

Supporting Information

Title Sweet-Tasting Ionic Conjugates of Local Anesthetics and Vasoconstrictors

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Data on compound structure for 3a-3e, 4a-4e and 6a-6b.

The following abbreviations are used to describe spin multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, brs = broad singlet, dd = doublet of doublets.

Mepivacaine acesulfamate 3a: White semisolid (97%, 0.396 g, 0.97 mmol); mp 84.0 – 86.0 °C; ¹H NMR (500 MHz, CD₃OD, δ): 7.21 – 7.09 (m, 3H), 5.53 (s, 1H), 4.17 (dd, *J* = 11.9, 3.2 Hz, 1H), 3.54 (d, *J* = 12.5 Hz, 1H), 3.18 (td, *J* = 12.4, 3.1 Hz, 1H), 2.93 (d, *J* = 1.1 Hz, 3H), 2.46 – 2.33 (m, 1H), 2.22 (d, *J* = 0.9 Hz, 6H), 2.02 (t, *J* = 1.0 Hz, 3H), 1.93 (s, 3H), 1.89 – 1.67 (m, 2H); ¹³C NMR (125 MHz, CD₃OD, δ): 173.2, 168.8, 164.4, 137.2, 134.7, 129.9, 129.5, 102.8, 68.8, 56.7, 43.6, 31.0, 24.6, 22.9, 20.4, 19.1. HRMS (ESI) *m/z*: [*M* + *H*]⁺ calcd for C₁₅H₂₂N₂O 246.3535, found 247.1800; HRMS (ESI) *m/z*: [*M* – *H*][–] calcd for C₄H₄NO₄S 161.9867, found 161.9873. Anal. Calcd for: C₁₉H₂₆N₃O₅S: C, 55.87; H, 6.42; N, 10.29%. Found: C, 55.76; H, 6.38; N, 10.34%. *Bupivacaine acesulfamate 3b*: Colorless oil (96%, 0.432 g, 0.96 mmol); ¹H NMR (500 MHz, CD₃OD, δ): 7.18 – 7.11 (m, 3H), 5.55 (s, 1H), 4.32 (d, *J* = 11.6 Hz, 1H), 3.69 (d, *J* = 12.2 Hz, 1H), 3.19 (dq, *J* = 16.5, 11.0, 8.5 Hz, 3H), 2.42 (d, *J* = 12.2 Hz, 1H), 2.24 (s, 6H), 2.04 (s, 3H), 1.99 – 1.70 (m, 7H), 1.41 (q, *J* = 7.4 Hz, 2H), 0.99 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (125 MHz, CD₃OD, δ): 173.2, 169.0, 164.4, 137.2, 134.7, 129.9, 129.9, 129.5, 102.9, 57.8, 53.7, 31.0, 27.3, 24.4, 21.5, 21.5, 20.4, 19.1, 14.4. HRMS (ESI) *m/z*: [*M* + *H*]⁺ calcd for C₁₈H₂₈N₂O 288.2196, found 289.2262; HRMS (ESI) *m/z*: [*M* – *H*][–] calcd for C₄H₄NO₄S 161.9867, found 161.9872. Anal. Calcd for: C₂₂H₃₂N₃O₅S: C, 58.65; H, 7.16; N, 9.33%. Found: C, 58.54; H, 7.09; N, 9.38%.

Prilocaine acesulfamate 3c: White solid (98%, 0.375 g, 0.98 mmol); mp 145.2 – 145.8 °C; ¹H NMR (500 MHz, CD₃OD, δ): 7.38 – 7.34 (m, 1H), 7.25 – 7.15 (m, 3H), 5.52 (s, 1H), 4.20 (q, *J* = 0.6 Hz, 1H), 3.12 – 2.92 (m, 2H), 2.26 (s, 3H), 2.02 (s, 3H), 1.71 (dd, *J* = 23.5, 7.3 Hz, 2H), 1.66 (d, *J* = 0.6 Hz, 3H), 1.02 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (125 MHz, CD₃OD, δ): 173.0, 169.6, 164.2,

136.1, 134.6, 132.0, 132.0, 128.3, 127.7, 127.1, 102.5, 57.9, 49.39, 21.1, 18.4, 17.2, 11.5. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{13}H_{20}N_2O$ 220.1576, found 221.1645; HRMS (ESI) m/z : $[M - H]^-$ calcd for $C_4H_4NO_4S$ 161.9867, found 161.9875. Anal. Calcd for: $C_{17}H_{24}N_3O_5S$: C, 53.39; H, 6.33; N, 10.99%. Found: C, 53.28; H, 6.30; N, 11.29%.

Articaine acesulfamate 3d: White solid (98%, 0.438 g, 0.98 mmol); mp 166.2 – 169.8 °C; 1H NMR (500 MHz, CD_3OD , δ): 7.41 – 7.40 (m, 1H), 3.83 – 3.82 (m 4H), 3.08 – 3.04 (m, 2H), 2.13 (t, J = 1.4 Hz, 3H), 2.04 – 2.03 (m, 4H), 1.78 – 1.70 (m, 5H), 1.06 – 1.01 (m, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 173.3, 169.8, 164.5, 163.6, 140.2, 138.5, 128.75, 125.4, 102.8, 58.1, 53.0, 49.78, 21.3, 20.4, 17.4, 14.6, 11.8. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{13}H_{20}N_2O_3S$ 284.1195, found 285.1261; HRMS (ESI) m/z : $[M - H]^-$ calcd for $C_4H_4NO_4S$ 161.9867, found 161.9875. Anal. Calcd for: $C_{17}H_{24}N_3O_7S_2$: C, 45.73; H, 5.42; N, 9.41%. Found: C, 45.67; H, 5.38; N, 9.50%.

Oxybuprocaine acesulfame 3e: Yellowish oil (98%, 0.462 g, 0.98 mmol); 1H NMR (500 MHz, CD_3OD , δ): 7.43 (d, J = 43.7 Hz, 2H), 6.68 (s, 1H), 5.44 (s, 1H), 4.56 (br s, 2H), 4.0 (br s, 2H), 3.56 (s, 2H), 1.97 (d, J = 12.1 Hz, 2H), 1.77 (br s, 2H), 1.5 (br s, 2H), 1.33 (br s, 6H), 0.98 (t, J = 10 Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 173.0, 168.2, 164.1, 146.9, 145.3, 126.0, 118.0, 114.1, 113.5, 102.5, 69.6, 60.0, 52.4, 32.7, 20.6, 20.1, 14.5, 9.5. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{17}H_{29}N_2O_3$ 309.2173, found 309.2172; HRMS (ESI) m/z : $[M - H]^-$ calcd for $C_4H_4NO_4S$ 161.9867, found 161.9870. Anal. Calcd for: $C_{21}H_{33}N_3O_7S$: C, 53.49; H, 7.05; N, 8.91%. Found: C, 53.40; H, 7.01; N, 8.98%.

Mepivacaine saccharinate 4a: Colorless oil (95%, 0.407 g, 0.95 mmol); 1H NMR (500 MHz, CD_3OD , δ): 7.82 – 7.76 (m, 2H), 7.75 – 7.65 (m, 2H), 7.18 – 7.09 (m, 3H), 4.20 (dd, J = 11.8, 3.3 Hz, 1H), 3.53 (d, J = 12.4 Hz, 1H), 3.18 (td, J = 12.5, 3.1 Hz, 1H), 2.94 (s, 3H), 2.39 (dd, J = 14.0, 3.5 Hz, 1H), 2.39 (d, J = 3.4 Hz, 1H), 2.27 (s, 6H), 1.95 (d, J = 12.6 Hz, 2H), 1.90 – 1.60 (m, 2H);

^{13}C NMR (125 MHz, CD_3OD , δ): 172.2, 168.5, 145.7, 136.9, 135.1, 134.4, 134.1, 133.7, 129.5, 129.2, 124.66, 121.2, 68.4, 56.4, 43.3, 30.6, 24.2, 22.5, 18.8. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{22}\text{N}_2\text{O}$ 246.1727, found 247.1799; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_7\text{H}_4\text{NO}_3\text{S}$ 181.9917, found 181.9924. Anal. Calcd for: $\text{C}_{22}\text{H}_{26}\text{N}_3\text{O}_4\text{S}$: C, 61.66; H, 6.12; N, 9.81%. Found: C, 61.65; H, 6.09; N, 9.84%.

Bupivacaine saccharinate 4b: White solid (97%, 0.456 g, 0.97 mmol); mp 162.4 – 164.8 °C. ^1H NMR (500 MHz, $\text{DMSO}-d_6$, δ): 10.17 (s, 1H), 9.70 (s, 1H), 7.64 – 7.57 (m, 1H), 7.58 (s, 1H), 7.13 (m, 3H), 4.07 (s, 1H), 3.52 (d, $J = 12.4$ Hz, 1H), 3.11 – 3.01 (m, 4H), 2.15 (s, 6H), 1.92 – 1.52 (m, 7H), 1.31 (q, $J = 7.4$ Hz, 2H), 0.90 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 172.4, 168.7, 145.8, 136.8, 136.8, 135.2, 134.4, 134.07, 133.7, 129.6, 129.2, 124.7, 121.2, 57.4, 53.3, 30.7, 27.0, 24.0, 21.2, 18.7, 14.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{28}\text{N}_2\text{O}$ 288.2196, found 289.2266; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_7\text{H}_4\text{NO}_3\text{S}$ 181.9917, found 181.9924. Anal. Calcd for: $\text{C}_{25}\text{H}_{32}\text{N}_3\text{O}_4\text{S}$: C, 63.81; H, 6.85; N, 8.93%. Found: C, 63.77; H, 6.82; N, 8.99%.

Prilocaine saccharinate 4c: White solid (96%, 0.386 g, 0.96 mmol); mp 122.0 – 123.4 °C; ^1H NMR (500 MHz, CD_3OD , δ): 7.81 – 7.69 (m, 3H), 7.41 – 7.38 (dd, $J = 7.3, 2.0$ Hz, 1H), 7.30 – 7.20 (m, 4H), 4.22 (q, $J = 7.0$ Hz, 1H), 3.11 – 3.05 (m, 2H), 2.29 (s, 3H), 1.78 (m, 5H), 1.06 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 172.7, 169.9, 146.1, 136.4, 135.5, 134.9, 134.4, 134.0, 132.4, 128.6, 128.1, 127.4, 125.0, 121.6, 58.3, 49.7, 21.5, 18.7, 17.6, 11.9. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{20}\text{N}_2\text{O}$ 220.1576, found 221.1646; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_7\text{H}_4\text{NO}_3\text{S}$ 181.9917, found 181.9923. Anal. Calcd for: $\text{C}_{20}\text{H}_{24}\text{N}_3\text{O}_4\text{S}$: C, 59.68; H, 6.01; N, 10.44%. Found: C, 59.64; H, 5.97; N, 10.49%.

Articaine saccharinate 4d: Yellow oil (99%, 0.462 g, 0.99 mmol); ^1H NMR (500 MHz, CD_3OD , δ): 8.79 – 8.76 (m, 2H), 8.69 – 8.66 (m, 2H), 8.39 (t, $J = 1.1$ Hz, 1H), 5.31 (d, $J = 6.0$ Hz, 1H),

4.81 – 4.80 (m, 3H), 4.10 – 4.05 (m, 2H), 3.11 (dt, $J = 2.1, 1.0$ Hz, 3H), 2.73 (d, $J = 7.0$ Hz, 5H), 2.01 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 172.7, 169.8, 163.5, 145.9, 140.1, 138.4, 138.4, 134.3, 133.9, 128.8, 124.9, 124.9, 121.5, 58.1, 53.0, 49.8, 21.3, 17.5, 14.6, 11.8. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{20}\text{N}_2\text{O}_3\text{S}$ 284.1195, found 285.1261; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_7\text{H}_4\text{NO}_3\text{S}$ 181.9917, found 181.9925. Anal. Calcd for: $\text{C}_{20}\text{H}_{24}\text{N}_3\text{O}_6\text{S}_2$: C, 51.49; H, 5.19; N, 9.01%. Found: C, 51.41; H, 5.12; N, 9.11%.

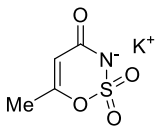
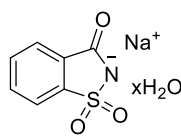
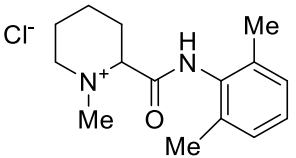
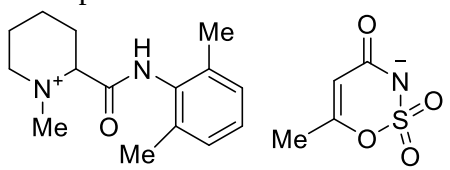
Oxybuprocaine saccharinate 4e: Yellow oil (97%, 0.462 g, 0.98 mmol); ^1H NMR (500 MHz, CD_3OD , δ): 7.76-7.59 (m, 4H), 7.49-7.34 (m, 2H), 6.65 (d, $J = 31.7$ Hz, 1H), 4.57 (m, 2H), 3.99 (m, 2H), 2.59 (m, 2H), 3.32 (m, 4H), 1.80 (br s, 2H), 1.52 (br s, 2H), 1.35 (t, $J = 15.0$ Hz, 6H), 1.01 (m, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 172.5, 168.2, 146.9, 145.8, 145.3, 135.2, 133.9, 133.5, 126.0, 124.7, 121.2, 118.0, 114.0, 113.4, 69.5, 60.0, 52.4, 32.7, 20.6, 14.5, 9.5. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{29}\text{N}_2\text{O}_3$ 309.2173, found 309.2171; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_4\text{H}_4\text{NO}_4\text{S}$ 181.9917, found 181.9920. Anal. Calcd for: $\text{C}_{24}\text{H}_{33}\text{N}_3\text{O}_6\text{S}$: C, 58.64; H, 6.77; N, 8.55%. Found: C, 58.49; H, 6.70; N, 8.65%.

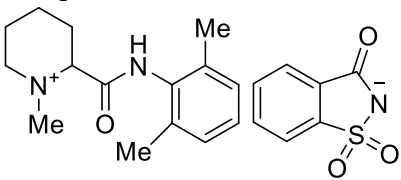
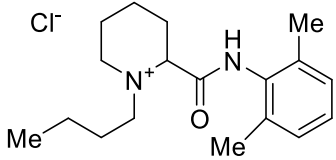
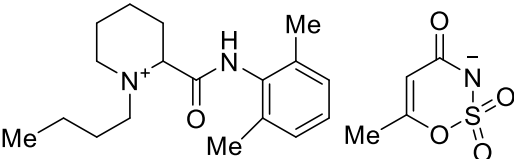
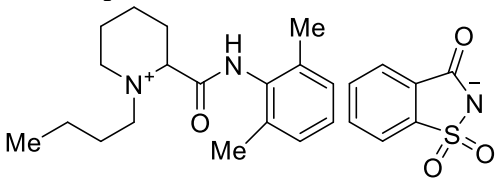
Epinephrine acesulfamate 6a: Colorless oil (99%, 0.343, 0.99 mmol); ^1H NMR (500 MHz, CD_3OD , δ): 6.88 (s, 1H), 6.79 – 6.72 (m, 2H), 5.53 (s, 1H), 4.83 – 4.79 (m, 1H), 3.18 – 3.04 (m, 2H), 2.74 (s, 3H), 2.05-2.04 (m 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 172.0, 163.2, 145.7, 145.6, 132.8, 117.7, 115.6, 113.4, 100.4, 69.0, 55.9, 33.0, 19.0. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_{14}\text{NO}_3$ 184.0968, found 184.0964; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_4\text{H}_4\text{NO}_4\text{S}$ 161.9867, found 161.9866. Anal. Calcd for: $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_7\text{S}$: C, 45.08; H, 5.24; N, 8.09%. Found: C, 45.00; H, 5.19; N, 8.16.

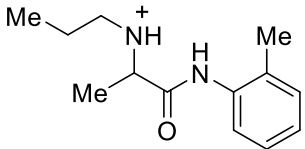
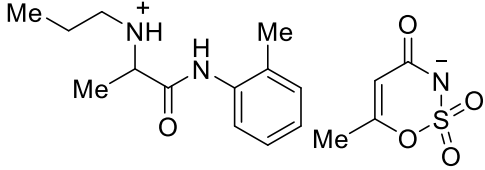
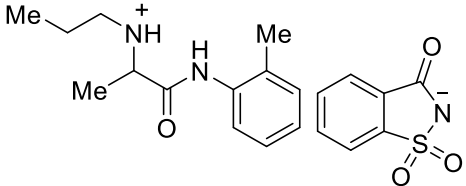
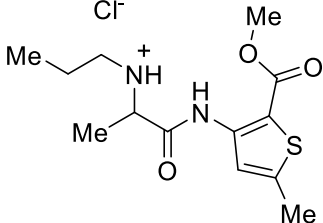
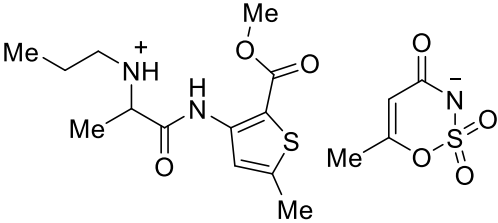
Epinephrine saccharinate 6b: Yellow solid (96%, 0.352 g, 0.96 mmol); mp 82.0 – 83.2 °C; ^1H NMR (500 MHz, CD_3OD , δ): 7.72 – 7.63 (m, 2H), 6.93 (d, $J = 2.0$ Hz, 1H), 6.82 – 6.72 (m, 2H),

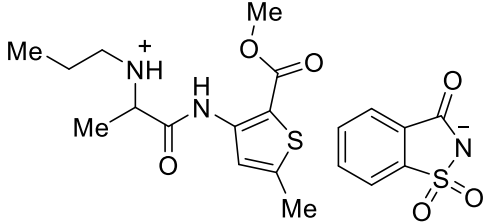
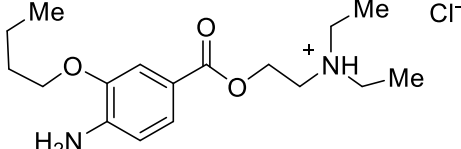
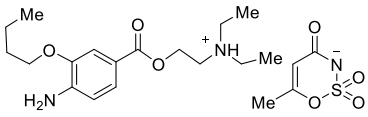
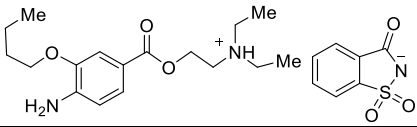
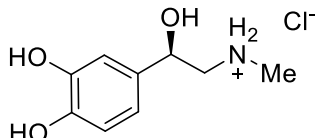
4.88 (dd, $J = 9.4, 3.9$ Hz, 3H), 2.77 (s, 3H), 2.02 (d, $J = 0.6$ Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD , δ): 171.3, 145.4, 145.3, 144.2, 133.7, 132.9, 132.6, 132.5, 123.5, 120.0, 117.7, 115.5, 113.3, 68.8, 55.7, 32.9. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_{14}\text{NO}_3$ 184.0968, found 184.0966; HRMS (ESI) m/z : $[\text{M} - \text{H}]^-$ calcd for $\text{C}_7\text{H}_4\text{NO}_3\text{S}$ 181.9917, found 181.9918. Anal. Calcd for: $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_6\text{S}$: C, 52.45; H, 4.95; N, 7.65%. Found: C, 52.39; H, 4.89; N, 7.74.

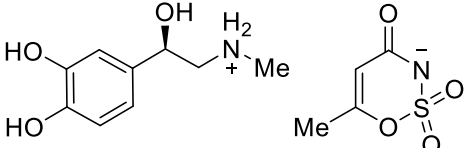
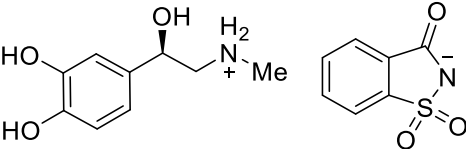
Table S1. *pH of synthesized salts and original compounds.*

Potassium acesulfame 2a 	Weight-by-volume conc.	pH
	10%	5.78
	5%	6.33
	2%	5.98
Sodium saccharin hydrate 2b 	Weight-by-volume conc.	pH
	10%	5.63
	5%	6.09
	2%	6.19
Mepivacaine hydrochloride 	Weight-by-volume conc.	pH
	10%	3.73
	5%	3.77
	2%	4.53
Mepivacaine acesulfamate 3a 	Weight-by-volume conc.	pH
	10%	4.00
	5%	4.87

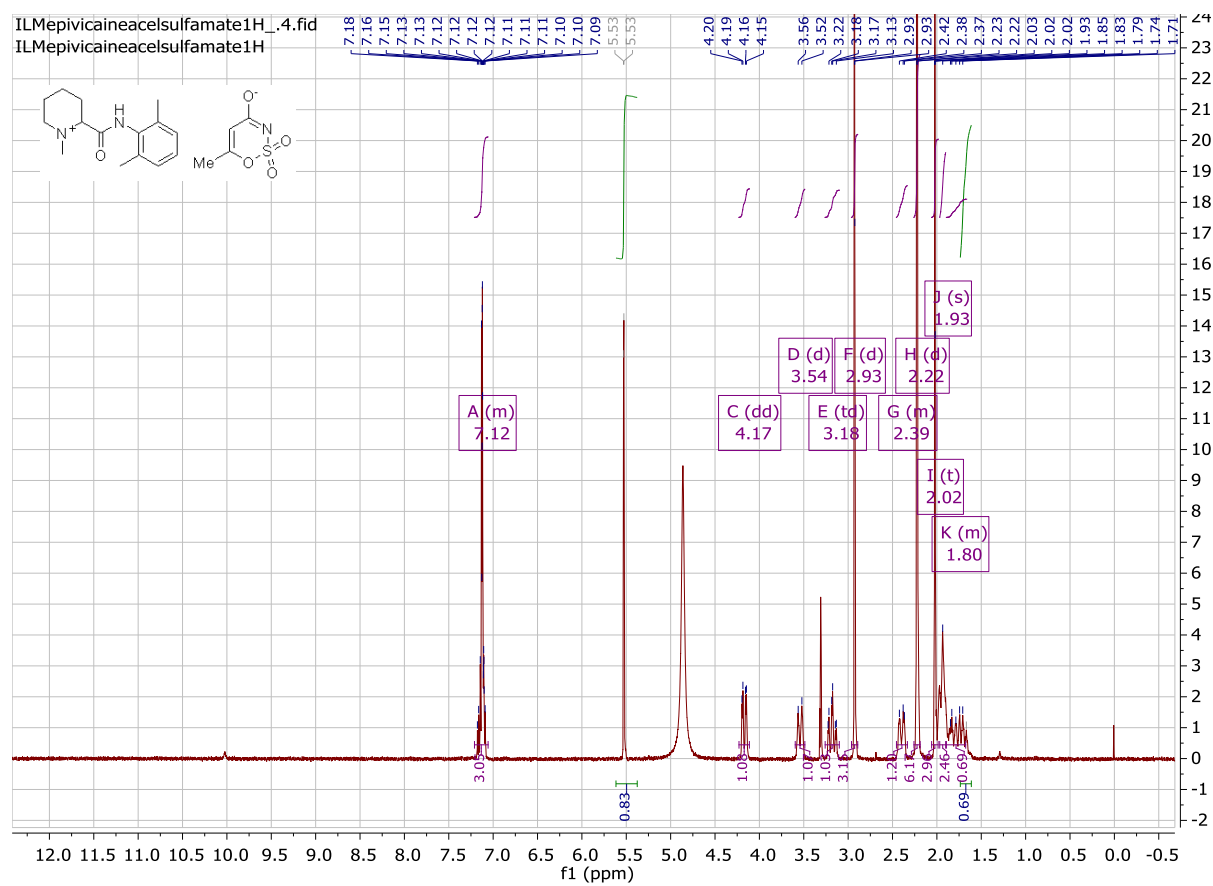
	2%	4.91
Mepivacaine saccharinate 4a 	Weight-by-volume conc.	pH
	10%	3.95
	5%	4.06
	2%	4.23
Bupivacaine hydrochloride  Cl ⁻ (low solubility in water)	Weight-by-volume conc.	pH
	10%	4.23
	5%	4.81
	2%	5.22
Bupivacaine acesulfamate 3b  (low solubility in water)	Weight-by-volume conc.	pH
	10%	4.25
	5%	5.13
	2%	5.38
Bupivacaine saccharinate 4b  (low solubility in water)	Weight-by-volume conc.	pH
	10%	3.84
	5%	3.66
	2%	5.19
	Weight-by-volume conc.	pH
	10%	2.10

	5%	3.42
	2%	4.60
Prilocaine acesulfamate 3c 	Weight-by-volume conc.	pH
	10%	4.71
	5%	5.00
	2%	5.16
Prilocaine saccharinate 4c 	Weight-by-volume conc..	pH
	10%	4.47
	5%	4.96
	2%	5.04
Articaine hydrochloride  (low solubility in water)	Weight-by-volume conc.	pH
	10%	4.22
	5%	4.62
	2%	4.78
Articaine acesulfamate 3d 	Weight-by-volume conc.	pH
	10%	3.50
	5%	3.79
	2%	3.95
Articaine saccharinate 4d	Weight-by-volume conc.	pH
	10%	3.83
	5%	3.95

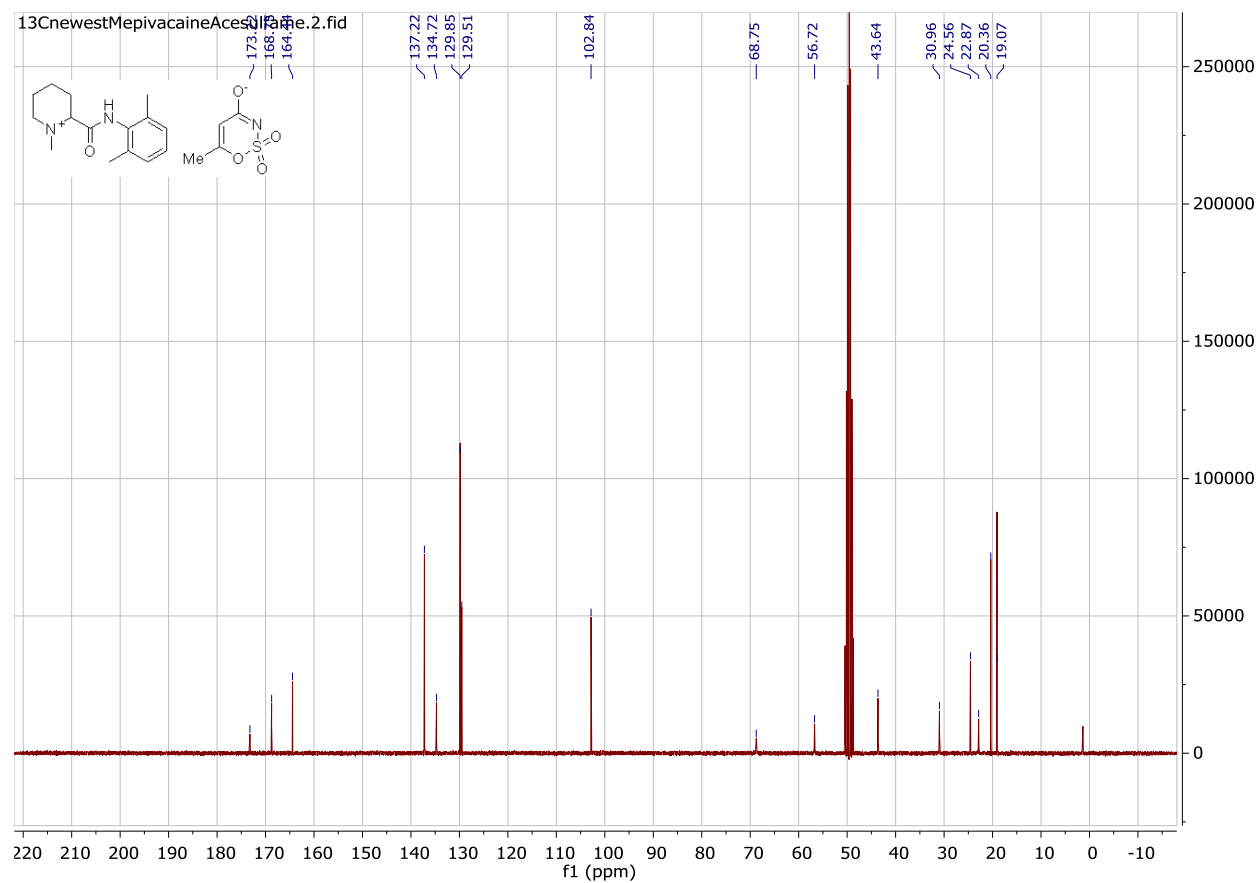
	2%	4.15
Oxybuprocaine hydrochloride 	Weight-by-volume conc.	pH
	10%	4.42
	5%	5.33
	2%	5.53
Oxybuprocaine acesulfamate 3e 	Weight-by-volume conc.	pH
	10%	4.68
	5%	5.22
	2%	5.56
Oxybuprocaine saccharinate 4e 	Weight-by-volume conc.	pH
	10%	4.70
	5%	5.21
	2%	5.71
Epinephrine hydrochloride 5 	Weight-by-volume conc.	pH
	10%	2.72
	5%	3.91
	2%	4.84
Epinephrine acesulfamate 6a 	Weight-by-volume conc.	pH
	10%	4.01

	5%	4.14
	2%	4.34
Epinephrine saccharinate 6b 	Weight-by-volume conc.	pH
	10%	3.57
	5%	4.03
	2%	4.41

¹H spectrum for mepivacaine acesulfamate 3a



¹³C spectrum for mepivacaine acesulfamate 3a



HRMS data for mepivacaine acesulfamate 3a

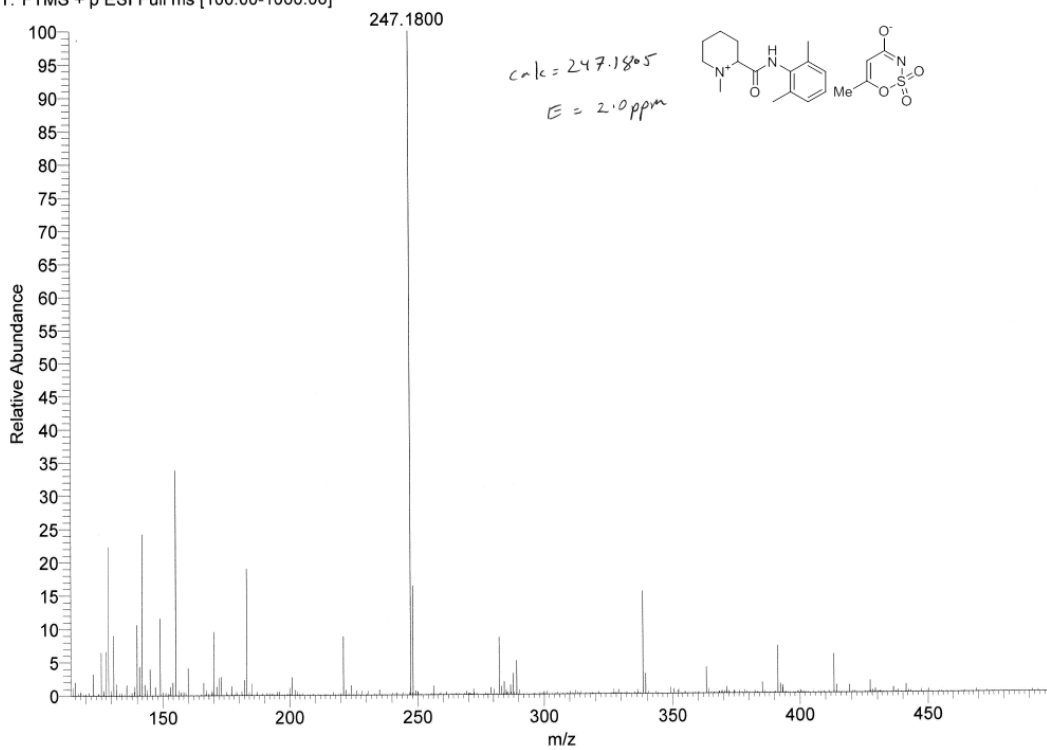
C:\Xcalibur\...IL061015H_150610143136

6/10/2015 4:46:48 PM

IL-19

IL061015H_150610143136 #76-102 RT: 0.70-0.91 AV: 27 NL: 1.15E6

T: FTMS + p ESI Full ms [100.00-1000.00]



HRMS data for mepivacaine acesulfamate 3a

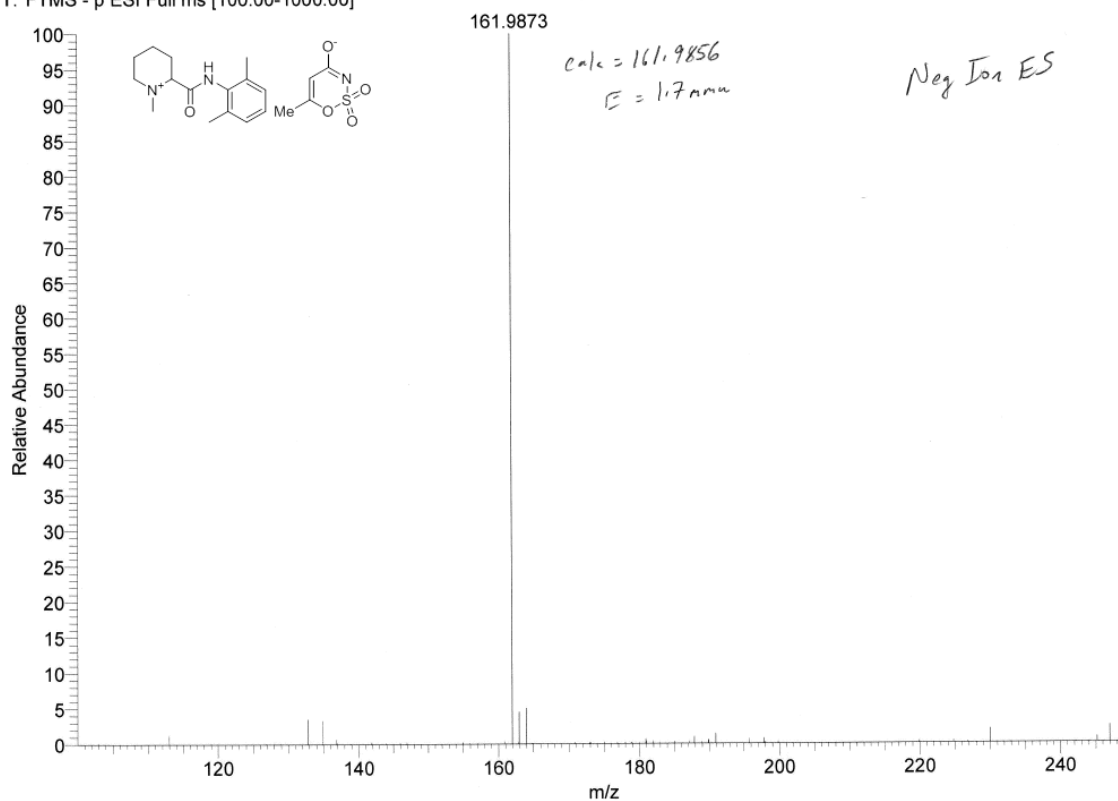
C:\Xcalibur\...\\IL061115O_150610143136

6/11/2015 2:15:54 PM

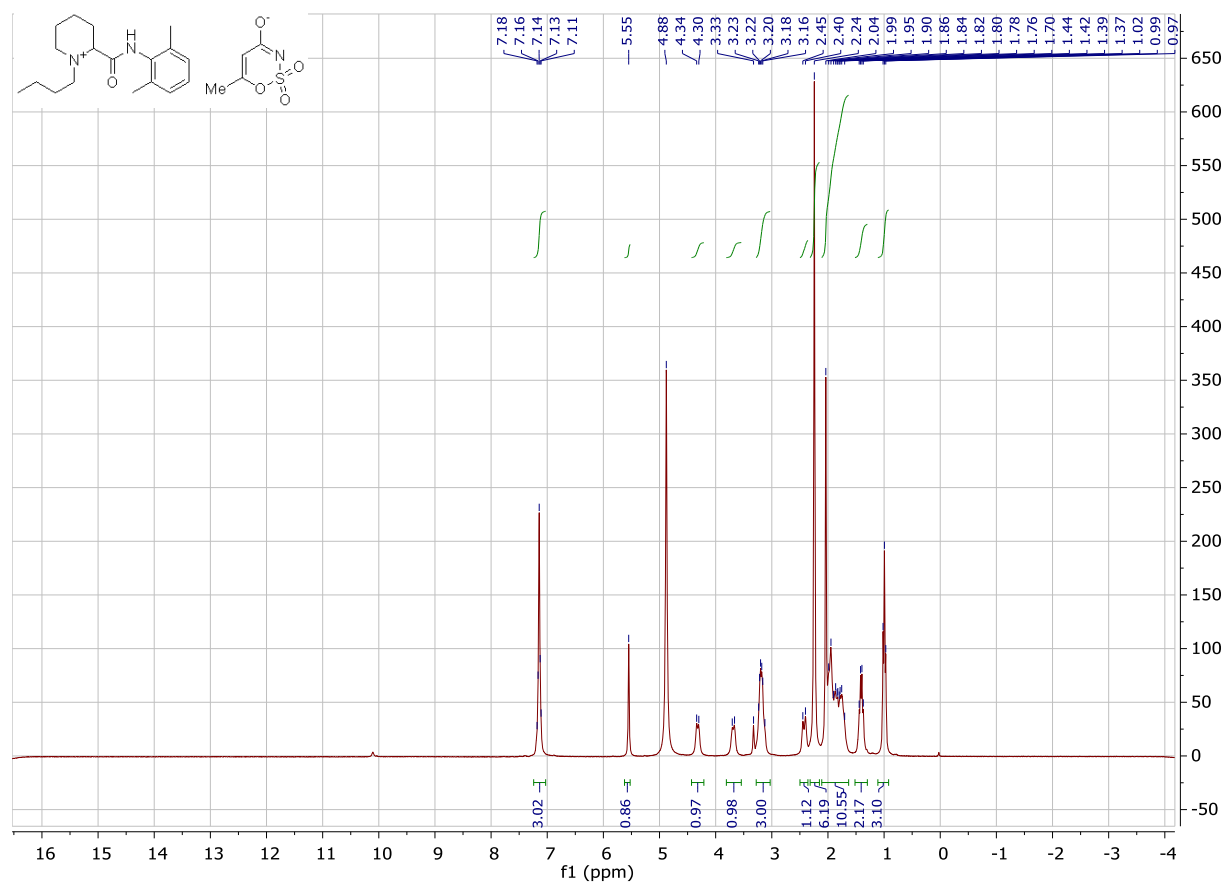
IL-19

IL061115O_150610143136 #179-205 RT: 2.79-3.06 AV: 27 SB: 37 1.57-2.21 NL: 1.44E6

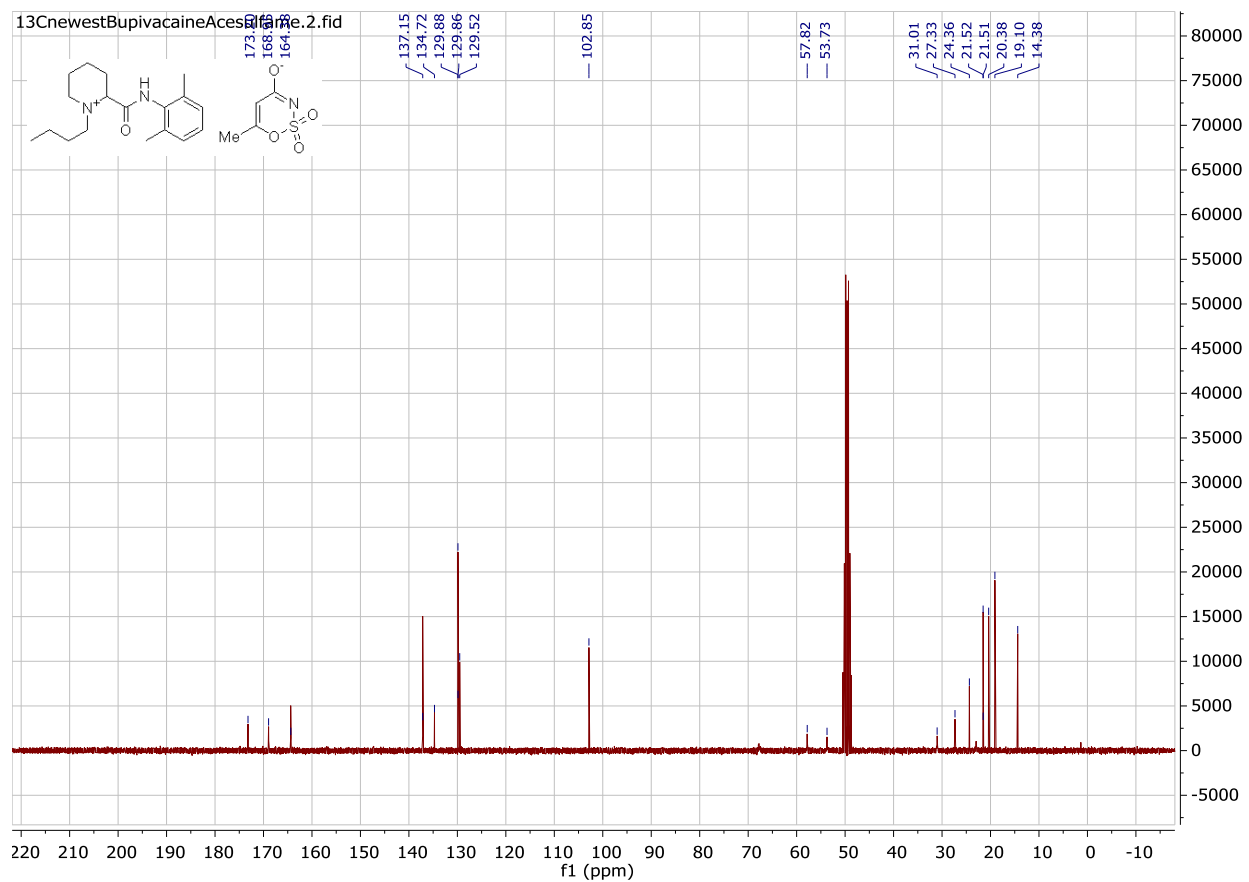
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for bupivacaine acesulfamate 3b



¹³C spectrum for bupivacaine acesulfamate 3b



HRMS data for bupivacaine acesulfamate 3b

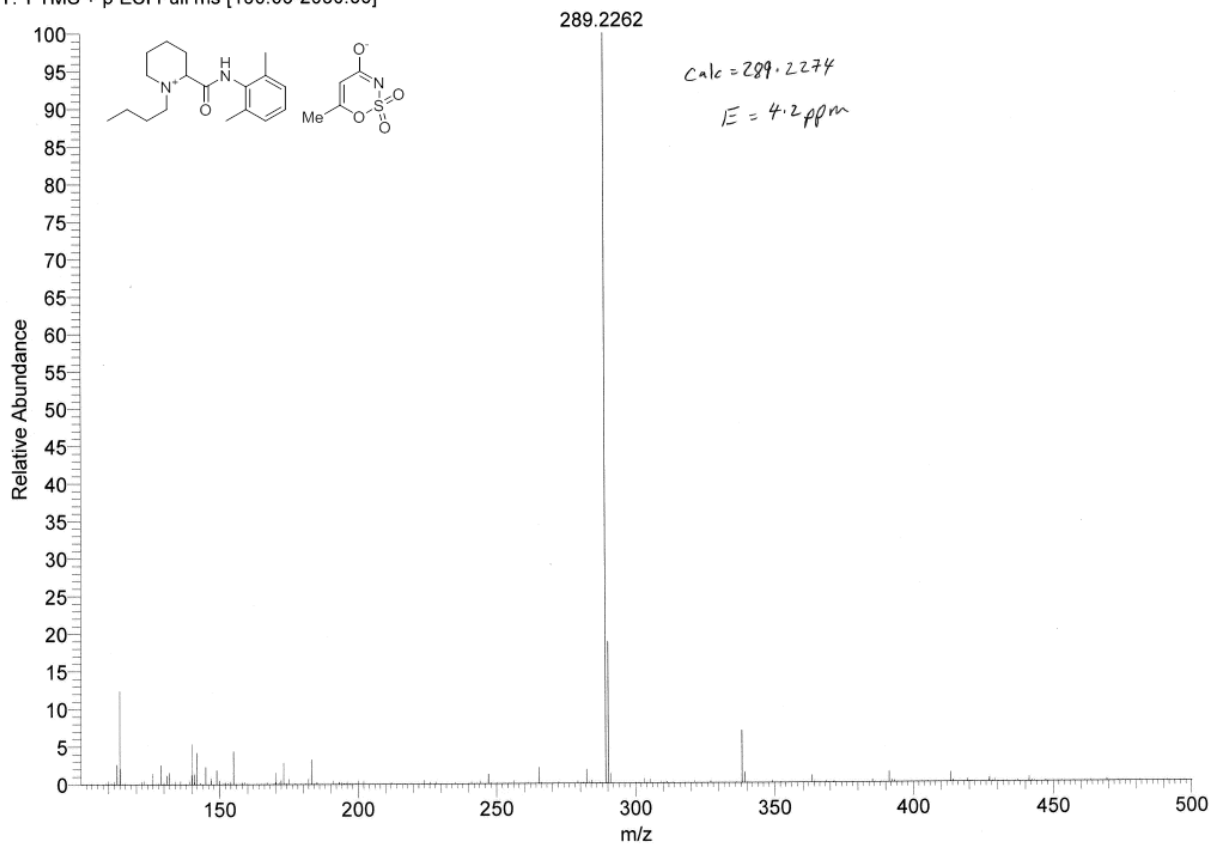
C:\Xcalibur\...\\IL061015b_150610143136

6/10/2015 2:57:56 PM

IL-13

IL061015b_150610143136 #115-128 RT: 0.95-1.05 AV: 14 NL: 4.71E6

T: FTMS + p ESI Full ms [100.00-2000.00]



HRMS data for bupivacaine acesulfamate 3b

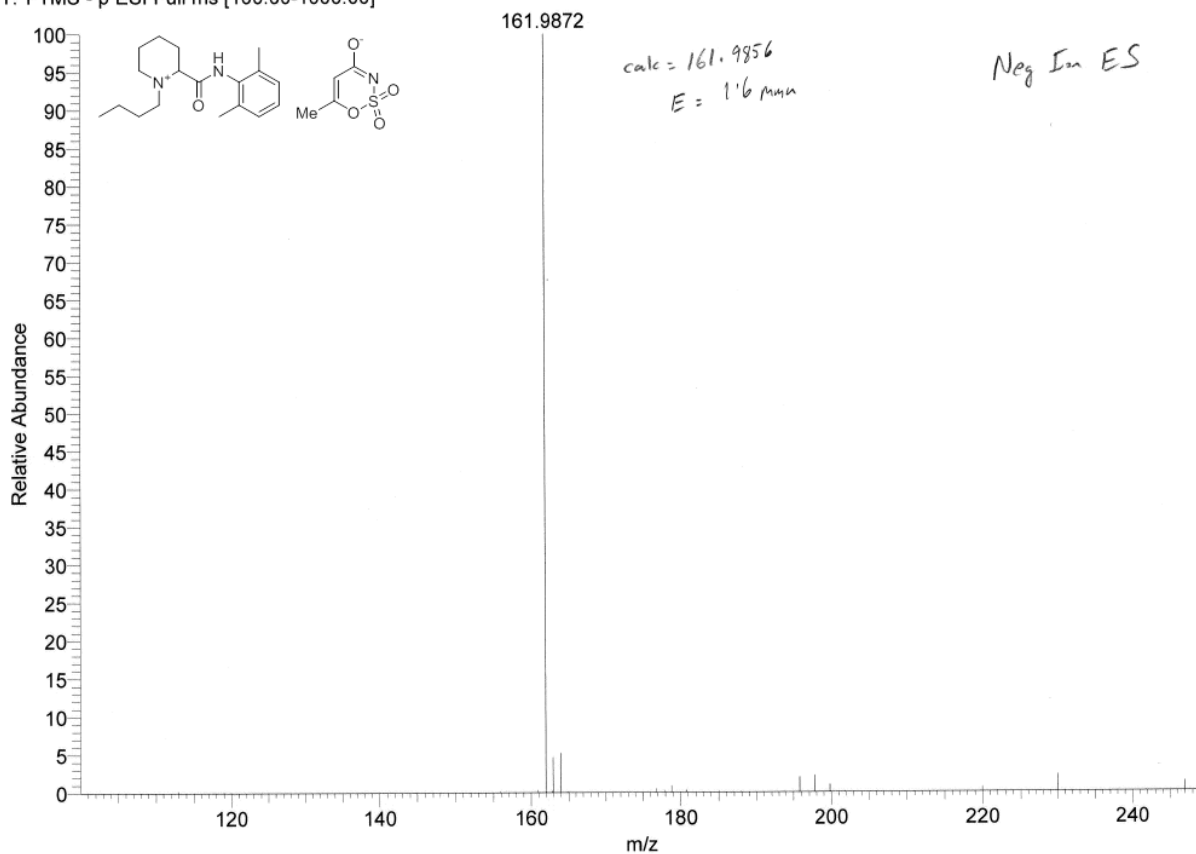
C:\Xcalibur\...\\L061115K_150610143136

6/11/2015 1:54:10 PM

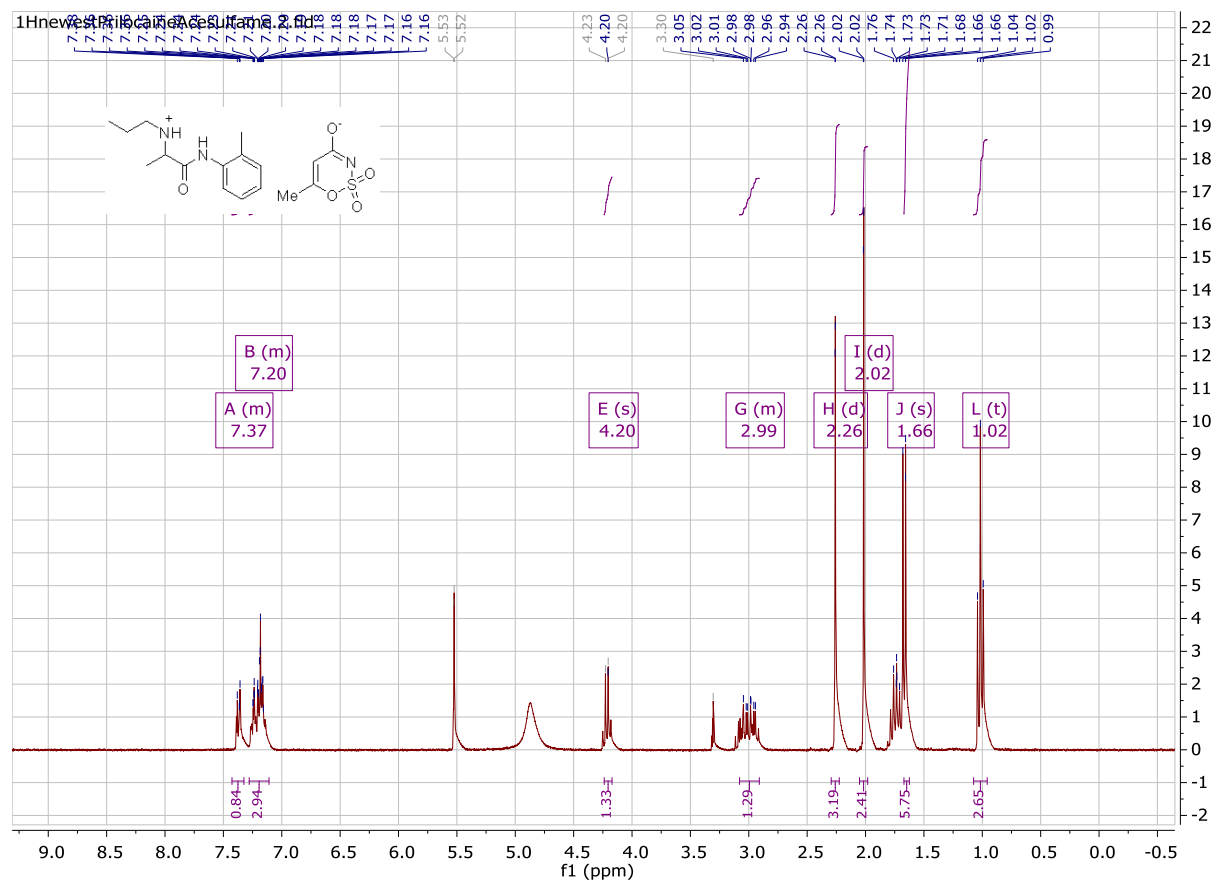
IL-13

IL061115K_150610143136 #59-62 RT: 0.87-0.90 AV: 4 SB: 43 0.10-0.69 NL: 2.40E6

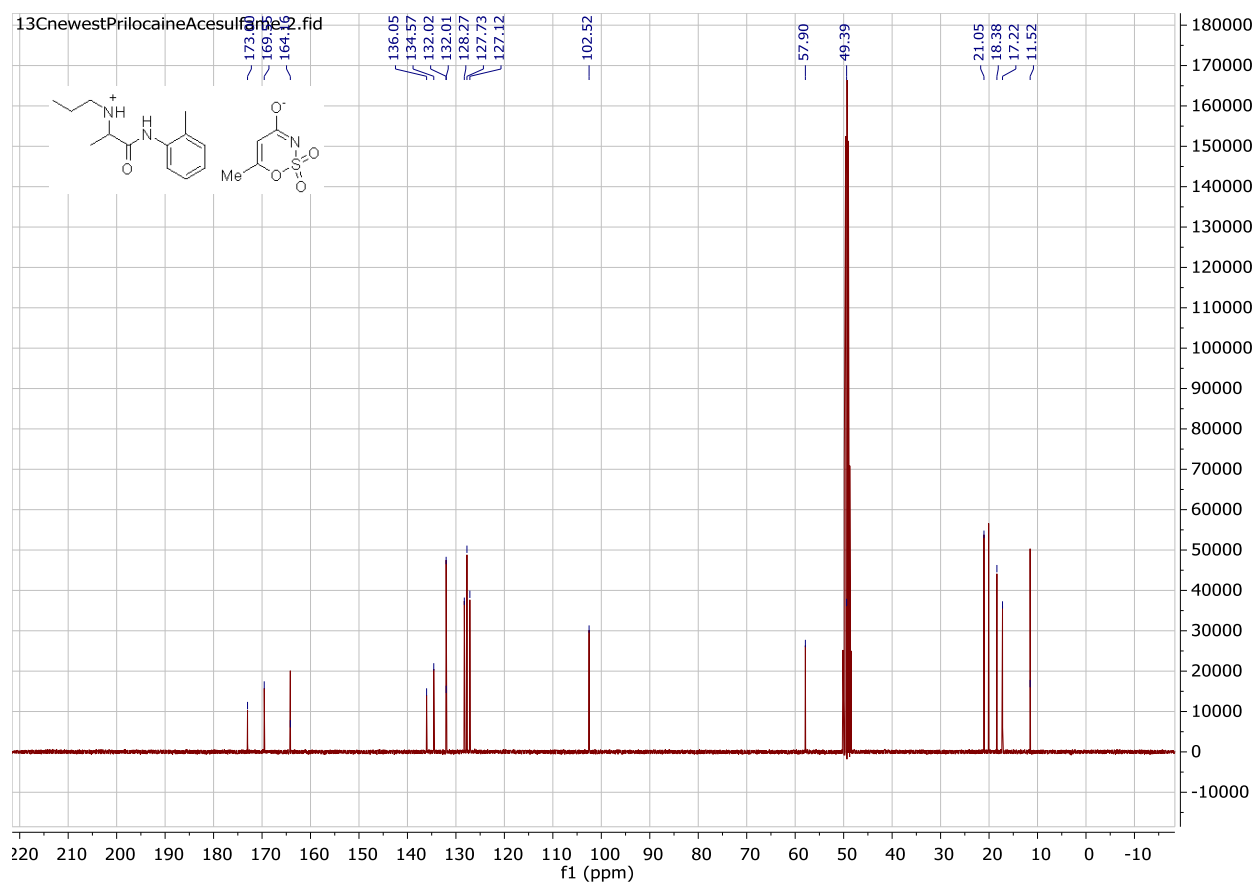
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for prilocaïne acesulfamate 3c



¹³C spectrum for prilocaine acesulfamate 3c



HRMS data for prilocaine acesulfamate 3c

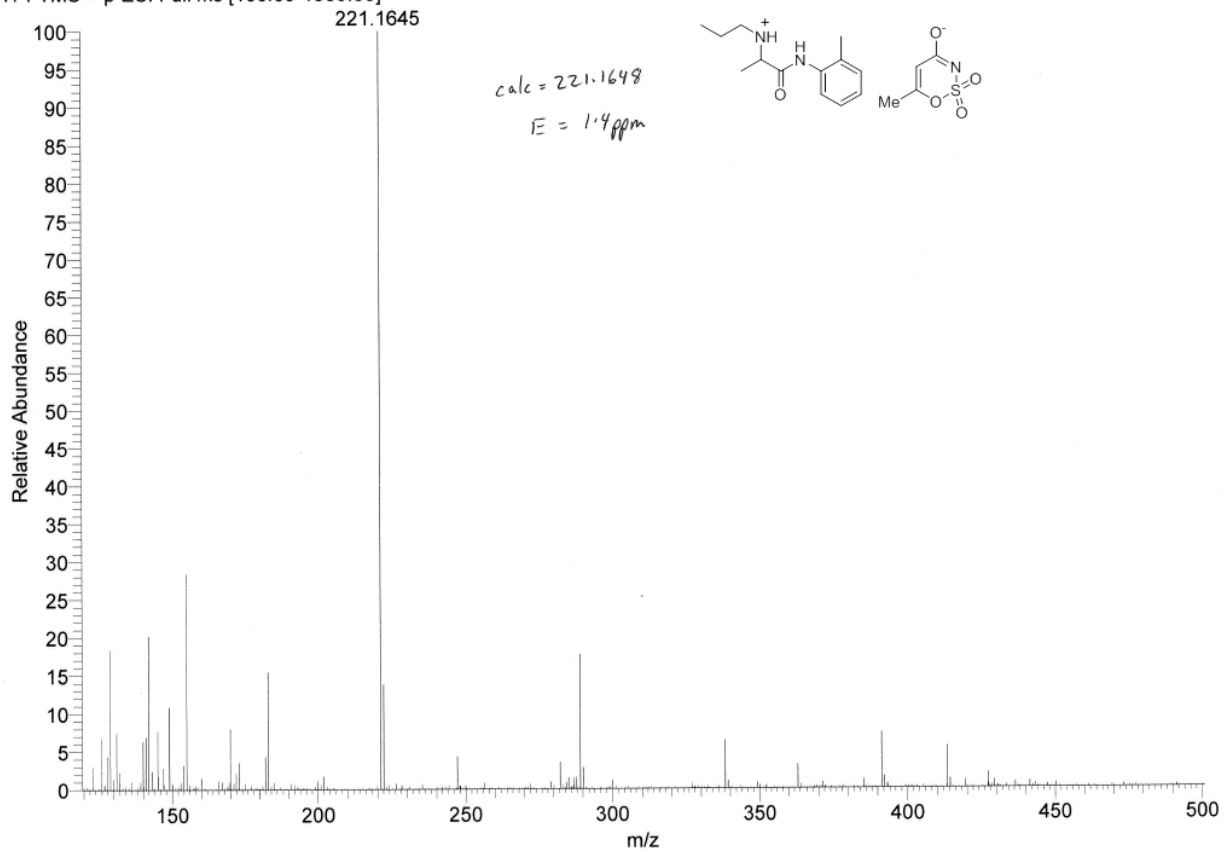
C:\Xcalibur\...IL061015D_150610143136

6/10/2015 3:47:57 PM

IL-15

IL061015D_150610143136 #74-78 RT: 0.66-0.69 AV: 5 NL: 1.71E6

T: FTMS + p ESI Full ms [100.00-1000.00]



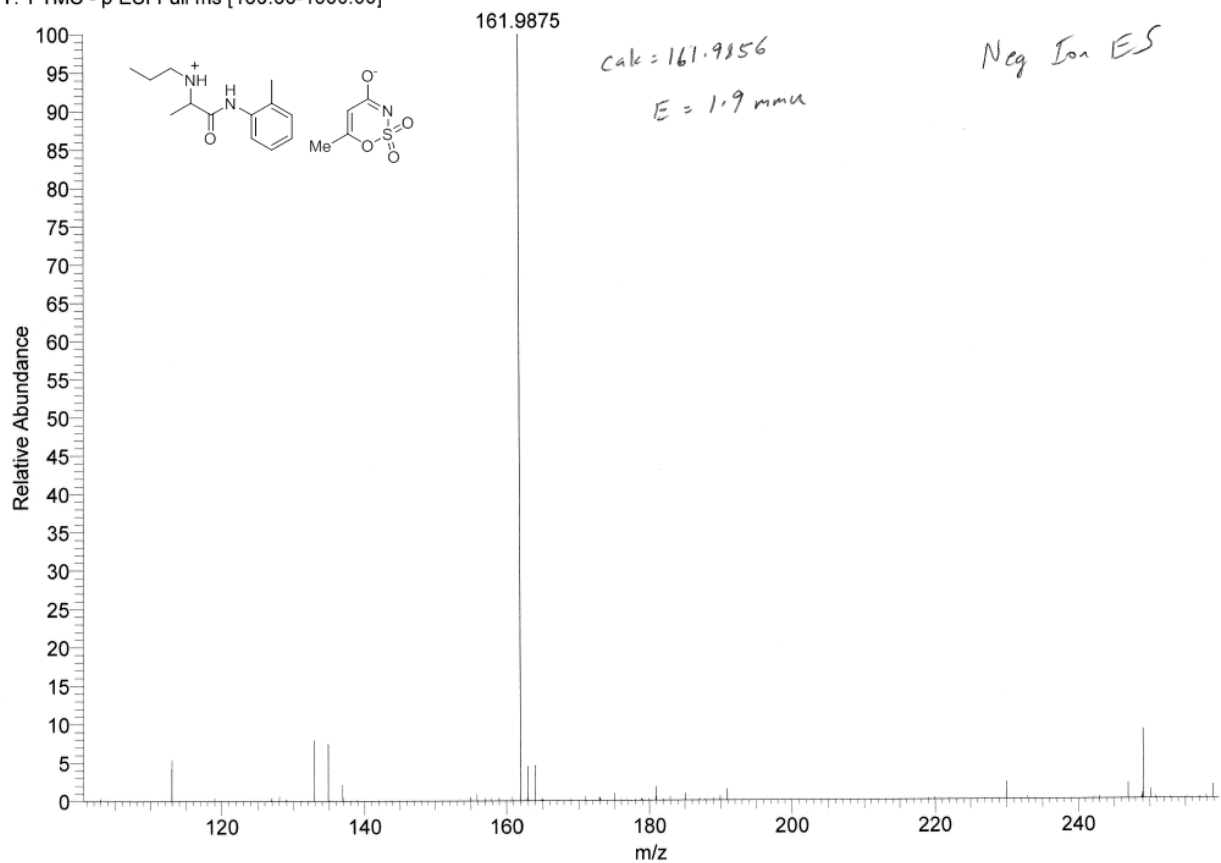
HRMS data for prilocaine acesulfamate 3c

C:\Xcalibur\...IL061115I_150610143136

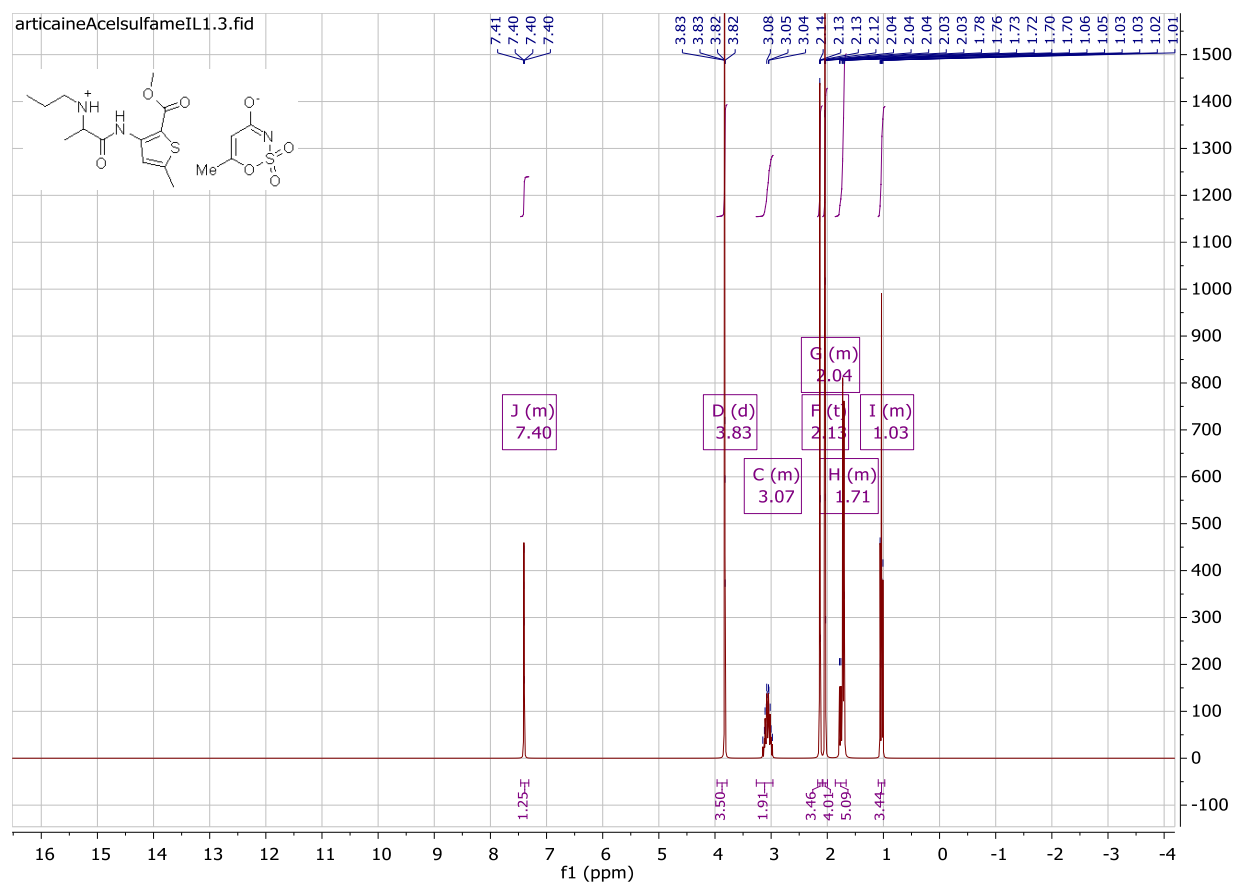
6/11/2015 1:43:37 PM

IL-15

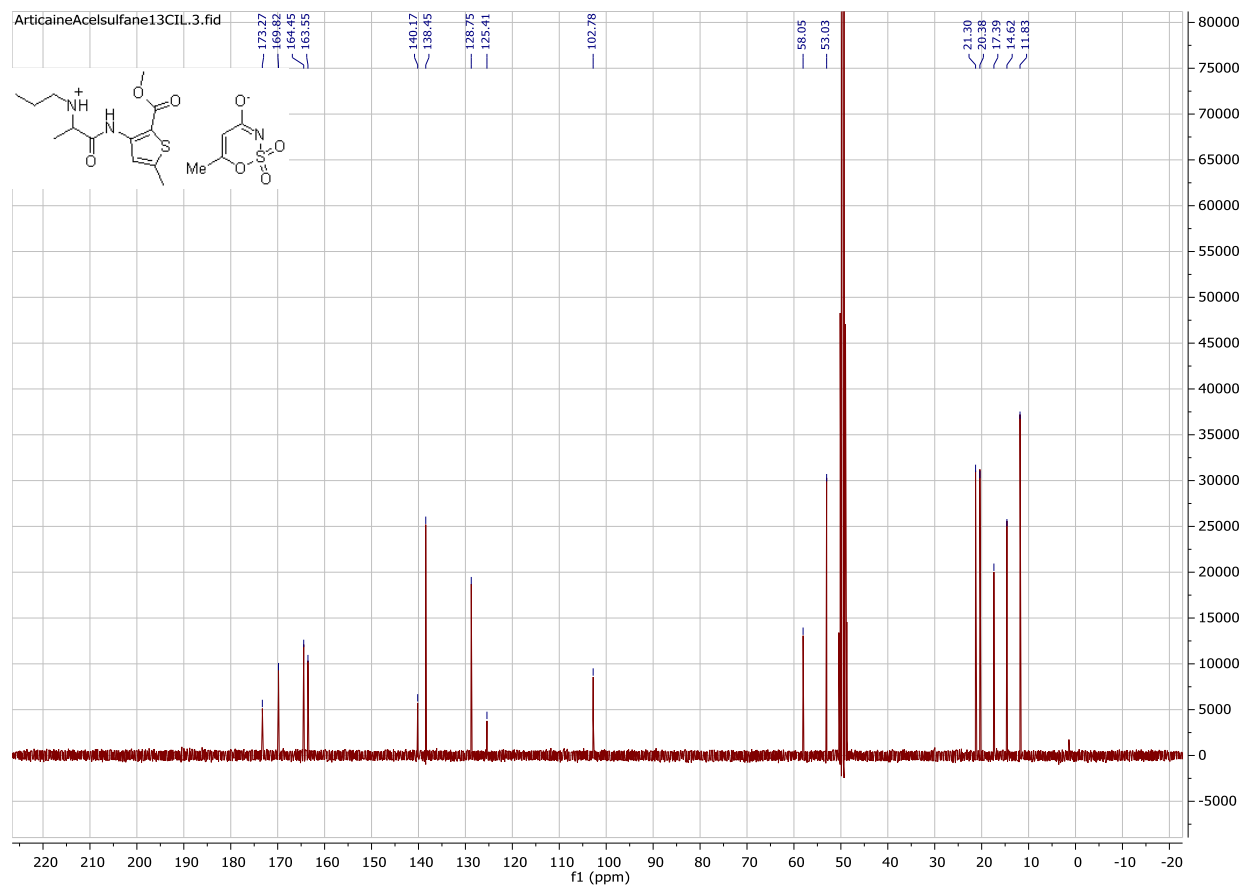
IL061115I_150610143136 #66-75 RT: 1.02-1.11 AV: 10 SB: 42 0.30-0.90 NL: 5.13E5
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for articaïne acesulfamate 3d



¹³C spectrum for artocaine acesulfamate 3d



HRMS data for artocaine acesulfamate 3d

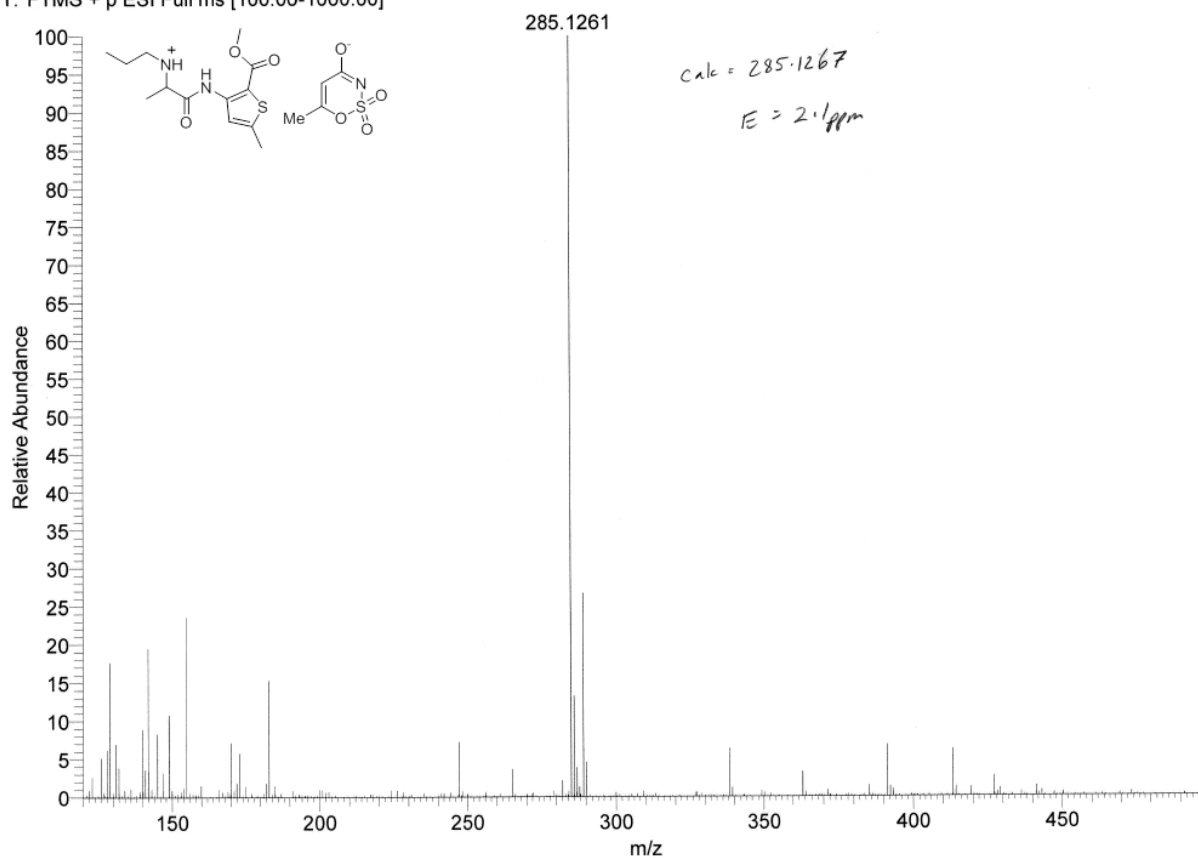
C:\Xcalibur\...IL061015C_150610143136

6/10/2015 3:11:48 PM

IL-11

IL061015C_150610143136 #92-102 RT: 0.77-0.85 AV: 11 NL: 1.90E6

T: FTMS + p ESI Full ms [100.00-1000.00]



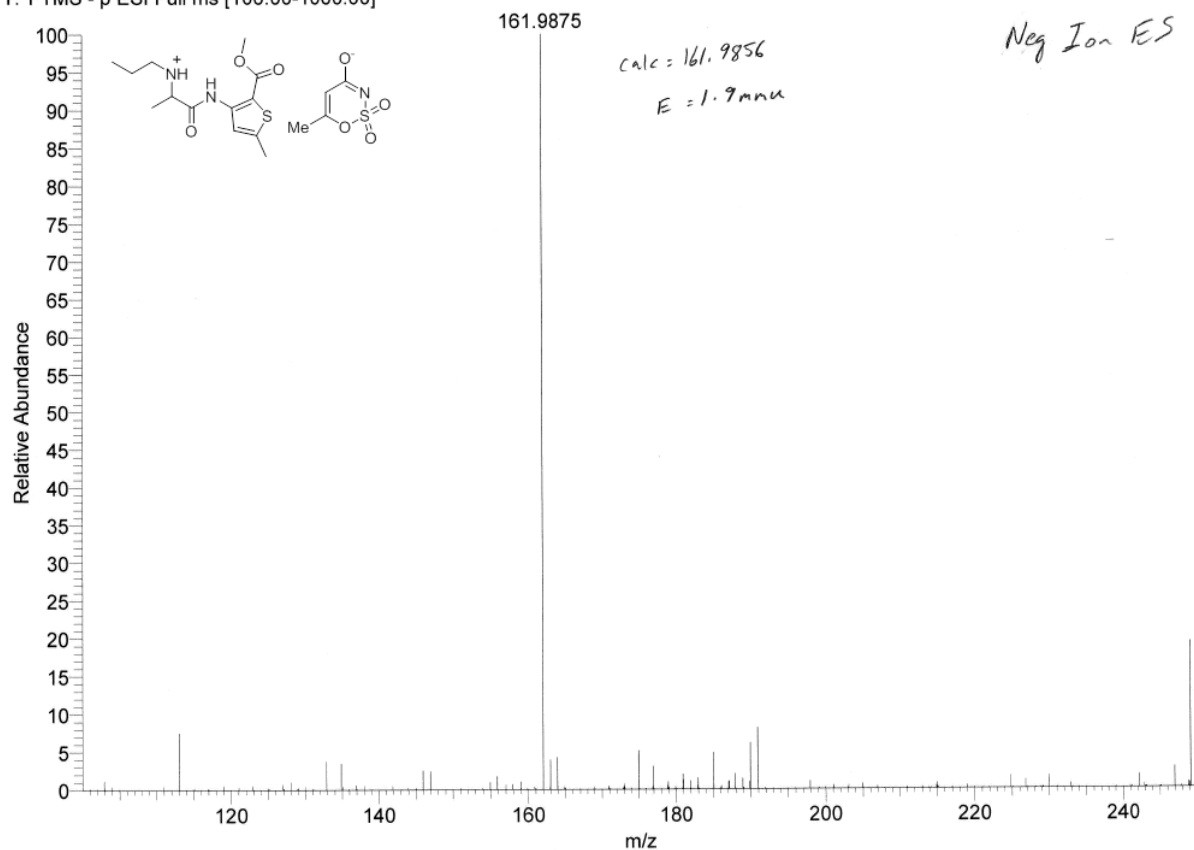
HRMS data for articaïne acesulfamate 3d

C:\Xcalibur\...\\L061115h_150610143136

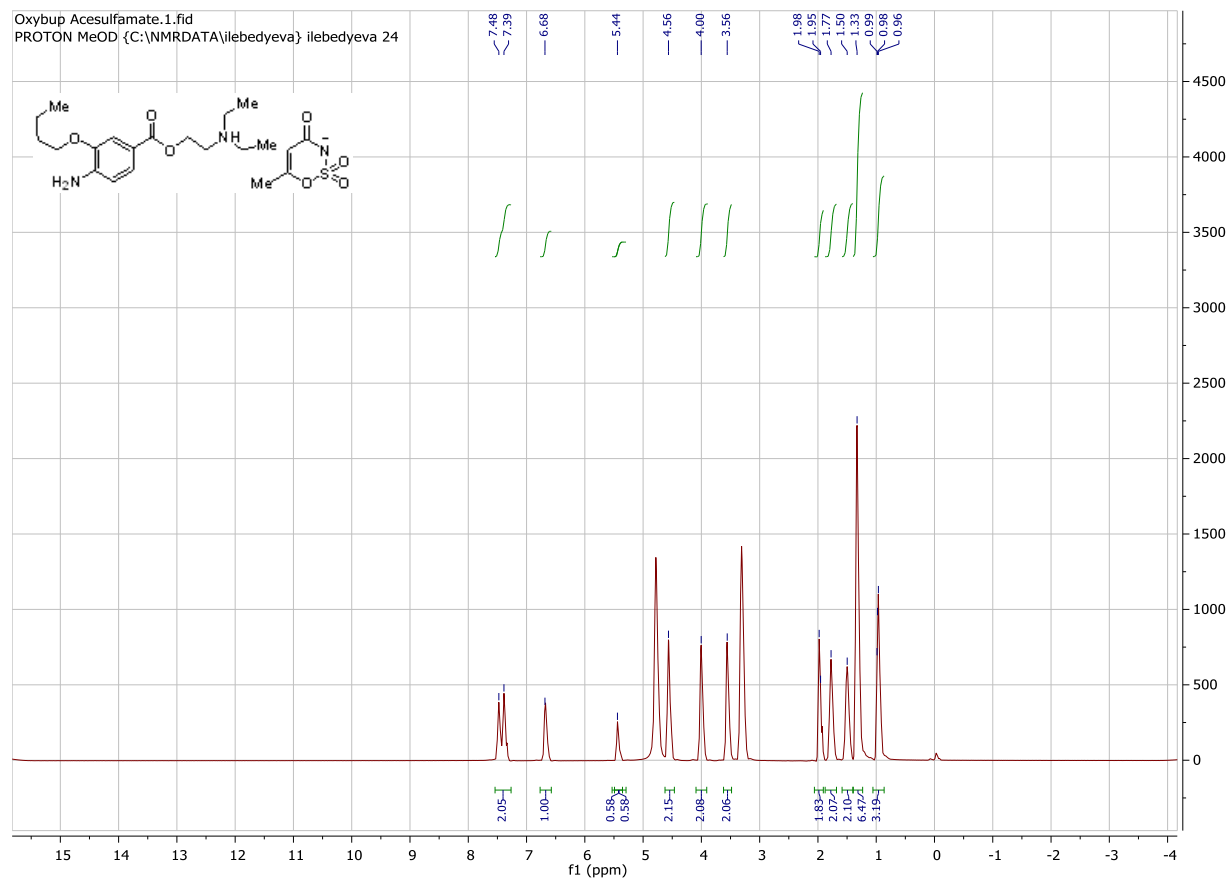
6/11/2015 1:35:41 PM

IL-11

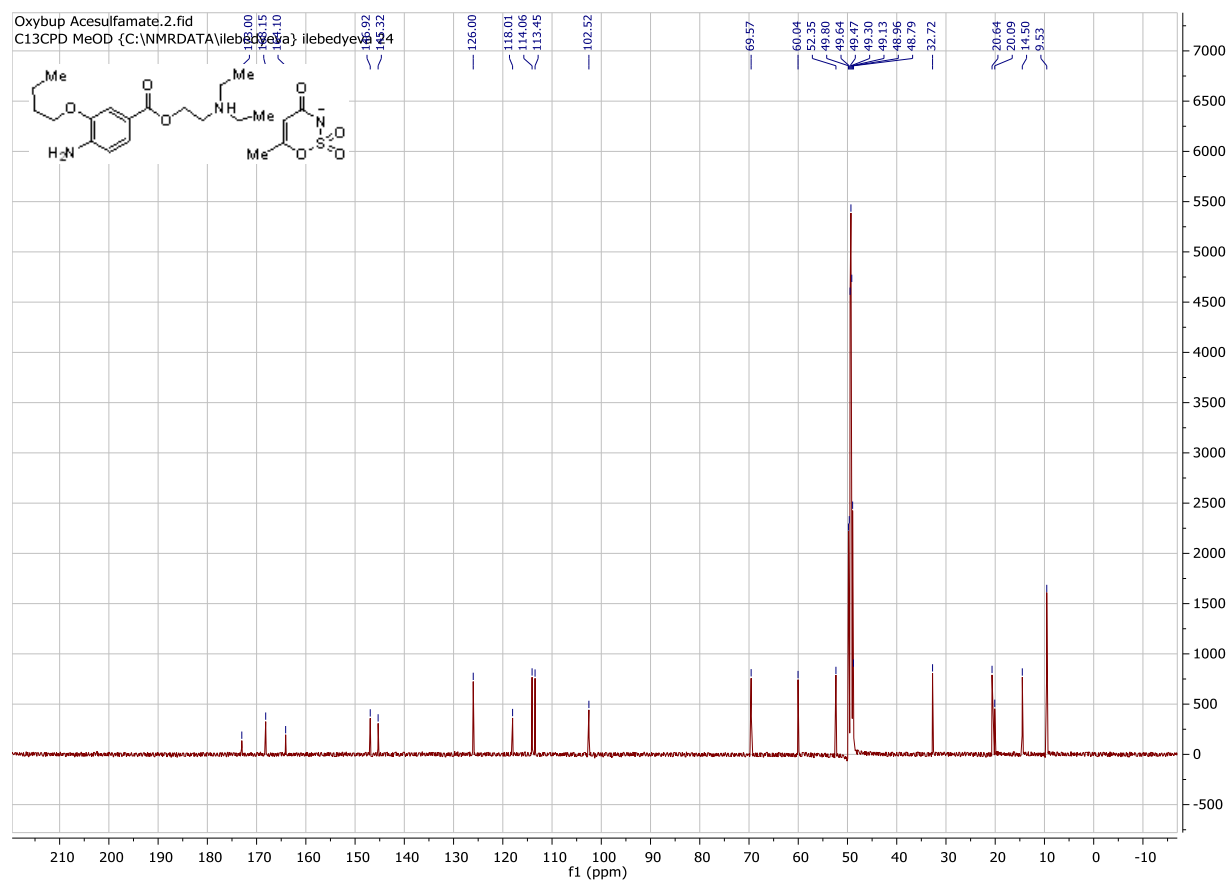
IL061115h_150610143136 #109-140 RT: 1.78-2.16 AV: 32 SB: 54 0.79-1.60 NL: 1.28E5
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for oxybuprocaine acesulfame 3e



¹³C spectrum for oxybuprocaine acesulfame 3e



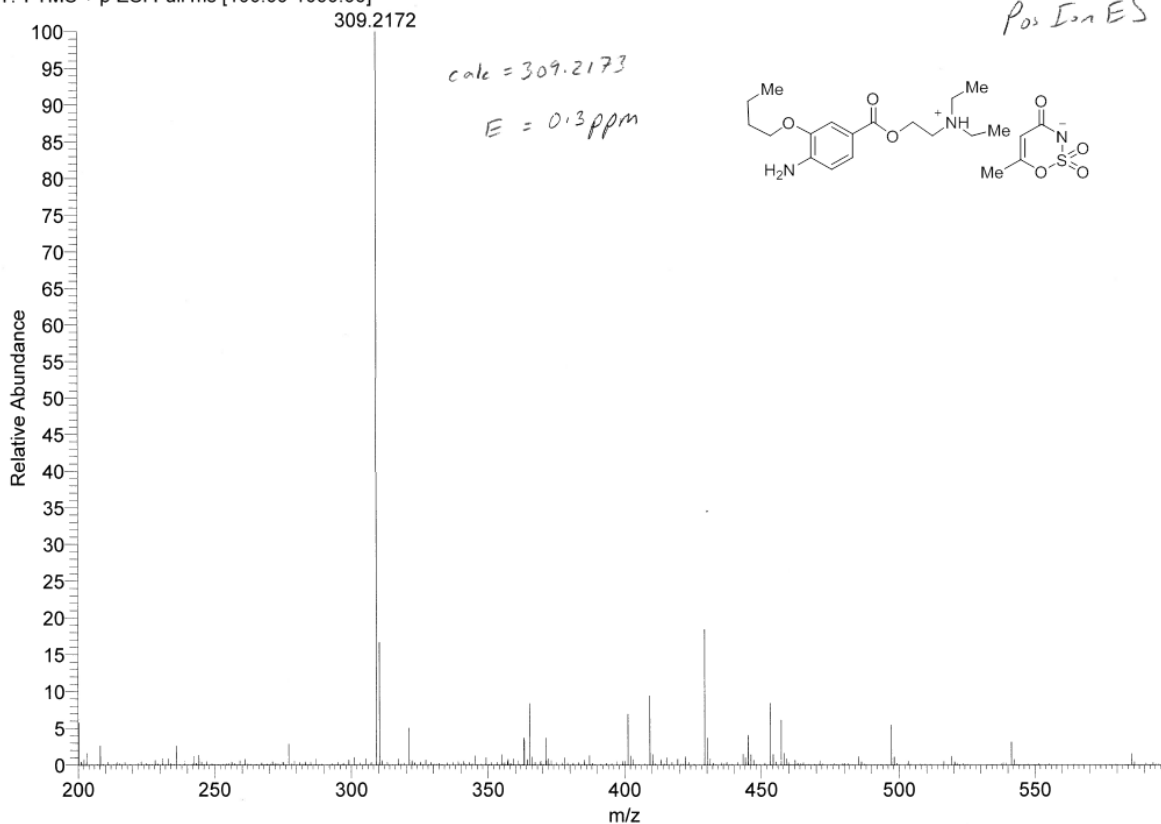
HRMS data for oxybuprocaine acesulfame 3e

C:\Xcalibur\...MassSpecLab03\1111416b

11/14/2016 2:35:50 PM

IL-277

1111416b #343-358 RT: 2.64-2.76 AV: 16 SB: 156 0.40-1.60 NL: 2.83E5
T: FTMS + p ESI Full ms [100.00-1000.00]



HRMS data for oxybuprocaine acesulfame 3e

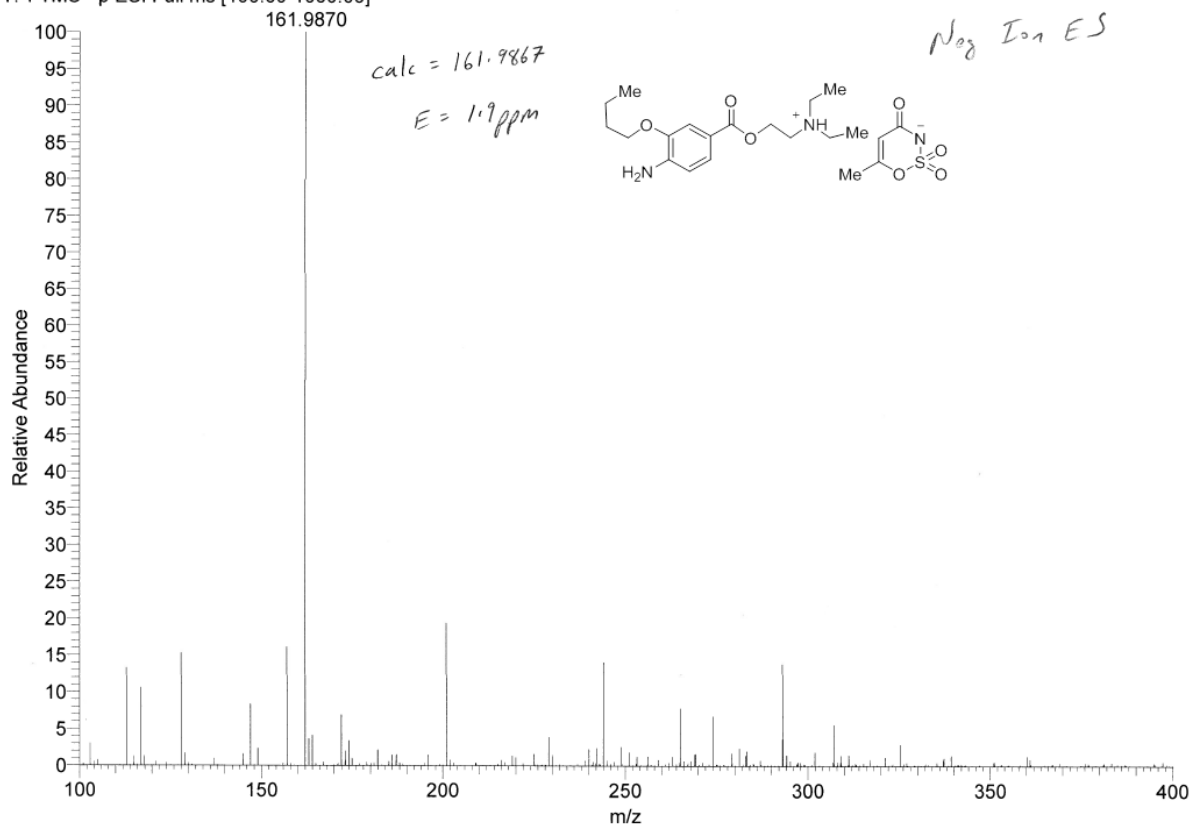
C:\Xcalibur\...\MassSpecLab03\il111416bc

11/14/2016 2:48:02 PM

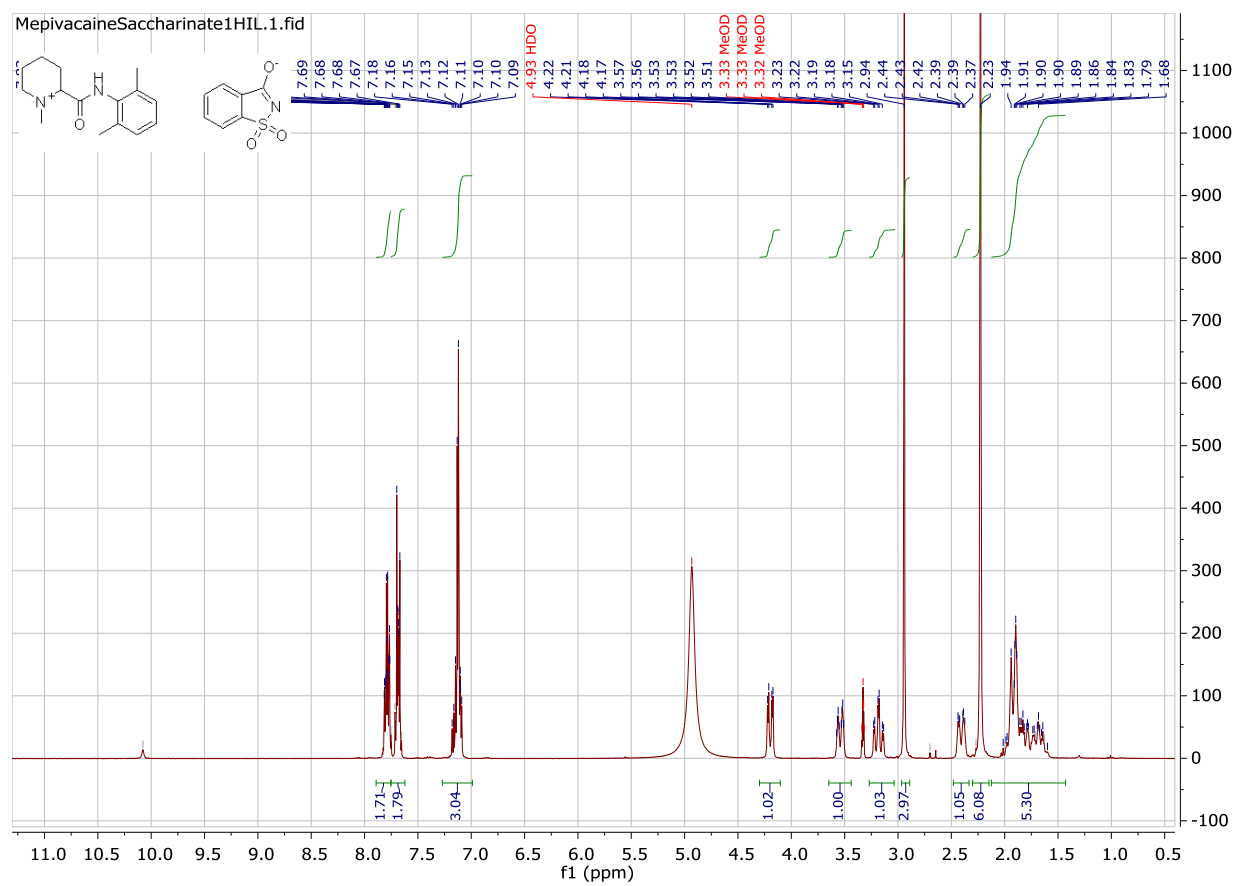
IL-277

il111416bc #163-168 RT: 1.99-2.05 AV: 6 SB: 146 0.10-1.90 NL: 2.94E5

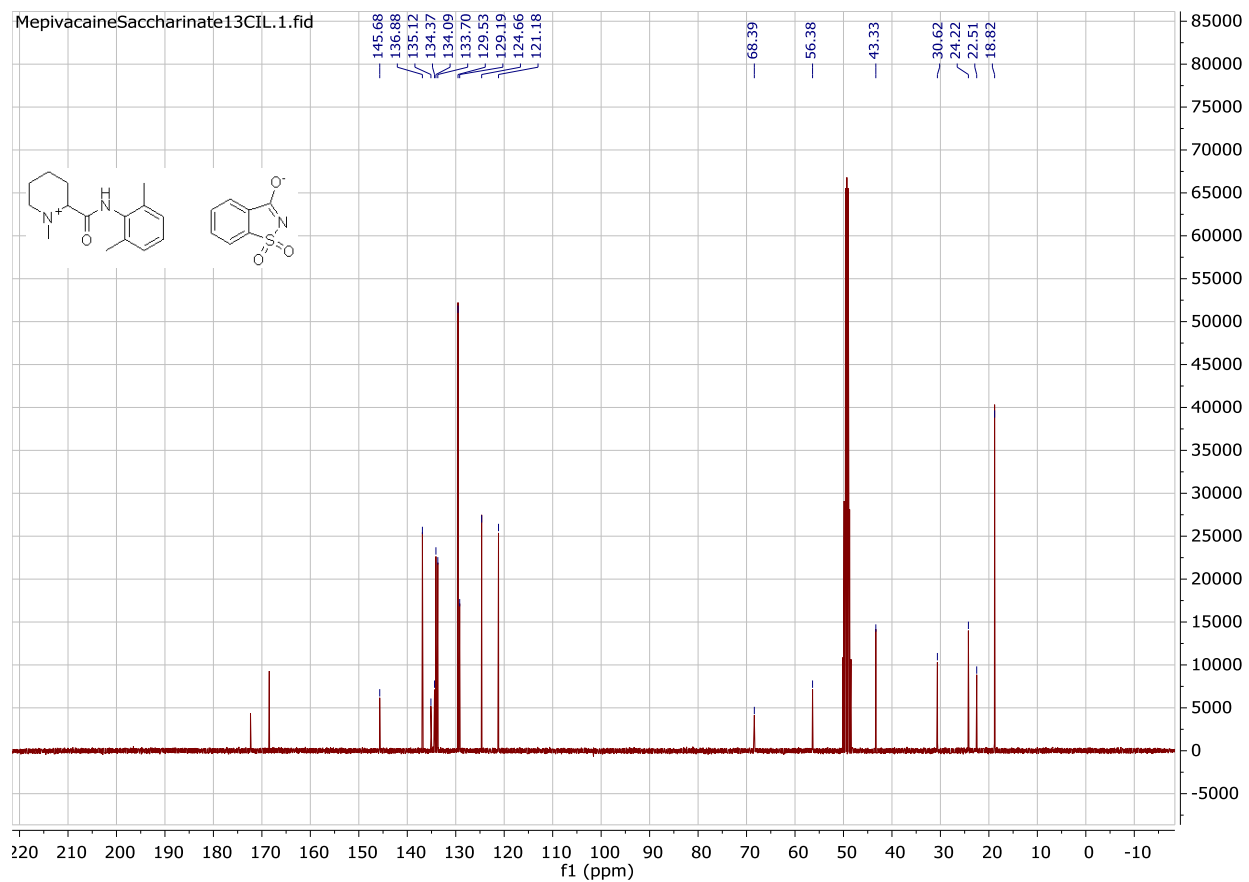
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for mepivacaine saccharinate 4a



¹³C spectrum for mepivacaine saccharinate 4a



HRMS data for mepivacaine saccharinate 4a

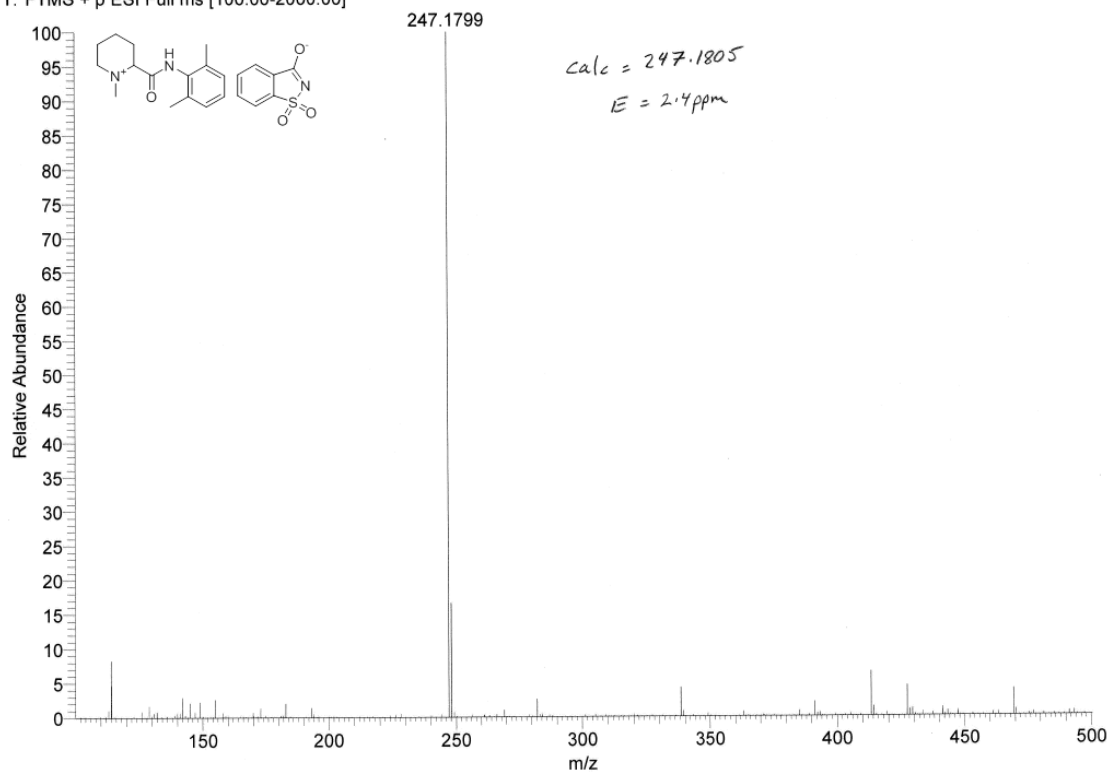
C:\Xcalibur\...IL061015a_150610143136

6/10/2015 2:31:36 PM

IL-12

IL061015a_150610143136 #456-477 RT: 3.58-3.73 AV: 22 NL: 7.39E6

T: FTMS + p ESI Full ms [100.00-2000.00]



HRMS data for mepivacaine saccharinate 4a

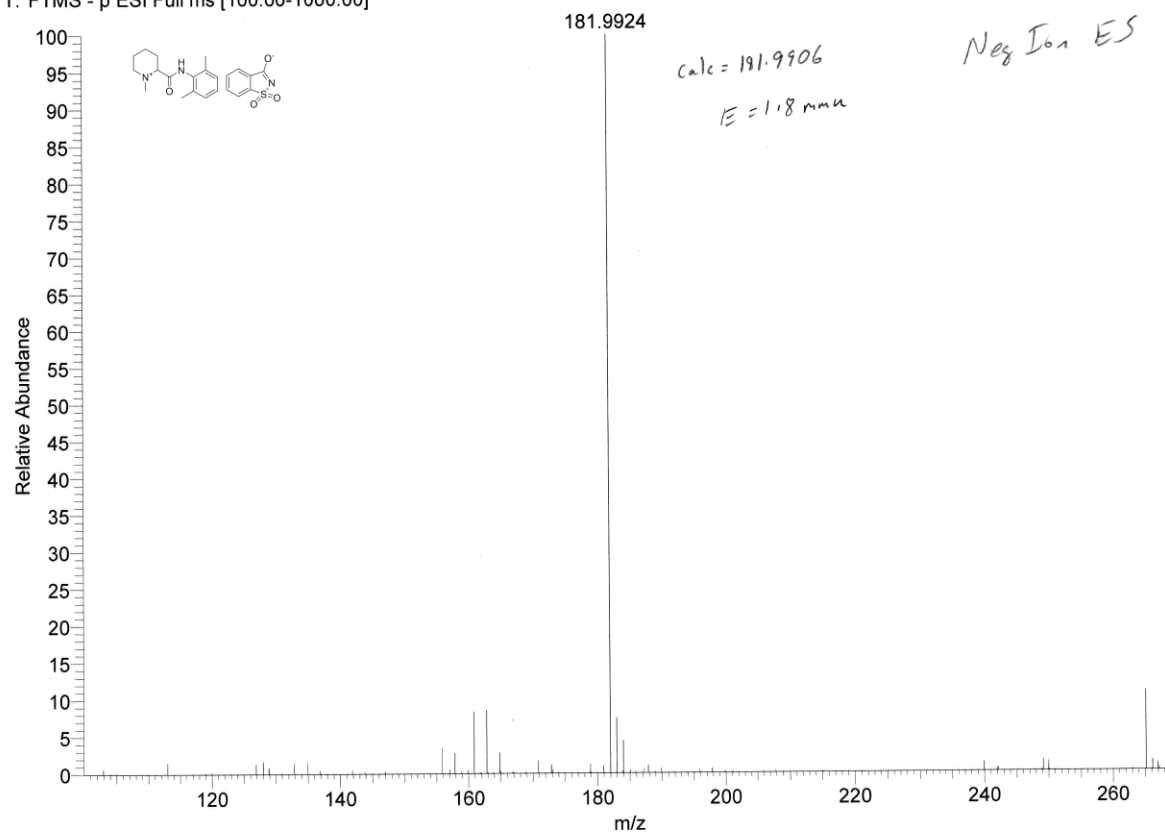
C:\Xcalibur\...IL061115J_150610143136

6/11/2015 1:49:08 PM

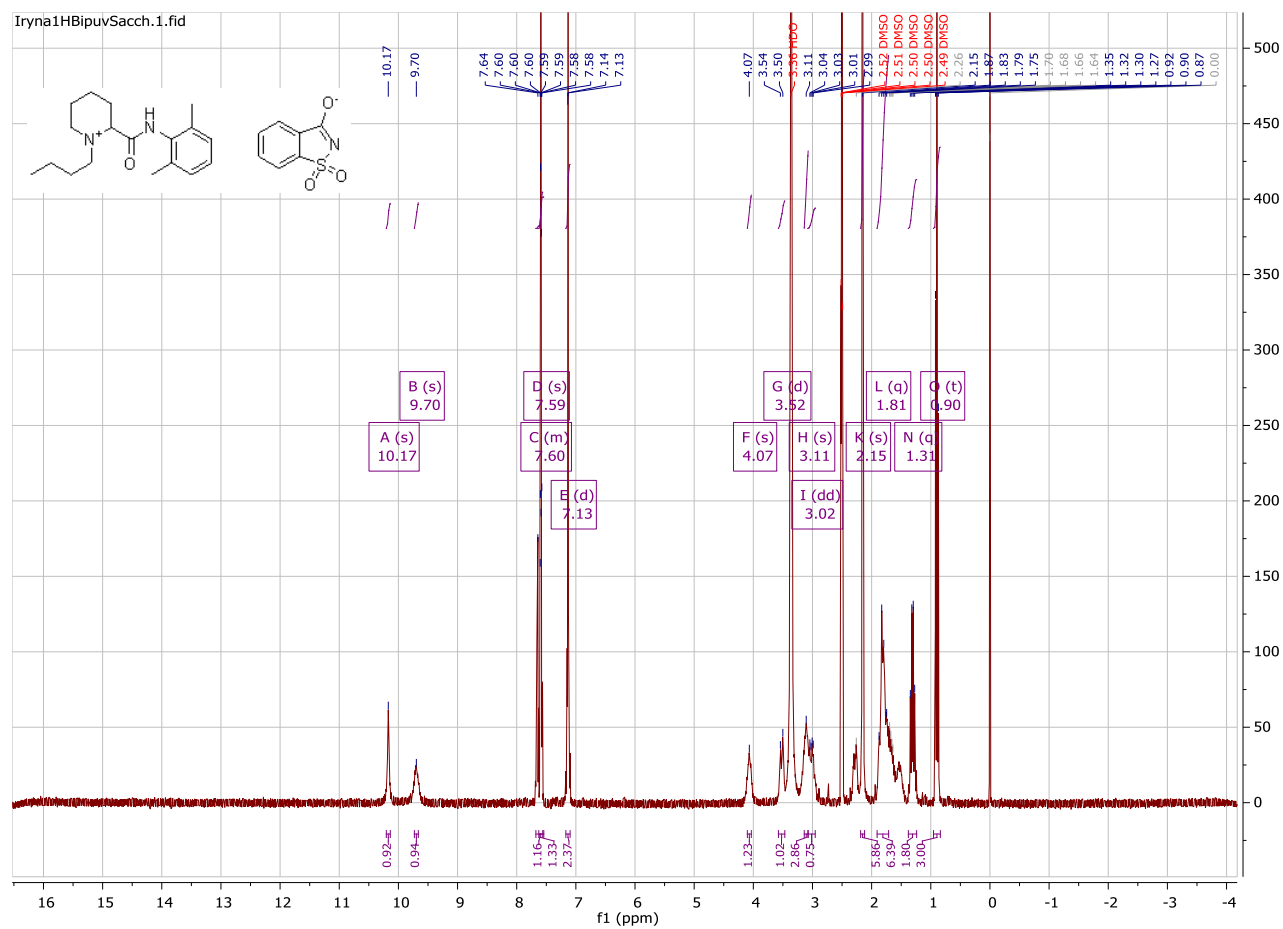
IL-12

IL061115J_150610143136 #56-72 RT: 0.84-1.00 AV: 17 SB: 41 0.10-0.70 NL: 1.27E6

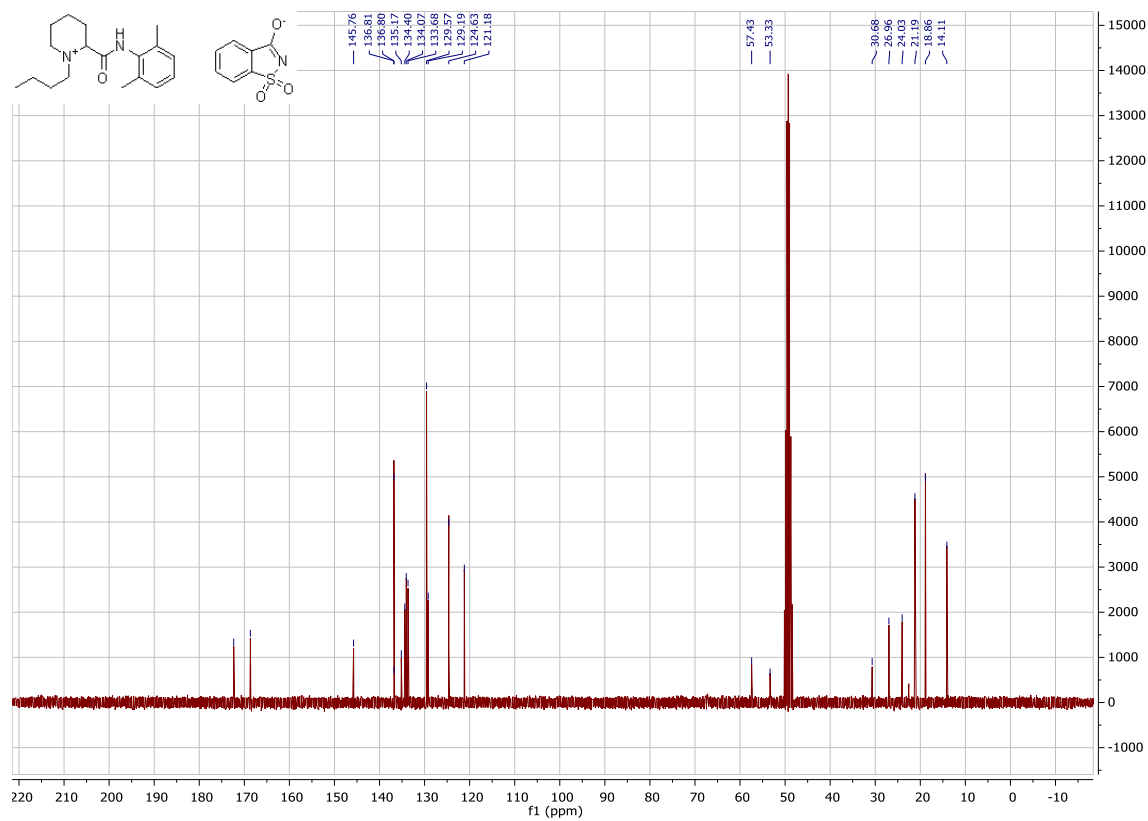
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for bupivacaine saccharinate 4b



¹³C spectrum for bupivacaine saccharinate 4b



HRMS data for bupivacaine saccharinate 4b

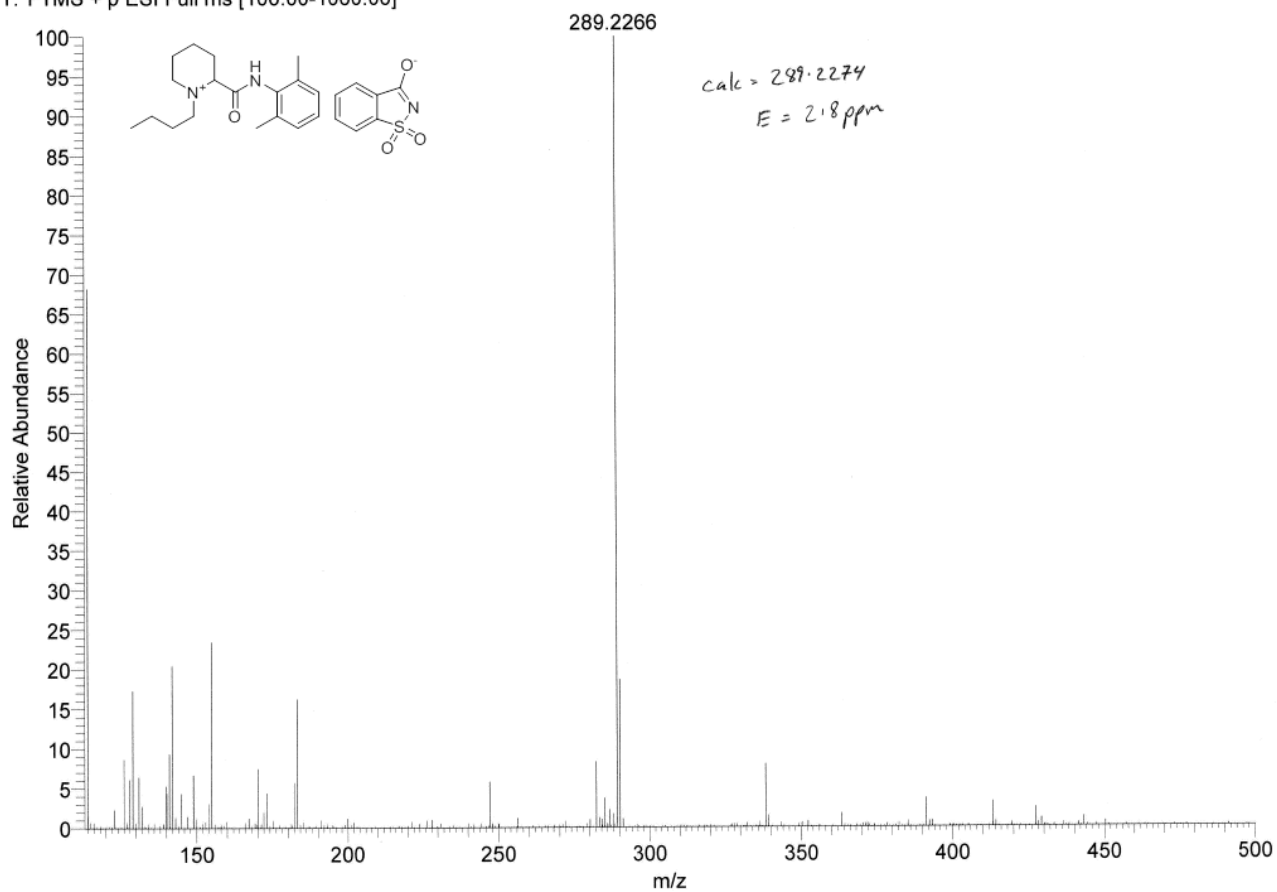
C:\Xcalibur\...IL061015F_150610143136

6/10/2015 4:34:37 PM

IL-17

IL061015F_150610143136 #95-115 RT: 0.86-1.01 AV: 21 NL: 2.49E6

T: FTMS + p ESI Full ms [100.00-1000.00]



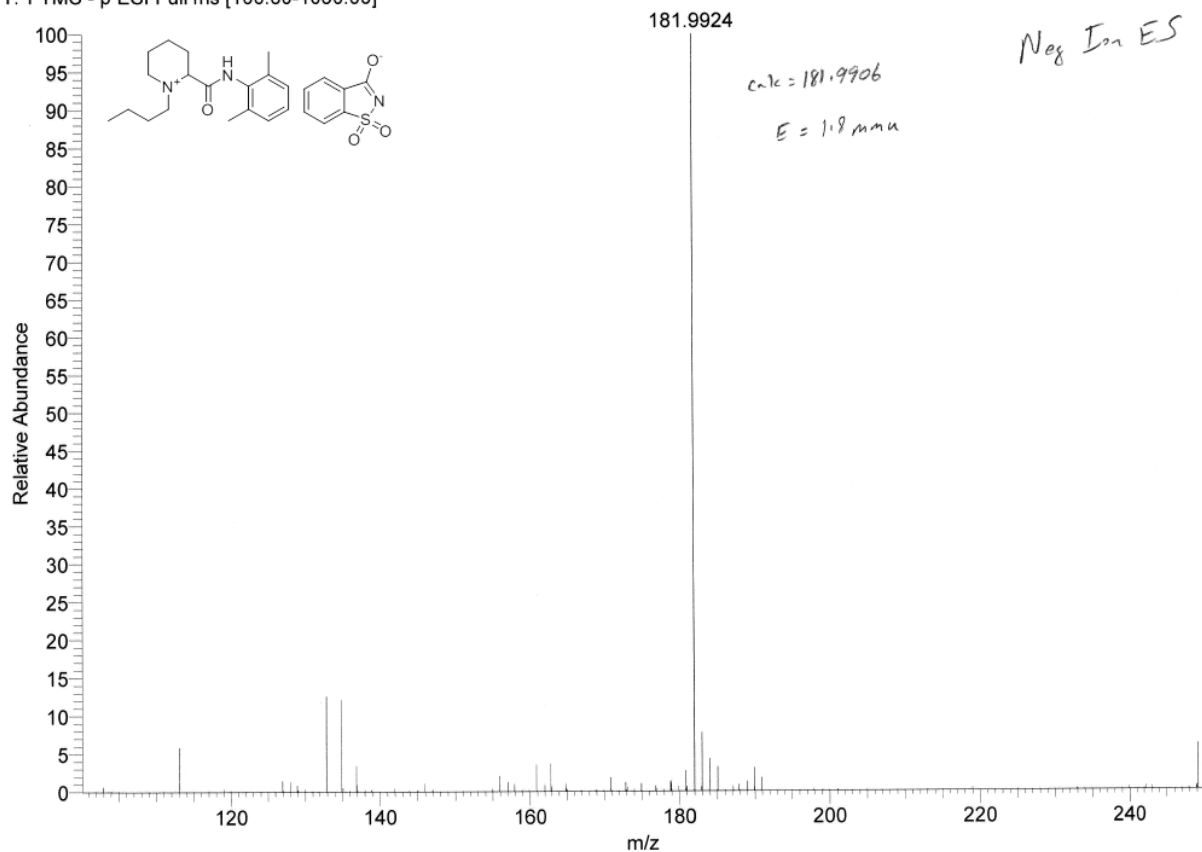
HRMS data for bupivacaine saccharinate 4b

C:\Xcalibur\...IL061115M_150610143136

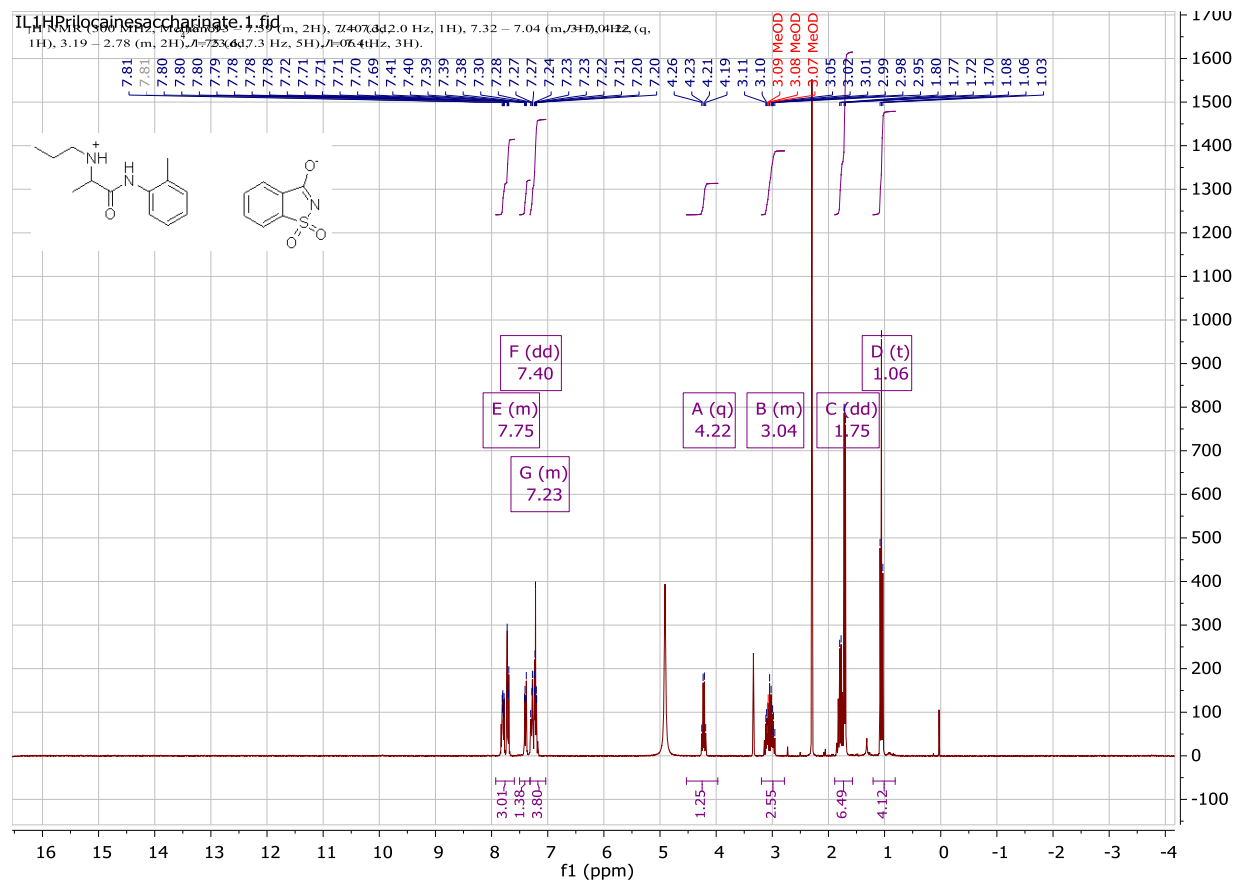
6/11/2015 2:07:42 PM

IL-17

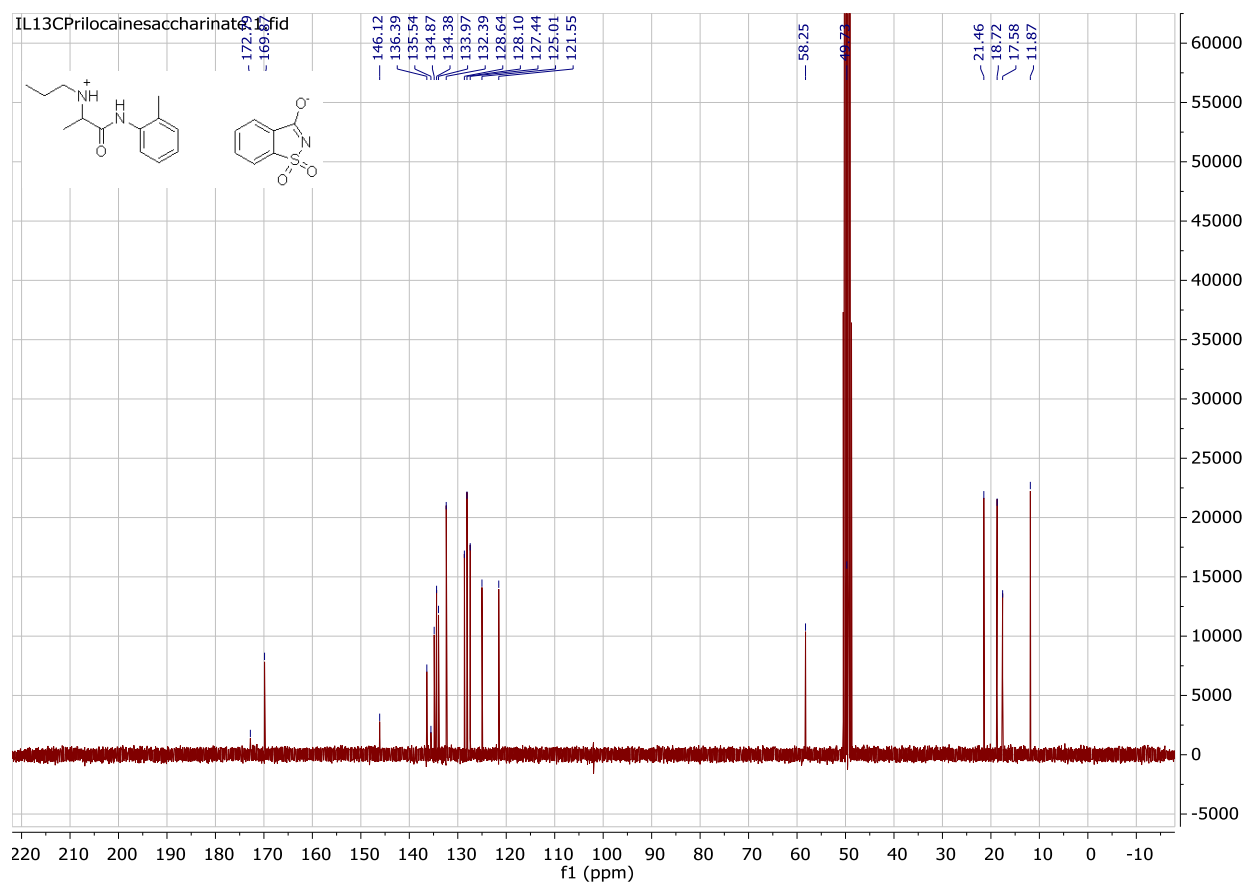
IL061115M_150610143136 #71-73 RT: 1.02-1.04 AV: 3 SB: 24 0.16-0.55 NL: 8.60E5
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for prilocaine saccharinate 4c



¹³C spectrum for prilocaine saccharinate 4c



HRMS data for prilocaine saccharinate 4c

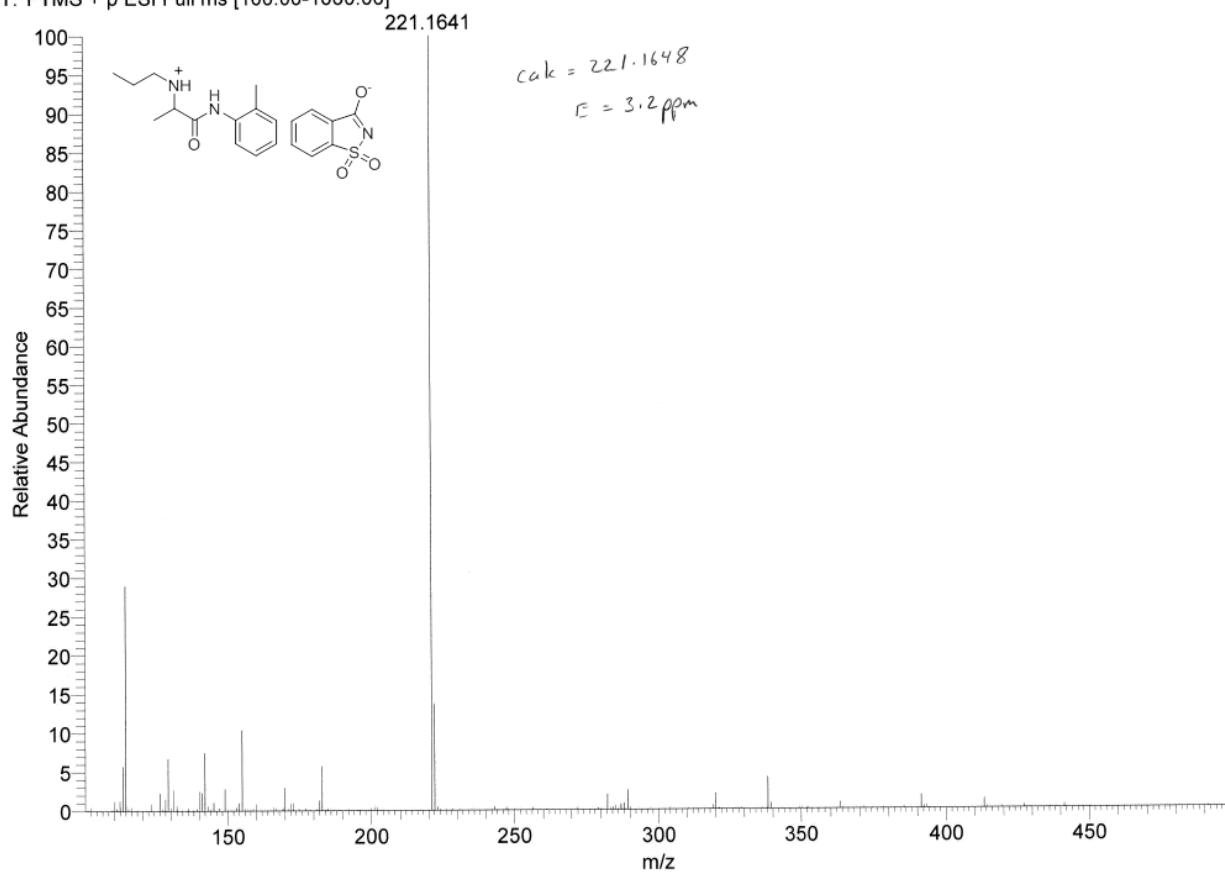
C:\Xcalibur\...\\L061015G_150610143136

6/10/2015 4:43:56 PM

IL-18

L061015G_150610143136 #80-93 RT: 0.73-0.83 AV: 14 NL: 4.90E6

T: FTMS + p ESI Full ms [100.00-1000.00]



HRMS data for prilocaine saccharinate 4c

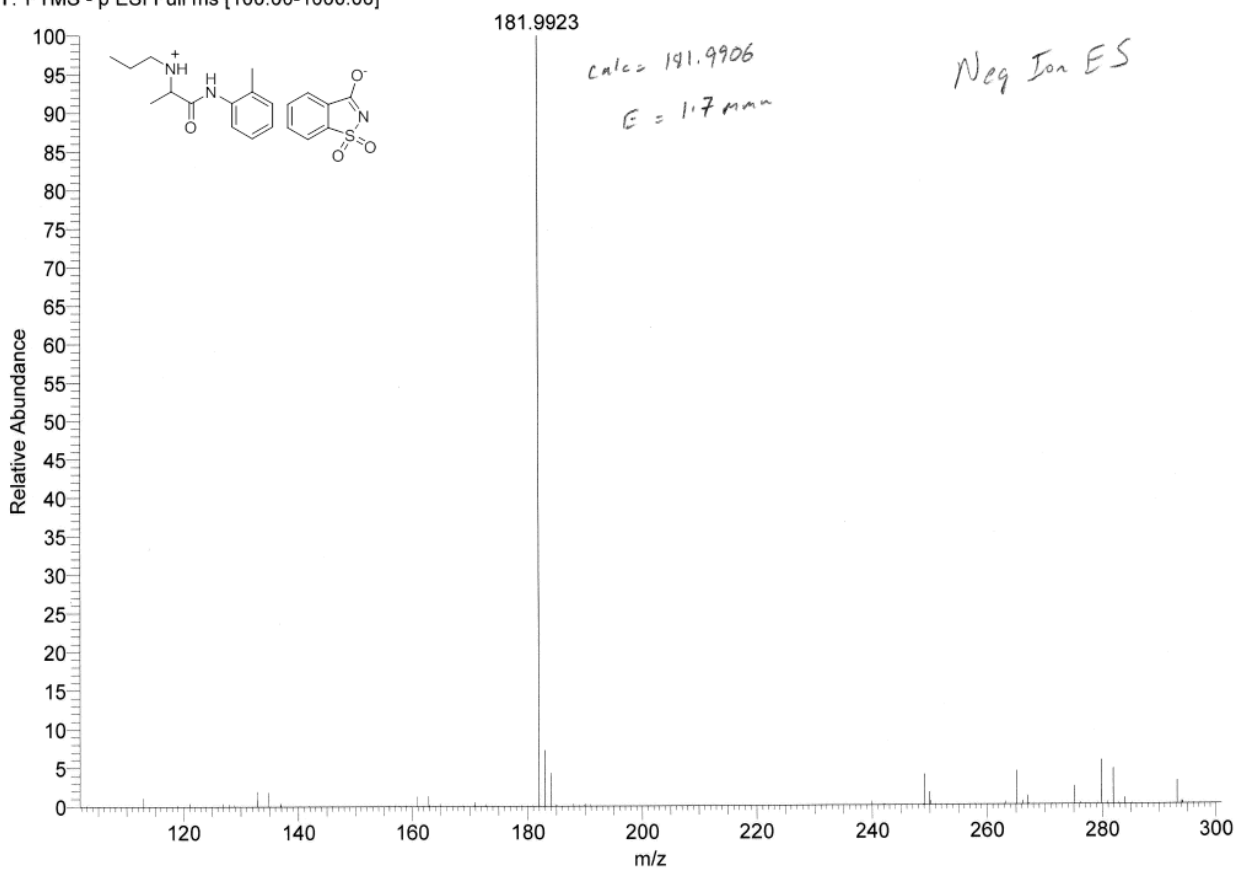
C:\Xcalibur\...IL061115N_150610143136

6/11/2015 2:12:23 PM

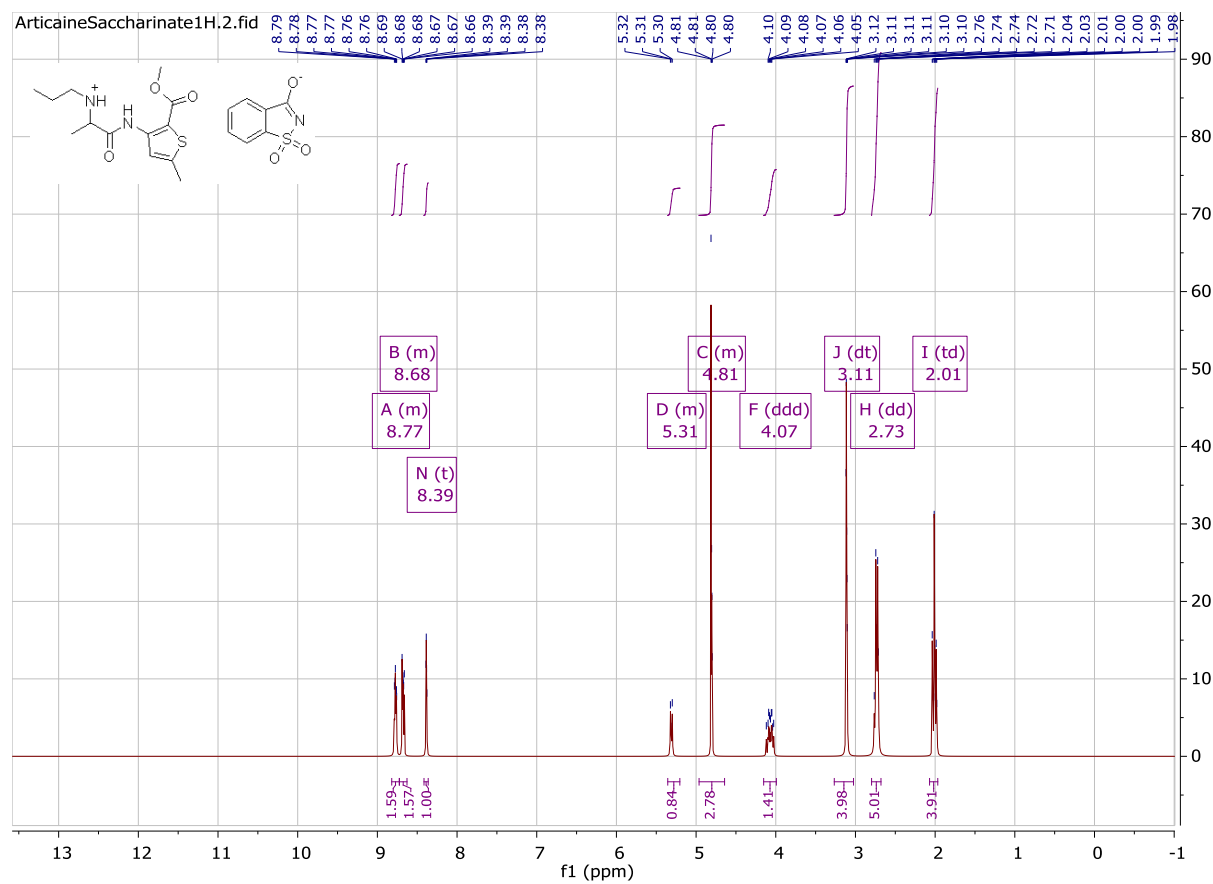
IL-18

IL061115N_150610143136 #67-74 RT: 0.98-1.04 AV: 8 SB: 31 0.27-0.71 NL: 1.85E6

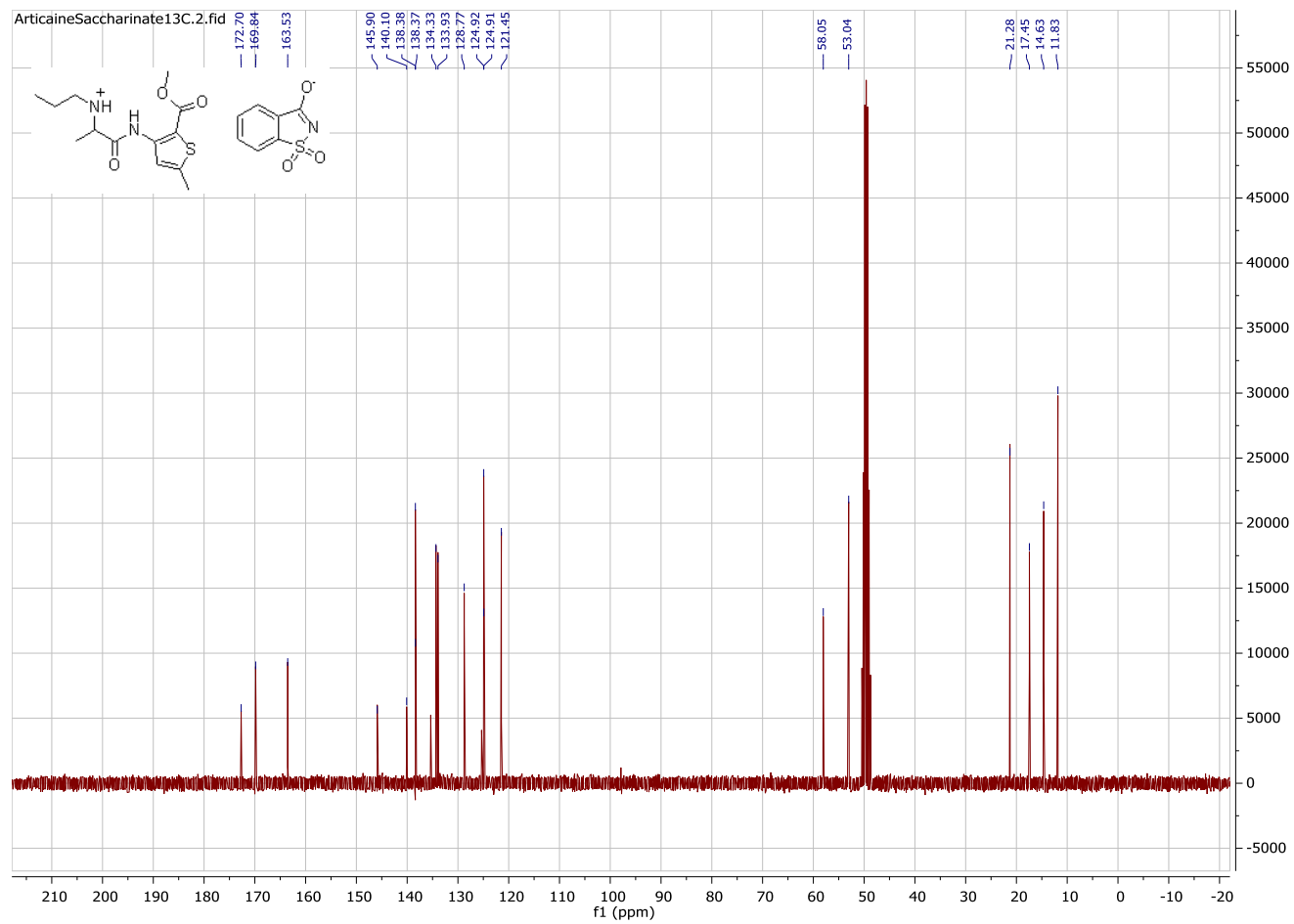
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for articaïne saccharinate 4d



¹³C spectrum for artocaine saccharinate 4d



HRMS data for artocaine saccharinate 4d

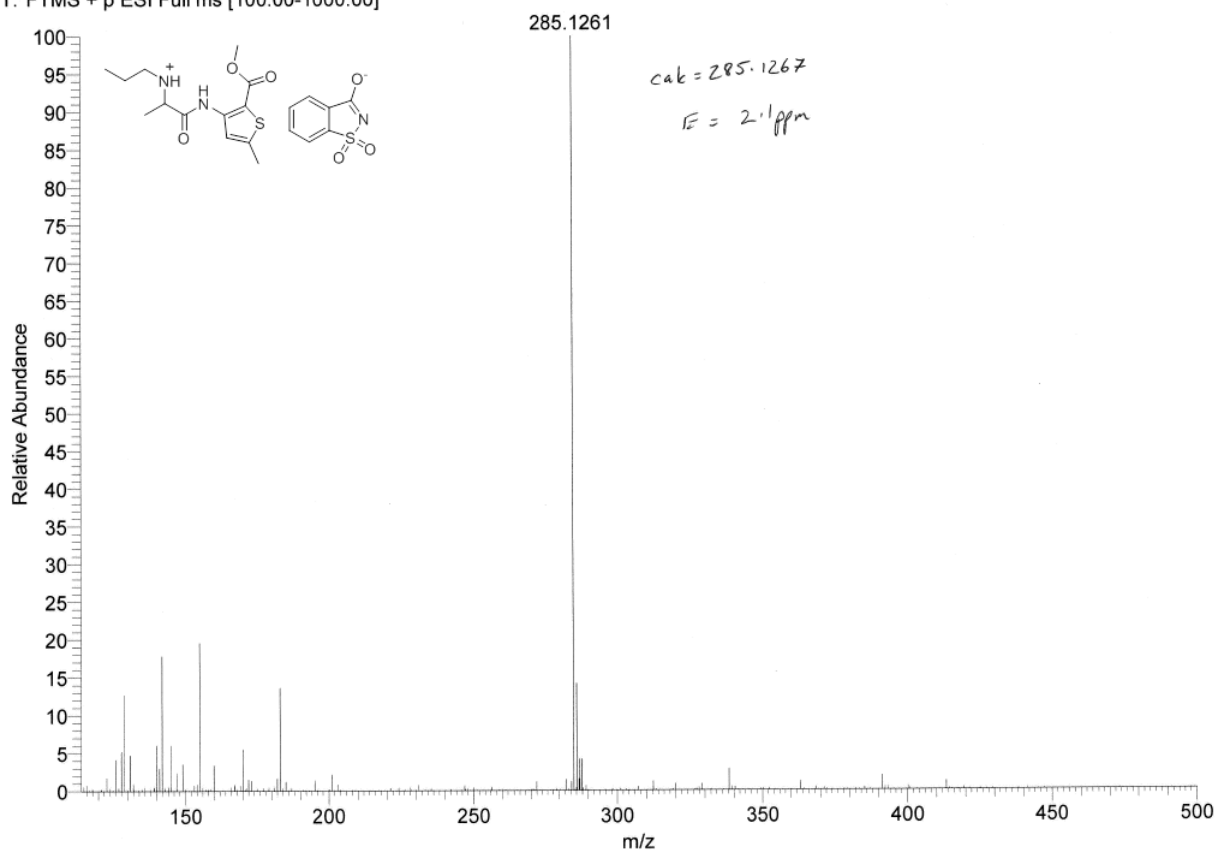
C:\Xcalibur\...VL061015E_150610143136

6/10/2015 4:27:40 PM

IL-16

IL061015E_150610143136 #68-74 RT: 0.60-0.66 AV: 7 NL: 3.10E6

T: FTMS + p ESI Full ms [100.00-1000.00]



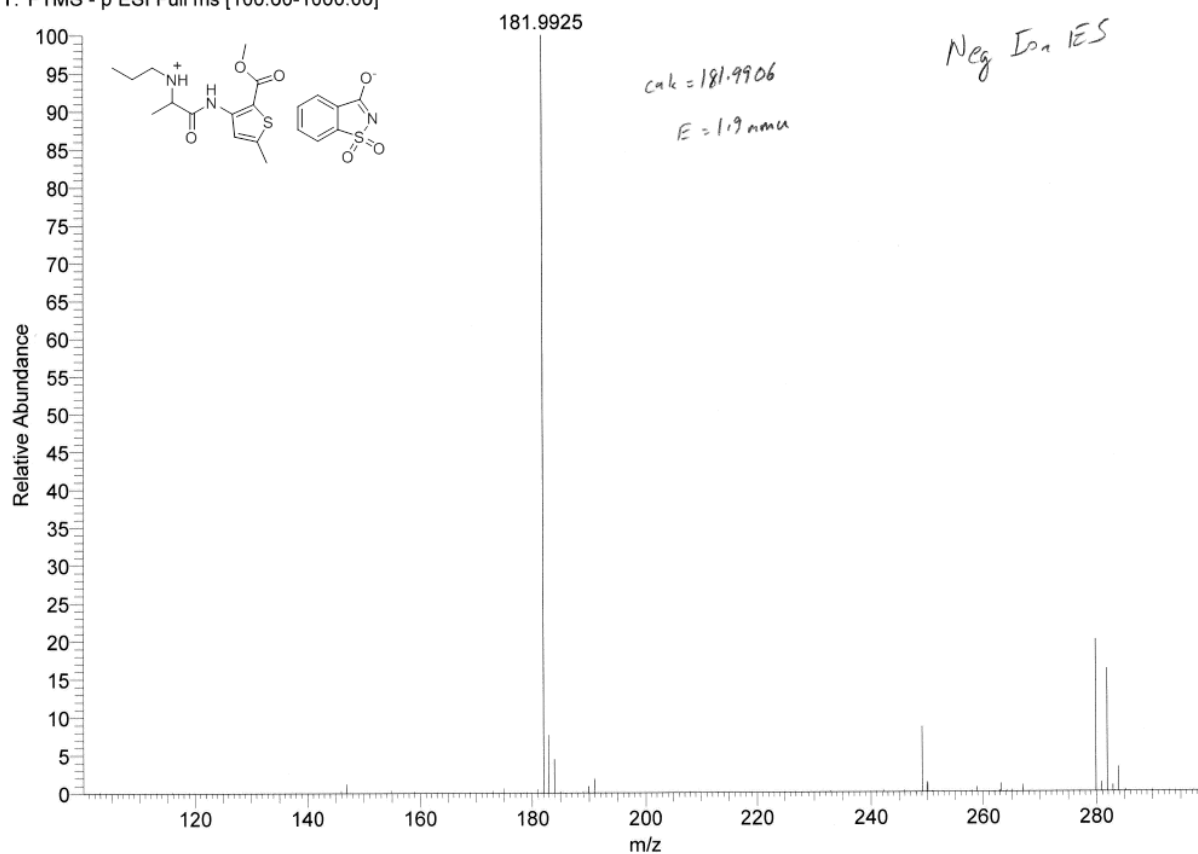
HRMS data for artocaine saccharinate 4d

C:\Xcalibur\...\\L061115L_150610143136

6/11/2015 2:02:15 PM

IL-16

IL061115L_150610143136 #62-69 RT: 0.90-0.98 AV: 8 SB: 1 0.63 NL: 6.89E5
T: FTMS - p ESI Full ms [100.00-1000.00]



Oxybup Saccharinate.1.fid
 PROTON MeOD {C:\NMRDATA\ilebedyeva} ilebedyeva 23

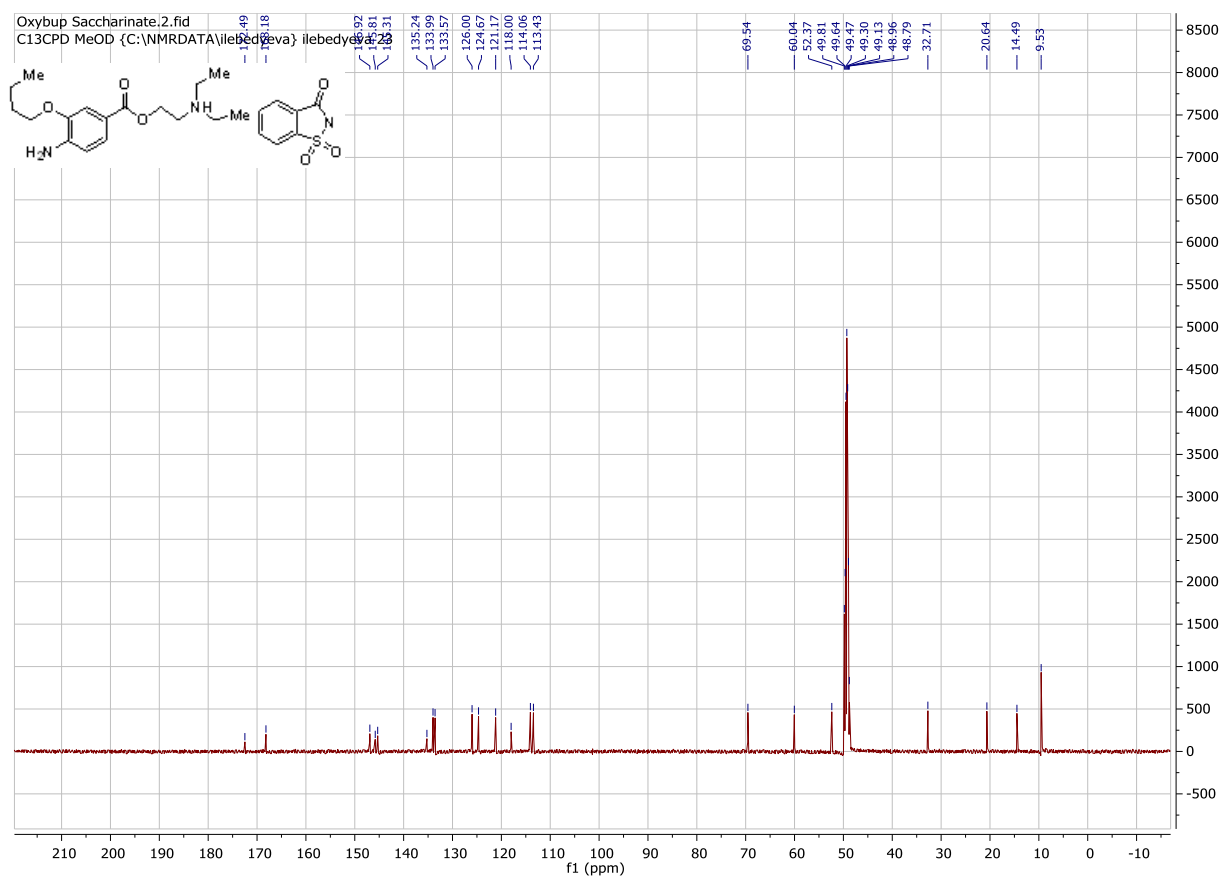
Chemical structures shown:

CCN(C)CCOC(=O)c1ccc(N)cc1
CCN(C)CCOC(=O)c1ccc(N)cc1

Integration values (from left to right):

- 3.69
- 2.15
- 1.00
- 2.24
- 2.14
- 2.14
- 4.82
- 2.09
- 2.09
- 6.81
- 3.32
- 3.54

¹³C spectrum for oxybuprocaine saccharinate 4e



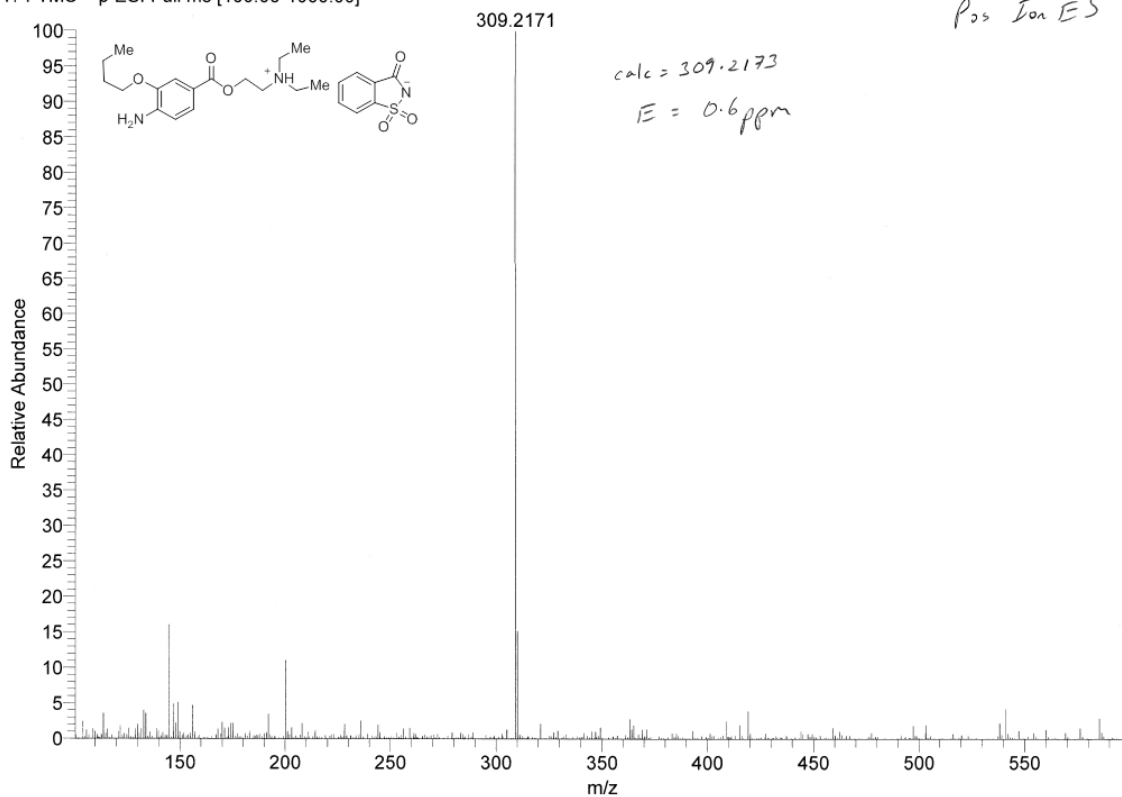
HRMS data for oxybuprocaine saccharinate 4e

C:\Xcalibur\...MassSpecLab03\1111416a

11/14/2016 2:25:58 PM

IL-278

1111416a #297-309 RT: 2.30-2.40 AV: 13 SB: 67 1.00-1.50 NL: 4.43E5
T: FTMS + p ESI Full ms [100.00-1000.00]



HRMS data for oxybuprocaine saccharinate 4e

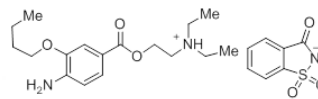
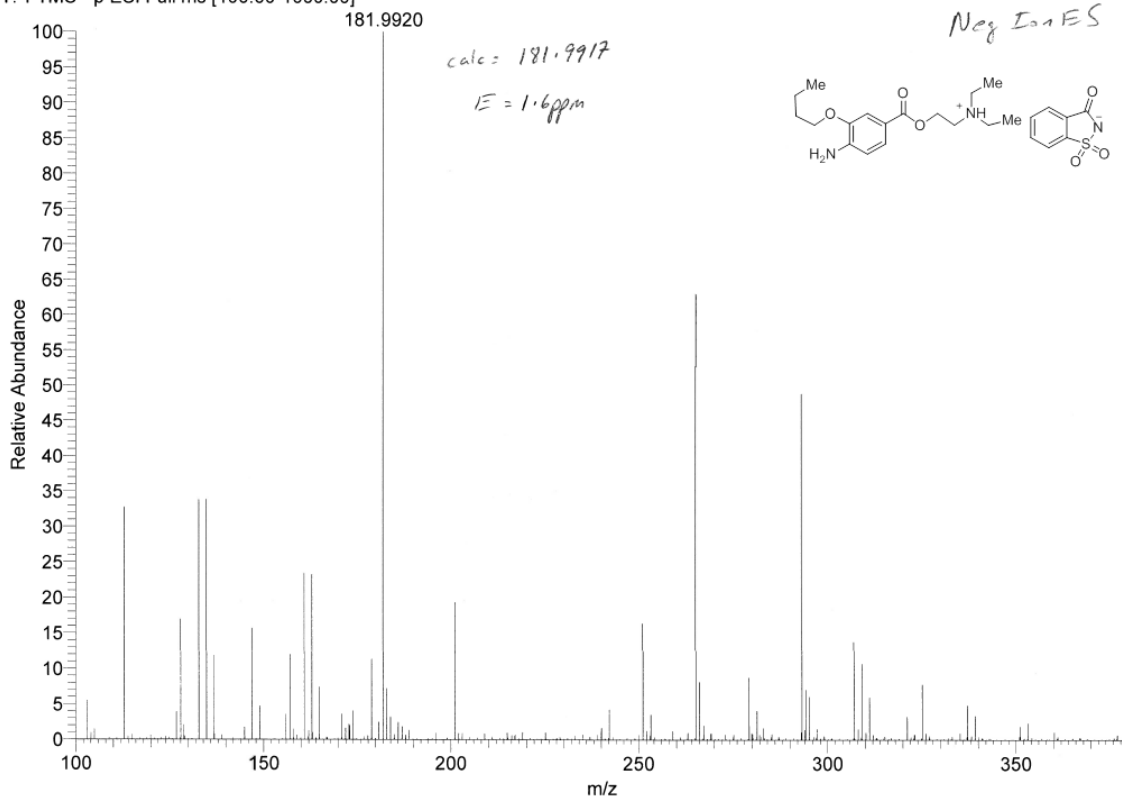
C:\Xcalibur\...\MassSpecLab03\il111416aa

11/14/2016 2:52:08 PM

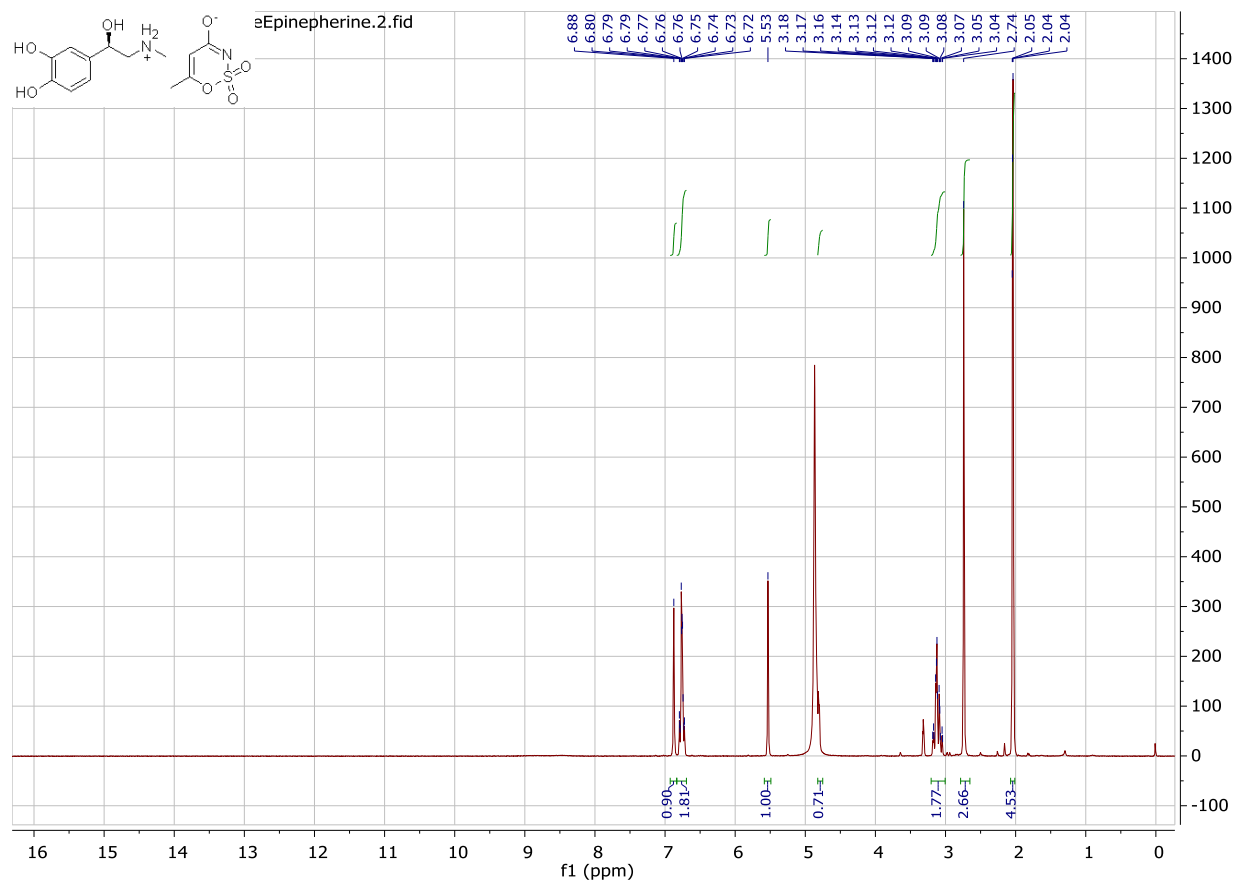
IL-278

il111416aa #133-140 RT: 1.66-1.74 AV: 8 SB: 87 0.10-1.20 NL: 2.76E5
T: FTMS - p ESI Full ms [100.00-1000.00]

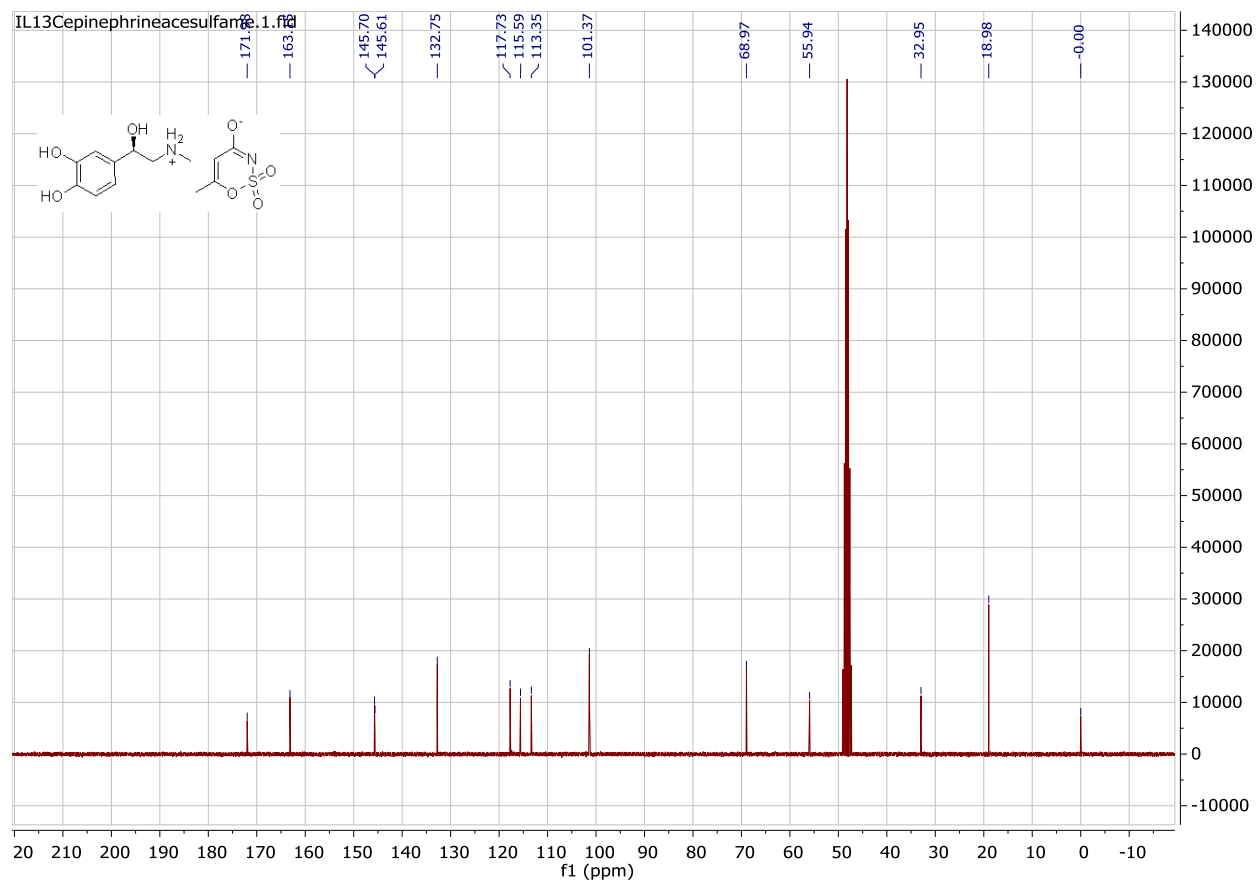
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for epinephrine acesulfamate 6a



¹³C spectrum for epinephrine acesulfamate 6a



HRMS data for epinephrine acesulfamate 6a

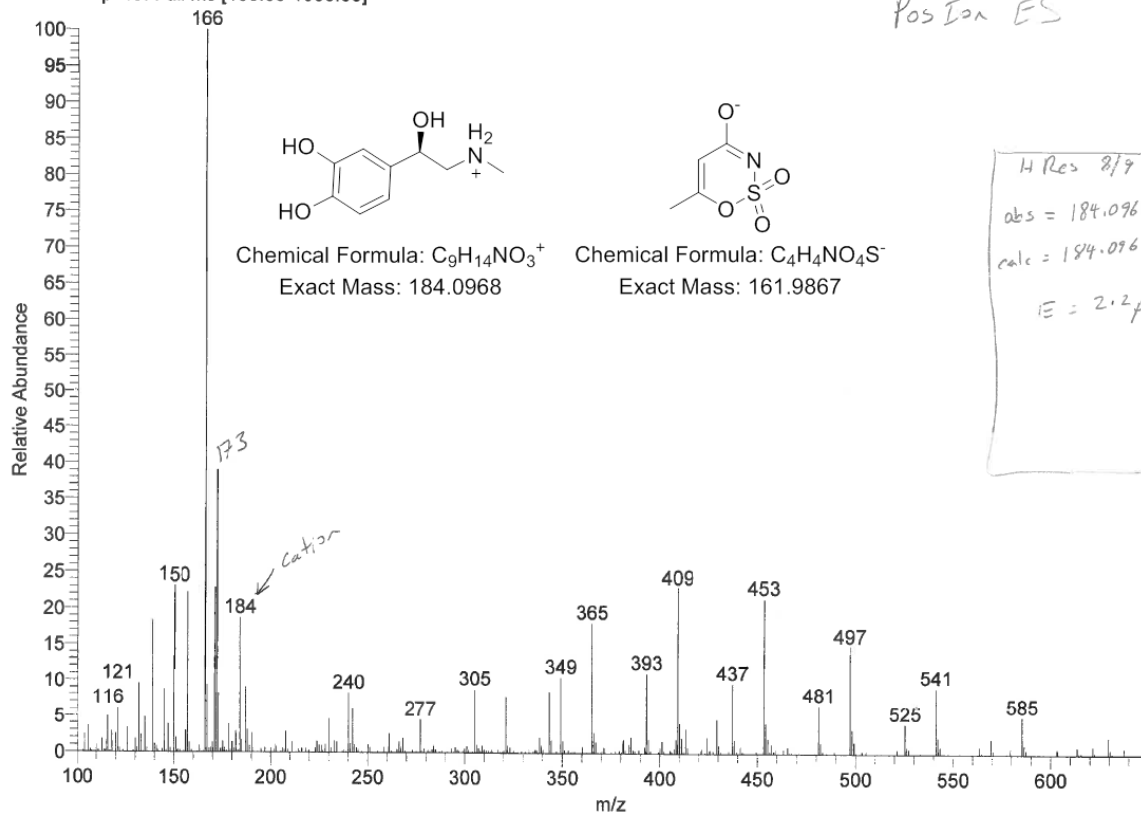
C:\Xcalibur\...MassSpecLab03\i080916a

8/9/2016 1:53:50 PM

IL-151

i080916a #516-657 RT: 1.57-2.01 AV: 142 SB: 366 0.20-1.30 NL: 2.00E6
T: FTMS + p ESI Full ms [100.00-1000.00]

Pos Ion ES



HRMS data for epinephrine acesulfamate 6a

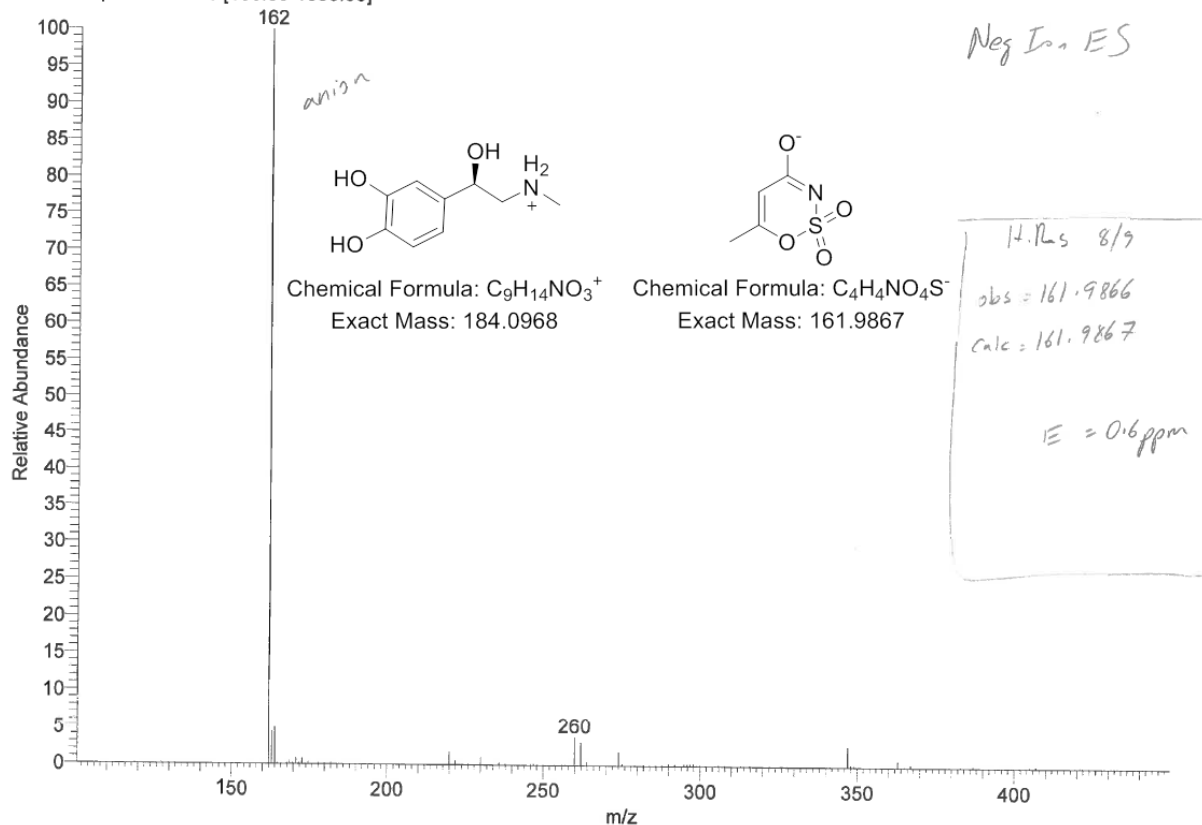
C:\Xcalibur\...MassSpecLab03\i1080916g

8/9/2016 3:30:14 PM

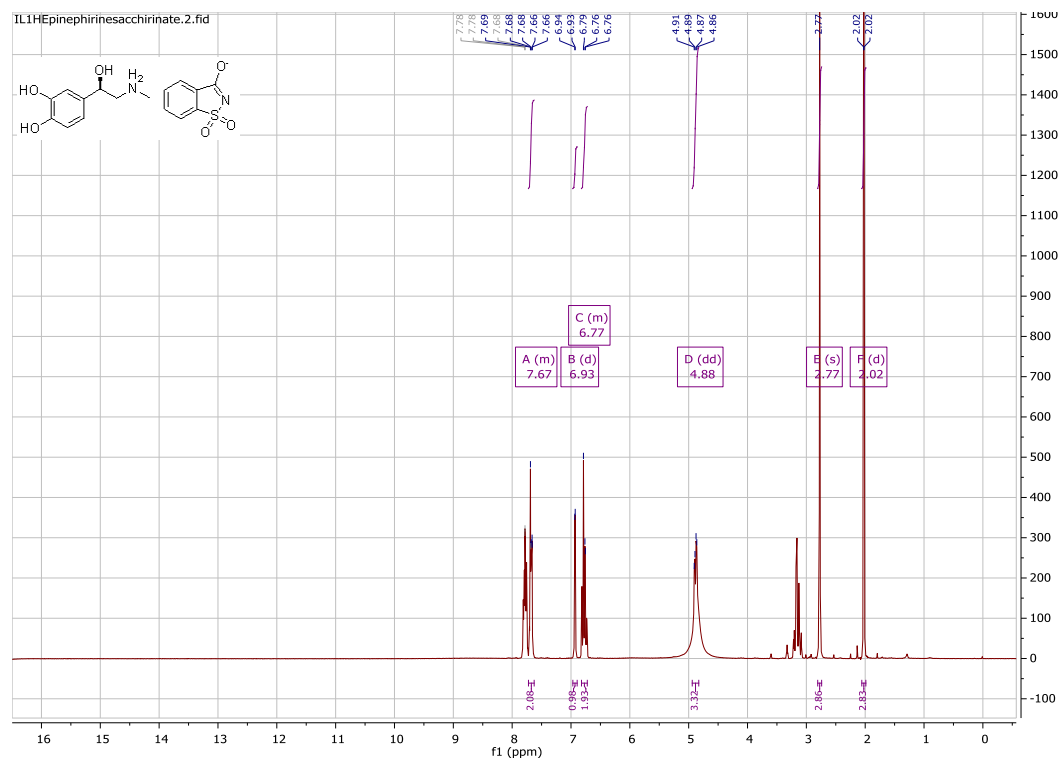
IL-151

i1080916g #92-98 RT: 2.05-2.16 AV: 7 SB: 48 0.18-1.30 NL: 4.27E5

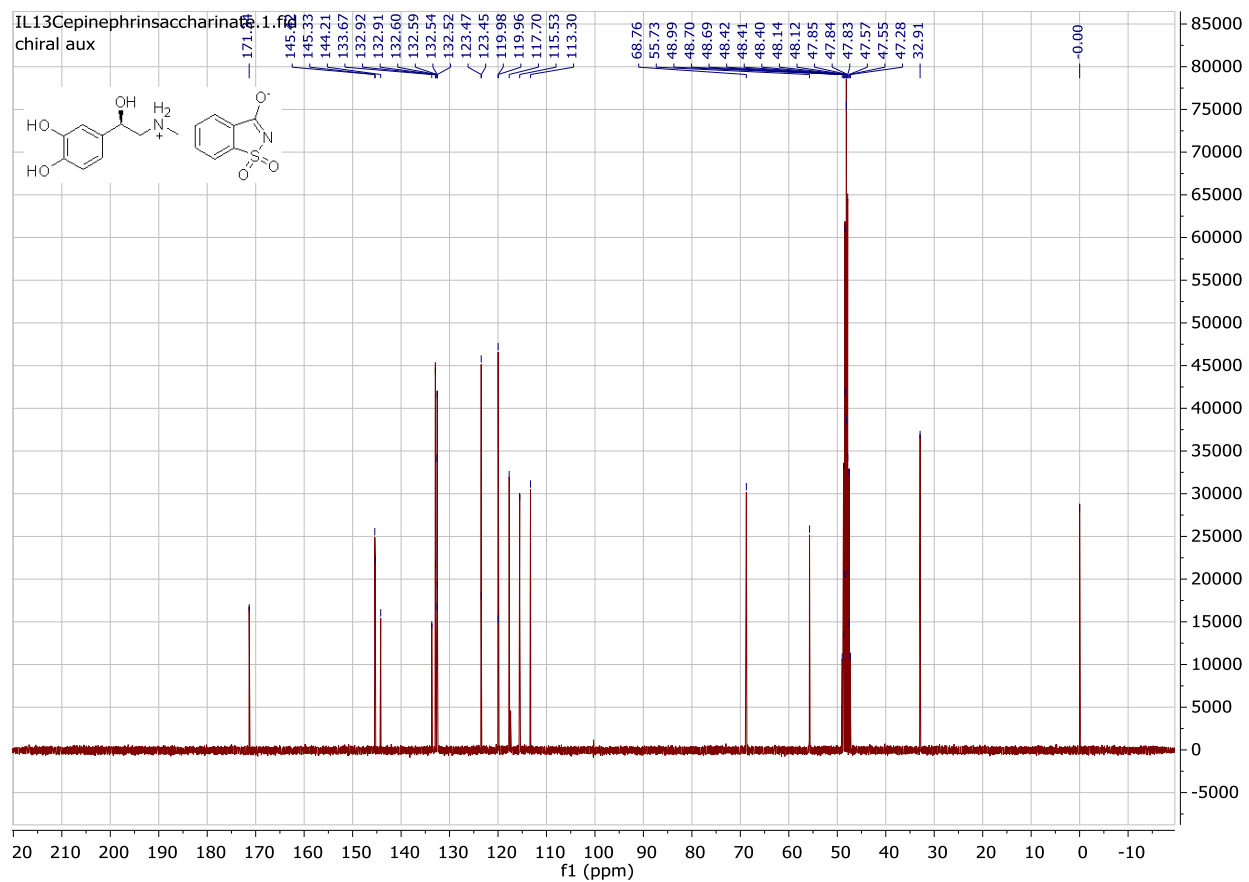
T: FTMS - p ESI Full ms [100.00-1000.00]



¹H spectrum for epinephrine saccharinate 6b



¹³C spectrum for epinephrine saccharinate 6b



HRMS data for epinephrine saccharinate 6b

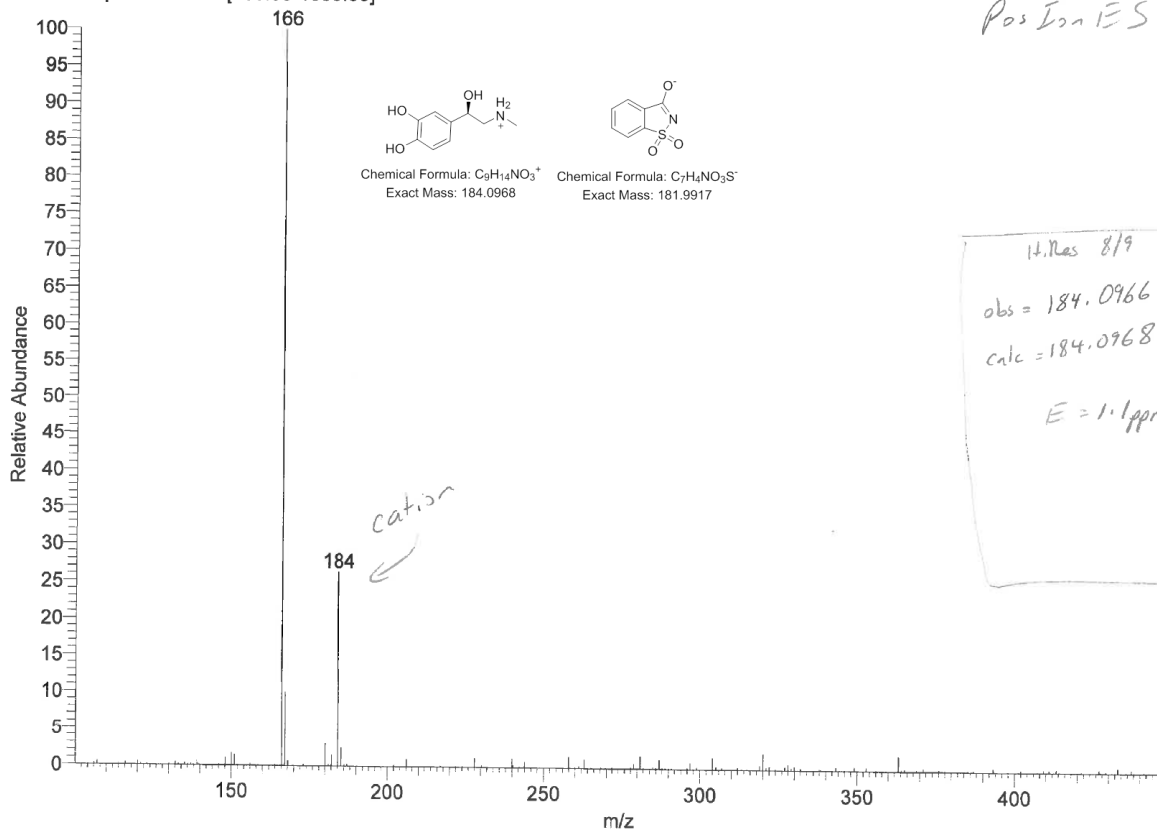
C:\Xcalibur\...MassSpecLab03\i1080916c

8/9/2016 2:12:20 PM

IL-150

i1080916c #632-651 RT: 2.07-2.12 AV: 20 SB: 121 0.20-0.60 NL: 1.46E7

T: FTMS + p ESI Full ms [100.00-1000.00]



HRMS data for epinephrine saccharinate 6b

C:\Xcalibur\...MassSpecLab03\i080916f

8/9/2016 3:22:22 PM

IL-150

i080916f #156-166 RT: 2.40-2.53 AV: 11 SB: 44 0.20-1.31 NL: 9.73E5

T: FTMS - p ESI Full ms [100.00-1000.00]

