW                    56.800 usec
DE                     6.50 usec
TE                    292.6 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W              13.81451130 W
SFO1              400.1320007 MHz
SI                     32768
SF                400.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00
```



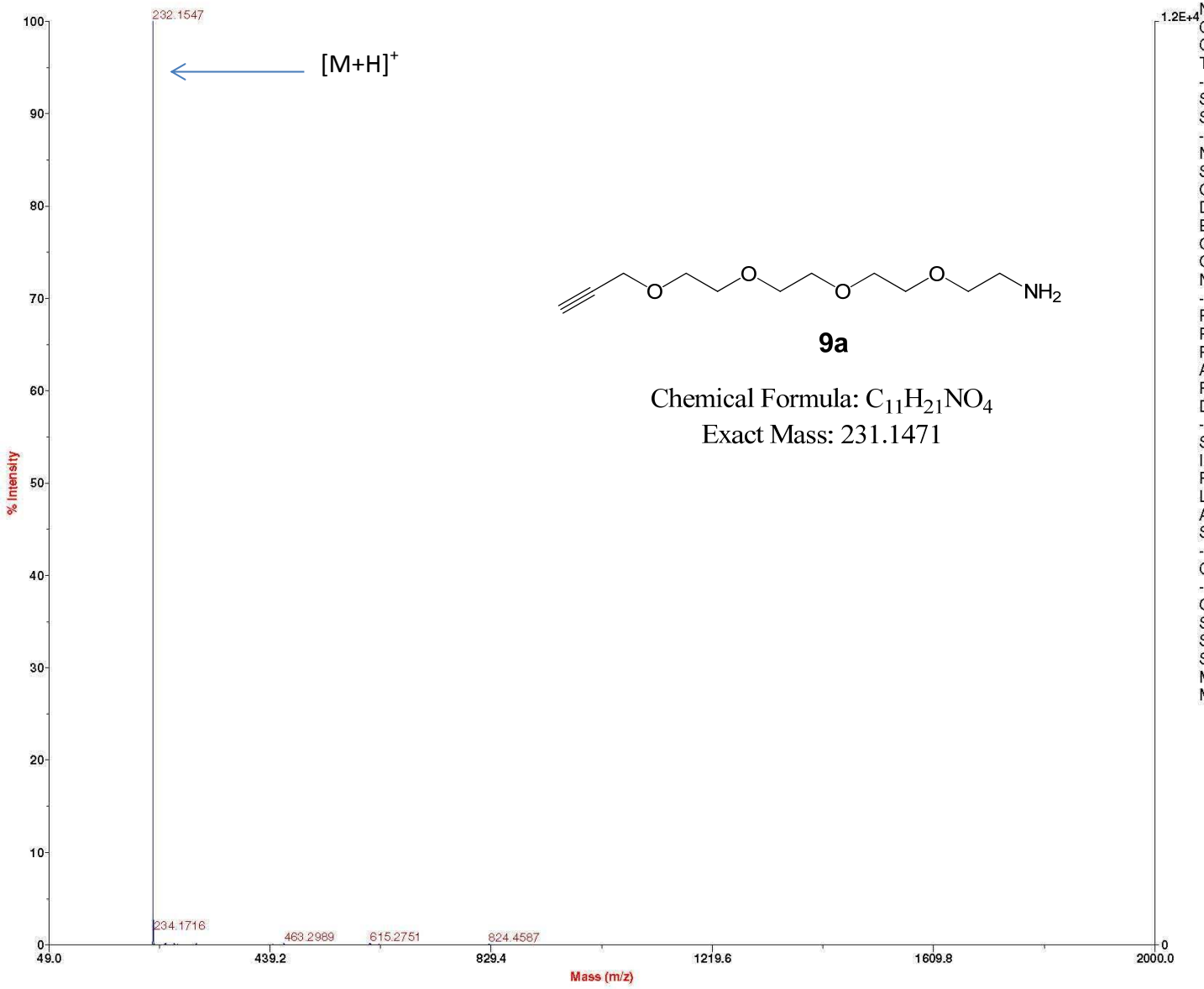

```
NAME      ZH3-132_Alk-P4-NH2
EXPNO                      2
PROCNO                     1
Date_               20111020
Time                   0.11
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                      80.6
DW                    20.800 usec
DE                     6.50 usec
TE                    294.5 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                     9.99 usec
PL1                    -3.00 dB
PL1W              73.67452240 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W              13.97447491 W
PL12W              0.54996562 W
PL13W              0.54996562 W
SFO2              400.1316005 MHz
SI                     32768
SF                100.6126885 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:30 (T /0.00:0.52) ASC[BP = 232.2, 12139]



9a

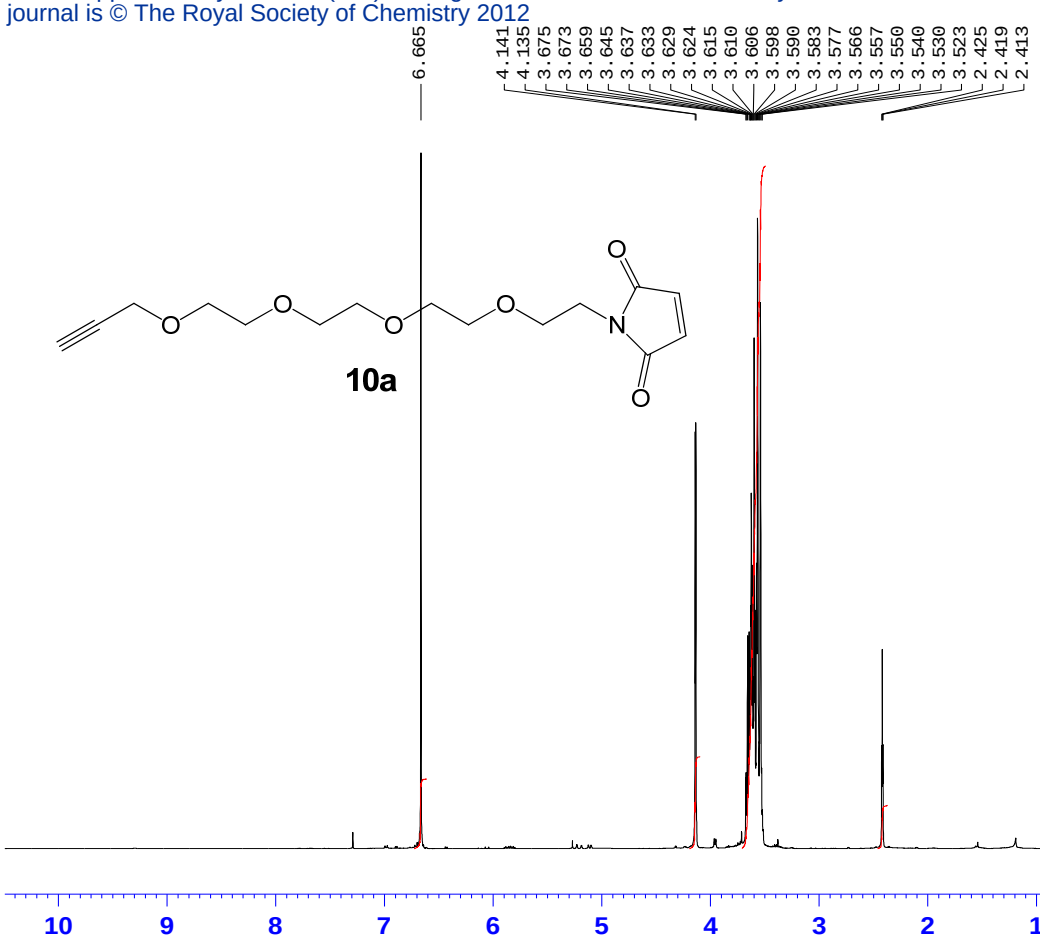
Chemical Formula: $C_{11}H_{21}NO_4$

Exact Mass: 231.1471

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0149194E-007
Calibration Constant B	78.267402
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	120.12
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	80.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

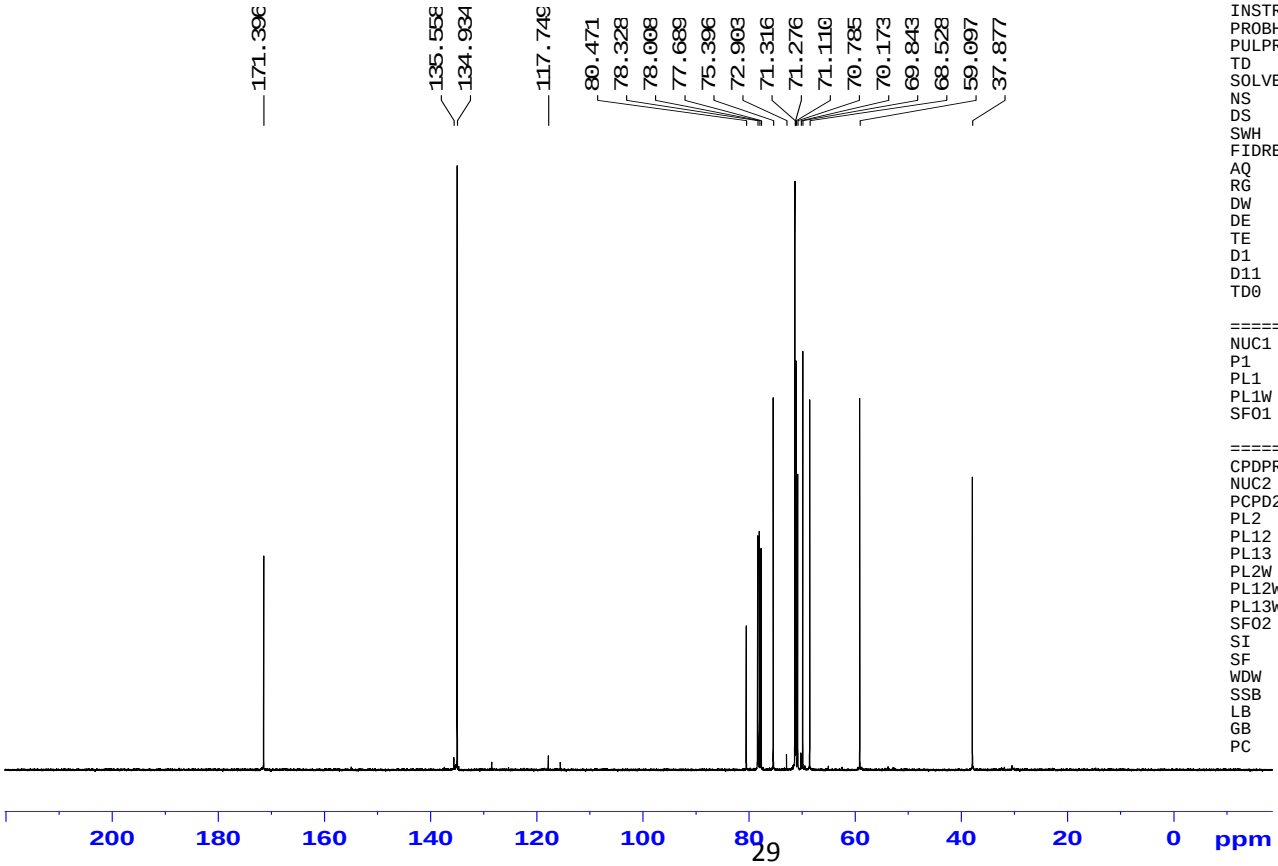
Acquired: Mar 12 13:50:00 2012
Mariner Mass Spectrum
C:\Mariner\Data\2012\Mar\12 Mon\ZH3-132001.dat

Printed: 13:52, March 12, 2012




```
NAME      ZH3-133-A_Alk-P4-Mal
EXPNO                    1
PROCNO                   1
Date_             20111025
Time                 1.20
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                   22.6
DW                 56.800 usec
DE                  6.50 usec
TE                 292.5 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.85 usec
PL1                 -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



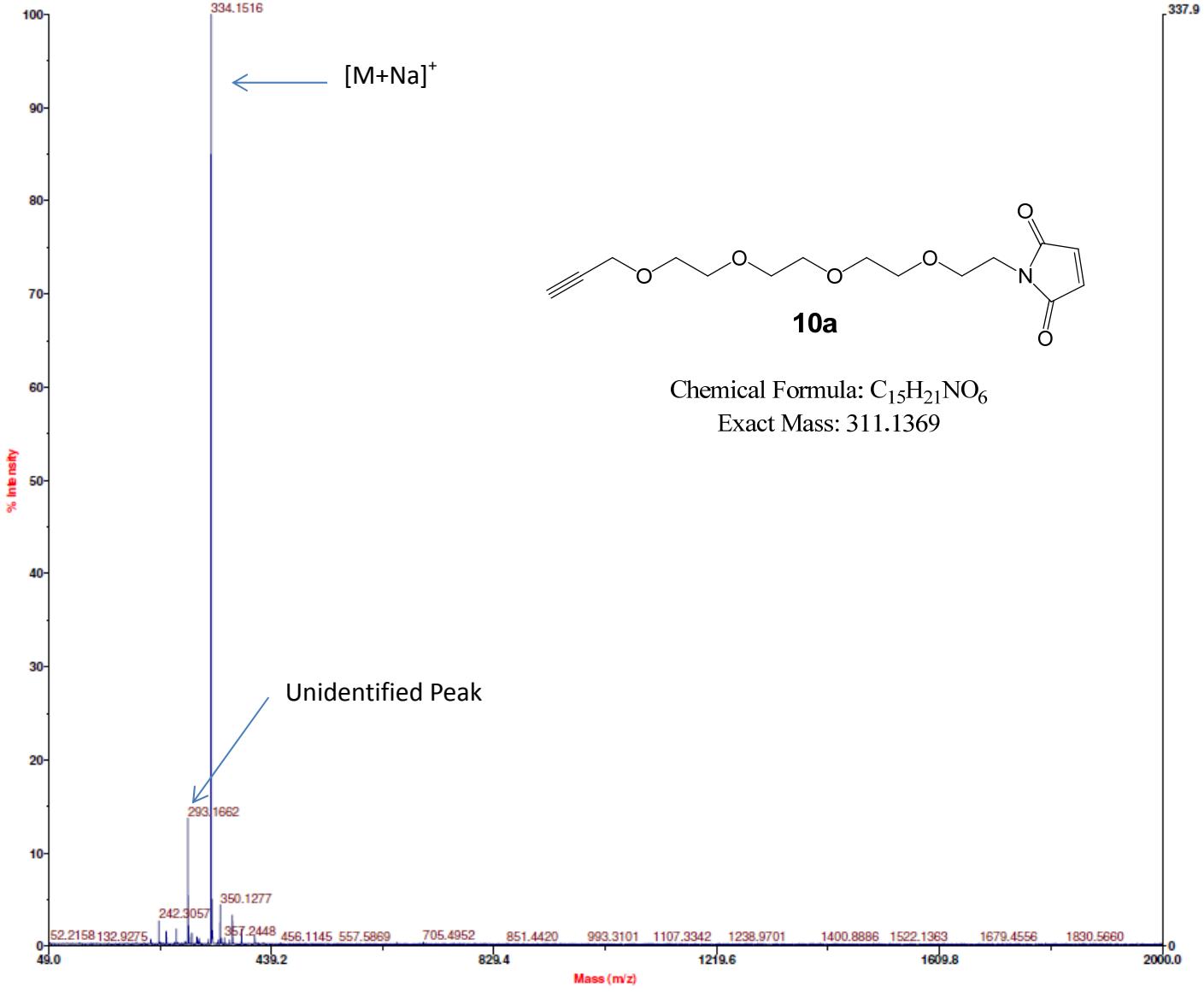

```
NAME      ZH3-133-A_Alk-P4-Mal
EXPNO                    2
PROCNO                   1
Date_             20111025
Time                 2.21
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    812
DW                 20.800 usec
DE                  6.50 usec
TE                 294.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.99 usec
PL1                 -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -0.65 dB
PL12                13.40 dB
PL13                13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6126885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:24 (T /0.00:0.41) ASC[BP = 334.2, 338]



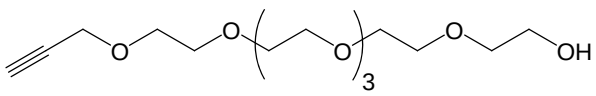
10a

Chemical Formula: $C_{15}H_{21}NO_6$
Exact Mass: 311.1369

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Oct 25 09:49:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\25 Tues\ZH3-133002.dat

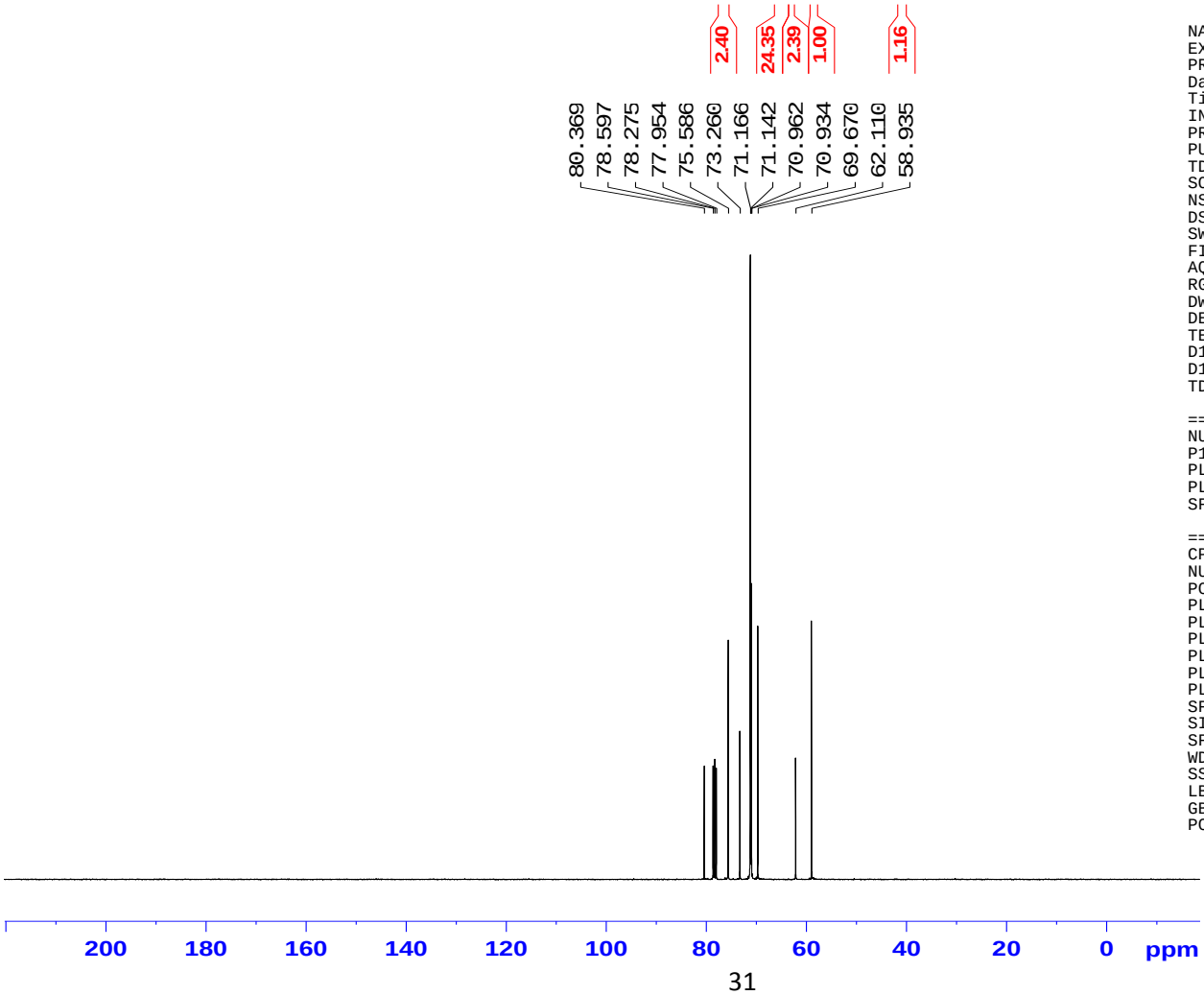
Printed: 09:50, October 25, 2011



2b


```
NAME      ZH3-134-C_Alk-P6-OH
EXPNO                       1
PROCNO                      1
Date_            20111024
Time                   23.15
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8802.817 Hz
FIDRES              0.134320 Hz
AQ                  3.7224948 sec
RG                        10
DW                     56.800 usec
DE                      6.50 usec
TE                     292.5 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W             13.81451130 W
SFO1             400.1320007 MHz
SI                     32768
SF               400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



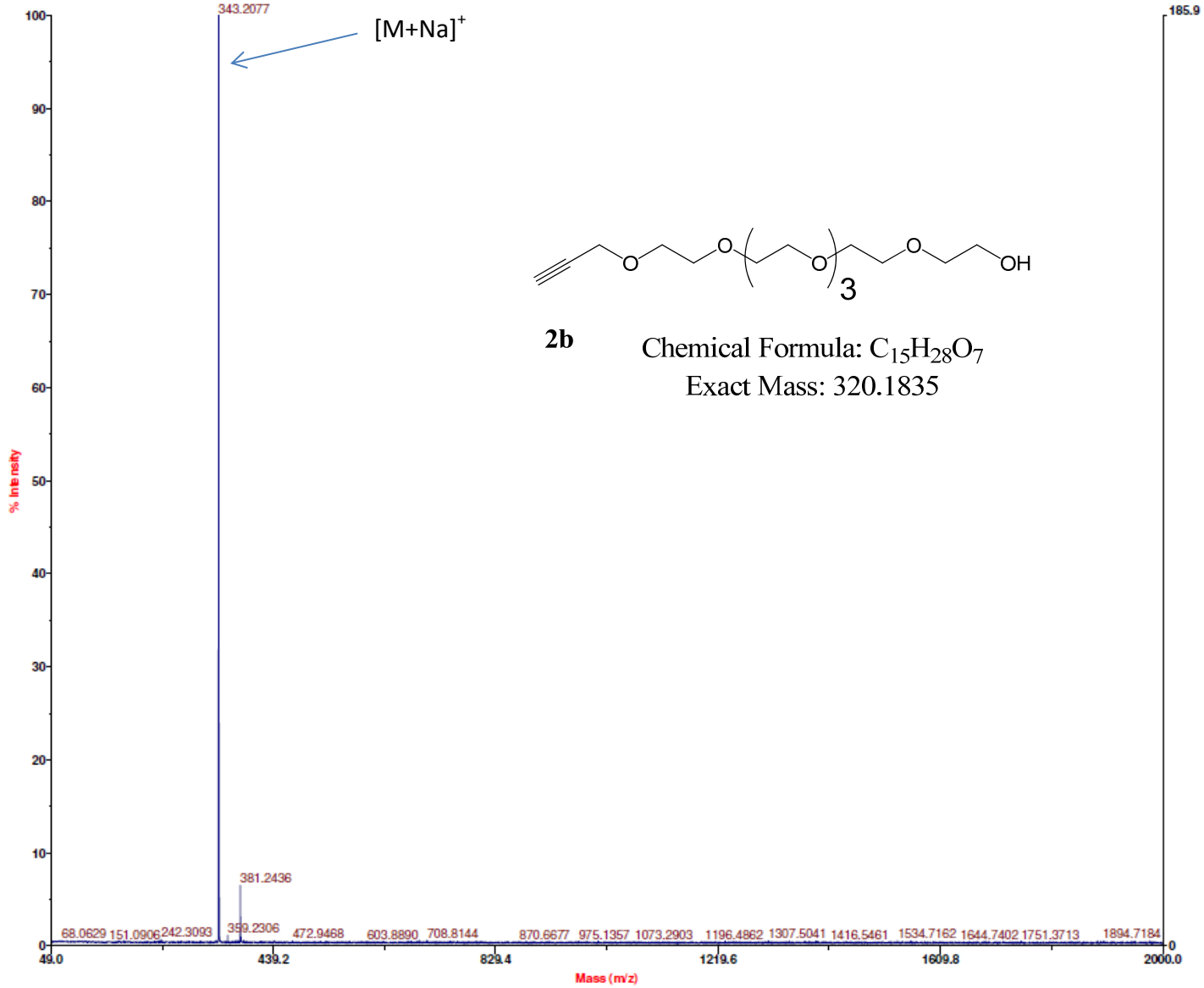

```
NAME      ZH3-134-C_Alk-P6-OH
EXPNO                       2
PROCNO                      1
Date_            20111025
Time                    0.15
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       575
DW                     20.800 usec
DE                      6.50 usec
TE                     294.4 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.99 usec
PL1                    -3.00 dB
PL1W             73.67452240 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W             13.97447491 W
PL12W             0.54996562 W
PL13W             0.54996562 W
SFO2             400.1316005 MHz
SI                     32768
SF               100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:34 (T /0.00:0.59) ASC[BP = 343.2, 186]



2b

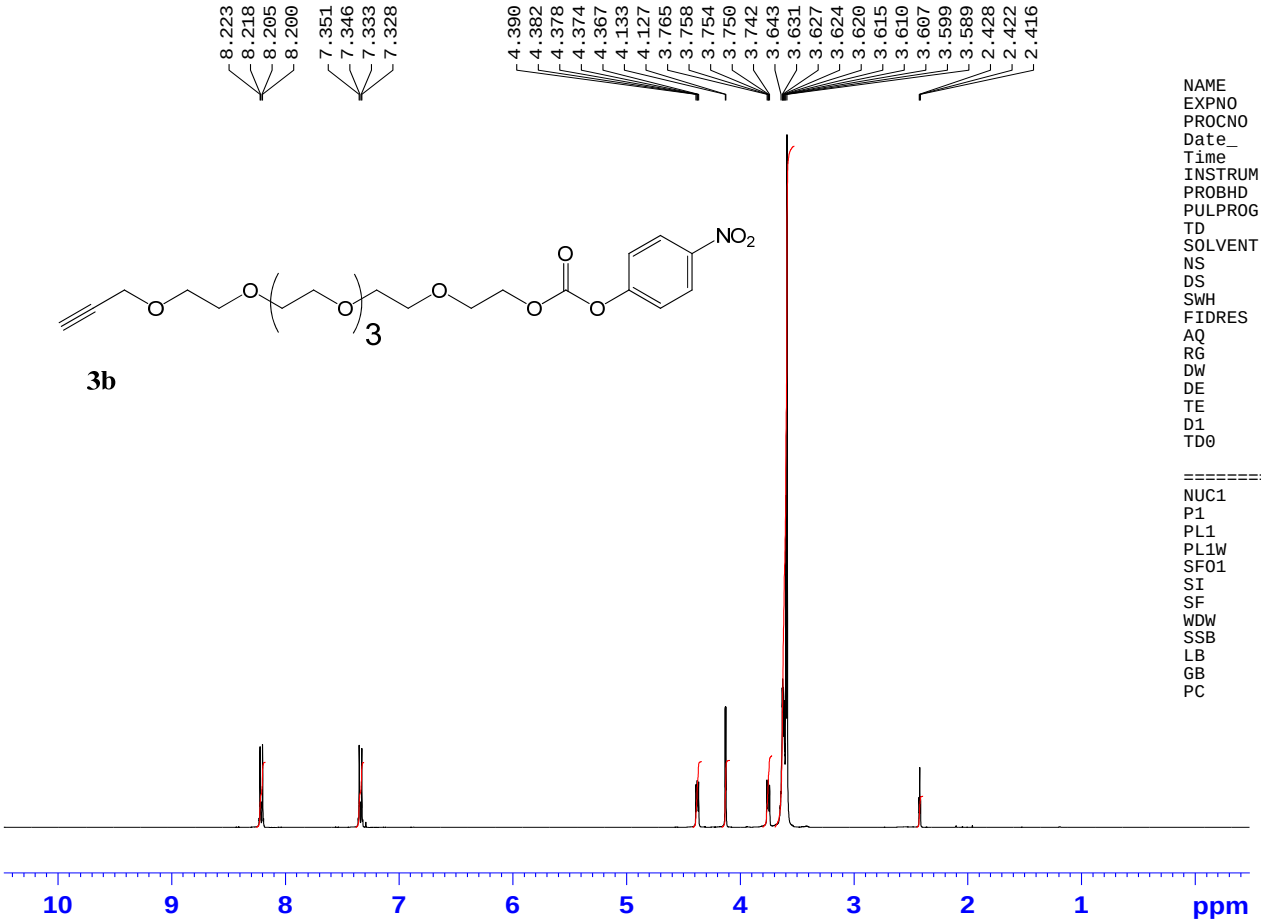
Chemical Formula: $C_{15}H_{28}O_7$

Exact Mass: 320.1835

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

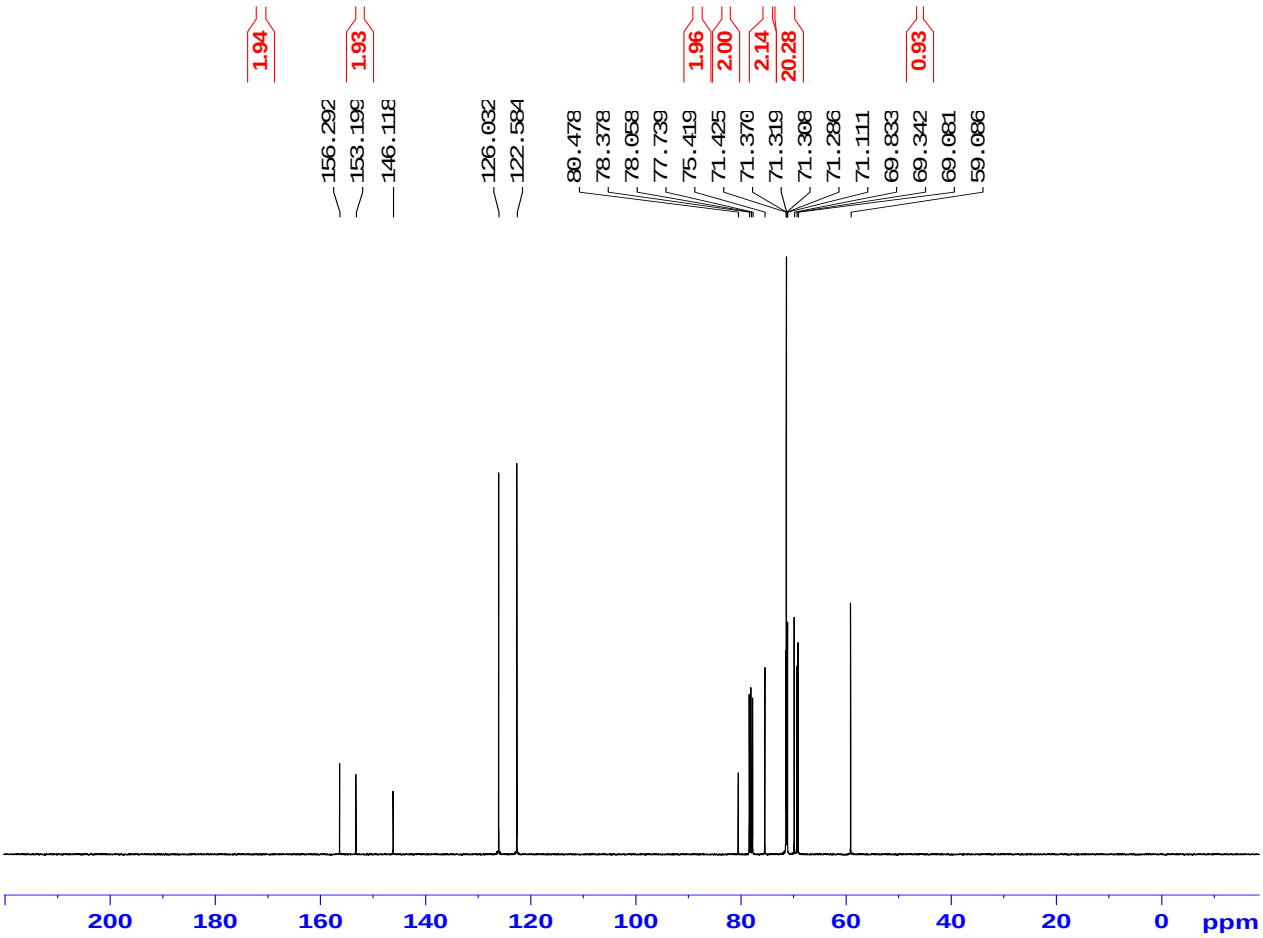
Acquired: Oct 25 09:51:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\25 Tues\ZH3-134001.dat

Printed: 09:52, October 25, 2011




```
NAME          ZH3-136_Alk-P6-PNPC
EXPNO                           1
PROCNO                          1
Date_                    20111026
Time                        21.59
INSTRUM                     spect
PROBHD          5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                      8802.817 Hz
FIDRES                   0.134320 Hz
AQ                       3.7224948 sec
RG                             18
DW                          56.800 usec
DE                           6.50 usec
TE                          292.9 K
D1                       1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                          14.85 usec
PL1                         -0.60 dB
PL1W                 13.81451130 W
SFO1                400.1320007 MHz
SI                          32768
SF                  400.1300000 MHz
WDW                            EM
SSB                             0
LB                           0.30 Hz
GB                              0
PC                           1.00
```



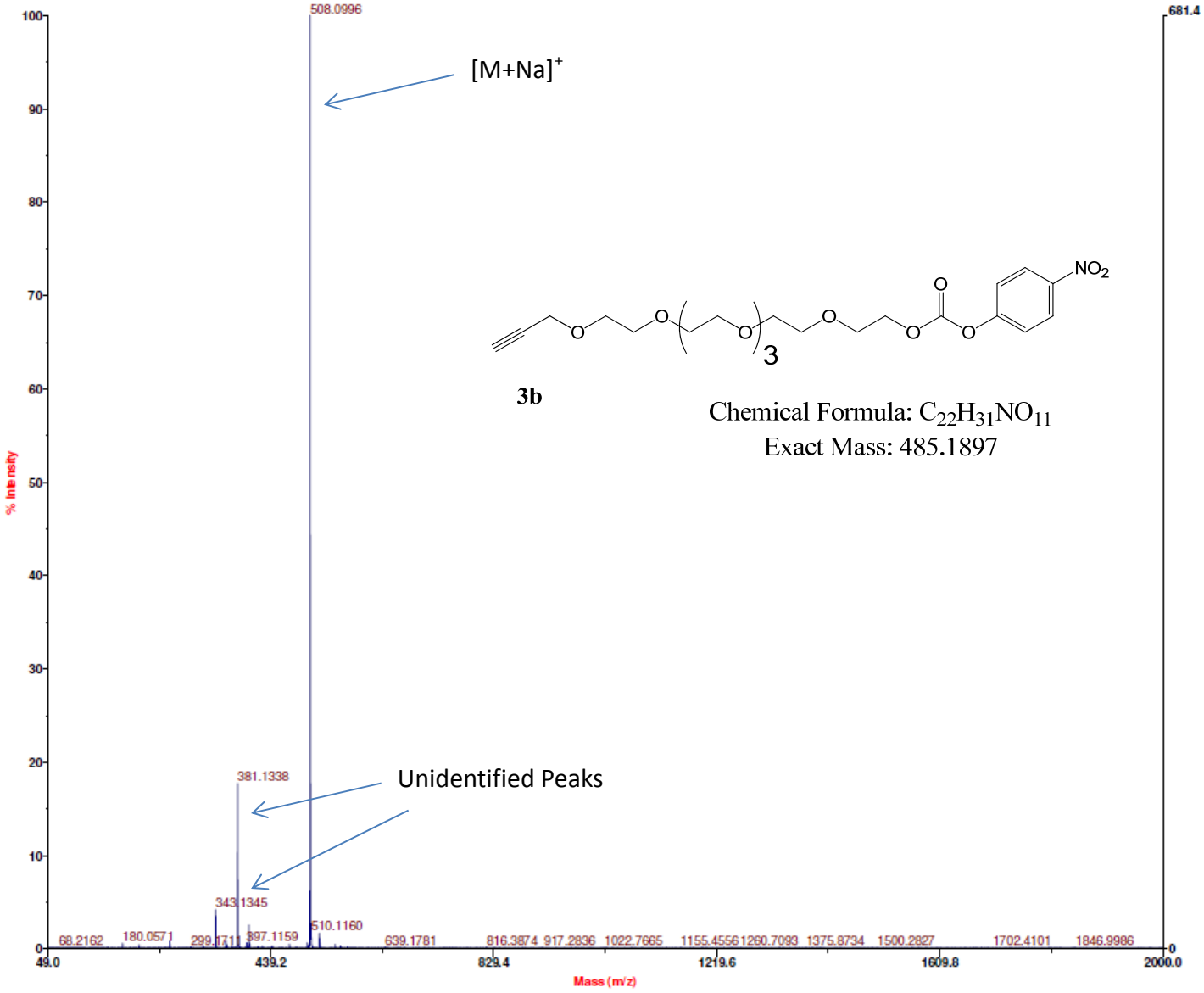

```
NAME          ZH3-136_Alk-P6-PNPC
EXPNO                           2
PROCNO                          1
Date_                    20111026
Time                        22.59
INSTRUM                     spect
PROBHD          5 mm PABBO BB-
PULPROG                   zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                           1024
DS                              4
SWH                  24038.461 Hz
FIDRES                   0.366798 Hz
AQ                       1.3631988 sec
RG                           1030
DW                          20.800 usec
DE                           6.50 usec
TE                          294.6 K
D1                       2.00000000 sec
D11                      0.03000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                          13C
P1                           9.99 usec
PL1                         -3.00 dB
PL1W                73.67452240 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                       80.00 usec
PL2                         -0.65 dB
PL12                        13.40 dB
PL13                        13.40 dB
PL2W                13.97447491 W
PL12W                0.54996562 W
PL13W                0.54996562 W
SFO2               400.1316005 MHz
SI                          32768
SF                 100.6126885 MHz
WDW                            EM
SSB                             0
LB                           1.00 Hz
GB                              0
PC                           1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:46 (T /0.00:0.81) ASC[BP = 508.1, 681]



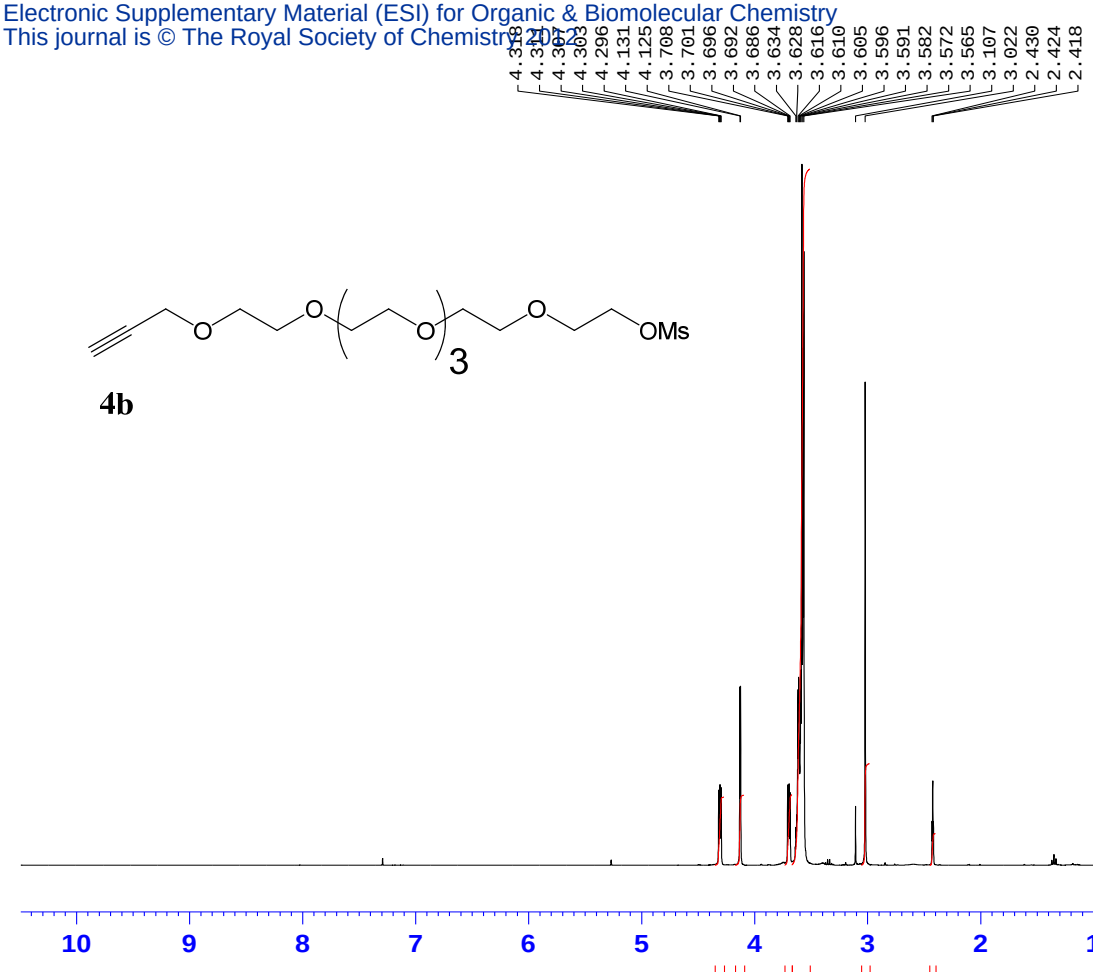
3b

Chemical Formula: $C_{22}H_{31}NO_{11}$
Exact Mass: 485.1897

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

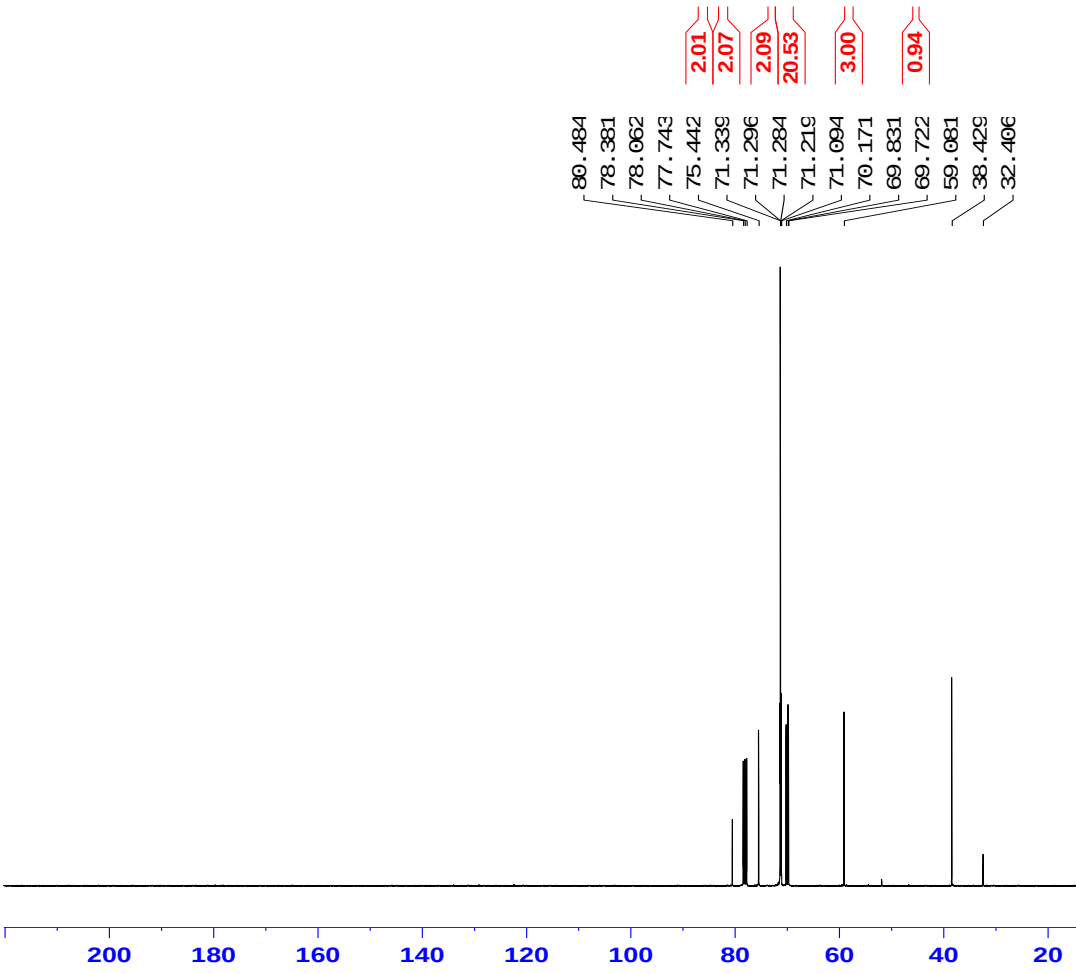
Acquired: Oct 27 09:35:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\27 Thur\ZH3-136001.dat

Printed: 09:37, October 27, 2011




```
NAME      ZH3-135_Alk-P6-OMs
EXPNO                      1
PROCNO                     1
Date_               20111025
Time                   21.04
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8802.817 Hz
FIDRES              0.134320 Hz
AQ                  3.7224948 sec
RG                        18
DW                     56.800 usec
DE                      6.50 usec
TE                     292.5 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W               13.81451130 W
SFO1               400.1320007 MHz
SI                     32768
SF                 400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



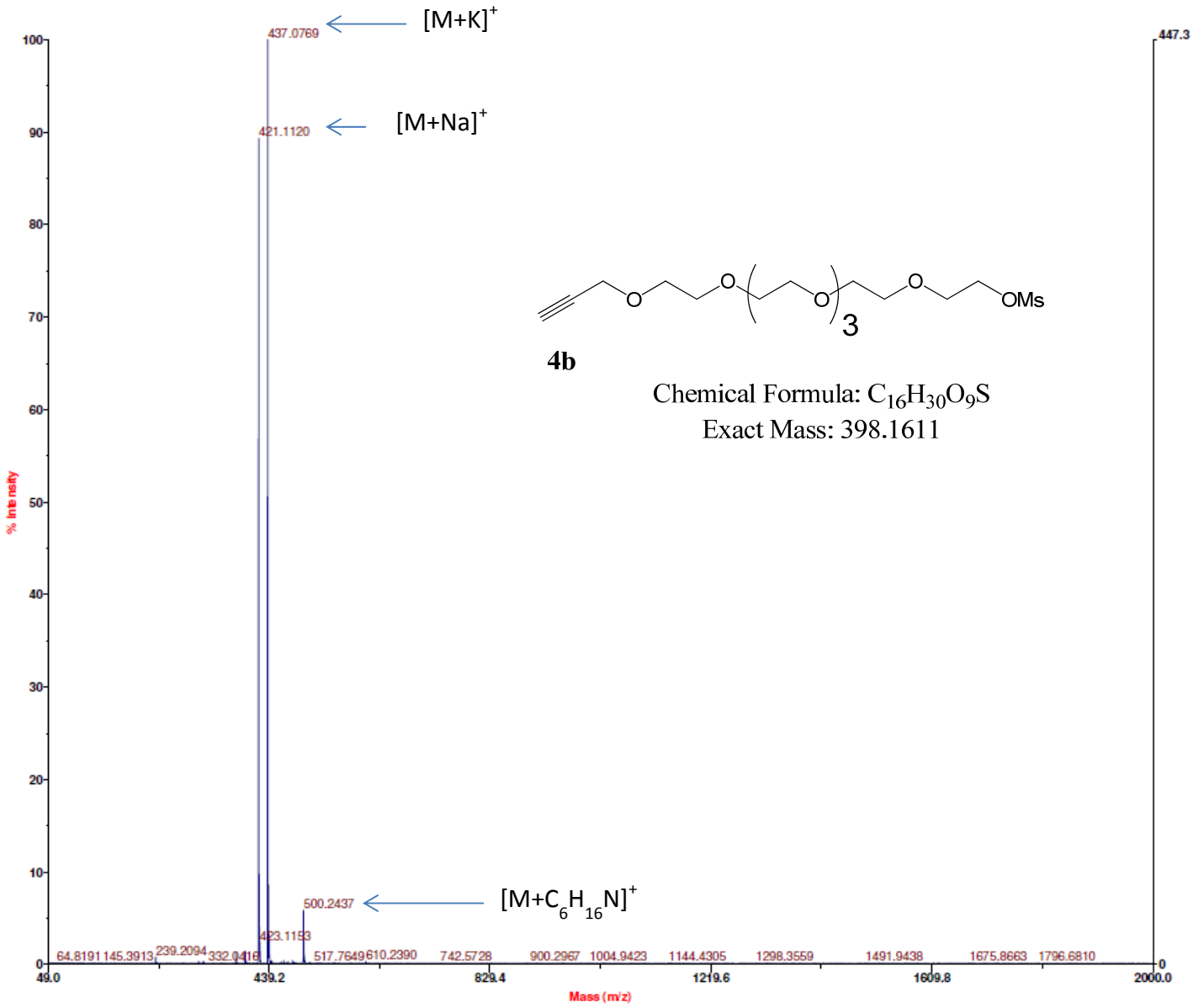

```
NAME      ZH3-135_Alk-P6-OMs
EXPNO                      2
PROCNO                     1
Date_               20111025
Time                   22.05
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       645
DW                     20.800 usec
DE                      6.50 usec
TE                     294.5 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.99 usec
PL1                    -3.00 dB
PL1W               73.67452240 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W               13.97447491 W
PL12W               0.54996562 W
PL13W               0.54996562 W
SFO2               400.1316005 MHz
SI                     32768
SF                 100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:67 (T /0.00:1.17) ASC[BP = 437.1, 447]



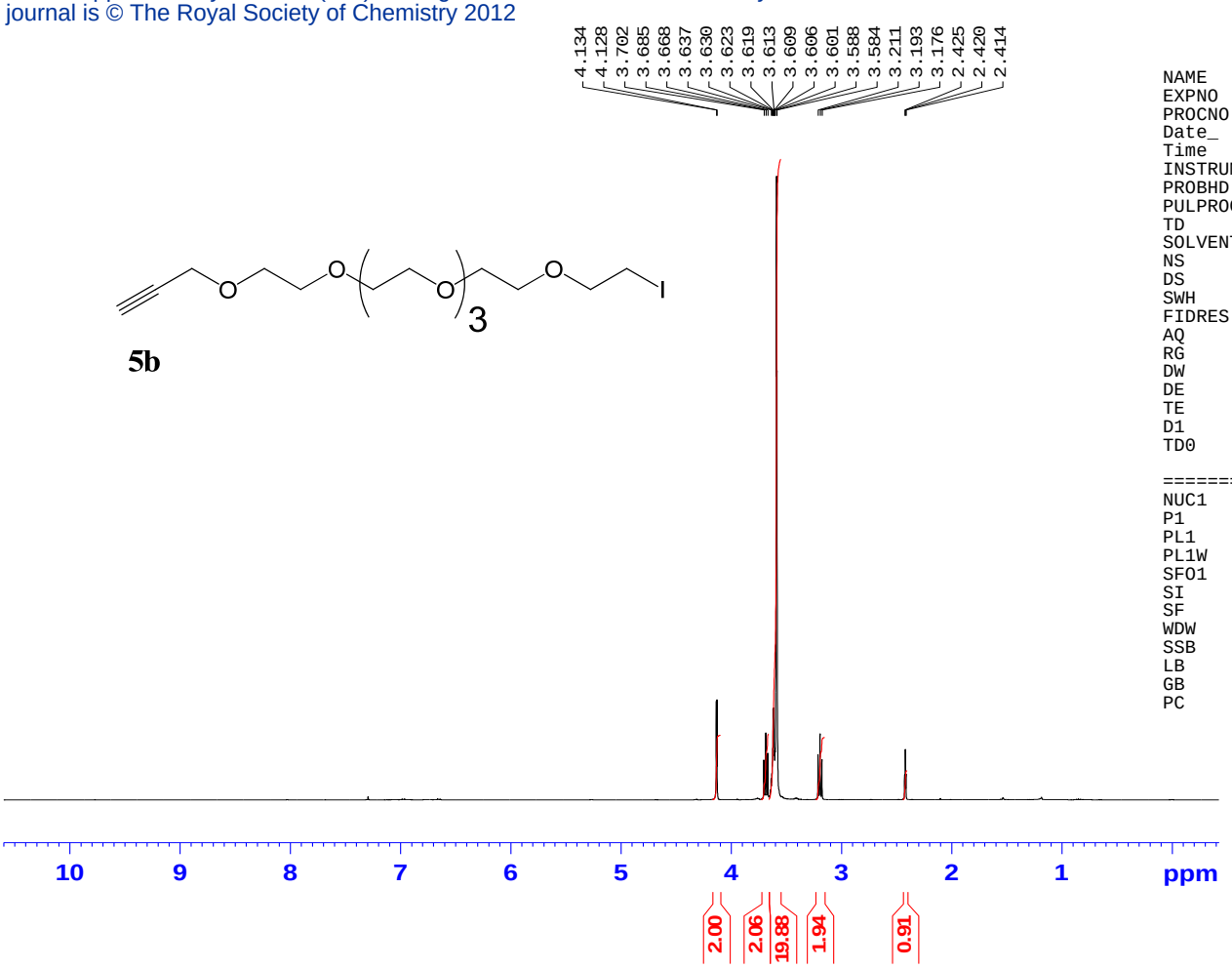
4b

Chemical Formula: $C_{16}H_{30}O_9S$
Exact Mass: 398.1611

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

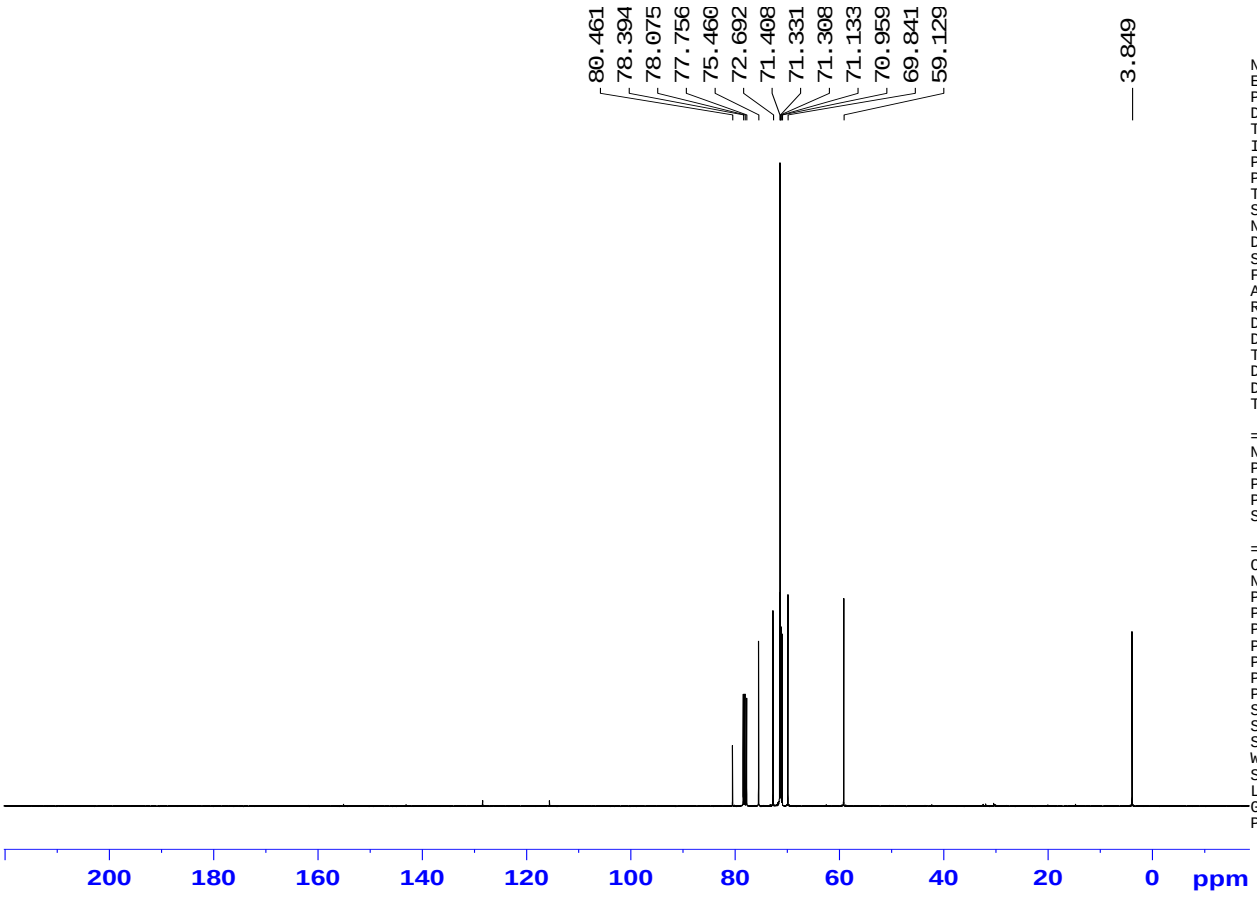
Acquired: Oct 26 09:52:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\26 Wed\ZH3-135001.dat

Printed: 09:54, October 26, 2011




```
NAME      ZH3-137_Alk-P6-I
EXPNO                    1
PROCNO                   1
Date_             20111027
Time                 0.03
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ                3.7224948 sec
RG                      18
DW                  56.800 usec
DE                   6.50 usec
TE                   292.6 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W           13.81451130 W
SFO1           400.1320007 MHz
SI                   32768
SF             400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



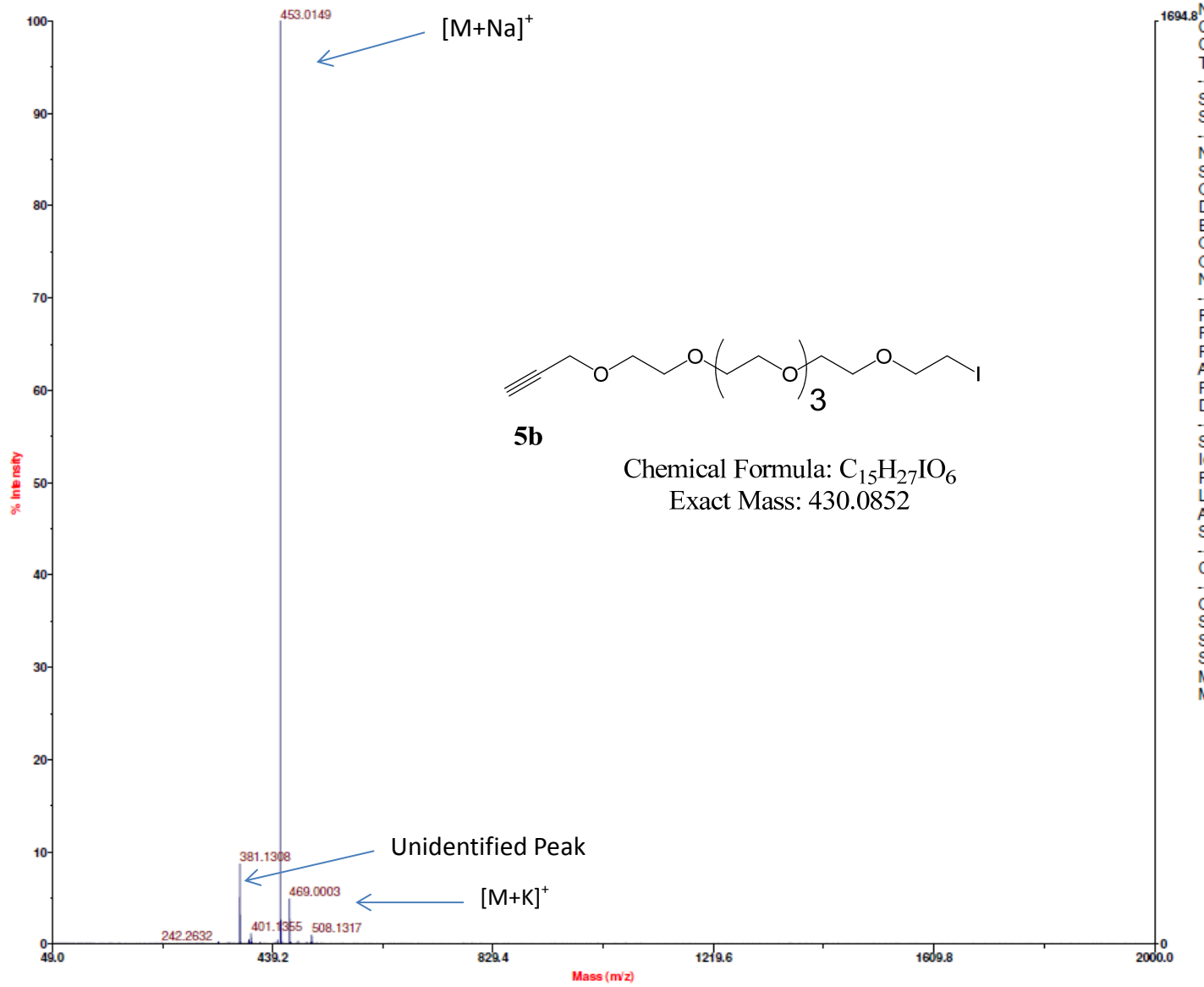

```
NAME      ZH3-137_Alk-P6-I
EXPNO                    2
PROCNO                   1
Date_             20111027
Time                 1.04
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     575
DW                  20.800 usec
DE                   6.50 usec
TE                   294.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W           73.67452240 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W           13.97447491 W
PL12W           0.54996562 W
PL13W           0.54996562 W
SFO2           400.1316005 MHz
SI                   32768
SF             100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:54 (T /0.00:0.95) ASC[BP = 453.0, 1695]



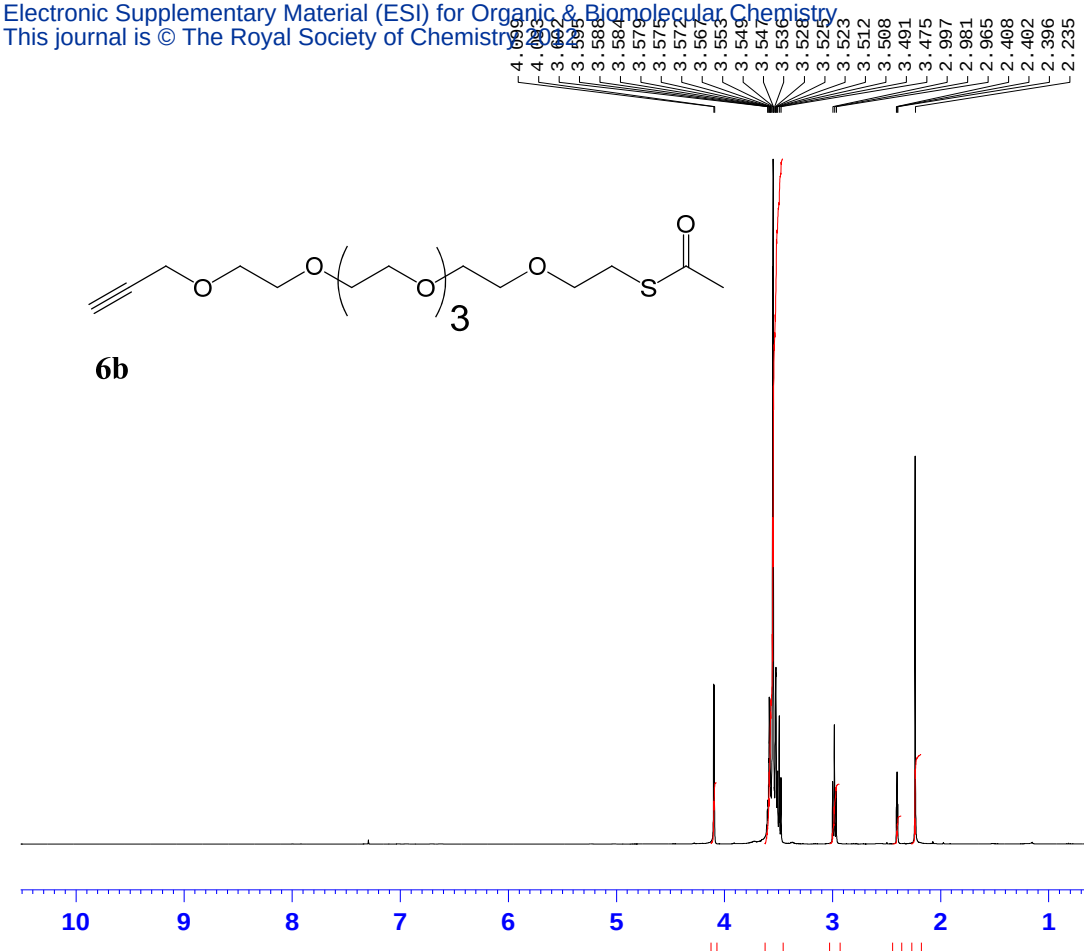
5b

Chemical Formula: $C_{15}H_{27}IO_6$
Exact Mass: 430.0852

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	149.90
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

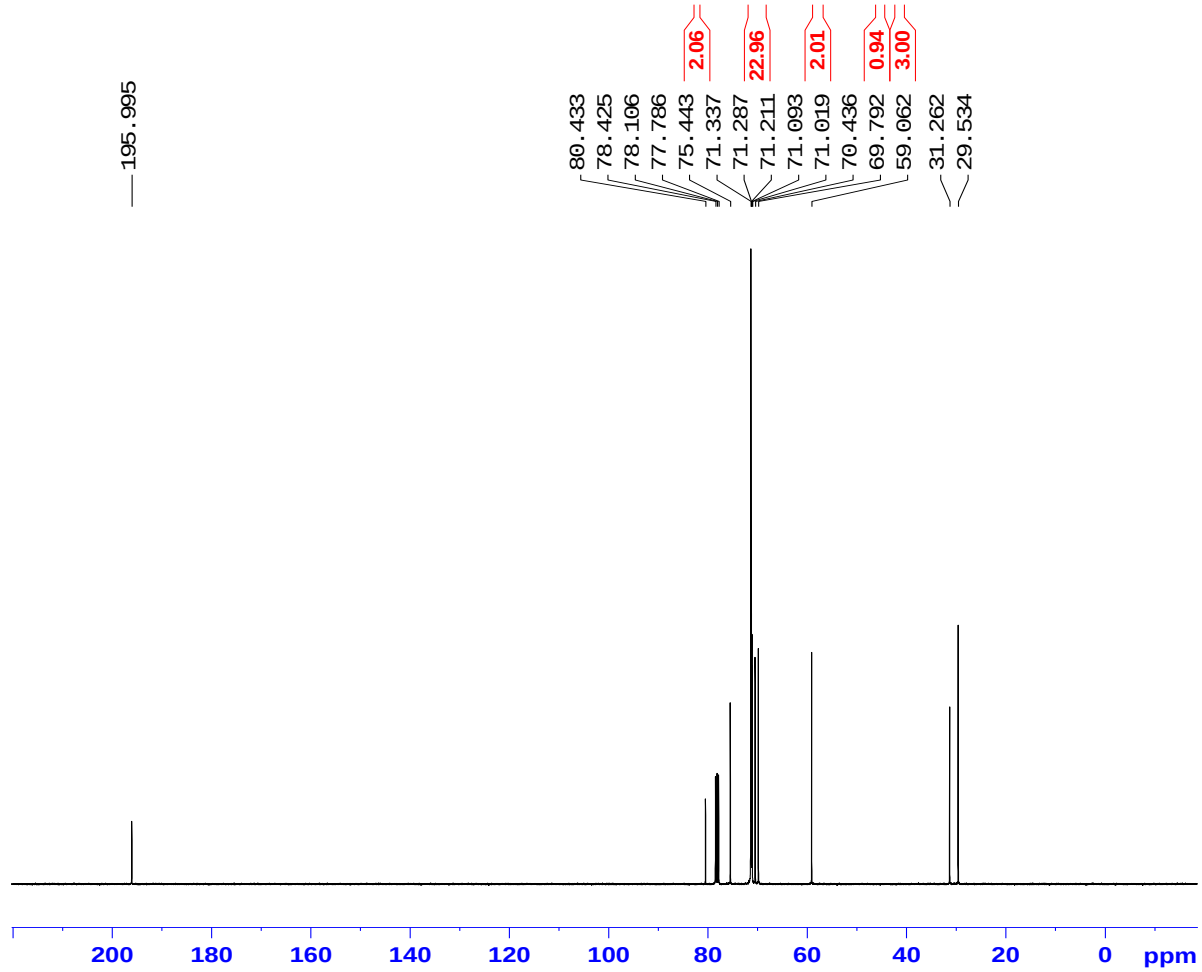
Acquired: Oct 27 09:56:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\27 Thur\ZH3-137001.dat

Printed: 09:58, October 27, 2011




```
NAME      LG-816_Alkyne-P6-SAc
EXPNO                    1
PROCNO                   1
Date_             20111027
Time                 15.11
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                    14.2
DW                  56.800 usec
DE                   6.50 usec
TE                  292.4 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.85 usec
PL1                 -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



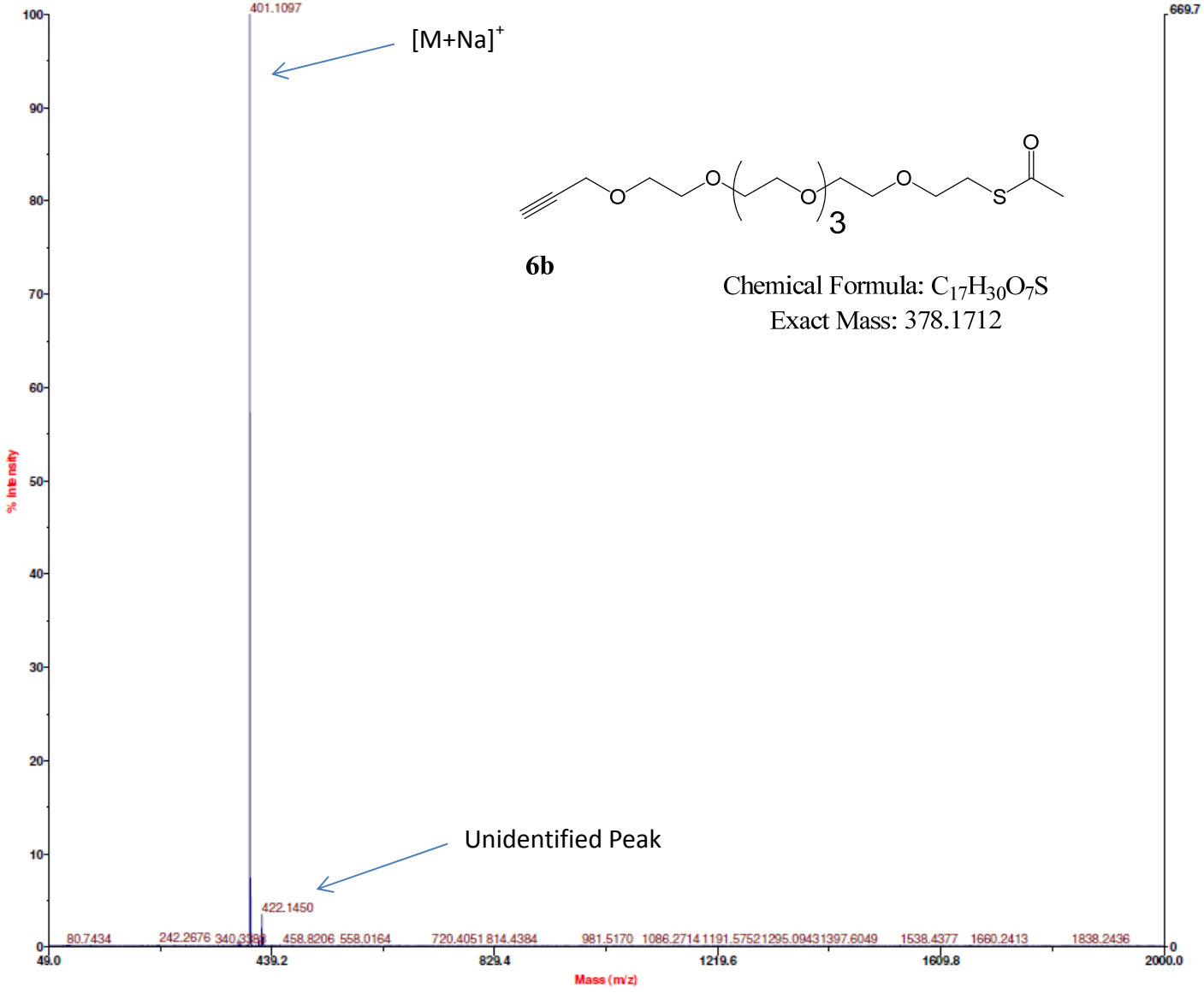

```
NAME      LG-816_Alkyne-P6-SAc
EXPNO                    2
PROCNO                   1
Date_             20111027
Time                 15.41
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    512
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    724
DW                  20.800 usec
DE                   6.50 usec
TE                  294.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.99 usec
PL1                 -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6126885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:29 (T /0.00:0.50) ASC[BP = 401.1, 670]



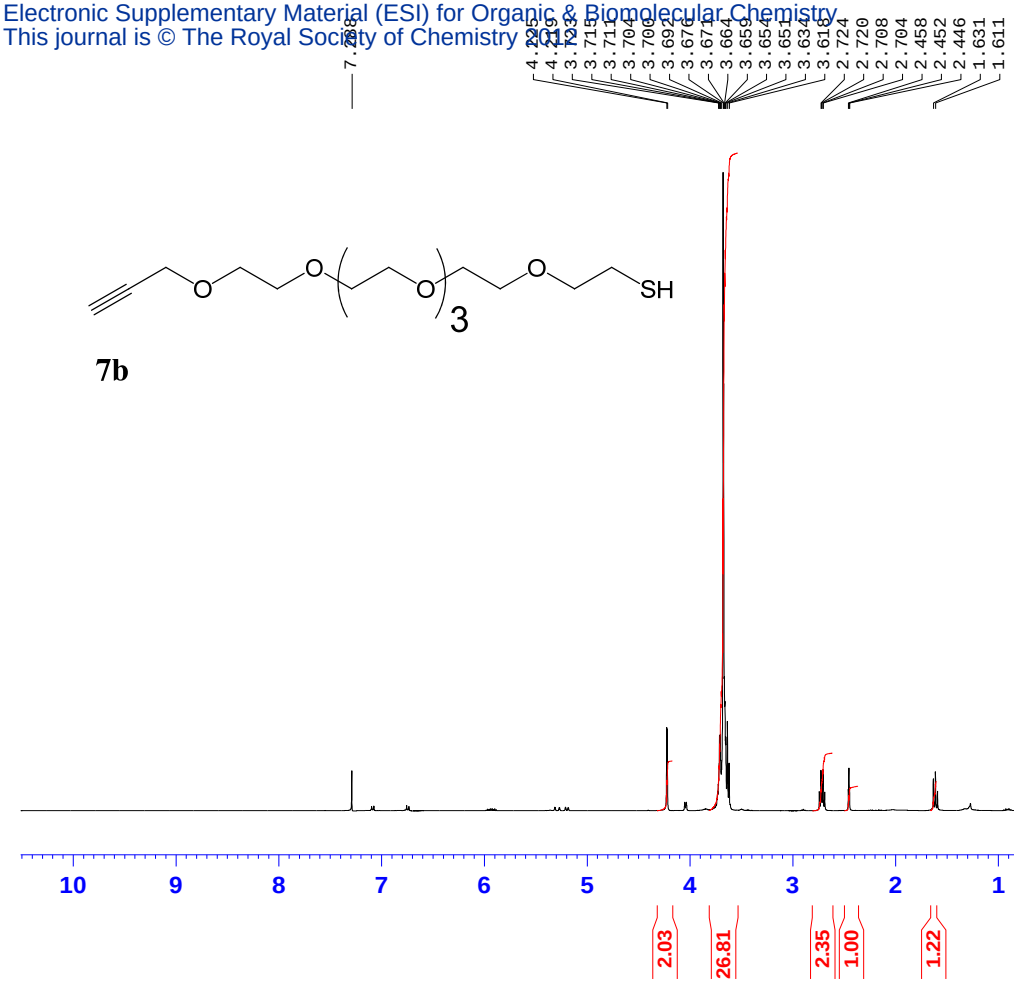
6b

Chemical Formula: $C_{17}H_{30}O_7S$
Exact Mass: 378.1712

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

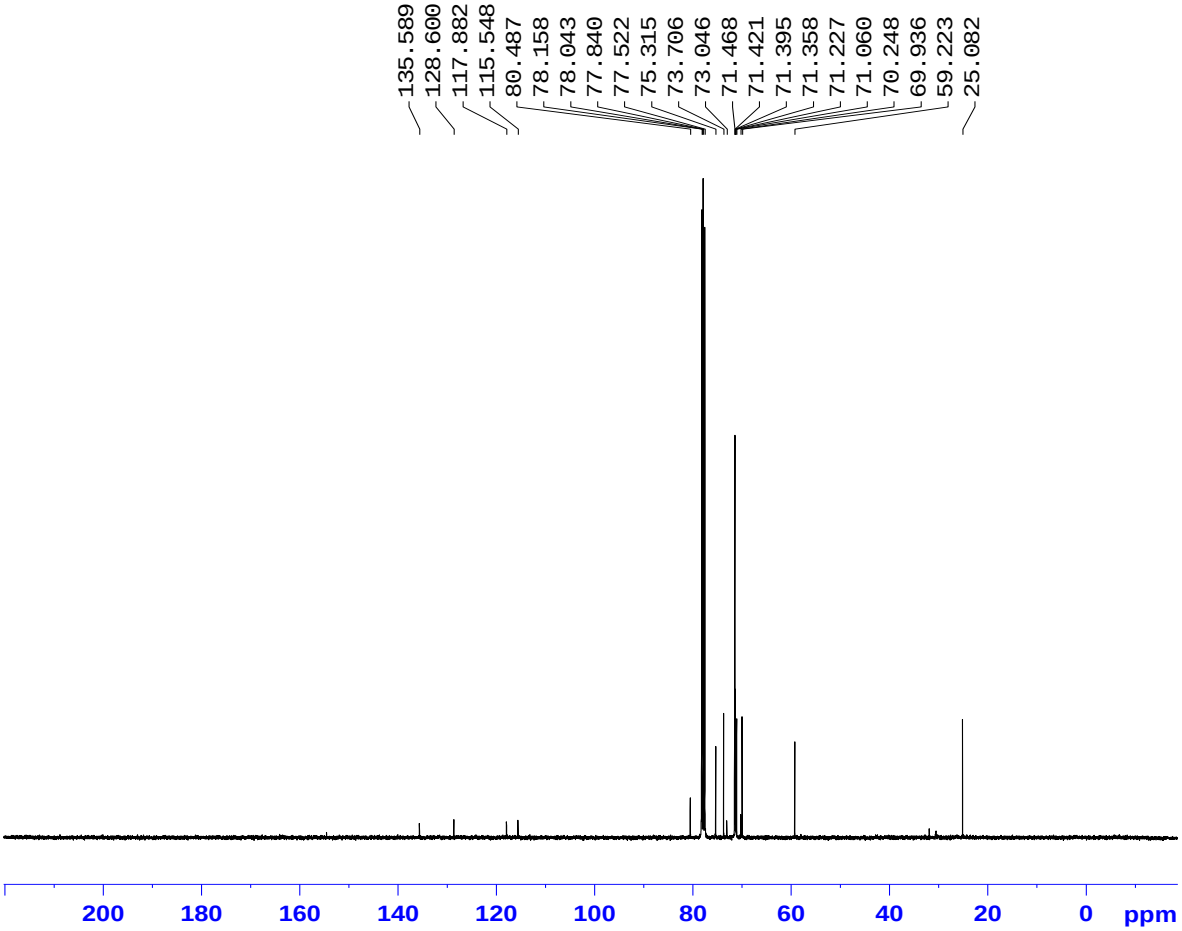
Acquired: Oct 27 16:22:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\27 Thur\LNG-816001.dat

Printed: 16:23, October 27, 2011




```
NAME      LG-819_Alkyne-P6-SH
EXPNO                    1
PROCNO                   1
Date_             20111031
Time                 19.52
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ               3.7224948 sec
RG                     128
DW                  56.800 usec
DE                   6.50 usec
TE                  292.5 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W           13.81451130 W
SFO1           400.1320007 MHz
SI                   32768
SF             400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



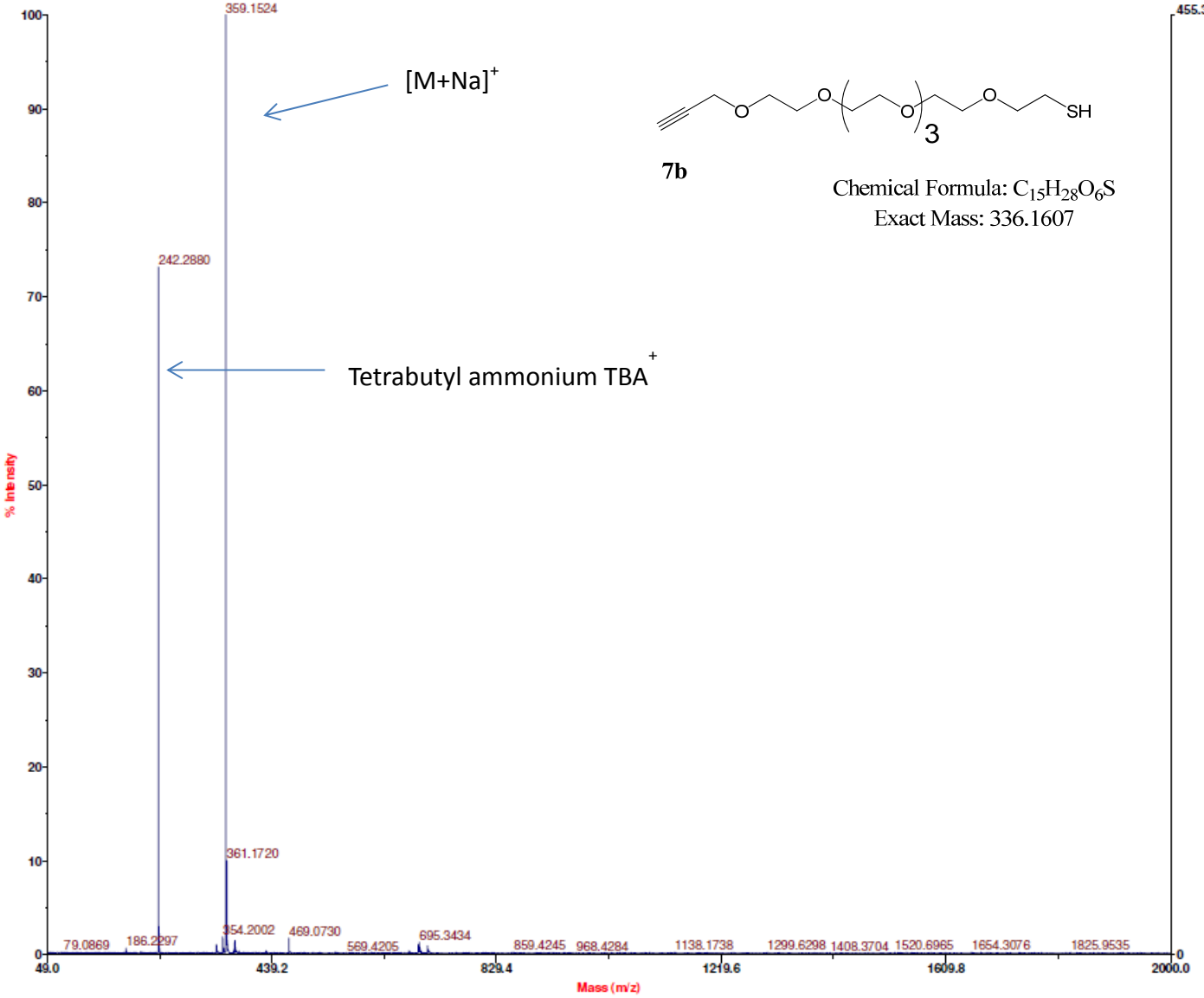

```
NAME      LG-819_Alkyne-P6-SH
EXPNO                    2
PROCNO                   1
Date_             20111031
Time                 21.48
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2000
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                     645
DW                  20.800 usec
DE                   6.50 usec
TE                  294.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W           73.67452240 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W           13.97447491 W
PL12W           0.54996562 W
PL13W           0.54996562 W
SFO2           400.1316005 MHz
SI                   32768
SF             100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:35 (T /0.00:0.61) ASC[BP = 359.2, 455]



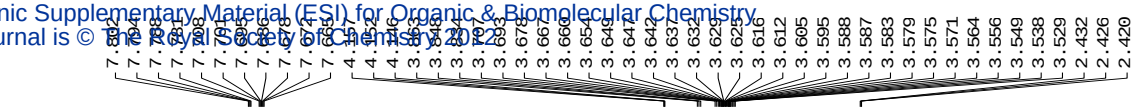
7b

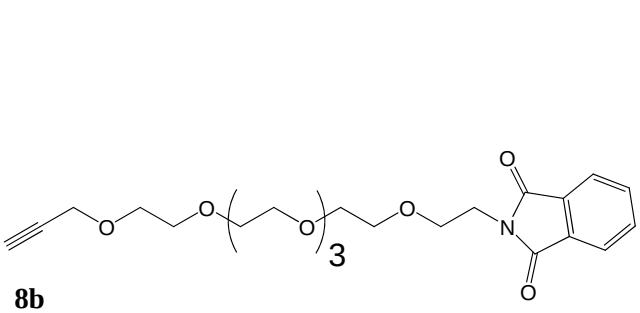
Chemical Formula: $C_{15}H_{28}O_6S$
Exact Mass: 336.1607

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Nov 01 10:41:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\01 Tue\LNG-819001.dat

Printed: 10:52, November 01, 2011

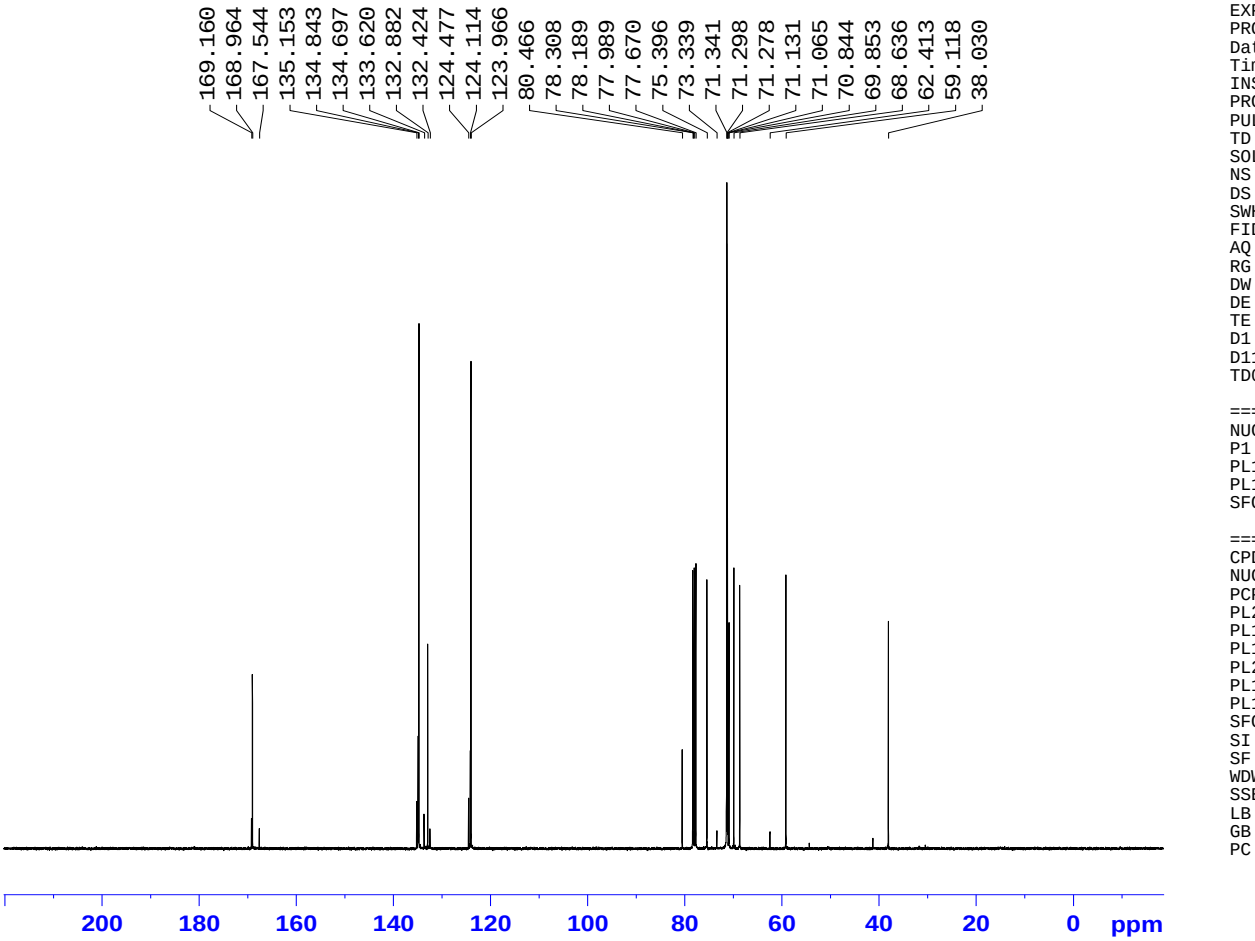




8b

```
NAME          LG-814M_Alkyne-P6-NPth
EXPNO                              1
PROCNO                             1
Date_                       20111027
Time                            3.12
INSTRUM                        spect
PROBHD    5 mm PABBO BB-
PULPROG                         zg30
TD                             65536
SOLVENT                        CDCl3
NS                                16
DS                                 2
SWH                        8802.817 Hz
FIDRES                     0.134320 Hz
AQ                         3.7224948 sec
RG                              22.6
DW                            56.800 usec
DE                             6.50 usec
TE                             292.6 K
D1                      1.00000000 sec
TD0                                1

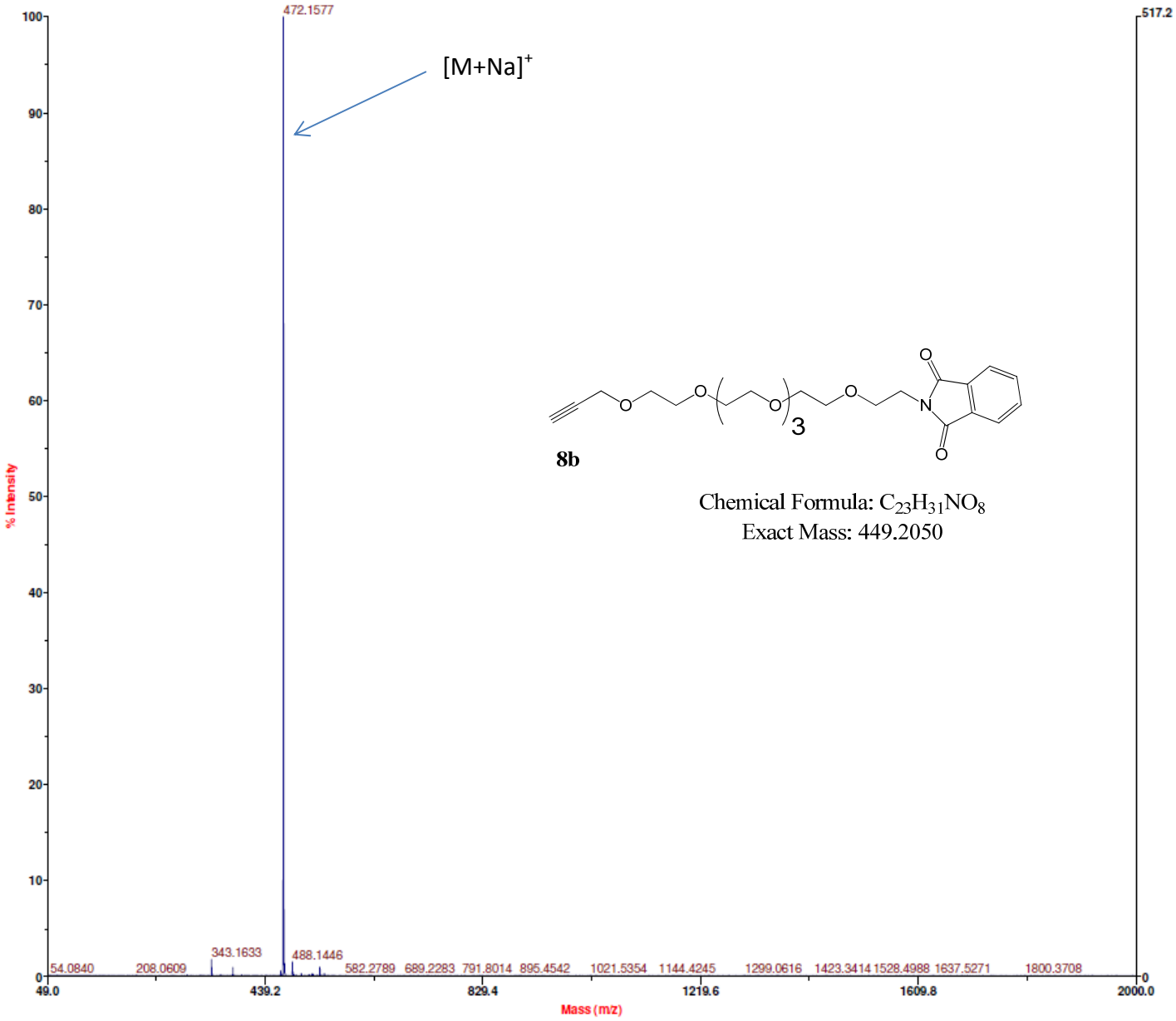
======== CHANNEL f1 ========
NUC1                              1H
P1                            14.85 usec
PL1                           -0.60 dB
PL1W                   13.81451130 W
SFO1                   400.1320007 MHz
SI                             32768
SF                     400.1300000 MHz
WDW                               EM
SSB                                0
LB                             0.30 Hz
GB                                 0
PC                             1.00
```


```
NAME          LG-814M_Alkyne-P6-NPth
EXPNO                              2
PROCNO                             1
Date_                       20111027
Time                            4.12
INSTRUM                        spect
PROBHD    5 mm PABBO BB-
PULPROG                       zgpg30
TD                             65536
SOLVENT                        CDCl3
NS                              1024
DS                                 4
SWH                       24038.461 Hz
FIDRES                     0.366798 Hz
AQ                         1.3631988 sec
RG                               575
DW                            20.800 usec
DE                             6.50 usec
TE                             294.5 K
D1                      2.00000000 sec
D11                     0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                              13C
P1                             9.99 usec
PL1                           -3.00 dB
PL1W                   73.67452240 W
SFO1                   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                    waltz16
NUC2                              1H
PCPD2                         80.00 usec
PL2                           -0.65 dB
PL12                          13.40 dB
PL13                          13.40 dB
PL2W                   13.97447491 W
PL12W                   0.54996562 W
PL13W                   0.54996562 W
SFO2                   400.1316005 MHz
SI                             32768
SF                     100.6126885 MHz
WDW                               EM
SSB                                0
LB                             1.00 Hz
GB                                 0
PC                             1.40
```



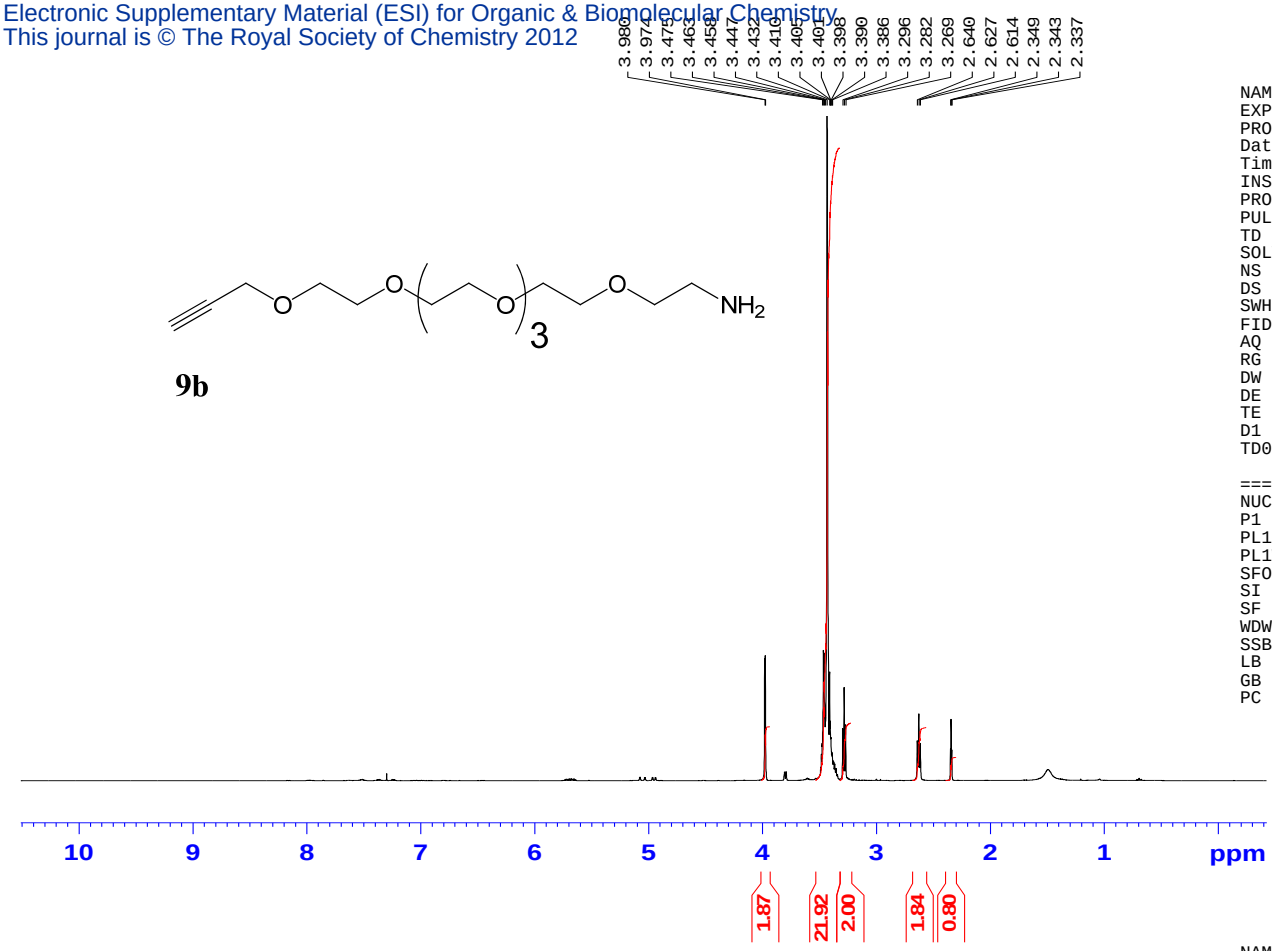
8b

Chemical Formula: $C_{23}H_{31}NO_8$
Exact Mass: 449.2050

Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

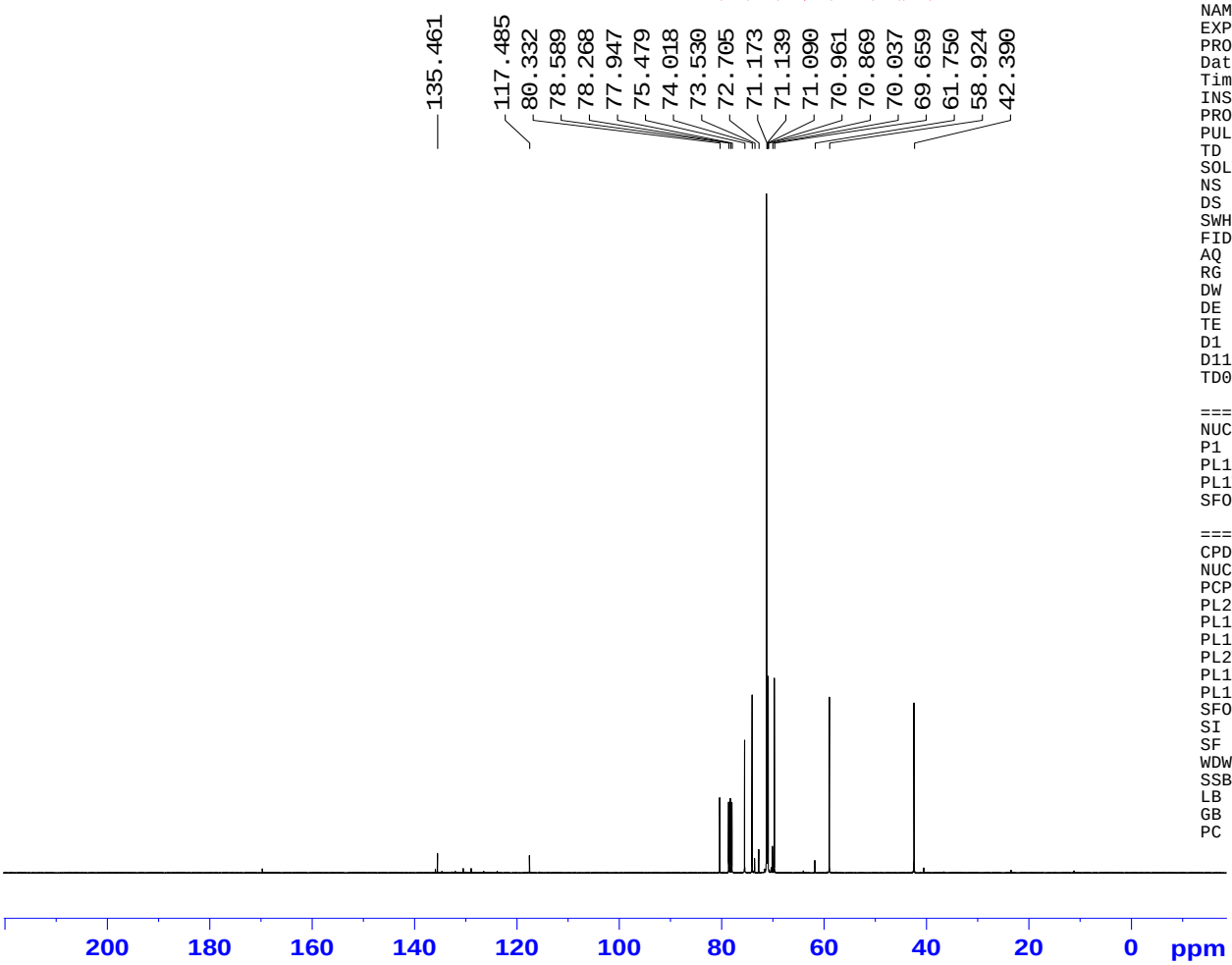
Acquired: Oct 26 16:14:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\26 Wed\LNG-814M001.dat

Printed: 16:15, October 26, 2011




```
NAME      LG-815M_Alkyne-P6-NH2
EXPNO                 1
PROCNO                1
Date_          20111027
Time               5.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8802.817 Hz
FIDRES         0.134320 Hz
AQ             3.7224948 sec
RG                   10
DW                56.800 usec
DE                 6.50 usec
TE                292.6 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.85 usec
PL1               -0.60 dB
PL1W        13.81451130 W
SFO1        400.1320007 MHz
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



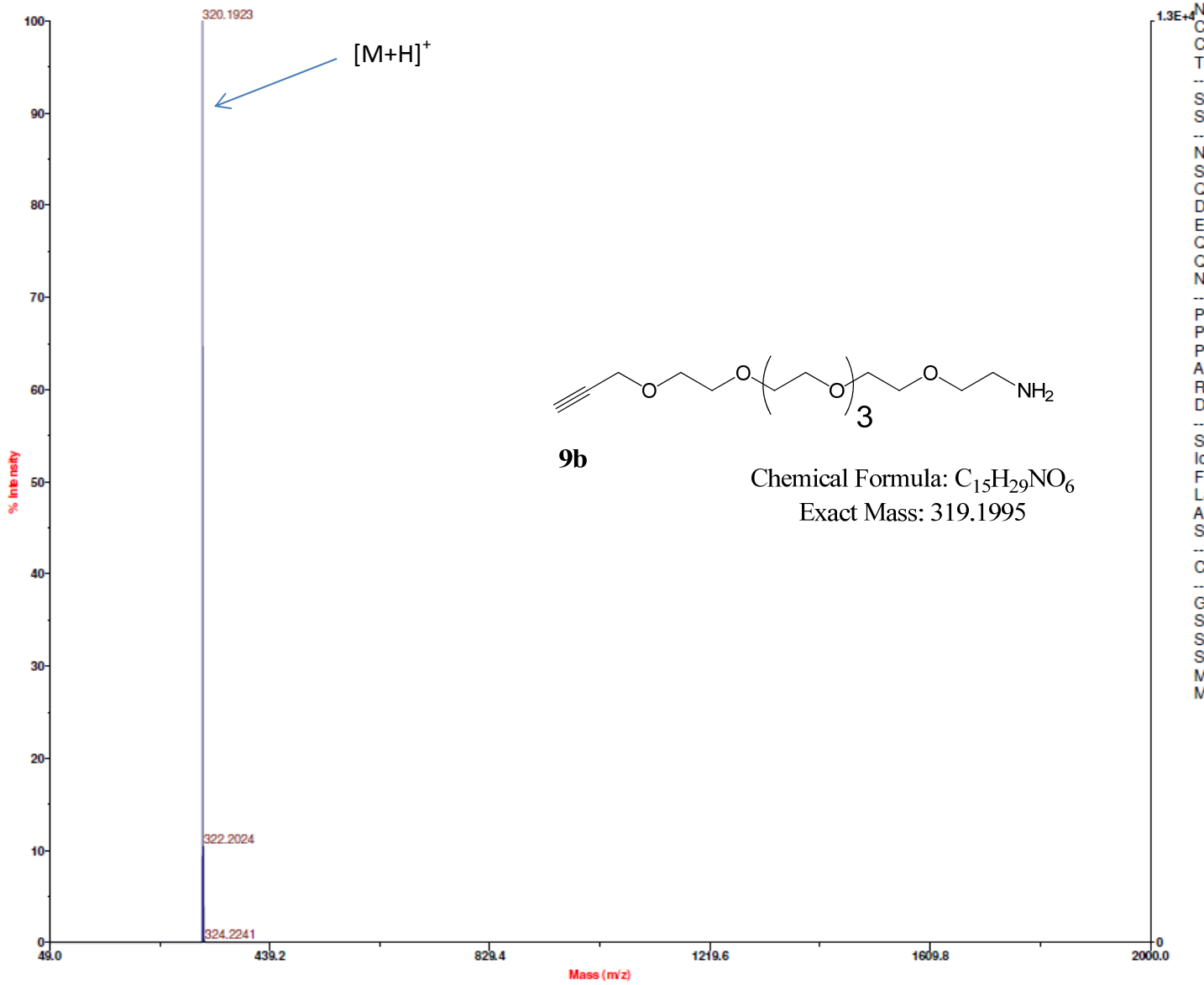

```
NAME      LG-815M_Alkyne-P6-NH2
EXPNO                 2
PROCNO                1
Date_          20111027
Time               6.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  812
DW                20.800 usec
DE                 6.50 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.99 usec
PL1               -3.00 dB
PL1W        73.67452240 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -0.65 dB
PL12              13.40 dB
PL13              13.40 dB
PL2W        13.97447491 W
PL12W        0.54996562 W
PL13W        0.54996562 W
SFO2        400.1316005 MHz
SI                32768
SF          100.6126885 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:39 (T /0.00:0.68) ASC[BP = 320.2, 13306]



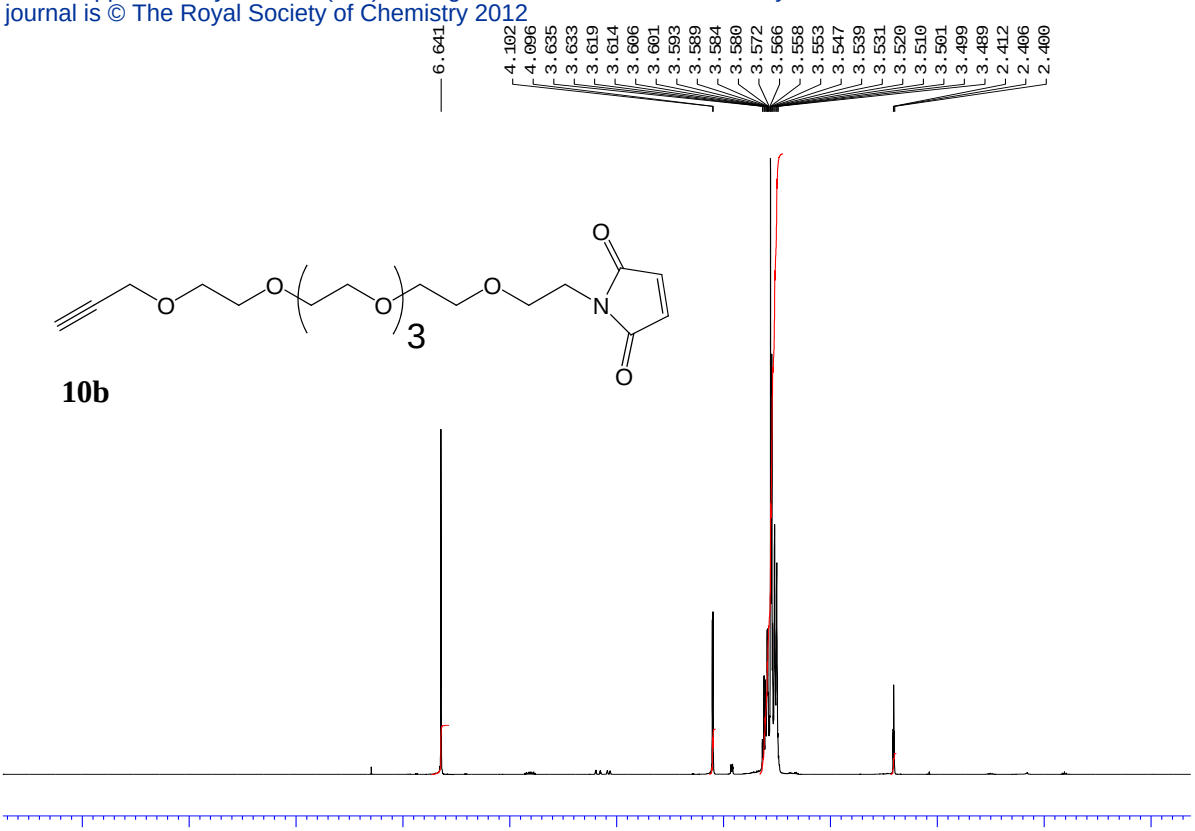
9b

Chemical Formula: $C_{15}H_{29}NO_6$
Exact Mass: 319.1995

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	149.90
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

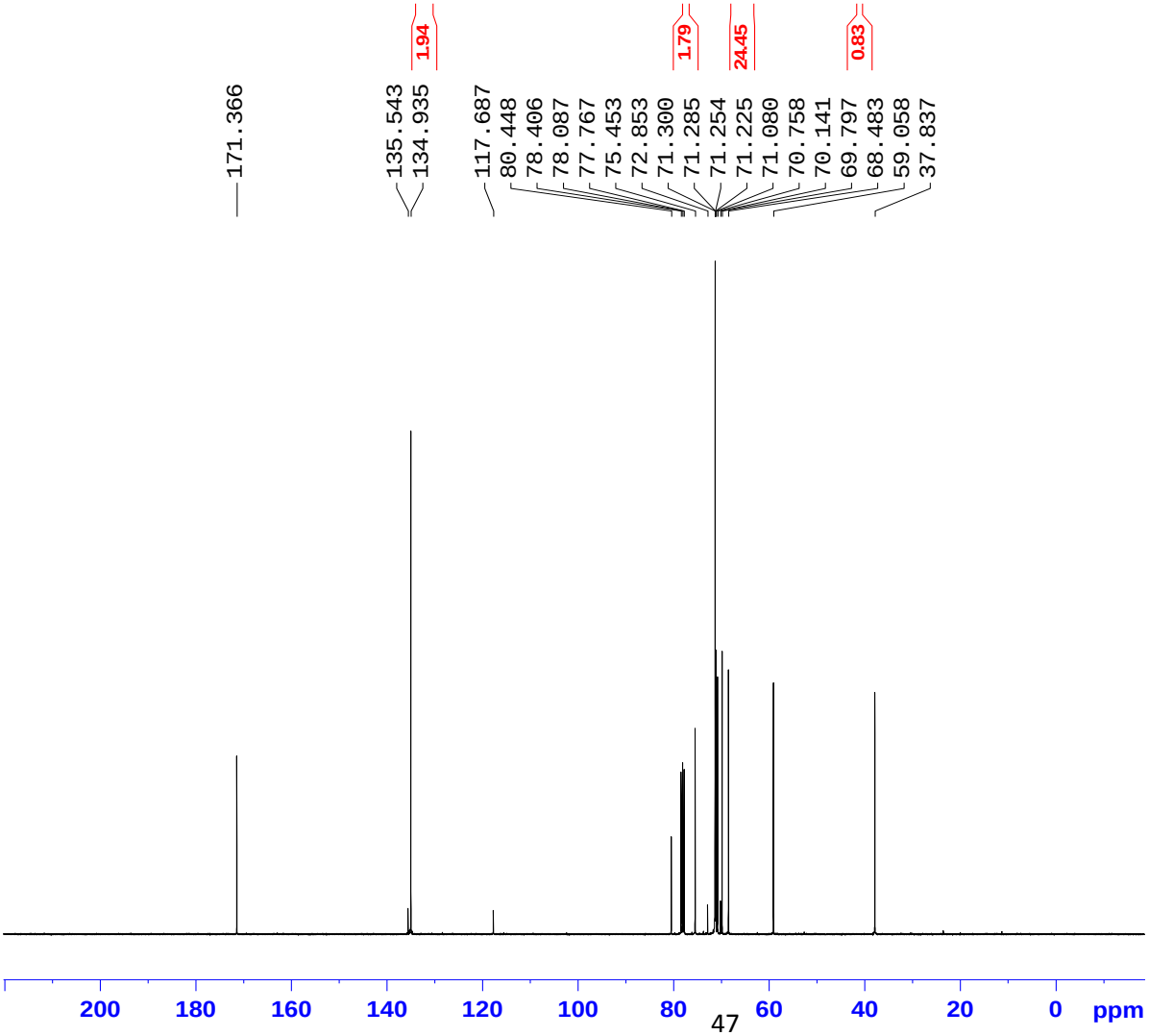
Acquired: Oct 27 10:29:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\27 Thur\LNG-815M001.dat

Printed: 10:30, October 27, 2011




```
NAME      ZH3-139_Alk-P6-Mal
EXPNO                      1
PROCNO                     1
Date_               20111027
Time                   21.05
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                       18
DW                    56.800 usec
DE                     6.50 usec
TE                    292.4 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W              13.81451130 W
SFO1             400.1320007 MHz
SI                     32768
SF               400.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```



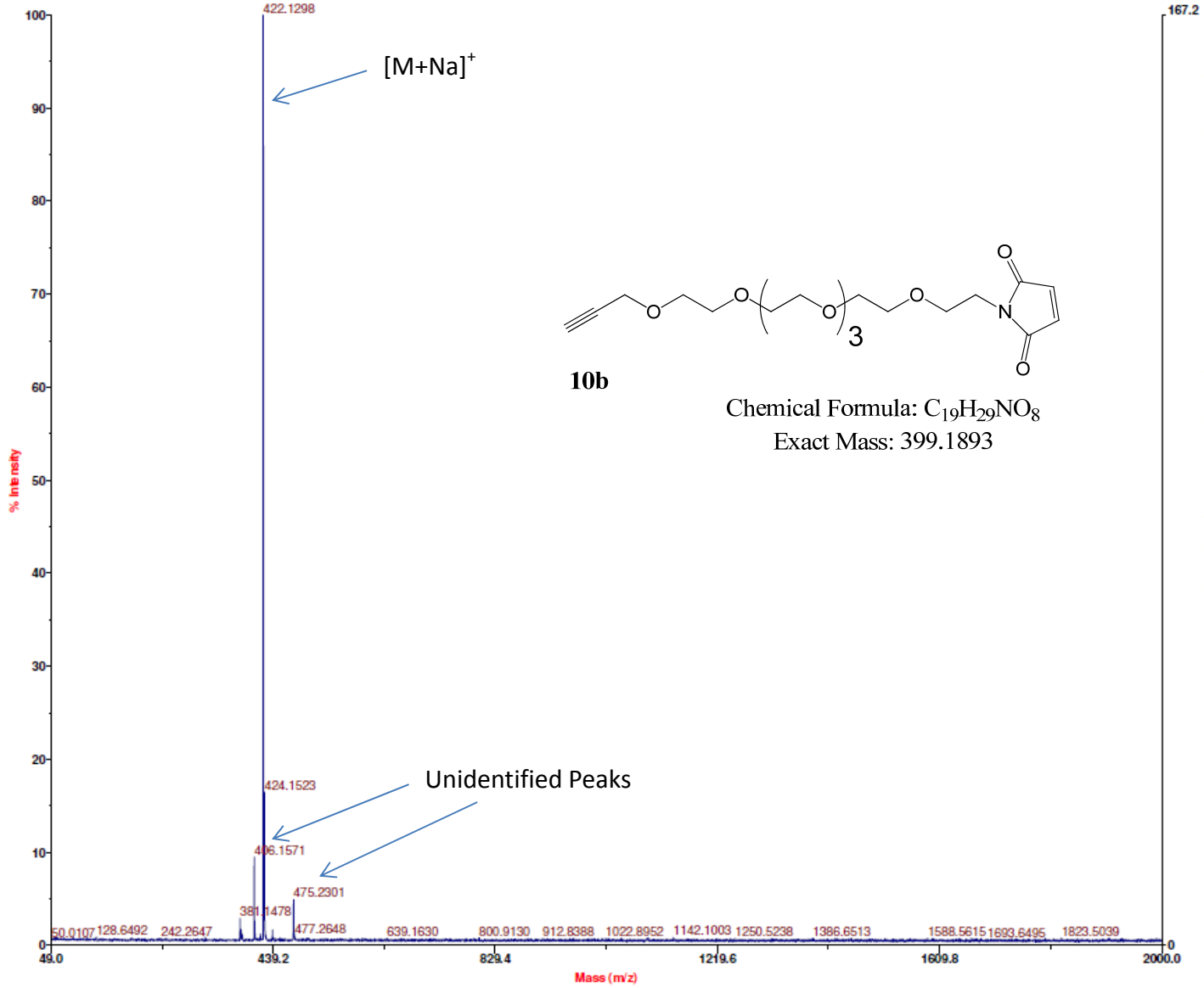

```
NAME      ZH3-139_Alk-P6-Mal
EXPNO                      2
PROCNO                     1
Date_               20111027
Time                   22.05
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       724
DW                    20.800 usec
DE                     6.50 usec
TE                    294.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.99 usec
PL1                   -3.00 dB
PL1W              73.67452240 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W              13.97447491 W
PL12W              0.54996562 W
PL13W              0.54996562 W
SFO2             400.1316005 MHz
SI                     32768
SF               100.6126885 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:25 (T /0.00:0.43) ASC[BP = 422.1, 167]



10b

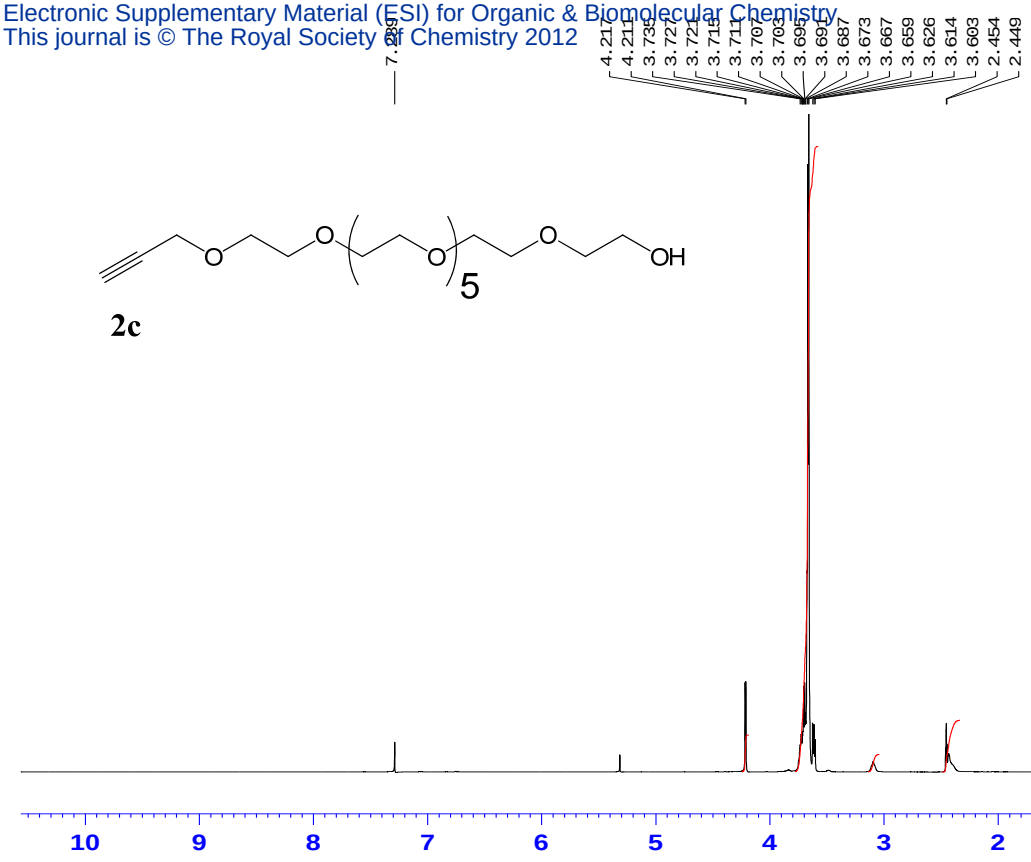
Chemical Formula: $C_{19}H_{29}NO_8$

Exact Mass: 399.1893

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

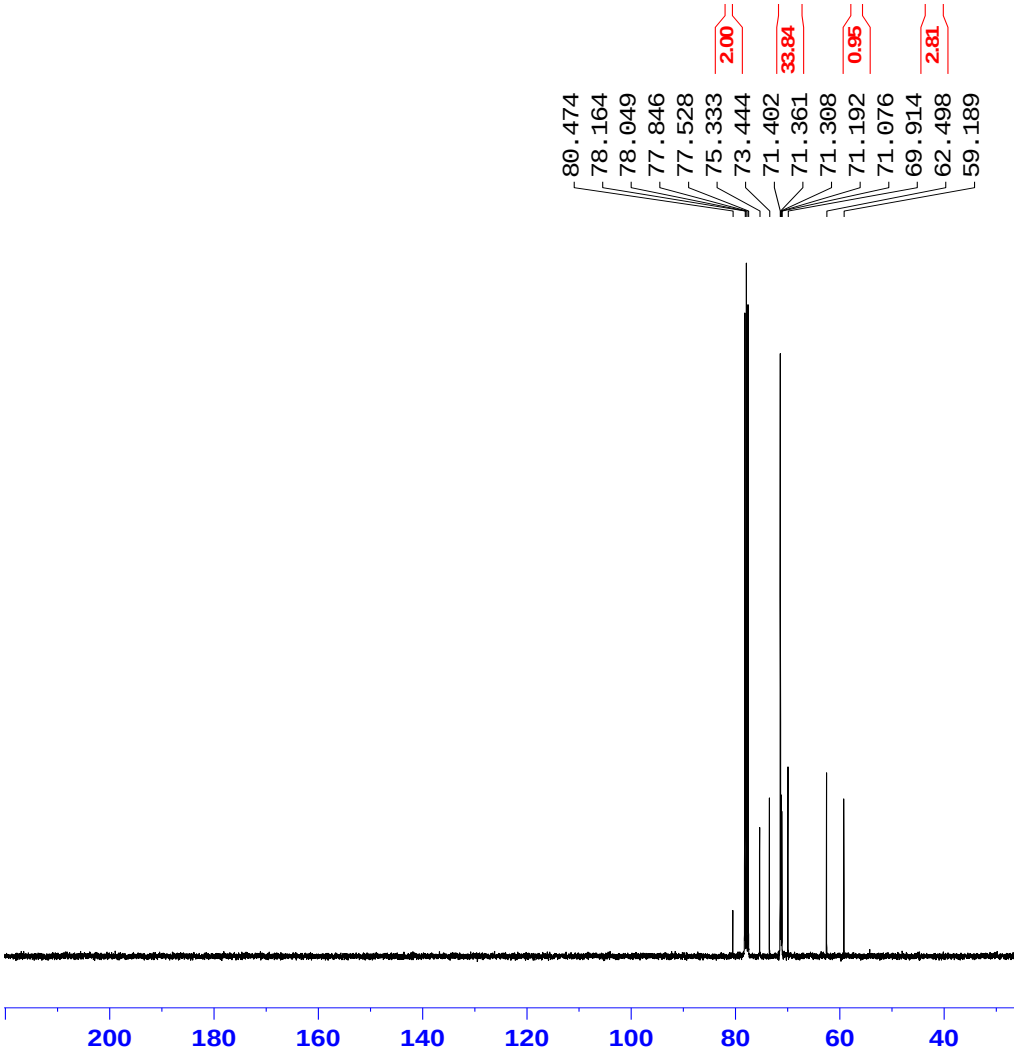
Acquired: Oct 27 16:17:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\27 Thur\ZH3-139001.dat

Printed: 16:19, October 27, 2011




```
NAME      LG-698_Alk-P8-OH
EXPNO                    1
PROCNO                   1
Date_             20110519
Time                 18.34
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ                3.7224948 sec
RG                    71.8
DW                   56.800 usec
DE                    6.50 usec
TE                   292.4 K
D1               1.00000000 sec
TD0                      1

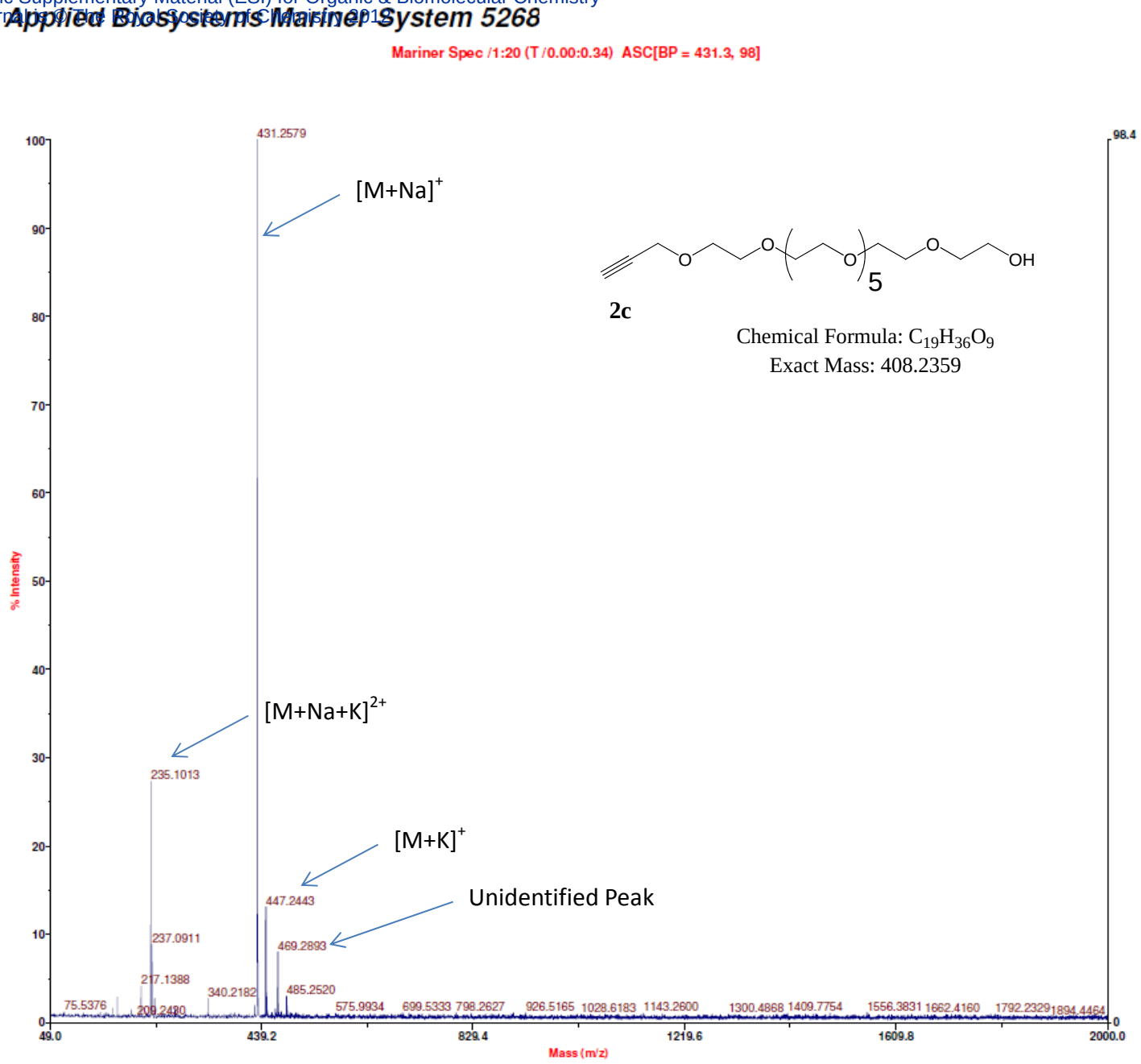
======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W           13.81451130 W
SFO1           400.1320007 MHz
SI                   32768
SF             400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      LG-698_Alk-P8-OH
EXPNO                    2
PROCNO                   1
Date_             20110519
Time                 19.35
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    71.8
DW                   20.800 usec
DE                    6.50 usec
TE                   294.9 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



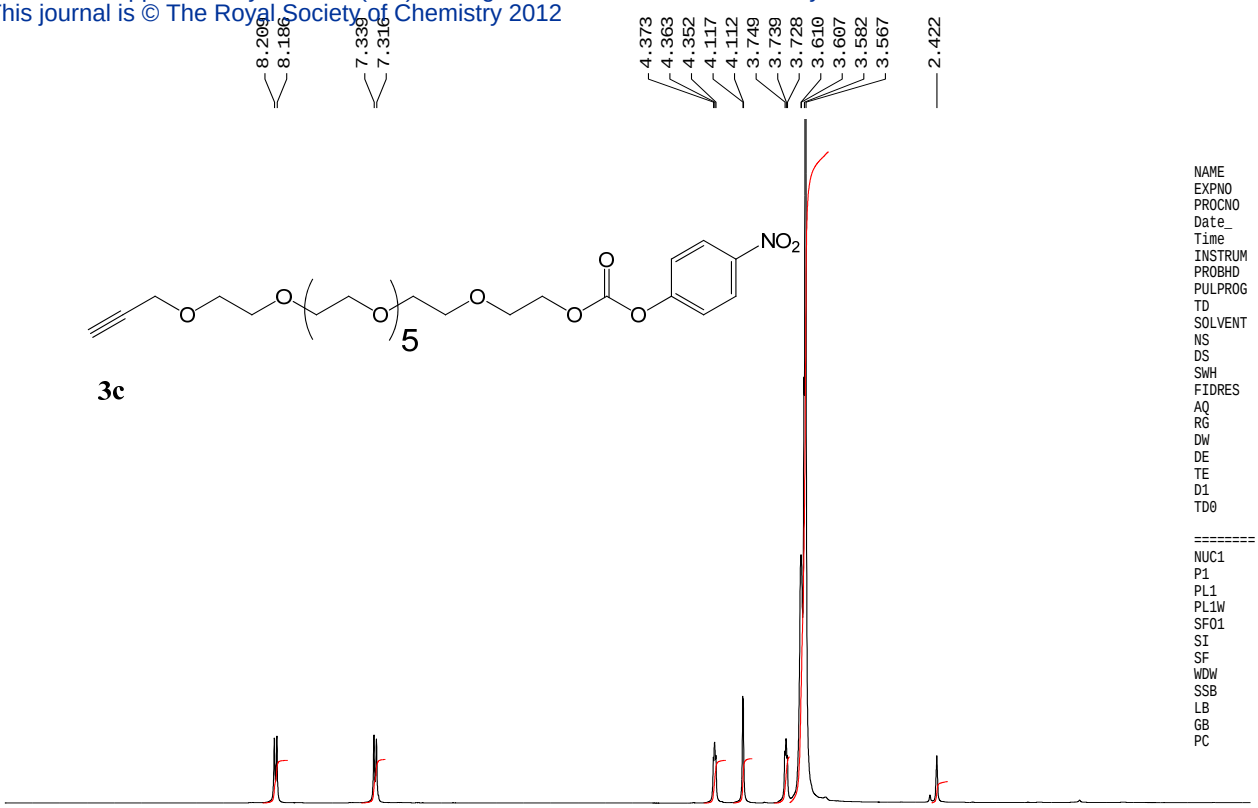
2c

Chemical Formula: $C_{19}H_{36}O_9$
Exact Mass: 408.2359

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0174991E-007
Calibration Constant B	78.221559
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	120.12
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.89
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

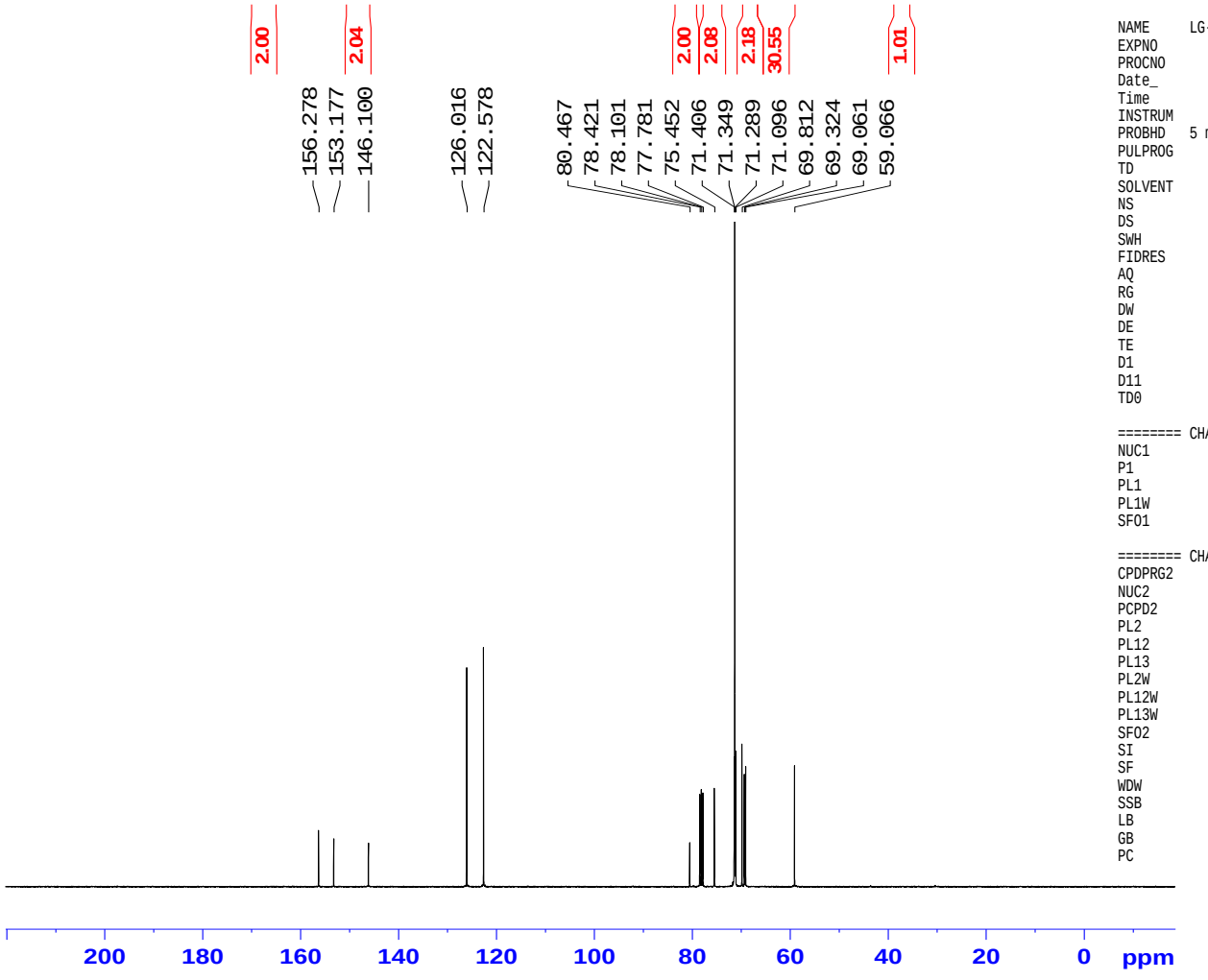
Acquired: May 20 14:16:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\May\20 Fri\LNG-698B001.dat

Printed: 14:17, May 20, 2011




```
NAME      LG-793P2_Alkyne-P8-p-NO2-Ph-carbonate
EXPNO                 1
PROCNO                1
Date_          20110928
Time              18.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8802.817 Hz
FIDRES         0.134320 Hz
AQ             3.7224948 sec
RG                   16
DW               56.800 usec
DE                6.50 usec
TE                292.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.85 usec
PL1               -0.60 dB
PL1W        13.81451130 W
SFO1        400.1320007 MHz
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                 1.00
```



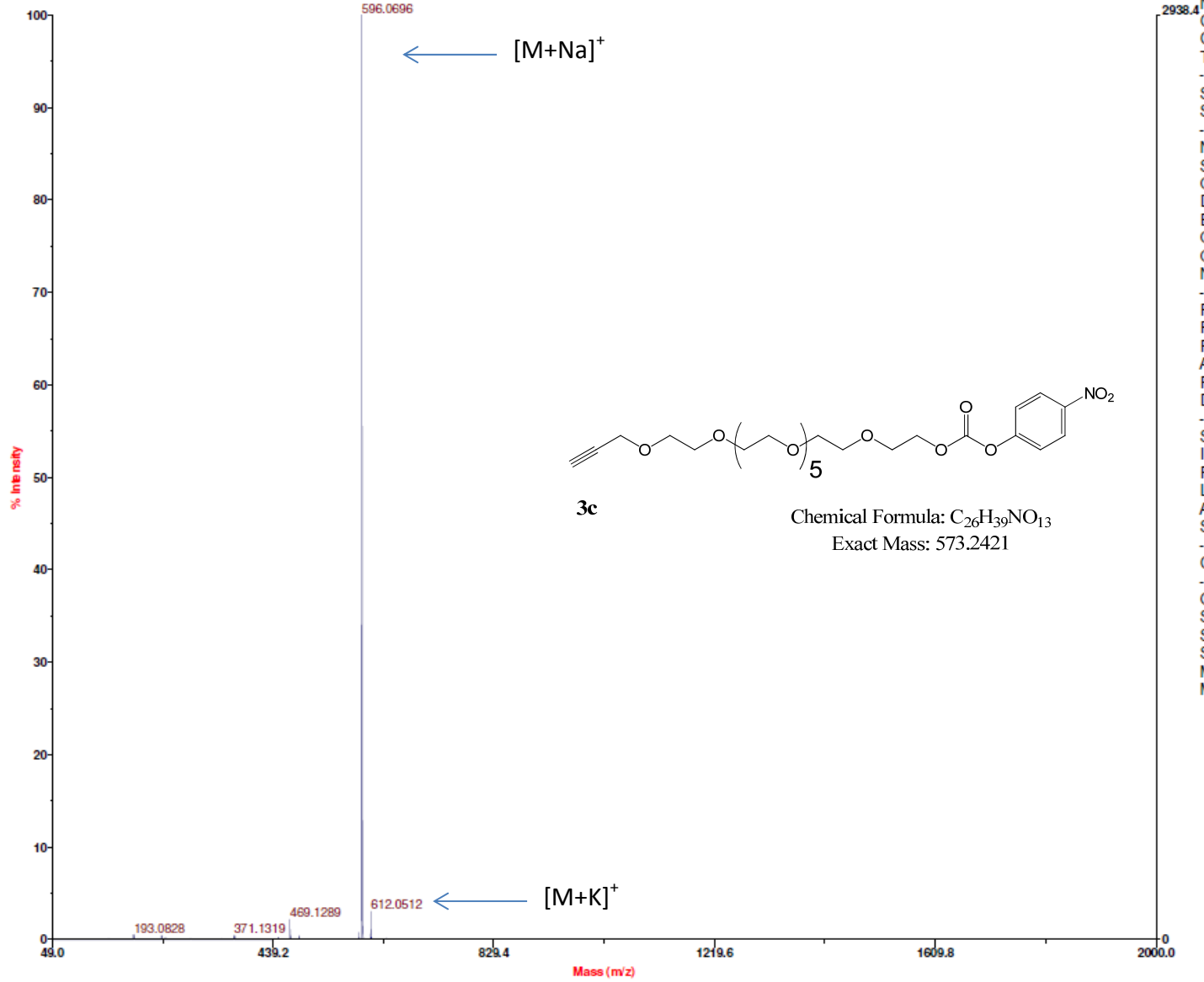

```
NAME      LG-793P2_Alkyne-P8-p-NO2-Ph-carbonate
EXPNO                 2
PROCNO                1
Date_          20110928
Time              19.36
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 1030
DW               20.800 usec
DE                6.50 usec
TE                294.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                9.99 usec
PL1               -3.00 dB
PL1W        73.67452240 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -0.65 dB
PL12              13.40 dB
PL13              13.40 dB
PL2W        13.97447491 W
PL12W        0.54996562 W
PL13W        0.54996562 W
SFO2        400.1316005 MHz
SI                32768
SF          100.6126885 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                 1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:59 (T /0.00:1.03) ASC[BP = 596.1, 2938]



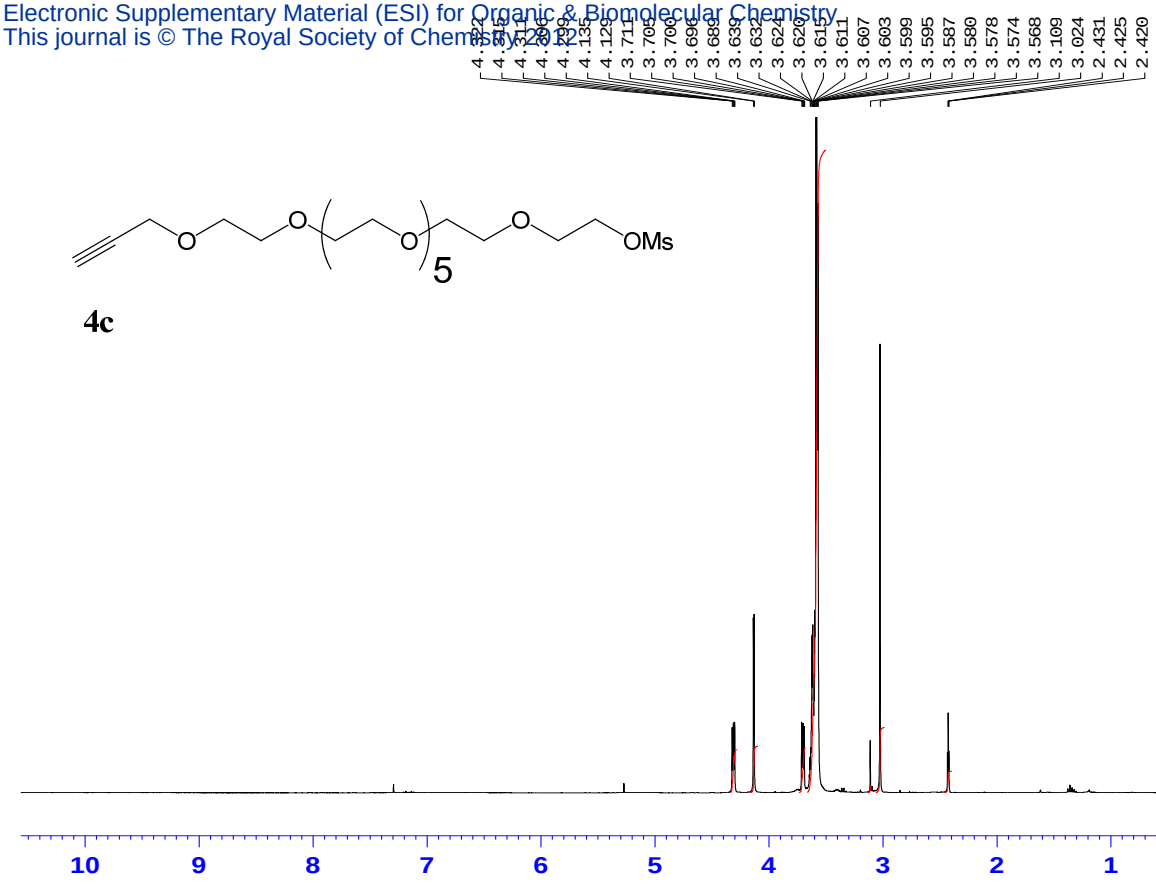
3c

Chemical Formula: $C_{26}H_{39}NO_{13}$
Exact Mass: 573.2421

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	120.12
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Sep 28 13:12:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Sep\28 Wed\LNG-793001.dat

Printed: 13:14, September 28, 2011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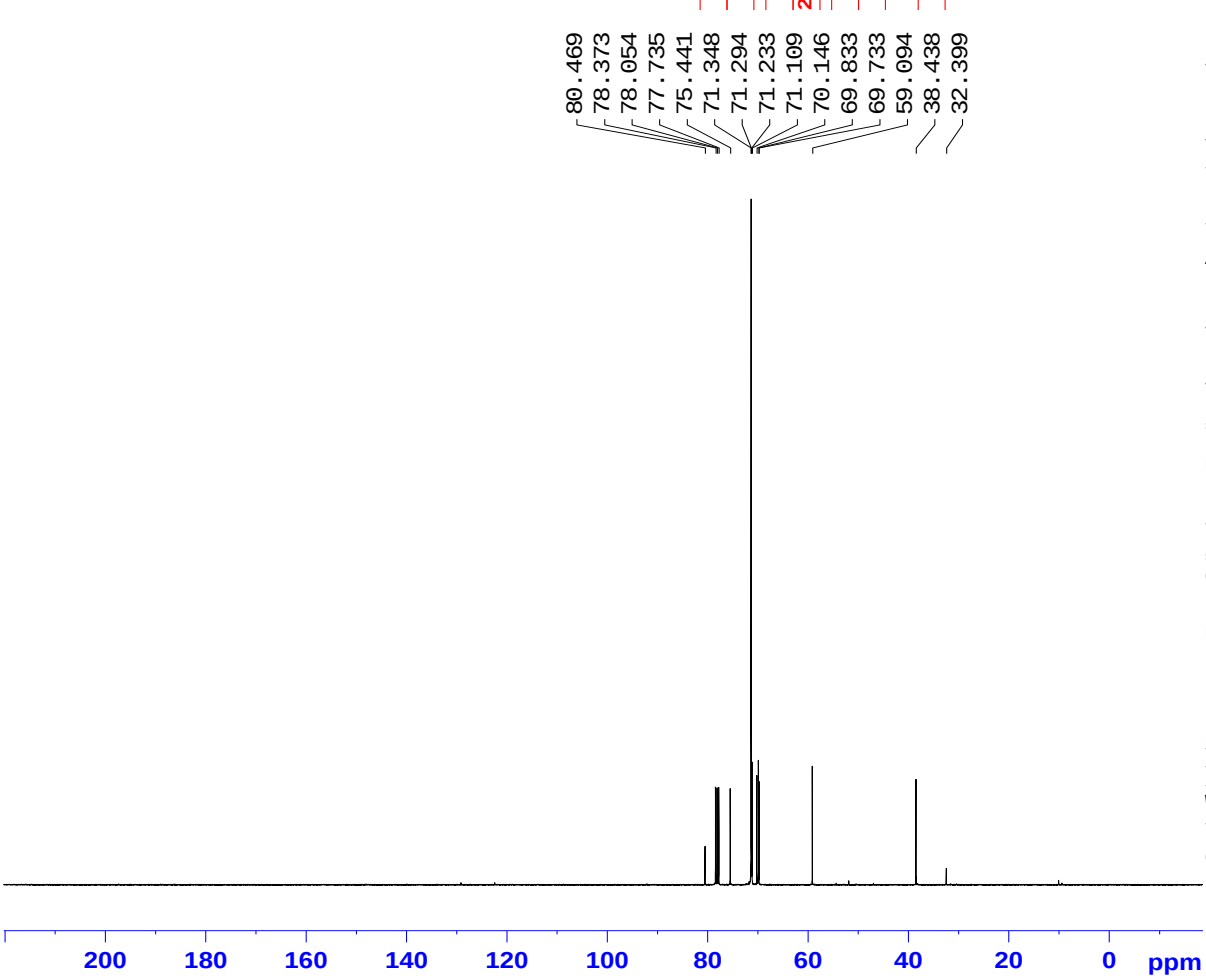
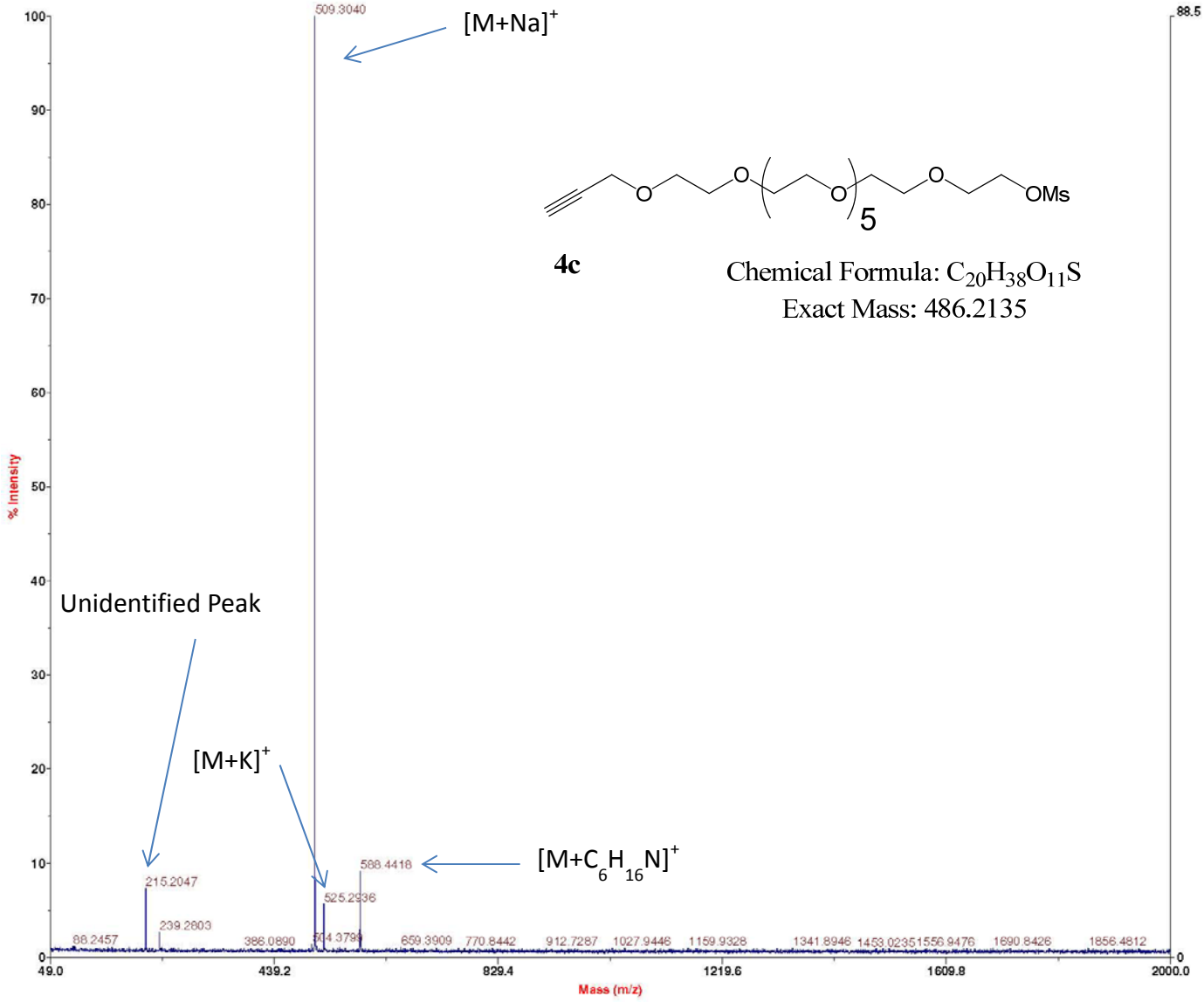
4.415
4.411
4.286
4.269
4.135
4.129
3.711
3.705
3.700
3.696
3.689
3.639
3.632
3.624
3.620
3.615
3.611
3.607
3.603
3.599
3.595
3.587
3.580
3.578
3.574
3.568
3.109
3.024
2.431
2.425
2.420
O
O
O
O
5
OMs
4c
NAME LG-719M_Alkyne-OEG-OMs
EXPNO 1
PROCNO 1
Date_ 20110614
Time 21.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224948 sec
RG 20.2
DW 56.800 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.85 usec
PL1 -0.60 dB
PL1W 13.81451130 W
SFO1 400.1320007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.16
2.10
29.76
0.33
3.02
1.00


80.469
78.373
78.054
77.735
75.441
71.348
71.294
71.233
71.109
70.146
69.833
69.733
59.094
38.438
32.399
NAME LG-719M_Alkyne-OEG-OMs
EXPNO 2
PROCNO 1
Date_ 20110614
Time 22.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 1030
DW 20.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.99 usec
PL1 -3.00 dB
PL1W 73.67452240 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.65 dB
PL12 13.40 dB
PL13 13.40 dB
PL2W 13.97447491 W
PL12W 0.54996562 W
PL13W 0.54996562 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6126885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

Applied Biosystems Mariner System 5268

Mariner Spec /1:38 (T /0.00:0.66) ASC[BP = 509.3, 88]



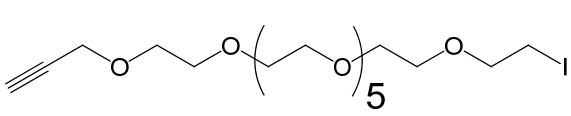
4c

Chemical Formula: $C_{20}H_{38}O_{11}S$
Exact Mass: 486.2135

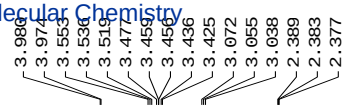
--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0174991E-007
Calibration Constant B	78.221559
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: May 24 11:33:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\May\24 Tues\LNG-700001.dat

Printed: 11:34, May 24, 2011

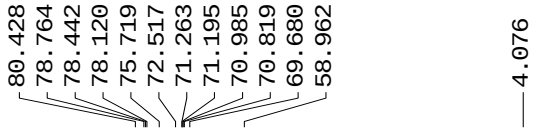


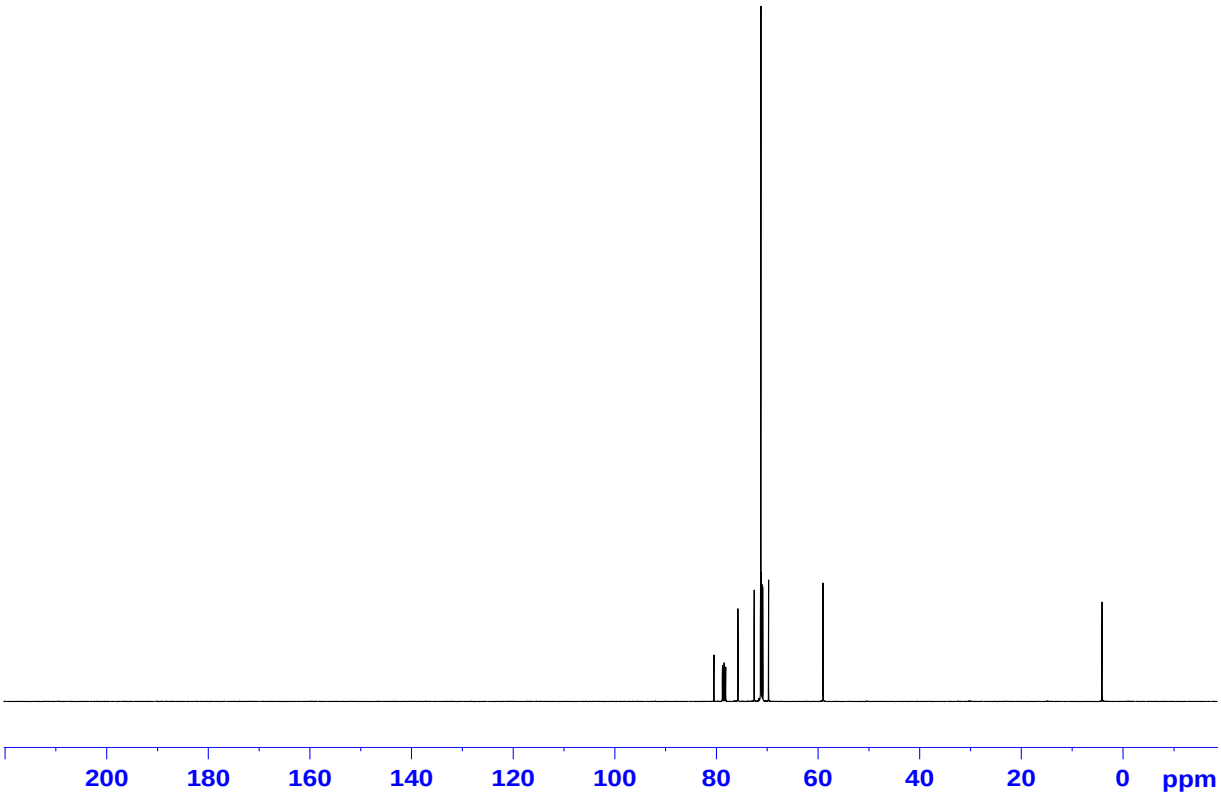
5c




```
NAME      ZH3-118_Alk-P8-I
EXPNO                    1
PROCNO                   1
Date_             20110927
Time                 21.04
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                        9
DW                   56.800 usec
DE                    6.50 usec
TE                   292.5 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.85 usec
PL1                   -0.60 dB
PL1W             13.81451130 W
SFO1             400.1320007 MHz
SI                    32768
SF               400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```





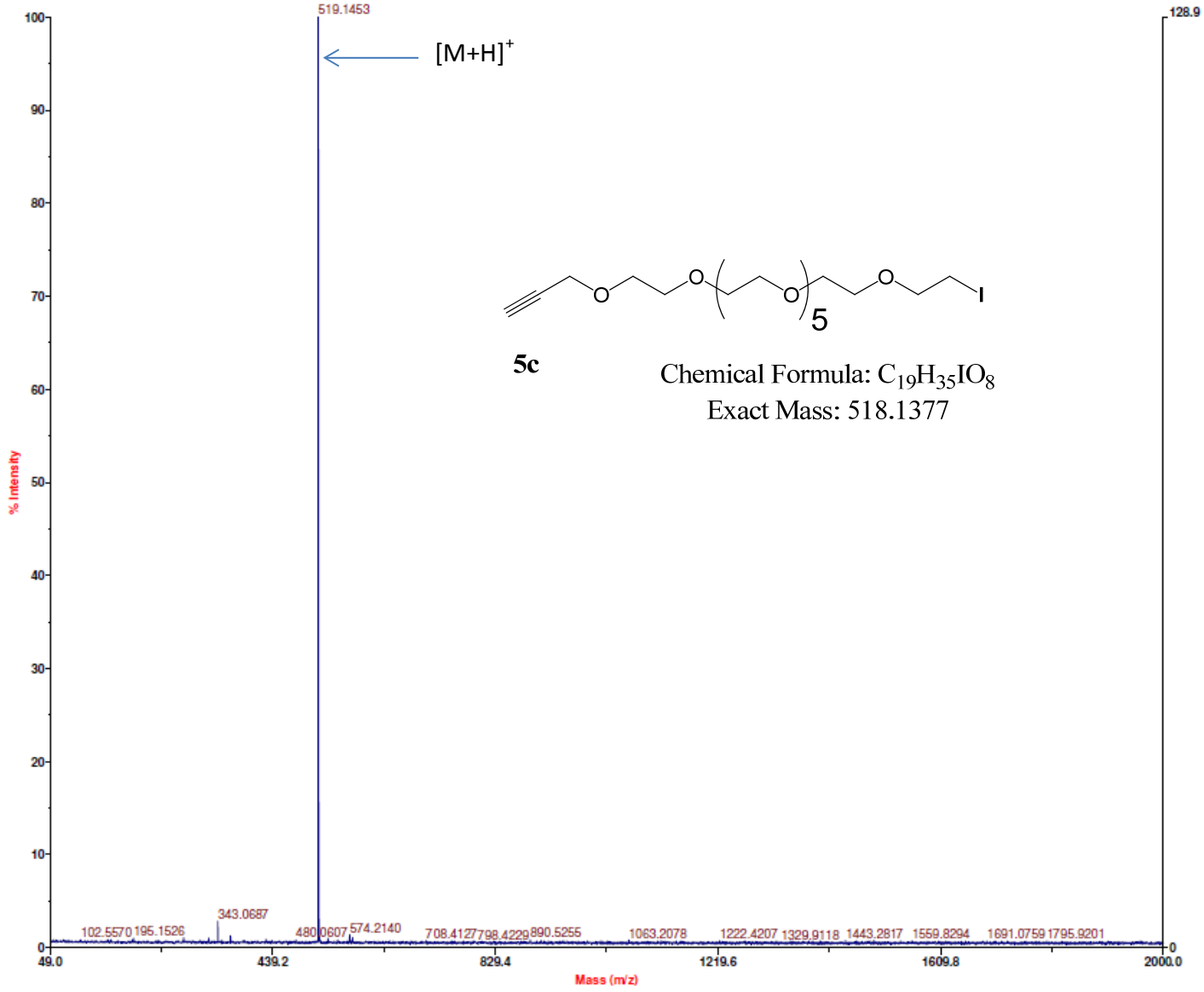

```
NAME      ZH3-118_Alk-P8-I
EXPNO                    2
PROCNO                   1
Date_             20110927
Time                 22.04
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      724
DW                   20.800 usec
DE                    6.50 usec
TE                   294.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W            73.67452240 W
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W            13.97447491 W
PL12W            0.54996562 W
PL13W            0.54996562 W
SFO2            400.1316005 MHz
SI                    32768
SF              100.6126885 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Applied Biosystems Mariner System 5219

Mariner Spec /1:27 (T /0.00:0.46) ASC[BP = 519.2, 129]



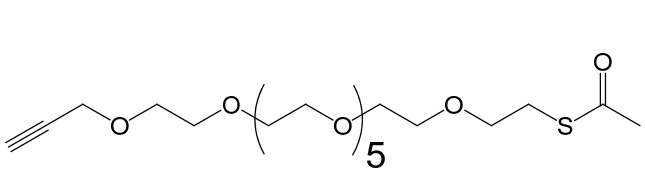
5c

Chemical Formula: $C_{19}H_{35}IO_8$
Exact Mass: 518.1377

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0149194E-007
Calibration Constant B	78.267402
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	80.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Jul 13 11:19:00 2012
Mariner Mass Spectrum
C:\Mariner\Data\2012\Jul\13 Fri\ZH3-118-APCI001.dat

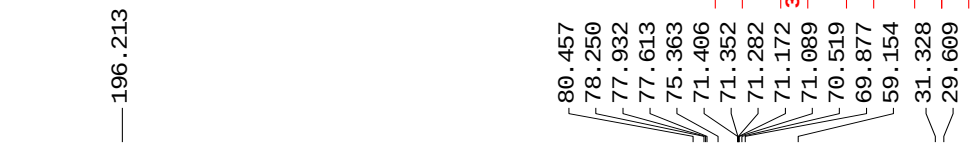
Printed: 11:20, July 13, 2012

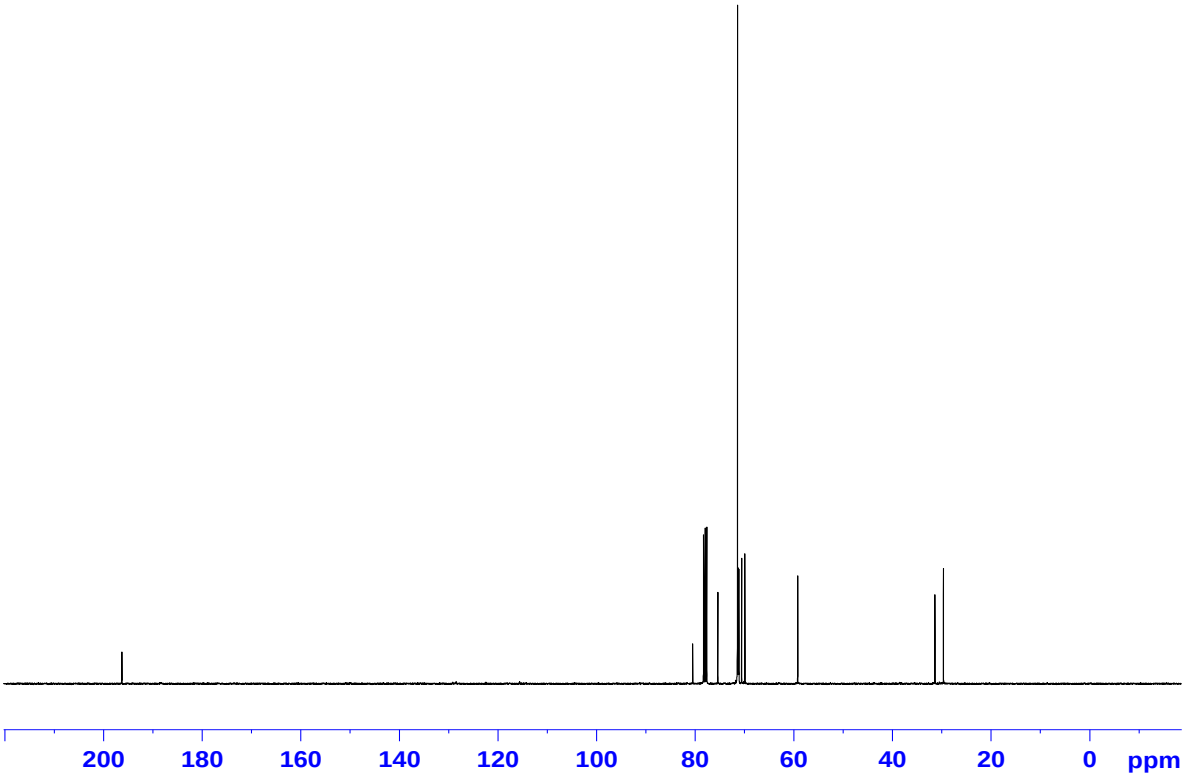


6c


```
NAME      ZH3-141_Alk-P8-SAc
EXPNO                      1
PROCNO                     1
Date_               20111101
Time                   21.04
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8802.817 Hz
FIDRES              0.134320 Hz
AQ                3.7224948 sec
RG                      28.5
DW                    56.800 usec
DE                     6.50 usec
TE                     292.4 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W              13.81451130 W
SFO1              400.1320007 MHz
SI                      32768
SF                400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```





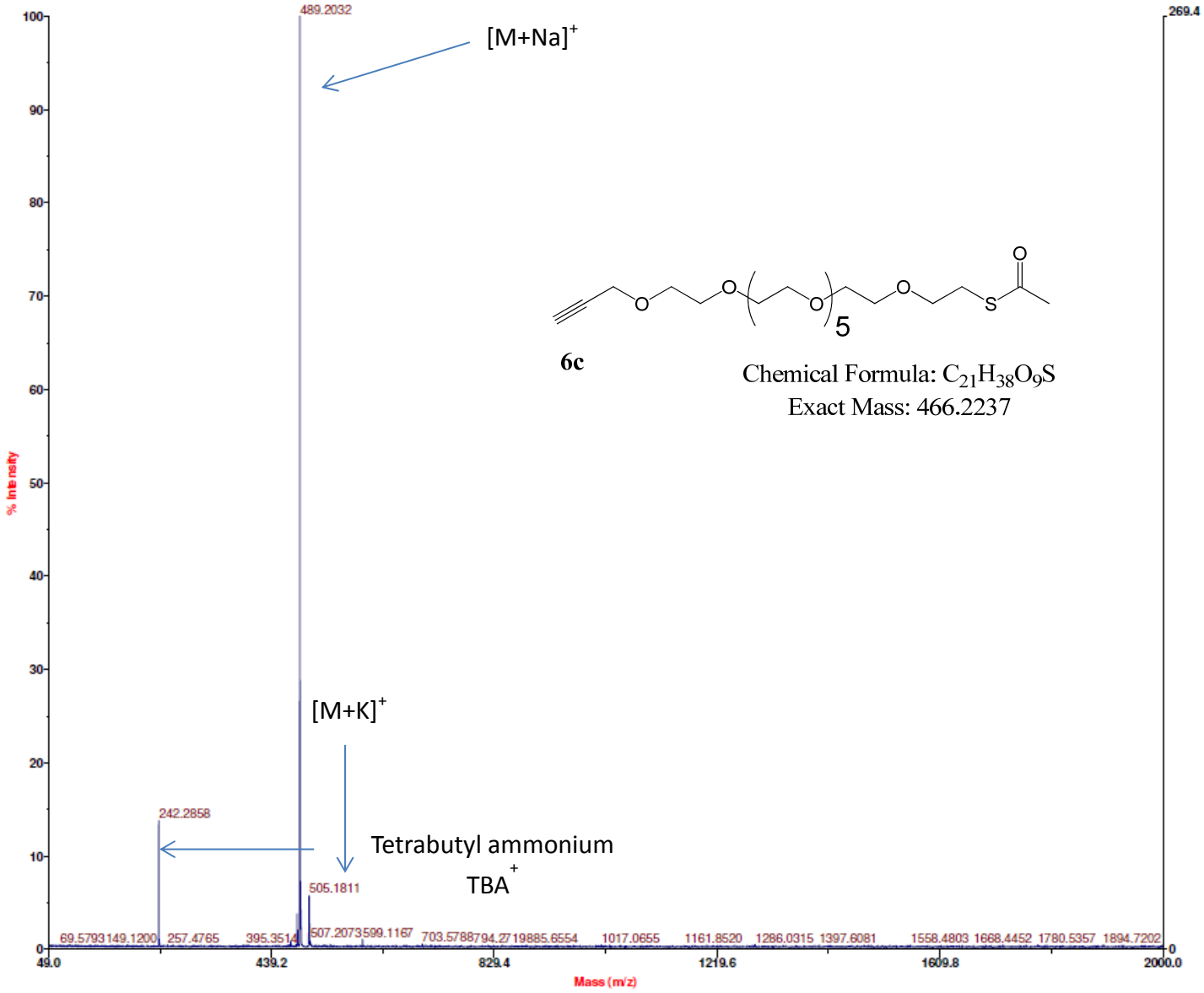

```
NAME      ZH3-141_Alk-P8-SAc
EXPNO                      2
PROCNO                     1
Date_               20111101
Time                   22.05
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                       724
DW                    20.800 usec
DE                     6.50 usec
TE                     294.4 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.99 usec
PL1                    -3.00 dB
PL1W              73.67452240 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W              13.97447491 W
PL12W              0.54996562 W
PL13W              0.54996562 W
SFO2             400.1316005 MHz
SI                      32768
SF                100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:23 (T /0.00:0.39) ASC[BP = 489.2, 269]



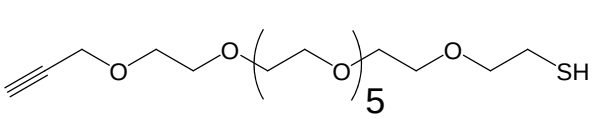
6c

Chemical Formula: $C_{21}H_{38}O_9S$
Exact Mass: 466.2237

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	80.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Nov 01 16:25:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\01 Tue\ZH3-141001.dat

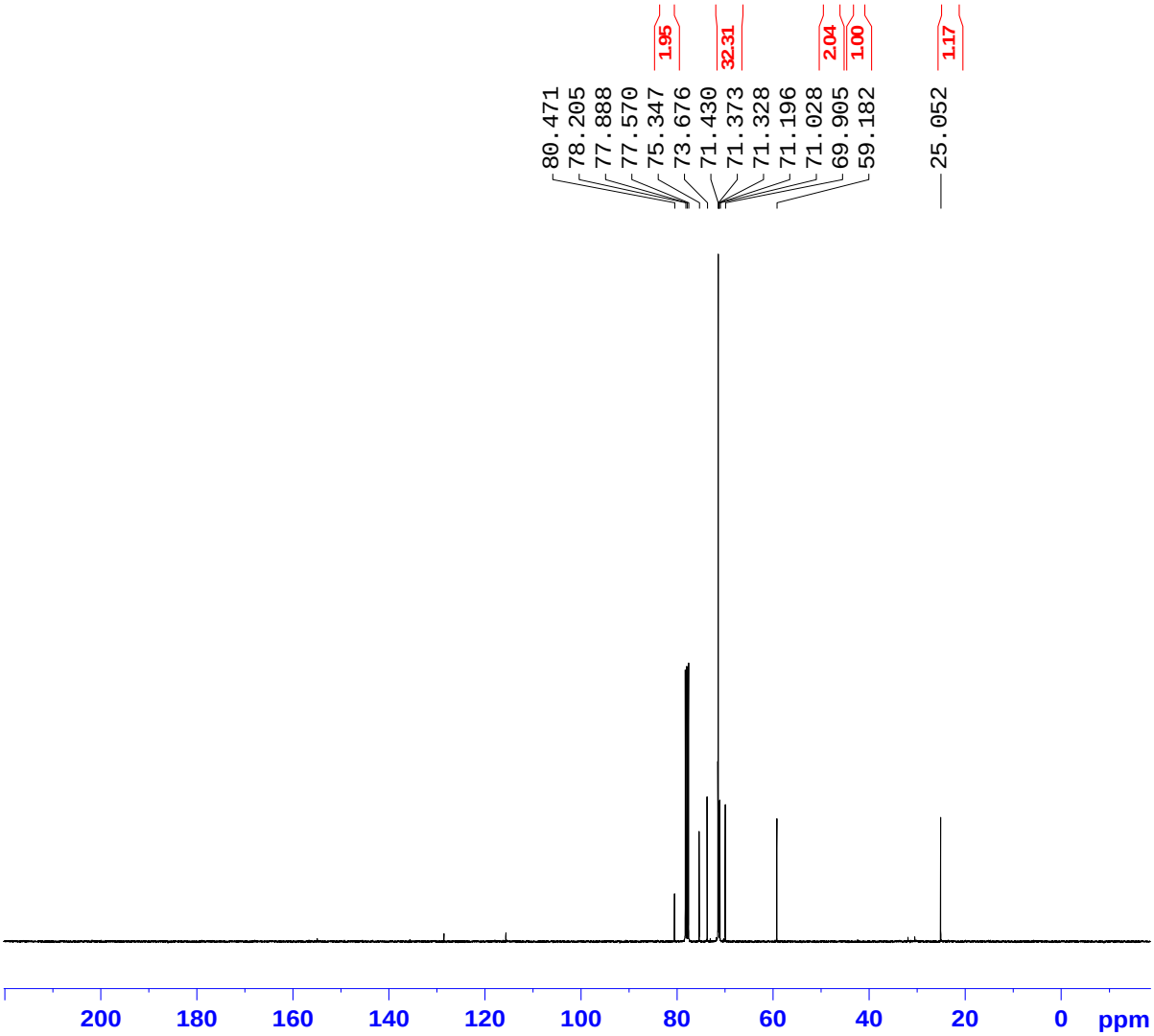
Printed: 16:26, November 01, 2011



7c


```
NAME      LG-820_Alkyne-P8-SH
EXPNO                       1
PROCNO                      1
Date_              20111102
Time                   18.56
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        64
DS                         2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                      71.8
DW                    56.800 usec
DE                     6.50 usec
TE                    292.4 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W            13.81451130 W
SFO1            400.1320007 MHz
SI                     32768
SF              400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



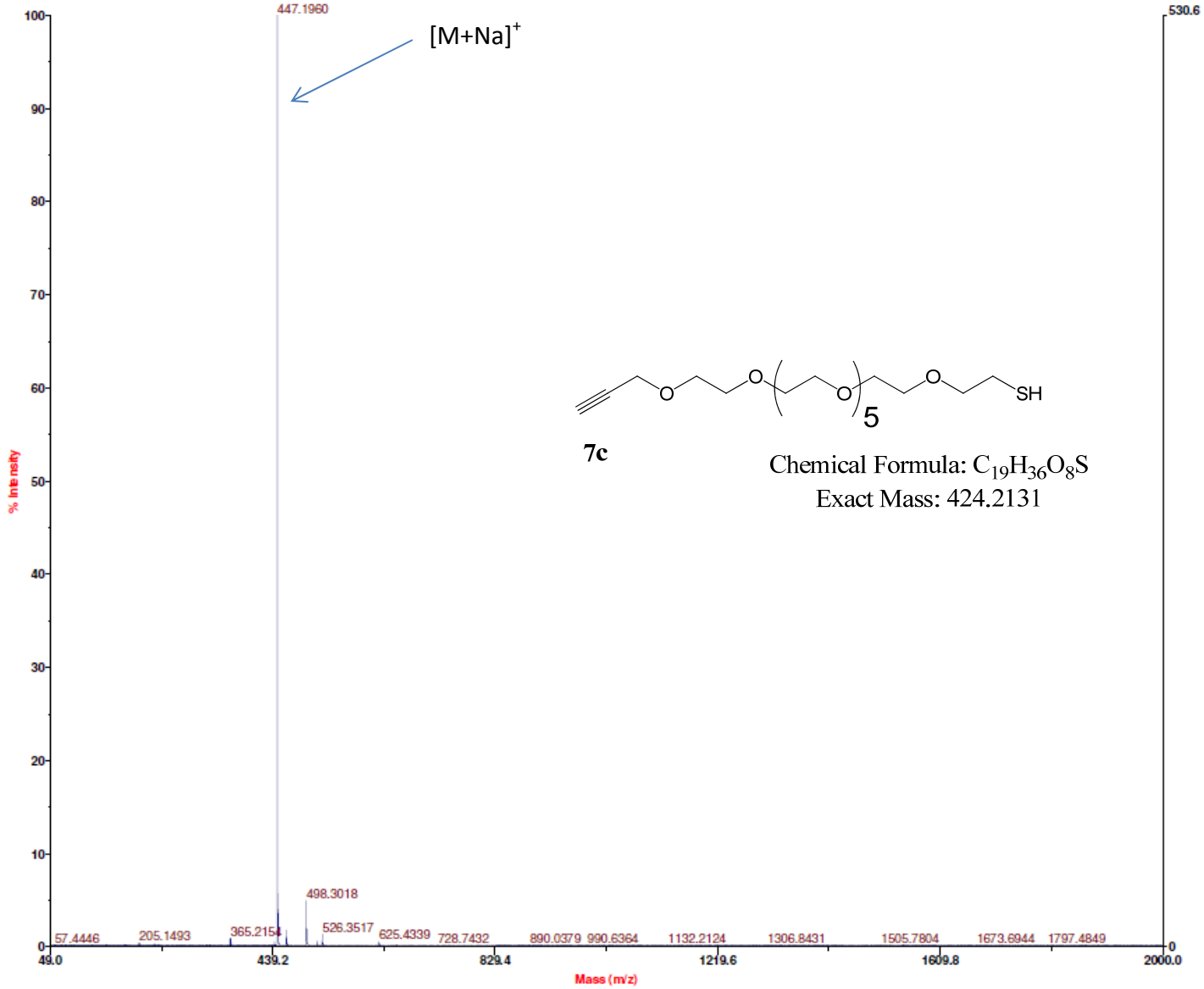

```
NAME      LG-820_Alkyne-P8-SH
EXPNO                       2
PROCNO                      1
Date_              20111102
Time                   22.58
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      2000
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      80.6
DW                    20.800 usec
DE                     6.50 usec
TE                    294.6 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.99 usec
PL1                    -3.00 dB
PL1W            73.67452240 W
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W            13.97447491 W
PL12W            0.54996562 W
PL13W            0.54996562 W
SFO2            400.1316005 MHz
SI                     32768
SF              100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:26 (T /0.00:0.45) ASC[BP = 447.2, 531]



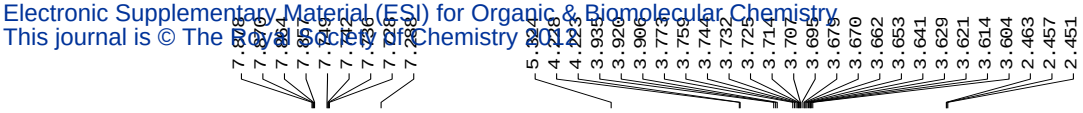
7c

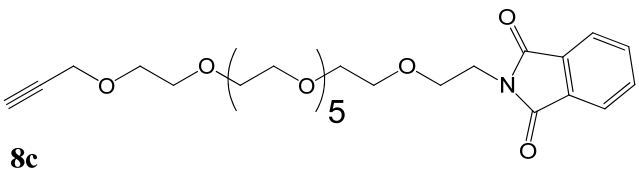
Chemical Formula: $C_{19}H_{36}O_8S$
Exact Mass: 424.2131

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	100.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Nov 03 12:55:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\03 Thur\LNG-820001.dat

Printed: 12:56, November 03, 2011

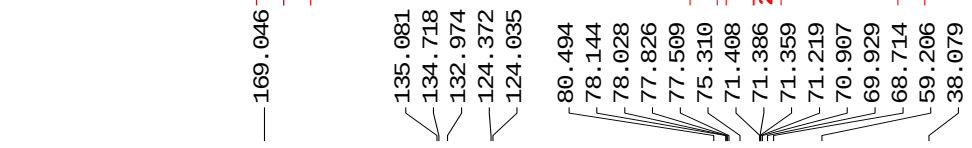


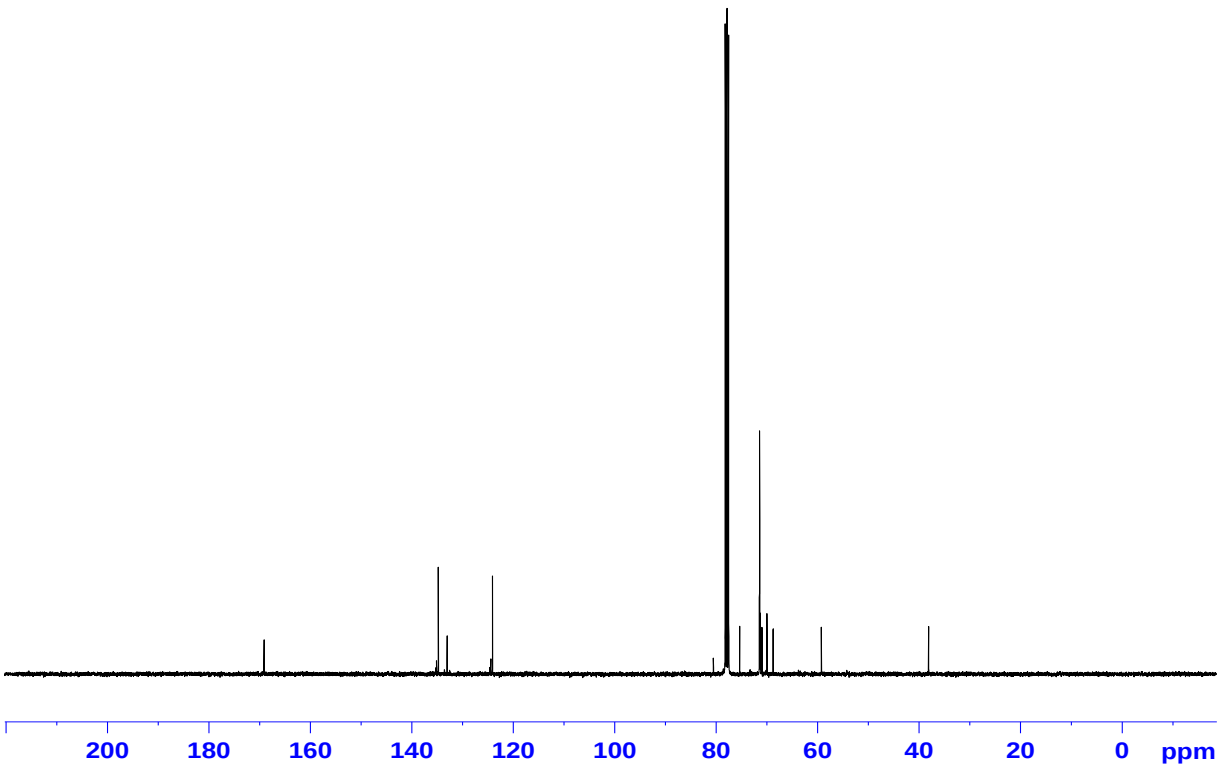


8c


```
NAME      ZH3-048_Alk-P8-NPth
EXPNO                    1
PROCNO                   1
Date_             20110601
Time                 13.16
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                       228
DW                    56.800 usec
DE                     6.50 usec
TE                    292.9 K
D1                 1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W           13.81451130 W
SFO1           400.1320007 MHz
SI                    32768
SF             400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```





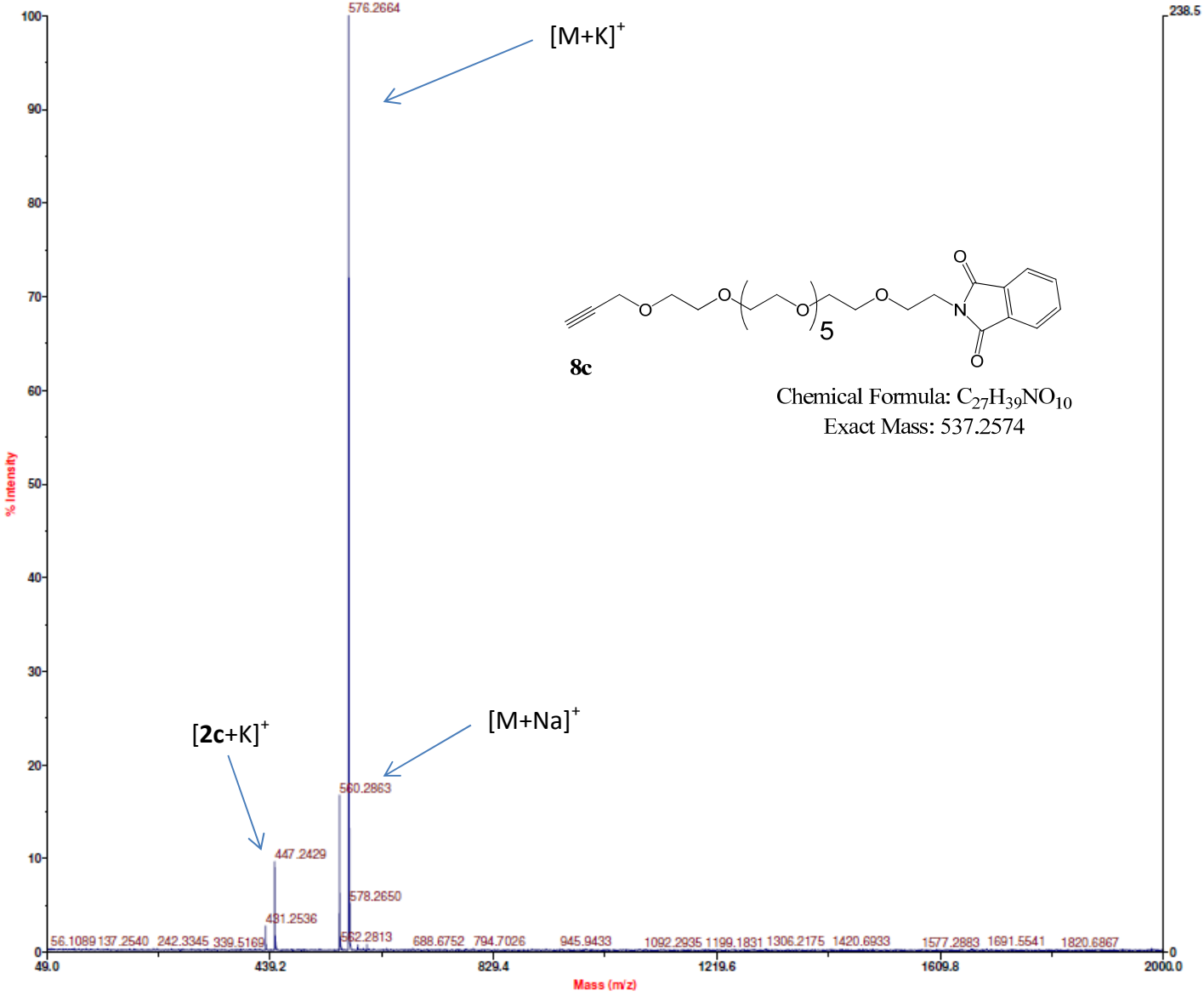

```
NAME      ZH3-048_Alk-P8-NPth
EXPNO                    2
PROCNO                   1
Date_             20110601
Time                 23.01
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                     80.6
DW                    20.800 usec
DE                     6.50 usec
TE                    294.6 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W           73.67452240 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W           13.97447491 W
PL12W           0.54996562 W
PL13W           0.54996562 W
SFO2           400.1316005 MHz
SI                    32768
SF             100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:26 (T /0.00:0.44) ASC[BP = 576.3, 238]



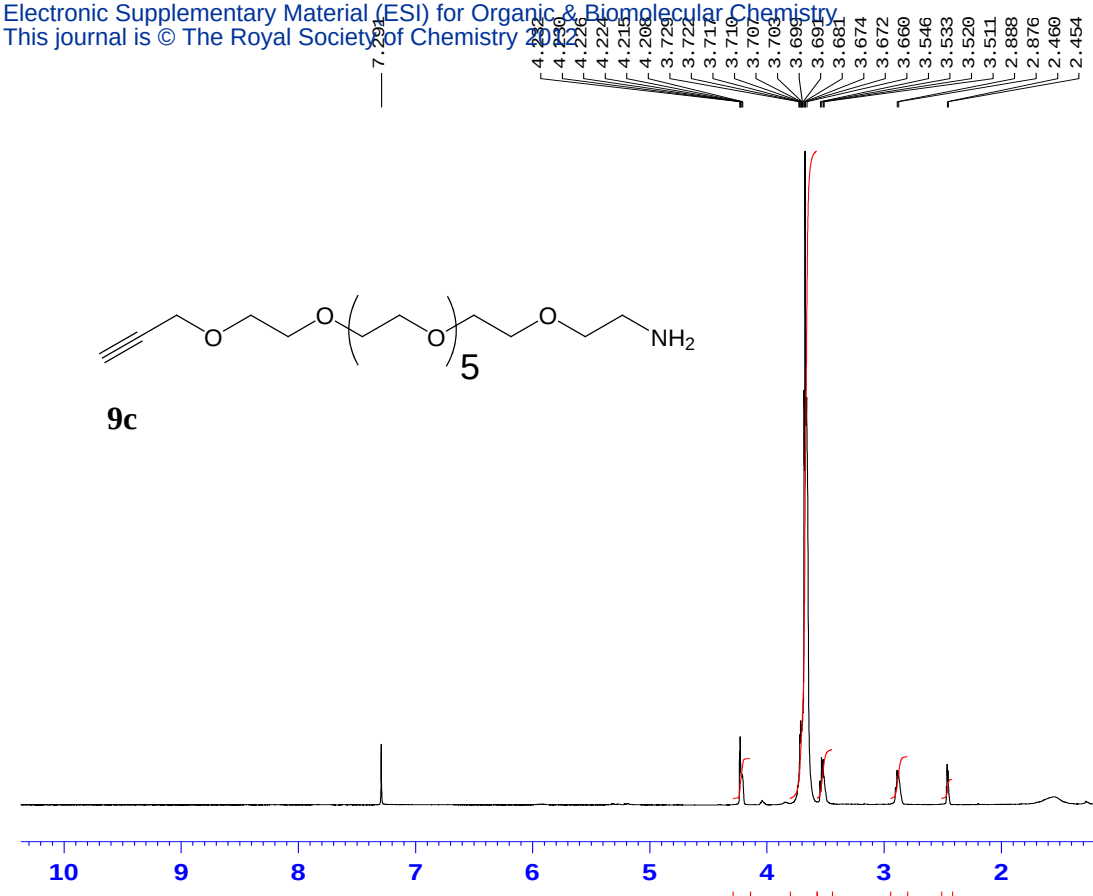
8c

Chemical Formula: $C_{27}H_{39}NO_{10}$
Exact Mass: 537.2574

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0174991E-007
Calibration Constant B	78.221559
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	120.12
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

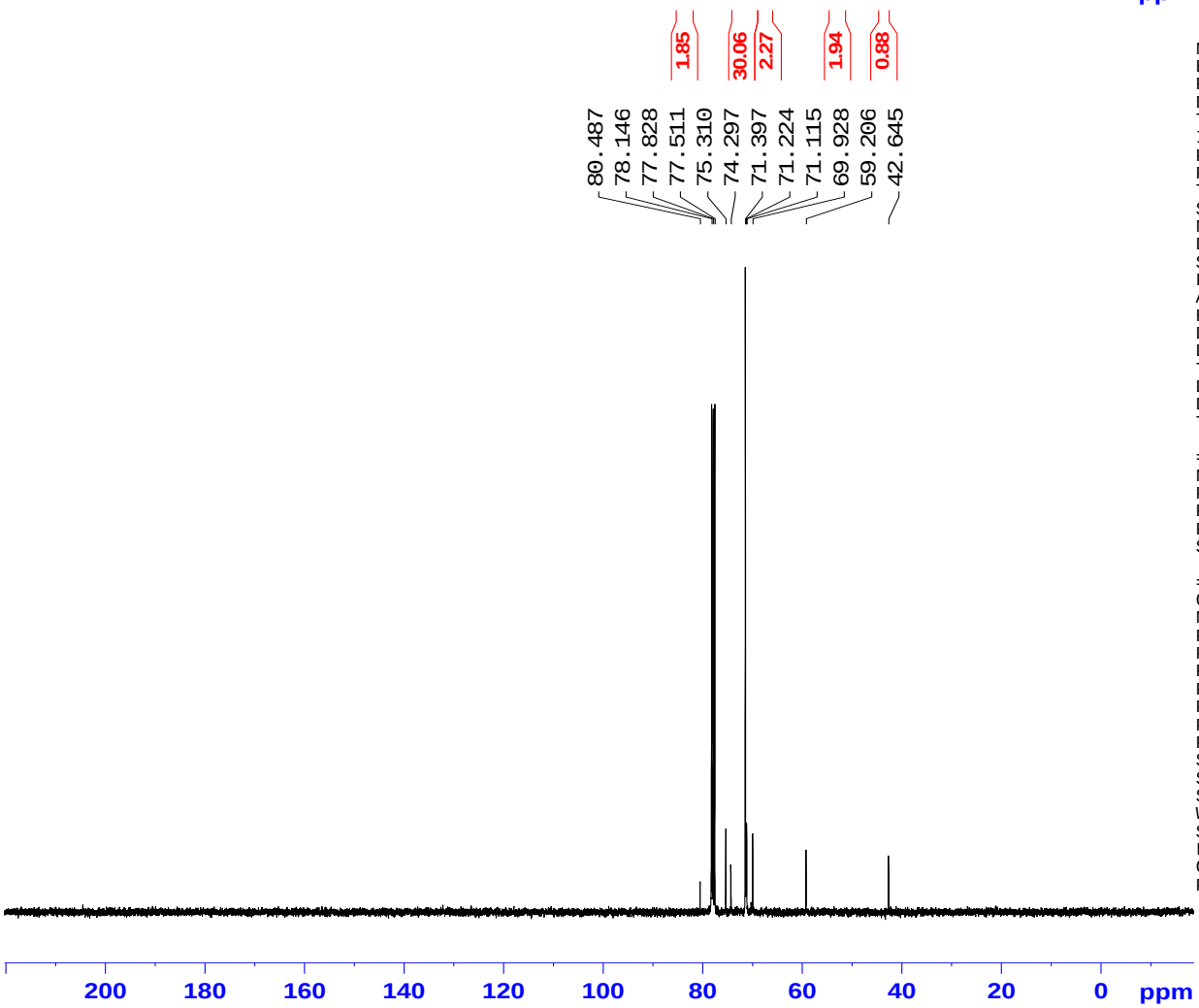
Acquired: May 25 15:34:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\May\25 Wed\LNG-701M001.dat

Printed: 15:37, May 25, 2011




```
NAME      ZH3-061_Alk-P8-NH2
EXPNO                      1
PROCNO                     1
Date_               20110616
Time                   21.44
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                       161
DW                    56.800 usec
DE                     6.50 usec
TE                    292.8 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W              13.81451130 W
SFO1              400.1320007 MHz
SI                     32768
SF                400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



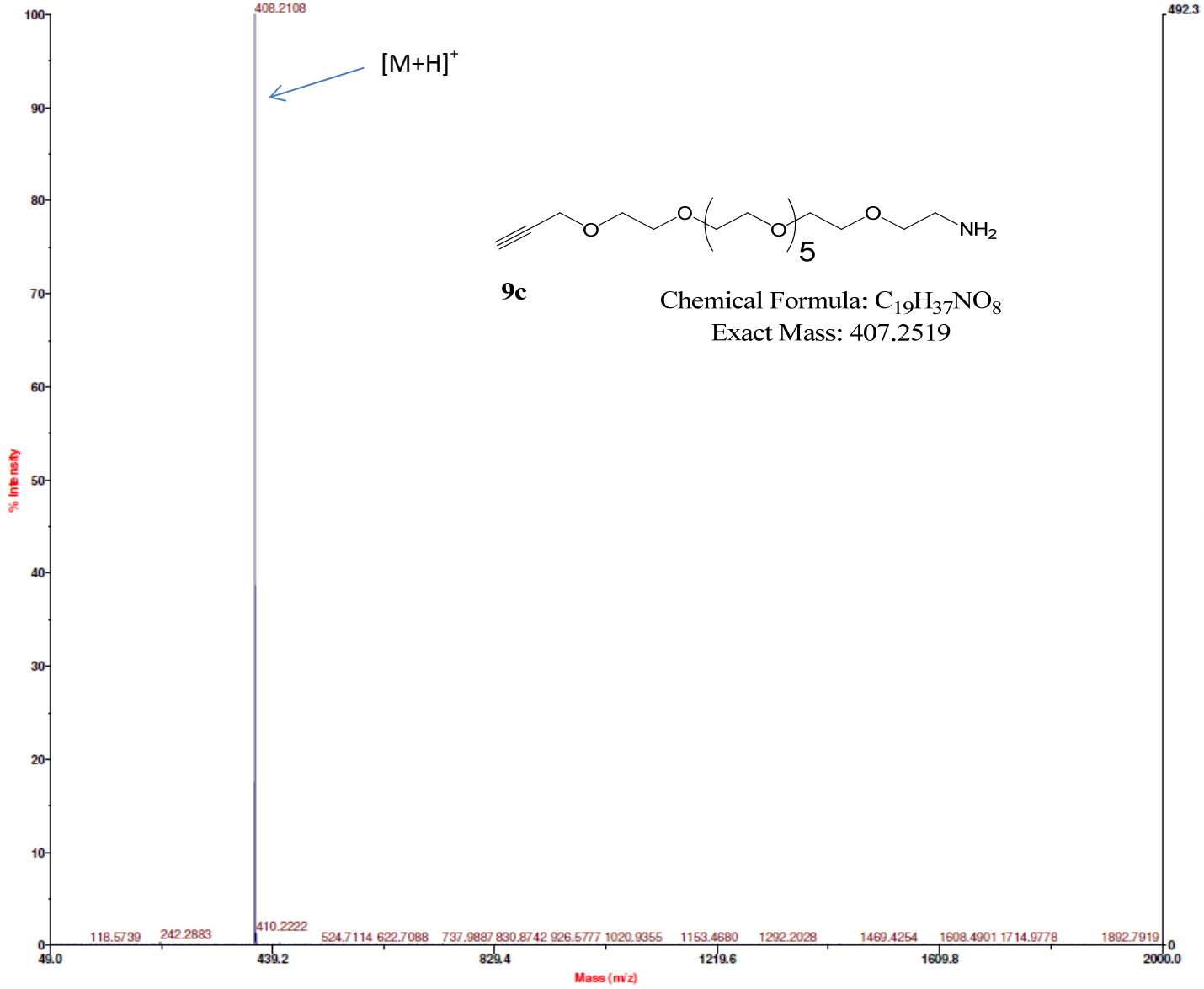

```
NAME      ZH3-061_Alk-P8-NH2
EXPNO                      2
PROCNO                     1
Date_               20110616
Time                   22.45
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       812
DW                    20.800 usec
DE                     6.50 usec
TE                    294.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                     9.99 usec
PL1                   -3.00 dB
PL1W              73.67452240 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W              13.97447491 W
PL12W              0.54996562 W
PL13W              0.54996562 W
SFO2             400.1316005 MHz
SI                     32768
SF               100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:23 (T /0.00:0.39) ASC[BP = 408.2, 492]



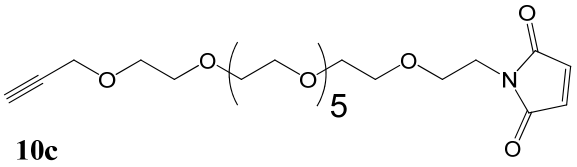
9c

Chemical Formula: $C_{19}H_{37}NO_8$
Exact Mass: 407.2519

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0126144E-007
Calibration Constant B	71.956893
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	149.90
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Aug 05 09:47:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Aug\05 Fri\ZH3-087001.dat

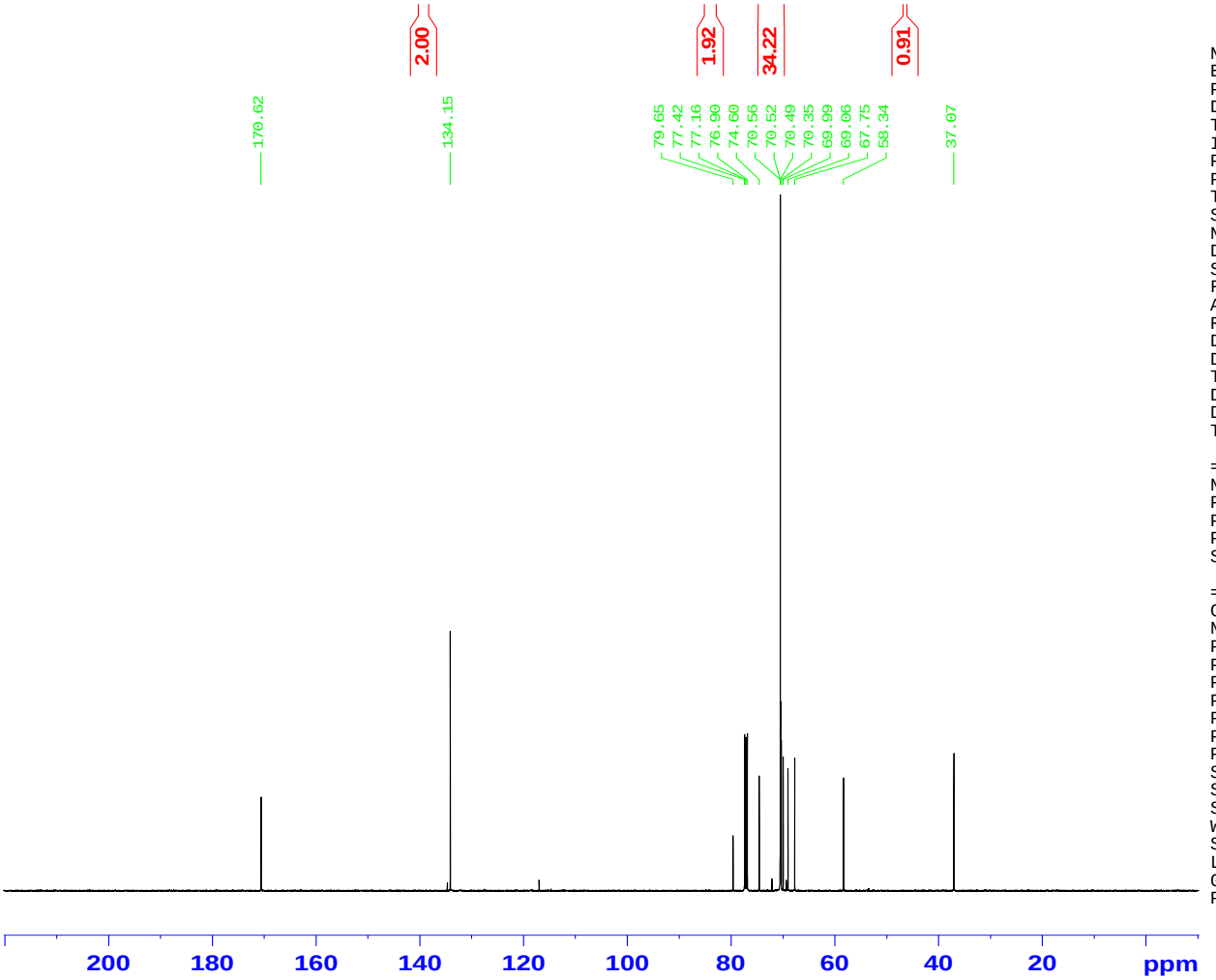
Printed: 09:48, August 05, 2011



10c


```
NAME      LG-725_Alkyne-P8-Maleimide
EXPNO                  1
PROCNO                 1
Date_           20110624
Time               12.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8802.817 Hz
FIDRES          0.134320 Hz
AQ              3.7224948 sec
RG                  22.6
DW                56.800 usec
DE                 6.50 usec
TE                292.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.85 usec
PL1               -0.60 dB
PL1W         13.81451130 W
SFO1         400.1320007 MHz
SI                 32768
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```



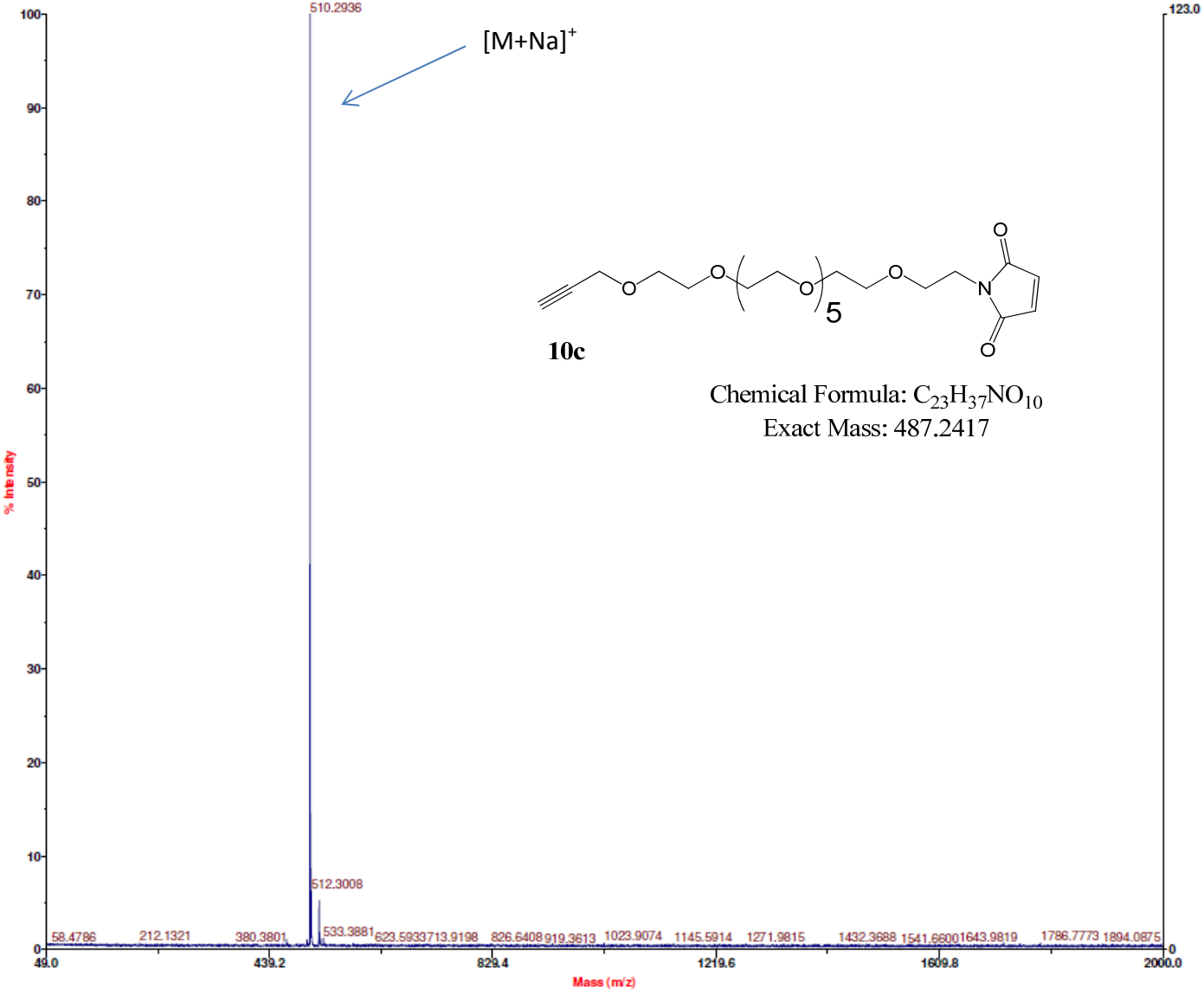

```
NAME      LG-725_Alk-P8-Mal
EXPNO                  2
PROCNO                 1
Date_           20111229
Time               14.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            28985.508 Hz
FIDRES          0.442284 Hz
AQ              1.1305633 sec
RG                  4096
DW                17.250 usec
DE                 6.50 usec
TE                296.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.83 usec
PL1                0.00 dB
PL1W         80.88274384 W
SFO1         125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 1.20 dB
PL12               15.40 dB
PL13               15.40 dB
PL2W         17.72078514 W
PL12W         0.67372549 W
PL13W         0.67372549 W
SFO2         500.1320005 MHz
SI                 32768
SF           125.7577890 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:29 (T /0.00:0.50) ASC[BP = 510.3, 123]



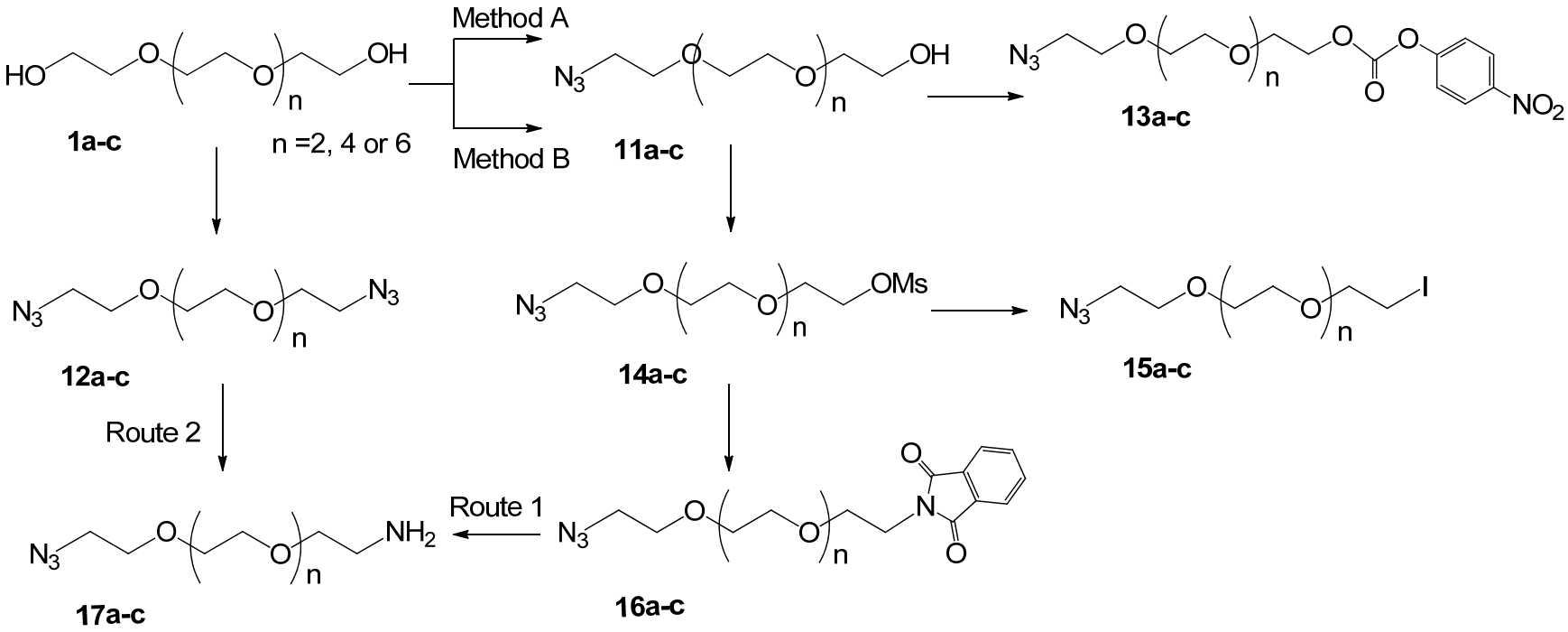
10c

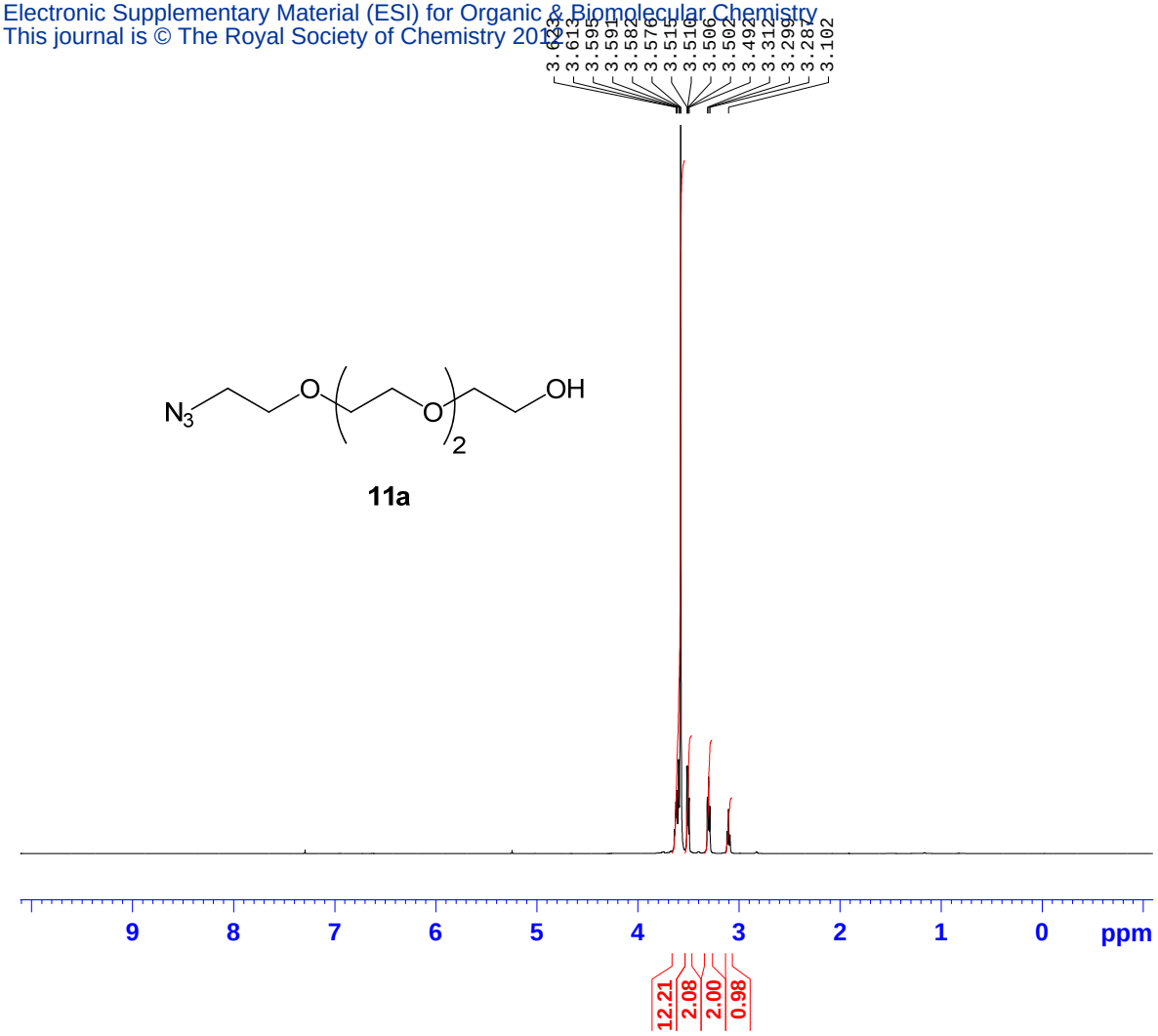
Chemical Formula: $C_{23}H_{37}NO_{10}$
Exact Mass: 487.2417

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0174991E-007
Calibration Constant B	78.221559
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Jun 24 15:09:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Jun\24 Fri\LNG-725001.dat

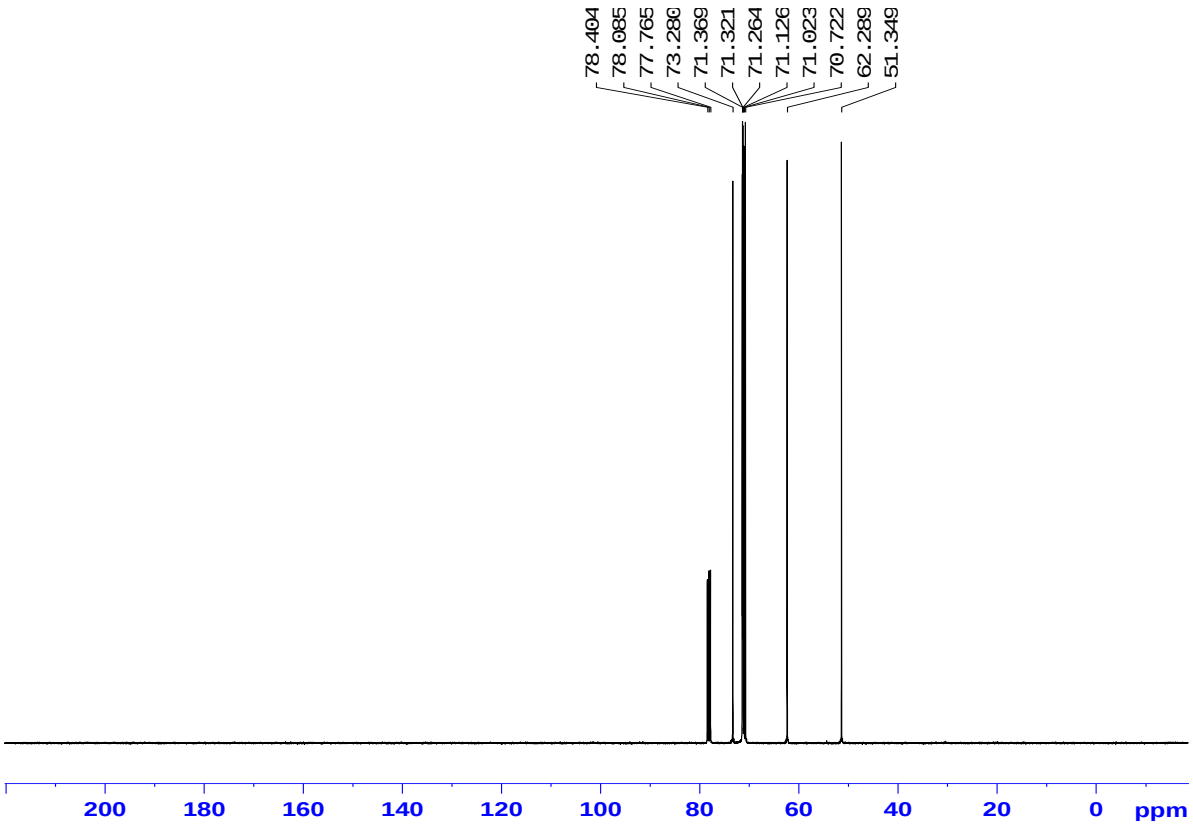
Printed: 15:10, June 24, 2011






```
NAME      ZH3-123-P_N3-P4-OH
EXPNO                      1
PROCNO                     1
Date_               20111010
Time                   21.04
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8802.817 Hz
FIDRES              0.134320 Hz
AQ                  3.7224948 sec
RG                        18
DW                     56.800 usec
DE                      6.50 usec
TE                     292.6 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W               13.81451130 W
SFO1               400.1320007 MHz
SI                     32768
SF                 400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



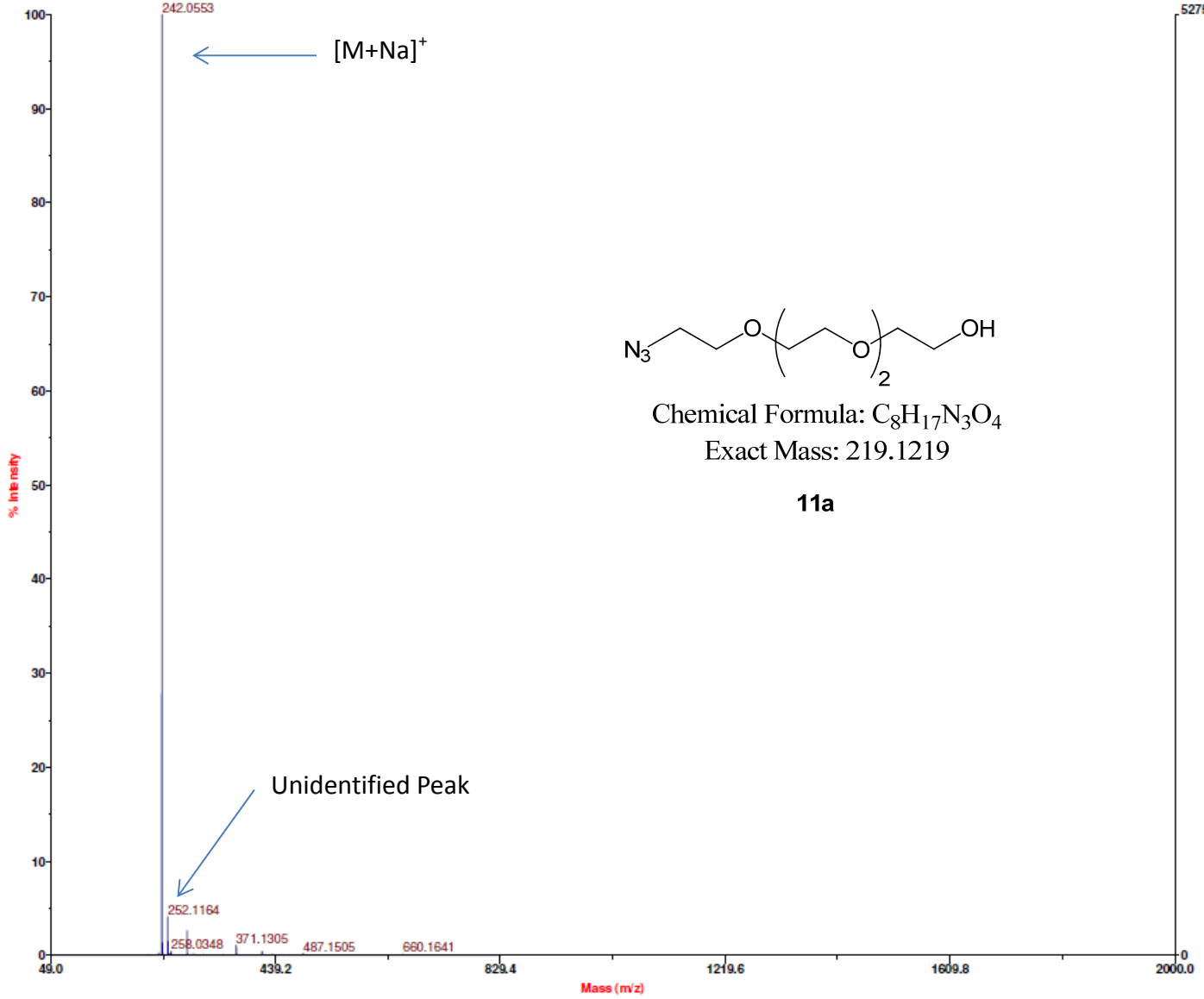

```
NAME      ZH3-123-P_N3-P4-OH
EXPNO                      2
PROCNO                     1
Date_               20111010
Time                   22.05
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       812
DW                     20.800 usec
DE                      6.50 usec
TE                     294.4 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.99 usec
PL1                    -3.00 dB
PL1W               73.67452240 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W               13.97447491 W
PL12W               0.54996562 W
PL13W               0.54996562 W
SFO2               400.1316005 MHz
SI                     32768
SF                 100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:46 (T /0.00:0.81) ASC[BP = 242.1, 5275]



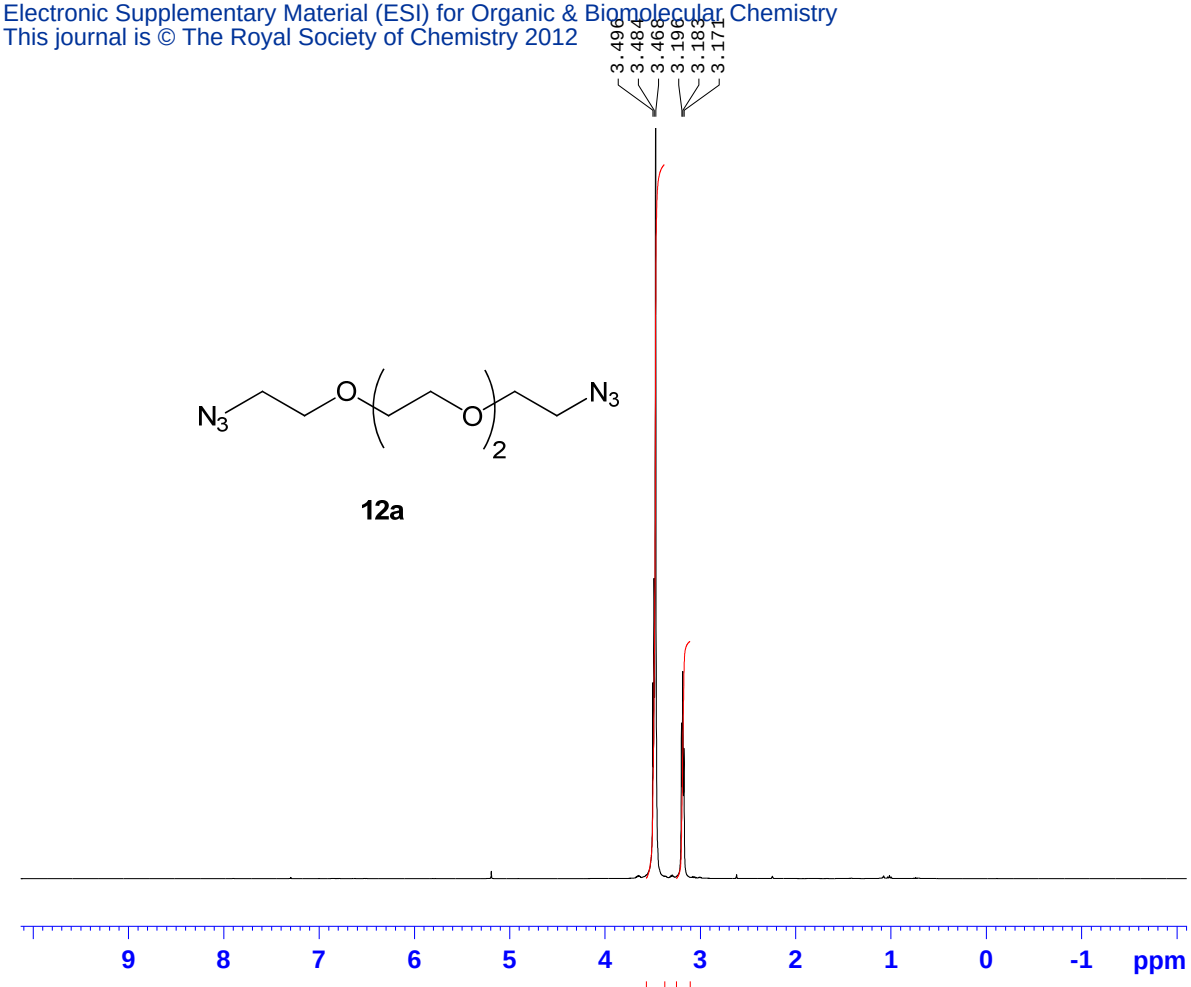
Chemical Formula: $C_8H_{17}N_3O_4$
Exact Mass: 219.1219

11a

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

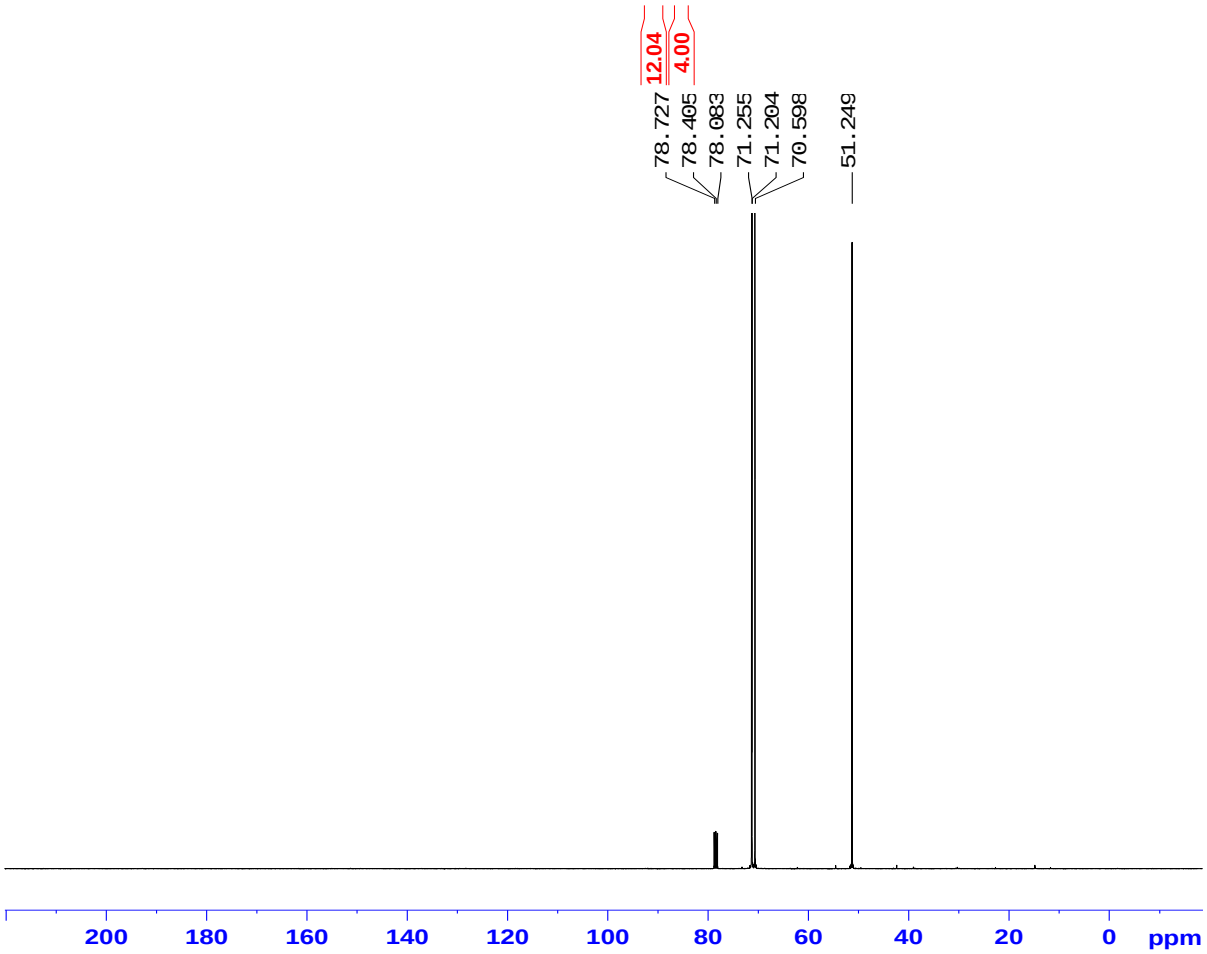
Acquired: Oct 11 11:20:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\11 Tue\ZH3-123001.dat

Printed: 11:22, October 11, 2011




```
NAME      ZH3-123-A_N3-P4-N3
EXPNO                    1
PROCNO                   1
Date_             20111007
Time                 14.08
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                      9
DW                 56.800 usec
DE                  6.50 usec
TE                 292.9 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.85 usec
PL1                 -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



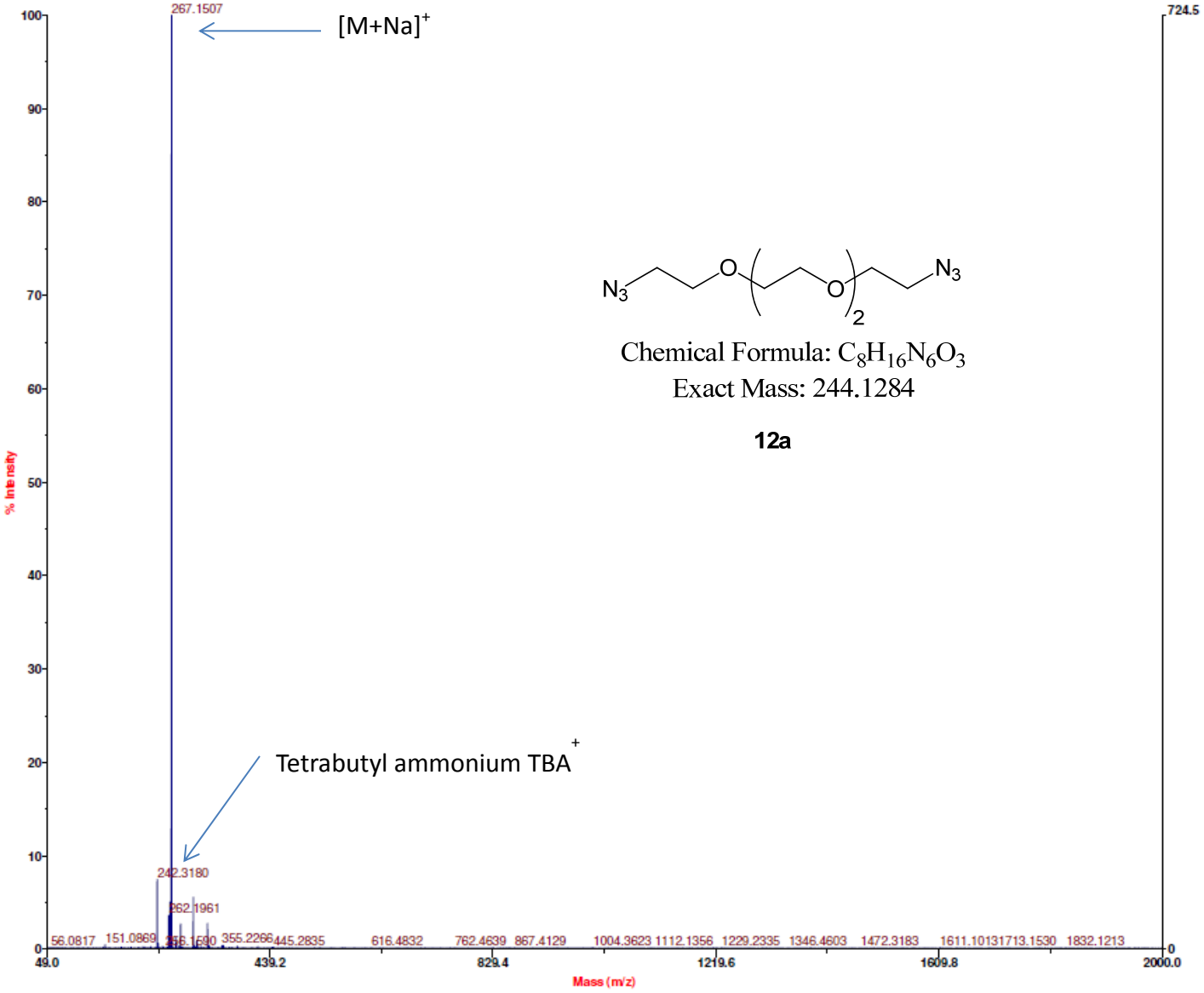

```
NAME      ZH3-123-A_N3-P4-N3
EXPNO                    2
PROCNO                   1
Date_             20111007
Time                 22.02
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    812
DW                 20.800 usec
DE                  6.50 usec
TE                 294.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.99 usec
PL1                 -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -0.65 dB
PL12                13.40 dB
PL13                13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6126885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:28 (T /0.00:0.48) ASC[BP = 267.2, 724]



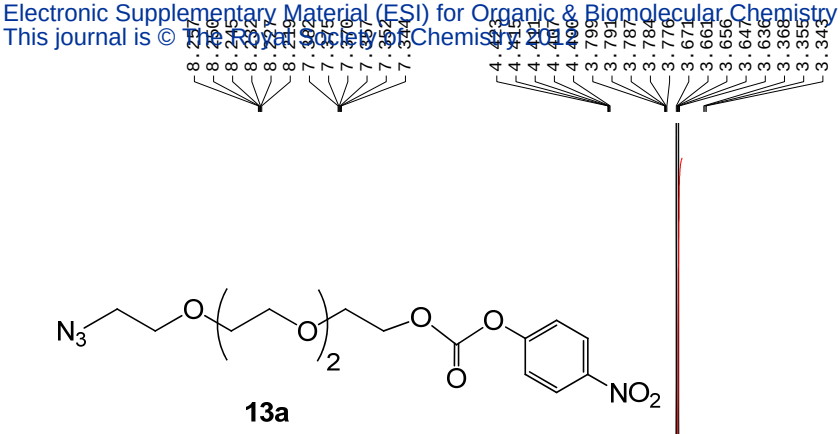
Chemical Formula: $C_8H_{16}N_6O_3$
Exact Mass: 244.1284

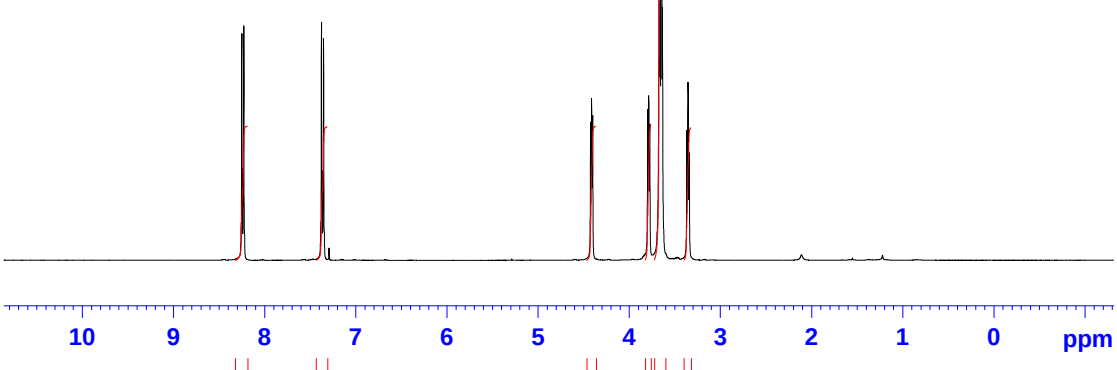
12a

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Dec 29 15:52:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\29 Thur\SJS-PEG4-diazide002.dat

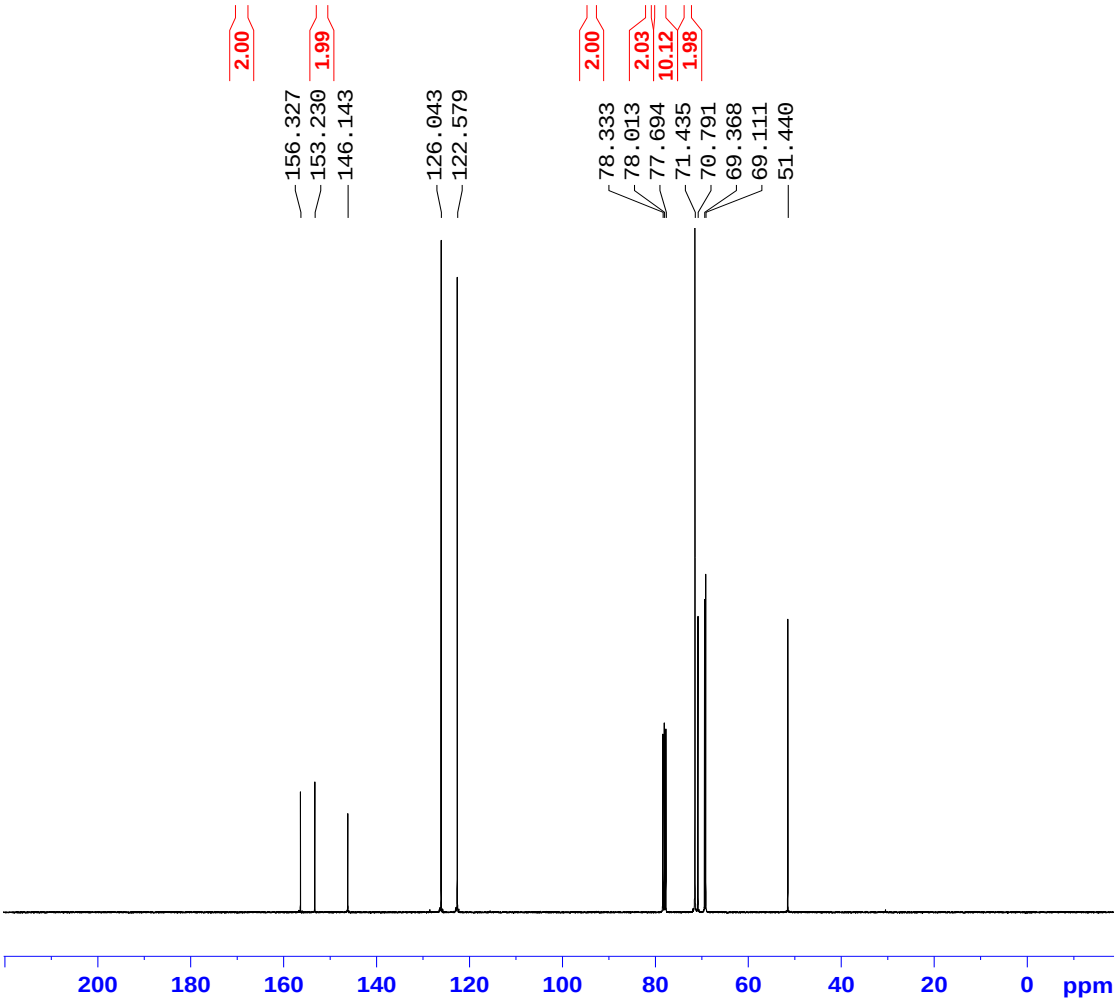
Printed: 15:53, December 29, 2011






```
NAME      ZH3-124-P_N3-P4-PNPC
EXPNO                    1
PROCNO                   1
Date_             20111012
Time                 21.23
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                      25.4
DW                    56.800 usec
DE                     6.50 usec
TE                    292.8 K
D1                 1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.85 usec
PL1                   -0.60 dB
PL1W             13.81451130 W
SFO1             400.1320007 MHz
SI                    32768
SF               400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



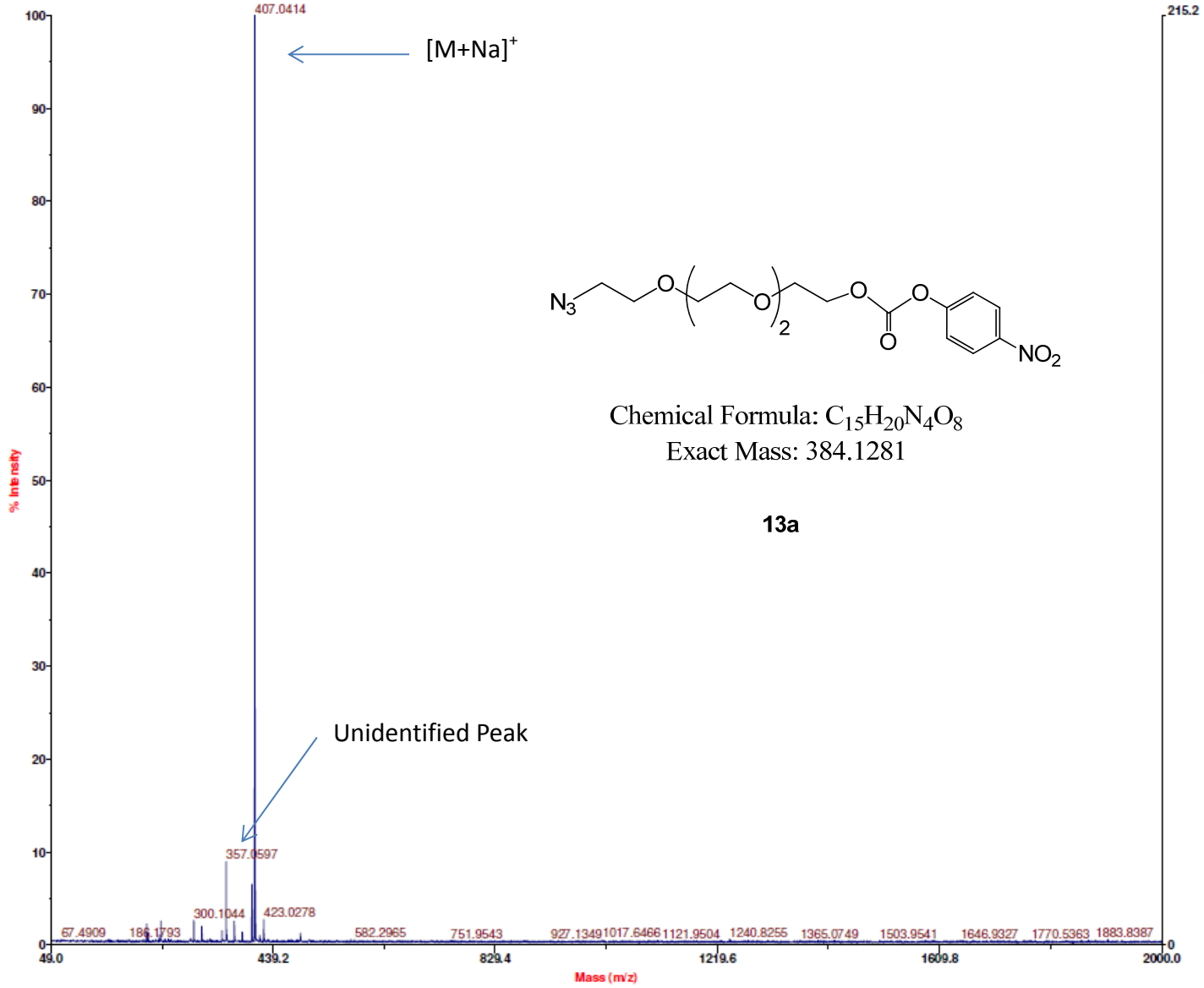

```
NAME      ZH3-124-P_N3-P4-PNPC
EXPNO                    2
PROCNO                   1
Date_             20111012
Time                 23.23
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      80.6
DW                    20.800 usec
DE                     6.50 usec
TE                    294.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.99 usec
PL1                   -3.00 dB
PL1W             73.67452240 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -0.65 dB
PL12                  13.40 dB
PL13                  13.40 dB
PL2W             13.97447491 W
PL12W             0.54996562 W
PL13W             0.54996562 W
SFO2             400.1316005 MHz
SI                    32768
SF               100.6126885 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:28 (T /0.00:0.48) ASC[BP = 407.0, 215]



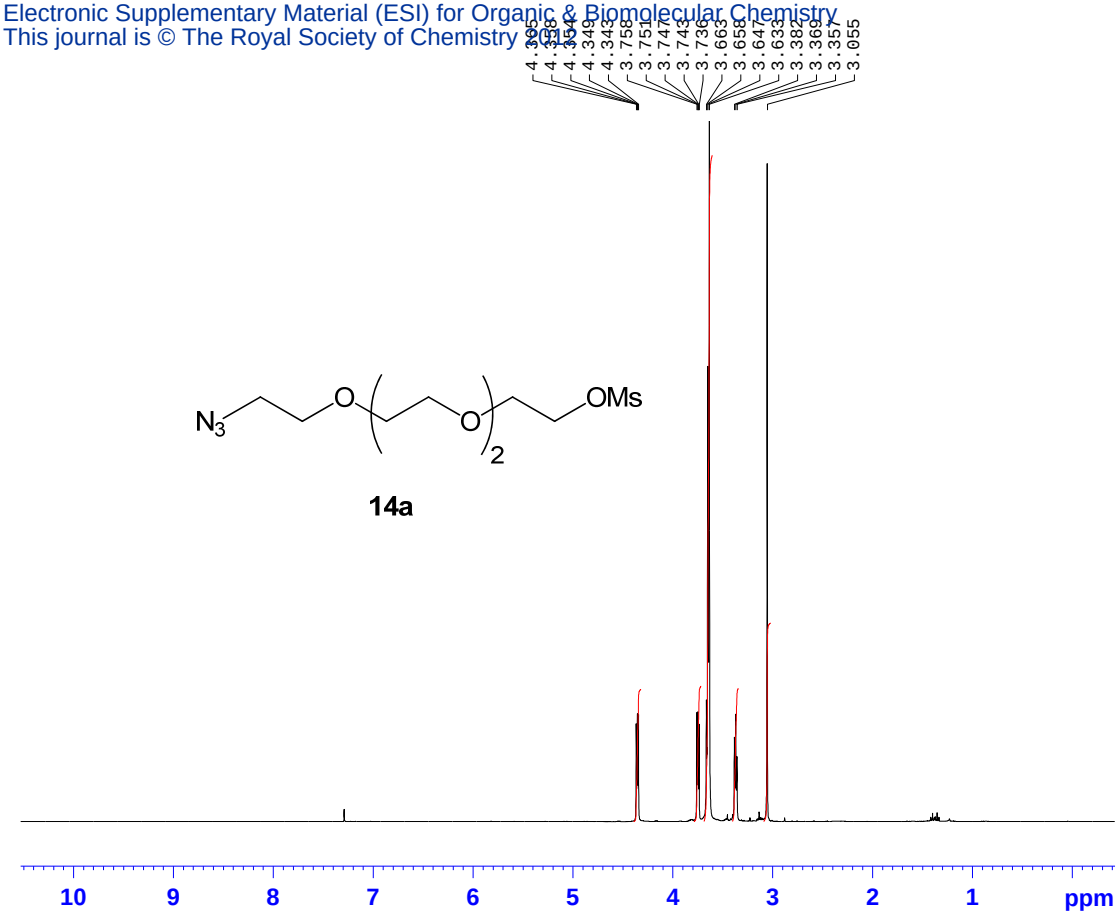
Chemical Formula: $C_{15}H_{20}N_4O_8$
Exact Mass: 384.1281

13a

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

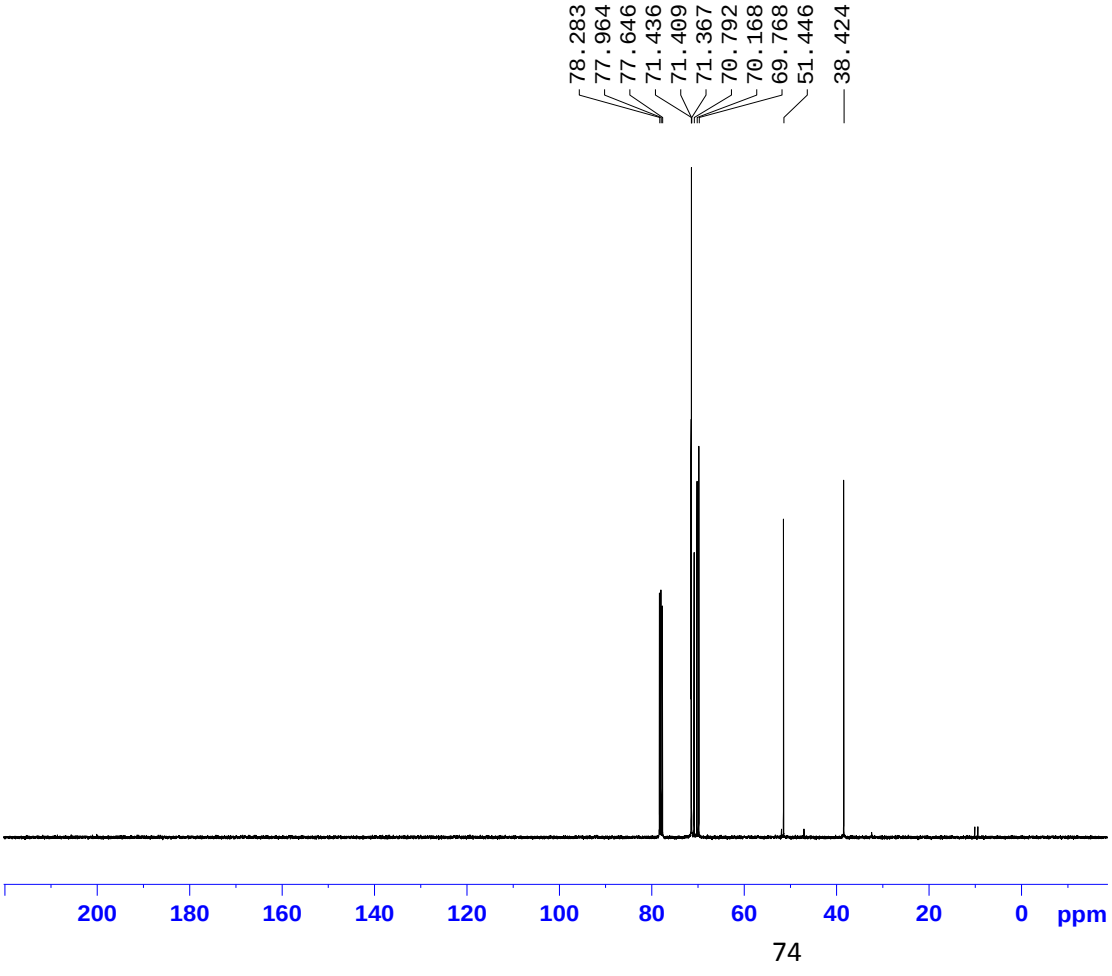
Acquired: Oct 14 09:16:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\14 Fri\ZH3-124001.dat

Printed: 09:17, October 14, 2011




```
NAME      LG-799M_N3-TEG-OMs
EXPNO                    4
PROCNO                   1
Date_             20111012
Time                 11.01
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                   28.5
DW                 56.800 usec
DE                  6.50 usec
TE                 292.3 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.85 usec
PL1                 -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



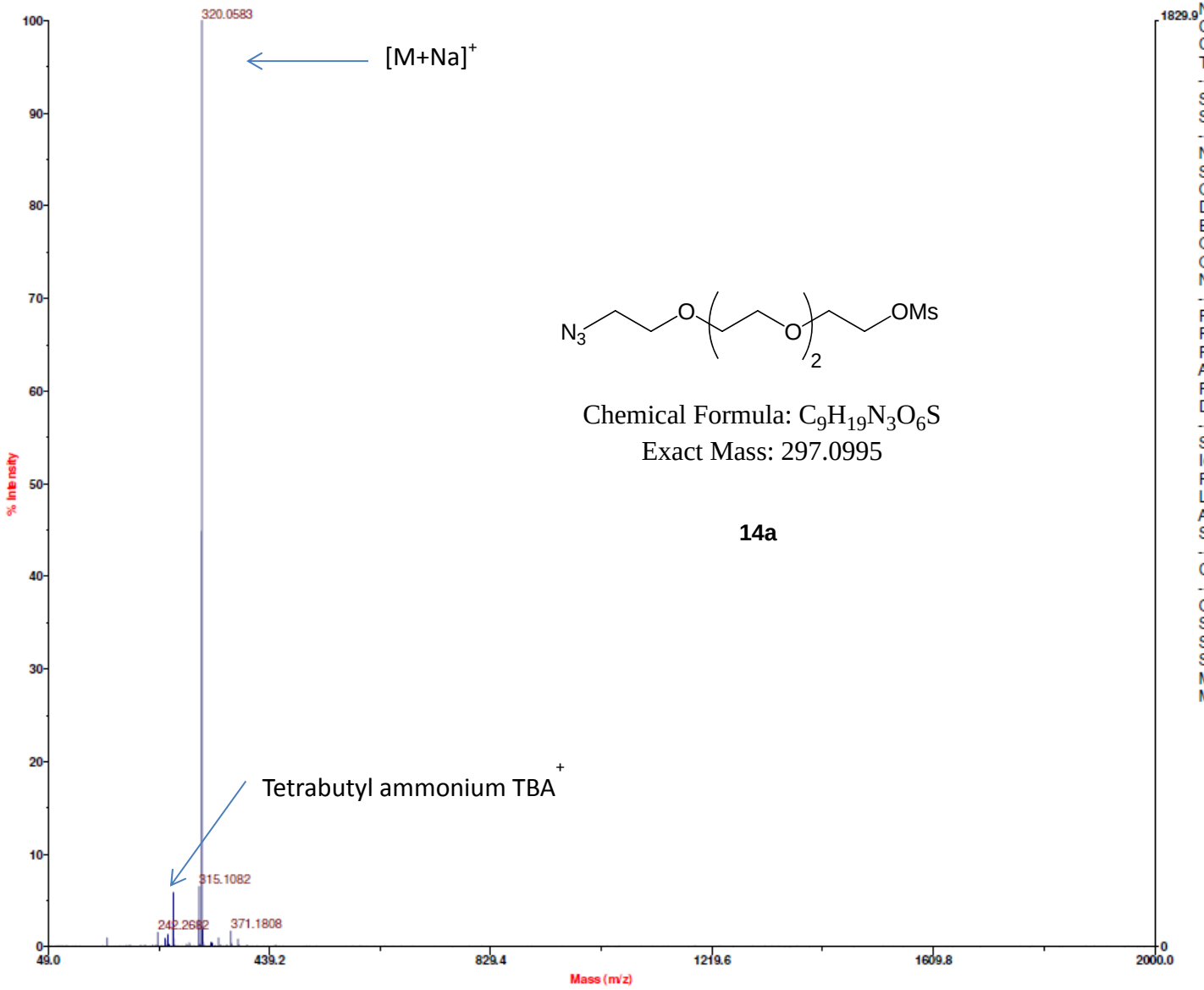

```
NAME      LG-799M_N3-TEG-OMs
EXPNO                    5
PROCNO                   1
Date_             20111012
Time                 11.57
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    512
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   80.6
DW                 20.800 usec
DE                  6.50 usec
TE                 294.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.99 usec
PL1                 -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -0.65 dB
PL12                13.40 dB
PL13                13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6126885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:25 (T /0.00:0.43) ASC[BP = 320.1, 1830]



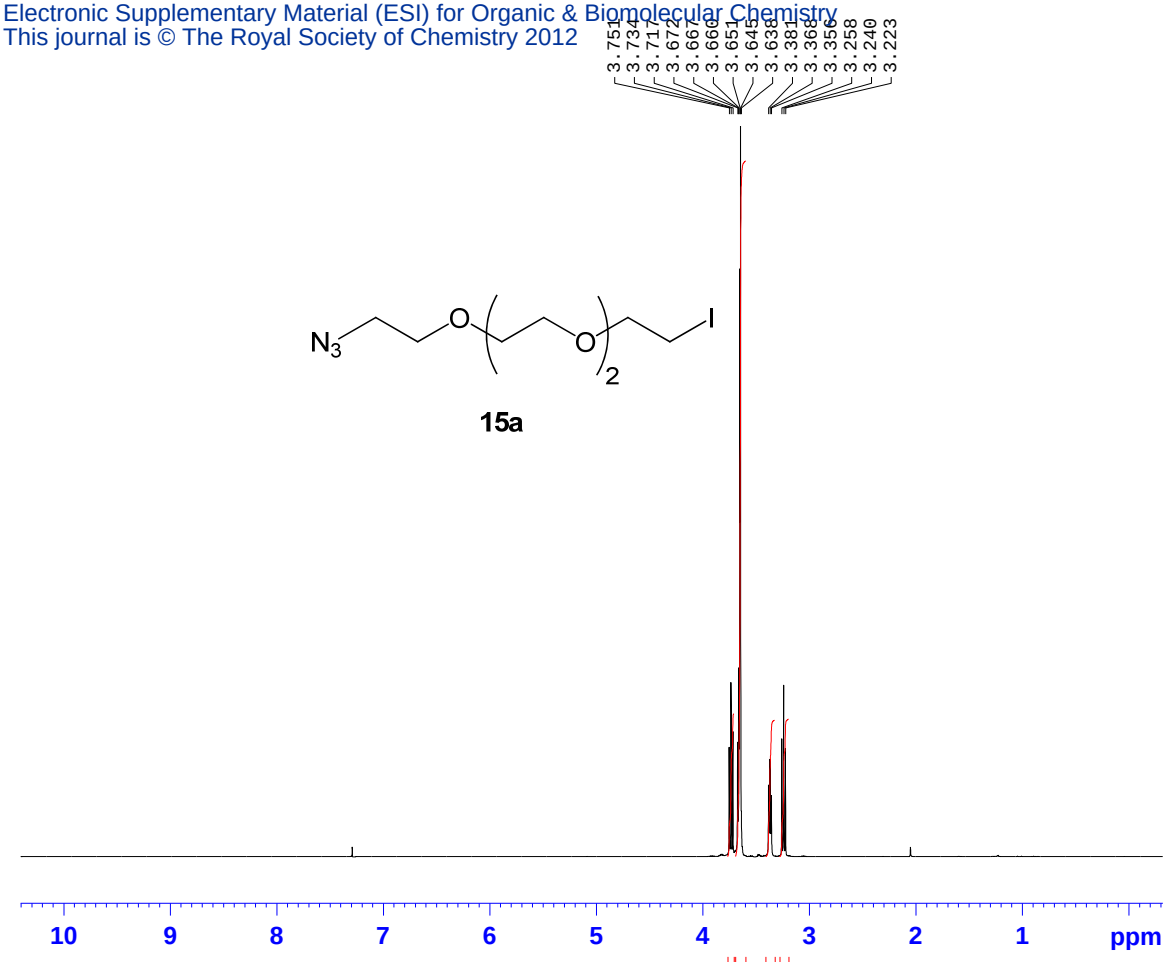
Chemical Formula: $C_9H_{19}N_3O_6S$
Exact Mass: 297.0995

14a

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

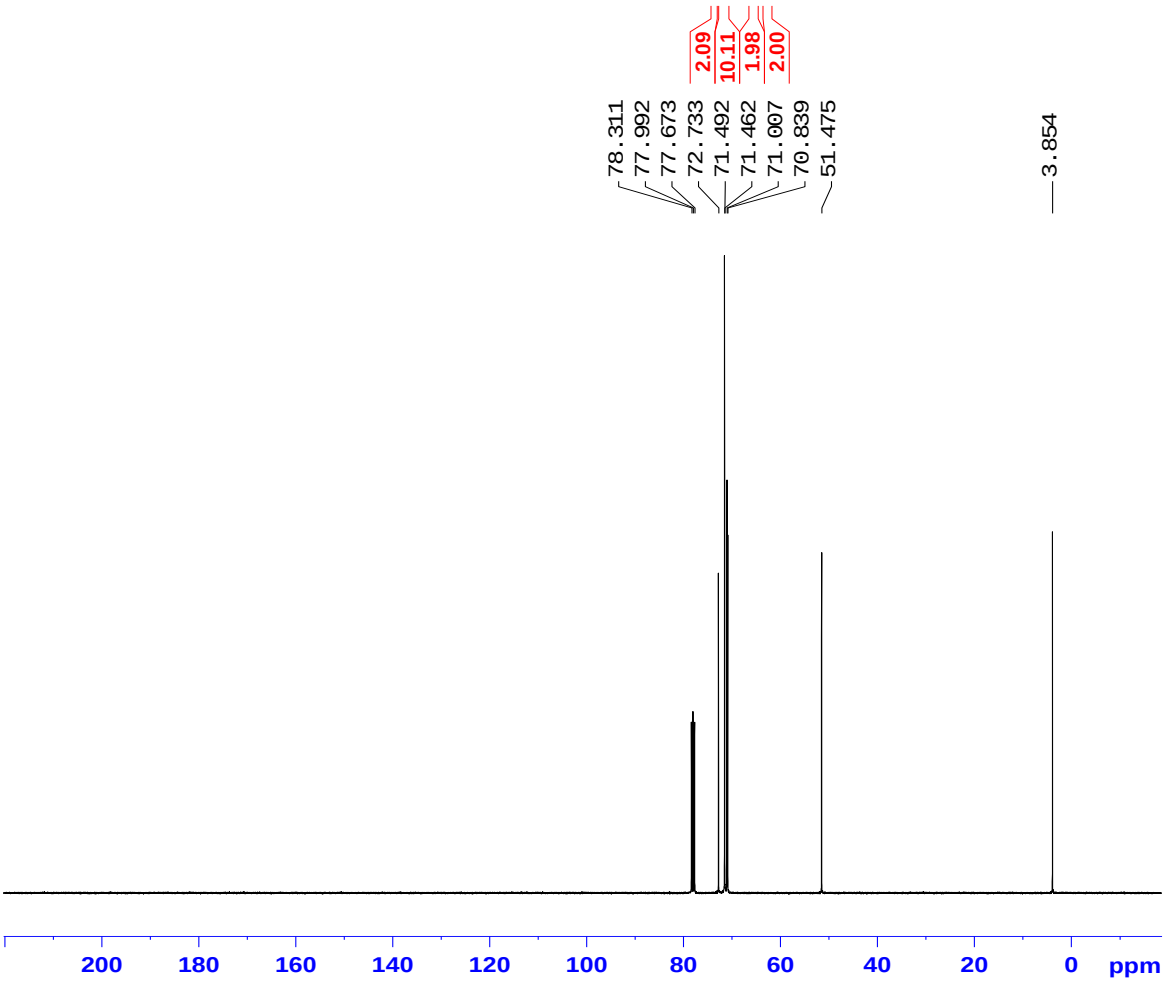
Acquired: Oct 13 11:20:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\13 Thur\LNG-799M002.dat

Printed: 11:21, October 13, 2011




```
NAME      LG-802_N3-TEG-Iodo
EXPNO                    1
PROCNO                   1
Date_             20111012
Time                 20.16
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                    28.5
DW                  56.800 usec
DE                   6.50 usec
TE                  292.6 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



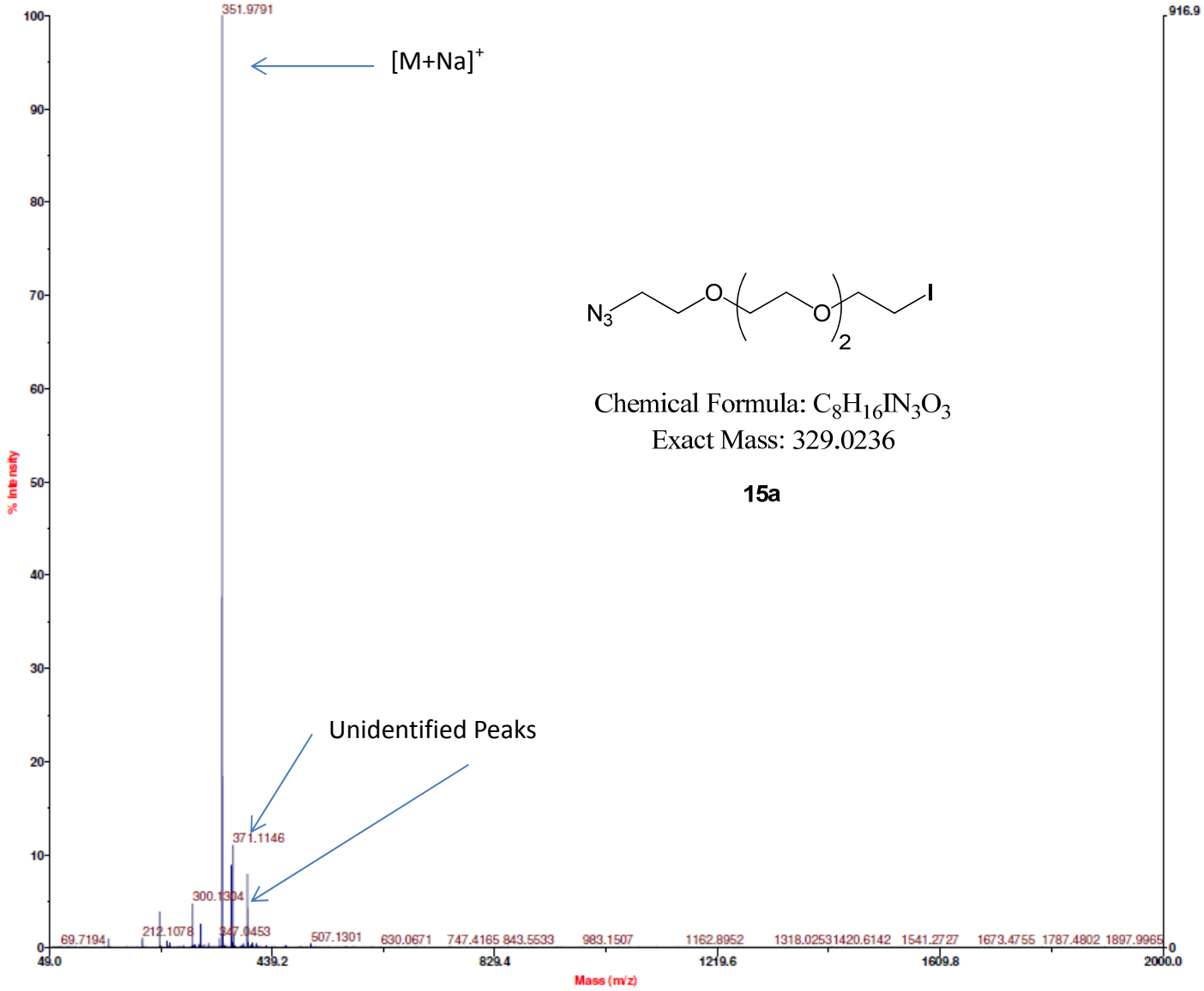

```
NAME      LG-802_N3-TEG-Iodo
EXPNO                    2
PROCNO                   1
Date_             20111012
Time                 21.17
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     912
DW                  20.800 usec
DE                   6.50 usec
TE                  294.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:35 (T /0.00:0.61) ASC[BP = 352.0, 917]



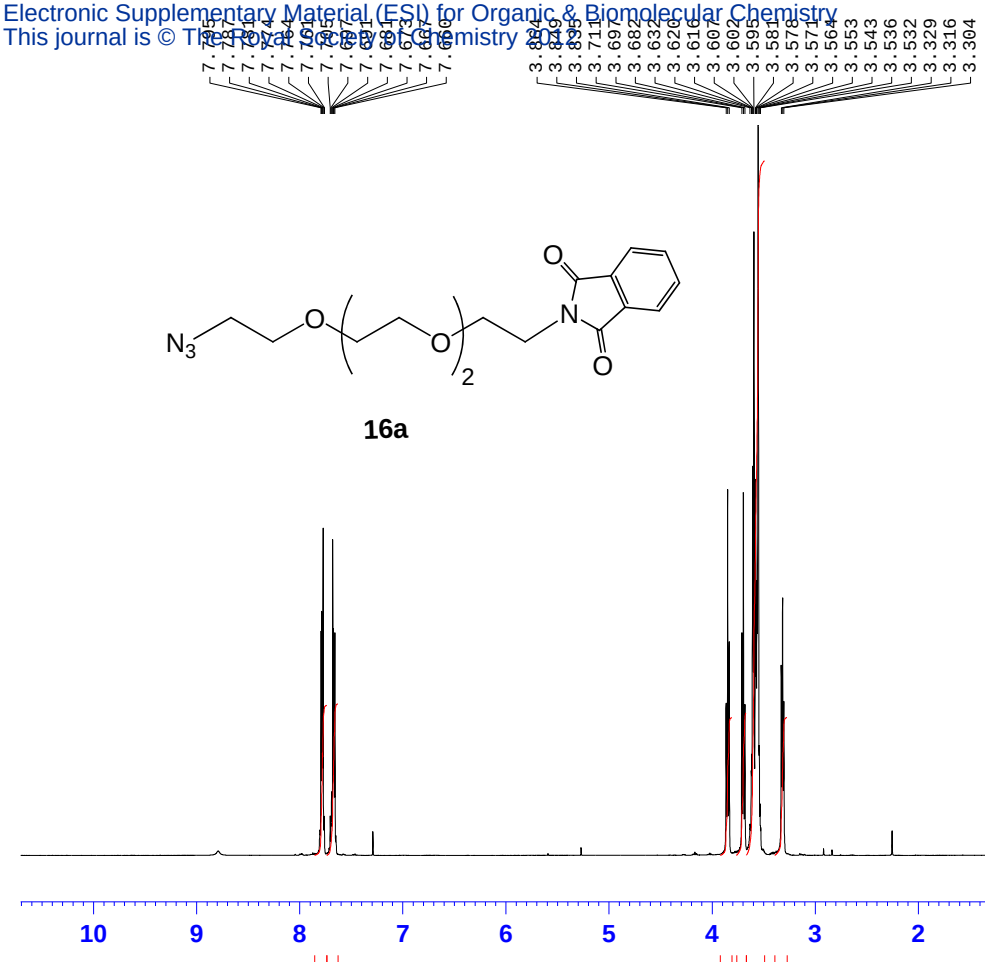
Chemical Formula: $C_8H_{16}IN_3O_3$
Exact Mass: 329.0236

15a

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

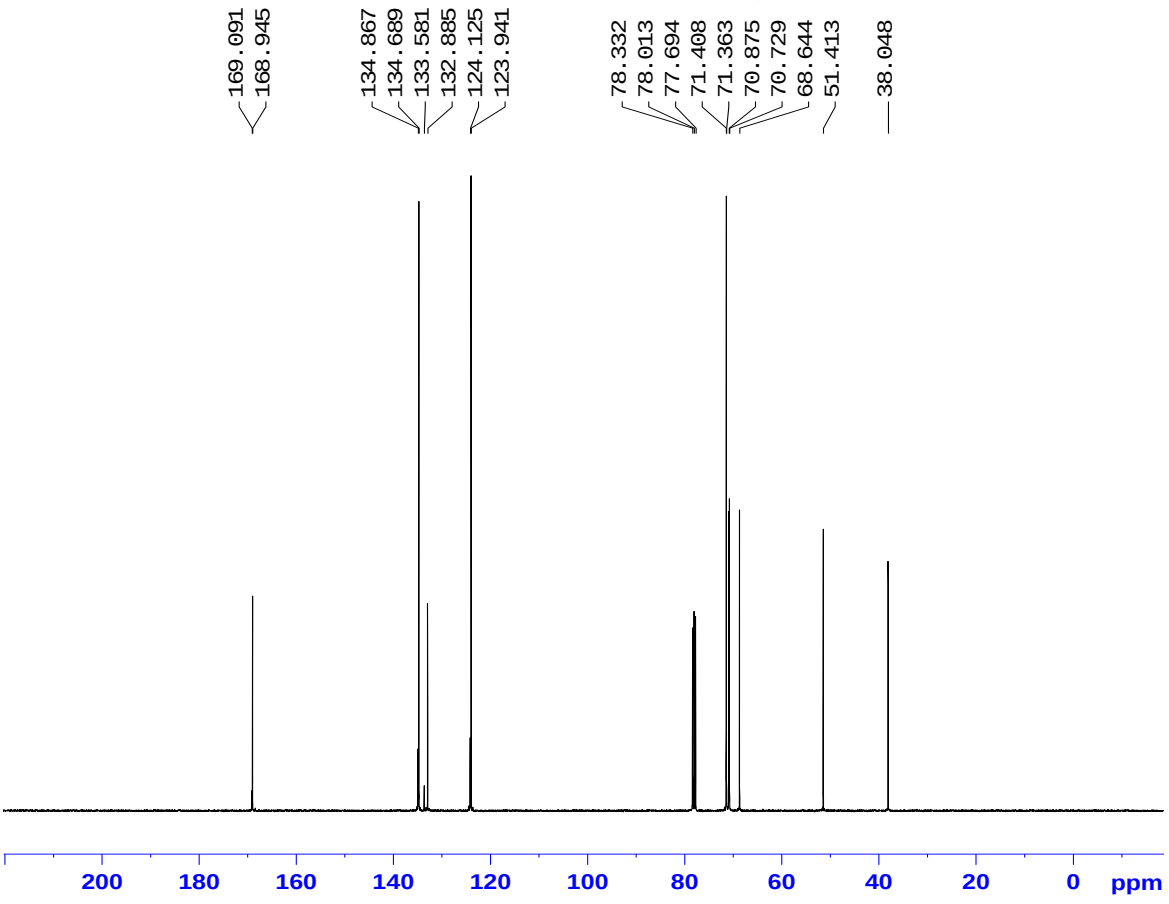
Acquired: Oct 13 11:43:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\13 Thur\LNG-802001.dat

Printed: 11:44, October 13, 2011




```
NAME      LG-801_N3-TEG-NPth
EXPNO                    1
PROCNO                   1
Date_             20111012
Time                 18.10
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ                3.7224948 sec
RG                    25.4
DW                  56.800 usec
DE                   6.50 usec
TE                  292.5 K
D1              1.00000000 sec
TD0                      1

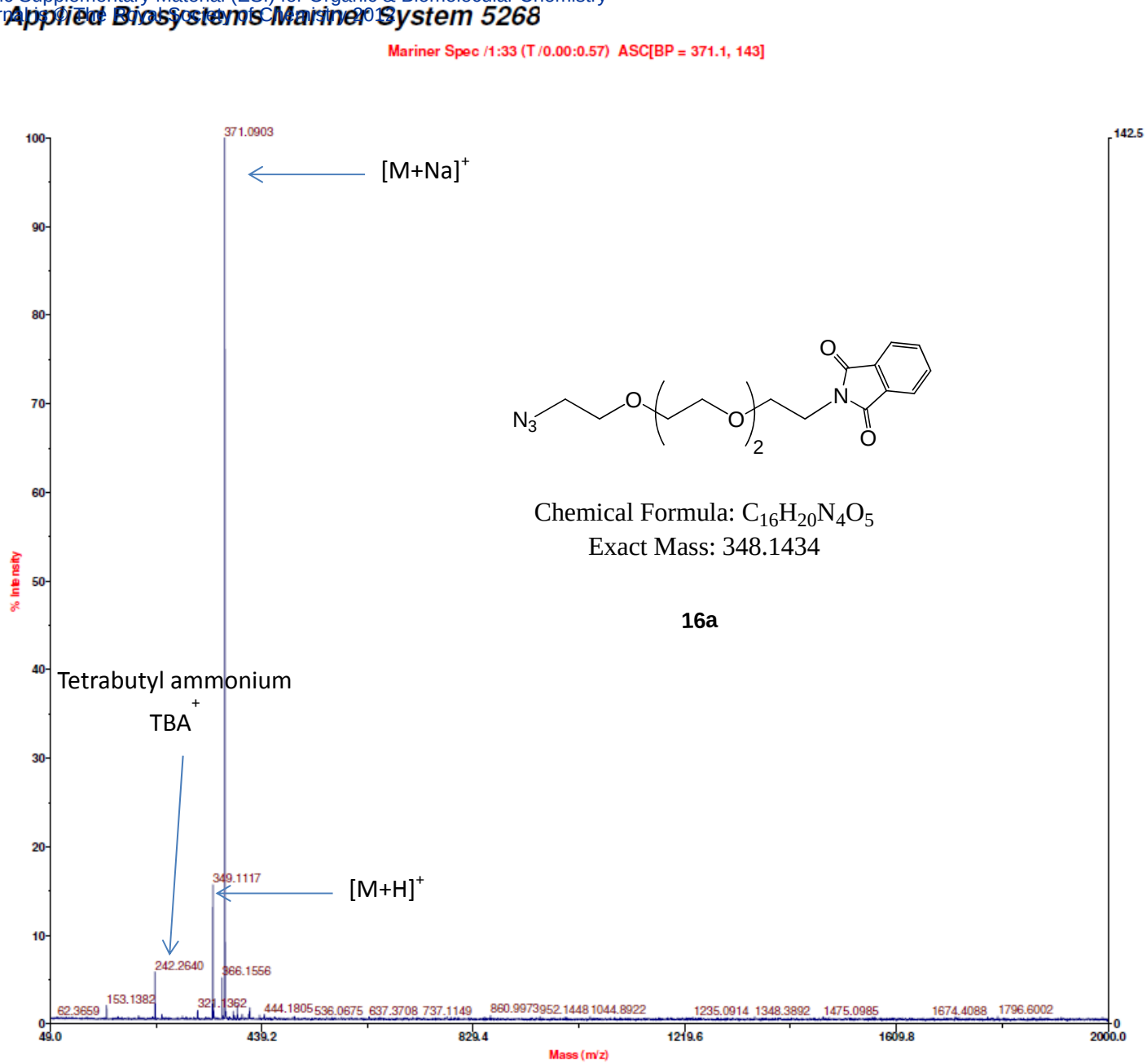
======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      LG-801_N3-TEG-NPth
EXPNO                    2
PROCNO                   1
Date_             20111012
Time                 19.12
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    80.6
DW                  20.800 usec
DE                   6.50 usec
TE                  294.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W         73.67452240 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W         13.97447491 W
PL12W         0.54996562 W
PL13W         0.54996562 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



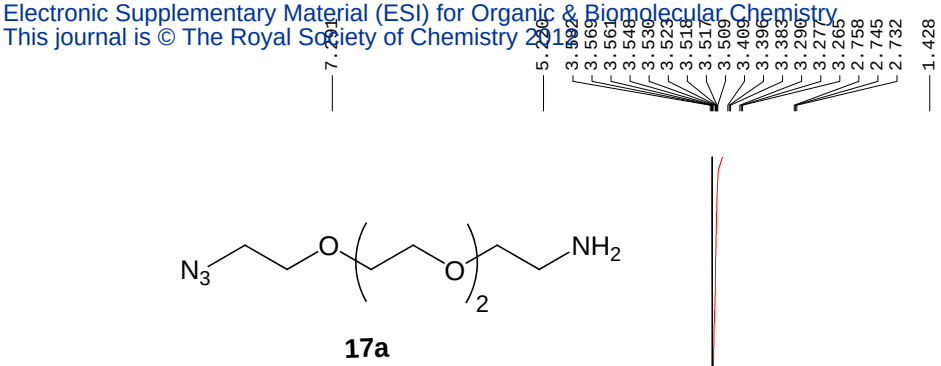
Chemical Formula: $C_{16}H_{20}N_4O_5$
Exact Mass: 348.1434

16a

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Oct 13 11:28:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\13 Thur\LNG-801001.dat

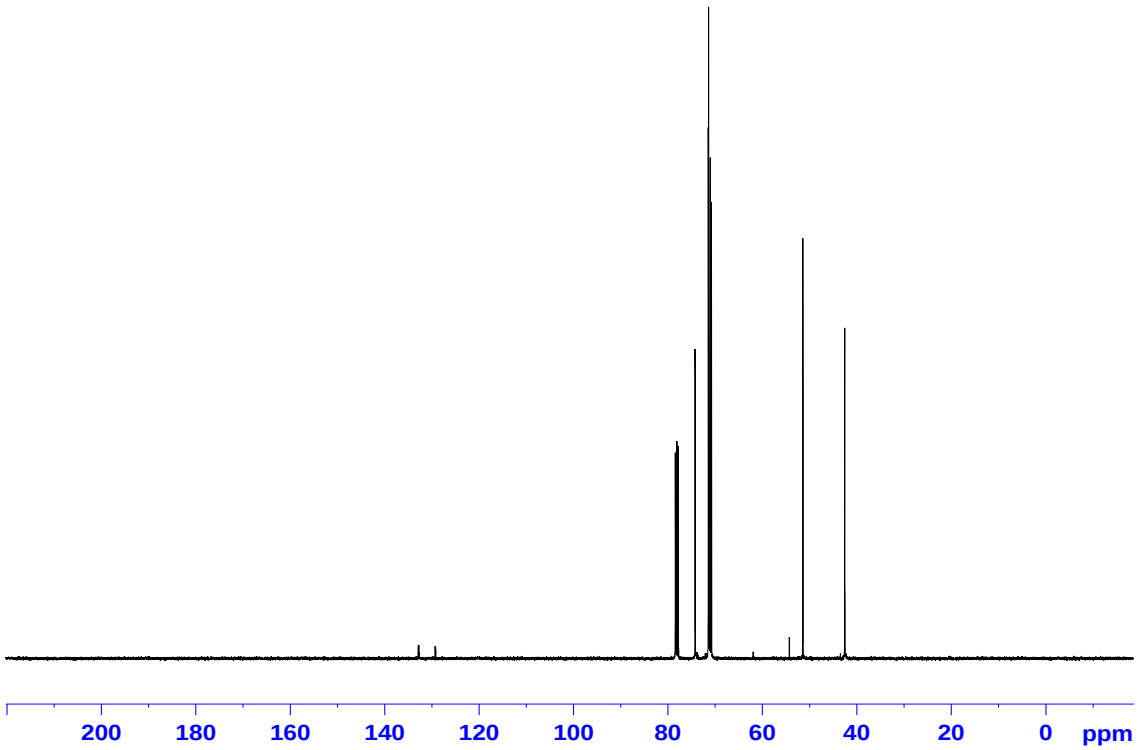
Printed: 11:30, October 13, 2011



17a


```
NAME      Jan20-2012_N3-P4-NH2
EXPNO                        1
PROCNO                       1
Date_             20120120
Time                    12.40
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                8802.817 Hz
FIDRES             0.134320 Hz
AQ                 3.7224948 sec
RG                      20.2
DW                    56.800 usec
DE                     6.50 usec
TE                    293.7 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.85 usec
PL1                    -0.60 dB
PL1W            13.81451130 W
SFO1            400.1320007 MHz
SI                     32768
SF              400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



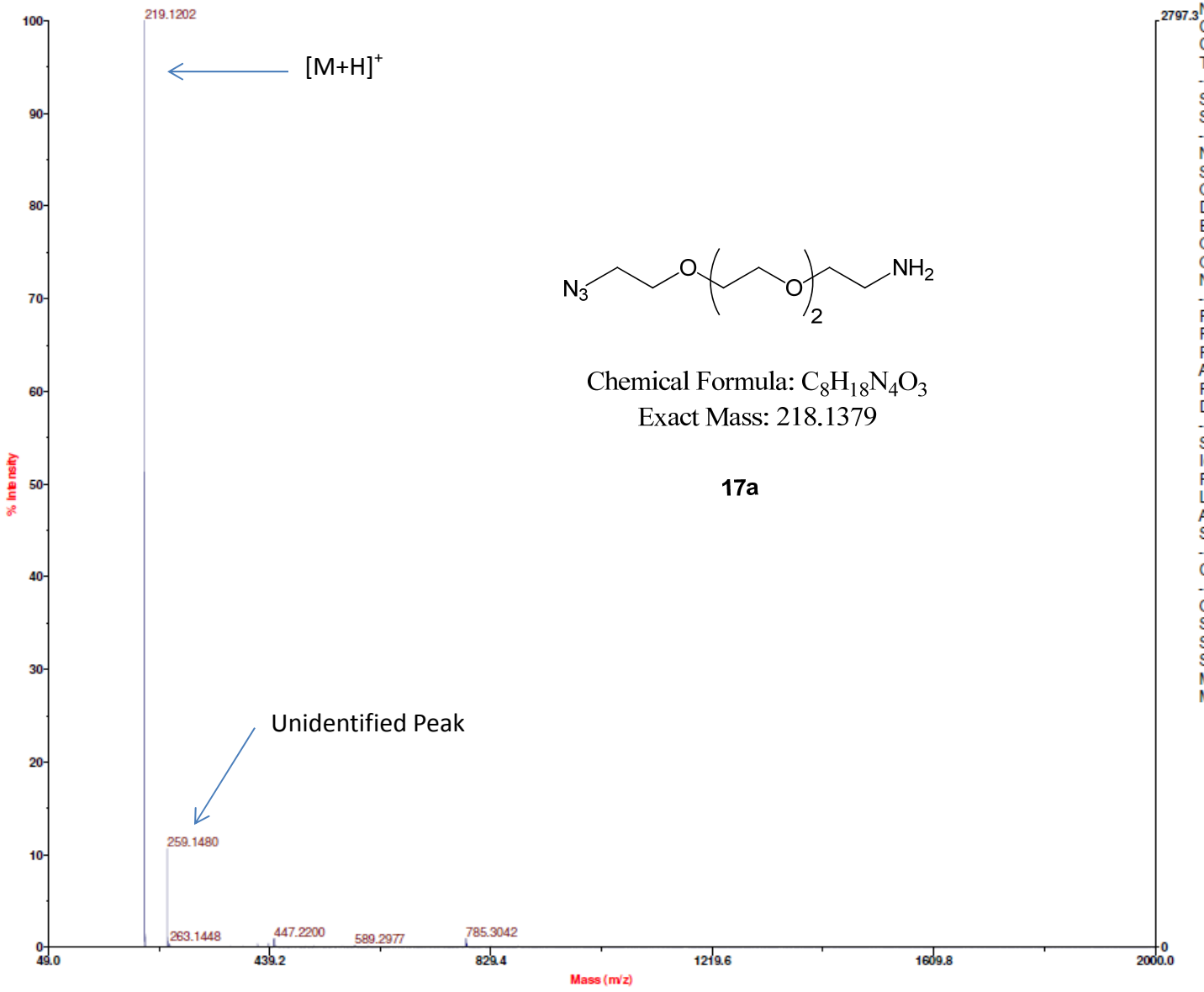

```
NAME      Jan20-2012_N3-P4-NH2
EXPNO                        2
PROCNO                       1
Date_             20120120
Time                    13.16
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       724
DW                    20.800 usec
DE                     6.50 usec
TE                    295.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.99 usec
PL1                   -3.00 dB
PL1W            73.67452240 W
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -0.65 dB
PL12                   13.40 dB
PL13                   13.40 dB
PL2W            13.97447491 W
PL12W            0.54996562 W
PL13W            0.54996562 W
SFO2            400.1316005 MHz
SI                     32768
SF              100.6126885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:47 (T /0.00:0.83) ASC[BP = 219.1, 2797]



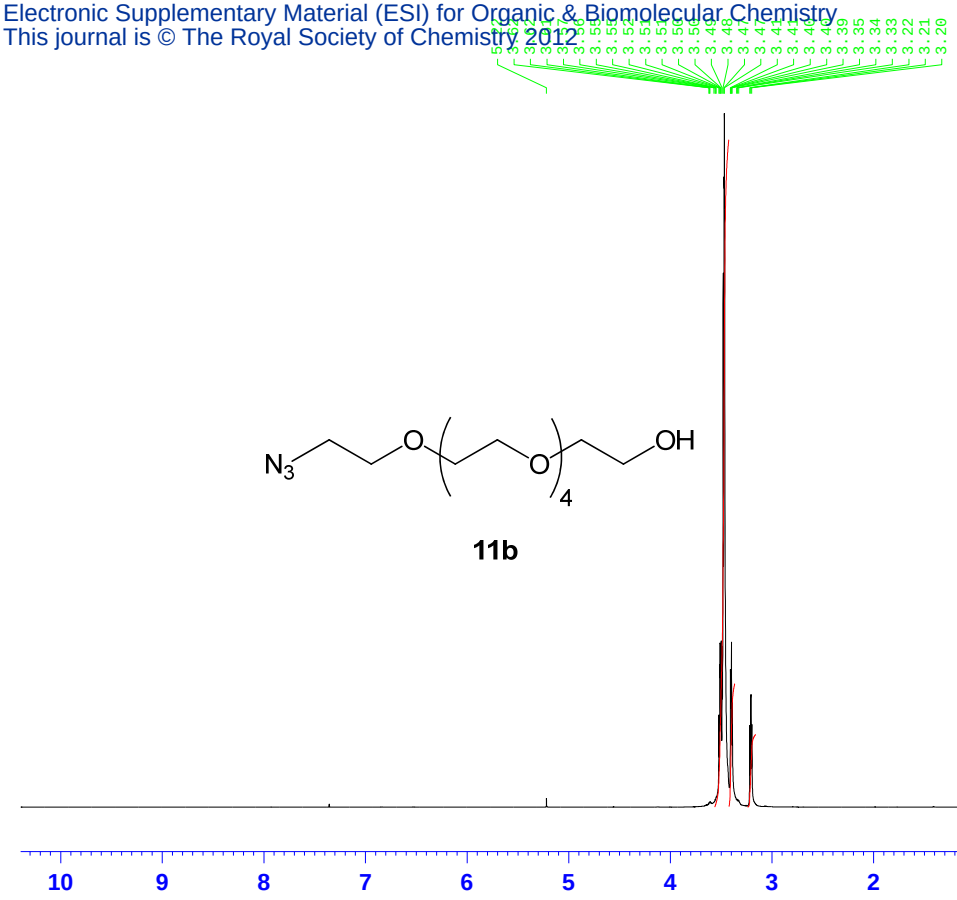
Chemical Formula: $C_8H_{18}N_4O_3$
Exact Mass: 218.1379

17a

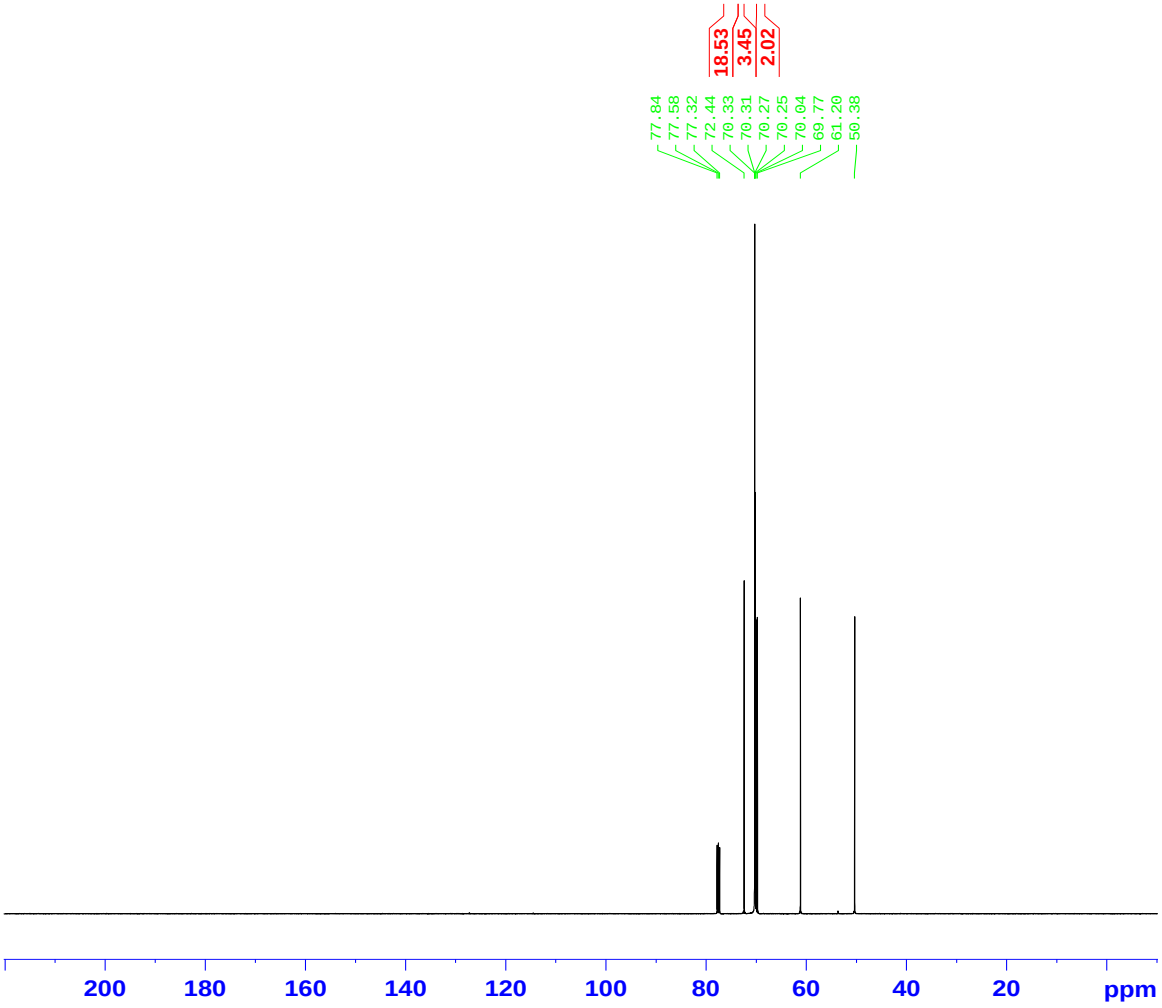
--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Oct 17 13:20:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Oct\17 Mon\LNG-804001.dat

Printed: 13:22, October 17, 2011



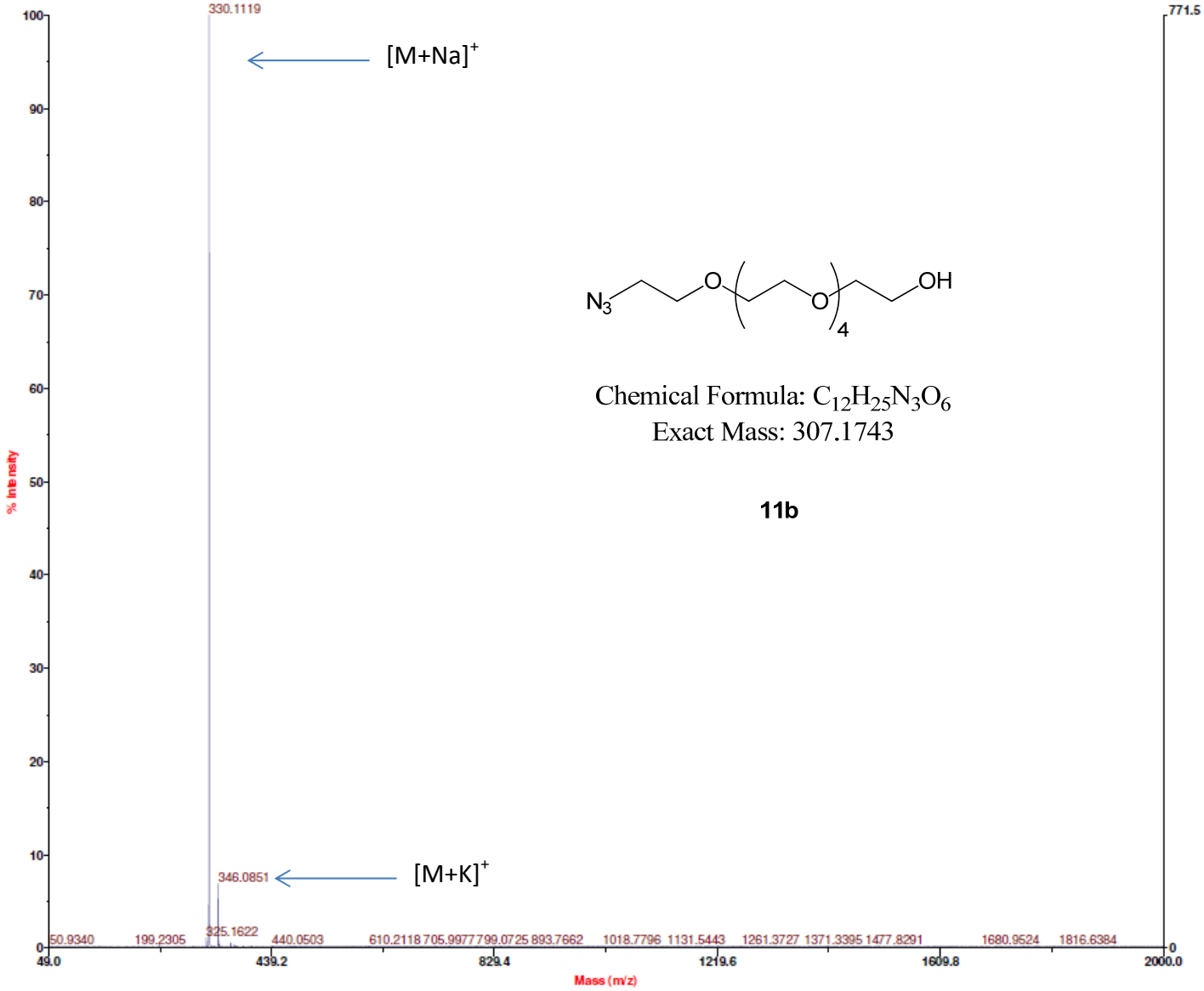
NAME	ZH3-143-C_N3-P6-OH
EXPNO	1
PROCNO	1
Date_	20111108
Time	21.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2769001 sec
RG	6.3
DW	50.000 usec
DE	6.50 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	1.20 dB
PL1W	17.72078514 W
SFO1	500.1330008 MHz
SI	32768
SF	500.1299631 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME	ZH3-143-C_N3-P6-OH
EXPNO	2
PROCNO	1
Date_	20111108
Time	22.05
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	28985.508 Hz
FIDRES	0.442284 Hz
AQ	1.1305633 sec
RG	4096
DW	17.250 usec
DE	6.50 usec
TE	296.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.83 usec
PL1	0.00 dB
PL1W	80.88274384 W
SFO1	125.7709936 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.20 dB
PL12	15.40 dB
PL13	15.40 dB
PL2W	17.72078514 W
PL12W	0.67372549 W
PL13W	0.67372549 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Applied Biosystems Mariner System 5268

Mariner Spec /1:40 (T /0.00:0.70) ASC[BP = 330.1, 771]



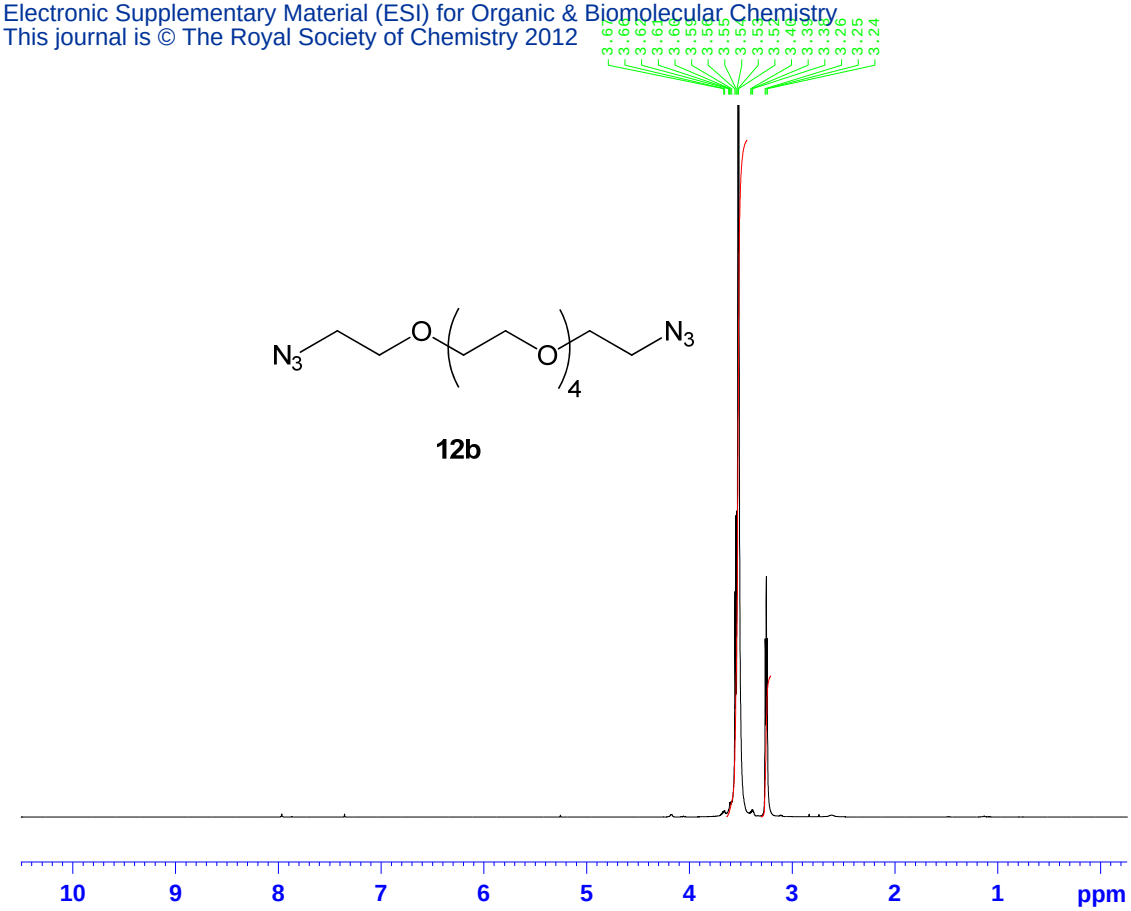
Chemical Formula: $C_{12}H_{25}N_3O_6$
Exact Mass: 307.1743

11b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

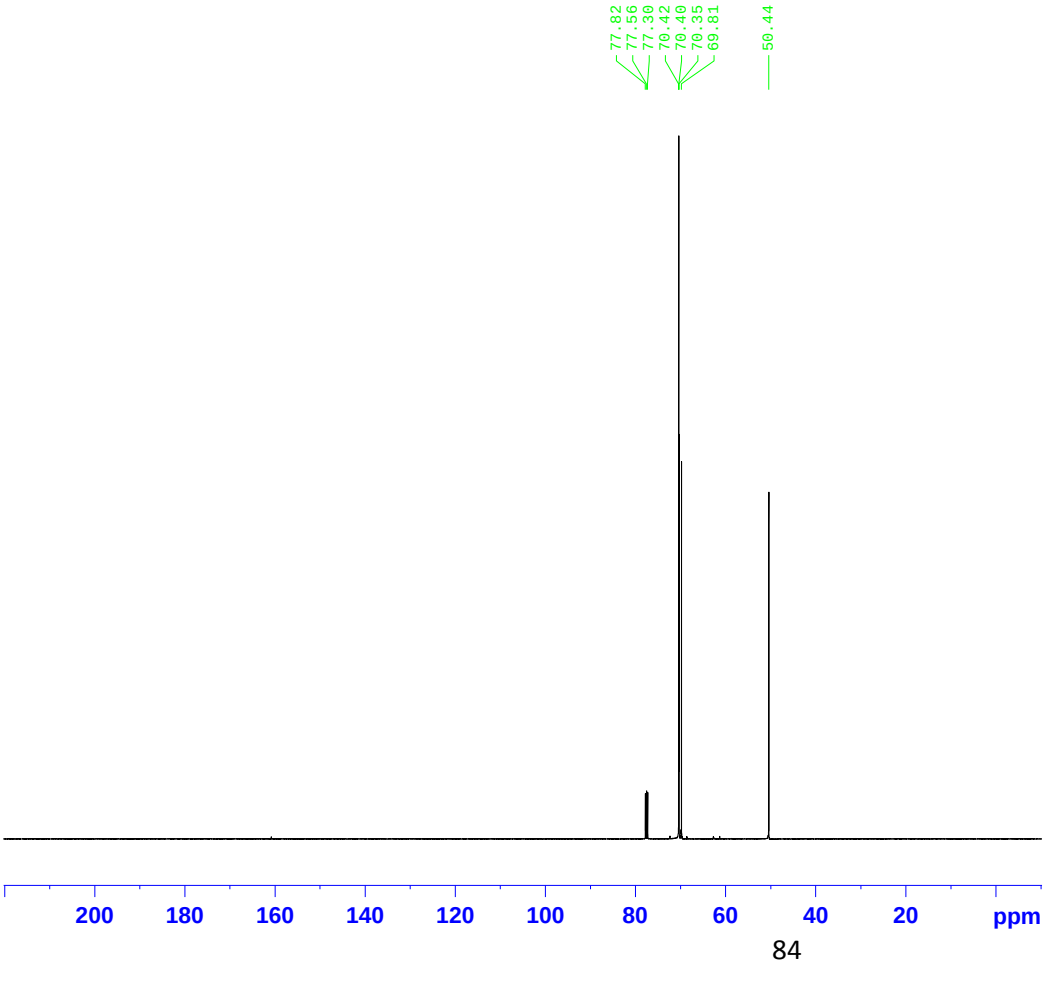
Acquired: Nov 09 21:27:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\09 Wed\ZH3-143-C001.dat

Printed: 21:29, November 09, 2011




```
NAME      ZH3-143-A_N3-P6-N3
EXPNO                  1
PROCNO                 1
Date_           20111108
Time               19.09
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.152588 Hz
AQ             3.2769001 sec
RG                   7.1
DW                50.000 usec
DE                 6.50 usec
TE                294.0 K
D1           1.00000000 sec
TD0                    1

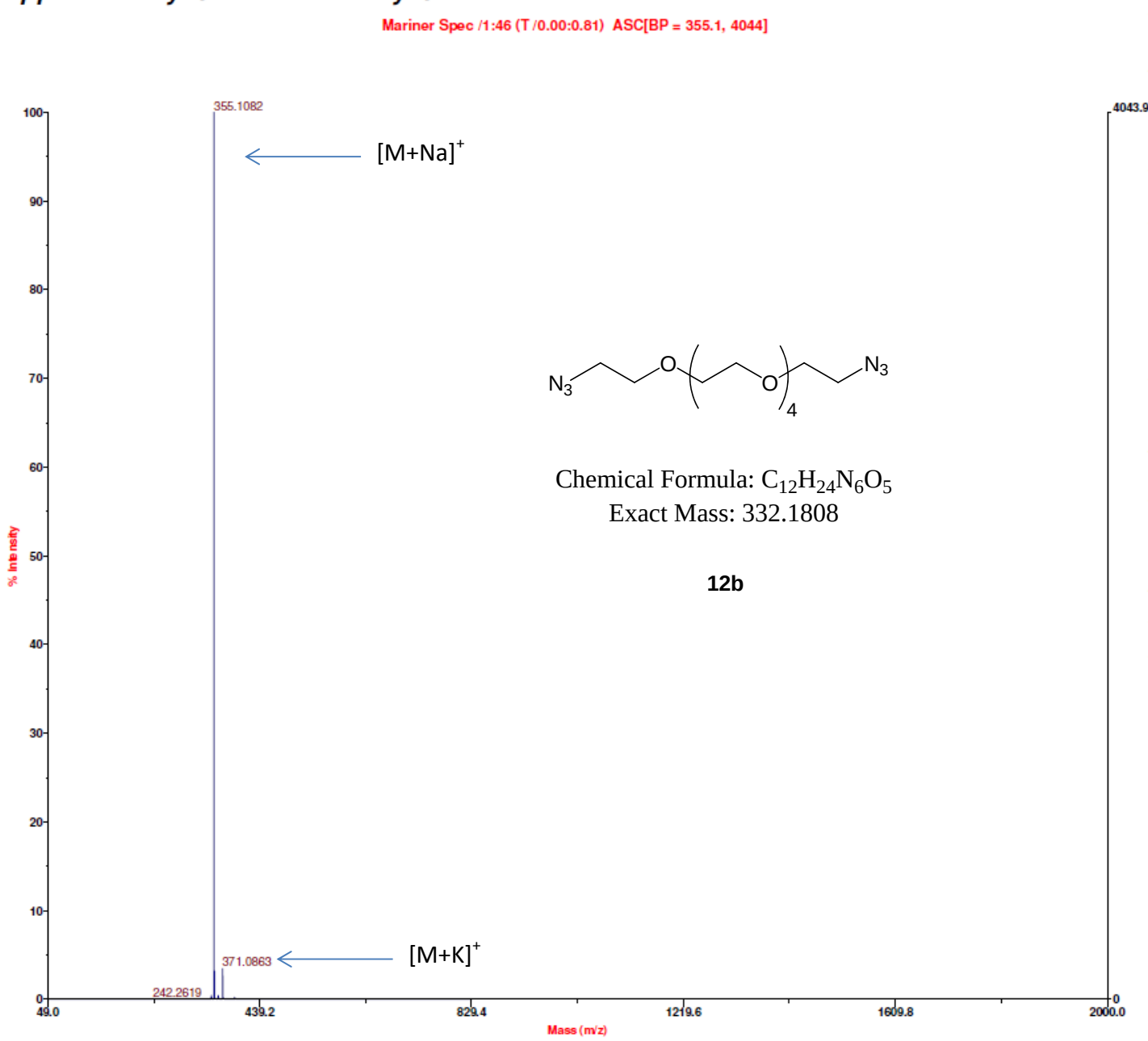
======== CHANNEL f1 ========
NUC1                  1H
P1                14.75 usec
PL1                1.20 dB
PL1W         17.72078514 W
SFO1         500.1330008 MHz
SI                 32768
SF           500.1299631 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
NAME      ZH3-143-A_N3-P6-N3
EXPNO                  2
PROCNO                 1
Date_           20111108
Time               20.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            28985.508 Hz
FIDRES          0.442284 Hz
AQ             1.1305633 sec
RG                  4096
DW                17.250 usec
DE                 6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.83 usec
PL1                0.00 dB
PL1W         80.88274384 W
SFO1         125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 1.20 dB
PL12               15.40 dB
PL13               15.40 dB
PL2W         17.72078514 W
PL12W         0.67372549 W
PL13W         0.67372549 W
SFO2         500.1320005 MHz
SI                 32768
SF           125.7577890 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



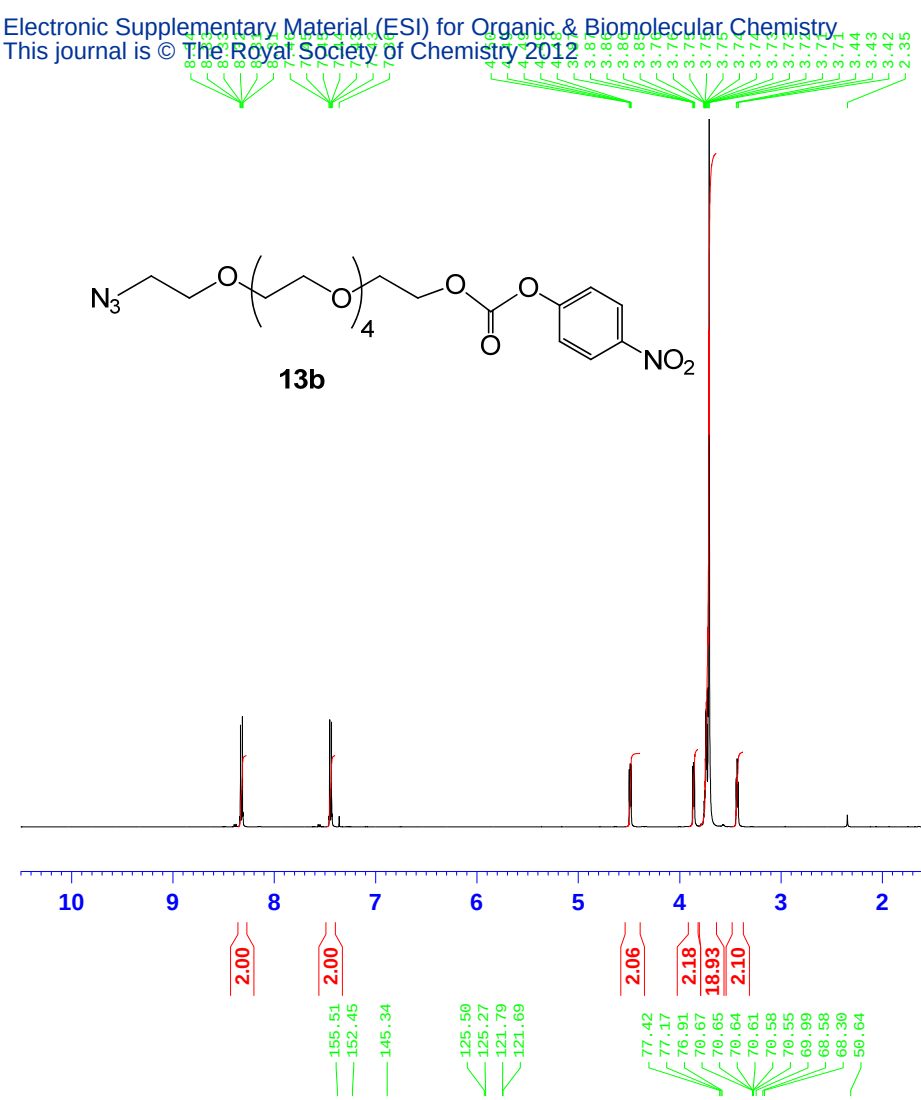
Chemical Formula: $C_{12}H_{24}N_6O_5$
Exact Mass: 332.1808

12b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

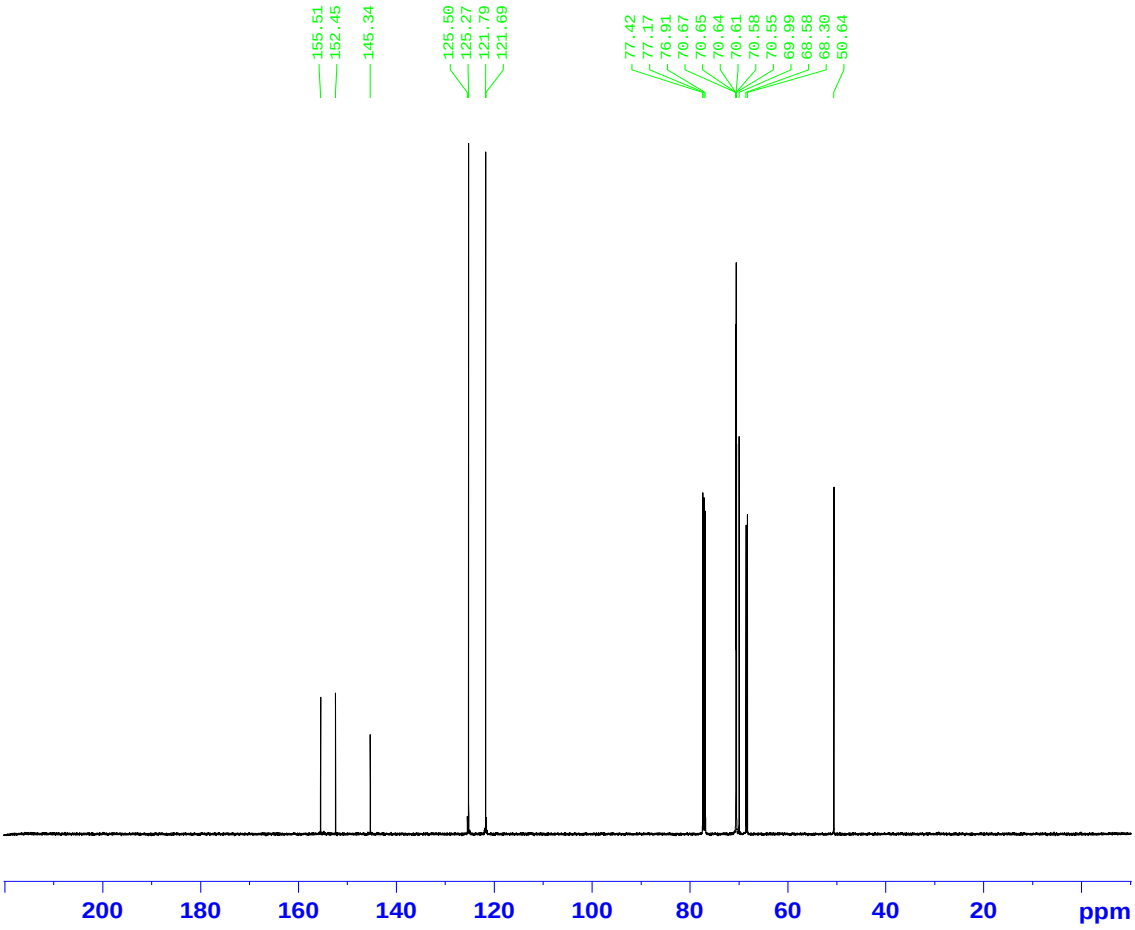
Acquired: Nov 09 21:05:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\09 Wed\ZH3-143-A001.dat

Printed: 21:07, November 09, 2011




```
NAME      LG-835_N3-P6-PNPC
EXPNO                     1
PROCNO                    1
Date_              20111201
Time                  21.32
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        2
SWH              10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2769001 sec
RG                     25.4
DW                  50.000 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   14.75 usec
PL1                   1.20 dB
PL1W           17.72078514 W
SFO1           500.1330008 MHz
SI                    32768
SF             500.1299631 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                    1.00
```



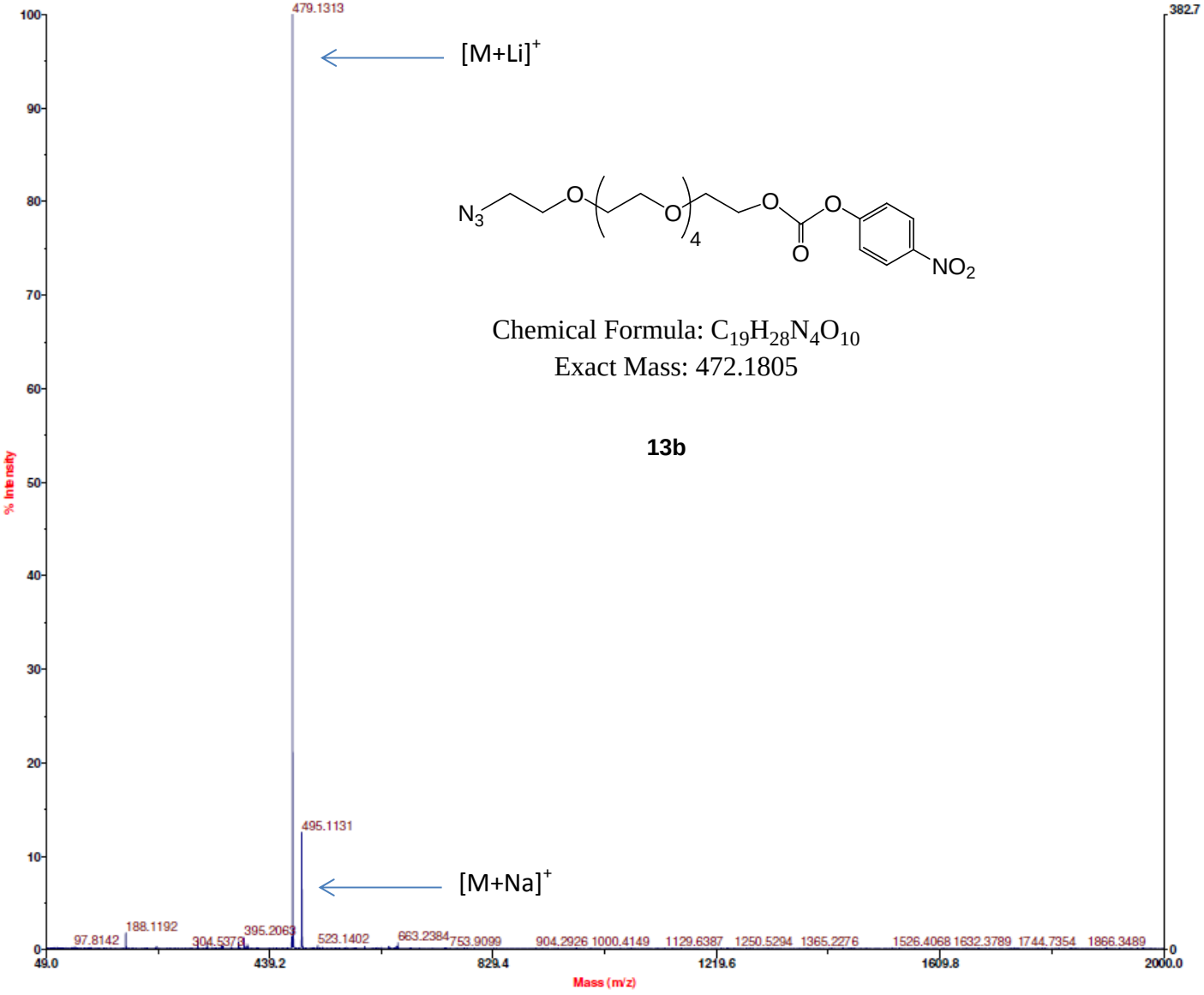

```
NAME      LG-835_N3-P6-PNPC
EXPNO                     2
PROCNO                    1
Date_              20111201
Time                  22.28
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              28985.508 Hz
FIDRES           0.442284 Hz
AQ               1.1305633 sec
RG                     4096
DW                  17.250 usec
DE                    6.50 usec
TE                   300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    8.83 usec
PL1                   0.00 dB
PL1W          80.88274384 W
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                   1.20 dB
PL12                 15.40 dB
PL13                 15.40 dB
PL2W          17.72078514 W
PL12W          0.67372549 W
PL13W          0.67372549 W
SFO2          500.1320005 MHz
SI                    32768
SF            125.7577890 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:23 (T /0.00:0.39) ASC[BP = 479.1, 383]



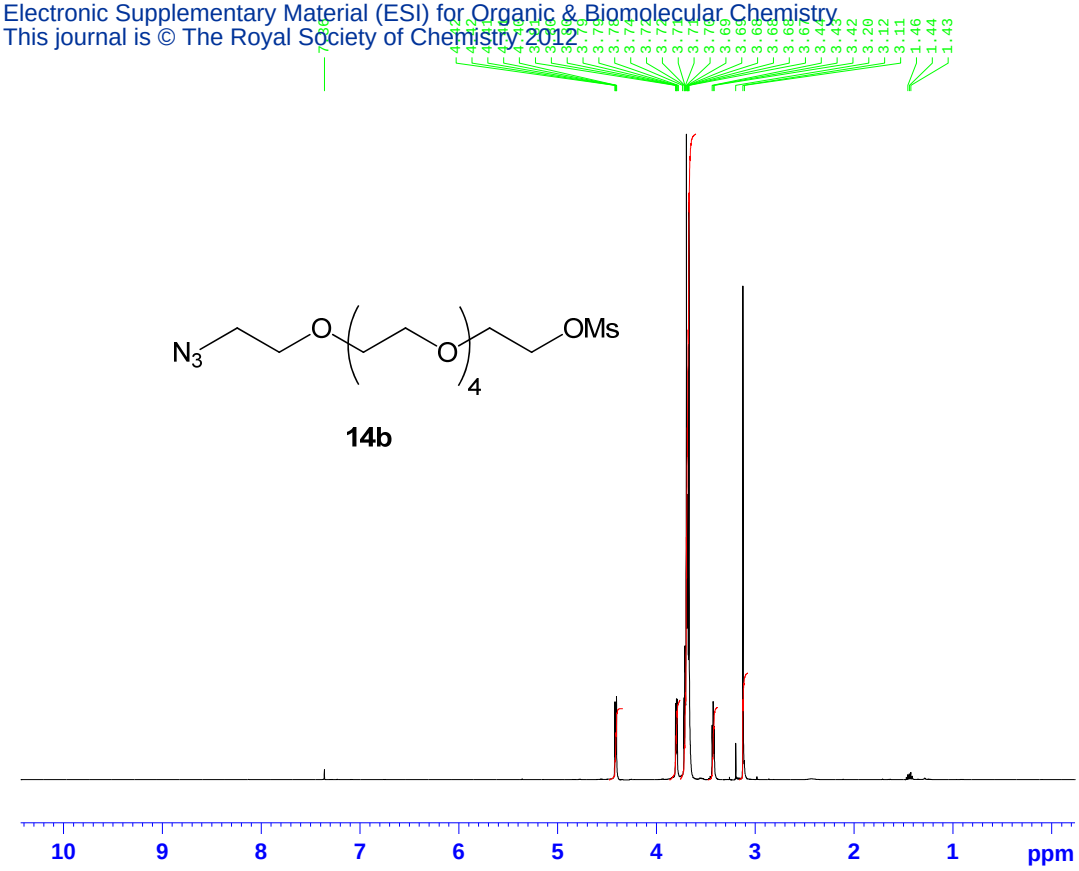
Chemical Formula: $C_{19}H_{28}N_4O_{10}$
Exact Mass: 472.1805

13b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

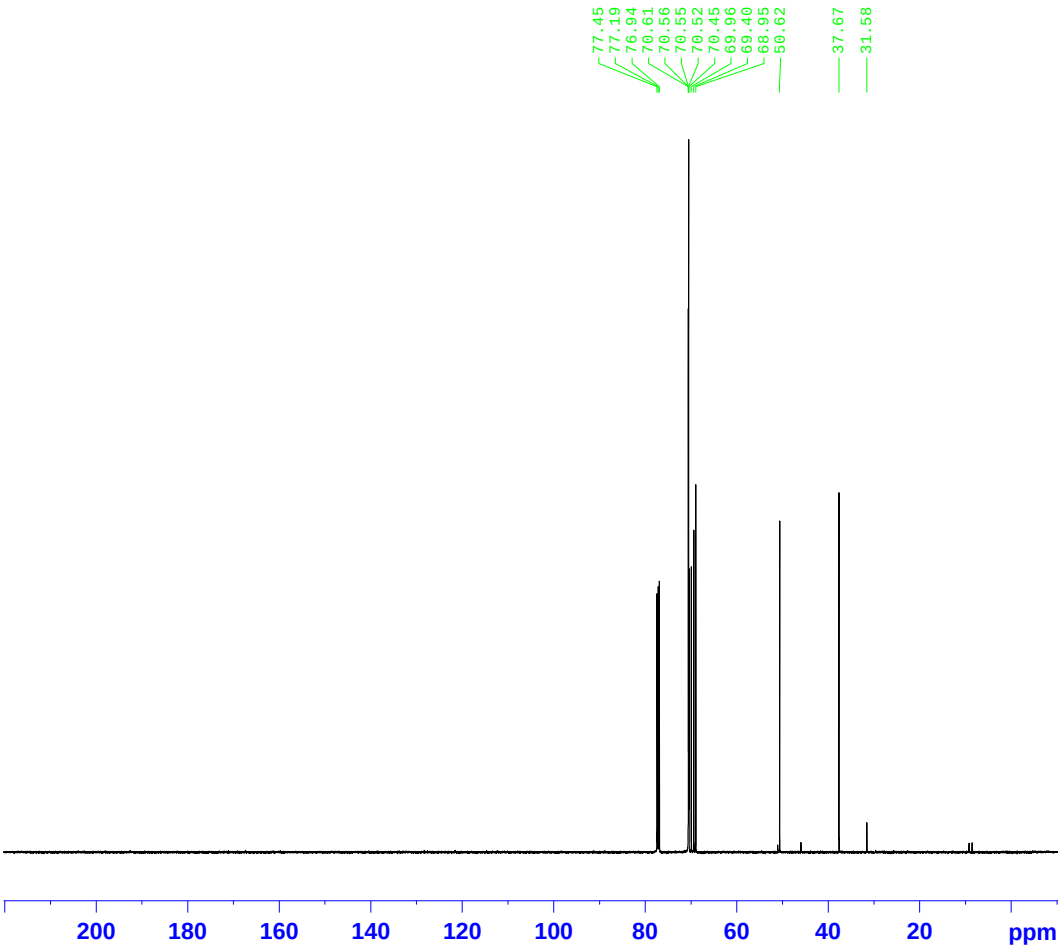
Acquired: Dec 02 10:00:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\02 Fri\LNG-835001.dat

Printed: 10:01, December 02, 2011




```
NAME      ZH3-144_N3-P6-OMs
EXPNO                    1
PROCNO                   1
Date_             20111206
Time                 19.07
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2769001 sec
RG                     22.6
DW                   50.000 usec
DE                    6.50 usec
TE                   294.2 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.75 usec
PL1                   1.20 dB
PL1W            17.72078514 W
SFO1           500.1330008 MHz
SI                    32768
SF             500.1299631 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



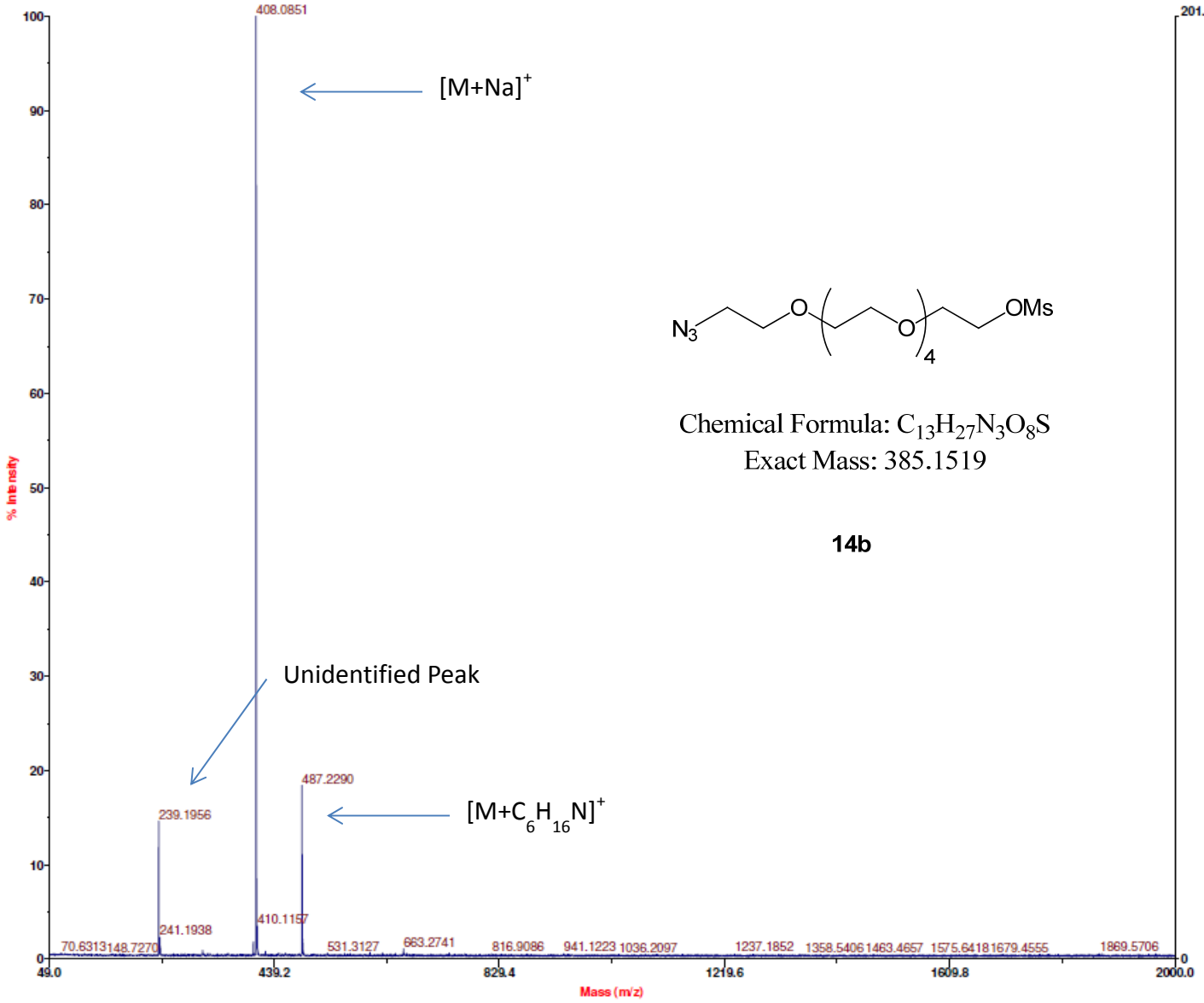

```
NAME      ZH3-144_N3-P6-OMs
EXPNO                    2
PROCNO                   1
Date_             20111206
Time                 20.04
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              28985.508 Hz
FIDRES                0.442284 Hz
AQ                1.1305633 sec
RG                     4096
DW                   17.250 usec
DE                    6.50 usec
TE                   296.7 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.83 usec
PL1                   0.00 dB
PL1W           80.88274384 W
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   1.20 dB
PL12                 15.40 dB
PL13                 15.40 dB
PL2W           17.72078514 W
PL12W           0.67372549 W
PL13W           0.67372549 W
SFO2          500.1320005 MHz
SI                    32768
SF             125.7577890 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:27 (T /0.00:0.47) ASC[BP = 408.1, 202]



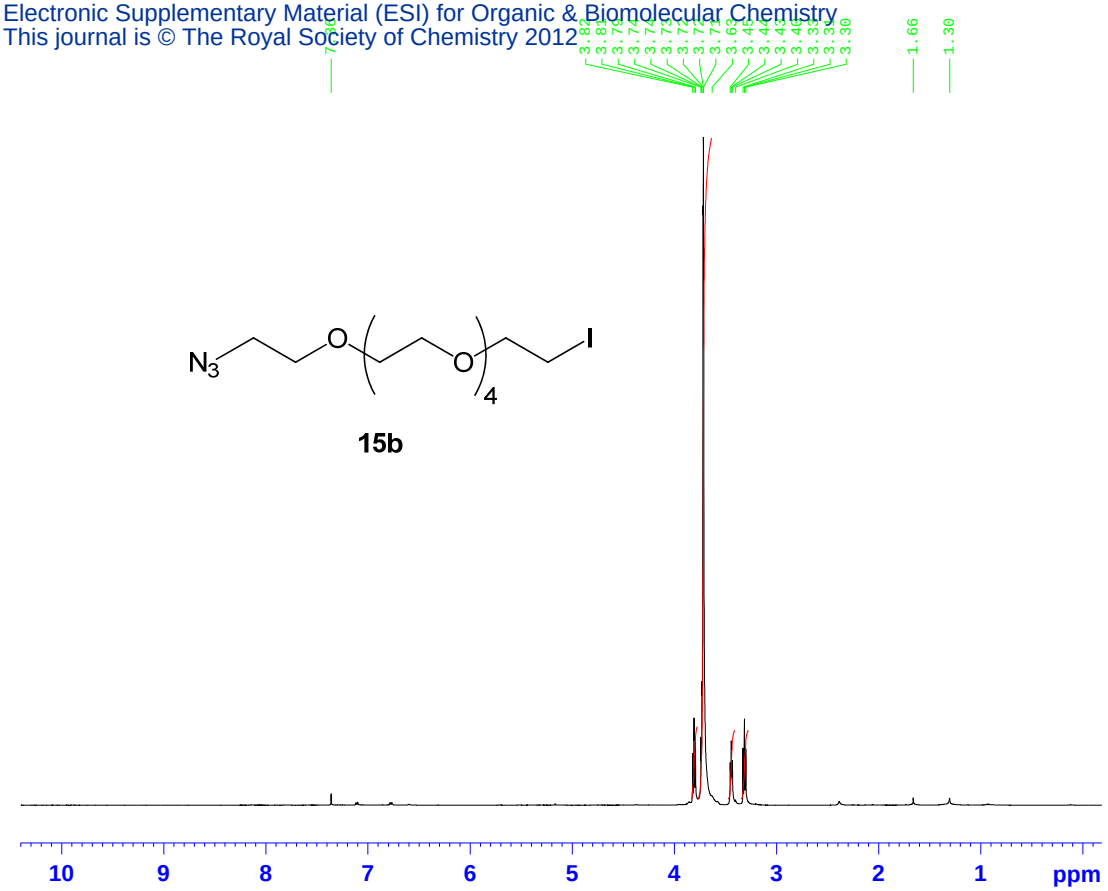
Chemical Formula: $C_{13}H_{27}N_3O_8S$
Exact Mass: 385.1519

14b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

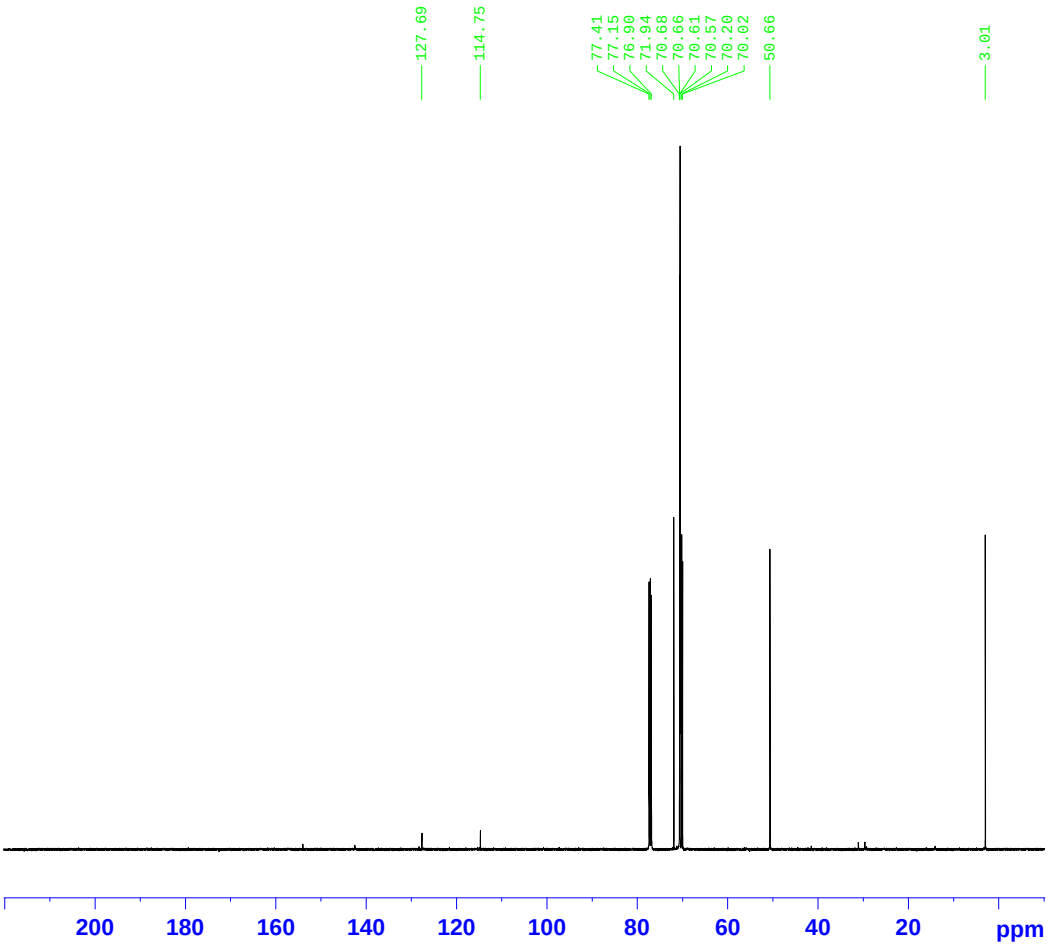
Acquired: Dec 06 15:49:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\06 Tue\ZH3-144002.dat

Printed: 15:50, December 06, 2011



NAME ZH3-145_N3-P6-I
EXPNO 1
PROCNO 1
Date_ 20111207
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 25.4
DW 50.000 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PL1 1.20 dB
PL1W 17.72078514 W
SFO1 500.1330008 MHz
SI 32768
SF 500.1299631 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



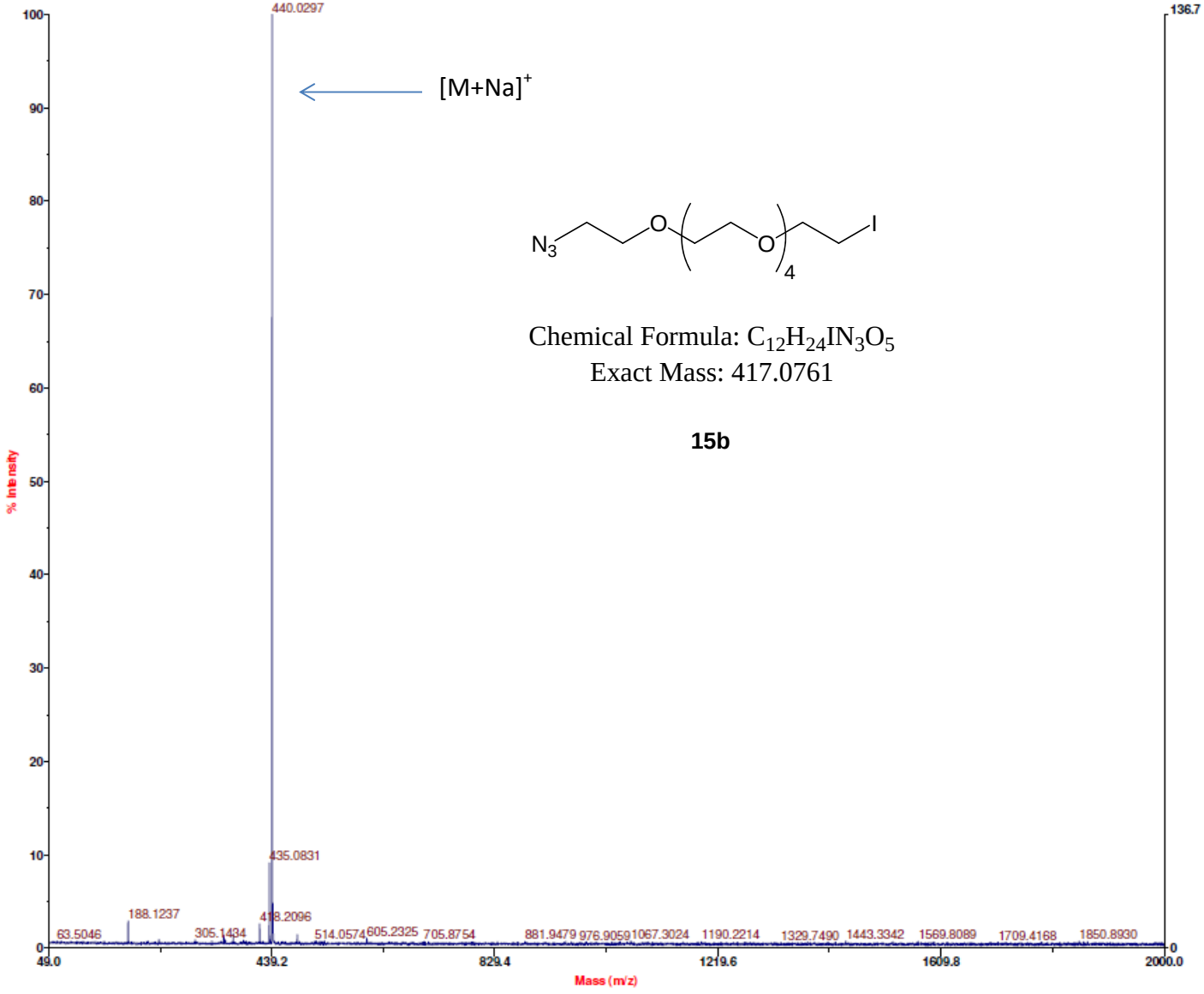
NAME ZH3-145_N3-P6-I
EXPNO 2
PROCNO 1
Date_ 20111207
Time 21.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 28985.508 Hz
FIDRES 0.442284 Hz
AQ 1.1305633 sec
RG 4096
DW 17.250 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.83 usec
PL1 0.00 dB
PL1W 80.88274384 W
SFO1 125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.20 dB
PL12 15.40 dB
PL13 15.40 dB
PL2W 17.72078514 W
PL12W 0.67372549 W
PL13W 0.67372549 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Applied Biosystems Mariner System 5268

Mariner Spec /1:27 (T /0.00:0.46) ASC[BP = 440.0, 137]



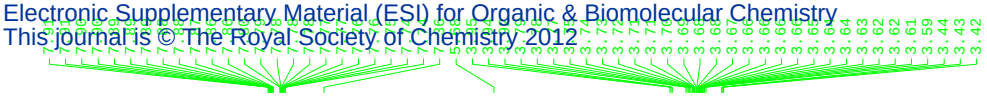
Chemical Formula: $C_{12}H_{24}IN_3O_5$
Exact Mass: 417.0761

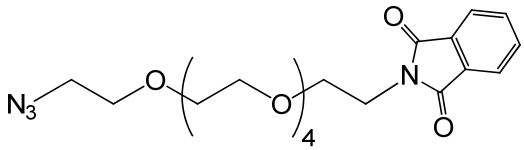
15b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Dec 08 09:07:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\08 Thur\ZH3-145001.dat

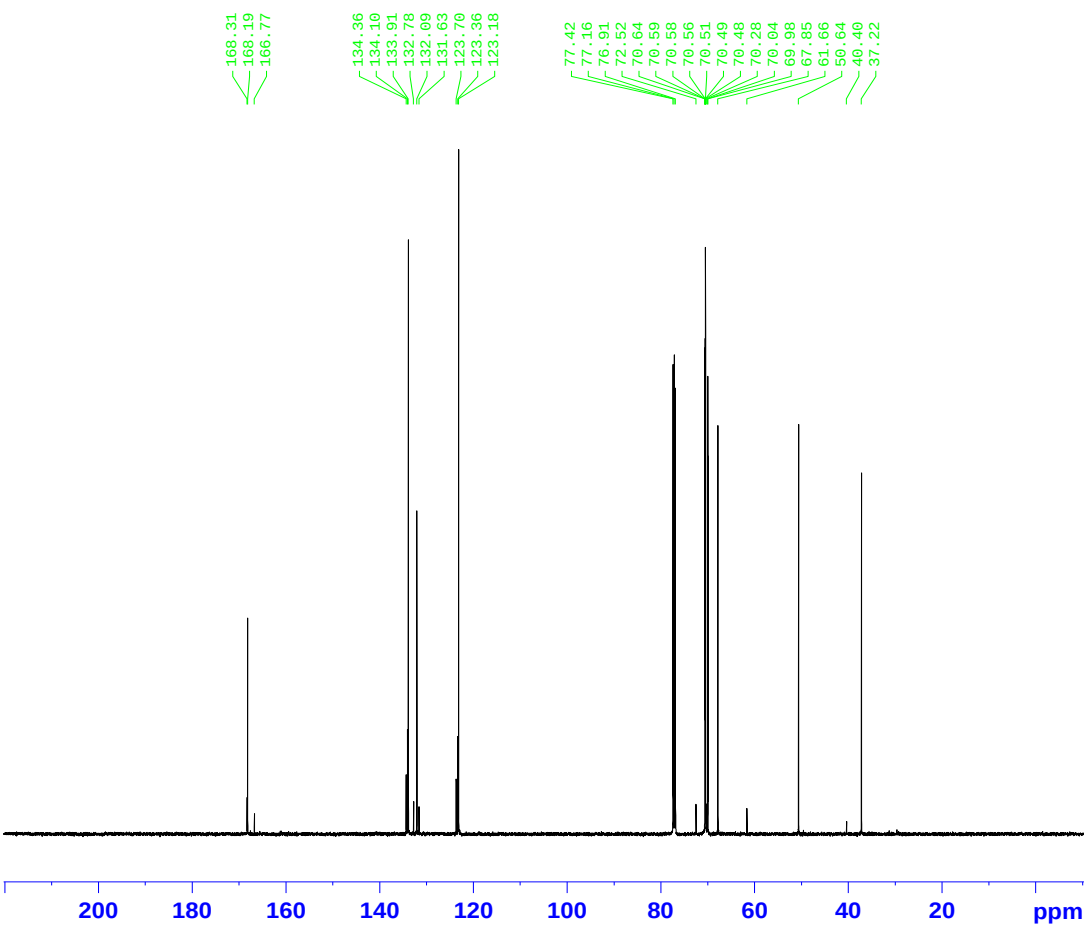
Printed: 09:08, December 08, 2011





16b

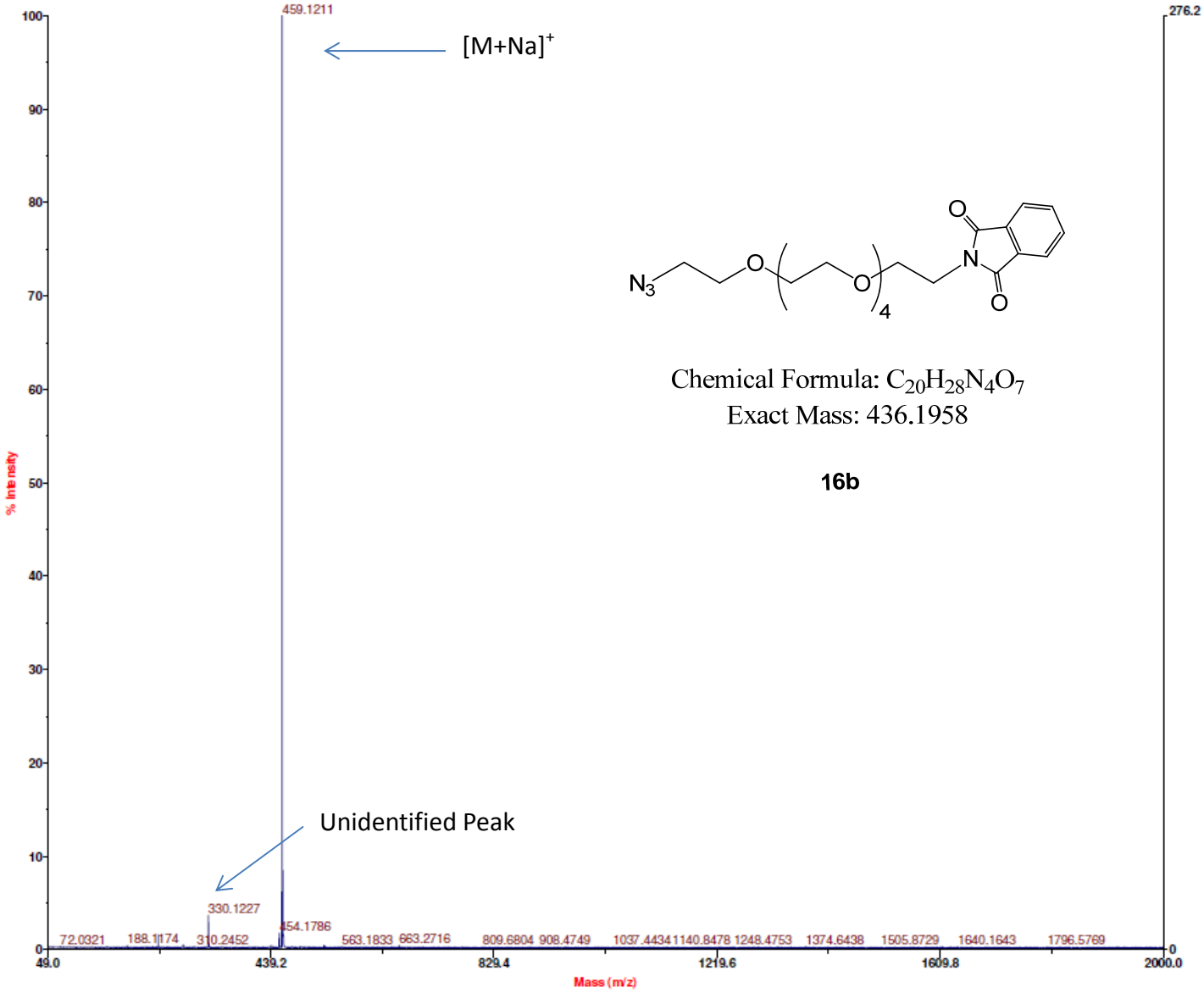
NAME	ZH3-146_N3-P6-NPth
EXPNO	1
PROCNO	1
Date_	20111207
Time	22.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2769001 sec
RG	25.4
DW	50.000 usec
DE	6.50 usec
TE	294.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	1.20 dB
PL1W	17.72078514 W
SFO1	500.1330008 MHz
SI	32768
SF	500.1299631 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME	ZH3-146_N3-P6-NPth
EXPNO	2
PROCNO	1
Date_	20111207
Time	23.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	28985.508 Hz
FIDRES	0.442284 Hz
AQ	1.1305633 sec
RG	4096
DW	17.250 usec
DE	6.50 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.83 usec
PL1	0.00 dB
PL1W	80.88274384 W
SFO1	125.7709936 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.20 dB
PL12	15.40 dB
PL13	15.40 dB
PL2W	17.72078514 W
PL12W	0.67372549 W
PL13W	0.67372549 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Applied Biosystems Mariner System 5268

Mariner Spec /1:52 (T /0.00:0.91) ASC[BP = 459.1, 276]



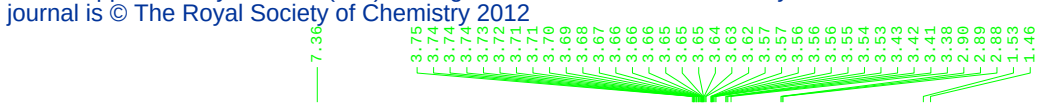
Chemical Formula: $C_{20}H_{28}N_4O_7$
Exact Mass: 436.1958

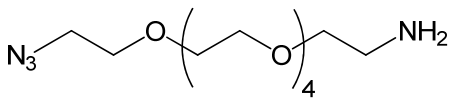
16b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

Acquired: Dec 08 09:33:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\08 Thur\ZH3-146002.dat

Printed: 09:34, December 08, 2011

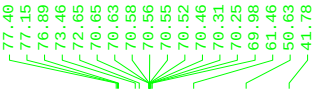


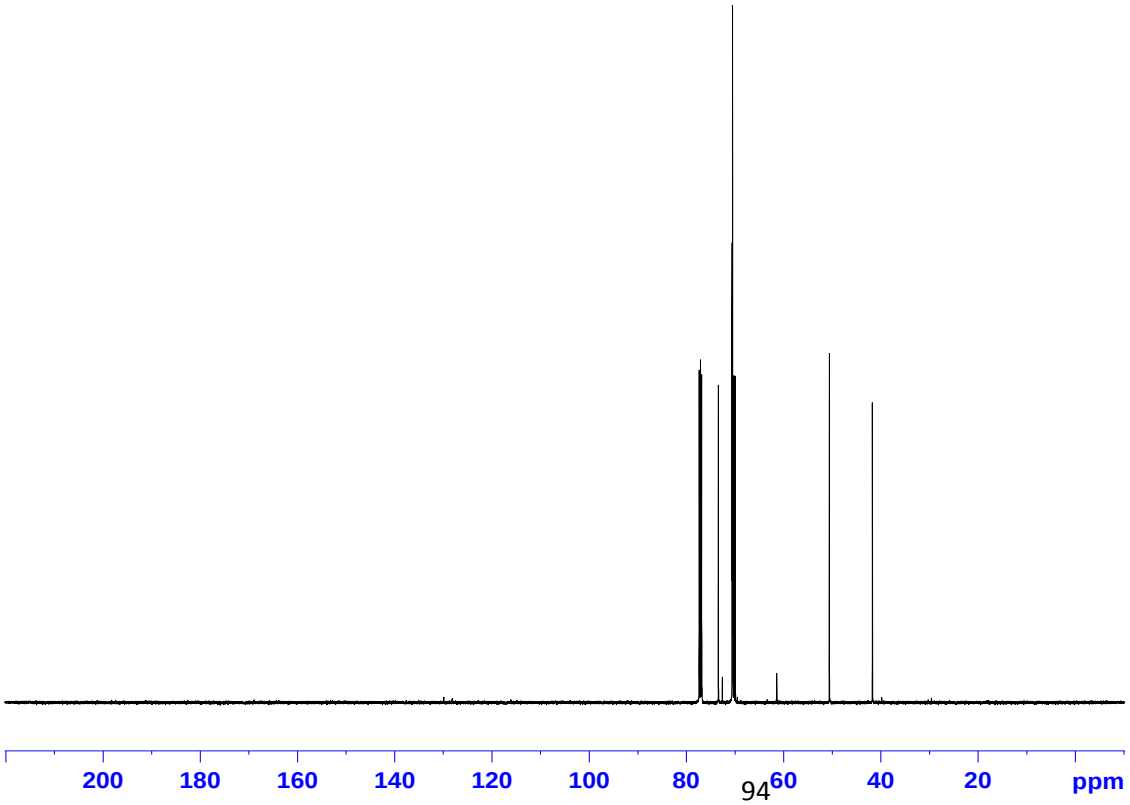


17b


```
NAME      ZH3-147_N3-P6-NH2
EXPNO                    1
PROCNO                   1
Date_             20111208
Time                 0.18
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2769001 sec
RG                  25.4
DW                50.000 usec
DE                 6.50 usec
TE                294.4 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.75 usec
PL1                  1.20 dB
PL1W        17.72078514 W
SFO1        500.1330008 MHz
SI                  32768
SF          500.1299631 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```





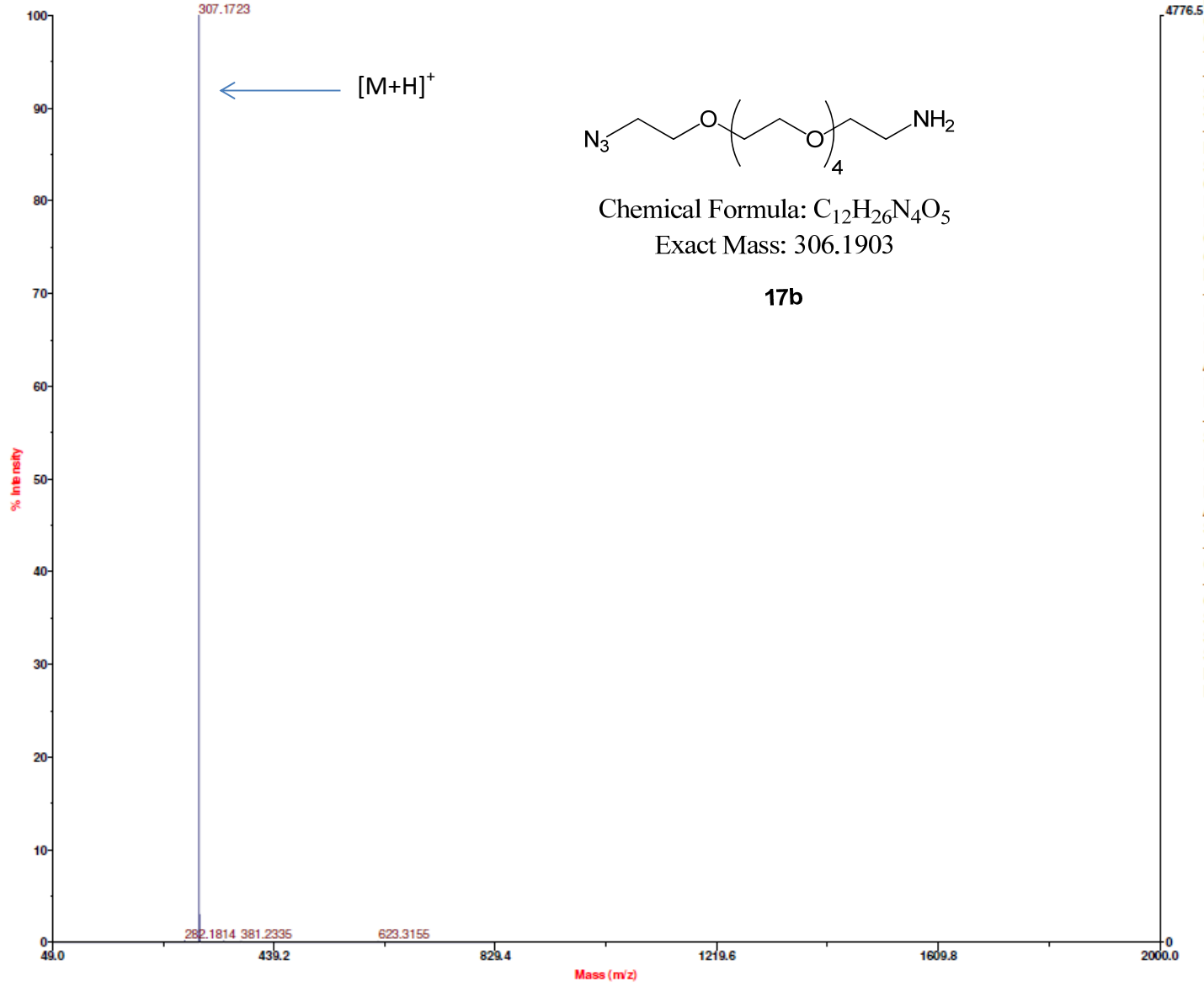

```
NAME      ZH3-147_N3-P6-NH2
EXPNO                    2
PROCNO                   1
Date_             20111208
Time                 1.14
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH           28985.508 Hz
FIDRES         0.442284 Hz
AQ             1.1305633 sec
RG                  4096
DW                17.250 usec
DE                 6.50 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.83 usec
PL1                  0.00 dB
PL1W        80.88274384 W
SFO1       125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  1.20 dB
PL12                15.40 dB
PL13                15.40 dB
PL2W        17.72078514 W
PL12W        0.67372549 W
PL13W        0.67372549 W
SFO2       500.1320005 MHz
SI                  32768
SF         125.7577890 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:33 (T /0.00:0.57) ASC[BP = 307.2, 4777]



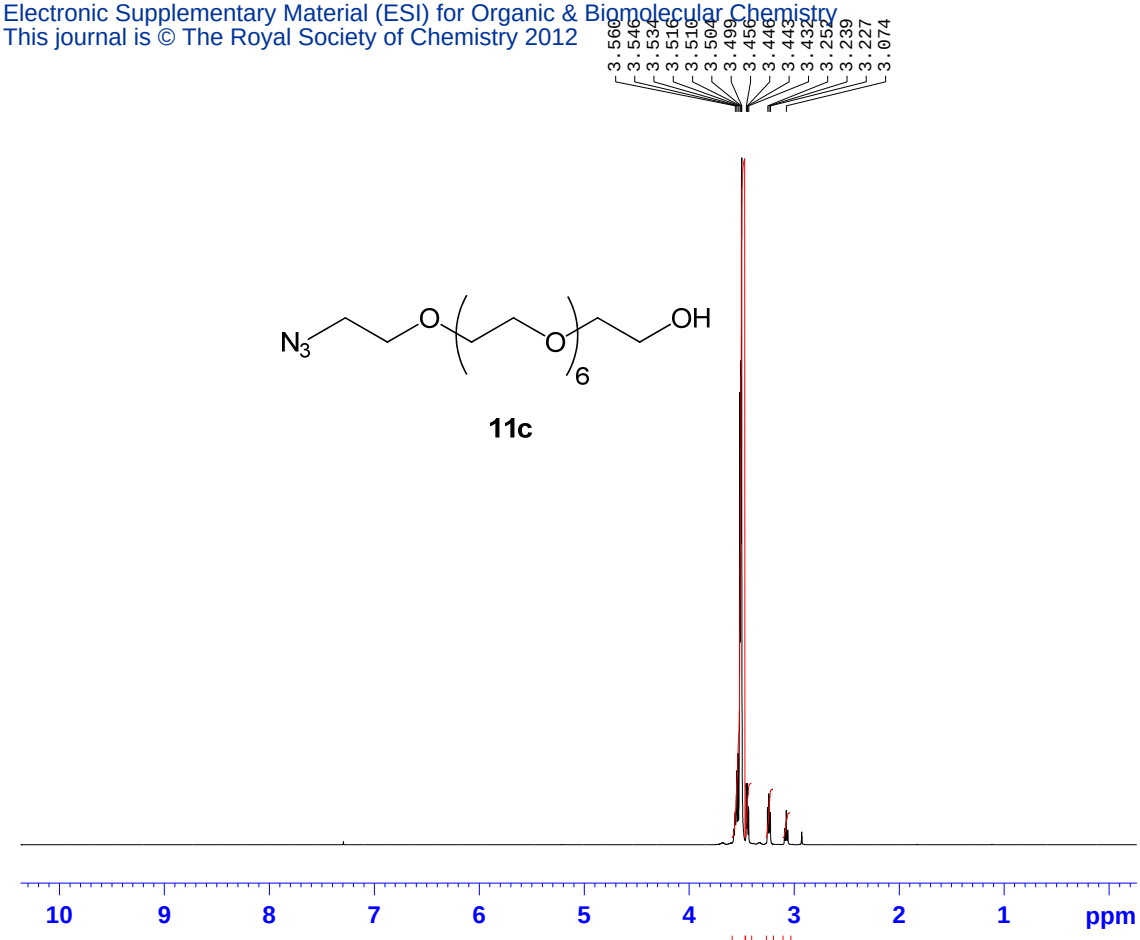
Chemical Formula: $C_{12}H_{26}N_4O_5$
Exact Mass: 306.1903

17b

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

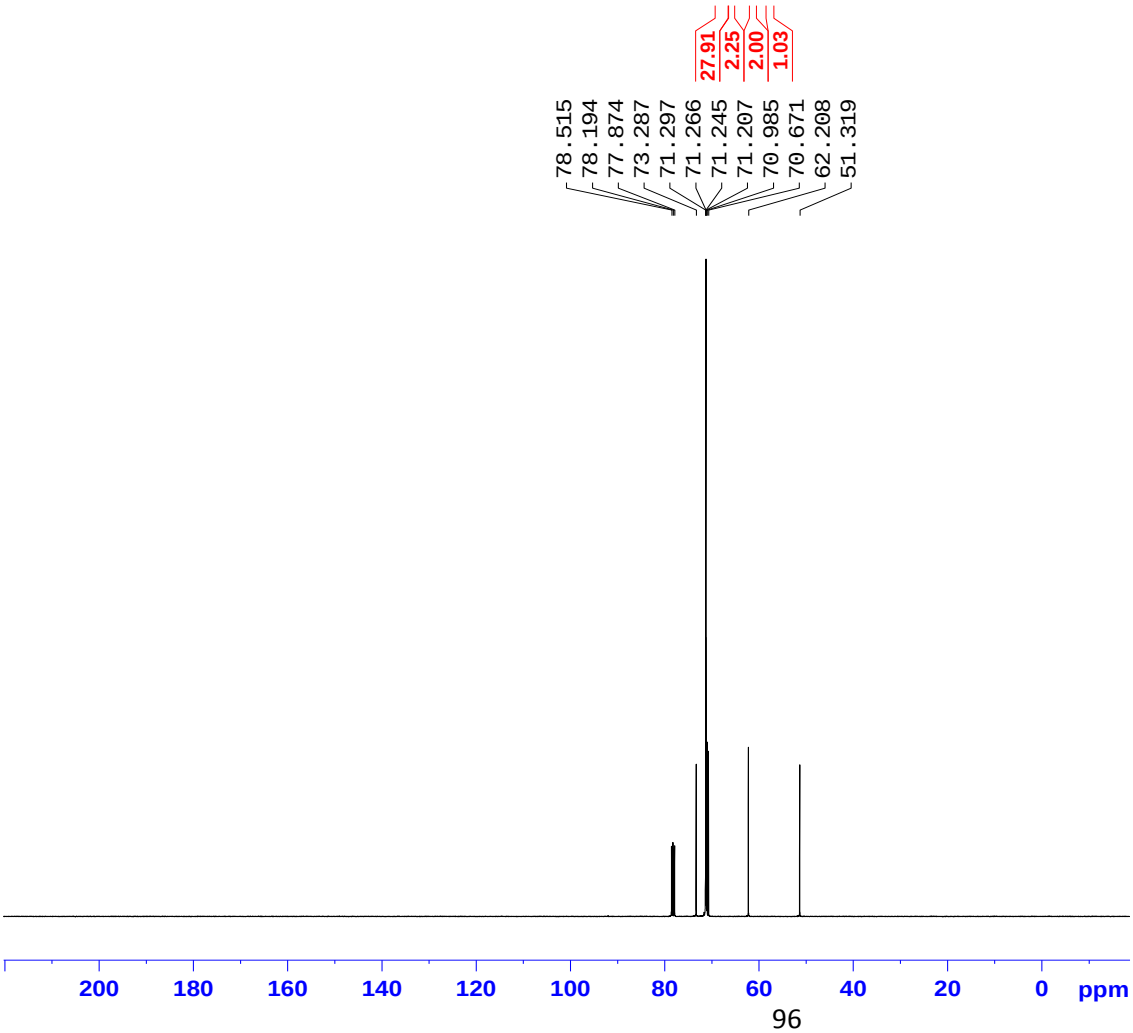
Acquired: Dec 08 09:50:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\08 Thur\ZH3-147002.dat

Printed: 09:51, December 08, 2011




```
NAME      LG-674_OEG-Mono-N3
EXPNO                  1
PROCNO                 1
Date_           20110413
Time               19.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8802.817 Hz
FIDRES          0.134320 Hz
AQ              3.7224948 sec
RG                  11.3
DW                 56.800 usec
DE                  6.50 usec
TE                 298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.85 usec
PL1                -0.60 dB
PL1W         13.81451130 W
SFO1         400.1320007 MHz
SI                 32768
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



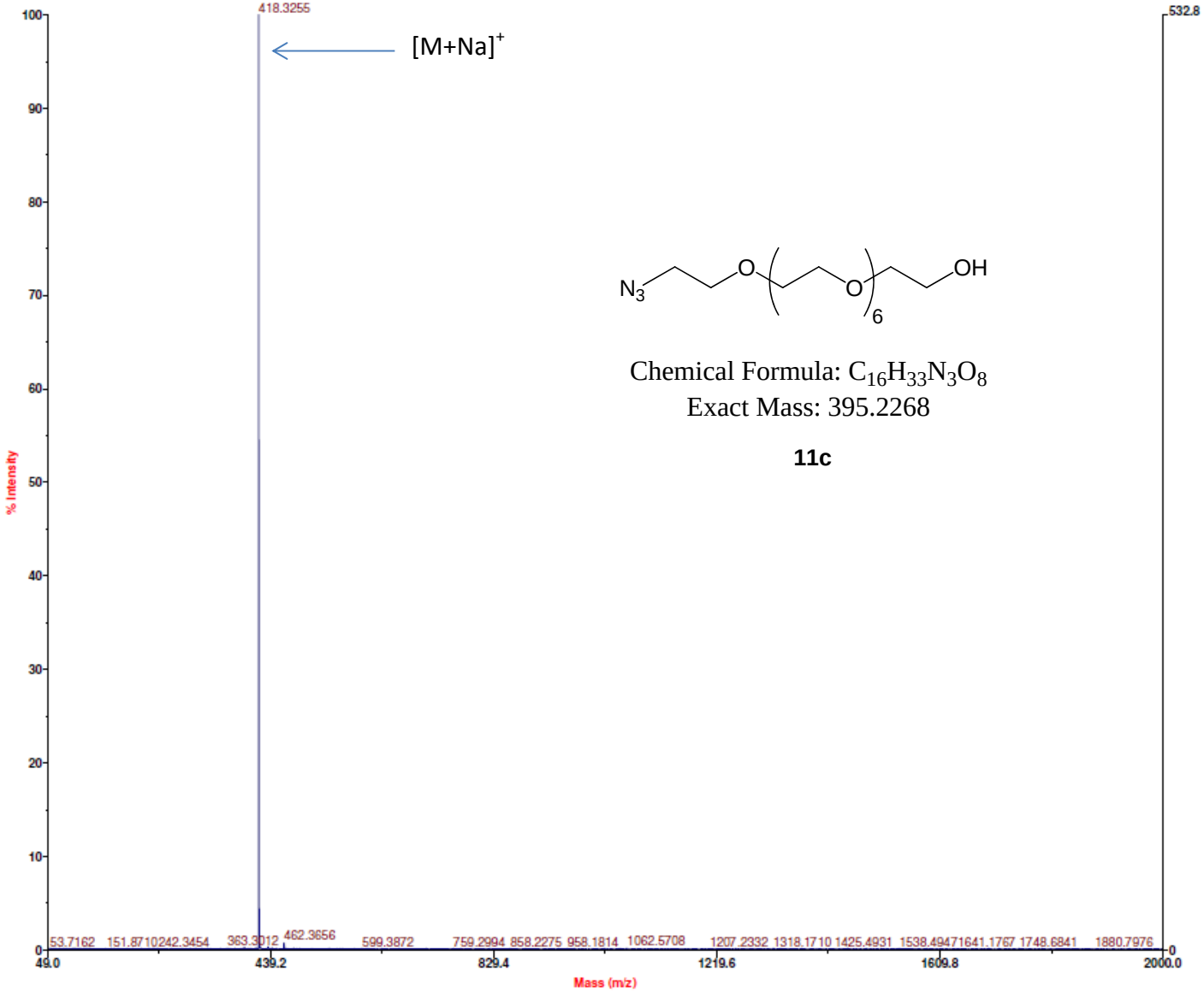

```
NAME      LG-674_OEG-Mono-N3
EXPNO                  2
PROCNO                 1
Date_           20110413
Time               20.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  1150
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.99 usec
PL1                -3.00 dB
PL1W         73.67452240 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -0.65 dB
PL12               13.40 dB
PL13               13.40 dB
PL2W         13.97447491 W
PL12W         0.54996562 W
PL13W         0.54996562 W
SFO2         400.1316005 MHz
SI                 32768
SF           100.6126885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:29 (T /0.00:0.50) ASC[BP = 418.3, 533]



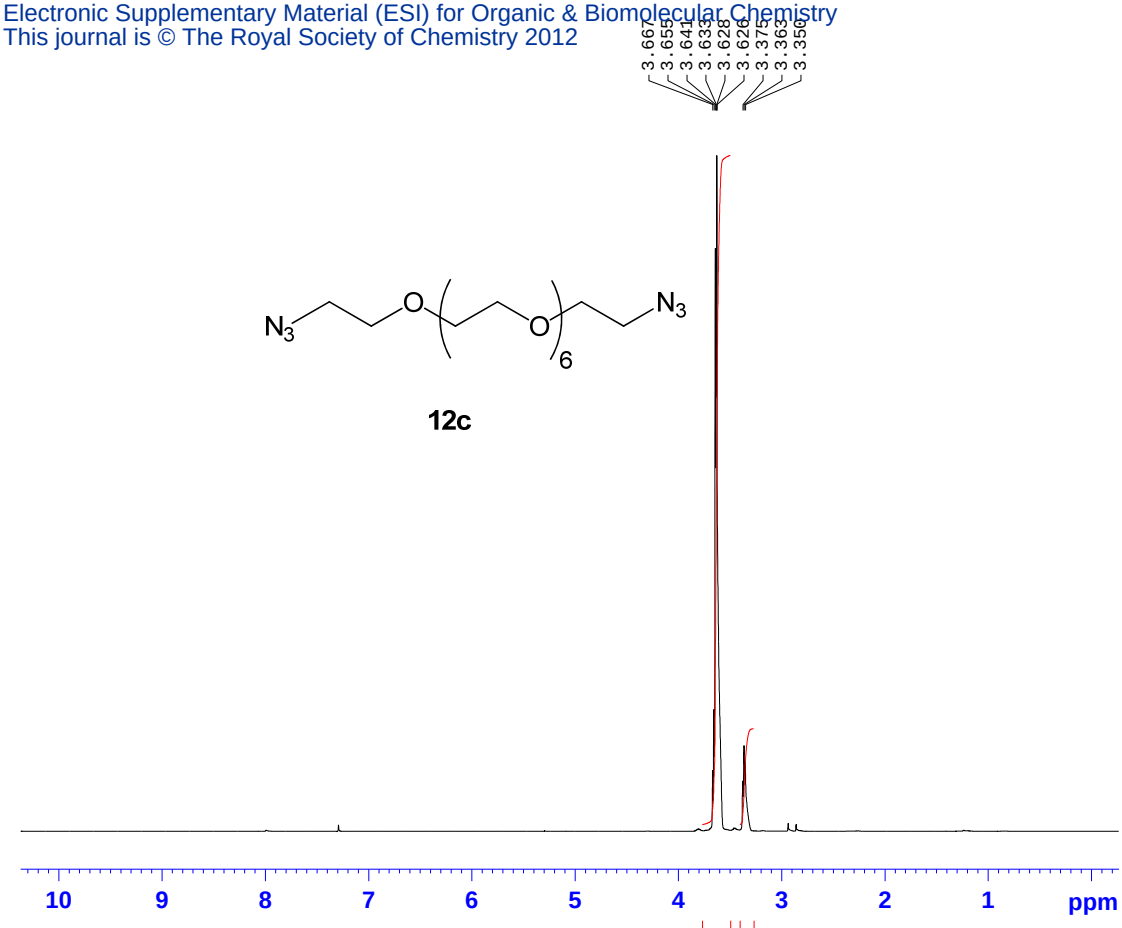
Chemical Formula: $C_{16}H_{33}N_3O_8$
Exact Mass: 395.2268

11c

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0174991E-007
Calibration Constant B	78.221559
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	149.90
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

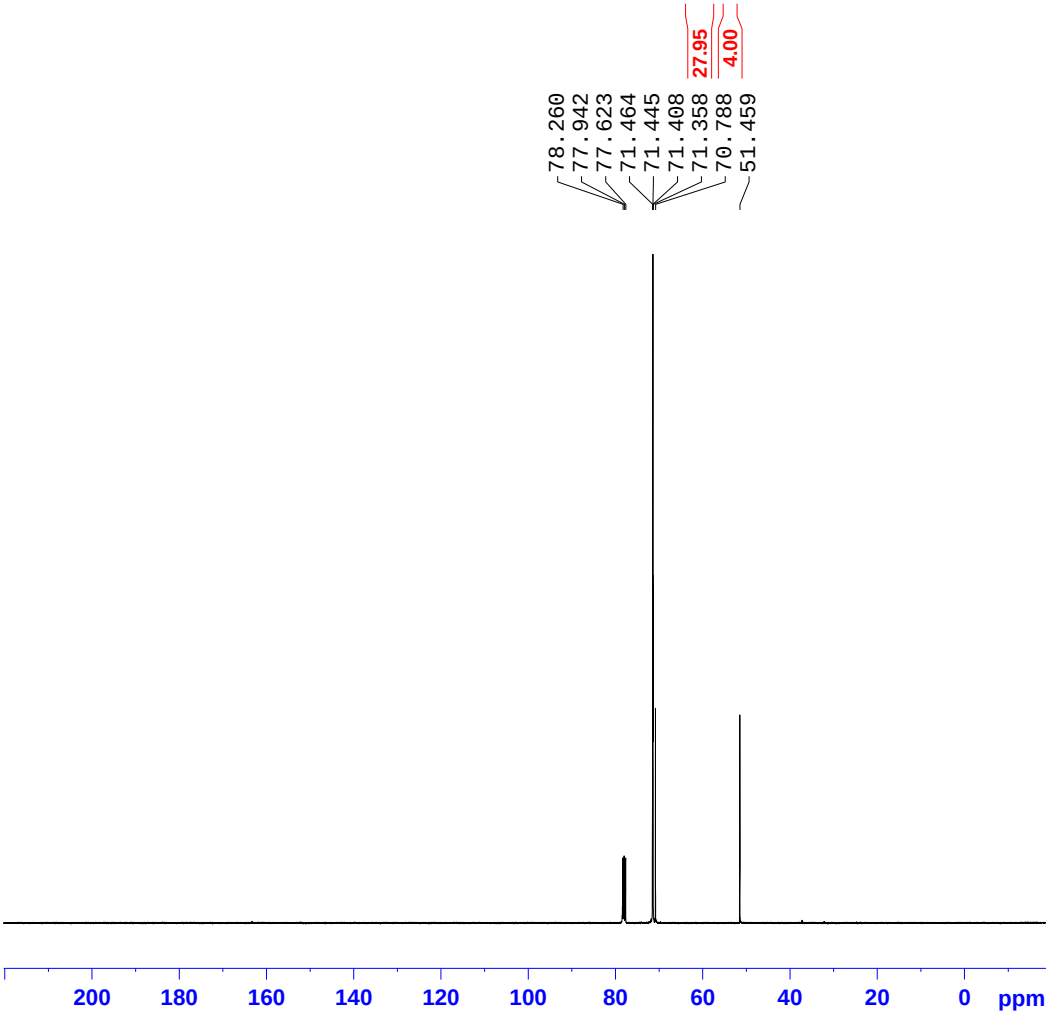
Acquired: Jun 17 11:19:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Jun\17 Fri\SJS-R12-frac4001.dat

Printed: 11:21, June 17, 2011




```
NAME      LG-674_OEG-Di-N3
EXPNO                    1
PROCNO                   1
Date_             20110413
Time                 17.55
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                   22.6
DW                 56.800 usec
DE                  6.50 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                      1

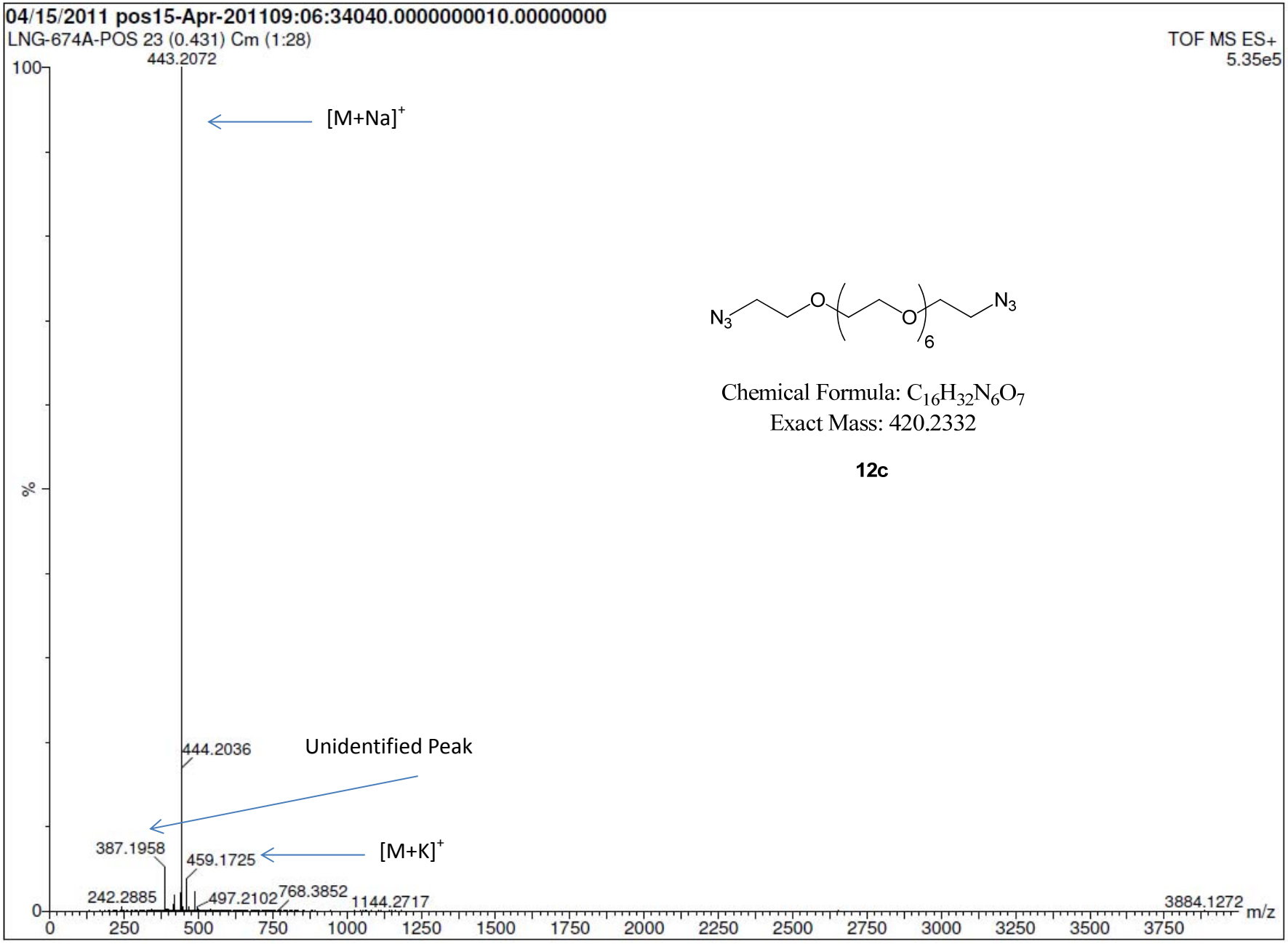
======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      LG-674_OEG-Di-N3
EXPNO                    2
PROCNO                   1
Date_             20110413
Time                 18.56
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   80.6
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

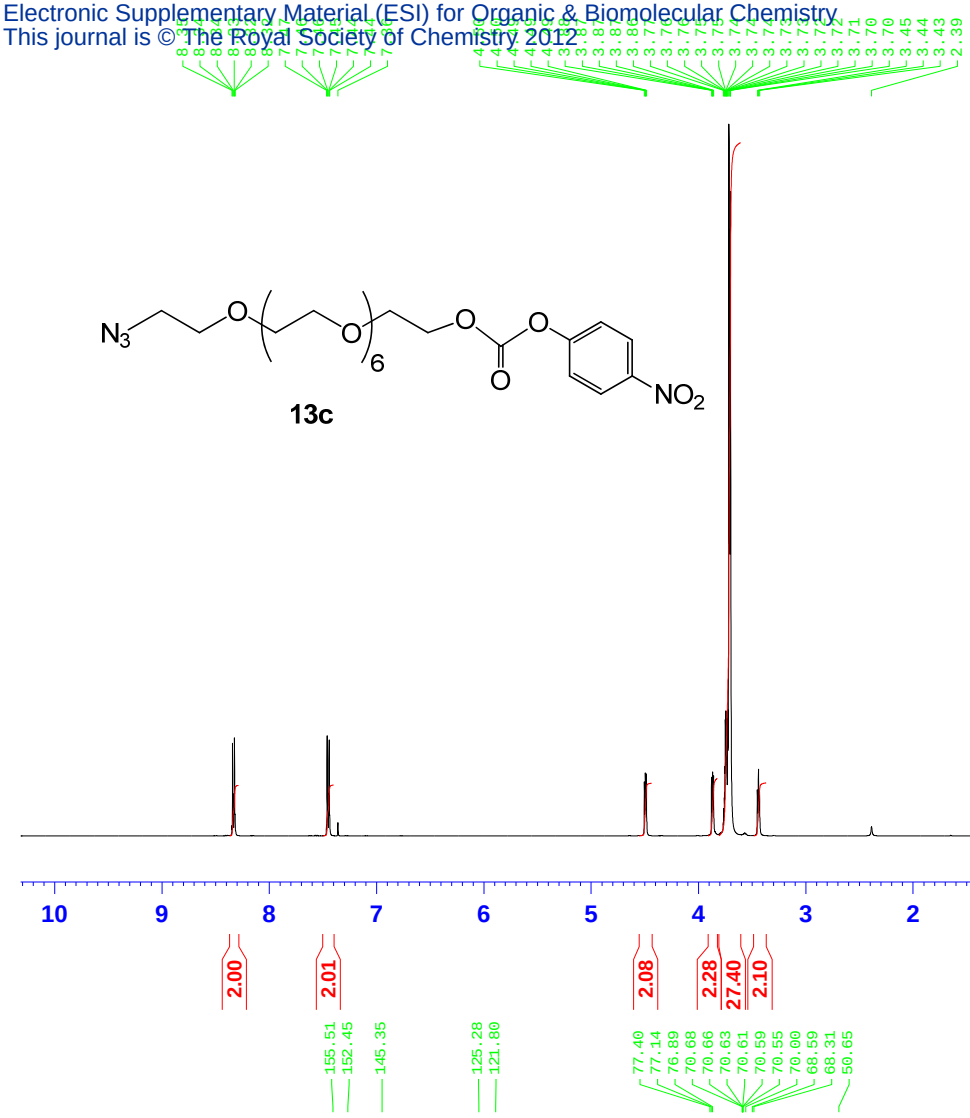
======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



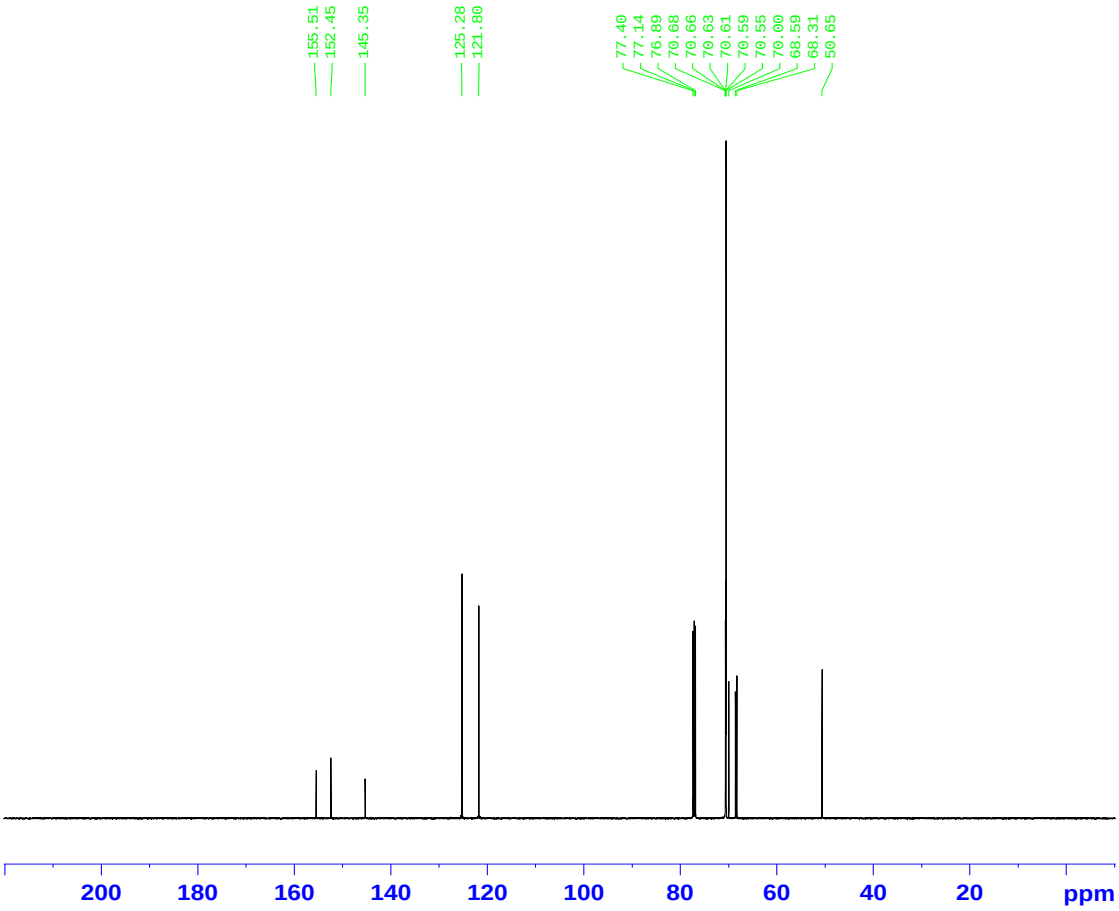
Chemical Formula: $C_{16}H_{32}N_6O_7$
Exact Mass: 420.2332

12c




```
NAME      LG-832_N3-OEG-PNPC
EXPNO                    1
PROCNO                   1
Date_             20111122
Time                 23.09
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        2
SWH              10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2769001 sec
RG                     28.5
DW                  50.000 usec
DE                   6.50 usec
TE                  294.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.75 usec
PL1                   1.20 dB
PL1W          17.72078514 W
SFO1          500.1330008 MHz
SI                    32768
SF            500.1299631 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



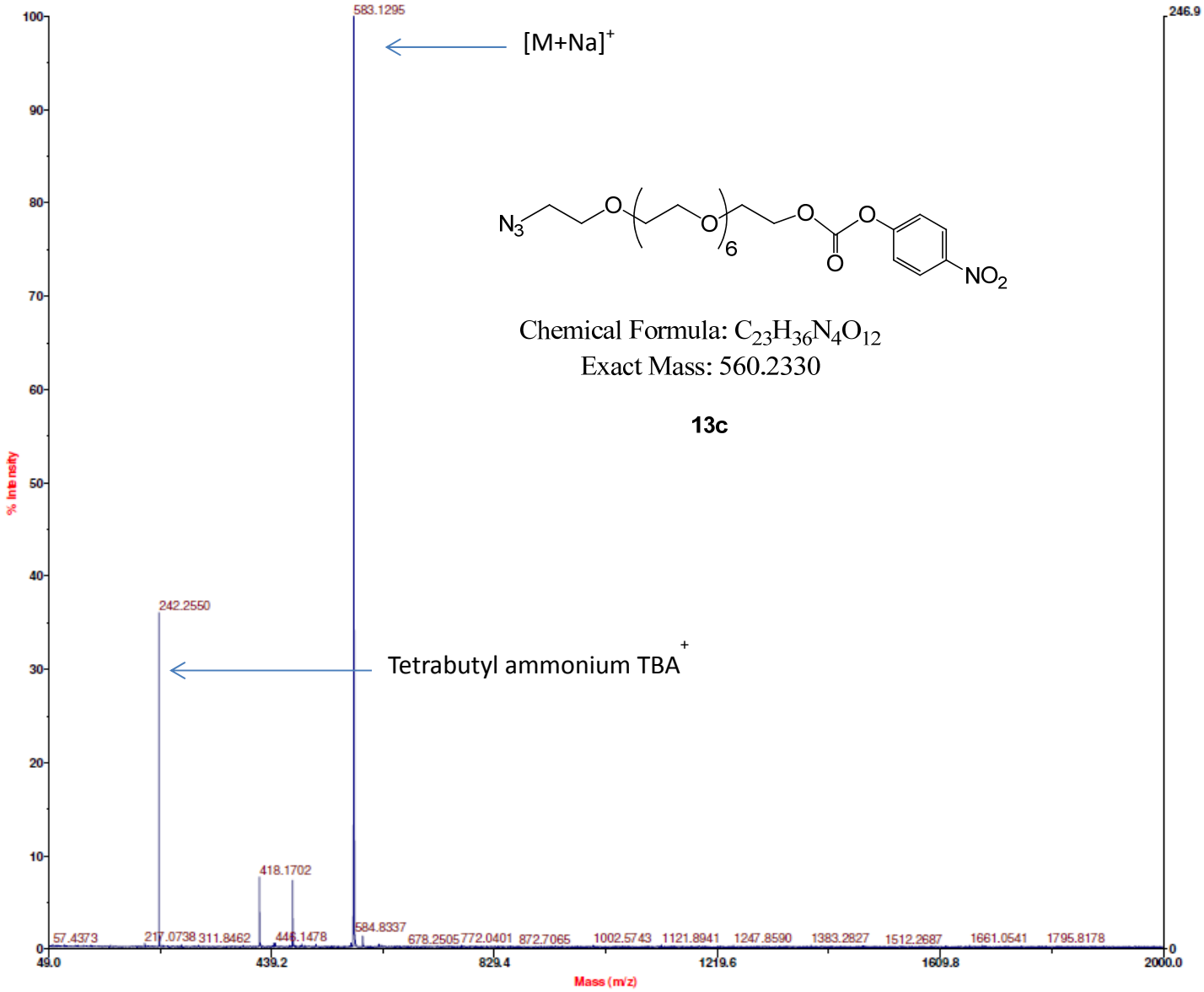

```
NAME      LG-832_N3-OEG-PNPC
EXPNO                    2
PROCNO                   1
Date_             20111123
Time                  0.06
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              28985.508 Hz
FIDRES           0.442284 Hz
AQ               1.1305633 sec
RG                     4096
DW                  17.250 usec
DE                   6.50 usec
TE                  296.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.83 usec
PL1                   0.00 dB
PL1W          80.88274384 W
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   1.20 dB
PL12                 15.40 dB
PL13                 15.40 dB
PL2W          17.72078514 W
PL12W          0.67372549 W
PL13W          0.67372549 W
SFO2          500.1320005 MHz
SI                    32768
SF            125.7577890 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:23 (T /0.00:0.39) ASC[BP = 583.1, 247]



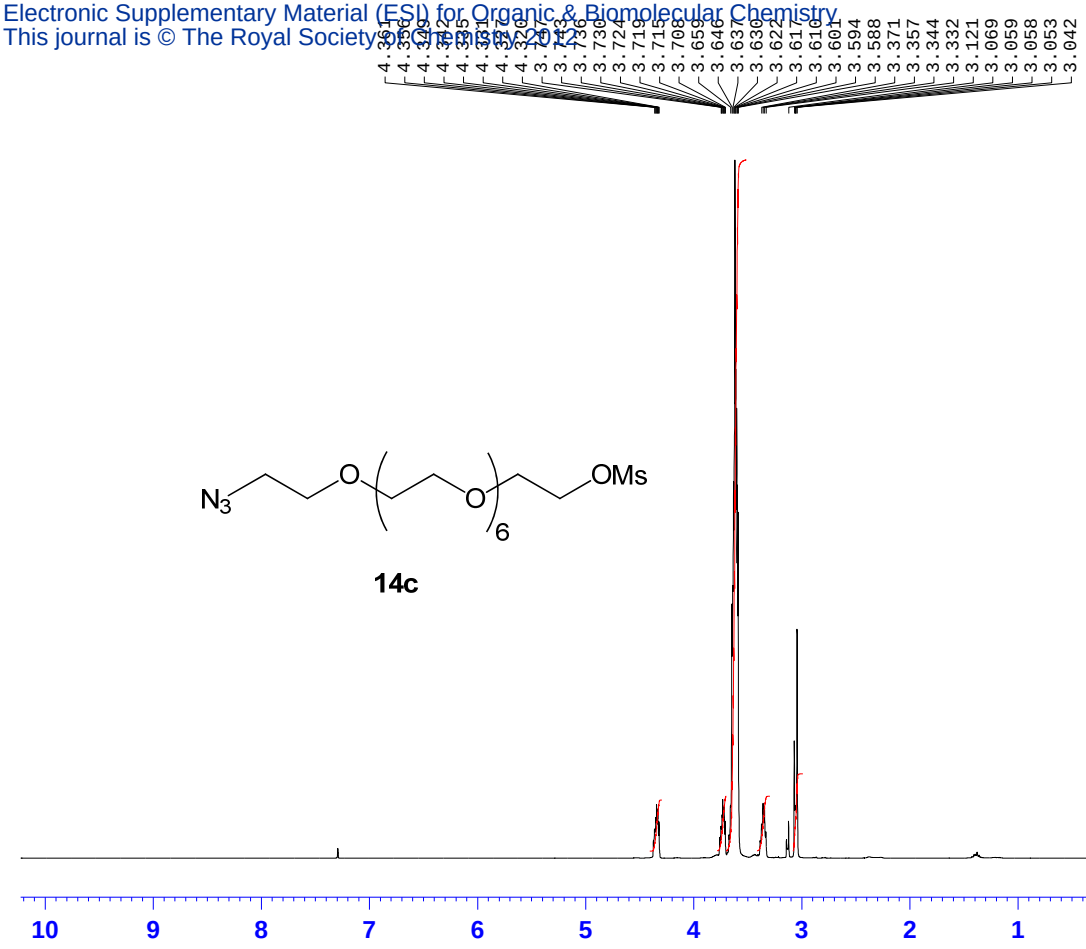
Chemical Formula: $C_{23}H_{36}N_4O_{12}$
Exact Mass: 560.2330

13c

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

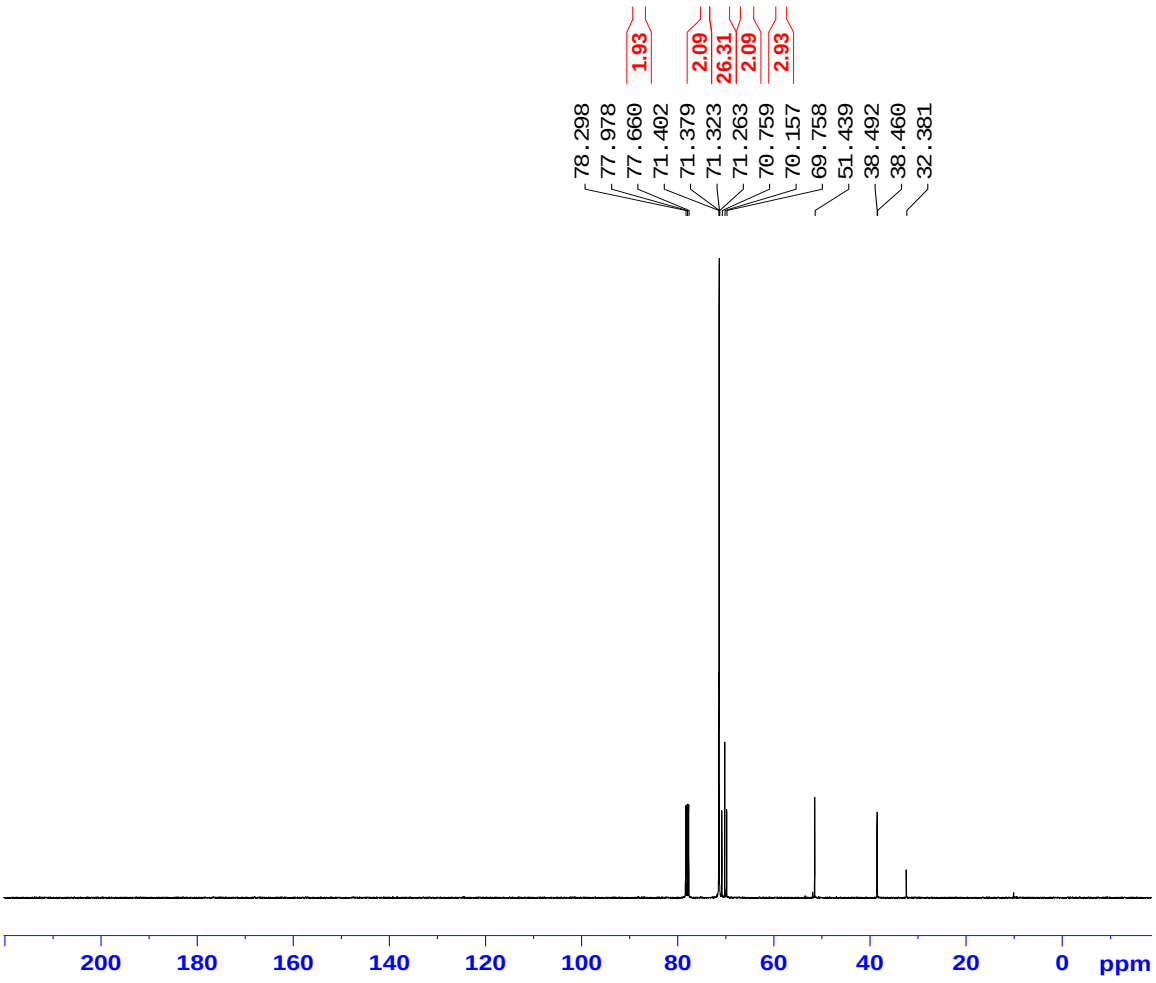
Acquired: Nov 22 15:15:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\22 Tue\LNG-832001.dat

Printed: 15:17, November 22, 2011




```
NAME      LG-678M_OMs-OEG-N3
EXPNO                    1
PROCNO                   1
Date_             20110419
Time                19.33
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     64
DS                      2
SWH              8802.817 Hz
FIDRES           0.134320 Hz
AQ               3.7224948 sec
RG                   25.4
DW                 56.800 usec
DE                  6.50 usec
TE                 292.6 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.85 usec
PL1                 -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

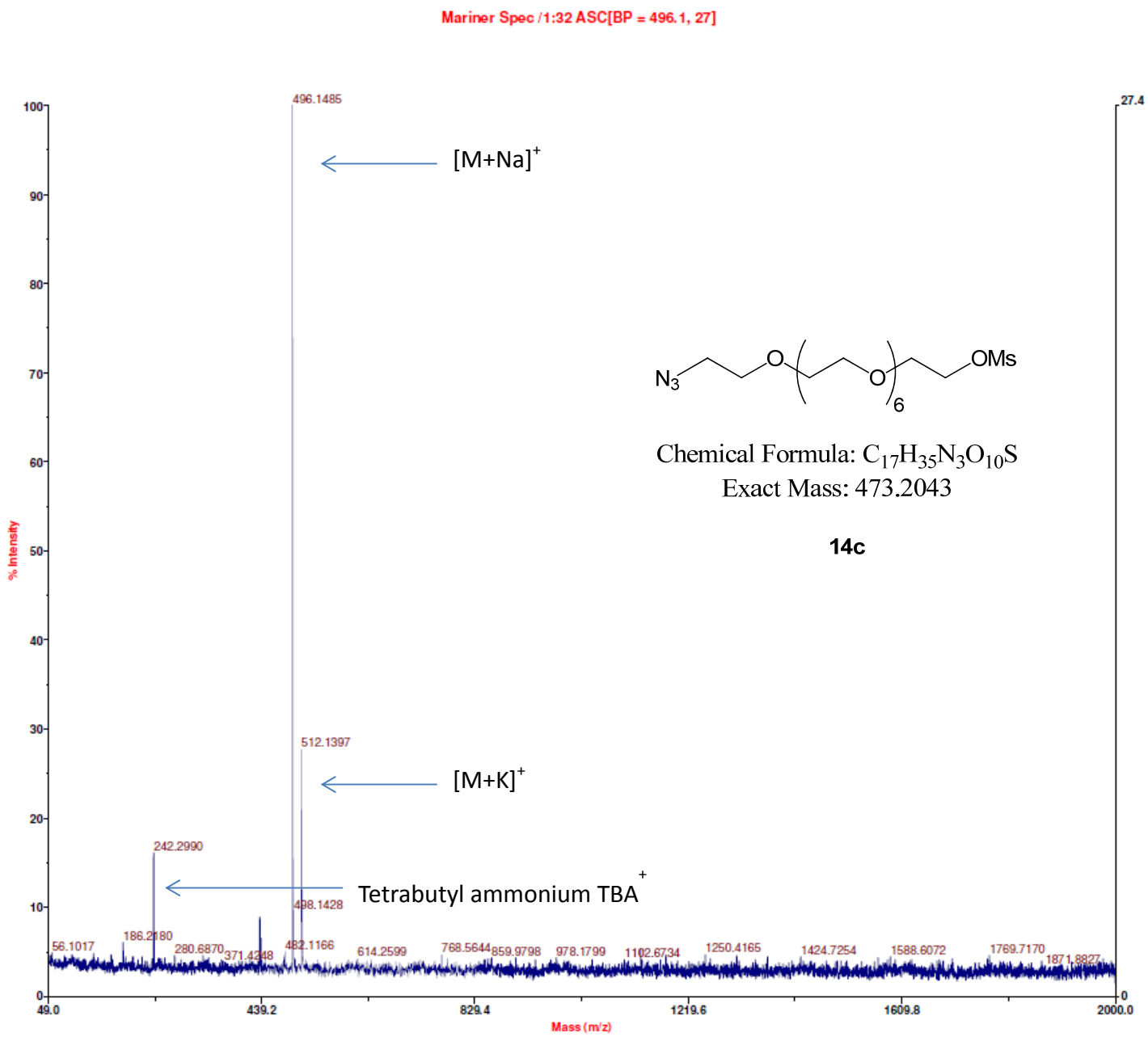



```
NAME      LG-678M_OMs-OEG-N3
EXPNO                    2
PROCNO                   1
Date_             20110419
Time                21.29
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2000
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    912
DW                 20.800 usec
DE                  6.50 usec
TE                 294.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.99 usec
PL1                 -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -0.65 dB
PL12                13.40 dB
PL13                13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6126885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268



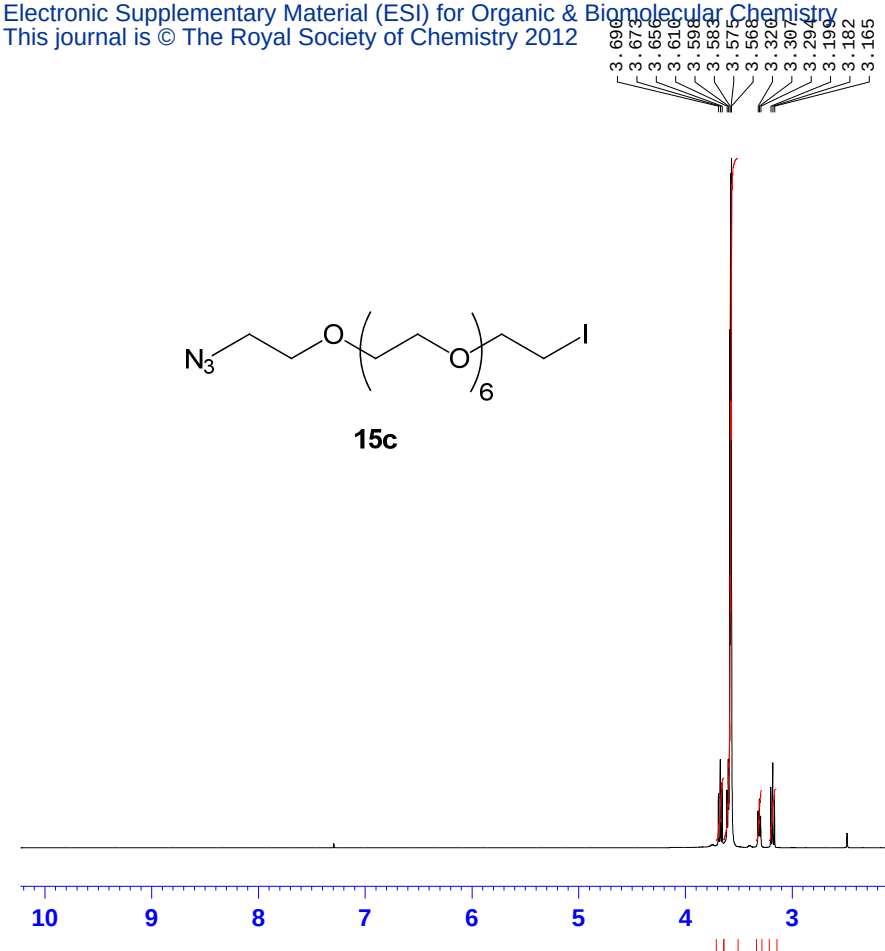
Chemical Formula: $C_{17}H_{35}N_3O_{10}S$
Exact Mass: 473.2043

14c

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0142059E-007
Calibration Constant B	75.342573
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	149.90
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

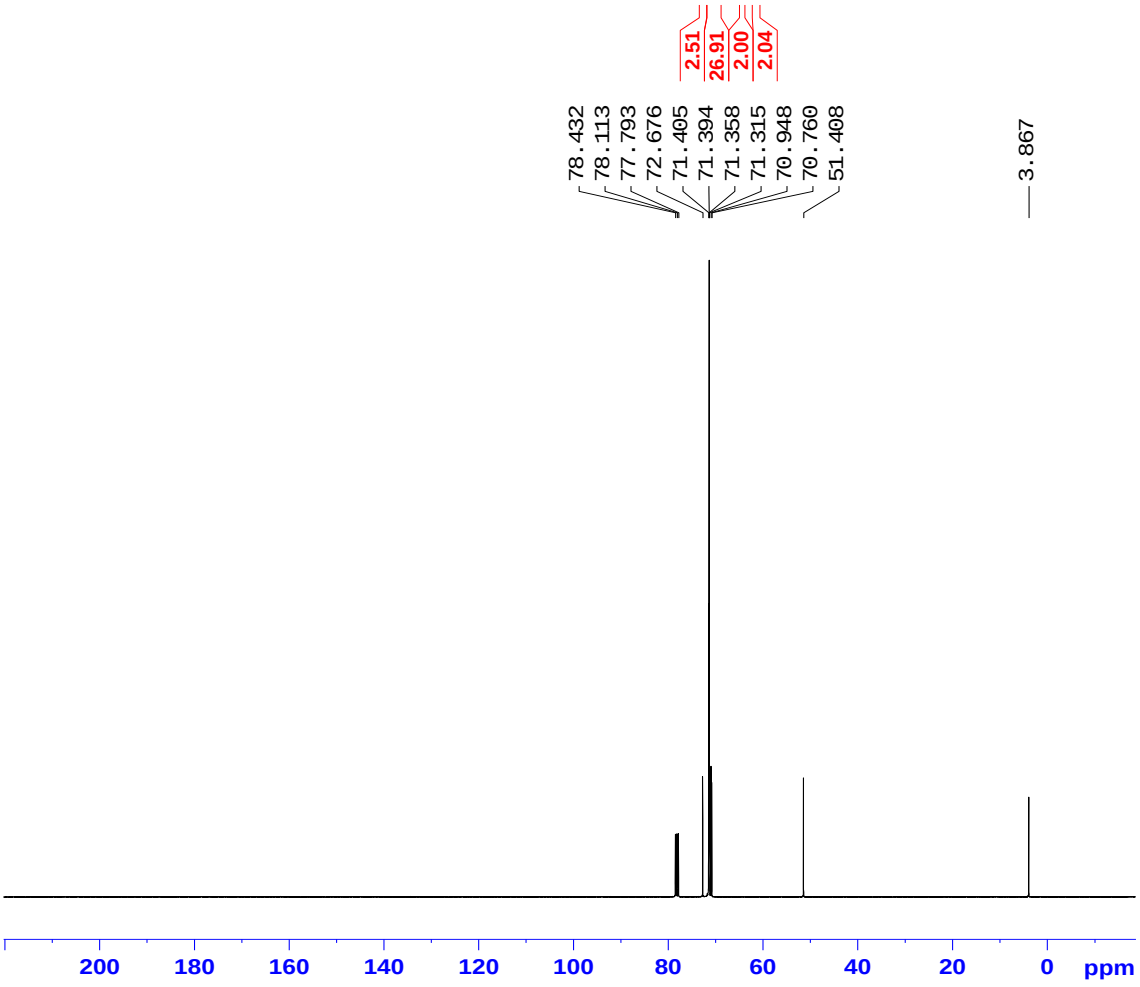
Acquired: Apr 20 11:02:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Apr\20 Wed\LNG-678M001.dat

Printed: 11:17, April 20, 2011




```
NAME      LG-679_Iodo-OEG-N3
EXPNO                    1
PROCNO                   1
Date_             20110420
Time                 19.41
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ               3.7224948 sec
RG                      16
DW                  56.800 usec
DE                   6.50 usec
TE                  292.9 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.85 usec
PL1                 -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```



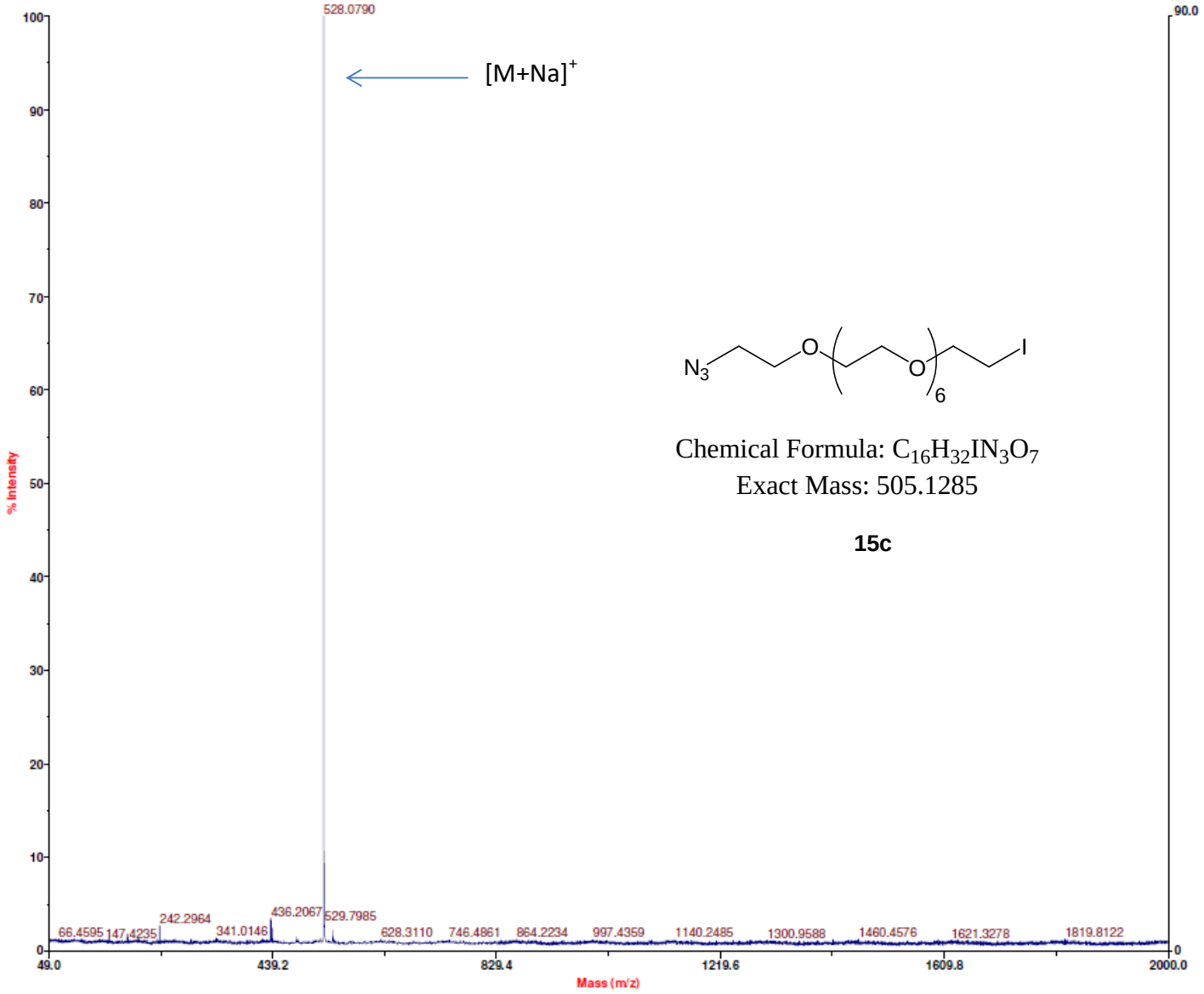

```
NAME      LG-679_Iodo-OEG-N3
EXPNO                    2
PROCNO                   1
Date_             20110420
Time                 20.41
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                     912
DW                  20.800 usec
DE                   6.50 usec
TE                  294.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.99 usec
PL1                 -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -0.65 dB
PL12                13.40 dB
PL13                13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6126885 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                  1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:71 ASC[BP = 528.1, 90]



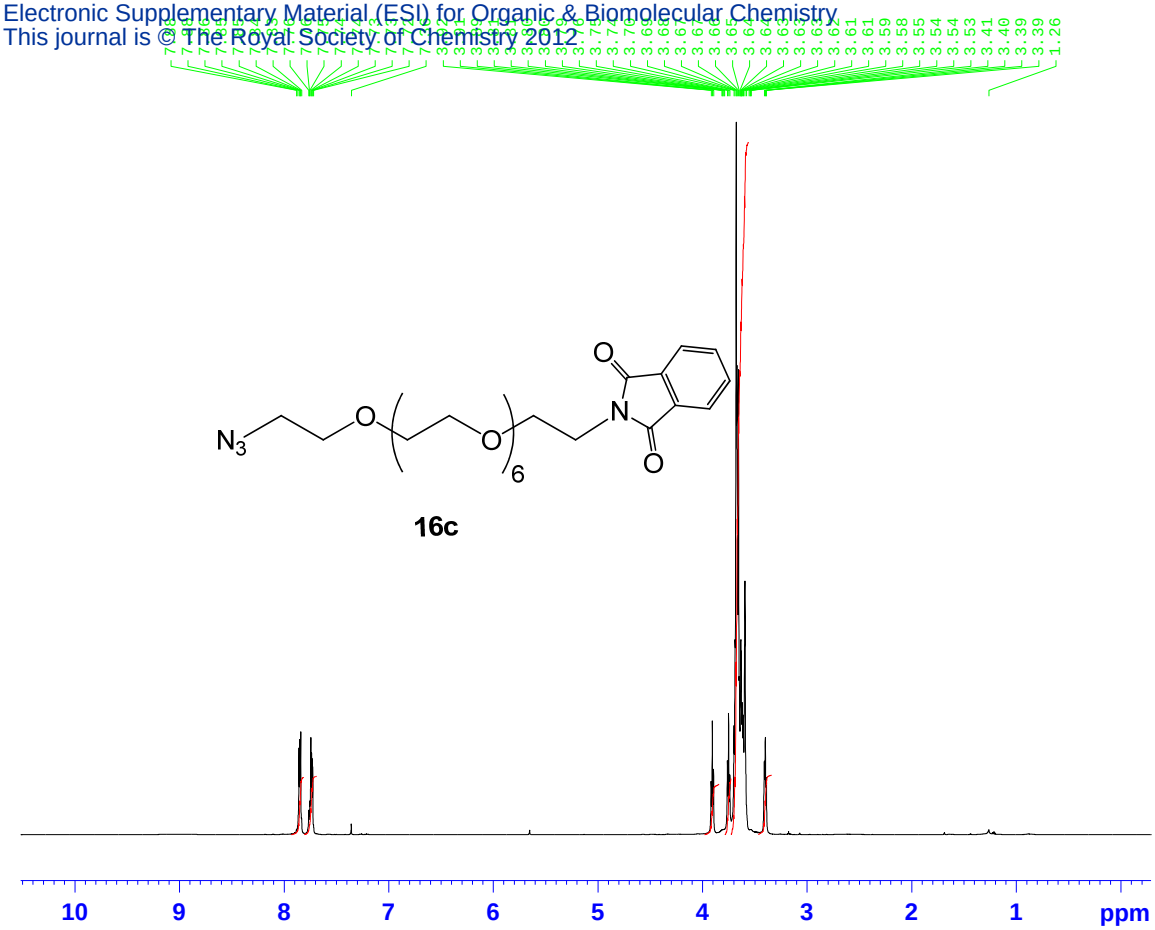
Chemical Formula: $C_{16}H_{32}IN_3O_7$
Exact Mass: 505.1285

15c

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0142059E-007
Calibration Constant B	75.342573
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

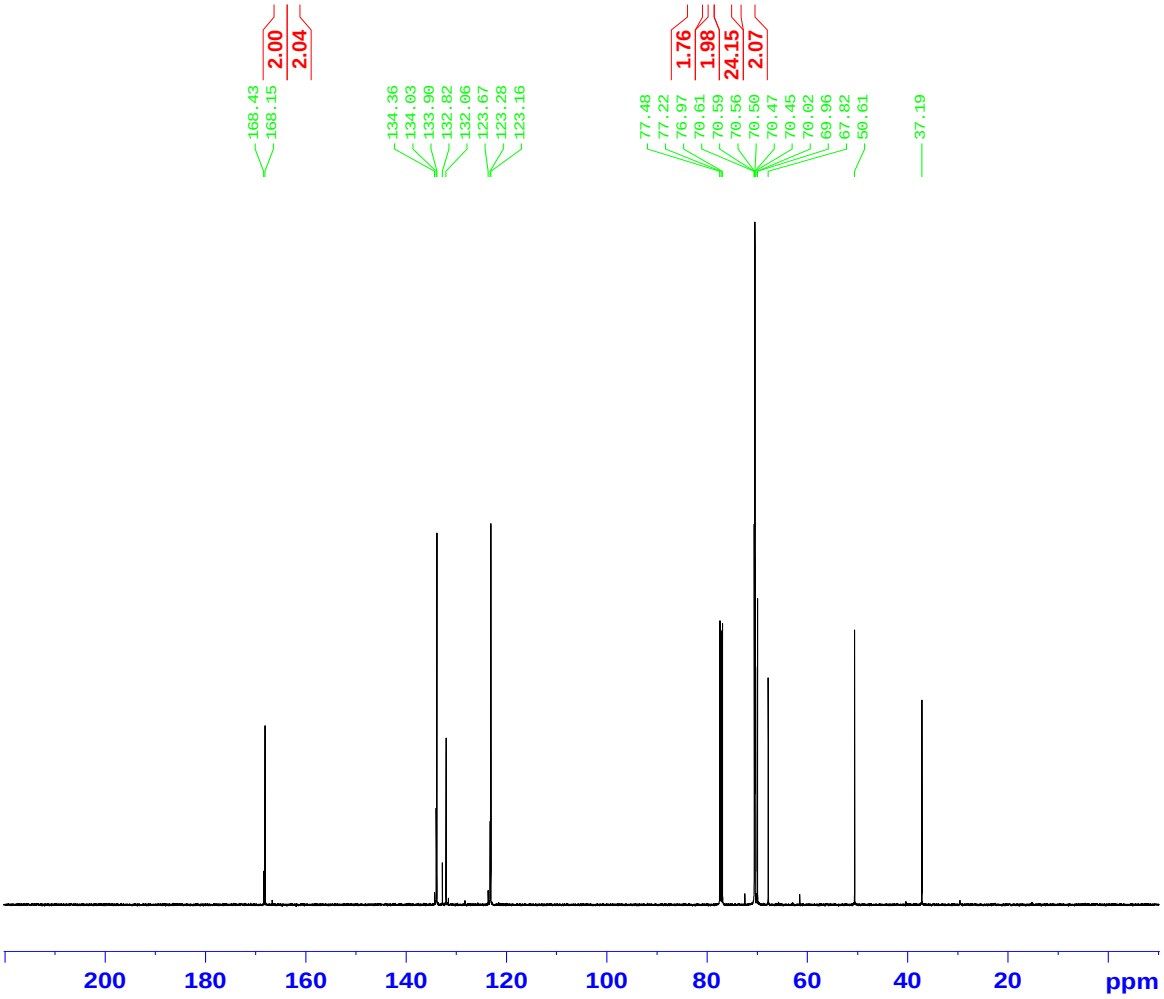
Acquired: Apr 20 13:58:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Apr\20 Wed\LNG-679M001.dat

Printed: 14:00, April 20, 2011




```
NAME      LG-833M_N3-OEG-NPth
EXPNO                       4
PROCNO                      1
Date_            20111123
Time                    23.41
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        64
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2769001 sec
RG                        18
DW                    50.000 usec
DE                     6.50 usec
TE                    294.5 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.75 usec
PL1                     1.20 dB
PL1W              17.72078514 W
SFO1              500.1330008 MHz
SI                     32768
SF                500.1299631 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



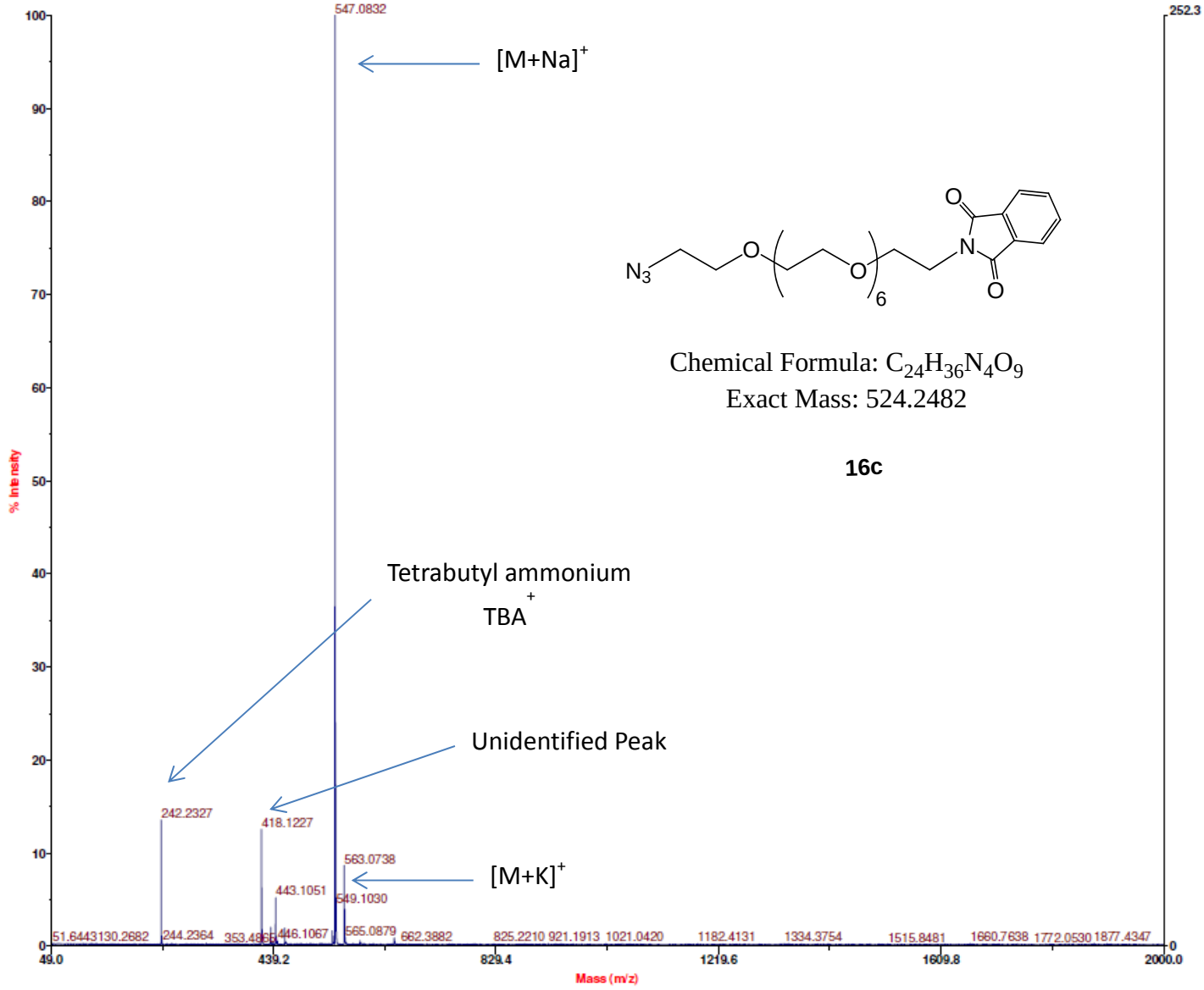

```
NAME      LG-833M_N3-OEG-NPth
EXPNO                       2
PROCNO                      1
Date_            20111123
Time                    22.42
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                28985.508 Hz
FIDRES             0.442284 Hz
AQ                 1.1305633 sec
RG                      4096
DW                    17.250 usec
DE                     6.50 usec
TE                    296.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.83 usec
PL1                     0.00 dB
PL1W              80.88274384 W
SFO1              125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     1.20 dB
PL12                   15.40 dB
PL13                   15.40 dB
PL2W              17.72078514 W
PL12W              0.67372549 W
PL13W              0.67372549 W
SFO2              500.1320005 MHz
SI                     32768
SF                125.7577890 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:31 (T /0.00:0.53) ASC[BP = 547.1, 252]



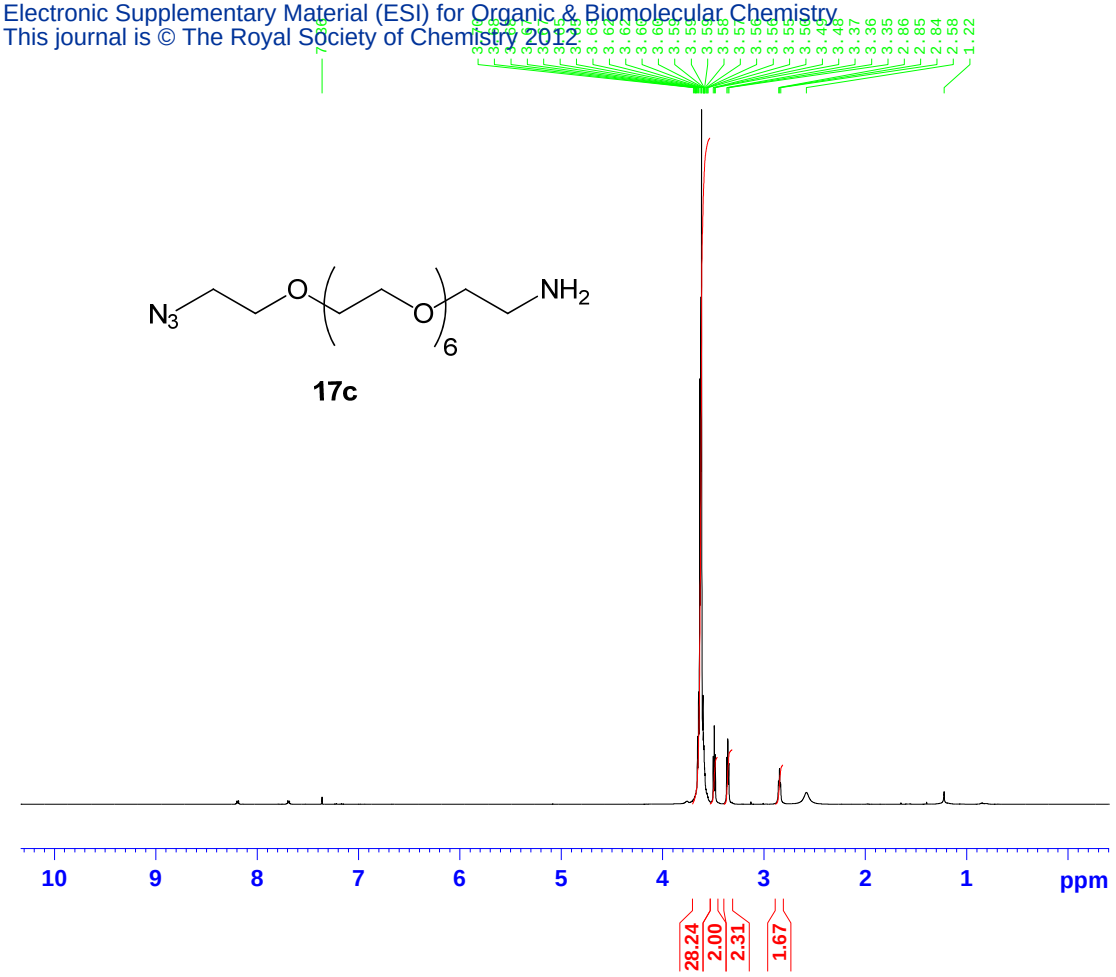
Chemical Formula: $C_{24}H_{36}N_4O_9$
Exact Mass: 524.2482

16c

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	120.12
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

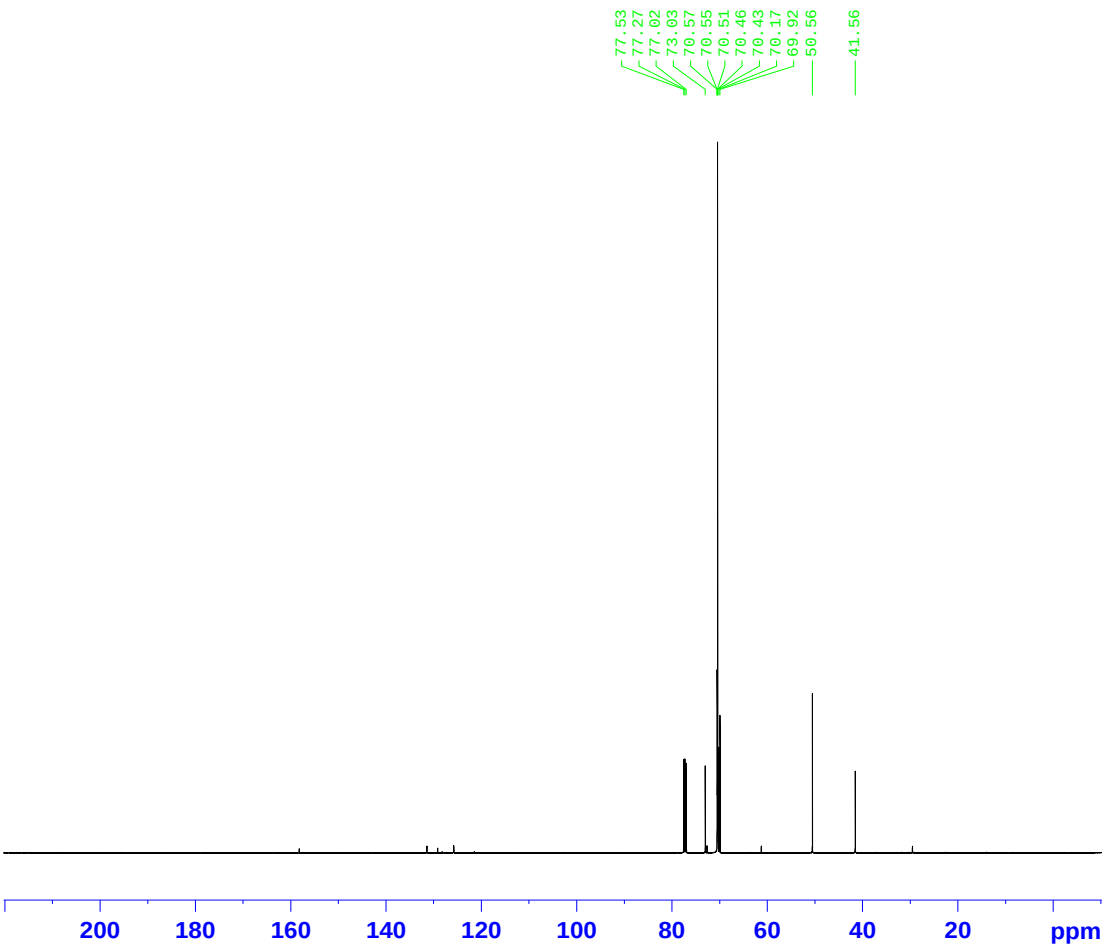
Acquired: Nov 23 11:25:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Nov\23 Wed\LNG-833M002.dat

Printed: 11:26, November 23, 2011




```
NAME      LG-834M_N3-P8-NH2
EXPNO                     5
PROCNO                    1
Date_              20111201
Time                 21.20
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       2
SWH             10000.000 Hz
FIDRES          0.152588 Hz
AQ              3.2769001 sec
RG                    11.3
DW                  50.000 usec
DE                   6.50 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.75 usec
PL1                  1.20 dB
PL1W          17.72078514 W
SFO1          500.1330008 MHz
SI                   32768
SF            500.1299631 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



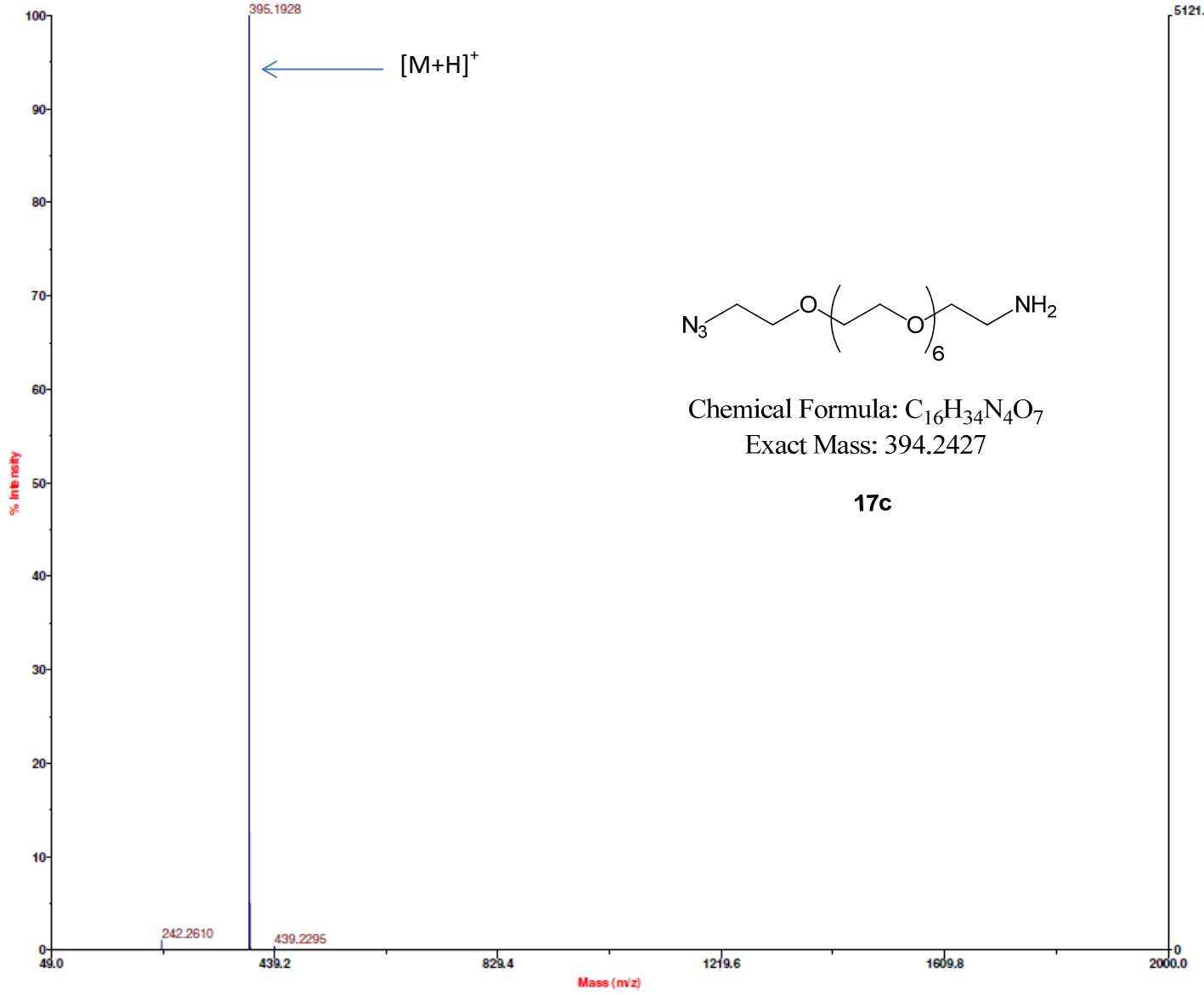

```
NAME      LG-834M_N3-P8-NH2
EXPNO                     2
PROCNO                    1
Date_              20111201
Time                 20.21
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             28985.508 Hz
FIDRES          0.442284 Hz
AQ              1.1305633 sec
RG                    4096
DW                  17.250 usec
DE                   6.50 usec
TE                  300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   8.83 usec
PL1                  0.00 dB
PL1W          80.88274384 W
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   1.20 dB
PL12                 15.40 dB
PL13                 15.40 dB
PL2W          17.72078514 W
PL12W          0.67372549 W
PL13W          0.67372549 W
SFO2          500.1320005 MHz
SI                   32768
SF            125.7577890 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Applied Biosystems Mariner System 5268

Mariner Spec /1:25 (T /0.00:0.43) ASC[BP = 395.2, 5122]



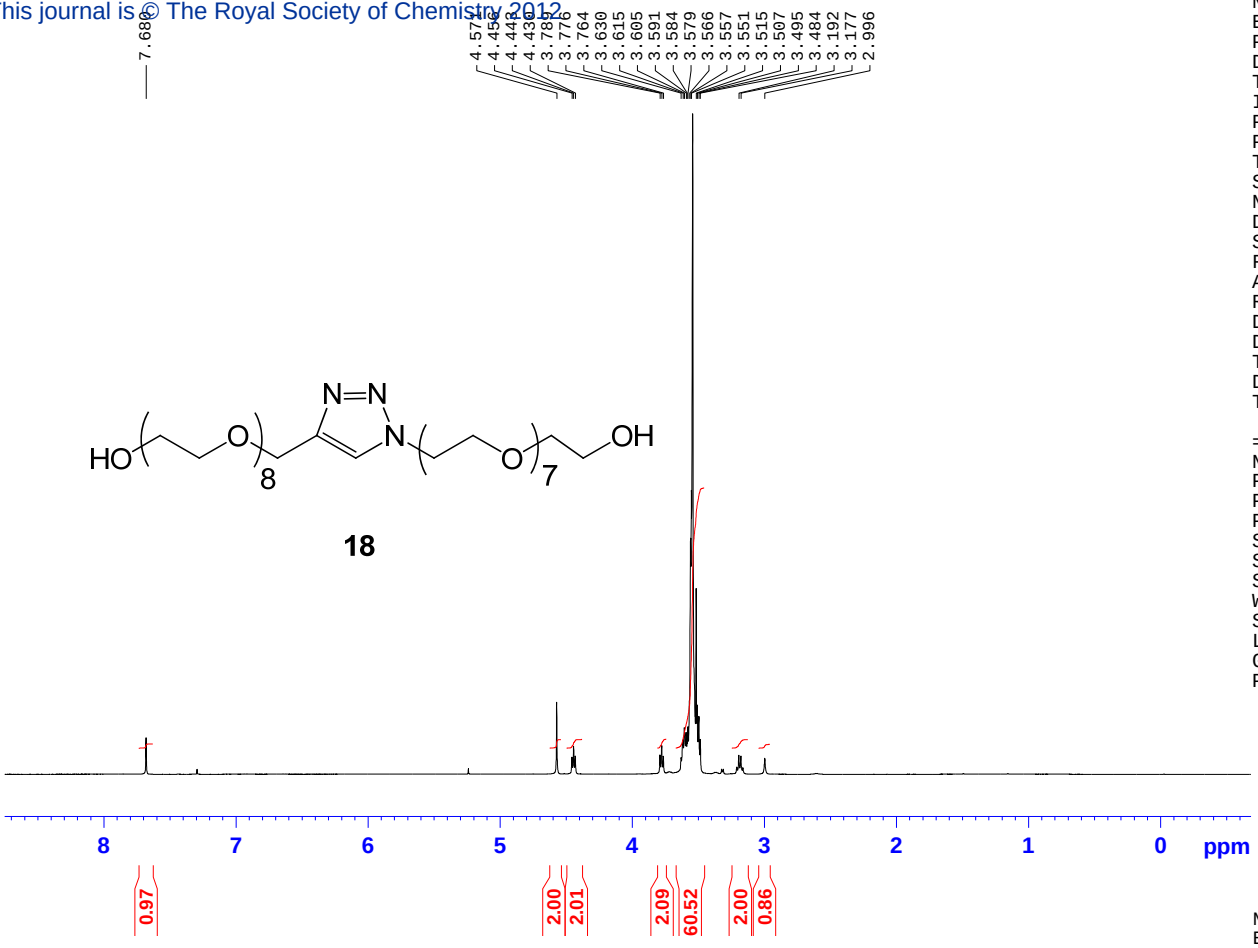
Chemical Formula: $C_{16}H_{34}N_4O_7$
Exact Mass: 394.2427

17c

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0146867E-007
Calibration Constant B	77.798312
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

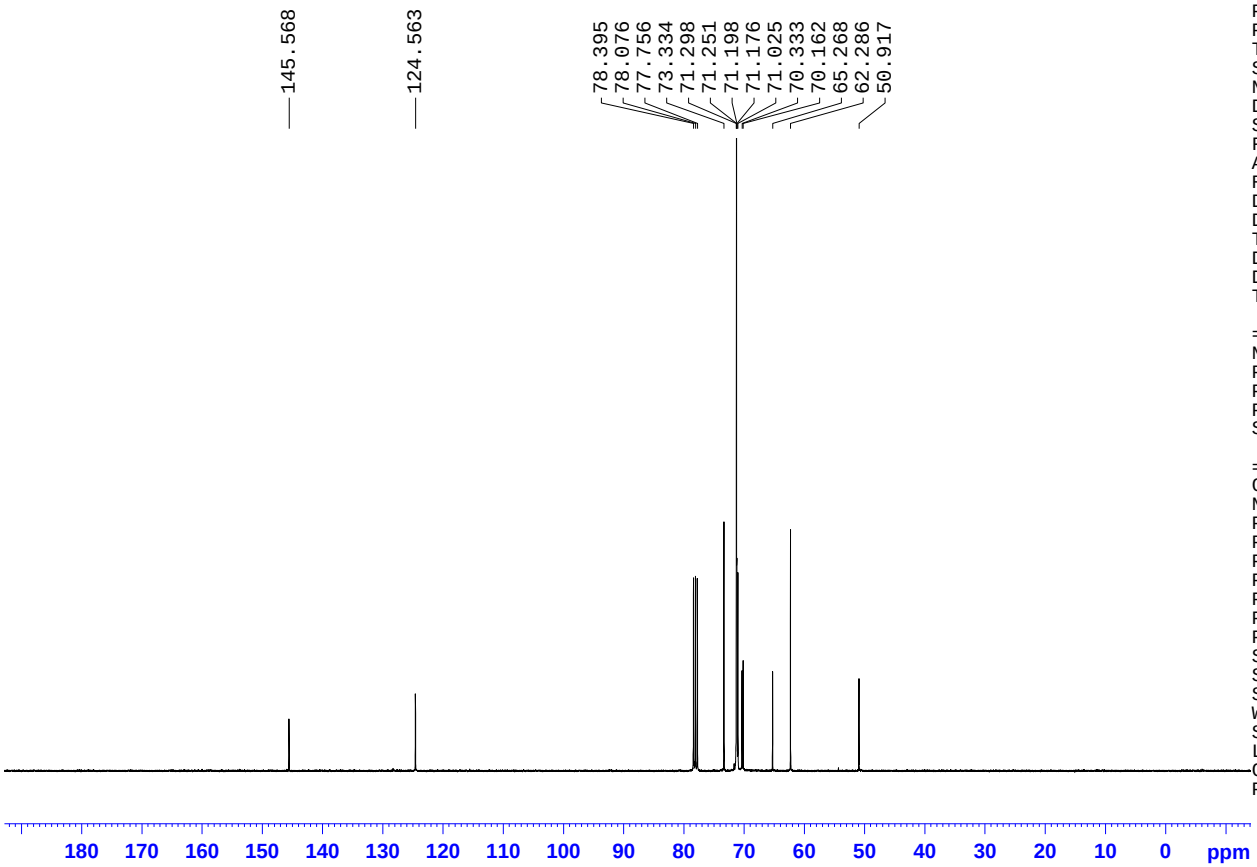
Acquired: Dec 01 10:19:00 2011
Mariner Mass Spectrum
C:\Mariner\Data\2011\Dec\01 Thur\LNG-834M001.dat

Printed: 10:21, December 01, 2011




```
NAME      LG-959_OH-P16-OH
EXPNO                    2
PROCNO                   1
Date_             20120615
Time                 18.32
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ                3.7224948 sec
RG                      18
DW                  56.800 usec
DE                   6.50 usec
TE                   293.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W          13.81451130 W
SFO1          400.1320007 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



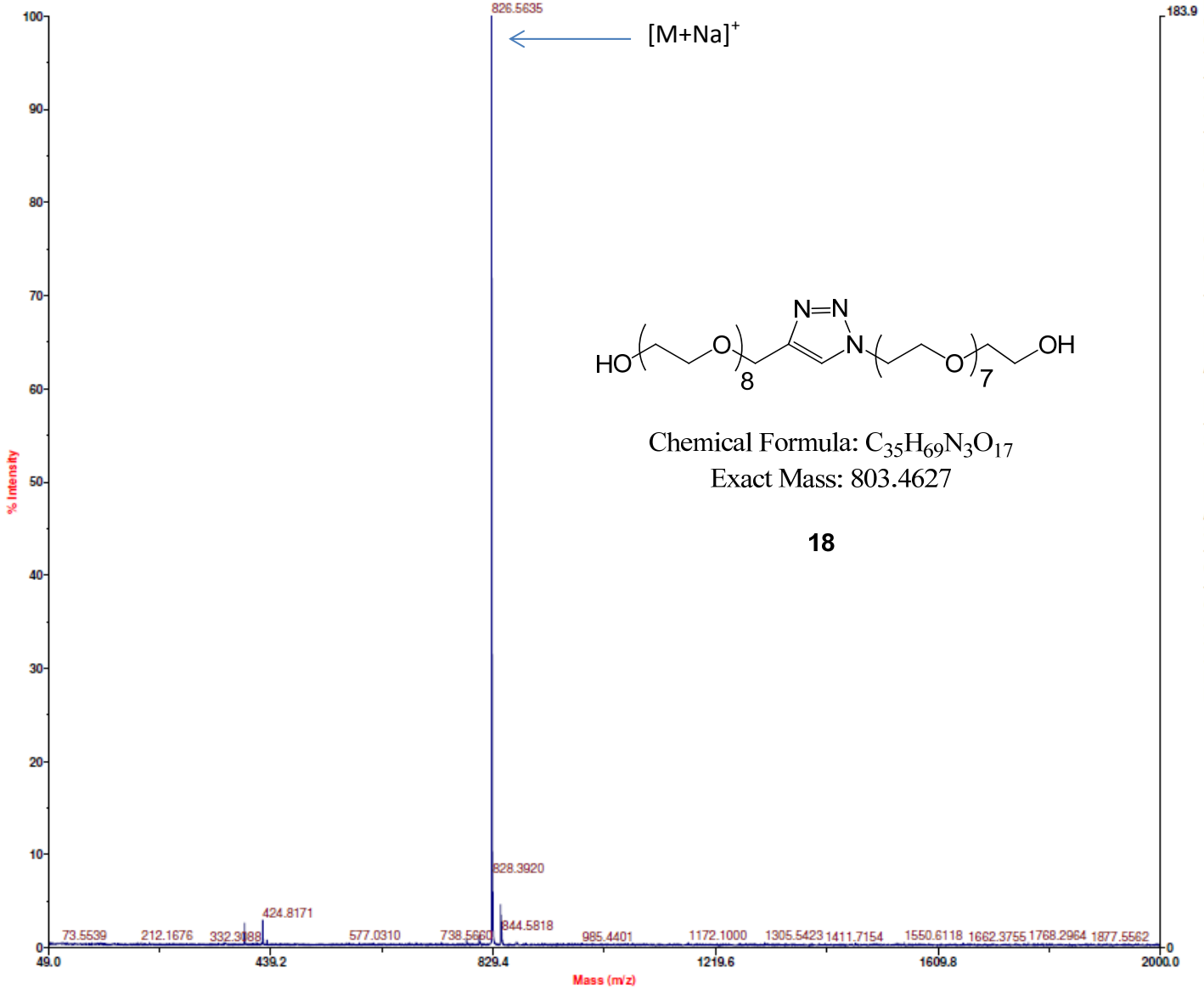

```
NAME      LG-959_OH-P16-OH
EXPNO                    3
PROCNO                   1
Date_             20120615
Time                 19.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    1030
DW                  20.800 usec
DE                   6.50 usec
TE                   296.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W          73.67452240 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W          13.97447491 W
PL12W          0.54996562 W
PL13W          0.54996562 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5219

Mariner Spec /1:24 (T /0.00:0.41) ASC[BP = 826.5, 184]



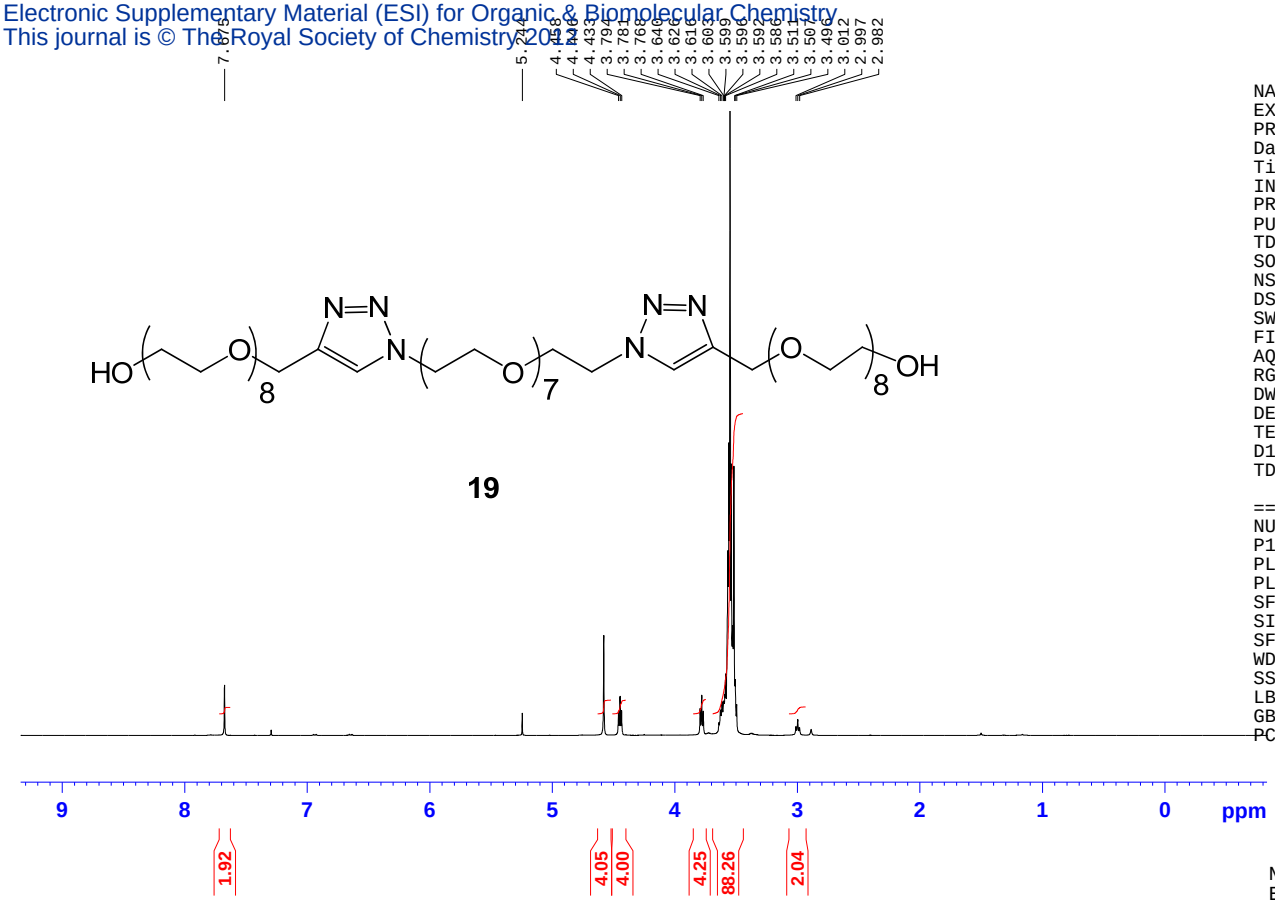
Chemical Formula: $C_{35}H_{69}N_3O_{17}$
Exact Mass: 803.4627

18

--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0149194E-007
Calibration Constant B	78.267402
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

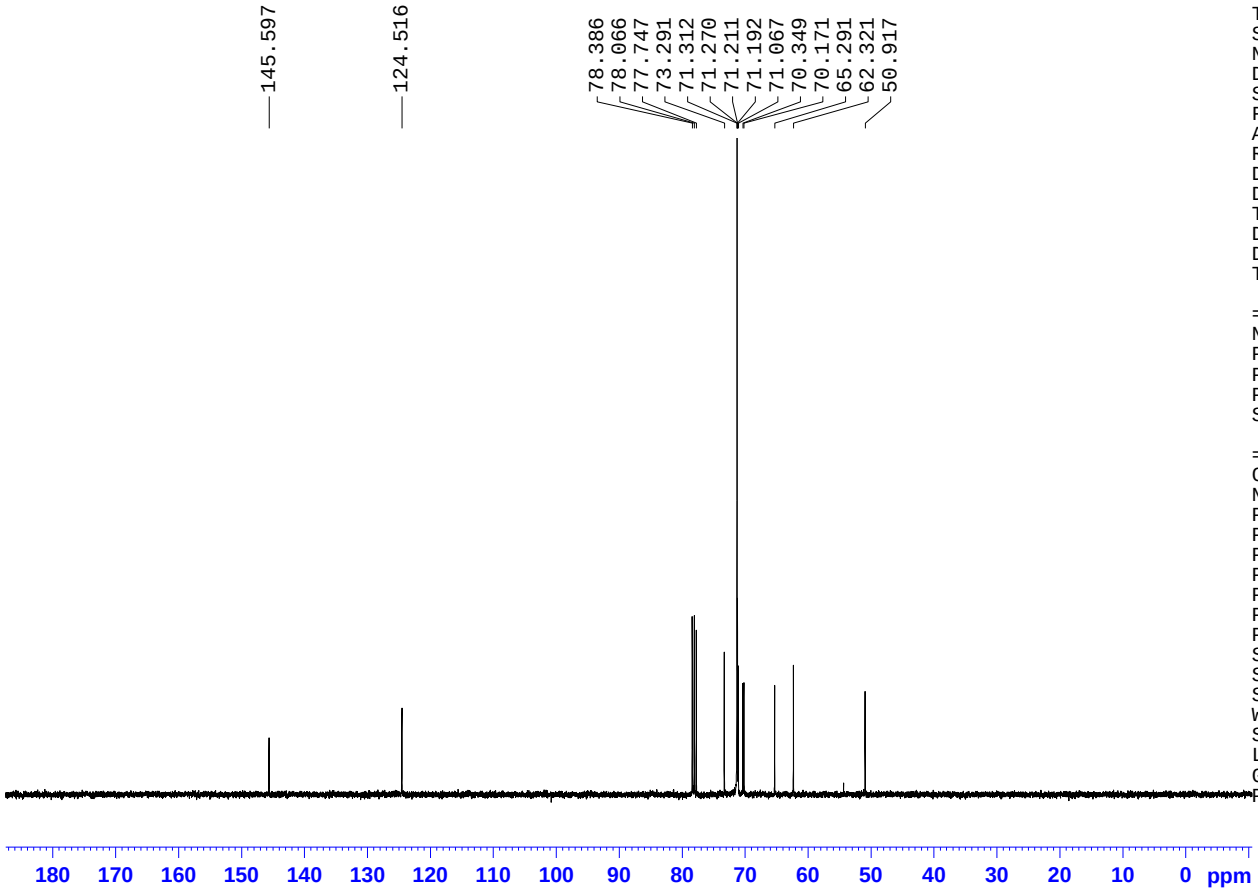
Acquired: Jun 15 13:22:00 2012
Mariner Mass Spectrum
C:\Mariner\Data\2012\June\15 Fri\LNG-959001.dat

Printed: 13:24, June 15, 2012




```
NAME      LG-953_OH-P24-OH
EXPNO                    2
PROCNO                   1
Date_             20120612
Time                 18.29
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8802.817 Hz
FIDRES            0.134320 Hz
AQ                3.7224948 sec
RG                      18
DW                  56.800 usec
DE                   6.50 usec
TE                  293.9 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.85 usec
PL1                  -0.60 dB
PL1W           13.81451130 W
SFO1           400.1320007 MHz
SI                   32768
SF               400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



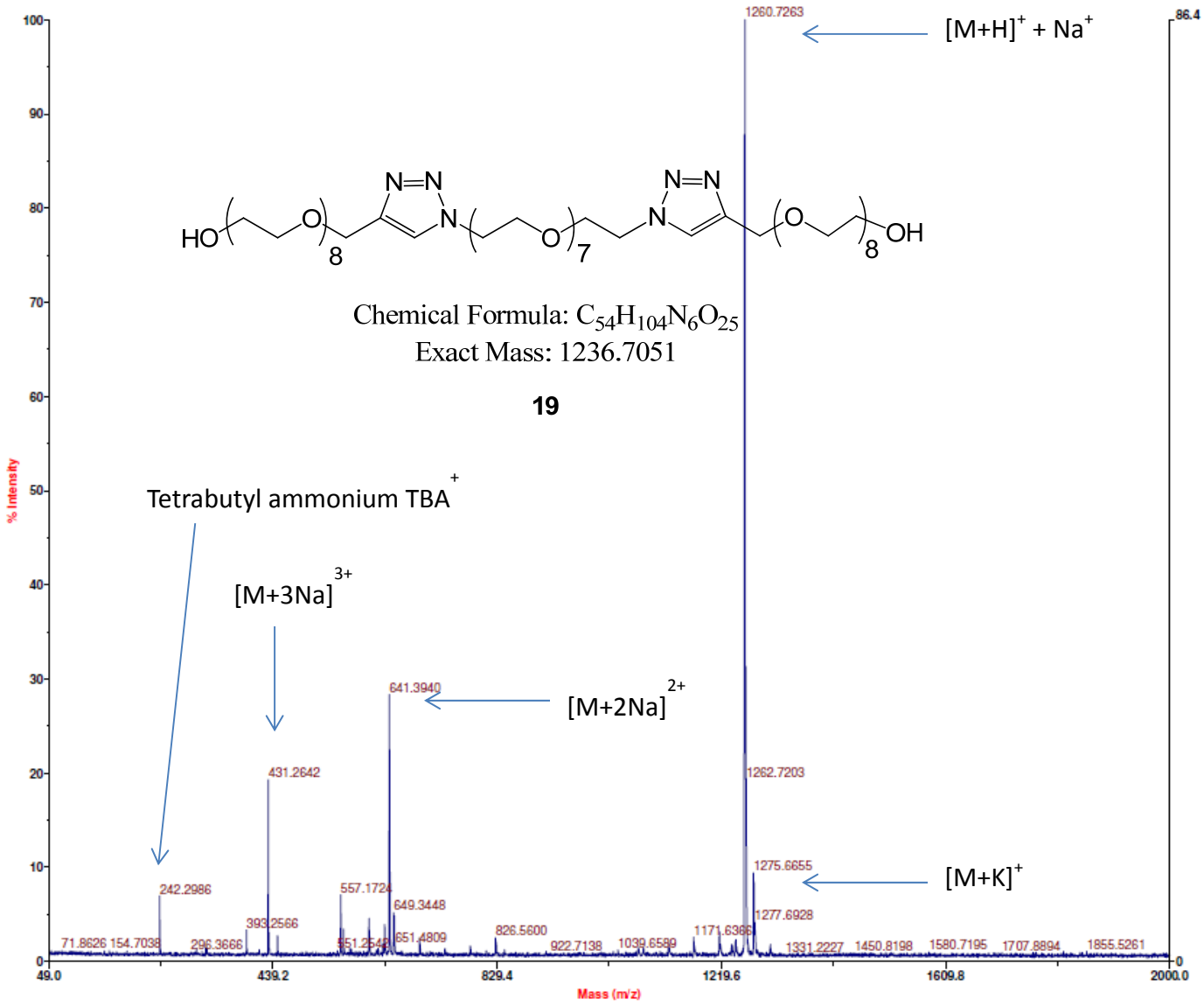

```
NAME      LG-953_OH-P24-OH
EXPNO                    3
PROCNO                   1
Date_             20120613
Time                  1.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                       1
DW                  20.800 usec
DE                   6.50 usec
TE                  296.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.99 usec
PL1                  -3.00 dB
PL1W           73.67452240 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -0.65 dB
PL12                 13.40 dB
PL13                 13.40 dB
PL2W           13.97447491 W
PL12W           0.54996562 W
PL13W           0.54996562 W
SFO2           400.1316005 MHz
SI                   32768
SF               100.6126885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Applied Biosystems Mariner System 5219

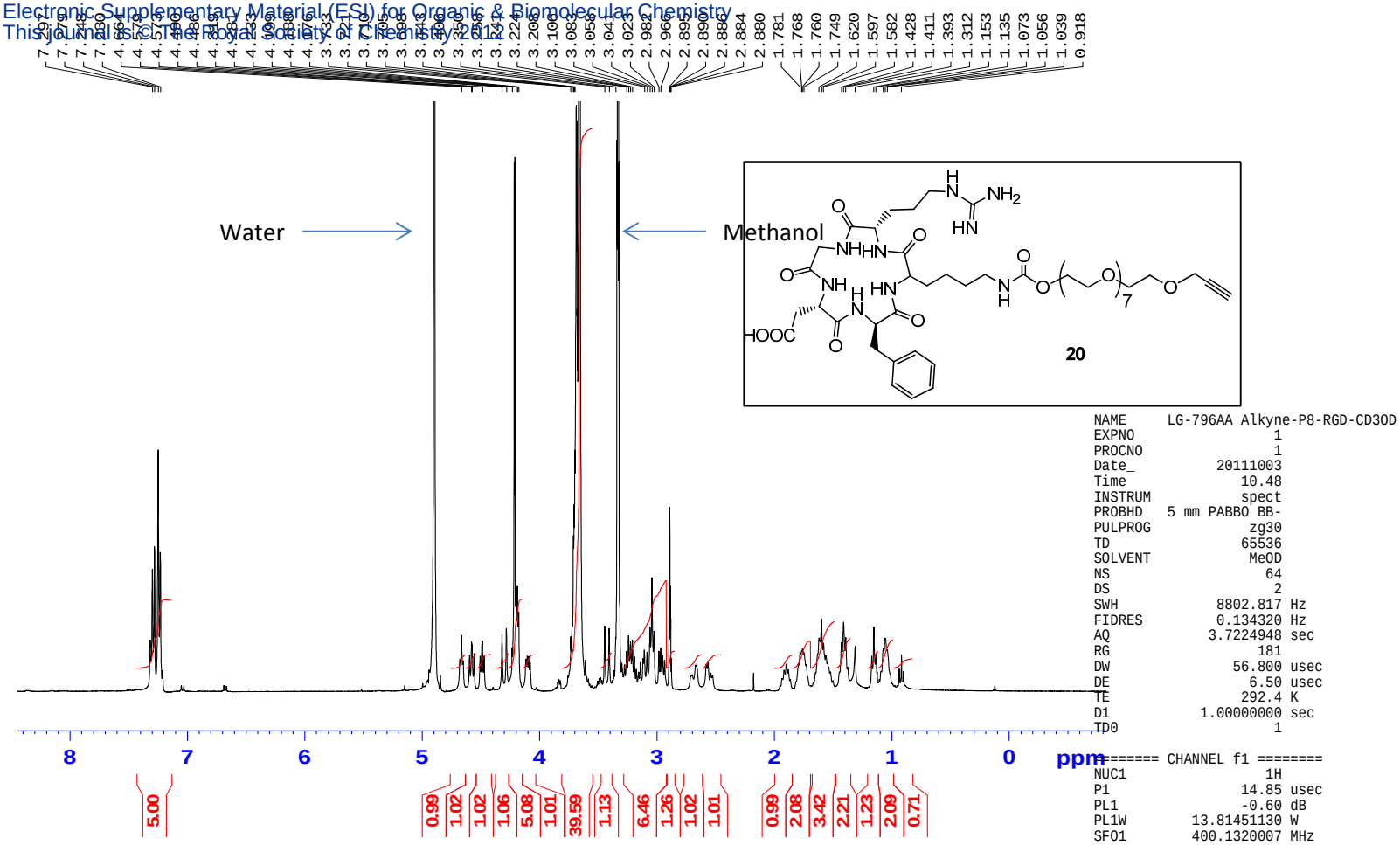
Mariner Spec /1:29 (T /0.00:0.50) ASC[BP = 1260.7, 86]



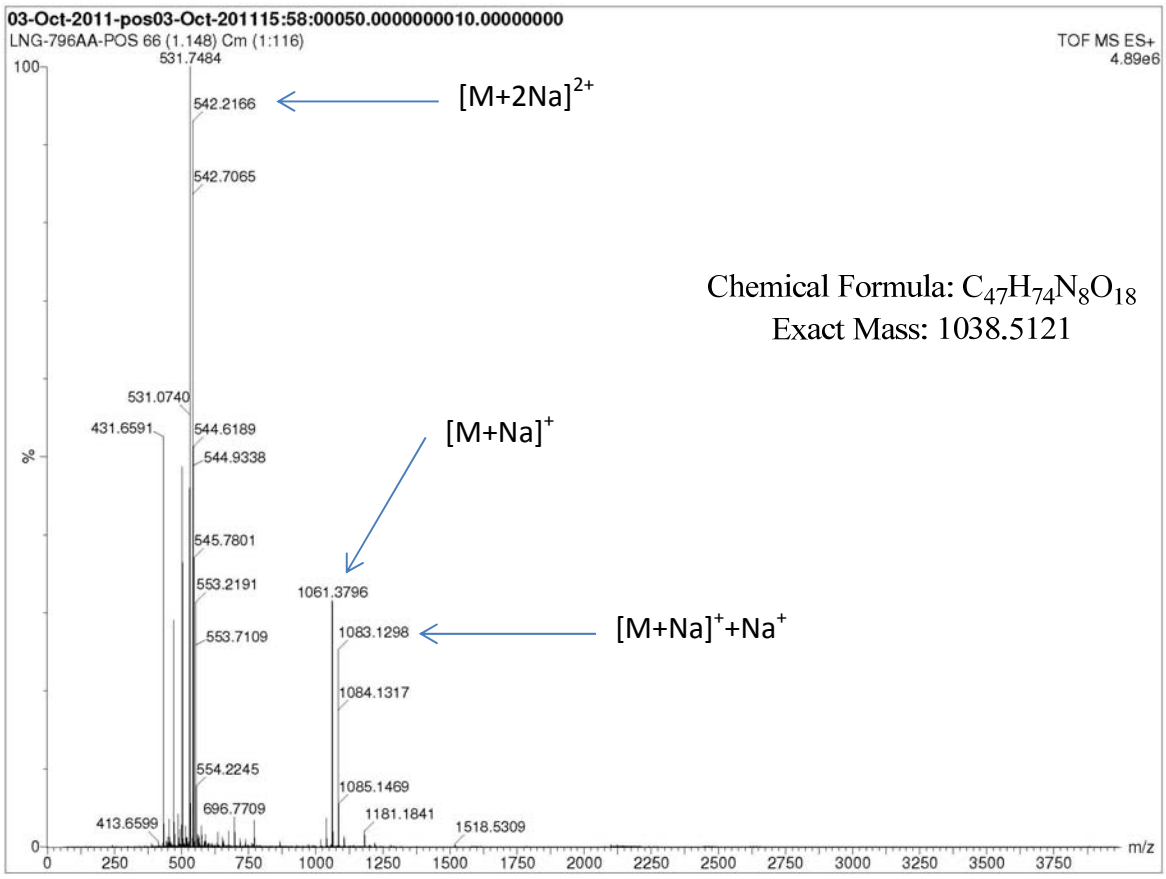
--> Mariner System State <--	
Instrument State	ON
Ion Polarity	POS
Auxillary Gas	ON
Curtain Gas	ON
Nebulizer Gas	ON
Calibration Constant A	5.0149194E-007
Calibration Constant B	78.267402
TDC Deadtime	10
--> Source Settings <--	
Spray Tip Potential	4509.96
SCIEX Heater	300.05
--> API Interface Settings <--	
Nozzle Potential	40.04
Skimmer 1 Potential	10.01
Quadrupole DC Potential	5.49
Deflection Voltage	0.10
Einzel Lens Potential	-24.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
--> Analyzer Settings <--	
Push Pulse Potential	490.00
Pull Pulse Potential	213.11
Pull Bias Potential	10.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1700.24
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	1.00
Ion Count Threshold	0.00
First Mass	50.00
Last Mass	2000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
Centroid Spectra	OFF
--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Manual
Syringe Pump Rate	50.00
Syringe Diameter	3.26
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

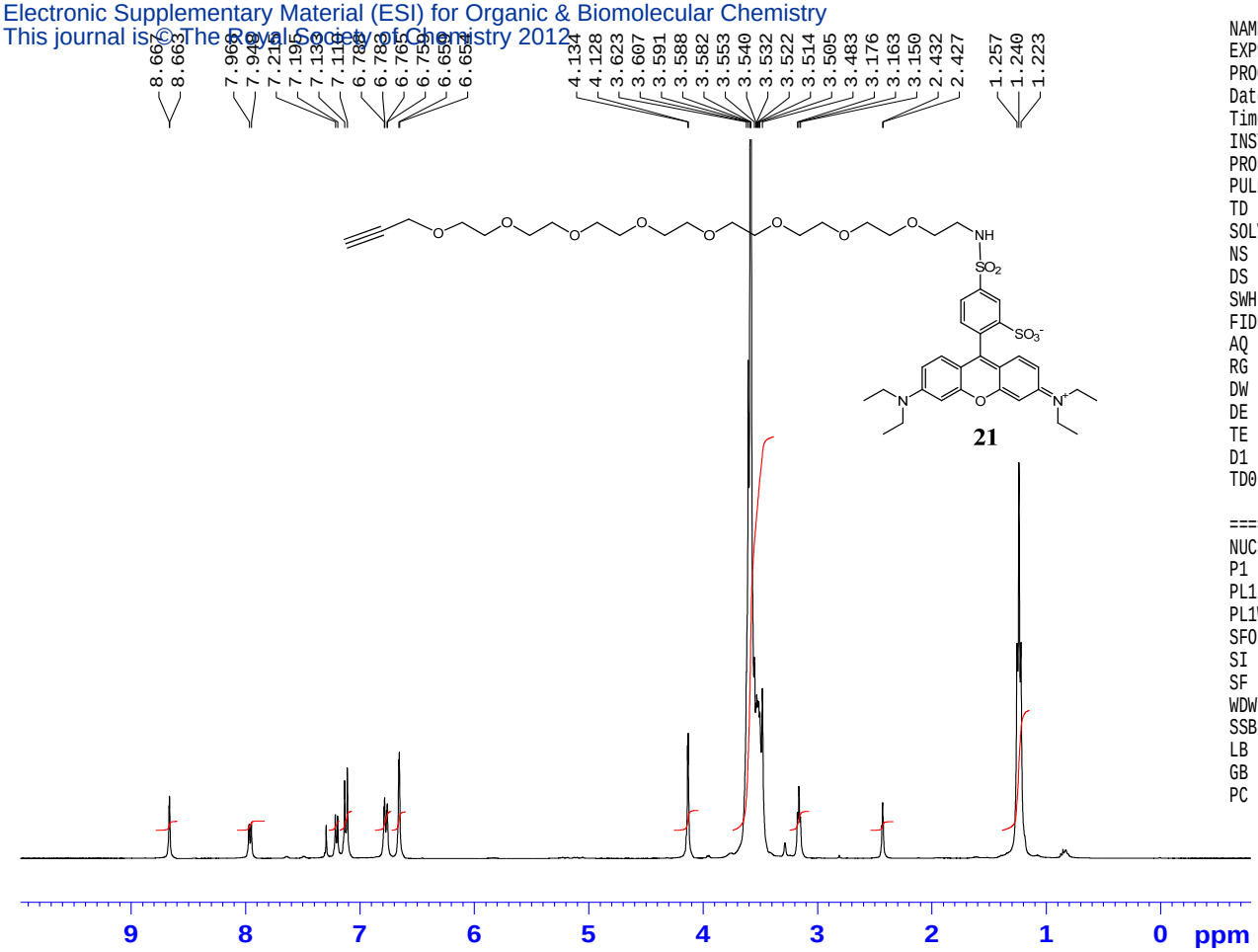
Acquired: Jun 12 14:00:00 2012
Mariner Mass Spectrum
C:\Mariner\Data\2012\June\12 Tue\LNG-953A002.dat

Printed: 14:02, June 12, 2012



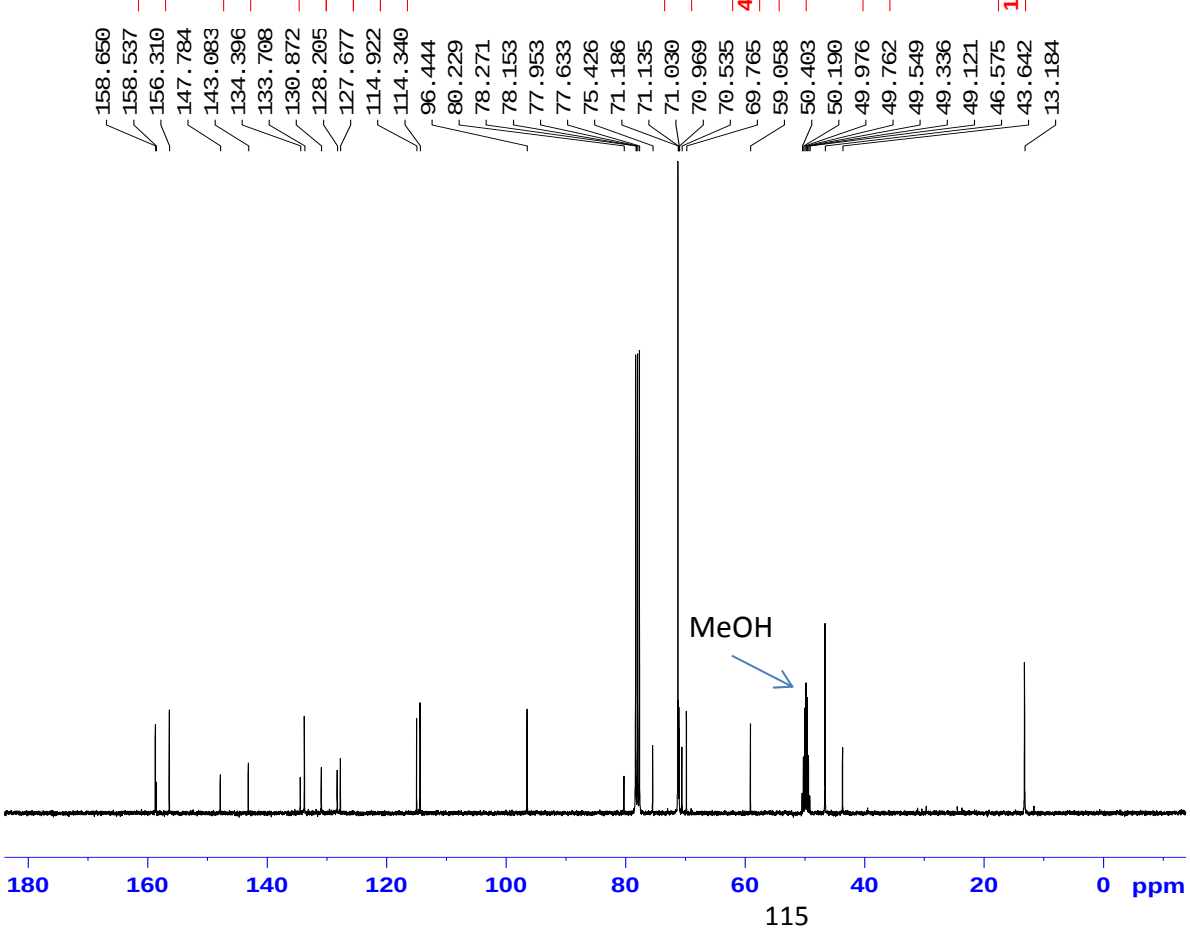

```
NAME          LG-796AA_Alkyne-P8-RGD-CD3OD
EXPNO                                    1
PROCNO                                   1
Date_                             20111003
Time                                10.48
INSTRUM                             spect
PROBHD       5 mm PABBO BB-
PULPROG                              zg30
TD                                  65536
SOLVENT                               MeOD
NS                                      64
DS                                       2
SWH                            8802.817 Hz
FIDRES                         0.134320 Hz
AQ                           3.7224948 sec
RG                                     181
DW                              56.800 usec
DE                               6.50 usec
TE                               292.4 K
D1                          1.00000000 sec
TD0                                      1
======== CHANNEL f1 ========
NUC1                                    1H
P1                              14.85 usec
PL1                              -0.60 dB
PL1W                      13.81451130 W
SFO1                      400.1320007 MHz
                                    32768
                          400.1300000 MHz
W                                      EM
B                                       0
                                 0.30 Hz
                                       0
                                    1.00
```






```
NAME      LG-785_Alkyne-P8-Rhoda
EXPNO                  1
PROCNO                 1
Date_           20110915
Time               17.57
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    64
DS                     2
SWH             8802.817 Hz
FIDRES          0.134320 Hz
AQ              3.7224948 sec
RG                  71.8
DW                56.800 usec
DE                 6.50 usec
TE                292.6 K
D1             1.00000000 sec
TD0                    1

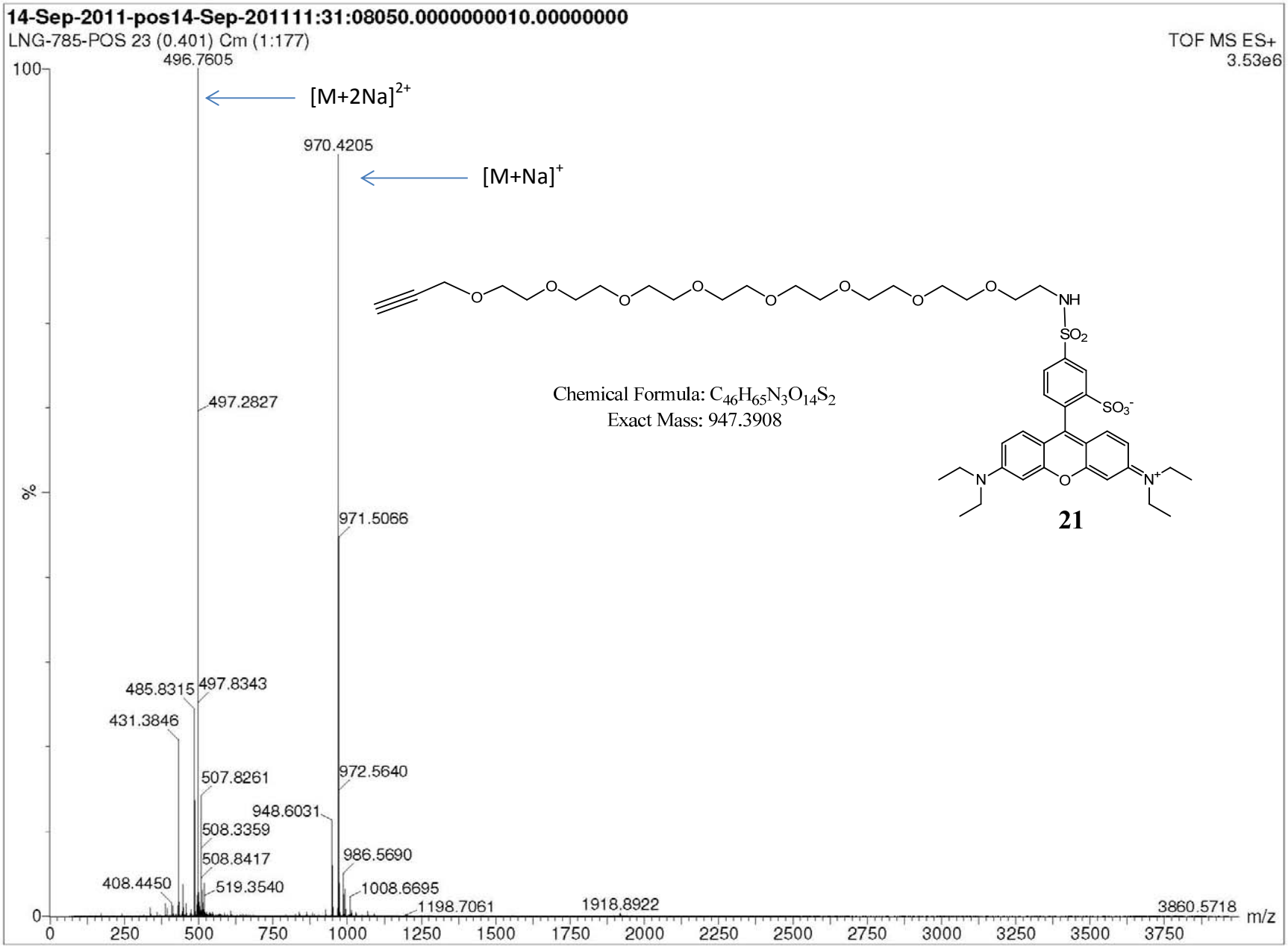
======== CHANNEL f1 ========
NUC1                  1H
P1                 14.85 usec
PL1                -0.60 dB
PL1W        13.81451130 W
SFO1        400.1320007 MHz
SI                 32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
NAME      LG-785_Alkyne-P8-Rhoda
EXPNO                  2
PROCNO                 1
Date_           20110915
Time               19.53
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2000
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  1820
DW                20.800 usec
DE                 6.50 usec
TE                294.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.99 usec
PL1                -3.00 dB
PL1W        73.67452240 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -0.65 dB
PL12               13.40 dB
PL13               13.40 dB
PL2W        13.97447491 W
PL12W        0.54996562 W
PL13W        0.54996562 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6126885 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


14-Sep-2011-pos14-Sep-201111:31:08050.0000000010.00000000
LNG-785-POS 23 (0.401) Cm (1:177)
TOF MS ES+
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496.7605
[M+2Na]2+
970.4205
[M+Na]+
497.2827
971.5066
485.8315
497.8343
431.3846
507.8261
972.5640
948.6031
508.3359
508.8417
986.5690
408.4450
519.3540
1008.6695
1198.7061
1918.8922
3860.5718
100
%
0
m/z
0
250
500
750
1000
1250
1500
1750
2000
2250
2500
2750
3000
3250
3500
3750
Chemical Formula: C46H65N3O14S2
Exact Mass: 947.3908
21